



wwPDB EM Validation Summary Report ⓘ

Mar 15, 2026 – 01:37 PM UTC

PDB ID : 9WYP / pdb_00009wyp
EMDB ID : EMD-66373
Title : The PSI-ACPI supercomplex from the cryptophyte Chroomonas placoidea
Authors : Li, X.Y.; Mao, Z.Y.; Han, G.Y.
Deposited on : 2025-09-27
Resolution : 2.25 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:

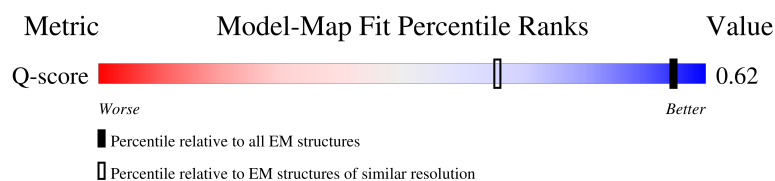
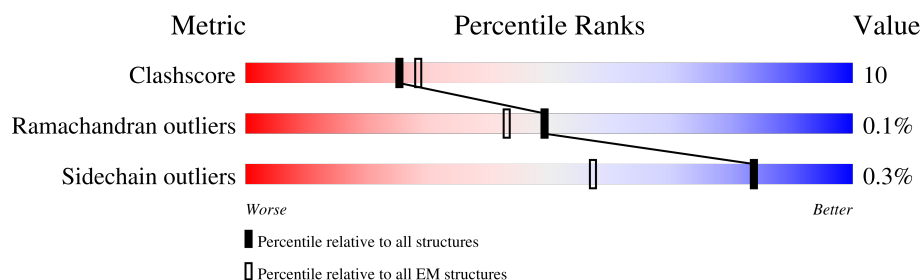
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.25 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.



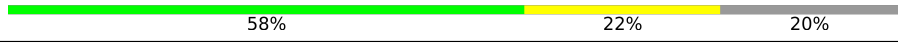
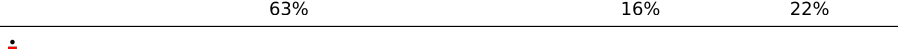
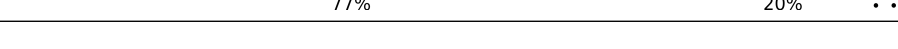
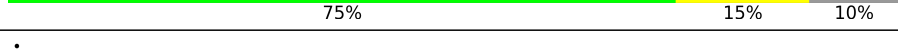
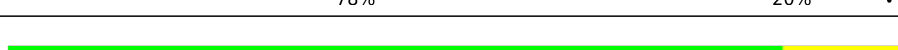
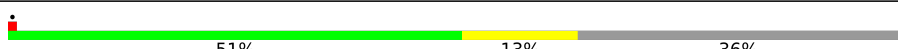
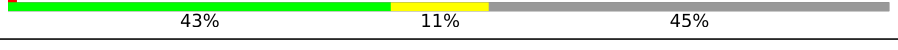
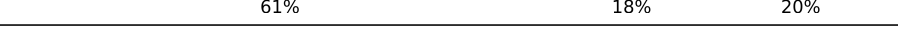
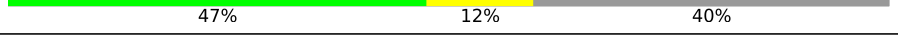
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3458 (1.75 - 2.75)

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

Mol	Chain	Length	Quality of chain
1	1	222	
2	2	216	
3	3	235	
4	4	217	

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Mol	Chain	Length	Quality of chain
5	5	229	
6	6	215	
7	7	230	
8	8	227	
9	9	220	
10	A	752	
11	B	734	
12	C	81	
13	D	141	
14	E	64	
15	F	183	
16	I	36	
17	J	42	
18	K	87	
19	L	153	
20	M	30	
21	O	155	
22	R	139	
23	Z	279	
24	a	215	
24	d	215	
25	b	218	
26	c	257	
27	e	208	
28	X	241	

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
29	CLA	1	601	X	-	-	-
29	CLA	1	602	X	-	-	-
29	CLA	1	603	X	-	-	-
29	CLA	1	604	X	-	-	-
29	CLA	1	605	X	-	-	-
29	CLA	1	606	X	-	-	-
29	CLA	1	607	X	-	-	-
29	CLA	1	608	X	-	-	-
29	CLA	1	609	X	-	-	-
29	CLA	1	611	X	-	-	-
29	CLA	1	612	X	-	-	-
29	CLA	1	613	X	-	-	-
29	CLA	2	601	X	-	-	-
29	CLA	2	602	X	-	-	-
29	CLA	2	603	X	-	-	-
29	CLA	2	604	X	-	-	-
29	CLA	2	605	X	-	-	-
29	CLA	2	606	X	-	-	-
29	CLA	2	607	X	-	-	-
29	CLA	2	608	X	-	-	-
29	CLA	2	609	X	-	-	-
29	CLA	2	611	X	-	-	-
29	CLA	2	612	X	-	-	-
29	CLA	3	302	X	-	-	-
29	CLA	3	303	X	-	-	-
29	CLA	3	304	X	-	-	-
29	CLA	3	305	X	-	-	-
29	CLA	3	306	X	-	-	-
29	CLA	3	308	X	-	-	-
29	CLA	3	309	X	-	-	-
29	CLA	3	310	X	-	-	-
29	CLA	3	311	X	-	-	-
29	CLA	3	312	X	-	-	-
29	CLA	3	313	X	-	-	-
29	CLA	4	601	X	-	-	-
29	CLA	4	602	X	-	-	-
29	CLA	4	603	X	-	-	-
29	CLA	4	604	X	-	-	-
29	CLA	4	606	X	-	-	-
29	CLA	4	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	4	608	X	-	-	-
29	CLA	4	609	X	-	-	-
29	CLA	4	610	X	-	-	-
29	CLA	4	611	X	-	-	-
29	CLA	5	601	X	-	-	-
29	CLA	5	602	X	-	-	-
29	CLA	5	603	X	-	-	-
29	CLA	5	604	X	-	-	-
29	CLA	5	605	X	-	-	-
29	CLA	5	606	X	-	-	-
29	CLA	5	607	X	-	-	-
29	CLA	5	608	X	-	-	-
29	CLA	5	609	X	-	-	-
29	CLA	5	611	X	-	-	-
29	CLA	5	612	X	-	-	-
29	CLA	5	613	X	-	-	-
29	CLA	6	601	X	-	-	-
29	CLA	6	602	X	-	-	-
29	CLA	6	603	X	-	-	-
29	CLA	6	604	X	-	-	-
29	CLA	6	605	X	-	-	-
29	CLA	6	606	X	-	-	-
29	CLA	6	607	X	-	-	-
29	CLA	6	608	X	-	-	-
29	CLA	6	609	X	-	-	-
29	CLA	6	611	X	-	-	-
29	CLA	6	612	X	-	-	-
29	CLA	7	302	X	-	-	-
29	CLA	7	303	X	-	-	-
29	CLA	7	304	X	-	-	-
29	CLA	7	305	X	-	-	-
29	CLA	7	306	X	-	-	-
29	CLA	7	307	X	-	-	-
29	CLA	7	308	X	-	-	-
29	CLA	7	309	X	-	-	-
29	CLA	7	311	X	-	-	-
29	CLA	7	312	X	-	-	-
29	CLA	8	301	X	-	-	-
29	CLA	8	302	X	-	-	-
29	CLA	8	303	X	-	-	-
29	CLA	8	304	X	-	-	-
29	CLA	8	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	8	306	X	-	-	-
29	CLA	8	307	X	-	-	-
29	CLA	8	308	X	-	-	-
29	CLA	8	317	X	-	-	-
29	CLA	9	302	X	-	-	-
29	CLA	9	303	X	-	-	-
29	CLA	9	304	X	-	-	-
29	CLA	9	305	X	-	-	-
29	CLA	9	306	X	-	-	-
29	CLA	9	307	X	-	-	-
29	CLA	9	308	X	-	-	-
29	CLA	9	309	X	-	-	-
29	CLA	9	310	X	-	-	-
29	CLA	9	312	X	-	-	-
29	CLA	9	313	X	-	-	-
29	CLA	9	314	X	-	-	-
29	CLA	9	315	X	-	-	-
29	CLA	A	801	X	-	-	-
29	CLA	A	802	X	-	-	-
29	CLA	A	803	X	-	-	-
29	CLA	A	804	X	-	-	-
29	CLA	A	805	X	-	-	-
29	CLA	A	806	X	-	-	-
29	CLA	A	807	X	-	-	-
29	CLA	A	808	X	-	-	-
29	CLA	A	809	X	-	-	-
29	CLA	A	810	X	-	-	-
29	CLA	A	811	X	-	-	-
29	CLA	A	812	X	-	-	-
29	CLA	A	813	X	-	-	-
29	CLA	A	814	X	-	-	-
29	CLA	A	815	X	-	-	-
29	CLA	A	816	X	-	-	-
29	CLA	A	817	X	-	-	-
29	CLA	A	818	X	-	-	-
29	CLA	A	819	X	-	-	-
29	CLA	A	820	X	-	-	-
29	CLA	A	821	X	-	-	-
29	CLA	A	822	X	-	-	-
29	CLA	A	823	X	-	-	-
29	CLA	A	824	X	-	-	-
29	CLA	A	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	A	827	X	-	-	-
29	CLA	A	828	X	-	-	-
29	CLA	A	829	X	-	-	-
29	CLA	A	830	X	-	-	-
29	CLA	A	831	X	-	-	-
29	CLA	A	832	X	-	-	-
29	CLA	A	833	X	-	-	-
29	CLA	A	834	X	-	-	-
29	CLA	A	835	X	-	-	-
29	CLA	A	836	X	-	-	-
29	CLA	A	837	X	-	-	-
29	CLA	A	838	X	-	-	-
29	CLA	A	839	X	-	-	-
29	CLA	A	840	X	-	-	-
29	CLA	A	841	X	-	-	-
29	CLA	A	842	X	-	-	-
29	CLA	A	843	X	-	-	-
29	CLA	A	853	X	-	-	-
29	CLA	A	854	X	-	-	-
29	CLA	A	855	X	-	-	-
29	CLA	B	802	X	-	-	-
29	CLA	B	803	X	-	-	-
29	CLA	B	804	X	-	-	-
29	CLA	B	805	X	-	-	-
29	CLA	B	806	X	-	-	-
29	CLA	B	807	X	-	-	-
29	CLA	B	808	X	-	-	-
29	CLA	B	809	X	-	-	-
29	CLA	B	810	X	-	-	-
29	CLA	B	811	X	-	-	-
29	CLA	B	812	X	-	-	-
29	CLA	B	813	X	-	-	-
29	CLA	B	814	X	-	-	-
29	CLA	B	815	X	-	-	-
29	CLA	B	816	X	-	-	-
29	CLA	B	817	X	-	-	-
29	CLA	B	818	X	-	-	-
29	CLA	B	819	X	-	-	-
29	CLA	B	820	X	-	-	-
29	CLA	B	821	X	-	-	-
29	CLA	B	822	X	-	-	-
29	CLA	B	823	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	B	824	X	-	-	-
29	CLA	B	825	X	-	-	-
29	CLA	B	826	X	-	-	-
29	CLA	B	827	X	-	-	-
29	CLA	B	828	X	-	-	-
29	CLA	B	829	X	-	-	-
29	CLA	B	830	X	-	-	-
29	CLA	B	831	X	-	-	-
29	CLA	B	832	X	-	-	-
29	CLA	B	833	X	-	-	-
29	CLA	B	834	X	-	-	-
29	CLA	B	835	X	-	-	-
29	CLA	B	836	X	-	-	-
29	CLA	B	837	X	-	-	-
29	CLA	B	838	X	-	-	-
29	CLA	B	839	X	-	-	-
29	CLA	B	840	X	-	-	-
29	CLA	B	841	X	-	-	-
29	CLA	F	201	X	-	-	-
29	CLA	F	202	X	-	-	-
29	CLA	J	103	X	-	-	-
29	CLA	K	101	X	-	-	-
29	CLA	K	102	X	-	-	-
29	CLA	L	201	X	-	-	-
29	CLA	L	202	X	-	-	-
29	CLA	L	203	X	-	-	-
29	CLA	O	201	X	-	-	-
29	CLA	O	202	X	-	-	-
29	CLA	O	203	X	-	-	-
29	CLA	O	204	X	-	-	-
29	CLA	R	202	X	-	-	-
29	CLA	X	301	X	-	-	-
29	CLA	Z	302	X	-	-	-
29	CLA	Z	303	X	-	-	-
29	CLA	Z	304	X	-	-	-
29	CLA	Z	305	X	-	-	-
29	CLA	a	601	X	-	-	-
29	CLA	a	602	X	-	-	-
29	CLA	a	603	X	-	-	-
29	CLA	a	604	X	-	-	-
29	CLA	a	605	X	-	-	-
29	CLA	a	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	a	607	X	-	-	-
29	CLA	a	608	X	-	-	-
29	CLA	a	609	X	-	-	-
29	CLA	a	611	X	-	-	-
29	CLA	a	612	X	-	-	-
29	CLA	b	601	X	-	-	-
29	CLA	b	602	X	-	-	-
29	CLA	b	603	X	-	-	-
29	CLA	b	604	X	-	-	-
29	CLA	b	606	X	-	-	-
29	CLA	b	607	X	-	-	-
29	CLA	b	608	X	-	-	-
29	CLA	b	610	X	-	-	-
29	CLA	b	611	X	-	-	-
29	CLA	c	601	X	-	-	-
29	CLA	c	602	X	-	-	-
29	CLA	c	603	X	-	-	-
29	CLA	c	604	X	-	-	-
29	CLA	c	605	X	-	-	-
29	CLA	c	606	X	-	-	-
29	CLA	c	607	X	-	-	-
29	CLA	c	608	X	-	-	-
29	CLA	c	609	X	-	-	-
29	CLA	c	612	X	-	-	-
29	CLA	c	613	X	-	-	-
29	CLA	c	615	X	-	-	-
29	CLA	d	601	X	-	-	-
29	CLA	d	602	X	-	-	-
29	CLA	d	603	X	-	-	-
29	CLA	d	604	X	-	-	-
29	CLA	d	605	X	-	-	-
29	CLA	d	606	X	-	-	-
29	CLA	d	607	X	-	-	-
29	CLA	d	608	X	-	-	-
29	CLA	d	609	X	-	-	-
29	CLA	d	611	X	-	-	-
29	CLA	d	612	X	-	-	-
29	CLA	e	601	X	-	-	-
29	CLA	e	602	X	-	-	-
29	CLA	e	603	X	-	-	-
29	CLA	e	604	X	-	-	-
29	CLA	e	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	e	607	X	-	-	-
29	CLA	e	608	X	-	-	-
29	CLA	e	610	X	-	-	-
29	CLA	e	611	X	-	-	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 61306 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ACPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	175	Total	C	N	O	S	0	0
			1316	848	222	238	8		

- Molecule 2 is a protein called ACPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	168	Total	C	N	O	S	0	0
			1320	872	215	230	3		

- Molecule 3 is a protein called ACPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	191	Total	C	N	O	S	0	0
			1433	920	243	259	11		

- Molecule 4 is a protein called ACPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	176	Total	C	N	O	S	0	0
			1366	891	224	245	6		

- Molecule 5 is a protein called ACPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	188	Total	C	N	O	S	0	0
			1403	908	234	253	8		

- Molecule 6 is a protein called ACPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	173	Total	C	N	O	S	0	0
			1305	846	217	232	10		

- Molecule 7 is a protein called ACPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	180	Total	C	N	O	S	0	0
			1358	874	234	242	8		

- Molecule 8 is a protein called ACPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	175	Total	C	N	O	S	0	0
			1313	852	219	237	5		

- Molecule 9 is a protein called ACPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	180	Total	C	N	O	S	0	0
			1349	864	230	243	12		

- Molecule 10 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	741	Total	C	N	O	S	0	0
			5824	3804	992	1000	28		

- Molecule 11 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	731	Total	C	N	O	S	0	0
			5828	3847	982	984	15		

- Molecule 12 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	80	Total	C	N	O	S	0	0
			591	361	103	115	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	137	Total	C	N	O	S	0	0
			1070	685	184	198	3		

- Molecule 14 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	E	61	Total	C	N	O	0	0
			491	312	85	94		

- Molecule 15 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	160	Total	C	N	O	S	0	0
			1258	814	214	228	2		

- Molecule 16 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	33	Total	C	N	O	S	0	0
			258	180	34	42	2		

- Molecule 17 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	42	Total	C	N	O	S	0	0
			342	232	49	58	3		

- Molecule 18 is a protein called Photosystem I reaction center subunit Psak.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	78	Total	C	N	O	S	0	0
			553	358	90	102	3		

- Molecule 19 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	150	Total	C	N	O	S	0	0
			1143	746	184	211	2		

- Molecule 20 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	30	Total	C	N	O	S	0	0
			227	152	35	39	1		

- Molecule 21 is a protein called Psao.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	99	Total	C	N	O	S	0	0
			766	518	113	134	1		

- Molecule 22 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	92	Total	C	N	O	S	0	0
			680	439	112	127	2		

- Molecule 23 is a protein called CCPI-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	153	Total	C	N	O	S	0	0
			1130	721	188	211	10		

- Molecule 24 is a protein called ACPI-13/10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	171	Total	C	N	O	S	0	0
			1271	823	207	231	10		
24	d	171	Total	C	N	O	S	0	0
			1271	823	207	231	10		

- Molecule 25 is a protein called ACPI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	176	Total	C	N	O	S	0	0
			1368	891	224	244	9		

- Molecule 26 is a protein called ACPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	215	Total	C	N	O	S	0	0
			1615	1053	265	283	14		

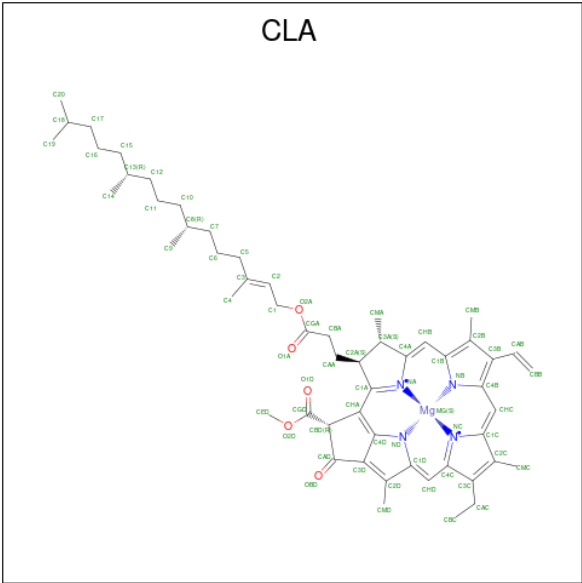
- Molecule 27 is a protein called ACPI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	168	Total	C	N	O	S	0	0
			1288	840	209	227	12		

- Molecule 28 is a protein called PsaQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	145	Total	C	N	O	S	0	0
			1034	655	176	199	4		

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	2	1	Total 59	C 49	Mg 1	N 4	O 5	0
29	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	3	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	4	1	Total 59	C 49	Mg 1	N 4	O 5	0
29	4	1	Total 54	C 44	Mg 1	N 4	O 5	0
29	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	5	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	7	1	Total 53	C 43	Mg 1	N 4	O 5	0
29	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	7	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	9	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	J	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	L	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
29	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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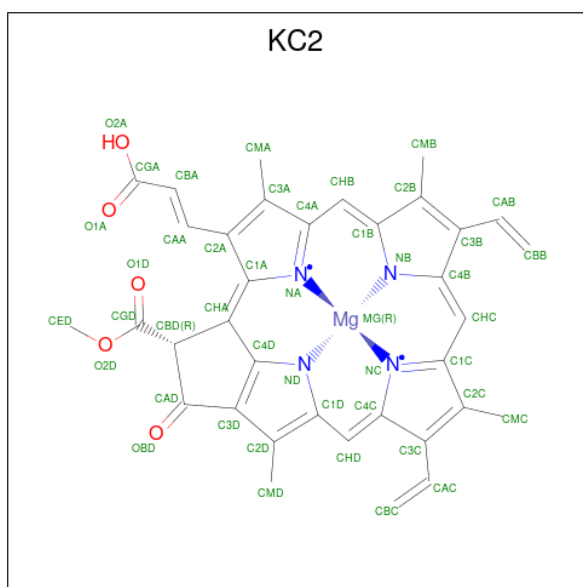
Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	e	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	X	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 30 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



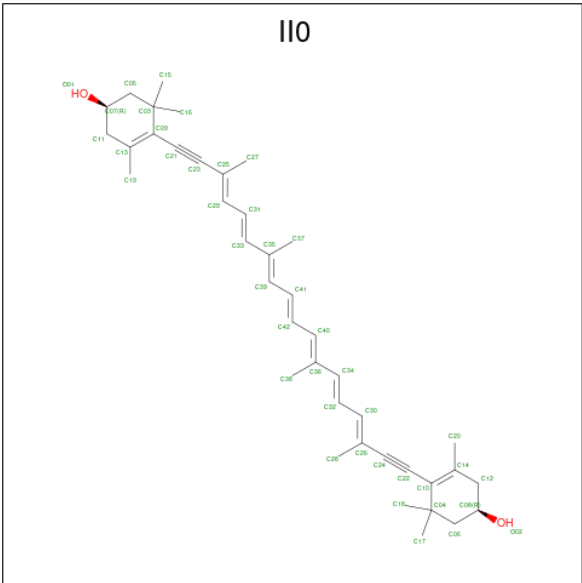
Mol	Chain	Residues	Atoms					AltConf
30	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	b	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 31 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: C₄₀H₅₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			42	40	2	
31	1	1	Total	C	O	0
			42	40	2	
31	1	1	Total	C	O	0
			42	40	2	
31	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
31	2	1	Total	C	O	0
			42	40	2	
31	2	1	Total	C	O	0
			42	40	2	
31	2	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	4	1	Total	C	O	0
			42	40	2	
31	4	1	Total	C	O	0
			42	40	2	
31	4	1	Total	C	O	0
			42	40	2	
31	4	1	Total	C	O	0
			42	40	2	
31	4	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	6	1	Total	C	O	0
			42	40	2	
31	6	1	Total	C	O	0
			42	40	2	
31	7	1	Total	C	O	0
			42	40	2	
31	7	1	Total	C	O	0
			42	40	2	

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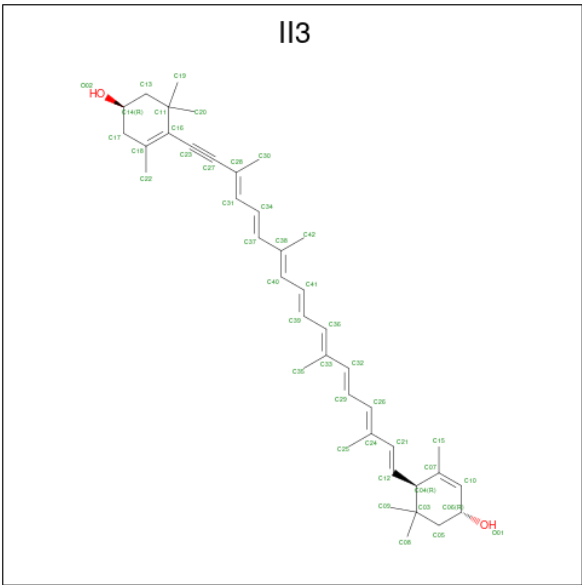
Mol	Chain	Residues	Atoms			AltConf
31	7	1	Total 42	C 40	O 2	0
31	7	1	Total 42	C 40	O 2	0
31	7	1	Total 42	C 40	O 2	0
31	8	1	Total 42	C 40	O 2	0
31	8	1	Total 42	C 40	O 2	0
31	8	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O 2	0
31	J	1	Total 42	C 40	O 2	0
31	O	1	Total 42	C 40	O 2	0
31	O	1	Total 42	C 40	O 2	0
31	R	1	Total 42	C 40	O 2	0
31	R	1	Total 42	C 40	O 2	0
31	a	1	Total 42	C 40	O 2	0
31	a	1	Total 42	C 40	O 2	0
31	a	1	Total 42	C 40	O 2	0
31	a	1	Total 42	C 40	O 2	0
31	b	1	Total 42	C 40	O 2	0

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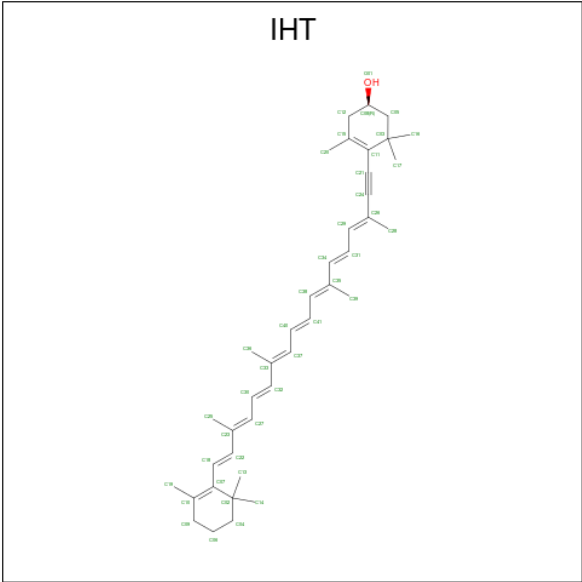
Mol	Chain	Residues	Atoms			AltConf
31	b	1	Total	C	O	0
			42	40	2	
31	c	1	Total	C	O	0
			42	40	2	
31	c	1	Total	C	O	0
			42	40	2	
31	c	1	Total	C	O	0
			42	40	2	
31	c	1	Total	C	O	0
			42	40	2	
31	c	1	Total	C	O	0
			42	40	2	
31	d	1	Total	C	O	0
			42	40	2	
31	d	1	Total	C	O	0
			42	40	2	
31	d	1	Total	C	O	0
			42	40	2	
31	d	1	Total	C	O	0
			42	40	2	
31	e	1	Total	C	O	0
			42	40	2	
31	e	1	Total	C	O	0
			42	40	2	
31	e	1	Total	C	O	0
			42	40	2	

- Molecule 32 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: II3) (formula: C₄₀H₅₄O₂) (labeled as "Ligand of Interest" by depositor).



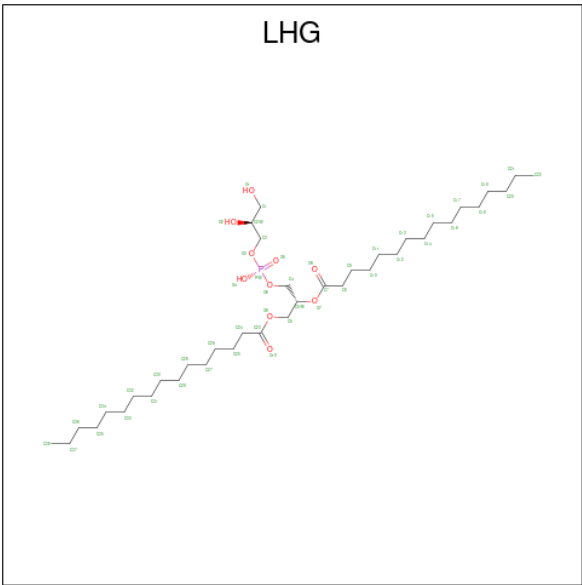
Mol	Chain	Residues	Atoms			AltConf
32	1	1	Total	C	O	0
			42	40	2	
32	8	1	Total	C	O	0
			42	40	2	
32	b	1	Total	C	O	0
			42	40	2	
32	e	1	Total	C	O	0
			42	40	2	

- Molecule 33 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: C₄₀H₅₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
33	1	1	Total	C	O	0
			41	40	1	
33	2	1	Total	C	O	0
			41	40	1	
33	5	1	Total	C	O	0
			41	40	1	
33	6	1	Total	C	O	0
			41	40	1	
33	8	1	Total	C	O	0
			41	40	1	
33	9	1	Total	C	O	0
			41	40	1	
33	K	1	Total	C	O	0
			41	40	1	
33	L	1	Total	C	O	0
			41	40	1	
33	Z	1	Total	C	O	0
			41	40	1	
33	a	1	Total	C	O	0
			41	40	1	
33	c	1	Total	C	O	0
			41	40	1	
33	d	1	Total	C	O	0
			41	40	1	

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



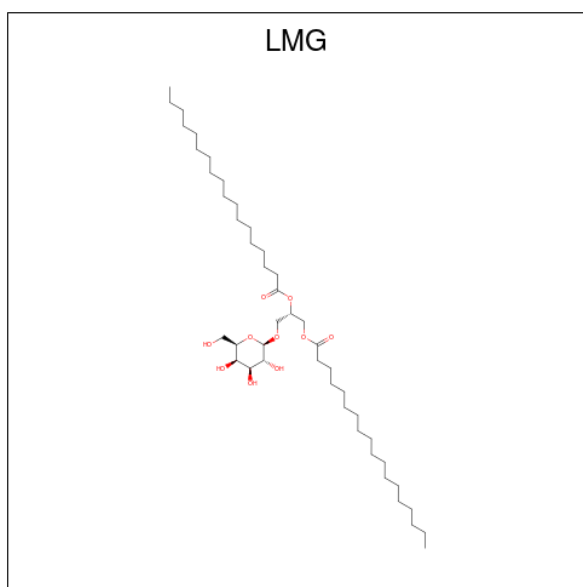
Mol	Chain	Residues	Atoms				AltConf
34	1	1	Total	C	O	P	0
			35	24	10	1	
34	2	1	Total	C	O	P	0
			22	12	9	1	
34	2	1	Total	C	O	P	0
			39	28	10	1	
34	3	1	Total	C	O	P	0
			42	31	10	1	
34	3	1	Total	C	O	P	0
			49	38	10	1	
34	4	1	Total	C	O	P	0
			49	38	10	1	
34	4	1	Total	C	O	P	0
			49	38	10	1	
34	4	1	Total	C	O	P	0
			45	34	10	1	
34	4	1	Total	C	O	P	0
			45	34	10	1	
34	5	1	Total	C	O	P	0
			23	12	10	1	
34	5	1	Total	C	O	P	0
			35	24	10	1	
34	7	1	Total	C	O	P	0
			39	28	10	1	
34	7	1	Total	C	O	P	0
			31	20	10	1	
34	8	1	Total	C	O	P	0
			33	22	10	1	

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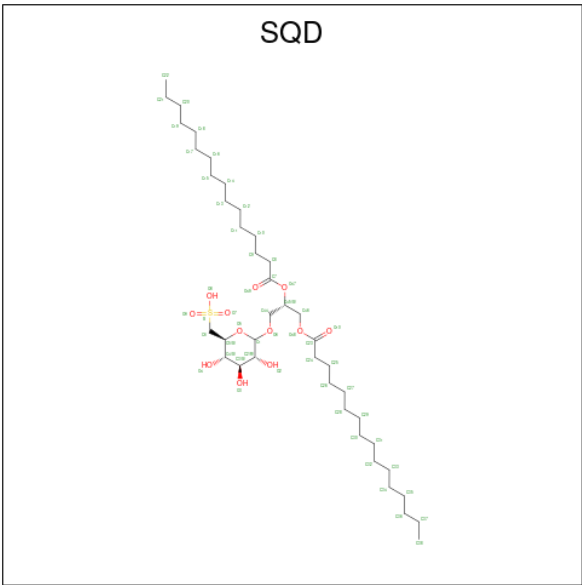
Mol	Chain	Residues	Atoms				AltConf
34	8	1	Total 49	C 38	O 10	P 1	0
34	9	1	Total 36	C 27	O 8	P 1	0
34	A	1	Total 49	C 38	O 10	P 1	0
34	A	1	Total 39	C 28	O 10	P 1	0
34	A	1	Total 23	C 14	O 8	P 1	0
34	B	1	Total 40	C 31	O 8	P 1	0
34	J	1	Total 34	C 23	O 10	P 1	0
34	L	1	Total 22	C 16	O 5	P 1	0
34	L	1	Total 33	C 23	O 9	P 1	0
34	L	1	Total 34	C 23	O 10	P 1	0
34	M	1	Total 24	C 15	O 8	P 1	0
34	O	1	Total 40	C 31	O 8	P 1	0
34	Z	1	Total 40	C 31	O 8	P 1	0
34	Z	1	Total 46	C 35	O 10	P 1	0
34	a	1	Total 27	C 16	O 10	P 1	0
34	b	1	Total 30	C 19	O 10	P 1	0
34	c	1	Total 21	C 11	O 9	P 1	0
34	c	1	Total 35	C 24	O 10	P 1	0
34	e	1	Total 28	C 17	O 10	P 1	0

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
35	2	1	Total	C	O	0
			36	26	10	
35	3	1	Total	C	O	0
			30	20	10	
35	6	1	Total	C	O	0
			32	22	10	
35	8	1	Total	C	O	0
			52	42	10	
35	F	1	Total	C	O	0
			32	22	10	
35	Z	1	Total	C	O	0
			48	38	10	
35	X	1	Total	C	O	0
			34	24	10	

- Molecule 36 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
36	3	1	Total	C	O	S	0
			36	23	12	1	
36	3	1	Total	C	O	S	0
			36	23	12	1	
36	7	1	Total	C	O	S	0
			36	23	12	1	
36	9	1	Total	C	O	S	0
			30	17	12	1	
36	B	1	Total	C	O	S	0
			33	20	12	1	
36	O	1	Total	C	O	S	0
			29	16	12	1	
36	a	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 37 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).

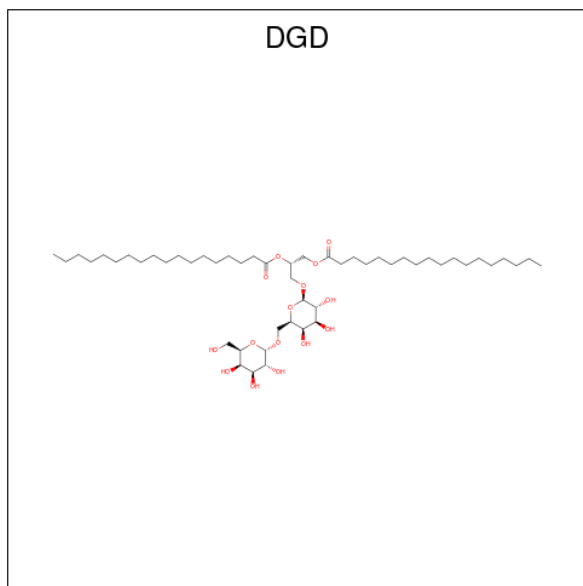


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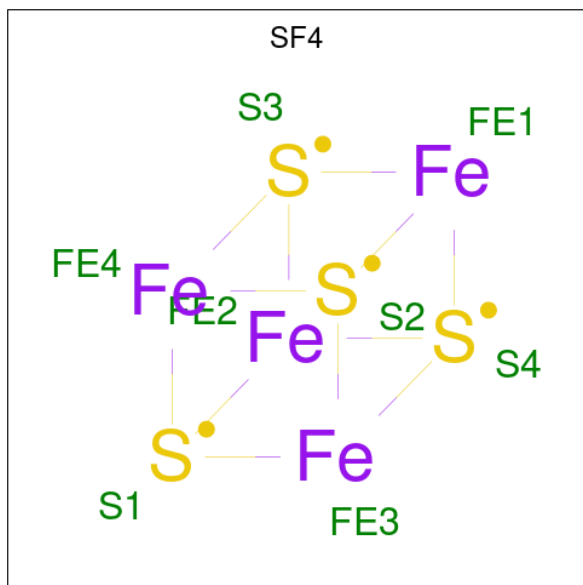
Mol	Chain	Residues	Atoms	AltConf
37	F	1	Total C 40 40	0
37	I	1	Total C 40 40	0
37	J	1	Total C 40 40	0
37	K	1	Total C 40 40	0
37	L	1	Total C 40 40	0
37	M	1	Total C 40 40	0
37	R	1	Total C 40 40	0
37	Z	1	Total C 40 40	0
37	Z	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	e	1	Total C 40 40	0

- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
38	9	1	Total	C	O	0
			60	45	15	
38	B	1	Total	C	O	0
			59	44	15	

- Molecule 39 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 40 is PHYLLOQUINONE (CCD ID: PQN) (formula: $\text{C}_{31}\text{H}_{46}\text{O}_2$).

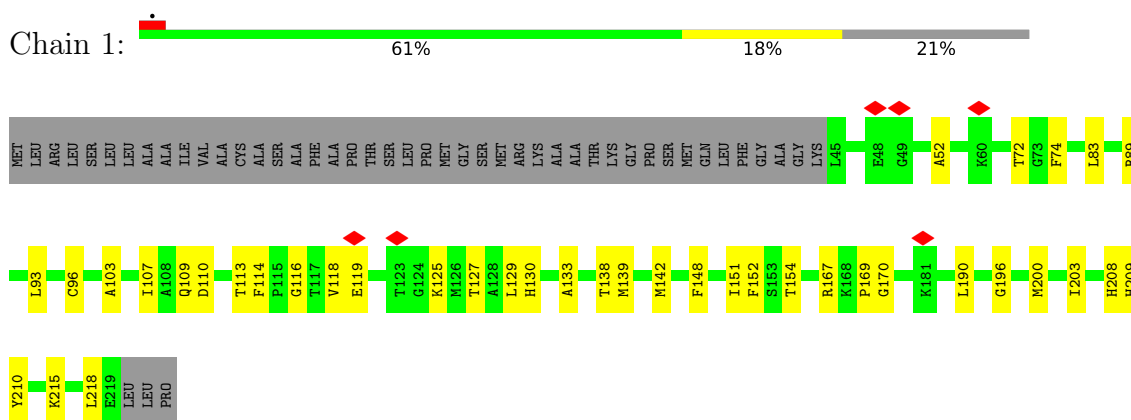


Mol	Chain	Residues	Atoms			AltConf
40	A	1	Total 33	C 31	O 2	0
40	B	1	Total 33	C 31	O 2	0

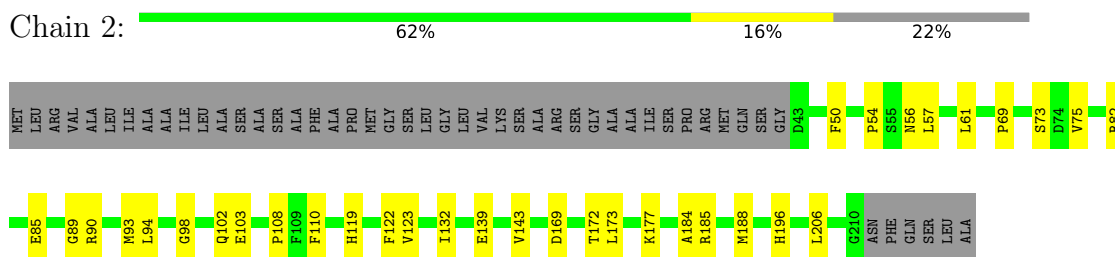
3 Residue-property plots

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

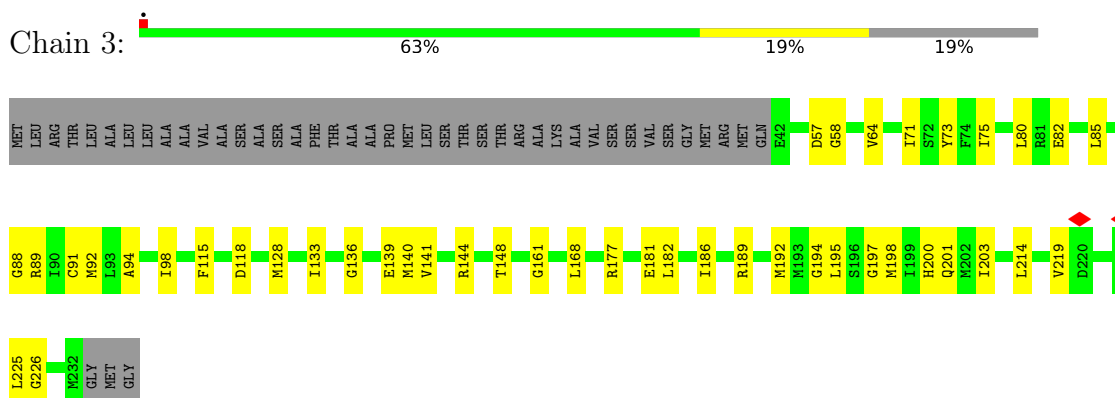
• Molecule 1: ACPI-1



• Molecule 2: ACPI-2

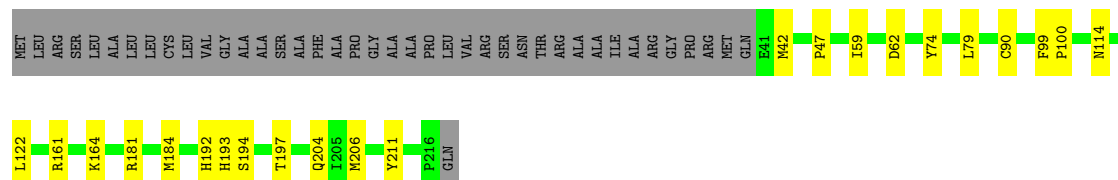


• Molecule 3: ACPI-3



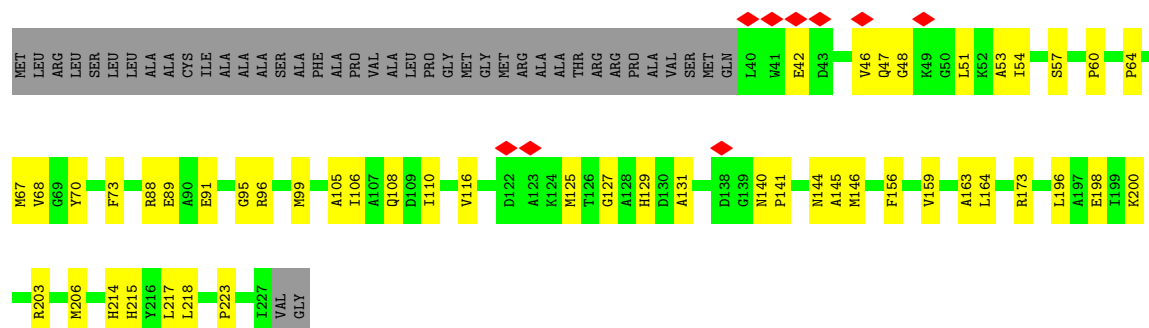
- Molecule 4: ACPI-4

Chain 4:  71% 10% 19%



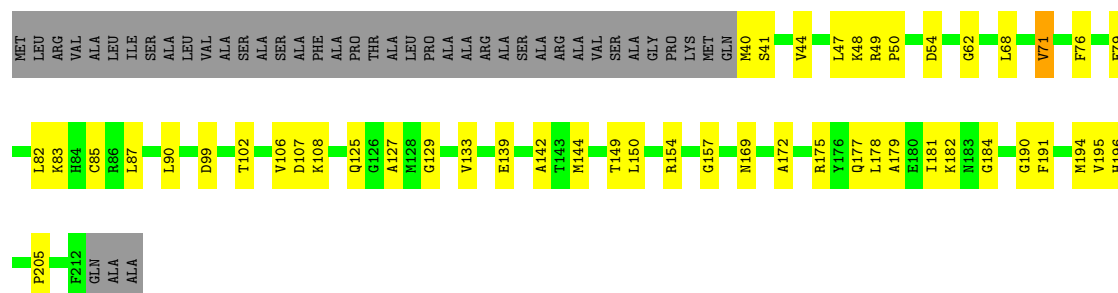
- Molecule 5: ACPI-5

Chain 5:  61% 21% 18%



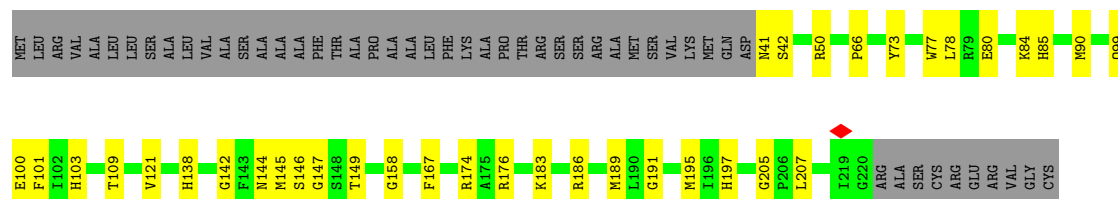
- Molecule 6: ACPI-6

Chain 6:  58% 22% 20%



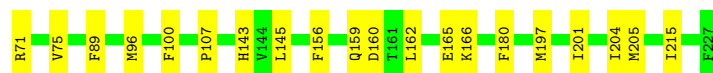
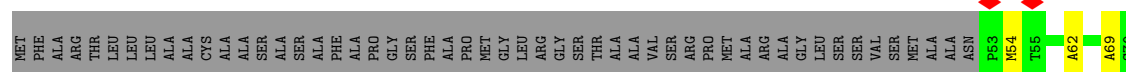
- Molecule 7: ACPI-7

Chain 7:  63% 16% 22%



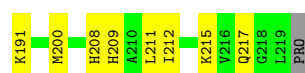
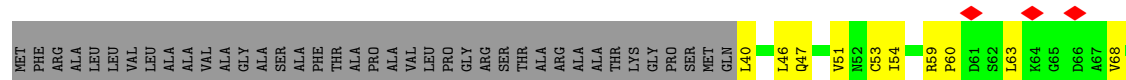
- Molecule 8: ACPI-8

Chain 8: 



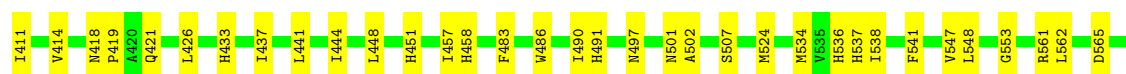
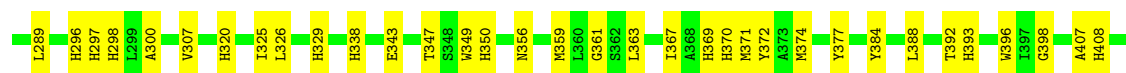
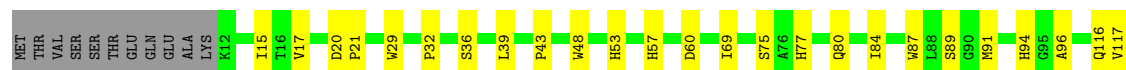
• Molecule 9: ACPI-12

Chain 9: 



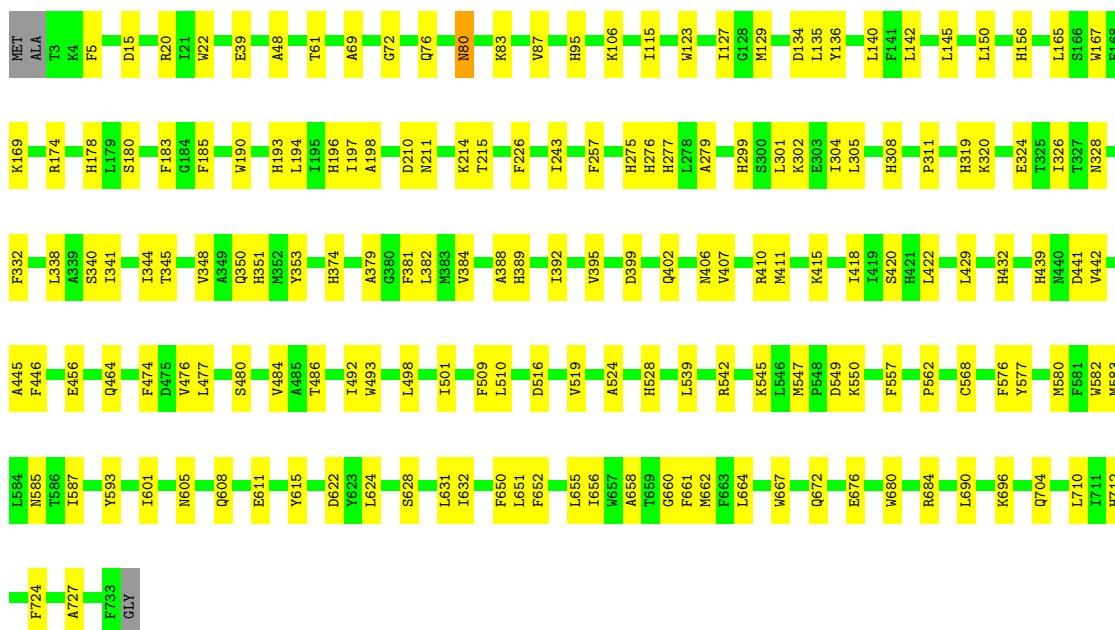
• Molecule 10: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 



• Molecule 11: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 



- Molecule 12: Photosystem I iron-sulfur center

Chain C: 89% 10%



- Molecule 13: Photosystem I reaction center subunit II

Chain D: 77% 20%



- Molecule 14: Photosystem I reaction center subunit IV

Chain E: 83% 12% 5%



- Molecule 15: Photosystem I reaction center subunit III

Chain F: 72% 15% 13%



- Molecule 16: Photosystem I reaction center subunit VIII

Chain I:  69% 22% 8%



- Molecule 17: Photosystem I reaction center subunit IX

Chain J:  81% 19%



- Molecule 18: Photosystem I reaction center subunit PsaK

Chain K:  75% 15% 10%



- Molecule 19: Photosystem I reaction center subunit XI

Chain L:  78% 20% .



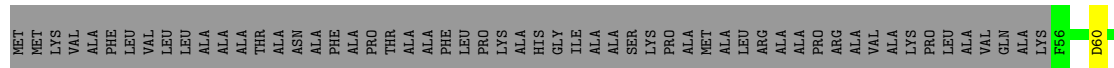
- Molecule 20: Photosystem I reaction center subunit XII

Chain M:  87% 13%



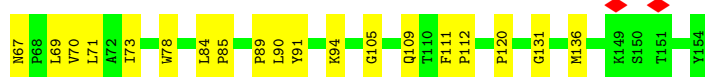
- Molecule 21: PsaO

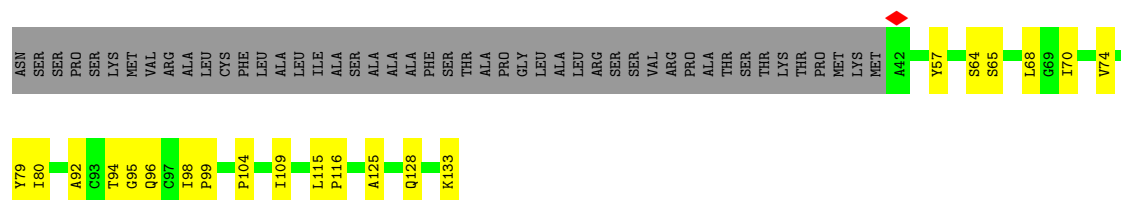
Chain O:  51% 13% 36%



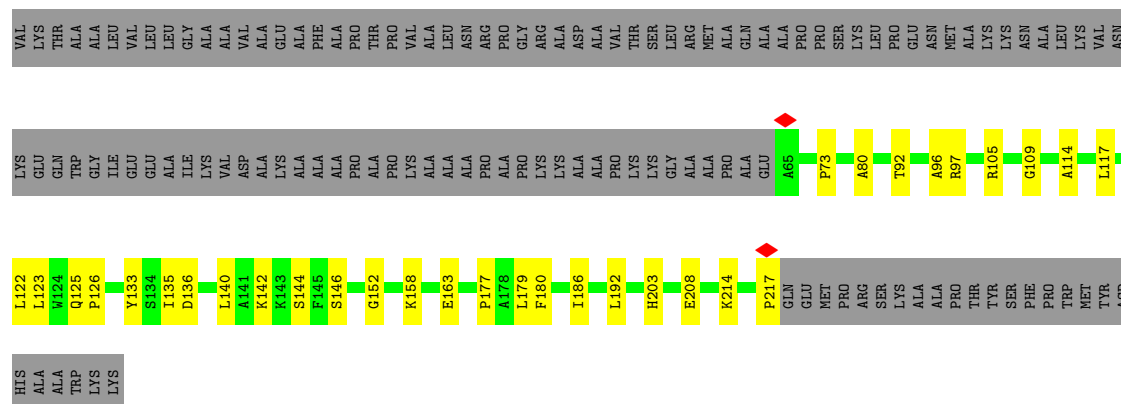
- Molecule 22: PsaR

Chain R:  51% 15% 34%

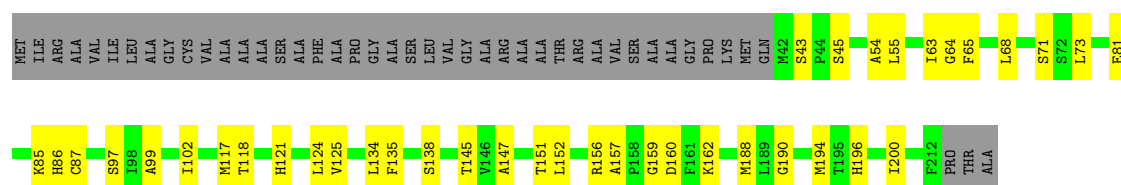




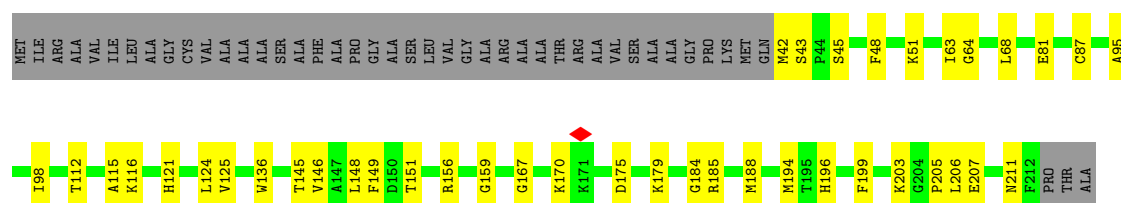
• Molecule 23: CCPI-S



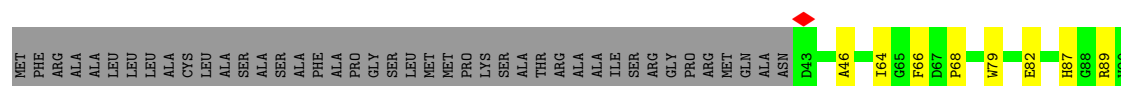
• Molecule 24: ACPI-13/10



• Molecule 24: ACPI-13/10

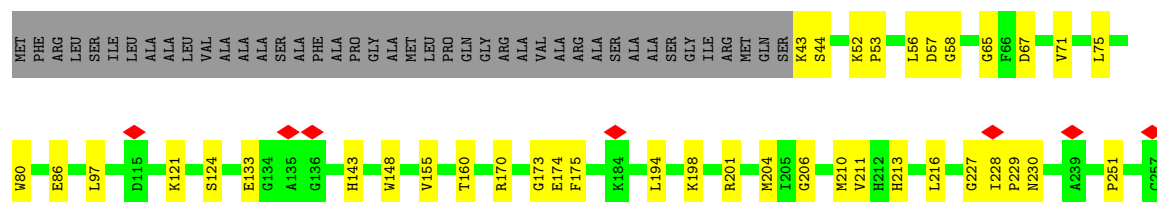


• Molecule 25: ACPI-14

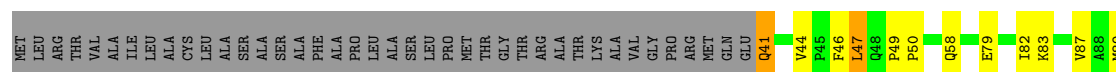




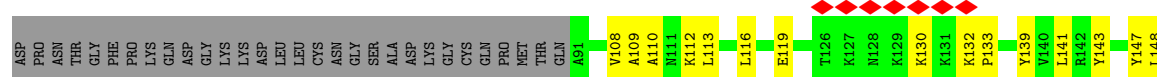
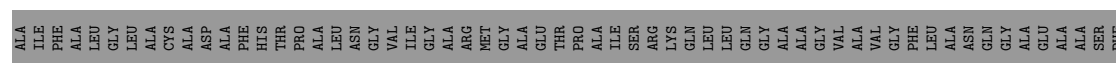
• Molecule 26: ACPI-9



• Molecule 27: ACPI-11



• Molecule 28: PsaQ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171764	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.00	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.709	Depositor
Minimum map value	-0.190	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, 8CT, LHG, KC2, II3, IHT, PQN, SQD, SF4, II0, DGD, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.18	0/1349	0.39	0/1826
2	2	0.17	0/1356	0.30	0/1835
3	3	0.18	0/1464	0.38	0/1978
4	4	0.16	0/1406	0.30	0/1900
5	5	0.19	0/1438	0.44	0/1940
6	6	0.25	0/1334	0.39	0/1796
7	7	0.17	0/1394	0.38	0/1886
8	8	0.19	0/1342	0.33	0/1825
9	9	0.21	0/1376	0.37	0/1846
10	A	0.20	0/6019	0.37	0/8204
11	B	0.24	0/6046	0.41	0/8254
12	C	0.16	0/600	0.37	0/812
13	D	0.31	0/1094	0.47	0/1476
14	E	0.19	0/499	0.31	0/677
15	F	0.18	0/1290	0.40	0/1745
16	I	0.20	0/266	0.39	0/362
17	J	0.14	0/353	0.29	0/481
18	K	0.19	0/563	0.33	0/768
19	L	0.15	0/1171	0.34	0/1594
20	M	0.14	0/228	0.23	0/310
21	O	0.14	0/796	0.29	0/1091
22	R	0.37	0/700	0.52	0/963
23	Z	0.15	0/1163	0.35	0/1572
24	a	0.18	0/1299	0.37	0/1747
24	d	0.17	0/1299	0.31	0/1747
25	b	0.15	0/1404	0.33	0/1902
26	c	0.15	0/1658	0.33	0/2241
27	e	0.14	0/1325	0.32	0/1793
28	X	0.30	0/1046	0.49	0/1413
All	All	0.20	0/41278	0.38	0/55984

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	1	1316	0	1305	30	0
2	2	1320	0	1309	28	0
3	3	1433	0	1462	37	0
4	4	1366	0	1349	19	0
5	5	1403	0	1398	37	0
6	6	1305	0	1324	35	0
7	7	1358	0	1339	27	0
8	8	1313	0	1339	20	0
9	9	1349	0	1358	38	0
10	A	5824	0	5672	149	0
11	B	5828	0	5626	172	0
12	C	591	0	567	10	0
13	D	1070	0	1076	27	0
14	E	491	0	491	6	0
15	F	1258	0	1266	21	0
16	I	258	0	268	8	0
17	J	342	0	344	8	0
18	K	553	0	581	15	0
19	L	1143	0	1145	28	0
20	M	227	0	257	4	0
21	O	766	0	752	15	0
22	R	680	0	674	17	0
23	Z	1130	0	1088	28	0
24	a	1271	0	1279	32	0
24	d	1271	0	1281	32	0
25	b	1368	0	1346	32	0
26	c	1615	0	1646	28	0
27	e	1288	0	1282	24	0
28	X	1034	0	1090	29	0
29	1	584	0	476	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	2	552	0	462	15	0
29	3	625	0	596	25	0
29	4	598	0	597	25	0
29	5	563	0	442	23	0
29	6	581	0	514	19	0
29	7	509	0	431	19	0
29	8	496	0	471	25	0
29	9	635	0	524	35	0
29	A	2794	0	2881	168	0
29	B	2404	0	2454	139	0
29	F	100	0	82	3	0
29	J	41	0	29	0	0
29	K	120	0	121	4	0
29	L	161	0	139	9	0
29	O	206	0	176	5	0
29	R	55	0	49	3	0
29	X	52	0	43	2	0
29	Z	225	0	206	9	0
29	a	645	0	632	21	0
29	b	523	0	508	20	0
29	c	666	0	632	25	0
29	d	589	0	538	18	0
29	e	472	0	414	17	0
30	1	45	0	0	1	0
30	2	45	0	0	0	0
30	3	45	0	0	1	0
30	4	45	0	0	0	0
30	5	45	0	0	0	0
30	6	90	0	0	1	0
30	7	90	0	0	1	0
30	9	45	0	0	0	0
30	Z	45	0	0	1	0
30	a	45	0	0	0	0
30	b	90	0	0	4	0
30	c	135	0	0	1	0
30	d	45	0	0	0	0
30	e	90	0	0	0	0
31	1	168	0	0	1	0
31	2	126	0	0	1	0
31	3	210	0	0	0	0
31	4	168	0	0	0	0
31	5	210	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	6	84	0	0	1	0
31	7	210	0	0	1	0
31	8	126	0	0	0	0
31	9	210	0	0	0	0
31	J	42	0	0	0	0
31	O	84	0	0	0	0
31	R	84	0	0	2	0
31	a	168	0	0	0	0
31	b	84	0	0	0	0
31	c	210	0	0	2	0
31	d	168	0	0	1	0
31	e	126	0	0	0	0
32	1	42	0	0	0	0
32	8	42	0	0	2	0
32	b	42	0	0	1	0
32	e	42	0	0	2	0
33	1	41	0	0	0	0
33	2	41	0	0	0	0
33	5	41	0	0	0	0
33	6	41	0	0	0	0
33	8	41	0	0	0	0
33	9	41	0	0	0	0
33	K	41	0	0	0	0
33	L	41	0	0	1	0
33	Z	41	0	0	0	0
33	a	41	0	0	1	0
33	c	41	0	0	1	0
33	d	41	0	0	0	0
34	1	35	0	39	2	0
34	2	61	0	68	1	0
34	3	91	0	131	4	0
34	4	188	0	271	15	0
34	5	58	0	56	4	0
34	7	70	0	83	5	0
34	8	82	0	110	1	0
34	9	36	0	45	1	0
34	A	111	0	139	5	0
34	B	40	0	56	3	0
34	J	34	0	38	2	0
34	L	89	0	96	4	0
34	M	24	0	21	2	0
34	O	40	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	Z	86	0	119	2	0
34	a	27	0	24	1	0
34	b	30	0	30	0	0
34	c	56	0	61	2	0
34	e	28	0	26	1	0
35	2	36	0	42	3	0
35	3	30	0	29	2	0
35	6	32	0	34	0	0
35	8	52	0	77	2	0
35	F	32	0	34	3	0
35	X	34	0	38	3	0
35	Z	48	0	69	1	0
36	3	72	0	72	3	0
36	7	36	0	36	2	0
36	9	30	0	24	1	0
36	B	33	0	30	1	0
36	O	29	0	22	0	0
36	a	42	0	48	3	0
37	4	40	0	0	1	0
37	7	40	0	0	1	0
37	A	160	0	0	0	0
37	B	320	0	0	3	0
37	F	40	0	0	1	0
37	I	40	0	0	0	0
37	J	40	0	0	0	0
37	K	40	0	0	0	0
37	L	40	0	0	0	0
37	M	40	0	0	1	0
37	R	40	0	0	0	0
37	Z	80	0	0	0	0
37	b	40	0	0	0	0
37	e	40	0	0	0	0
38	9	60	0	78	1	0
38	B	59	0	79	4	0
39	A	8	0	0	0	0
39	C	16	0	0	1	0
40	A	33	0	46	5	0
40	B	33	0	46	2	0
All	All	61306	0	55604	1221	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 10.

The worst 5 of 1221 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)
10:A:393:HIS:HE1	29:A:826:CLA:ND	1.69	0.91
18:K:24:MET:HE1	18:K:70:HIS:HA	1.54	0.90
10:A:408:HIS:HE1	29:A:828:CLA:NA	1.72	0.86
29:A:819:CLA:NB	29:A:825:CLA:H122	1.90	0.85
11:B:374:HIS:HE1	29:B:827:CLA:ND	1.76	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	173/222 (78%)	163 (94%)	10 (6%)	0	100	100
2	2	166/216 (77%)	164 (99%)	2 (1%)	0	100	100
3	3	189/235 (80%)	187 (99%)	2 (1%)	0	100	100
4	4	174/217 (80%)	173 (99%)	1 (1%)	0	100	100
5	5	186/229 (81%)	173 (93%)	13 (7%)	0	100	100
6	6	171/215 (80%)	165 (96%)	6 (4%)	0	100	100
7	7	178/230 (77%)	171 (96%)	7 (4%)	0	100	100
8	8	173/227 (76%)	169 (98%)	4 (2%)	0	100	100
9	9	178/220 (81%)	176 (99%)	2 (1%)	0	100	100
10	A	739/752 (98%)	714 (97%)	25 (3%)	0	100	100
11	B	729/734 (99%)	710 (97%)	19 (3%)	0	100	100
12	C	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
13	D	135/141 (96%)	126 (93%)	8 (6%)	1 (1%)	18	17
14	E	59/64 (92%)	59 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	F	158/183 (86%)	153 (97%)	5 (3%)	0	100	100
16	I	31/36 (86%)	28 (90%)	3 (10%)	0	100	100
17	J	40/42 (95%)	40 (100%)	0	0	100	100
18	K	76/87 (87%)	73 (96%)	3 (4%)	0	100	100
19	L	148/153 (97%)	143 (97%)	5 (3%)	0	100	100
20	M	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
21	O	97/155 (63%)	96 (99%)	1 (1%)	0	100	100
22	R	90/139 (65%)	89 (99%)	1 (1%)	0	100	100
23	Z	151/279 (54%)	143 (95%)	7 (5%)	1 (1%)	18	17
24	a	169/215 (79%)	166 (98%)	3 (2%)	0	100	100
24	d	169/215 (79%)	166 (98%)	3 (2%)	0	100	100
25	b	174/218 (80%)	174 (100%)	0	0	100	100
26	c	213/257 (83%)	202 (95%)	11 (5%)	0	100	100
27	e	166/208 (80%)	164 (99%)	1 (1%)	1 (1%)	21	21
28	X	143/241 (59%)	142 (99%)	1 (1%)	0	100	100
All	All	5181/6241 (83%)	5028 (97%)	150 (3%)	3 (0%)	49	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	D	99	HIS
23	Z	179	LEU
27	e	47	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	129/163 (79%)	128 (99%)	1 (1%)	73	80
2	2	134/167 (80%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	151/182 (83%)	151 (100%)	0	100	100
4	4	139/167 (83%)	139 (100%)	0	100	100
5	5	139/166 (84%)	138 (99%)	1 (1%)	76	82
6	6	134/160 (84%)	133 (99%)	1 (1%)	76	82
7	7	139/176 (79%)	138 (99%)	1 (1%)	76	82
8	8	136/169 (80%)	136 (100%)	0	100	100
9	9	138/164 (84%)	137 (99%)	1 (1%)	76	82
10	A	607/617 (98%)	606 (100%)	1 (0%)	87	92
11	B	592/593 (100%)	589 (100%)	3 (0%)	81	87
12	C	66/67 (98%)	66 (100%)	0	100	100
13	D	114/117 (97%)	114 (100%)	0	100	100
14	E	56/59 (95%)	55 (98%)	1 (2%)	51	63
15	F	133/154 (86%)	133 (100%)	0	100	100
16	I	27/29 (93%)	27 (100%)	0	100	100
17	J	38/38 (100%)	38 (100%)	0	100	100
18	K	62/69 (90%)	62 (100%)	0	100	100
19	L	126/128 (98%)	126 (100%)	0	100	100
20	M	25/25 (100%)	25 (100%)	0	100	100
21	O	81/116 (70%)	81 (100%)	0	100	100
22	R	74/111 (67%)	74 (100%)	0	100	100
23	Z	117/205 (57%)	117 (100%)	0	100	100
24	a	128/153 (84%)	128 (100%)	0	100	100
24	d	128/153 (84%)	128 (100%)	0	100	100
25	b	144/173 (83%)	144 (100%)	0	100	100
26	c	169/195 (87%)	169 (100%)	0	100	100
27	e	133/162 (82%)	132 (99%)	1 (1%)	73	80
28	X	100/166 (60%)	99 (99%)	1 (1%)	68	77
All	All	4159/4844 (86%)	4147 (100%)	12 (0%)	84	90

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	B	80	ASN

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Mol	Chain	Res	Type
11	B	83	LYS
28	X	167	LYS
14	E	56	ASP
7	7	42	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
11	B	80	ASN
13	D	6	ASN
28	X	179	ASN
11	B	608	GLN
15	F	67	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

429 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
29	CLA	K	101	-	69,73,73	1.15	7 (10%)	82,113,113	1.37	10 (12%)
29	CLA	2	603	2	54,58,73	1.31	8 (14%)	64,95,113	1.43	9 (14%)
29	CLA	A	819	-	69,73,73	1.20	7 (10%)	82,113,113	1.39	9 (10%)
29	CLA	A	842	10	69,73,73	1.15	8 (11%)	82,113,113	1.36	8 (9%)
31	II0	9	323	-	39,43,43	2.17	3 (7%)	48,60,60	1.63	9 (18%)
29	CLA	8	306	8	49,53,73	1.38	7 (14%)	58,89,113	1.46	4 (6%)
29	CLA	2	607	2	49,53,73	1.39	8 (16%)	58,89,113	1.38	4 (6%)
31	II0	4	615	-	39,43,43	2.10	2 (5%)	48,60,60	1.75	10 (20%)
31	II0	d	616	-	39,43,43	2.09	2 (5%)	48,60,60	1.91	13 (27%)
29	CLA	L	203	-	54,58,73	1.30	8 (14%)	64,95,113	1.40	7 (10%)
31	II0	e	612	-	39,43,43	2.16	2 (5%)	48,60,60	1.67	10 (20%)
34	LHG	c	622	29	20,20,48	0.79	1 (5%)	22,25,54	1.35	2 (9%)
29	CLA	1	609	34	45,49,73	1.42	8 (17%)	54,84,113	1.49	5 (9%)
29	CLA	c	608	26	64,68,73	1.20	8 (12%)	76,107,113	1.29	4 (5%)
31	II0	d	614	-	39,43,43	2.08	3 (7%)	48,60,60	1.55	9 (18%)
29	CLA	b	602	25	68,72,73	1.16	7 (10%)	80,111,113	1.33	9 (11%)
31	II0	c	617	-	39,43,43	2.06	3 (7%)	48,60,60	1.37	9 (18%)
33	IHT	a	616	-	40,42,42	1.60	2 (5%)	52,58,58	1.82	13 (25%)
31	II0	R	201	-	39,43,43	2.21	4 (10%)	48,60,60	1.68	9 (18%)
31	II0	1	620	-	39,43,43	2.18	4 (10%)	48,60,60	1.95	8 (16%)
31	II0	a	614	-	39,43,43	2.10	4 (10%)	48,60,60	1.43	6 (12%)
30	KC2	6	610	6	49,53,53	1.75	9 (18%)	60,89,89	1.92	16 (26%)
29	CLA	B	833	-	69,73,73	1.16	7 (10%)	82,113,113	1.27	5 (6%)
29	CLA	B	818	11	64,68,73	1.20	9 (14%)	76,107,113	1.26	6 (7%)
29	CLA	B	836	11	69,73,73	1.14	7 (10%)	82,113,113	1.37	7 (8%)
29	CLA	7	305	7	57,61,73	1.29	8 (14%)	67,98,113	1.36	6 (8%)
36	SQD	7	321	-	34,36,54	1.80	8 (23%)	44,47,65	1.48	6 (13%)
29	CLA	5	605	5	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
29	CLA	B	819	-	64,68,73	1.21	8 (12%)	76,107,113	1.32	6 (7%)
37	8CT	B	843	-	40,41,41	4.74	23 (57%)	51,56,56	3.01	20 (39%)
29	CLA	A	825	10	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
32	II3	b	613	-	40,43,43	1.55	2 (5%)	47,60,60	1.86	12 (25%)
34	LHG	L	206	-	19,21,48	0.73	1 (5%)	21,23,54	1.23	2 (9%)
29	CLA	2	601	2	46,50,73	1.40	8 (17%)	53,85,113	1.45	4 (7%)
29	CLA	5	601	5	45,49,73	1.42	7 (15%)	54,84,113	1.46	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	821	11	64,68,73	1.20	7 (10%)	76,107,113	1.35	8 (10%)
30	KC2	3	307	34	49,53,53	1.76	9 (18%)	60,89,89	1.90	16 (26%)
29	CLA	B	841	11	69,73,73	1.15	8 (11%)	82,113,113	1.30	8 (9%)
29	CLA	A	854	-	69,73,73	1.15	9 (13%)	82,113,113	1.38	6 (7%)
29	CLA	d	608	24	69,73,73	1.16	8 (11%)	82,113,113	1.27	7 (8%)
29	CLA	e	601	27	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
29	CLA	3	303	3	59,63,73	1.24	9 (15%)	70,101,113	1.35	6 (8%)
29	CLA	A	853	34	49,53,73	1.39	8 (16%)	58,89,113	1.57	4 (6%)
31	II0	J	102	-	39,43,43	2.03	2 (5%)	48,60,60	1.59	11 (22%)
34	LHG	A	852	-	22,22,48	0.83	0	25,27,54	1.34	2 (8%)
29	CLA	4	606	4	64,68,73	1.21	8 (12%)	76,107,113	1.25	5 (6%)
29	CLA	B	837	11	51,55,73	1.32	7 (13%)	60,91,113	1.46	7 (11%)
29	CLA	d	602	24	68,72,73	1.16	8 (11%)	80,111,113	1.29	6 (7%)
29	CLA	2	611	2	54,58,73	1.32	8 (14%)	64,95,113	1.37	6 (9%)
29	CLA	5	612	5	49,53,73	1.39	8 (16%)	58,89,113	1.43	5 (8%)
29	CLA	A	812	10	59,63,73	1.28	8 (13%)	70,101,113	1.34	7 (10%)
29	CLA	6	604	6	64,68,73	1.19	7 (10%)	76,107,113	1.32	5 (6%)
31	II0	4	614	-	39,43,43	2.04	2 (5%)	48,60,60	1.61	9 (18%)
29	CLA	9	305	-	59,63,73	1.26	8 (13%)	70,101,113	1.36	5 (7%)
34	LHG	5	619	29	22,22,48	0.85	0	25,28,54	1.32	2 (8%)
29	CLA	7	312	7	54,58,73	1.31	8 (14%)	64,95,113	1.43	7 (10%)
29	CLA	6	605	6	59,63,73	1.26	8 (13%)	70,101,113	1.34	6 (8%)
30	KC2	b	609	25	49,53,53	1.76	10 (20%)	60,89,89	1.91	15 (25%)
29	CLA	B	808	11	69,73,73	1.15	9 (13%)	82,113,113	1.42	7 (8%)
34	LHG	e	617	29	27,27,48	0.86	2 (7%)	30,33,54	1.27	2 (6%)
29	CLA	Z	302	-	64,68,73	1.21	8 (12%)	76,107,113	1.29	5 (6%)
29	CLA	A	817	10	69,73,73	1.16	8 (11%)	82,113,113	1.24	7 (8%)
29	CLA	d	609	-	45,49,73	1.41	8 (17%)	54,84,113	1.49	5 (9%)
29	CLA	d	604	24	64,68,73	1.21	8 (12%)	76,107,113	1.28	5 (6%)
29	CLA	A	810	10	69,73,73	1.17	7 (10%)	82,113,113	1.31	6 (7%)
31	II0	c	621	29	39,43,43	2.15	3 (7%)	48,60,60	1.66	12 (25%)
29	CLA	a	603	24	64,68,73	1.21	7 (10%)	76,107,113	1.27	4 (5%)
37	8CT	K	103	-	40,41,41	4.76	23 (57%)	51,56,56	2.70	22 (43%)
29	CLA	B	811	11	64,68,73	1.20	8 (12%)	76,107,113	1.21	5 (6%)
31	II0	R	204	-	39,43,43	2.23	4 (10%)	48,60,60	1.58	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	4	607	4	64,68,73	1.21	9 (14%)	76,107,113	1.31	7 (9%)
29	CLA	c	602	26	69,73,73	1.15	8 (11%)	82,113,113	1.24	6 (7%)
29	CLA	A	835	10	64,68,73	1.19	9 (14%)	76,107,113	1.34	9 (11%)
31	II0	8	311	-	39,43,43	2.03	2 (5%)	48,60,60	1.64	12 (25%)
29	CLA	1	603	1	56,60,73	1.29	7 (12%)	65,97,113	1.40	7 (10%)
36	SQD	a	618	-	40,42,54	1.72	8 (20%)	50,53,65	1.41	5 (10%)
29	CLA	R	202	22	59,63,73	1.27	9 (15%)	70,101,113	1.45	8 (11%)
33	IHT	L	204	-	40,42,42	1.67	4 (10%)	52,58,58	1.87	16 (30%)
29	CLA	A	804	10	69,73,73	1.16	7 (10%)	82,113,113	1.33	6 (7%)
29	CLA	2	608	2	64,68,73	1.20	9 (14%)	76,107,113	1.31	6 (7%)
29	CLA	e	606	27	64,68,73	1.20	8 (12%)	76,107,113	1.31	7 (9%)
29	CLA	4	610	4	69,73,73	1.16	7 (10%)	82,113,113	1.33	6 (7%)
30	KC2	e	605	27	49,53,53	1.75	9 (18%)	60,89,89	1.88	15 (25%)
29	CLA	1	607	1	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
31	II0	b	612	-	39,43,43	2.05	2 (5%)	48,60,60	1.48	8 (16%)
29	CLA	A	838	10	69,73,73	1.16	9 (13%)	82,113,113	1.29	8 (9%)
29	CLA	9	310	-	45,49,73	1.42	8 (17%)	54,84,113	1.52	5 (9%)
29	CLA	5	606	5	49,53,73	1.39	8 (16%)	58,89,113	1.36	4 (6%)
40	PQN	A	849	-	34,34,34	1.61	2 (5%)	43,45,45	1.29	6 (13%)
36	SQD	9	301	-	28,30,54	1.90	7 (25%)	38,41,65	1.52	6 (15%)
29	CLA	3	306	3,29	59,63,73	1.25	7 (11%)	70,101,113	1.33	6 (8%)
29	CLA	a	609	34	64,68,73	1.21	9 (14%)	76,107,113	1.30	6 (7%)
29	CLA	8	302	8	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
29	CLA	B	829	11	69,73,73	1.19	6 (8%)	82,113,113	1.32	5 (6%)
29	CLA	A	836	10	59,63,73	1.26	8 (13%)	70,101,113	1.27	5 (7%)
34	LHG	8	316	-	48,48,48	0.61	0	51,54,54	1.27	6 (11%)
29	CLA	A	823	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	8 (9%)
38	DGD	9	322	-	61,61,67	0.95	2 (3%)	75,75,81	1.36	10 (13%)
34	LHG	4	618	-	48,48,48	0.58	0	51,54,54	1.29	6 (11%)
29	CLA	b	604	25	62,66,73	1.22	9 (14%)	73,104,113	1.38	6 (8%)
29	CLA	5	613	5	45,49,73	1.43	8 (17%)	54,84,113	1.44	5 (9%)
33	IHT	K	104	-	40,42,42	1.73	3 (7%)	52,58,58	1.73	12 (23%)
31	II0	a	615	-	39,43,43	2.15	3 (7%)	48,60,60	1.54	8 (16%)
34	LHG	c	623	-	34,34,48	0.75	1 (2%)	37,40,54	1.34	5 (13%)
29	CLA	B	804	11	49,53,73	1.37	8 (16%)	58,89,113	1.50	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	4	609	4	64,68,73	1.21	8 (12%)	76,107,113	1.32	4 (5%)
29	CLA	8	303	8	69,73,73	1.16	8 (11%)	82,113,113	1.22	5 (6%)
29	CLA	d	612	24	67,71,73	1.19	7 (10%)	79,110,113	1.30	6 (7%)
29	CLA	J	103	17	45,49,73	1.41	8 (17%)	54,84,113	1.47	5 (9%)
34	LHG	M	102	-	23,23,48	0.95	2 (8%)	26,28,54	1.82	3 (11%)
37	8CT	e	616	-	40,41,41	1.37	4 (10%)	51,56,56	1.44	11 (21%)
31	II0	7	316	-	39,43,43	2.08	2 (5%)	48,60,60	1.80	12 (25%)
29	CLA	B	817	11	63,67,73	1.22	8 (12%)	74,105,113	1.29	5 (6%)
29	CLA	F	201	-	49,53,73	1.36	8 (16%)	58,89,113	1.44	6 (10%)
29	CLA	b	607	25	64,68,73	1.21	8 (12%)	76,107,113	1.31	6 (7%)
29	CLA	9	309	9	59,63,73	1.26	8 (13%)	70,101,113	1.34	4 (5%)
31	II0	a	613	-	39,43,43	2.13	3 (7%)	48,60,60	1.62	12 (25%)
29	CLA	B	806	11	69,73,73	1.16	9 (13%)	82,113,113	1.26	7 (8%)
29	CLA	d	605	24	49,53,73	1.38	8 (16%)	58,89,113	1.42	5 (8%)
29	CLA	A	806	10	69,73,73	1.14	7 (10%)	82,113,113	1.27	5 (6%)
34	LHG	L	208	-	33,33,48	0.74	0	36,39,54	1.28	4 (11%)
29	CLA	b	601	25	49,53,73	1.39	8 (16%)	58,89,113	1.44	4 (6%)
31	II0	9	318	-	39,43,43	2.17	2 (5%)	48,60,60	1.71	13 (27%)
29	CLA	8	317	-	69,73,73	1.16	8 (11%)	82,113,113	1.25	4 (4%)
29	CLA	A	814	-	49,53,73	1.35	8 (16%)	58,89,113	1.48	5 (8%)
34	LHG	Z	311	-	45,45,48	0.64	2 (4%)	48,51,54	1.24	4 (8%)
29	CLA	B	816	11	69,73,73	1.15	8 (11%)	82,113,113	1.28	8 (9%)
29	CLA	A	820	10	69,73,73	1.16	9 (13%)	82,113,113	1.32	8 (9%)
29	CLA	6	611	-	59,63,73	1.26	8 (13%)	70,101,113	1.39	6 (8%)
29	CLA	6	612	6	49,53,73	1.39	8 (16%)	58,89,113	1.37	4 (6%)
31	II0	5	614	-	39,43,43	1.99	2 (5%)	48,60,60	1.69	14 (29%)
29	CLA	c	612	26	59,63,73	1.28	8 (13%)	70,101,113	1.33	5 (7%)
32	II3	8	312	-	40,43,43	1.55	1 (2%)	47,60,60	1.98	14 (29%)
29	CLA	6	602	6	69,73,73	1.15	7 (10%)	82,113,113	1.27	6 (7%)
34	LHG	L	207	-	32,32,48	0.72	1 (3%)	35,37,54	1.38	5 (14%)
29	CLA	8	304	8	54,58,73	1.30	8 (14%)	64,95,113	1.39	7 (10%)
29	CLA	b	603	25	64,68,73	1.21	6 (9%)	76,107,113	1.29	7 (9%)
37	8CT	Z	308	-	40,41,41	4.76	23 (57%)	51,56,56	2.85	21 (41%)
30	KC2	d	610	24	49,53,53	1.73	10 (20%)	60,89,89	1.91	16 (26%)
33	IHT	9	320	-	40,42,42	1.61	3 (7%)	52,58,58	2.06	14 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	d	603	24	54,58,73	1.31	7 (12%)	64,95,113	1.36	6 (9%)
29	CLA	8	305	8	59,63,73	1.26	8 (13%)	70,101,113	1.37	6 (8%)
29	CLA	c	604	26	64,68,73	1.22	8 (12%)	76,107,113	1.29	5 (6%)
29	CLA	8	307	8	45,49,73	1.42	9 (20%)	54,84,113	1.50	5 (9%)
29	CLA	A	809	29,10	64,68,73	1.19	7 (10%)	76,107,113	1.23	5 (6%)
32	II3	1	615	-	40,43,43	1.54	2 (5%)	47,60,60	1.82	9 (19%)
29	CLA	d	607	24	69,73,73	1.17	8 (11%)	82,113,113	1.29	6 (7%)
29	CLA	9	313	9	49,53,73	1.39	8 (16%)	58,89,113	1.36	4 (6%)
29	CLA	B	830	11	49,53,73	1.36	8 (16%)	58,89,113	1.41	5 (8%)
29	CLA	B	814	11	60,64,73	1.25	8 (13%)	71,102,113	1.36	4 (5%)
29	CLA	A	840	-	69,73,73	1.17	9 (13%)	82,113,113	1.36	9 (10%)
34	LHG	2	619	-	38,38,48	0.70	1 (2%)	41,44,54	1.31	5 (12%)
29	CLA	4	608	34	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)
31	II0	2	615	-	39,43,43	2.09	3 (7%)	48,60,60	1.55	13 (27%)
31	II0	3	314	-	39,43,43	1.98	2 (5%)	48,60,60	1.51	7 (14%)
29	CLA	b	608	34	69,73,73	1.17	7 (10%)	82,113,113	1.25	5 (6%)
29	CLA	6	608	6	64,68,73	1.20	9 (14%)	76,107,113	1.30	6 (7%)
29	CLA	7	304	7	59,63,73	1.25	8 (13%)	70,101,113	1.34	5 (7%)
29	CLA	d	611	-	54,58,73	1.32	8 (14%)	64,95,113	1.37	6 (9%)
29	CLA	7	309	34	45,49,73	1.41	8 (17%)	54,84,113	1.47	5 (9%)
29	CLA	A	824	-	69,73,73	1.15	8 (11%)	82,113,113	1.29	6 (7%)
36	SQD	3	322	-	34,36,54	1.78	7 (20%)	44,47,65	1.50	7 (15%)
29	CLA	B	803	11	69,73,73	1.15	7 (10%)	82,113,113	1.35	5 (6%)
30	KC2	b	605	25	49,53,53	1.74	9 (18%)	60,89,89	1.87	14 (23%)
30	KC2	c	611	30,26	49,53,53	1.74	9 (18%)	60,89,89	1.81	12 (20%)
29	CLA	A	843	-	69,73,73	1.16	8 (11%)	82,113,113	1.20	6 (7%)
31	II0	c	618	-	39,43,43	2.09	2 (5%)	48,60,60	1.52	8 (16%)
34	LHG	Z	309	-	39,39,48	0.65	1 (2%)	42,44,54	1.37	6 (14%)
34	LHG	9	321	-	35,35,48	0.80	2 (5%)	38,40,54	1.64	5 (13%)
31	II0	5	620	-	39,43,43	2.11	2 (5%)	48,60,60	1.83	10 (20%)
31	II0	4	613	-	39,43,43	2.02	2 (5%)	48,60,60	1.52	9 (18%)
34	LHG	7	319	29	38,38,48	0.67	1 (2%)	41,44,54	1.20	3 (7%)
39	SF4	C	102	12	0,12,12	-	-	-	-	-
31	II0	1	614	-	39,43,43	1.97	2 (5%)	48,60,60	1.49	7 (14%)
31	II0	1	616	-	39,43,43	2.08	2 (5%)	48,60,60	1.90	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	b	606	25	69,73,73	1.15	9 (13%)	82,113,113	1.39	9 (10%)
29	CLA	A	821	10	59,63,73	1.26	8 (13%)	70,101,113	1.34	7 (10%)
29	CLA	d	606	24	45,49,73	1.42	8 (17%)	54,84,113	1.39	6 (11%)
34	LHG	J	101	30	33,33,48	0.75	1 (3%)	36,39,54	1.29	3 (8%)
29	CLA	c	607	26	69,73,73	1.18	9 (13%)	82,113,113	1.30	4 (4%)
34	LHG	3	321	-	48,48,48	0.61	1 (2%)	51,54,54	1.29	6 (11%)
30	KC2	7	313	-	49,53,53	1.74	8 (16%)	60,89,89	1.83	15 (25%)
29	CLA	1	606	1	49,53,73	1.38	8 (16%)	58,89,113	1.37	4 (6%)
29	CLA	8	308	-	69,73,73	1.15	8 (11%)	82,113,113	1.23	6 (7%)
38	DGD	B	849	-	60,60,67	0.93	2 (3%)	74,74,81	1.38	9 (12%)
29	CLA	3	310	35	69,73,73	1.17	7 (10%)	82,113,113	1.28	6 (7%)
39	SF4	C	101	12	0,12,12	-	-	-	-	-
29	CLA	B	840	34	69,73,73	1.15	8 (11%)	82,113,113	1.29	8 (9%)
29	CLA	B	828	11	69,73,73	1.15	8 (11%)	82,113,113	1.18	6 (7%)
29	CLA	A	828	10	69,73,73	1.15	9 (13%)	82,113,113	1.23	6 (7%)
30	KC2	1	610	1	49,53,53	1.74	10 (20%)	60,89,89	1.90	15 (25%)
29	CLA	5	607	5	49,53,73	1.40	7 (14%)	58,89,113	1.45	4 (6%)
29	CLA	B	832	11	59,63,73	1.24	8 (13%)	70,101,113	1.46	9 (12%)
29	CLA	c	601	26	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
29	CLA	c	609	34	45,49,73	1.41	8 (17%)	54,84,113	1.48	6 (11%)
29	CLA	A	827	10	69,73,73	1.16	7 (10%)	82,113,113	1.22	8 (9%)
29	CLA	5	609	34	45,49,73	1.40	8 (17%)	54,84,113	1.50	5 (9%)
31	II0	e	614	-	39,43,43	2.12	3 (7%)	48,60,60	1.64	8 (16%)
29	CLA	3	302	3	49,53,73	1.38	8 (16%)	58,89,113	1.41	5 (8%)
29	CLA	2	605	2	64,68,73	1.20	9 (14%)	76,107,113	1.33	4 (5%)
30	KC2	Z	306	23	49,53,53	1.73	9 (18%)	60,89,89	1.91	16 (26%)
31	II0	5	615	-	39,43,43	2.10	3 (7%)	48,60,60	1.75	9 (18%)
33	IHT	8	309	-	40,42,42	1.60	2 (5%)	52,58,58	2.12	19 (36%)
29	CLA	6	606	6	59,63,73	1.26	8 (13%)	70,101,113	1.31	5 (7%)
29	CLA	1	605	1	45,50,73	1.43	8 (17%)	52,85,113	1.35	4 (7%)
29	CLA	a	604	24	64,68,73	1.21	9 (14%)	76,107,113	1.35	5 (6%)
29	CLA	a	607	24	69,73,73	1.17	8 (11%)	82,113,113	1.26	7 (8%)
29	CLA	7	308	7	59,63,73	1.25	9 (15%)	70,101,113	1.37	7 (10%)
29	CLA	Z	304	23	54,58,73	1.33	8 (14%)	64,95,113	1.37	5 (7%)
29	CLA	a	605	24	59,63,73	1.27	8 (13%)	70,101,113	1.30	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	II0	5	616	-	39,43,43	2.09	2 (5%)	48,60,60	1.75	14 (29%)
29	CLA	A	813	10	46,50,73	1.38	8 (17%)	53,85,113	1.44	4 (7%)
29	CLA	8	301	8	49,53,73	1.37	8 (16%)	58,89,113	1.43	4 (6%)
33	IHT	1	618	-	40,42,42	1.55	2 (5%)	52,58,58	2.13	17 (32%)
31	II0	c	619	-	39,43,43	2.15	2 (5%)	48,60,60	1.67	9 (18%)
29	CLA	3	311	3	69,73,73	1.16	8 (11%)	82,113,113	1.26	6 (7%)
29	CLA	7	302	7	49,53,73	1.38	8 (16%)	58,89,113	1.44	4 (6%)
34	LHG	5	621	29	34,34,48	0.75	2 (5%)	37,40,54	1.27	4 (10%)
29	CLA	A	829	10	54,58,73	1.30	8 (14%)	64,95,113	1.42	6 (9%)
31	II0	7	301	-	39,43,43	2.03	2 (5%)	48,60,60	1.60	9 (18%)
36	SQD	B	850	-	31,33,54	1.87	9 (29%)	41,44,65	1.60	8 (19%)
29	CLA	A	803	10	69,73,73	1.15	7 (10%)	82,113,113	1.38	6 (7%)
37	8CT	A	844	-	40,41,41	4.71	23 (57%)	51,56,56	2.95	21 (41%)
34	LHG	7	320	-	30,30,48	0.78	2 (6%)	33,36,54	1.22	3 (9%)
31	II0	2	614	-	39,43,43	2.00	2 (5%)	48,60,60	1.55	8 (16%)
29	CLA	c	615	-	59,63,73	1.27	8 (13%)	70,101,113	1.33	6 (8%)
29	CLA	B	827	11	69,73,73	1.15	7 (10%)	82,113,113	1.25	5 (6%)
29	CLA	O	201	34	59,63,73	1.26	8 (13%)	70,101,113	1.36	7 (10%)
29	CLA	B	809	11	69,73,73	1.16	8 (11%)	82,113,113	1.35	8 (9%)
29	CLA	3	304	3	64,68,73	1.20	7 (10%)	76,107,113	1.24	8 (10%)
37	8CT	M	101	-	40,41,41	4.75	23 (57%)	51,56,56	3.03	20 (39%)
29	CLA	3	312	3	54,58,73	1.31	8 (14%)	64,95,113	1.48	6 (9%)
31	II0	9	317	-	39,43,43	2.09	3 (7%)	48,60,60	1.60	10 (20%)
34	LHG	2	617	29	21,21,48	0.79	1 (4%)	23,26,54	1.30	2 (8%)
29	CLA	2	602	2	63,67,73	1.20	8 (12%)	74,105,113	1.36	7 (9%)
29	CLA	4	611	4	69,73,73	1.16	7 (10%)	82,113,113	1.29	7 (8%)
31	II0	a	619	-	39,43,43	2.16	3 (7%)	48,60,60	1.64	9 (18%)
37	8CT	B	846	-	40,41,41	4.75	23 (57%)	51,56,56	2.83	19 (37%)
29	CLA	e	602	27	59,63,73	1.25	8 (13%)	70,101,113	1.36	8 (11%)
29	CLA	A	831	10	69,73,73	1.15	8 (11%)	82,113,113	1.26	5 (6%)
29	CLA	1	602	1	63,67,73	1.20	7 (11%)	74,105,113	1.32	8 (10%)
31	II0	d	613	-	39,43,43	2.09	3 (7%)	48,60,60	1.56	7 (14%)
29	CLA	B	807	11	69,73,73	1.15	8 (11%)	82,113,113	1.29	6 (7%)
29	CLA	4	603	4	58,62,73	1.25	7 (12%)	68,99,113	1.38	9 (13%)
29	CLA	e	603	27	54,58,73	1.31	8 (14%)	64,95,113	1.40	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMG	8	314	-	52,52,55	0.78	1 (1%)	60,60,63	1.36	7 (11%)
29	CLA	1	608	1	64,68,73	1.21	8 (12%)	76,107,113	1.33	7 (9%)
29	CLA	2	604	2	59,63,73	1.26	8 (13%)	70,101,113	1.44	6 (8%)
37	8CT	Z	307	-	40,41,41	4.82	23 (57%)	51,56,56	2.36	22 (43%)
29	CLA	4	601	4	59,63,73	1.26	8 (13%)	70,101,113	1.38	8 (11%)
29	CLA	9	315	-	45,49,73	1.42	8 (17%)	54,84,113	1.49	5 (9%)
29	CLA	L	201	19	55,59,73	1.29	8 (14%)	64,96,113	1.41	5 (7%)
29	CLA	A	808	10	59,63,73	1.24	8 (13%)	70,101,113	1.34	7 (10%)
29	CLA	e	604	-	64,68,73	1.21	8 (12%)	76,107,113	1.35	6 (7%)
37	8CT	7	318	-	40,41,41	1.34	6 (15%)	51,56,56	1.59	11 (21%)
29	CLA	9	303	9	59,63,73	1.25	7 (11%)	70,101,113	1.35	6 (8%)
31	II0	3	317	-	39,43,43	2.05	2 (5%)	48,60,60	1.50	7 (14%)
29	CLA	e	607	27	49,53,73	1.38	8 (16%)	58,89,113	1.43	5 (8%)
29	CLA	6	601	6	49,53,73	1.39	8 (16%)	58,89,113	1.41	5 (8%)
34	LHG	4	619	29	44,44,48	0.64	1 (2%)	47,50,54	1.28	5 (10%)
29	CLA	A	805	10	54,58,73	1.31	8 (14%)	64,95,113	1.35	6 (9%)
29	CLA	O	203	21	59,63,73	1.26	9 (15%)	70,101,113	1.36	6 (8%)
30	KC2	c	610	26	49,53,53	1.74	10 (20%)	60,89,89	1.90	17 (28%)
29	CLA	B	815	11	46,50,73	1.37	8 (17%)	53,85,113	1.40	4 (7%)
35	LMG	Z	310	-	48,48,55	0.78	2 (4%)	56,56,63	1.39	9 (16%)
29	CLA	a	608	24	64,68,73	1.20	7 (10%)	76,107,113	1.32	8 (10%)
29	CLA	a	612	24	69,73,73	1.17	7 (10%)	82,113,113	1.25	8 (9%)
29	CLA	A	811	10	69,73,73	1.18	9 (13%)	82,113,113	1.27	6 (7%)
34	LHG	O	208	-	39,39,48	0.76	2 (5%)	42,44,54	1.61	7 (16%)
31	II0	6	615	-	39,43,43	2.08	2 (5%)	48,60,60	1.66	9 (18%)
37	8CT	A	846	-	40,41,41	4.73	23 (57%)	51,56,56	3.02	20 (39%)
29	CLA	e	610	-	55,59,73	1.31	8 (14%)	64,96,113	1.37	6 (9%)
31	II0	O	205	-	39,43,43	2.19	2 (5%)	48,60,60	1.56	10 (20%)
37	8CT	B	847	-	40,41,41	4.73	23 (57%)	51,56,56	2.89	26 (50%)
29	CLA	B	802	-	59,63,73	1.24	7 (11%)	70,101,113	1.29	7 (10%)
29	CLA	B	826	11	69,73,73	1.15	9 (13%)	82,113,113	1.31	9 (10%)
29	CLA	d	601	24	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
37	8CT	F	203	-	40,41,41	4.75	23 (57%)	51,56,56	3.05	21 (41%)
31	II0	e	615	-	39,43,43	2.11	3 (7%)	48,60,60	1.55	9 (18%)
29	CLA	e	611	27	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMG	3	319	29	30,30,55	1.04	1 (3%)	38,38,63	1.23	5 (13%)
31	II0	8	310	-	39,43,43	2.06	2 (5%)	48,60,60	1.66	12 (25%)
29	CLA	O	202	-	45,49,73	1.40	7 (15%)	54,84,113	1.50	6 (11%)
29	CLA	B	805	11	69,73,73	1.14	7 (10%)	82,113,113	1.30	7 (8%)
34	LHG	A	851	29	38,38,48	0.70	1 (2%)	41,44,54	1.33	5 (12%)
37	8CT	A	845	-	40,41,41	4.76	23 (57%)	51,56,56	2.65	23 (45%)
31	II0	c	616	-	39,43,43	2.09	3 (7%)	48,60,60	1.54	10 (20%)
34	LHG	b	616	29	29,29,48	0.74	1 (3%)	32,35,54	1.26	3 (9%)
29	CLA	1	612	1	64,68,73	1.22	7 (10%)	76,107,113	1.28	5 (6%)
29	CLA	B	834	-	49,53,73	1.38	8 (16%)	58,89,113	1.46	5 (8%)
35	LMG	X	302	-	34,34,55	0.93	0	42,42,63	1.23	5 (11%)
29	CLA	A	833	10	69,73,73	1.16	7 (10%)	82,113,113	1.23	4 (4%)
34	LHG	4	617	29	48,48,48	0.66	1 (2%)	51,54,54	1.35	8 (15%)
29	CLA	A	855	-	64,68,73	1.21	7 (10%)	76,107,113	1.30	5 (6%)
29	CLA	4	602	4	63,67,73	1.20	7 (11%)	74,105,113	1.30	7 (9%)
37	8CT	B	852	-	40,41,41	4.72	23 (57%)	51,56,56	3.05	23 (45%)
29	CLA	5	602	5	59,63,73	1.24	9 (15%)	70,101,113	1.34	5 (7%)
37	8CT	J	104	-	40,41,41	4.74	23 (57%)	51,56,56	2.85	24 (47%)
29	CLA	2	609	34	45,49,73	1.41	8 (17%)	54,84,113	1.49	5 (9%)
34	LHG	3	301	29	41,41,48	0.67	1 (2%)	44,47,54	1.25	4 (9%)
29	CLA	b	610	25	55,59,73	1.30	7 (12%)	64,96,113	1.41	5 (7%)
29	CLA	a	611	-	59,63,73	1.25	9 (15%)	70,101,113	1.35	6 (8%)
29	CLA	Z	305	23	64,68,73	1.21	9 (14%)	76,107,113	1.27	5 (6%)
29	CLA	B	838	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	6 (7%)
31	II0	9	316	-	39,43,43	2.13	3 (7%)	48,60,60	1.61	10 (20%)
29	CLA	5	603	5	49,53,73	1.39	7 (14%)	58,89,113	1.38	4 (6%)
36	SQD	3	320	-	34,36,54	1.77	7 (20%)	44,47,65	1.40	6 (13%)
34	LHG	8	315	-	32,32,48	0.76	2 (6%)	35,38,54	1.25	3 (8%)
29	CLA	7	311	-	59,63,73	1.26	7 (11%)	70,101,113	1.34	6 (8%)
29	CLA	A	822	10	69,73,73	1.16	9 (13%)	82,113,113	1.23	4 (4%)
29	CLA	4	604	-	59,63,73	1.27	8 (13%)	70,101,113	1.39	7 (10%)
34	LHG	a	617	29	26,26,48	0.81	1 (3%)	29,32,54	1.33	3 (10%)
29	CLA	A	830	10	64,68,73	1.20	9 (14%)	76,107,113	1.29	9 (11%)
37	8CT	B	845	-	40,41,41	4.81	23 (57%)	51,56,56	2.52	19 (37%)
31	II0	4	612	-	39,43,43	1.99	2 (5%)	48,60,60	1.52	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMG	F	204	-	32,32,55	0.94	2 (6%)	40,40,63	1.36	6 (15%)
29	CLA	B	824	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	4 (4%)
31	II0	3	316	-	39,43,43	2.10	2 (5%)	48,60,60	1.99	13 (27%)
29	CLA	c	613	26	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
29	CLA	1	611	1	49,53,73	1.38	8 (16%)	58,89,113	1.47	4 (6%)
29	CLA	A	832	10	69,73,73	1.15	8 (11%)	82,113,113	1.26	6 (7%)
33	IHT	2	616	-	40,42,42	1.58	2 (5%)	52,58,58	2.03	15 (28%)
31	II0	8	313	-	39,43,43	2.10	3 (7%)	48,60,60	1.32	5 (10%)
29	CLA	A	837	10	69,73,73	1.18	8 (11%)	82,113,113	1.36	7 (8%)
29	CLA	F	202	15	59,63,73	1.25	8 (13%)	70,101,113	1.34	6 (8%)
31	II0	1	617	-	39,43,43	2.09	2 (5%)	48,60,60	1.67	12 (25%)
40	PQN	B	842	-	34,34,34	1.60	2 (5%)	43,45,45	1.16	5 (11%)
31	II0	b	614	-	39,43,43	2.14	3 (7%)	48,60,60	1.50	10 (20%)
31	II0	9	319	-	39,43,43	2.11	2 (5%)	48,60,60	1.48	10 (20%)
33	IHT	5	618	-	40,42,42	1.53	2 (5%)	52,58,58	1.91	11 (21%)
29	CLA	c	606	26	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
29	CLA	c	603	31,26	69,73,73	1.17	7 (10%)	82,113,113	1.24	8 (9%)
33	IHT	d	617	-	40,42,42	1.62	3 (7%)	52,58,58	1.92	15 (28%)
32	II3	e	613	-	40,43,43	1.57	2 (5%)	47,60,60	1.90	11 (23%)
29	CLA	5	604	5	59,63,73	1.24	8 (13%)	70,101,113	1.35	7 (10%)
31	II0	2	613	-	39,43,43	2.03	2 (5%)	48,60,60	1.59	9 (18%)
34	LHG	A	850	-	48,48,48	0.63	1 (2%)	51,54,54	1.27	5 (9%)
29	CLA	A	807	10	54,58,73	1.29	7 (12%)	64,95,113	1.47	7 (10%)
29	CLA	A	841	10	69,73,73	1.17	9 (13%)	82,113,113	1.29	6 (7%)
29	CLA	B	822	11	64,68,73	1.19	8 (12%)	76,107,113	1.29	6 (7%)
29	CLA	Z	303	23,29	59,63,73	1.26	8 (13%)	70,101,113	1.32	5 (7%)
29	CLA	c	605	26	49,53,73	1.38	8 (16%)	58,89,113	1.41	4 (6%)
29	CLA	3	308	3	64,68,73	1.22	9 (14%)	76,107,113	1.38	5 (6%)
29	CLA	9	306	9	49,53,73	1.39	8 (16%)	58,89,113	1.34	4 (6%)
30	KC2	4	605	4	49,53,53	1.74	9 (18%)	60,89,89	1.85	14 (23%)
29	CLA	B	823	11	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
29	CLA	b	611	25	59,63,73	1.25	8 (13%)	70,101,113	1.35	6 (8%)
31	II0	6	614	-	39,43,43	2.02	2 (5%)	48,60,60	1.59	11 (22%)
29	CLA	1	604	1	49,53,73	1.38	7 (14%)	58,89,113	1.47	5 (8%)
29	CLA	a	606	24	69,73,73	1.18	9 (13%)	82,113,113	1.19	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	2	612	2	49,53,73	1.39	8 (16%)	58,89,113	1.44	5 (8%)
33	IHT	c	620	-	40,42,42	1.71	2 (5%)	52,58,58	1.97	15 (28%)
37	8CT	R	203	-	40,41,41	4.75	23 (57%)	51,56,56	3.03	23 (45%)
29	CLA	6	607	6	59,63,73	1.29	7 (11%)	70,101,113	1.30	5 (7%)
29	CLA	3	313	3	49,53,73	1.38	8 (16%)	58,89,113	1.46	4 (6%)
29	CLA	e	608	34	45,49,73	1.42	8 (17%)	54,84,113	1.45	6 (11%)
33	IHT	Z	301	-	40,42,42	1.54	1 (2%)	52,58,58	2.21	15 (28%)
29	CLA	B	812	11	59,63,73	1.25	9 (15%)	70,101,113	1.34	6 (8%)
30	KC2	e	609	27	49,53,53	1.73	9 (18%)	60,89,89	1.88	15 (25%)
29	CLA	9	314	9	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
29	CLA	K	102	18	59,63,73	1.27	9 (15%)	70,101,113	1.30	4 (5%)
30	KC2	2	610	2	49,53,53	1.75	10 (20%)	60,89,89	1.93	16 (26%)
31	II0	3	315	-	39,43,43	1.98	2 (5%)	48,60,60	1.45	8 (16%)
30	KC2	7	310	7	49,53,53	1.72	9 (18%)	60,89,89	1.90	15 (25%)
29	CLA	A	802	29,10	59,63,73	1.25	8 (13%)	70,101,113	1.30	5 (7%)
29	CLA	L	202	19	64,68,73	1.18	7 (10%)	76,107,113	1.34	7 (9%)
31	II0	7	314	-	39,43,43	1.99	2 (5%)	48,60,60	1.60	10 (20%)
29	CLA	A	826	10	69,73,73	1.16	6 (8%)	82,113,113	1.22	6 (7%)
29	CLA	9	312	9	45,49,73	1.41	8 (17%)	54,84,113	1.48	5 (9%)
31	II0	7	317	-	39,43,43	2.11	2 (5%)	48,60,60	1.61	11 (22%)
37	8CT	B	848	-	40,41,41	4.81	23 (57%)	51,56,56	2.67	19 (37%)
37	8CT	4	616	-	40,41,41	1.35	8 (20%)	51,56,56	1.60	11 (21%)
29	CLA	1	601	1	49,53,73	1.40	7 (14%)	58,89,113	1.49	5 (8%)
29	CLA	B	820	11	64,68,73	1.21	8 (12%)	76,107,113	1.29	7 (9%)
29	CLA	a	601	24	49,53,73	1.40	9 (18%)	58,89,113	1.39	4 (6%)
29	CLA	A	818	10	69,73,73	1.16	8 (11%)	82,113,113	1.28	5 (6%)
29	CLA	B	831	11	64,68,73	1.18	7 (10%)	76,107,113	1.25	7 (9%)
29	CLA	7	306	7	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
31	II0	3	318	-	39,43,43	2.05	2 (5%)	48,60,60	1.54	10 (20%)
29	CLA	6	603	6	49,53,73	1.38	8 (16%)	58,89,113	1.41	6 (10%)
29	CLA	B	825	-	64,68,73	1.20	9 (14%)	76,107,113	1.32	9 (11%)
31	II0	d	615	-	39,43,43	2.18	2 (5%)	48,60,60	1.62	8 (16%)
29	CLA	B	835	11	59,63,73	1.25	8 (13%)	70,101,113	1.31	8 (11%)
30	KC2	6	613	6	49,53,53	1.74	10 (20%)	60,89,89	1.89	15 (25%)
29	CLA	B	810	11	69,73,73	1.17	8 (11%)	82,113,113	1.29	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	II0	7	315	-	39,43,43	1.98	2 (5%)	48,60,60	1.52	8 (16%)
29	CLA	9	307	9	61,65,73	1.24	7 (11%)	72,103,113	1.25	7 (9%)
37	8CT	I	101	-	40,41,41	4.79	23 (57%)	51,56,56	2.68	21 (41%)
34	LHG	4	620	-	44,44,48	0.66	2 (4%)	47,50,54	1.25	4 (8%)
29	CLA	7	307	7	49,53,73	1.37	8 (16%)	58,89,113	1.49	4 (6%)
29	CLA	5	611	5	49,53,73	1.38	7 (14%)	58,89,113	1.42	4 (6%)
37	8CT	b	615	-	40,41,41	1.42	4 (10%)	51,56,56	1.41	10 (19%)
30	KC2	c	614	30	49,53,53	1.79	8 (16%)	60,89,89	1.75	14 (23%)
37	8CT	B	851	-	40,41,41	4.77	23 (57%)	51,56,56	2.93	19 (37%)
37	8CT	B	844	-	40,41,41	4.78	23 (57%)	51,56,56	2.94	19 (37%)
29	CLA	O	204	-	59,63,73	1.26	9 (15%)	70,101,113	1.33	7 (10%)
37	8CT	L	205	-	40,41,41	4.74	23 (57%)	51,56,56	2.90	22 (43%)
29	CLA	A	815	10	66,70,73	1.17	8 (12%)	78,109,113	1.30	7 (8%)
34	LHG	1	619	29	34,34,48	0.66	0	37,40,54	1.30	4 (10%)
29	CLA	a	602	24	59,63,73	1.25	9 (15%)	70,101,113	1.32	5 (7%)
29	CLA	B	839	11	69,73,73	1.15	7 (10%)	82,113,113	1.26	4 (4%)
29	CLA	9	304	9	49,53,73	1.38	9 (18%)	58,89,113	1.40	4 (6%)
29	CLA	A	839	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	6 (7%)
33	IHT	6	616	-	40,42,42	1.52	1 (2%)	52,58,58	1.70	11 (21%)
36	SQD	O	207	-	27,29,54	1.93	7 (25%)	37,40,65	1.55	7 (18%)
29	CLA	3	309	3	64,68,73	1.21	9 (14%)	76,107,113	1.24	5 (6%)
29	CLA	6	609	34	45,49,73	1.41	8 (17%)	54,84,113	1.50	6 (11%)
29	CLA	A	834	10	59,63,73	1.25	7 (11%)	70,101,113	1.35	5 (7%)
29	CLA	X	301	-	56,60,73	1.29	8 (14%)	65,97,113	1.33	5 (7%)
39	SF4	A	848	10,11	0,12,12	-	-	-	-	-
29	CLA	A	801	10	69,73,73	1.16	6 (8%)	82,113,113	1.30	7 (8%)
30	KC2	5	610	5	49,53,53	1.74	10 (20%)	60,89,89	1.90	15 (25%)
29	CLA	3	305	3	69,73,73	1.15	7 (10%)	82,113,113	1.27	6 (7%)
31	II0	O	206	-	39,43,43	2.10	2 (5%)	48,60,60	1.51	8 (16%)
29	CLA	2	606	2	49,53,73	1.38	9 (18%)	58,89,113	1.41	4 (6%)
35	LMG	6	617	-	32,32,55	1.05	3 (9%)	40,40,63	1.28	6 (15%)
29	CLA	5	608	5	64,68,73	1.21	9 (14%)	76,107,113	1.31	6 (7%)
29	CLA	9	308	-	69,73,73	1.20	8 (11%)	82,113,113	1.27	6 (7%)
30	KC2	9	311	9	49,53,53	1.73	10 (20%)	60,89,89	1.87	15 (25%)
34	LHG	B	801	-	39,39,48	0.75	1 (2%)	42,44,54	1.62	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	813	11	69,73,73	1.18	9 (13%)	82,113,113	1.24	7 (8%)
29	CLA	1	613	1	49,53,73	1.40	8 (16%)	58,89,113	1.42	5 (8%)
30	KC2	a	610	24	49,53,53	1.73	9 (18%)	60,89,89	1.91	15 (25%)
29	CLA	7	303	7	69,73,73	1.15	8 (11%)	82,113,113	1.29	8 (9%)
35	LMG	2	618	-	36,36,55	0.84	1 (2%)	44,44,63	1.36	7 (15%)
29	CLA	9	302	9	49,53,73	1.39	7 (14%)	58,89,113	1.43	4 (6%)
29	CLA	A	816	10	64,68,73	1.20	8 (12%)	76,107,113	1.32	6 (7%)
31	II0	5	617	-	39,43,43	2.08	2 (5%)	48,60,60	1.56	12 (25%)
37	8CT	A	847	-	40,41,41	4.72	23 (57%)	51,56,56	2.94	22 (43%)

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
29	CLA	K	101	-	1/1/15/20	8/39/115/115	-
29	CLA	2	603	2	1/1/12/20	6/21/97/115	-
29	CLA	A	819	-	1/1/15/20	5/39/115/115	-
29	CLA	A	842	10	1/1/15/20	12/39/115/115	-
31	II0	9	323	-	-	4/21/67/67	0/2/2/2
29	CLA	8	306	8	1/1/11/20	3/15/91/115	-
29	CLA	2	607	2	1/1/11/20	6/15/91/115	-
31	II0	4	615	-	-	3/21/67/67	0/2/2/2
31	II0	d	616	-	-	3/21/67/67	0/2/2/2
29	CLA	L	203	-	1/1/12/20	4/21/97/115	-
31	II0	e	612	-	-	6/21/67/67	0/2/2/2
34	LHG	c	622	29	-	13/23/23/53	-
29	CLA	1	609	34	1/1/10/20	4/10/86/115	-
29	CLA	c	608	26	1/1/14/20	8/33/109/115	-
31	II0	d	614	-	-	0/21/67/67	0/2/2/2
29	CLA	b	602	25	1/1/14/20	15/38/114/115	-
31	II0	c	617	-	-	1/21/67/67	0/2/2/2
33	IHT	a	616	-	-	4/25/65/65	0/2/2/2
31	II0	R	201	-	-	0/21/67/67	0/2/2/2
31	II0	1	620	-	-	5/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	II0	a	614	-	-	2/21/67/67	0/2/2/2
30	KC2	6	610	6	-	10/15/71/71	-
29	CLA	B	833	-	1/1/15/20	12/39/115/115	-
29	CLA	B	818	11	1/1/14/20	4/33/109/115	-
29	CLA	B	836	11	1/1/15/20	11/39/115/115	-
29	CLA	7	305	7	1/1/12/20	5/25/101/115	-
36	SQD	7	321	-	-	15/31/51/69	0/1/1/1
29	CLA	5	605	5	1/1/11/20	5/15/91/115	-
29	CLA	B	819	-	1/1/14/20	6/33/109/115	-
37	8CT	B	843	-	-	11/29/63/63	0/2/2/2
29	CLA	A	825	10	-	13/39/115/115	-
32	II3	b	613	-	-	2/25/67/67	0/2/2/2
34	LHG	L	206	-	-	8/22/23/53	-
29	CLA	2	601	2	1/1/10/20	3/12/88/115	-
29	CLA	5	601	5	1/1/10/20	4/10/86/115	-
29	CLA	B	821	11	1/1/14/20	8/33/109/115	-
30	KC2	3	307	34	-	10/15/71/71	-
29	CLA	B	841	11	1/1/15/20	1/39/115/115	-
29	CLA	A	854	-	1/1/15/20	19/39/115/115	-
29	CLA	d	608	24	1/1/15/20	13/39/115/115	-
29	CLA	e	601	27	1/1/11/20	4/15/91/115	-
29	CLA	3	303	3	1/1/13/20	4/27/103/115	-
29	CLA	A	853	34	1/1/11/20	10/15/91/115	-
31	II0	J	102	-	-	6/21/67/67	0/2/2/2
34	LHG	A	852	-	-	11/26/26/53	-
29	CLA	4	606	4	1/1/14/20	3/33/109/115	-
29	CLA	B	837	11	1/1/11/20	0/18/94/115	-
29	CLA	d	602	24	1/1/14/20	14/38/114/115	-
29	CLA	2	611	2	1/1/12/20	5/21/97/115	-
29	CLA	5	612	5	1/1/11/20	7/15/91/115	-
29	CLA	A	812	10	1/1/13/20	2/27/103/115	-
29	CLA	6	604	6	1/1/14/20	12/33/109/115	-
31	II0	4	614	-	-	4/21/67/67	0/2/2/2
29	CLA	9	305	-	1/1/13/20	5/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LHG	5	619	29	-	12/26/26/53	-
29	CLA	7	312	7	1/1/12/20	8/21/97/115	-
29	CLA	6	605	6	1/1/13/20	9/27/103/115	-
30	KC2	b	609	25	-	3/15/71/71	-
29	CLA	B	808	11	1/1/15/20	21/39/115/115	-
34	LHG	e	617	29	-	17/32/32/53	-
29	CLA	Z	302	-	1/1/14/20	13/33/109/115	-
29	CLA	A	817	10	1/1/15/20	12/39/115/115	-
29	CLA	d	609	-	1/1/10/20	2/10/86/115	-
29	CLA	d	604	24	1/1/14/20	7/33/109/115	-
29	CLA	A	810	10	1/1/15/20	14/39/115/115	-
31	II0	c	621	29	-	0/21/67/67	0/2/2/2
29	CLA	a	603	24	1/1/14/20	9/33/109/115	-
37	8CT	K	103	-	-	10/29/63/63	0/2/2/2
29	CLA	B	811	11	1/1/14/20	7/33/109/115	-
31	II0	R	204	-	-	0/21/67/67	0/2/2/2
29	CLA	4	607	4	1/1/14/20	9/33/109/115	-
29	CLA	c	602	26	1/1/15/20	18/39/115/115	-
29	CLA	A	835	10	1/1/14/20	4/33/109/115	-
31	II0	8	311	-	-	6/21/67/67	0/2/2/2
29	CLA	1	603	1	1/1/12/20	7/24/100/115	-
36	SQD	a	618	-	-	17/37/57/69	0/1/1/1
29	CLA	R	202	22	1/1/13/20	10/27/103/115	-
33	IHT	L	204	-	-	0/25/65/65	0/2/2/2
29	CLA	A	804	10	1/1/15/20	15/39/115/115	-
29	CLA	2	608	2	1/1/14/20	7/33/109/115	-
29	CLA	e	606	27	1/1/14/20	9/33/109/115	-
29	CLA	4	610	4	1/1/15/20	12/39/115/115	-
30	KC2	e	605	27	-	8/15/71/71	-
29	CLA	1	607	1	1/1/11/20	6/15/91/115	-
31	II0	b	612	-	-	3/21/67/67	0/2/2/2
29	CLA	A	838	10	1/1/15/20	7/39/115/115	-
29	CLA	9	310	-	1/1/10/20	4/10/86/115	-
29	CLA	5	606	5	1/1/11/20	4/15/91/115	-
40	PQN	A	849	-	-	2/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	SQD	9	301	-	-	10/25/45/69	0/1/1/1
29	CLA	3	306	3,29	1/1/13/20	7/27/103/115	-
29	CLA	a	609	34	1/1/14/20	9/33/109/115	-
29	CLA	8	302	8	1/1/15/20	16/39/115/115	-
29	CLA	B	829	11	1/1/15/20	17/39/115/115	-
29	CLA	A	836	10	1/1/13/20	7/27/103/115	-
34	LHG	8	316	-	-	29/53/53/53	-
29	CLA	A	823	-	1/1/15/20	11/39/115/115	-
38	DGD	9	322	-	-	19/49/89/95	0/2/2/2
34	LHG	4	618	-	-	30/53/53/53	-
29	CLA	b	604	25	1/1/13/20	8/31/107/115	-
29	CLA	5	613	5	1/1/10/20	6/10/86/115	-
33	IHT	K	104	-	-	4/25/65/65	0/2/2/2
31	II0	a	615	-	-	6/21/67/67	0/2/2/2
34	LHG	c	623	-	-	23/38/38/53	-
29	CLA	B	804	11	1/1/11/20	7/15/91/115	-
29	CLA	4	609	4	1/1/14/20	6/33/109/115	-
29	CLA	8	303	8	1/1/15/20	16/39/115/115	-
29	CLA	d	612	24	1/1/14/20	10/37/113/115	-
29	CLA	J	103	17	1/1/10/20	2/10/86/115	-
34	LHG	M	102	-	-	10/25/25/53	-
37	8CT	e	616	-	-	11/29/63/63	0/2/2/2
31	II0	7	316	-	-	3/21/67/67	0/2/2/2
29	CLA	B	817	11	1/1/13/20	14/32/108/115	-
29	CLA	F	201	-	1/1/11/20	3/15/91/115	-
29	CLA	b	607	25	1/1/14/20	5/33/109/115	-
29	CLA	9	309	9	1/1/13/20	10/27/103/115	-
31	II0	a	613	-	-	1/21/67/67	0/2/2/2
29	CLA	B	806	11	1/1/15/20	13/39/115/115	-
29	CLA	d	605	24	1/1/11/20	4/15/91/115	-
29	CLA	A	806	10	1/1/15/20	15/39/115/115	-
34	LHG	L	208	-	-	22/38/38/53	-
29	CLA	b	601	25	1/1/11/20	2/15/91/115	-
31	II0	9	318	-	-	3/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	8	317	-	1/1/15/20	11/39/115/115	-
29	CLA	A	814	-	1/1/11/20	7/15/91/115	-
34	LHG	Z	311	-	-	23/50/50/53	-
29	CLA	B	816	11	1/1/15/20	10/39/115/115	-
29	CLA	A	820	10	1/1/15/20	13/39/115/115	-
29	CLA	6	611	-	1/1/13/20	1/27/103/115	-
29	CLA	6	612	6	1/1/11/20	5/15/91/115	-
31	II0	5	614	-	-	1/21/67/67	0/2/2/2
29	CLA	c	612	26	1/1/13/20	8/27/103/115	-
32	II3	8	312	-	-	8/25/67/67	0/2/2/2
29	CLA	6	602	6	1/1/15/20	12/39/115/115	-
34	LHG	L	207	-	-	16/36/36/53	-
29	CLA	8	304	8	1/1/12/20	2/21/97/115	-
29	CLA	b	603	25	1/1/14/20	6/33/109/115	-
37	8CT	Z	308	-	-	11/29/63/63	0/2/2/2
30	KC2	d	610	24	-	10/15/71/71	-
33	IHT	9	320	-	-	7/25/65/65	0/2/2/2
29	CLA	d	603	24	1/1/12/20	4/21/97/115	-
29	CLA	8	305	8	1/1/13/20	8/27/103/115	-
29	CLA	c	604	26	1/1/14/20	10/33/109/115	-
29	CLA	8	307	8	1/1/10/20	6/10/86/115	-
29	CLA	A	809	29,10	1/1/14/20	7/33/109/115	-
32	II3	1	615	-	-	0/25/67/67	0/2/2/2
29	CLA	d	607	24	1/1/15/20	7/39/115/115	-
29	CLA	9	313	9	1/1/11/20	7/15/91/115	-
29	CLA	B	830	11	1/1/11/20	2/15/91/115	-
29	CLA	B	814	11	1/1/13/20	11/29/105/115	-
29	CLA	A	840	-	1/1/15/20	12/39/115/115	-
34	LHG	2	619	-	-	21/43/43/53	-
29	CLA	4	608	34	1/1/15/20	10/39/115/115	-
31	II0	2	615	-	-	5/21/67/67	0/2/2/2
31	II0	3	314	-	-	1/21/67/67	0/2/2/2
29	CLA	b	608	34	1/1/15/20	13/39/115/115	-
29	CLA	6	608	6	1/1/14/20	4/33/109/115	-
29	CLA	7	304	7	1/1/13/20	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	d	611	-	1/1/12/20	5/21/97/115	-
29	CLA	7	309	34	1/1/10/20	4/10/86/115	-
29	CLA	A	824	-	1/1/15/20	8/39/115/115	-
36	SQD	3	322	-	-	15/31/51/69	0/1/1/1
29	CLA	B	803	11	1/1/15/20	19/39/115/115	-
30	KC2	b	605	25	-	7/15/71/71	-
30	KC2	c	611	30,26	-	4/15/71/71	-
29	CLA	A	843	-	1/1/15/20	8/39/115/115	-
31	II0	c	618	-	-	1/21/67/67	0/2/2/2
34	LHG	Z	309	-	-	17/43/43/53	-
34	LHG	9	321	-	-	19/37/37/53	-
31	II0	5	620	-	-	3/21/67/67	0/2/2/2
31	II0	4	613	-	-	2/21/67/67	0/2/2/2
34	LHG	7	319	29	-	25/43/43/53	-
39	SF4	C	102	12	-	-	0/6/5/5
31	II0	1	614	-	-	3/21/67/67	0/2/2/2
31	II0	1	616	-	-	5/21/67/67	0/2/2/2
29	CLA	b	606	25	1/1/15/20	16/39/115/115	-
29	CLA	A	821	10	1/1/13/20	5/27/103/115	-
29	CLA	d	606	24	1/1/10/20	0/10/86/115	-
34	LHG	J	101	30	-	12/38/38/53	-
29	CLA	c	607	26	1/1/15/20	12/39/115/115	-
34	LHG	3	321	-	-	23/53/53/53	-
30	KC2	7	313	-	-	9/15/71/71	-
29	CLA	1	606	1	1/1/11/20	4/15/91/115	-
29	CLA	8	308	-	1/1/15/20	6/39/115/115	-
38	DGD	B	849	-	-	18/48/88/95	0/2/2/2
29	CLA	3	310	35	1/1/15/20	4/39/115/115	-
39	SF4	C	101	12	-	-	0/6/5/5
29	CLA	B	840	34	1/1/15/20	6/39/115/115	-
29	CLA	B	828	11	1/1/15/20	6/39/115/115	-
29	CLA	A	828	10	1/1/15/20	10/39/115/115	-
30	KC2	1	610	1	-	3/15/71/71	-
29	CLA	5	607	5	1/1/11/20	6/15/91/115	-
29	CLA	B	832	11	1/1/13/20	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	c	601	26	1/1/11/20	8/15/91/115	-
29	CLA	c	609	34	1/1/10/20	4/10/86/115	-
29	CLA	A	827	10	1/1/15/20	8/39/115/115	-
29	CLA	5	609	34	1/1/10/20	2/10/86/115	-
31	II0	e	614	-	-	1/21/67/67	0/2/2/2
29	CLA	3	302	3	1/1/11/20	6/15/91/115	-
29	CLA	2	605	2	1/1/14/20	7/33/109/115	-
30	KC2	Z	306	23	-	4/15/71/71	-
31	II0	5	615	-	-	4/21/67/67	0/2/2/2
33	IHT	8	309	-	-	6/25/65/65	0/2/2/2
29	CLA	6	606	6	1/1/13/20	10/27/103/115	-
29	CLA	1	605	1	1/1/10/20	4/11/87/115	-
29	CLA	a	604	24	1/1/14/20	9/33/109/115	-
29	CLA	a	607	24	1/1/15/20	8/39/115/115	-
29	CLA	7	308	7	1/1/13/20	9/27/103/115	-
29	CLA	Z	304	23	1/1/12/20	4/21/97/115	-
29	CLA	a	605	24	1/1/13/20	9/27/103/115	-
31	II0	5	616	-	-	1/21/67/67	0/2/2/2
29	CLA	A	813	10	1/1/10/20	1/12/88/115	-
29	CLA	8	301	8	1/1/11/20	7/15/91/115	-
33	IHT	1	618	-	-	3/25/65/65	0/2/2/2
31	II0	c	619	-	-	4/21/67/67	0/2/2/2
29	CLA	3	311	3	1/1/15/20	10/39/115/115	-
29	CLA	7	302	7	1/1/11/20	2/15/91/115	-
34	LHG	5	621	29	-	14/39/39/53	-
29	CLA	A	829	10	1/1/12/20	8/21/97/115	-
31	II0	7	301	-	-	4/21/67/67	0/2/2/2
36	SQD	B	850	-	-	15/28/48/69	0/1/1/1
29	CLA	A	803	10	1/1/15/20	3/39/115/115	-
37	8CT	A	844	-	-	7/29/63/63	0/2/2/2
34	LHG	7	320	-	-	17/35/35/53	-
31	II0	2	614	-	-	1/21/67/67	0/2/2/2
29	CLA	c	615	-	1/1/13/20	8/27/103/115	-
29	CLA	B	827	11	1/1/15/20	13/39/115/115	-
29	CLA	O	201	34	1/1/13/20	5/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	809	11	1/1/15/20	11/39/115/115	-
29	CLA	3	304	3	1/1/14/20	8/33/109/115	-
37	8CT	M	101	-	-	8/29/63/63	0/2/2/2
29	CLA	3	312	3	1/1/12/20	7/21/97/115	-
31	II0	9	317	-	-	0/21/67/67	0/2/2/2
34	LHG	2	617	29	-	10/24/24/53	-
29	CLA	2	602	2	1/1/13/20	9/32/108/115	-
29	CLA	4	611	4	1/1/15/20	9/39/115/115	-
31	II0	a	619	-	-	1/21/67/67	0/2/2/2
37	8CT	B	846	-	-	9/29/63/63	0/2/2/2
29	CLA	e	602	27	1/1/13/20	7/27/103/115	-
29	CLA	A	831	10	1/1/15/20	14/39/115/115	-
29	CLA	1	602	1	1/1/13/20	3/32/108/115	-
31	II0	d	613	-	-	0/21/67/67	0/2/2/2
29	CLA	B	807	11	1/1/15/20	7/39/115/115	-
29	CLA	4	603	4	1/1/12/20	7/26/102/115	-
29	CLA	e	603	27	1/1/12/20	6/21/97/115	-
35	LMG	8	314	-	-	15/47/67/70	0/1/1/1
29	CLA	1	608	1	1/1/14/20	10/33/109/115	-
29	CLA	2	604	2	1/1/13/20	8/27/103/115	-
37	8CT	Z	307	-	-	7/29/63/63	0/2/2/2
29	CLA	4	601	4	1/1/13/20	4/27/103/115	-
29	CLA	9	315	-	1/1/10/20	4/10/86/115	-
29	CLA	L	201	19	1/1/12/20	7/23/99/115	-
29	CLA	A	808	10	1/1/13/20	8/27/103/115	-
29	CLA	e	604	-	1/1/14/20	7/33/109/115	-
37	8CT	7	318	-	-	14/29/63/63	0/2/2/2
29	CLA	9	303	9	1/1/13/20	11/27/103/115	-
31	II0	3	317	-	-	3/21/67/67	0/2/2/2
29	CLA	e	607	27	1/1/11/20	2/15/91/115	-
29	CLA	6	601	6	1/1/11/20	6/15/91/115	-
34	LHG	4	619	29	-	19/49/49/53	-
29	CLA	A	805	10	1/1/12/20	0/21/97/115	-
29	CLA	O	203	21	1/1/13/20	9/27/103/115	-
30	KC2	c	610	26	-	8/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	815	11	1/1/10/20	3/12/88/115	-
35	LMG	Z	310	-	-	20/43/63/70	0/1/1/1
29	CLA	a	608	24	1/1/14/20	10/33/109/115	-
29	CLA	a	612	24	1/1/15/20	9/39/115/115	-
29	CLA	A	811	10	1/1/15/20	11/39/115/115	-
34	LHG	O	208	-	-	17/41/41/53	-
31	II0	6	615	-	-	3/21/67/67	0/2/2/2
37	8CT	A	846	-	-	8/29/63/63	0/2/2/2
29	CLA	e	610	-	1/1/12/20	5/23/99/115	-
31	II0	O	205	-	-	1/21/67/67	0/2/2/2
37	8CT	B	847	-	-	3/29/63/63	0/2/2/2
29	CLA	B	802	-	1/1/13/20	4/27/103/115	-
29	CLA	B	826	11	1/1/15/20	4/39/115/115	-
29	CLA	d	601	24	1/1/11/20	7/15/91/115	-
37	8CT	F	203	-	-	9/29/63/63	0/2/2/2
31	II0	e	615	-	-	3/21/67/67	0/2/2/2
29	CLA	e	611	27	1/1/15/20	14/39/115/115	-
35	LMG	3	319	29	-	17/25/45/70	0/1/1/1
31	II0	8	310	-	-	5/21/67/67	0/2/2/2
29	CLA	O	202	-	1/1/10/20	4/10/86/115	-
29	CLA	B	805	11	1/1/15/20	13/39/115/115	-
34	LHG	A	851	29	-	18/43/43/53	-
37	8CT	A	845	-	-	5/29/63/63	0/2/2/2
31	II0	c	616	-	-	1/21/67/67	0/2/2/2
34	LHG	b	616	29	-	17/34/34/53	-
29	CLA	1	612	1	1/1/14/20	7/33/109/115	-
29	CLA	B	834	-	1/1/11/20	2/15/91/115	-
35	LMG	X	302	-	-	9/29/49/70	0/1/1/1
29	CLA	A	833	10	1/1/15/20	6/39/115/115	-
34	LHG	4	617	29	-	25/53/53/53	-
29	CLA	A	855	-	1/1/14/20	9/33/109/115	-
29	CLA	4	602	4	1/1/13/20	4/32/108/115	-
37	8CT	B	852	-	-	14/29/63/63	0/2/2/2
29	CLA	5	602	5	1/1/13/20	2/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	8CT	J	104	-	-	9/29/63/63	0/2/2/2
29	CLA	2	609	34	1/1/10/20	4/10/86/115	-
34	LHG	3	301	29	-	13/46/46/53	-
29	CLA	b	610	25	1/1/12/20	7/23/99/115	-
29	CLA	a	611	-	1/1/13/20	9/27/103/115	-
29	CLA	Z	305	23	1/1/14/20	13/33/109/115	-
29	CLA	B	838	-	1/1/15/20	5/39/115/115	-
31	II0	9	316	-	-	0/21/67/67	0/2/2/2
29	CLA	5	603	5	1/1/11/20	2/15/91/115	-
36	SQD	3	320	-	-	13/31/51/69	0/1/1/1
34	LHG	8	315	-	-	23/37/37/53	-
29	CLA	7	311	-	1/1/13/20	4/27/103/115	-
29	CLA	A	822	10	1/1/15/20	13/39/115/115	-
29	CLA	4	604	-	1/1/13/20	11/27/103/115	-
34	LHG	a	617	29	-	15/31/31/53	-
29	CLA	A	830	10	1/1/14/20	7/33/109/115	-
37	8CT	B	845	-	-	6/29/63/63	0/2/2/2
31	II0	4	612	-	-	2/21/67/67	0/2/2/2
35	LMG	F	204	-	-	8/27/47/70	0/1/1/1
29	CLA	B	824	-	1/1/15/20	16/39/115/115	-
31	II0	3	316	-	-	4/21/67/67	0/2/2/2
29	CLA	c	613	26	1/1/11/20	9/15/91/115	-
29	CLA	1	611	1	1/1/11/20	7/15/91/115	-
29	CLA	A	832	10	1/1/15/20	5/39/115/115	-
33	IHT	2	616	-	-	3/25/65/65	0/2/2/2
31	II0	8	313	-	-	4/21/67/67	0/2/2/2
29	CLA	A	837	10	1/1/15/20	11/39/115/115	-
29	CLA	F	202	15	1/1/13/20	7/27/103/115	-
31	II0	1	617	-	-	5/21/67/67	0/2/2/2
40	PQN	B	842	-	-	3/23/43/43	0/2/2/2
31	II0	b	614	-	-	3/21/67/67	0/2/2/2
31	II0	9	319	-	-	5/21/67/67	0/2/2/2
33	IHT	5	618	-	-	1/25/65/65	0/2/2/2
29	CLA	c	606	26	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	c	603	31,26	1/1/15/20	12/39/115/115	-
33	IHT	d	617	-	-	0/25/65/65	0/2/2/2
32	II3	e	613	-	-	1/25/67/67	0/2/2/2
29	CLA	5	604	5	1/1/13/20	14/27/103/115	-
31	II0	2	613	-	-	3/21/67/67	0/2/2/2
34	LHG	A	850	-	-	22/53/53/53	-
29	CLA	A	807	10	1/1/12/20	5/21/97/115	-
29	CLA	A	841	10	1/1/15/20	11/39/115/115	-
29	CLA	B	822	11	1/1/14/20	9/33/109/115	-
29	CLA	Z	303	23,29	1/1/13/20	8/27/103/115	-
29	CLA	c	605	26	1/1/11/20	8/15/91/115	-
29	CLA	3	308	3	1/1/14/20	17/33/109/115	-
29	CLA	9	306	9	1/1/11/20	0/15/91/115	-
30	KC2	4	605	4	-	7/15/71/71	-
29	CLA	B	823	11	1/1/15/20	13/39/115/115	-
29	CLA	b	611	25	1/1/13/20	7/27/103/115	-
31	II0	6	614	-	-	0/21/67/67	0/2/2/2
29	CLA	1	604	1	1/1/11/20	2/15/91/115	-
29	CLA	a	606	24	1/1/15/20	10/39/115/115	-
29	CLA	2	612	2	1/1/11/20	8/15/91/115	-
33	IHT	c	620	-	-	4/25/65/65	0/2/2/2
37	8CT	R	203	-	-	4/29/63/63	0/2/2/2
29	CLA	6	607	6	1/1/13/20	10/27/103/115	-
29	CLA	3	313	3	1/1/11/20	5/15/91/115	-
29	CLA	e	608	34	1/1/10/20	4/10/86/115	-
33	IHT	Z	301	-	-	7/25/65/65	0/2/2/2
29	CLA	B	812	11	1/1/13/20	5/27/103/115	-
30	KC2	e	609	27	-	7/15/71/71	-
29	CLA	9	314	9	1/1/11/20	5/15/91/115	-
29	CLA	K	102	18	1/1/13/20	7/27/103/115	-
30	KC2	2	610	2	-	10/15/71/71	-
31	II0	3	315	-	-	1/21/67/67	0/2/2/2
30	KC2	7	310	7	-	9/15/71/71	-
29	CLA	A	802	29,10	1/1/13/20	3/27/103/115	-
29	CLA	L	202	19	1/1/14/20	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	II0	7	314	-	-	1/21/67/67	0/2/2/2
29	CLA	A	826	10	1/1/15/20	8/39/115/115	-
29	CLA	9	312	9	1/1/10/20	4/10/86/115	-
31	II0	7	317	-	-	3/21/67/67	0/2/2/2
37	8CT	B	848	-	-	8/29/63/63	0/2/2/2
37	8CT	4	616	-	-	14/29/63/63	0/2/2/2
29	CLA	1	601	1	1/1/11/20	7/15/91/115	-
29	CLA	B	820	11	1/1/14/20	12/33/109/115	-
29	CLA	a	601	24	1/1/11/20	7/15/91/115	-
29	CLA	A	818	10	1/1/15/20	10/39/115/115	-
29	CLA	B	831	11	1/1/14/20	11/33/109/115	-
29	CLA	7	306	7	1/1/11/20	7/15/91/115	-
31	II0	3	318	-	-	3/21/67/67	0/2/2/2
29	CLA	6	603	6	1/1/11/20	4/15/91/115	-
29	CLA	B	825	-	1/1/14/20	6/33/109/115	-
31	II0	d	615	-	-	1/21/67/67	0/2/2/2
29	CLA	B	835	11	1/1/13/20	3/27/103/115	-
30	KC2	6	613	6	-	11/15/71/71	-
29	CLA	B	810	11	1/1/15/20	18/39/115/115	-
31	II0	7	315	-	-	0/21/67/67	0/2/2/2
29	CLA	9	307	9	1/1/13/20	9/30/106/115	-
37	8CT	I	101	-	-	9/29/63/63	0/2/2/2
34	LHG	4	620	-	-	22/49/49/53	-
29	CLA	7	307	7	1/1/11/20	5/15/91/115	-
29	CLA	5	611	5	1/1/11/20	6/15/91/115	-
37	8CT	b	615	-	-	14/29/63/63	0/2/2/2
30	KC2	c	614	30	-	6/15/71/71	-
37	8CT	B	851	-	-	12/29/63/63	0/2/2/2
37	8CT	B	844	-	-	9/29/63/63	0/2/2/2
29	CLA	O	204	-	1/1/13/20	6/27/103/115	-
37	8CT	L	205	-	-	11/29/63/63	0/2/2/2
29	CLA	A	815	10	1/1/14/20	2/36/112/115	-
34	LHG	1	619	29	-	20/39/39/53	-
29	CLA	a	602	24	1/1/13/20	11/27/103/115	-
29	CLA	B	839	11	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	9	304	9	1/1/11/20	6/15/91/115	-
29	CLA	A	839	-	1/1/15/20	16/39/115/115	-
33	IHT	6	616	-	-	6/25/65/65	0/2/2/2
36	SQD	O	207	-	-	14/24/44/69	0/1/1/1
29	CLA	3	309	3	1/1/14/20	5/33/109/115	-
29	CLA	6	609	34	1/1/10/20	0/10/86/115	-
29	CLA	A	834	10	1/1/13/20	7/27/103/115	-
29	CLA	X	301	-	1/1/12/20	5/24/100/115	-
39	SF4	A	848	10,11	-	-	0/6/5/5
29	CLA	A	801	10	1/1/15/20	20/39/115/115	-
30	KC2	5	610	5	-	9/15/71/71	-
29	CLA	3	305	3	1/1/15/20	6/39/115/115	-
31	II0	O	206	-	-	0/21/67/67	0/2/2/2
29	CLA	2	606	2	1/1/11/20	5/15/91/115	-
35	LMG	6	617	-	-	10/27/47/70	0/1/1/1
29	CLA	5	608	5	1/1/14/20	13/33/109/115	-
29	CLA	9	308	-	1/1/15/20	19/39/115/115	-
30	KC2	9	311	9	-	8/15/71/71	-
34	LHG	B	801	-	-	24/41/41/53	-
29	CLA	B	813	11	1/1/15/20	13/39/115/115	-
29	CLA	1	613	1	1/1/11/20	8/15/91/115	-
30	KC2	a	610	24	-	9/15/71/71	-
29	CLA	7	303	7	1/1/15/20	8/39/115/115	-
35	LMG	2	618	-	-	9/31/51/70	0/1/1/1
29	CLA	9	302	9	1/1/11/20	5/15/91/115	-
29	CLA	A	816	10	1/1/14/20	19/33/109/115	-
31	II0	5	617	-	-	6/21/67/67	0/2/2/2
37	8CT	A	847	-	-	10/29/63/63	0/2/2/2

The worst 5 of 2997 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B	847	8CT	C02-C03	15.12	1.59	1.34
37	Z	307	8CT	C02-C03	15.03	1.59	1.34
37	B	845	8CT	C02-C03	14.91	1.59	1.34
37	Z	308	8CT	C02-C03	14.83	1.59	1.34
37	I	101	8CT	C02-C03	14.81	1.59	1.34

The worst 5 of 3323 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B	843	8CT	C33-C32-C31	-12.10	113.28	124.83
37	L	205	8CT	C33-C32-C31	-12.08	113.30	124.83
37	A	844	8CT	C33-C32-C31	-11.85	113.51	124.83
37	A	846	8CT	C33-C32-C31	-11.71	113.66	124.83
37	M	101	8CT	C33-C32-C31	-11.68	113.68	124.83

5 of 254 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	1	601	CLA	ND
29	1	602	CLA	ND
29	1	603	CLA	ND
29	1	604	CLA	ND
29	1	605	CLA	ND

5 of 3412 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	1	607	CLA	C1A-C2A-CAA-CBA
29	1	608	CLA	C4-C3-C5-C6
29	1	611	CLA	CHA-CBD-CGD-O1D
29	1	611	CLA	CHA-CBD-CGD-O2D
29	1	612	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

297 monomers are involved in 691 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	2	603	CLA	2	0
29	A	819	CLA	5	0
29	A	842	CLA	6	0
29	8	306	CLA	2	0
29	2	607	CLA	1	0
29	L	203	CLA	4	0
29	1	609	CLA	2	0
29	c	608	CLA	2	0
29	b	602	CLA	3	0
33	a	616	IHT	1	0
29	B	818	CLA	3	0
29	B	836	CLA	3	0
36	7	321	SQD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	5	605	CLA	2	0
29	B	819	CLA	1	0
29	A	825	CLA	7	0
32	b	613	II3	1	0
34	L	206	LHG	1	0
29	5	601	CLA	2	0
29	B	821	CLA	3	0
30	3	307	KC2	1	0
29	B	841	CLA	3	0
29	A	854	CLA	9	0
29	d	608	CLA	2	0
29	3	303	CLA	2	0
29	A	853	CLA	5	0
34	A	852	LHG	1	0
29	4	606	CLA	2	0
29	B	837	CLA	7	0
29	d	602	CLA	4	0
29	5	612	CLA	2	0
29	A	812	CLA	7	0
29	6	604	CLA	1	0
29	9	305	CLA	2	0
29	7	312	CLA	4	0
30	b	609	KC2	4	0
29	B	808	CLA	5	0
34	e	617	LHG	1	0
29	Z	302	CLA	4	0
29	A	817	CLA	5	0
29	d	604	CLA	2	0
29	A	810	CLA	4	0
31	c	621	II0	1	0
29	a	603	CLA	1	0
29	B	811	CLA	4	0
31	R	204	II0	2	0
29	4	607	CLA	1	0
29	c	602	CLA	5	0
29	A	835	CLA	4	0
29	1	603	CLA	3	0
36	a	618	SQD	3	0
29	R	202	CLA	3	0
33	L	204	IHT	1	0
29	A	804	CLA	5	0
29	2	608	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	e	606	CLA	3	0
29	4	610	CLA	4	0
29	1	607	CLA	1	0
29	A	838	CLA	6	0
29	9	310	CLA	4	0
29	5	606	CLA	2	0
40	A	849	PQN	5	0
36	9	301	SQD	1	0
29	3	306	CLA	1	0
29	8	302	CLA	5	0
29	B	829	CLA	6	0
29	A	836	CLA	5	0
34	8	316	LHG	1	0
29	A	823	CLA	1	0
38	9	322	DGD	1	0
34	4	618	LHG	6	0
29	b	604	CLA	1	0
29	5	613	CLA	1	0
34	c	623	LHG	2	0
29	B	804	CLA	1	0
29	4	609	CLA	1	0
29	8	303	CLA	2	0
29	d	612	CLA	2	0
34	M	102	LHG	2	0
29	B	817	CLA	10	0
29	F	201	CLA	2	0
29	9	309	CLA	4	0
29	B	806	CLA	4	0
29	d	605	CLA	2	0
29	A	806	CLA	2	0
34	L	208	LHG	1	0
29	b	601	CLA	2	0
29	8	317	CLA	4	0
29	A	814	CLA	1	0
29	B	816	CLA	5	0
29	A	820	CLA	4	0
29	6	612	CLA	1	0
29	c	612	CLA	4	0
32	8	312	II3	2	0
29	6	602	CLA	4	0
34	L	207	LHG	2	0
29	8	304	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	b	603	CLA	2	0
29	d	603	CLA	2	0
29	8	305	CLA	1	0
29	c	604	CLA	1	0
29	8	307	CLA	2	0
29	A	809	CLA	5	0
29	d	607	CLA	2	0
29	9	313	CLA	3	0
29	B	814	CLA	8	0
29	A	840	CLA	5	0
34	2	619	LHG	1	0
29	4	608	CLA	5	0
29	b	608	CLA	3	0
29	6	608	CLA	1	0
29	7	304	CLA	4	0
29	7	309	CLA	1	0
29	A	824	CLA	4	0
36	3	322	SQD	1	0
29	B	803	CLA	4	0
30	c	611	KC2	1	0
29	A	843	CLA	8	0
34	Z	309	LHG	2	0
34	9	321	LHG	1	0
34	7	319	LHG	2	0
39	C	102	SF4	1	0
31	1	614	II0	1	0
29	b	606	CLA	4	0
29	A	821	CLA	3	0
29	d	606	CLA	1	0
34	J	101	LHG	2	0
29	c	607	CLA	6	0
34	3	321	LHG	2	0
29	1	606	CLA	1	0
29	8	308	CLA	4	0
38	B	849	DGD	4	0
29	3	310	CLA	4	0
29	B	840	CLA	5	0
29	B	828	CLA	1	0
29	A	828	CLA	4	0
30	1	610	KC2	1	0
29	5	607	CLA	2	0
29	B	832	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	c	601	CLA	1	0
29	A	827	CLA	3	0
29	3	302	CLA	2	0
29	2	605	CLA	2	0
30	Z	306	KC2	1	0
31	5	615	II0	1	0
29	6	606	CLA	3	0
29	1	605	CLA	2	0
29	a	604	CLA	2	0
29	a	607	CLA	3	0
29	7	308	CLA	5	0
29	Z	304	CLA	1	0
29	a	605	CLA	2	0
29	A	813	CLA	1	0
29	8	301	CLA	1	0
29	3	311	CLA	2	0
34	5	621	LHG	4	0
29	A	829	CLA	4	0
36	B	850	SQD	1	0
29	A	803	CLA	5	0
34	7	320	LHG	3	0
29	c	615	CLA	1	0
29	B	827	CLA	8	0
29	O	201	CLA	2	0
29	B	809	CLA	4	0
29	3	304	CLA	1	0
37	M	101	8CT	1	0
29	3	312	CLA	1	0
29	2	602	CLA	2	0
29	4	611	CLA	7	0
29	e	602	CLA	5	0
29	A	831	CLA	4	0
29	B	807	CLA	2	0
29	4	603	CLA	2	0
35	8	314	LMG	2	0
29	1	608	CLA	1	0
29	2	604	CLA	2	0
29	4	601	CLA	2	0
29	L	201	CLA	3	0
29	A	808	CLA	4	0
29	e	604	CLA	2	0
37	7	318	8CT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	9	303	CLA	4	0
29	e	607	CLA	1	0
29	6	601	CLA	2	0
34	4	619	LHG	2	0
29	A	805	CLA	2	0
29	B	815	CLA	3	0
35	Z	310	LMG	1	0
29	a	612	CLA	5	0
29	A	811	CLA	4	0
29	B	802	CLA	3	0
29	B	826	CLA	4	0
29	d	601	CLA	2	0
37	F	203	8CT	1	0
29	e	611	CLA	5	0
35	3	319	LMG	2	0
29	O	202	CLA	2	0
29	B	805	CLA	2	0
34	A	851	LHG	2	0
31	c	616	II0	1	0
29	1	612	CLA	1	0
29	B	834	CLA	3	0
35	X	302	LMG	3	0
29	A	833	CLA	5	0
34	4	617	LHG	5	0
29	A	855	CLA	1	0
29	4	602	CLA	1	0
37	B	852	8CT	1	0
29	5	602	CLA	2	0
34	3	301	LHG	2	0
29	b	610	CLA	1	0
29	a	611	CLA	1	0
29	Z	305	CLA	3	0
29	B	838	CLA	1	0
29	5	603	CLA	3	0
36	3	320	SQD	2	0
29	7	311	CLA	1	0
29	A	822	CLA	4	0
29	4	604	CLA	1	0
34	a	617	LHG	1	0
29	A	830	CLA	3	0
35	F	204	LMG	3	0
29	B	824	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	1	611	CLA	1	0
29	A	832	CLA	4	0
29	A	837	CLA	6	0
29	F	202	CLA	1	0
40	B	842	PQN	2	0
29	c	606	CLA	3	0
29	c	603	CLA	4	0
32	e	613	II3	2	0
29	5	604	CLA	5	0
31	2	613	II0	1	0
34	A	850	LHG	2	0
29	A	807	CLA	3	0
29	A	841	CLA	5	0
29	B	822	CLA	6	0
29	Z	303	CLA	1	0
29	c	605	CLA	1	0
29	3	308	CLA	8	0
29	B	823	CLA	5	0
29	b	611	CLA	4	0
31	6	614	II0	1	0
29	1	604	CLA	2	0
29	a	606	CLA	2	0
29	2	612	CLA	1	0
33	c	620	IHT	1	0
29	6	607	CLA	4	0
29	3	313	CLA	2	0
29	e	608	CLA	1	0
29	9	314	CLA	1	0
29	K	102	CLA	4	0
30	7	310	KC2	1	0
29	A	802	CLA	3	0
29	L	202	CLA	3	0
31	7	314	II0	1	0
29	A	826	CLA	6	0
29	9	312	CLA	1	0
37	4	616	8CT	1	0
29	1	601	CLA	3	0
29	B	820	CLA	4	0
29	a	601	CLA	3	0
29	A	818	CLA	5	0
29	B	831	CLA	3	0
29	6	603	CLA	1	0

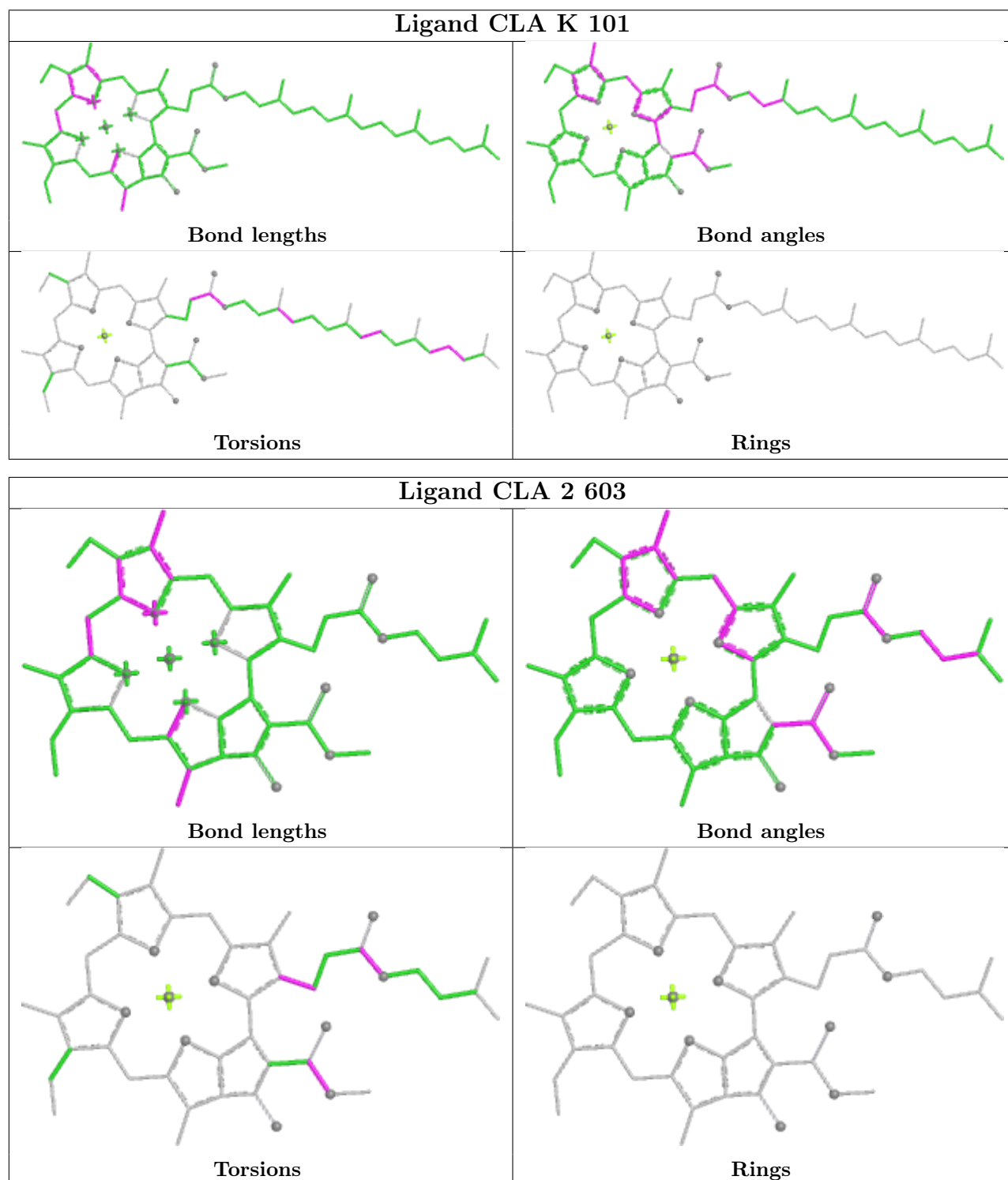
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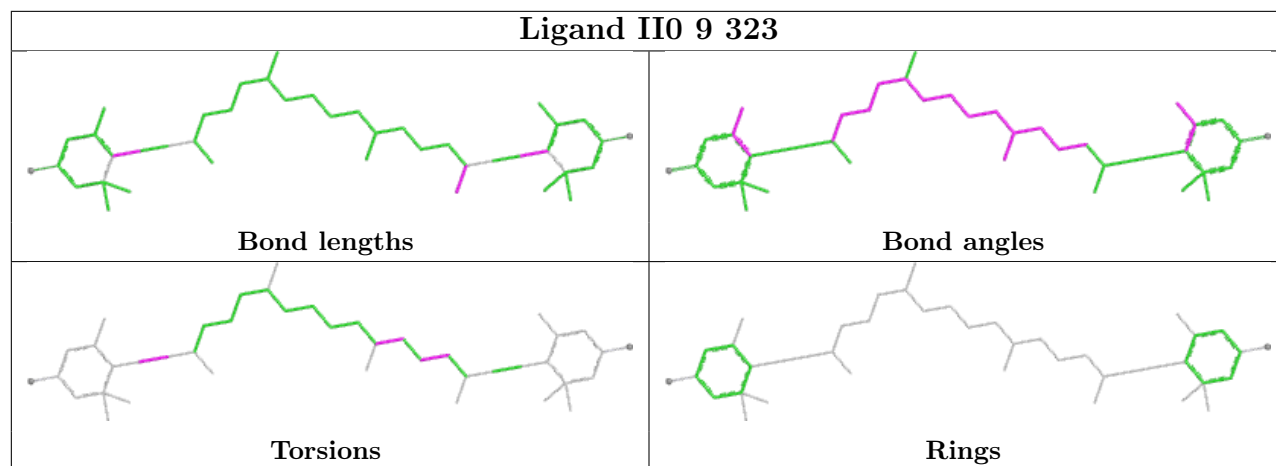
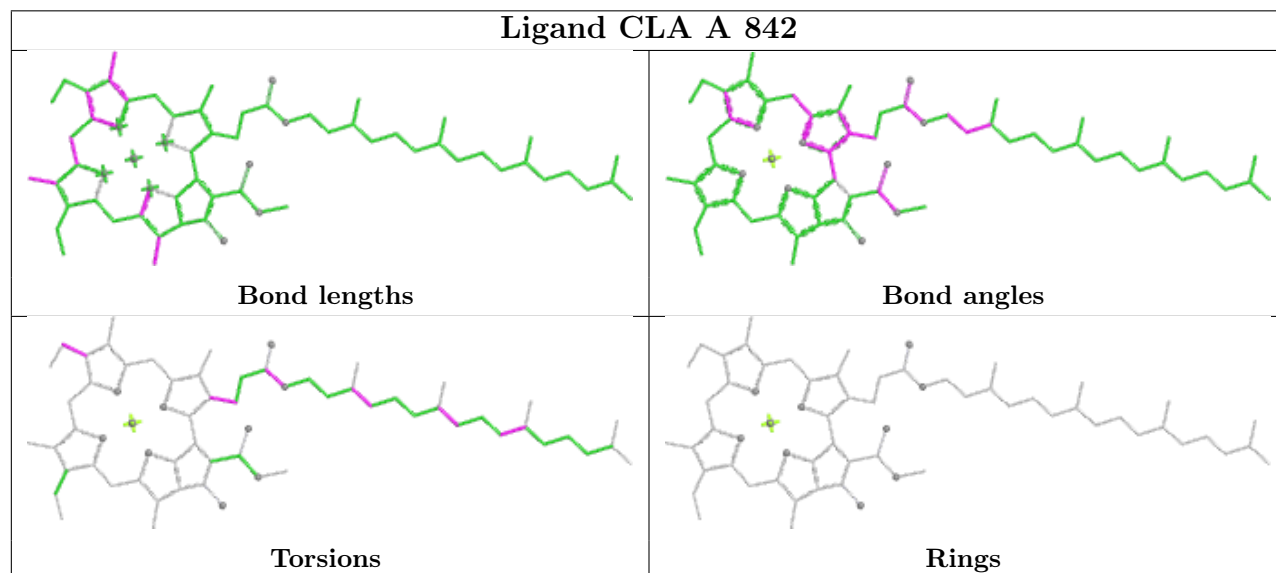
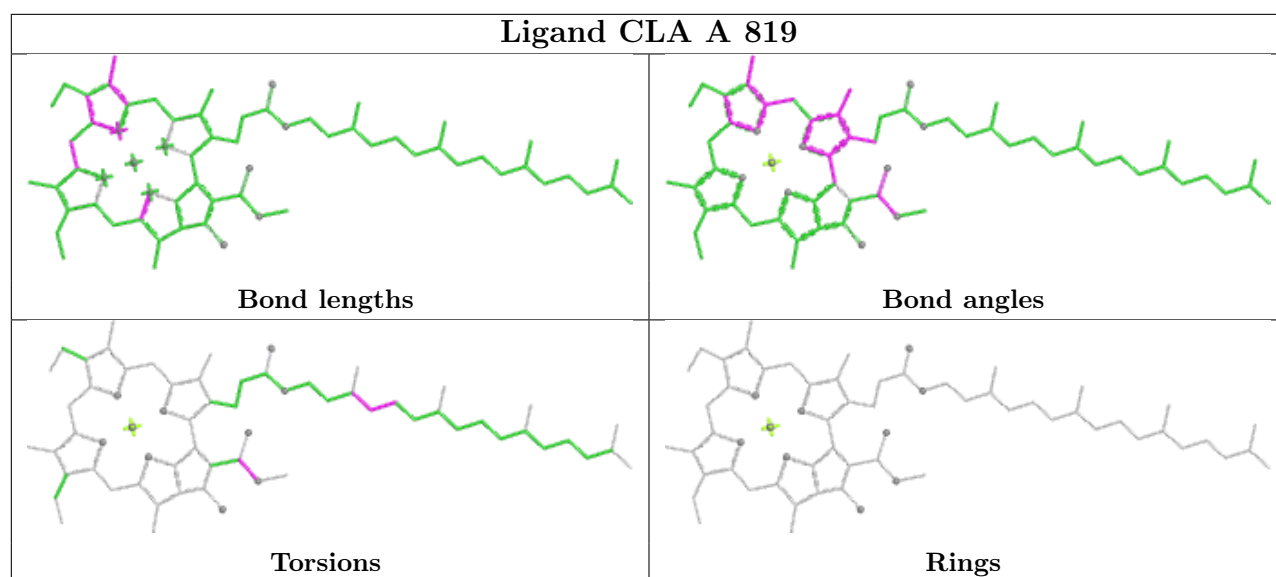
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	825	CLA	2	0
31	d	615	II0	1	0
30	6	613	KC2	1	0
29	B	810	CLA	11	0
29	9	307	CLA	4	0
34	4	620	LHG	2	0
29	7	307	CLA	4	0
29	5	611	CLA	3	0
37	B	851	8CT	1	0
37	B	844	8CT	1	0
29	O	204	CLA	1	0
29	A	815	CLA	6	0
34	1	619	LHG	2	0
29	a	602	CLA	2	0
29	B	839	CLA	4	0
29	9	304	CLA	3	0
29	A	839	CLA	3	0
29	3	309	CLA	2	0
29	6	609	CLA	3	0
29	A	834	CLA	2	0
29	X	301	CLA	2	0
29	A	801	CLA	2	0
29	3	305	CLA	1	0
29	2	606	CLA	4	0
29	5	608	CLA	2	0
29	9	308	CLA	9	0
34	B	801	LHG	3	0
29	B	813	CLA	4	0
29	7	303	CLA	1	0
35	2	618	LMG	3	0
29	9	302	CLA	2	0
29	A	816	CLA	6	0

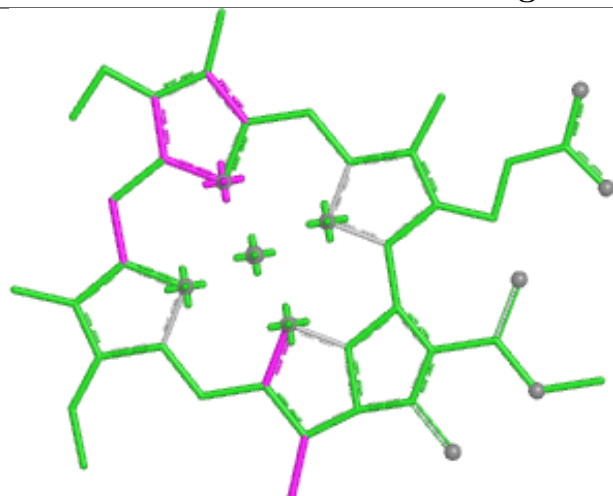
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

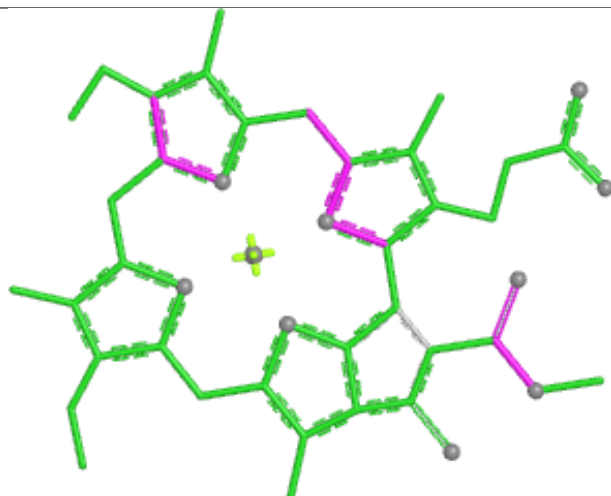




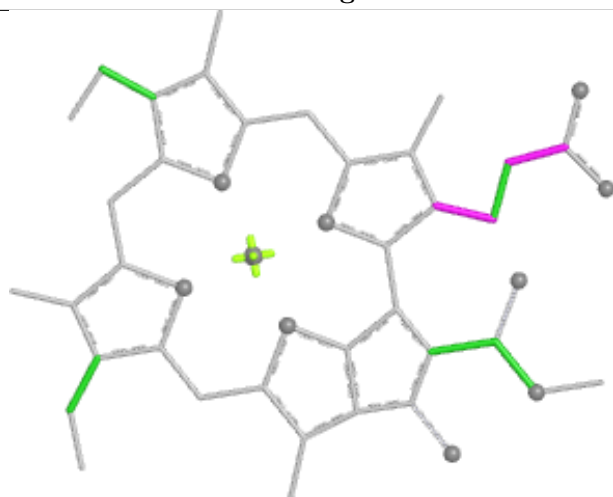
Ligand CLA 8 306



Bond lengths



Bond angles

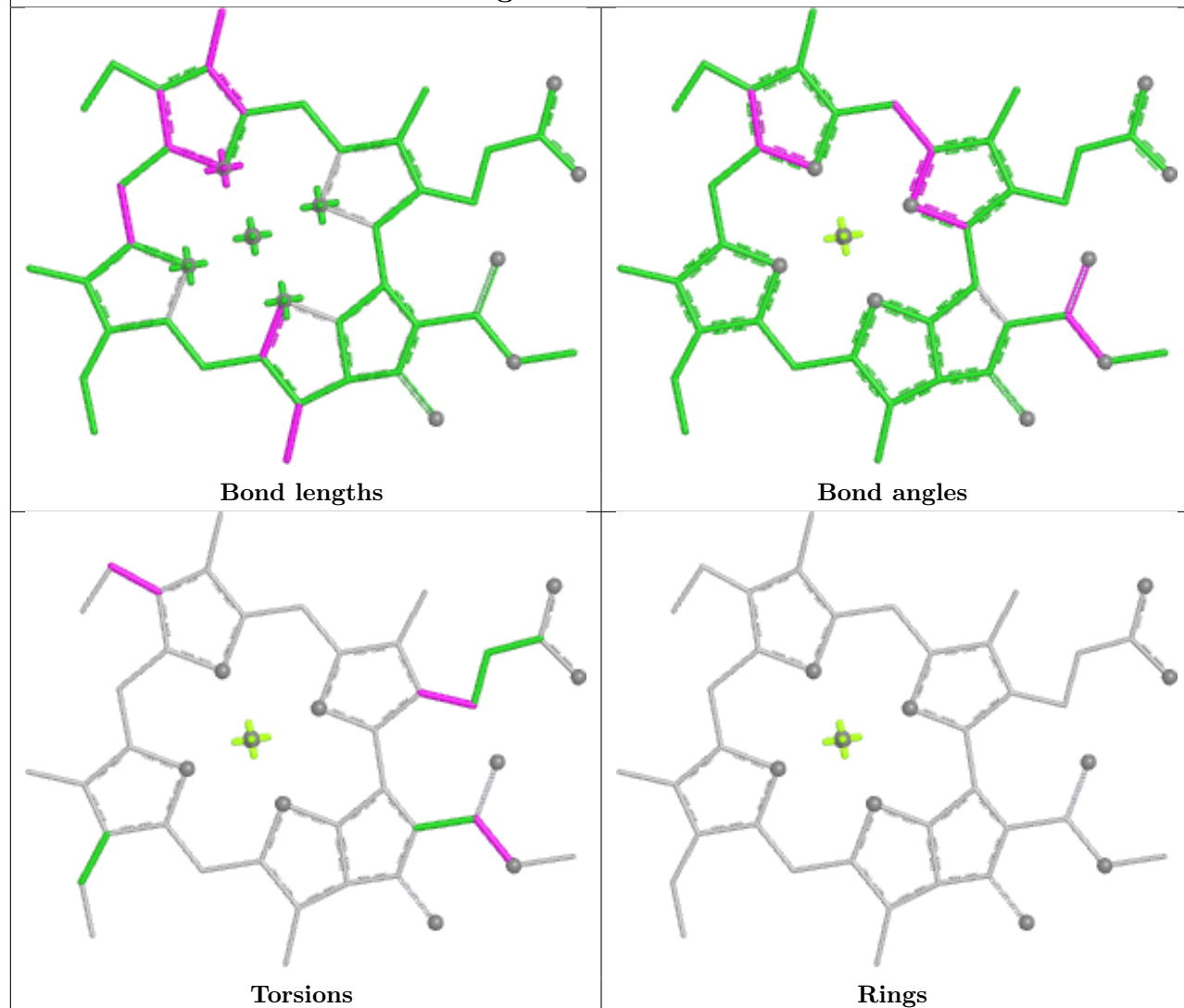


Torsions

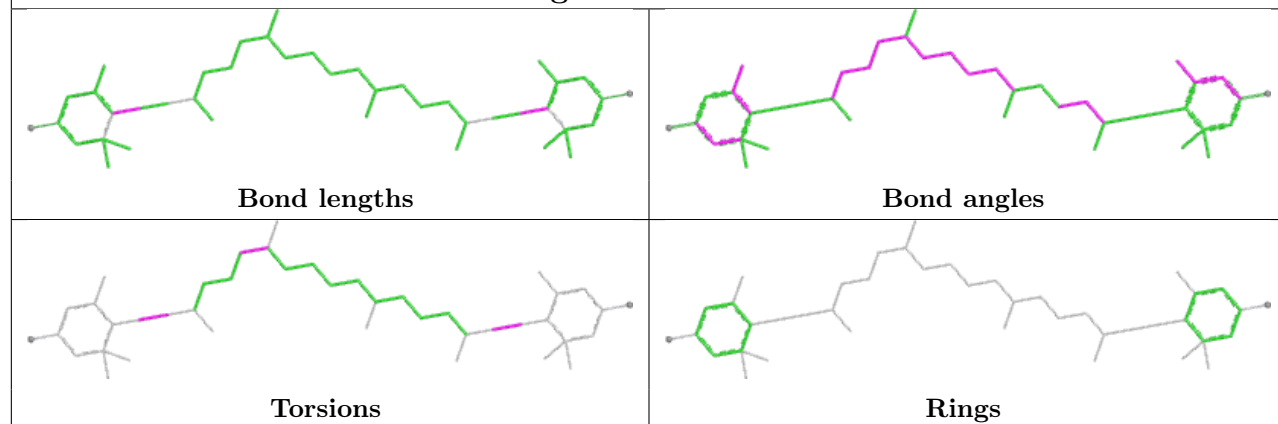


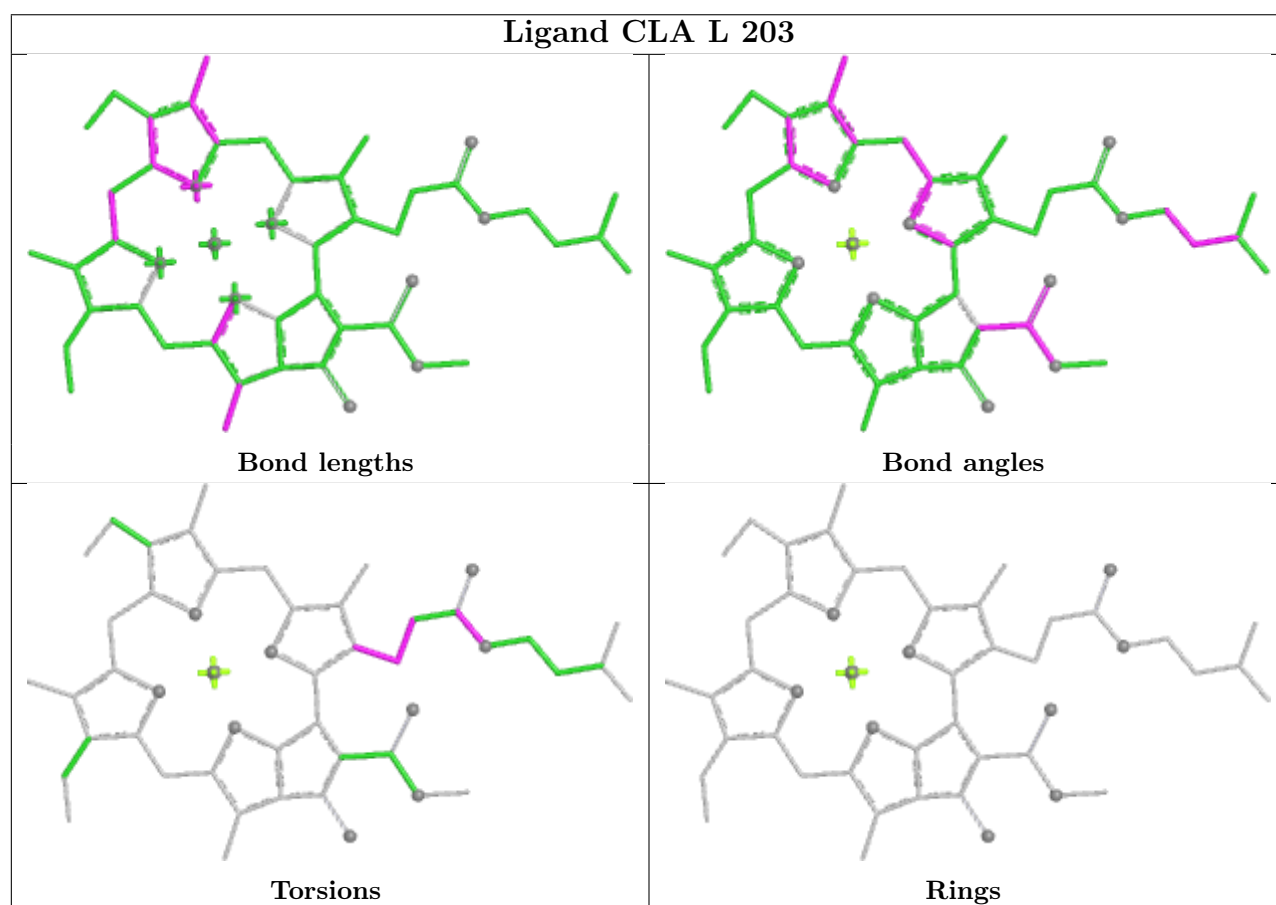
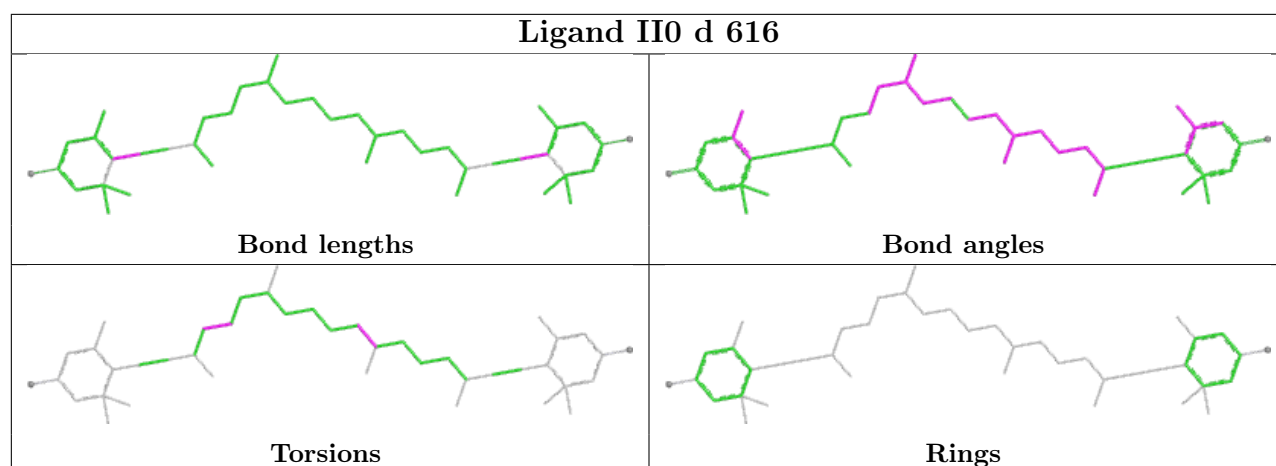
Rings

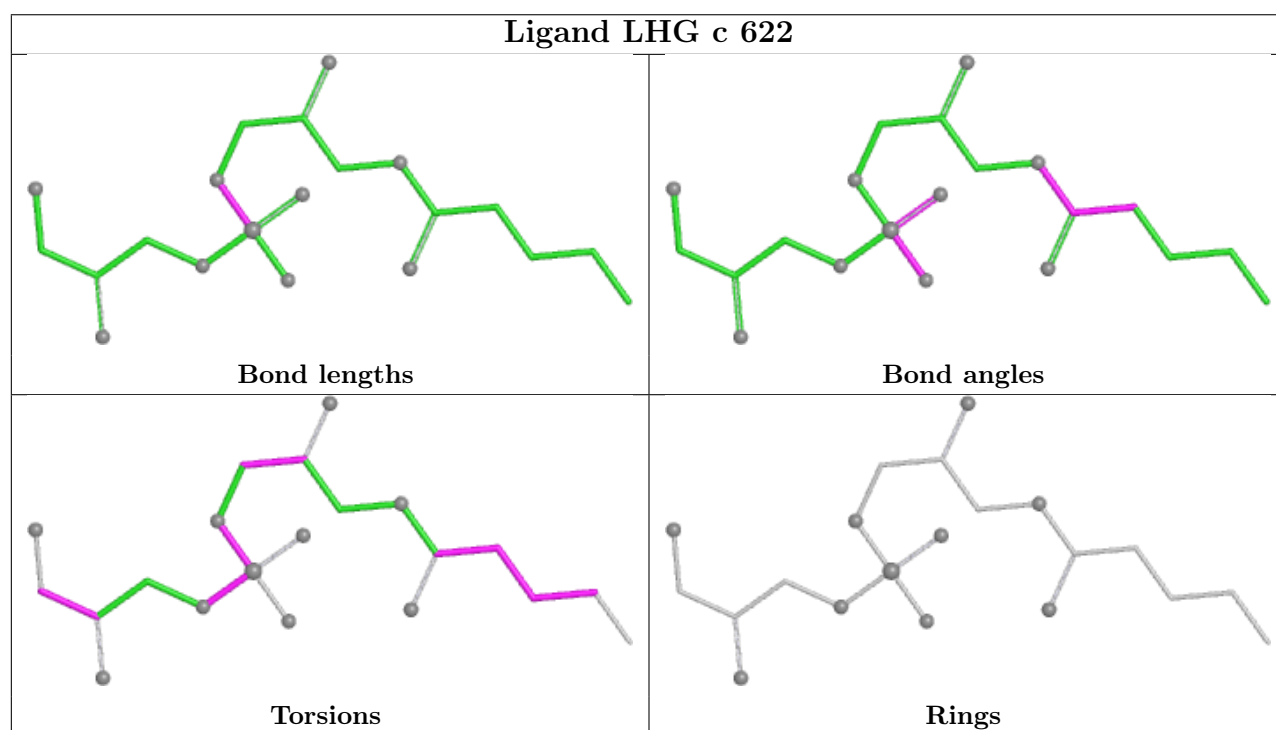
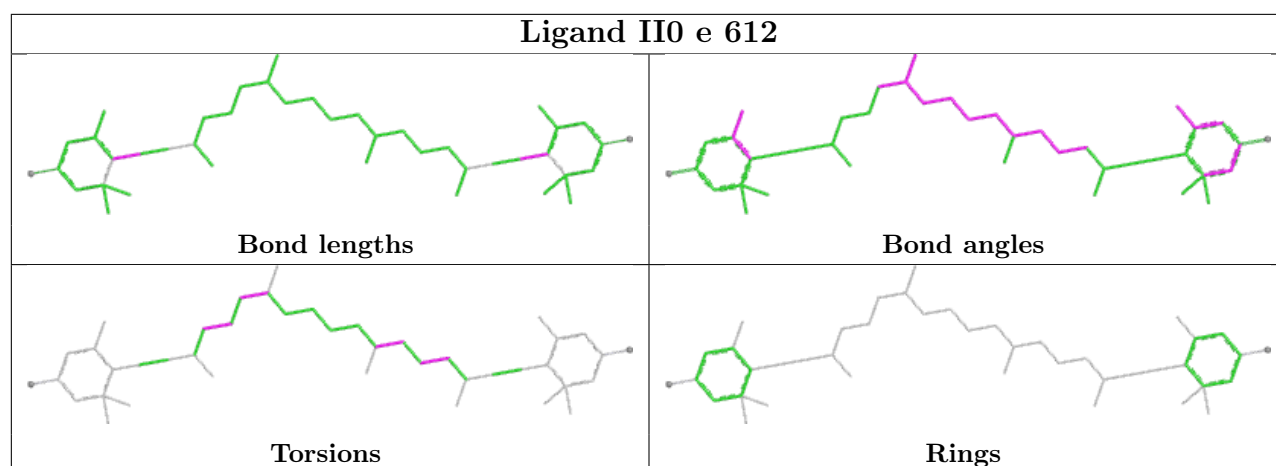
Ligand CLA 2 607



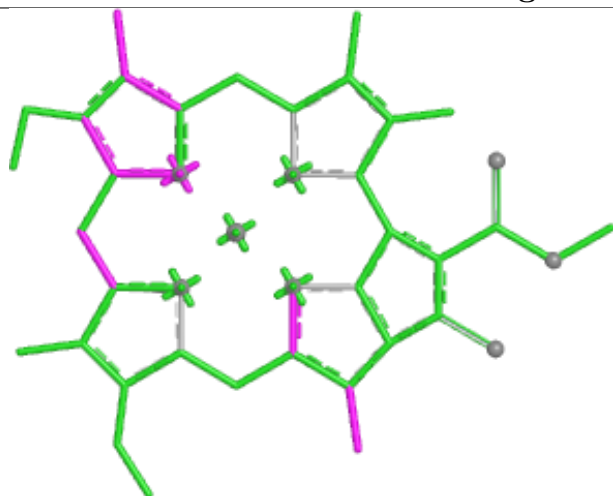
Ligand II0 4 615



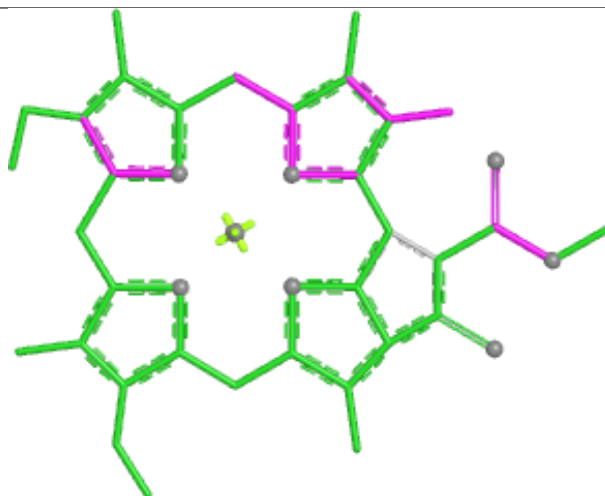




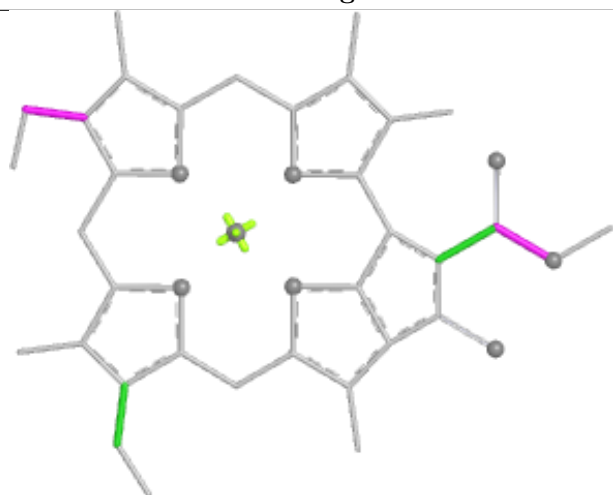
Ligand CLA 1 609



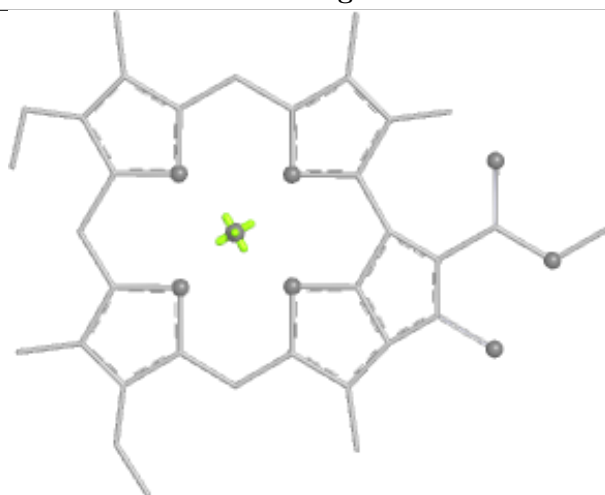
Bond lengths



Bond angles

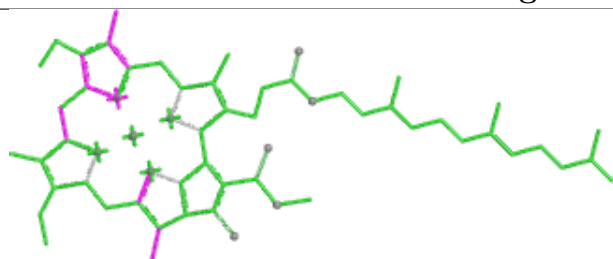


Torsions

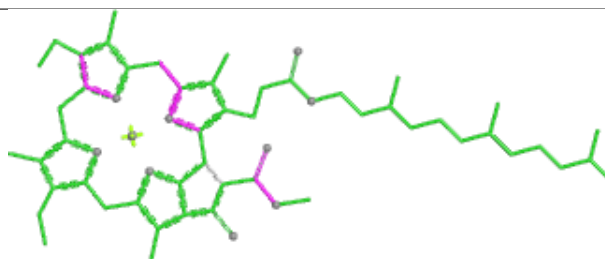


Rings

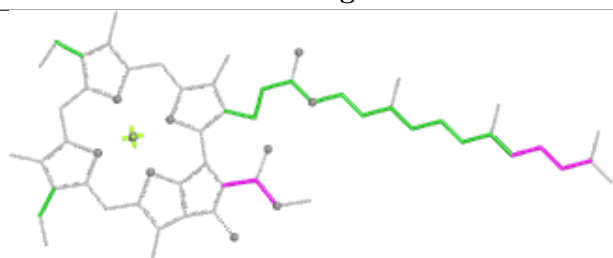
Ligand CLA c 608



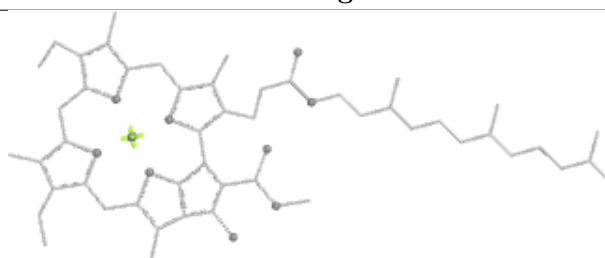
Bond lengths



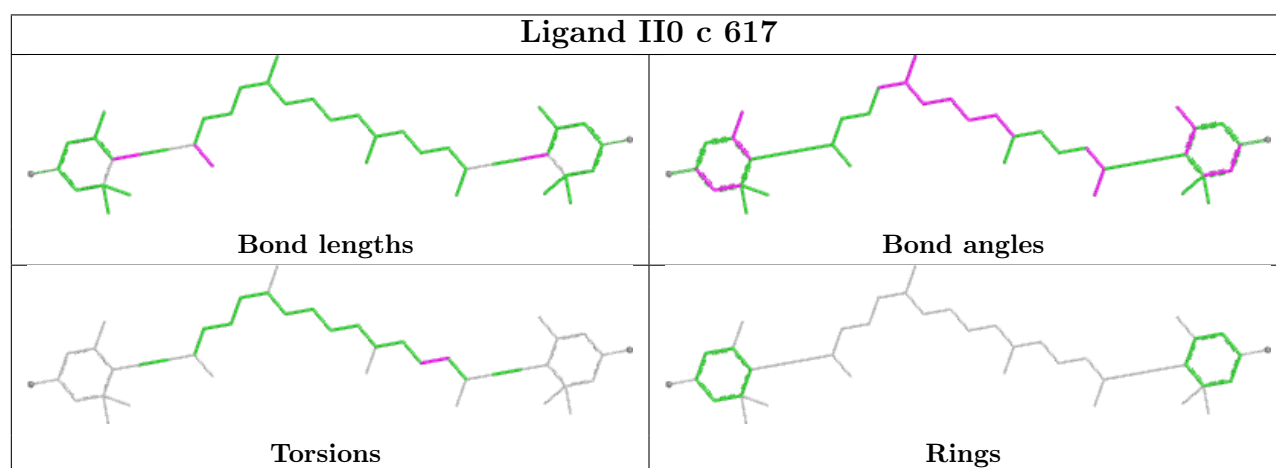
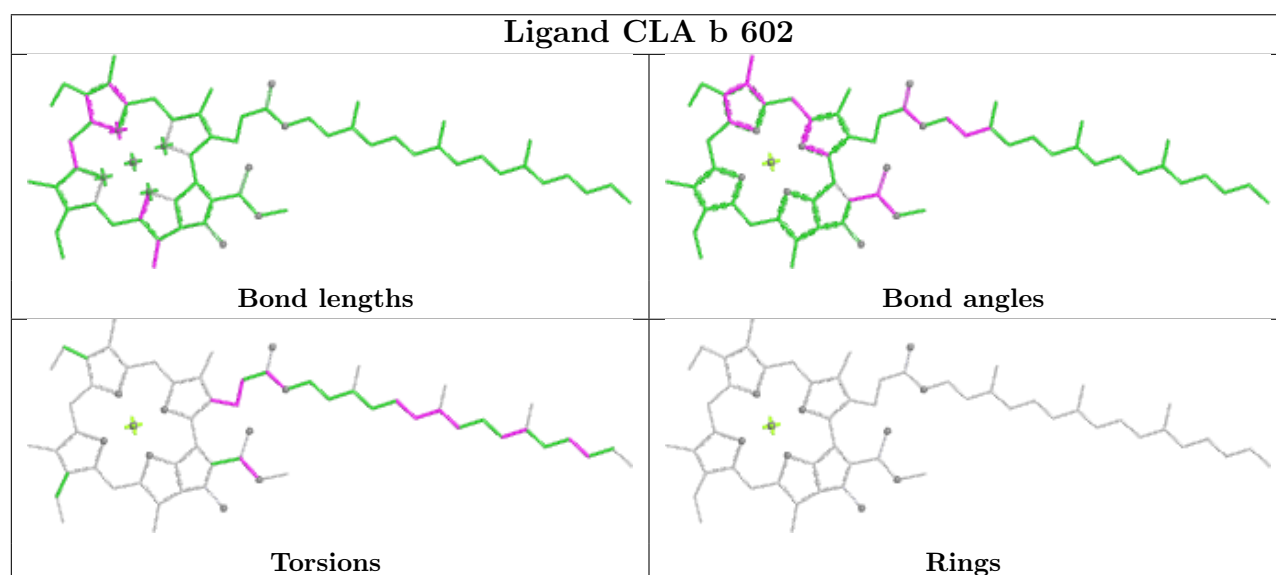
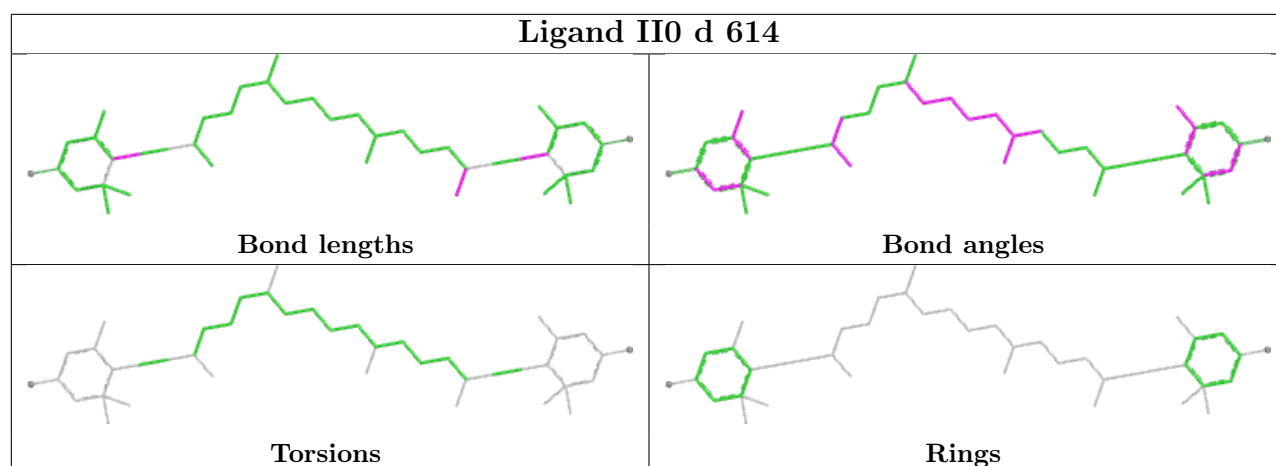
Bond angles

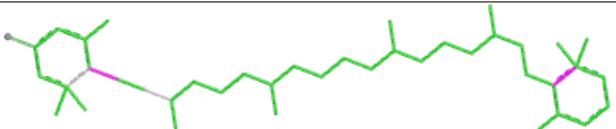
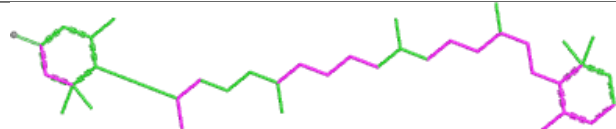
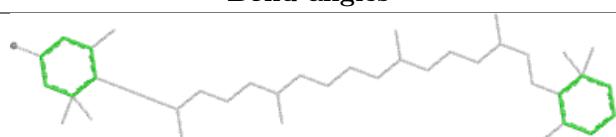


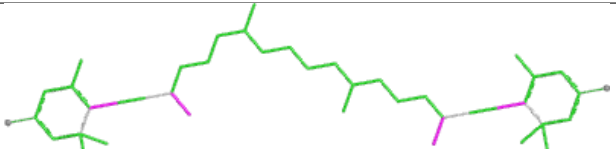
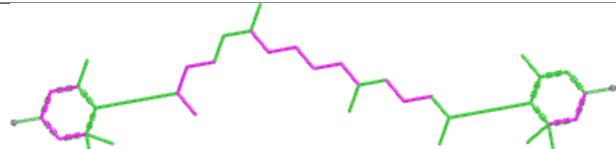
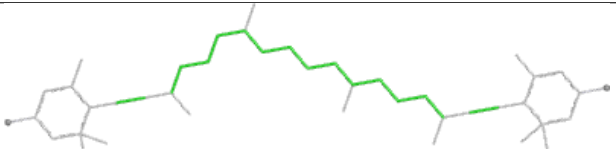
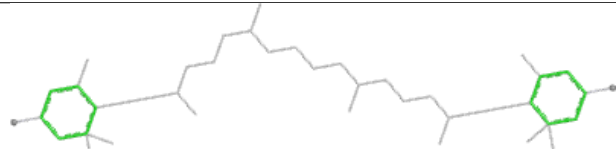
Torsions

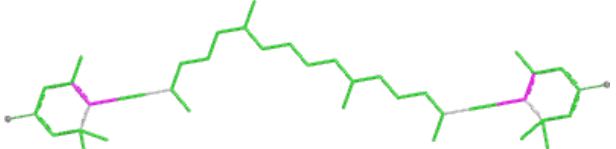
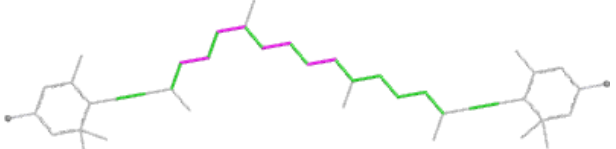
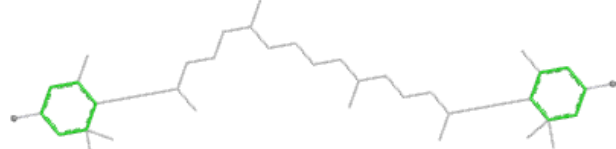


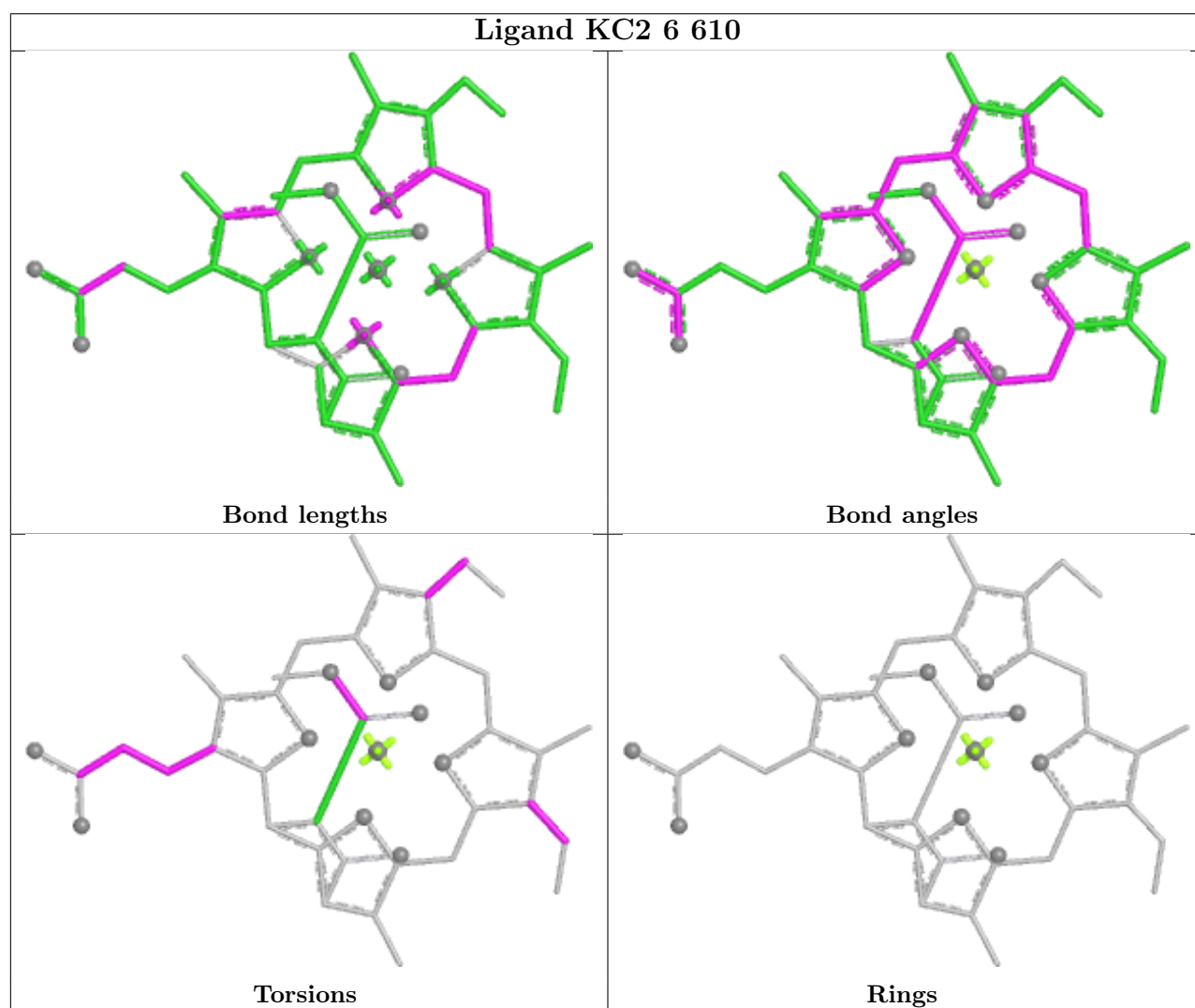
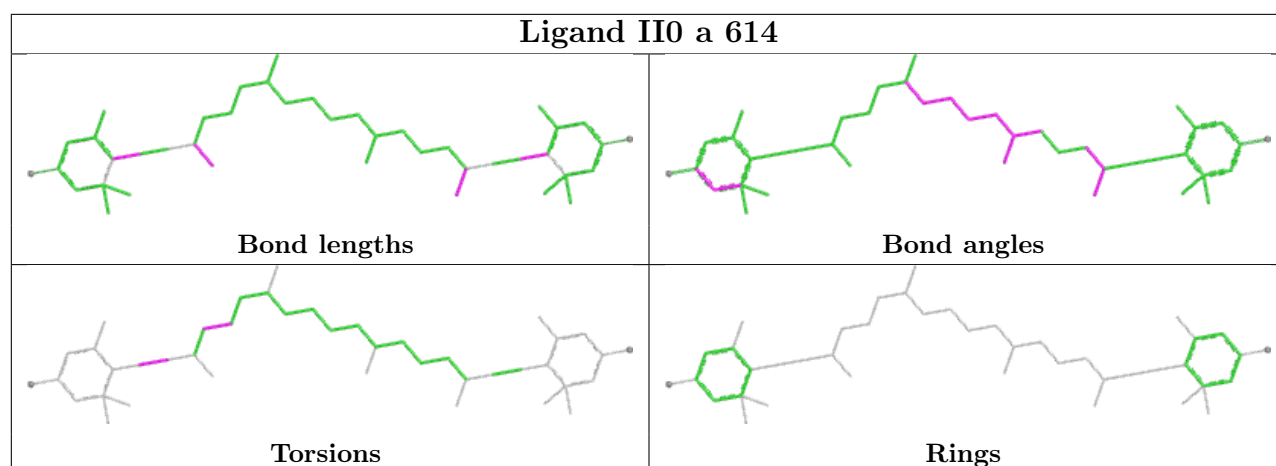
Rings

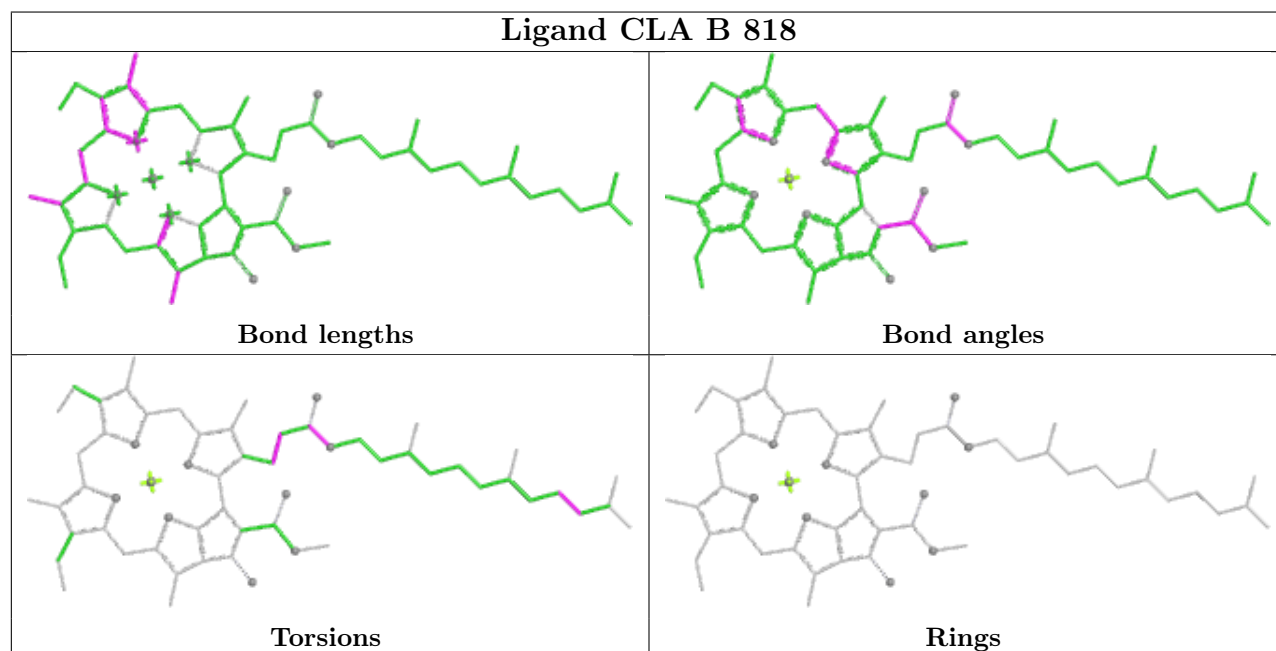
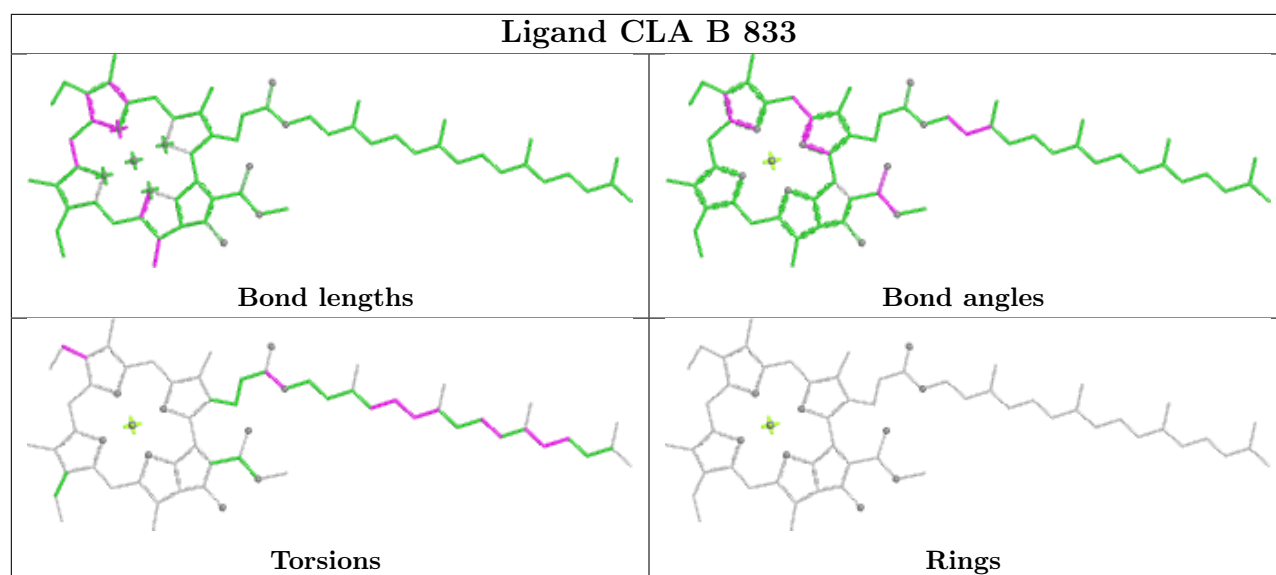


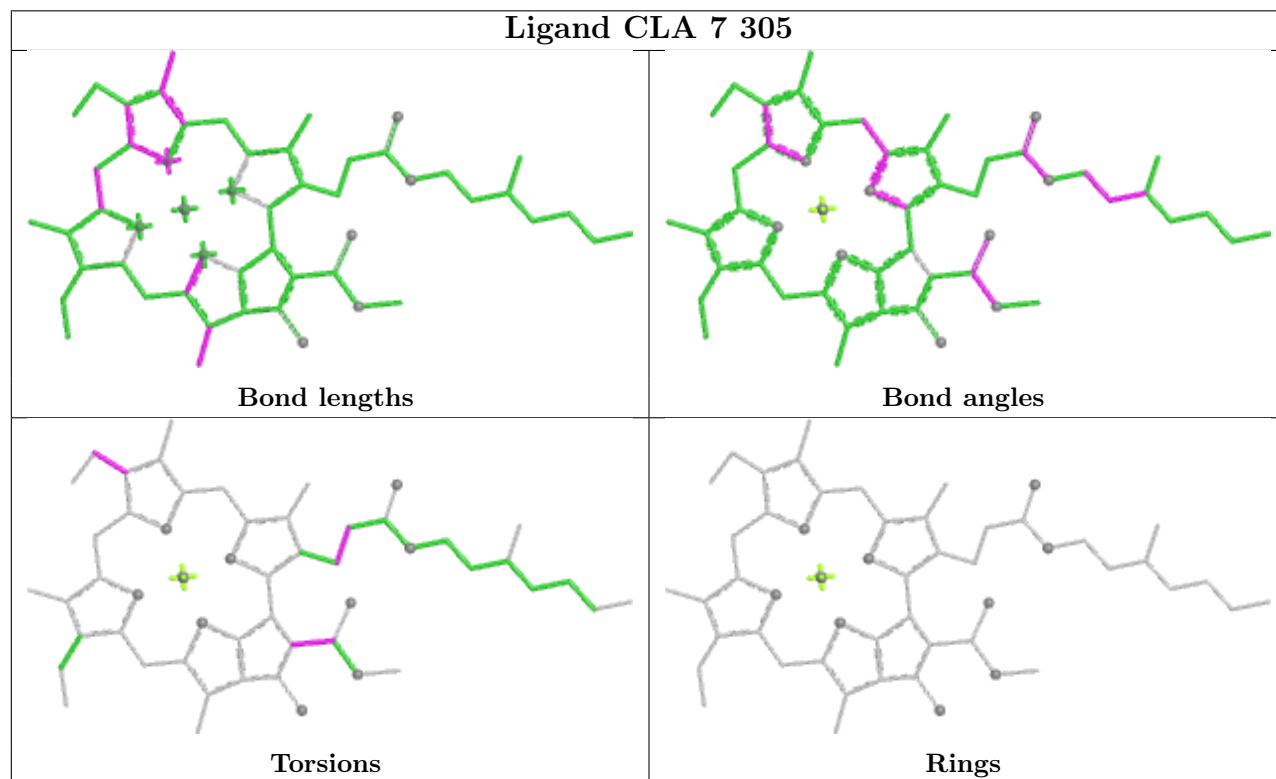
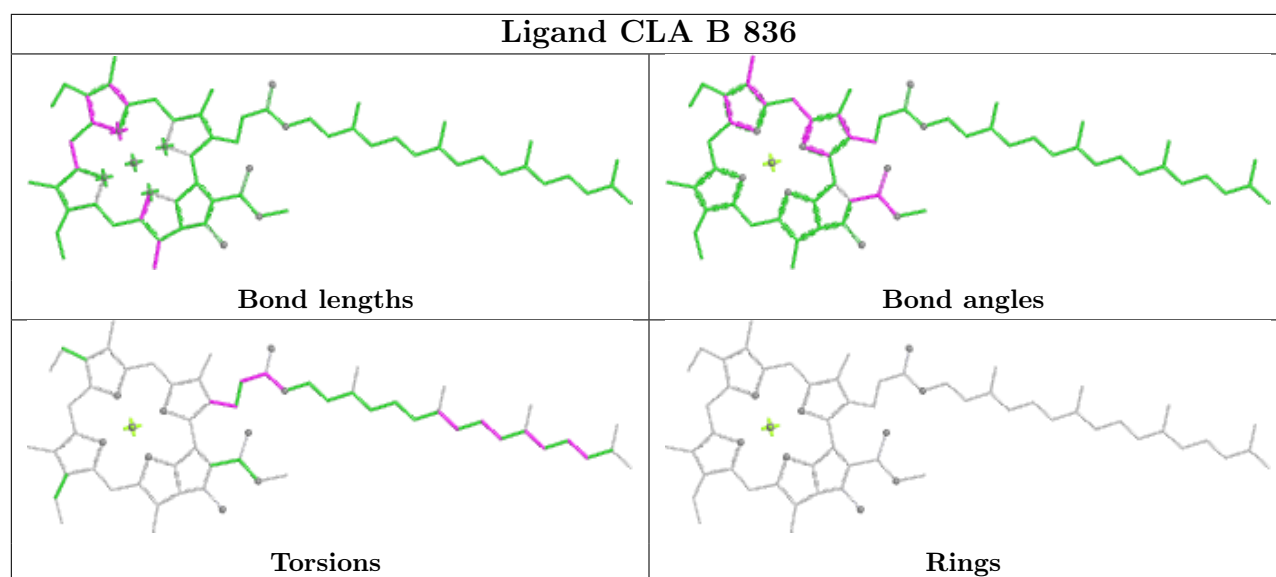
Ligand IHT a 616	
	Bond lengths
	Bond angles
	Torsions
	Rings

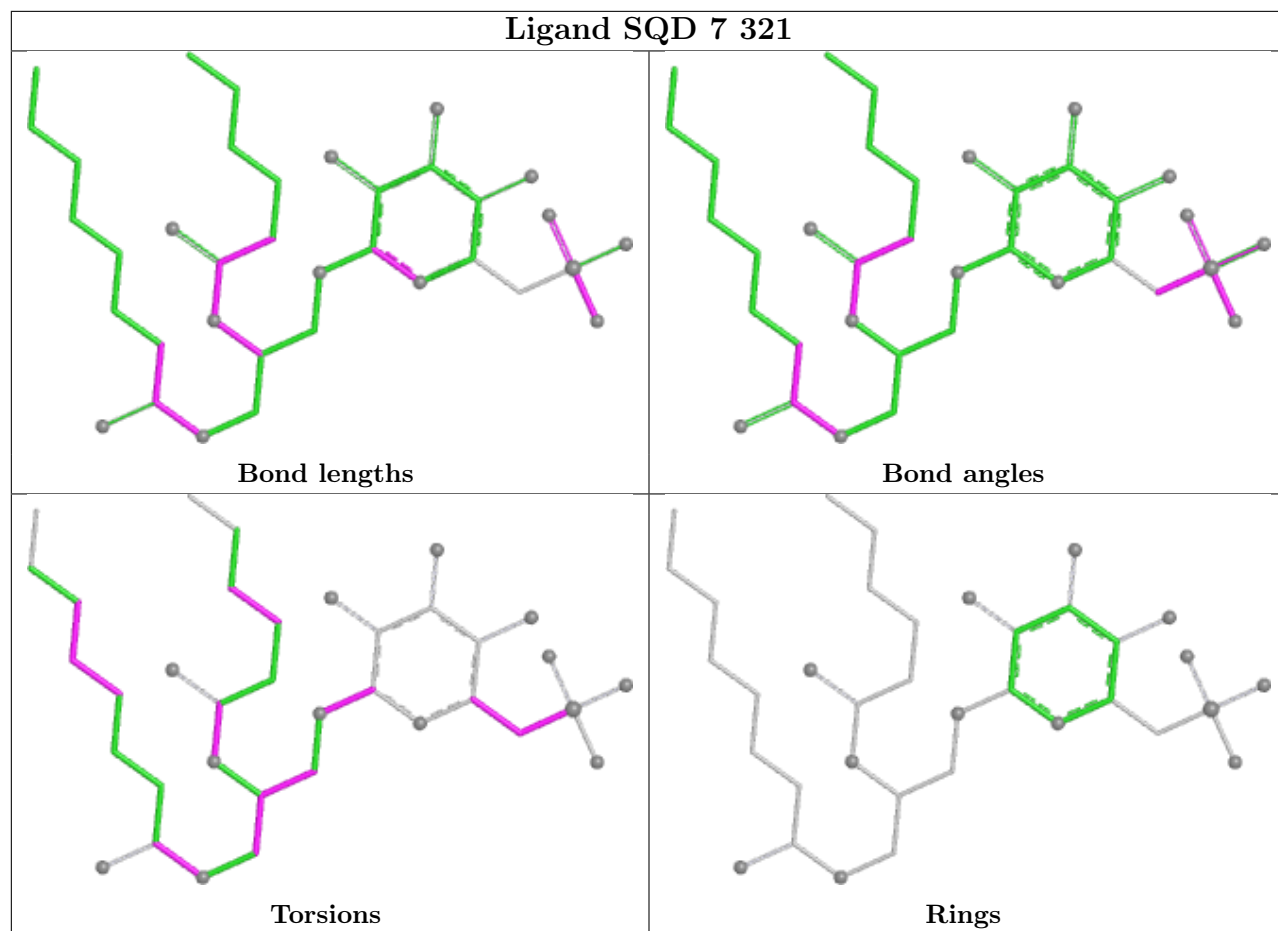
Ligand II0 R 201	
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	Bond angles
	Torsions
	Rings

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	Rings

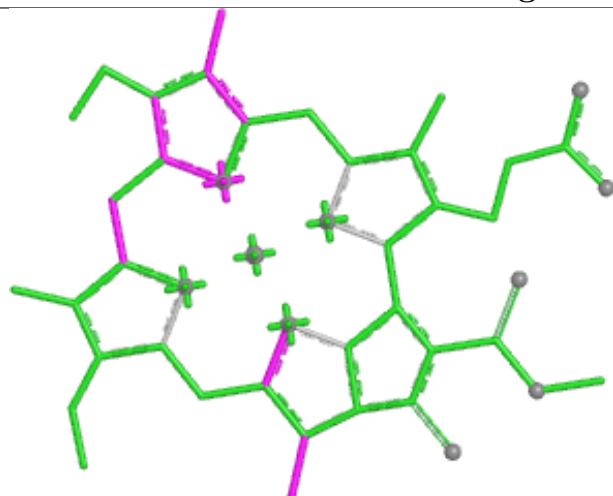




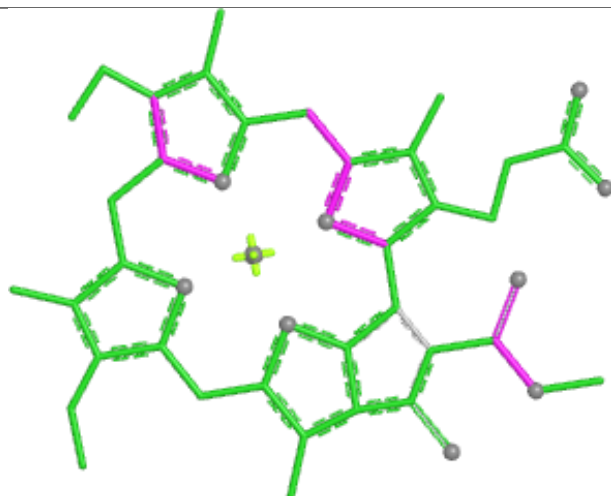




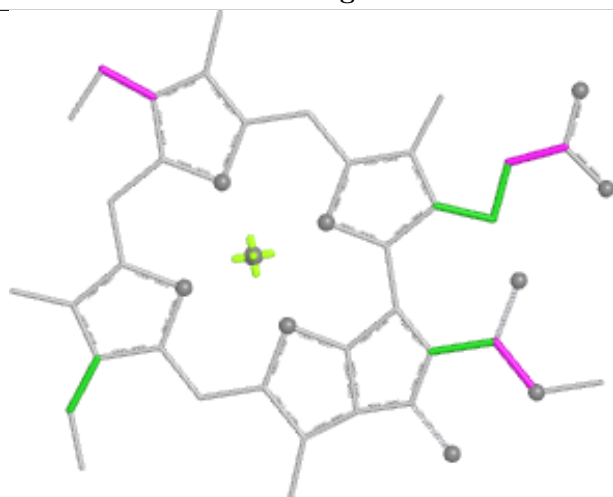
Ligand CLA 5 605



Bond lengths



Bond angles

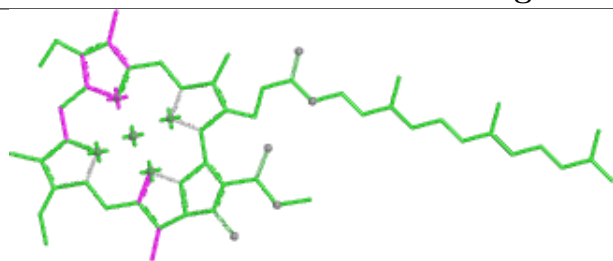


Torsions

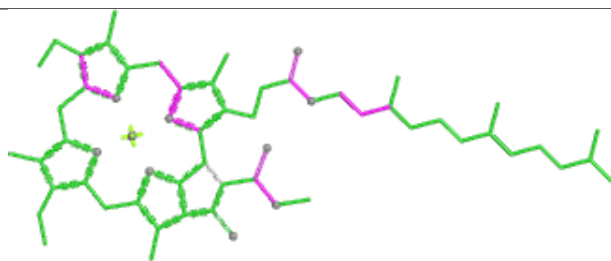


Rings

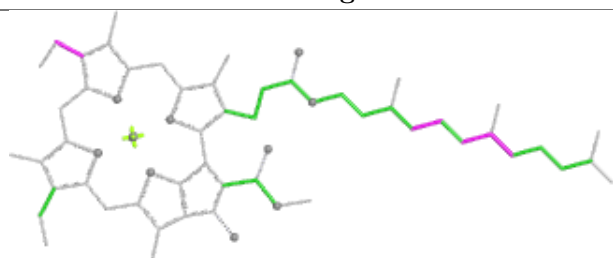
Ligand CLA B 819



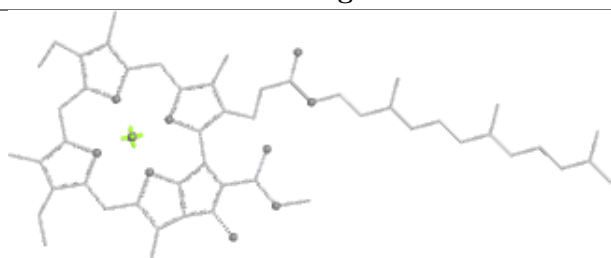
Bond lengths



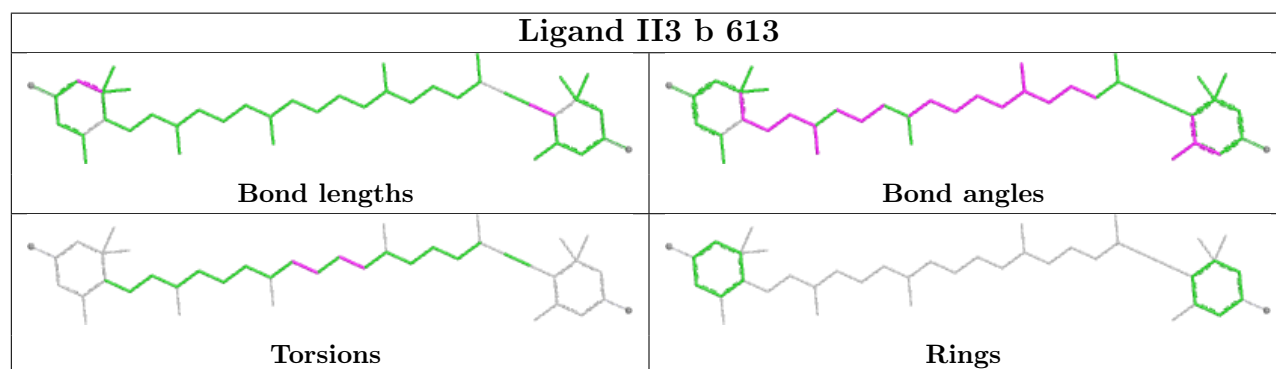
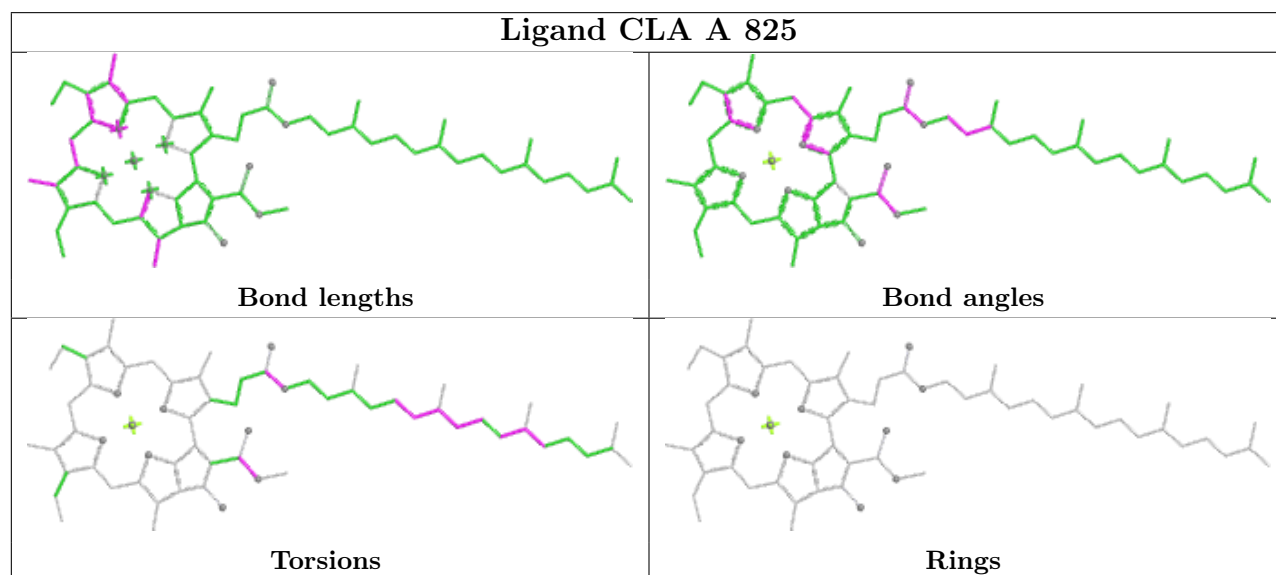
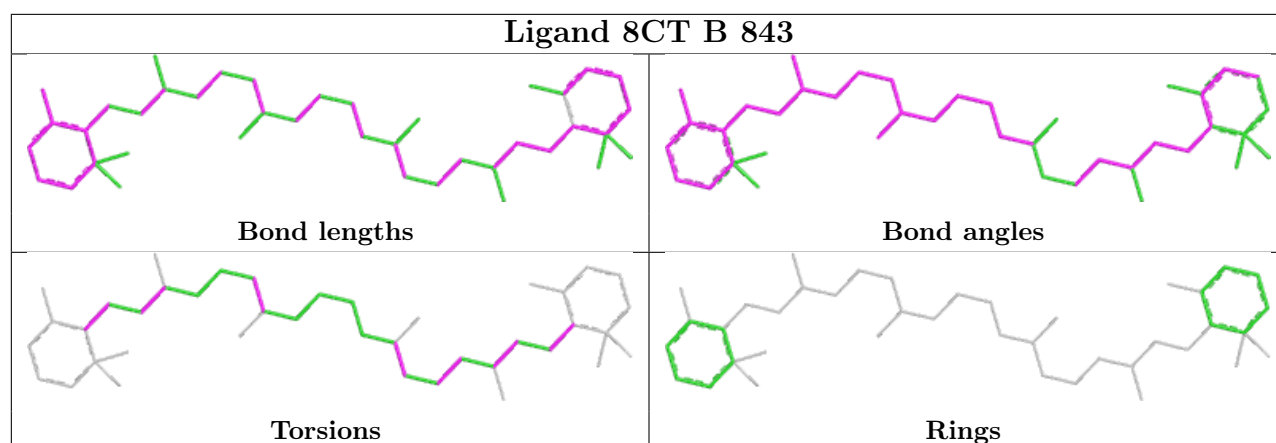
Bond angles

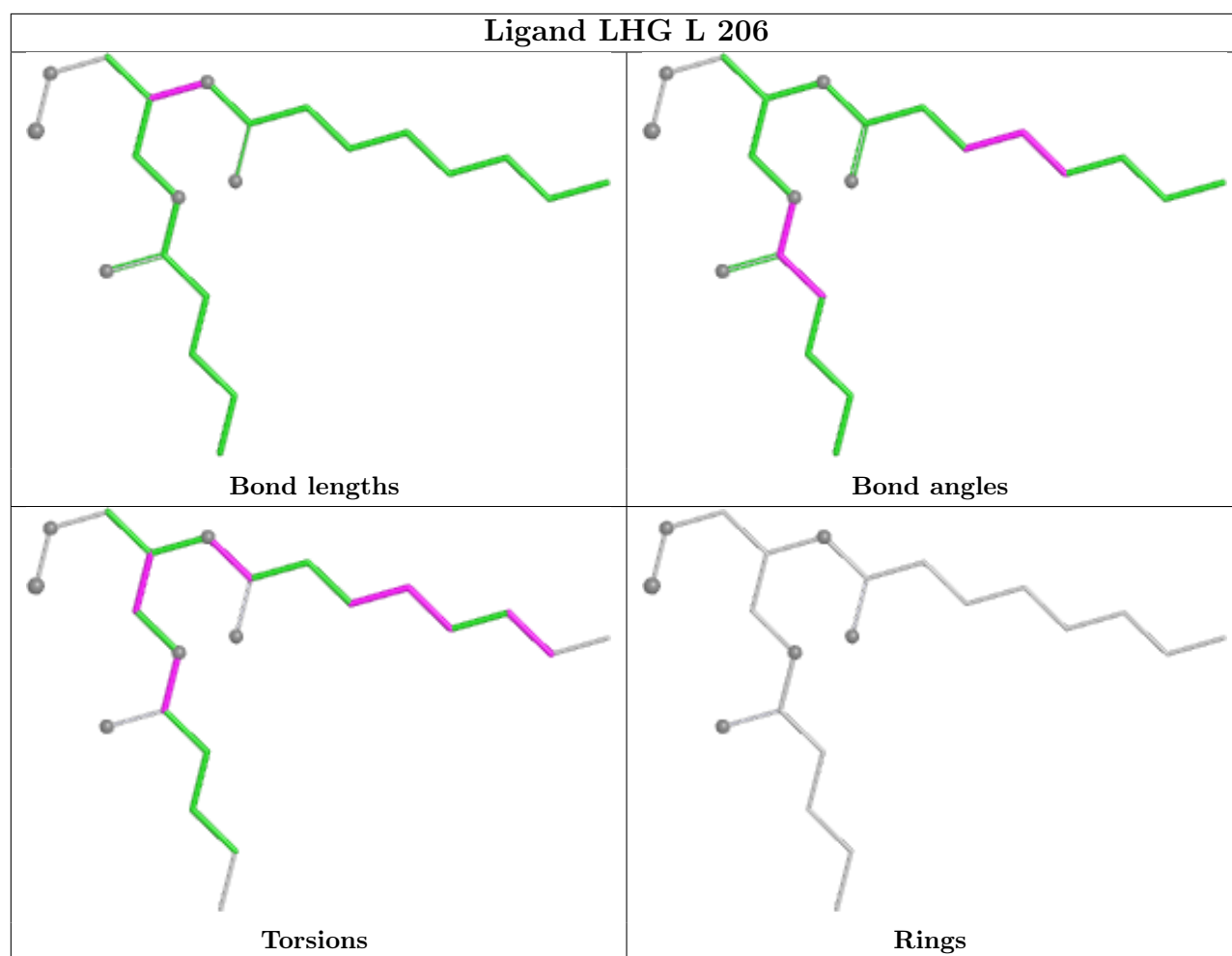


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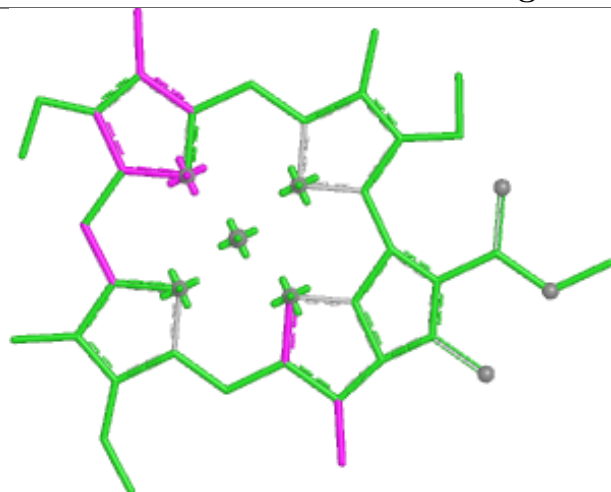


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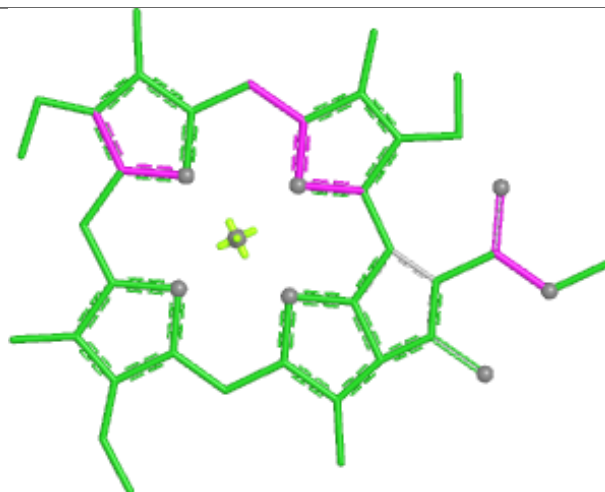




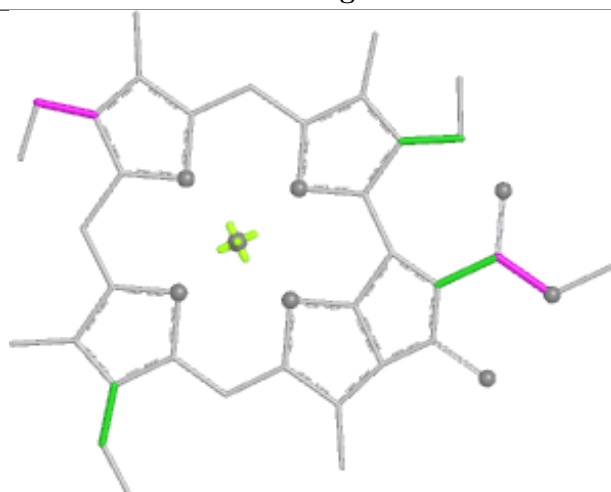
Ligand CLA 2 601



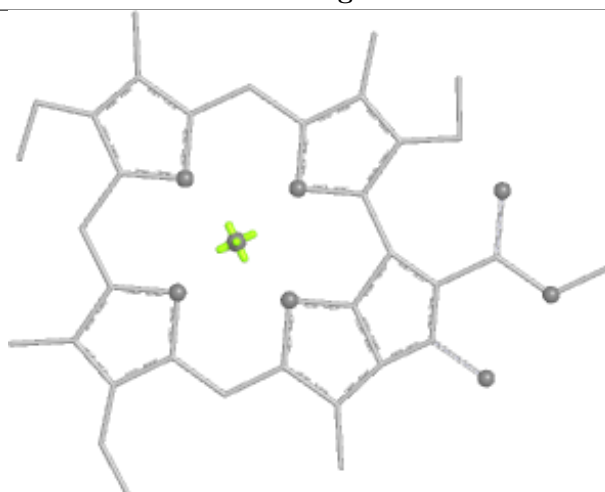
Bond lengths



Bond angles

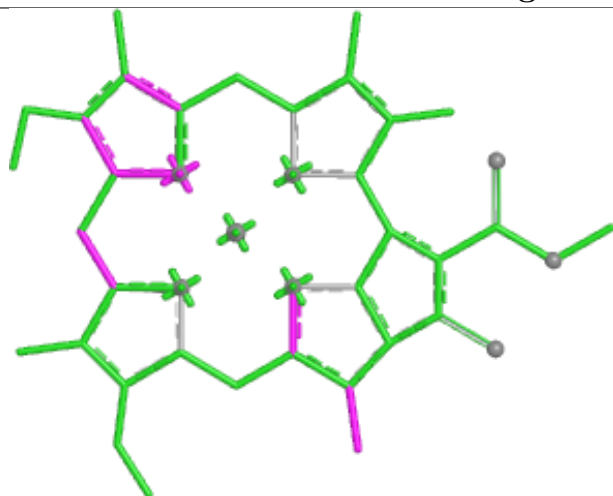


Torsions

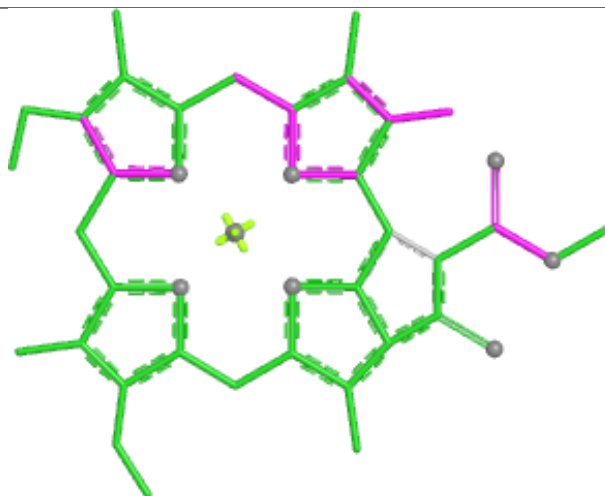


Rings

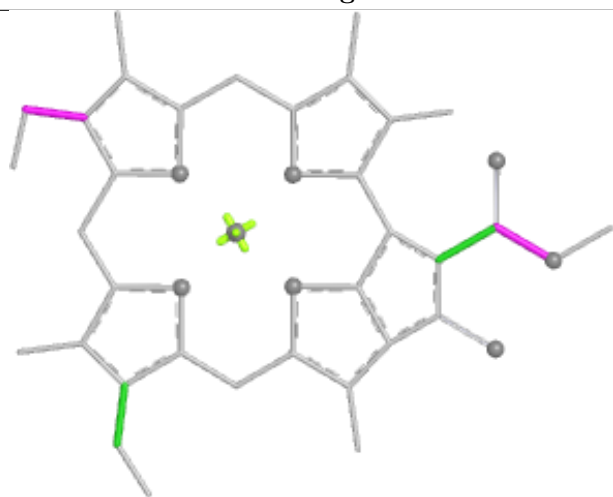
Ligand CLA 5 601



Bond lengths



Bond angles

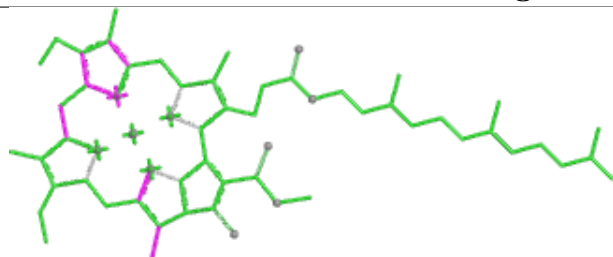


Torsions

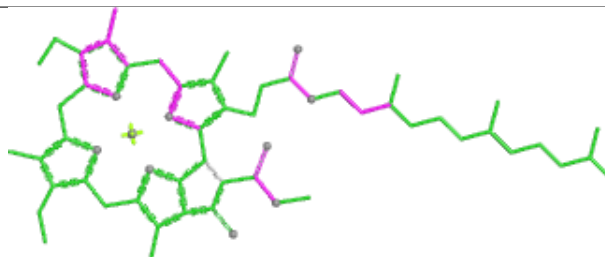


Rings

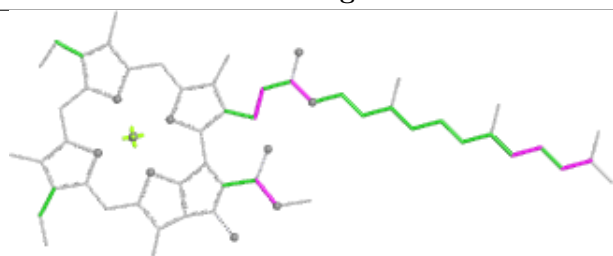
Ligand CLA B 821



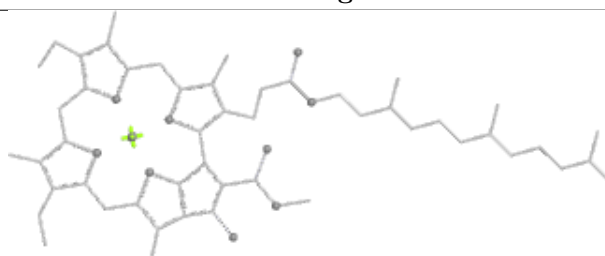
Bond lengths



Bond angles

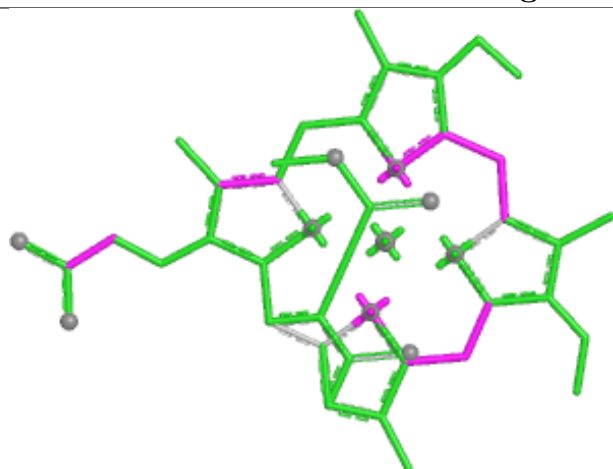


Torsions

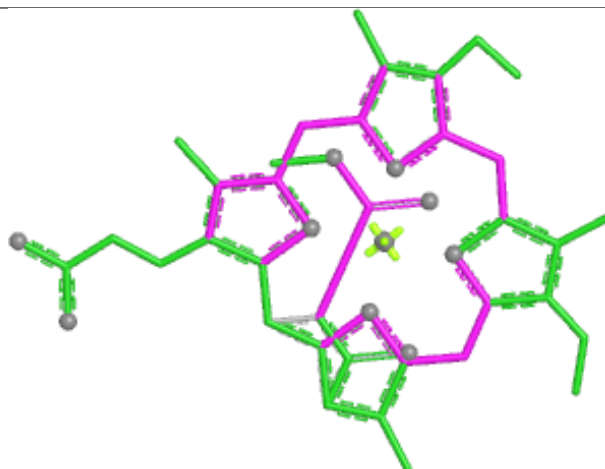


Rings

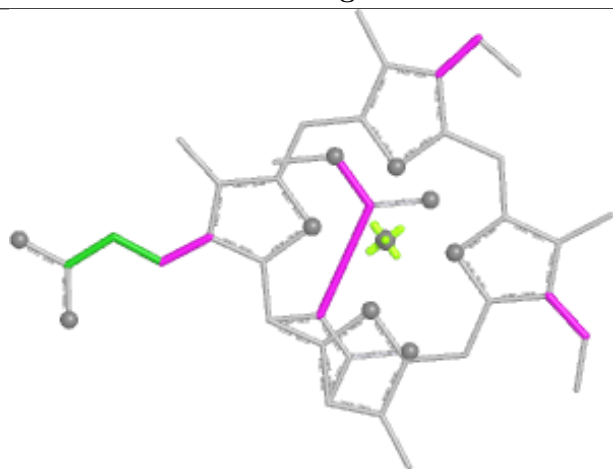
Ligand KC2 3 307



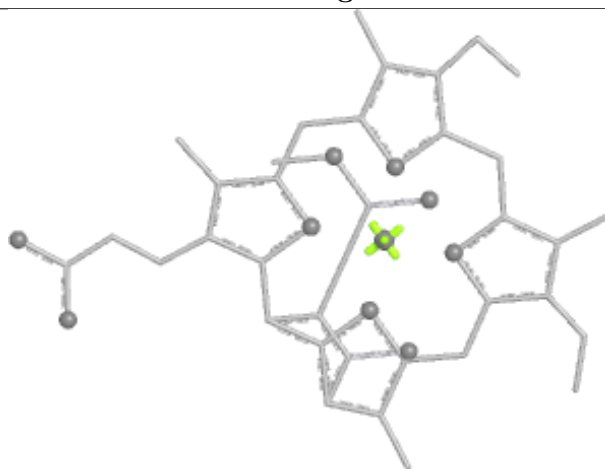
Bond lengths



Bond angles

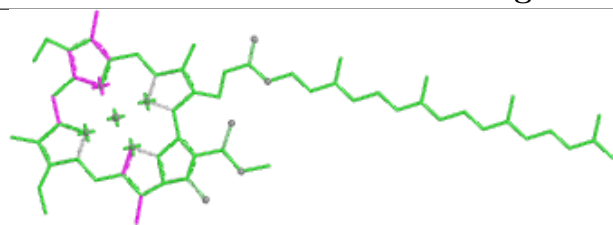


Torsions

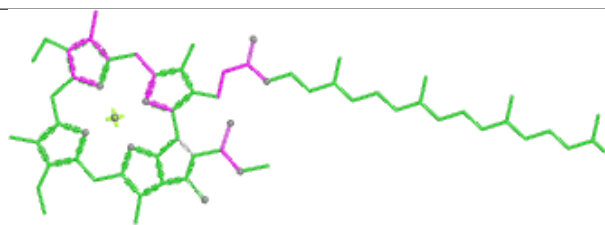


Rings

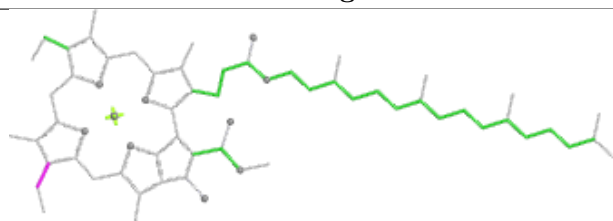
Ligand CLA B 841



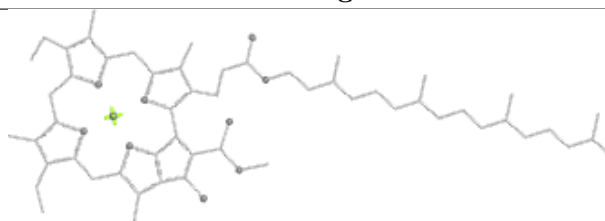
Bond lengths



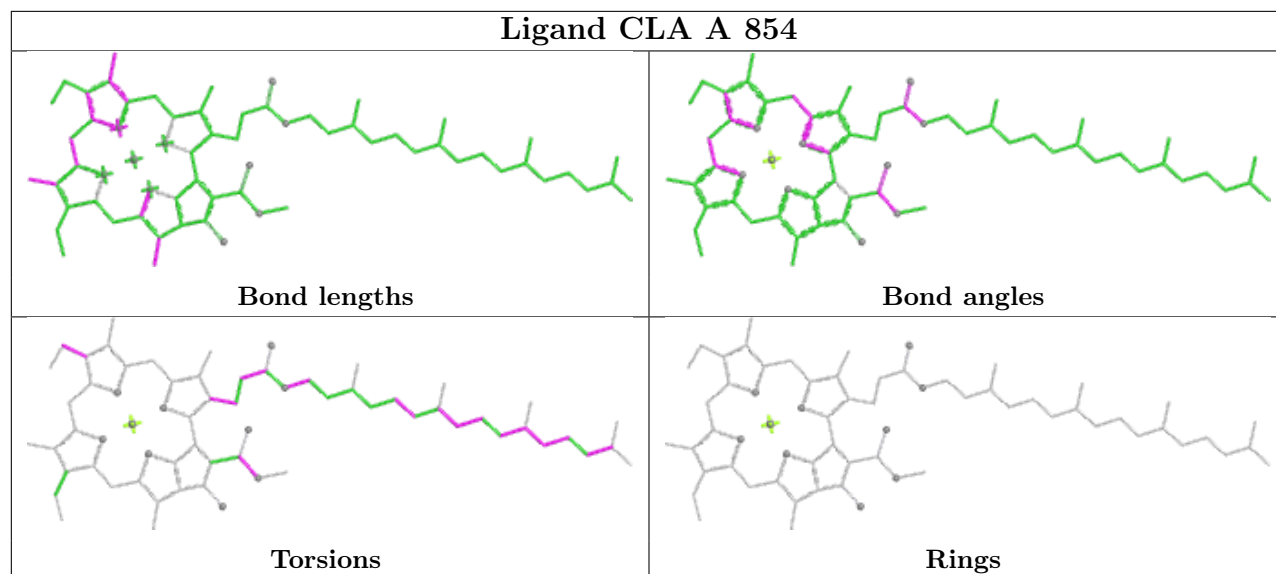
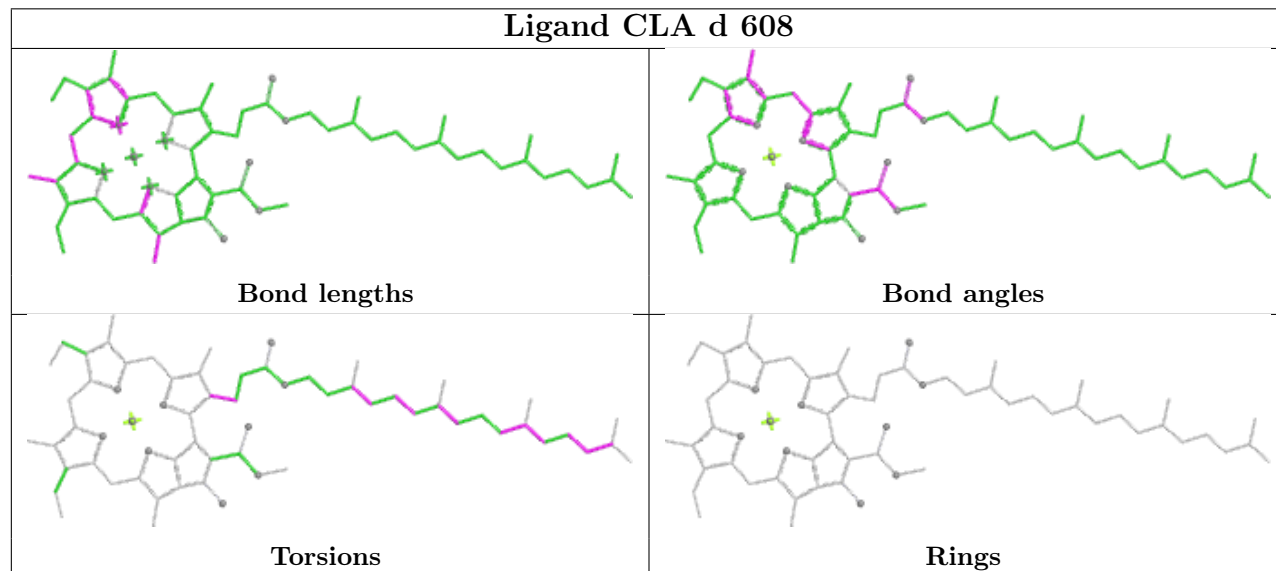
Bond angles



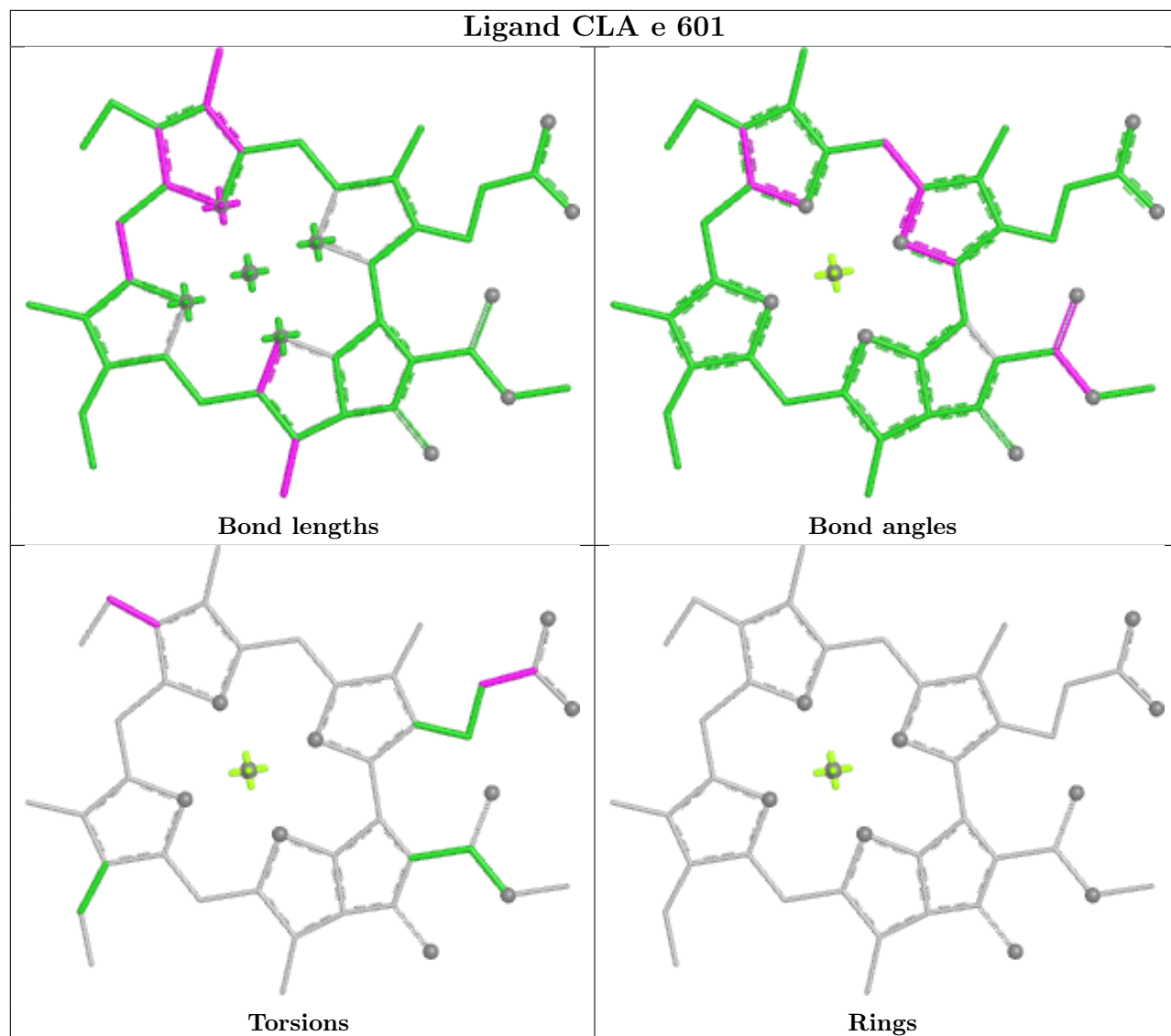
Torsions

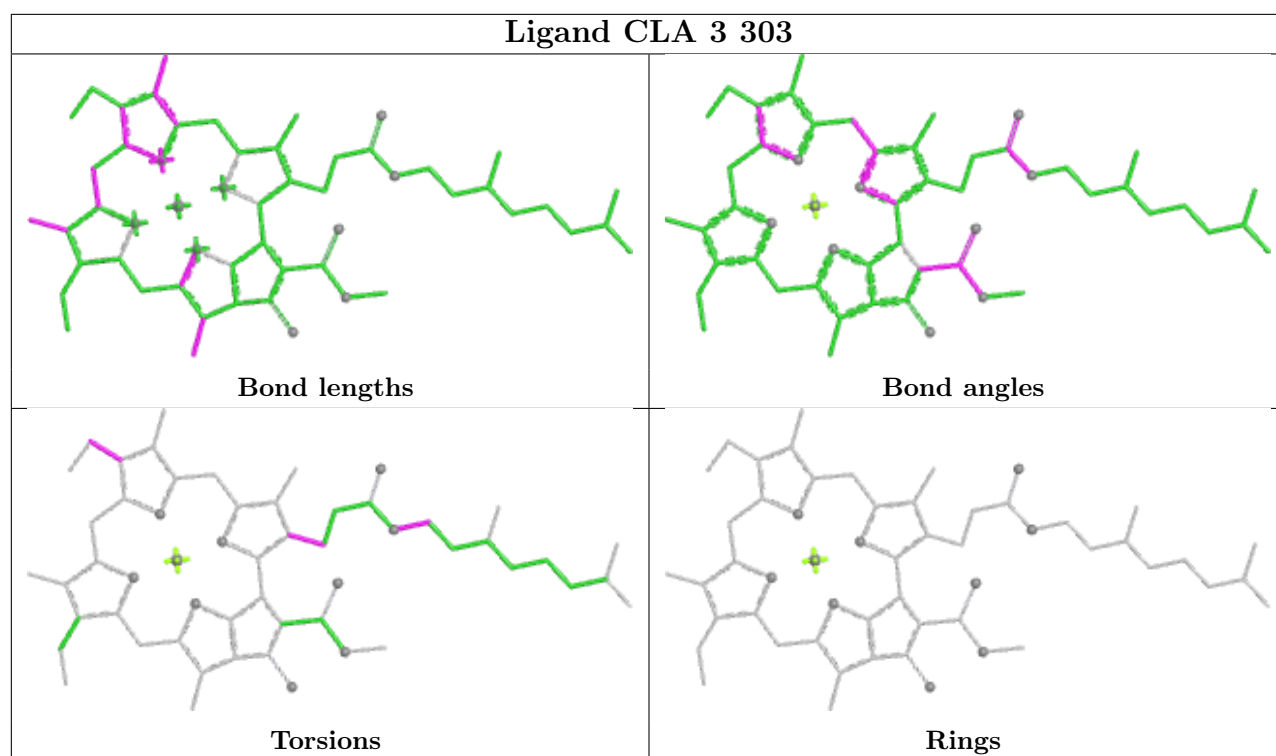


Rings

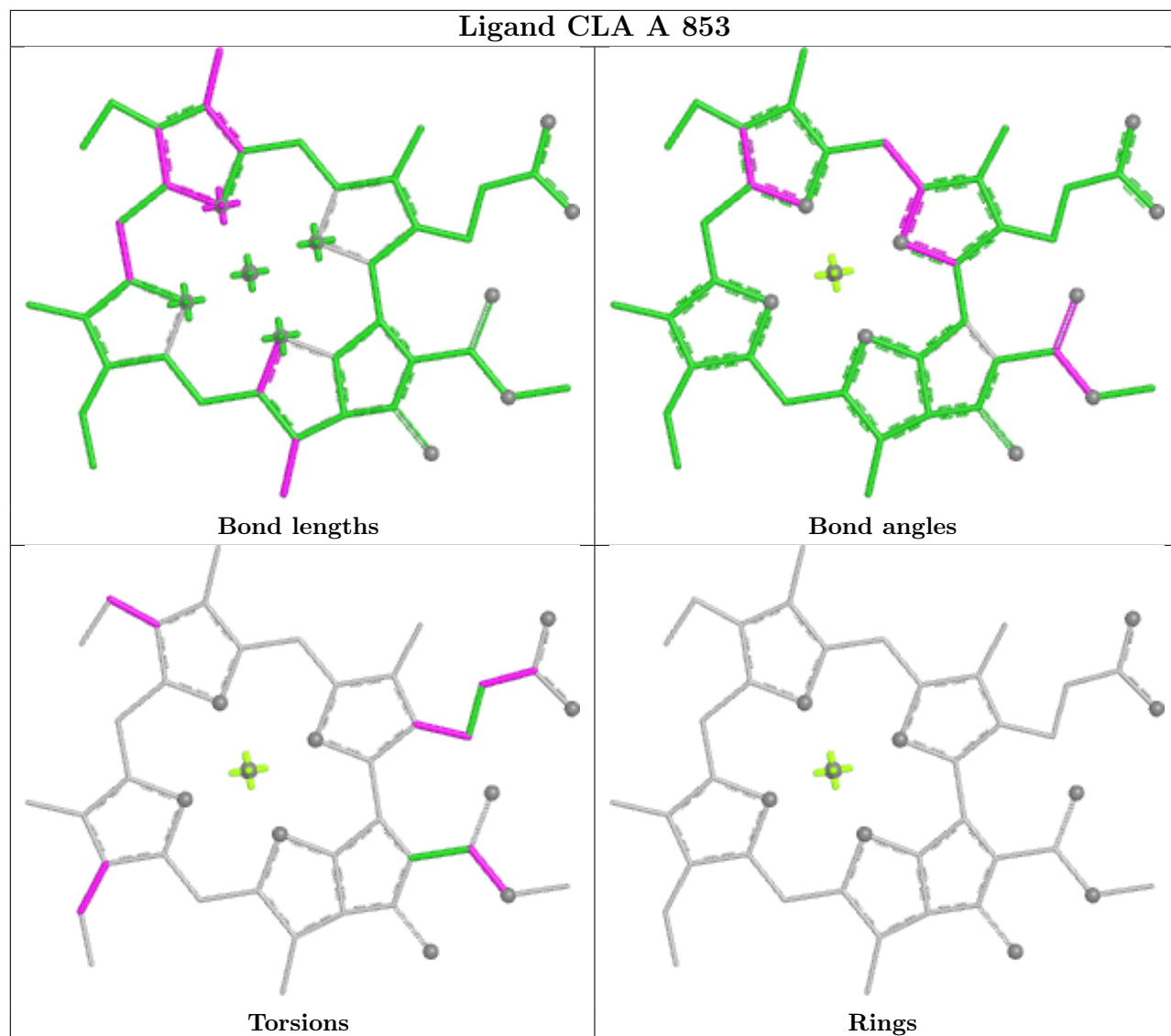
Ligand CLA A 854**Ligand CLA d 608**

Ligand CLA e 601

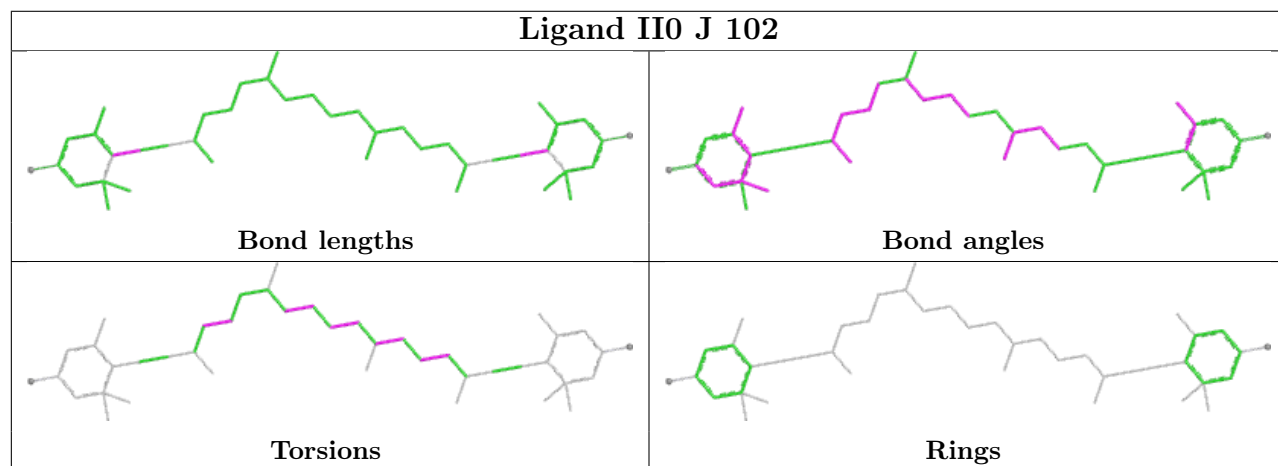


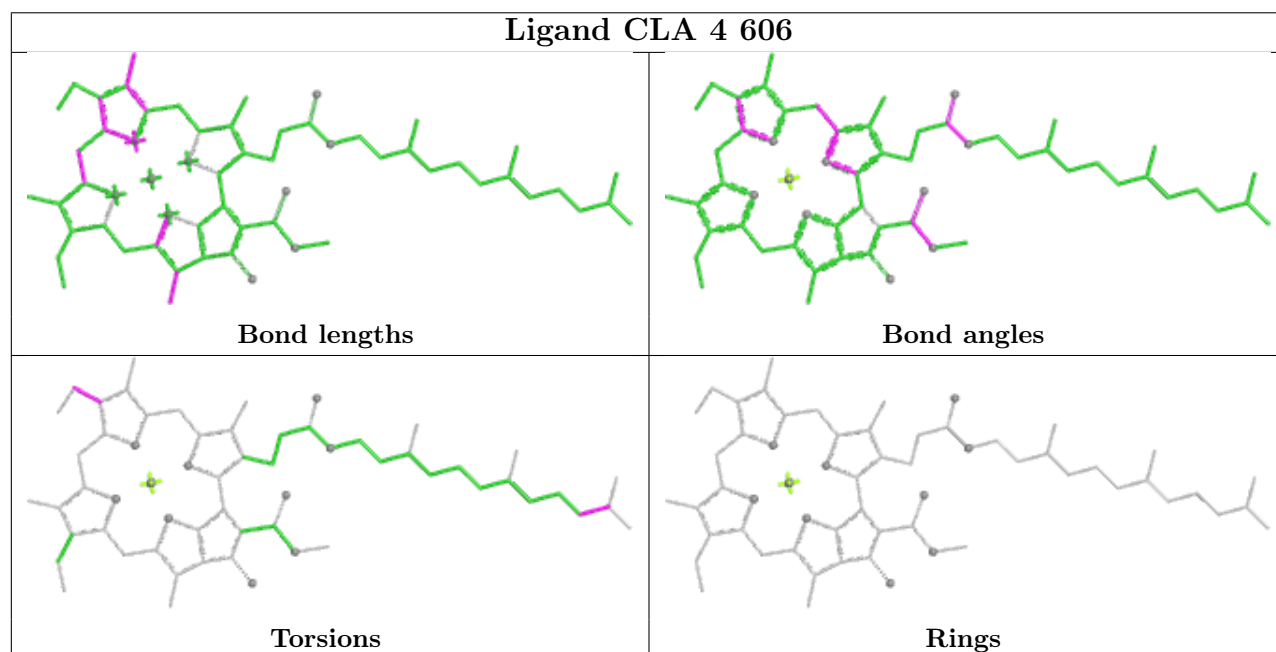
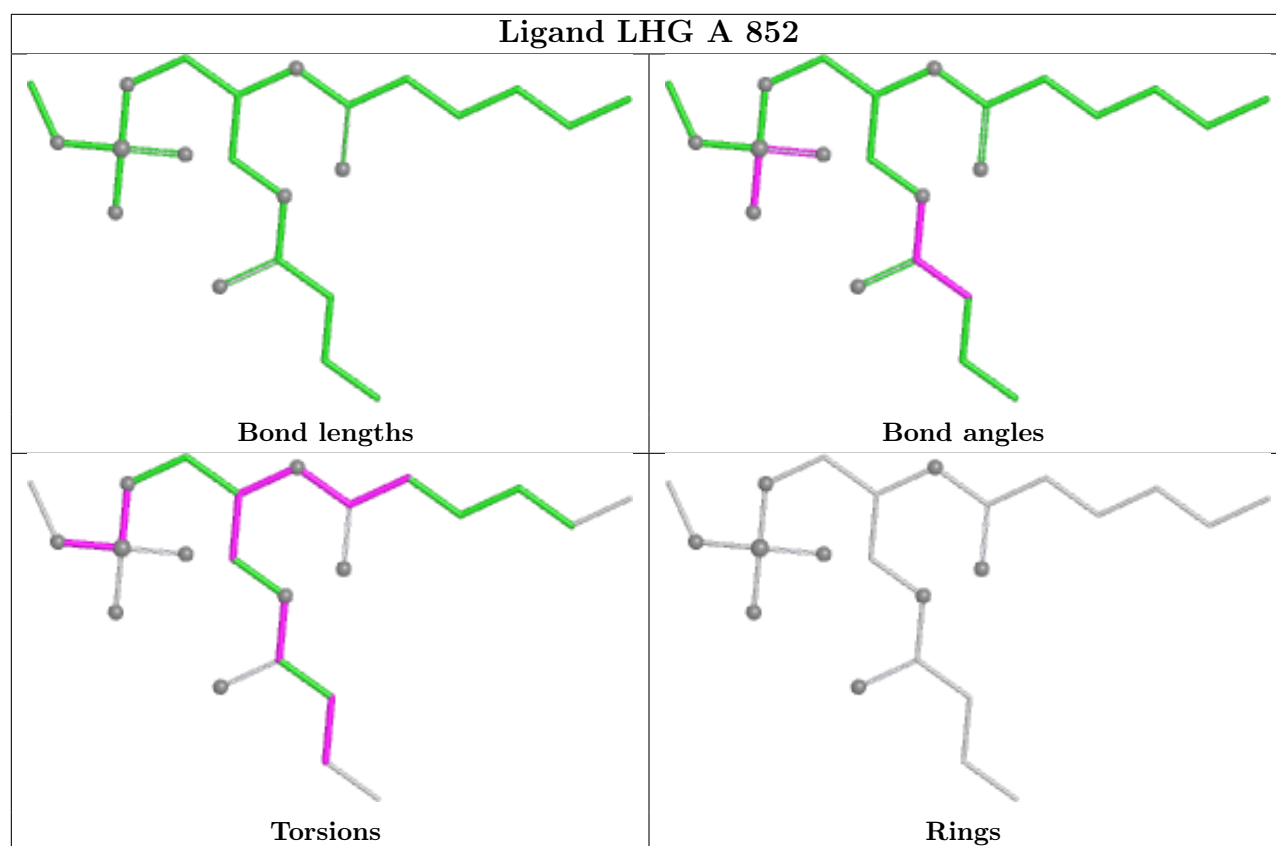


Ligand CLA A 853

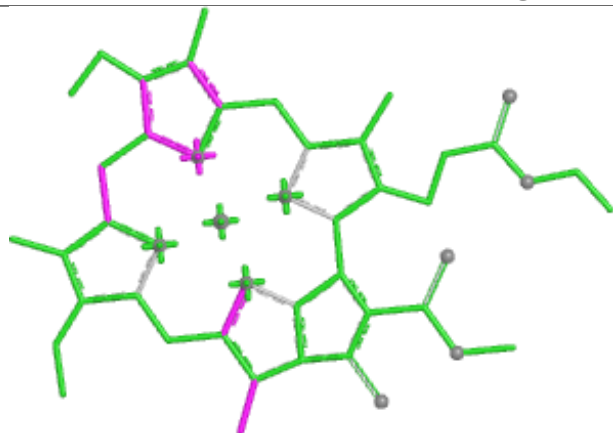


Ligand II0 J 102

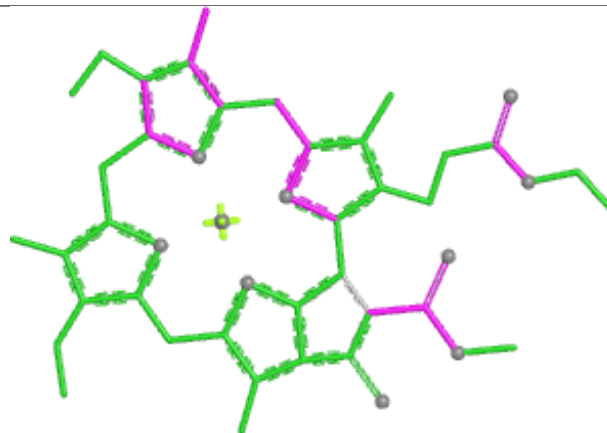




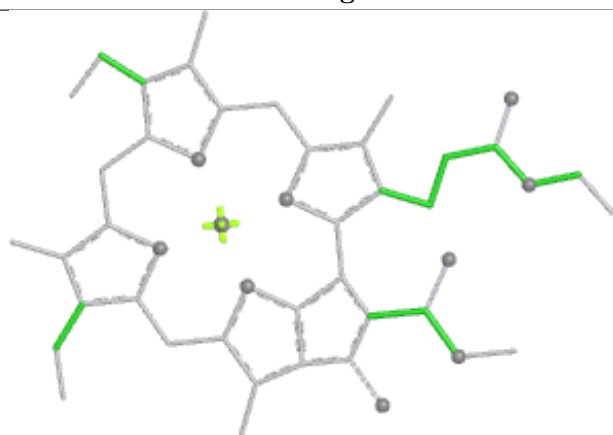
Ligand CLA B 837



Bond lengths



Bond angles

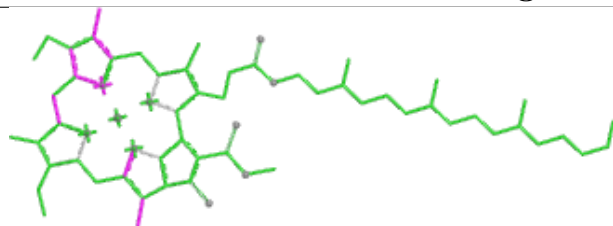


Torsions

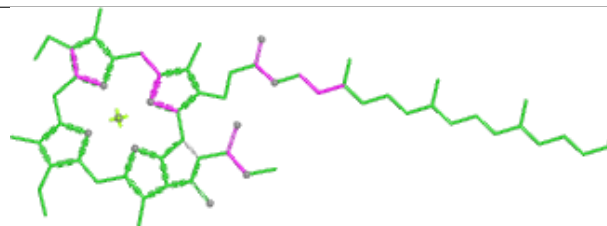


Rings

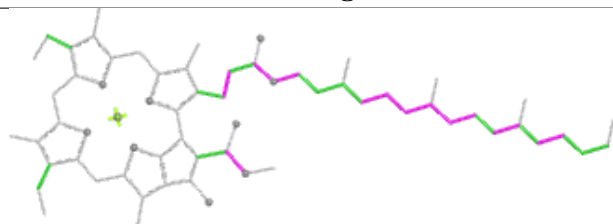
Ligand CLA d 602



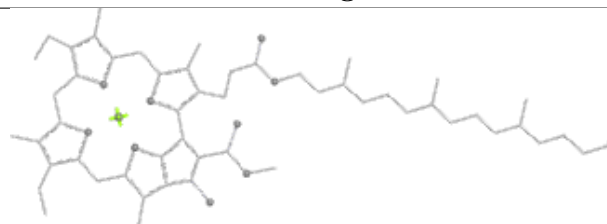
Bond lengths



Bond angles

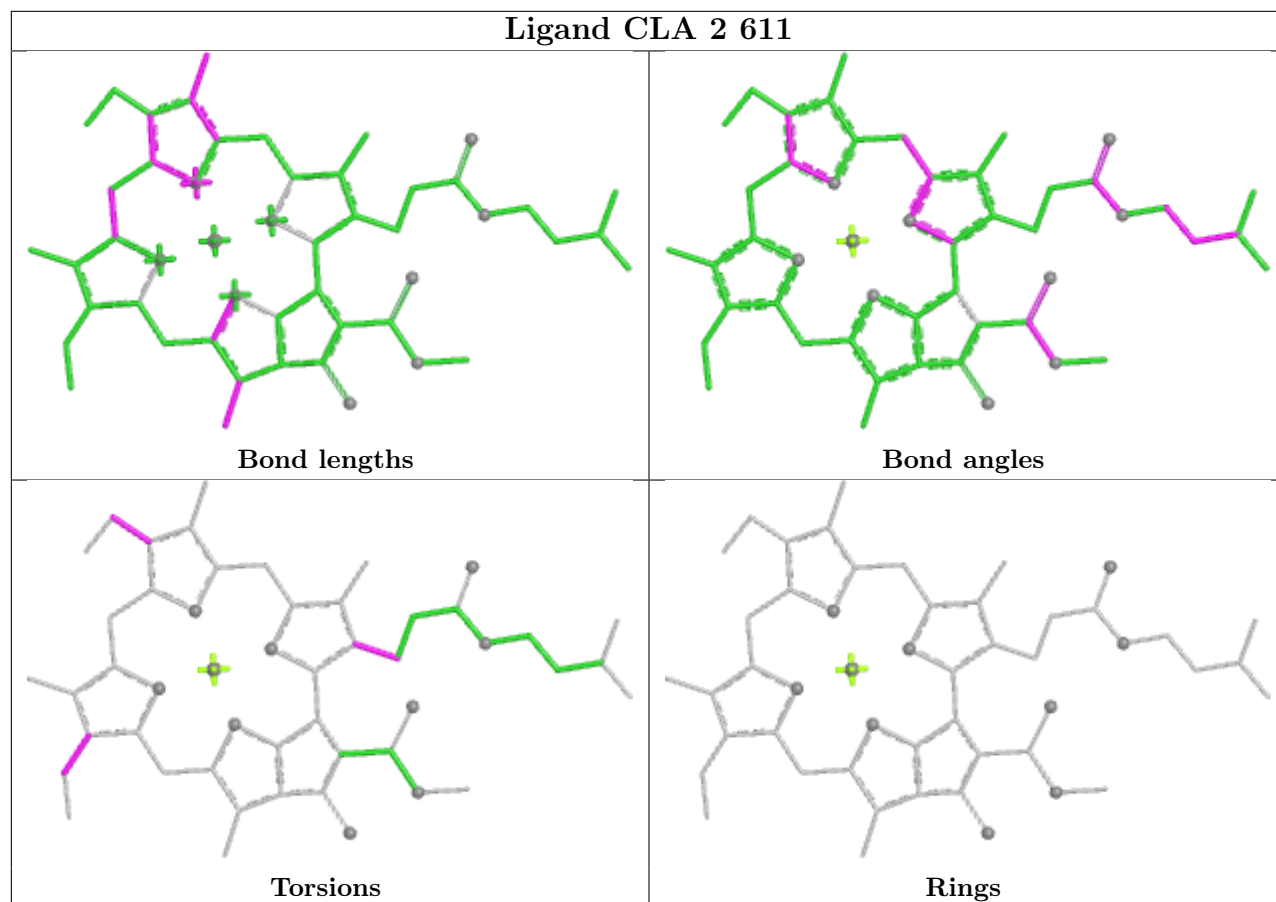


Torsions

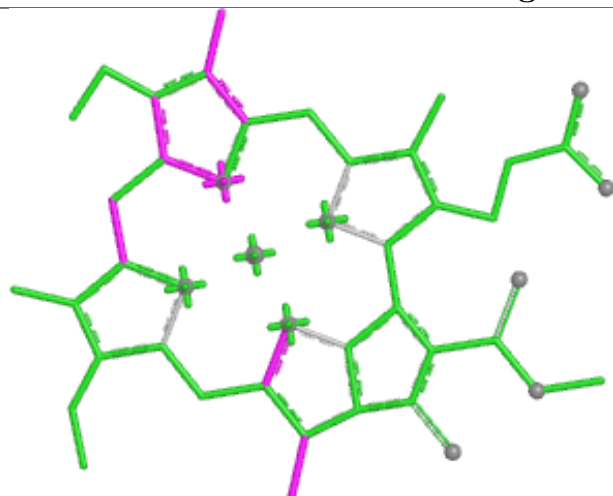


Rings

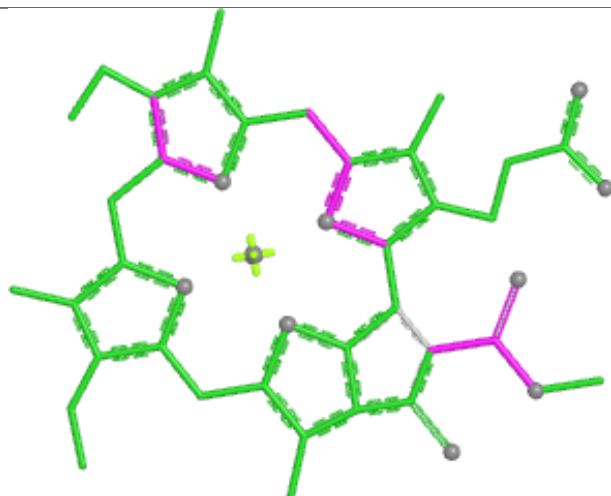
Ligand CLA 2 611



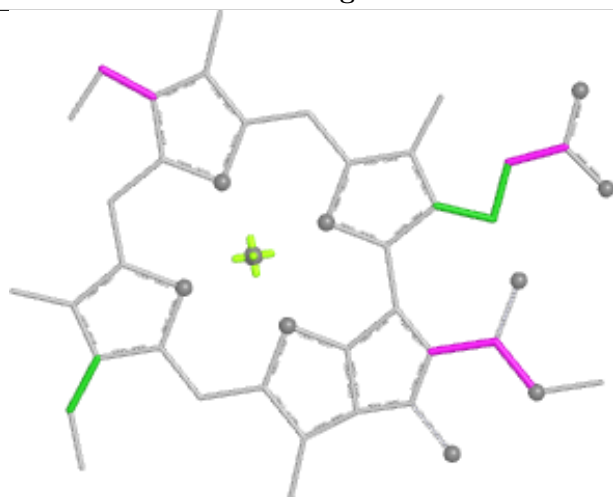
Ligand CLA 5 612



Bond lengths



Bond angles

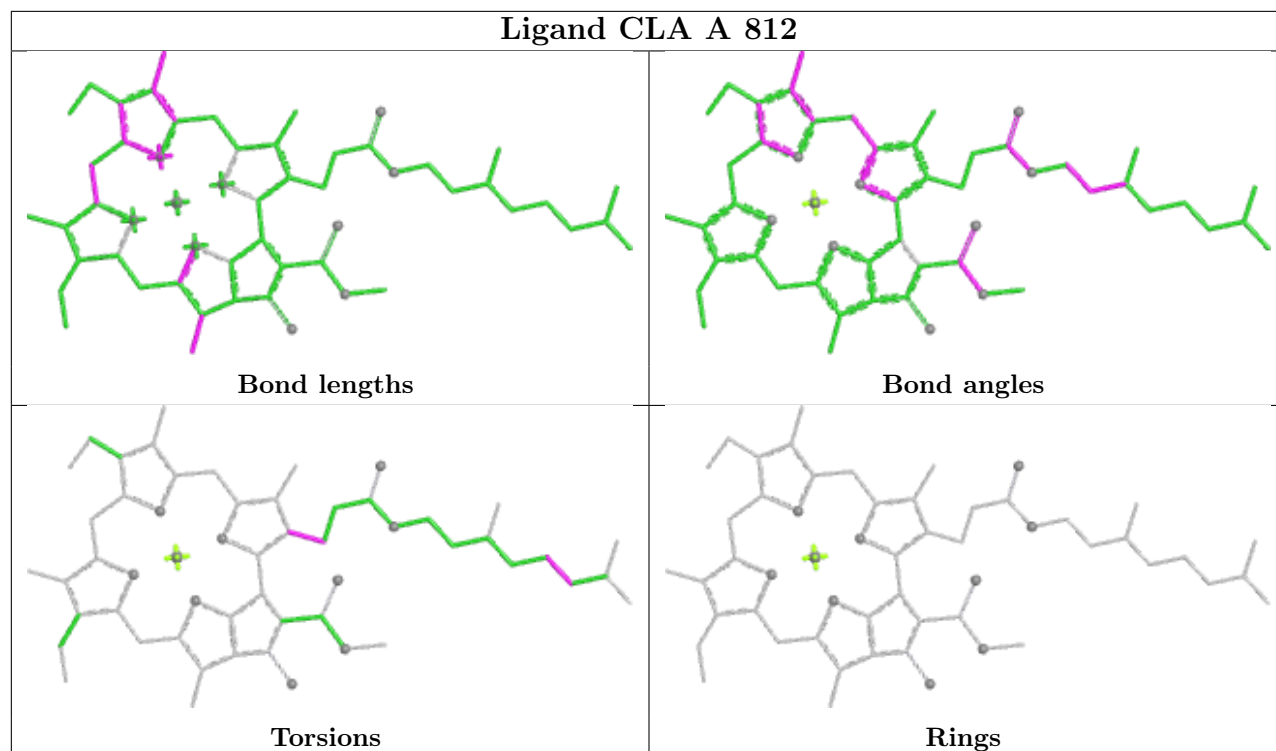


Torsions

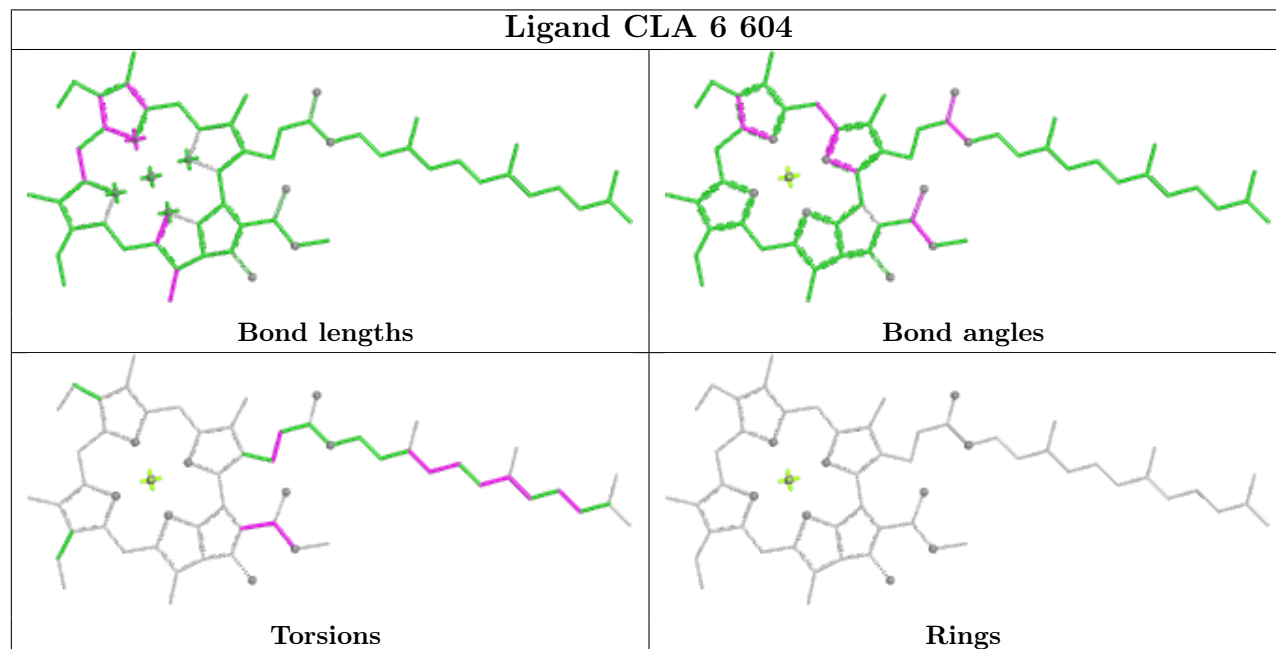


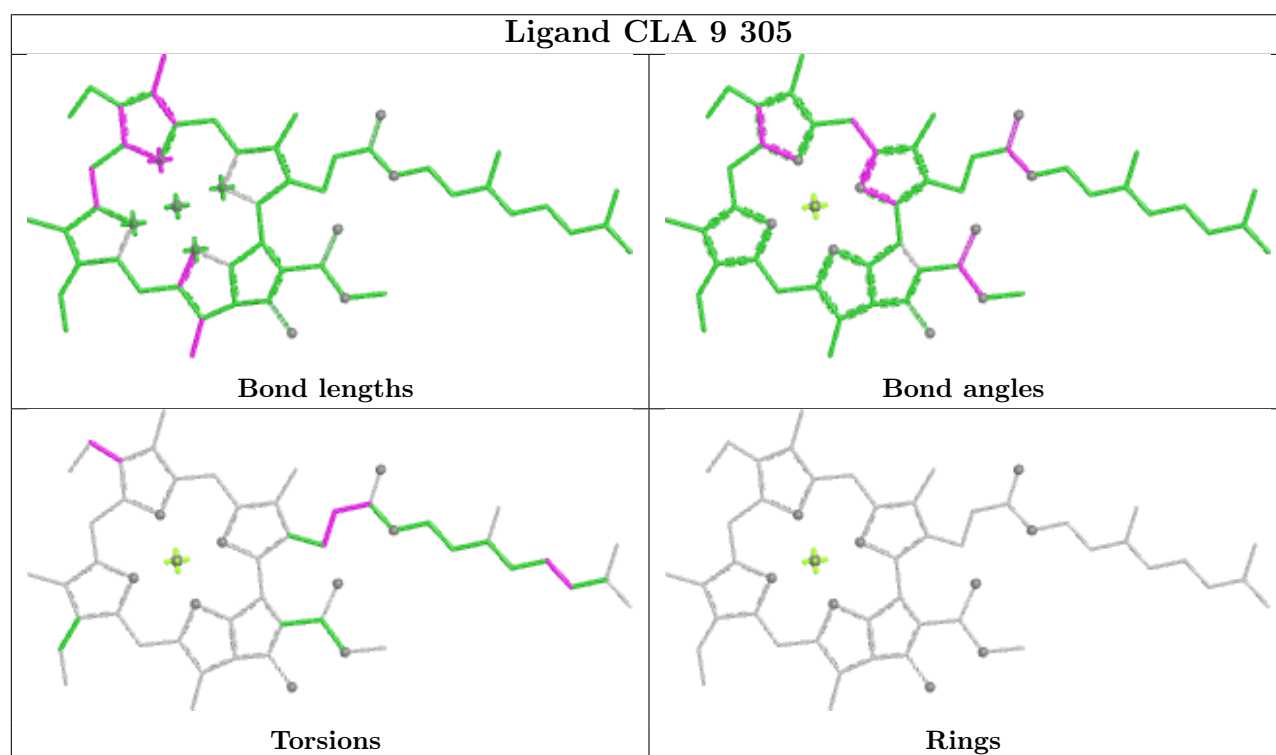
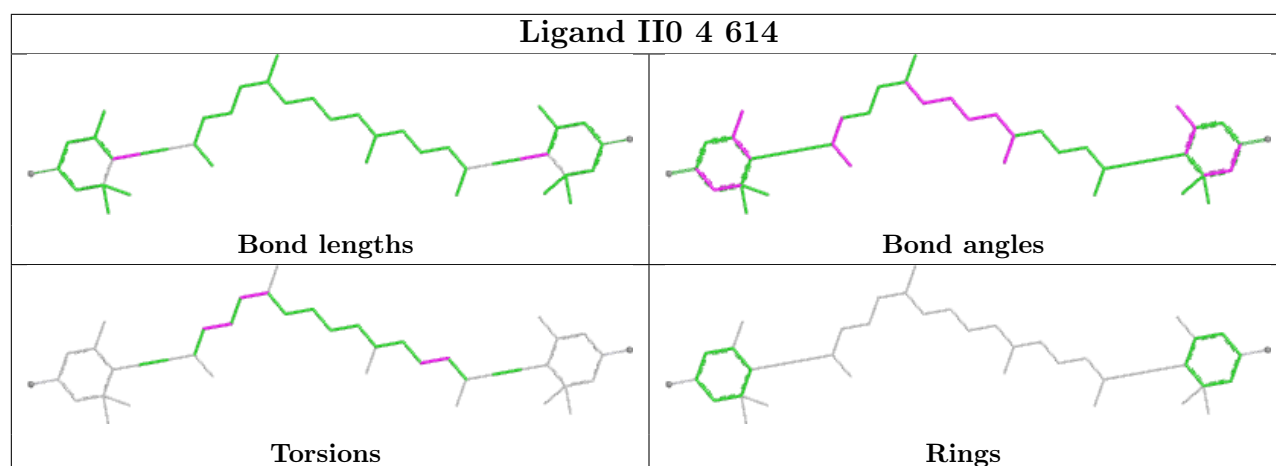
Rings

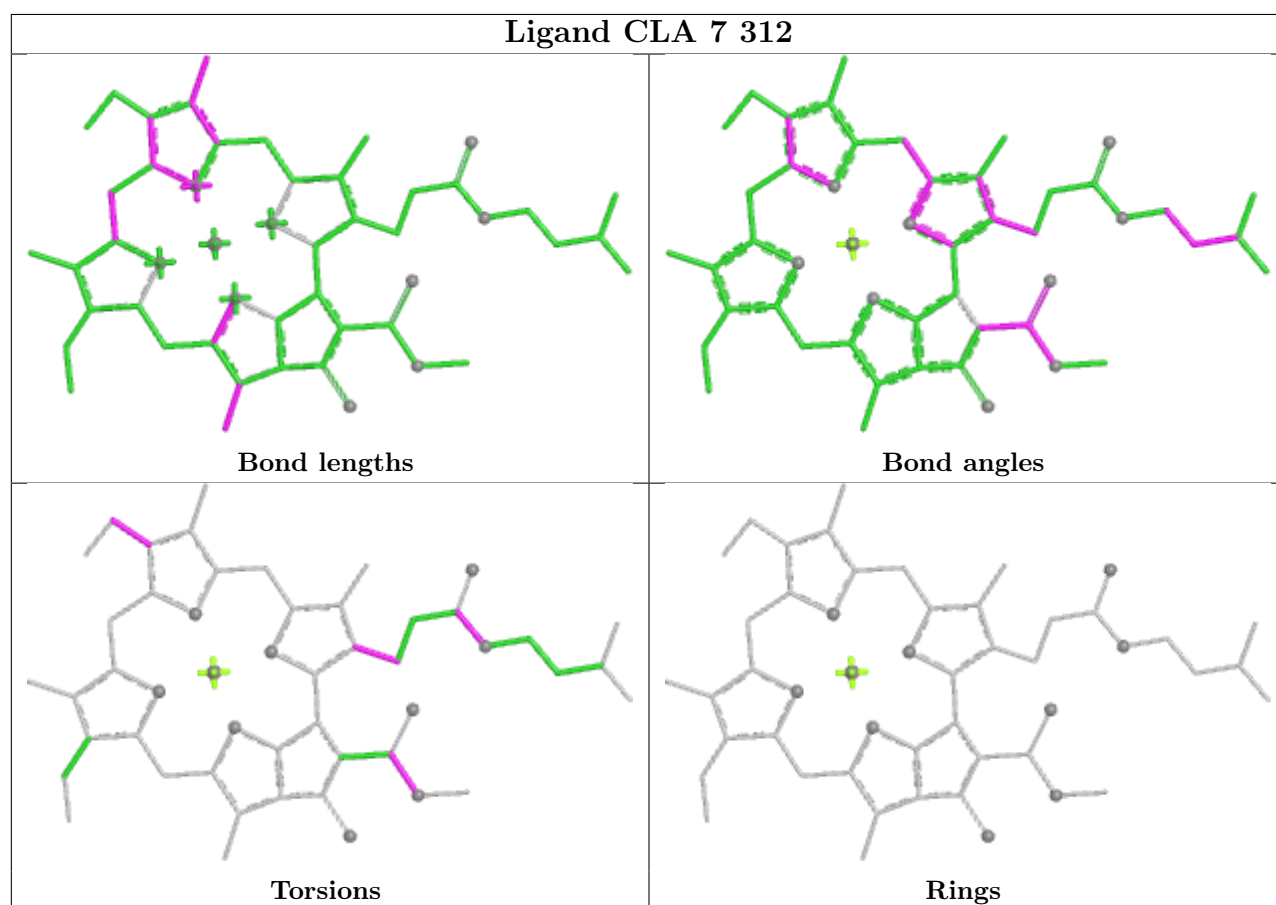
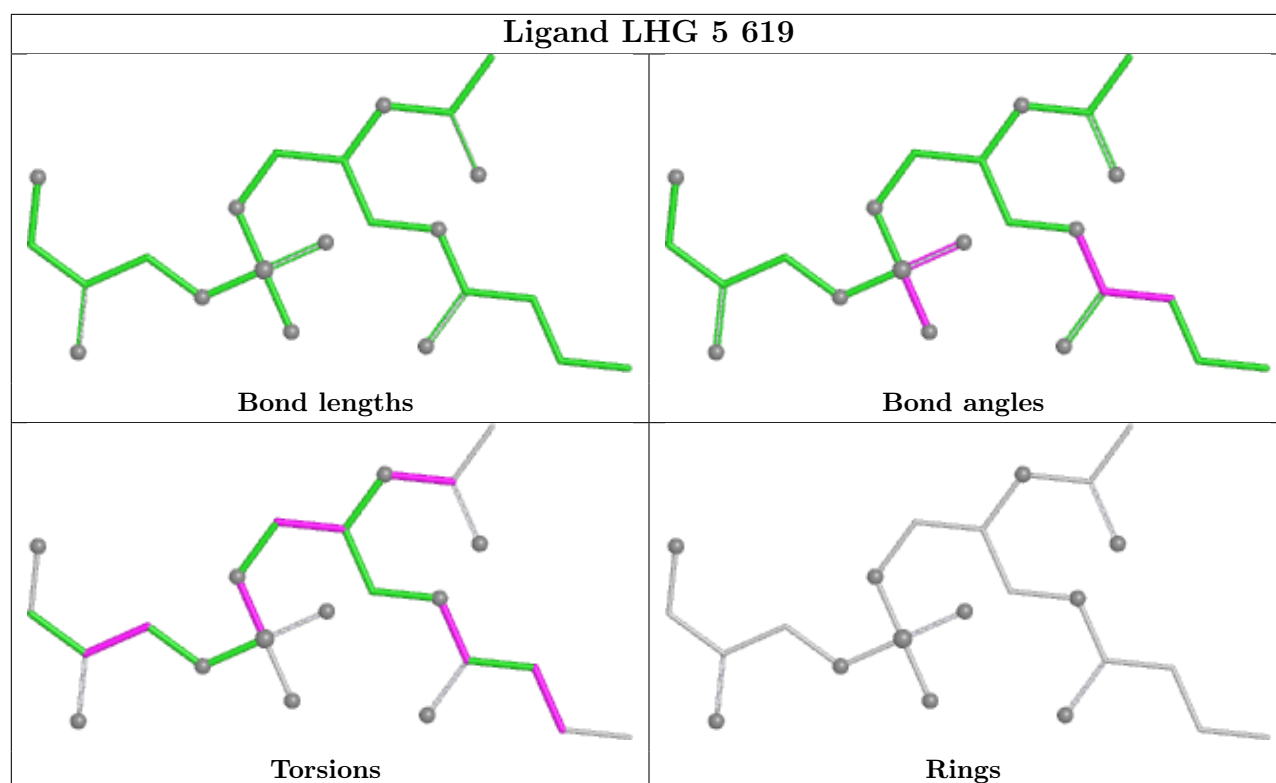
Ligand CLA A 812

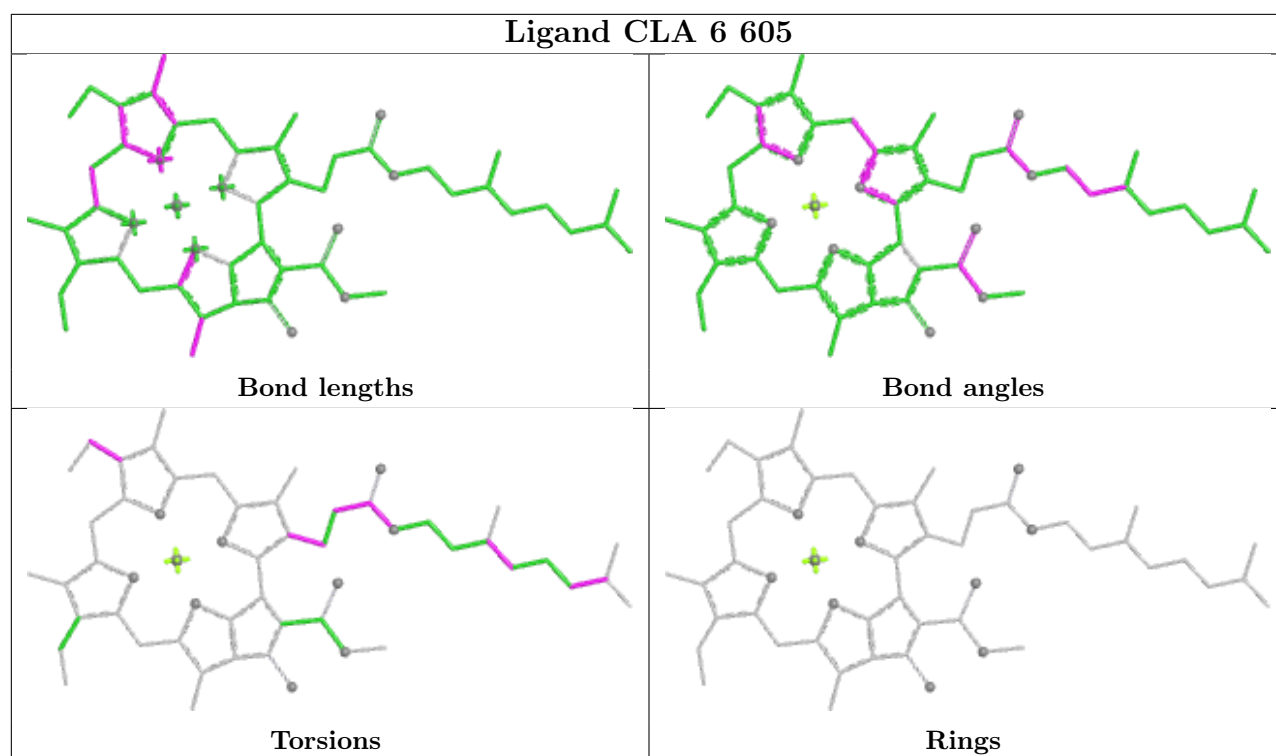


Ligand CLA 6 604

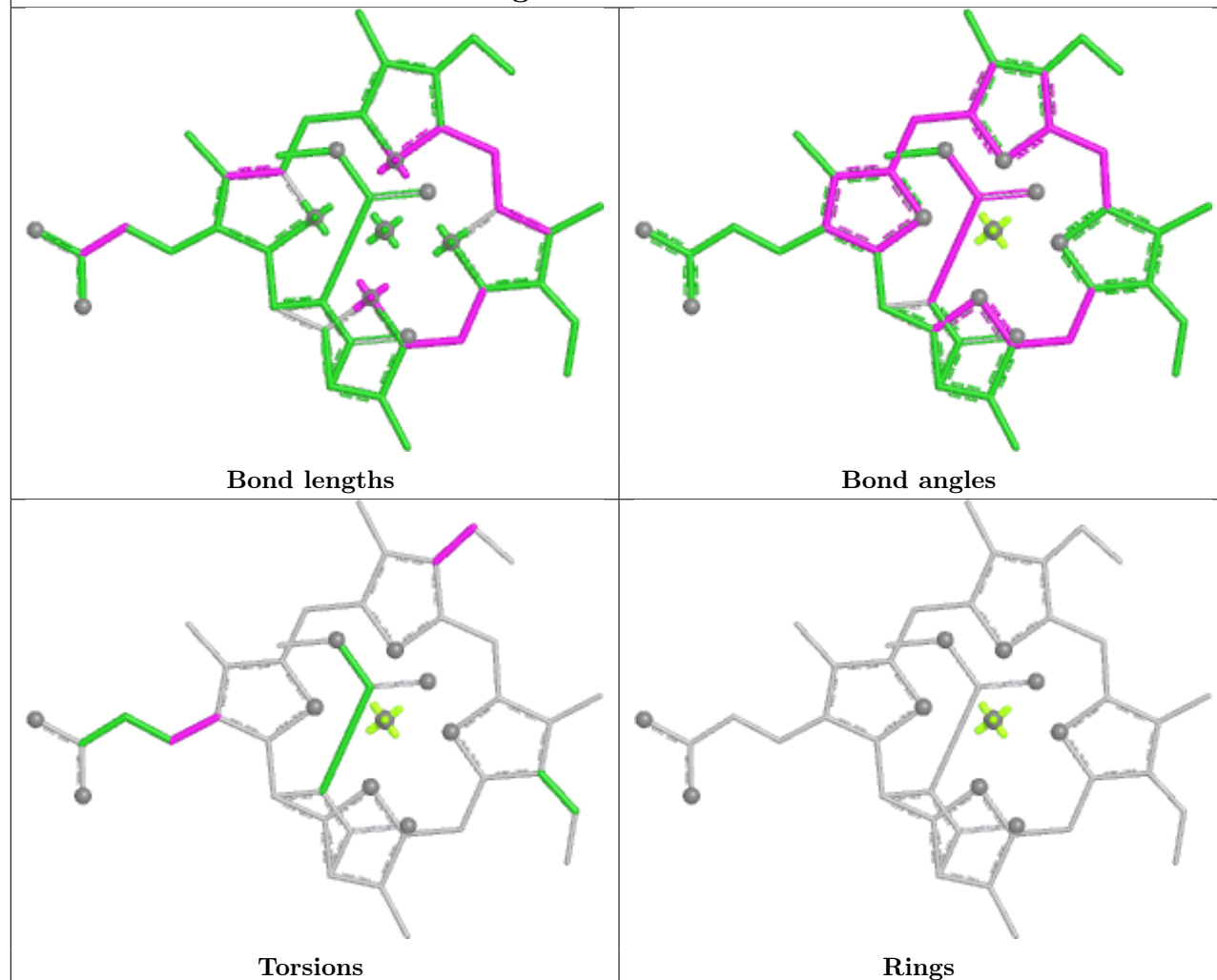




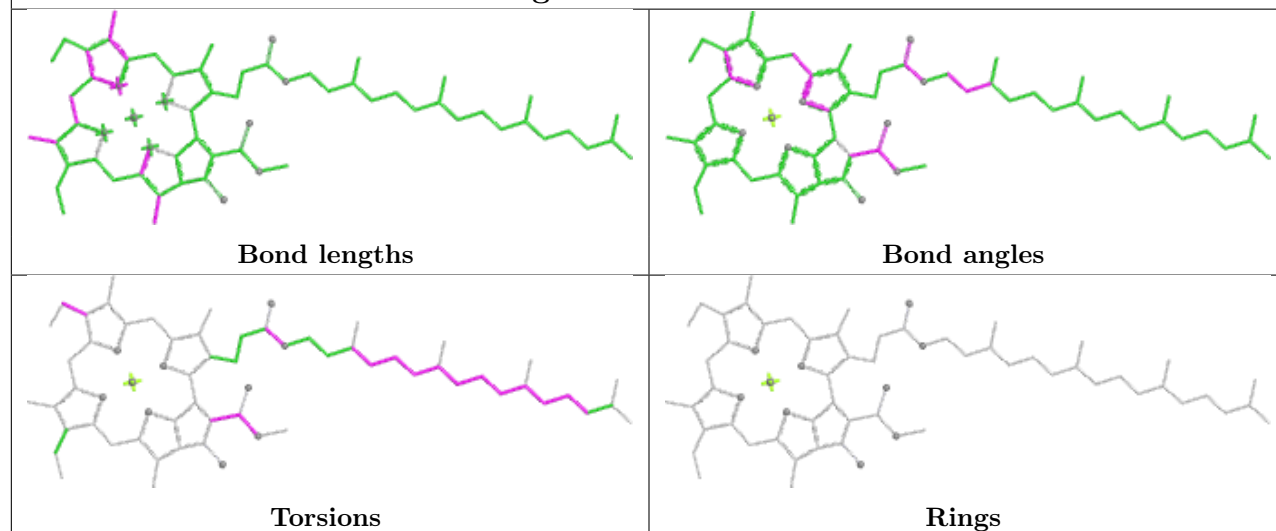


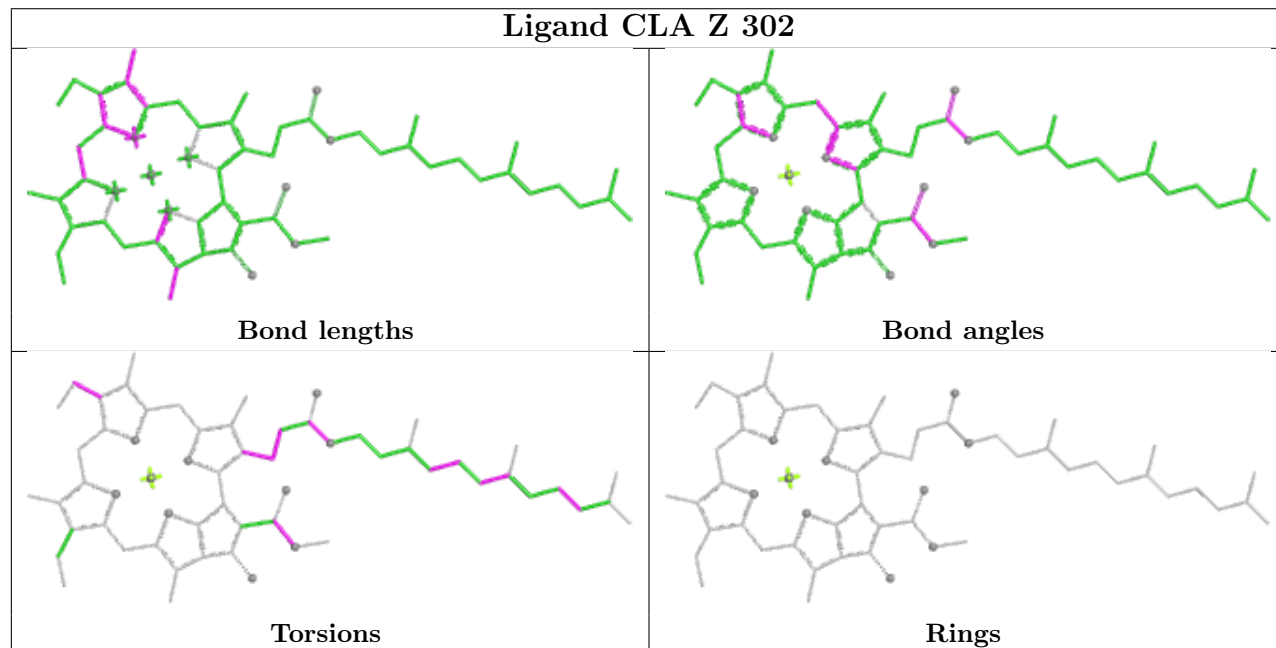
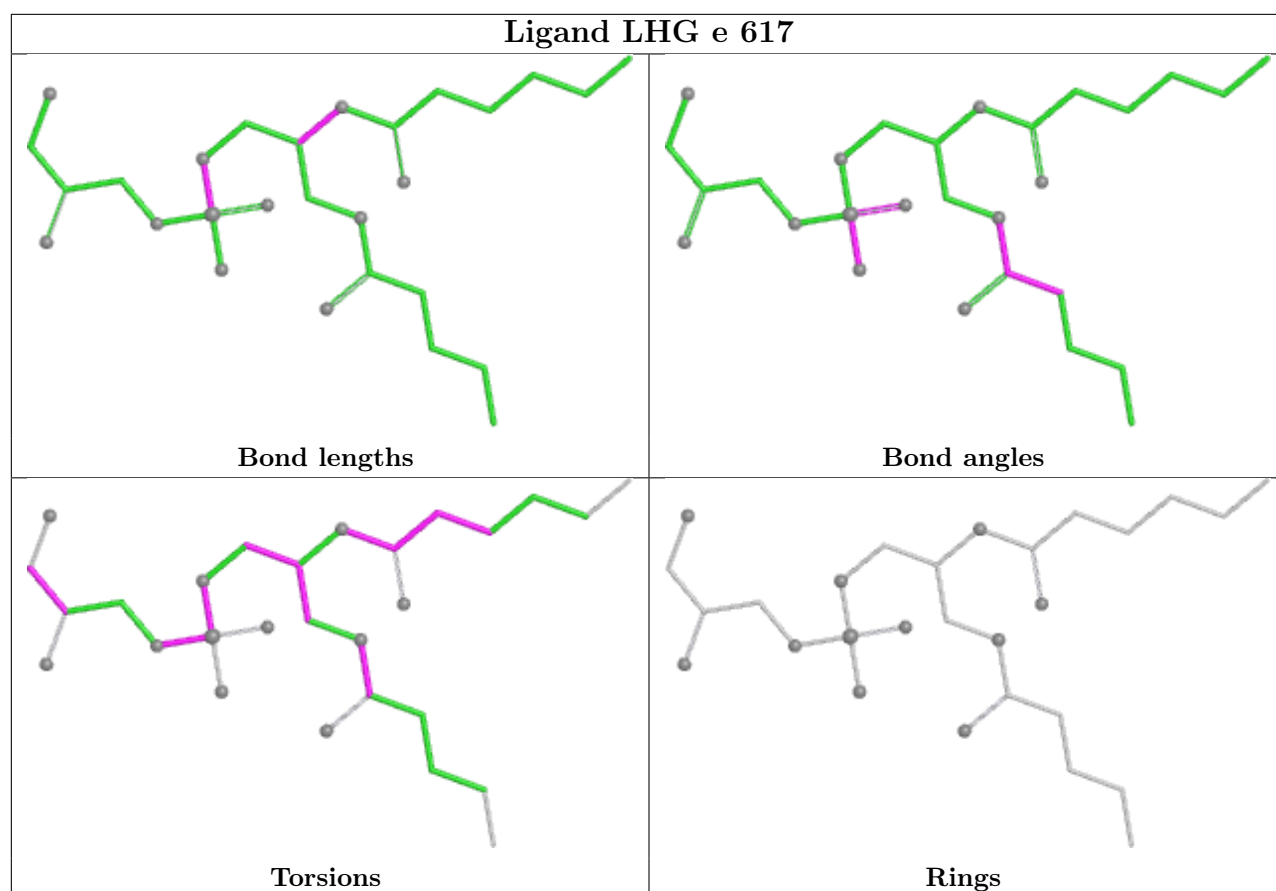


Ligand KC2 b 609

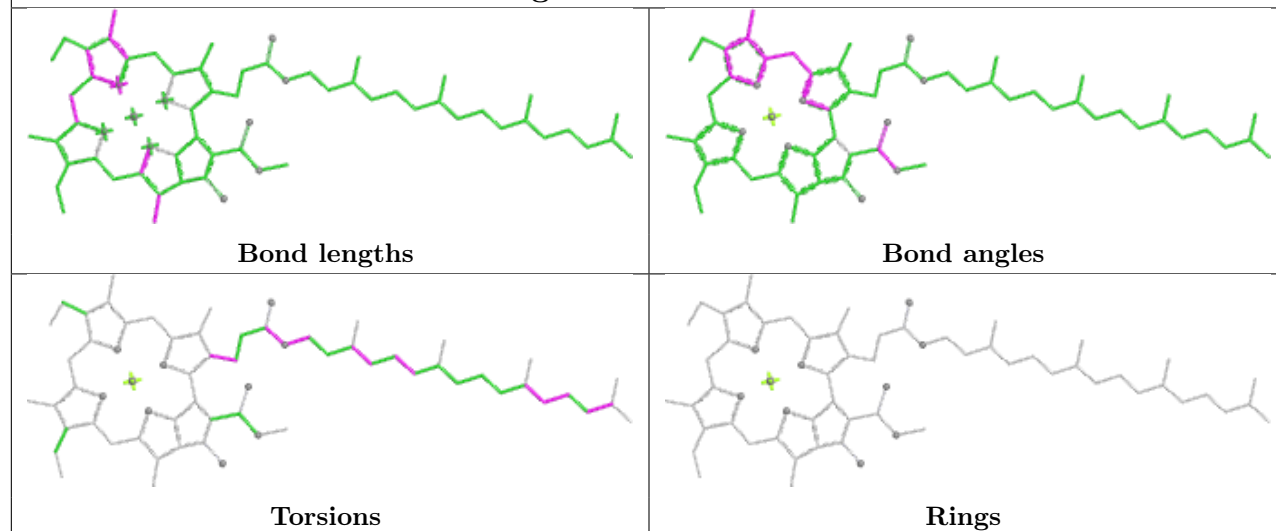


Ligand CLA B 808

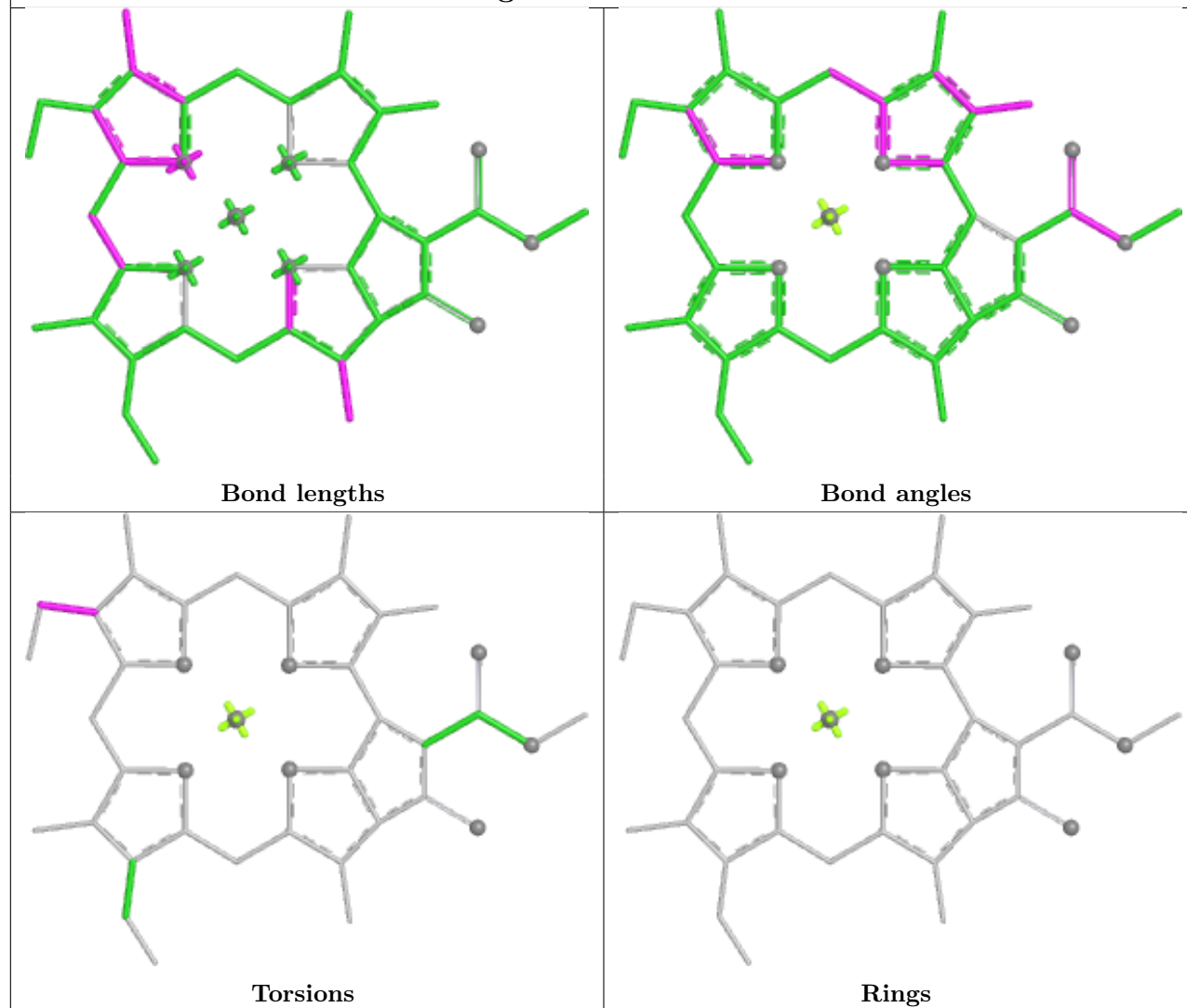


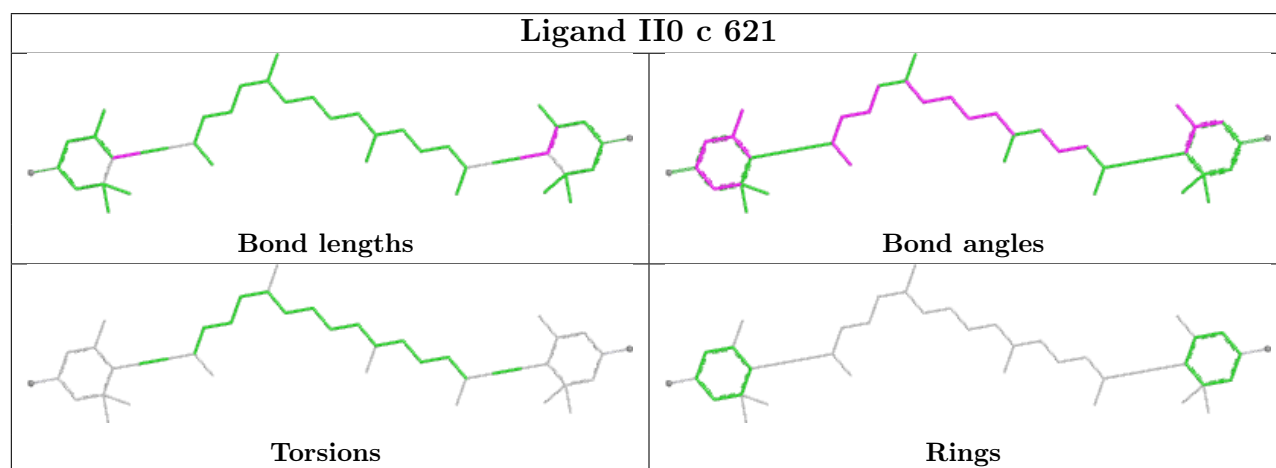
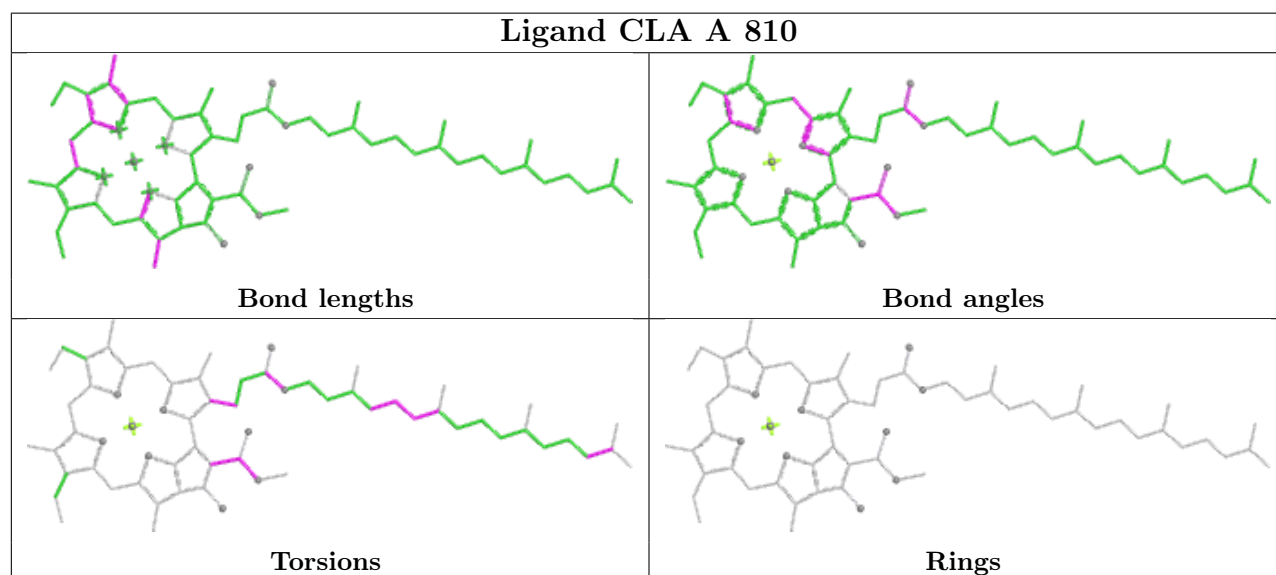
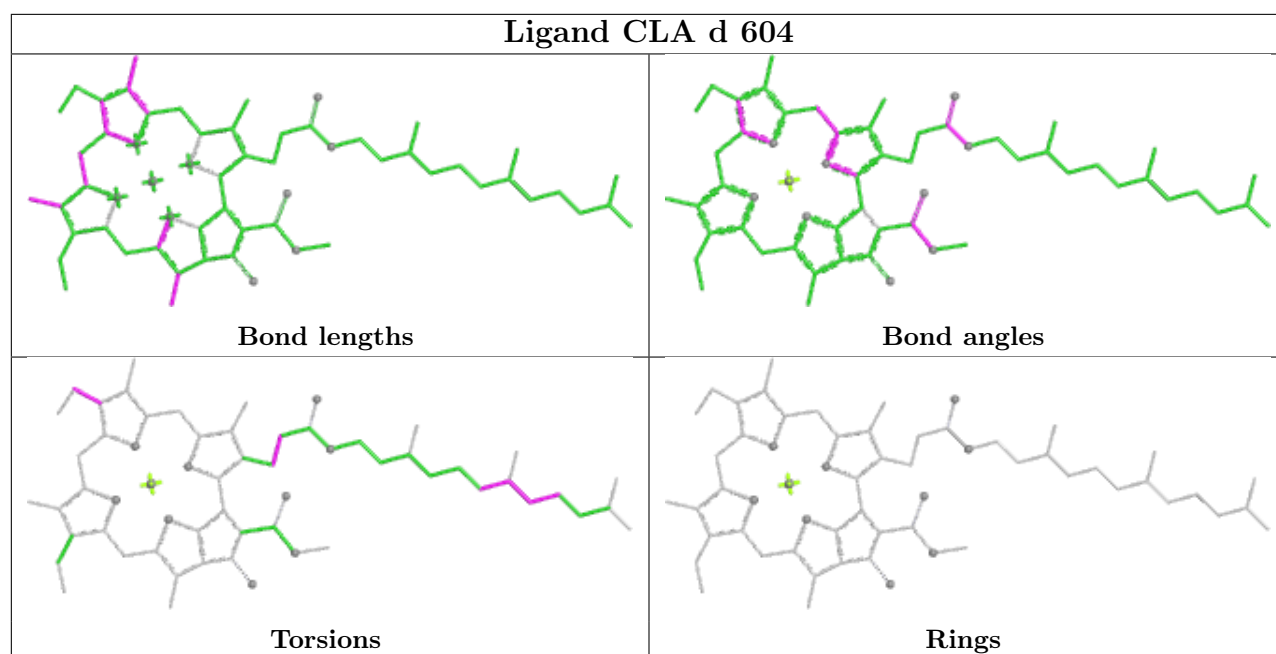


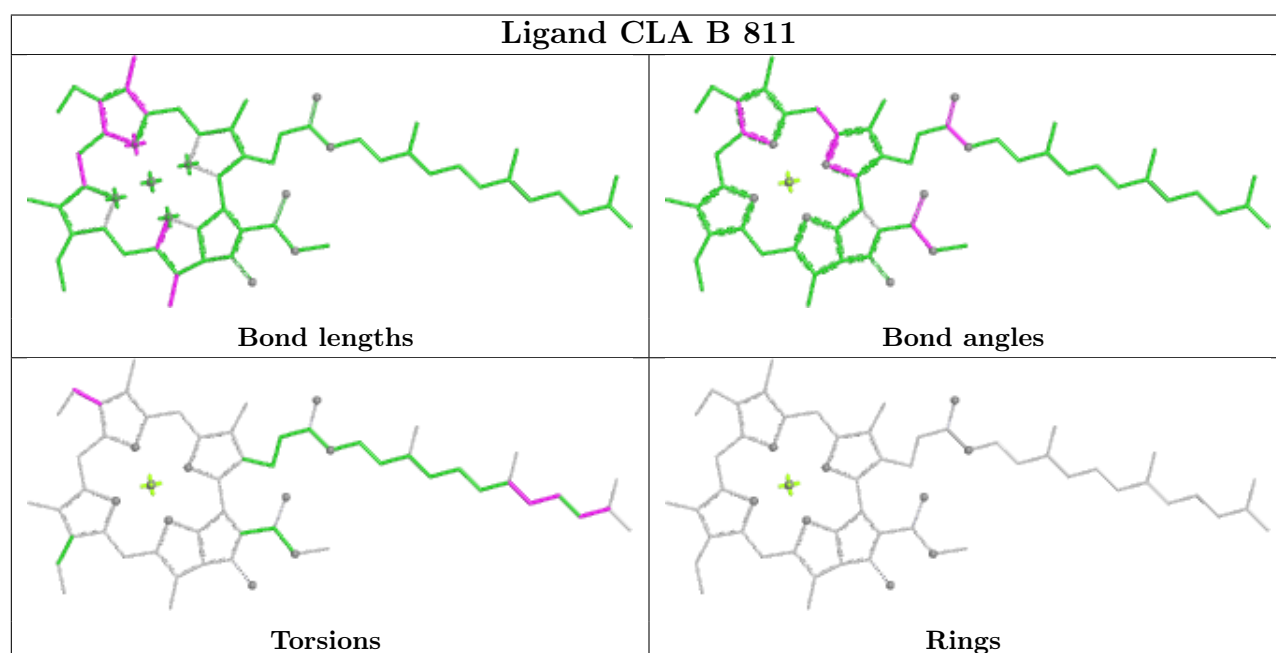
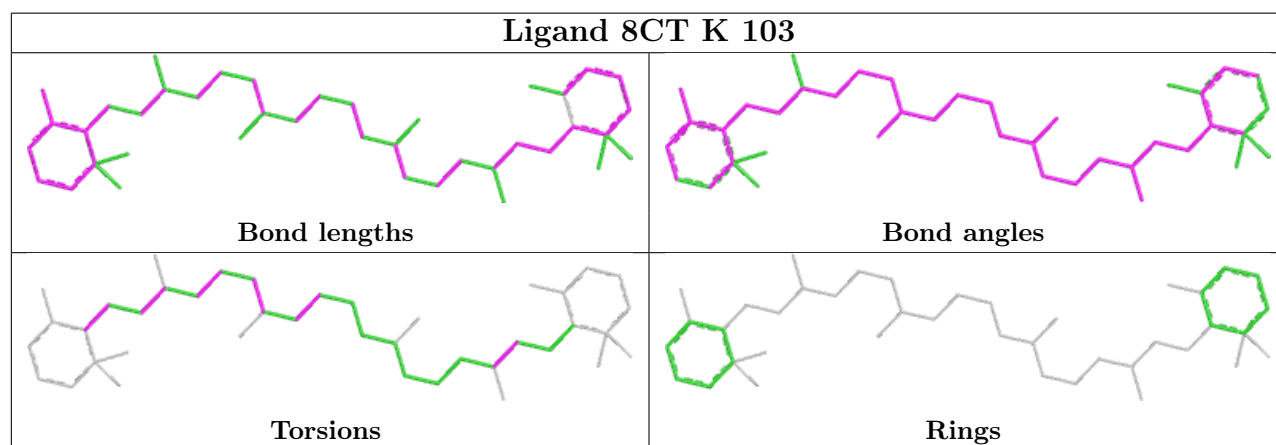
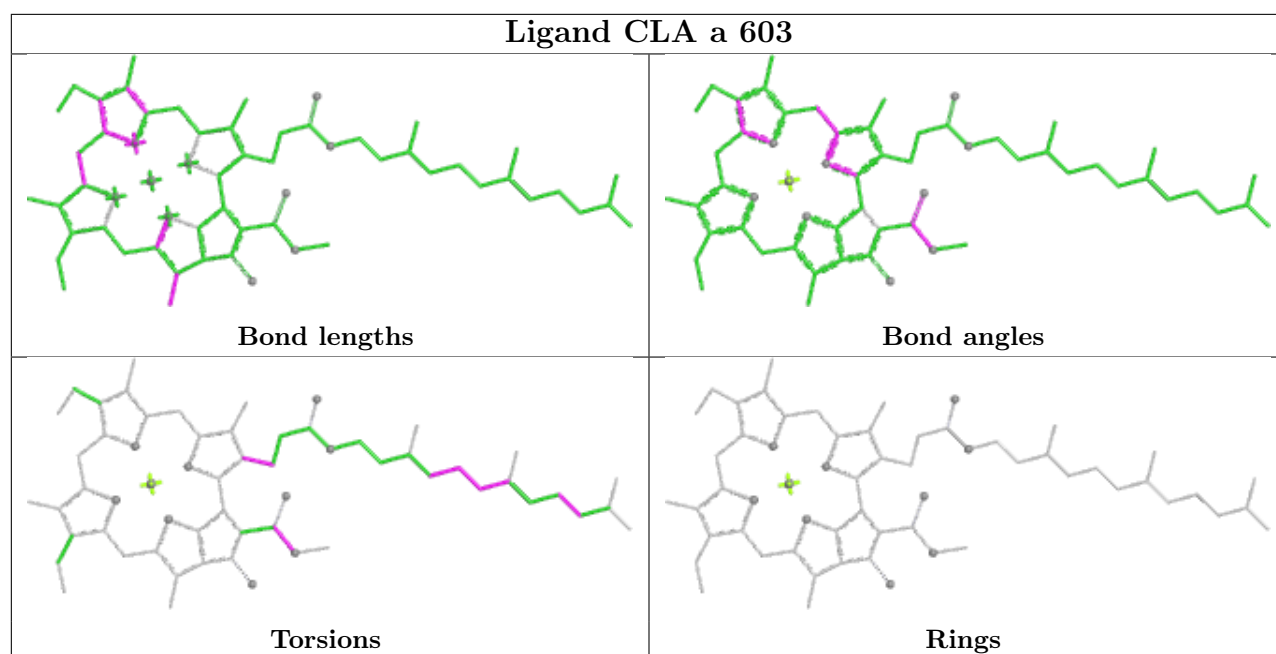
Ligand CLA A 817

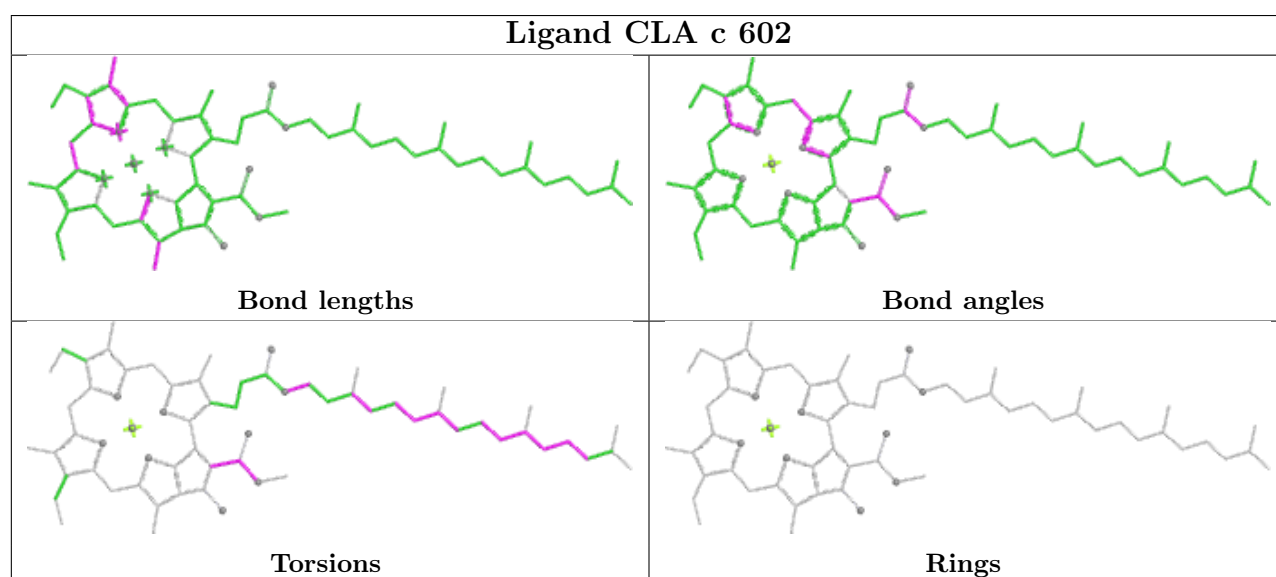
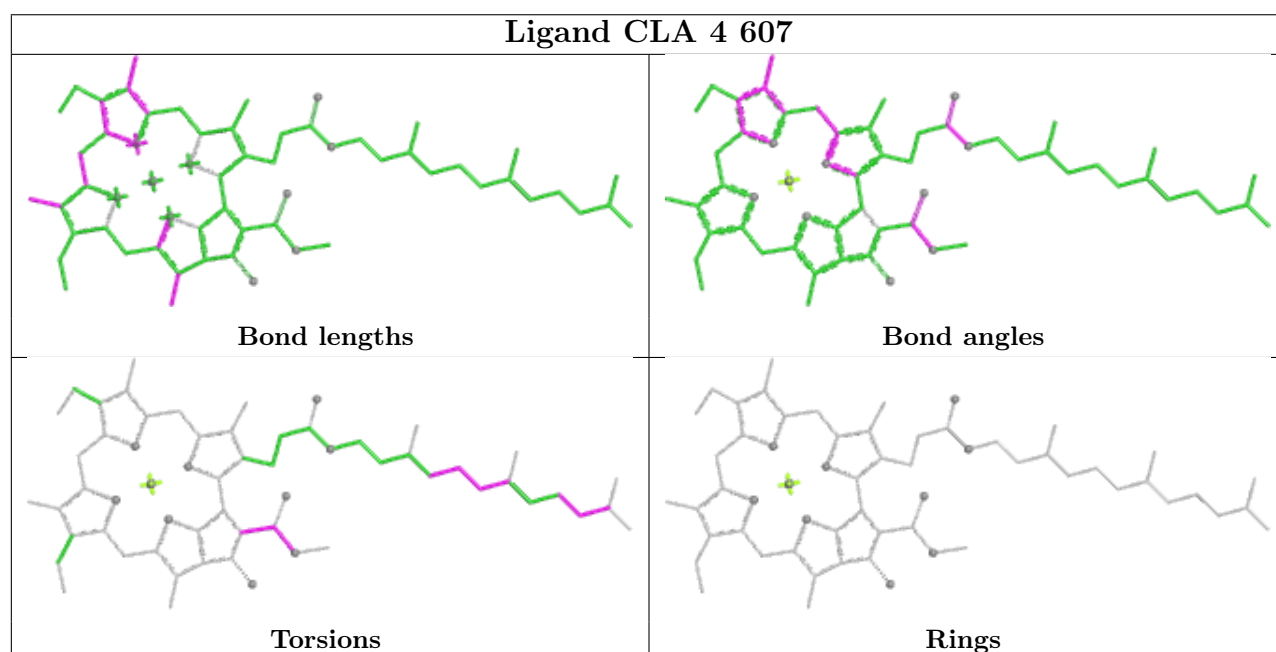
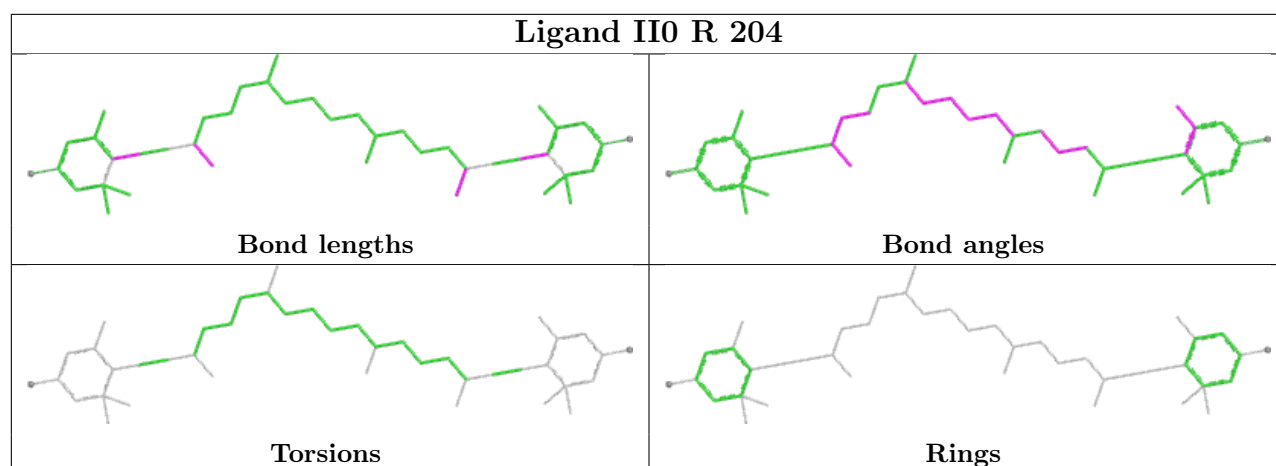


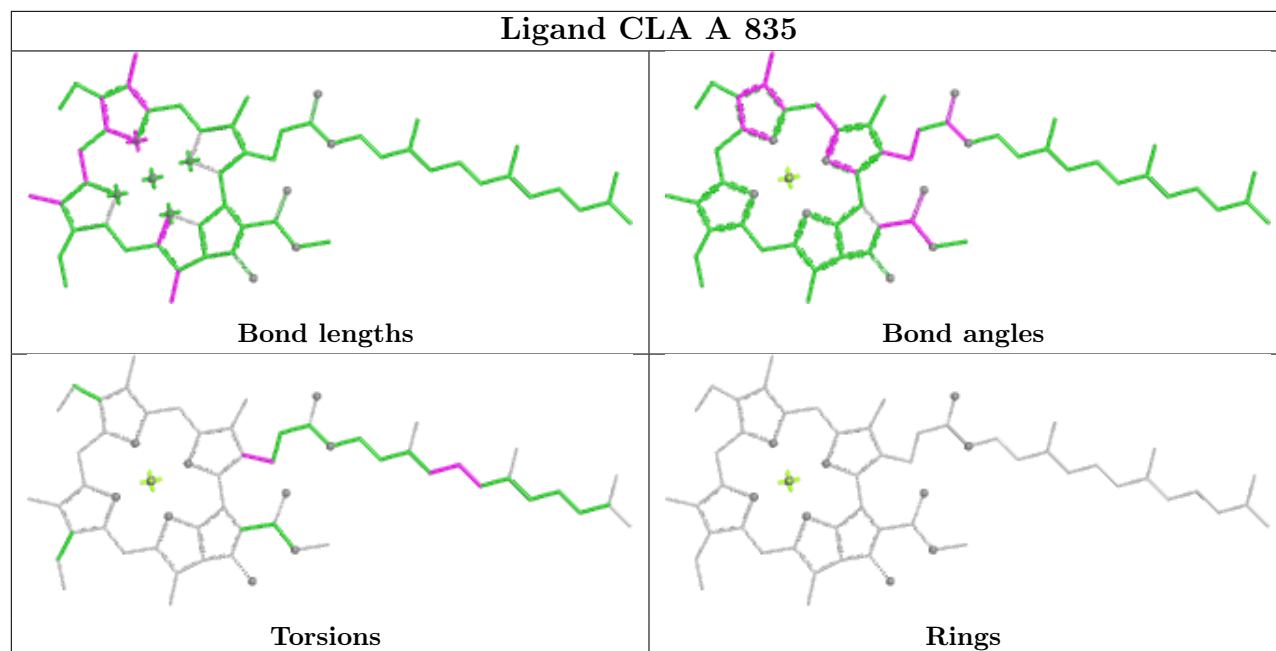
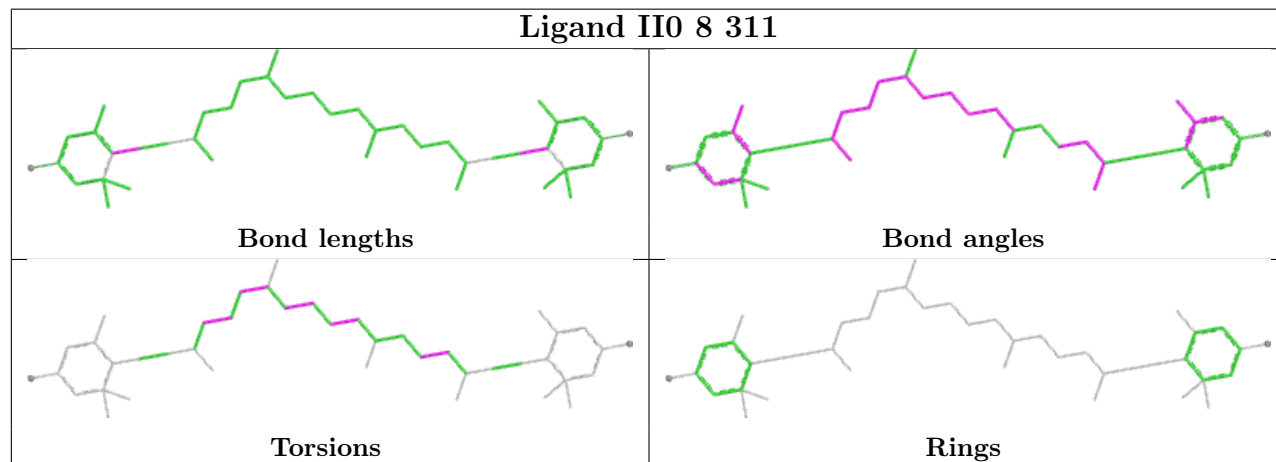
Ligand CLA d 609



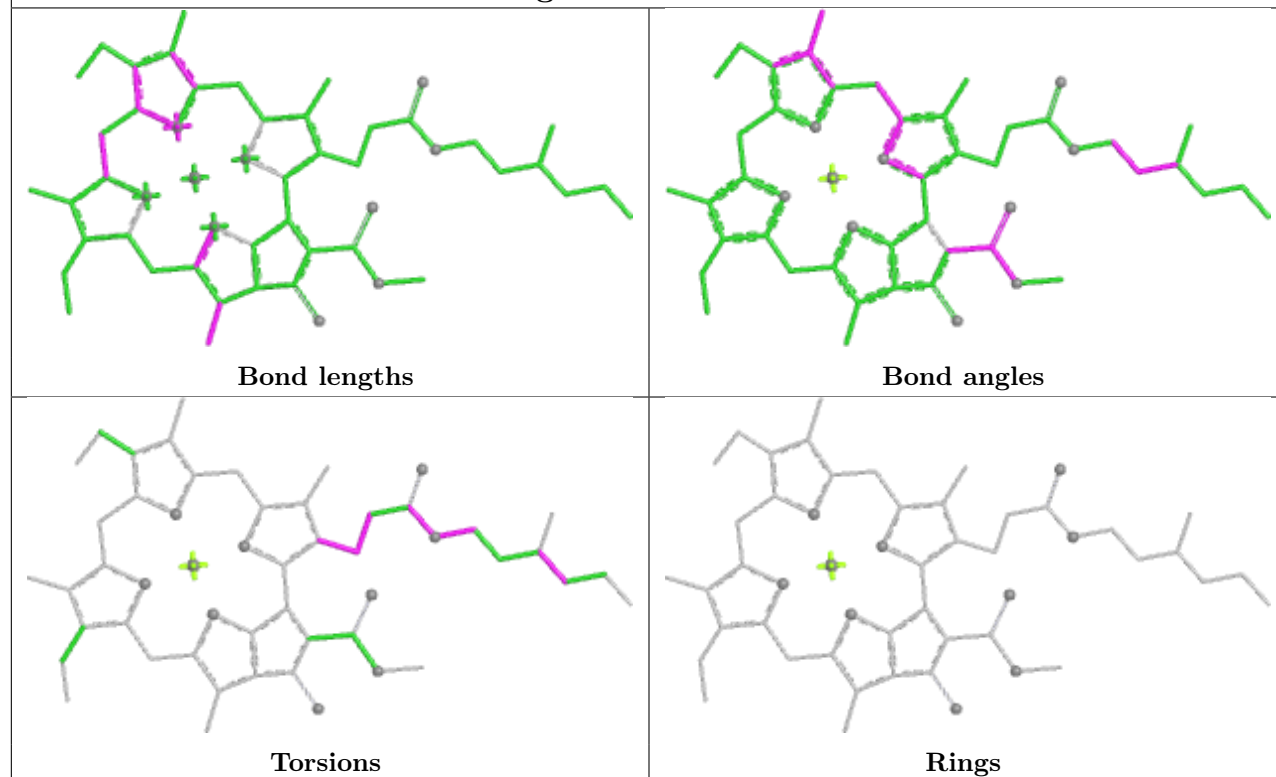




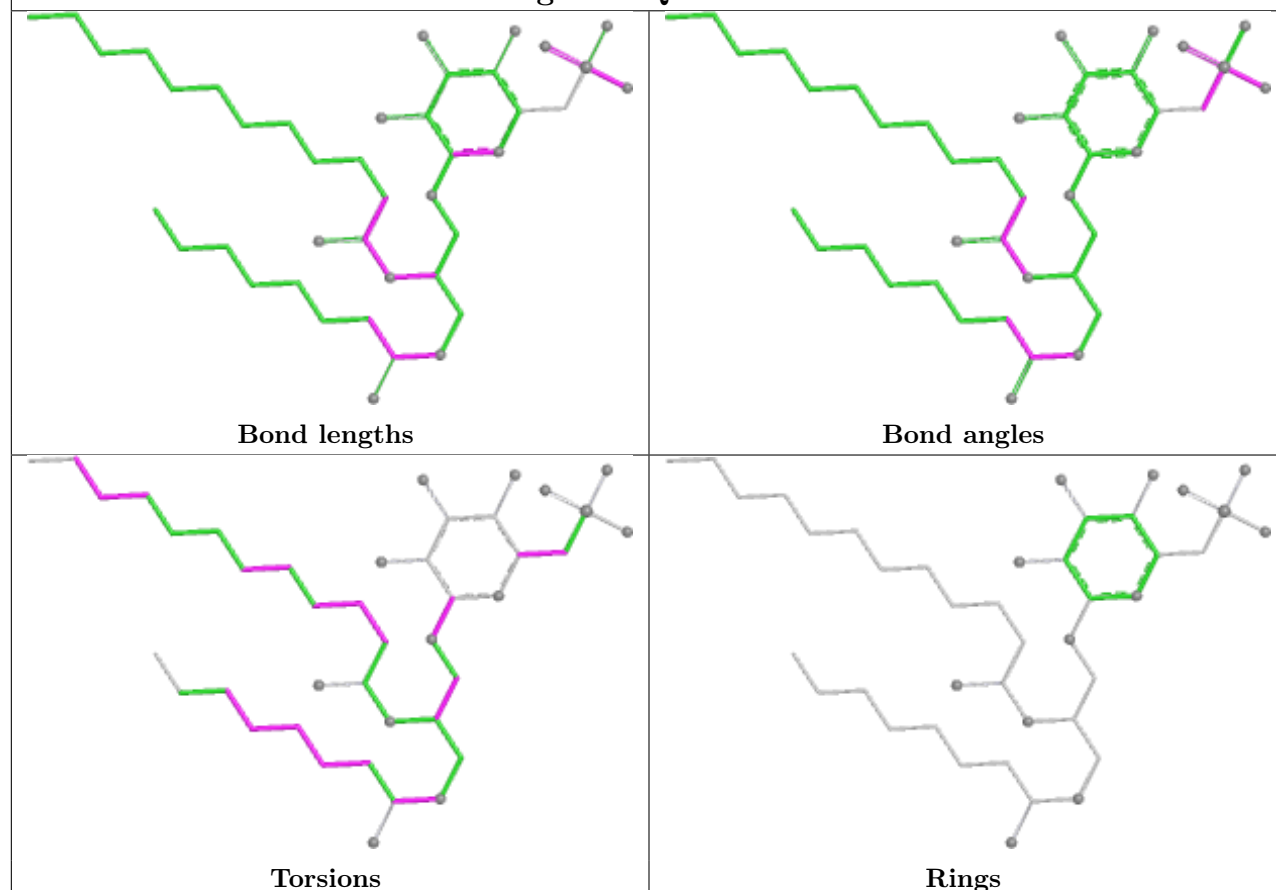


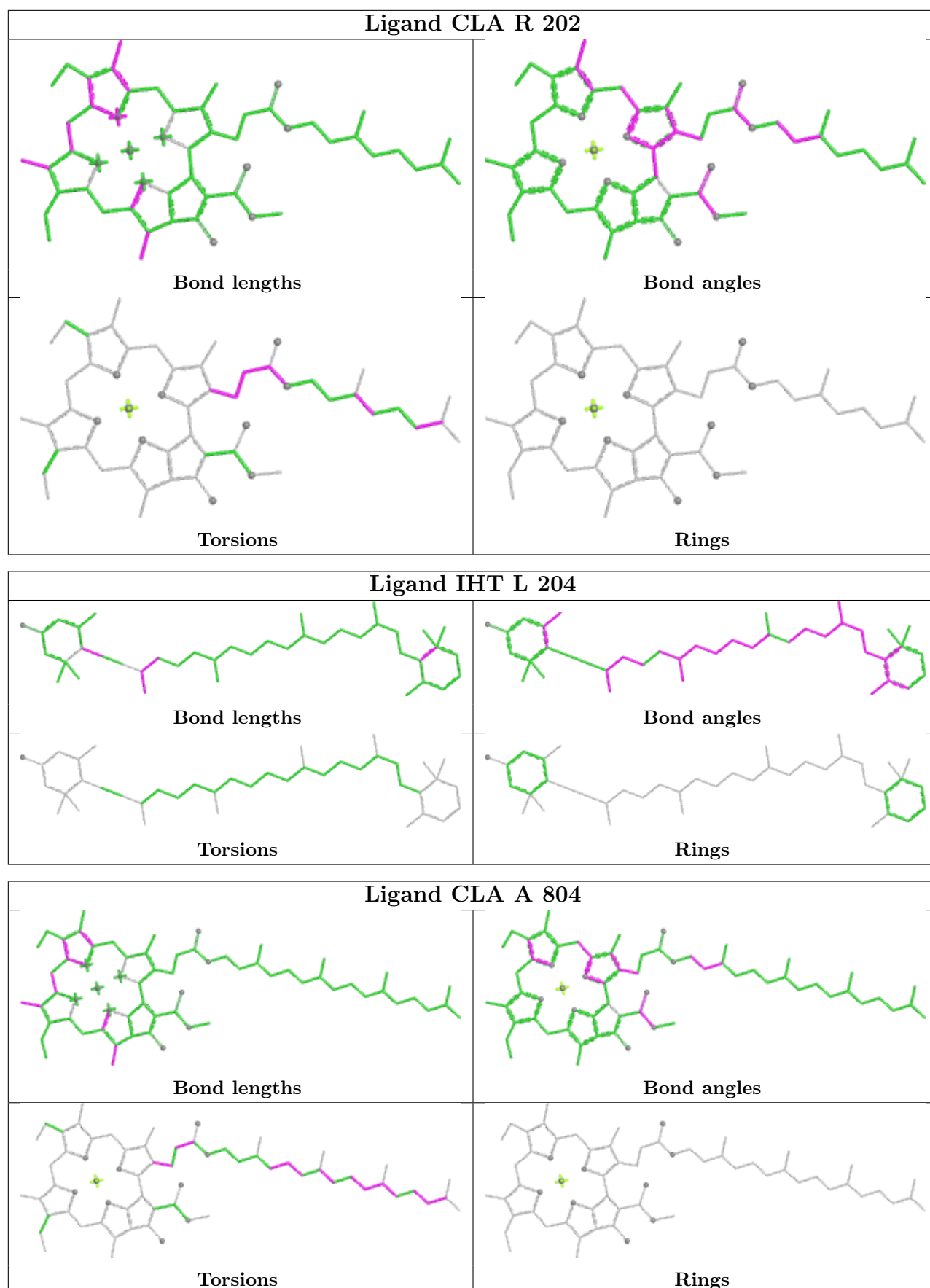
Ligand CLA A 835**Ligand II0 8 311**

Ligand CLA 1 603

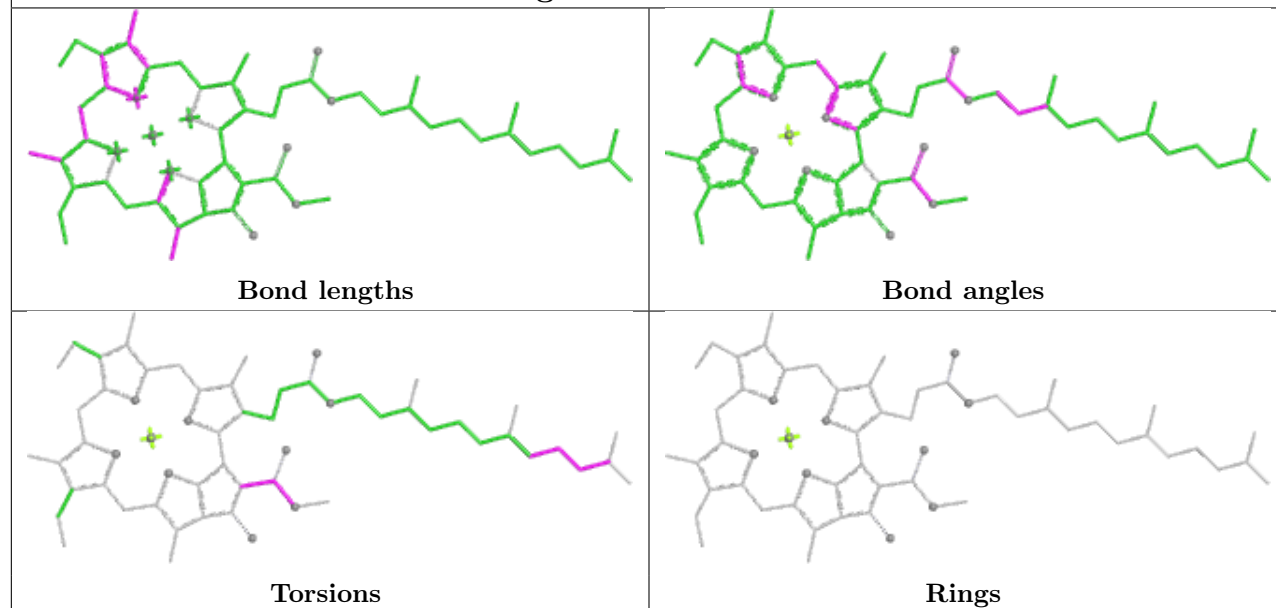


Ligand SQD a 618

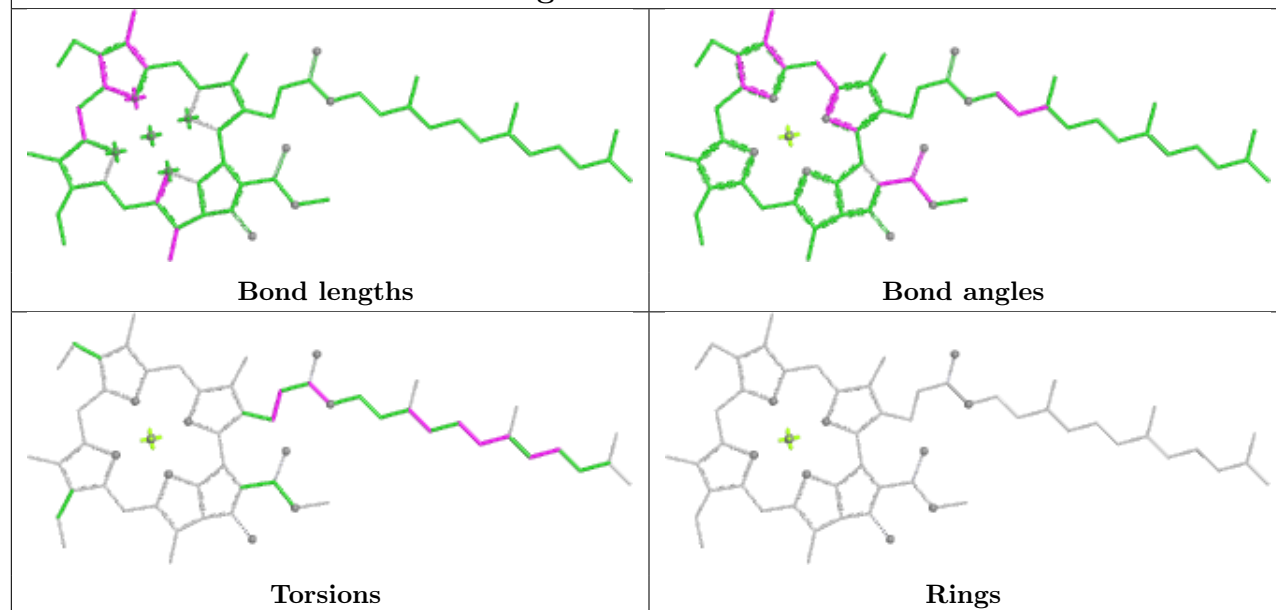




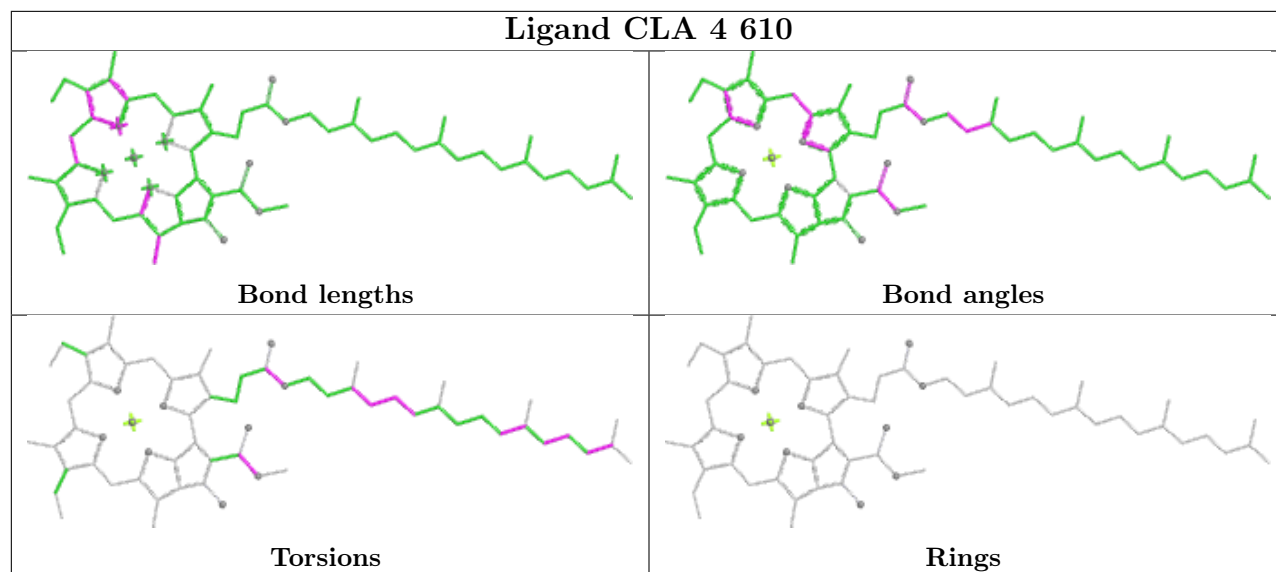
Ligand CLA 2 608



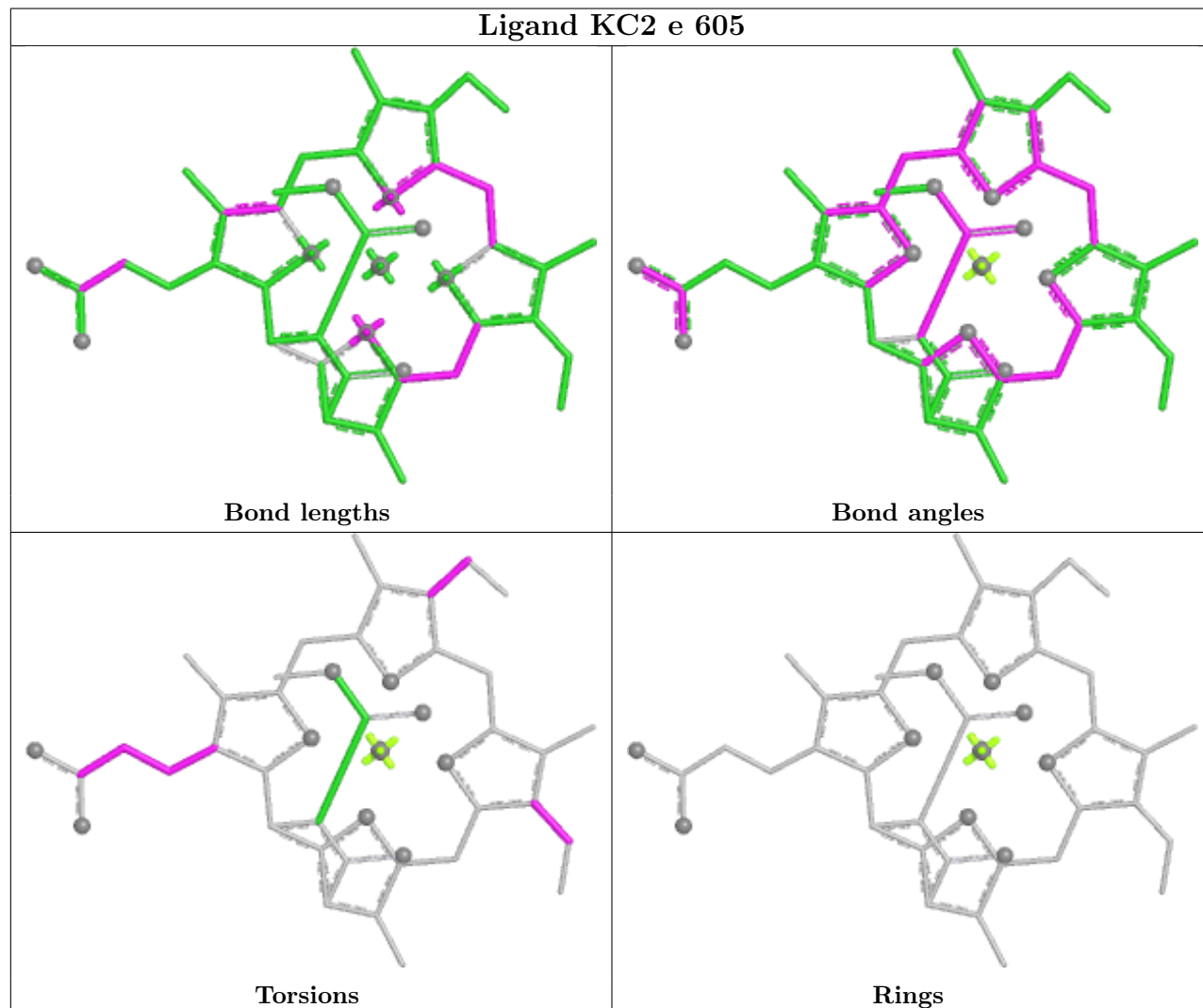
Ligand CLA e 606



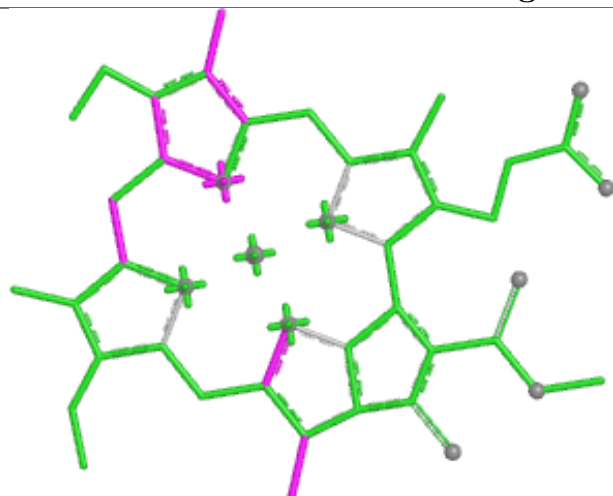
Ligand CLA 4 610



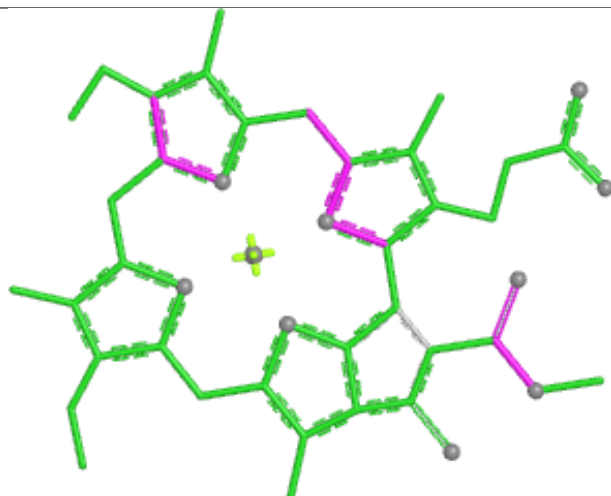
Ligand KC2 e 605



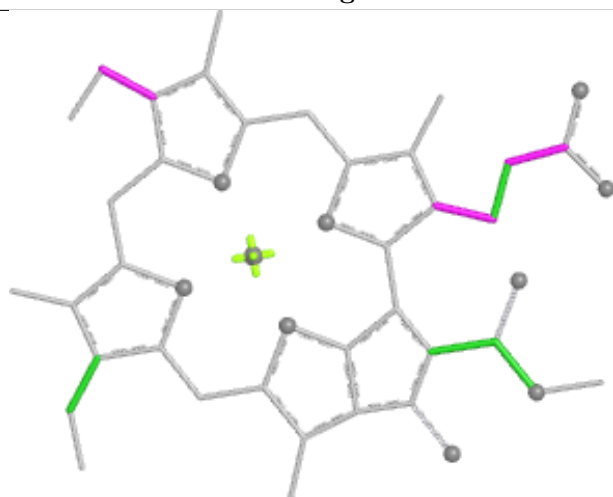
Ligand CLA 1 607



Bond lengths



Bond angles

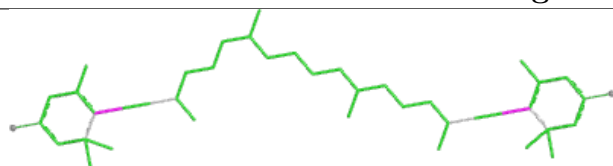


Torsions

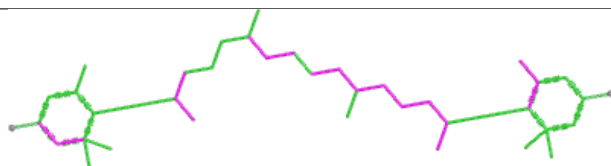


Rings

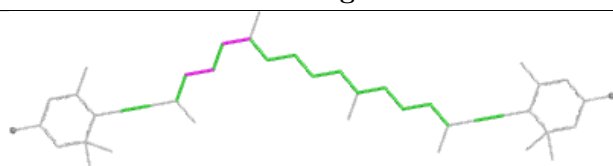
Ligand II0 b 612



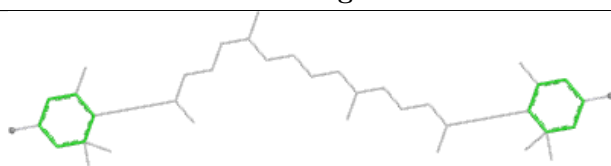
Bond lengths



Bond angles

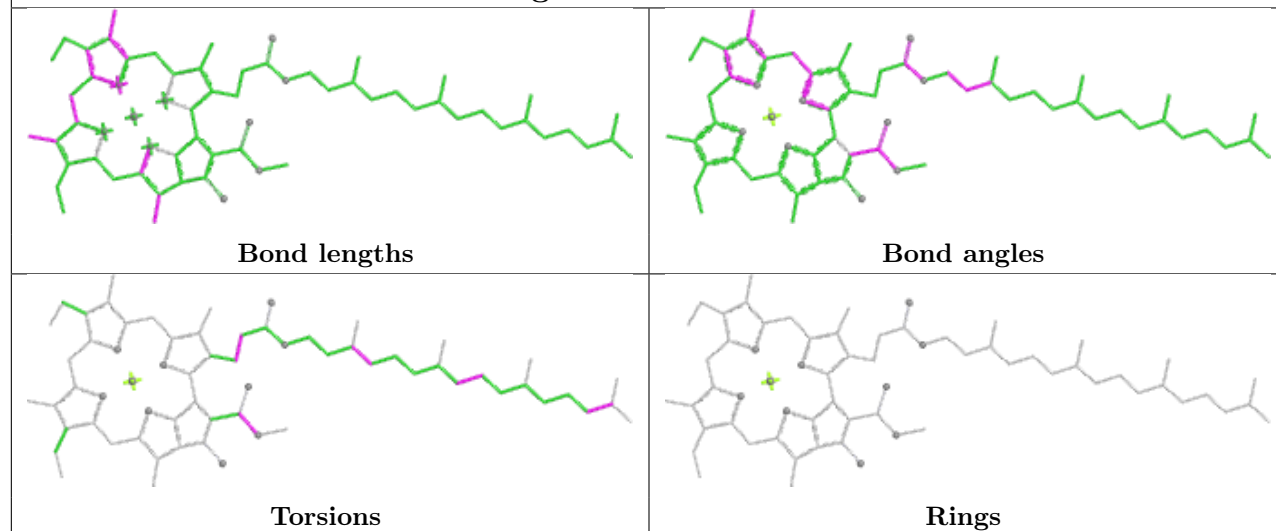


Torsions

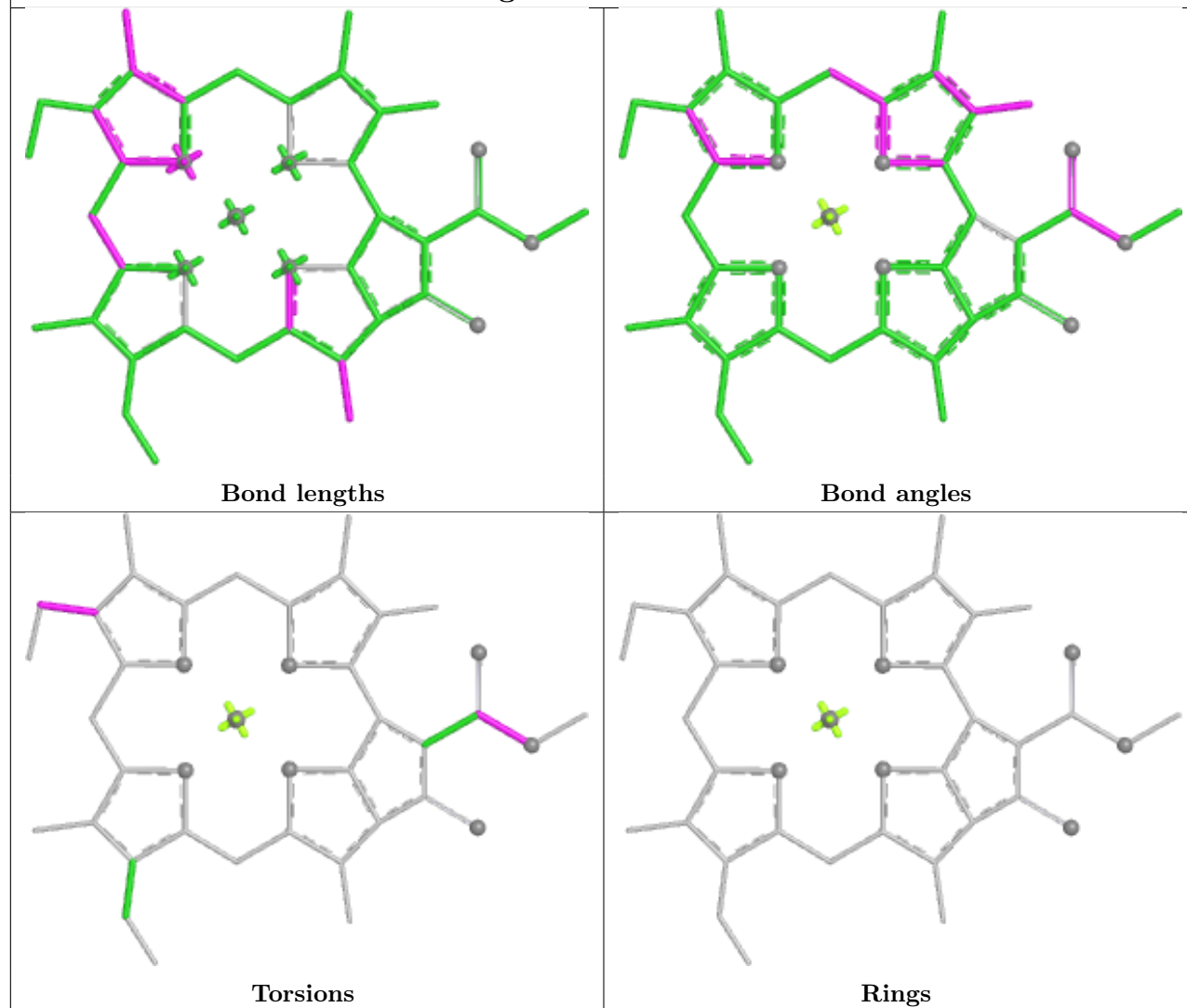


Rings

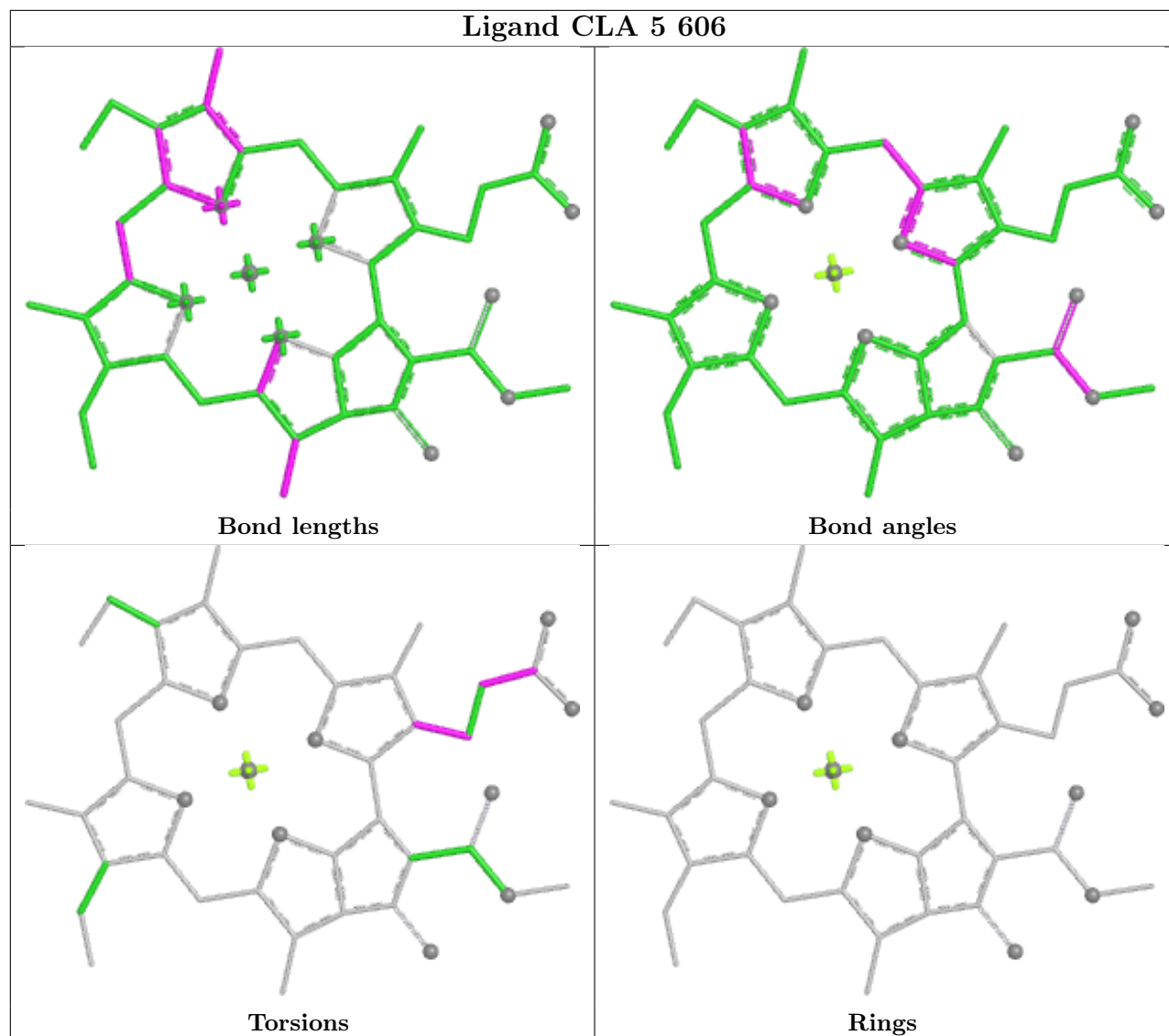
Ligand CLA A 838



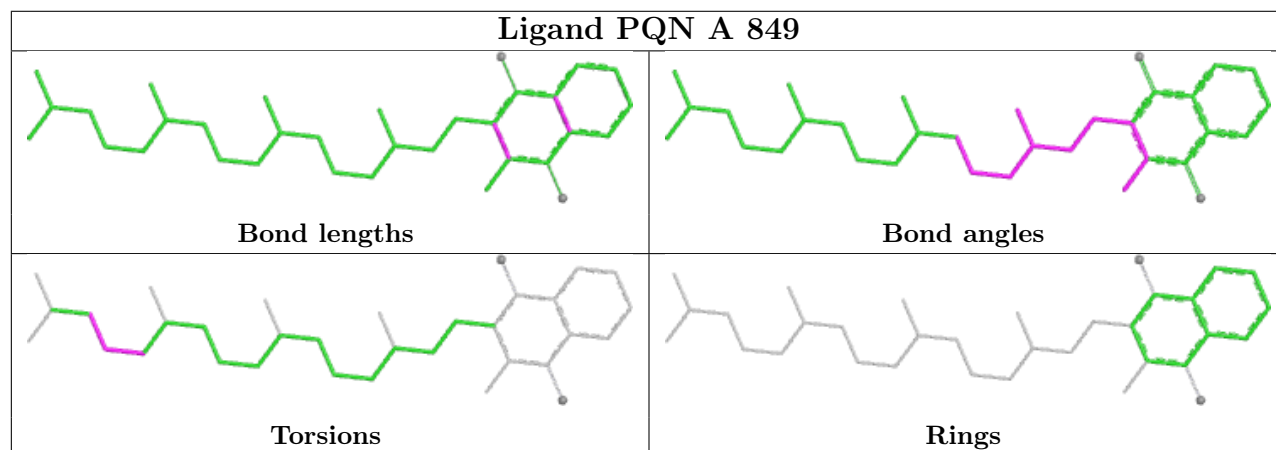
Ligand CLA 9 310



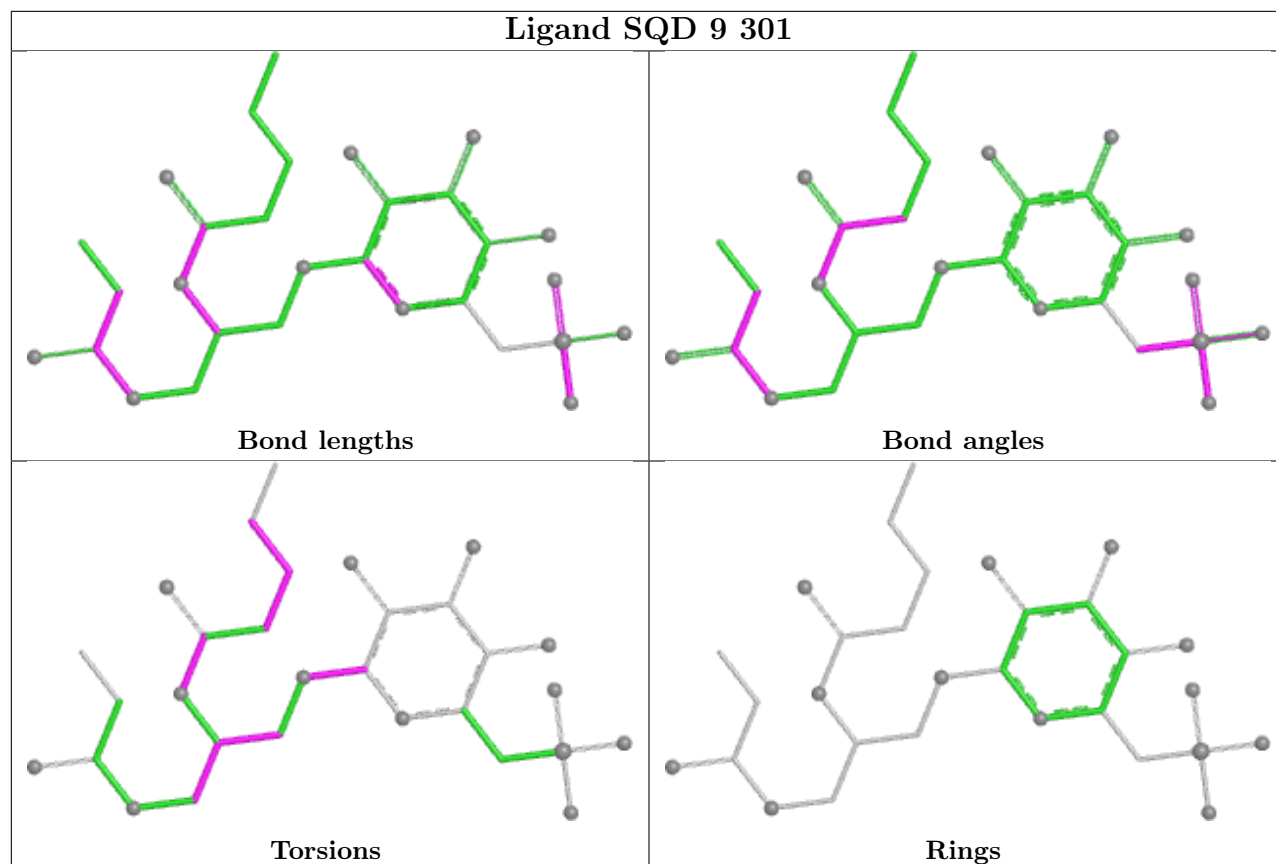
Ligand CLA 5 606



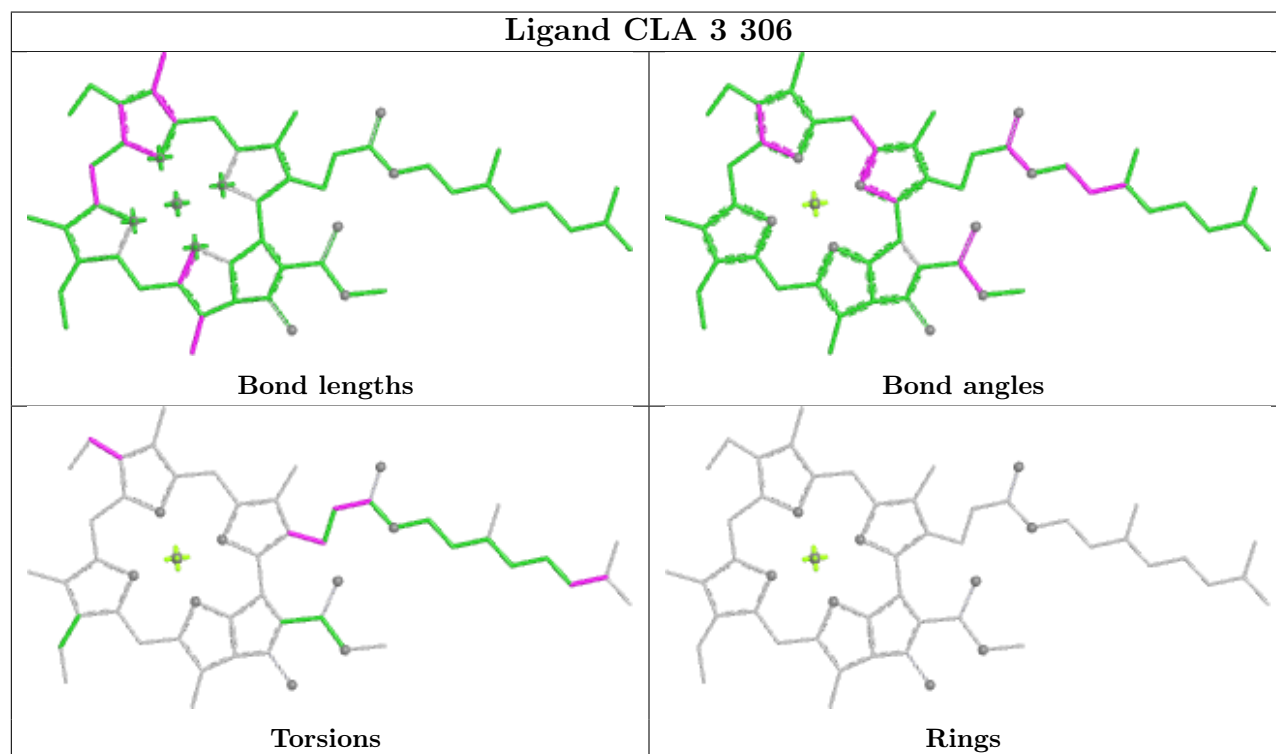
Ligand PQN A 849

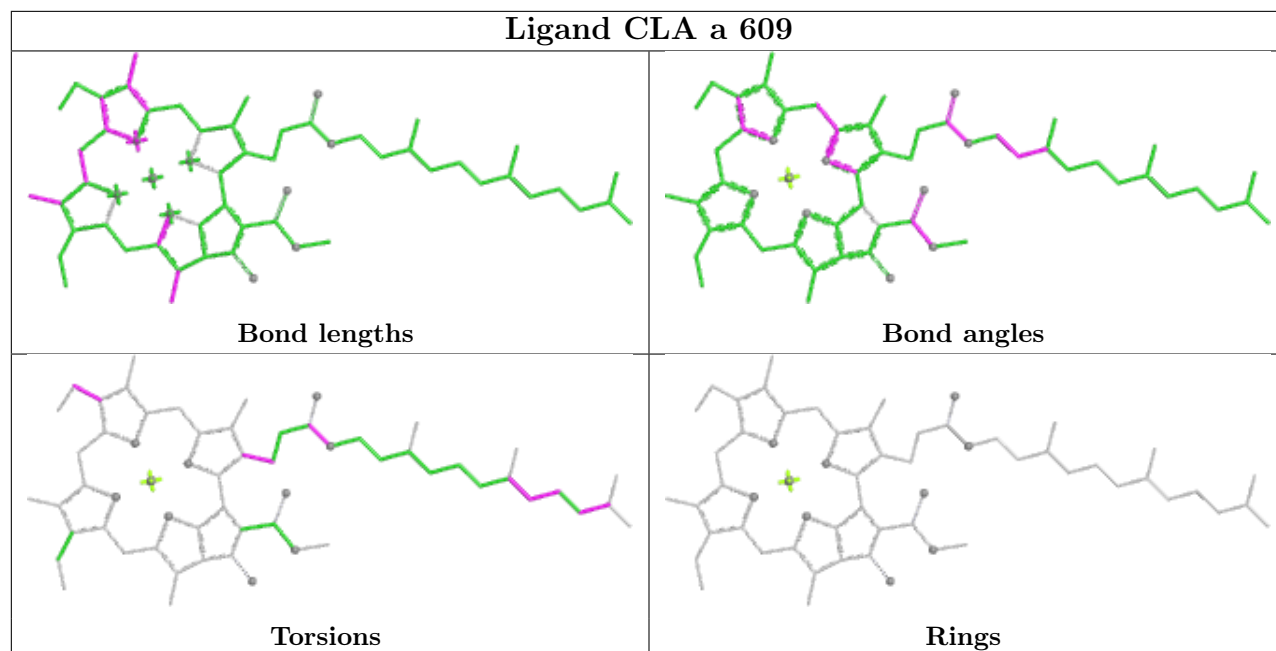
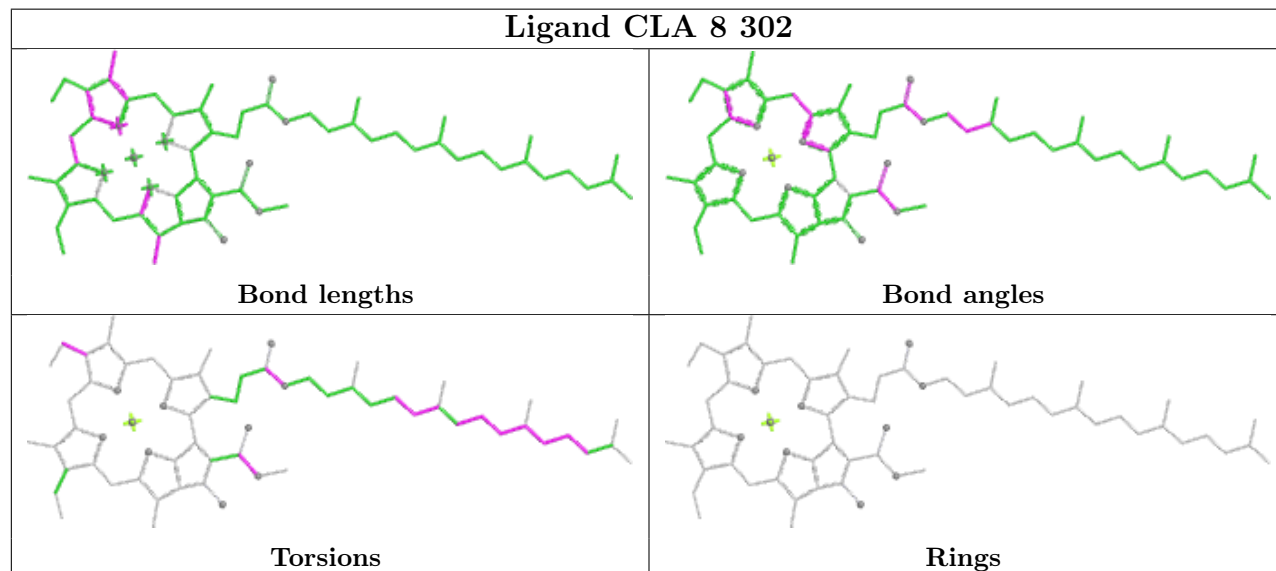


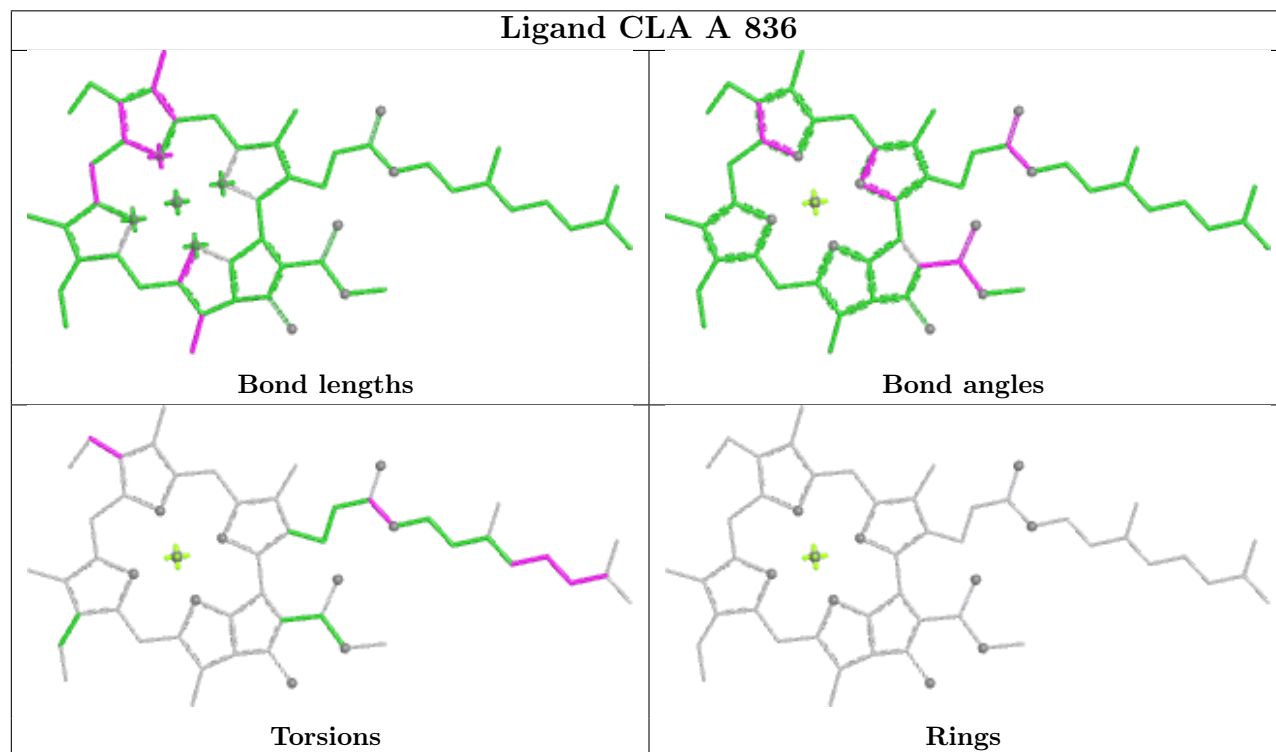
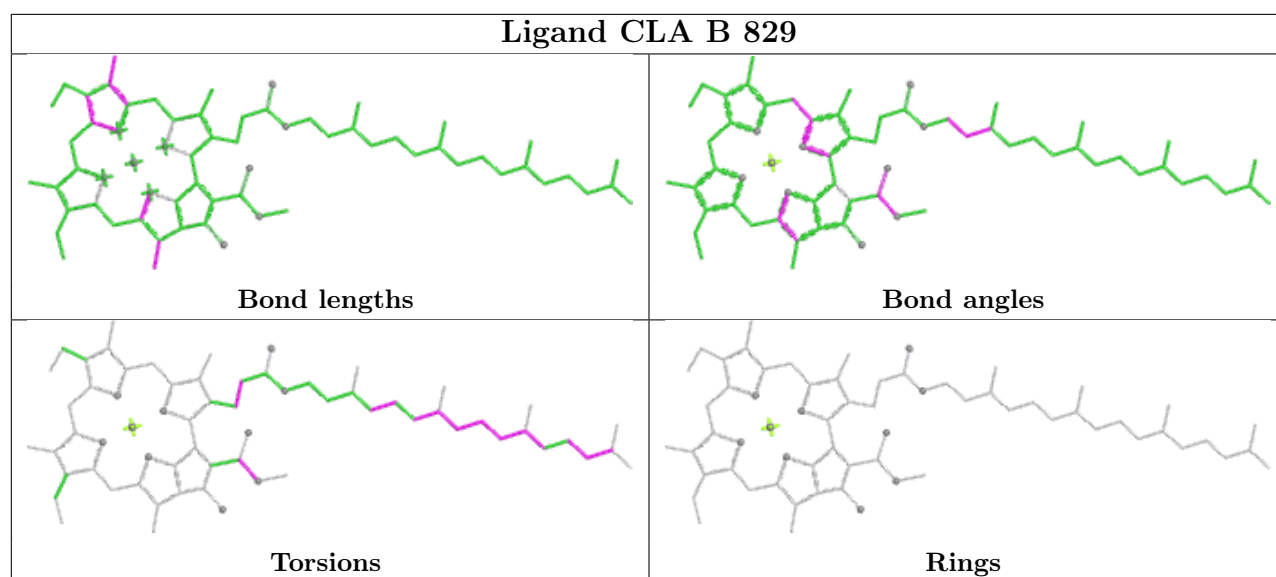
Ligand SQD 9 301

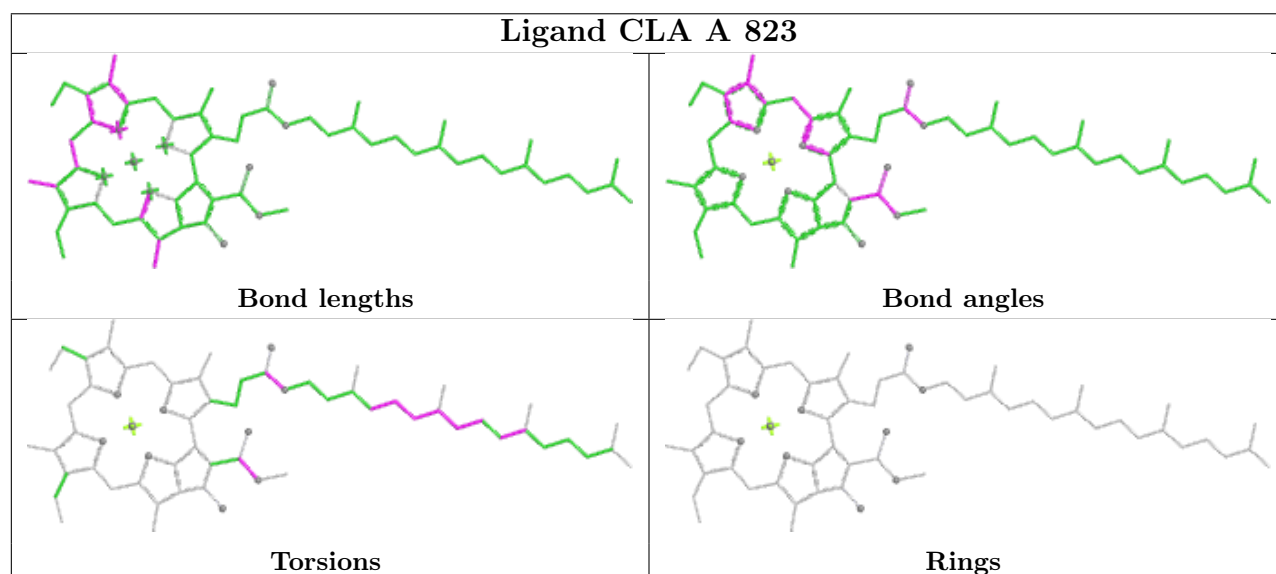
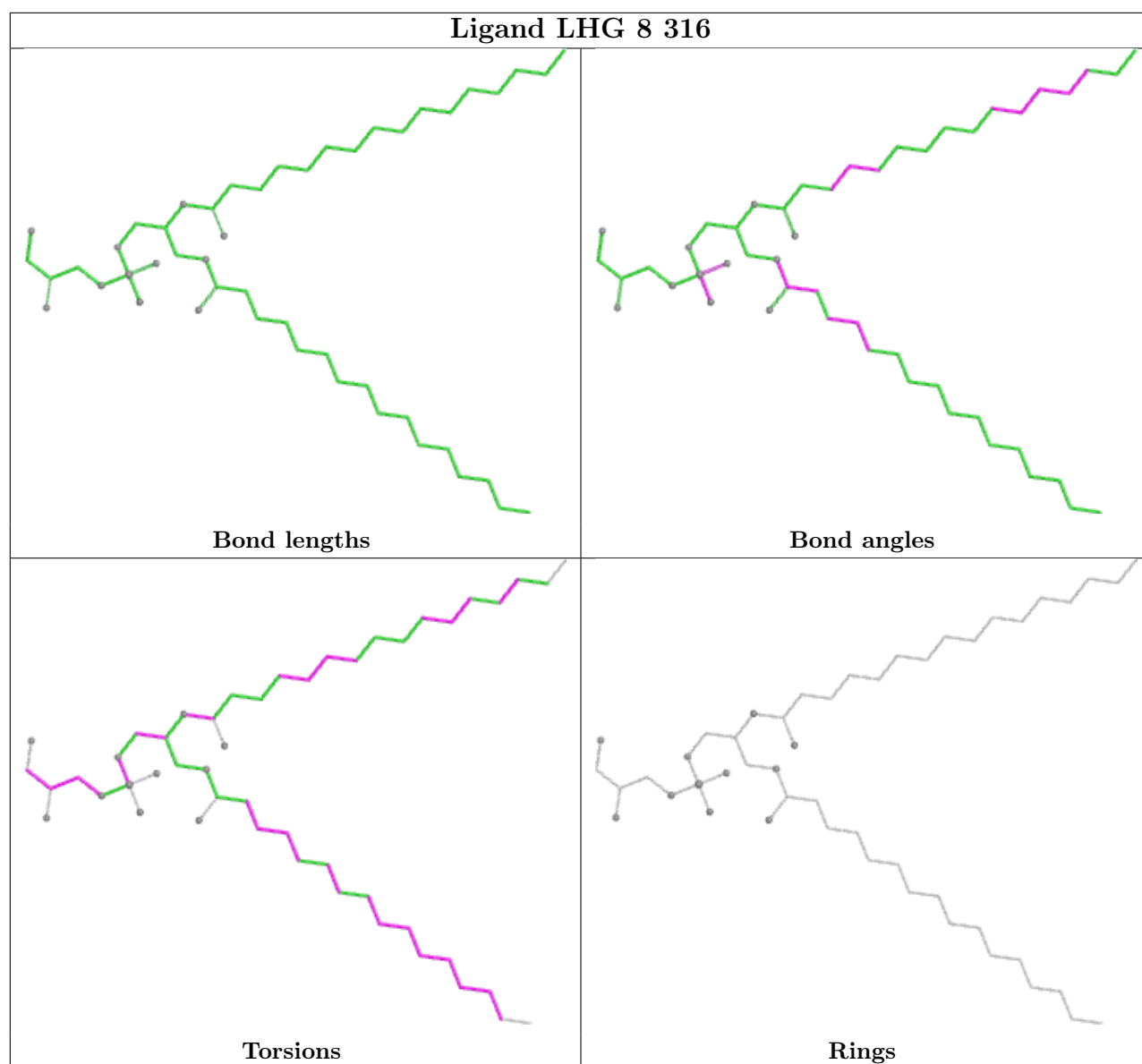


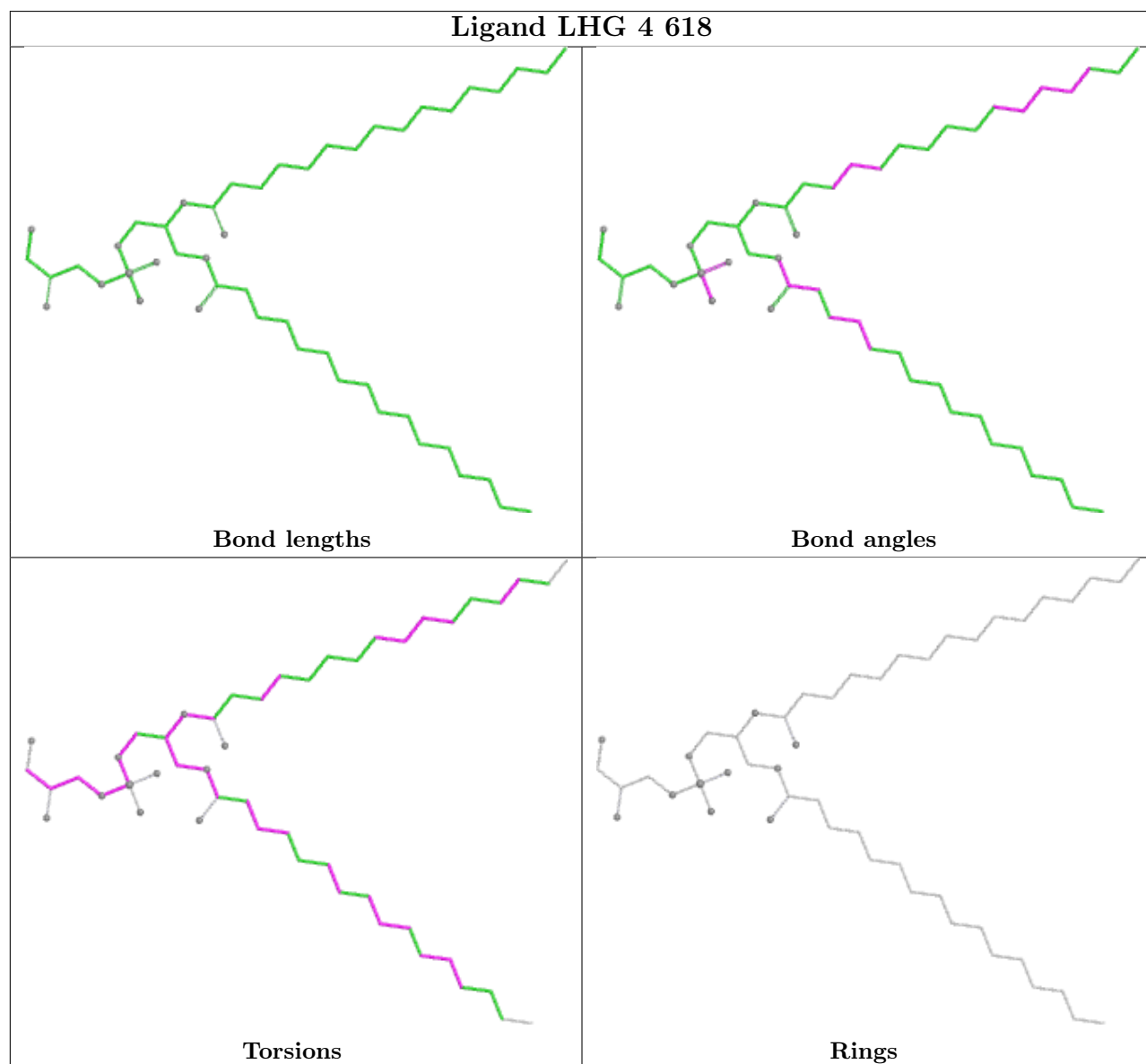
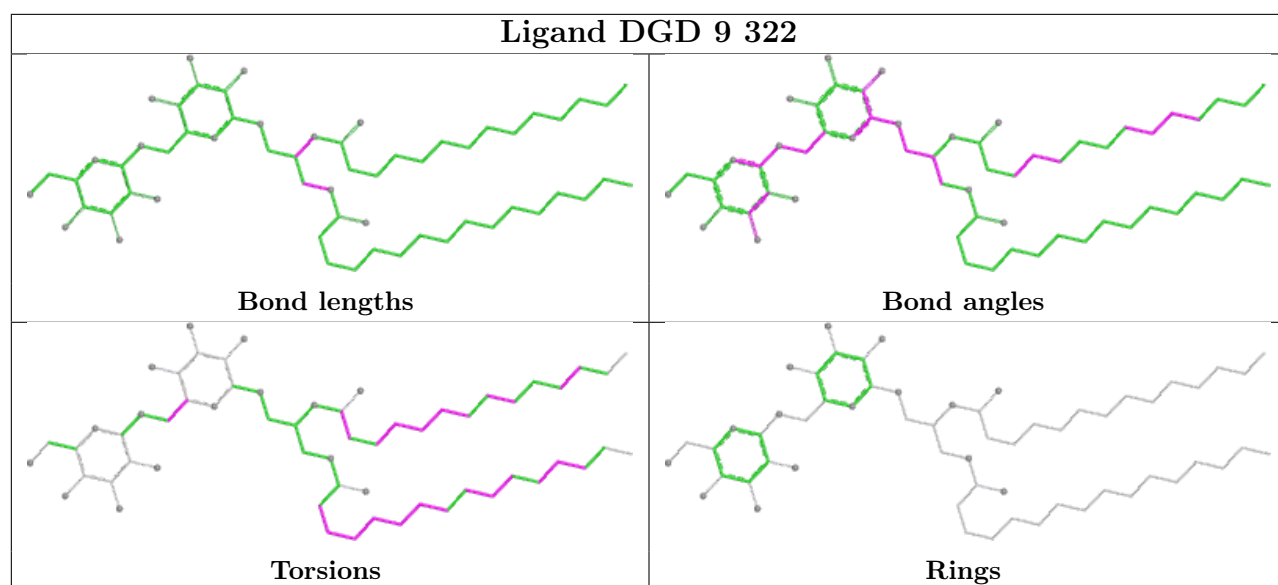
Ligand CLA 3 306



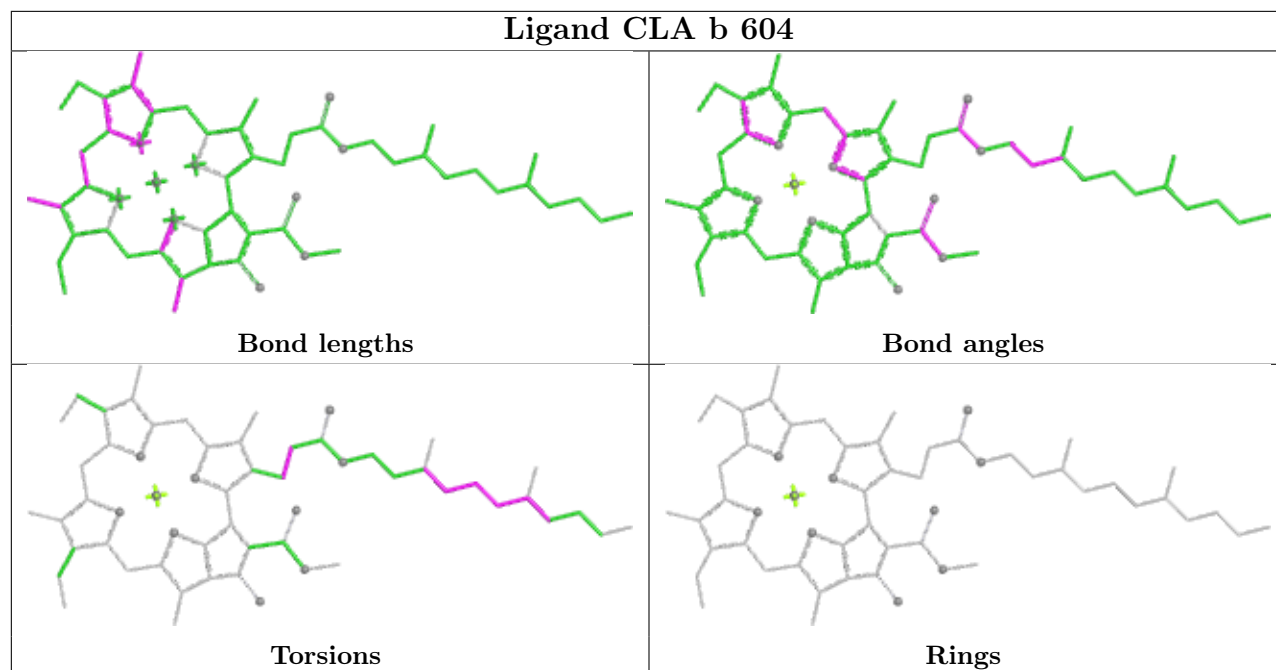
Ligand CLA a 609**Ligand CLA 8 302**



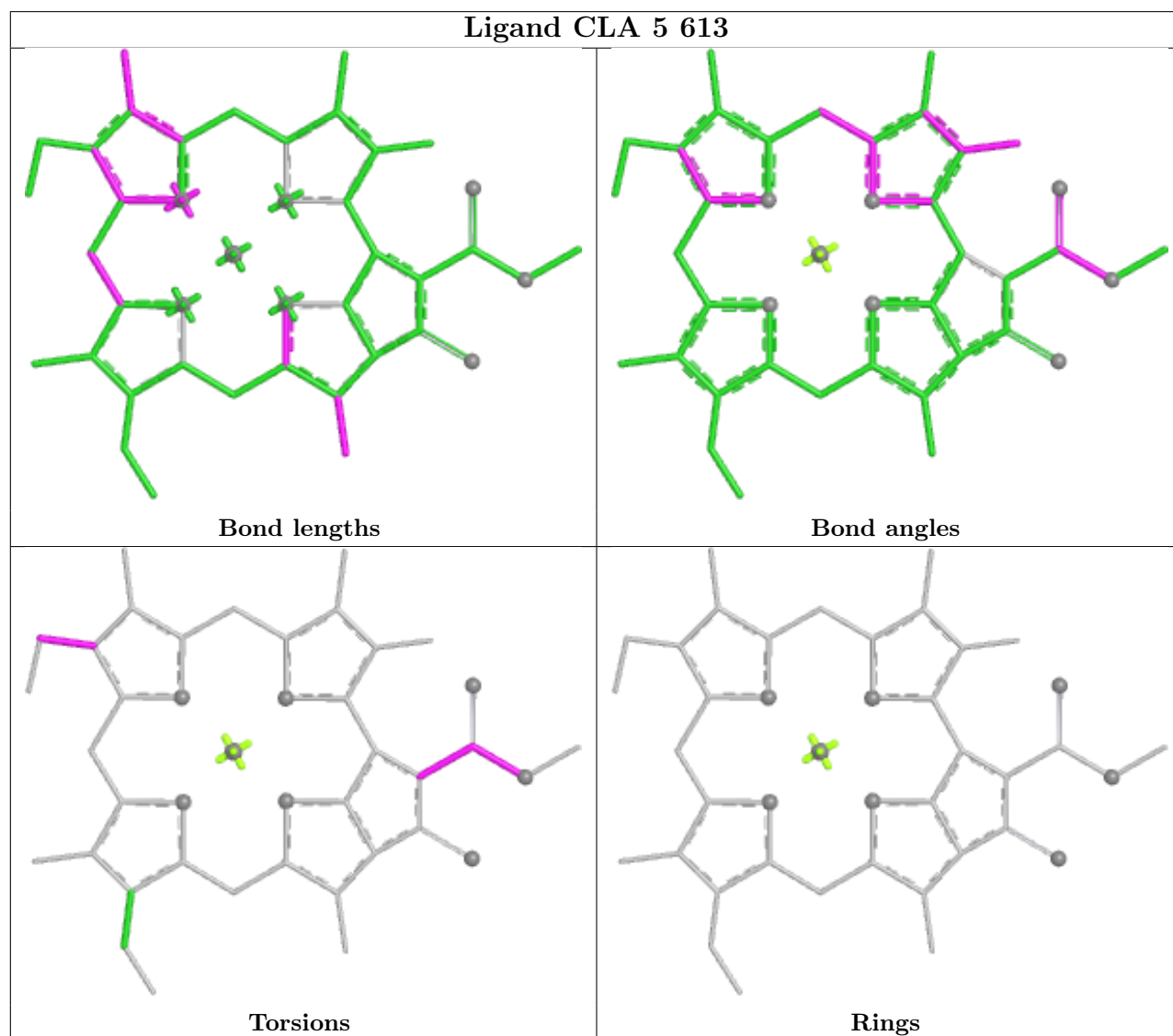


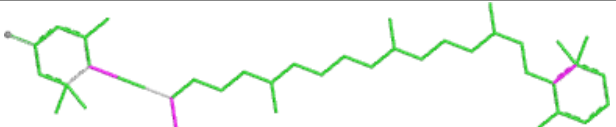
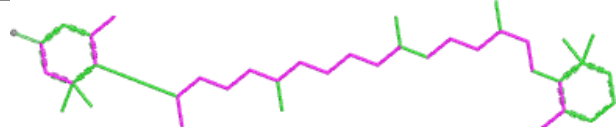
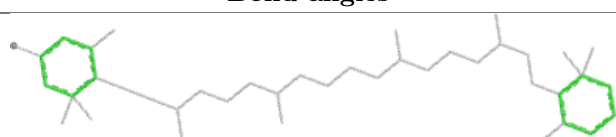


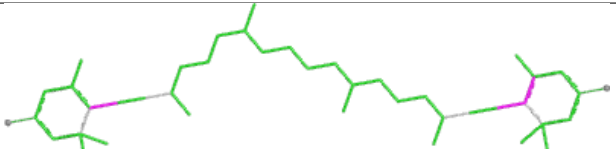
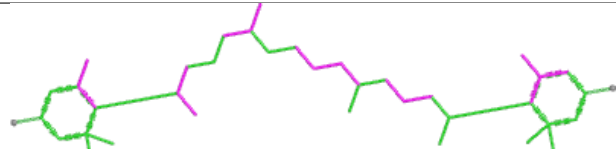
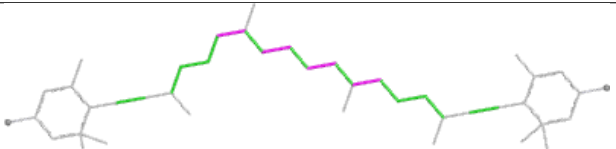
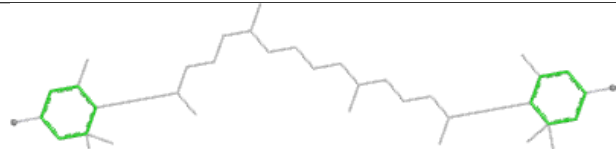
Ligand CLA b 604

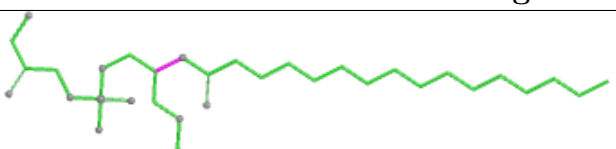
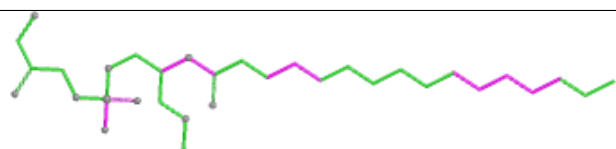
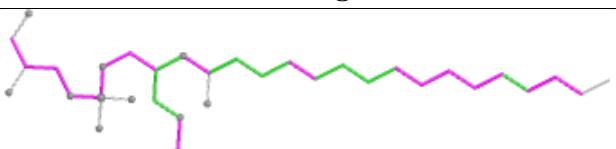
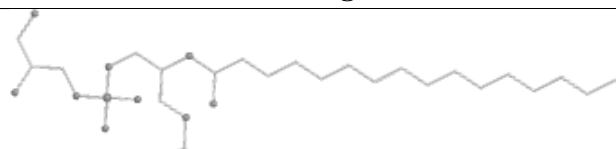


Ligand CLA 5 613

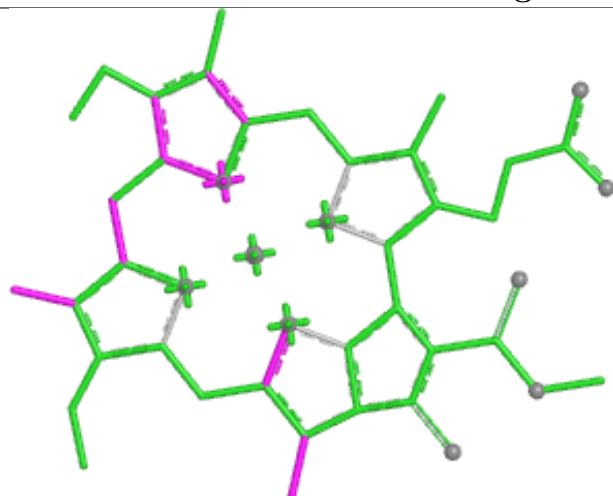


Ligand IHT K 104	
	Bond lengths
	Bond angles
	Torsions
	Rings

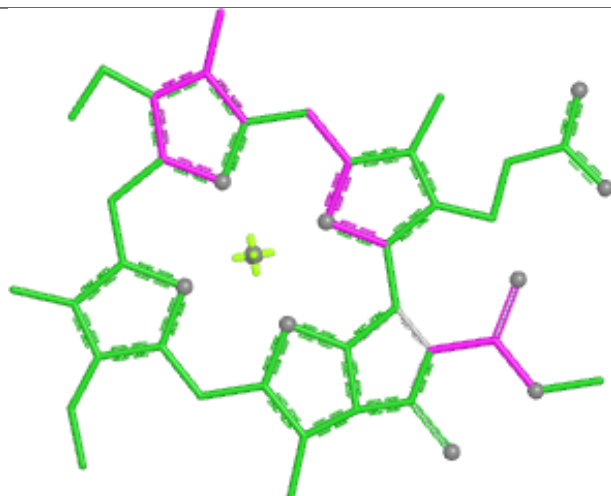
Ligand II0 a 615	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand LHG c 623	
	Bond lengths
	Bond angles
	Torsions
	Rings

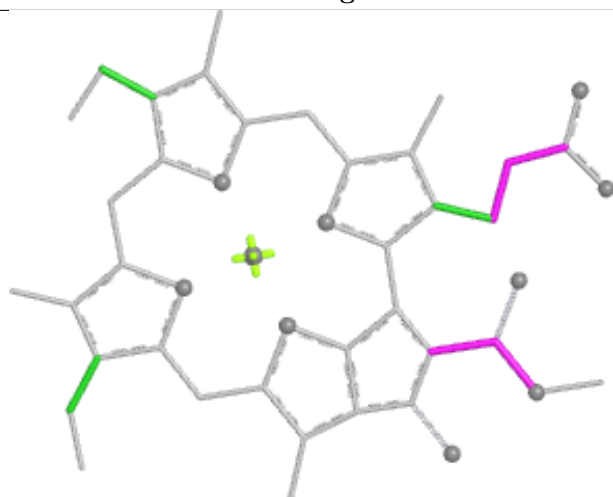
Ligand CLA B 804



Bond lengths



Bond angles

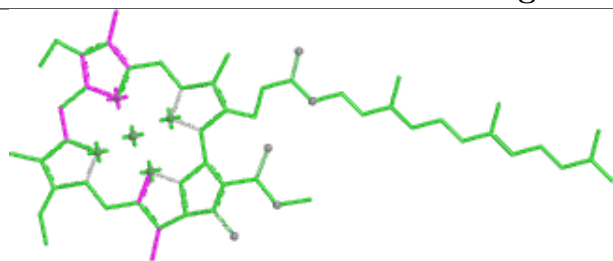


Torsions

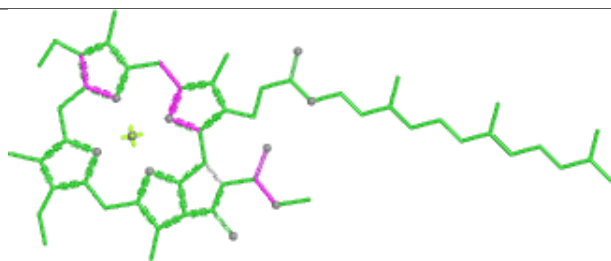


Rings

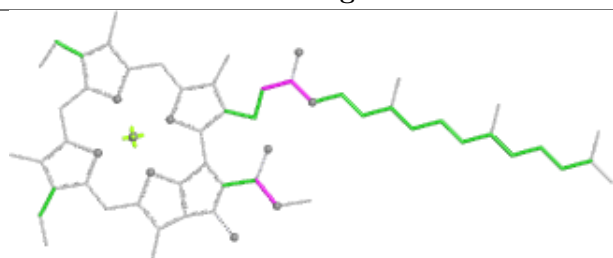
Ligand CLA 4 609



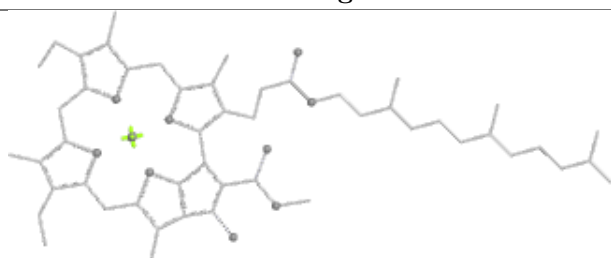
Bond lengths



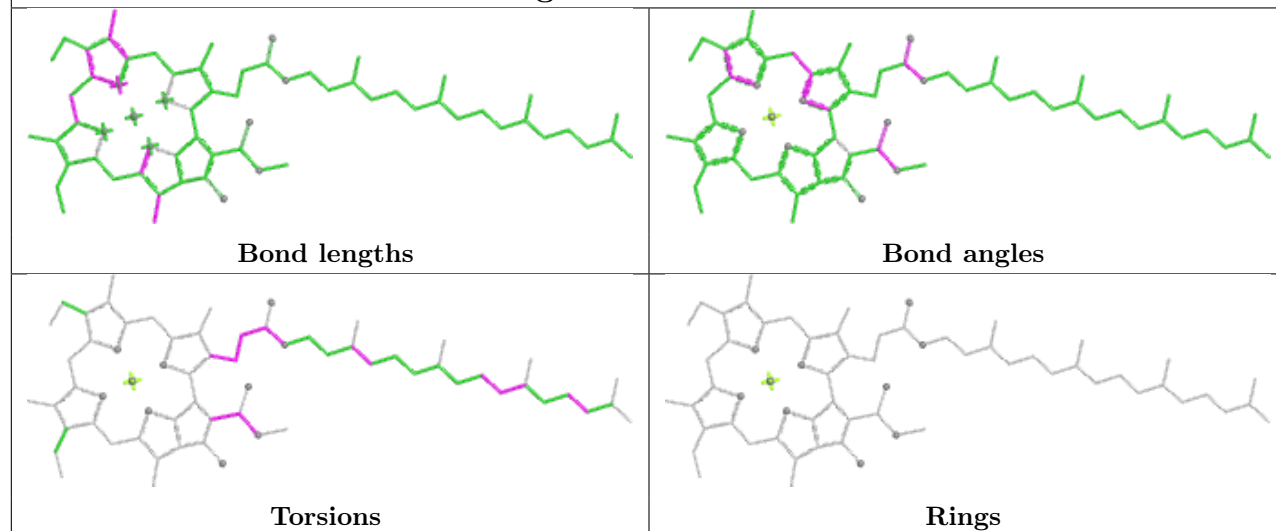
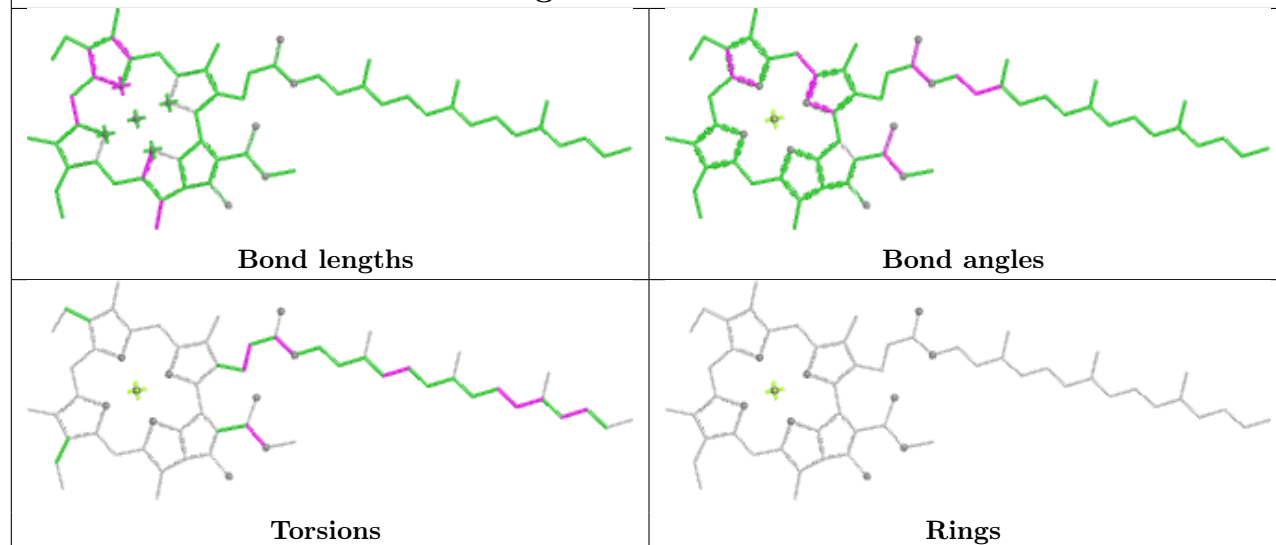
Bond angles



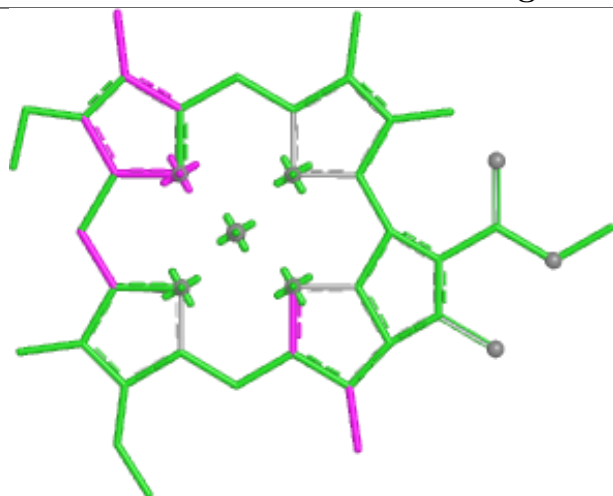
Torsions



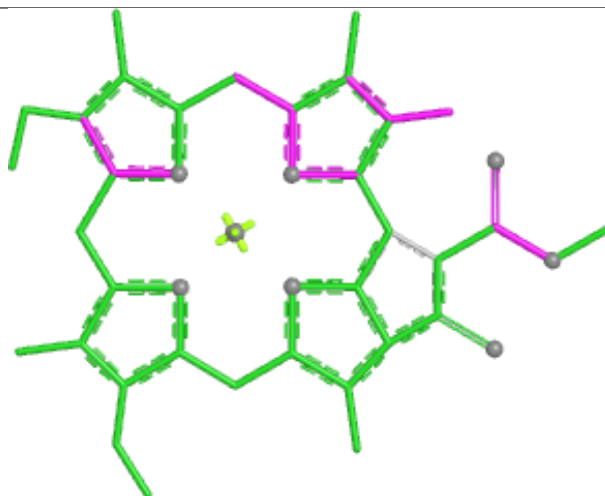
Rings

Ligand CLA 8 303**Ligand CLA d 612**

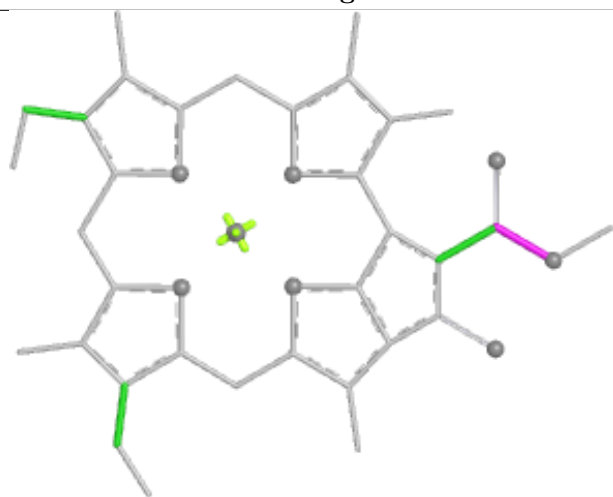
Ligand CLA J 103



Bond lengths



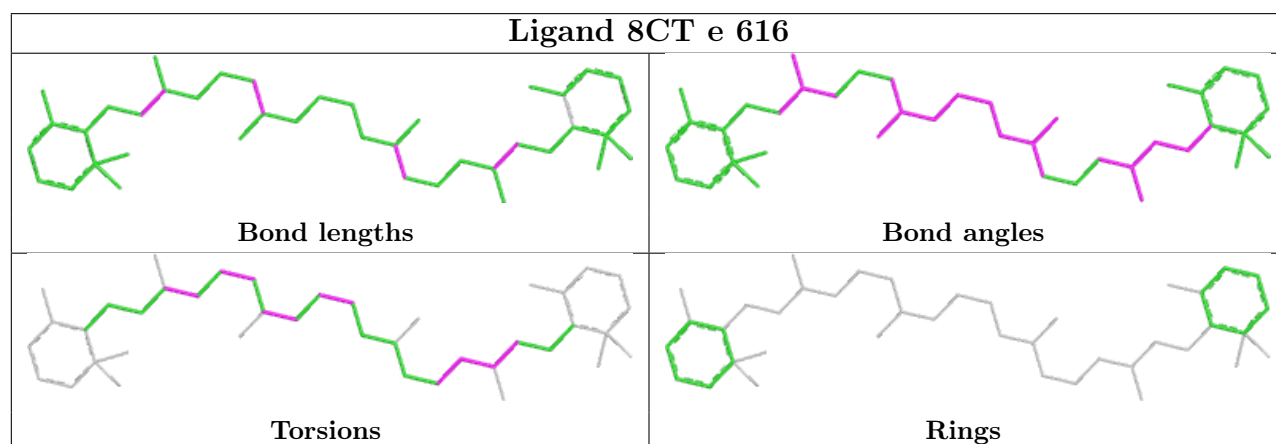
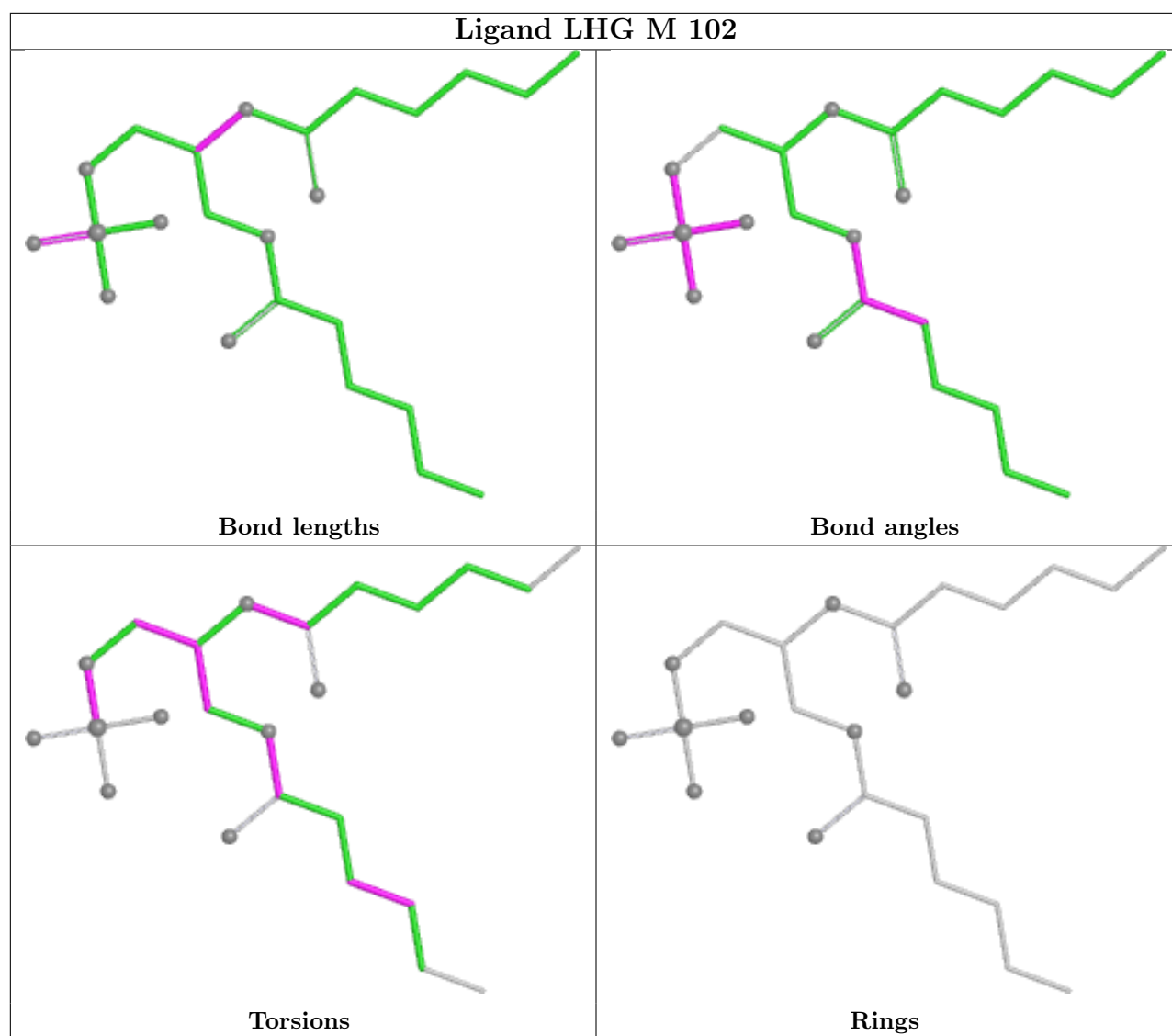
Bond angles

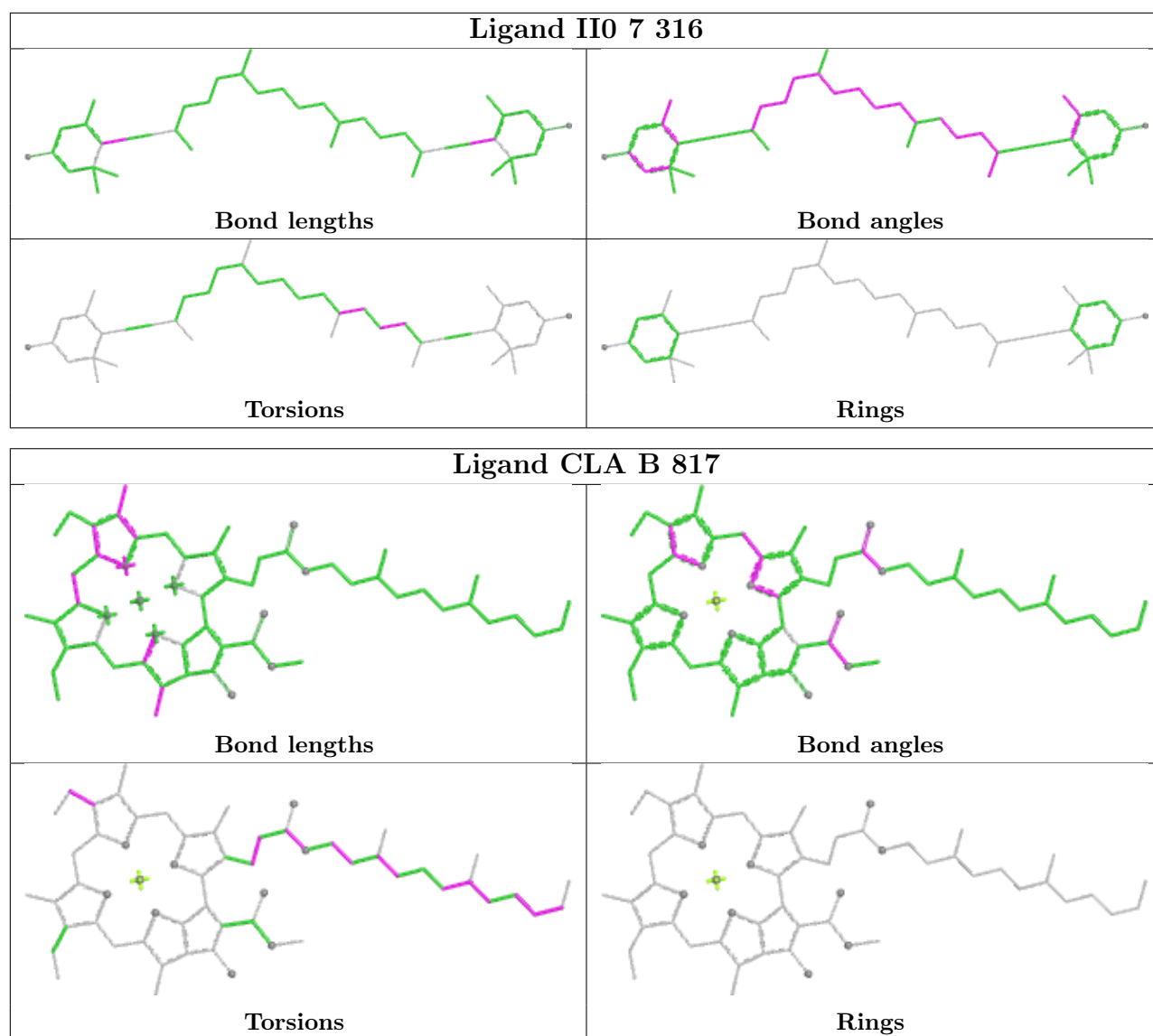


Torsions

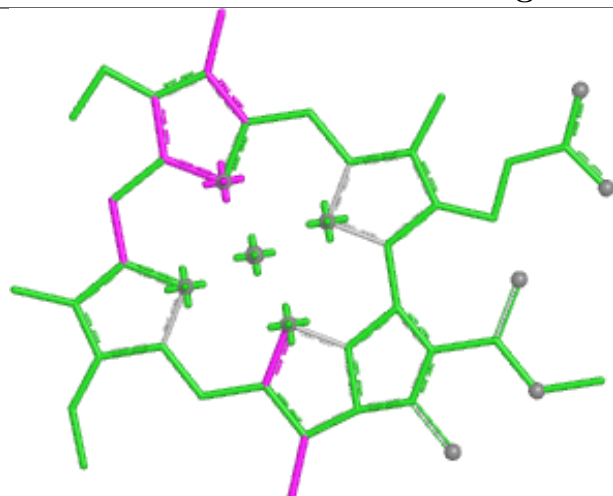


Rings

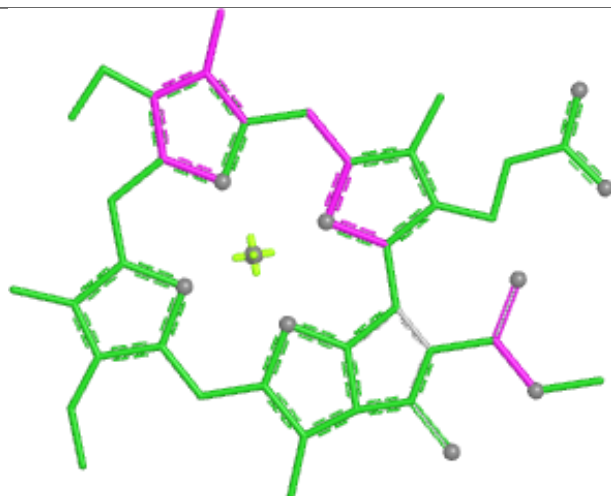




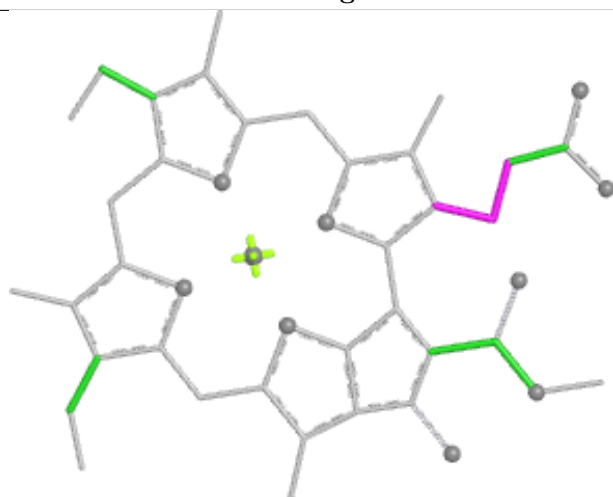
Ligand CLA F 201



Bond lengths



Bond angles

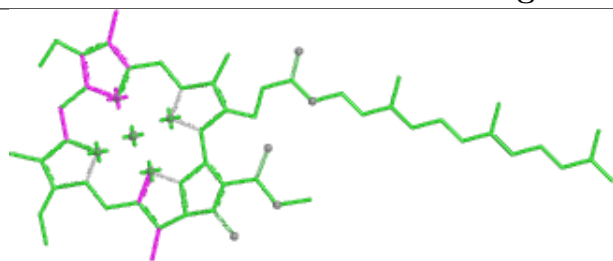


Torsions

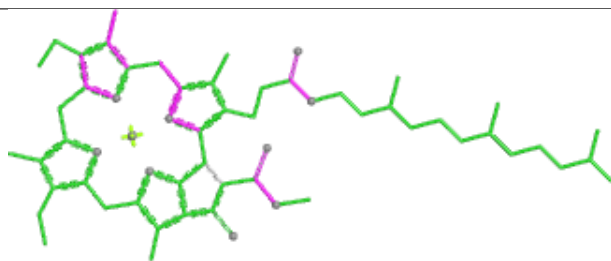


Rings

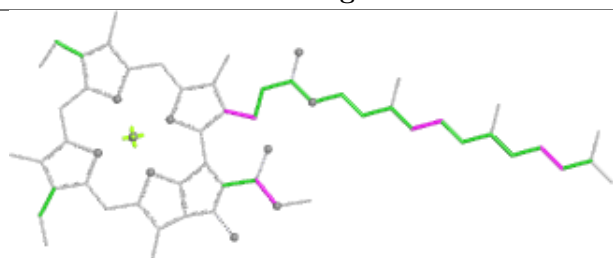
Ligand CLA b 607



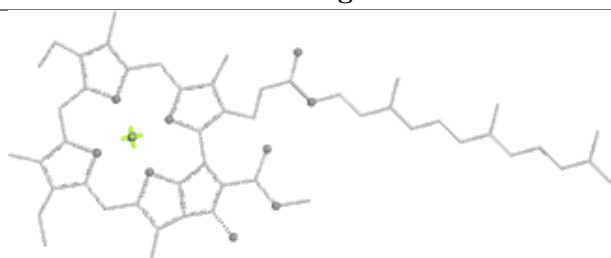
Bond lengths



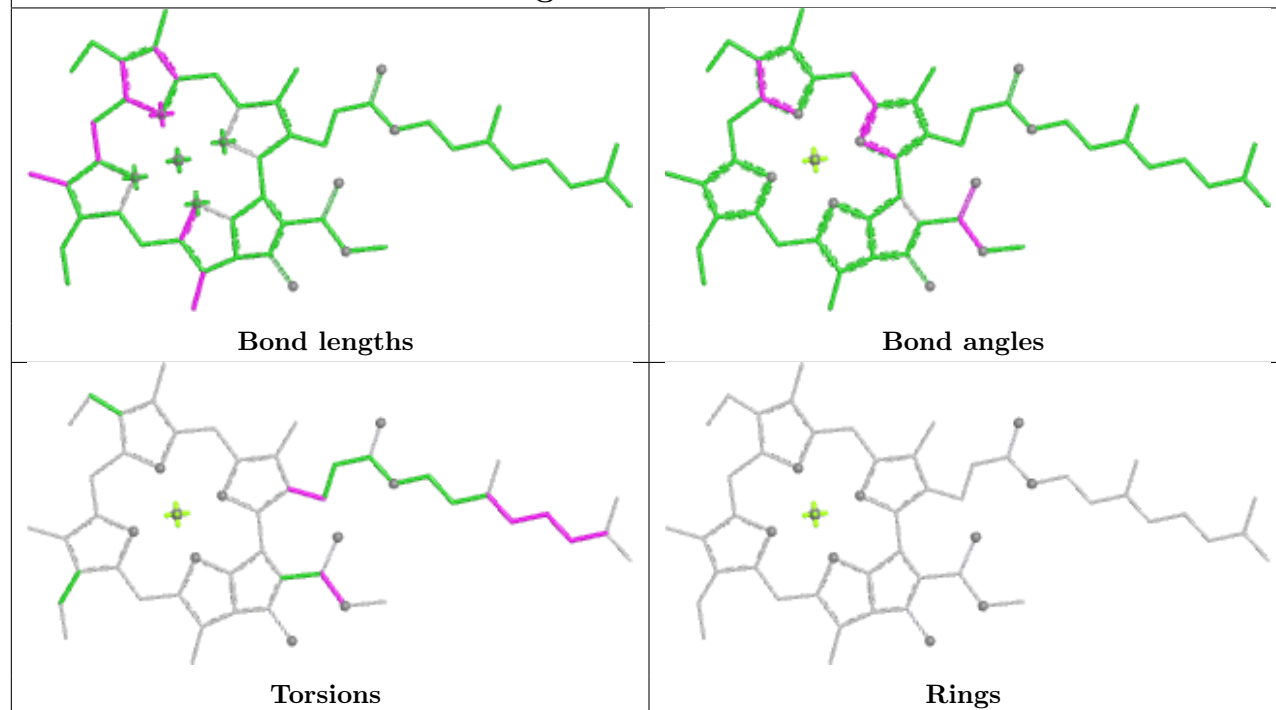
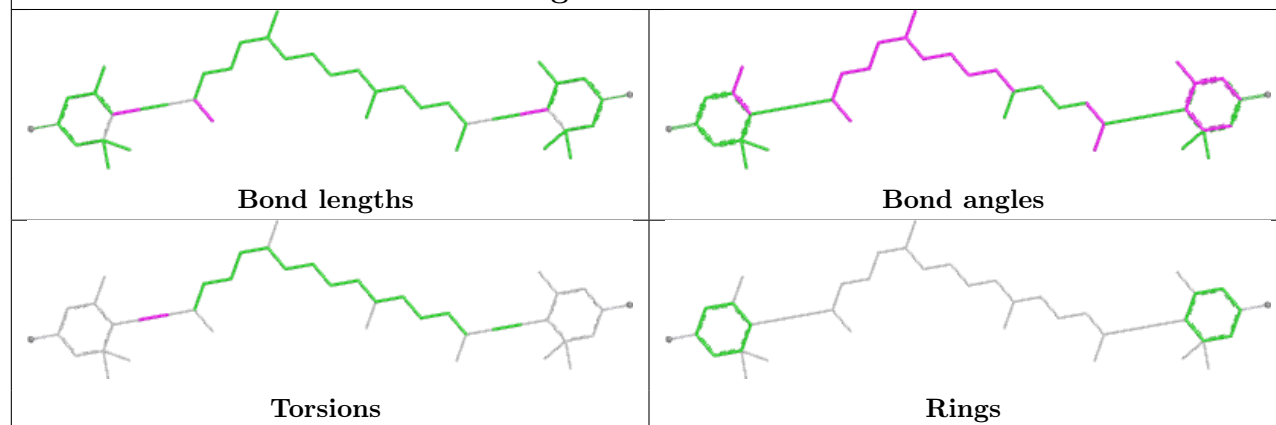
Bond angles



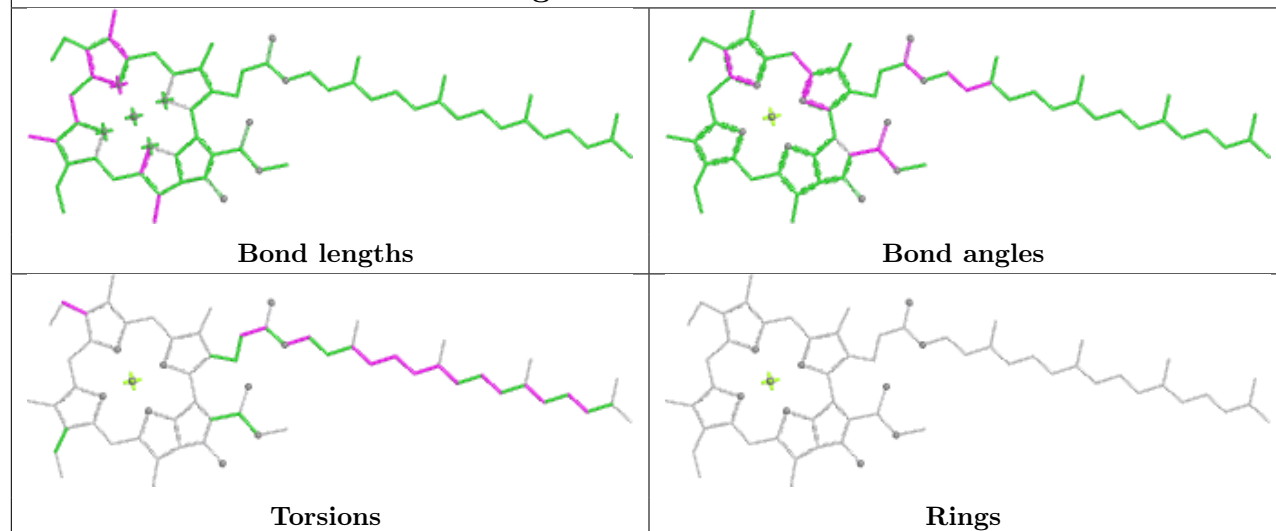
Torsions



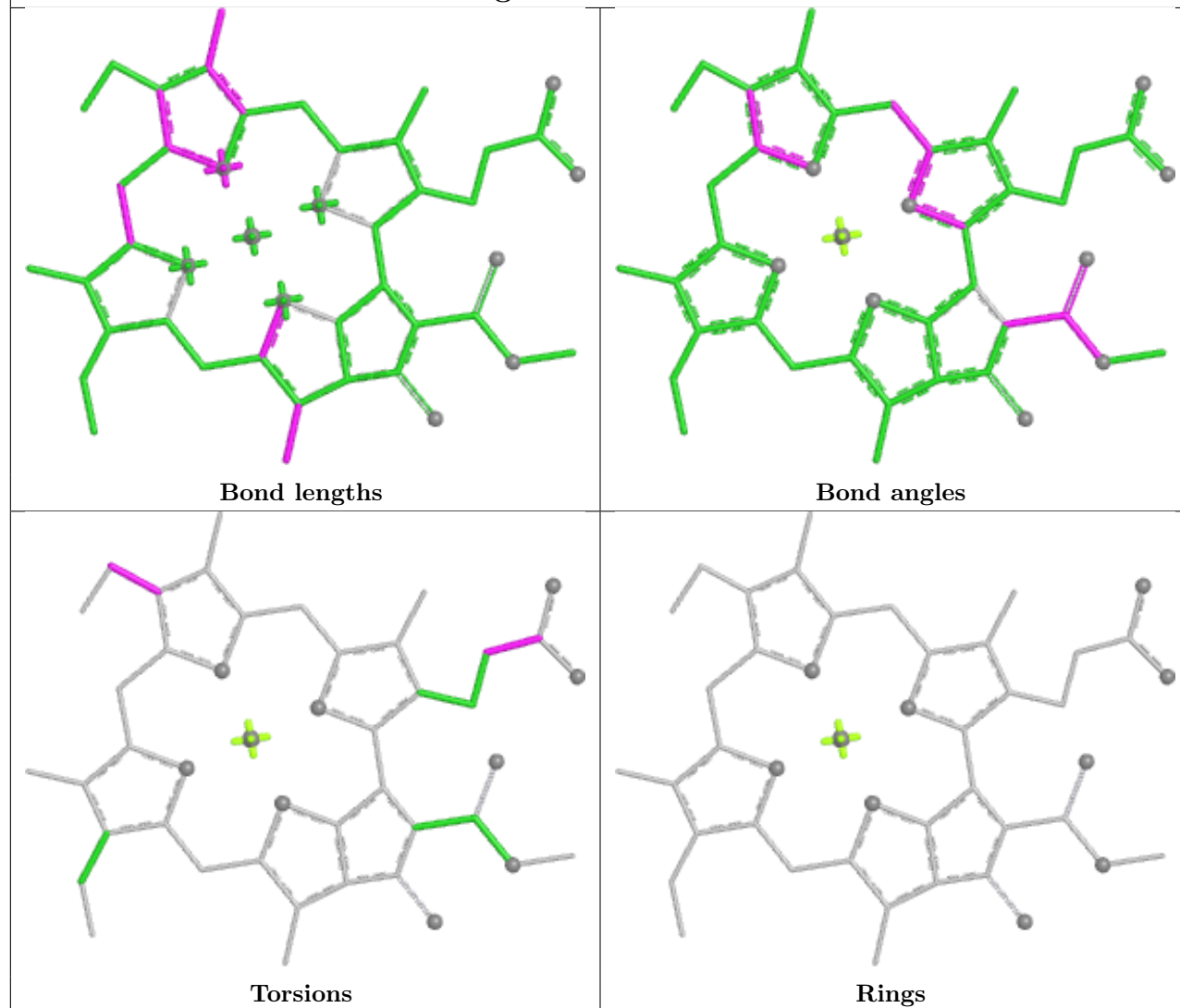
Rings

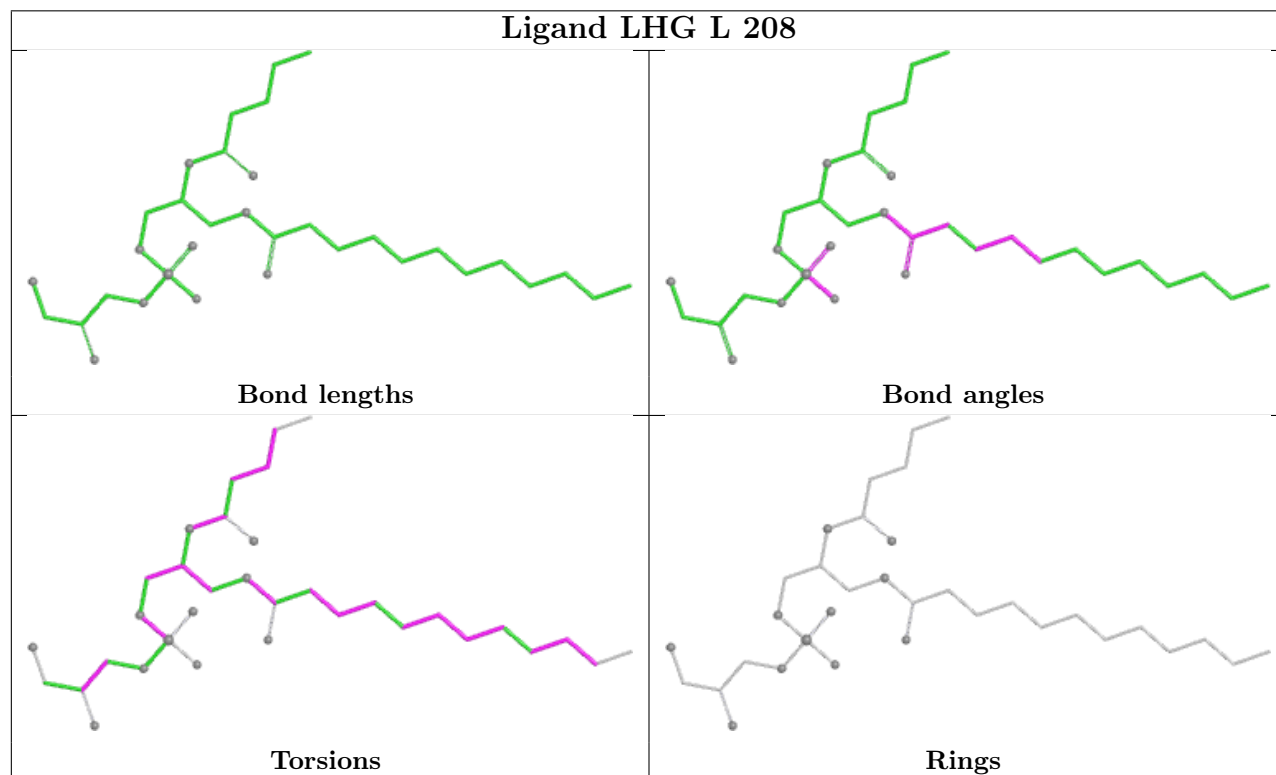
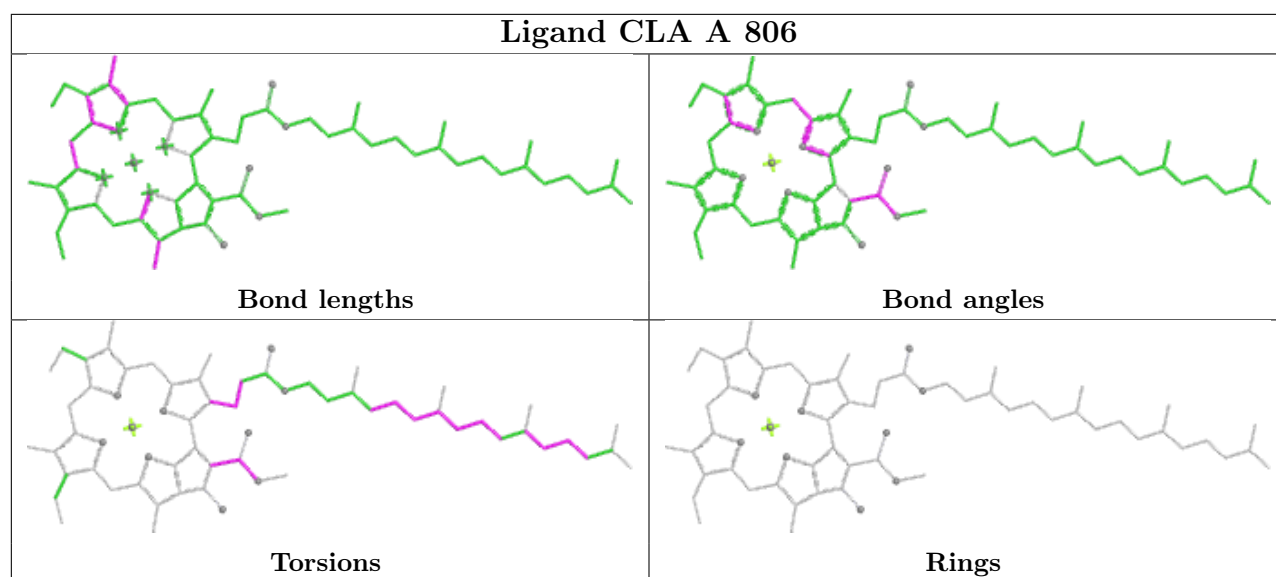
Ligand CLA 9 309**Ligand II0 a 613**

Ligand CLA B 806

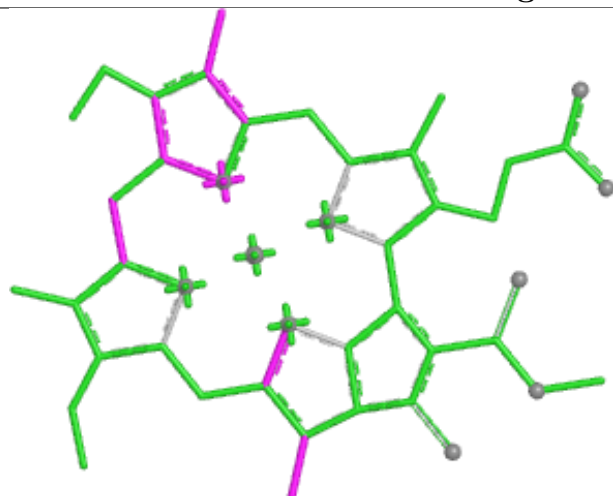


Ligand CLA d 605

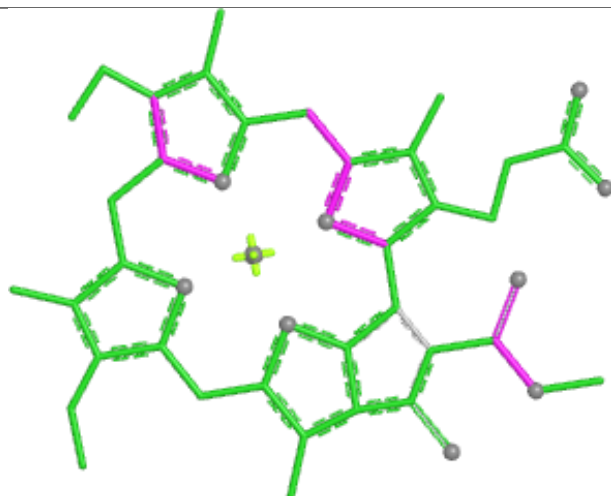




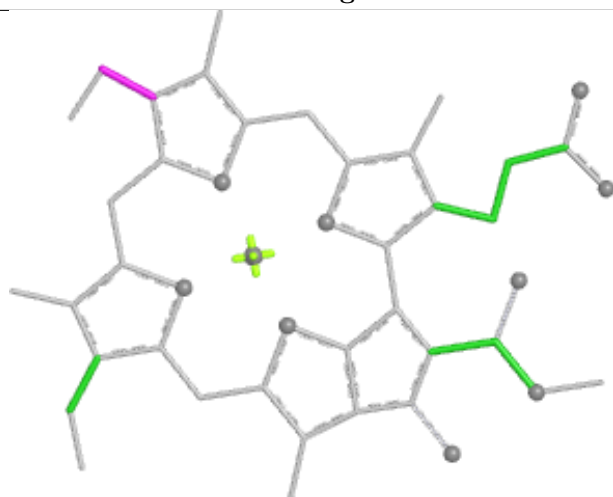
Ligand CLA b 601



Bond lengths



Bond angles

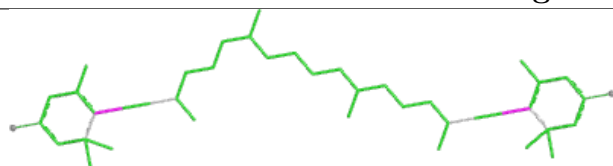


Torsions

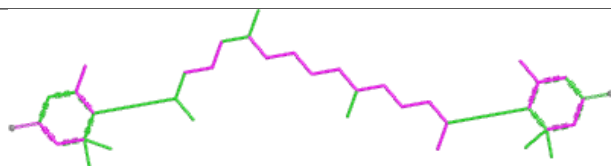


Rings

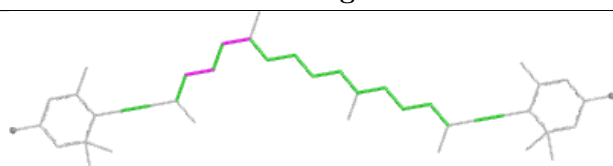
Ligand II0 9 318



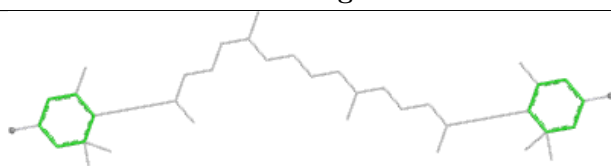
Bond lengths



Bond angles

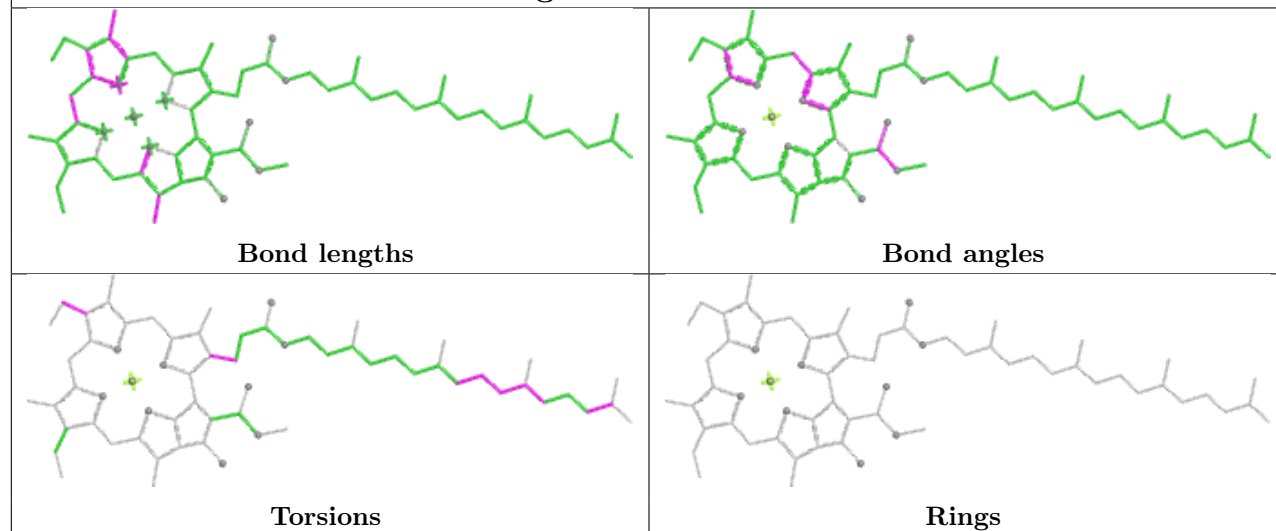


Torsions

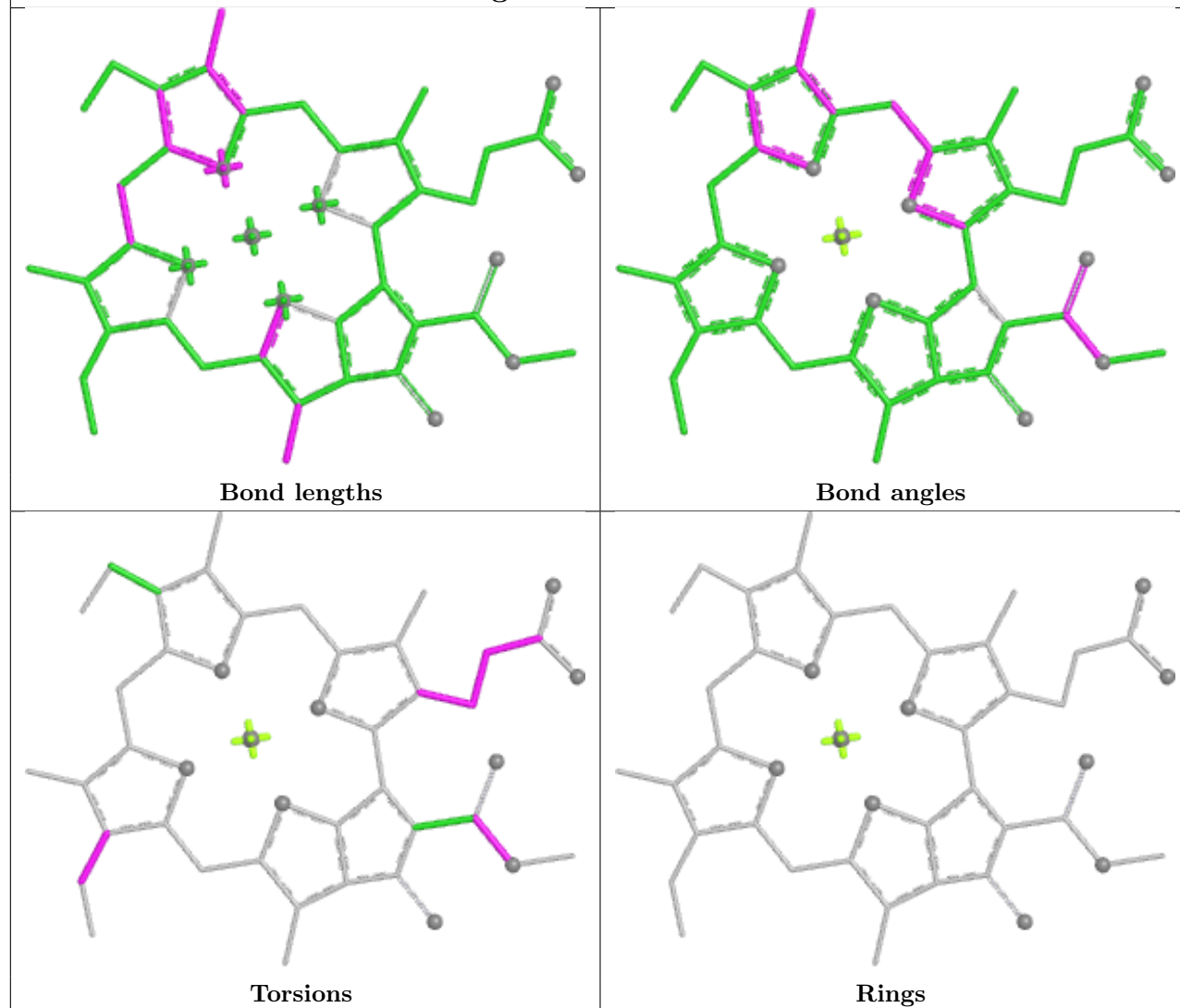


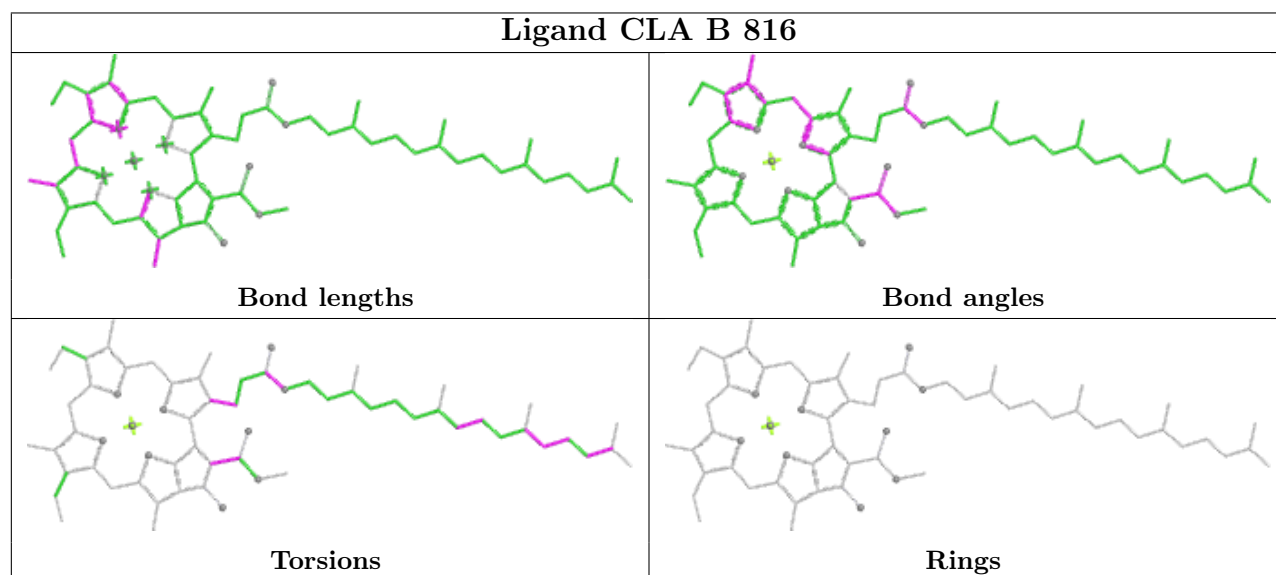
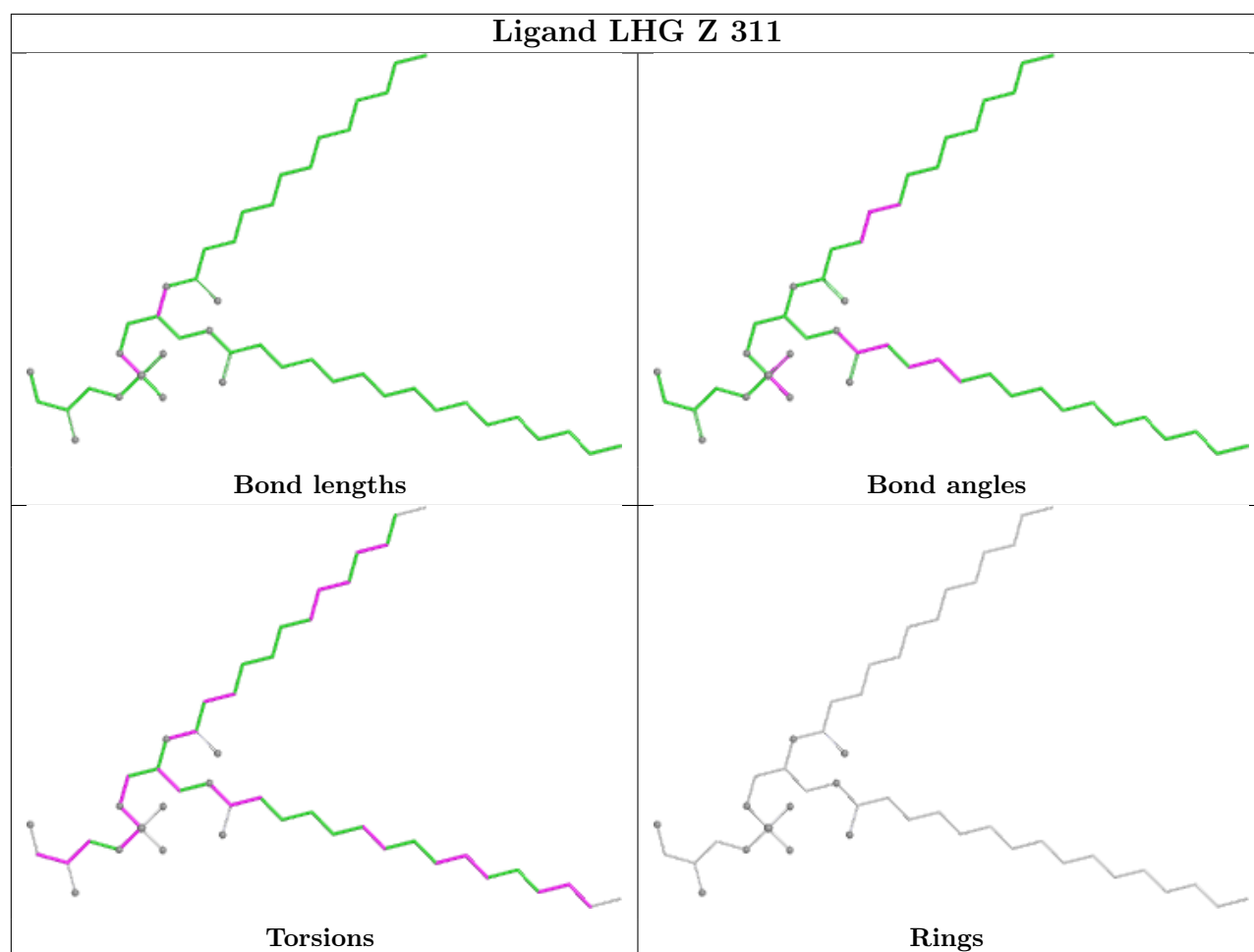
Rings

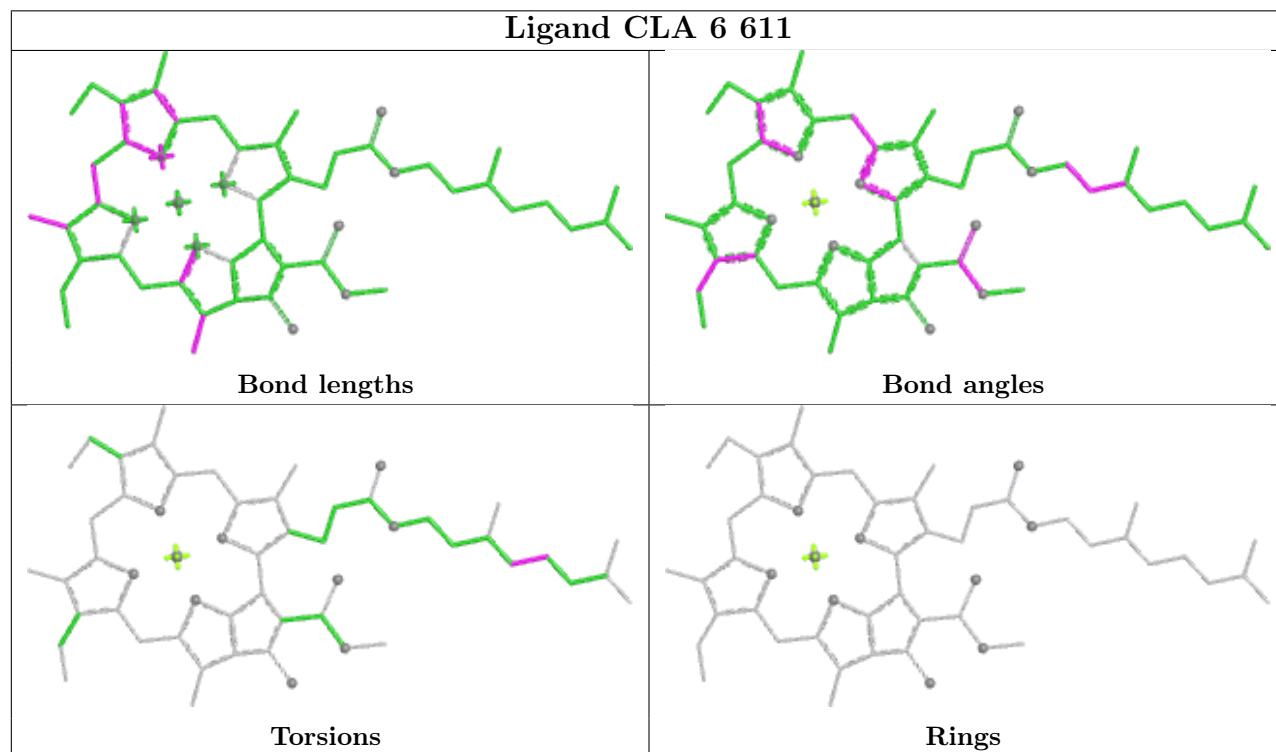
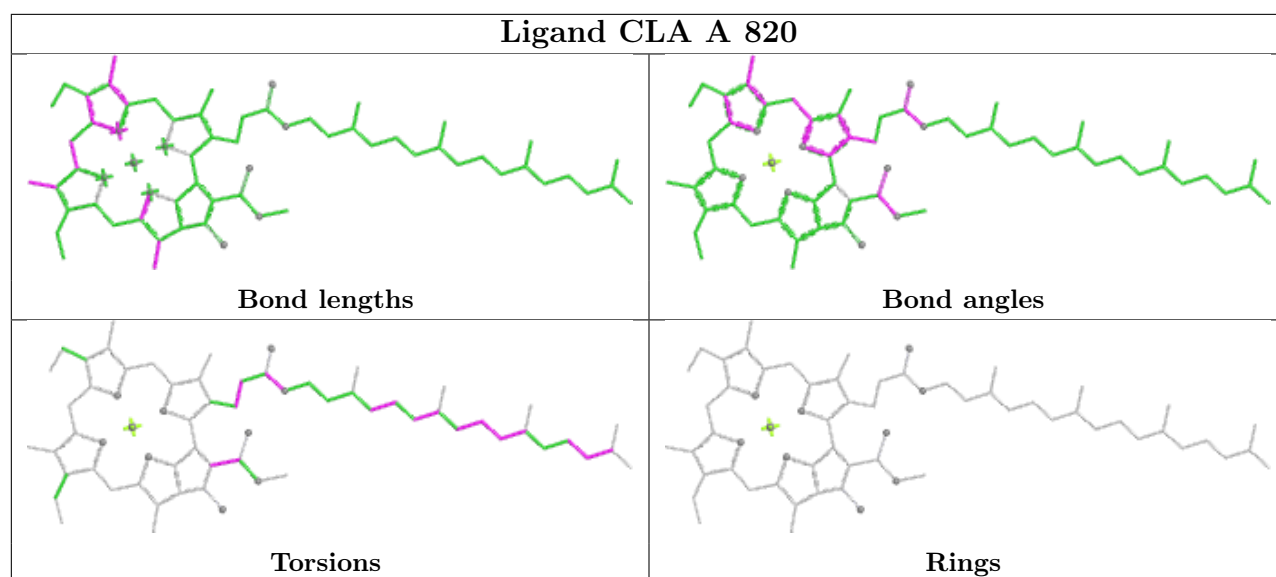
Ligand CLA 8 317



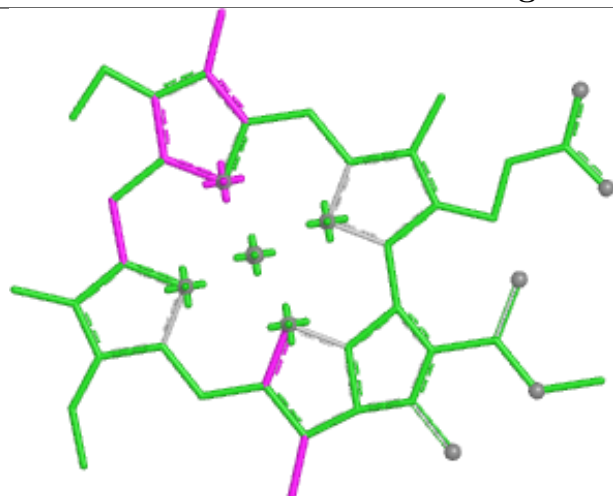
Ligand CLA A 814



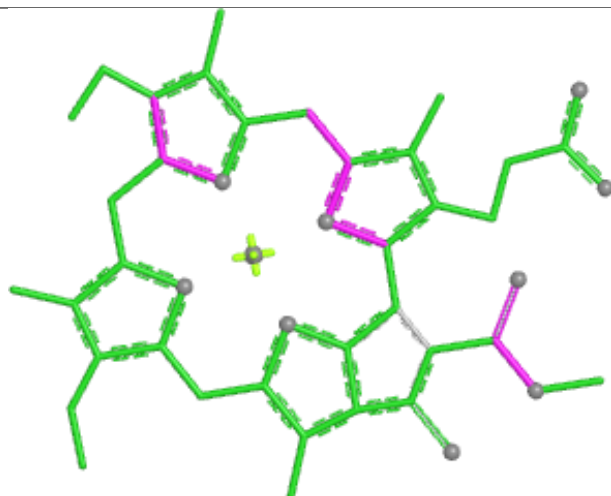




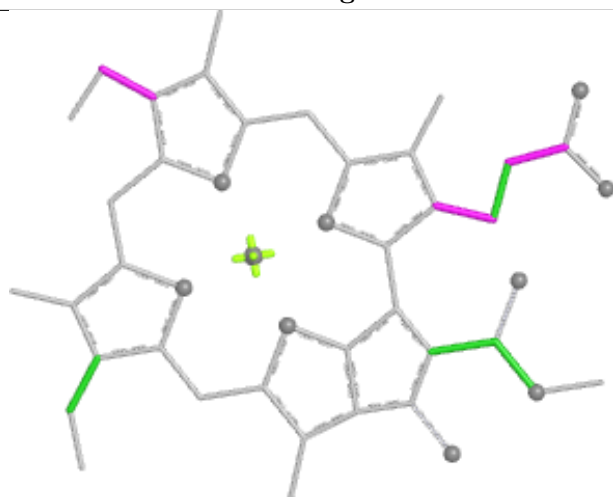
Ligand CLA 6 612



Bond lengths



Bond angles

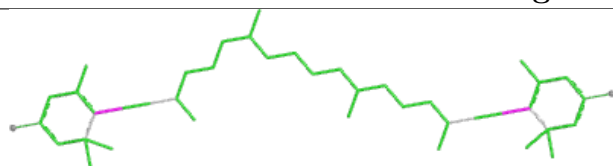


Torsions

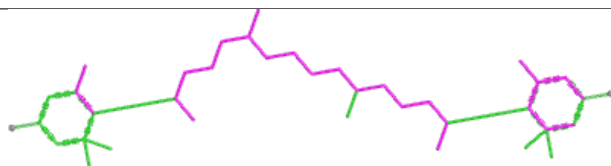


Rings

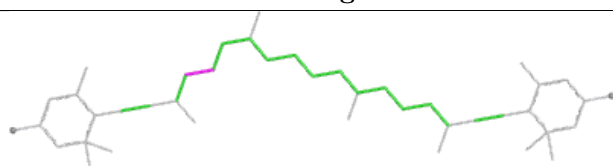
Ligand II0 5 614



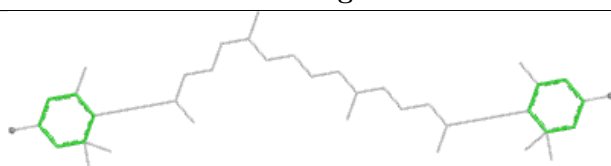
Bond lengths



Bond angles

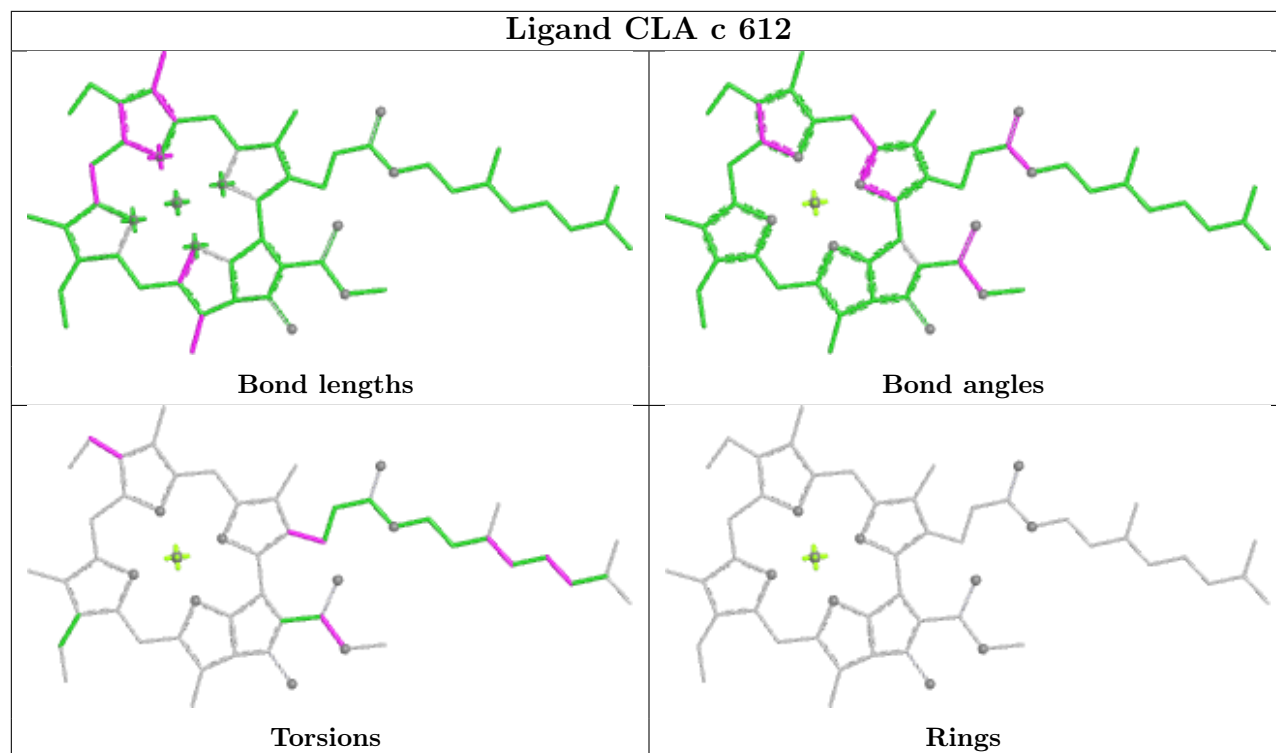


Torsions

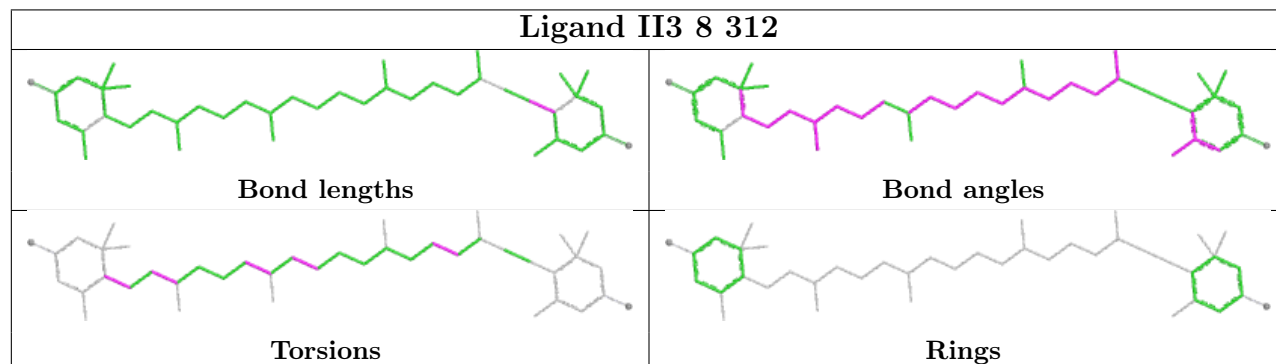


Rings

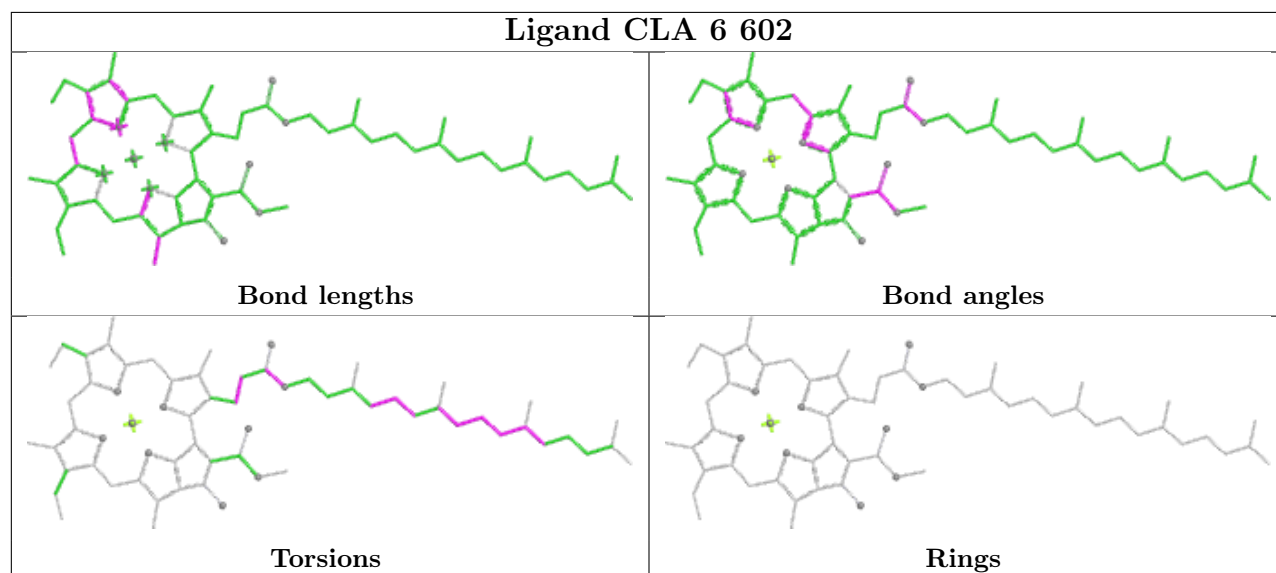
Ligand CLA c 612

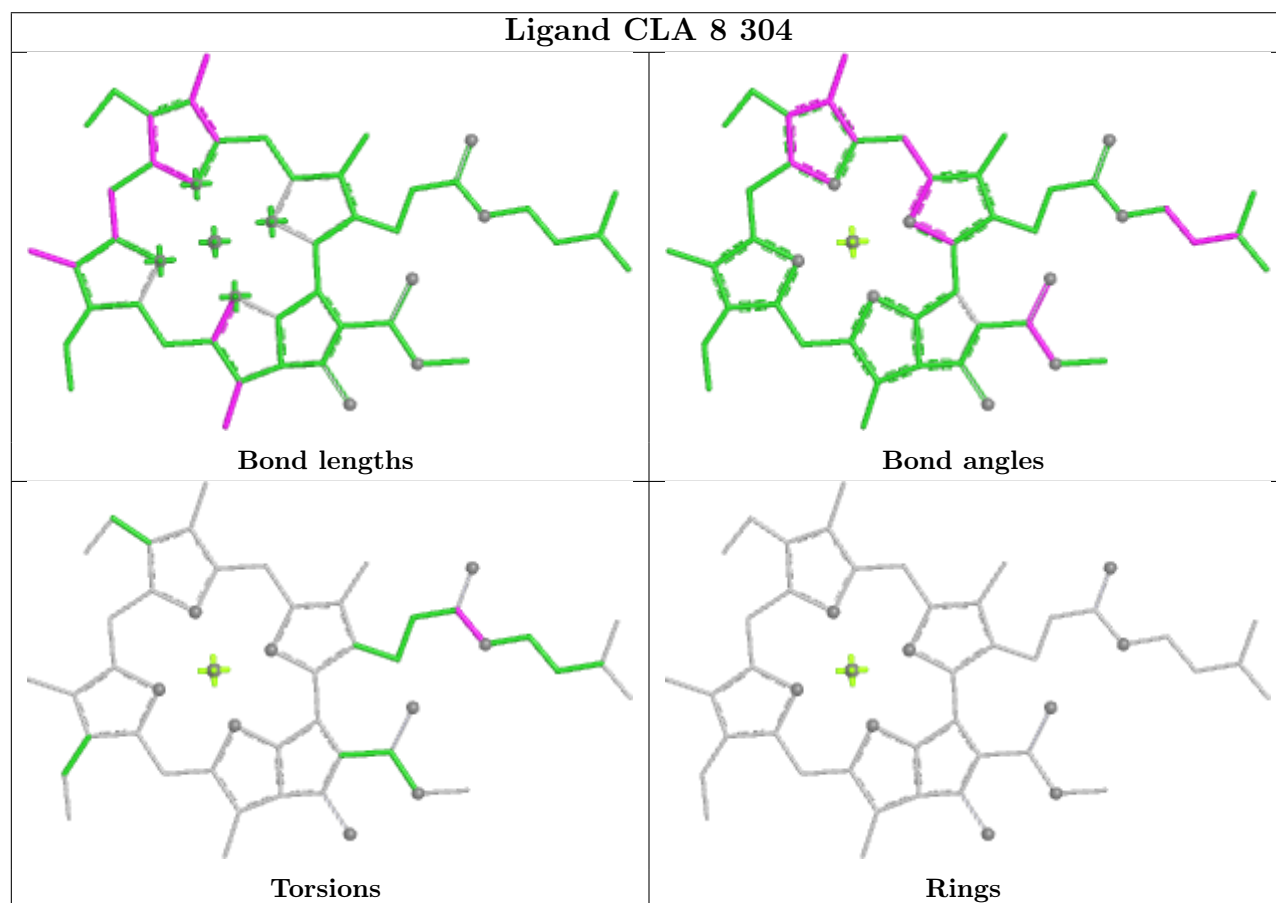
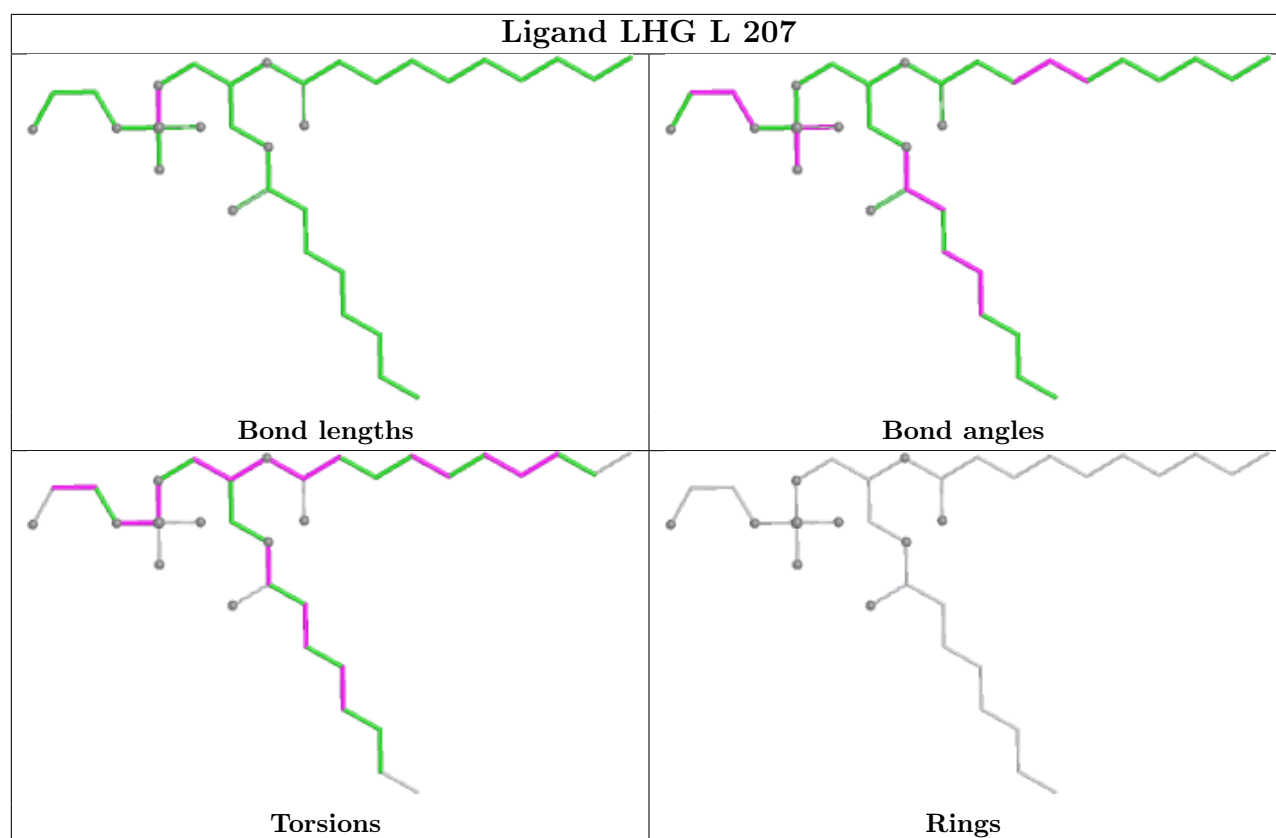


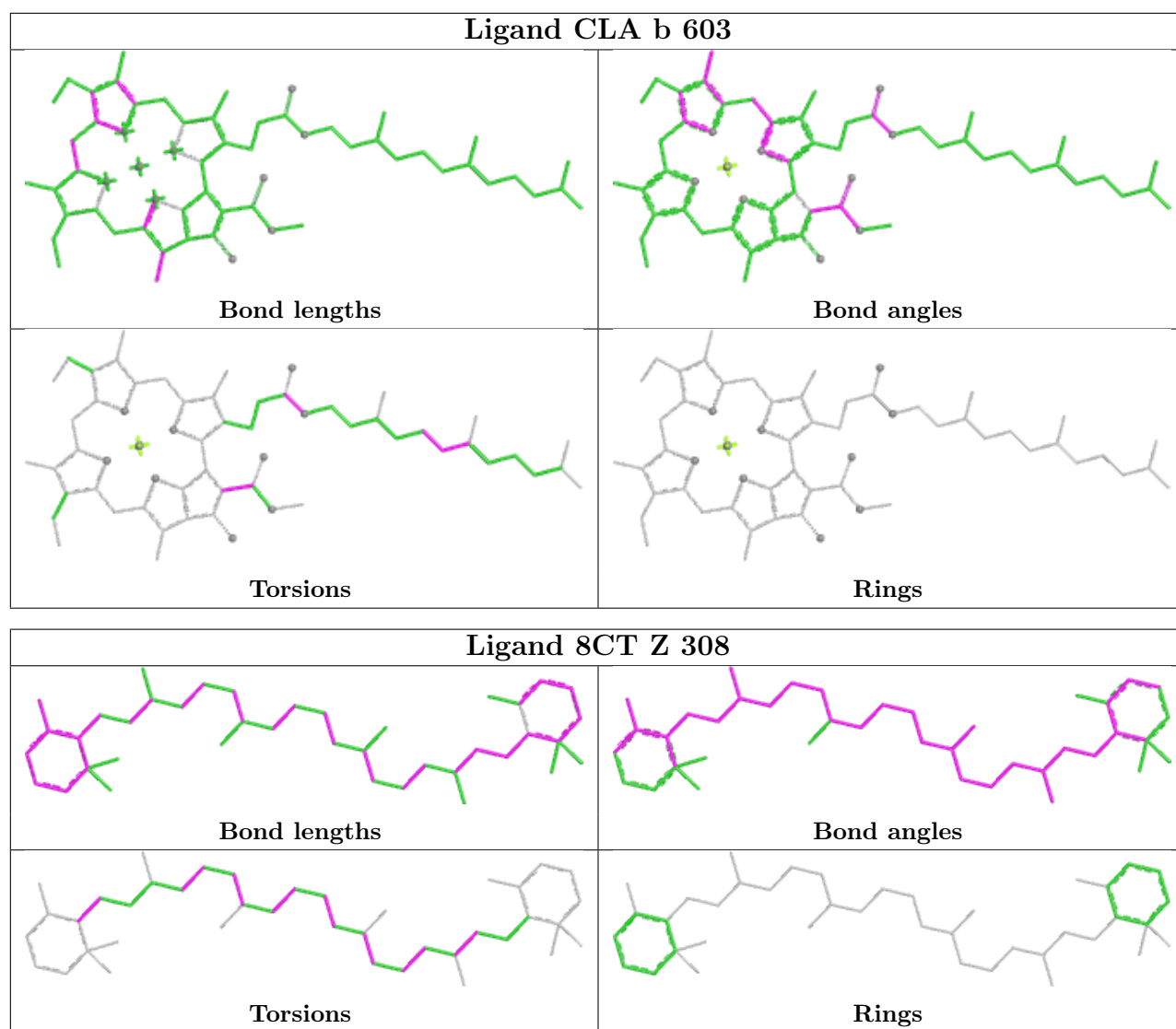
Ligand II3 8 312



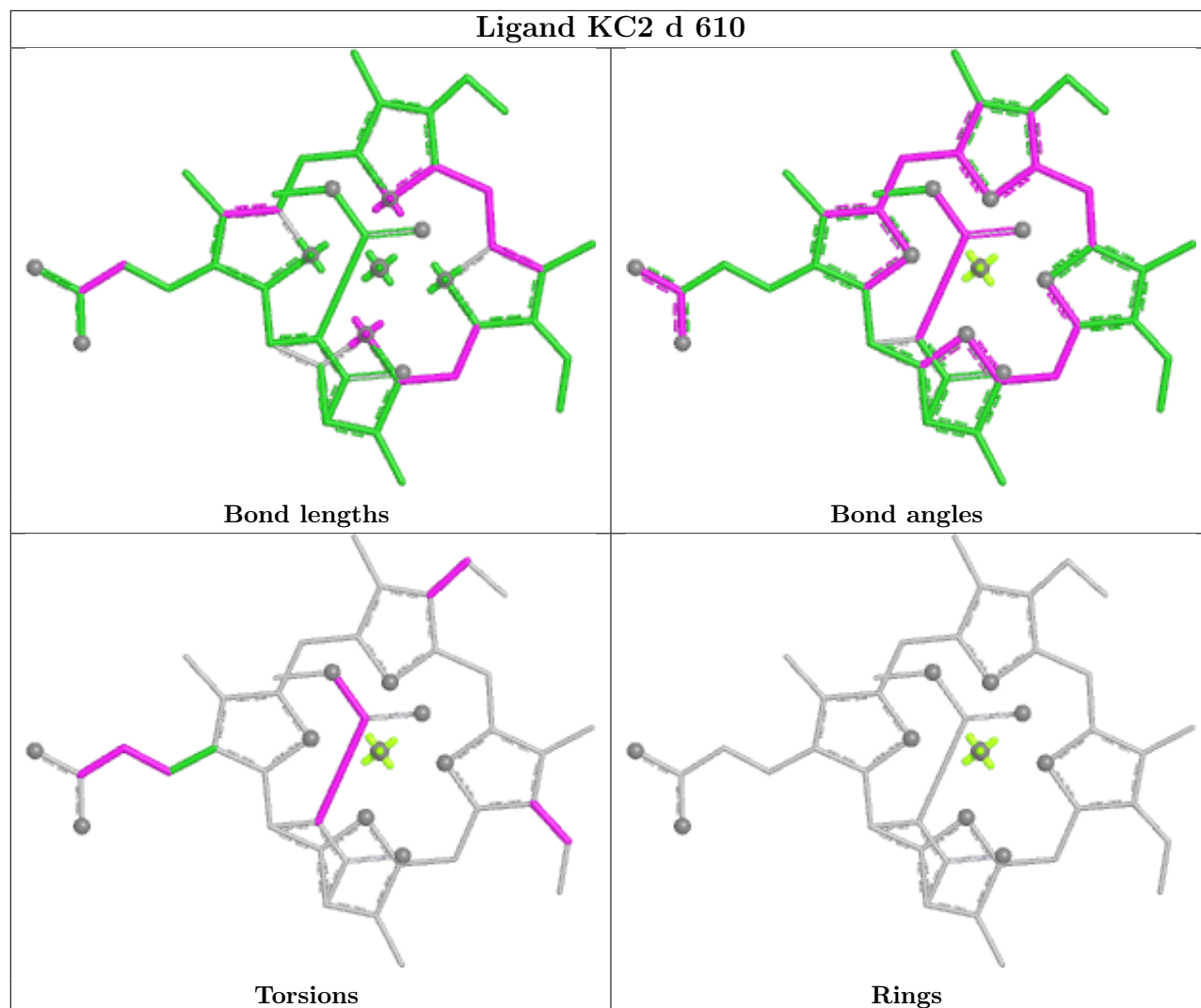
Ligand CLA 6 602



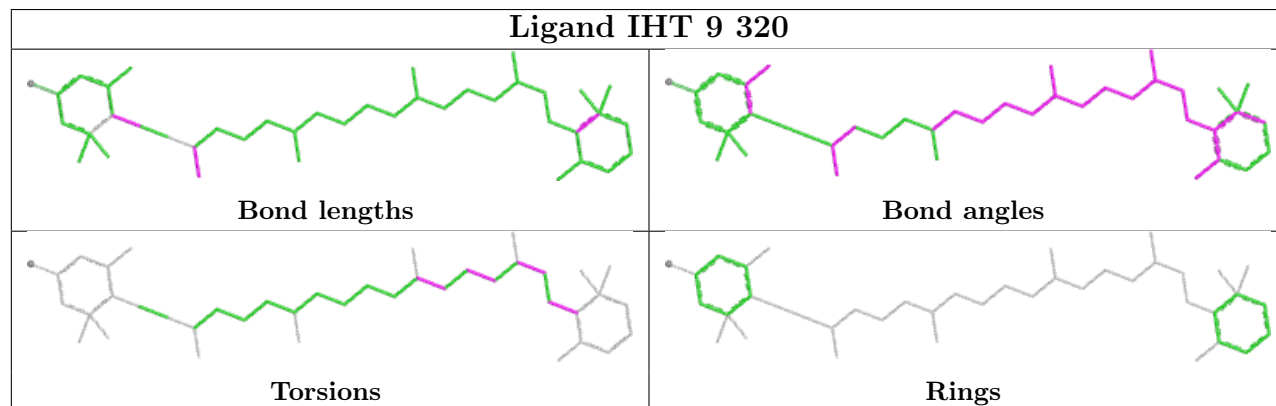




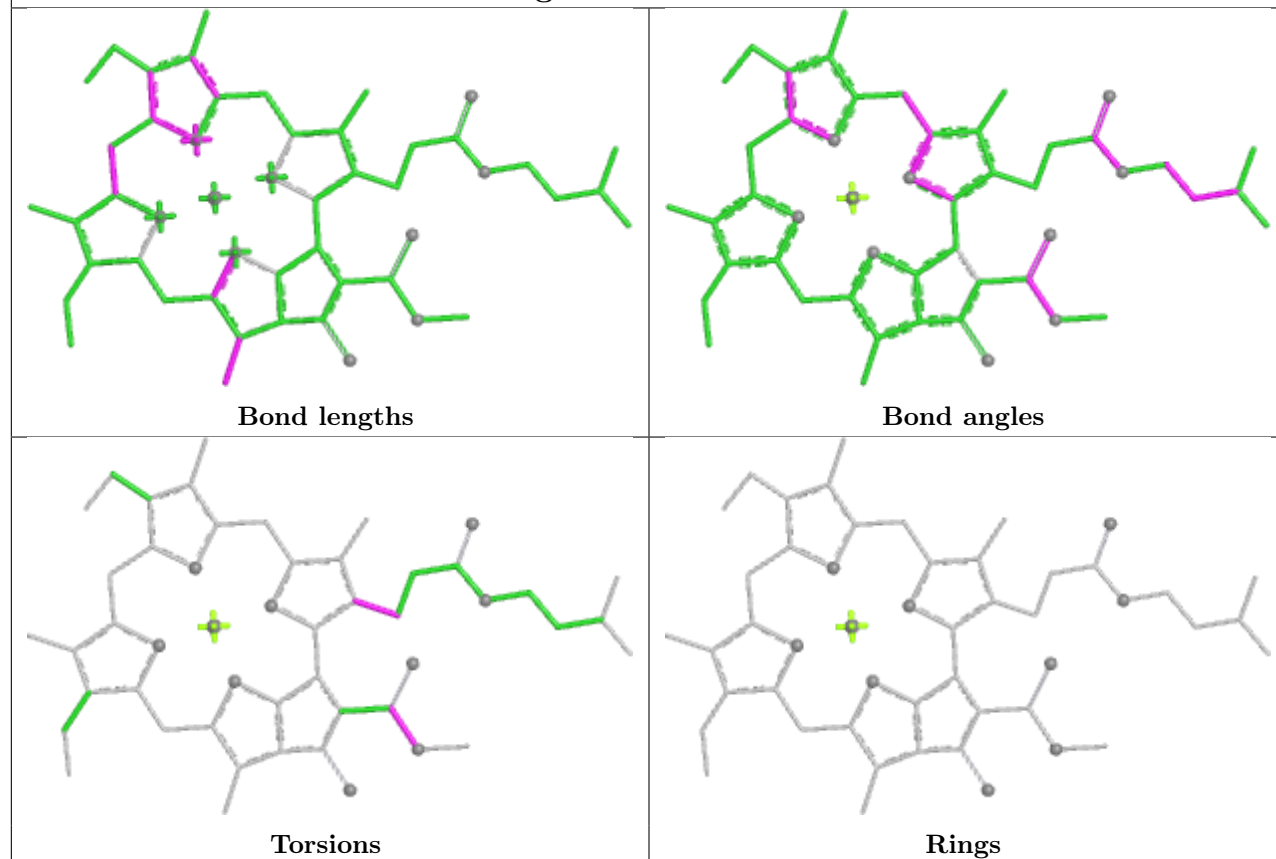
Ligand KC2 d 610



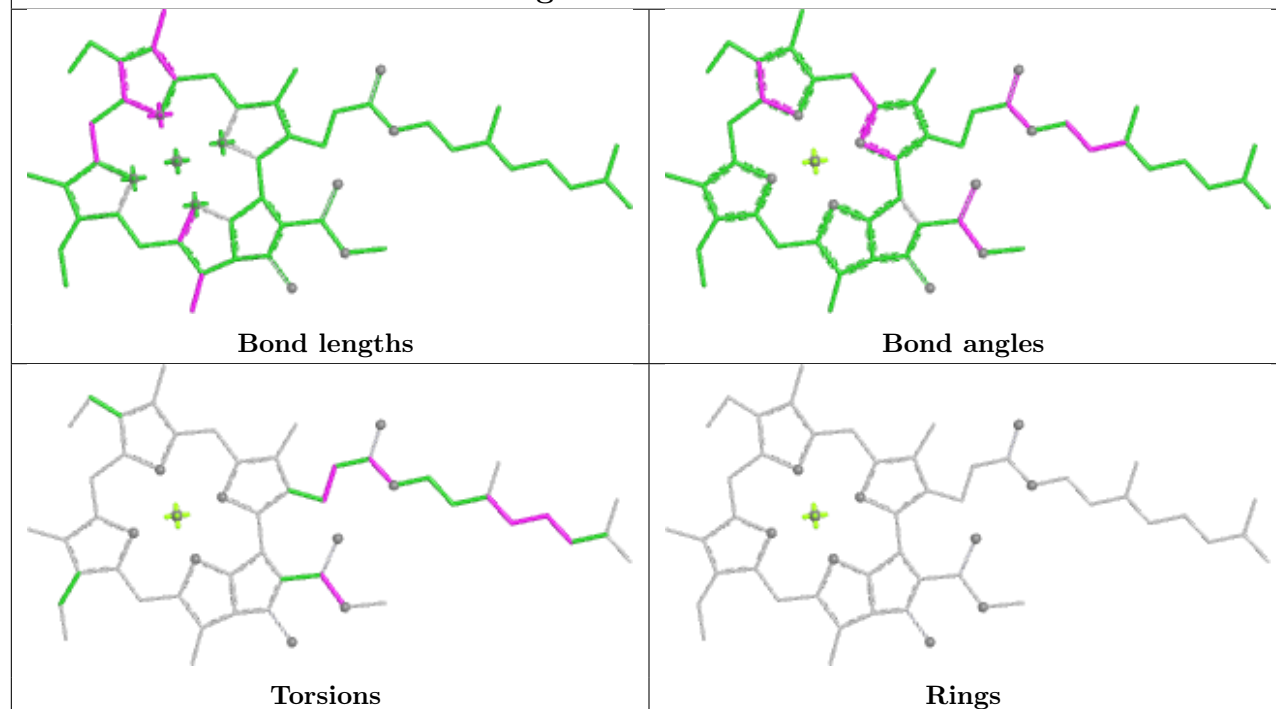
Ligand IHT 9 320



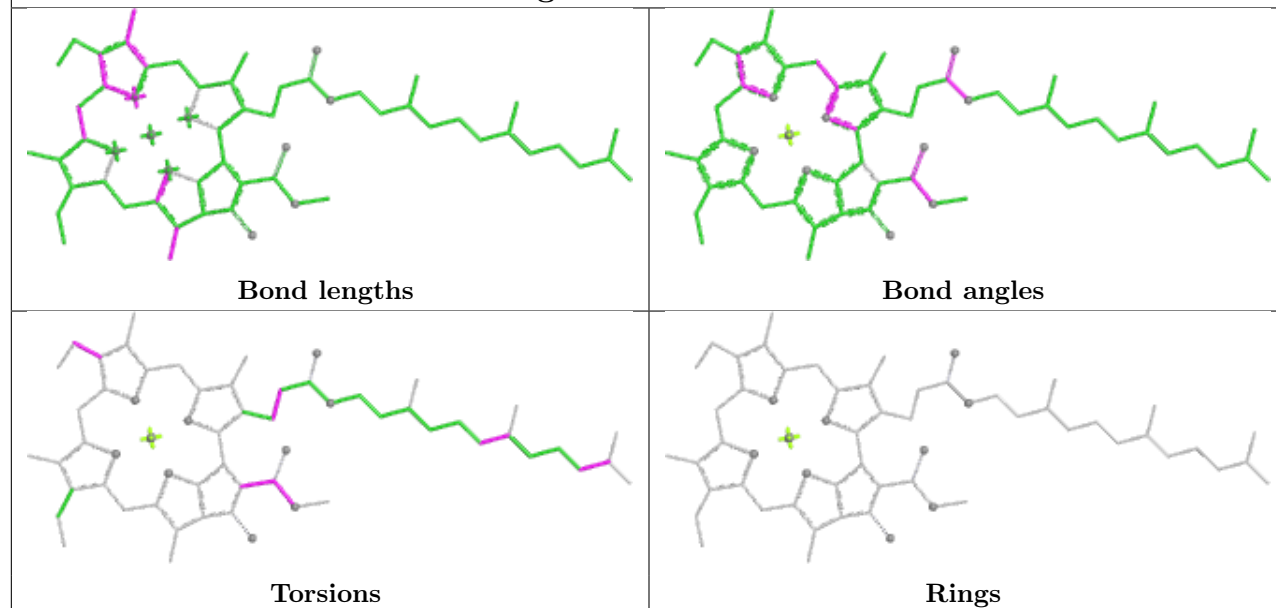
Ligand CLA d 603



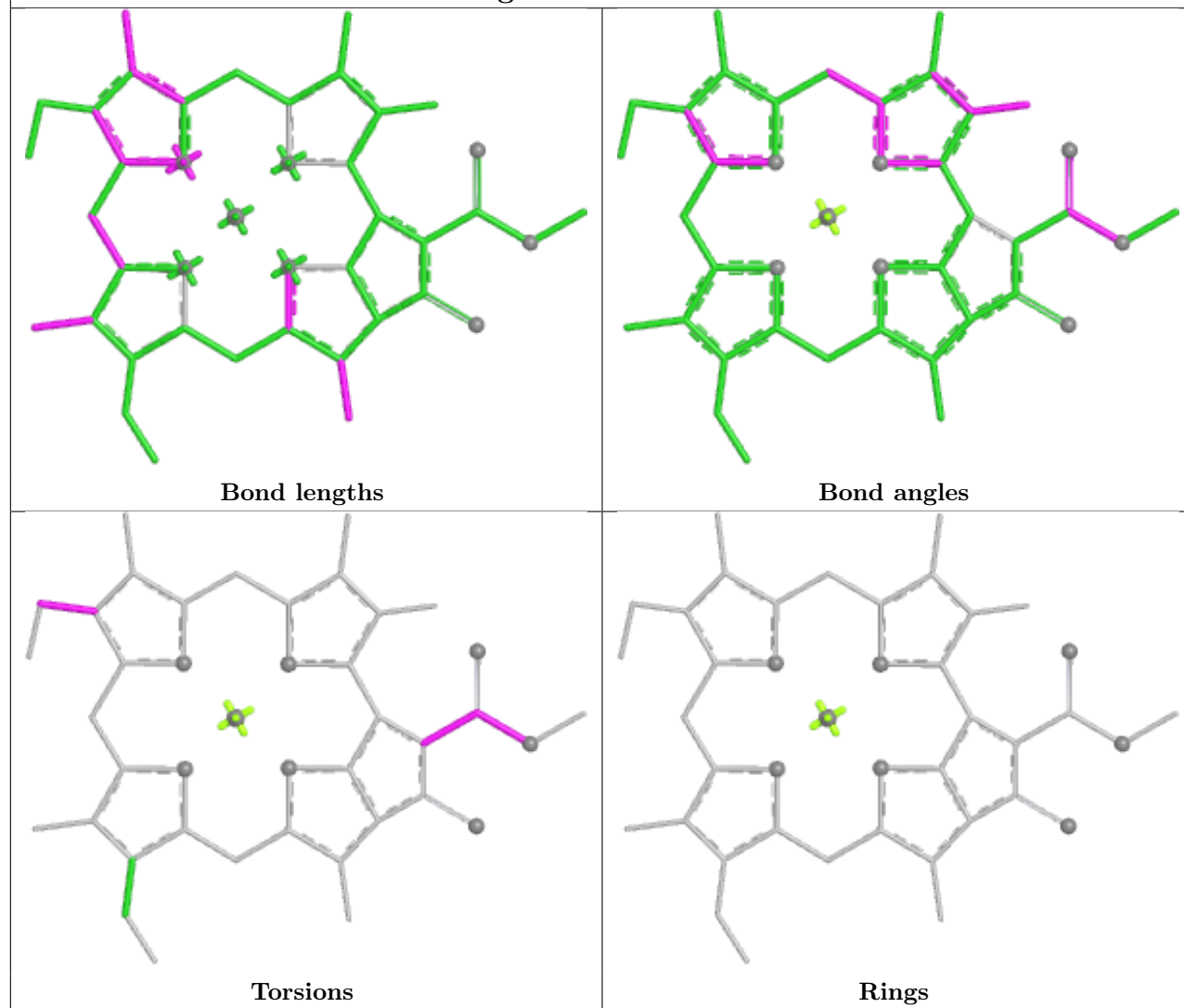
Ligand CLA 8 305

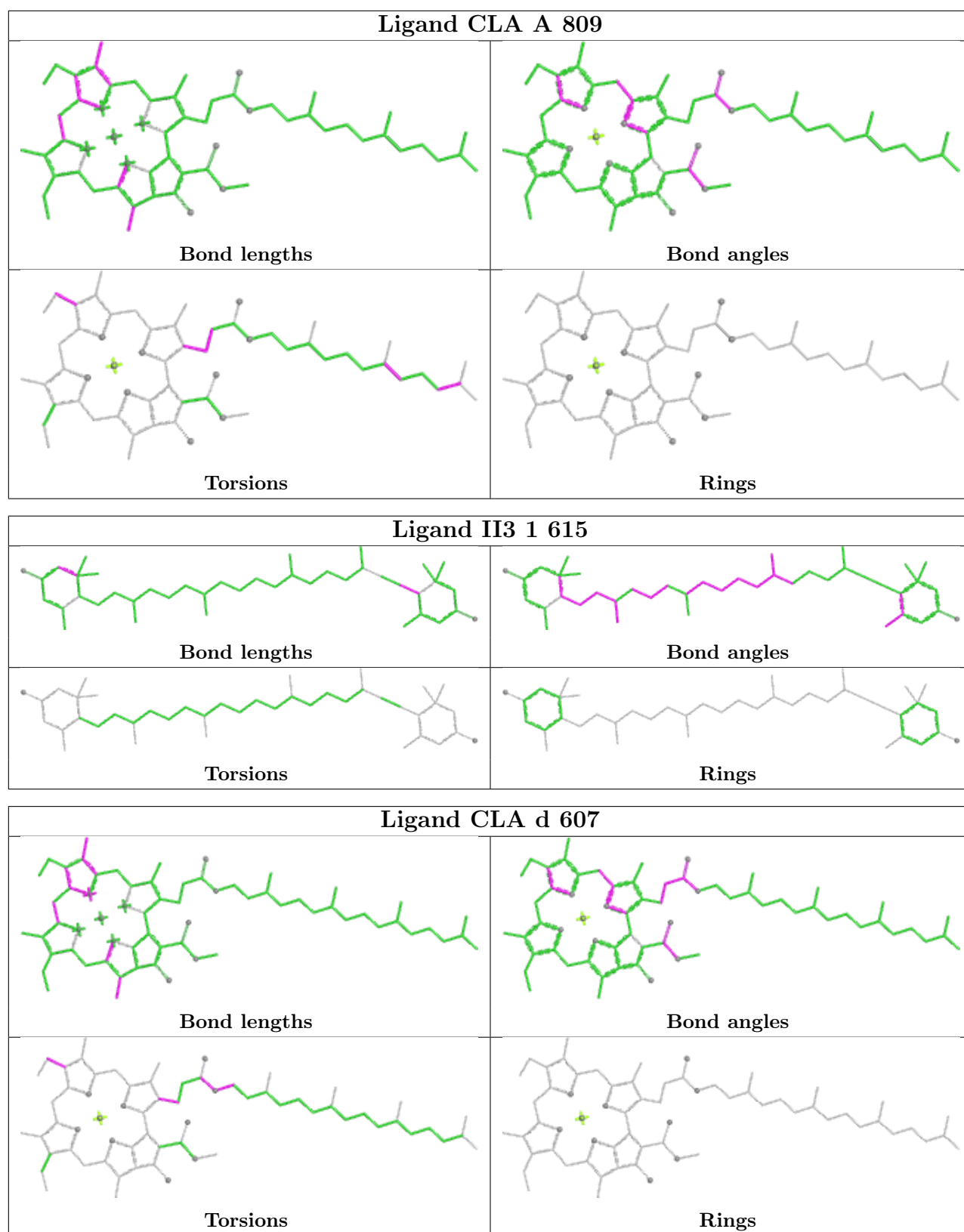


Ligand CLA c 604

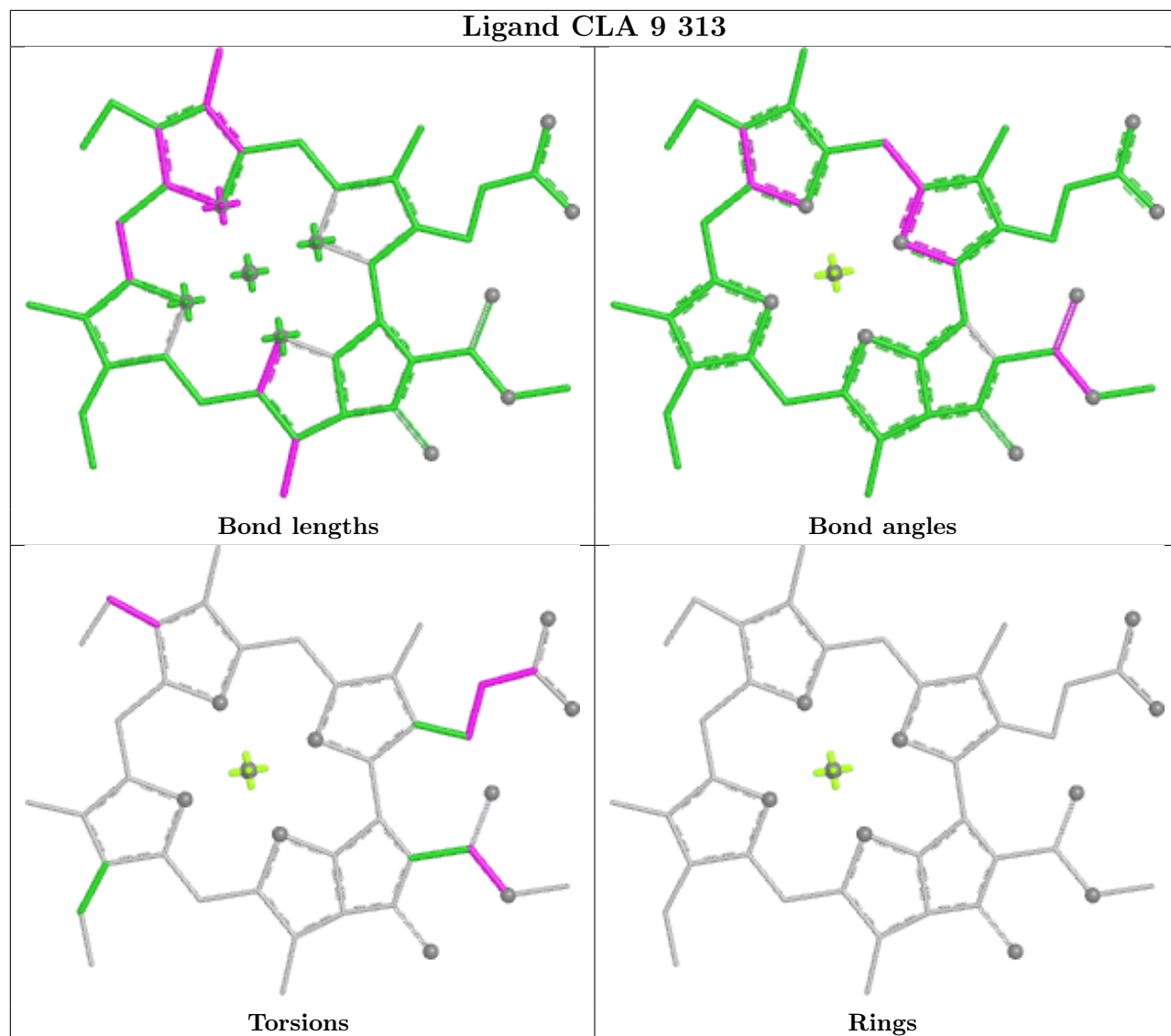


Ligand CLA 8 307

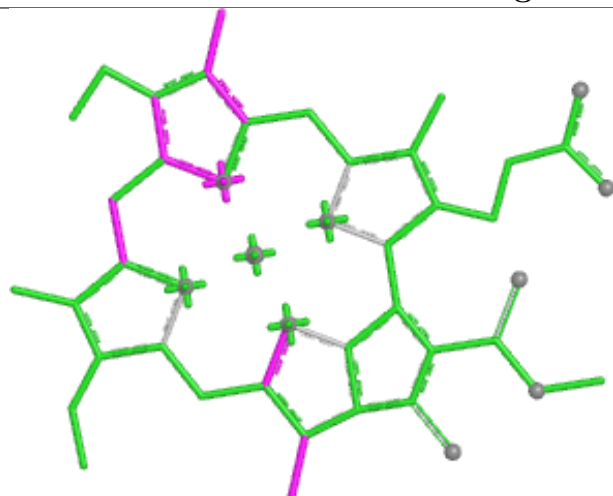




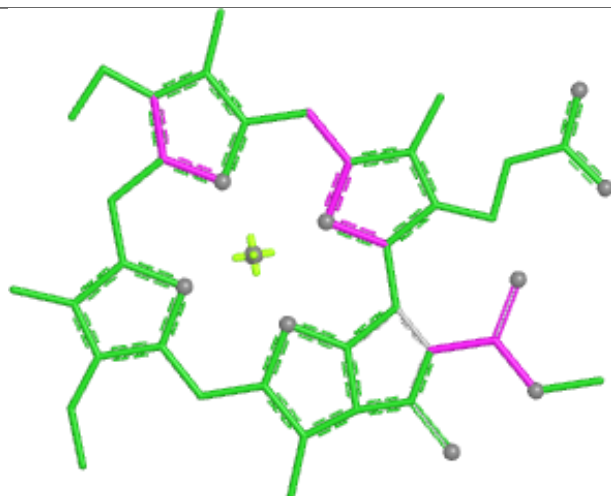
Ligand CLA 9 313



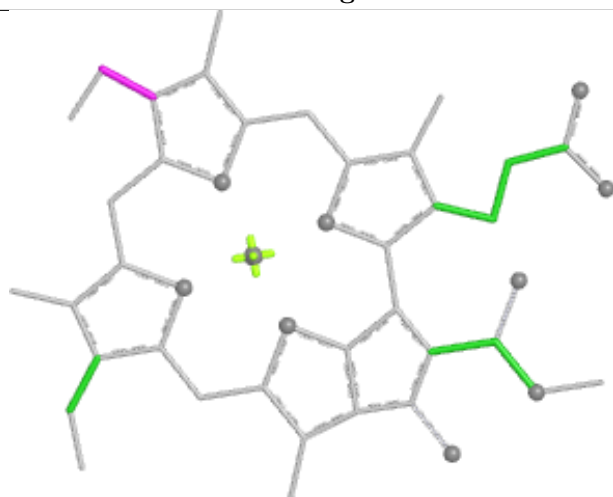
Ligand CLA B 830



Bond lengths



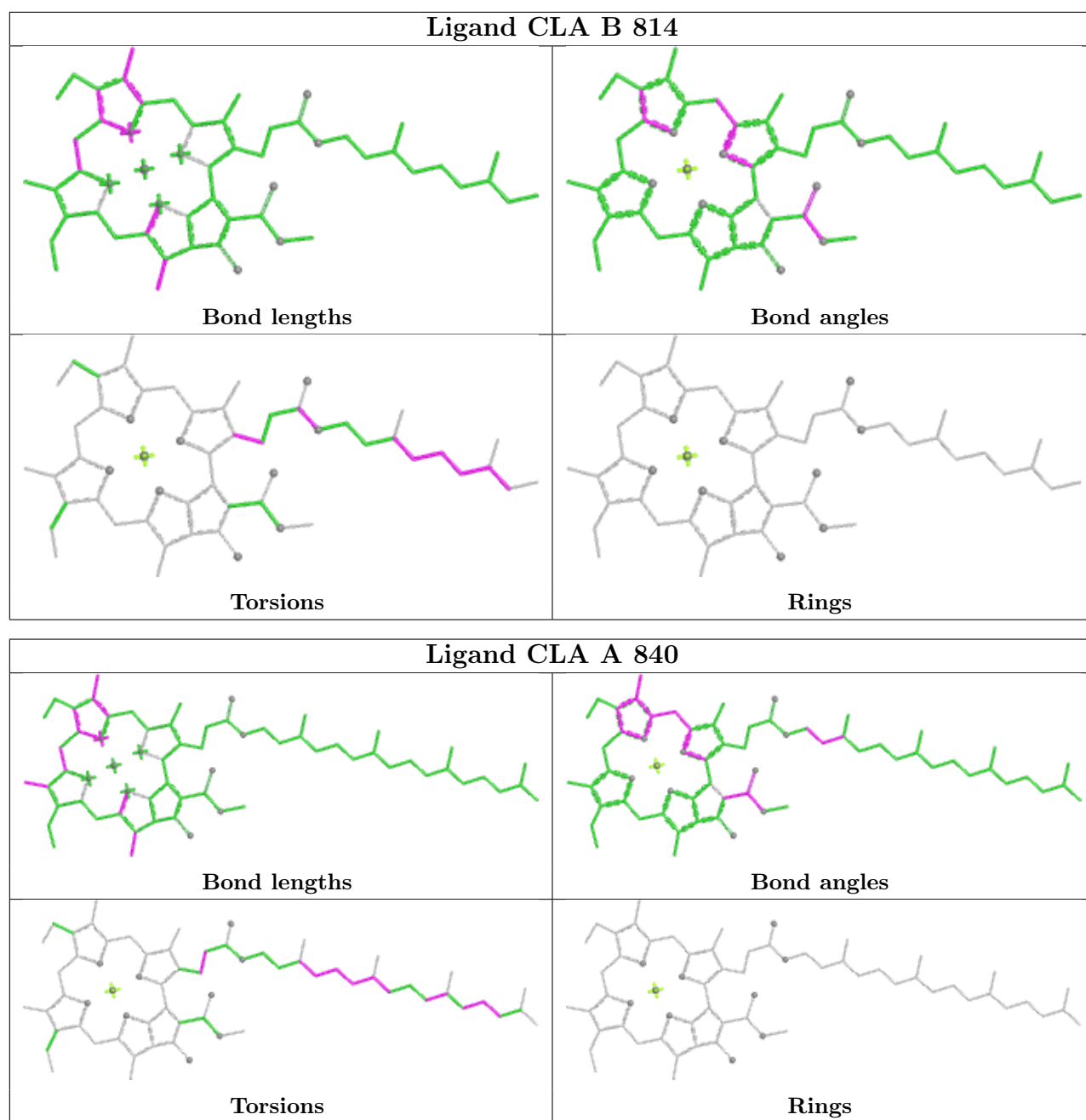
Bond angles



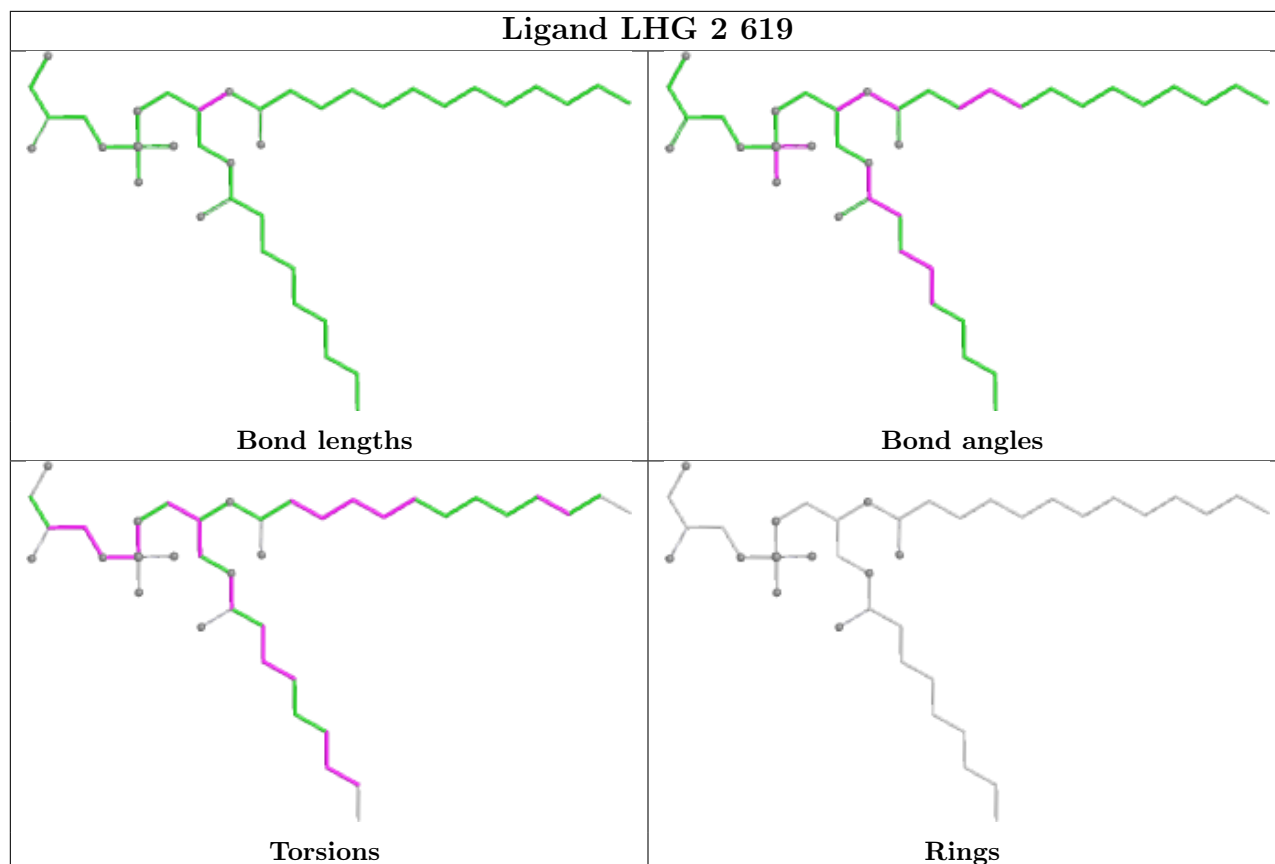
Torsions



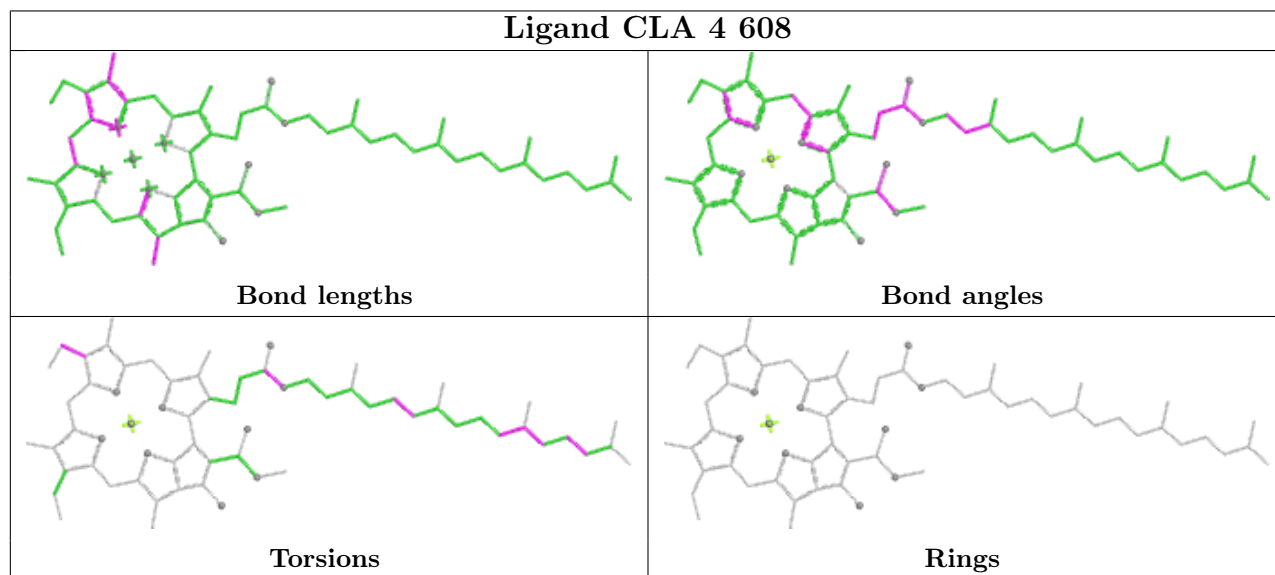
Rings

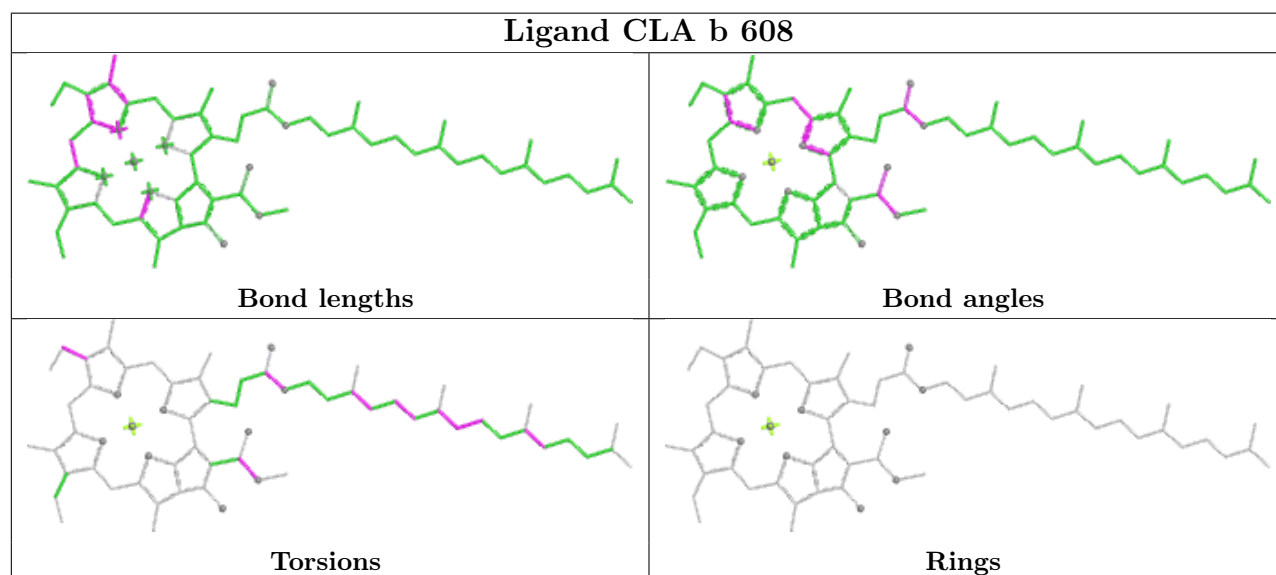
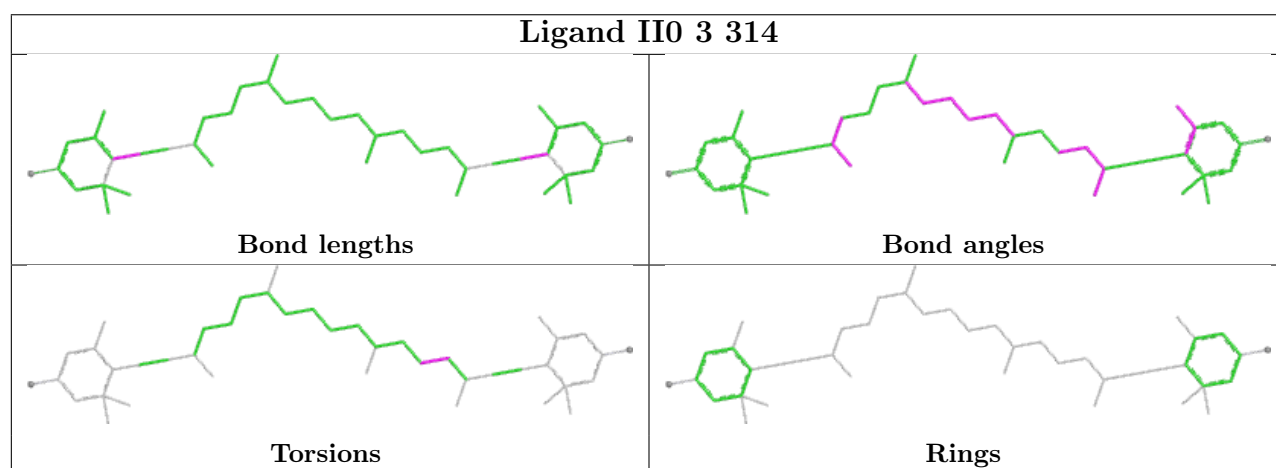
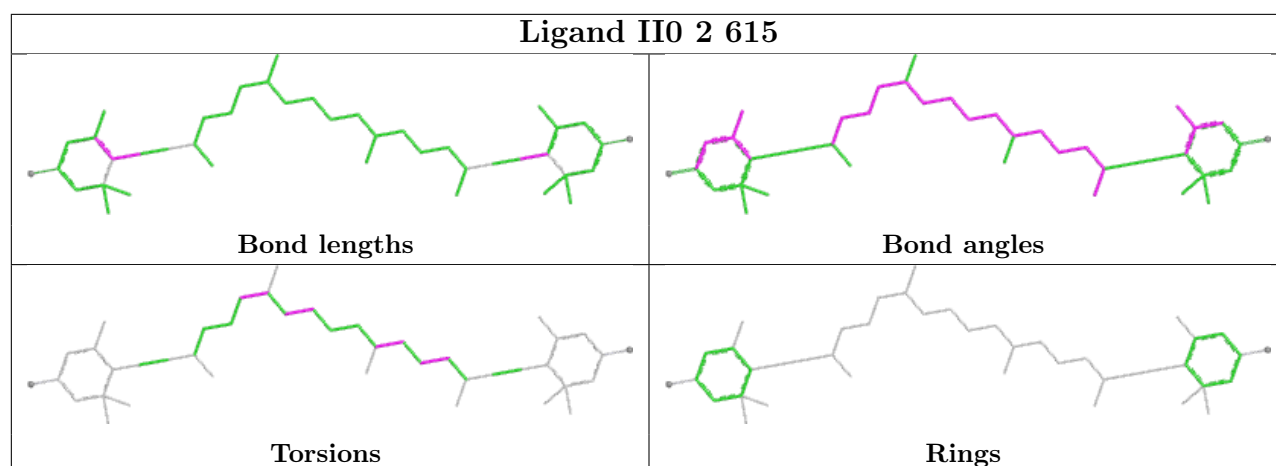


Ligand LHG 2 619

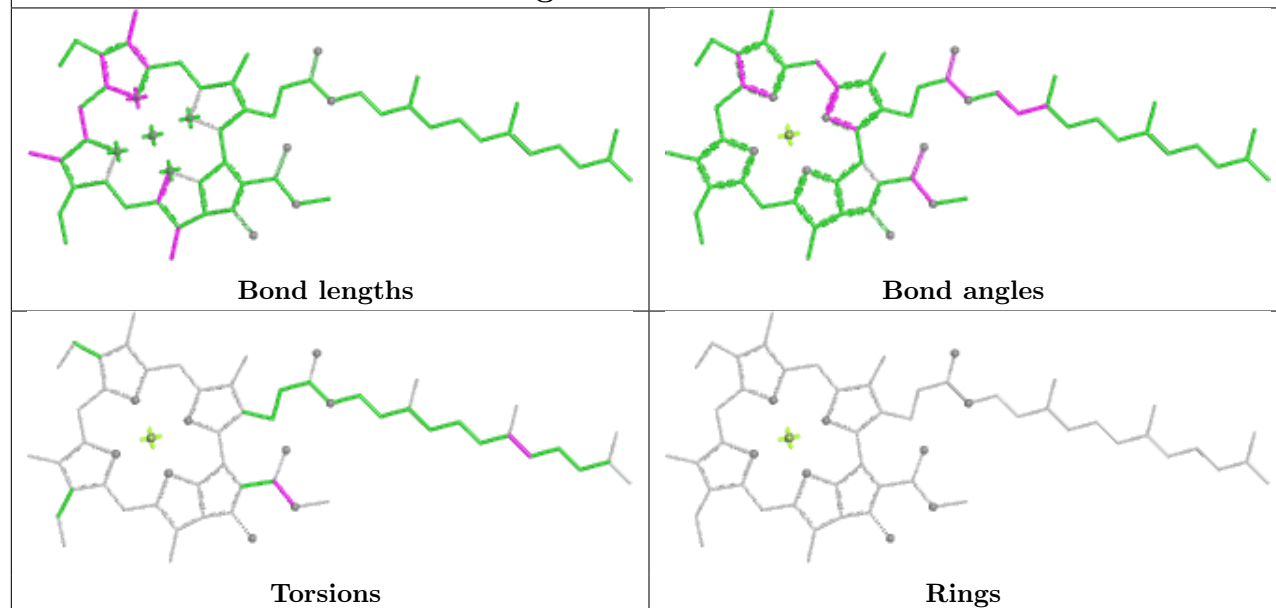


Ligand CLA 4 608

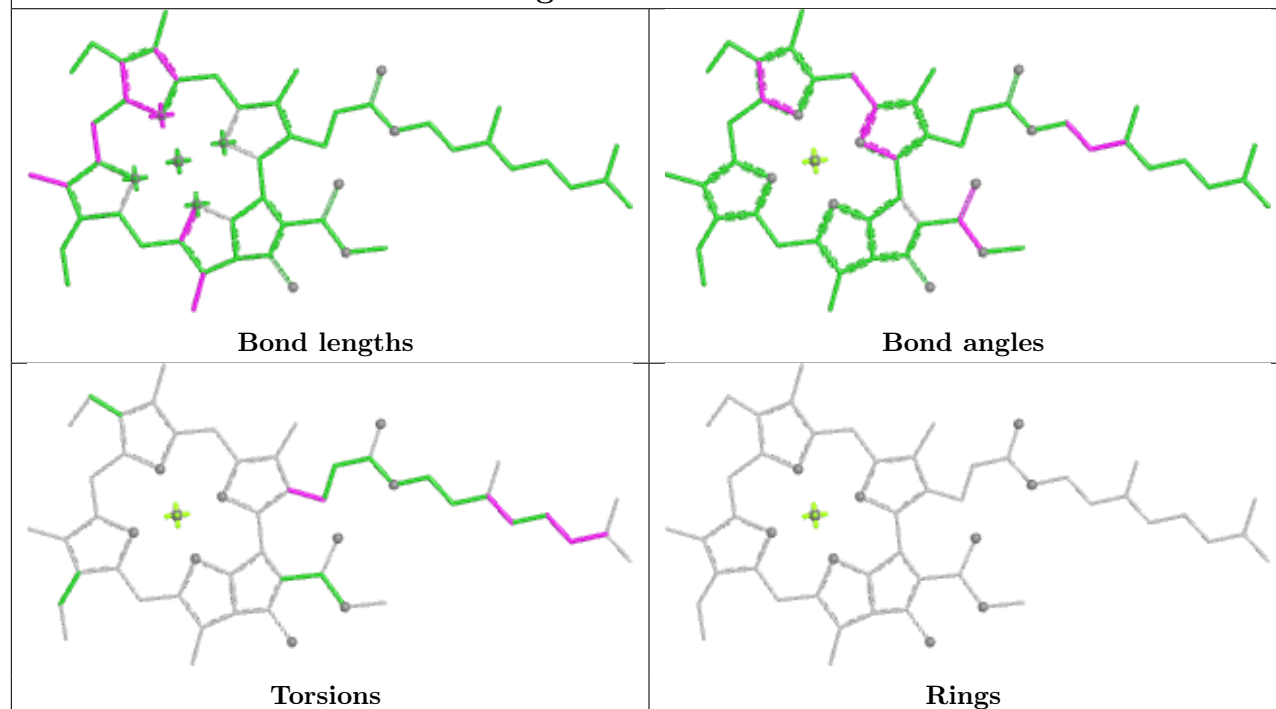




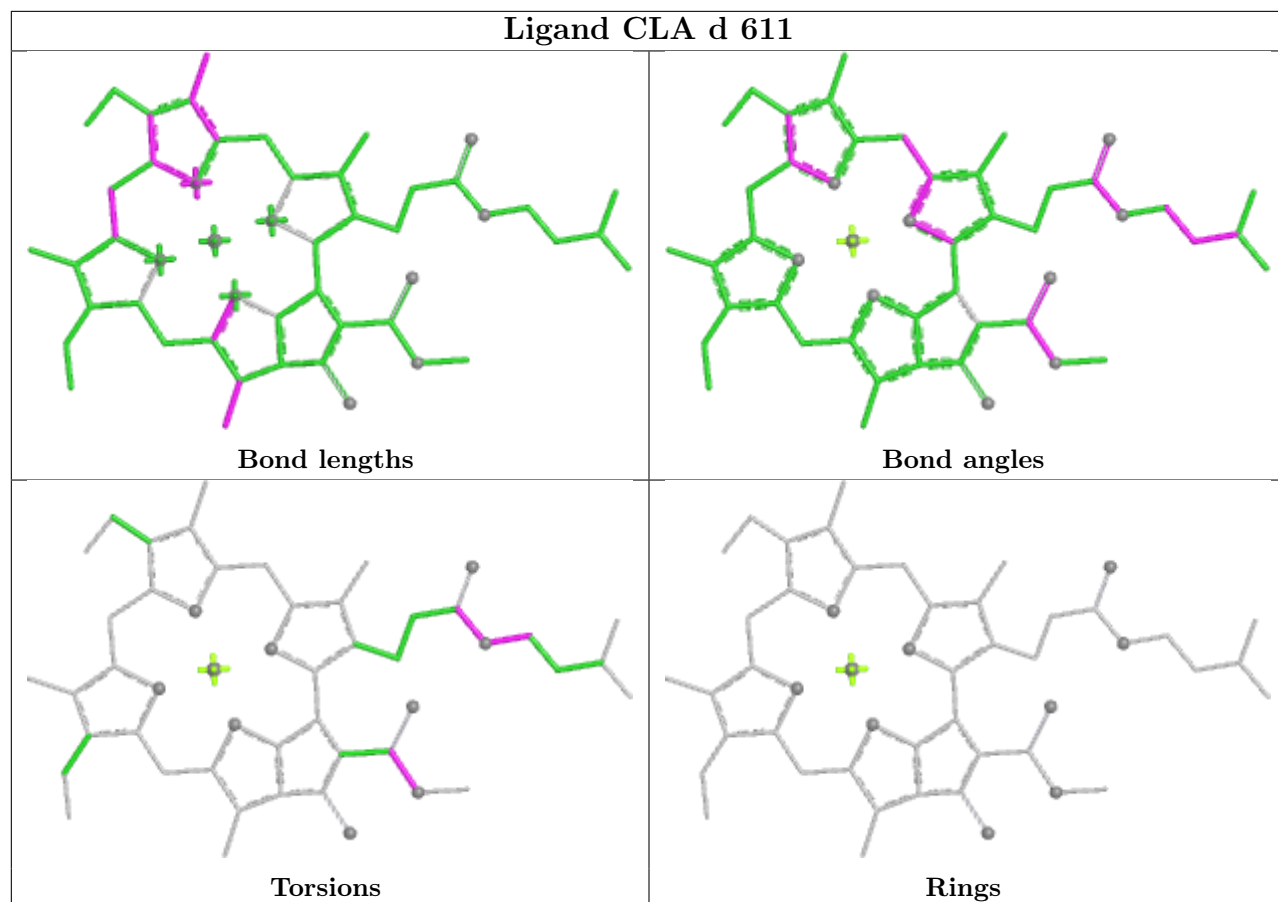
Ligand CLA 6 608



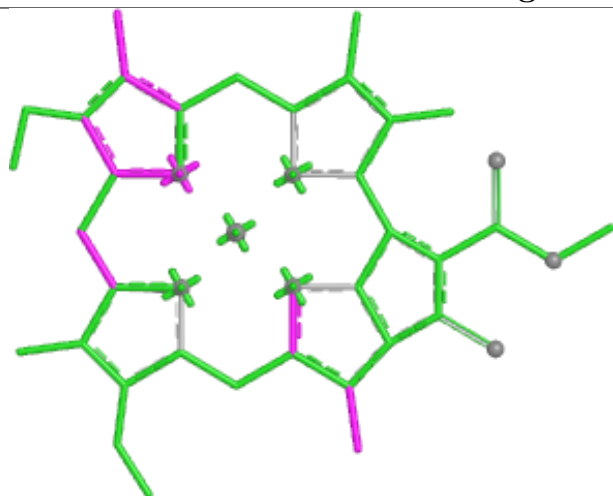
Ligand CLA 7 304



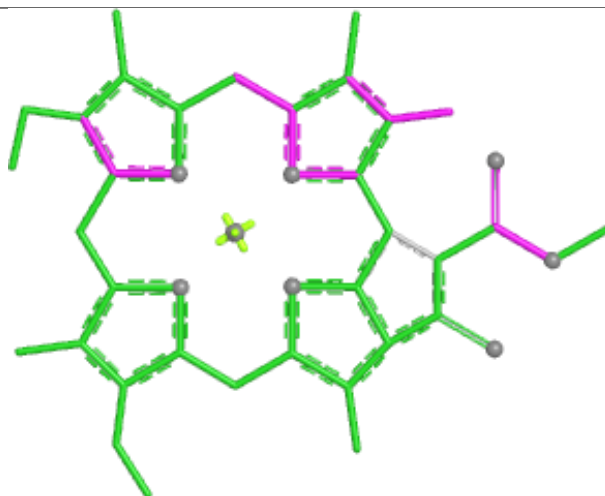
Ligand CLA d 611



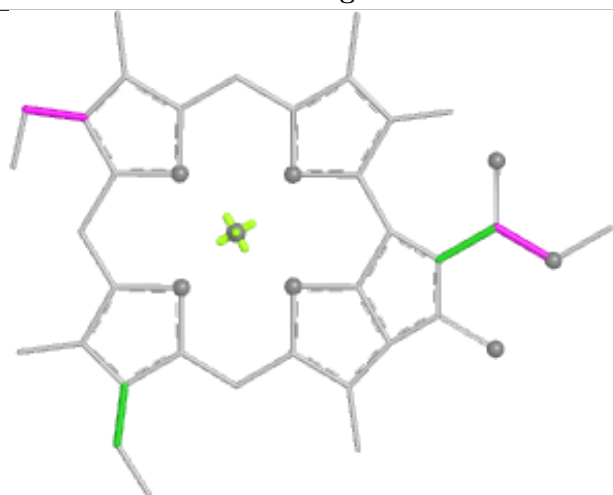
Ligand CLA 7 309



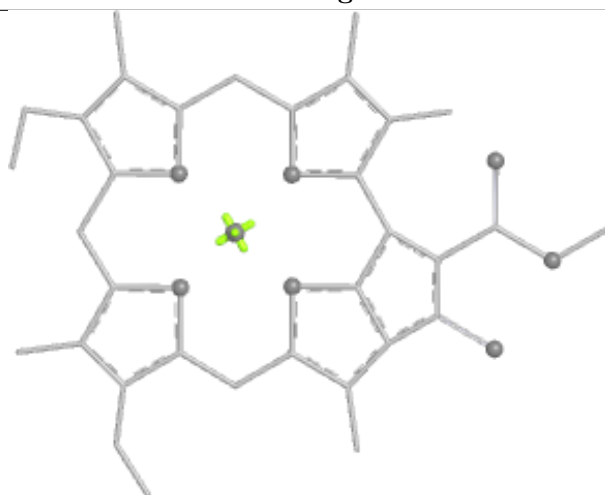
Bond lengths



Bond angles

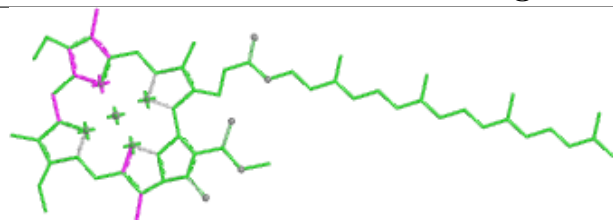


Torsions

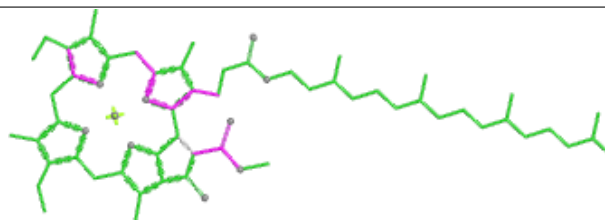


Rings

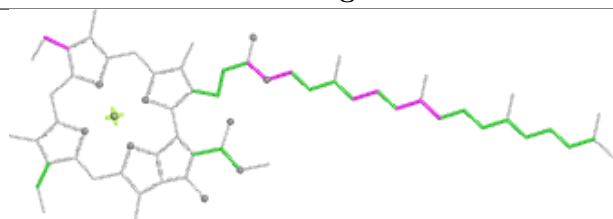
Ligand CLA A 824



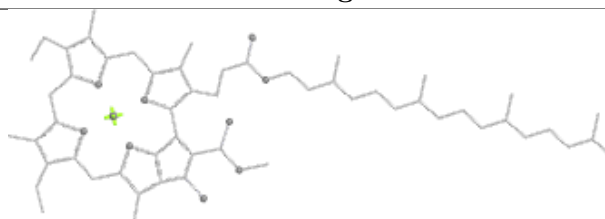
Bond lengths



Bond angles

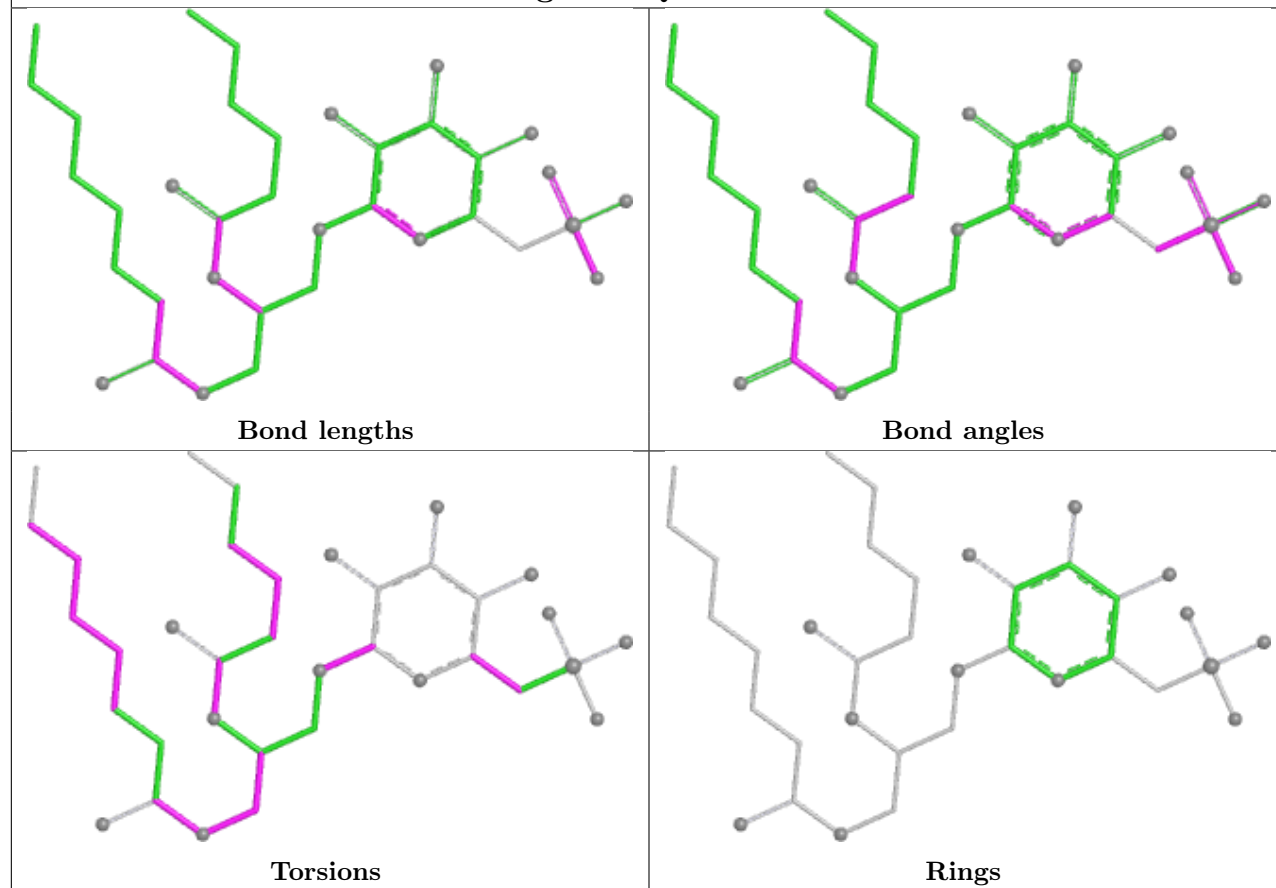


Torsions

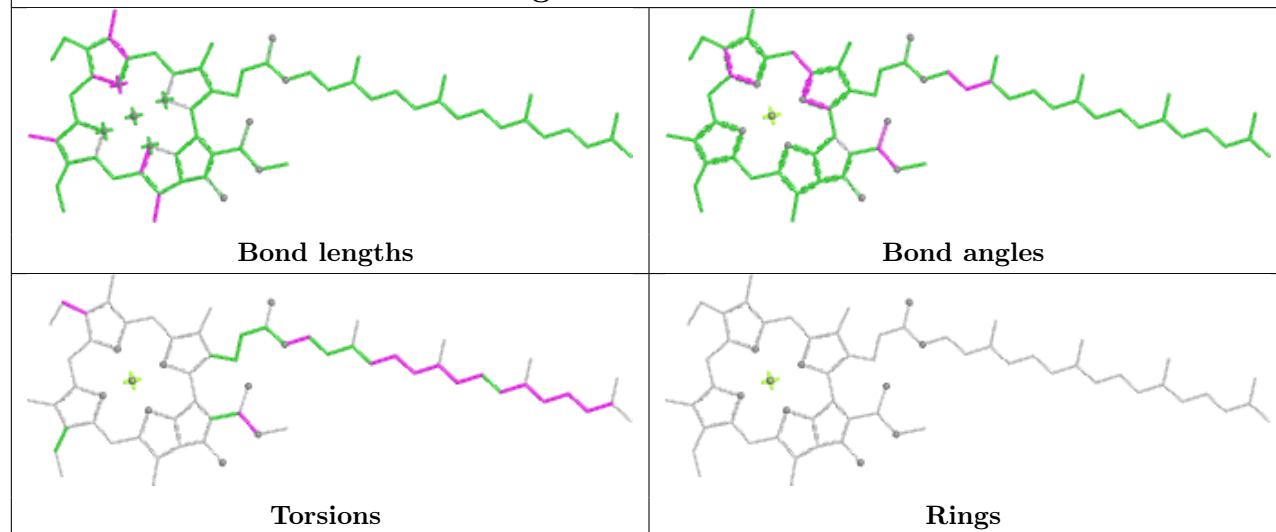


Rings

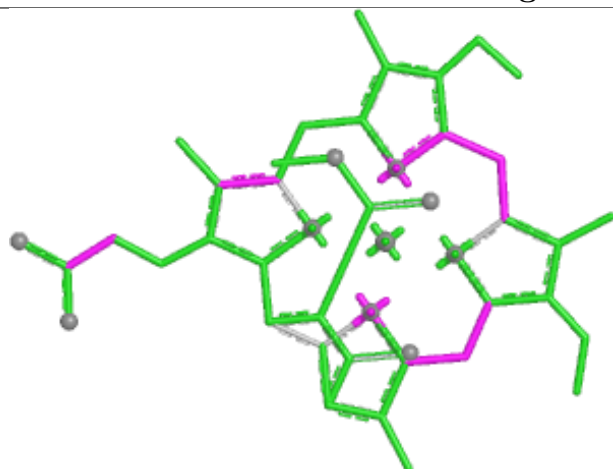
Ligand SQD 3 322



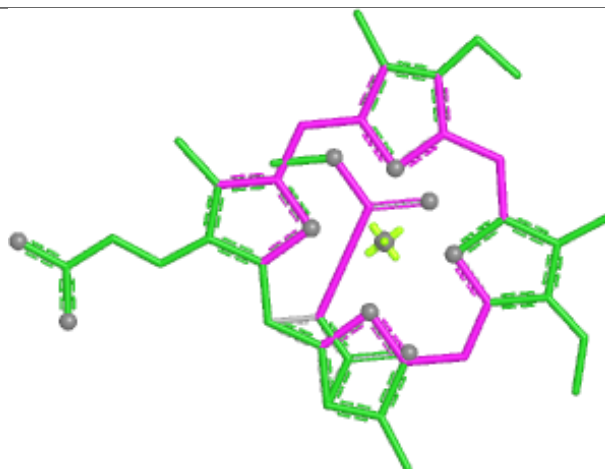
Ligand CLA B 803



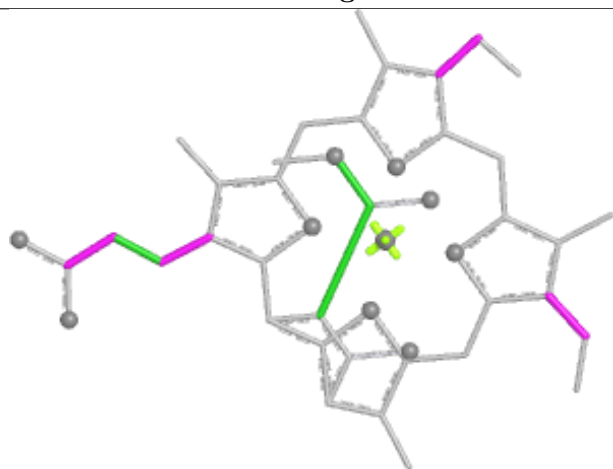
Ligand KC2 b 605



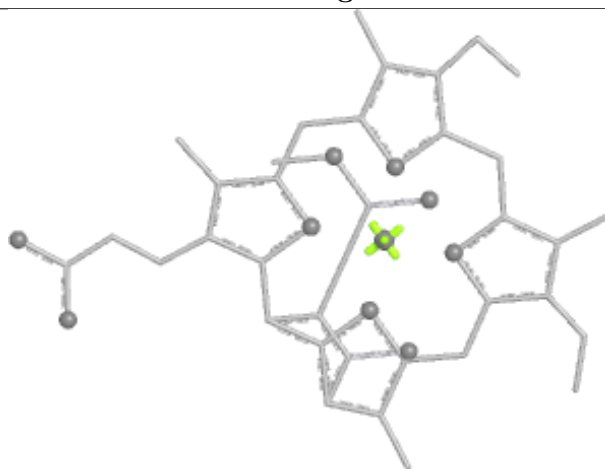
Bond lengths



Bond angles

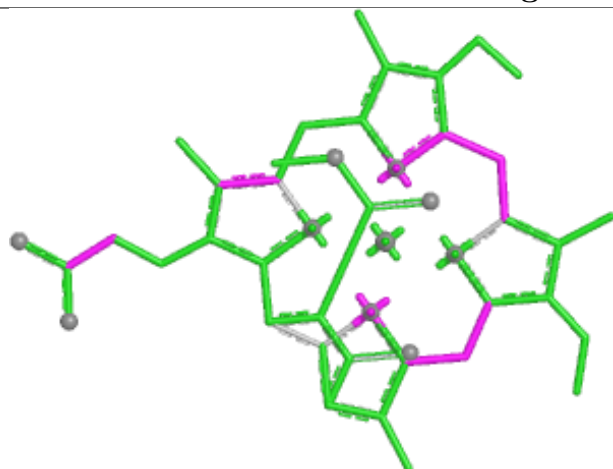


Torsions

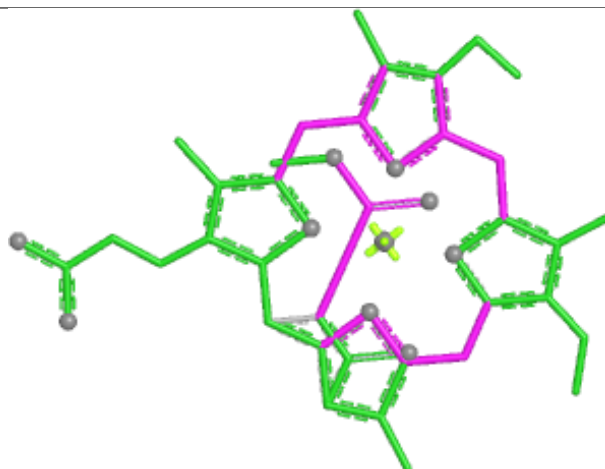


Rings

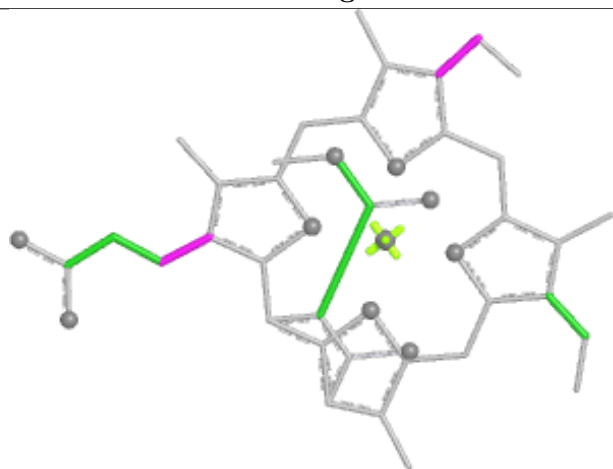
Ligand KC2 c 611



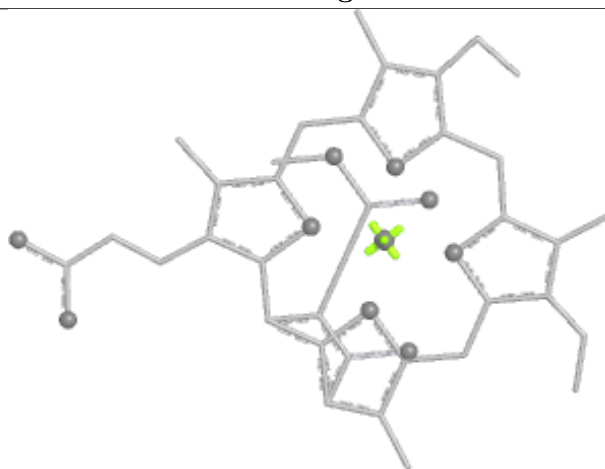
Bond lengths



Bond angles

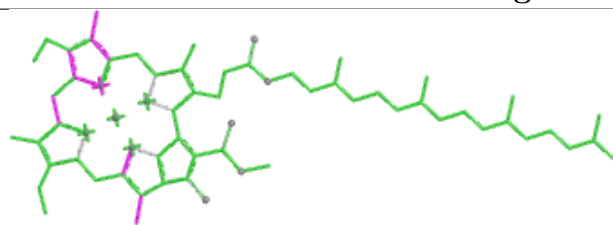


Torsions

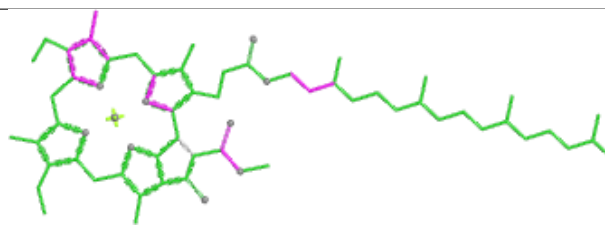


Rings

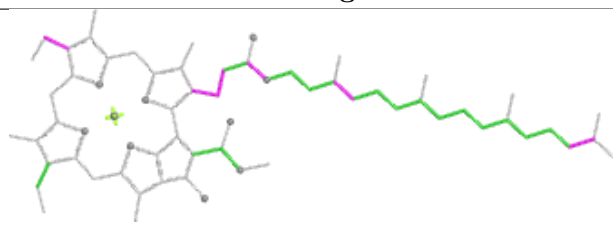
Ligand CLA A 843



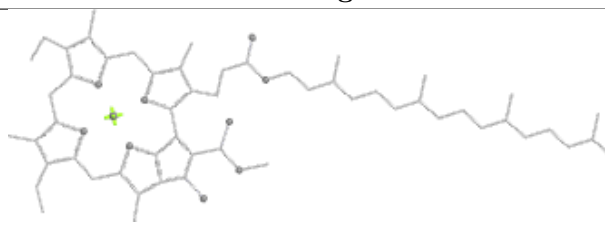
Bond lengths



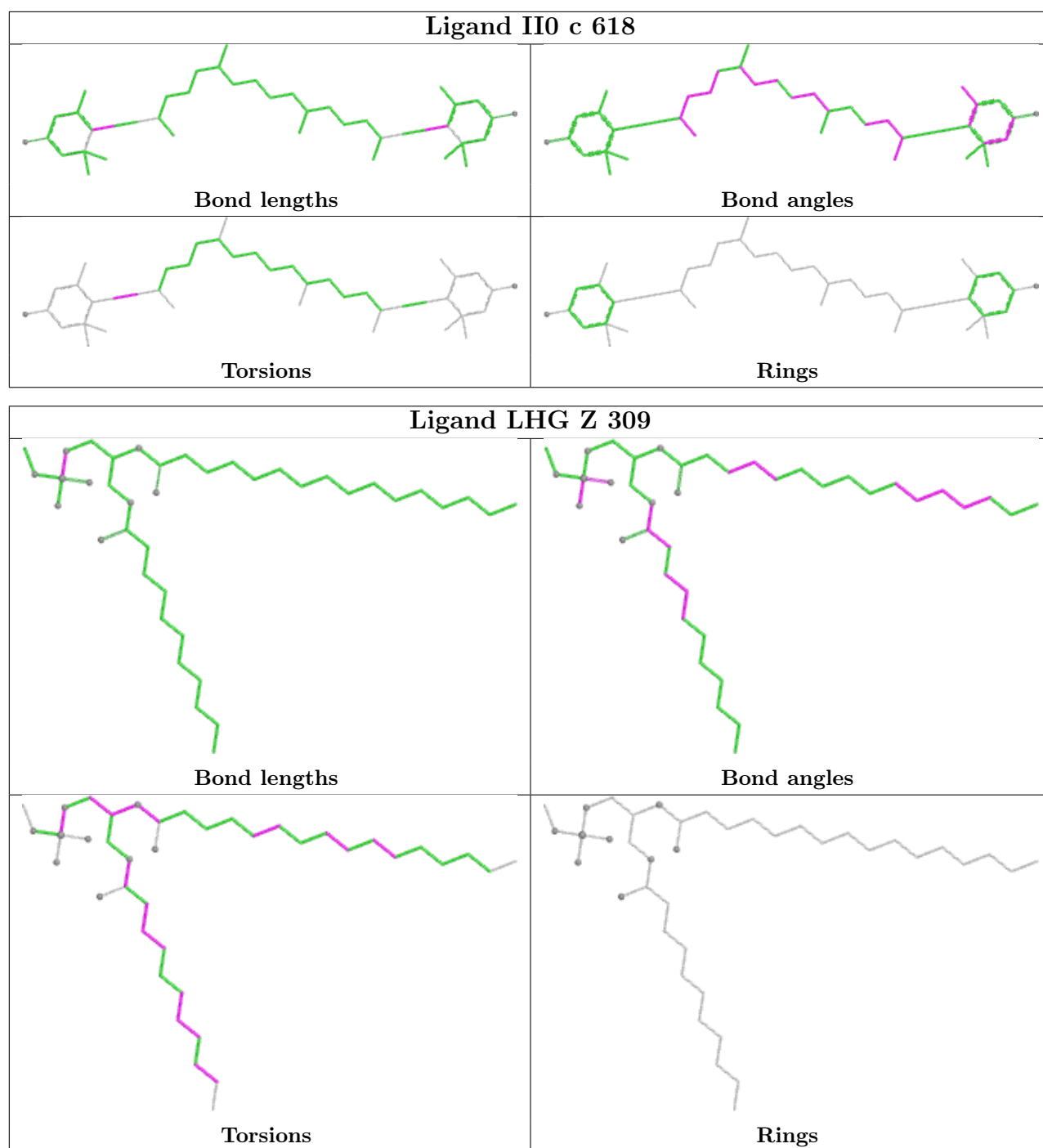
Bond angles



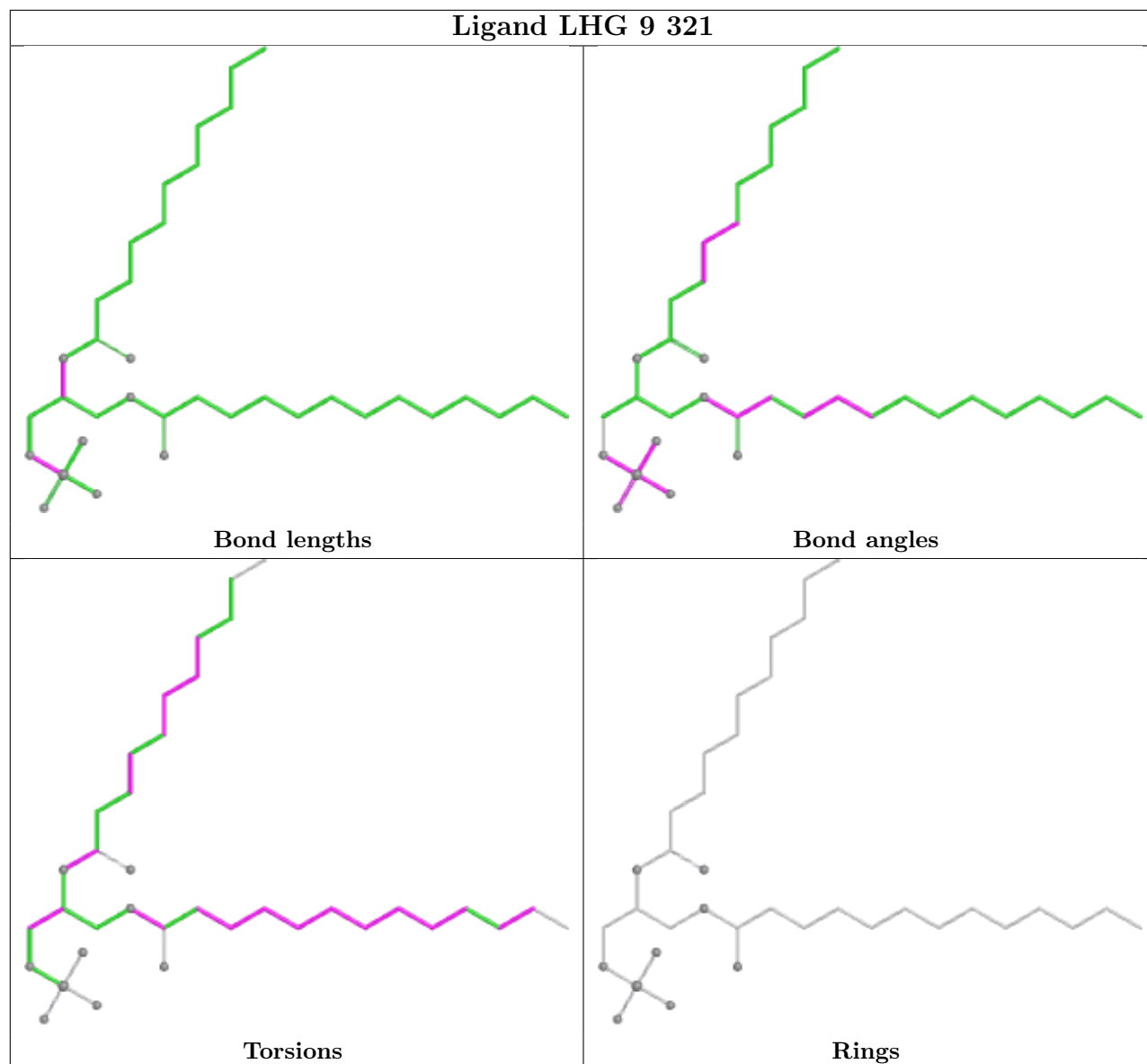
Torsions



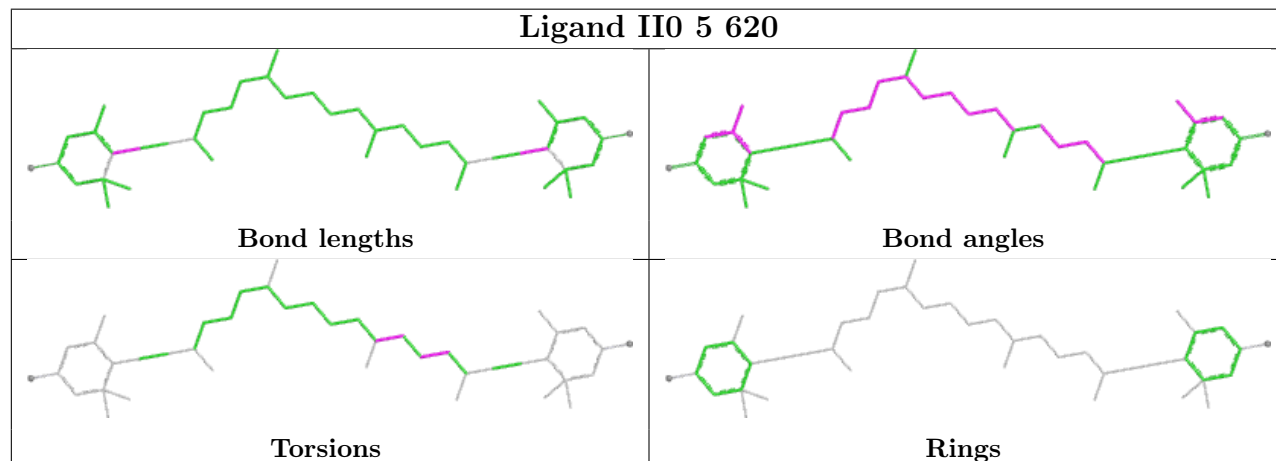
Rings

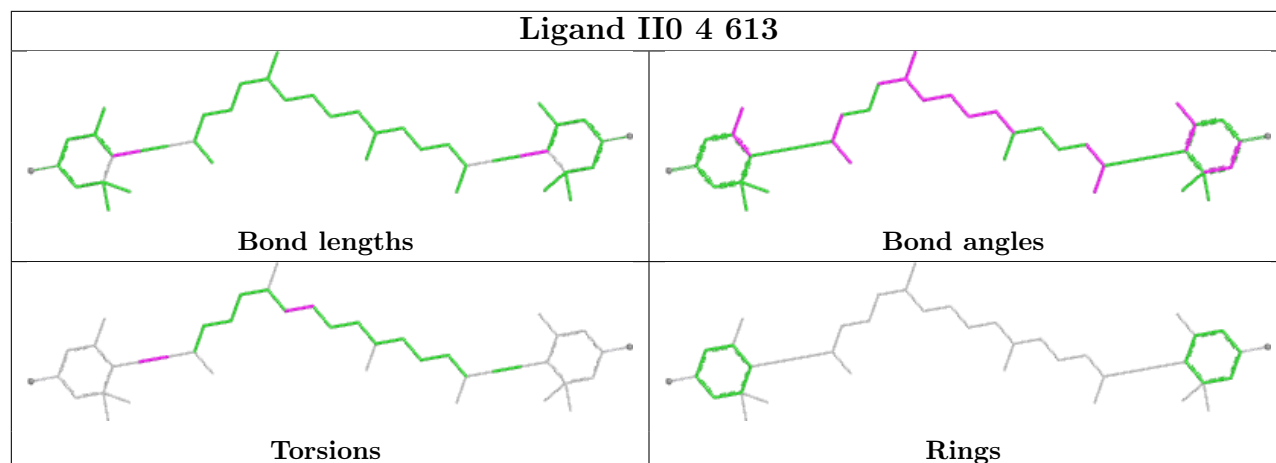
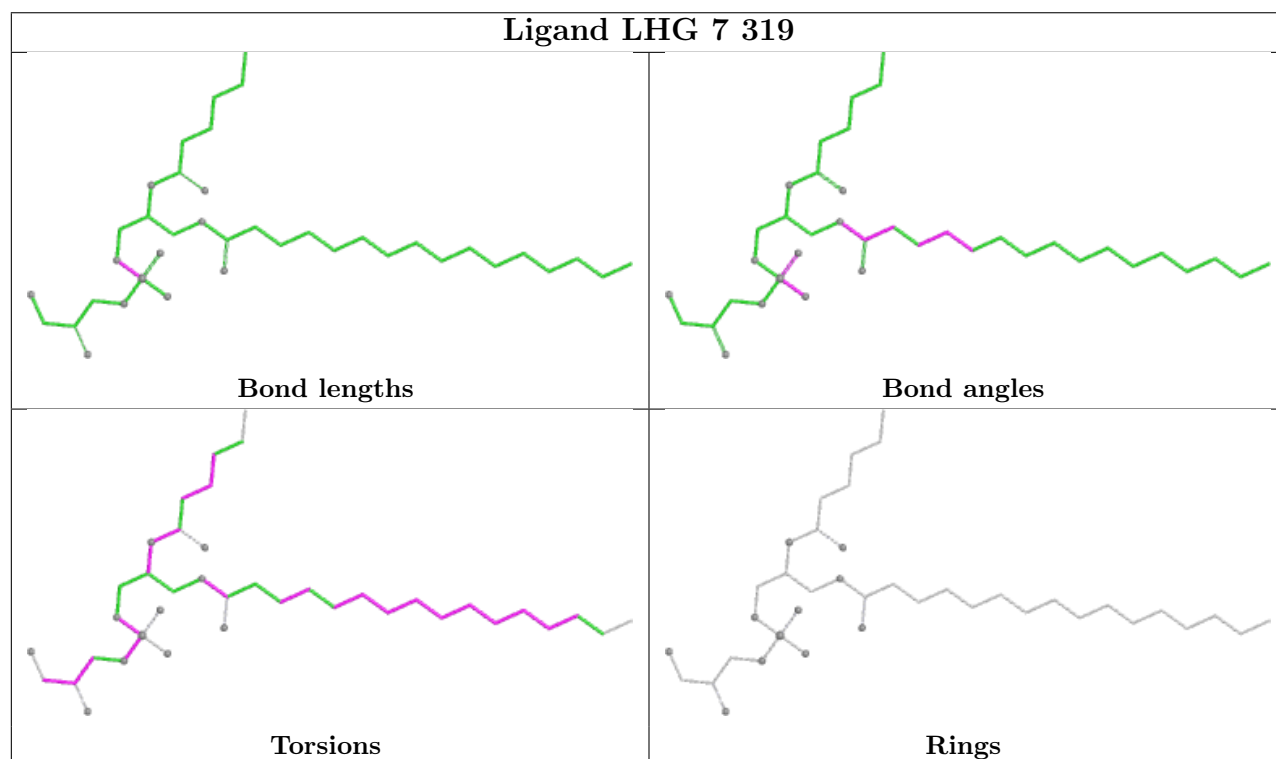
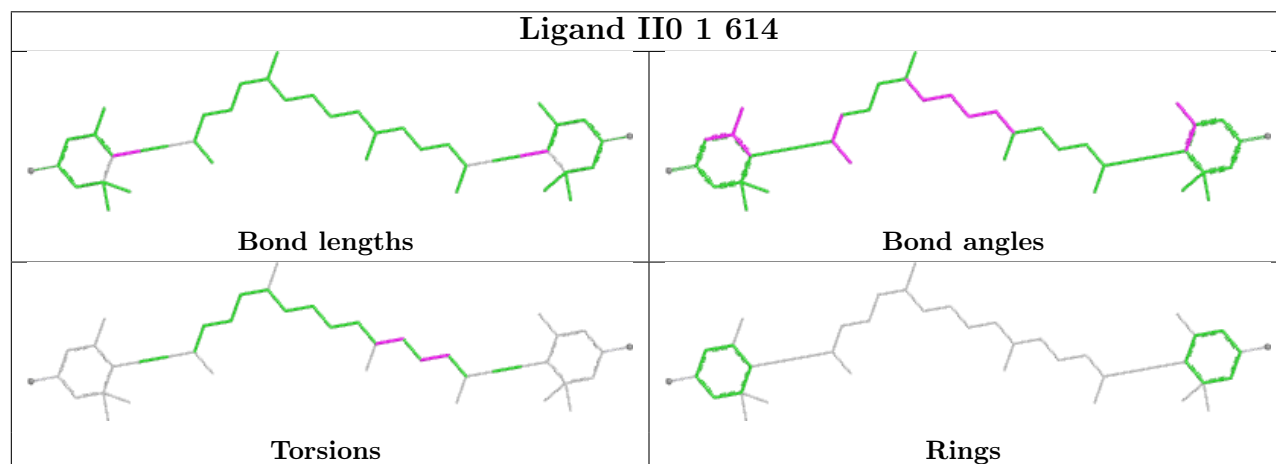


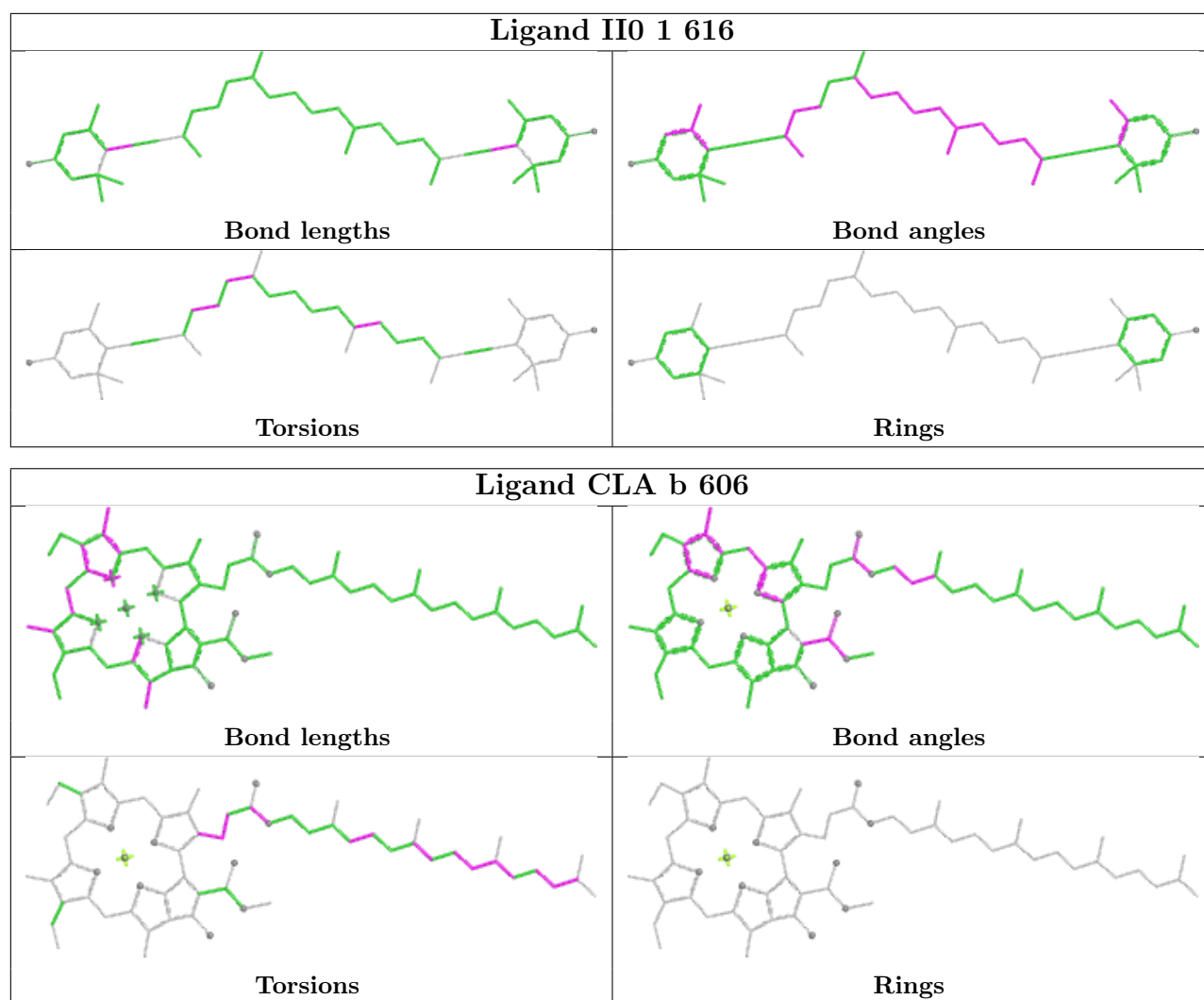
Ligand LHG 9 321

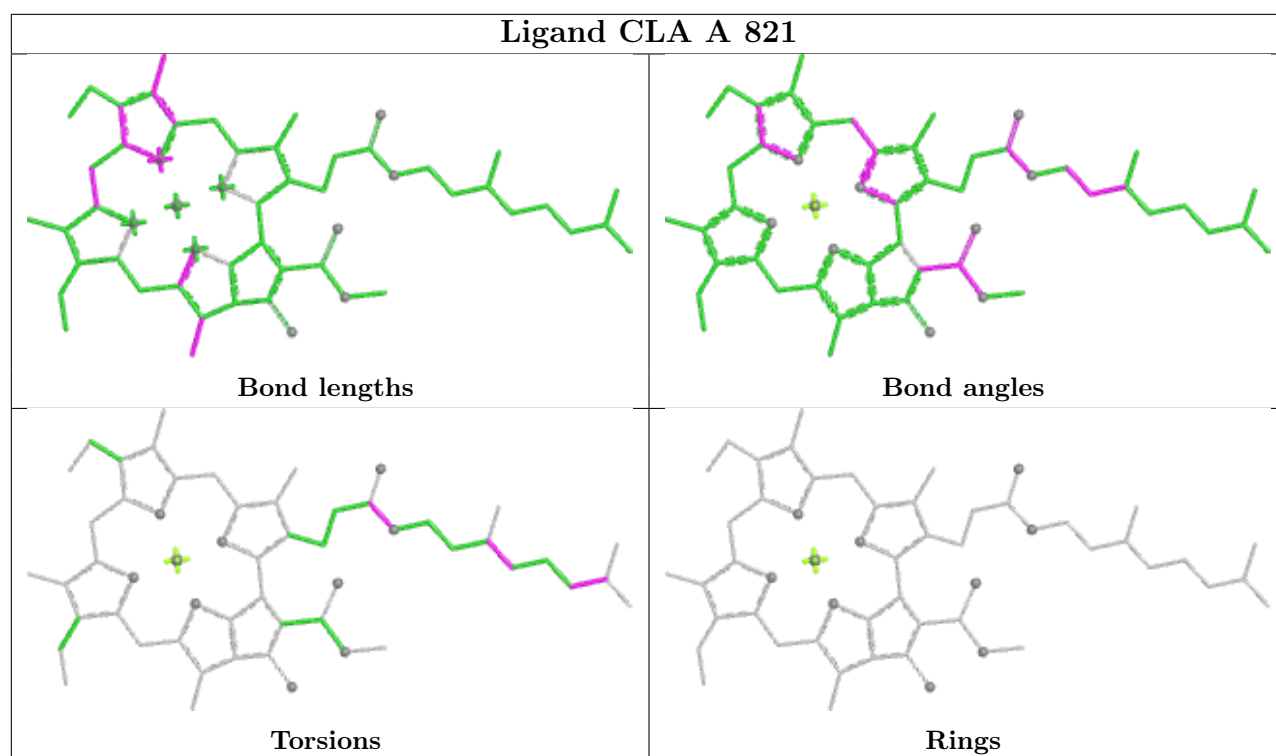


Ligand II0 5 620

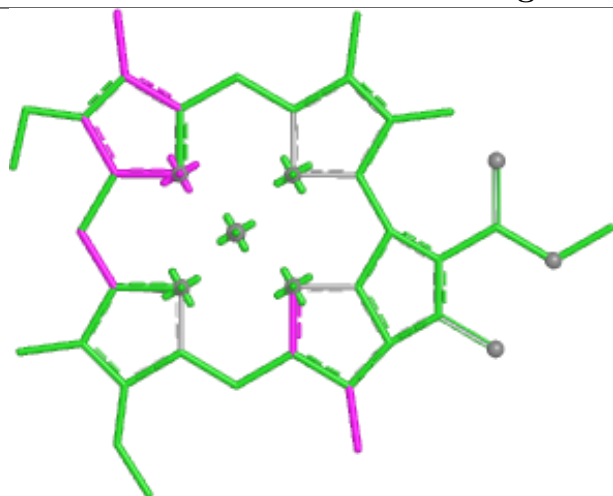


Ligand II0 4 613**Ligand LHG 7 319****Ligand II0 1 614**

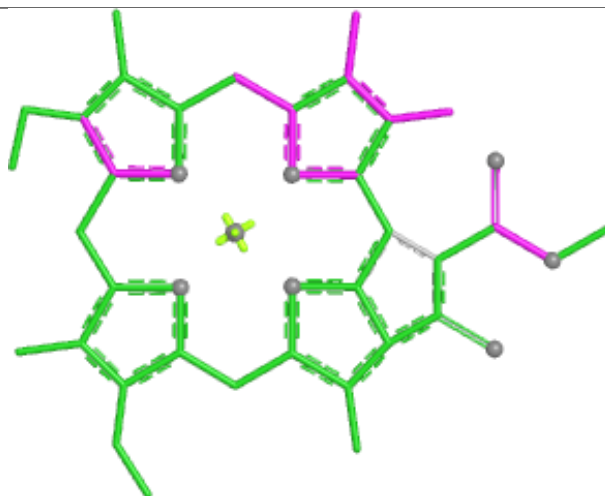




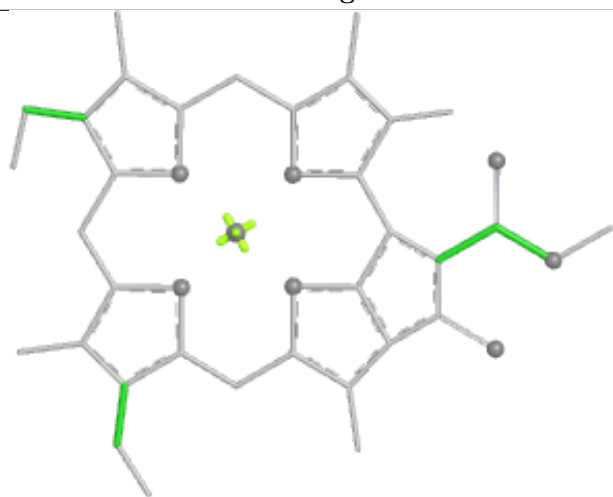
Ligand CLA d 606



Bond lengths



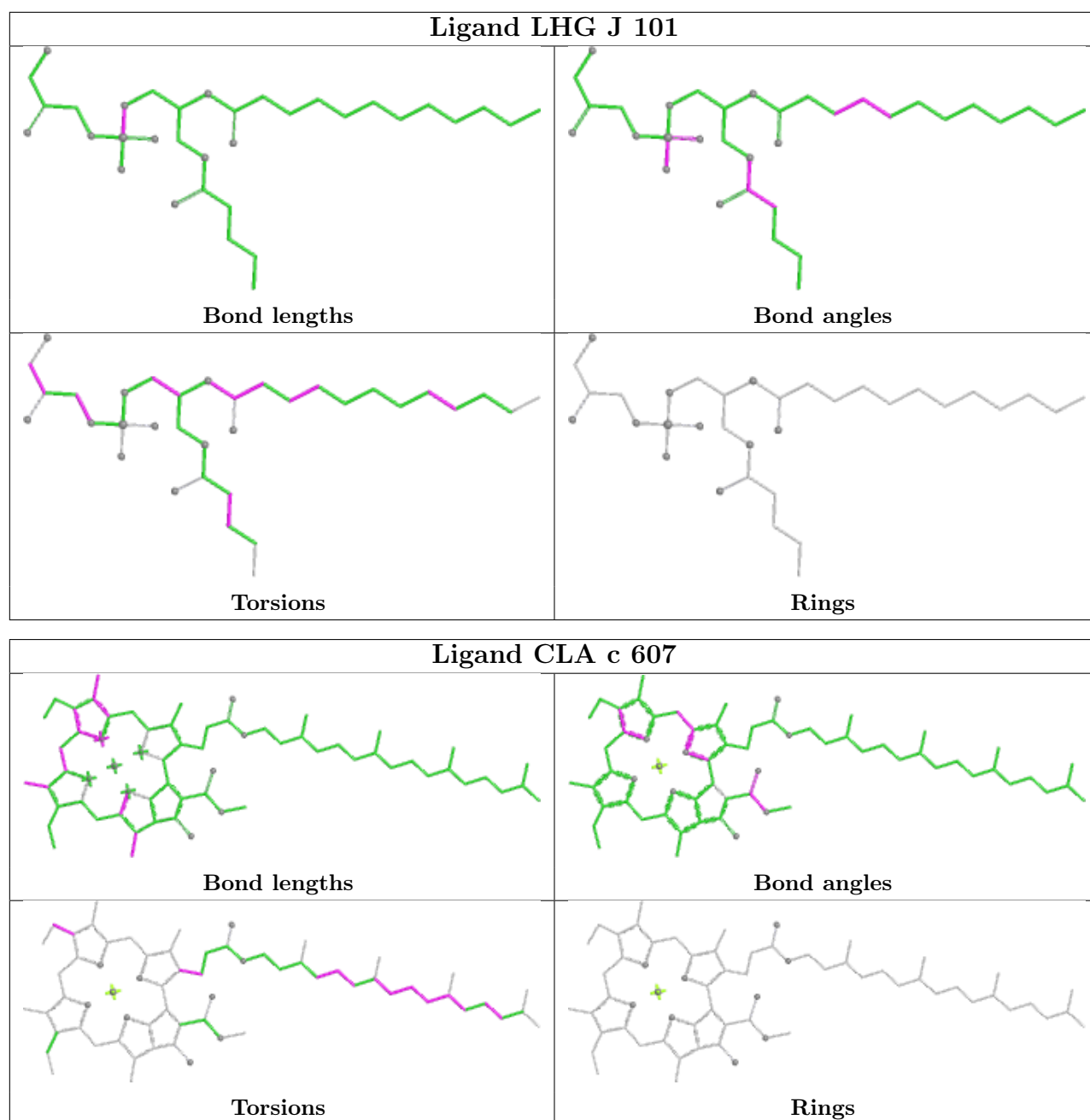
Bond angles

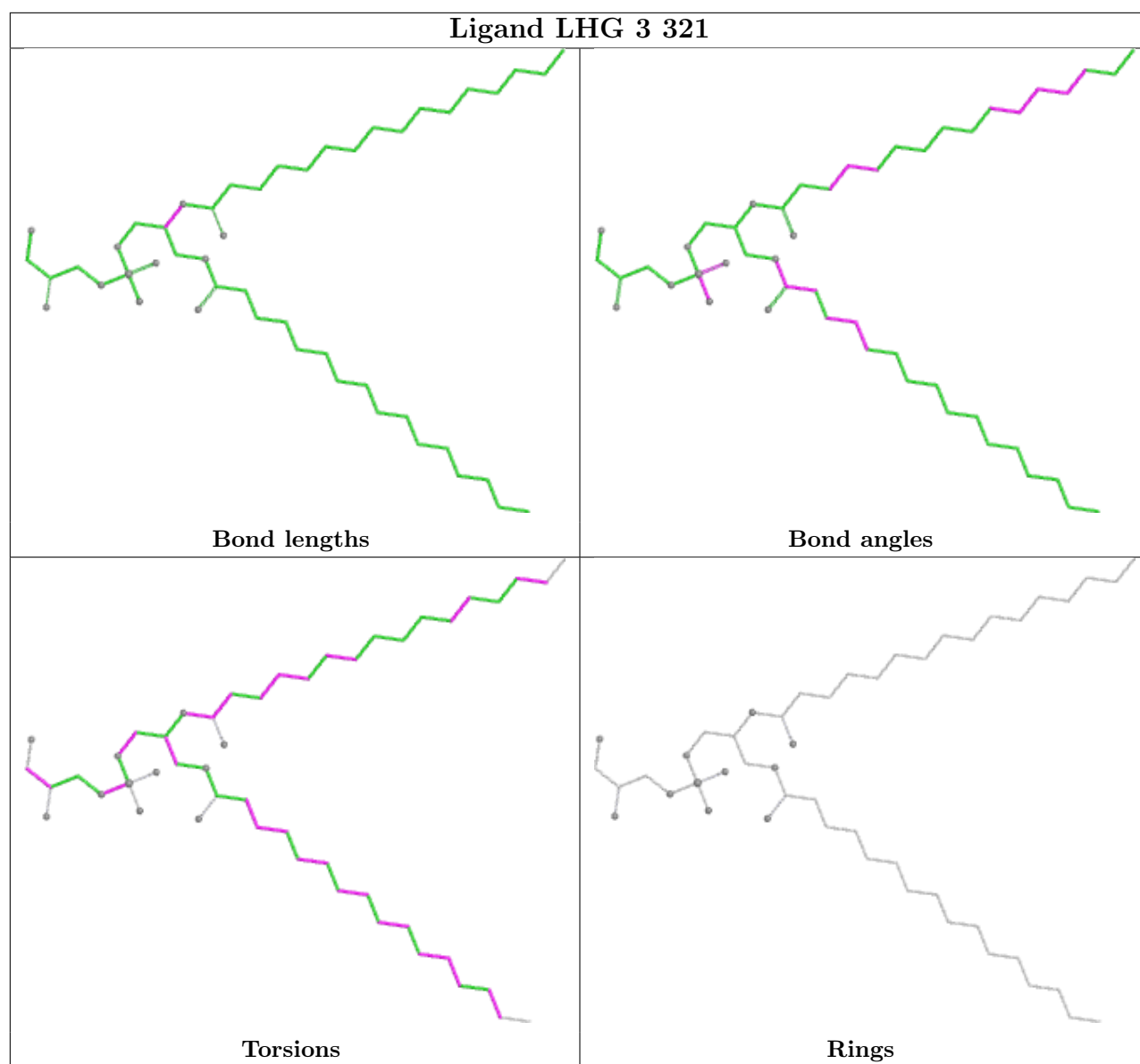


Torsions

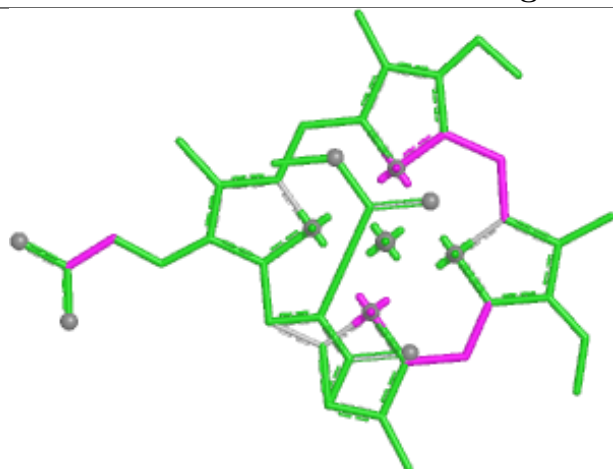


Rings

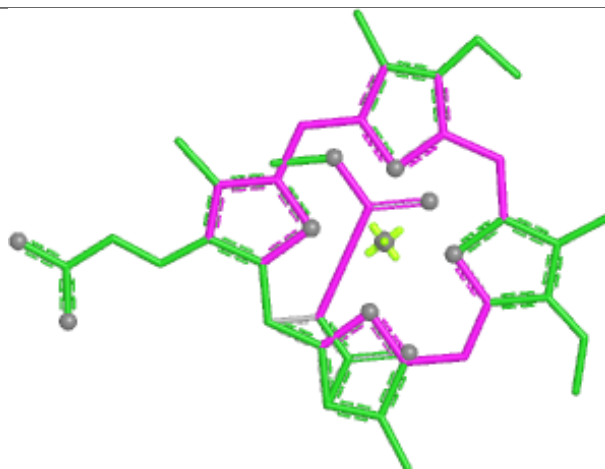




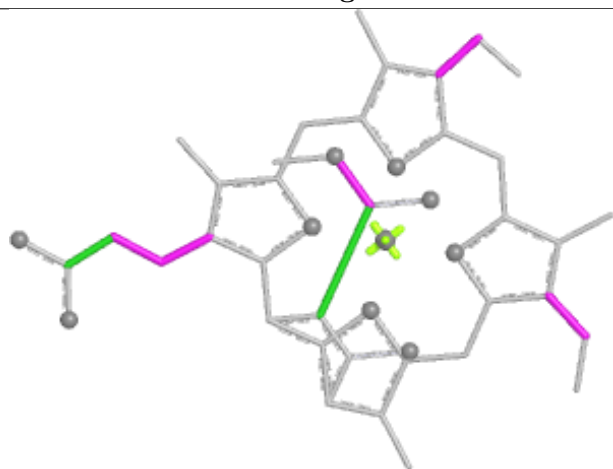
Ligand KC2 7 313



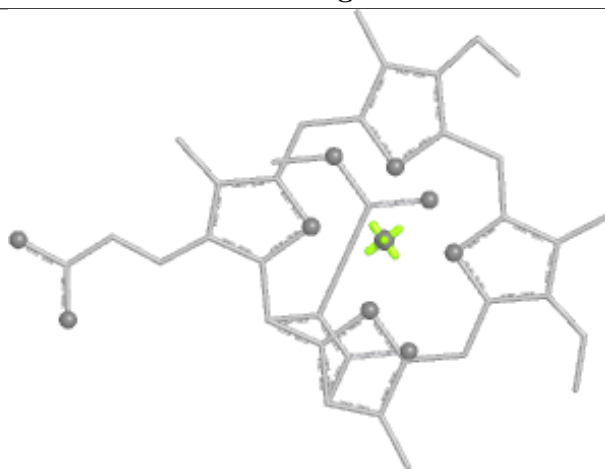
Bond lengths



Bond angles

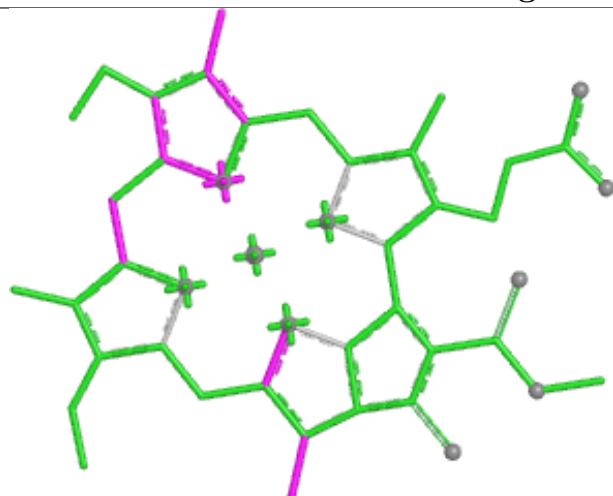


Torsions

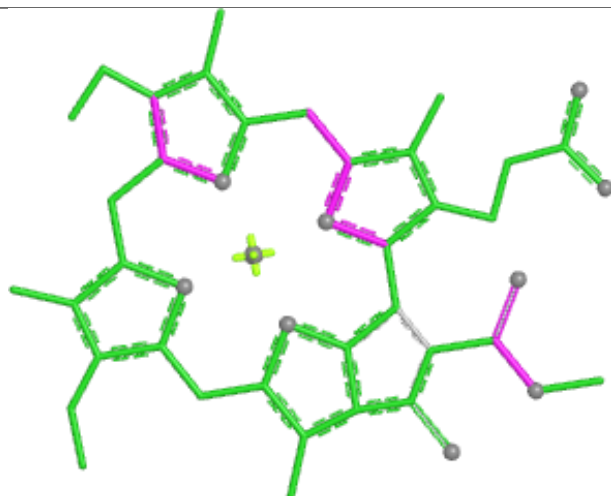


Rings

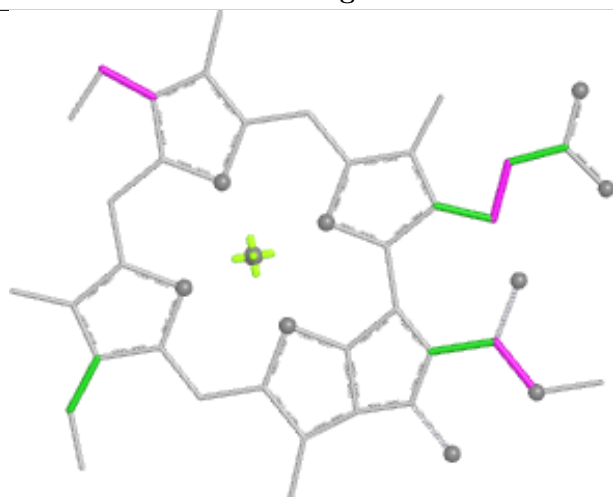
Ligand CLA 1 606



Bond lengths



Bond angles

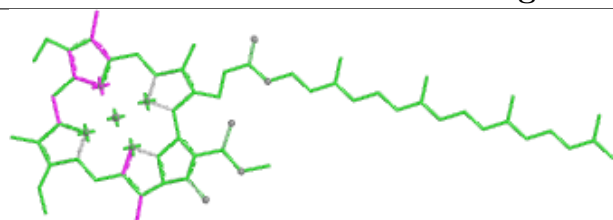


Torsions

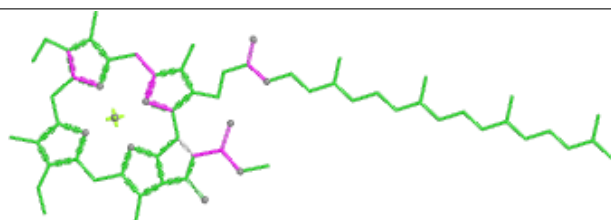


Rings

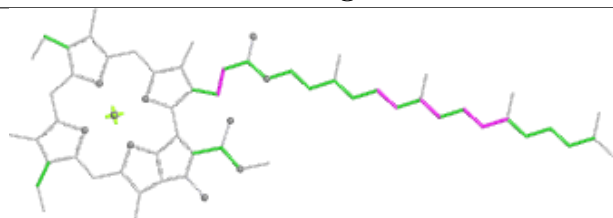
Ligand CLA 8 308



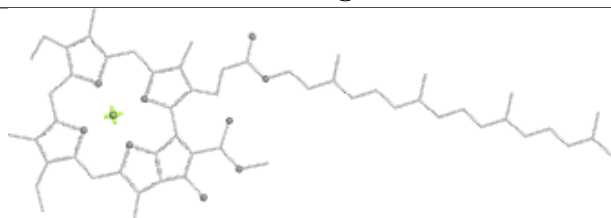
Bond lengths



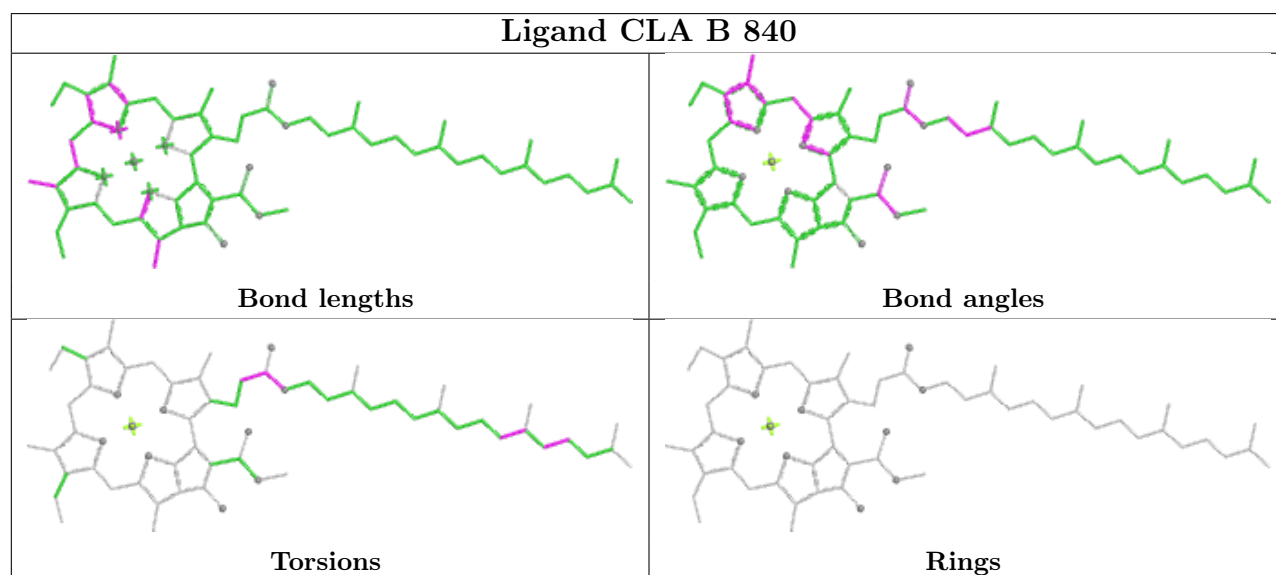
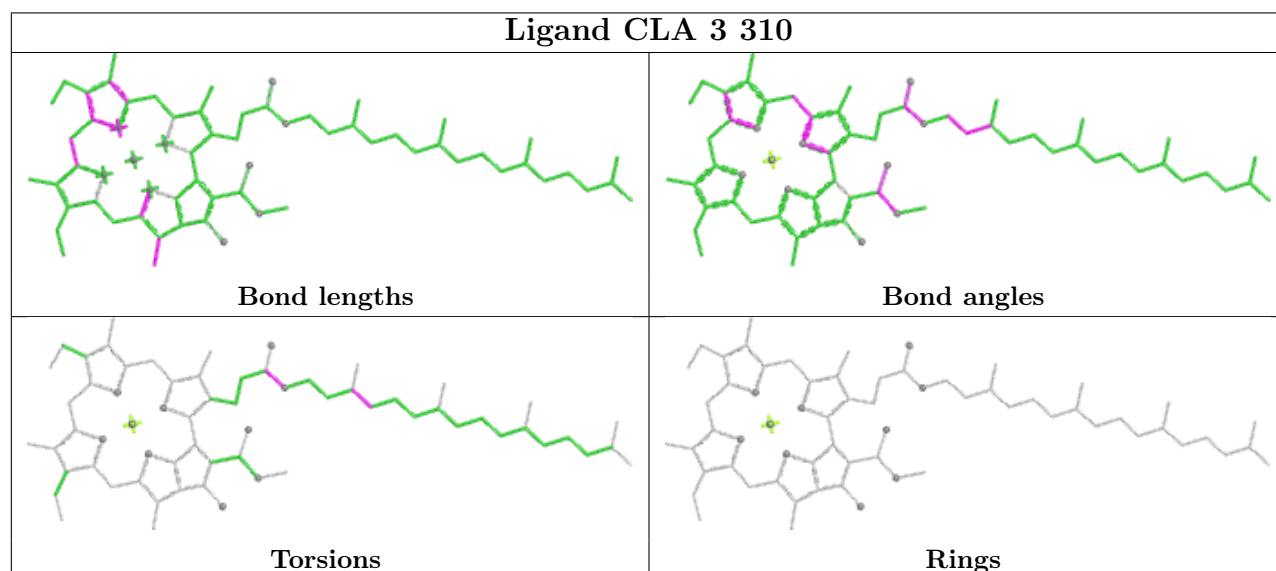
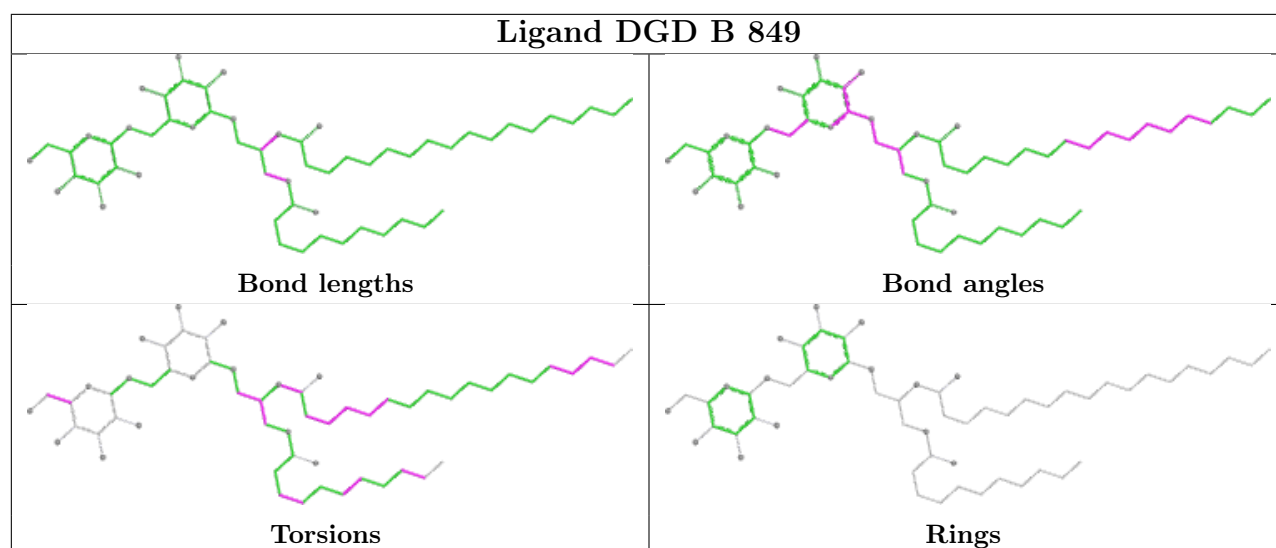
Bond angles

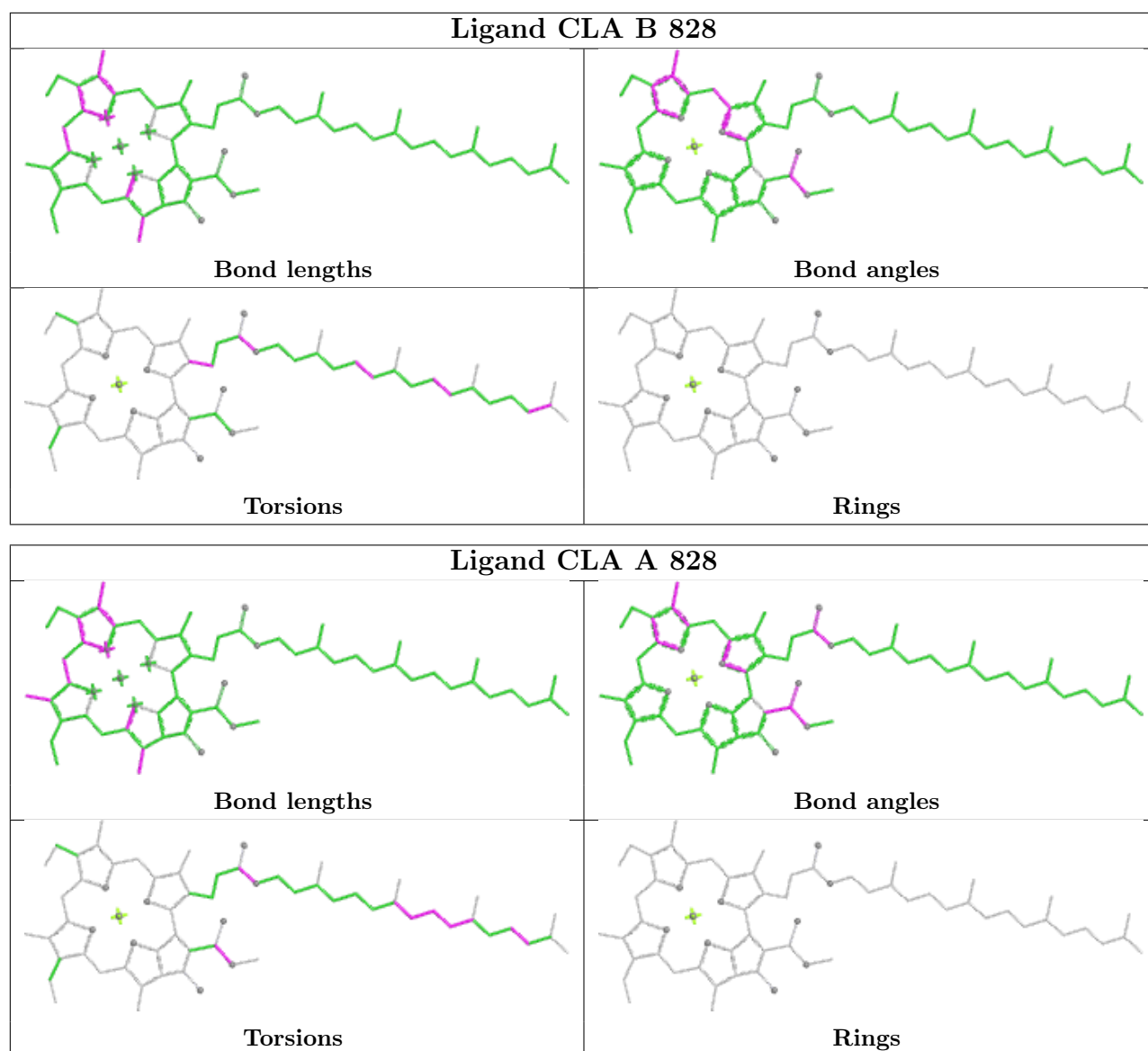


Torsions

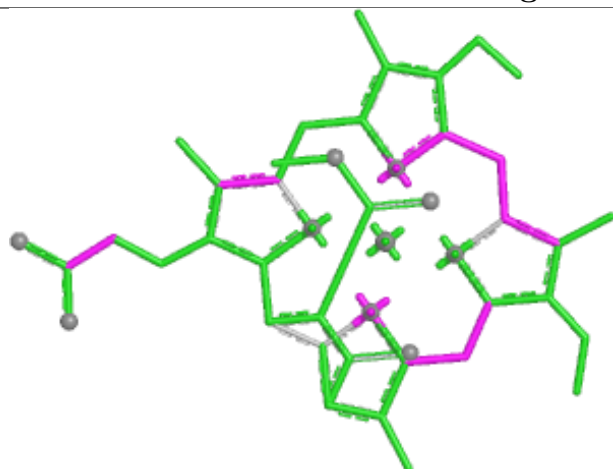


Rings

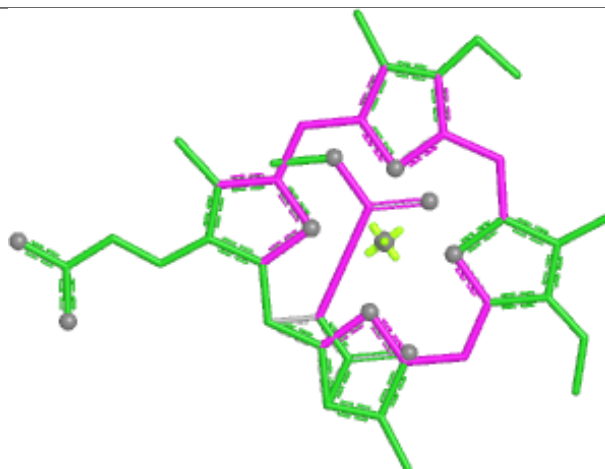




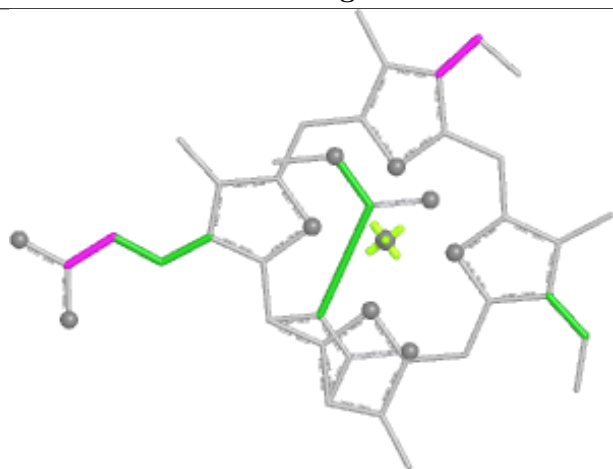
Ligand KC2 1 610



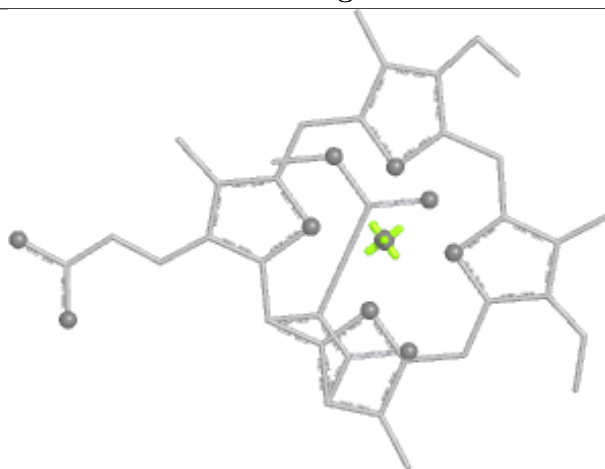
Bond lengths



Bond angles

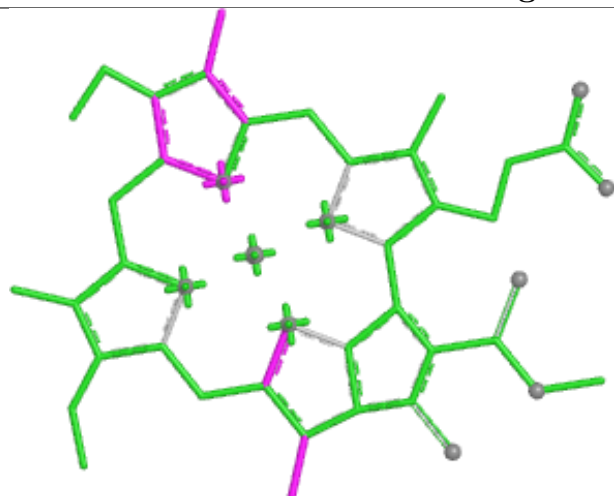


Torsions

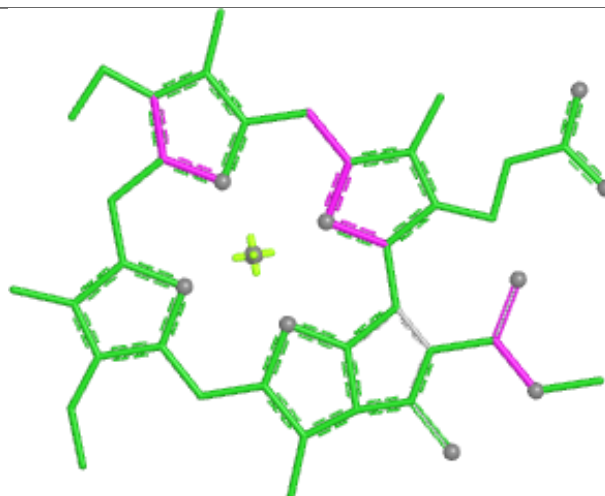


Rings

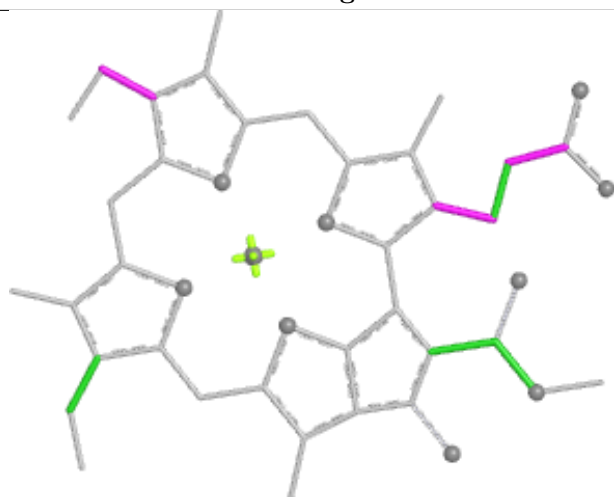
Ligand CLA 5 607



Bond lengths



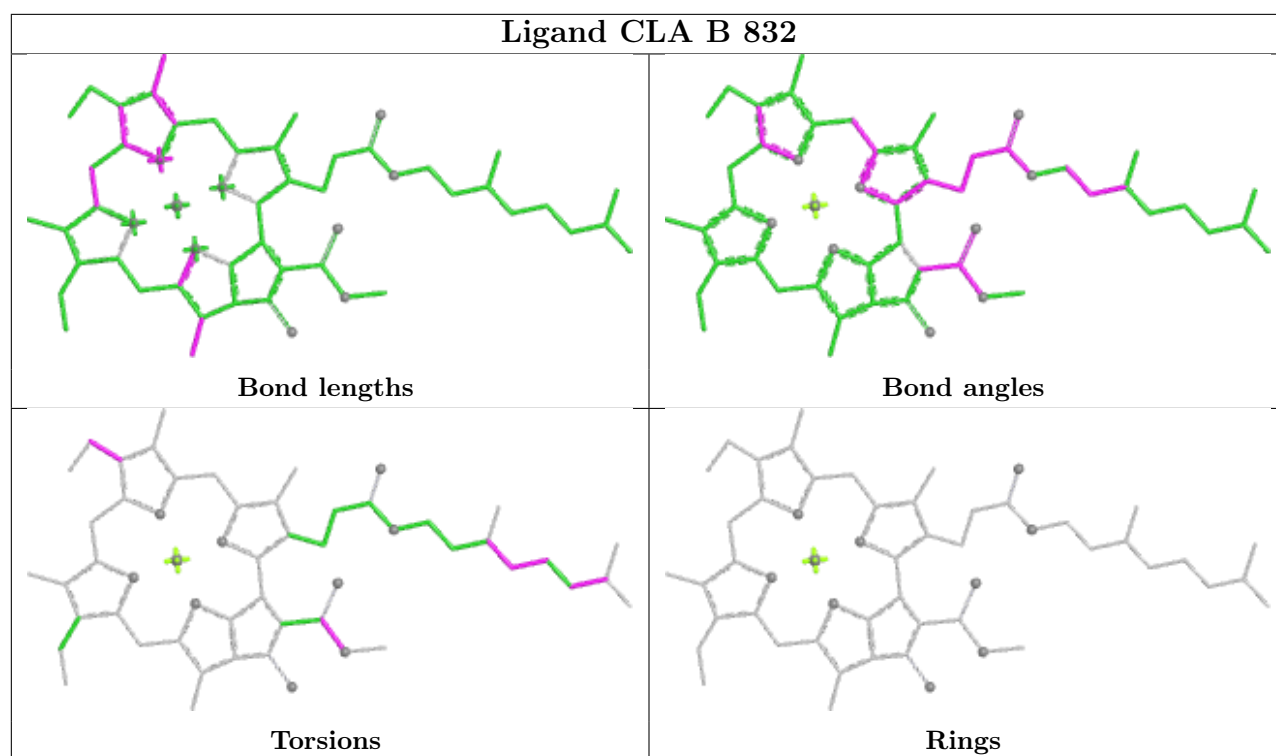
Bond angles



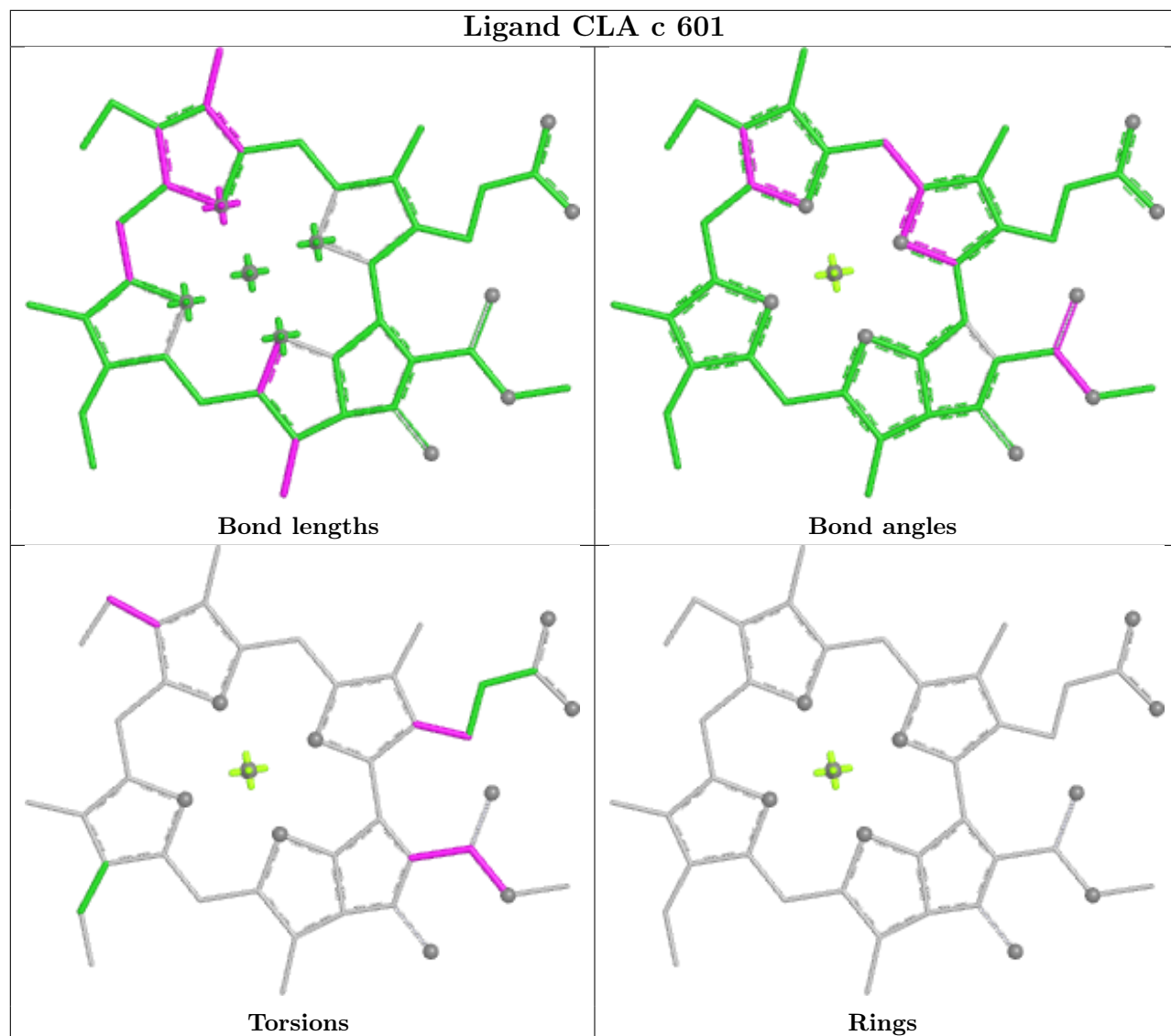
Torsions



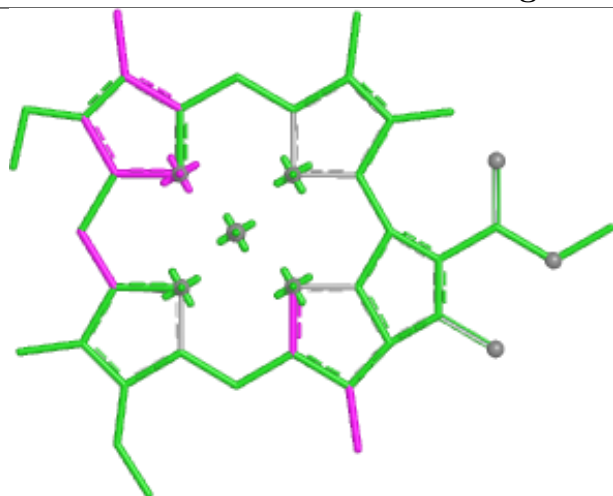
Rings



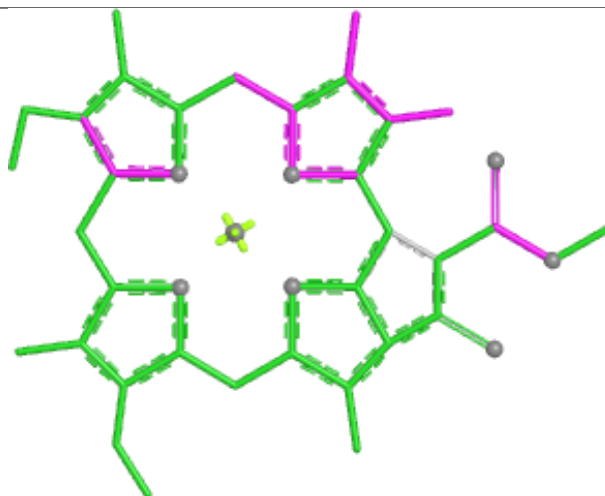
Ligand CLA c 601



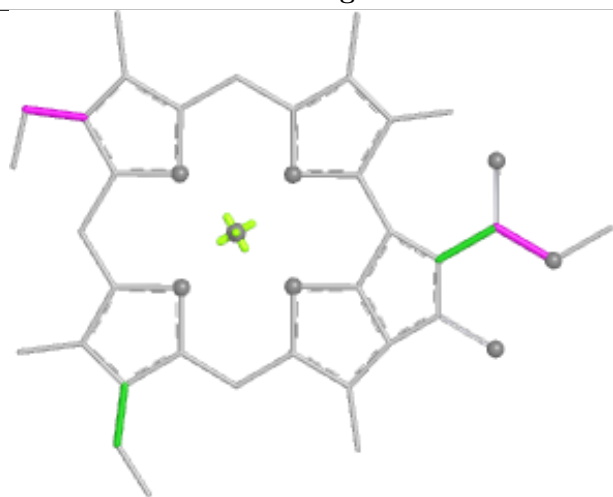
Ligand CLA c 609



Bond lengths



Bond angles

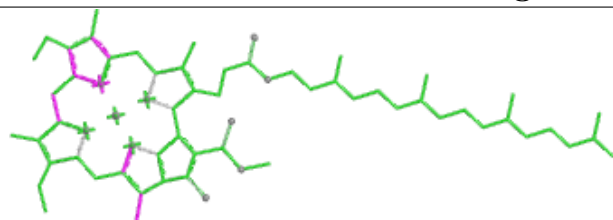


Torsions

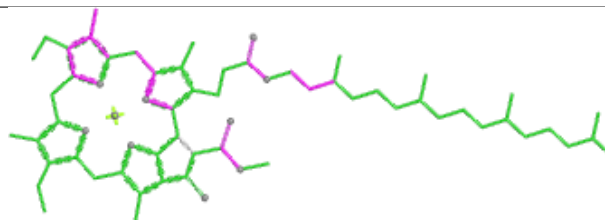


Rings

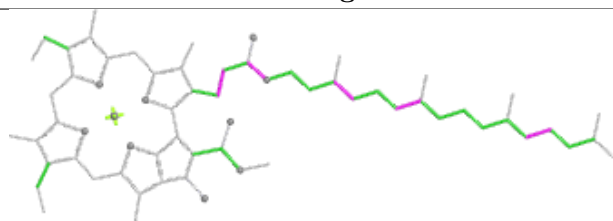
Ligand CLA A 827



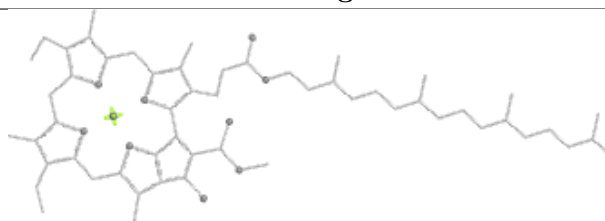
Bond lengths



Bond angles

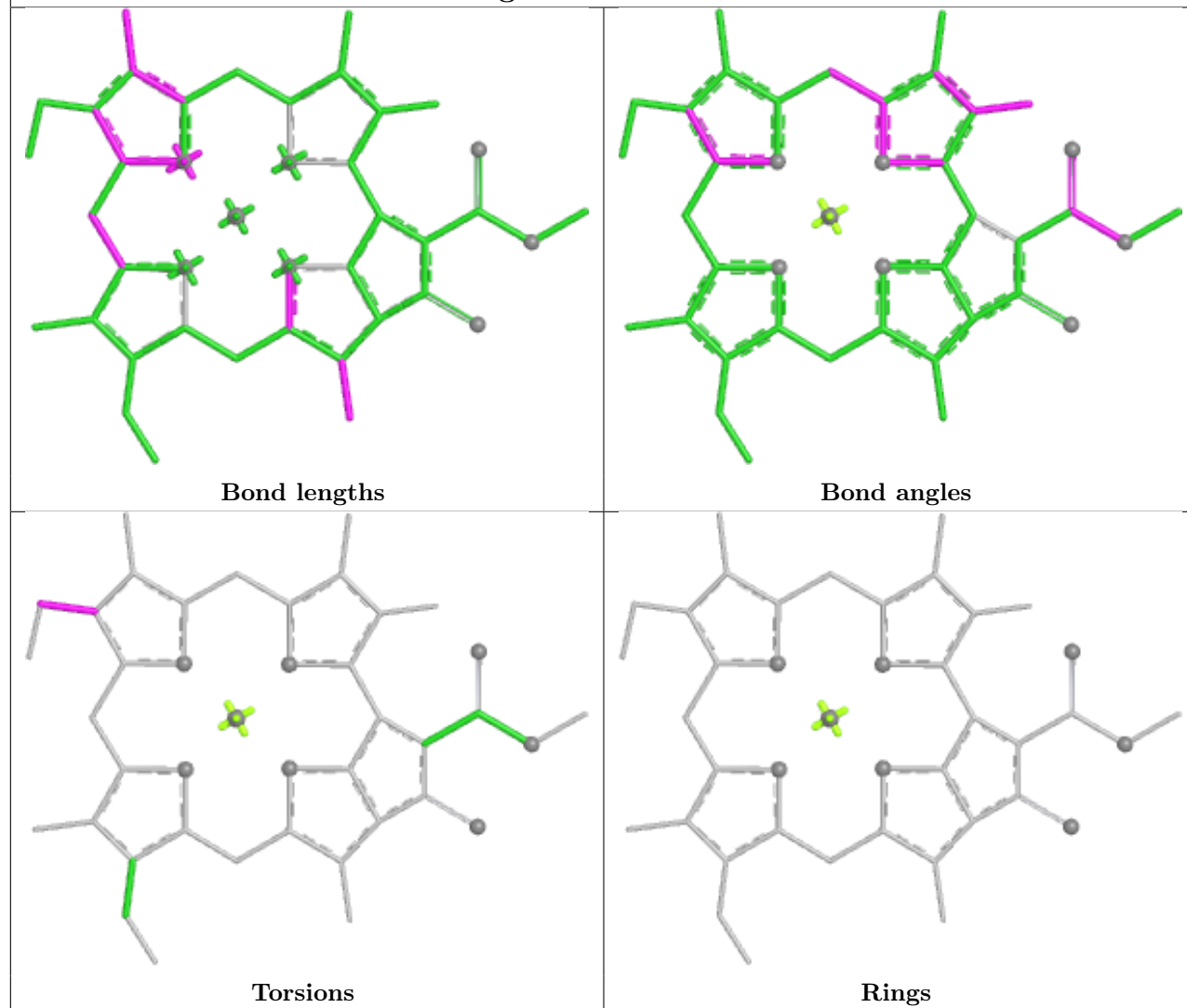


Torsions

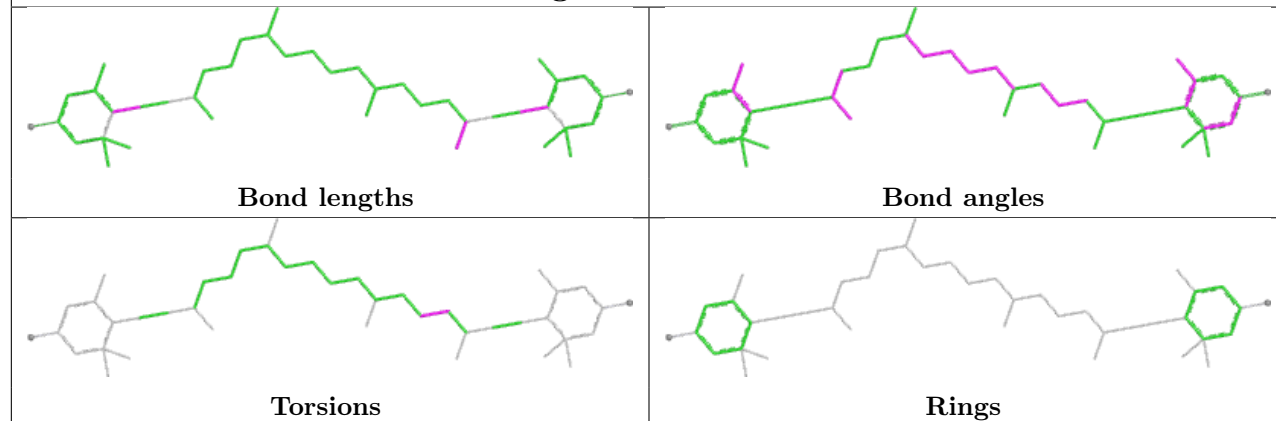


Rings

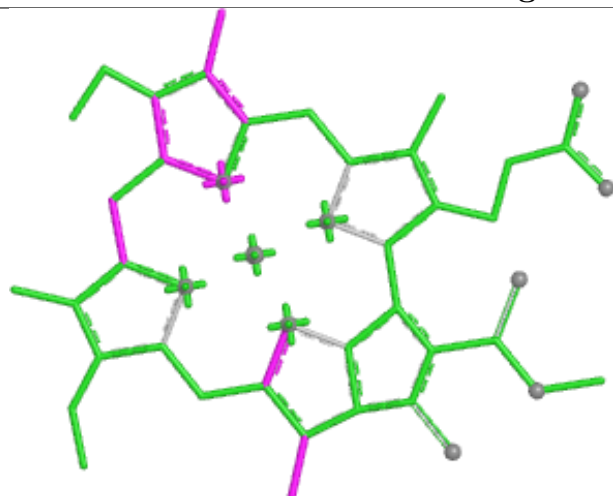
Ligand CLA 5 609



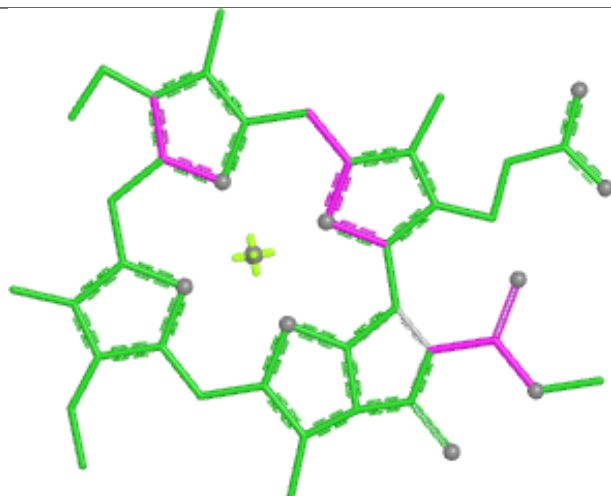
Ligand II0 e 614



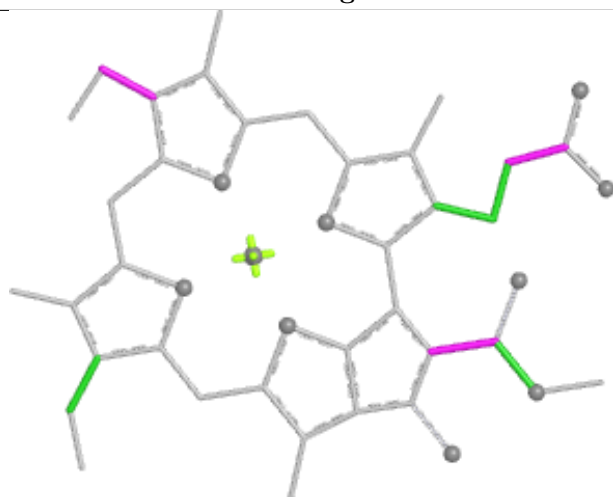
Ligand CLA 3 302



Bond lengths



Bond angles

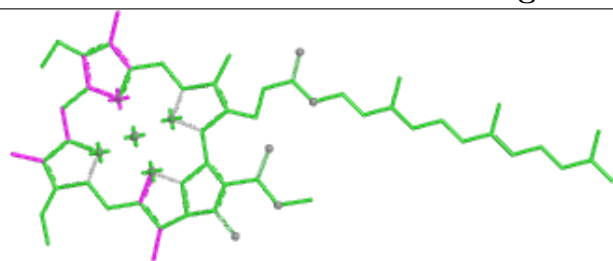


Torsions

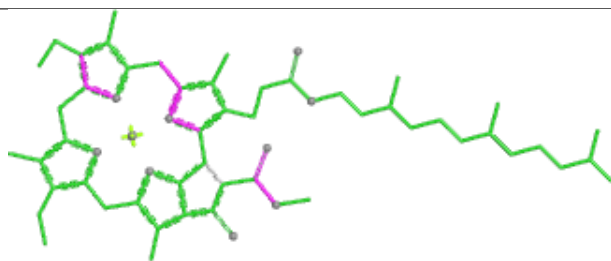


Rings

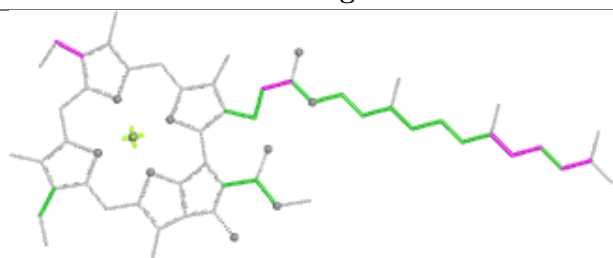
Ligand CLA 2 605



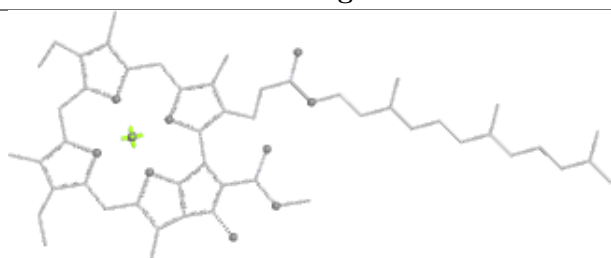
Bond lengths



Bond angles

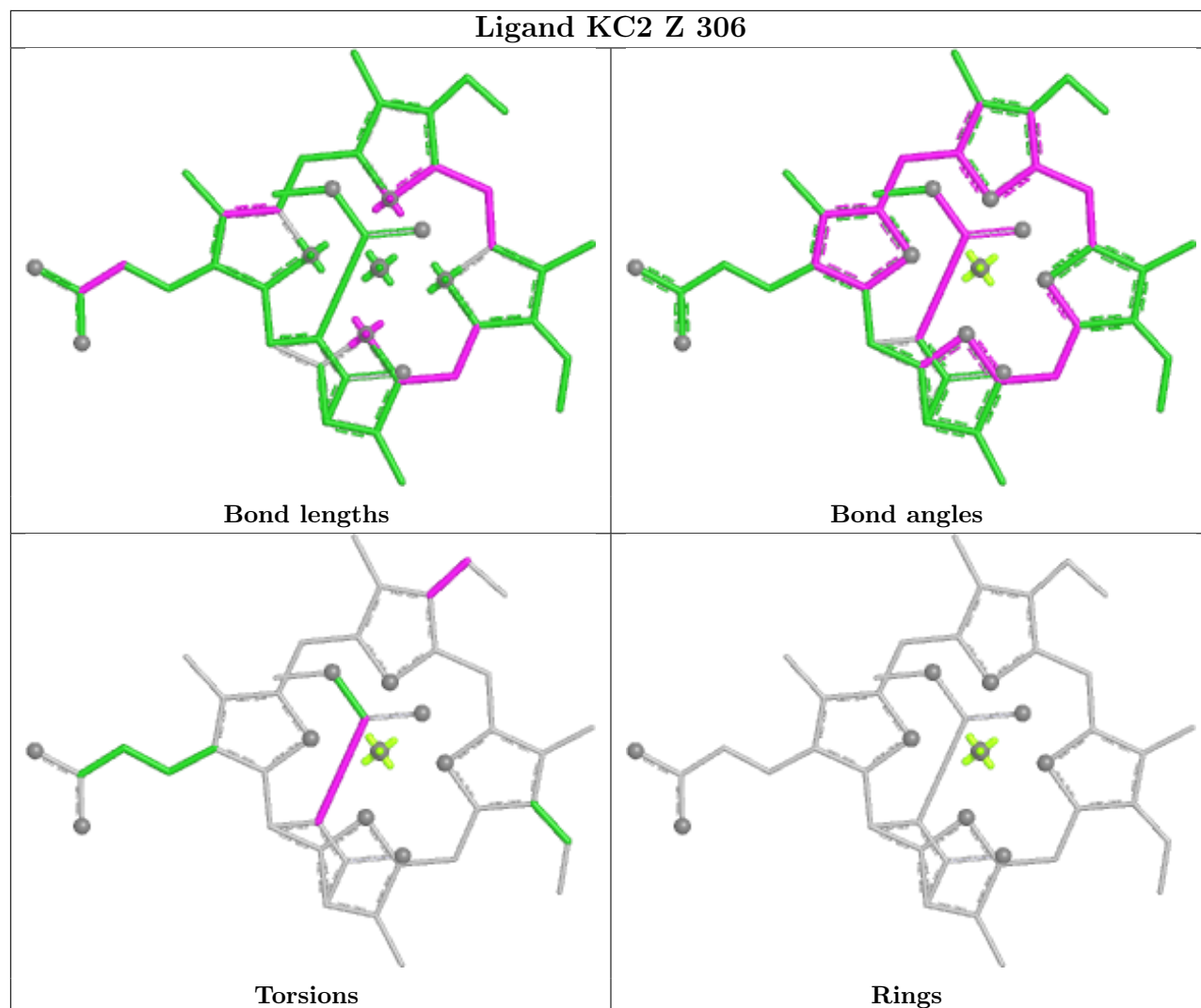


Torsions

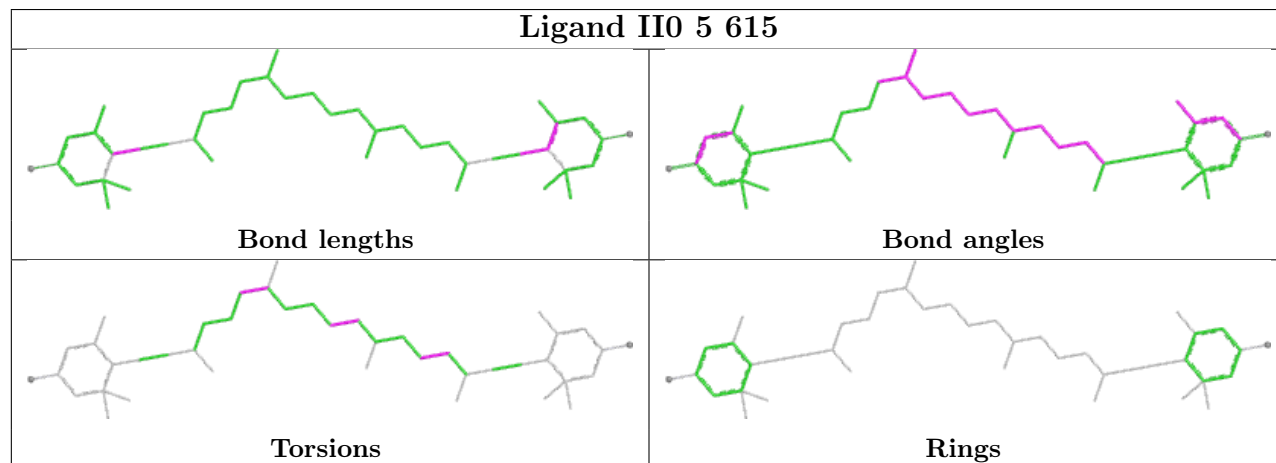


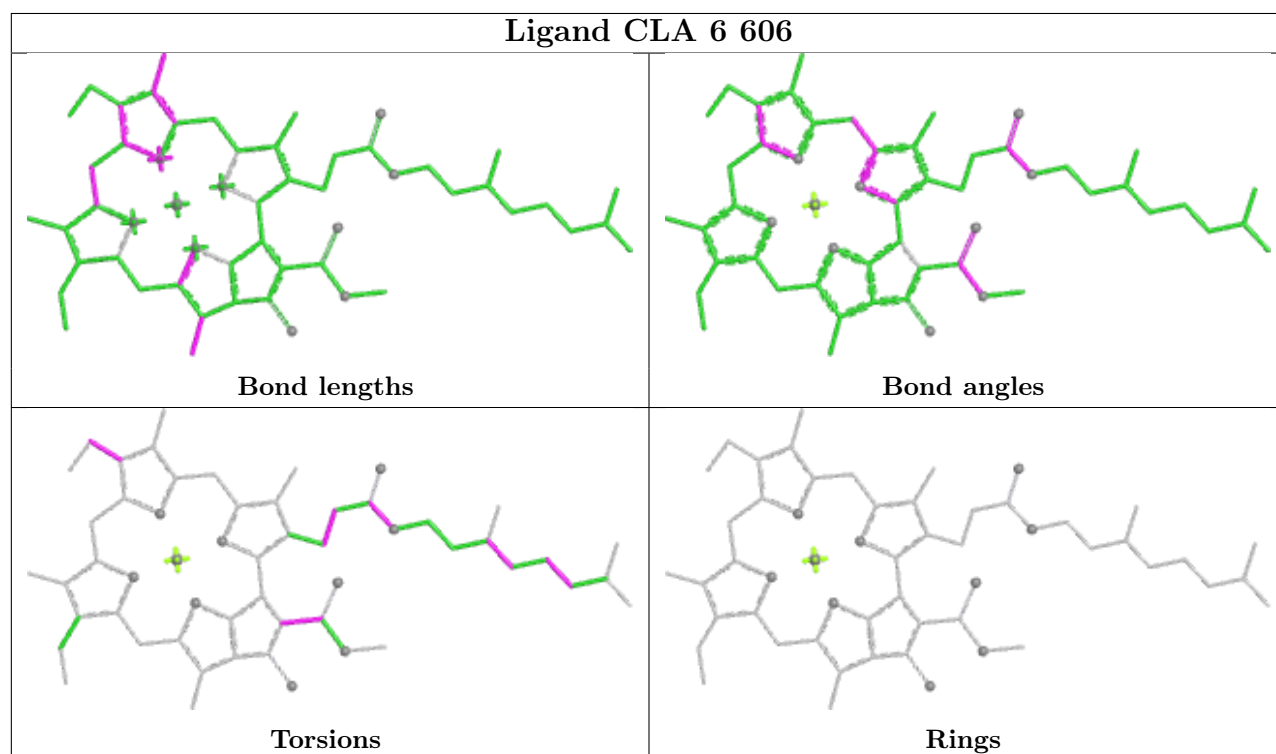
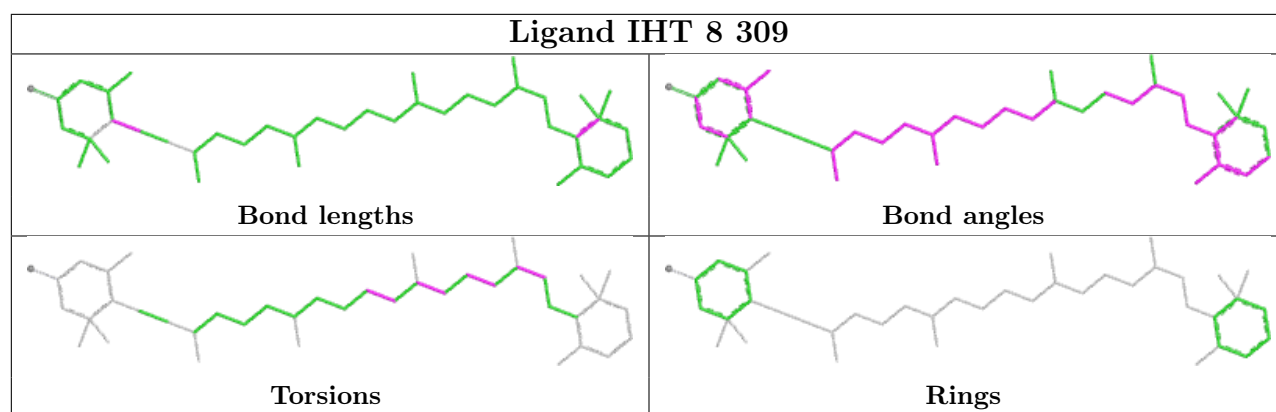
Rings

Ligand KC2 Z 306

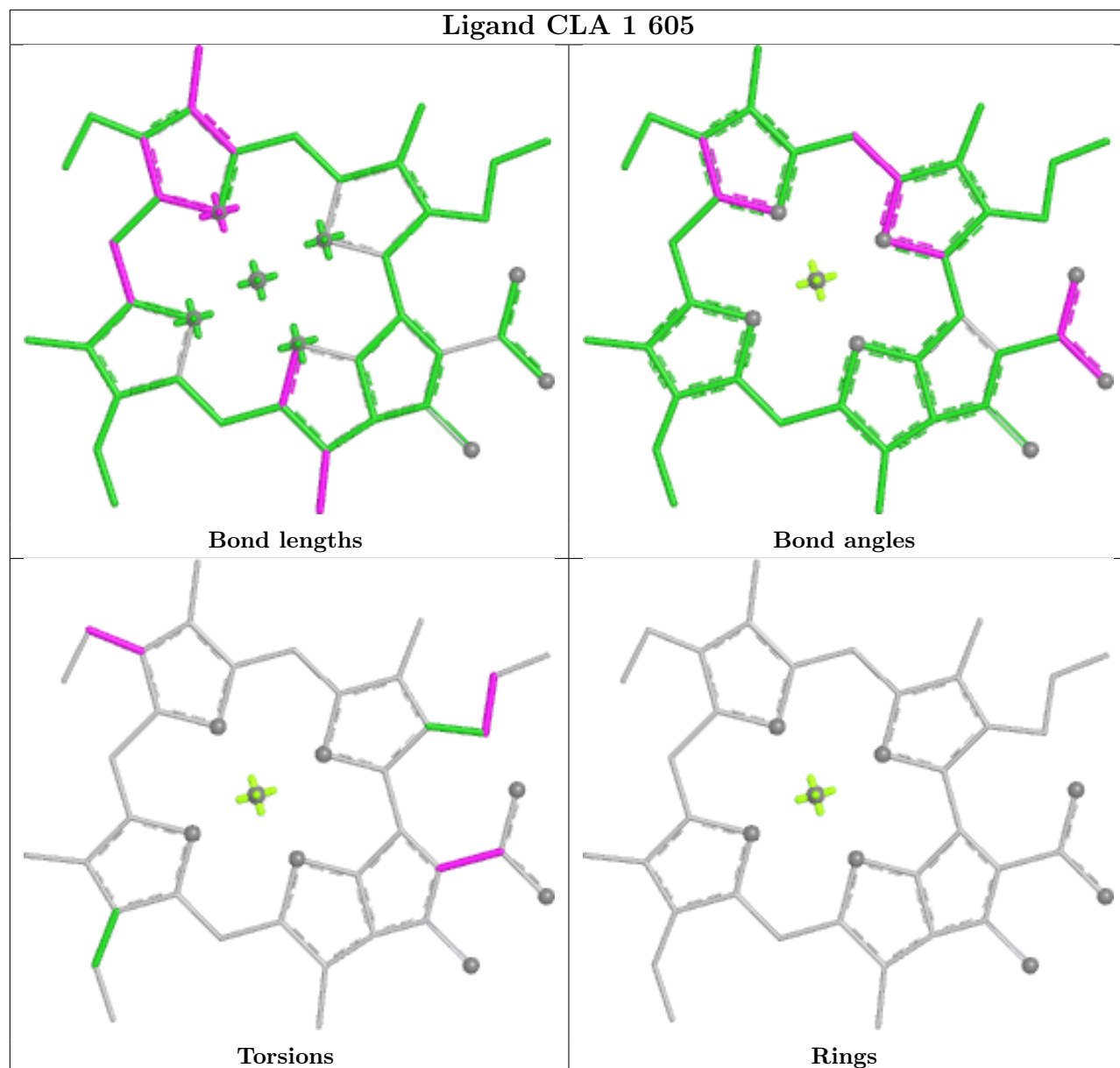


Ligand II0 5 615

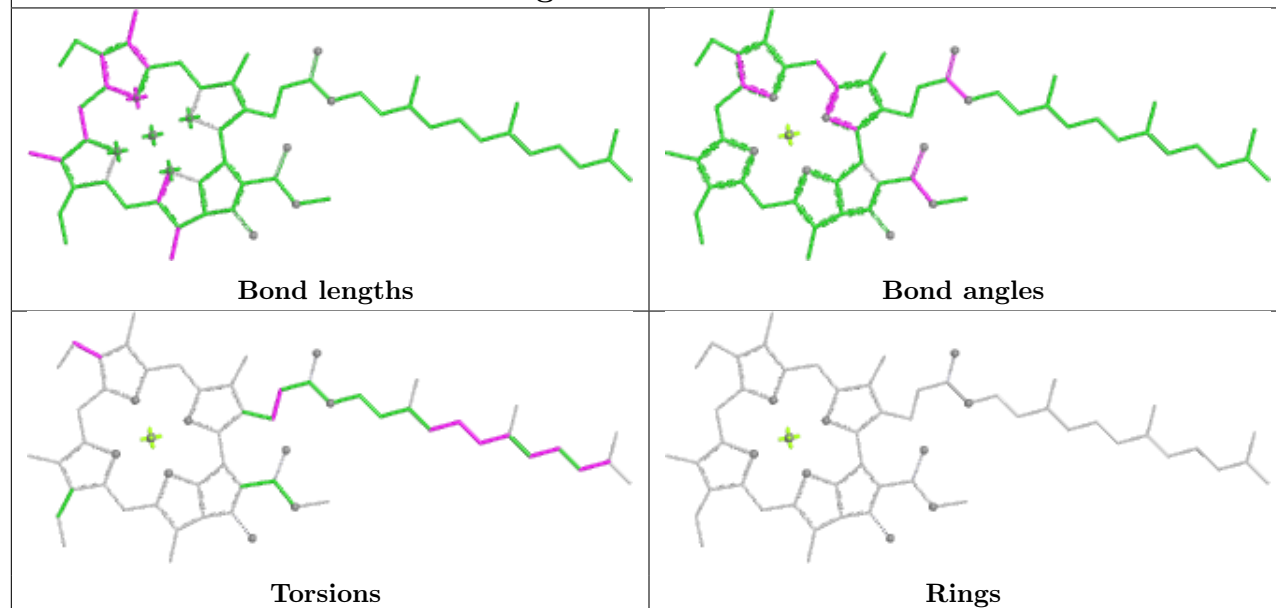




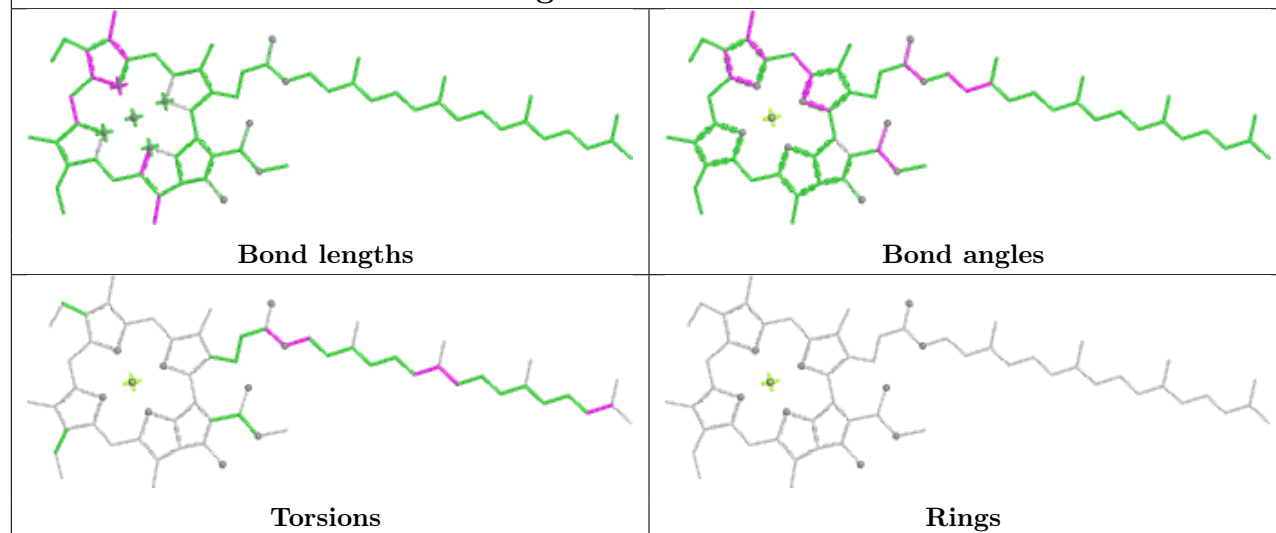
Ligand CLA 1 605



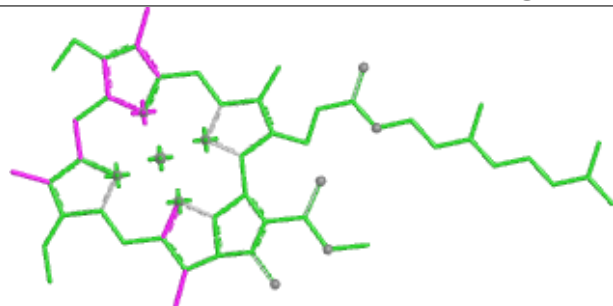
Ligand CLA a 604



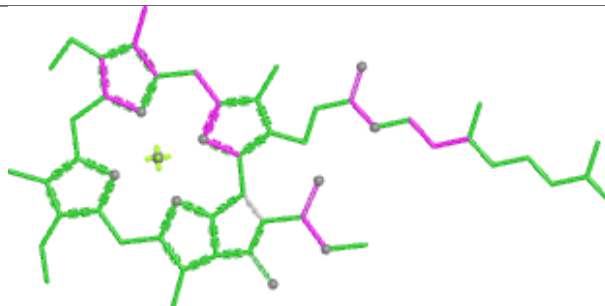
Ligand CLA a 607



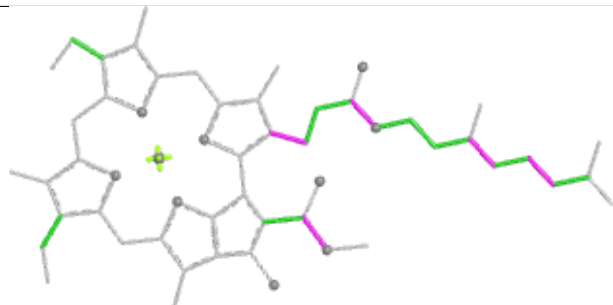
Ligand CLA 7 308



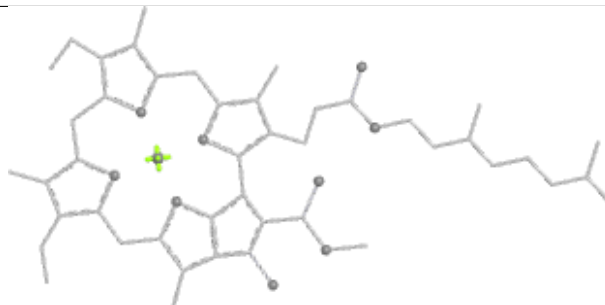
Bond lengths



Bond angles

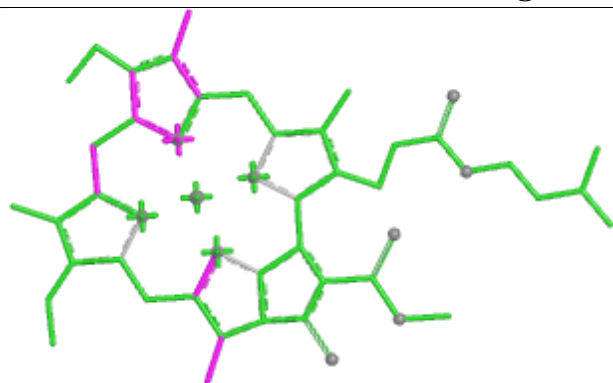


Torsions

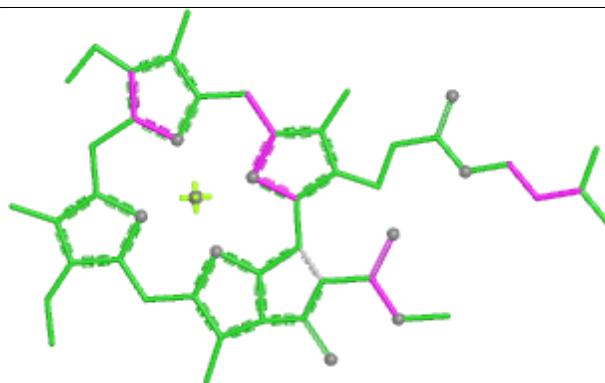


Rings

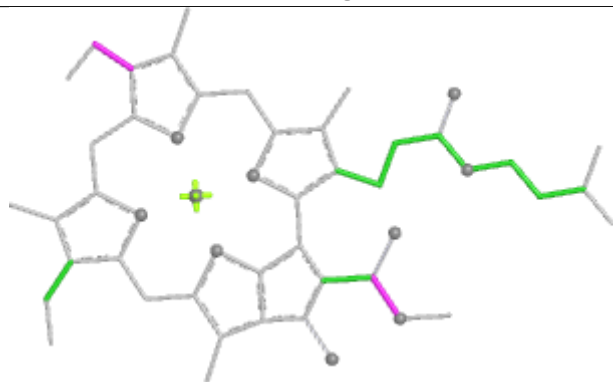
Ligand CLA Z 304



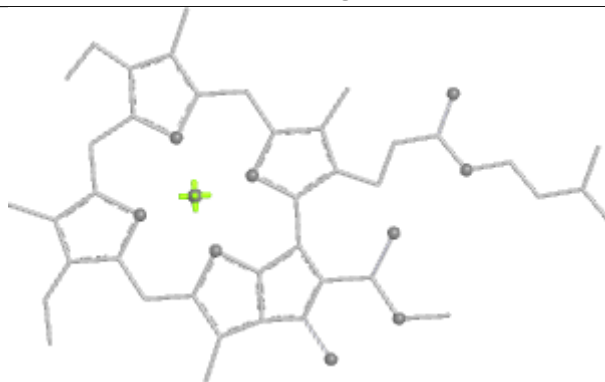
Bond lengths



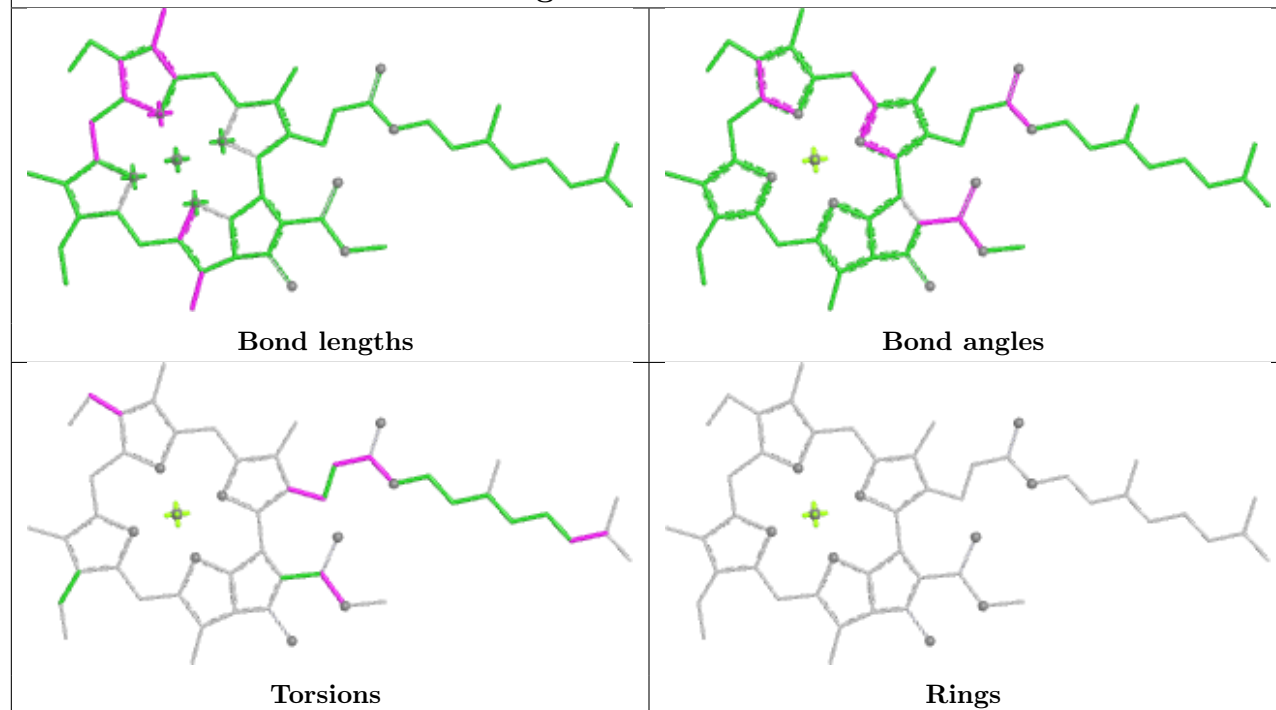
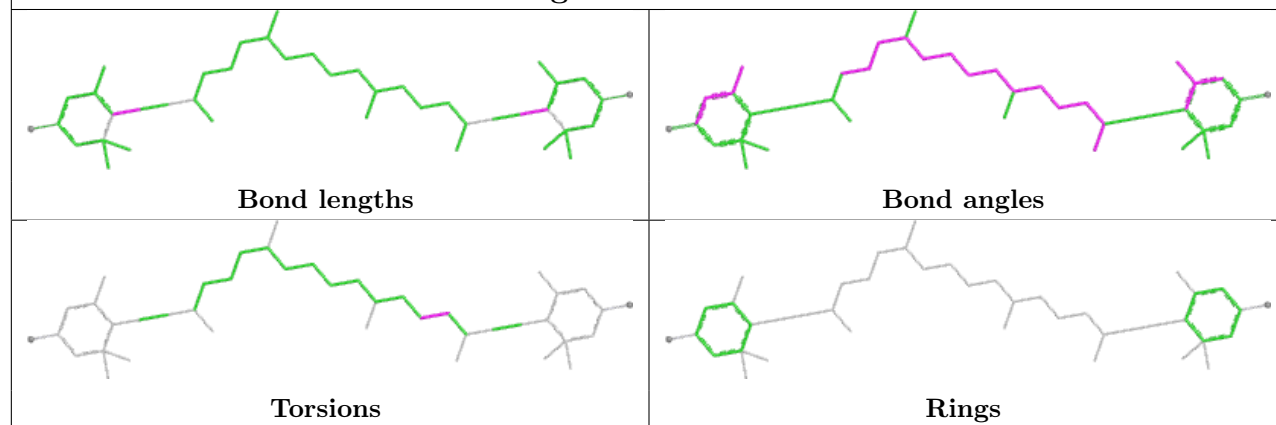
Bond angles



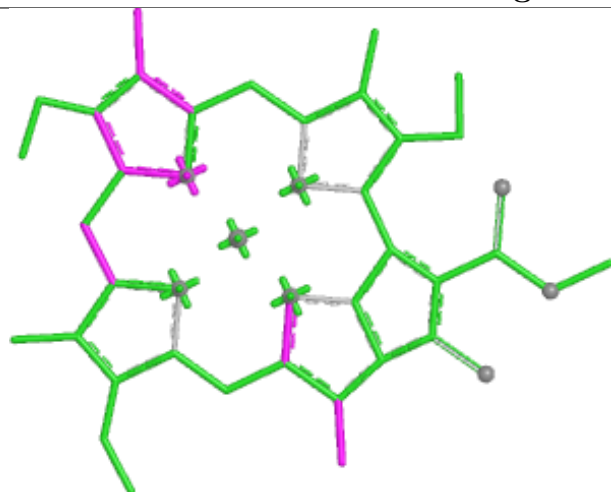
Torsions



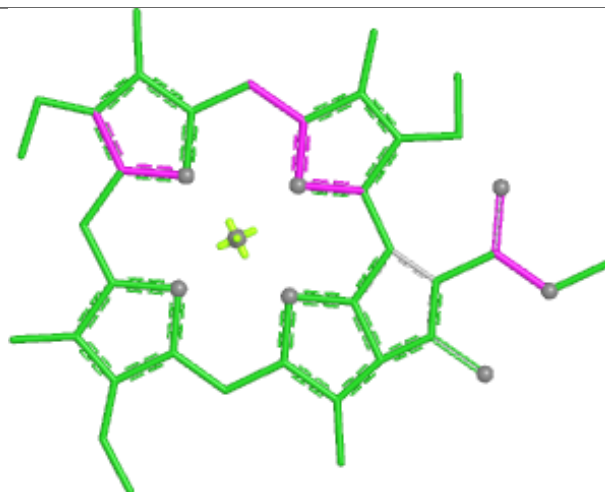
Rings

Ligand CLA a 605**Ligand II0 5 616**

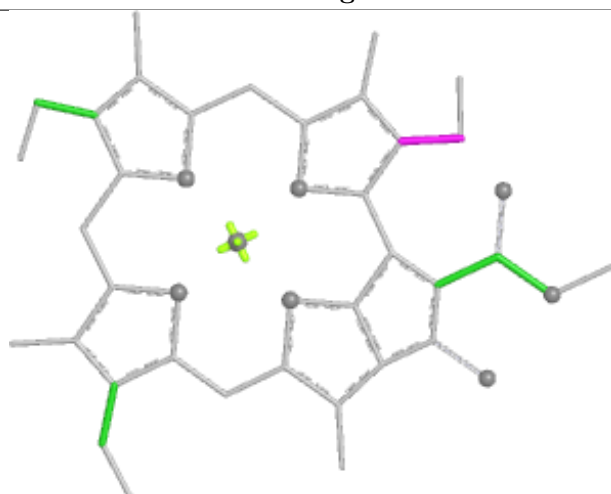
Ligand CLA A 813



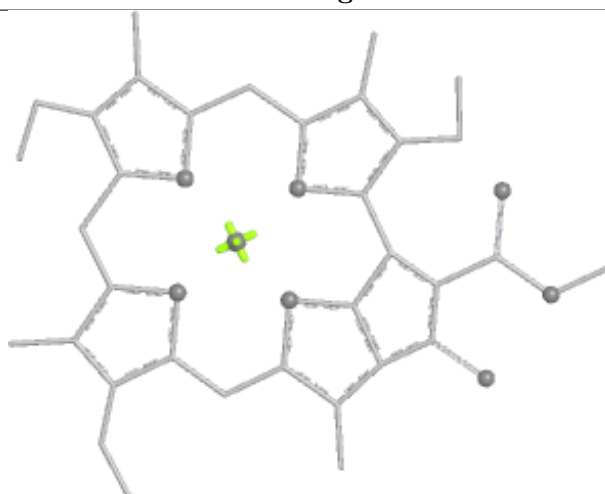
Bond lengths



Bond angles

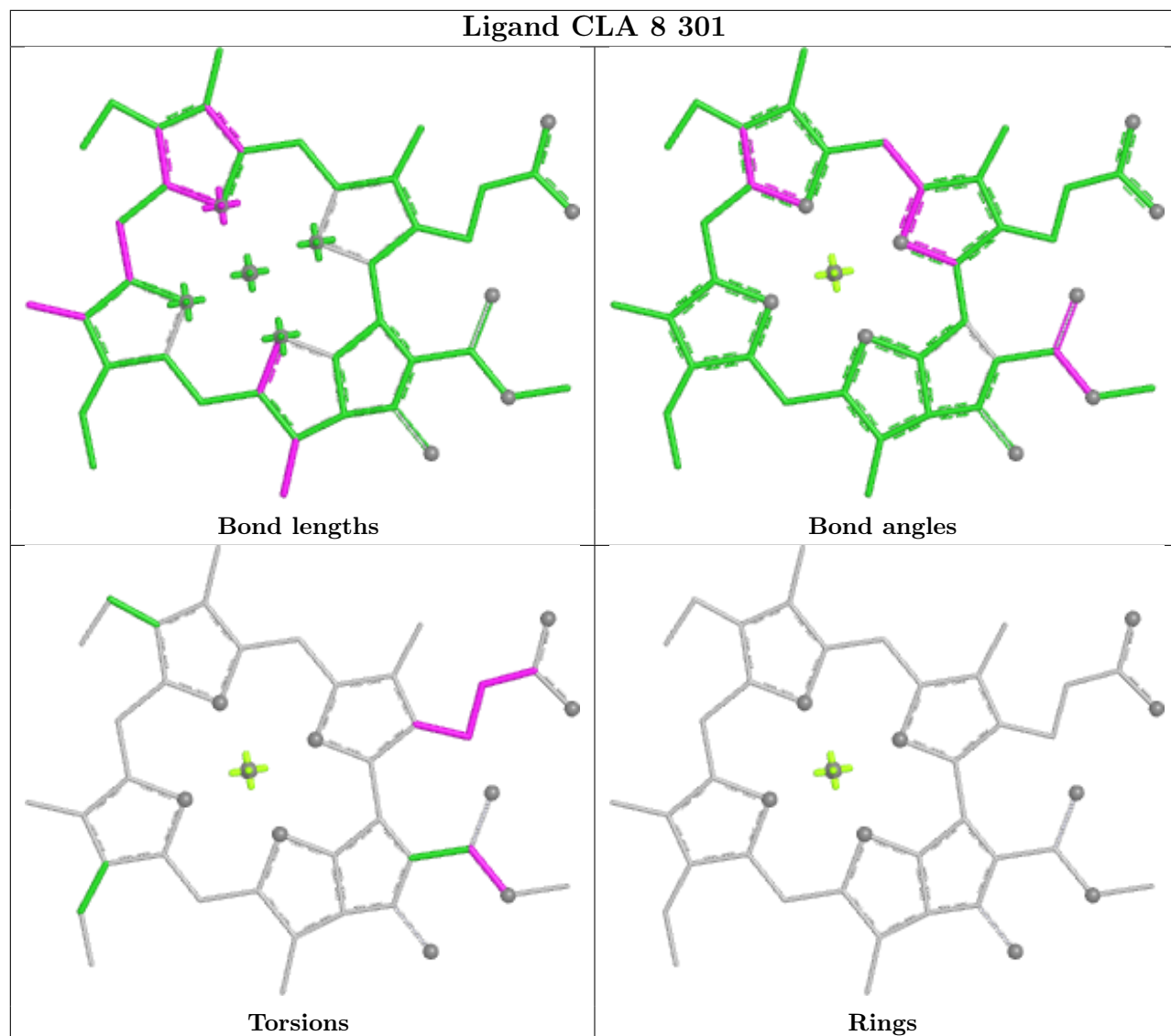


Torsions

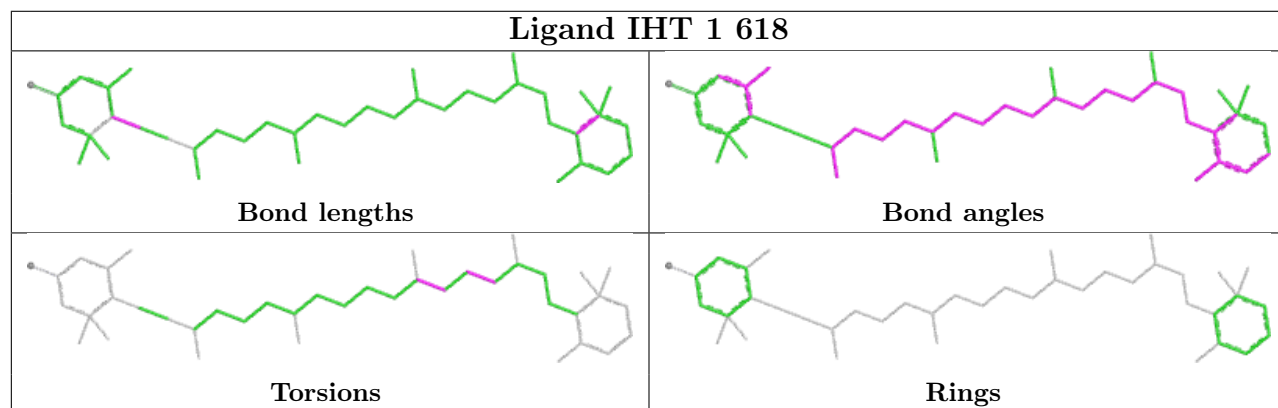


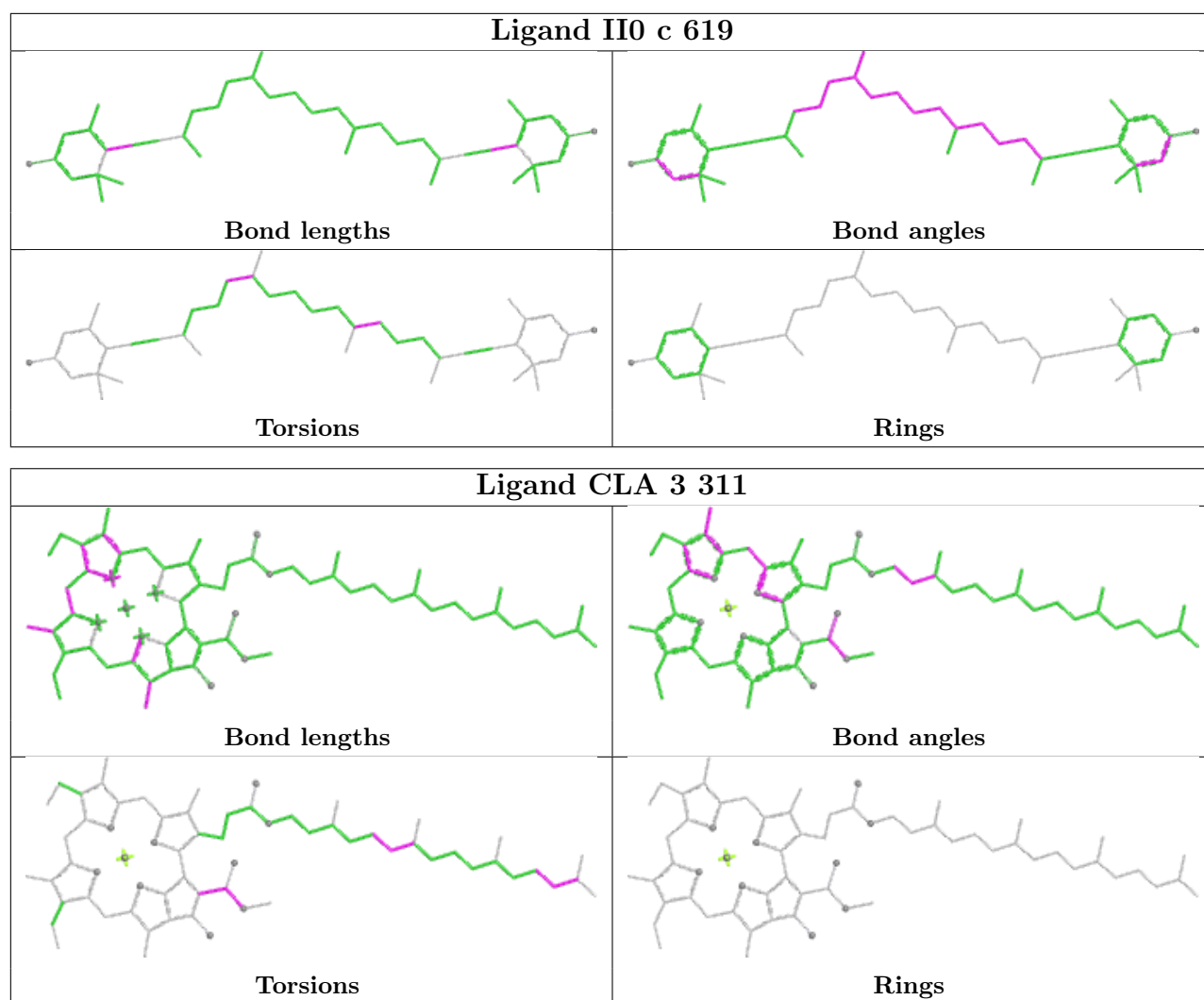
Rings

Ligand CLA 8 301

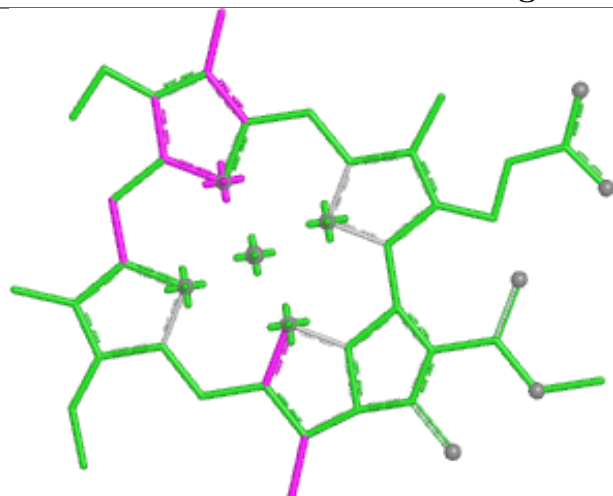


Ligand IHT 1 618

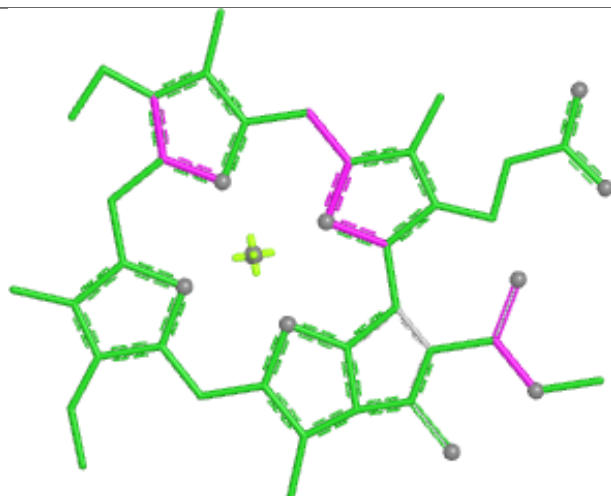




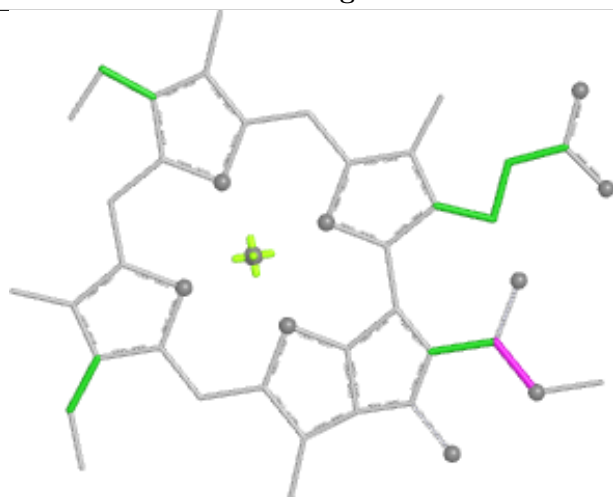
Ligand CLA 7 302



Bond lengths



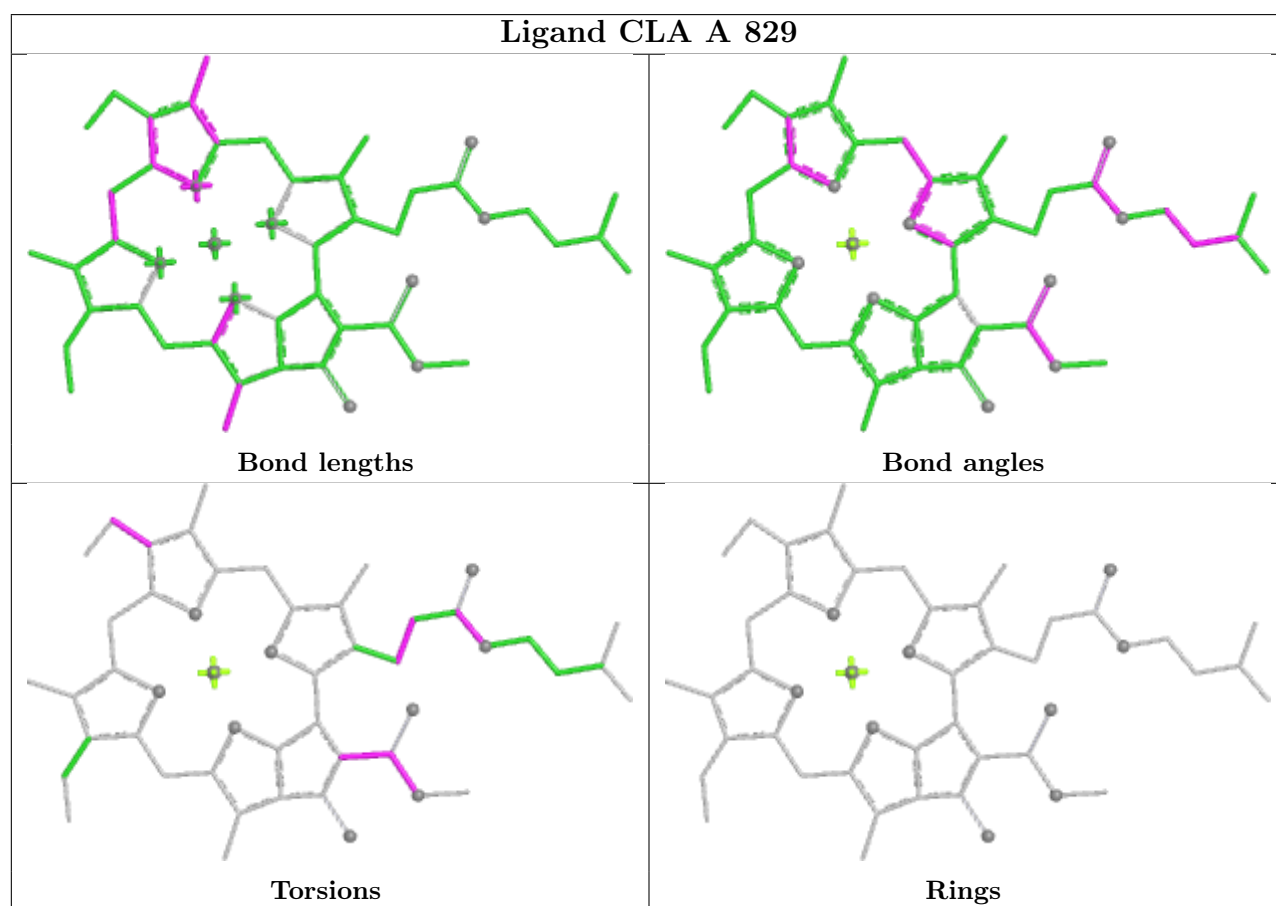
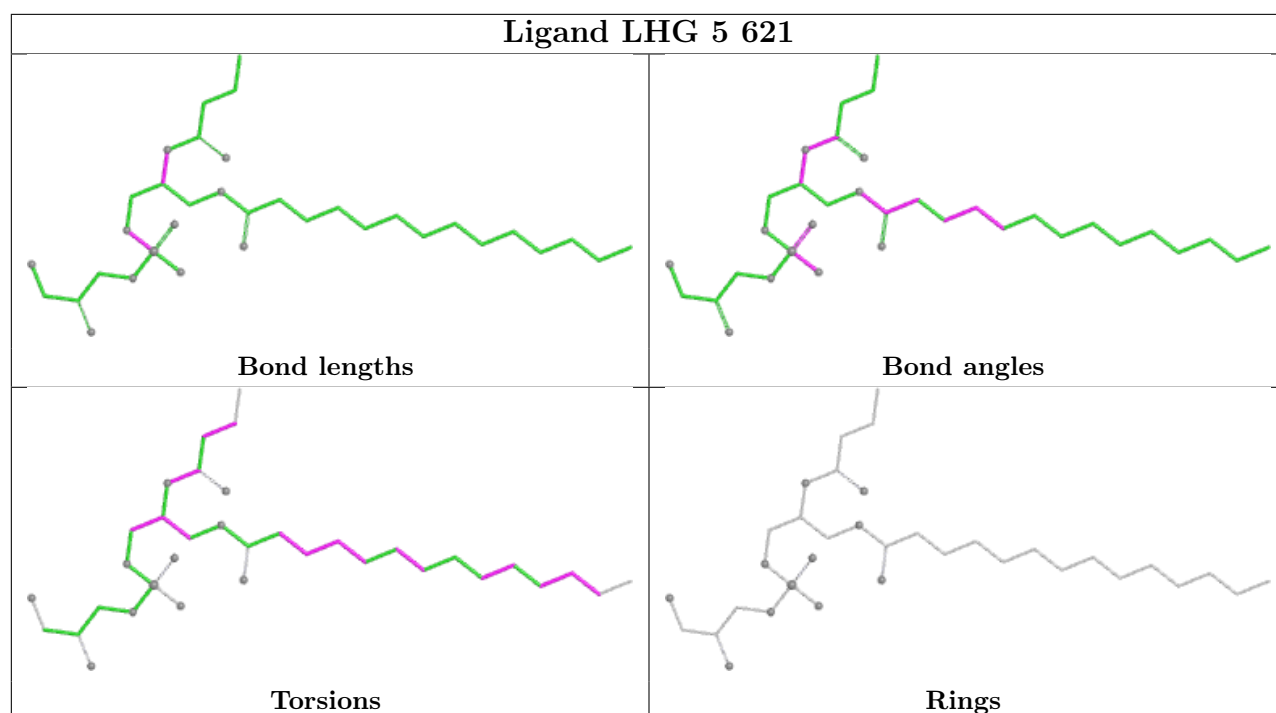
Bond angles

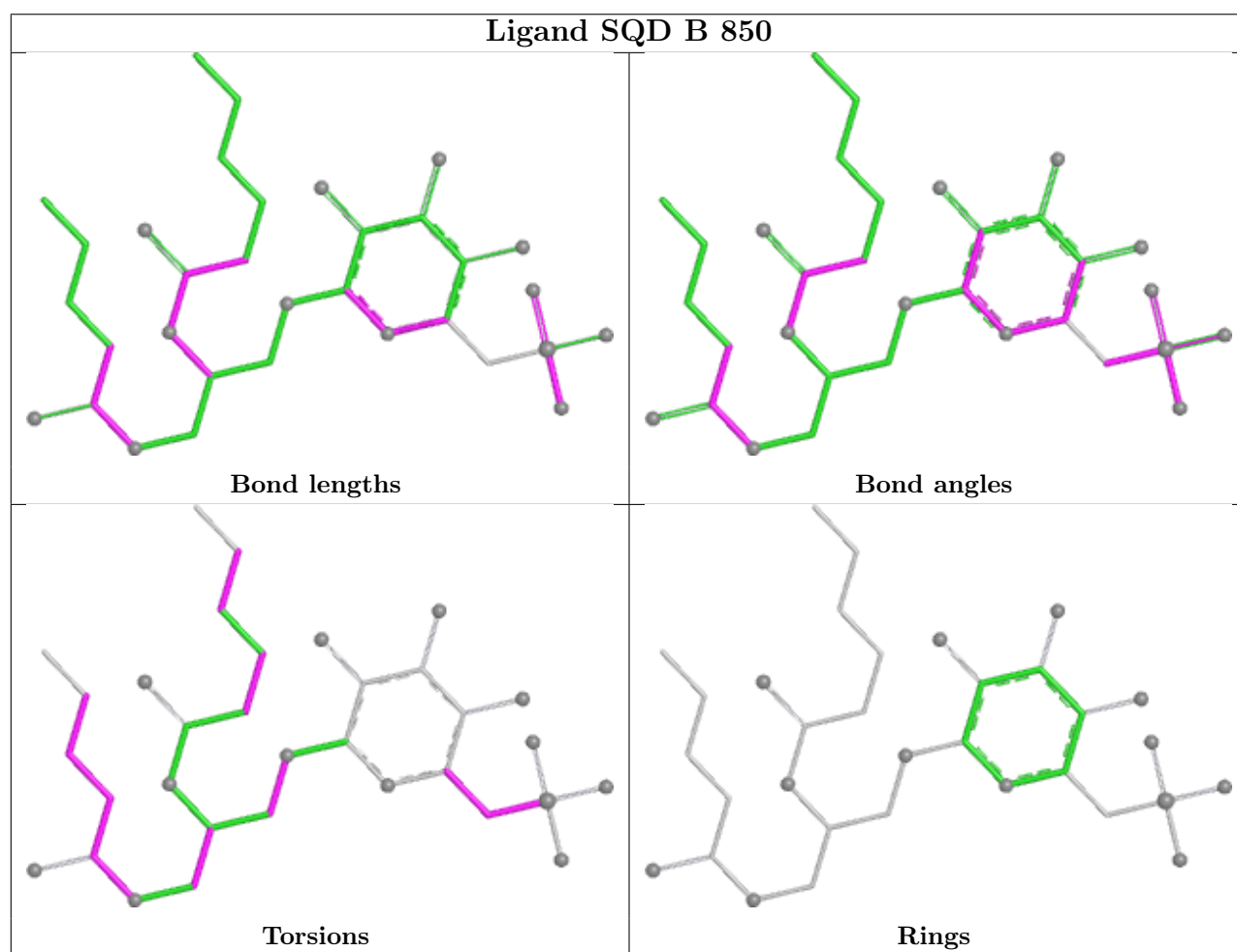
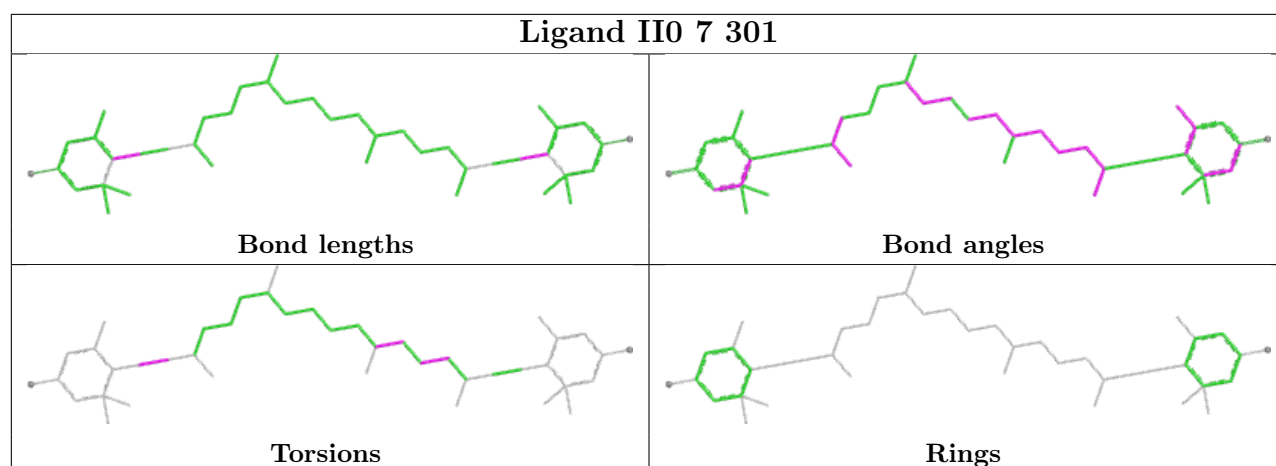


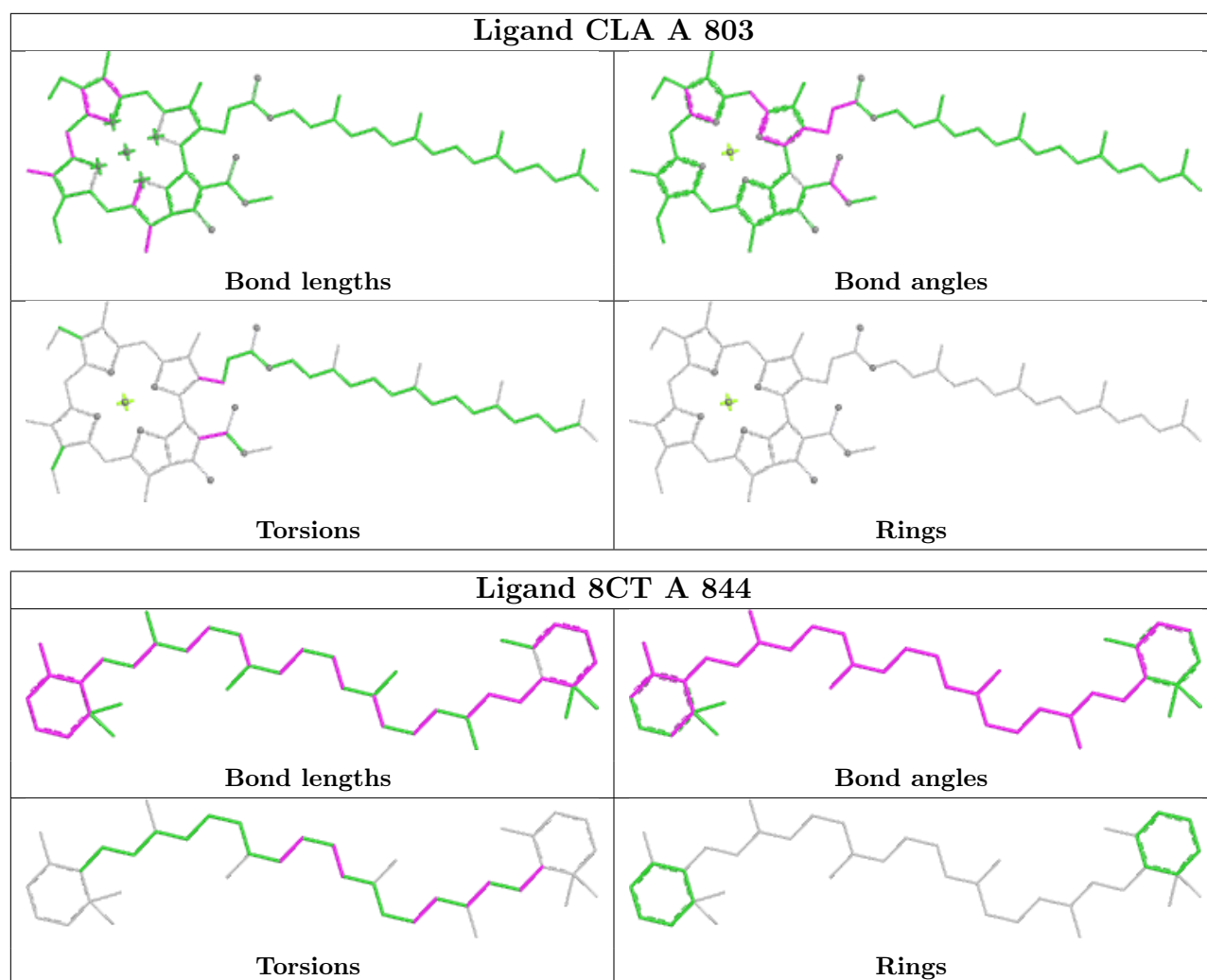
Torsions

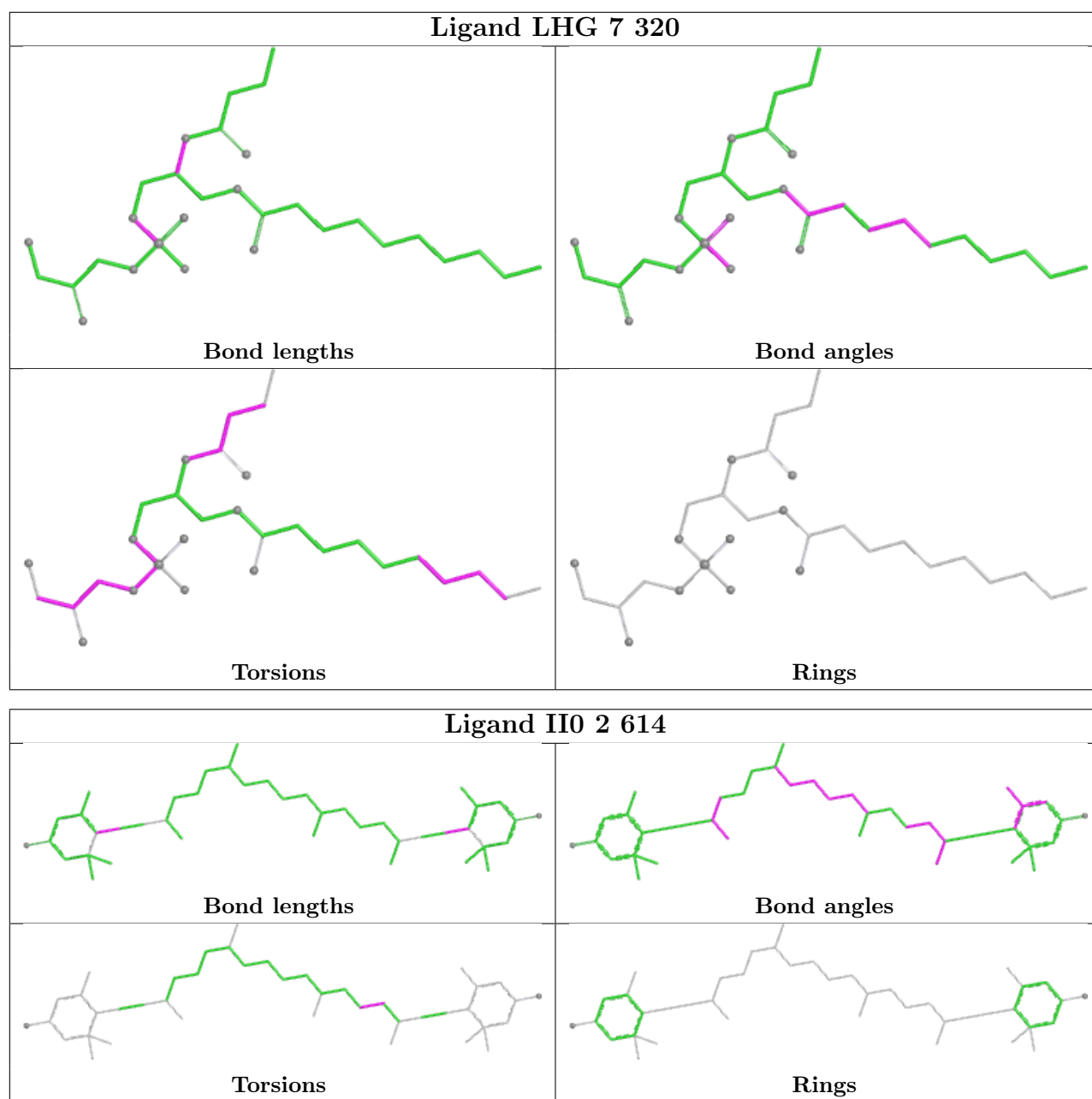


Rings

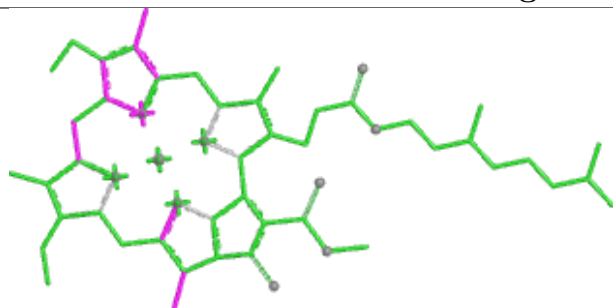




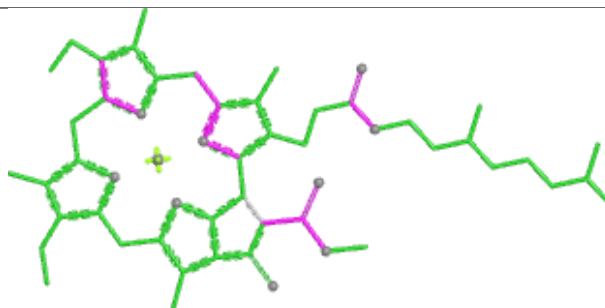




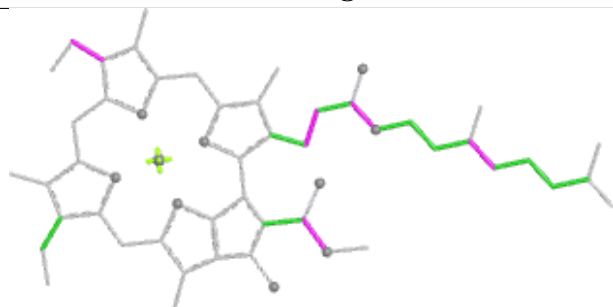
Ligand CLA c 615



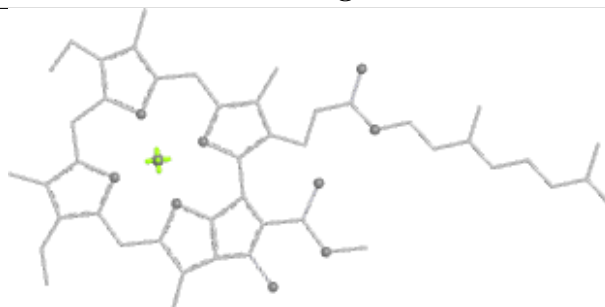
Bond lengths



Bond angles

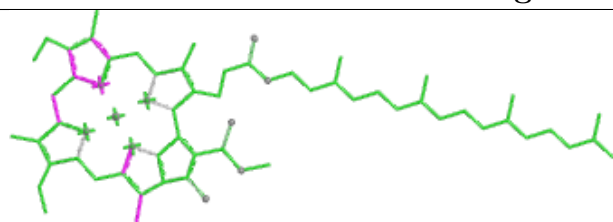


Torsions

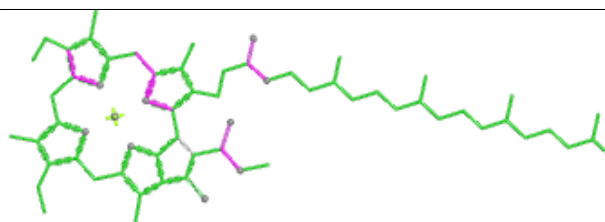


Rings

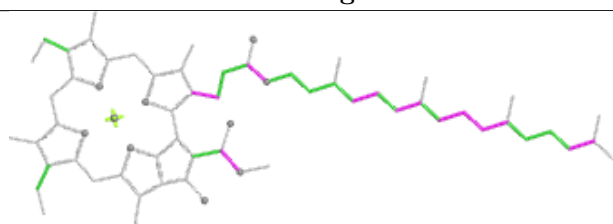
Ligand CLA B 827



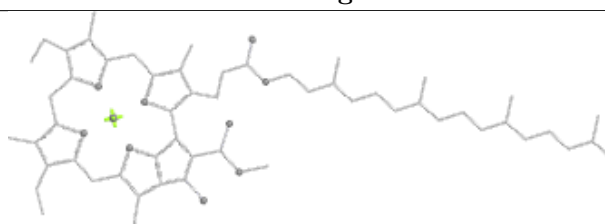
Bond lengths



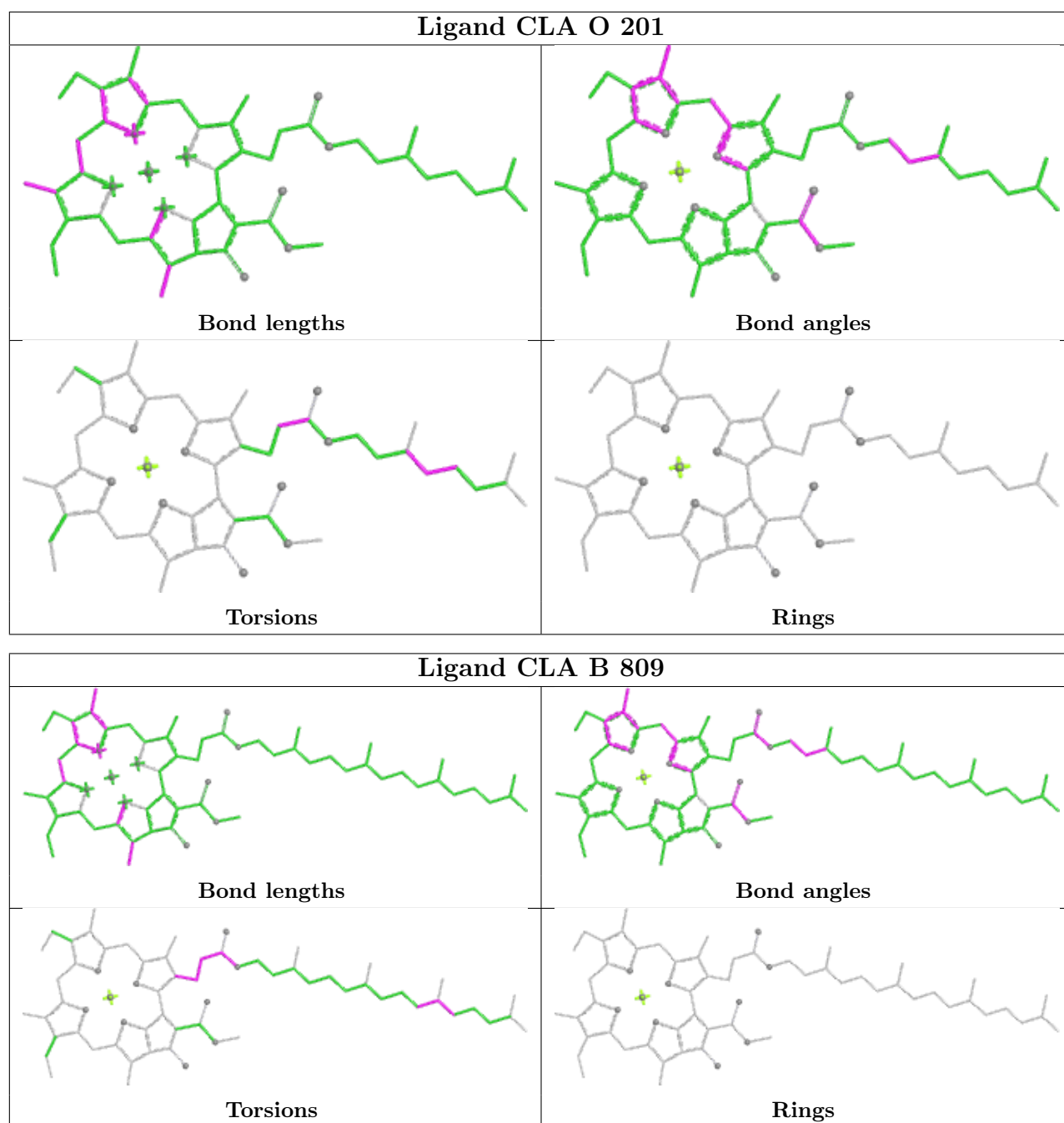
Bond angles

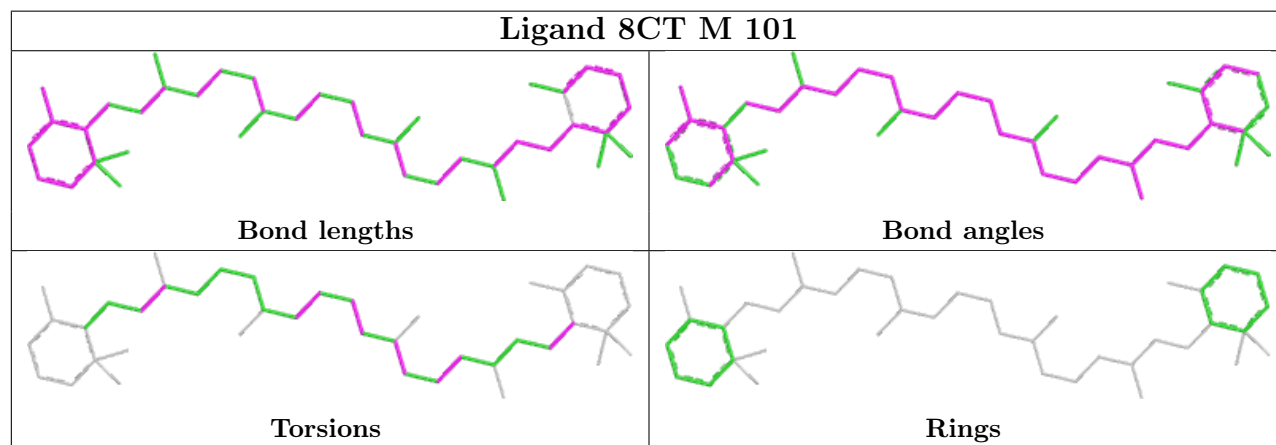
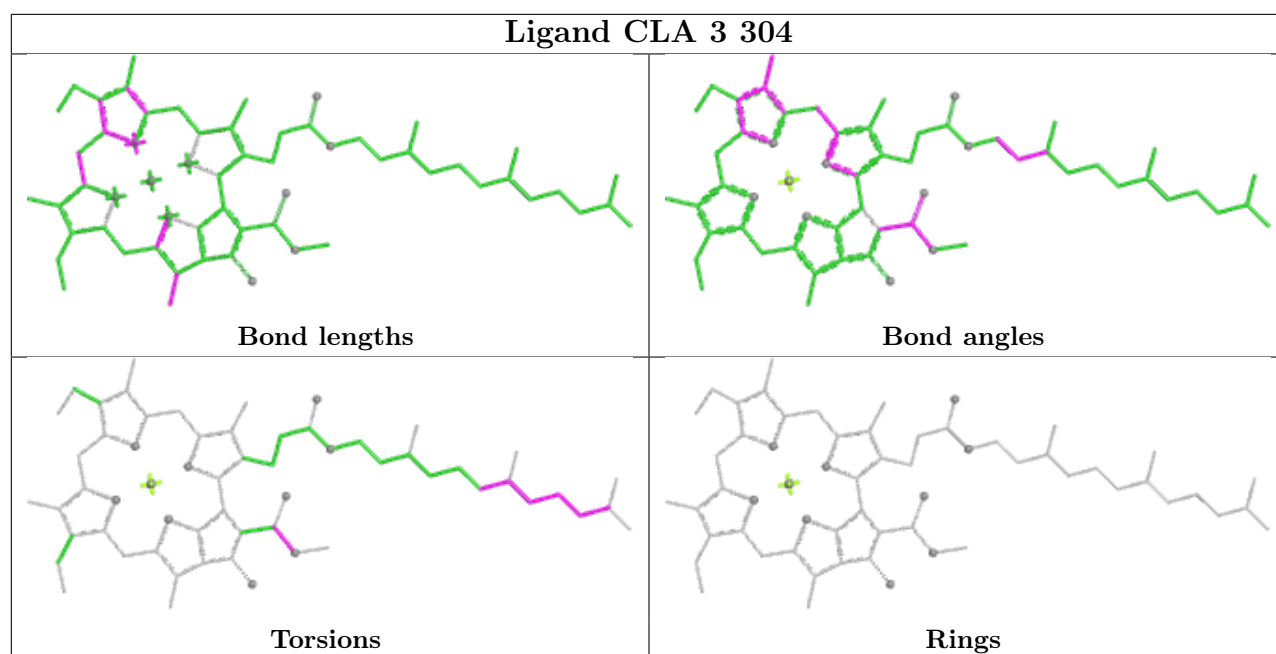


Torsions

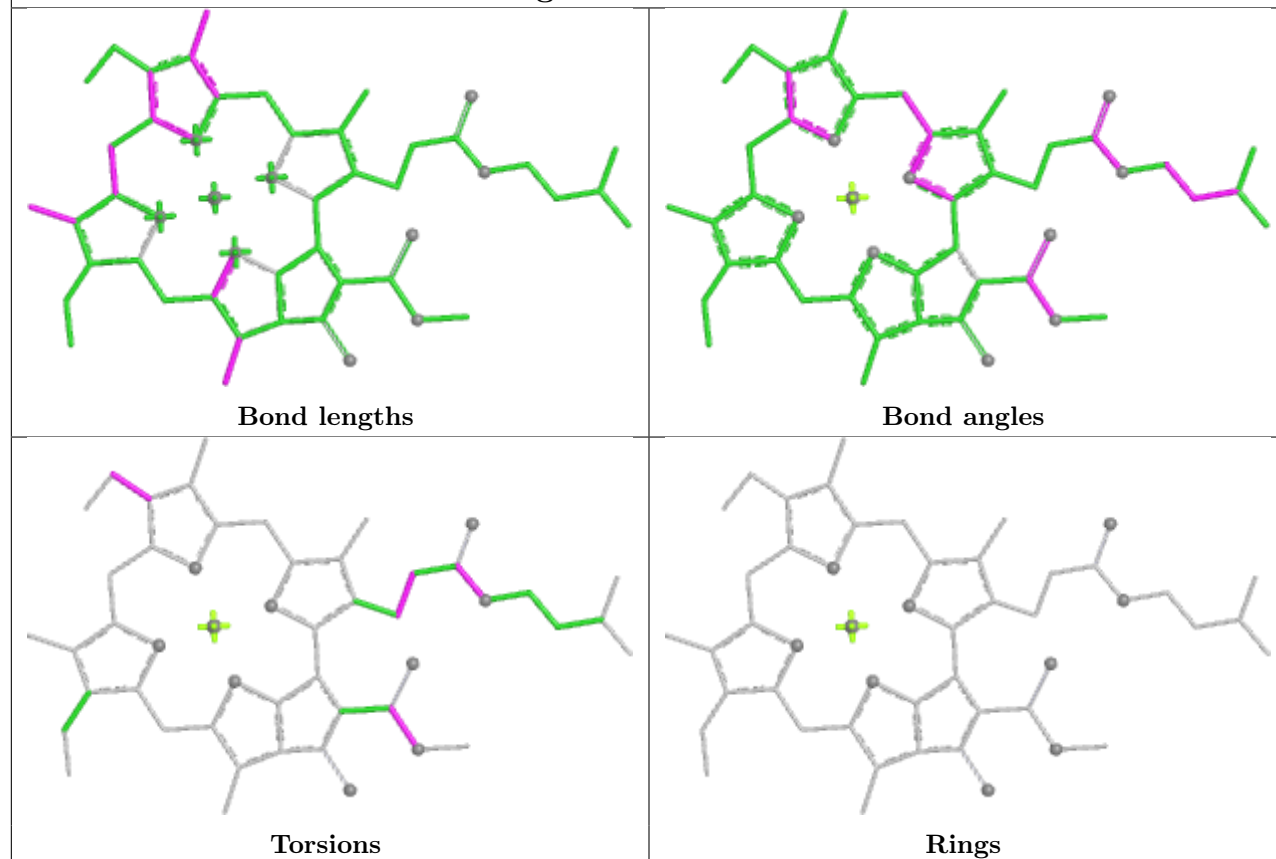


Rings

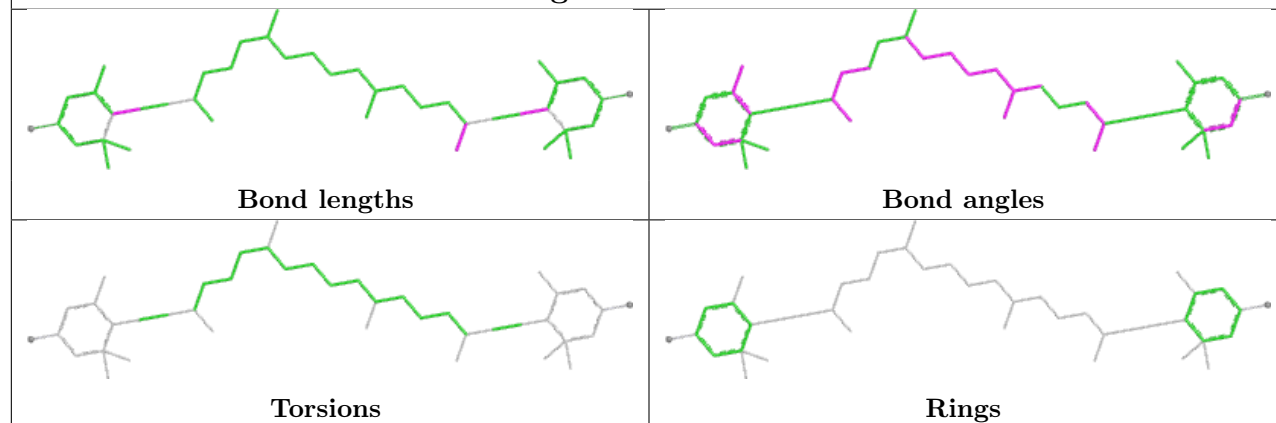


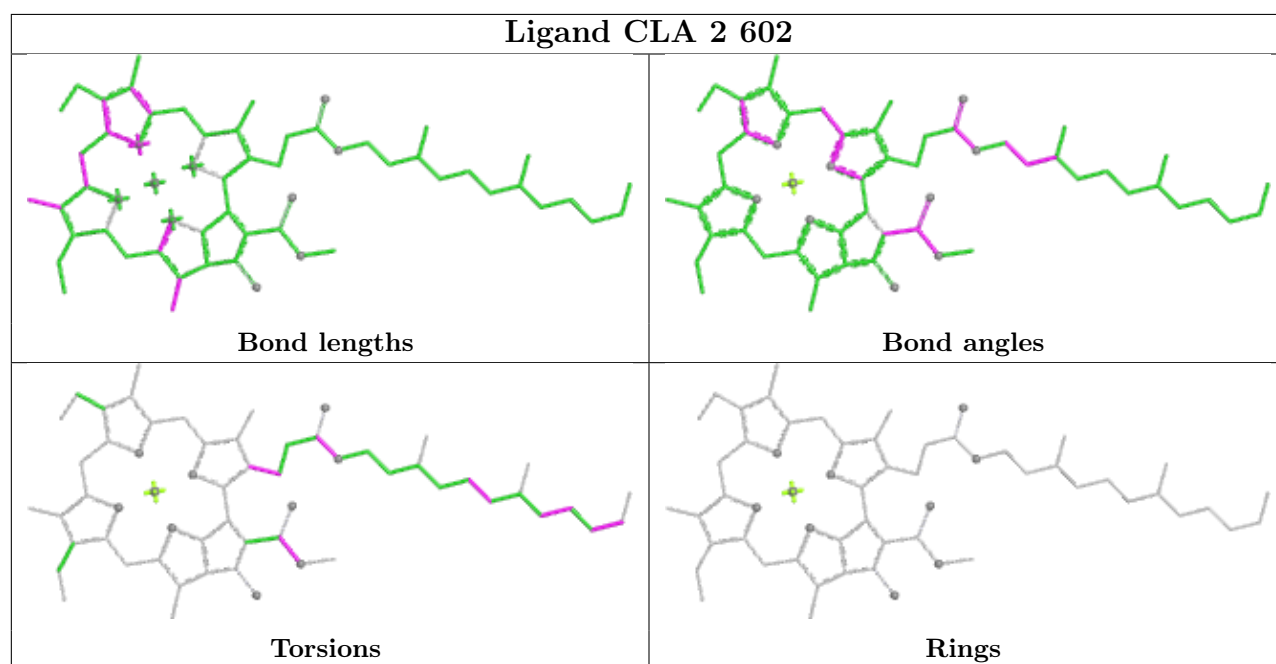
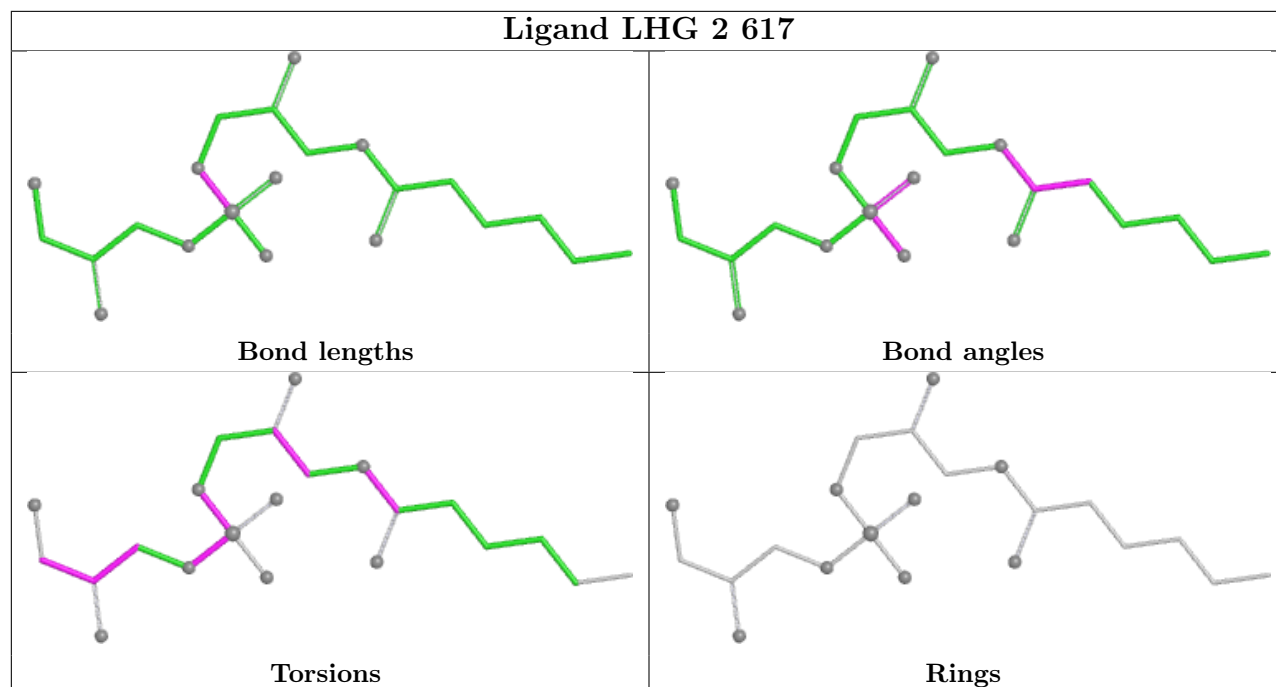


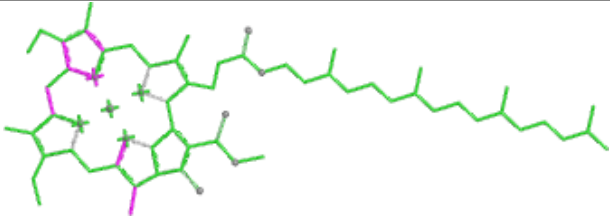
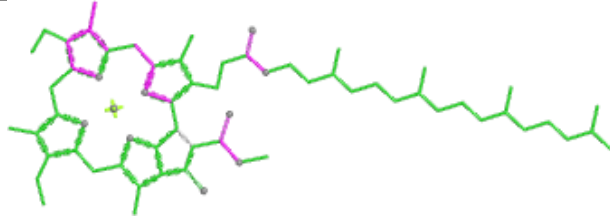
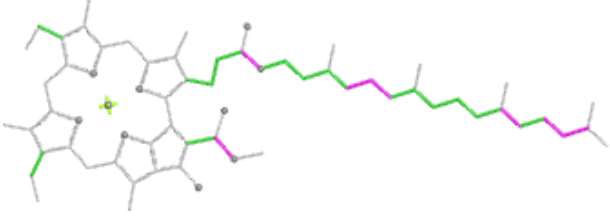
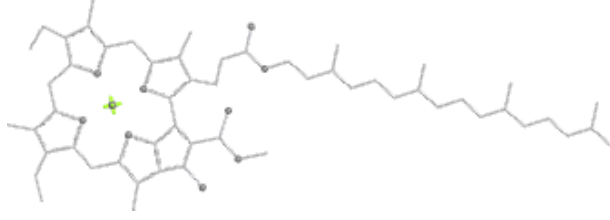
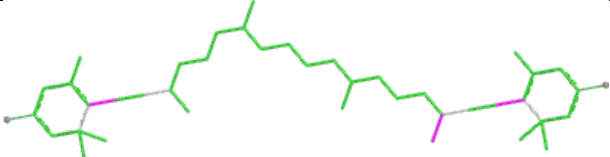
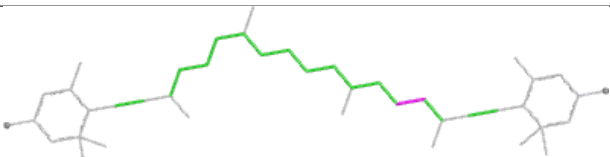
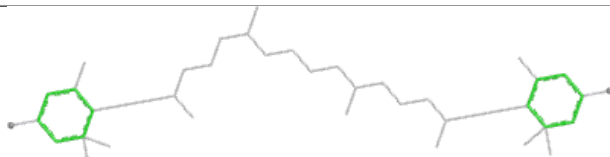
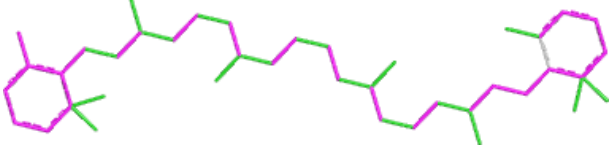
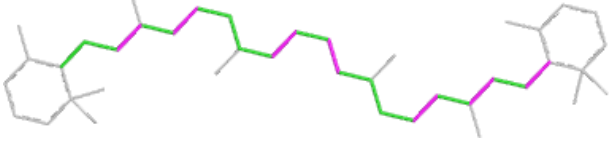
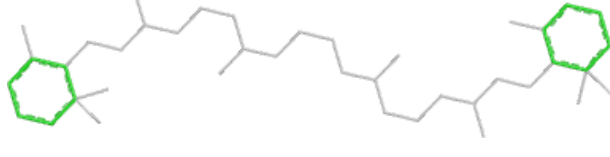
Ligand CLA 3 312

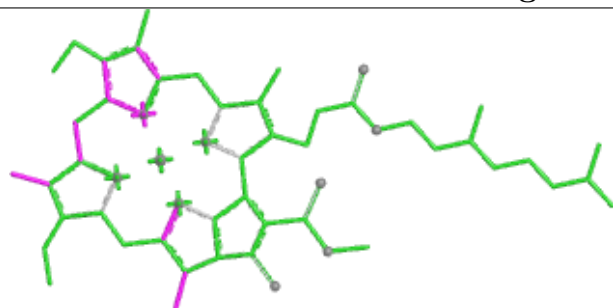


Ligand II0 9 317

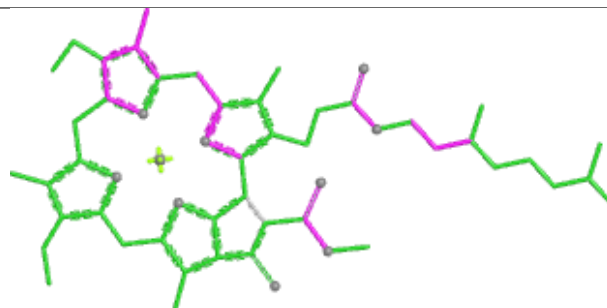




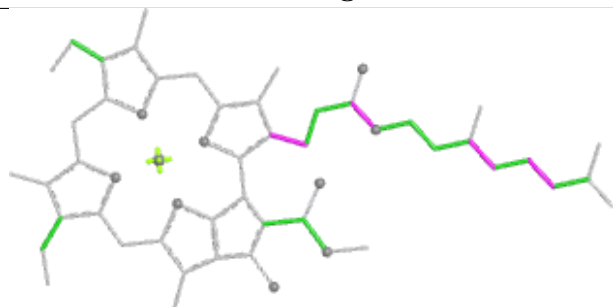
Ligand CLA 4 611	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand II0 a 619	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand 8CT B 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA e 602

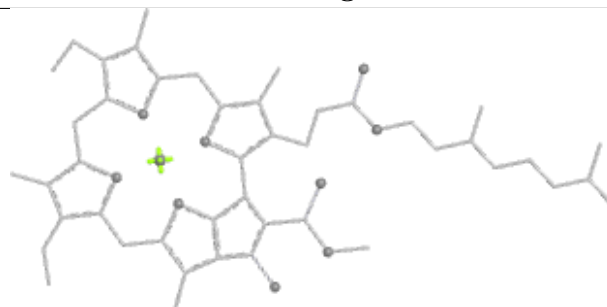
Bond lengths



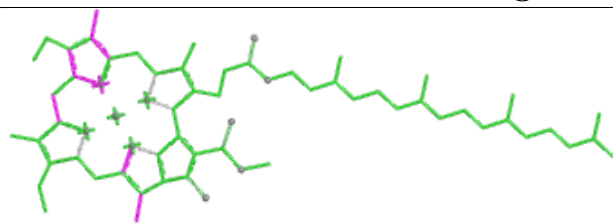
Bond angles



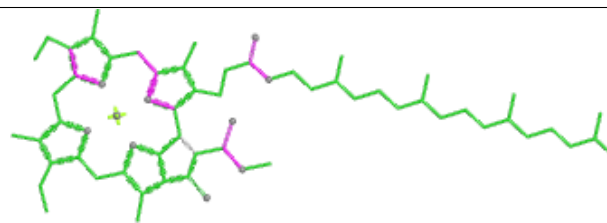
Torsions



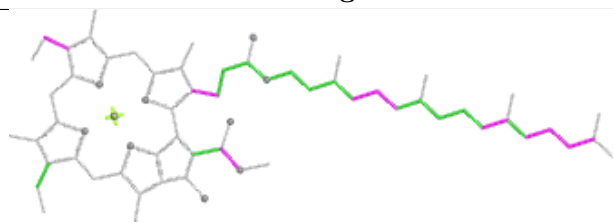
Rings

Ligand CLA A 831

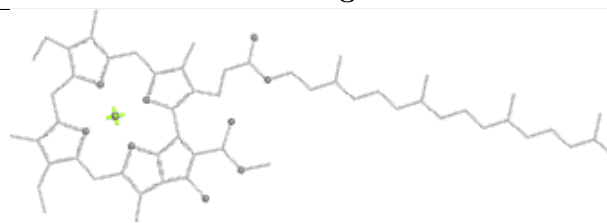
Bond lengths



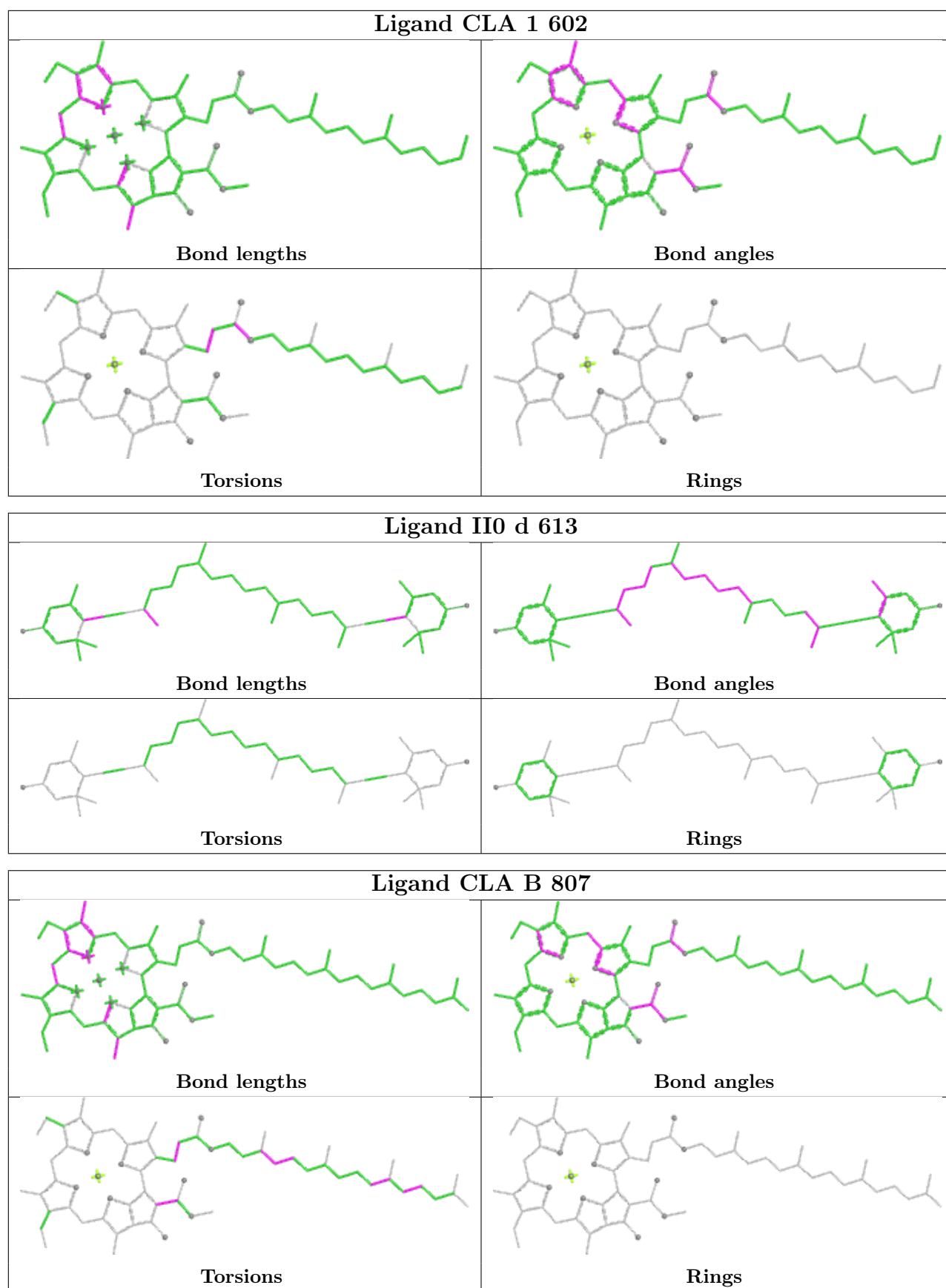
Bond angles



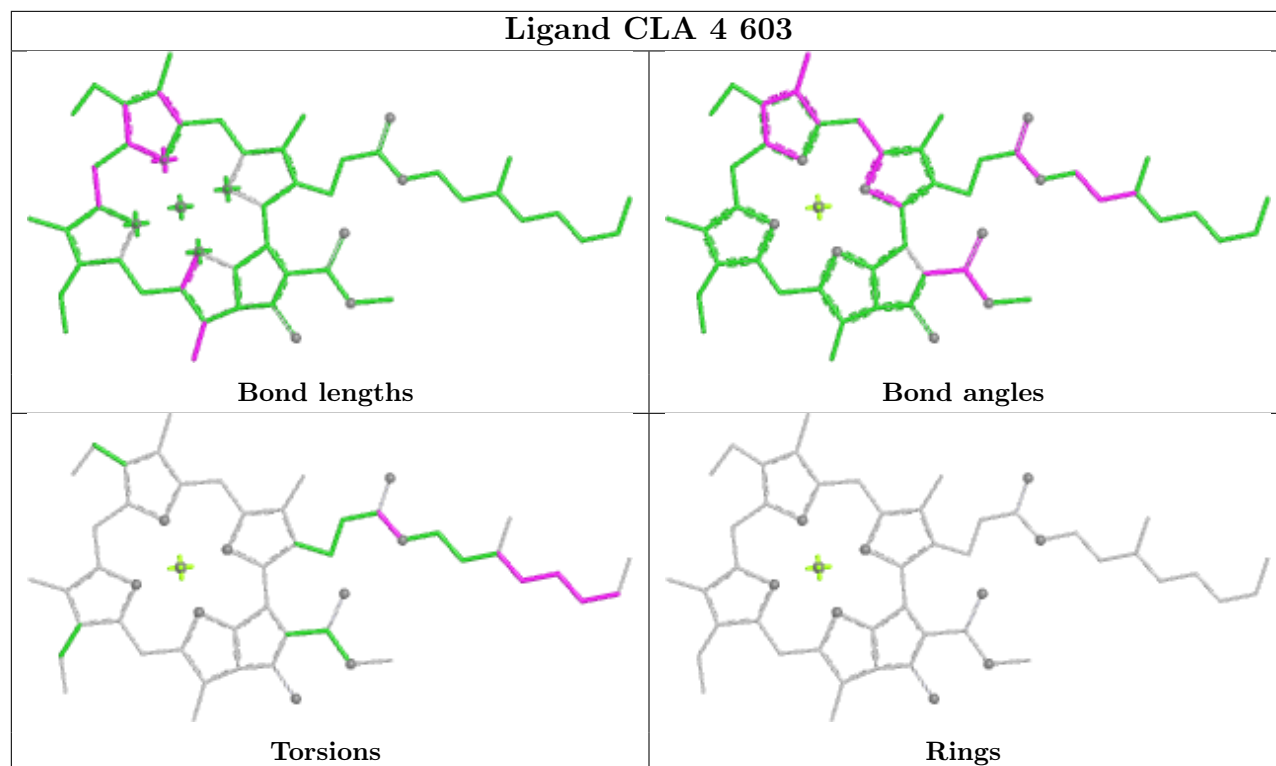
Torsions



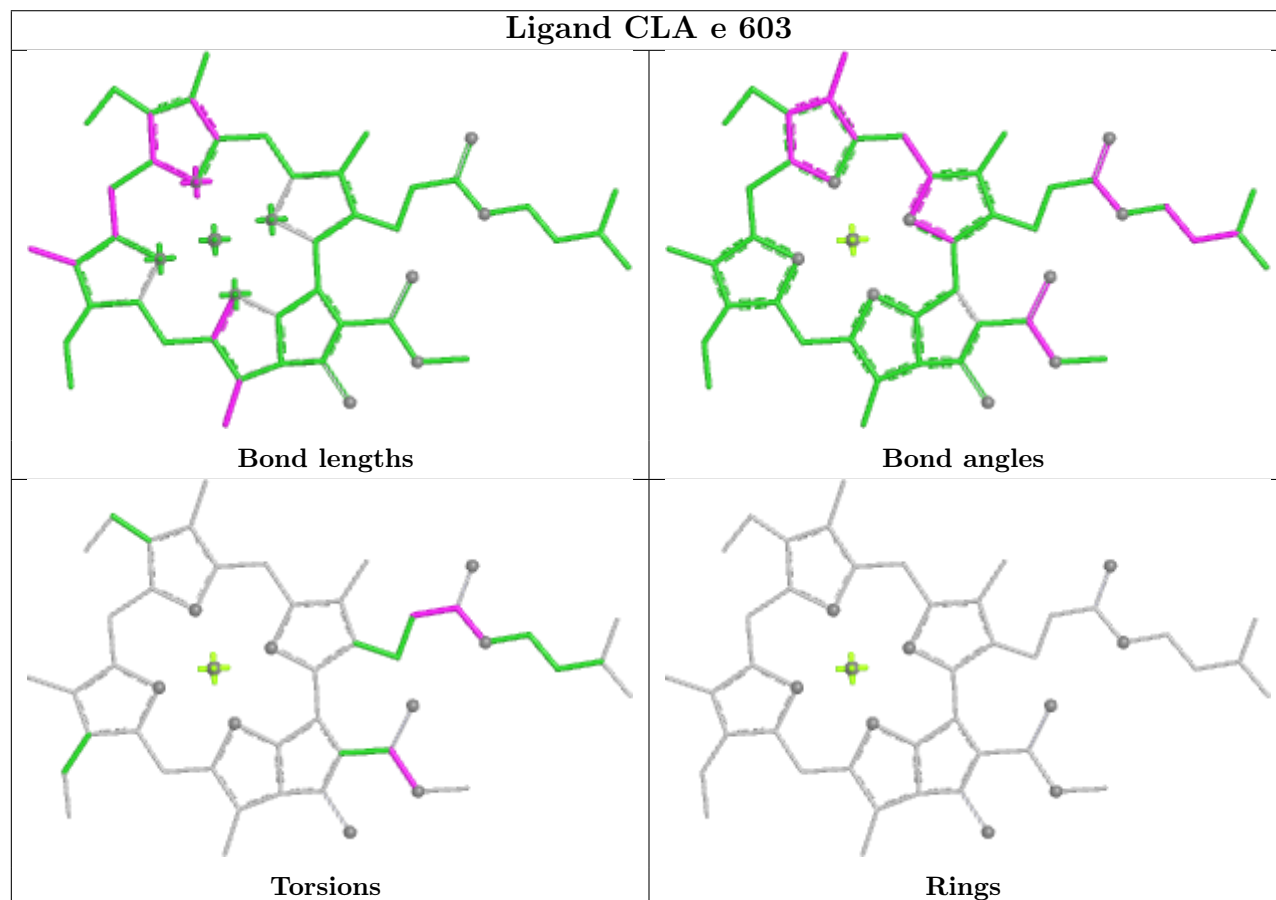
Rings

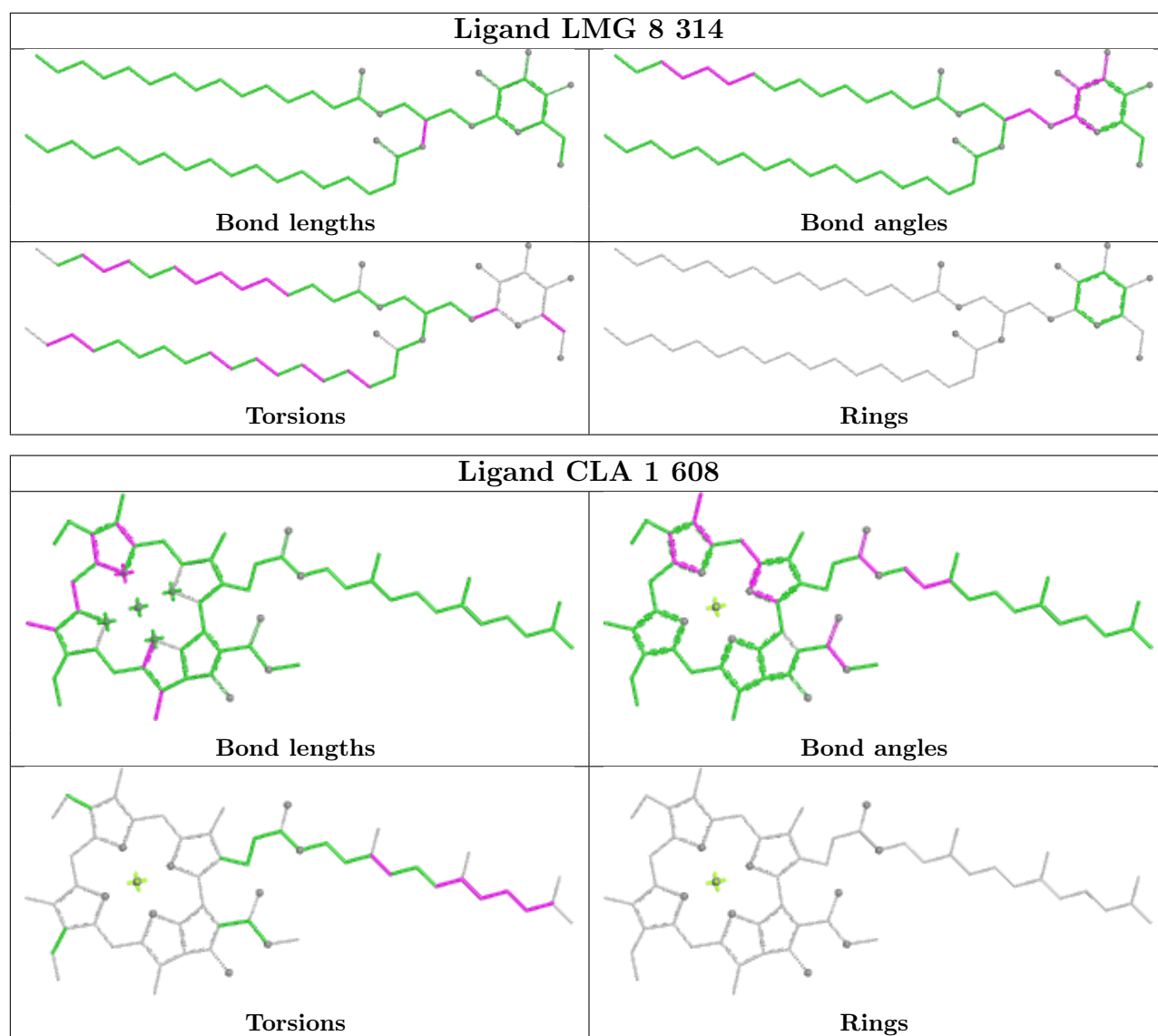


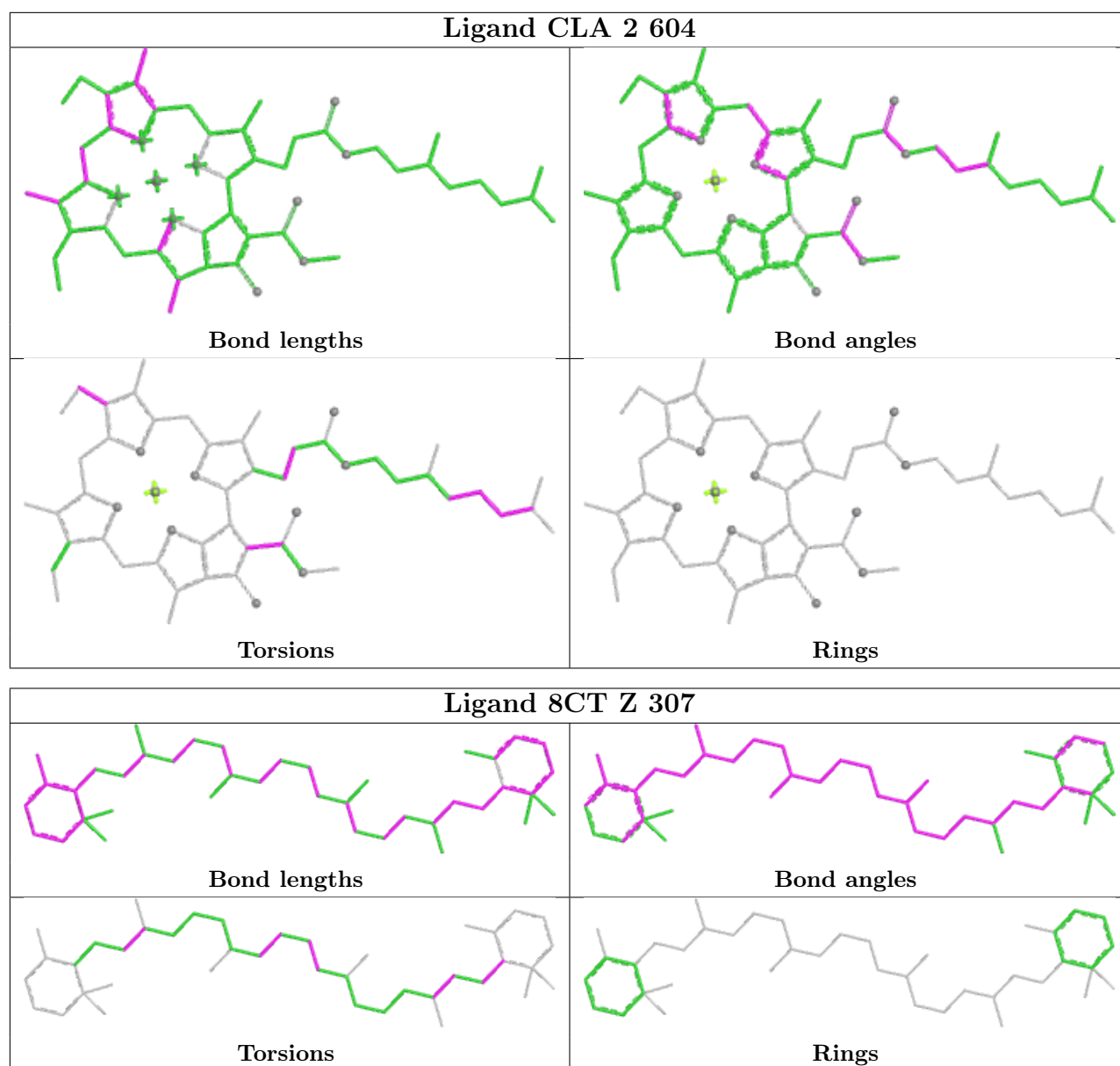
Ligand CLA 4 603

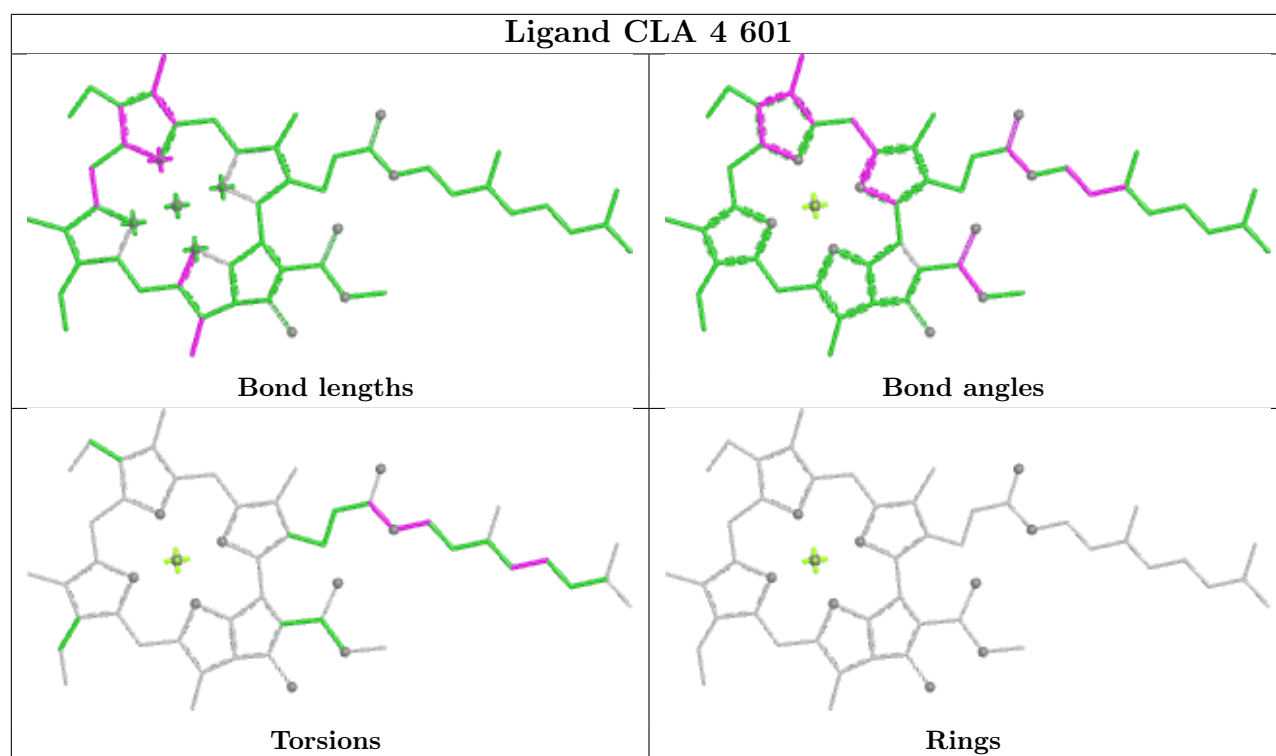


Ligand CLA e 603

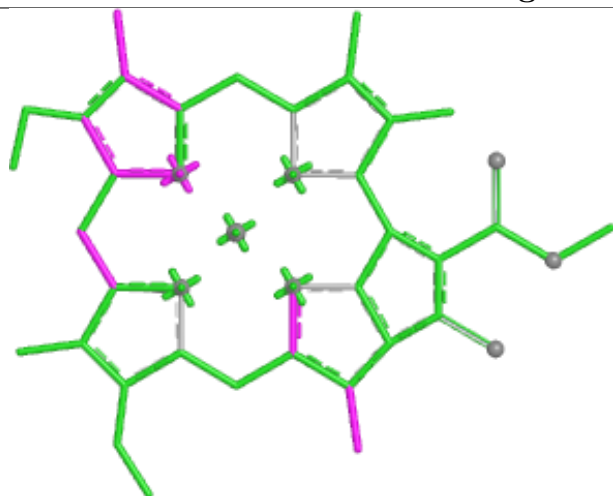




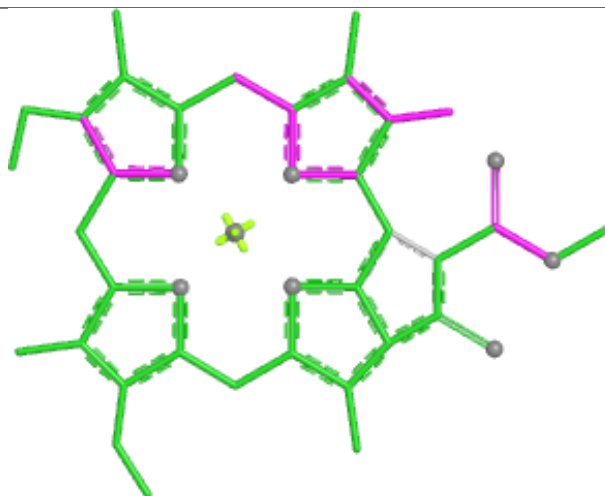




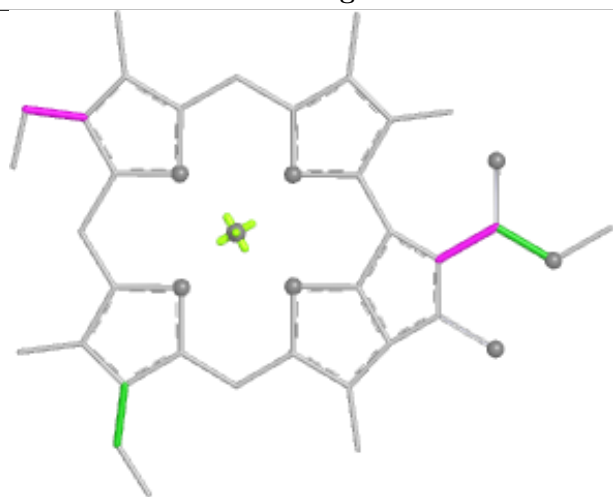
Ligand CLA 9 315



Bond lengths



Bond angles

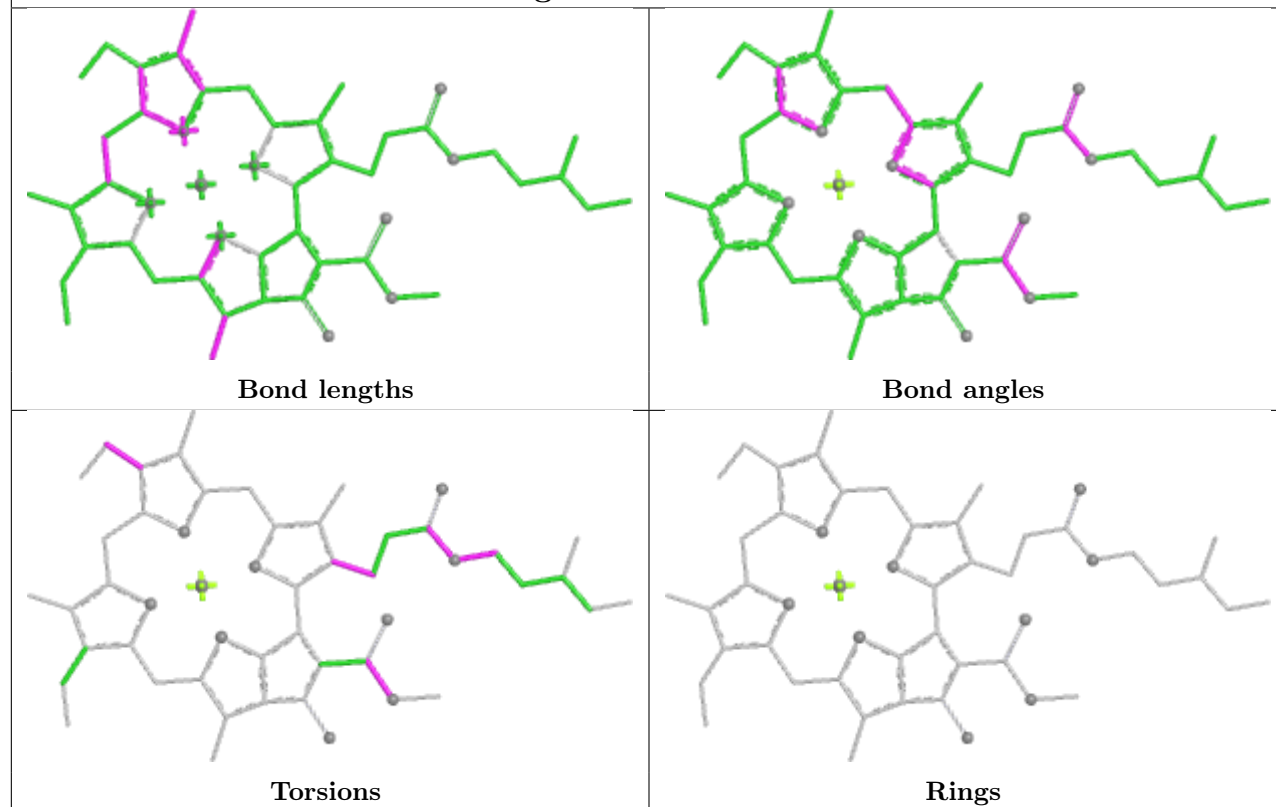


Torsions

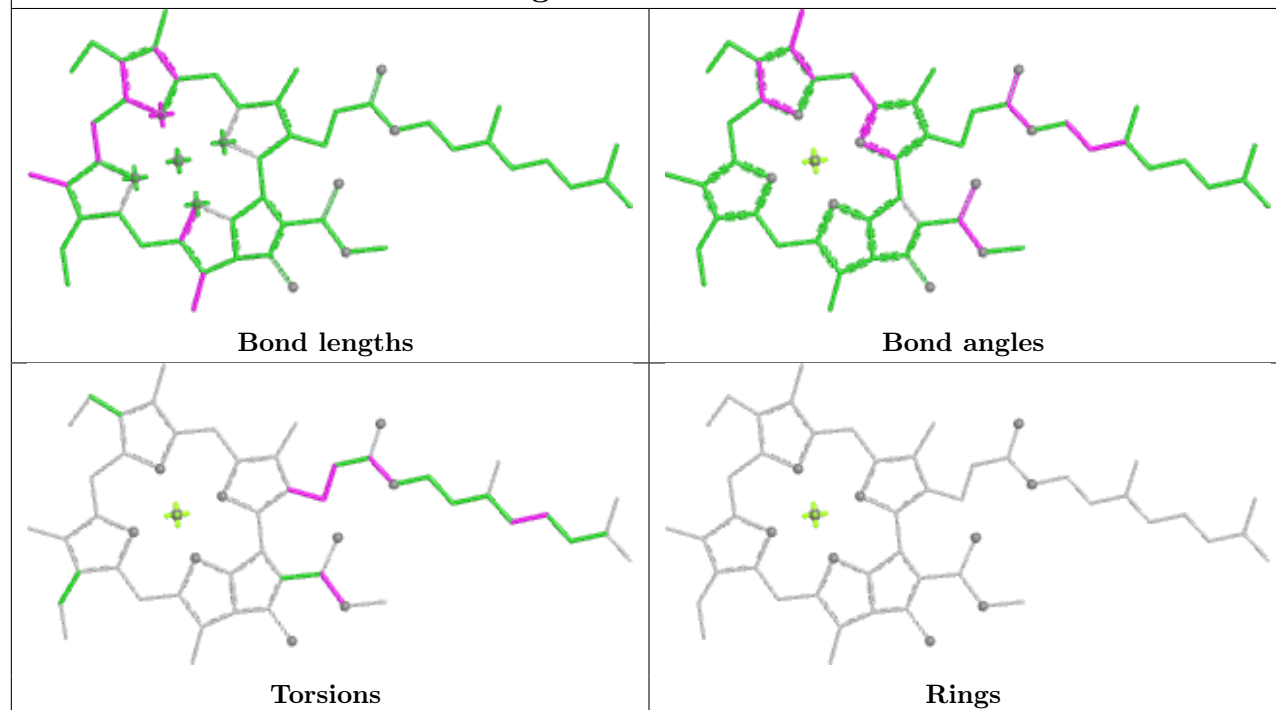


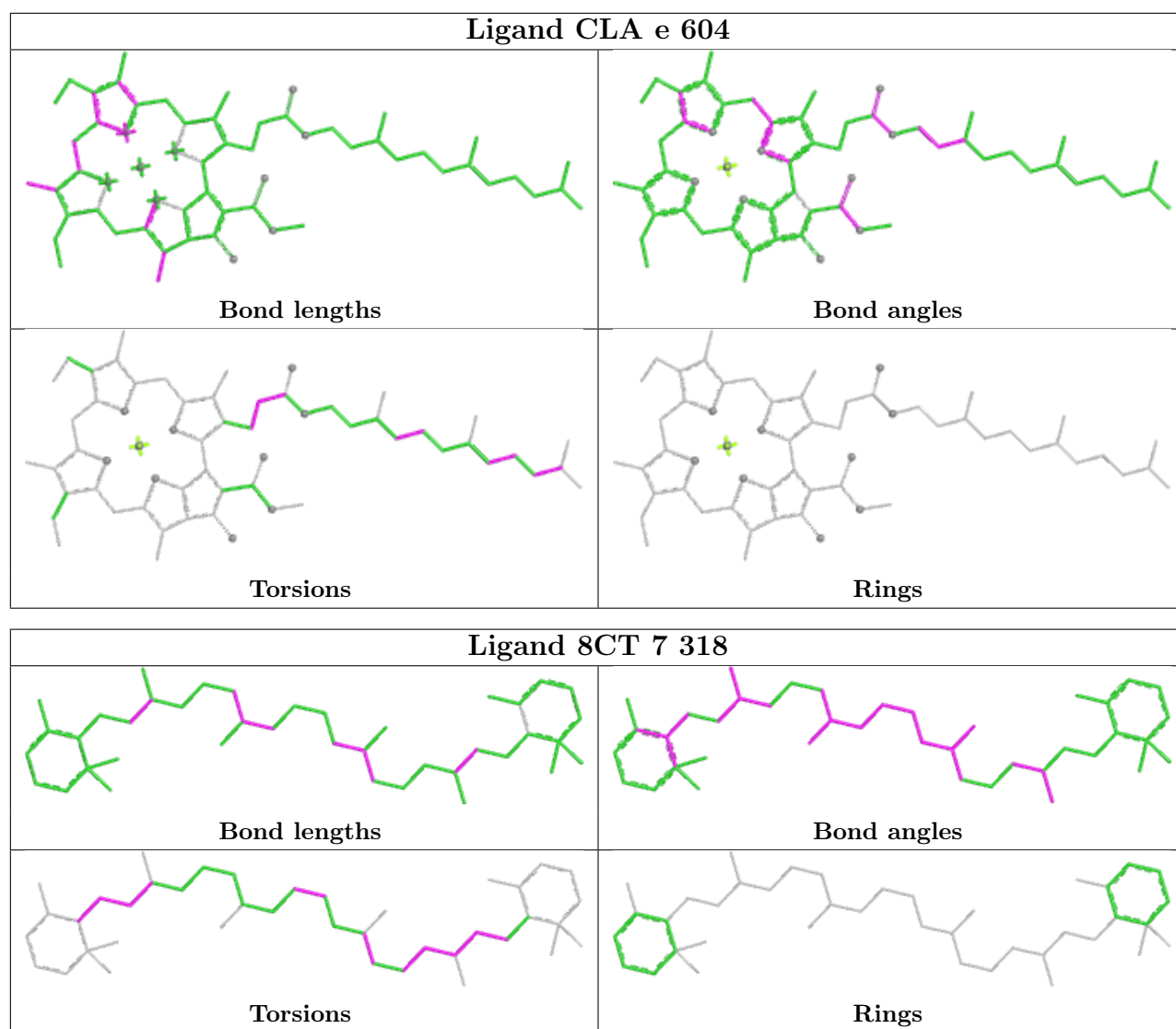
Rings

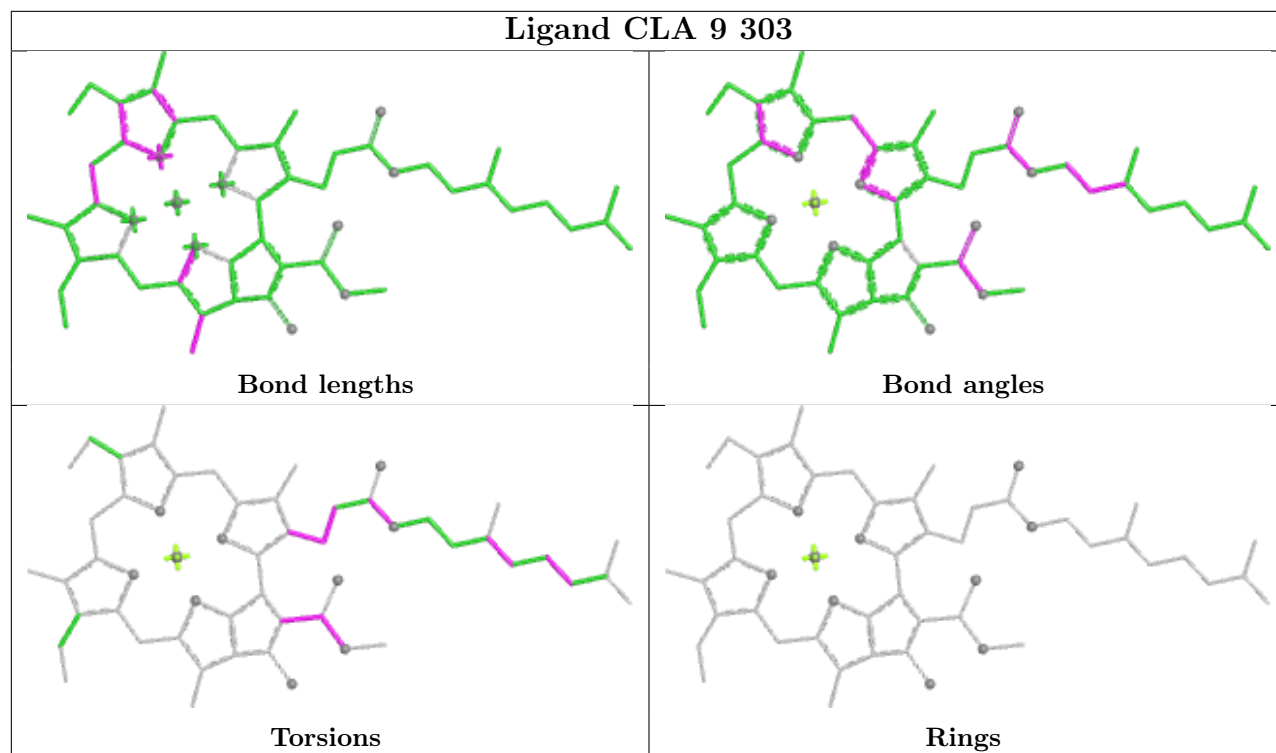
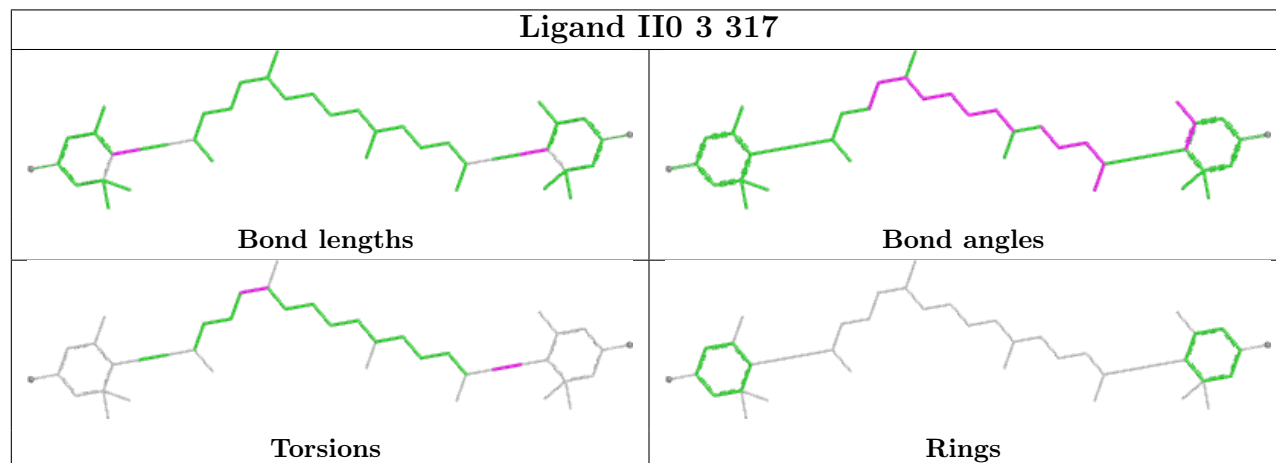
Ligand CLA L 201



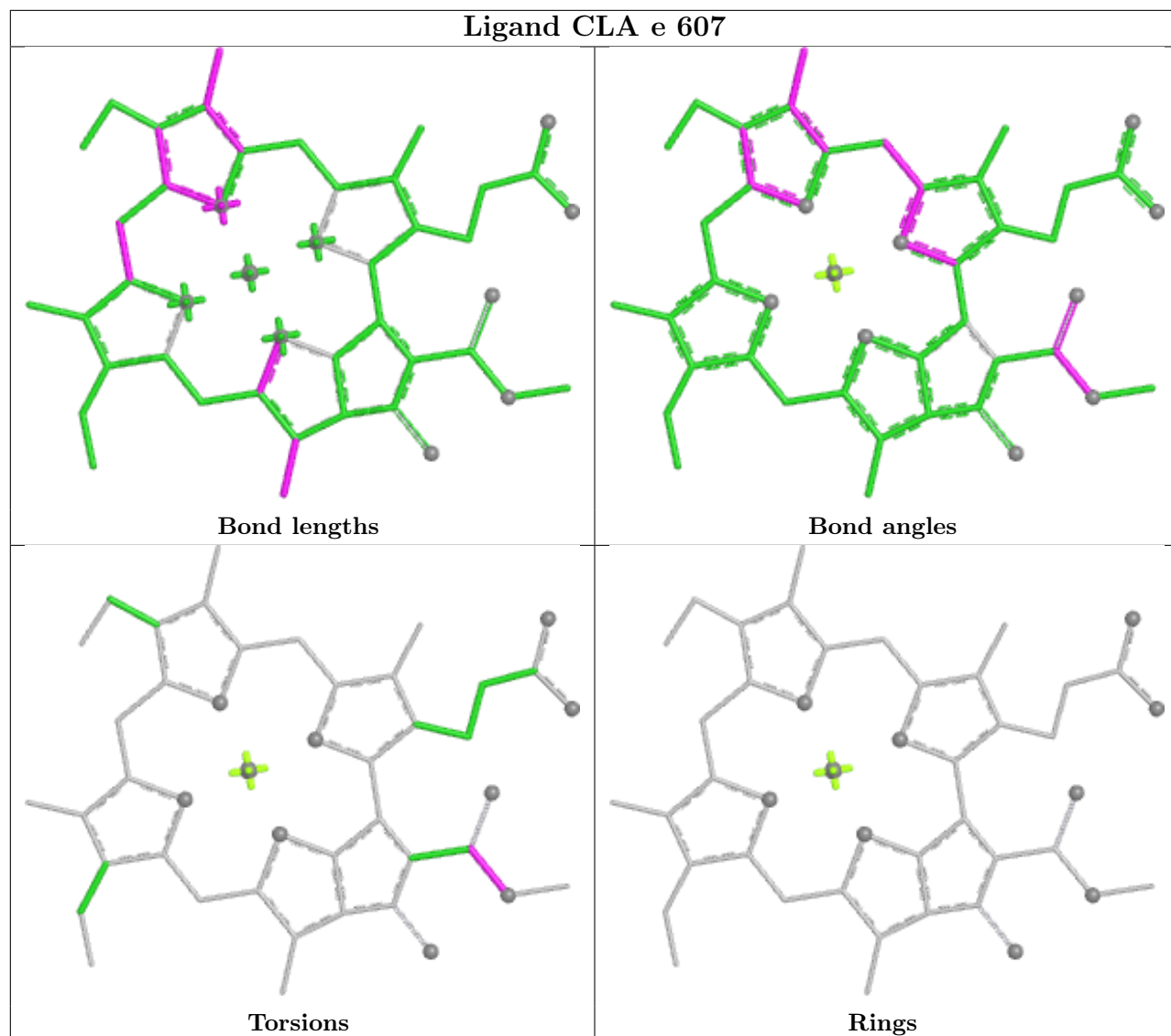
Ligand CLA A 808



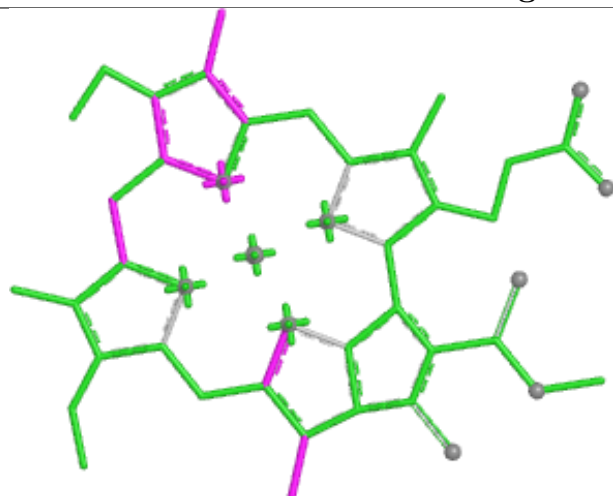


Ligand CLA 9 303**Ligand II0 3 317**

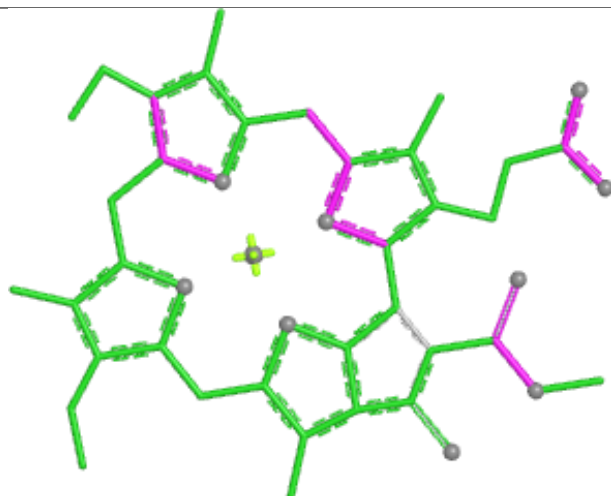
Ligand CLA e 607



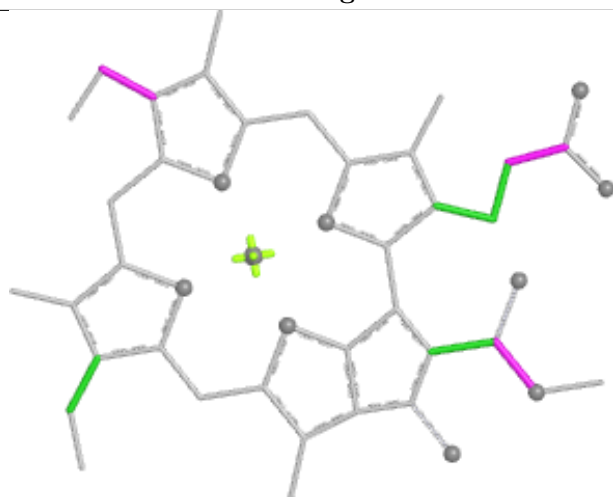
Ligand CLA 6 601



Bond lengths



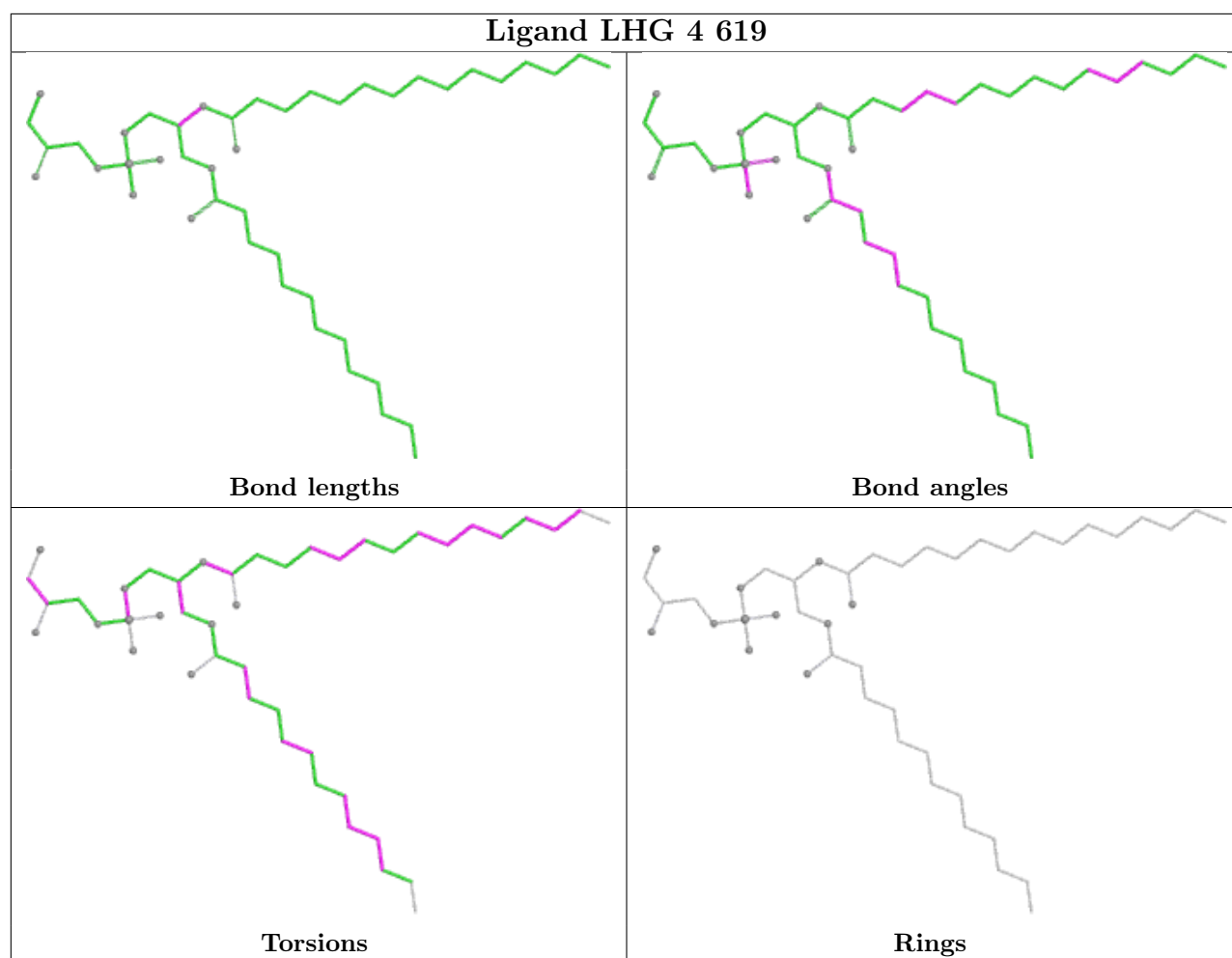
Bond angles



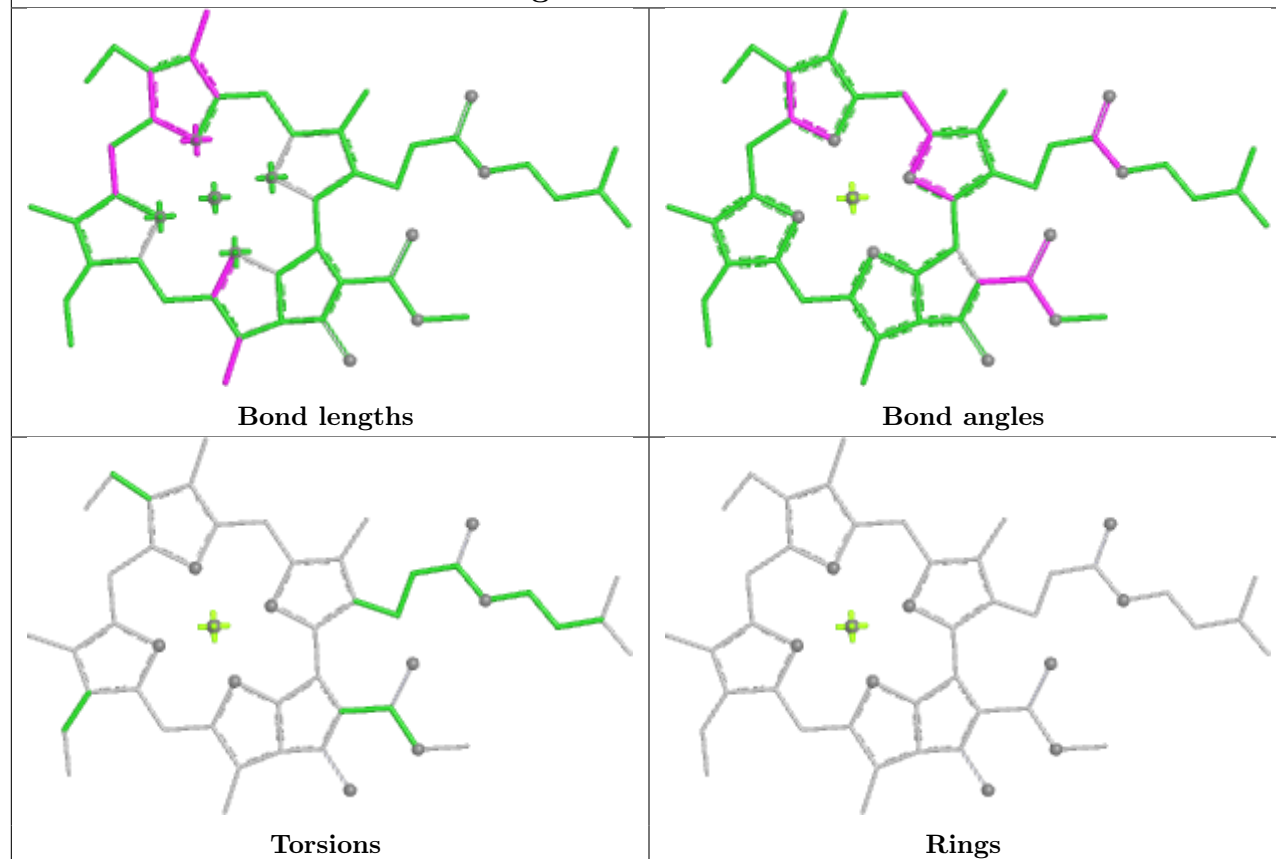
Torsions



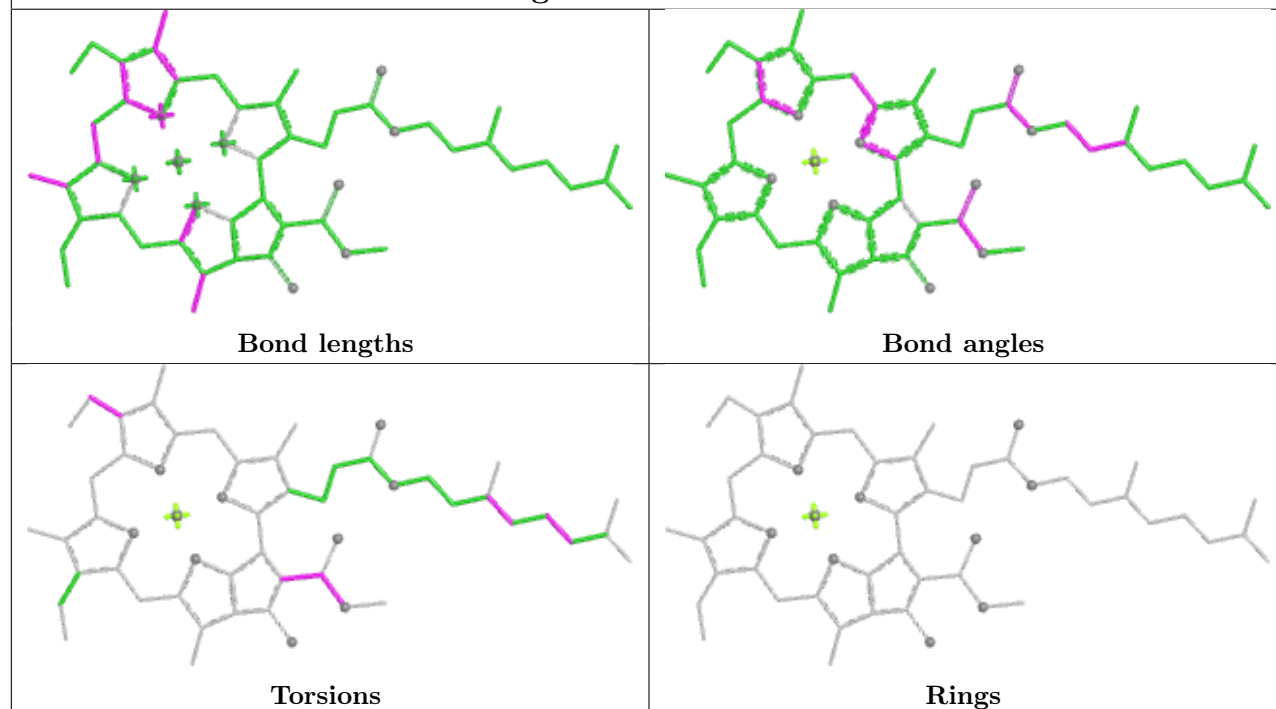
Rings



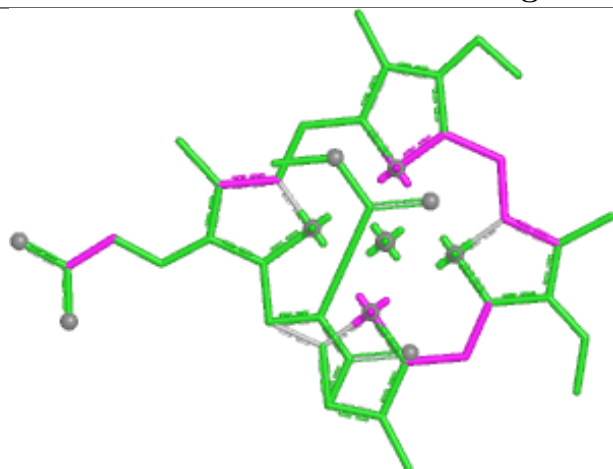
Ligand CLA A 805



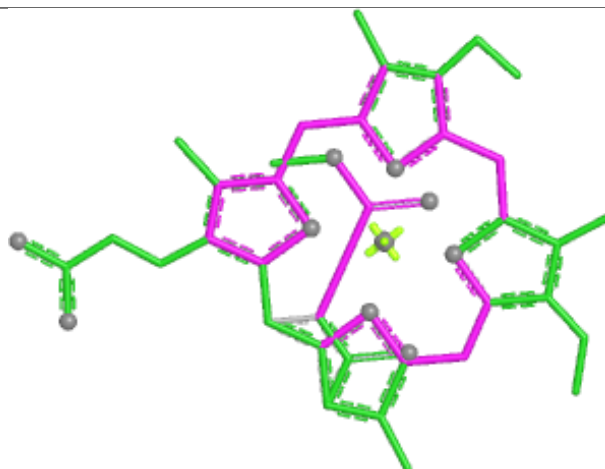
Ligand CLA O 203



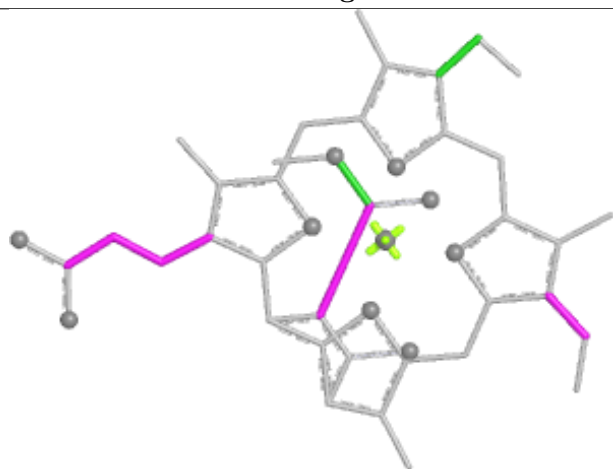
Ligand KC2 c 610



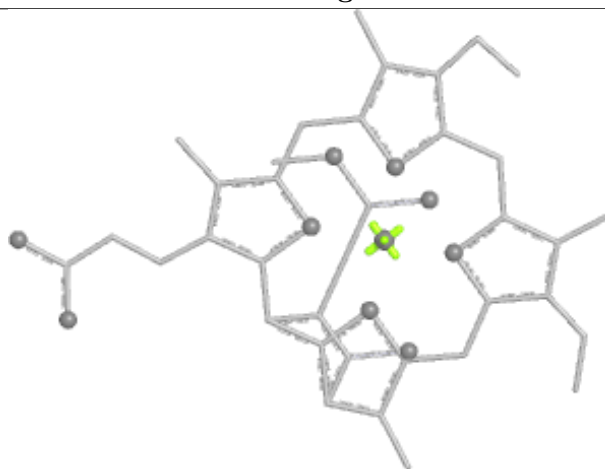
Bond lengths



Bond angles

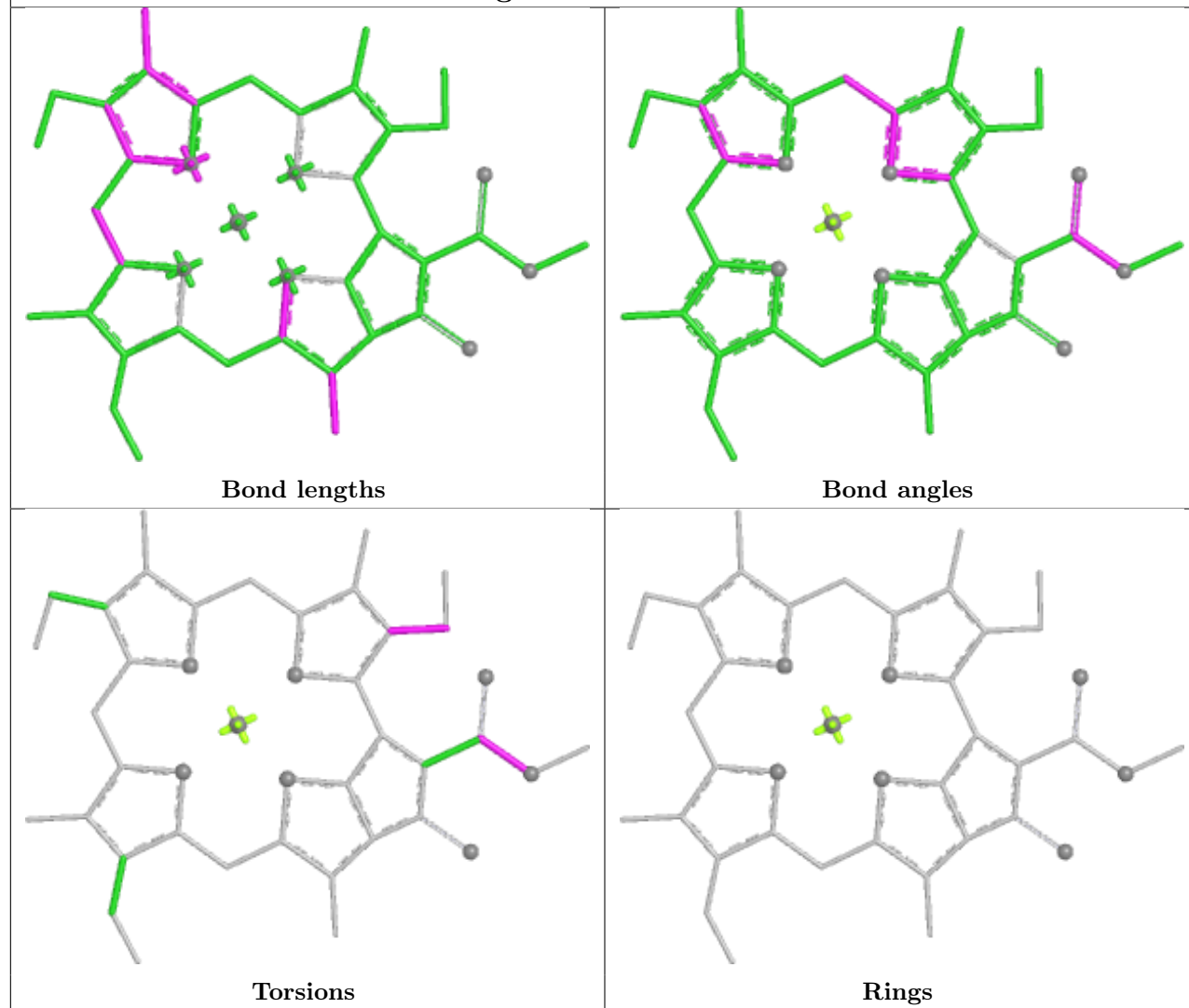


Torsions

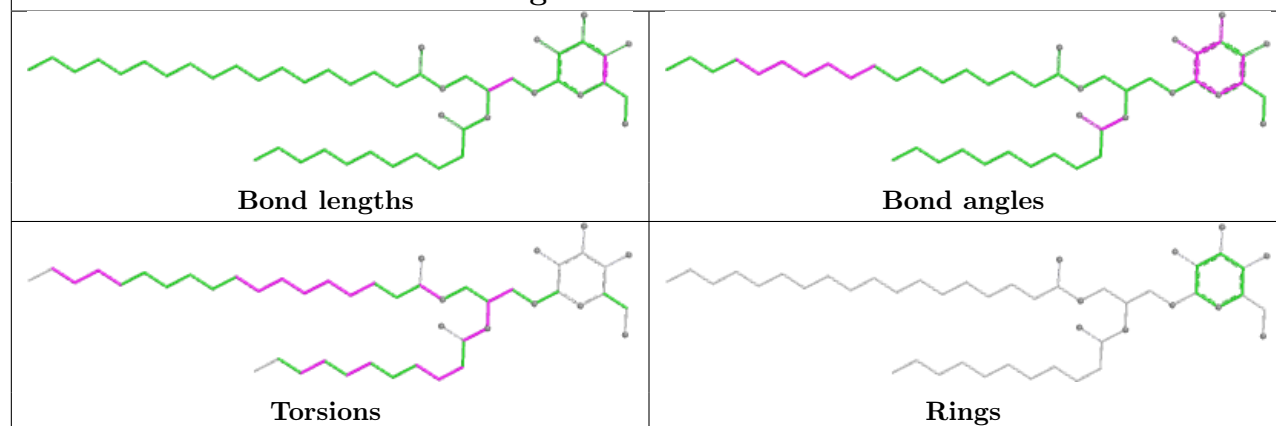


Rings

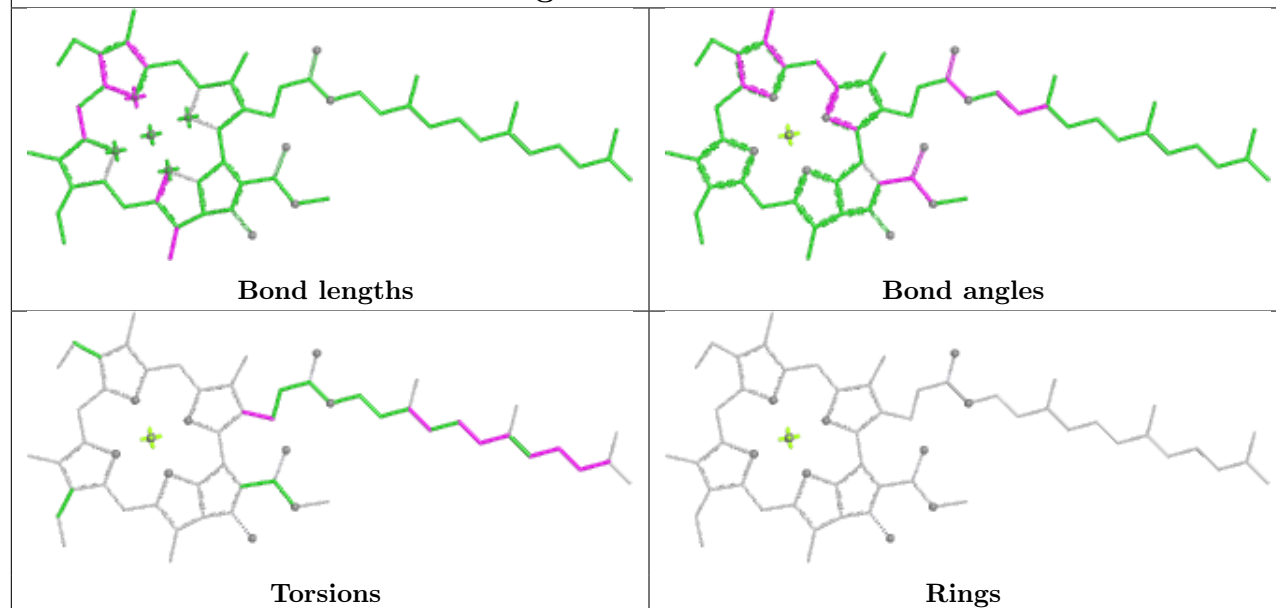
Ligand CLA B 815



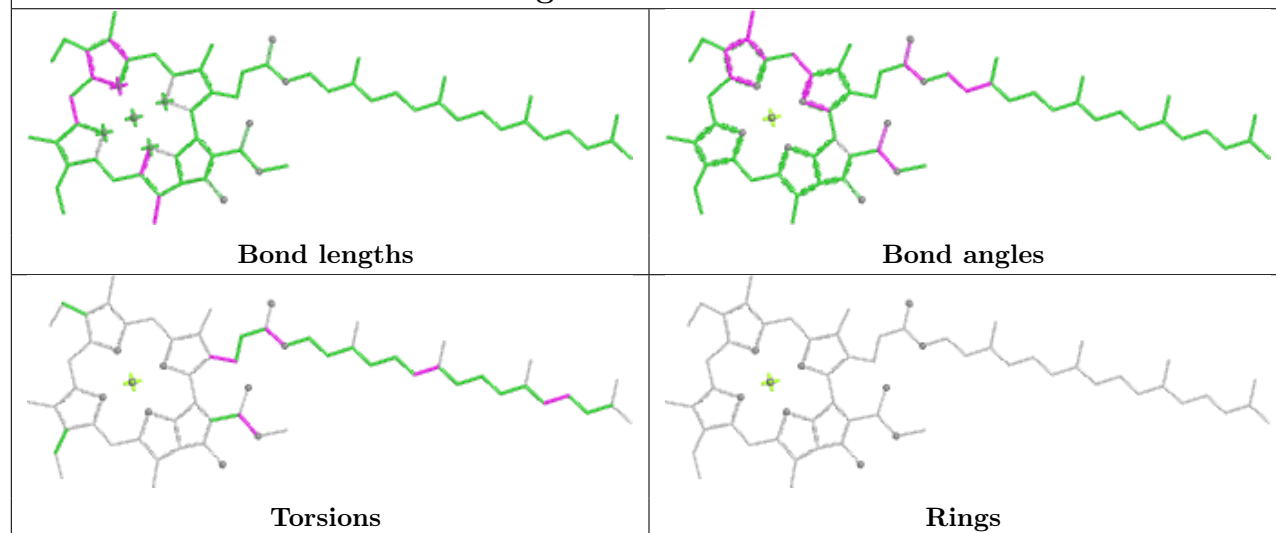
Ligand LMG Z 310

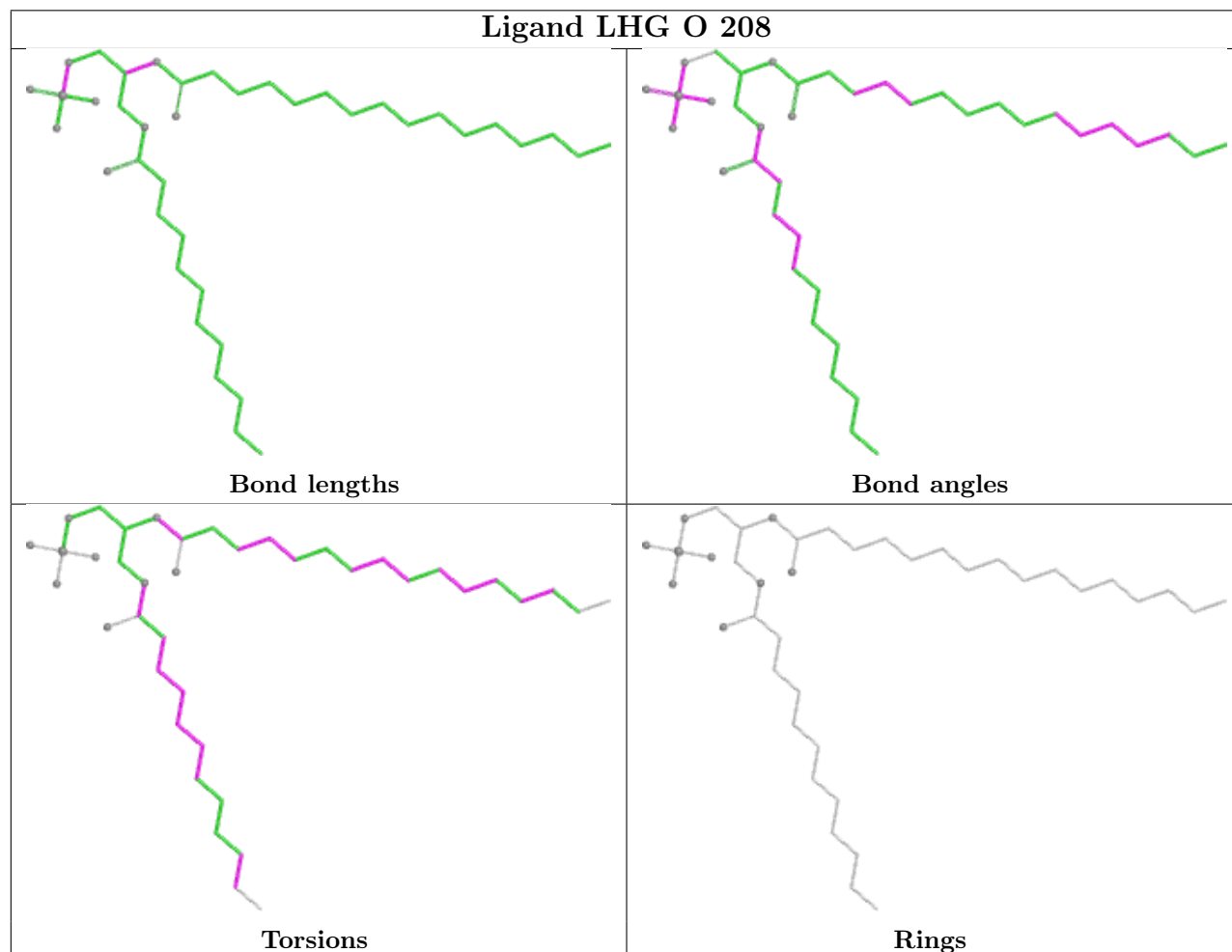
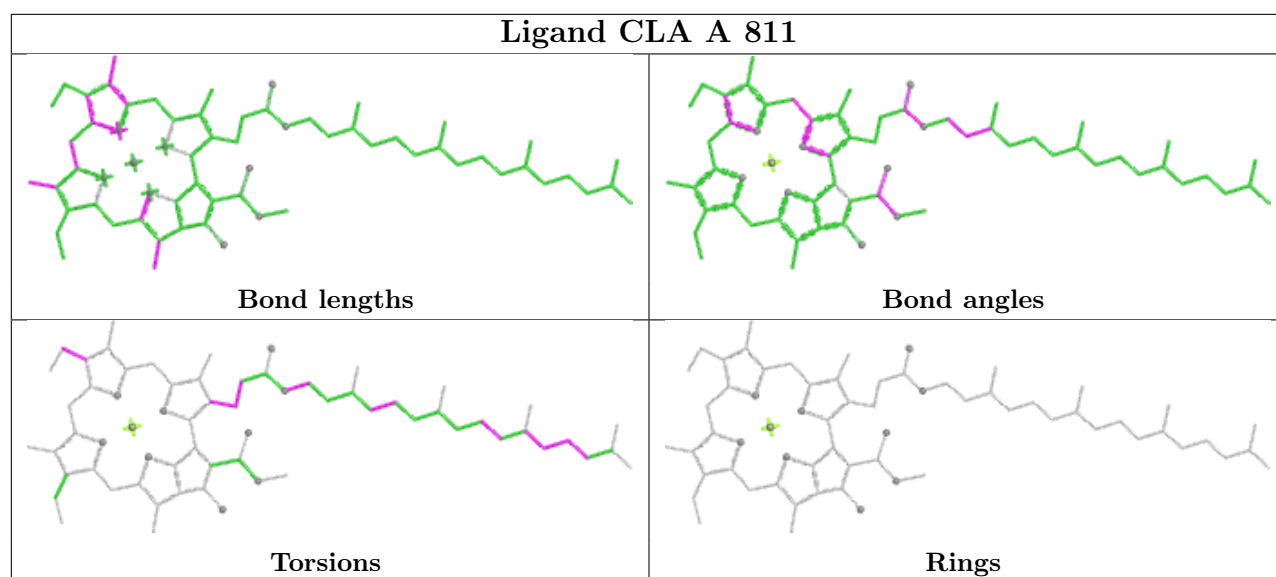


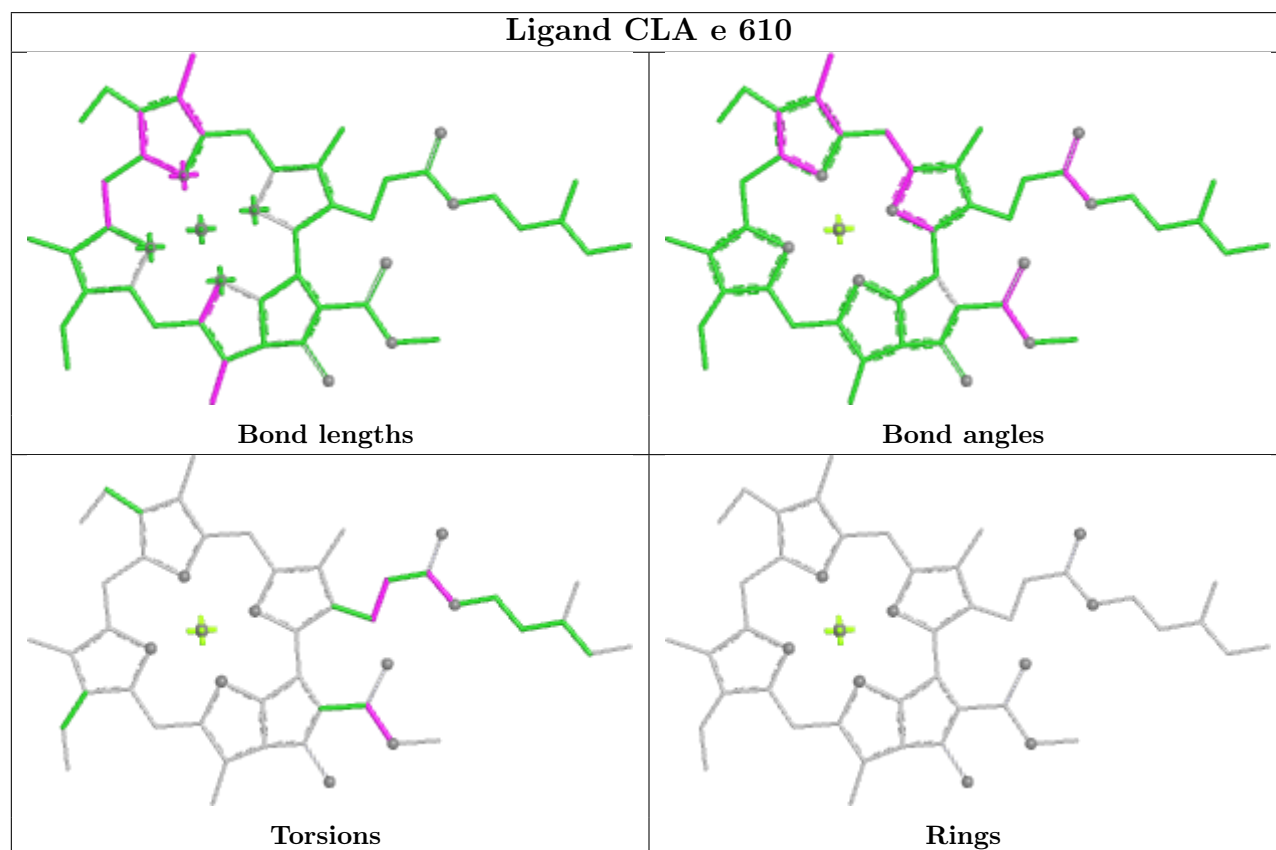
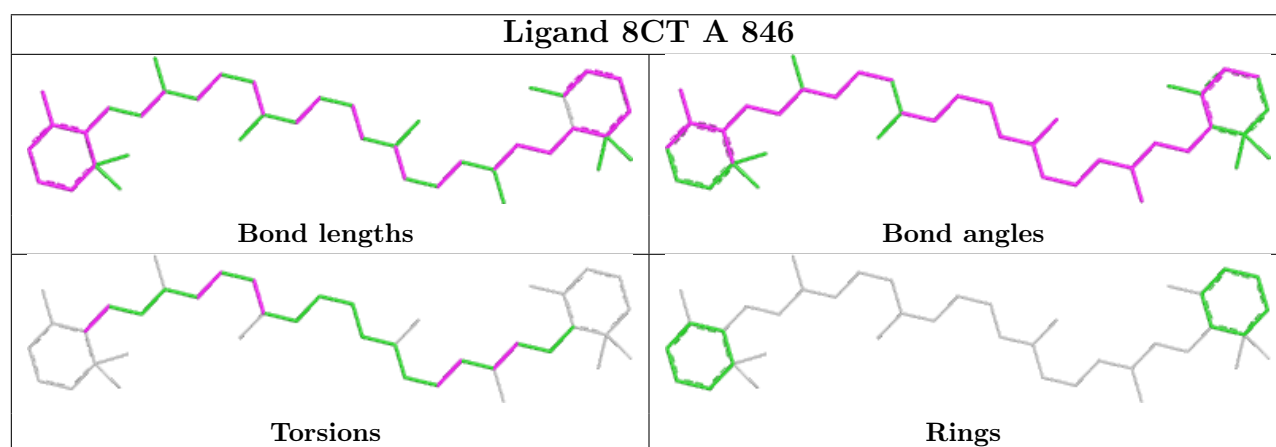
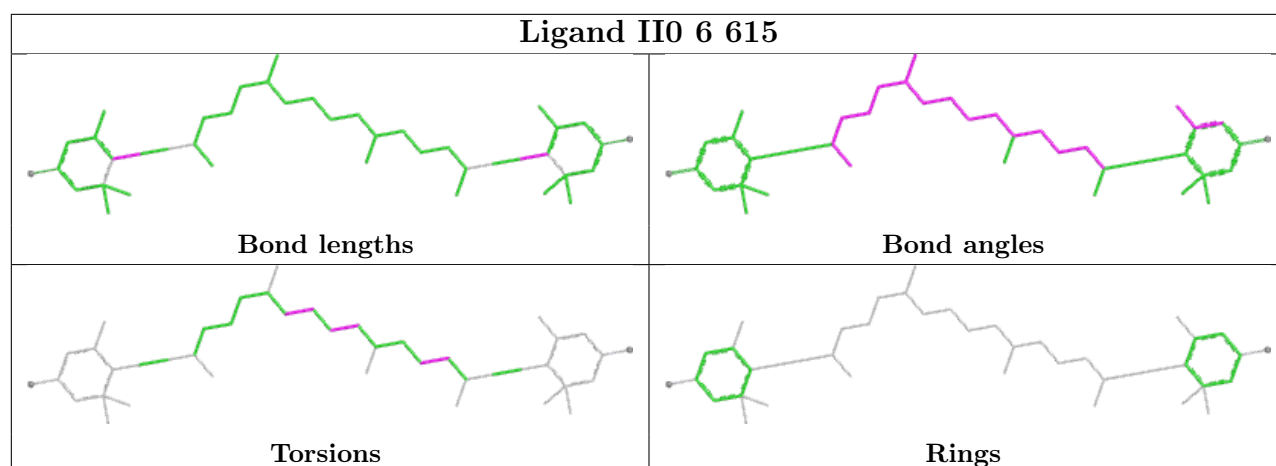
Ligand CLA a 608



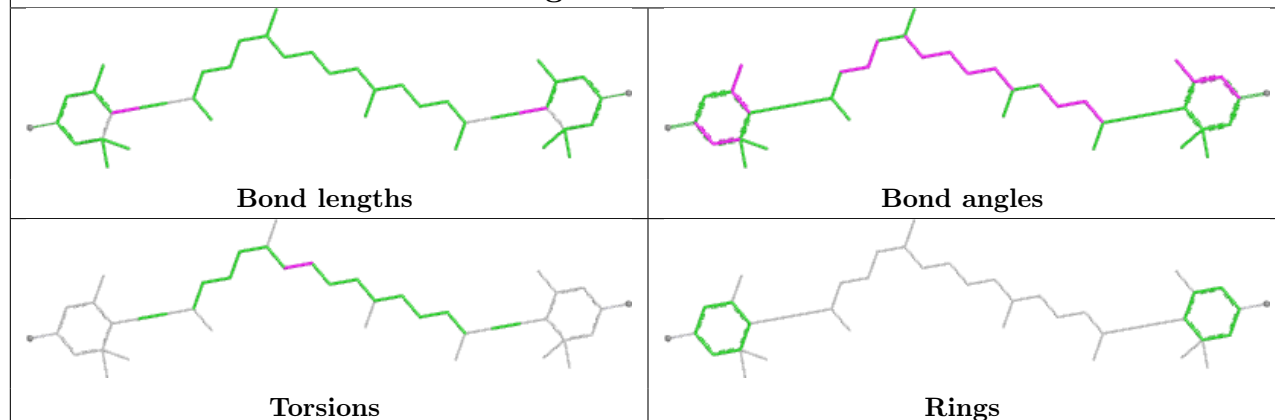
Ligand CLA a 612



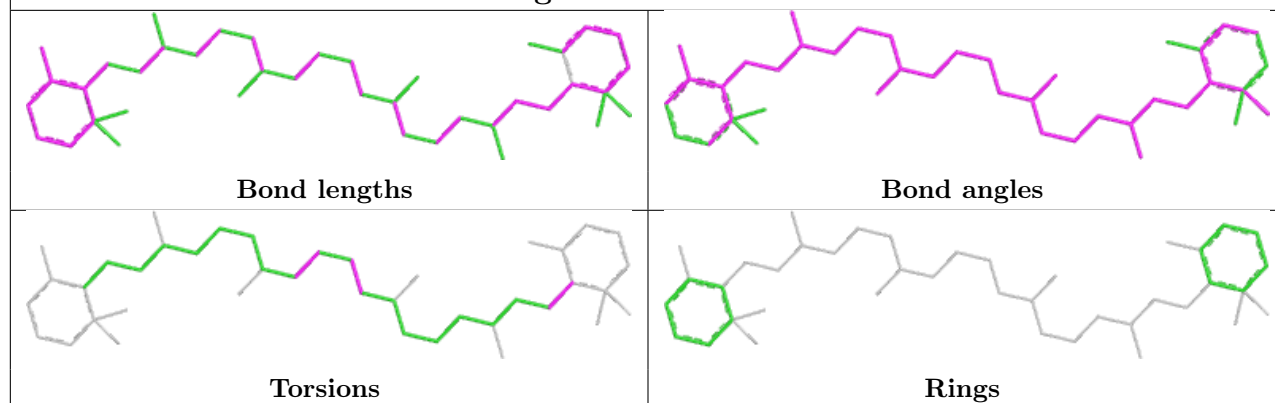




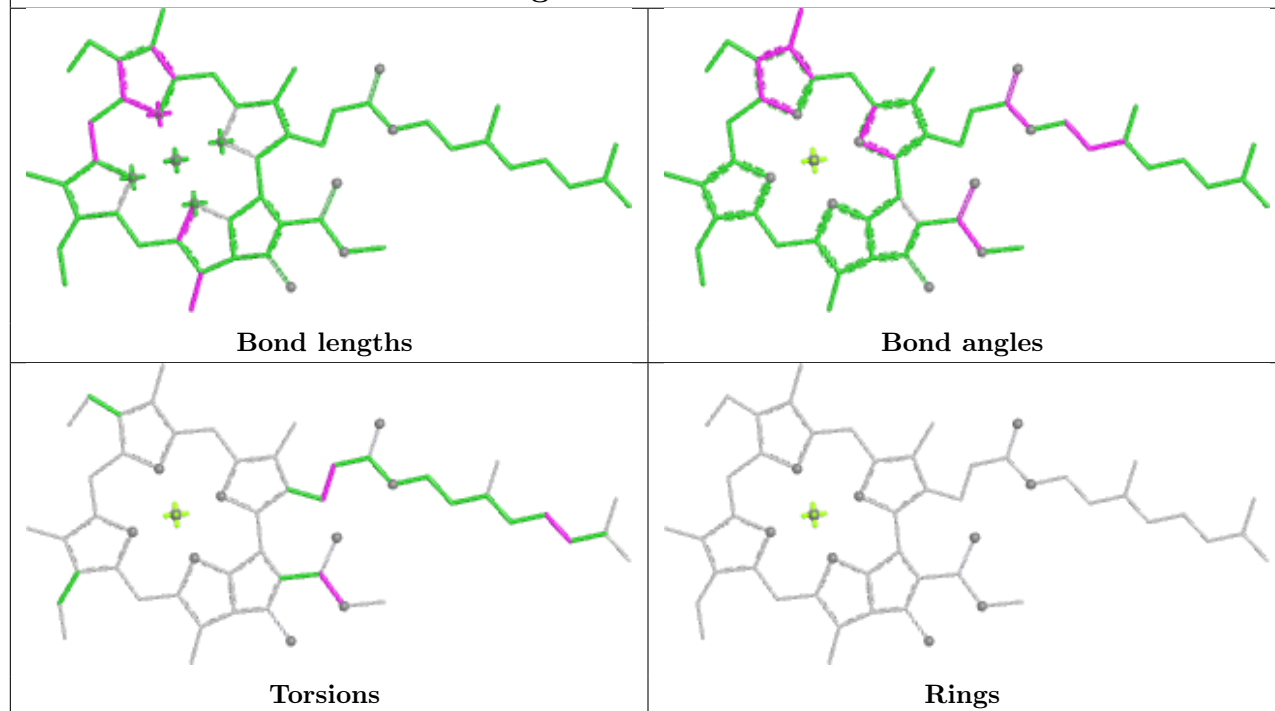
Ligand II0 O 205



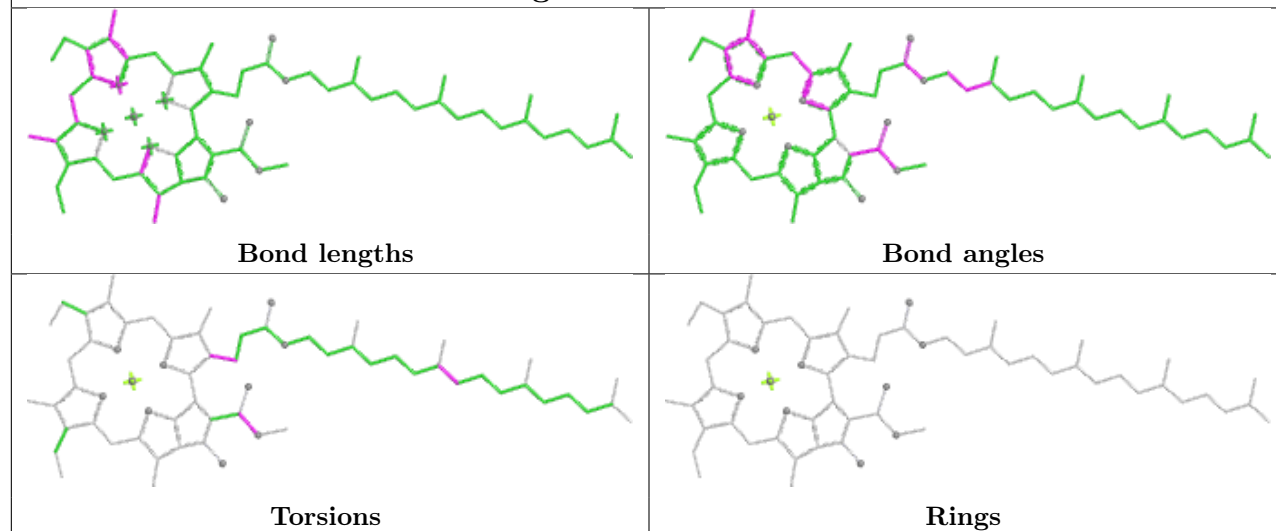
Ligand 8CT B 847



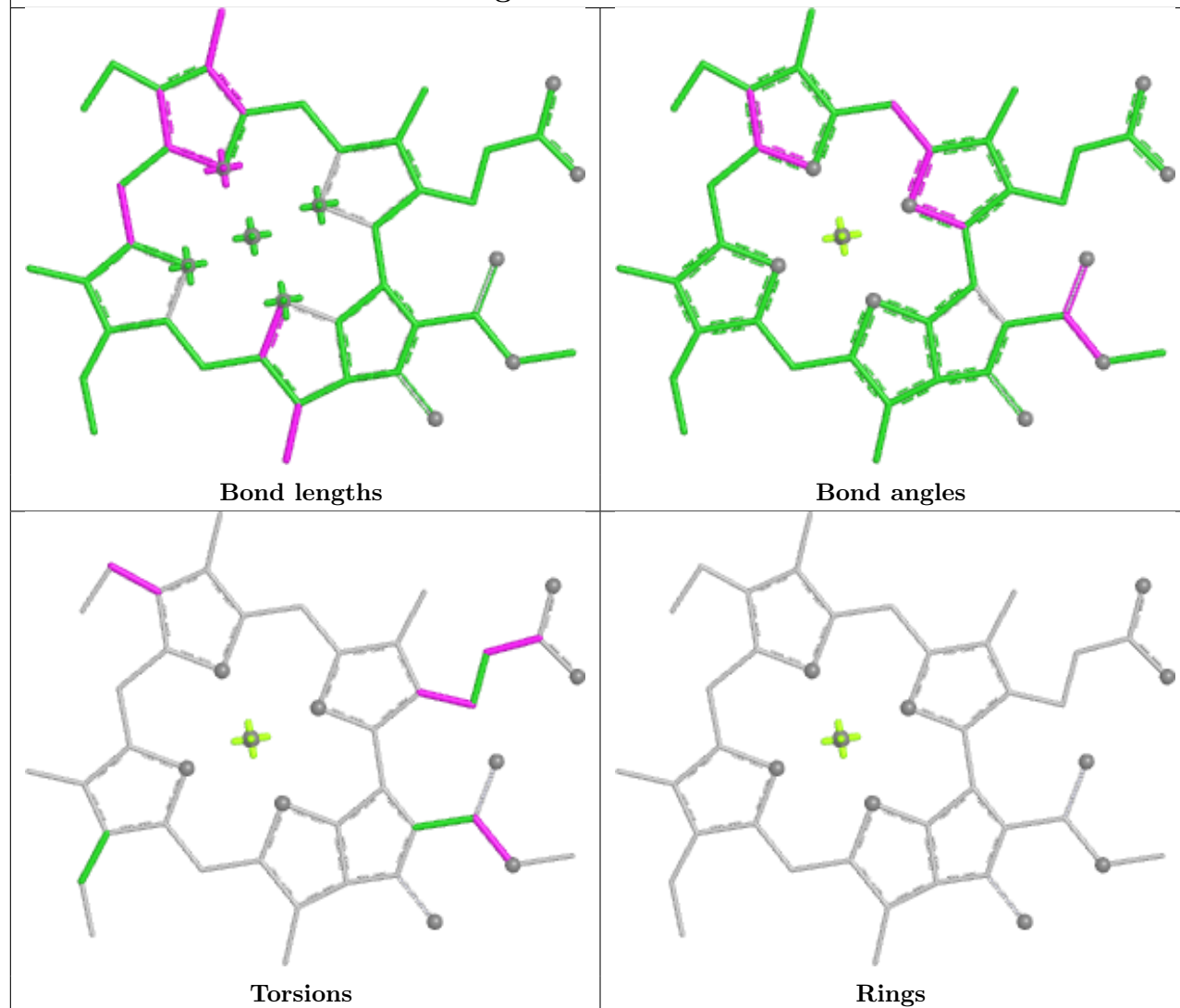
Ligand CLA B 802

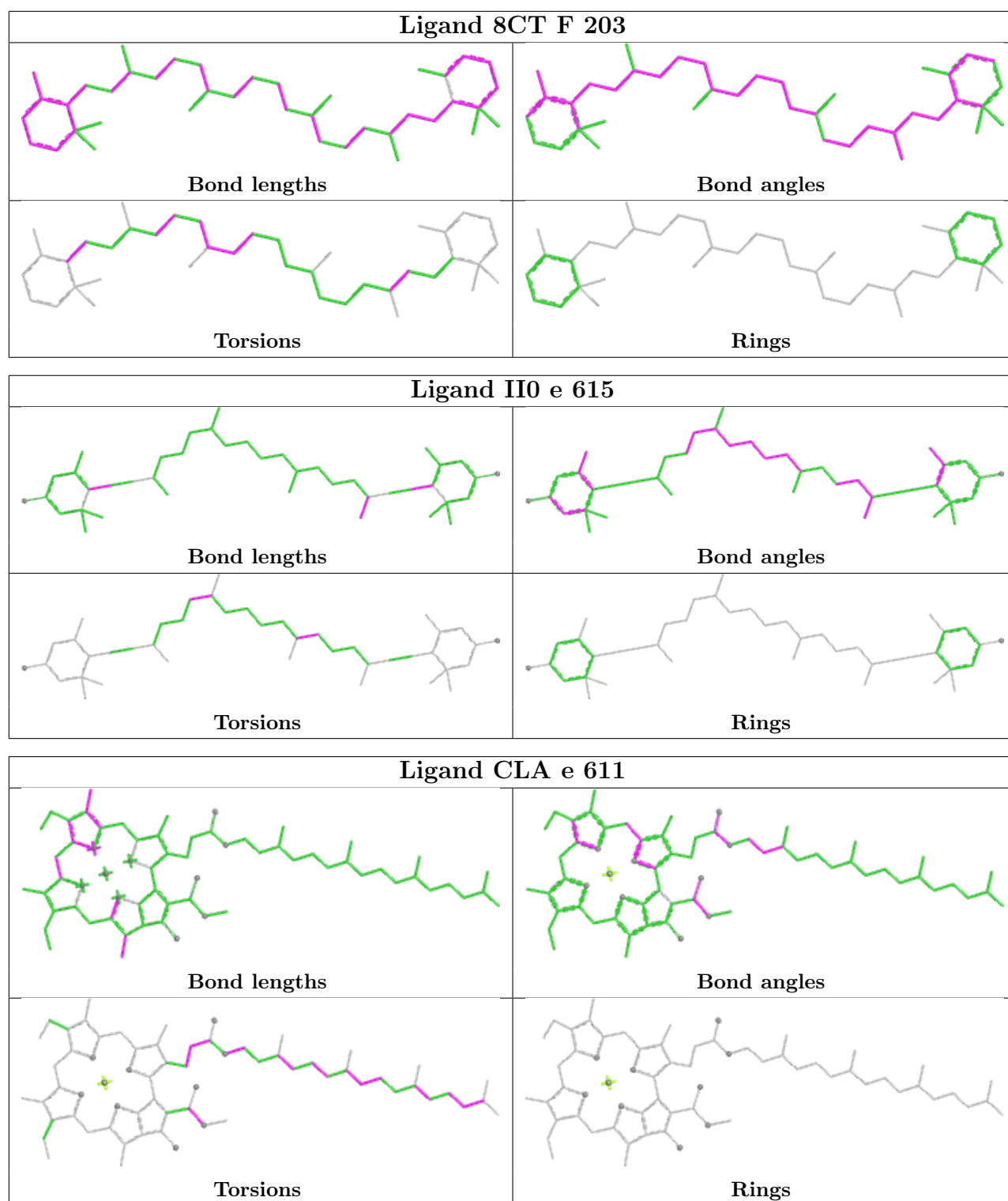


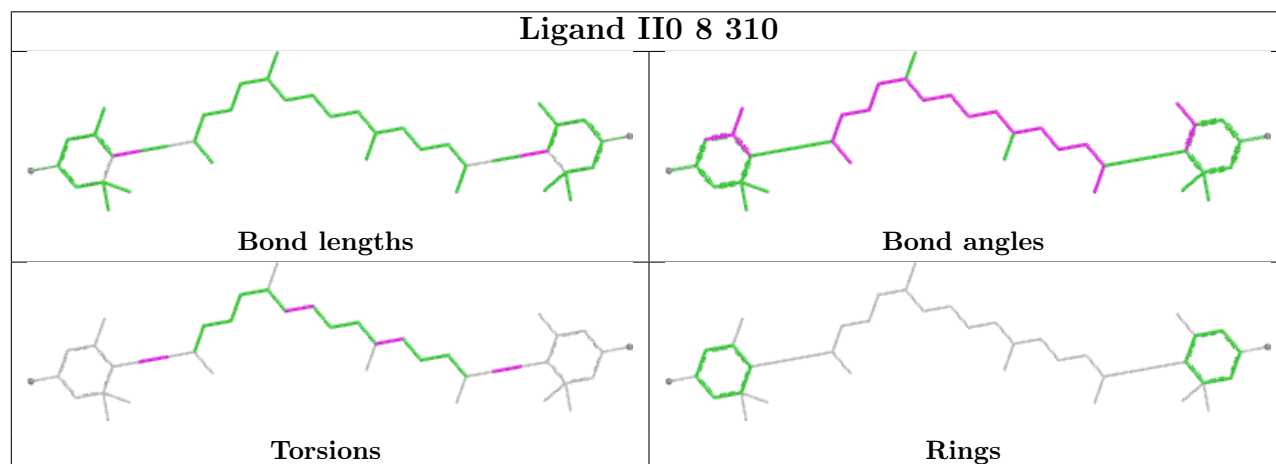
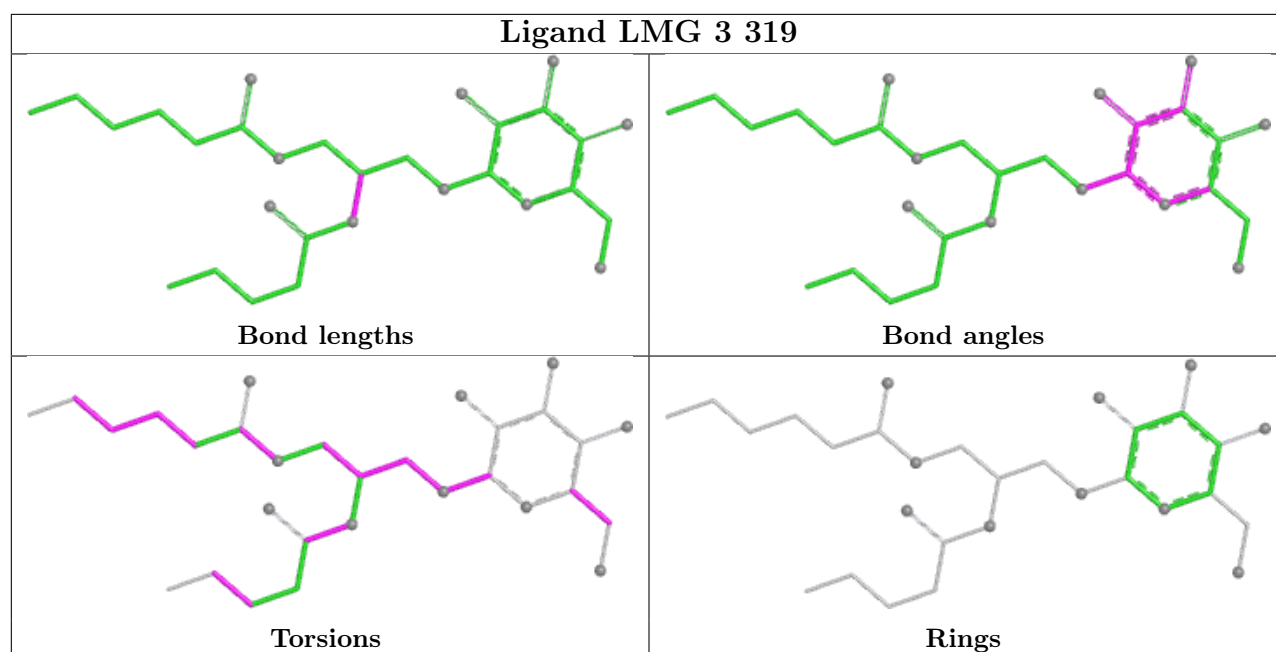
Ligand CLA B 826



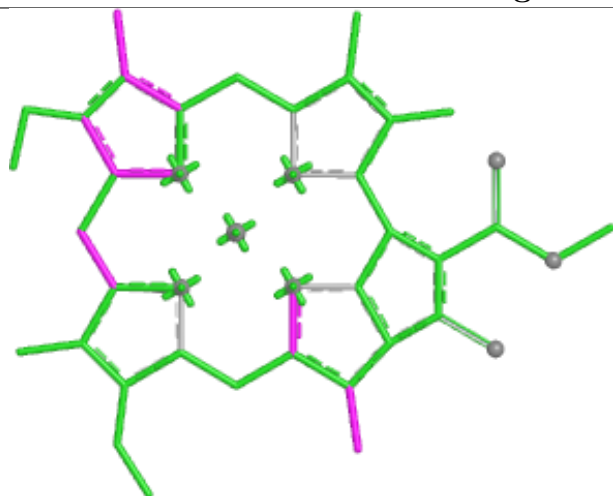
Ligand CLA d 601



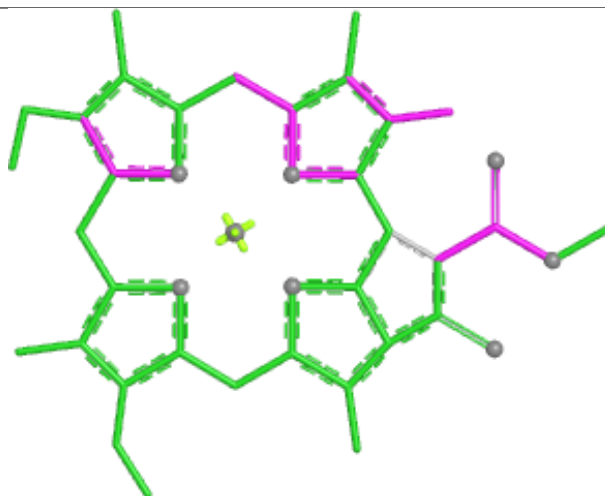




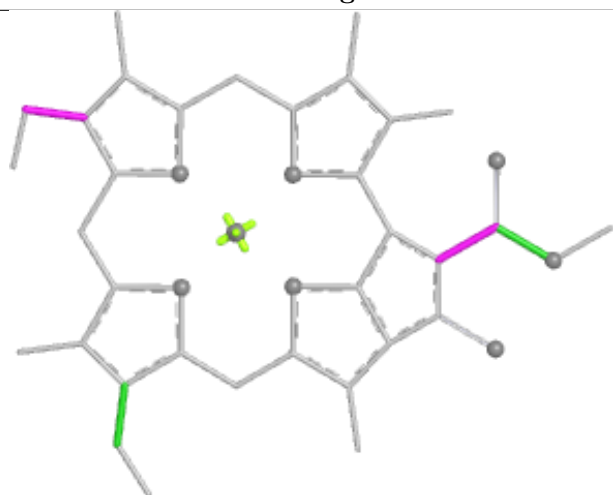
Ligand CLA O 202



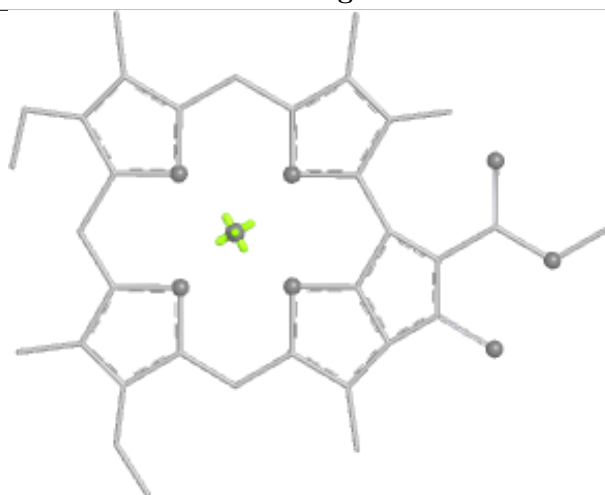
Bond lengths



Bond angles

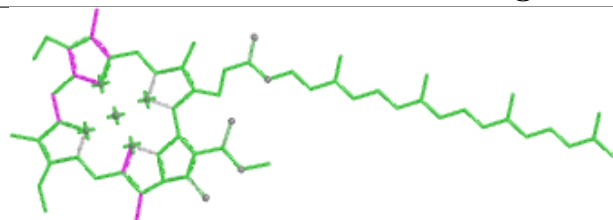


Torsions

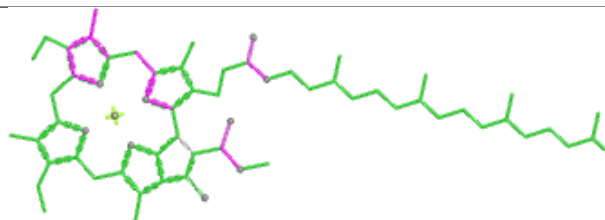


Rings

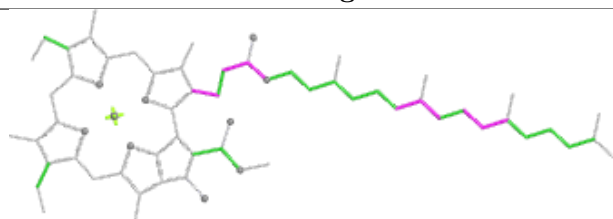
Ligand CLA B 805



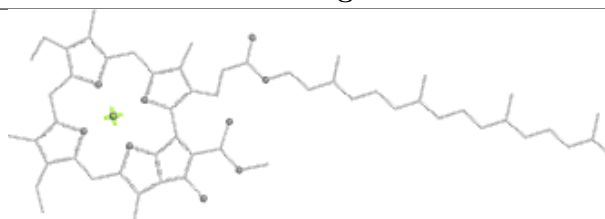
Bond lengths



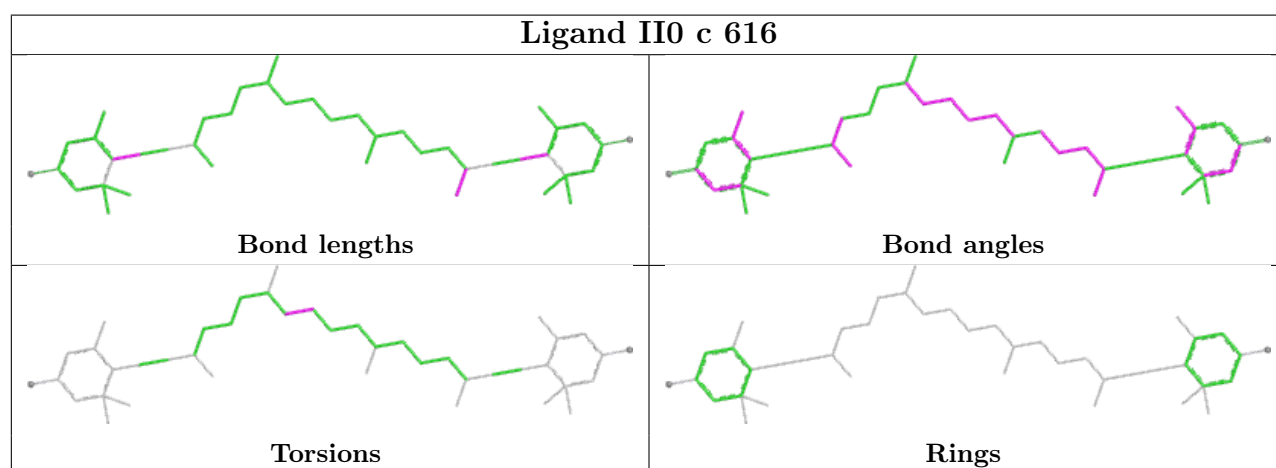
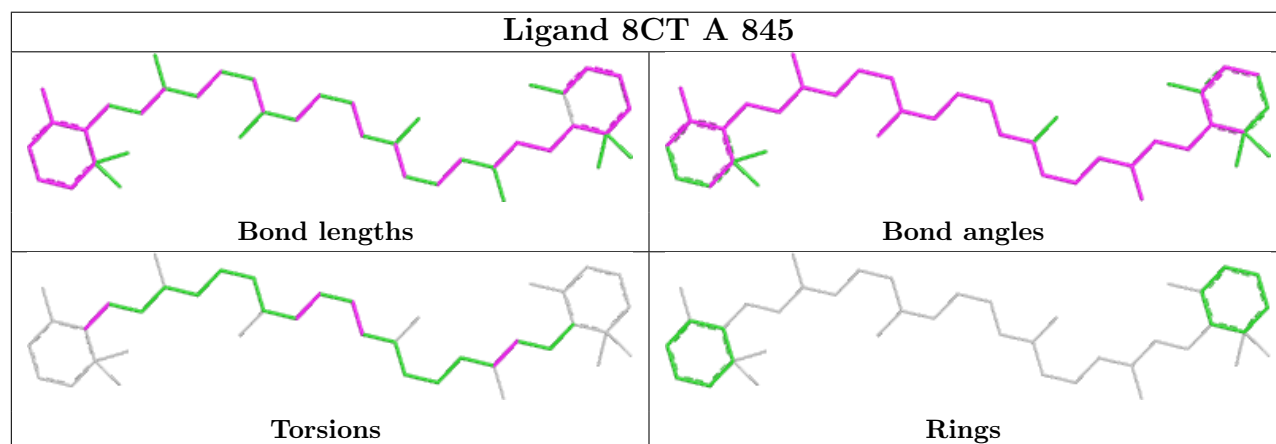
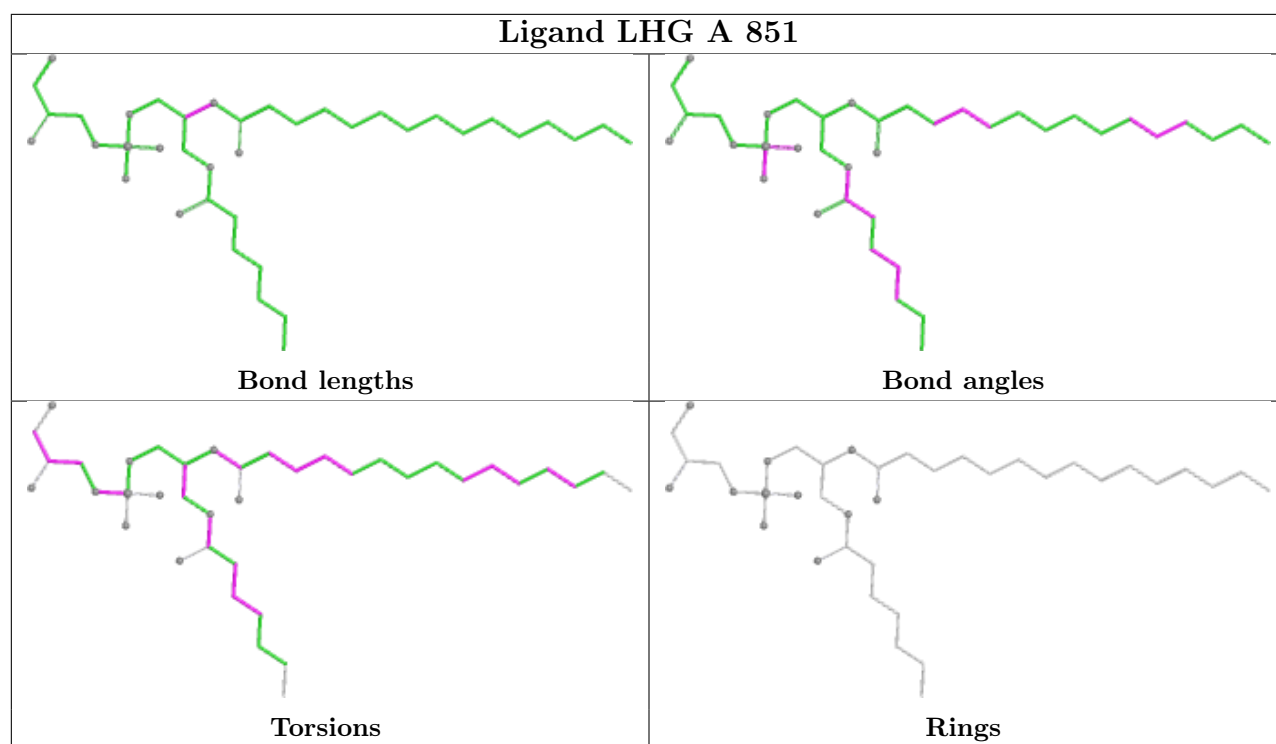
Bond angles

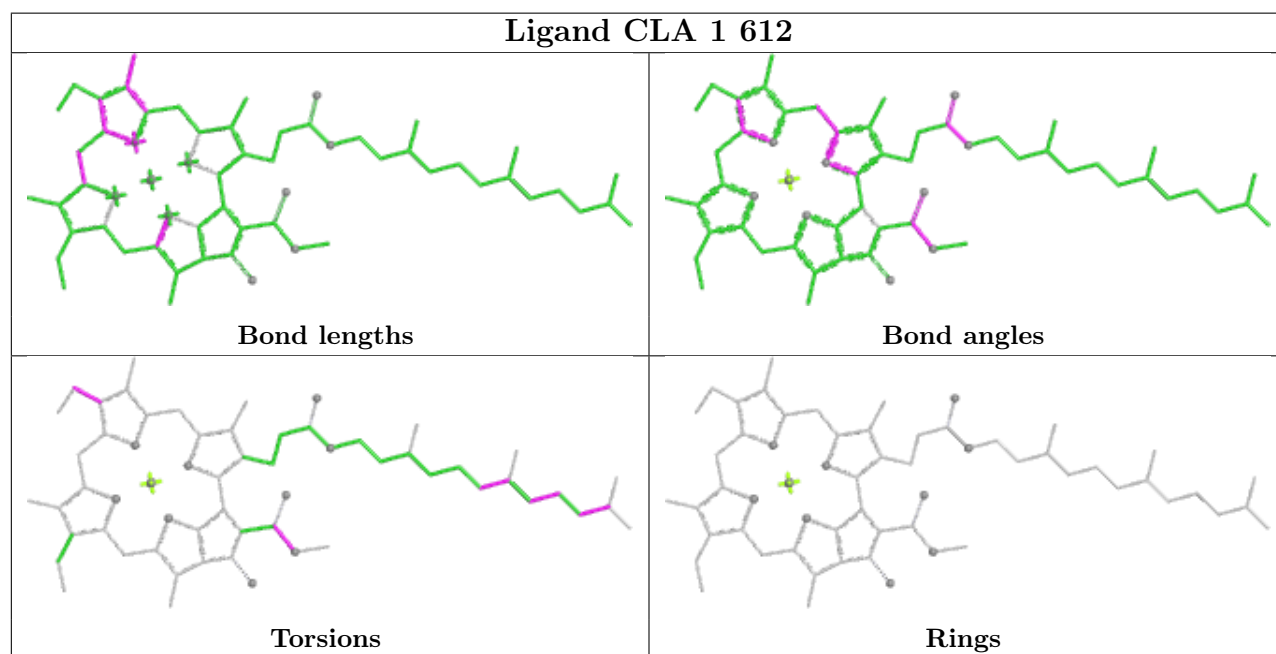
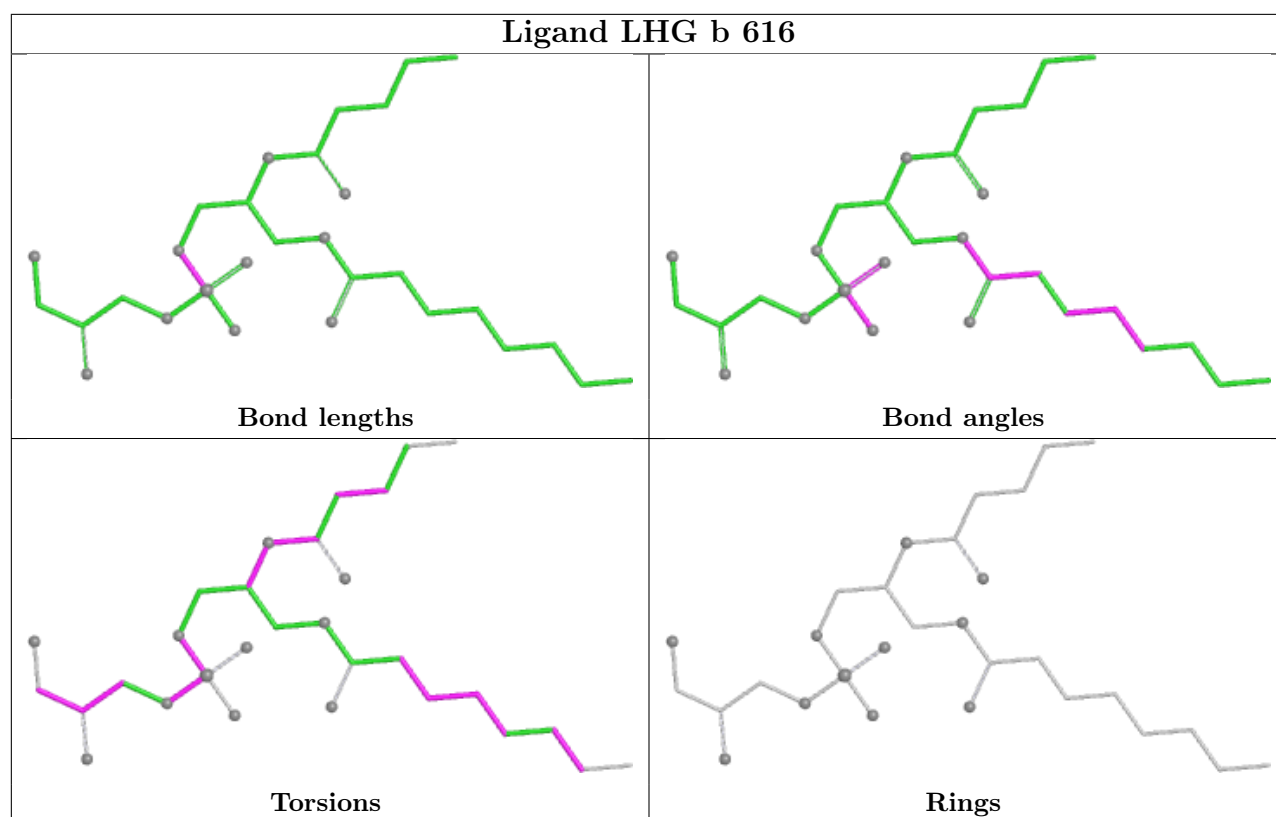


Torsions

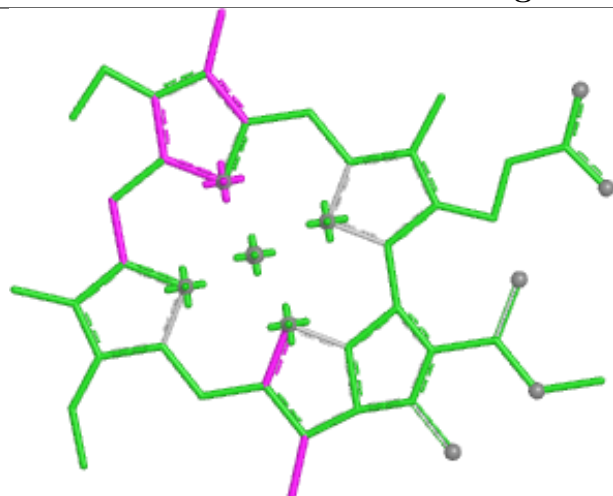


Rings

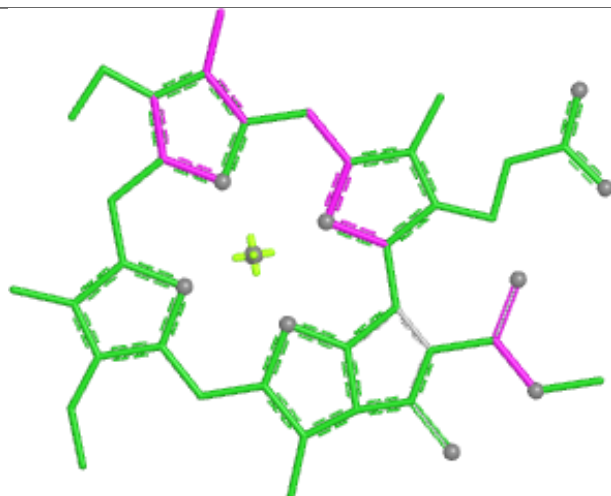




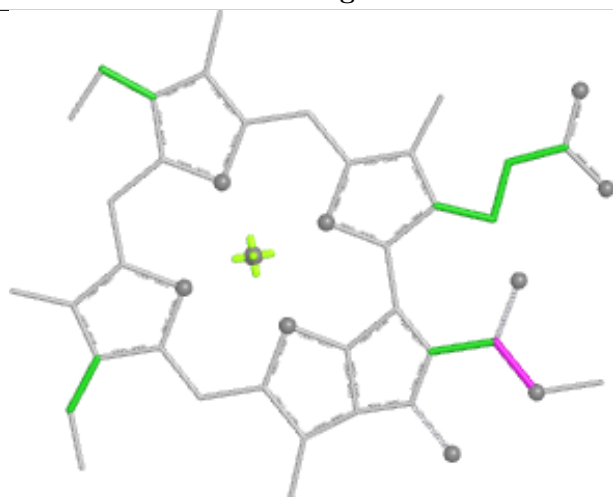
Ligand CLA B 834



Bond lengths



Bond angles

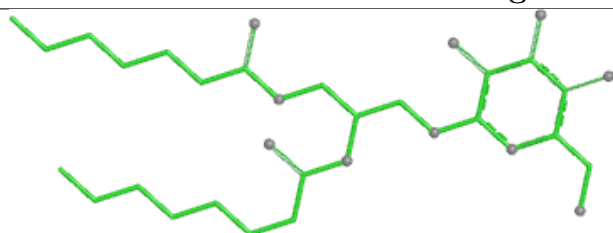


Torsions

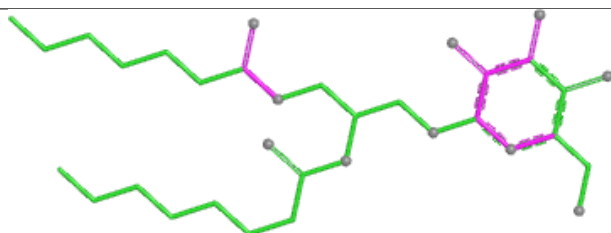


Rings

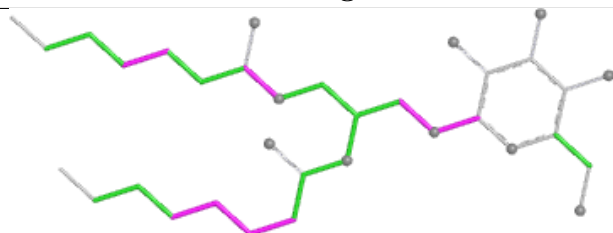
Ligand LMG X 302



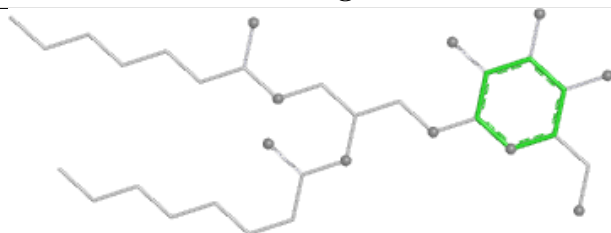
Bond lengths



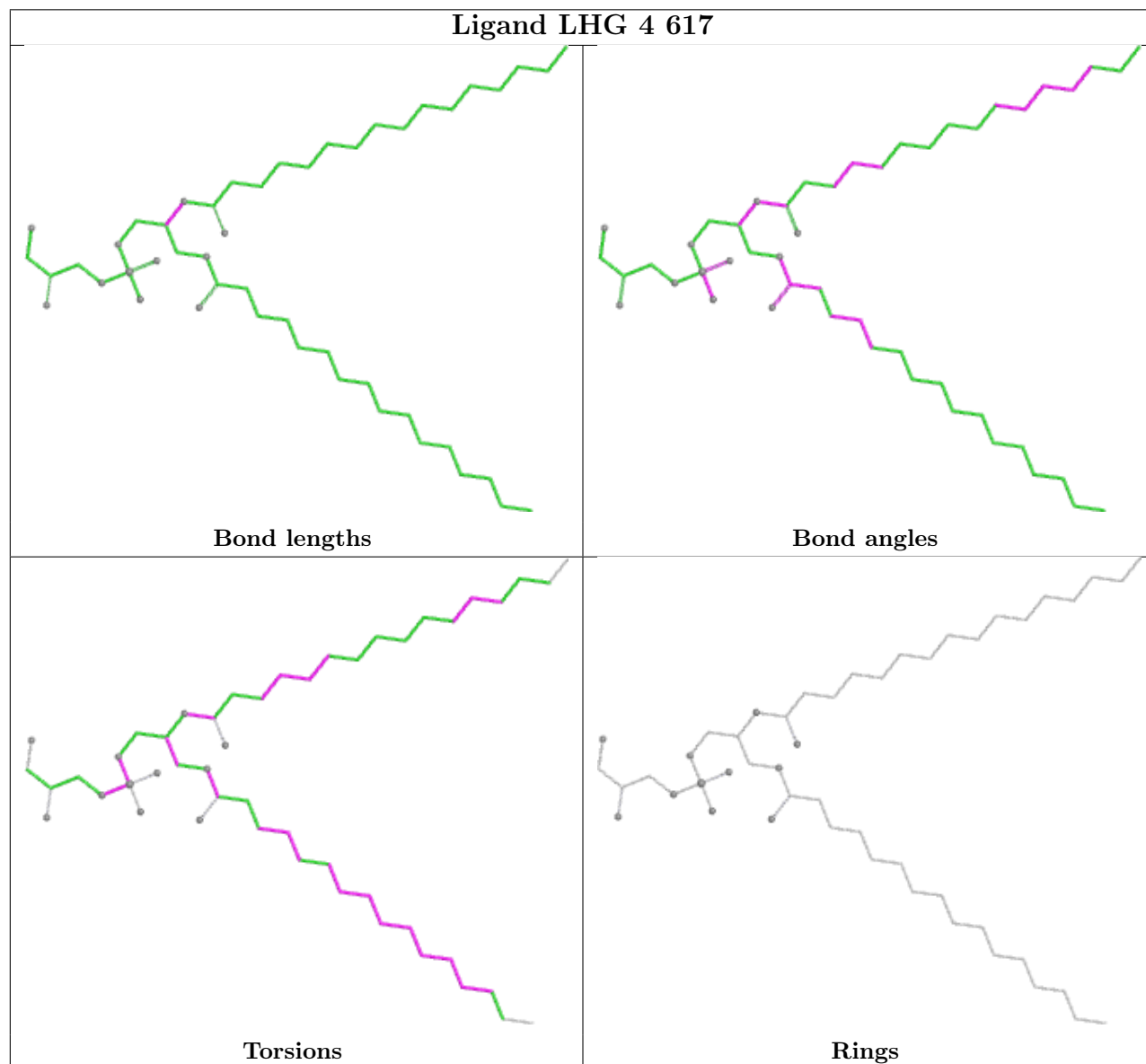
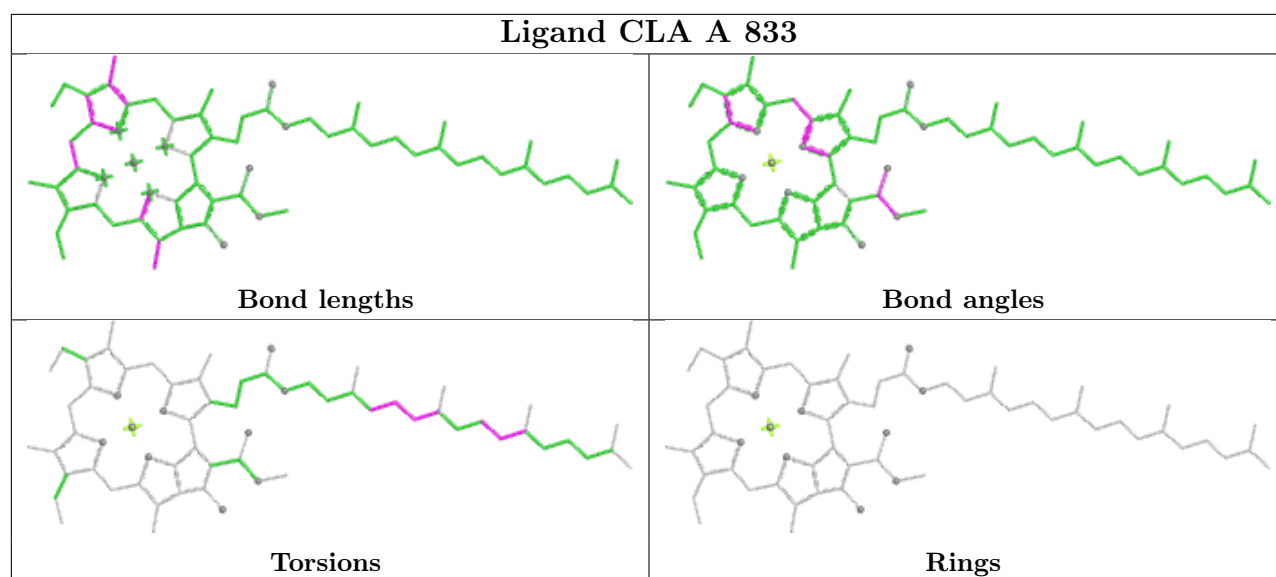
Bond angles



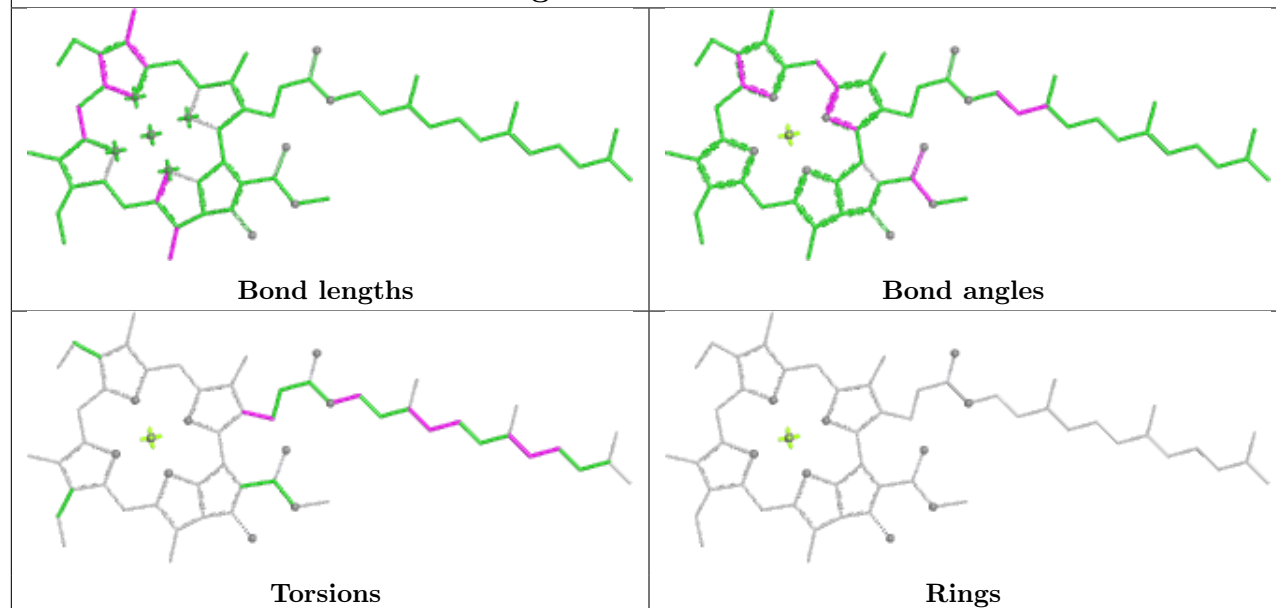
Torsions



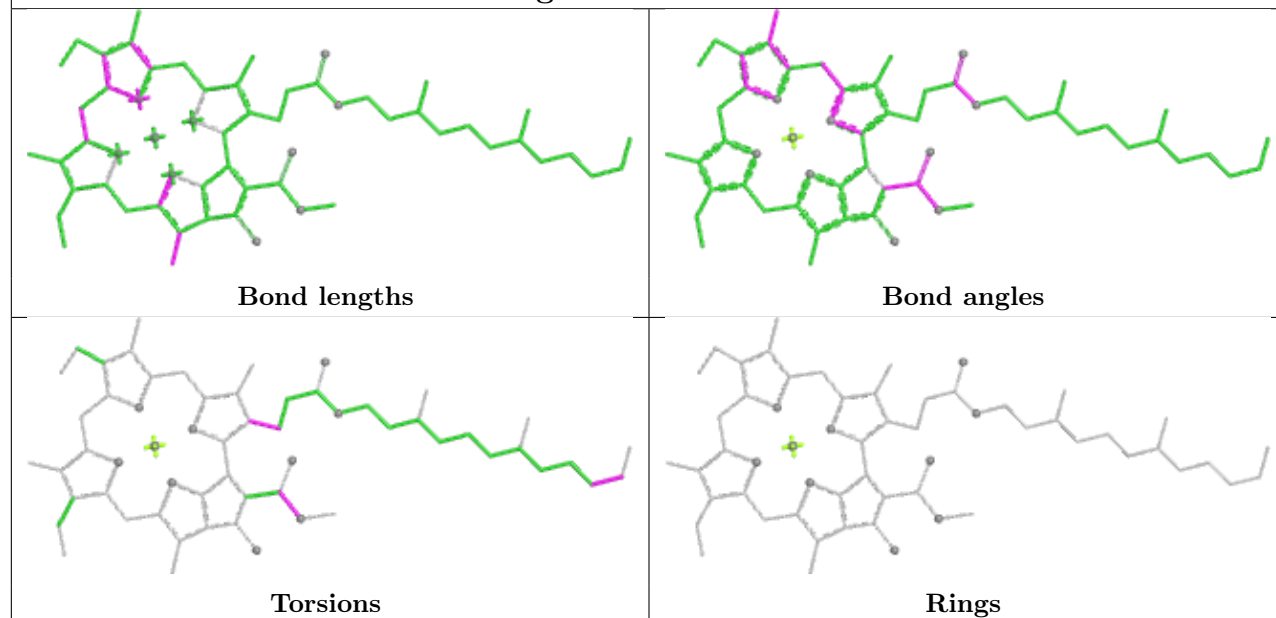
Rings



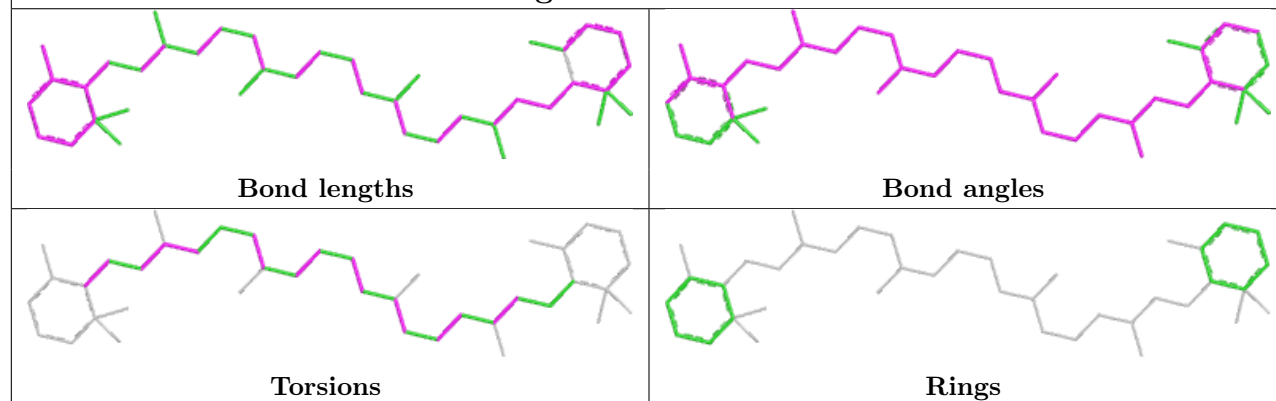
Ligand CLA A 855

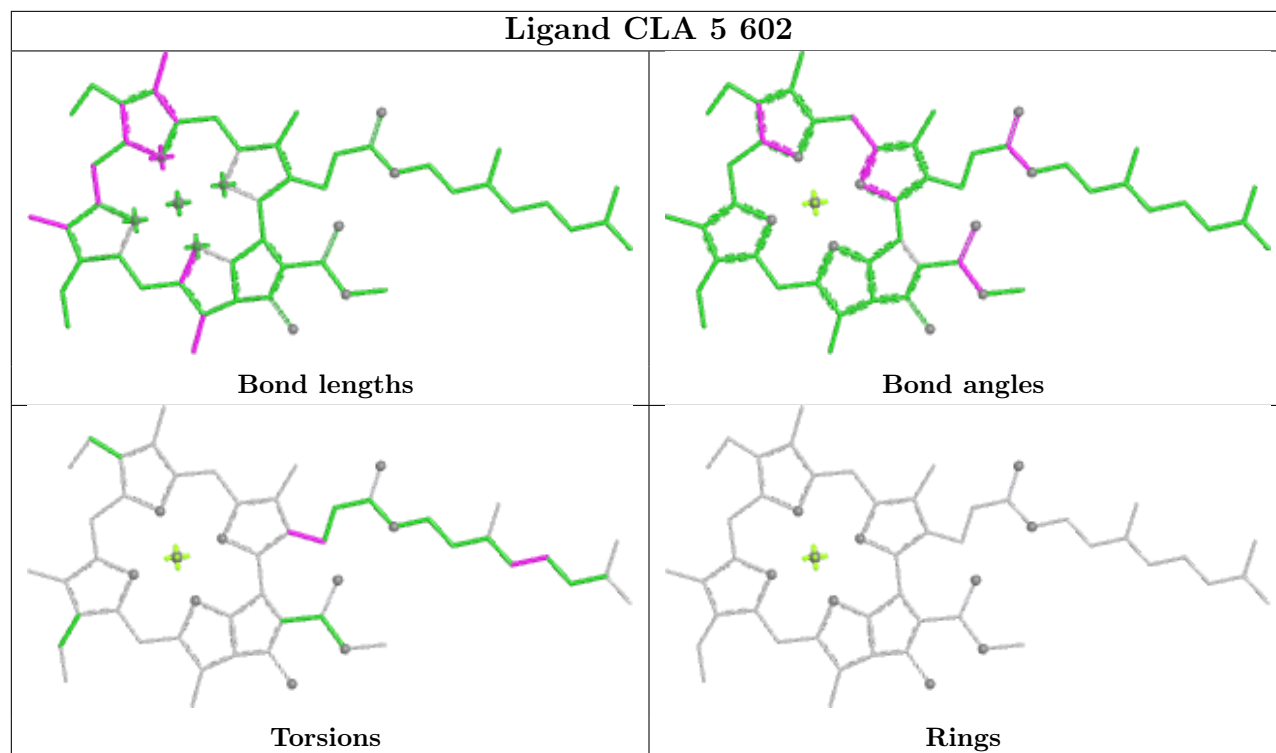
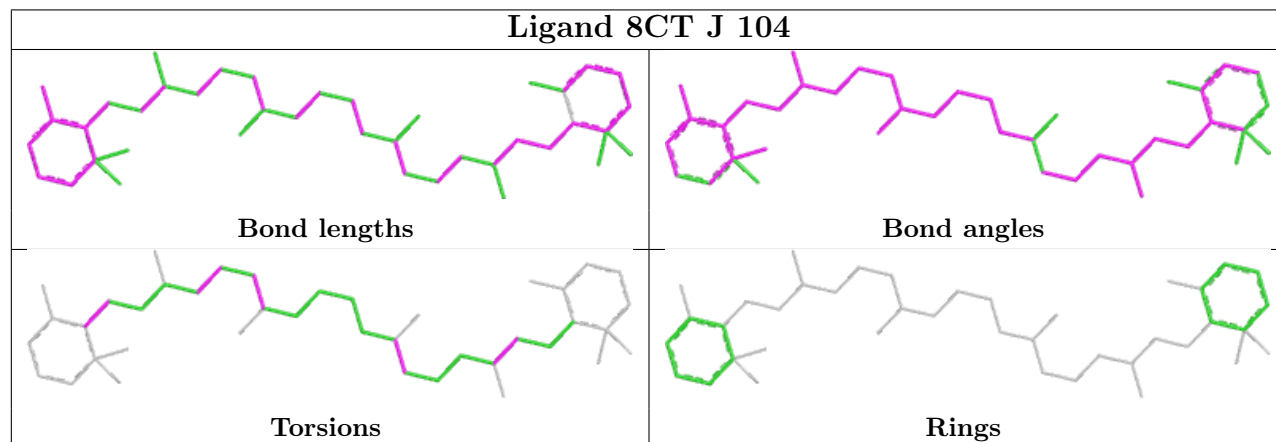


Ligand CLA 4 602

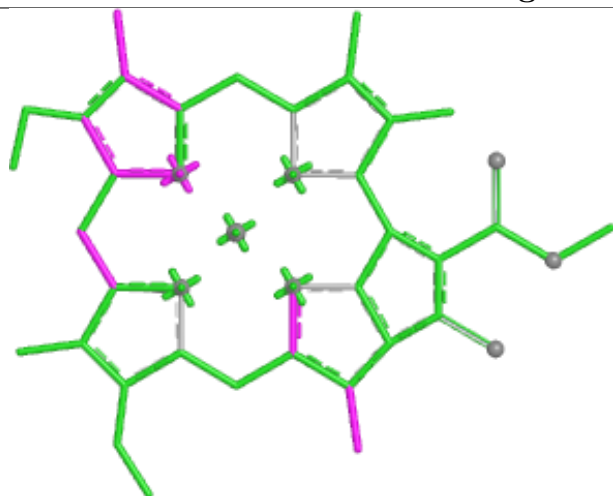


Ligand 8CT B 852

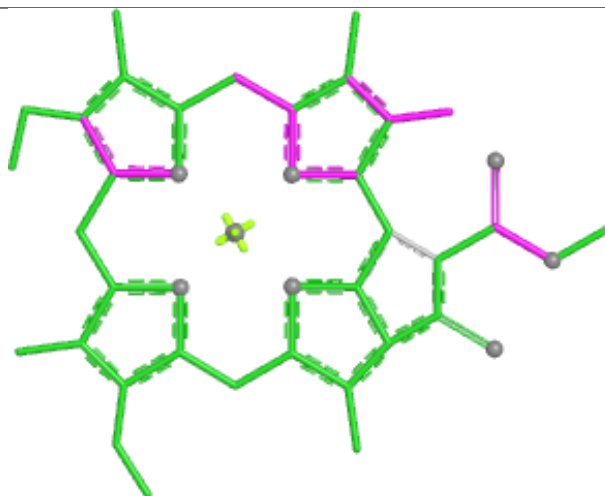


Ligand CLA 5 602**Ligand 8CT J 104**

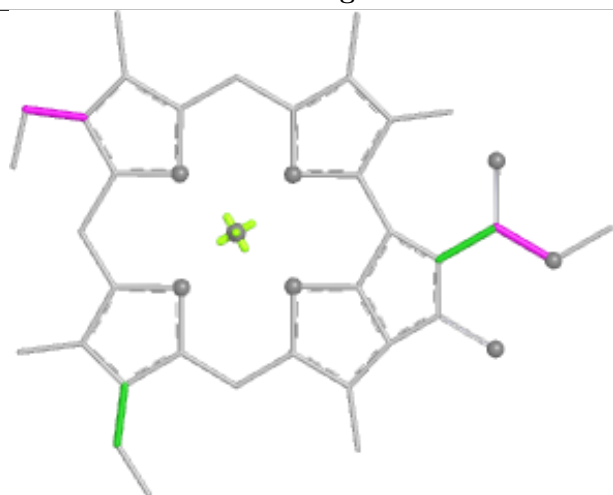
Ligand CLA 2 609



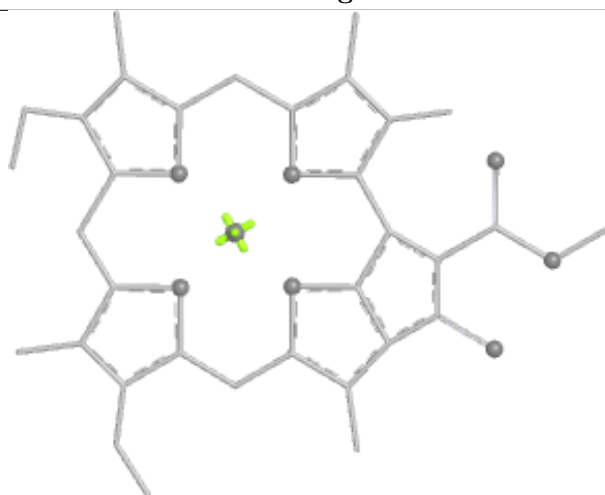
Bond lengths



Bond angles

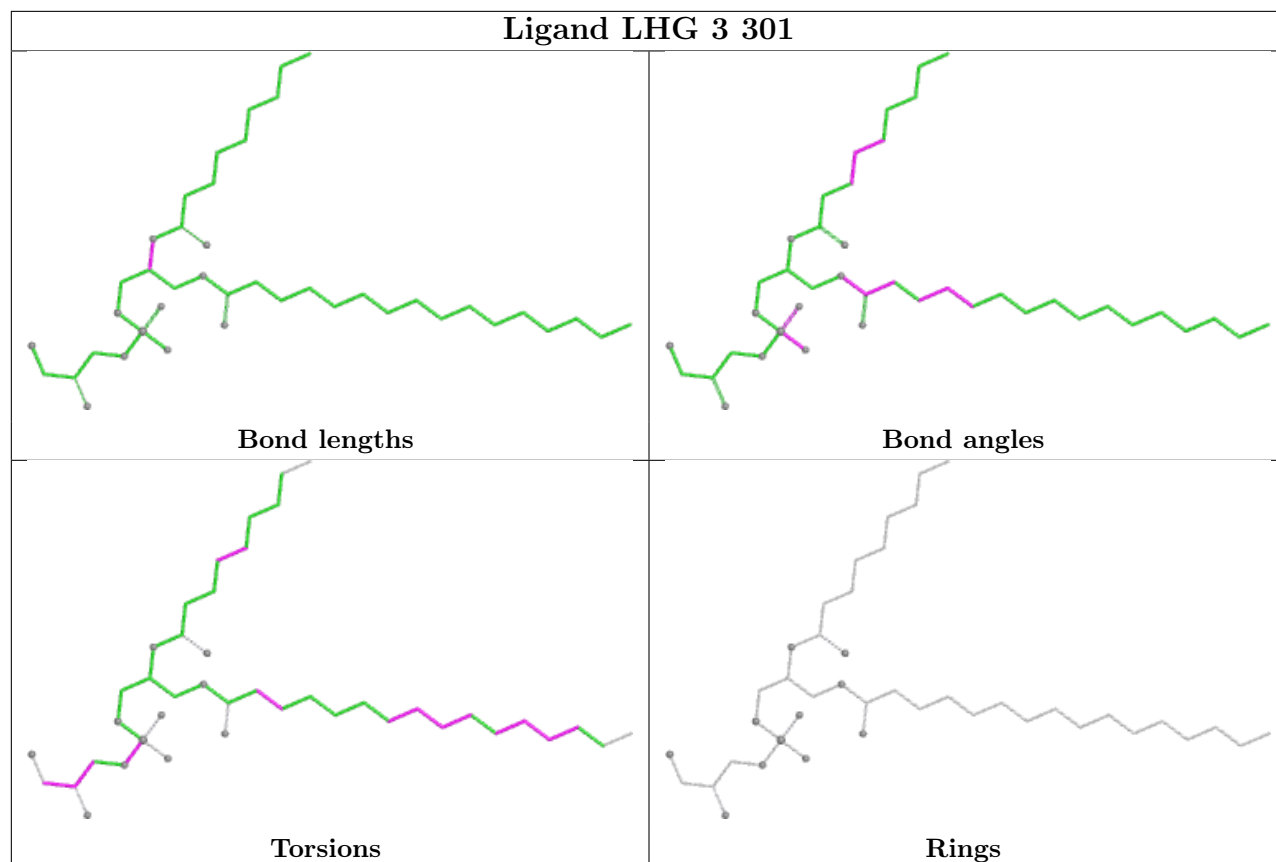


Torsions

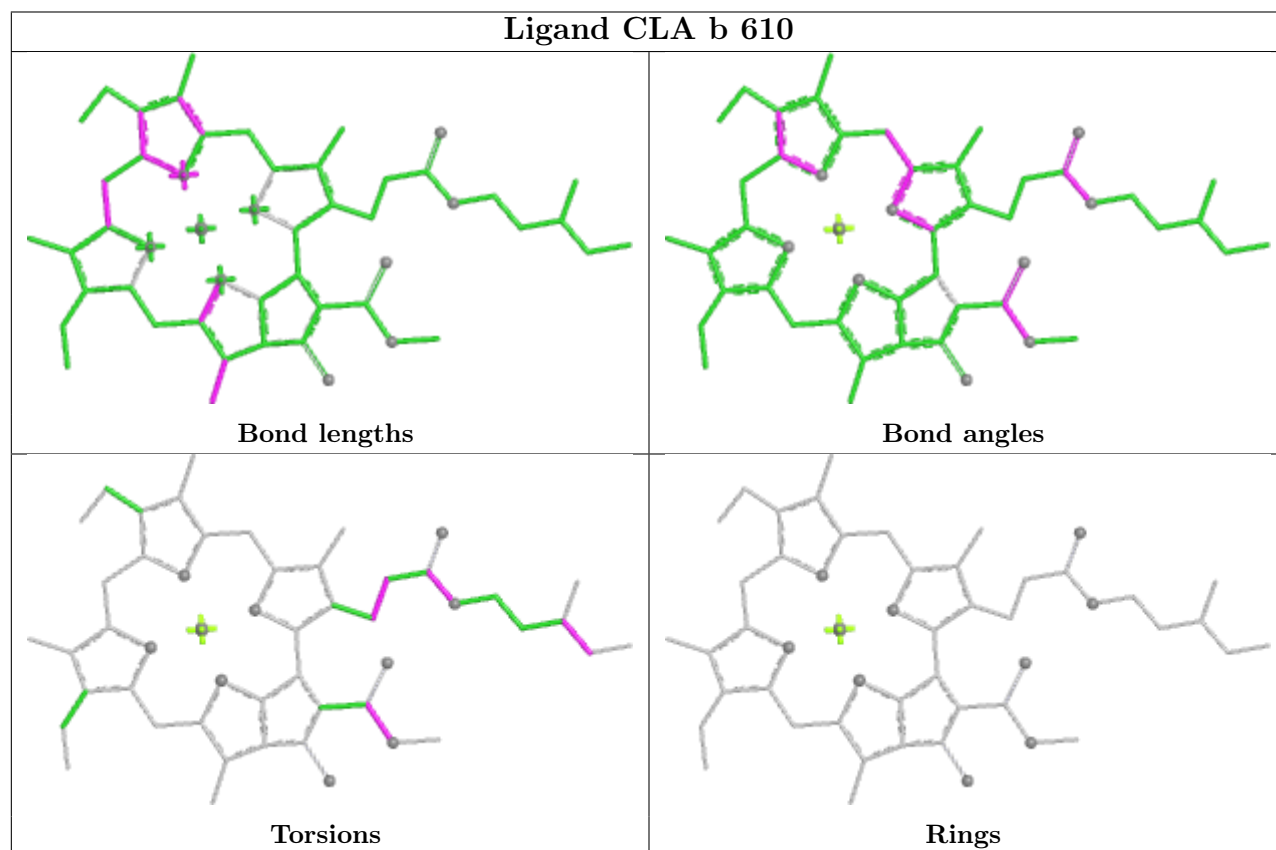


Rings

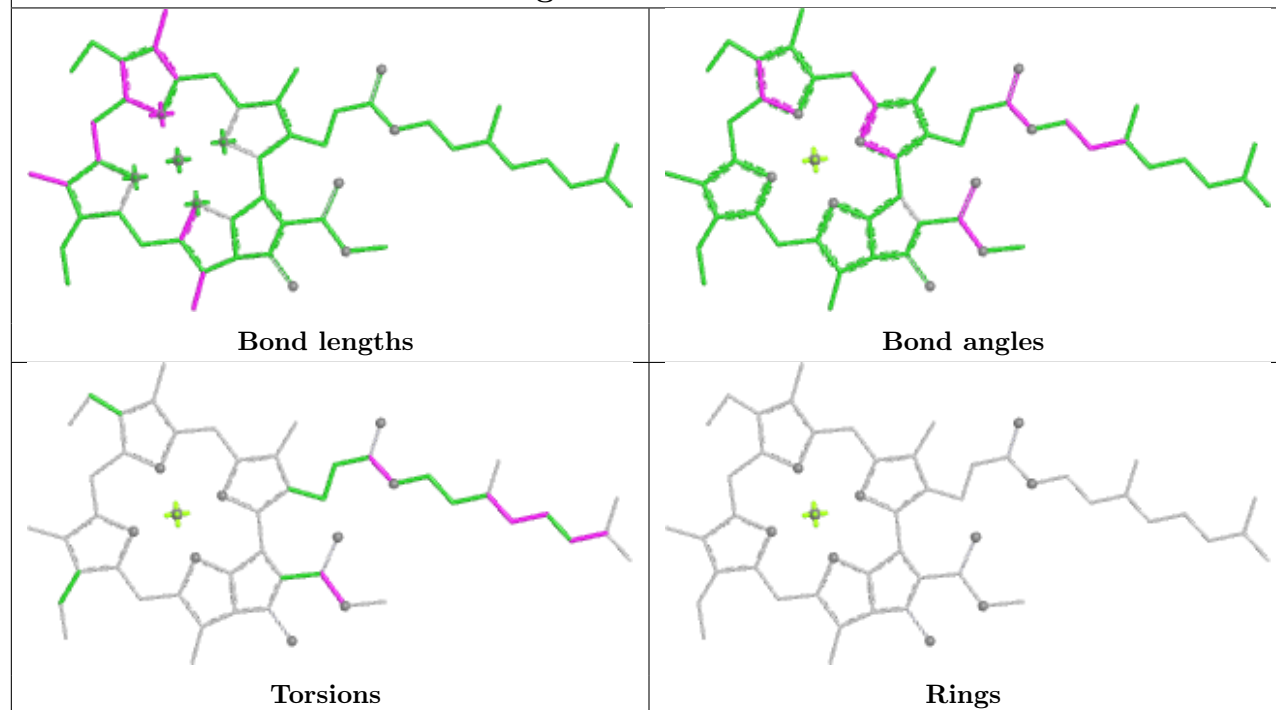
Ligand LHG 3 301



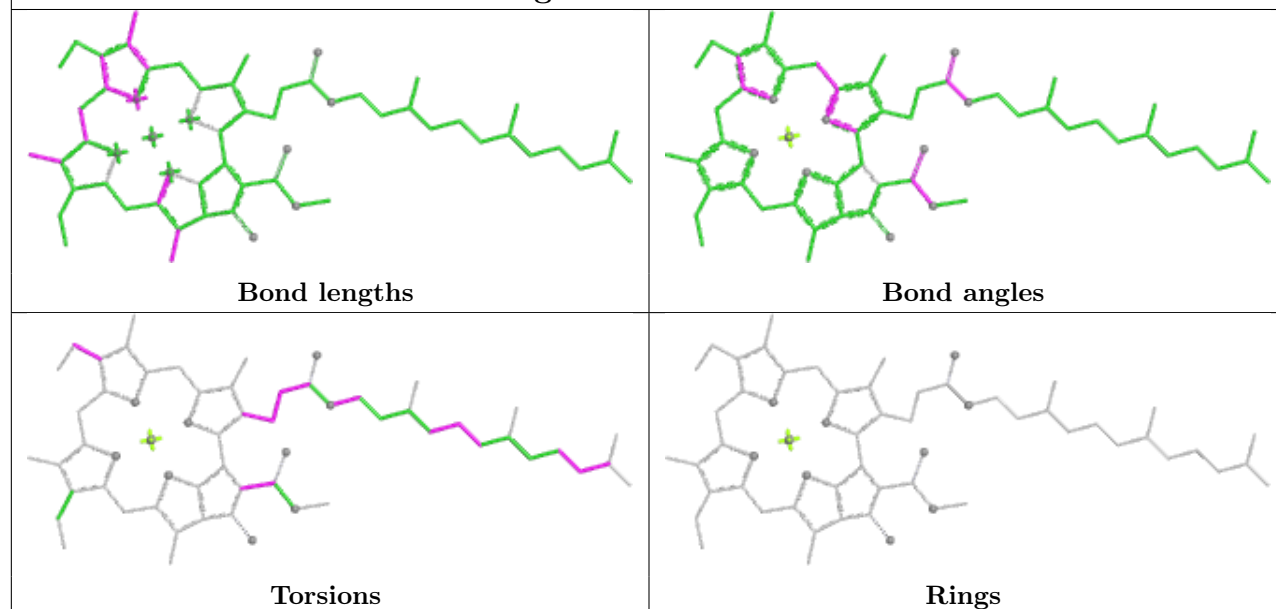
Ligand CLA b 610

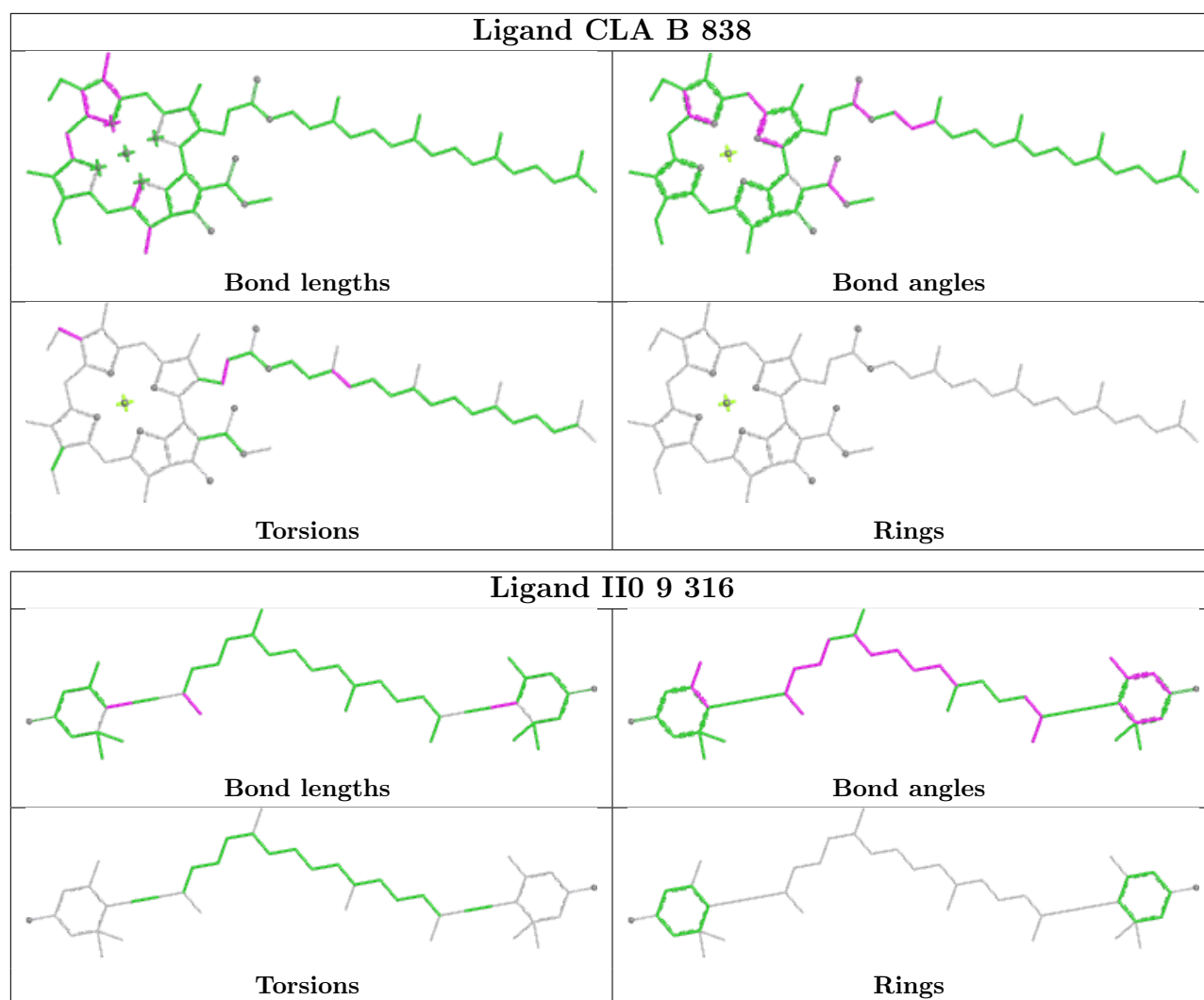


Ligand CLA a 611

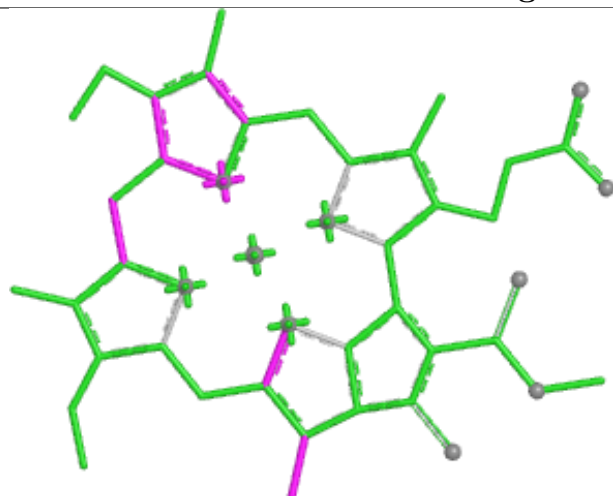


Ligand CLA Z 305

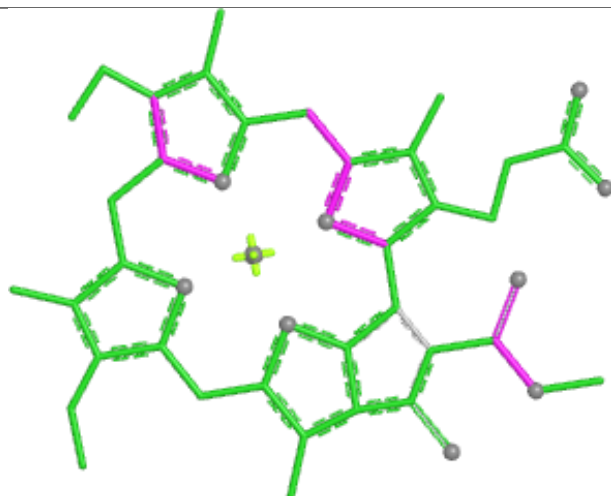




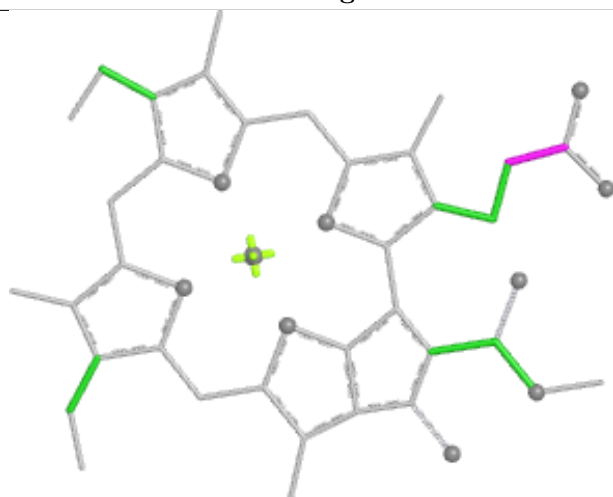
Ligand CLA 5 603



Bond lengths



Bond angles

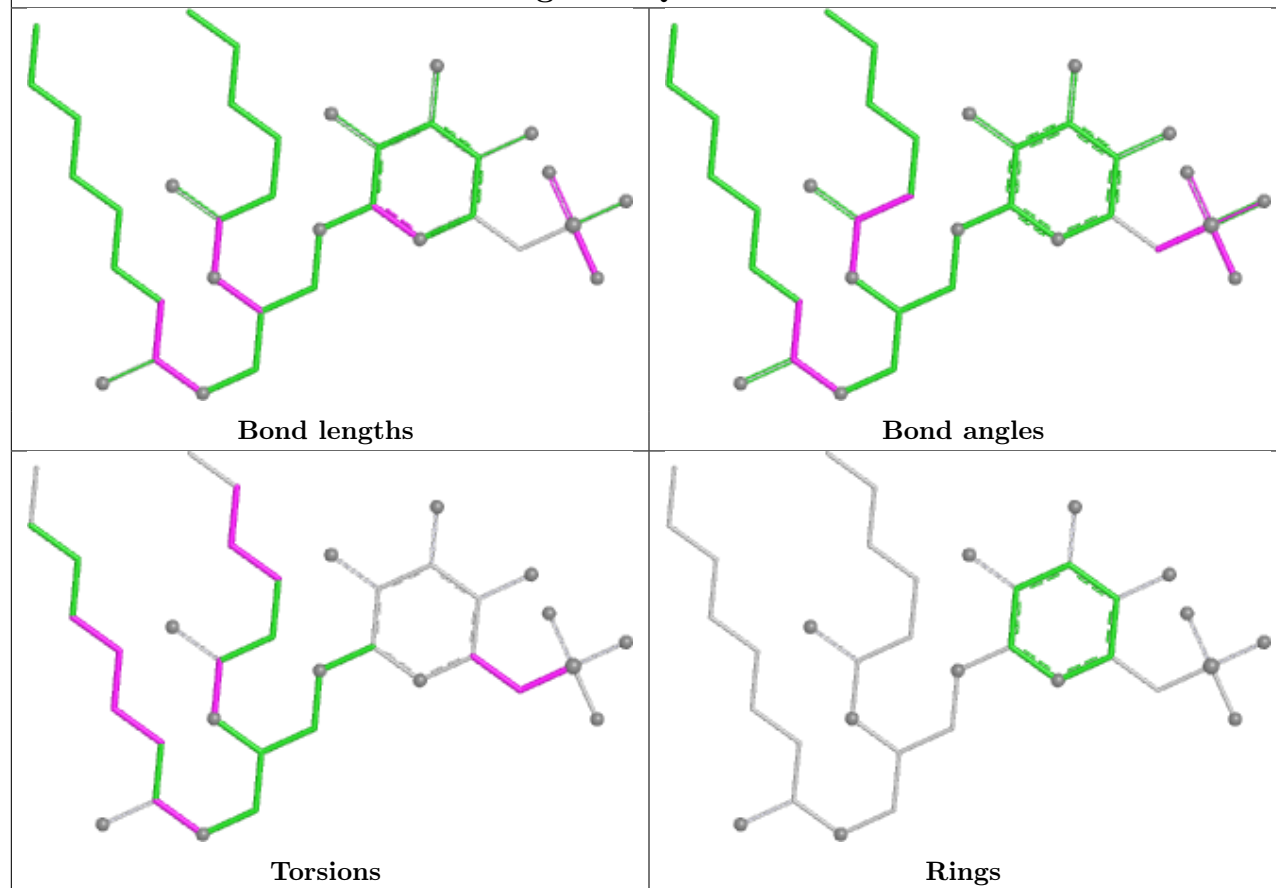


Torsions

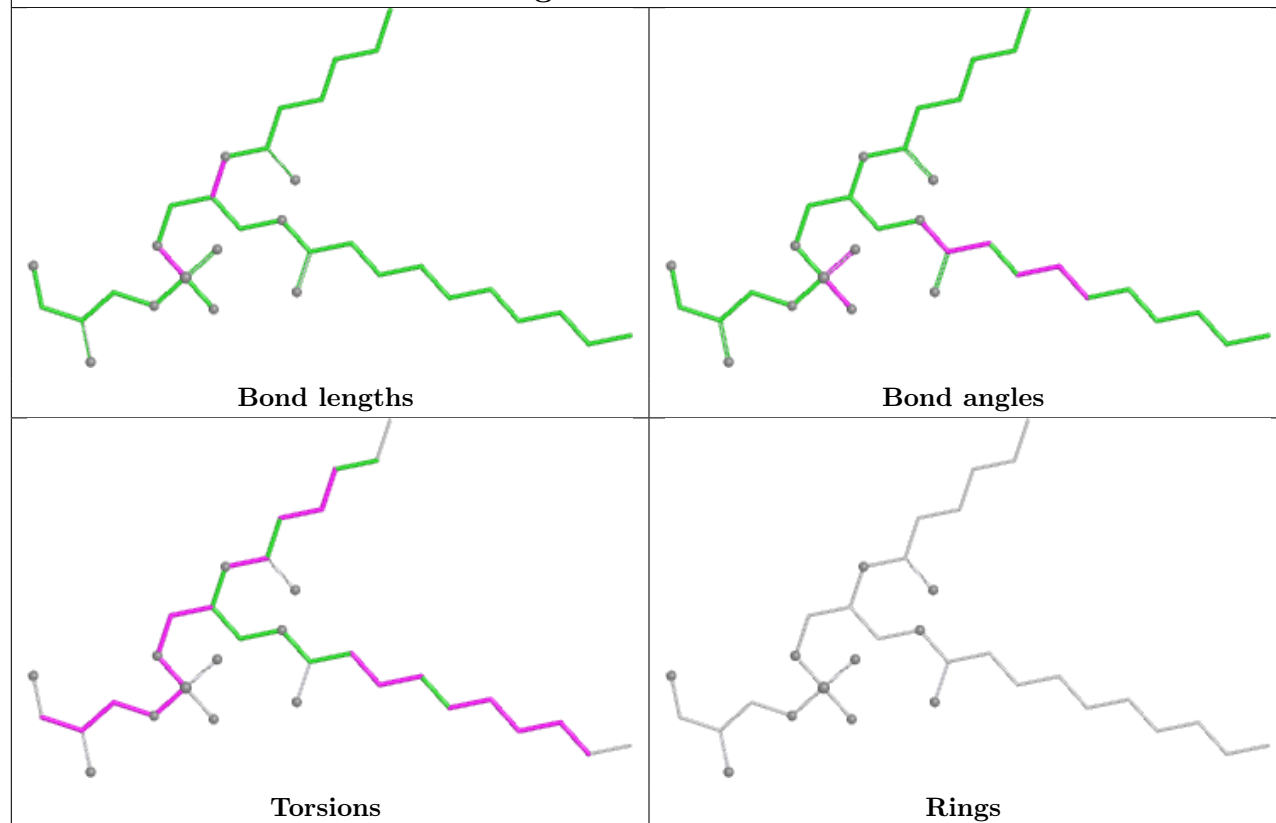


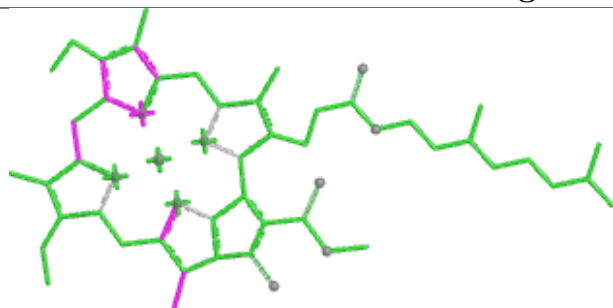
Rings

Ligand SQD 3 320

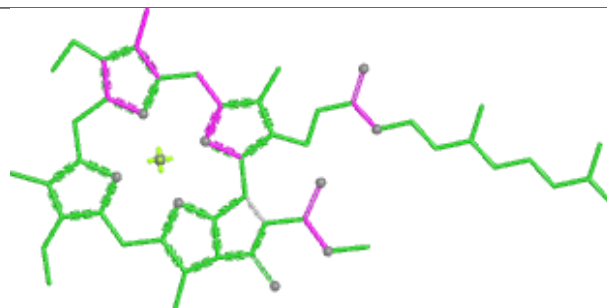


Ligand LHG 8 315

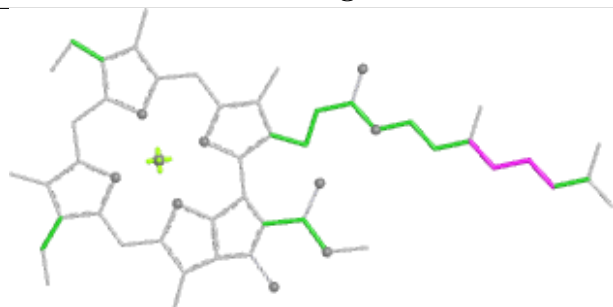


Ligand CLA 7 311

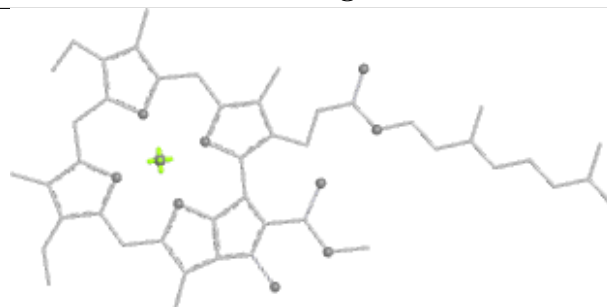
Bond lengths



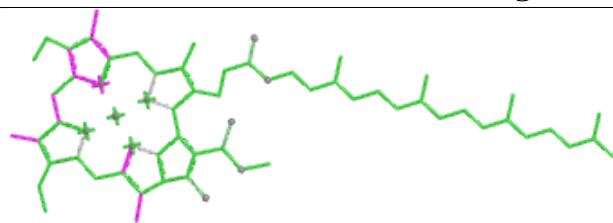
Bond angles



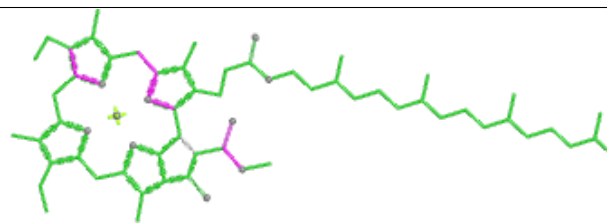
Torsions



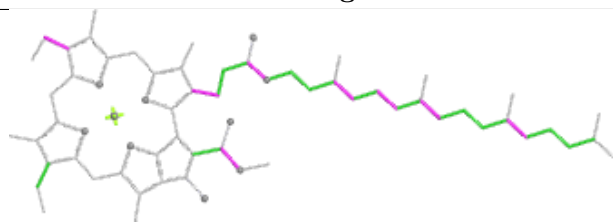
Rings

Ligand CLA A 822

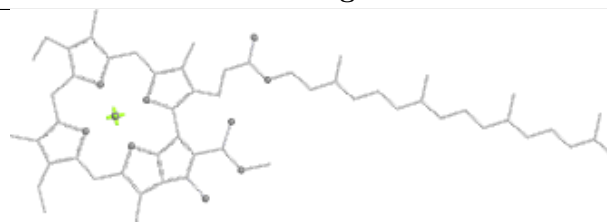
Bond lengths



Bond angles

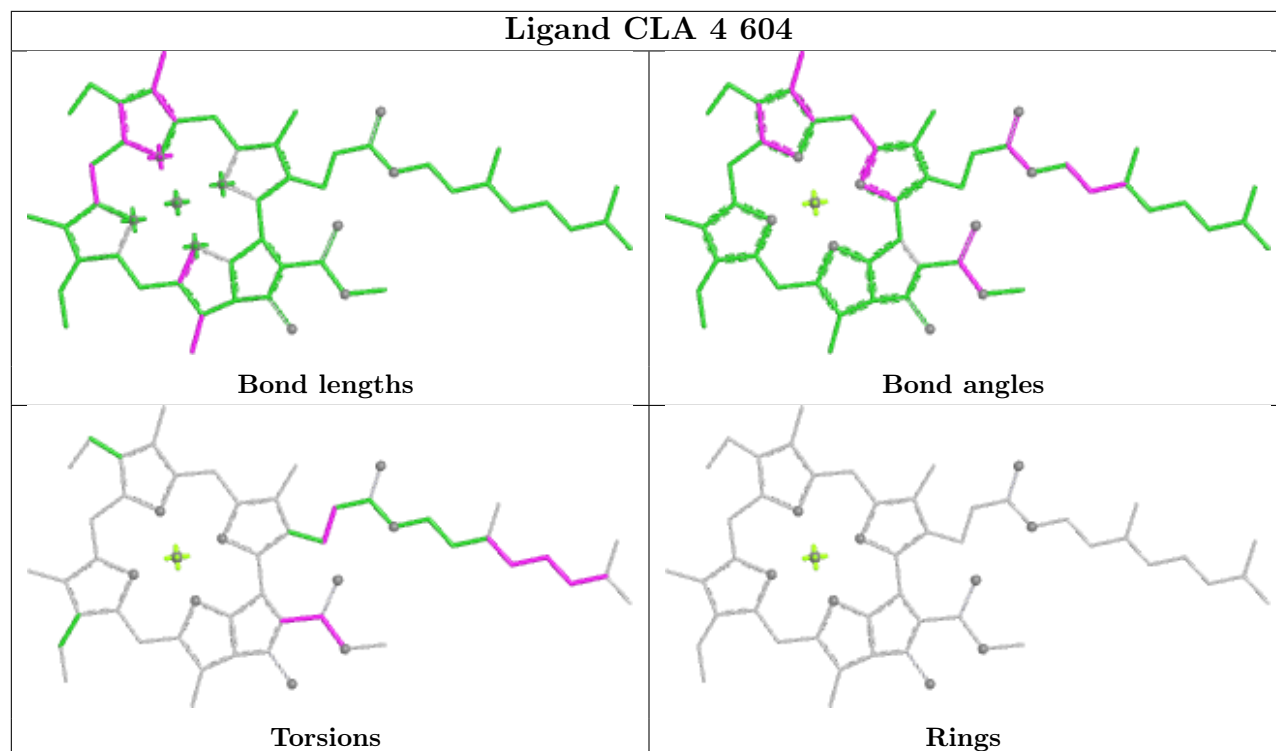


Torsions

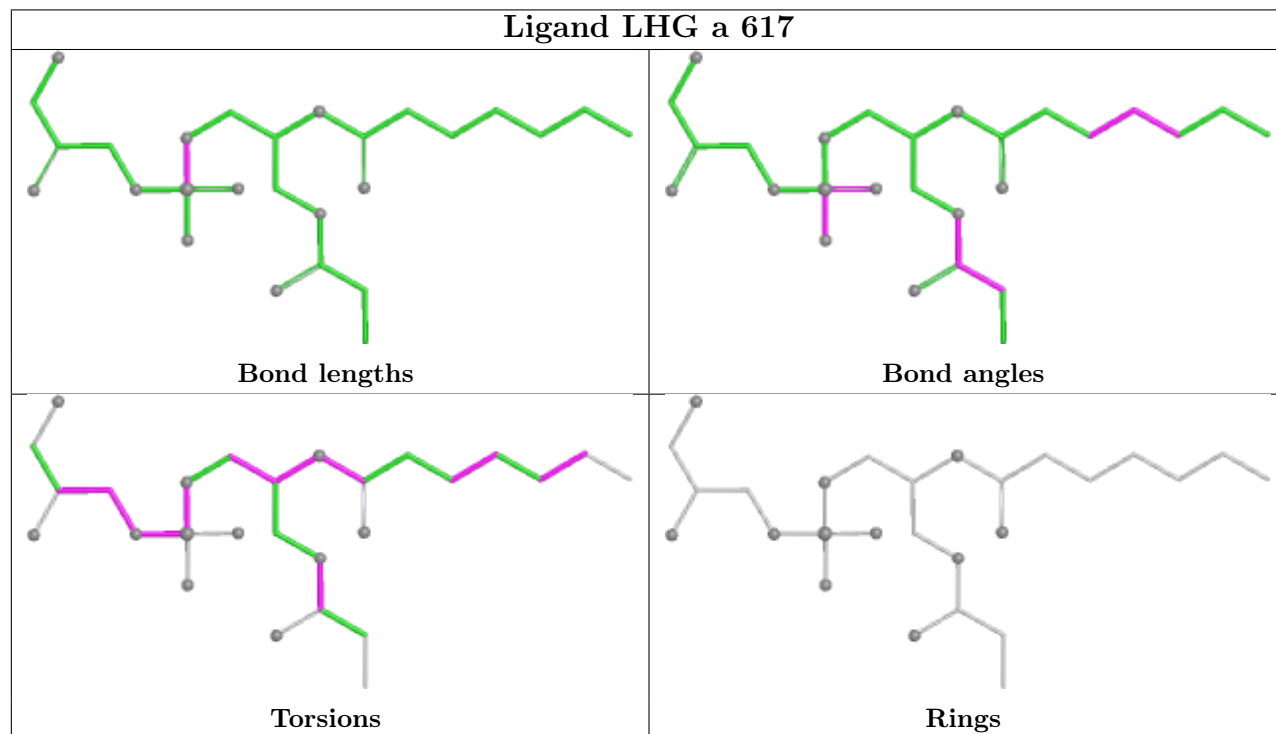


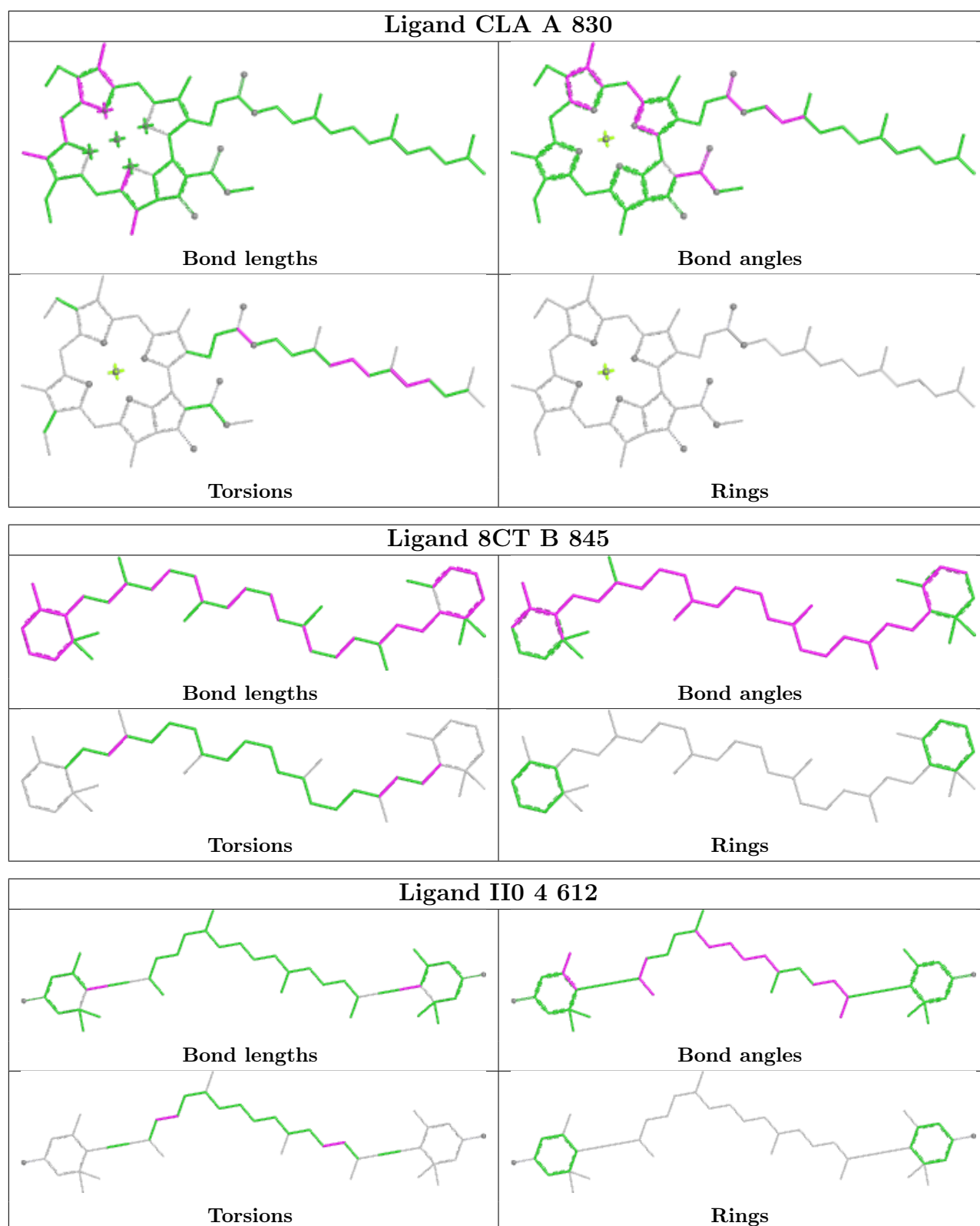
Rings

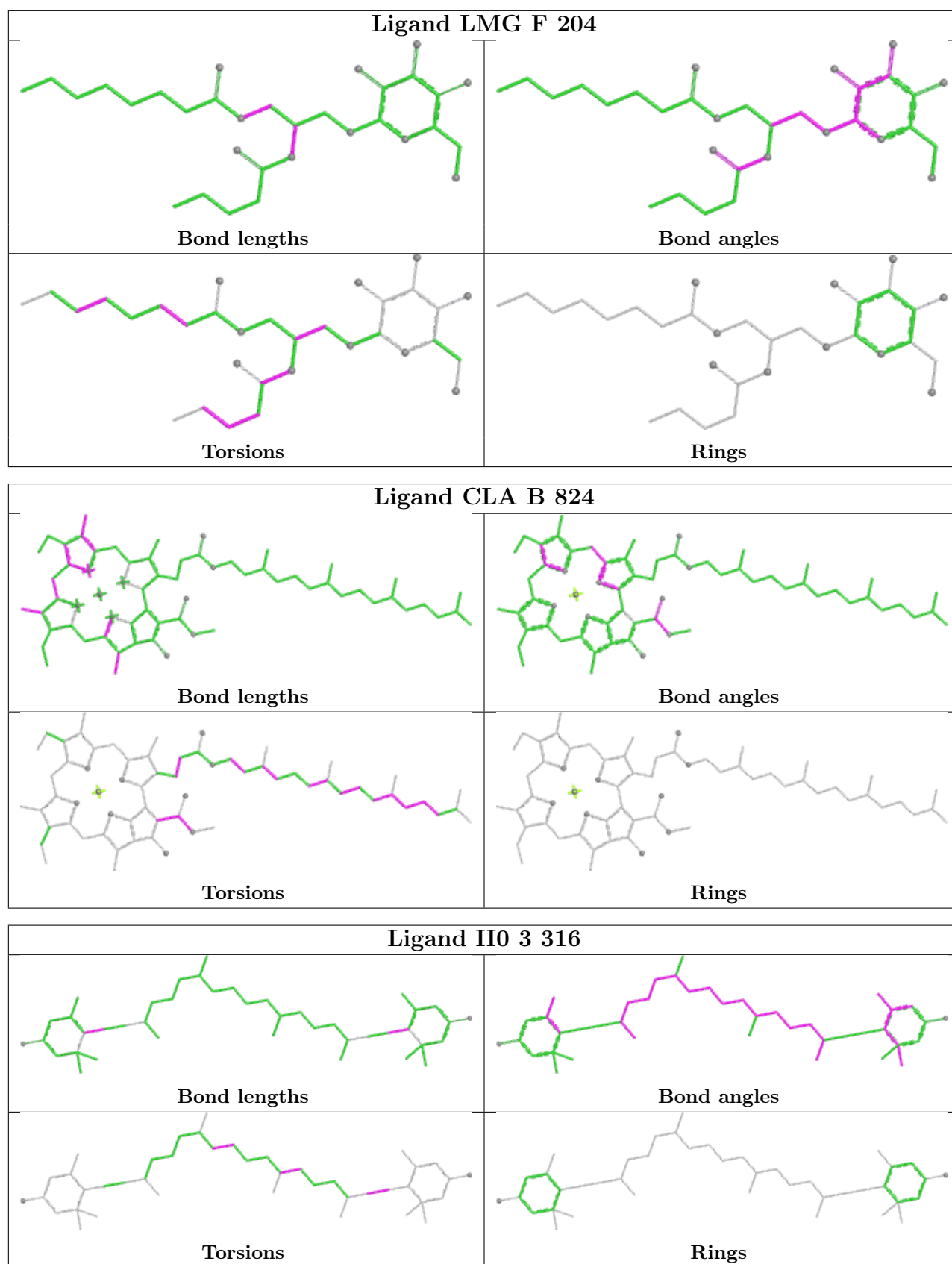
Ligand CLA 4 604



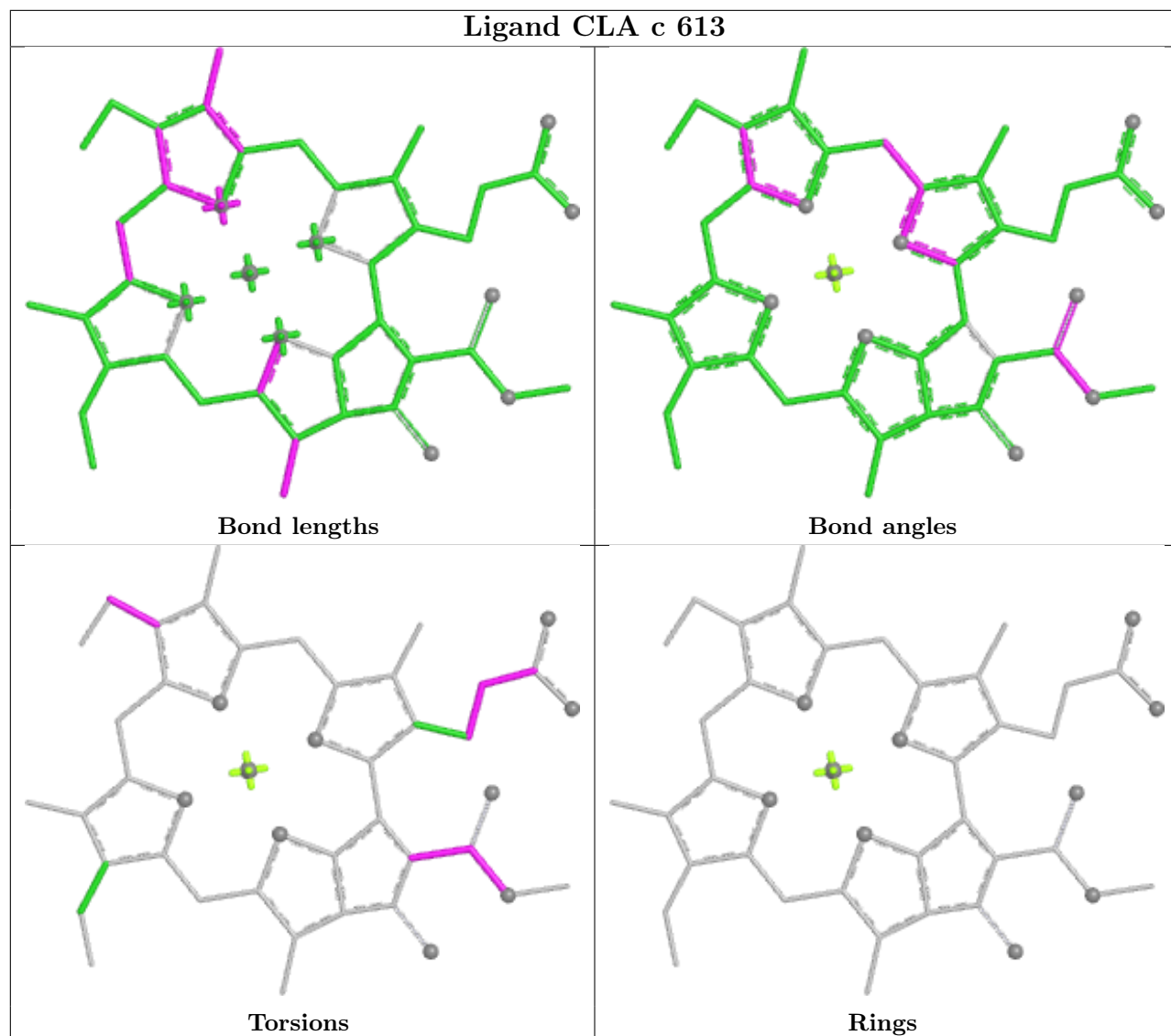
Ligand LHG a 617



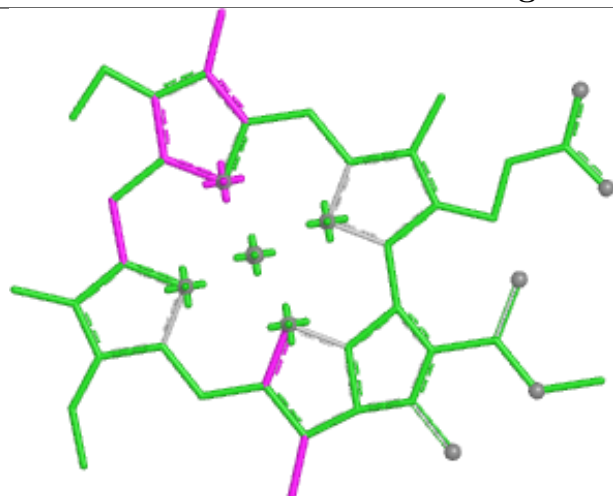




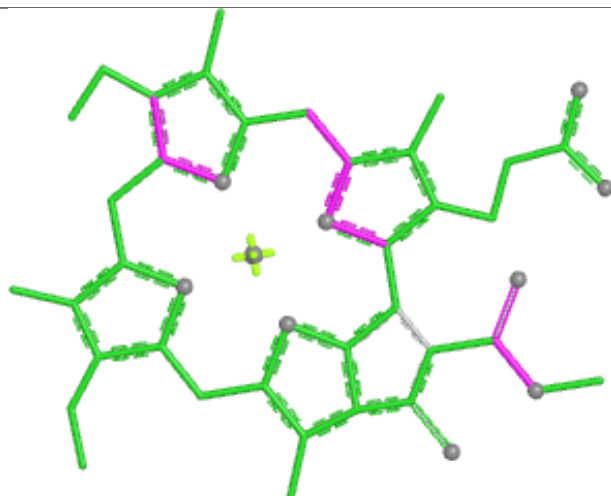
Ligand CLA c 613



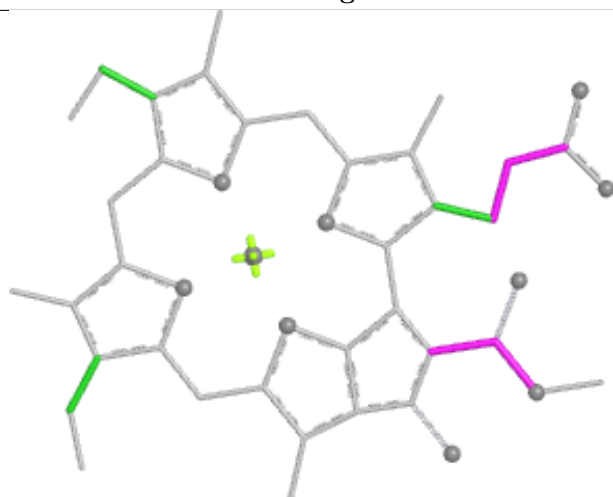
Ligand CLA 1 611



Bond lengths



Bond angles

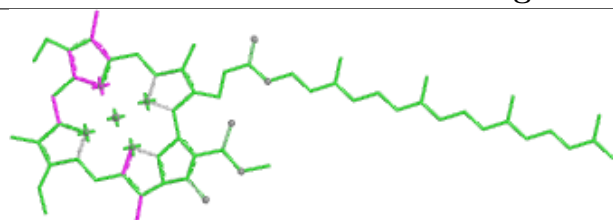


Torsions

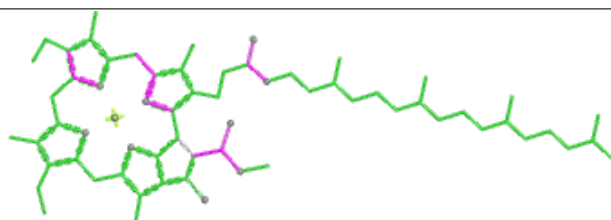


Rings

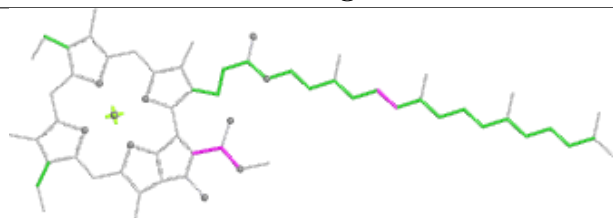
Ligand CLA A 832



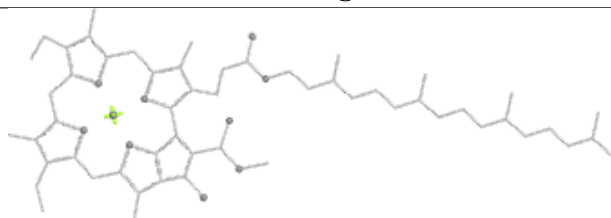
Bond lengths



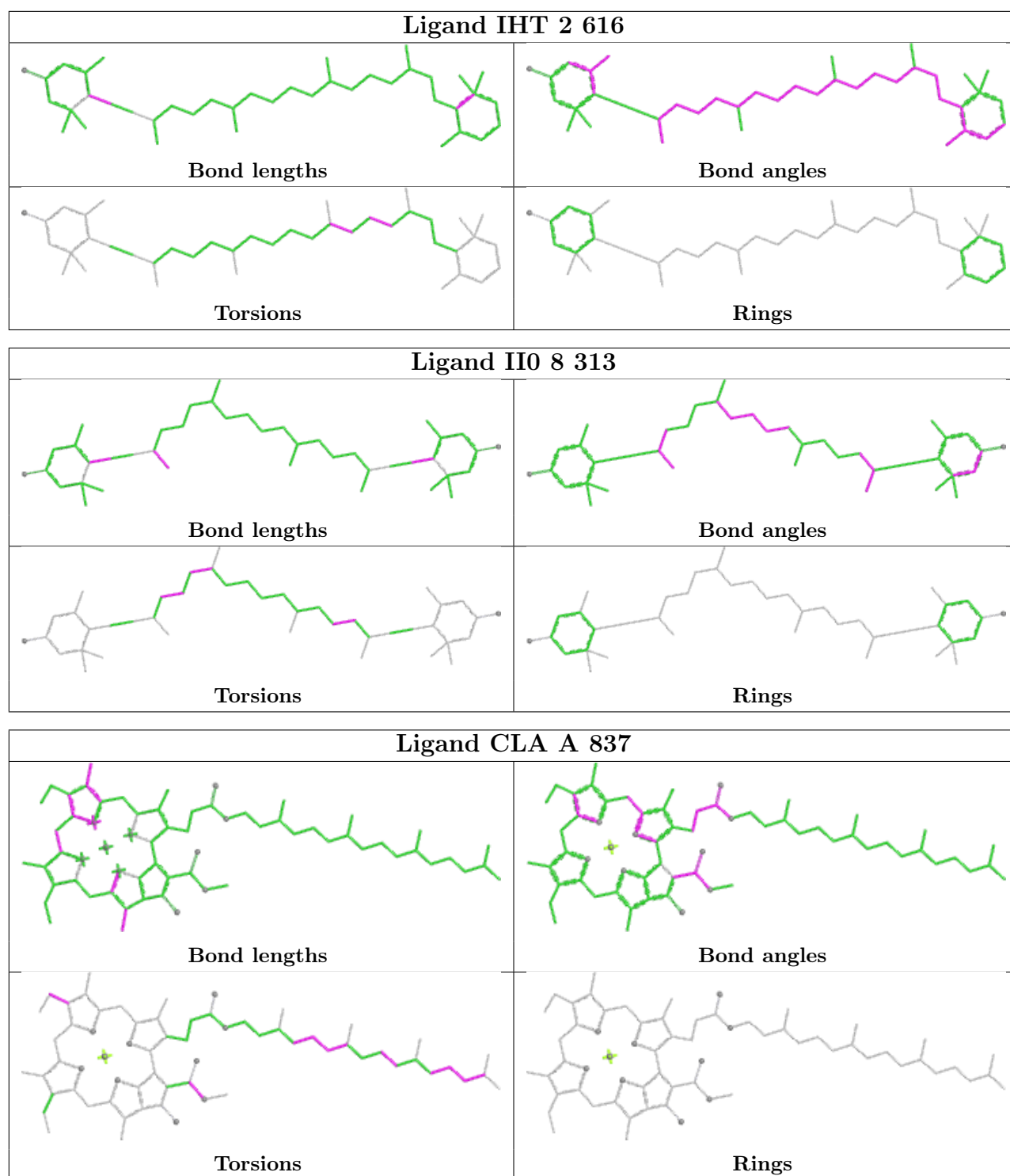
Bond angles

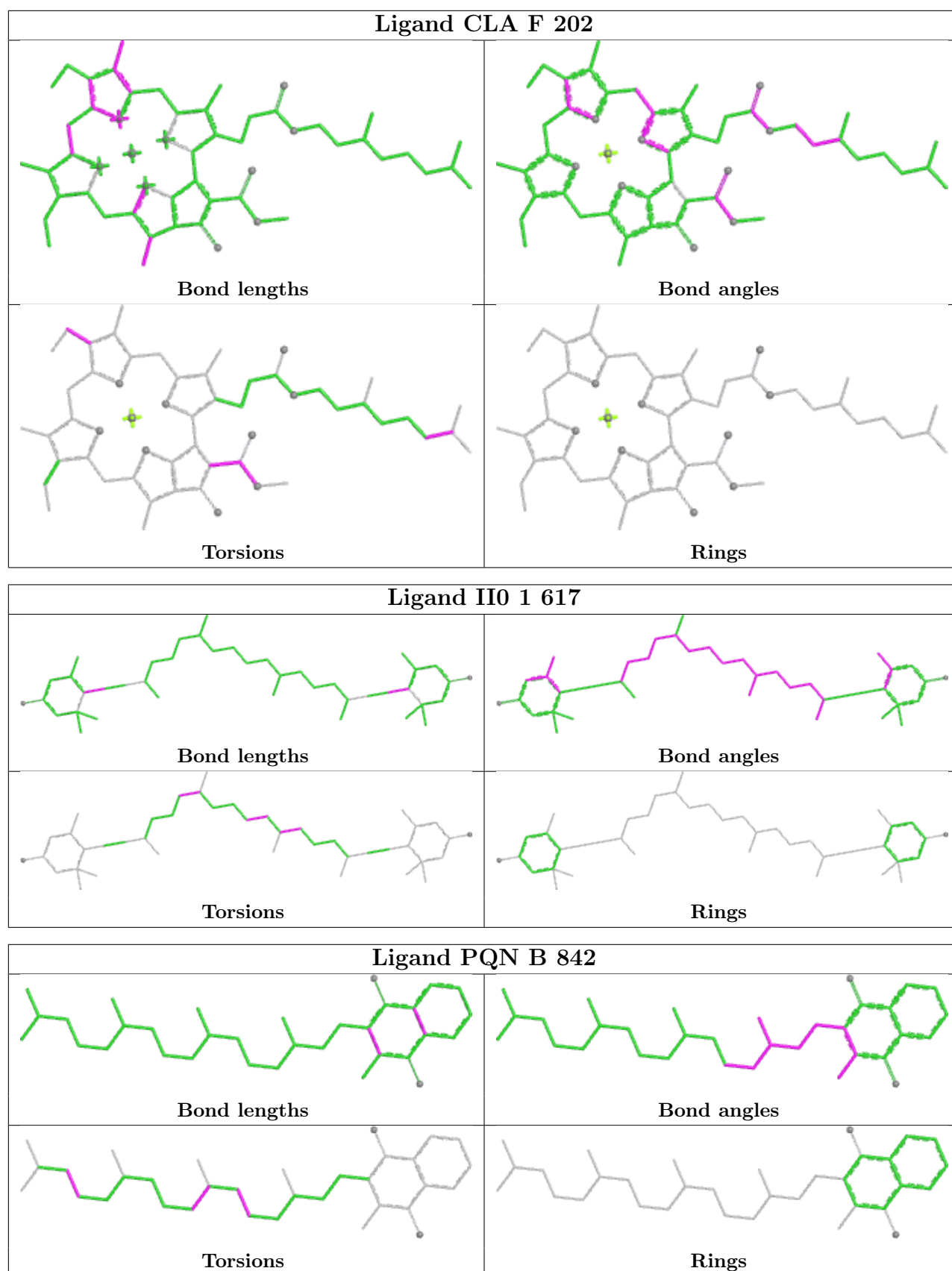


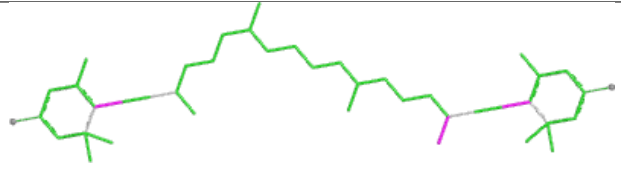
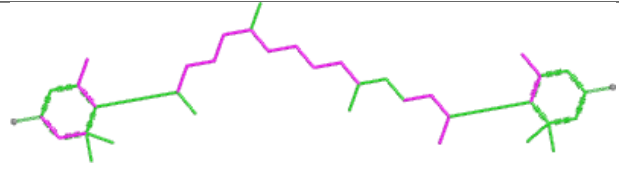
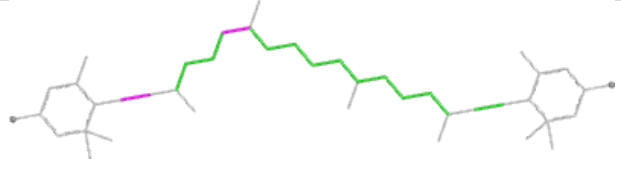
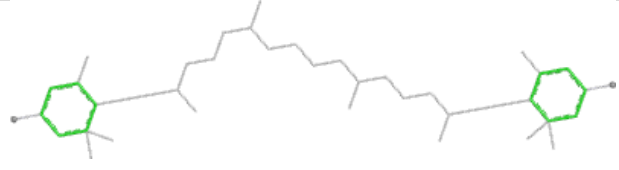
Torsions

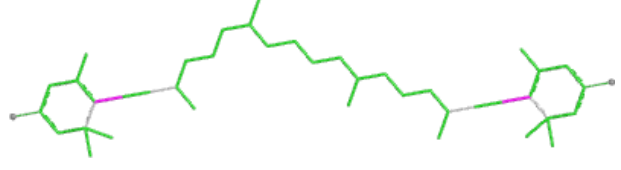
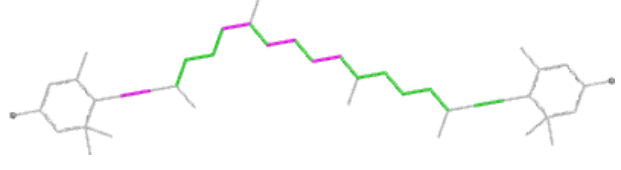
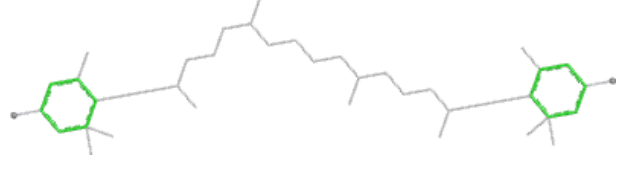


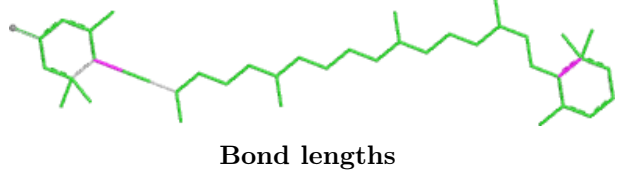
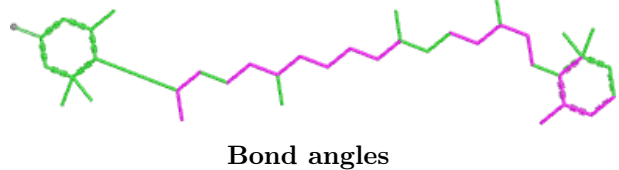
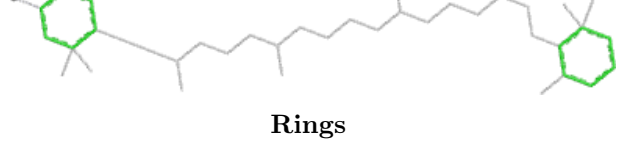
Rings

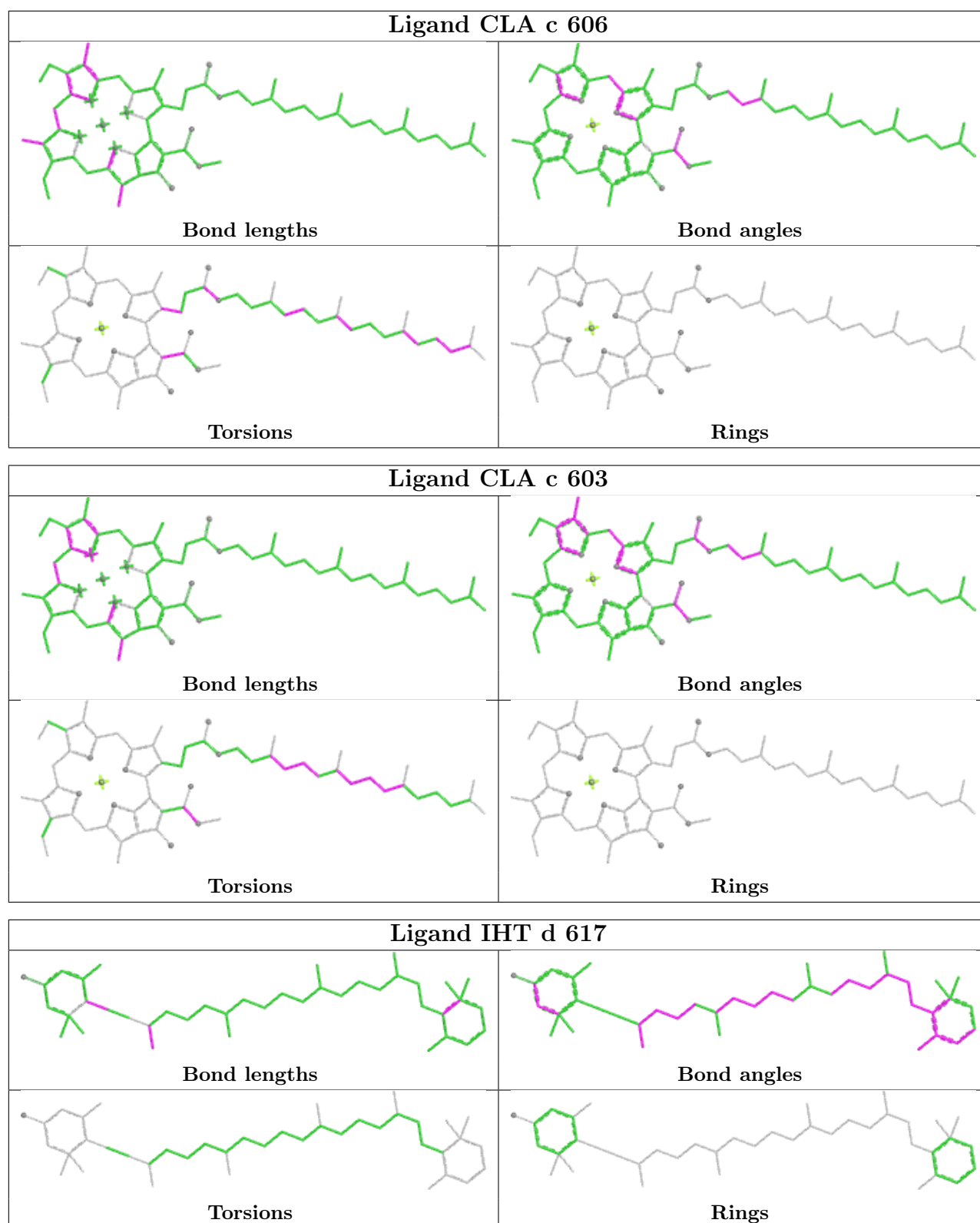


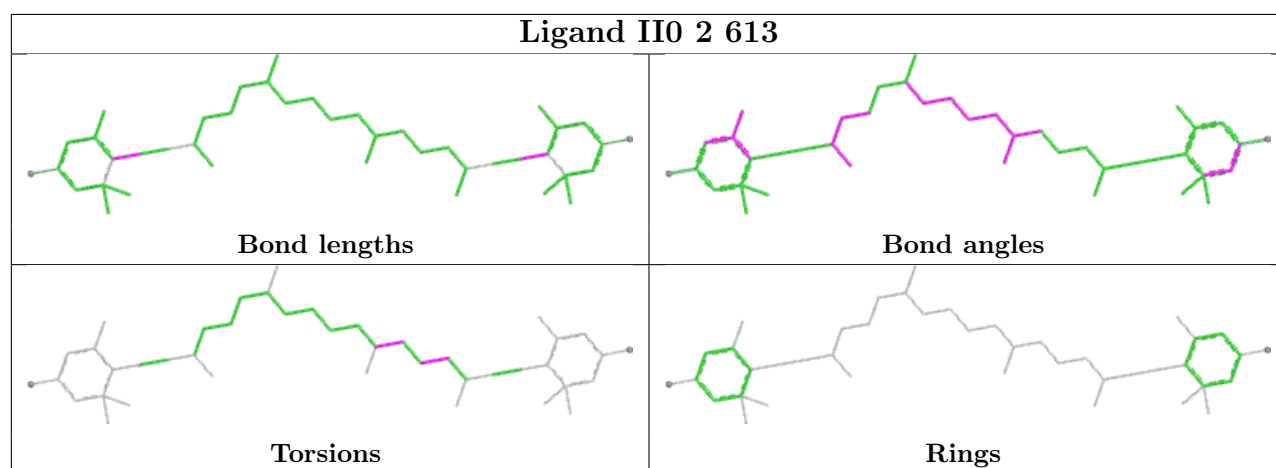
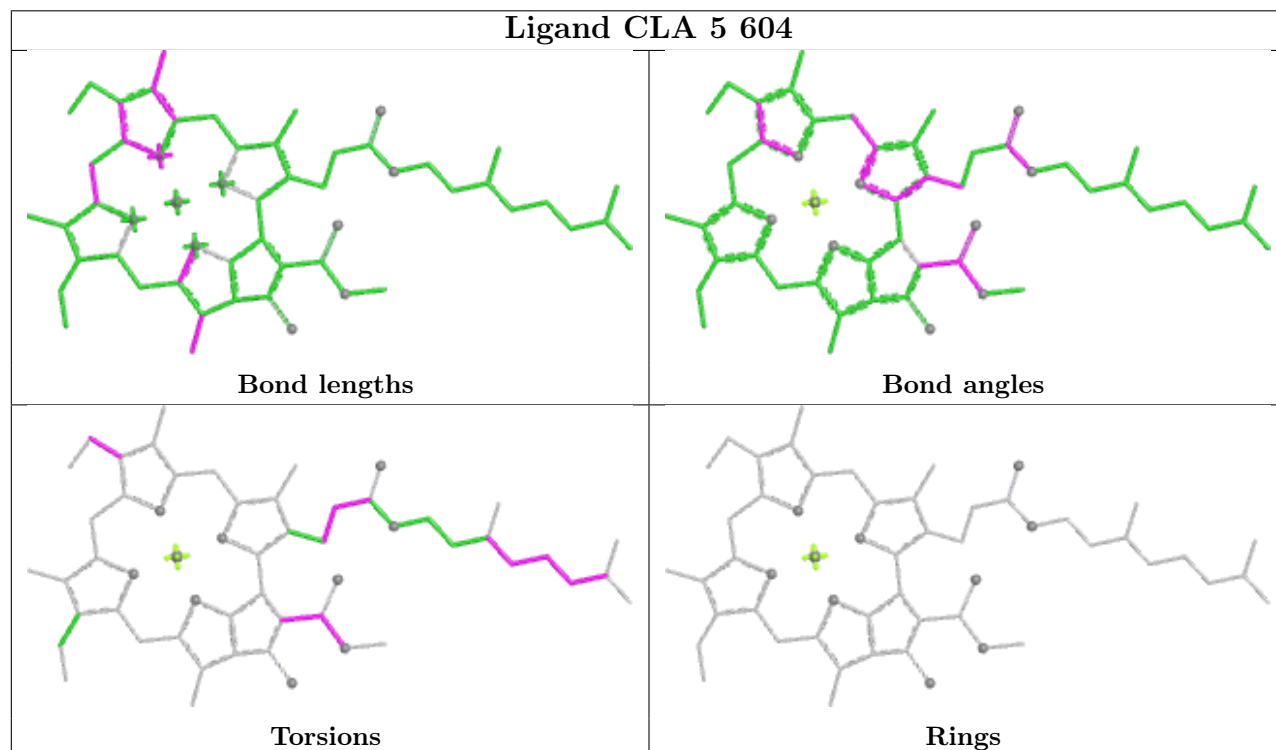
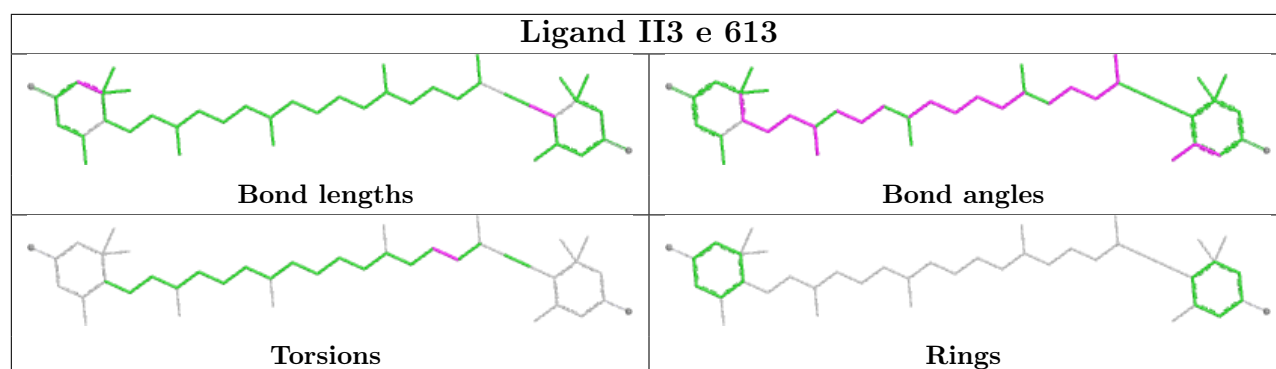


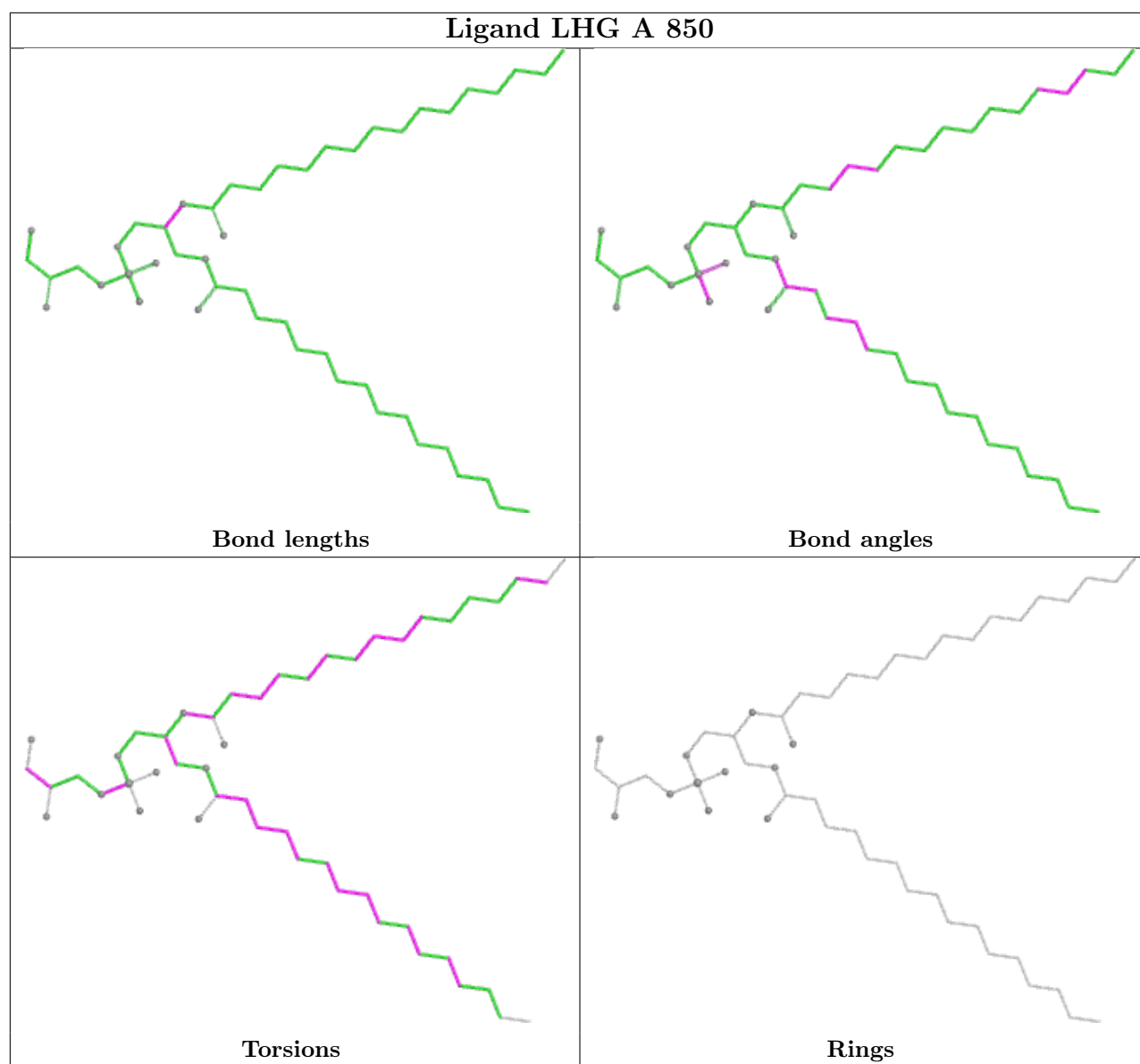
Ligand II0 b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 9 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

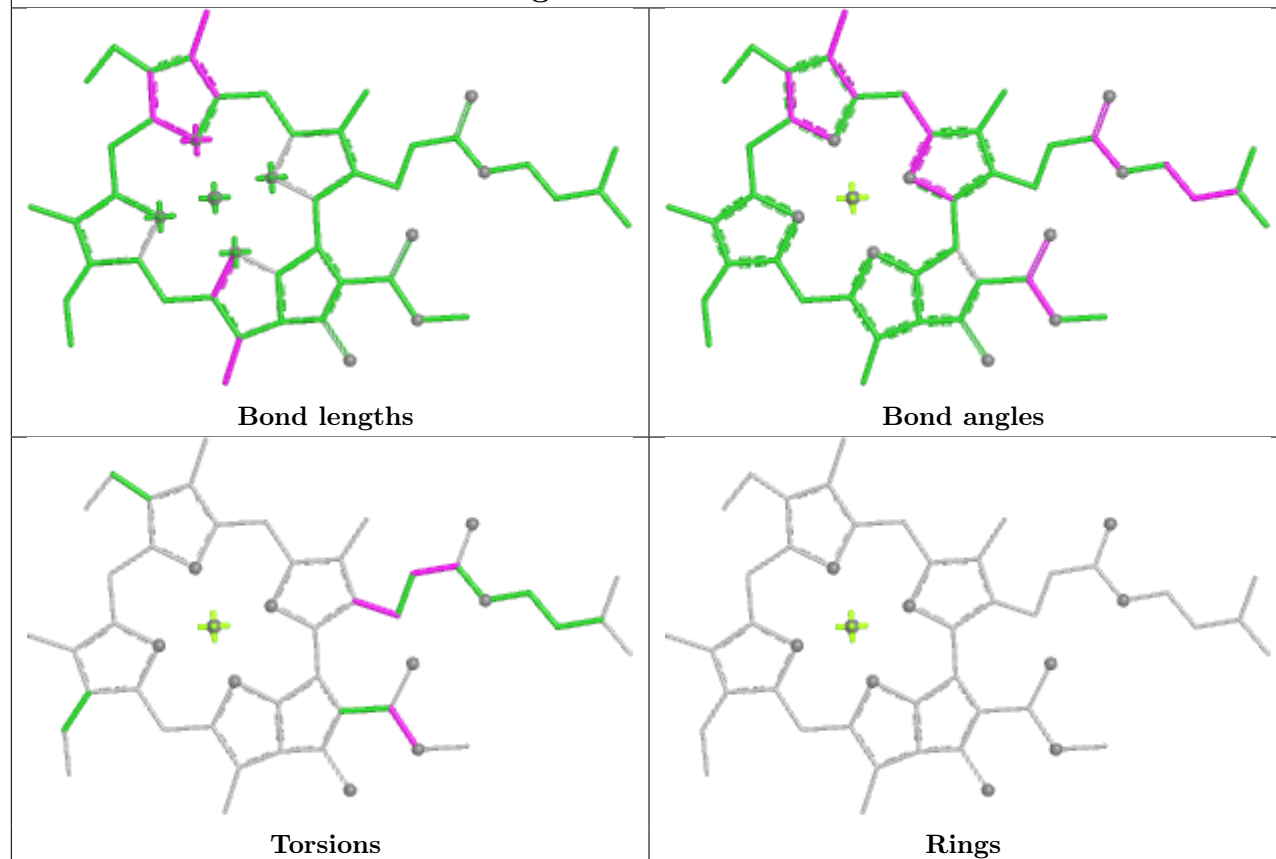
Ligand IHT 5 618	
	
Bond lengths	Bond angles
	
Torsions	Rings



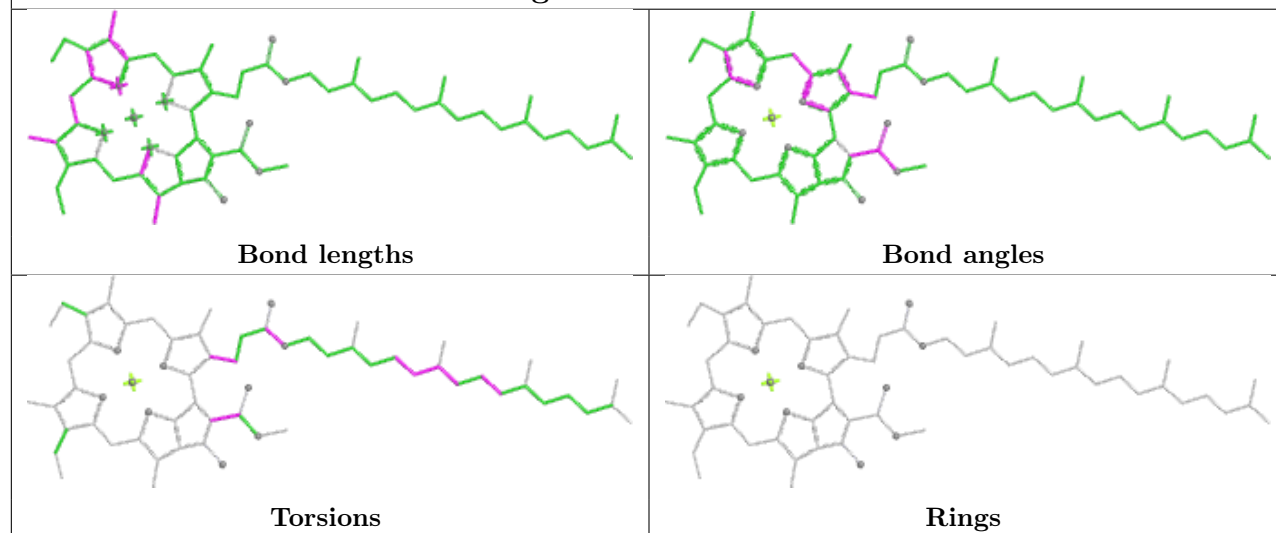


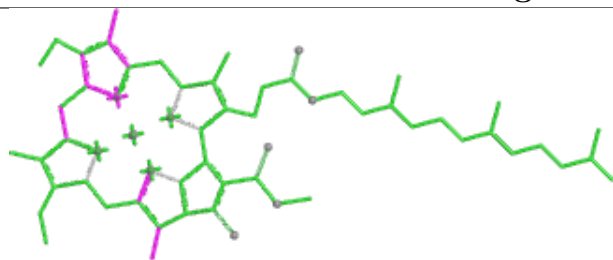


Ligand CLA A 807

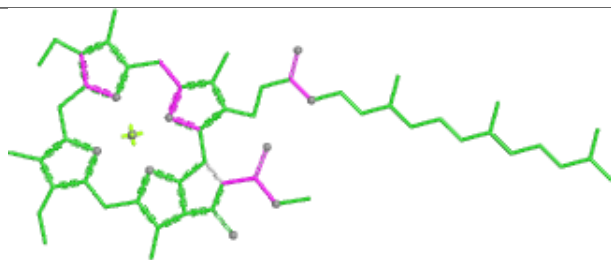


Ligand CLA A 841

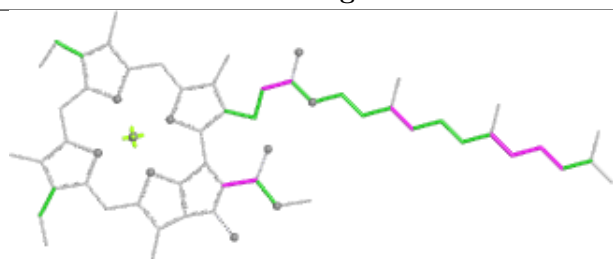


Ligand CLA B 822

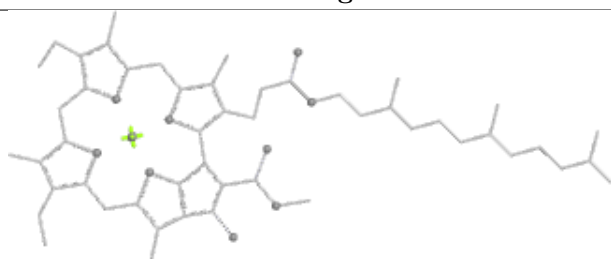
Bond lengths



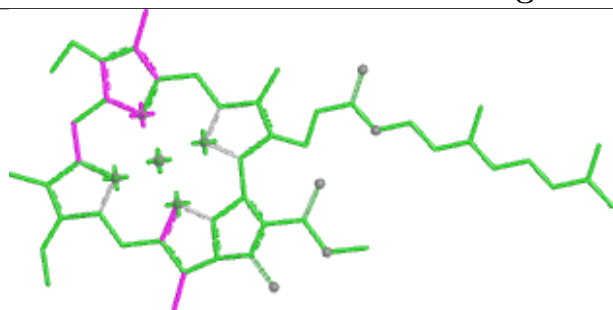
Bond angles



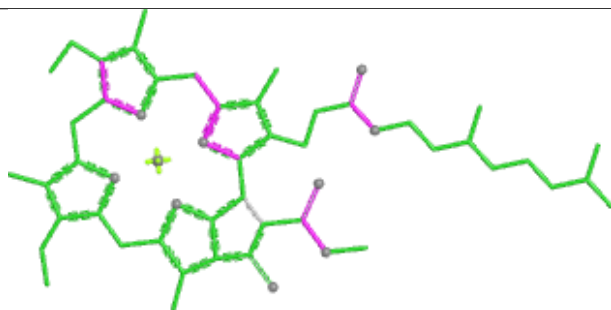
Torsions



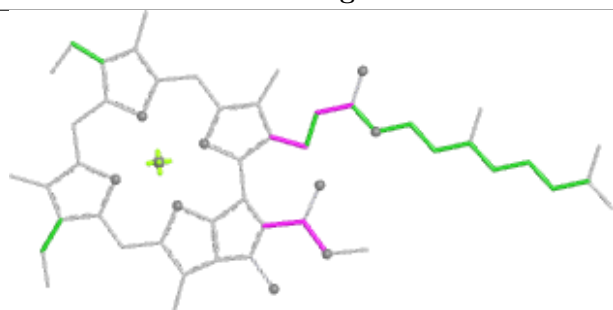
Rings

Ligand CLA Z 303

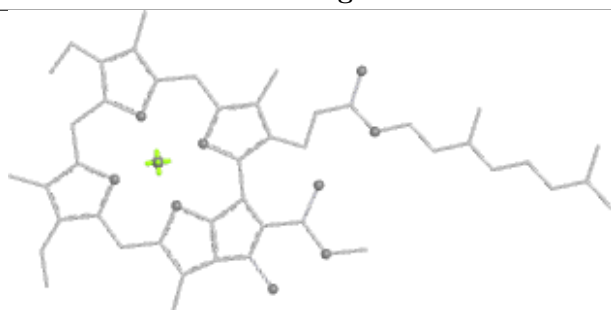
Bond lengths



Bond angles

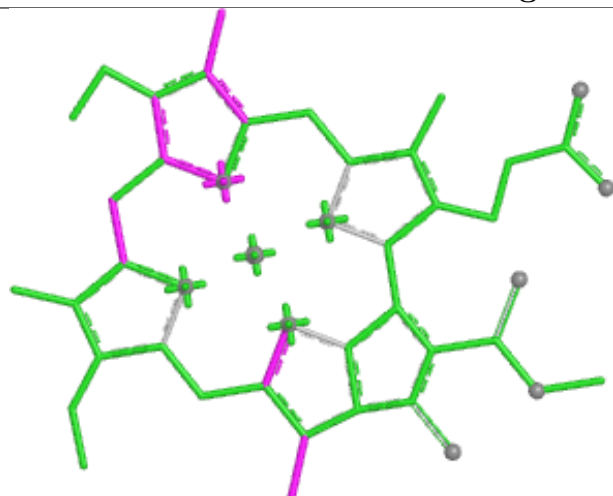


Torsions

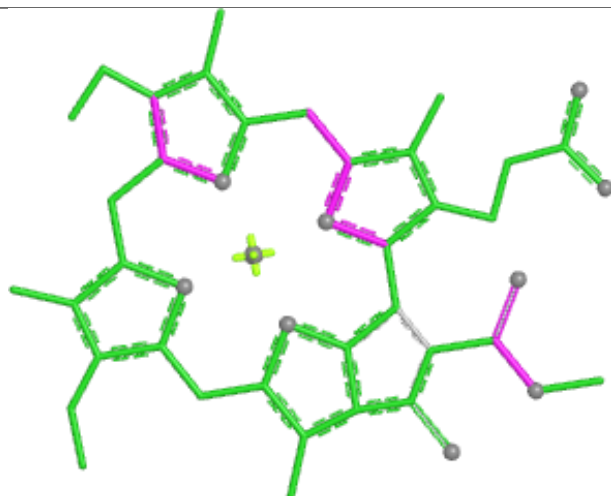


Rings

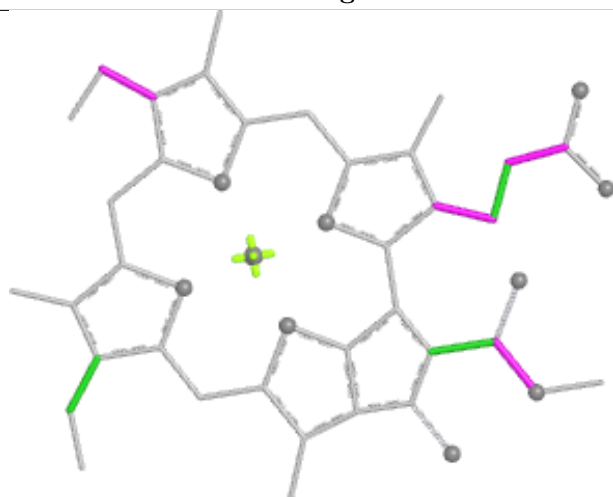
Ligand CLA c 605



Bond lengths



Bond angles

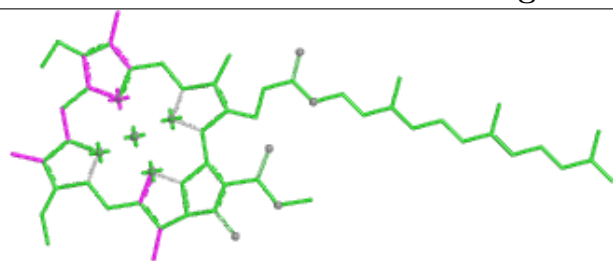


Torsions

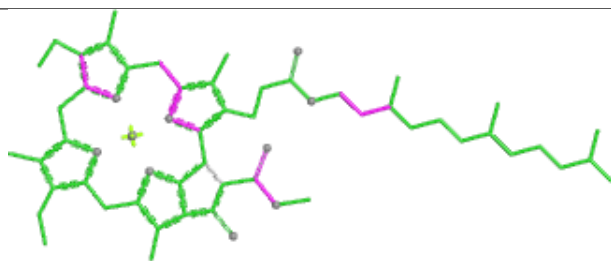


Rings

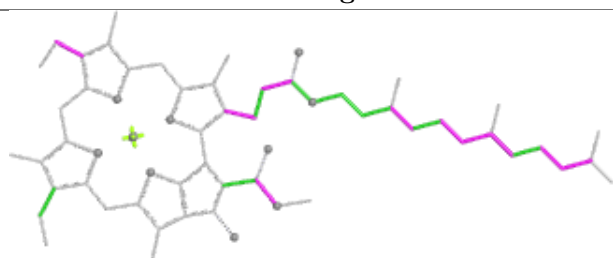
Ligand CLA 3 308



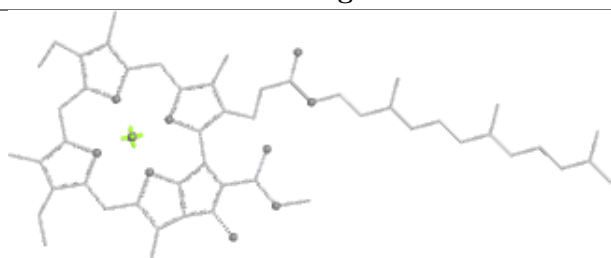
Bond lengths



Bond angles

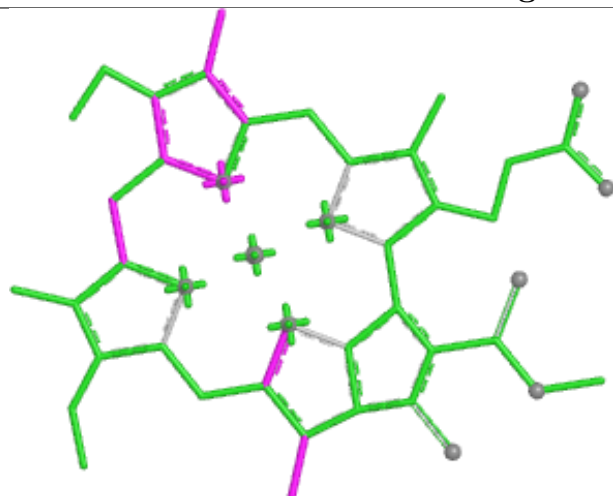


Torsions

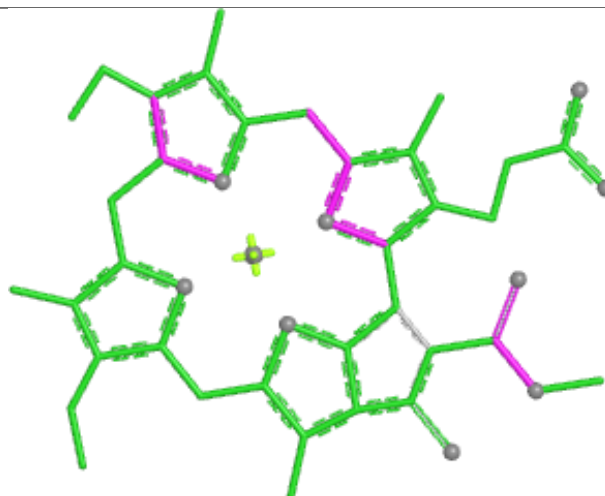


Rings

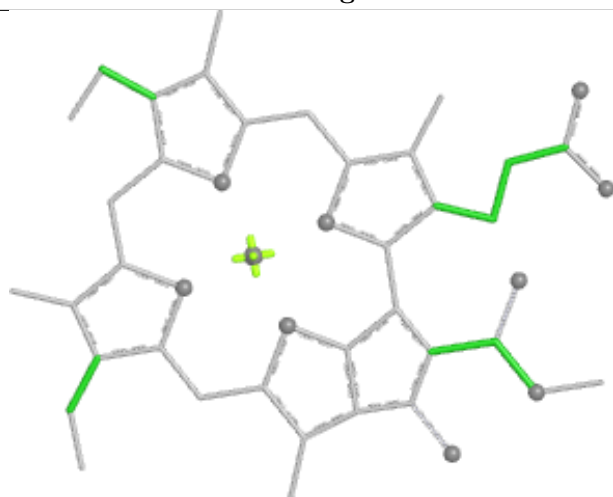
Ligand CLA 9 306



Bond lengths



Bond angles

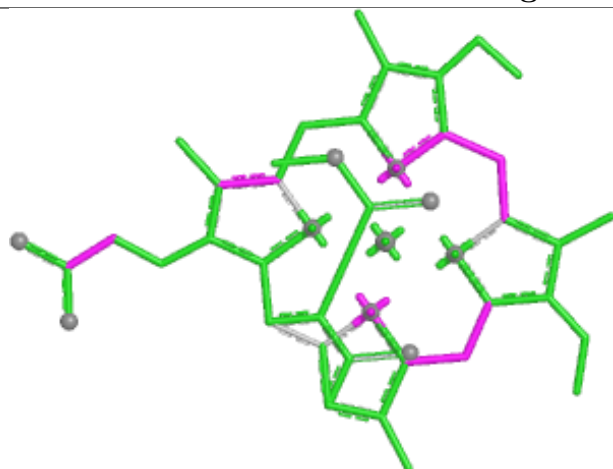


Torsions

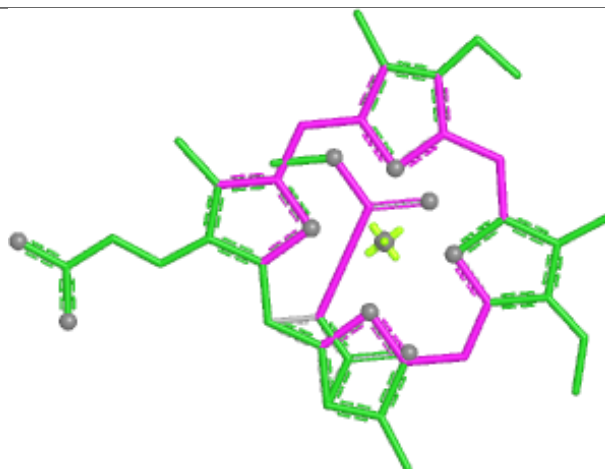


Rings

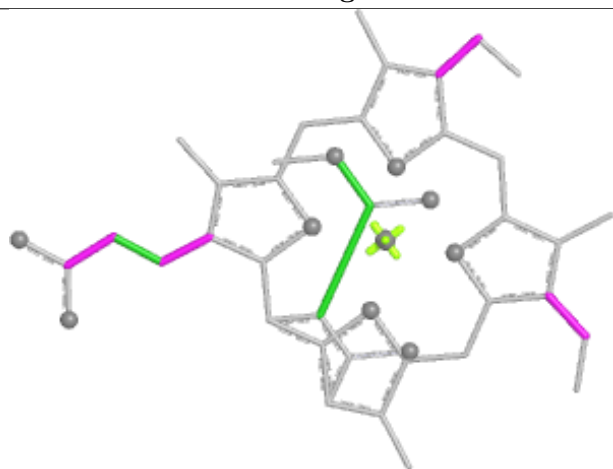
Ligand KC2 4 605



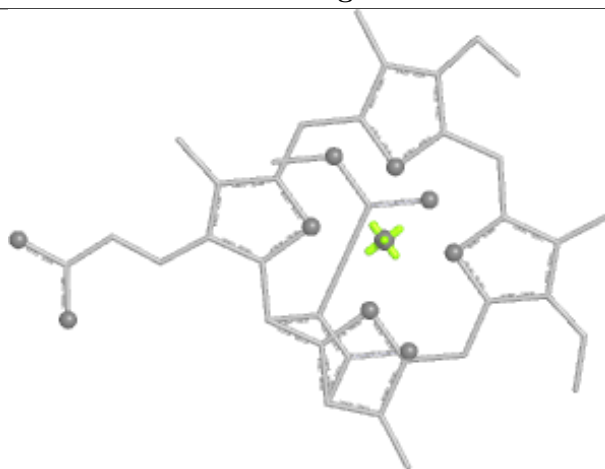
Bond lengths



Bond angles

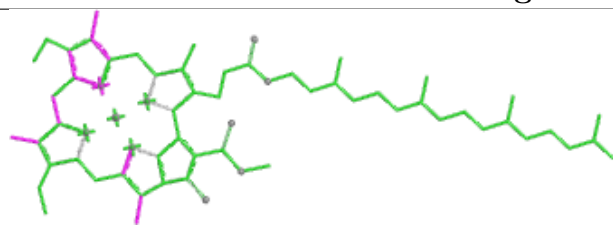


Torsions

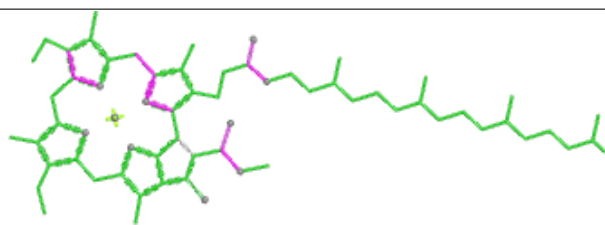


Rings

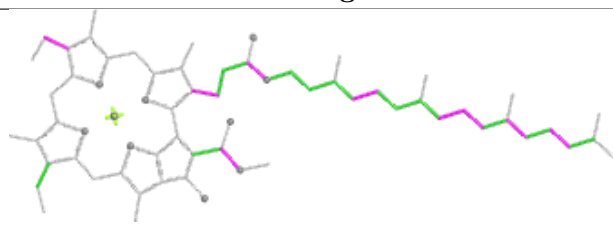
Ligand CLA B 823



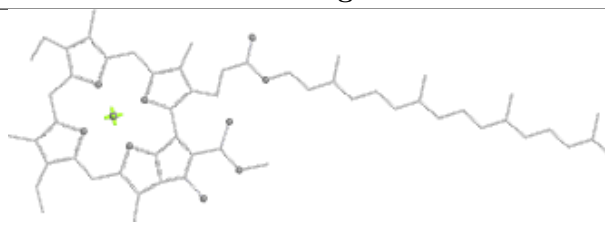
Bond lengths



Bond angles

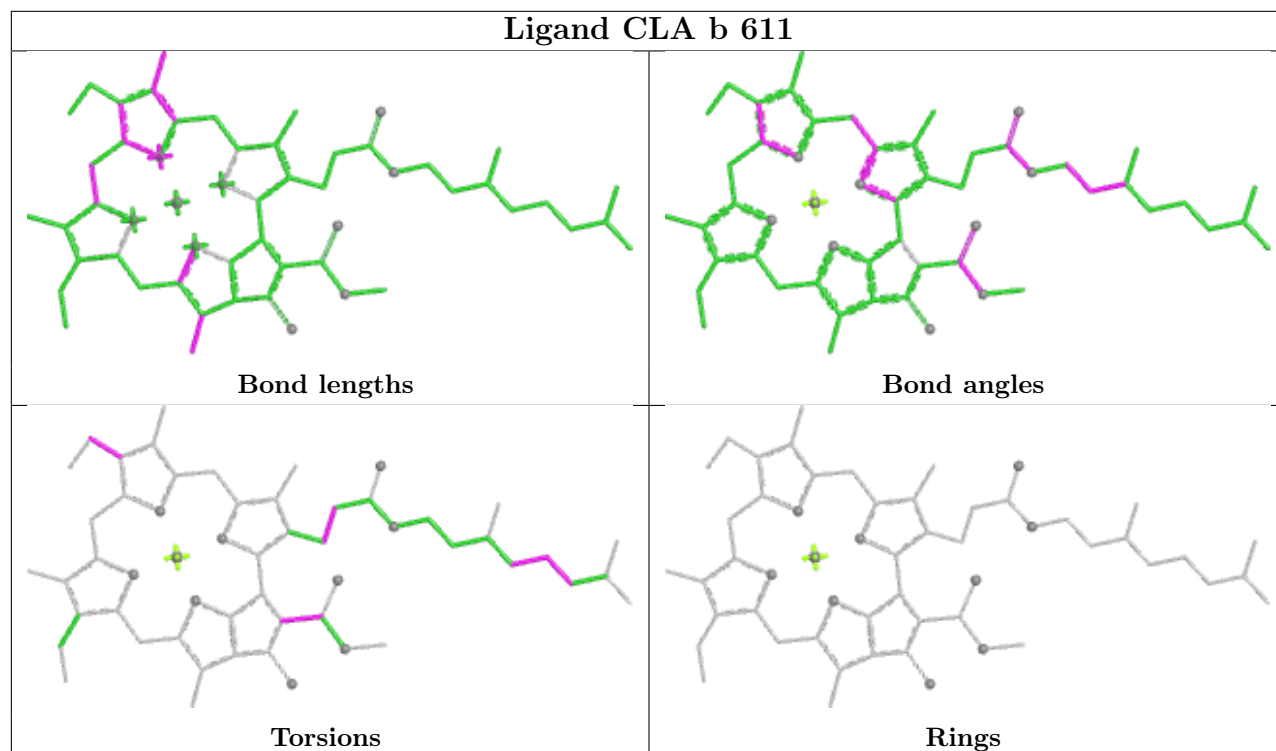


Torsions

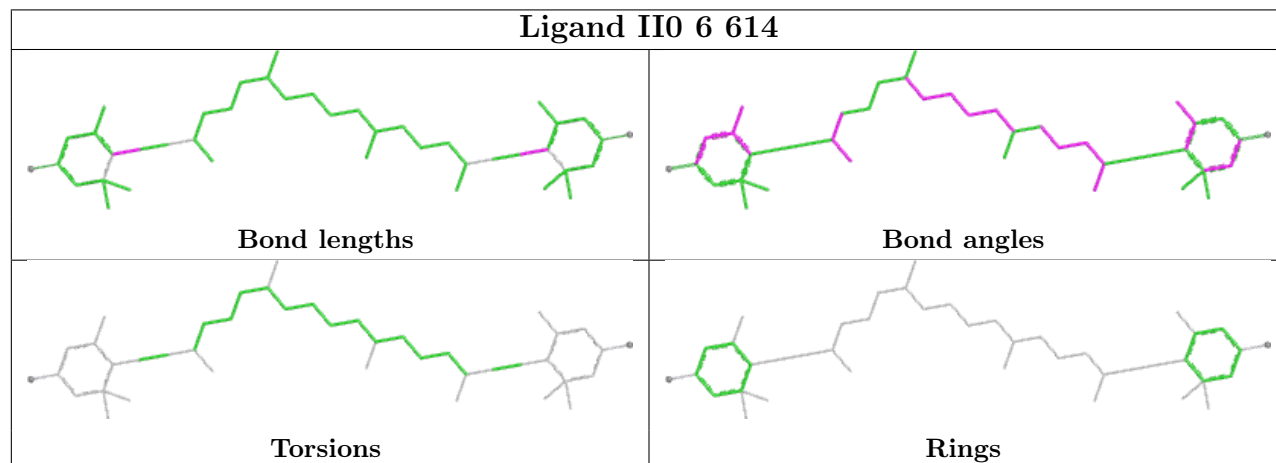


Rings

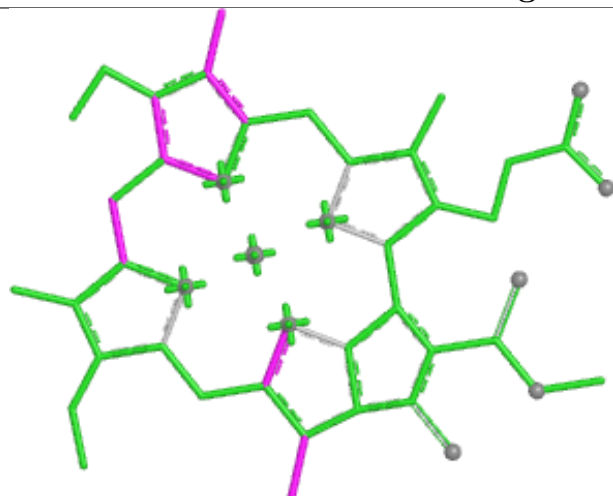
Ligand CLA b 611



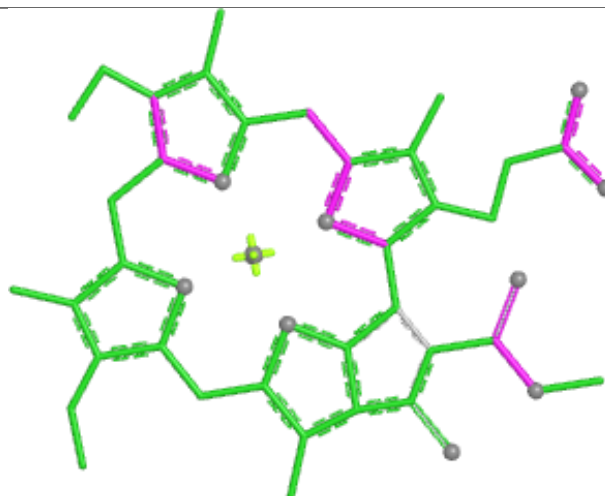
Ligand II0 6 614



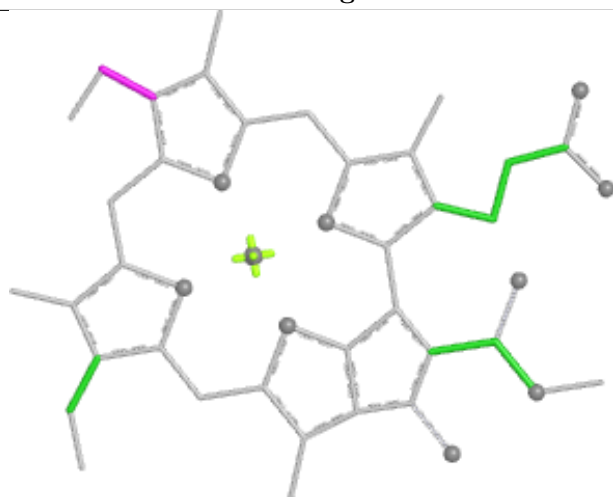
Ligand CLA 1 604



Bond lengths



Bond angles

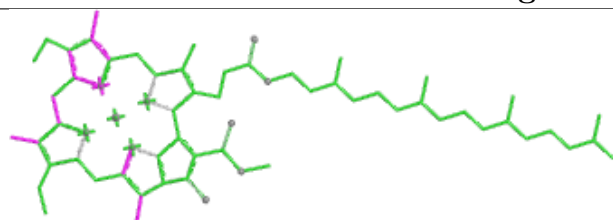


Torsions

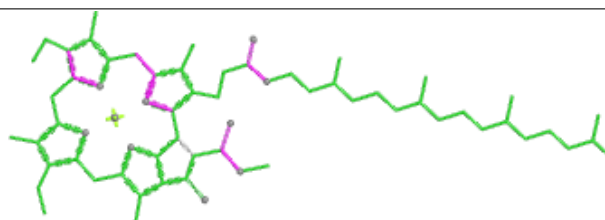


Rings

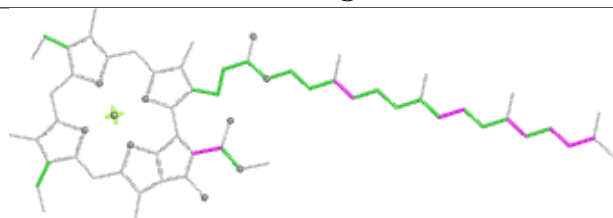
Ligand CLA a 606



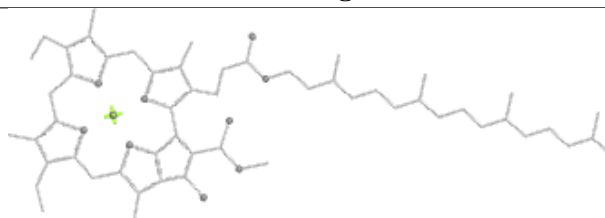
Bond lengths



Bond angles

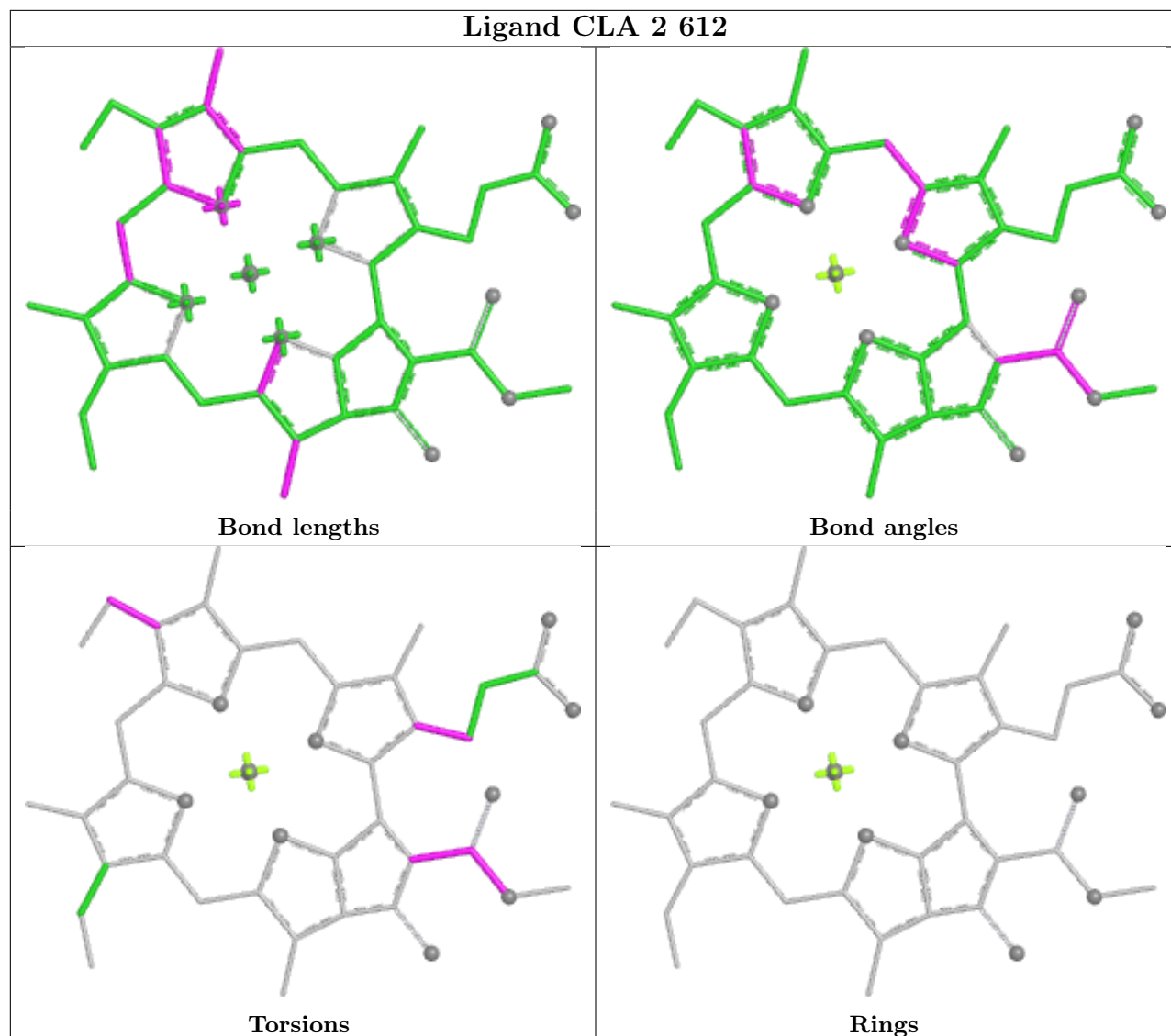


Torsions

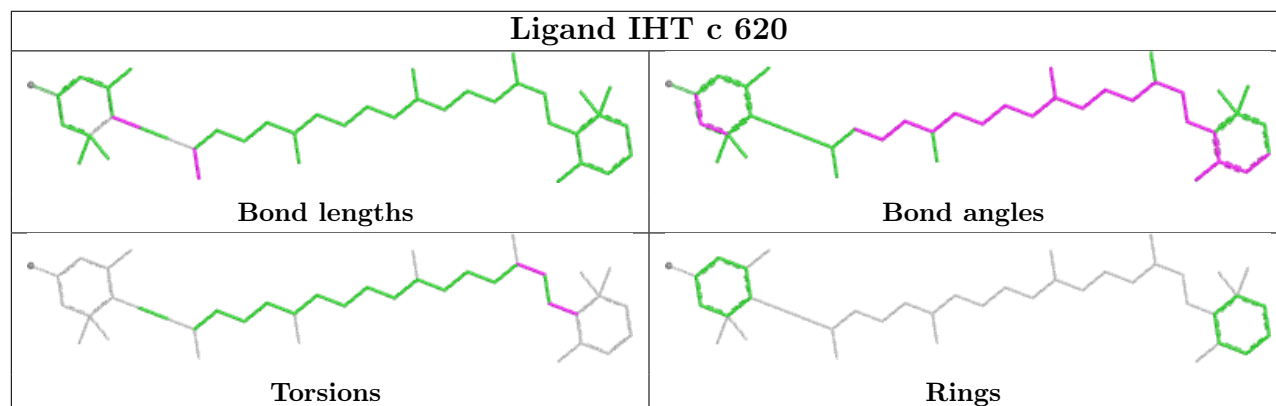


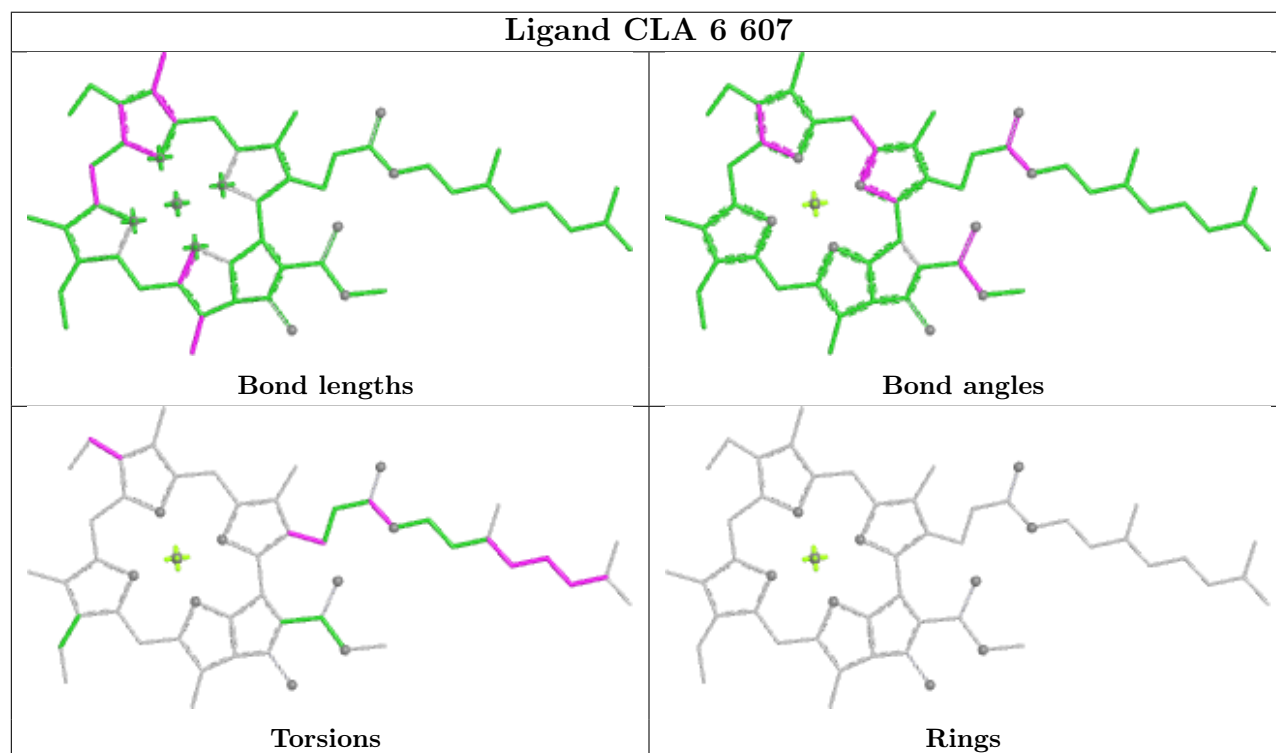
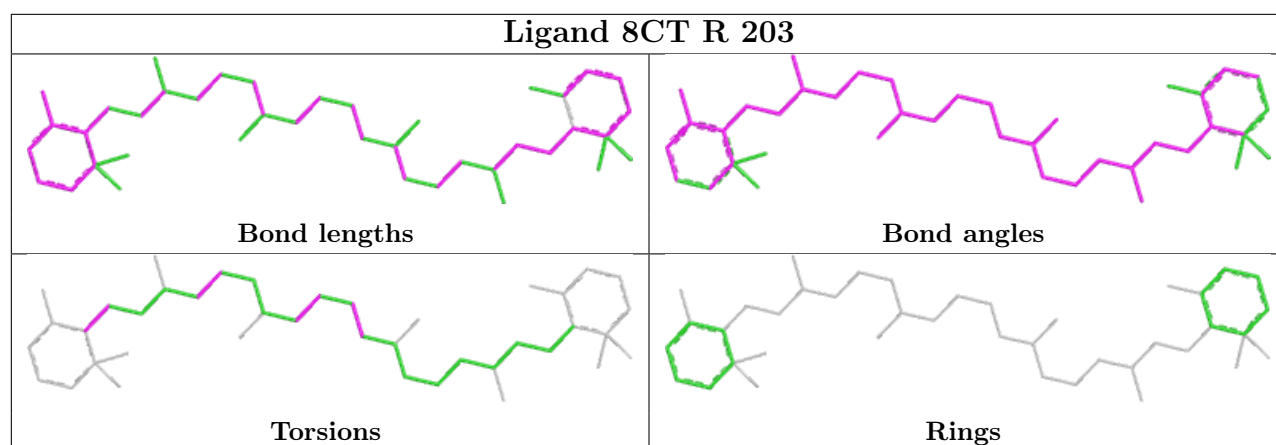
Rings

Ligand CLA 2 612

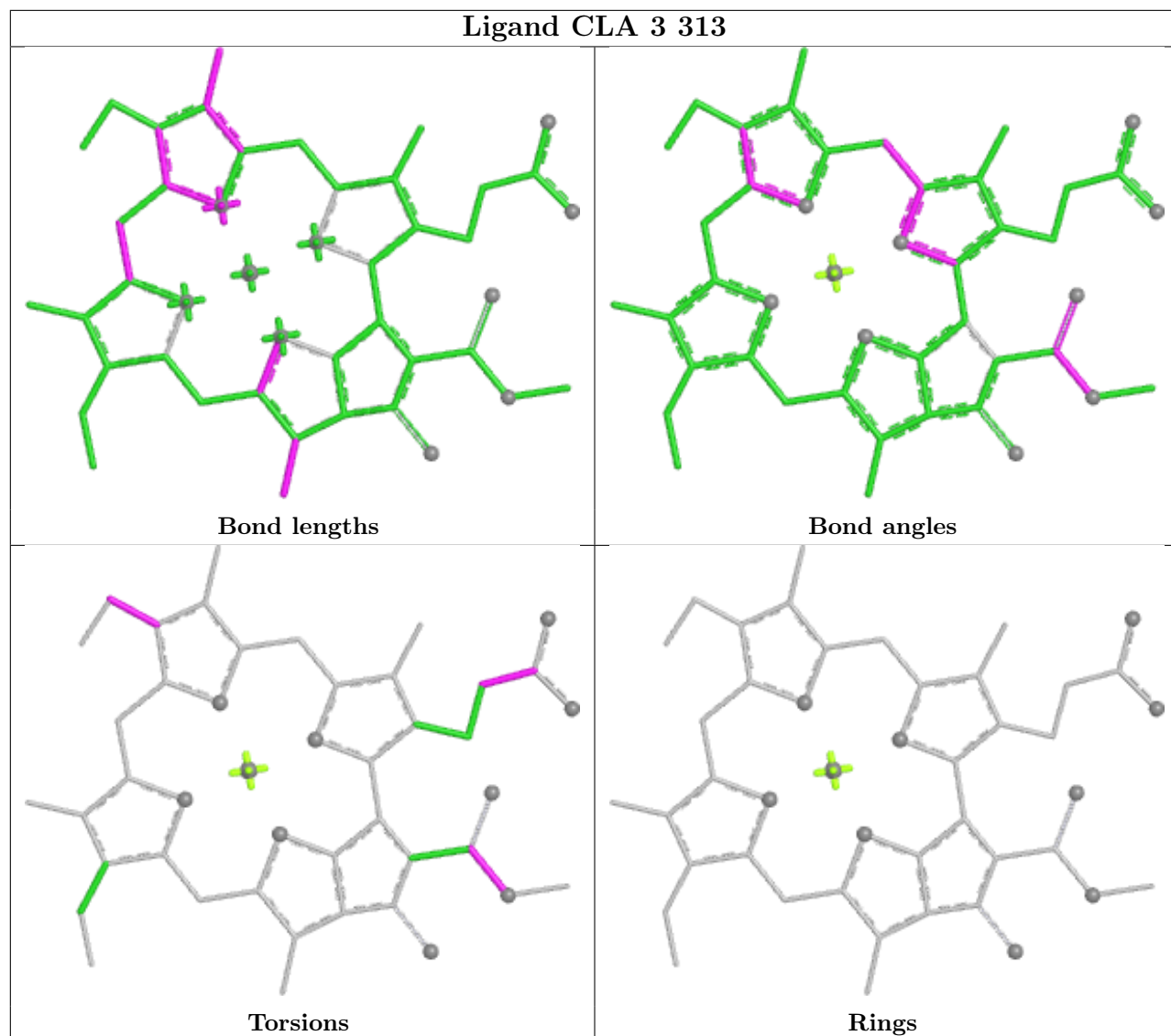


Ligand IHT c 620

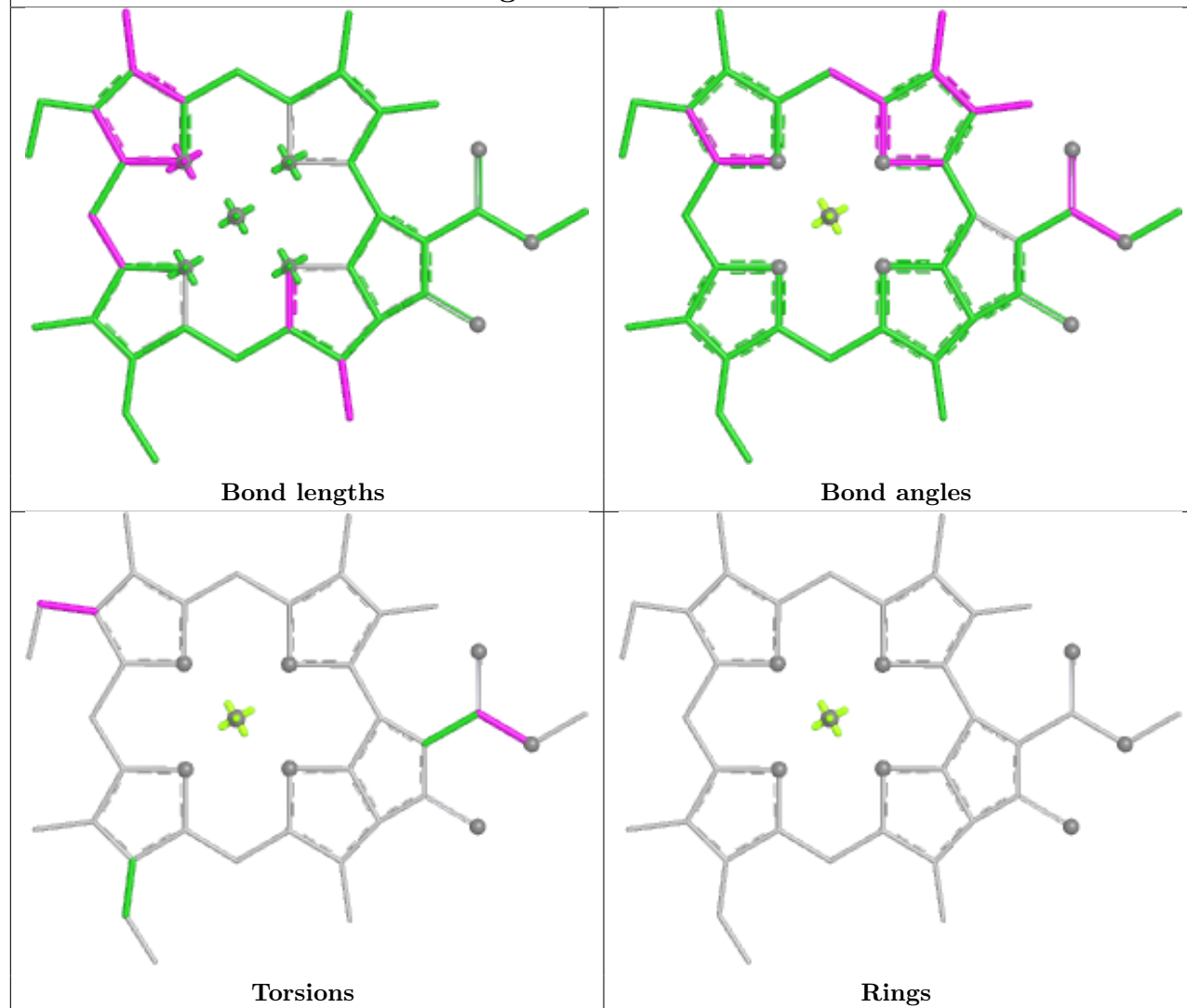




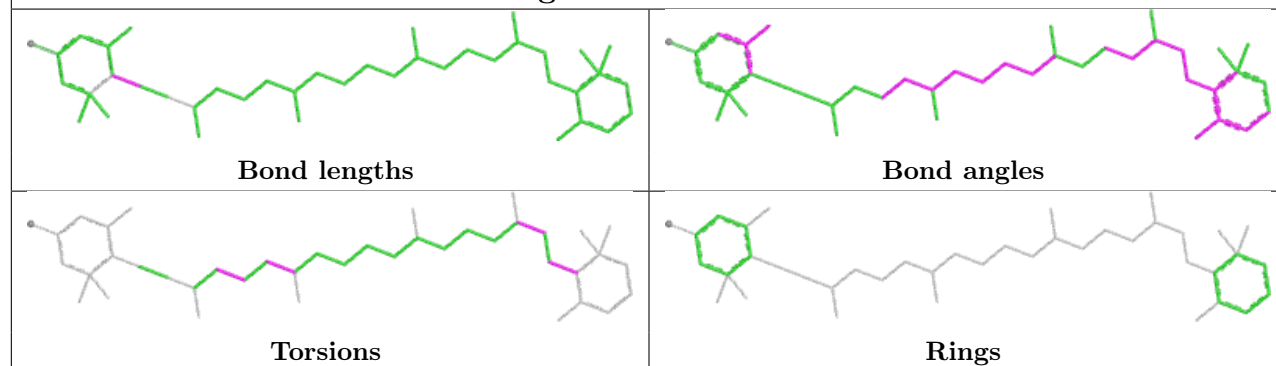
Ligand CLA 3 313

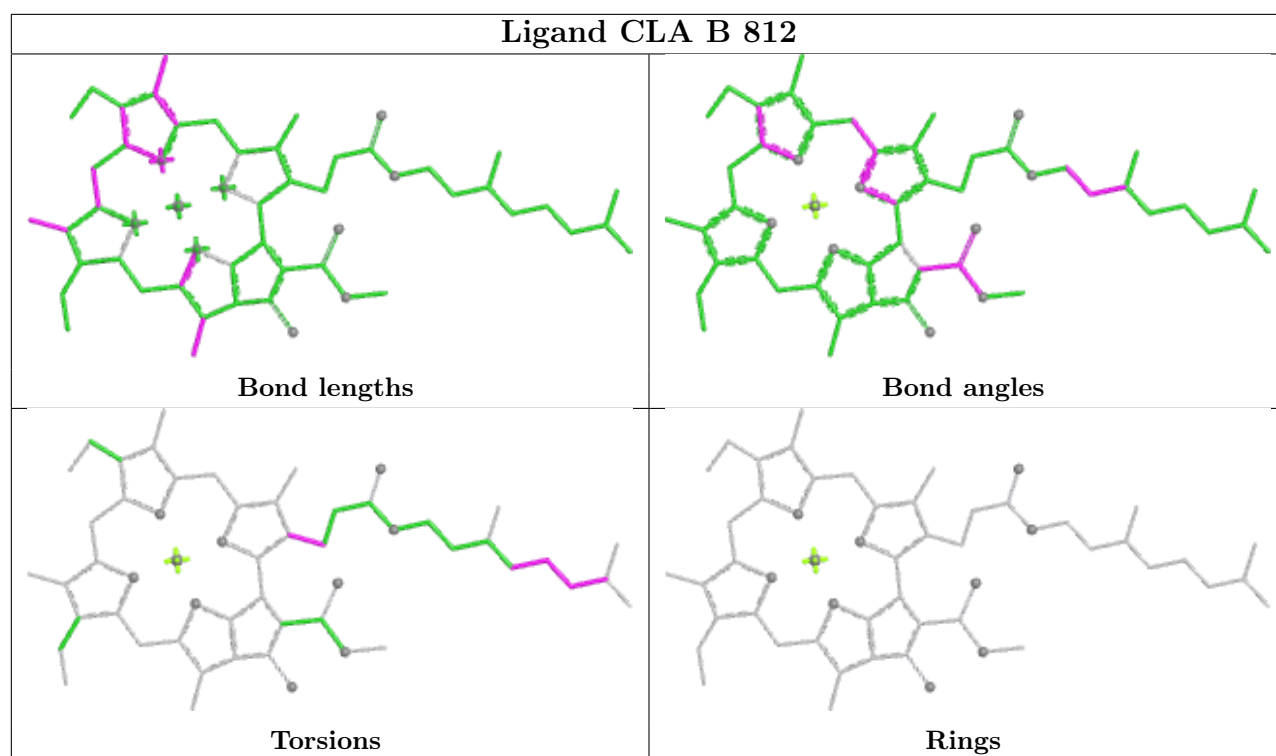


Ligand CLA e 608

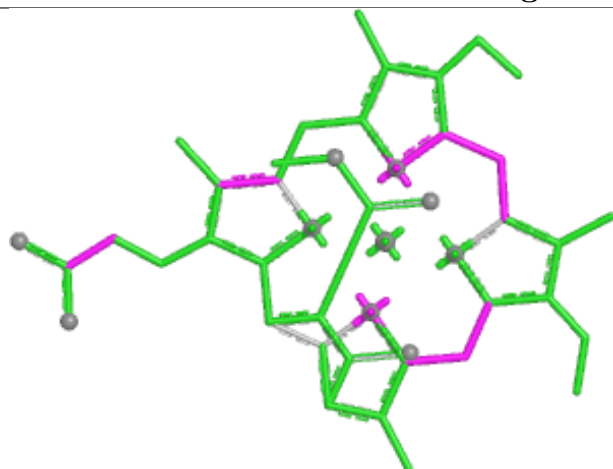


Ligand IHT Z 301

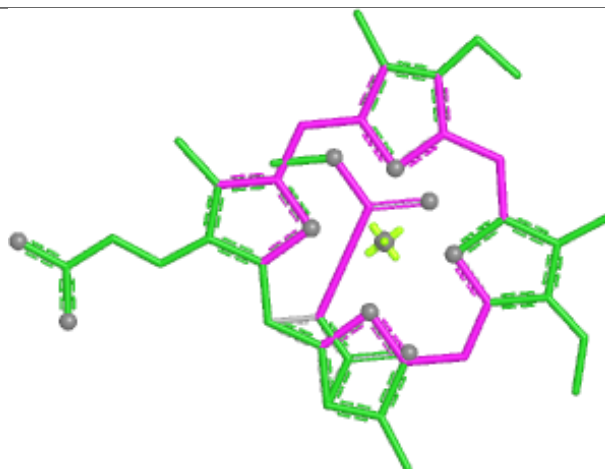




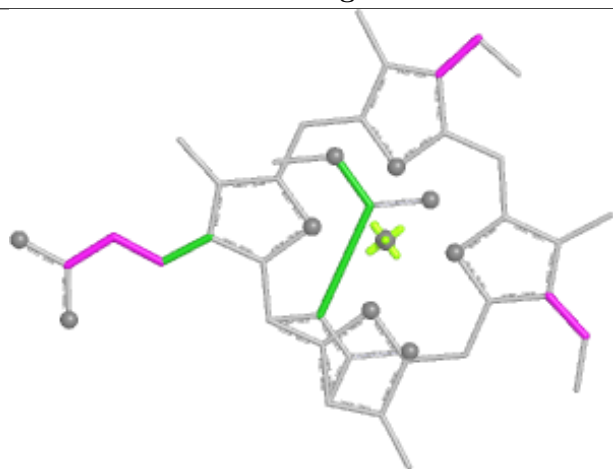
Ligand KC2 e 609



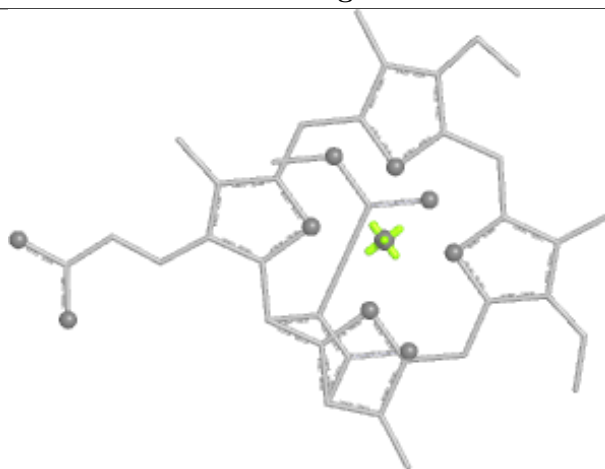
Bond lengths



Bond angles

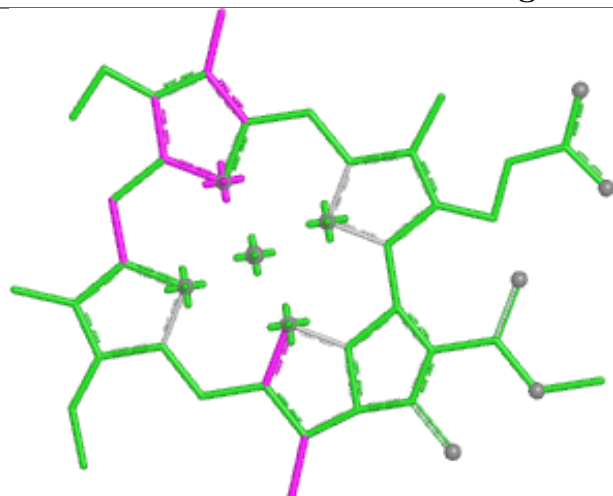


Torsions

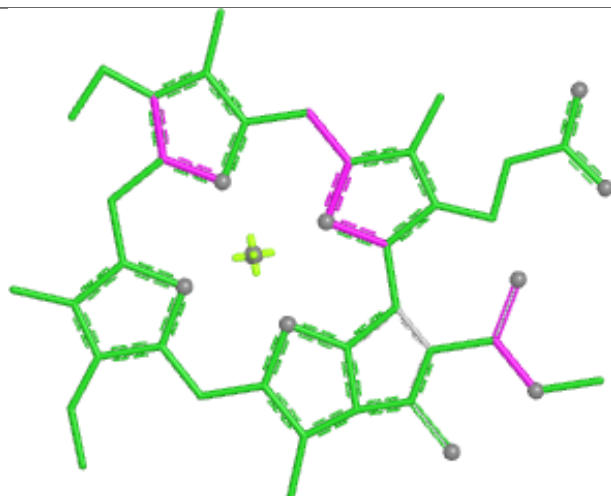


Rings

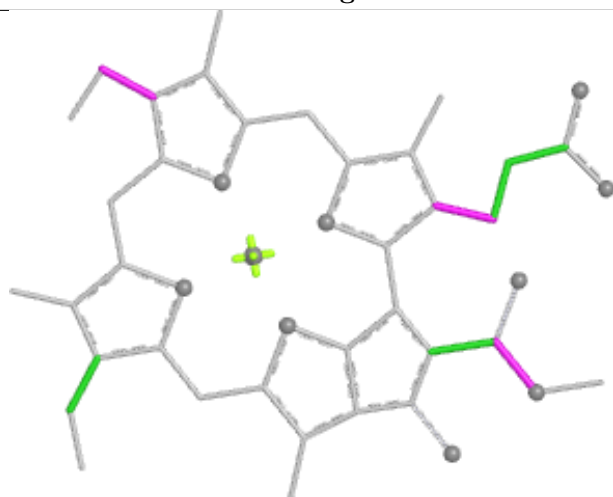
Ligand CLA 9 314



Bond lengths



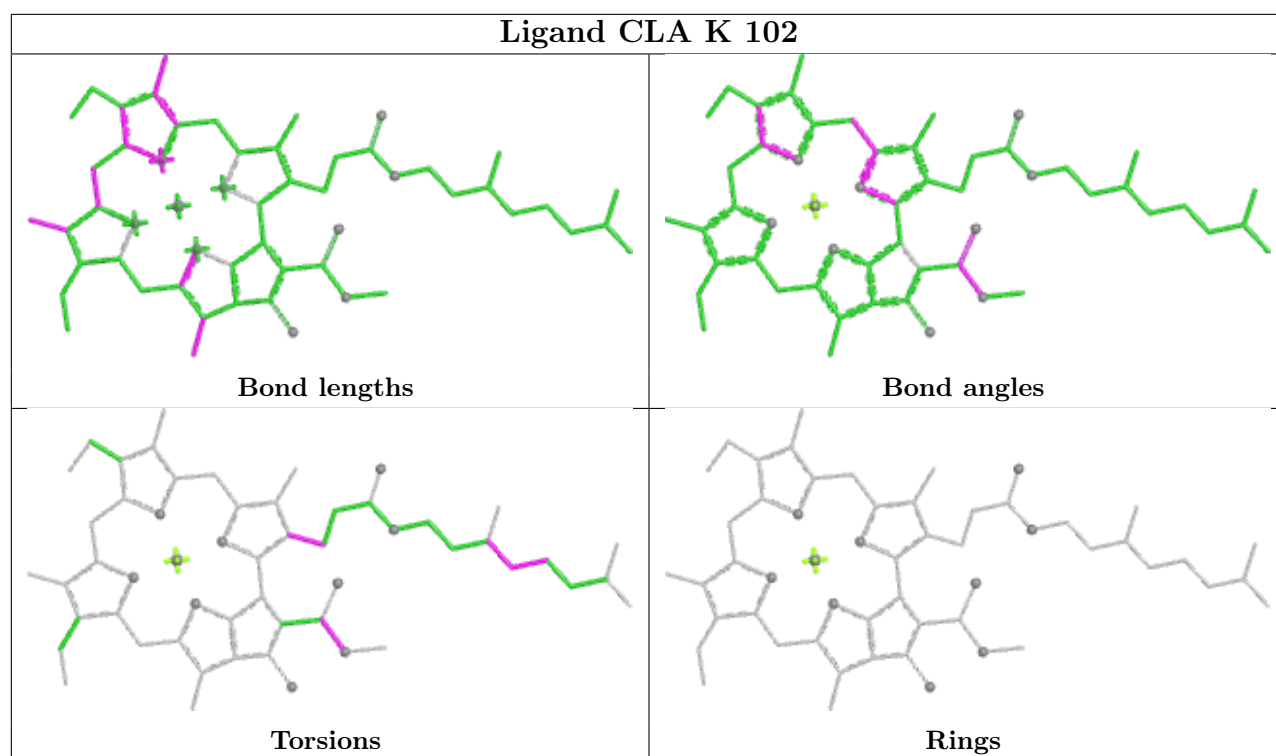
Bond angles



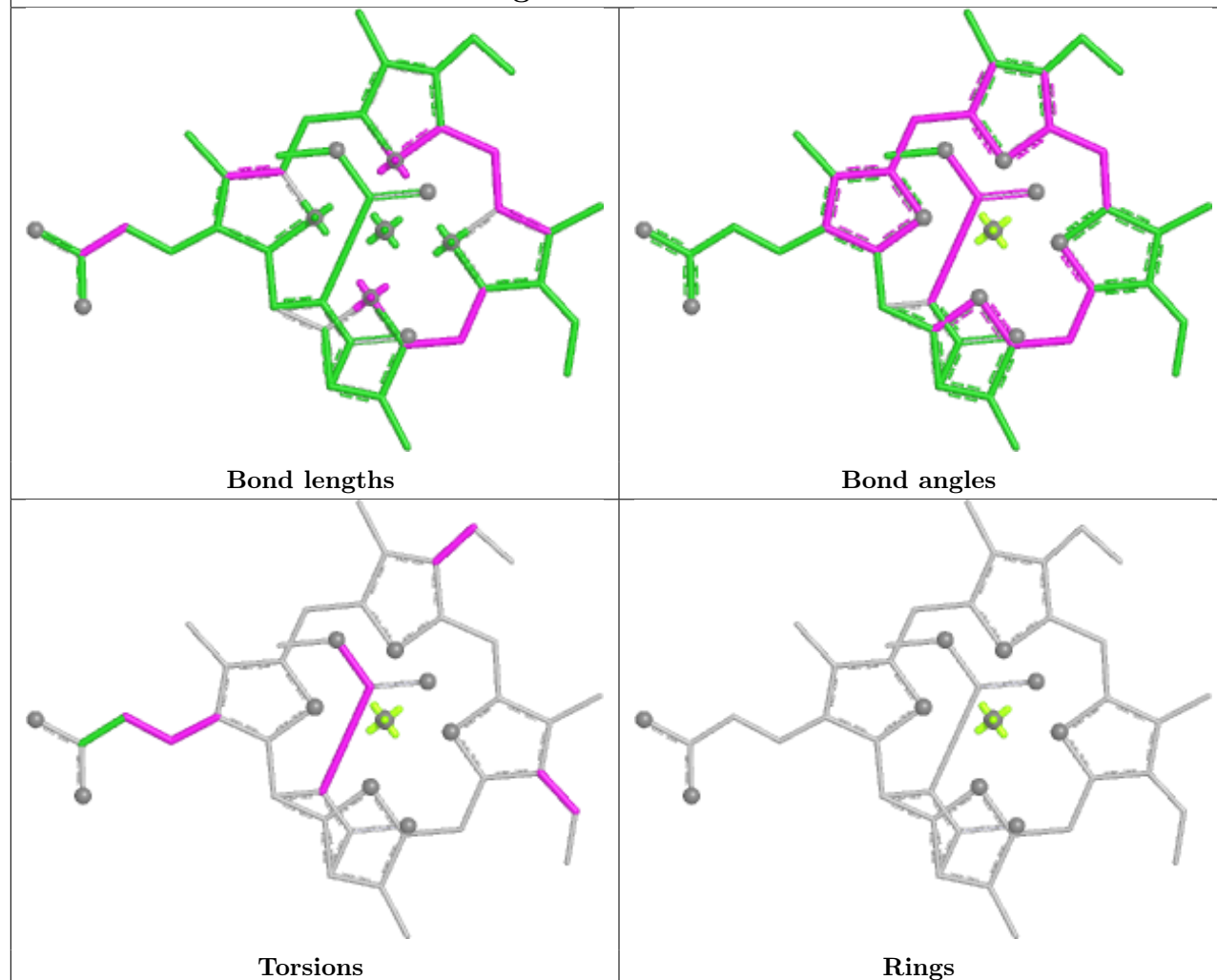
Torsions



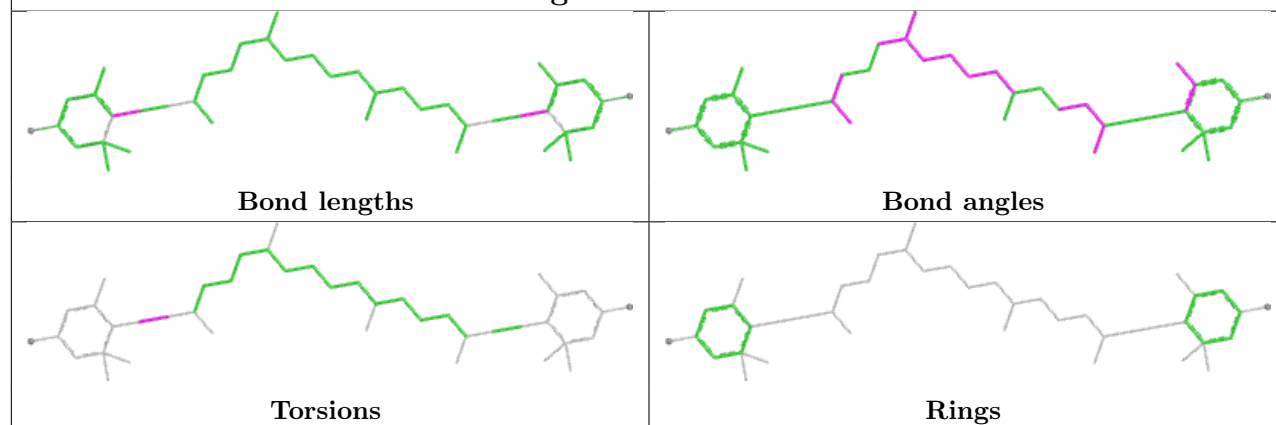
Rings



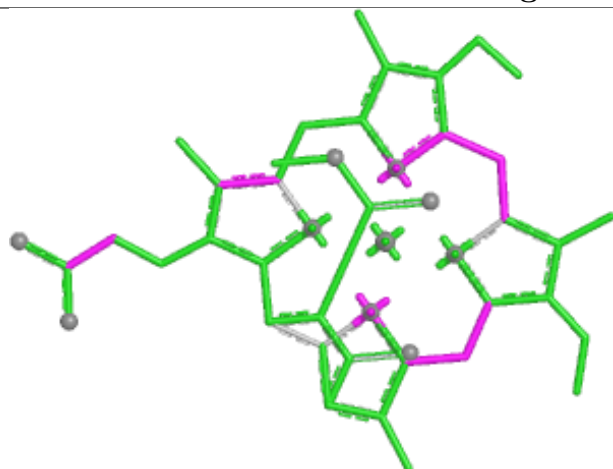
Ligand KC2 2 610



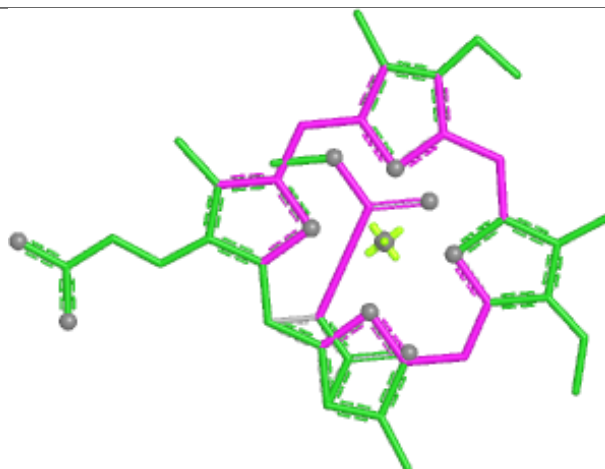
Ligand II0 3 315



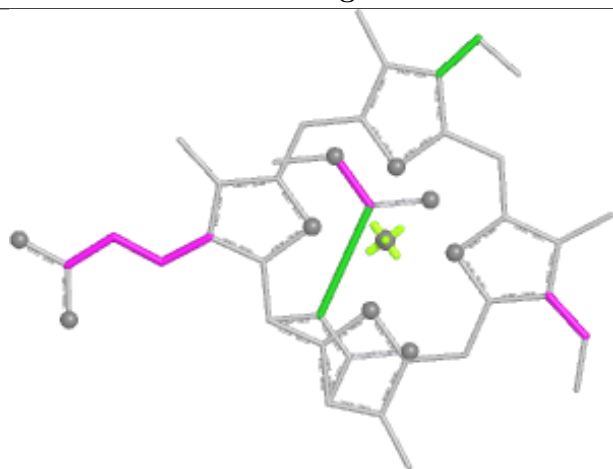
Ligand KC2 7 310



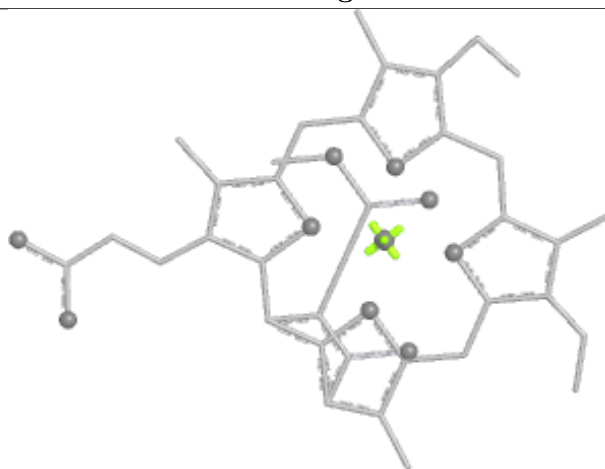
Bond lengths



Bond angles

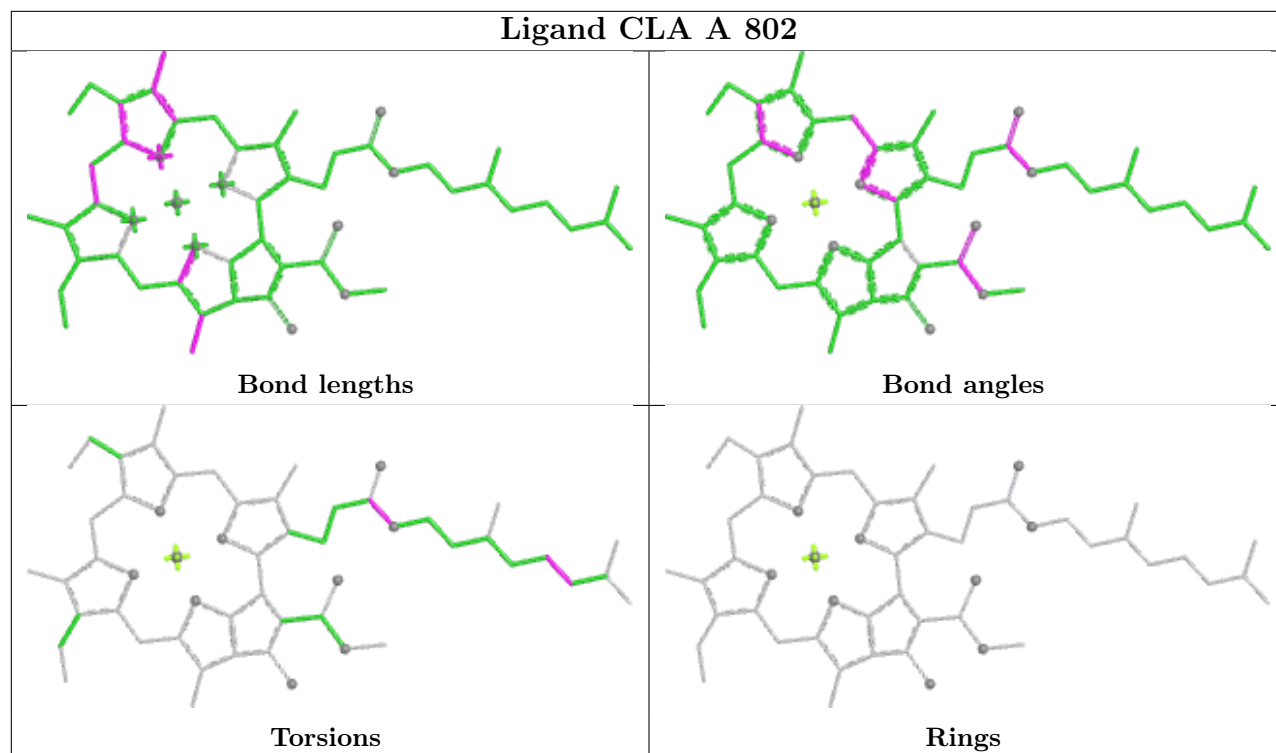


Torsions

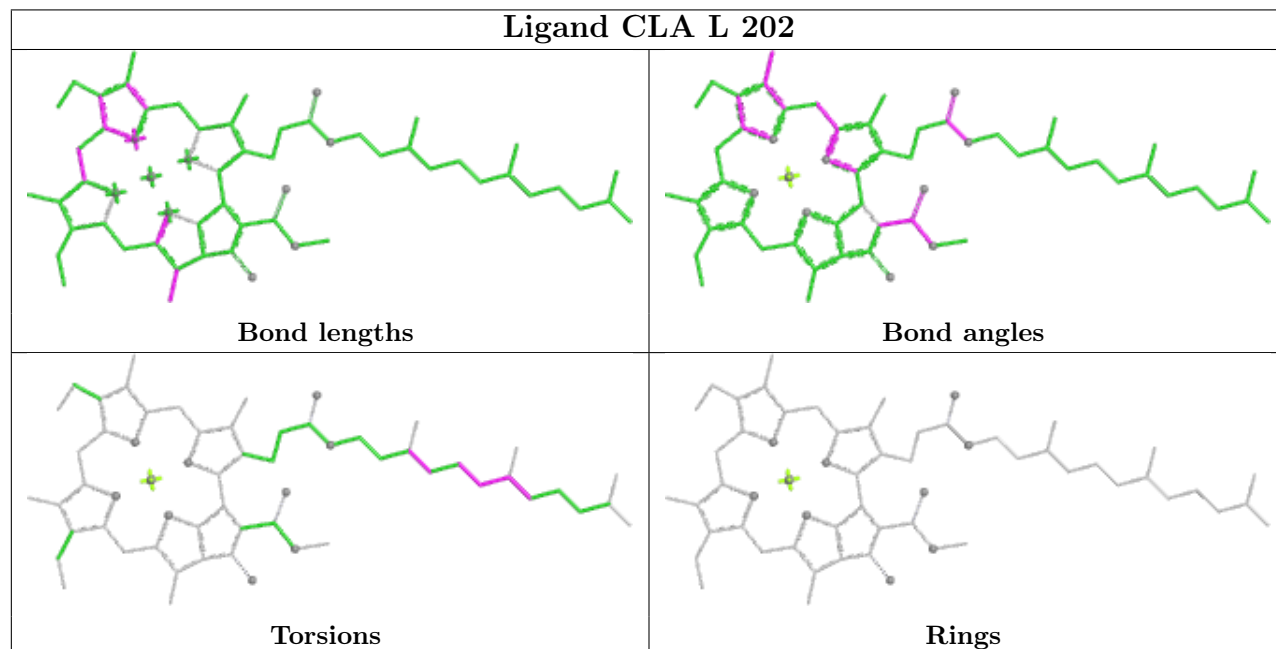


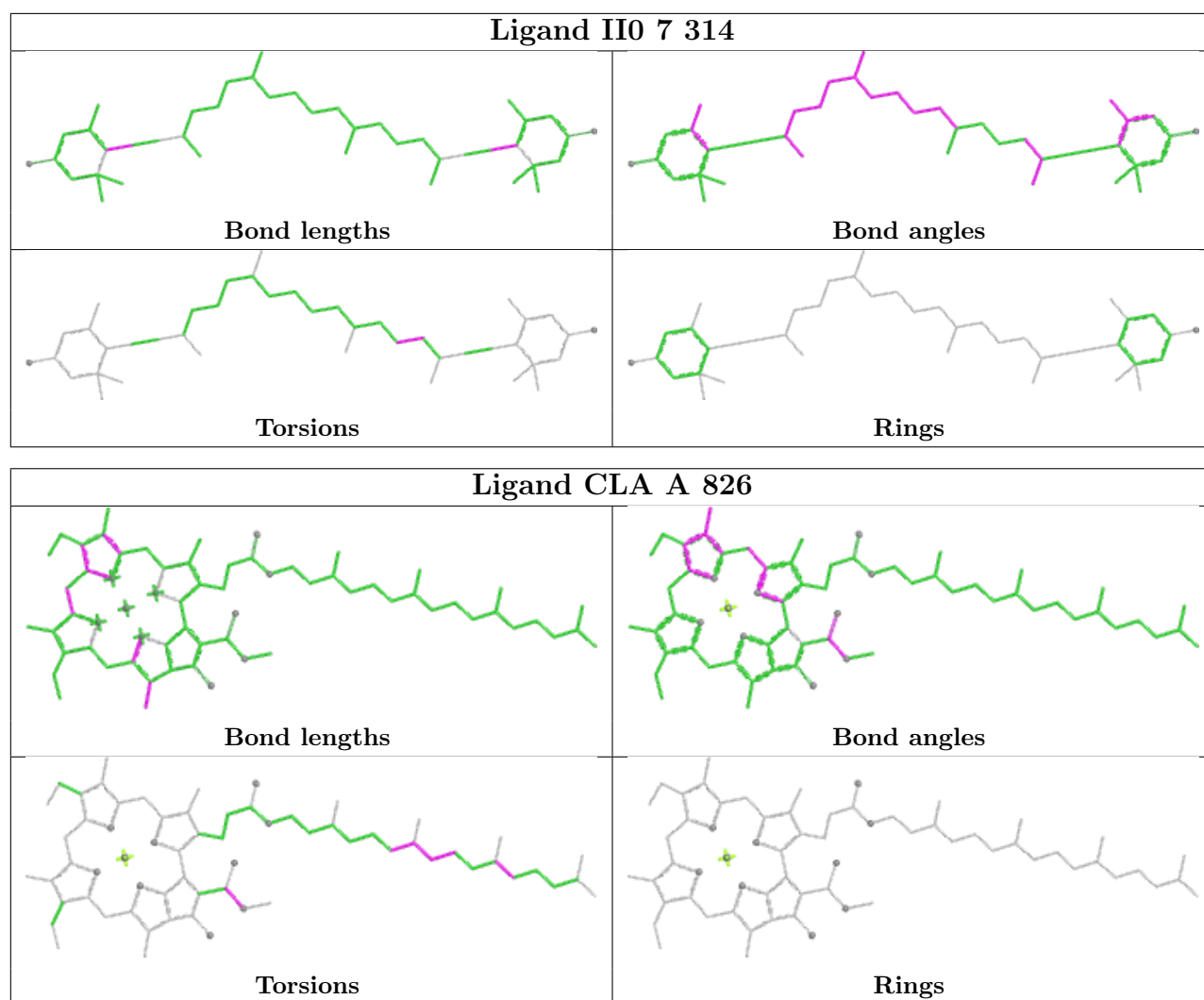
Rings

Ligand CLA A 802

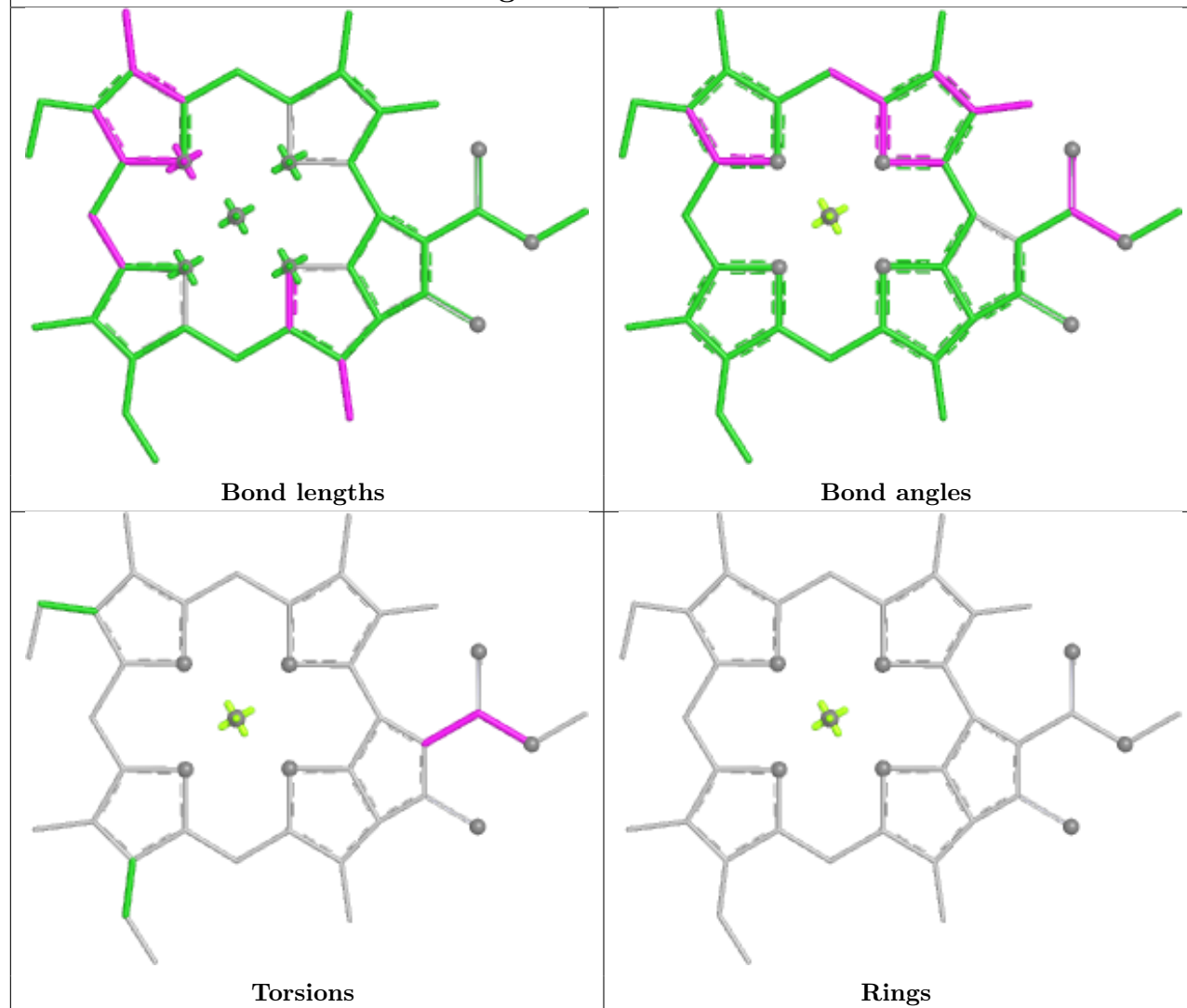


Ligand CLA L 202

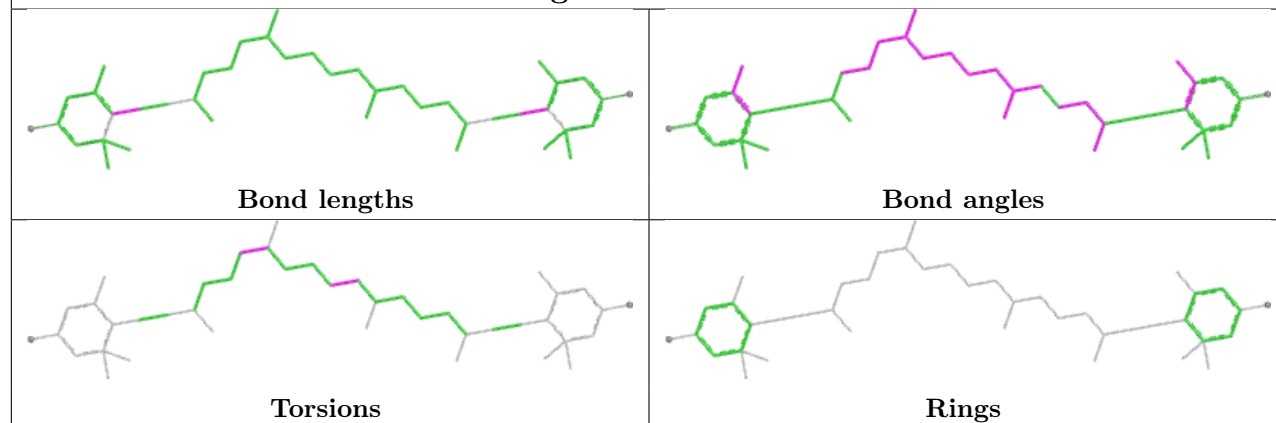


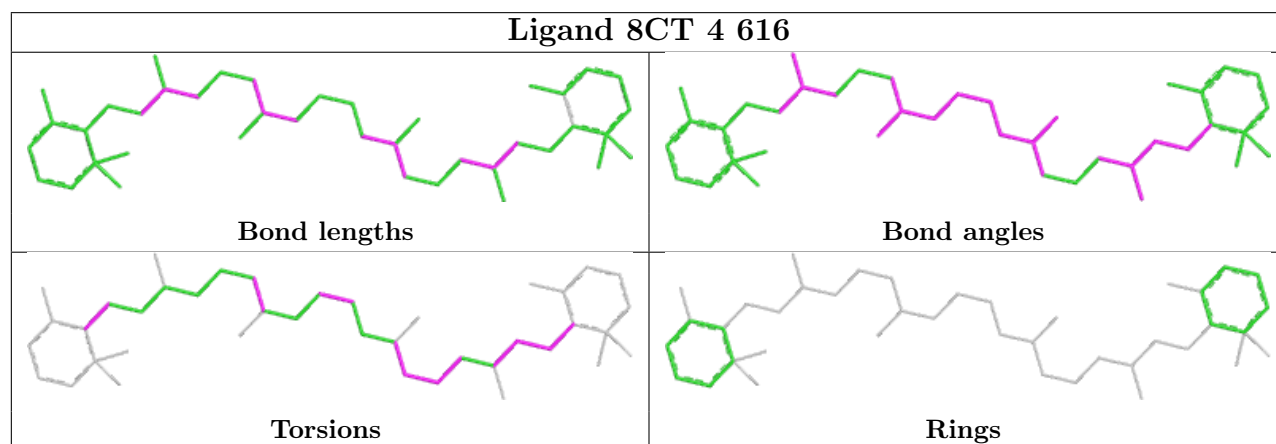
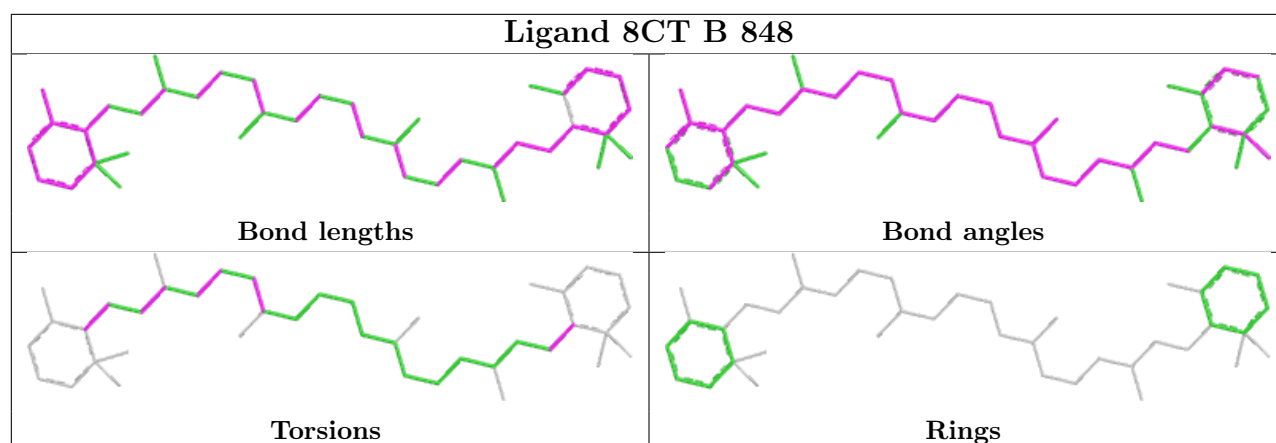


Ligand CLA 9 312

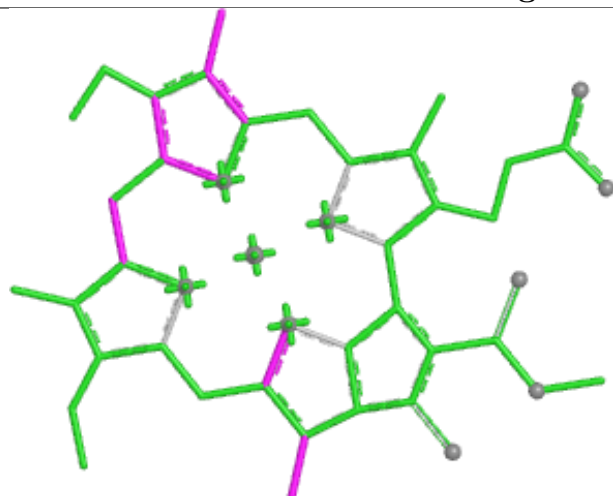


Ligand II0 7 317

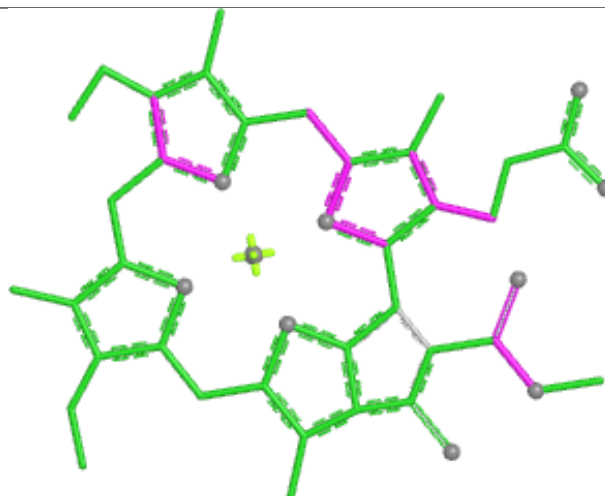




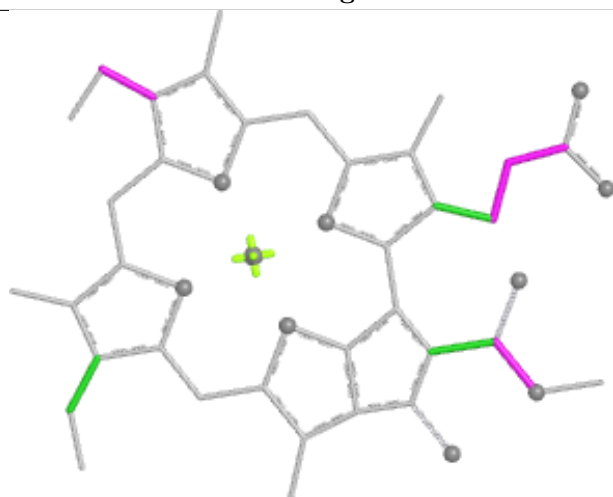
Ligand CLA 1 601



Bond lengths



Bond angles

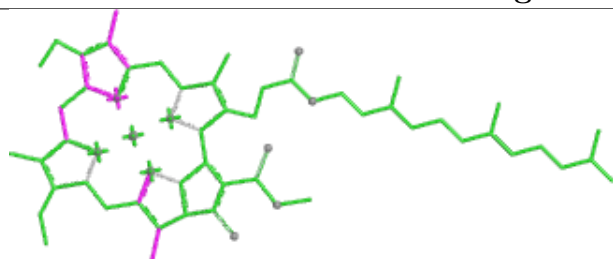


Torsions

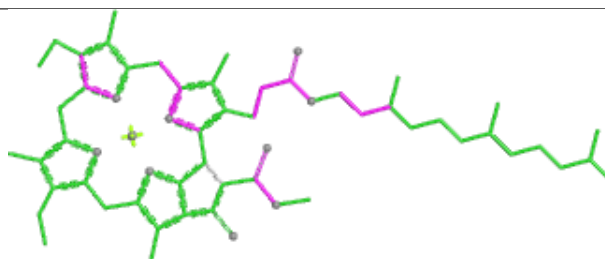


Rings

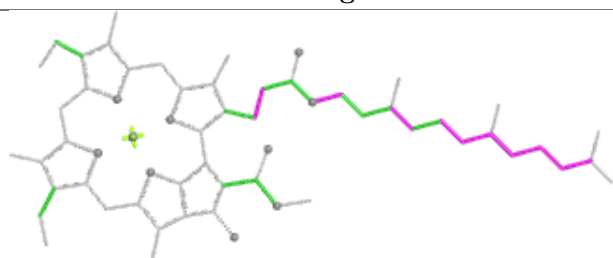
Ligand CLA B 820



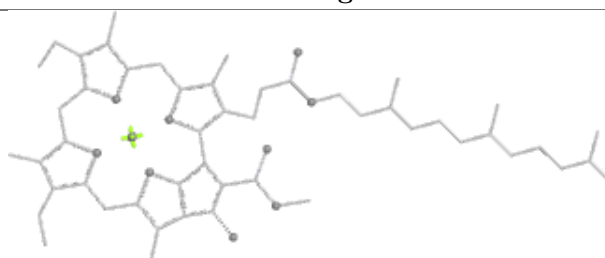
Bond lengths



Bond angles

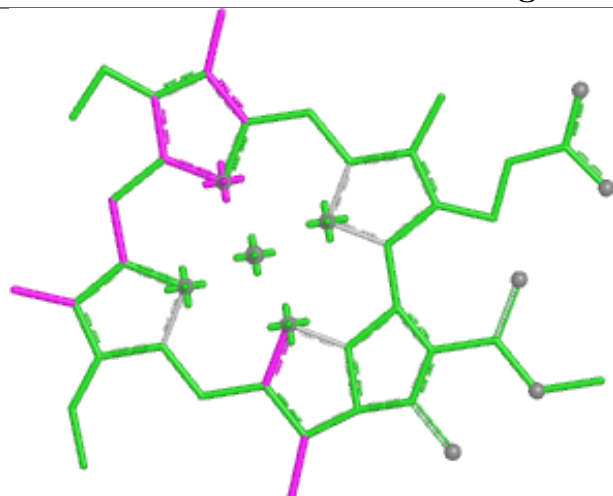


Torsions

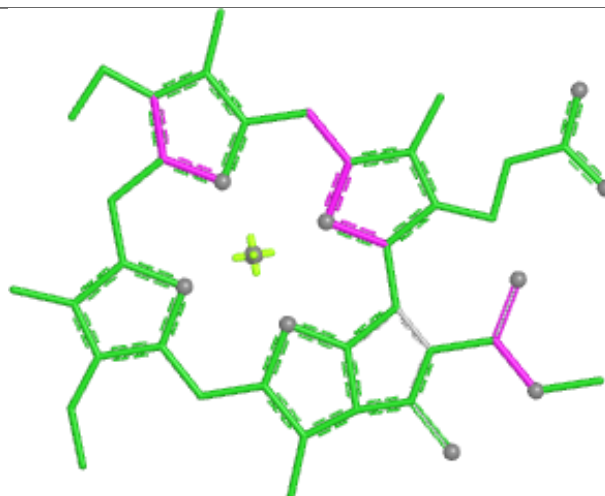


Rings

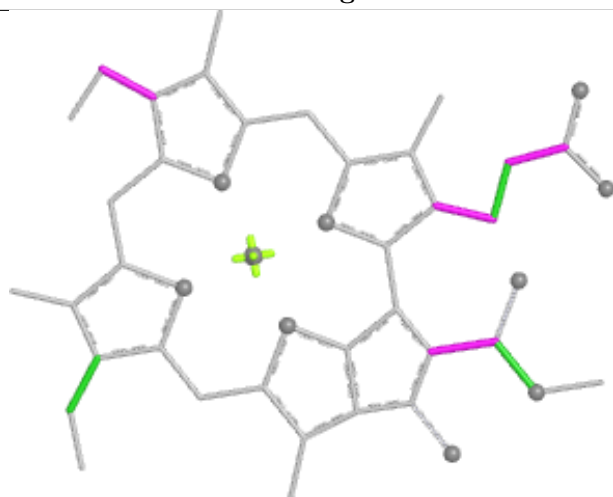
Ligand CLA a 601



Bond lengths



Bond angles

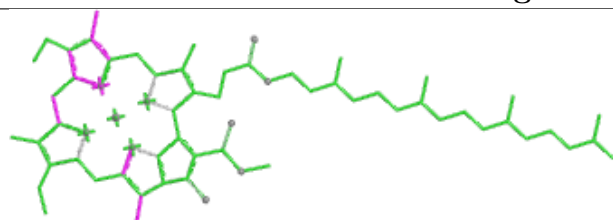


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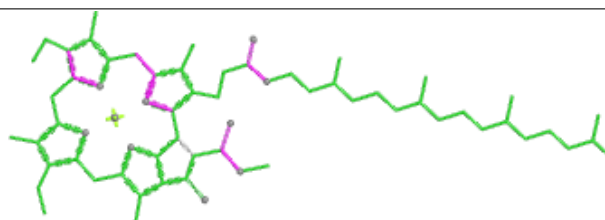


Rings

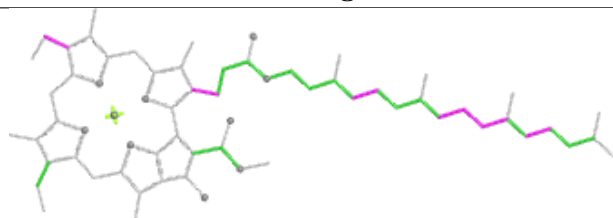
Ligand CLA A 818



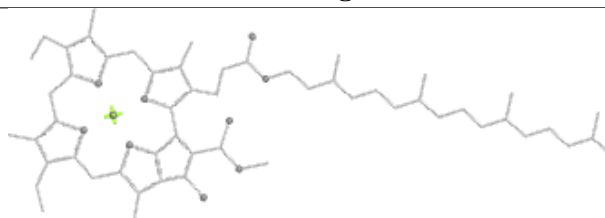
Bond lengths



Bond angles

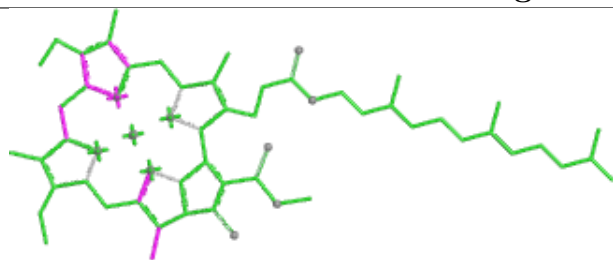


Torsions

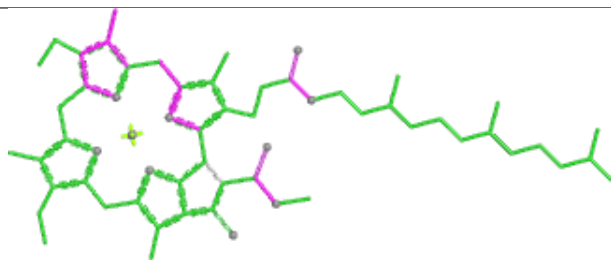


Rings

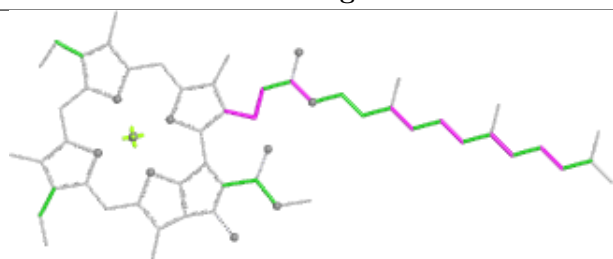
Ligand CLA B 831



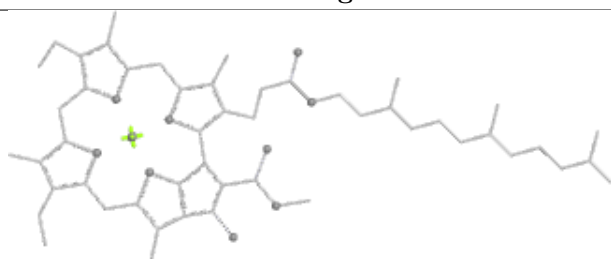
Bond lengths



Bond angles

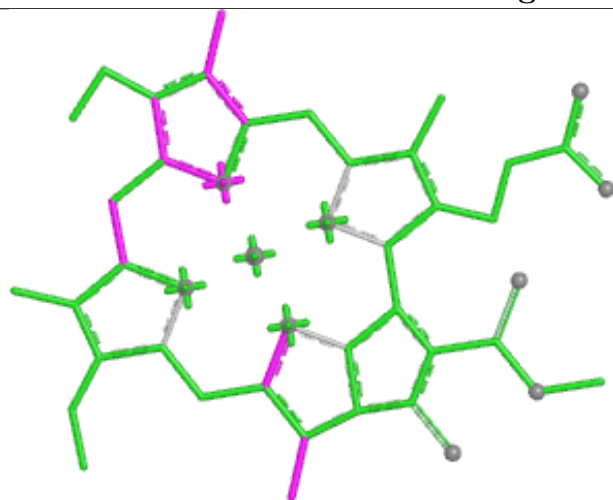


Torsions

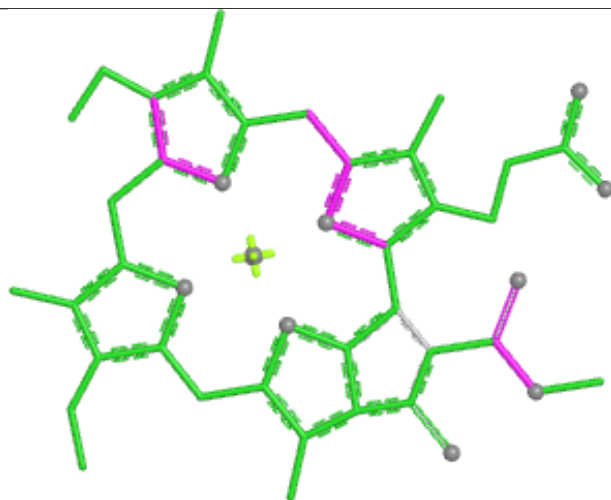


Rings

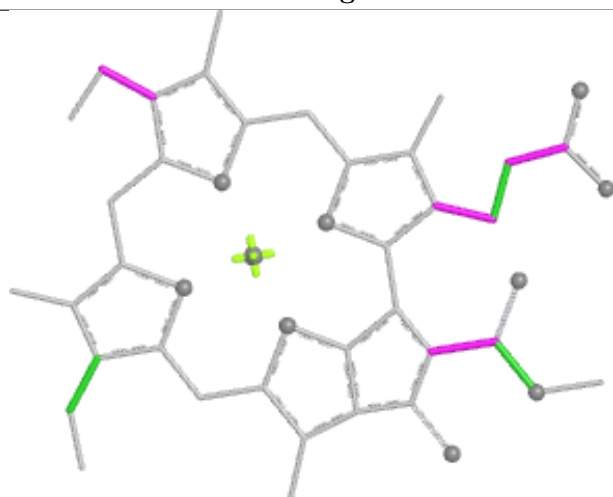
Ligand CLA 7 306



Bond lengths



Bond angles

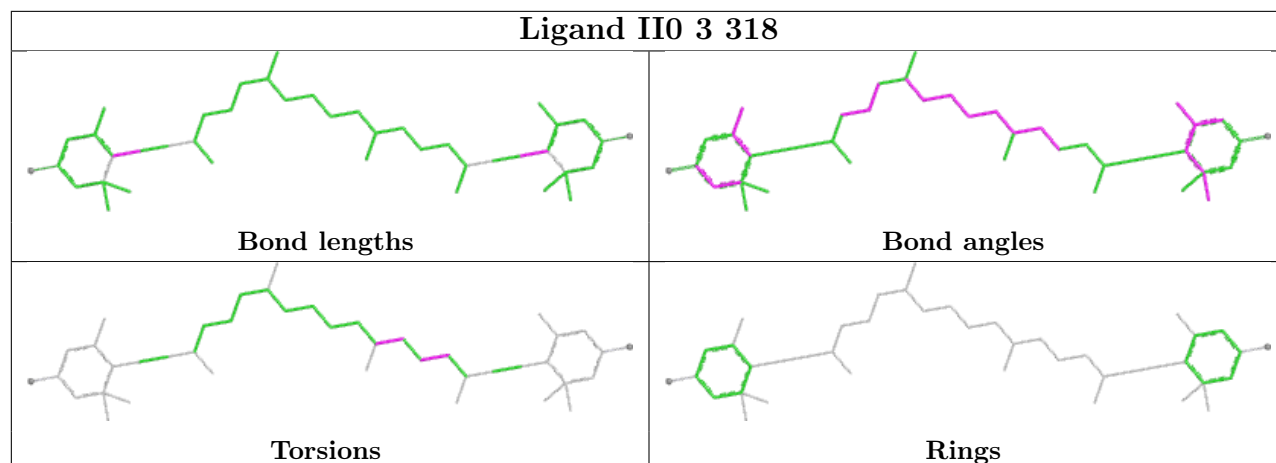


Torsions

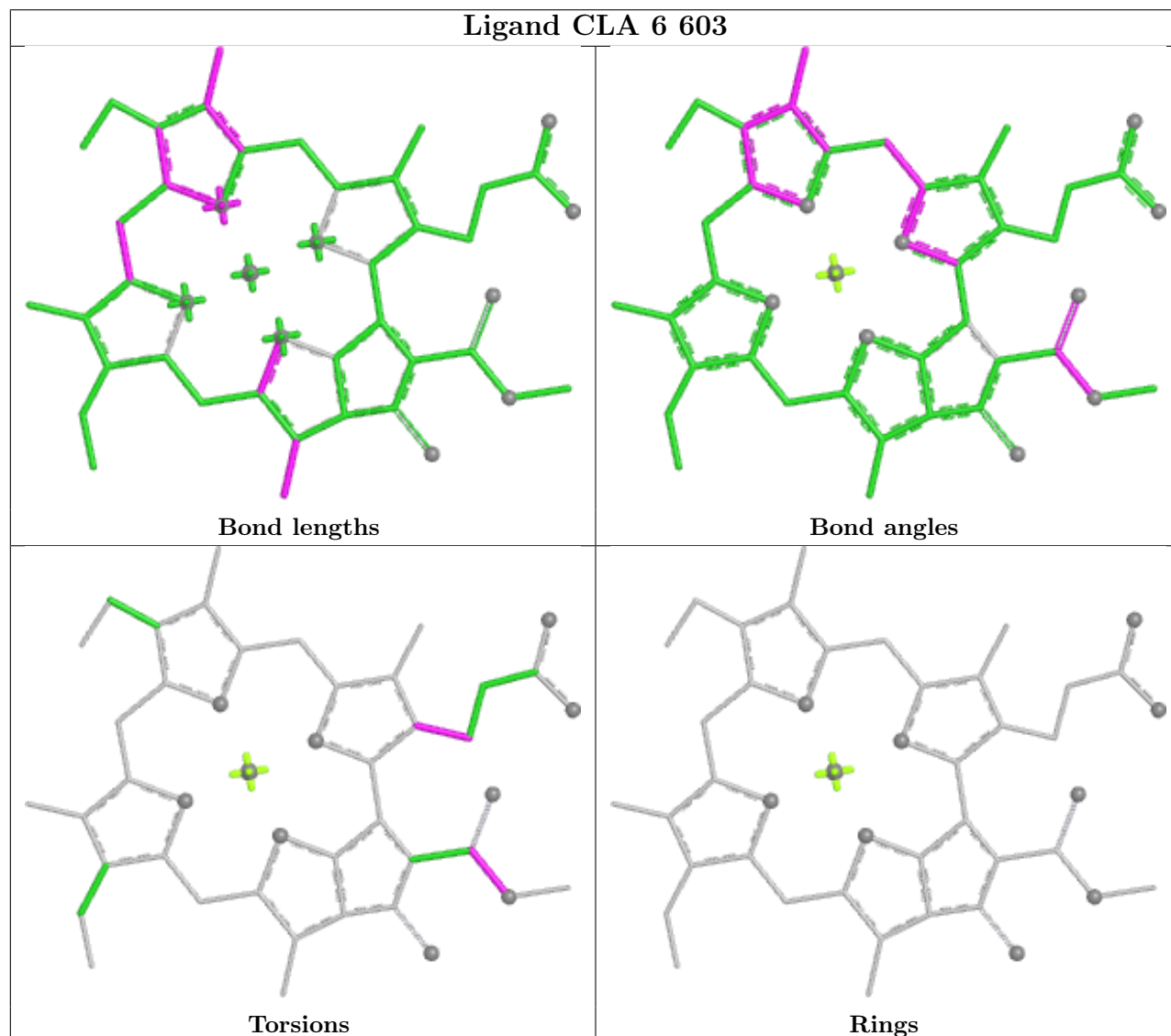


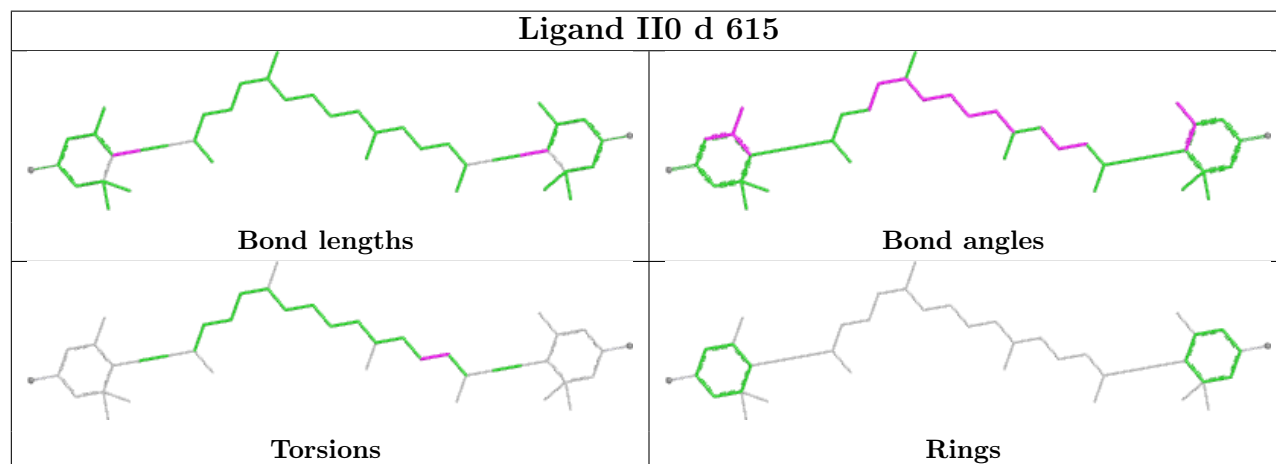
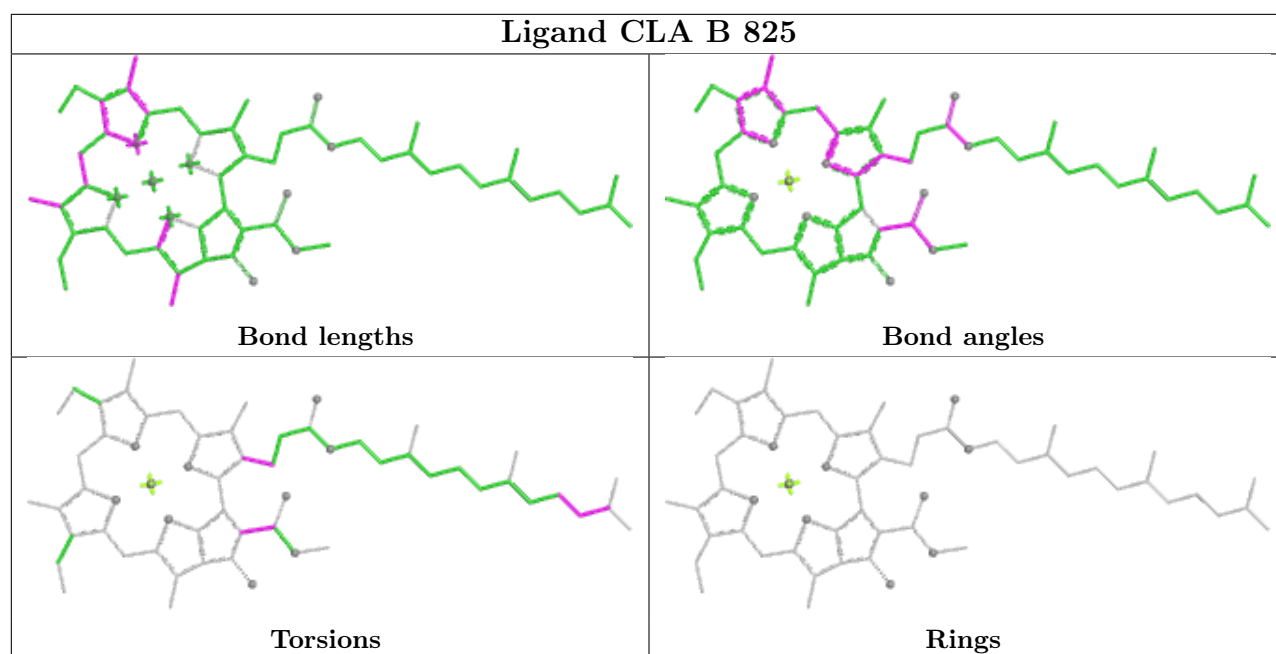
Rings

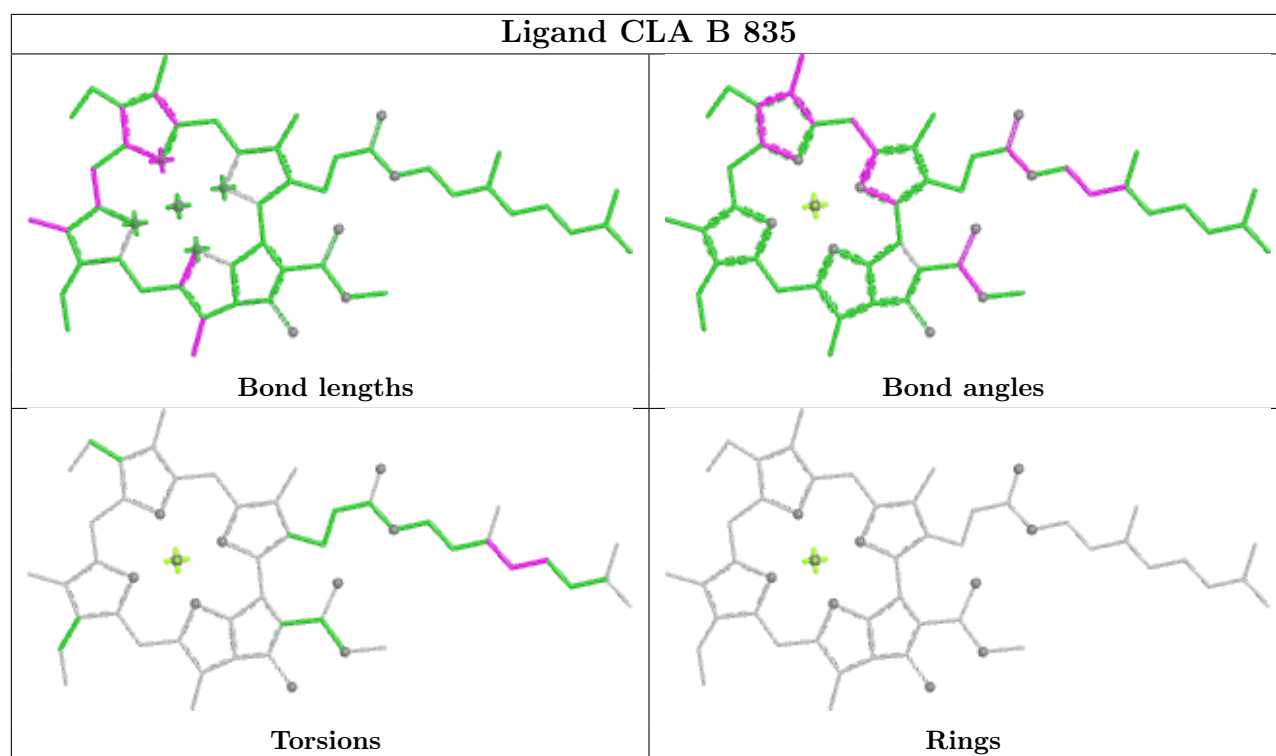
Ligand II0 3 318



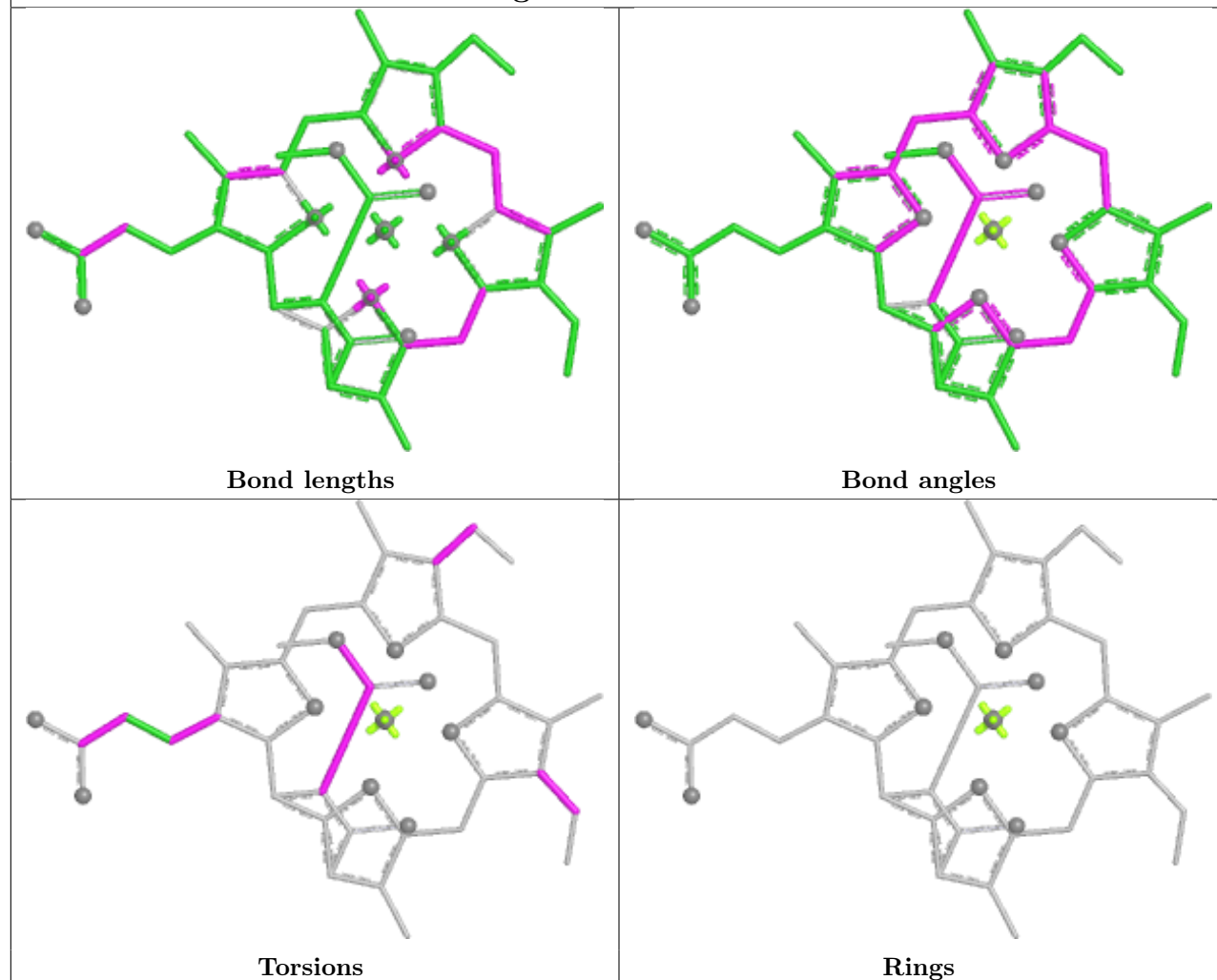
Ligand CLA 6 603



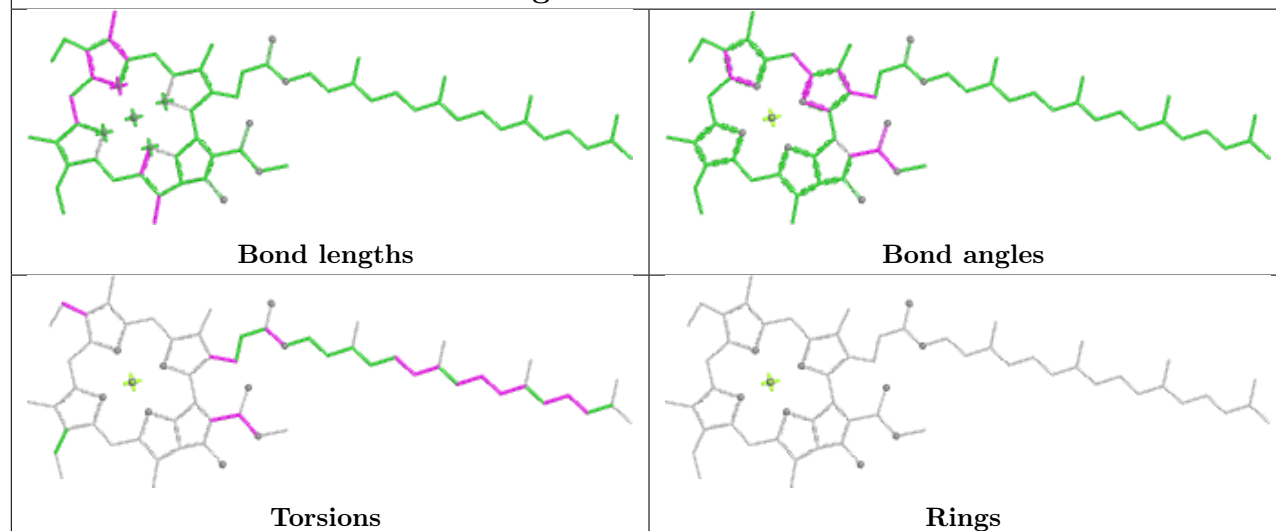


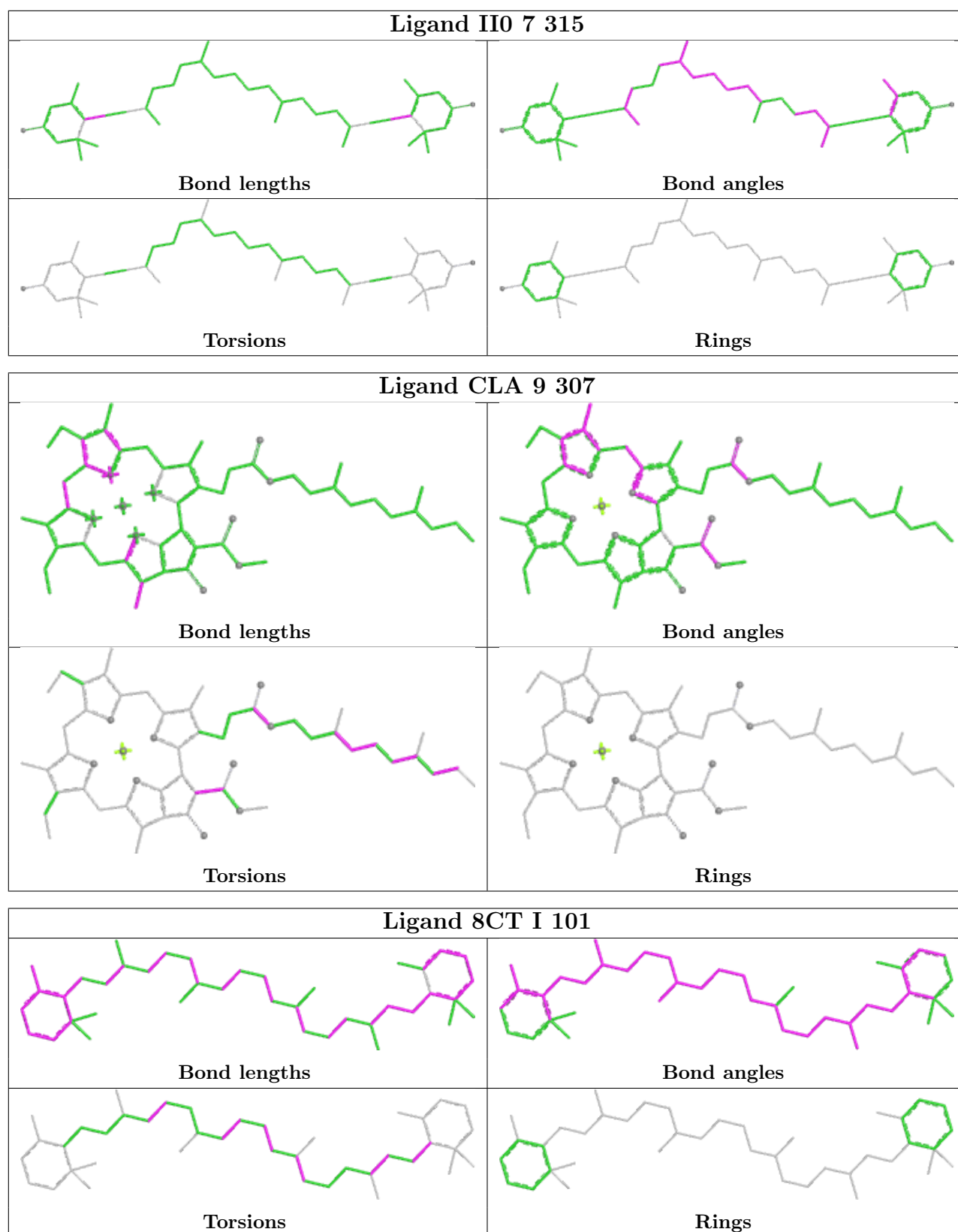


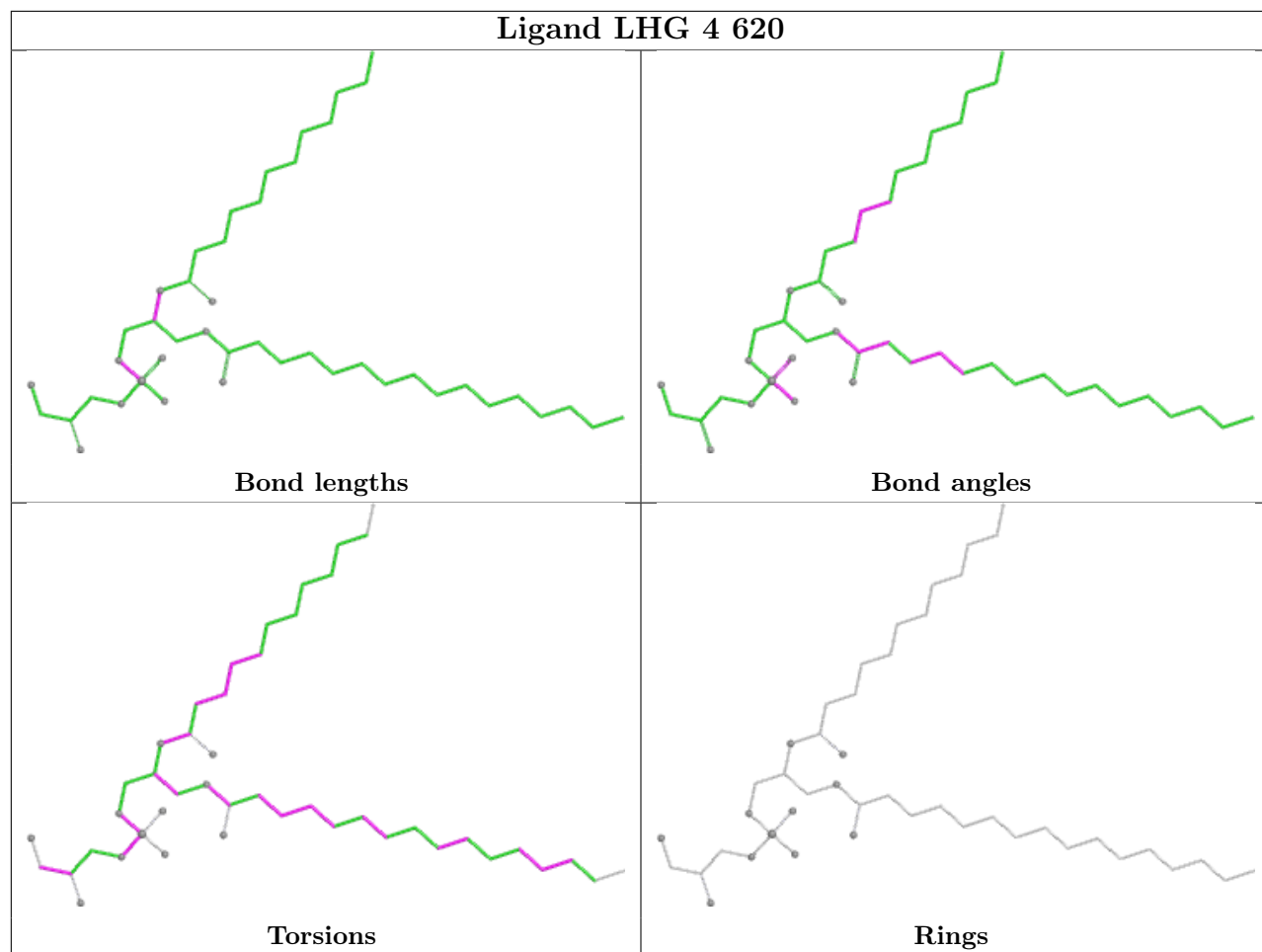
Ligand KC2 6 613



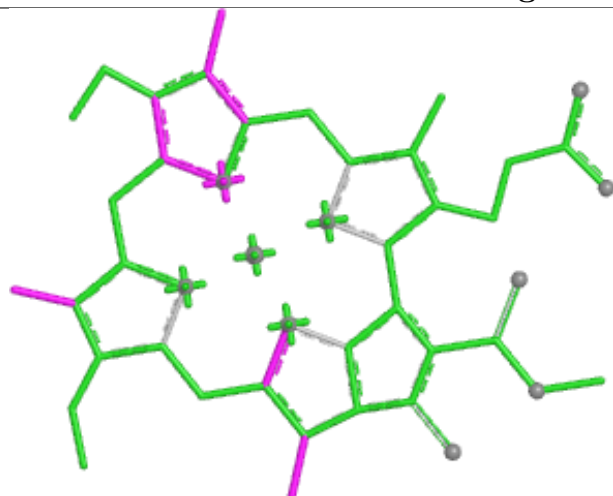
Ligand CLA B 810



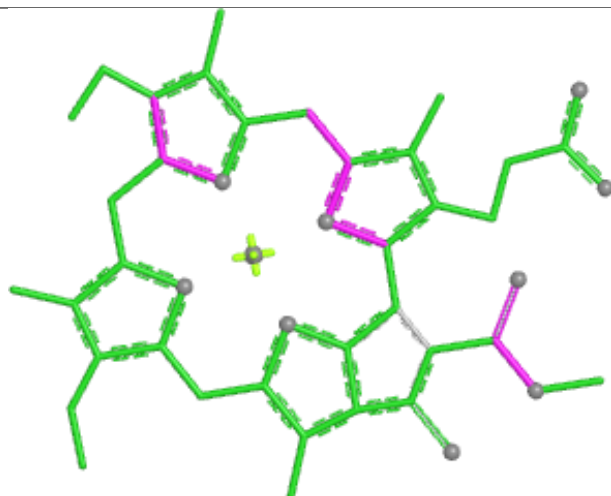




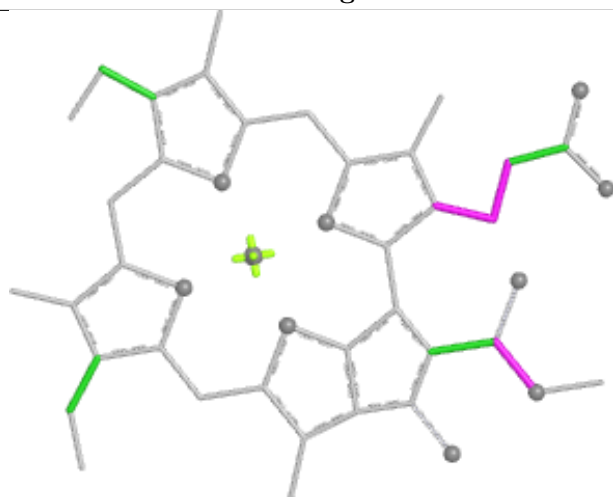
Ligand CLA 7 307



Bond lengths



Bond angles

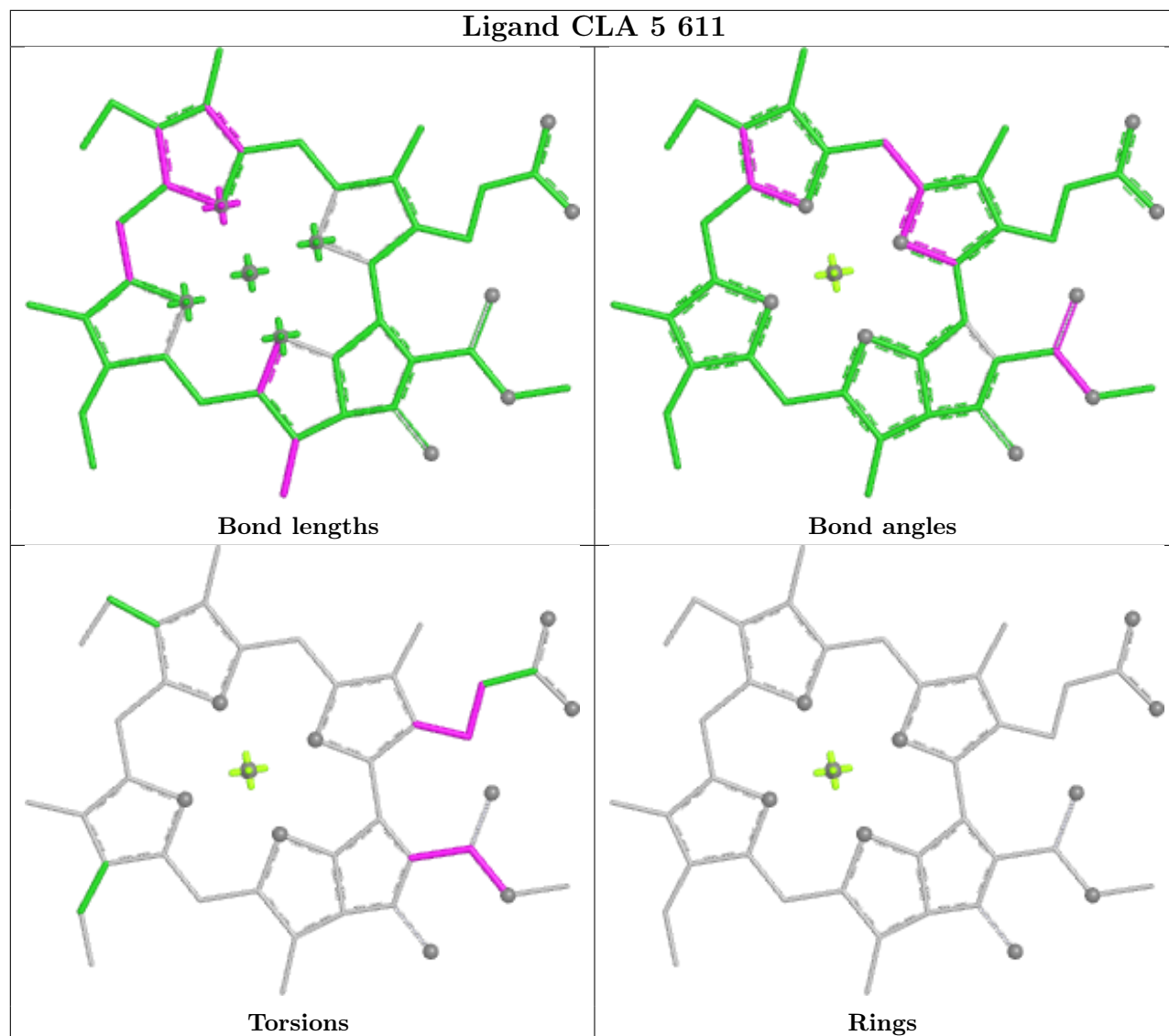


Torsions

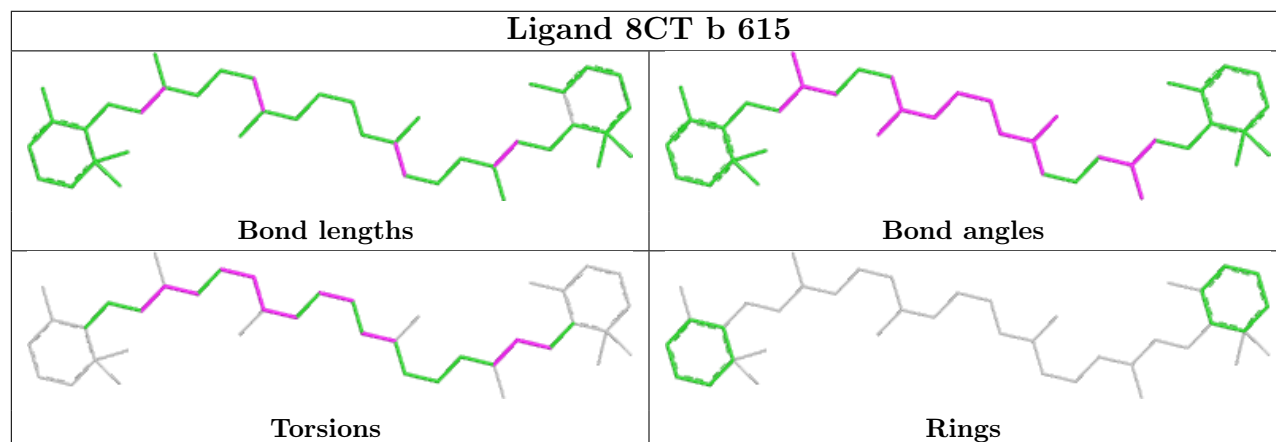


Rings

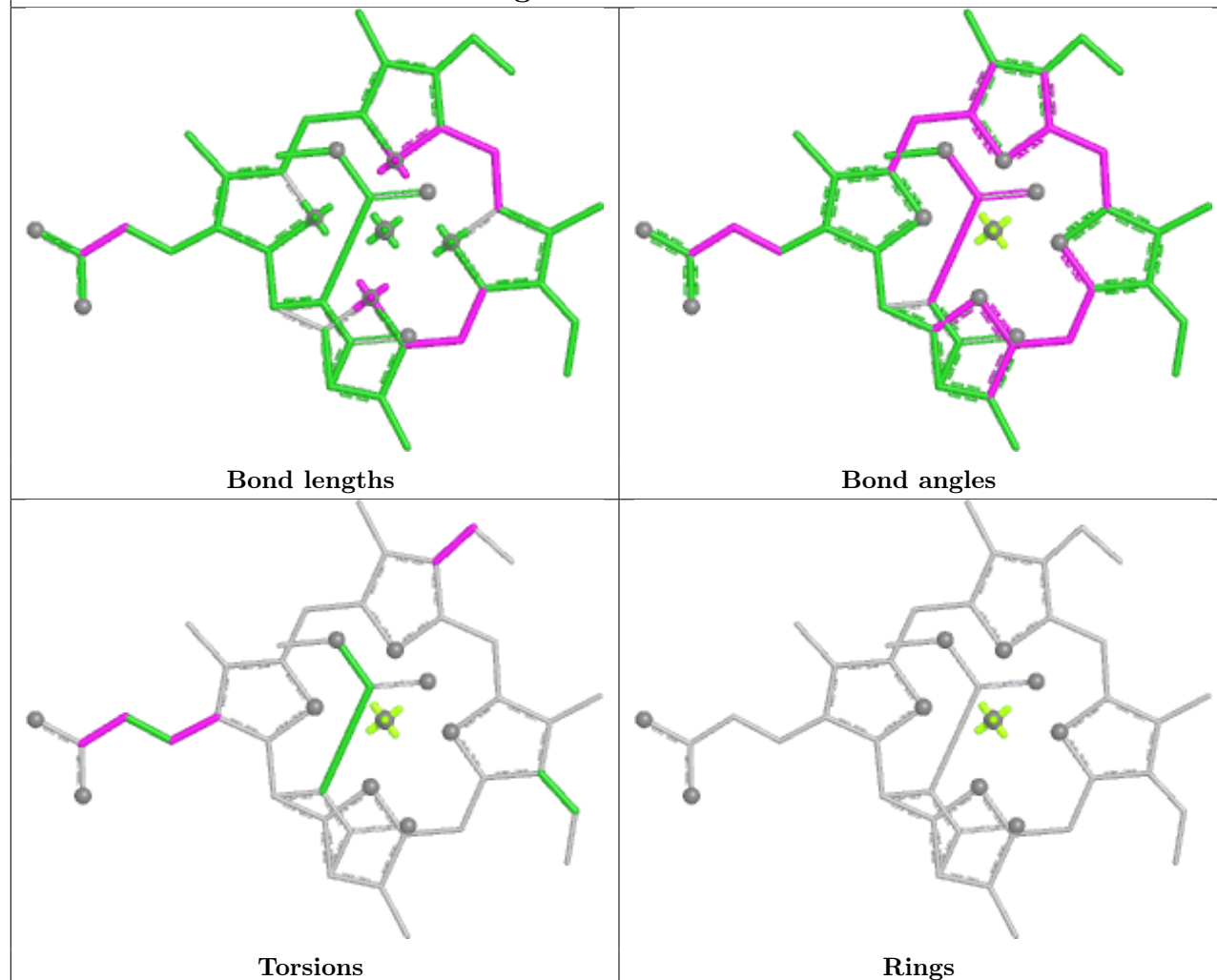
Ligand CLA 5 611



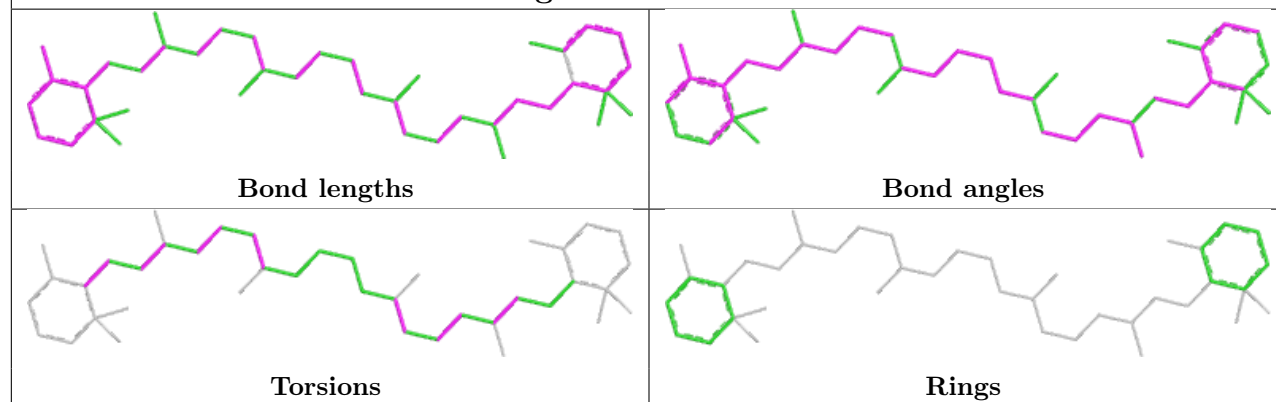
Ligand 8CT b 615

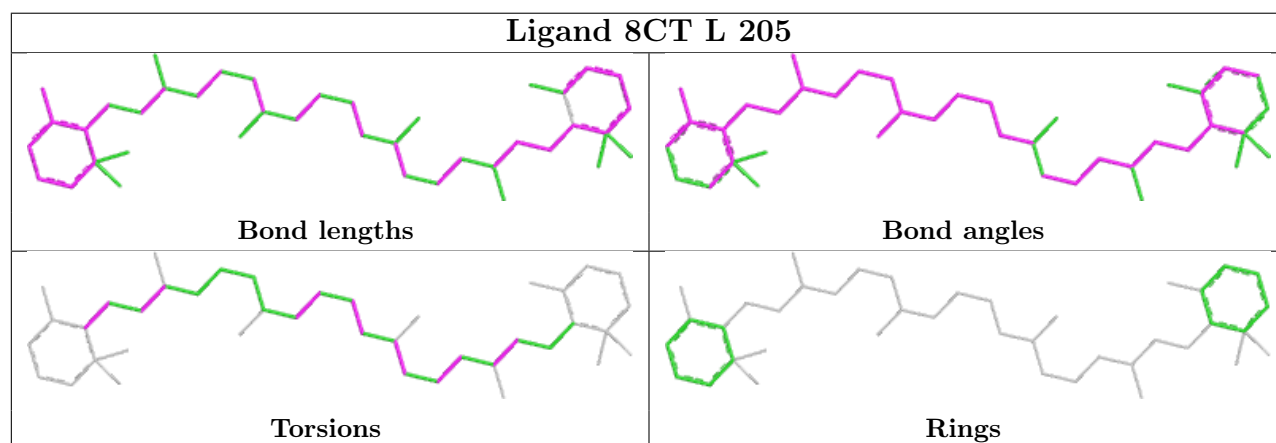
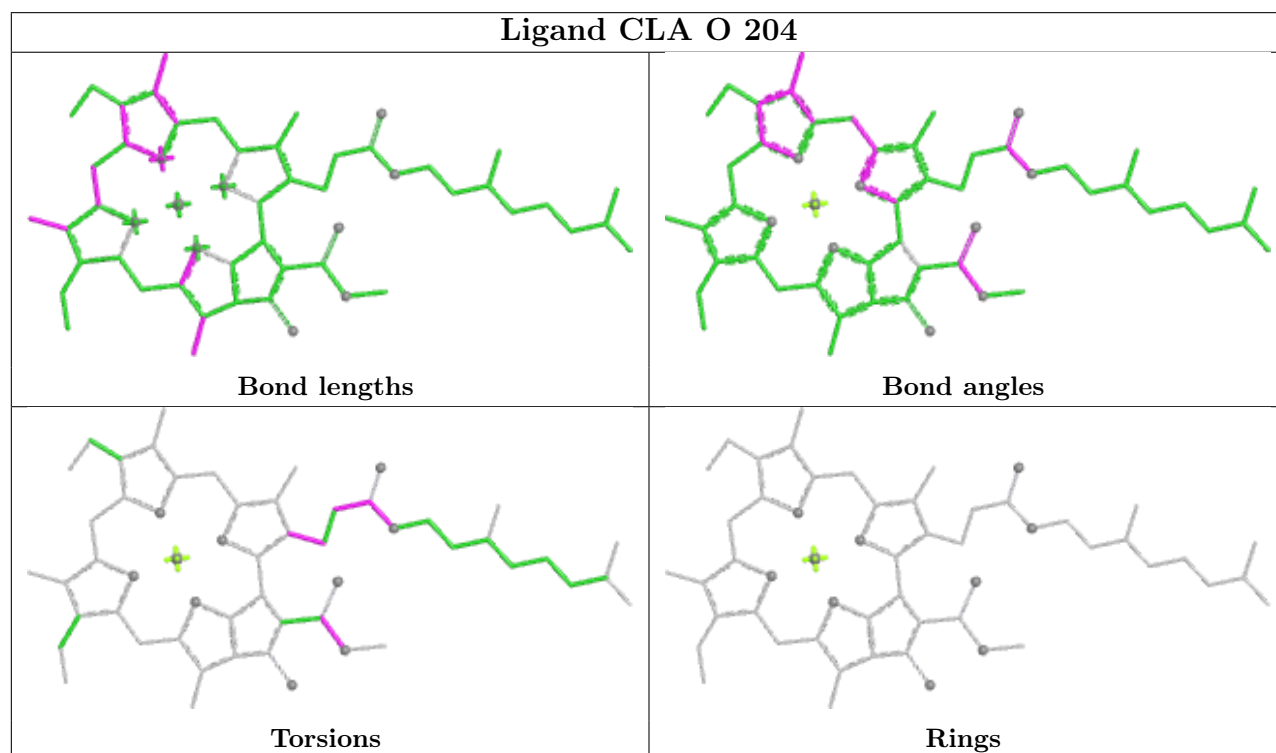
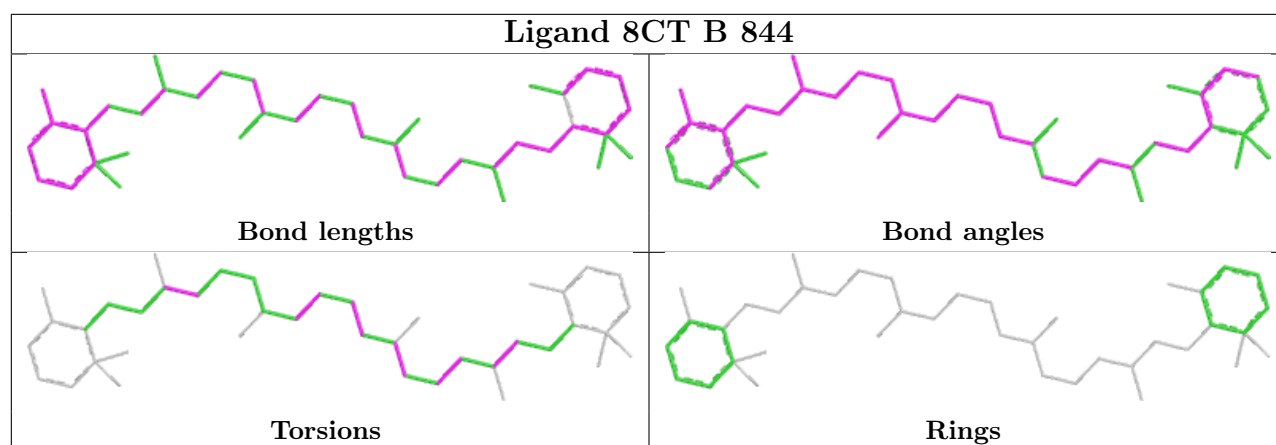


Ligand KC2 c 614

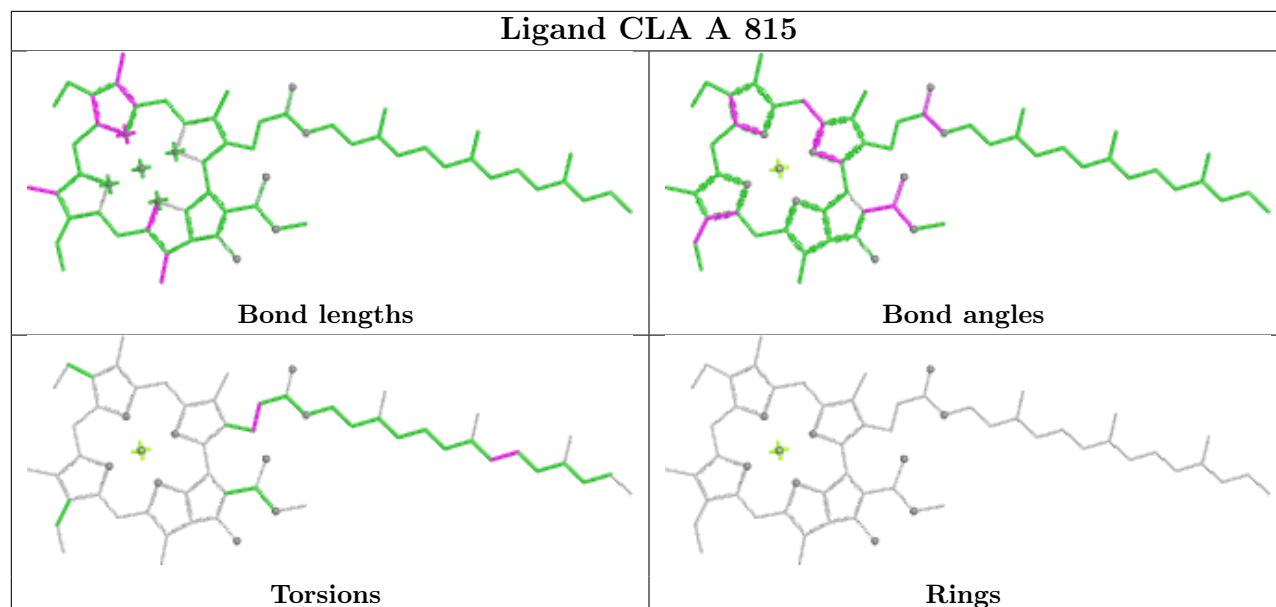


Ligand 8CT B 851

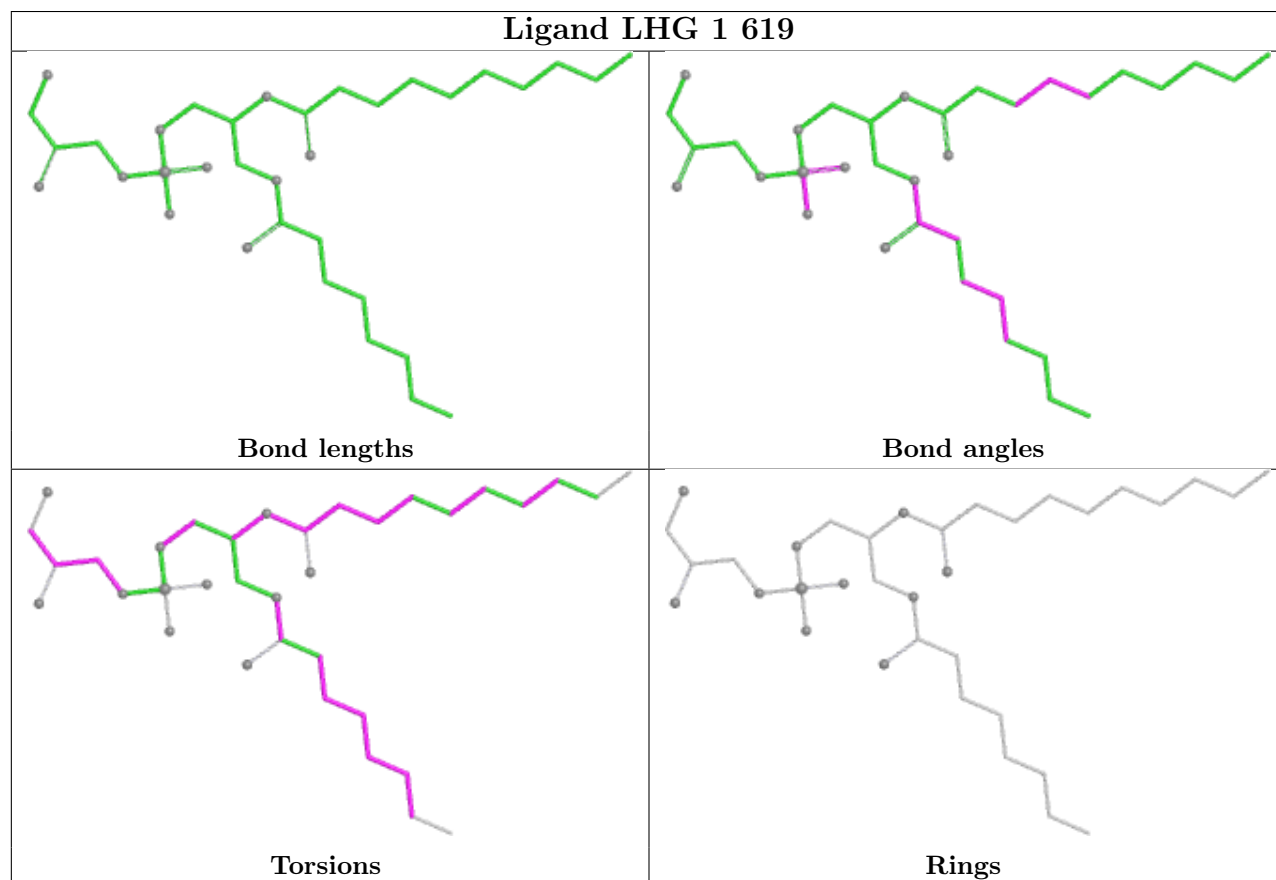


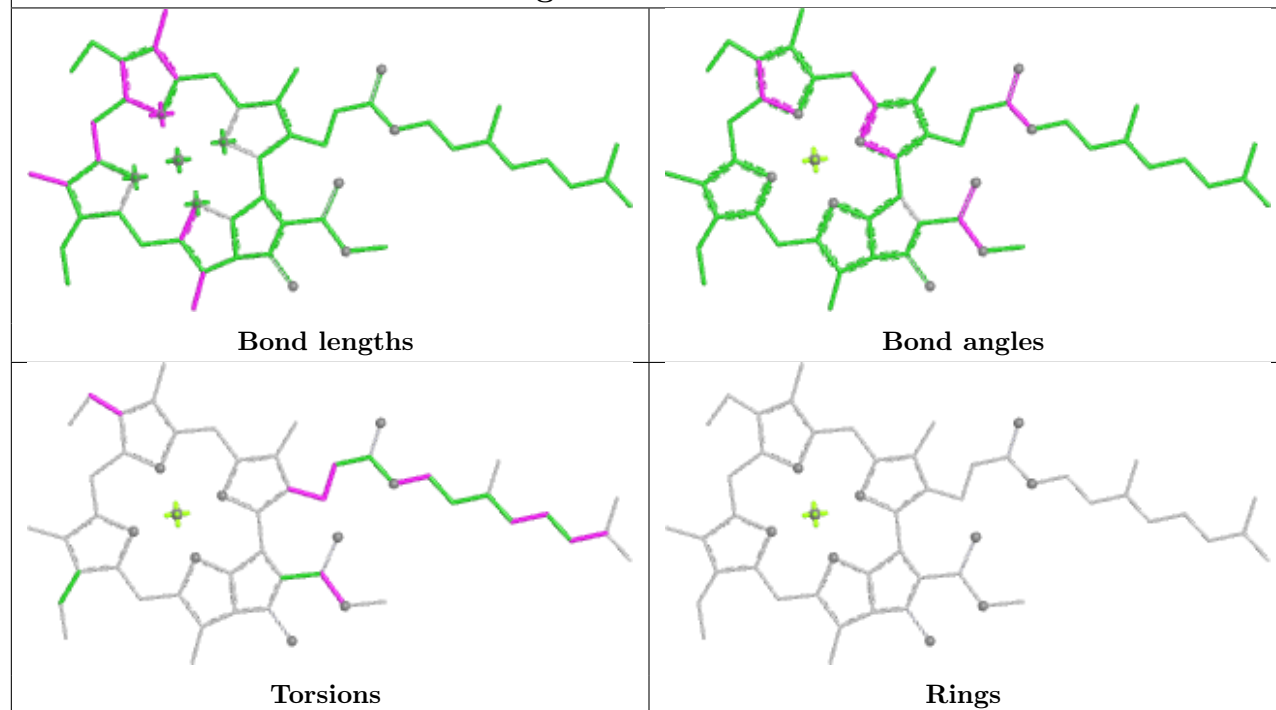
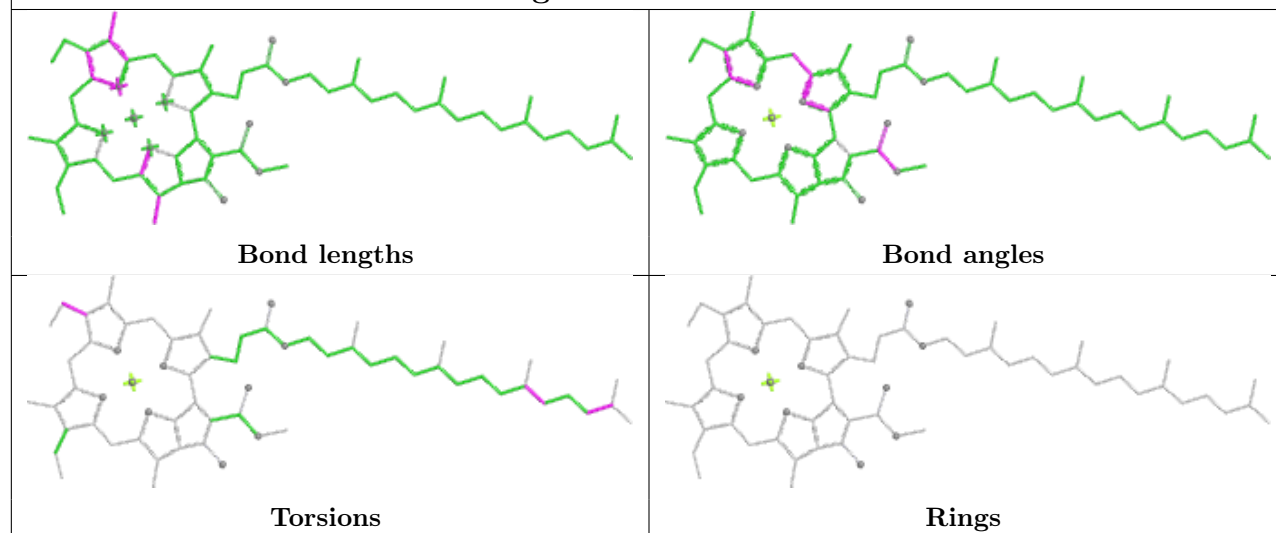


Ligand CLA A 815

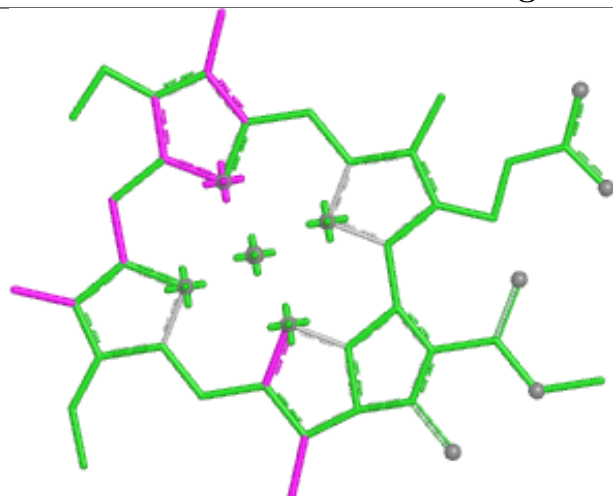


Ligand LHG 1 619

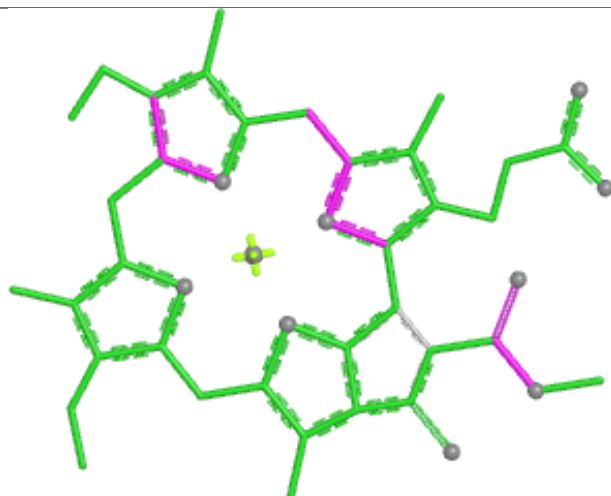


Ligand CLA a 602**Ligand CLA B 839**

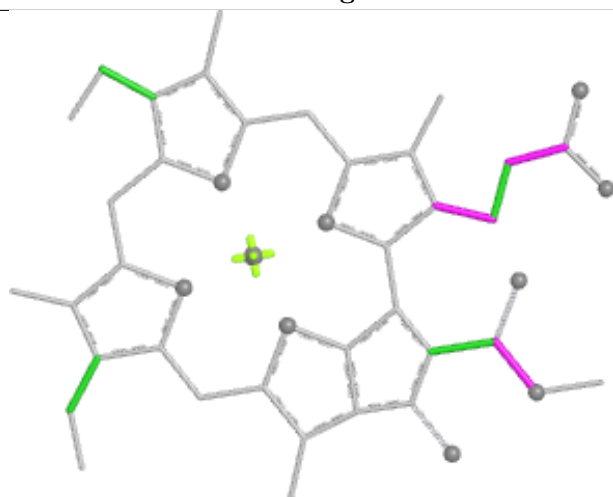
Ligand CLA 9 304



Bond lengths



Bond angles

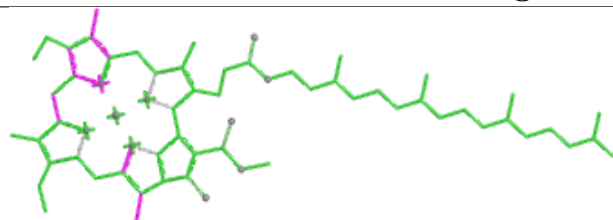


Torsions

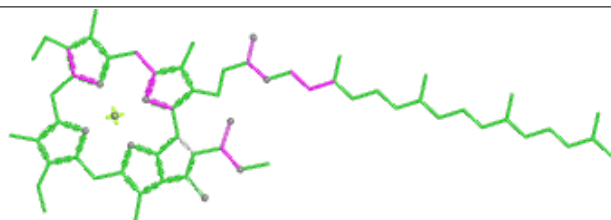


Rings

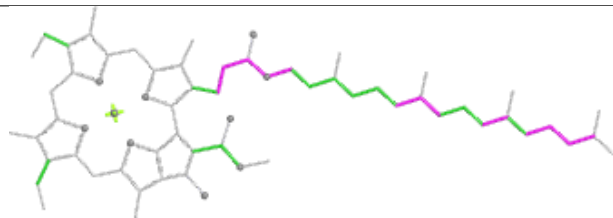
Ligand CLA A 839



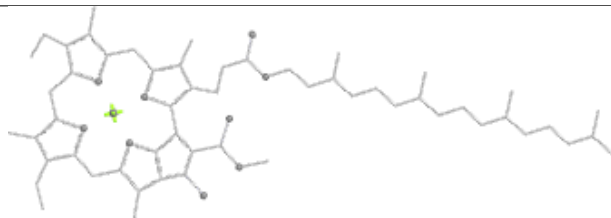
Bond lengths



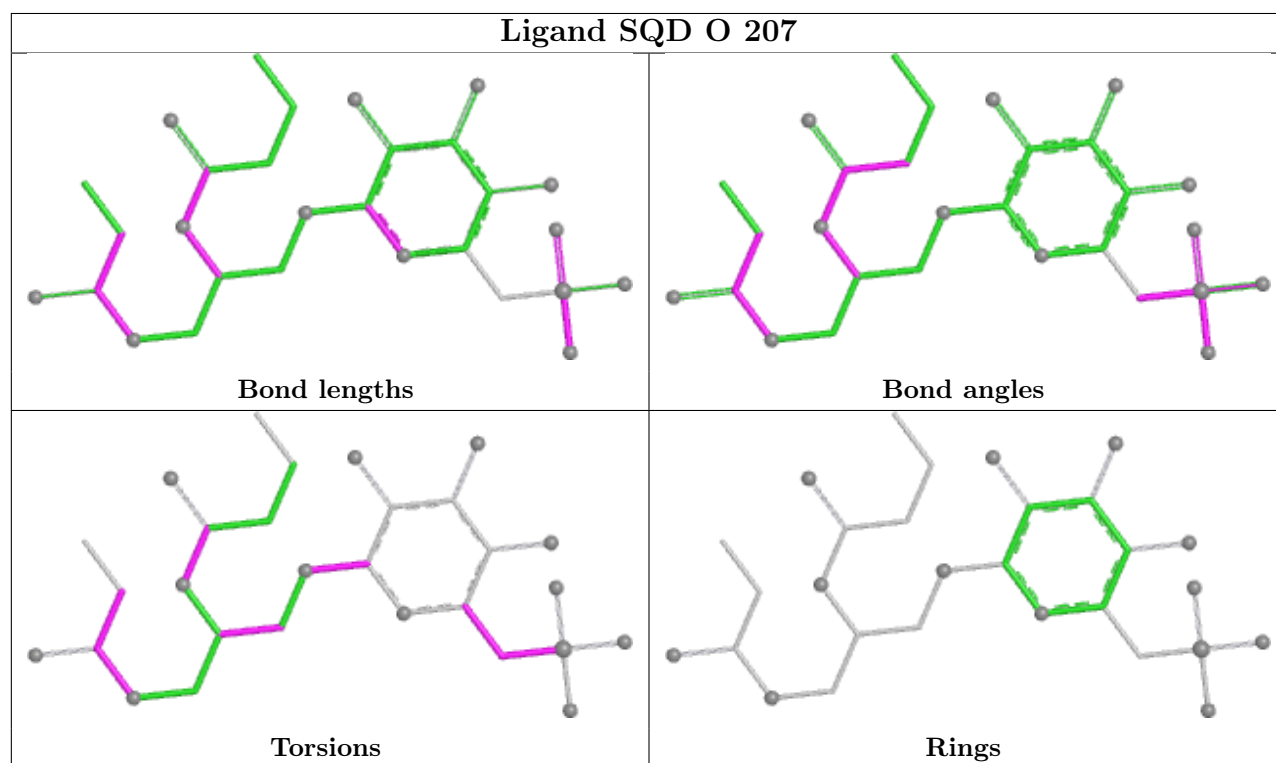
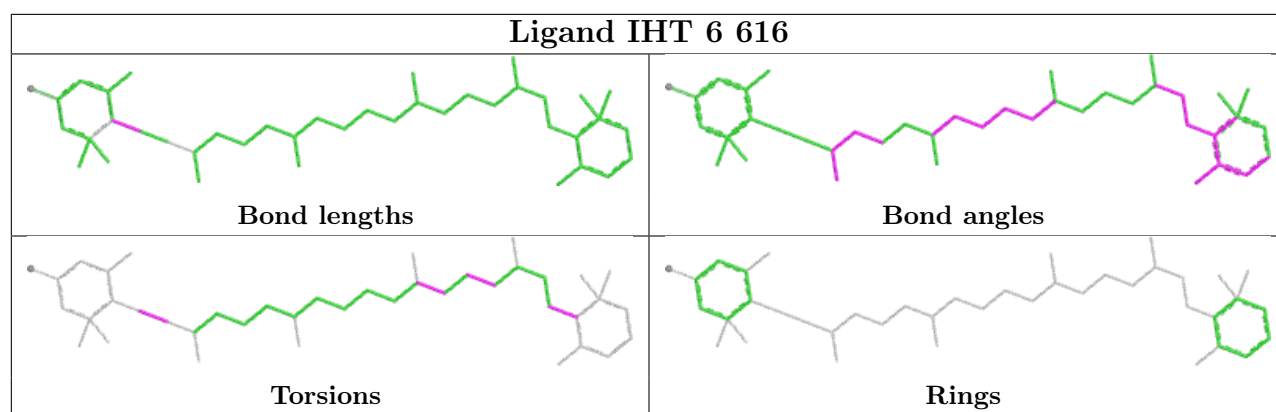
Bond angles



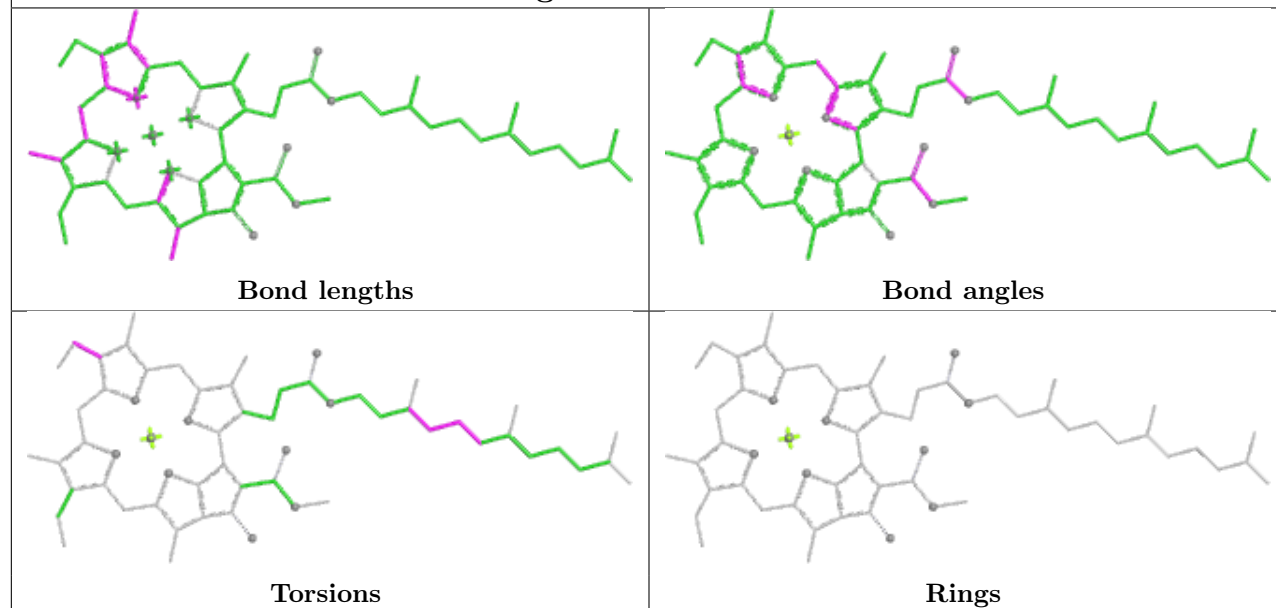
Torsions



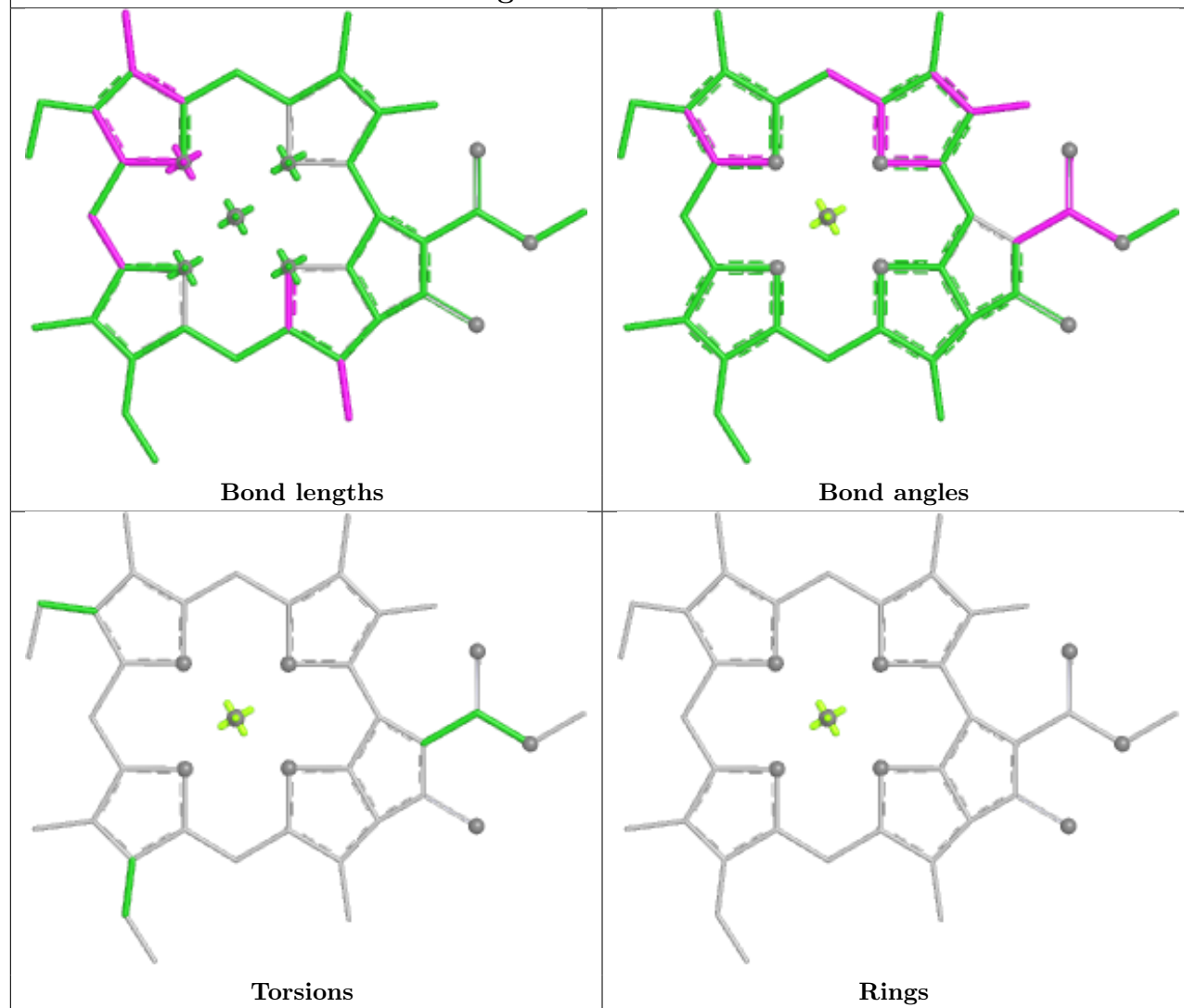
Rings



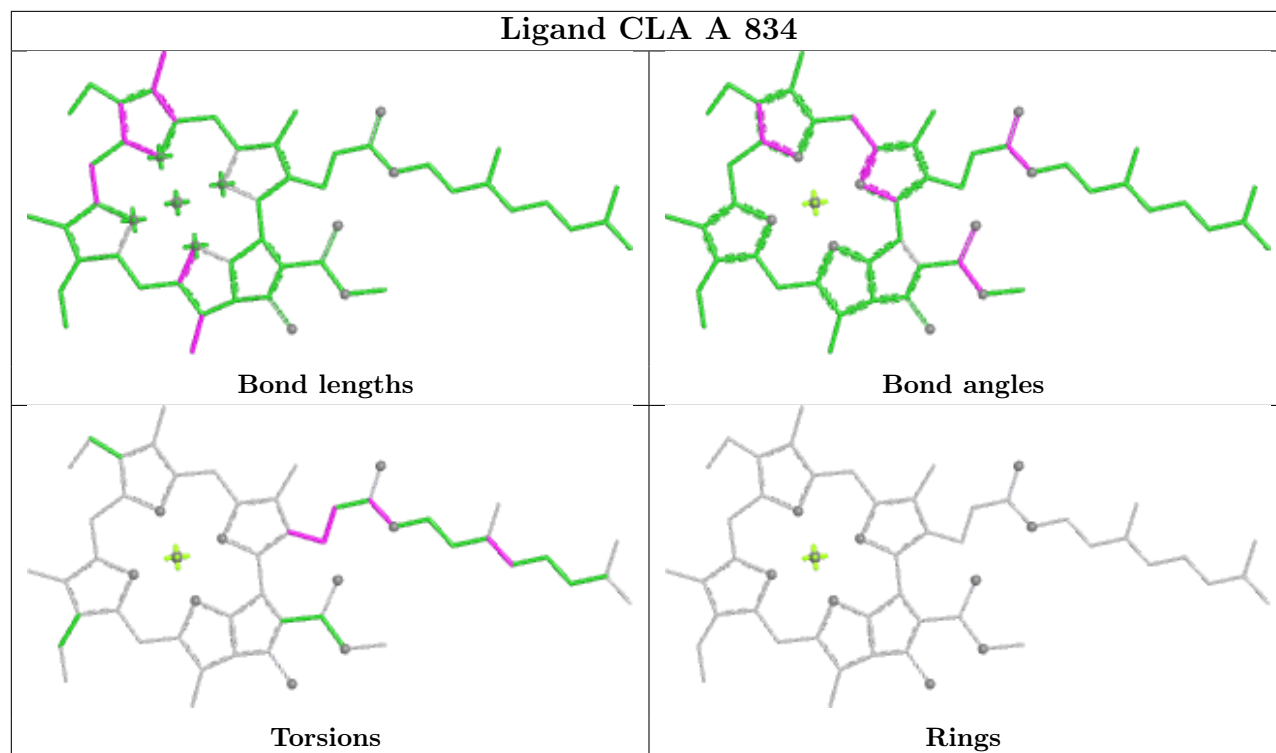
Ligand CLA 3 309



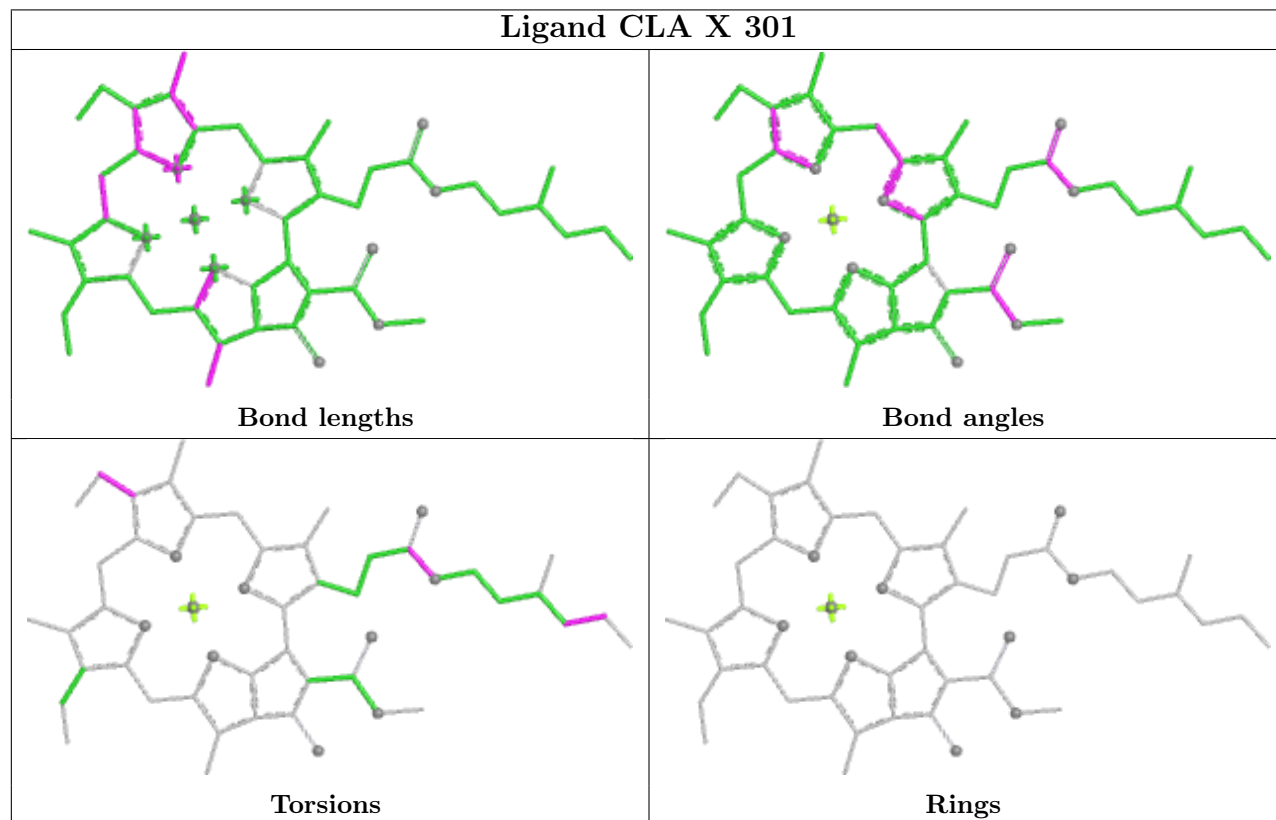
Ligand CLA 6 609



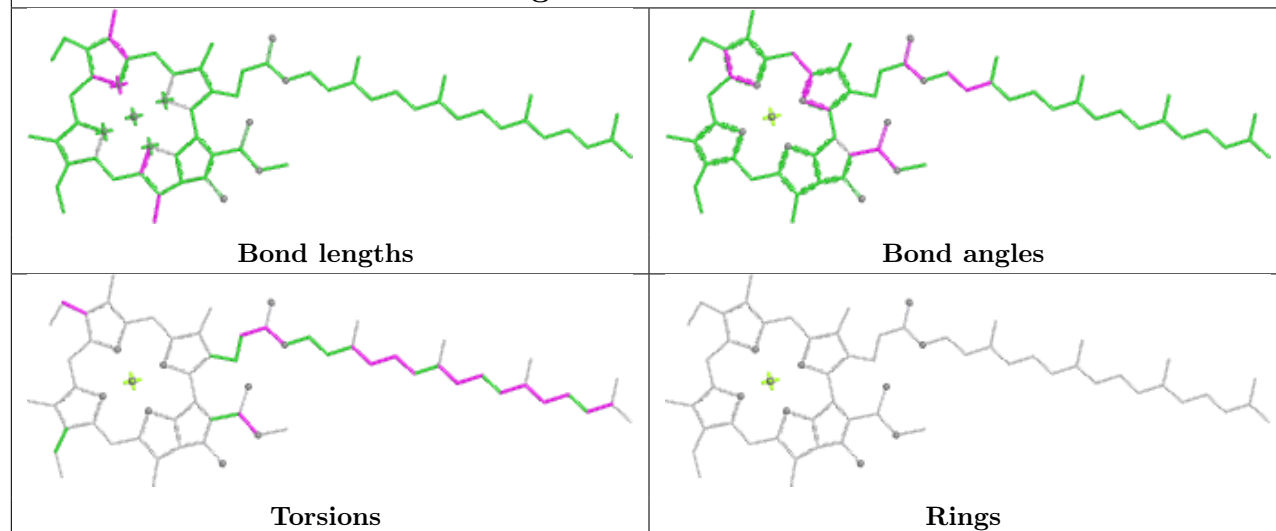
Ligand CLA A 834



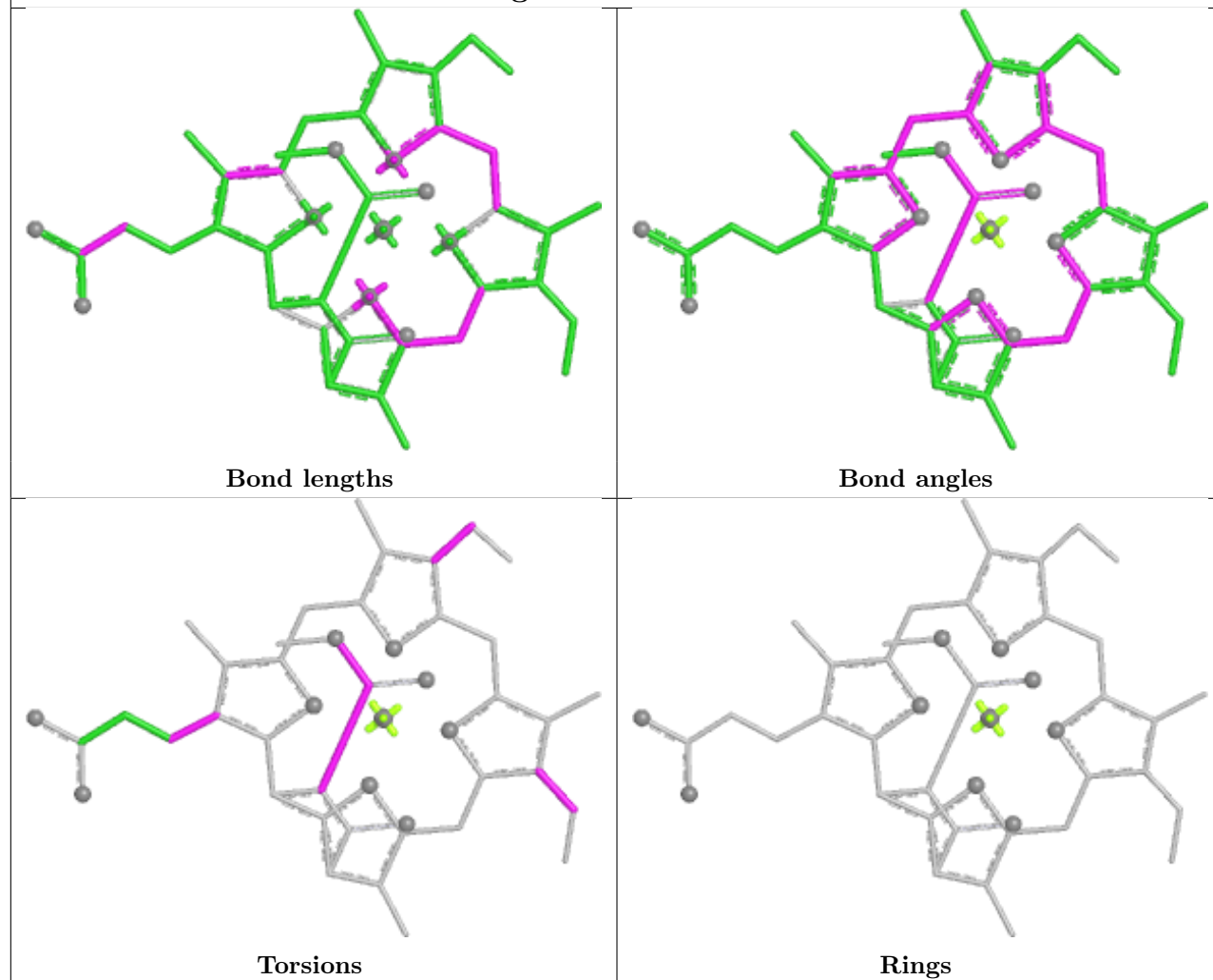
Ligand CLA X 301

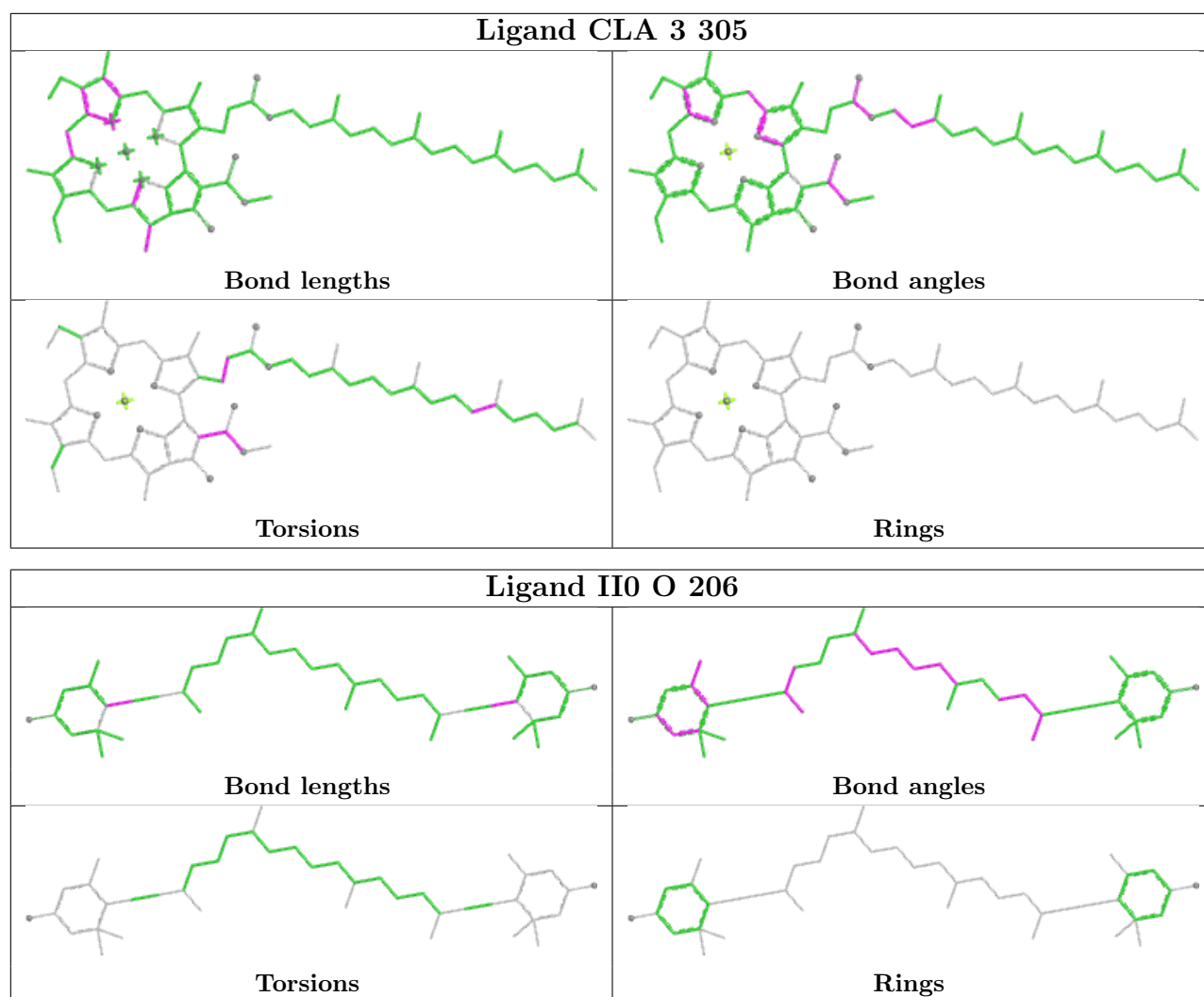


Ligand CLA A 801

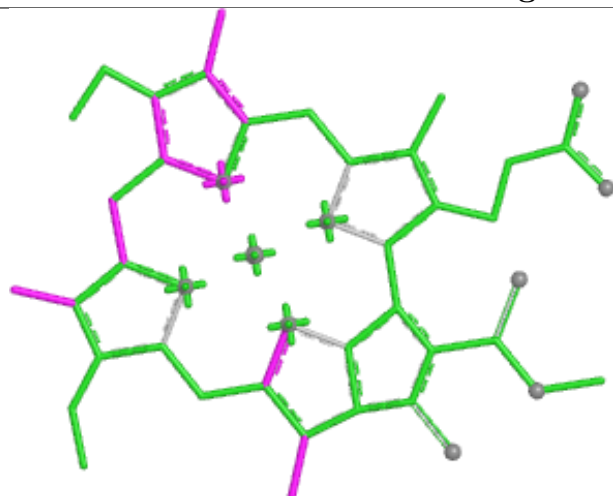


Ligand KC2 5 610

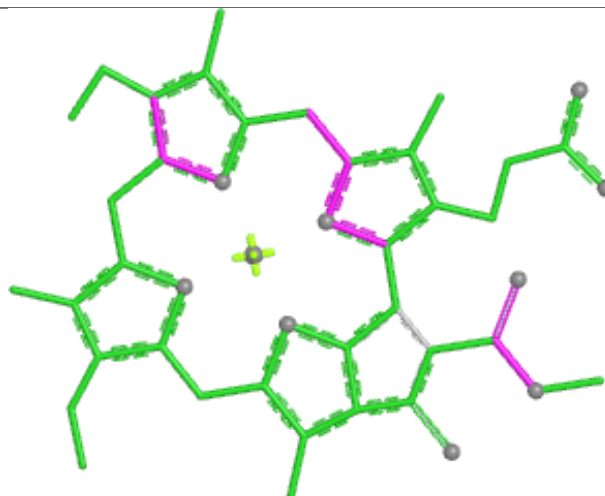




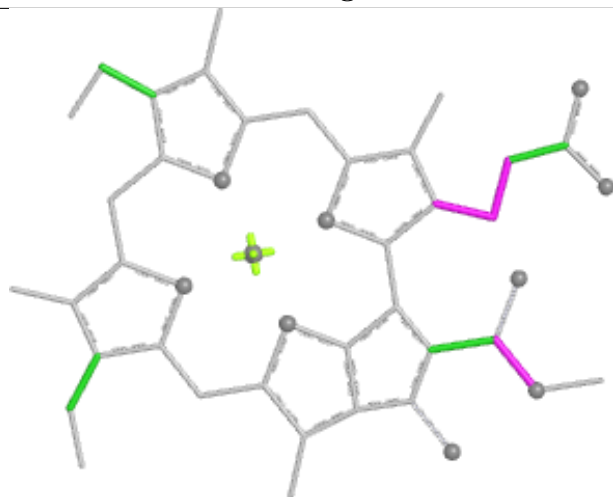
Ligand CLA 2 606



Bond lengths



Bond angles

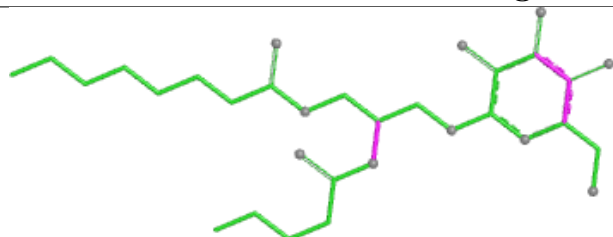


Torsions

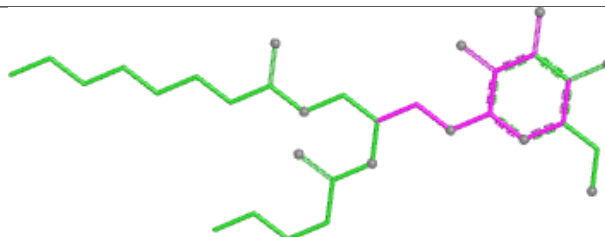


Rings

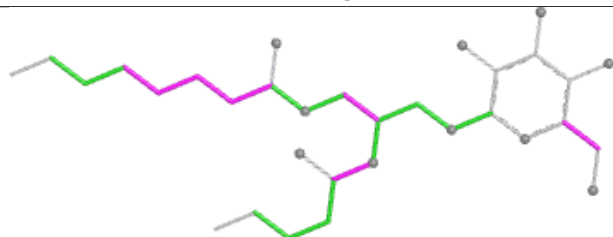
Ligand LMG 6 617



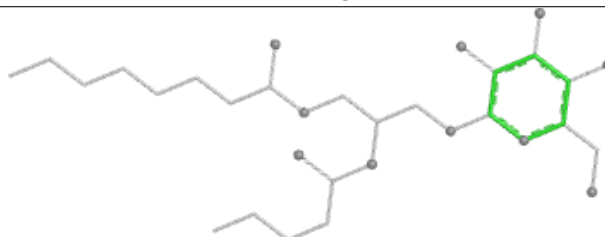
Bond lengths



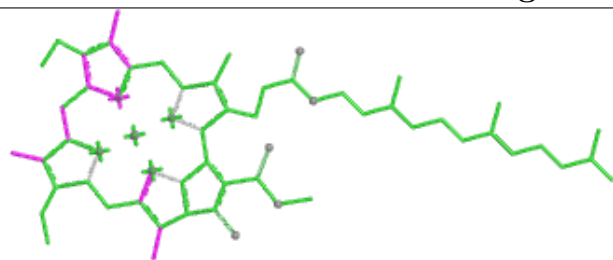
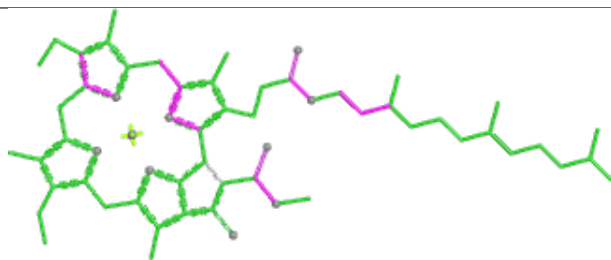
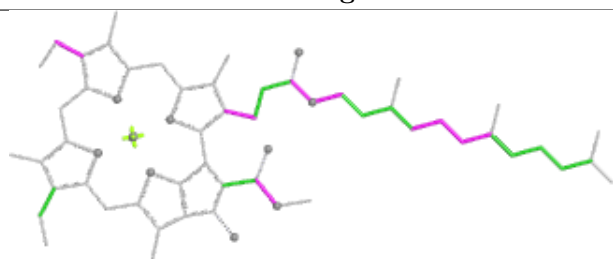
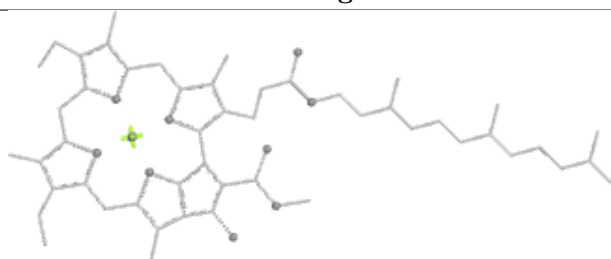
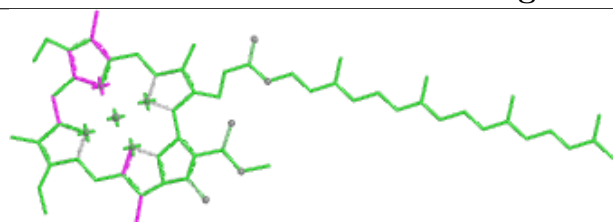
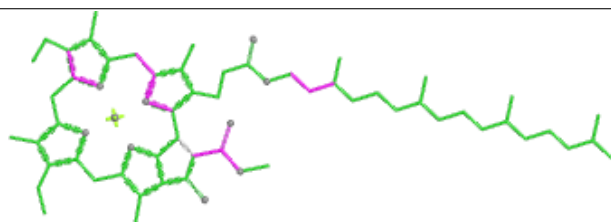
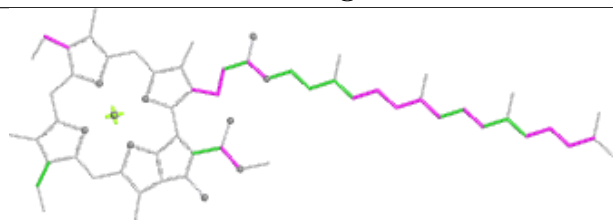
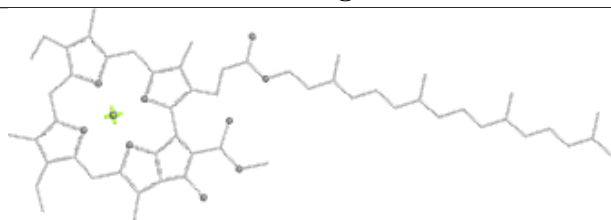
Bond angles



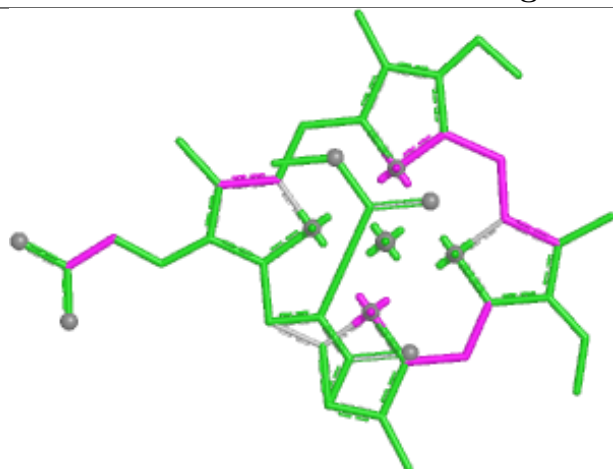
Torsions



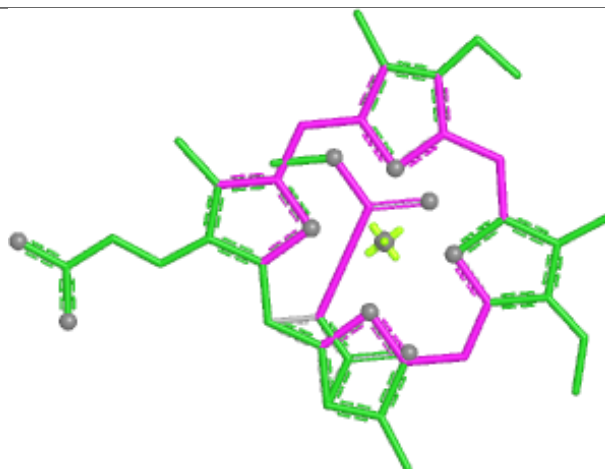
Rings

Ligand CLA 5 608**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 9 308****Bond lengths****Bond angles****Torsions****Rings**

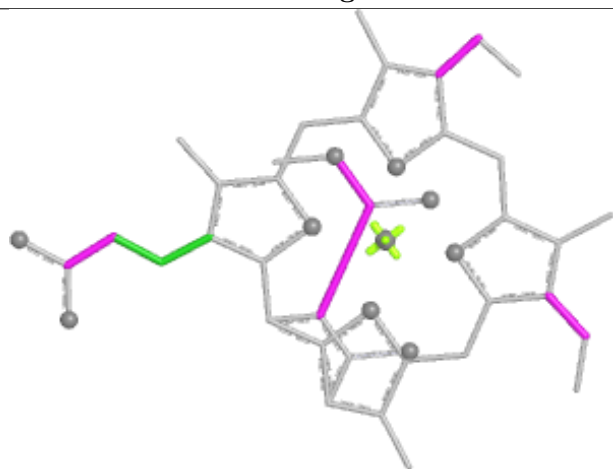
Ligand KC2 9 311



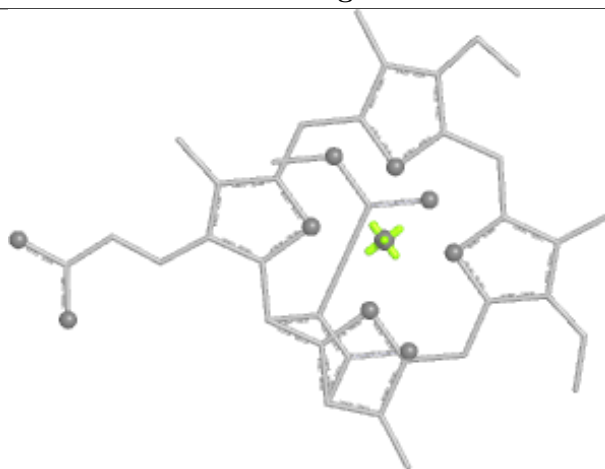
Bond lengths



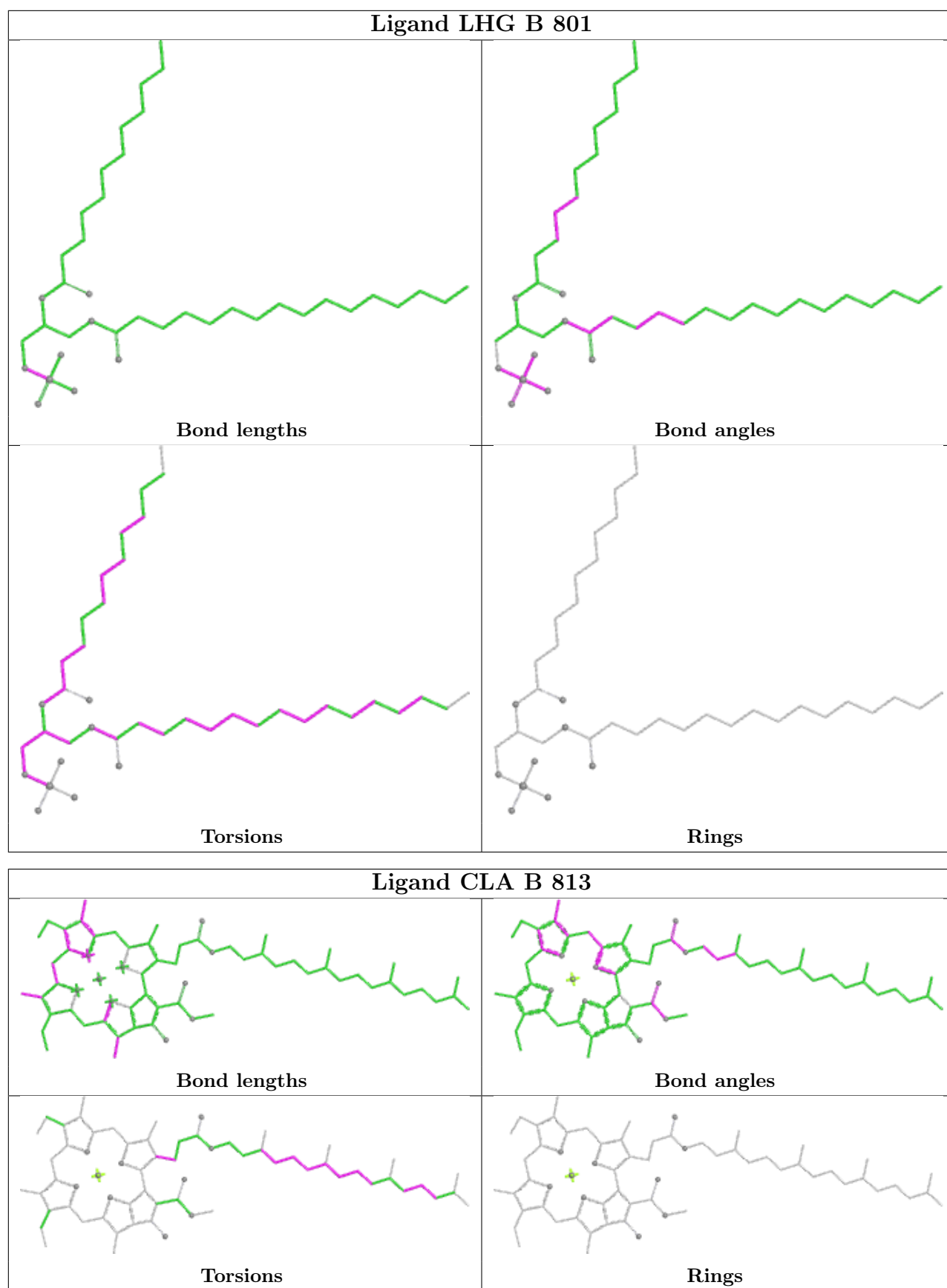
Bond angles



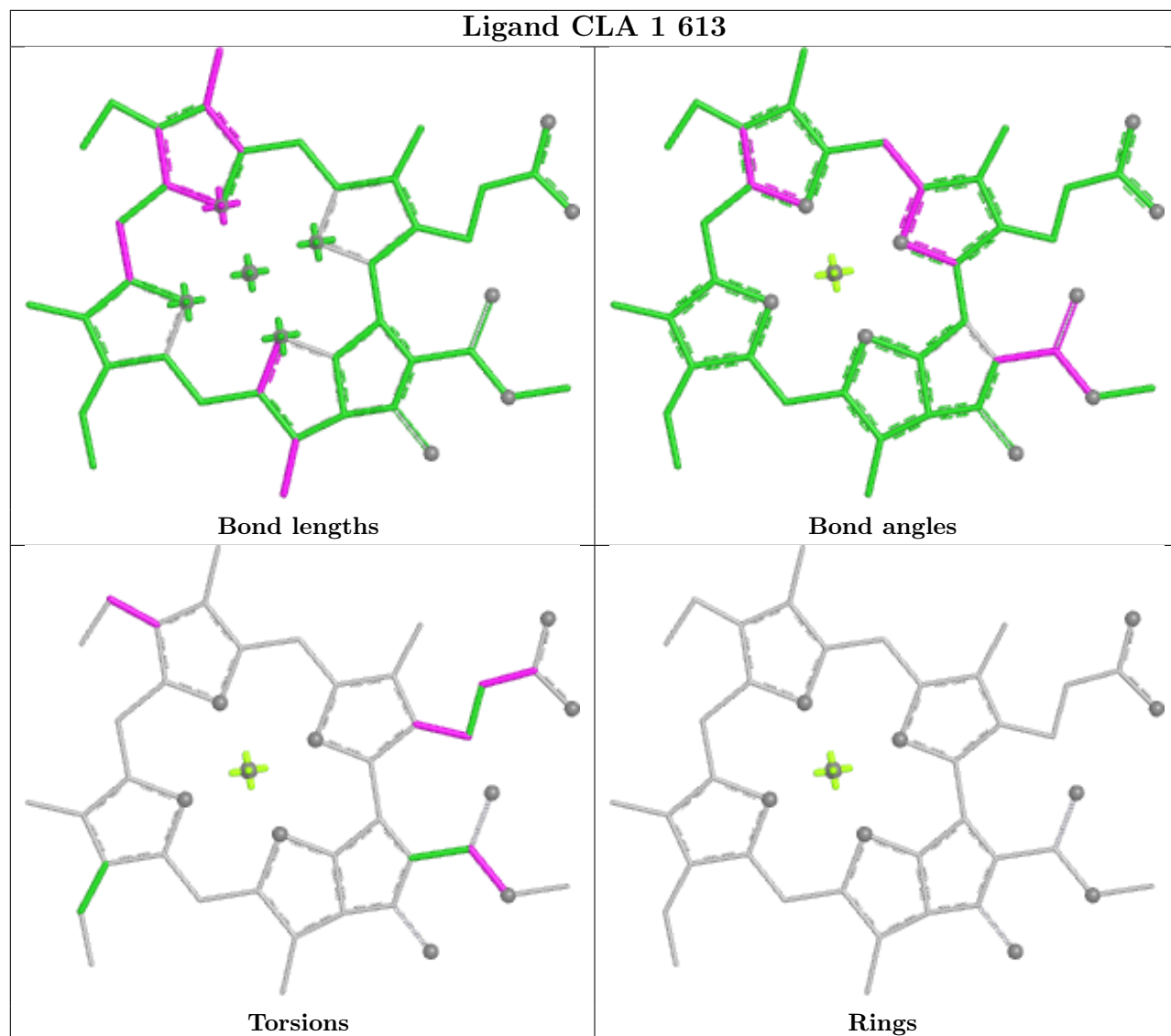
Torsions



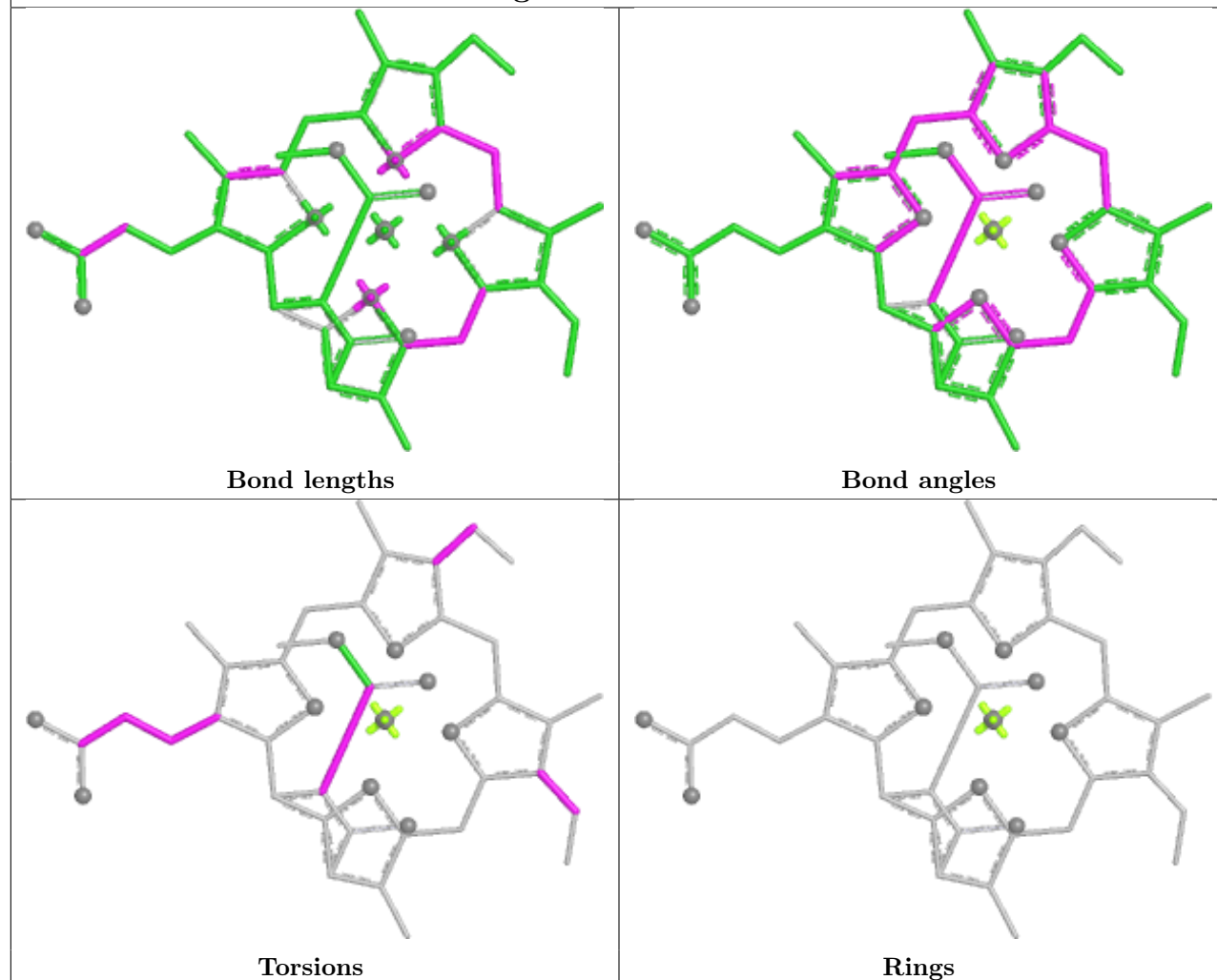
Rings



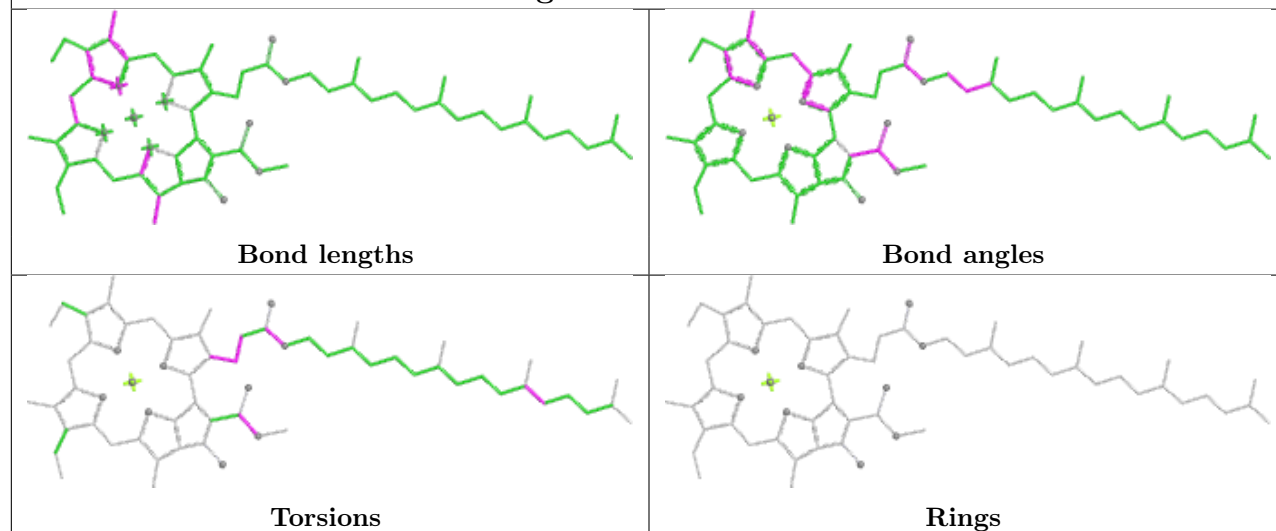
Ligand CLA 1 613

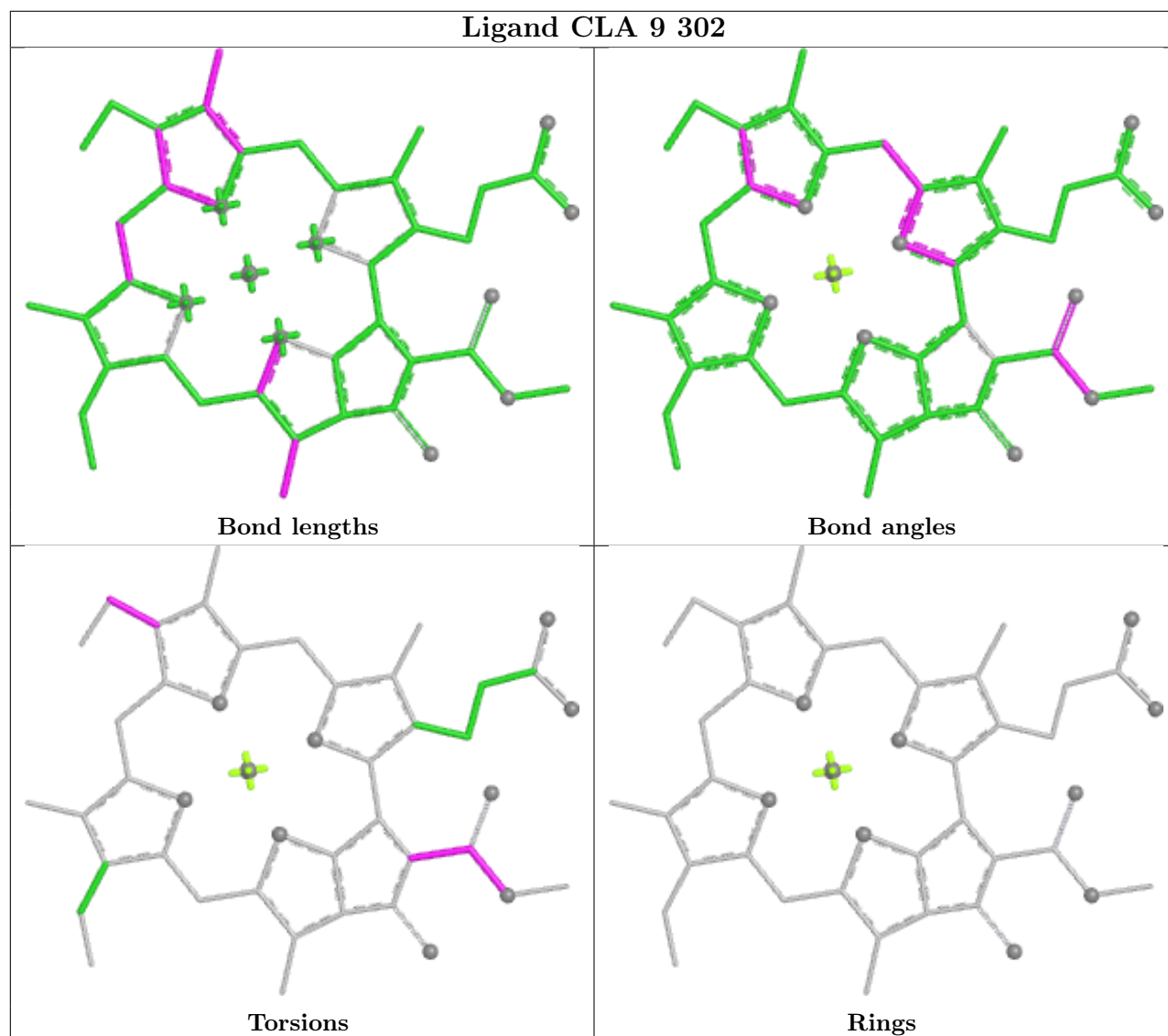
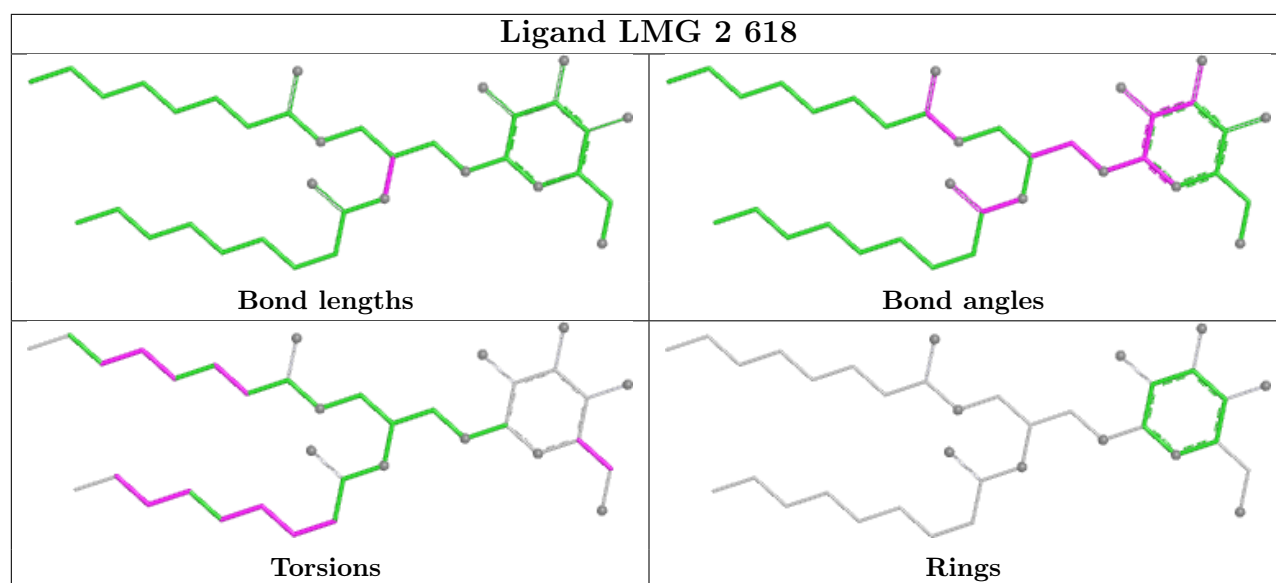


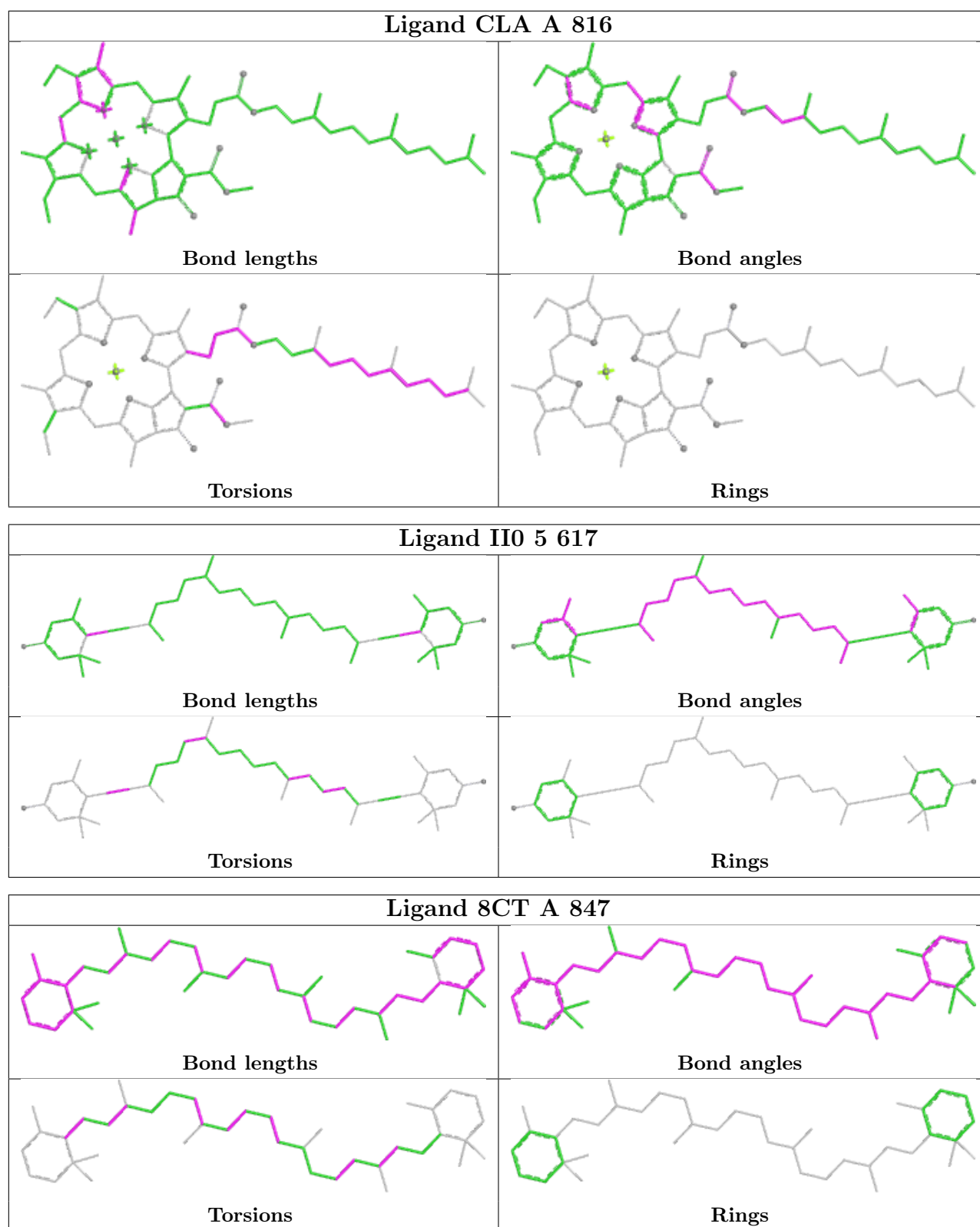
Ligand KC2 a 610



Ligand CLA 7 303







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

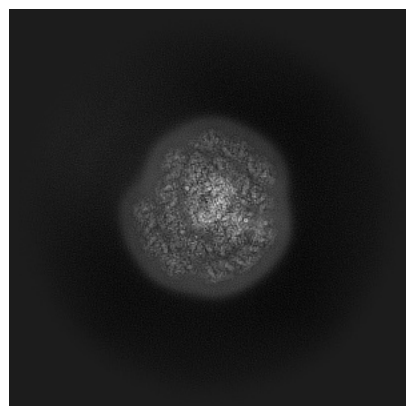
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66373. These allow visual inspection of the internal detail of the map and identification of artifacts.

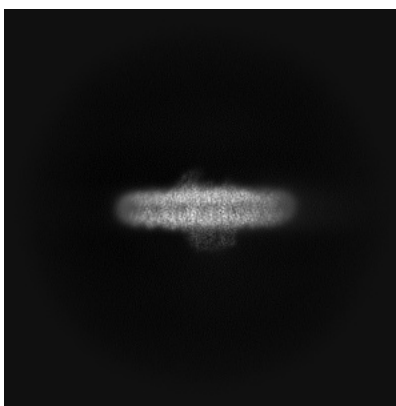
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

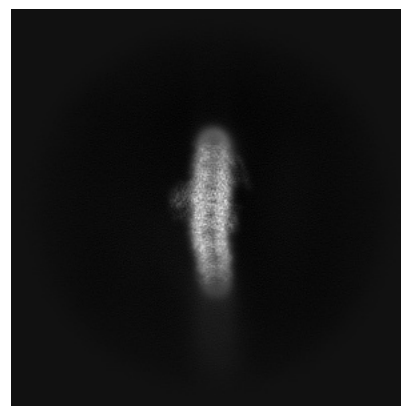
6.1.1 Primary map



X

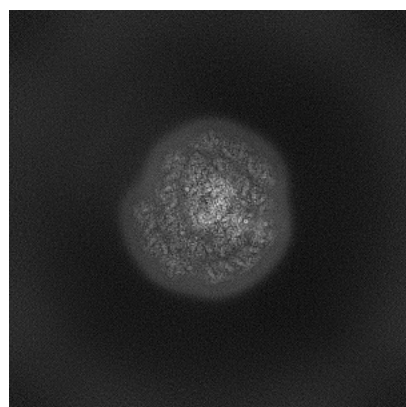


Y

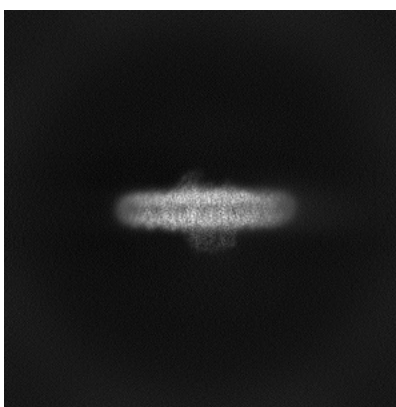


Z

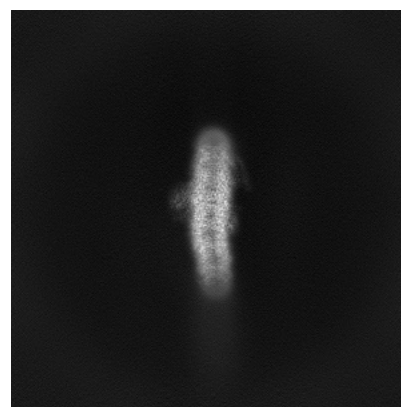
6.1.2 Raw map



X



Y

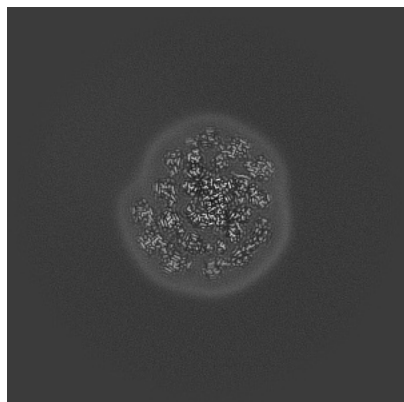


Z

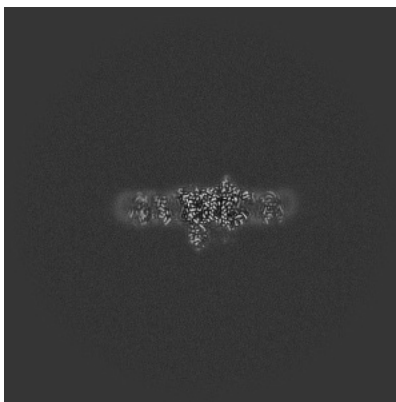
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

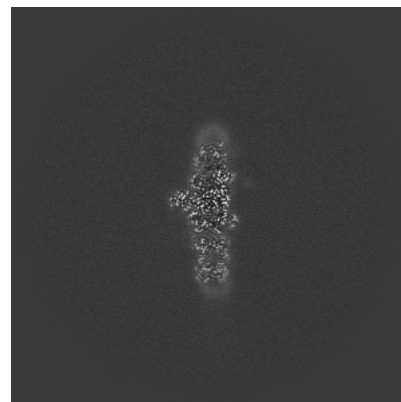
6.2.1 Primary map



X Index: 256

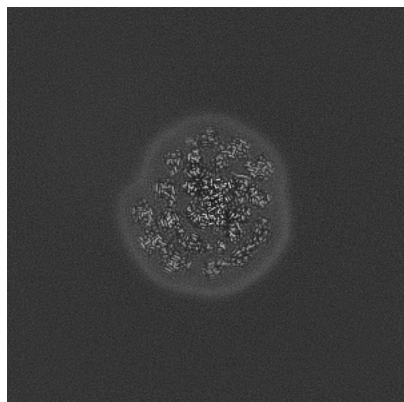


Y Index: 256

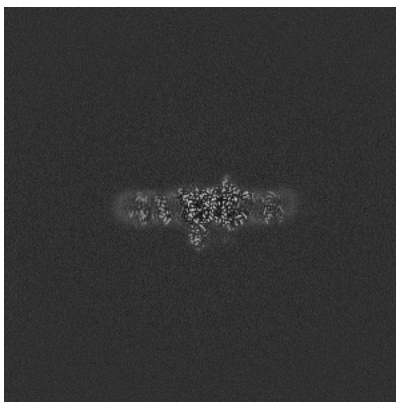


Z Index: 256

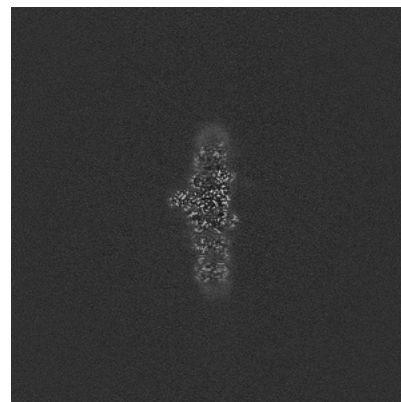
6.2.2 Raw map



X Index: 256



Y Index: 256

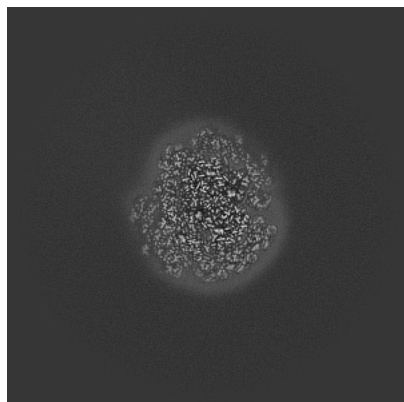


Z Index: 256

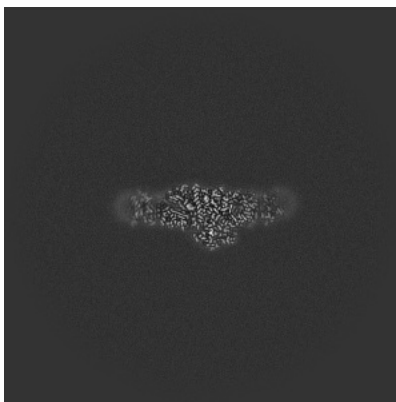
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

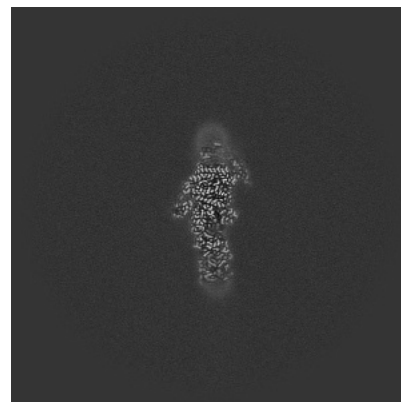
6.3.1 Primary map



X Index: 243

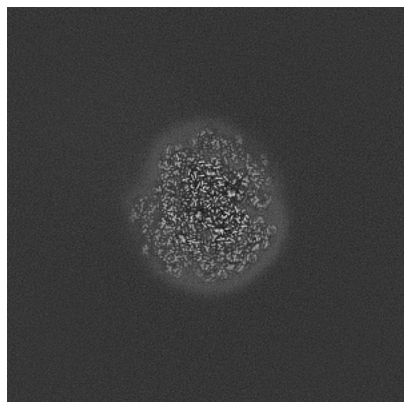


Y Index: 269

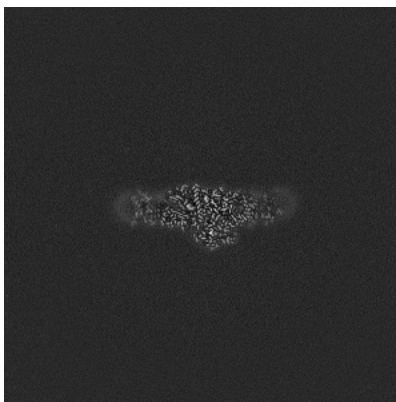


Z Index: 242

6.3.2 Raw map



X Index: 243



Y Index: 269

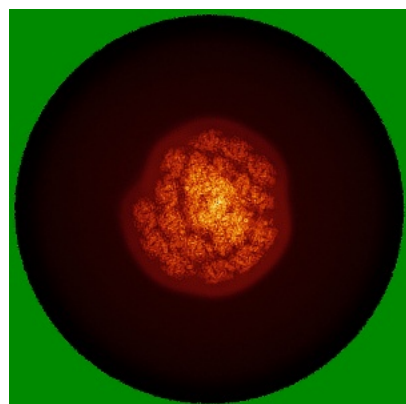


Z Index: 242

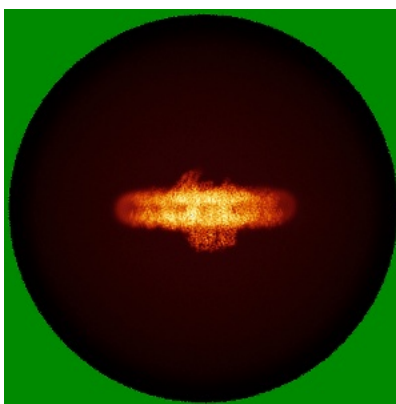
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

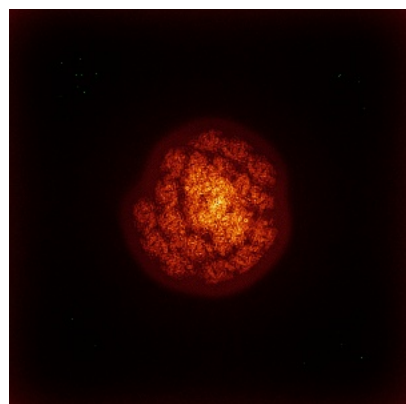


Y

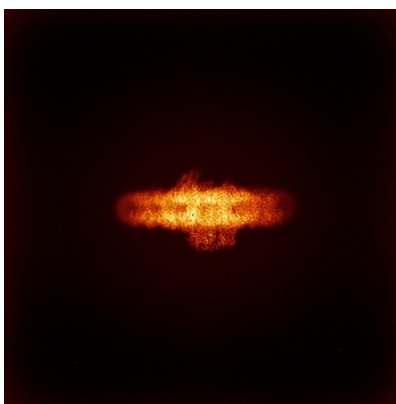


Z

6.4.2 Raw map



X



Y

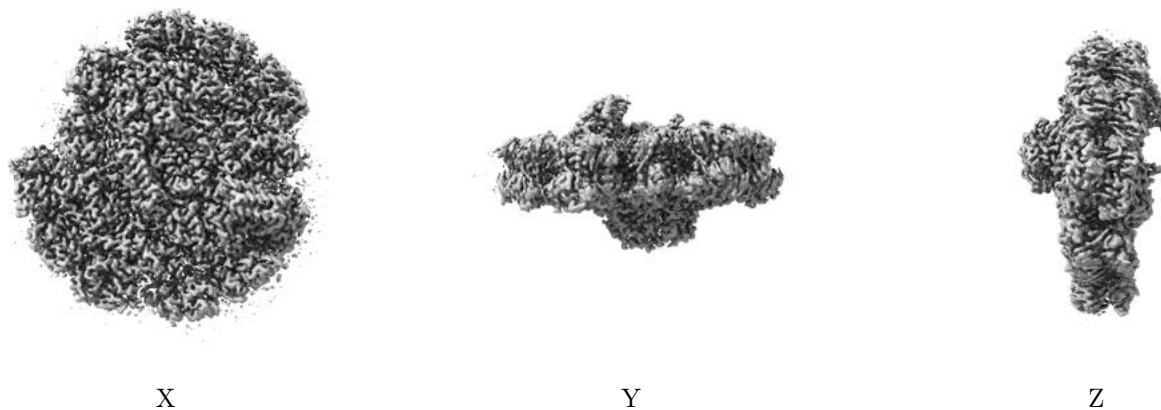


Z

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.

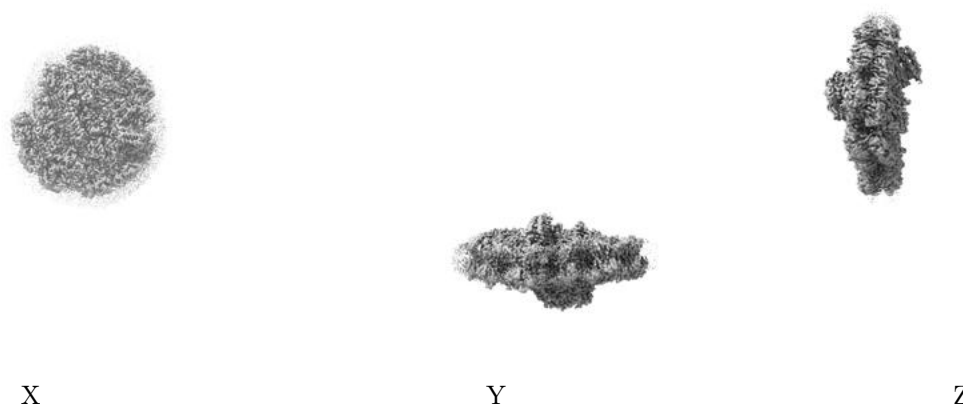
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

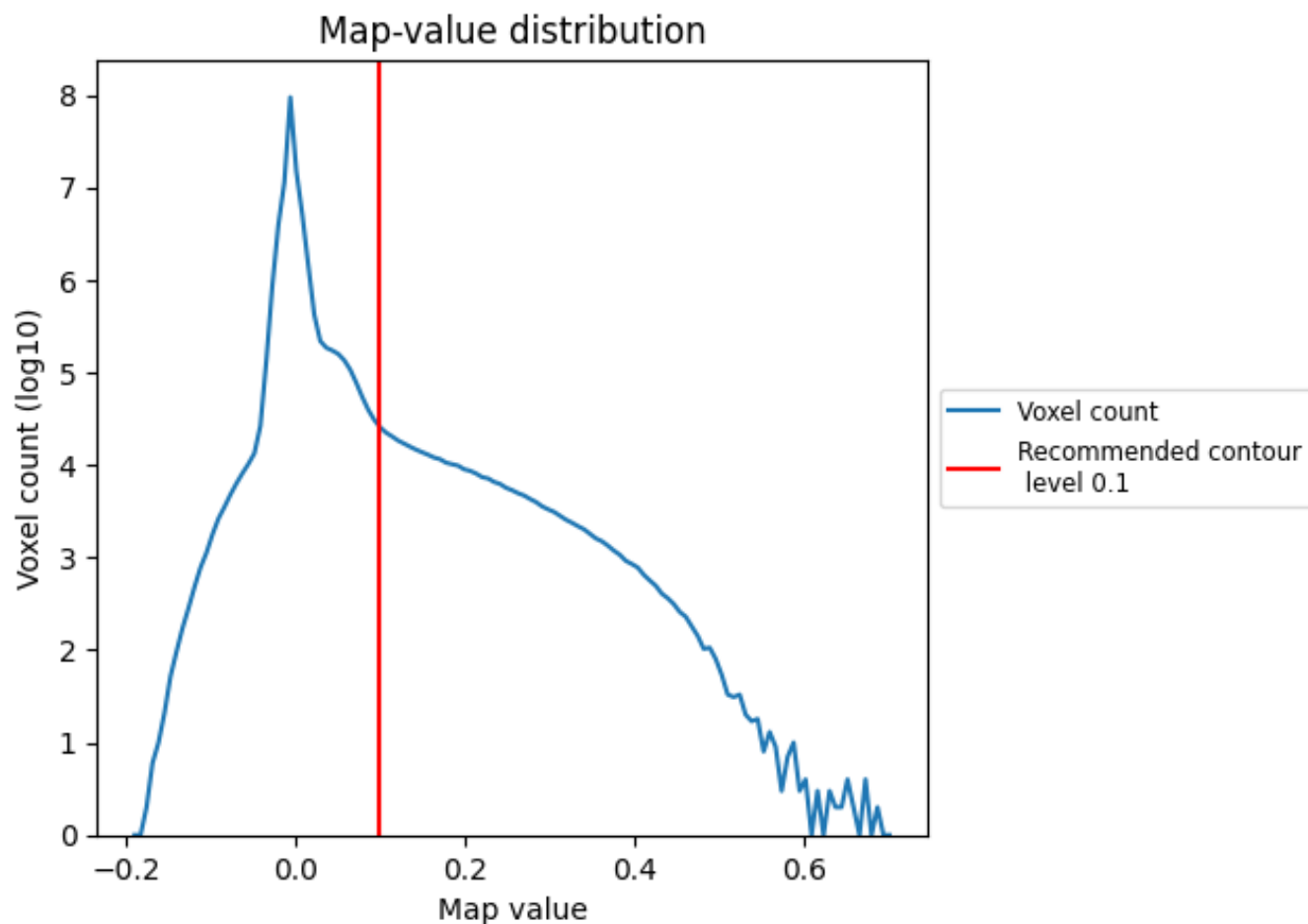
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

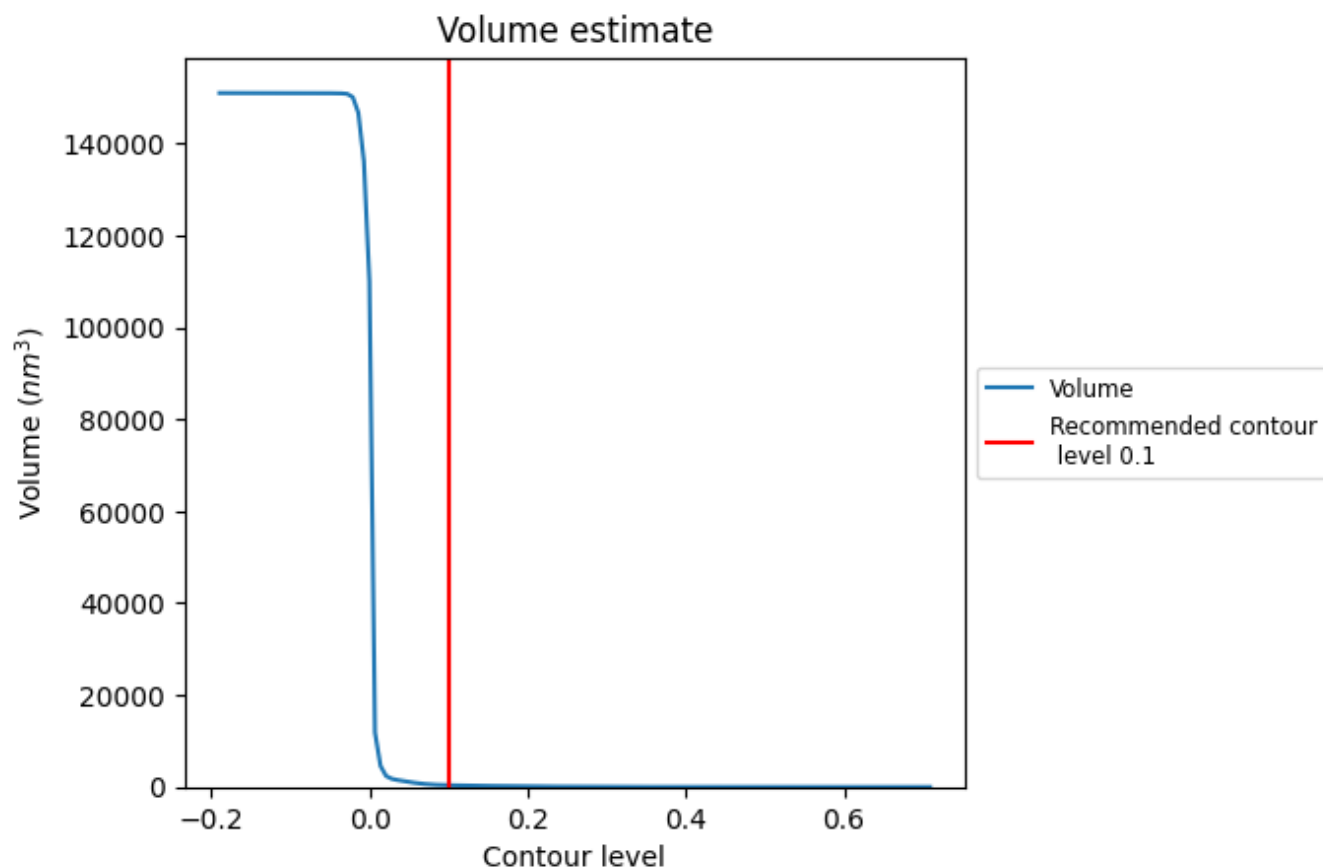
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

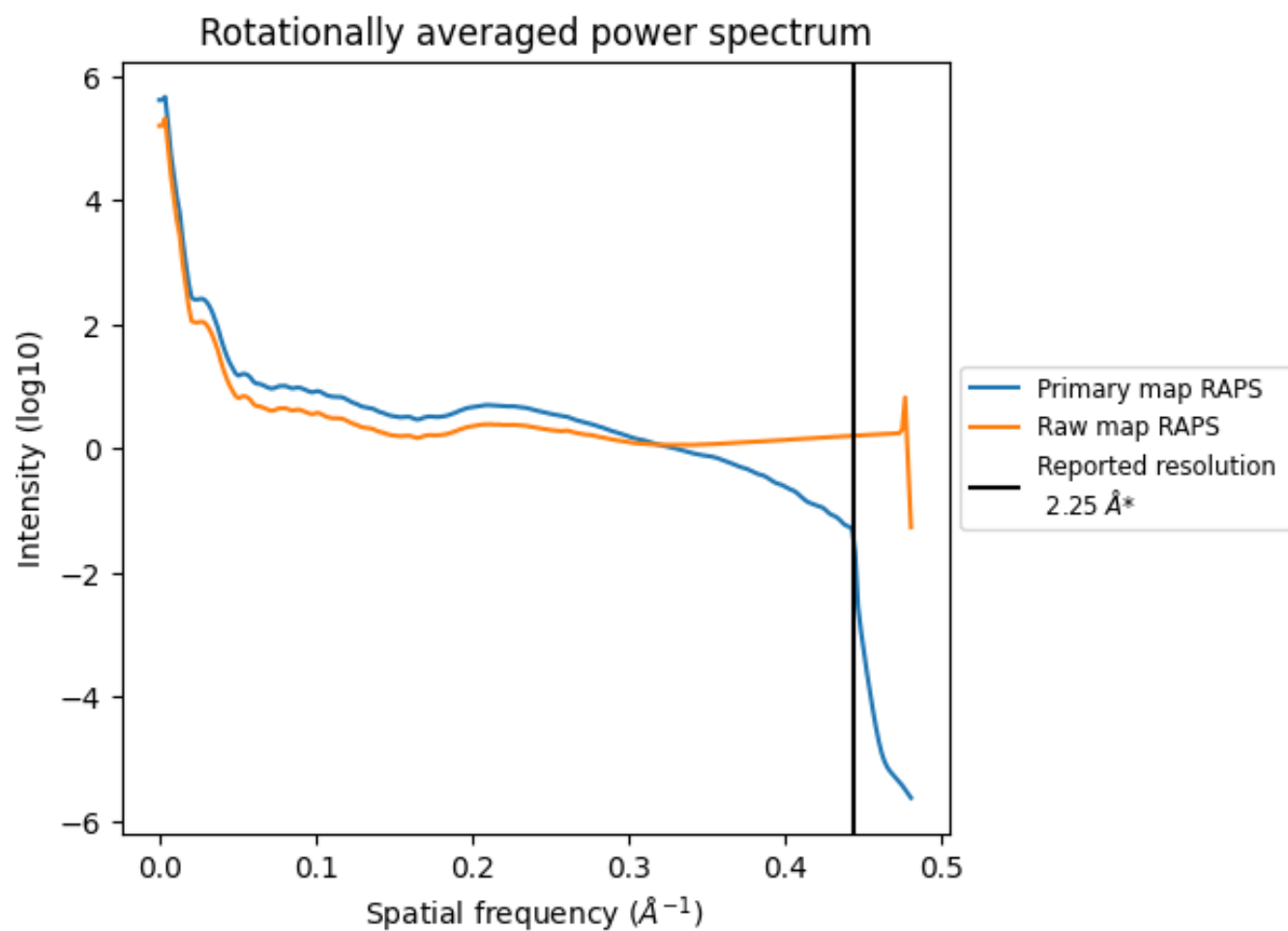
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm^3 ; this corresponds to an approximate mass of 341 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 ⓘ

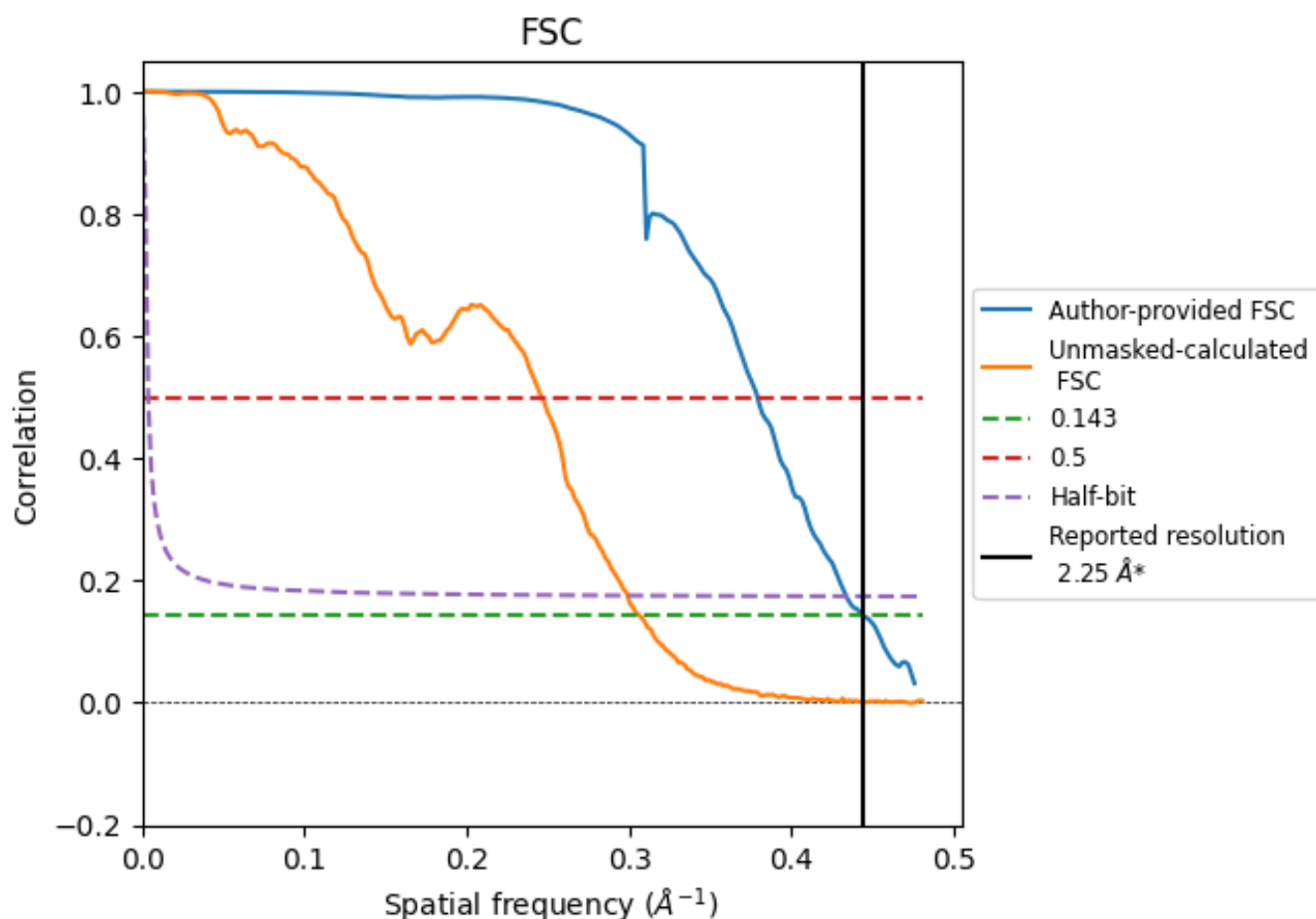


*Reported resolution corresponds to spatial frequency of $0.444 \text{ \AA}^{-1}$

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 0.444 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

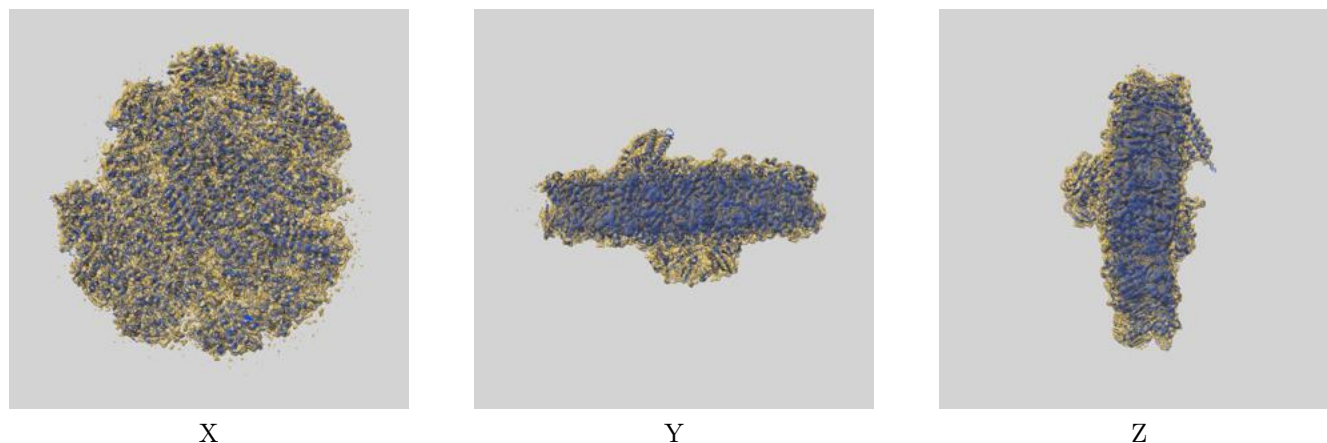
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.25	2.64	2.30
Unmasked-calculated*	3.27	4.06	3.34

*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 3.27 differs from the reported value 2.25 by more than 10 %

9 Map-model fit [i](#)

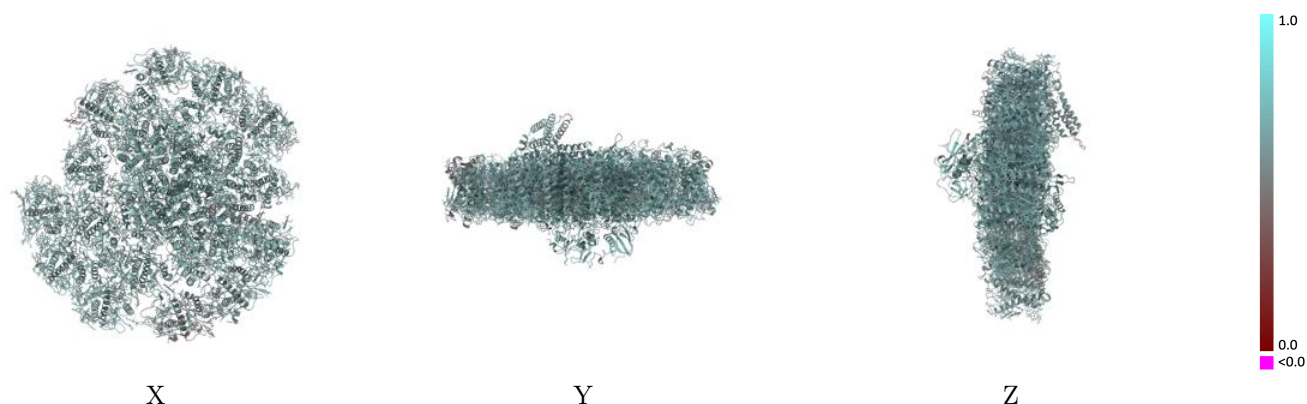
This section contains information regarding the fit between EMDB map EMD-66373 and PDB model 9WYP. Per-residue inclusion information can be found in [section 3](#) on [page 43](#).

9.1 Map-model overlay [i](#)



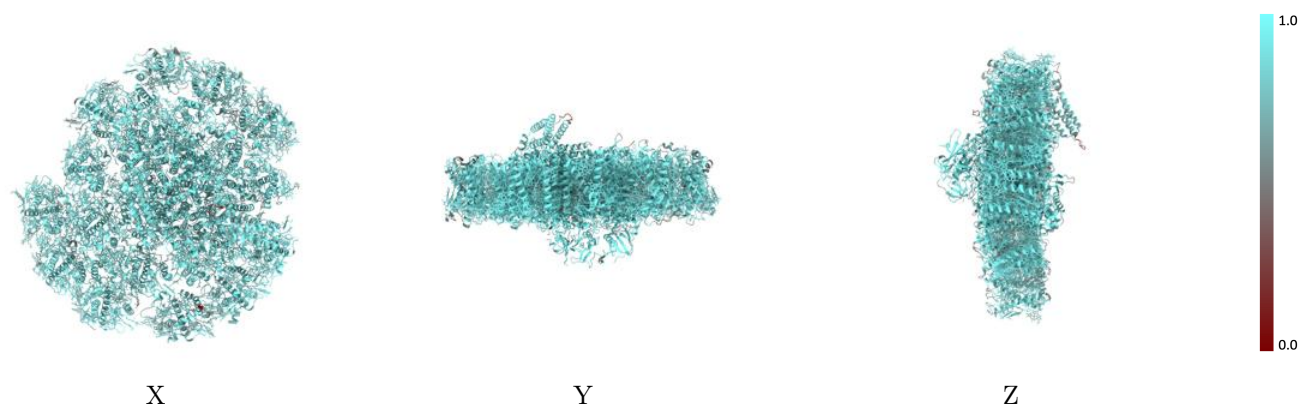
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



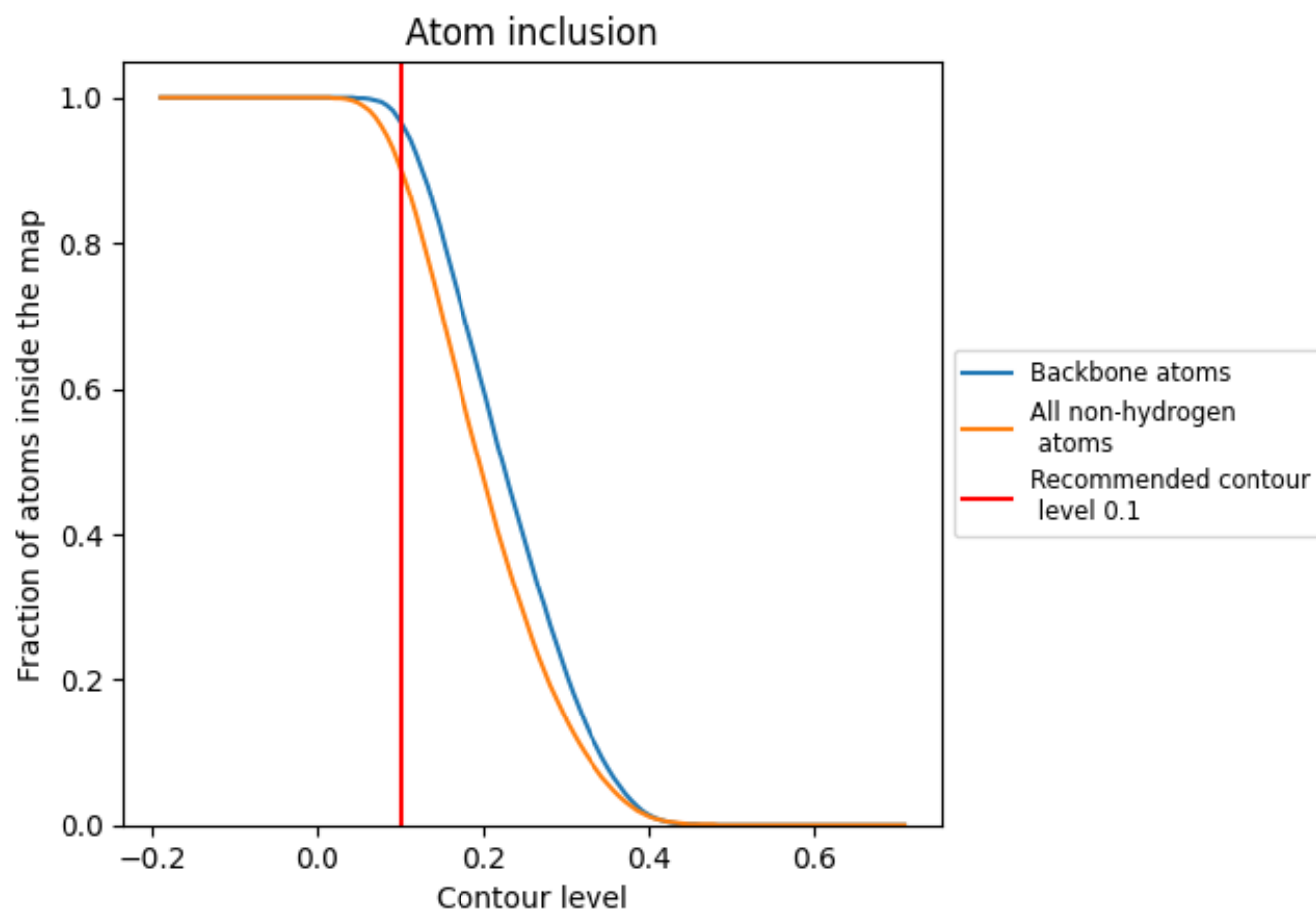
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 90% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9040	 0.6200
1	 0.8350	 0.5750
2	 0.9170	 0.6150
3	 0.9330	 0.6340
4	 0.9310	 0.6320
5	 0.7930	 0.5440
6	 0.8870	 0.5920
7	 0.9110	 0.5960
8	 0.8910	 0.6070
9	 0.8420	 0.6060
A	 0.9590	 0.6500
B	 0.9660	 0.6510
C	 0.9760	 0.6440
D	 0.9180	 0.6230
E	 0.9100	 0.6200
F	 0.9150	 0.6210
I	 0.9430	 0.6220
J	 0.9630	 0.6390
K	 0.9160	 0.6140
L	 0.9240	 0.6290
M	 0.9270	 0.6310
O	 0.9150	 0.6270
R	 0.9430	 0.6290
X	 0.8100	 0.5710
Z	 0.8620	 0.6150
a	 0.8790	 0.6160
b	 0.8800	 0.6070
c	 0.8240	 0.6010
d	 0.8440	 0.6140
e	 0.8300	 0.5990

