



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 03:52 PM JST

PDB ID : 5XNL
EMDB ID : EMD-6741
Title : Structure of stacked C2S2M2-type PSII-LHCII supercomplex from *Pisum sativum*
Authors : Su, X.D.; Ma, J.; Wei, X.P.; Cao, P.; Zhu, D.J.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on : 2017-05-23
Resolution : 2.70 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:

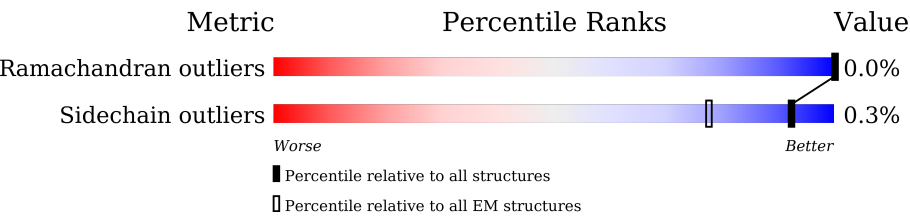
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 2.70 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	232	<div><div>93%</div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>6%</div></div>
1	2	232	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>93%</div><div>• 6%</div></div>
1	5	232	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>94%</div><div>6%</div></div>
1	6	232	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>93%</div><div>• 6%</div></div>
1	G	232	<div><div>27%</div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>6%</div></div>
1	N	232	<div><div>18%</div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>6%</div></div>
1	Y	232	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>6%</div></div>
1	g	232	<div><div>26%</div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>6%</div></div>
1	n	232	<div><div>18%</div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>6%</div></div>

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Mol	Chain	Length	Quality of chain
1	y	232	
2	3	243	
2	7	243	
3	4	210	
3	8	210	
4	A	344	
4	a	344	
5	B	507	
5	b	507	
6	C	473	
6	c	473	
7	D	353	
7	d	353	
8	E	83	
8	e	83	
9	F	39	
9	f	39	
10	H	73	
10	h	73	
11	I	36	
11	i	36	
12	J	40	
12	j	40	
13	K	61	
13	k	61	

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Mol	Chain	Length	Quality of chain
14	L	38	
14	l	38	
15	M	34	
15	m	34	
16	O	248	
16	o	248	
17	P	186	
17	p	186	
18	Q	148	
18	q	148	
19	R	246	
19	r	246	
20	S	244	
20	s	244	
21	T	35	
21	t	35	
22	W	54	
22	w	54	
23	X	86	
23	x	86	
24	Z	62	
24	z	62	

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
25	CHL	1	601	X	-	-	-
25	CHL	1	605	X	-	-	-
25	CHL	1	606	X	-	-	-
25	CHL	1	607	X	-	-	-
25	CHL	1	608	X	-	-	-
25	CHL	1	609	X	-	-	-
25	CHL	2	601	X	-	-	-
25	CHL	2	605	X	-	-	-
25	CHL	2	606	X	-	-	-
25	CHL	2	607	X	-	-	-
25	CHL	2	608	X	-	-	-
25	CHL	2	609	X	-	-	-
25	CHL	3	601	X	-	-	-
25	CHL	3	605	X	-	-	-
25	CHL	3	606	X	-	-	-
25	CHL	3	607	X	-	-	-
25	CHL	3	608	X	-	-	-
25	CHL	3	609	X	-	-	-
25	CHL	4	601	X	-	-	-
25	CHL	4	606	X	-	-	-
25	CHL	4	607	X	-	-	-
25	CHL	4	608	X	-	-	-
25	CHL	4	609	X	-	-	-
25	CHL	5	601	X	-	-	-
25	CHL	5	605	X	-	-	-
25	CHL	5	606	X	-	-	-
25	CHL	5	607	X	-	-	-
25	CHL	5	608	X	-	-	-
25	CHL	5	609	X	-	-	-
25	CHL	6	601	X	-	-	-
25	CHL	6	605	X	-	-	-
25	CHL	6	606	X	-	-	-
25	CHL	6	607	X	-	-	-
25	CHL	6	608	X	-	-	-
25	CHL	6	609	X	-	-	-
25	CHL	7	601	X	-	-	-
25	CHL	7	605	X	-	-	-
25	CHL	7	606	X	-	-	-
25	CHL	7	607	X	-	-	-
25	CHL	7	608	X	-	-	-
25	CHL	7	609	X	-	-	-
25	CHL	8	601	X	-	-	-
25	CHL	8	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CHL	8	607	X	-	-	-
25	CHL	8	608	X	-	-	-
25	CHL	8	609	X	-	-	-
25	CHL	G	601	X	-	-	-
25	CHL	G	605	X	-	-	-
25	CHL	G	606	X	-	-	-
25	CHL	G	607	X	-	-	-
25	CHL	G	608	X	-	-	-
25	CHL	G	609	X	-	-	-
25	CHL	N	601	X	-	-	-
25	CHL	N	605	X	-	-	-
25	CHL	N	606	X	-	-	-
25	CHL	N	607	X	-	-	-
25	CHL	N	608	X	-	-	-
25	CHL	N	609	X	-	-	-
25	CHL	R	606	X	-	-	-
25	CHL	R	607	X	-	-	-
25	CHL	R	608	X	-	-	-
25	CHL	R	614	X	-	-	-
25	CHL	S	601	X	-	-	-
25	CHL	S	606	X	-	-	-
25	CHL	S	607	X	-	-	-
25	CHL	S	608	X	-	-	-
25	CHL	Y	601	X	-	-	-
25	CHL	Y	605	X	-	-	-
25	CHL	Y	606	X	-	-	-
25	CHL	Y	607	X	-	-	-
25	CHL	Y	608	X	-	-	-
25	CHL	Y	609	X	-	-	-
25	CHL	g	601	X	-	-	-
25	CHL	g	605	X	-	-	-
25	CHL	g	606	X	-	-	-
25	CHL	g	607	X	-	-	-
25	CHL	g	608	X	-	-	-
25	CHL	g	609	X	-	-	-
25	CHL	n	601	X	-	-	-
25	CHL	n	605	X	-	-	-
25	CHL	n	606	X	-	-	-
25	CHL	n	607	X	-	-	-
25	CHL	n	608	X	-	-	-
25	CHL	n	609	X	-	-	-
25	CHL	r	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CHL	r	607	X	-	-	-
25	CHL	r	608	X	-	-	-
25	CHL	r	614	X	-	-	-
25	CHL	s	601	X	-	-	-
25	CHL	s	606	X	-	-	-
25	CHL	s	607	X	-	-	-
25	CHL	s	608	X	-	-	-
25	CHL	y	601	X	-	-	-
25	CHL	y	605	X	-	-	-
25	CHL	y	606	X	-	-	-
25	CHL	y	607	X	-	-	-
25	CHL	y	608	X	-	-	-
25	CHL	y	609	X	-	-	-
26	CLA	1	602	X	-	-	-
26	CLA	1	603	X	-	-	-
26	CLA	1	610	X	-	-	-
26	CLA	1	611	X	-	-	-
26	CLA	1	612	X	-	-	-
26	CLA	1	614	X	-	-	-
26	CLA	2	602	X	-	-	-
26	CLA	2	603	X	-	-	-
26	CLA	2	604	X	-	-	-
26	CLA	2	610	X	-	-	-
26	CLA	2	612	X	-	-	-
26	CLA	2	614	X	-	-	-
26	CLA	3	602	X	-	-	-
26	CLA	3	603	X	-	-	-
26	CLA	3	604	X	-	-	-
26	CLA	3	610	X	-	-	-
26	CLA	3	611	X	-	-	-
26	CLA	3	612	X	-	-	-
26	CLA	3	613	X	-	-	-
26	CLA	3	614	X	-	-	-
26	CLA	4	602	X	-	-	-
26	CLA	4	603	X	-	-	-
26	CLA	4	610	X	-	-	-
26	CLA	4	611	X	-	-	-
26	CLA	4	612	X	-	-	-
26	CLA	5	602	X	-	-	-
26	CLA	5	603	X	-	-	-
26	CLA	5	610	X	-	-	-
26	CLA	5	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	5	612	X	-	-	-
26	CLA	5	614	X	-	-	-
26	CLA	6	602	X	-	-	-
26	CLA	6	603	X	-	-	-
26	CLA	6	604	X	-	-	-
26	CLA	6	610	X	-	-	-
26	CLA	6	612	X	-	-	-
26	CLA	6	614	X	-	-	-
26	CLA	7	602	X	-	-	-
26	CLA	7	603	X	-	-	-
26	CLA	7	604	X	-	-	-
26	CLA	7	610	X	-	-	-
26	CLA	7	611	X	-	-	-
26	CLA	7	612	X	-	-	-
26	CLA	7	613	X	-	-	-
26	CLA	7	614	X	-	-	-
26	CLA	8	602	X	-	-	-
26	CLA	8	603	X	-	-	-
26	CLA	8	610	X	-	-	-
26	CLA	8	611	X	-	-	-
26	CLA	8	612	X	-	-	-
26	CLA	A	405	X	-	-	-
26	CLA	A	406	X	-	-	-
26	CLA	A	410	X	-	-	-
26	CLA	B	602	X	-	-	-
26	CLA	B	603	X	-	-	-
26	CLA	B	604	X	-	-	-
26	CLA	B	605	X	-	-	-
26	CLA	B	606	X	-	-	-
26	CLA	B	607	X	-	-	-
26	CLA	B	608	X	-	-	-
26	CLA	B	611	X	-	-	-
26	CLA	B	612	X	-	-	-
26	CLA	B	613	X	-	-	-
26	CLA	B	614	X	-	-	-
26	CLA	B	615	X	-	-	-
26	CLA	B	616	X	-	-	-
26	CLA	B	617	X	-	-	-
26	CLA	C	501	X	-	-	-
26	CLA	C	502	X	-	-	-
26	CLA	C	503	X	-	-	-
26	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	C	505	X	-	-	-
26	CLA	C	506	X	-	-	-
26	CLA	C	507	X	-	-	-
26	CLA	C	508	X	-	-	-
26	CLA	C	509	X	-	-	-
26	CLA	C	510	X	-	-	-
26	CLA	C	511	X	-	-	-
26	CLA	C	512	X	-	-	-
26	CLA	D	402	X	-	-	-
26	CLA	G	602	X	-	-	-
26	CLA	G	603	X	-	-	-
26	CLA	G	604	X	-	-	-
26	CLA	G	610	X	-	-	-
26	CLA	G	611	X	-	-	-
26	CLA	G	612	X	-	-	-
26	CLA	G	613	X	-	-	-
26	CLA	G	614	X	-	-	-
26	CLA	N	602	X	-	-	-
26	CLA	N	603	X	-	-	-
26	CLA	N	604	X	-	-	-
26	CLA	N	610	X	-	-	-
26	CLA	N	611	X	-	-	-
26	CLA	N	612	X	-	-	-
26	CLA	N	613	X	-	-	-
26	CLA	N	614	X	-	-	-
26	CLA	R	601	X	-	-	-
26	CLA	R	602	X	-	-	-
26	CLA	R	603	X	-	-	-
26	CLA	R	604	X	-	-	-
26	CLA	R	609	X	-	-	-
26	CLA	R	610	X	-	-	-
26	CLA	R	611	X	-	-	-
26	CLA	R	612	X	-	-	-
26	CLA	R	613	X	-	-	-
26	CLA	S	602	X	-	-	-
26	CLA	S	603	X	-	-	-
26	CLA	S	604	X	-	-	-
26	CLA	S	609	X	-	-	-
26	CLA	S	610	X	-	-	-
26	CLA	S	611	X	-	-	-
26	CLA	S	612	X	-	-	-
26	CLA	S	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	S	614	X	-	-	-
26	CLA	Y	602	X	-	-	-
26	CLA	Y	603	X	-	-	-
26	CLA	Y	604	X	-	-	-
26	CLA	Y	610	X	-	-	-
26	CLA	Y	611	X	-	-	-
26	CLA	Y	612	X	-	-	-
26	CLA	Y	613	X	-	-	-
26	CLA	Y	614	X	-	-	-
26	CLA	a	405	X	-	-	-
26	CLA	a	406	X	-	-	-
26	CLA	a	410	X	-	-	-
26	CLA	b	602	X	-	-	-
26	CLA	b	603	X	-	-	-
26	CLA	b	604	X	-	-	-
26	CLA	b	605	X	-	-	-
26	CLA	b	606	X	-	-	-
26	CLA	b	607	X	-	-	-
26	CLA	b	608	X	-	-	-
26	CLA	b	611	X	-	-	-
26	CLA	b	612	X	-	-	-
26	CLA	b	613	X	-	-	-
26	CLA	b	614	X	-	-	-
26	CLA	b	615	X	-	-	-
26	CLA	b	616	X	-	-	-
26	CLA	b	617	X	-	-	-
26	CLA	c	501	X	-	-	-
26	CLA	c	502	X	-	-	-
26	CLA	c	503	X	-	-	-
26	CLA	c	504	X	-	-	-
26	CLA	c	505	X	-	-	-
26	CLA	c	506	X	-	-	-
26	CLA	c	507	X	-	-	-
26	CLA	c	508	X	-	-	-
26	CLA	c	509	X	-	-	-
26	CLA	c	510	X	-	-	-
26	CLA	c	511	X	-	-	-
26	CLA	c	512	X	-	-	-
26	CLA	d	402	X	-	-	-
26	CLA	g	602	X	-	-	-
26	CLA	g	603	X	-	-	-
26	CLA	g	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	g	610	X	-	-	-
26	CLA	g	611	X	-	-	-
26	CLA	g	612	X	-	-	-
26	CLA	g	613	X	-	-	-
26	CLA	g	614	X	-	-	-
26	CLA	n	602	X	-	-	-
26	CLA	n	603	X	-	-	-
26	CLA	n	604	X	-	-	-
26	CLA	n	610	X	-	-	-
26	CLA	n	611	X	-	-	-
26	CLA	n	612	X	-	-	-
26	CLA	n	613	X	-	-	-
26	CLA	n	614	X	-	-	-
26	CLA	r	601	X	-	-	-
26	CLA	r	602	X	-	-	-
26	CLA	r	603	X	-	-	-
26	CLA	r	604	X	-	-	-
26	CLA	r	609	X	-	-	-
26	CLA	r	610	X	-	-	-
26	CLA	r	611	X	-	-	-
26	CLA	r	612	X	-	-	-
26	CLA	r	613	X	-	-	-
26	CLA	s	602	X	-	-	-
26	CLA	s	603	X	-	-	-
26	CLA	s	604	X	-	-	-
26	CLA	s	609	X	-	-	-
26	CLA	s	610	X	-	-	-
26	CLA	s	611	X	-	-	-
26	CLA	s	612	X	-	-	-
26	CLA	s	613	X	-	-	-
26	CLA	s	614	X	-	-	-
26	CLA	y	602	X	-	-	-
26	CLA	y	603	X	-	-	-
26	CLA	y	604	X	-	-	-
26	CLA	y	610	X	-	-	-
26	CLA	y	611	X	-	-	-
26	CLA	y	612	X	-	-	-
26	CLA	y	613	X	-	-	-
26	CLA	y	614	X	-	-	-

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 98986 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 Chlorophyll a-b binding protein 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	2	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		
1	G	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	N	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	Y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	5	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	6	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		
1	g	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	n	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		
2	7	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		

- Molecule 3 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

- Molecule 4 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		
4	a	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		

- Molecule 5 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	503	Total	C	N	O	S	0	0
			3948	2581	669	686	12		
5	b	503	Total	C	N	O	S	0	0
			3948	2581	669	686	12		

- Molecule 6 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		
6	c	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		

- Molecule 7 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	341	Total	C	N	O	S	0	0
			2712	1790	444	466	12		
7	d	341	Total	C	N	O	S	0	0
			2712	1790	444	466	12		

- Molecule 8 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	75	Total	C	N	O	0	0
			612	400	100	112		
8	e	75	Total	C	N	O	0	0
			612	400	100	112		

- Molecule 9 is a protein called Cytochrome b559 subunit beta, PsbF.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	30	Total	C	N	O	S	0	0
			241	162	41	37	1		
9	f	30	Total	C	N	O	S	0	0
			241	162	41	37	1		

- Molecule 10 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	60	Total	C	N	O	S	0	0
			452	296	72	81	3		
10	h	60	Total	C	N	O	S	0	0
			452	296	72	81	3		

- Molecule 11 is a protein called Photosystem II reaction center protein I, PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	34	Total	C	N	O	S	0	0
			278	191	43	43	1		
11	i	34	Total	C	N	O	S	0	0
			278	191	43	43	1		

- Molecule 12 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	35	Total	C	N	O	0	0
			256	174	39	43		
12	j	35	Total	C	N	O	0	0
			256	174	39	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	37	Total	C	N	O	S	0	0
			306	215	44	46	1		
13	k	37	Total	C	N	O	S	0	0
			306	215	44	46	1		

- Molecule 14 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	37	Total	C	N	O	0	0
			311	205	49	57		
14	l	37	Total	C	N	O	0	0
			311	205	49	57		

- Molecule 15 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	33	Total	C	N	O	S	0	0
			256	176	36	43	1		
15	m	33	Total	C	N	O	S	0	0
			256	176	36	43	1		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		
16	o	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		

- Molecule 17 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	186	Total	C	N	O	S	0	0
			1434	909	238	286	1		
17	p	186	Total	C	N	O	S	0	0
			1434	909	238	286	1		

- Molecule 18 is a protein called Oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Q	129	Total	C	N	O	0	0
			1034	661	177	196		
18	q	129	Total	C	N	O	0	0
			1034	661	177	196		

- Molecule 19 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	234	Total	C	N	O	S	0	0
			1835	1194	297	341	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	r	234	Total	C	N	O	S	0	0
			1835	1194	297	341	3		

- Molecule 20 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	218	Total	C	N	O	S	0	0
			1689	1107	273	305	4		
20	s	218	Total	C	N	O	S	0	0
			1689	1107	273	305	4		

- Molecule 21 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	32	Total	C	N	O	S	0	0
			261	182	37	41	1		
21	t	32	Total	C	N	O	S	0	0
			261	182	37	41	1		

- Molecule 22 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	54	Total	C	N	O	S	0	0
			419	275	61	82	1		
22	w	54	Total	C	N	O	S	0	0
			419	275	61	82	1		

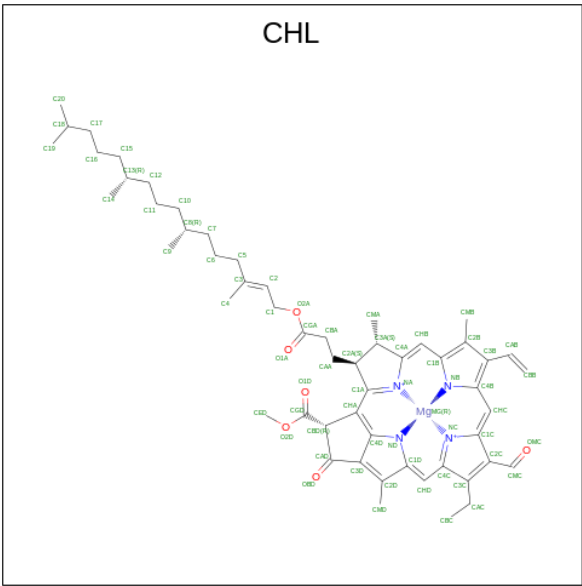
- Molecule 23 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	39	Total	C	N	O	0	0
			276	180	46	50		
23	x	39	Total	C	N	O	0	0
			276	180	46	50		

- Molecule 24 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	62	Total	C	N	O	S	0	0
			464	312	69	82	1		
24	z	62	Total	C	N	O	S	0	0
			464	312	69	82	1		

- Molecule 25 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
			Total	C	Mg	N	O	
			309	243	6	24	36	
			Total	C	Mg	N	O	
25	1	1	309	243	6	24	36	0
			Total	C	Mg	N	O	
			309	243	6	24	36	
			Total	C	Mg	N	O	
			309	243	6	24	36	
25	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
			Total	C	Mg	N	O	
			309	243	6	24	36	
			Total	C	Mg	N	O	
25	1	1	309	243	6	24	36	0
			Total	C	Mg	N	O	
			306	240	6	24	36	
			Total	C	Mg	N	O	
			306	240	6	24	36	
25	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
			Total	C	Mg	N	O	
			306	240	6	24	36	
			Total	C	Mg	N	O	
25	2	1	306	240	6	24	36	0
			Total	C	Mg	N	O	
			306	240	6	24	36	
			Total	C	Mg	N	O	
			306	240	6	24	36	
25	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
			Total	C	Mg	N	O	
			306	240	6	24	36	
			Total	C	Mg	N	O	
25	2	1	306	240	6	24	36	0
			Total	C	Mg	N	O	
			306	240	6	24	36	
			Total	C	Mg	N	O	
			306	240	6	24	36	
25	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
			Total	C	Mg	N	O	
			316	250	6	24	36	
			Total	C	Mg	N	O	

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	R	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	R	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	R	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	R	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	S	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	S	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	S	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	S	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	Y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	Y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	Y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	Y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	Y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	Y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	5	1	Total 309	C 243	Mg 6	N 24	O 36	0
25	5	1	Total 309	C 243	Mg 6	N 24	O 36	0
25	5	1	Total 309	C 243	Mg 6	N 24	O 36	0
25	5	1	Total 309	C 243	Mg 6	N 24	O 36	0
25	5	1	Total 309	C 243	Mg 6	N 24	O 36	0
25	5	1	Total 309	C 243	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0

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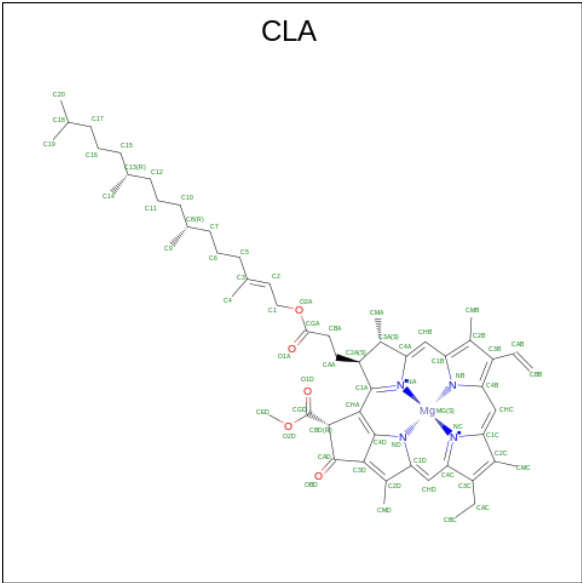
Mol	Chain	Residues	Atoms					AltConf
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	r	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	r	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	r	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	r	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	y	1	362	296	6	24	36	0

- Molecule 26 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	1	1	Total 412	332	8	32	40	0
26	1	1	Total 412	332	8	32	40	0
26	1	1	Total 412	332	8	32	40	0
26	1	1	Total 412	332	8	32	40	0
26	1	1	Total 412	332	8	32	40	0
26	1	1	Total 412	332	8	32	40	0
26	1	1	Total 412	332	8	32	40	0
26	1	1	Total 412	332	8	32	40	0
26	2	1	Total 391	311	8	32	40	0
26	2	1	Total 391	311	8	32	40	0

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Mol	Chain	Residues	Atoms					AltConf
26	2	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	2	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	2	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	2	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	2	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	2	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	4	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	4	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	4	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	4	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	4	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	4	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	4	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	A	1	Total 240	C 200	Mg 4	N 16	O 20	0

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Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	D	1	Total 130	C 110	Mg 2	N 8	O 10	0
26	D	1	Total 130	C 110	Mg 2	N 8	O 10	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0

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Mol	Chain	Residues	Atoms					AltConf
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	8	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	8	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	8	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	8	1	Total 270	C 210	Mg 6	N 24	O 30	0

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Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
26	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	

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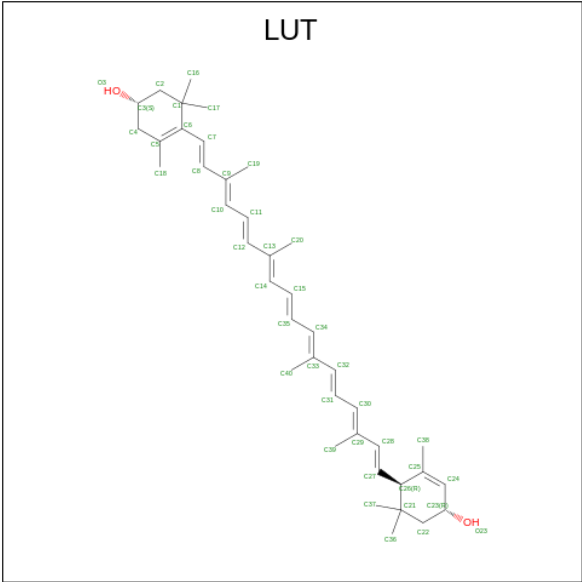
Mol	Chain	Residues	Atoms					AltConf
26	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0

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Mol	Chain	Residues	Atoms					AltConf
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0

- Molecule 27 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



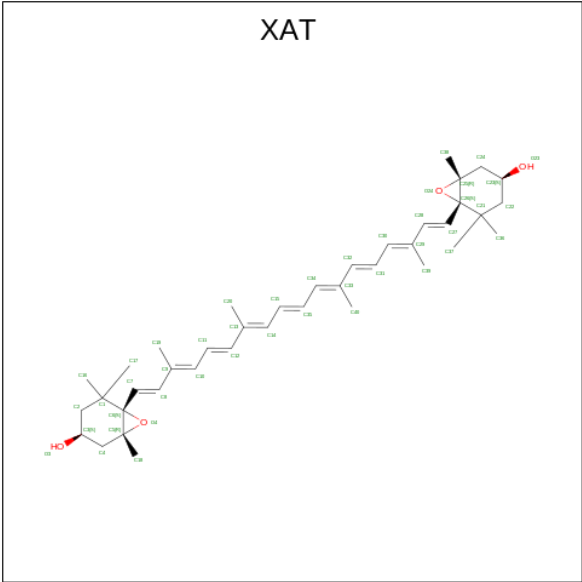
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			84	80	4	
27	1	1	Total	C	O	0
			84	80	4	
27	2	1	Total	C	O	0
			84	80	4	
27	2	1	Total	C	O	0
			84	80	4	
27	3	1	Total	C	O	0
			84	80	4	
27	3	1	Total	C	O	0
			84	80	4	
27	4	1	Total	C	O	0
			42	40	2	
27	G	1	Total	C	O	0
			84	80	4	
27	G	1	Total	C	O	0
			84	80	4	
27	N	1	Total	C	O	0
			84	80	4	
27	N	1	Total	C	O	0
			84	80	4	
27	R	1	Total	C	O	0
			42	40	2	
27	S	1	Total	C	O	0
			84	80	4	
27	S	1	Total	C	O	0
			84	80	4	

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Mol	Chain	Residues	Atoms			AltConf
27	Y	1	Total	C	O	0
			84	80	4	
27	Y	1	Total	C	O	0
			84	80	4	
27	5	1	Total	C	O	0
			84	80	4	
27	5	1	Total	C	O	0
			84	80	4	
27	6	1	Total	C	O	0
			84	80	4	
27	6	1	Total	C	O	0
			84	80	4	
27	7	1	Total	C	O	0
			84	80	4	
27	7	1	Total	C	O	0
			84	80	4	
27	8	1	Total	C	O	0
			42	40	2	
27	g	1	Total	C	O	0
			84	80	4	
27	g	1	Total	C	O	0
			84	80	4	
27	n	1	Total	C	O	0
			84	80	4	
27	n	1	Total	C	O	0
			84	80	4	
27	r	1	Total	C	O	0
			42	40	2	
27	s	1	Total	C	O	0
			84	80	4	
27	s	1	Total	C	O	0
			84	80	4	
27	y	1	Total	C	O	0
			84	80	4	
27	y	1	Total	C	O	0
			84	80	4	

- Molecule 28 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



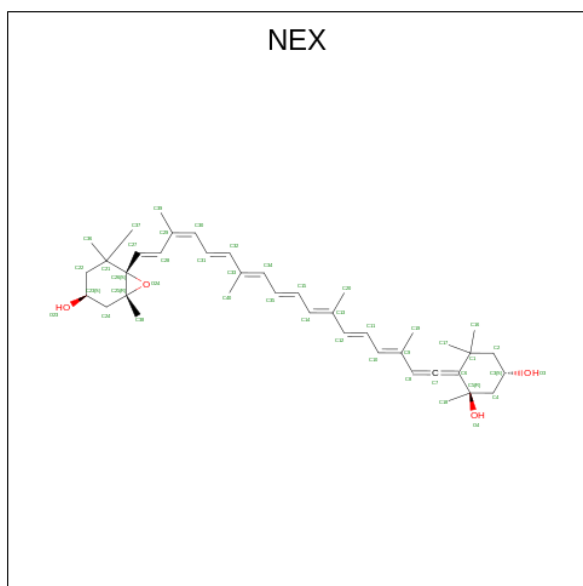
Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total	C	O	0
			44	40	4	
28	2	1	Total	C	O	0
			44	40	4	
28	3	1	Total	C	O	0
			44	40	4	
28	4	1	Total	C	O	0
			44	40	4	
28	G	1	Total	C	O	0
			44	40	4	
28	N	1	Total	C	O	0
			44	40	4	
28	R	1	Total	C	O	0
			44	40	4	
28	Y	1	Total	C	O	0
			44	40	4	
28	5	1	Total	C	O	0
			44	40	4	
28	6	1	Total	C	O	0
			44	40	4	
28	7	1	Total	C	O	0
			44	40	4	
28	8	1	Total	C	O	0
			44	40	4	
28	g	1	Total	C	O	0
			44	40	4	
28	n	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
28	r	1	Total	C	O	0
			44	40	4	
28	y	1	Total	C	O	0
			44	40	4	

- Molecule 29 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



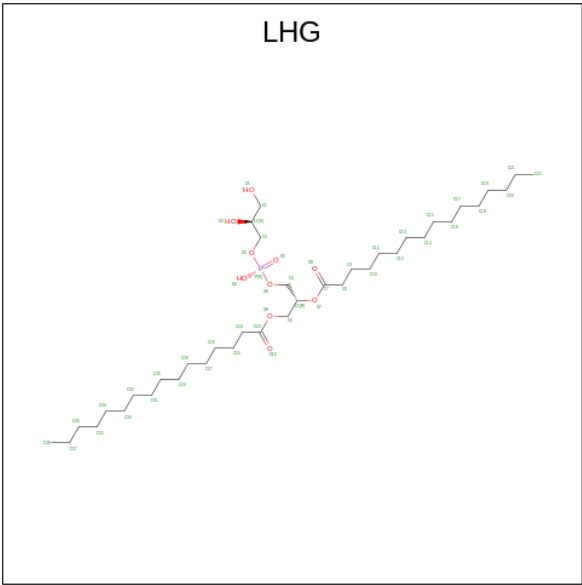
Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			44	40	4	
29	2	1	Total	C	O	0
			44	40	4	
29	3	1	Total	C	O	0
			44	40	4	
29	G	1	Total	C	O	0
			44	40	4	
29	N	1	Total	C	O	0
			44	40	4	
29	R	1	Total	C	O	0
			44	40	4	
29	S	1	Total	C	O	0
			44	40	4	
29	Y	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
29	5	1	Total	C	O	0
			44	40	4	
29	6	1	Total	C	O	0
			44	40	4	
29	7	1	Total	C	O	0
			44	40	4	
29	g	1	Total	C	O	0
			44	40	4	
29	n	1	Total	C	O	0
			44	40	4	
29	r	1	Total	C	O	0
			44	40	4	
29	s	1	Total	C	O	0
			44	40	4	
29	y	1	Total	C	O	0
			44	40	4	

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
30	1	1	Total	C	O	P	0
			41	30	10	1	
30	2	1	Total	C	O	P	0
			37	26	10	1	
30	3	1	Total	C	O	P	0
			47	36	10	1	

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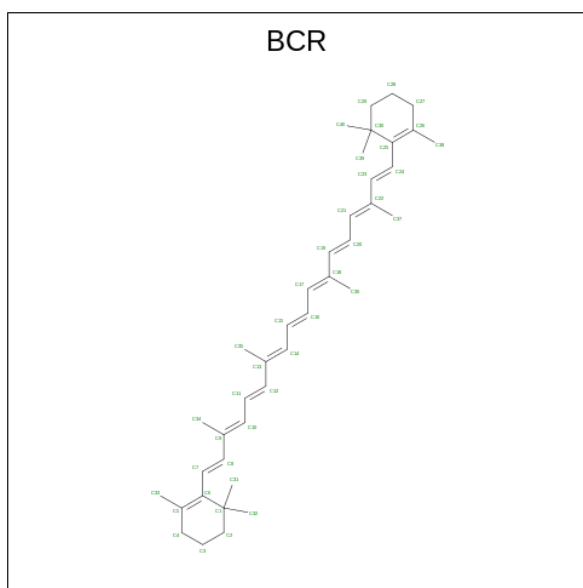
Mol	Chain	Residues	Atoms				AltConf
30	4	1	Total	C	O	P	0
			21	10	10	1	
30	B	1	Total	C	O	P	0
			96	74	20	2	
30	B	1	Total	C	O	P	0
			96	74	20	2	
30	C	1	Total	C	O	P	0
			147	114	30	3	
30	C	1	Total	C	O	P	0
			147	114	30	3	
30	C	1	Total	C	O	P	0
			147	114	30	3	
30	D	1	Total	C	O	P	0
			138	105	30	3	
30	D	1	Total	C	O	P	0
			138	105	30	3	
30	D	1	Total	C	O	P	0
			138	105	30	3	
30	G	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	N	1	Total	C	O	P	0
			49	38	10	1	
30	R	1	Total	C	O	P	0
			42	31	10	1	
30	S	1	Total	C	O	P	0
			49	38	10	1	
30	Y	1	Total	C	O	P	0
			49	38	10	1	
30	5	1	Total	C	O	P	0
			41	30	10	1	
30	6	1	Total	C	O	P	0
			37	26	10	1	
30	7	1	Total	C	O	P	0
			47	36	10	1	
30	8	1	Total	C	O	P	0
			21	10	10	1	
30	b	1	Total	C	O	P	0
			96	74	20	2	
30	b	1	Total	C	O	P	0
			96	74	20	2	

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Mol	Chain	Residues	Atoms				AltConf
30	c	1	Total	C	O	P	0
			147	114	30	3	
30	c	1	Total	C	O	P	0
			147	114	30	3	
30	c	1	Total	C	O	P	0
			147	114	30	3	
30	d	1	Total	C	O	P	0
			138	105	30	3	
30	d	1	Total	C	O	P	0
			138	105	30	3	
30	d	1	Total	C	O	P	0
			138	105	30	3	
30	g	1	Total	C	O	P	0
			49	38	10	1	
30	l	1	Total	C	O	P	0
			49	38	10	1	
30	n	1	Total	C	O	P	0
			49	38	10	1	
30	r	1	Total	C	O	P	0
			42	31	10	1	
30	s	1	Total	C	O	P	0
			49	38	10	1	
30	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



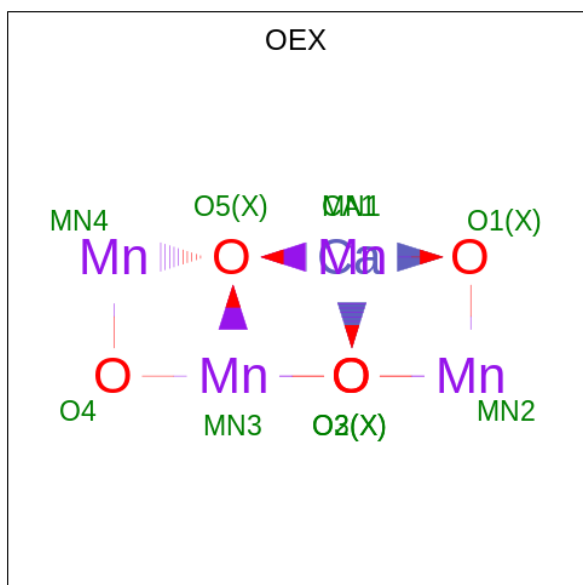
Mol	Chain	Residues	Atoms	AltConf
31	4	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	B	1	Total C 120 120	0
31	B	1	Total C 120 120	0
31	B	1	Total C 120 120	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	D	1	Total C 40 40	0
31	H	1	Total C 40 40	0
31	T	1	Total C 40 40	0
31	8	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 120 120	0
31	b	1	Total C 120 120	0
31	b	1	Total C 120 120	0
31	c	1	Total C 160 160	0
31	c	1	Total C 160 160	0
31	c	1	Total C 160 160	0
31	c	1	Total C 160 160	0
31	d	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
31	h	1	Total	C	0
			40	40	
31	t	1	Total	C	0
			40	40	

- Molecule 32 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
32	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 33 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total	Fe	0
			1	1	
33	a	1	Total	Fe	0
			1	1	

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

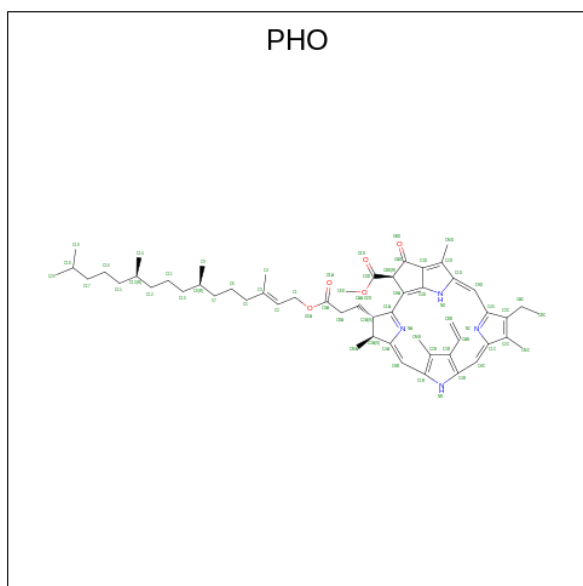
Mol	Chain	Residues	Atoms		AltConf
34	A	2	Total	Cl	0
			2	2	

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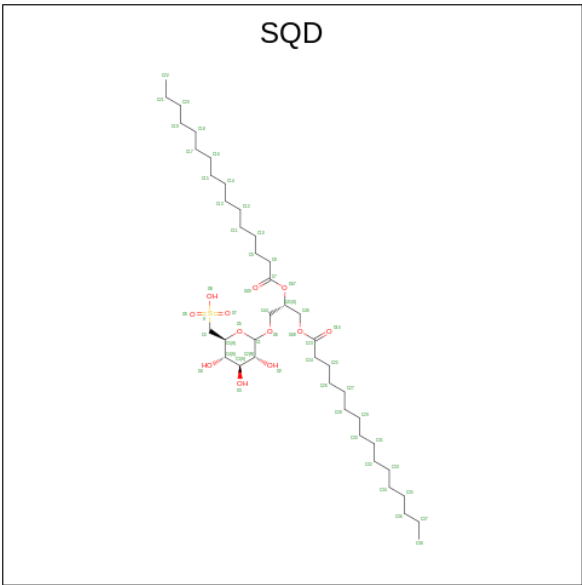
Mol	Chain	Residues	Atoms		AltConf
34	a	2	Total	Cl	0
			2	2	

- Molecule 35 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



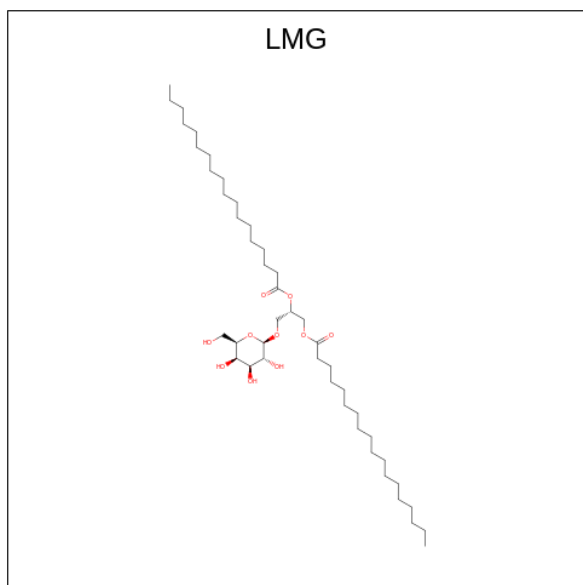
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	N	O	0
			128	110	8	10	
35	A	1	Total	C	N	O	0
			128	110	8	10	
35	a	1	Total	C	N	O	0
			128	110	8	10	
35	a	1	Total	C	N	O	0
			128	110	8	10	

- Molecule 36 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



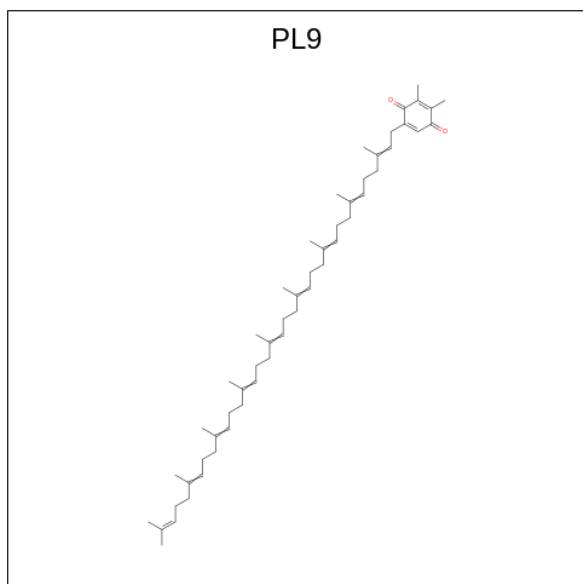
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	O	S	0
			104	78	24	2	
36	A	1	Total	C	O	S	0
			104	78	24	2	
36	B	1	Total	C	O	S	0
			96	70	24	2	
36	B	1	Total	C	O	S	0
			96	70	24	2	
36	a	1	Total	C	O	S	0
			104	78	24	2	
36	a	1	Total	C	O	S	0
			104	78	24	2	
36	b	1	Total	C	O	S	0
			96	70	24	2	
36	b	1	Total	C	O	S	0
			96	70	24	2	

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



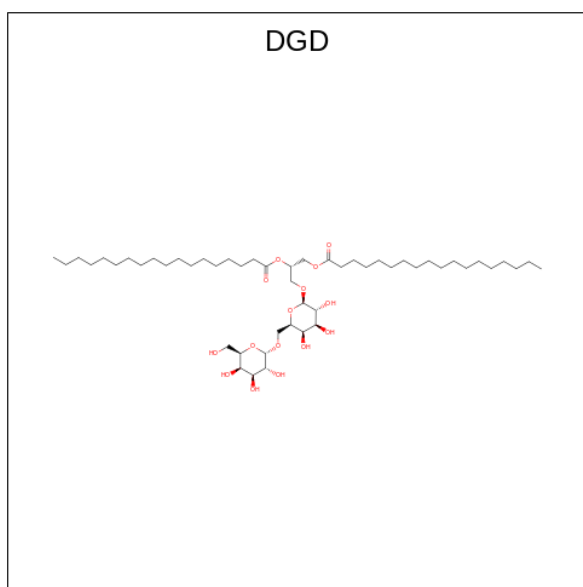
Mol	Chain	Residues	Atoms			AltConf
37	A	1	Total	C	O	0
			88	68	20	
37	A	1	Total	C	O	0
			88	68	20	
37	B	1	Total	C	O	0
			106	86	20	
37	B	1	Total	C	O	0
			106	86	20	
37	C	1	Total	C	O	0
			51	41	10	
37	D	1	Total	C	O	0
			46	36	10	
37	Z	1	Total	C	O	0
			51	41	10	
37	a	1	Total	C	O	0
			88	68	20	
37	a	1	Total	C	O	0
			88	68	20	
37	b	1	Total	C	O	0
			106	86	20	
37	b	1	Total	C	O	0
			106	86	20	
37	c	1	Total	C	O	0
			51	41	10	
37	d	1	Total	C	O	0
			46	36	10	
37	z	1	Total	C	O	0
			51	41	10	

- Molecule 38 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



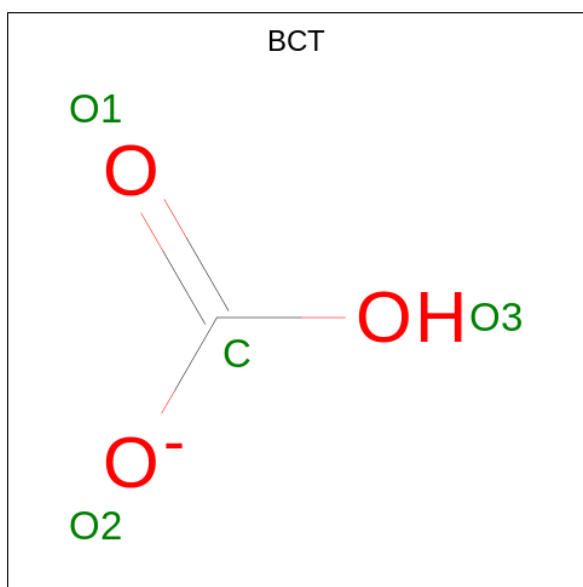
Mol	Chain	Residues	Atoms			AltConf
38	A	1	Total	C	O	0
			13	11	2	
38	D	1	Total	C	O	0
			55	53	2	
38	a	1	Total	C	O	0
			13	11	2	
38	d	1	Total	C	O	0
			55	53	2	

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



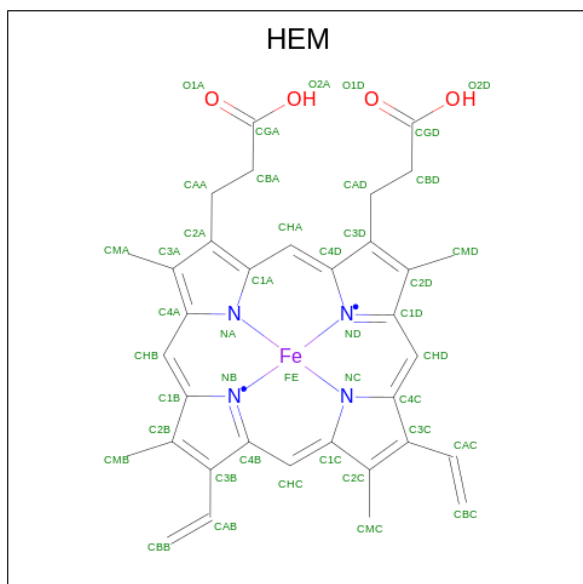
Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			59	44	15	
39	C	1	Total	C	O	0
			177	132	45	
39	C	1	Total	C	O	0
			177	132	45	
39	C	1	Total	C	O	0
			177	132	45	
39	H	1	Total	C	O	0
			62	47	15	
39	b	1	Total	C	O	0
			59	44	15	
39	c	1	Total	C	O	0
			177	132	45	
39	c	1	Total	C	O	0
			177	132	45	
39	c	1	Total	C	O	0
			177	132	45	
39	h	1	Total	C	O	0
			62	47	15	

- Molecule 40 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
40	D	1	Total	C	O	0
			4	1	3	
40	d	1	Total	C	O	0
			4	1	3	

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
41	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
41	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		AltConf
42	A	96	Total	O	0
			96	96	
42	B	89	Total	O	0
			89	89	
42	C	68	Total	O	0
			68	68	
42	D	58	Total	O	0
			58	58	
42	E	10	Total	O	0
			10	10	
42	F	2	Total	O	0
			2	2	
42	G	15	Total	O	0
			15	15	
42	H	16	Total	O	0
			16	16	
42	J	3	Total	O	0
			3	3	
42	K	2	Total	O	0
			2	2	
42	L	10	Total	O	0
			10	10	
42	M	4	Total	O	0
			4	4	
42	N	20	Total	O	0
			20	20	
42	O	31	Total	O	0
			31	31	
42	P	16	Total	O	0
			16	16	
42	R	30	Total	O	0
			30	30	
42	S	14	Total	O	0
			14	14	
42	T	2	Total	O	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
42	W	4	Total O 4 4	0
42	X	5	Total O 5 5	0
42	Y	39	Total O 39 39	0
42	Z	4	Total O 4 4	0
42	a	96	Total O 96 96	0
42	b	89	Total O 89 89	0
42	c	68	Total O 68 68	0
42	d	58	Total O 58 58	0
42	e	10	Total O 10 10	0
42	f	2	Total O 2 2	0
42	g	15	Total O 15 15	0
42	h	16	Total O 16 16	0
42	j	3	Total O 3 3	0
42	k	2	Total O 2 2	0
42	l	10	Total O 10 10	0
42	m	4	Total O 4 4	0
42	n	20	Total O 20 20	0
42	o	31	Total O 31 31	0
42	p	16	Total O 16 16	0
42	r	30	Total O 30 30	0
42	s	14	Total O 14 14	0

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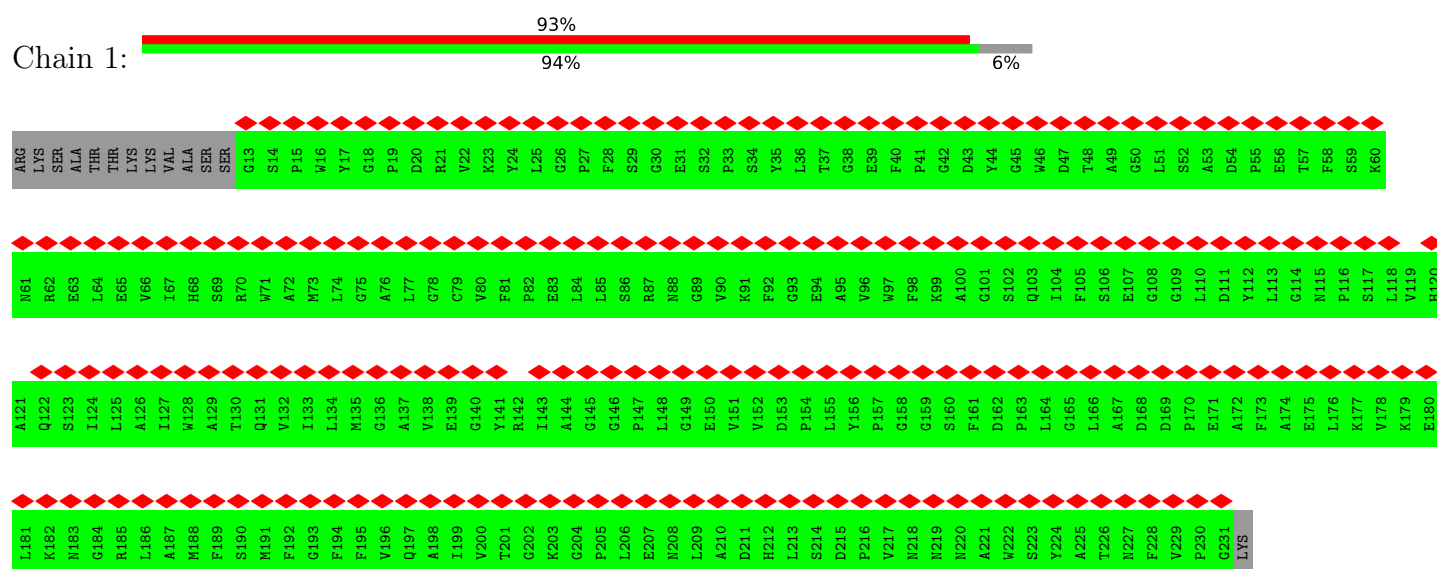
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Mol	Chain	Residues	Atoms		AltConf
42	t	2	Total 2	O 2	0
42	w	4	Total 4	O 4	0
42	x	5	Total 5	O 5	0
42	y	39	Total 39	O 39	0
42	z	4	Total 4	O 4	0

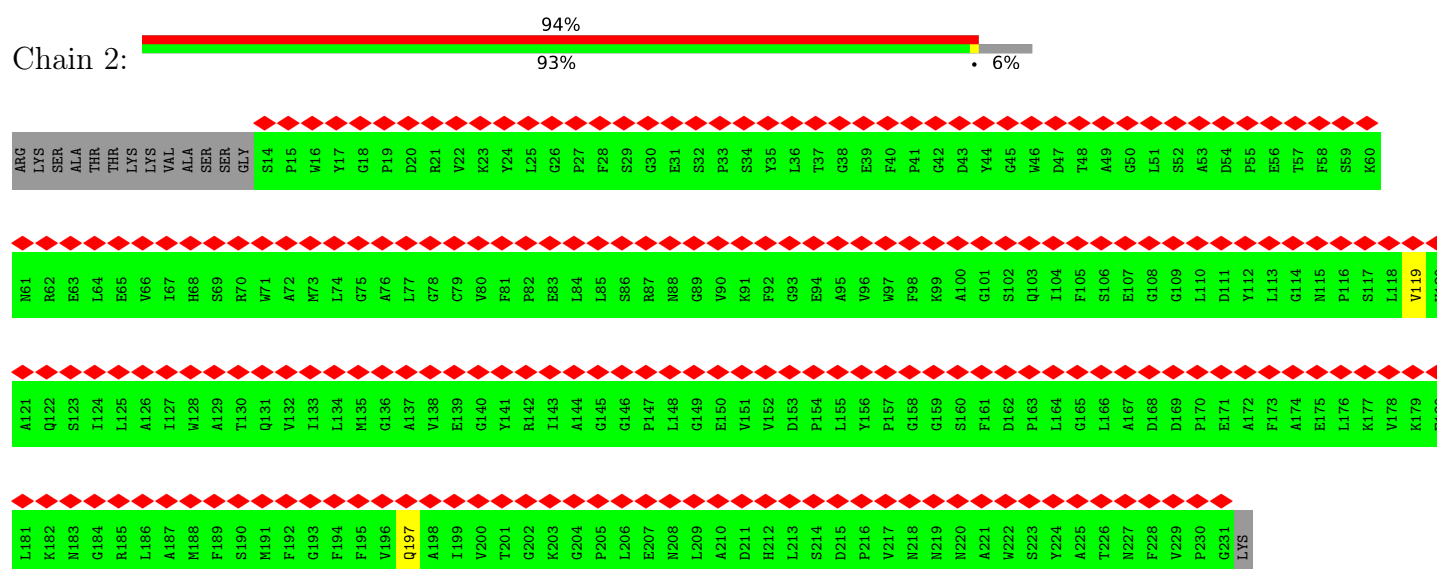
3 Residue-property plots

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.

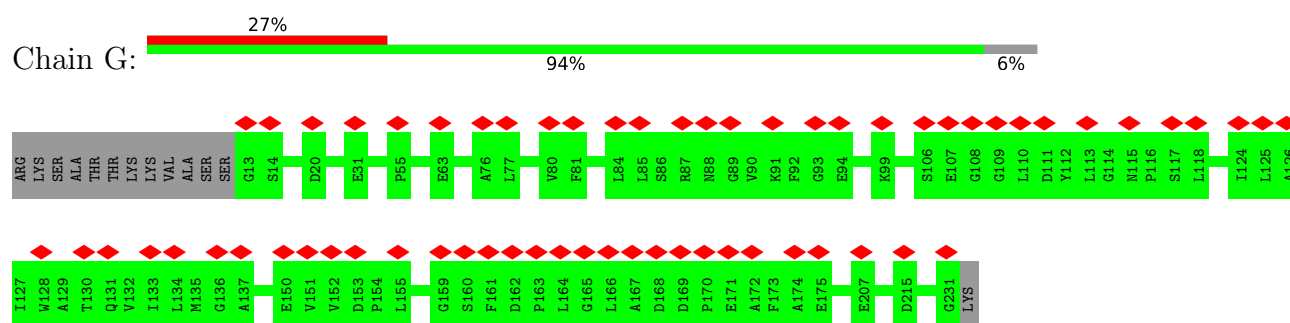
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



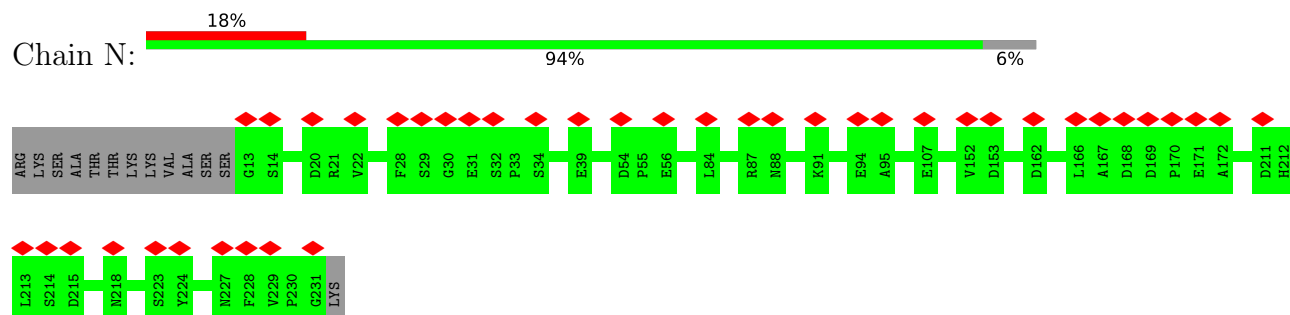
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



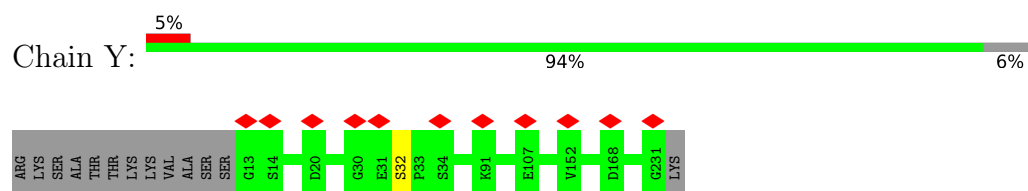
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



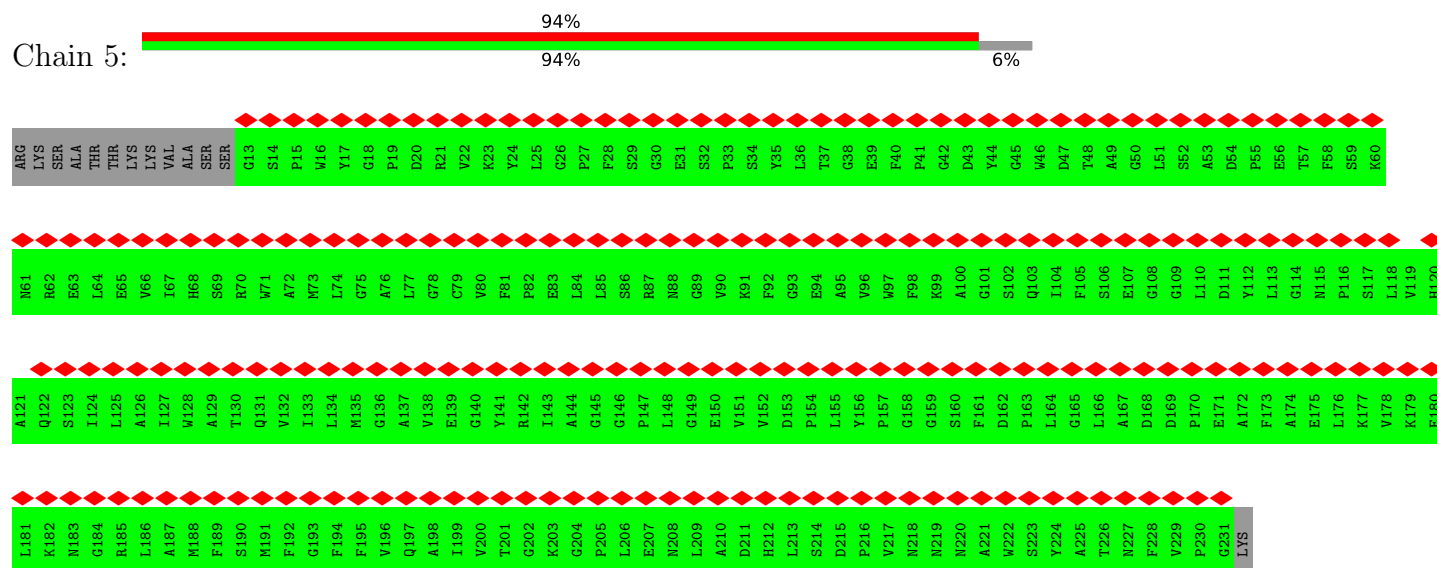
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



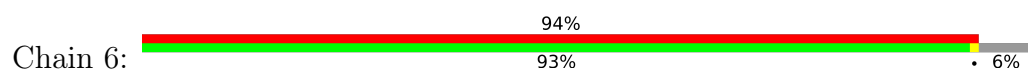
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

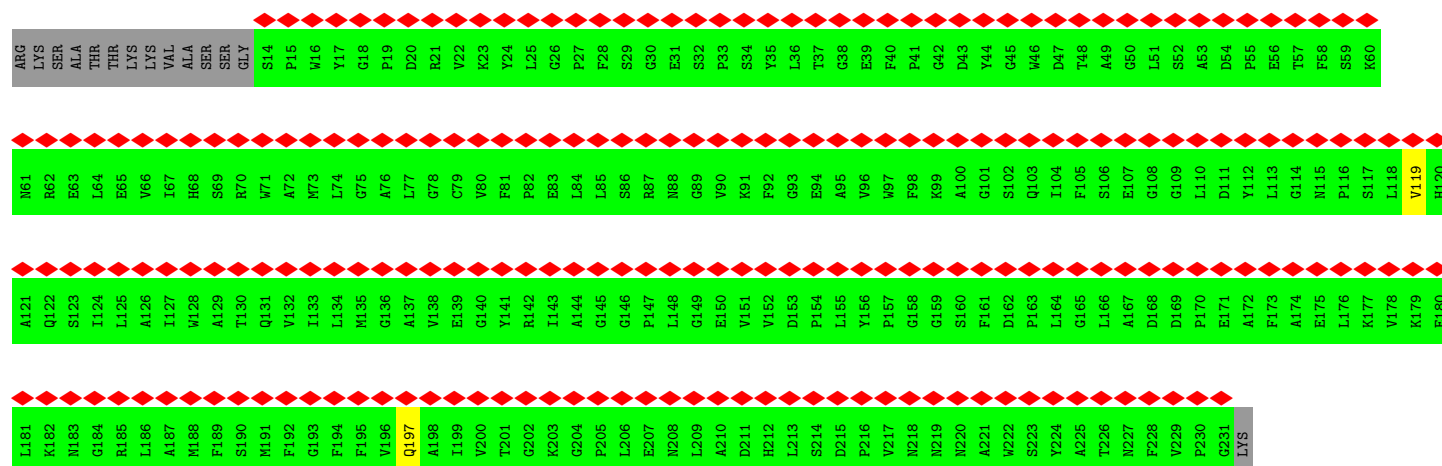


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

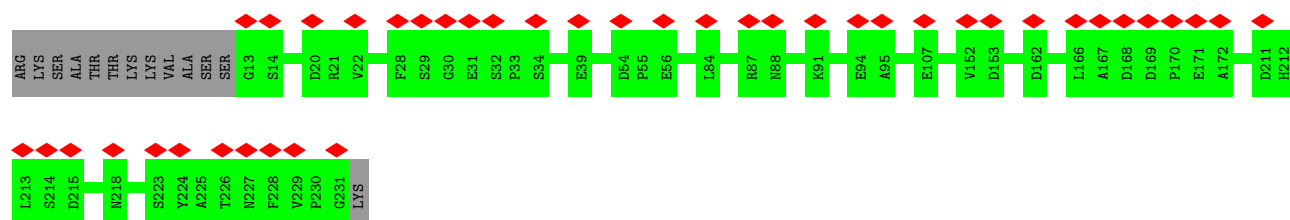




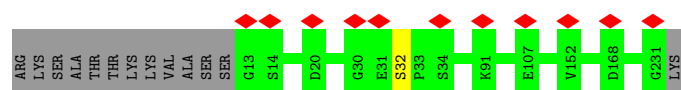
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



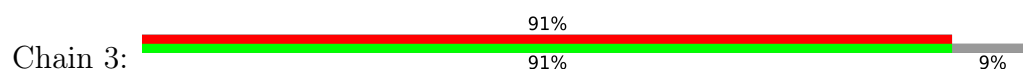
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

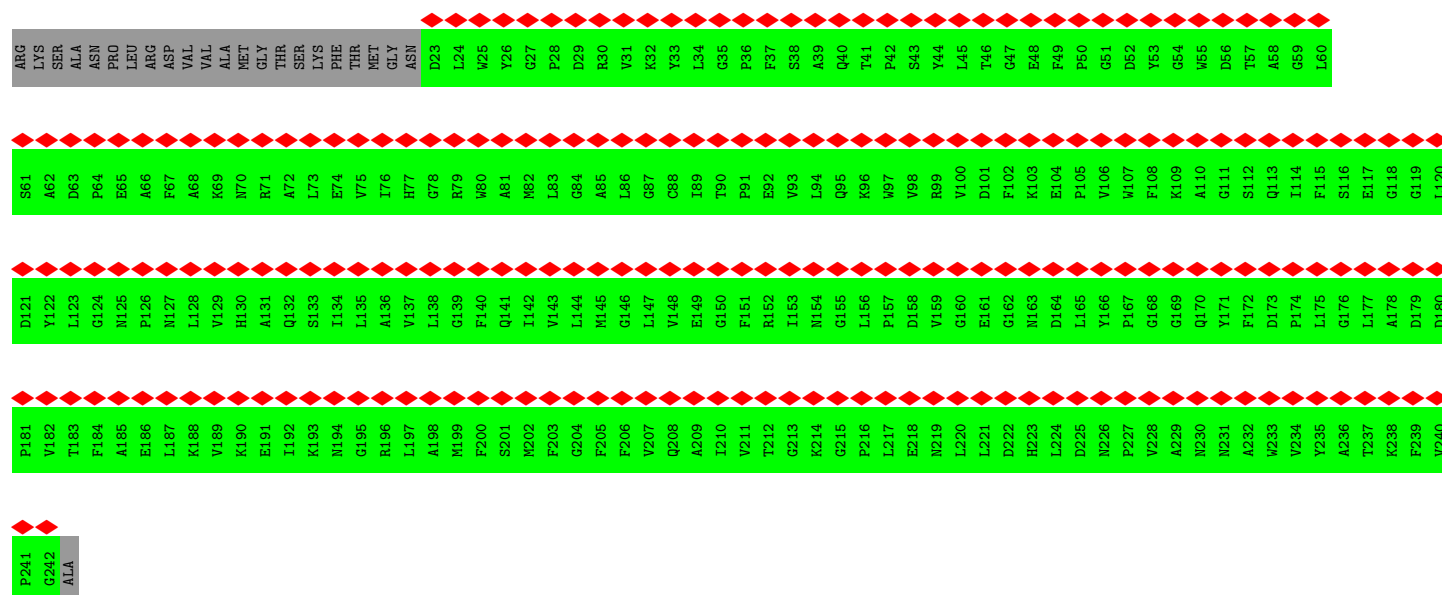


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

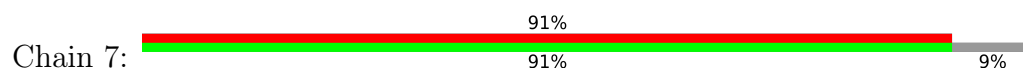


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

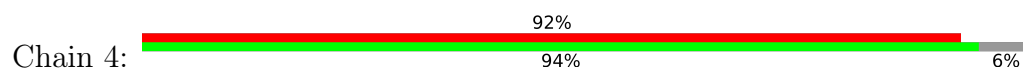


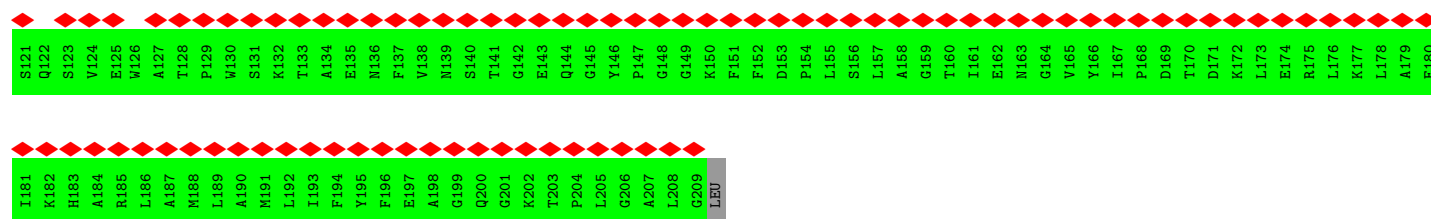


• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

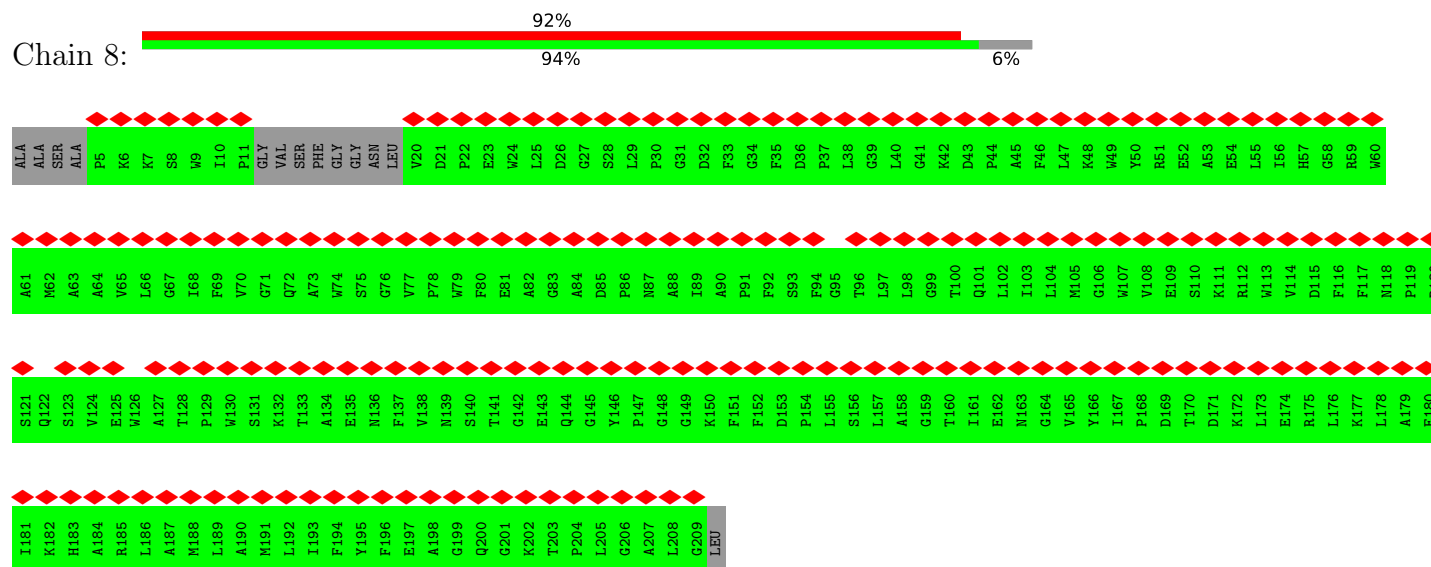


• Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

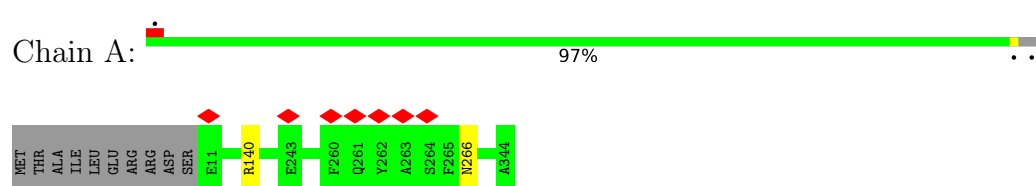




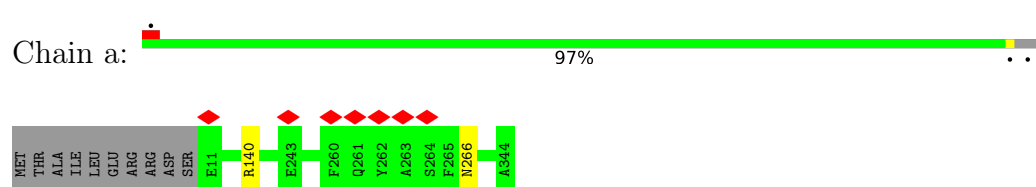
- Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24



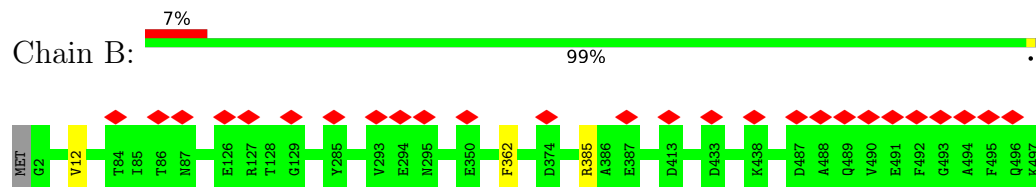
- Molecule 4: Photosystem II protein D1



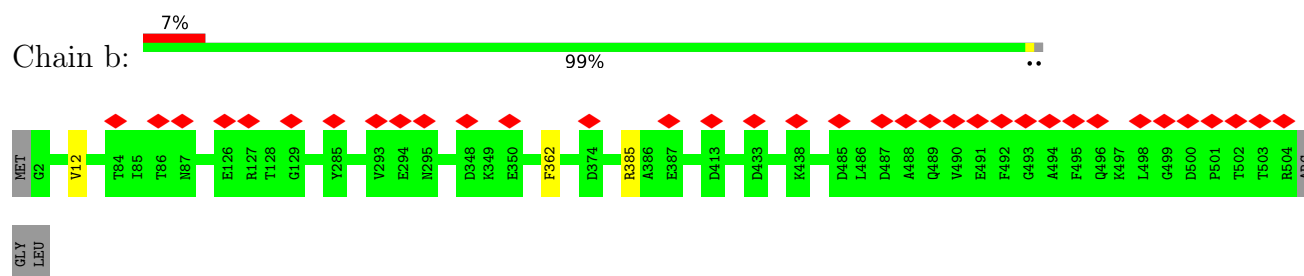
- Molecule 4: Photosystem II protein D1



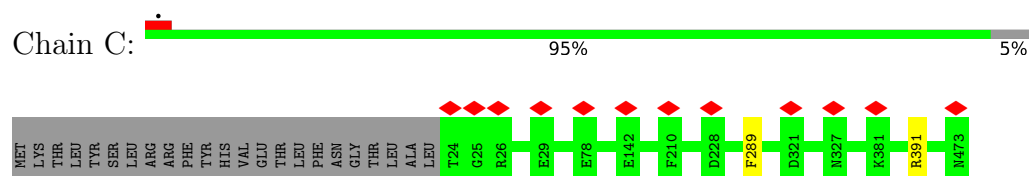
- Molecule 5: Photosystem II CP47 reaction center protein



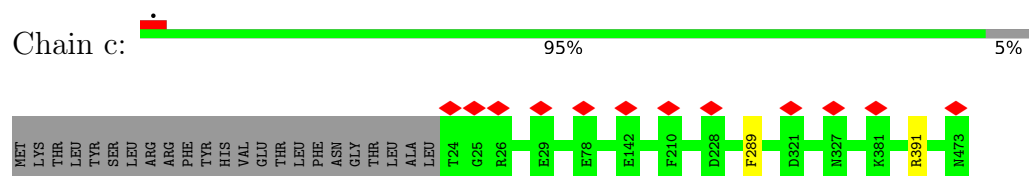
- Molecule 5: Photosystem II CP47 reaction center protein



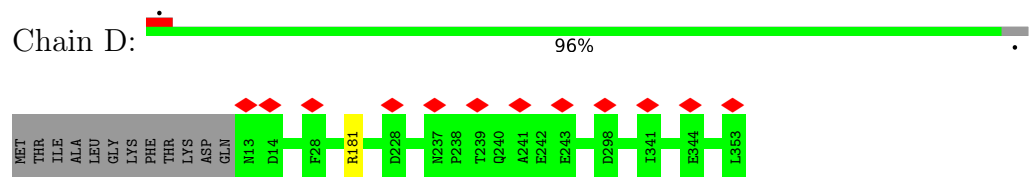
- Molecule 6: Photosystem II CP43 reaction center protein



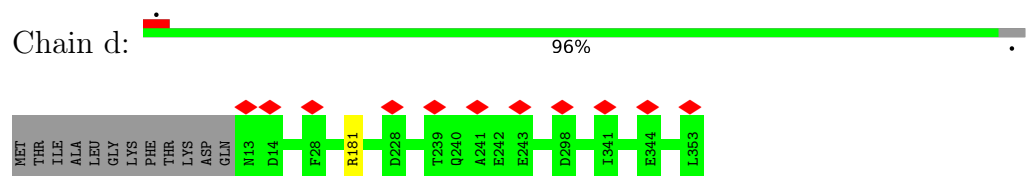
- Molecule 6: Photosystem II CP43 reaction center protein



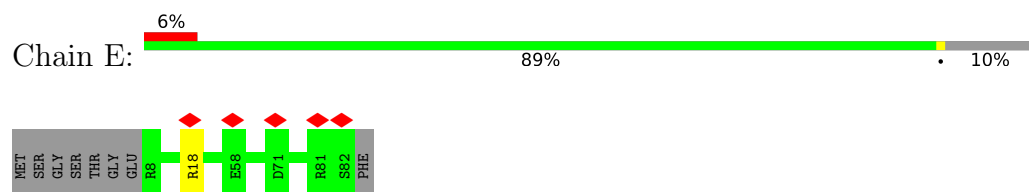
- Molecule 7: Photosystem II D2 protein



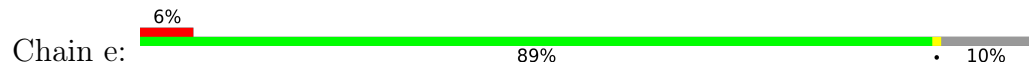
- Molecule 7: Photosystem II D2 protein

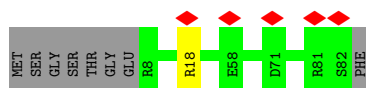


- Molecule 8: Cytochrome b559 subunit alpha

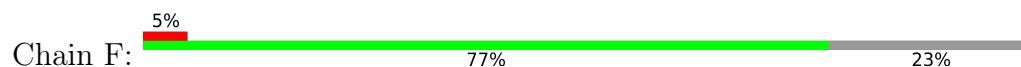


- Molecule 8: Cytochrome b559 subunit alpha

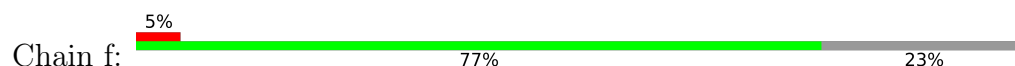




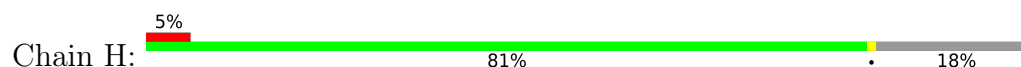
- Molecule 9: Cytochrome b559 subunit beta, PsbF



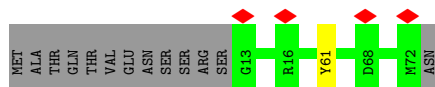
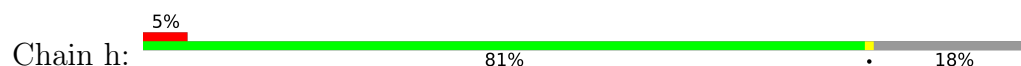
- Molecule 9: Cytochrome b559 subunit beta, PsbF



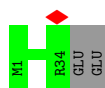
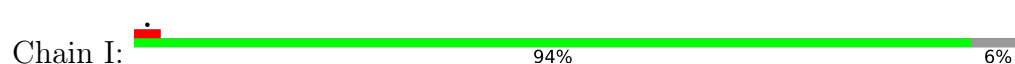
- Molecule 10: Photosystem II reaction center protein H



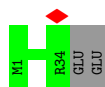
- Molecule 10: Photosystem II reaction center protein H



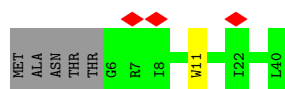
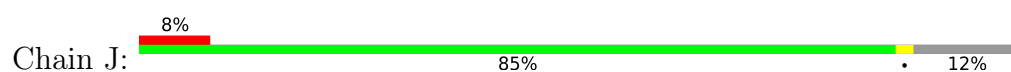
- Molecule 11: Photosystem II reaction center protein I, PsbI



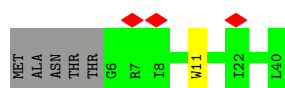
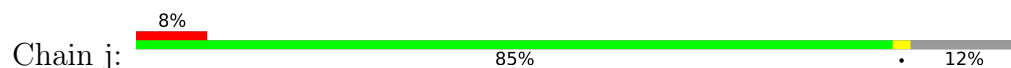
- Molecule 11: Photosystem II reaction center protein I, PsbI



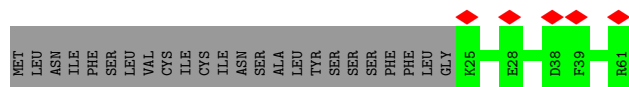
- Molecule 12: Photosystem II reaction center protein J



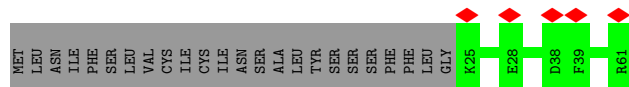
- Molecule 12: Photosystem II reaction center protein J



- Molecule 13: Photosystem II reaction center protein K



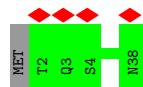
- Molecule 13: Photosystem II reaction center protein K



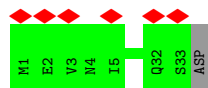
- Molecule 14: Photosystem II reaction center protein L



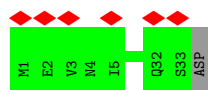
- Molecule 14: Photosystem II reaction center protein L



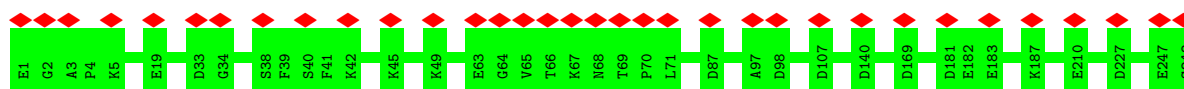
- Molecule 15: Photosystem II reaction center protein M



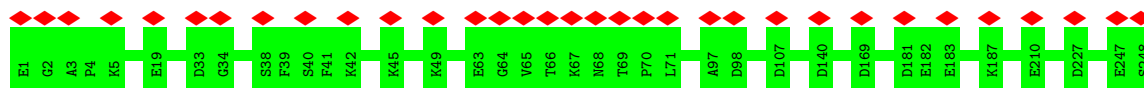
- Molecule 15: Photosystem II reaction center protein M



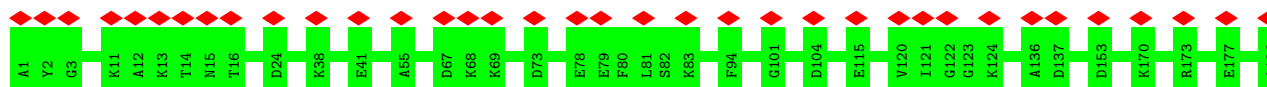
- Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic



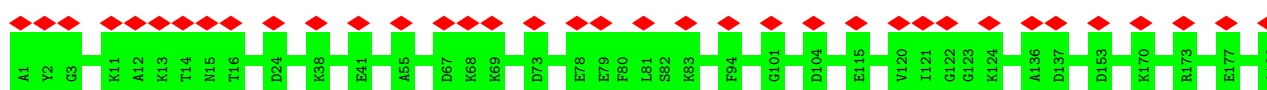
- Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic



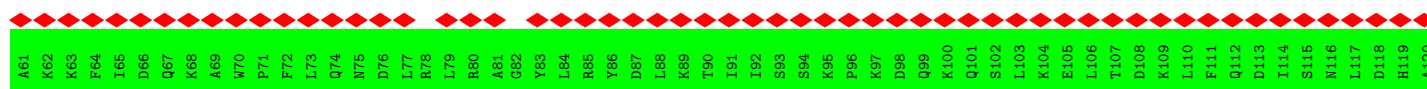
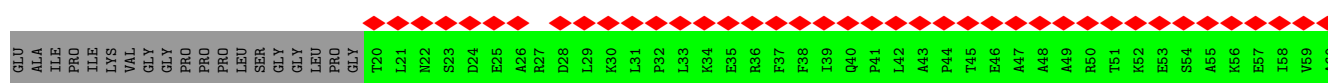
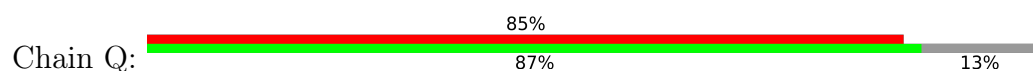
- Molecule 17: Oxygen-evolving enhancer protein 2, chloroplastic

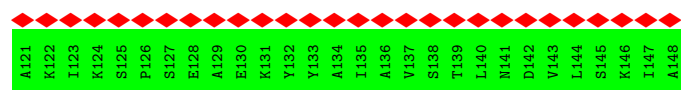


- Molecule 17: Oxygen-evolving enhancer protein 2, chloroplastic

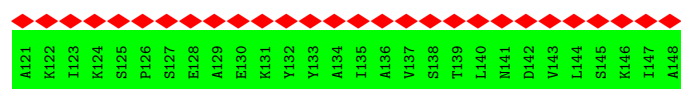
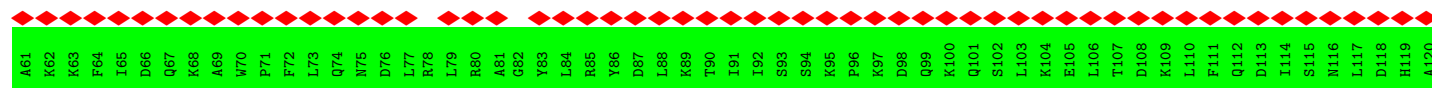
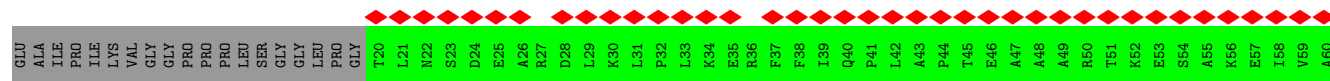
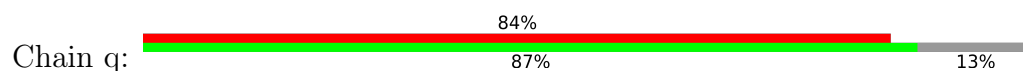


- Molecule 18: Oxygen-evolving enhancer protein 3

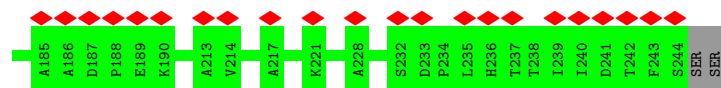
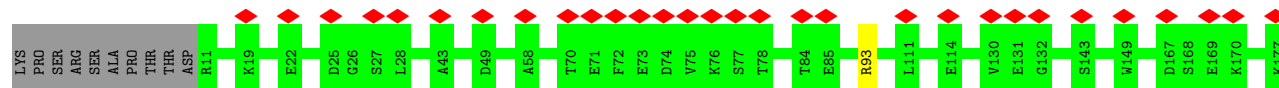




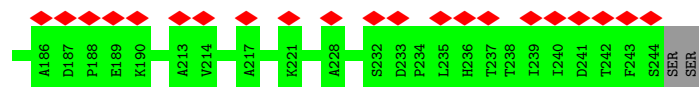
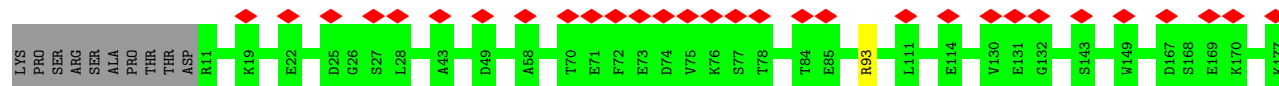
• Molecule 18: Oxygen-evolving enhancer protein 3



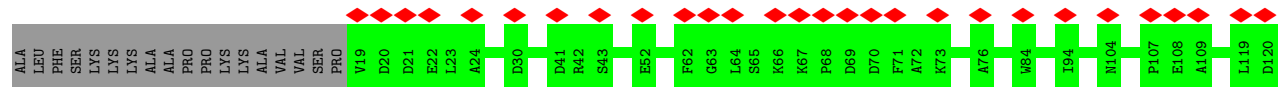
• Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29

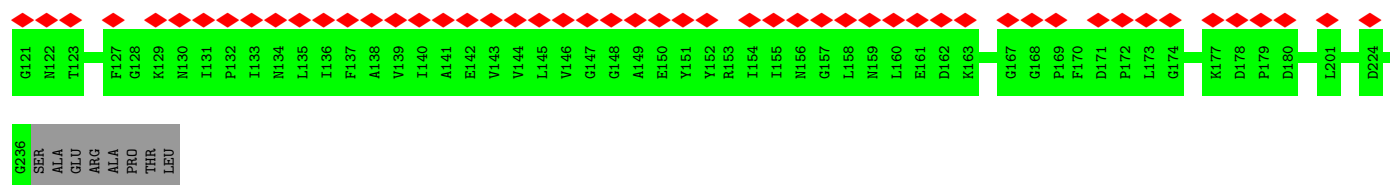


• Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29

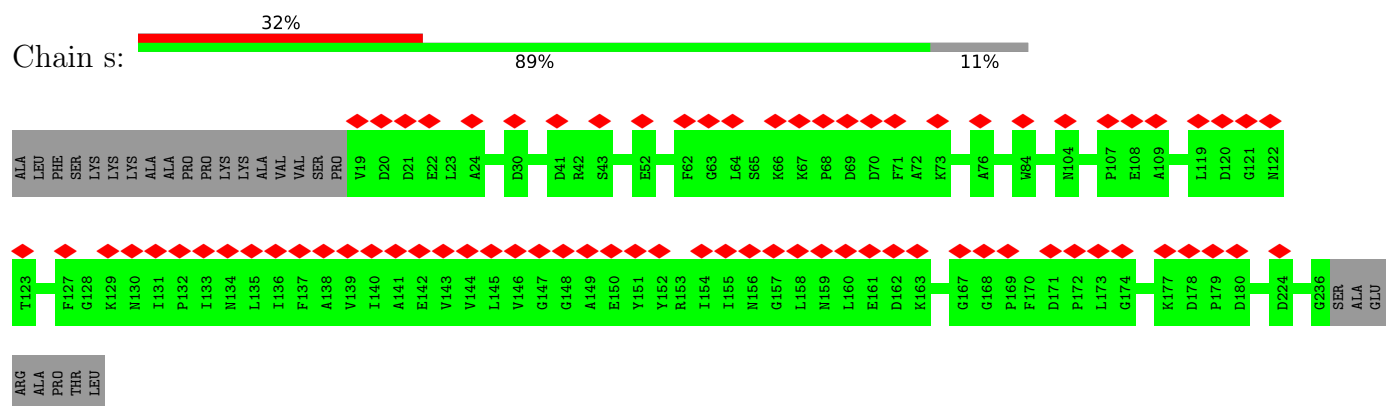


• Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

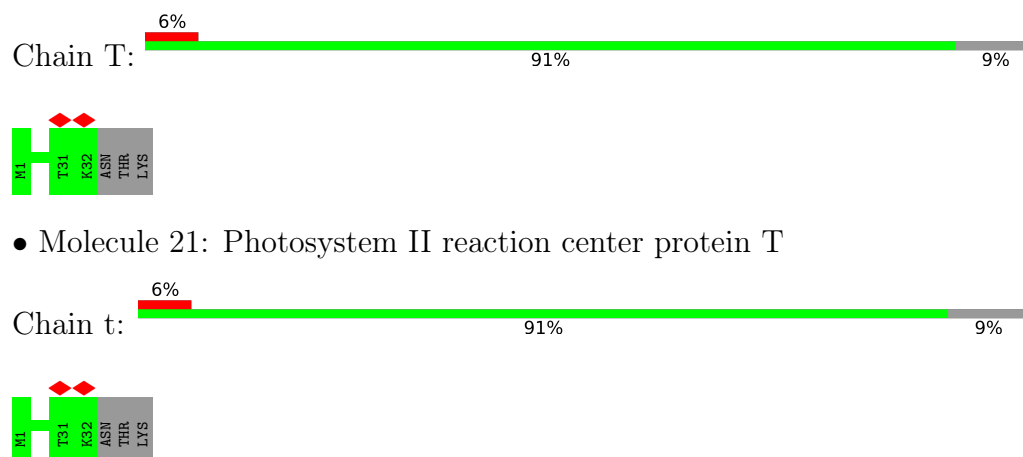




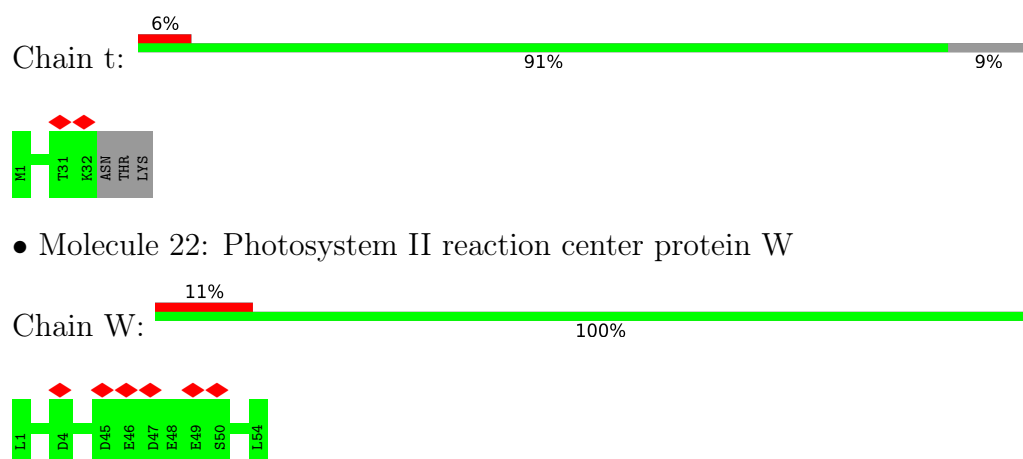
- Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26



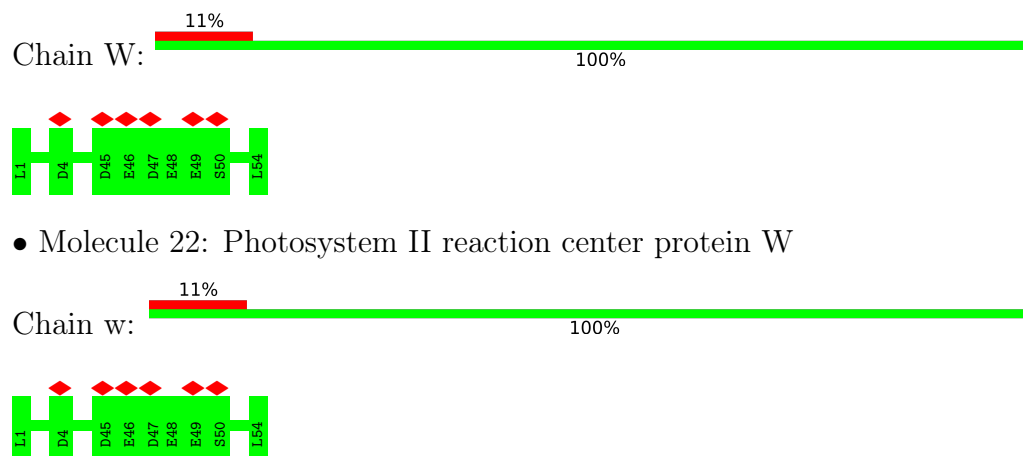
- Molecule 21: Photosystem II reaction center protein T



- Molecule 21: Photosystem II reaction center protein T

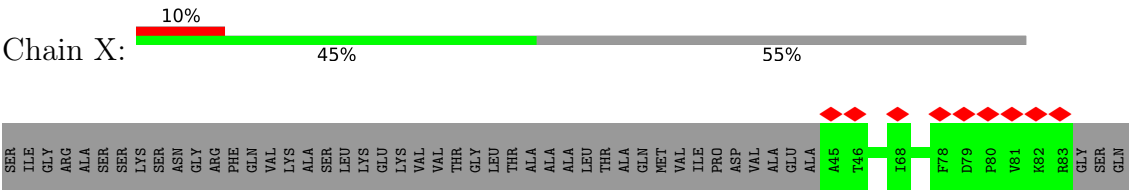


- Molecule 22: Photosystem II reaction center protein W

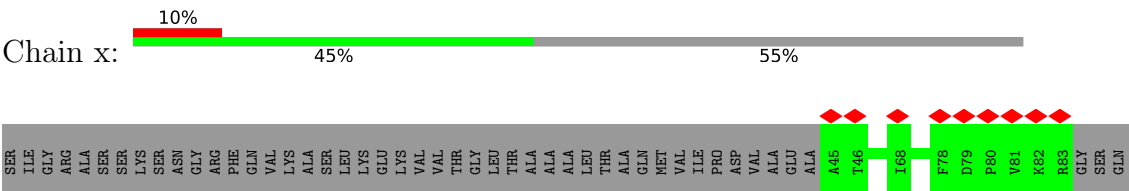


- Molecule 22: Photosystem II reaction center protein W

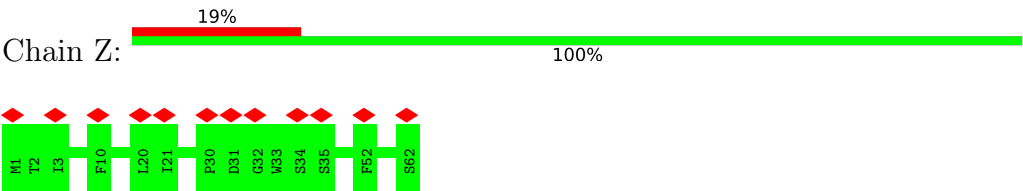
● Molecule 23: Photosystem II reaction center protein X



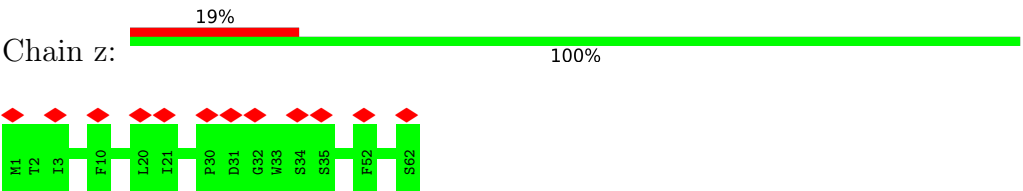
● Molecule 23: Photosystem II reaction center protein X



● Molecule 24: Photosystem II reaction center protein Z



● Molecule 24: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	136521	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	168.730	Depositor
Minimum map value	-94.103	Depositor
Average map value	0.061	Depositor
Map value standard deviation	6.582	Depositor
Recommended contour level	17.5	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, XAT, FE2, HEM, NEX, SQD, LUT, DGD, BCR, PL9, BCT, PHO, CHL, CLA, LMG, CL, OEX

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	0.36	0/1720	0.50	0/2342
1	2	0.32	0/1716	0.51	1/2337 (0.0%)
1	5	0.37	0/1720	0.50	0/2342
1	6	0.33	0/1716	0.51	1/2337 (0.0%)
1	G	0.39	0/1720	0.52	0/2342
1	N	0.44	0/1720	0.56	0/2342
1	Y	0.43	0/1720	0.55	0/2342
1	g	0.39	0/1720	0.52	0/2342
1	n	0.45	0/1720	0.56	0/2342
1	y	0.43	0/1720	0.55	0/2342
2	3	0.37	0/1759	0.53	0/2396
2	7	0.37	0/1759	0.53	0/2396
3	4	0.34	0/1586	0.55	0/2158
3	8	0.34	0/1586	0.55	0/2158
4	A	0.54	0/2697	0.62	1/3677 (0.0%)
4	a	0.54	0/2697	0.62	1/3677 (0.0%)
5	B	0.54	0/4081	0.60	0/5556
5	b	0.54	0/4081	0.61	0/5556
6	C	0.58	0/3614	0.63	0/4922
6	c	0.58	0/3614	0.63	0/4922
7	D	0.47	0/2804	0.61	0/3823
7	d	0.48	0/2804	0.61	0/3823
8	E	0.47	0/630	0.52	0/857
8	e	0.48	0/630	0.52	0/857
9	F	0.60	0/248	0.64	0/335
9	f	0.60	0/248	0.64	0/335
10	H	0.50	0/461	0.56	0/626
10	h	0.50	0/461	0.56	0/626
11	I	0.52	0/286	0.68	0/386
11	i	0.52	0/286	0.68	0/386
12	J	0.58	1/262 (0.4%)	0.70	0/354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
12	j	0.58	1/262 (0.4%)	0.70	0/354
13	K	0.48	0/318	0.63	0/434
13	k	0.48	0/318	0.63	0/434
14	L	0.57	0/319	0.59	0/434
14	l	0.57	0/319	0.59	0/434
15	M	0.44	0/260	0.66	0/355
15	m	0.44	0/260	0.66	0/355
16	O	0.43	0/1906	0.60	0/2575
16	o	0.43	0/1906	0.60	0/2575
17	P	0.54	0/1464	0.63	0/1978
17	p	0.54	0/1464	0.63	0/1978
18	Q	0.29	0/1051	0.59	0/1414
18	q	0.29	0/1051	0.59	0/1414
19	R	0.50	0/1886	0.59	0/2569
19	r	0.50	0/1886	0.59	0/2569
20	S	0.43	0/1736	0.65	0/2359
20	s	0.43	0/1736	0.65	0/2359
21	T	0.46	0/269	0.51	0/365
21	t	0.46	0/269	0.51	0/365
22	W	0.55	0/429	0.63	0/581
22	w	0.55	0/429	0.63	0/581
23	X	0.33	0/279	0.48	0/380
23	x	0.33	0/279	0.48	0/380
24	Z	0.42	0/474	0.55	0/648
24	z	0.42	0/474	0.55	0/648
All	All	0.47	2/74830 (0.0%)	0.59	4/101774 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	j	11	TRP	CB-CG	-5.25	1.40	1.50
12	J	11	TRP	CB-CG	-5.24	1.40	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	197	GLN	CA-CB-CG	5.70	125.94	113.40
1	2	197	GLN	CA-CB-CG	5.69	125.92	113.40
4	A	140	ARG	NE-CZ-NH1	-5.28	117.66	120.30
4	a	140	ARG	NE-CZ-NH1	-5.28	117.66	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	217/232 (94%)	209 (96%)	8 (4%)	0	100	100
1	2	216/232 (93%)	210 (97%)	5 (2%)	1 (0%)	29	54
1	5	217/232 (94%)	209 (96%)	8 (4%)	0	100	100
1	6	216/232 (93%)	210 (97%)	5 (2%)	1 (0%)	29	54
1	G	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	N	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	Y	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	g	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	n	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	y	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
2	3	218/243 (90%)	209 (96%)	9 (4%)	0	100	100
2	7	218/243 (90%)	209 (96%)	9 (4%)	0	100	100
3	4	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
3	8	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
4	A	332/344 (96%)	326 (98%)	6 (2%)	0	100	100
4	a	332/344 (96%)	326 (98%)	6 (2%)	0	100	100
5	B	501/507 (99%)	493 (98%)	8 (2%)	0	100	100
5	b	501/507 (99%)	493 (98%)	8 (2%)	0	100	100
6	C	448/473 (95%)	441 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	c	448/473 (95%)	442 (99%)	6 (1%)	0	100	100
7	D	339/353 (96%)	335 (99%)	4 (1%)	0	100	100
7	d	339/353 (96%)	335 (99%)	4 (1%)	0	100	100
8	E	73/83 (88%)	73 (100%)	0	0	100	100
8	e	73/83 (88%)	73 (100%)	0	0	100	100
9	F	28/39 (72%)	28 (100%)	0	0	100	100
9	f	28/39 (72%)	28 (100%)	0	0	100	100
10	H	58/73 (80%)	58 (100%)	0	0	100	100
10	h	58/73 (80%)	58 (100%)	0	0	100	100
11	I	32/36 (89%)	32 (100%)	0	0	100	100
11	i	32/36 (89%)	32 (100%)	0	0	100	100
12	J	33/40 (82%)	33 (100%)	0	0	100	100
12	j	33/40 (82%)	33 (100%)	0	0	100	100
13	K	35/61 (57%)	35 (100%)	0	0	100	100
13	k	35/61 (57%)	35 (100%)	0	0	100	100
14	L	35/38 (92%)	35 (100%)	0	0	100	100
14	l	35/38 (92%)	35 (100%)	0	0	100	100
15	M	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
15	m	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
16	O	246/248 (99%)	240 (98%)	6 (2%)	0	100	100
16	o	246/248 (99%)	240 (98%)	6 (2%)	0	100	100
17	P	184/186 (99%)	183 (100%)	1 (0%)	0	100	100
17	p	184/186 (99%)	183 (100%)	1 (0%)	0	100	100
18	Q	127/148 (86%)	125 (98%)	2 (2%)	0	100	100
18	q	127/148 (86%)	125 (98%)	2 (2%)	0	100	100
19	R	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
19	r	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
20	S	216/244 (88%)	209 (97%)	7 (3%)	0	100	100
20	s	216/244 (88%)	208 (96%)	8 (4%)	0	100	100
21	T	30/35 (86%)	30 (100%)	0	0	100	100
21	t	30/35 (86%)	30 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	W	52/54 (96%)	52 (100%)	0	0	100	100
22	w	52/54 (96%)	52 (100%)	0	0	100	100
23	X	37/86 (43%)	36 (97%)	1 (3%)	0	100	100
23	x	37/86 (43%)	36 (97%)	1 (3%)	0	100	100
24	Z	60/62 (97%)	60 (100%)	0	0	100	100
24	z	60/62 (97%)	60 (100%)	0	0	100	100
All	All	9248/10006 (92%)	9056 (98%)	190 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	119	VAL
1	6	119	VAL

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	171/182 (94%)	171 (100%)	0	100	100
1	2	171/182 (94%)	171 (100%)	0	100	100
1	5	171/182 (94%)	171 (100%)	0	100	100
1	6	171/182 (94%)	171 (100%)	0	100	100
1	G	171/182 (94%)	171 (100%)	0	100	100
1	N	171/182 (94%)	171 (100%)	0	100	100
1	Y	171/182 (94%)	170 (99%)	1 (1%)	86	95
1	g	171/182 (94%)	171 (100%)	0	100	100
1	n	171/182 (94%)	171 (100%)	0	100	100
1	y	171/182 (94%)	170 (99%)	1 (1%)	86	95
2	3	175/193 (91%)	175 (100%)	0	100	100
2	7	175/193 (91%)	175 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	4	154/162 (95%)	154 (100%)	0	100	100
3	8	154/162 (95%)	154 (100%)	0	100	100
4	A	270/279 (97%)	269 (100%)	1 (0%)	91	97
4	a	270/279 (97%)	269 (100%)	1 (0%)	91	97
5	B	400/403 (99%)	397 (99%)	3 (1%)	81	93
5	b	400/403 (99%)	397 (99%)	3 (1%)	81	93
6	C	352/373 (94%)	350 (99%)	2 (1%)	86	95
6	c	352/373 (94%)	350 (99%)	2 (1%)	86	95
7	D	275/285 (96%)	274 (100%)	1 (0%)	91	97
7	d	275/285 (96%)	274 (100%)	1 (0%)	91	97
8	E	67/73 (92%)	66 (98%)	1 (2%)	65	86
8	e	67/73 (92%)	66 (98%)	1 (2%)	65	86
9	F	25/34 (74%)	25 (100%)	0	100	100
9	f	25/34 (74%)	25 (100%)	0	100	100
10	H	49/61 (80%)	48 (98%)	1 (2%)	55	81
10	h	49/61 (80%)	48 (98%)	1 (2%)	55	81
11	I	31/33 (94%)	31 (100%)	0	100	100
11	i	31/33 (94%)	31 (100%)	0	100	100
12	J	26/30 (87%)	26 (100%)	0	100	100
12	j	26/30 (87%)	26 (100%)	0	100	100
13	K	32/54 (59%)	32 (100%)	0	100	100
13	k	32/54 (59%)	32 (100%)	0	100	100
14	L	35/36 (97%)	35 (100%)	0	100	100
14	l	35/36 (97%)	35 (100%)	0	100	100
15	M	29/30 (97%)	29 (100%)	0	100	100
15	m	29/30 (97%)	29 (100%)	0	100	100
16	O	204/204 (100%)	204 (100%)	0	100	100
16	o	204/204 (100%)	204 (100%)	0	100	100
17	P	150/150 (100%)	150 (100%)	0	100	100
17	p	150/150 (100%)	150 (100%)	0	100	100
18	Q	112/125 (90%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	q	112/125 (90%)	112 (100%)	0	100	100
19	R	191/202 (95%)	190 (100%)	1 (0%)	88	96
19	r	191/202 (95%)	190 (100%)	1 (0%)	88	96
20	S	170/190 (90%)	170 (100%)	0	100	100
20	s	170/190 (90%)	170 (100%)	0	100	100
21	T	29/32 (91%)	29 (100%)	0	100	100
21	t	29/32 (91%)	29 (100%)	0	100	100
22	W	44/44 (100%)	44 (100%)	0	100	100
22	w	44/44 (100%)	44 (100%)	0	100	100
23	X	32/67 (48%)	32 (100%)	0	100	100
23	x	32/67 (48%)	32 (100%)	0	100	100
24	Z	54/54 (100%)	54 (100%)	0	100	100
24	z	54/54 (100%)	54 (100%)	0	100	100
All	All	7522/8048 (94%)	7500 (100%)	22 (0%)	92	98

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	b	385	ARG
7	d	181	ARG
6	c	391	ARG
8	e	18	ARG
7	D	181	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	88	ASN
19	r	56	ASN
4	a	234	ASN
19	r	47	GLN
9	f	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 490 ligands modelled in this entry, 6 are monoatomic - leaving 484 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	CHL	R	608	42	61,69,74	1.90	10 (16%)	67,108,114	2.92	24 (35%)
26	CLA	r	613	19	60,68,73	1.59	8 (13%)	70,107,113	1.29	8 (11%)
28	XAT	4	622	-	39,47,47	0.93	1 (2%)	54,74,74	2.62	21 (38%)
26	CLA	s	603	20	45,53,73	1.78	10 (22%)	52,89,113	1.92	12 (23%)
26	CLA	g	610	1	64,72,73	1.50	6 (9%)	74,111,113	1.37	8 (10%)
37	LMG	D	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.46	4 (7%)
26	CLA	y	613	1	65,73,73	1.49	9 (13%)	76,113,113	1.43	9 (11%)
26	CLA	5	613	1	55,63,73	1.65	9 (16%)	64,101,113	1.35	6 (9%)
26	CLA	y	614	1	48,56,73	1.67	10 (20%)	55,92,113	1.60	9 (16%)
30	LHG	R	2630	26	41,41,48	0.70	1 (2%)	44,47,54	1.27	6 (13%)
36	SQD	a	418	-	53,54,54	0.92	5 (9%)	62,65,65	1.67	14 (22%)
25	CHL	1	609	1	62,70,74	1.94	14 (22%)	68,109,114	2.72	20 (29%)
26	CLA	B	604	5	65,73,73	1.51	11 (16%)	76,113,113	1.46	10 (13%)
26	CLA	N	610	1	65,73,73	1.42	8 (12%)	76,113,113	1.42	10 (13%)
26	CLA	B	616	5	65,73,73	1.46	10 (15%)	76,113,113	1.45	12 (15%)
26	CLA	C	504	42	65,73,73	1.40	10 (15%)	76,113,113	1.68	8 (10%)
25	CHL	1	601	1	46,54,74	2.35	15 (32%)	49,90,114	3.07	21 (42%)
26	CLA	g	613	1	65,73,73	1.49	8 (12%)	76,113,113	1.35	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	NEX	7	1623	-	38,46,46	0.87	1 (2%)	50,70,70	2.39	16 (32%)
30	LHG	d	409	-	48,48,48	0.75	1 (2%)	51,54,54	1.31	7 (13%)
26	CLA	B	612	5	65,73,73	1.50	8 (12%)	76,113,113	1.67	10 (13%)
30	LHG	b	2631	-	48,48,48	0.68	2 (4%)	51,54,54	1.22	6 (11%)
25	CHL	1	606	-	46,54,74	2.24	15 (32%)	49,90,114	3.08	20 (40%)
25	CHL	S	608	-	46,54,74	2.25	15 (32%)	49,90,114	3.15	16 (32%)
27	LUT	Y	1621	-	42,43,43	0.88	1 (2%)	51,60,60	1.69	13 (25%)
37	LMG	C	521	-	51,51,55	0.80	3 (5%)	59,59,63	1.38	6 (10%)
27	LUT	G	1621	-	42,43,43	0.89	1 (2%)	51,60,60	1.96	17 (33%)
25	CHL	G	605	1	46,54,74	2.27	15 (32%)	49,90,114	3.33	20 (40%)
26	CLA	4	611	30	45,53,73	1.81	8 (17%)	52,89,113	1.49	7 (13%)
27	LUT	N	1620	-	42,43,43	0.81	0	51,60,60	1.69	12 (23%)
25	CHL	N	609	1	66,74,74	1.88	14 (21%)	73,114,114	2.72	23 (31%)
26	CLA	Y	602	1	65,73,73	1.43	8 (12%)	76,113,113	1.53	10 (13%)
26	CLA	7	613	2	58,66,73	1.61	10 (17%)	67,104,113	1.42	8 (11%)
27	LUT	5	1621	-	42,43,43	0.90	2 (4%)	51,60,60	1.73	15 (29%)
26	CLA	B	609	5	65,73,73	1.40	8 (12%)	76,113,113	1.68	12 (15%)
26	CLA	n	611	30	60,68,73	1.55	7 (11%)	70,107,113	1.45	7 (10%)
25	CHL	3	609	2	61,69,74	2.02	14 (22%)	67,108,114	2.61	21 (31%)
31	BCR	c	515	-	41,41,41	0.93	2 (4%)	56,56,56	2.01	16 (28%)
27	LUT	g	1621	-	42,43,43	0.89	1 (2%)	51,60,60	1.95	17 (33%)
26	CLA	G	604	42	50,58,73	1.78	10 (20%)	58,95,113	1.71	10 (17%)
28	XAT	r	622	-	39,47,47	0.97	1 (2%)	54,74,74	2.77	21 (38%)
28	XAT	g	1622	-	39,47,47	0.98	2 (5%)	54,74,74	2.91	22 (40%)
26	CLA	n	612	1	60,68,73	1.55	7 (11%)	70,107,113	1.43	8 (11%)
26	CLA	b	606	5	65,73,73	1.54	12 (18%)	76,113,113	1.67	11 (14%)
26	CLA	5	611	30	45,53,73	1.79	9 (20%)	52,89,113	1.42	6 (11%)
26	CLA	3	603	2	55,63,73	1.56	11 (20%)	64,101,113	1.56	10 (15%)
25	CHL	Y	601	1	66,74,74	1.84	13 (19%)	73,114,114	2.86	22 (30%)
26	CLA	g	611	30	60,68,73	1.61	7 (11%)	70,107,113	1.60	7 (10%)
26	CLA	Y	614	1	48,56,73	1.67	10 (20%)	55,92,113	1.60	9 (16%)
41	HEM	f	101	9,8	41,50,50	1.46	4 (9%)	45,82,82	1.37	7 (15%)
26	CLA	Y	612	1	60,68,73	1.57	9 (15%)	70,107,113	1.42	7 (10%)
25	CHL	6	606	-	46,54,74	2.27	15 (32%)	49,90,114	3.09	17 (34%)
26	CLA	3	604	-	45,53,73	1.81	9 (20%)	52,89,113	1.51	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	Y	613	1	65,73,73	1.48	9 (13%)	76,113,113	1.43	9 (11%)
26	CLA	5	614	1	45,53,73	1.79	7 (15%)	52,89,113	1.47	8 (15%)
25	CHL	y	606	42	50,58,74	2.04	13 (26%)	52,94,114	3.18	19 (36%)
26	CLA	b	609	5	65,73,73	1.40	8 (12%)	76,113,113	1.69	12 (15%)
26	CLA	5	612	1	45,53,73	1.84	10 (22%)	52,89,113	1.50	9 (17%)
26	CLA	B	614	5	65,73,73	1.43	9 (13%)	76,113,113	1.45	7 (9%)
26	CLA	r	612	19	49,57,73	1.74	7 (14%)	55,93,113	1.61	7 (12%)
27	LUT	8	620	-	42,43,43	0.80	0	51,60,60	1.87	18 (35%)
26	CLA	S	610	20	55,63,73	1.63	8 (14%)	64,101,113	1.58	10 (15%)
26	CLA	S	603	20	45,53,73	1.77	10 (22%)	52,89,113	1.92	12 (23%)
26	CLA	1	610	1	56,64,73	1.61	9 (16%)	65,102,113	1.25	6 (9%)
25	CHL	3	605	2	46,54,74	2.29	15 (32%)	49,90,114	3.13	21 (42%)
28	XAT	G	1622	-	39,47,47	0.98	2 (5%)	54,74,74	2.91	23 (42%)
25	CHL	Y	609	1	66,74,74	1.86	14 (21%)	73,114,114	2.72	22 (30%)
25	CHL	2	605	1	46,54,74	2.30	16 (34%)	49,90,114	3.15	19 (38%)
26	CLA	1	604	-	50,58,73	1.74	9 (18%)	58,95,113	1.52	9 (15%)
26	CLA	r	609	19	58,66,73	1.62	8 (13%)	67,104,113	1.54	7 (10%)
26	CLA	B	615	5	65,73,73	1.40	10 (15%)	76,113,113	1.46	10 (13%)
25	CHL	5	607	-	63,71,74	1.89	13 (20%)	69,110,114	2.87	20 (28%)
25	CHL	7	605	2	46,54,74	2.29	15 (32%)	49,90,114	3.13	21 (42%)
30	LHG	r	2630	26	41,41,48	0.70	1 (2%)	44,47,54	1.27	6 (13%)
26	CLA	Y	604	42	50,58,73	1.73	10 (20%)	58,95,113	1.77	8 (13%)
27	LUT	s	1621	-	42,43,43	0.85	1 (2%)	51,60,60	1.78	17 (33%)
26	CLA	r	601	19	49,57,73	1.64	5 (10%)	55,93,113	1.92	11 (20%)
26	CLA	4	603	3	45,53,73	1.80	9 (20%)	52,89,113	1.60	8 (15%)
26	CLA	S	612	20	49,57,73	1.64	7 (14%)	55,93,113	1.68	6 (10%)
30	LHG	G	2630	26	48,48,48	0.66	1 (2%)	51,54,54	1.28	6 (11%)
26	CLA	B	608	42	65,73,73	1.53	10 (15%)	76,113,113	1.68	11 (14%)
35	PHO	a	408	-	51,69,69	1.13	6 (11%)	47,99,99	1.46	10 (21%)
26	CLA	A	410	4	60,68,73	1.48	10 (16%)	70,107,113	1.63	9 (12%)
25	CHL	3	608	-	46,54,74	2.20	15 (32%)	49,90,114	3.28	18 (36%)
26	CLA	A	407	42	50,58,73	1.61	10 (20%)	58,95,113	1.68	10 (17%)
26	CLA	b	607	5	65,73,73	1.50	11 (16%)	76,113,113	1.60	13 (17%)
25	CHL	n	605	1	48,56,74	2.20	14 (29%)	51,92,114	3.24	20 (39%)
26	CLA	G	603	1	65,73,73	1.52	11 (16%)	76,113,113	1.58	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	s	611	30	56,64,73	1.55	9 (16%)	65,102,113	1.48	7 (10%)
27	LUT	G	1620	-	42,43,43	0.76	0	51,60,60	1.64	12 (23%)
36	SQD	A	412	-	49,50,54	0.96	6 (12%)	58,61,65	1.74	11 (18%)
30	LHG	c	523	-	48,48,48	0.66	1 (2%)	51,54,54	1.20	5 (9%)
26	CLA	C	513	6	65,73,73	1.39	7 (10%)	76,113,113	1.60	14 (18%)
25	CHL	5	601	1	46,54,74	2.34	15 (32%)	49,90,114	3.07	21 (42%)
26	CLA	g	603	1	65,73,73	1.52	11 (16%)	76,113,113	1.58	13 (17%)
26	CLA	b	615	5	65,73,73	1.40	10 (15%)	76,113,113	1.46	10 (13%)
25	CHL	G	608	42	66,74,74	1.84	16 (24%)	73,114,114	2.73	21 (28%)
29	NEX	G	1623	-	38,46,46	1.00	2 (5%)	50,70,70	2.39	14 (28%)
26	CLA	S	609	20	45,53,73	1.82	6 (13%)	52,89,113	1.41	9 (17%)
25	CHL	n	607	42	66,74,74	1.80	13 (19%)	73,114,114	2.84	20 (27%)
28	XAT	Y	1622	-	39,47,47	1.08	4 (10%)	54,74,74	3.00	21 (38%)
30	LHG	8	2630	26	20,20,48	0.91	0	23,26,54	1.29	2 (8%)
25	CHL	N	606	42	50,58,74	2.16	15 (30%)	52,94,114	3.03	21 (40%)
27	LUT	2	1621	-	42,43,43	0.84	1 (2%)	51,60,60	1.68	15 (29%)
37	LMG	b	2633	-	55,55,55	0.78	3 (5%)	63,63,63	1.32	7 (11%)
26	CLA	c	509	6	65,73,73	1.45	11 (16%)	76,113,113	1.73	11 (14%)
25	CHL	5	608	-	46,54,74	2.17	14 (30%)	49,90,114	3.26	14 (28%)
25	CHL	Y	607	42	66,74,74	1.80	13 (19%)	73,114,114	2.72	21 (28%)
30	LHG	g	2630	26	48,48,48	0.66	1 (2%)	51,54,54	1.28	6 (11%)
27	LUT	1	1621	-	42,43,43	0.90	2 (4%)	51,60,60	1.73	15 (29%)
30	LHG	c	522	-	48,48,48	0.69	1 (2%)	51,54,54	1.26	6 (11%)
29	NEX	n	1623	-	38,46,46	0.90	1 (2%)	50,70,70	2.36	15 (30%)
31	BCR	b	619	-	41,41,41	0.80	0	56,56,56	1.81	17 (30%)
26	CLA	c	508	6	65,73,73	1.47	11 (16%)	76,113,113	1.84	12 (15%)
25	CHL	6	601	1	46,54,74	2.26	13 (28%)	49,90,114	3.22	22 (44%)
26	CLA	2	611	30	45,53,73	1.79	7 (15%)	52,89,113	1.53	7 (13%)
26	CLA	8	603	3	45,53,73	1.80	9 (20%)	52,89,113	1.60	8 (15%)
26	CLA	5	610	1	56,64,73	1.61	9 (16%)	65,102,113	1.25	6 (9%)
28	XAT	n	1622	-	39,47,47	0.93	0	54,74,74	3.00	24 (44%)
26	CLA	a	405	4	65,73,73	1.49	10 (15%)	76,113,113	1.67	12 (15%)
26	CLA	A	406	42	65,73,73	1.42	8 (12%)	76,113,113	1.76	16 (21%)
26	CLA	c	504	42	65,73,73	1.40	10 (15%)	76,113,113	1.67	8 (10%)
26	CLA	R	613	19	60,68,73	1.59	7 (11%)	70,107,113	1.28	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LUT	s	1620	-	42,43,43	0.78	0	51,60,60	1.76	12 (23%)
26	CLA	2	614	1	45,53,73	1.82	6 (13%)	52,89,113	1.45	7 (13%)
35	PHO	A	408	-	51,69,69	1.13	6 (11%)	47,99,99	1.46	11 (23%)
26	CLA	4	604	-	45,53,73	1.81	8 (17%)	52,89,113	1.45	7 (13%)
26	CLA	g	602	1	65,73,73	1.45	8 (12%)	76,113,113	1.58	11 (14%)
30	LHG	N	2630	26	48,48,48	0.66	1 (2%)	51,54,54	1.30	6 (11%)
25	CHL	Y	608	42	66,74,74	1.80	13 (19%)	73,114,114	2.74	23 (31%)
25	CHL	S	607	42	58,66,74	1.93	12 (20%)	63,104,114	2.86	20 (31%)
31	BCR	8	623	-	41,41,41	0.74	0	56,56,56	2.31	17 (30%)
26	CLA	y	612	1	60,68,73	1.57	9 (15%)	70,107,113	1.42	8 (11%)
26	CLA	a	407	42	50,58,73	1.61	10 (20%)	58,95,113	1.67	10 (17%)
25	CHL	3	607	-	53,61,74	2.24	16 (30%)	57,98,114	2.89	23 (40%)
26	CLA	g	604	42	50,58,73	1.78	10 (20%)	58,95,113	1.71	10 (17%)
26	CLA	5	603	1	55,63,73	1.57	11 (20%)	64,101,113	1.57	9 (14%)
37	LMG	c	521	-	51,51,55	0.79	3 (5%)	59,59,63	1.37	6 (10%)
26	CLA	c	502	6	65,73,73	1.40	9 (13%)	76,113,113	1.70	8 (10%)
27	LUT	n	1620	-	42,43,43	0.80	0	51,60,60	1.69	12 (23%)
26	CLA	d	402	7	65,73,73	1.55	10 (15%)	76,113,113	1.71	10 (13%)
25	CHL	2	607	-	61,69,74	1.96	15 (24%)	67,108,114	2.73	21 (31%)
25	CHL	s	608	-	46,54,74	2.24	15 (32%)	49,90,114	3.15	16 (32%)
26	CLA	4	612	3	45,53,73	1.77	7 (15%)	52,89,113	1.50	9 (17%)
30	LHG	s	2630	26	48,48,48	0.74	1 (2%)	51,54,54	1.26	7 (13%)
26	CLA	3	611	30	55,63,73	1.66	10 (18%)	64,101,113	1.51	11 (17%)
25	CHL	g	605	1	46,54,74	2.27	15 (32%)	49,90,114	3.32	20 (40%)
31	BCR	C	516	-	41,41,41	0.74	0	56,56,56	1.98	17 (30%)
26	CLA	6	602	1	61,69,73	1.52	8 (13%)	71,108,113	1.34	8 (11%)
27	LUT	2	1620	-	42,43,43	0.81	0	51,60,60	1.81	15 (29%)
28	XAT	1	1622	-	39,47,47	0.90	0	54,74,74	2.77	22 (40%)
26	CLA	3	614	2	48,56,73	1.72	8 (16%)	55,92,113	1.28	7 (12%)
26	CLA	C	511	6	65,73,73	1.44	8 (12%)	76,113,113	1.56	9 (11%)
26	CLA	7	603	2	55,63,73	1.56	11 (20%)	64,101,113	1.57	10 (15%)
30	LHG	L	101	-	48,48,48	0.90	1 (2%)	51,54,54	1.31	6 (11%)
25	CHL	5	609	1	62,70,74	1.93	14 (22%)	68,109,114	2.72	20 (29%)
26	CLA	1	602	1	61,69,73	1.51	10 (16%)	71,108,113	1.27	8 (11%)
30	LHG	y	2630	26	48,48,48	0.79	2 (4%)	51,54,54	1.23	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	R	616	19	45,53,73	1.83	7 (15%)	52,89,113	1.44	5 (9%)
26	CLA	D	403	7	65,73,73	1.42	7 (10%)	76,113,113	1.69	11 (14%)
26	CLA	7	610	2	60,68,73	1.58	9 (15%)	70,107,113	1.28	8 (11%)
26	CLA	6	614	1	45,53,73	1.82	6 (13%)	52,89,113	1.45	6 (11%)
26	CLA	Y	611	30	60,68,73	1.58	9 (15%)	70,107,113	1.53	9 (12%)
26	CLA	c	505	6	65,73,73	1.43	10 (15%)	76,113,113	1.75	11 (14%)
26	CLA	n	604	42	50,58,73	1.79	10 (20%)	58,95,113	1.75	9 (15%)
31	BCR	4	623	-	41,41,41	0.74	0	56,56,56	2.31	17 (30%)
26	CLA	c	512	6	65,73,73	1.42	10 (15%)	76,113,113	1.51	7 (9%)
36	SQD	b	623	-	41,42,54	1.09	5 (12%)	50,53,65	1.77	10 (20%)
26	CLA	b	616	5	65,73,73	1.46	10 (15%)	76,113,113	1.45	12 (15%)
37	LMG	Z	101	-	51,51,55	0.84	1 (1%)	59,59,63	1.32	5 (8%)
26	CLA	s	613	20	55,63,73	1.56	7 (12%)	64,101,113	1.55	7 (10%)
30	LHG	D	408	-	45,45,48	0.77	1 (2%)	48,51,54	1.28	5 (10%)
39	DGD	c	519	-	63,63,67	1.11	5 (7%)	77,77,81	1.47	12 (15%)
26	CLA	r	604	42	48,56,73	1.64	8 (16%)	55,92,113	1.77	10 (18%)
26	CLA	R	612	19	49,57,73	1.74	7 (14%)	55,93,113	1.61	7 (12%)
26	CLA	8	602	3	45,53,73	1.75	9 (20%)	52,89,113	1.59	7 (13%)
26	CLA	b	614	5	65,73,73	1.43	10 (15%)	76,113,113	1.45	7 (9%)
26	CLA	1	614	1	45,53,73	1.79	7 (15%)	52,89,113	1.47	7 (13%)
26	CLA	1	612	1	45,53,73	1.84	10 (22%)	52,89,113	1.50	9 (17%)
31	BCR	A	411	-	41,41,41	0.79	0	56,56,56	1.78	13 (23%)
29	NEX	2	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.39	15 (30%)
25	CHL	g	608	42	66,74,74	1.84	16 (24%)	73,114,114	2.73	21 (28%)
26	CLA	C	507	42	65,73,73	1.47	12 (18%)	76,113,113	1.74	11 (14%)
25	CHL	4	607	-	46,54,74	2.31	15 (32%)	49,90,114	3.04	18 (36%)
26	CLA	R	602	19	60,68,73	1.49	6 (10%)	70,107,113	1.64	9 (12%)
26	CLA	g	614	1	48,56,73	1.74	6 (12%)	55,92,113	1.48	7 (12%)
25	CHL	G	601	1	66,74,74	1.82	12 (18%)	73,114,114	2.90	24 (32%)
26	CLA	g	612	1	60,68,73	1.55	7 (11%)	70,107,113	1.35	8 (11%)
31	BCR	c	516	-	41,41,41	0.73	0	56,56,56	1.98	17 (30%)
26	CLA	a	406	42	65,73,73	1.42	8 (12%)	76,113,113	1.76	16 (21%)
30	LHG	b	2630	-	46,46,48	0.66	1 (2%)	49,52,54	1.28	6 (12%)
26	CLA	2	613	1	45,53,73	1.82	9 (20%)	52,89,113	1.43	7 (13%)
26	CLA	1	603	1	55,63,73	1.57	11 (20%)	64,101,113	1.57	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	2	603	1	55,63,73	1.63	10 (18%)	64,101,113	1.52	10 (15%)
25	CHL	6	609	1	61,69,74	1.98	14 (22%)	67,108,114	2.74	20 (29%)
26	CLA	C	503	6	65,73,73	1.48	9 (13%)	76,113,113	1.43	10 (13%)
26	CLA	G	613	1	65,73,73	1.49	8 (12%)	76,113,113	1.36	7 (9%)
26	CLA	R	603	19	60,68,73	1.45	9 (15%)	70,107,113	1.67	12 (17%)
39	DGD	C	520	-	61,61,67	1.17	8 (13%)	75,75,81	1.47	12 (16%)
37	LMG	a	413	-	48,48,55	0.79	0	56,56,63	1.31	6 (10%)
26	CLA	5	602	1	61,69,73	1.51	10 (16%)	71,108,113	1.28	8 (11%)
26	CLA	5	604	-	50,58,73	1.74	9 (18%)	58,95,113	1.52	9 (15%)
26	CLA	b	604	5	65,73,73	1.50	11 (16%)	76,113,113	1.46	10 (13%)
26	CLA	1	611	30	45,53,73	1.79	9 (20%)	52,89,113	1.41	6 (11%)
39	DGD	c	520	-	61,61,67	1.17	8 (13%)	75,75,81	1.47	12 (16%)
25	CHL	2	606	-	46,54,74	2.26	15 (32%)	49,90,114	3.08	18 (36%)
25	CHL	R	606	42	66,74,74	1.87	14 (21%)	73,114,114	2.78	22 (30%)
30	LHG	B	2630	-	46,46,48	0.65	1 (2%)	49,52,54	1.28	6 (12%)
30	LHG	1	2630	26	40,40,48	0.72	1 (2%)	43,46,54	1.34	6 (13%)
26	CLA	c	510	6	65,73,73	1.44	7 (10%)	76,113,113	1.58	10 (13%)
27	LUT	r	620	-	42,43,43	0.87	2 (4%)	51,60,60	1.82	14 (27%)
25	CHL	6	607	-	61,69,74	1.95	15 (24%)	67,108,114	2.73	21 (31%)
27	LUT	4	620	-	42,43,43	0.80	0	51,60,60	1.87	18 (35%)
40	BCT	D	401	33	2,3,3	1.32	0	2,3,3	4.20	2 (100%)
26	CLA	S	611	30	56,64,73	1.55	9 (16%)	65,102,113	1.47	7 (10%)
26	CLA	A	405	4	65,73,73	1.49	10 (15%)	76,113,113	1.68	12 (15%)
25	CHL	n	608	42	66,74,74	1.82	13 (19%)	73,114,114	2.77	25 (34%)
25	CHL	5	606	-	46,54,74	2.24	15 (32%)	49,90,114	3.08	20 (40%)
26	CLA	N	613	1	60,68,73	1.49	8 (13%)	70,107,113	1.58	7 (10%)
26	CLA	N	603	1	65,73,73	1.54	11 (16%)	76,113,113	1.61	15 (19%)
31	BCR	c	514	-	41,41,41	0.90	2 (4%)	56,56,56	1.74	13 (23%)
25	CHL	S	606	42	46,54,74	2.27	15 (32%)	49,90,114	3.37	19 (38%)
26	CLA	B	605	5	65,73,73	1.54	11 (16%)	76,113,113	2.03	24 (31%)
26	CLA	N	604	42	50,58,73	1.79	10 (20%)	58,95,113	1.74	9 (15%)
26	CLA	s	612	20	49,57,73	1.64	7 (14%)	55,93,113	1.68	6 (10%)
37	LMG	A	413	-	48,48,55	0.79	0	56,56,63	1.31	6 (10%)
30	LHG	C	522	-	48,48,48	0.69	1 (2%)	51,54,54	1.26	6 (11%)
26	CLA	C	509	6	65,73,73	1.45	11 (16%)	76,113,113	1.73	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	r	608	42	61,69,74	1.90	10 (16%)	67,108,114	2.91	23 (34%)
30	LHG	n	2630	26	48,48,48	0.66	1 (2%)	51,54,54	1.30	6 (11%)
40	BCT	d	401	33	2,3,3	1.32	0	2,3,3	4.19	2 (100%)
26	CLA	R	610	19	65,73,73	1.47	9 (13%)	76,113,113	1.38	11 (14%)
37	LMG	a	415	-	40,40,55	0.86	0	48,48,63	1.29	5 (10%)
31	BCR	a	411	-	41,41,41	0.79	0	56,56,56	1.78	13 (23%)
26	CLA	s	609	20	45,53,73	1.81	6 (13%)	52,89,113	1.41	9 (17%)
38	PL9	a	414	-	13,13,55	0.87	0	17,17,69	1.68	4 (23%)
25	CHL	N	601	1	66,74,74	1.84	14 (21%)	73,114,114	2.82	23 (31%)
25	CHL	s	607	42	58,66,74	1.93	12 (20%)	63,104,114	2.86	20 (31%)
25	CHL	g	607	42	66,74,74	1.88	13 (19%)	73,114,114	2.66	22 (30%)
25	CHL	Y	605	1	48,56,74	2.15	14 (29%)	51,92,114	3.33	17 (33%)
26	CLA	8	612	3	45,53,73	1.78	7 (15%)	52,89,113	1.51	9 (17%)
25	CHL	G	606	42	50,58,74	2.21	15 (30%)	52,94,114	3.06	22 (42%)
26	CLA	2	612	1	45,53,73	1.85	7 (15%)	52,89,113	1.50	8 (15%)
29	NEX	g	1623	-	38,46,46	1.00	3 (7%)	50,70,70	2.39	14 (28%)
25	CHL	s	606	42	46,54,74	2.27	15 (32%)	49,90,114	3.37	19 (38%)
26	CLA	b	605	5	65,73,73	1.55	11 (16%)	76,113,113	2.03	24 (31%)
26	CLA	y	604	42	50,58,73	1.73	10 (20%)	58,95,113	1.77	8 (13%)
25	CHL	8	607	-	46,54,74	2.31	15 (32%)	49,90,114	3.05	18 (36%)
28	XAT	8	622	-	39,47,47	0.93	1 (2%)	54,74,74	2.62	21 (38%)
26	CLA	c	501	6	65,73,73	1.48	9 (13%)	76,113,113	1.37	10 (13%)
25	CHL	n	606	42	50,58,74	2.16	15 (30%)	52,94,114	3.04	21 (40%)
25	CHL	y	609	1	66,74,74	1.86	14 (21%)	73,114,114	2.72	22 (30%)
37	LMG	B	2633	-	55,55,55	0.78	3 (5%)	63,63,63	1.32	7 (11%)
26	CLA	r	611	30	49,57,73	1.65	8 (16%)	55,93,113	1.74	12 (21%)
25	CHL	8	606	-	46,54,74	2.29	15 (32%)	49,90,114	3.19	22 (44%)
28	XAT	5	1622	-	39,47,47	0.90	0	54,74,74	2.77	22 (40%)
39	DGD	B	626	-	60,60,67	1.04	3 (5%)	74,74,81	1.39	12 (16%)
26	CLA	6	613	1	45,53,73	1.82	9 (20%)	52,89,113	1.43	7 (13%)
31	BCR	C	515	-	41,41,41	0.93	2 (4%)	56,56,56	2.01	16 (28%)
26	CLA	C	506	6	65,73,73	1.45	10 (15%)	76,113,113	1.58	11 (14%)
26	CLA	R	609	19	58,66,73	1.62	8 (13%)	67,104,113	1.54	7 (10%)
26	CLA	S	602	20	61,69,73	1.51	8 (13%)	71,108,113	1.46	11 (15%)
25	CHL	y	601	1	66,74,74	1.84	13 (19%)	73,114,114	2.86	22 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	4	609	3	46,54,74	2.31	15 (32%)	49,90,114	3.07	17 (34%)
25	CHL	8	609	3	46,54,74	2.31	15 (32%)	49,90,114	3.08	17 (34%)
26	CLA	B	610	5	65,73,73	1.41	9 (13%)	76,113,113	1.60	9 (11%)
26	CLA	C	502	6	65,73,73	1.40	9 (13%)	76,113,113	1.70	9 (11%)
30	LHG	c	2630	-	48,48,48	0.66	1 (2%)	51,54,54	1.31	7 (13%)
30	LHG	C	523	-	48,48,48	0.66	1 (2%)	51,54,54	1.20	5 (9%)
25	CHL	8	601	3	44,53,74	2.43	16 (36%)	46,89,114	3.02	16 (34%)
39	DGD	b	626	-	60,60,67	1.05	3 (5%)	74,74,81	1.39	12 (16%)
25	CHL	r	607	42	56,64,74	2.01	12 (21%)	61,102,114	3.09	21 (34%)
37	LMG	d	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.45	4 (7%)
26	CLA	b	610	5	65,73,73	1.41	9 (13%)	76,113,113	1.59	9 (11%)
37	LMG	A	415	-	40,40,55	0.86	0	48,48,63	1.28	5 (10%)
30	LHG	C	2630	-	48,48,48	0.66	1 (2%)	51,54,54	1.31	7 (13%)
25	CHL	G	609	1	61,69,74	1.93	14 (22%)	67,108,114	2.78	22 (32%)
25	CHL	1	605	1	46,54,74	2.25	15 (32%)	49,90,114	3.22	21 (42%)
25	CHL	S	601	20	46,54,74	2.28	13 (28%)	49,90,114	3.13	20 (40%)
26	CLA	r	603	19	60,68,73	1.45	9 (15%)	70,107,113	1.66	12 (17%)
26	CLA	c	513	6	65,73,73	1.39	7 (10%)	76,113,113	1.60	14 (18%)
39	DGD	h	102	-	63,63,67	1.08	7 (11%)	77,77,81	1.41	11 (14%)
27	LUT	N	1621	-	42,43,43	0.89	2 (4%)	51,60,60	1.83	14 (27%)
26	CLA	b	608	42	65,73,73	1.53	10 (15%)	76,113,113	1.69	11 (14%)
29	NEX	Y	1623	-	38,46,46	0.94	2 (5%)	50,70,70	2.59	18 (36%)
27	LUT	3	1621	-	42,43,43	0.85	1 (2%)	51,60,60	1.60	11 (21%)
26	CLA	B	602	42	65,73,73	1.50	9 (13%)	76,113,113	1.41	7 (9%)
25	CHL	n	609	1	66,74,74	1.88	14 (21%)	73,114,114	2.72	23 (31%)
32	OEX	A	401	4,6	0,15,15	-	-	-	-	-
30	LHG	3	2630	26	46,46,48	0.70	1 (2%)	49,52,54	1.24	5 (10%)
28	XAT	N	1622	-	39,47,47	0.92	0	54,74,74	3.00	24 (44%)
25	CHL	1	607	-	63,71,74	1.89	13 (20%)	69,110,114	2.87	20 (28%)
26	CLA	b	612	5	65,73,73	1.50	8 (12%)	76,113,113	1.66	9 (11%)
25	CHL	y	608	42	66,74,74	1.80	13 (19%)	73,114,114	2.74	23 (31%)
26	CLA	b	613	5	65,73,73	1.47	9 (13%)	76,113,113	1.85	13 (17%)
26	CLA	N	611	30	60,68,73	1.54	7 (11%)	70,107,113	1.45	7 (10%)
25	CHL	n	601	1	66,74,74	1.85	14 (21%)	73,114,114	2.82	23 (31%)
30	LHG	Y	2630	26	48,48,48	0.79	2 (4%)	51,54,54	1.23	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCR	H	101	-	41,41,41	0.78	0	56,56,56	1.90	10 (17%)
26	CLA	n	613	1	60,68,73	1.49	8 (13%)	70,107,113	1.58	7 (10%)
26	CLA	n	603	1	65,73,73	1.55	10 (15%)	76,113,113	1.61	15 (19%)
26	CLA	3	610	2	60,68,73	1.57	9 (15%)	70,107,113	1.28	8 (11%)
41	HEM	F	101	9,8	41,50,50	1.46	4 (9%)	45,82,82	1.37	7 (15%)
26	CLA	Y	603	1	65,73,73	1.59	10 (15%)	76,113,113	1.56	13 (17%)
27	LUT	S	1620	-	42,43,43	0.79	0	51,60,60	1.76	12 (23%)
25	CHL	g	609	1	61,69,74	1.93	14 (22%)	67,108,114	2.78	22 (32%)
30	LHG	4	2630	26	20,20,48	0.91	1 (5%)	23,26,54	1.30	2 (8%)
26	CLA	C	505	6	65,73,73	1.43	10 (15%)	76,113,113	1.75	11 (14%)
38	PL9	d	405	-	55,55,55	1.83	12 (21%)	68,69,69	1.57	12 (17%)
30	LHG	6	2630	26	36,36,48	0.74	1 (2%)	39,42,54	1.27	4 (10%)
26	CLA	C	512	6	65,73,73	1.42	10 (15%)	76,113,113	1.51	8 (10%)
25	CHL	1	608	-	46,54,74	2.17	14 (30%)	49,90,114	3.27	14 (28%)
25	CHL	4	606	-	46,54,74	2.29	15 (32%)	49,90,114	3.18	23 (46%)
26	CLA	C	501	6	65,73,73	1.48	9 (13%)	76,113,113	1.37	10 (13%)
25	CHL	s	601	20	46,54,74	2.28	14 (30%)	49,90,114	3.12	20 (40%)
31	BCR	c	517	-	41,41,41	0.89	1 (2%)	56,56,56	2.09	11 (19%)
26	CLA	G	610	1	64,72,73	1.50	7 (10%)	74,111,113	1.37	8 (10%)
30	LHG	l	101	-	48,48,48	0.90	1 (2%)	51,54,54	1.31	7 (13%)
31	BCR	h	101	-	41,41,41	0.78	0	56,56,56	1.89	10 (17%)
26	CLA	G	602	1	65,73,73	1.45	8 (12%)	76,113,113	1.59	11 (14%)
31	BCR	B	620	-	41,41,41	0.79	0	56,56,56	1.99	16 (28%)
26	CLA	R	601	19	49,57,73	1.64	5 (10%)	55,93,113	1.92	11 (20%)
35	PHO	A	409	-	51,69,69	1.09	4 (7%)	47,99,99	1.36	7 (14%)
26	CLA	6	603	1	55,63,73	1.63	11 (20%)	64,101,113	1.53	10 (15%)
26	CLA	6	611	30	45,53,73	1.79	8 (17%)	52,89,113	1.52	7 (13%)
28	XAT	R	622	-	39,47,47	0.97	1 (2%)	54,74,74	2.76	21 (38%)
25	CHL	2	609	1	61,69,74	1.98	15 (24%)	67,108,114	2.74	20 (29%)
29	NEX	6	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.38	15 (30%)
27	LUT	3	1620	-	42,43,43	0.85	0	51,60,60	1.72	13 (25%)
29	NEX	R	623	-	38,46,46	1.05	3 (7%)	50,70,70	2.51	19 (38%)
25	CHL	6	605	1	46,54,74	2.29	16 (34%)	49,90,114	3.15	19 (38%)
26	CLA	R	611	30	49,57,73	1.65	8 (16%)	55,93,113	1.75	12 (21%)
25	CHL	y	605	1	48,56,74	2.15	14 (29%)	51,92,114	3.33	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	3	602	2	60,68,73	1.55	9 (15%)	70,107,113	1.34	8 (11%)
29	NEX	3	1623	-	38,46,46	0.87	1 (2%)	50,70,70	2.40	16 (32%)
25	CHL	5	605	1	46,54,74	2.25	15 (32%)	49,90,114	3.21	21 (42%)
26	CLA	G	612	1	60,68,73	1.54	8 (13%)	70,107,113	1.35	8 (11%)
29	NEX	1	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.42	15 (30%)
25	CHL	2	601	1	46,54,74	2.26	13 (28%)	49,90,114	3.23	22 (44%)
35	PHO	a	409	-	51,69,69	1.09	4 (7%)	47,99,99	1.36	7 (14%)
28	XAT	3	1622	-	39,47,47	1.03	2 (5%)	54,74,74	2.85	24 (44%)
29	NEX	S	1623	-	38,46,46	0.91	2 (5%)	50,70,70	2.24	15 (30%)
26	CLA	B	606	5	65,73,73	1.54	12 (18%)	76,113,113	1.67	11 (14%)
26	CLA	B	611	42	65,73,73	1.45	10 (15%)	76,113,113	1.70	13 (17%)
25	CHL	y	607	42	66,74,74	1.80	13 (19%)	73,114,114	2.72	21 (28%)
27	LUT	7	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.60	11 (21%)
28	XAT	y	1622	-	39,47,47	1.08	3 (7%)	54,74,74	3.00	21 (38%)
26	CLA	Y	610	1	60,68,73	1.55	10 (16%)	70,107,113	1.28	8 (11%)
26	CLA	r	616	19	45,53,73	1.82	7 (15%)	52,89,113	1.44	5 (9%)
26	CLA	B	603	5	65,73,73	1.43	7 (10%)	76,113,113	1.51	8 (10%)
26	CLA	2	602	1	61,69,73	1.52	8 (13%)	71,108,113	1.34	8 (11%)
31	BCR	C	517	-	41,41,41	0.89	1 (2%)	56,56,56	2.08	11 (19%)
25	CHL	7	606	-	46,54,74	2.20	15 (32%)	49,90,114	3.15	19 (38%)
26	CLA	y	611	30	60,68,73	1.58	9 (15%)	70,107,113	1.53	9 (12%)
27	LUT	y	1620	-	42,43,43	0.88	1 (2%)	51,60,60	1.72	13 (25%)
26	CLA	B	613	5	65,73,73	1.48	9 (13%)	76,113,113	1.84	13 (17%)
26	CLA	C	510	6	65,73,73	1.44	7 (10%)	76,113,113	1.59	10 (13%)
30	LHG	B	2631	-	48,48,48	0.68	2 (4%)	51,54,54	1.22	6 (11%)
26	CLA	c	506	6	65,73,73	1.45	10 (15%)	76,113,113	1.58	10 (13%)
26	CLA	7	602	2	60,68,73	1.55	9 (15%)	70,107,113	1.34	8 (11%)
31	BCR	C	514	-	41,41,41	0.90	1 (2%)	56,56,56	1.75	13 (23%)
30	LHG	S	2630	26	48,48,48	0.73	1 (2%)	51,54,54	1.26	7 (13%)
27	LUT	n	1621	-	42,43,43	0.89	2 (4%)	51,60,60	1.83	14 (27%)
25	CHL	7	609	2	61,69,74	2.02	15 (24%)	67,108,114	2.61	21 (31%)
26	CLA	6	610	1	50,58,73	1.67	9 (18%)	58,95,113	1.37	9 (15%)
26	CLA	y	603	1	65,73,73	1.59	10 (15%)	76,113,113	1.56	13 (17%)
26	CLA	y	610	1	60,68,73	1.55	10 (16%)	70,107,113	1.28	8 (11%)
28	XAT	6	1622	-	39,47,47	0.91	1 (2%)	54,74,74	2.81	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	s	604	42	50,58,73	1.65	7 (14%)	58,95,113	1.97	9 (15%)
32	OEX	a	401	4,6	0,15,15	-	-	-		
25	CHL	g	606	42	50,58,74	2.20	15 (30%)	52,94,114	3.06	22 (42%)
25	CHL	r	614	19	42,50,74	2.33	14 (33%)	44,85,114	3.45	19 (43%)
26	CLA	N	602	1	65,73,73	1.44	8 (12%)	76,113,113	1.58	11 (14%)
26	CLA	n	602	1	65,73,73	1.44	8 (12%)	76,113,113	1.58	11 (14%)
31	BCR	d	404	-	41,41,41	0.74	0	56,56,56	1.84	12 (21%)
25	CHL	7	601	2	64,72,74	1.91	12 (18%)	70,111,114	2.88	23 (32%)
26	CLA	G	614	1	48,56,73	1.73	6 (12%)	55,92,113	1.48	7 (12%)
26	CLA	7	614	2	48,56,73	1.72	8 (16%)	55,92,113	1.28	7 (12%)
36	SQD	B	621	-	53,54,54	0.94	4 (7%)	62,65,65	1.64	13 (20%)
26	CLA	4	610	3	45,53,73	1.81	9 (20%)	52,89,113	1.30	6 (11%)
26	CLA	8	604	-	45,53,73	1.81	8 (17%)	52,89,113	1.44	7 (13%)
30	LHG	D	409	-	48,48,48	0.75	1 (2%)	51,54,54	1.31	7 (13%)
25	CHL	N	605	1	48,56,74	2.19	14 (29%)	51,92,114	3.24	20 (39%)
30	LHG	5	2630	26	40,40,48	0.72	1 (2%)	43,46,54	1.33	6 (13%)
27	LUT	6	1620	-	42,43,43	0.81	0	51,60,60	1.80	15 (29%)
26	CLA	c	507	42	65,73,73	1.48	12 (18%)	76,113,113	1.73	11 (14%)
26	CLA	s	614	20	49,57,73	1.63	6 (12%)	55,93,113	1.75	10 (18%)
38	PL9	A	414	-	13,13,55	0.87	0	17,17,69	1.68	4 (23%)
39	DGD	c	518	-	56,56,67	1.17	7 (12%)	70,70,81	1.56	12 (17%)
26	CLA	n	614	1	48,56,73	1.66	6 (12%)	55,92,113	1.69	8 (14%)
25	CHL	G	607	42	66,74,74	1.88	13 (19%)	73,114,114	2.66	23 (31%)
31	BCR	B	619	-	41,41,41	0.80	0	56,56,56	1.81	17 (30%)
26	CLA	2	604	-	45,53,73	1.81	8 (17%)	52,89,113	1.50	6 (11%)
26	CLA	b	617	5	65,73,73	1.45	9 (13%)	76,113,113	1.62	11 (14%)
25	CHL	4	601	3	44,53,74	2.42	16 (36%)	46,89,114	3.02	16 (34%)
36	SQD	a	412	-	49,50,54	0.96	6 (12%)	58,61,65	1.75	11 (18%)
26	CLA	C	508	6	65,73,73	1.47	11 (16%)	76,113,113	1.84	11 (14%)
27	LUT	1	1620	-	42,43,43	0.79	0	51,60,60	1.66	14 (27%)
25	CHL	N	608	42	66,74,74	1.82	13 (19%)	73,114,114	2.77	25 (34%)
25	CHL	6	608	-	46,54,74	2.23	15 (32%)	49,90,114	3.26	17 (34%)
26	CLA	7	604	-	45,53,73	1.81	9 (20%)	52,89,113	1.51	7 (13%)
29	NEX	y	1623	-	38,46,46	0.94	2 (5%)	50,70,70	2.59	18 (36%)
26	CLA	b	611	42	65,73,73	1.44	10 (15%)	76,113,113	1.69	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	NEX	r	623	-	38,46,46	1.04	3 (7%)	50,70,70	2.51	19 (38%)
25	CHL	3	601	2	64,72,74	1.91	12 (18%)	70,111,114	2.89	23 (32%)
25	CHL	8	608	-	46,54,74	2.16	14 (30%)	49,90,114	3.32	18 (36%)
27	LUT	g	1620	-	42,43,43	0.77	0	51,60,60	1.63	12 (23%)
31	BCR	b	618	-	41,41,41	0.84	1 (2%)	56,56,56	1.85	14 (25%)
26	CLA	d	403	7	65,73,73	1.42	7 (10%)	76,113,113	1.69	11 (14%)
26	CLA	4	602	3	45,53,73	1.75	9 (20%)	52,89,113	1.58	7 (13%)
26	CLA	b	603	5	65,73,73	1.42	7 (10%)	76,113,113	1.51	8 (10%)
27	LUT	6	1621	-	42,43,43	0.84	1 (2%)	51,60,60	1.68	15 (29%)
25	CHL	r	606	42	66,74,74	1.87	14 (21%)	73,114,114	2.78	22 (30%)
31	BCR	D	404	-	41,41,41	0.75	0	56,56,56	1.83	12 (21%)
25	CHL	2	608	-	46,54,74	2.23	15 (32%)	49,90,114	3.26	17 (34%)
26	CLA	1	613	1	55,63,73	1.64	9 (16%)	64,101,113	1.34	6 (9%)
30	LHG	2	2630	26	36,36,48	0.74	1 (2%)	39,42,54	1.27	4 (10%)
36	SQD	A	418	-	53,54,54	0.92	5 (9%)	62,65,65	1.67	14 (22%)
27	LUT	S	1621	-	42,43,43	0.85	1 (2%)	51,60,60	1.78	17 (33%)
25	CHL	3	606	-	46,54,74	2.20	15 (32%)	49,90,114	3.15	19 (38%)
38	PL9	D	405	-	55,55,55	1.83	12 (21%)	68,69,69	1.57	12 (17%)
30	LHG	d	408	-	45,45,48	0.78	1 (2%)	48,51,54	1.28	5 (10%)
25	CHL	7	607	-	53,61,74	2.24	16 (30%)	57,98,114	2.88	23 (40%)
31	BCR	T	101	-	41,41,41	0.75	0	56,56,56	2.55	19 (33%)
26	CLA	8	611	30	45,53,73	1.81	8 (17%)	52,89,113	1.50	7 (13%)
26	CLA	s	610	20	55,63,73	1.63	8 (14%)	64,101,113	1.58	10 (15%)
37	LMG	B	622	-	51,51,55	0.83	1 (1%)	59,59,63	1.30	4 (6%)
37	LMG	z	101	-	51,51,55	0.84	1 (1%)	59,59,63	1.32	5 (8%)
29	NEX	N	1623	-	38,46,46	0.90	1 (2%)	50,70,70	2.36	15 (30%)
26	CLA	3	612	2	45,53,73	1.78	10 (22%)	52,89,113	1.51	10 (19%)
25	CHL	Y	606	42	50,58,74	2.04	13 (26%)	52,94,114	3.18	19 (36%)
30	LHG	d	410	-	42,42,48	0.68	1 (2%)	45,48,54	1.22	4 (8%)
26	CLA	D	402	7	65,73,73	1.55	10 (15%)	76,113,113	1.71	10 (13%)
27	LUT	Y	1620	-	42,43,43	0.87	1 (2%)	51,60,60	1.73	13 (25%)
26	CLA	S	613	20	55,63,73	1.56	7 (12%)	64,101,113	1.55	7 (10%)
26	CLA	n	610	1	65,73,73	1.43	8 (12%)	76,113,113	1.42	10 (13%)
26	CLA	c	511	6	65,73,73	1.45	8 (12%)	76,113,113	1.55	9 (11%)
31	BCR	t	101	-	41,41,41	0.76	0	56,56,56	2.55	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	g	601	1	66,74,74	1.82	12 (18%)	73,114,114	2.90	24 (32%)
26	CLA	S	614	20	49,57,73	1.62	6 (12%)	55,93,113	1.76	10 (18%)
27	LUT	5	1620	-	42,43,43	0.80	0	51,60,60	1.66	15 (29%)
26	CLA	G	611	30	60,68,73	1.61	7 (11%)	70,107,113	1.60	7 (10%)
26	CLA	7	611	30	55,63,73	1.66	10 (18%)	64,101,113	1.51	11 (17%)
37	LMG	b	622	-	51,51,55	0.83	1 (1%)	59,59,63	1.30	4 (6%)
25	CHL	7	608	-	46,54,74	2.20	15 (32%)	49,90,114	3.28	19 (38%)
31	BCR	b	620	-	41,41,41	0.80	0	56,56,56	1.99	16 (28%)
25	CHL	R	614	19	42,50,74	2.32	14 (33%)	44,85,114	3.45	19 (43%)
26	CLA	B	607	5	65,73,73	1.50	11 (16%)	76,113,113	1.60	12 (15%)
26	CLA	c	503	6	65,73,73	1.49	9 (13%)	76,113,113	1.44	9 (11%)
30	LHG	7	2630	26	46,46,48	0.70	1 (2%)	49,52,54	1.25	5 (10%)
26	CLA	r	610	19	65,73,73	1.48	9 (13%)	76,113,113	1.38	11 (14%)
39	DGD	C	518	-	56,56,67	1.17	7 (12%)	70,70,81	1.56	13 (18%)
31	BCR	B	618	-	41,41,41	0.84	1 (2%)	56,56,56	1.85	14 (25%)
26	CLA	s	602	20	61,69,73	1.51	8 (13%)	71,108,113	1.46	11 (15%)
29	NEX	s	1623	-	38,46,46	0.90	2 (5%)	50,70,70	2.24	15 (30%)
26	CLA	r	602	19	60,68,73	1.50	7 (11%)	70,107,113	1.65	9 (12%)
36	SQD	B	623	-	41,42,54	1.10	5 (12%)	50,53,65	1.77	10 (20%)
26	CLA	R	604	42	48,56,73	1.64	8 (16%)	55,92,113	1.77	10 (18%)
25	CHL	R	607	42	56,64,74	2.01	13 (23%)	61,102,114	3.09	21 (34%)
26	CLA	7	612	2	45,53,73	1.77	10 (22%)	52,89,113	1.51	10 (19%)
39	DGD	C	519	-	63,63,67	1.11	5 (7%)	77,77,81	1.47	12 (15%)
26	CLA	N	614	1	48,56,73	1.66	6 (12%)	55,92,113	1.68	8 (14%)
26	CLA	N	612	1	60,68,73	1.55	7 (11%)	70,107,113	1.43	8 (11%)
27	LUT	7	1620	-	42,43,43	0.84	0	51,60,60	1.71	12 (23%)
26	CLA	y	602	1	65,73,73	1.43	8 (12%)	76,113,113	1.53	10 (13%)
36	SQD	b	621	-	53,54,54	0.94	4 (7%)	62,65,65	1.64	13 (20%)
26	CLA	S	604	42	50,58,73	1.64	7 (14%)	58,95,113	1.96	8 (13%)
28	XAT	7	1622	-	39,47,47	1.03	2 (5%)	54,74,74	2.85	24 (44%)
25	CHL	4	608	-	46,54,74	2.16	14 (30%)	49,90,114	3.30	18 (36%)
26	CLA	3	613	2	58,66,73	1.61	10 (17%)	67,104,113	1.42	8 (11%)
26	CLA	8	610	3	45,53,73	1.81	9 (20%)	52,89,113	1.30	6 (11%)
26	CLA	B	617	5	65,73,73	1.45	9 (13%)	76,113,113	1.62	11 (14%)
27	LUT	y	1621	-	42,43,43	0.88	1 (2%)	51,60,60	1.69	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	XAT	2	1622	-	39,47,47	0.91	1 (2%)	54,74,74	2.82	21 (38%)
25	CHL	N	607	42	66,74,74	1.80	13 (19%)	73,114,114	2.84	20 (27%)
26	CLA	2	610	1	50,58,73	1.67	9 (18%)	58,95,113	1.37	9 (15%)
26	CLA	6	604	-	45,53,73	1.81	8 (17%)	52,89,113	1.50	6 (11%)
26	CLA	a	410	4	60,68,73	1.48	10 (16%)	70,107,113	1.64	9 (12%)
30	LHG	D	410	-	42,42,48	0.68	1 (2%)	45,48,54	1.22	4 (8%)
27	LUT	R	620	-	42,43,43	0.86	2 (4%)	51,60,60	1.82	14 (27%)
26	CLA	6	612	1	45,53,73	1.85	8 (17%)	52,89,113	1.50	8 (15%)
26	CLA	b	602	42	65,73,73	1.50	9 (13%)	76,113,113	1.41	7 (9%)
29	NEX	5	1623	-	38,46,46	0.98	2 (5%)	50,70,70	2.41	16 (32%)
39	DGD	H	102	-	63,63,67	1.08	7 (11%)	77,77,81	1.40	11 (14%)

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
25	CHL	R	608	42	4/4/19/26	17/33/131/137	-
26	CLA	r	613	19	1/1/14/20	10/31/109/115	-
28	XAT	4	622	-	-	2/31/93/93	0/4/4/4
26	CLA	s	603	20	1/1/11/20	5/13/91/115	-
26	CLA	g	610	1	1/1/14/20	13/36/114/115	-
37	LMG	D	411	-	-	15/41/61/70	0/1/1/1
26	CLA	y	613	1	1/1/15/20	10/37/115/115	-
26	CLA	5	613	1	-	8/25/103/115	-
26	CLA	y	614	1	1/1/11/20	3/17/95/115	-
30	LHG	R	2630	26	-	19/46/46/53	-
36	SQD	a	418	-	-	22/49/69/69	0/1/1/1
25	CHL	1	609	1	4/4/19/26	16/35/133/137	-
26	CLA	B	604	5	1/1/15/20	10/37/115/115	-
26	CLA	N	610	1	1/1/15/20	12/37/115/115	-
26	CLA	B	616	5	1/1/15/20	13/37/115/115	-
26	CLA	C	504	42	1/1/15/20	18/37/115/115	-
25	CHL	1	601	1	3/3/16/26	6/15/113/137	-
26	CLA	g	613	1	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	NEX	7	1623	-	-	4/27/83/83	0/3/3/3
30	LHG	d	409	-	-	27/53/53/53	-
26	CLA	B	612	5	1/1/15/20	13/37/115/115	-
30	LHG	b	2631	-	-	22/53/53/53	-
25	CHL	1	606	-	3/3/16/26	8/15/113/137	-
25	CHL	S	608	-	3/3/16/26	4/15/113/137	-
27	LUT	Y	1621	-	-	1/29/67/67	0/2/2/2
37	LMG	C	521	-	-	22/46/66/70	0/1/1/1
27	LUT	G	1621	-	-	3/29/67/67	0/2/2/2
25	CHL	G	605	1	3/3/16/26	9/15/113/137	-
26	CLA	4	611	30	1/1/11/20	4/13/91/115	-
27	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
25	CHL	N	609	1	4/4/20/26	13/39/137/137	-
26	CLA	Y	602	1	1/1/15/20	10/37/115/115	-
26	CLA	7	613	2	1/1/13/20	9/29/107/115	-
27	LUT	5	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	n	611	30	1/1/14/20	4/31/109/115	-
26	CLA	B	609	5	-	9/37/115/115	-
25	CHL	3	609	2	4/4/19/26	13/33/131/137	-
31	BCR	c	515	-	-	6/29/63/63	0/2/2/2
27	LUT	g	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	G	604	42	1/1/12/20	5/19/97/115	-
28	XAT	r	622	-	-	3/31/93/93	0/4/4/4
28	XAT	g	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	n	612	1	1/1/14/20	9/31/109/115	-
26	CLA	b	606	5	1/1/15/20	14/37/115/115	-
26	CLA	5	611	30	1/1/11/20	6/13/91/115	-
26	CLA	3	603	2	1/1/13/20	13/25/103/115	-
25	CHL	Y	601	1	4/4/20/26	16/39/137/137	-
26	CLA	g	611	30	1/1/14/20	11/31/109/115	-
26	CLA	Y	614	1	1/1/11/20	3/17/95/115	-
41	HEM	f	101	9,8	-	1/12/54/54	-
26	CLA	Y	612	1	1/1/14/20	15/31/109/115	-
25	CHL	6	606	-	3/3/16/26	6/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	3	604	-	1/1/11/20	9/13/91/115	-
26	CLA	Y	613	1	1/1/15/20	10/37/115/115	-
26	CLA	5	614	1	1/1/11/20	2/13/91/115	-
25	CHL	y	606	42	3/3/16/26	6/20/118/137	-
26	CLA	b	609	5	-	9/37/115/115	-
26	CLA	5	612	1	1/1/11/20	3/13/91/115	-
26	CLA	B	614	5	1/1/15/20	13/37/115/115	-
26	CLA	r	612	19	1/1/11/20	6/18/96/115	-
27	LUT	8	620	-	-	4/29/67/67	0/2/2/2
26	CLA	S	610	20	1/1/13/20	4/25/103/115	-
26	CLA	S	603	20	1/1/11/20	5/13/91/115	-
26	CLA	1	610	1	1/1/13/20	5/27/105/115	-
25	CHL	3	605	2	3/3/16/26	9/15/113/137	-
28	XAT	G	1622	-	-	2/31/93/93	0/4/4/4
25	CHL	Y	609	1	4/4/20/26	13/39/137/137	-
25	CHL	2	605	1	3/3/16/26	9/15/113/137	-
26	CLA	r	609	19	1/1/13/20	3/29/107/115	-
26	CLA	1	604	-	-	10/19/97/115	-
26	CLA	B	615	5	1/1/15/20	13/37/115/115	-
25	CHL	5	607	-	4/4/19/26	20/36/134/137	-
25	CHL	7	605	2	3/3/16/26	9/15/113/137	-
30	LHG	r	2630	26	-	19/46/46/53	-
26	CLA	Y	604	42	1/1/12/20	3/19/97/115	-
27	LUT	s	1621	-	-	2/29/67/67	0/2/2/2
26	CLA	r	601	19	1/1/11/20	14/18/96/115	-
26	CLA	4	603	3	1/1/11/20	4/13/91/115	-
26	CLA	S	612	20	1/1/11/20	5/18/96/115	-
30	LHG	G	2630	26	-	26/53/53/53	-
26	CLA	B	608	42	1/1/15/20	11/37/115/115	-
35	PHO	a	408	-	-	12/37/103/103	0/5/6/6
26	CLA	A	410	4	1/1/14/20	5/31/109/115	-
25	CHL	3	608	-	3/3/16/26	3/15/113/137	-
26	CLA	b	607	5	1/1/15/20	9/37/115/115	-
26	CLA	A	407	42	-	3/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	n	605	1	3/3/16/26	9/18/116/137	-
26	CLA	G	603	1	1/1/15/20	11/37/115/115	-
26	CLA	s	611	30	1/1/13/20	9/27/105/115	-
27	LUT	G	1620	-	-	2/29/67/67	0/2/2/2
36	SQD	A	412	-	-	13/45/65/69	0/1/1/1
30	LHG	c	523	-	-	21/53/53/53	-
26	CLA	C	513	6	-	10/37/115/115	-
25	CHL	5	601	1	3/3/16/26	6/15/113/137	-
26	CLA	g	603	1	1/1/15/20	11/37/115/115	-
26	CLA	b	615	5	1/1/15/20	12/37/115/115	-
25	CHL	G	608	42	4/4/20/26	15/39/137/137	-
29	NEX	G	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	S	609	20	1/1/11/20	5/13/91/115	-
25	CHL	n	607	42	4/4/20/26	14/39/137/137	-
28	XAT	Y	1622	-	-	2/31/93/93	0/4/4/4
30	LHG	8	2630	26	-	8/23/23/53	-
25	CHL	N	606	42	3/3/16/26	6/20/118/137	-
27	LUT	2	1621	-	-	3/29/67/67	0/2/2/2
37	LMG	b	2633	-	-	24/50/70/70	0/1/1/1
26	CLA	c	509	6	1/1/15/20	8/37/115/115	-
25	CHL	5	608	-	3/3/16/26	7/15/113/137	-
25	CHL	Y	607	42	4/4/20/26	16/39/137/137	-
30	LHG	g	2630	26	-	26/53/53/53	-
27	LUT	1	1621	-	-	3/29/67/67	0/2/2/2
30	LHG	c	522	-	-	20/53/53/53	-
29	NEX	n	1623	-	-	4/27/83/83	0/3/3/3
31	BCR	b	619	-	-	2/29/63/63	0/2/2/2
26	CLA	c	508	6	1/1/15/20	11/37/115/115	-
25	CHL	6	601	1	3/3/16/26	6/15/113/137	-
26	CLA	2	611	30	-	3/13/91/115	-
26	CLA	8	603	3	1/1/11/20	4/13/91/115	-
26	CLA	5	610	1	1/1/13/20	5/27/105/115	-
28	XAT	n	1622	-	-	3/31/93/93	0/4/4/4
26	CLA	a	405	4	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	406	42	1/1/15/20	12/37/115/115	-
26	CLA	c	504	42	1/1/15/20	18/37/115/115	-
26	CLA	R	613	19	1/1/14/20	10/31/109/115	-
27	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	2	614	1	1/1/11/20	5/13/91/115	-
35	PHO	A	408	-	-	12/37/103/103	0/5/6/6
26	CLA	4	604	-	-	8/13/91/115	-
26	CLA	g	602	1	1/1/15/20	12/37/115/115	-
30	LHG	N	2630	26	-	24/53/53/53	-
25	CHL	Y	608	42	4/4/20/26	15/39/137/137	-
25	CHL	S	607	42	4/4/18/26	19/30/128/137	-
31	BCR	8	623	-	-	9/29/63/63	0/2/2/2
26	CLA	y	612	1	1/1/14/20	15/31/109/115	-
26	CLA	a	407	42	-	3/19/97/115	-
25	CHL	3	607	-	3/3/17/26	8/24/122/137	-
26	CLA	g	604	42	1/1/12/20	5/19/97/115	-
26	CLA	5	603	1	1/1/13/20	12/25/103/115	-
37	LMG	c	521	-	-	22/46/66/70	0/1/1/1
26	CLA	c	502	6	1/1/15/20	20/37/115/115	-
27	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	d	402	7	1/1/15/20	4/37/115/115	-
25	CHL	2	607	-	4/4/19/26	14/33/131/137	-
25	CHL	s	608	-	3/3/16/26	4/15/113/137	-
26	CLA	4	612	3	1/1/11/20	5/13/91/115	-
30	LHG	s	2630	26	-	27/53/53/53	-
26	CLA	3	611	30	1/1/13/20	7/25/103/115	-
25	CHL	g	605	1	3/3/16/26	9/15/113/137	-
31	BCR	C	516	-	-	7/29/63/63	0/2/2/2
26	CLA	6	602	1	1/1/14/20	12/33/111/115	-
27	LUT	2	1620	-	-	2/29/67/67	0/2/2/2
28	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	3	614	2	1/1/11/20	9/17/95/115	-
26	CLA	C	511	6	1/1/15/20	14/37/115/115	-
26	CLA	7	603	2	1/1/13/20	13/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	L	101	-	-	20/53/53/53	-
25	CHL	5	609	1	4/4/19/26	16/35/133/137	-
26	CLA	1	602	1	1/1/14/20	12/33/111/115	-
30	LHG	y	2630	26	-	24/53/53/53	-
26	CLA	R	616	19	-	6/13/91/115	-
26	CLA	D	403	7	-	12/37/115/115	-
26	CLA	7	610	2	1/1/14/20	7/31/109/115	-
26	CLA	6	614	1	1/1/11/20	5/13/91/115	-
26	CLA	Y	611	30	1/1/14/20	8/31/109/115	-
26	CLA	c	505	6	1/1/15/20	17/37/115/115	-
26	CLA	n	604	42	1/1/12/20	5/19/97/115	-
31	BCR	4	623	-	-	9/29/63/63	0/2/2/2
26	CLA	c	512	6	1/1/15/20	11/37/115/115	-
36	SQD	b	623	-	-	17/37/57/69	0/1/1/1
26	CLA	b	616	5	1/1/15/20	13/37/115/115	-
37	LMG	Z	101	-	-	24/46/66/70	0/1/1/1
26	CLA	s	613	20	1/1/13/20	6/25/103/115	-
30	LHG	D	408	-	-	19/50/50/53	-
39	DGD	c	519	-	-	26/51/91/95	0/2/2/2
26	CLA	r	604	42	1/1/11/20	6/17/95/115	-
26	CLA	R	612	19	1/1/11/20	6/18/96/115	-
26	CLA	8	602	3	1/1/11/20	7/13/91/115	-
26	CLA	b	614	5	1/1/15/20	13/37/115/115	-
26	CLA	1	614	1	1/1/11/20	2/13/91/115	-
26	CLA	1	612	1	1/1/11/20	3/13/91/115	-
31	BCR	A	411	-	-	6/29/63/63	0/2/2/2
29	NEX	2	1623	-	-	7/27/83/83	0/3/3/3
25	CHL	g	608	42	4/4/20/26	15/39/137/137	-
26	CLA	C	507	42	1/1/15/20	23/37/115/115	-
25	CHL	4	607	-	3/3/16/26	8/15/113/137	-
26	CLA	R	602	19	1/1/14/20	8/31/109/115	-
26	CLA	g	614	1	1/1/11/20	3/17/95/115	-
25	CHL	G	601	1	4/4/20/26	16/39/137/137	-
26	CLA	g	612	1	1/1/14/20	11/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	c	516	-	-	7/29/63/63	0/2/2/2
26	CLA	a	406	42	1/1/15/20	12/37/115/115	-
30	LHG	b	2630	-	-	31/51/51/53	-
26	CLA	2	613	1	-	5/13/91/115	-
26	CLA	1	603	1	1/1/13/20	12/25/103/115	-
26	CLA	2	603	1	1/1/13/20	11/25/103/115	-
25	CHL	6	609	1	4/4/19/26	11/33/131/137	-
26	CLA	C	503	6	1/1/15/20	14/37/115/115	-
26	CLA	G	613	1	1/1/15/20	12/37/115/115	-
26	CLA	R	603	19	1/1/14/20	14/31/109/115	-
39	DGD	C	520	-	-	21/49/89/95	0/2/2/2
37	LMG	a	413	-	-	28/43/63/70	0/1/1/1
26	CLA	5	602	1	1/1/14/20	12/33/111/115	-
26	CLA	5	604	-	-	10/19/97/115	-
26	CLA	b	604	5	1/1/15/20	10/37/115/115	-
26	CLA	1	611	30	1/1/11/20	6/13/91/115	-
39	DGD	c	520	-	-	21/49/89/95	0/2/2/2
25	CHL	2	606	-	3/3/16/26	6/15/113/137	-
25	CHL	R	606	42	4/4/20/26	19/39/137/137	-
30	LHG	B	2630	-	-	31/51/51/53	-
30	LHG	1	2630	26	-	15/45/45/53	-
26	CLA	c	510	6	1/1/15/20	14/37/115/115	-
27	LUT	r	620	-	-	3/29/67/67	0/2/2/2
25	CHL	6	607	-	4/4/19/26	14/33/131/137	-
27	LUT	4	620	-	-	4/29/67/67	0/2/2/2
26	CLA	S	611	30	1/1/13/20	9/27/105/115	-
26	CLA	A	405	4	1/1/15/20	7/37/115/115	-
25	CHL	n	608	42	4/4/20/26	13/39/137/137	-
25	CHL	5	606	-	3/3/16/26	8/15/113/137	-
26	CLA	N	613	1	1/1/14/20	8/31/109/115	-
26	CLA	N	603	1	1/1/15/20	15/37/115/115	-
31	BCR	c	514	-	-	4/29/63/63	0/2/2/2
25	CHL	S	606	42	3/3/16/26	10/15/113/137	-
26	CLA	B	605	5	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	N	604	42	1/1/12/20	5/19/97/115	-
26	CLA	s	612	20	1/1/11/20	5/18/96/115	-
37	LMG	A	413	-	-	28/43/63/70	0/1/1/1
30	LHG	C	522	-	-	20/53/53/53	-
26	CLA	C	509	6	1/1/15/20	8/37/115/115	-
25	CHL	r	608	42	4/4/19/26	17/33/131/137	-
30	LHG	n	2630	26	-	24/53/53/53	-
26	CLA	R	610	19	1/1/15/20	13/37/115/115	-
37	LMG	a	415	-	-	14/35/55/70	0/1/1/1
31	BCR	a	411	-	-	6/29/63/63	0/2/2/2
26	CLA	s	609	20	1/1/11/20	5/13/91/115	-
38	PL9	a	414	-	-	1/5/18/73	0/1/1/1
25	CHL	N	601	1	4/4/20/26	16/39/137/137	-
25	CHL	s	607	42	4/4/18/26	19/30/128/137	-
25	CHL	g	607	42	4/4/20/26	16/39/137/137	-
25	CHL	Y	605	1	3/3/16/26	8/18/116/137	-
26	CLA	8	612	3	1/1/11/20	5/13/91/115	-
25	CHL	G	606	42	3/3/16/26	9/20/118/137	-
26	CLA	2	612	1	1/1/11/20	5/13/91/115	-
29	NEX	g	1623	-	-	5/27/83/83	0/3/3/3
25	CHL	s	606	42	3/3/16/26	10/15/113/137	-
26	CLA	b	605	5	1/1/15/20	14/37/115/115	-
26	CLA	y	604	42	1/1/12/20	3/19/97/115	-
25	CHL	8	607	-	3/3/16/26	8/15/113/137	-
28	XAT	8	622	-	-	2/31/93/93	0/4/4/4
26	CLA	c	501	6	1/1/15/20	17/37/115/115	-
25	CHL	n	606	42	3/3/16/26	6/20/118/137	-
25	CHL	y	609	1	4/4/20/26	13/39/137/137	-
37	LMG	B	2633	-	-	24/50/70/70	0/1/1/1
26	CLA	r	611	30	1/1/11/20	8/18/96/115	-
25	CHL	8	606	-	3/3/16/26	8/15/113/137	-
28	XAT	5	1622	-	-	2/31/93/93	0/4/4/4
39	DGD	B	626	-	-	24/48/88/95	0/2/2/2
26	CLA	6	613	1	-	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	C	515	-	-	6/29/63/63	0/2/2/2
26	CLA	C	506	6	1/1/15/20	22/37/115/115	-
26	CLA	R	609	19	1/1/13/20	3/29/107/115	-
26	CLA	S	602	20	1/1/14/20	14/33/111/115	-
25	CHL	y	601	1	4/4/20/26	16/39/137/137	-
25	CHL	4	609	3	3/3/16/26	4/15/113/137	-
25	CHL	8	609	3	3/3/16/26	4/15/113/137	-
26	CLA	B	610	5	-	11/37/115/115	-
26	CLA	C	502	6	1/1/15/20	20/37/115/115	-
30	LHG	c	2630	-	-	27/53/53/53	-
30	LHG	C	523	-	-	21/53/53/53	-
25	CHL	8	601	3	3/3/16/26	7/13/111/137	-
39	DGD	b	626	-	-	24/48/88/95	0/2/2/2
25	CHL	r	607	42	4/4/18/26	9/27/125/137	-
37	LMG	d	411	-	-	15/41/61/70	0/1/1/1
26	CLA	b	610	5	-	11/37/115/115	-
37	LMG	A	415	-	-	14/35/55/70	0/1/1/1
30	LHG	C	2630	-	-	27/53/53/53	-
25	CHL	G	609	1	4/4/19/26	10/33/131/137	-
25	CHL	1	605	1	3/3/16/26	8/15/113/137	-
25	CHL	S	601	20	3/3/16/26	7/15/113/137	-
26	CLA	r	603	19	1/1/14/20	14/31/109/115	-
26	CLA	c	513	6	-	10/37/115/115	-
39	DGD	h	102	-	-	21/51/91/95	0/2/2/2
27	LUT	N	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	b	608	42	1/1/15/20	11/37/115/115	-
29	NEX	Y	1623	-	-	6/27/83/83	0/3/3/3
27	LUT	3	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	B	602	42	1/1/15/20	15/37/115/115	-
25	CHL	n	609	1	4/4/20/26	14/39/137/137	-
30	LHG	3	2630	26	-	24/51/51/53	-
28	XAT	N	1622	-	-	3/31/93/93	0/4/4/4
25	CHL	1	607	-	4/4/19/26	20/36/134/137	-
26	CLA	b	612	5	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	y	608	42	4/4/20/26	15/39/137/137	-
26	CLA	b	613	5	1/1/15/20	16/37/115/115	-
26	CLA	N	611	30	1/1/14/20	4/31/109/115	-
25	CHL	n	601	1	4/4/20/26	16/39/137/137	-
30	LHG	Y	2630	26	-	24/53/53/53	-
31	BCR	H	101	-	-	4/29/63/63	0/2/2/2
26	CLA	n	613	1	1/1/14/20	8/31/109/115	-
26	CLA	n	603	1	1/1/15/20	15/37/115/115	-
26	CLA	3	610	2	1/1/14/20	7/31/109/115	-
41	HEM	F	101	9,8	-	1/12/54/54	-
26	CLA	Y	603	1	1/1/15/20	13/37/115/115	-
27	LUT	S	1620	-	-	2/29/67/67	0/2/2/2
25	CHL	g	609	1	4/4/19/26	10/33/131/137	-
30	LHG	4	2630	26	-	8/23/23/53	-
26	CLA	C	505	6	1/1/15/20	17/37/115/115	-
38	PL9	d	405	-	-	10/53/73/73	0/1/1/1
30	LHG	6	2630	26	-	16/41/41/53	-
26	CLA	C	512	6	1/1/15/20	11/37/115/115	-
25	CHL	1	608	-	3/3/16/26	7/15/113/137	-
25	CHL	4	606	-	3/3/16/26	8/15/113/137	-
26	CLA	C	501	6	1/1/15/20	17/37/115/115	-
25	CHL	s	601	20	3/3/16/26	7/15/113/137	-
31	BCR	c	517	-	-	4/29/63/63	0/2/2/2
26	CLA	G	610	1	1/1/14/20	13/36/114/115	-
30	LHG	l	101	-	-	20/53/53/53	-
31	BCR	h	101	-	-	4/29/63/63	0/2/2/2
26	CLA	G	602	1	1/1/15/20	12/37/115/115	-
31	BCR	B	620	-	-	6/29/63/63	0/2/2/2
26	CLA	R	601	19	1/1/11/20	14/18/96/115	-
35	PHO	A	409	-	-	7/37/103/103	0/5/6/6
26	CLA	6	603	1	1/1/13/20	11/25/103/115	-
26	CLA	6	611	30	-	3/13/91/115	-
28	XAT	R	622	-	-	3/31/93/93	0/4/4/4
25	CHL	2	609	1	4/4/19/26	11/33/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	NEX	6	1623	-	-	7/27/83/83	0/3/3/3
27	LUT	3	1620	-	-	2/29/67/67	0/2/2/2
29	NEX	R	623	-	-	4/27/83/83	0/3/3/3
25	CHL	6	605	1	3/3/16/26	9/15/113/137	-
26	CLA	R	611	30	1/1/11/20	8/18/96/115	-
25	CHL	y	605	1	3/3/16/26	8/18/116/137	-
26	CLA	3	602	2	1/1/14/20	14/31/109/115	-
29	NEX	3	1623	-	-	4/27/83/83	0/3/3/3
25	CHL	5	605	1	3/3/16/26	8/15/113/137	-
26	CLA	G	612	1	1/1/14/20	11/31/109/115	-
29	NEX	1	1623	-	-	6/27/83/83	0/3/3/3
25	CHL	2	601	1	3/3/16/26	6/15/113/137	-
35	PHO	a	409	-	-	7/37/103/103	0/5/6/6
28	XAT	3	1622	-	-	2/31/93/93	0/4/4/4
29	NEX	S	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	B	606	5	1/1/15/20	14/37/115/115	-
26	CLA	B	611	42	1/1/15/20	10/37/115/115	-
25	CHL	y	607	42	4/4/20/26	16/39/137/137	-
27	LUT	7	1621	-	-	3/29/67/67	0/2/2/2
28	XAT	y	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	Y	610	1	1/1/14/20	7/31/109/115	-
26	CLA	r	616	19	-	6/13/91/115	-
26	CLA	B	603	5	1/1/15/20	9/37/115/115	-
26	CLA	2	602	1	1/1/14/20	12/33/111/115	-
31	BCR	C	517	-	-	4/29/63/63	0/2/2/2
25	CHL	7	606	-	3/3/16/26	9/15/113/137	-
26	CLA	y	611	30	1/1/14/20	8/31/109/115	-
27	LUT	y	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	B	613	5	1/1/15/20	16/37/115/115	-
26	CLA	C	510	6	1/1/15/20	15/37/115/115	-
30	LHG	B	2631	-	-	23/53/53/53	-
26	CLA	c	506	6	1/1/15/20	22/37/115/115	-
26	CLA	7	602	2	1/1/14/20	14/31/109/115	-
31	BCR	C	514	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	S	2630	26	-	27/53/53/53	-
27	LUT	n	1621	-	-	3/29/67/67	0/2/2/2
25	CHL	7	609	2	4/4/19/26	13/33/131/137	-
26	CLA	6	610	1	1/1/12/20	4/19/97/115	-
26	CLA	y	603	1	1/1/15/20	13/37/115/115	-
26	CLA	y	610	1	1/1/14/20	7/31/109/115	-
28	XAT	6	1622	-	-	3/31/93/93	0/4/4/4
26	CLA	s	604	42	1/1/12/20	6/19/97/115	-
25	CHL	g	606	42	3/3/16/26	9/20/118/137	-
25	CHL	r	614	19	3/3/15/26	6/10/108/137	-
26	CLA	N	602	1	1/1/15/20	12/37/115/115	-
26	CLA	n	602	1	1/1/15/20	11/37/115/115	-
31	BCR	d	404	-	-	7/29/63/63	0/2/2/2
25	CHL	7	601	2	4/4/19/26	18/37/135/137	-
26	CLA	G	614	1	1/1/11/20	3/17/95/115	-
26	CLA	7	614	2	1/1/11/20	9/17/95/115	-
36	SQD	B	621	-	-	32/49/69/69	0/1/1/1
26	CLA	4	610	3	1/1/11/20	4/13/91/115	-
26	CLA	8	604	-	-	8/13/91/115	-
30	LHG	D	409	-	-	27/53/53/53	-
25	CHL	N	605	1	3/3/16/26	9/18/116/137	-
30	LHG	5	2630	26	-	15/45/45/53	-
27	LUT	6	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	c	507	42	1/1/15/20	23/37/115/115	-
26	CLA	s	614	20	1/1/11/20	3/18/96/115	-
38	PL9	A	414	-	-	1/5/18/73	0/1/1/1
39	DGD	c	518	-	-	15/44/84/95	0/2/2/2
26	CLA	n	614	1	1/1/11/20	6/17/95/115	-
25	CHL	G	607	42	4/4/20/26	16/39/137/137	-
31	BCR	B	619	-	-	2/29/63/63	0/2/2/2
26	CLA	2	604	-	1/1/11/20	8/13/91/115	-
26	CLA	b	617	5	1/1/15/20	18/37/115/115	-
25	CHL	4	601	3	3/3/16/26	7/13/111/137	-
36	SQD	a	412	-	-	13/45/65/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	C	508	6	1/1/15/20	11/37/115/115	-
27	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
25	CHL	N	608	42	4/4/20/26	13/39/137/137	-
25	CHL	6	608	-	3/3/16/26	7/15/113/137	-
26	CLA	7	604	-	1/1/11/20	9/13/91/115	-
29	NEX	y	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	b	611	42	1/1/15/20	10/37/115/115	-
29	NEX	r	623	-	-	4/27/83/83	0/3/3/3
25	CHL	3	601	2	4/4/19/26	18/37/135/137	-
25	CHL	8	608	-	3/3/16/26	5/15/113/137	-
27	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
31	BCR	b	618	-	-	2/29/63/63	0/2/2/2
26	CLA	d	403	7	-	12/37/115/115	-
26	CLA	4	602	3	1/1/11/20	7/13/91/115	-
26	CLA	b	603	5	1/1/15/20	9/37/115/115	-
27	LUT	6	1621	-	-	3/29/67/67	0/2/2/2
25	CHL	r	606	42	4/4/20/26	19/39/137/137	-
31	BCR	D	404	-	-	7/29/63/63	0/2/2/2
25	CHL	2	608	-	3/3/16/26	7/15/113/137	-
26	CLA	1	613	1	-	8/25/103/115	-
30	LHG	2	2630	26	-	16/41/41/53	-
36	SQD	A	418	-	-	22/49/69/69	0/1/1/1
27	LUT	S	1621	-	-	2/29/67/67	0/2/2/2
25	CHL	3	606	-	3/3/16/26	9/15/113/137	-
38	PL9	D	405	-	-	10/53/73/73	0/1/1/1
30	LHG	d	408	-	-	19/50/50/53	-
25	CHL	7	607	-	3/3/17/26	8/24/122/137	-
31	BCR	T	101	-	-	13/29/63/63	0/2/2/2
26	CLA	8	611	30	1/1/11/20	4/13/91/115	-
26	CLA	s	610	20	1/1/13/20	4/25/103/115	-
37	LMG	B	622	-	-	23/46/66/70	0/1/1/1
37	LMG	z	101	-	-	24/46/66/70	0/1/1/1
29	NEX	N	1623	-	-	4/27/83/83	0/3/3/3
26	CLA	3	612	2	1/1/11/20	8/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	Y	606	42	3/3/16/26	6/20/118/137	-
30	LHG	d	410	-	-	30/47/47/53	-
26	CLA	D	402	7	1/1/15/20	4/37/115/115	-
27	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	S	613	20	1/1/13/20	6/25/103/115	-
26	CLA	n	610	1	1/1/15/20	12/37/115/115	-
26	CLA	c	511	6	1/1/15/20	14/37/115/115	-
31	BCR	t	101	-	-	13/29/63/63	0/2/2/2
25	CHL	g	601	1	4/4/20/26	16/39/137/137	-
26	CLA	S	614	20	1/1/11/20	3/18/96/115	-
27	LUT	5	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	G	611	30	1/1/14/20	11/31/109/115	-
26	CLA	7	611	30	1/1/13/20	7/25/103/115	-
37	LMG	b	622	-	-	23/46/66/70	0/1/1/1
25	CHL	7	608	-	3/3/16/26	3/15/113/137	-
31	BCR	b	620	-	-	6/29/63/63	0/2/2/2
25	CHL	R	614	19	3/3/15/26	6/10/108/137	-
26	CLA	B	607	5	1/1/15/20	9/37/115/115	-
26	CLA	c	503	6	1/1/15/20	14/37/115/115	-
30	LHG	7	2630	26	-	24/51/51/53	-
26	CLA	r	610	19	1/1/15/20	13/37/115/115	-
39	DGD	C	518	-	-	15/44/84/95	0/2/2/2
31	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	CLA	s	602	20	1/1/14/20	14/33/111/115	-
29	NEX	s	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	r	602	19	1/1/14/20	8/31/109/115	-
36	SQD	B	623	-	-	17/37/57/69	0/1/1/1
26	CLA	R	604	42	1/1/11/20	6/17/95/115	-
25	CHL	R	607	42	4/4/18/26	9/27/125/137	-
26	CLA	7	612	2	1/1/11/20	8/13/91/115	-
39	DGD	C	519	-	-	26/51/91/95	0/2/2/2
26	CLA	N	614	1	1/1/11/20	6/17/95/115	-
26	CLA	N	612	1	1/1/14/20	9/31/109/115	-
27	LUT	7	1620	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	y	602	1	1/1/15/20	10/37/115/115	-
36	SQD	b	621	-	-	32/49/69/69	0/1/1/1
26	CLA	S	604	42	1/1/12/20	6/19/97/115	-
28	XAT	7	1622	-	-	2/31/93/93	0/4/4/4
25	CHL	4	608	-	3/3/16/26	5/15/113/137	-
26	CLA	3	613	2	1/1/13/20	9/29/107/115	-
26	CLA	8	610	3	1/1/11/20	4/13/91/115	-
26	CLA	B	617	5	1/1/15/20	18/37/115/115	-
27	LUT	y	1621	-	-	1/29/67/67	0/2/2/2
28	XAT	2	1622	-	-	3/31/93/93	0/4/4/4
25	CHL	N	607	42	4/4/20/26	14/39/137/137	-
26	CLA	2	610	1	1/1/12/20	4/19/97/115	-
26	CLA	6	604	-	1/1/11/20	8/13/91/115	-
26	CLA	a	410	4	1/1/14/20	5/31/109/115	-
30	LHG	D	410	-	-	29/47/47/53	-
27	LUT	R	620	-	-	4/29/67/67	0/2/2/2
26	CLA	6	612	1	1/1/11/20	5/13/91/115	-
26	CLA	b	602	42	1/1/15/20	15/37/115/115	-
29	NEX	5	1623	-	-	6/27/83/83	0/3/3/3
39	DGD	H	102	-	-	21/51/91/95	0/2/2/2

The worst 5 of 3567 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	612	CLA	C4B-NB	8.06	1.42	1.35
26	R	609	CLA	C4B-NB	8.04	1.42	1.35
26	6	612	CLA	C4B-NB	8.04	1.42	1.35
26	r	609	CLA	C4B-NB	8.04	1.42	1.35
26	R	612	CLA	C4B-NB	7.91	1.42	1.35

The worst 5 of 5990 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	607	CHL	C2C-C3C-C4C	-10.86	98.75	106.49
25	n	607	CHL	C2C-C3C-C4C	-10.86	98.75	106.49
25	y	601	CHL	CMD-C2D-C1D	10.85	143.84	124.71
25	Y	601	CHL	CMD-C2D-C1D	10.83	143.81	124.71
25	G	601	CHL	CMD-C2D-C1D	10.64	143.47	124.71

5 of 532 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	1	601	CHL	ND
25	1	601	CHL	NA
25	1	601	CHL	NC
25	1	605	CHL	ND
25	1	605	CHL	NA

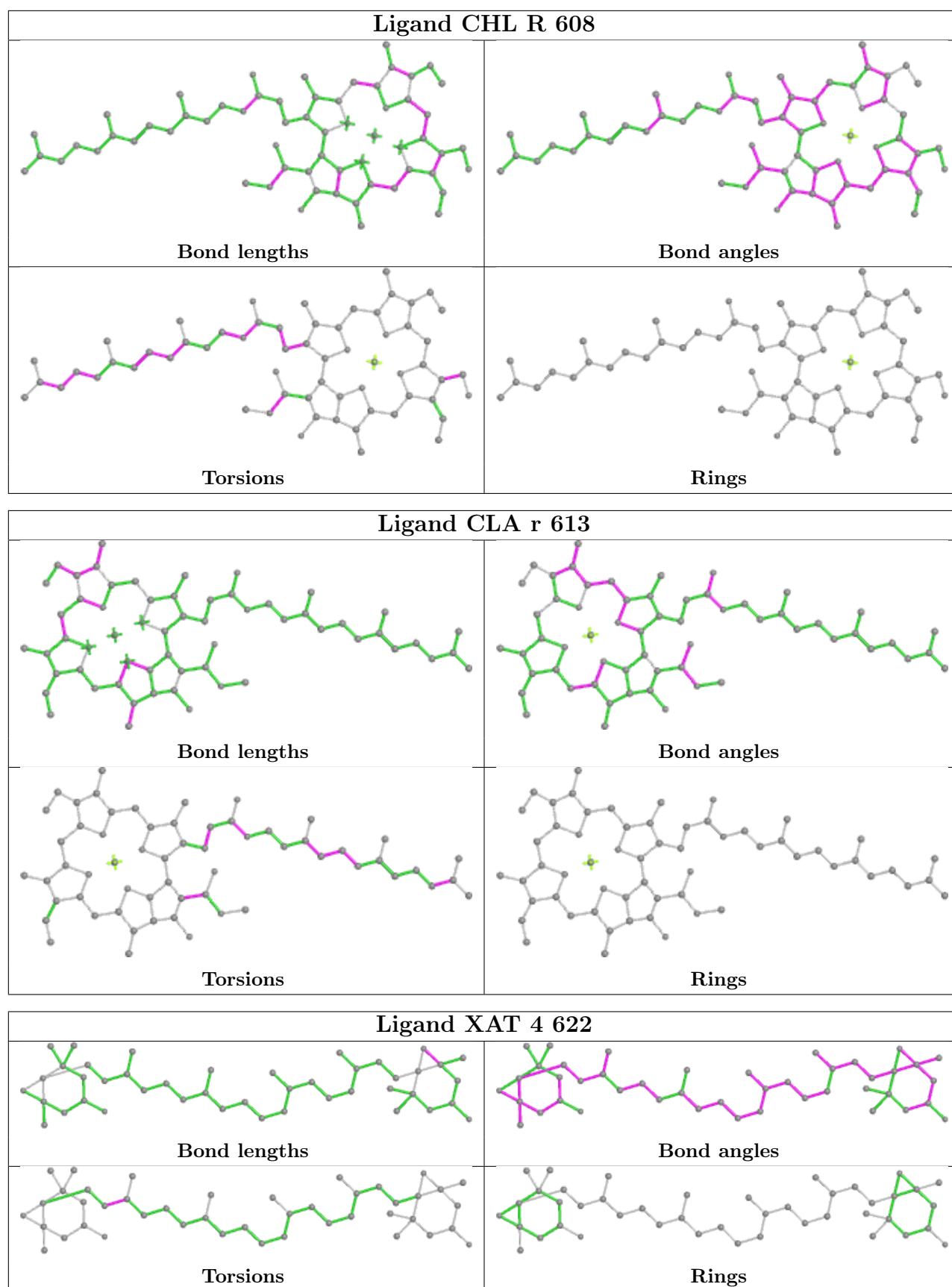
5 of 4969 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	1	601	CHL	C1C-C2C-CMC-OMC
25	1	601	CHL	C3C-C2C-CMC-OMC
25	1	601	CHL	CHA-CBD-CGD-O1D
25	1	601	CHL	CHA-CBD-CGD-O2D
25	1	605	CHL	C1C-C2C-CMC-OMC

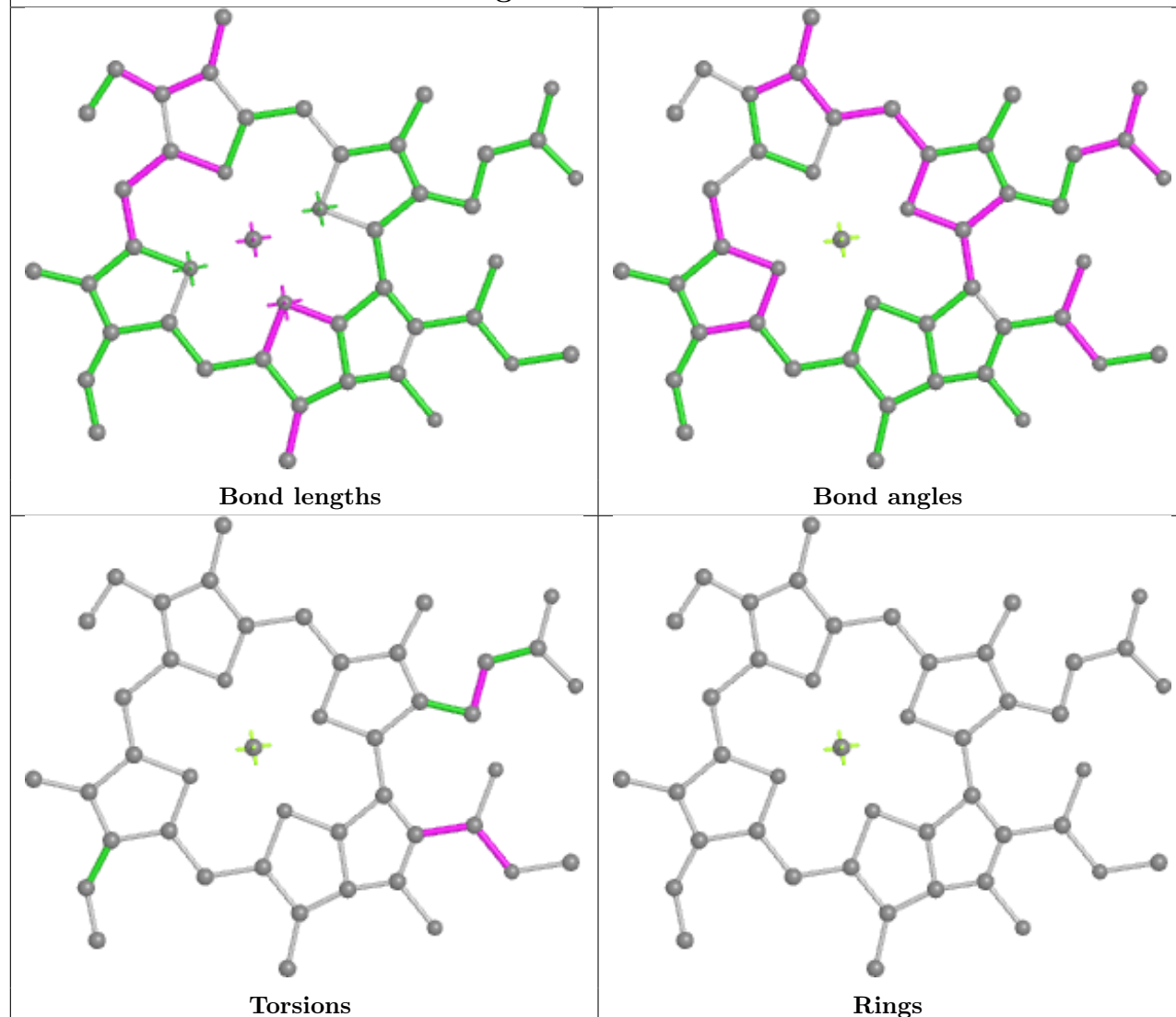
There are no ring outliers.

No monomer is involved in short contacts.

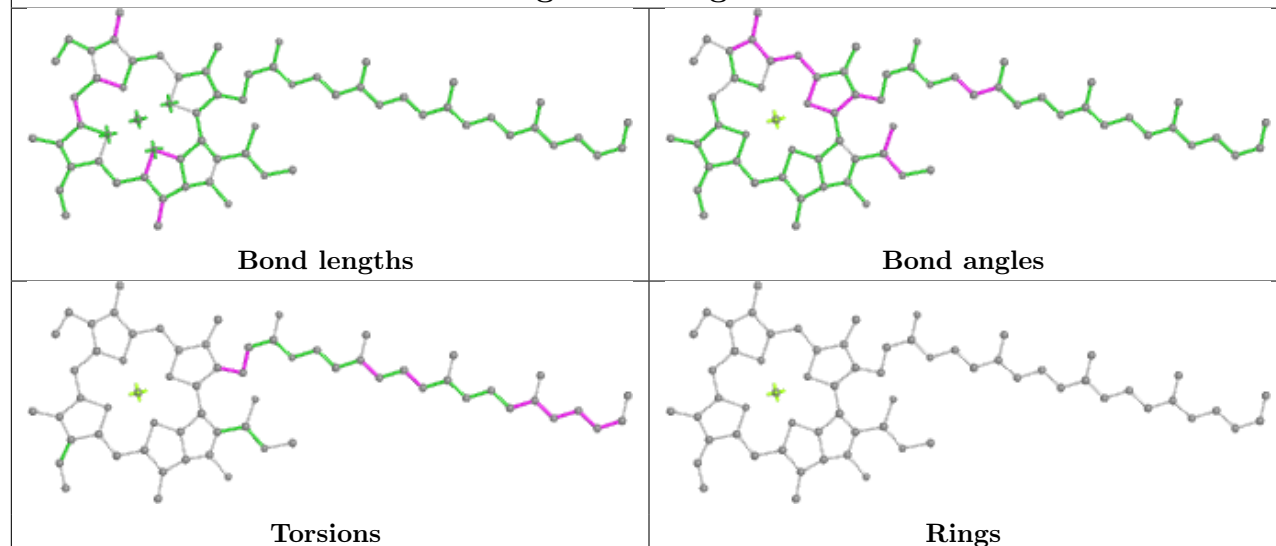
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

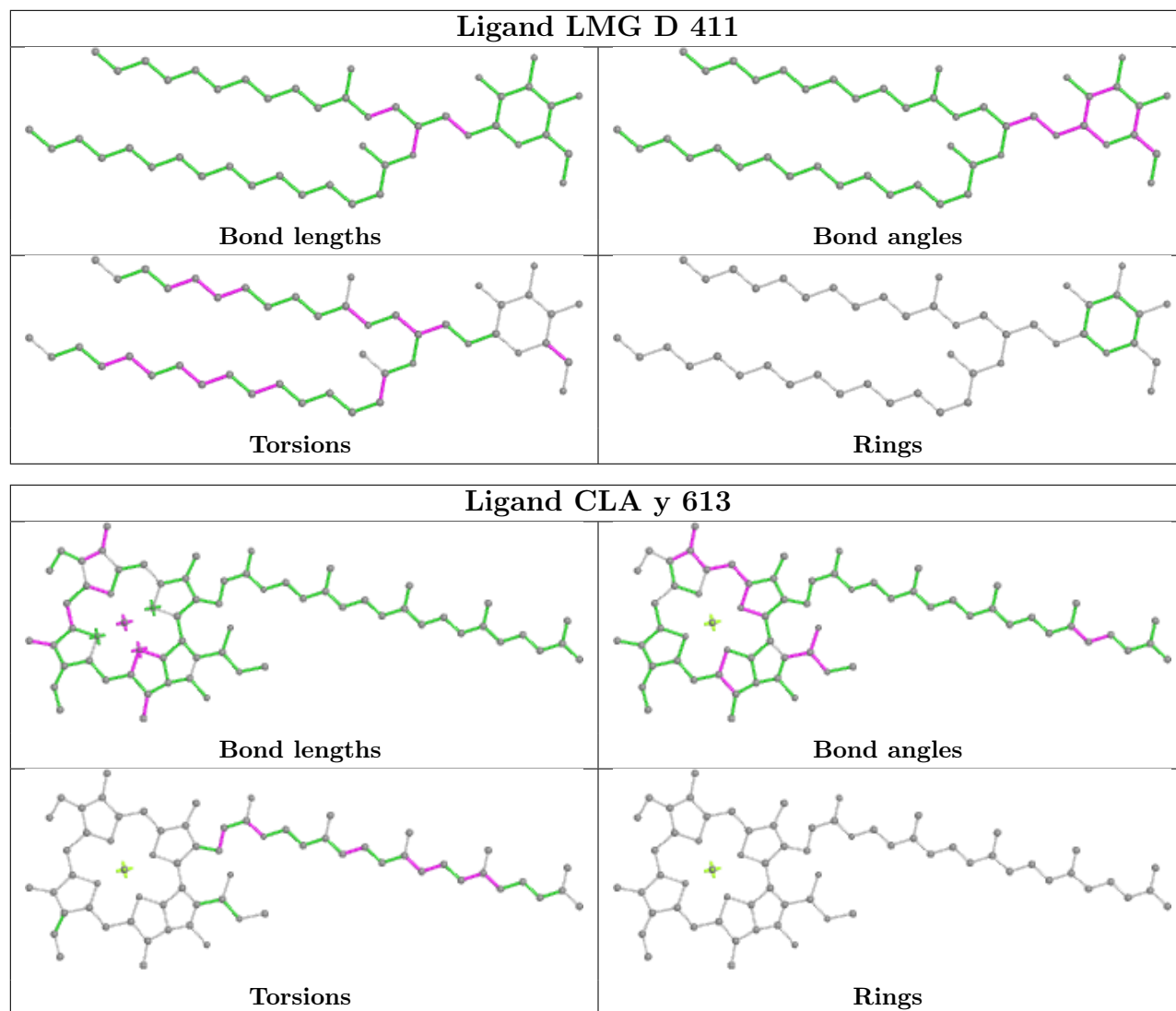


Ligand CLA s 603

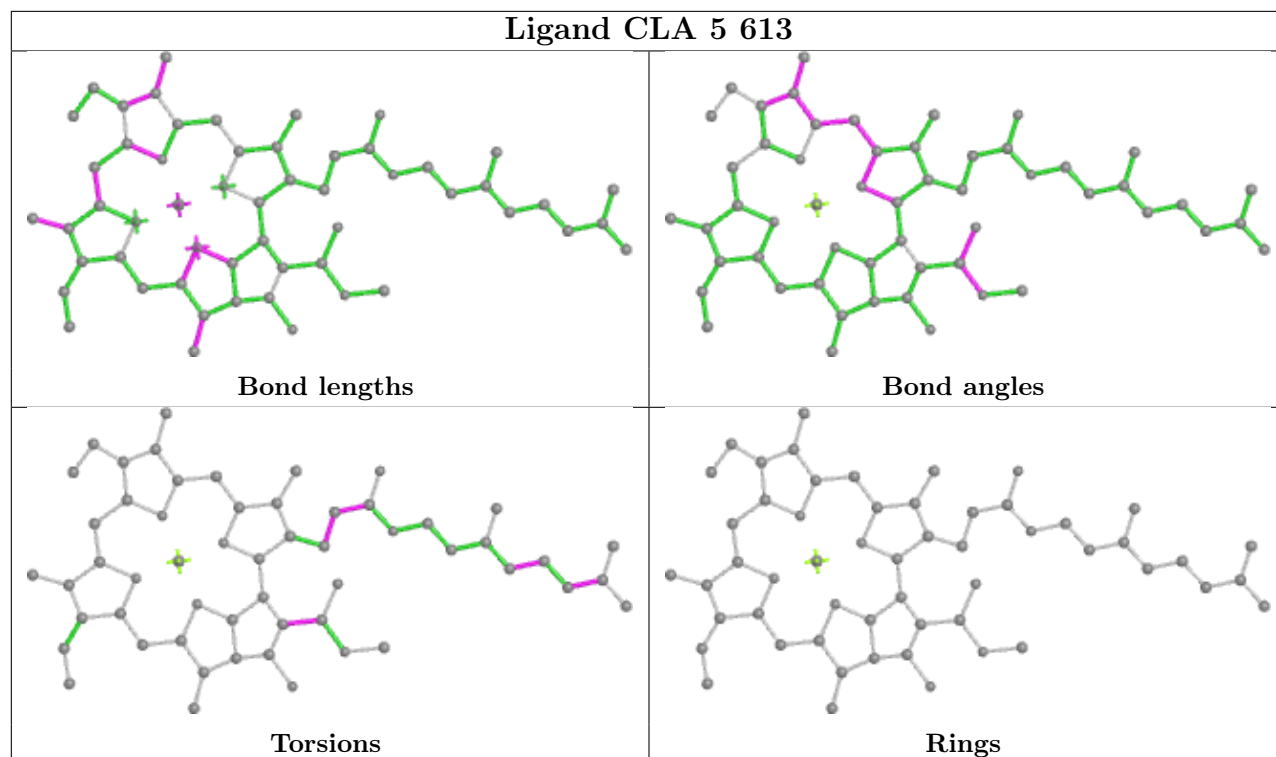


Ligand CLA g 610

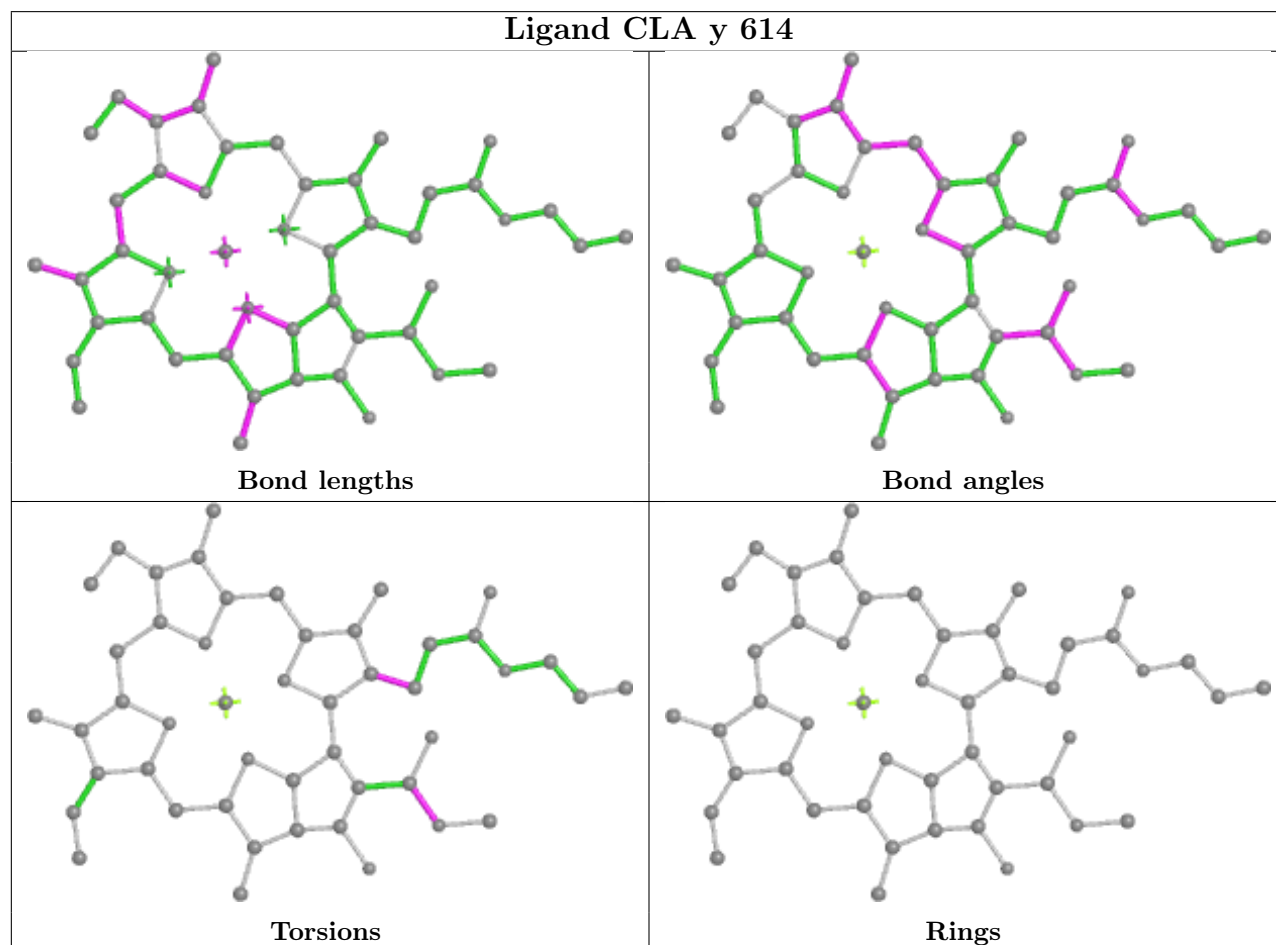


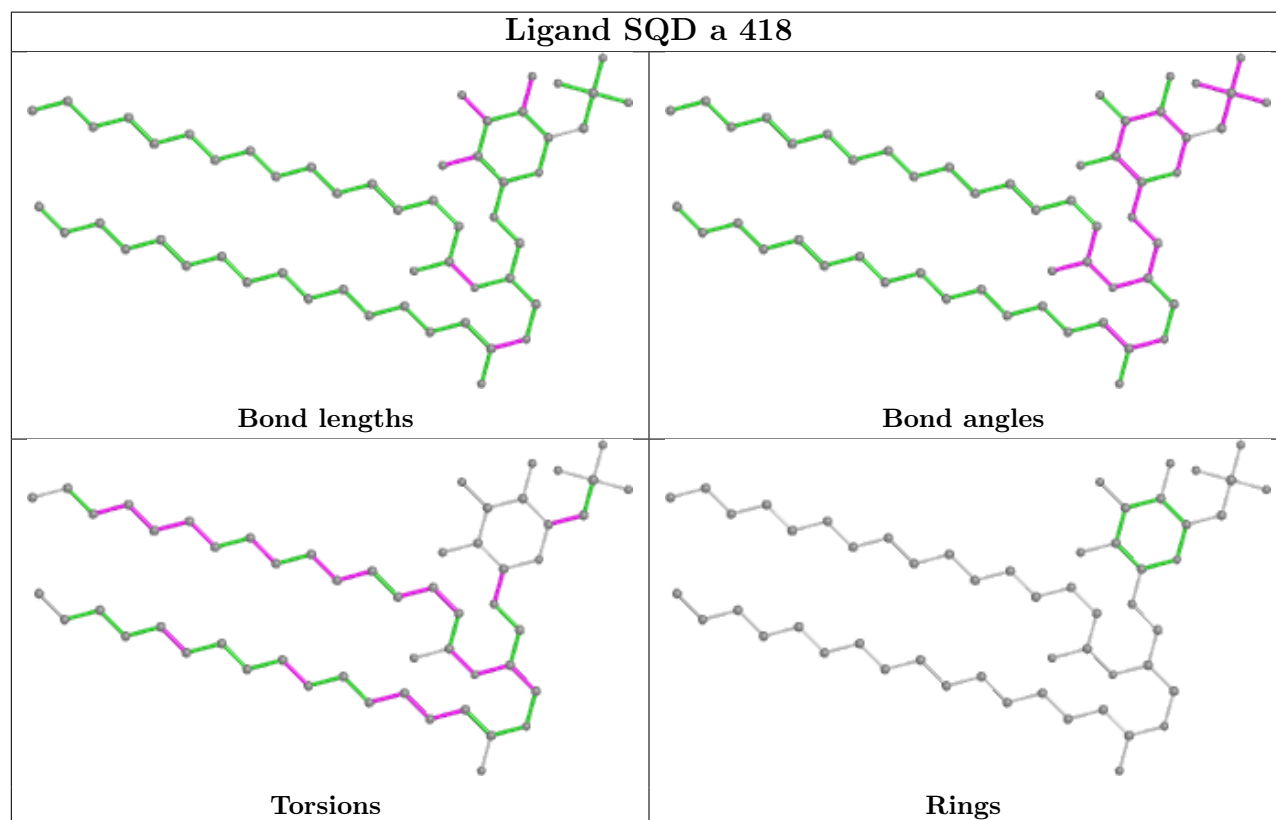
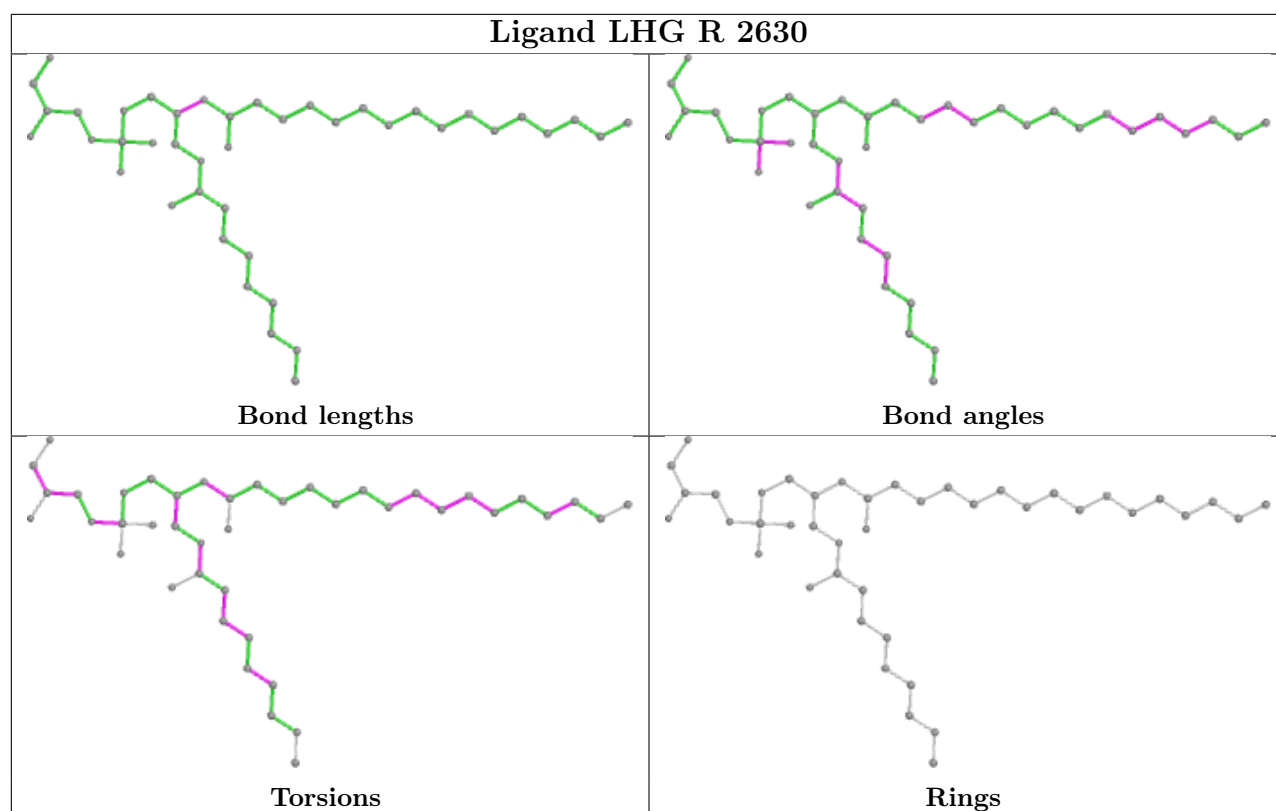


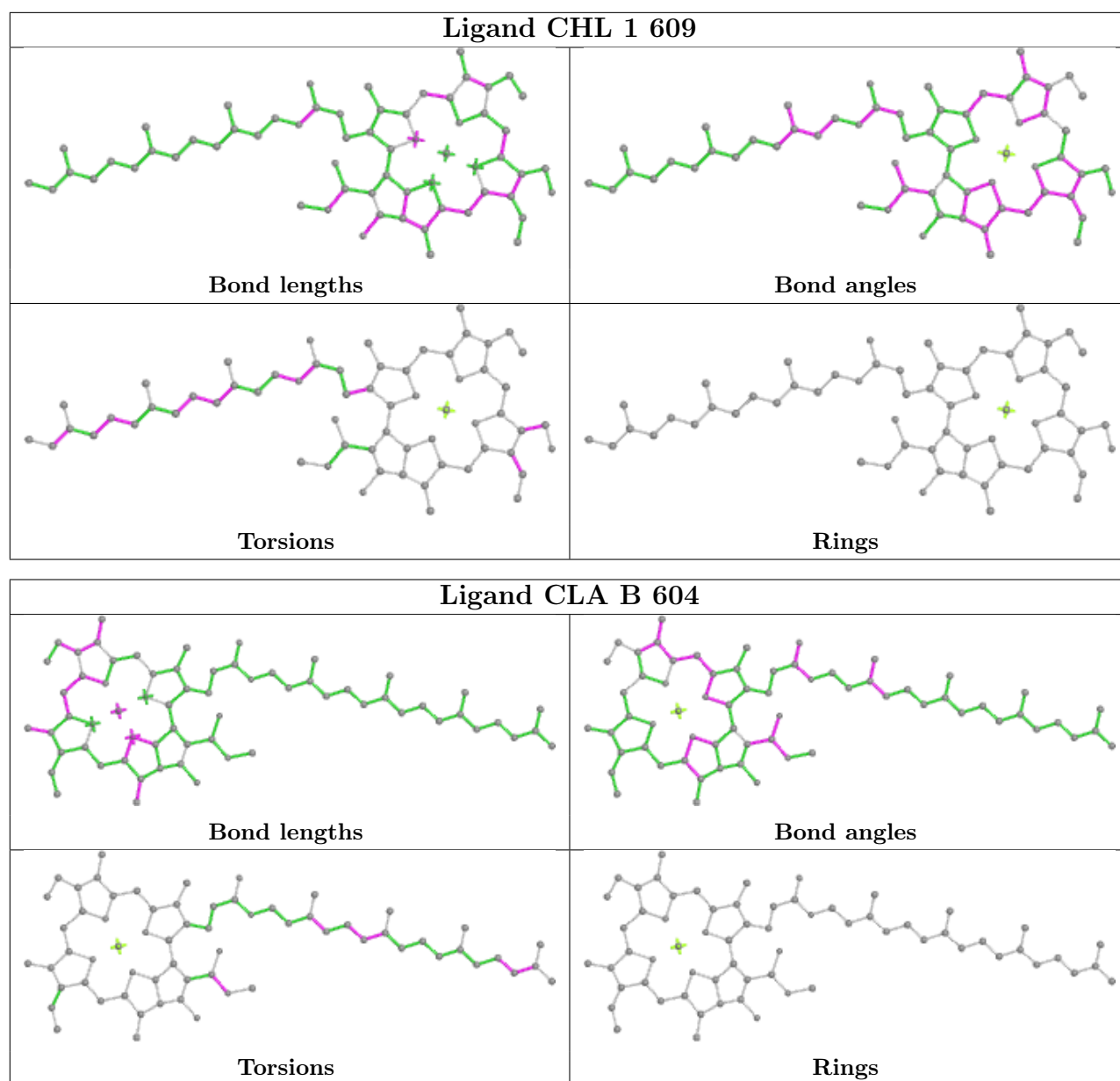
Ligand CLA 5 613

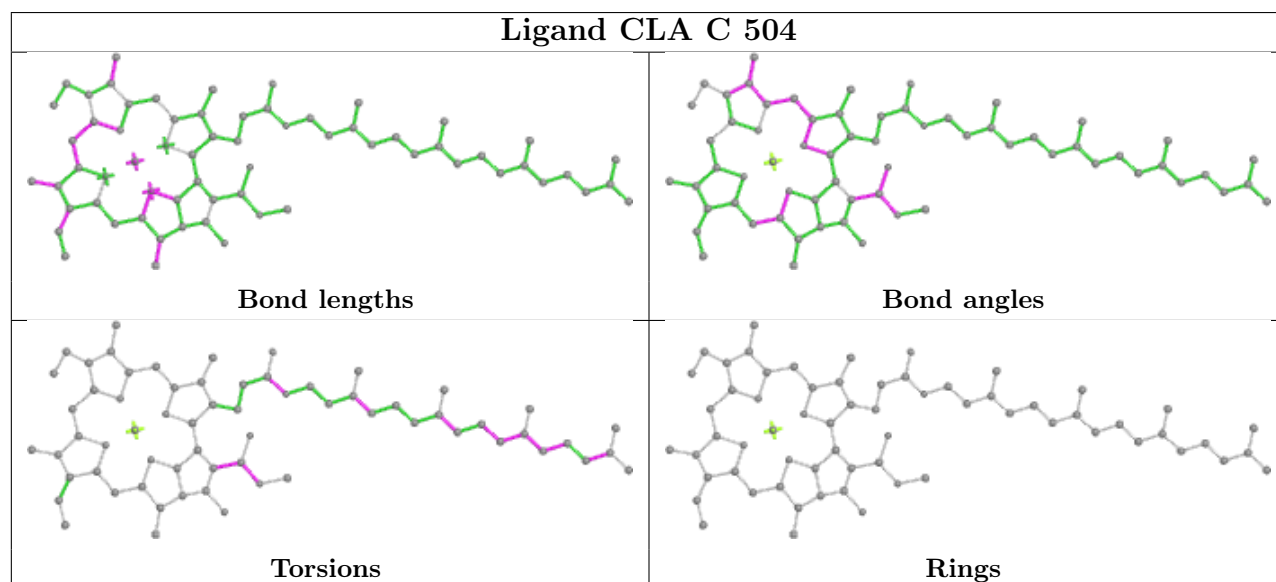
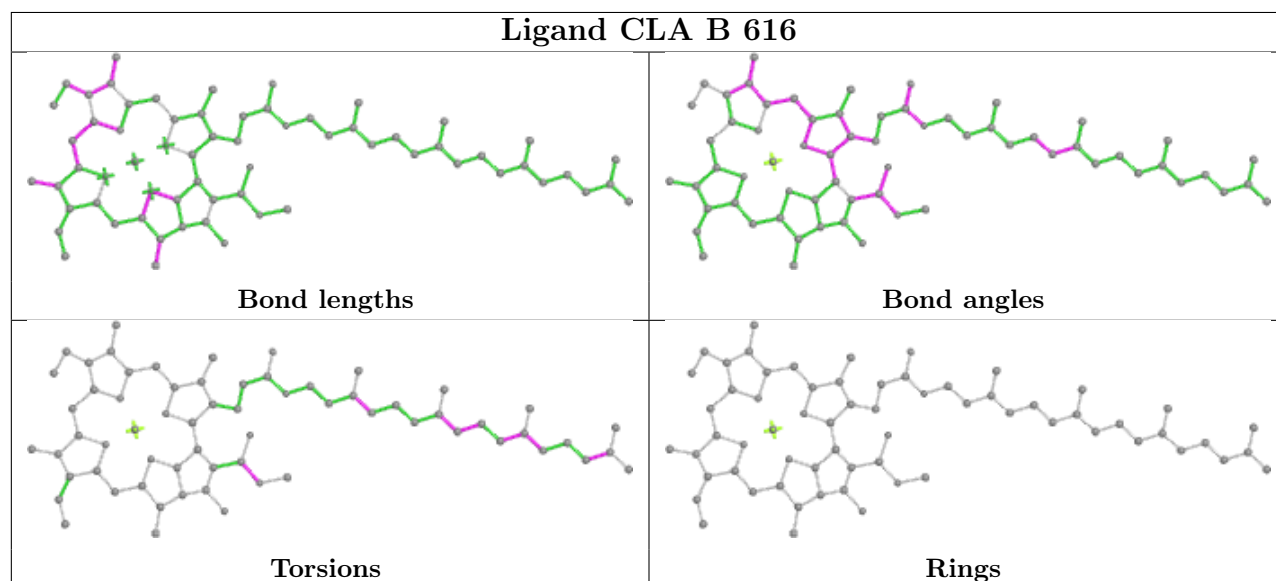
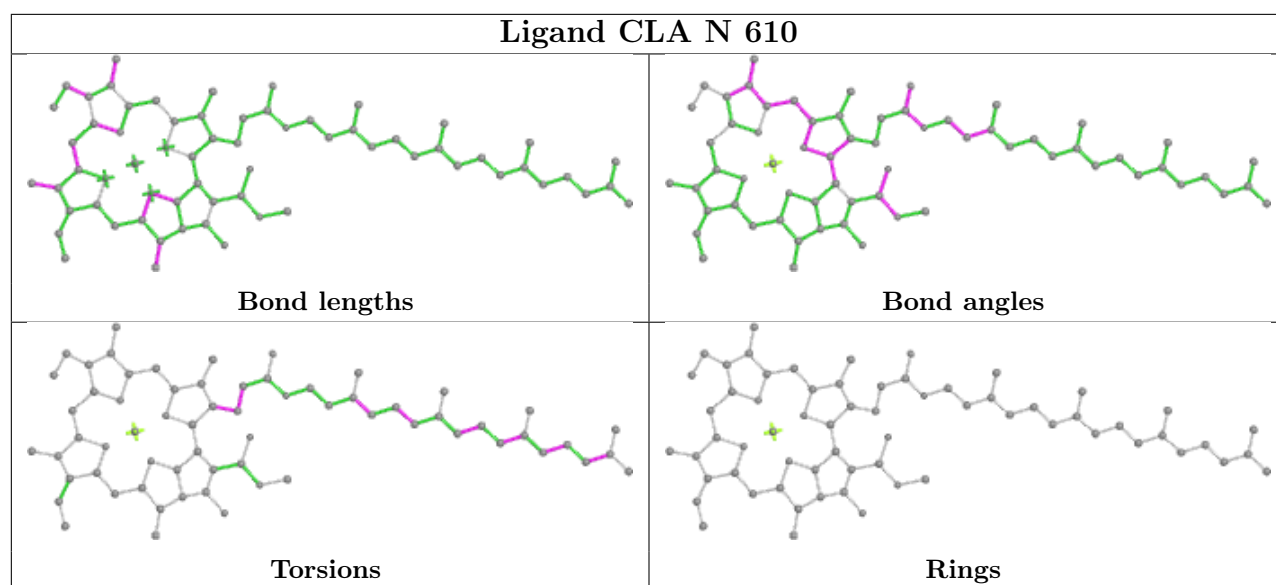


Ligand CLA y 614

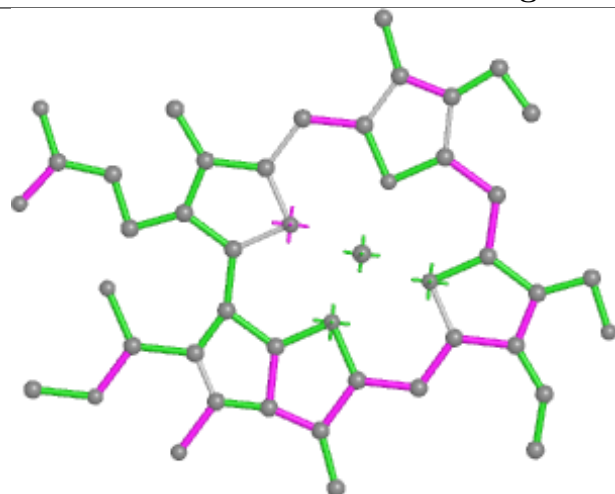




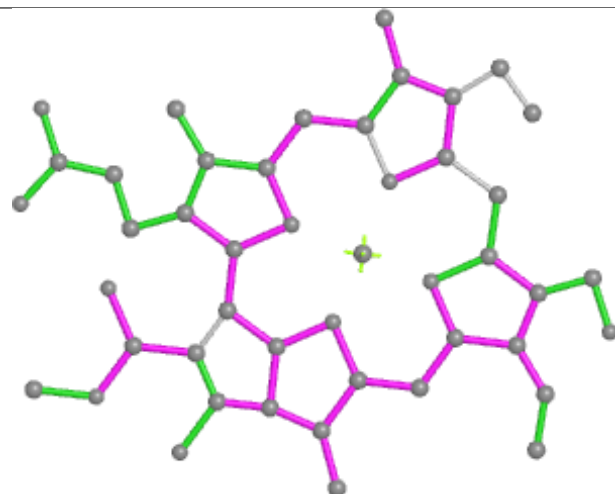




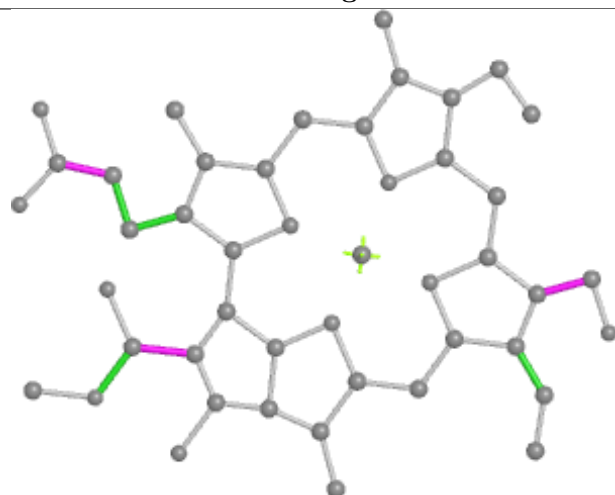
Ligand CHL 1 601



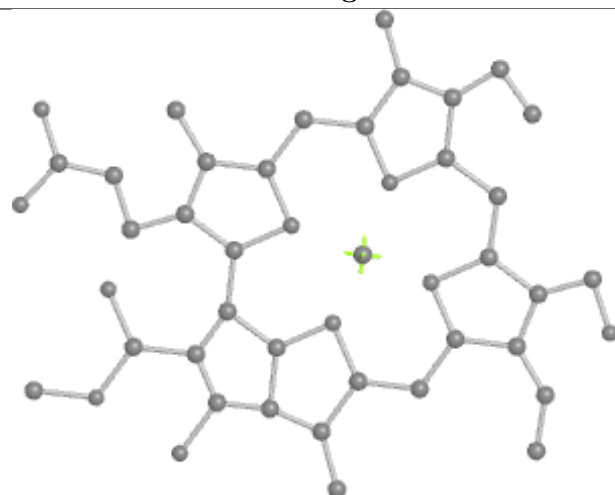
Bond lengths



Bond angles

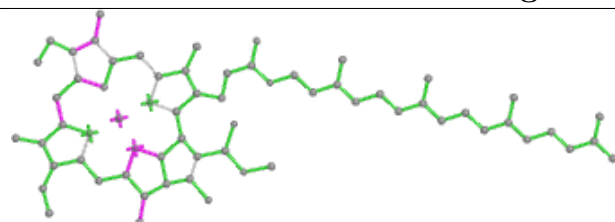


Torsions

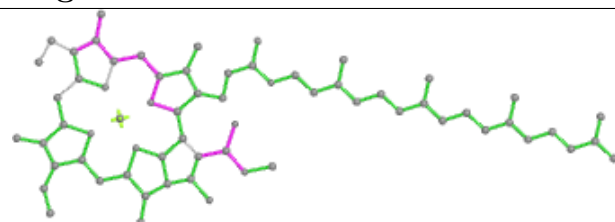


Rings

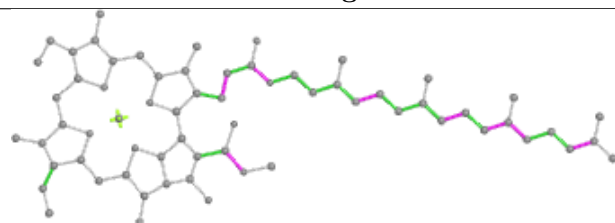
Ligand CLA g 613



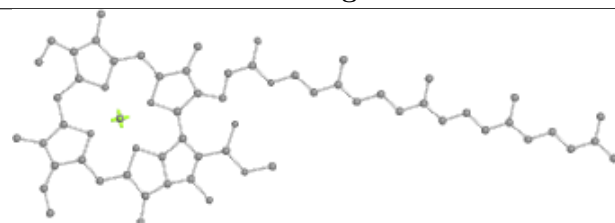
Bond lengths



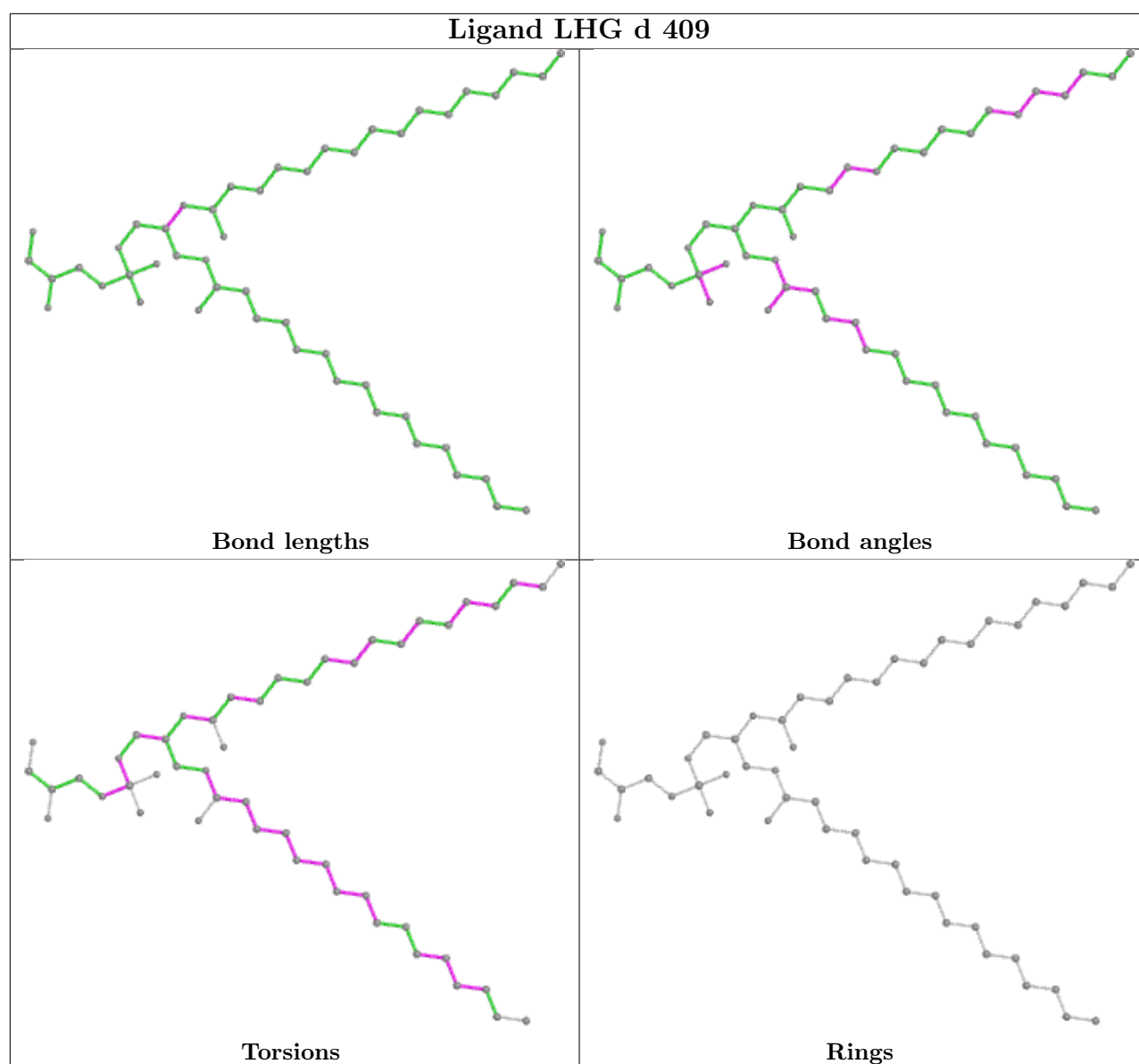
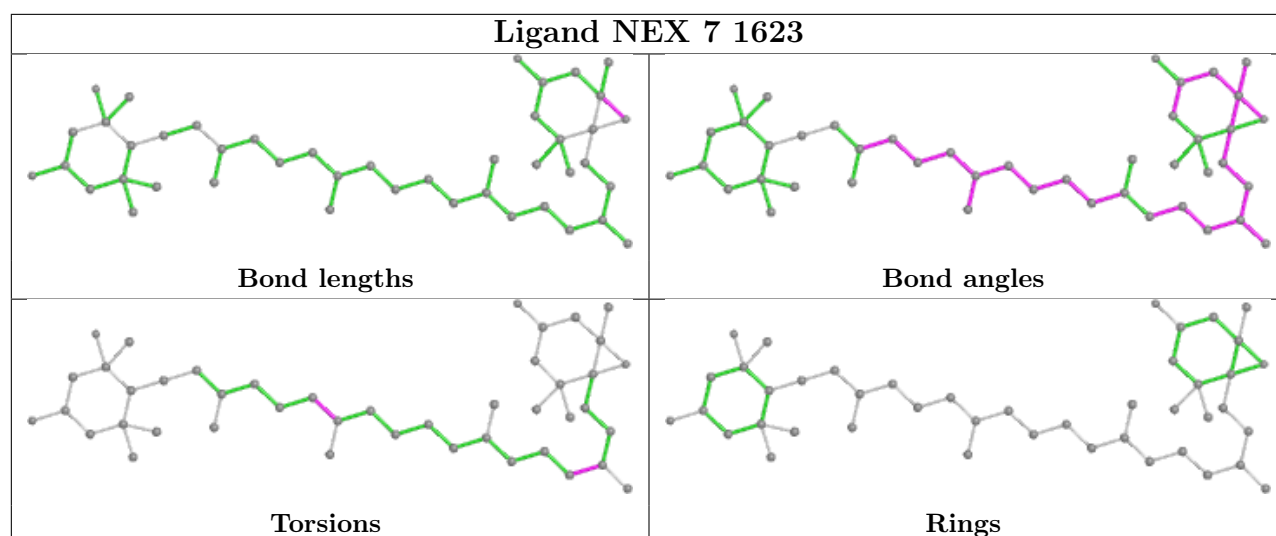
Bond angles

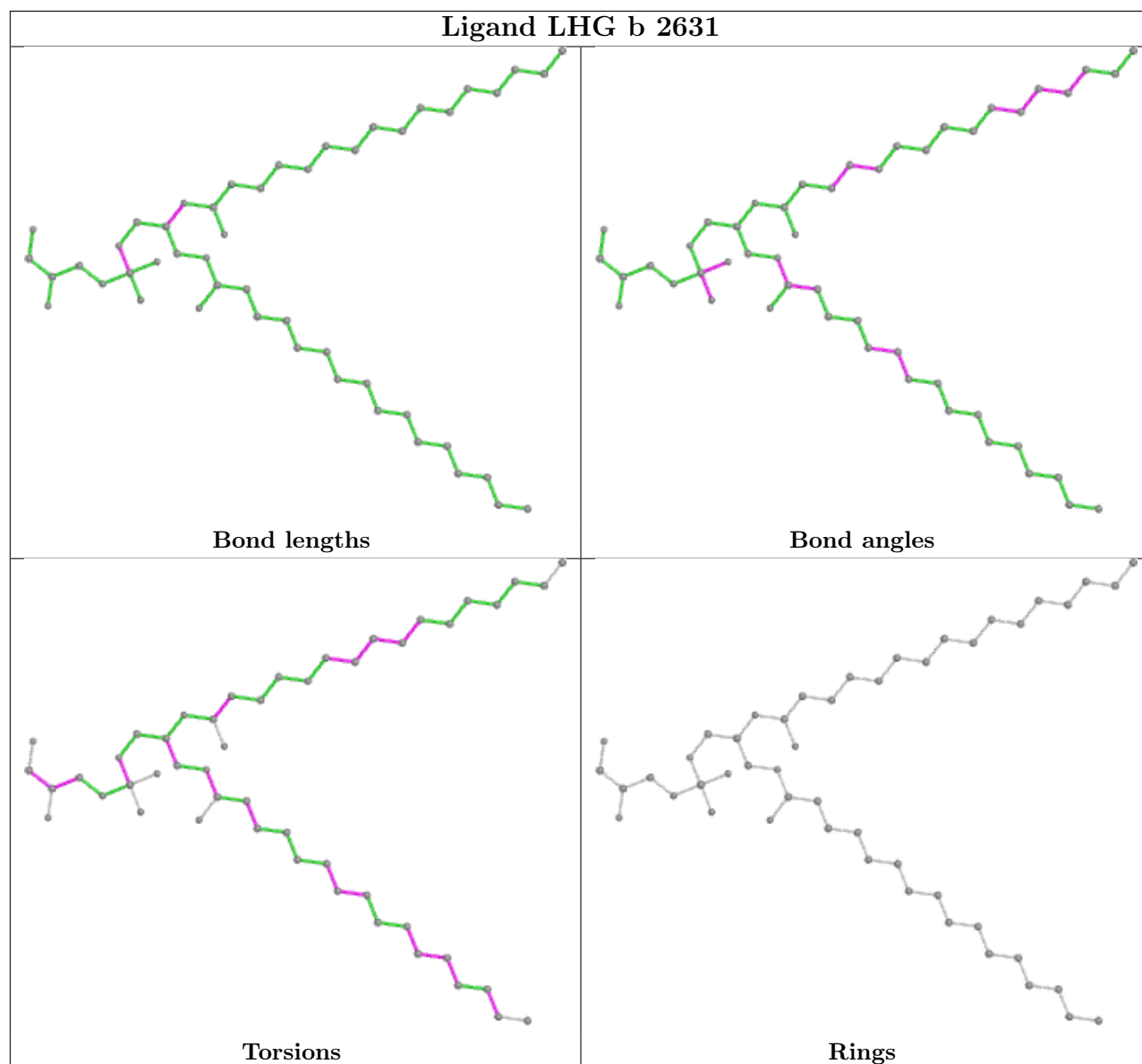
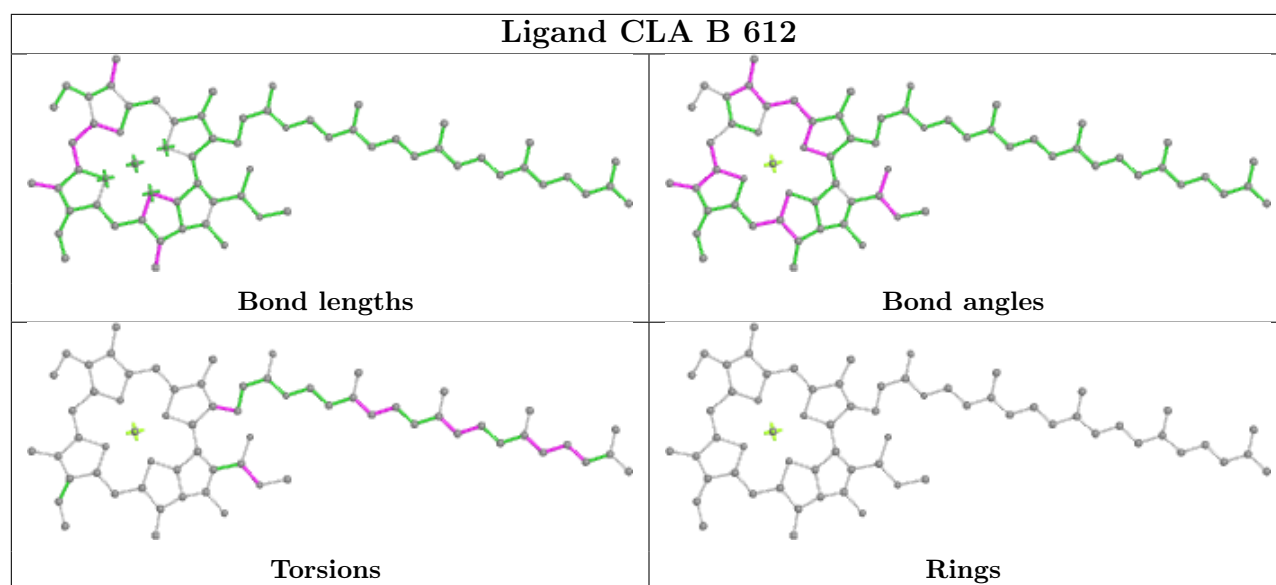


Torsions

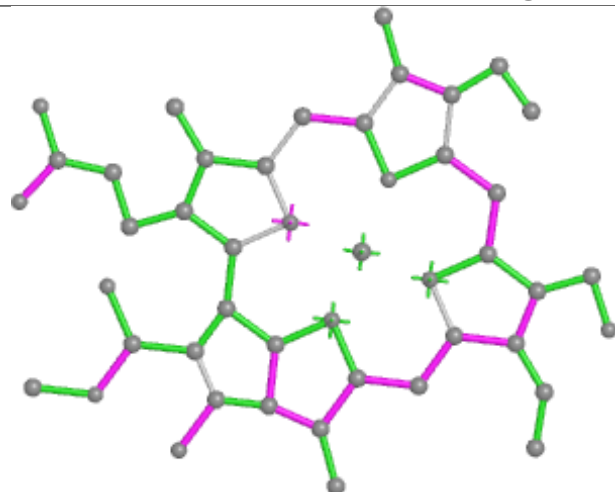


Rings

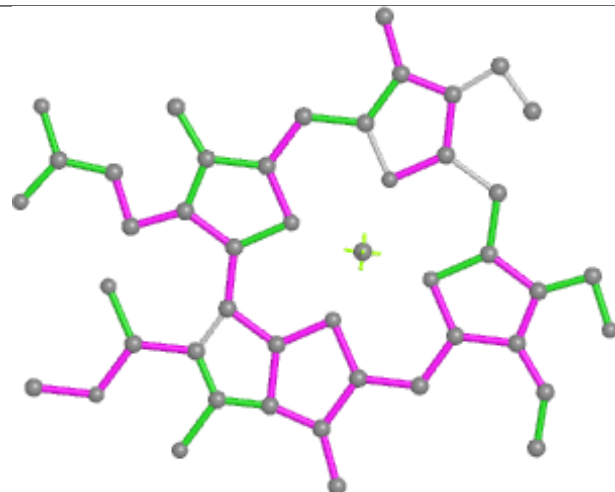




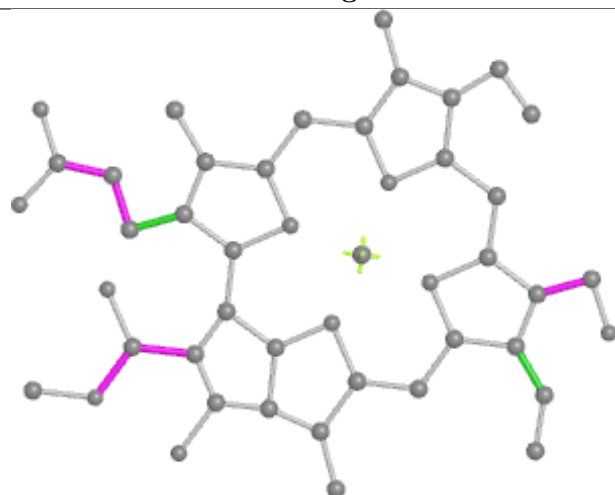
Ligand CHL 1 606



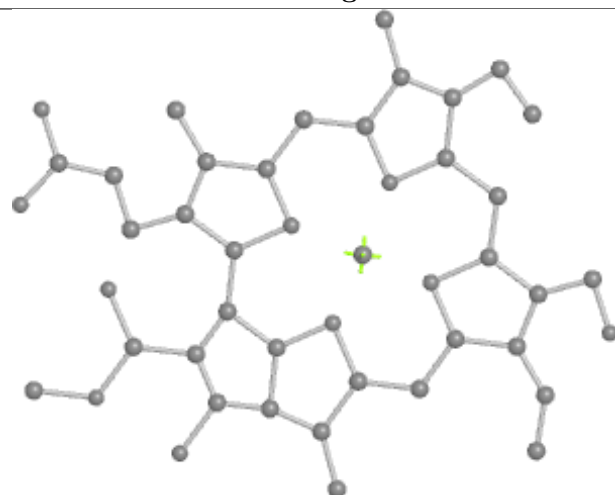
Bond lengths



Bond angles

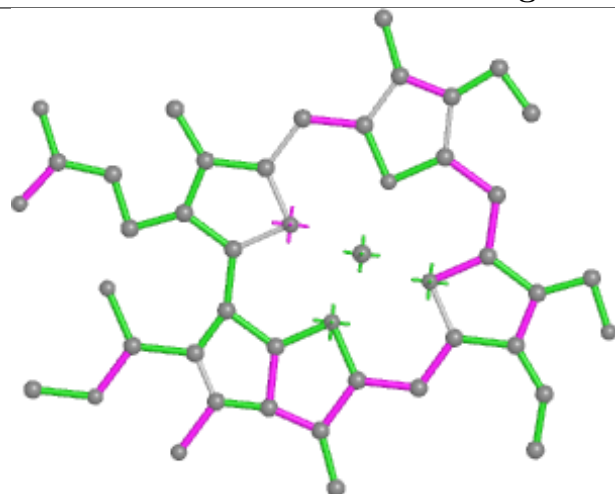


Torsions

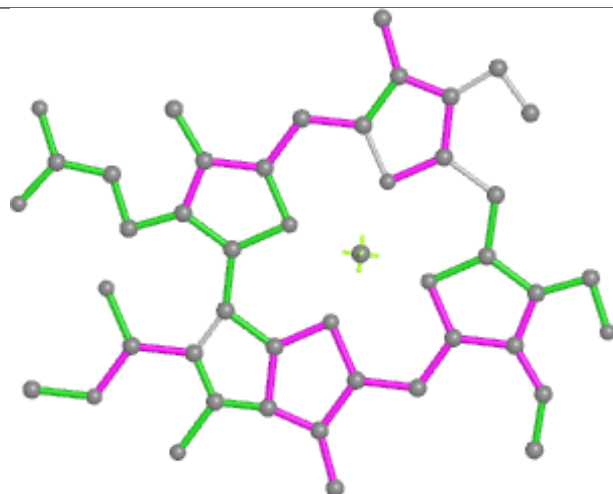


Rings

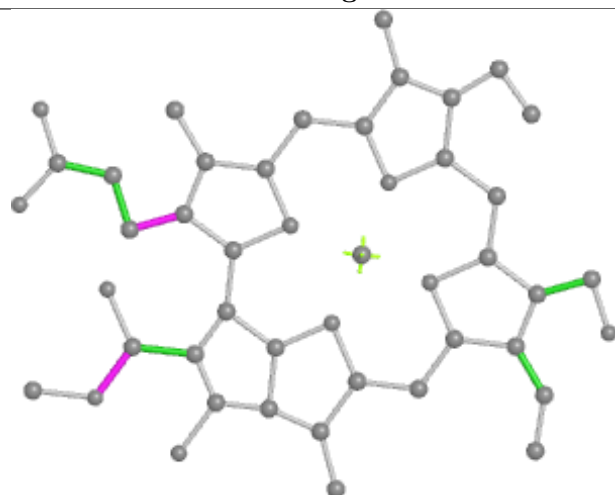
Ligand CHL S 608



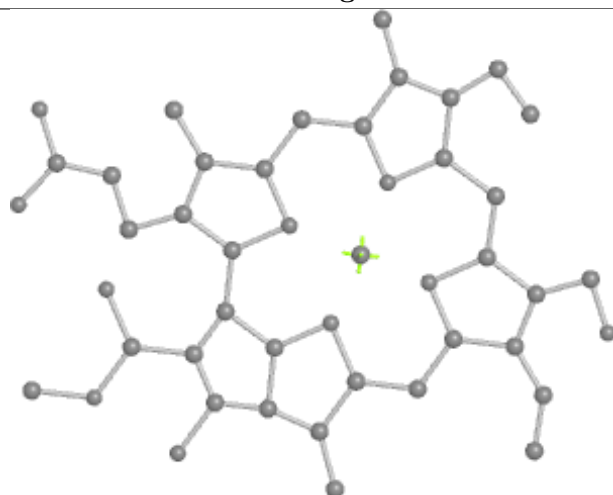
Bond lengths



Bond angles

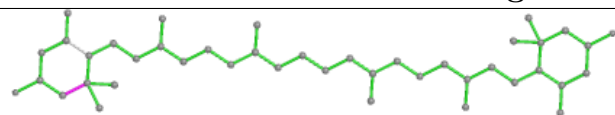


Torsions

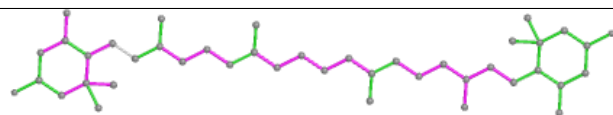


Rings

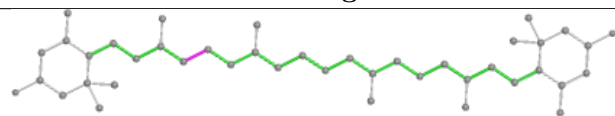
Ligand LUT Y 1621



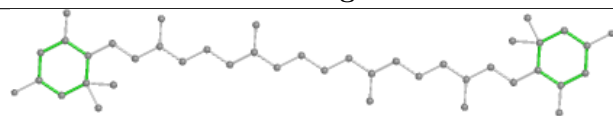
Bond lengths



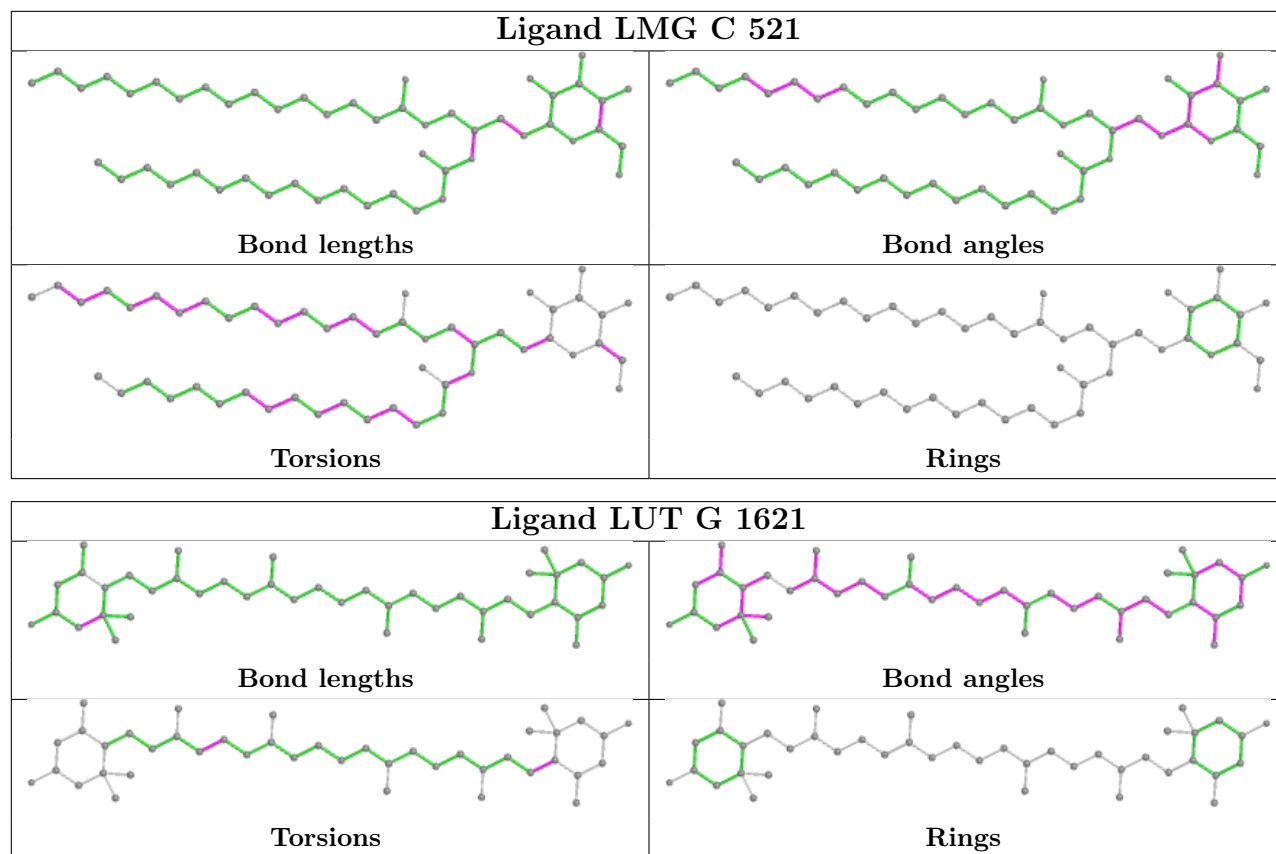
Bond angles

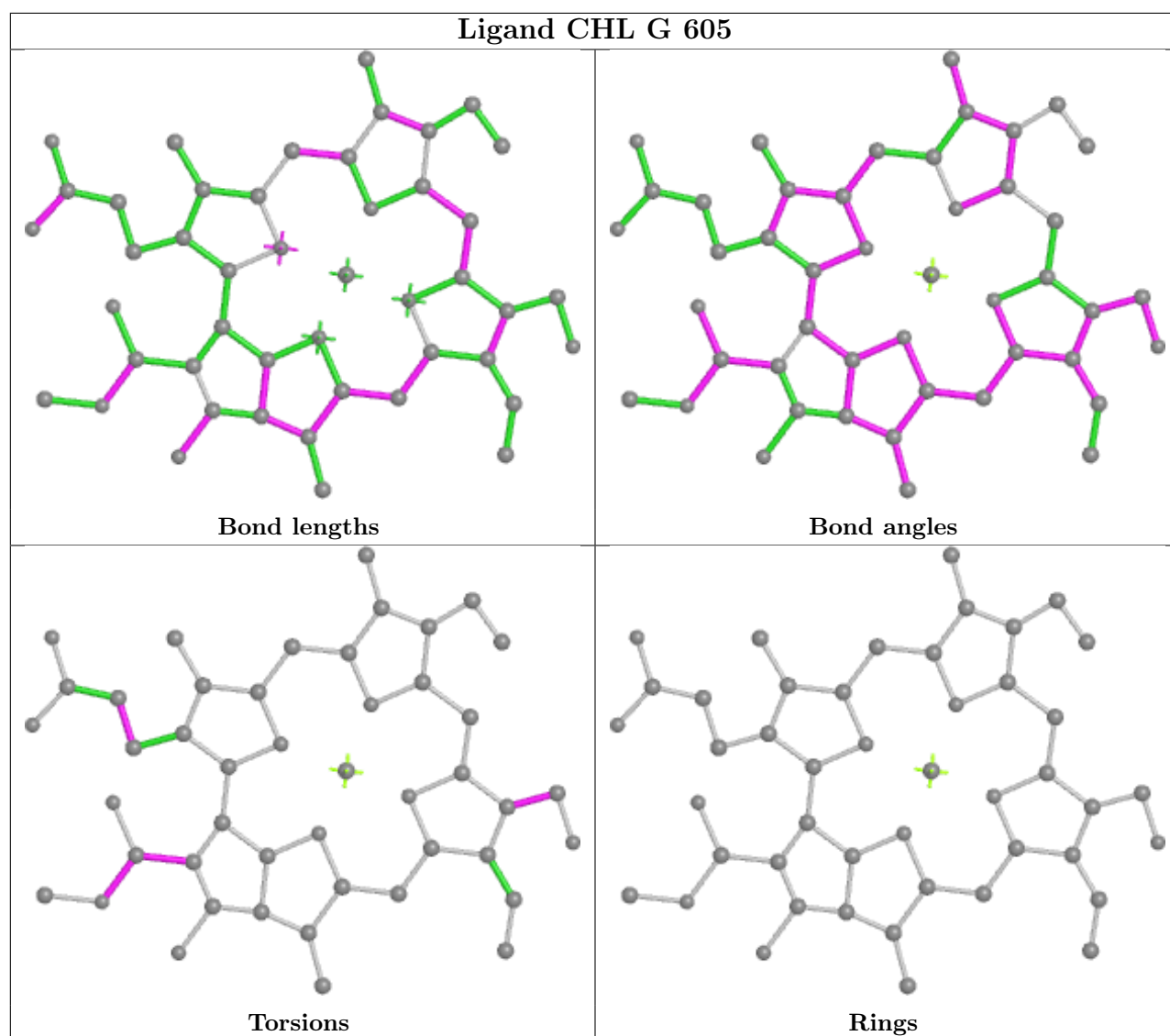


Torsions

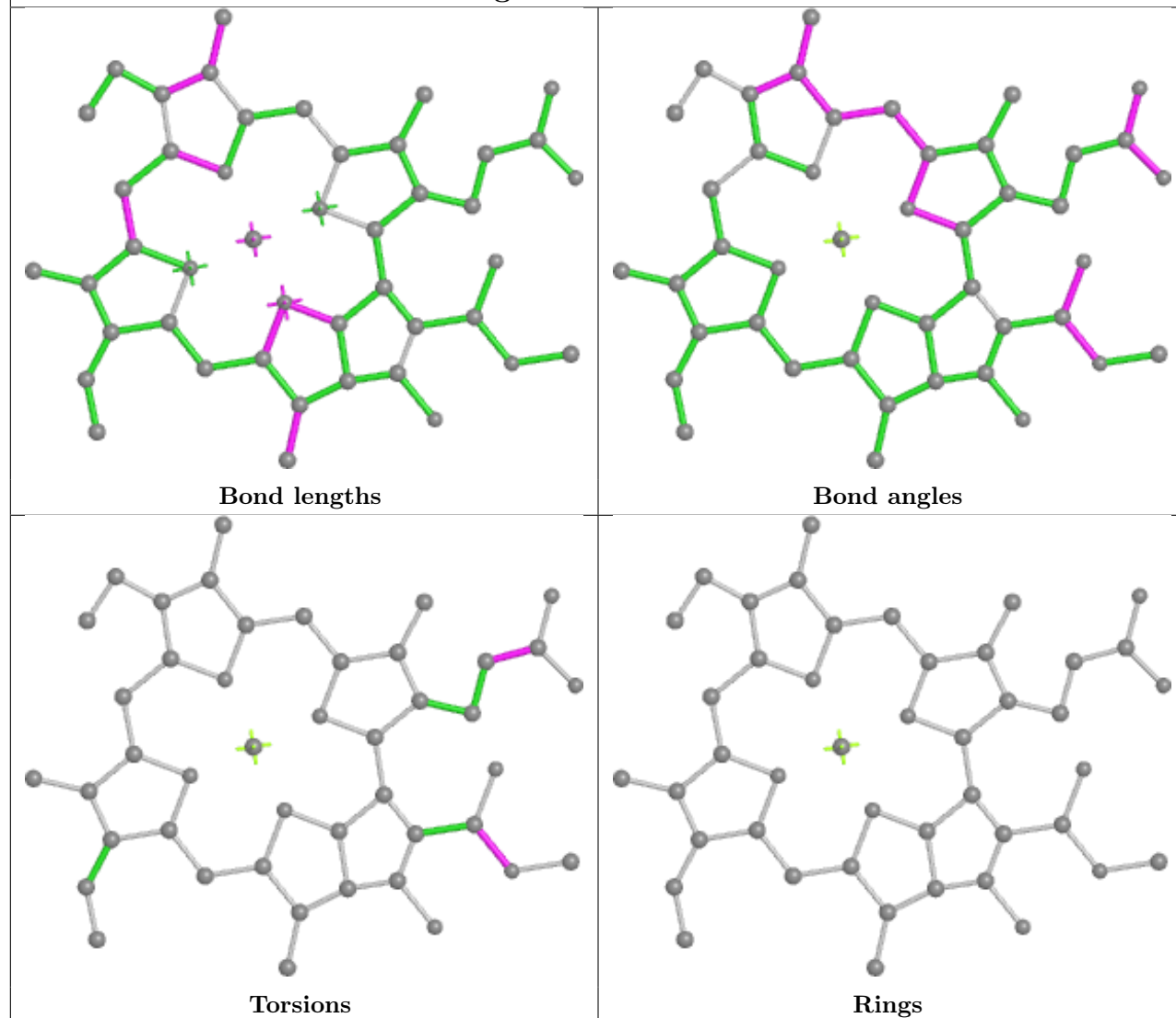


Rings

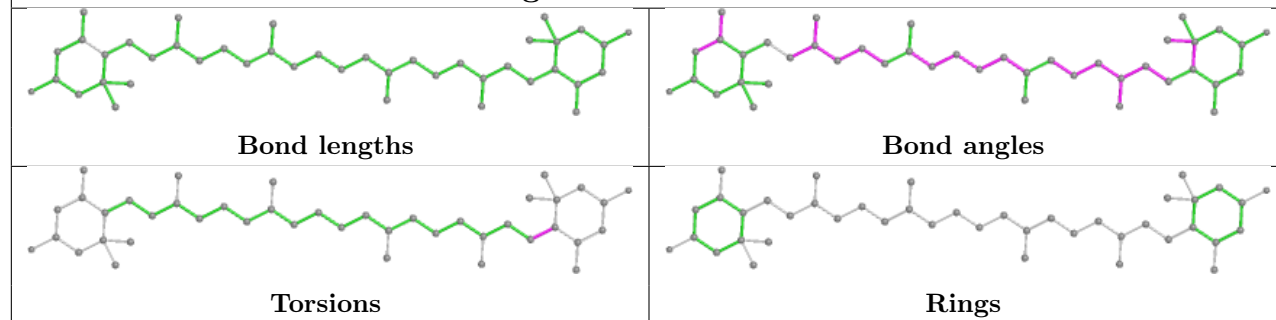


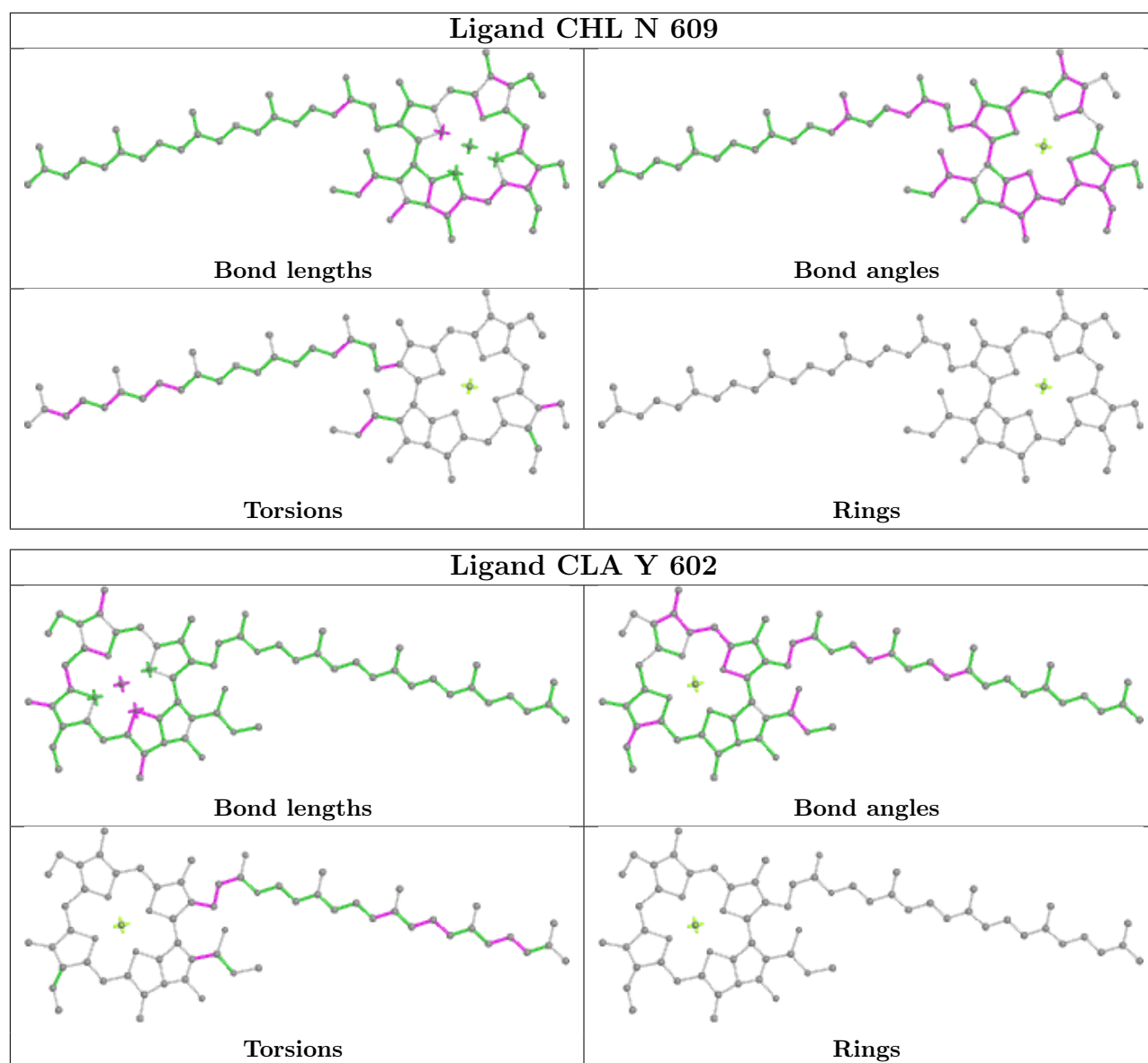


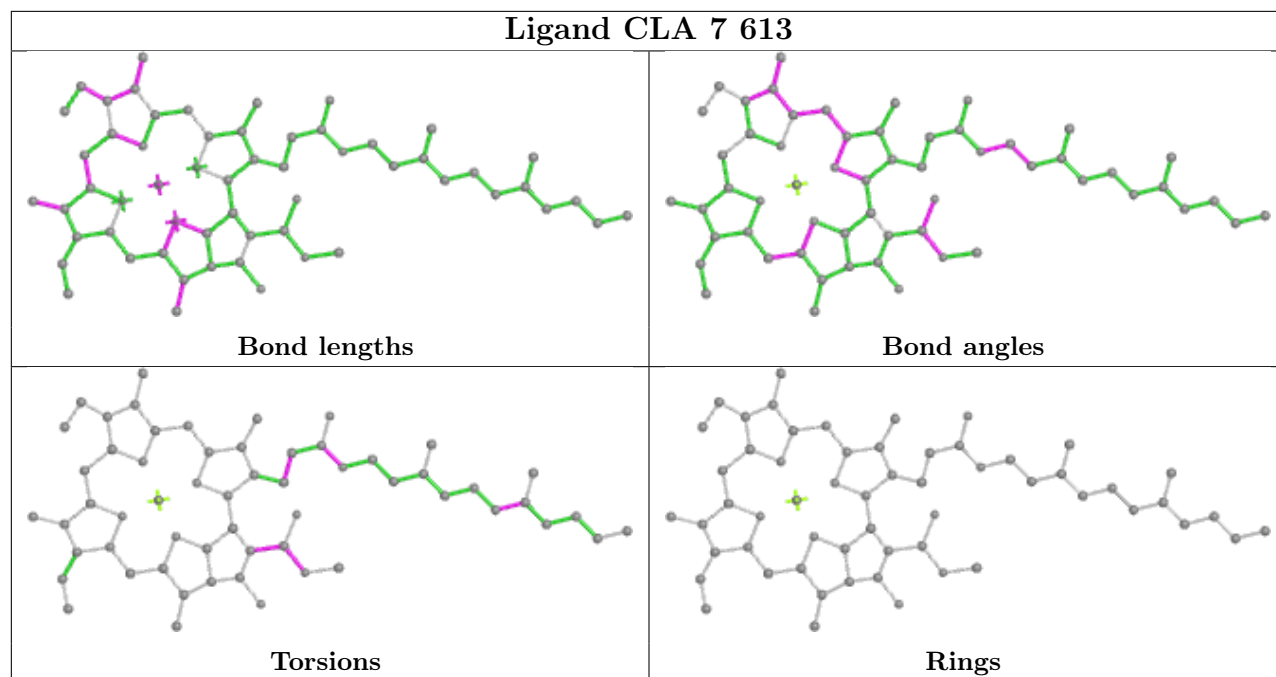
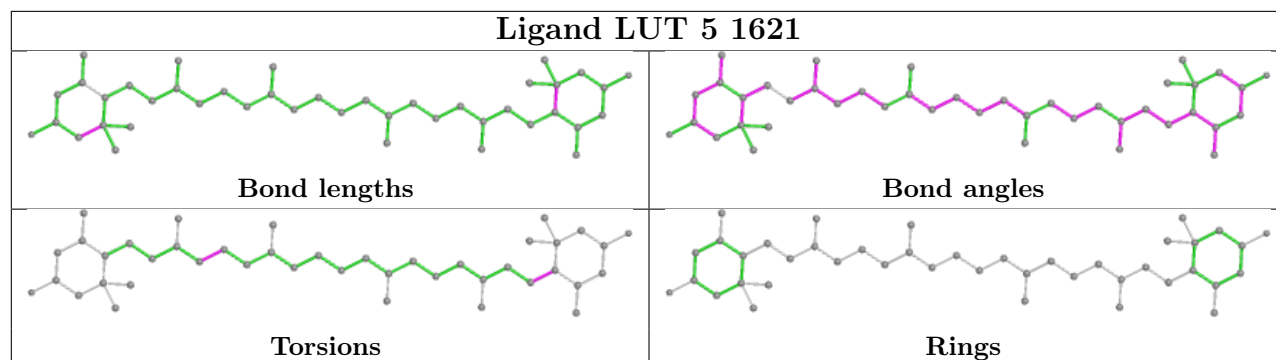
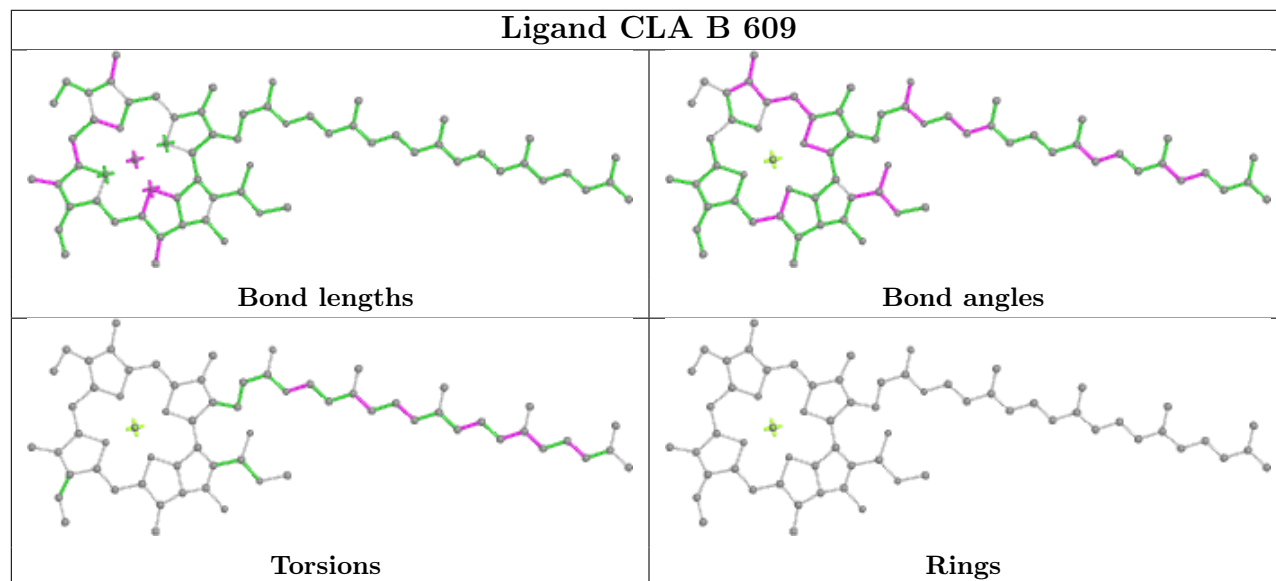
Ligand CLA 4 611

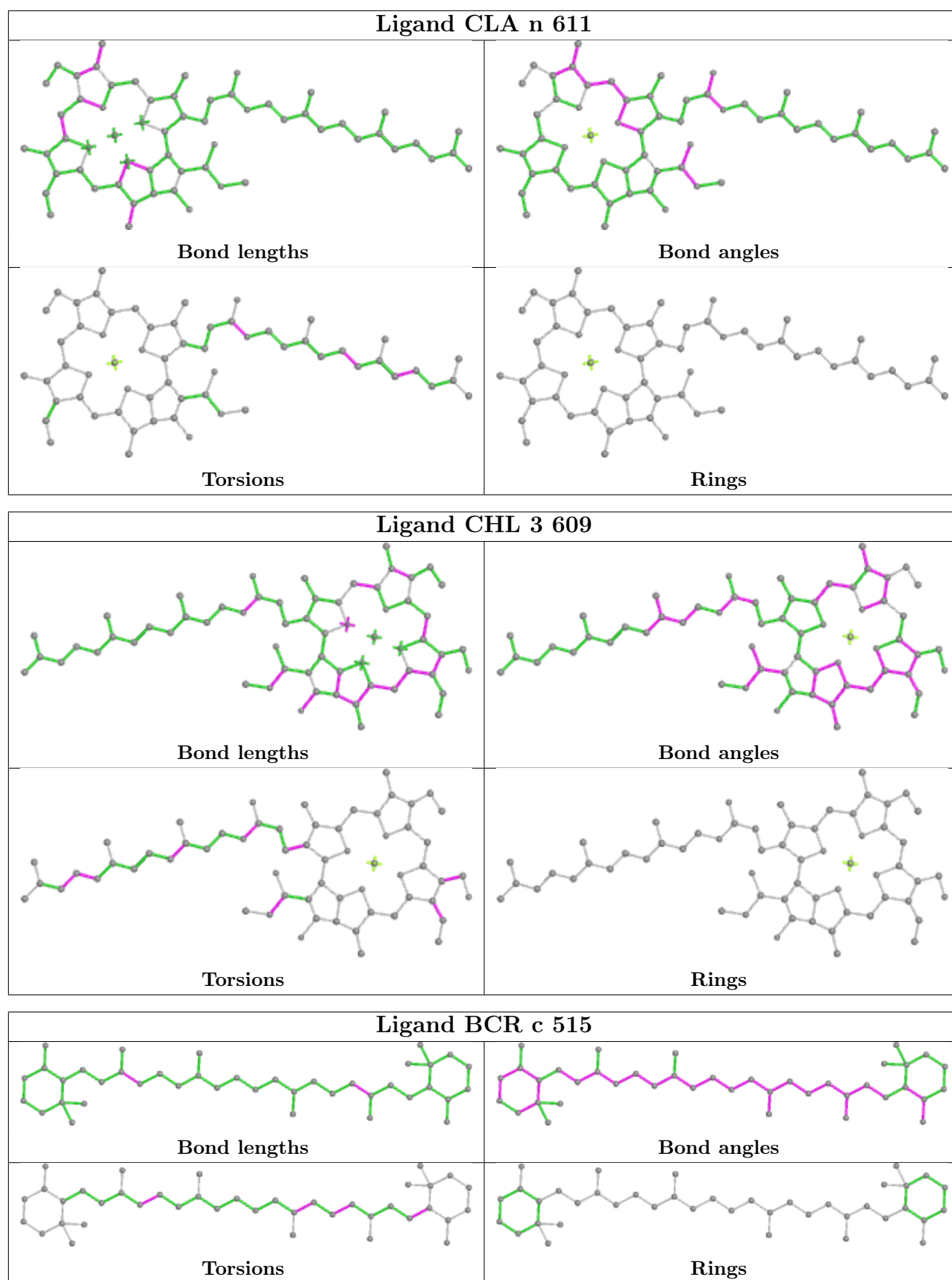


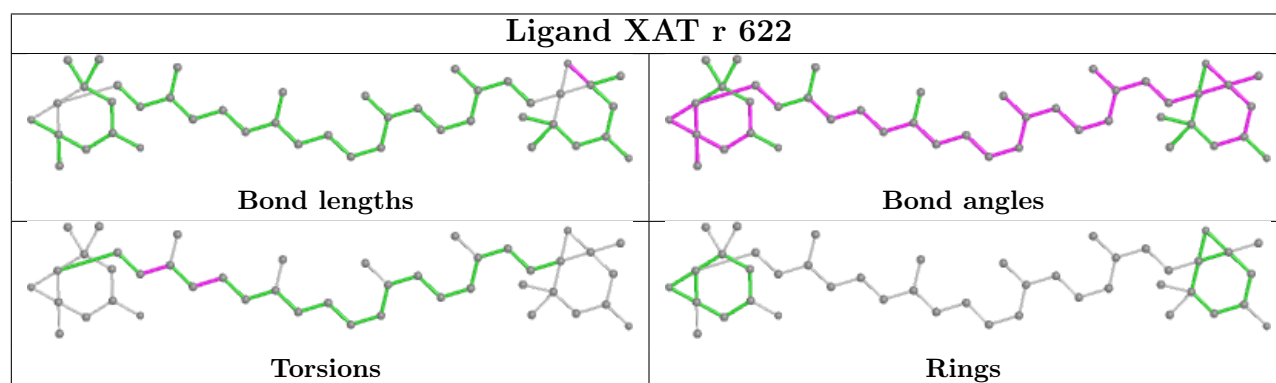
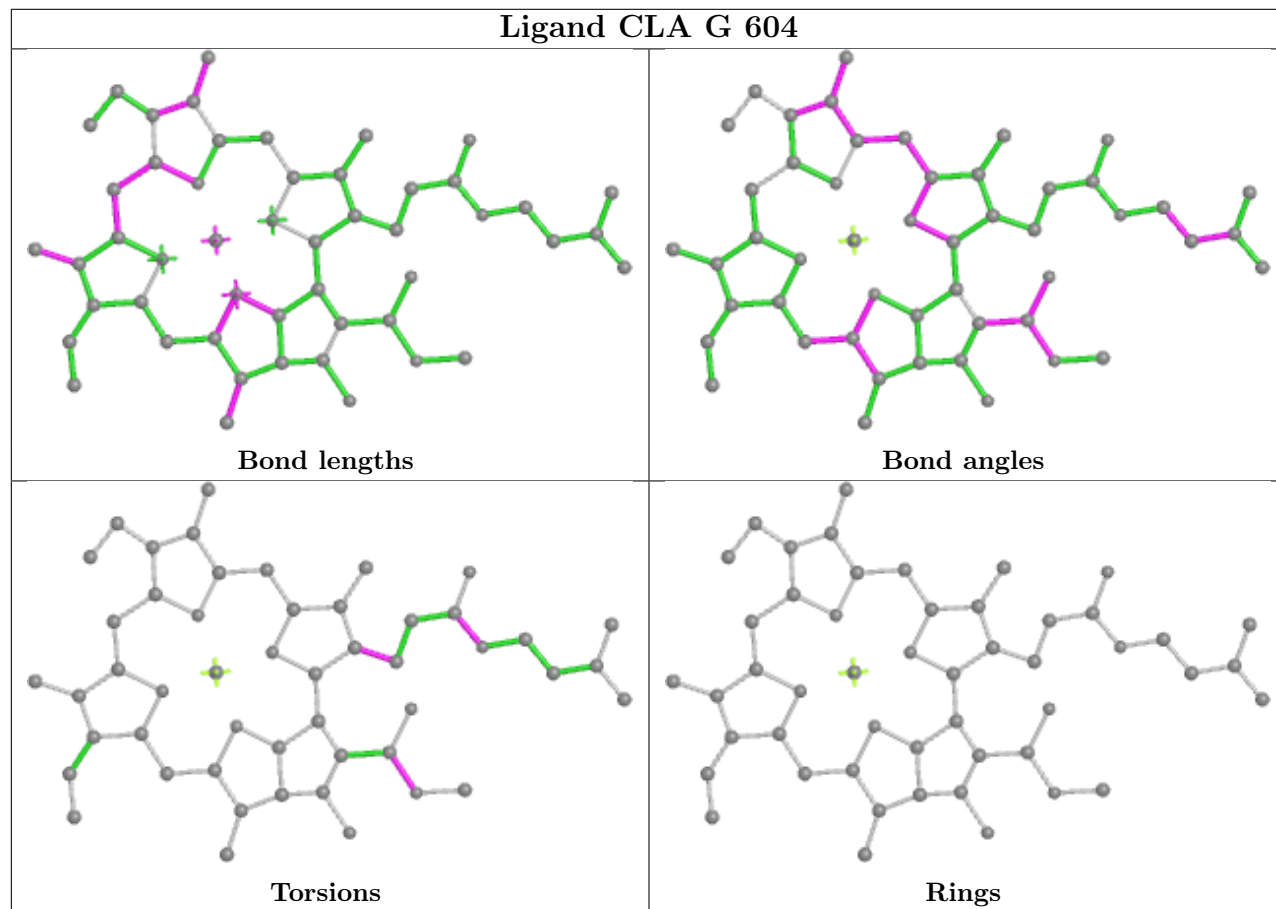
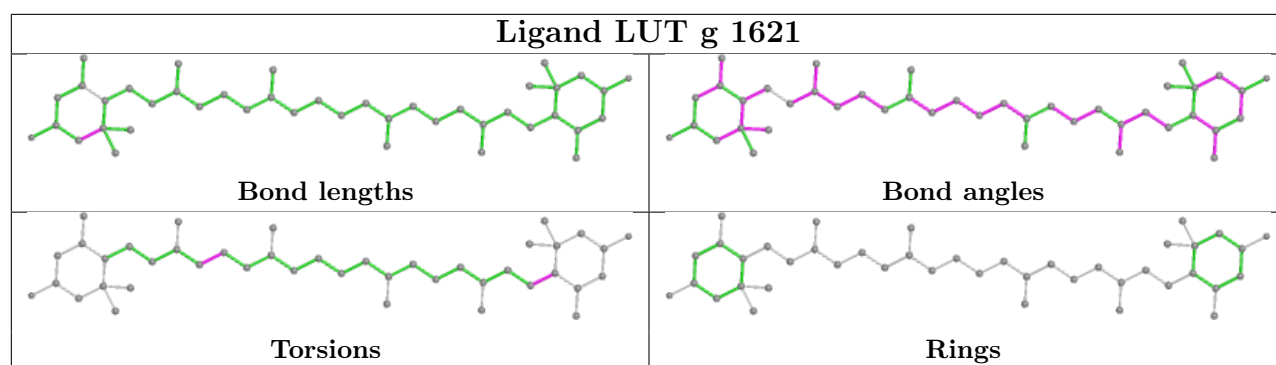
Ligand LUT N 1620

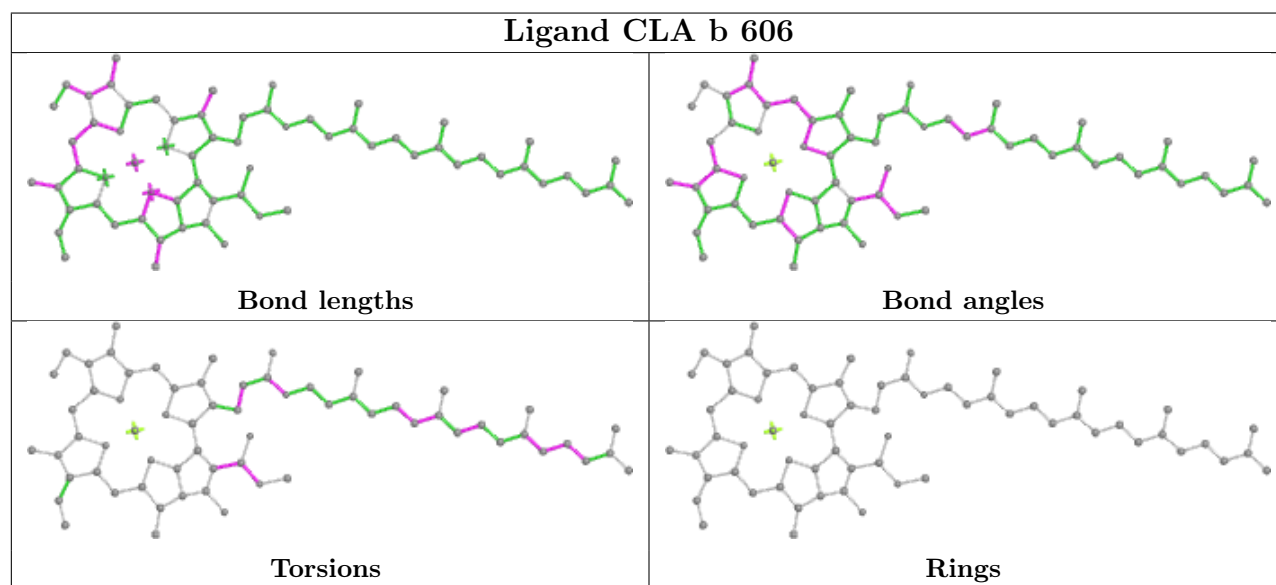
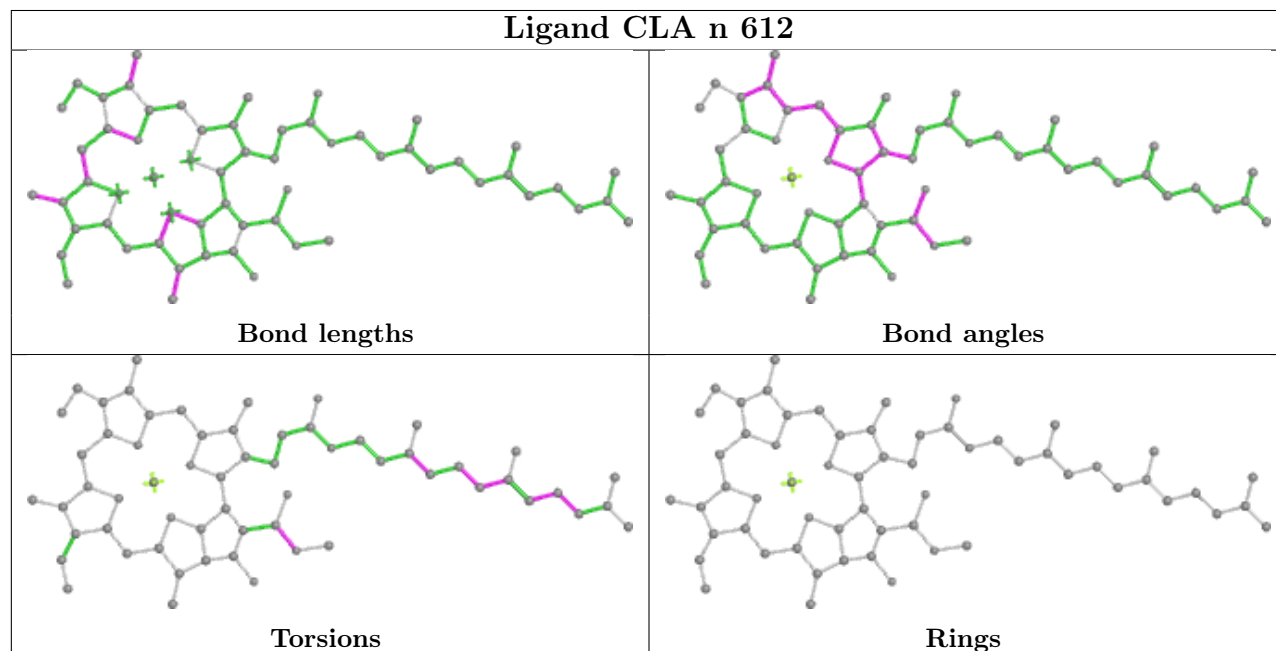
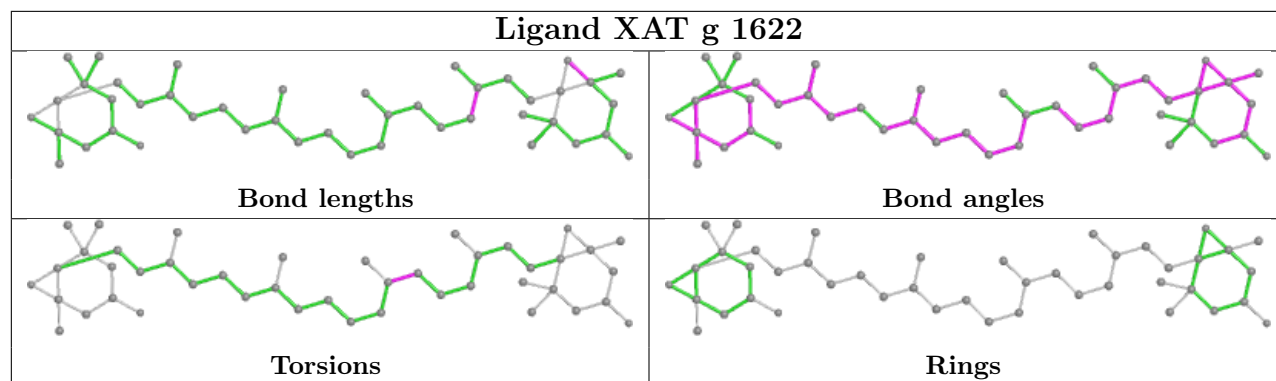




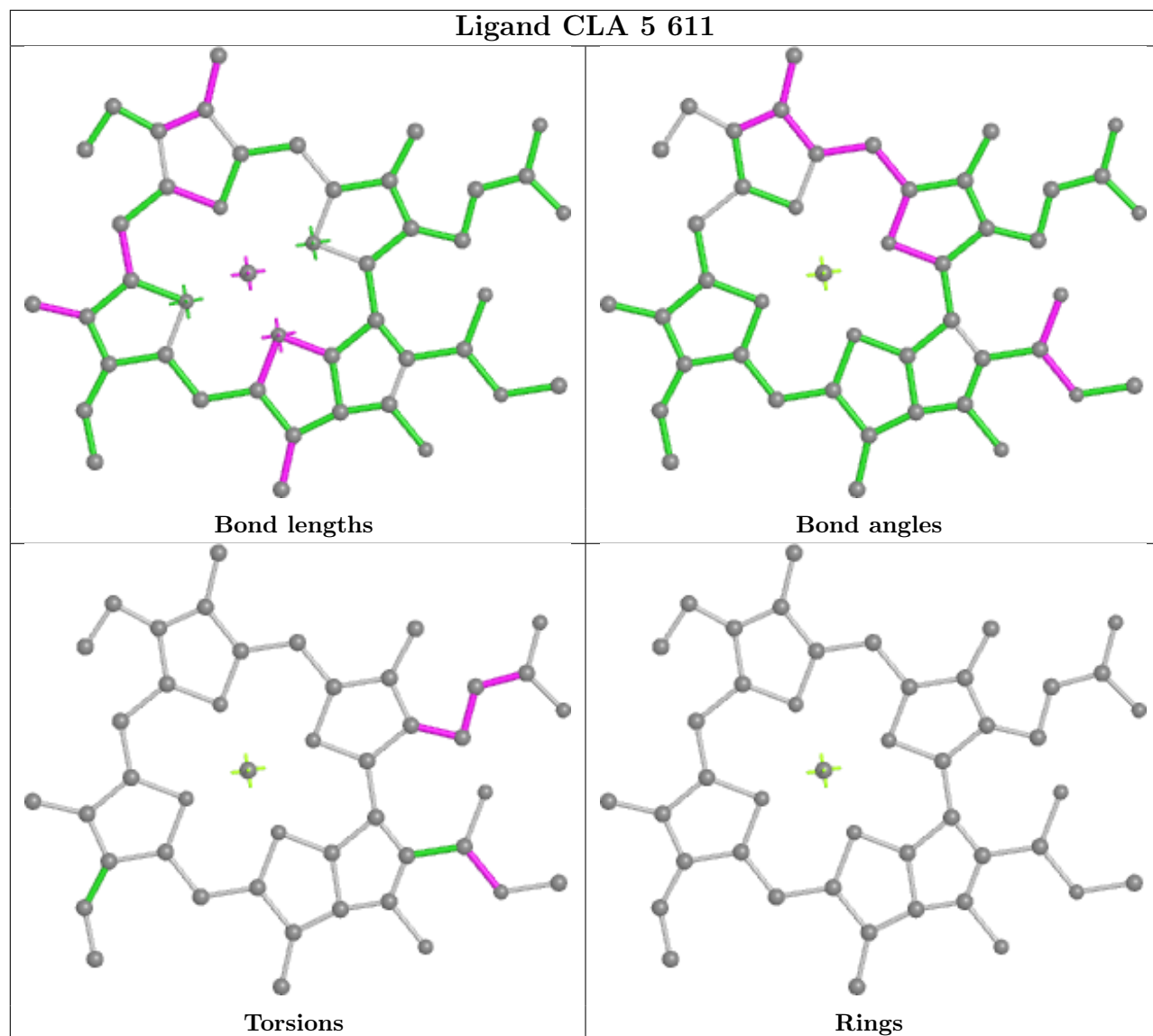
Ligand CLA 7 613**Ligand LUT 5 1621****Ligand CLA B 609**

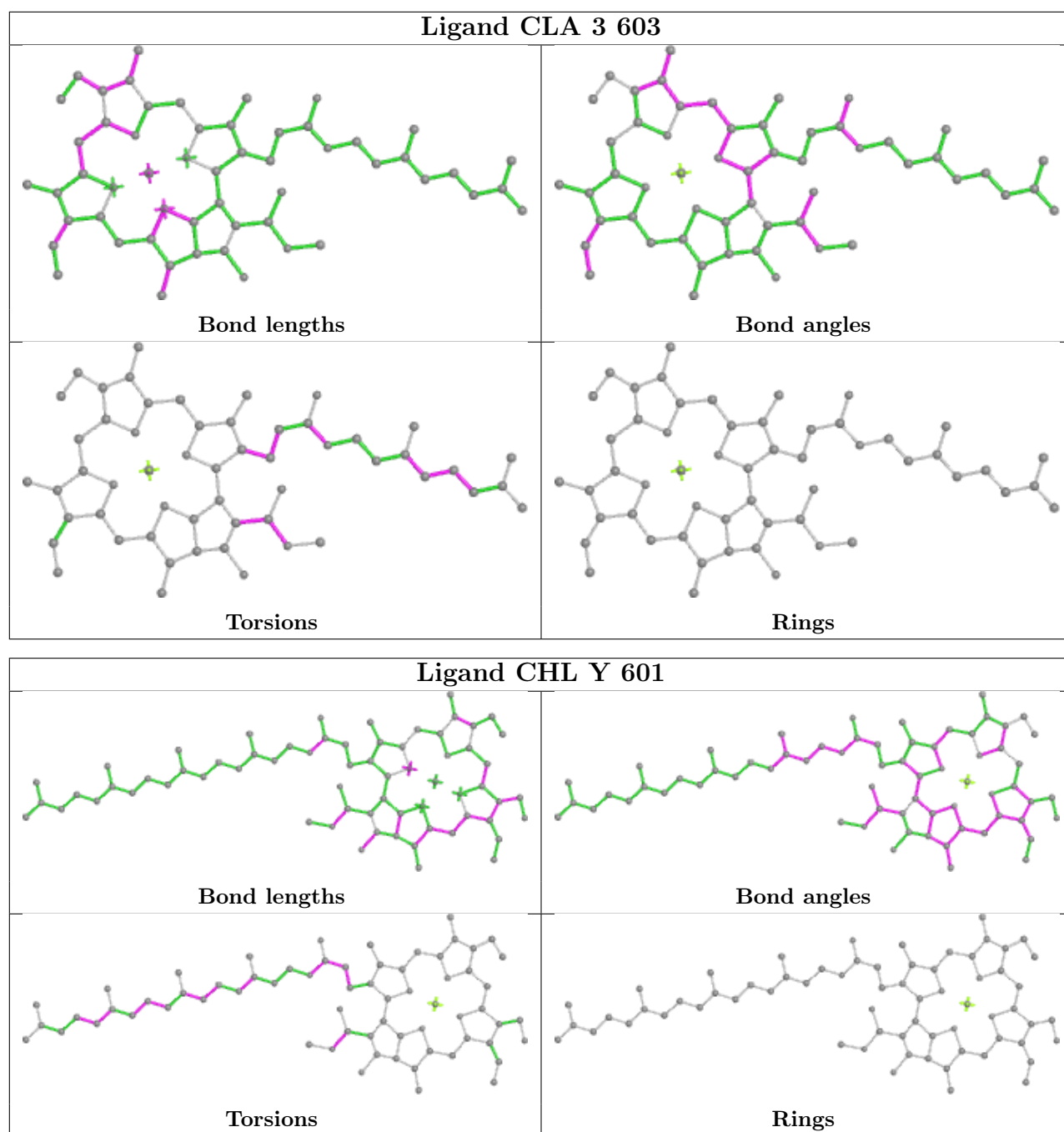




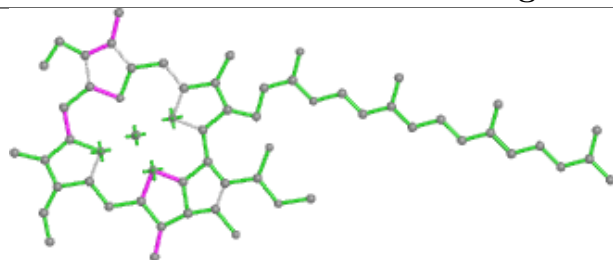


Ligand CLA 5 611

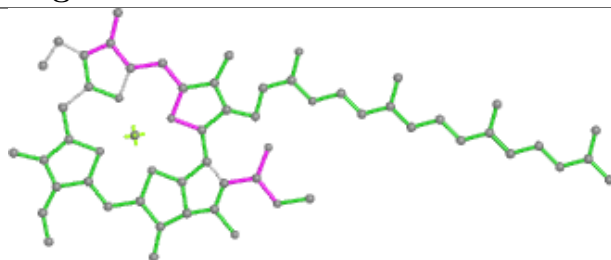




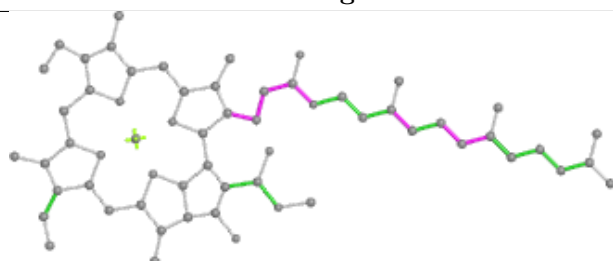
Ligand CLA g 611



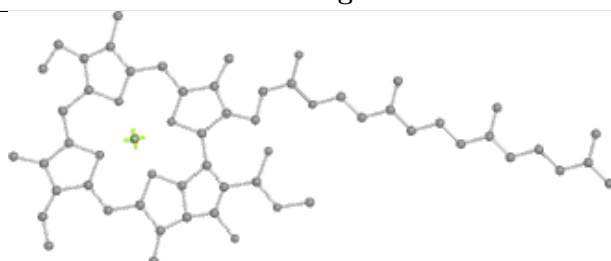
Bond lengths



Bond angles

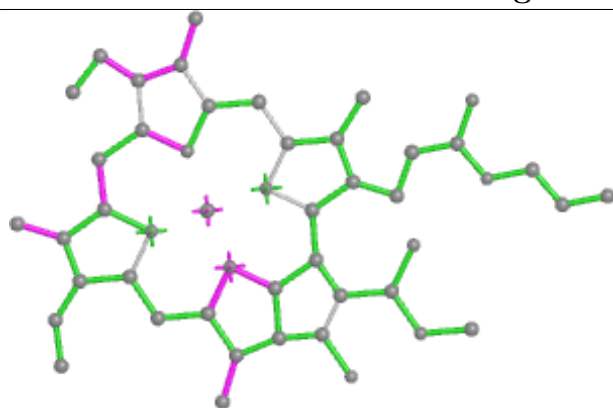


Torsions

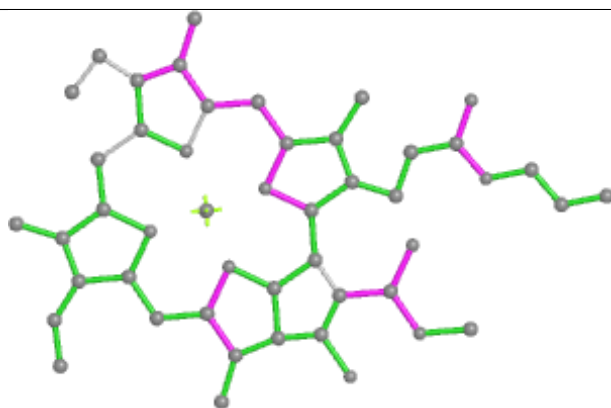


Rings

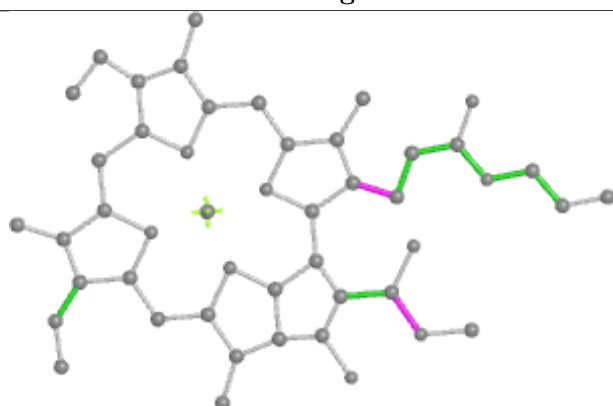
Ligand CLA Y 614



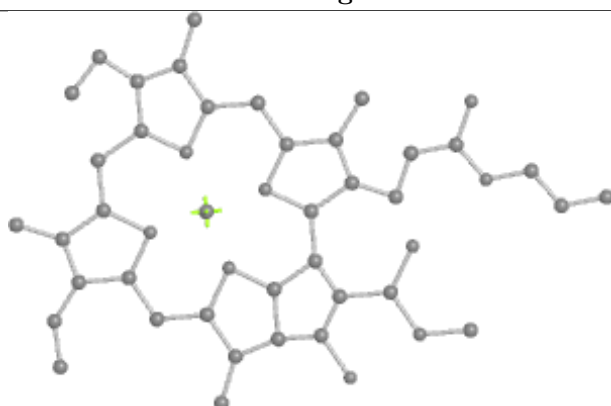
Bond lengths



Bond angles

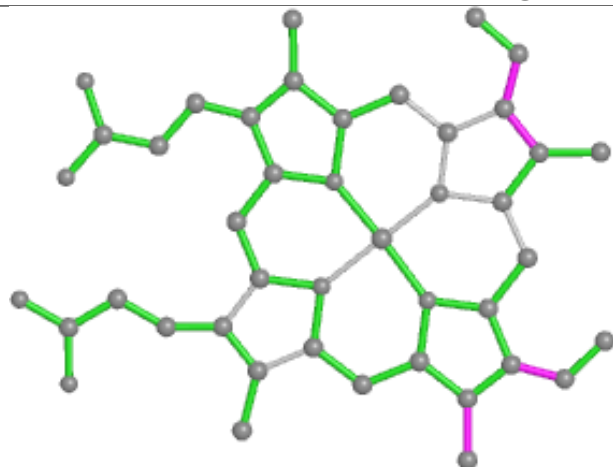


Torsions

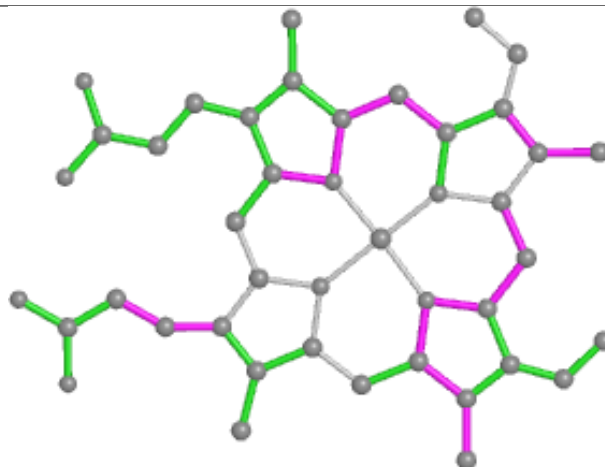


Rings

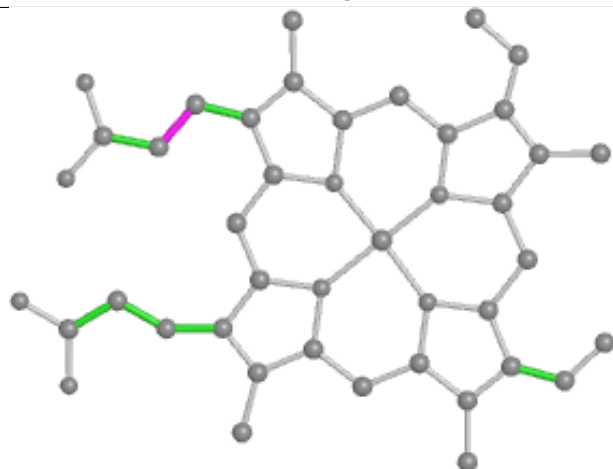
Ligand HEM f 101



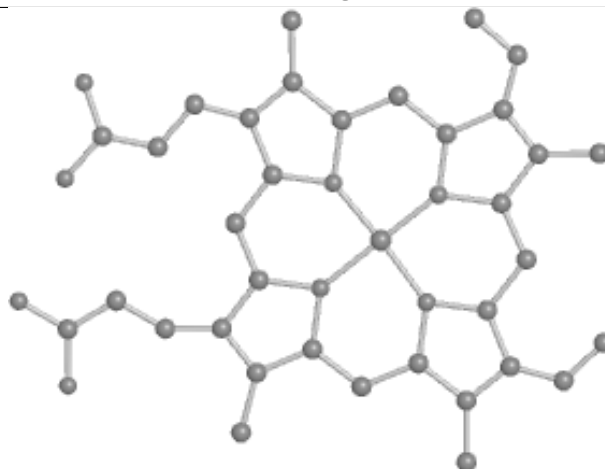
Bond lengths



Bond angles

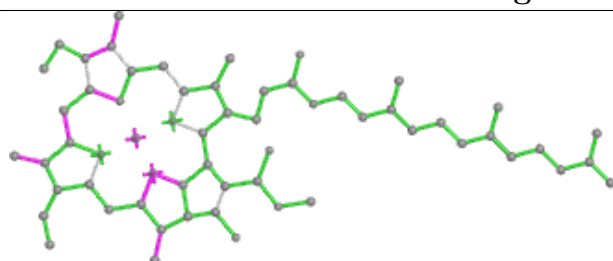


Torsions

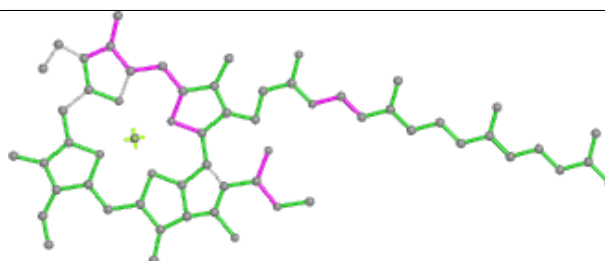


Rings

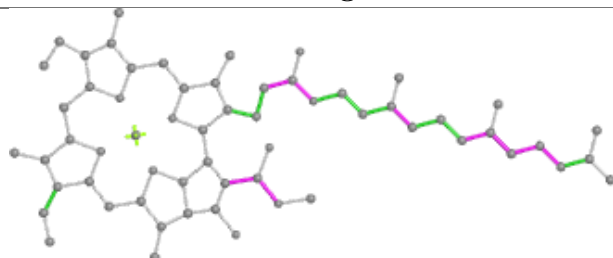
Ligand CLA Y 612



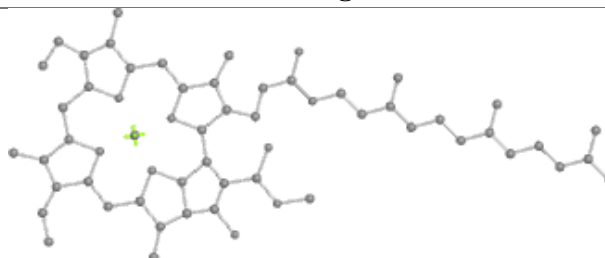
Bond lengths



Bond angles

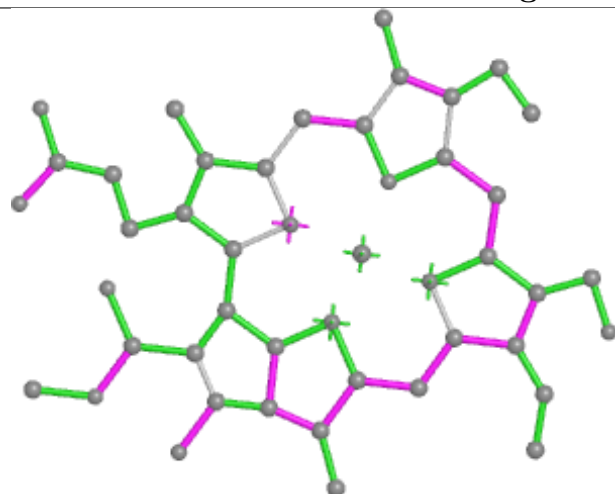


Torsions

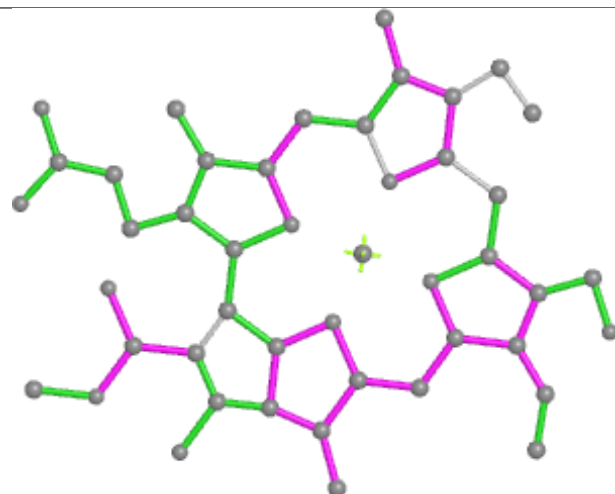


Rings

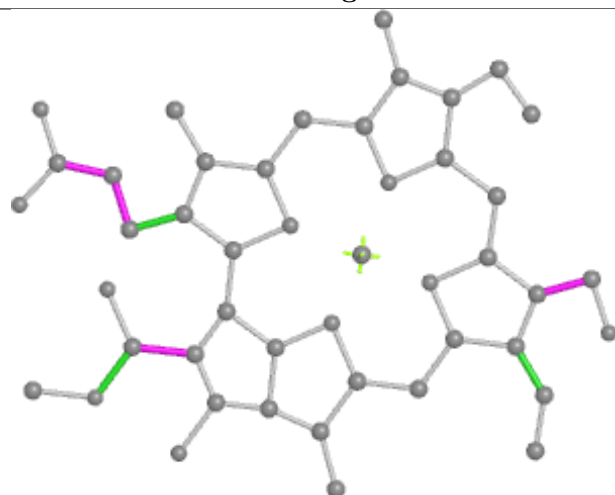
Ligand CHL 6 606



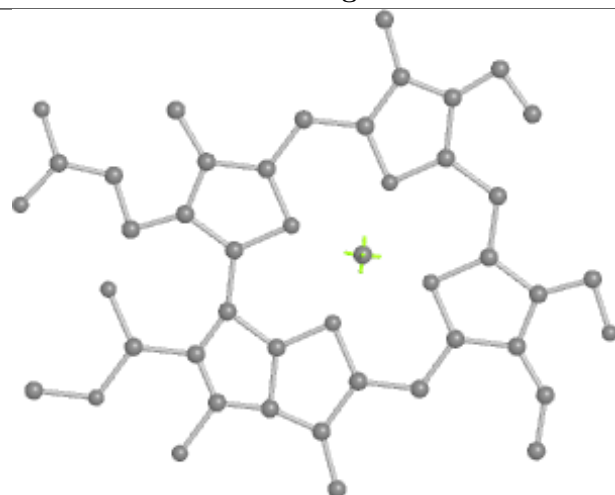
Bond lengths



Bond angles

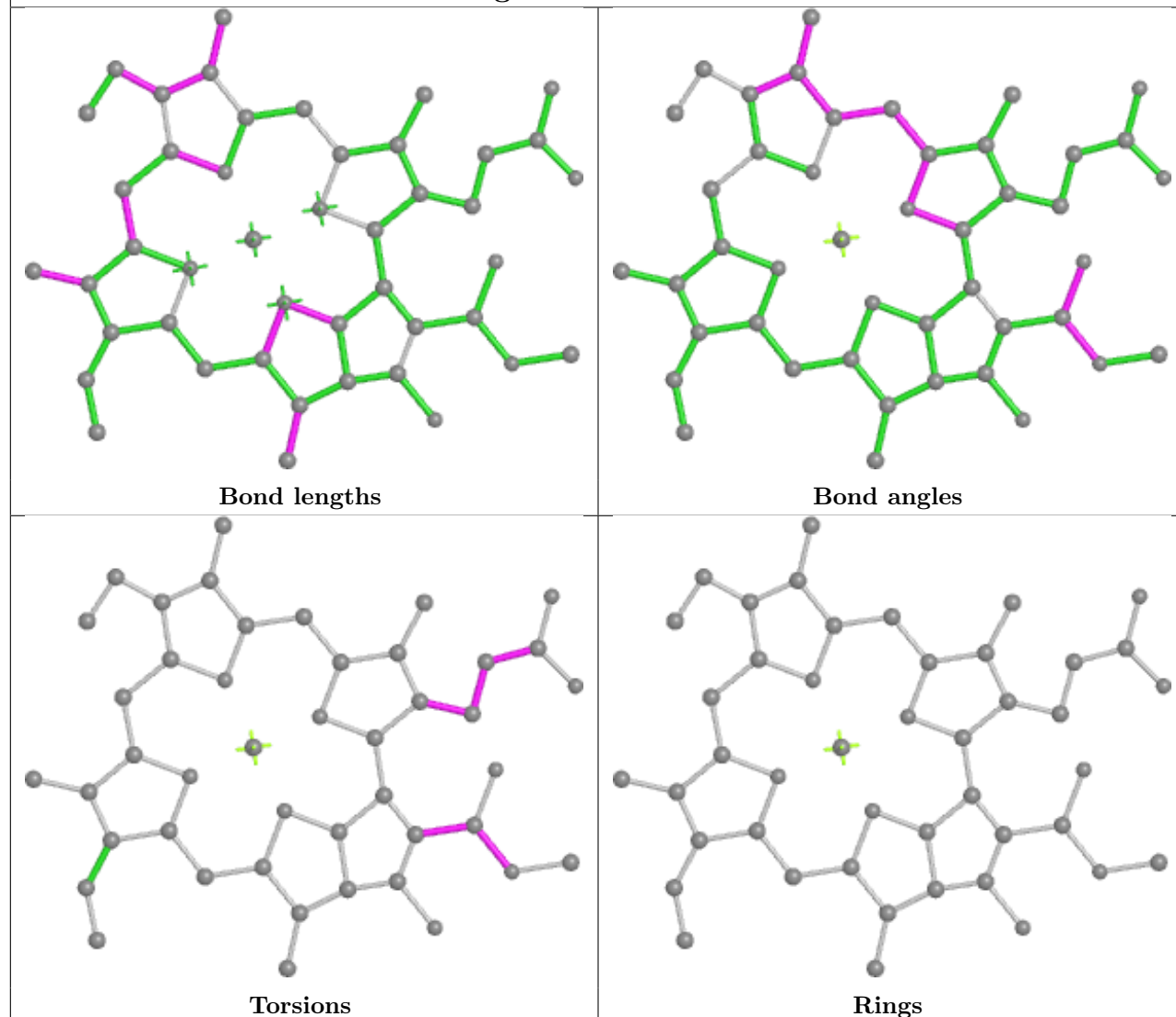


Torsions

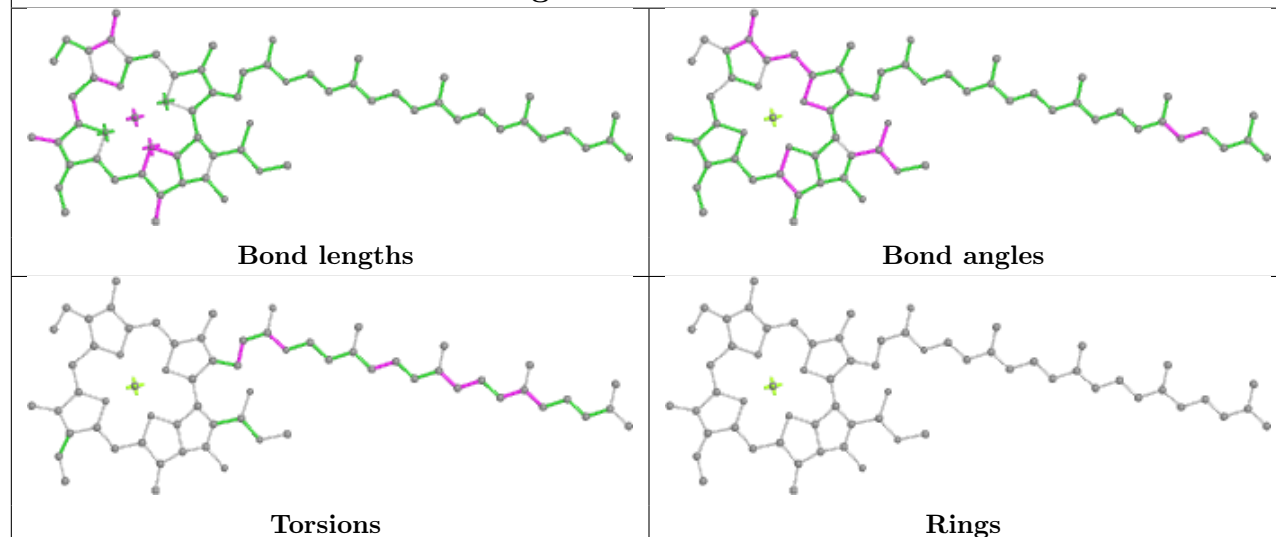


Rings

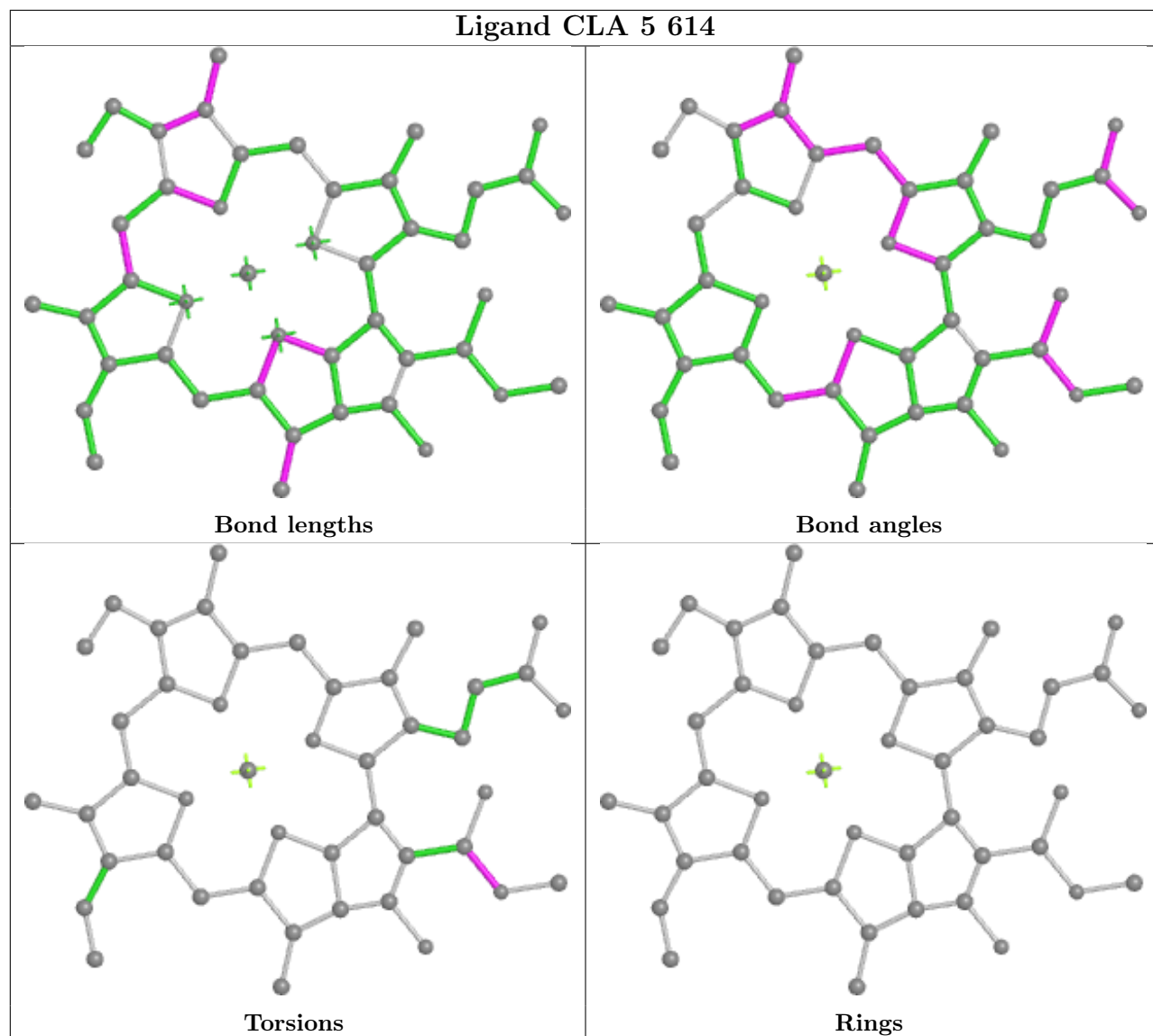
Ligand CLA 3 604

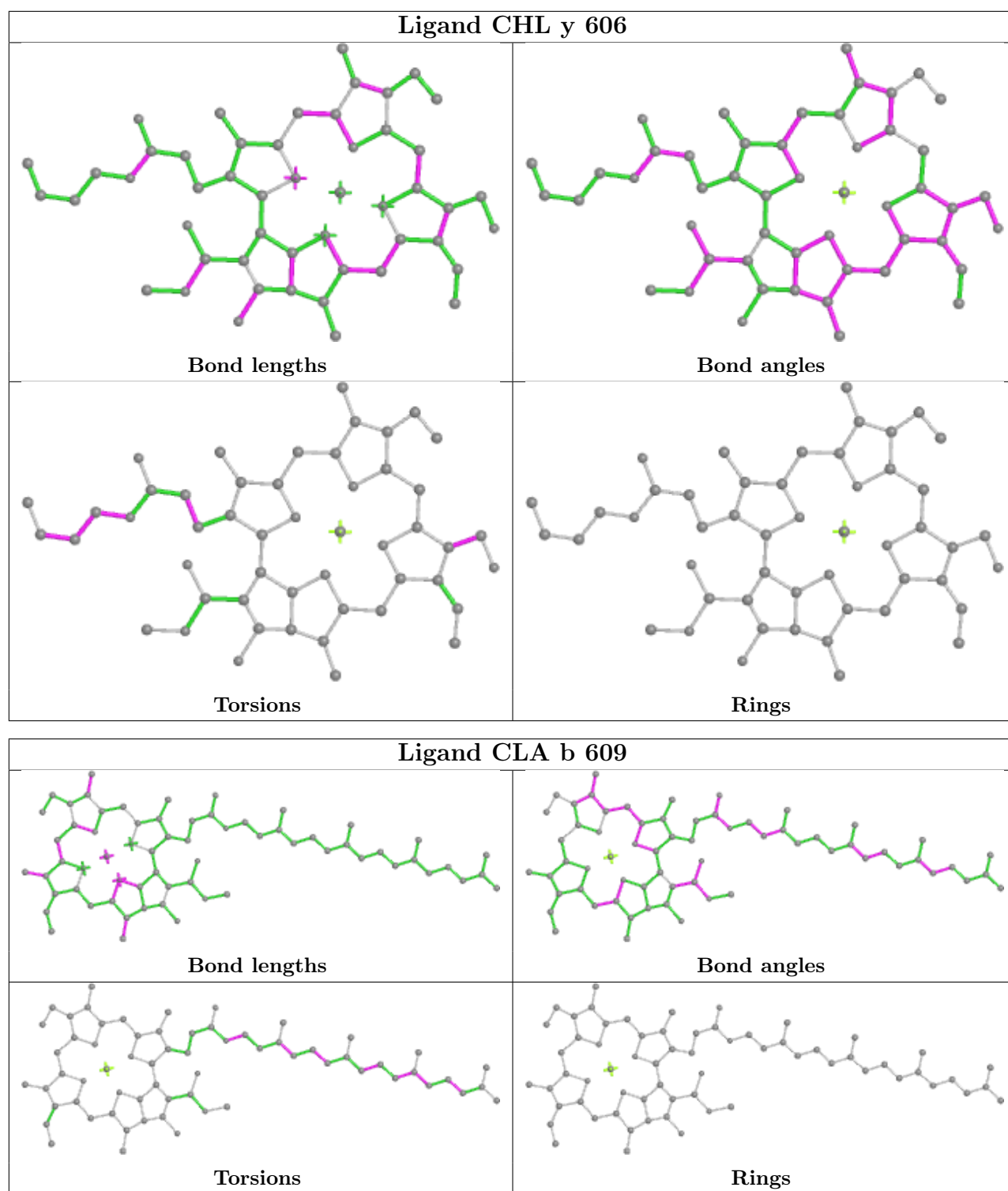


Ligand CLA Y 613

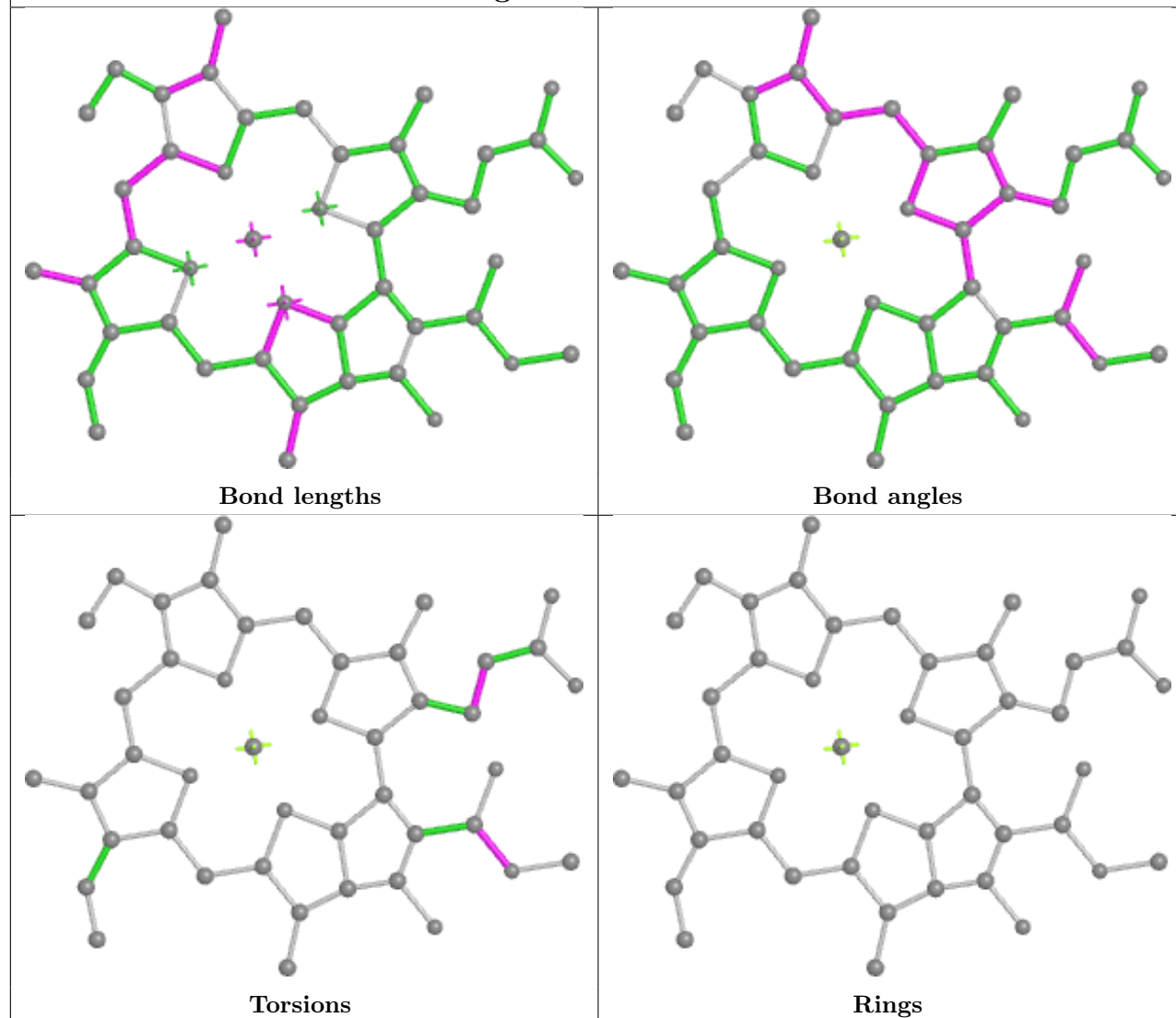


Ligand CLA 5 614

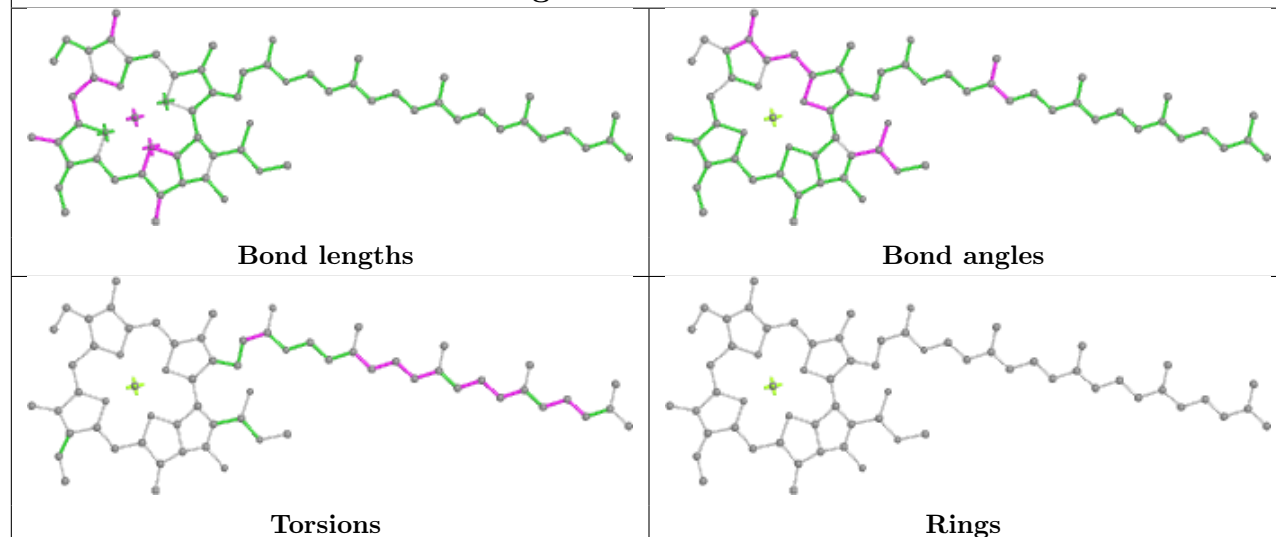




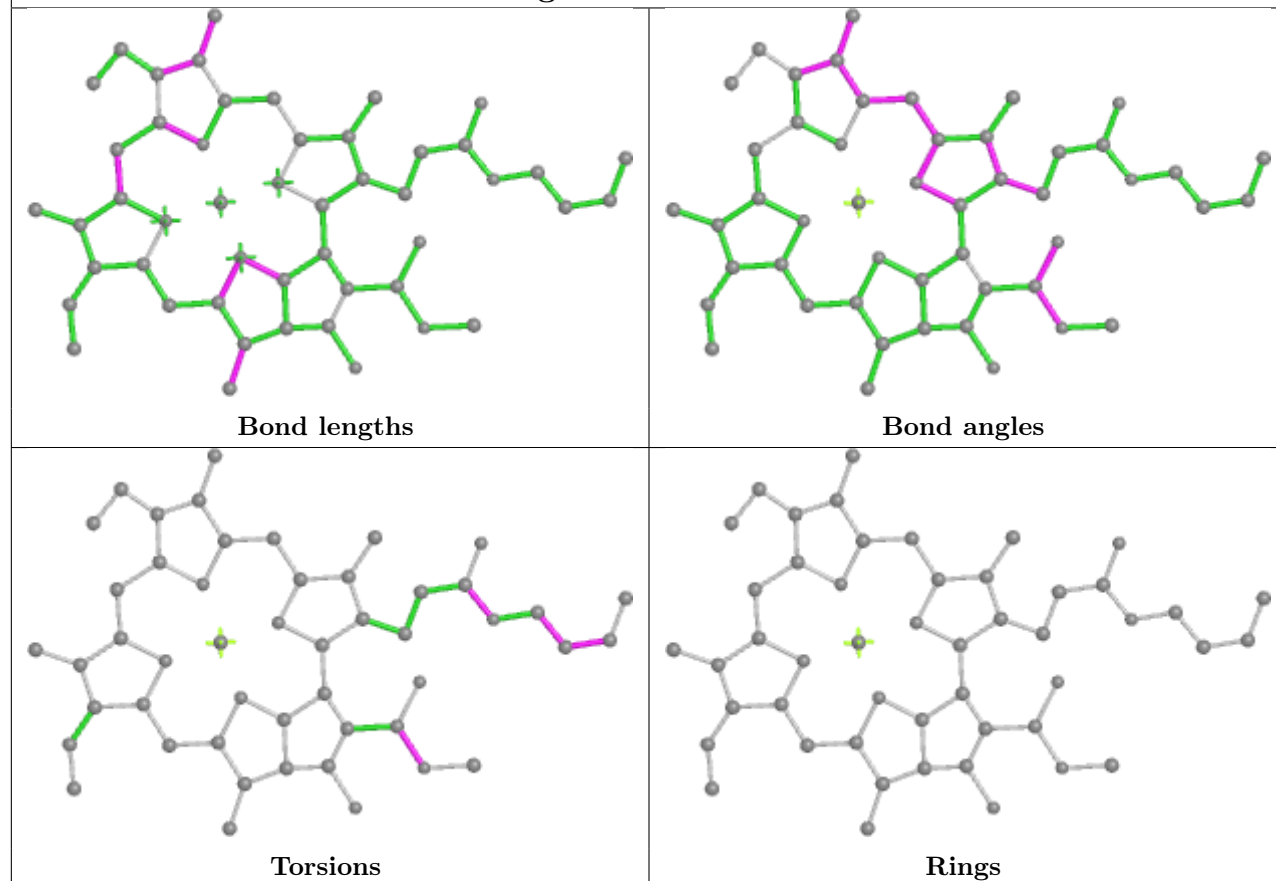
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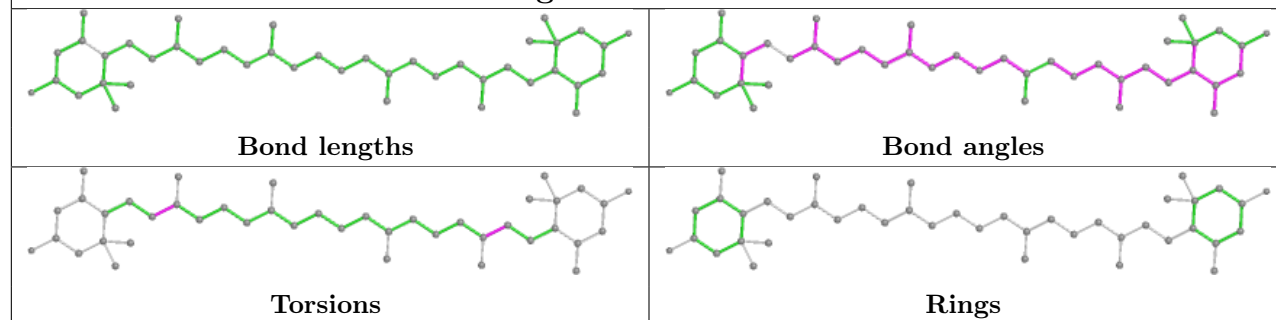
Ligand CLA B 614

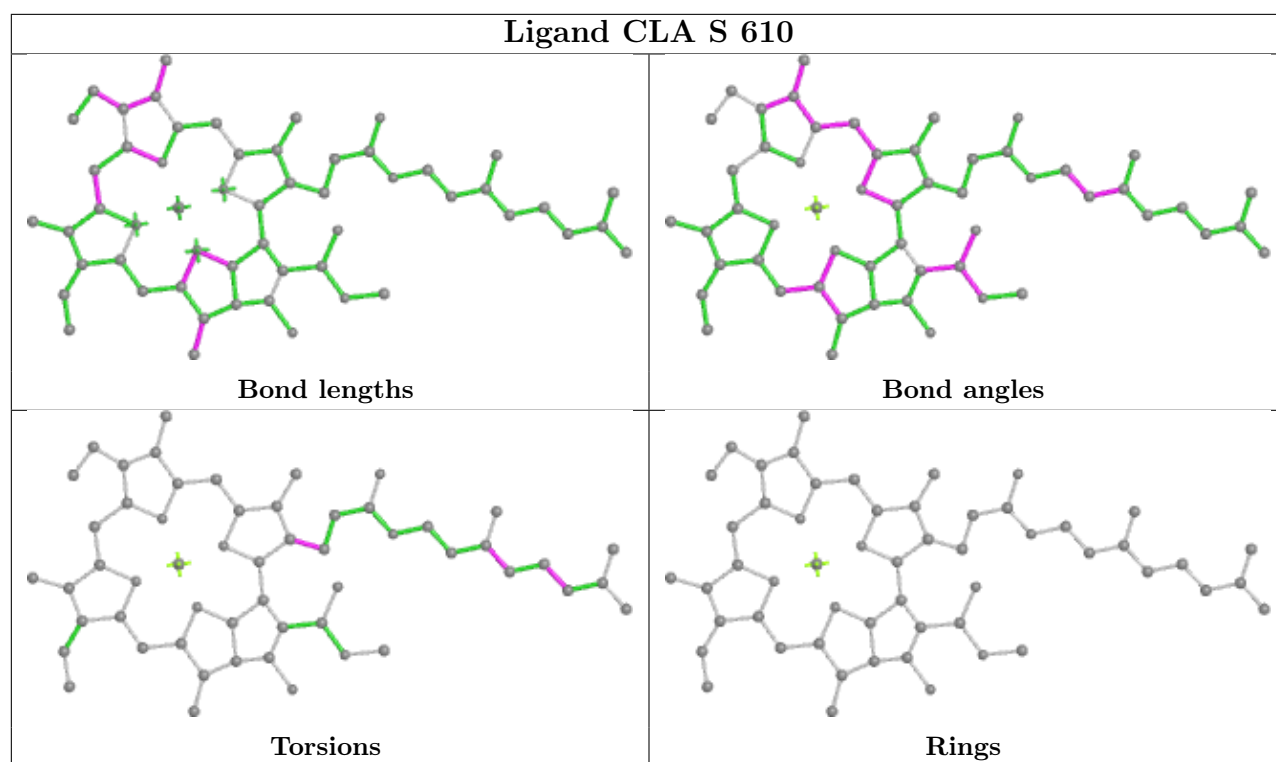


Ligand CLA r 612

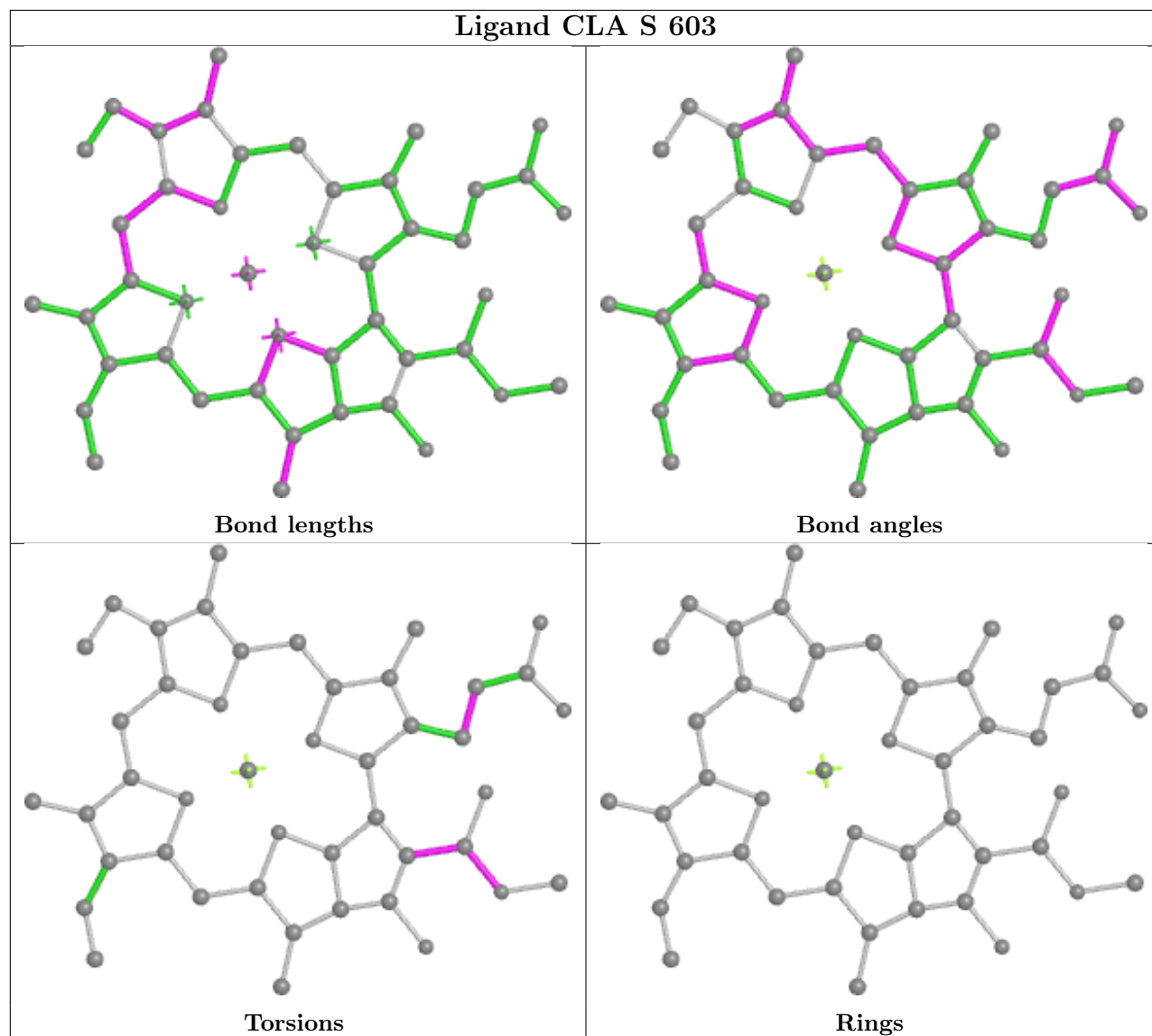


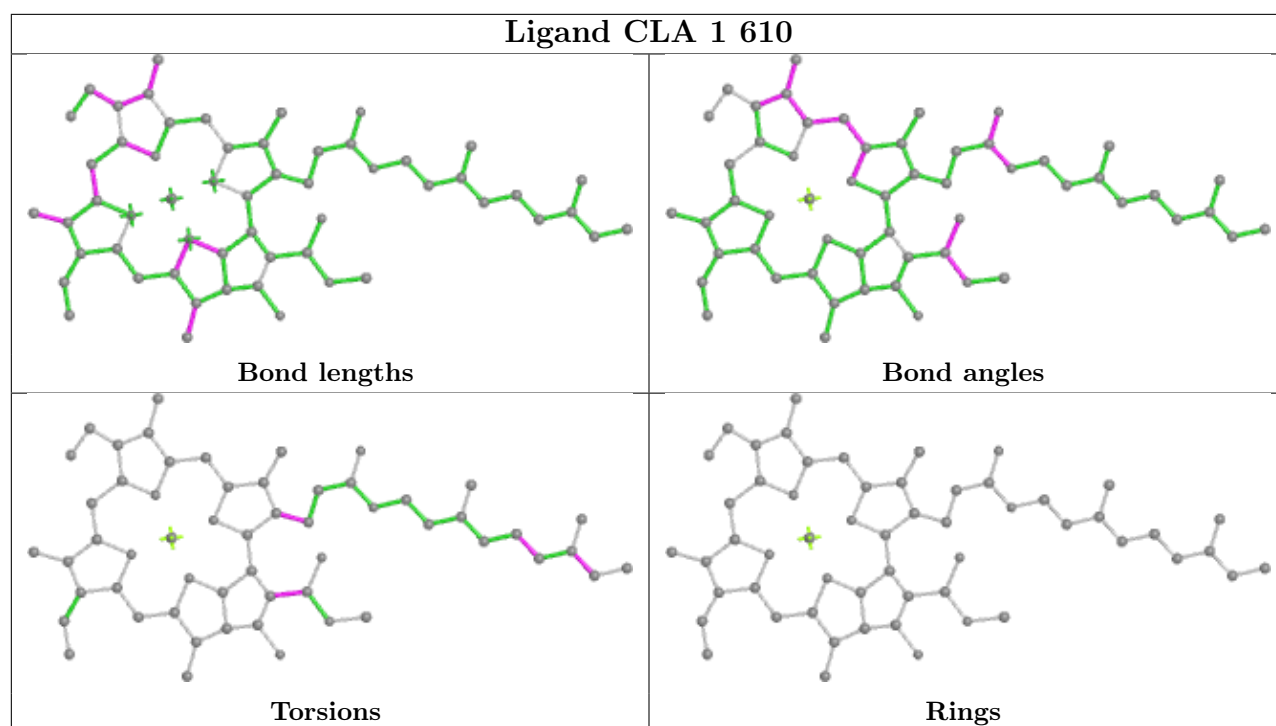
Ligand LUT 8 620



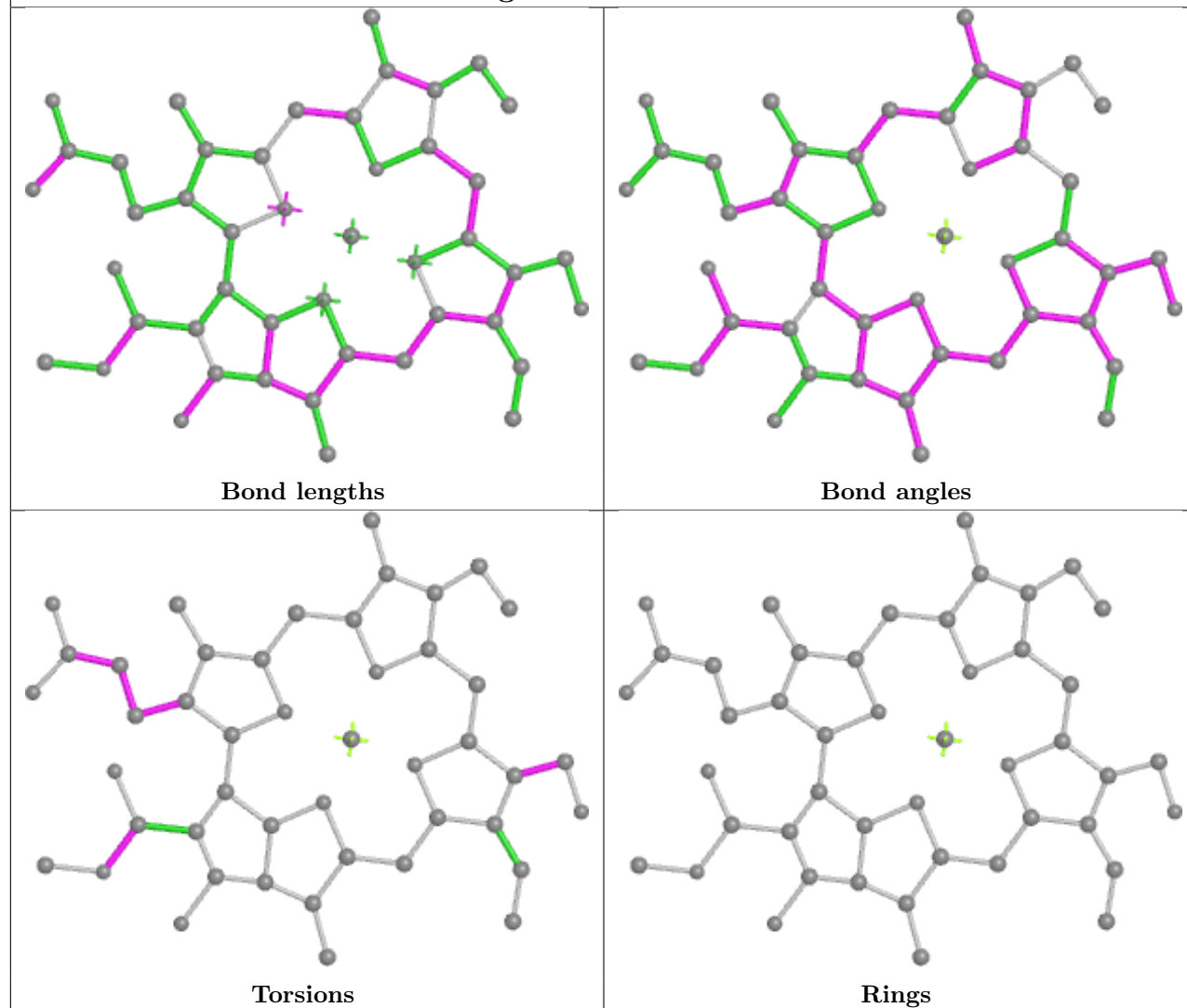


Ligand CLA S 603

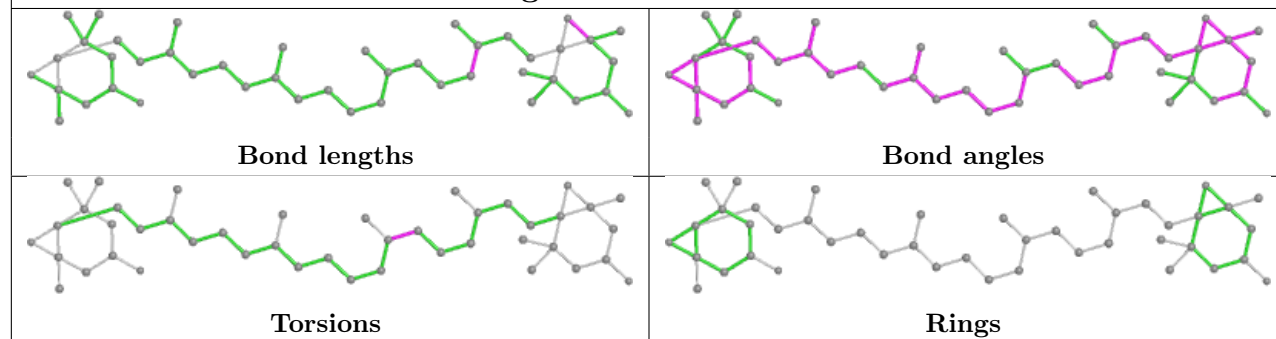


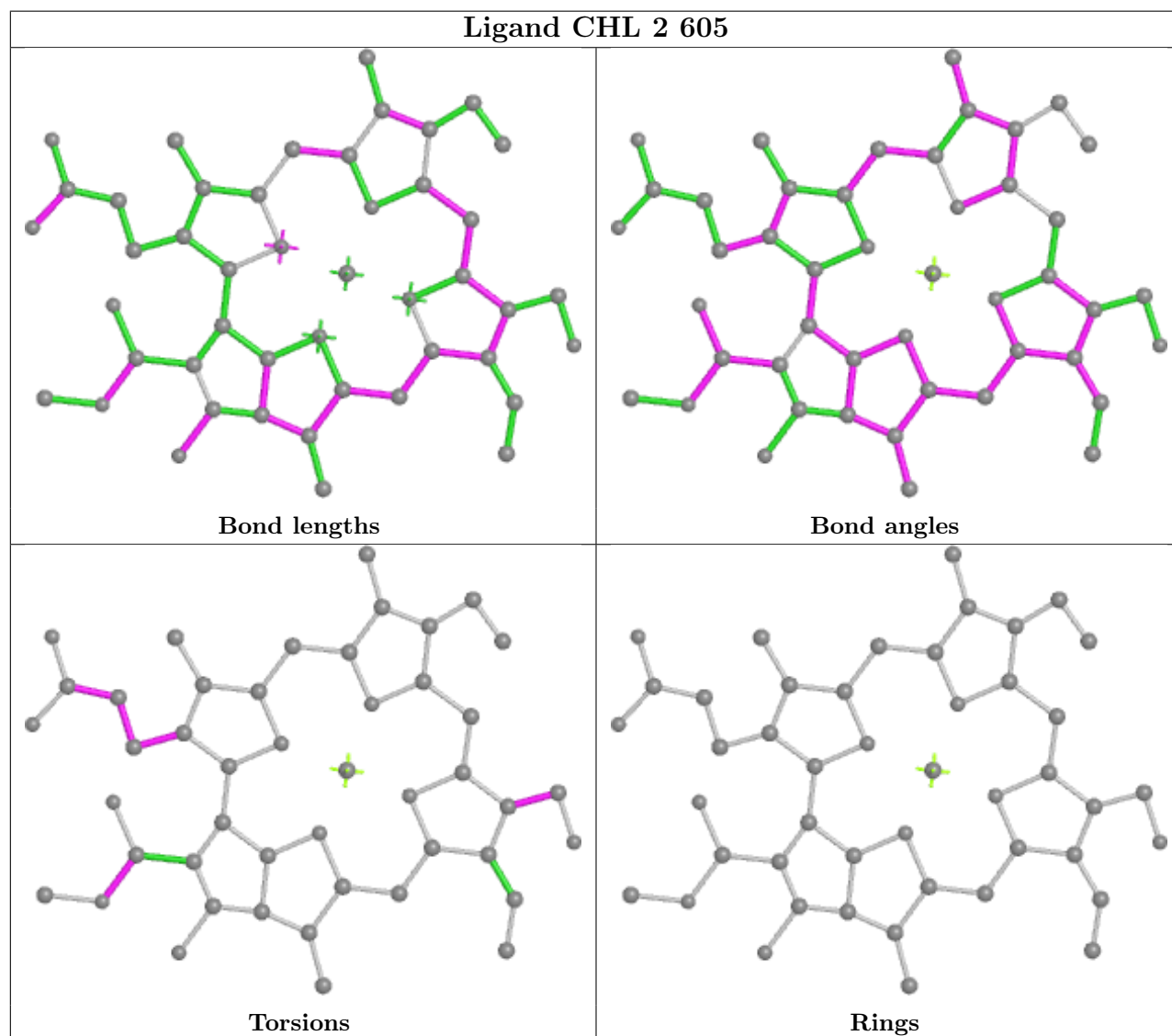
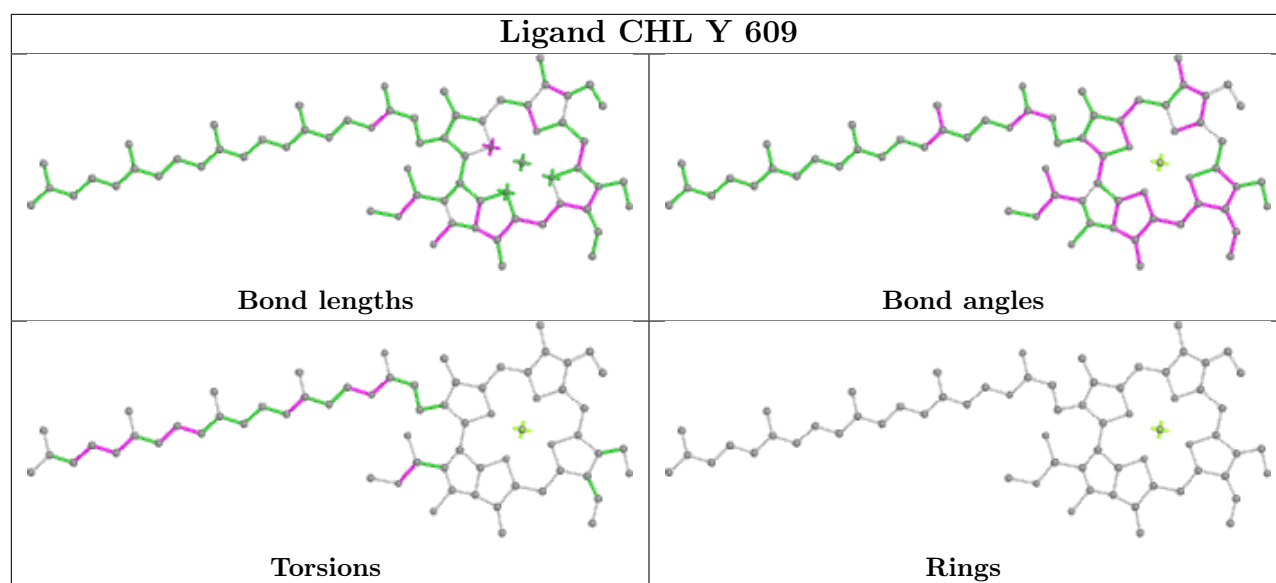


Ligand CHL 3 605

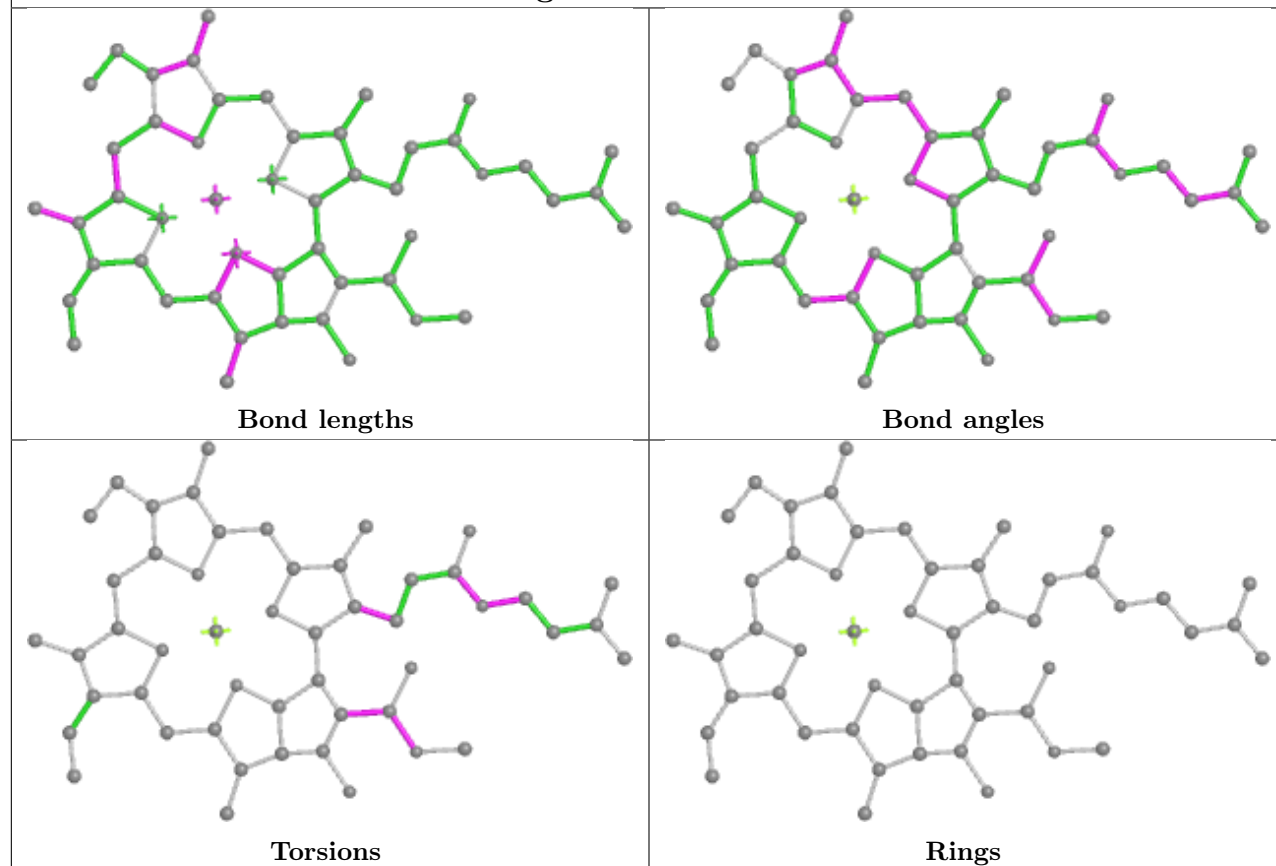


Ligand XAT G 1622

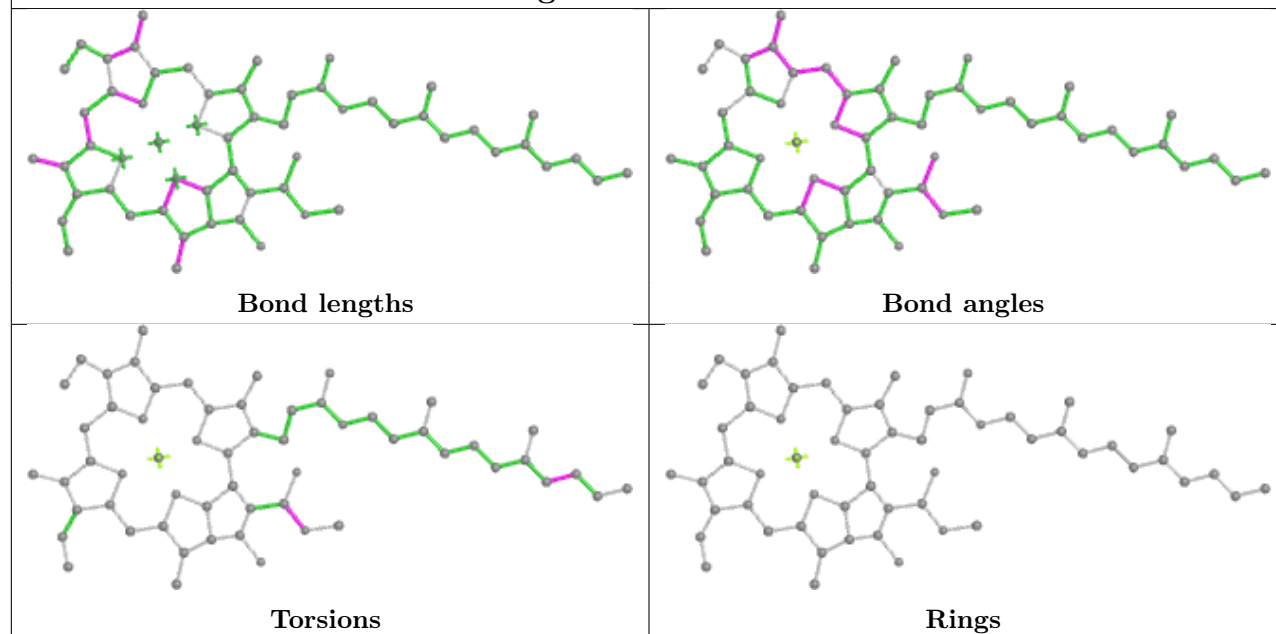


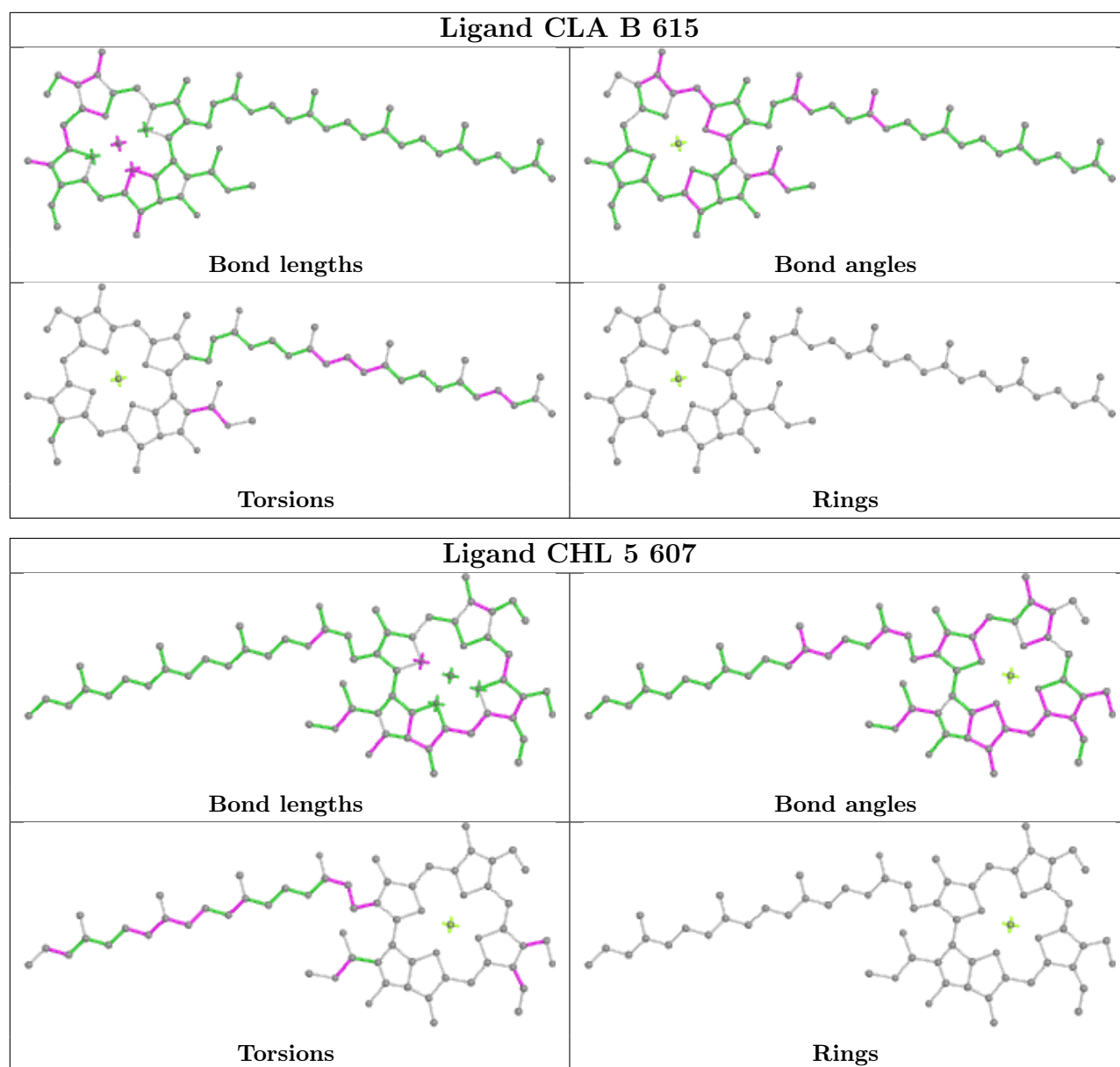


Ligand CLA 1 604

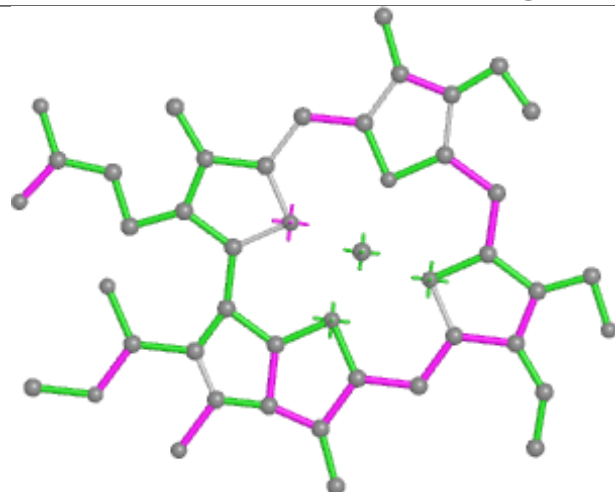


Ligand CLA r 609

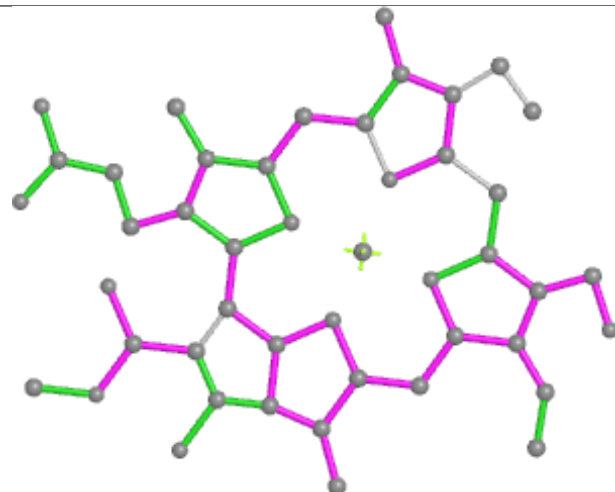




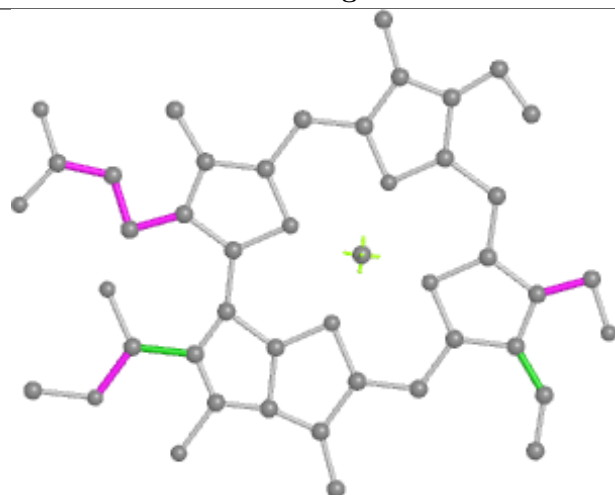
Ligand CHL 7 605



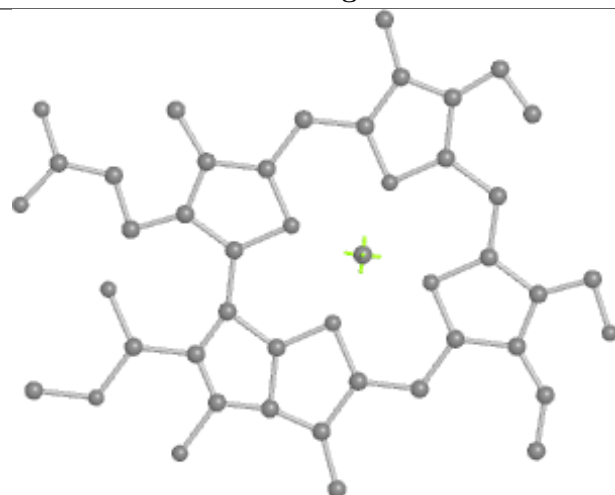
Bond lengths



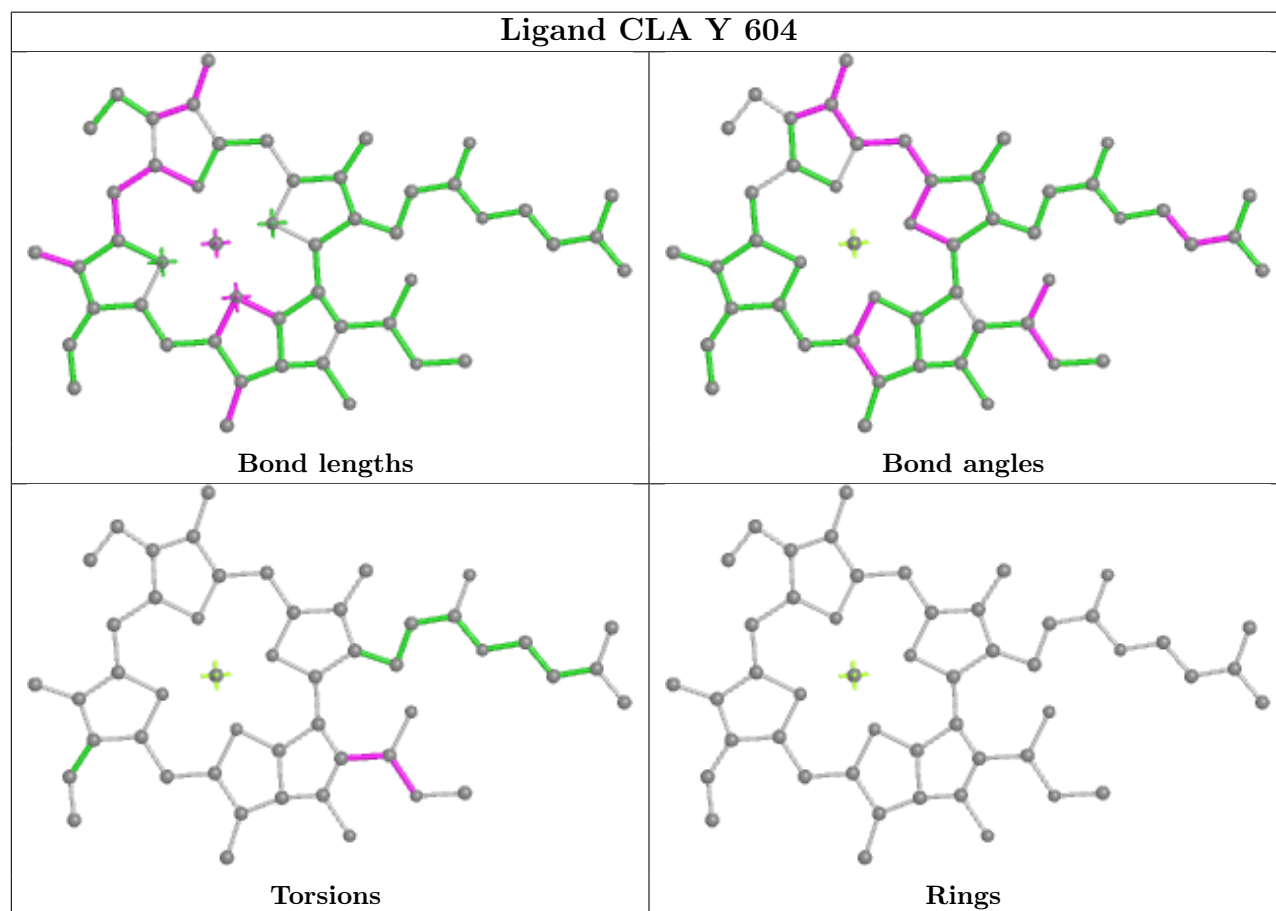
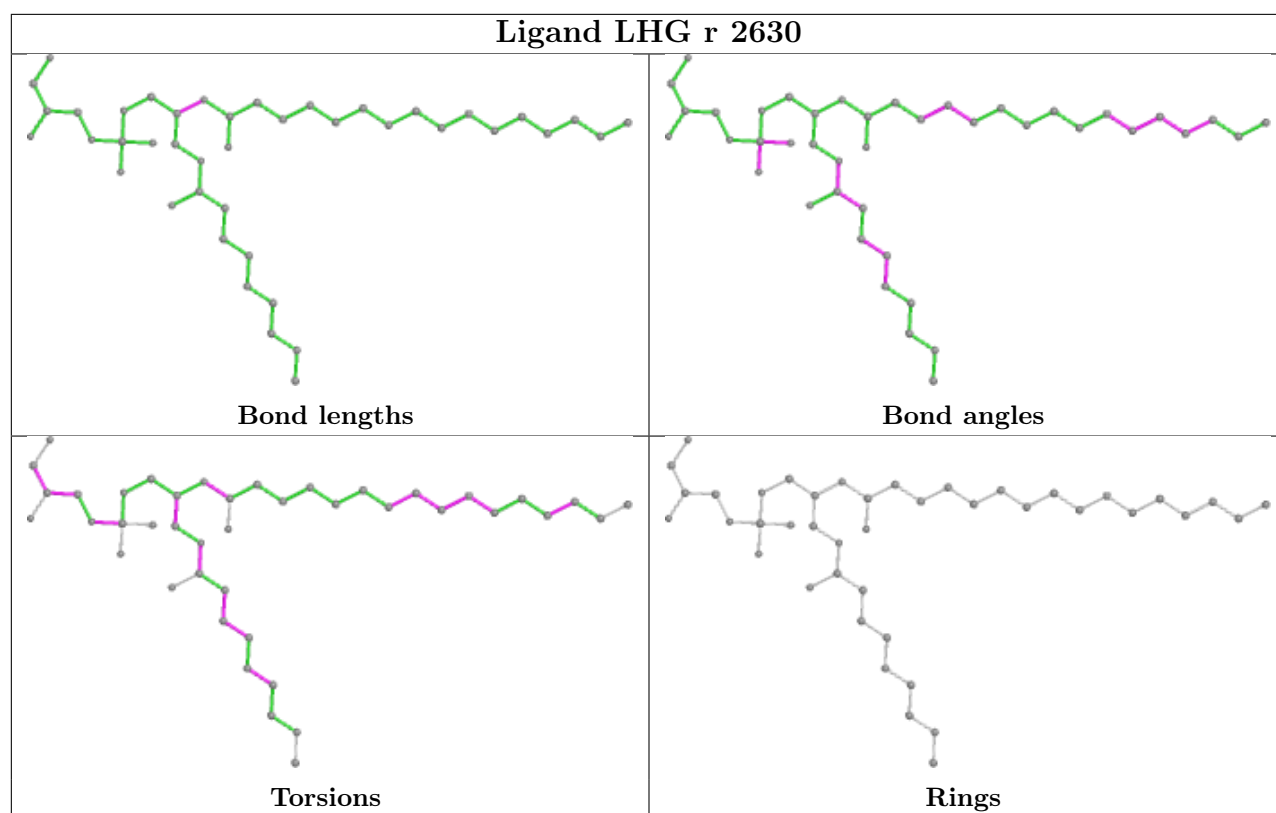
Bond angles

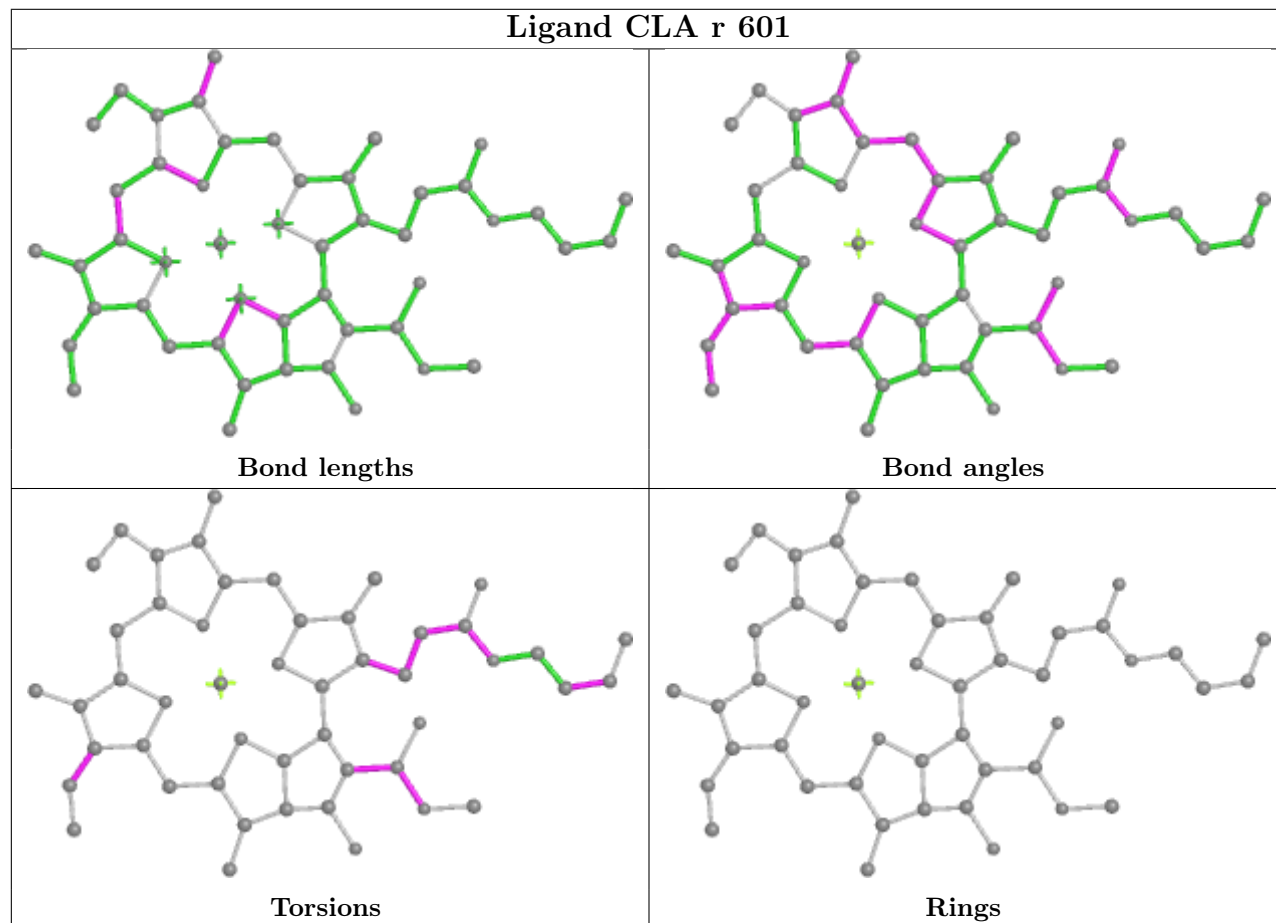
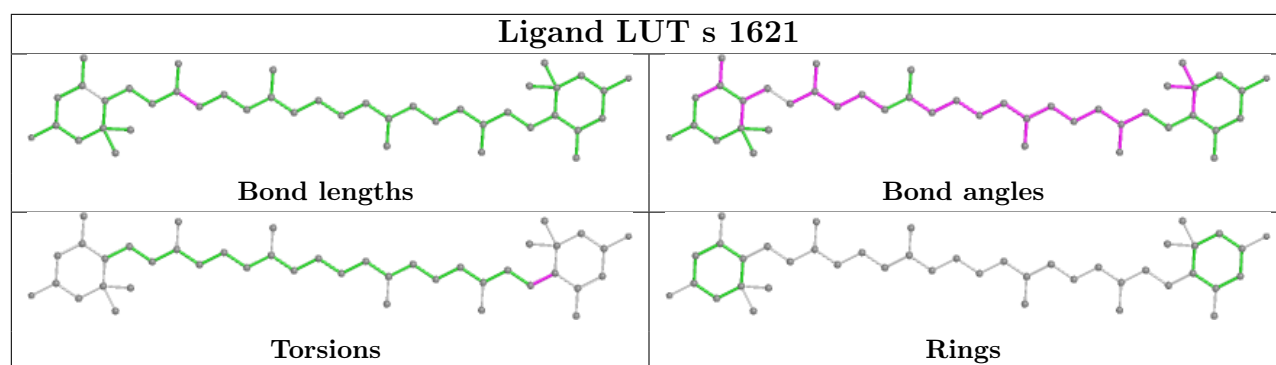


Torsions

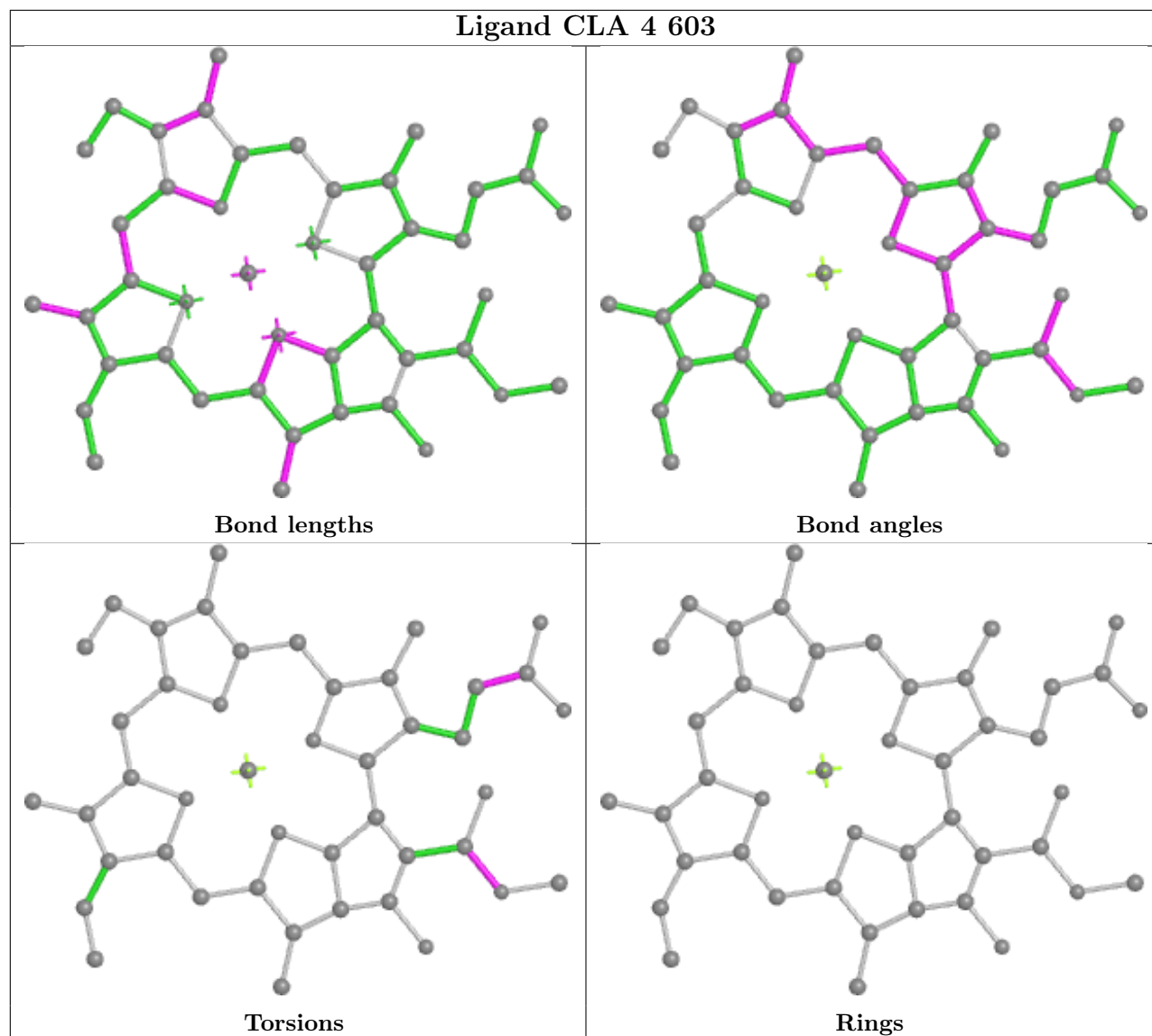


Rings

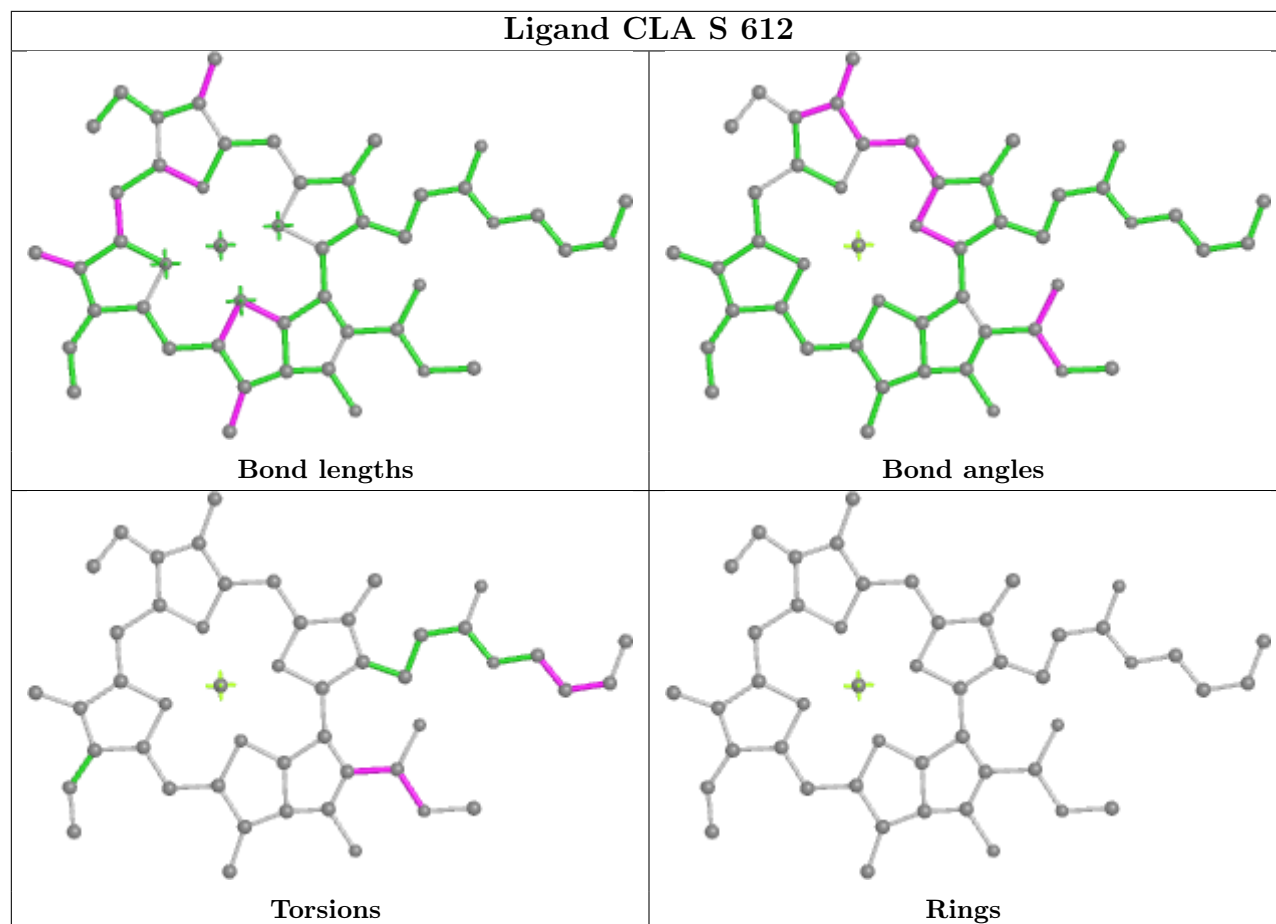


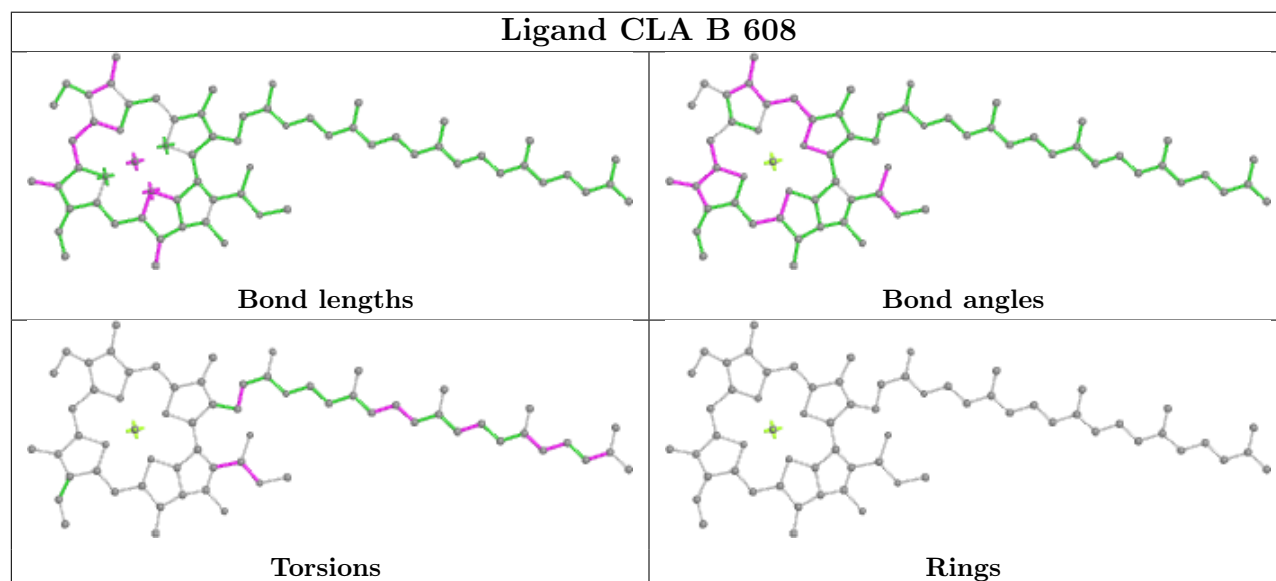
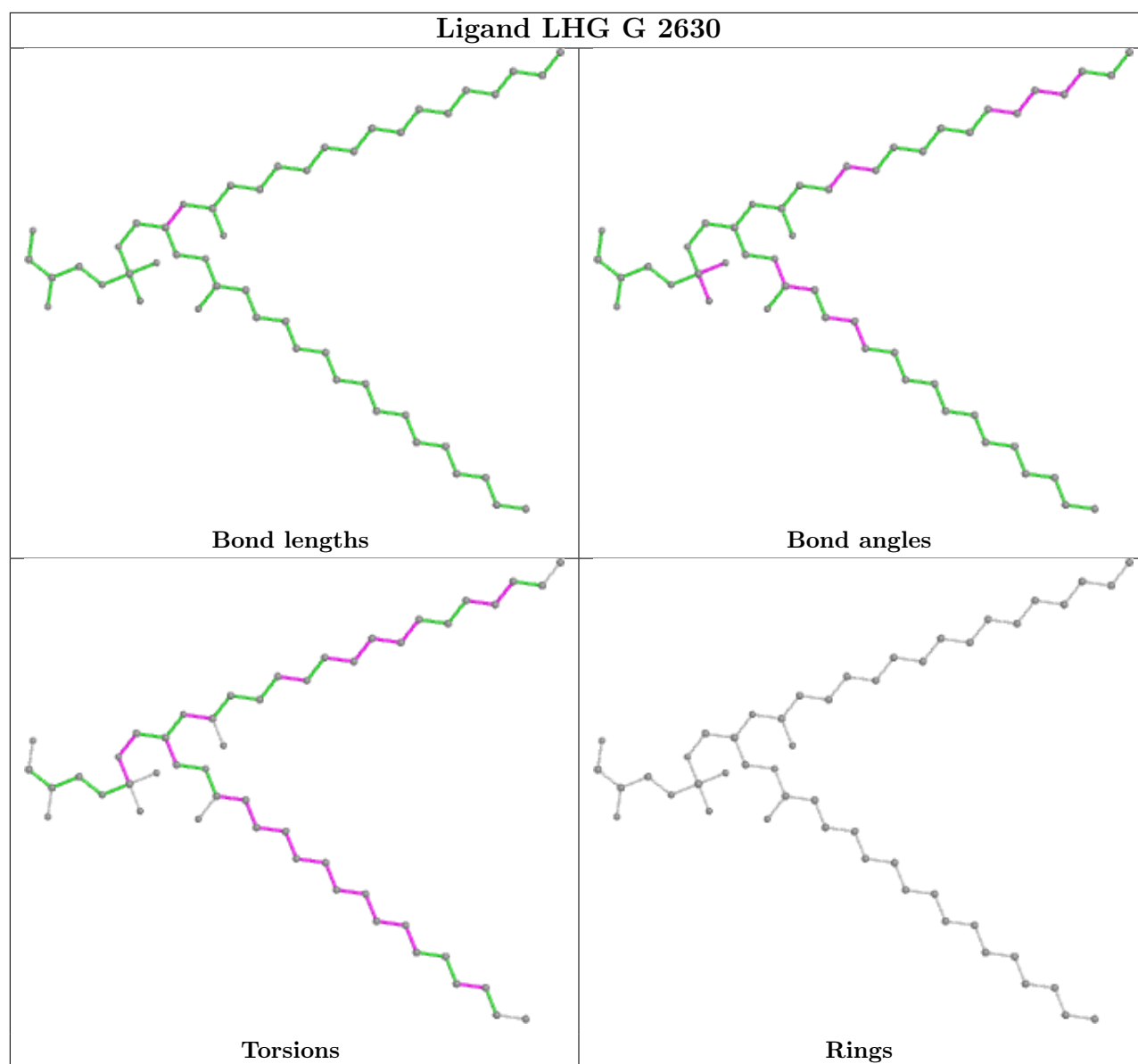


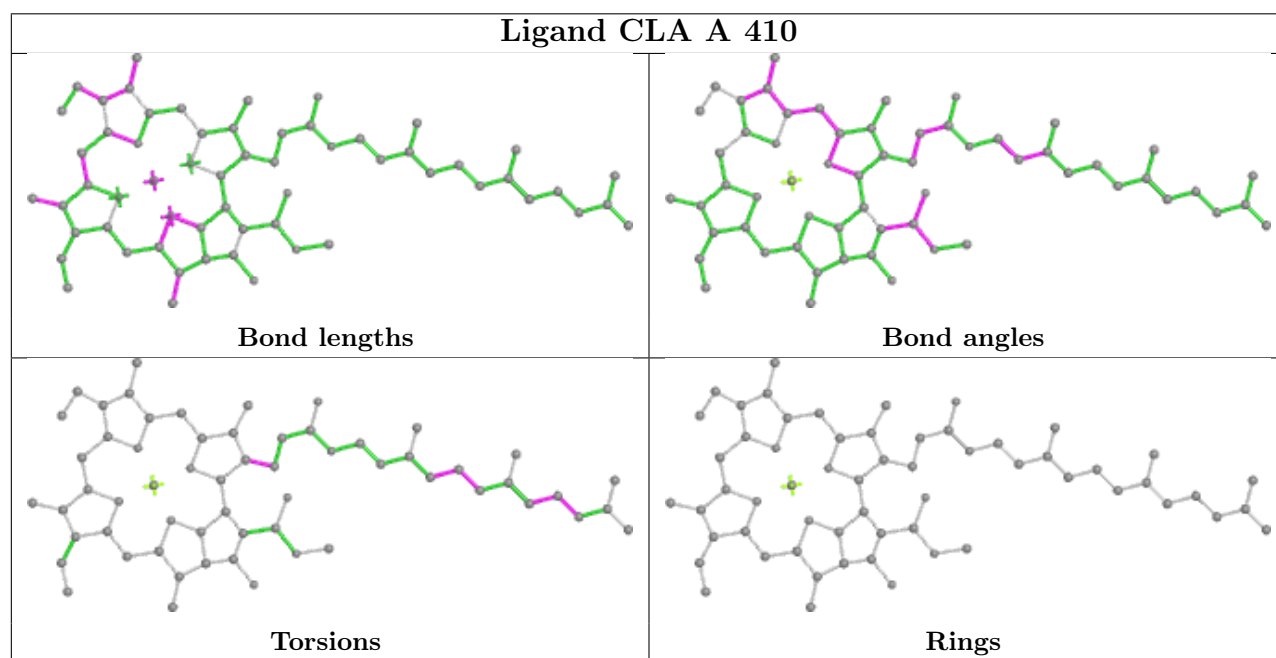
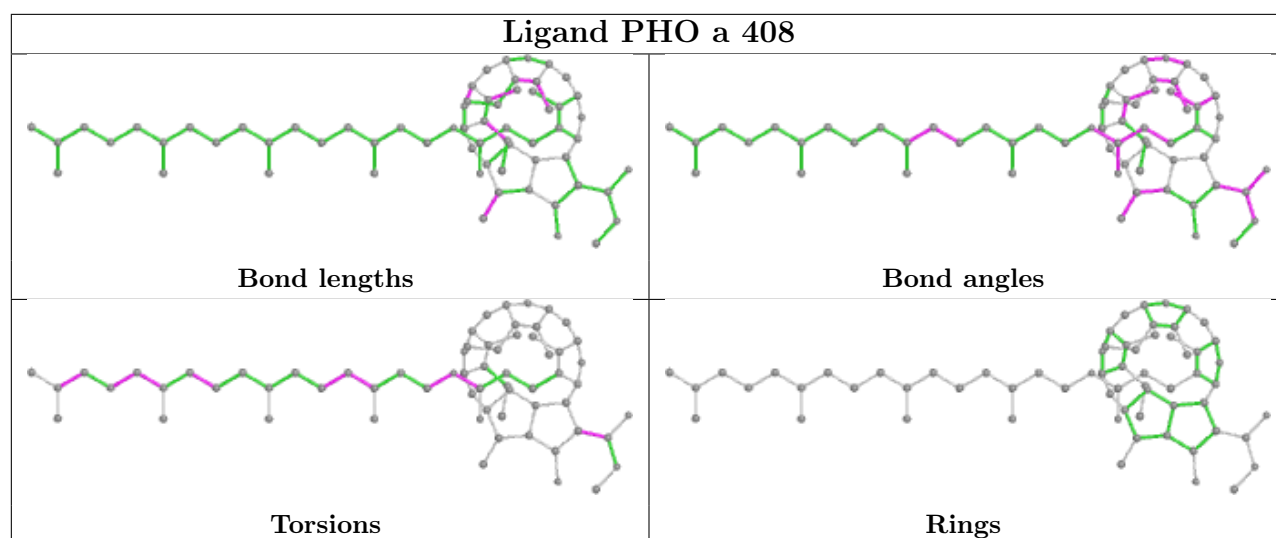
Ligand CLA 4 603



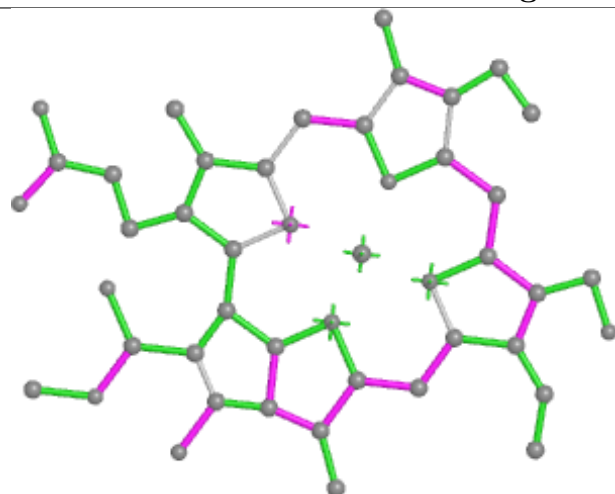
Ligand CLA S 612



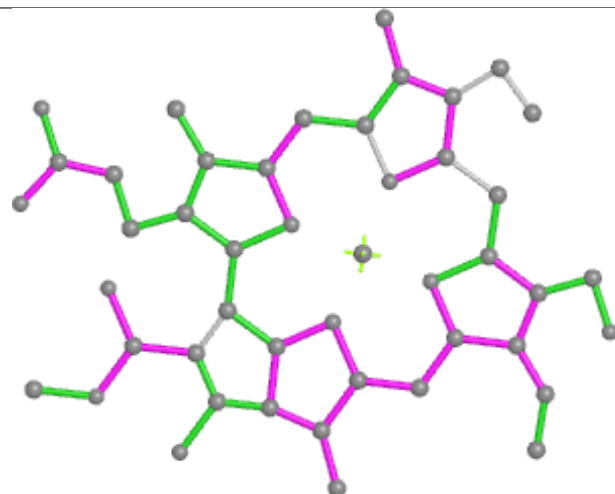




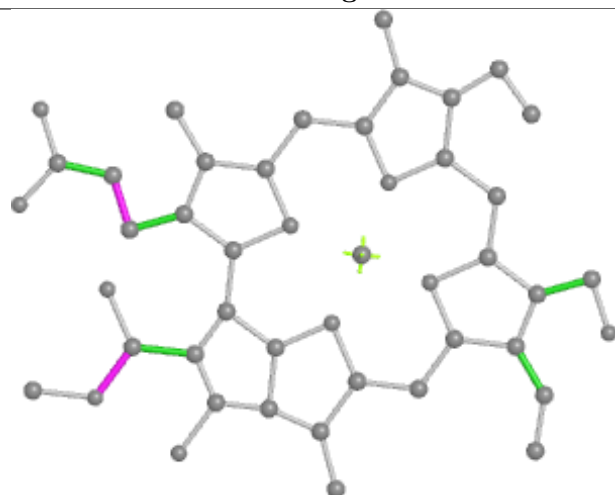
Ligand CHL 3 608



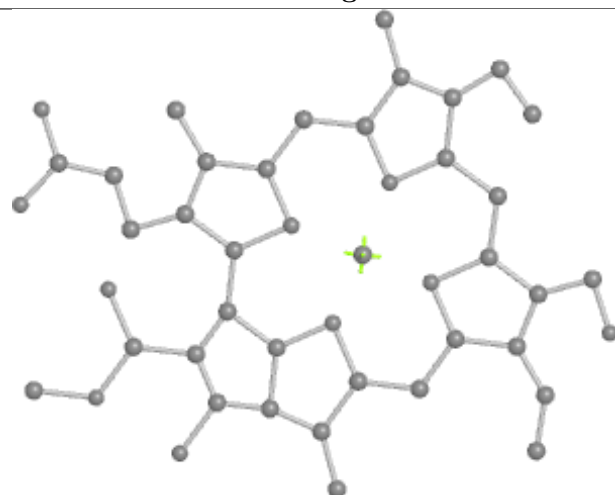
Bond lengths



Bond angles

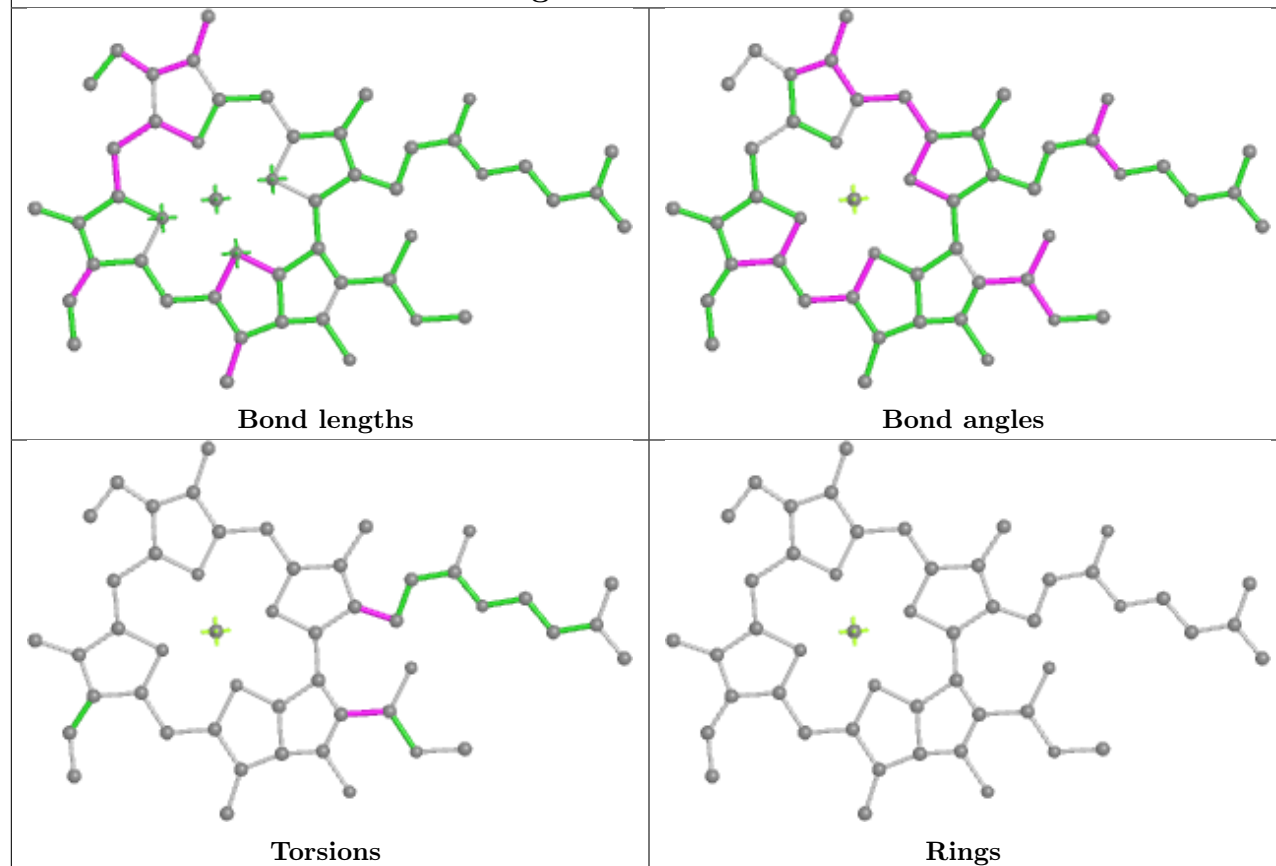


Torsions

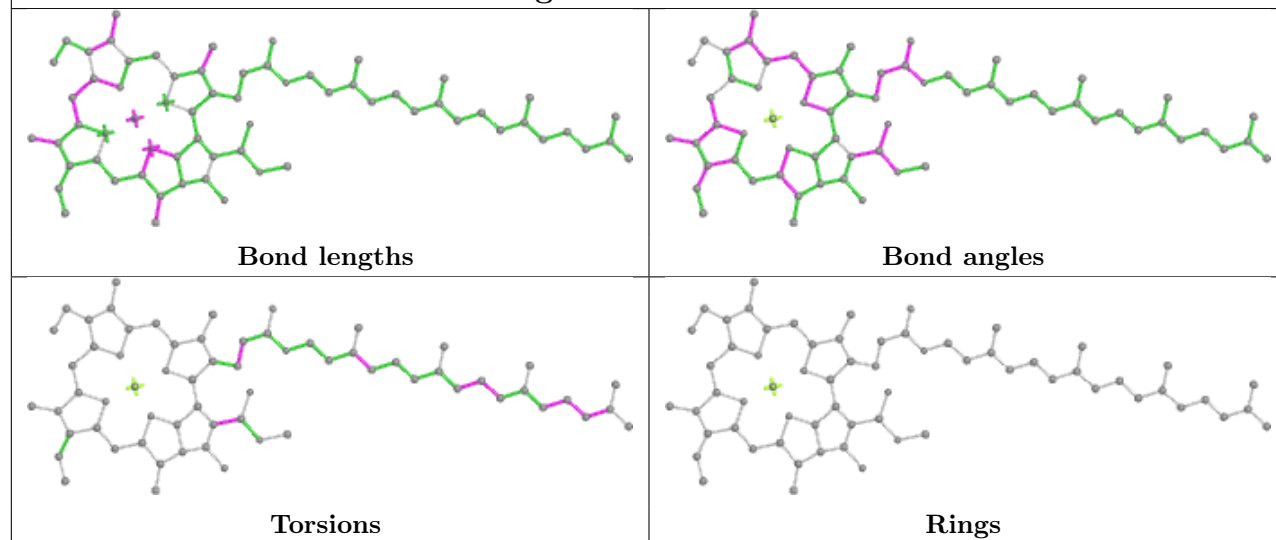


Rings

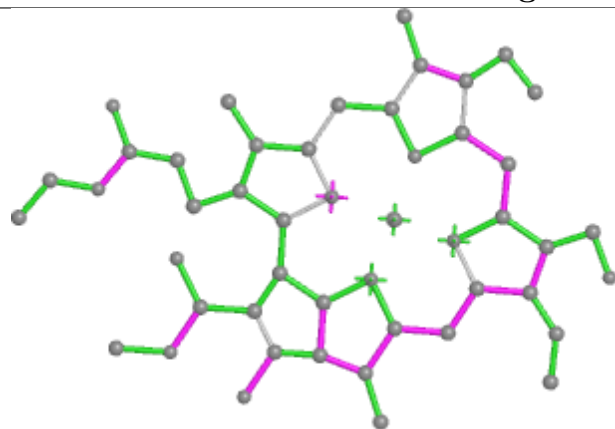
Ligand CLA A 407



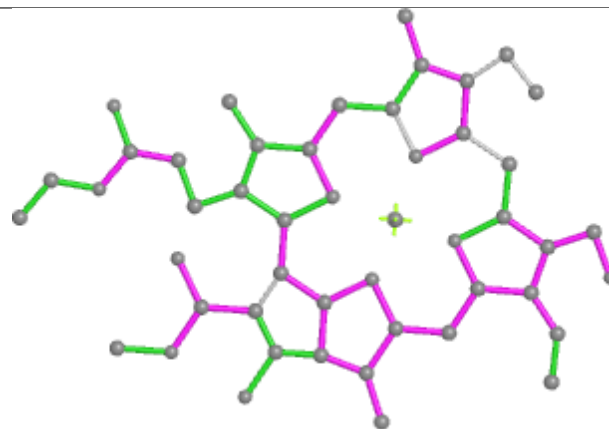
Ligand CLA b 607



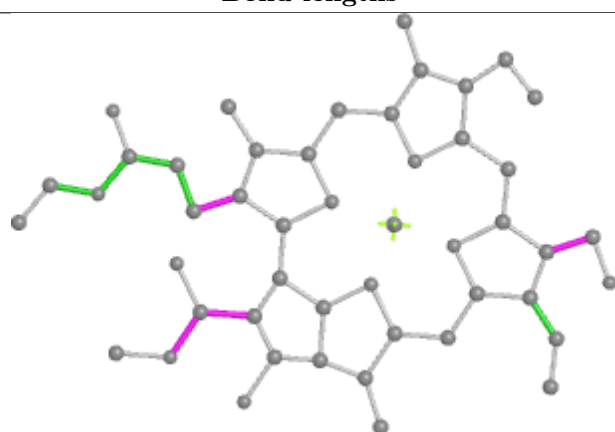
Ligand CHL n 605



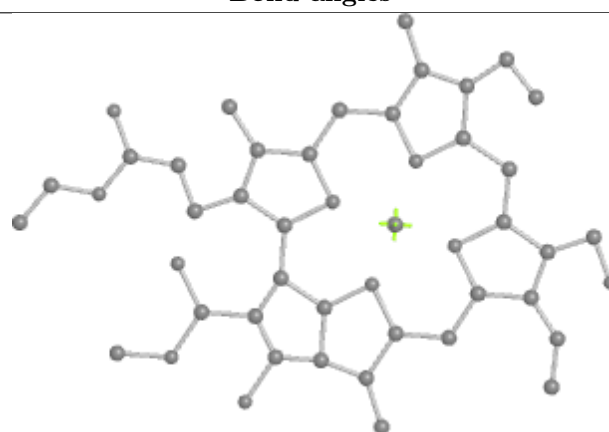
Bond lengths



Bond angles

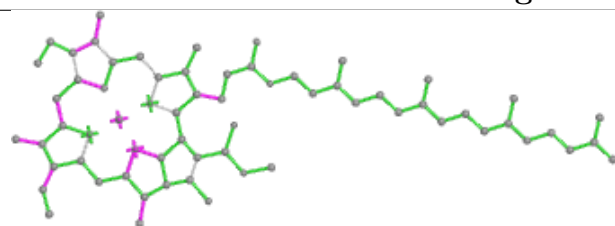


Torsions

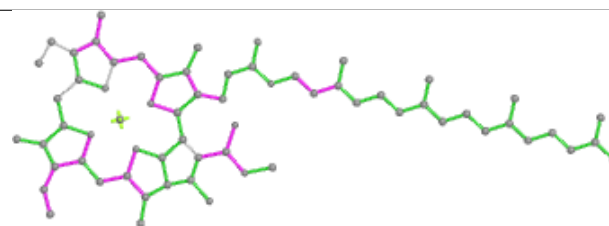


Rings

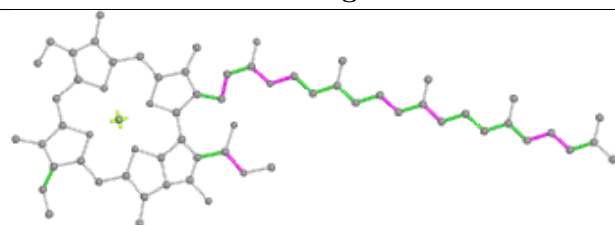
Ligand CLA G 603



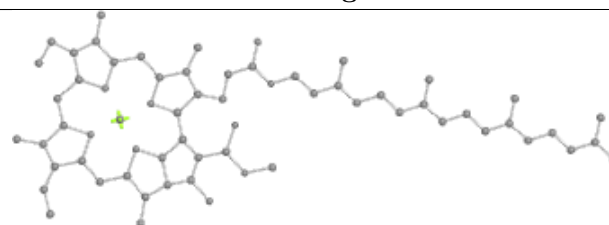
Bond lengths



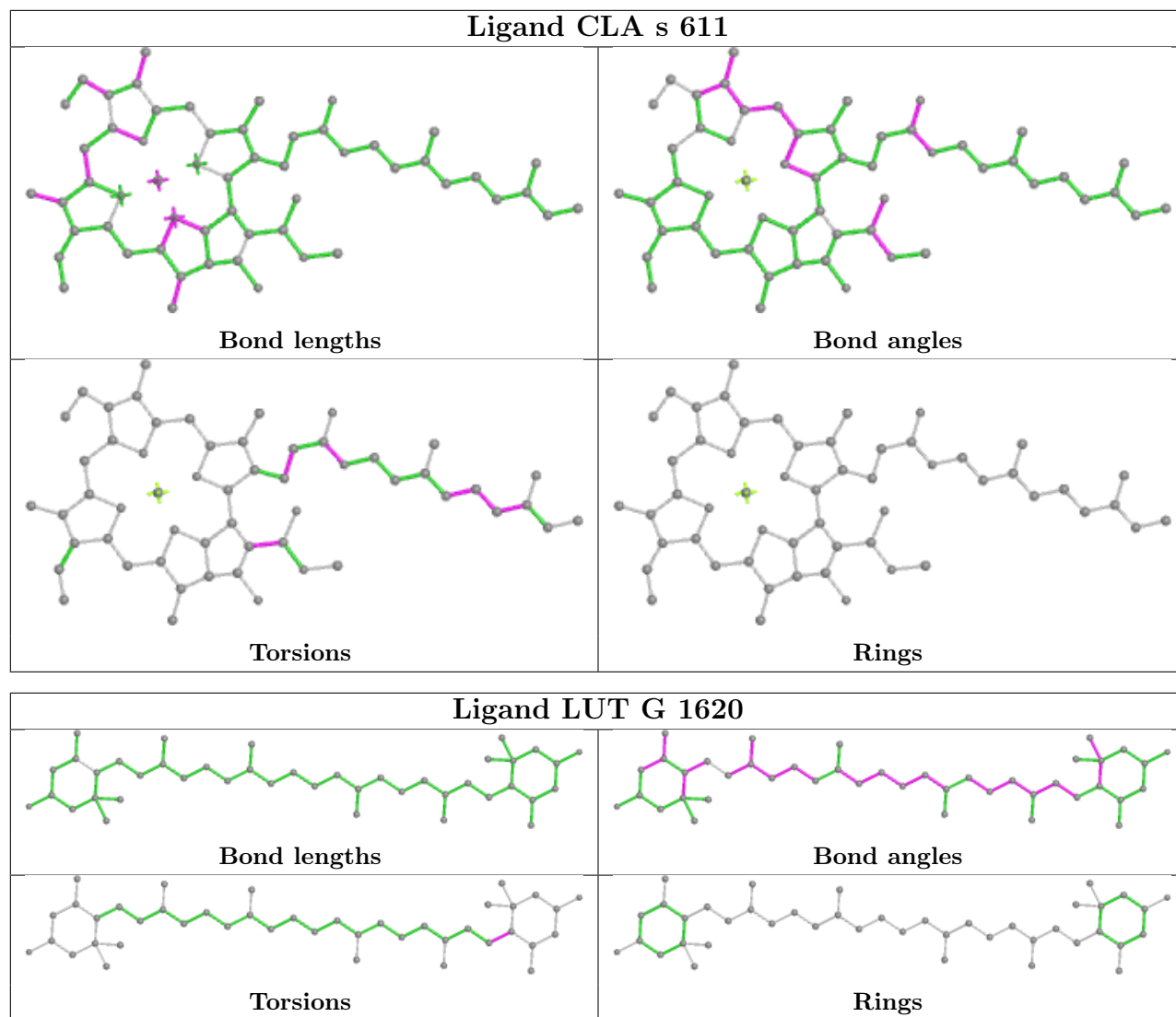
Bond angles

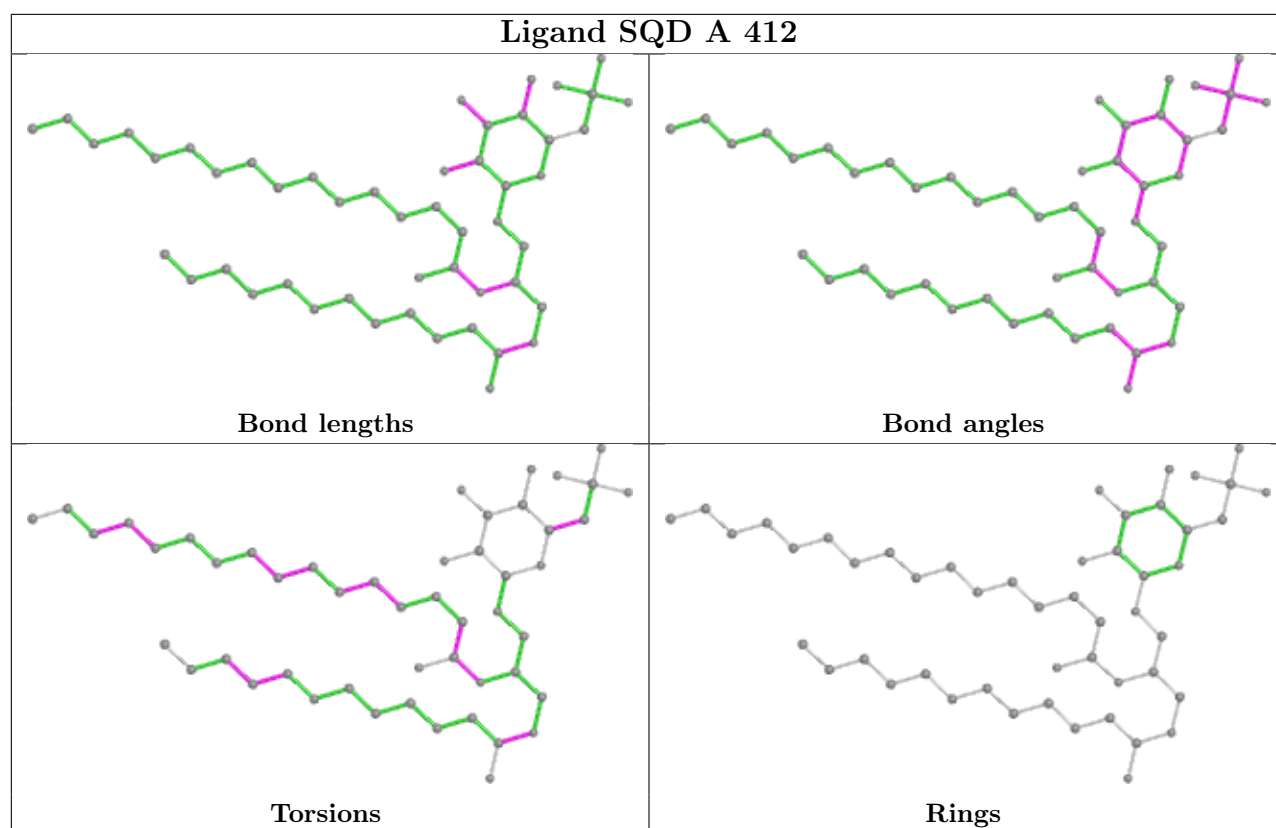


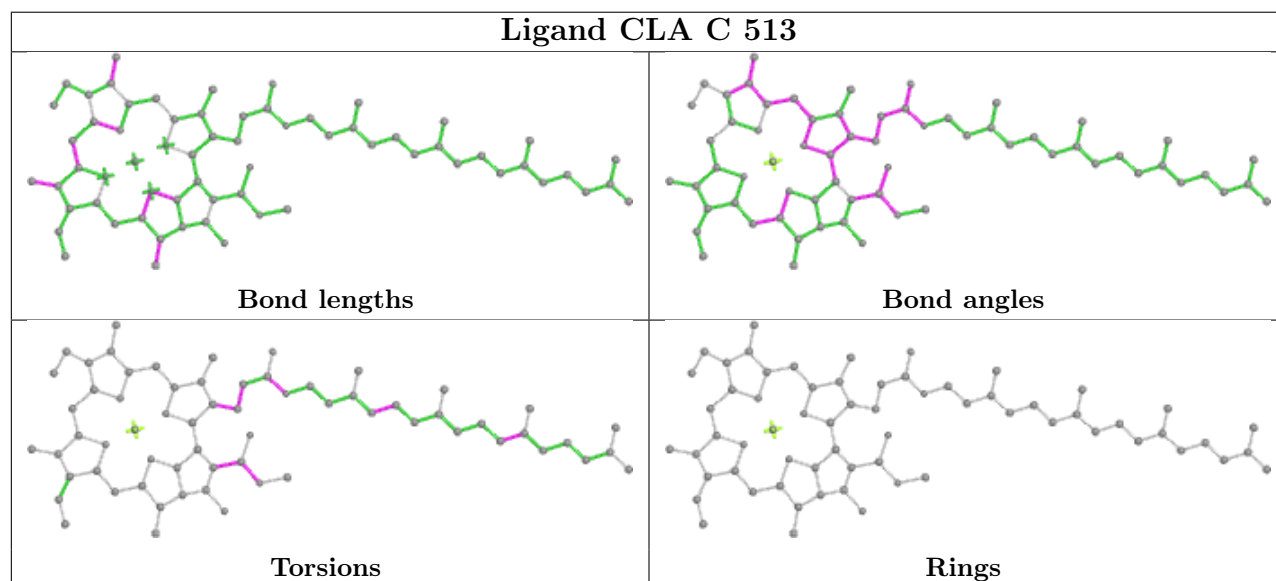
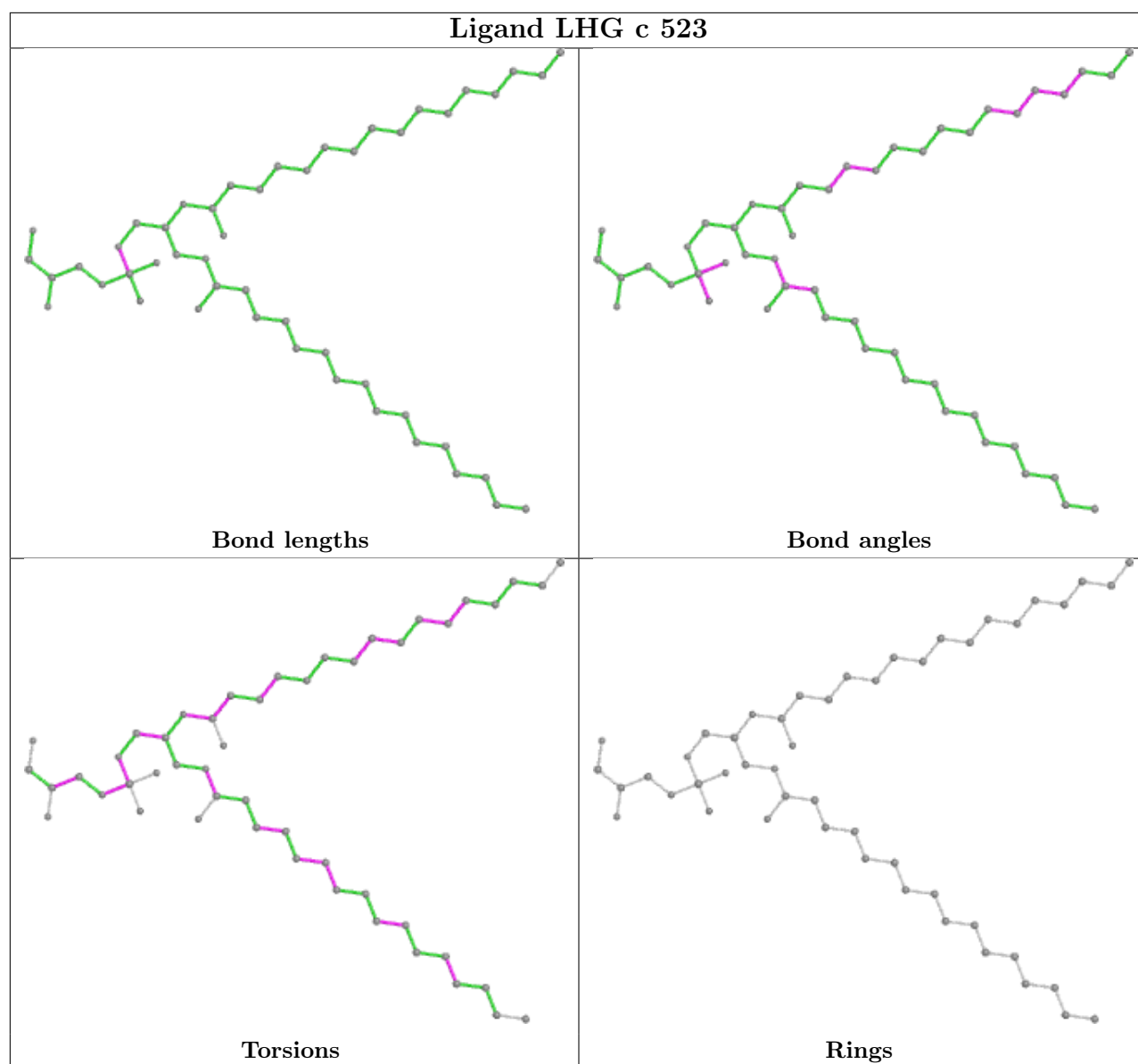
Torsions



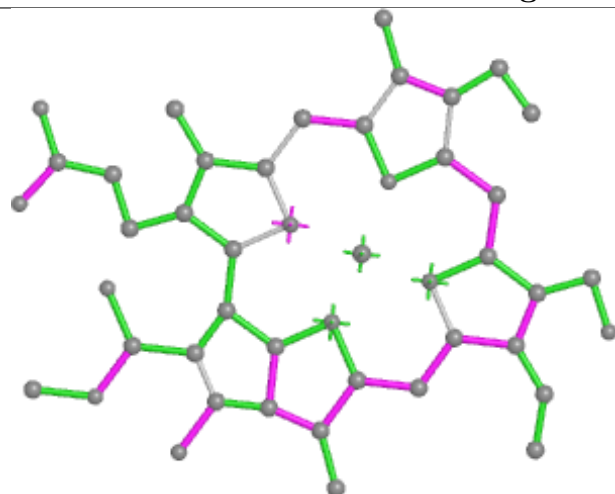
Rings



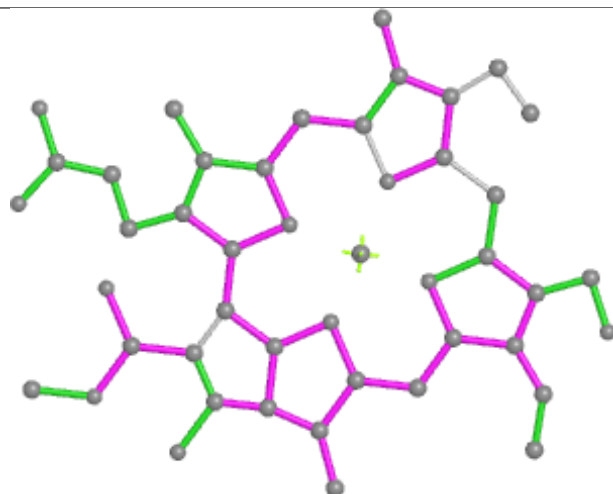




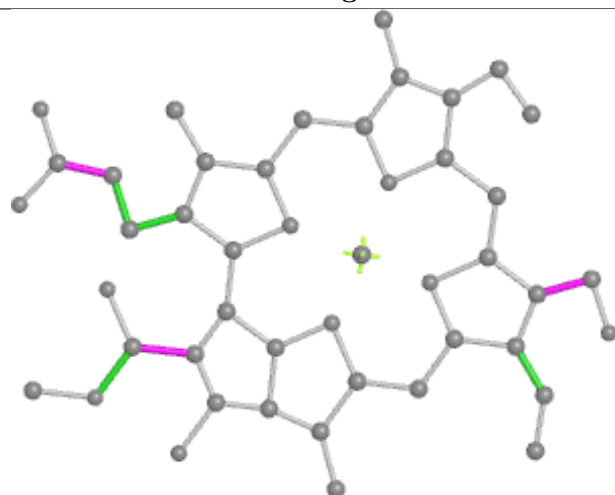
Ligand CHL 5 601



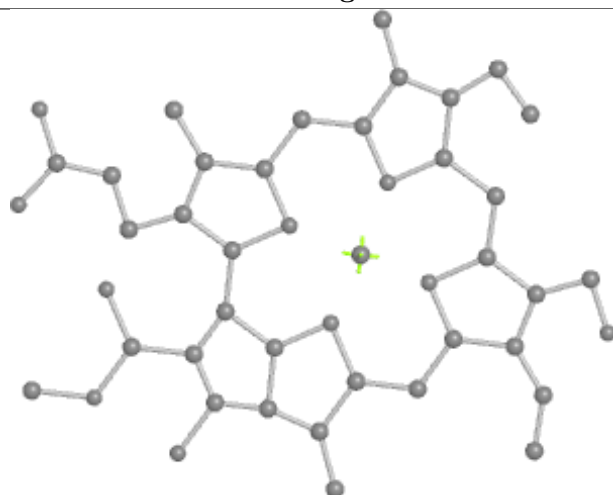
Bond lengths



Bond angles

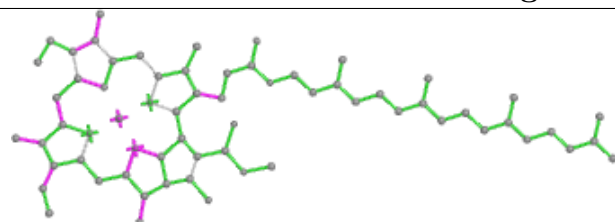


Torsions

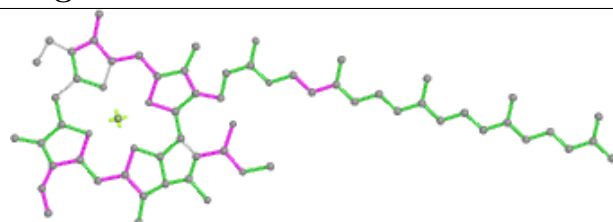


Rings

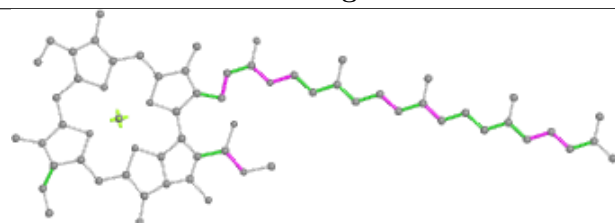
Ligand CLA g 603



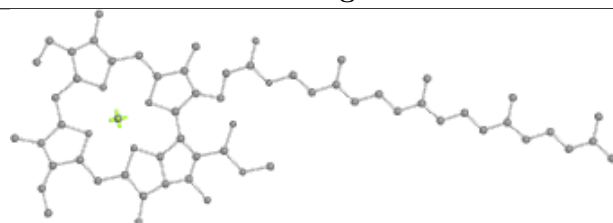
Bond lengths



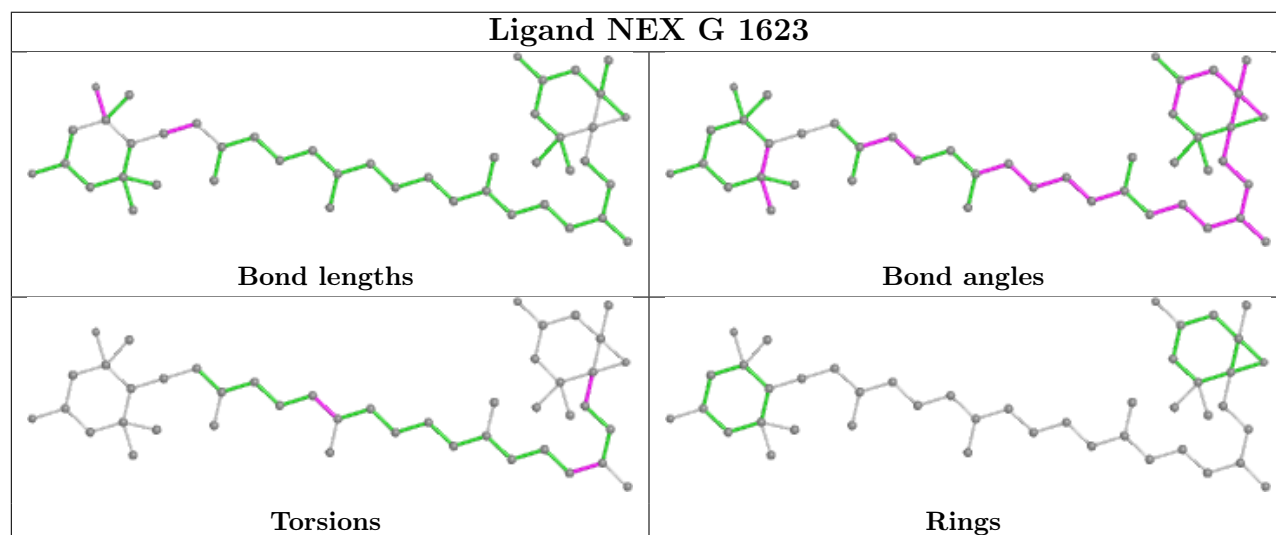
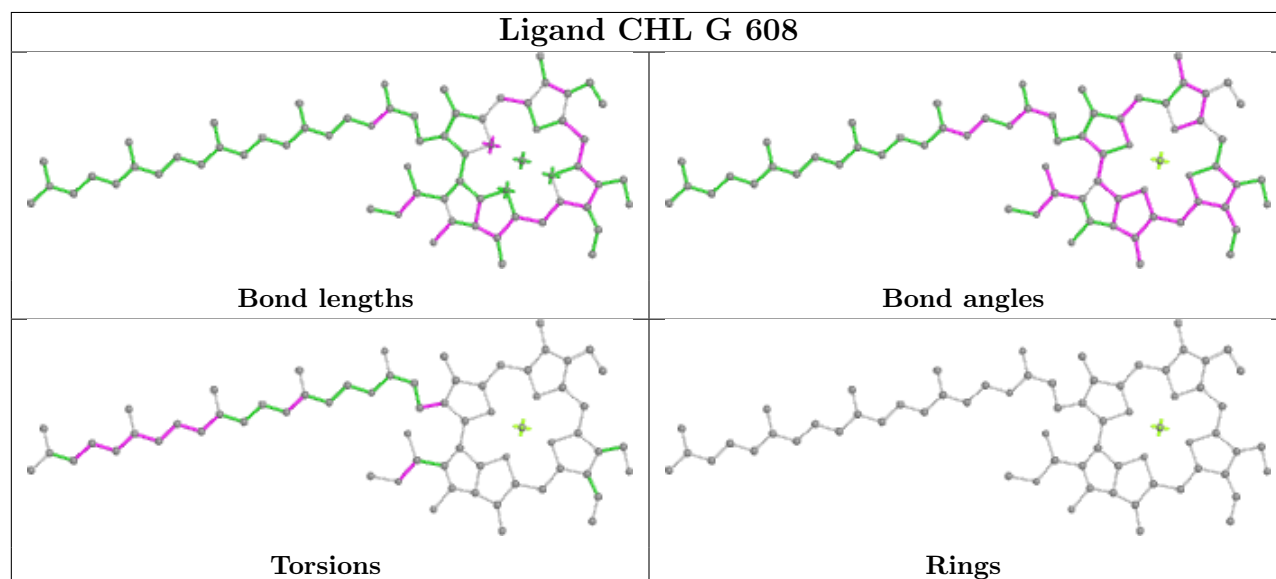
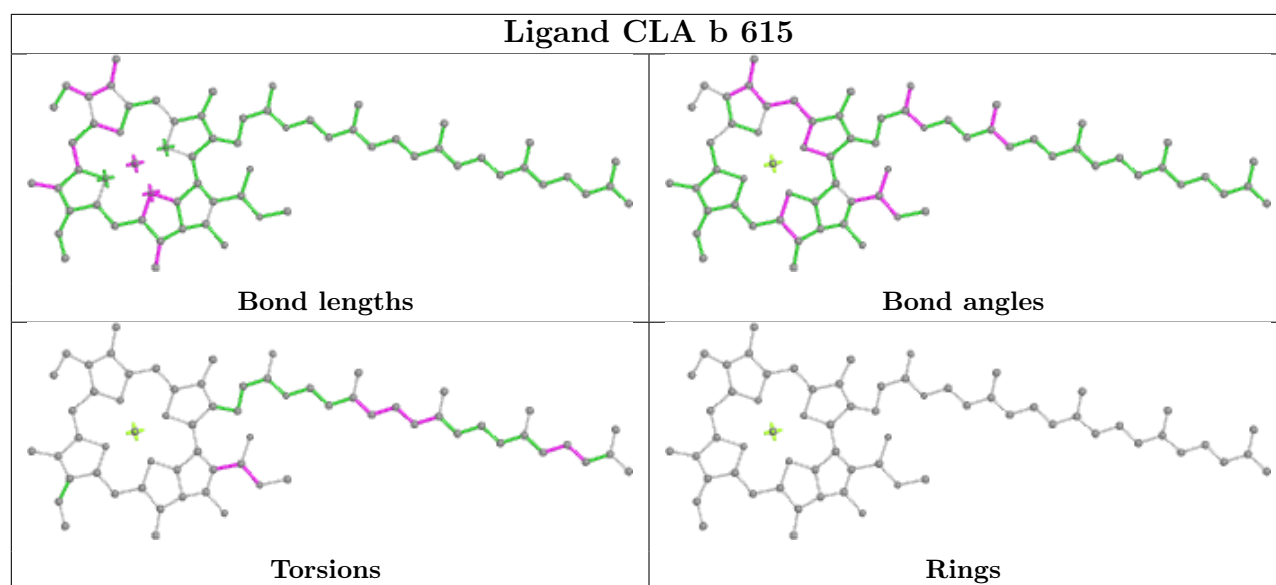
Bond angles



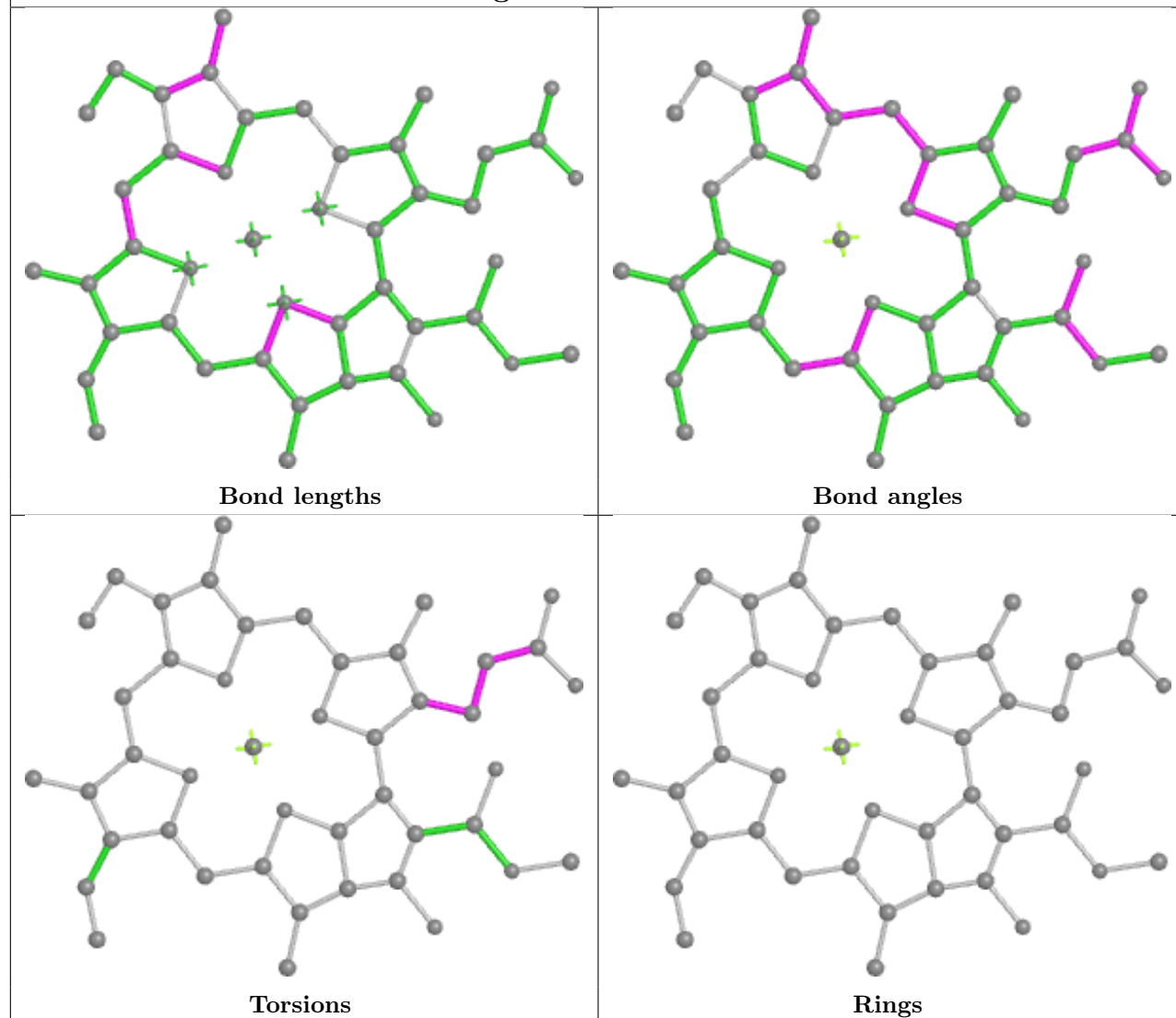
Torsions



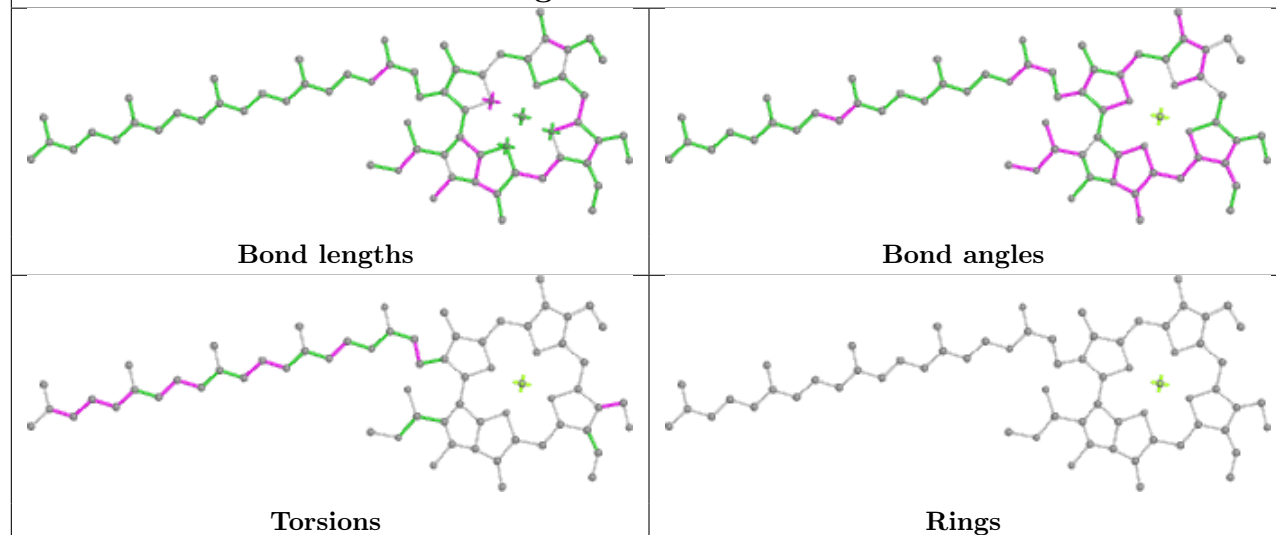
Rings

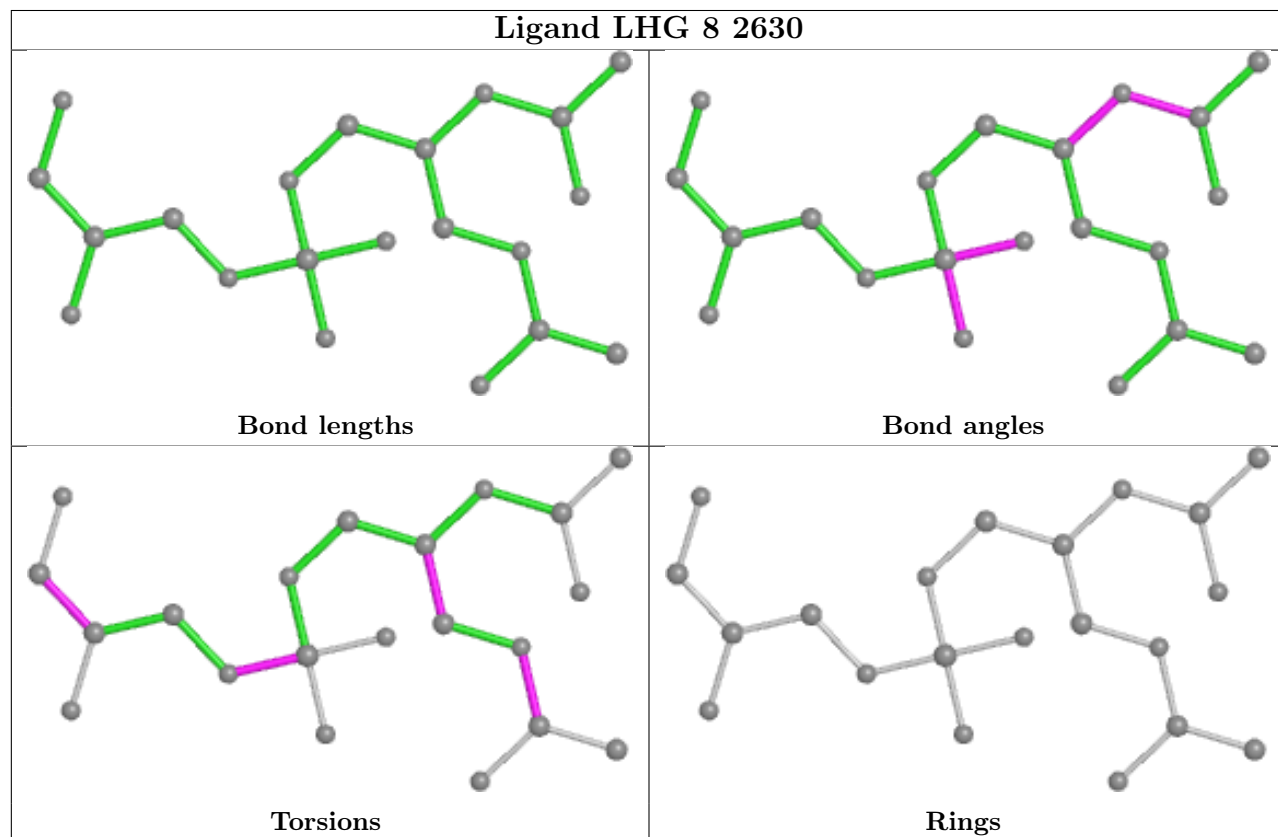
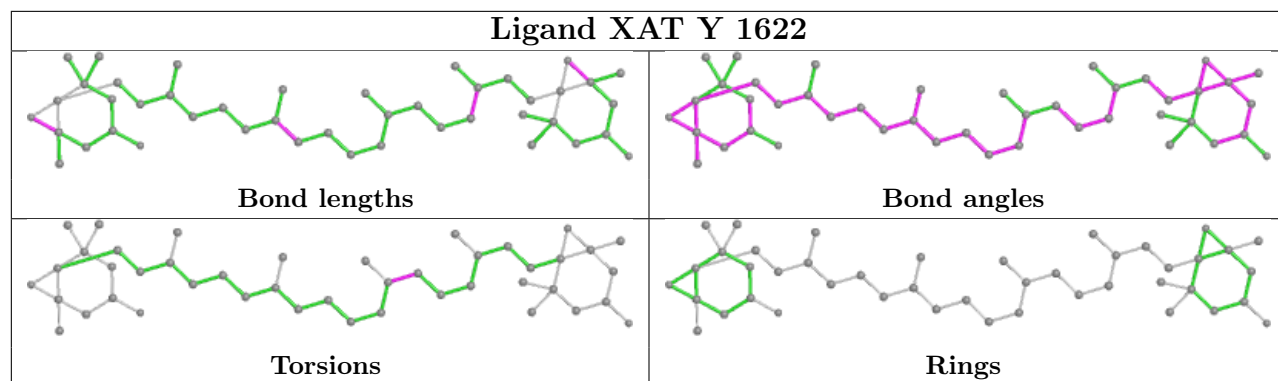


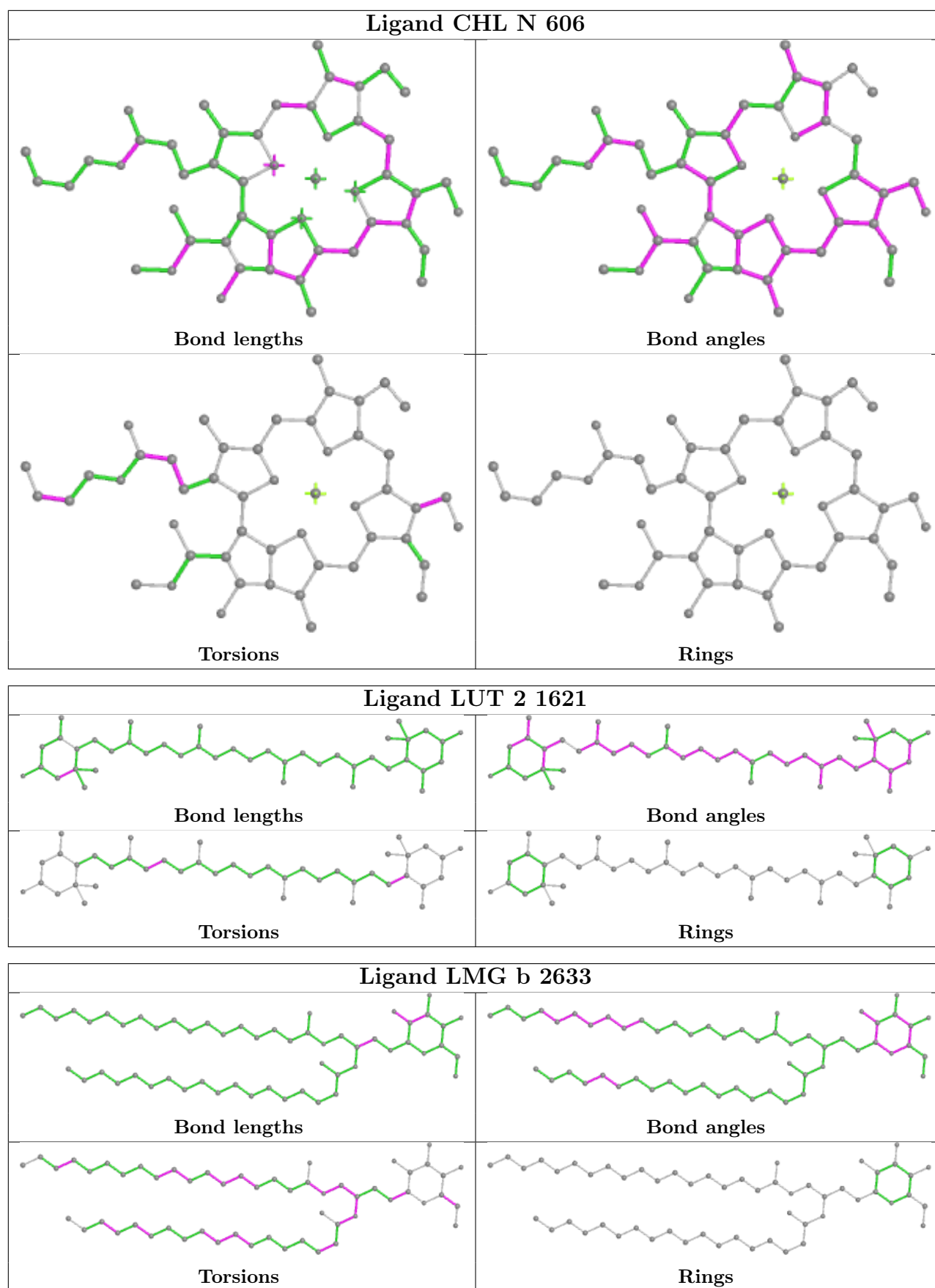
Ligand CLA S 609



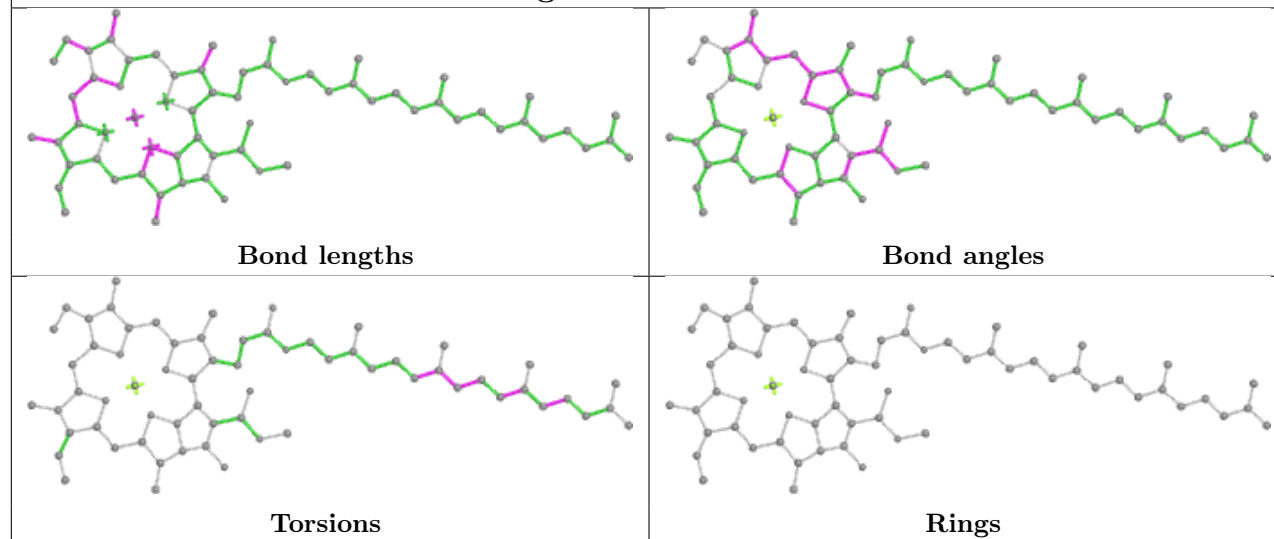
Ligand CHL n 607



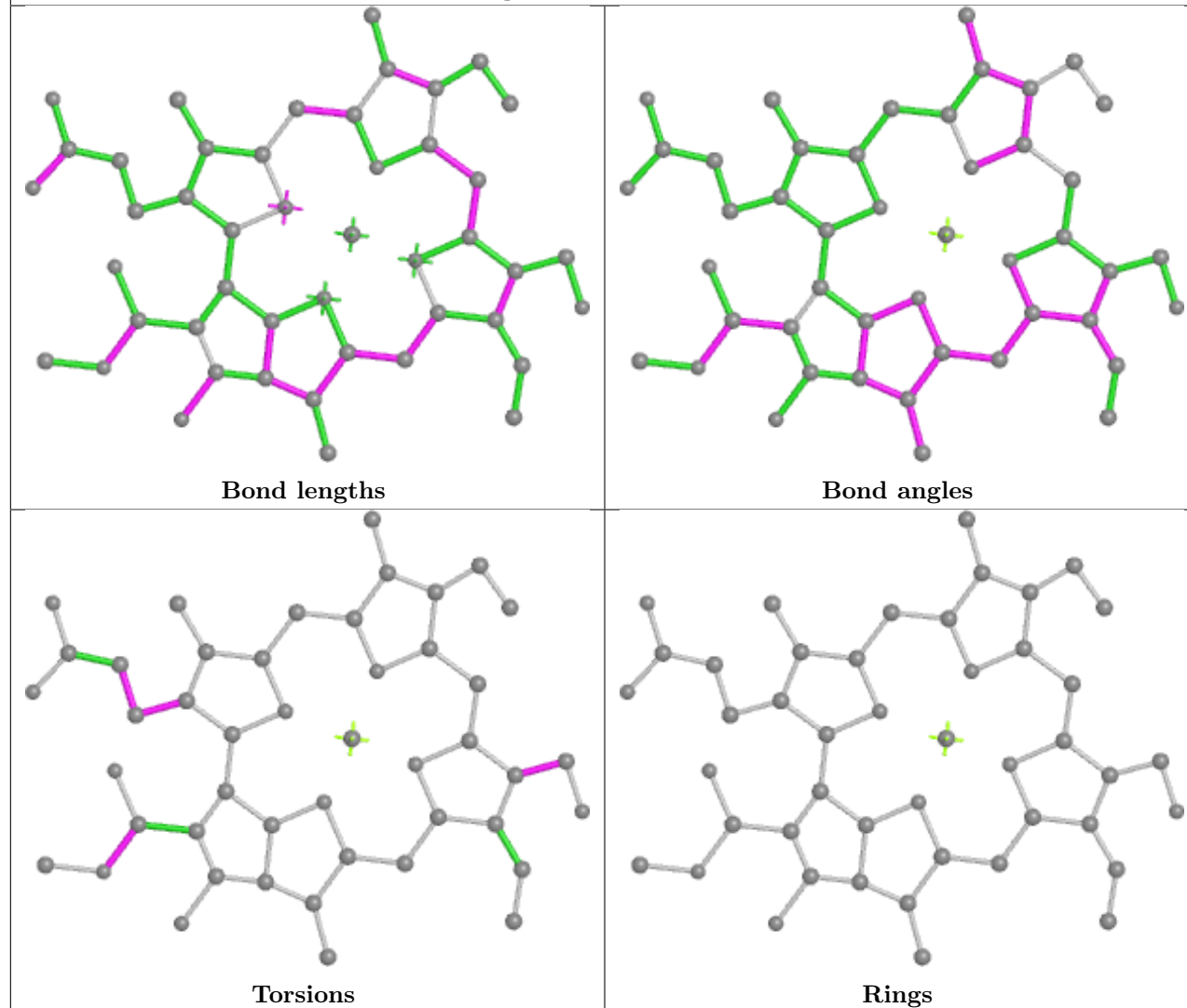


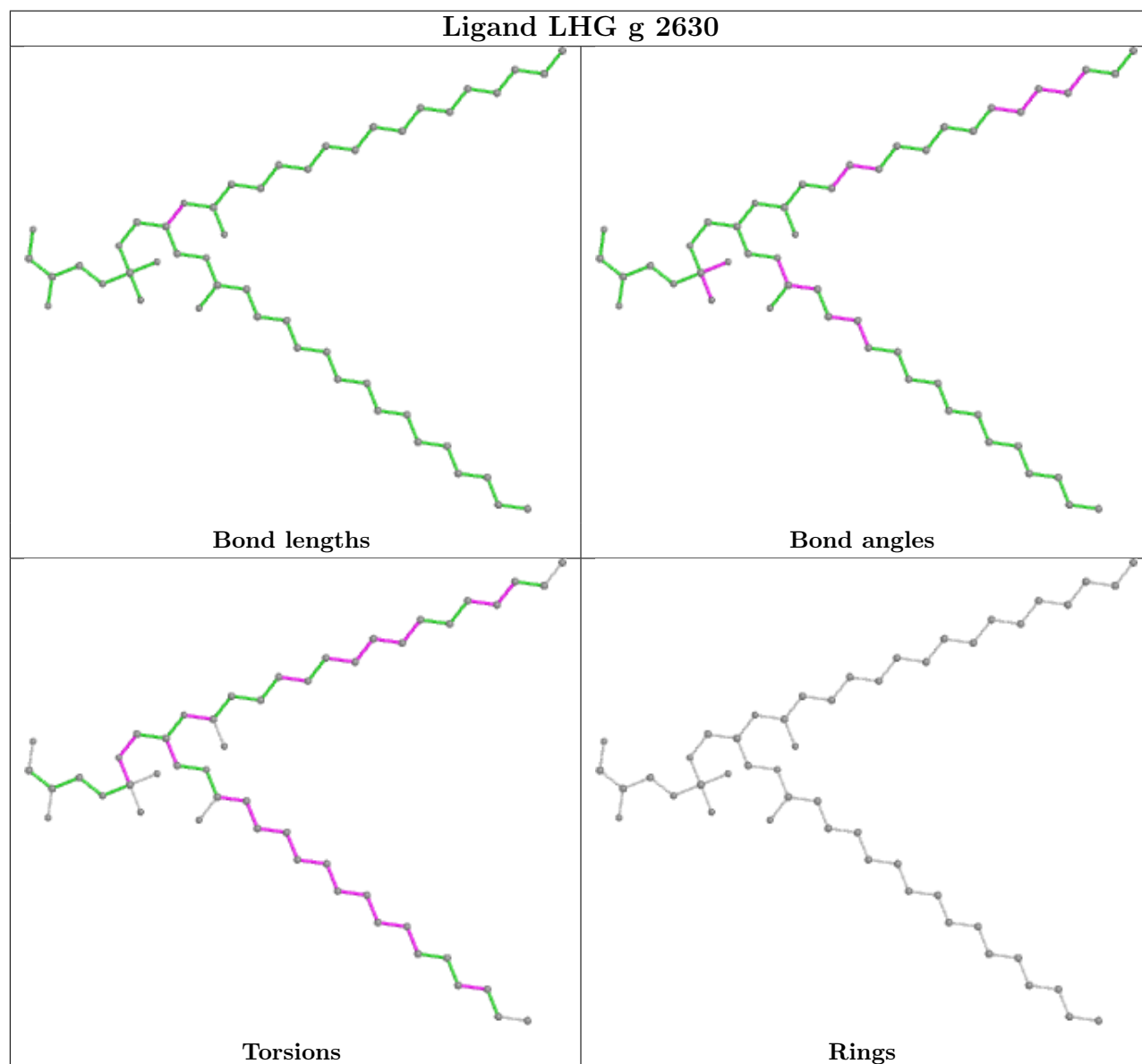
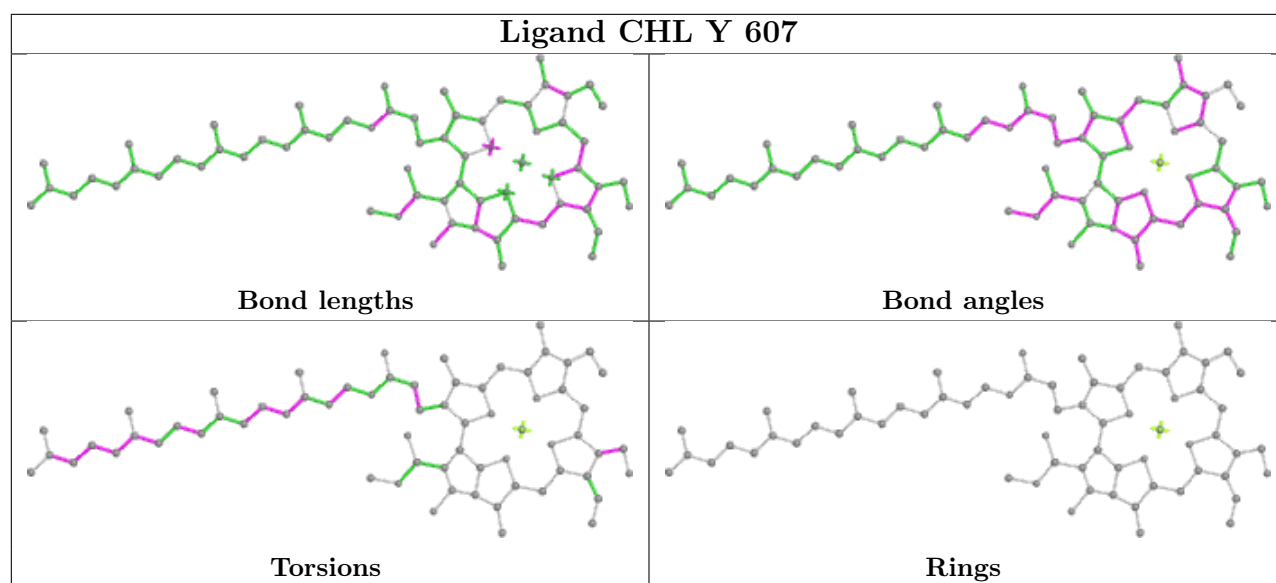


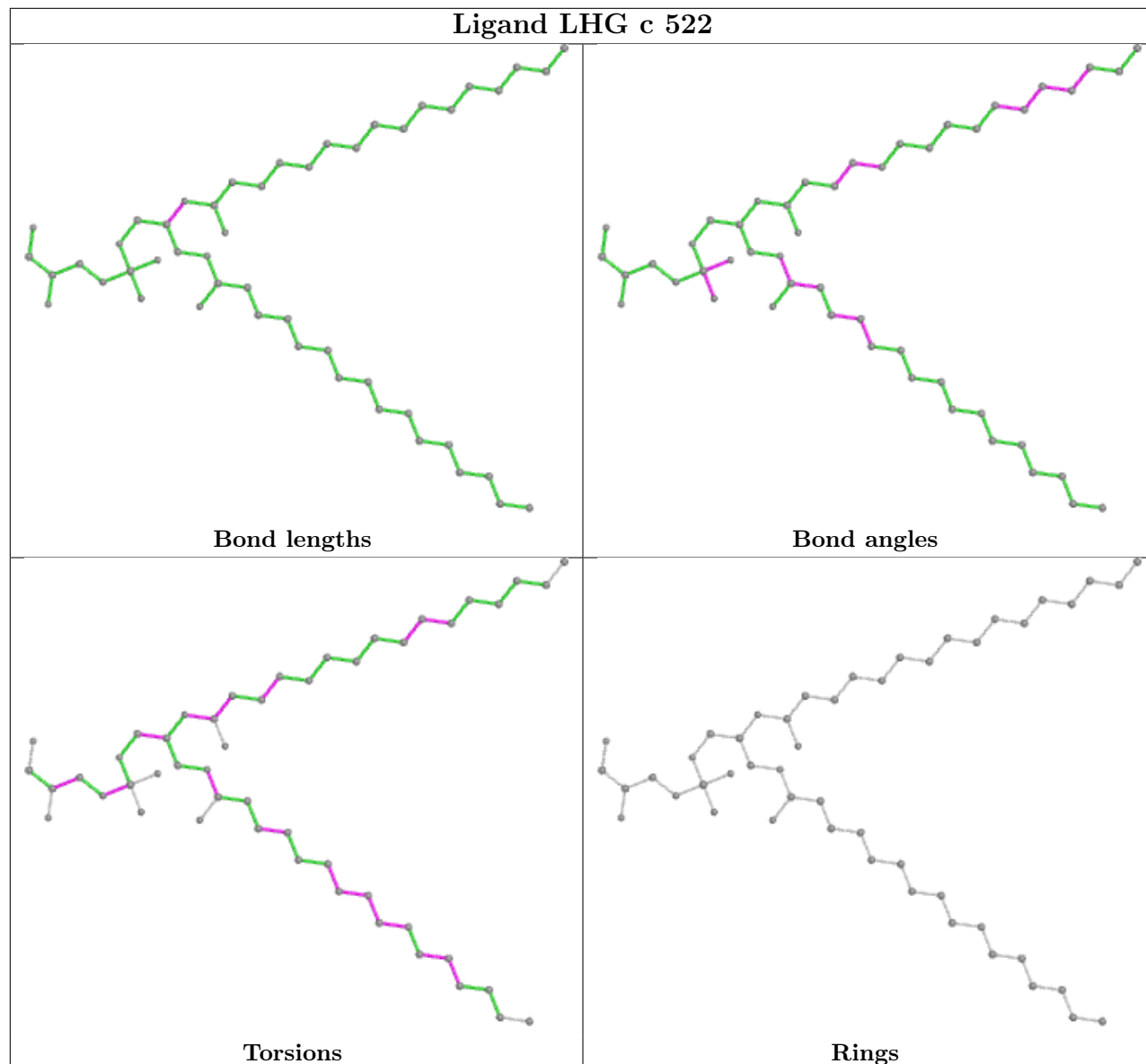
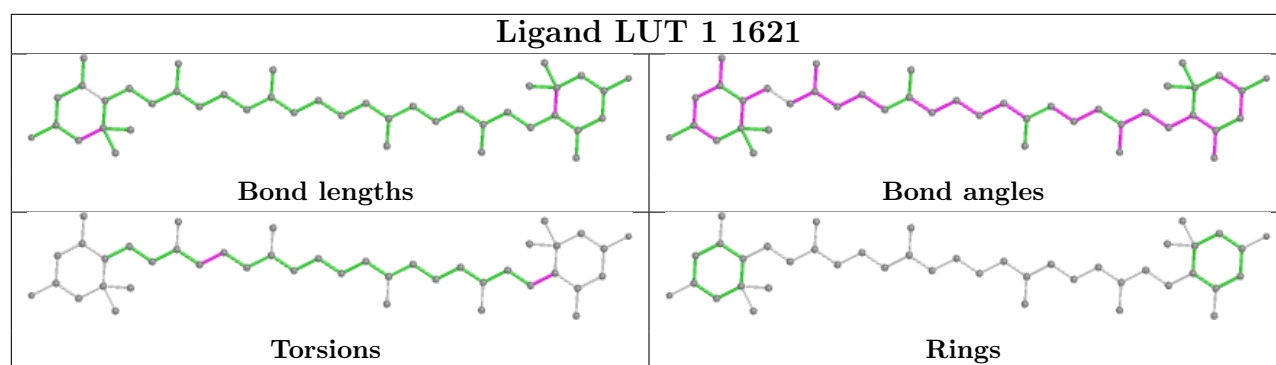
Ligand CLA c 509

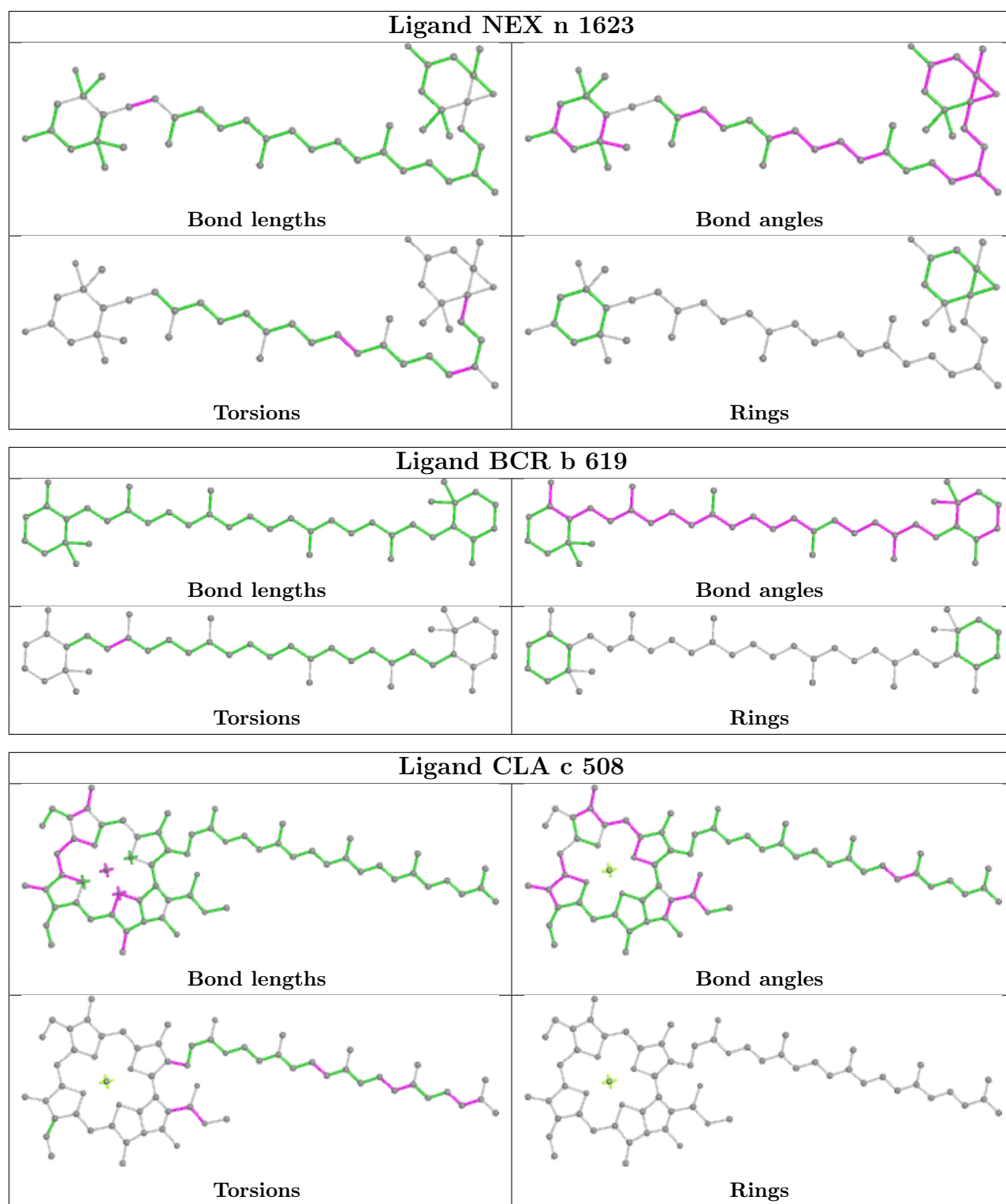


Ligand CHL 5 608

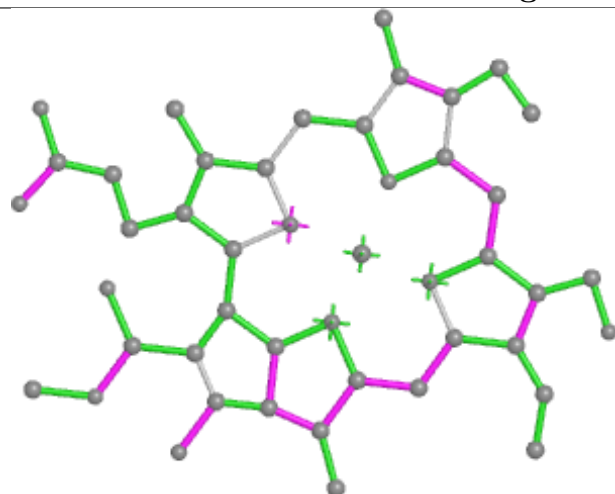




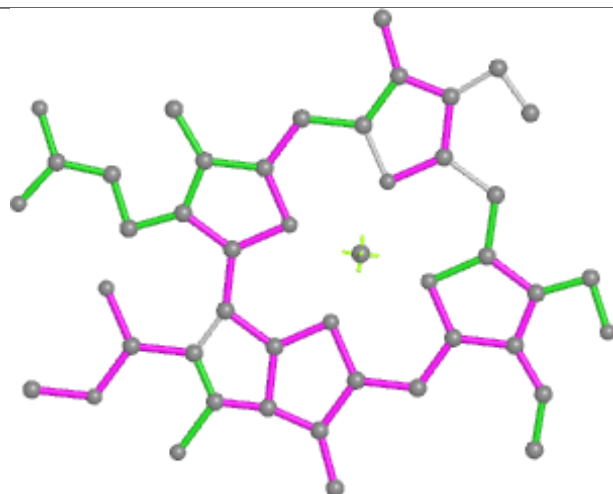




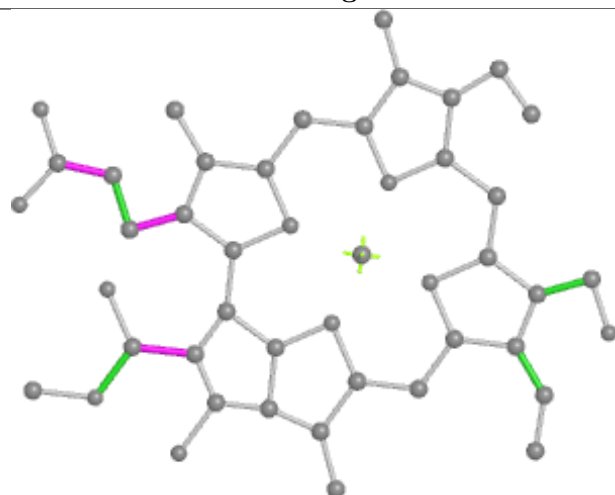
Ligand CHL 6 601



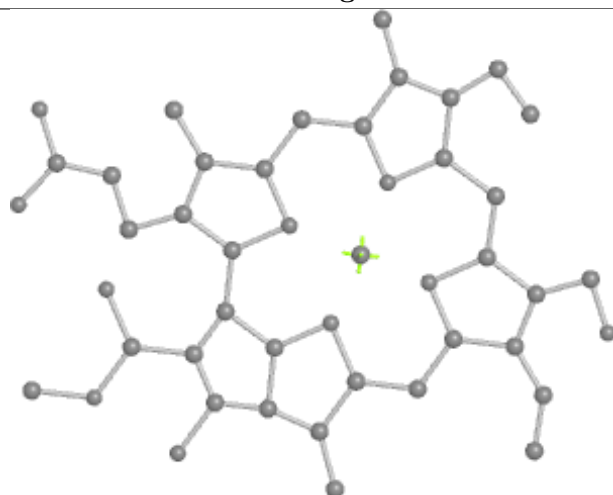
Bond lengths



Bond angles

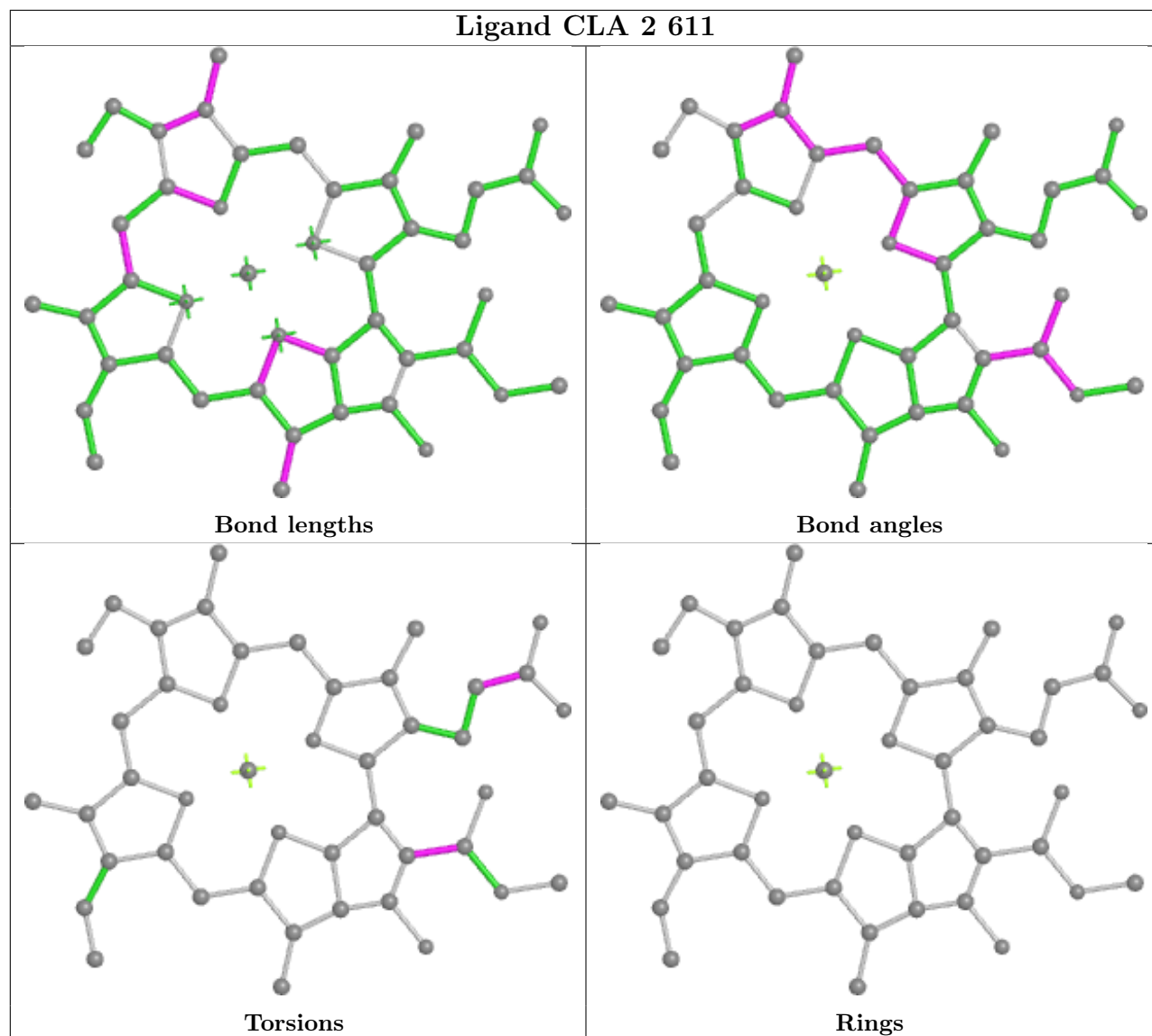


Torsions

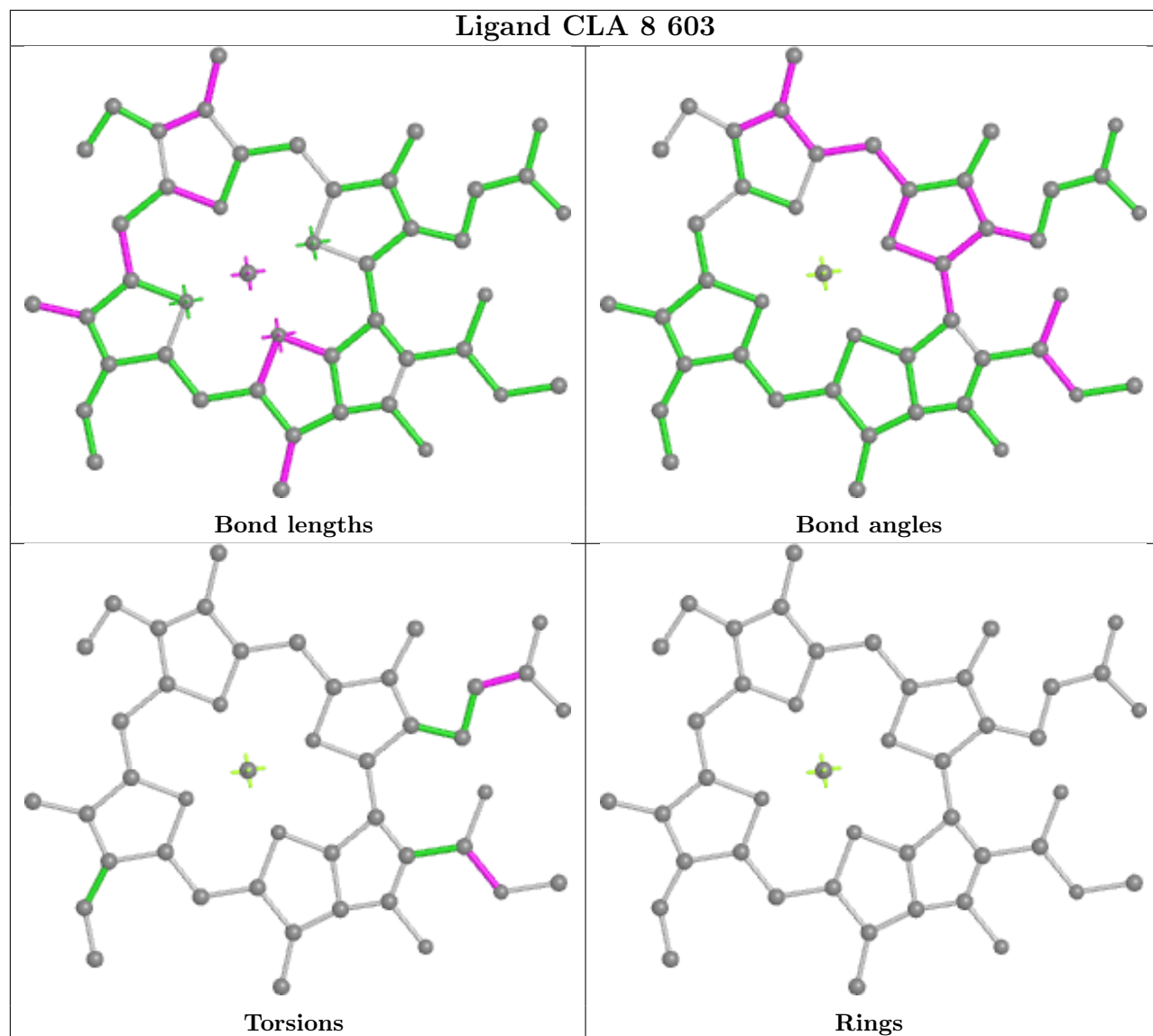


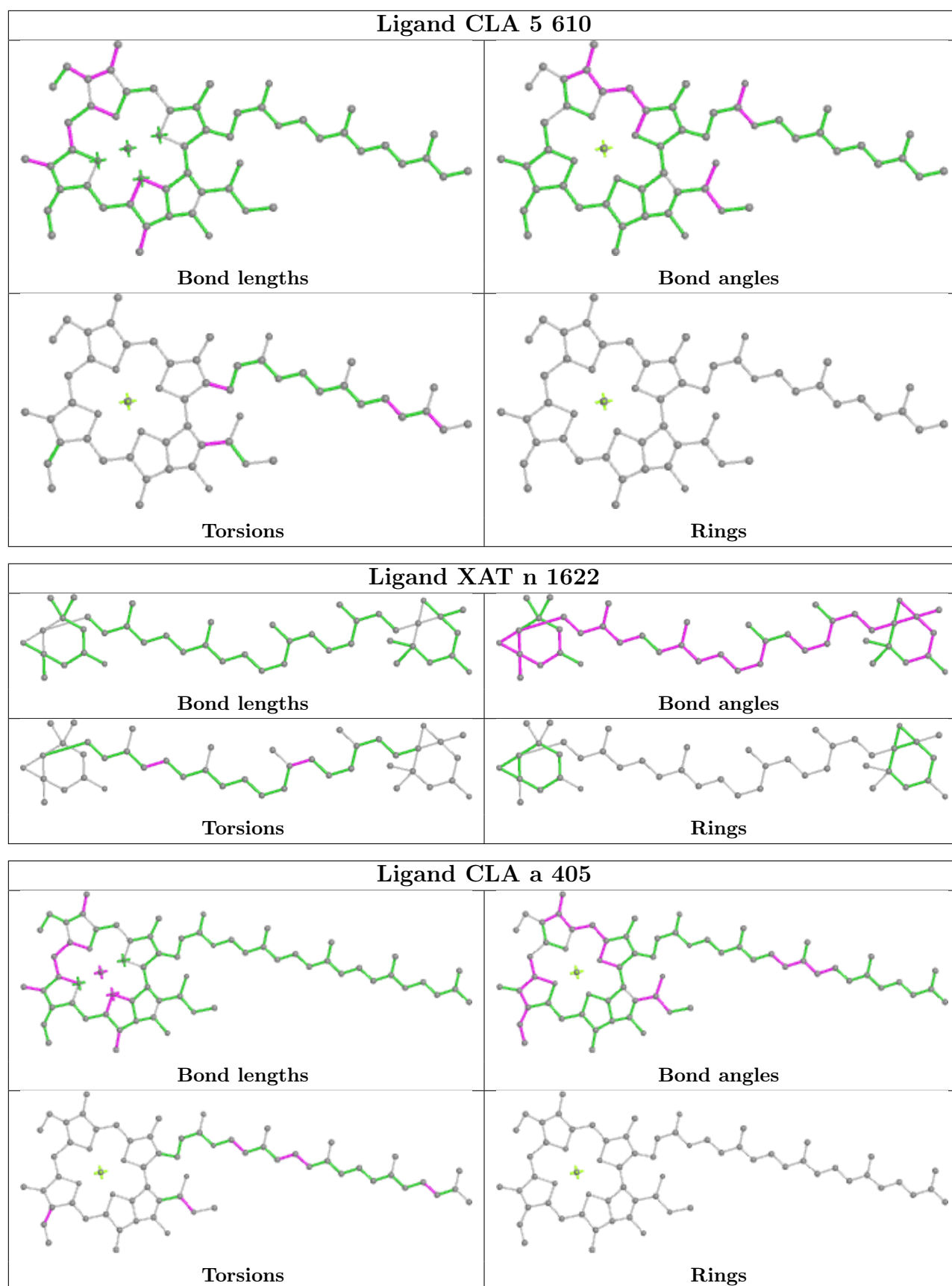
Rings

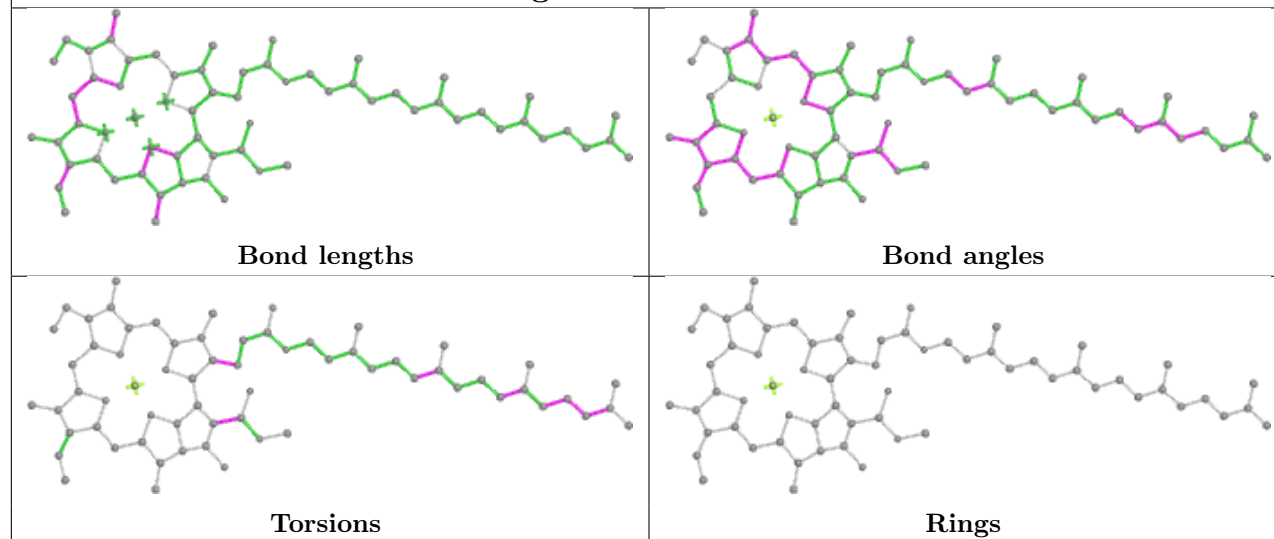
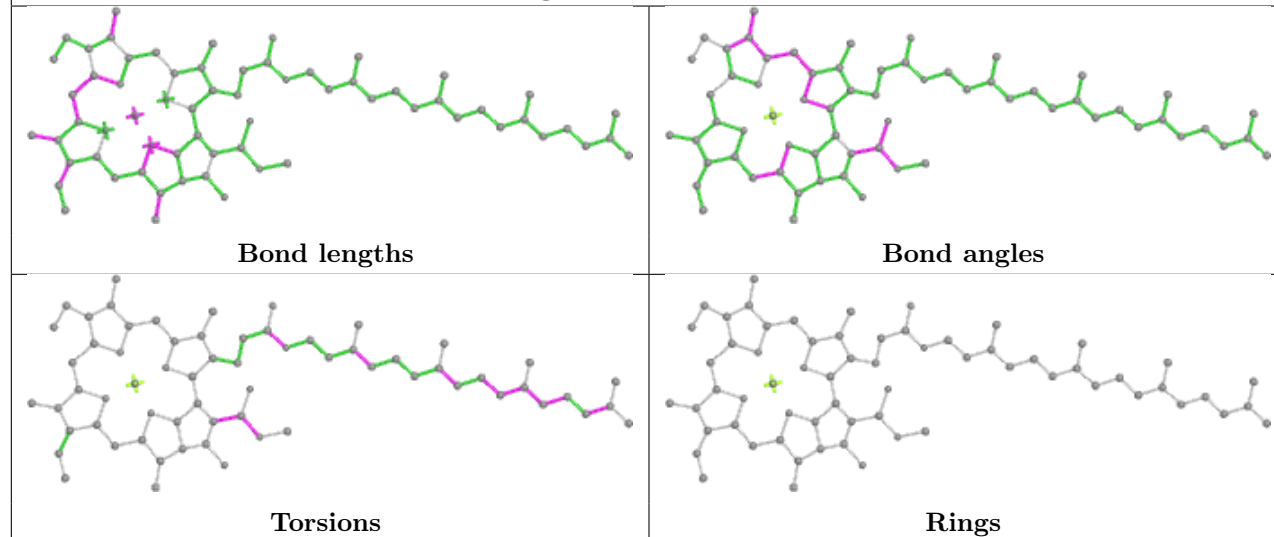
Ligand CLA 2 611

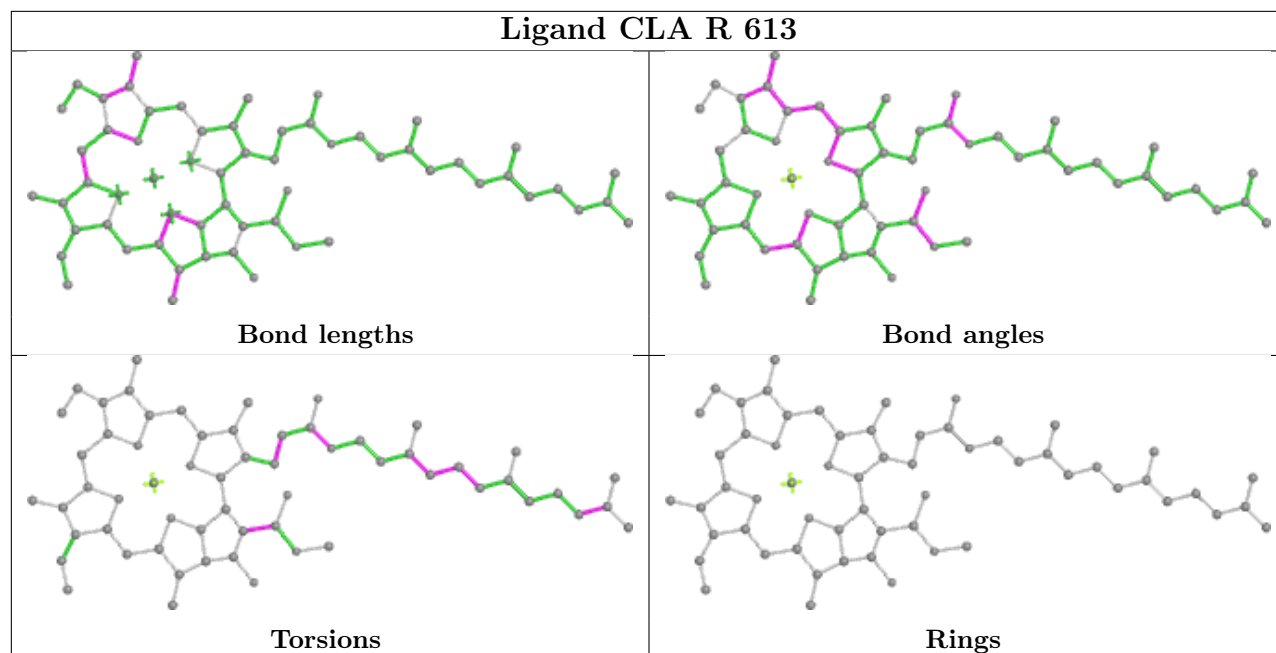
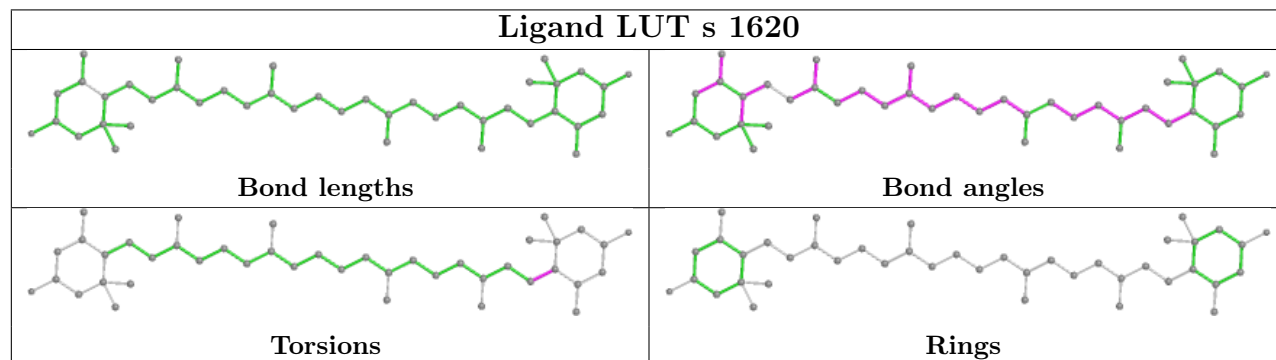


Ligand CLA 8 603

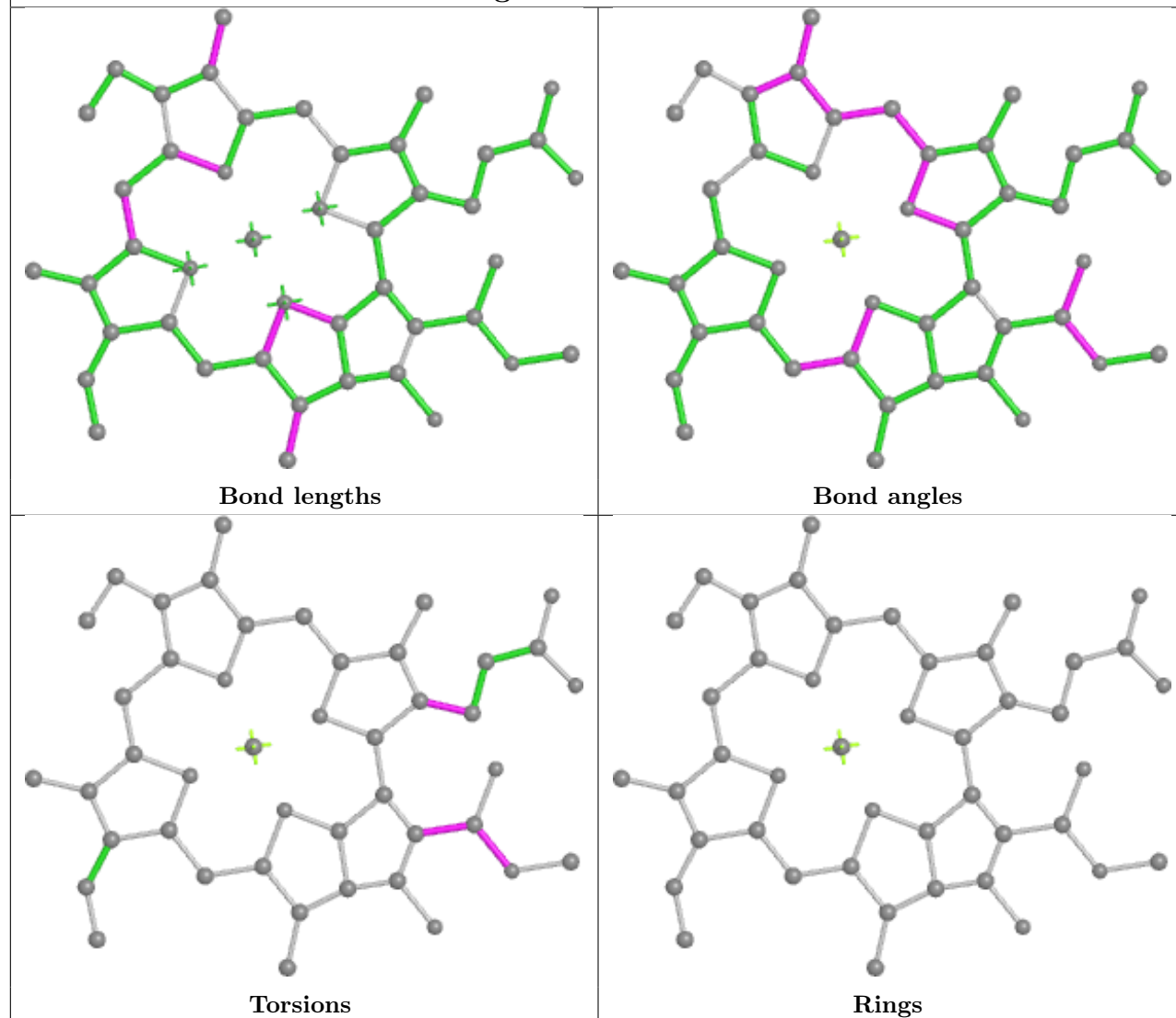




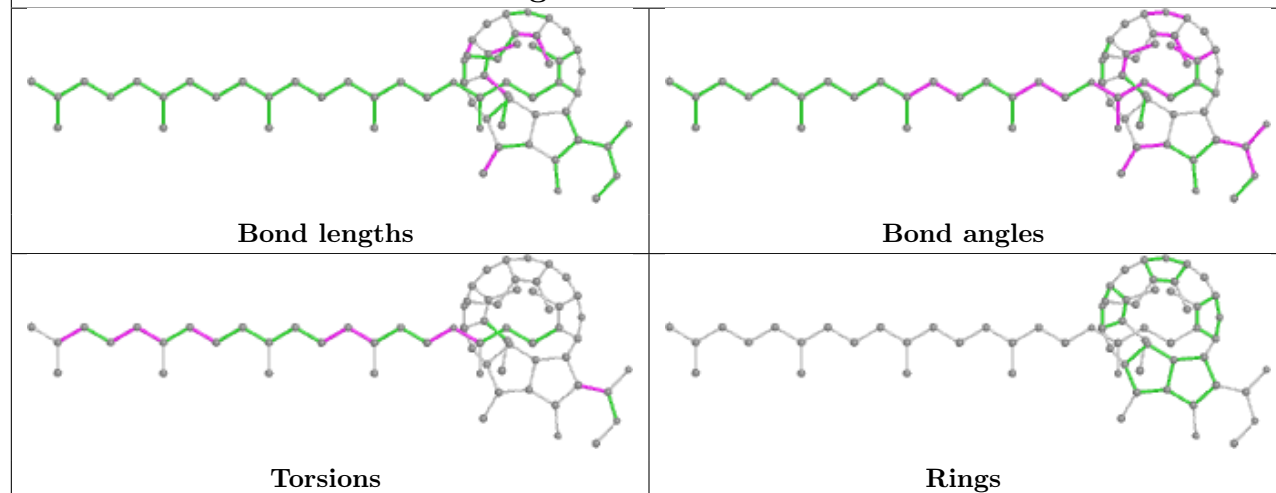
Ligand CLA A 406**Ligand CLA c 504**

Ligand CLA R 613**Ligand LUT s 1620**

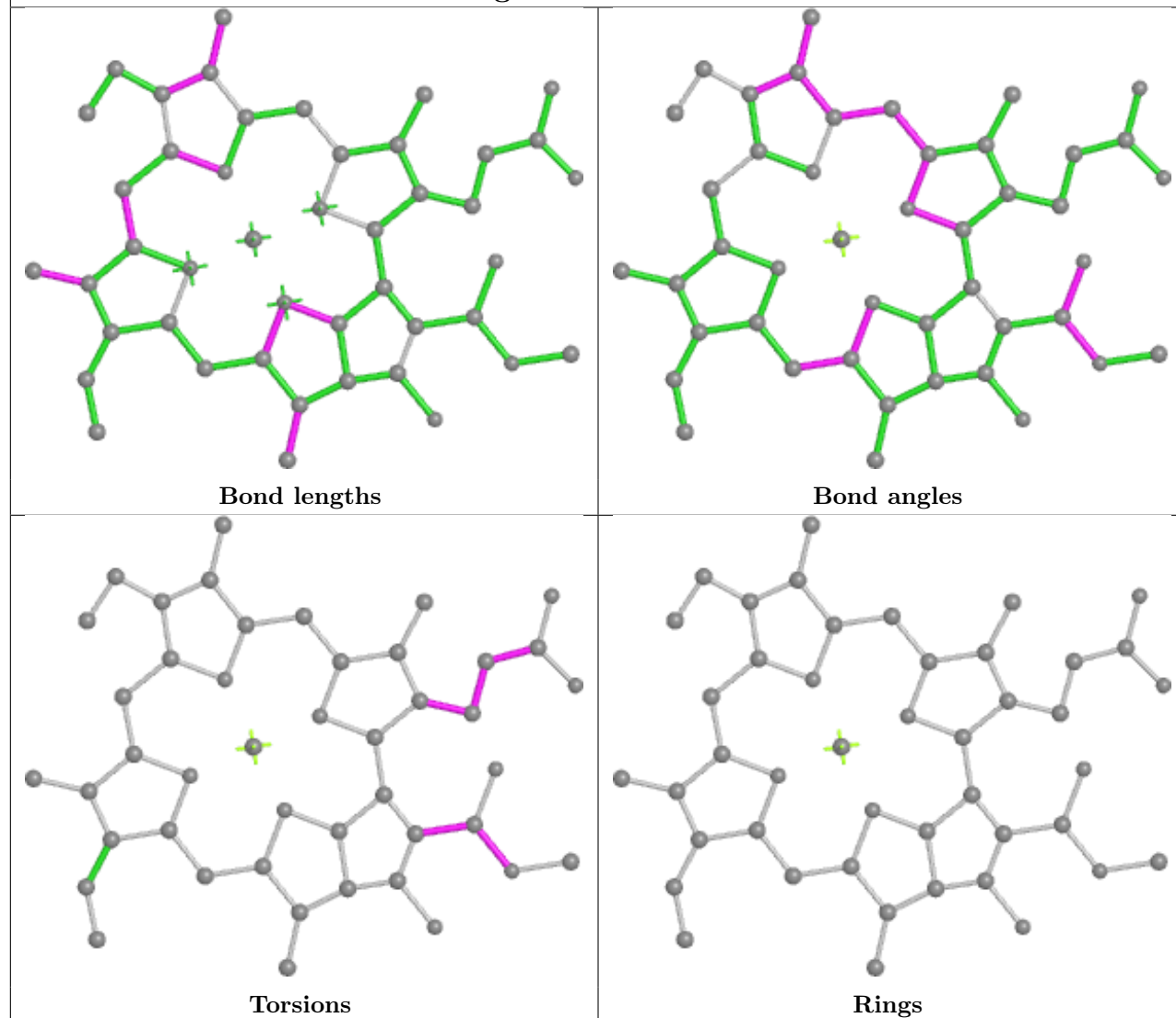
Ligand CLA 2 614



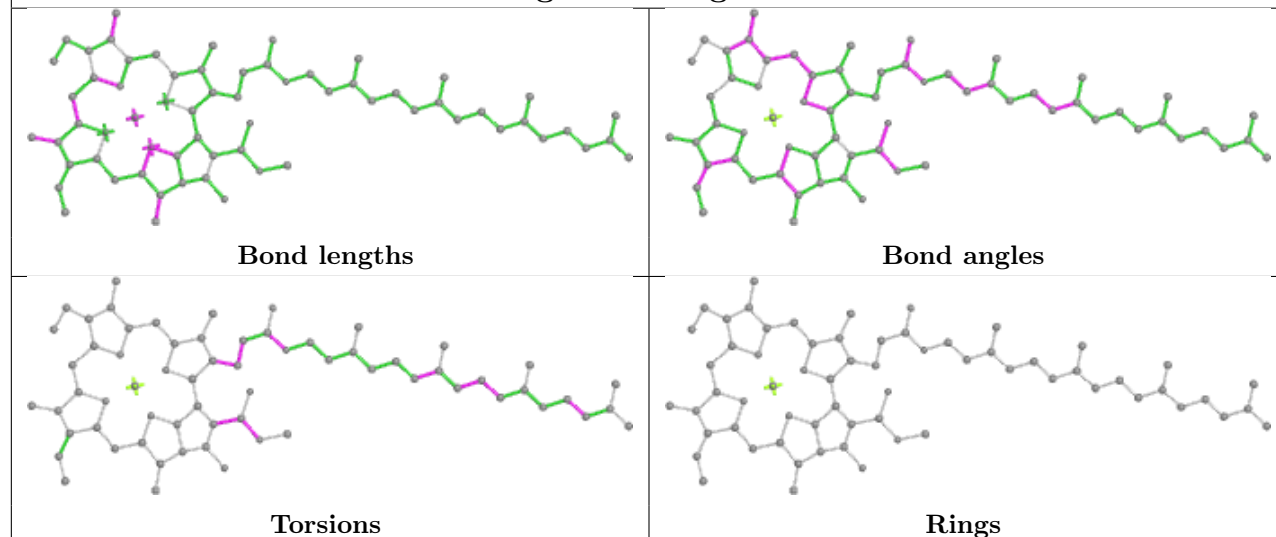
Ligand PHO A 408

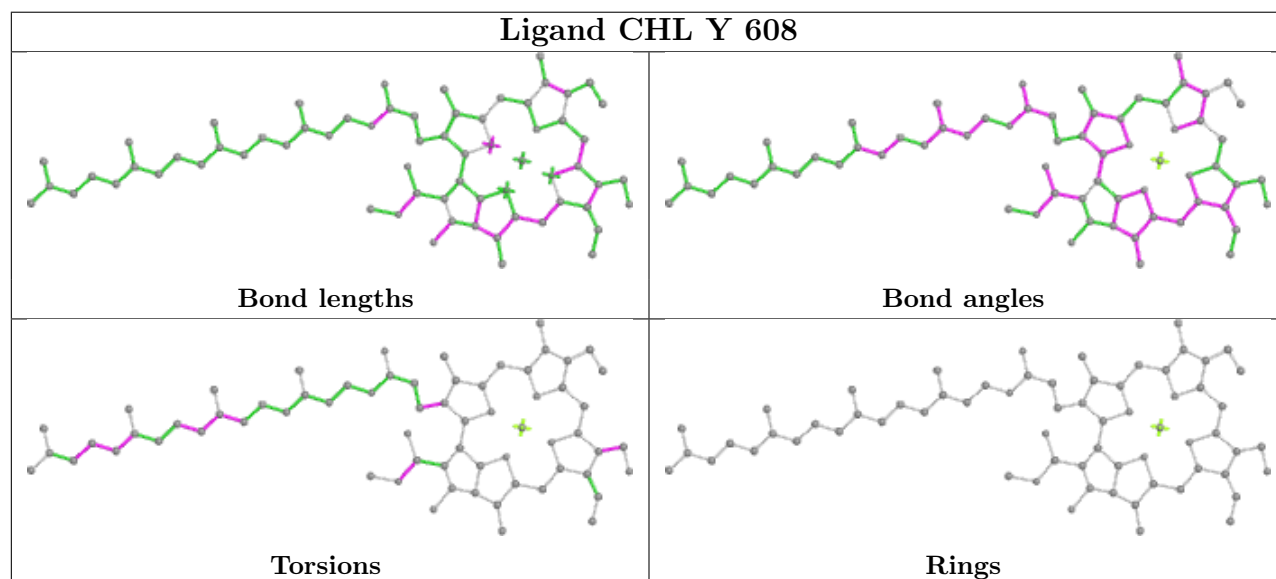
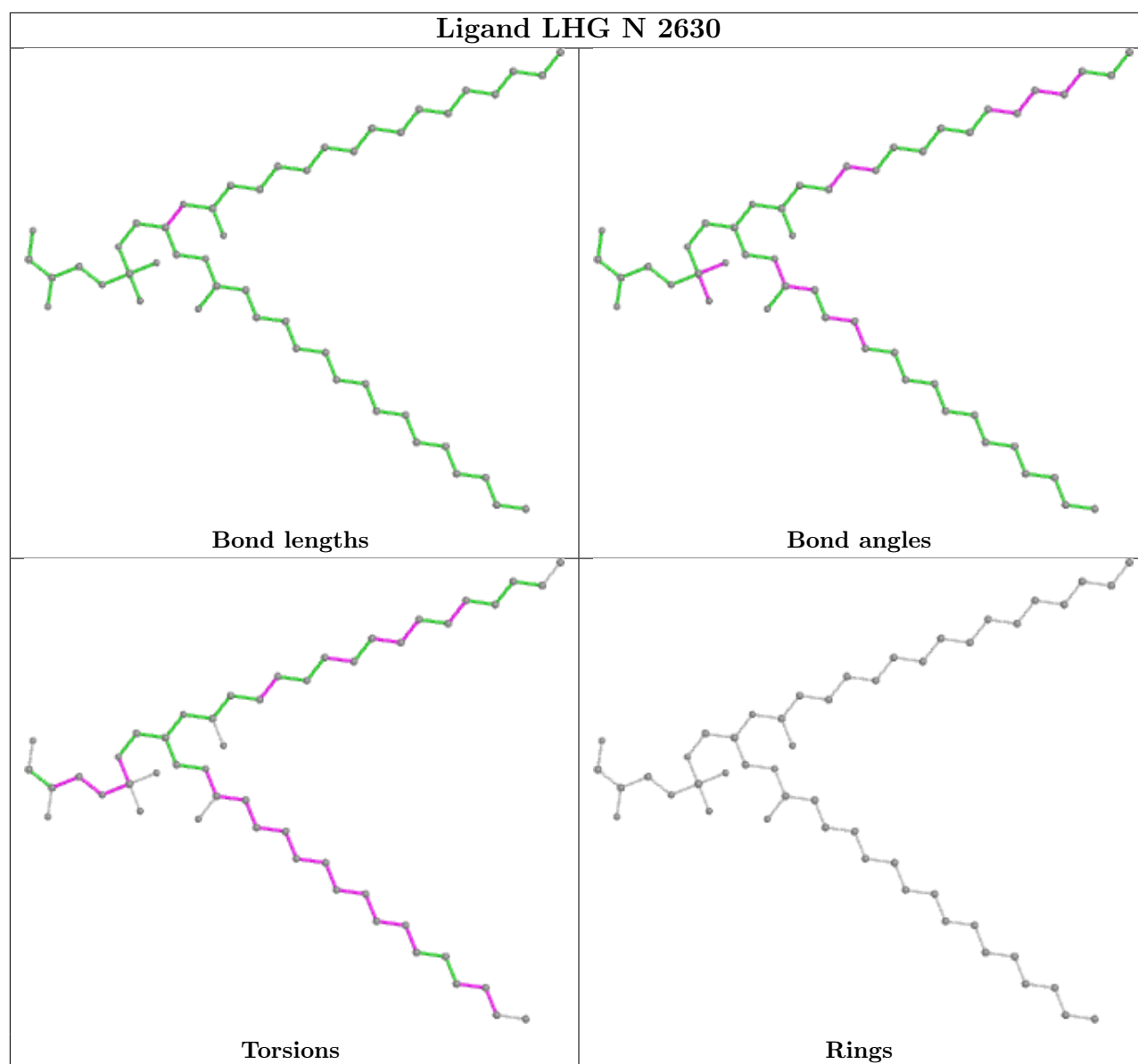


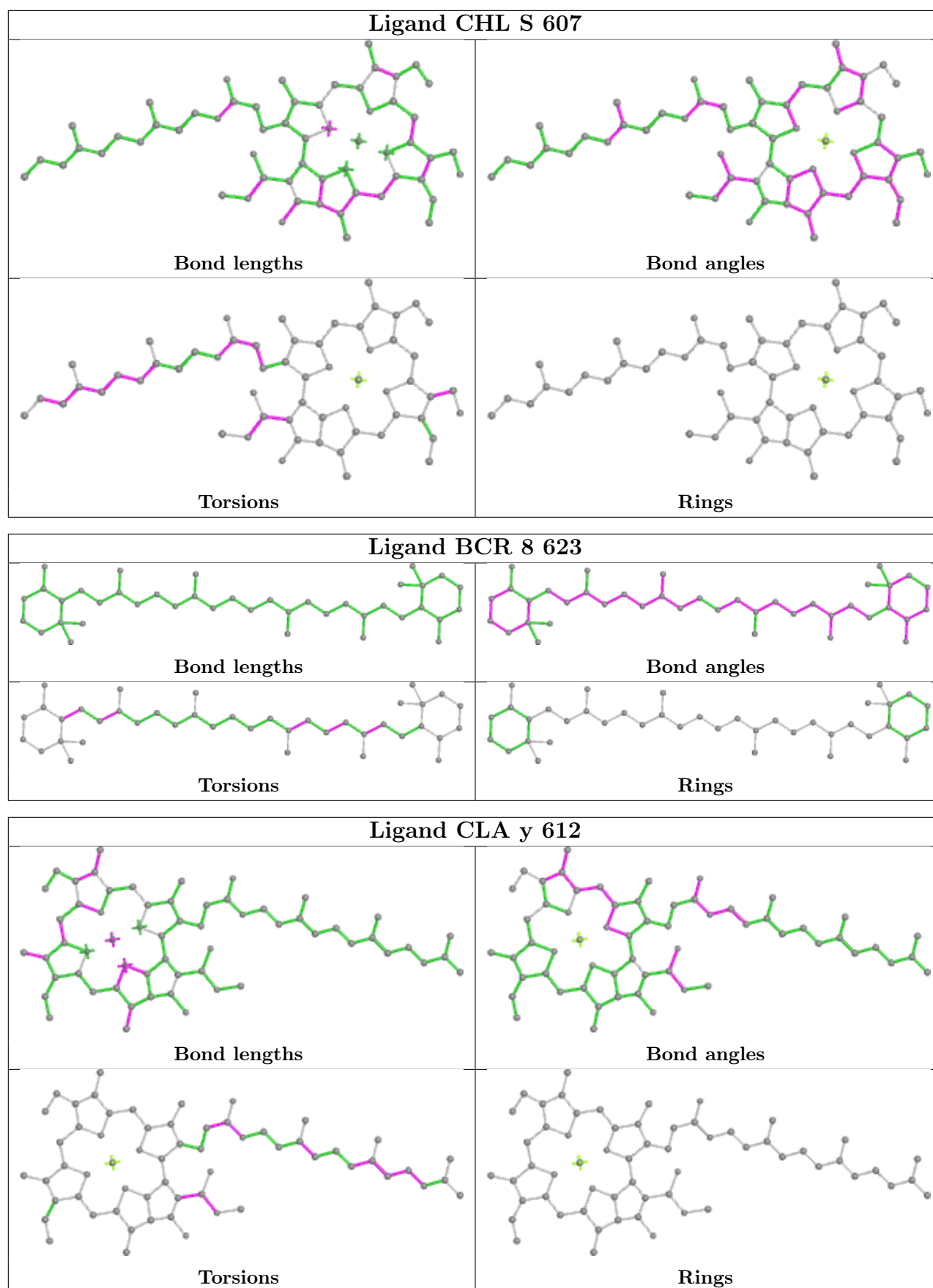
Ligand CLA 4 604



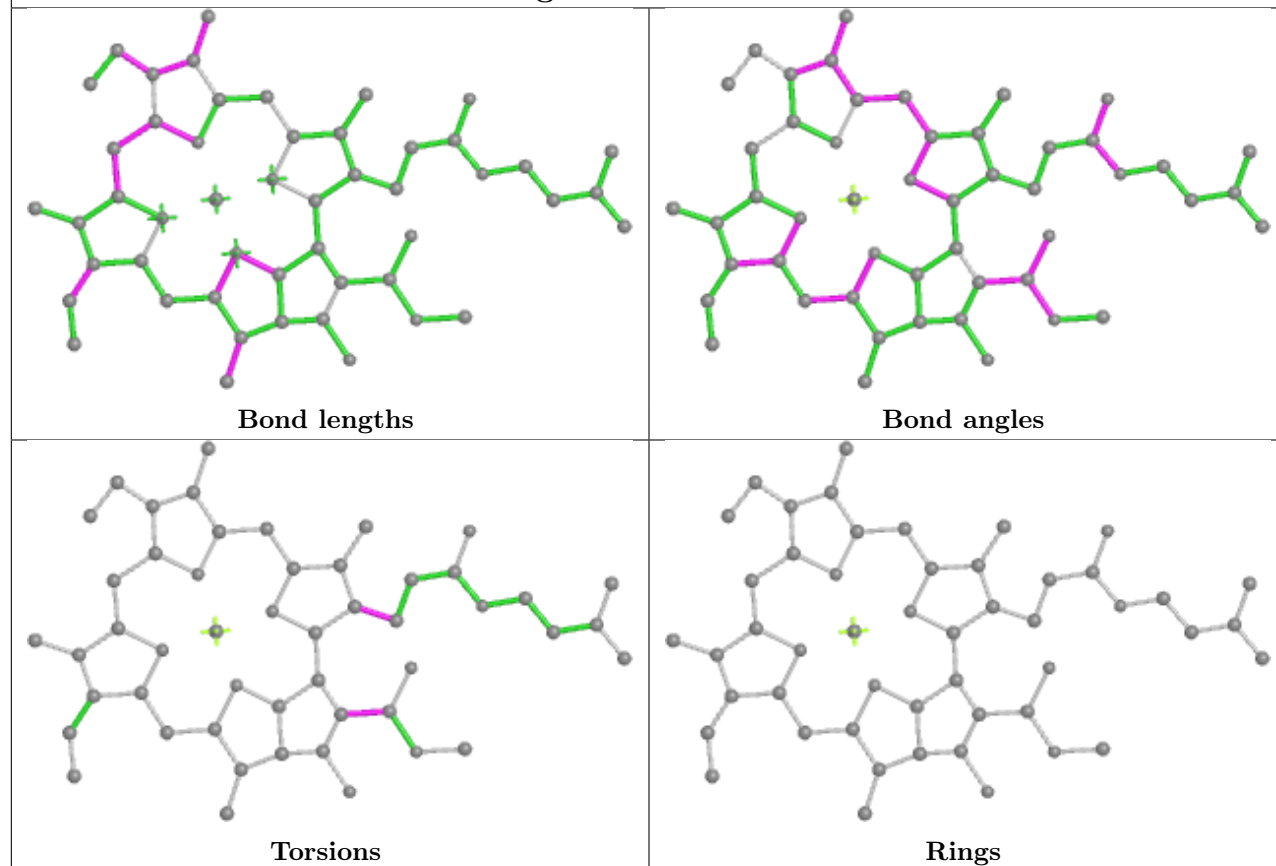
Ligand CLA g 602



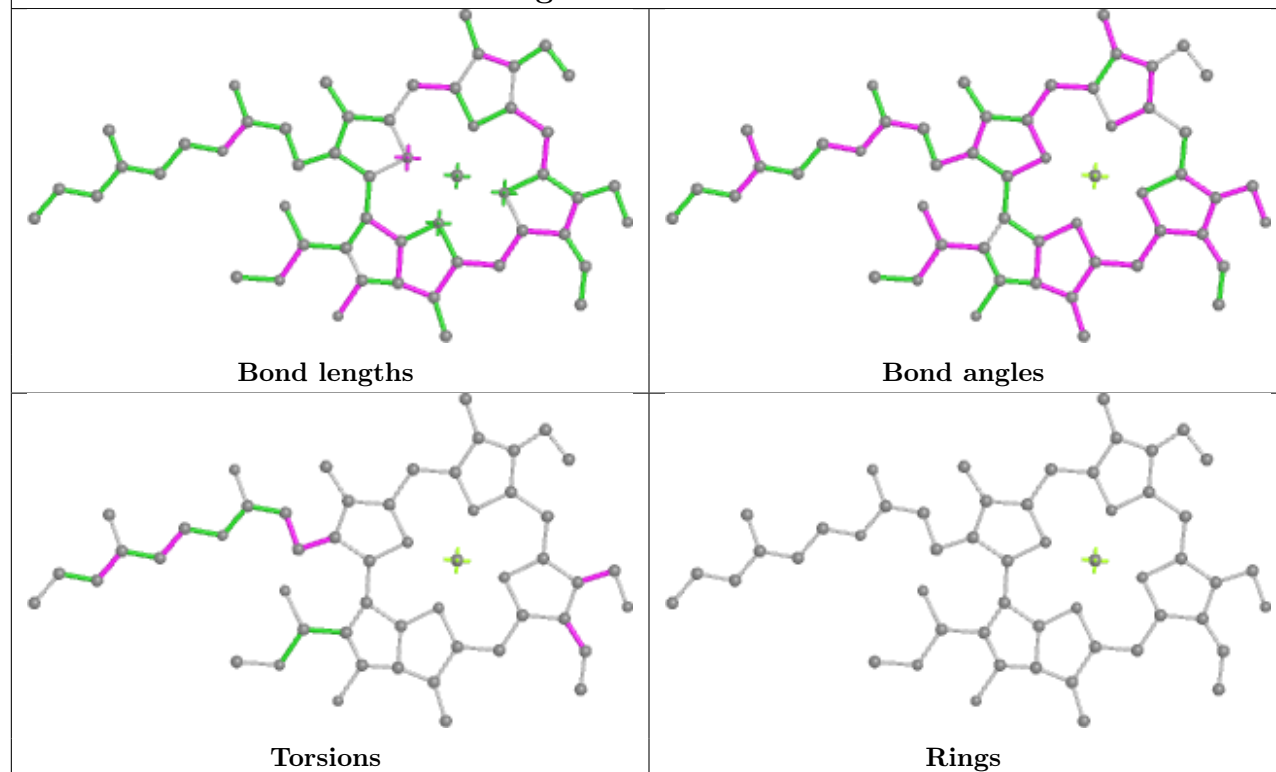




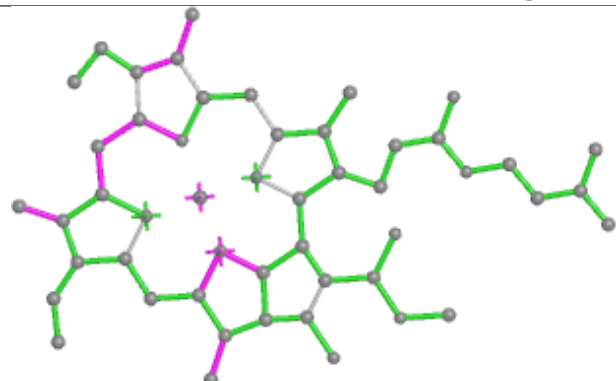
Ligand CLA a 407



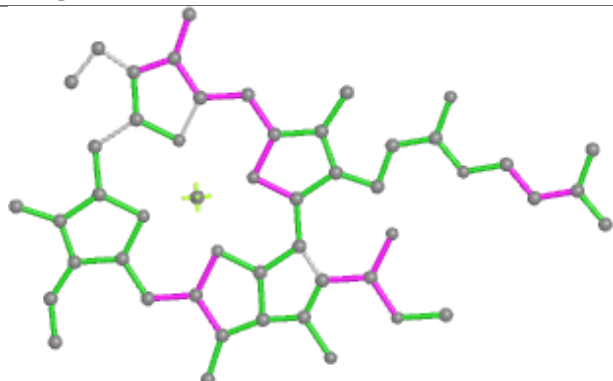
Ligand CHL 3 607



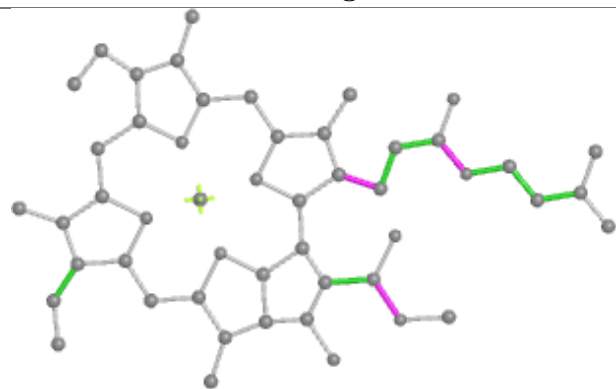
Ligand CLA g 604



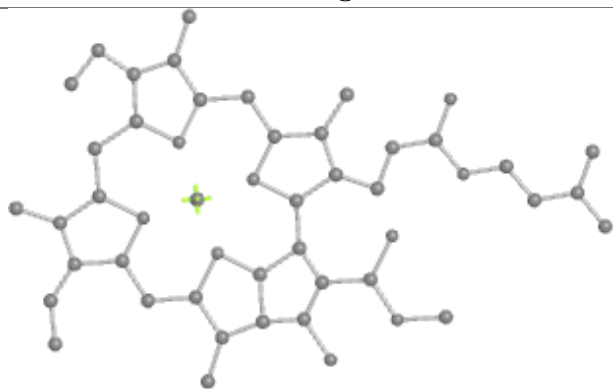
Bond lengths



Bond angles

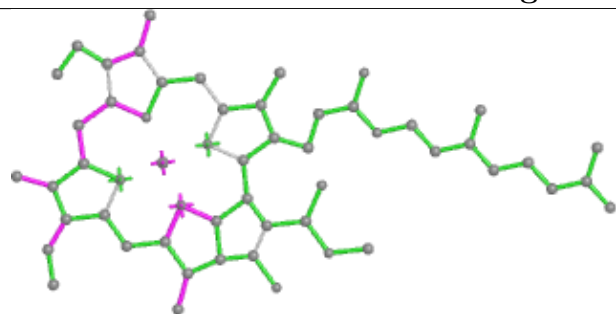


Torsions

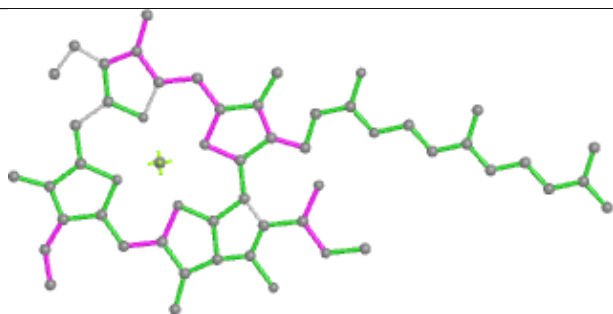


Rings

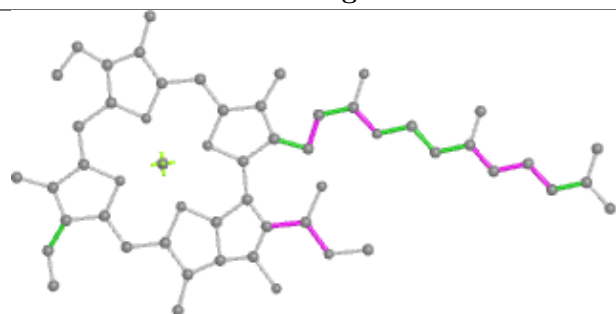
Ligand CLA 5 603



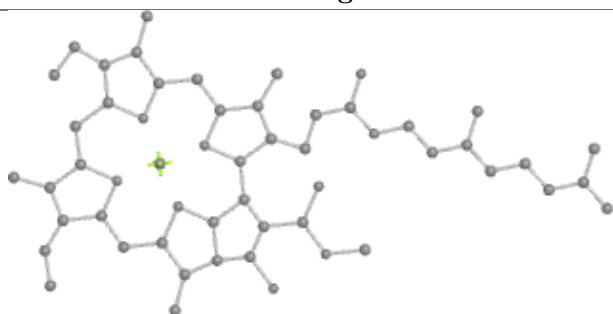
Bond lengths



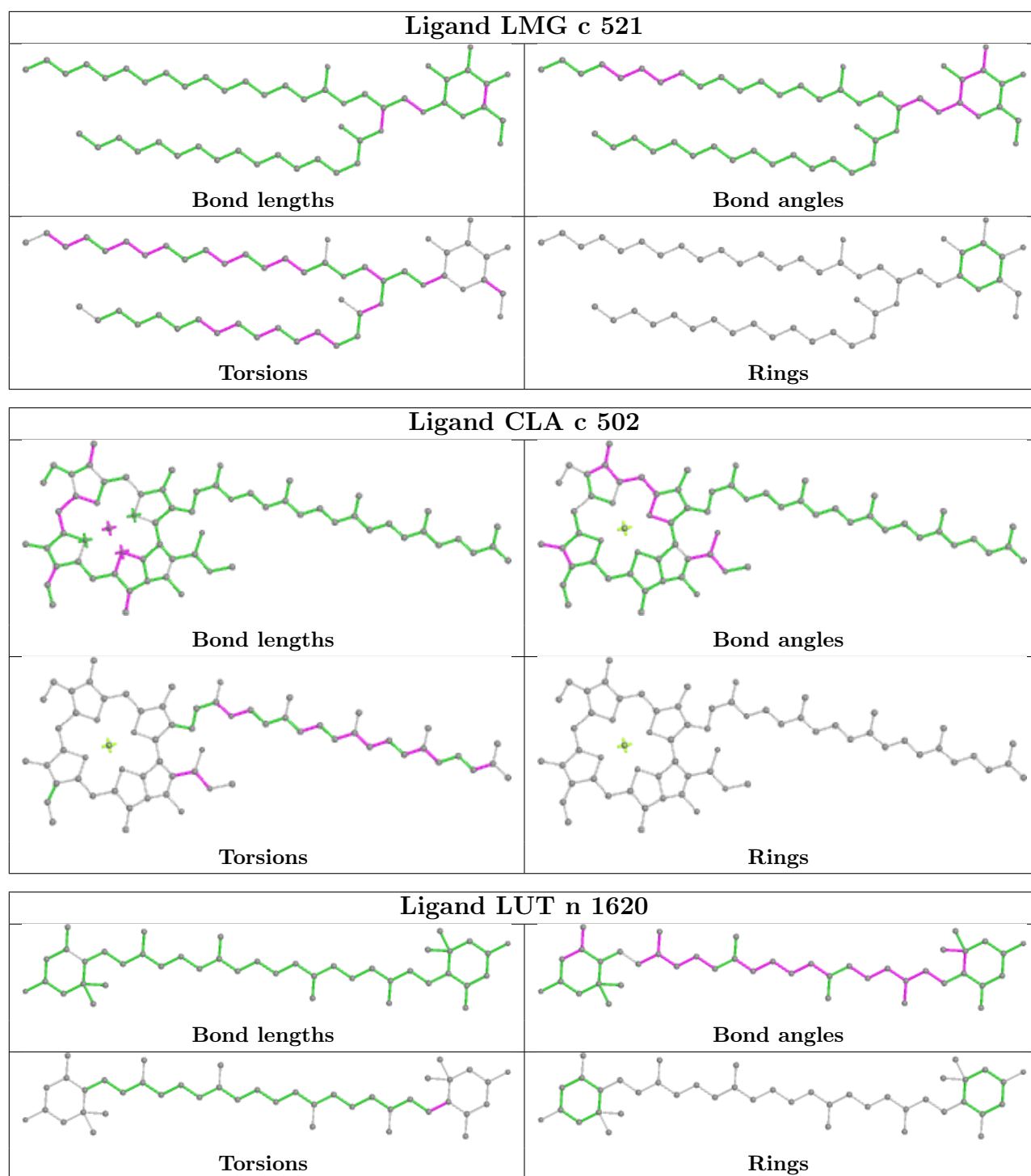
Bond angles

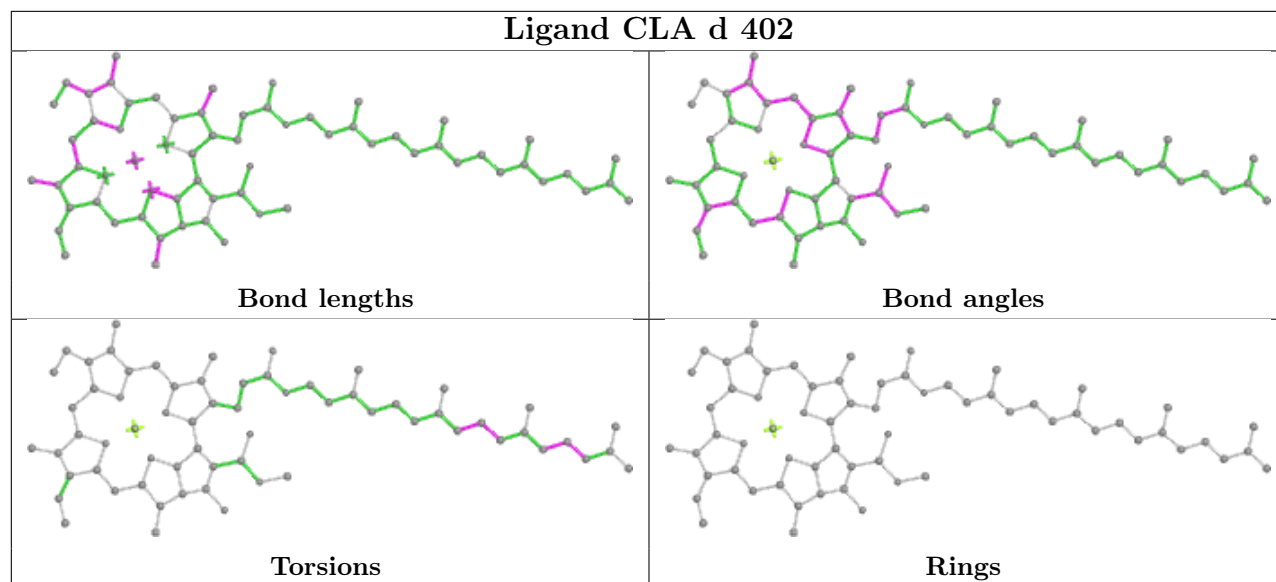
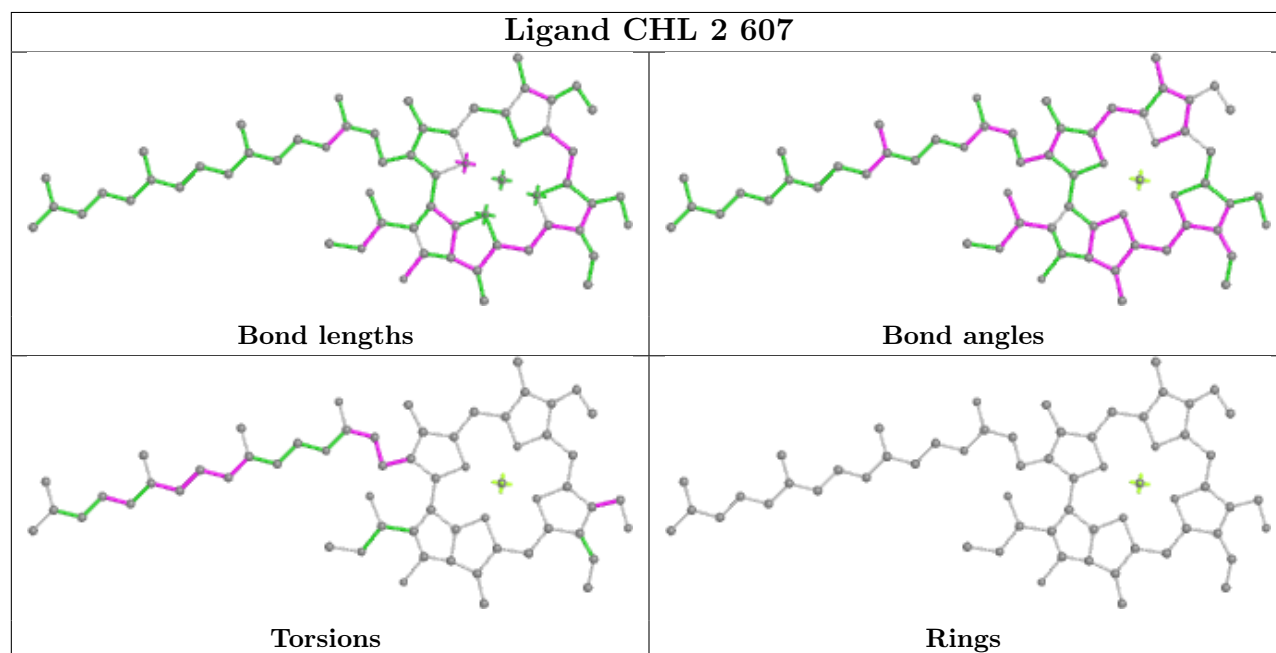


Torsions

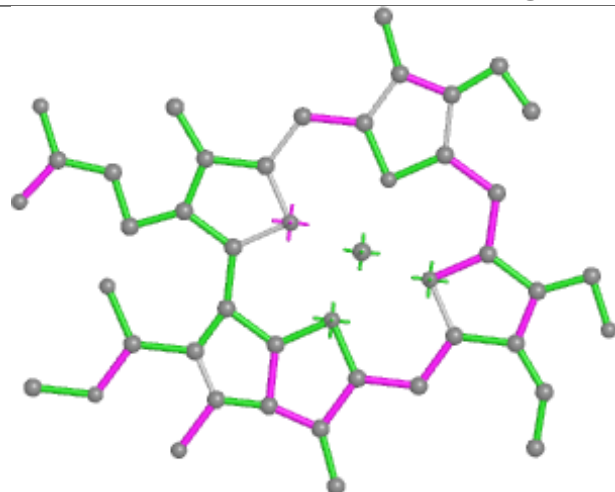


Rings

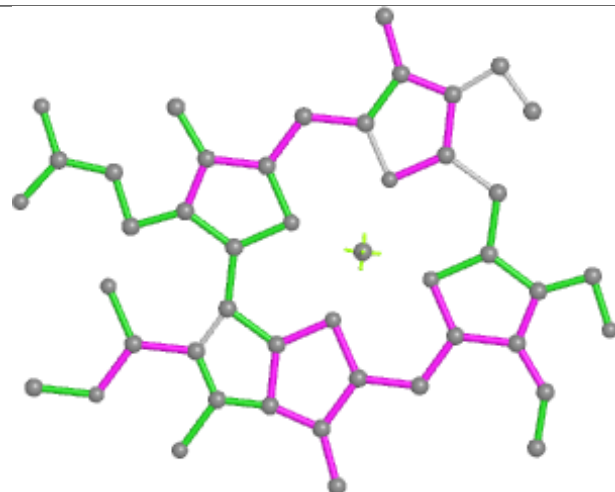


Ligand CLA d 402**Ligand CHL 2 607**

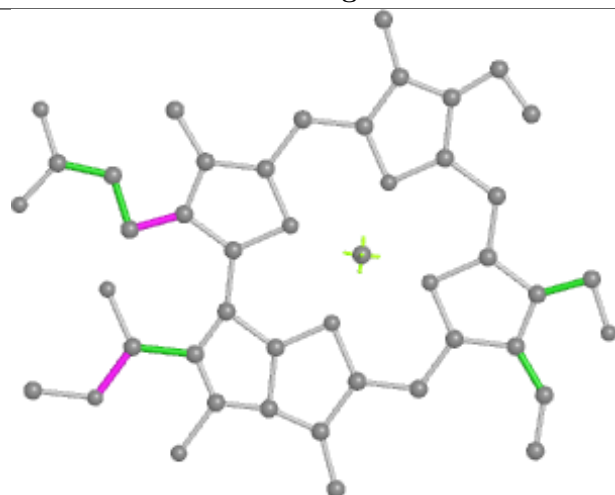
Ligand CHL s 608



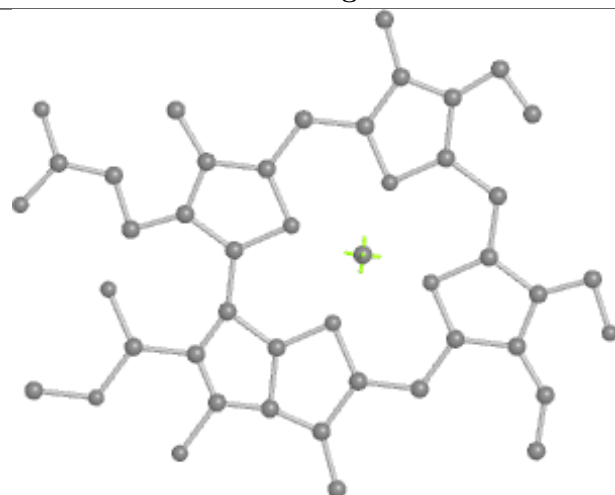
Bond lengths



Bond angles

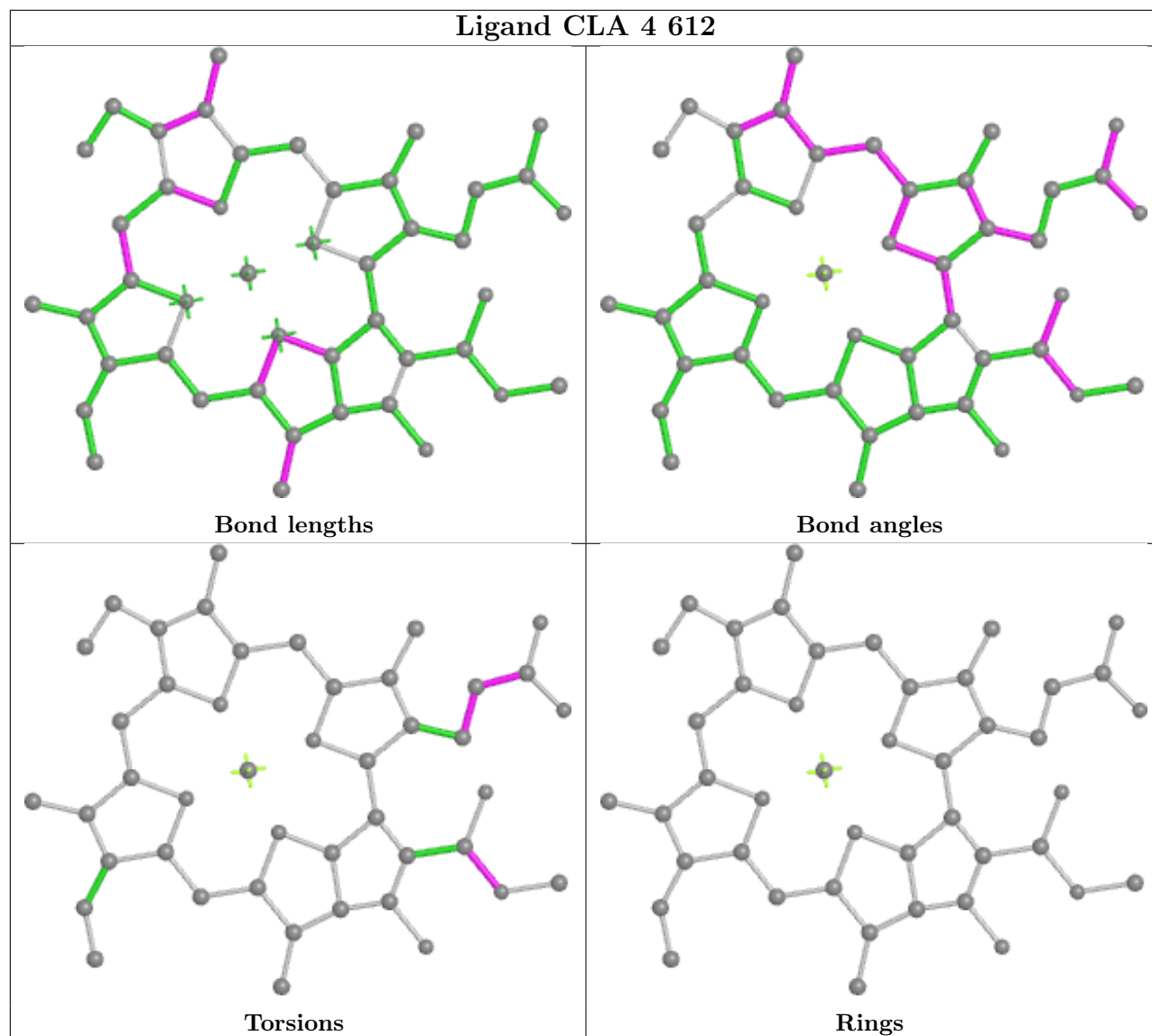


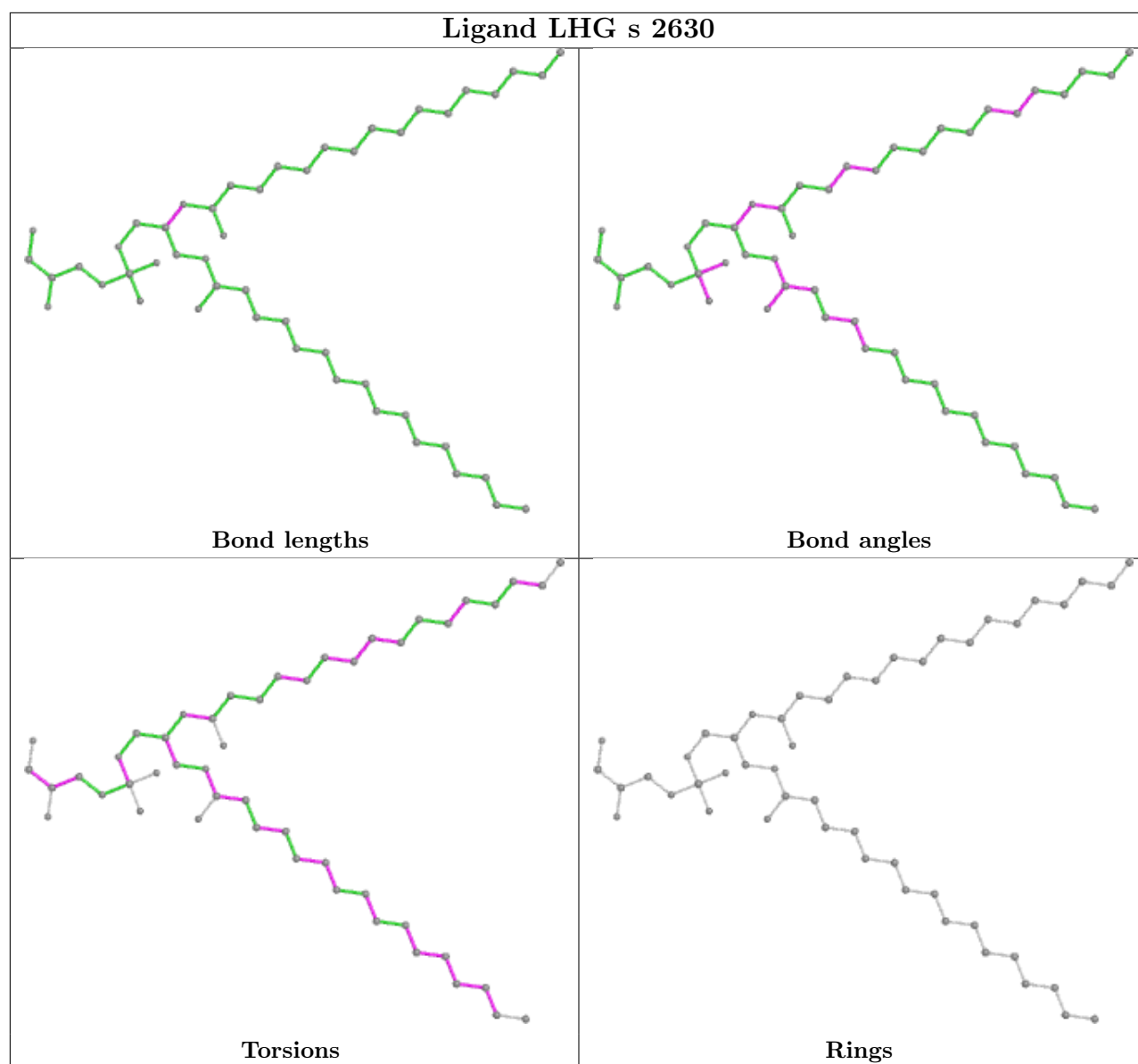
Torsions

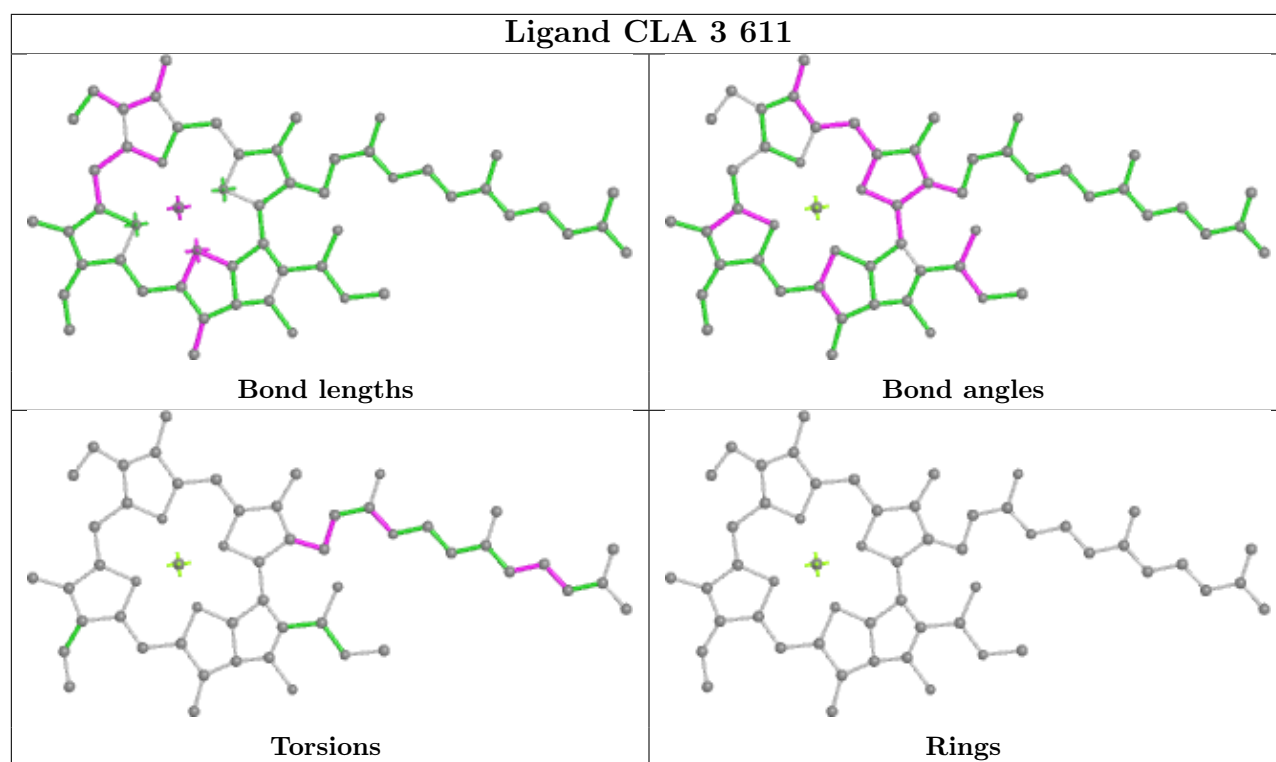


Rings

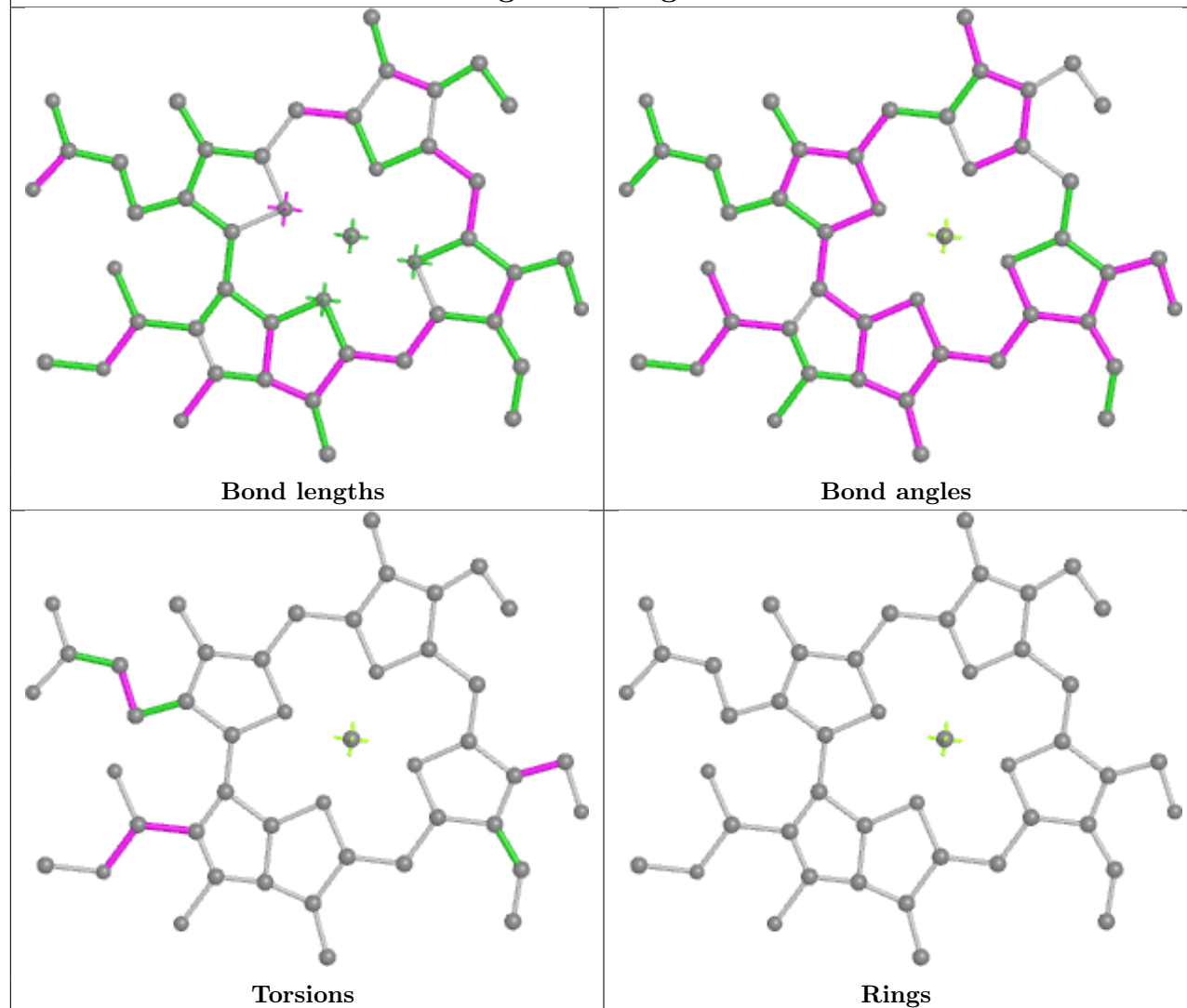
Ligand CLA 4 612



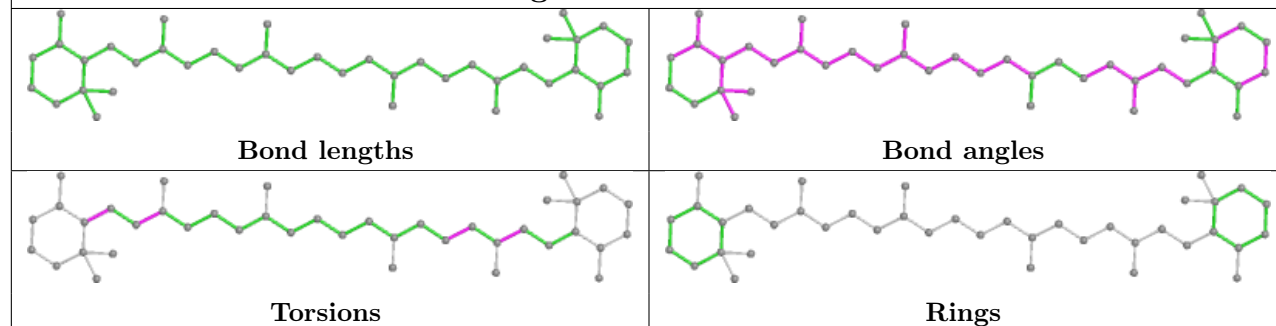


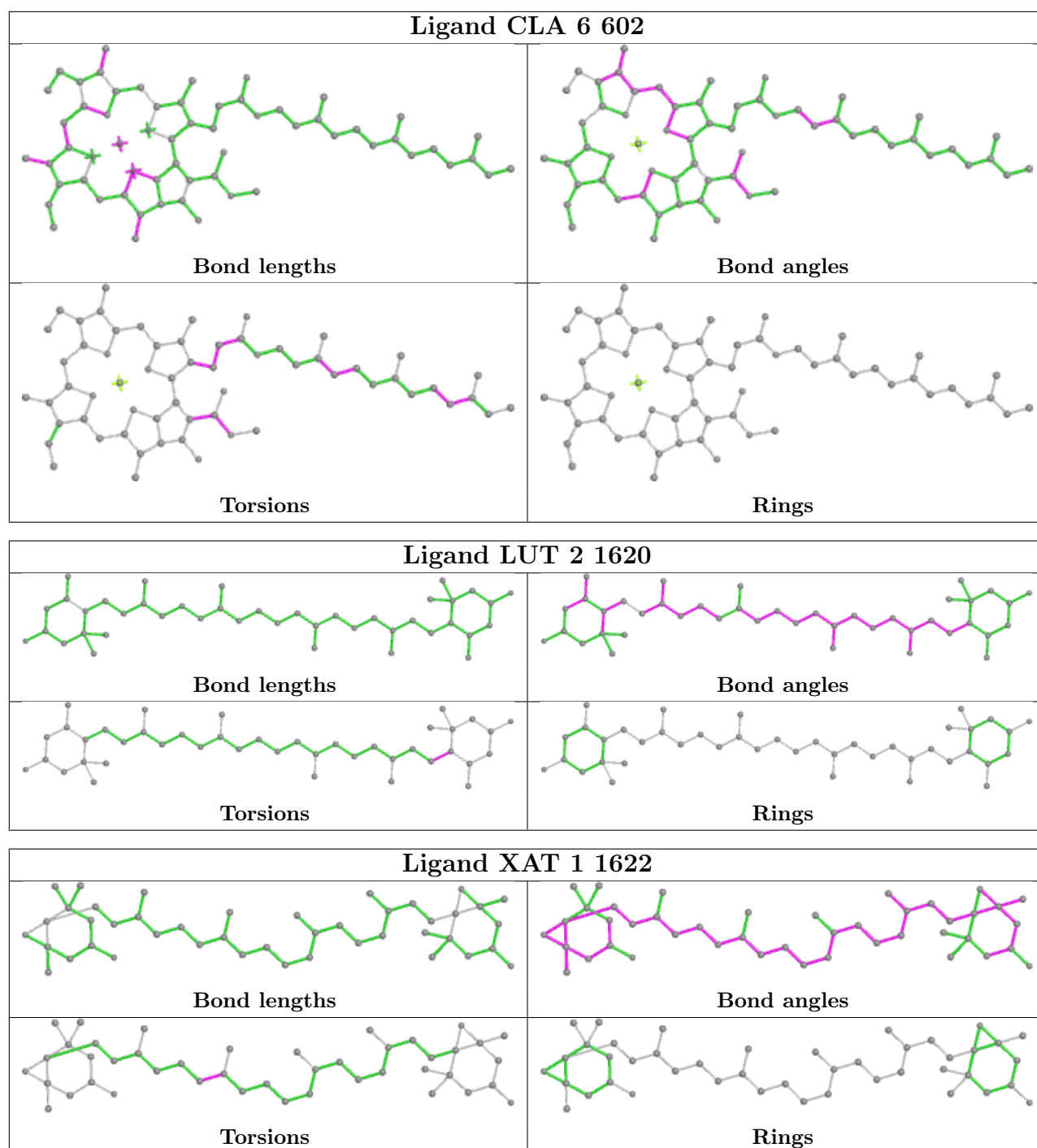


Ligand CHL g 605

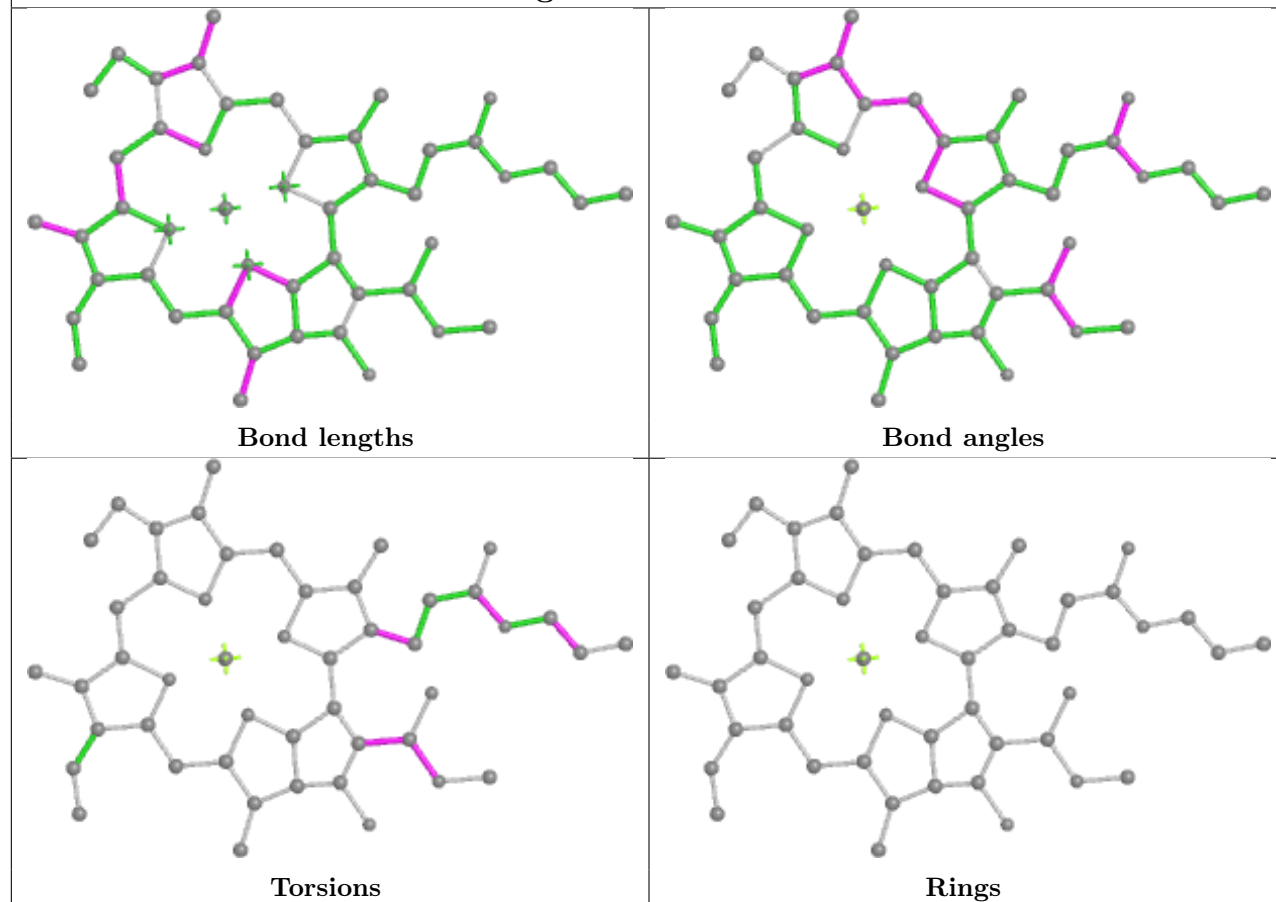


Ligand BCR C 516

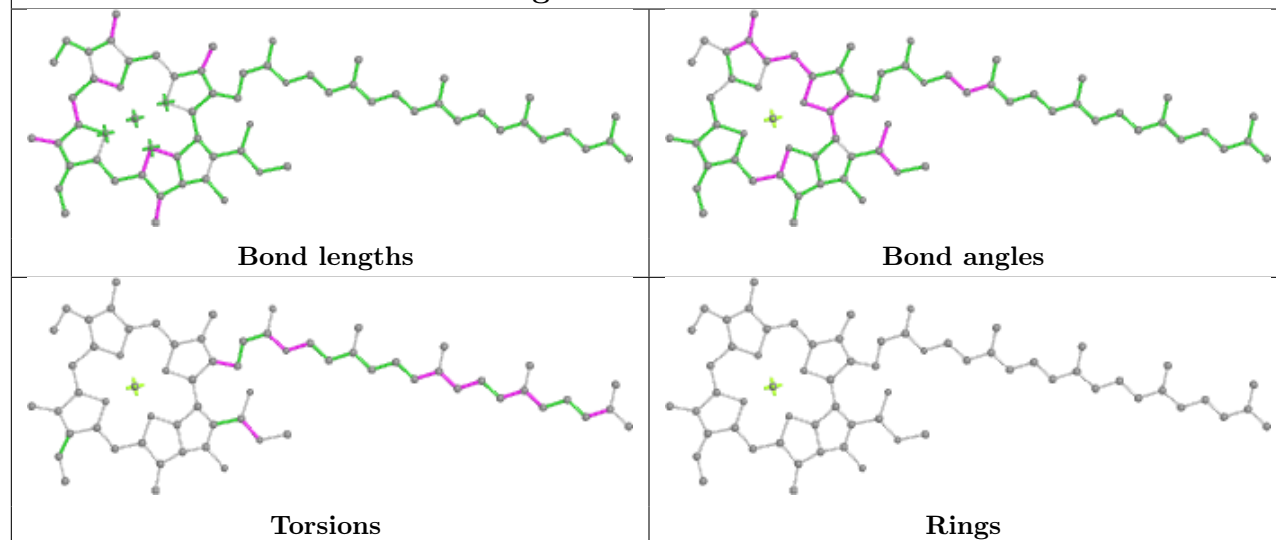


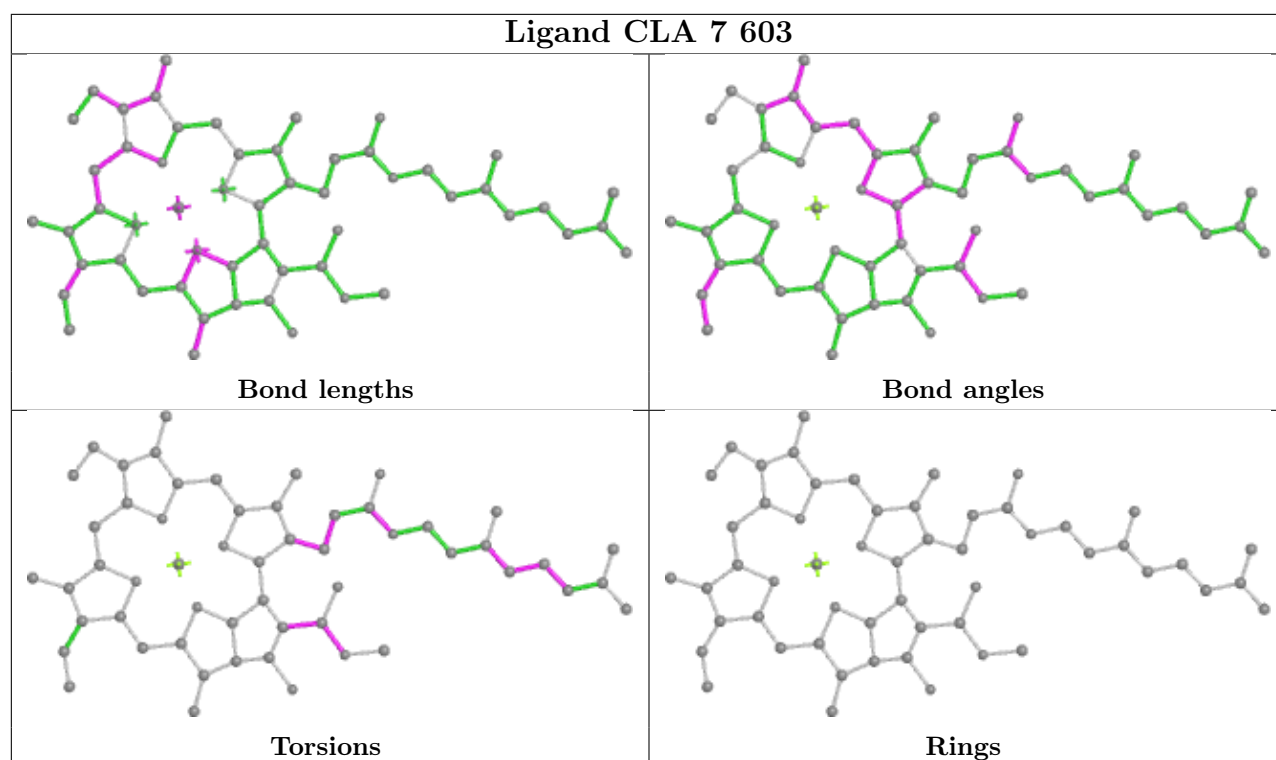


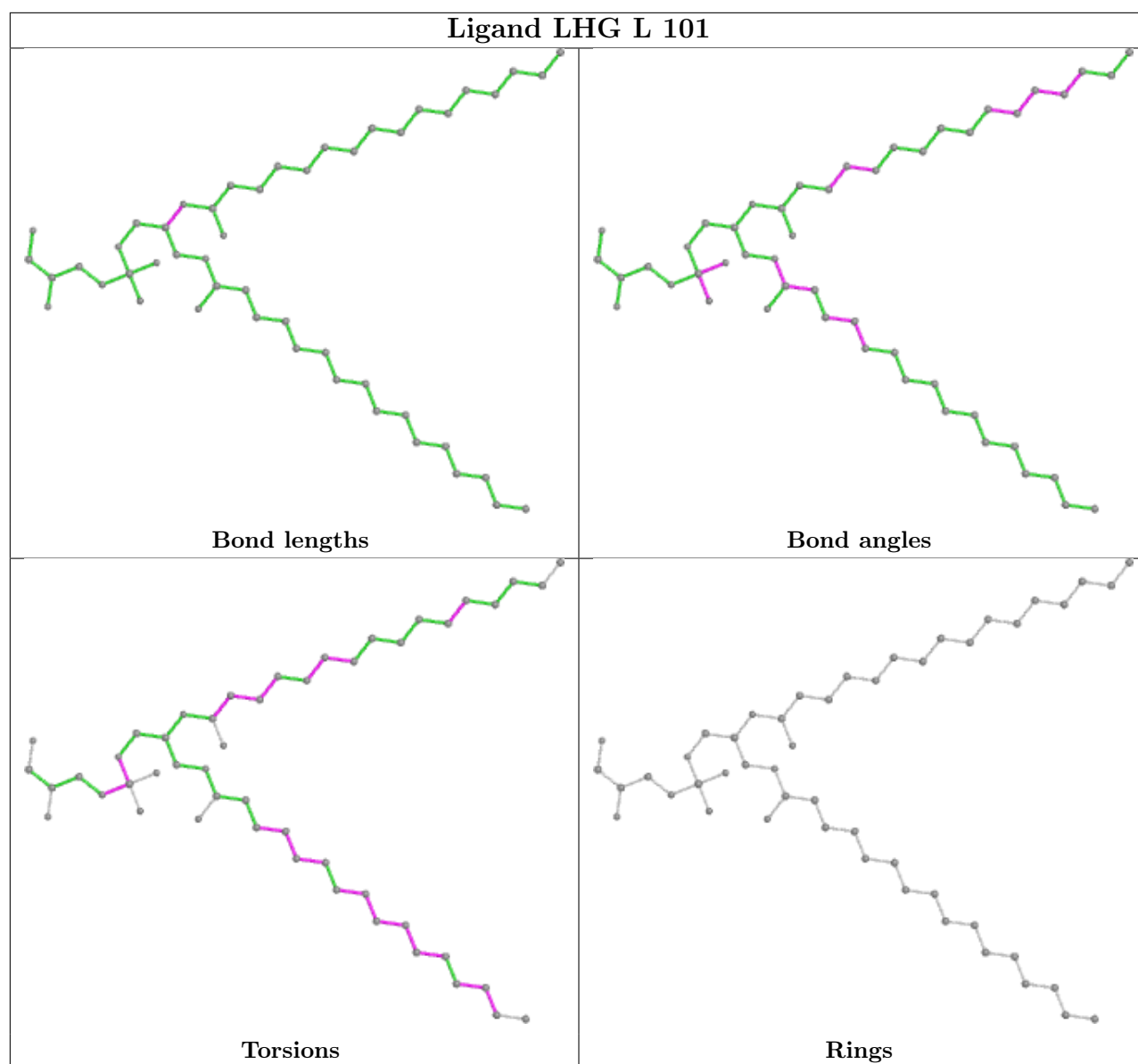
Ligand CLA 3 614

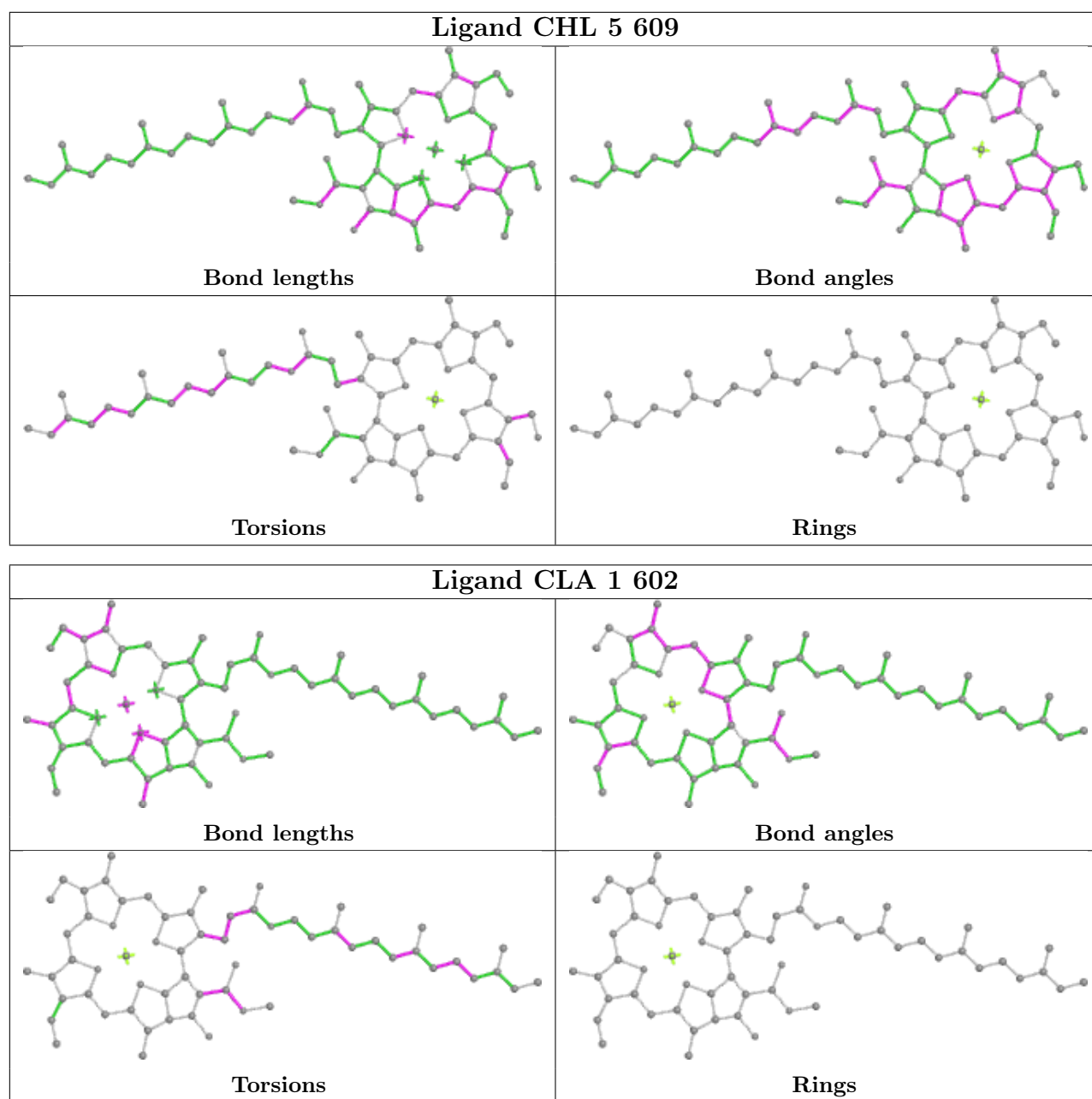


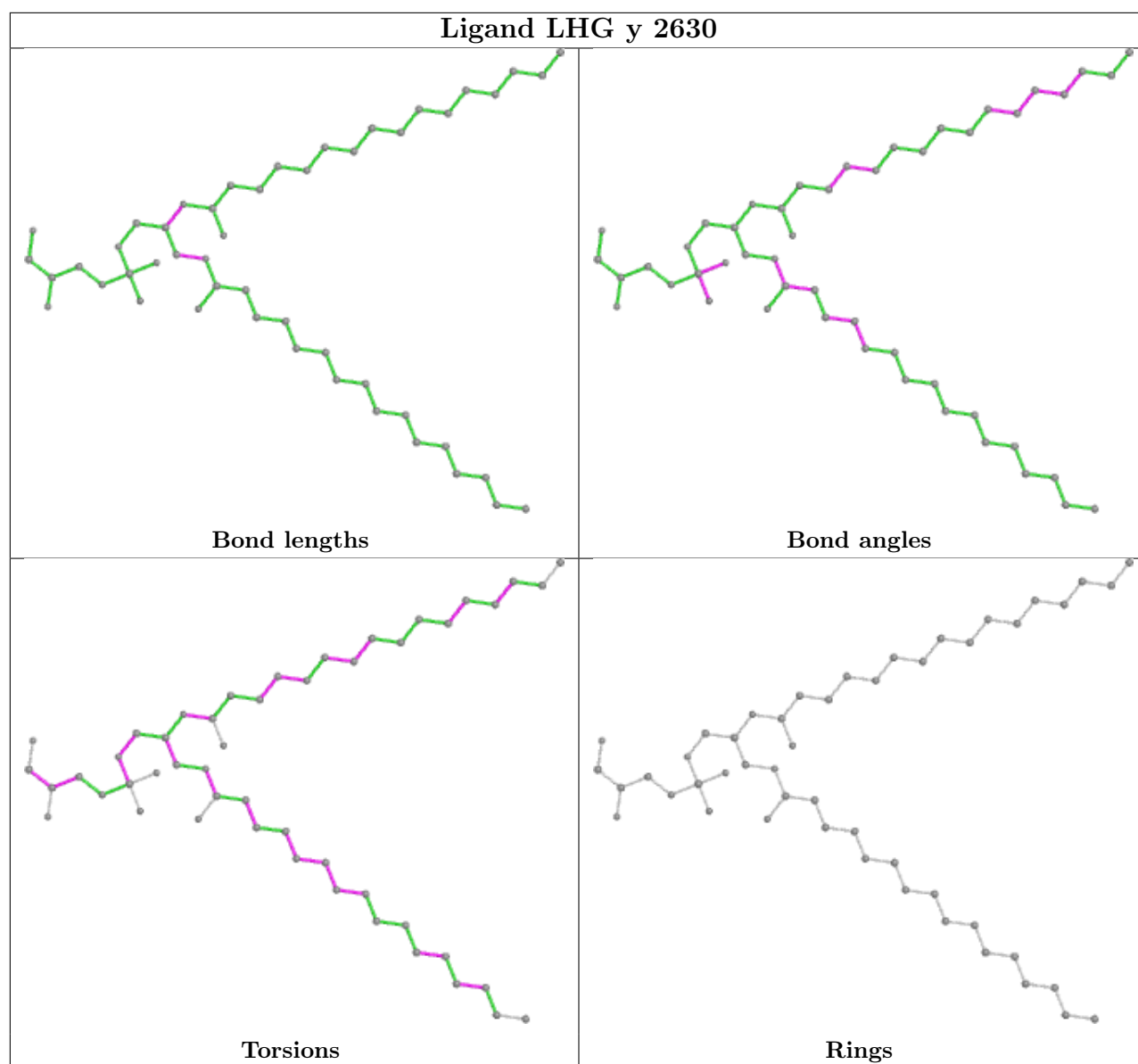
Ligand CLA C 511



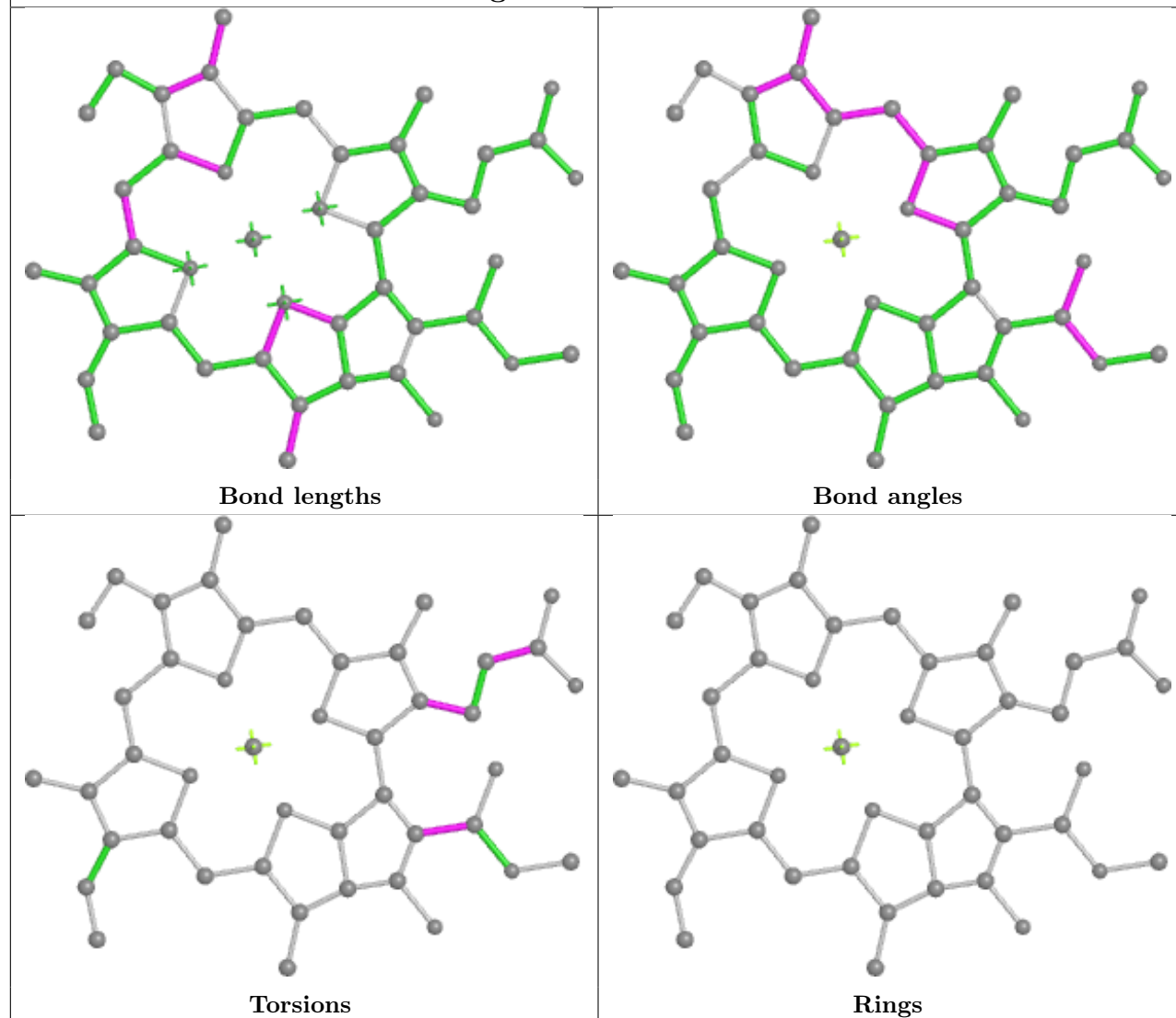




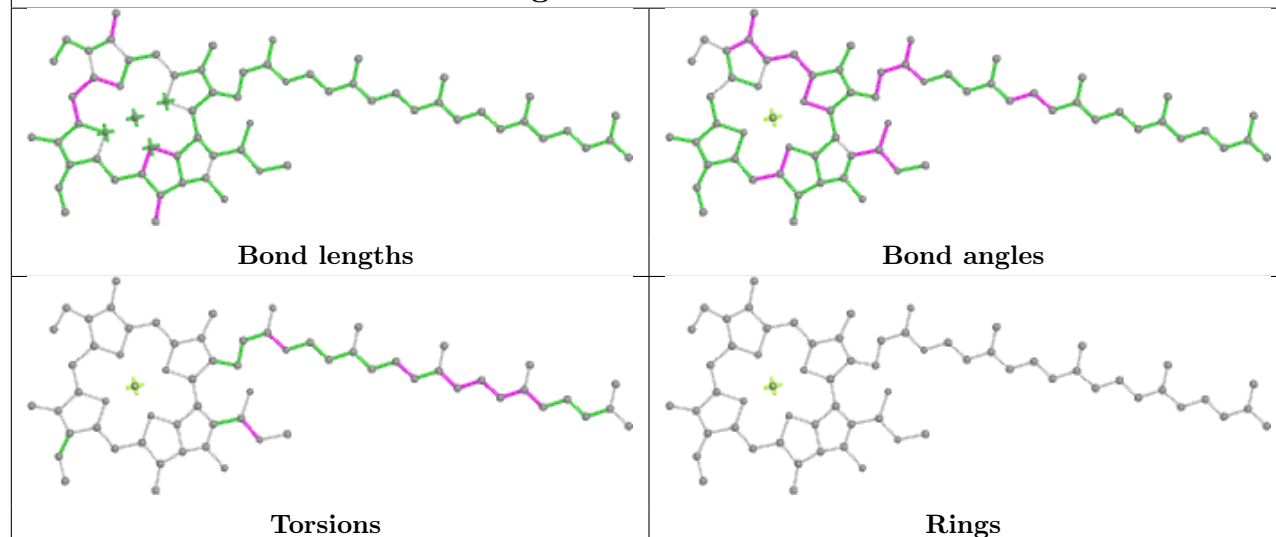




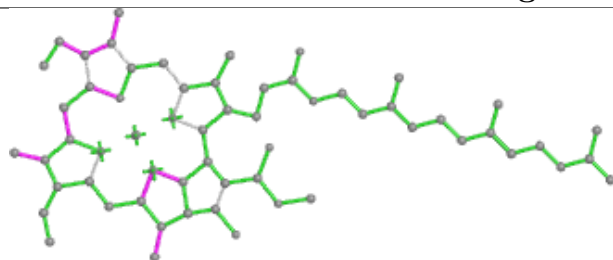
Ligand CLA R 616



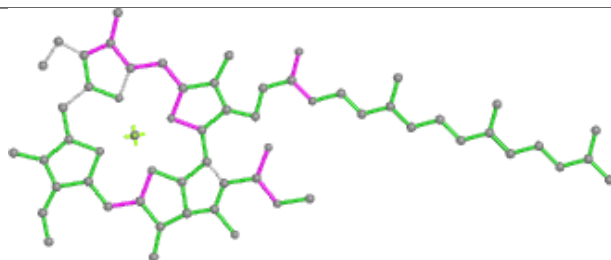
Ligand CLA D 403



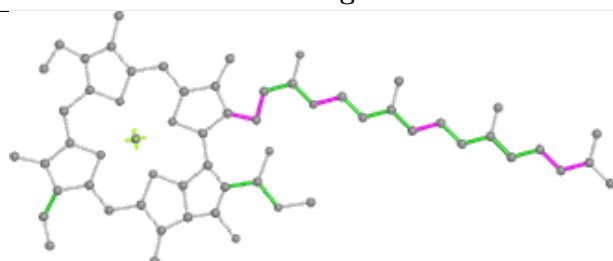
Ligand CLA 7 610



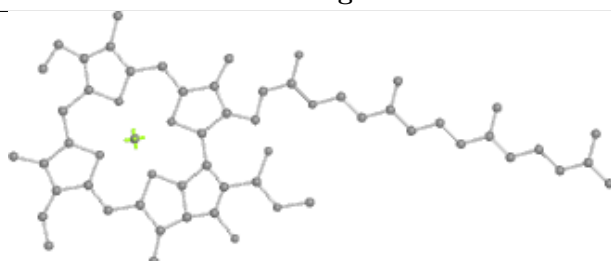
Bond lengths



Bond angles

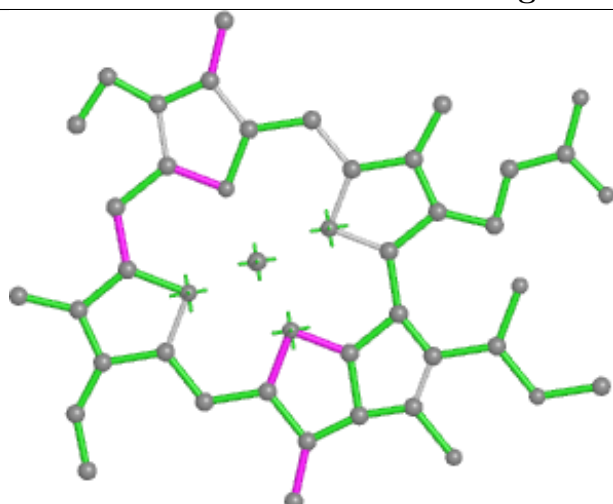


Torsions

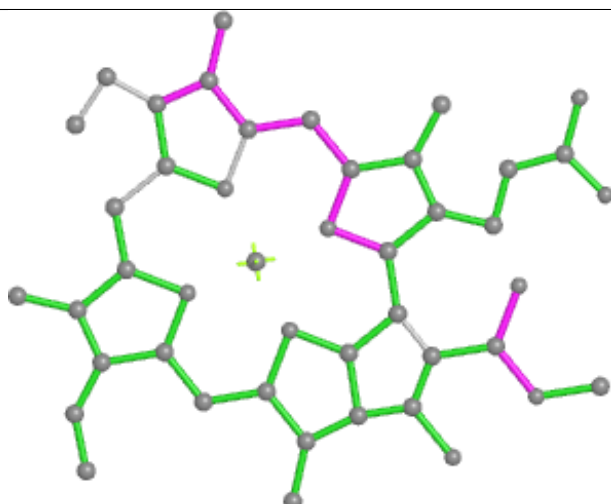


Rings

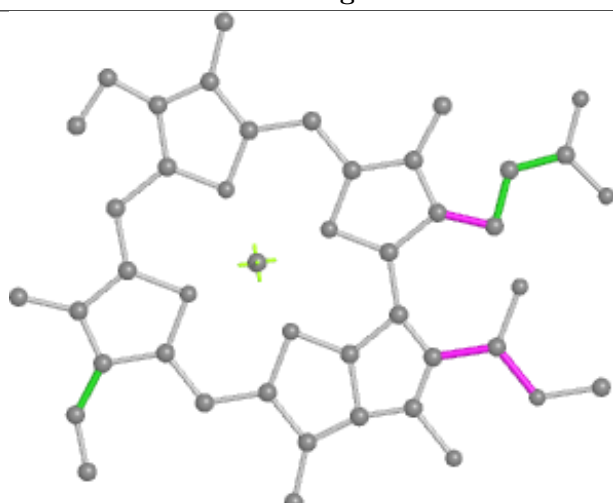
Ligand CLA 6 614



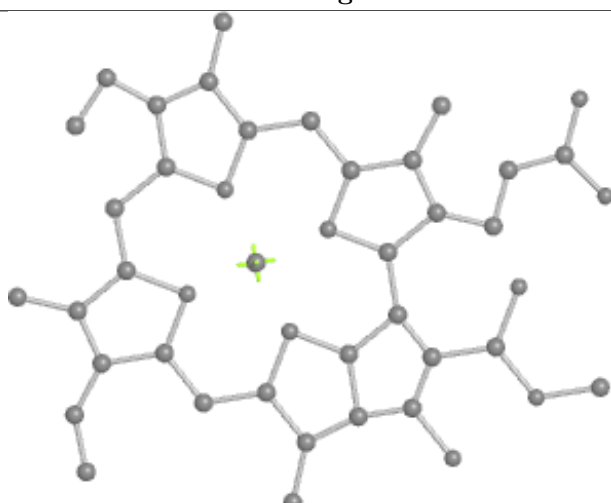
Bond lengths



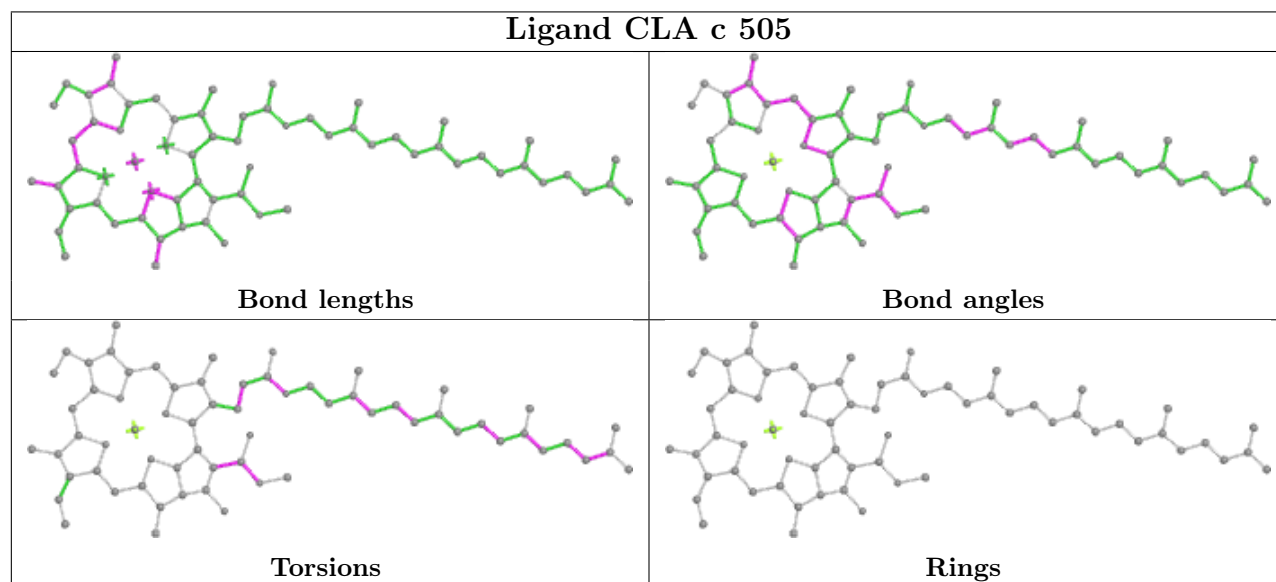
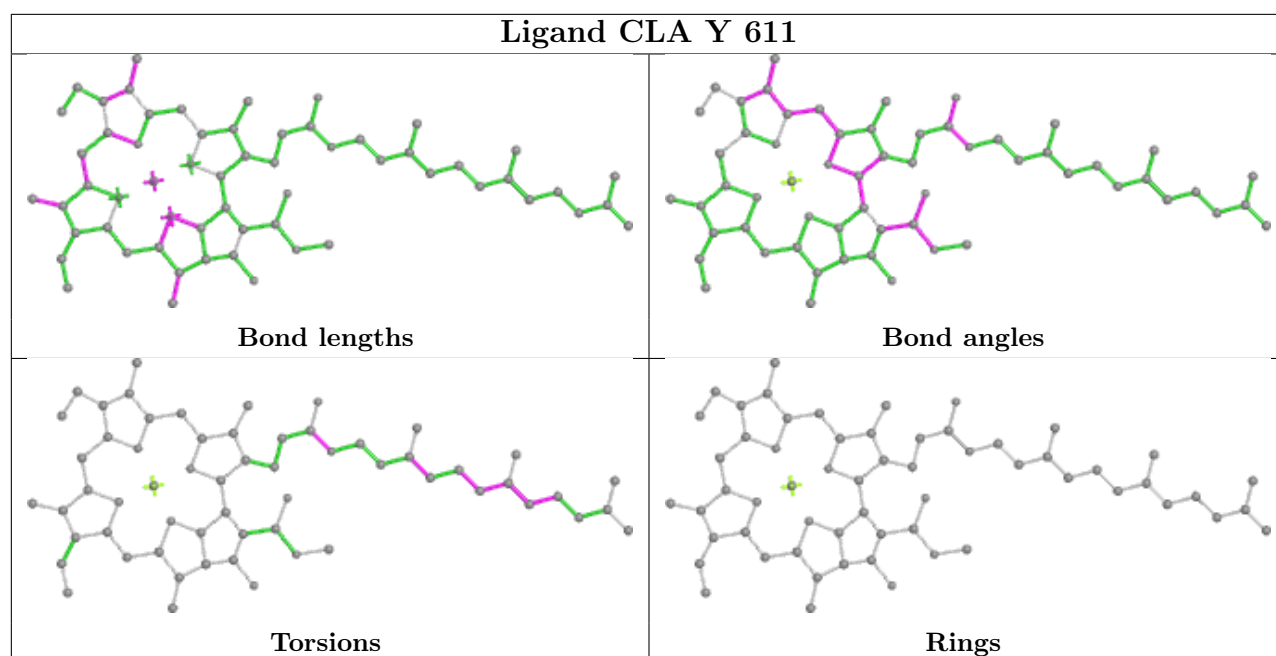
Bond angles



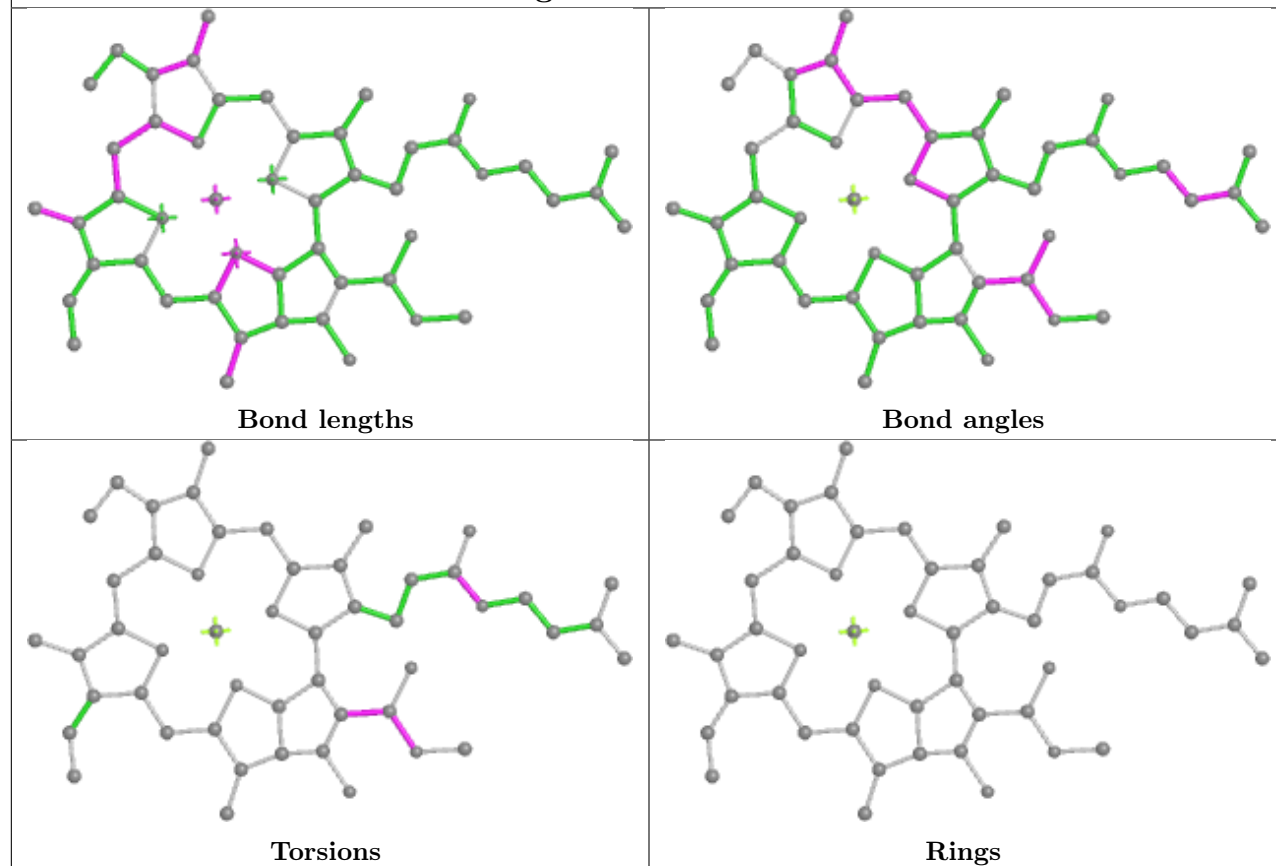
Torsions



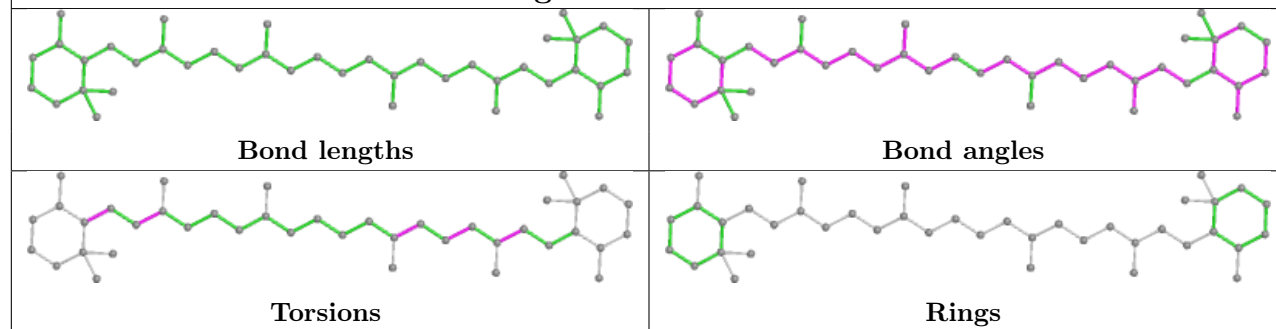
Rings



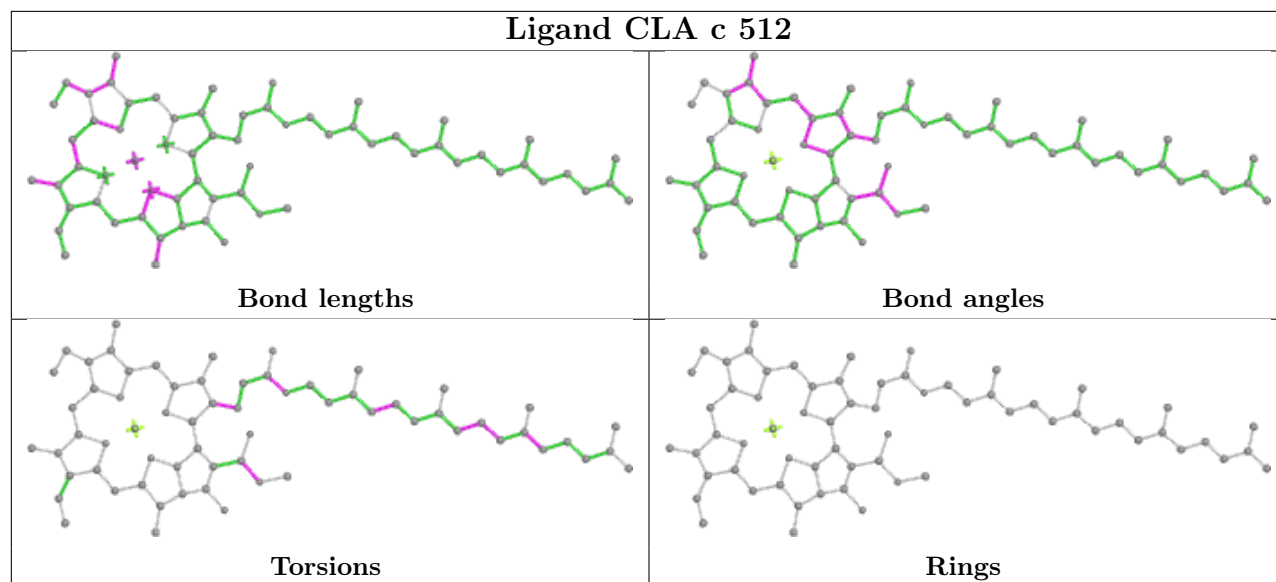
Ligand CLA n 604



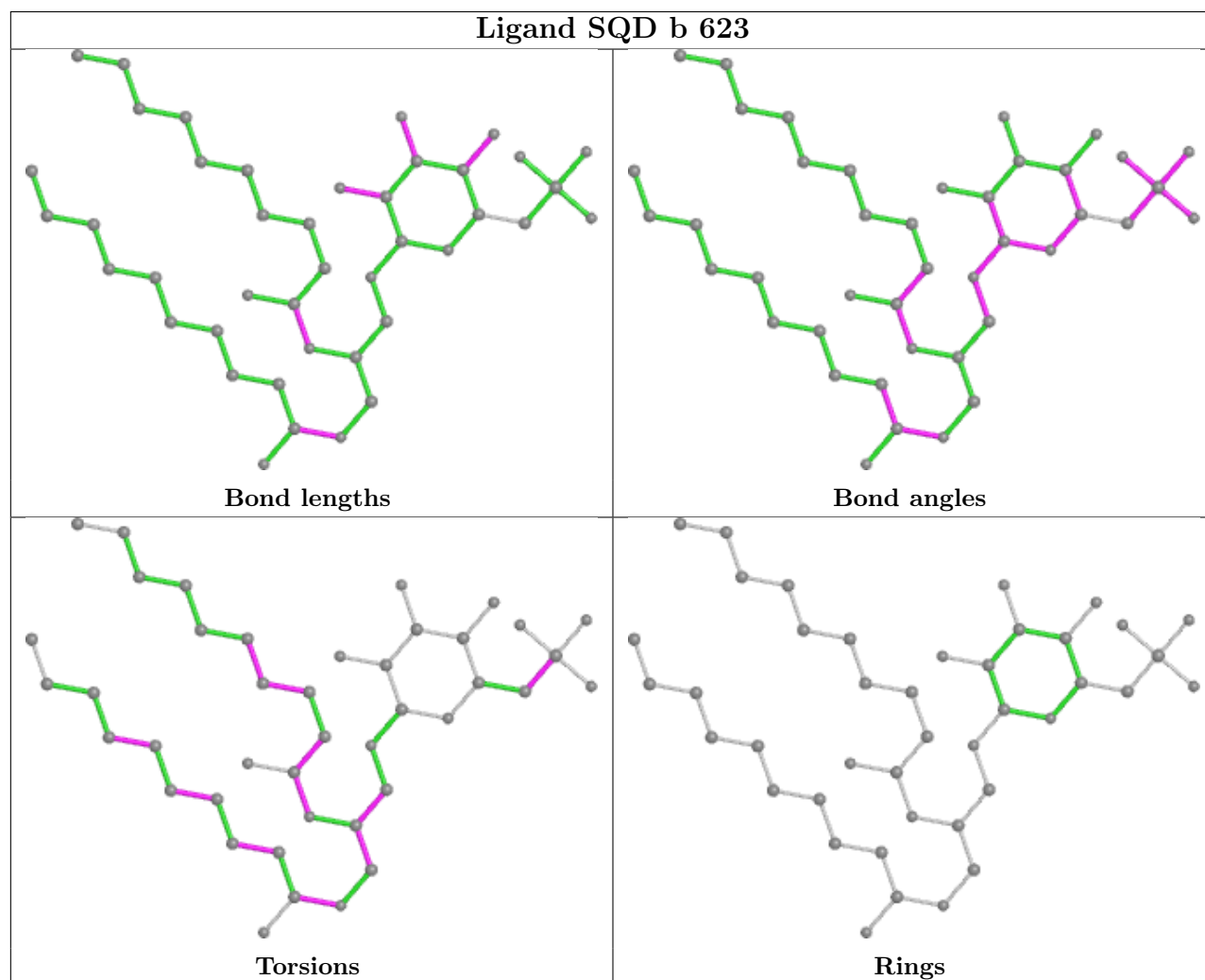
Ligand BCR 4 623

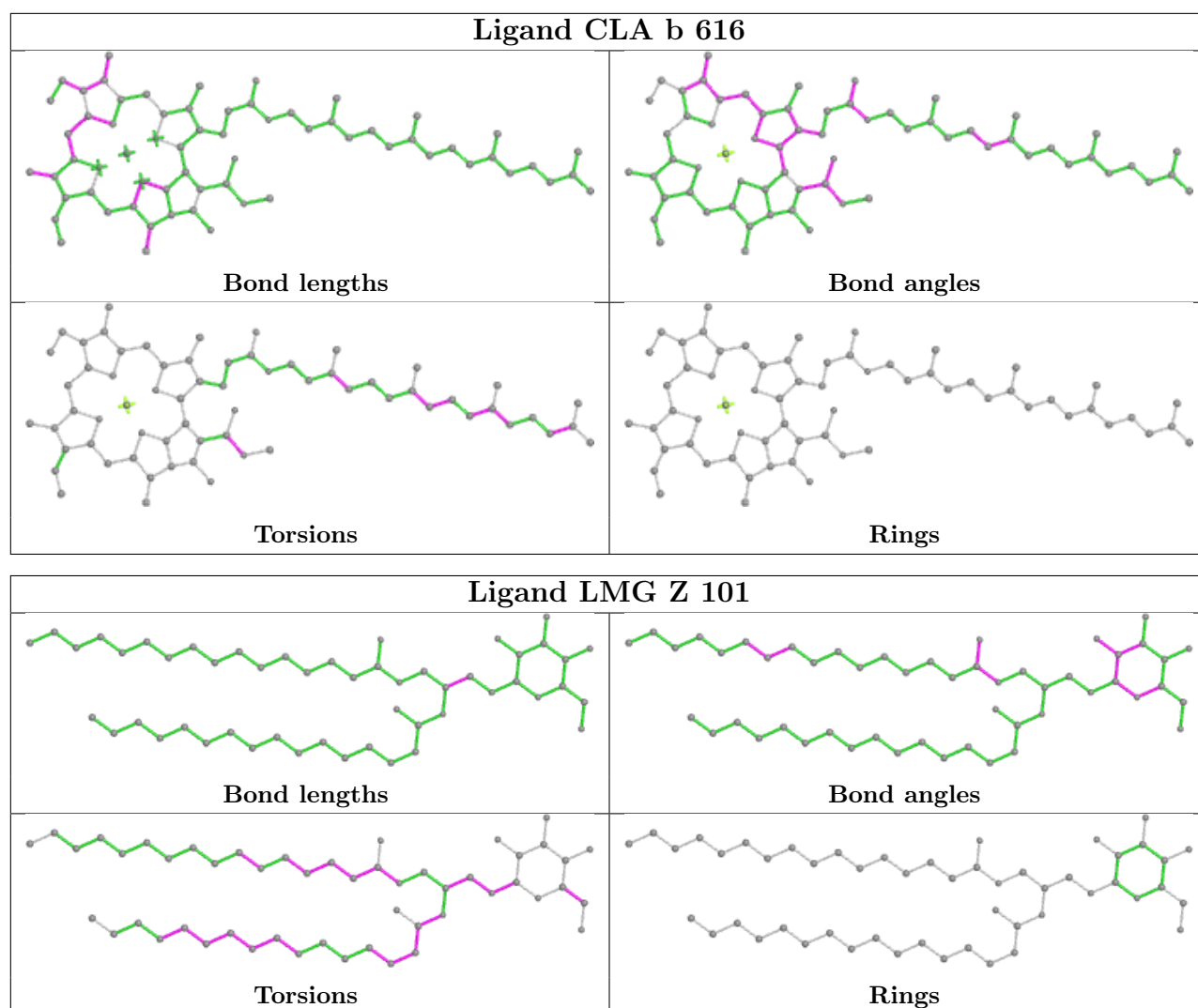


Ligand CLA c 512

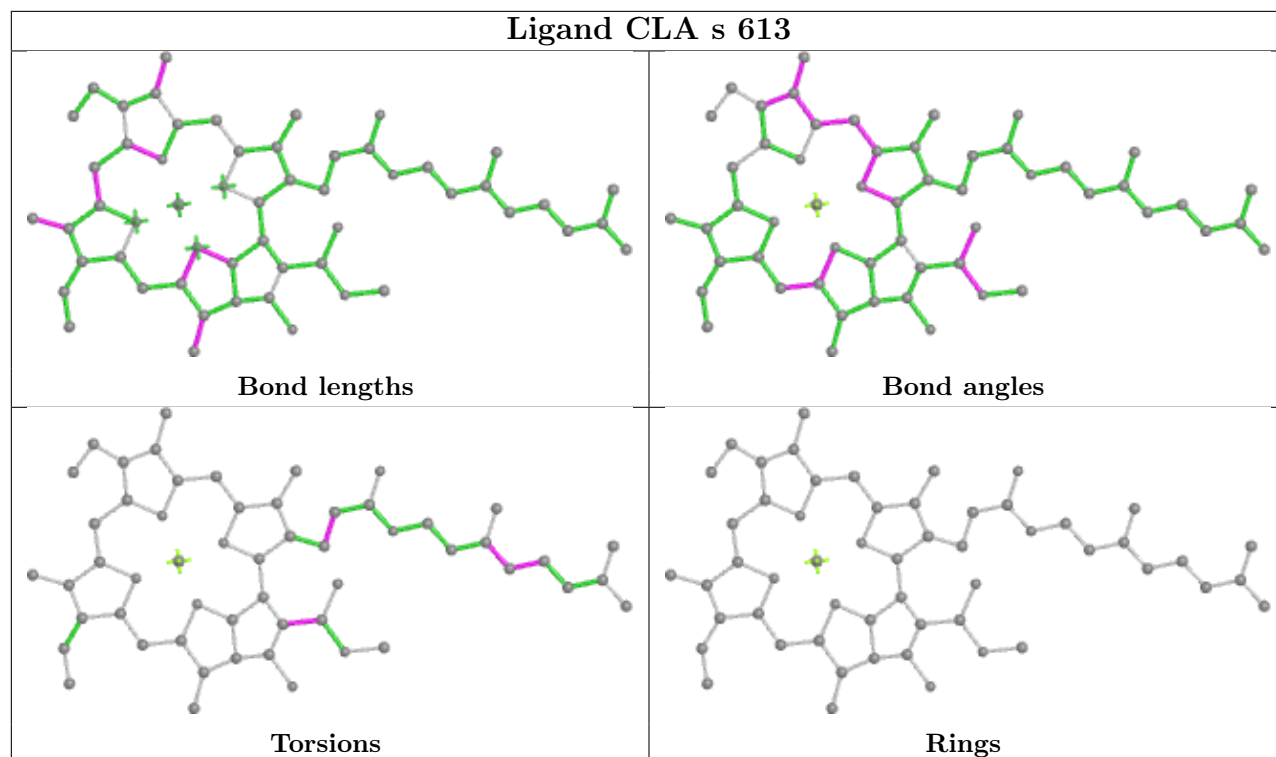


Ligand SQD b 623

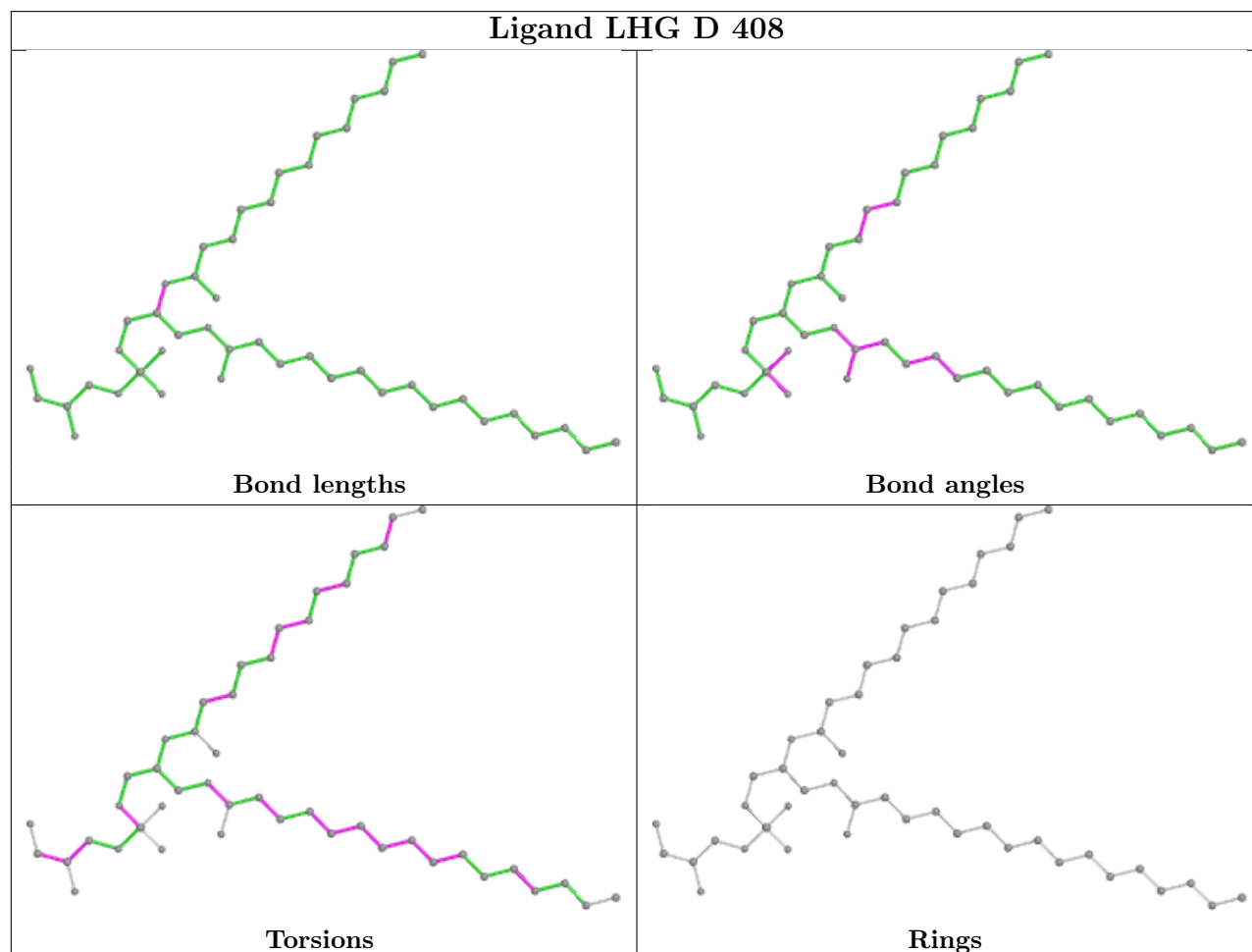


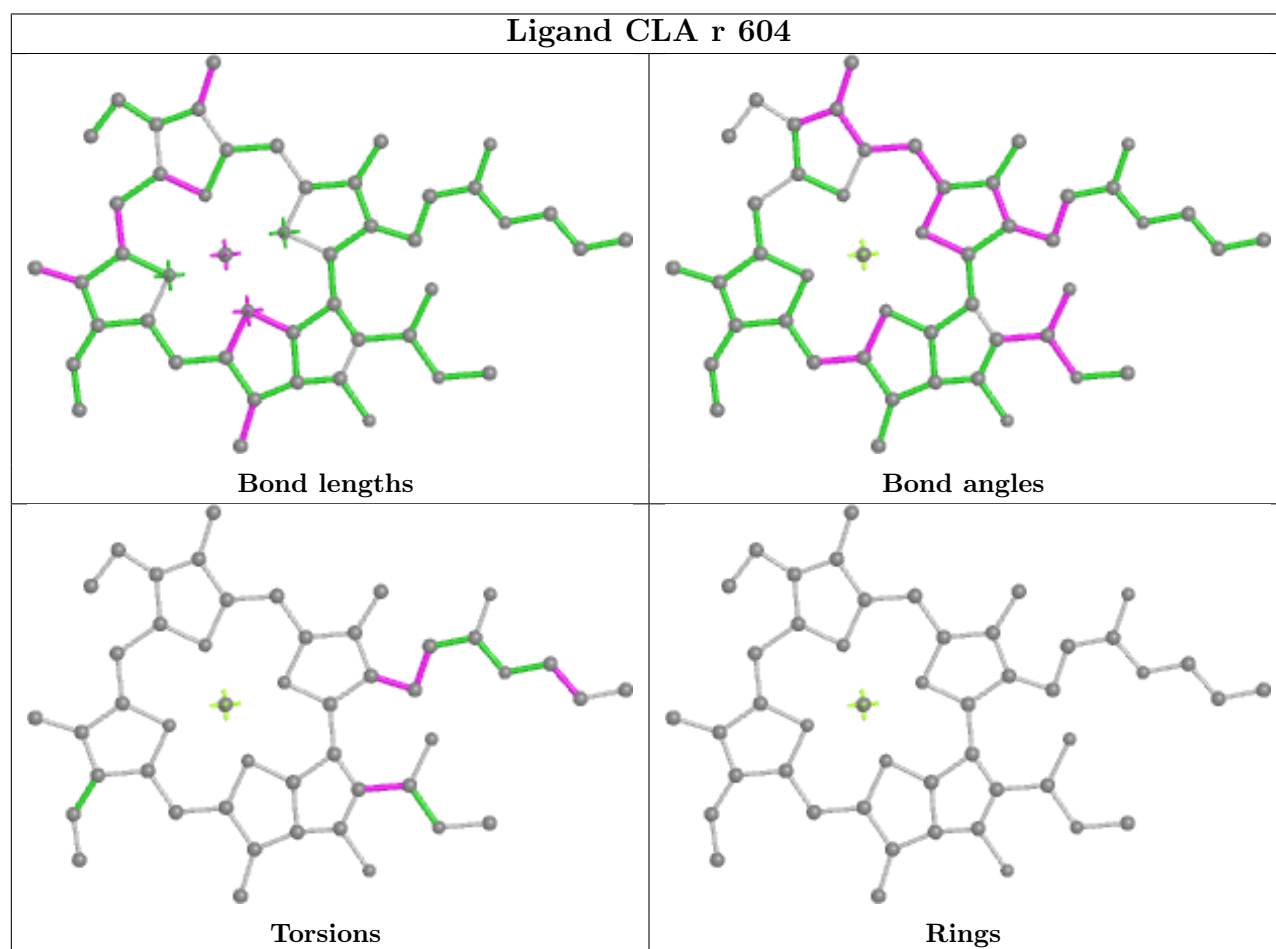
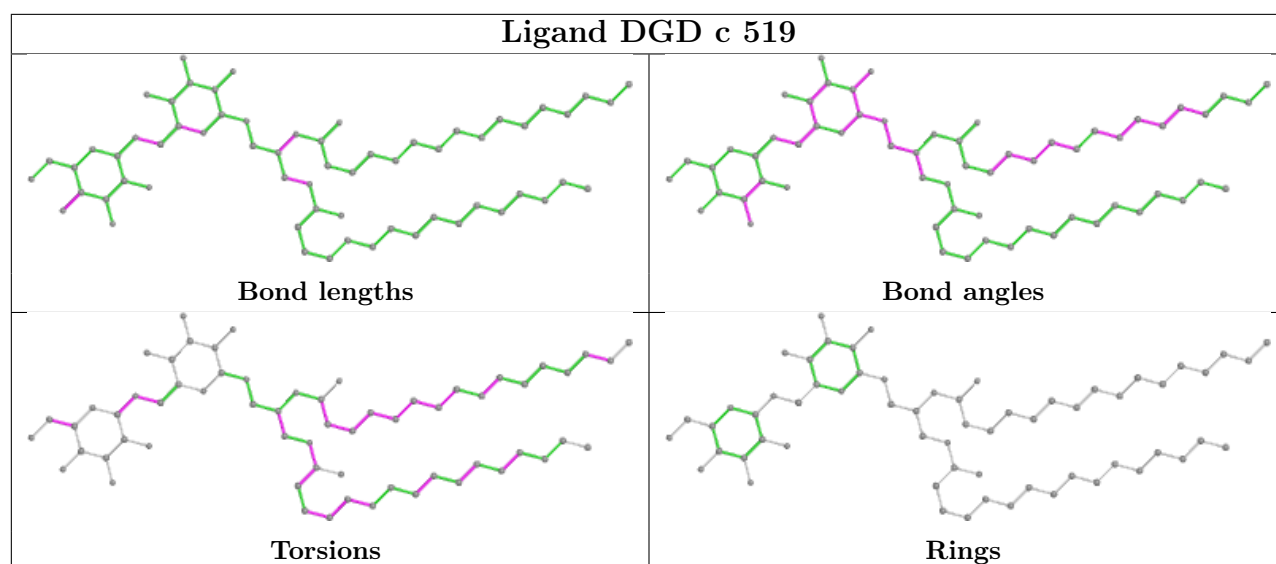


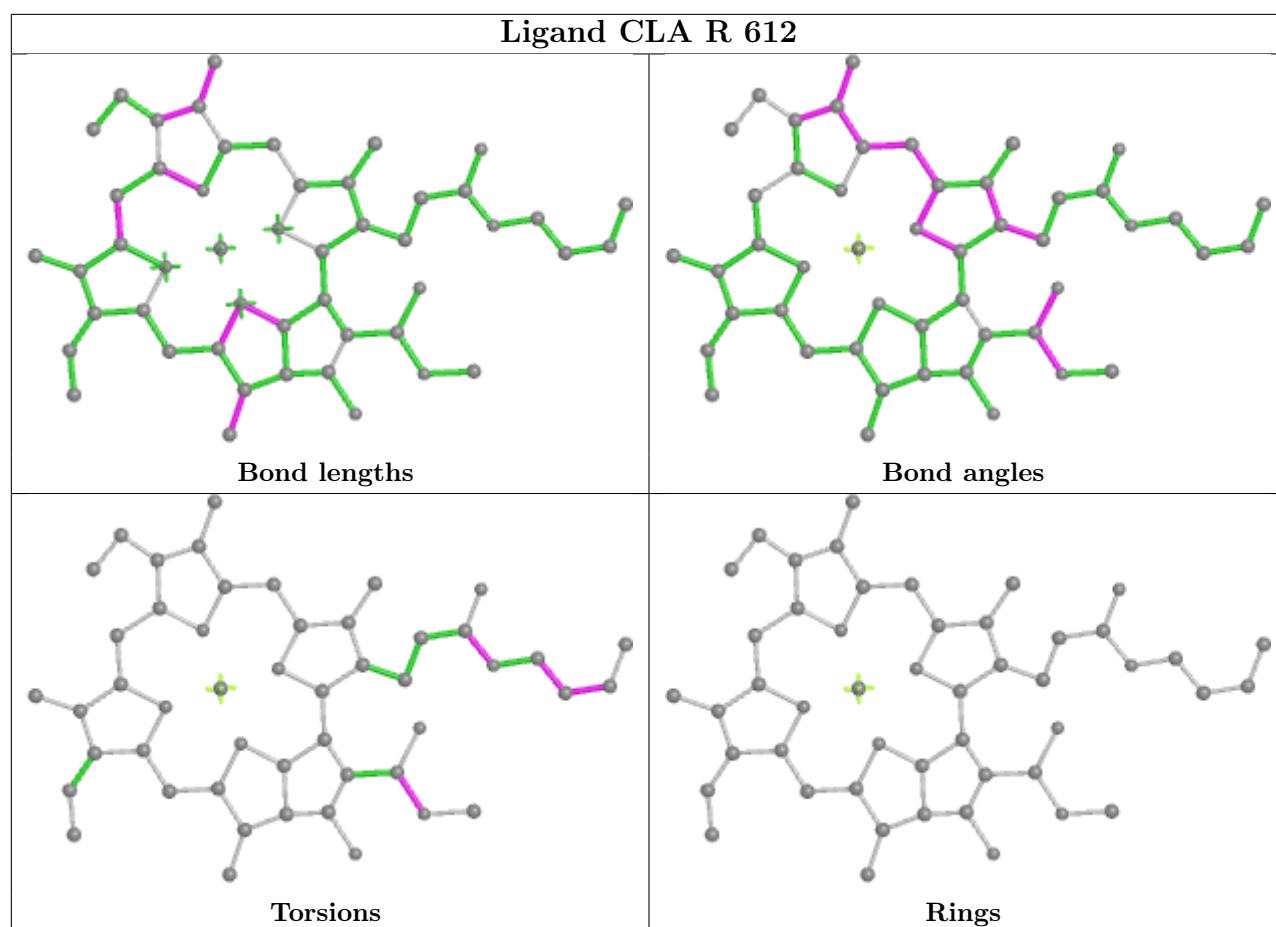
Ligand CLA s 613



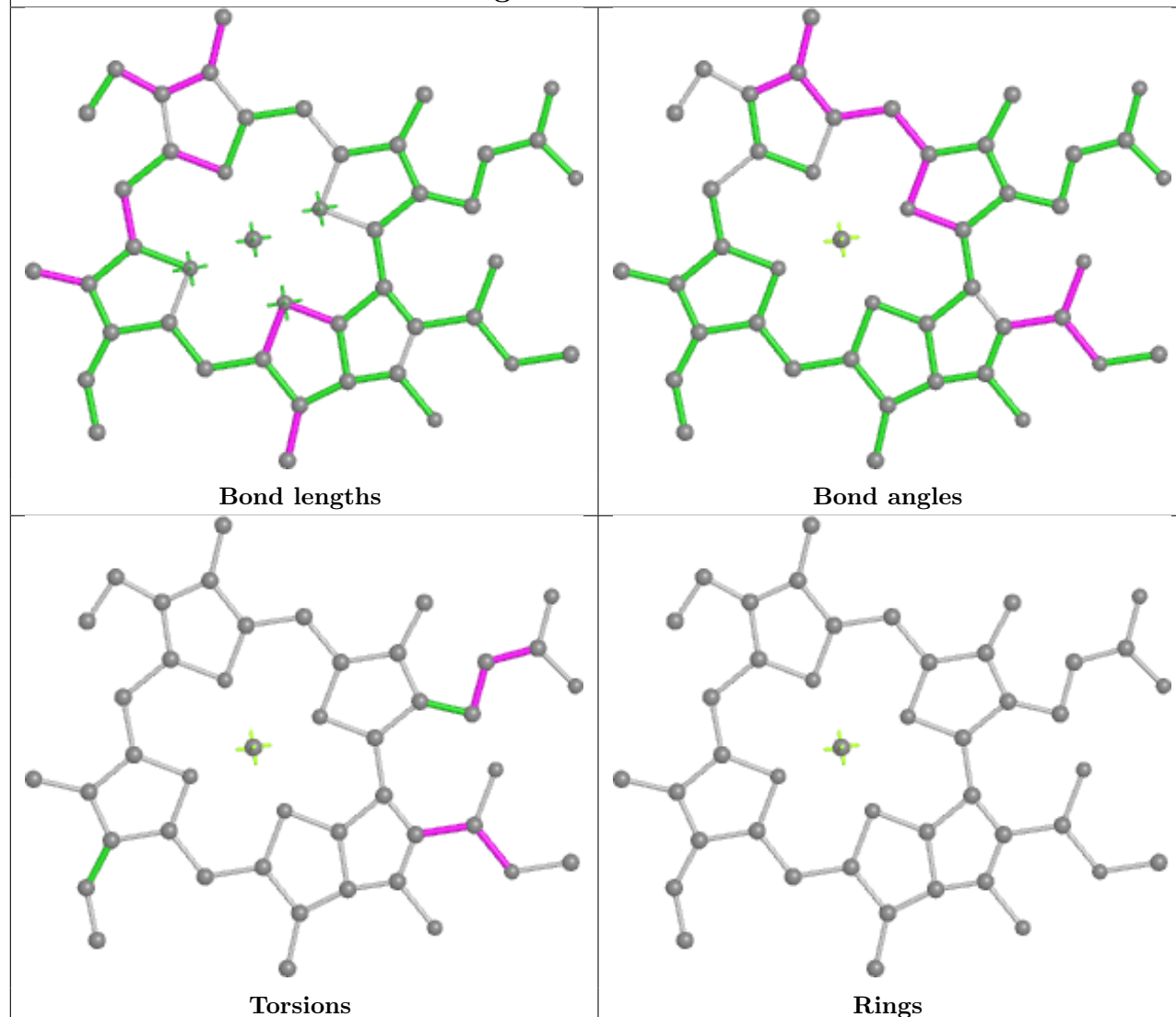
Ligand LHG D 408



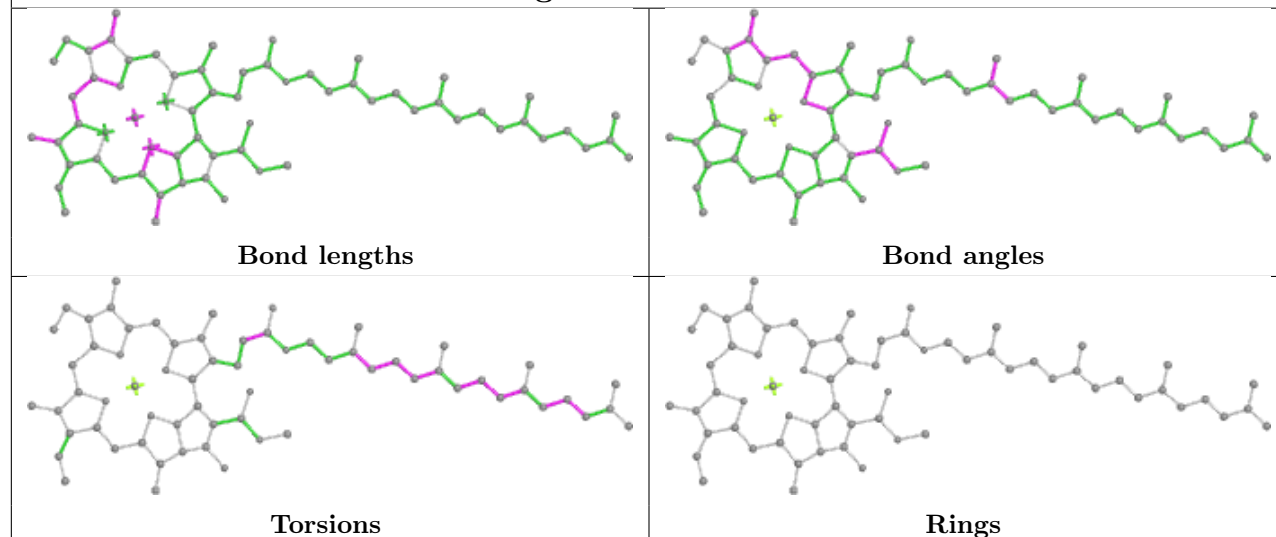




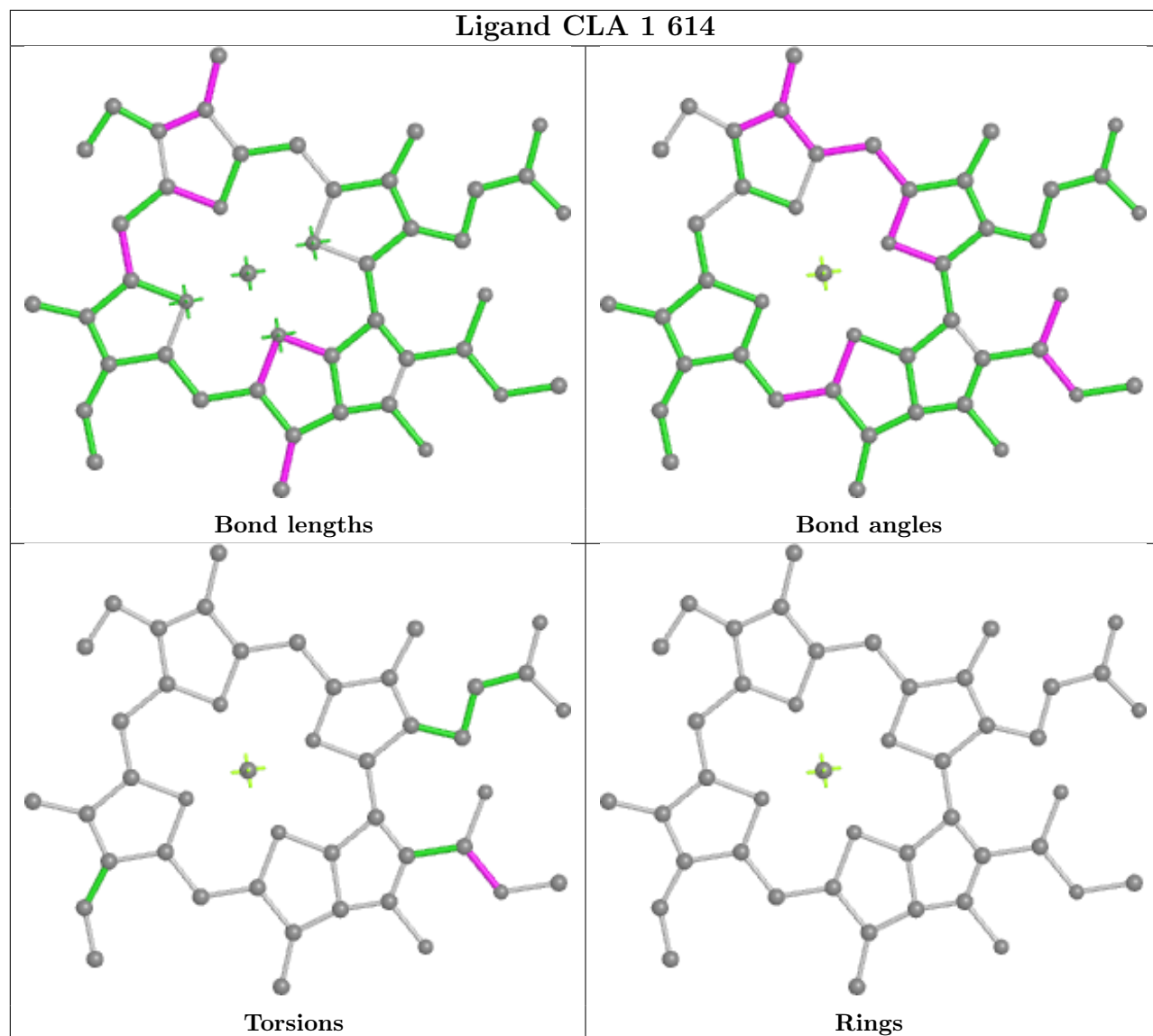
Ligand CLA 8 602



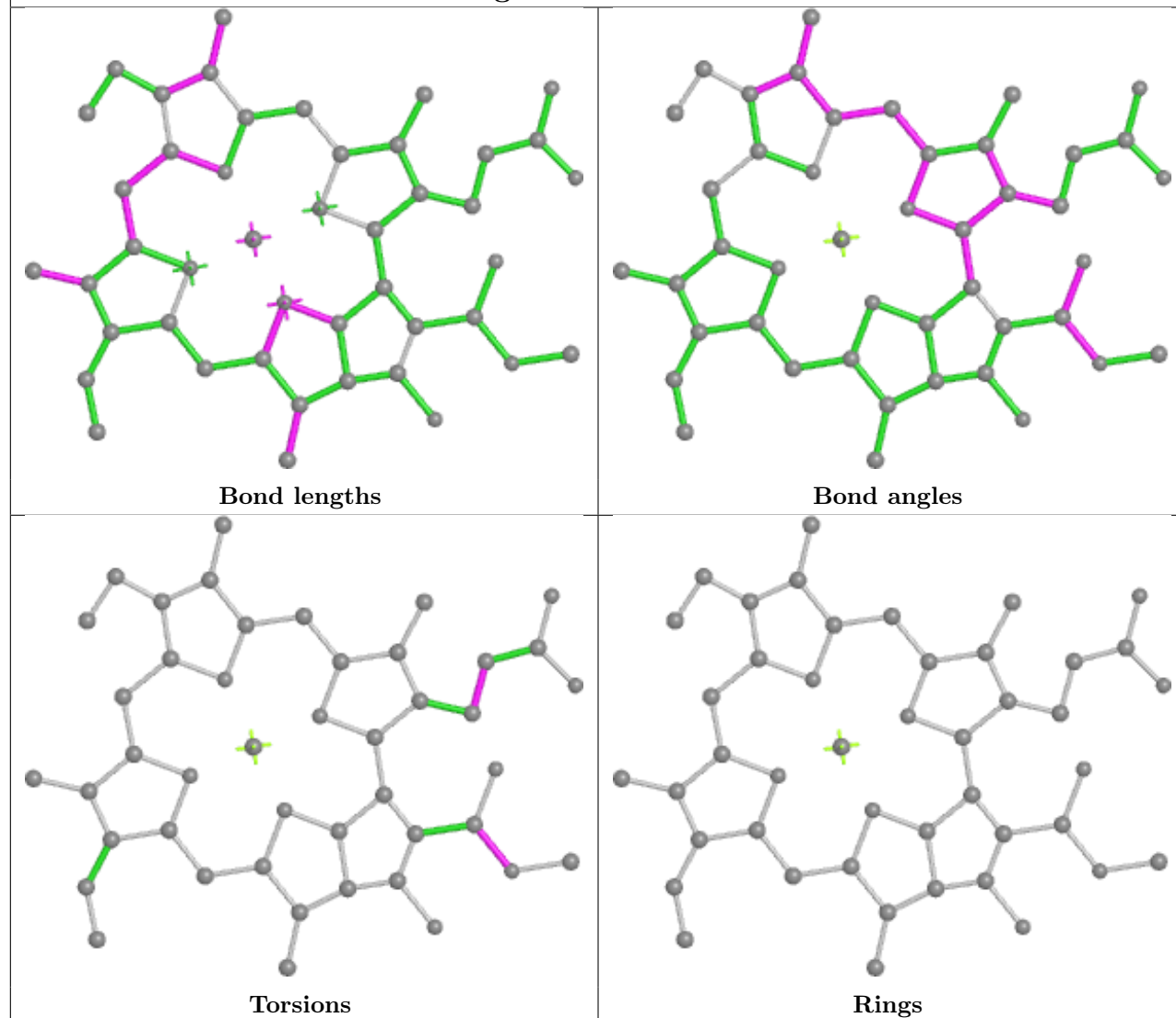
Ligand CLA b 614



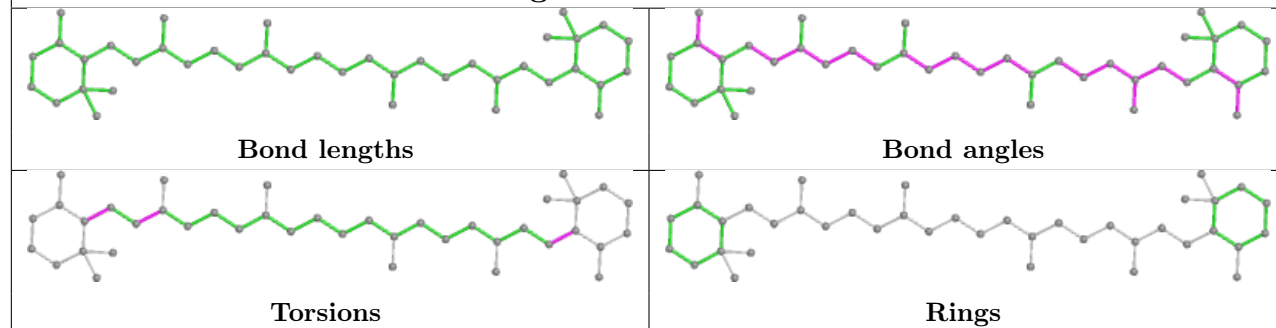
Ligand CLA 1 614

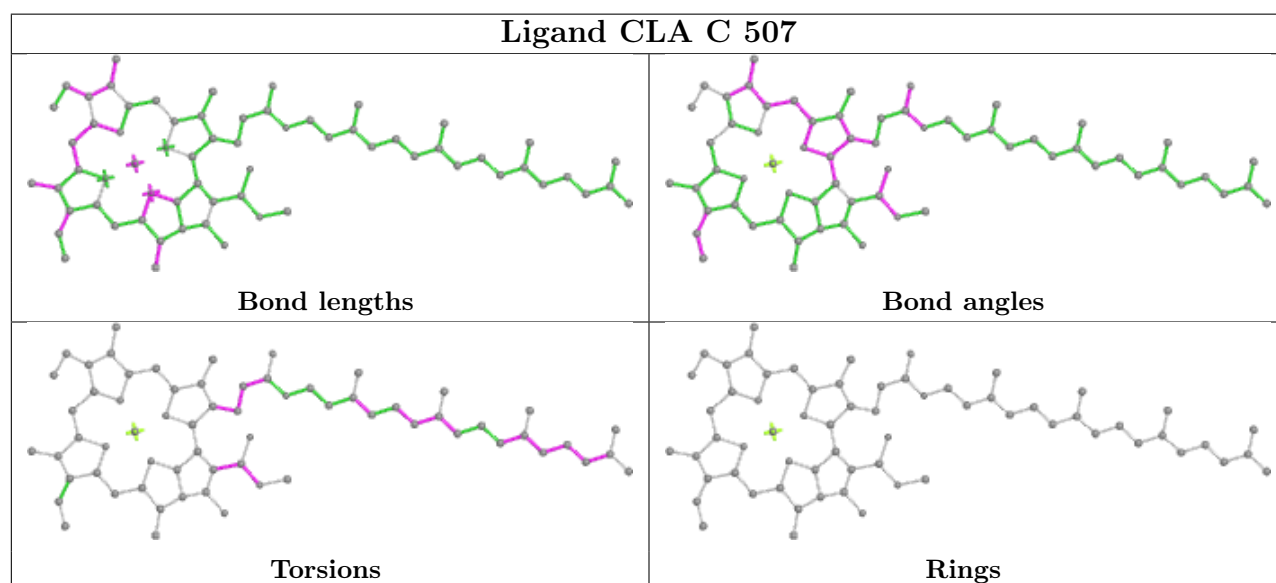
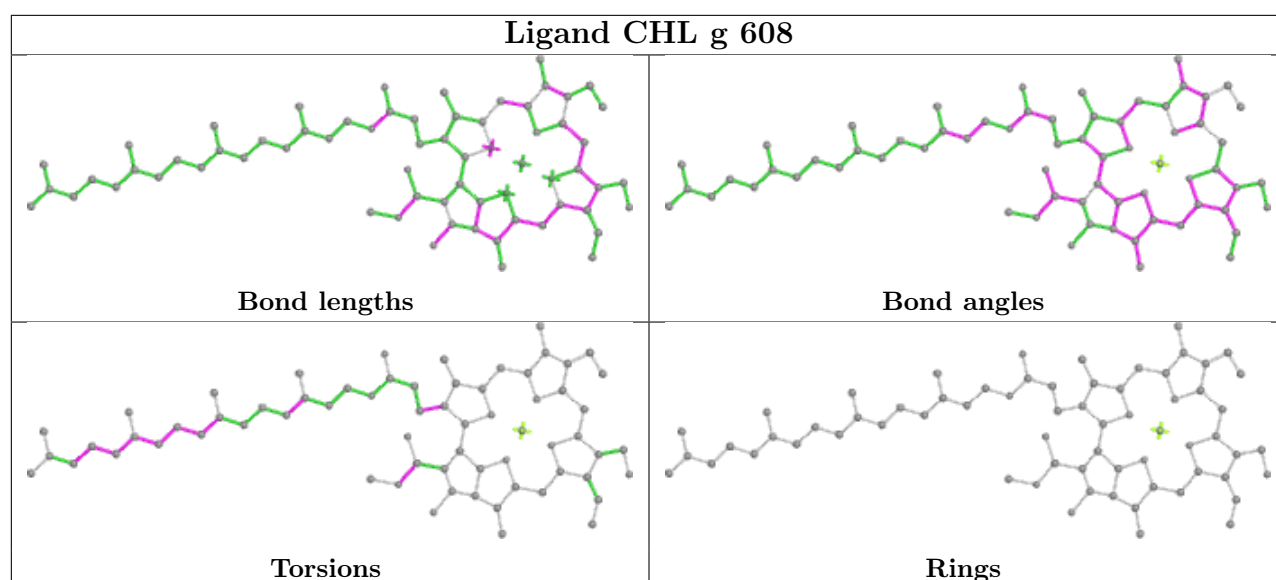
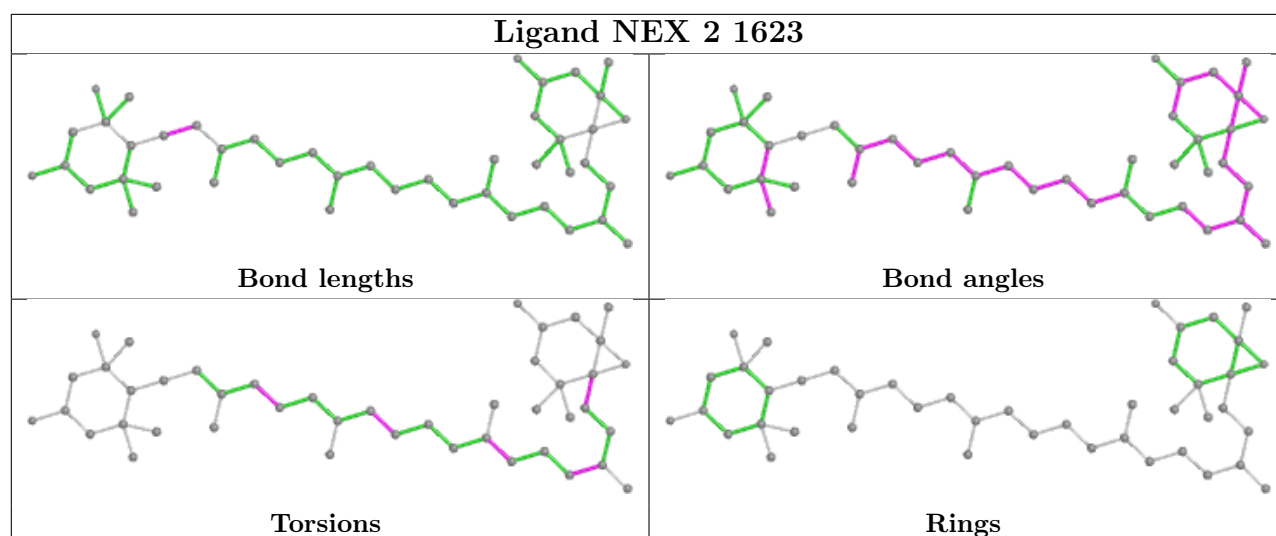


Ligand CLA 1 612

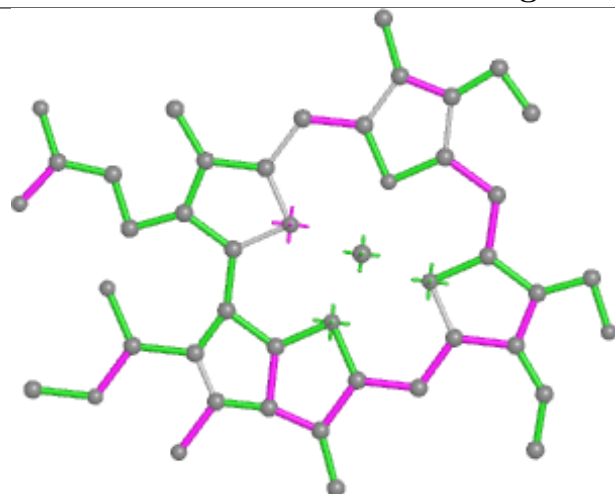


Ligand BCR A 411

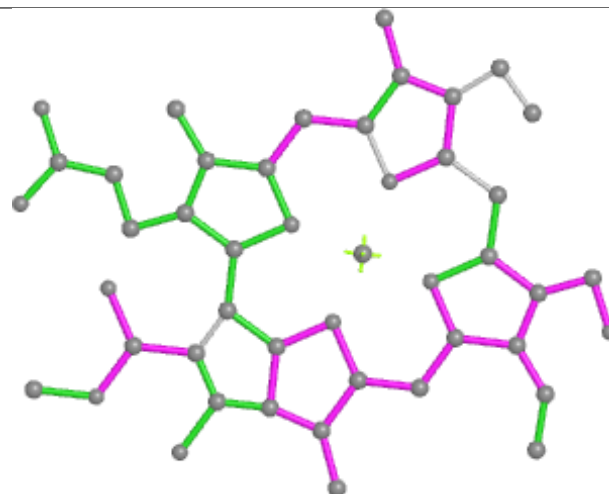




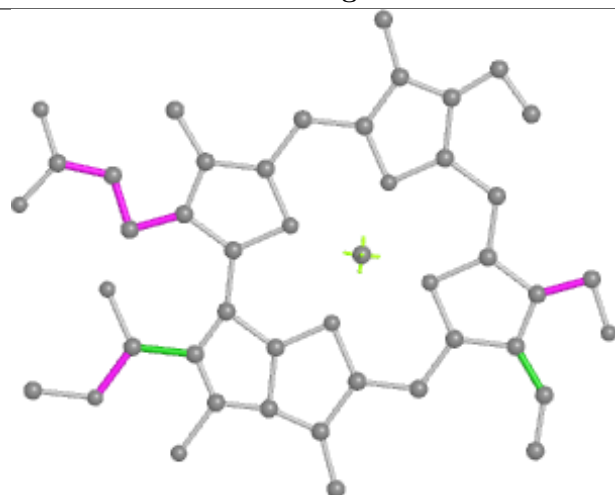
Ligand CHL 4 607



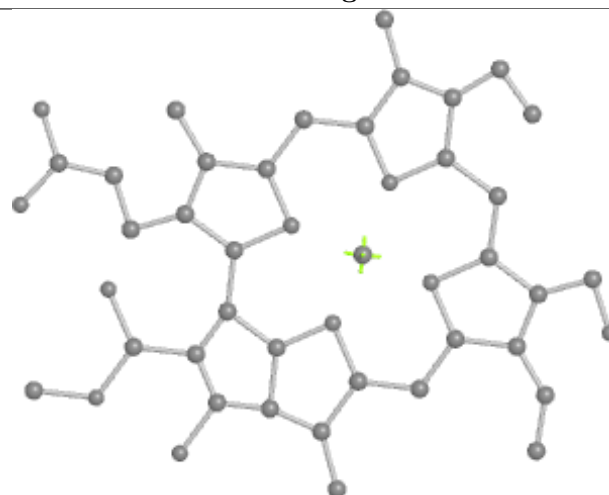
Bond lengths



Bond angles

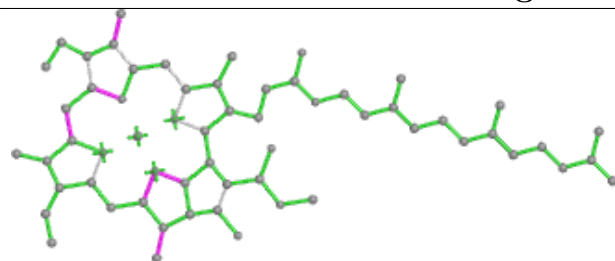


Torsions

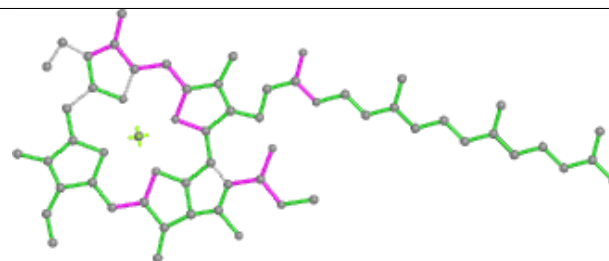


Rings

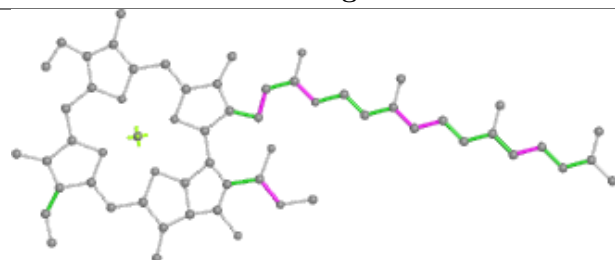
Ligand CLA R 602



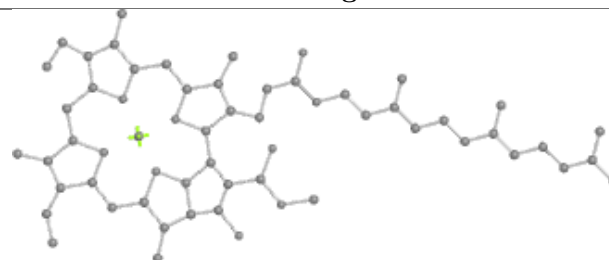
Bond lengths



Bond angles

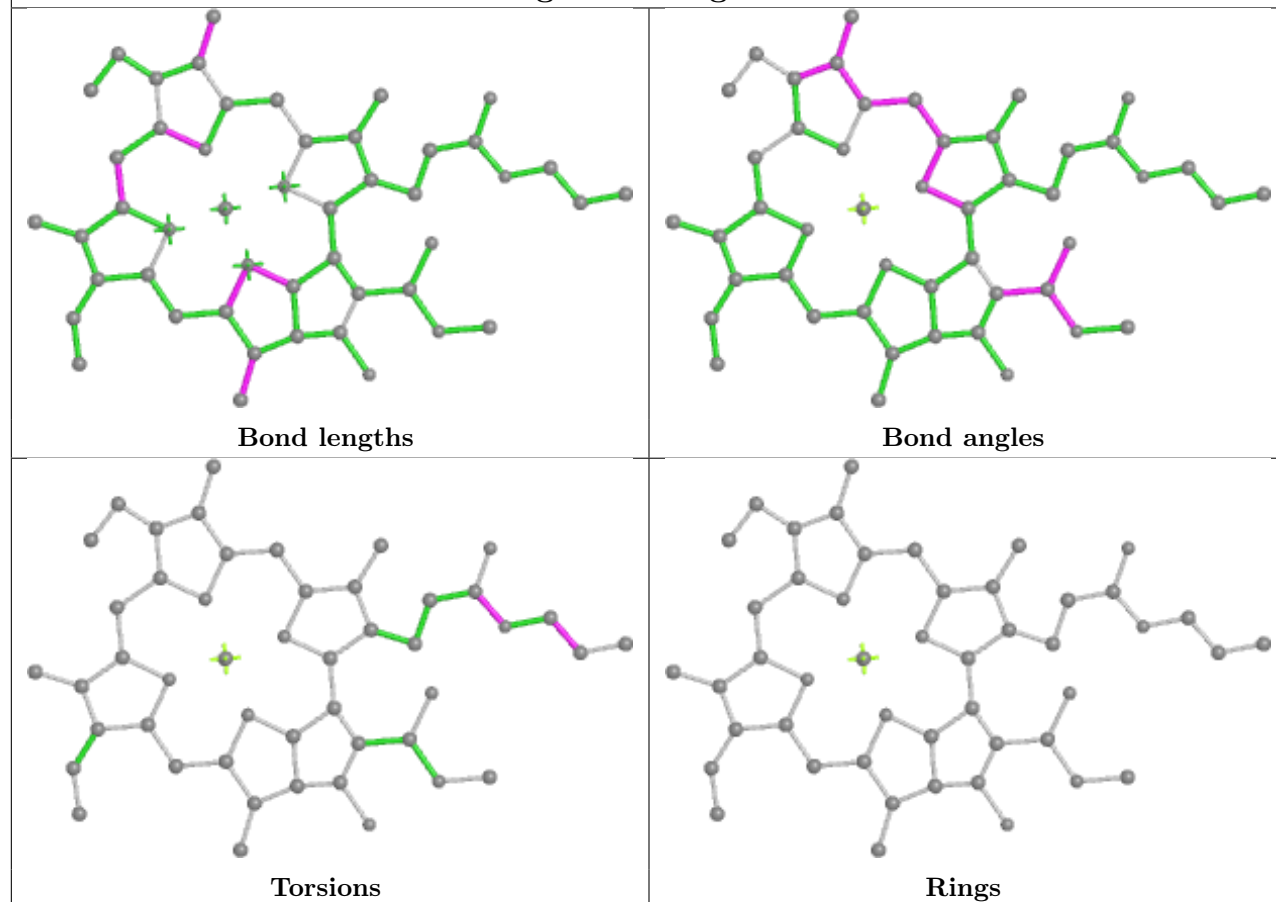


Torsions

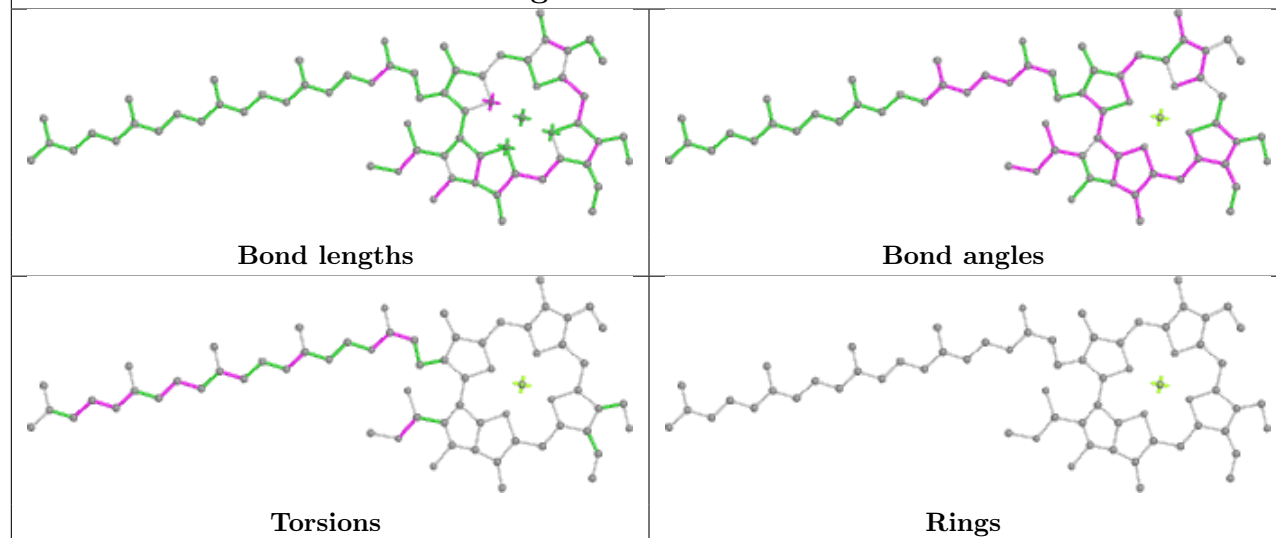


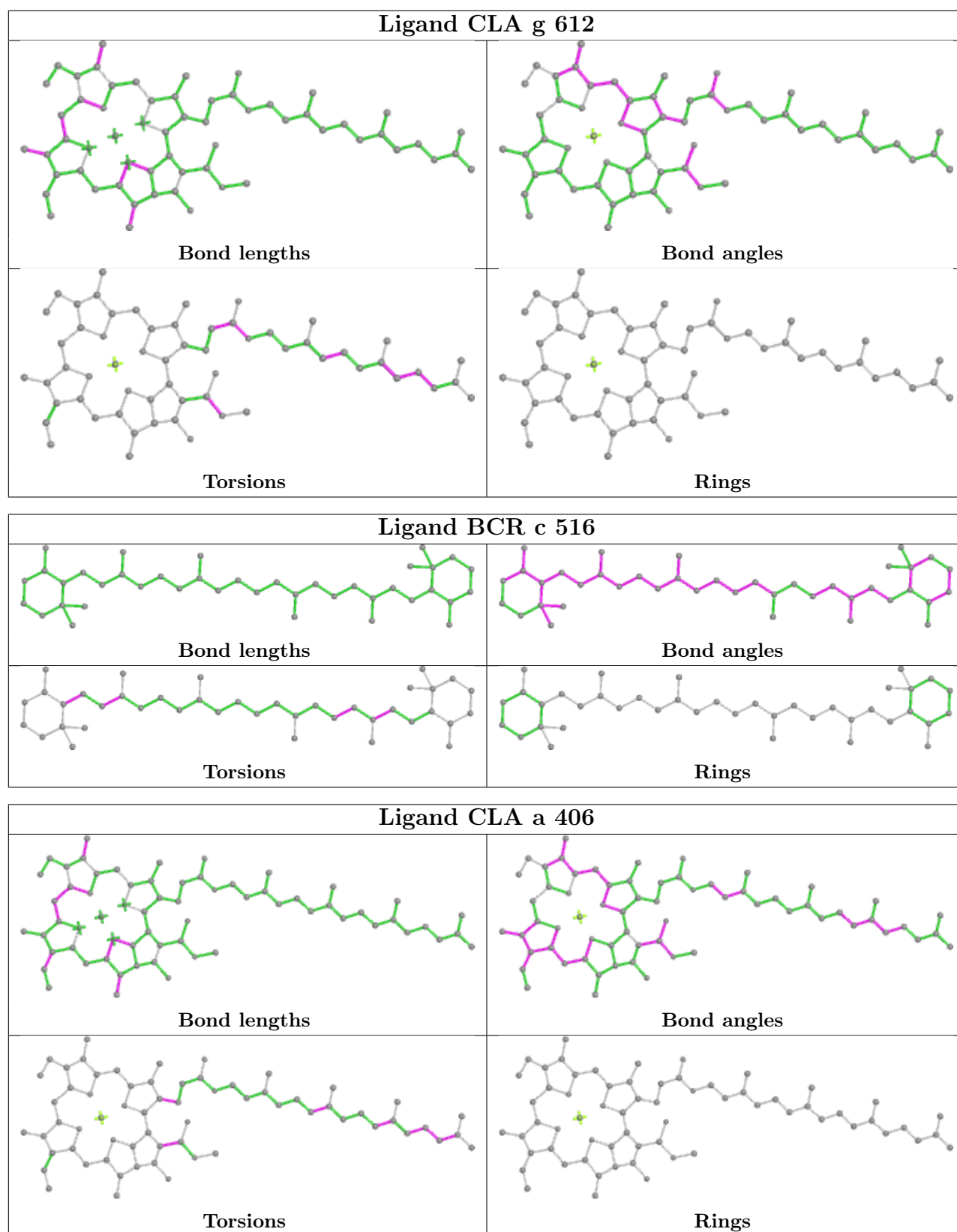
Rings

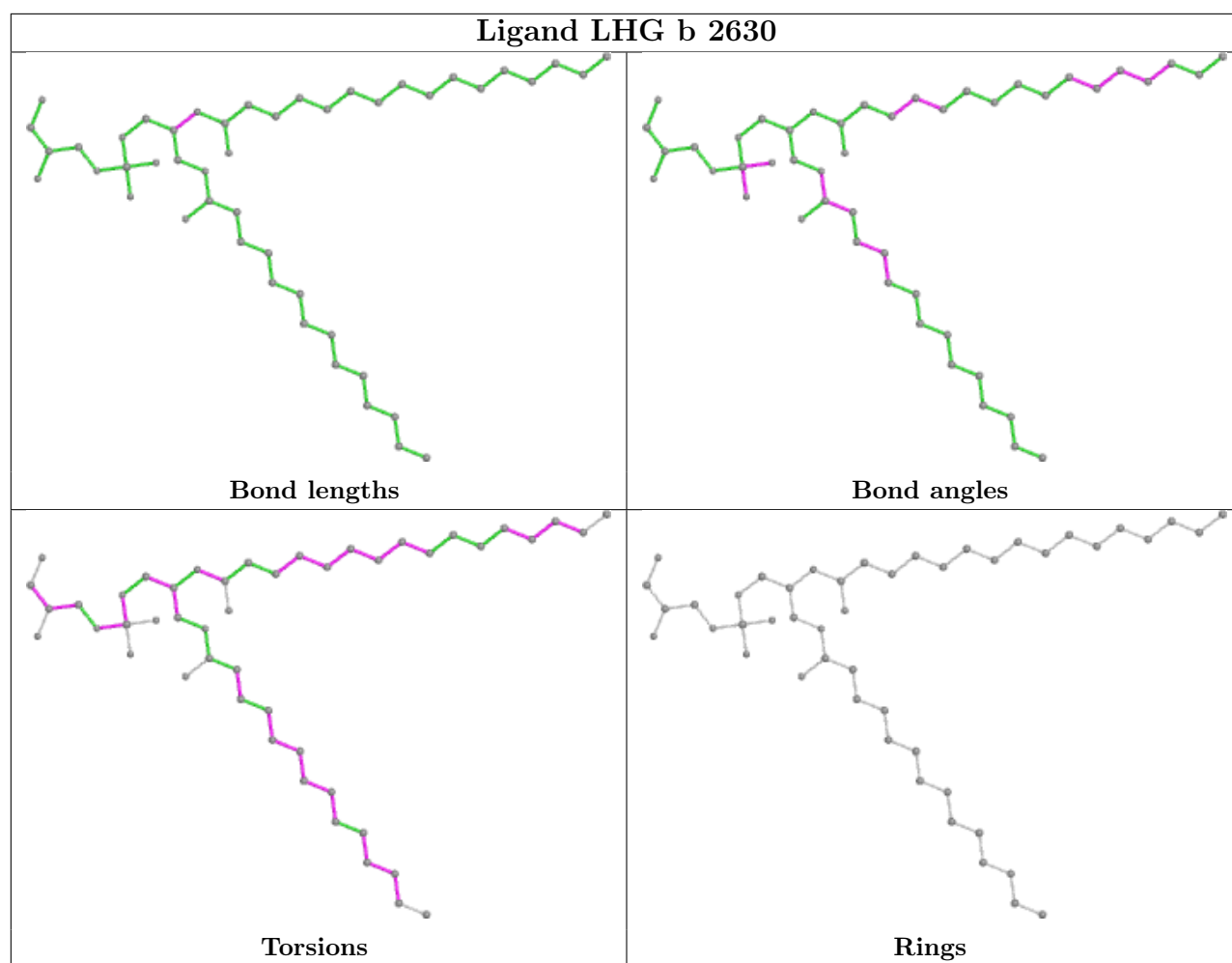
Ligand CLA g 614



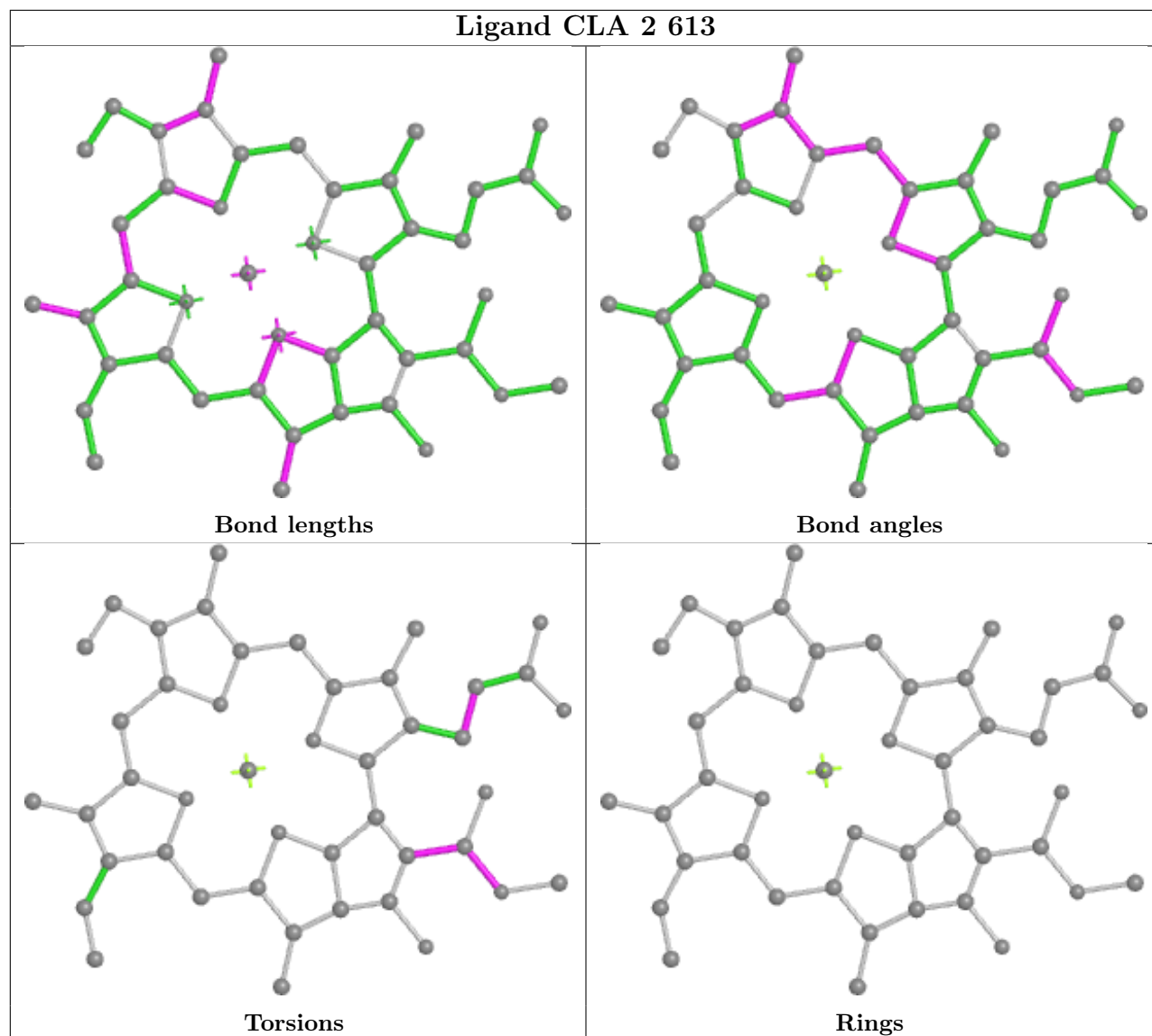
Ligand CHL G 601



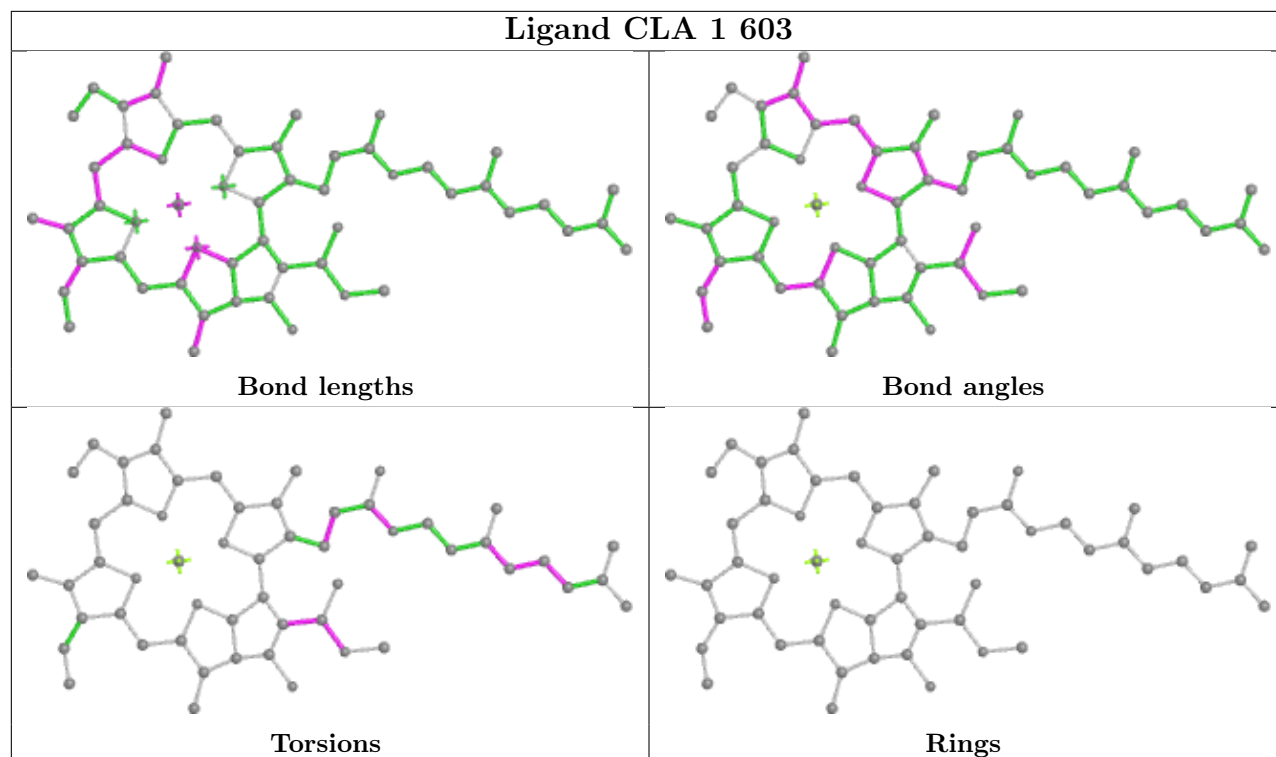




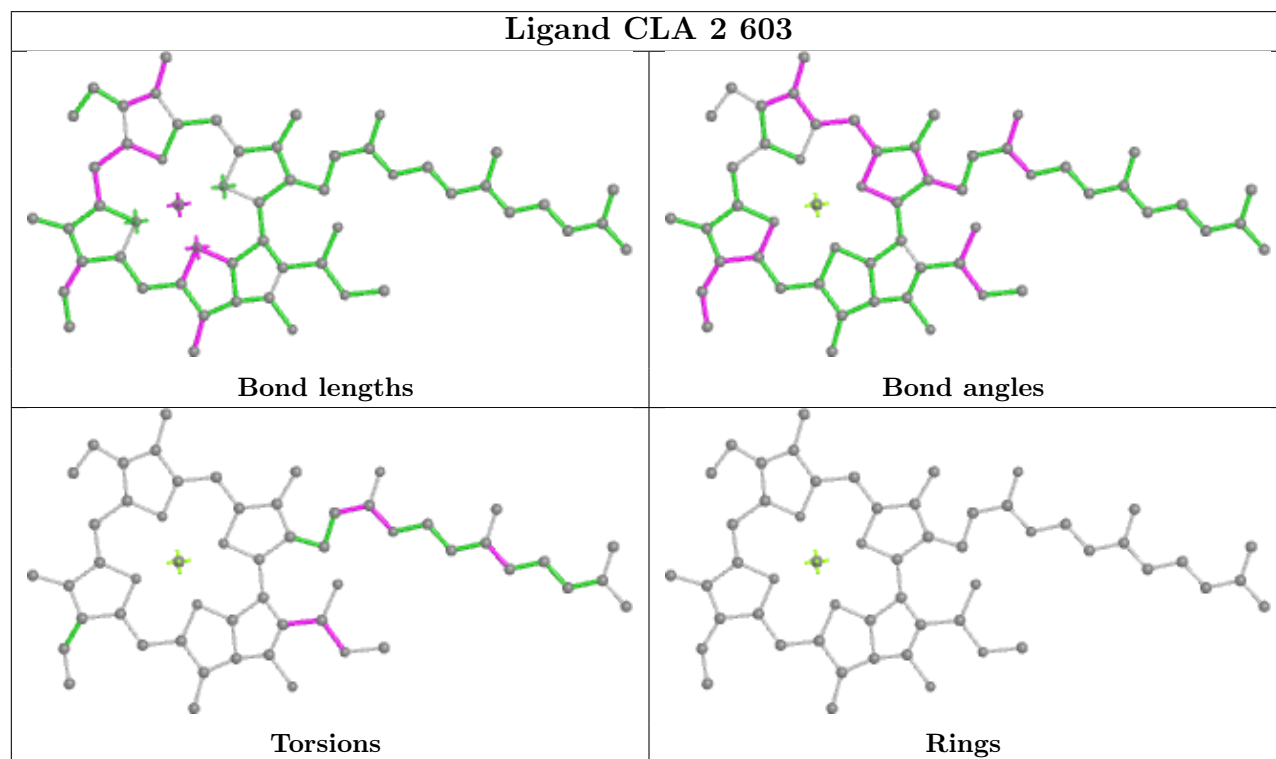
Ligand CLA 2 613

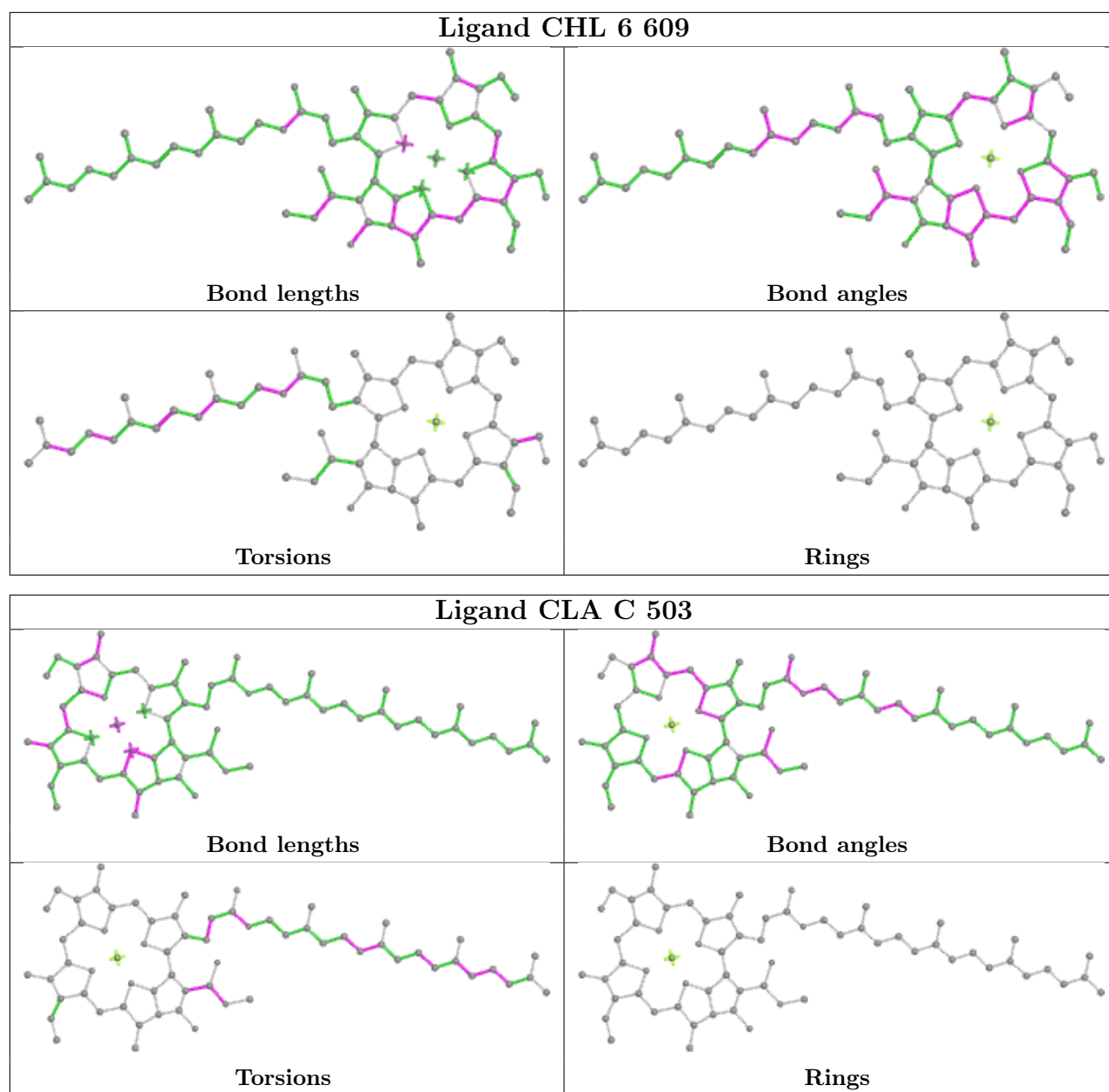


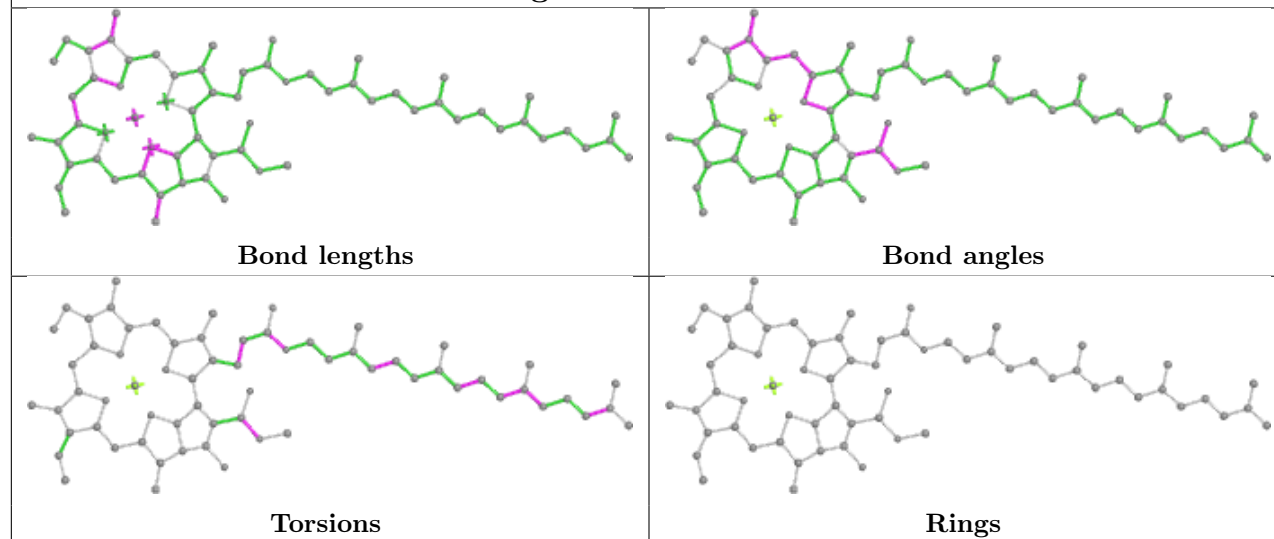
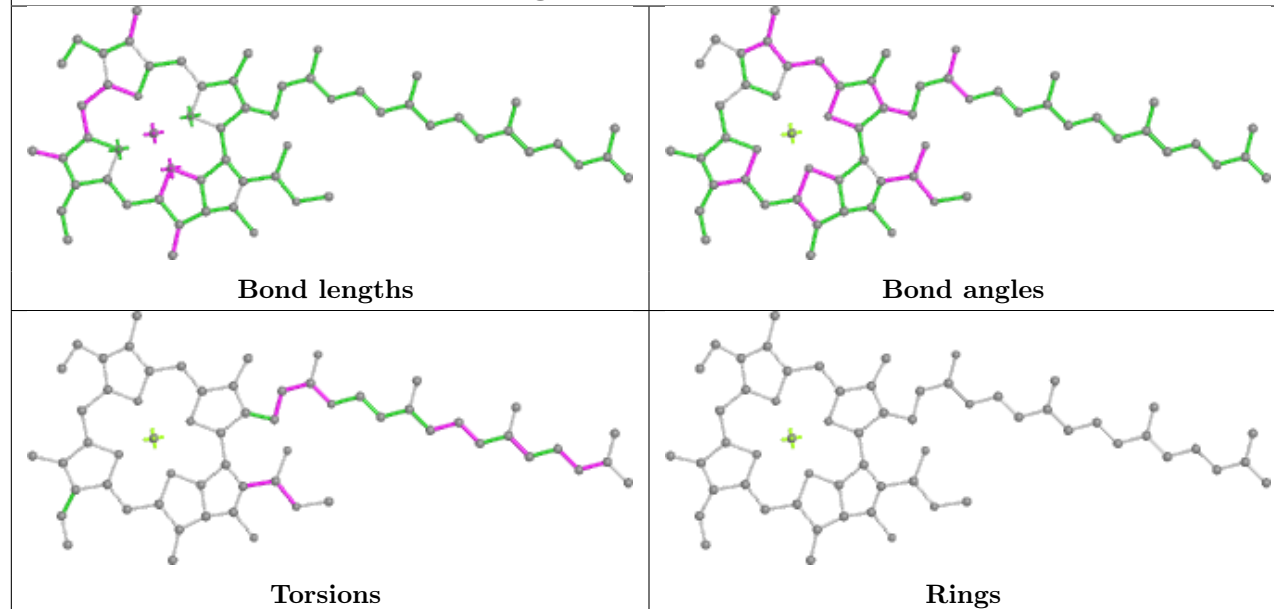
Ligand CLA 1 603

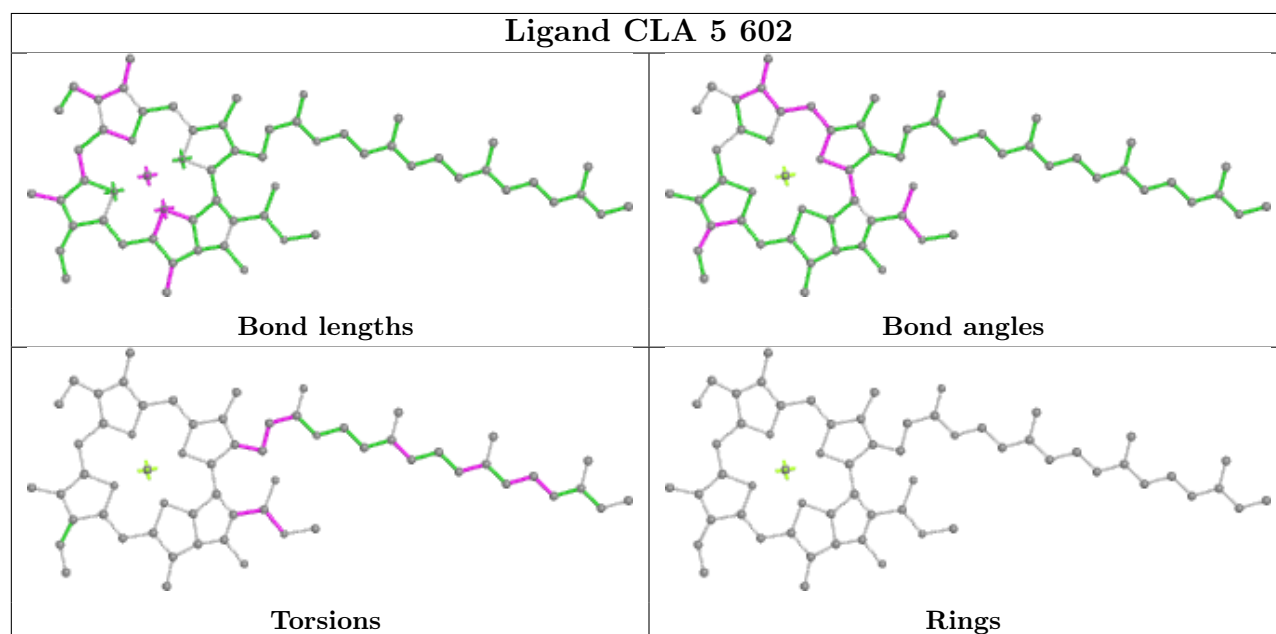
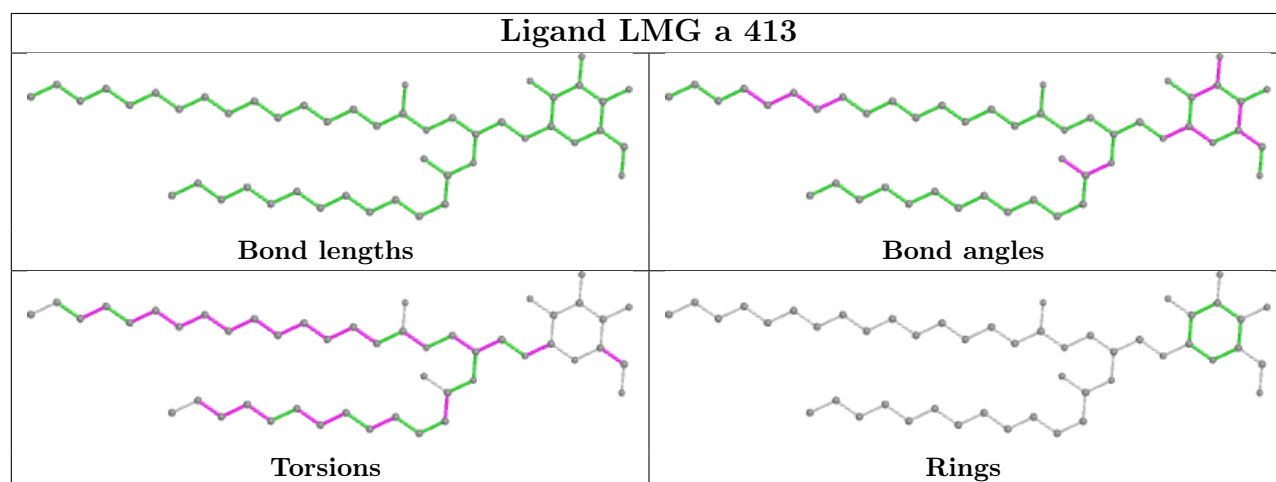
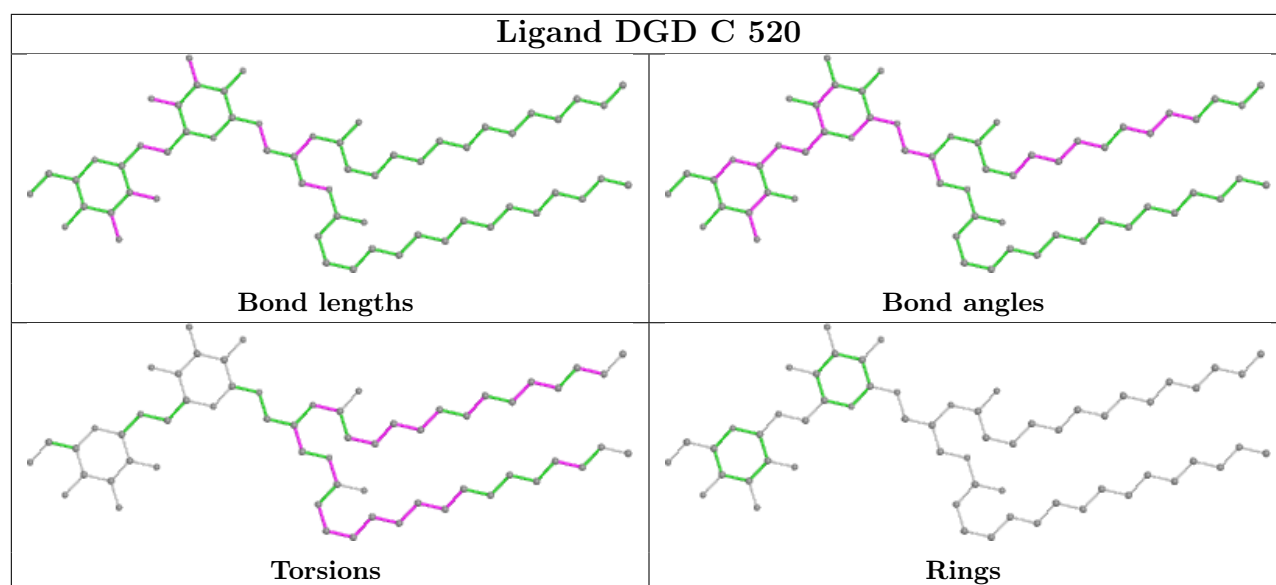


Ligand CLA 2 603

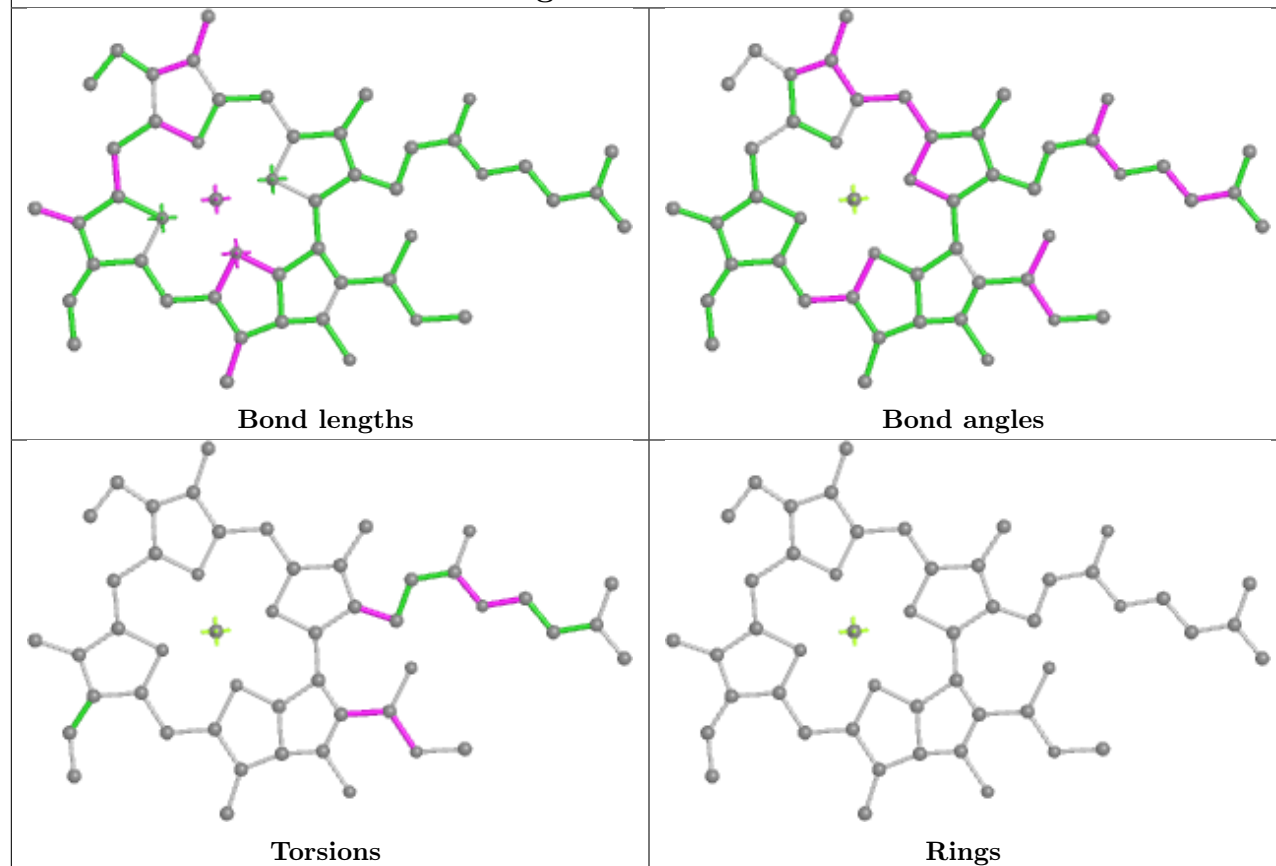




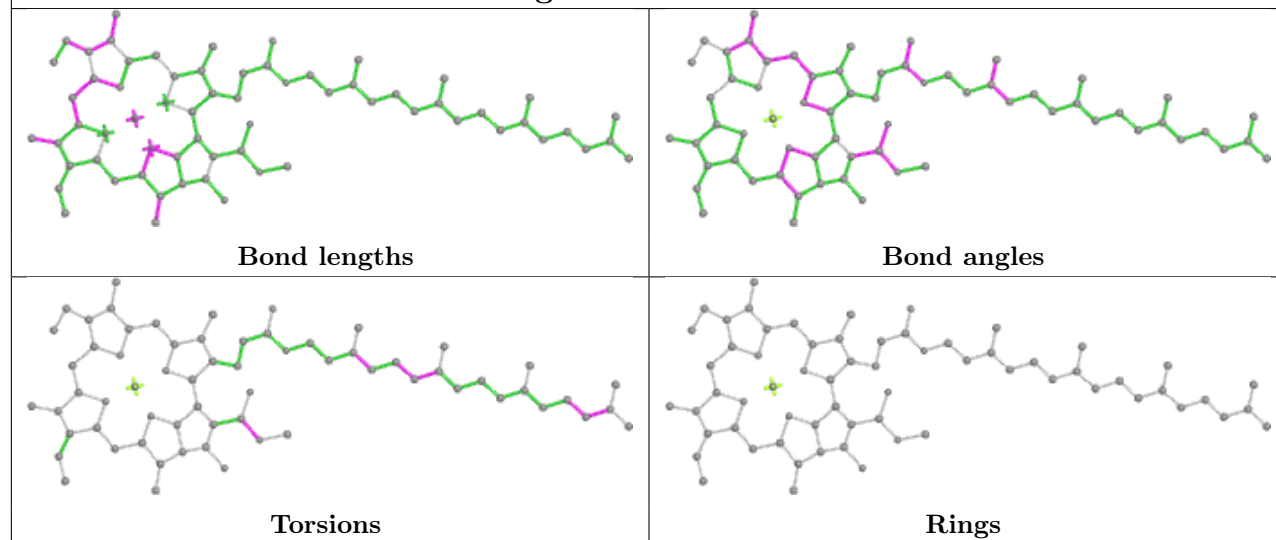
Ligand CLA G 613**Ligand CLA R 603**



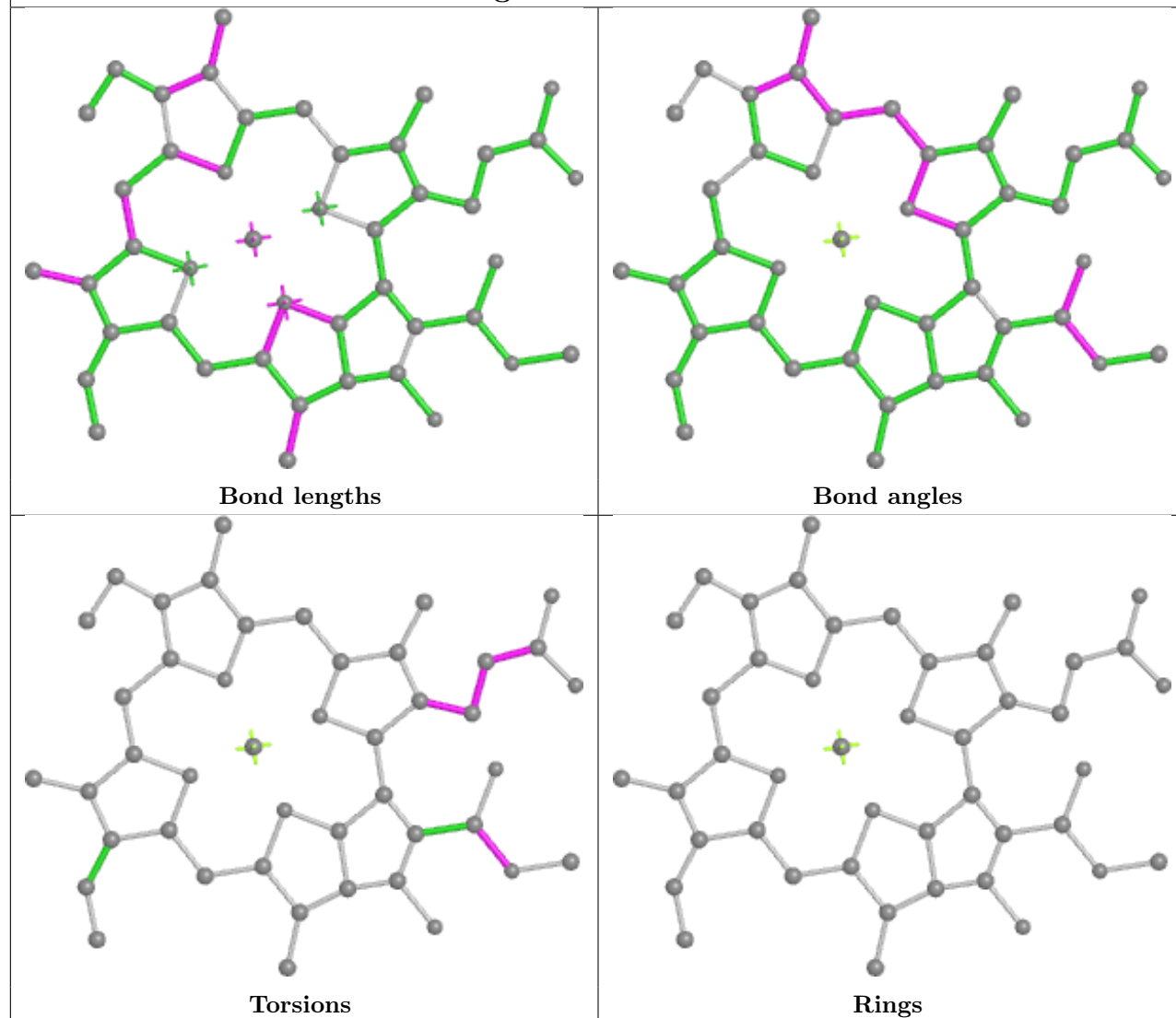
Ligand CLA 5 604



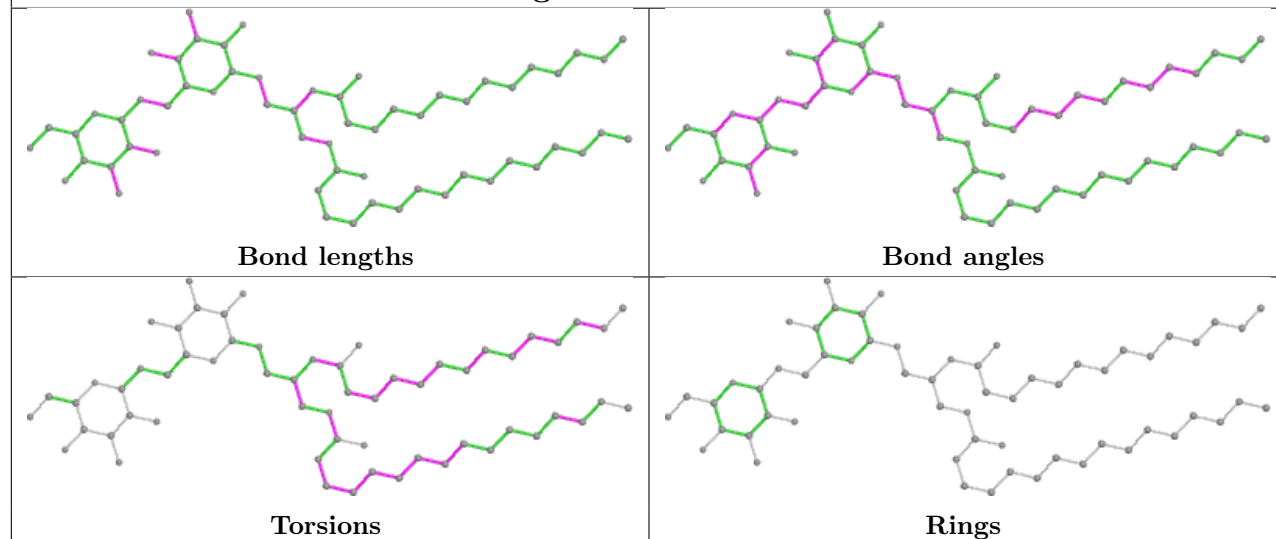
Ligand CLA b 604



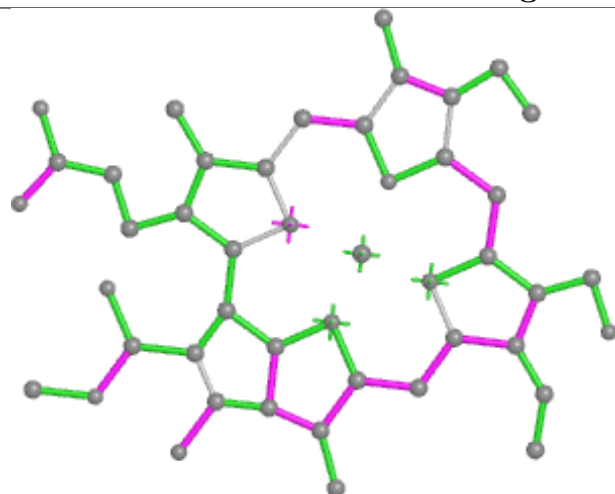
Ligand CLA 1 611



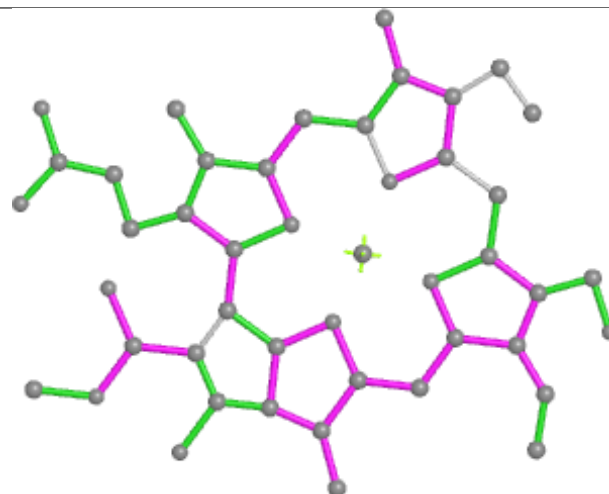
Ligand DGD c 520



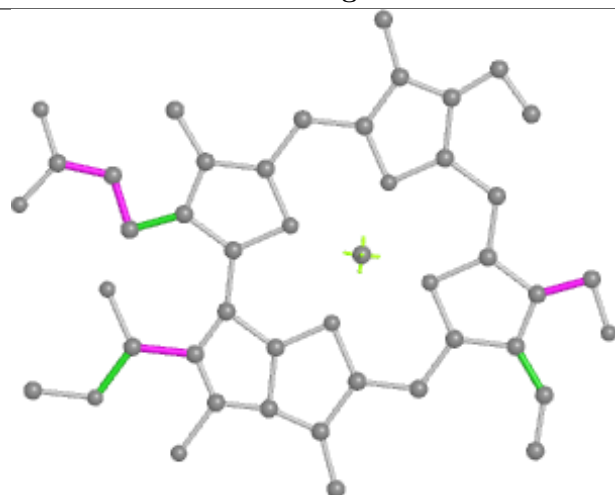
Ligand CHL 2 606



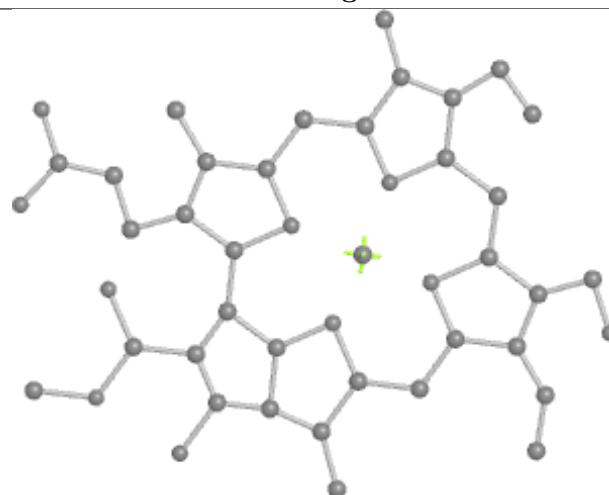
Bond lengths



Bond angles

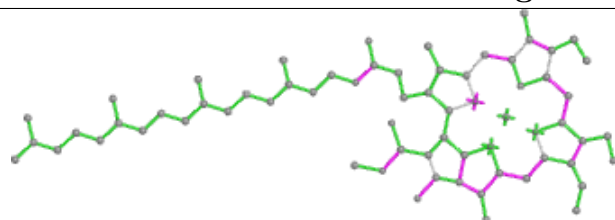


Torsions

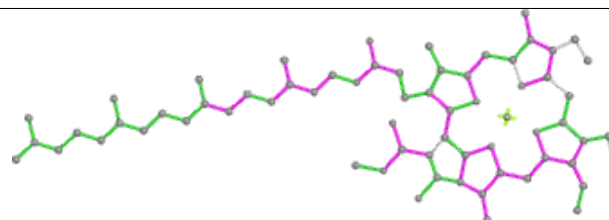


Rings

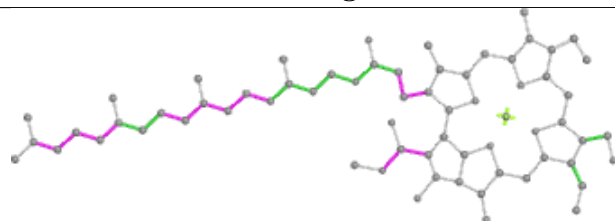
Ligand CHL R 606



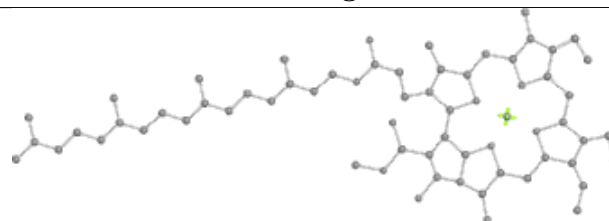
Bond lengths



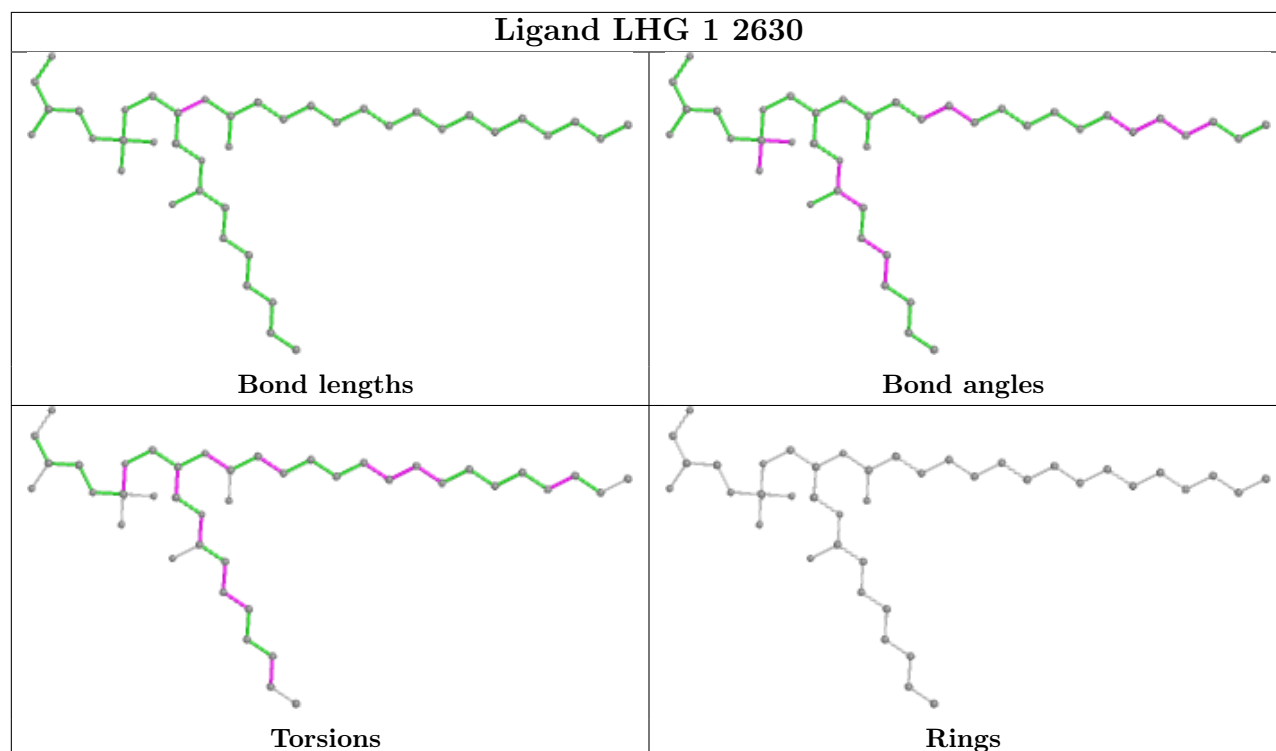
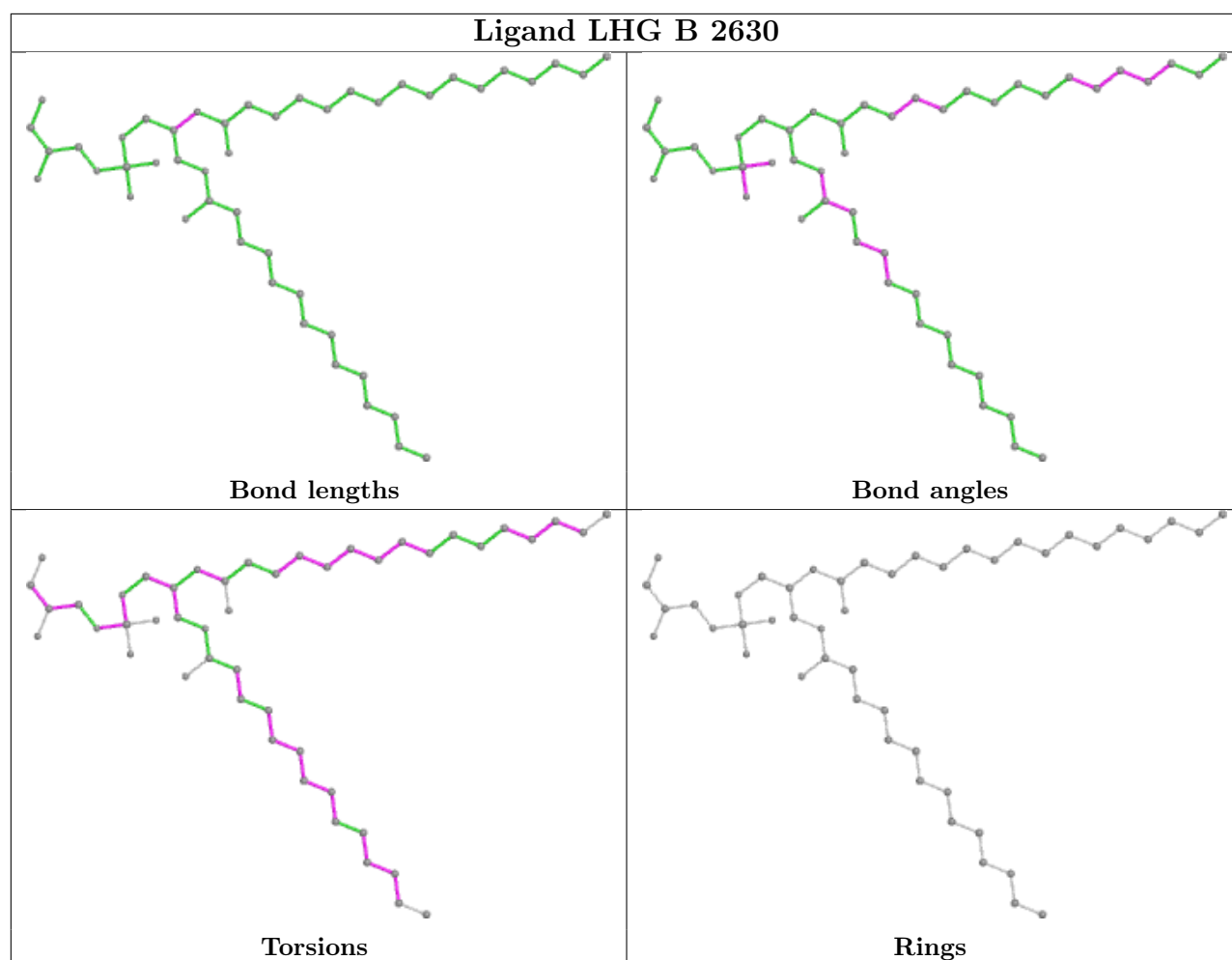
Bond angles

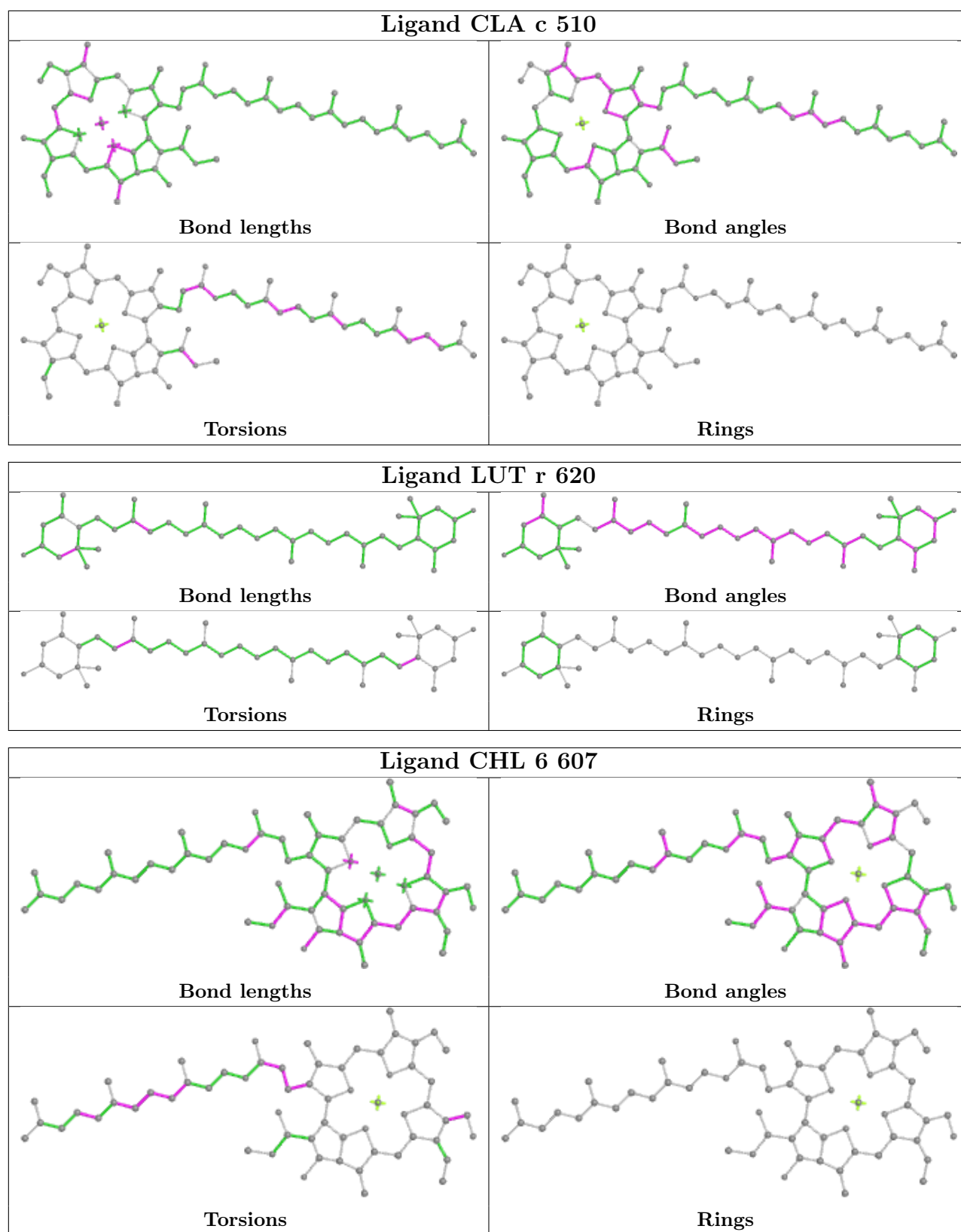


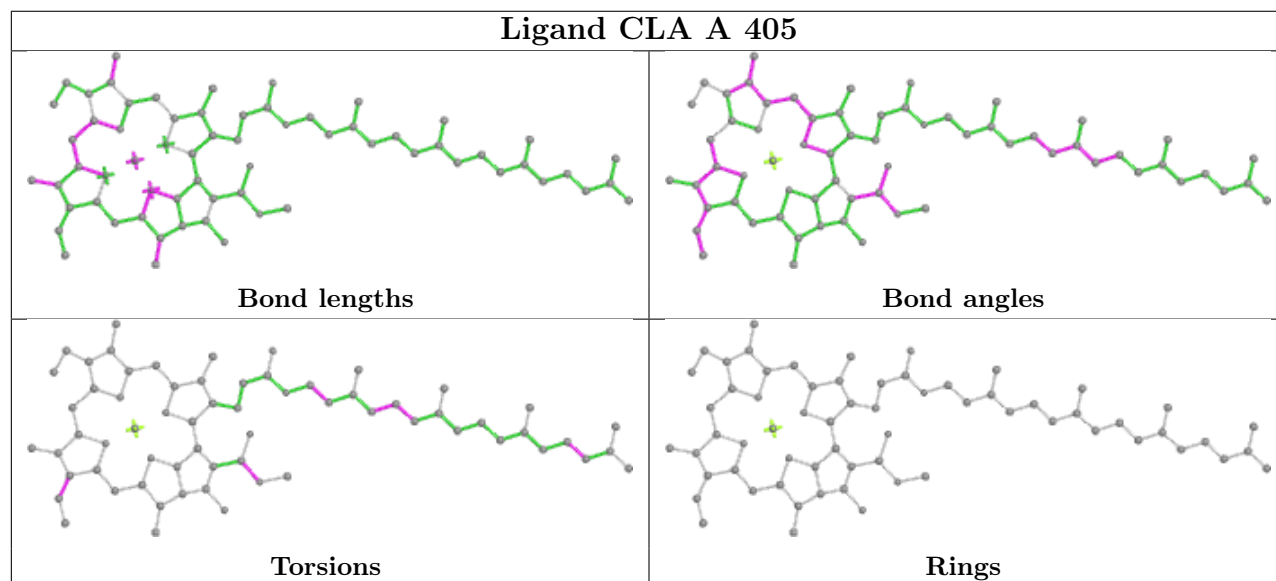
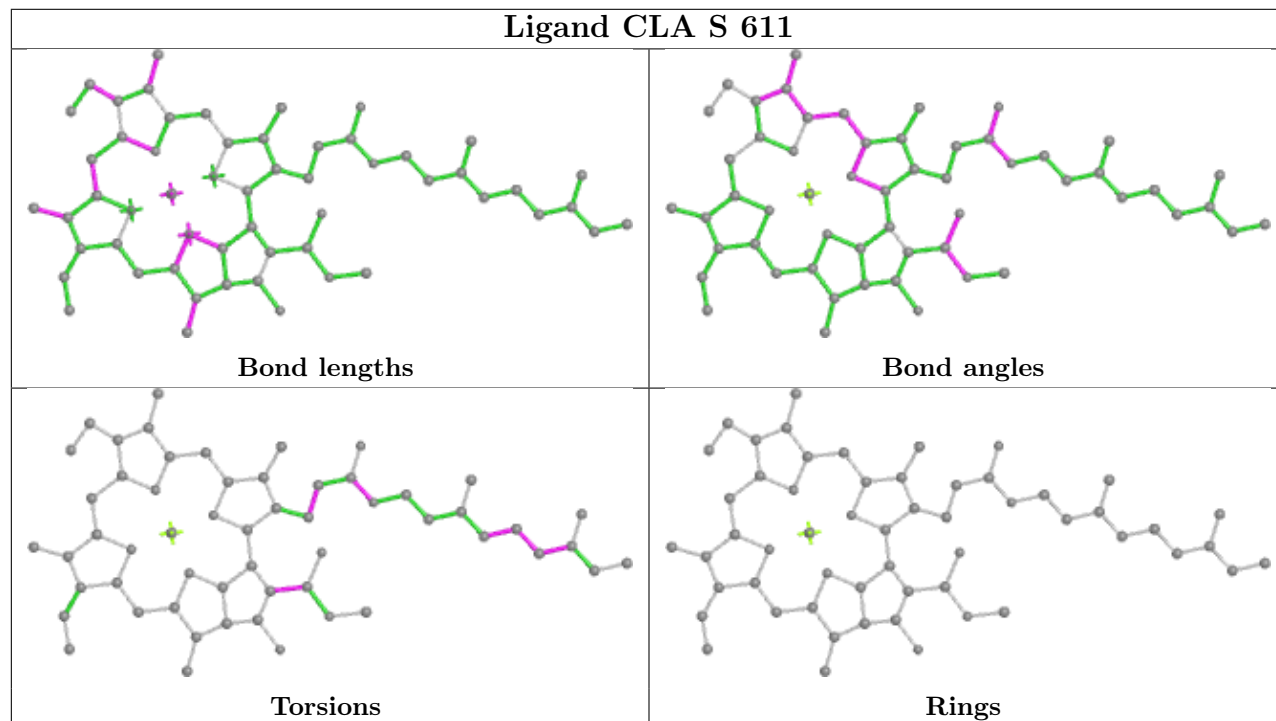
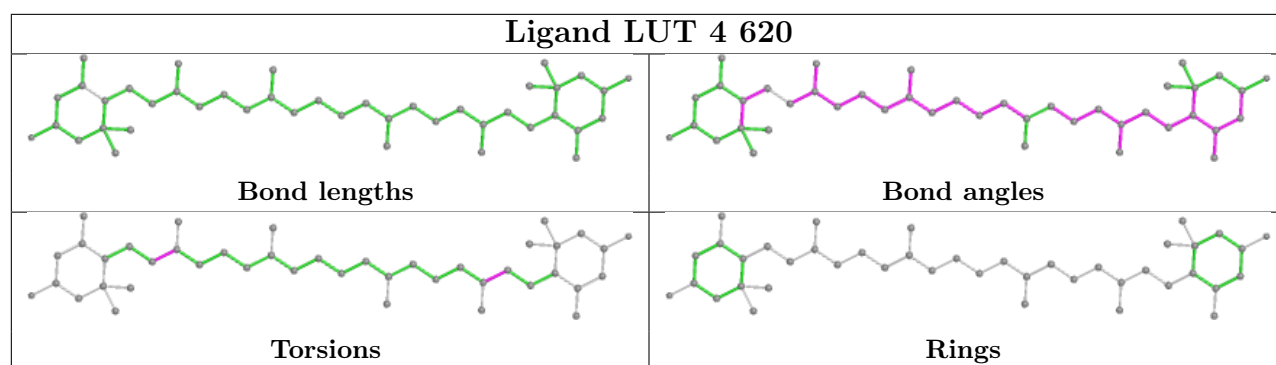
Torsions

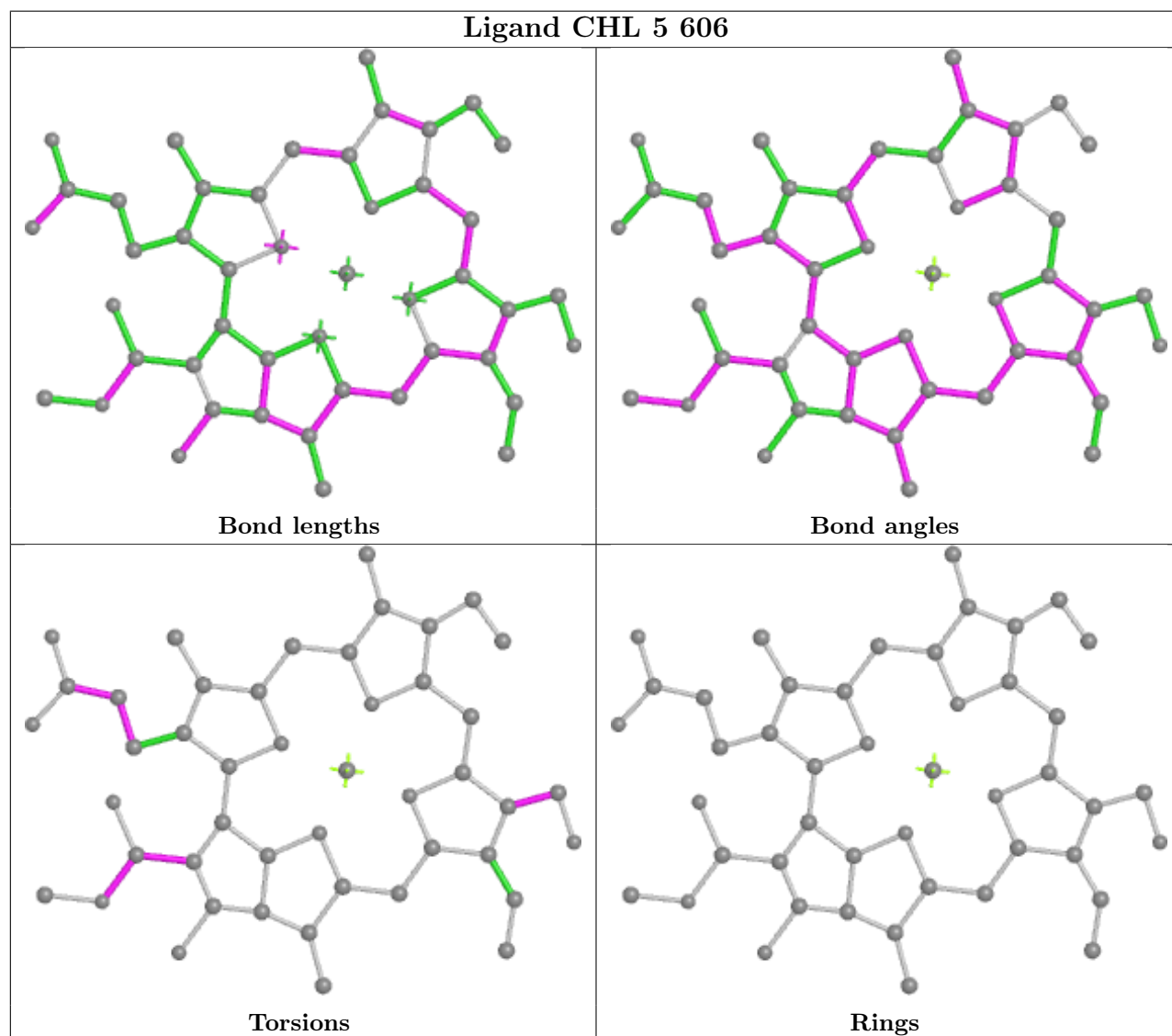
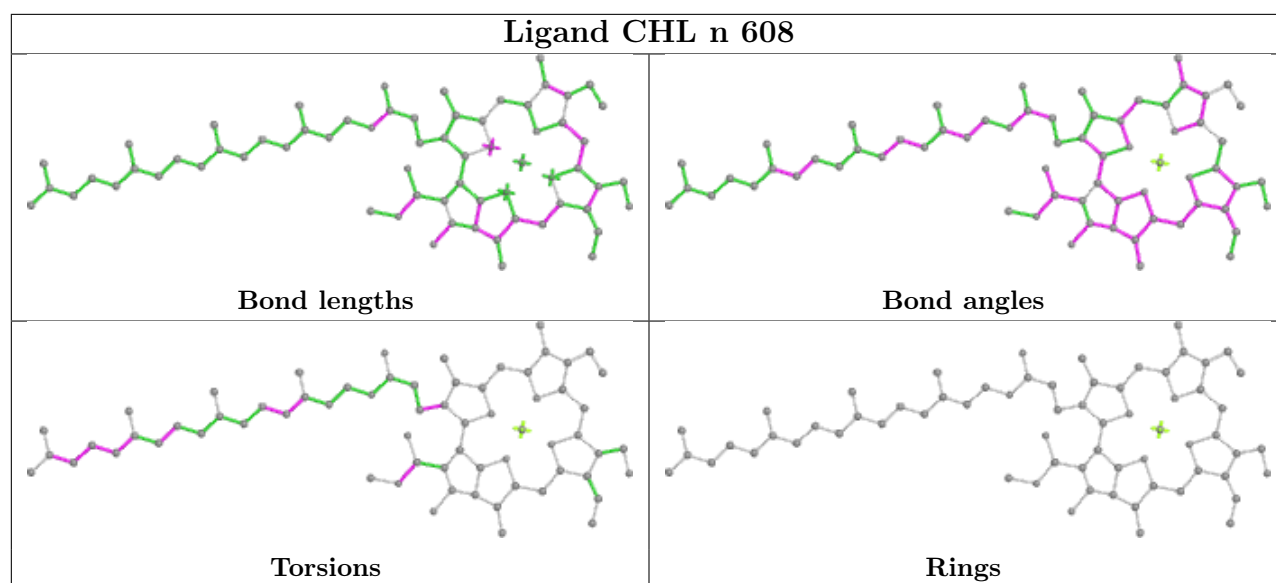


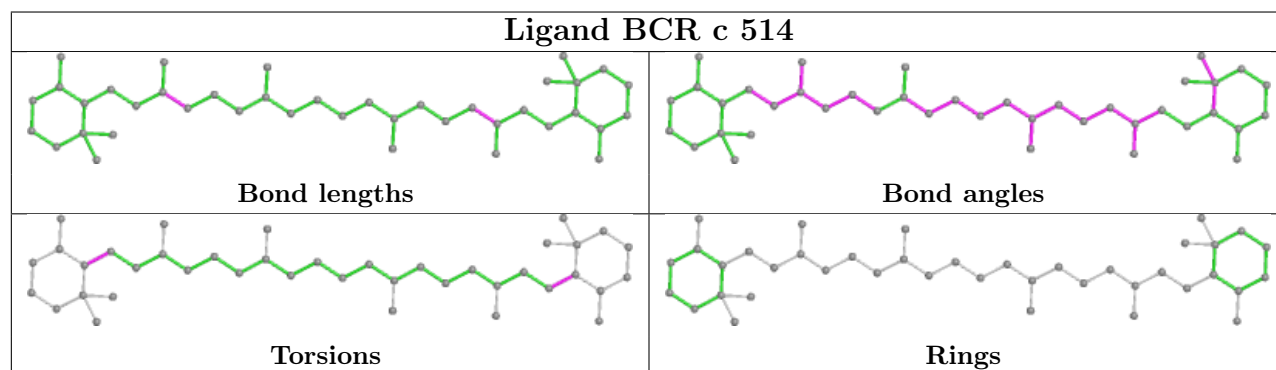
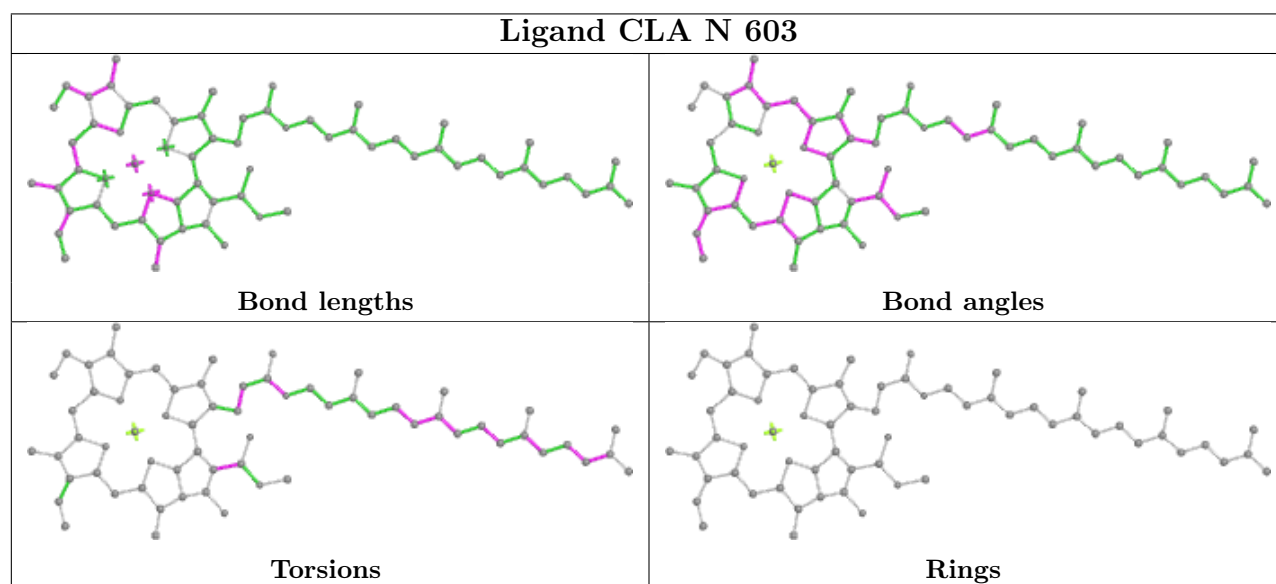
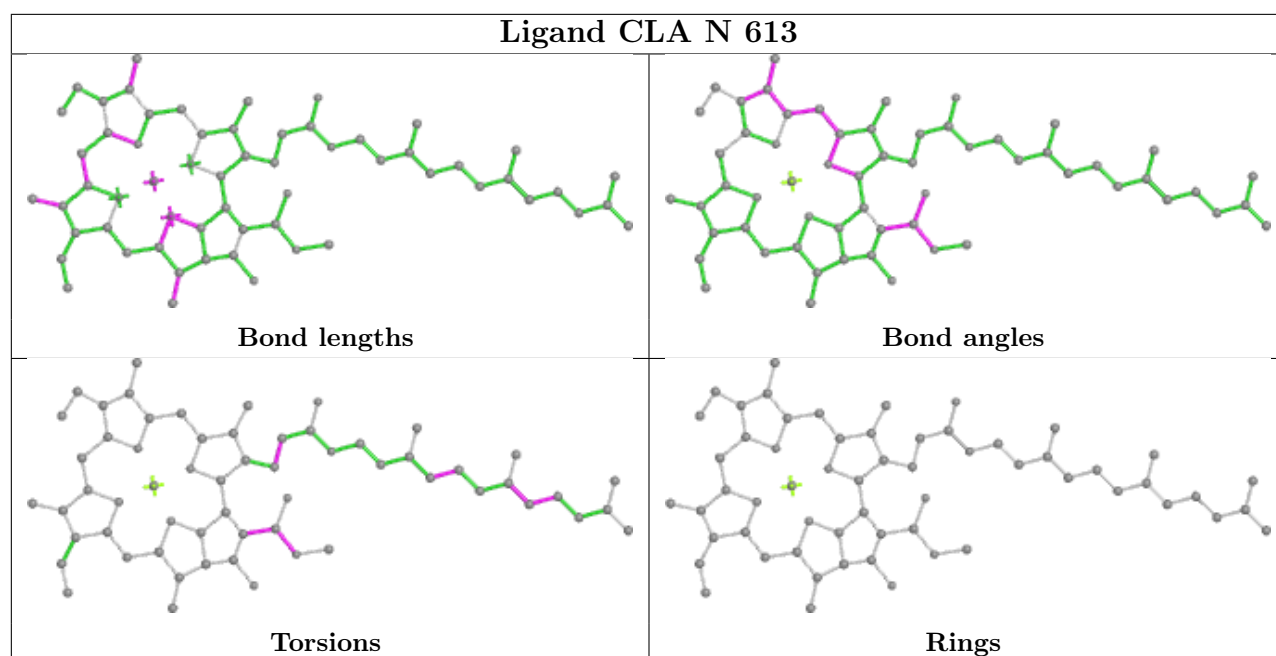
Rings



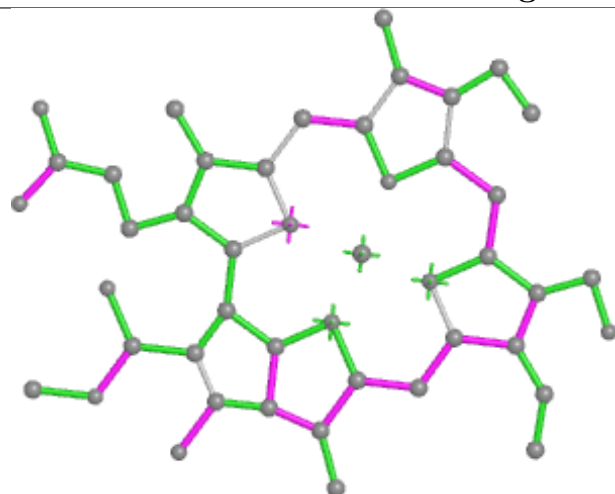




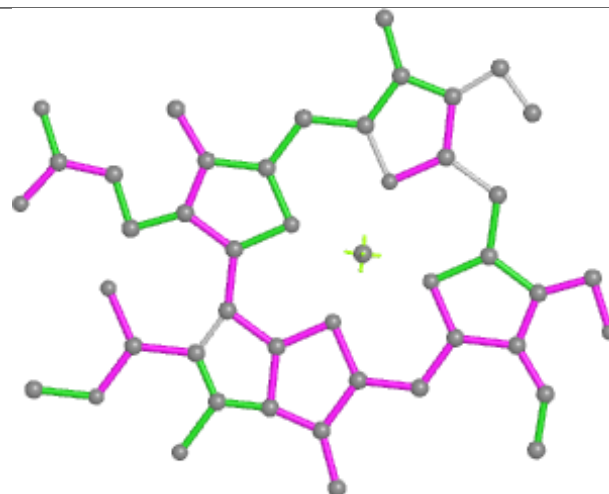




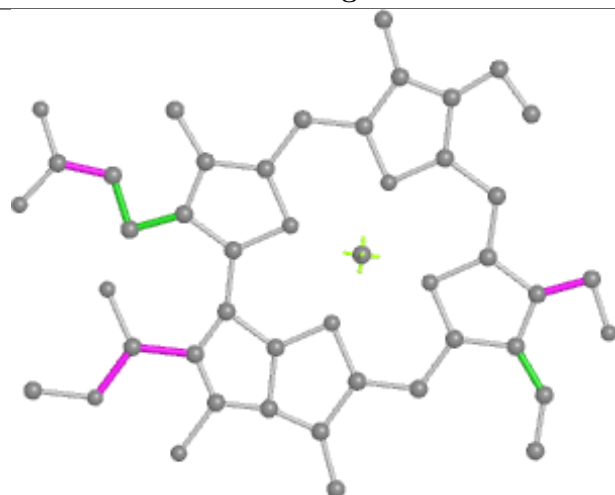
Ligand CHL S 606



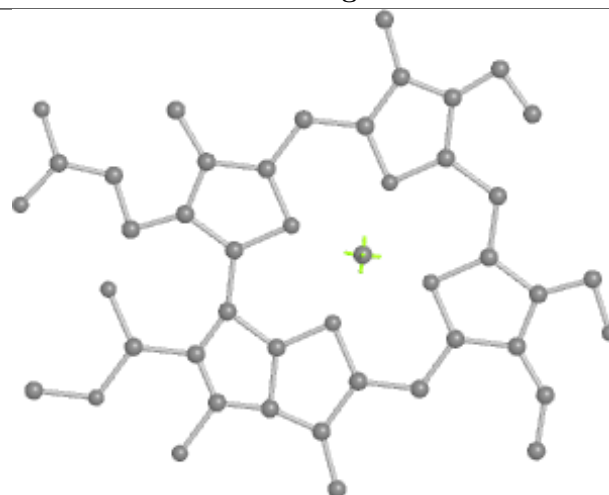
Bond lengths



Bond angles

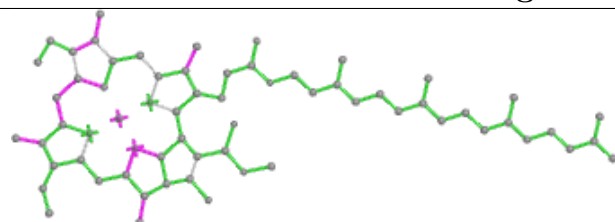


Torsions

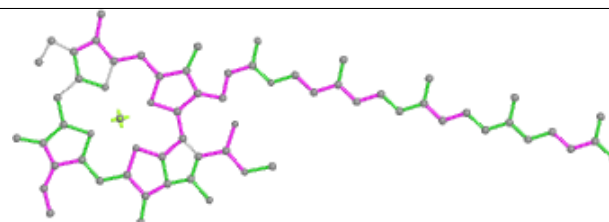


Rings

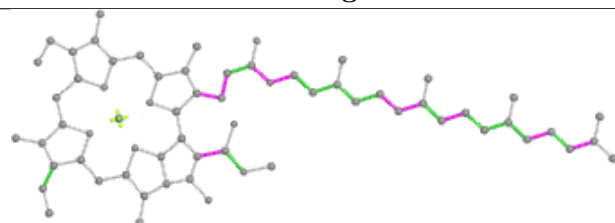
Ligand CLA B 605



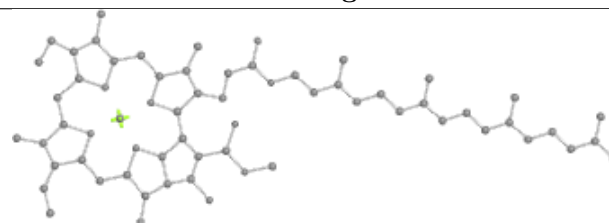
Bond lengths



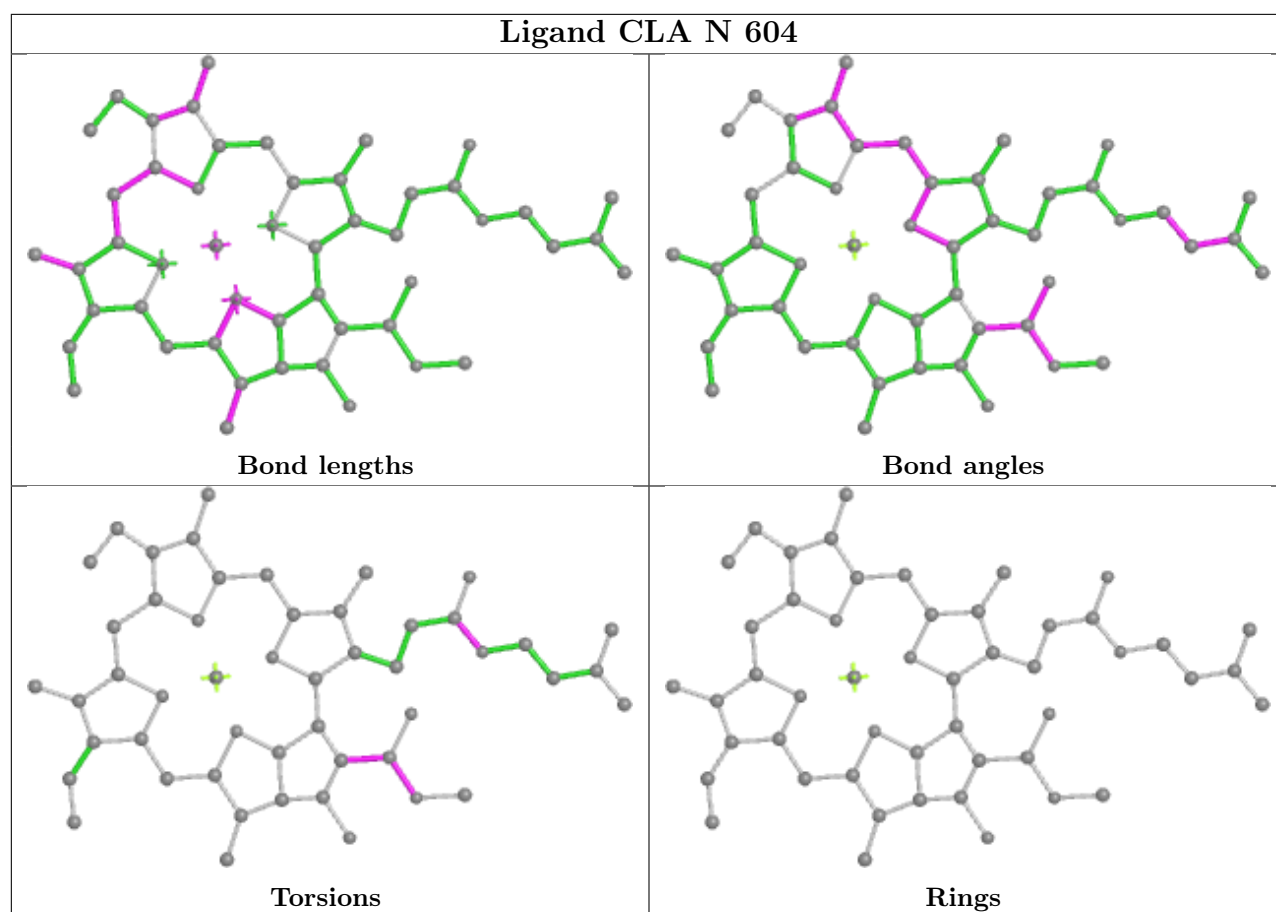
Bond angles



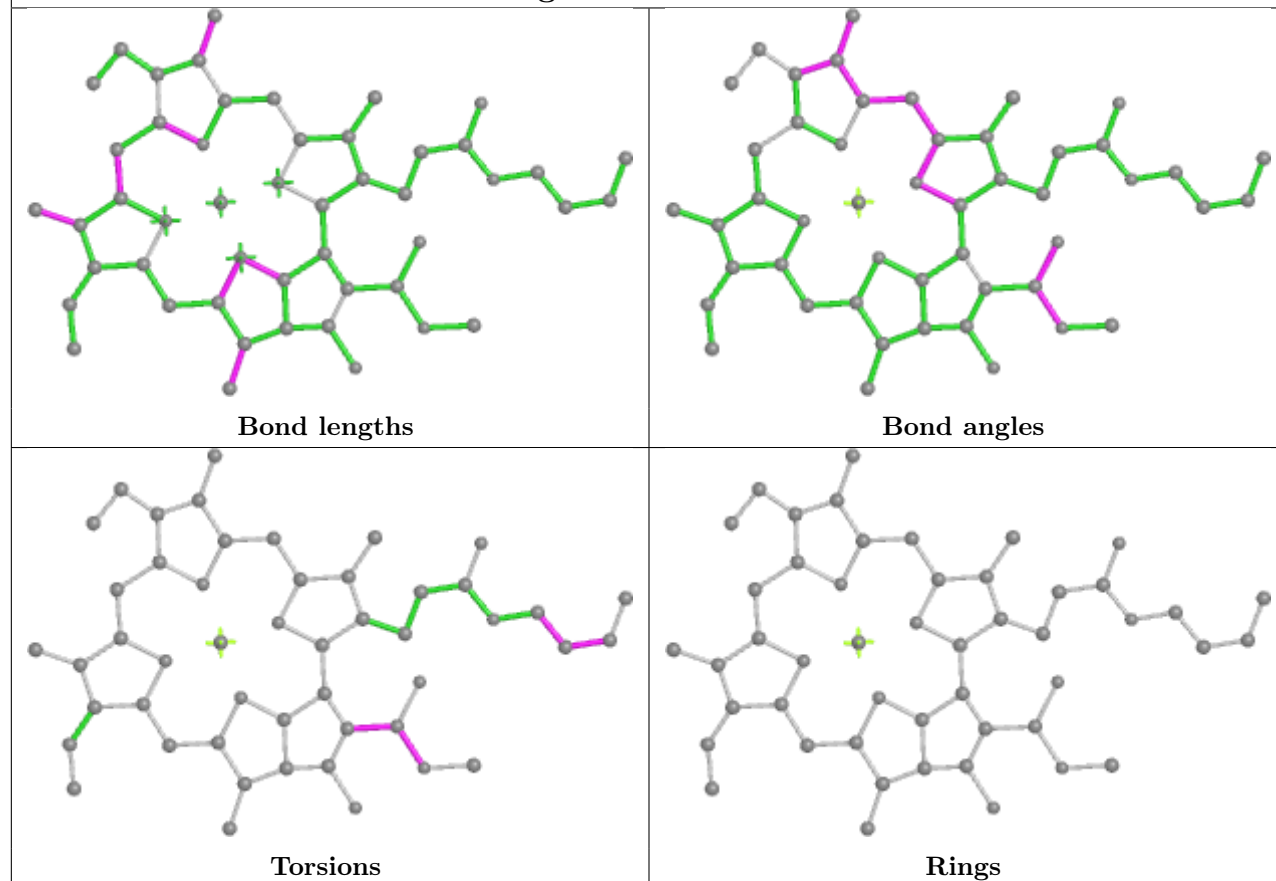
Torsions



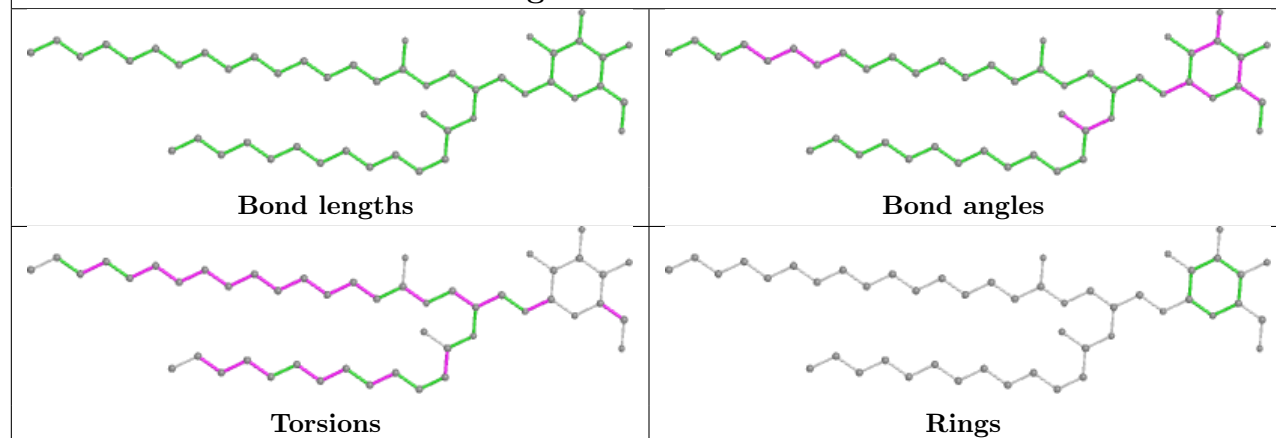
Rings

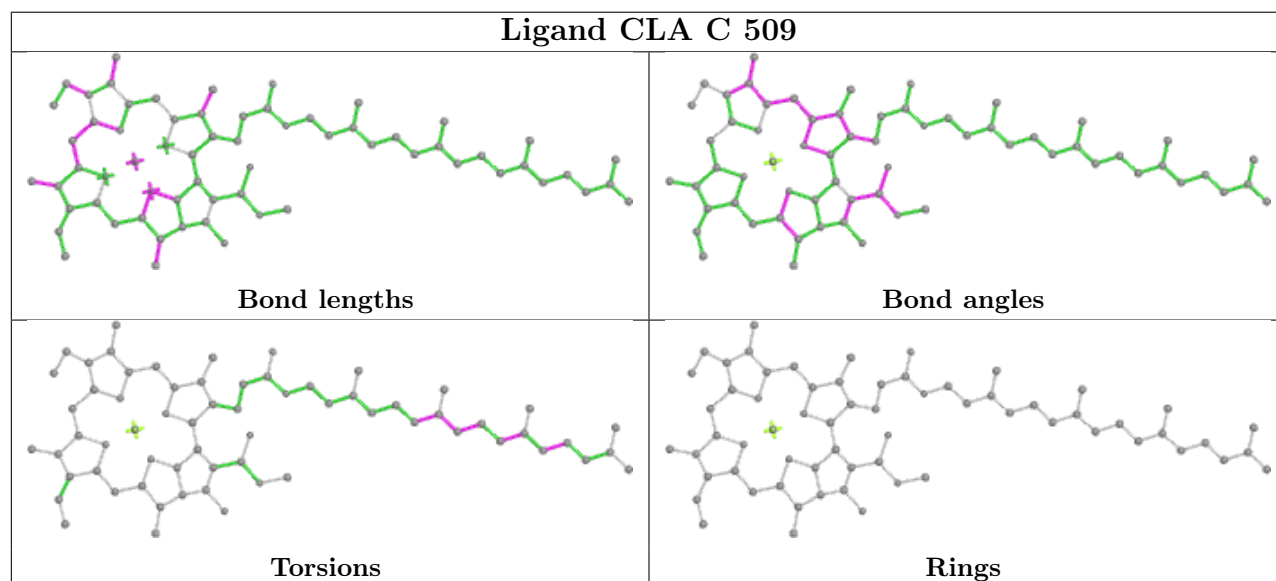
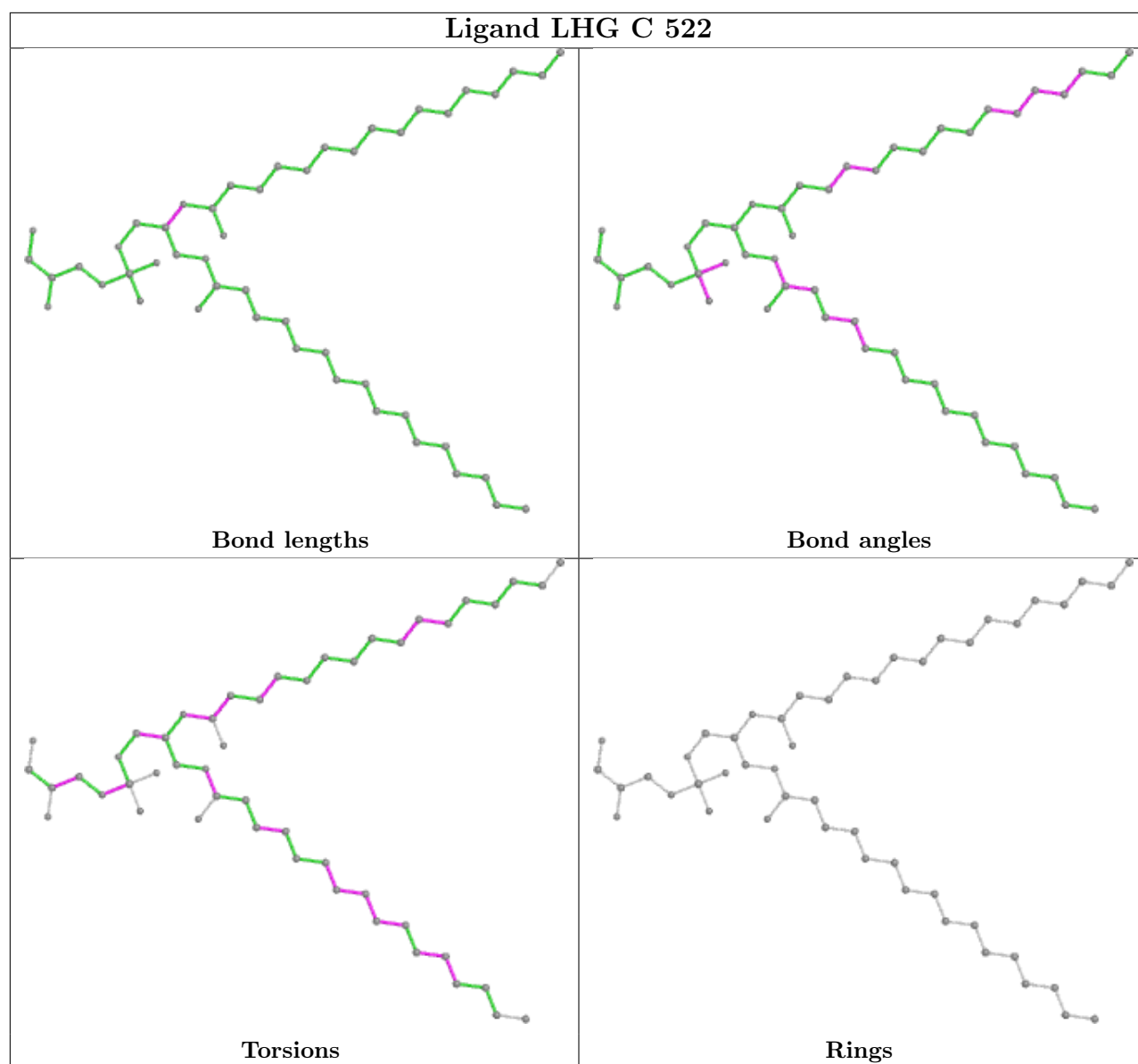


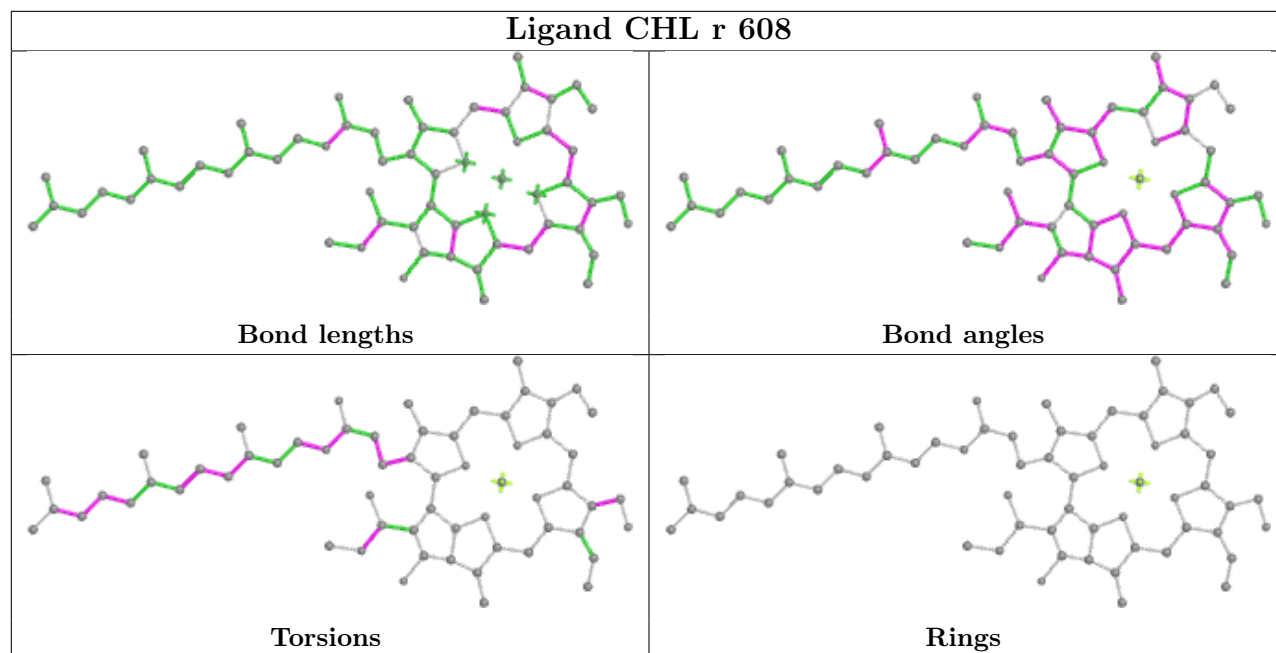
Ligand CLA s 612

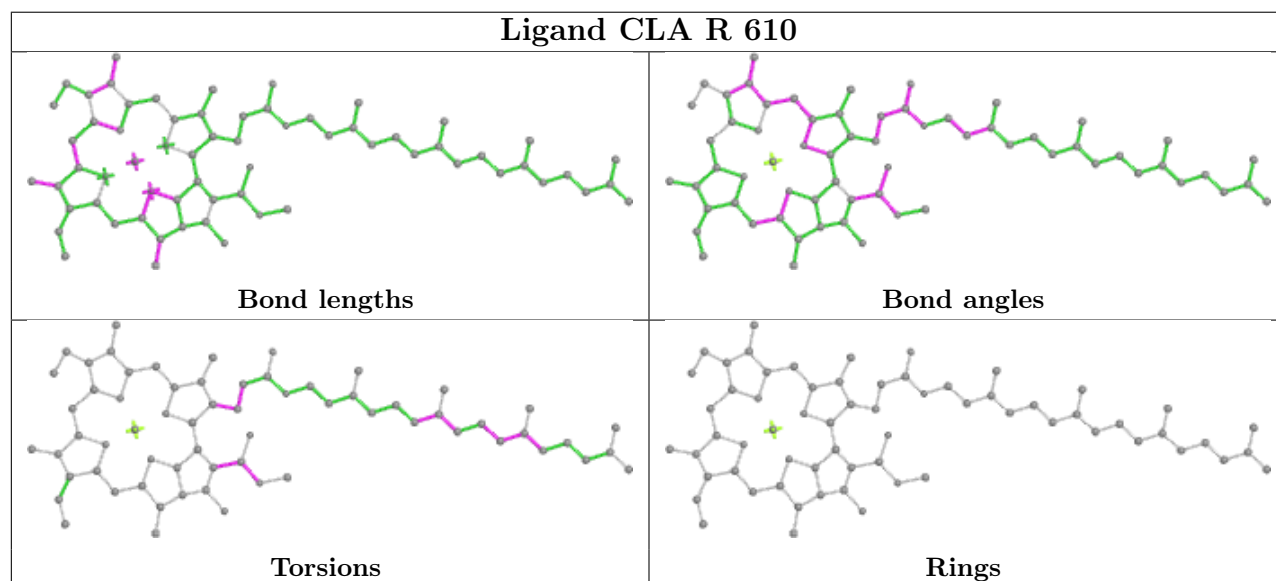
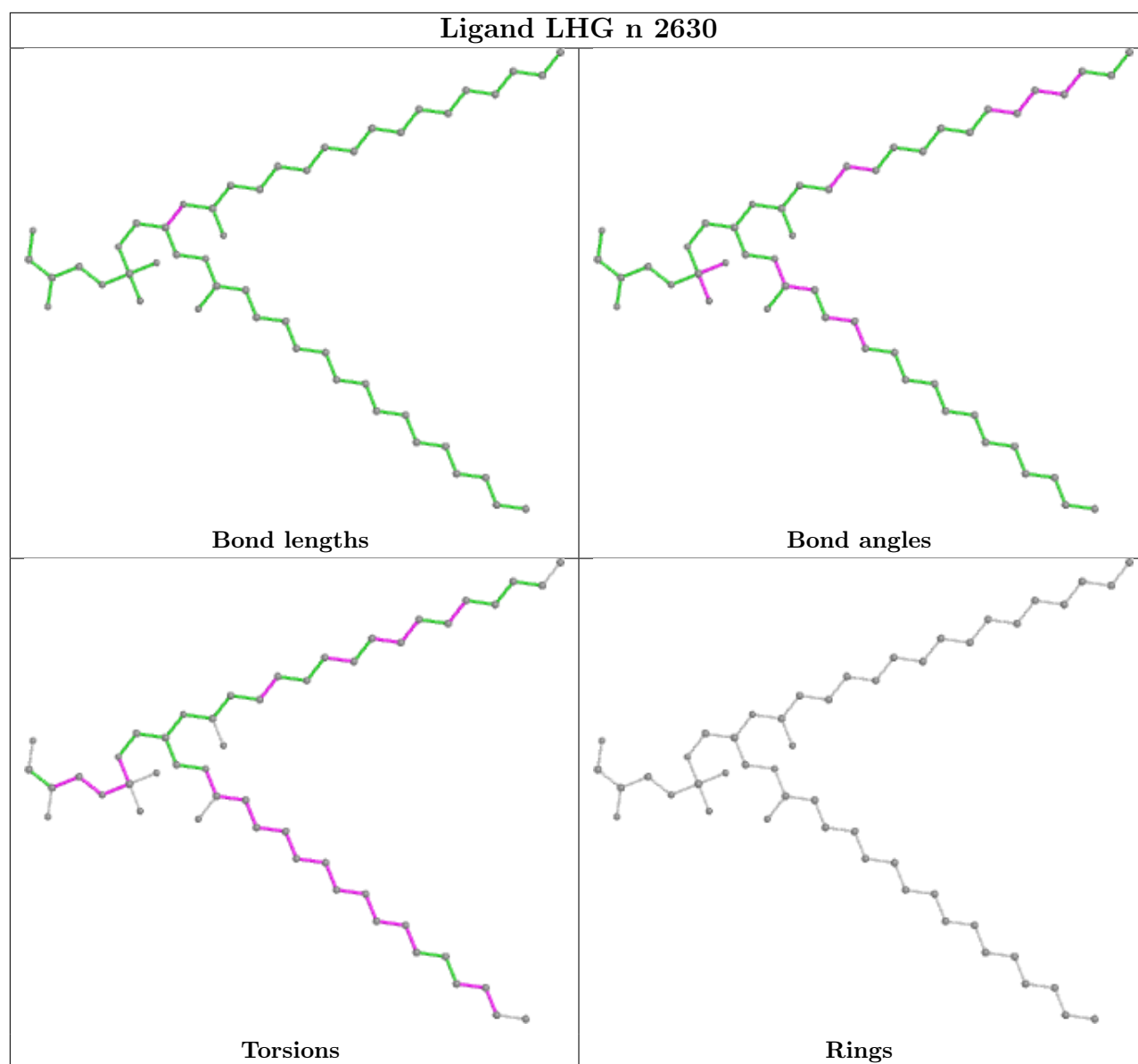


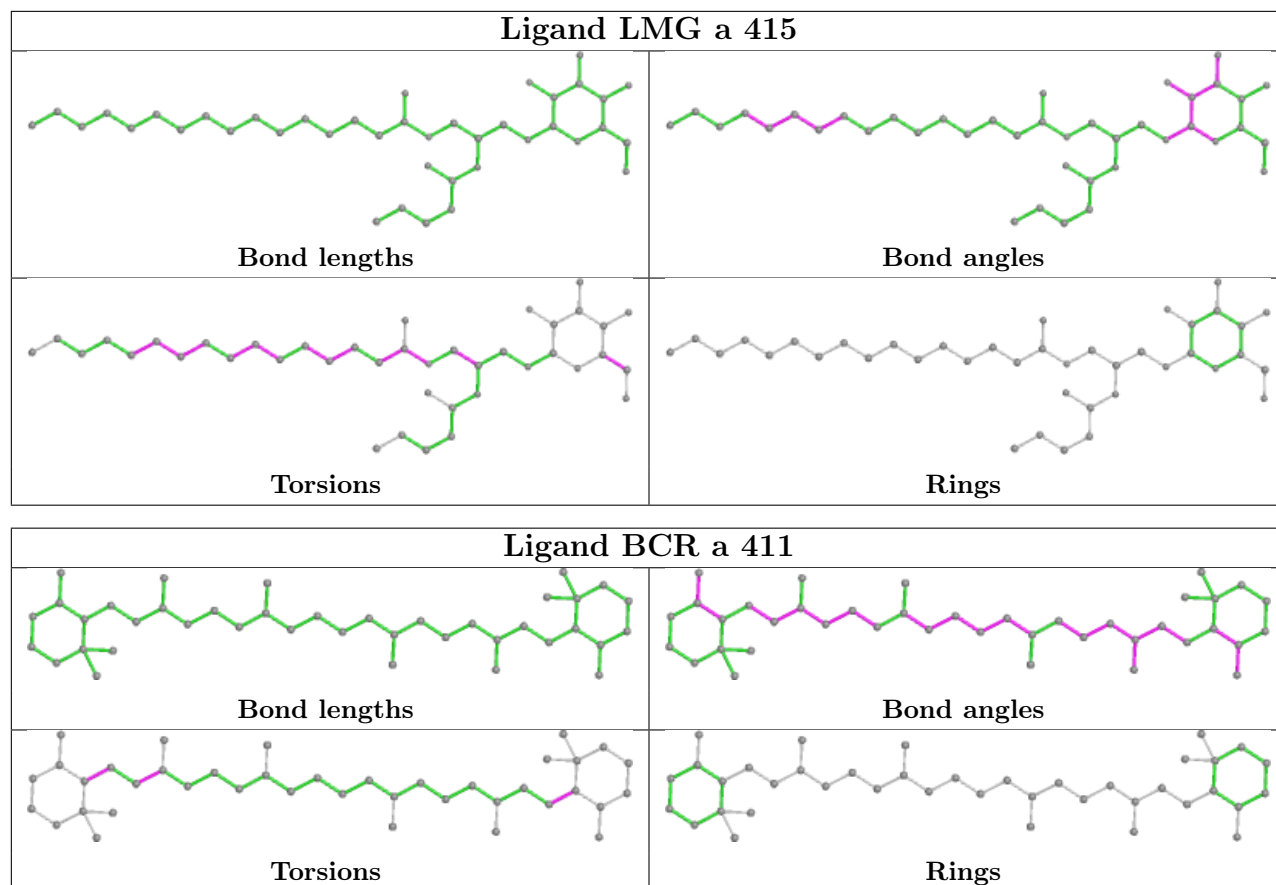
Ligand LMG A 413



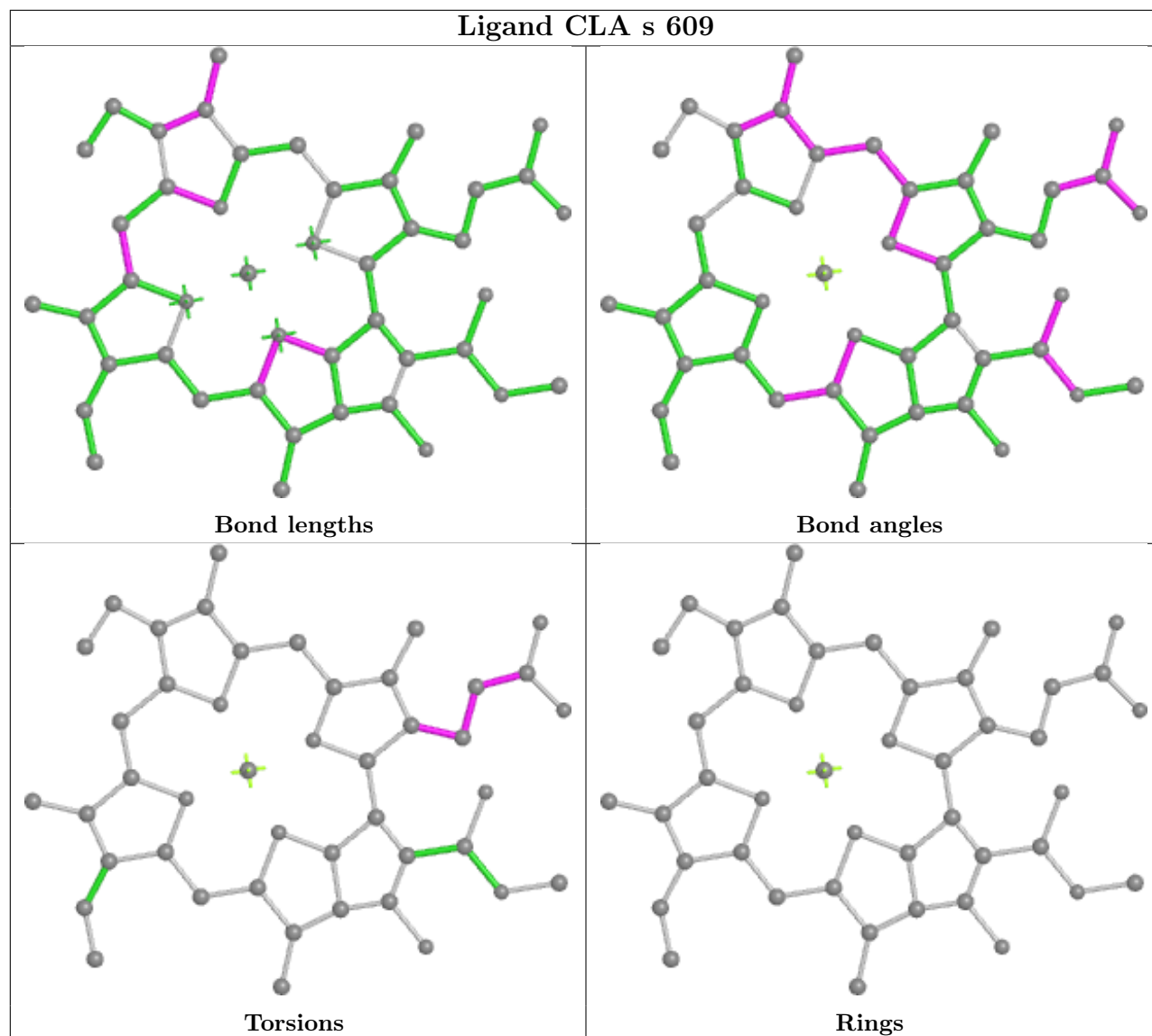


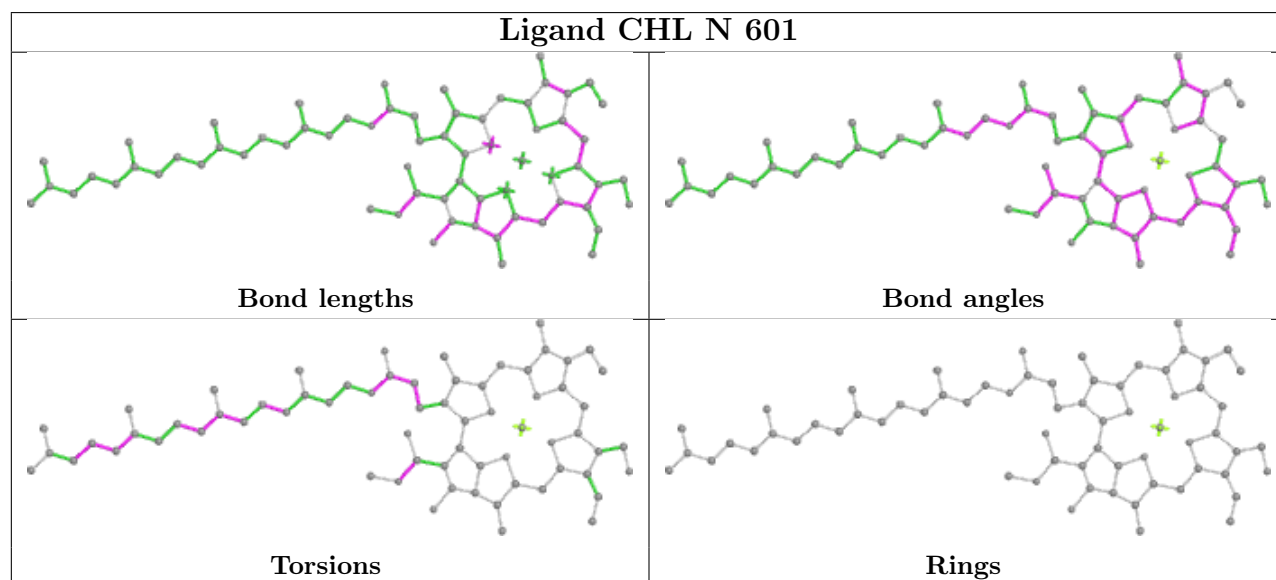
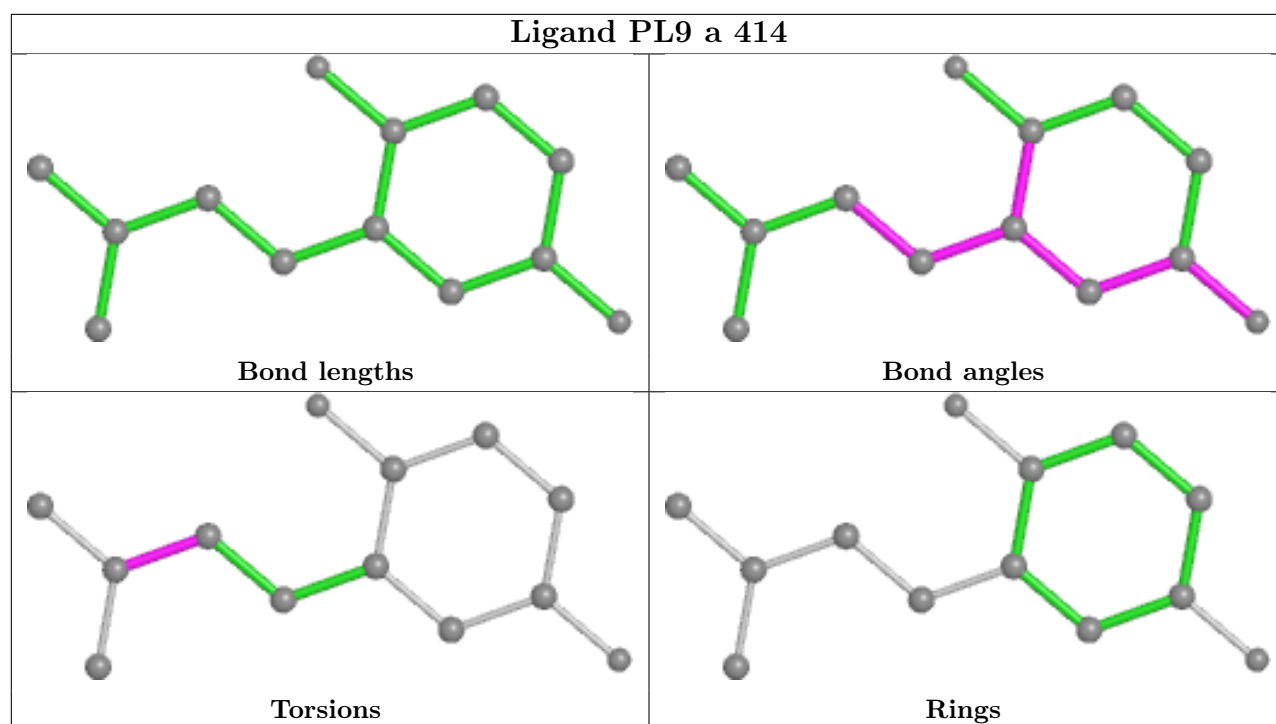


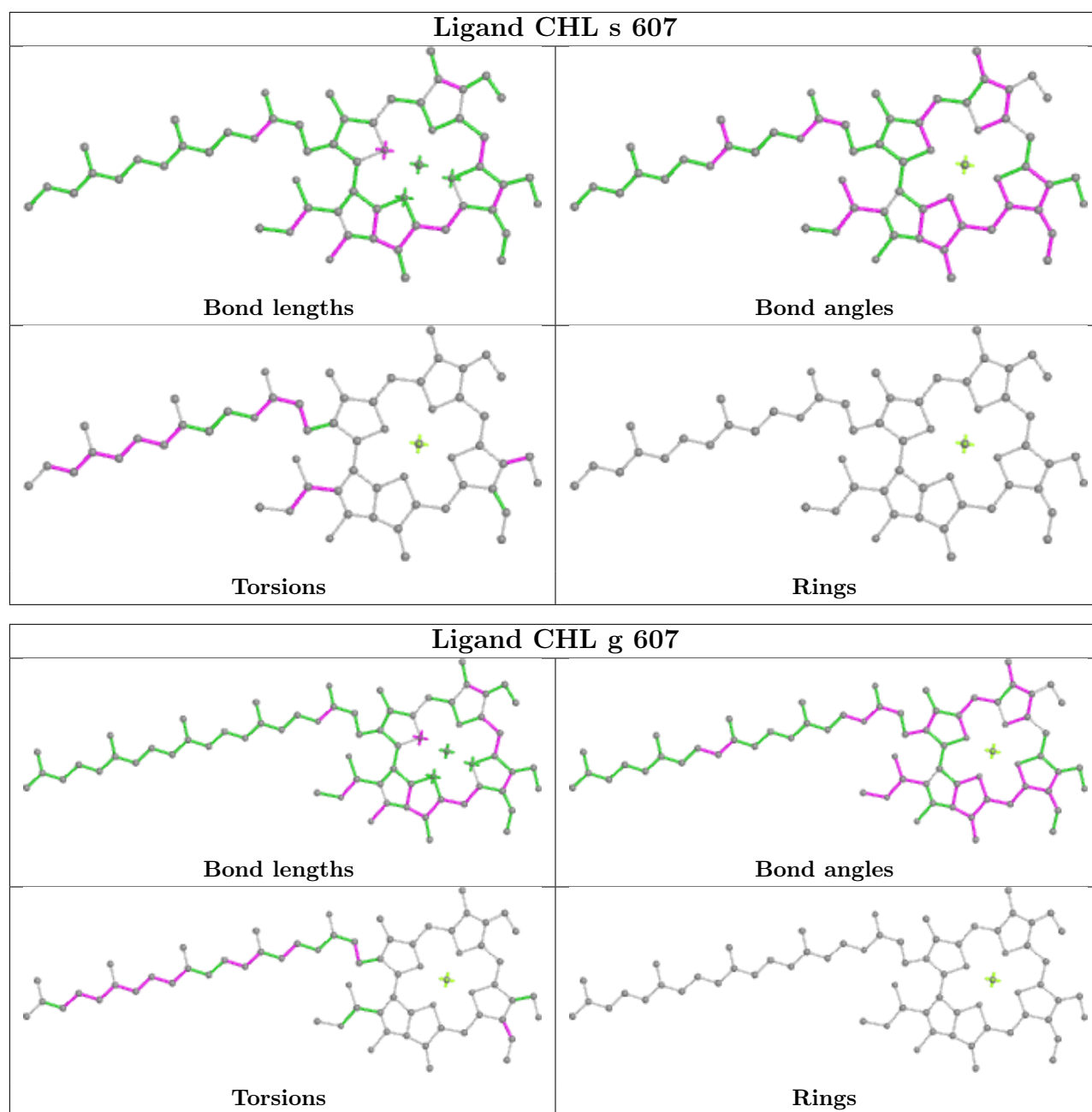


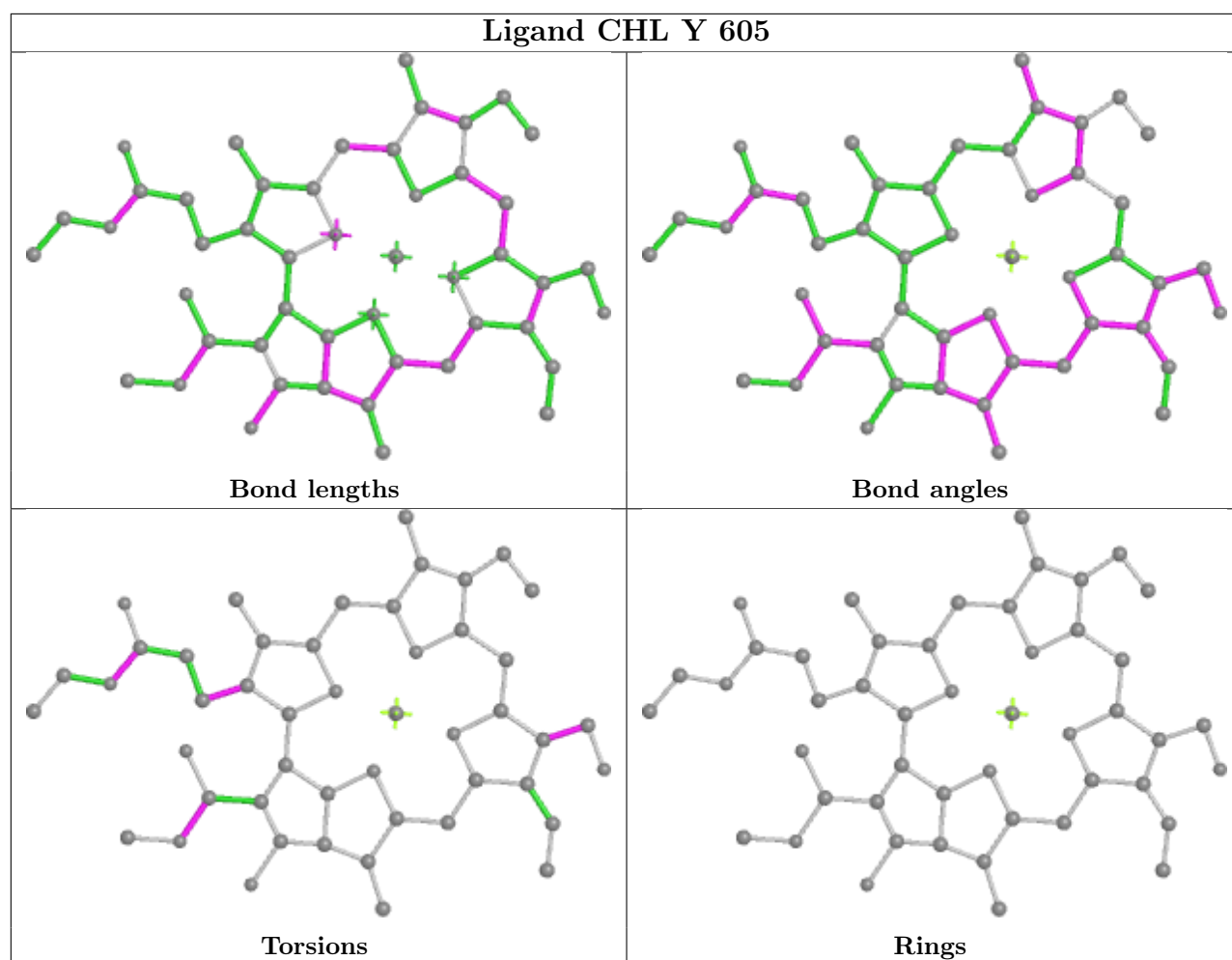


Ligand CLA s 609

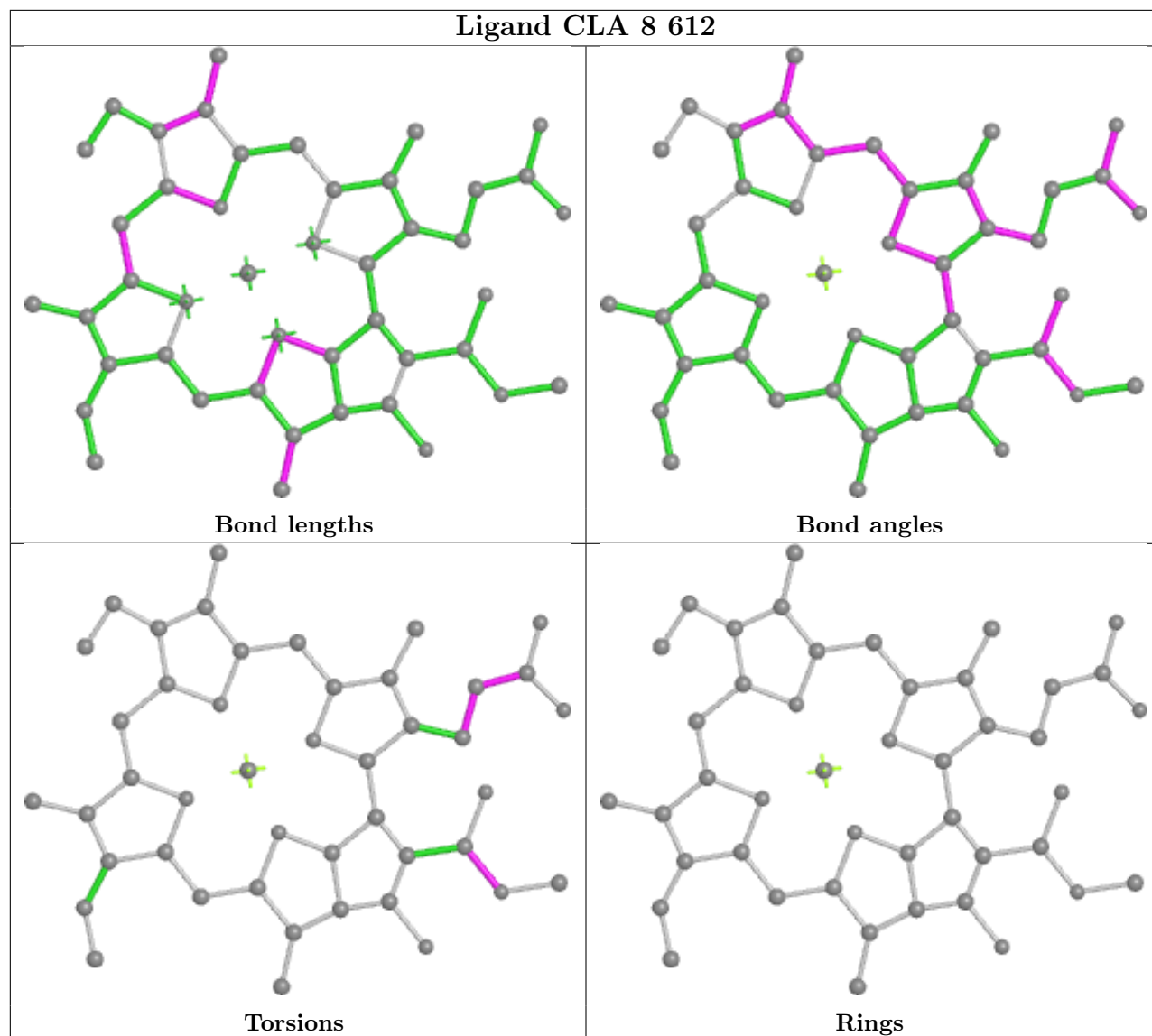


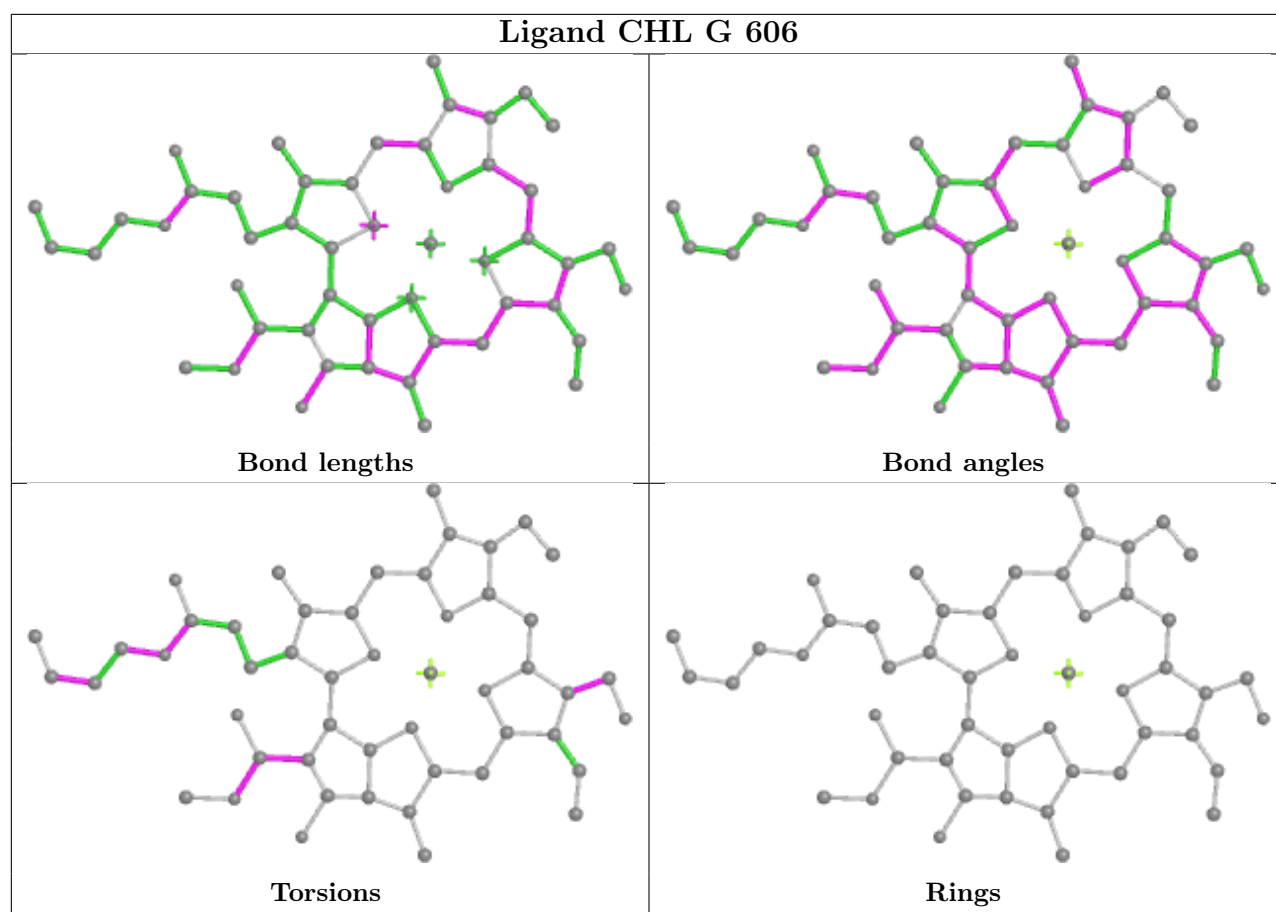




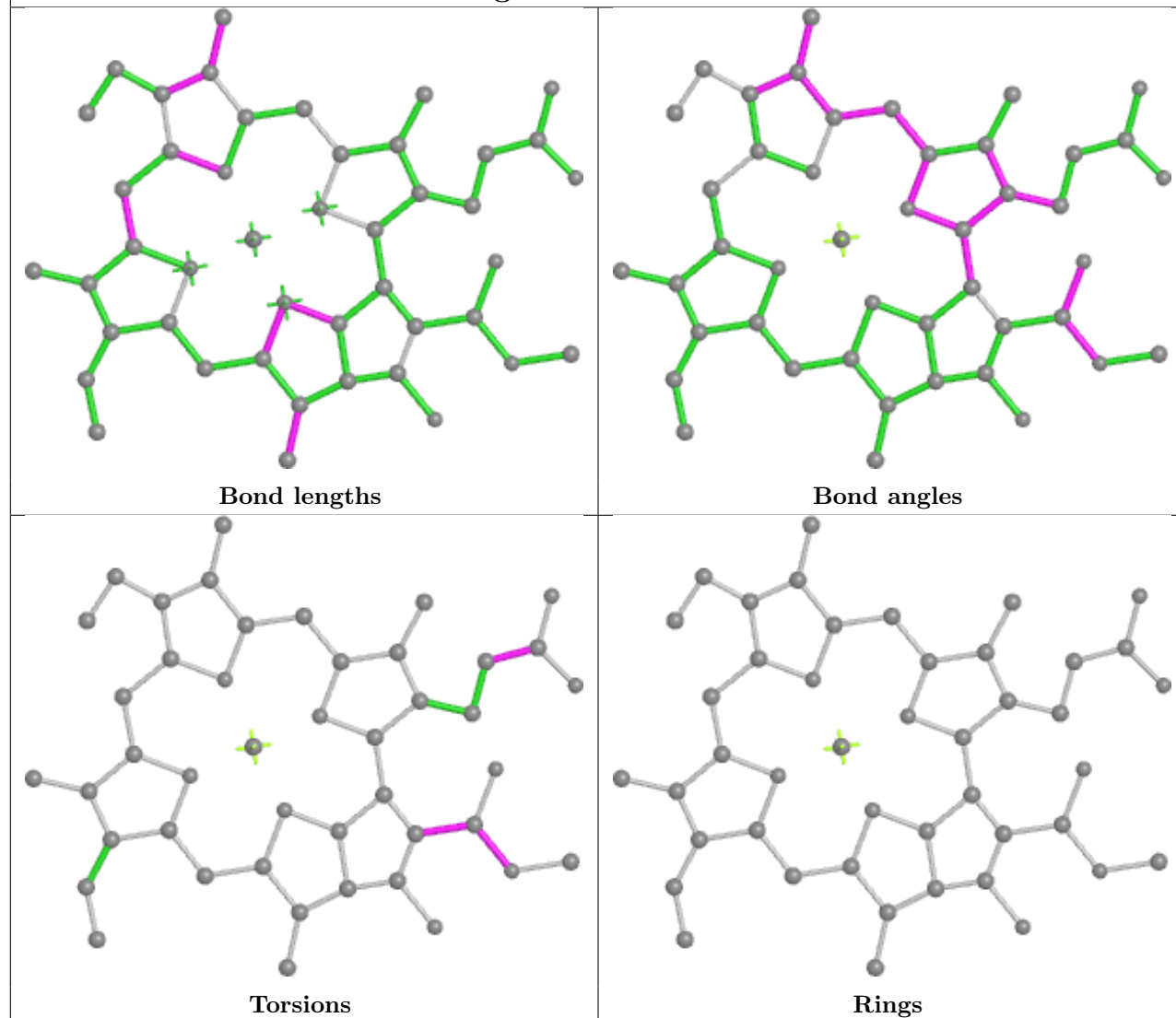


Ligand CLA 8 612

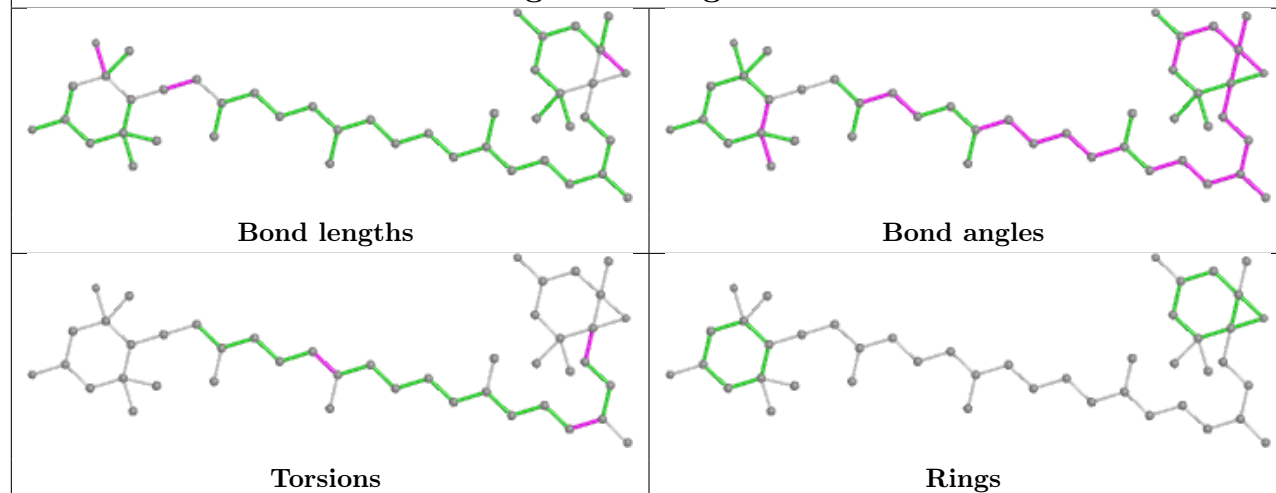




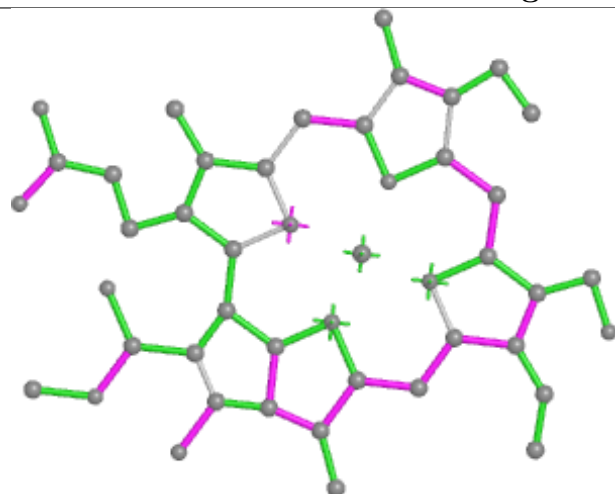
Ligand CLA 2 612



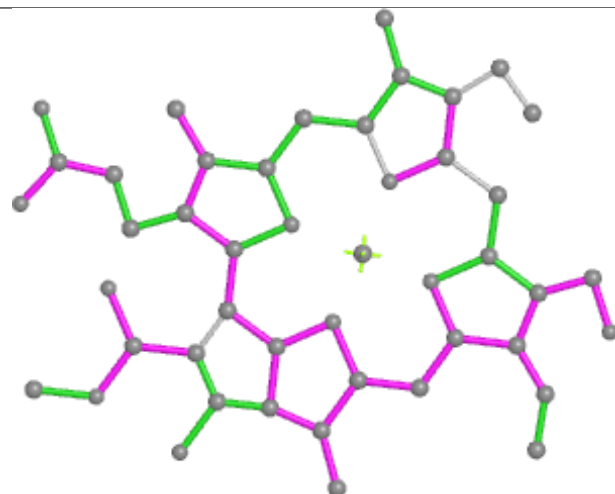
Ligand NEX g 1623



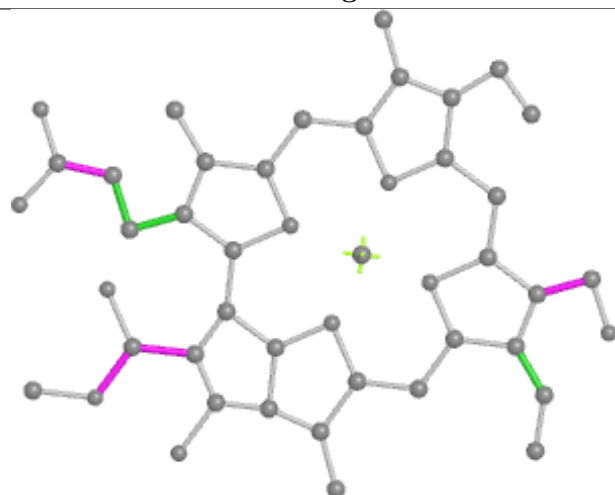
Ligand CHL s 606



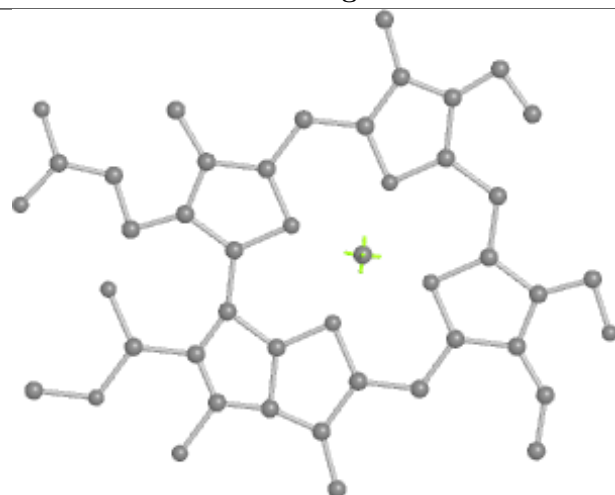
Bond lengths



Bond angles

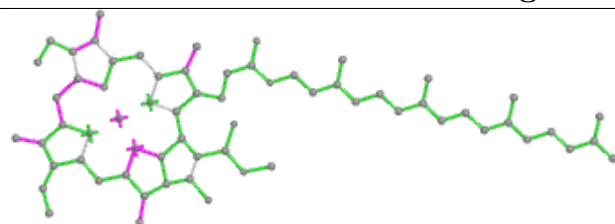


Torsions

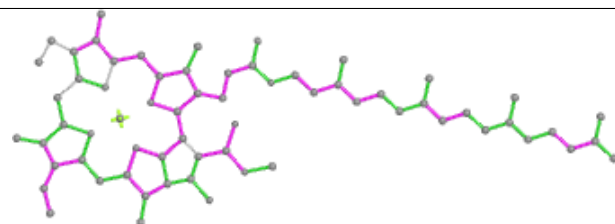


Rings

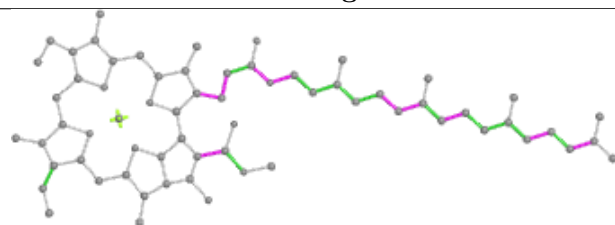
Ligand CLA b 605



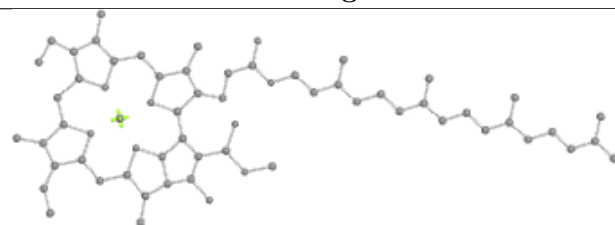
Bond lengths



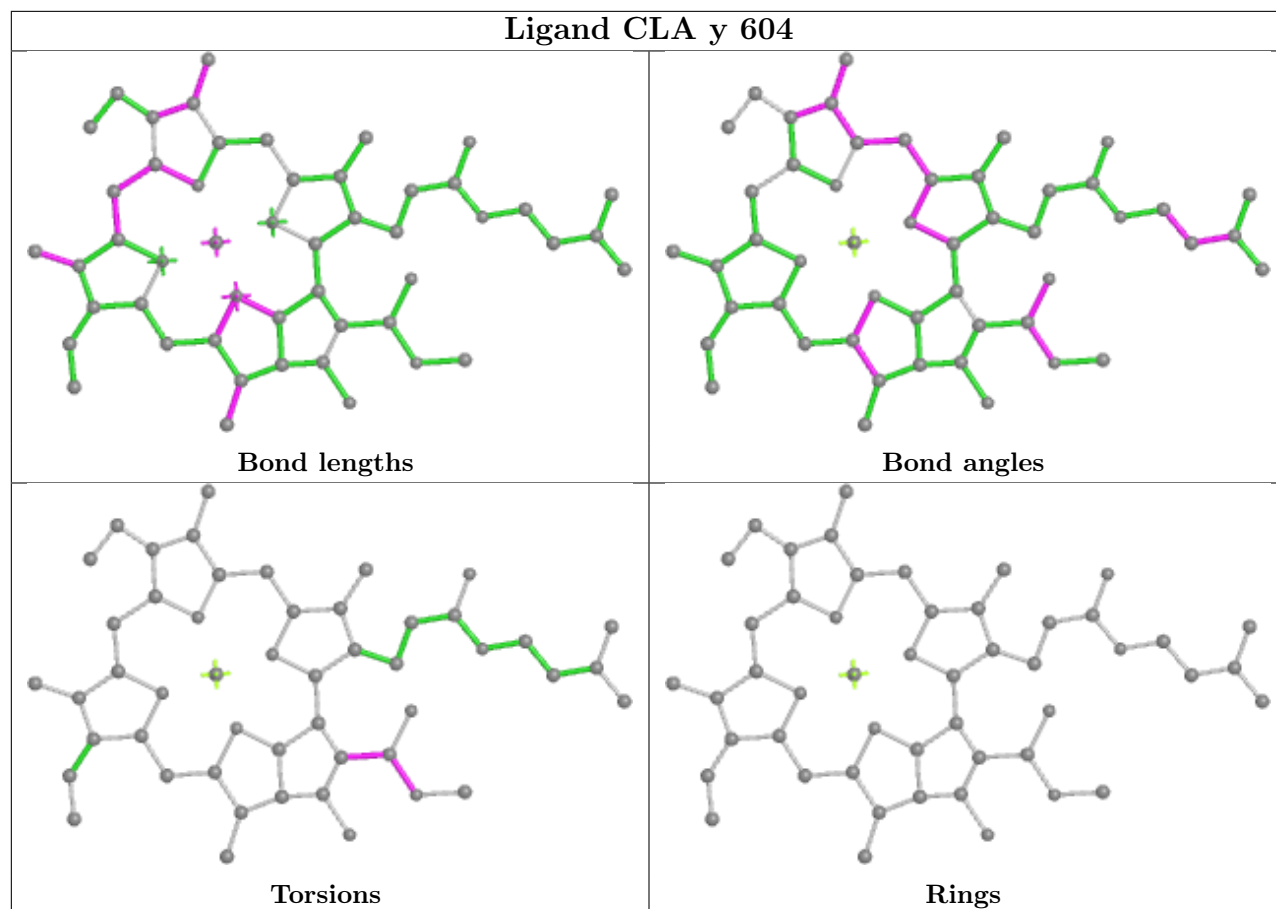
Bond angles



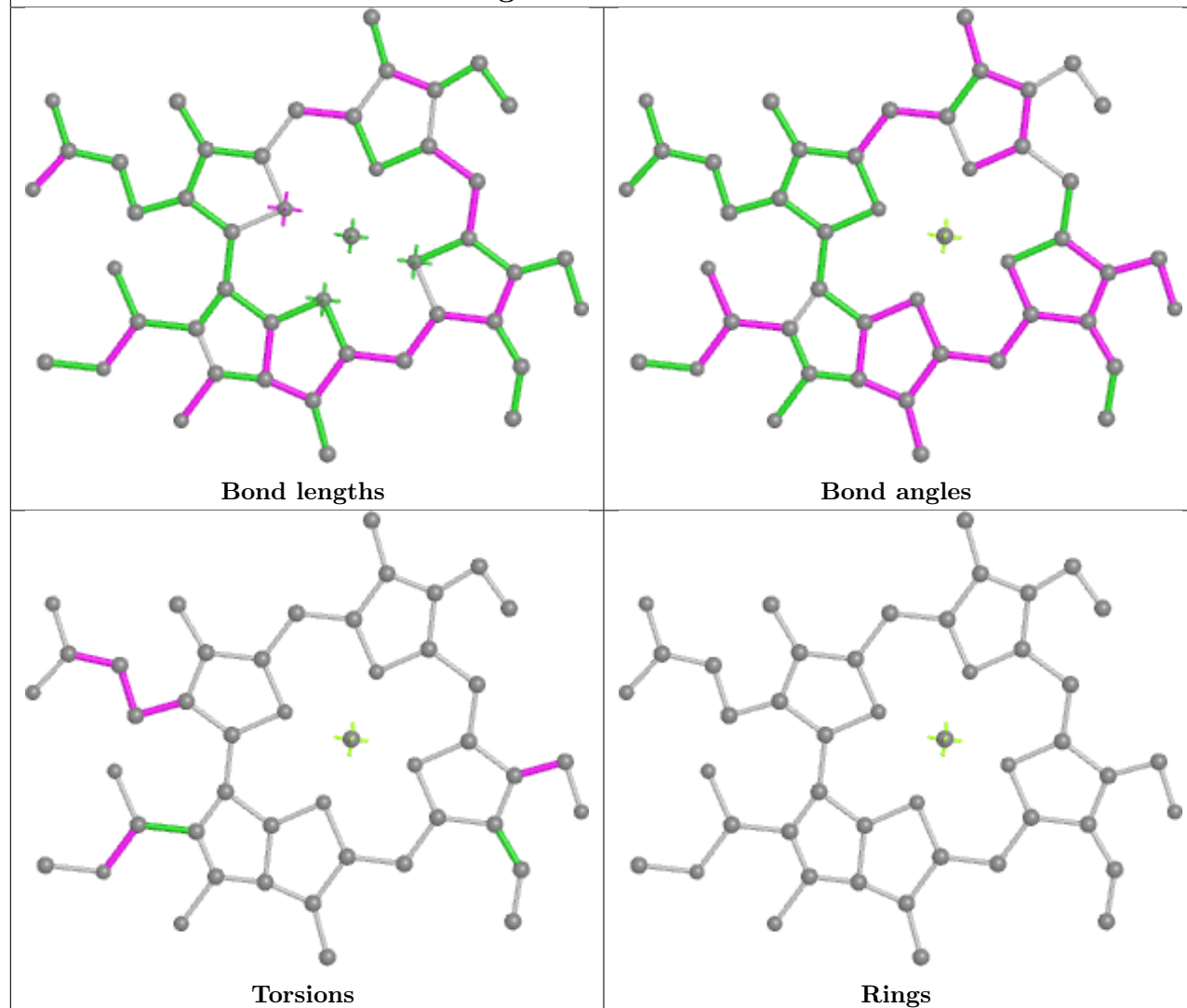
Torsions



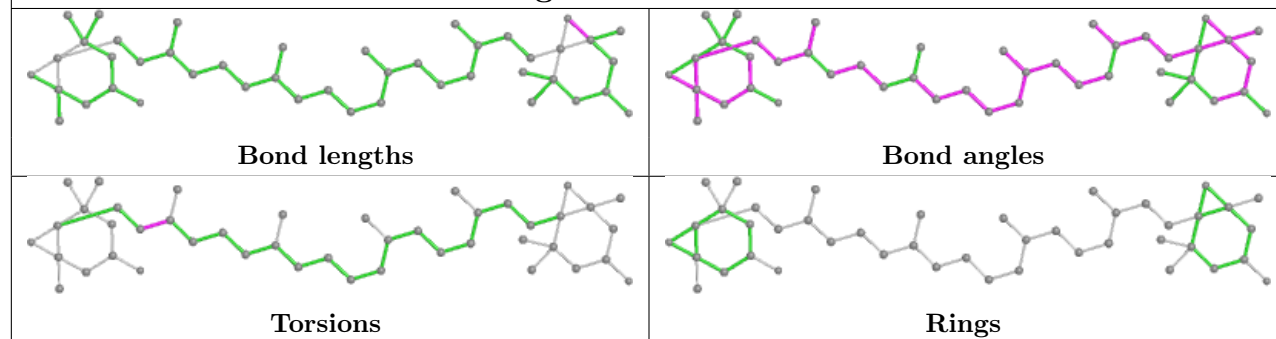
Rings



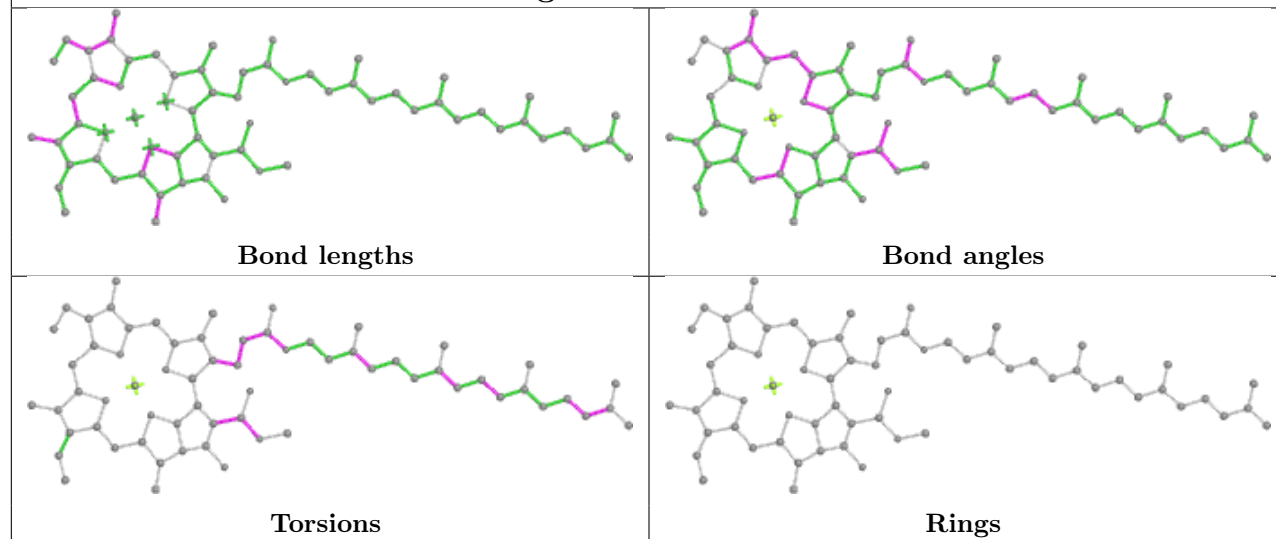
Ligand CHL 8 607



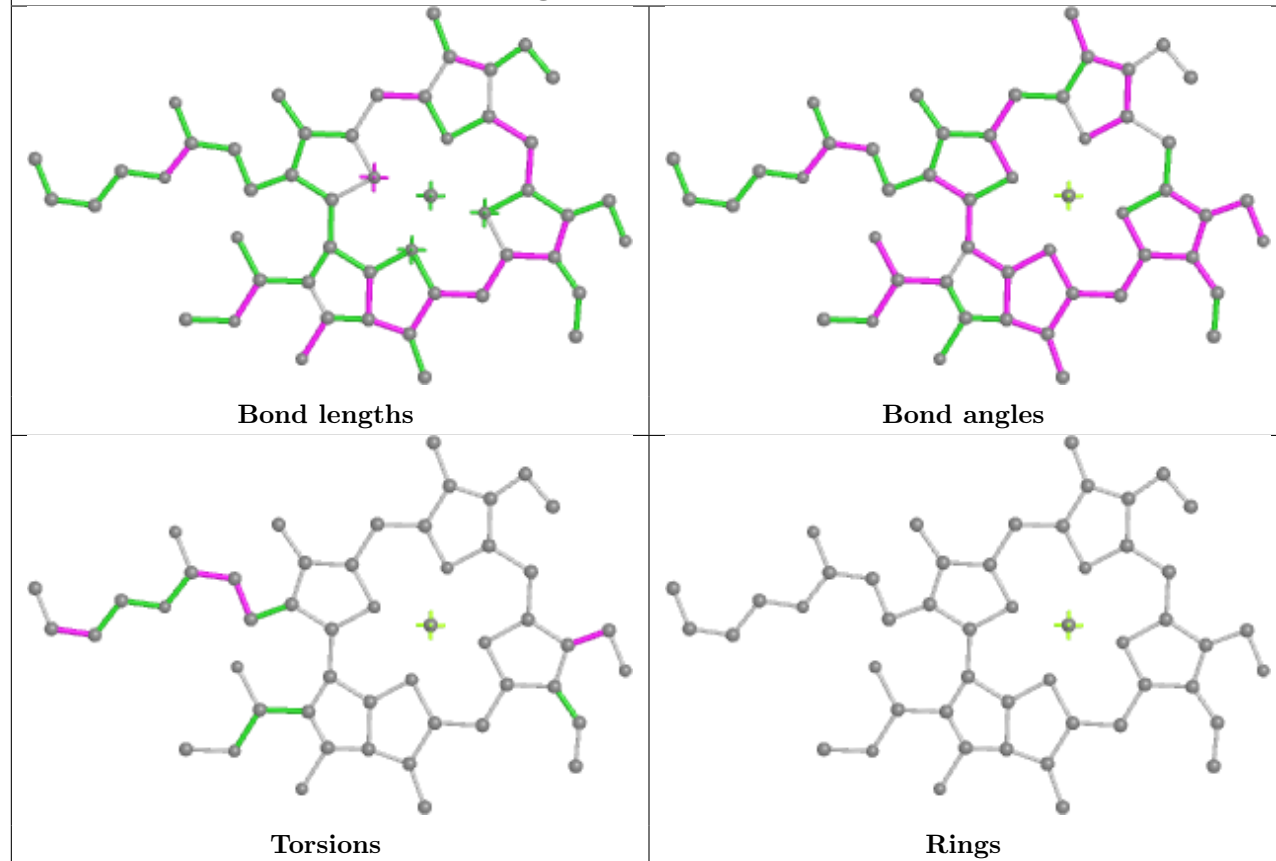
Ligand XAT 8 622

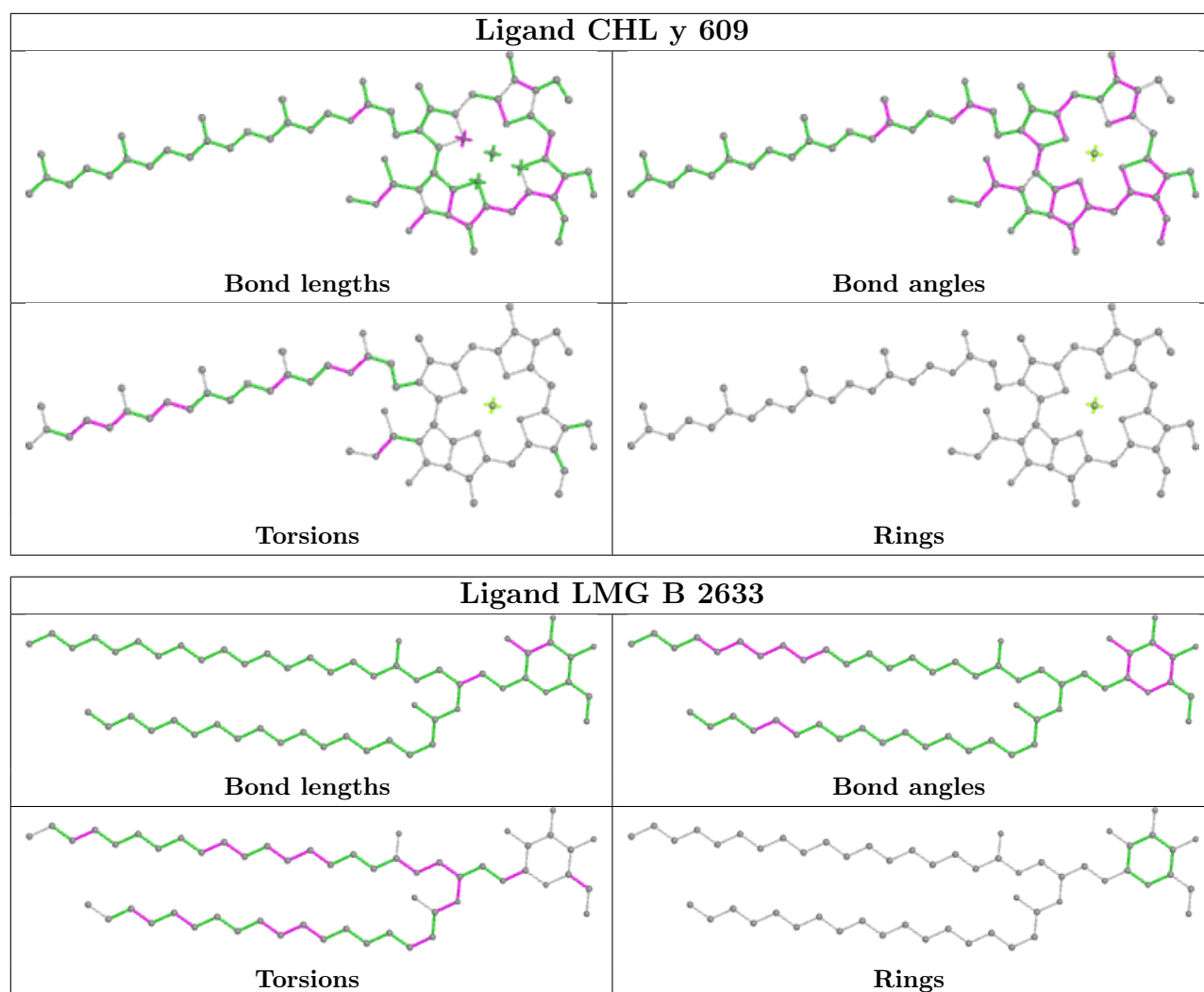


Ligand CLA c 501

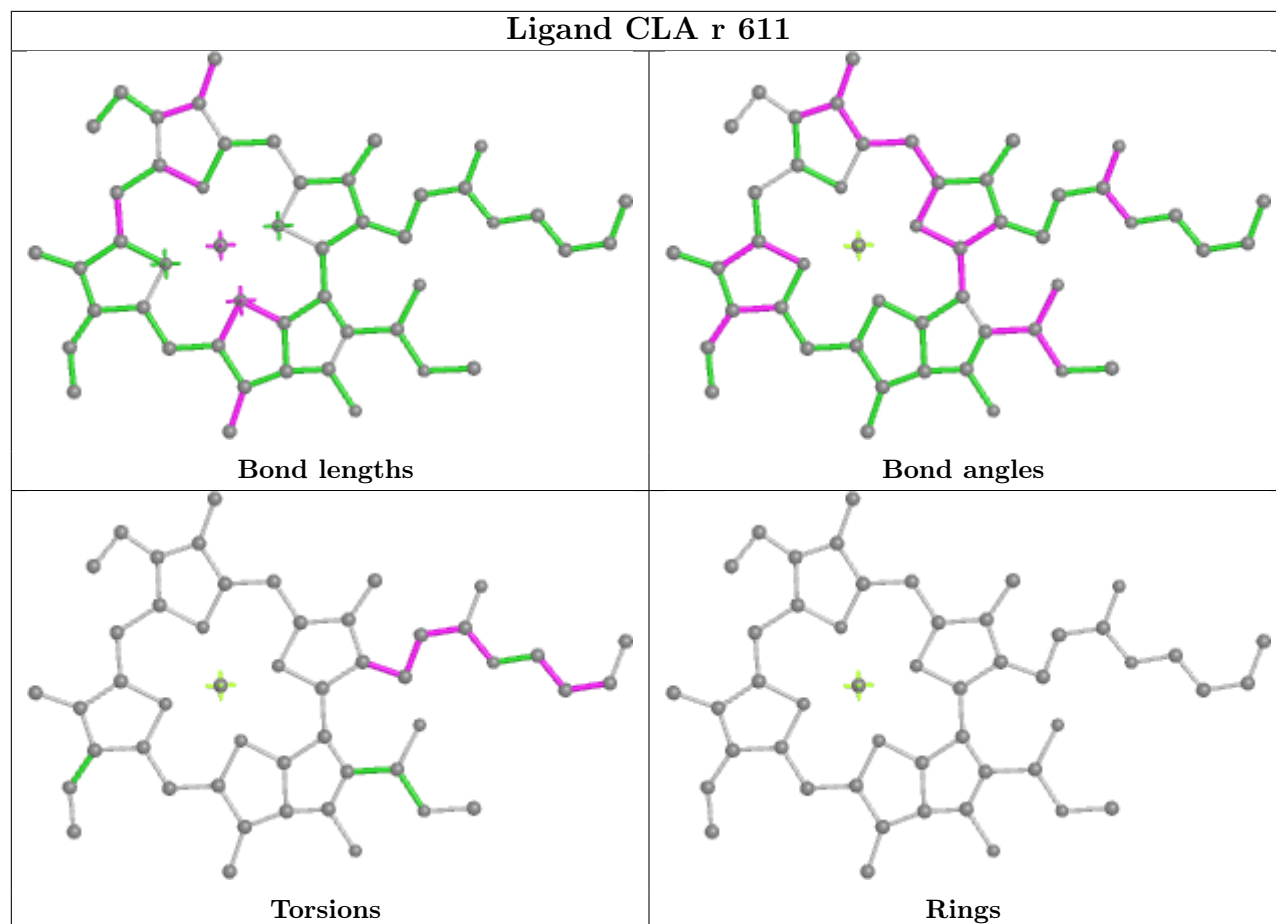


Ligand CHL n 606

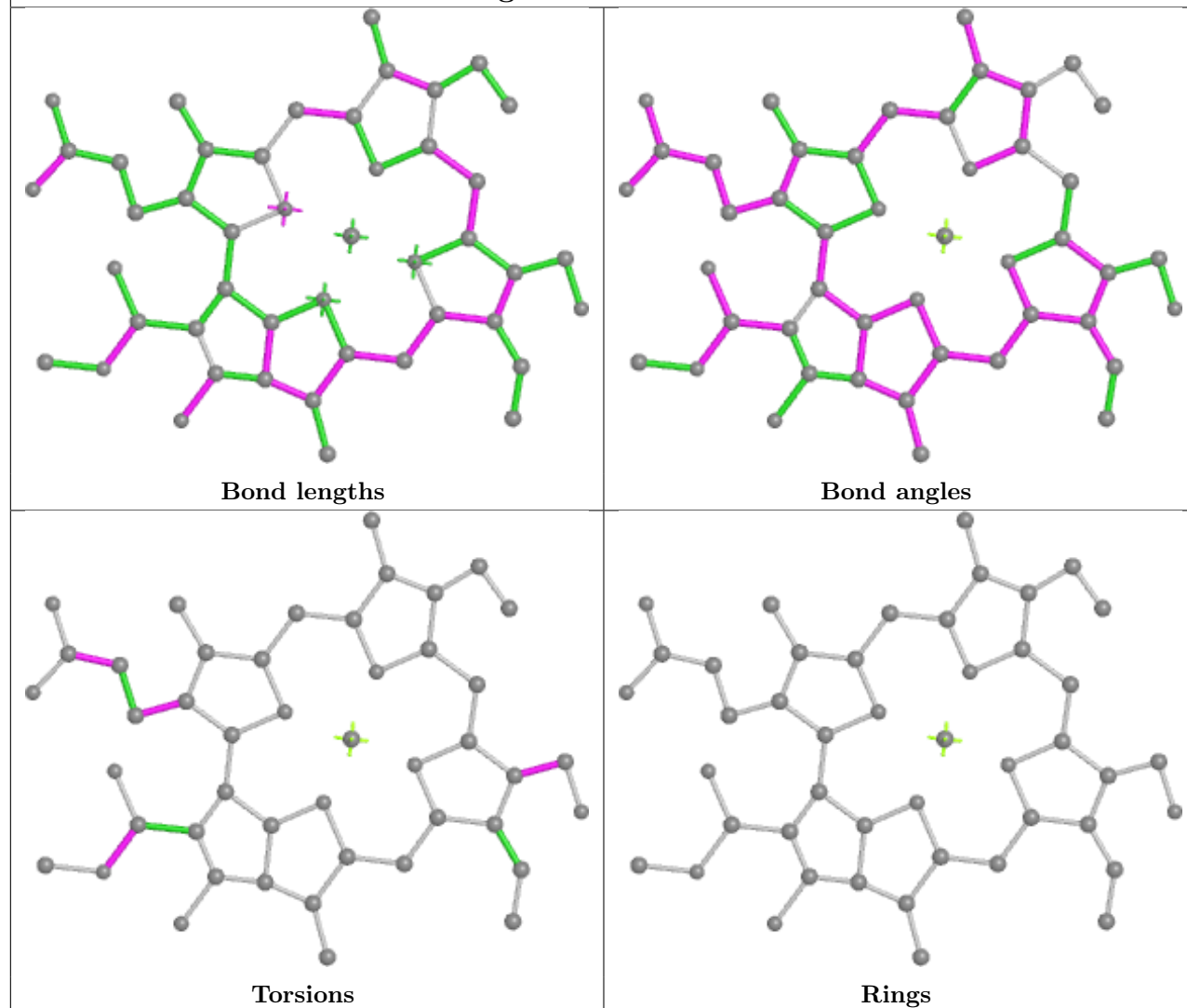




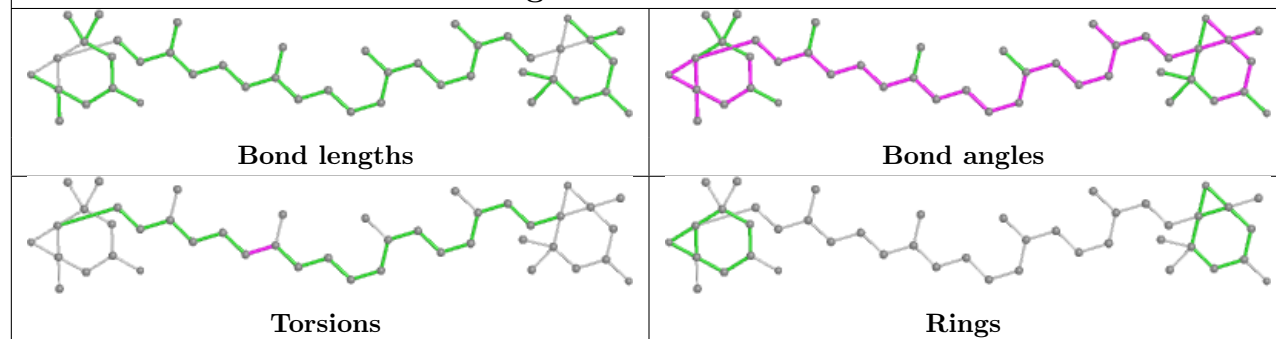
Ligand CLA r 611

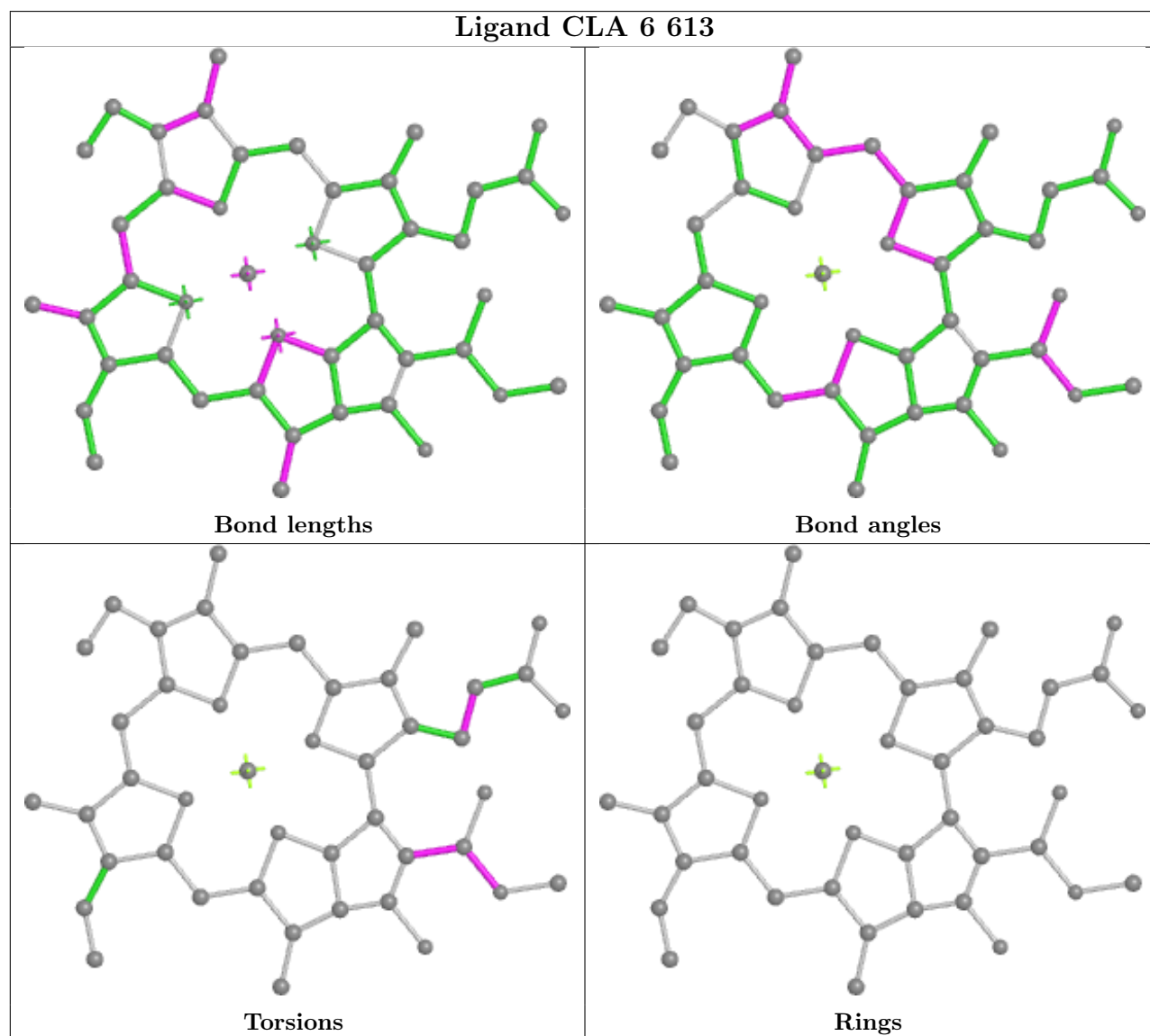
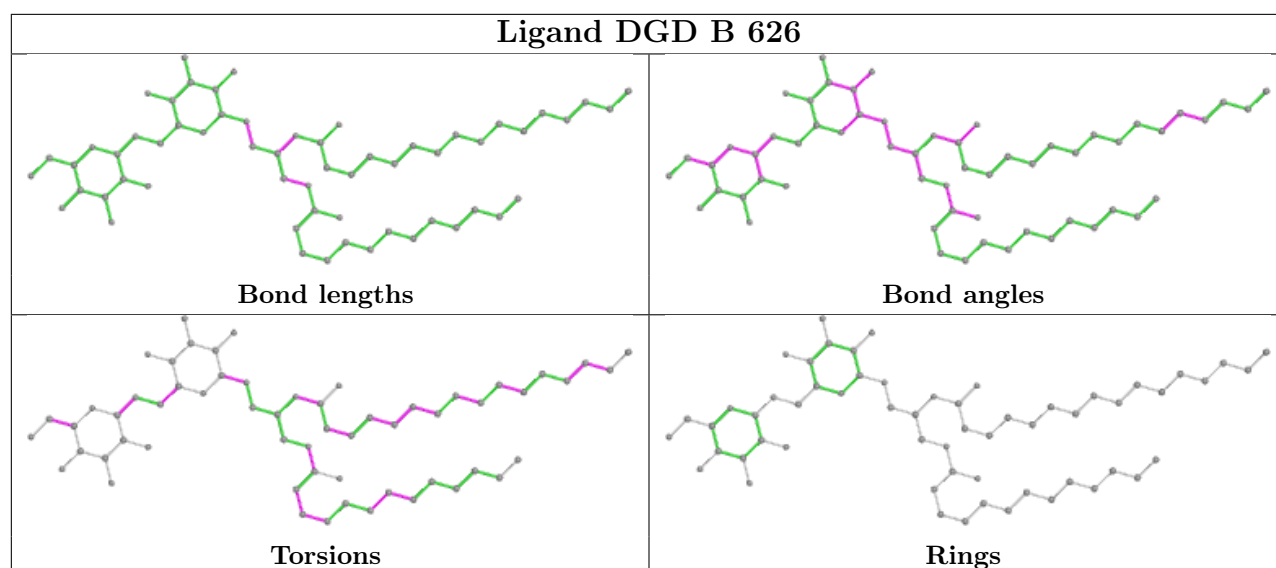


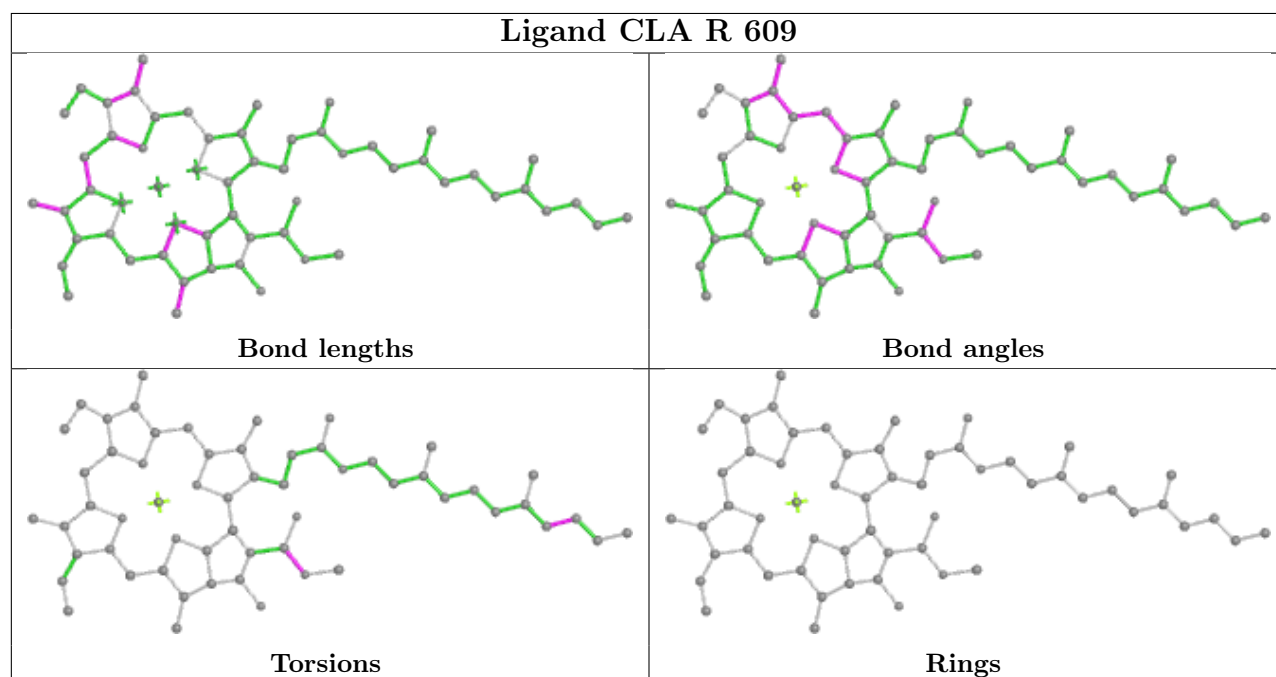
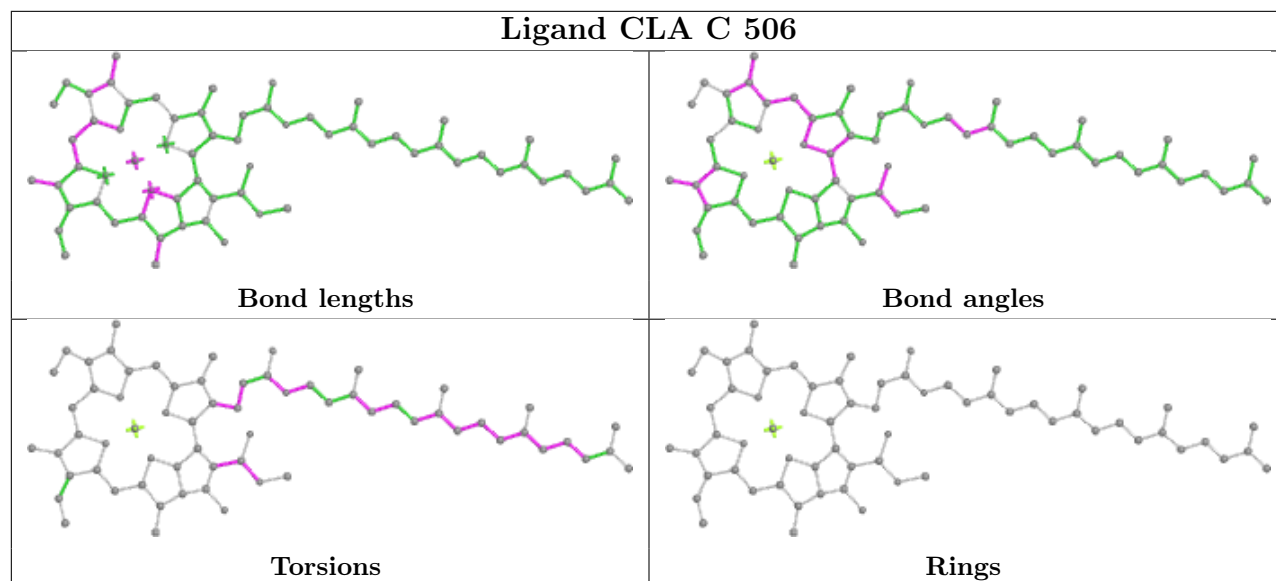
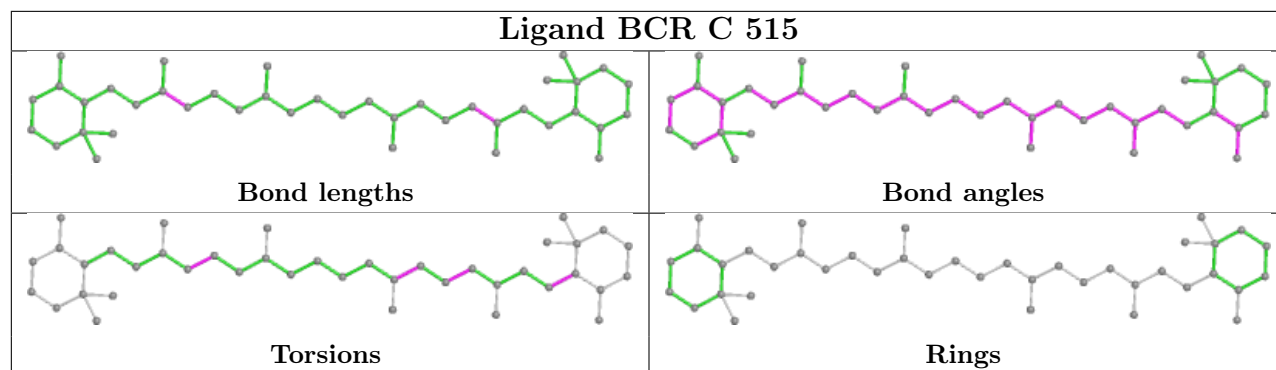
Ligand CHL 8 606

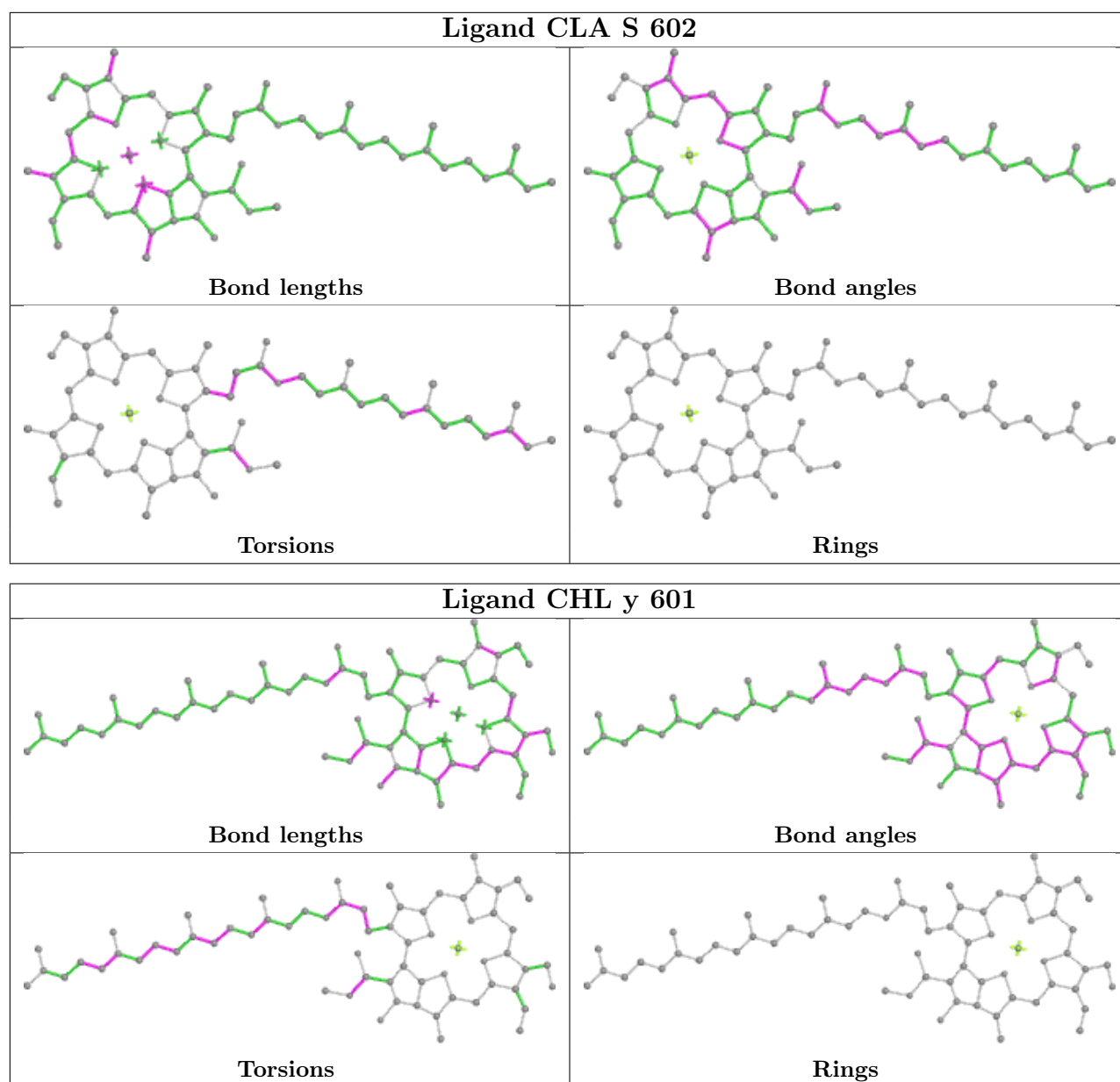


Ligand XAT 5 1622

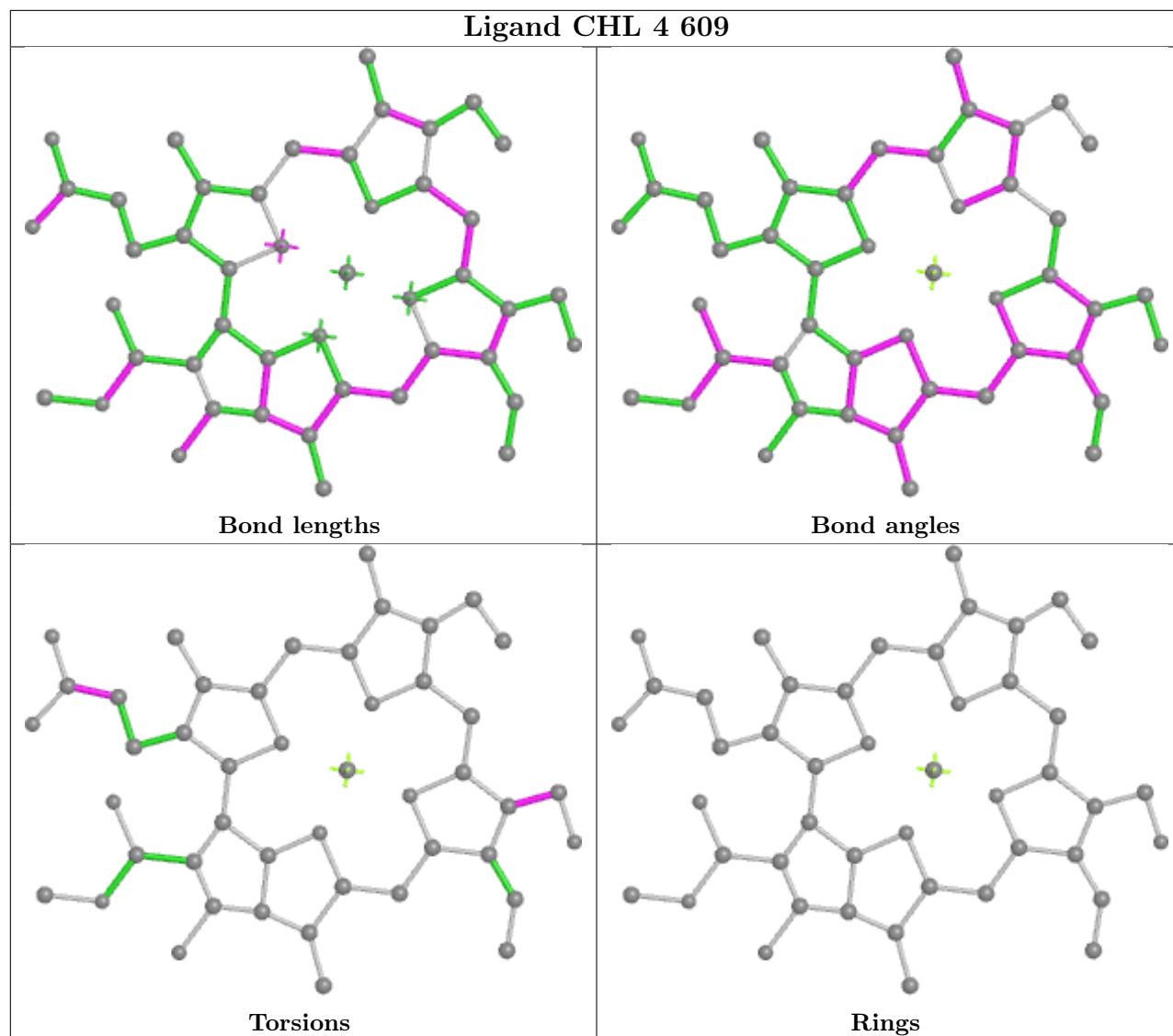




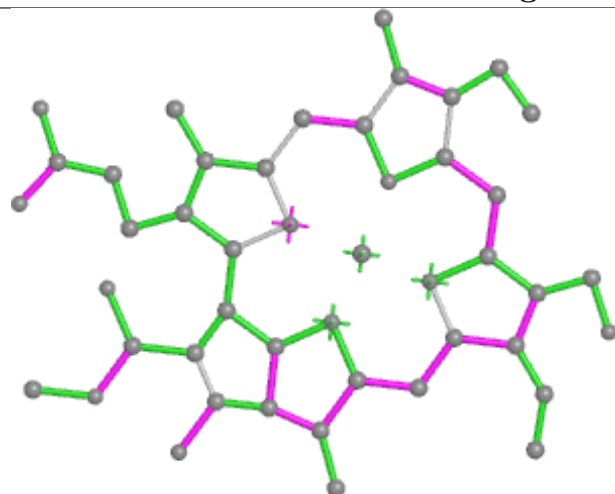




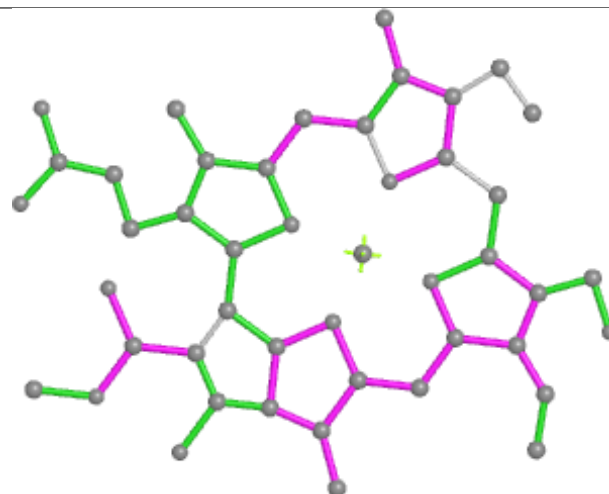
Ligand CHL 4 609



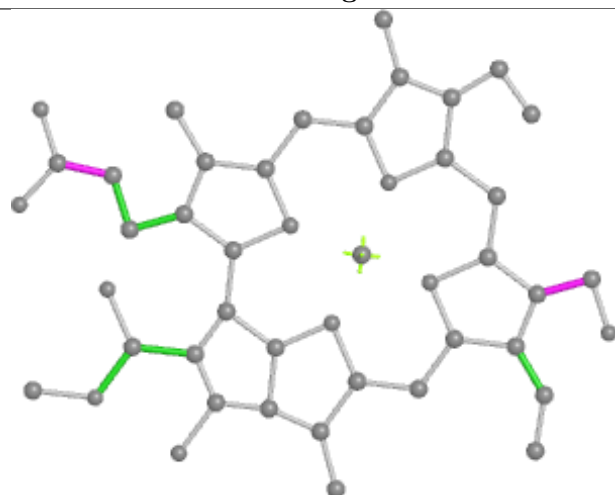
Ligand CHL 8 609



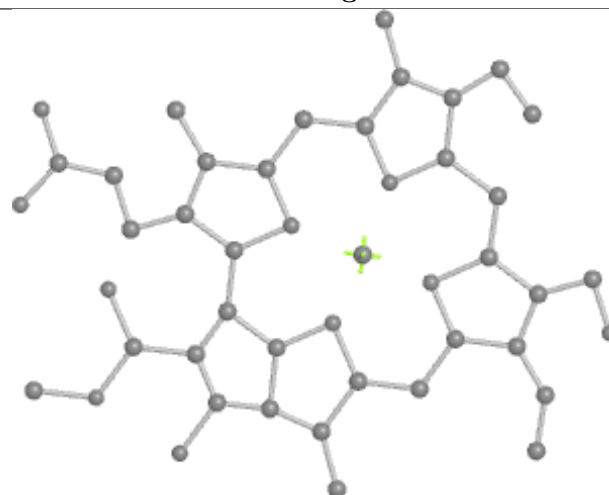
Bond lengths



Bond angles

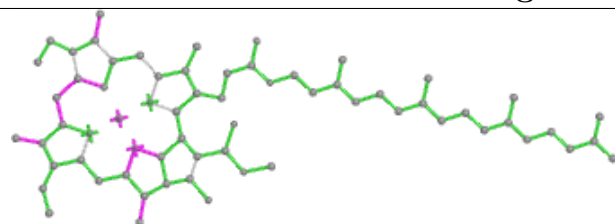


Torsions

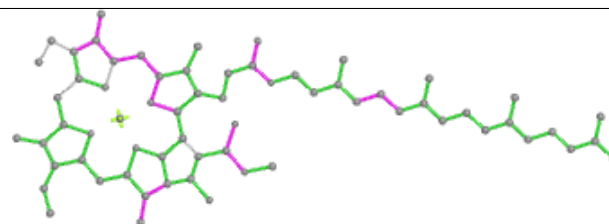


Rings

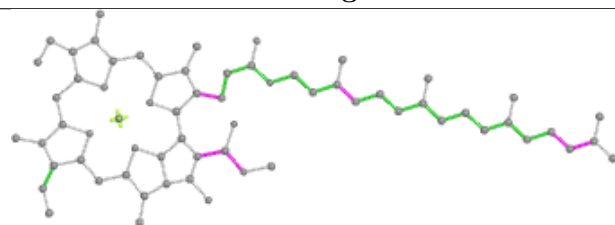
Ligand CLA B 610



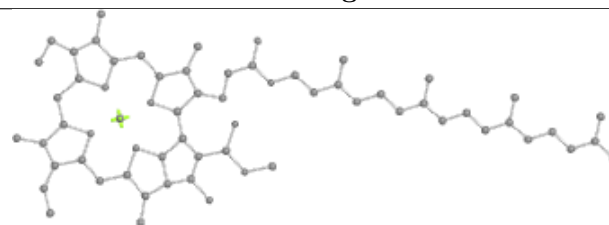
Bond lengths



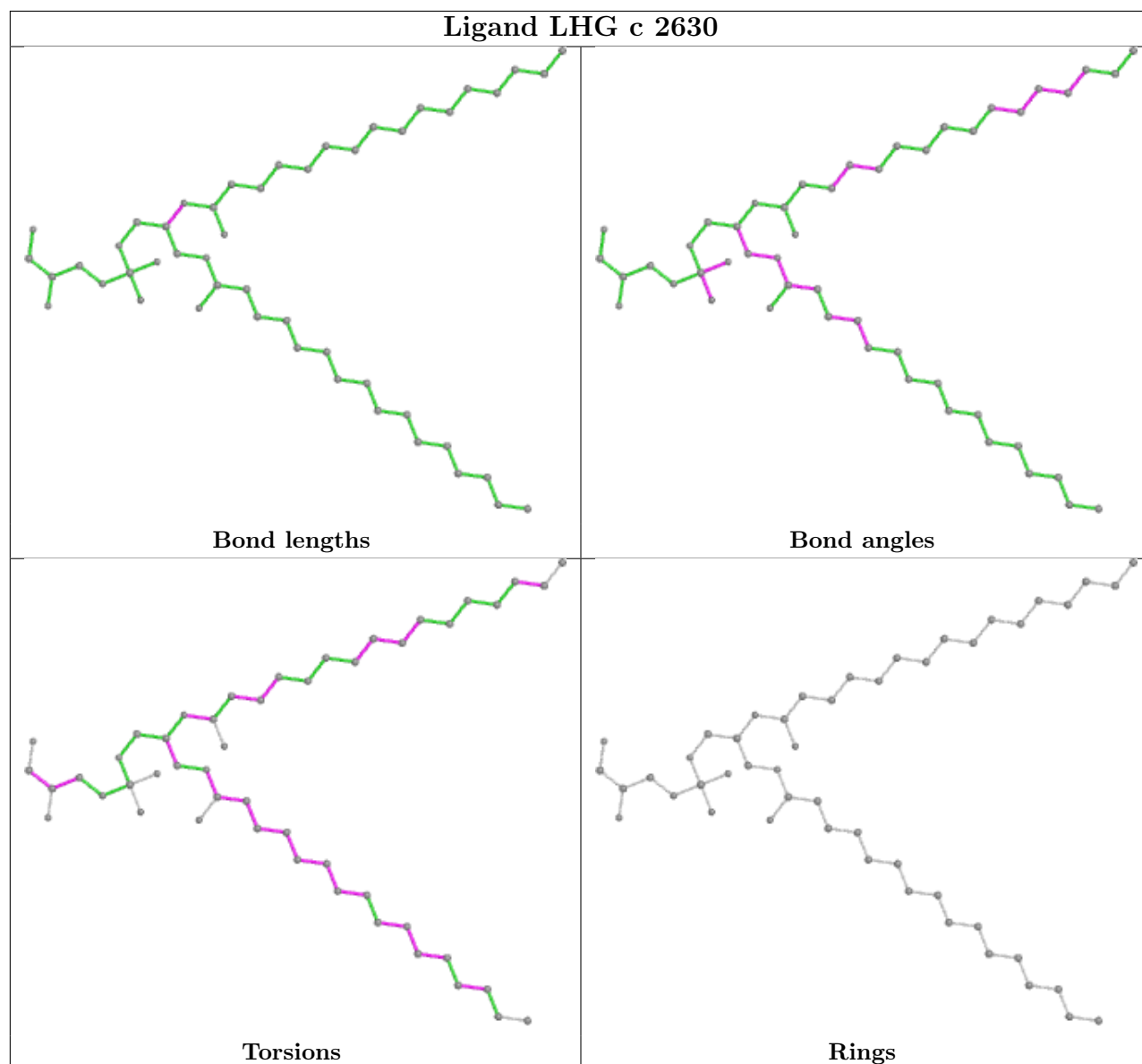
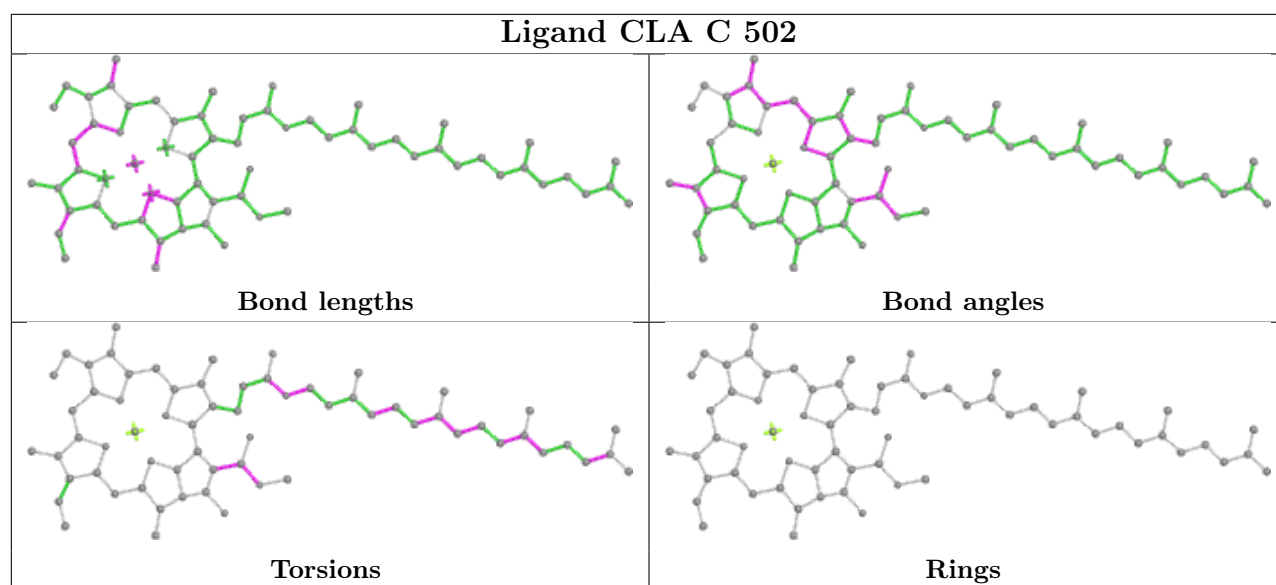
Bond angles

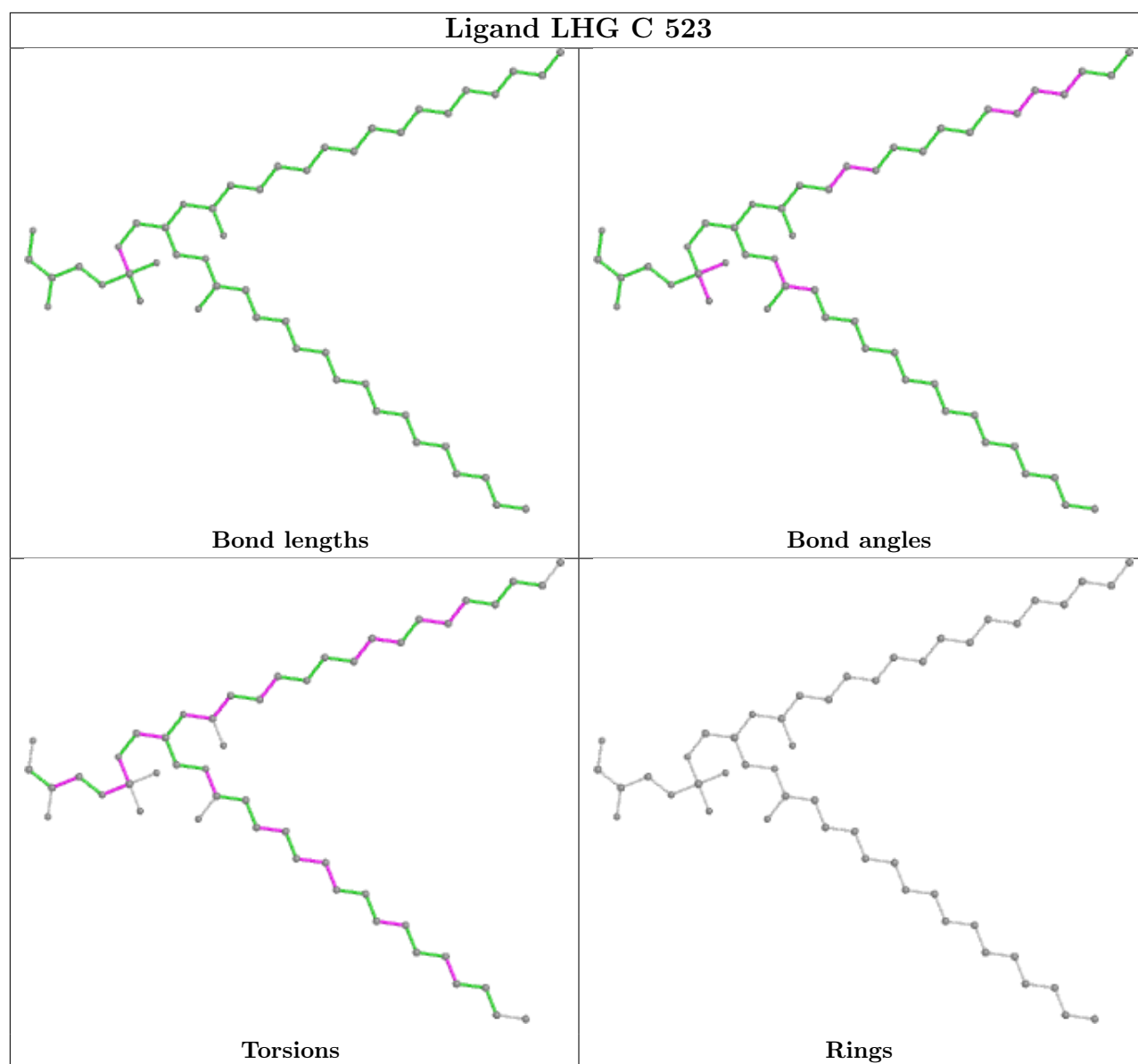


Torsions

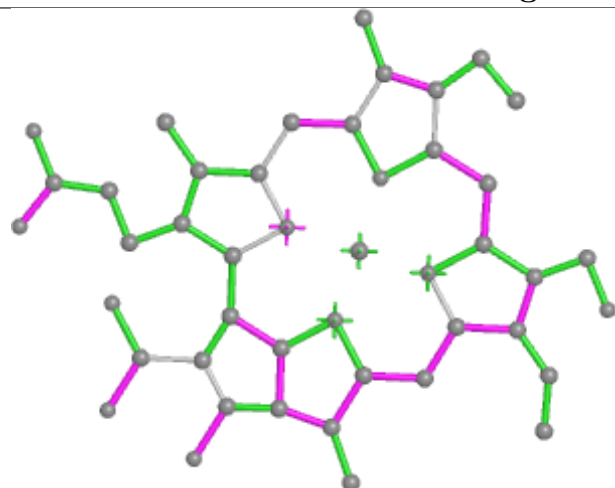


Rings

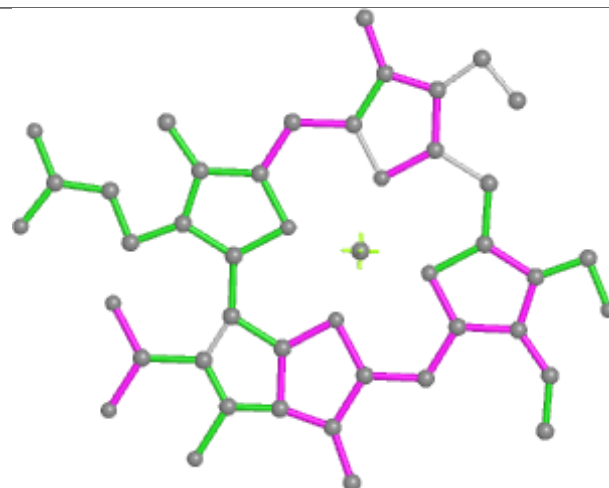




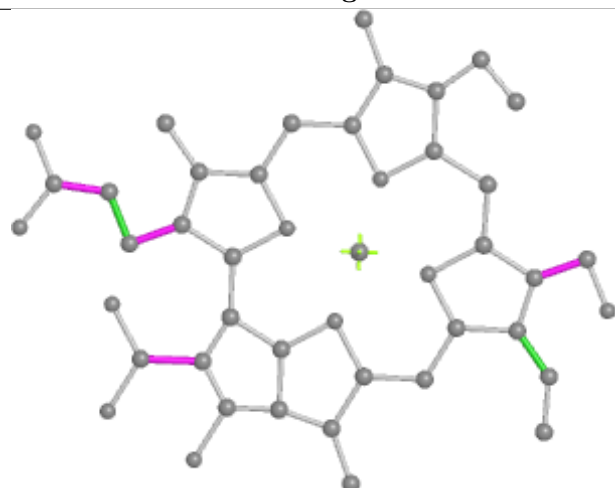
Ligand CHL 8 601



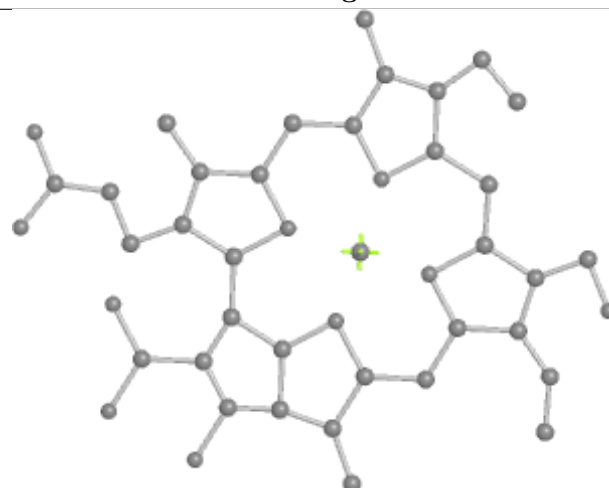
Bond lengths



Bond angles

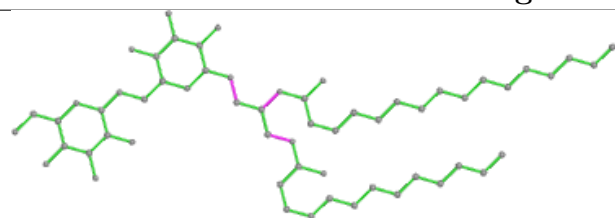


Torsions

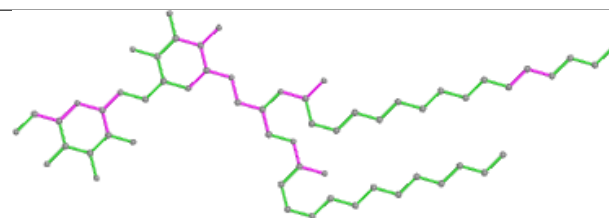


Rings

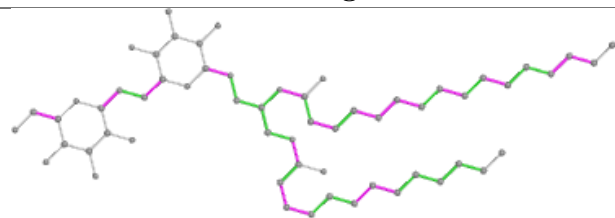
Ligand DGD b 626



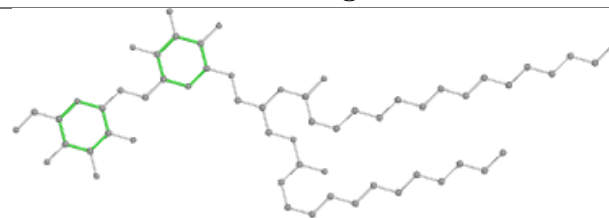
Bond lengths



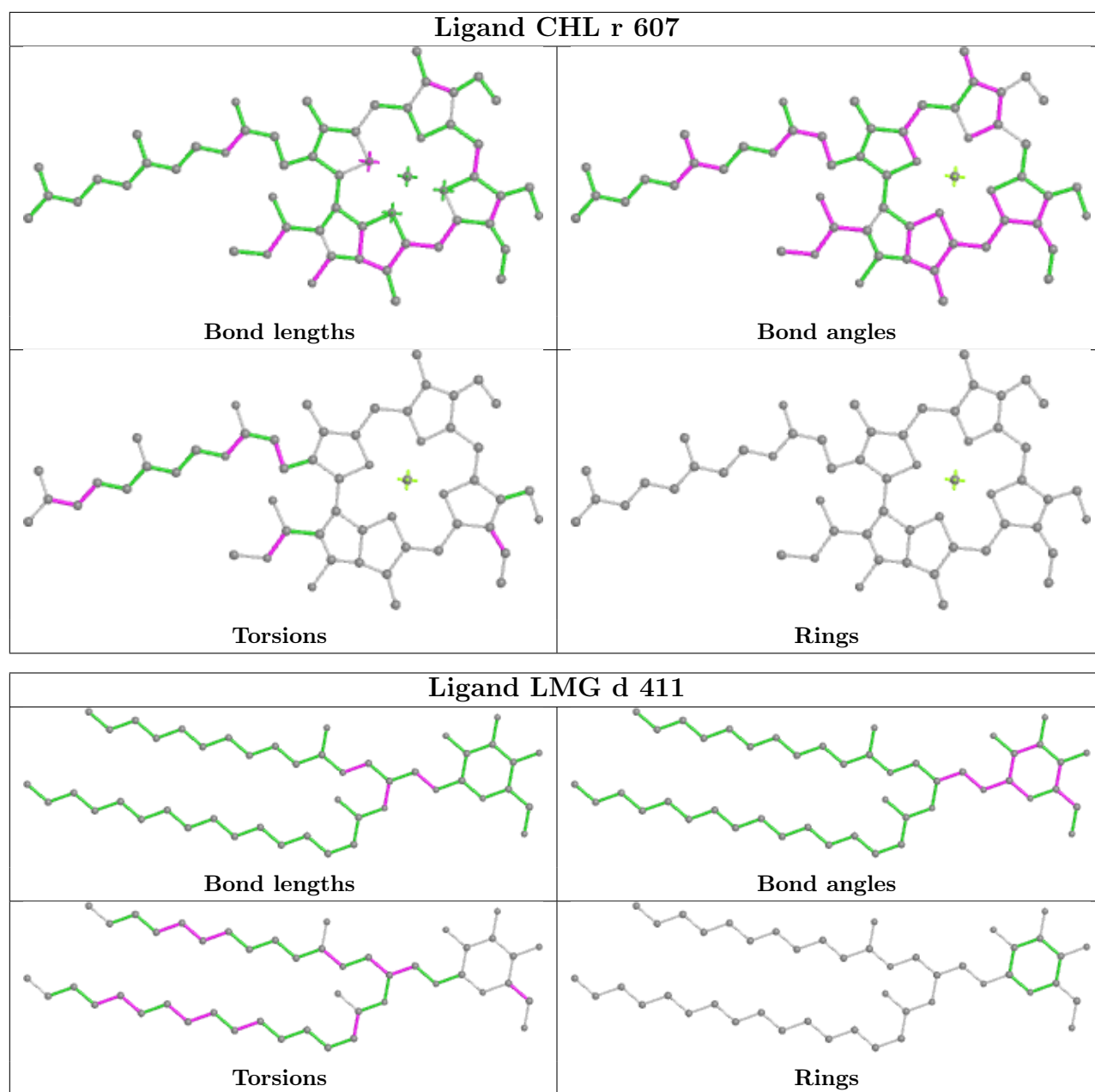
Bond angles

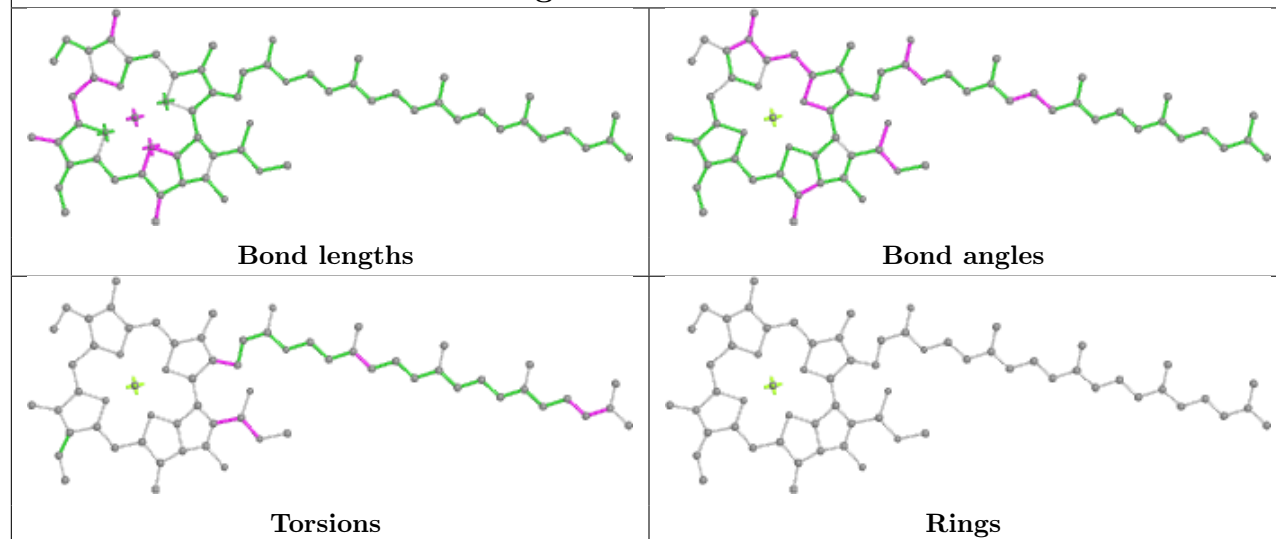
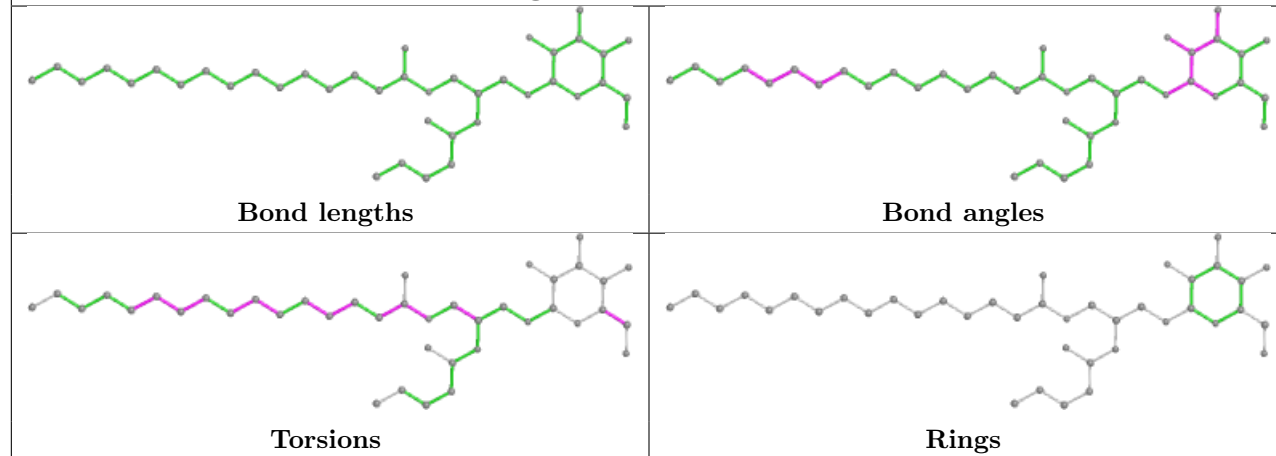


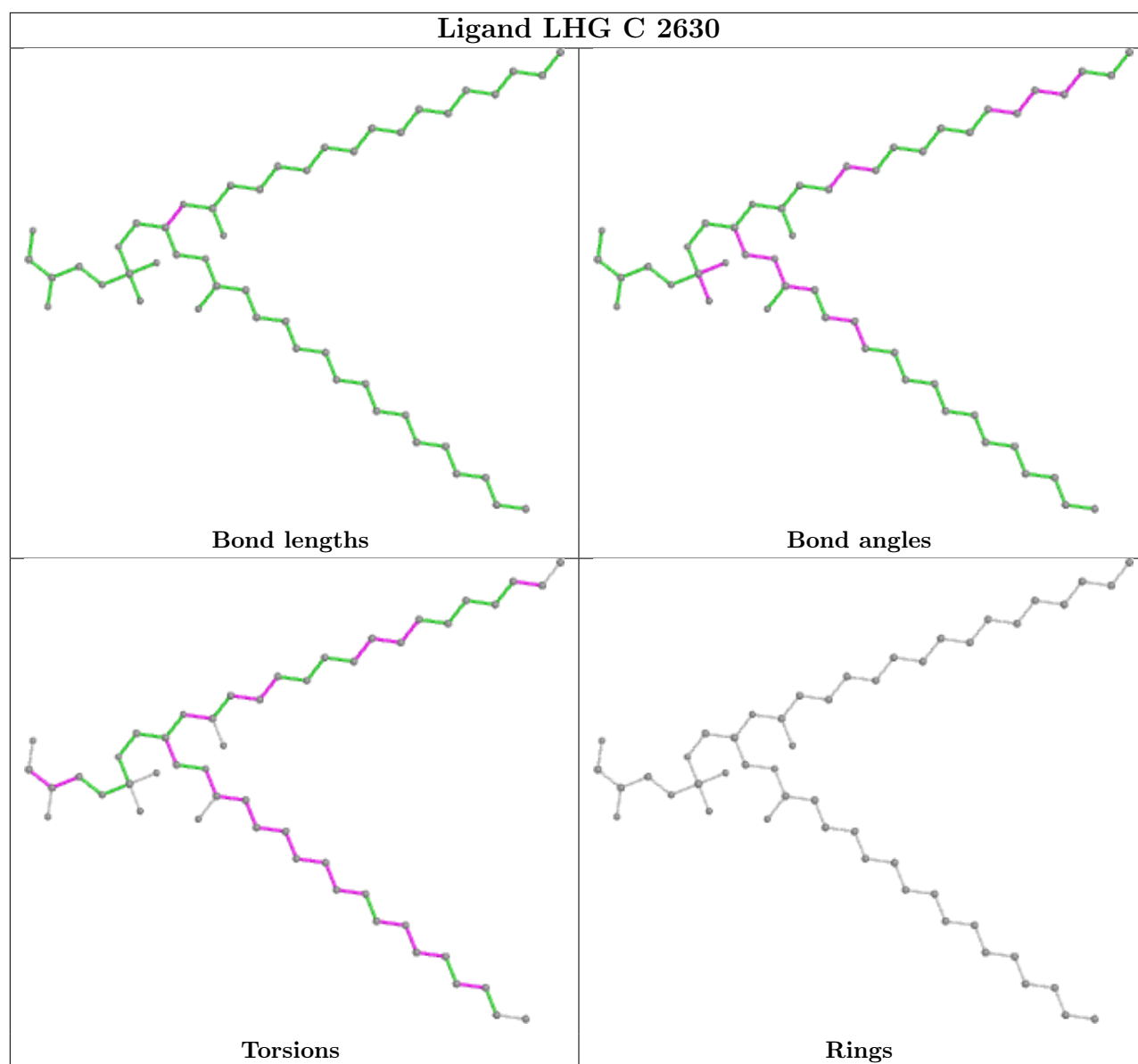
Torsions

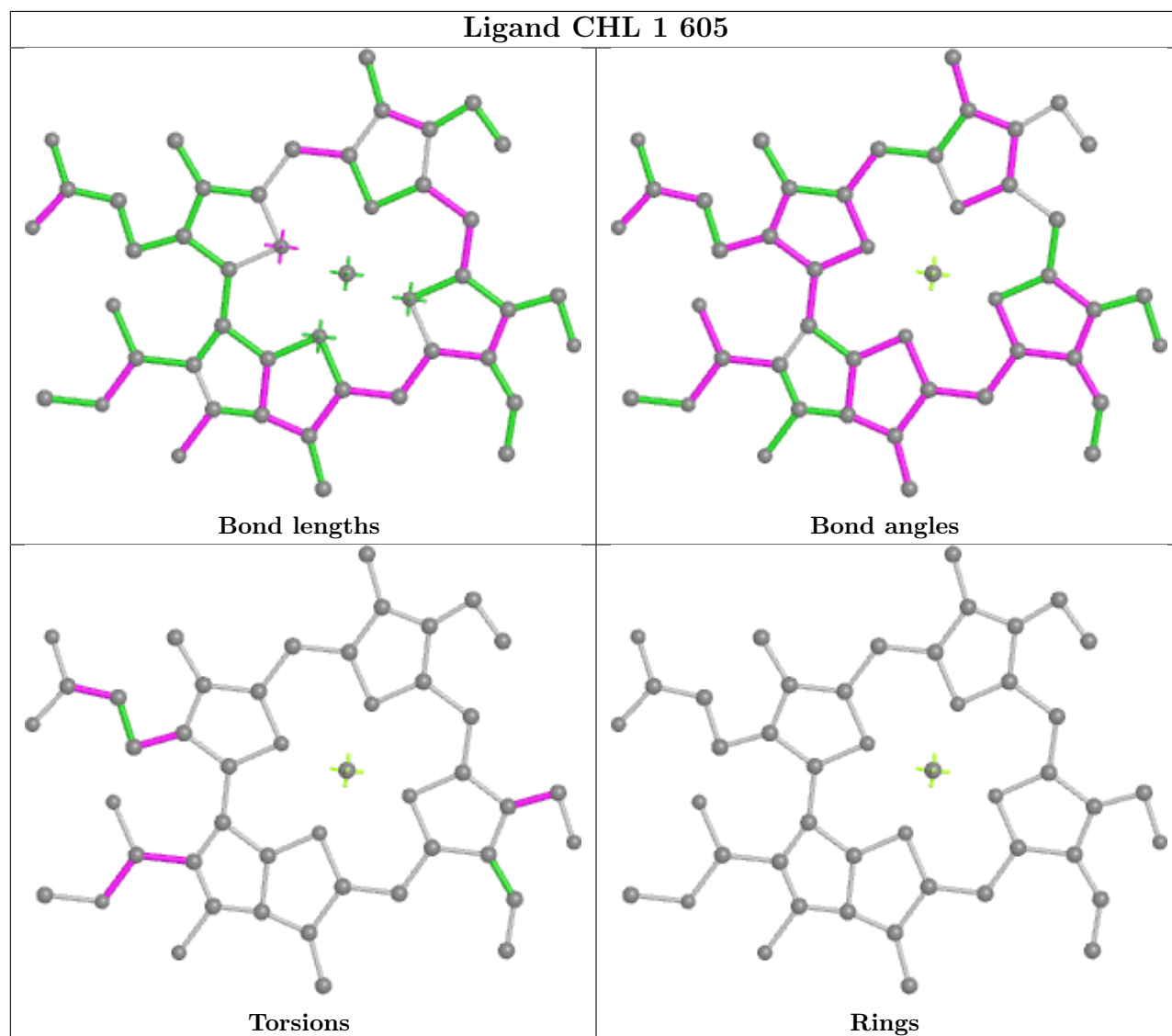
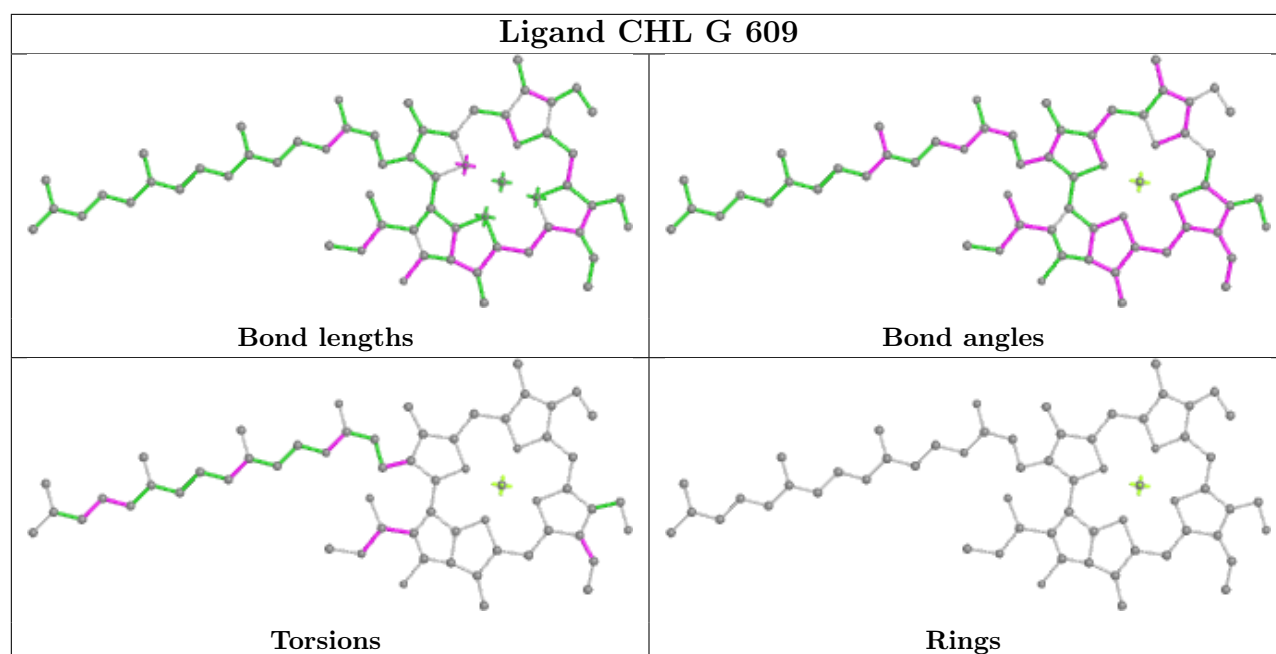


Rings

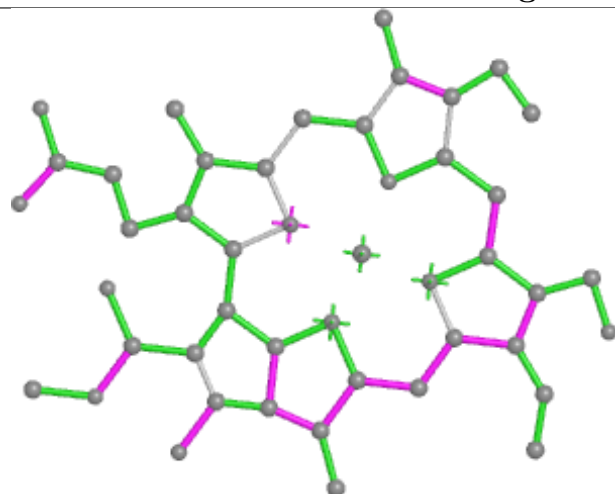


Ligand CLA b 610**Ligand LMG A 415**

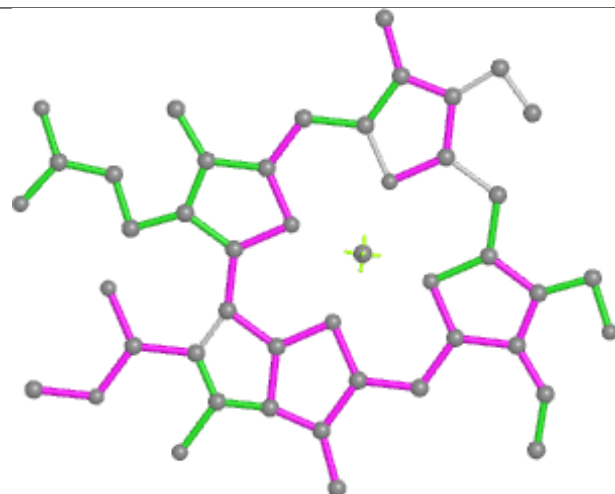




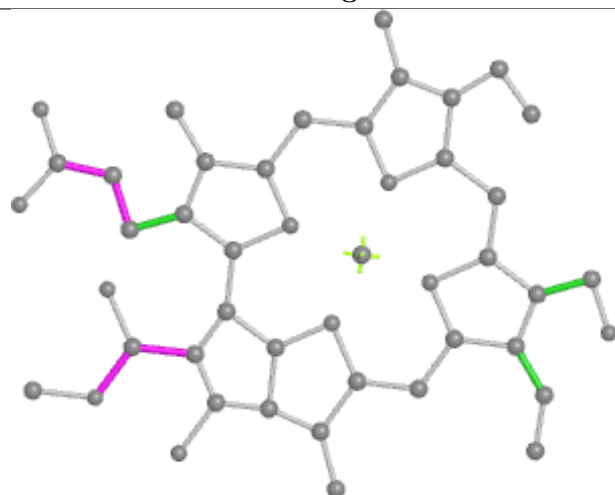
Ligand CHL S 601



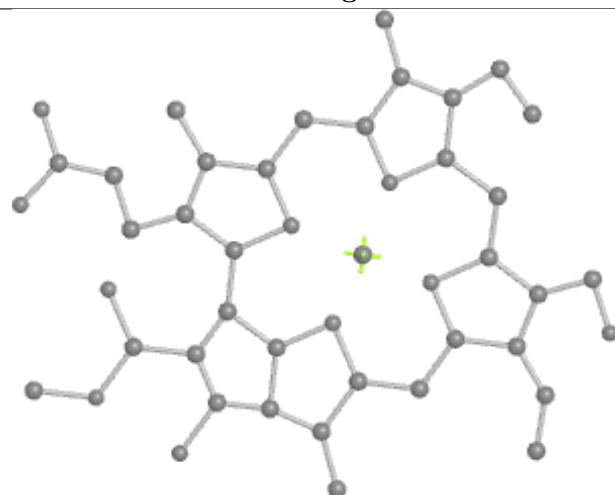
Bond lengths



Bond angles

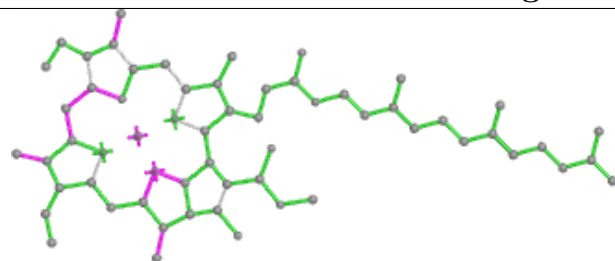


Torsions

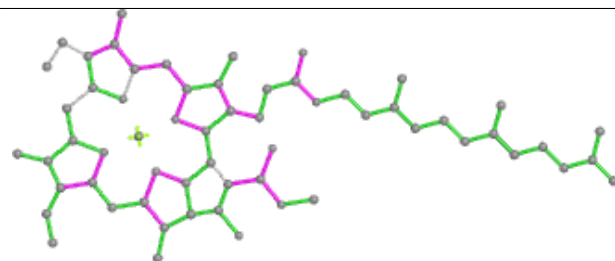


Rings

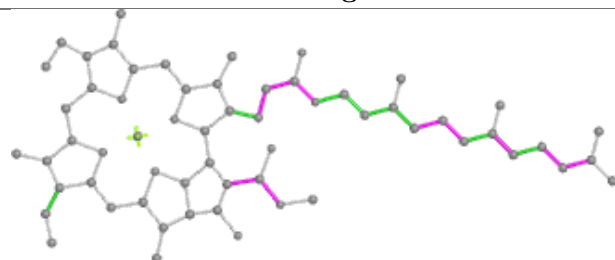
Ligand CLA r 603



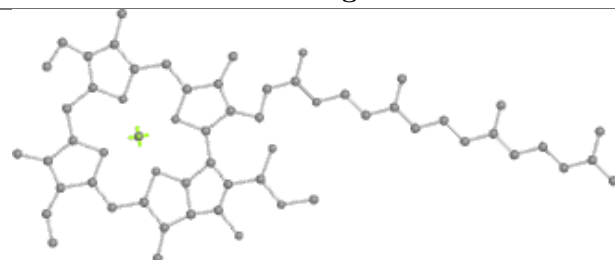
Bond lengths



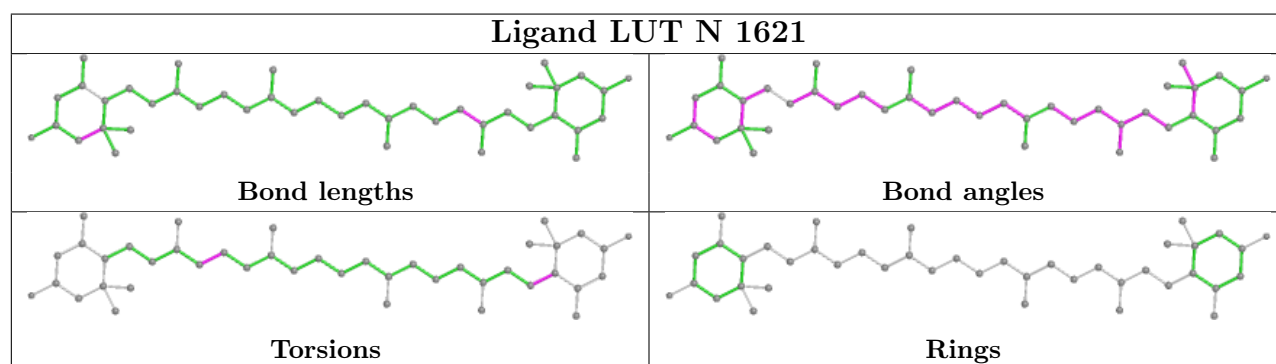
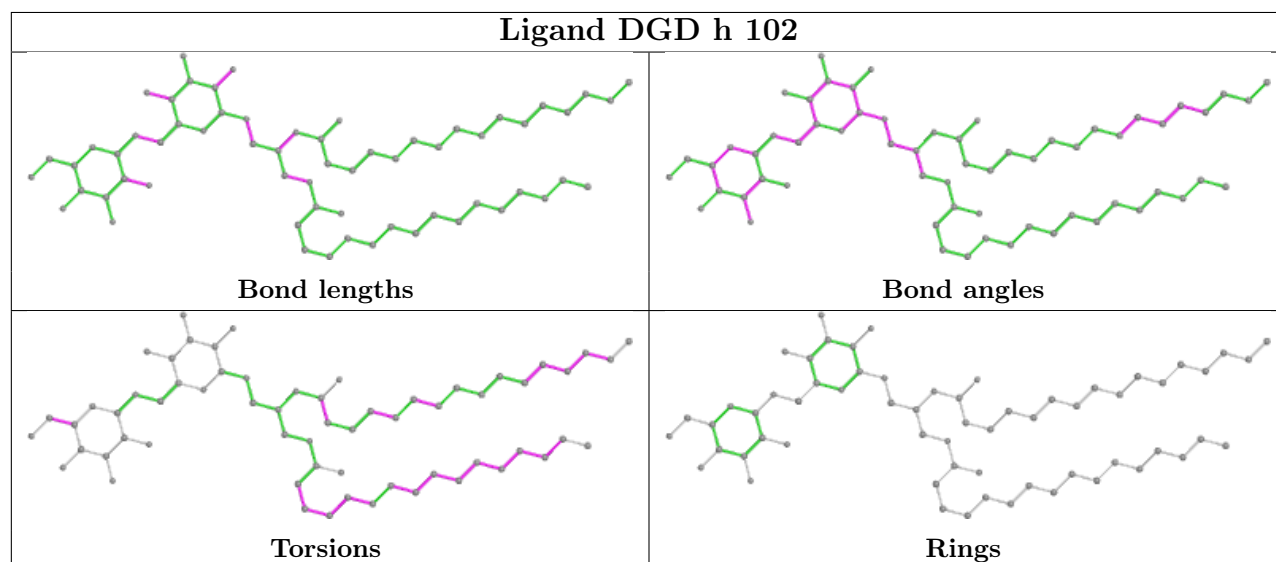
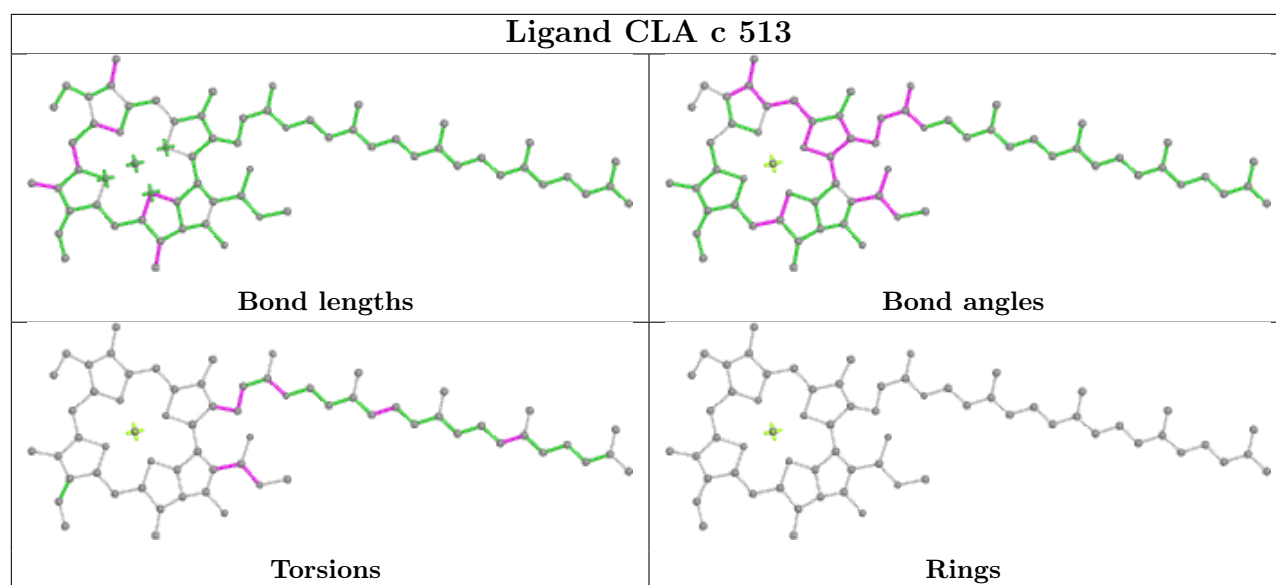
Bond angles

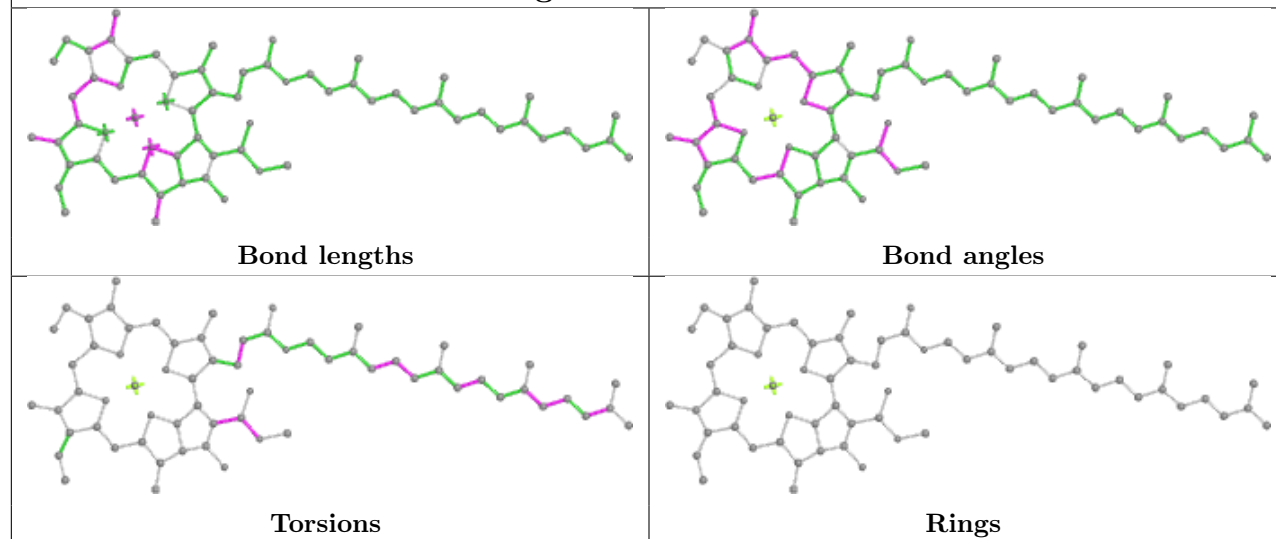
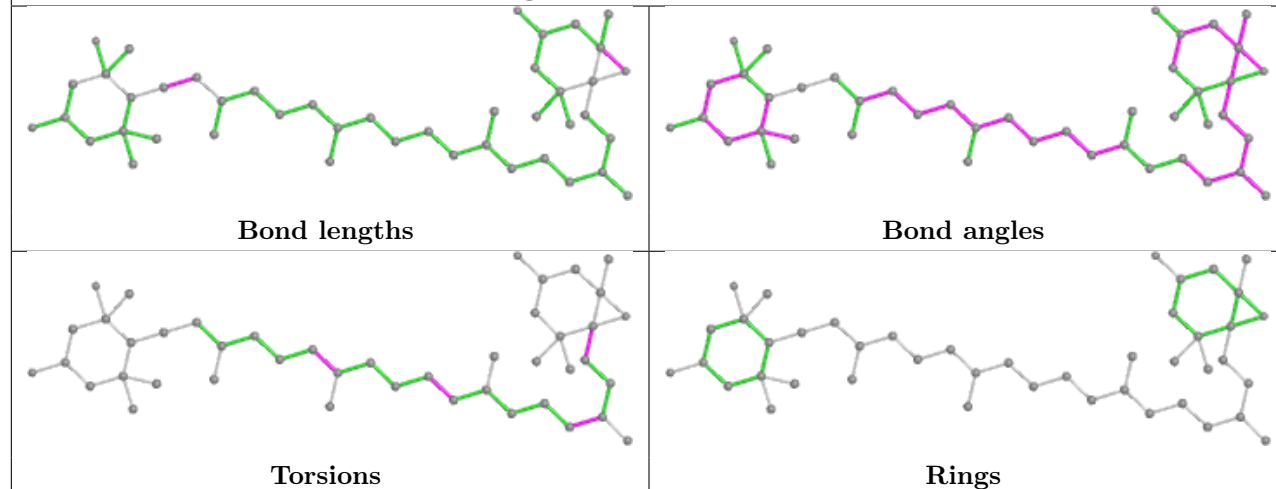
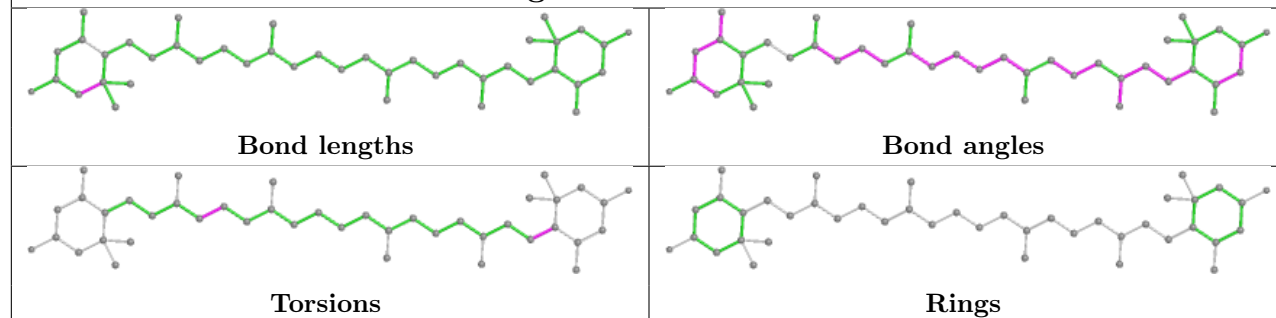


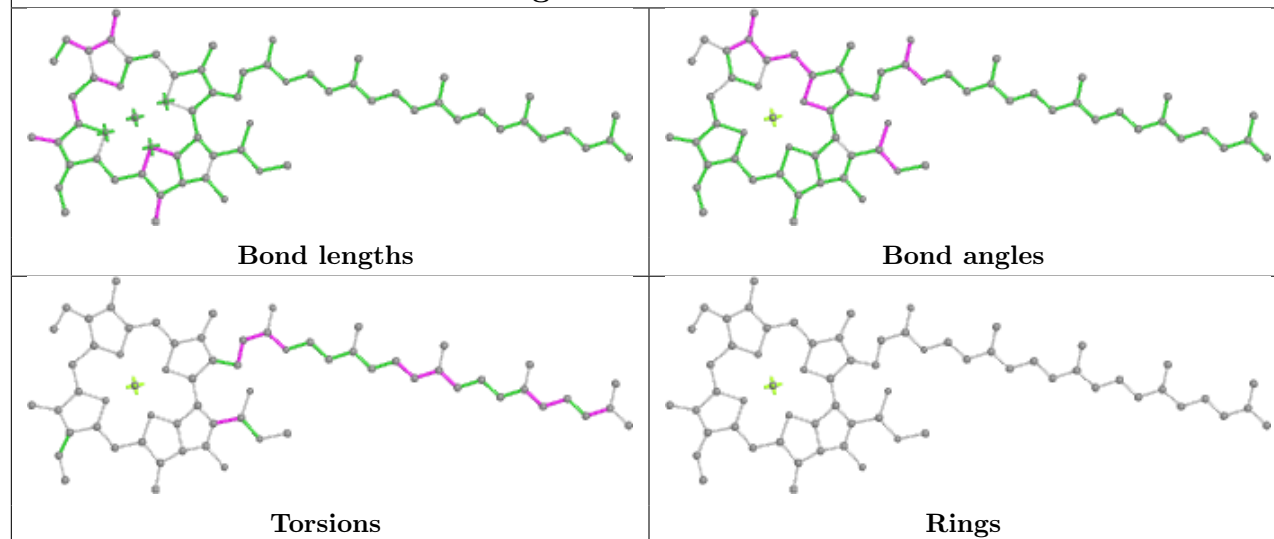
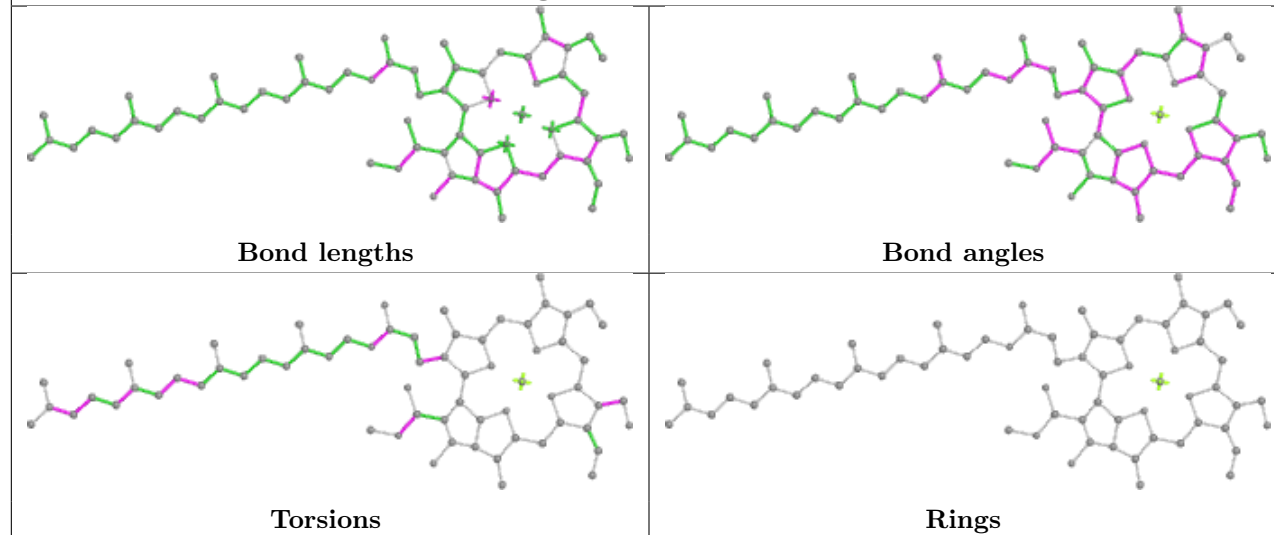
Torsions

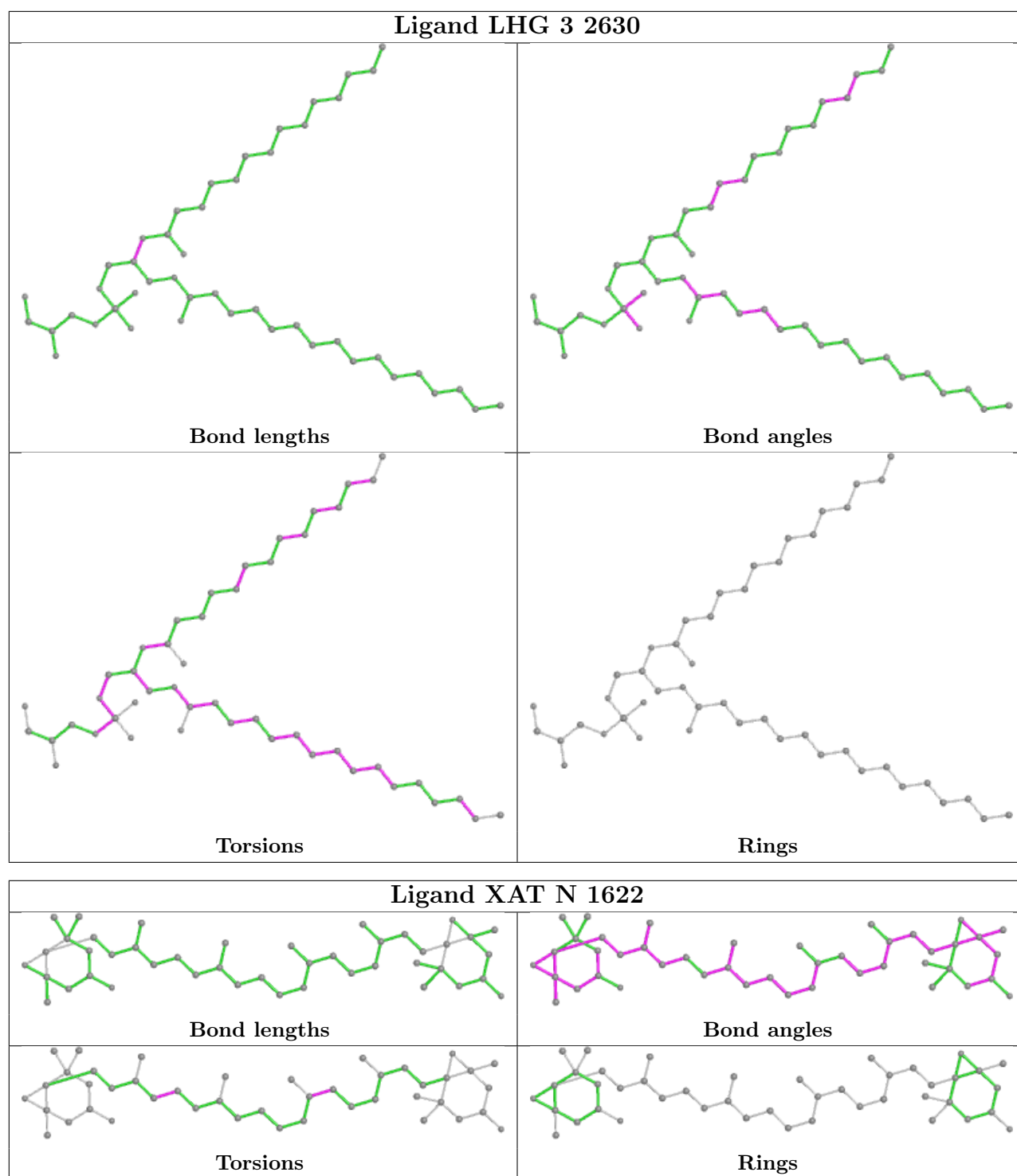


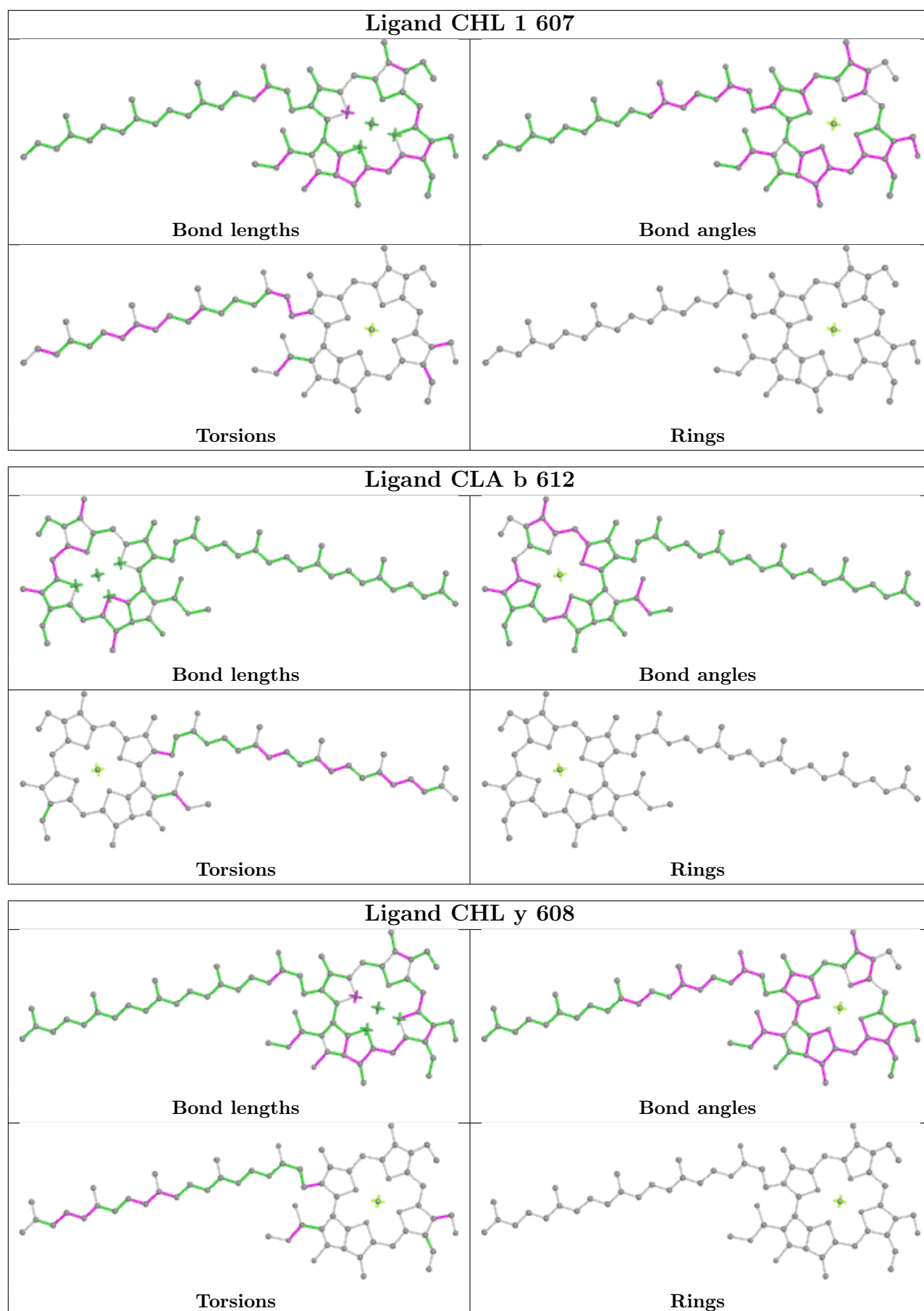
Rings

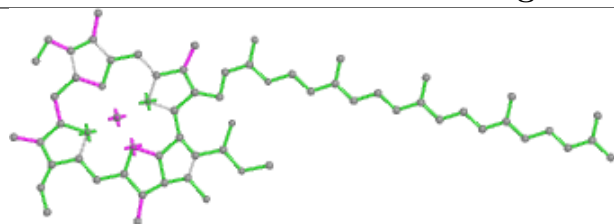
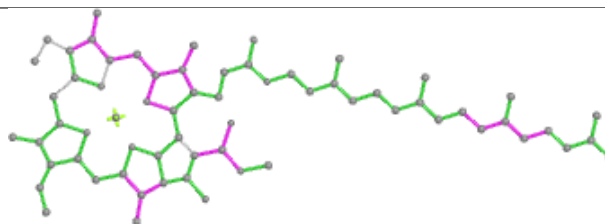
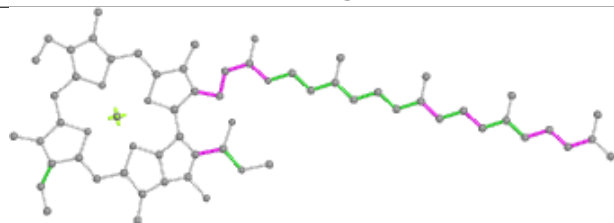
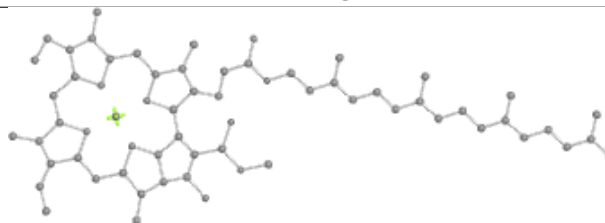
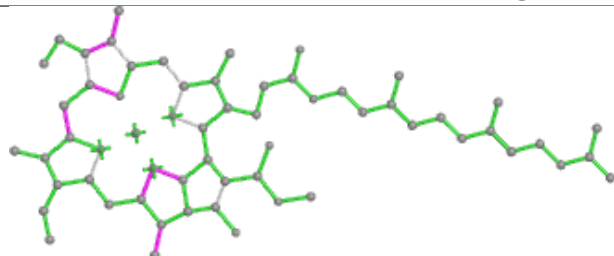
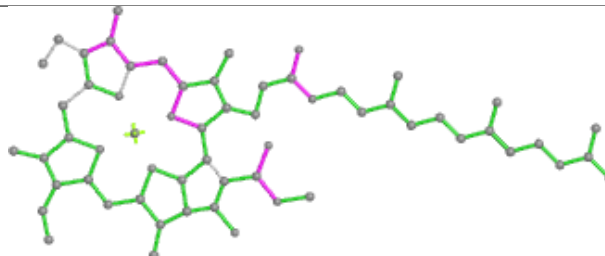
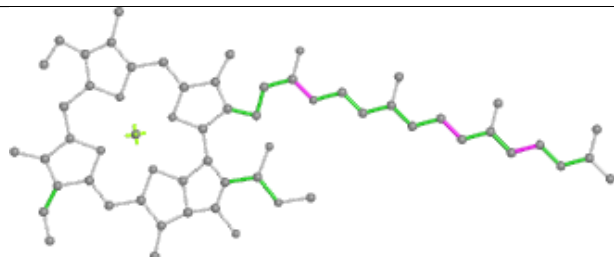
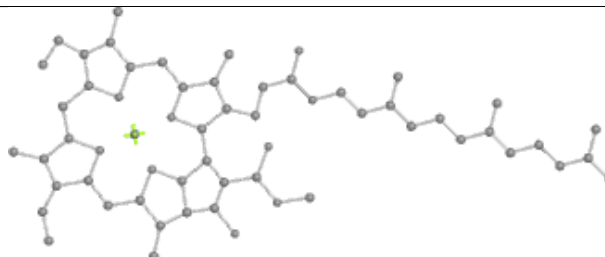


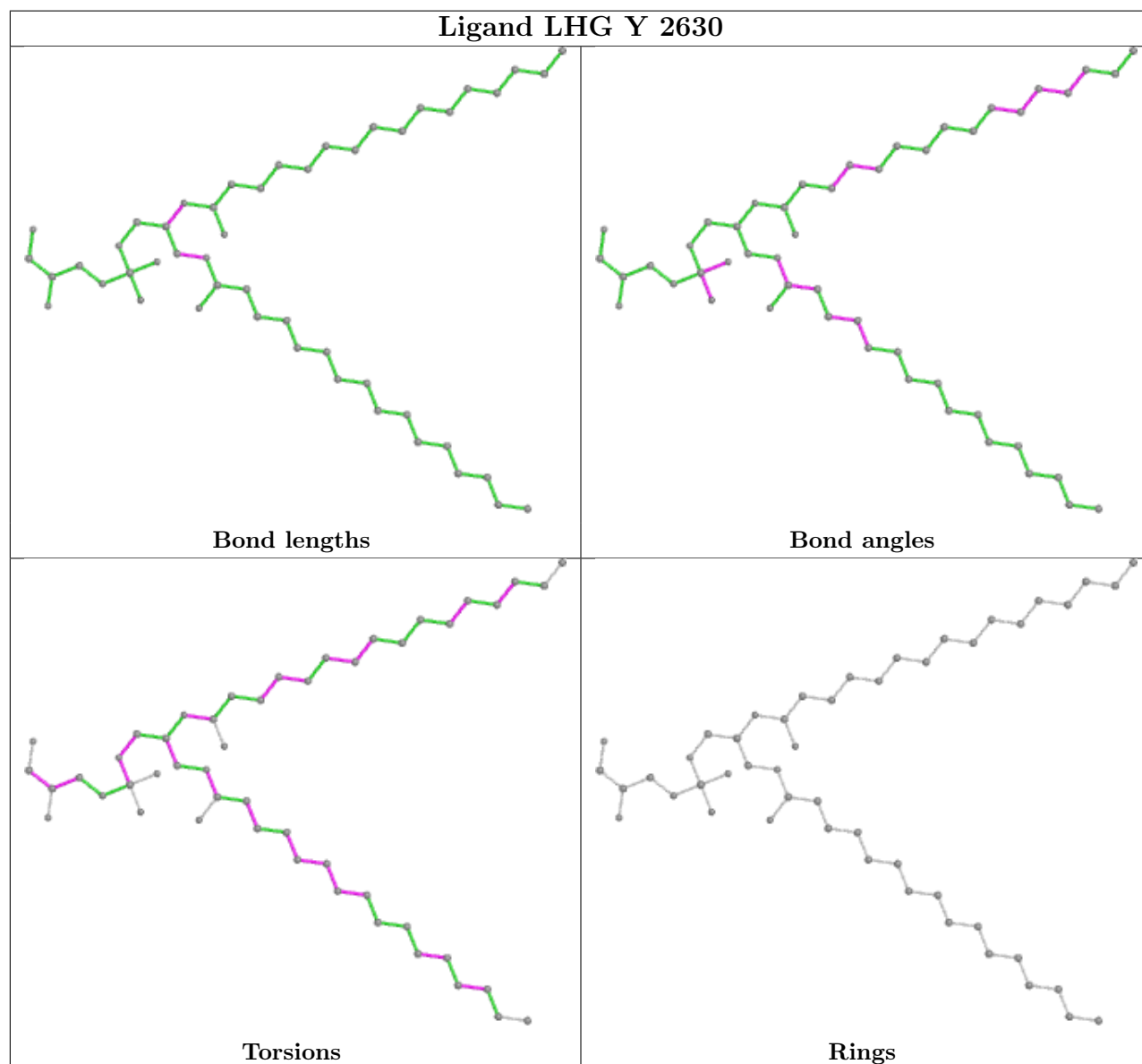
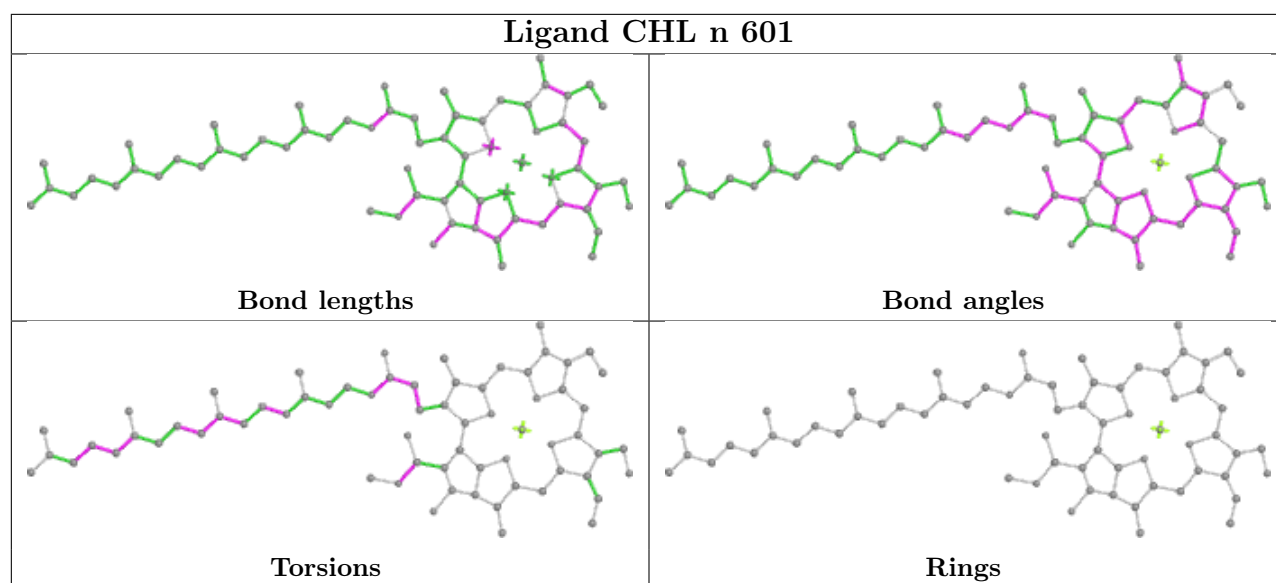
Ligand CLA b 608**Ligand NEX Y 1623****Ligand LUT 3 1621**

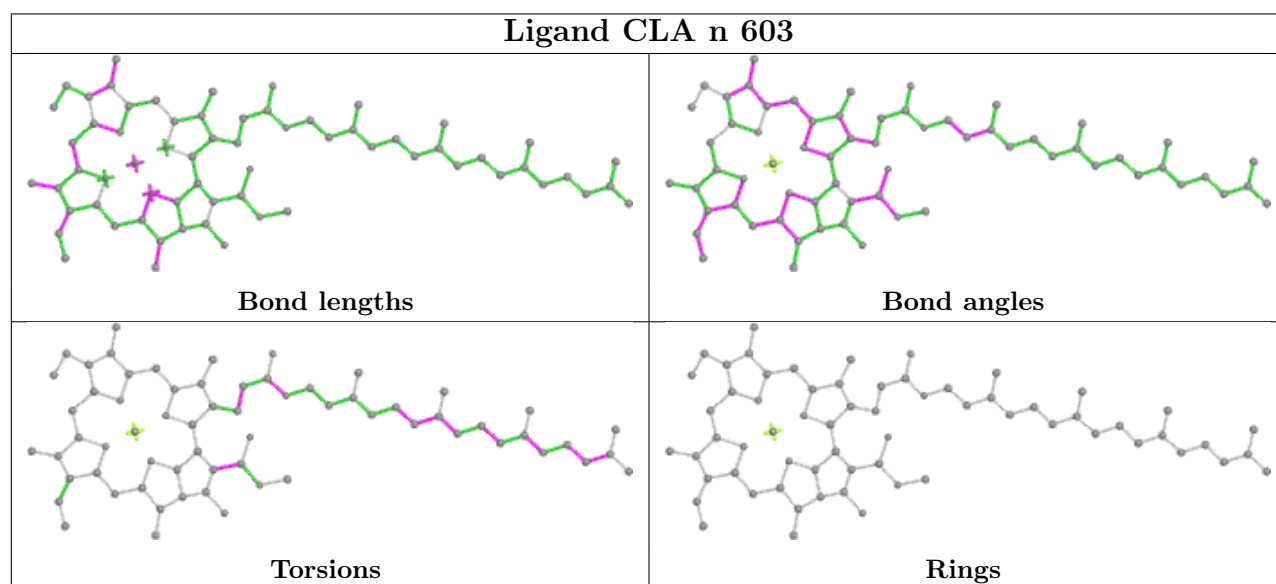
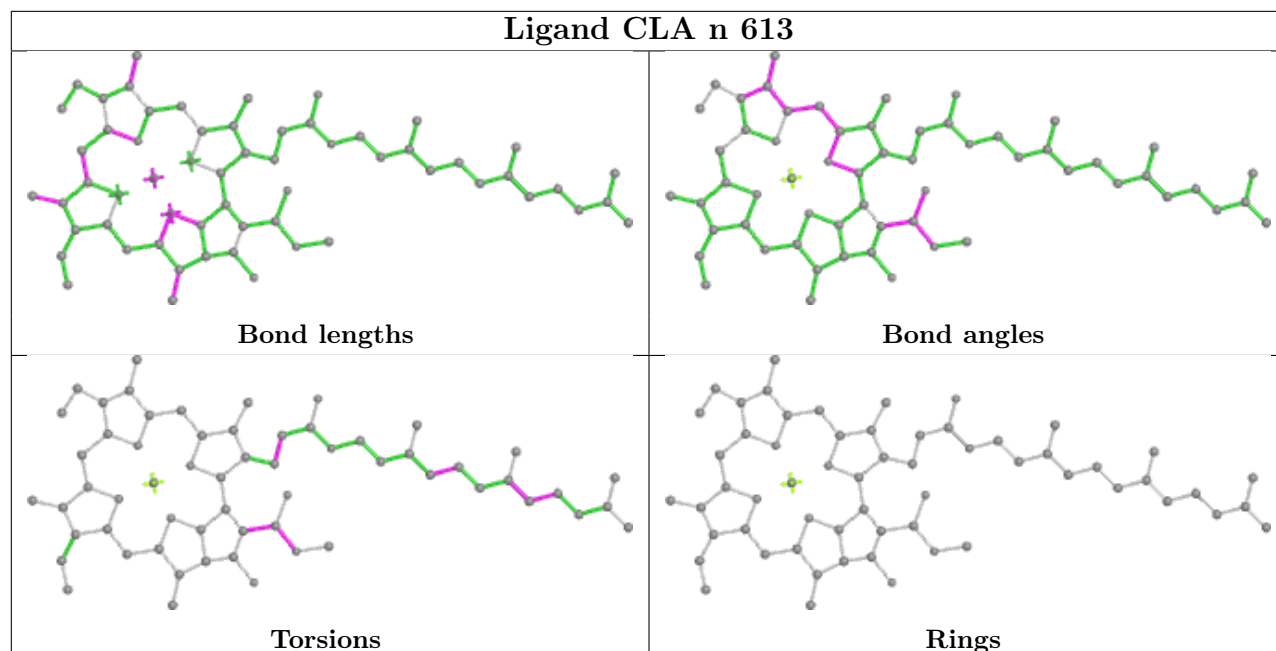
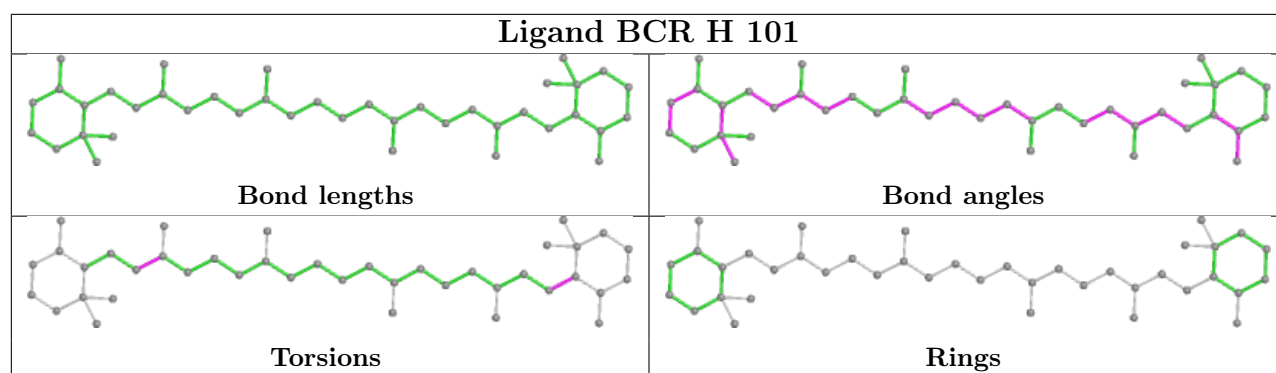
Ligand CLA B 602**Ligand CHL n 609**



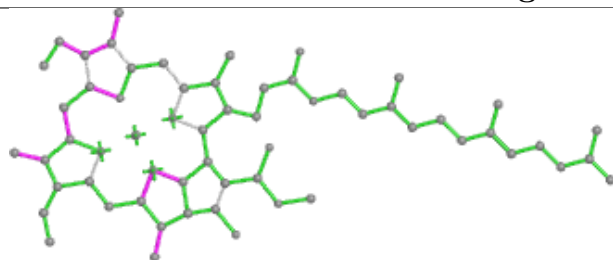


Ligand CLA b 613**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA N 611****Bond lengths****Bond angles****Torsions****Rings**

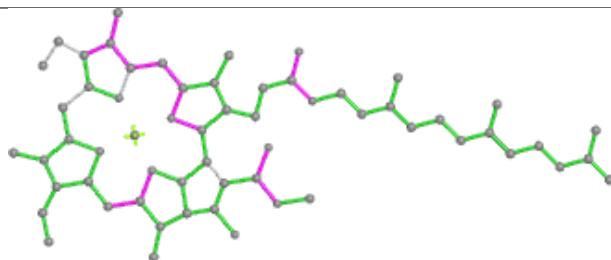




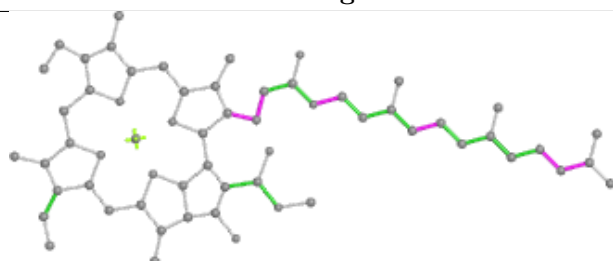
Ligand CLA 3 610



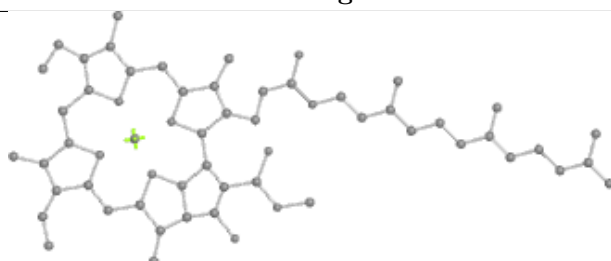
Bond lengths



Bond angles

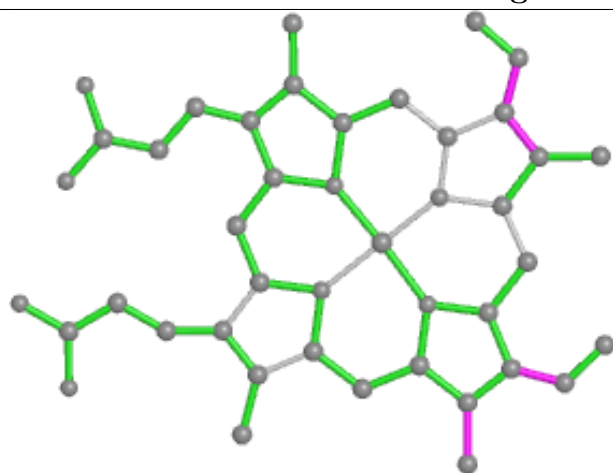


Torsions

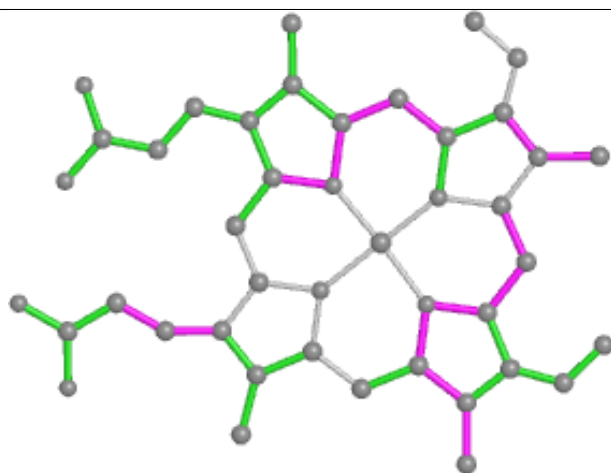


Rings

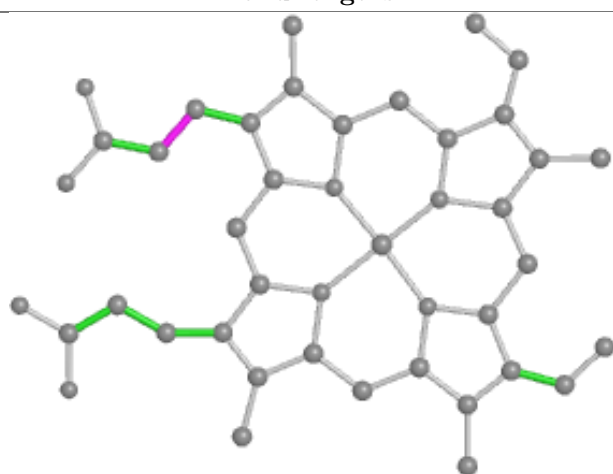
Ligand HEM F 101



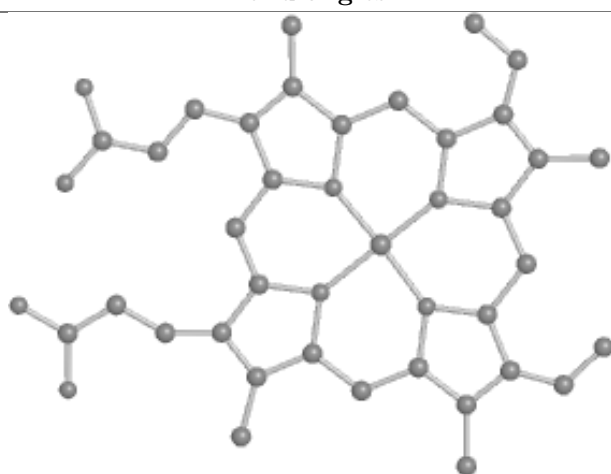
Bond lengths



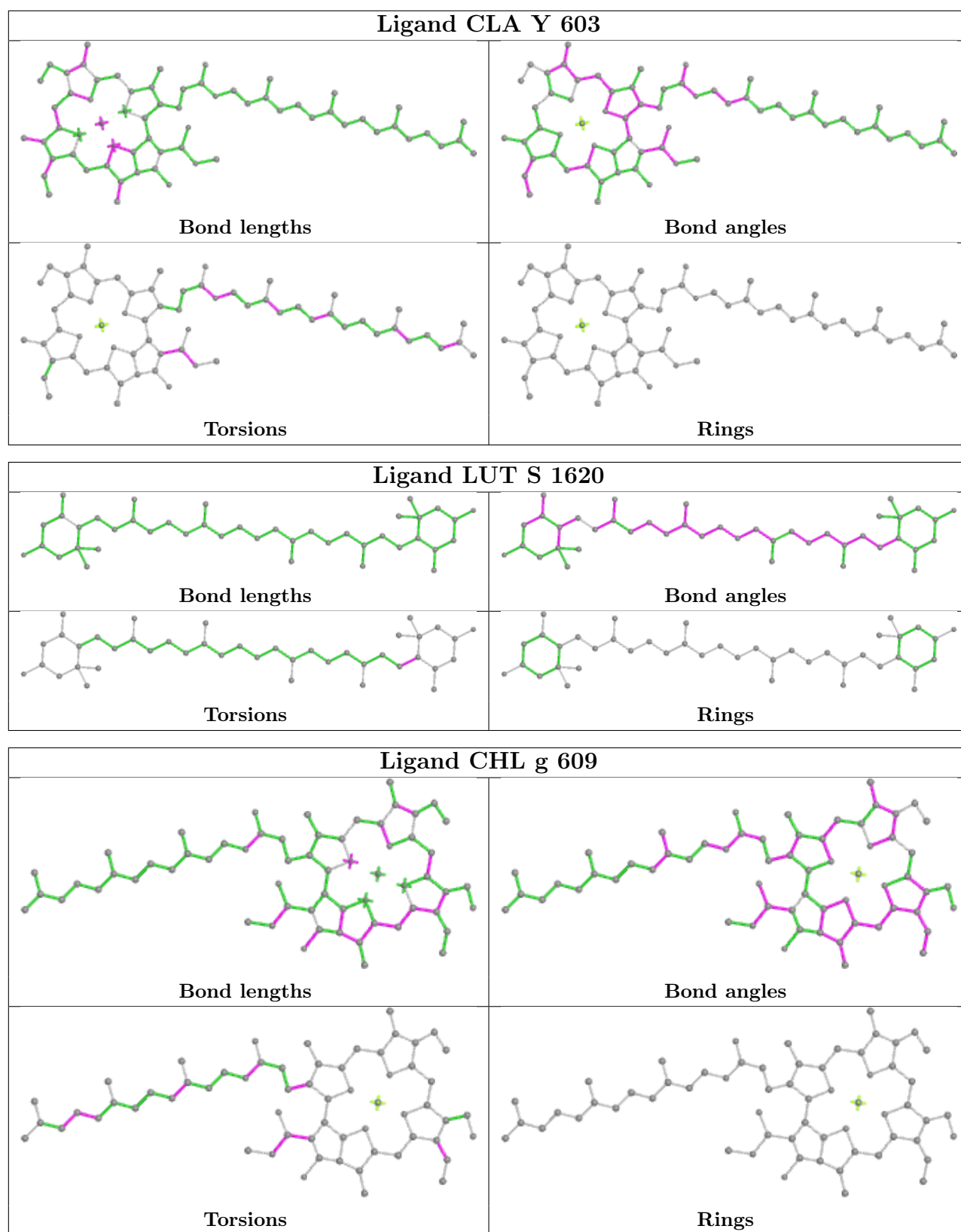
Bond angles

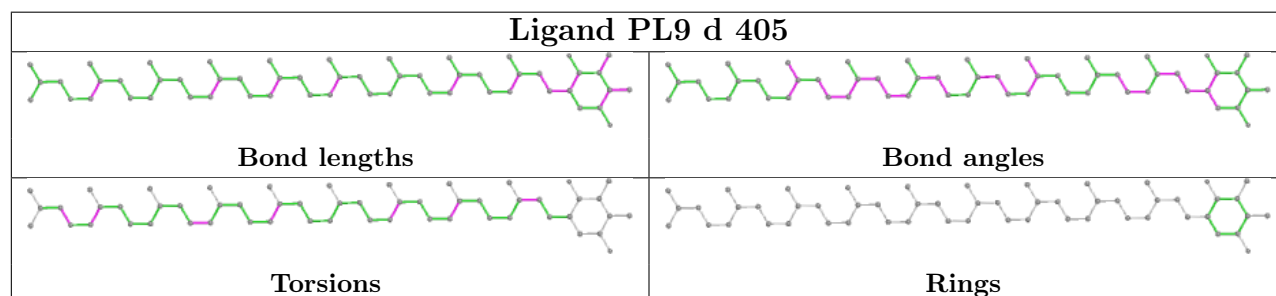
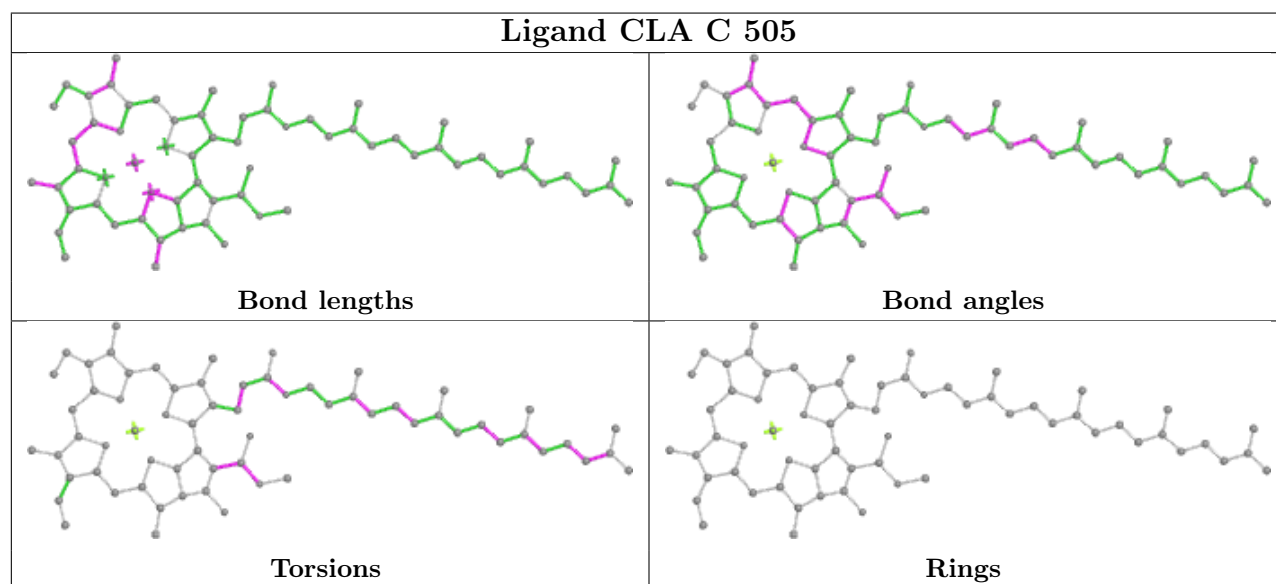
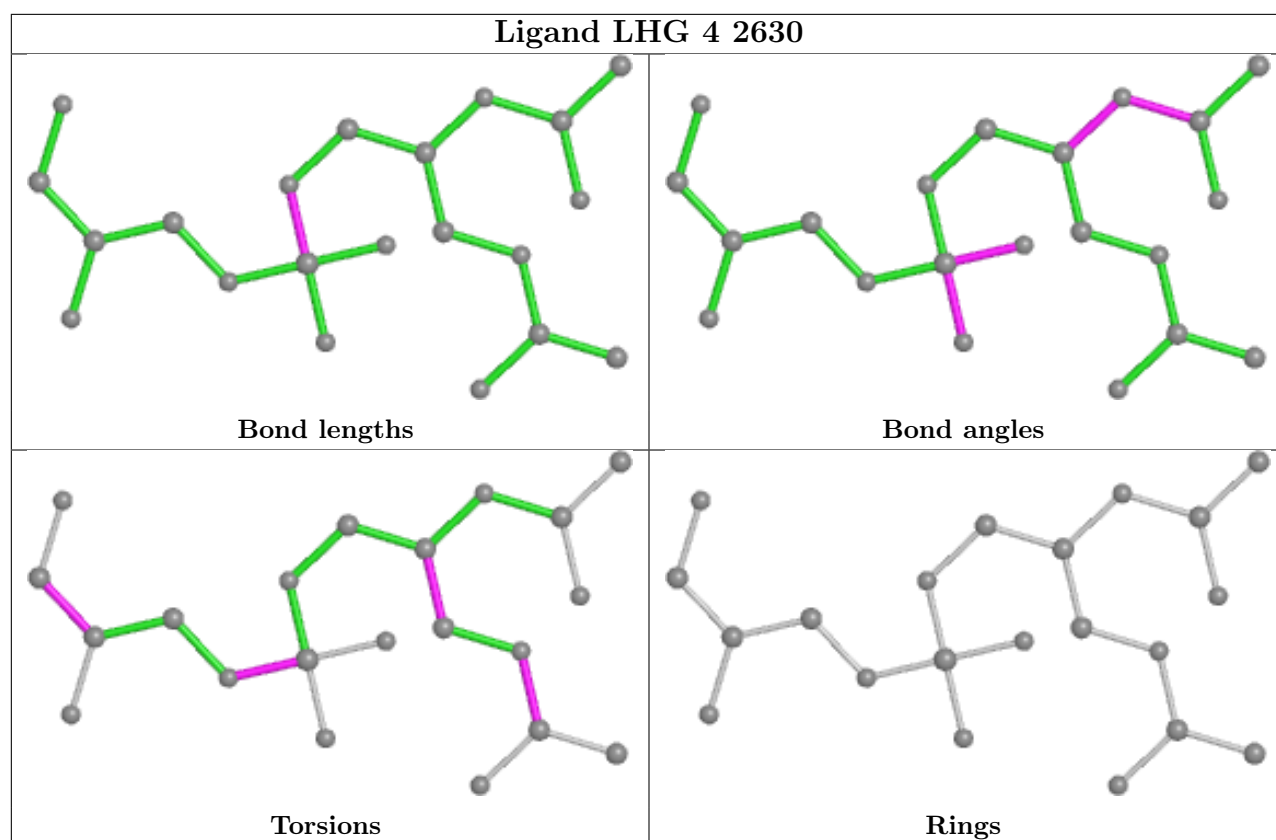


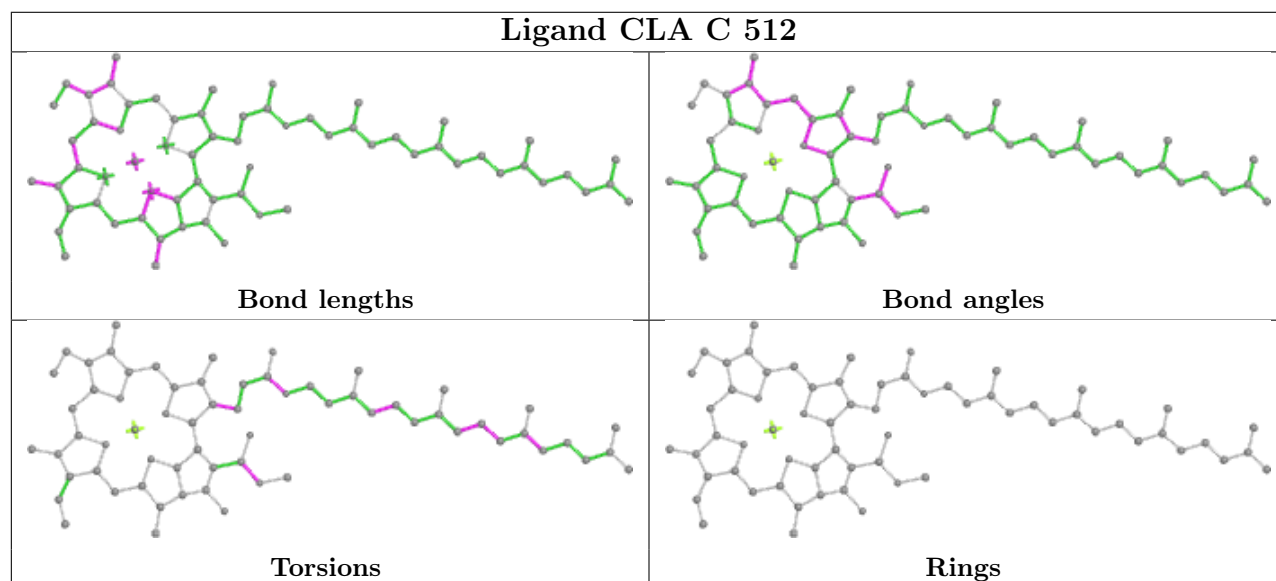
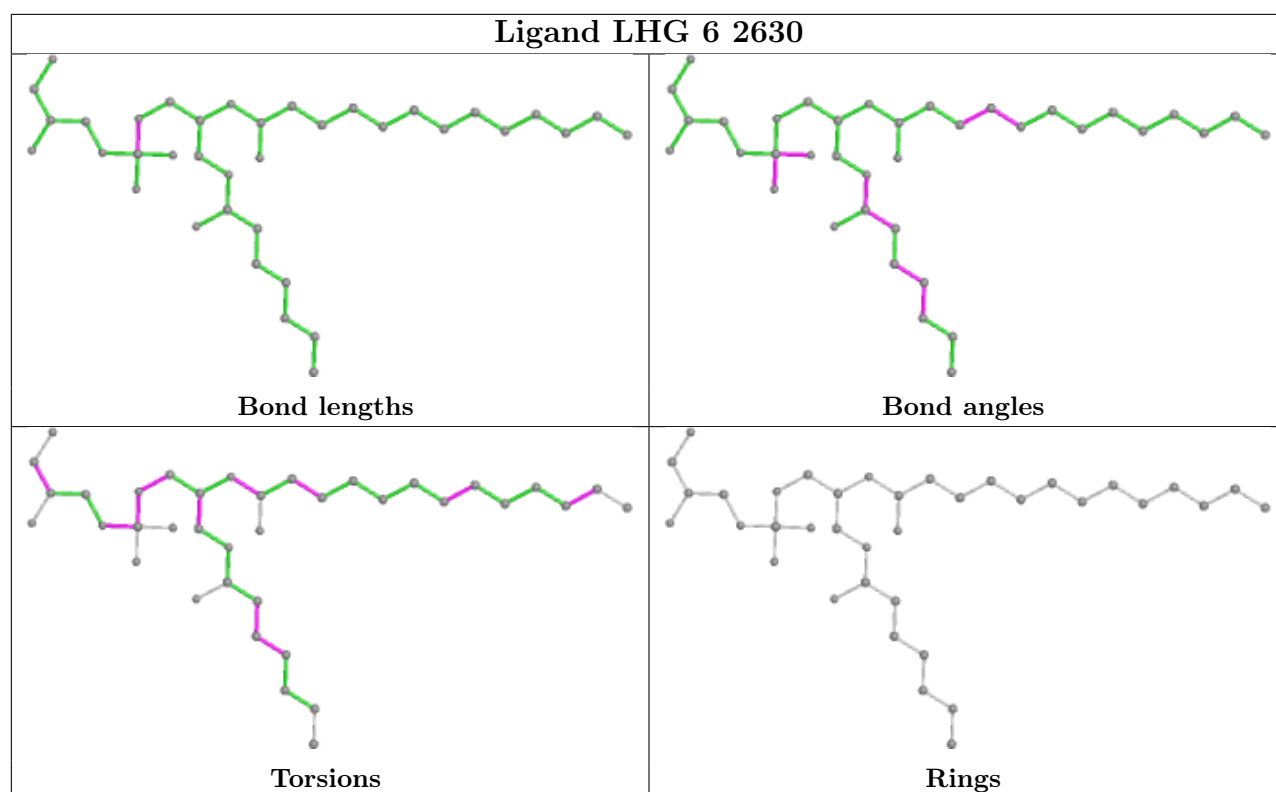
Torsions



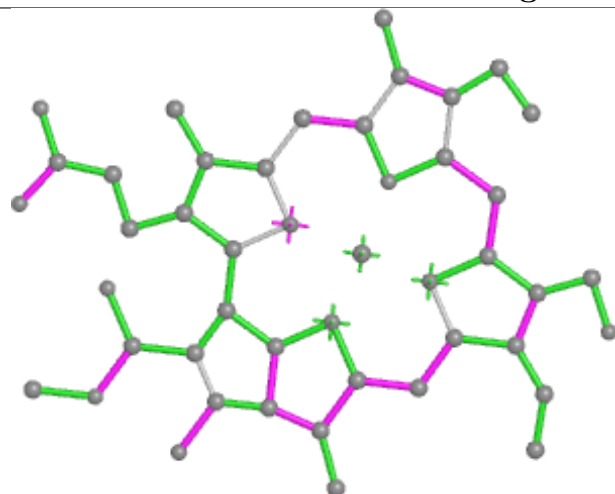
Rings



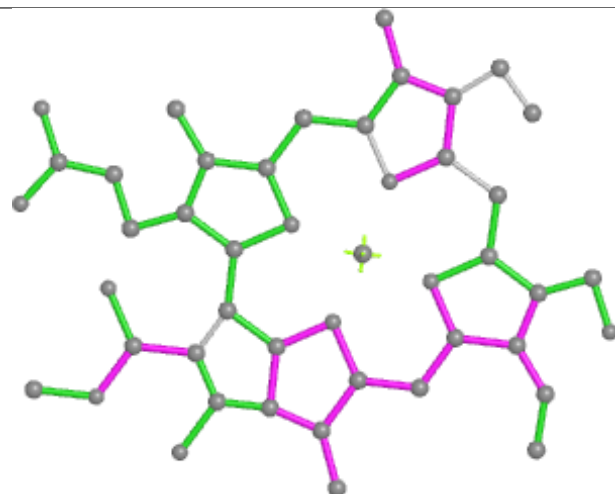




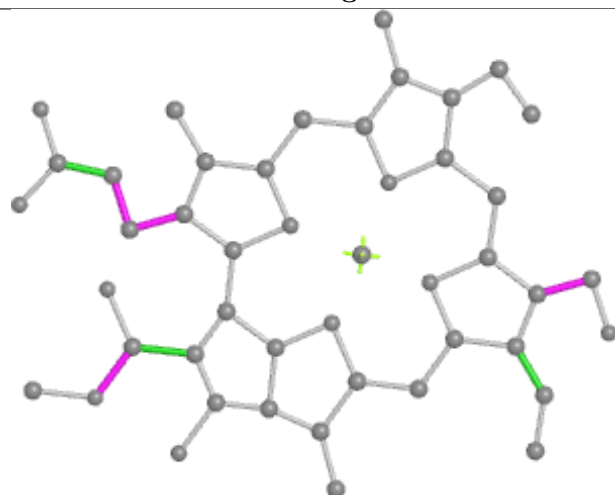
Ligand CHL 1 608



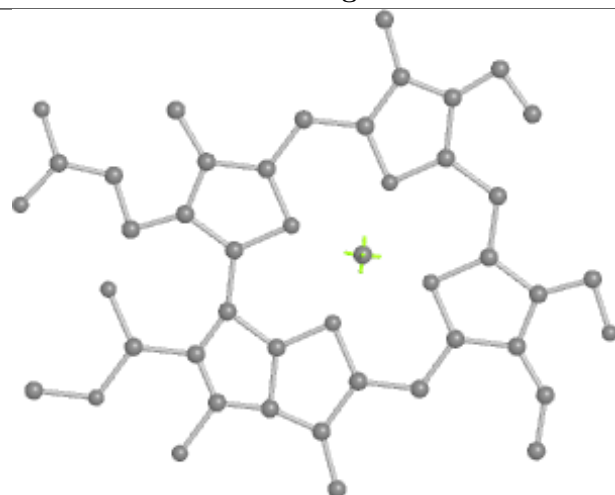
Bond lengths



Bond angles

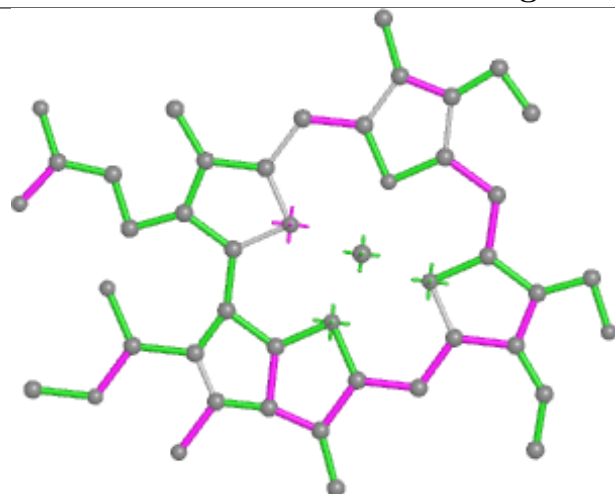


Torsions

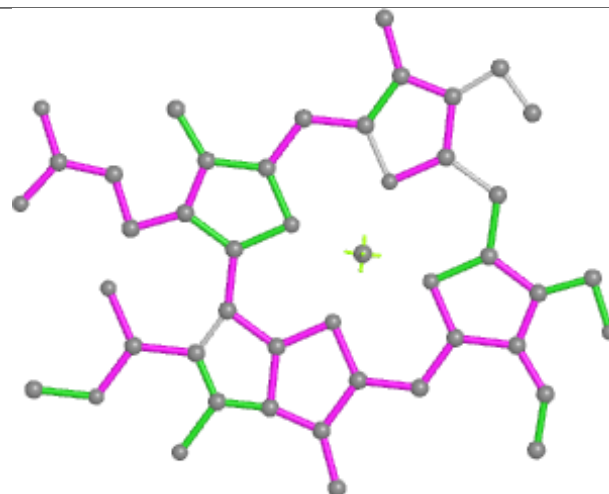


Rings

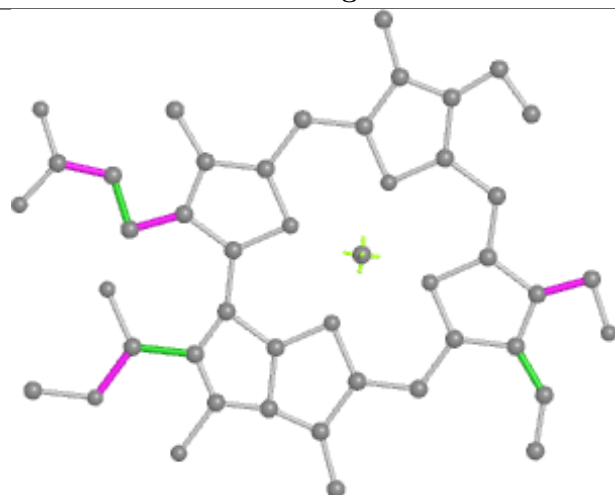
Ligand CHL 4 606



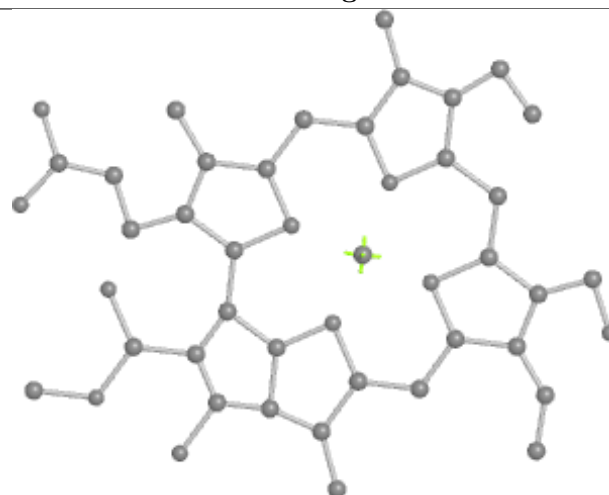
Bond lengths



Bond angles

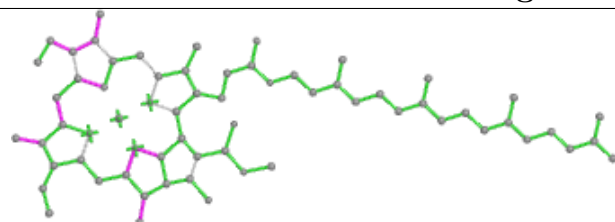


Torsions

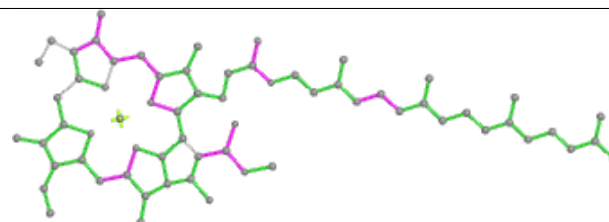


Rings

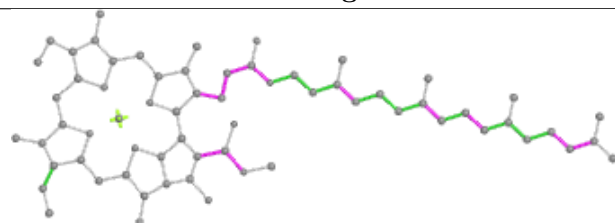
Ligand CLA C 501



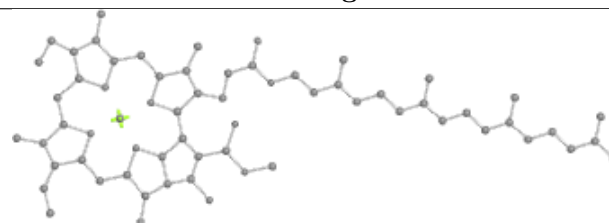
Bond lengths



Bond angles

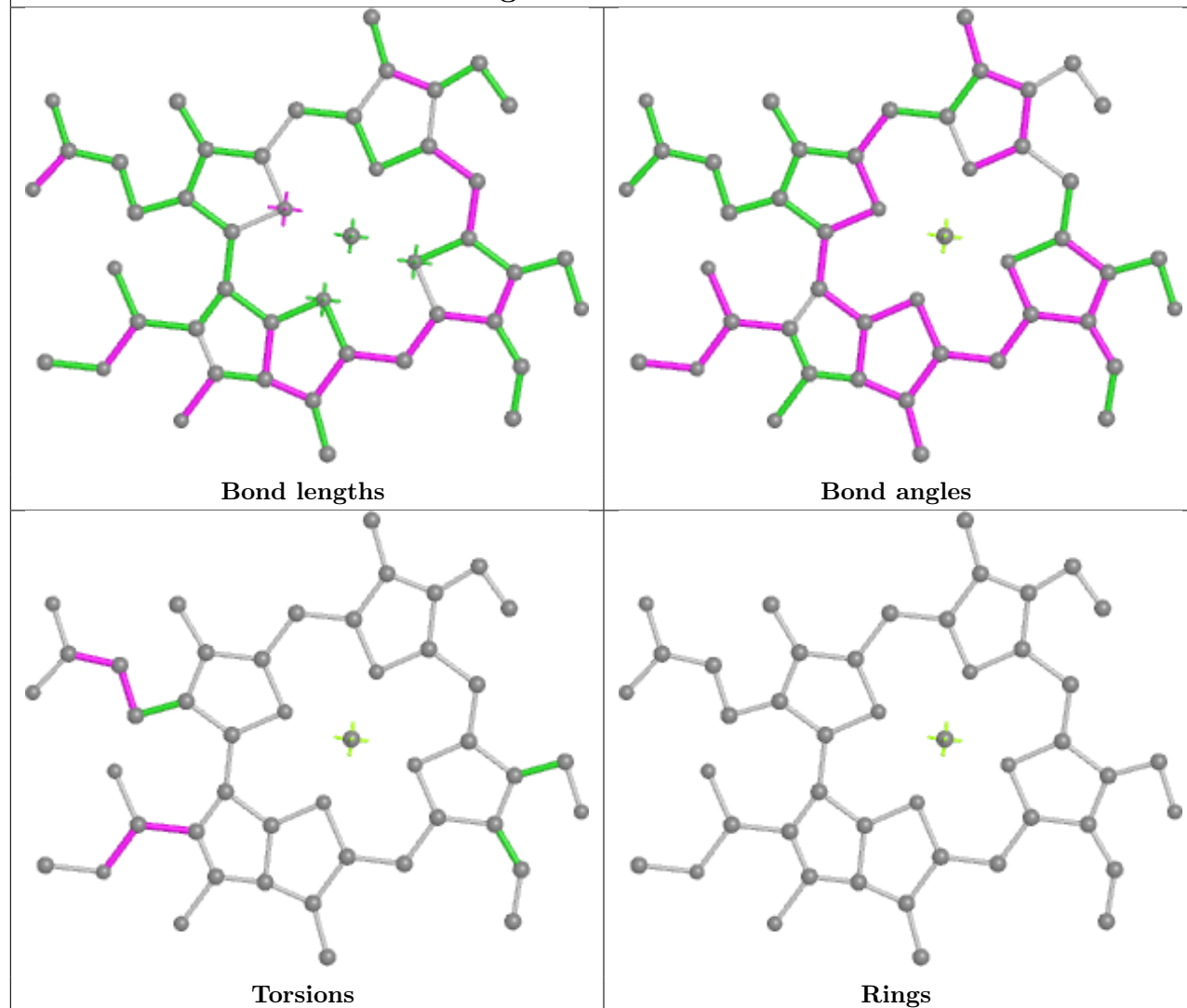


Torsions

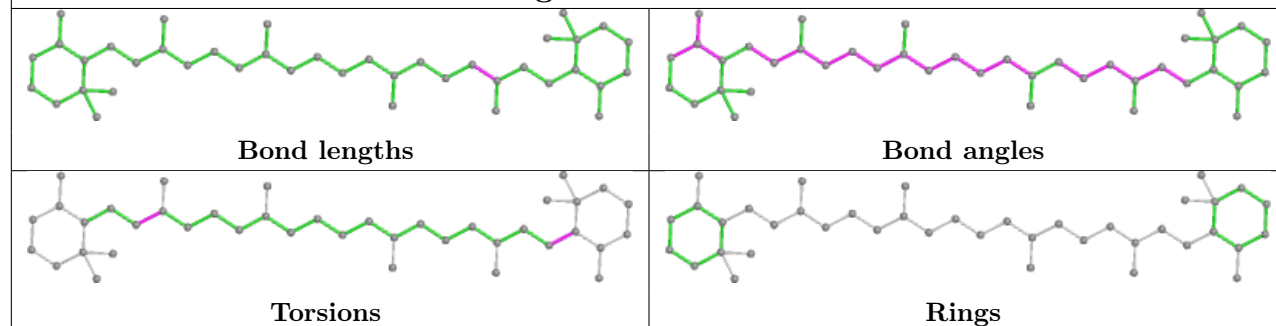


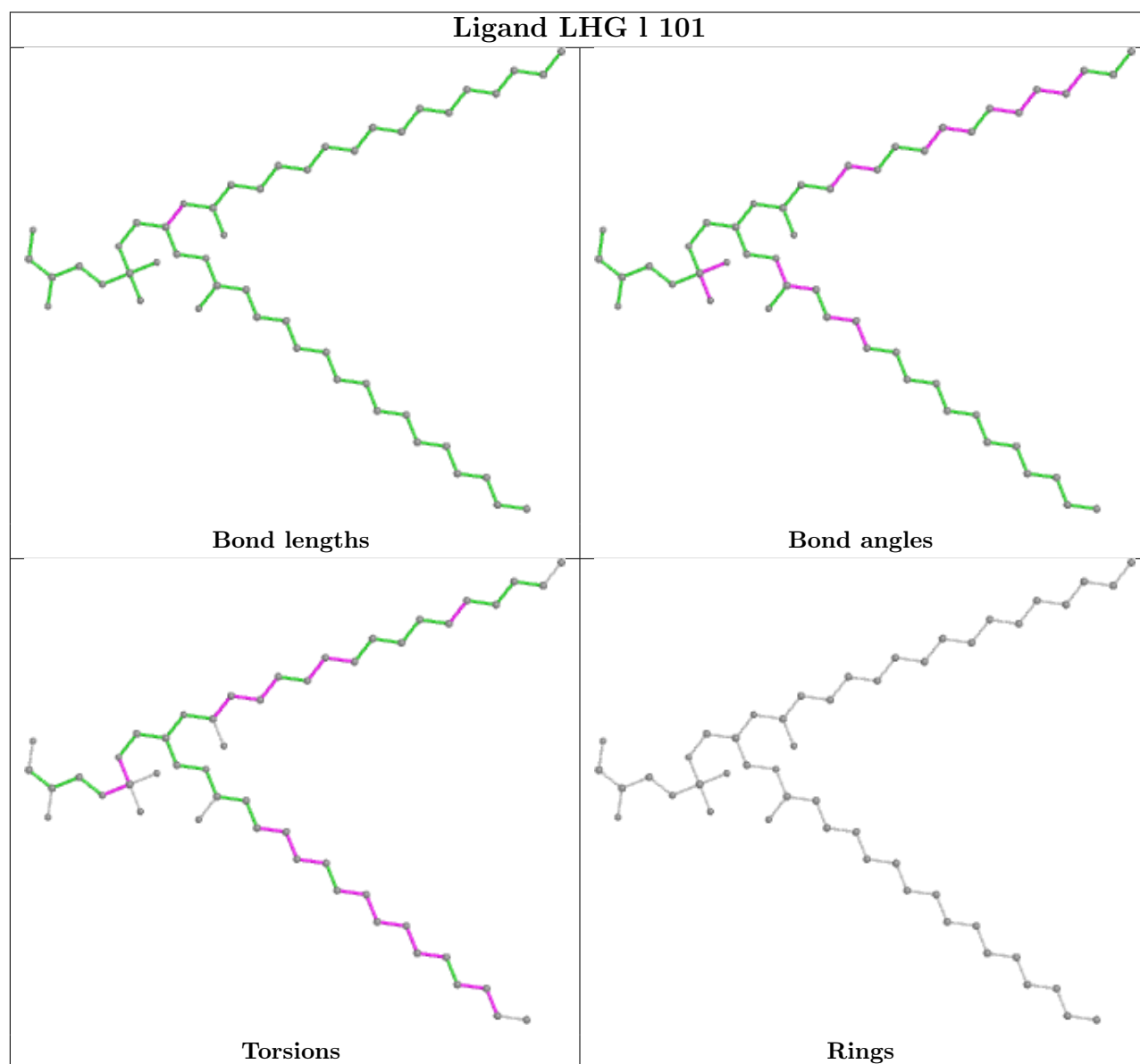
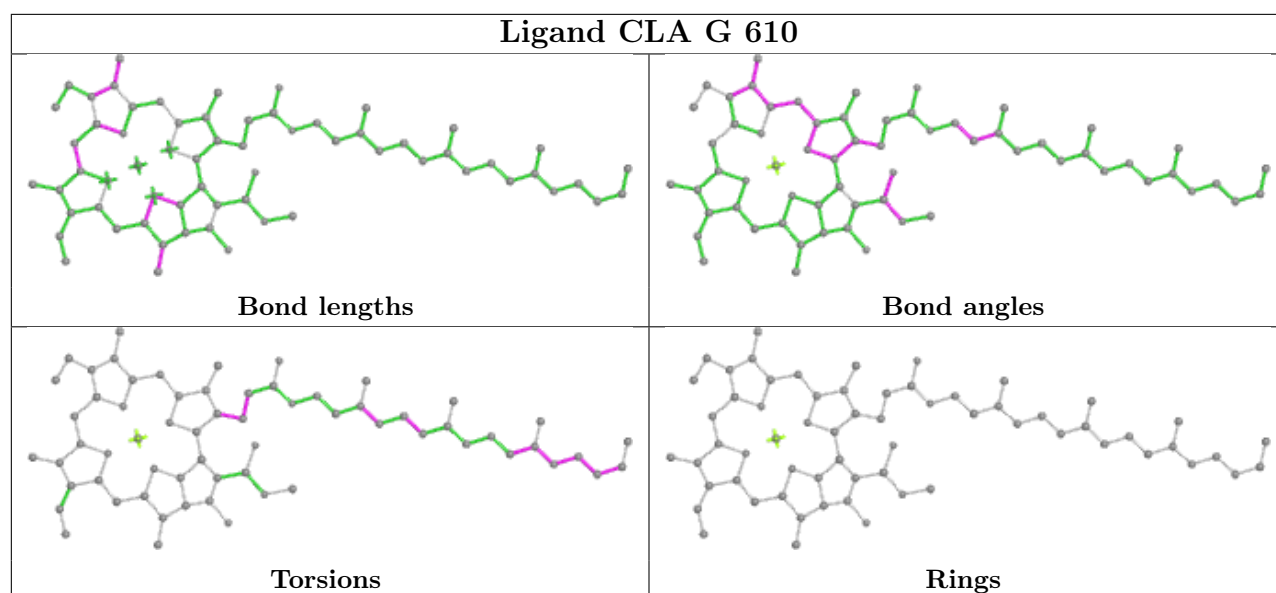
Rings

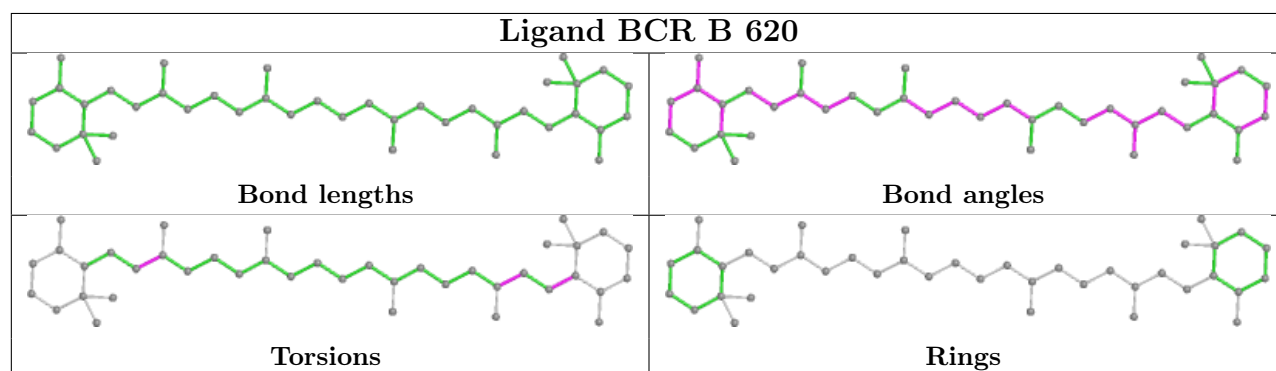
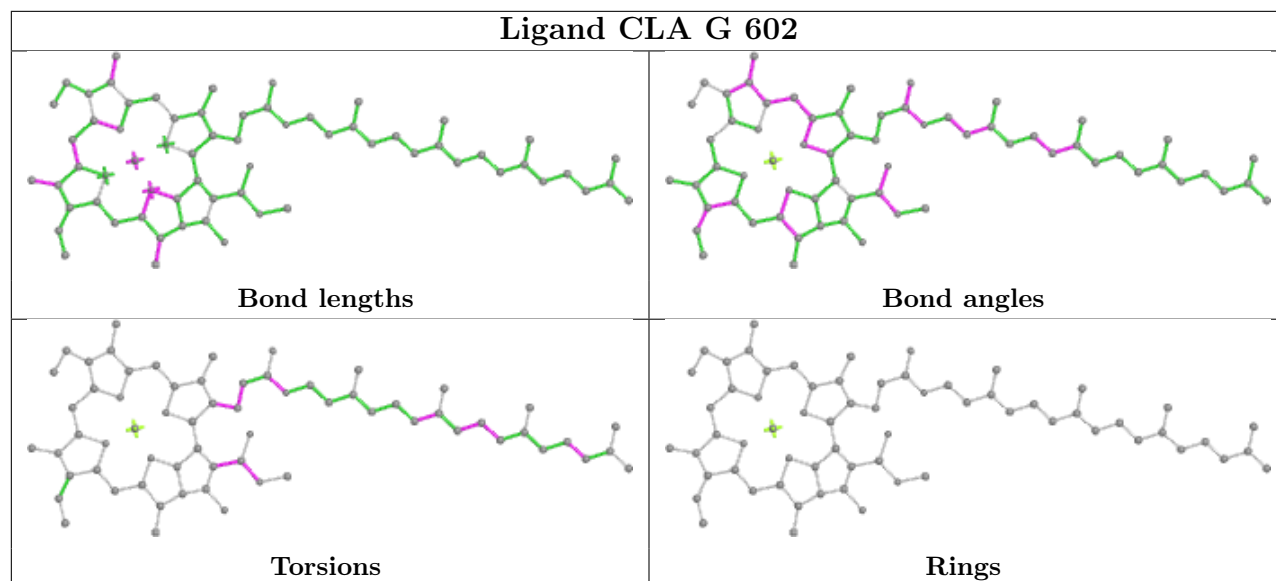
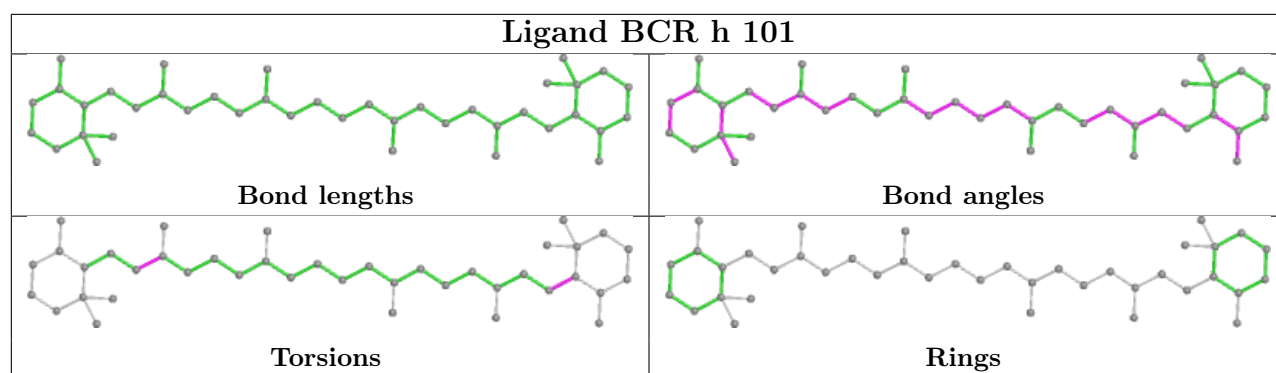
Ligand CHL s 601



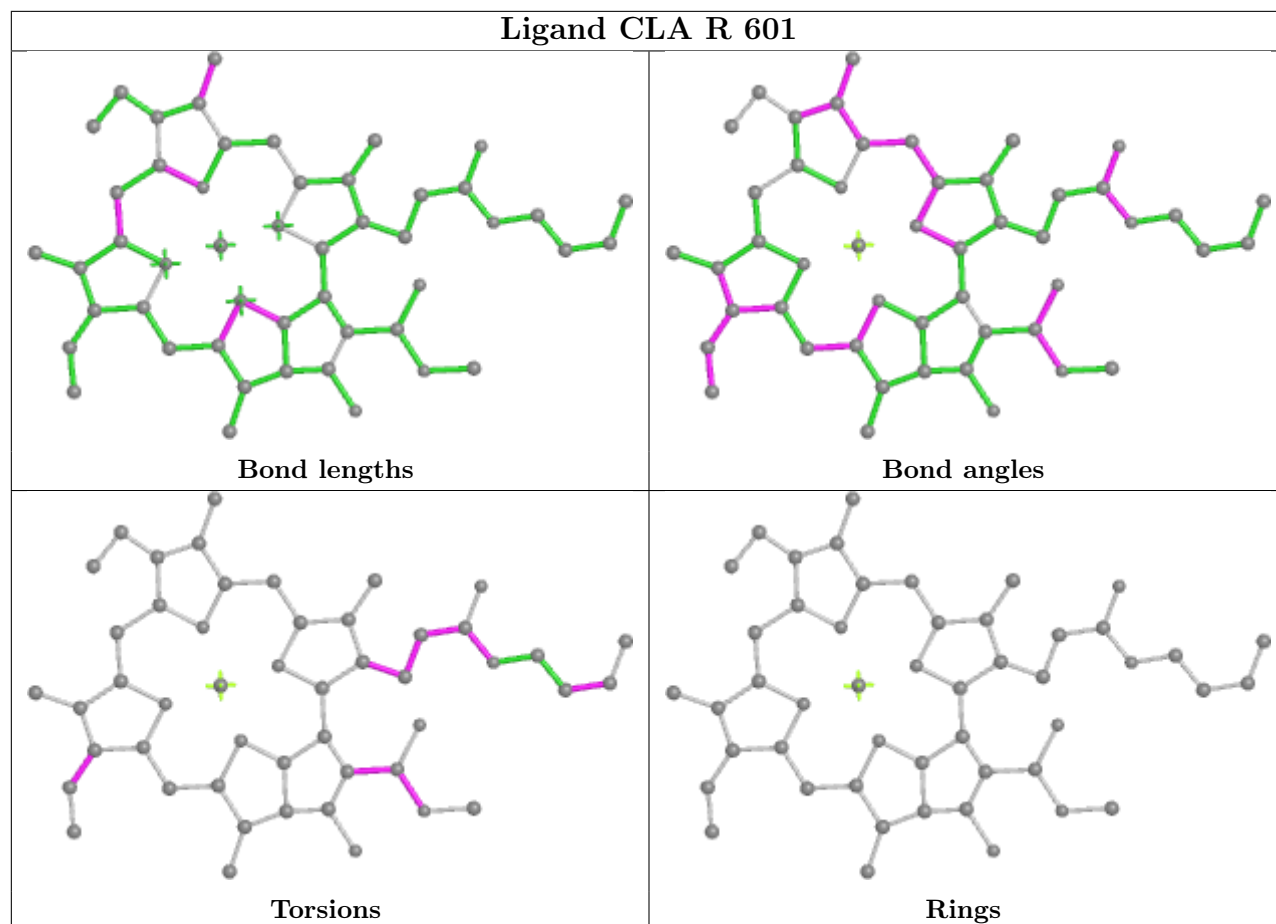
Ligand BCR c 517



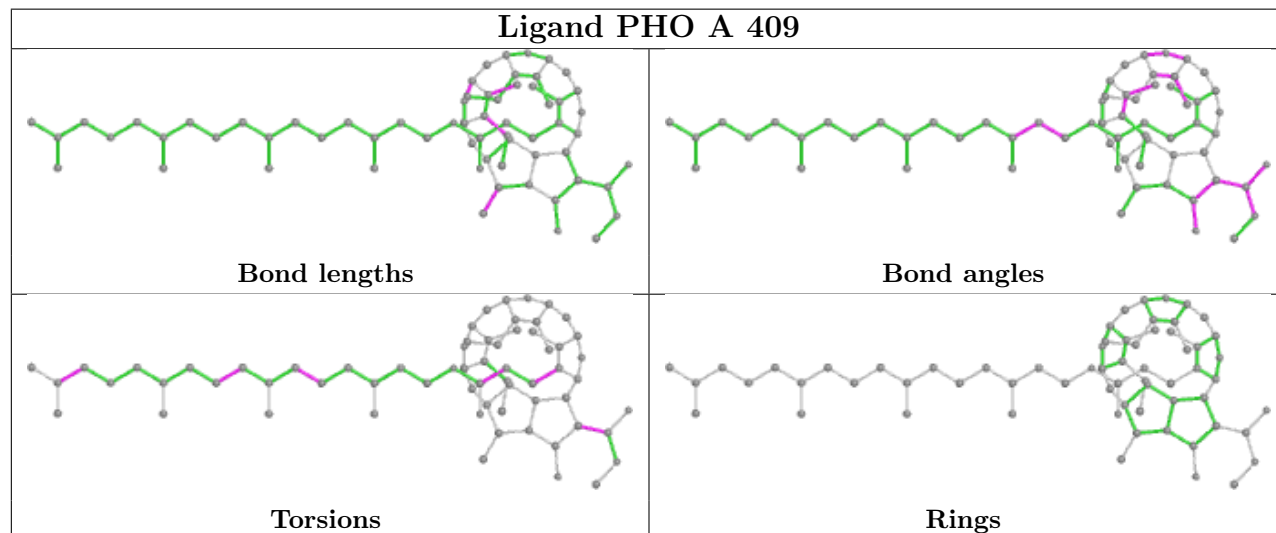


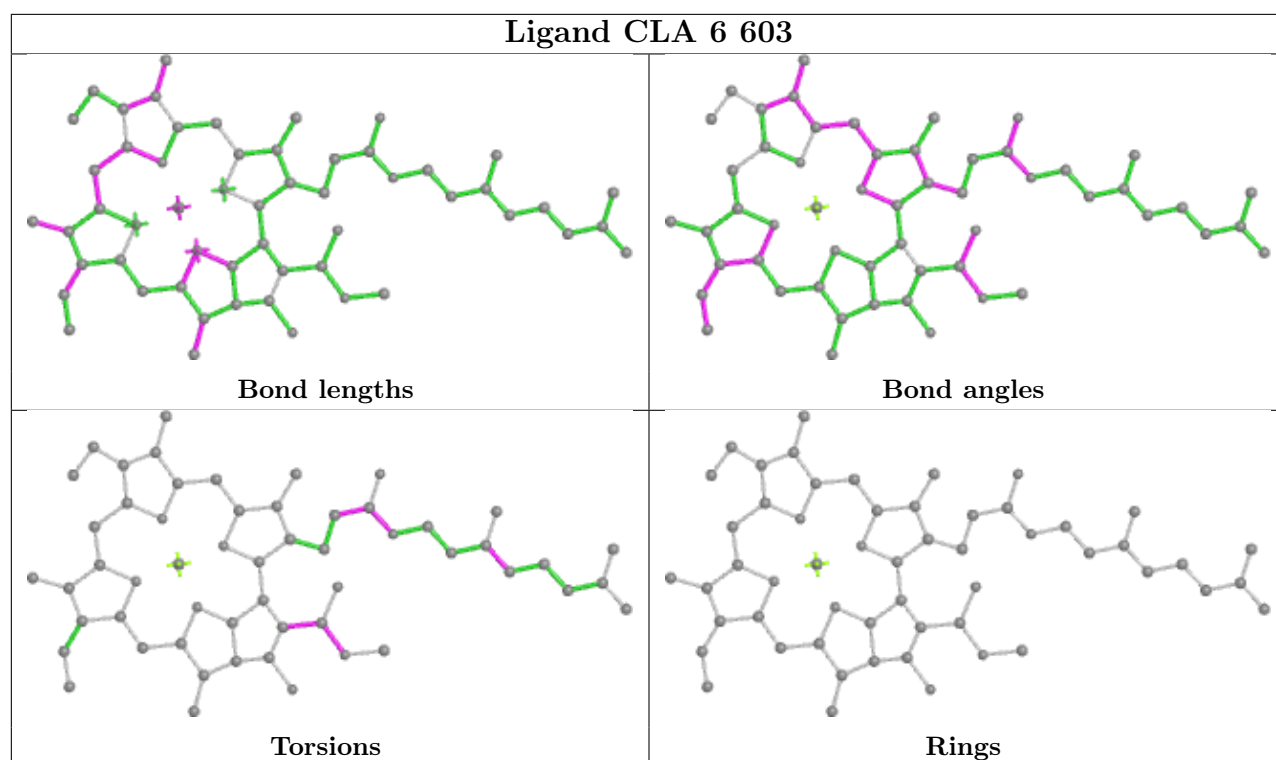


Ligand CLA R 601

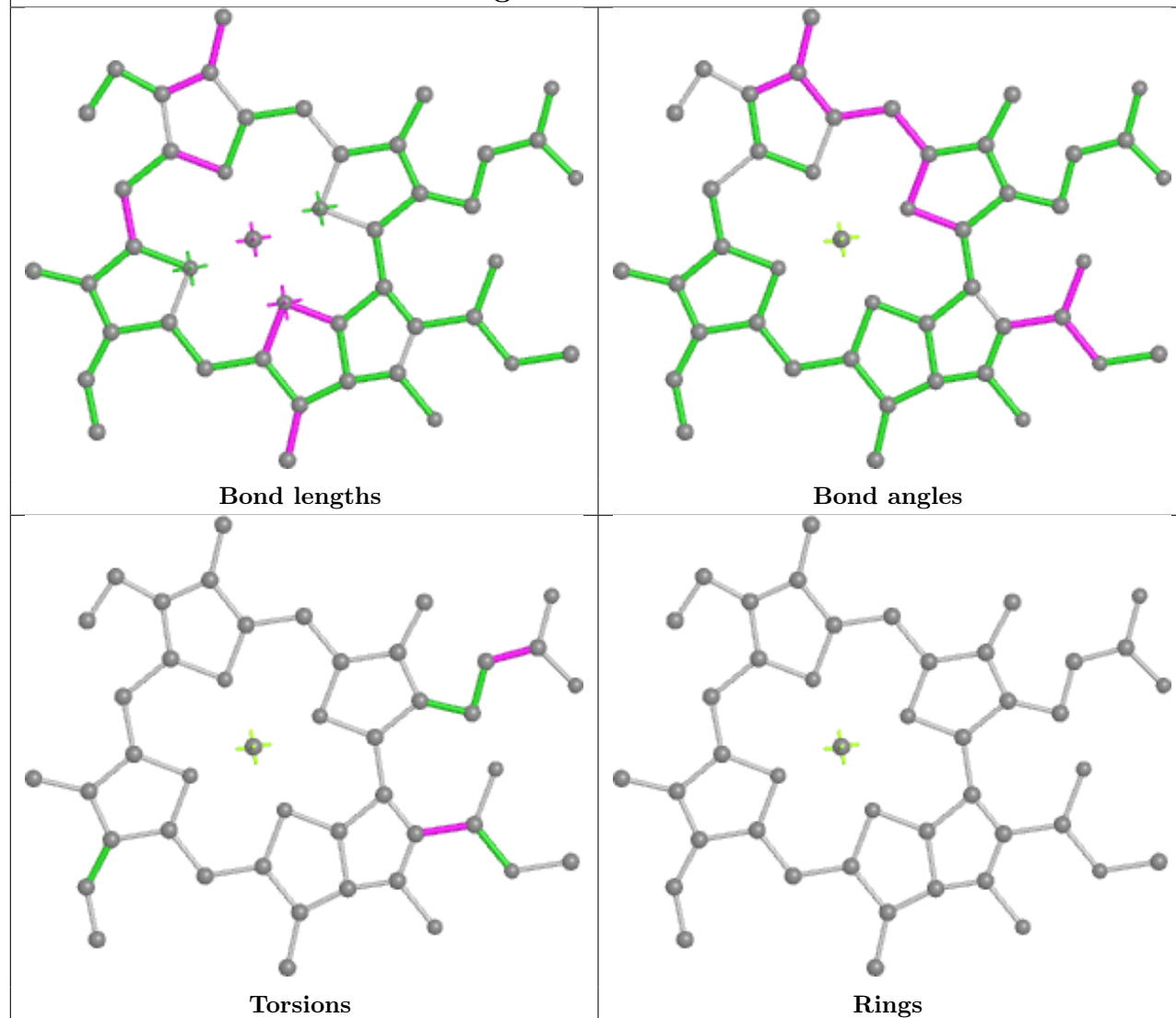


Ligand PHO A 409

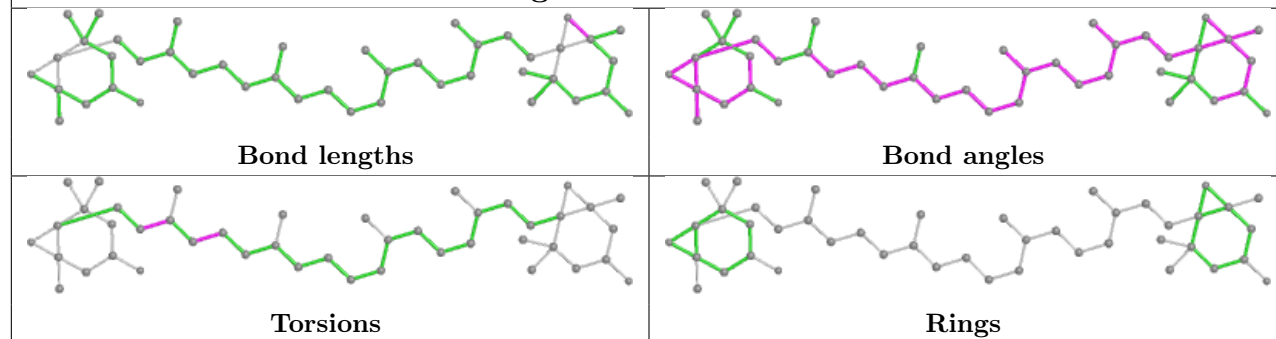


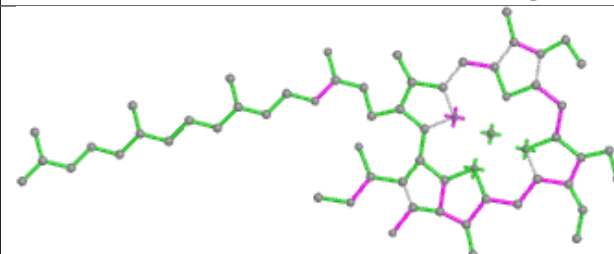
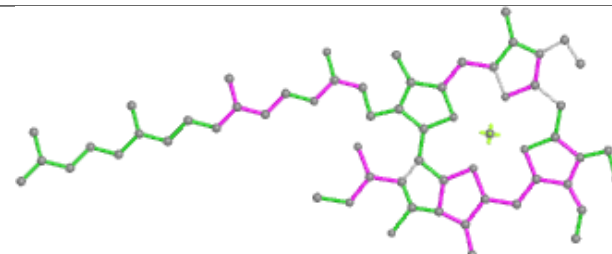
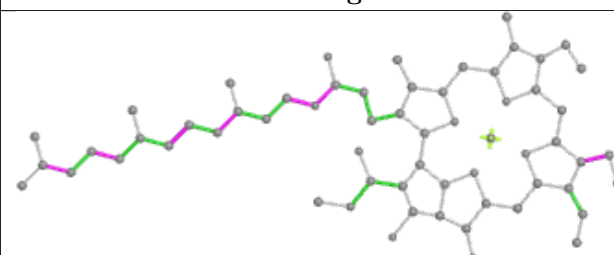
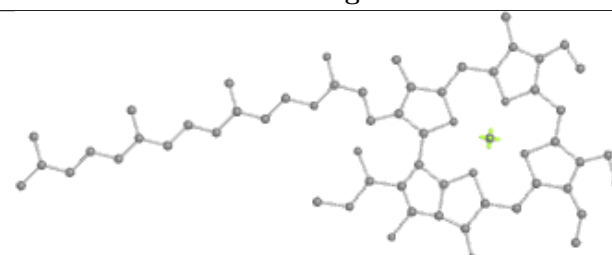


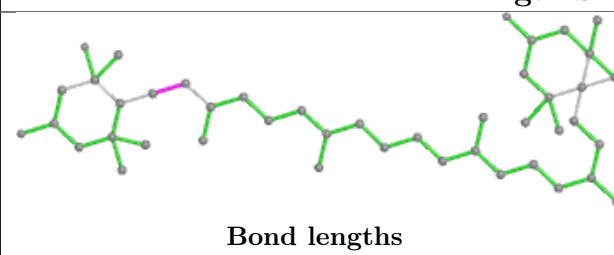
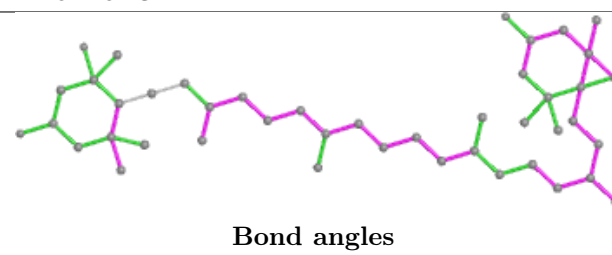
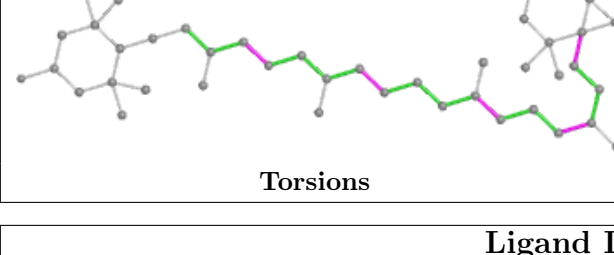
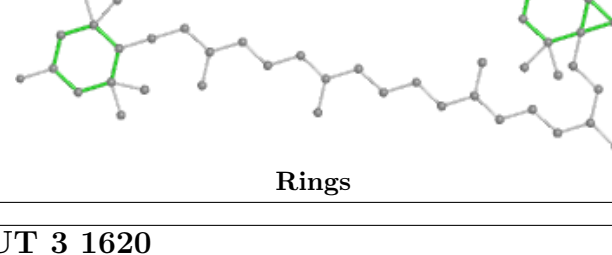
Ligand CLA 6 611

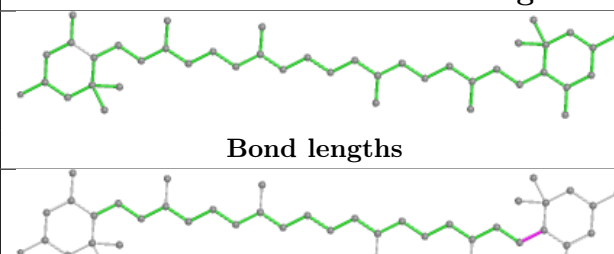
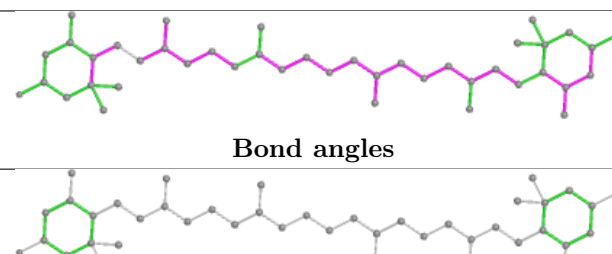
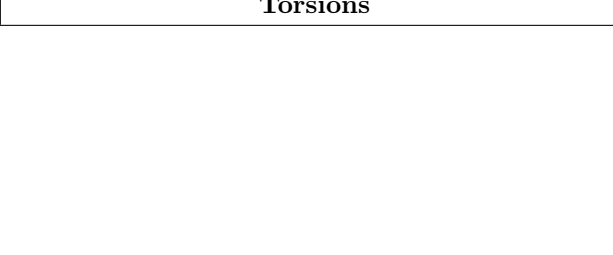
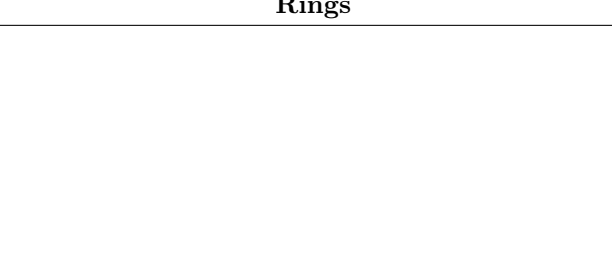


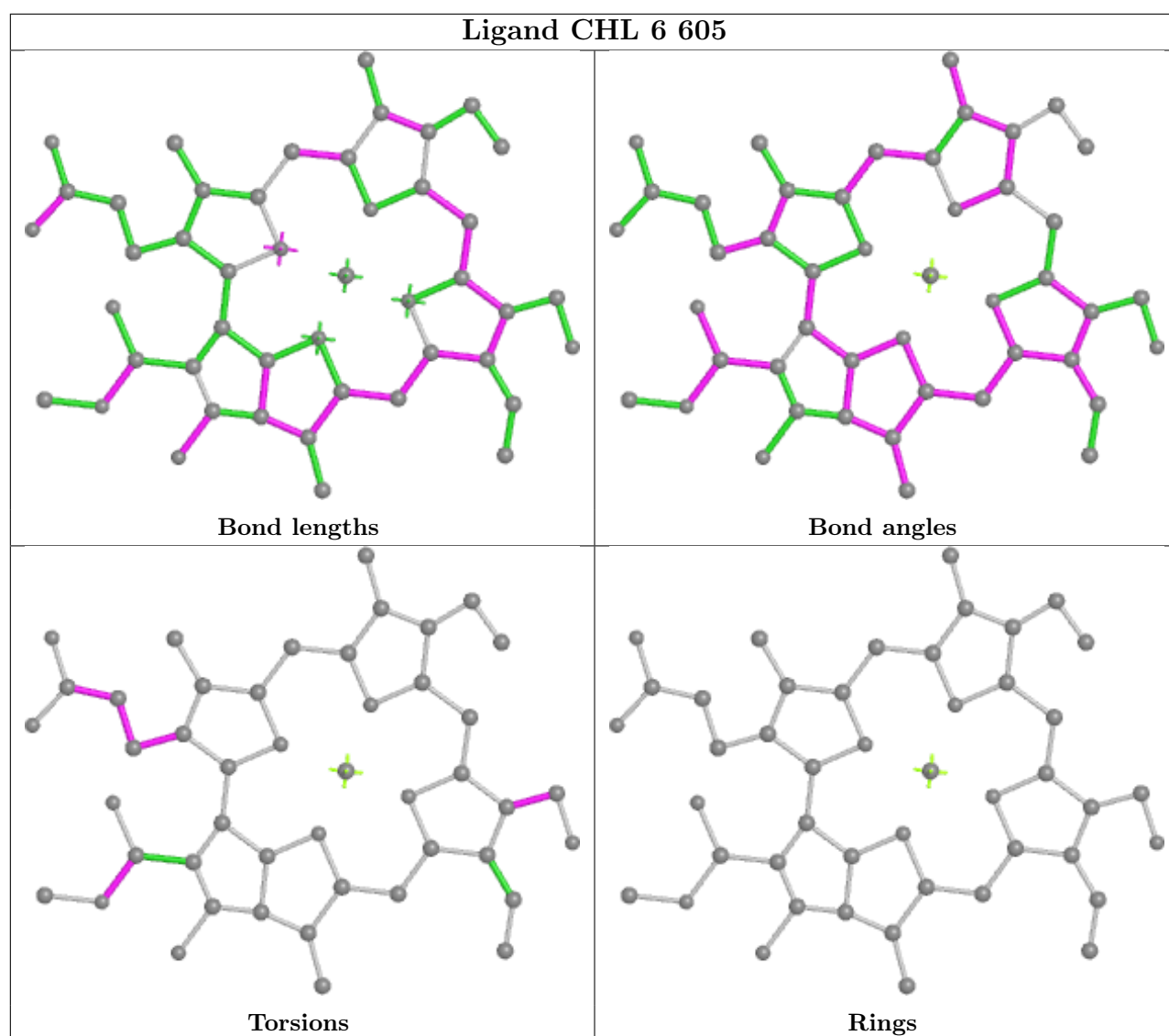
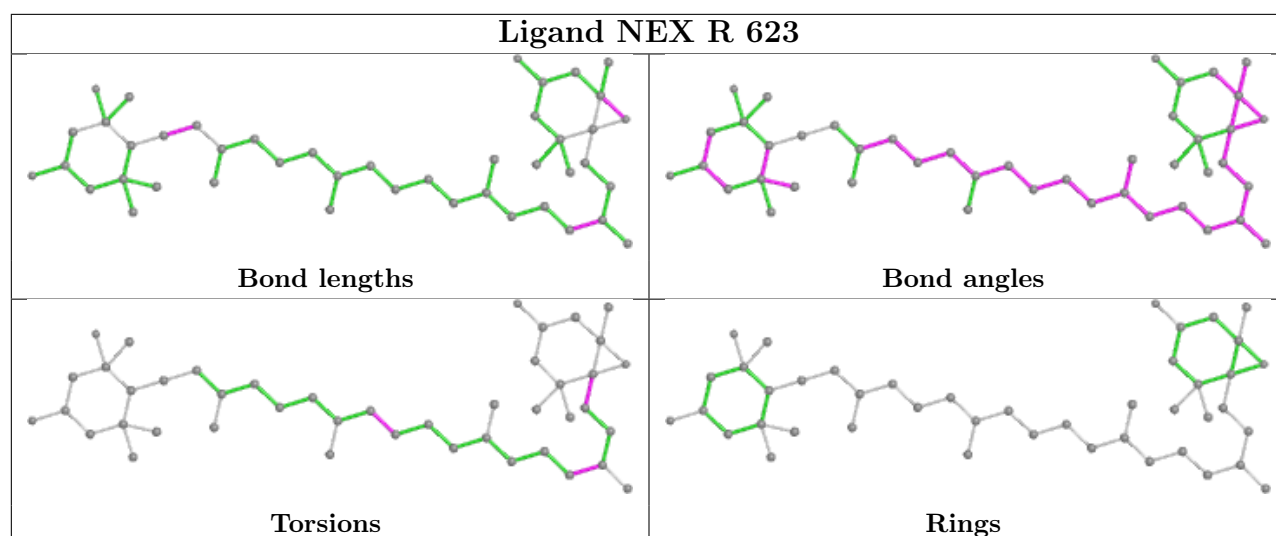
Ligand XAT R 622

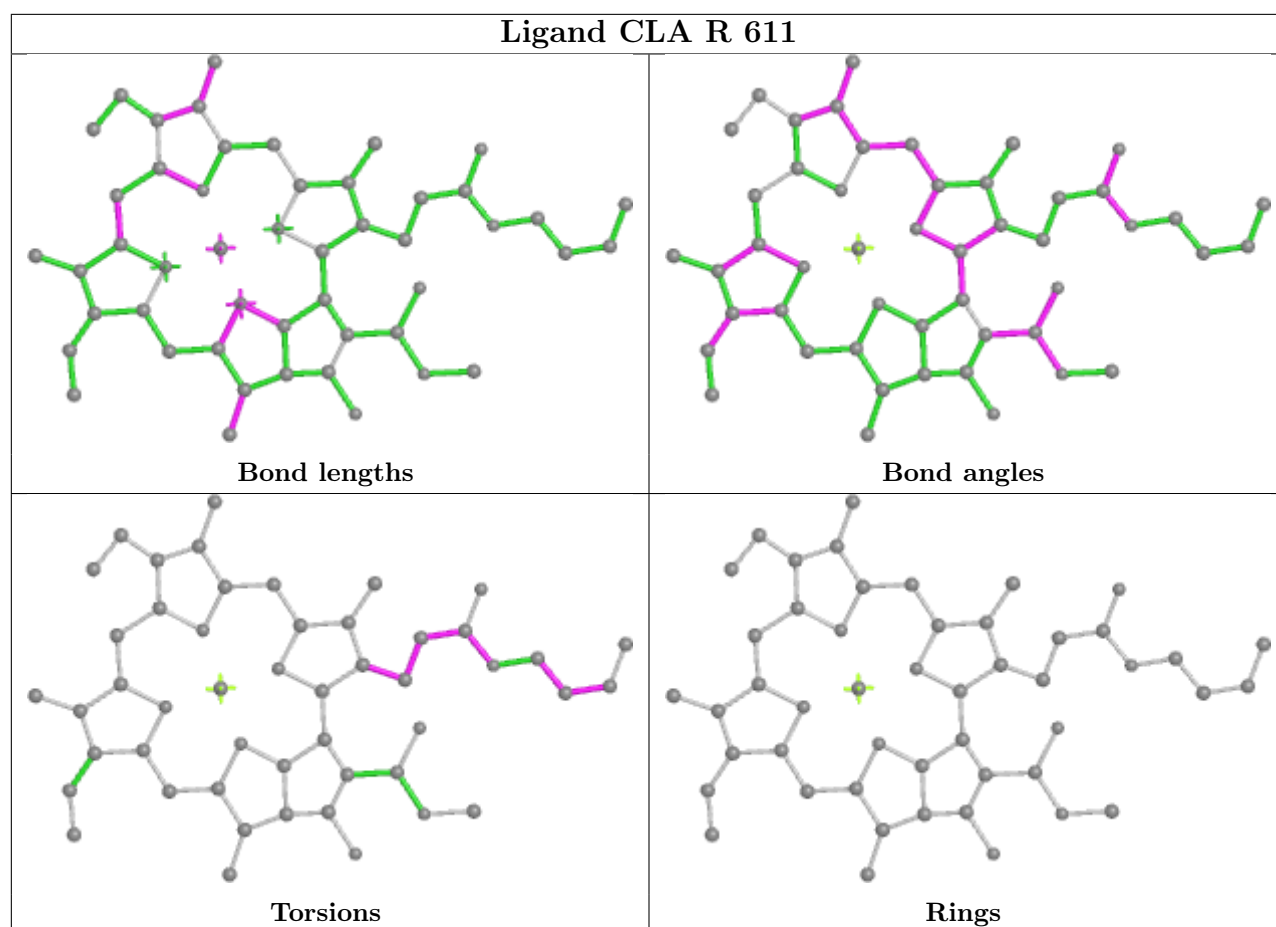


Ligand CHL 2 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

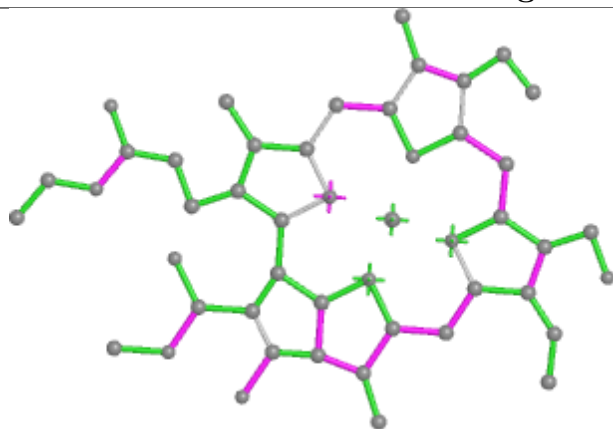
Ligand NEX 6 1623	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 3 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

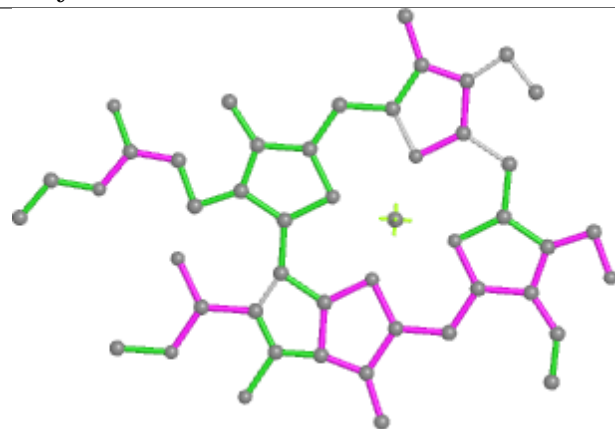




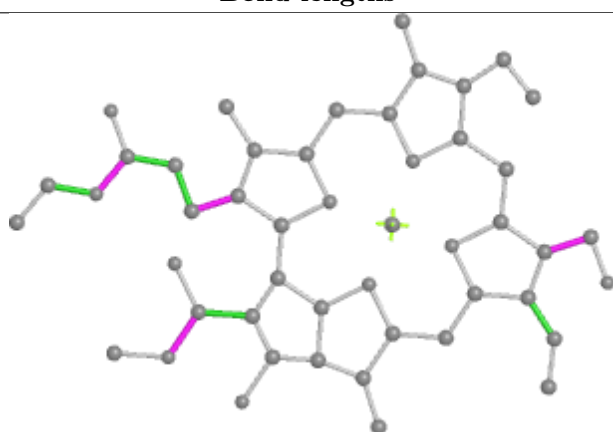
Ligand CHL y 605



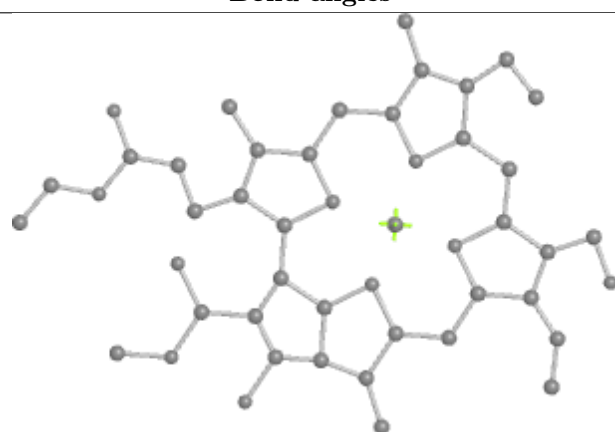
Bond lengths



Bond angles

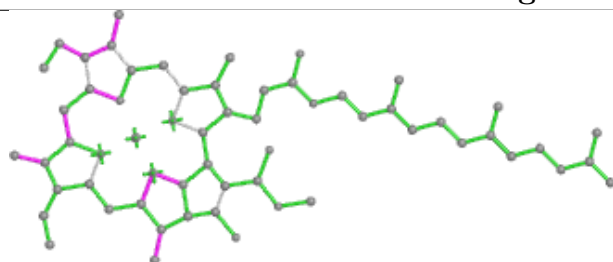


Torsions

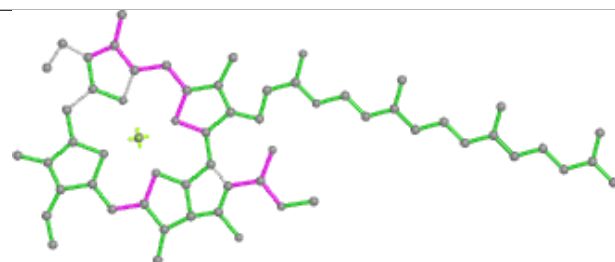


Rings

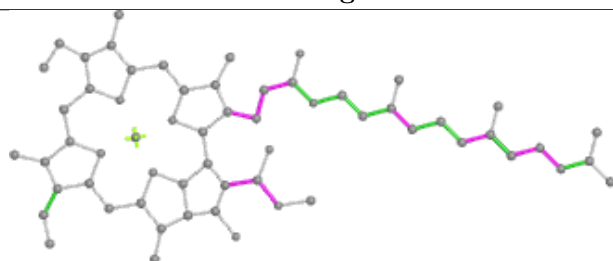
Ligand CLA 3 602



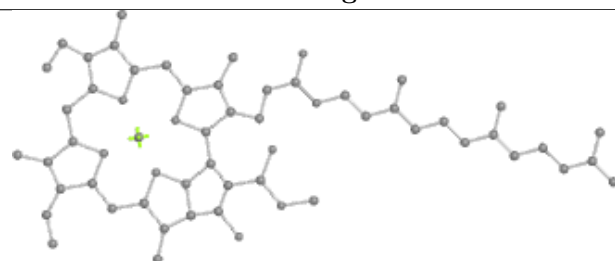
Bond lengths



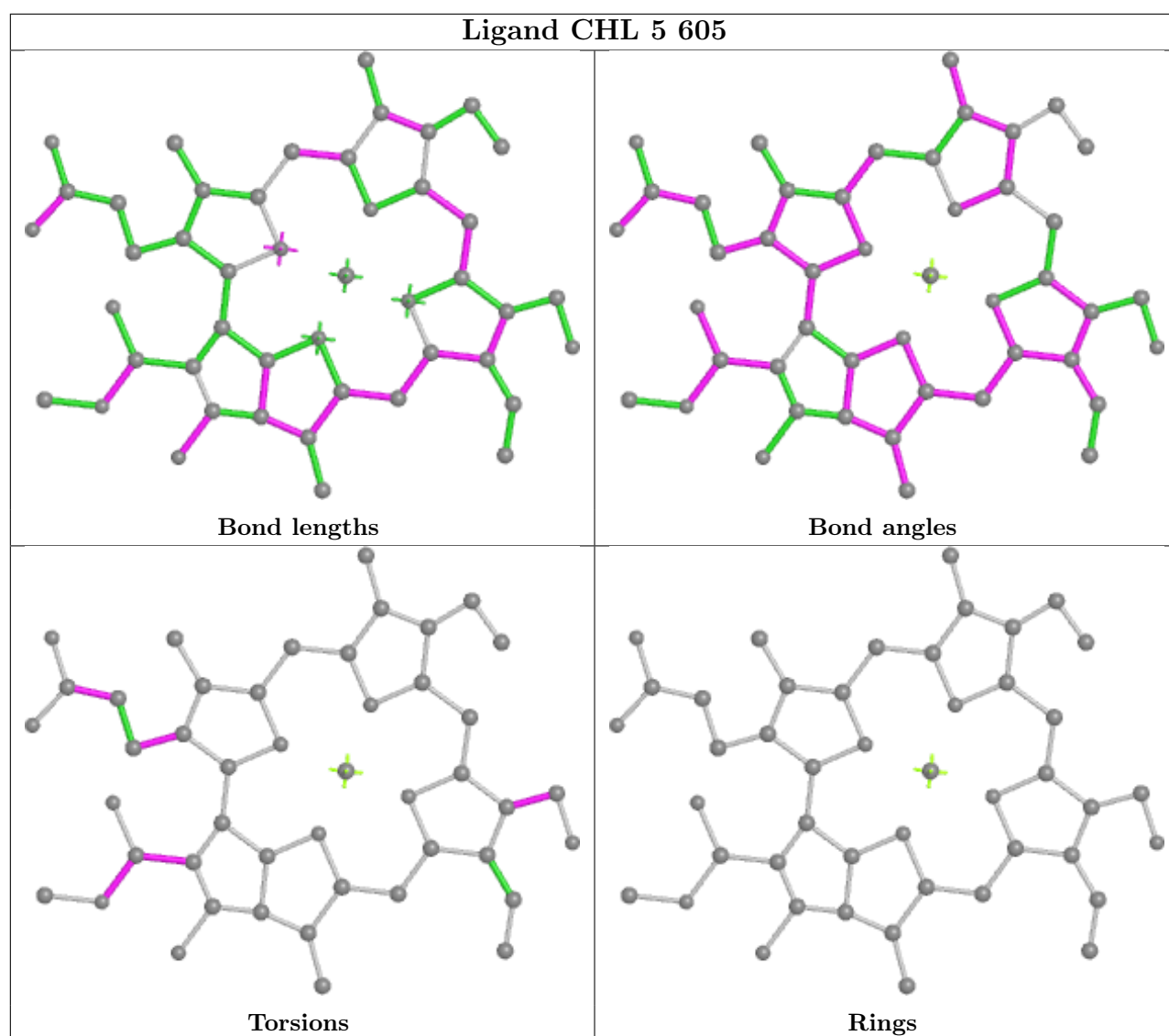
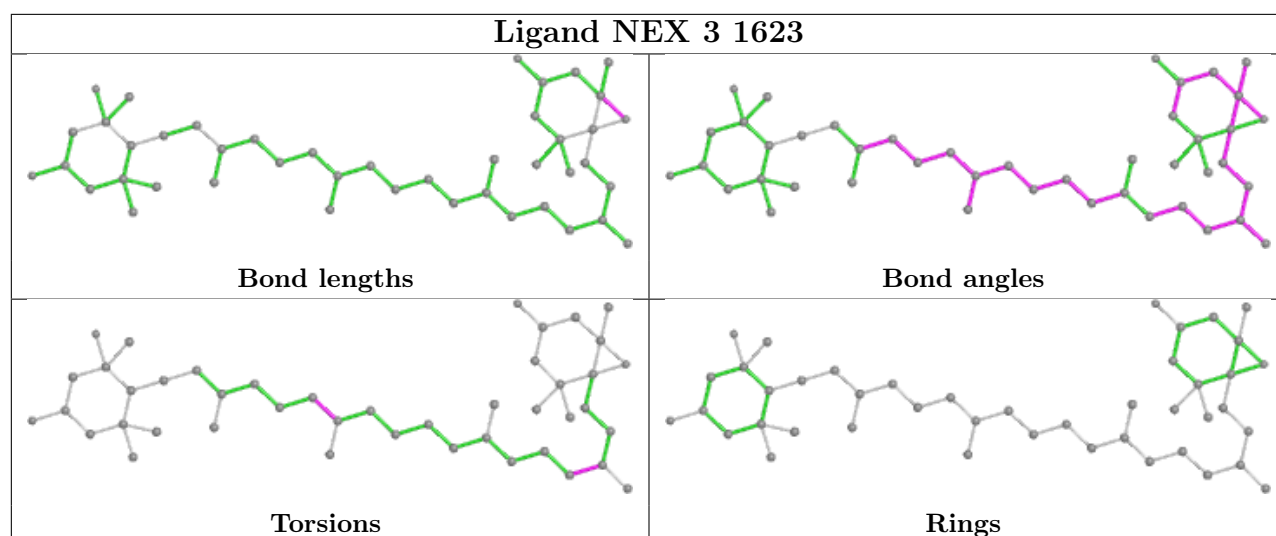
Bond angles

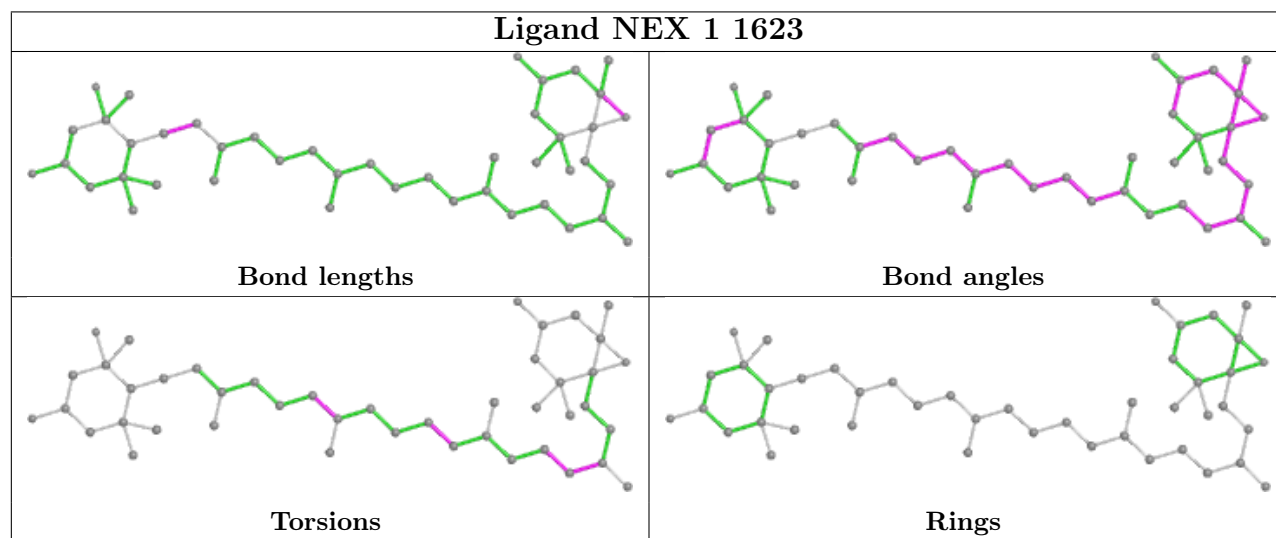
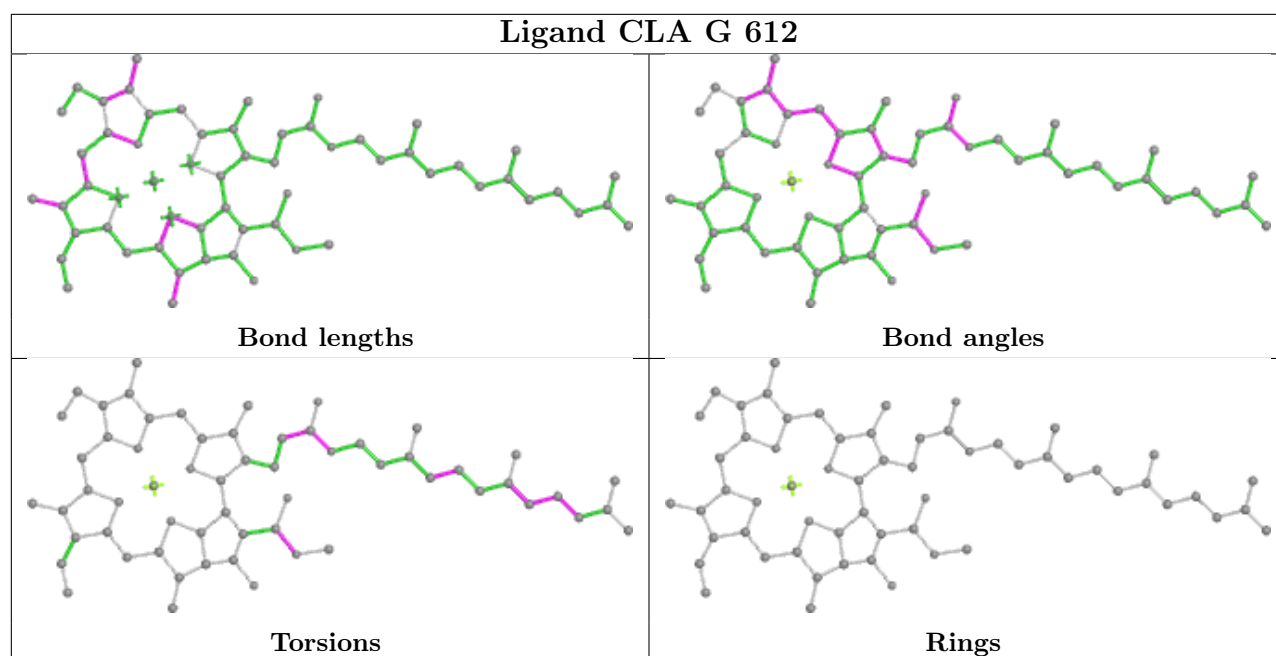


Torsions

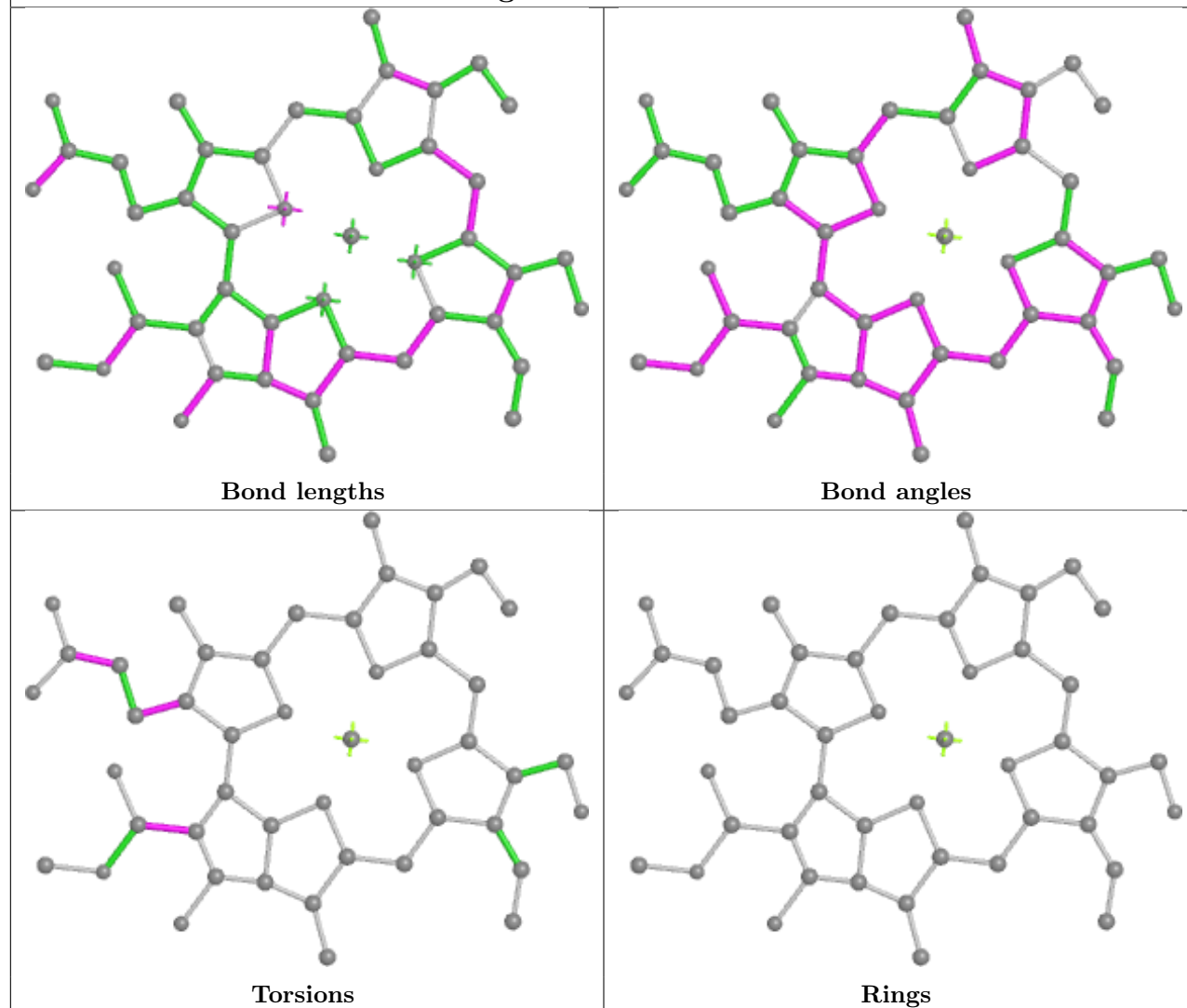


Rings

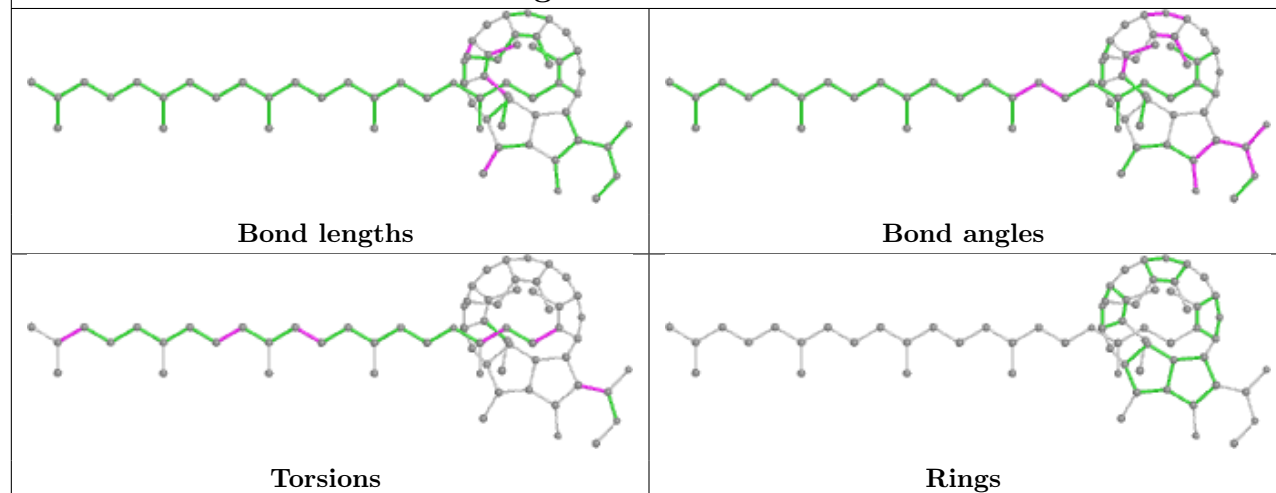


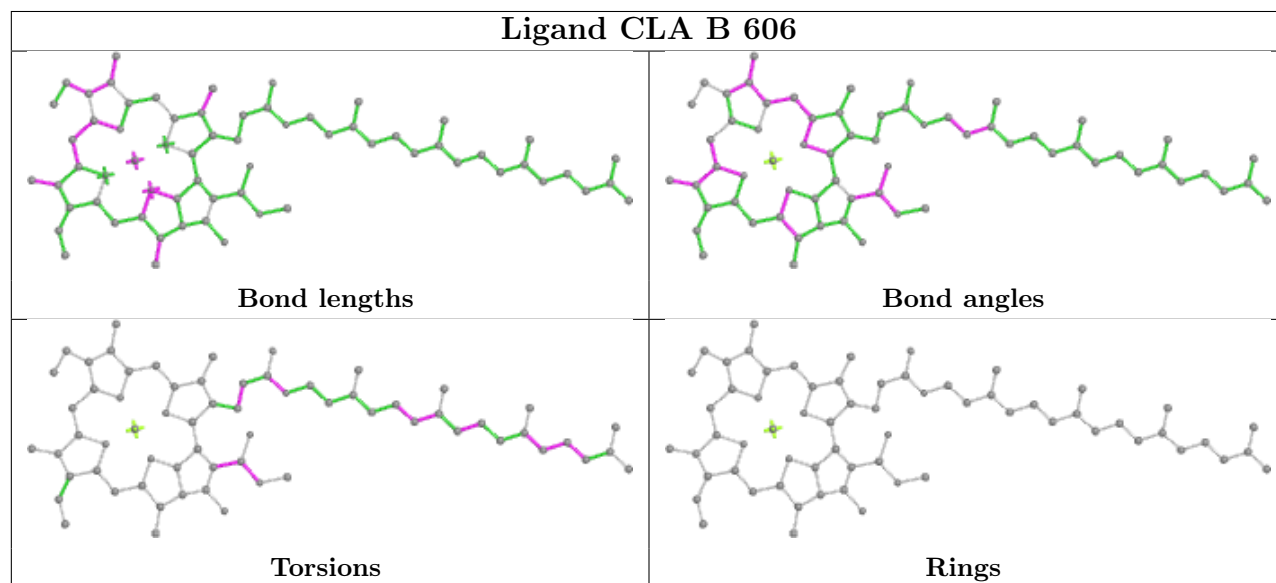
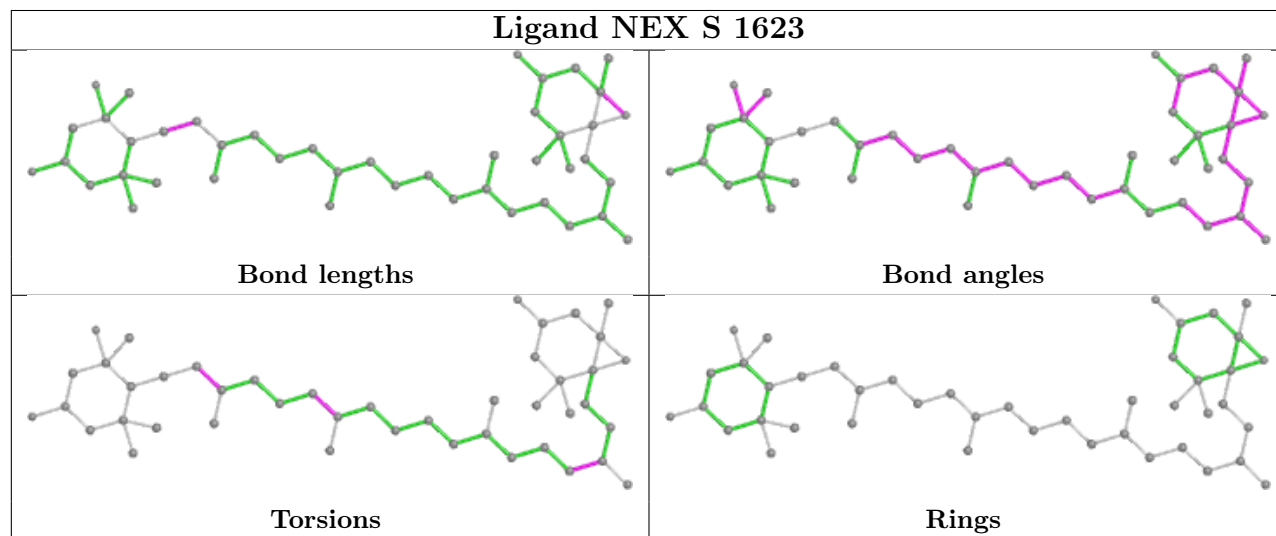
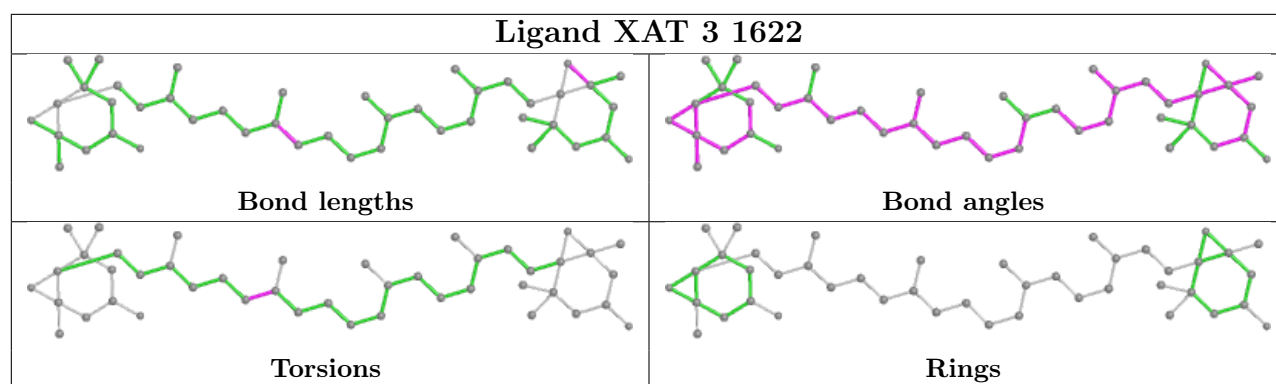


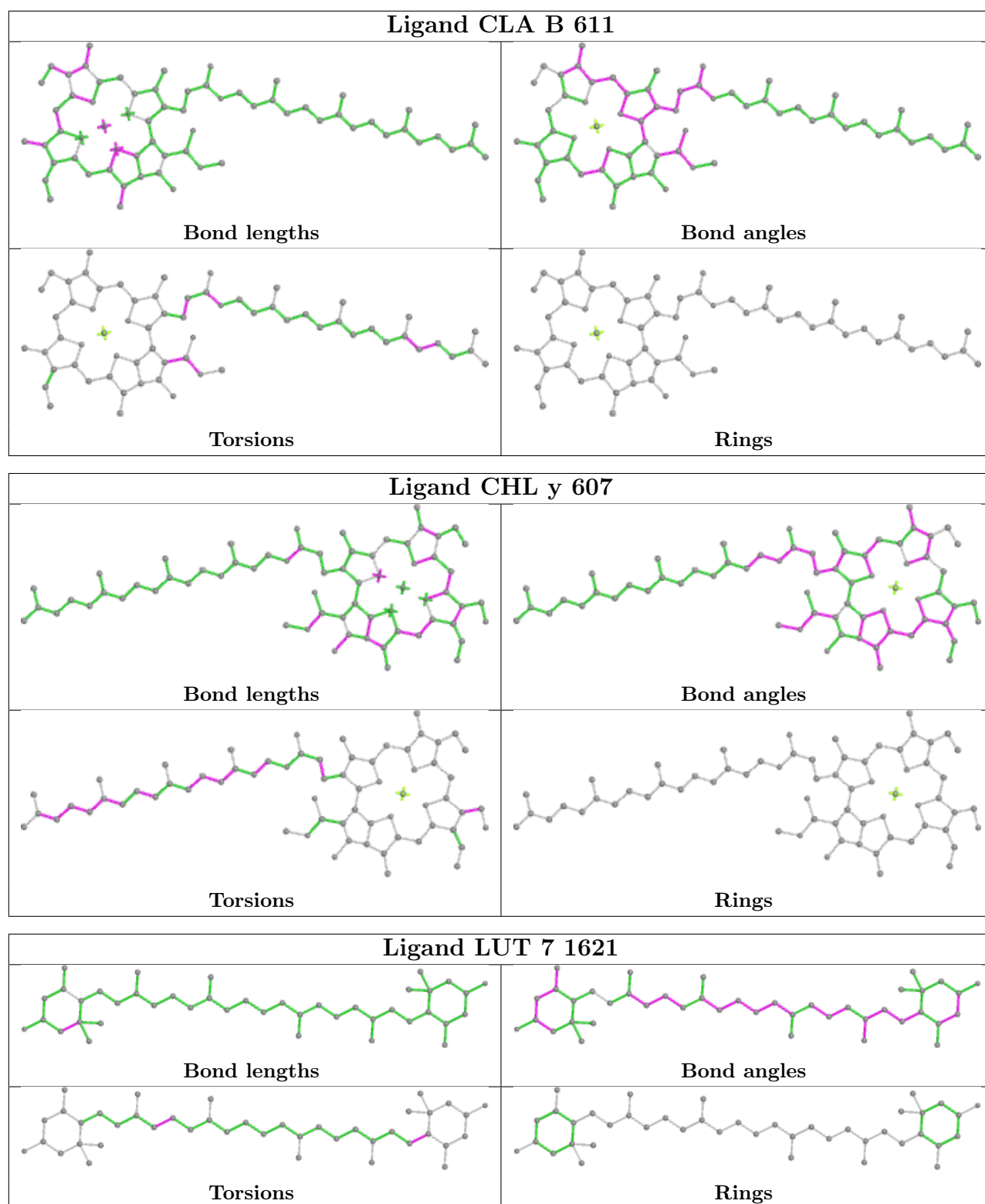
Ligand CHL 2 601

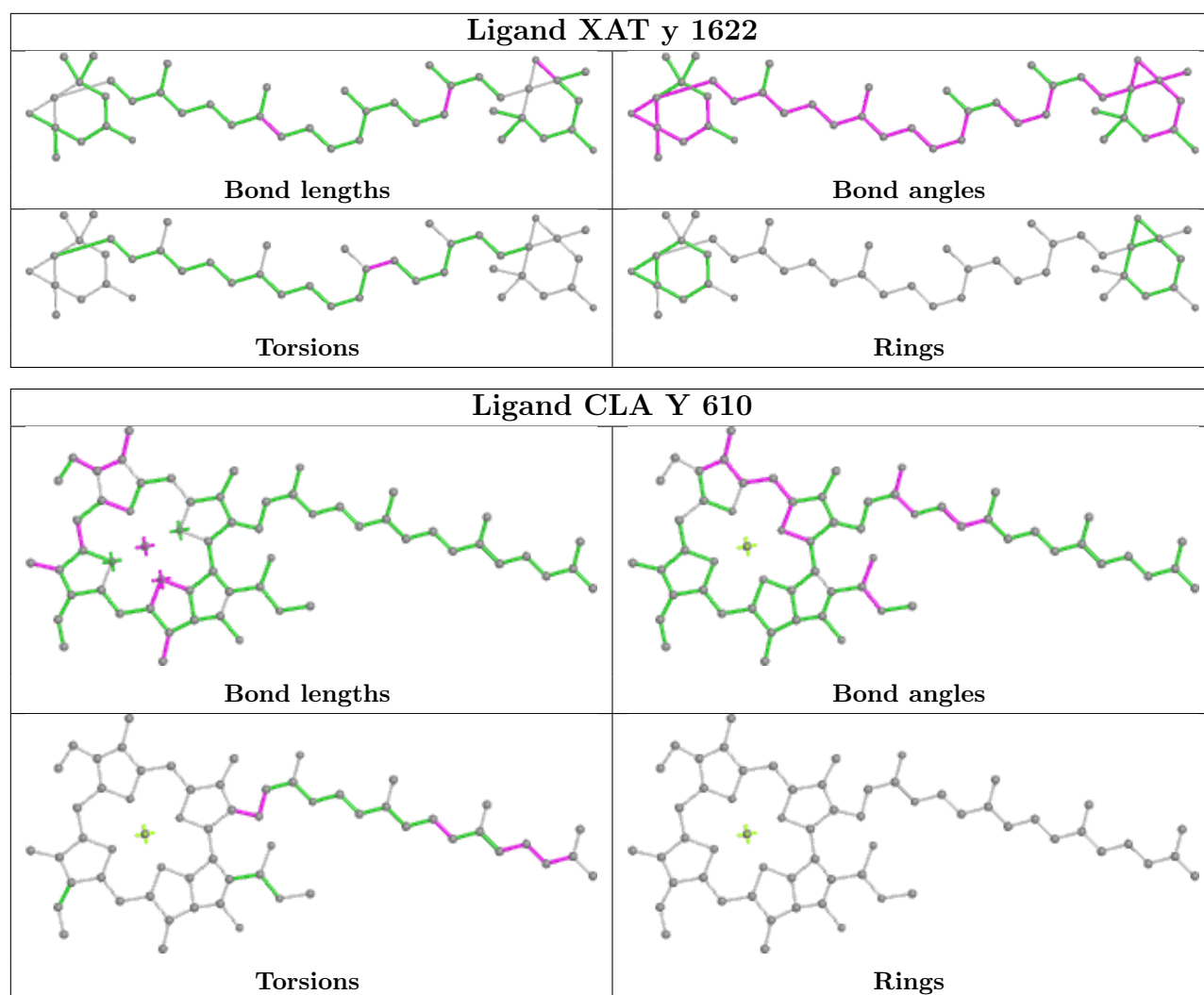


Ligand PHO a 409

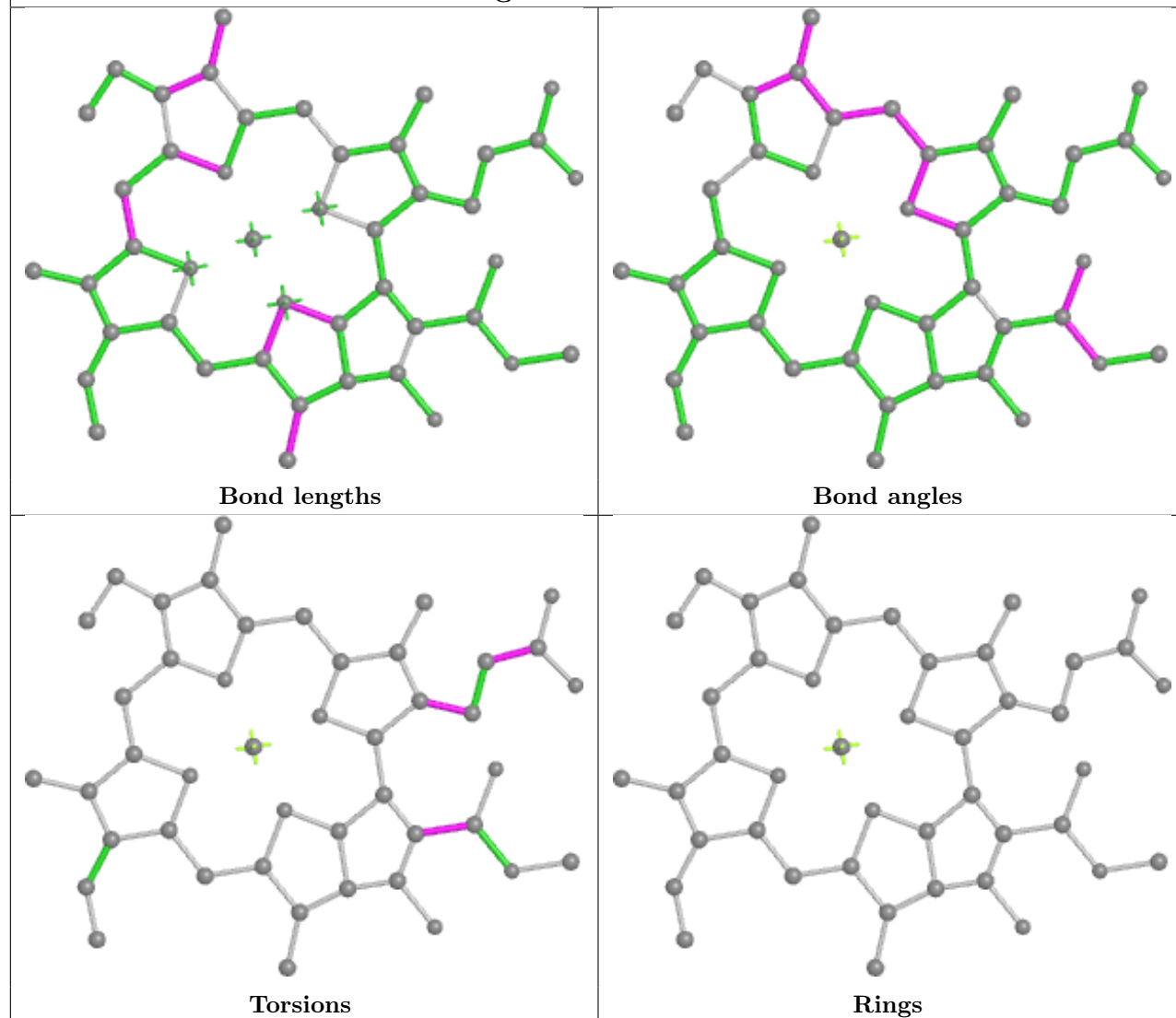




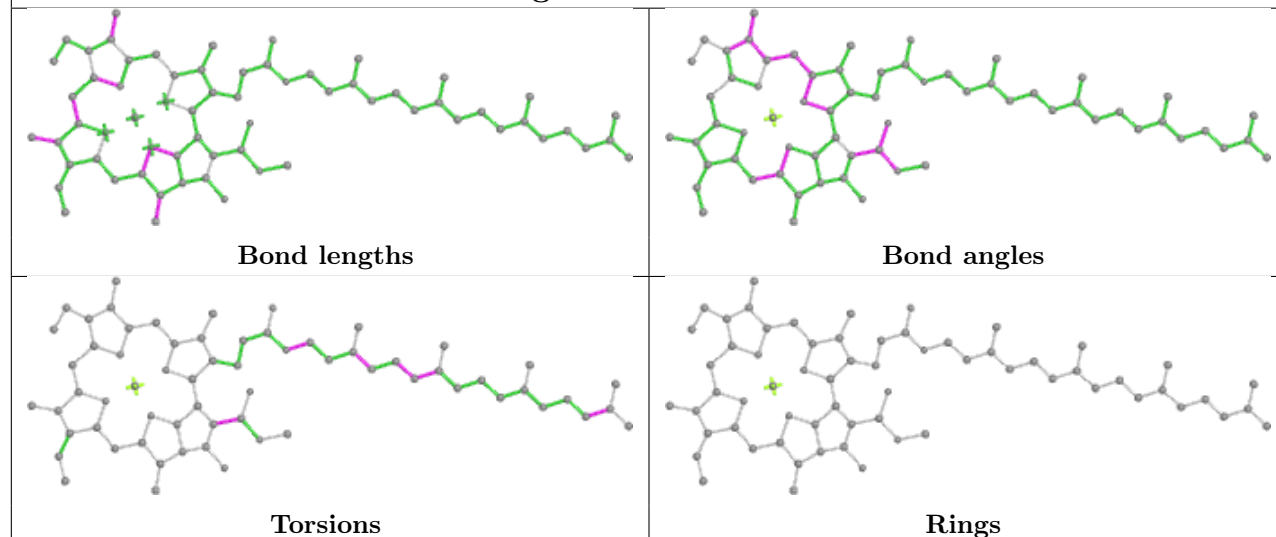


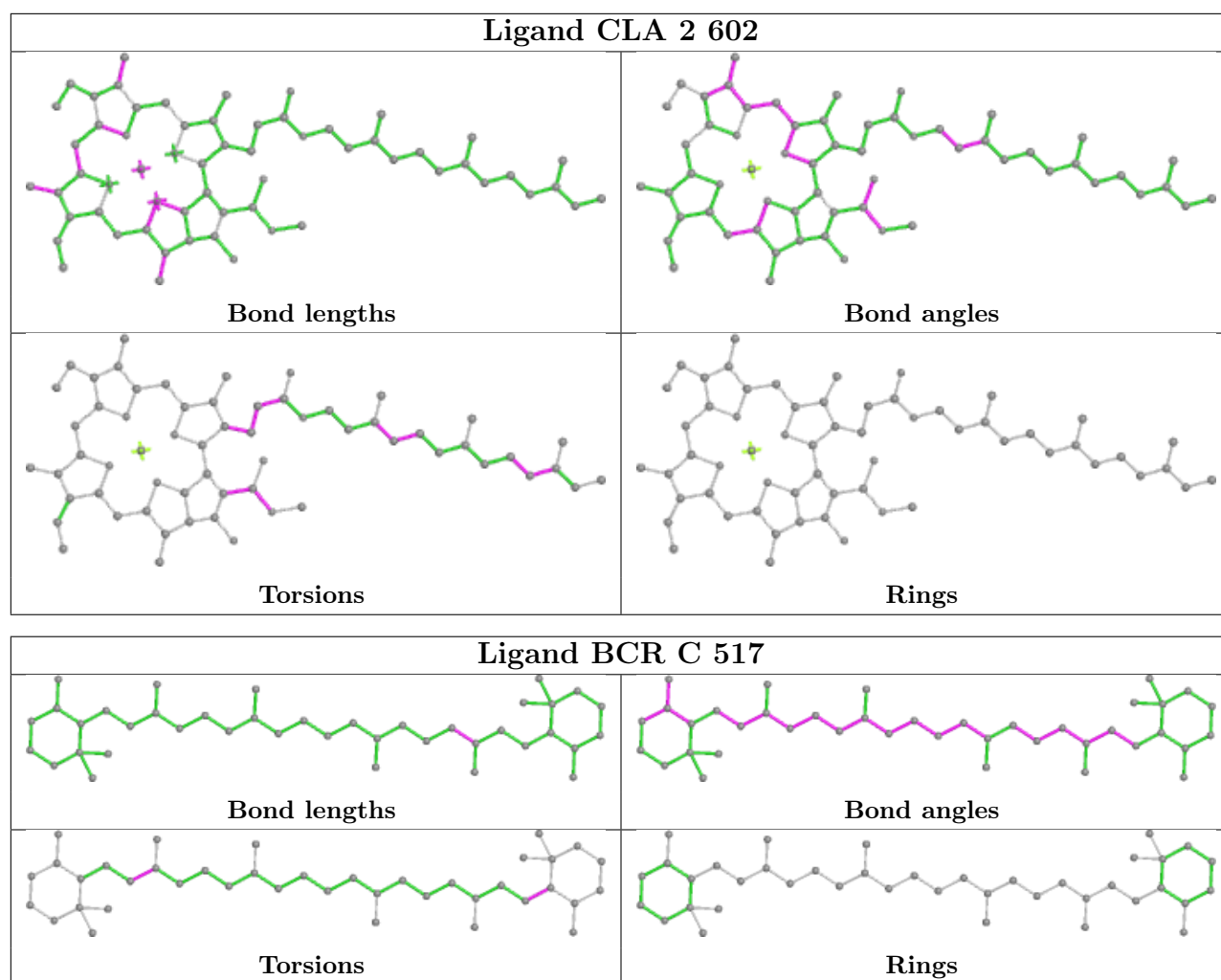


Ligand CLA r 616

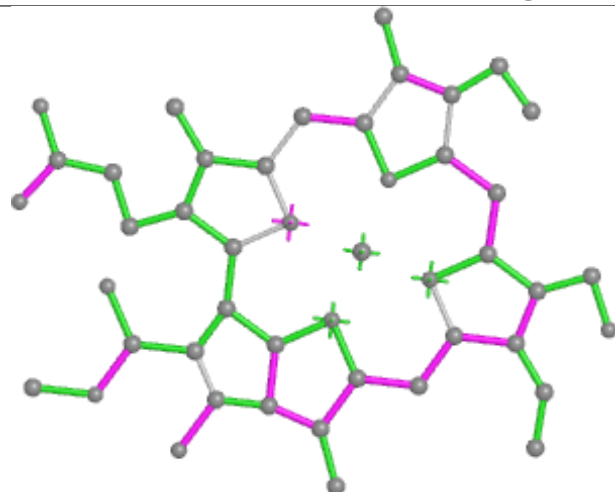


Ligand CLA B 603

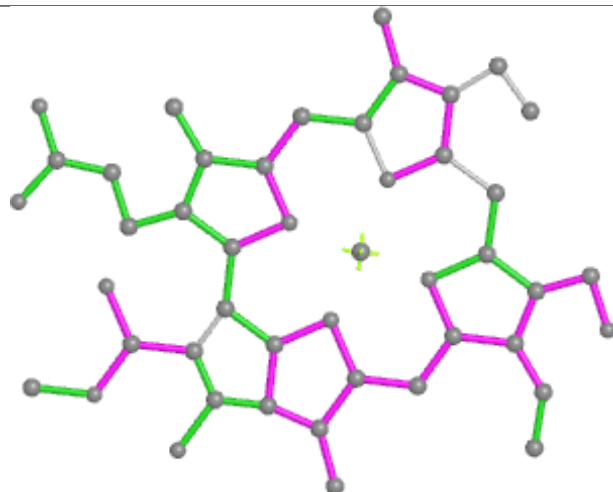




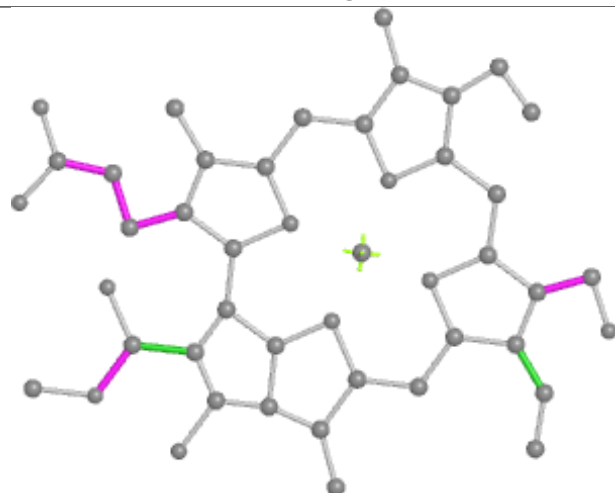
Ligand CHL 7 606



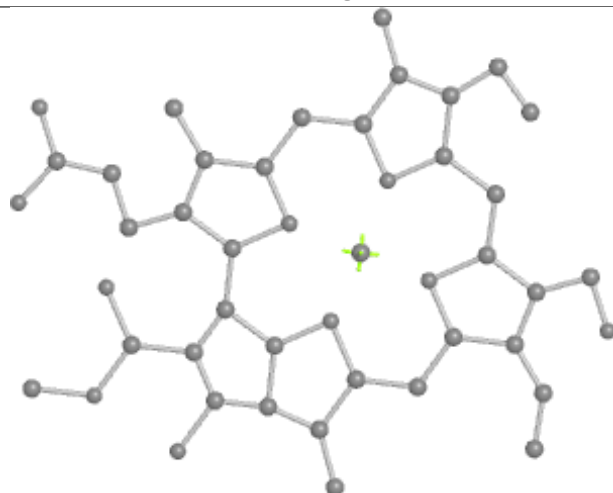
Bond lengths



Bond angles

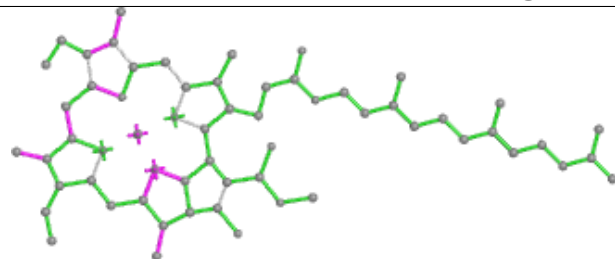


Torsions

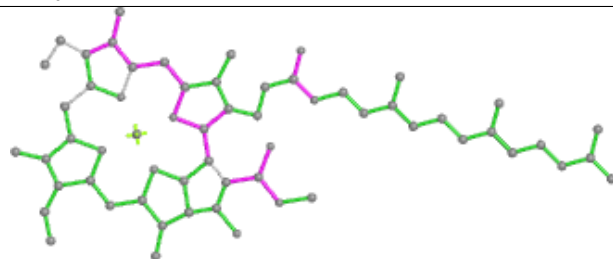


Rings

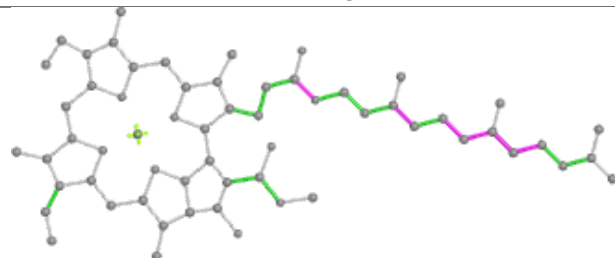
Ligand CLA y 611



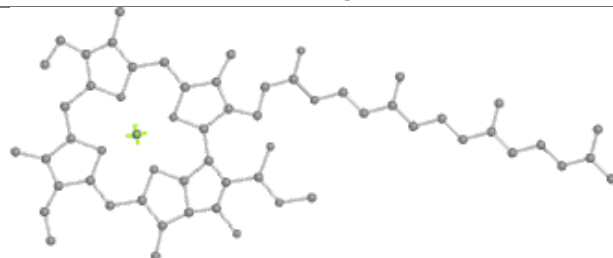
Bond lengths



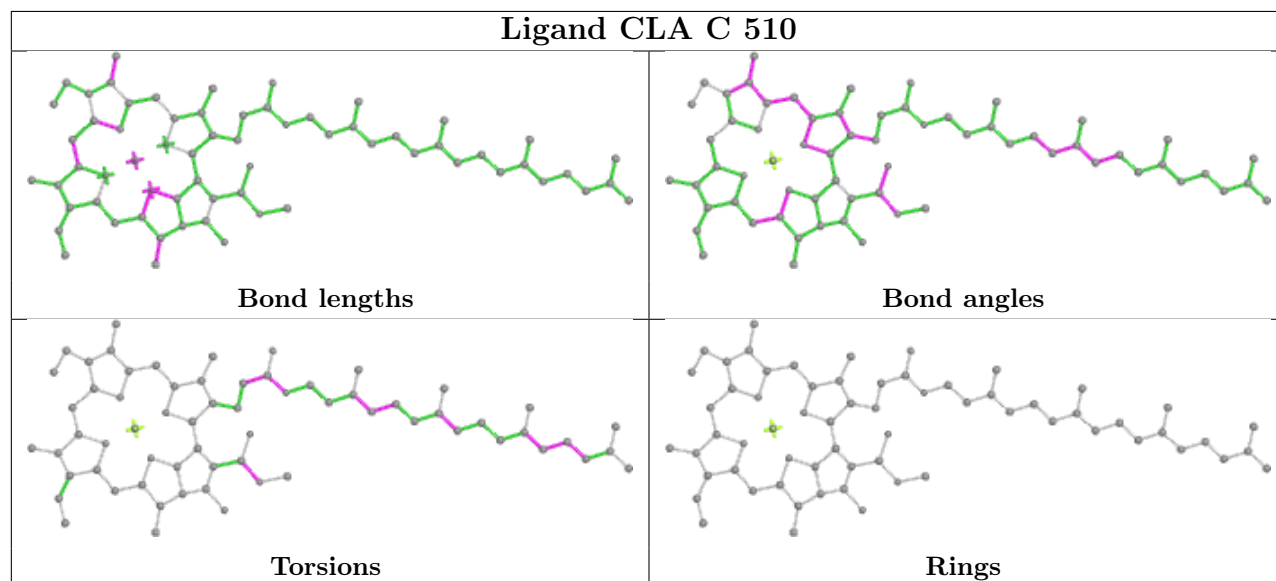
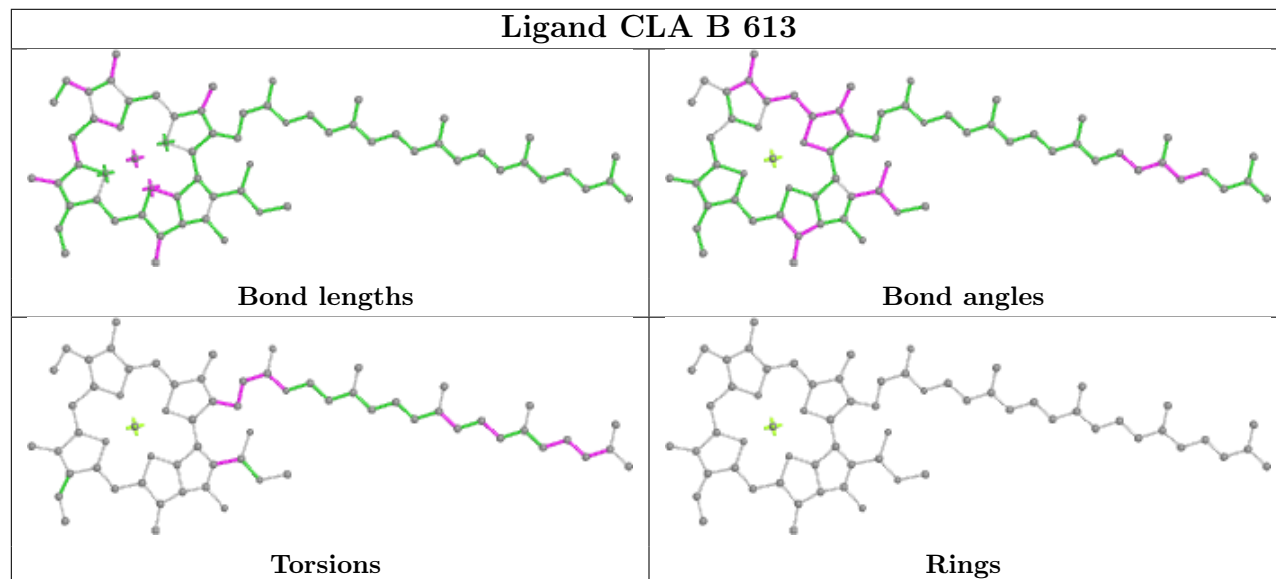
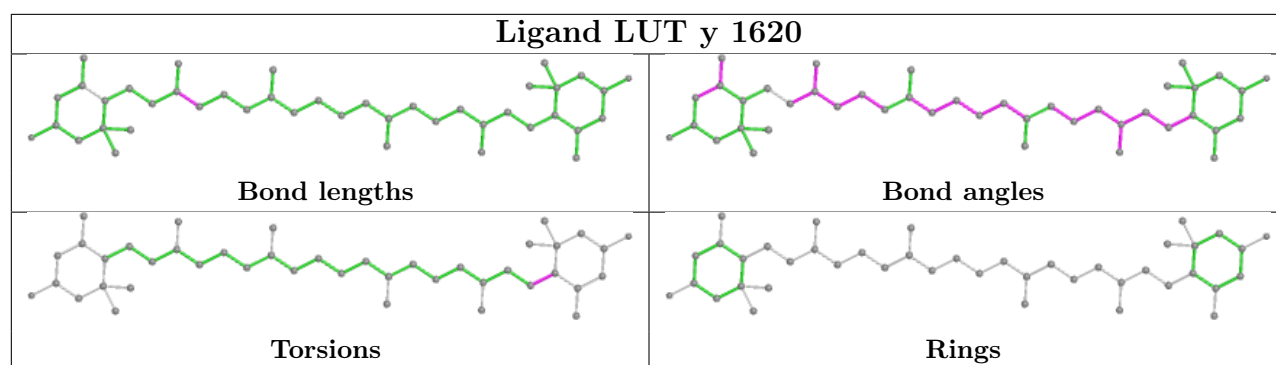
Bond angles

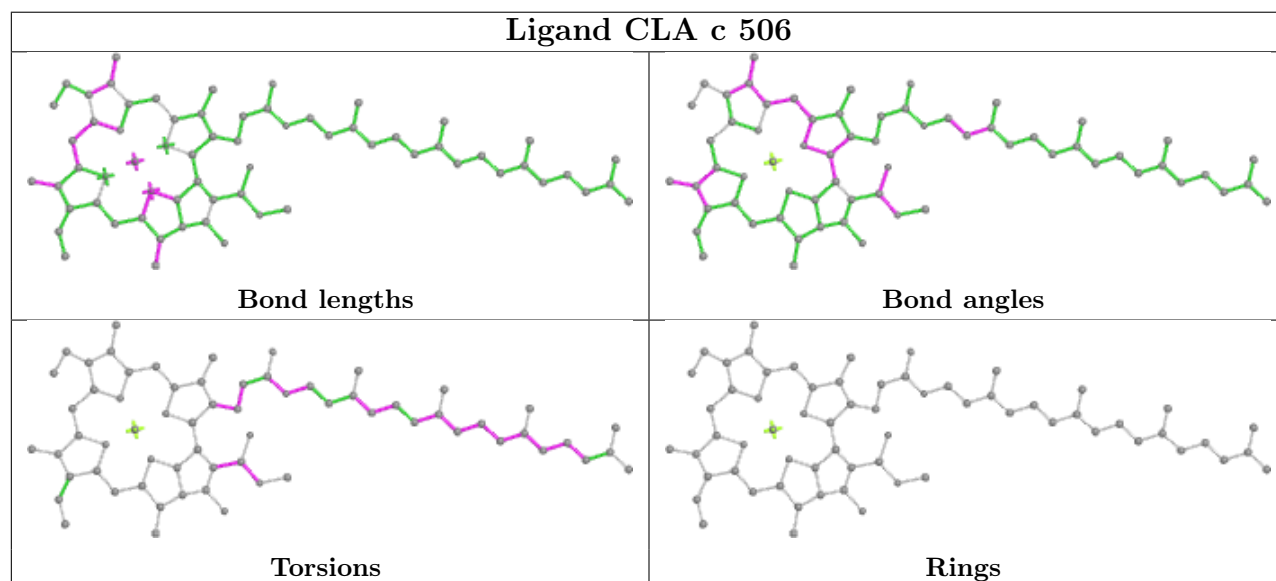
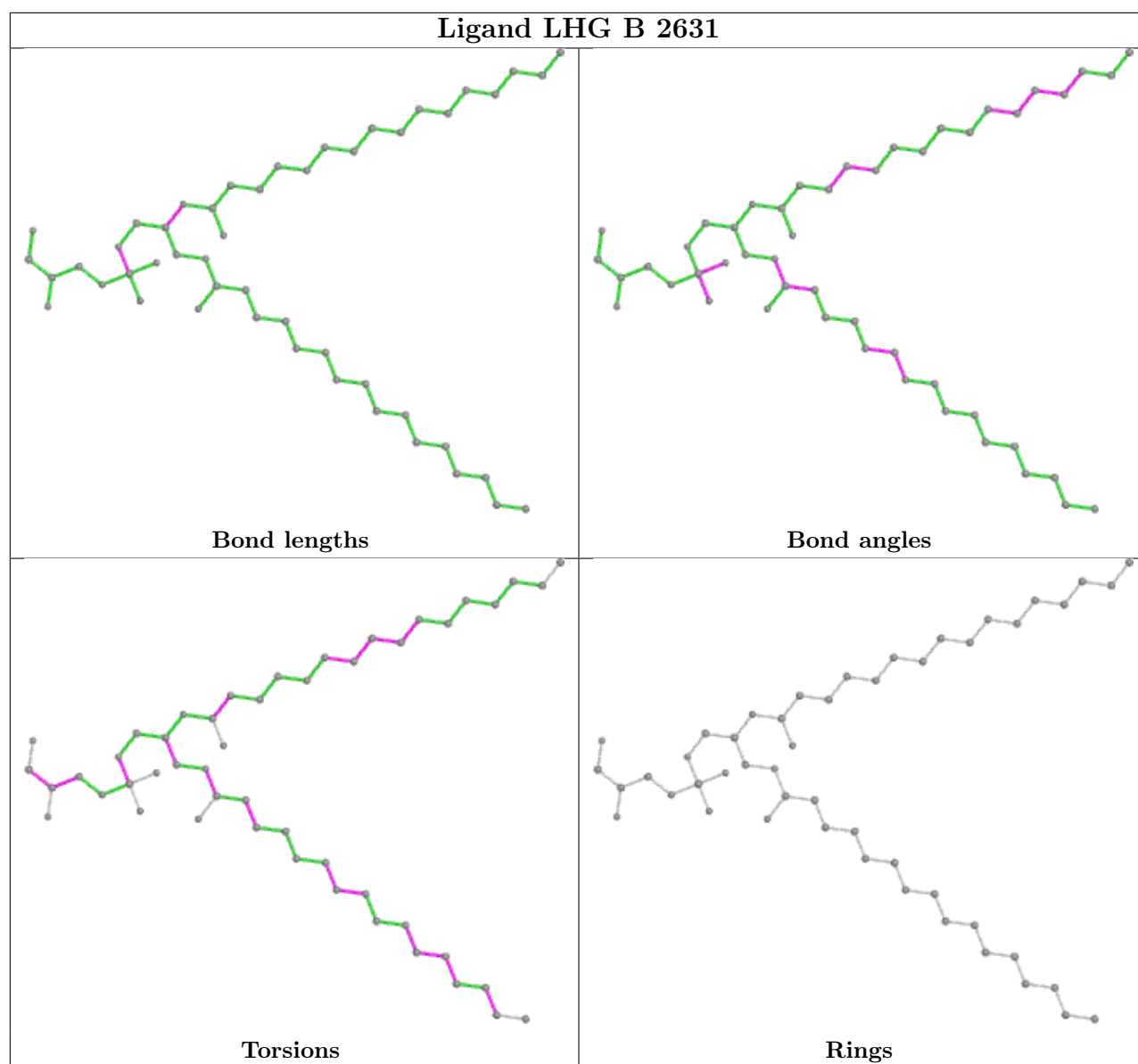


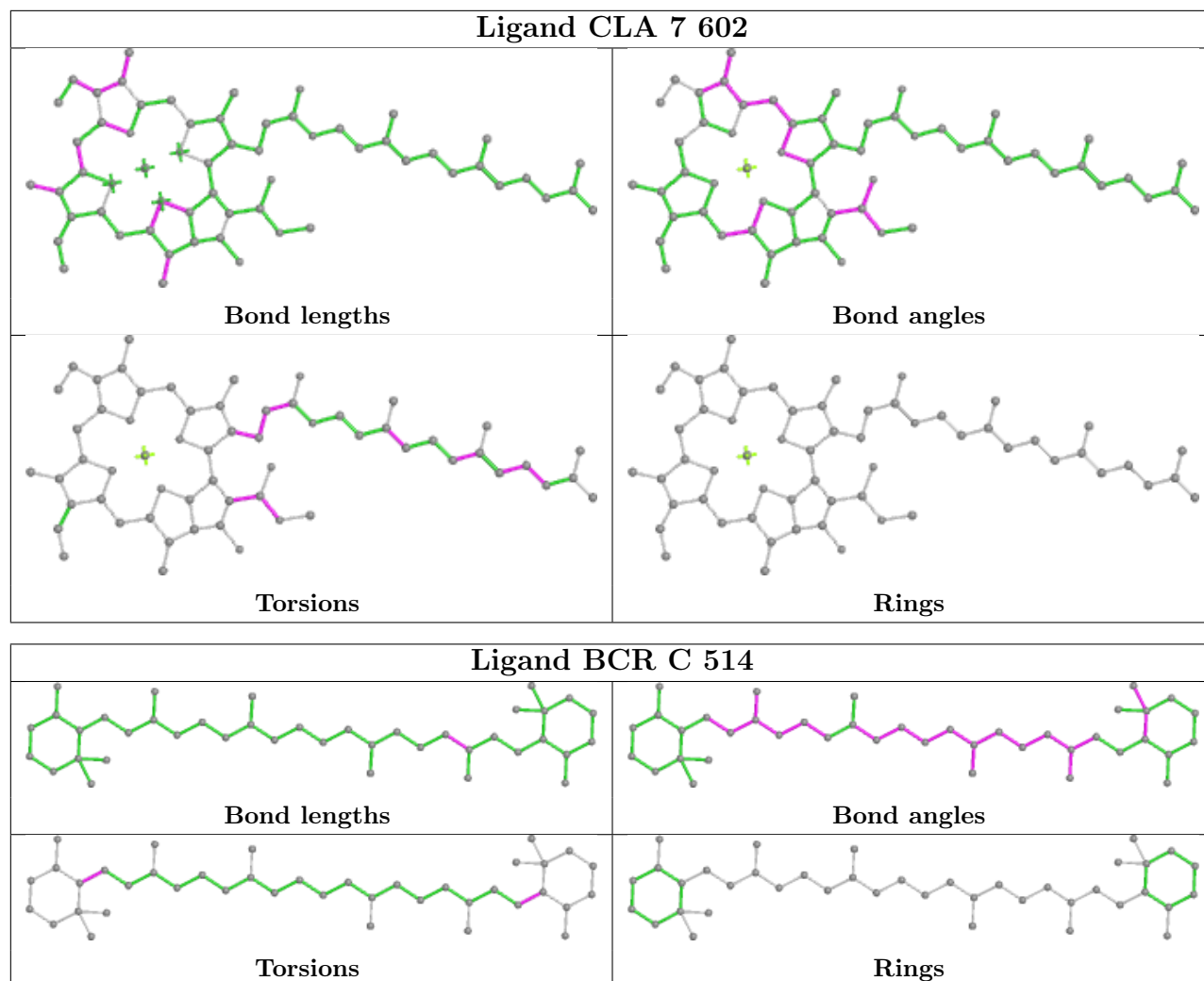
Torsions

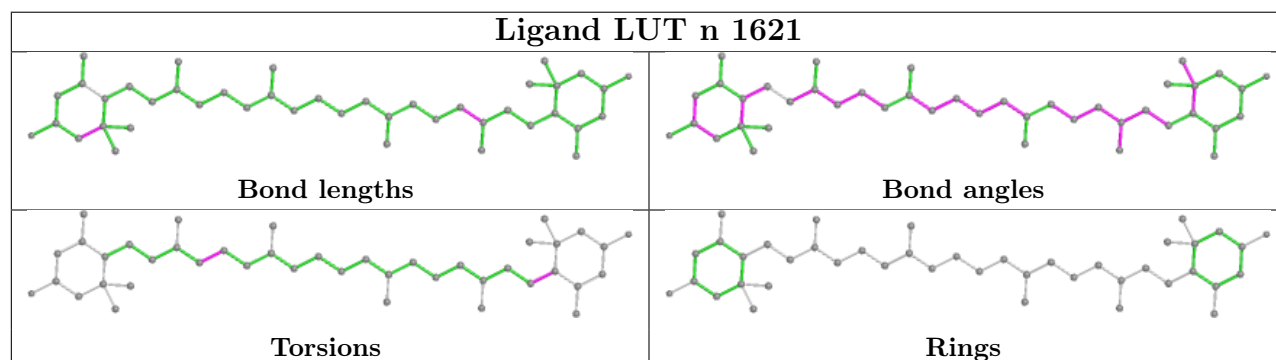
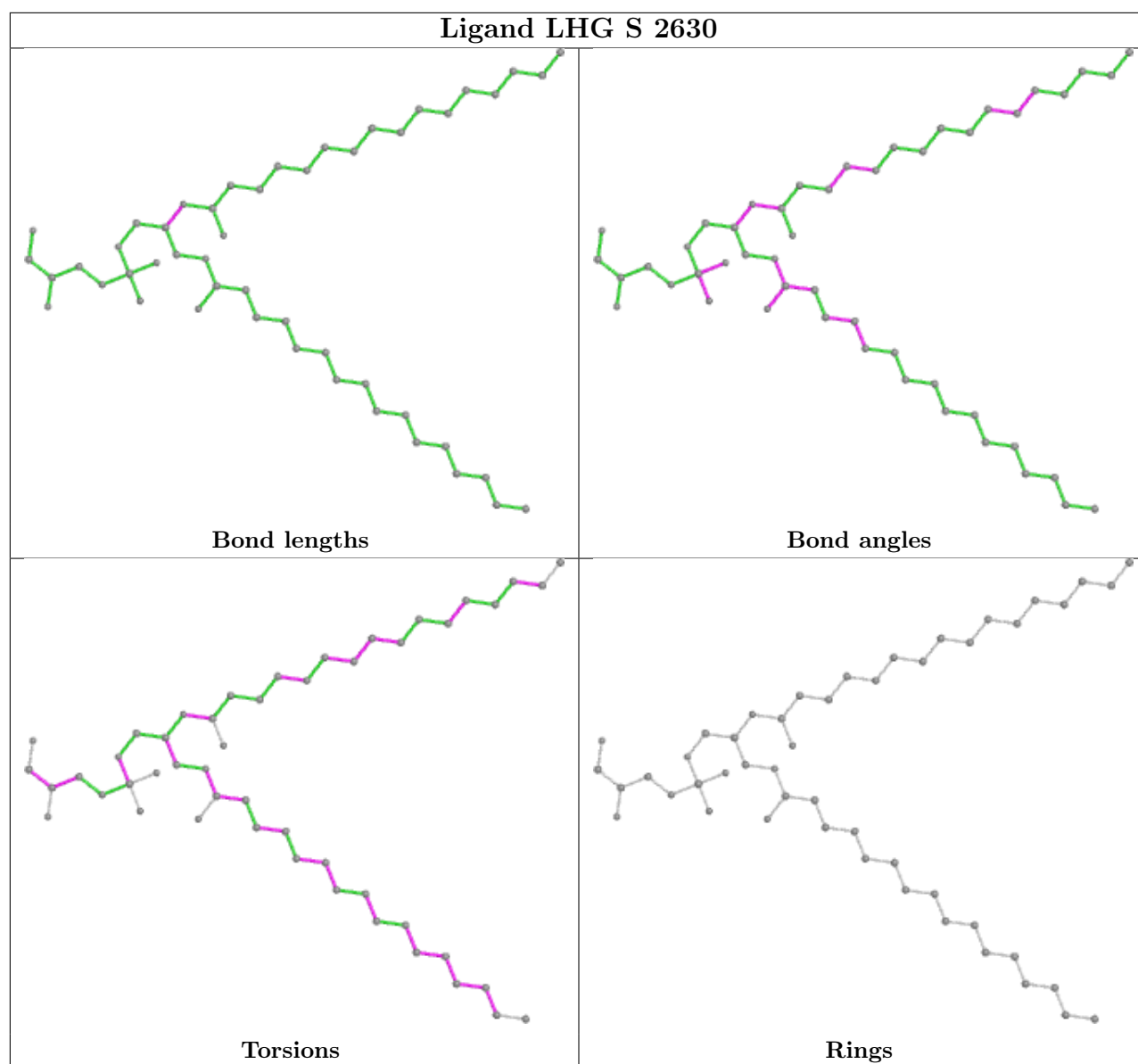


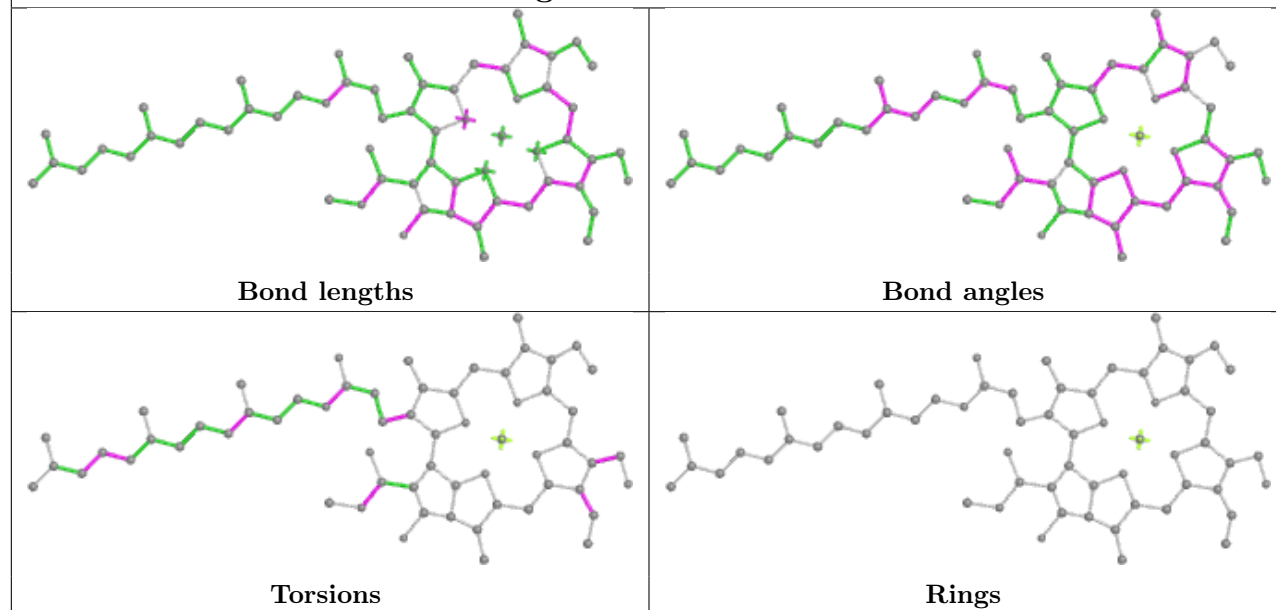
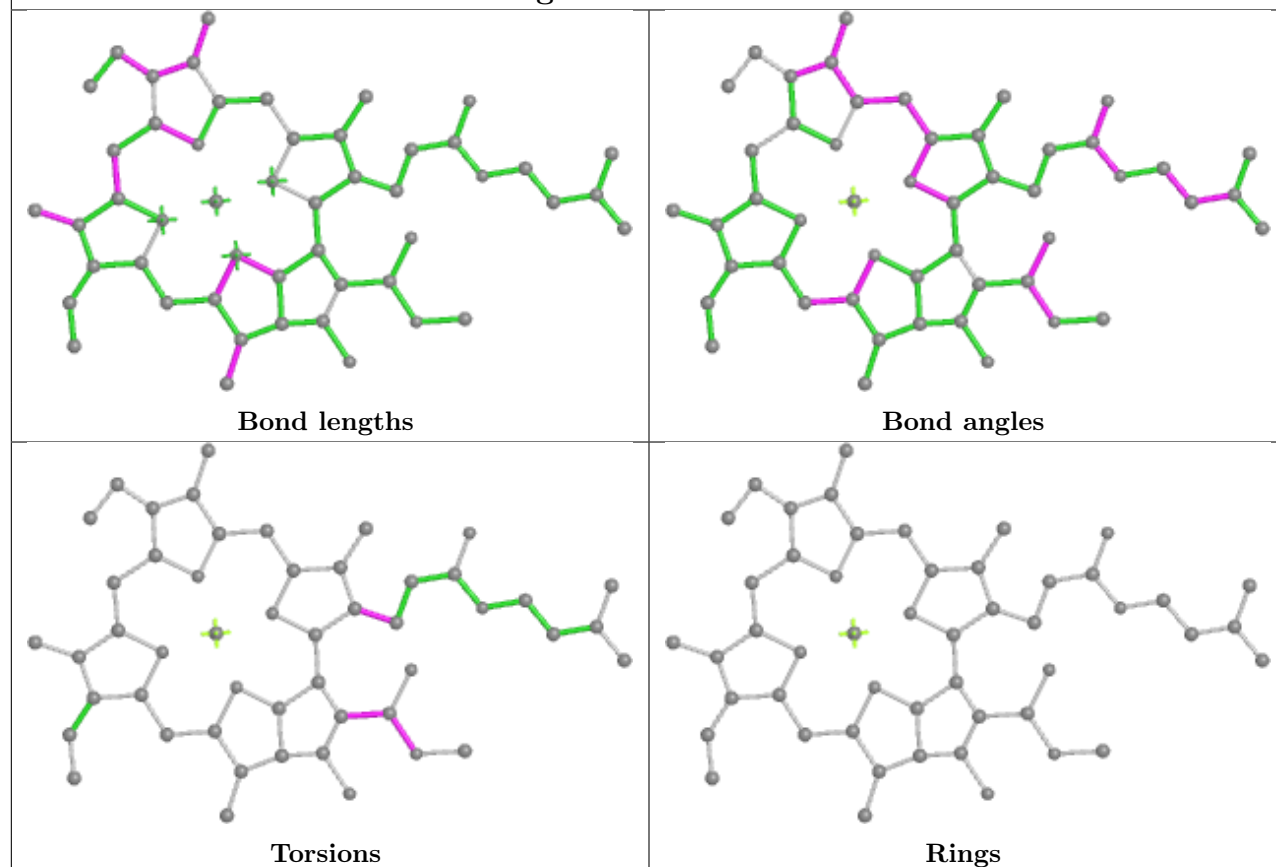
Rings

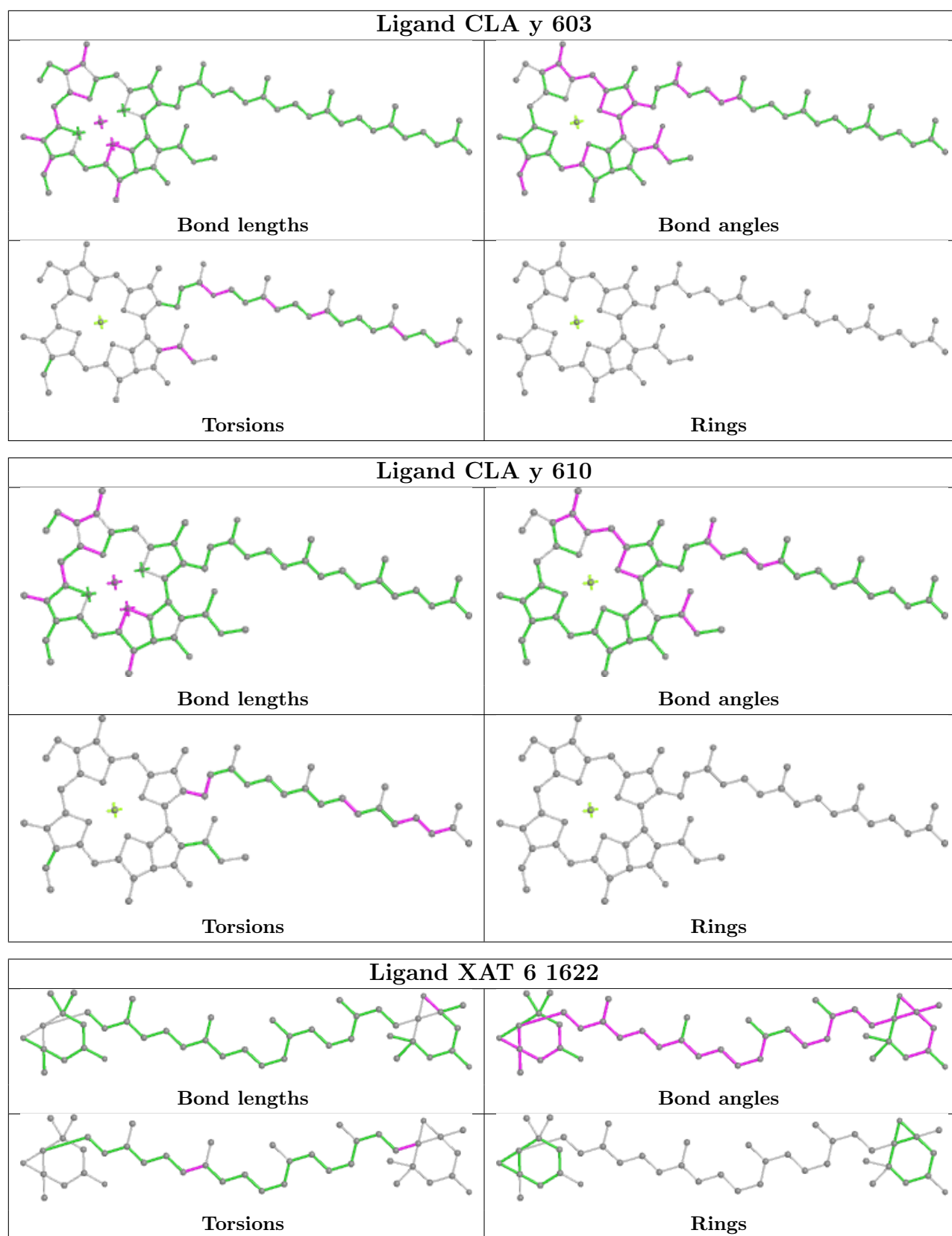




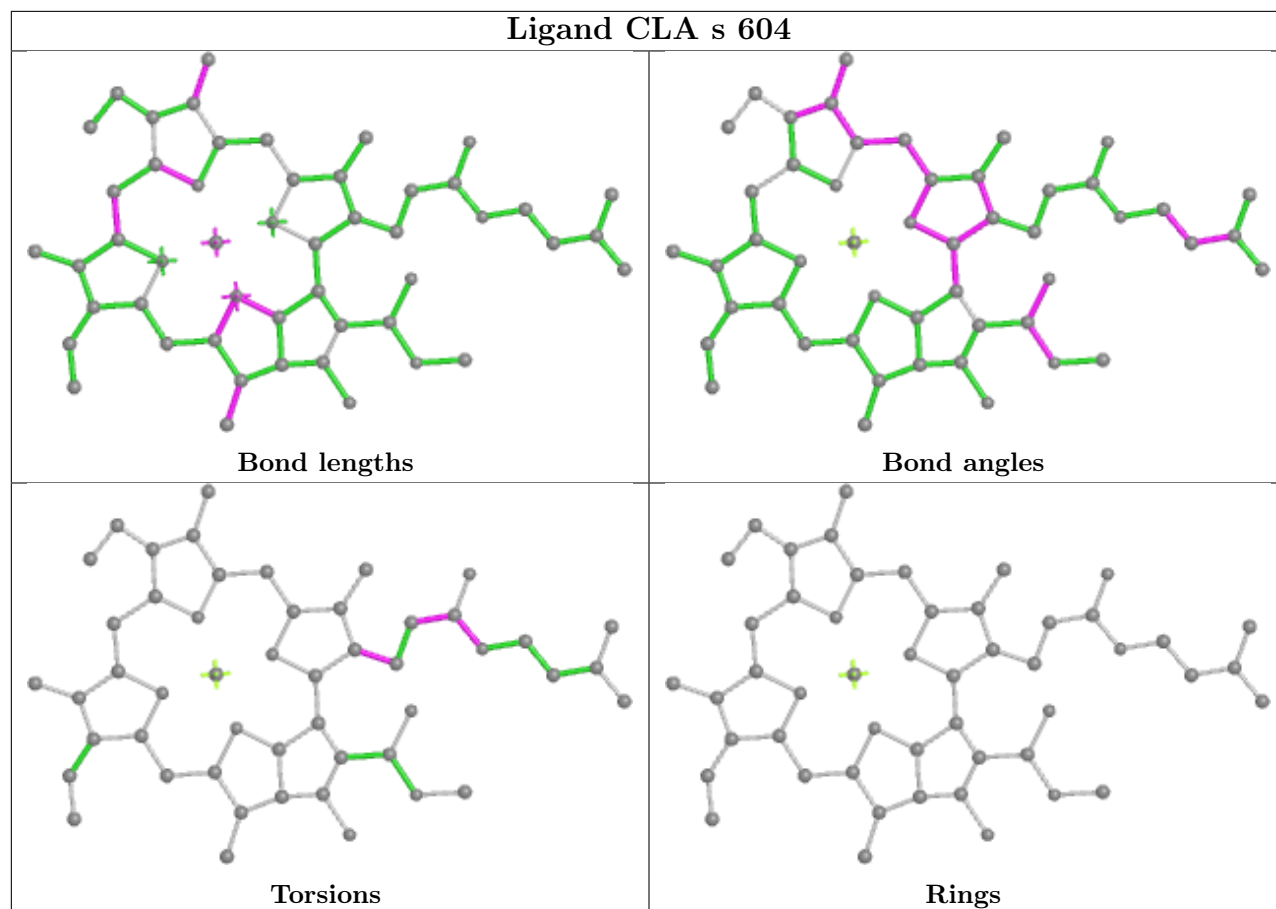




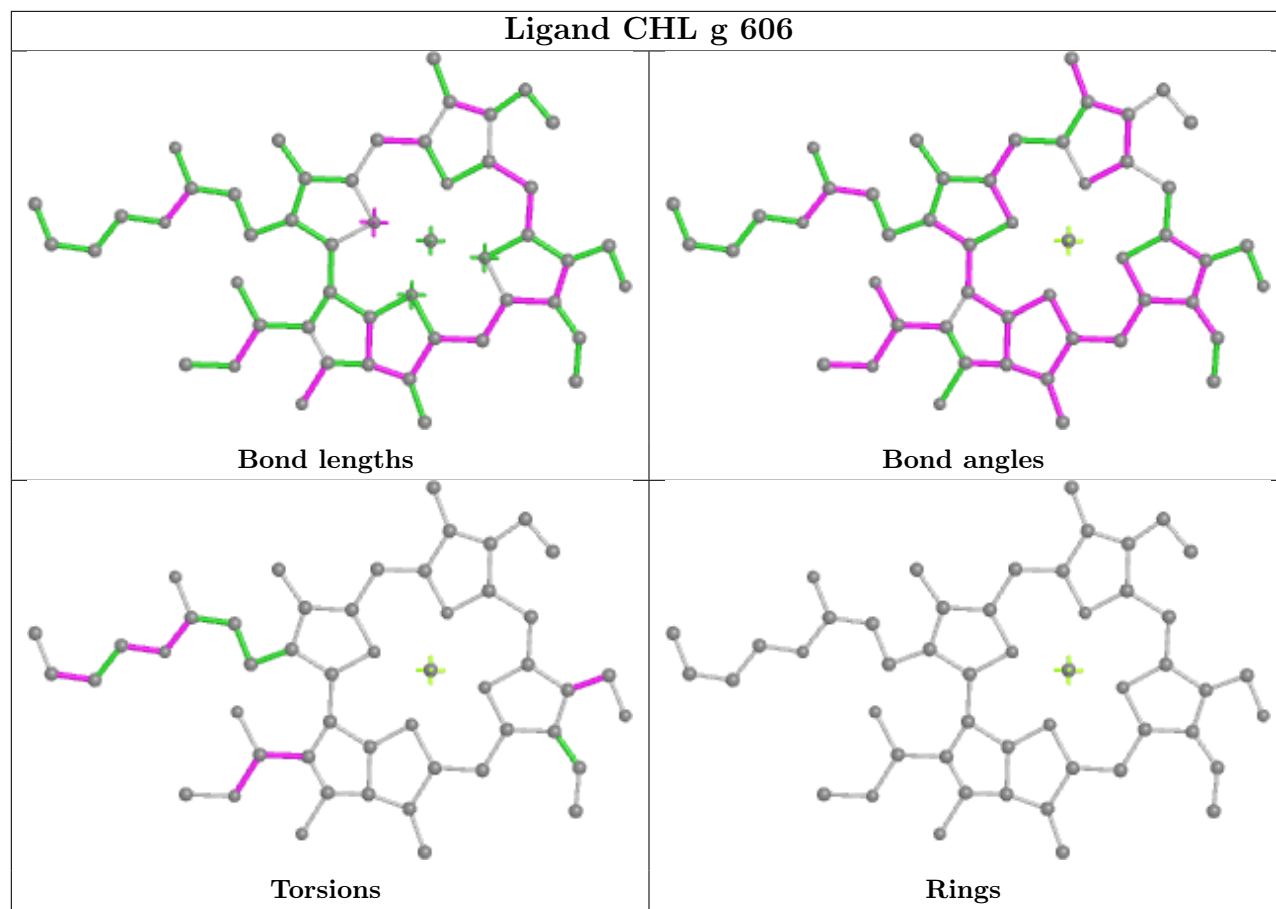
Ligand CHL 7 609**Ligand CLA 6 610**

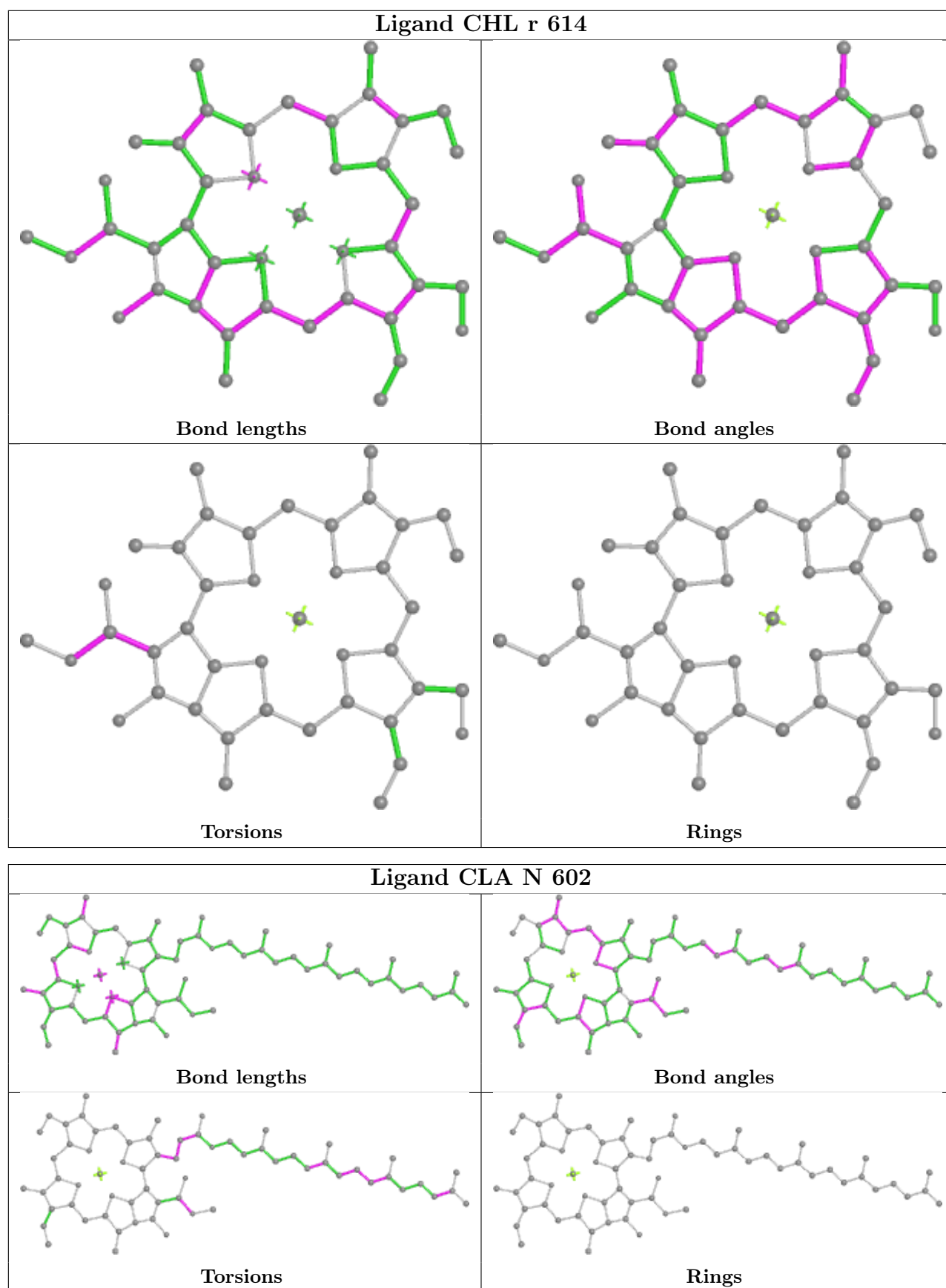


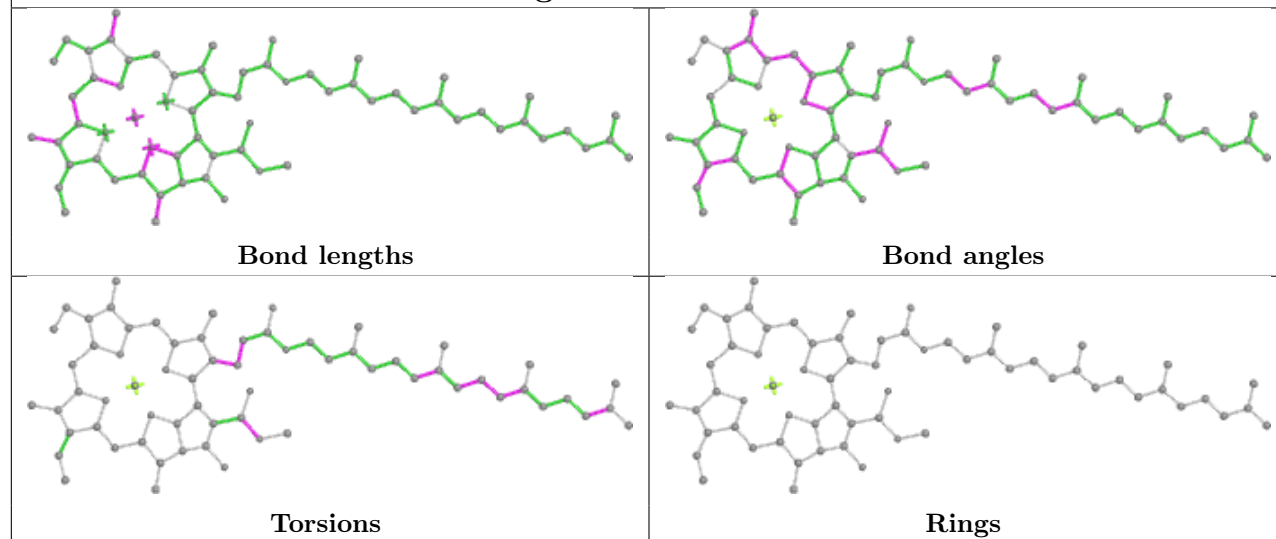
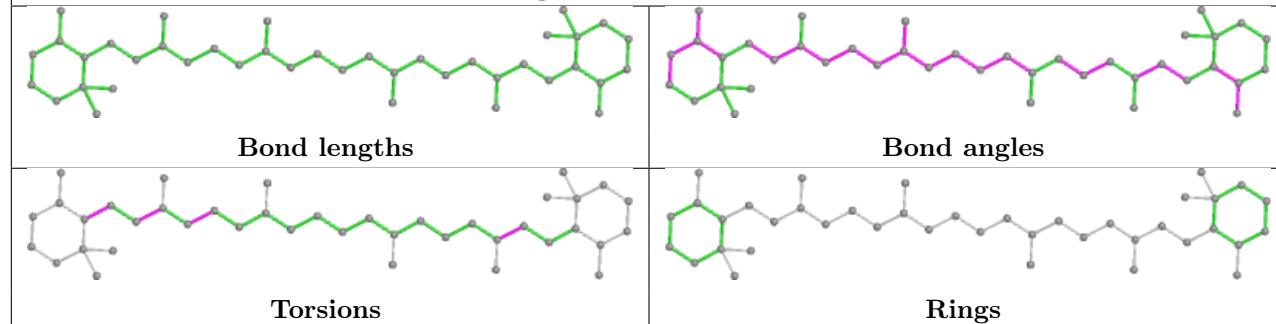
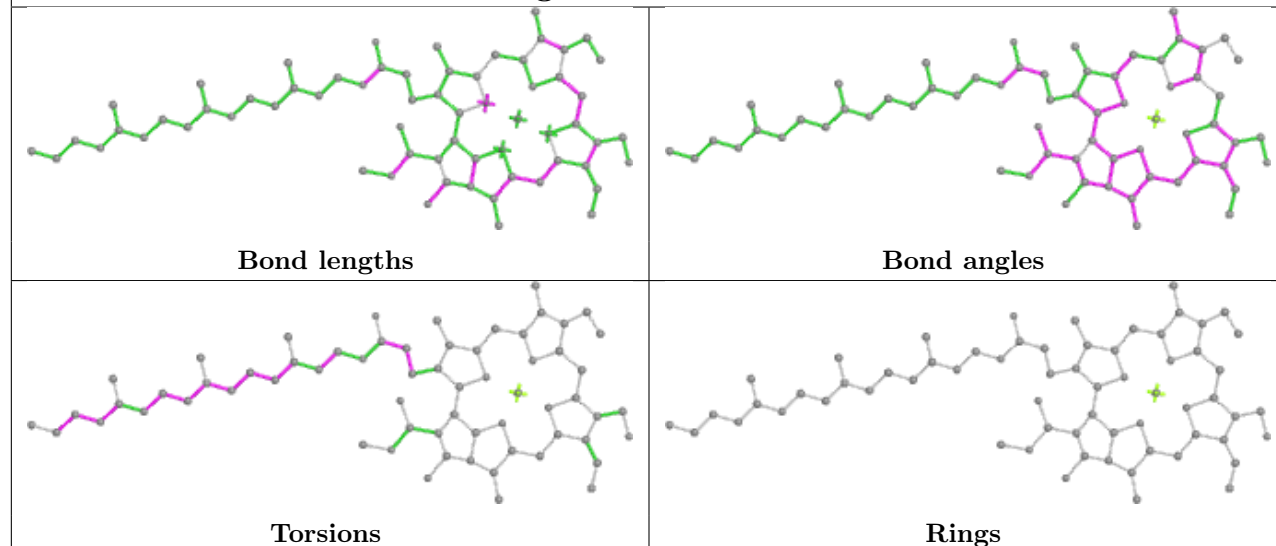
Ligand CLA s 604

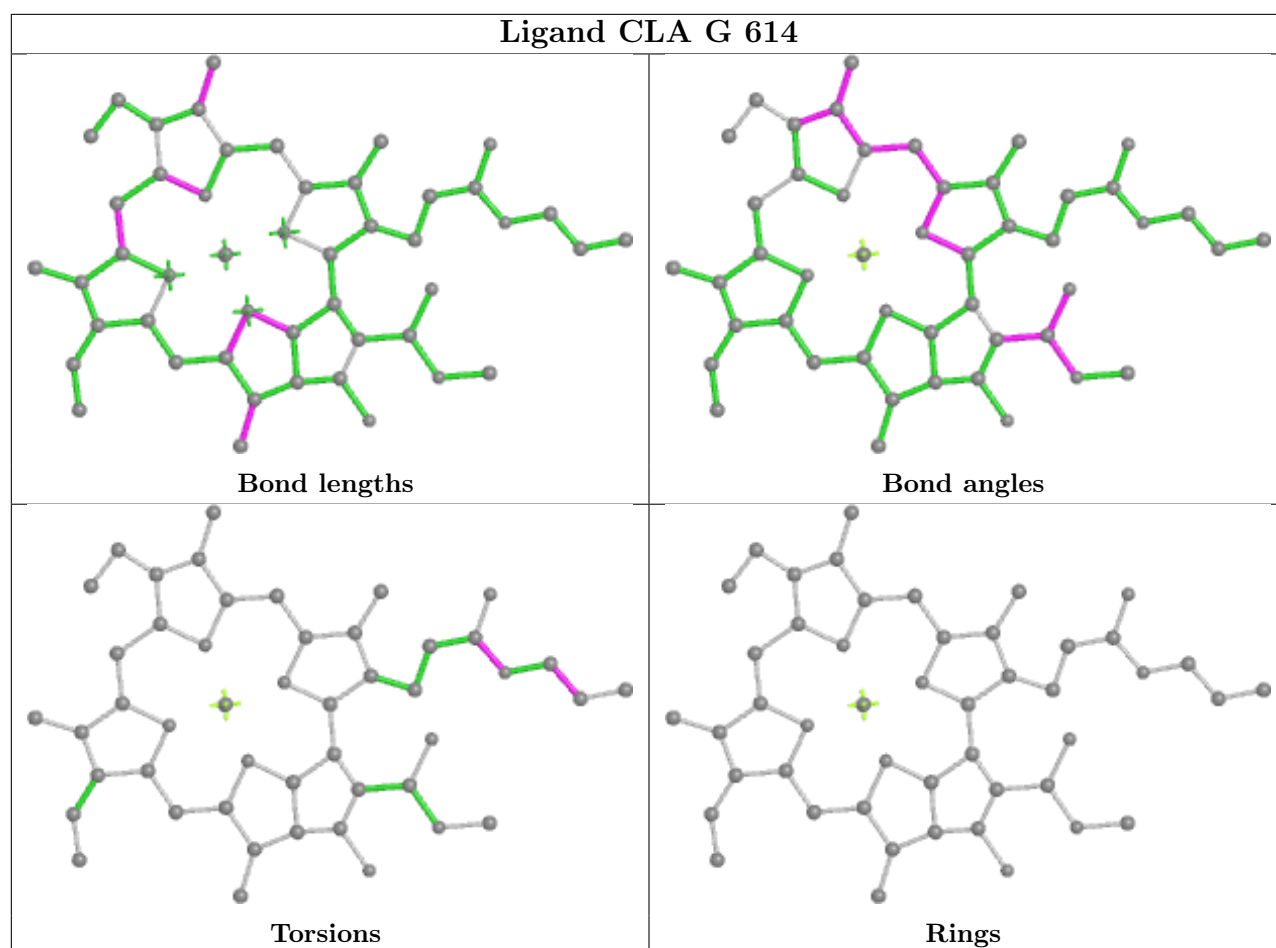


Ligand CHL g 606

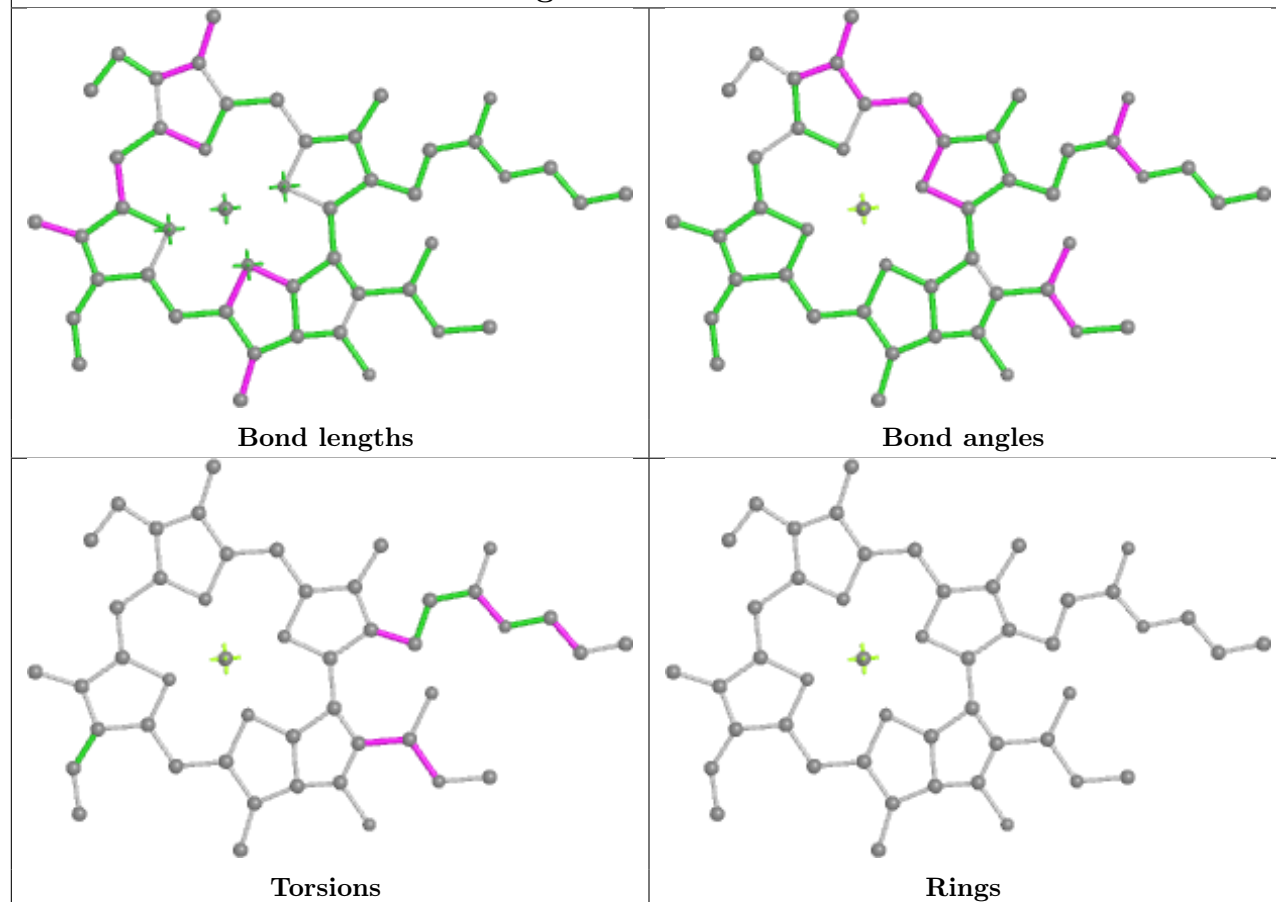




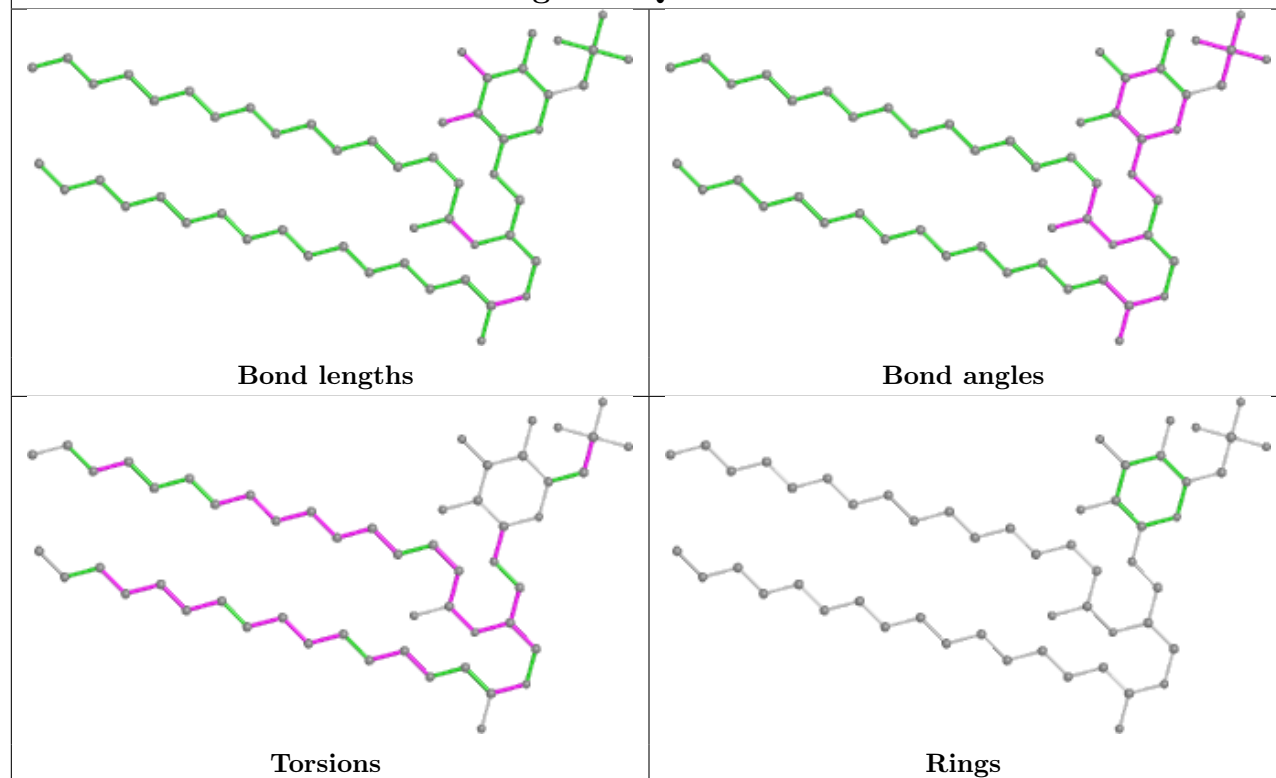
Ligand CLA n 602**Ligand BCR d 404****Ligand CHL 7 601**



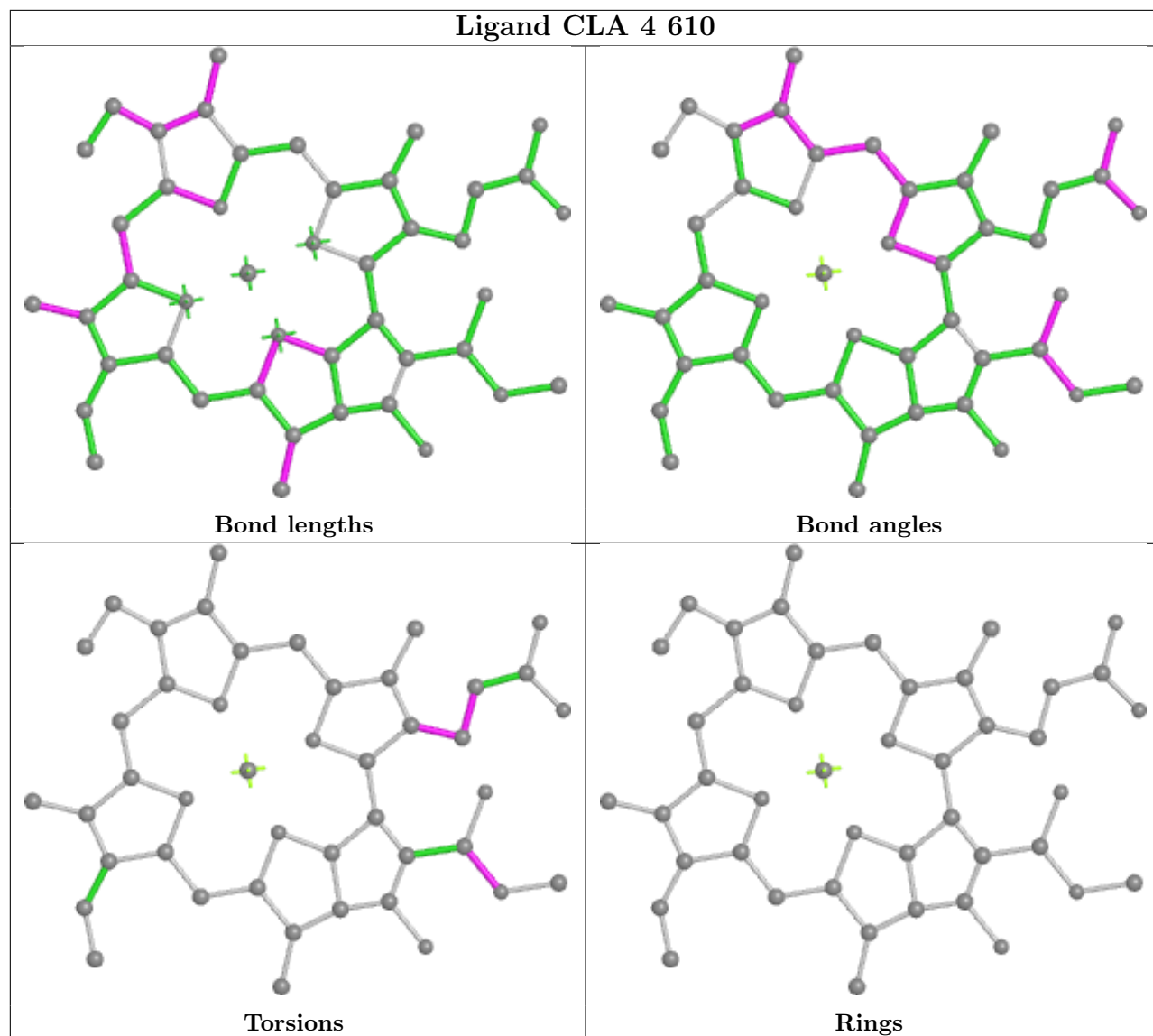
Ligand CLA 7 614



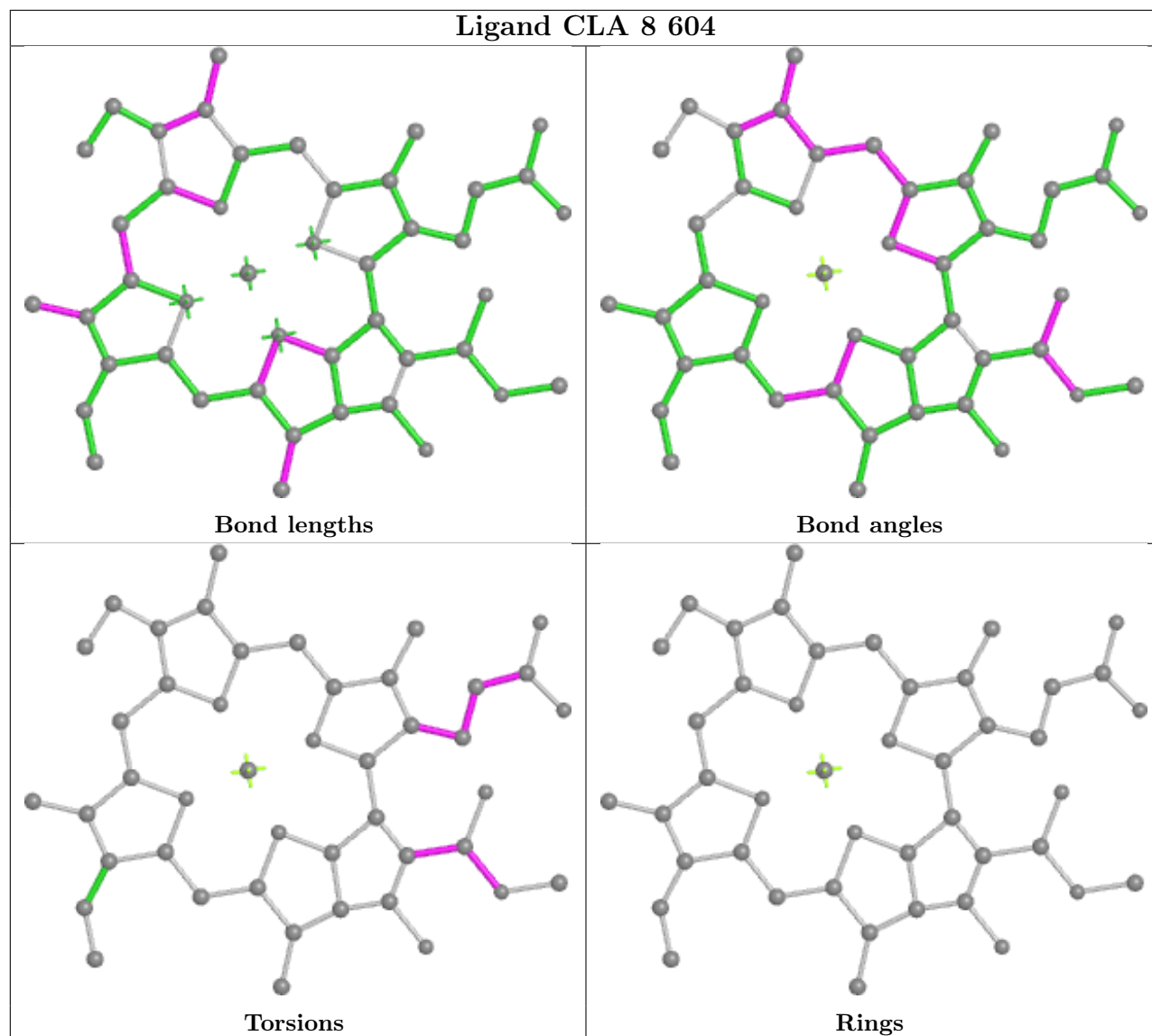
Ligand SQD B 621

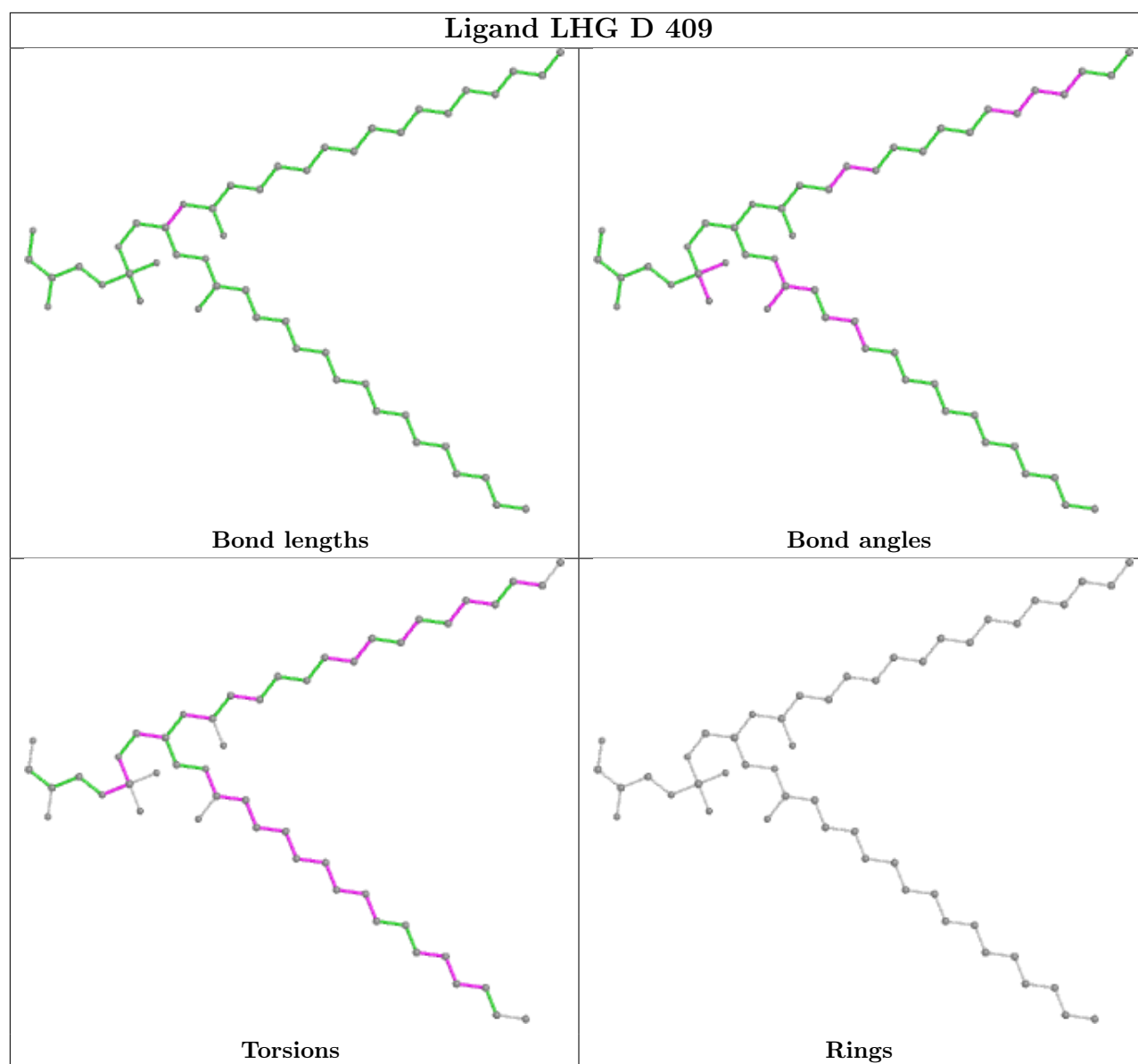


Ligand CLA 4 610

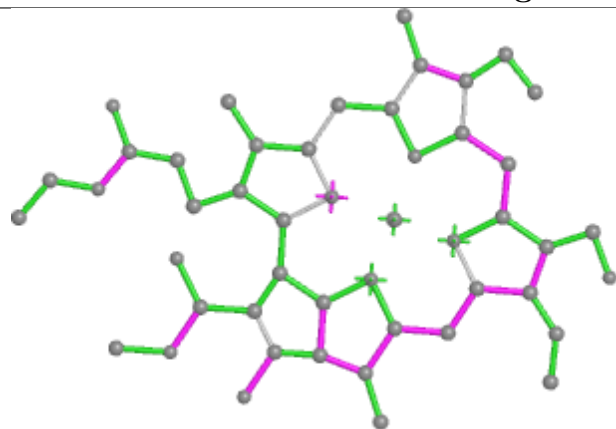


Ligand CLA 8 604

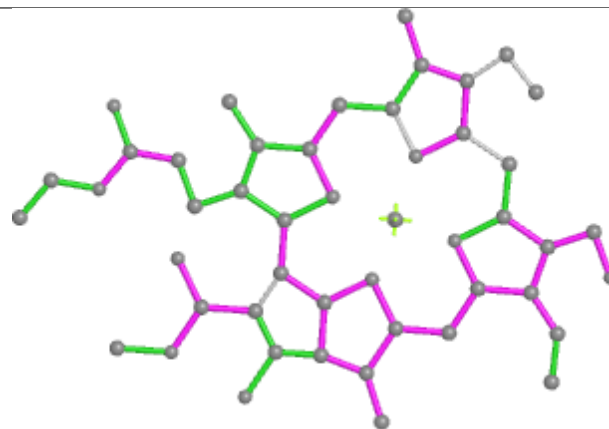




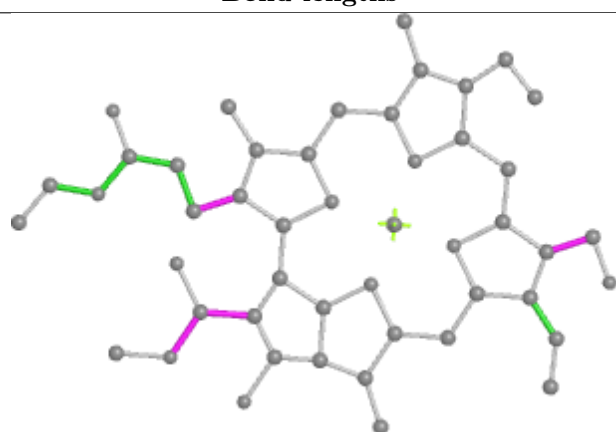
Ligand CHL N 605



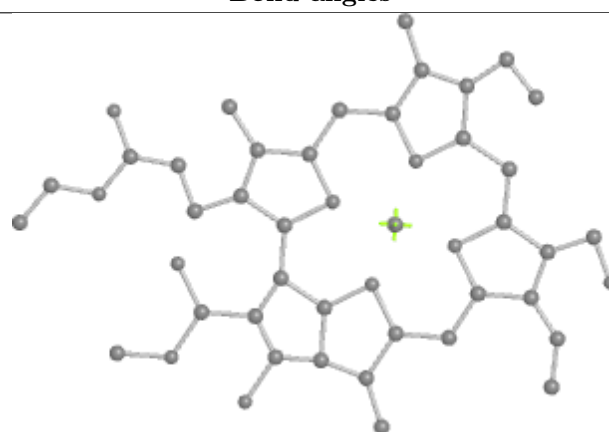
Bond lengths



Bond angles

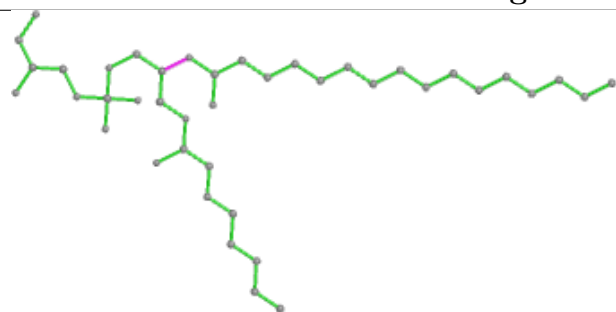


Torsions

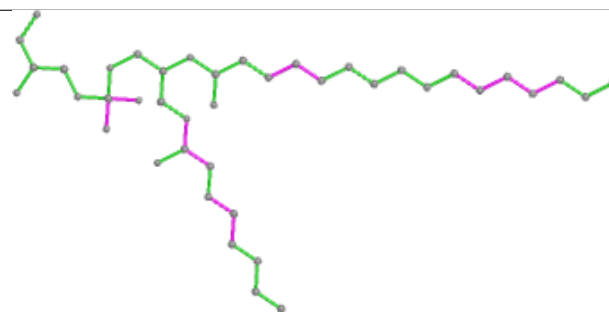


Rings

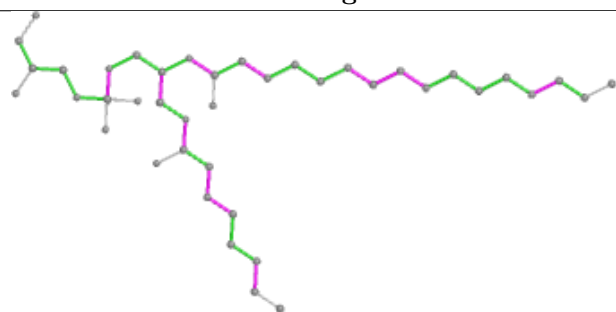
Ligand LHG 5 2630



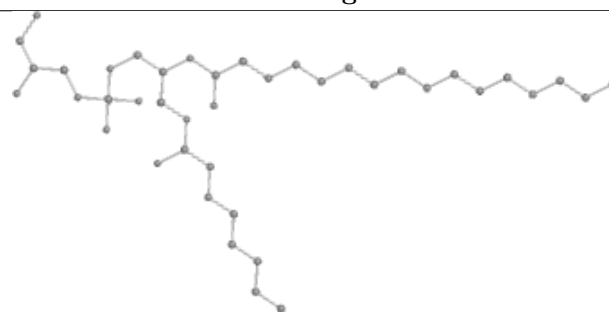
Bond lengths



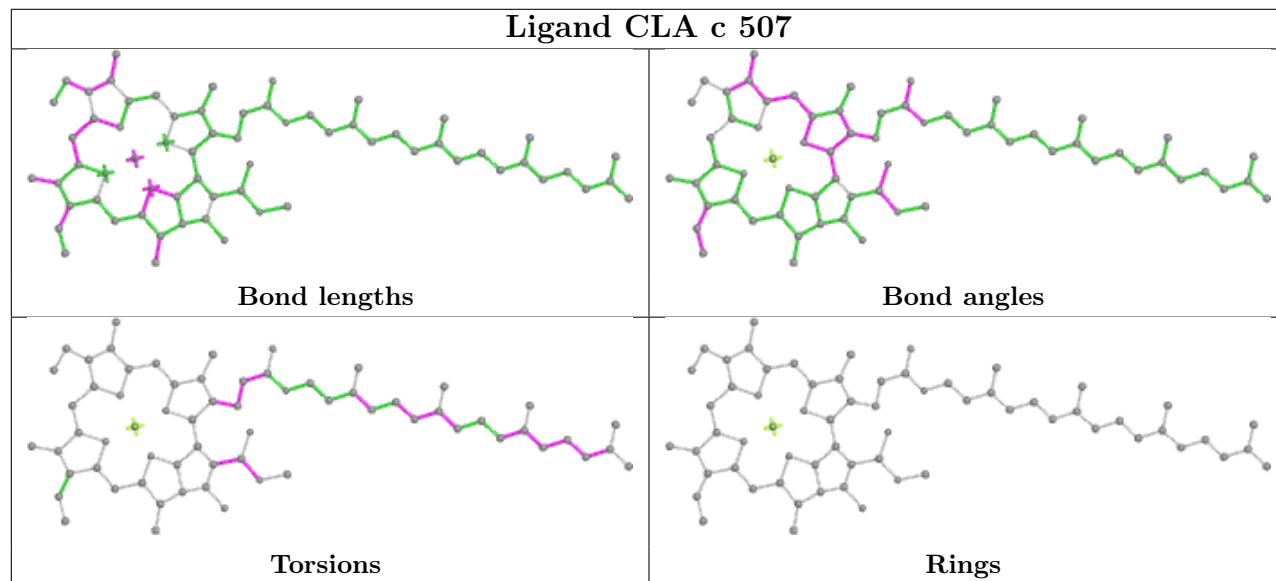
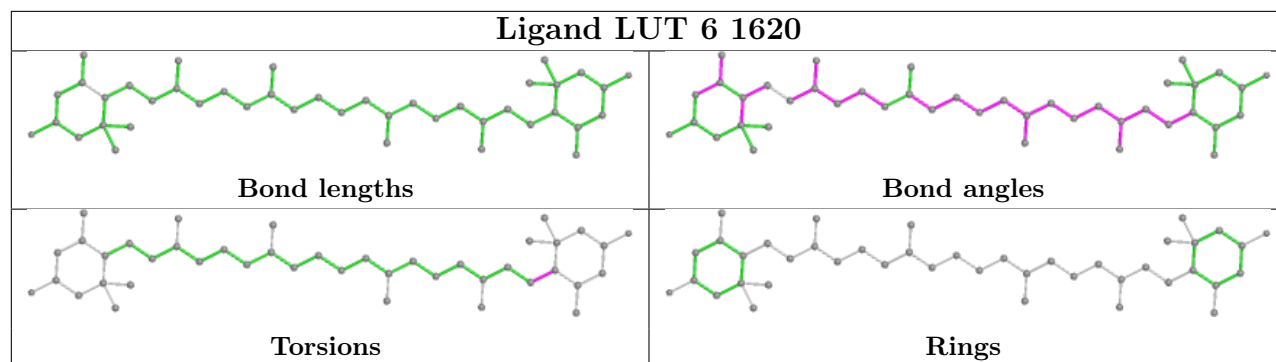
Bond angles



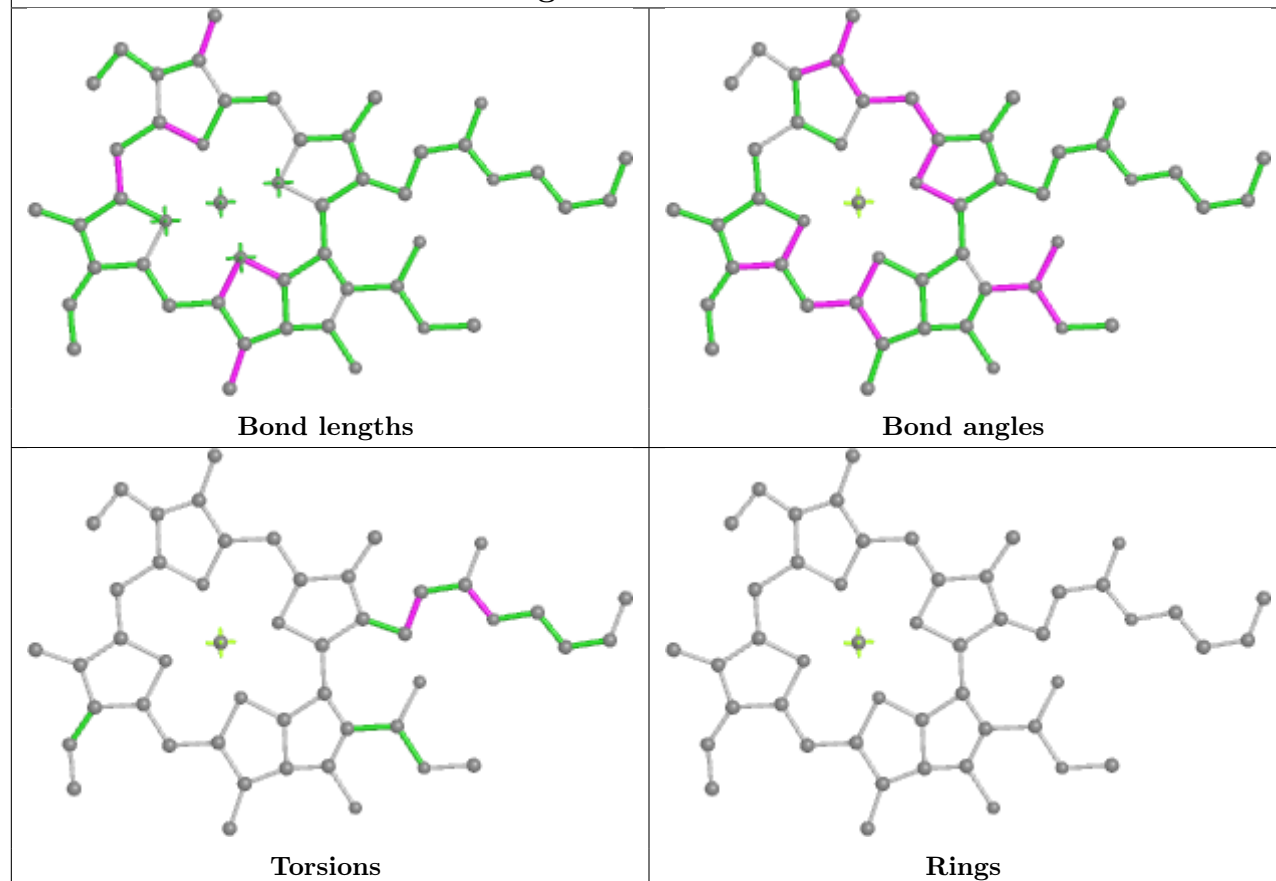
Torsions



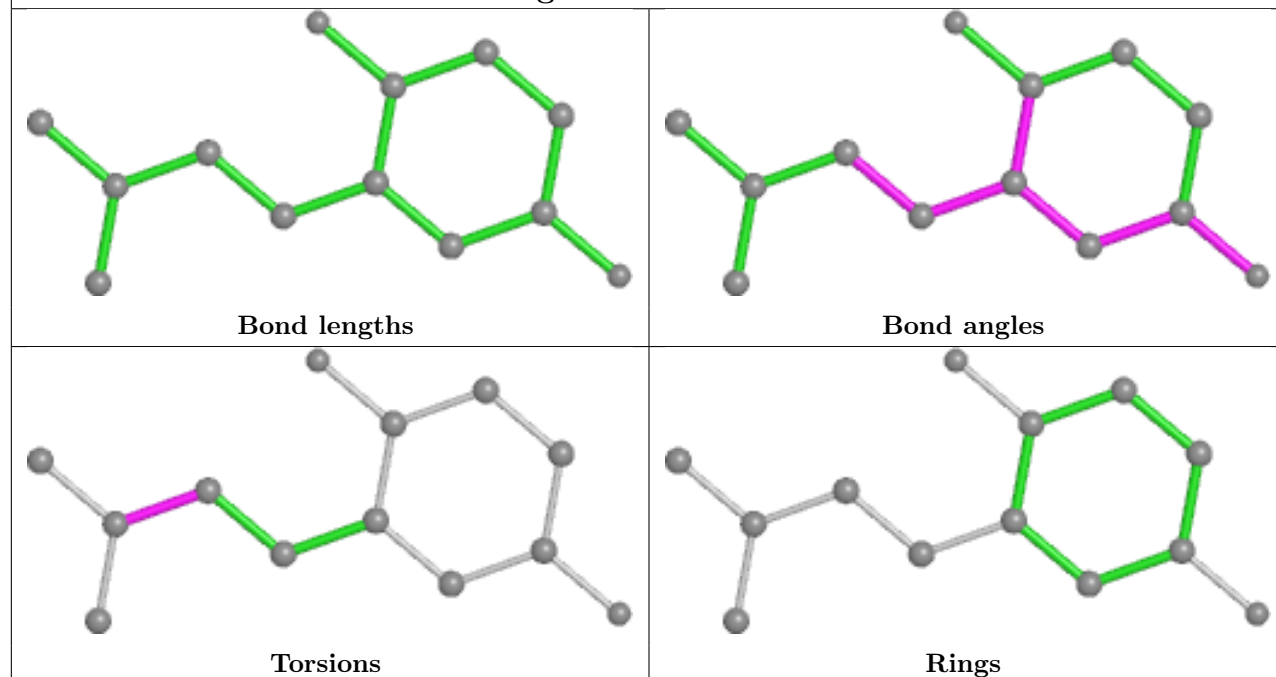
Rings



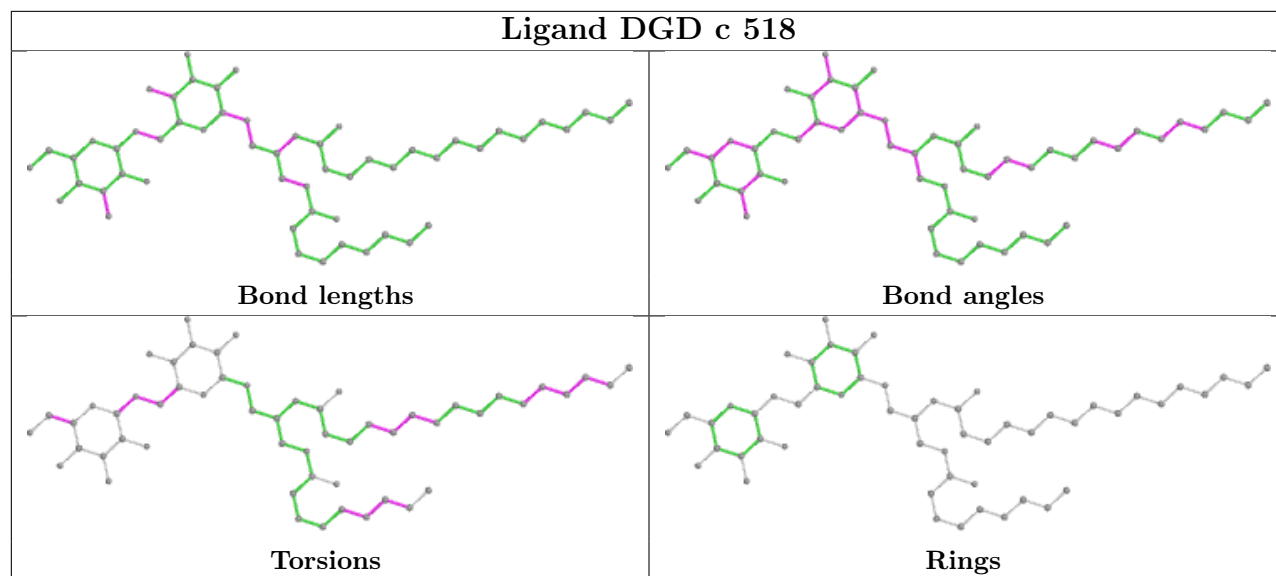
Ligand CLA s 614



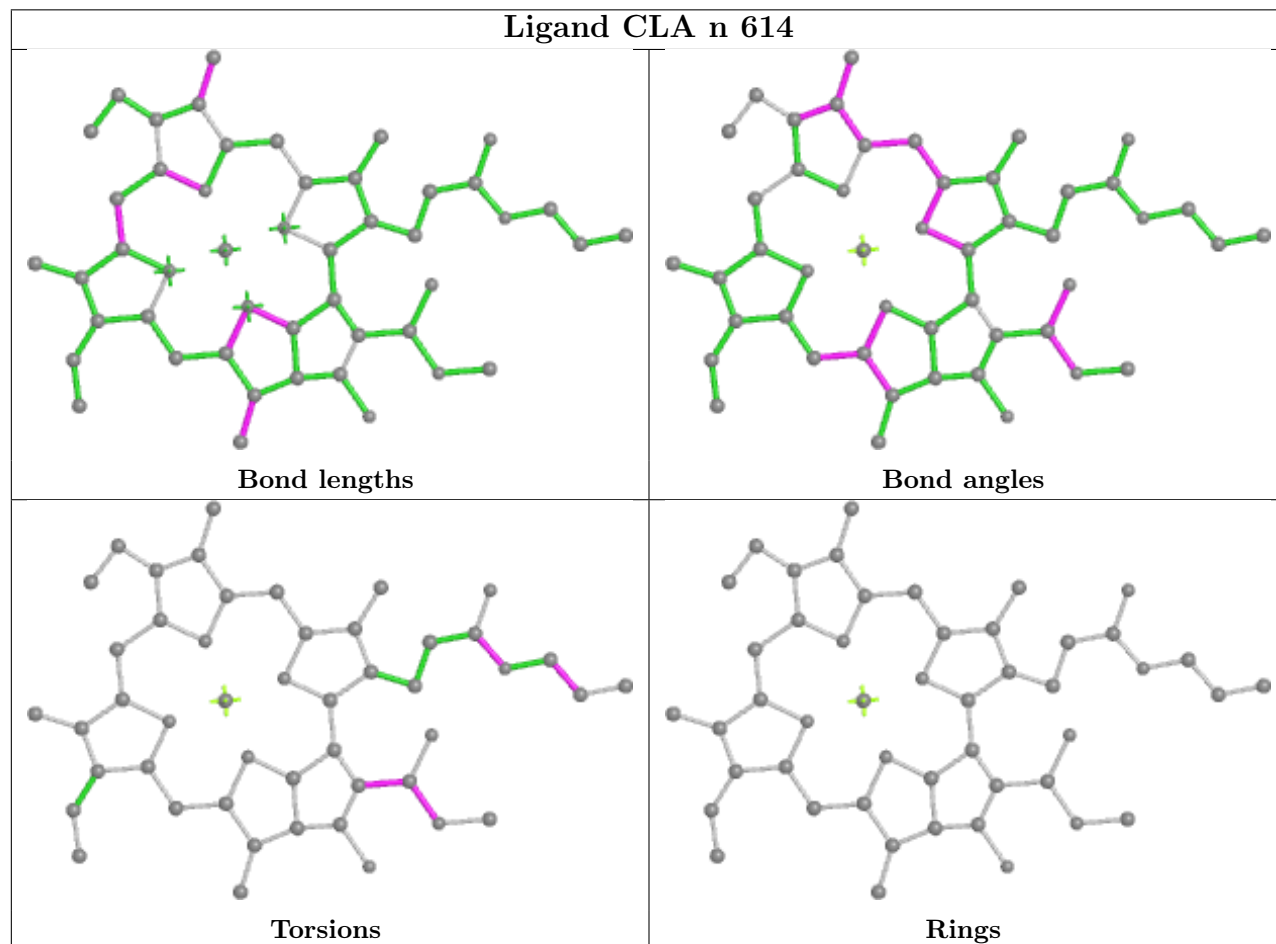
Ligand PL9 A 414

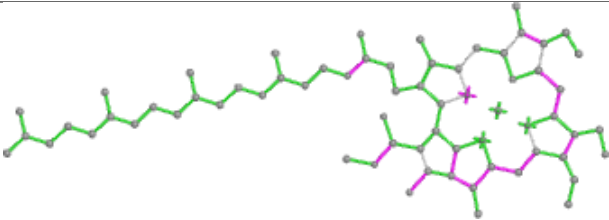
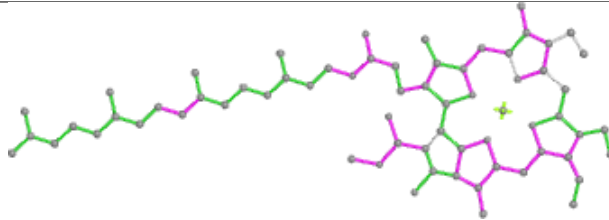
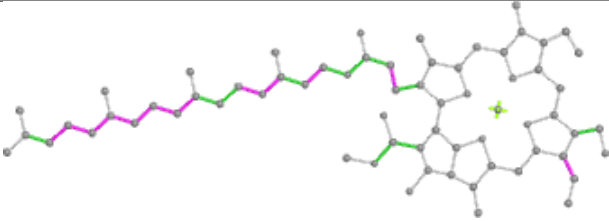
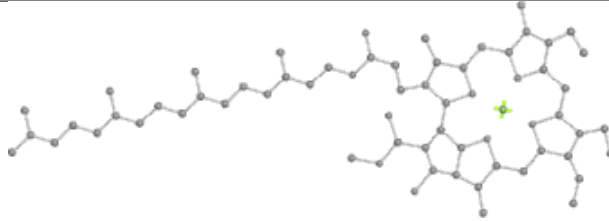
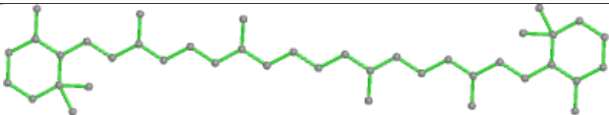
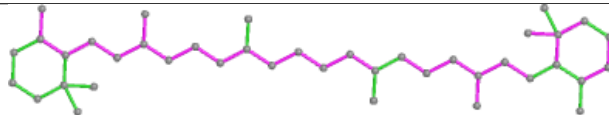
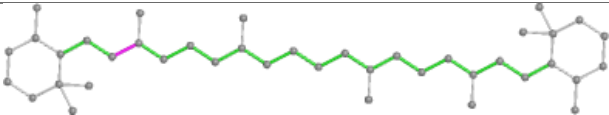
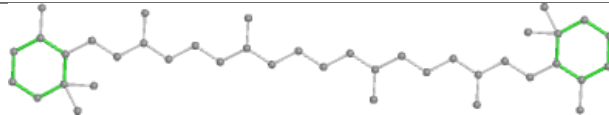


Ligand DGD c 518

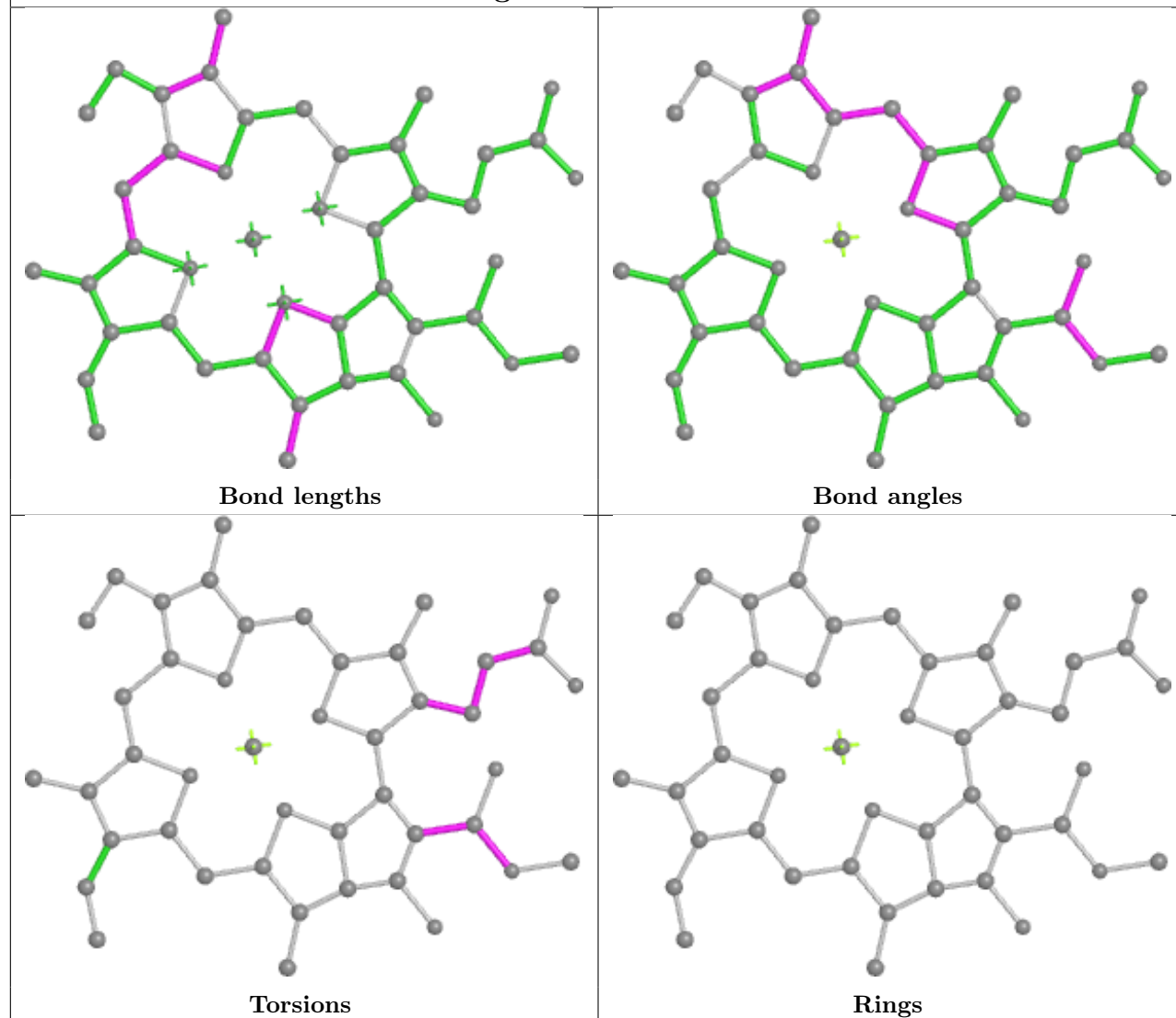


Ligand CLA n 614

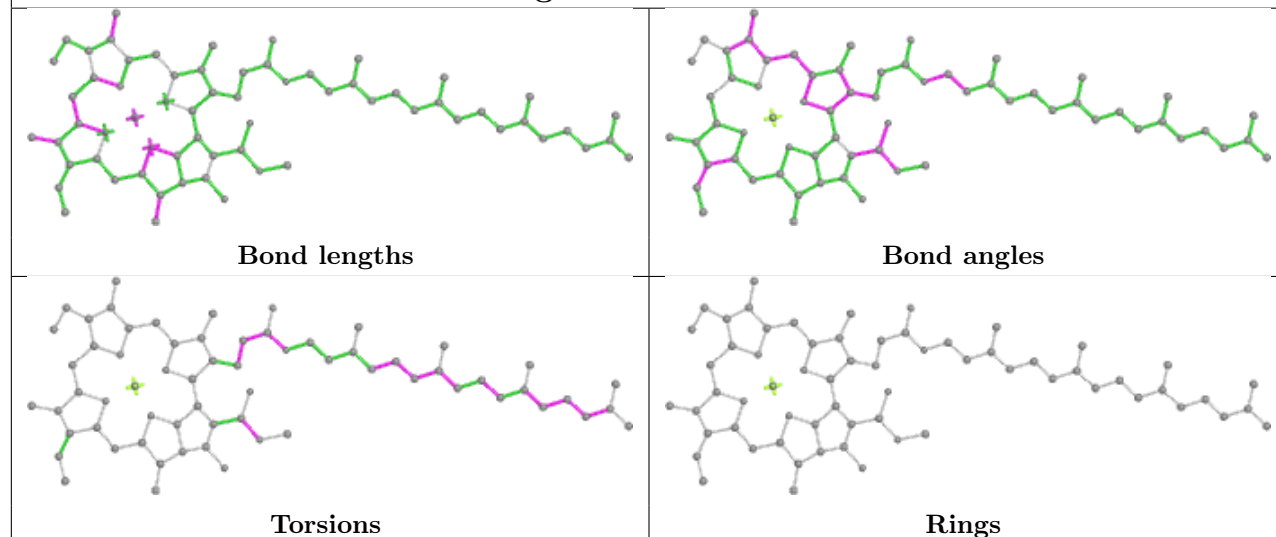


Ligand CHL G 607	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

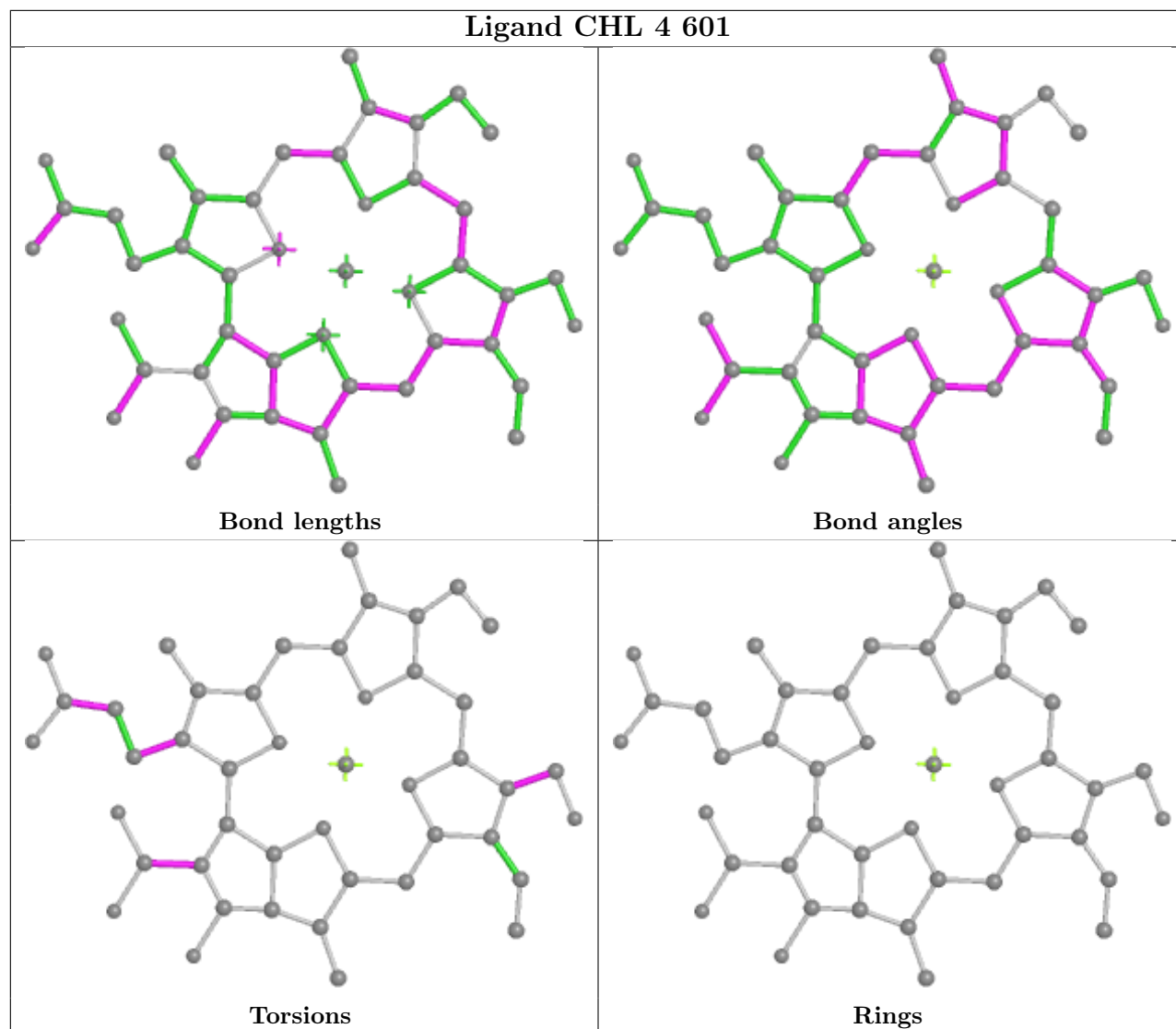
Ligand CLA 2 604

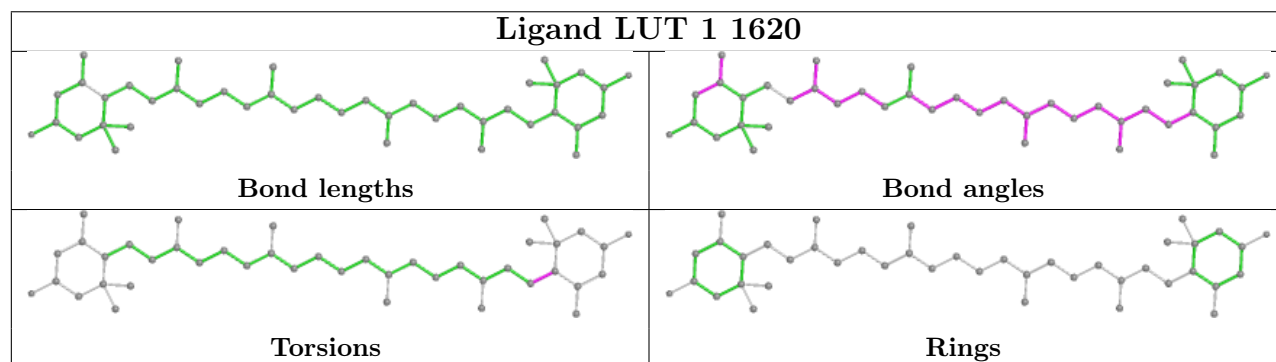
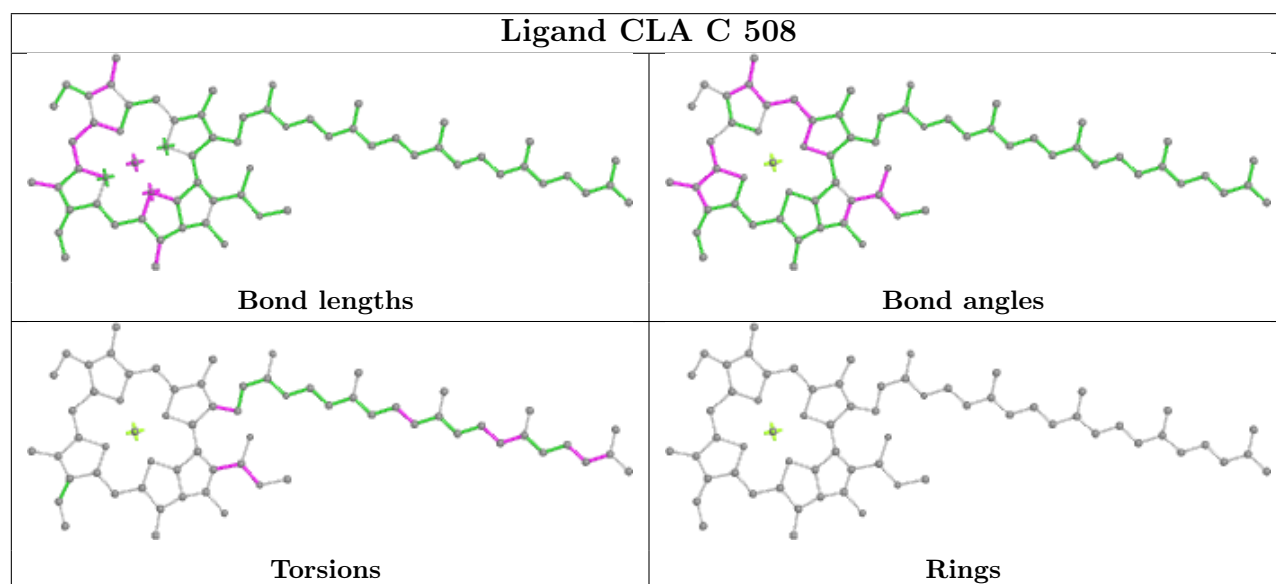
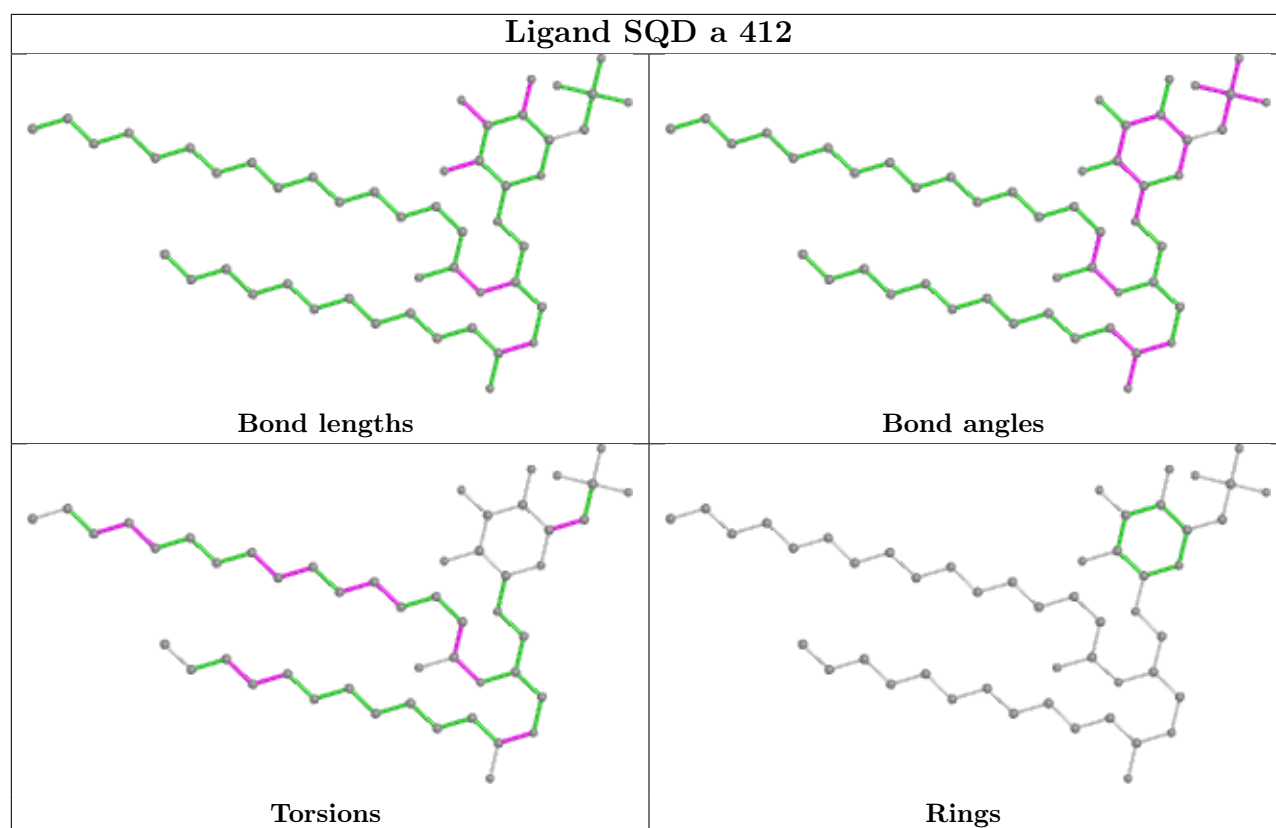


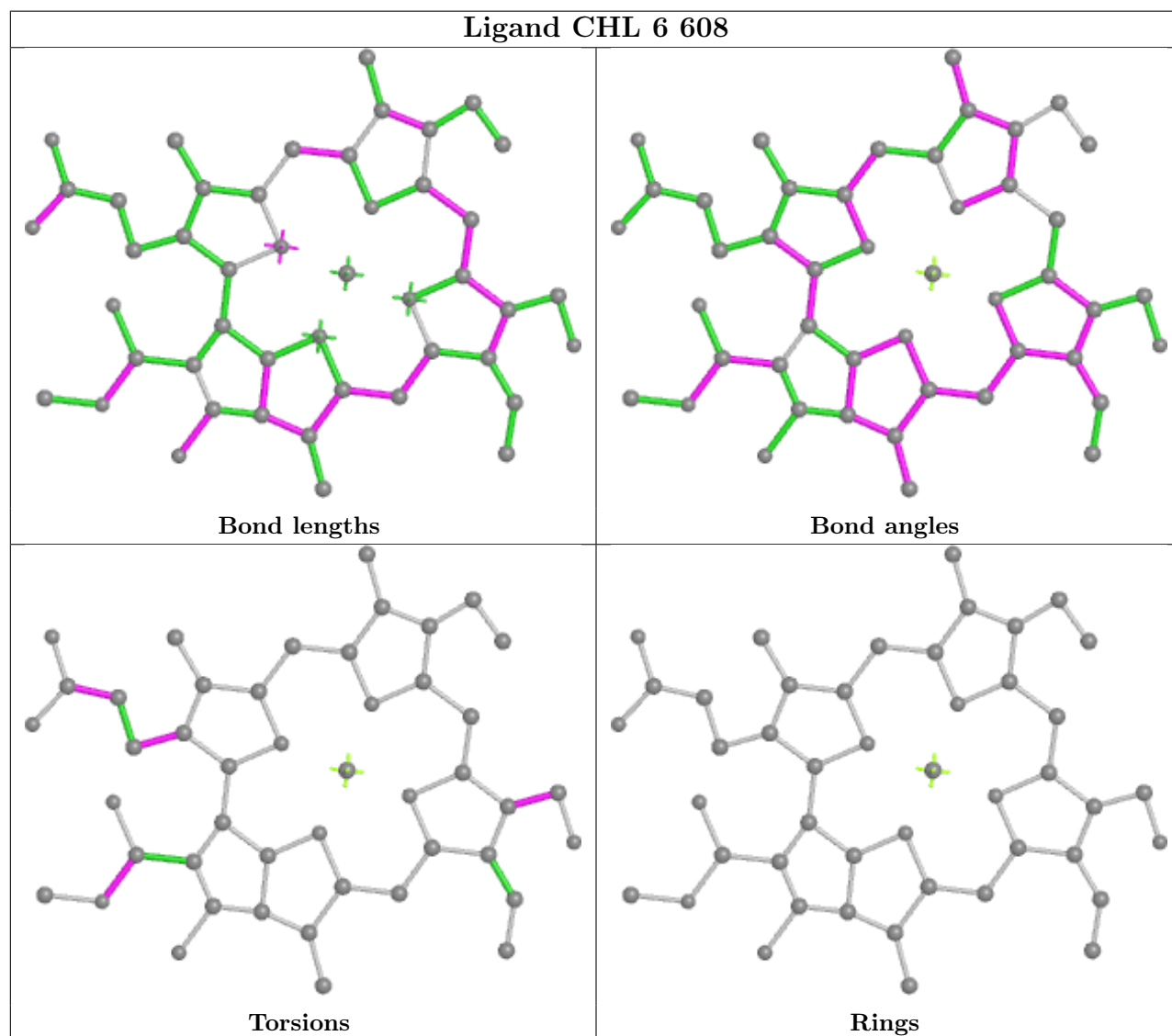
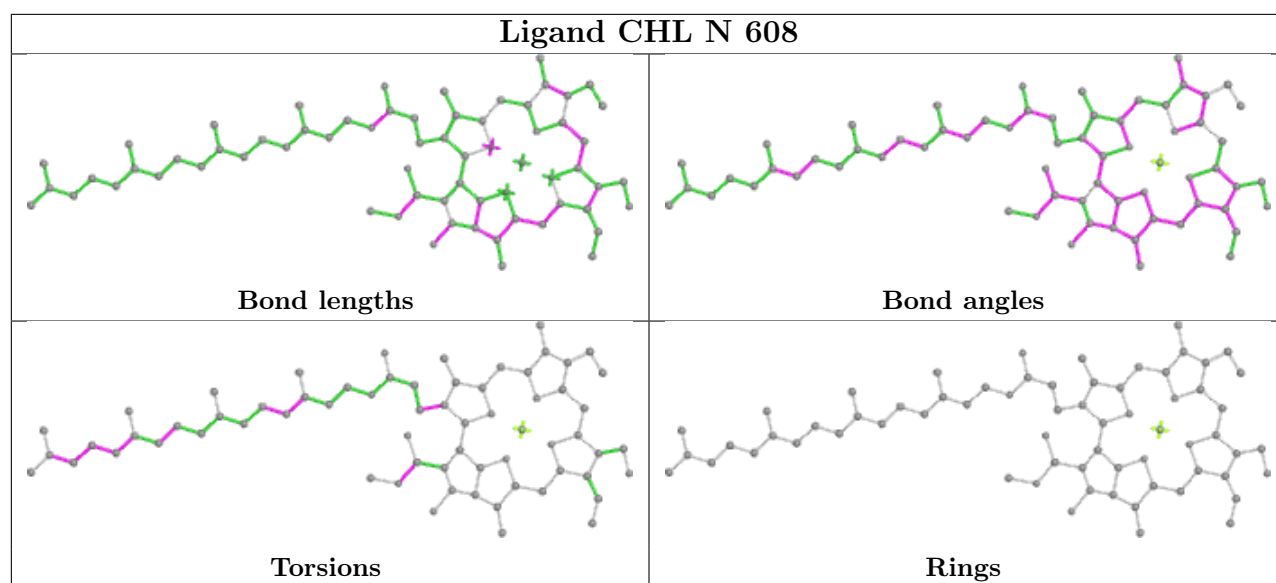
Ligand CLA b 617



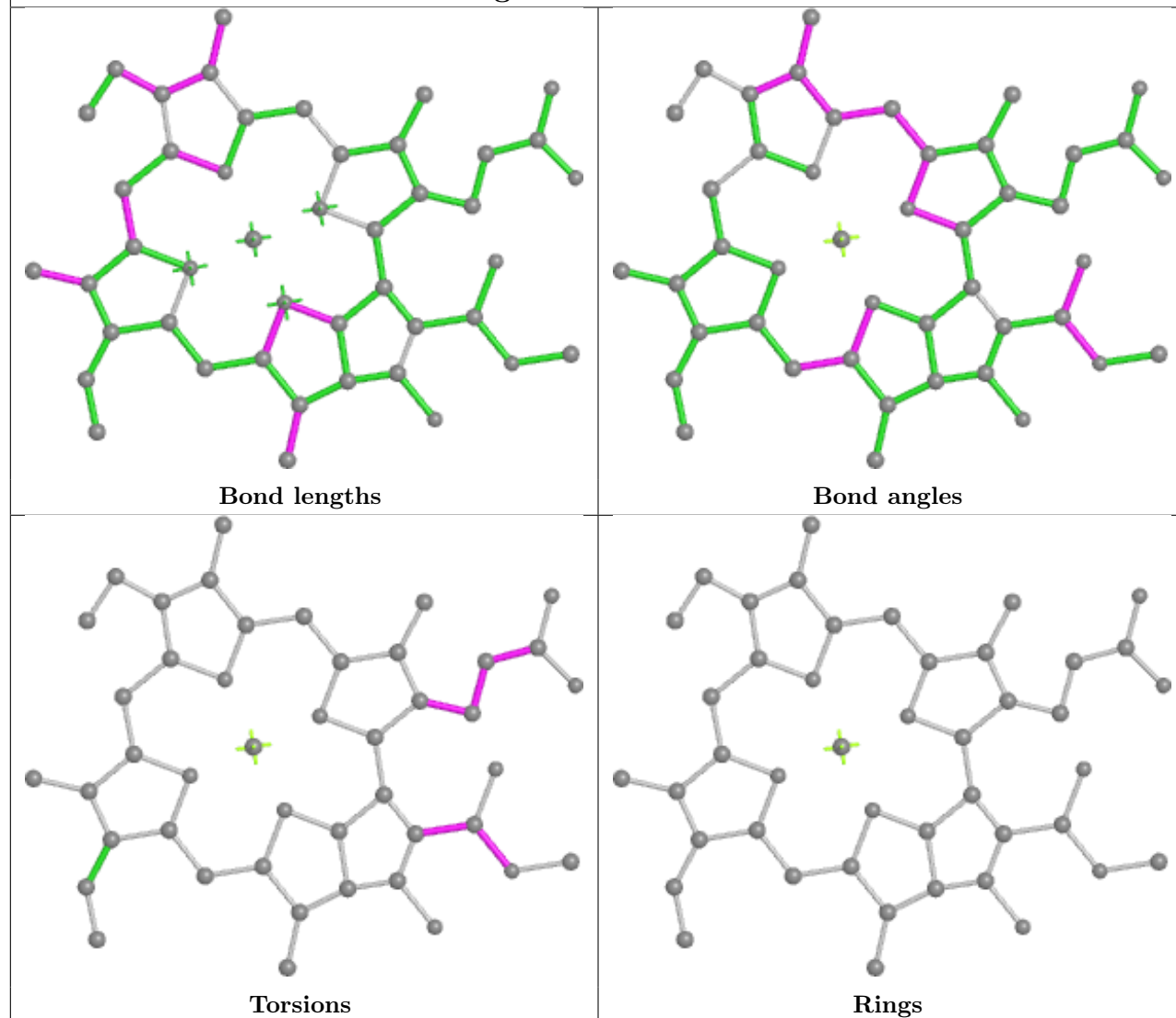
Ligand CHL 4 601



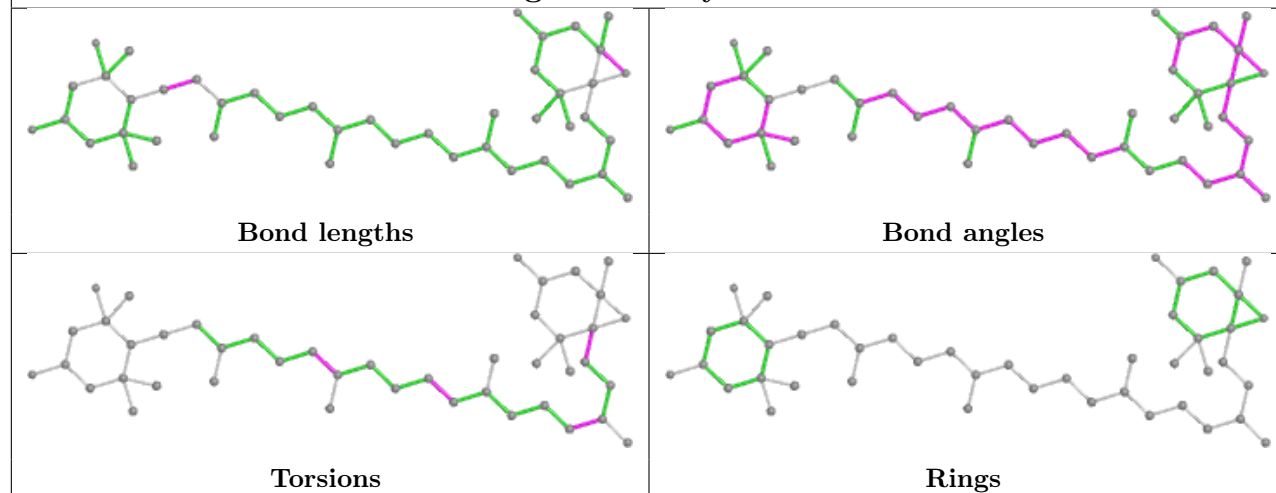




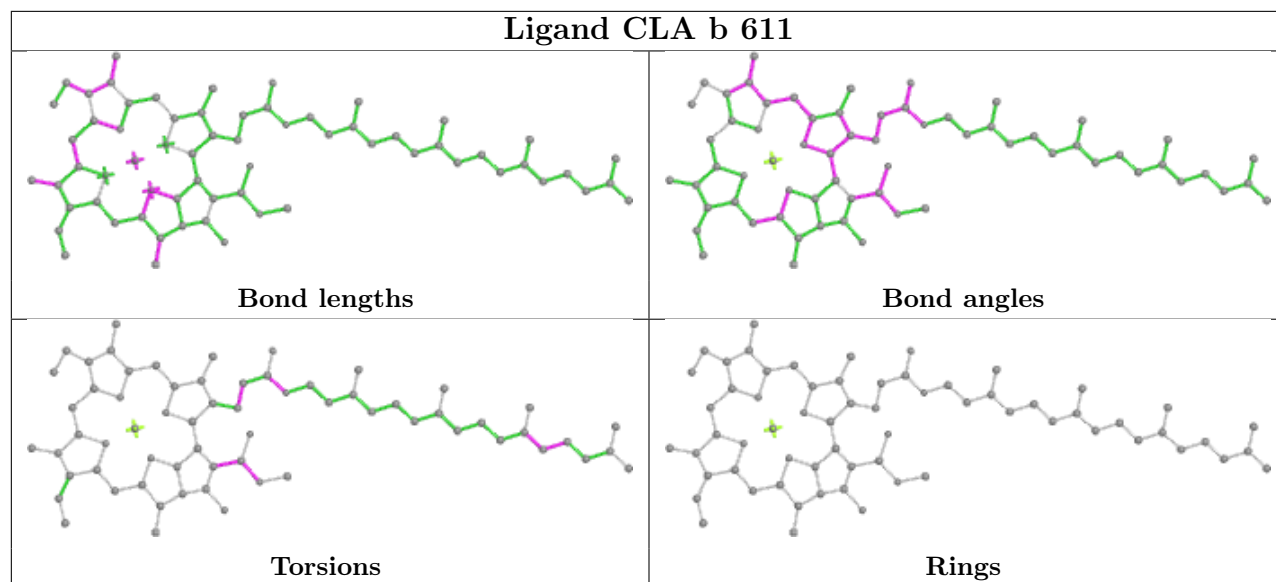
Ligand CLA 7 604



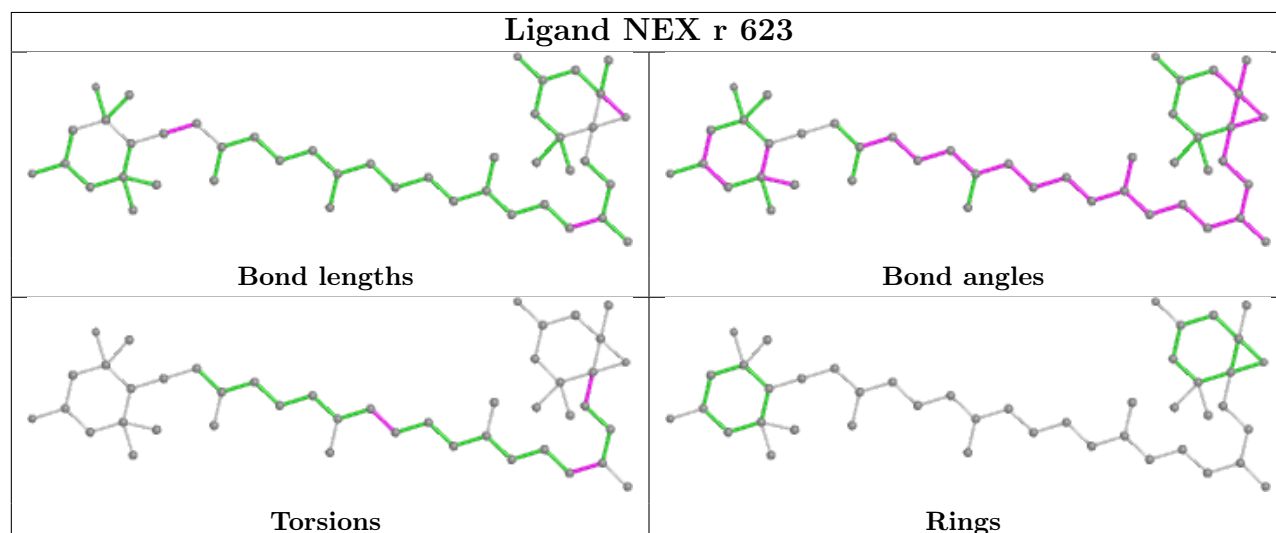
Ligand NEX y 1623



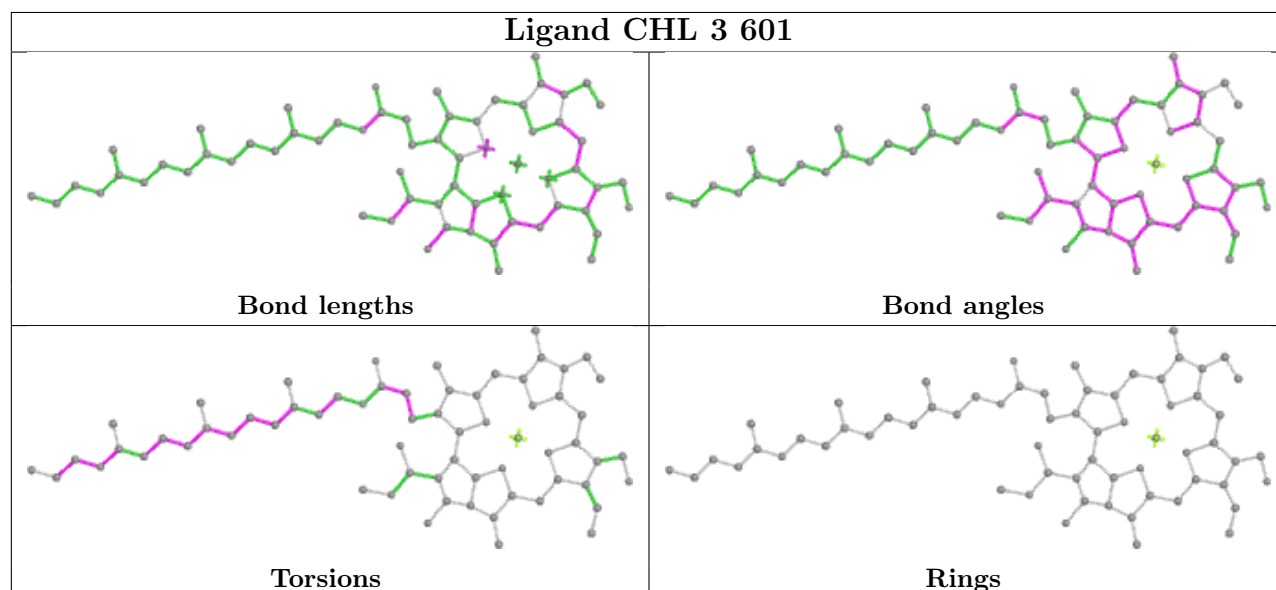
Ligand CLA b 611



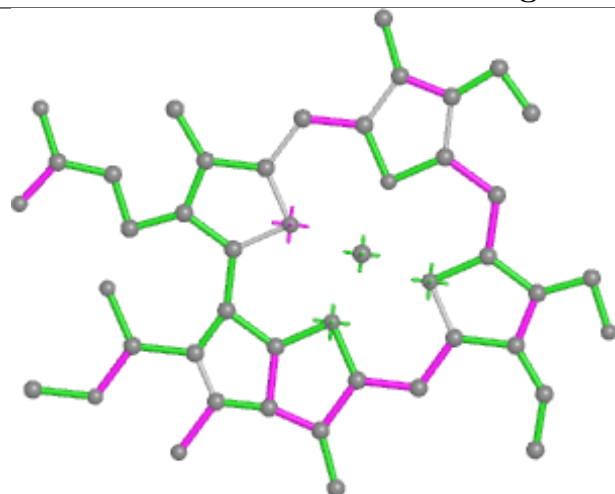
Ligand NEX r 623



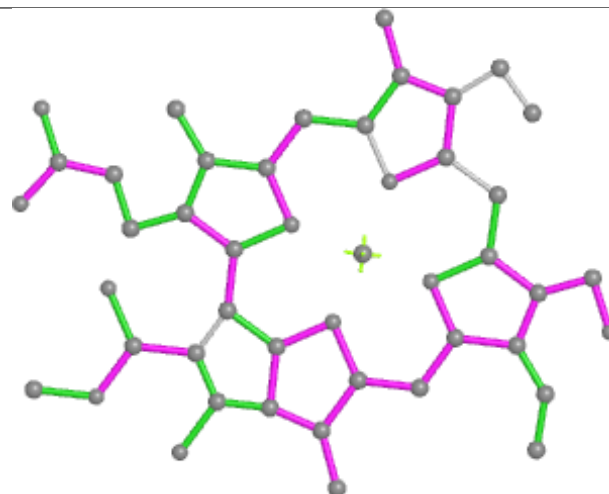
Ligand CHL 3 601



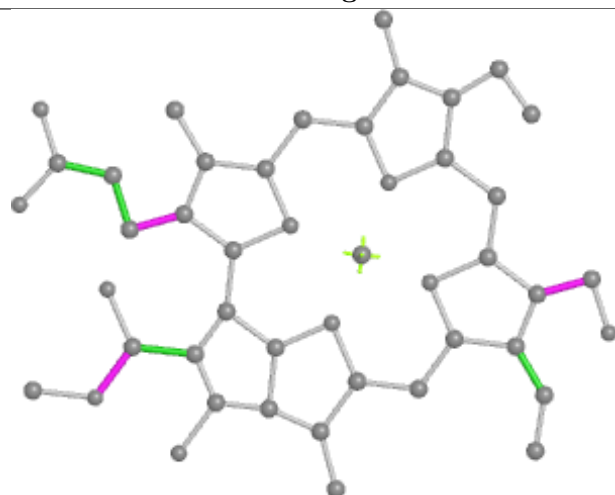
Ligand CHL 8 608



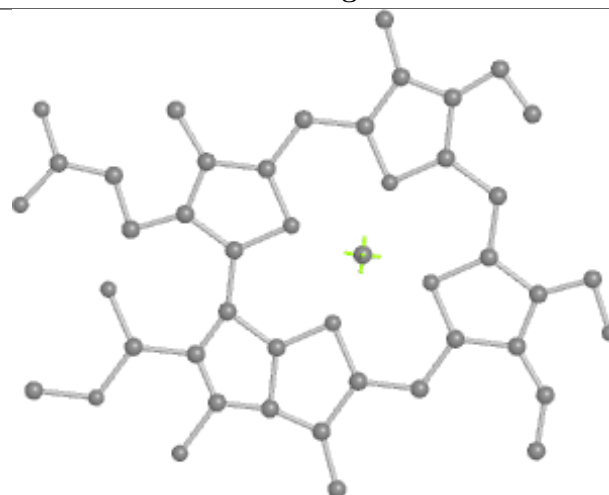
Bond lengths



Bond angles

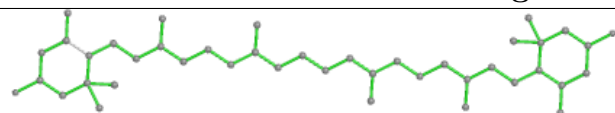


Torsions

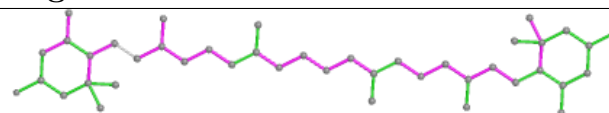


Rings

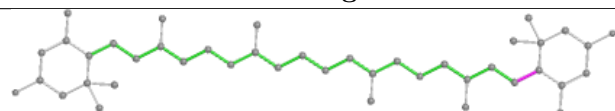
Ligand LUT g 1620



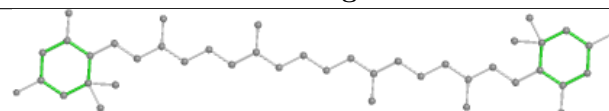
Bond lengths



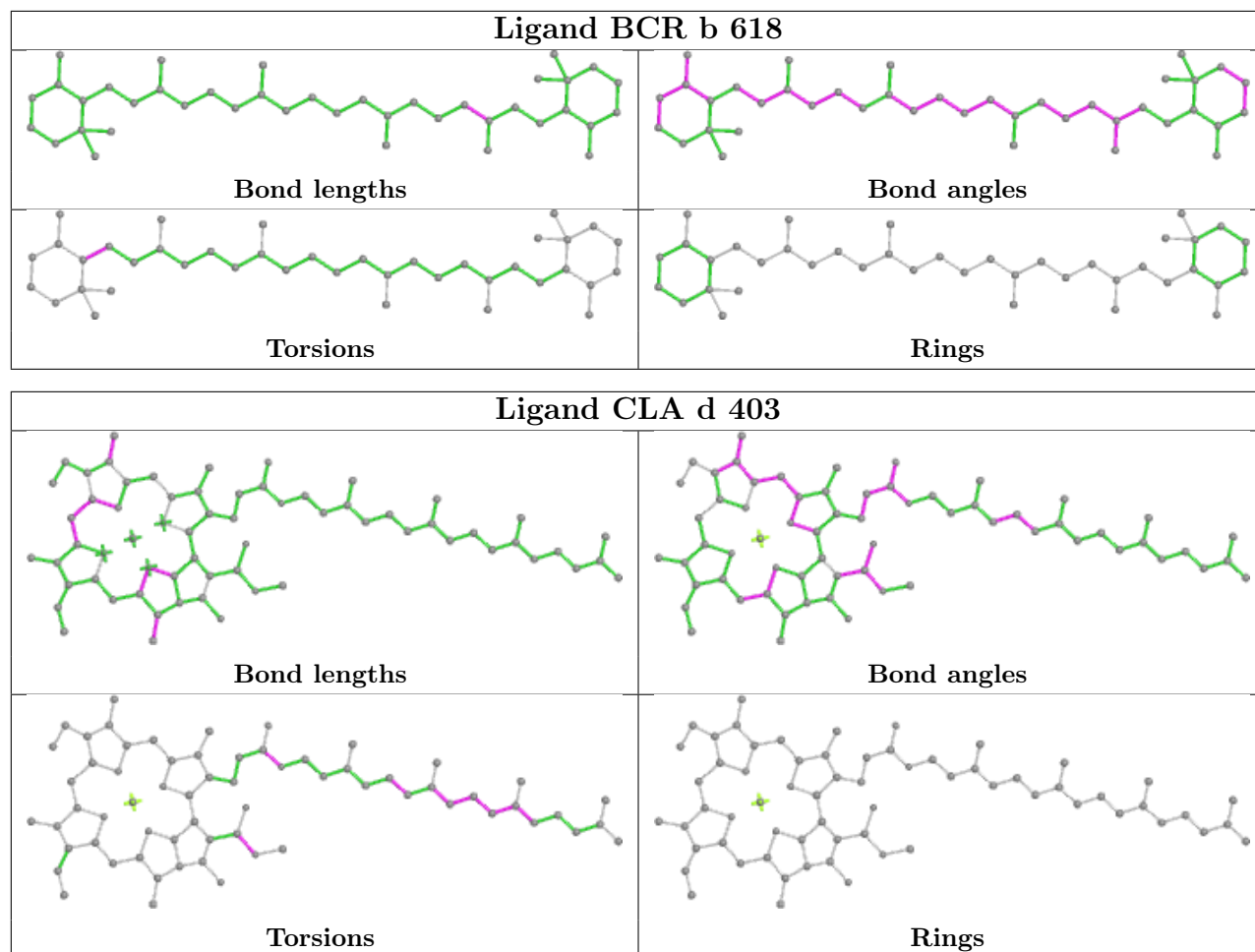
Bond angles



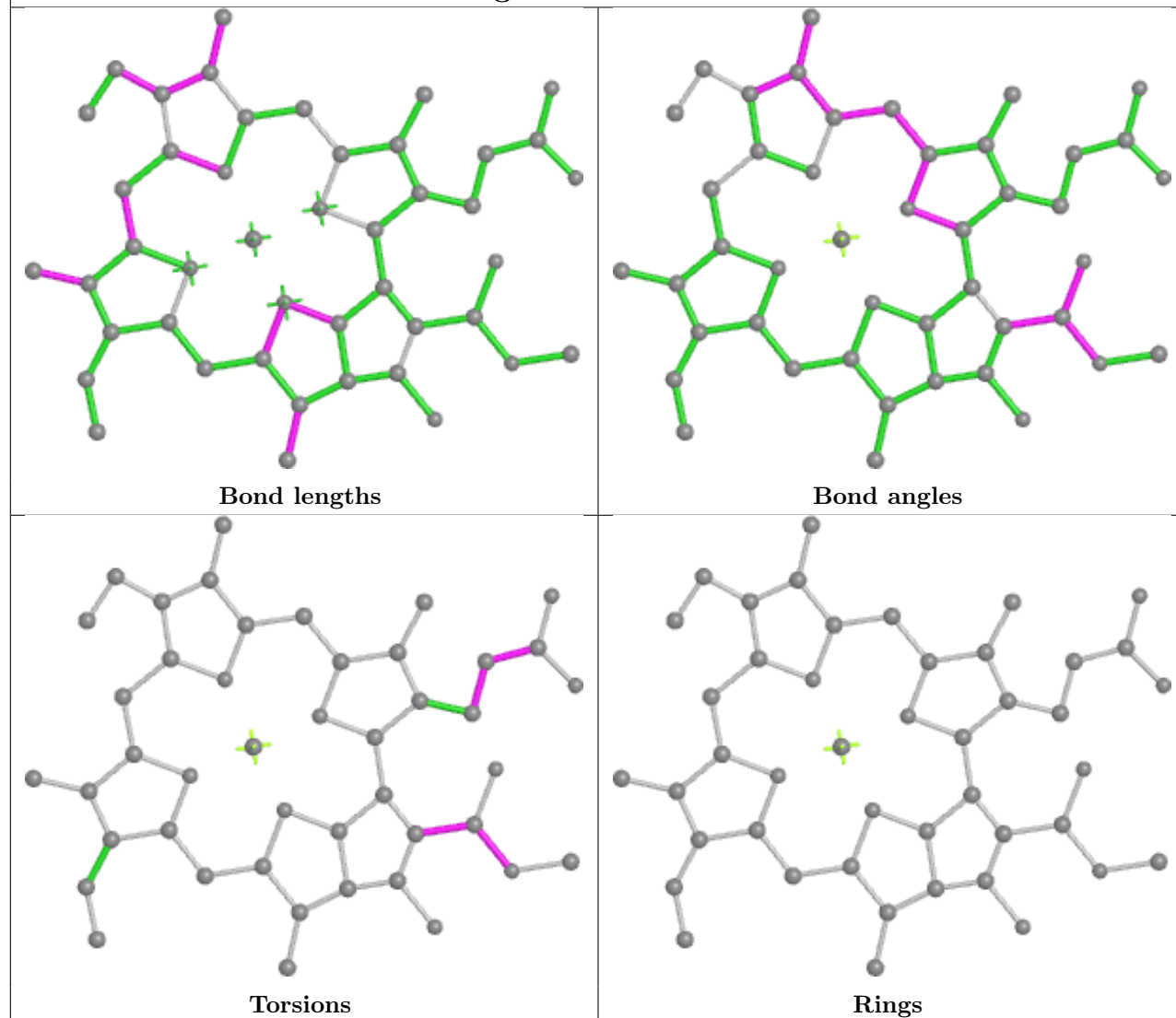
Torsions



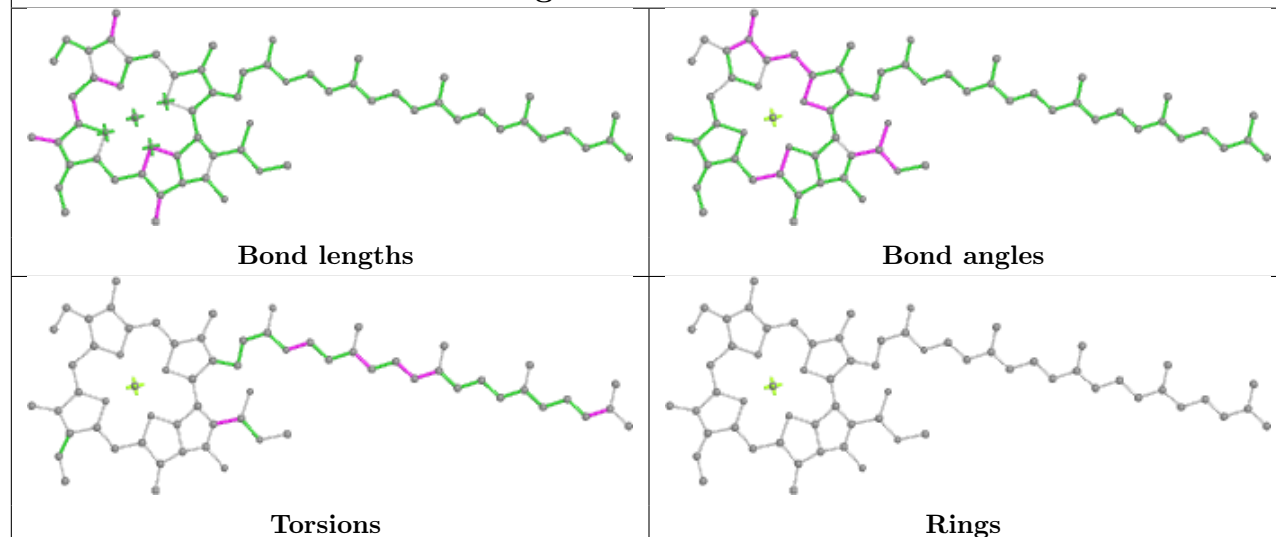
Rings

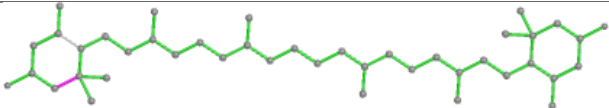
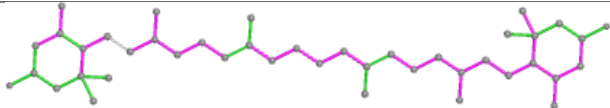
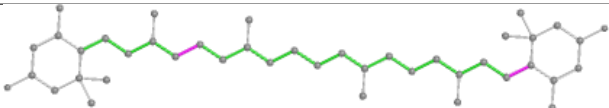
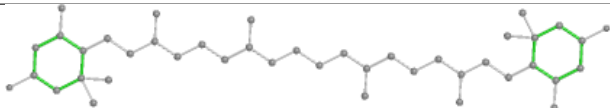


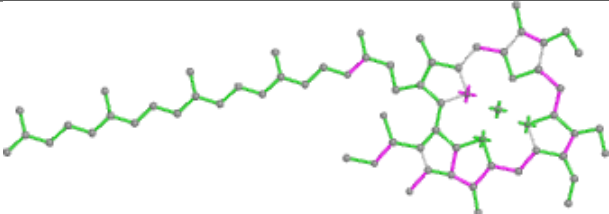
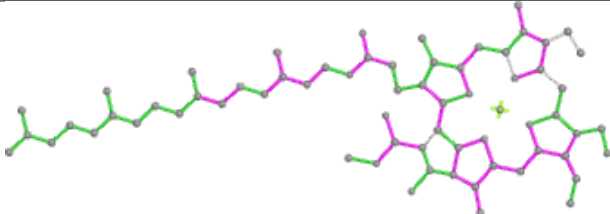
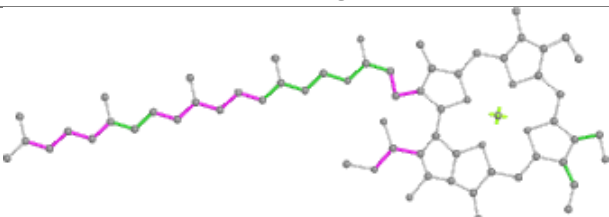
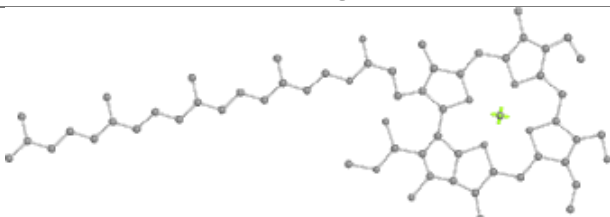
Ligand CLA 4 602

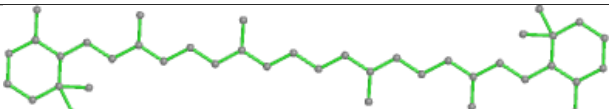
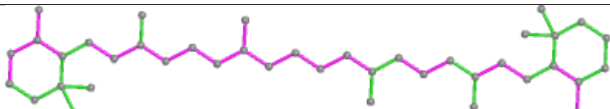
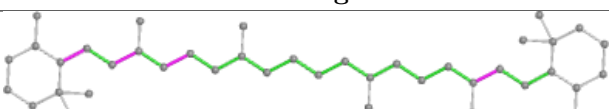



Ligand CLA b 603

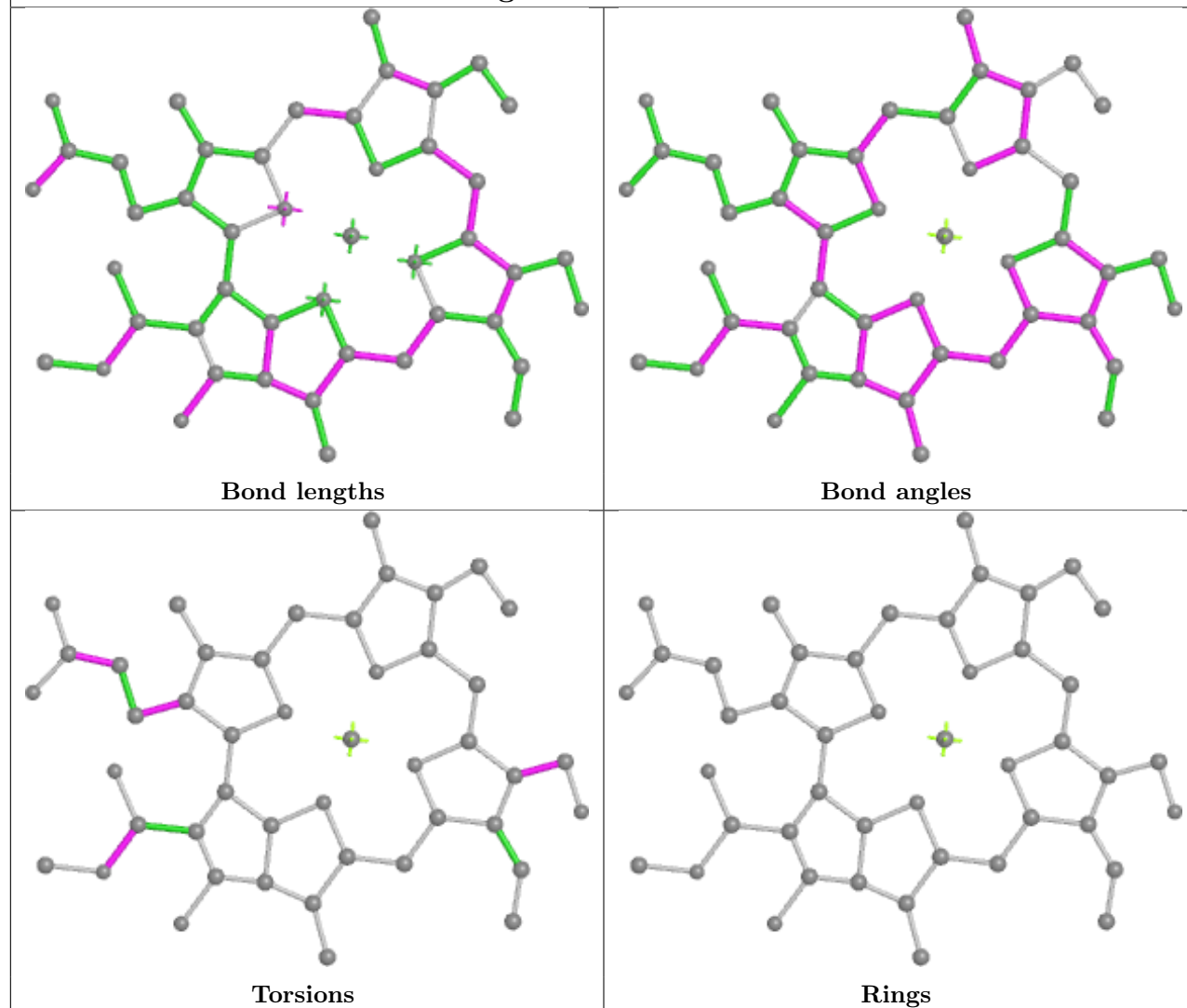


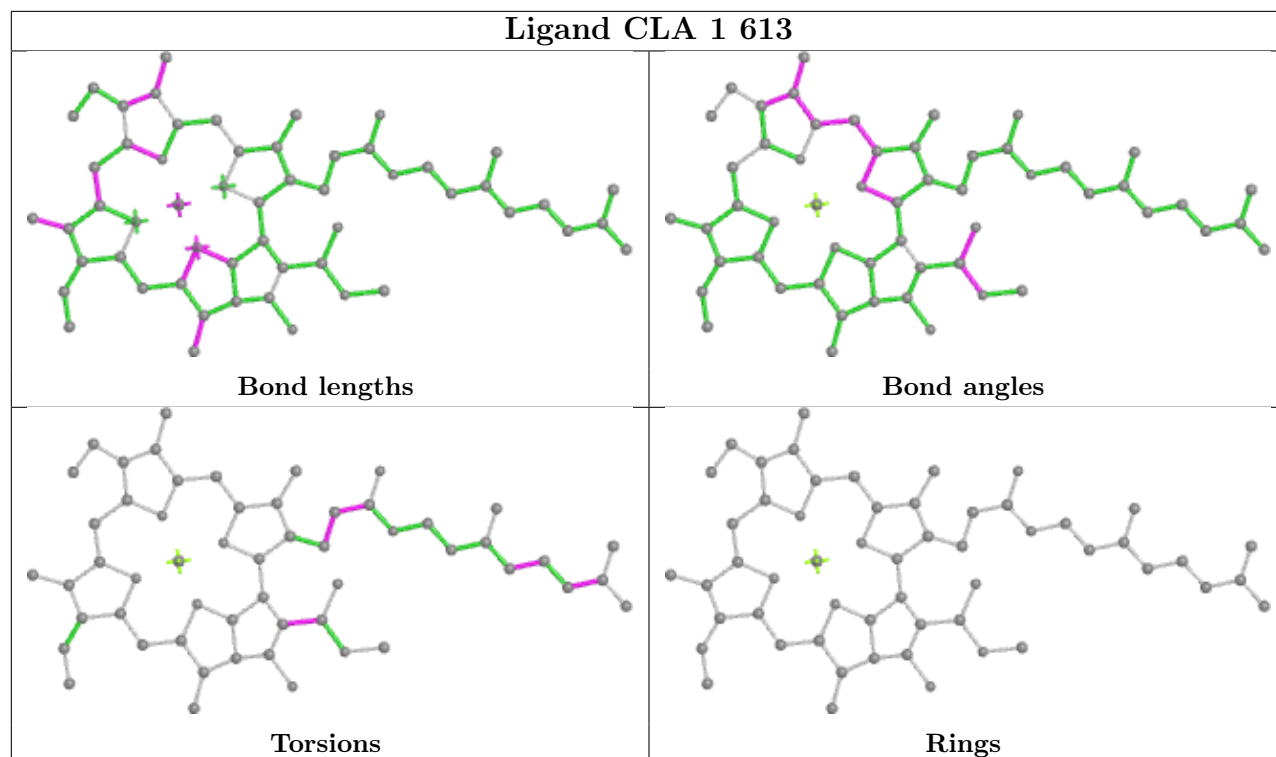
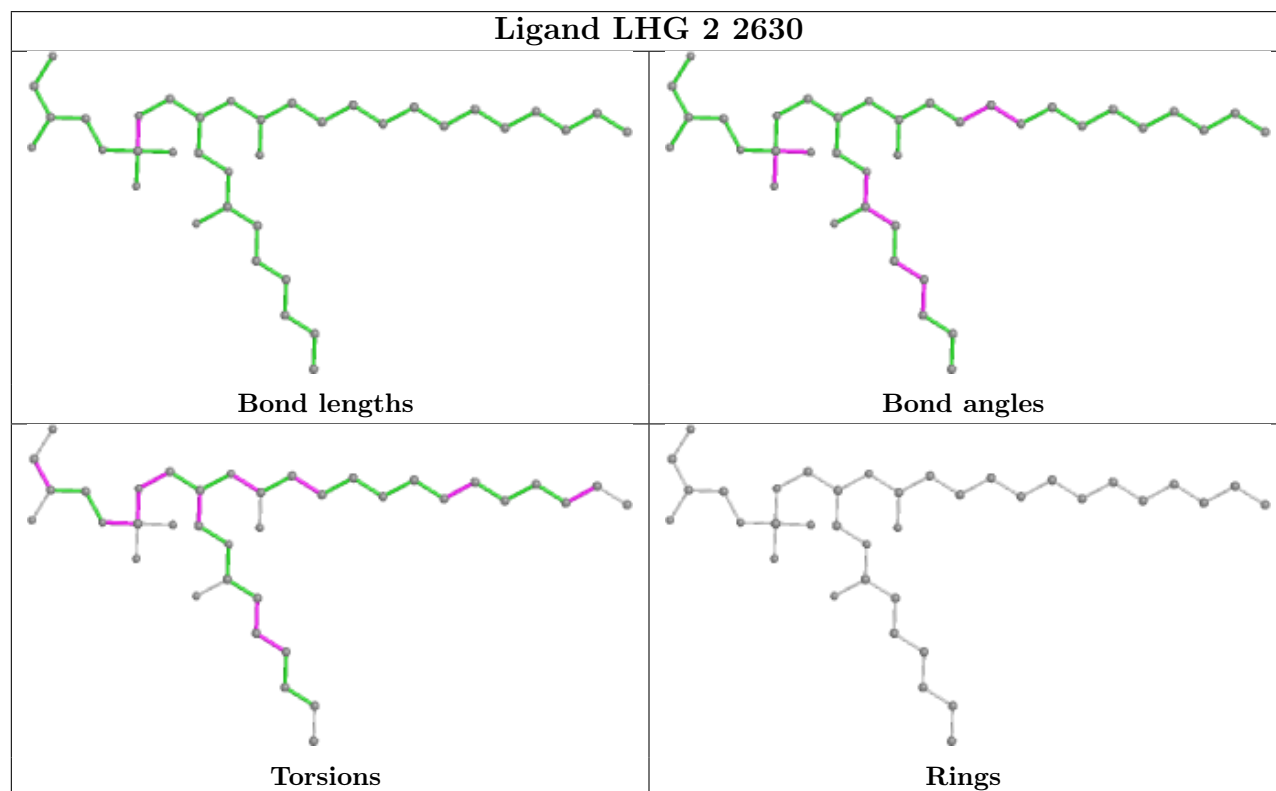
Ligand LUT 6 1621	
	
Bond lengths	Bond angles
	
Torsions	Rings

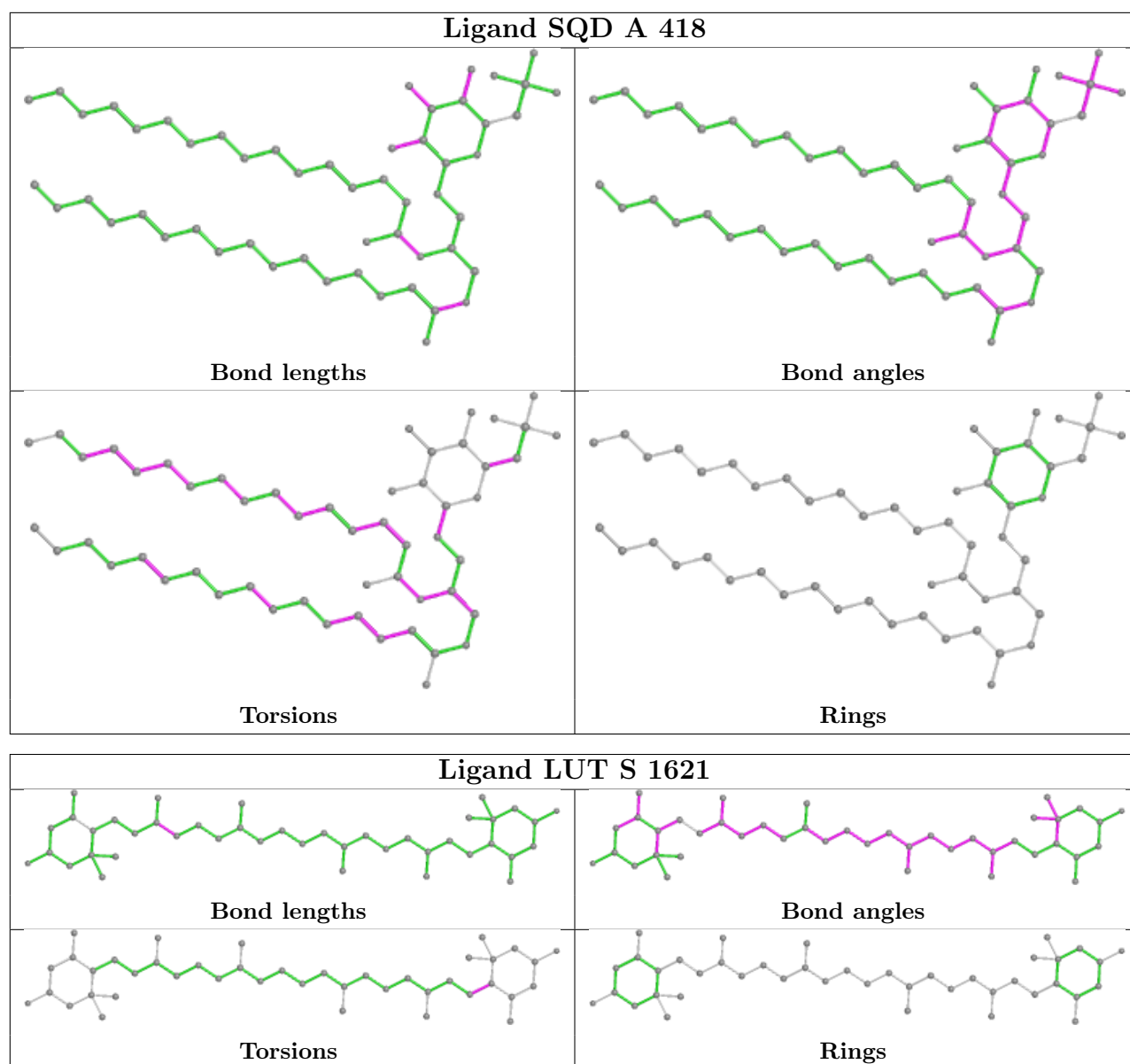
Ligand CHL r 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

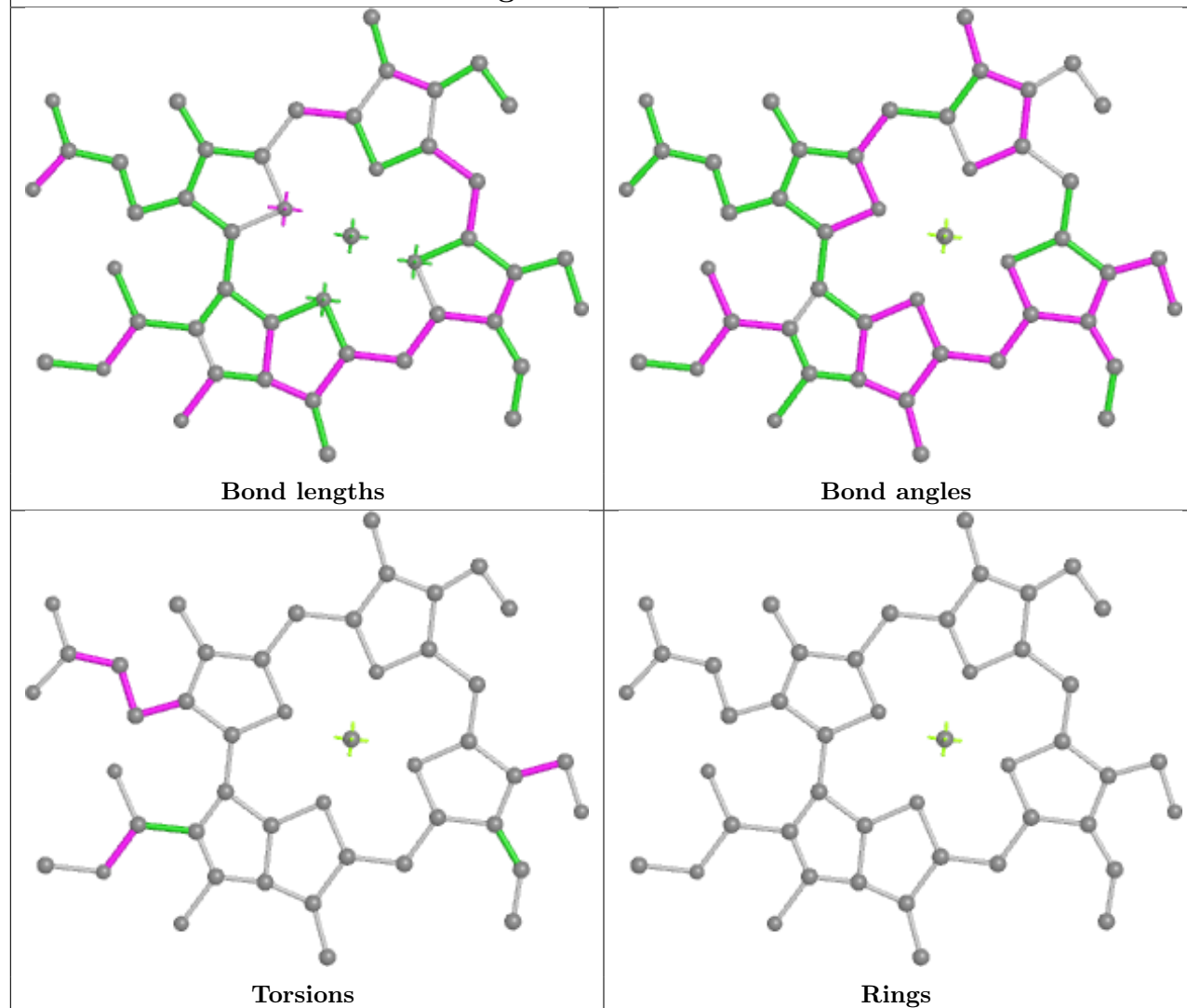
Ligand CHL 2 608



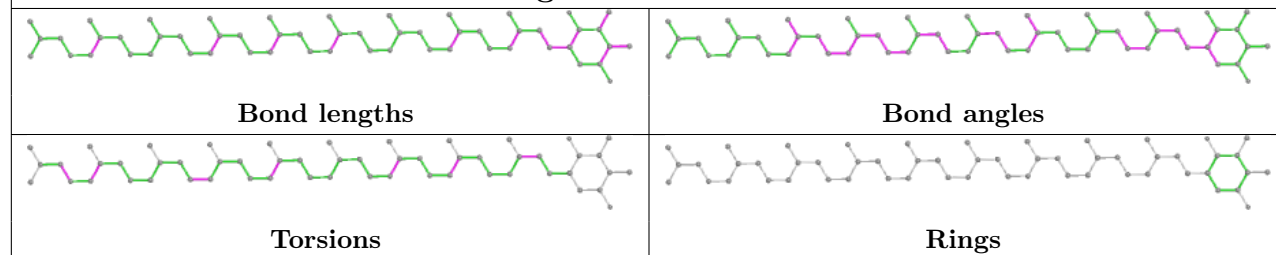
Ligand CLA 1 613**Ligand LHG 2 2630**



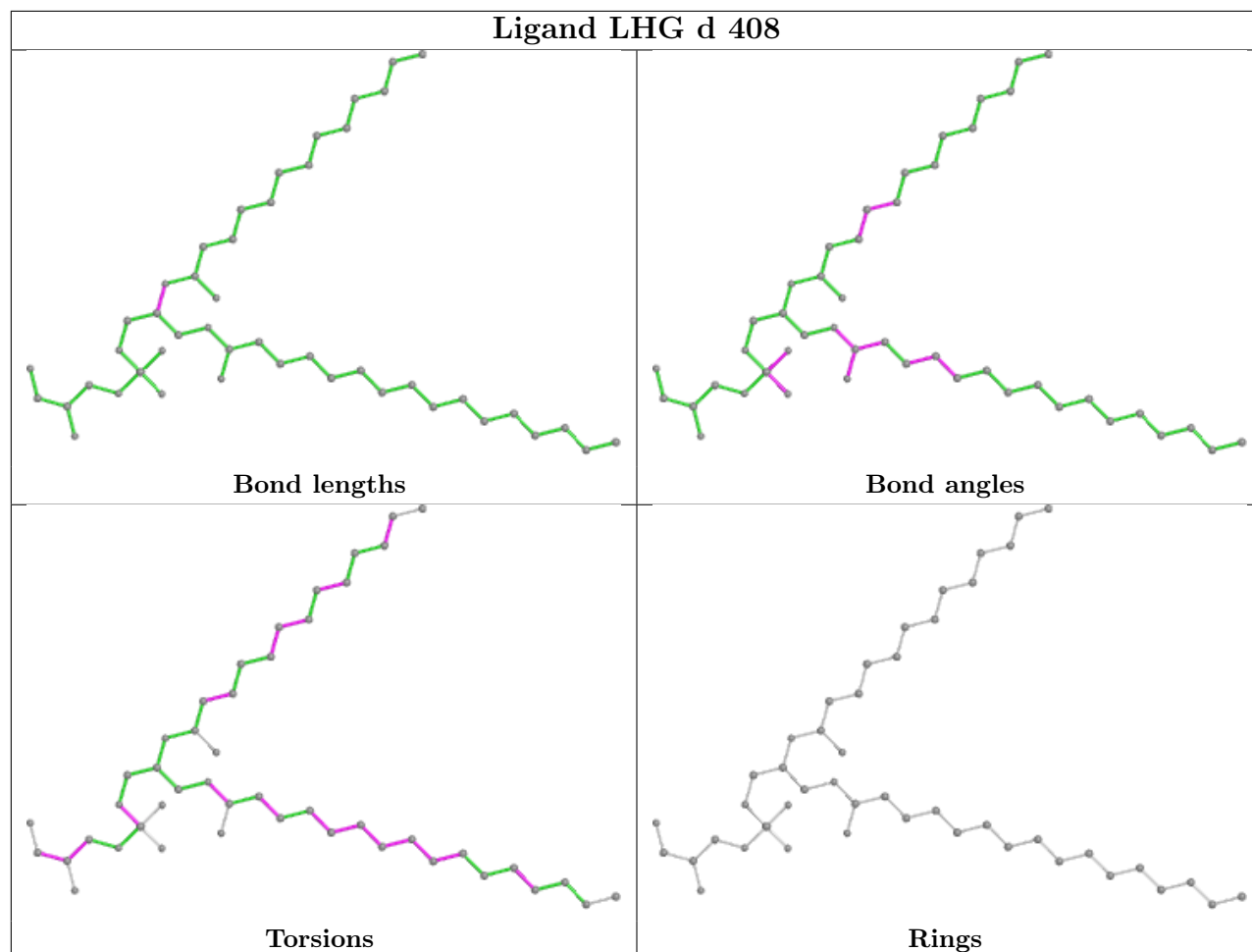
Ligand CHL 3 606



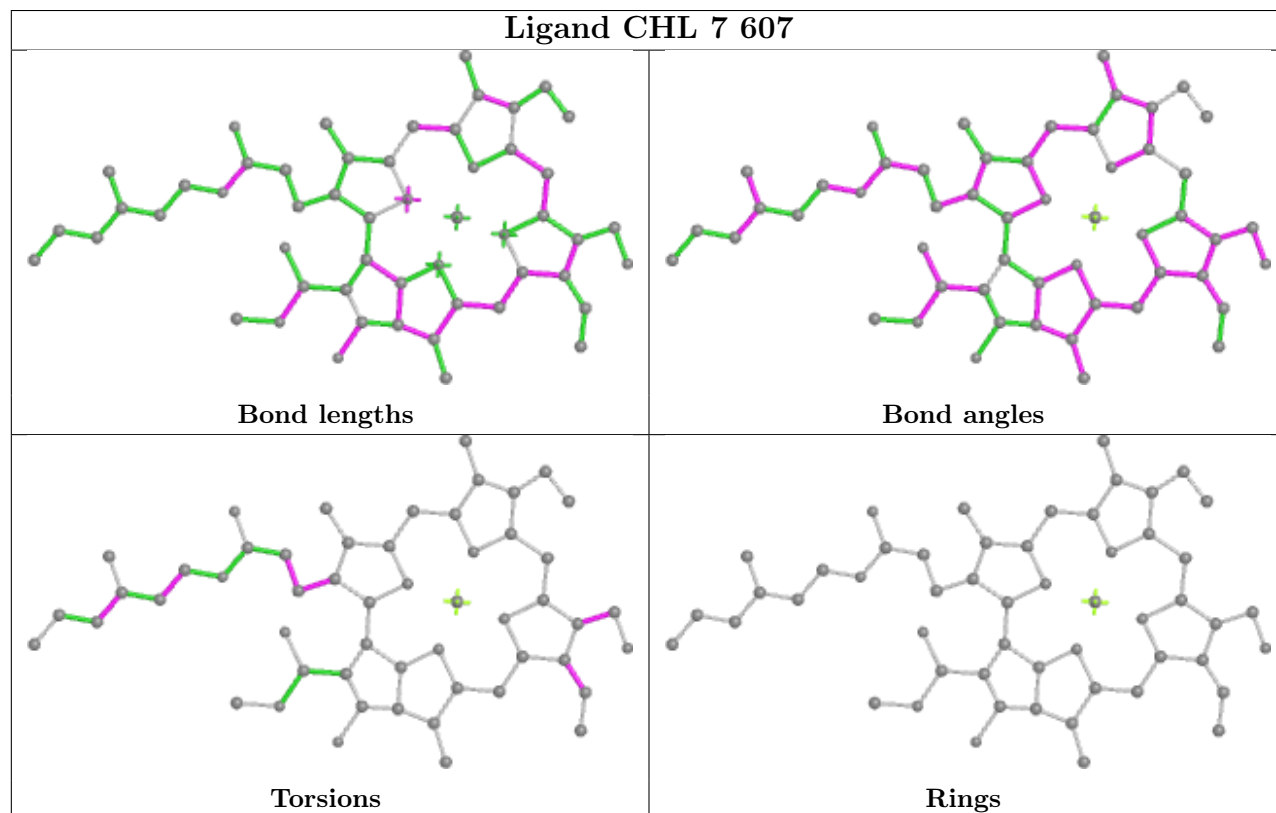
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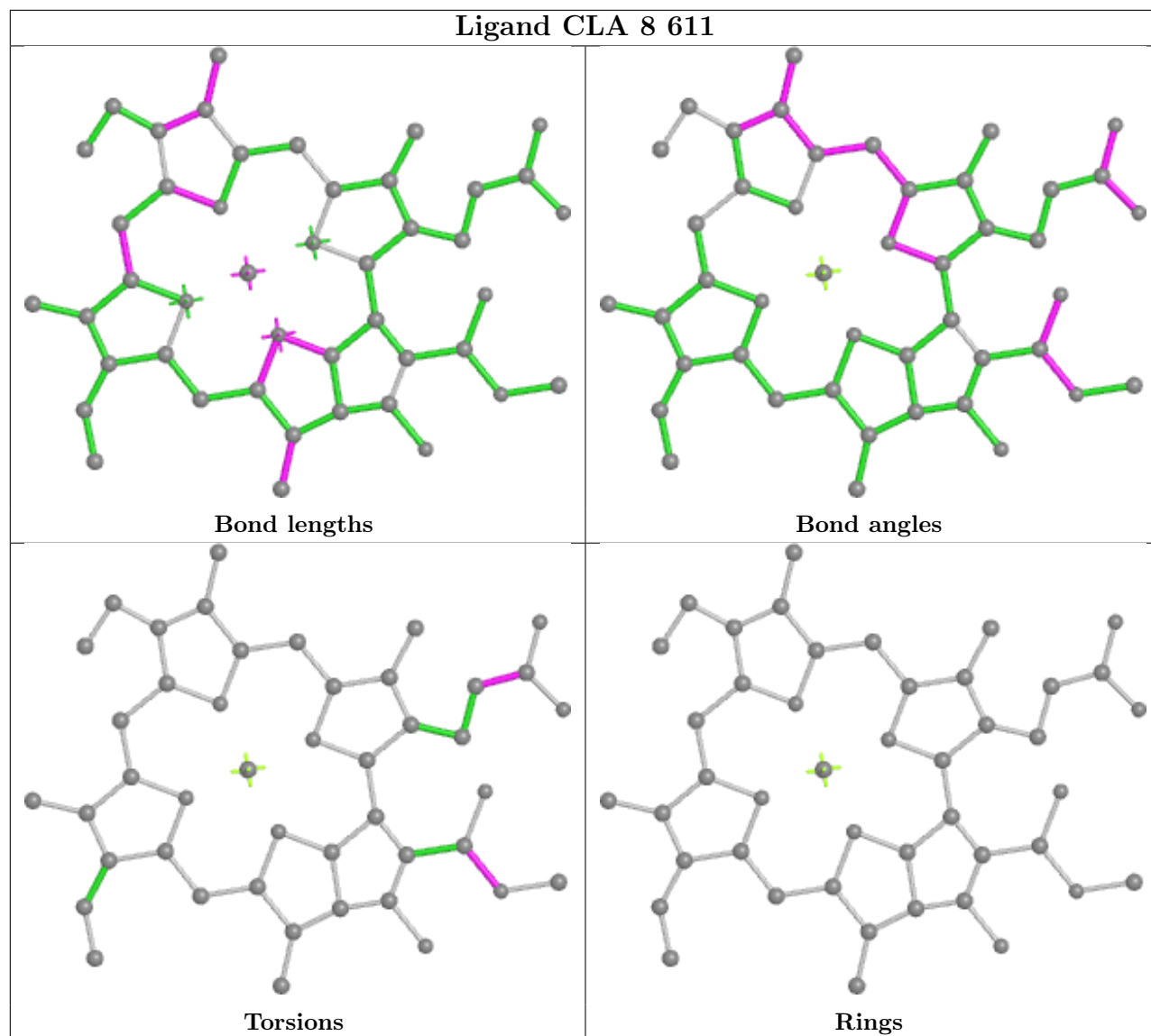
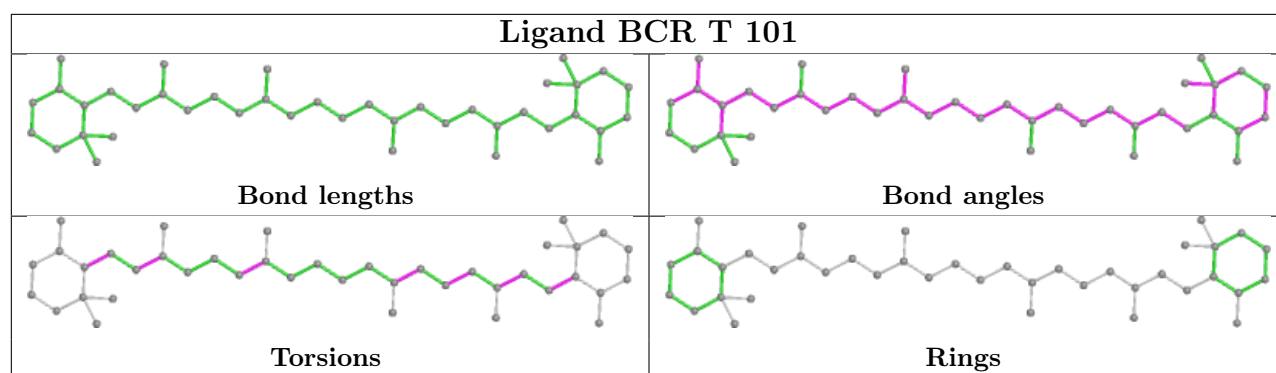


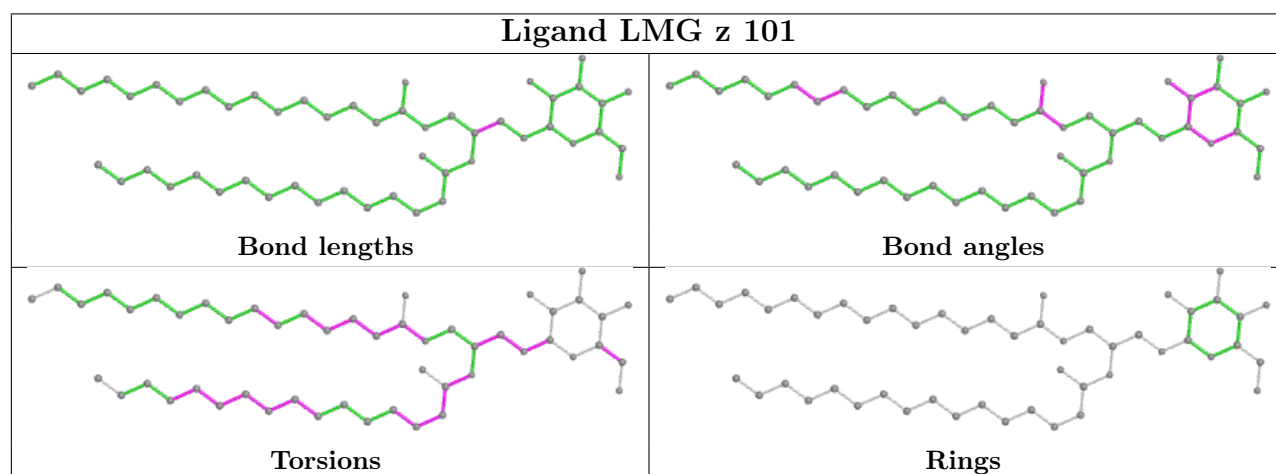
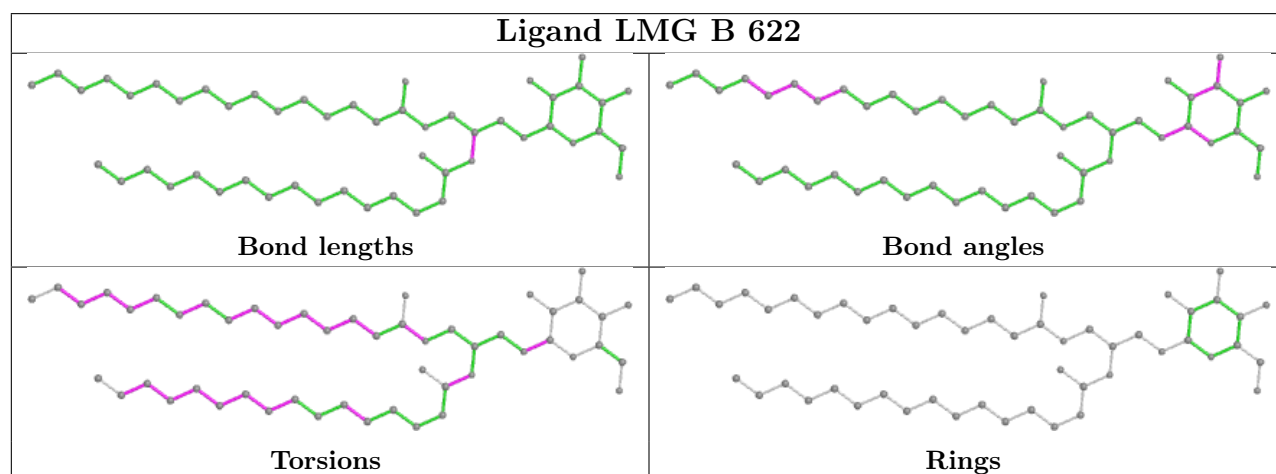
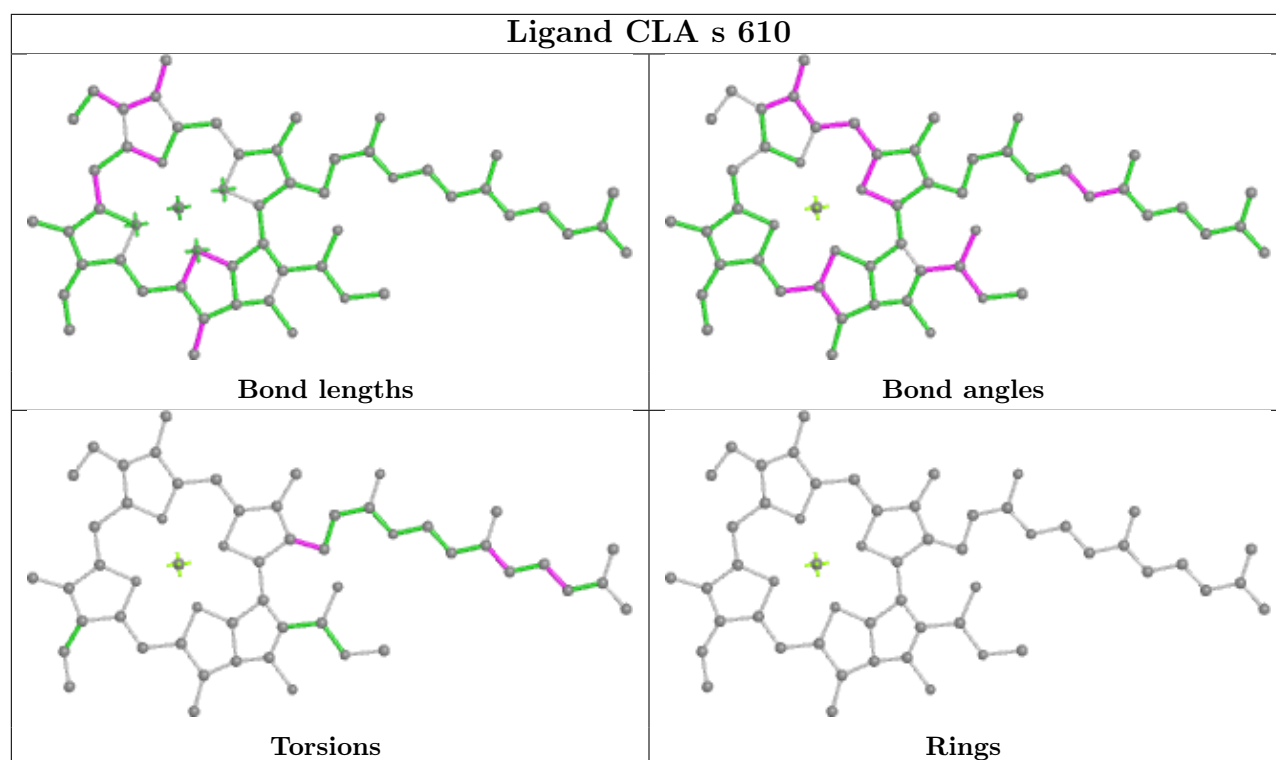
Ligand LHG d 408

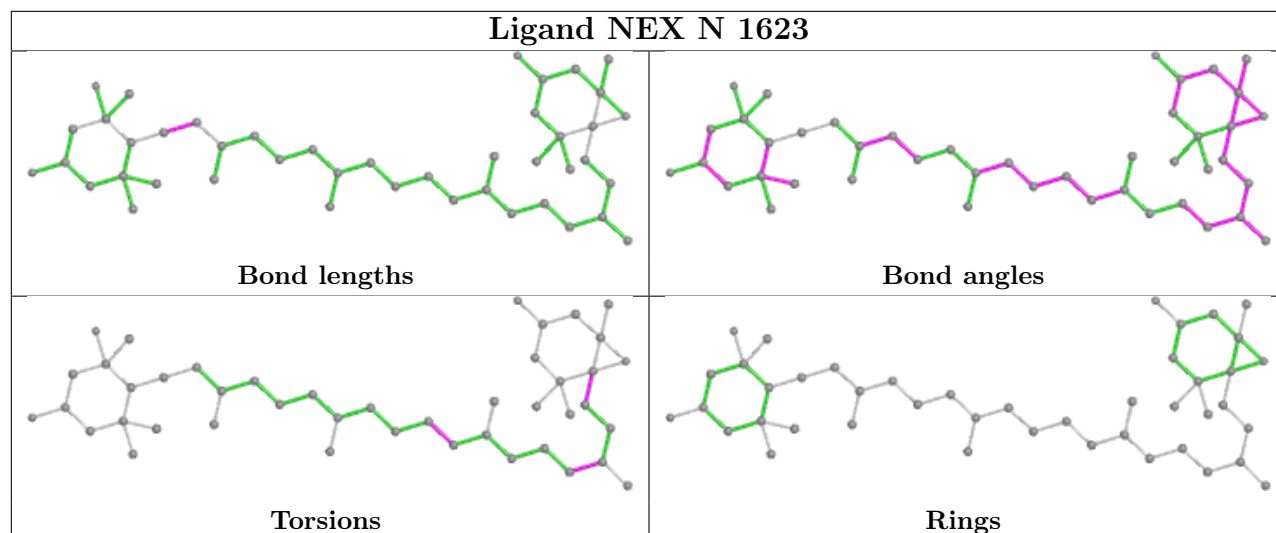
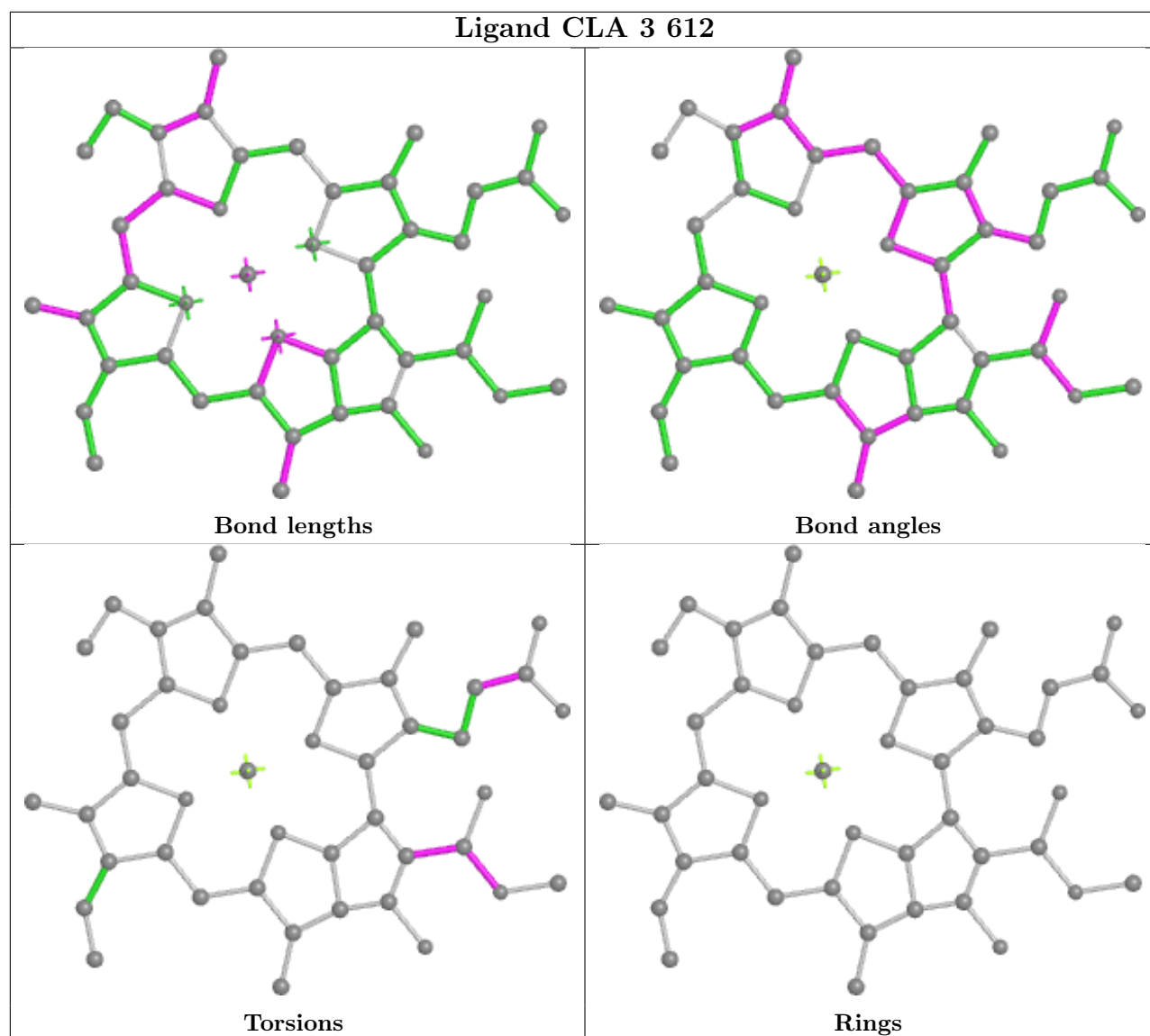


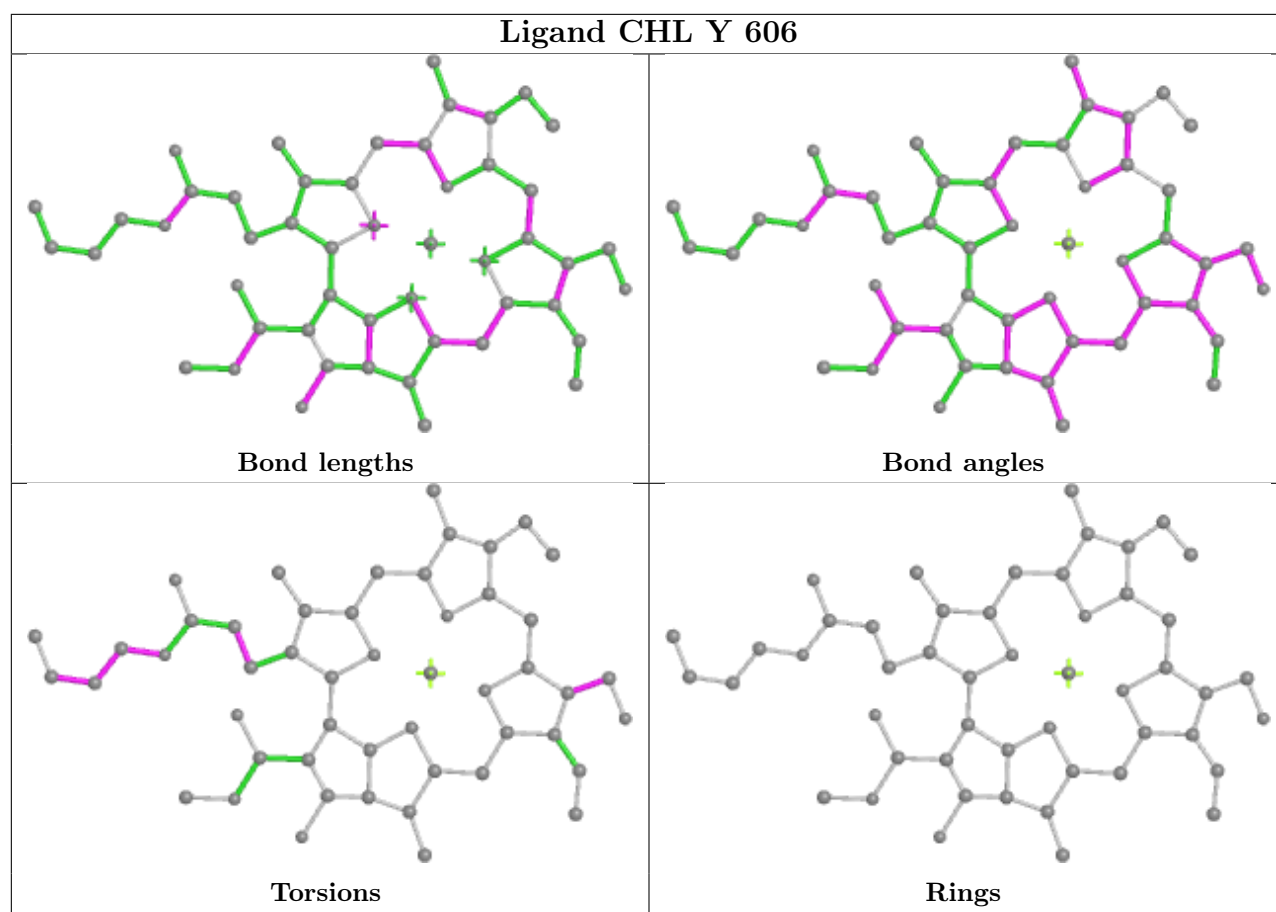
Ligand CHL 7 607

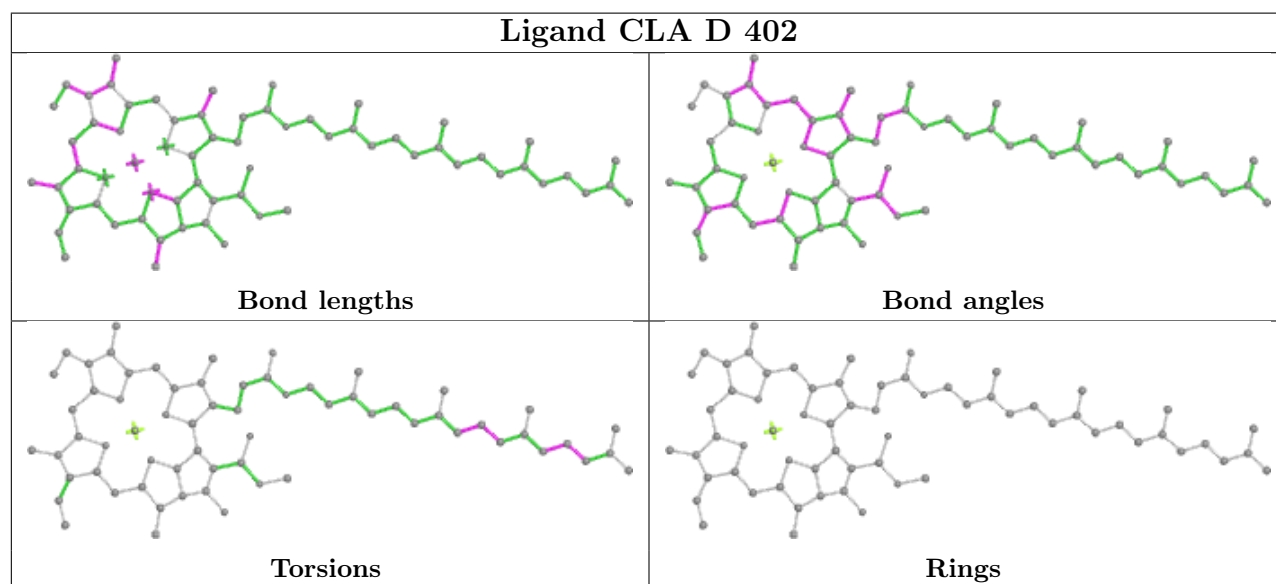
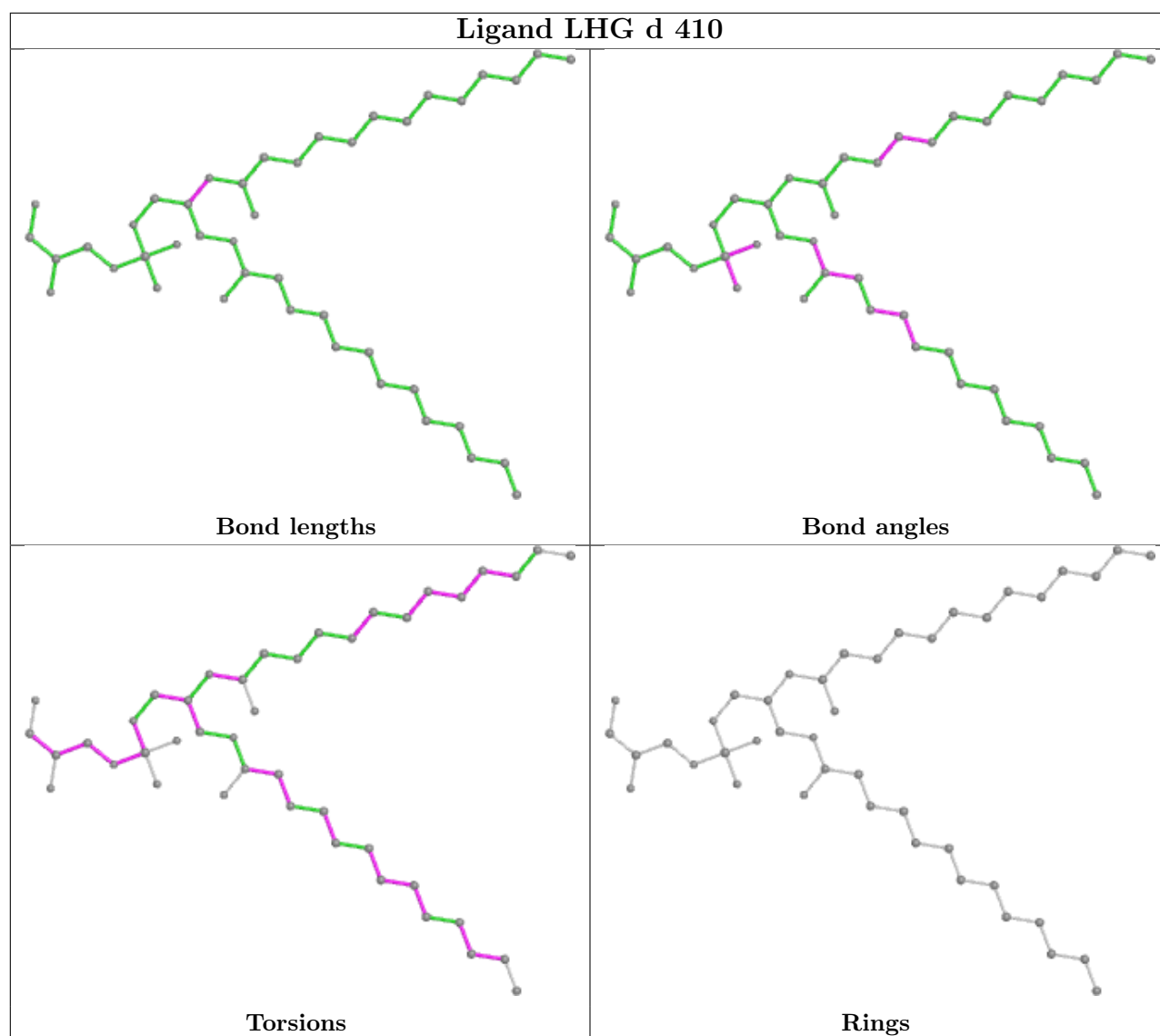


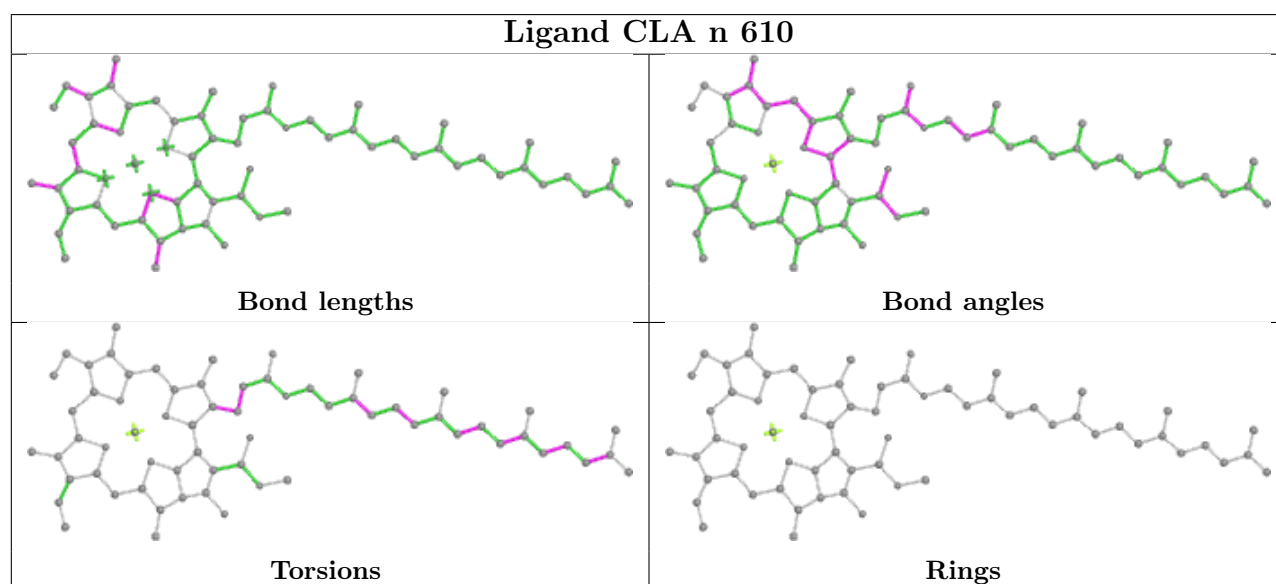
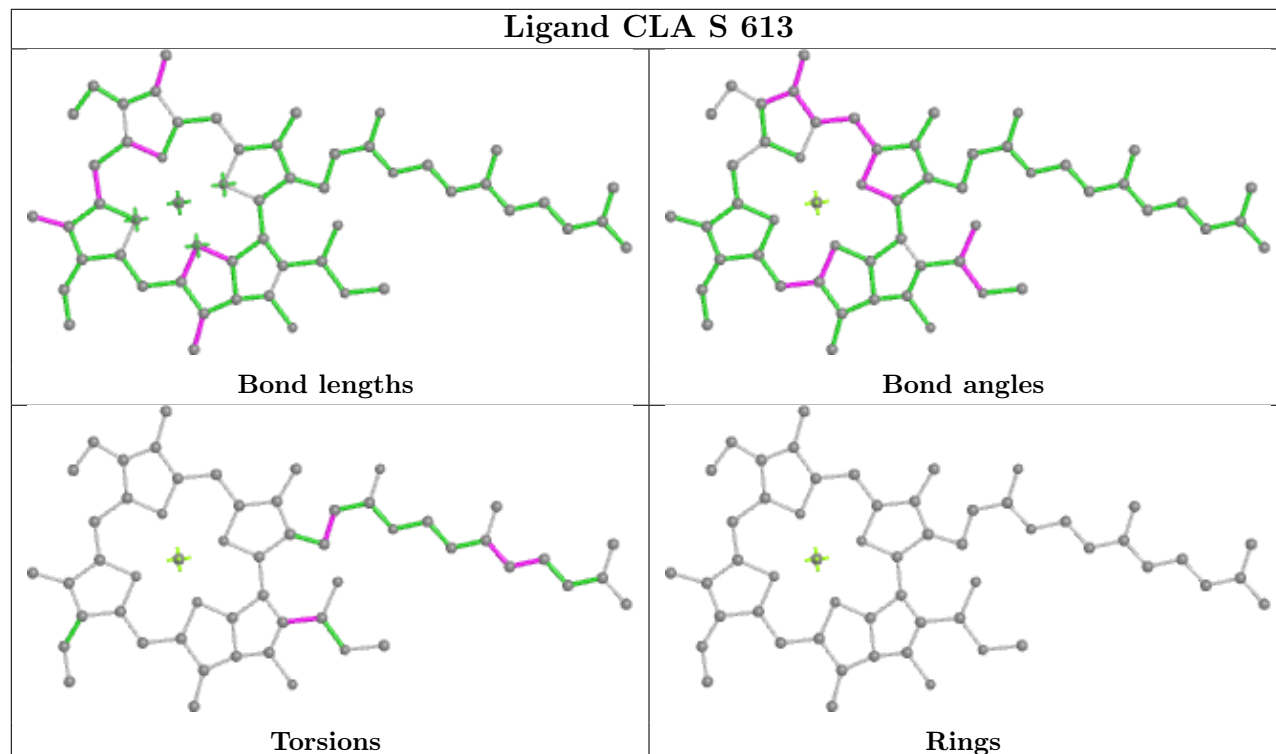
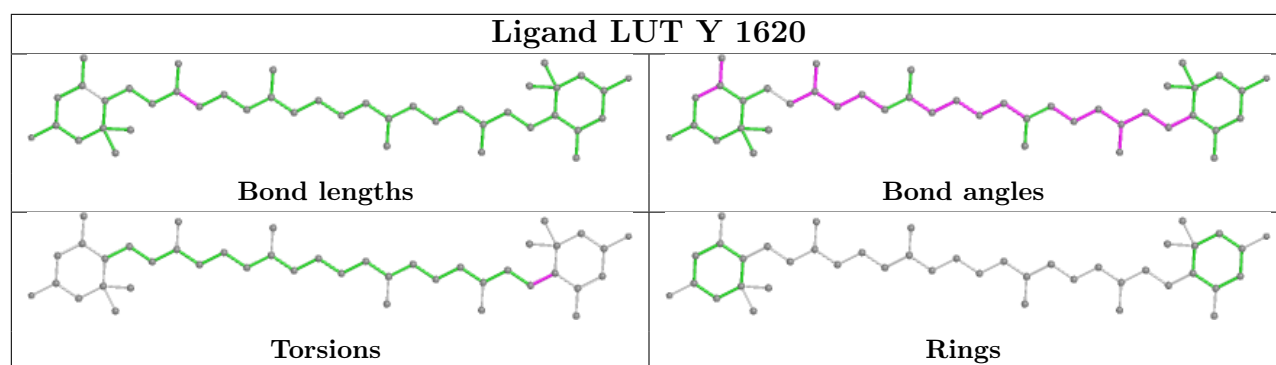


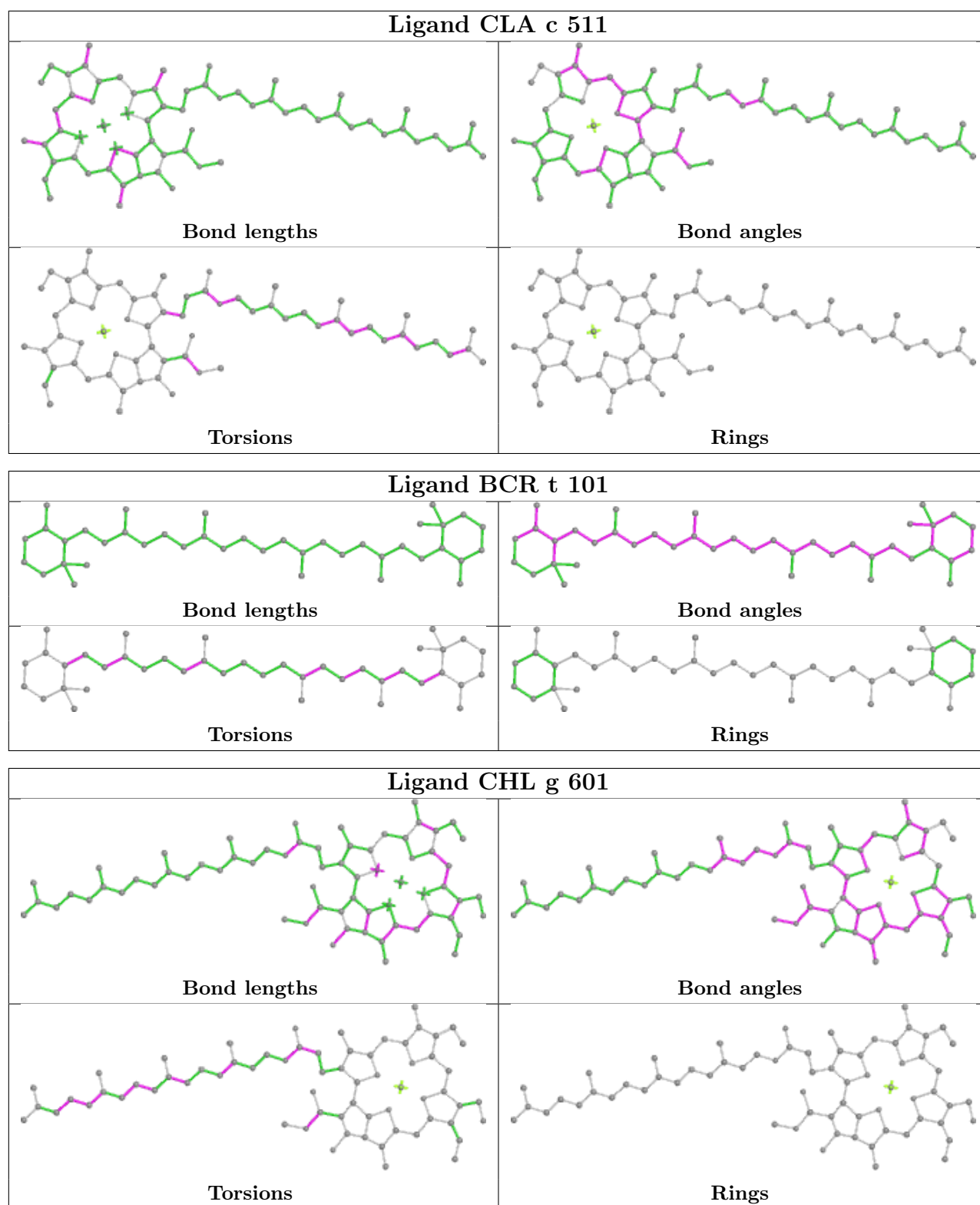


Ligand NEX N 1623**Ligand CLA 3 612**

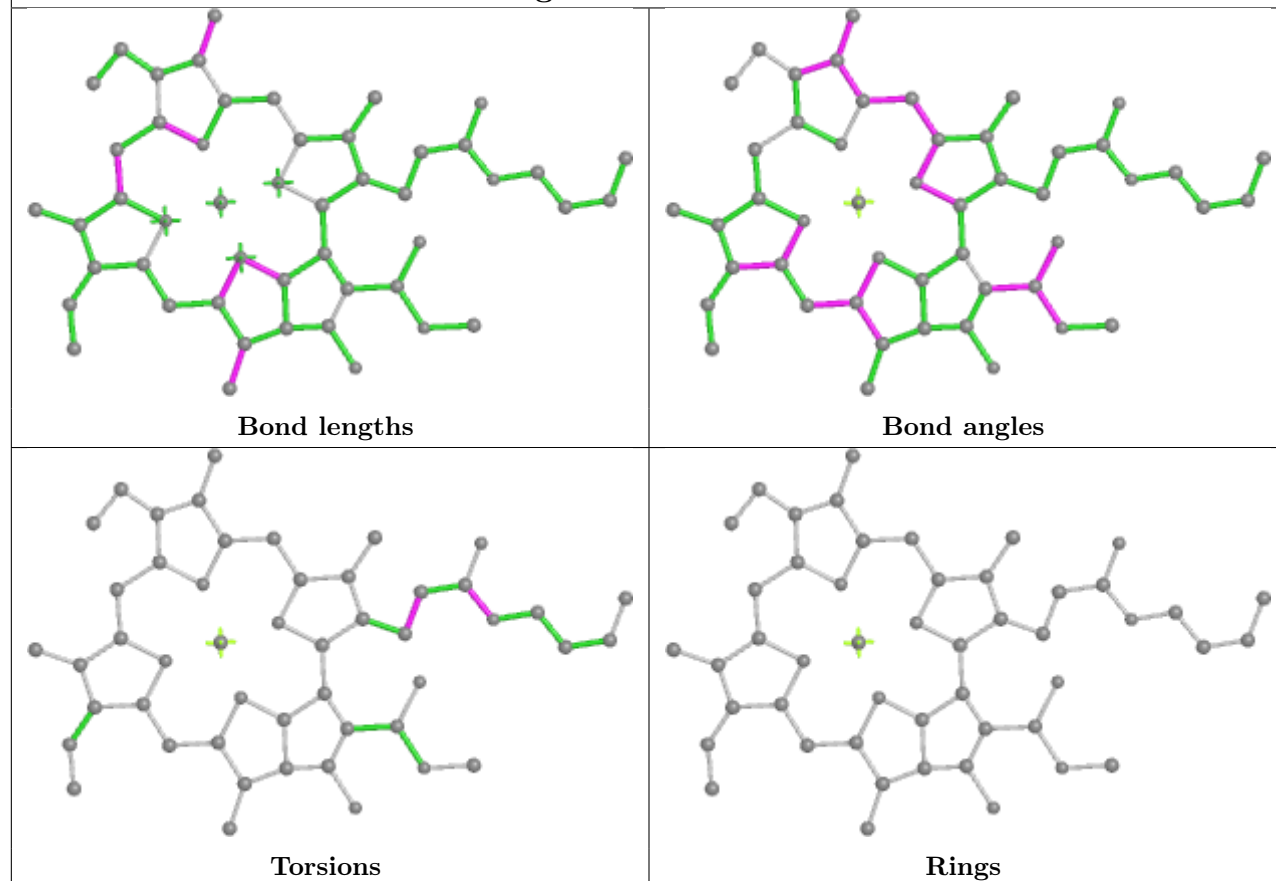




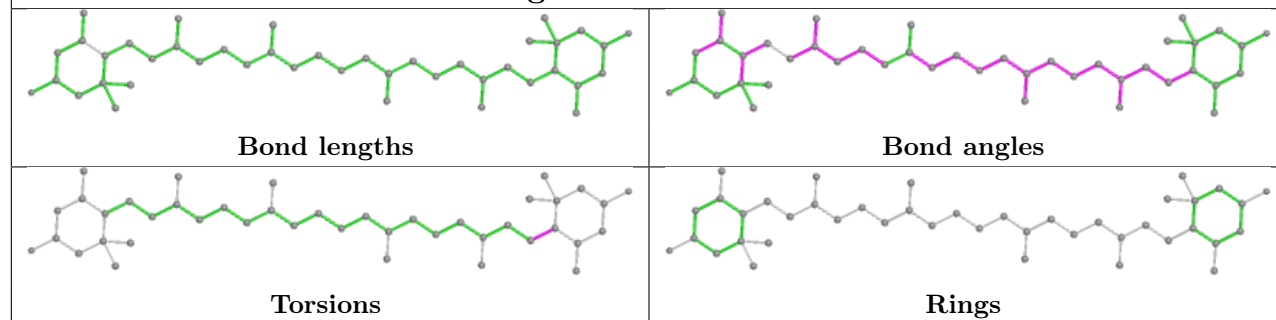




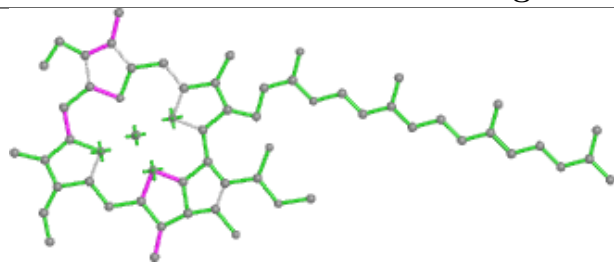
Ligand CLA S 614



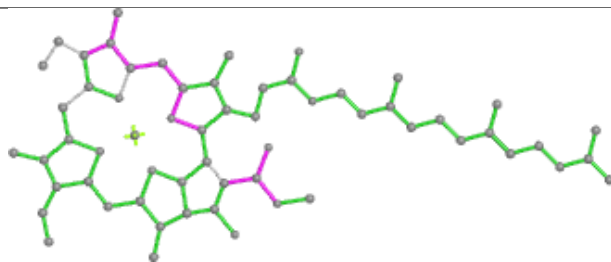
Ligand LUT 5 1620



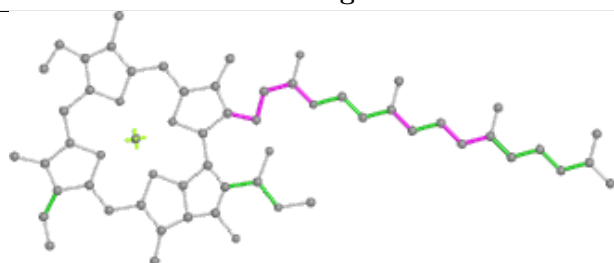
Ligand CLA G 611



Bond lengths



Bond angles

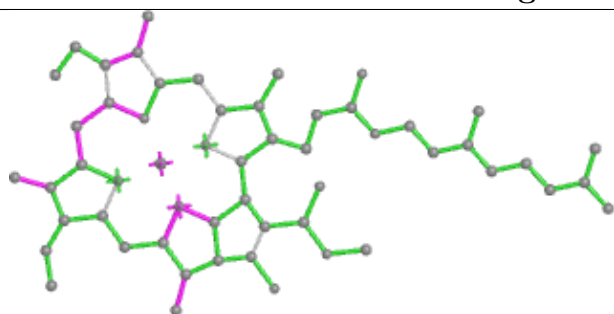


Torsions

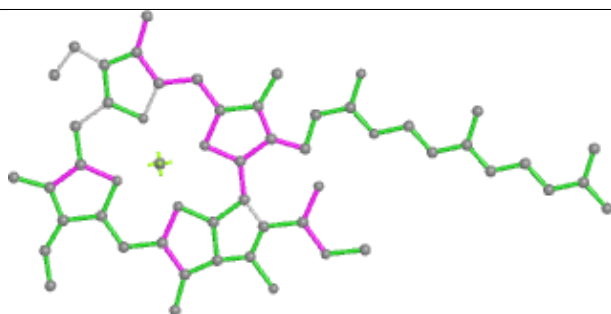


Rings

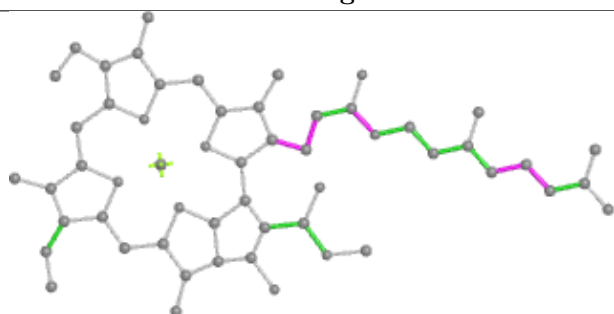
Ligand CLA 7 611



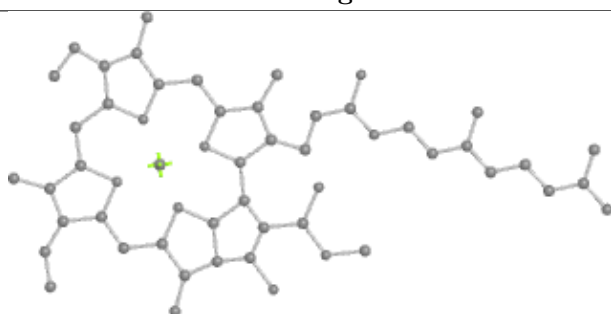
Bond lengths



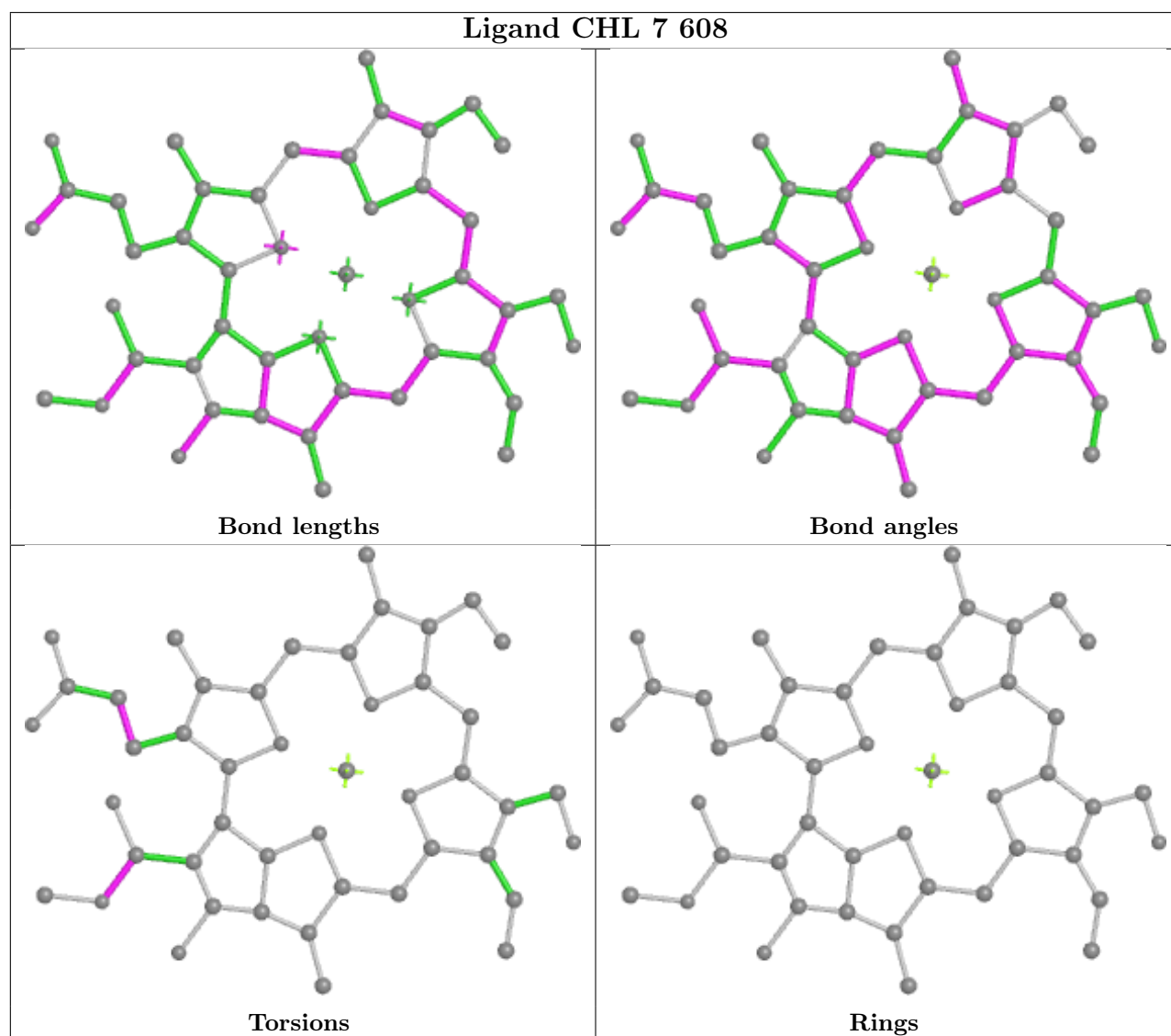
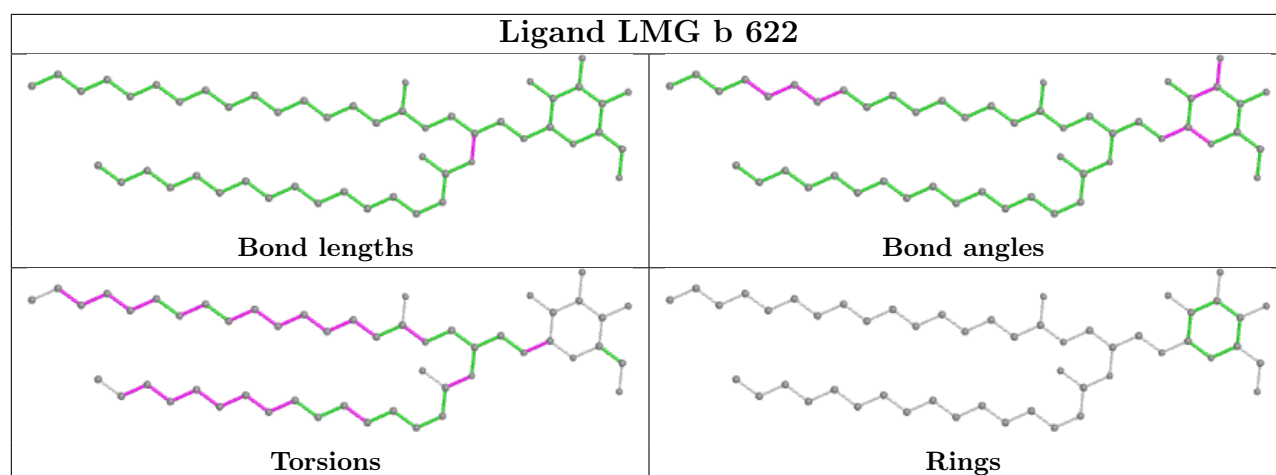
Bond angles

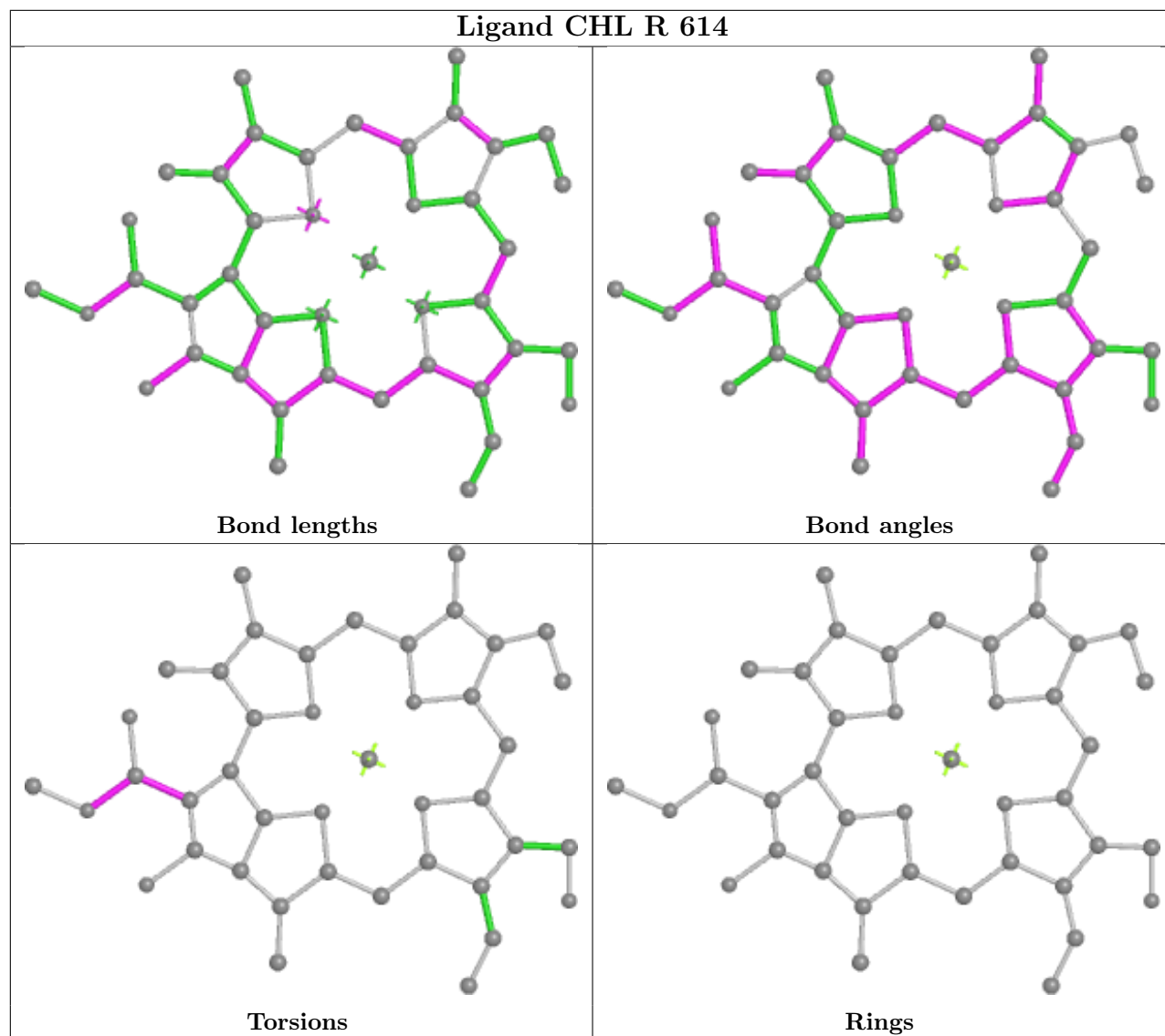
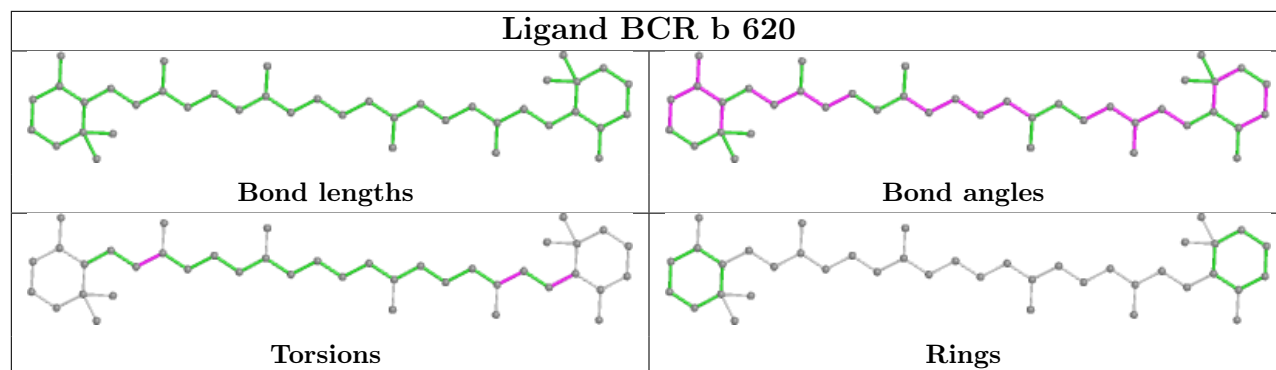


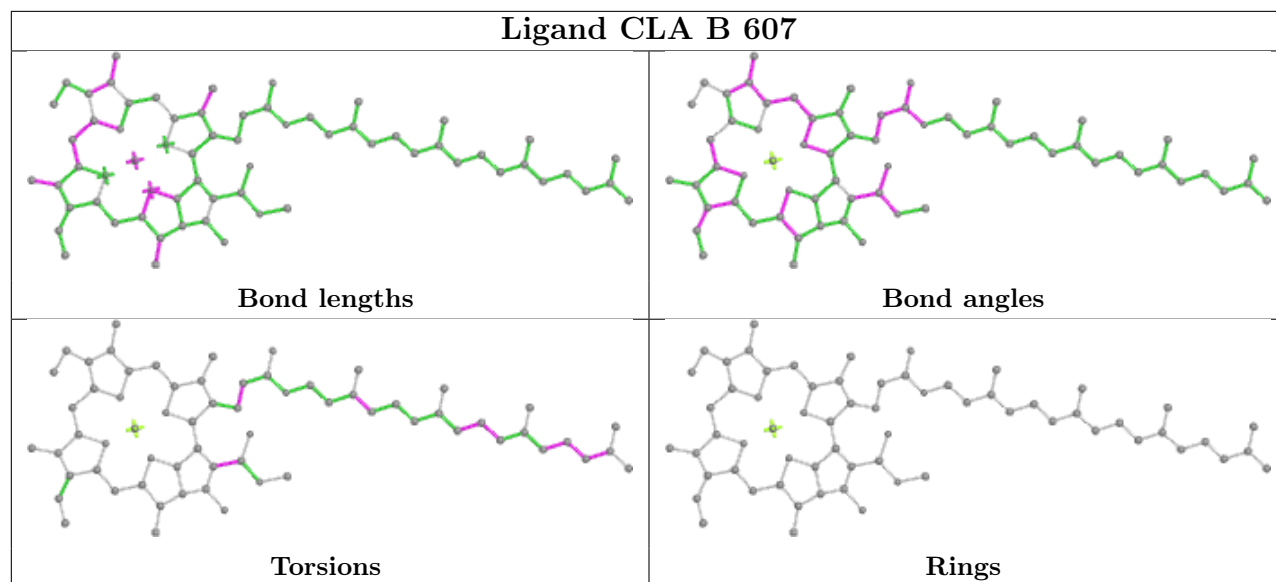
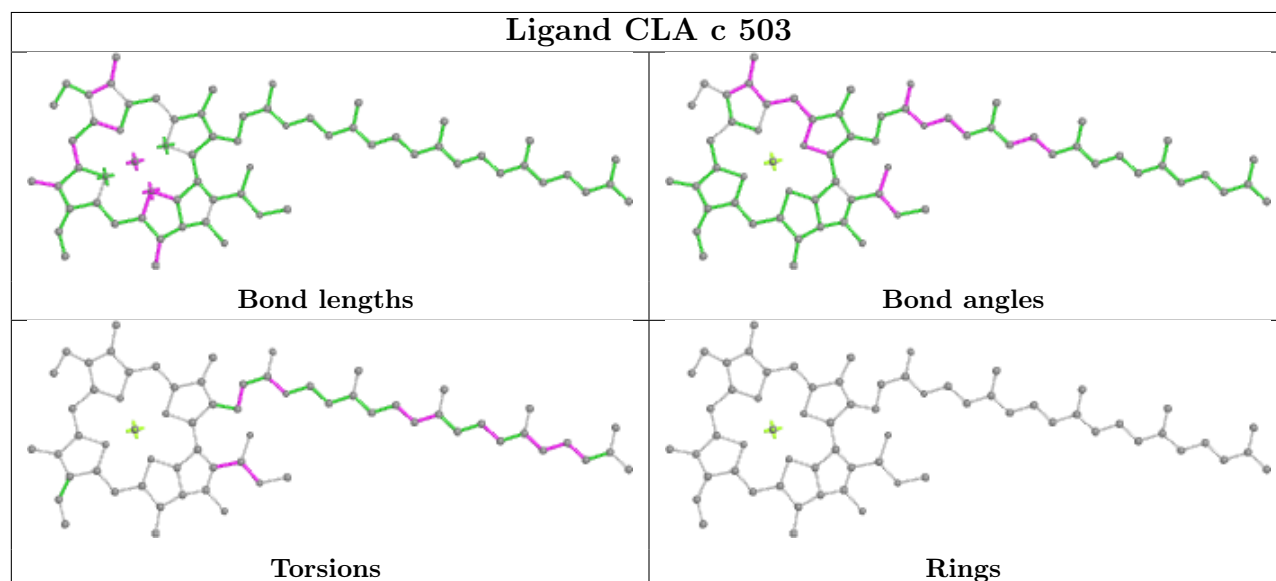
Torsions

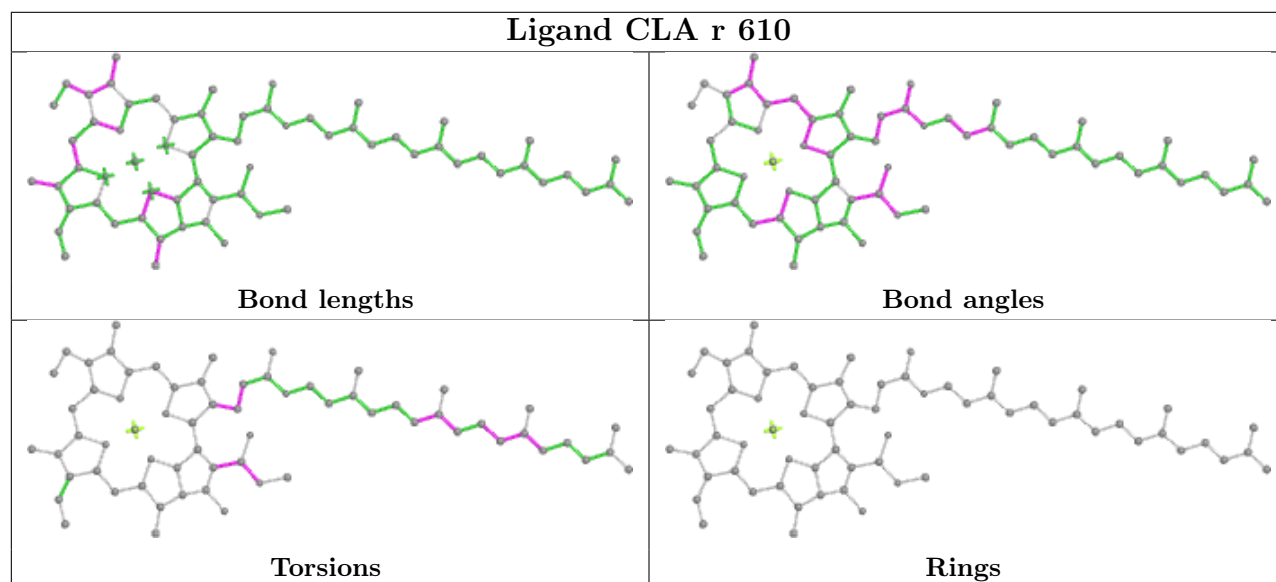
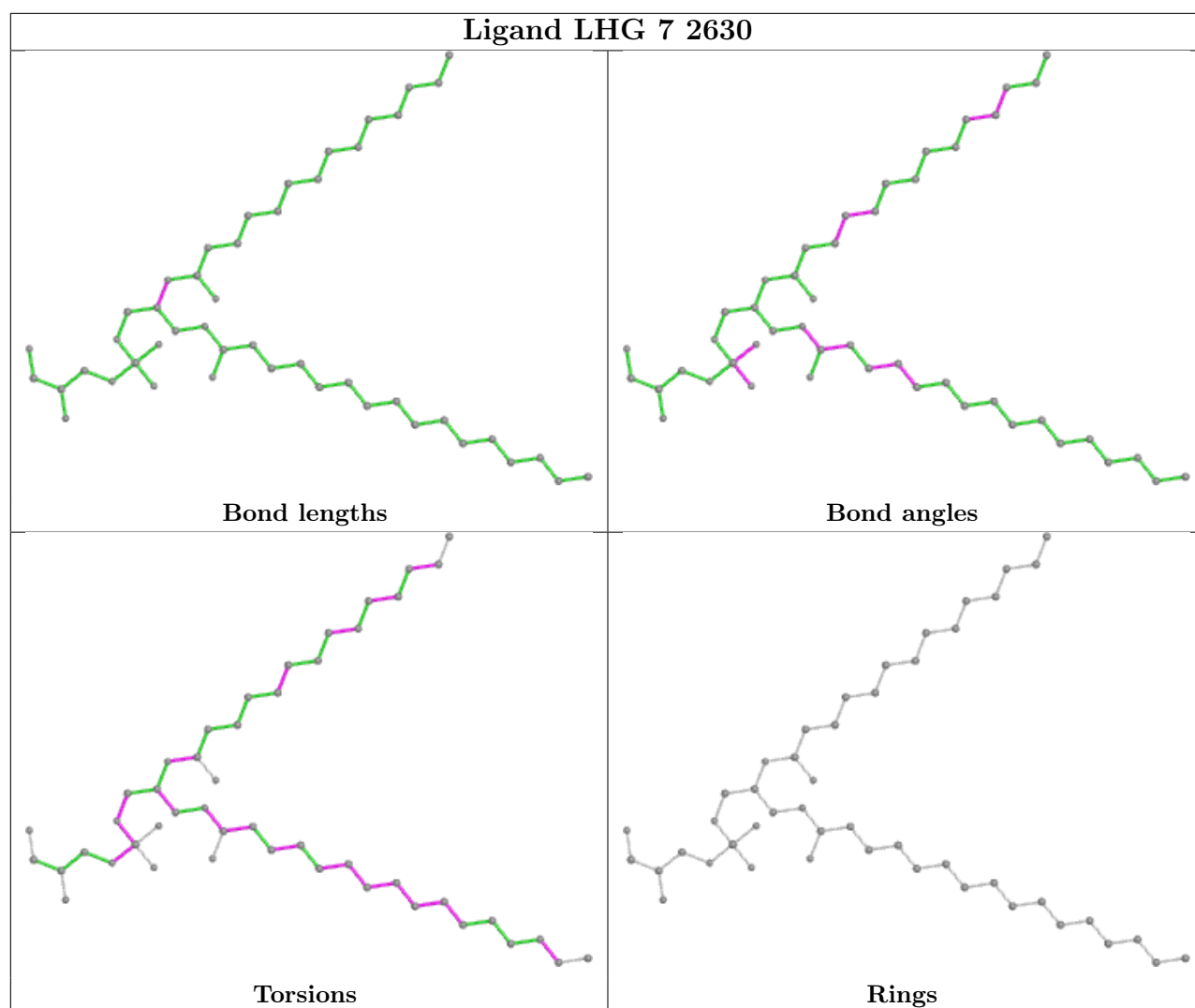


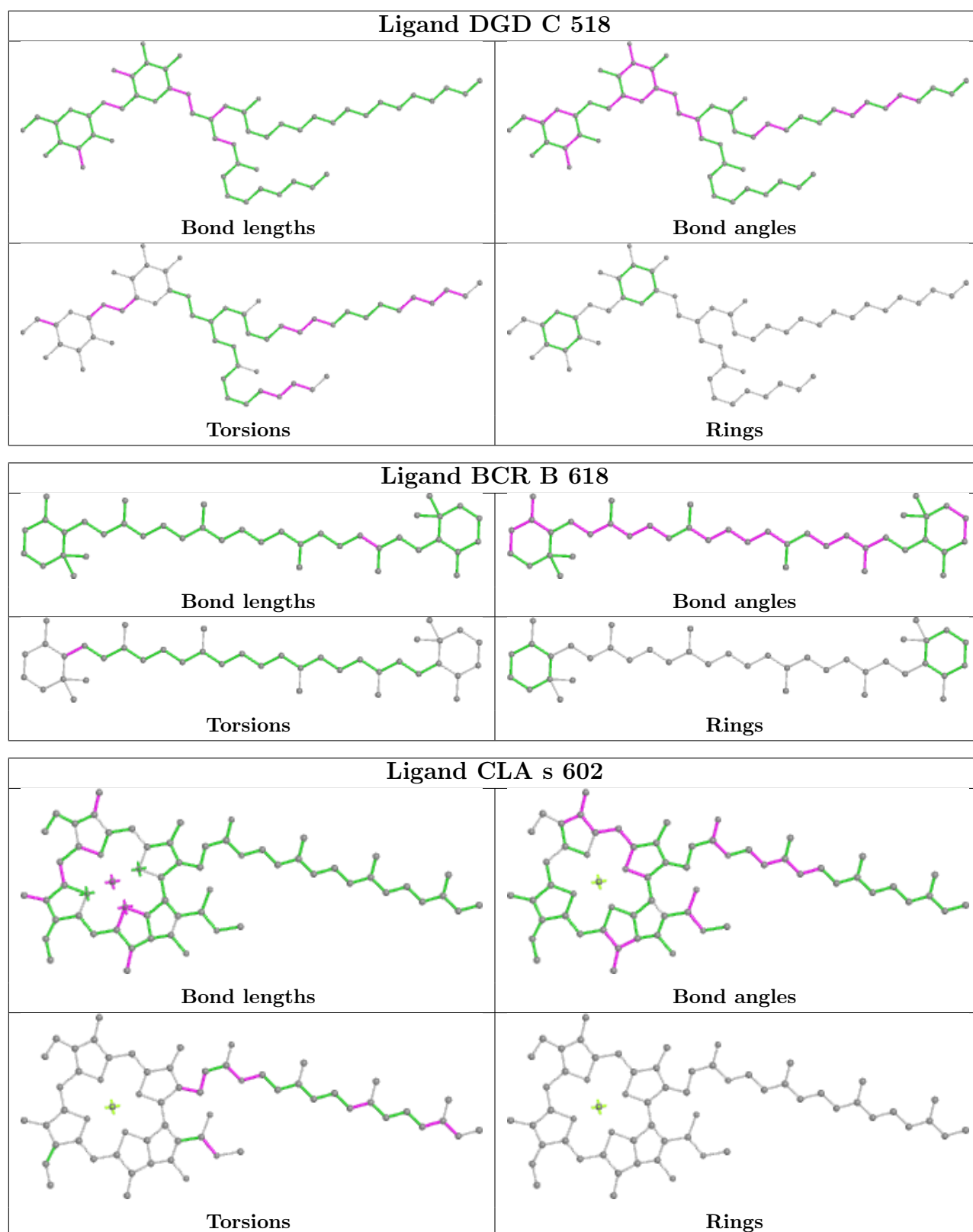
Rings

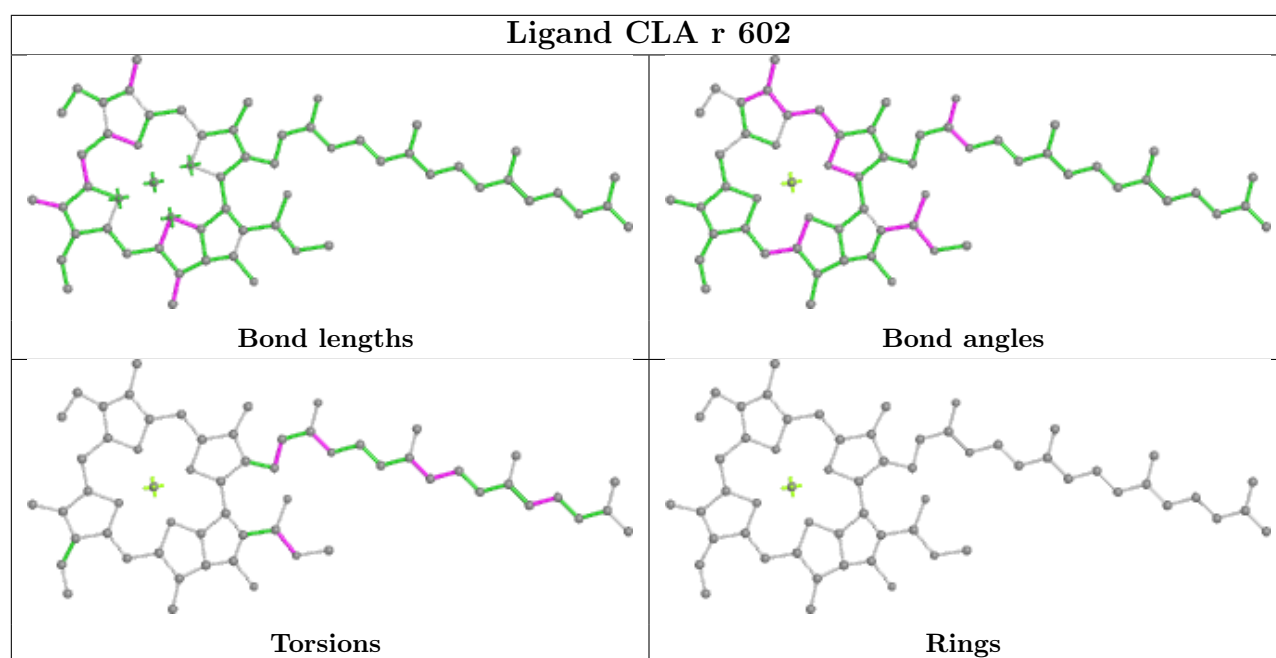
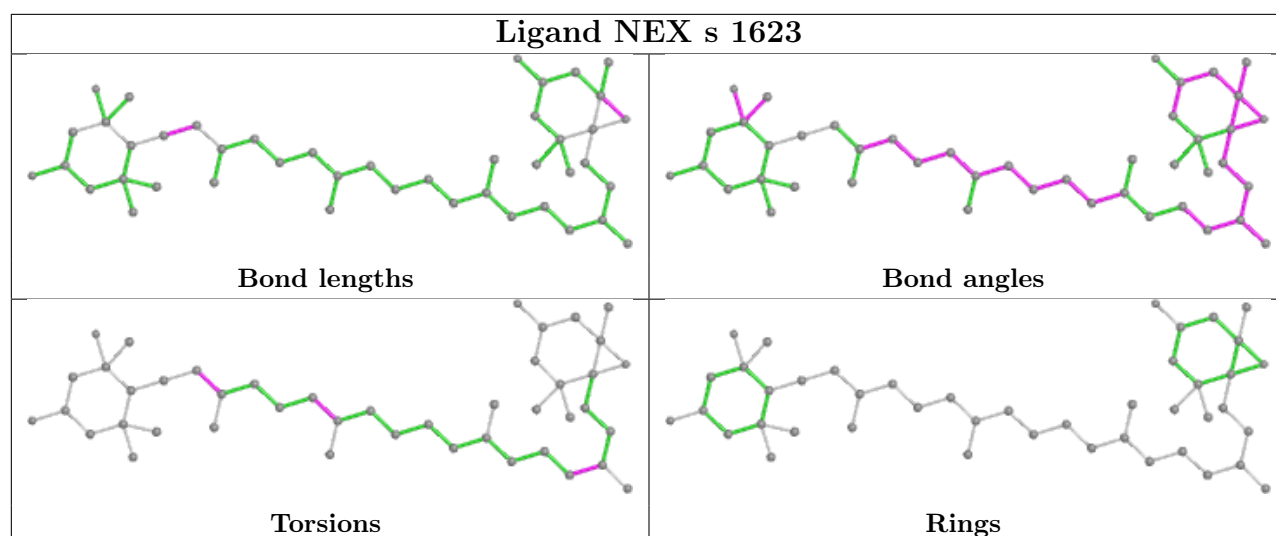


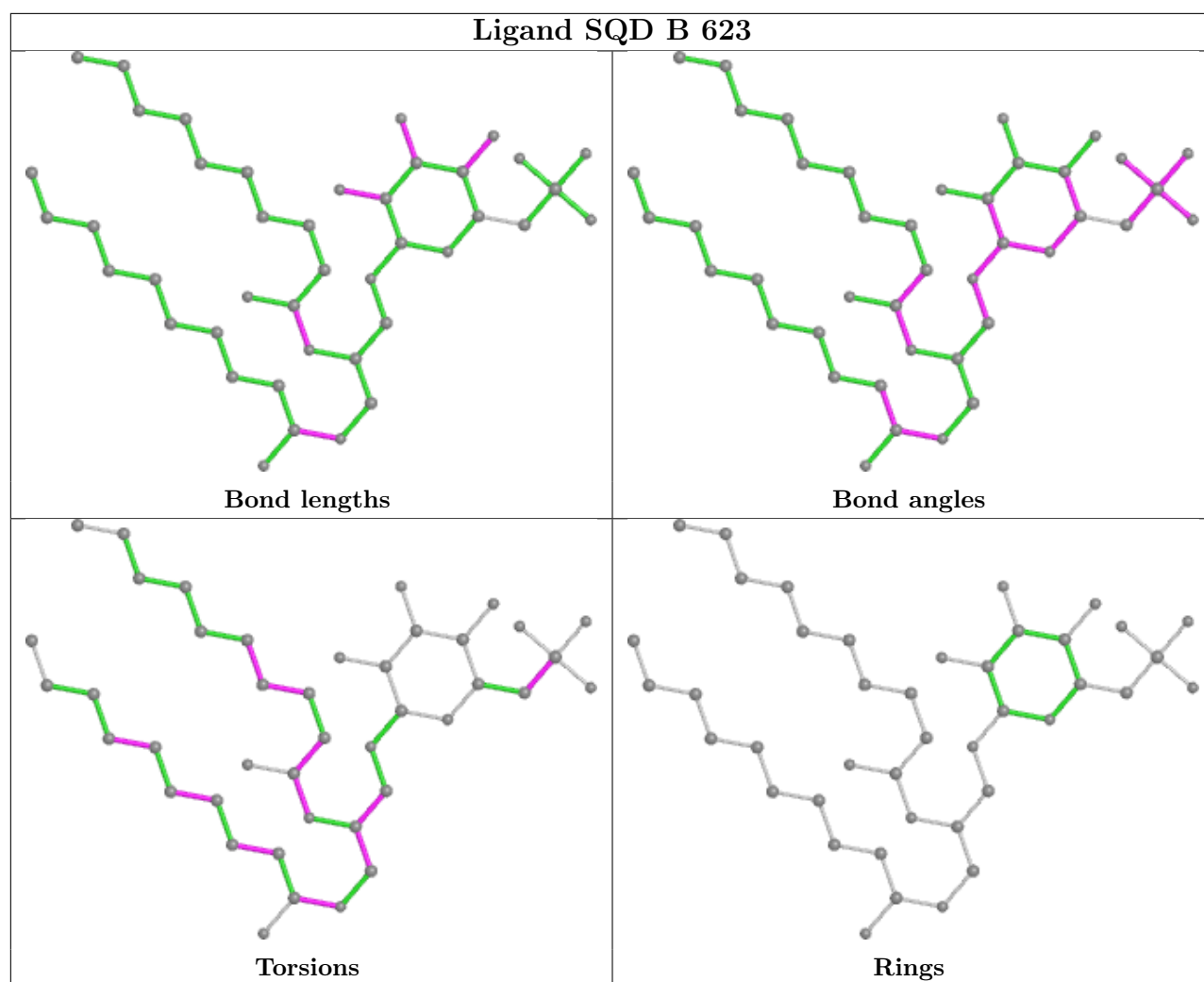


Ligand CLA B 607**Ligand CLA c 503**

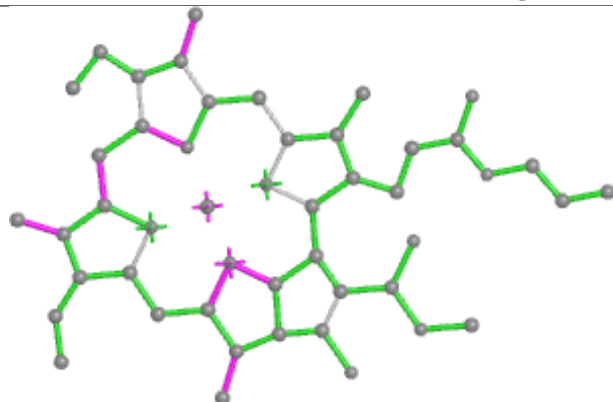




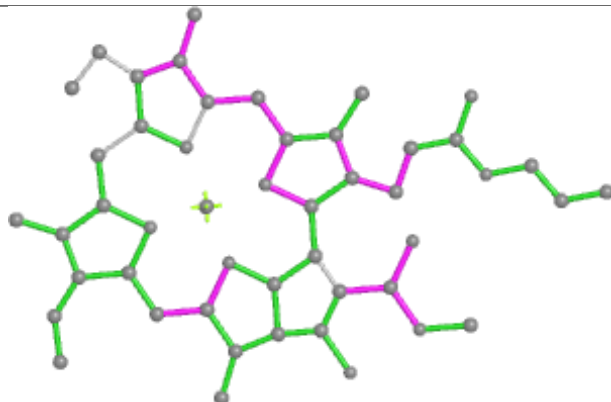




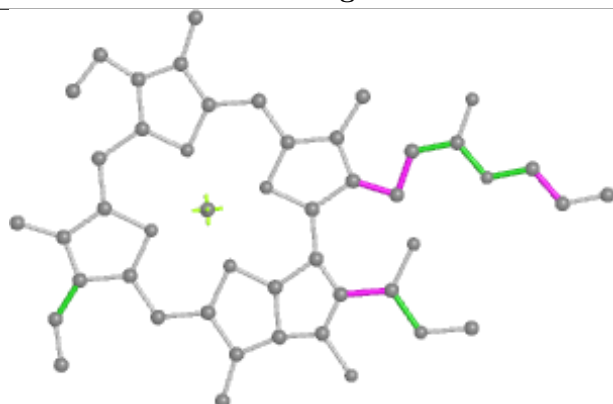
Ligand CLA R 604



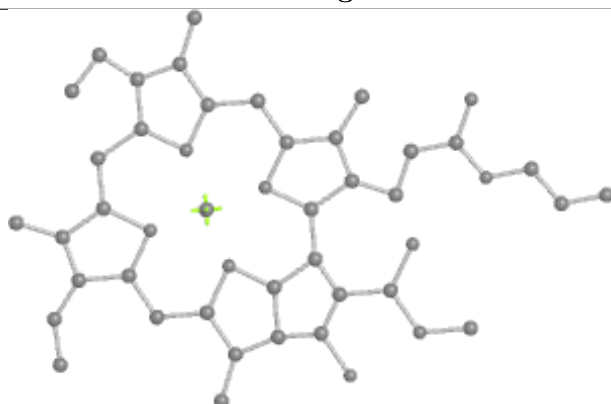
Bond lengths



Bond angles

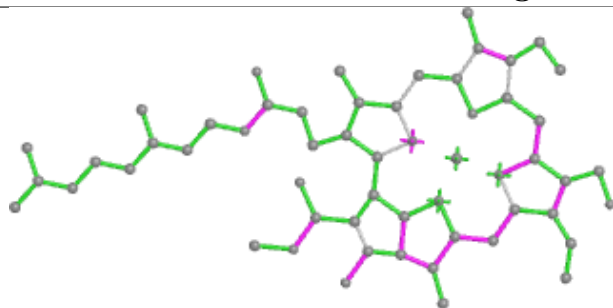


Torsions

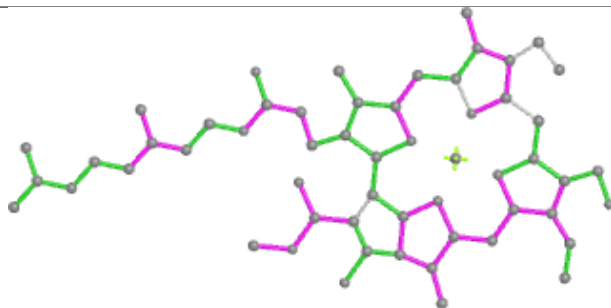


Rings

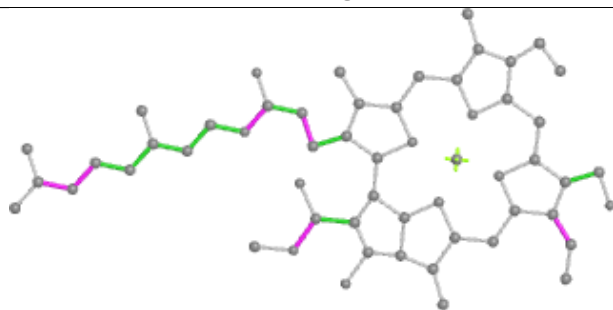
Ligand CHL R 607



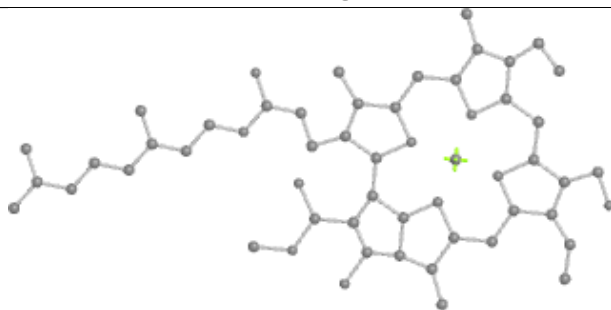
Bond lengths



Bond angles

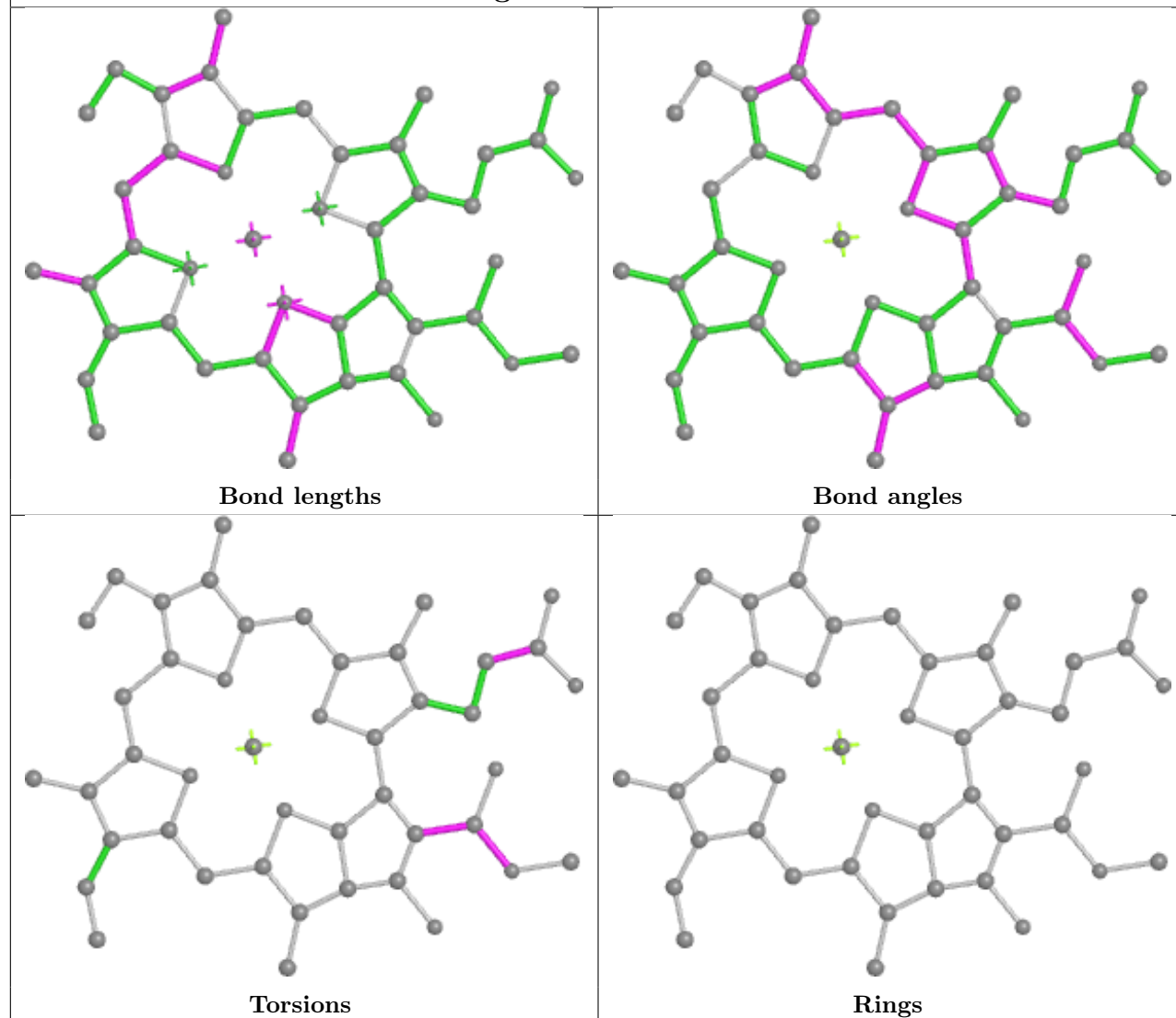


Torsions

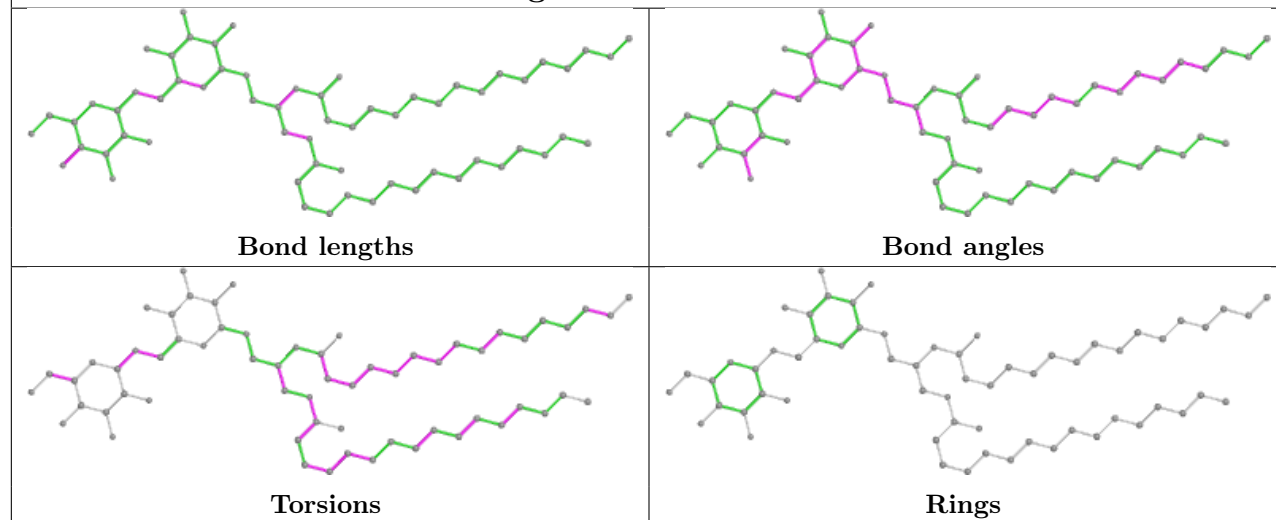


Rings

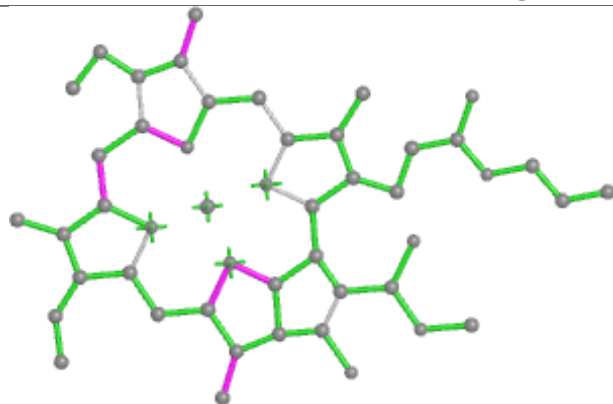
Ligand CLA 7 612



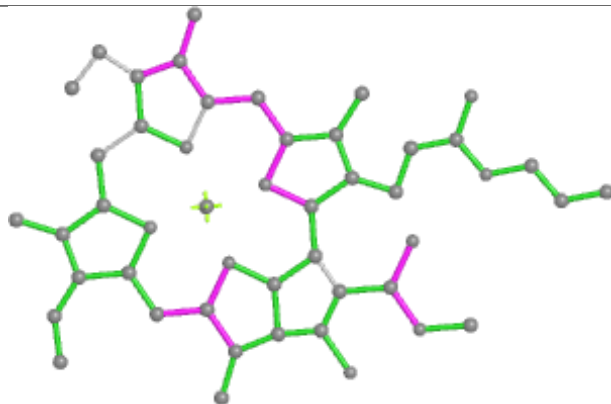
Ligand DGD C 519



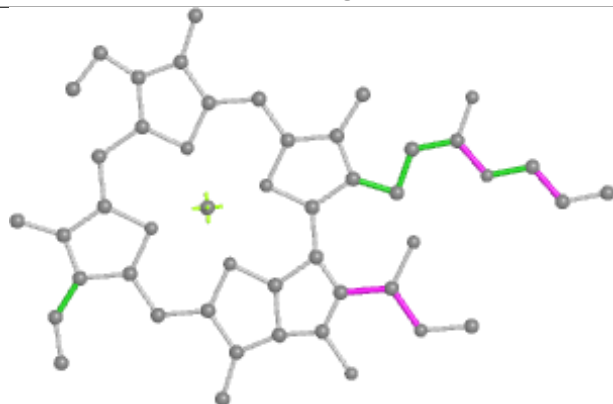
Ligand CLA N 614



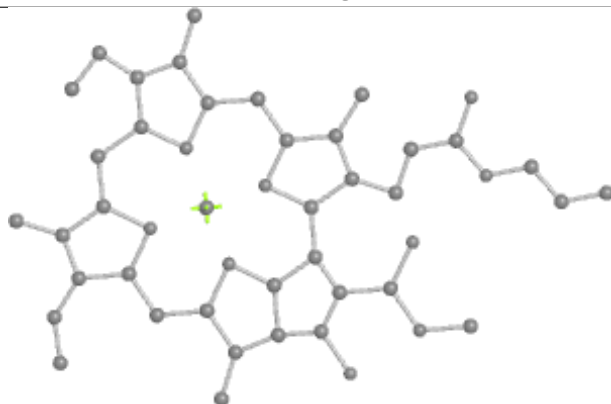
Bond lengths



Bond angles

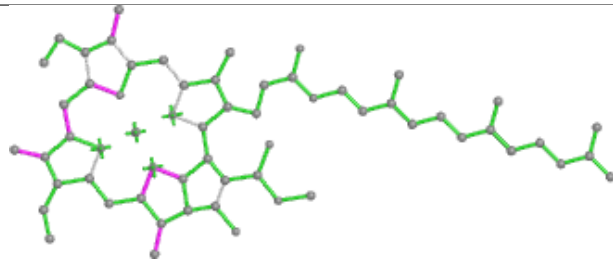


Torsions

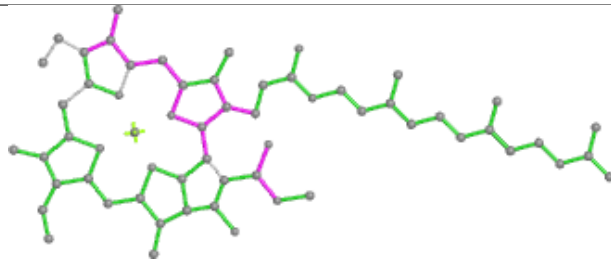


Rings

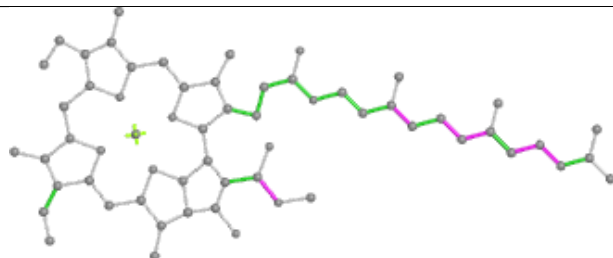
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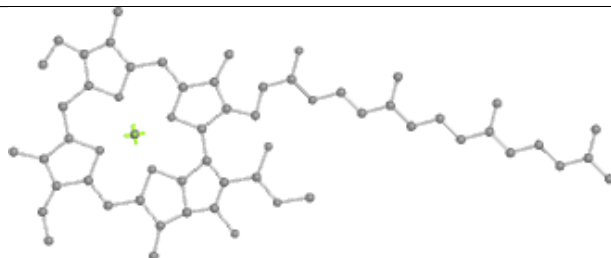
Bond lengths



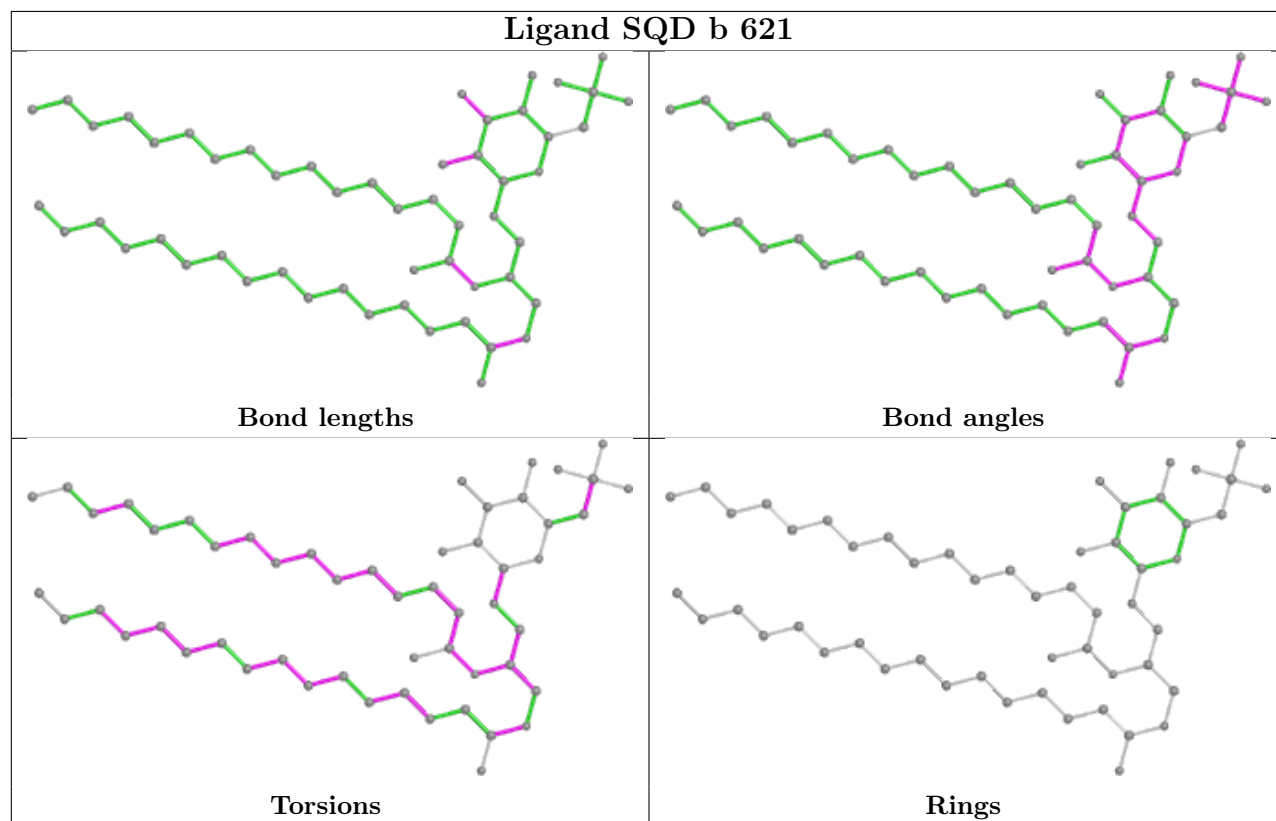
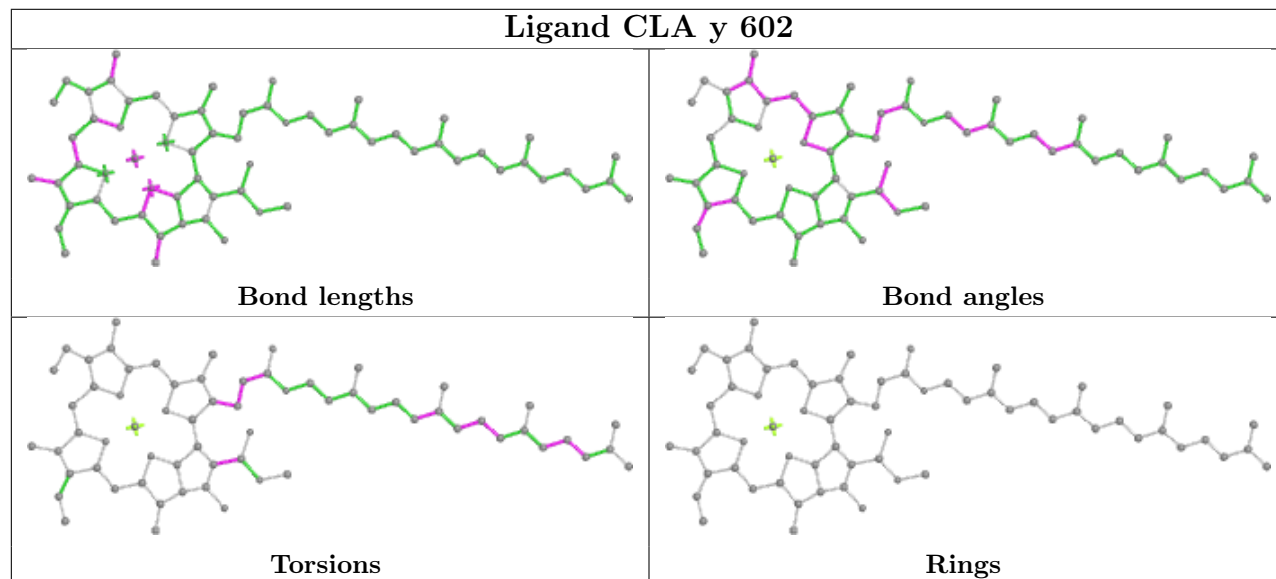
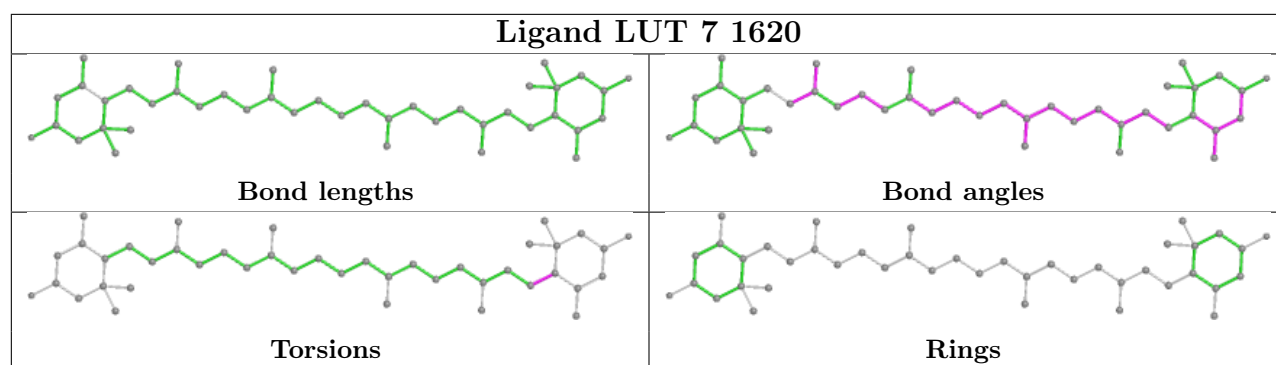
Bond angles



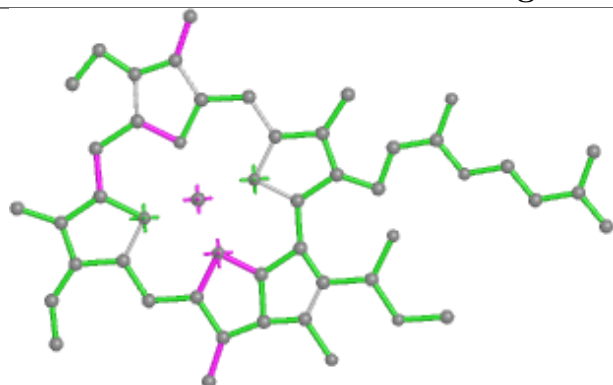
Torsions



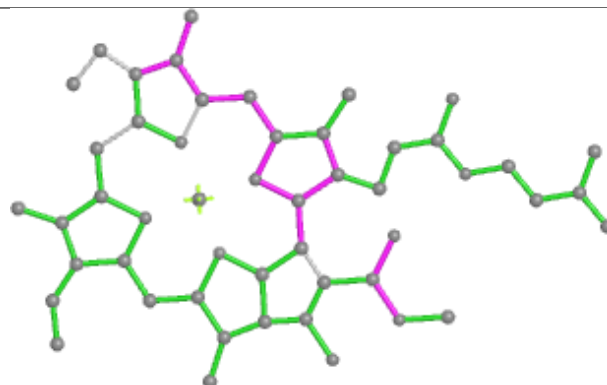
Rings



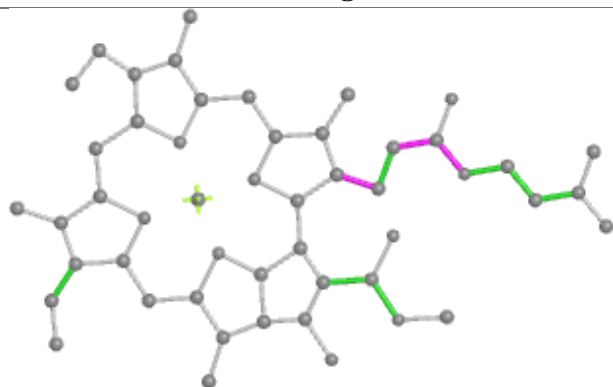
Ligand CLA S 604



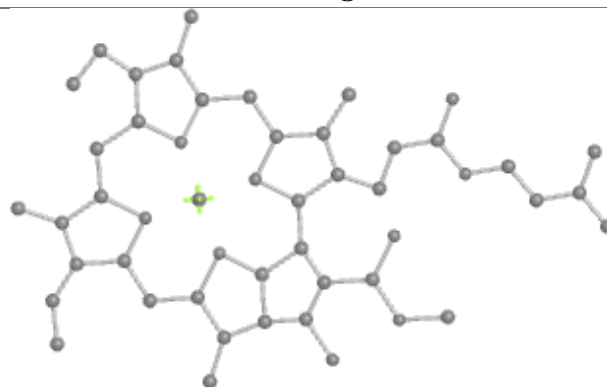
Bond lengths



Bond angles

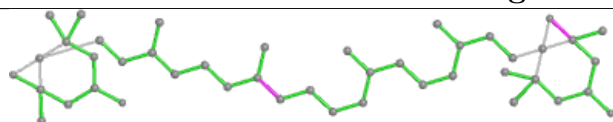


Torsions

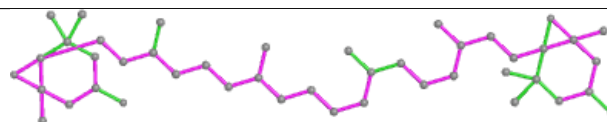


Rings

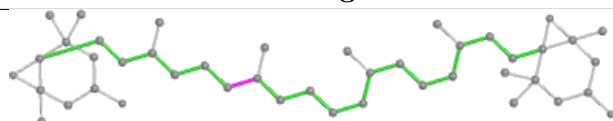
Ligand XAT 7 1622



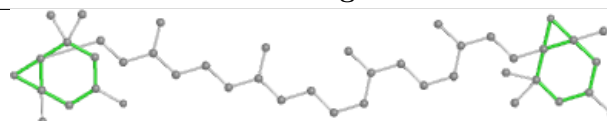
Bond lengths



Bond angles

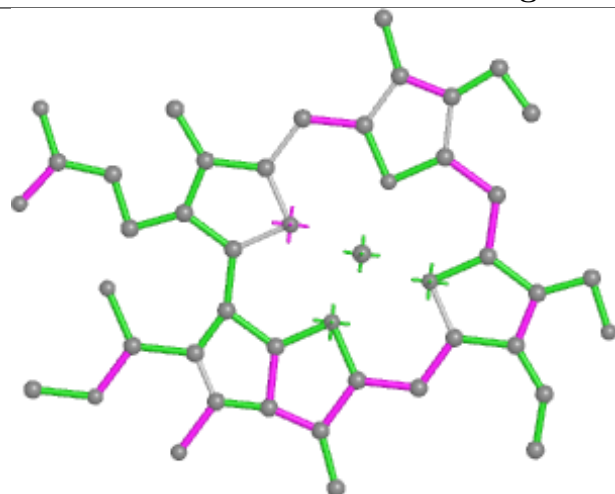


Torsions

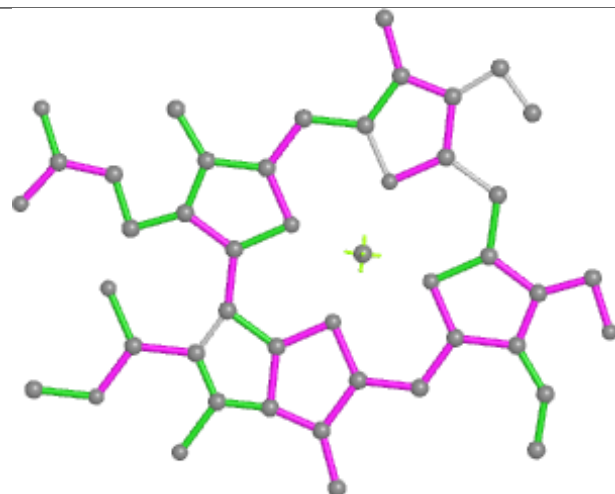


Rings

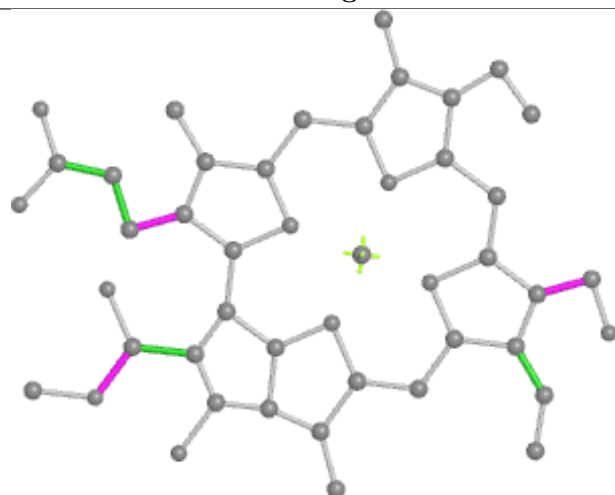
Ligand CHL 4 608



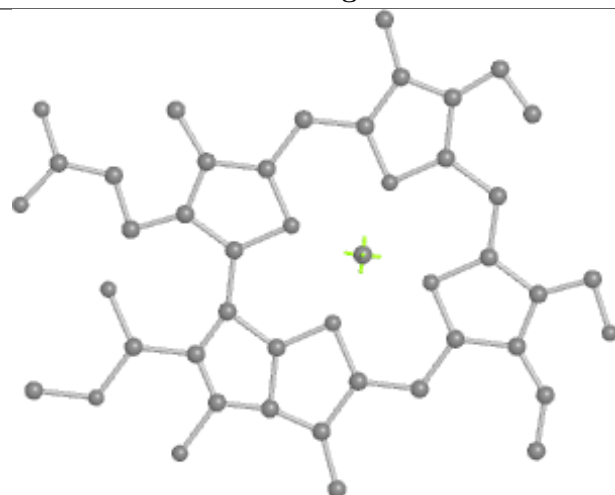
Bond lengths



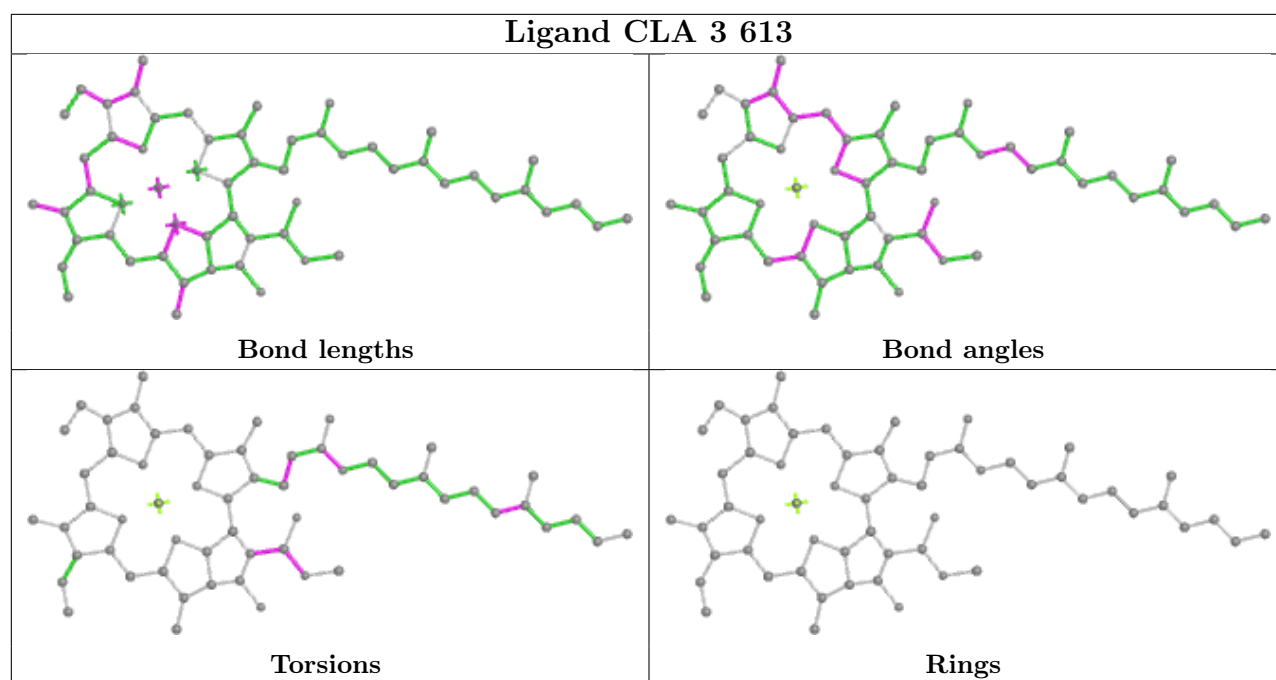
Bond angles



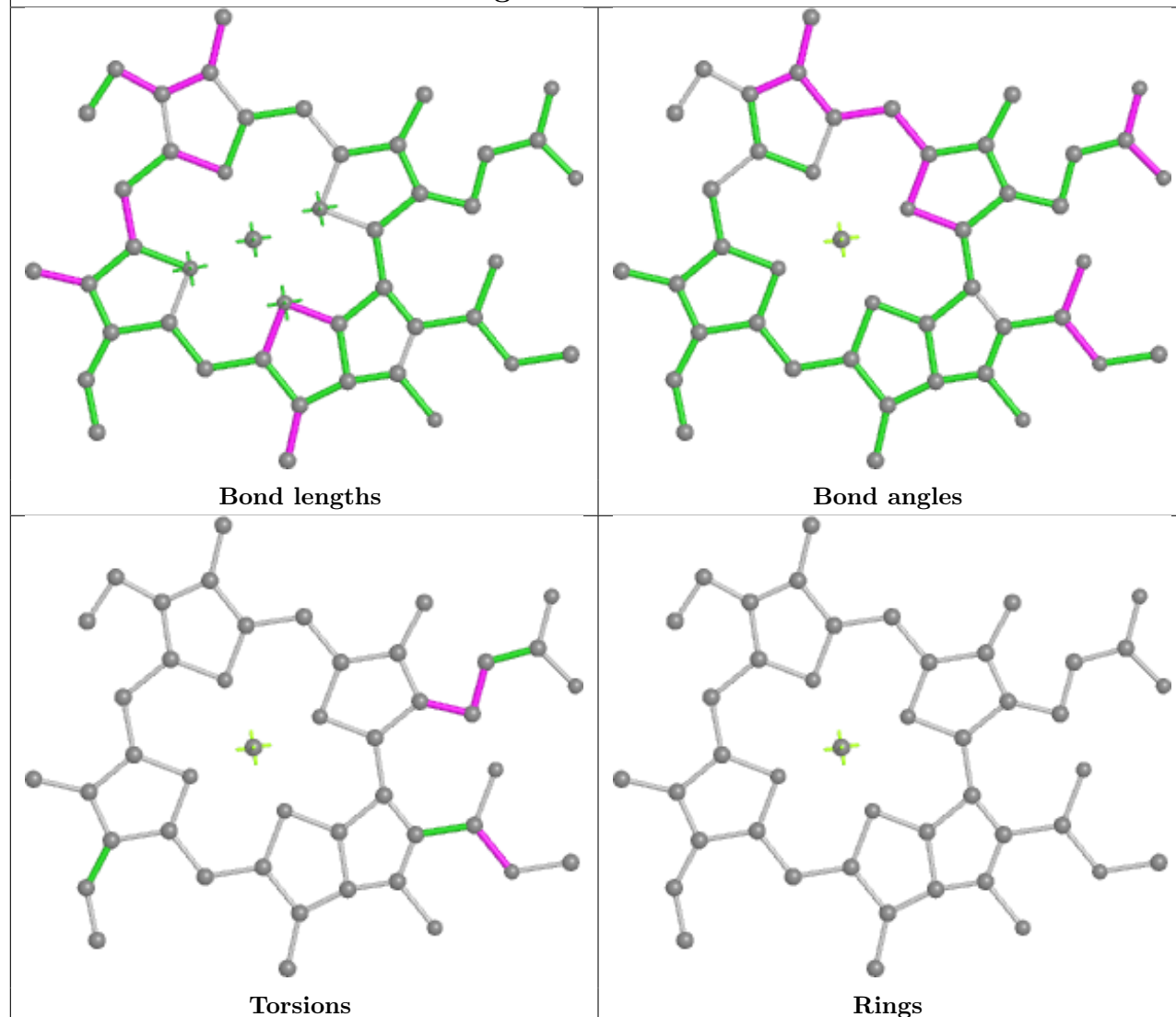
Torsions



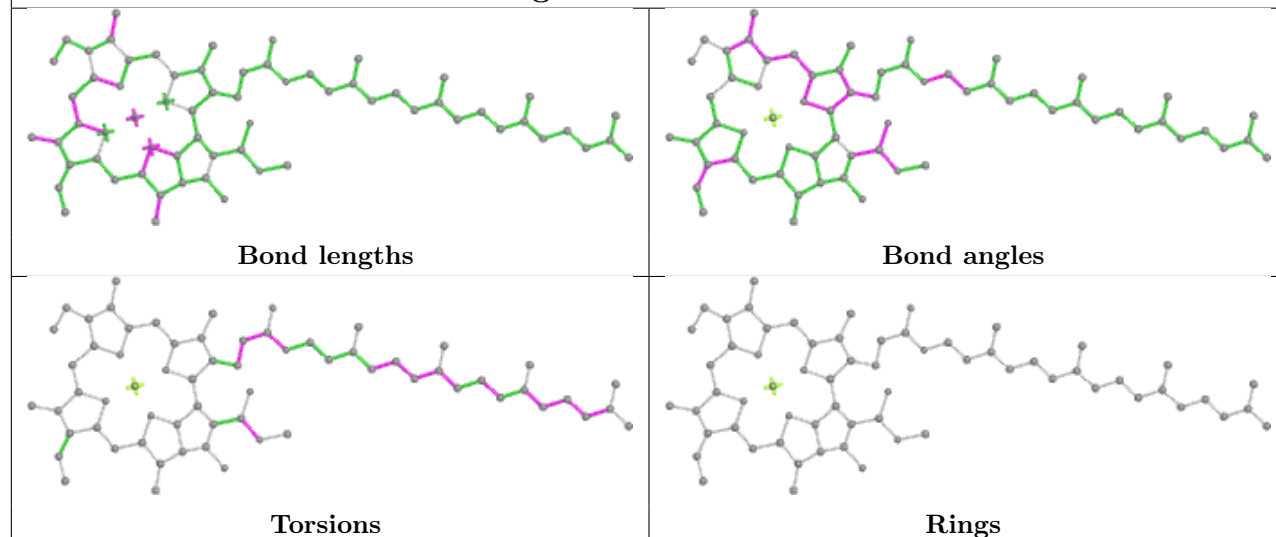
Rings

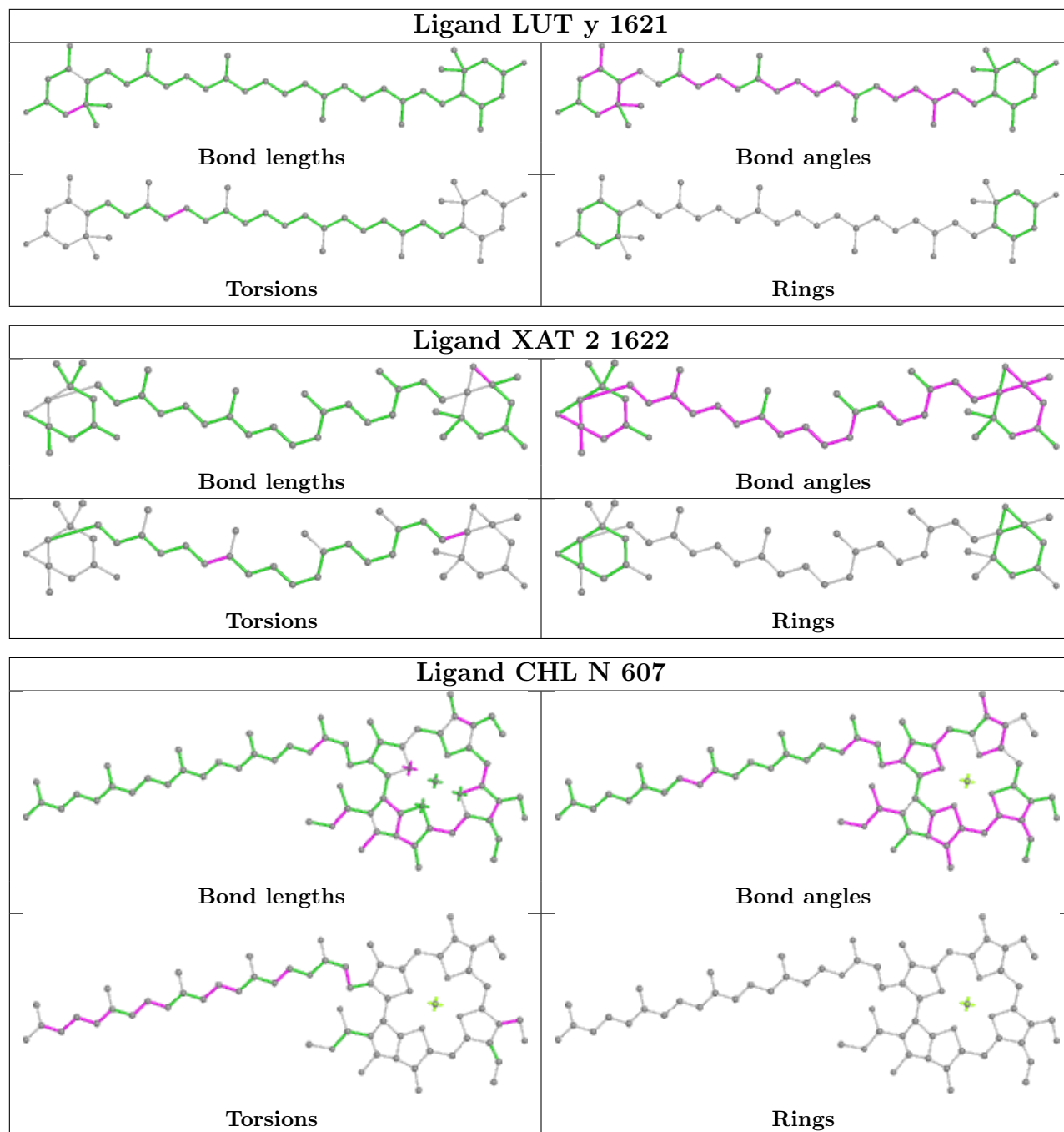


Ligand CLA 8 610

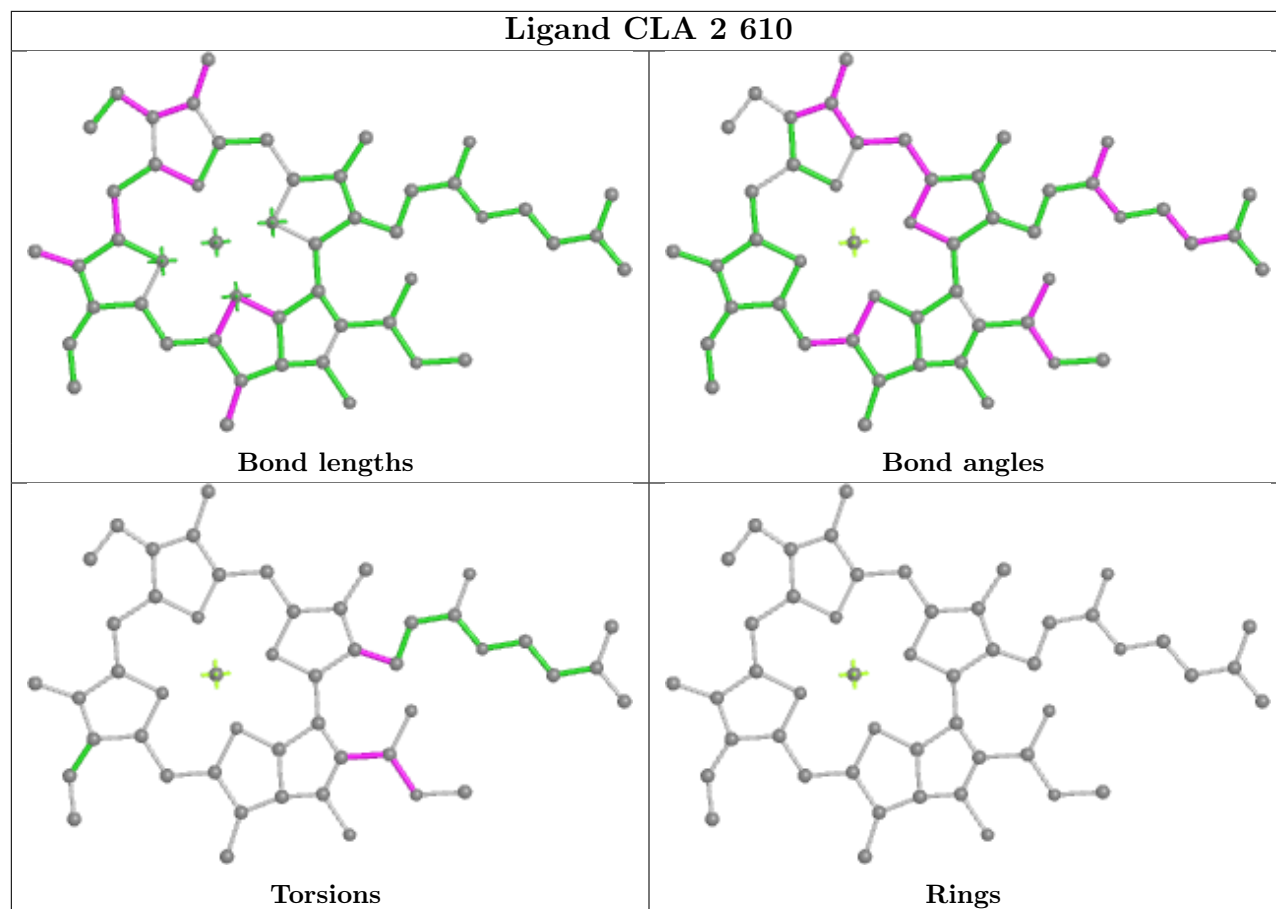


Ligand CLA B 617

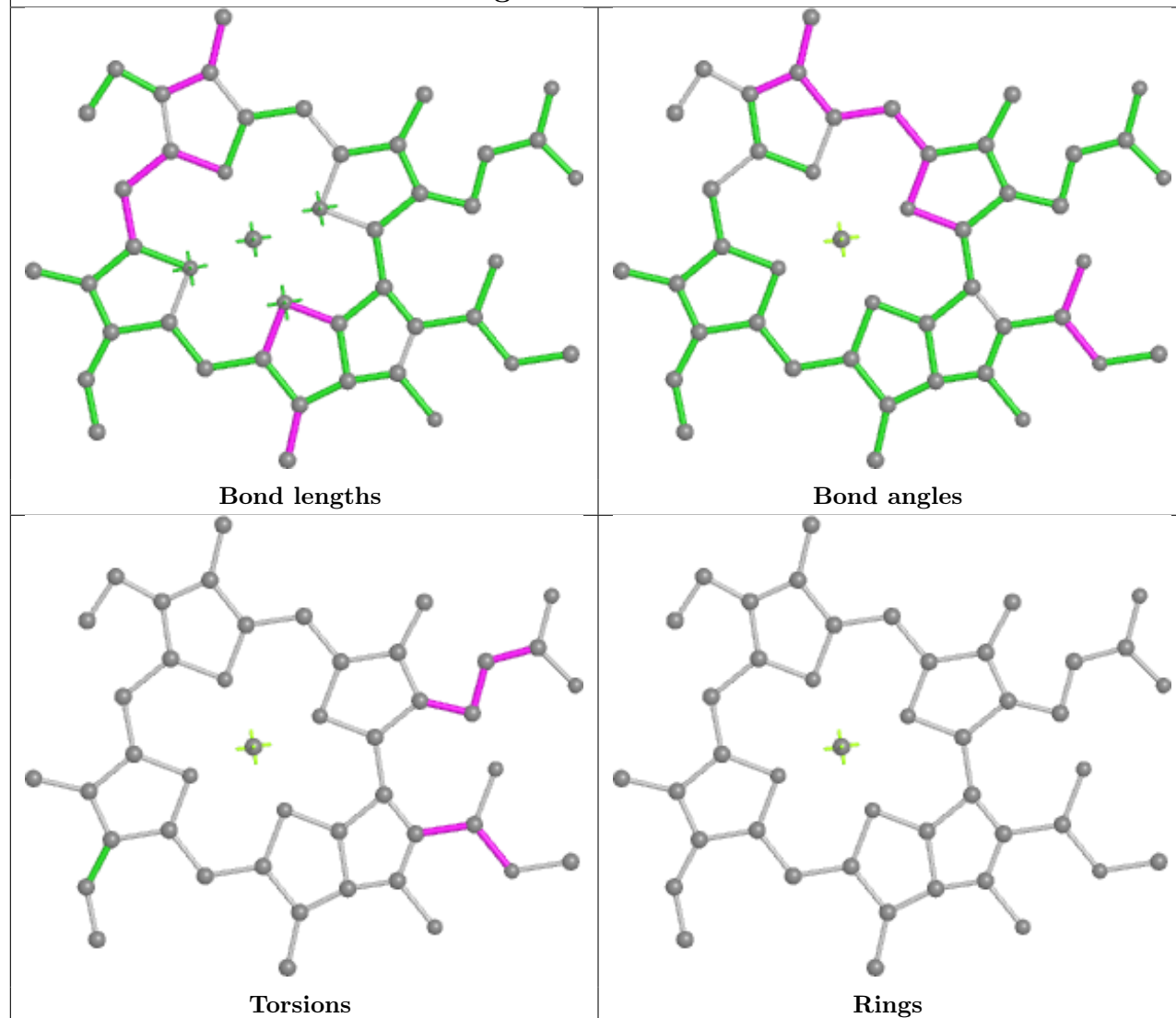




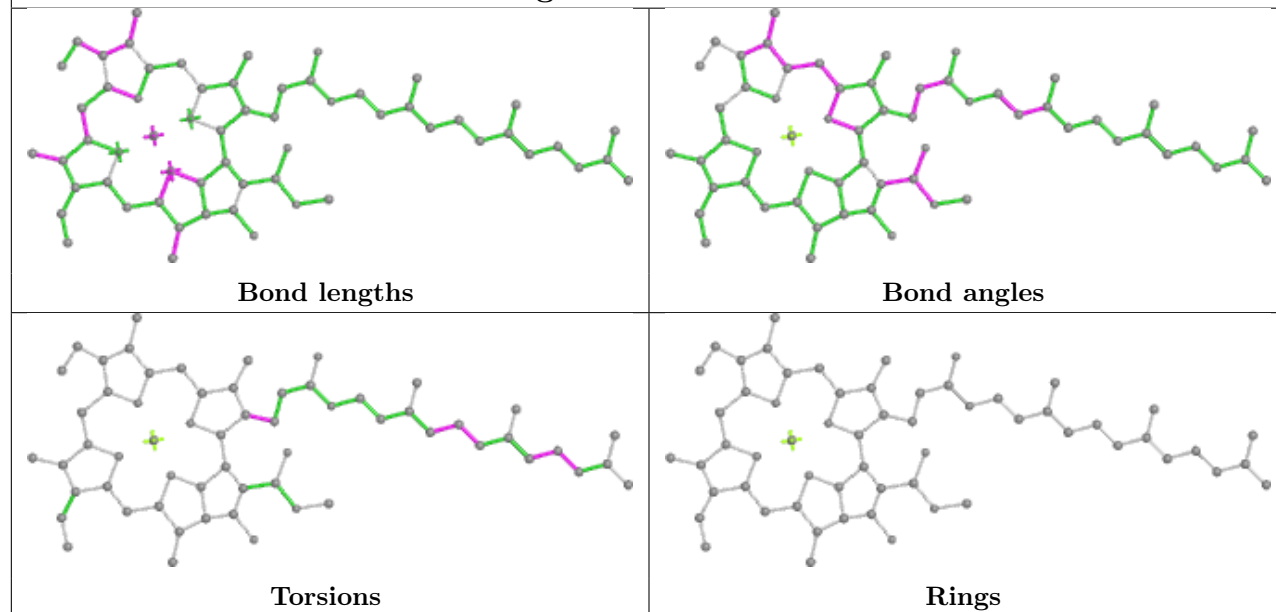
Ligand CLA 2 610

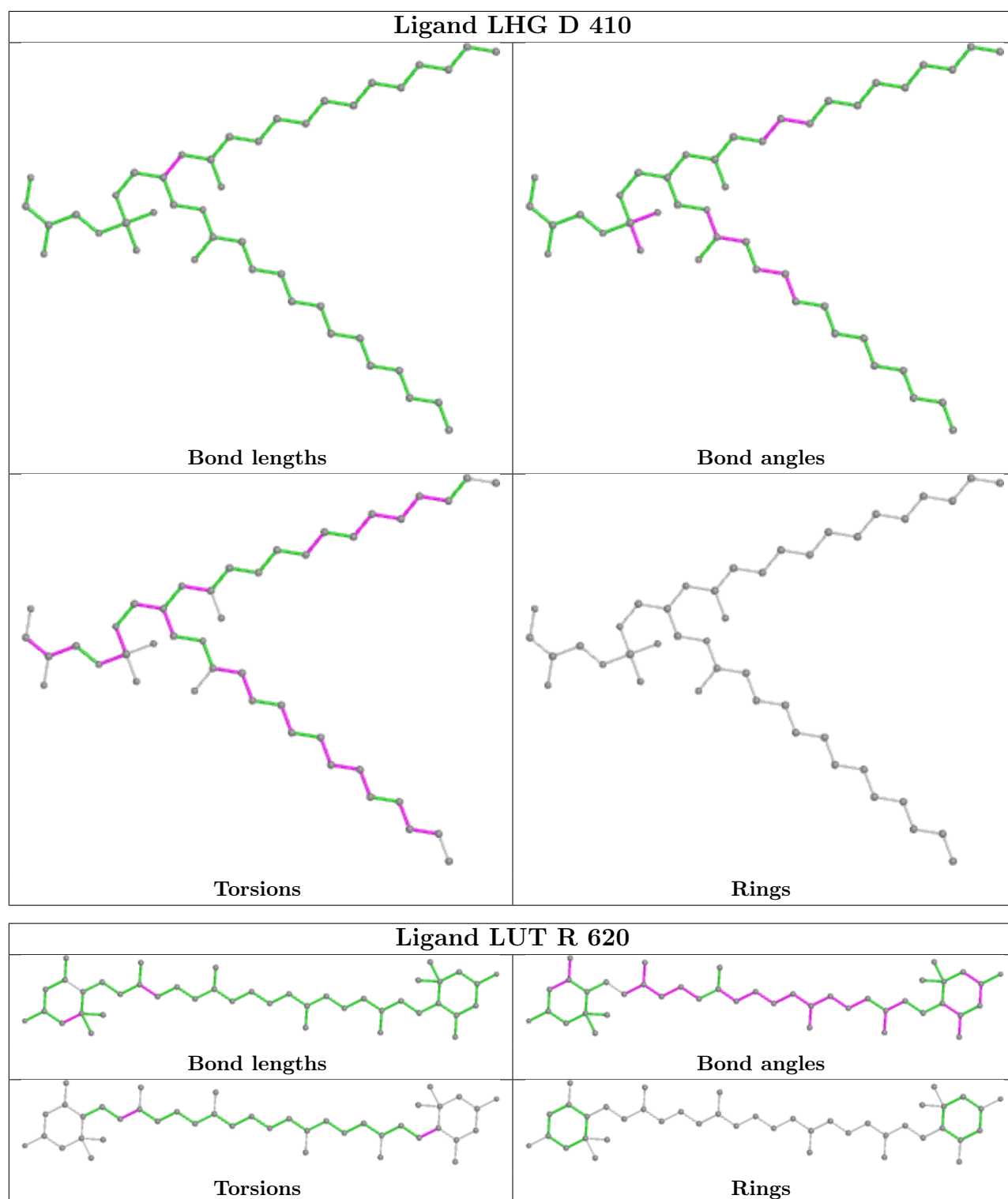


Ligand CLA 6 604

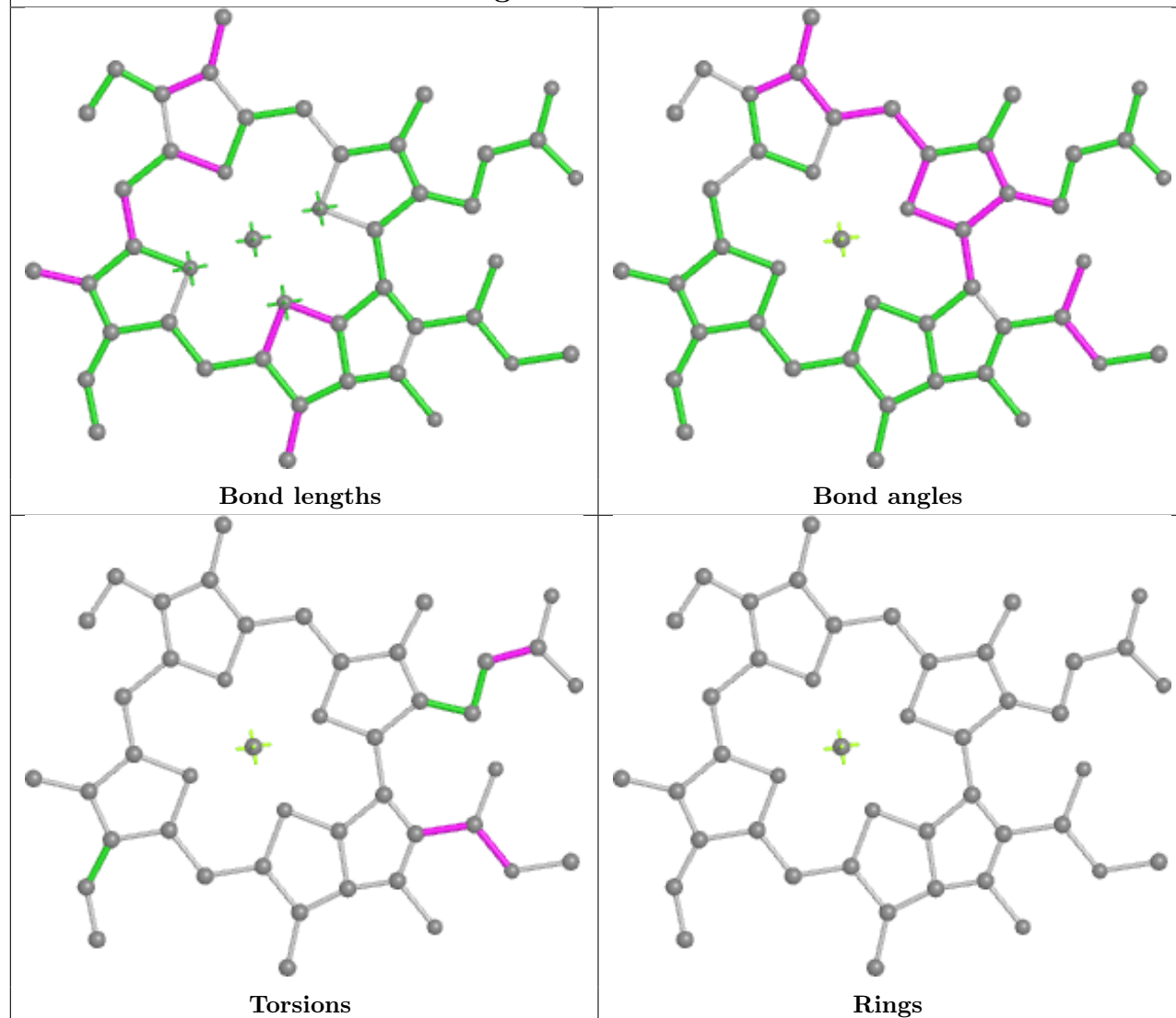


Ligand CLA a 410

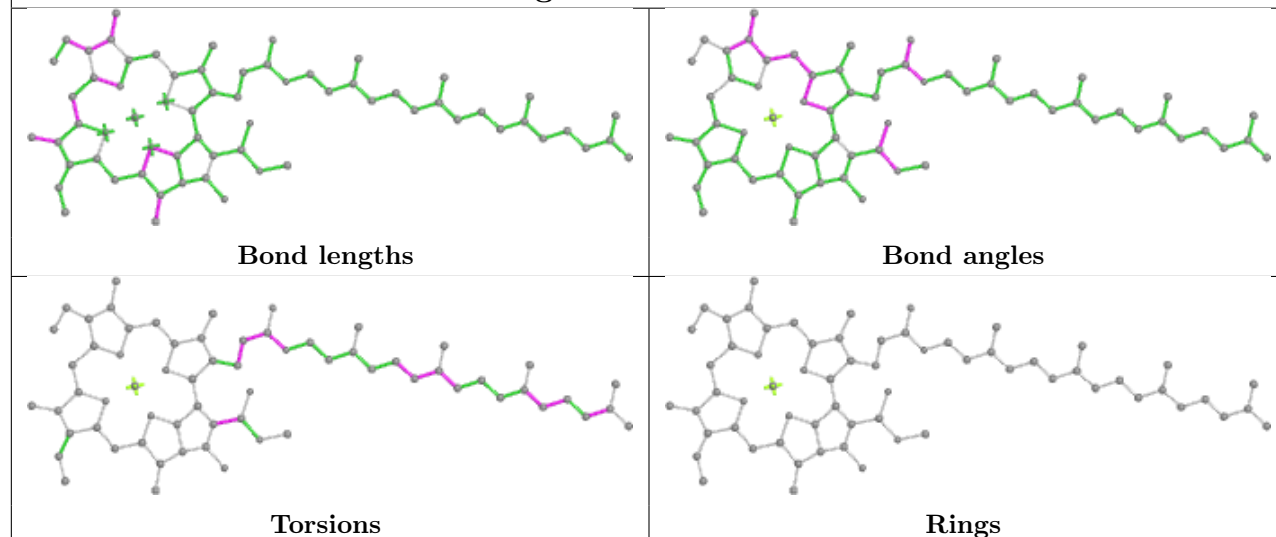


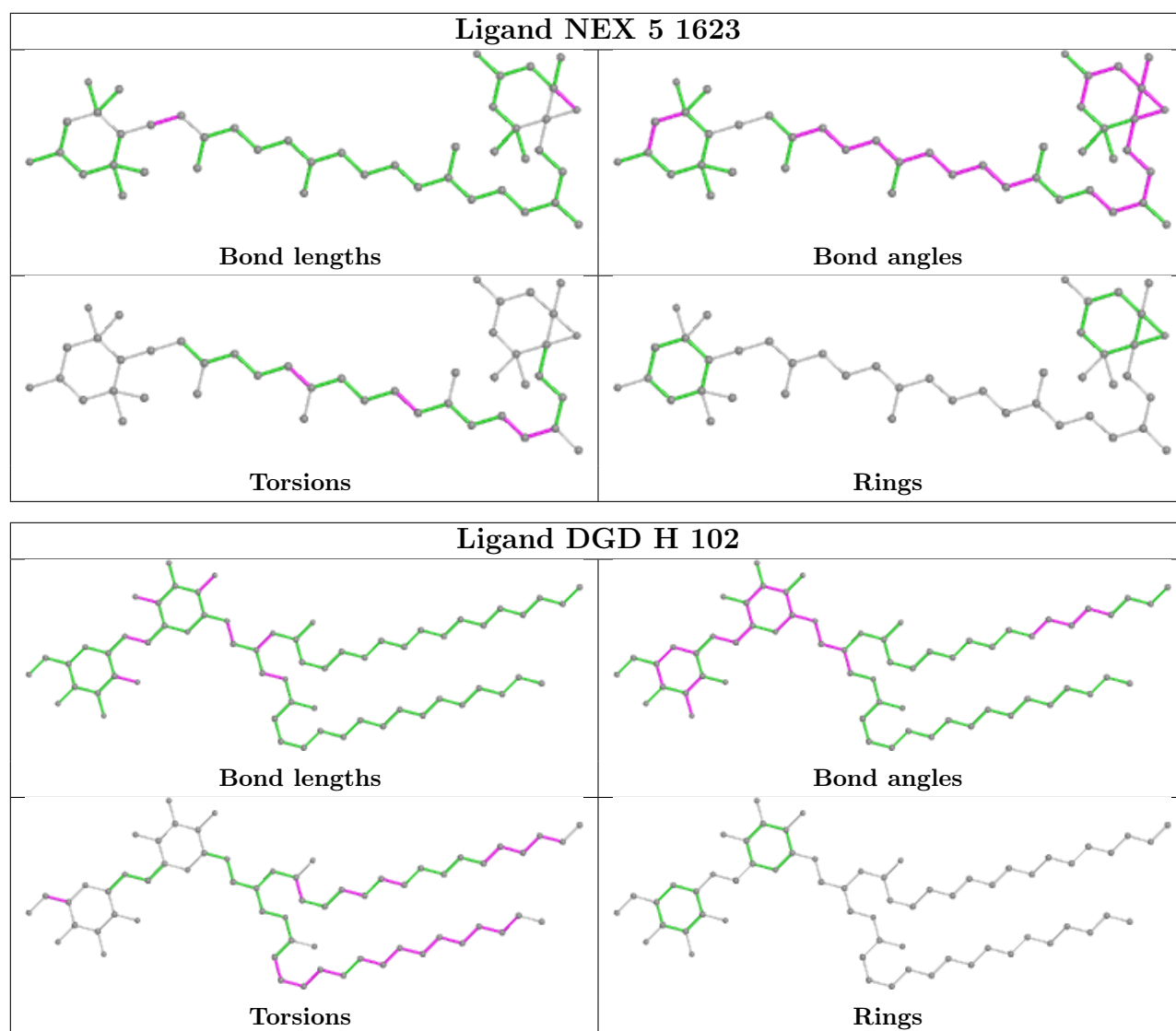


Ligand CLA 6 612



Ligand CLA b 602





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

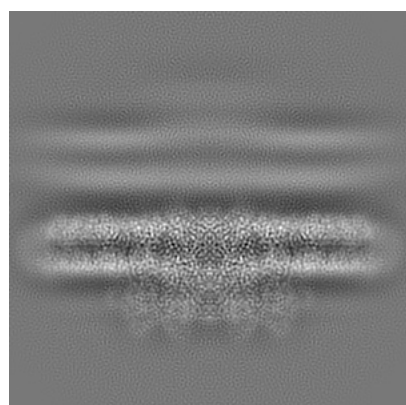
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6741. These allow visual inspection of the internal detail of the map and identification of artifacts.

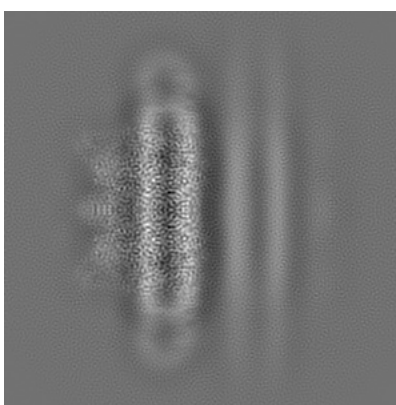
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

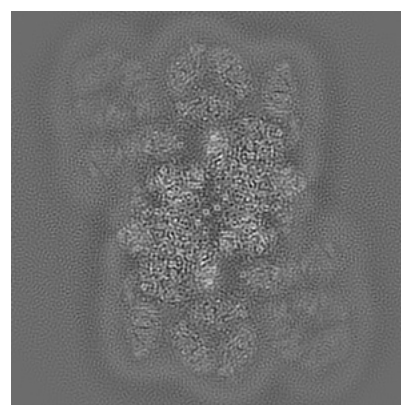
6.1.1 Primary map



X



Y

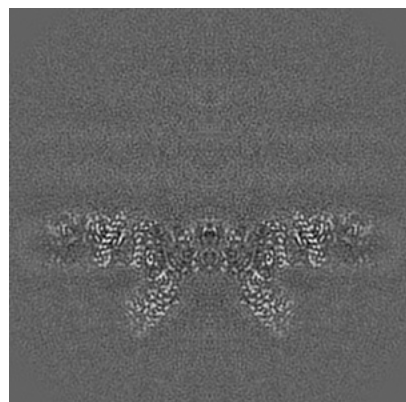


Z

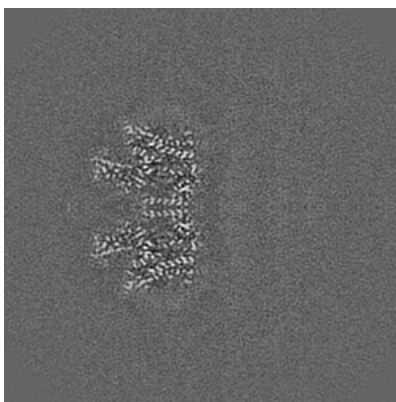
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

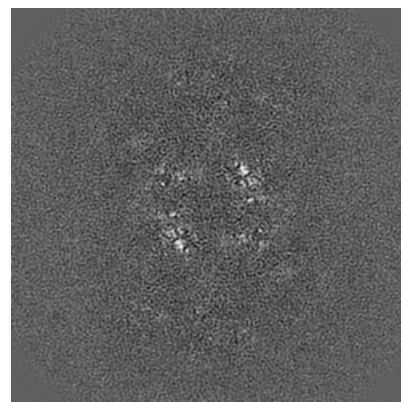
6.2.1 Primary map



X Index: 150



Y Index: 150

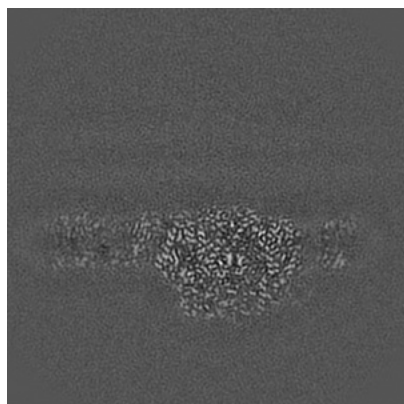


Z Index: 150

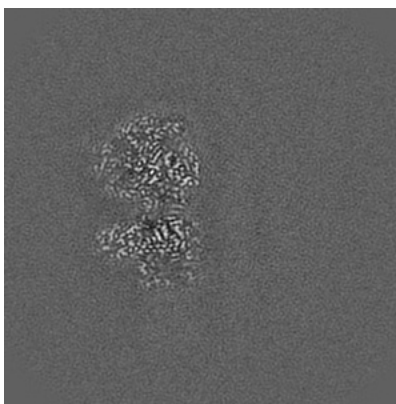
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

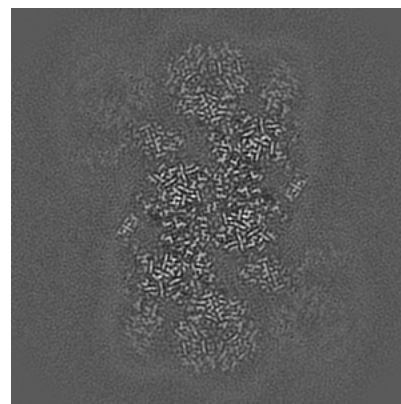
6.3.1 Primary map



X Index: 178



Y Index: 162

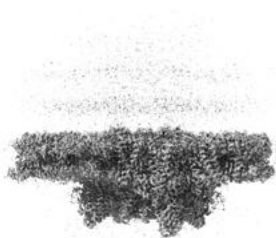


Z Index: 130

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

6.4 Orthogonal surface views [i](#)

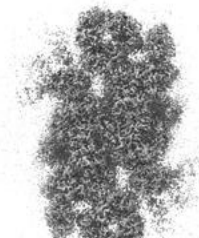
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 17.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

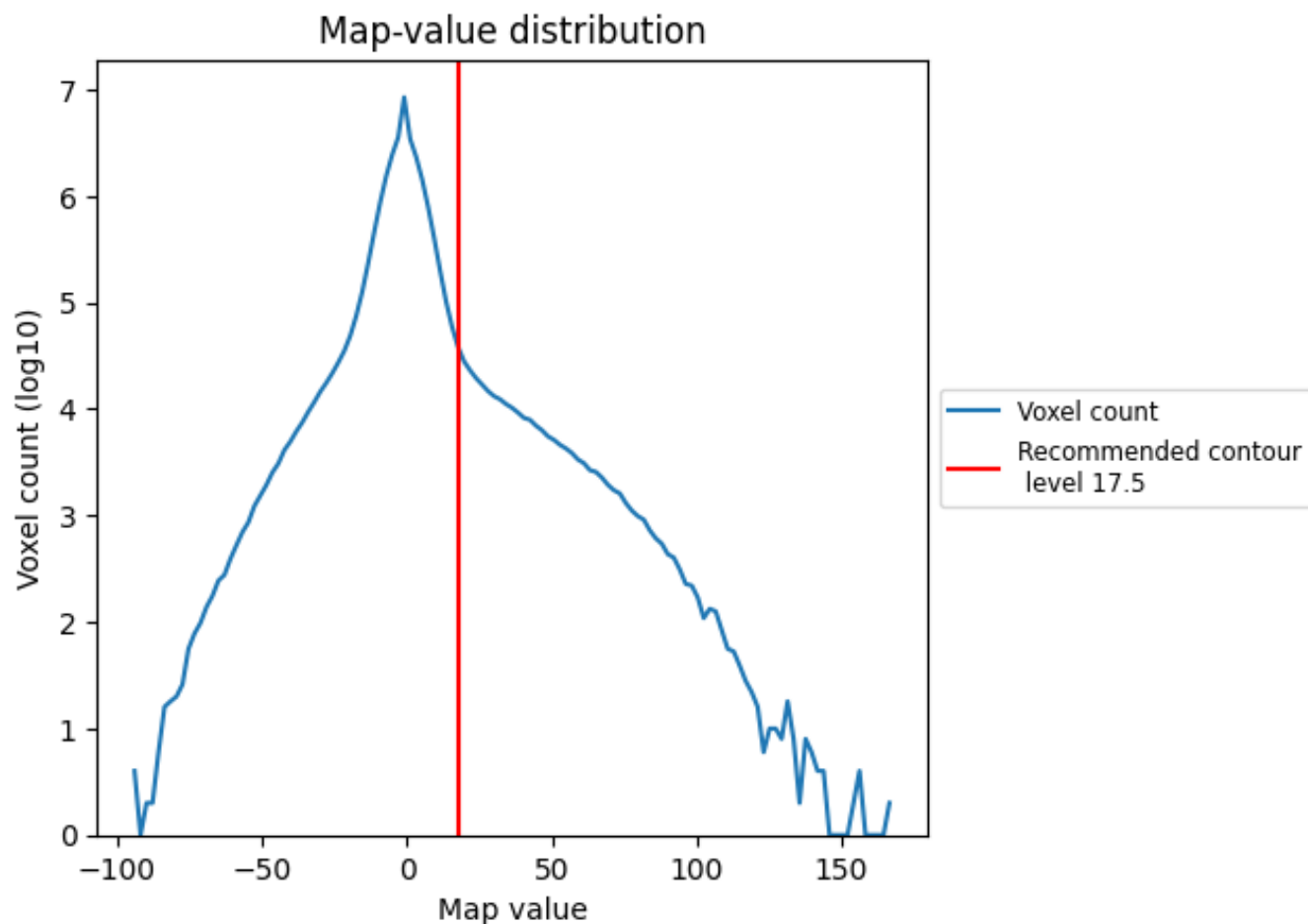
6.5 Mask visualisation

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

7 Map analysis [i](#)

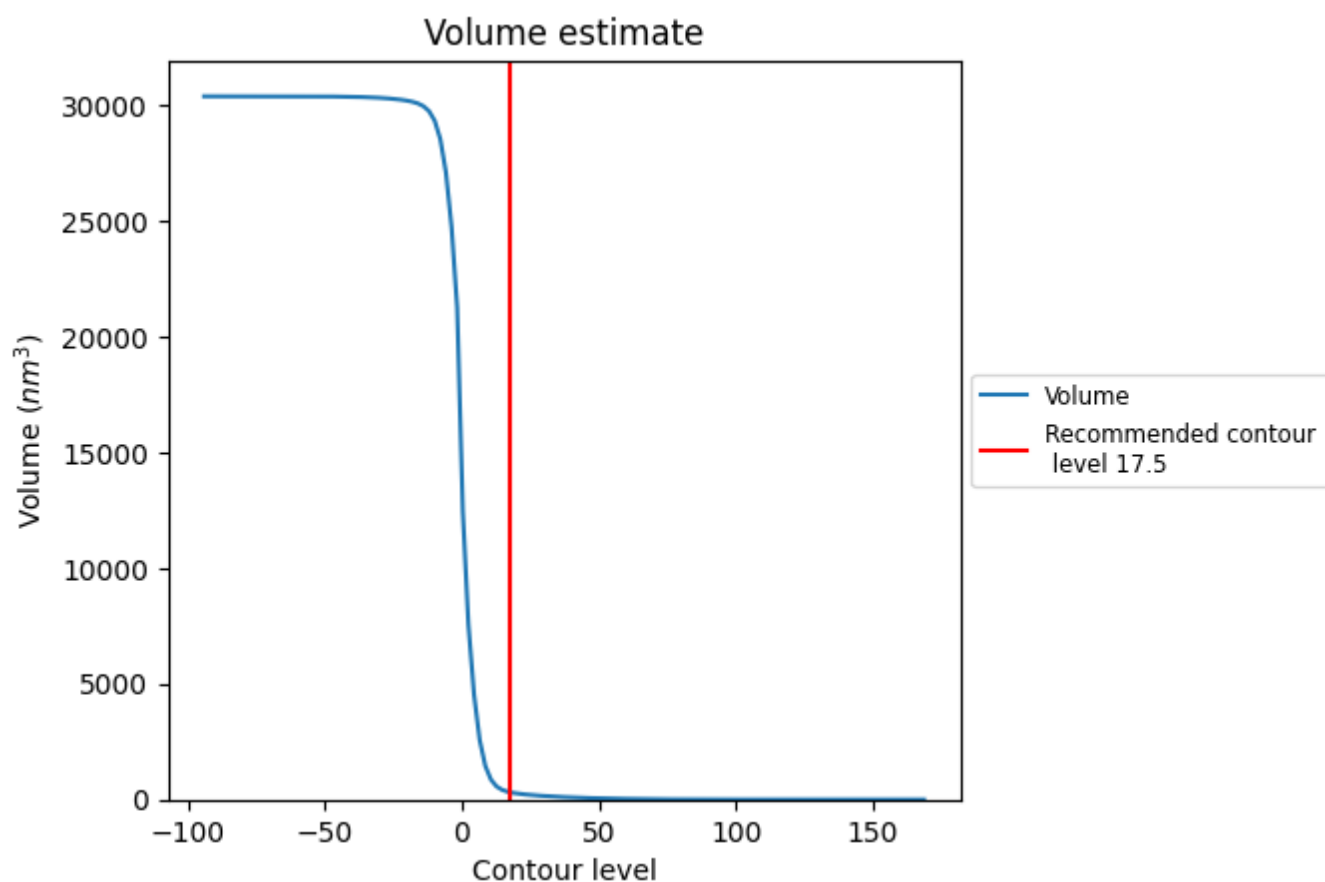
This section contains the results of statistical analysis of the map.

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.

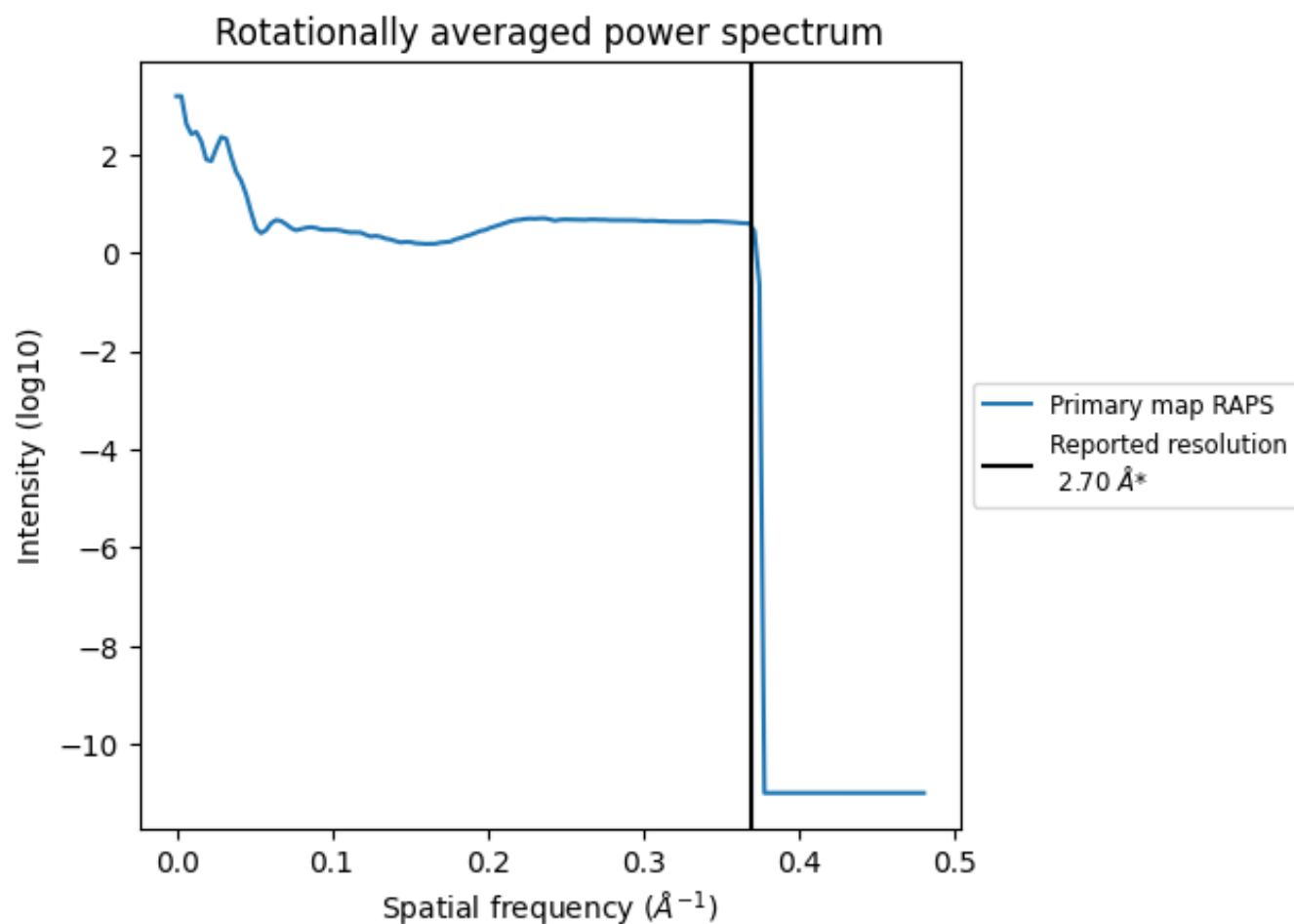
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 319 nm³; this corresponds to an approximate mass of 288 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 0.370 Å⁻¹

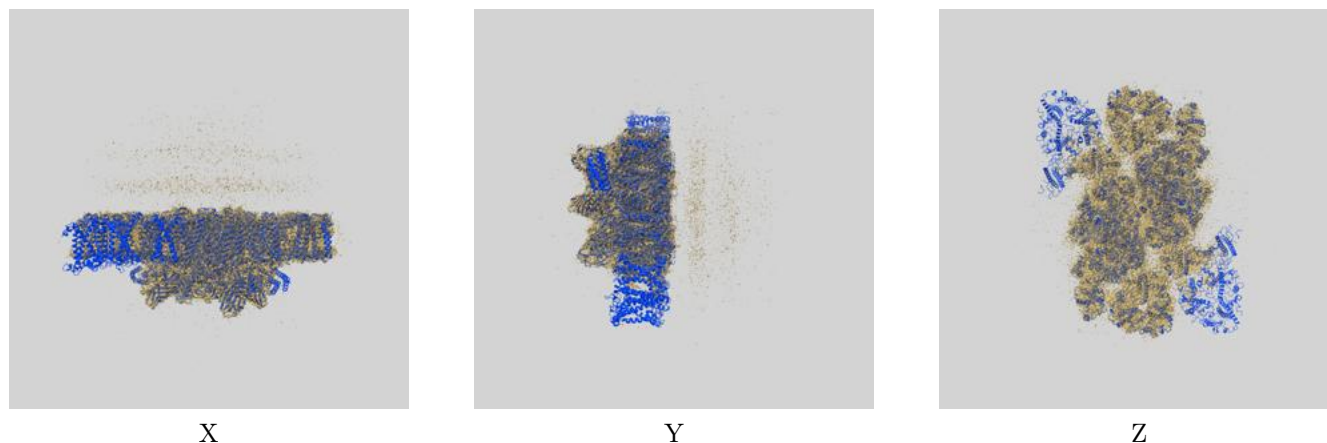
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

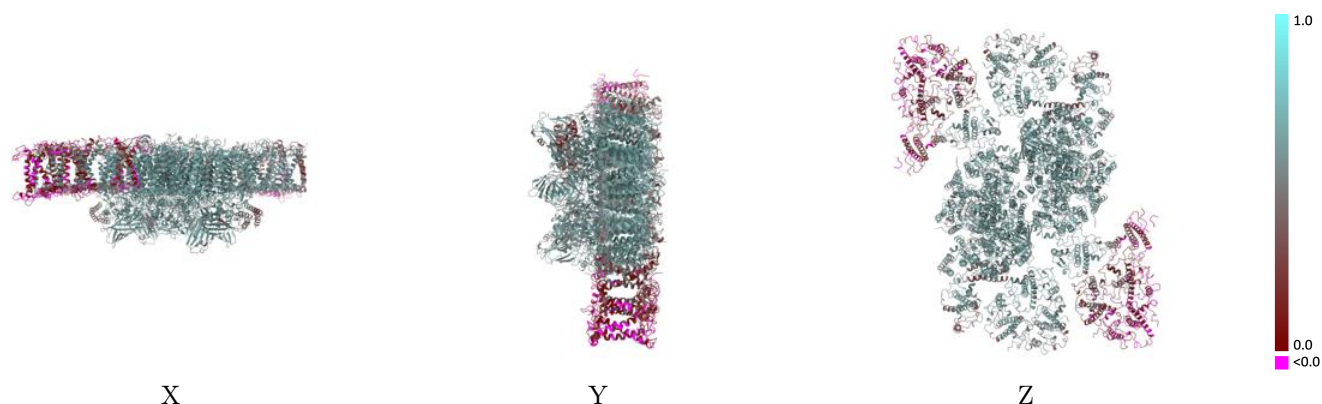
This section contains information regarding the fit between EMDB map EMD-6741 and PDB model 5XNL. Per-residue inclusion information can be found in section 3 on page 51.

9.1 Map-model overlay [i](#)



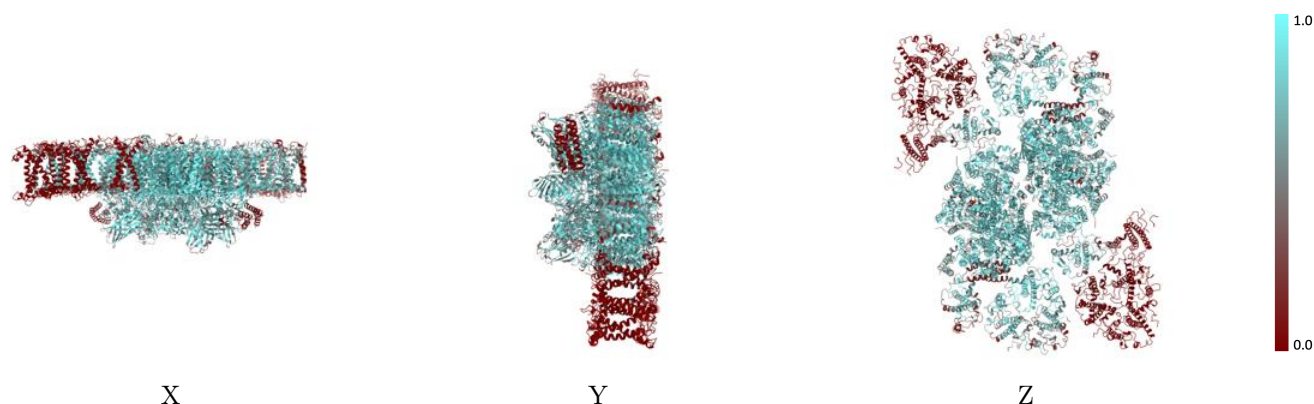
The images above show the 3D surface view of the map at the recommended contour level 17.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



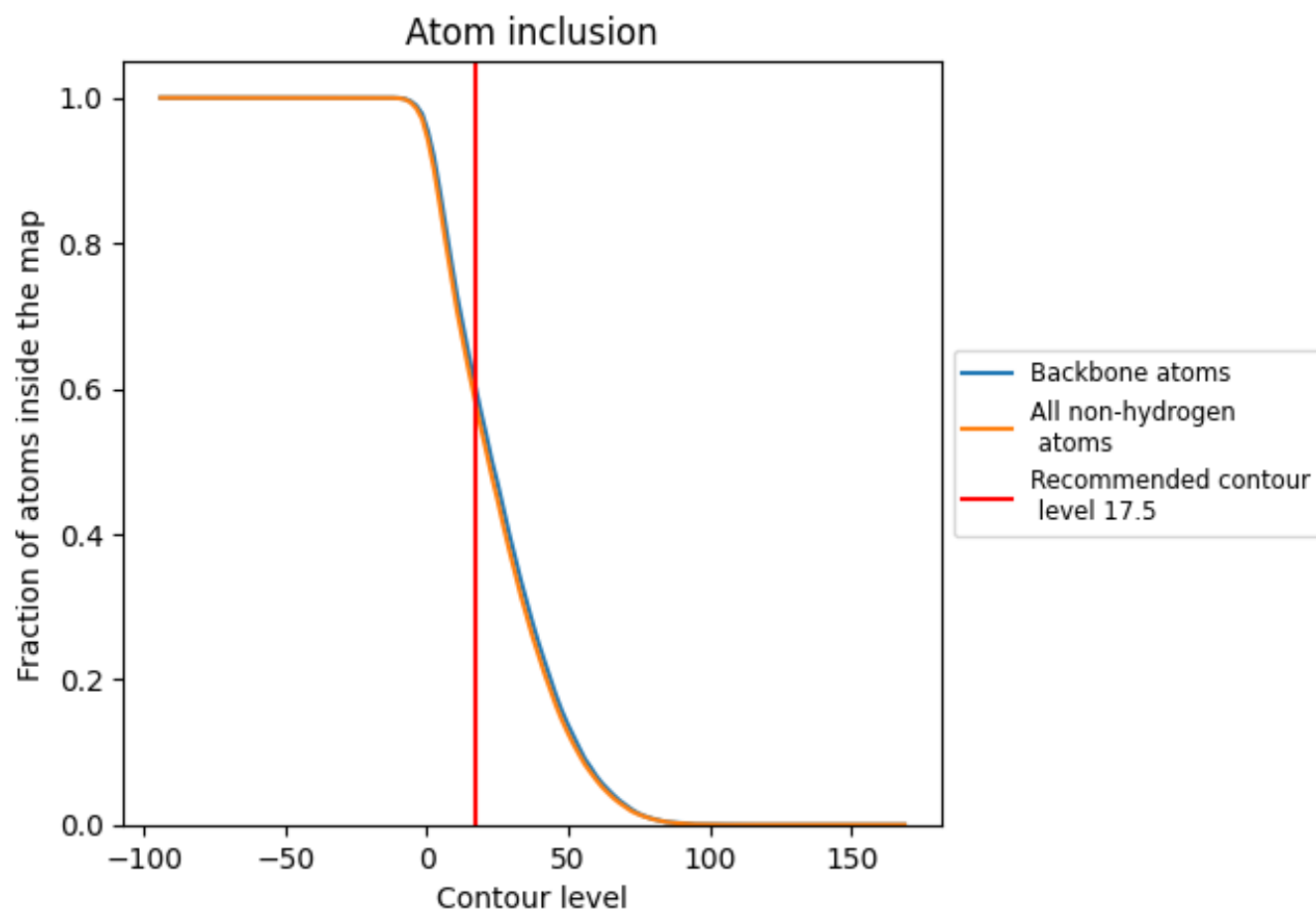
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (17.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 57% 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 (17.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5743	 0.5080
1	 0.0440	 0.2350
2	 0.0004	 0.0900
3	 0.0193	 0.2140
4	 0.0374	 0.1910
5	 0.0444	 0.2370
6	 0.0000	 0.0880
7	 0.0193	 0.2130
8	 0.0369	 0.1890
A	 0.8729	 0.6430
B	 0.8093	 0.6200
C	 0.8211	 0.6290
D	 0.8650	 0.6370
E	 0.7798	 0.6010
F	 0.7891	 0.6140
G	 0.5388	 0.5460
H	 0.8026	 0.6150
I	 0.8755	 0.6340
J	 0.6813	 0.5830
K	 0.7318	 0.5880
L	 0.8085	 0.6190
M	 0.6745	 0.5720
N	 0.6003	 0.5620
O	 0.7227	 0.5810
P	 0.6242	 0.5760
Q	 0.0757	 0.4090
R	 0.6353	 0.5630
S	 0.5200	 0.5220
T	 0.7013	 0.6000
W	 0.6925	 0.5860
X	 0.5876	 0.5550
Y	 0.7971	 0.6100
Z	 0.5575	 0.5360
a	 0.8719	 0.6420
b	 0.8082	 0.6200



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Chain	Atom inclusion	Q-score
c	 0.8196	 0.6300
d	 0.8643	 0.6370
e	 0.7798	 0.6010
f	 0.7927	 0.6130
g	 0.5411	 0.5450
h	 0.8007	 0.6110
i	 0.8755	 0.6330
j	 0.6773	 0.5810
k	 0.7318	 0.5800
l	 0.8056	 0.6240
m	 0.6667	 0.5710
n	 0.5988	 0.5610
o	 0.7211	 0.5820
p	 0.6256	 0.5770
q	 0.0767	 0.4070
r	 0.6361	 0.5650
s	 0.5220	 0.5210
t	 0.6879	 0.6000
w	 0.6925	 0.5880
x	 0.5876	 0.5590
y	 0.7967	 0.6110
z	 0.5536	 0.5340