



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 07:56 PM JST

PDB ID : 8WM6
EMDB ID : EMD-37642
Title : The structure of PSI-CAC(L-14) of R. salina at 2.7 angstroms resolution
Authors : Zhang, S.M.; Si, L.; Li, M.
Deposited on : 2023-10-03
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.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

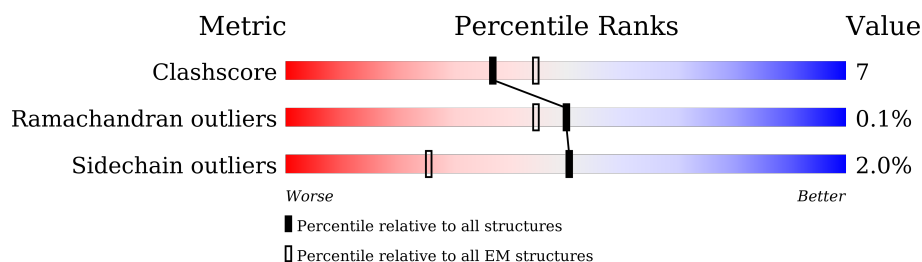
1 Overall quality at a glance

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.




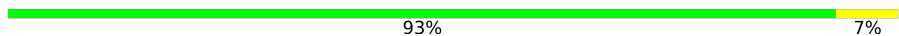







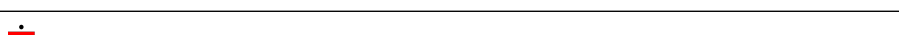
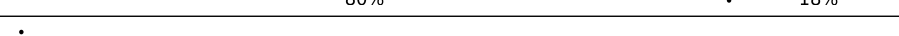
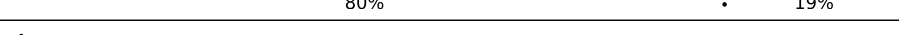
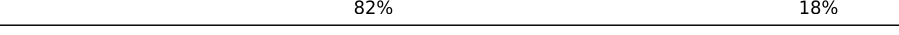








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	752	 87% 11% .
2	B	734	 88% 11% .
3	C	81	 85% 14% .
4	D	141	 80% 18% ..
5	E	64	 84% 9% 6%
6	F	188	 76% 10% 14%
7	I	36	 83% 11% 6%
8	J	42	 90% 10%

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Mol	Chain	Length	Quality of chain
9	L	153	
10	M	30	
11	O	146	
12	K	87	
13	s	269	
14	c	216	
15	a	216	
16	b	223	
17	h	225	
18	f	212	
18	j	212	
18	m	212	
19	e	203	
20	l	238	
21	k	241	
22	i	218	
23	d	213	
24	g	255	
25	R	129	
26	n	219	
27	Q	234	

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
28	CLA	A	801	X	-	-	-
28	CLA	A	802	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	A	803	X	-	-	-
28	CLA	A	804	X	-	-	-
28	CLA	A	805	X	-	-	-
28	CLA	A	806	X	-	-	-
28	CLA	A	807	X	-	-	-
28	CLA	A	808	X	-	-	-
28	CLA	A	809	X	-	-	-
28	CLA	A	810	X	-	-	-
28	CLA	A	812	X	-	-	-
28	CLA	A	813	X	-	-	-
28	CLA	A	815	X	-	-	-
28	CLA	A	816	X	-	-	-
28	CLA	A	817	X	-	-	-
28	CLA	A	818	X	-	-	-
28	CLA	A	819	X	-	-	-
28	CLA	A	820	X	-	-	-
28	CLA	A	822	X	-	-	-
28	CLA	A	824	X	-	-	-
28	CLA	A	826	X	-	-	-
28	CLA	A	827	X	-	-	-
28	CLA	A	829	X	-	-	-
28	CLA	A	831	X	-	-	-
28	CLA	A	832	X	-	-	-
28	CLA	A	833	X	-	-	-
28	CLA	A	834	X	-	-	-
28	CLA	A	835	X	-	-	-
28	CLA	A	837	X	-	-	-
28	CLA	A	838	X	-	-	-
28	CLA	A	839	X	-	-	-
28	CLA	A	840	X	-	-	-
28	CLA	A	841	X	-	-	-
28	CLA	A	851	X	-	-	-
28	CLA	A	852	X	-	-	-
28	CLA	A	854	X	-	-	-
28	CLA	A	855	X	-	-	-
28	CLA	B	801	X	-	-	-
28	CLA	B	802	X	-	-	-
28	CLA	B	803	X	-	-	-
28	CLA	B	804	X	-	-	-
28	CLA	B	805	X	-	-	-
28	CLA	B	806	X	-	-	-
28	CLA	B	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	B	808	X	-	-	-
28	CLA	B	809	X	-	-	-
28	CLA	B	810	X	-	-	-
28	CLA	B	811	X	-	-	-
28	CLA	B	812	X	-	-	-
28	CLA	B	813	X	-	-	-
28	CLA	B	815	X	-	-	-
28	CLA	B	817	X	-	-	-
28	CLA	B	820	X	-	-	-
28	CLA	B	821	X	-	-	-
28	CLA	B	823	X	-	-	-
28	CLA	B	824	X	-	-	-
28	CLA	B	825	X	-	-	-
28	CLA	B	826	X	-	-	-
28	CLA	B	828	X	-	-	-
28	CLA	B	830	X	-	-	-
28	CLA	B	831	X	-	-	-
28	CLA	B	832	X	-	-	-
28	CLA	B	833	X	-	-	-
28	CLA	B	834	X	-	-	-
28	CLA	B	835	X	-	-	-
28	CLA	B	836	X	-	-	-
28	CLA	B	837	X	-	-	-
28	CLA	B	838	X	-	-	-
28	CLA	B	839	X	-	-	-
28	CLA	B	840	X	-	-	-
28	CLA	F	201	X	-	-	-
28	CLA	F	202	X	-	-	-
28	CLA	J	103	X	-	-	-
28	CLA	K	101	X	-	-	-
28	CLA	K	103	X	-	-	-
28	CLA	L	202	X	-	-	-
28	CLA	L	207	X	-	-	-
28	CLA	O	201	X	-	-	-
28	CLA	O	202	X	-	-	-
28	CLA	O	206	X	-	-	-
28	CLA	Q	302	X	-	-	-
28	CLA	Q	303	X	-	-	-
28	CLA	R	203	X	-	-	-
28	CLA	a	303	X	-	-	-
28	CLA	a	304	X	-	-	-
28	CLA	a	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	a	306	X	-	-	-
28	CLA	a	307	X	-	-	-
28	CLA	a	308	X	-	-	-
28	CLA	a	309	X	-	-	-
28	CLA	a	310	X	-	-	-
28	CLA	a	311	X	-	-	-
28	CLA	a	312	X	-	-	-
28	CLA	b	601	X	-	-	-
28	CLA	b	602	X	-	-	-
28	CLA	b	603	X	-	-	-
28	CLA	b	605	X	-	-	-
28	CLA	b	606	X	-	-	-
28	CLA	b	607	X	-	-	-
28	CLA	b	608	X	-	-	-
28	CLA	b	609	X	-	-	-
28	CLA	b	610	X	-	-	-
28	CLA	b	611	X	-	-	-
28	CLA	b	612	X	-	-	-
28	CLA	c	601	X	-	-	-
28	CLA	c	602	X	-	-	-
28	CLA	c	603	X	-	-	-
28	CLA	c	605	X	-	-	-
28	CLA	c	607	X	-	-	-
28	CLA	c	608	X	-	-	-
28	CLA	c	609	X	-	-	-
28	CLA	c	612	X	-	-	-
28	CLA	d	301	X	-	-	-
28	CLA	d	302	X	-	-	-
28	CLA	d	303	X	-	-	-
28	CLA	d	304	X	-	-	-
28	CLA	d	305	X	-	-	-
28	CLA	d	306	X	-	-	-
28	CLA	d	307	X	-	-	-
28	CLA	d	308	X	-	-	-
28	CLA	d	309	X	-	-	-
28	CLA	e	601	X	-	-	-
28	CLA	e	603	X	-	-	-
28	CLA	e	606	X	-	-	-
28	CLA	e	607	X	-	-	-
28	CLA	e	608	X	-	-	-
28	CLA	e	610	X	-	-	-
28	CLA	e	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	f	601	X	-	-	-
28	CLA	f	602	X	-	-	-
28	CLA	f	603	X	-	-	-
28	CLA	f	604	X	-	-	-
28	CLA	f	608	X	-	-	-
28	CLA	f	609	X	-	-	-
28	CLA	f	610	X	-	-	-
28	CLA	f	612	X	-	-	-
28	CLA	f	613	X	-	-	-
28	CLA	g	302	X	-	-	-
28	CLA	g	303	X	-	-	-
28	CLA	g	304	X	-	-	-
28	CLA	g	306	X	-	-	-
28	CLA	g	307	X	-	-	-
28	CLA	g	308	X	-	-	-
28	CLA	g	309	X	-	-	-
28	CLA	g	310	X	-	-	-
28	CLA	g	311	X	-	-	-
28	CLA	g	315	X	-	-	-
28	CLA	g	322	X	-	-	-
28	CLA	h	302	X	-	-	-
28	CLA	h	303	X	-	-	-
28	CLA	h	304	X	-	-	-
28	CLA	h	305	X	-	-	-
28	CLA	h	306	X	-	-	-
28	CLA	h	307	X	-	-	-
28	CLA	h	308	X	-	-	-
28	CLA	h	313	X	-	-	-
28	CLA	i	302	X	-	-	-
28	CLA	i	303	X	-	-	-
28	CLA	i	304	X	-	-	-
28	CLA	i	306	X	-	-	-
28	CLA	i	307	X	-	-	-
28	CLA	i	308	X	-	-	-
28	CLA	i	309	X	-	-	-
28	CLA	i	311	X	-	-	-
28	CLA	i	312	X	-	-	-
28	CLA	j	601	X	-	-	-
28	CLA	j	602	X	-	-	-
28	CLA	j	603	X	-	-	-
28	CLA	j	605	X	-	-	-
28	CLA	j	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	j	607	X	-	-	-
28	CLA	j	608	X	-	-	-
28	CLA	j	609	X	-	-	-
28	CLA	j	610	X	-	-	-
28	CLA	j	612	X	-	-	-
28	CLA	j	613	X	-	-	-
28	CLA	k	602	X	-	-	-
28	CLA	k	603	X	-	-	-
28	CLA	k	604	X	-	-	-
28	CLA	k	605	X	-	-	-
28	CLA	k	607	X	-	-	-
28	CLA	k	608	X	-	-	-
28	CLA	k	609	X	-	-	-
28	CLA	k	610	X	-	-	-
28	CLA	k	614	X	-	-	-
28	CLA	l	302	X	-	-	-
28	CLA	l	303	X	-	-	-
28	CLA	l	304	X	-	-	-
28	CLA	l	305	X	-	-	-
28	CLA	l	306	X	-	-	-
28	CLA	l	307	X	-	-	-
28	CLA	l	308	X	-	-	-
28	CLA	l	309	X	-	-	-
28	CLA	l	311	X	-	-	-
28	CLA	m	601	X	-	-	-
28	CLA	m	602	X	-	-	-
28	CLA	m	603	X	-	-	-
28	CLA	m	606	X	-	-	-
28	CLA	m	607	X	-	-	-
28	CLA	m	608	X	-	-	-
28	CLA	m	609	X	-	-	-
28	CLA	m	610	X	-	-	-
28	CLA	m	612	X	-	-	-
28	CLA	m	613	X	-	-	-
28	CLA	n	601	X	-	-	-
28	CLA	n	603	X	-	-	-
28	CLA	n	604	X	-	-	-
28	CLA	n	605	X	-	-	-
28	CLA	n	606	X	-	-	-
28	CLA	n	607	X	-	-	-
28	CLA	n	608	X	-	-	-
28	CLA	n	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	n	610	X	-	-	-
28	CLA	n	613	X	-	-	-
28	CLA	s	202	X	-	-	-
28	CLA	s	206	X	-	-	-
28	CLA	s	208	X	-	-	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 61164 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5825	3802	994	1001	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	1	0
			5826	3844	982	985	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			592	361	103	116	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1084	692	186	203	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	60	Total	C	N	O	0	0
			484	309	84	91		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	161	Total	C	N	O	S	0	0
			1254	814	212	226	2		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	34	Total	C	N	O	S	0	0
			264	182	35	45	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	42	Total	C	N	O	S	0	0
			351	240	49	59	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	151	Total	C	N	O	S	0	0
			1146	753	182	208	3		

- Molecule 10 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	30	Total	C	N	O	S	0	0
			232	155	38	38	1		

- Molecule 11 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	104	Total	C	N	O	S	0	0
			773	515	117	138	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	69	Total	C	N	O	S	0	0
			488	319	80	87	2		

- Molecule 13 is a protein called chain s.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	s	154	Total	C	N	O	S	0	0
			1140	719	195	217	9		

- Molecule 14 is a protein called cac-c.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	170	Total	C	N	O	S	0	0
			1357	897	221	236	3		

- Molecule 15 is a protein called cac-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	175	Total	C	N	O	S	0	0
			1361	889	217	245	10		

- Molecule 16 is a protein called cac-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	b	194	Total	C	N	O	S	0	0
			1439	916	251	258	14		

- Molecule 17 is a protein called cac-h.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	h	162	Total	C	N	O	S	0	0
			1200	778	202	214	6		

- Molecule 18 is a protein called cac-f.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	m	174	Total	C	N	O	S	0	0
			1309	846	214	241	8		
18	f	174	Total	C	N	O	S	0	0
			1302	842	212	240	8		
18	j	172	Total	C	N	O	S	0	0
			1293	834	212	239	8		

- Molecule 19 is a protein called cac-e.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	169	Total	C	N	O	S	0	0
			1286	843	207	228	8		

- Molecule 20 is a protein called cac-l.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	175	Total	C	N	O	S	0	0
			1344	869	230	238	7		

- Molecule 21 is a protein called cac-k.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	k	180	Total	C	N	O	S	0	0
			1346	872	223	239	12		

- Molecule 22 is a protein called cac-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	i	175	Total	C	N	O	S	0	0
			1324	849	227	237	11		

- Molecule 23 is a protein called cac-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	129	Total	C	N	O	S	0	0
			974	624	169	171	10		

- Molecule 24 is a protein called cac-g.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	g	219	Total	C	N	O	S	0	0
			1630	1060	267	292	11		

- Molecule 25 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	90	Total	C	N	O	S	0	0
			664	434	105	124	1		

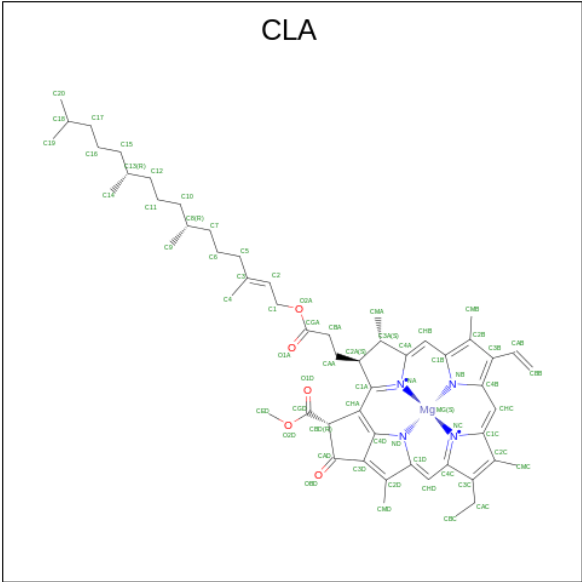
- Molecule 26 is a protein called cac-n.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	n	181	Total	C	N	O	S	0	0
			1350	870	228	242	10		

- Molecule 27 is a protein called PsaQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	179	Total	C	N	O	S	0	0
			1294	814	222	252	6		

- Molecule 28 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
28	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	F	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
28	L	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
28	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	s	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	c	1	Total 52	C 42	Mg 1	N 4	O 5	0
28	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	a	1	Total 52	C 42	Mg 1	N 4	O 5	0
28	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
28	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
28	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	h	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	h	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	h	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	h	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
28	m	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
28	m	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
28	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	e	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	e	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	l	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	l	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	l	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	l	1	Total 61	C 51	Mg 1	N 4	O 5	0
28	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	k	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	k	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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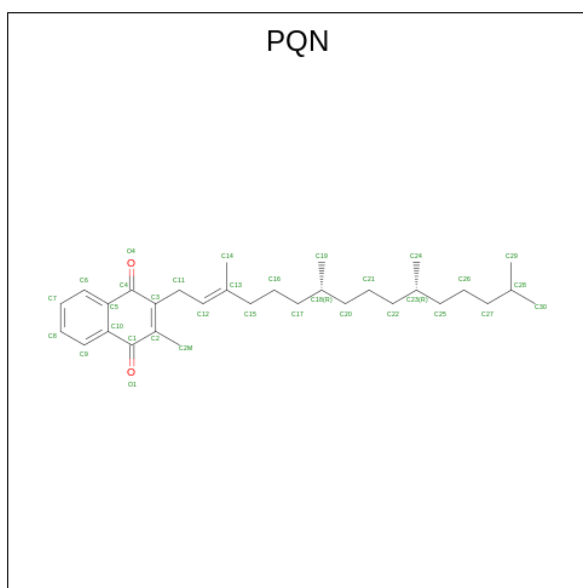
Mol	Chain	Residues	Atoms					AltConf
28	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	d	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
28	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	g	1	Total 54	C 44	Mg 1	N 4	O 5	0
28	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	R	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	n	1	Total 45	C 35	Mg 1	N 4	O 5	0

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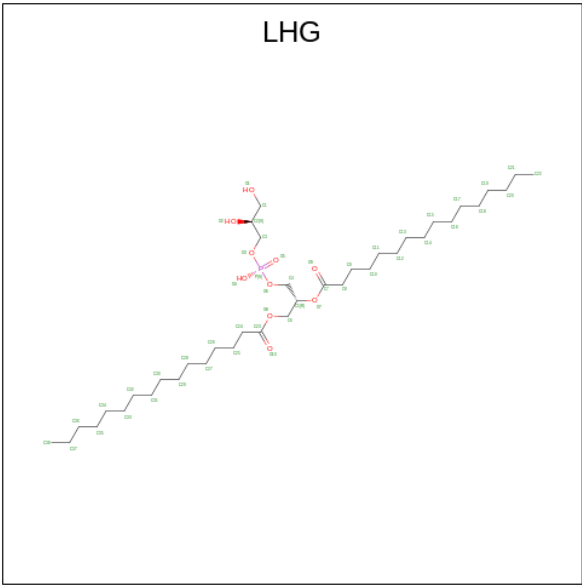
Mol	Chain	Residues	Atoms					AltConf
28	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 29 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

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



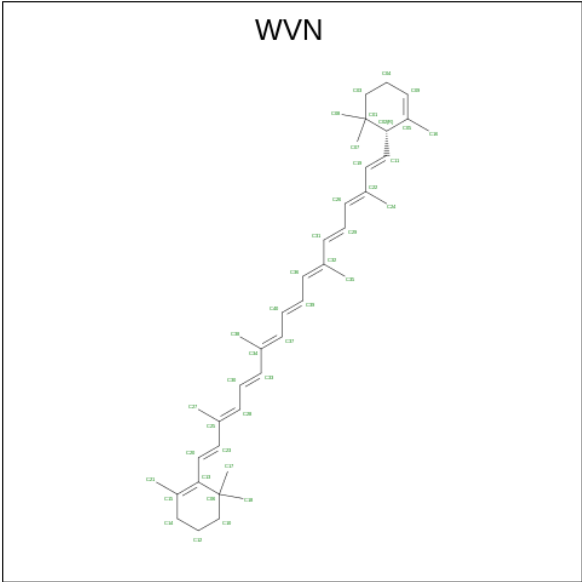
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			48	37	10	1	
30	A	1	Total	C	O	P	0
			27	16	10	1	
30	A	1	Total	C	O	P	0
			38	27	10	1	
30	J	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	c	1	Total	C	O	P	0
			37	26	10	1	
30	c	1	Total	C	O	P	0
			37	26	10	1	
30	a	1	Total	C	O	P	0
			49	38	10	1	
30	a	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
30	b	1	Total	C	O	P	0
			49	38	10	1	
30	b	1	Total	C	O	P	0
			31	20	10	1	
30	m	1	Total	C	O	P	0
			37	26	10	1	
30	e	1	Total	C	O	P	0
			37	26	10	1	
30	l	1	Total	C	O	P	0
			32	21	10	1	
30	k	1	Total	C	O	P	0
			37	26	10	1	
30	f	1	Total	C	O	P	0
			49	38	10	1	
30	i	1	Total	C	O	P	0
			37	26	10	1	
30	j	1	Total	C	O	P	0
			30	19	10	1	
30	d	1	Total	C	O	P	0
			37	26	10	1	
30	g	1	Total	C	O	P	0
			37	26	10	1	
30	g	1	Total	C	O	P	0
			37	26	10	1	
30	n	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 31 is 1,3,3-trimethyl-2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-[(1R)-2,6,6-trimethylcyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohexene (three-letter code: WVN) (formula: C₄₀H₅₆).



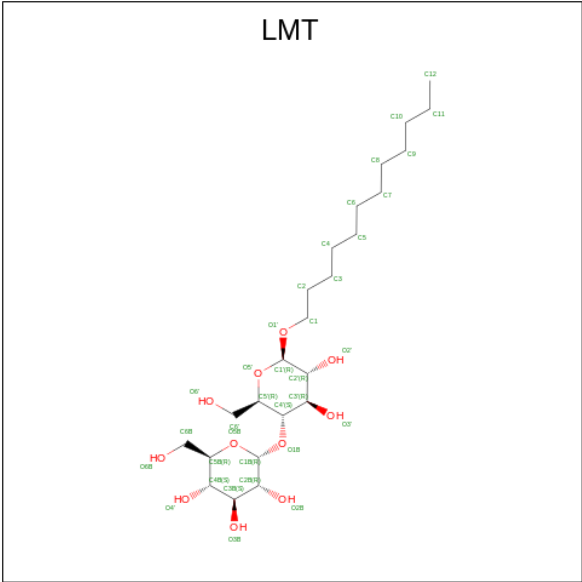
Mol	Chain	Residues	Atoms		AltConf
31	A	1	Total	C	0
			40	40	
31	A	1	Total	C	0
			40	40	
31	A	1	Total	C	0
			40	40	
31	A	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	F	1	Total	C	0
			40	40	
31	F	1	Total	C	0
			40	40	
31	I	1	Total	C	0
			40	40	
31	J	1	Total	C	0
			40	40	
31	J	1	Total	C	0
			40	40	

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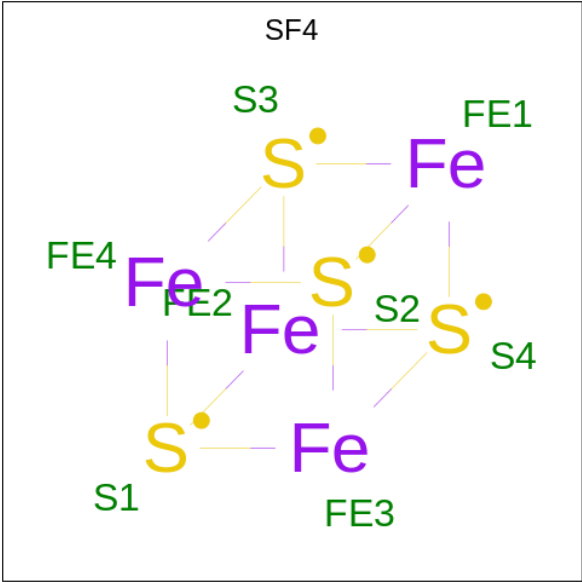
Mol	Chain	Residues	Atoms	AltConf
31	L	1	Total C 40 40	0
31	L	1	Total C 40 40	0
31	L	1	Total C 40 40	0
31	M	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	s	1	Total C 40 40	0
31	s	1	Total C 40 40	0
31	h	1	Total C 40 40	0
31	e	1	Total C 40 40	0
31	l	1	Total C 40 40	0
31	l	1	Total C 40 40	0
31	i	1	Total C 40 40	0
31	R	1	Total C 40 40	0
31	R	1	Total C 40 40	0

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



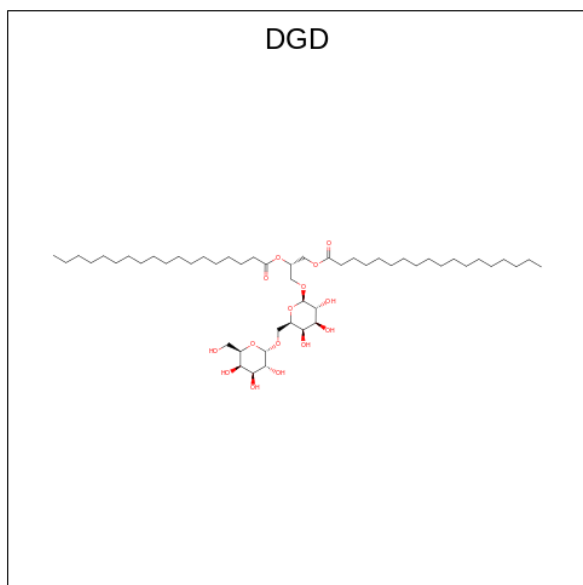
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			35	24	11	
32	a	1	Total	C	O	0
			24	18	6	
32	a	1	Total	C	O	0
			35	24	11	
32	b	1	Total	C	O	0
			24	18	6	

- Molecule 33 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



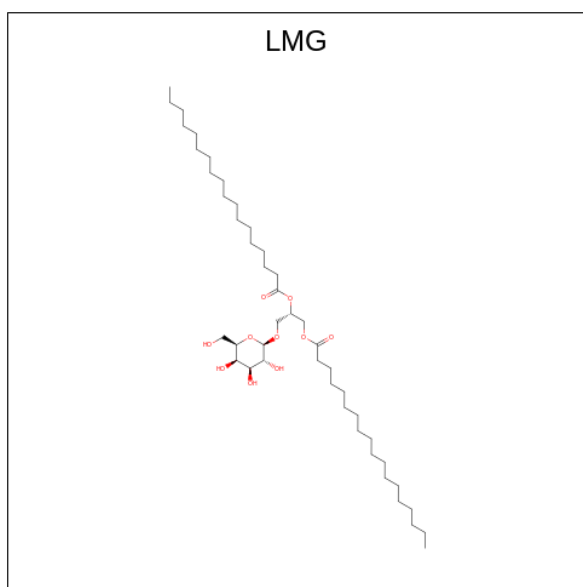
Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	Fe	S	0
			8	4	4	
33	C	1	Total	Fe	S	0
			8	4	4	
33	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



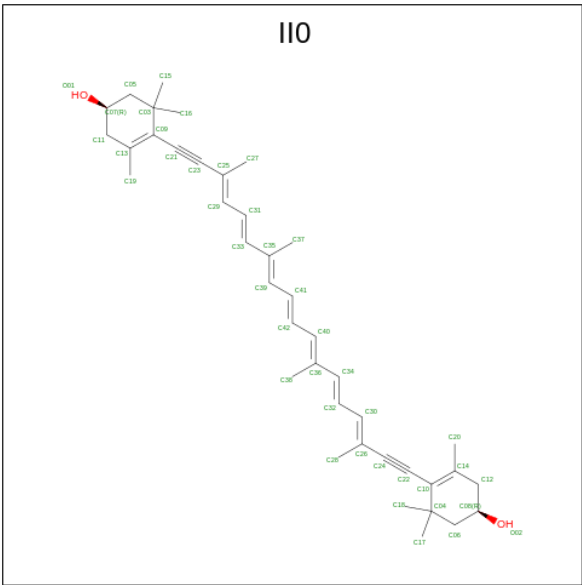
Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			60	45	15	

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
35	F	1	Total	C	O	0
			48	38	10	
35	J	1	Total	C	O	0
			55	45	10	
35	L	1	Total	C	O	0
			55	45	10	
35	O	1	Total	C	O	0
			26	16	10	
35	c	1	Total	C	O	0
			55	45	10	
35	b	1	Total	C	O	0
			49	39	10	
35	n	1	Total	C	O	0
			55	45	10	
35	Q	1	Total	C	O	0
			38	28	10	

- Molecule 36 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (three-letter code: II0) (formula: C₄₀H₅₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
36	J	1	Total	C	O	0
			42	40	2	
36	O	1	Total	C	O	0
			42	40	2	
36	c	1	Total	C	O	0
			42	40	2	
36	c	1	Total	C	O	0
			42	40	2	
36	c	1	Total	C	O	0
			42	40	2	
36	c	1	Total	C	O	0
			42	40	2	
36	a	1	Total	C	O	0
			42	40	2	
36	a	1	Total	C	O	0
			42	40	2	
36	a	1	Total	C	O	0
			42	40	2	
36	a	1	Total	C	O	0
			42	40	2	
36	b	1	Total	C	O	0
			42	40	2	
36	b	1	Total	C	O	0
			42	40	2	
36	b	1	Total	C	O	0
			42	40	2	
36	h	1	Total	C	O	0
			28	27	1	

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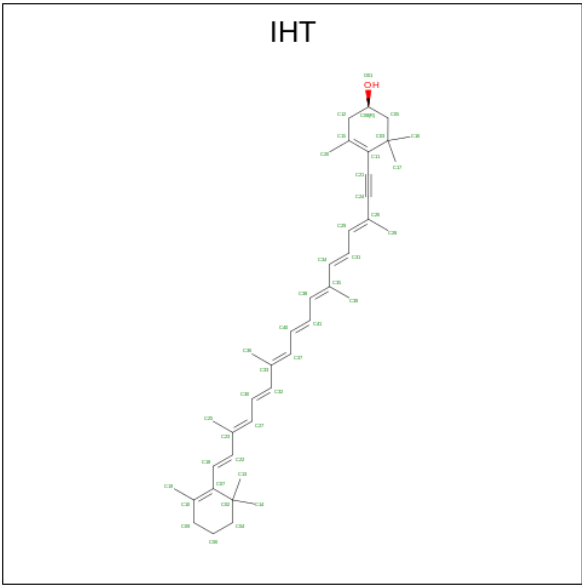
Mol	Chain	Residues	Atoms			AltConf
36	h	1	Total	C	O	0
			42	40	2	
36	h	1	Total	C	O	0
			42	40	2	
36	m	1	Total	C	O	0
			42	40	2	
36	m	1	Total	C	O	0
			42	40	2	
36	m	1	Total	C	O	0
			42	40	2	
36	m	1	Total	C	O	0
			42	40	2	
36	e	1	Total	C	O	0
			42	40	2	
36	e	1	Total	C	O	0
			42	40	2	
36	e	1	Total	C	O	0
			42	40	2	
36	e	1	Total	C	O	0
			42	40	2	
36	l	1	Total	C	O	0
			42	40	2	
36	l	1	Total	C	O	0
			42	40	2	
36	l	1	Total	C	O	0
			42	40	2	
36	l	1	Total	C	O	0
			42	40	2	
36	k	1	Total	C	O	0
			42	40	2	
36	k	1	Total	C	O	0
			42	40	2	
36	k	1	Total	C	O	0
			42	40	2	
36	k	1	Total	C	O	0
			42	40	2	
36	k	1	Total	C	O	0
			42	40	2	
36	f	1	Total	C	O	0
			42	40	2	
36	f	1	Total	C	O	0
			42	40	2	

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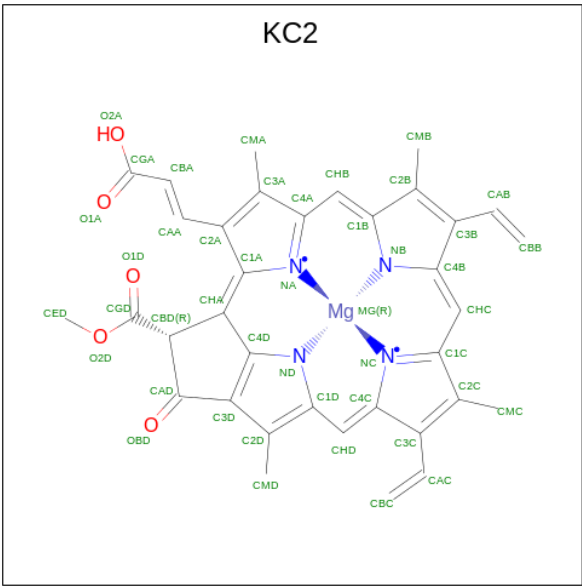
Mol	Chain	Residues	Atoms			AltConf
36	f	1	Total	C	O	0
			42	40	2	
36	f	1	Total	C	O	0
			42	40	2	
36	i	1	Total	C	O	0
			42	40	2	
36	i	1	Total	C	O	0
			42	40	2	
36	i	1	Total	C	O	0
			42	40	2	
36	i	1	Total	C	O	0
			42	40	2	
36	i	1	Total	C	O	0
			42	40	2	
36	j	1	Total	C	O	0
			42	40	2	
36	j	1	Total	C	O	0
			42	40	2	
36	d	1	Total	C	O	0
			42	40	2	
36	d	1	Total	C	O	0
			42	40	2	
36	d	1	Total	C	O	0
			42	40	2	
36	d	1	Total	C	O	0
			42	40	2	
36	g	1	Total	C	O	0
			42	40	2	
36	g	1	Total	C	O	0
			42	40	2	
36	g	1	Total	C	O	0
			42	40	2	
36	g	1	Total	C	O	0
			42	40	2	
36	n	1	Total	C	O	0
			42	40	2	
36	n	1	Total	C	O	0
			42	40	2	
36	n	1	Total	C	O	0
			42	40	2	
36	n	1	Total	C	O	0
			42	40	2	

- Molecule 37 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (three-letter code: IHT) (formula: C₄₀H₅₄O).



Mol	Chain	Residues	Atoms			AltConf
37	O	1	Total	C	O	0
			41	40	1	
37	c	1	Total	C	O	0
			41	40	1	
37	a	1	Total	C	O	0
			41	40	1	
37	b	1	Total	C	O	0
			41	40	1	
37	b	1	Total	C	O	0
			41	40	1	
37	m	1	Total	C	O	0
			41	40	1	
37	k	1	Total	C	O	0
			41	40	1	
37	f	1	Total	C	O	0
			41	40	1	
37	j	1	Total	C	O	0
			41	40	1	
37	g	1	Total	C	O	0
			41	40	1	
37	R	1	Total	C	O	0
			41	40	1	
37	n	1	Total	C	O	0
			41	40	1	

- Molecule 38 is Chlorophyll c2 (three-letter code: KC2) (formula: C₃₅H₂₈MgN₄O₅).



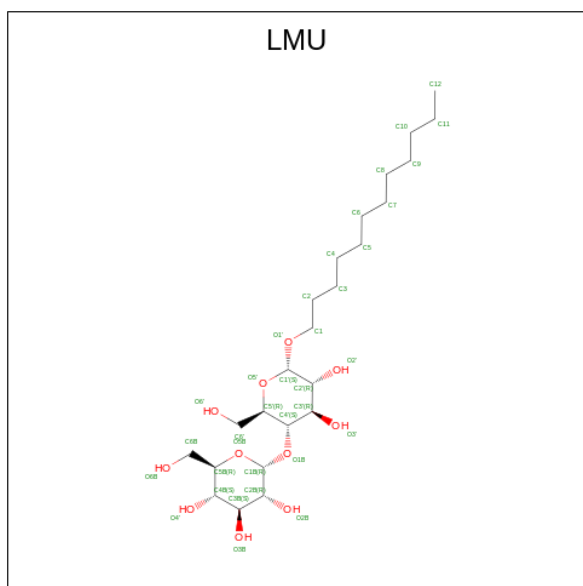
Mol	Chain	Residues	Atoms					AltConf
38	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	i	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	i	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
38	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 39 is DODECYL-ALPHA-D-MALTOSE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
39	i	1	Total	C	O	0
			35	24	11	

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	A	50	Total	O	0
			50	50	

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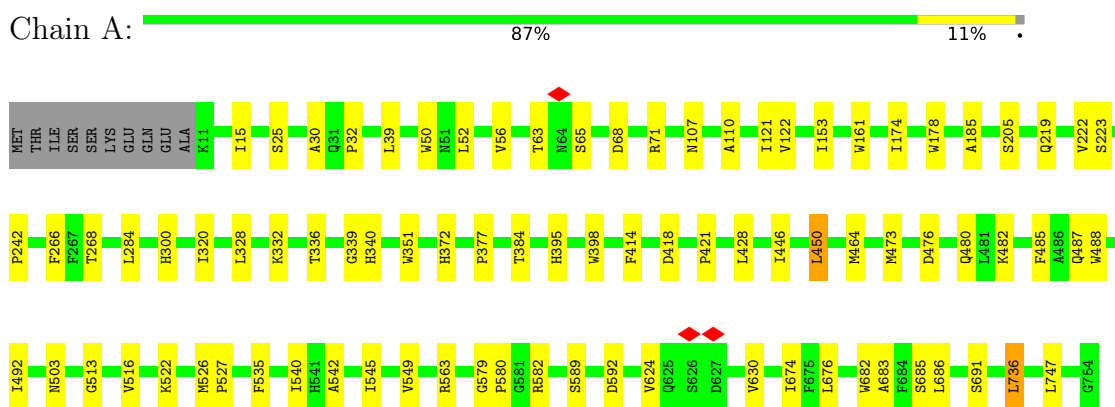
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Mol	Chain	Residues	Atoms		AltConf
40	B	57	Total 57	O 57	0
40	C	8	Total 8	O 8	0
40	D	1	Total 1	O 1	0
40	F	2	Total 2	O 2	0
40	I	1	Total 1	O 1	0
40	J	1	Total 1	O 1	0
40	L	1	Total 1	O 1	0
40	O	1	Total 1	O 1	0
40	K	1	Total 1	O 1	0
40	a	3	Total 3	O 3	0
40	b	2	Total 2	O 2	0
40	h	1	Total 1	O 1	0
40	m	1	Total 1	O 1	0
40	e	4	Total 4	O 4	0
40	R	1	Total 1	O 1	0
40	n	3	Total 3	O 3	0
40	Q	1	Total 1	O 1	0

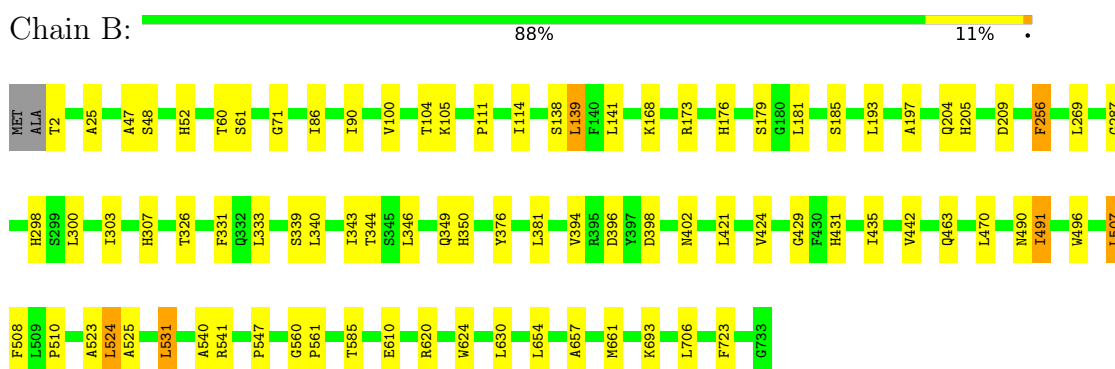
3 Residue-property plots

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

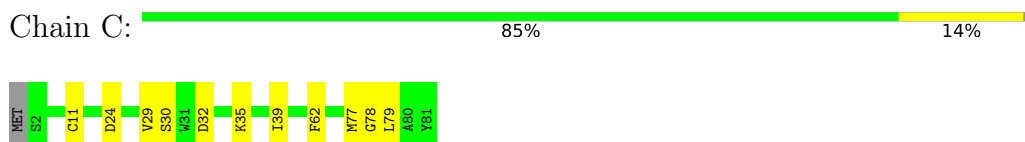
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center




- Molecule 4: Photosystem I reaction center subunit II

Chain D:  80% 18% ..



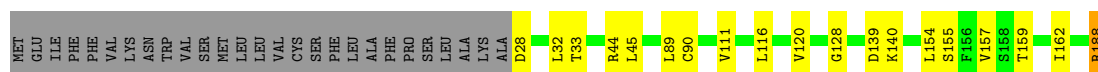
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  84% 9% 6%




- Molecule 6: Photosystem I reaction center subunit III

Chain F:  76% 10% 14%




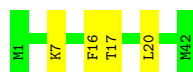
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  83% 11% 6%




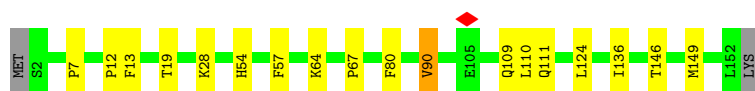
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  90% 10%



- Molecule 9: Photosystem I reaction center subunit XI

Chain L:  87% 11% ..

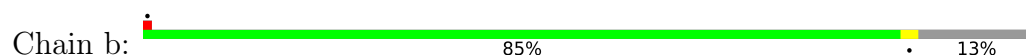


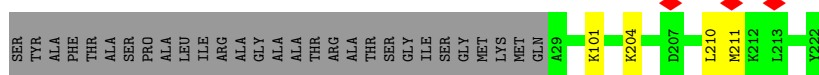
- Molecule 10: Photosystem I reaction center subunit XII

Chain M:  93% 7%

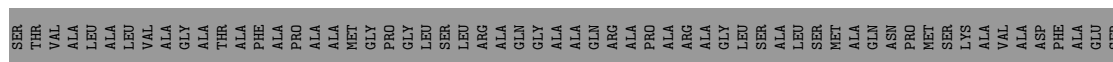


- Molecule 11: PsaO

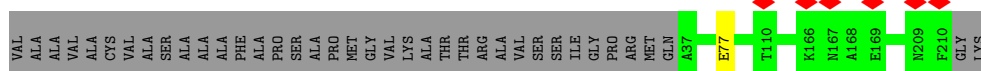
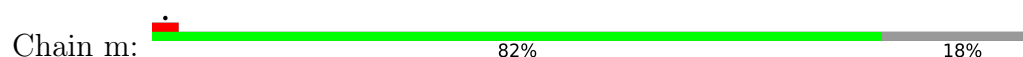




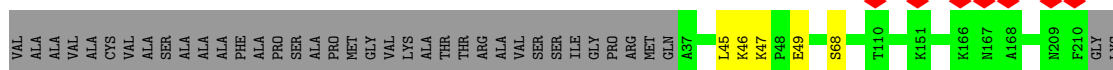
- Molecule 17: cac-h



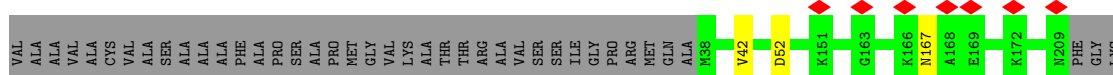
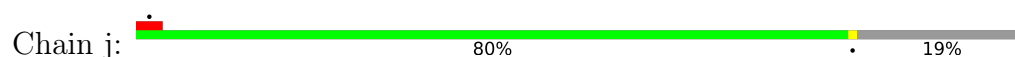
- Molecule 18: cac-f



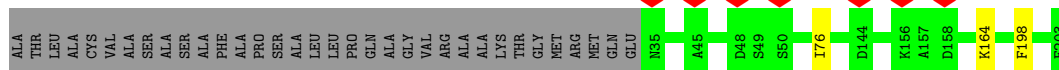
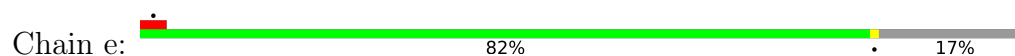
- Molecule 18: cac-f



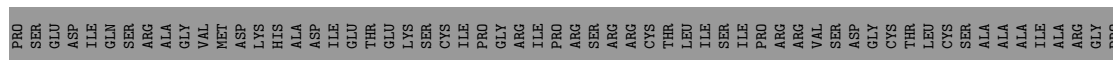
- Molecule 18: cac-f

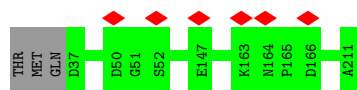


- Molecule 19: cac-e

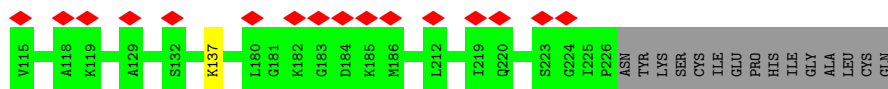
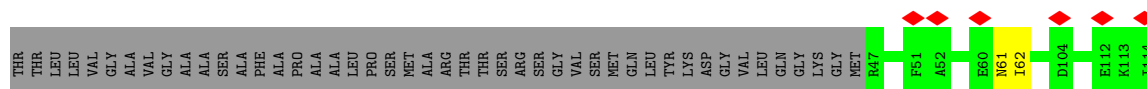
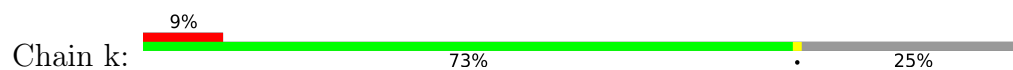


- Molecule 20: cac-l

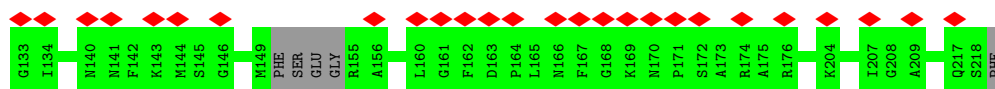
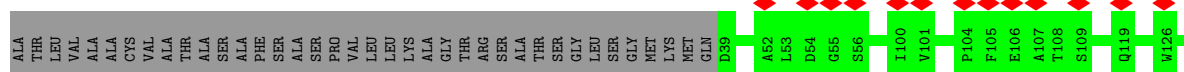
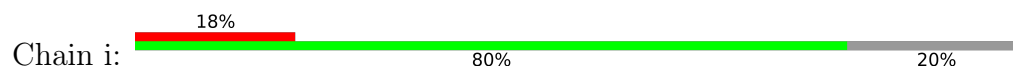




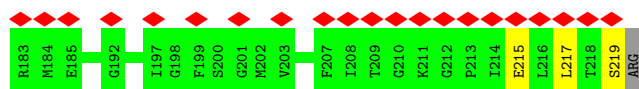
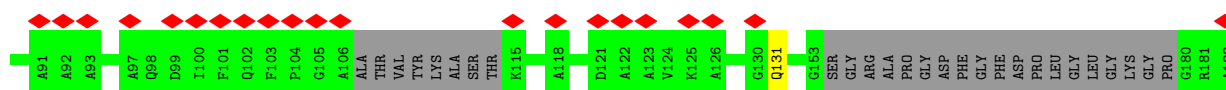
- Molecule 21: cac-k



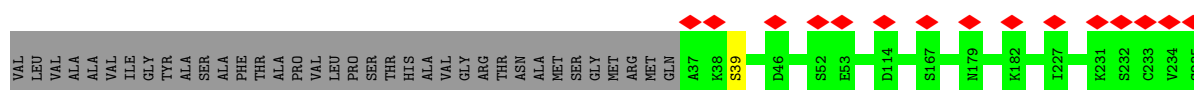
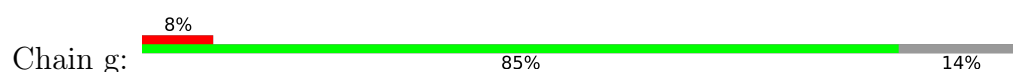
- Molecule 22: cac-i

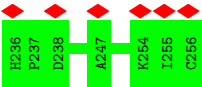


- Molecule 23: cac-d



- Molecule 24: cac-g

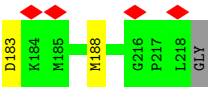
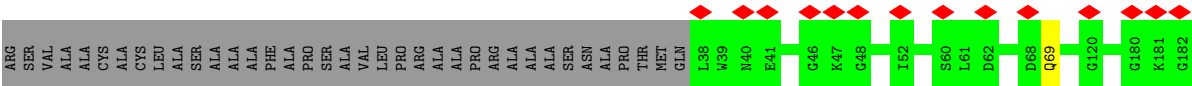
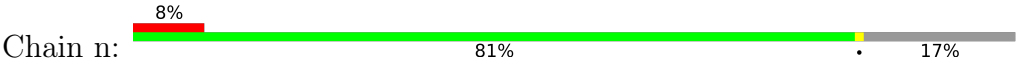




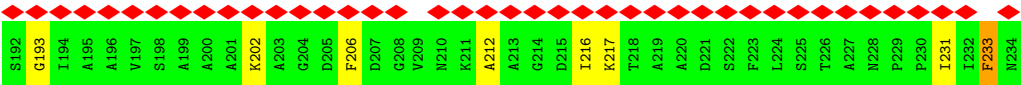
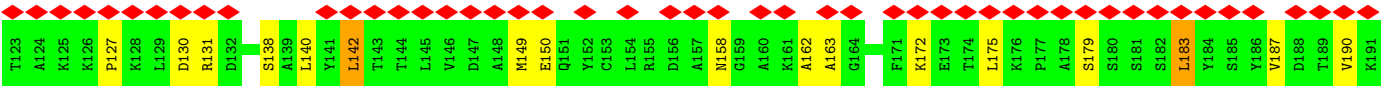
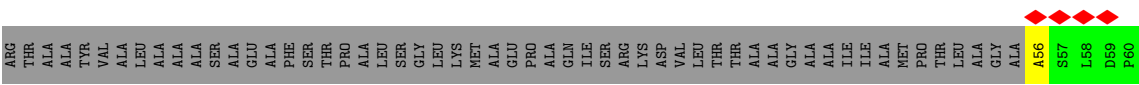
• Molecule 25: PsaR



• Molecule 26: cac-n



• Molecule 27: PsaQ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86231	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)	1200	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.296	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	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: II0, SF4, PQN, WVN, DGD, LMT, LHG, IHT, LMU, LMG, KC2, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/6019	0.57	0/8204
2	B	0.44	0/6045	0.59	0/8254
3	C	0.44	0/601	0.64	0/813
4	D	0.45	0/1109	0.58	0/1500
5	E	0.46	0/492	0.57	0/666
6	F	0.45	0/1287	0.60	0/1747
7	I	0.43	0/271	0.62	0/370
8	J	0.48	0/364	0.63	0/495
9	L	0.40	0/1175	0.55	0/1599
10	M	0.32	0/233	0.55	0/315
11	O	0.51	0/799	0.64	0/1094
12	K	0.39	0/495	0.59	0/672
13	s	0.41	0/1170	0.62	0/1580
14	c	0.43	0/1396	0.57	0/1889
15	a	0.45	0/1406	0.58	0/1903
16	b	0.44	0/1469	0.64	0/1983
17	h	0.39	0/1226	0.59	0/1667
18	f	0.42	0/1328	0.59	0/1790
18	j	0.43	0/1318	0.60	0/1775
18	m	0.39	0/1335	0.55	0/1798
19	e	0.40	0/1324	0.55	0/1795
20	l	0.39	0/1379	0.53	0/1863
21	k	0.38	0/1380	0.59	0/1869
22	i	0.42	0/1359	0.62	0/1835
23	d	0.39	0/993	0.58	0/1335
24	g	0.43	0/1673	0.59	0/2264
25	R	0.39	0/686	0.55	0/940
26	n	0.42	0/1383	0.62	0/1867
27	Q	0.40	0/1313	0.59	0/1775
All	All	0.43	0/41028	0.59	0/55657

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5825	0	5677	64	0
2	B	5826	0	5640	62	0
3	C	592	0	567	6	0
4	D	1084	0	1080	15	0
5	E	484	0	486	4	0
6	F	1254	0	1264	17	0
7	I	264	0	276	3	0
8	J	351	0	344	5	0
9	L	1146	0	1160	11	0
10	M	232	0	265	2	0
11	O	773	0	765	24	0
12	K	488	0	516	7	0
13	s	1140	0	1099	0	0
14	c	1357	0	1337	0	0
15	a	1361	0	1305	0	0
16	b	1439	0	1456	0	0
17	h	1200	0	1228	0	0
18	f	1302	0	1320	0	0
18	j	1293	0	1321	0	0
18	m	1309	0	1335	0	0
19	e	1286	0	1262	0	0
20	l	1344	0	1315	0	0
21	k	1346	0	1349	0	0
22	i	1324	0	1298	0	0
23	d	974	0	978	0	0
24	g	1630	0	1644	0	0
25	R	664	0	647	4	0
26	n	1350	0	1348	0	0
27	Q	1294	0	1333	20	0
28	A	2706	0	2777	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	B	2454	0	2485	82	0
28	F	117	0	115	4	0
28	J	42	0	31	0	0
28	K	93	0	72	1	0
28	L	215	0	191	11	0
28	O	182	0	187	13	0
28	Q	110	0	105	7	0
28	R	51	0	41	1	0
28	a	619	0	588	0	0
28	b	724	0	737	0	0
28	c	586	0	520	0	0
28	d	498	0	407	0	0
28	e	582	0	578	0	0
28	f	700	0	695	0	0
28	g	661	0	611	0	0
28	h	505	0	470	0	0
28	i	528	0	451	0	0
28	j	637	0	556	0	0
28	k	596	0	534	0	0
28	l	535	0	538	0	0
28	m	651	0	606	0	0
28	n	605	0	552	0	0
28	s	246	0	257	0	0
29	A	33	0	46	1	0
29	B	33	0	46	1	0
30	A	113	0	142	5	0
30	J	49	0	74	6	0
30	L	49	0	74	2	0
30	a	98	0	148	0	0
30	b	80	0	106	0	0
30	c	74	0	88	0	0
30	d	37	0	44	0	0
30	e	37	0	44	0	0
30	f	49	0	74	0	0
30	g	74	0	88	0	0
30	i	37	0	44	0	0
30	j	30	0	30	0	0
30	k	37	0	44	0	0
30	l	32	0	34	0	0
30	m	37	0	44	0	0
30	n	43	0	59	0	0
31	A	160	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	B	200	0	0	1	0
31	F	80	0	0	0	0
31	I	40	0	0	2	0
31	J	80	0	0	1	0
31	K	80	0	0	1	0
31	L	120	0	0	1	0
31	M	40	0	0	0	0
31	R	80	0	0	7	0
31	e	40	0	0	0	0
31	h	40	0	0	0	0
31	i	40	0	0	0	0
31	l	80	0	0	0	0
31	s	80	0	0	0	0
32	A	35	0	45	2	0
32	a	59	0	78	0	0
32	b	24	0	34	0	0
33	A	8	0	0	0	0
33	C	16	0	0	0	0
34	B	60	0	81	2	0
35	F	48	0	69	3	0
35	J	55	0	86	2	0
35	L	55	0	86	4	0
35	O	26	0	22	0	0
35	Q	38	0	46	4	0
35	b	49	0	71	0	0
35	c	55	0	86	0	0
35	n	55	0	86	0	0
36	J	42	0	0	0	0
36	O	42	0	0	0	0
36	a	168	0	0	0	0
36	b	126	0	0	0	0
36	c	168	0	0	0	0
36	d	168	0	0	0	0
36	e	168	0	0	0	0
36	f	168	0	0	0	0
36	g	168	0	0	0	0
36	h	112	0	0	0	0
36	i	210	0	0	0	0
36	j	84	0	0	0	0
36	k	210	0	0	0	0
36	l	168	0	0	0	0
36	m	168	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	n	168	0	0	0	0
37	O	41	0	0	0	0
37	R	41	0	0	0	0
37	a	41	0	0	0	0
37	b	82	0	0	0	0
37	c	41	0	0	0	0
37	f	41	0	0	0	0
37	g	41	0	0	0	0
37	j	41	0	0	0	0
37	k	41	0	0	0	0
37	m	41	0	0	0	0
37	n	41	0	0	0	0
38	c	45	0	0	0	0
38	d	90	0	0	0	0
38	e	45	0	0	0	0
38	f	45	0	0	0	0
38	g	135	0	0	0	0
38	i	90	0	0	0	0
38	j	45	0	0	0	0
38	k	135	0	0	0	0
38	l	45	0	0	0	0
38	m	45	0	0	0	0
38	n	90	0	0	0	0
38	s	90	0	0	0	0
39	i	35	0	46	0	0
40	A	50	0	0	0	0
40	B	57	0	0	0	0
40	C	8	0	0	0	0
40	D	1	0	0	0	0
40	F	2	0	0	0	0
40	I	1	0	0	0	0
40	J	1	0	0	0	0
40	K	1	0	0	0	0
40	L	1	0	0	0	0
40	O	1	0	0	0	0
40	Q	1	0	0	0	0
40	R	1	0	0	0	0
40	a	3	0	0	0	0
40	b	2	0	0	0	0
40	e	4	0	0	0	0
40	h	1	0	0	0	0
40	m	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	n	3	0	0	0	0
All	All	61164	0	55784	395	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 395 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:813:CLA:H61	31:R:202:WVN:C17	1.71	1.21
28:B:813:CLA:H8	31:R:202:WVN:C14	1.78	1.13
11:O:24:VAL:HG22	11:O:44:VAL:HG11	1.15	1.08
28:B:813:CLA:C6	31:R:202:WVN:C17	2.42	0.97
11:O:24:VAL:HG22	11:O:44:VAL:CG1	2.01	0.91

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/752 (98%)	722 (98%)	18 (2%)	0	100	100
2	B	731/734 (100%)	707 (97%)	23 (3%)	1 (0%)	48	73
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
5	E	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
6	F	159/188 (85%)	155 (98%)	4 (2%)	0	100	100
7	I	32/36 (89%)	32 (100%)	0	0	100	100
8	J	40/42 (95%)	39 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	L	149/153 (97%)	147 (99%)	2 (1%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
11	O	102/146 (70%)	97 (95%)	5 (5%)	0	100	100
12	K	65/87 (75%)	65 (100%)	0	0	100	100
13	s	152/269 (56%)	144 (95%)	8 (5%)	0	100	100
14	c	168/216 (78%)	163 (97%)	5 (3%)	0	100	100
15	a	173/216 (80%)	167 (96%)	6 (4%)	0	100	100
16	b	192/223 (86%)	190 (99%)	2 (1%)	0	100	100
17	h	160/225 (71%)	156 (98%)	3 (2%)	1 (1%)	22	45
18	f	172/212 (81%)	167 (97%)	5 (3%)	0	100	100
18	j	170/212 (80%)	163 (96%)	7 (4%)	0	100	100
18	m	172/212 (81%)	164 (95%)	8 (5%)	0	100	100
19	e	167/203 (82%)	164 (98%)	3 (2%)	0	100	100
20	l	173/238 (73%)	169 (98%)	4 (2%)	0	100	100
21	k	178/241 (74%)	172 (97%)	6 (3%)	0	100	100
22	i	171/218 (78%)	161 (94%)	10 (6%)	0	100	100
23	d	123/213 (58%)	122 (99%)	1 (1%)	0	100	100
24	g	217/255 (85%)	206 (95%)	11 (5%)	0	100	100
25	R	88/129 (68%)	86 (98%)	2 (2%)	0	100	100
26	n	179/219 (82%)	170 (95%)	9 (5%)	0	100	100
27	Q	177/234 (76%)	163 (92%)	12 (7%)	2 (1%)	12	30
All	All	5151/6189 (83%)	4987 (97%)	160 (3%)	4 (0%)	50	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	Q	75	CYS
27	Q	130	ASP
17	h	164	LYS
2	B	491	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	607/616 (98%)	604 (100%)	3 (0%)	86	95
2	B	593/593 (100%)	582 (98%)	11 (2%)	52	79
3	C	67/68 (98%)	64 (96%)	3 (4%)	23	50
4	D	116/117 (99%)	112 (97%)	4 (3%)	32	61
5	E	54/58 (93%)	54 (100%)	0	100	100
6	F	133/157 (85%)	132 (99%)	1 (1%)	79	91
7	I	28/29 (97%)	28 (100%)	0	100	100
8	J	39/39 (100%)	39 (100%)	0	100	100
9	L	124/126 (98%)	121 (98%)	3 (2%)	44	73
10	M	25/25 (100%)	25 (100%)	0	100	100
11	O	81/110 (74%)	76 (94%)	5 (6%)	15	36
12	K	52/66 (79%)	50 (96%)	2 (4%)	28	56
13	s	116/195 (60%)	115 (99%)	1 (1%)	75	90
14	c	138/171 (81%)	134 (97%)	4 (3%)	37	67
15	a	139/165 (84%)	133 (96%)	6 (4%)	25	52
16	b	149/168 (89%)	145 (97%)	4 (3%)	40	69
17	h	123/162 (76%)	121 (98%)	2 (2%)	58	82
18	f	135/161 (84%)	130 (96%)	5 (4%)	29	58
18	j	136/161 (84%)	133 (98%)	3 (2%)	47	76
18	m	137/161 (85%)	136 (99%)	1 (1%)	81	93
19	e	130/155 (84%)	127 (98%)	3 (2%)	45	74
20	l	137/191 (72%)	137 (100%)	0	100	100
21	k	138/186 (74%)	135 (98%)	3 (2%)	47	76
22	i	138/168 (82%)	138 (100%)	0	100	100
23	d	97/157 (62%)	93 (96%)	4 (4%)	26	54
24	g	171/199 (86%)	170 (99%)	1 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	R	69/98 (70%)	69 (100%)	0	100	100
26	n	140/163 (86%)	137 (98%)	3 (2%)	48	76
27	Q	134/168 (80%)	123 (92%)	11 (8%)	9	23
All	All	4146/4833 (86%)	4063 (98%)	83 (2%)	50	78

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	f	46	LYS
26	n	188	MET
18	f	49	GLU
23	d	215	GLU
27	Q	73	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	420	ASN
11	O	27	GLN
18	m	128	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

415 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	A	851	-	65,73,73	1.56	9 (13%)	76,113,113	1.47	10 (13%)
28	CLA	k	604	21	65,73,73	1.52	7 (10%)	76,113,113	1.45	9 (11%)
28	CLA	B	831	40	45,53,73	1.84	7 (15%)	52,89,113	1.49	6 (11%)
28	CLA	l	309	30	61,69,73	1.50	6 (9%)	71,108,113	1.49	8 (11%)
31	WVN	K	102	-	40,41,41	1.83	14 (35%)	50,56,56	1.98	14 (28%)
36	II0	g	316	-	39,43,43	6.82	22 (56%)	50,60,60	2.24	15 (30%)
39	LMU	i	301	-	36,36,36	1.18	3 (8%)	47,47,47	1.15	5 (10%)
35	LMG	O	205	-	26,26,55	1.26	2 (7%)	34,34,63	1.23	3 (8%)
28	CLA	j	605	18	45,53,73	1.87	6 (13%)	52,89,113	1.69	9 (17%)
28	CLA	i	305	22	65,73,73	1.47	5 (7%)	76,113,113	1.42	9 (11%)
38	KC2	k	612	-	48,53,53	3.15	22 (45%)	54,89,89	4.41	33 (61%)
36	II0	i	313	-	39,43,43	6.70	21 (53%)	50,60,60	2.51	19 (38%)
28	CLA	A	810	28	62,70,73	1.54	8 (12%)	72,109,113	1.32	8 (11%)
35	LMG	n	620	-	55,55,55	0.88	2 (3%)	63,63,63	0.90	2 (3%)
28	CLA	m	607	-	51,59,73	1.71	8 (15%)	59,96,113	1.52	9 (15%)
37	IHT	a	317	-	40,42,42	6.27	26 (65%)	53,58,58	2.10	16 (30%)
28	CLA	b	604	-	65,73,73	1.50	8 (12%)	76,113,113	1.25	8 (10%)
30	LHG	A	843	-	47,47,48	0.95	2 (4%)	50,53,54	1.08	3 (6%)
30	LHG	g	321	28	36,36,48	1.07	2 (5%)	39,42,54	1.42	9 (23%)
29	PQN	A	842	-	34,34,34	1.85	5 (14%)	42,45,45	1.32	5 (11%)
28	CLA	K	103	-	42,50,73	1.81	9 (21%)	48,85,113	1.66	12 (25%)
28	CLA	A	832	-	65,73,73	1.45	8 (12%)	76,113,113	1.73	13 (17%)
28	CLA	h	303	17	50,58,73	1.69	8 (16%)	58,95,113	1.53	10 (17%)
28	CLA	a	303	15	52,60,73	1.66	6 (11%)	60,97,113	1.63	7 (11%)
38	KC2	s	201	13	48,53,53	3.00	21 (43%)	54,89,89	4.43	32 (59%)
28	CLA	j	601	18	51,59,73	1.68	6 (11%)	59,96,113	1.39	7 (11%)
28	CLA	A	823	-	55,63,73	1.57	7 (12%)	64,101,113	1.41	9 (14%)
28	CLA	b	603	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	9 (11%)
28	CLA	j	609	18	51,59,73	1.63	5 (9%)	59,96,113	1.53	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PQN	B	842	-	34,34,34	1.76	5 (14%)	42,45,45	1.34	5 (11%)
28	CLA	B	818	-	46,54,73	1.69	6 (13%)	53,90,113	1.66	9 (16%)
28	CLA	f	603	-	51,59,73	1.63	7 (13%)	59,96,113	1.57	7 (11%)
30	LHG	A	844	28	26,26,48	1.25	2 (7%)	29,32,54	1.39	5 (17%)
36	II0	b	613	-	39,43,43	6.77	22 (56%)	50,60,60	2.18	19 (38%)
38	KC2	i	310	22	48,53,53	3.11	21 (43%)	54,89,89	4.41	30 (55%)
30	LHG	J	106	28	48,48,48	0.93	2 (4%)	51,54,54	1.09	3 (5%)
28	CLA	c	605	14	51,59,73	1.67	8 (15%)	59,96,113	1.68	10 (16%)
28	CLA	n	606	26	51,59,73	1.70	6 (11%)	59,96,113	1.55	9 (15%)
28	CLA	h	306	17	65,73,73	1.51	7 (10%)	76,113,113	1.34	9 (11%)
28	CLA	i	304	-	51,59,73	1.69	6 (11%)	59,96,113	1.50	9 (15%)
28	CLA	g	309	24	65,73,73	1.53	6 (9%)	76,113,113	1.38	9 (11%)
28	CLA	s	206	40	65,73,73	1.47	6 (9%)	76,113,113	1.52	11 (14%)
38	KC2	e	609	19	48,53,53	3.10	21 (43%)	54,89,89	4.54	32 (59%)
28	CLA	f	605	18	45,53,73	1.82	6 (13%)	52,89,113	1.55	8 (15%)
28	CLA	i	306	-	51,59,73	1.70	8 (15%)	59,96,113	1.56	7 (11%)
28	CLA	g	322	35	65,73,73	1.49	6 (9%)	76,113,113	1.44	12 (15%)
28	CLA	n	608	26	51,59,73	1.75	7 (13%)	59,96,113	1.49	8 (13%)
38	KC2	f	611	18	48,53,53	3.09	22 (45%)	54,89,89	4.49	32 (59%)
36	II0	a	314	-	39,43,43	6.65	23 (58%)	50,60,60	2.08	19 (38%)
28	CLA	A	840	40	65,73,73	1.45	6 (9%)	76,113,113	1.36	9 (11%)
28	CLA	n	604	26	60,68,73	1.56	5 (8%)	70,107,113	1.54	10 (14%)
28	CLA	a	305	-	51,59,73	1.64	7 (13%)	59,96,113	1.56	9 (15%)
35	LMG	b	621	-	49,49,55	0.96	3 (6%)	57,57,63	1.21	5 (8%)
37	IHT	g	319	-	40,42,42	6.30	25 (62%)	53,58,58	3.05	21 (39%)
36	II0	f	614	-	39,43,43	6.78	23 (58%)	50,60,60	2.08	15 (30%)
28	CLA	c	603	-	51,59,73	1.62	6 (11%)	59,96,113	1.61	7 (11%)
28	CLA	a	308	15	65,73,73	1.46	6 (9%)	76,113,113	1.43	11 (14%)
28	CLA	i	311	-	51,59,73	1.80	9 (17%)	59,96,113	1.48	8 (13%)
28	CLA	c	606	-	52,60,73	1.71	10 (19%)	60,97,113	1.59	9 (15%)
31	WVN	K	104	-	40,41,41	1.89	14 (35%)	50,56,56	1.97	15 (30%)
28	CLA	d	302	-	51,59,73	1.61	7 (13%)	59,96,113	1.64	8 (13%)
28	CLA	A	804	-	65,73,73	1.45	7 (10%)	76,113,113	1.60	8 (10%)
28	CLA	B	806	-	65,73,73	1.37	6 (9%)	76,113,113	1.55	7 (9%)
28	CLA	d	303	-	65,73,73	1.52	6 (9%)	76,113,113	1.38	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	II0	n	616	-	39,43,43	6.85	23 (58%)	50,60,60	2.10	14 (28%)
30	LHG	l	317	28	31,31,48	1.15	2 (6%)	34,37,54	1.18	4 (11%)
28	CLA	A	805	1	65,73,73	1.42	7 (10%)	76,113,113	1.49	9 (11%)
31	WVN	F	203	-	40,41,41	1.92	14 (35%)	50,56,56	2.46	20 (40%)
28	CLA	d	306	-	51,59,73	1.72	6 (11%)	59,96,113	1.52	7 (11%)
28	CLA	A	807	1	65,73,73	1.41	6 (9%)	76,113,113	1.49	9 (11%)
28	CLA	b	610	16	65,73,73	1.46	8 (12%)	76,113,113	1.39	8 (10%)
28	CLA	k	607	-	51,59,73	1.72	7 (13%)	59,96,113	1.58	12 (20%)
28	CLA	B	805	-	65,73,73	1.44	8 (12%)	76,113,113	1.43	8 (10%)
28	CLA	h	304	-	51,59,73	1.61	6 (11%)	59,96,113	1.61	10 (16%)
28	CLA	m	602	18	56,64,73	1.57	9 (16%)	65,102,113	1.49	10 (15%)
28	CLA	c	604	14	65,73,73	1.49	7 (10%)	76,113,113	1.47	7 (9%)
36	II0	n	618	-	39,43,43	6.83	21 (53%)	50,60,60	2.23	19 (38%)
28	CLA	A	830	-	50,58,73	1.65	7 (14%)	58,95,113	1.66	7 (12%)
36	II0	f	615	-	39,43,43	6.74	23 (58%)	50,60,60	2.10	18 (36%)
38	KC2	d	311	-	48,53,53	3.12	21 (43%)	54,89,89	4.34	32 (59%)
28	CLA	F	201	40	65,73,73	1.53	8 (12%)	76,113,113	1.26	7 (9%)
38	KC2	k	611	21	48,53,53	3.10	22 (45%)	54,89,89	4.59	31 (57%)
36	II0	j	615	-	39,43,43	6.80	22 (56%)	50,60,60	2.09	20 (40%)
28	CLA	f	601	18	47,55,73	1.75	7 (14%)	54,91,113	1.64	9 (16%)
28	CLA	b	605	40,28	65,73,73	1.43	8 (12%)	76,113,113	1.49	9 (11%)
36	II0	k	619	-	39,43,43	6.74	22 (56%)	50,60,60	2.38	20 (40%)
28	CLA	A	809	-	56,64,73	1.54	7 (12%)	65,102,113	1.41	7 (10%)
28	CLA	a	312	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	9 (11%)
28	CLA	k	602	21	50,58,73	1.69	6 (12%)	58,95,113	1.68	10 (17%)
38	KC2	g	313	38	48,53,53	3.11	22 (45%)	54,89,89	4.48	32 (59%)
28	CLA	e	610	40	65,73,73	1.48	6 (9%)	76,113,113	1.39	9 (11%)
28	CLA	A	854	40	65,73,73	1.56	9 (13%)	76,113,113	1.49	10 (13%)
28	CLA	c	607	14	46,54,73	1.77	6 (13%)	53,90,113	1.48	7 (13%)
28	CLA	g	307	24	51,59,73	1.67	6 (11%)	59,96,113	1.45	8 (13%)
28	CLA	A	819	-	45,53,73	1.77	8 (17%)	52,89,113	1.83	12 (23%)
28	CLA	h	302	17	50,58,73	1.66	7 (14%)	58,95,113	1.64	7 (12%)
30	LHG	A	849	-	37,37,48	1.03	2 (5%)	40,43,54	1.13	4 (10%)
28	CLA	n	603	-	51,59,73	1.66	8 (15%)	59,96,113	1.51	10 (16%)
28	CLA	O	206	-	65,73,73	1.46	9 (13%)	76,113,113	1.72	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	WVN	A	845	-	40,41,41	1.90	13 (32%)	50,56,56	1.97	14 (28%)
35	LMG	J	105	-	55,55,55	0.85	2 (3%)	63,63,63	0.92	5 (7%)
36	II0	l	313	-	39,43,43	6.90	22 (56%)	50,60,60	2.44	16 (32%)
28	CLA	j	603	-	51,59,73	1.63	5 (9%)	59,96,113	1.60	8 (13%)
28	CLA	A	836	-	65,73,73	1.41	7 (10%)	76,113,113	1.62	10 (13%)
28	CLA	c	602	14	50,58,73	1.65	7 (14%)	58,95,113	1.77	10 (17%)
28	CLA	c	609	30	45,53,73	1.81	6 (13%)	52,89,113	1.42	8 (15%)
28	CLA	l	311	20	65,73,73	1.52	6 (9%)	76,113,113	1.29	9 (11%)
28	CLA	B	816	-	57,65,73	1.56	6 (10%)	66,103,113	1.46	9 (13%)
28	CLA	A	838	1	65,73,73	1.52	7 (10%)	76,113,113	1.39	8 (10%)
28	CLA	j	606	18	51,59,73	1.66	8 (15%)	59,96,113	1.58	8 (13%)
28	CLA	g	310	24	51,59,73	1.64	7 (13%)	59,96,113	1.63	10 (16%)
28	CLA	B	804	-	65,73,73	1.39	6 (9%)	76,113,113	1.59	10 (13%)
31	WVN	L	201	-	40,41,41	1.93	15 (37%)	50,56,56	2.44	17 (34%)
28	CLA	h	313	40	65,73,73	1.50	6 (9%)	76,113,113	1.37	7 (9%)
28	CLA	k	601	21	51,59,73	1.68	6 (11%)	59,96,113	1.64	9 (15%)
28	CLA	k	609	21	65,73,73	1.47	7 (10%)	76,113,113	1.59	9 (11%)
28	CLA	B	812	-	60,68,73	1.56	7 (11%)	70,107,113	1.45	9 (12%)
28	CLA	d	305	23	51,59,73	2.00	8 (15%)	59,96,113	1.61	11 (18%)
28	CLA	f	609	18	65,73,73	1.47	7 (10%)	76,113,113	1.47	11 (14%)
28	CLA	g	308	-	65,73,73	1.43	8 (12%)	76,113,113	1.55	8 (10%)
28	CLA	k	608	21	65,73,73	1.52	7 (10%)	76,113,113	1.39	10 (13%)
36	II0	h	311	-	39,43,43	6.68	21 (53%)	50,60,60	2.13	17 (34%)
36	II0	m	618	-	39,43,43	6.86	21 (53%)	50,60,60	3.26	20 (40%)
28	CLA	B	835	40	65,73,73	1.52	8 (12%)	76,113,113	1.28	8 (10%)
28	CLA	c	601	14	51,59,73	1.68	6 (11%)	59,96,113	1.47	7 (11%)
36	II0	m	615	-	39,43,43	6.66	23 (58%)	50,60,60	2.13	20 (40%)
28	CLA	l	308	20	51,59,73	1.65	7 (13%)	59,96,113	1.63	11 (18%)
31	WVN	B	845	-	40,41,41	1.79	13 (32%)	50,56,56	1.95	12 (24%)
28	CLA	h	307	17	57,65,73	1.63	6 (10%)	66,103,113	1.31	7 (10%)
28	CLA	a	304	15	50,58,73	1.64	7 (14%)	58,95,113	1.64	10 (17%)
28	CLA	l	305	20	65,73,73	1.44	8 (12%)	76,113,113	1.53	11 (14%)
28	CLA	a	311	15	65,73,73	1.45	7 (10%)	76,113,113	1.51	10 (13%)
28	CLA	j	604	18	65,73,73	1.47	6 (9%)	76,113,113	1.44	10 (13%)
37	IHT	m	617	-	40,42,42	6.14	26 (65%)	53,58,58	2.43	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	A	802	-	65,73,73	1.44	7 (10%)	76,113,113	1.72	11 (14%)
35	LMG	L	209	28	55,55,55	0.84	2 (3%)	63,63,63	1.42	10 (15%)
28	CLA	B	820	-	53,61,73	1.64	8 (15%)	61,98,113	1.44	9 (14%)
28	CLA	i	303	22	50,58,73	1.64	7 (14%)	58,95,113	1.74	9 (15%)
28	CLA	A	827	-	62,70,73	1.47	6 (9%)	72,109,113	1.42	7 (9%)
32	LMT	b	618	-	24,24,36	1.11	3 (12%)	29,29,47	1.08	0
28	CLA	d	301	23	50,58,73	1.67	6 (12%)	58,95,113	1.62	8 (13%)
37	IHT	b	615	-	40,42,42	6.19	25 (62%)	53,58,58	2.45	18 (33%)
28	CLA	B	802	-	65,73,73	1.43	7 (10%)	76,113,113	1.35	10 (13%)
38	KC2	i	319	-	48,53,53	3.12	22 (45%)	54,89,89	4.62	32 (59%)
28	CLA	e	605	19	65,73,73	1.50	7 (10%)	76,113,113	1.34	9 (11%)
28	CLA	d	304	23	51,59,73	1.68	6 (11%)	59,96,113	1.66	6 (10%)
28	CLA	B	827	-	50,58,73	1.67	7 (14%)	58,95,113	1.44	10 (17%)
28	CLA	B	817	40	65,73,73	1.48	8 (12%)	76,113,113	1.46	7 (9%)
28	CLA	b	602	16	55,63,73	1.59	6 (10%)	64,101,113	1.60	10 (15%)
28	CLA	b	609	-	51,59,73	1.49	7 (13%)	59,96,113	1.90	9 (15%)
31	WVN	B	846	-	40,41,41	1.87	14 (35%)	50,56,56	1.98	13 (26%)
28	CLA	n	607	-	65,73,73	1.43	7 (10%)	76,113,113	1.50	8 (10%)
28	CLA	B	830	40	65,73,73	1.47	6 (9%)	76,113,113	1.39	9 (11%)
38	KC2	n	611	26	48,53,53	3.05	22 (45%)	54,89,89	4.53	30 (55%)
33	SF4	A	853	1,2	0,12,12	-	-	-	-	-
37	IHT	f	617	-	40,42,42	6.20	25 (62%)	53,58,58	2.22	15 (28%)
28	CLA	A	808	1	65,73,73	1.40	8 (12%)	76,113,113	1.53	13 (17%)
37	IHT	k	618	-	40,42,42	6.19	26 (65%)	53,58,58	2.41	20 (37%)
36	II0	e	612	-	39,43,43	6.80	22 (56%)	50,60,60	2.28	15 (30%)
28	CLA	b	601	16	51,59,73	1.63	7 (13%)	59,96,113	1.71	13 (22%)
28	CLA	A	855	30	41,49,73	1.92	8 (19%)	47,84,113	2.23	12 (25%)
36	II0	d	313	-	39,43,43	6.73	22 (56%)	50,60,60	2.35	18 (36%)
36	II0	f	618	-	39,43,43	6.80	22 (56%)	50,60,60	2.39	19 (38%)
28	CLA	A	833	-	50,58,73	1.63	7 (14%)	58,95,113	1.49	7 (12%)
28	CLA	e	607	19	65,73,73	1.51	7 (10%)	76,113,113	1.34	8 (10%)
30	LHG	c	618	28	36,36,48	1.11	2 (5%)	39,42,54	1.18	3 (7%)
31	WVN	I	101	-	40,41,41	1.86	13 (32%)	50,56,56	1.75	13 (26%)
28	CLA	i	307	22	61,69,73	1.52	6 (9%)	71,108,113	1.45	8 (11%)
36	II0	d	314	-	39,43,43	6.85	21 (53%)	50,60,60	2.29	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	A	803	28	55,63,73	1.57	7 (12%)	64,101,113	1.61	9 (14%)
36	II0	l	316	-	39,43,43	6.82	23 (58%)	50,60,60	1.95	17 (34%)
38	KC2	d	310	23	48,53,53	3.13	22 (45%)	54,89,89	4.55	31 (57%)
36	II0	g	317	-	39,43,43	6.72	23 (58%)	50,60,60	2.41	16 (32%)
36	II0	k	615	-	39,43,43	6.79	22 (56%)	50,60,60	2.20	16 (32%)
28	CLA	B	819	-	55,63,73	1.60	8 (14%)	64,101,113	1.36	7 (10%)
28	CLA	b	612	30	51,59,73	1.62	8 (15%)	59,96,113	1.78	10 (16%)
28	CLA	m	603	-	65,73,73	1.45	8 (12%)	76,113,113	1.55	8 (10%)
28	CLA	B	808	2	65,73,73	1.47	8 (12%)	76,113,113	1.59	10 (13%)
30	LHG	d	317	28	36,36,48	1.11	2 (5%)	39,42,54	1.02	2 (5%)
28	CLA	l	302	20	47,55,73	1.73	8 (17%)	54,91,113	1.44	7 (12%)
36	II0	j	614	-	39,43,43	6.77	22 (56%)	50,60,60	2.26	17 (34%)
28	CLA	L	204	40	50,58,73	1.68	7 (14%)	58,95,113	1.57	10 (17%)
37	IHT	n	617	-	40,42,42	6.15	26 (65%)	53,58,58	2.29	17 (32%)
38	KC2	c	610	-	48,53,53	3.07	22 (45%)	54,89,89	4.47	31 (57%)
28	CLA	k	603	-	51,59,73	1.62	5 (9%)	59,96,113	1.70	10 (16%)
36	II0	m	614	-	39,43,43	6.84	22 (56%)	50,60,60	1.94	16 (32%)
38	KC2	m	611	18	48,53,53	3.08	22 (45%)	54,89,89	4.56	31 (57%)
28	CLA	B	836	-	65,73,73	1.47	7 (10%)	76,113,113	1.55	14 (18%)
28	CLA	d	307	23	46,54,73	1.80	6 (13%)	53,90,113	1.49	6 (11%)
28	CLA	j	607	-	51,59,73	1.70	9 (17%)	59,96,113	1.48	9 (15%)
28	CLA	j	612	-	51,59,73	1.89	7 (13%)	59,96,113	1.72	10 (16%)
28	CLA	n	609	26	65,73,73	1.44	6 (9%)	76,113,113	1.52	12 (15%)
31	WVN	B	844	-	40,41,41	1.87	13 (32%)	50,56,56	2.42	16 (32%)
28	CLA	Q	302	40	65,73,73	1.50	7 (10%)	76,113,113	1.37	10 (13%)
36	II0	i	320	-	39,43,43	6.70	22 (56%)	50,60,60	2.25	14 (28%)
28	CLA	m	613	-	43,51,73	1.74	8 (18%)	49,86,113	1.78	13 (26%)
38	KC2	s	204	-	48,53,53	3.07	22 (45%)	54,89,89	4.43	32 (59%)
28	CLA	K	101	40	51,59,73	1.62	5 (9%)	59,96,113	1.85	13 (22%)
28	CLA	i	312	-	51,59,73	1.64	6 (11%)	59,96,113	1.56	10 (16%)
28	CLA	A	825	40	65,73,73	1.40	7 (10%)	76,113,113	1.35	6 (7%)
28	CLA	d	312	-	51,59,73	1.67	6 (11%)	59,96,113	1.61	12 (20%)
31	WVN	s	205	-	40,41,41	1.81	13 (32%)	50,56,56	2.23	21 (42%)
28	CLA	e	602	19	50,58,73	1.70	6 (12%)	58,95,113	1.53	9 (15%)
36	II0	b	617	-	39,43,43	6.67	20 (51%)	50,60,60	2.28	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	A	835	-	65,73,73	1.46	6 (9%)	76,113,113	1.35	6 (7%)
38	KC2	g	314	38	48,53,53	3.12	22 (45%)	54,89,89	4.58	31 (57%)
28	CLA	A	837	-	65,73,73	1.42	7 (10%)	76,113,113	1.40	10 (13%)
28	CLA	F	202	6	52,60,73	1.65	8 (15%)	60,97,113	1.61	9 (15%)
28	CLA	s	203	28,13	65,73,73	1.46	7 (10%)	76,113,113	1.51	10 (13%)
28	CLA	B	829	-	50,58,73	1.75	8 (16%)	58,95,113	1.40	9 (15%)
28	CLA	m	601	18	42,50,73	1.86	7 (16%)	48,85,113	1.47	8 (16%)
28	CLA	h	301	40	65,73,73	1.57	9 (13%)	76,113,113	1.39	9 (11%)
28	CLA	k	614	-	51,59,73	1.72	6 (11%)	59,96,113	1.47	10 (16%)
28	CLA	n	613	-	51,59,73	1.69	6 (11%)	59,96,113	1.38	7 (11%)
28	CLA	B	815	-	59,67,73	1.50	8 (13%)	68,105,113	1.38	7 (10%)
28	CLA	A	831	-	65,73,73	1.47	9 (13%)	76,113,113	1.41	9 (11%)
28	CLA	m	608	18	65,73,73	1.49	6 (9%)	76,113,113	1.45	8 (10%)
28	CLA	i	308	22	51,59,73	1.67	7 (13%)	59,96,113	1.63	8 (13%)
36	II0	l	312	-	39,43,43	6.79	22 (56%)	50,60,60	2.10	16 (32%)
28	CLA	f	607	-	65,73,73	1.50	7 (10%)	76,113,113	1.36	9 (11%)
30	LHG	g	301	28	36,36,48	1.10	2 (5%)	39,42,54	1.21	3 (7%)
28	CLA	e	601	19	45,53,73	1.73	7 (15%)	52,89,113	1.64	8 (15%)
36	II0	g	320	-	39,43,43	6.81	23 (58%)	50,60,60	2.24	18 (36%)
28	CLA	a	309	15	65,73,73	1.35	7 (10%)	76,113,113	1.69	10 (13%)
31	WVN	A	846	-	40,41,41	1.94	13 (32%)	50,56,56	2.97	20 (40%)
28	CLA	A	820	40	65,73,73	1.46	7 (10%)	76,113,113	1.54	7 (9%)
35	LMG	Q	301	-	38,38,55	1.03	2 (5%)	46,46,63	1.18	2 (4%)
28	CLA	O	201	30	52,60,73	1.56	8 (15%)	60,97,113	1.64	10 (16%)
31	WVN	L	206	-	40,41,41	1.82	13 (32%)	50,56,56	2.37	20 (40%)
36	II0	m	616	-	39,43,43	6.71	22 (56%)	50,60,60	2.18	15 (30%)
28	CLA	f	608	18	65,73,73	1.56	7 (10%)	76,113,113	1.55	10 (13%)
28	CLA	m	612	40	51,59,73	1.65	9 (17%)	59,96,113	1.57	12 (20%)
28	CLA	e	603	19	51,59,73	1.65	6 (11%)	59,96,113	1.60	9 (15%)
28	CLA	l	303	20	65,73,73	1.48	7 (10%)	76,113,113	1.47	11 (14%)
36	II0	i	317	-	39,43,43	6.88	21 (53%)	50,60,60	2.23	16 (32%)
28	CLA	O	202	-	65,73,73	1.48	7 (10%)	76,113,113	1.46	11 (14%)
28	CLA	j	602	18	50,58,73	1.64	7 (14%)	58,95,113	1.63	8 (13%)
28	CLA	B	826	-	51,59,73	1.70	7 (13%)	59,96,113	1.71	10 (16%)
28	CLA	f	612	18	51,59,73	1.71	8 (15%)	59,96,113	1.55	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	A	814	-	50,58,73	1.67	7 (14%)	58,95,113	1.60	10 (17%)
28	CLA	e	604	40	65,73,73	1.45	6 (9%)	76,113,113	1.53	11 (14%)
28	CLA	l	306	20	65,73,73	1.53	7 (10%)	76,113,113	1.53	12 (15%)
28	CLA	e	608	30	46,54,73	1.72	5 (10%)	53,90,113	1.64	8 (15%)
37	IHT	O	204	-	40,42,42	6.22	25 (62%)	53,58,58	2.38	19 (35%)
28	CLA	B	840	-	65,73,73	1.49	5 (7%)	76,113,113	1.43	8 (10%)
28	CLA	m	610	30	55,63,73	1.63	6 (10%)	64,101,113	1.49	11 (17%)
36	II0	c	614	-	39,43,43	6.73	22 (56%)	50,60,60	2.24	20 (40%)
31	WVN	R	201	-	40,41,41	1.86	14 (35%)	50,56,56	1.88	11 (22%)
36	II0	k	621	-	39,43,43	6.74	22 (56%)	50,60,60	2.33	13 (26%)
28	CLA	B	838	-	57,65,73	1.55	7 (12%)	66,103,113	1.41	9 (13%)
36	II0	e	613	-	39,43,43	6.79	23 (58%)	50,60,60	2.21	20 (40%)
36	II0	f	616	-	39,43,43	6.74	22 (56%)	50,60,60	2.33	16 (32%)
28	CLA	B	833	-	65,73,73	1.42	5 (7%)	76,113,113	1.50	11 (14%)
30	LHG	a	301	28	48,48,48	0.92	2 (4%)	51,54,54	1.15	4 (7%)
28	CLA	m	609	18	51,59,73	1.62	7 (13%)	59,96,113	1.56	9 (15%)
36	II0	g	318	-	39,43,43	6.84	21 (53%)	50,60,60	2.09	17 (34%)
32	LMT	a	320	-	36,36,36	1.25	6 (16%)	47,47,47	1.29	7 (14%)
30	LHG	b	620	-	30,30,48	1.12	2 (6%)	33,36,54	1.18	3 (9%)
28	CLA	f	604	18	65,73,73	1.45	6 (9%)	76,113,113	1.40	6 (7%)
30	LHG	n	619	-	42,42,48	0.98	2 (4%)	45,48,54	1.13	2 (4%)
28	CLA	B	811	-	65,73,73	1.42	7 (10%)	76,113,113	1.57	14 (18%)
28	CLA	a	306	40	65,73,73	1.44	7 (10%)	76,113,113	1.44	8 (10%)
36	II0	e	616	-	39,43,43	6.77	22 (56%)	50,60,60	2.12	18 (36%)
28	CLA	s	208	-	51,59,73	1.67	6 (11%)	59,96,113	1.51	9 (15%)
28	CLA	B	809	-	54,62,73	1.68	7 (12%)	67,100,113	1.42	11 (16%)
28	CLA	m	606	-	65,73,73	1.47	7 (10%)	76,113,113	1.32	8 (10%)
31	WVN	l	301	-	40,41,41	1.86	14 (35%)	50,56,56	2.19	19 (38%)
28	CLA	B	821	40	65,73,73	1.52	8 (12%)	76,113,113	2.06	19 (25%)
35	LMG	F	205	-	48,48,55	0.97	2 (4%)	56,56,63	1.24	5 (8%)
31	WVN	B	848	-	40,41,41	1.97	14 (35%)	50,56,56	2.04	19 (38%)
31	WVN	J	102	-	40,41,41	1.87	14 (35%)	50,56,56	1.93	14 (28%)
35	LMG	c	619	-	55,55,55	0.97	2 (3%)	63,63,63	1.48	10 (15%)
36	II0	n	614	-	39,43,43	6.86	22 (56%)	50,60,60	2.37	15 (30%)
36	II0	a	316	-	39,43,43	6.66	21 (53%)	50,60,60	2.40	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	m	619	28	36,36,48	1.08	2 (5%)	39,42,54	1.11	3 (7%)
31	WVN	l	315	-	40,41,41	1.88	14 (35%)	50,56,56	2.24	17 (34%)
30	LHG	L	208	-	48,48,48	0.94	2 (4%)	51,54,54	1.01	3 (5%)
31	WVN	s	207	-	40,41,41	1.89	14 (35%)	50,56,56	2.15	13 (26%)
28	CLA	L	202	9	49,57,73	1.69	6 (12%)	55,93,113	1.55	7 (12%)
36	II0	O	203	-	39,43,43	6.72	22 (56%)	50,60,60	2.30	16 (32%)
28	CLA	A	824	40	65,73,73	1.43	6 (9%)	76,113,113	1.47	9 (11%)
31	WVN	B	847	-	40,41,41	1.88	13 (32%)	50,56,56	1.98	14 (28%)
36	II0	h	312	-	39,43,43	6.82	21 (53%)	50,60,60	2.05	17 (34%)
28	CLA	c	612	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	8 (10%)
28	CLA	A	817	-	65,73,73	1.49	10 (15%)	76,113,113	1.42	9 (11%)
37	IHT	c	616	-	40,42,42	6.23	26 (65%)	53,58,58	2.25	17 (32%)
31	WVN	M	101	-	40,41,41	1.91	15 (37%)	50,56,56	2.16	16 (32%)
28	CLA	k	610	30	51,59,73	1.66	7 (13%)	59,96,113	1.59	7 (11%)
36	II0	a	318	-	39,43,43	6.96	22 (56%)	50,60,60	2.61	16 (32%)
36	II0	k	616	-	39,43,43	6.79	23 (58%)	50,60,60	2.35	20 (40%)
38	KC2	j	611	18	48,53,53	3.07	22 (45%)	54,89,89	4.58	32 (59%)
28	CLA	g	302	24	42,50,73	1.81	6 (14%)	48,85,113	1.68	9 (18%)
28	CLA	a	313	-	48,56,73	1.76	7 (14%)	55,92,113	1.45	8 (14%)
36	II0	i	315	-	39,43,43	6.80	21 (53%)	50,60,60	2.34	17 (34%)
28	CLA	c	611	14	45,53,73	1.96	9 (20%)	52,89,113	1.74	8 (15%)
28	CLA	A	834	-	51,59,73	1.62	6 (11%)	59,96,113	1.74	12 (20%)
28	CLA	A	801	-	65,73,73	1.47	6 (9%)	76,113,113	1.32	8 (10%)
32	LMT	a	302	-	24,24,36	1.07	2 (8%)	29,29,47	0.81	0
28	CLA	j	613	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
36	II0	c	617	-	39,43,43	6.70	21 (53%)	50,60,60	2.25	13 (26%)
28	CLA	A	815	40	45,53,73	1.73	9 (20%)	52,89,113	1.97	8 (15%)
28	CLA	A	841	-	65,73,73	1.43	8 (12%)	76,113,113	1.57	11 (14%)
28	CLA	B	801	40	65,73,73	1.47	8 (12%)	76,113,113	1.58	9 (11%)
28	CLA	k	605	21	45,53,73	1.77	7 (15%)	52,89,113	1.73	12 (23%)
31	WVN	L	205	-	40,41,41	1.92	14 (35%)	50,56,56	2.06	15 (30%)
28	CLA	A	826	-	65,73,73	1.43	6 (9%)	76,113,113	1.62	10 (13%)
28	CLA	B	841	30	65,73,73	1.45	6 (9%)	76,113,113	1.47	10 (13%)
28	CLA	s	202	13	65,73,73	1.52	7 (10%)	76,113,113	1.51	11 (14%)
28	CLA	L	203	-	65,73,73	1.46	8 (12%)	76,113,113	1.35	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	A	829	-	65,73,73	1.52	8 (12%)	76,113,113	1.51	7 (9%)
28	CLA	b	608	30	65,73,73	1.50	6 (9%)	76,113,113	1.39	10 (13%)
38	KC2	g	312	24	48,53,53	3.10	20 (41%)	54,89,89	4.54	30 (55%)
28	CLA	A	839	-	65,73,73	1.40	7 (10%)	76,113,113	1.40	7 (9%)
30	LHG	e	617	28	36,36,48	1.09	2 (5%)	39,42,54	1.32	5 (12%)
36	II0	l	314	-	39,43,43	6.77	22 (56%)	50,60,60	2.22	19 (38%)
28	CLA	B	839	-	65,73,73	1.50	7 (10%)	76,113,113	1.47	12 (15%)
28	CLA	f	610	30	65,73,73	1.50	6 (9%)	76,113,113	1.29	10 (13%)
28	CLA	l	304	-	51,59,73	1.68	5 (9%)	59,96,113	1.51	7 (11%)
28	CLA	h	308	17	51,59,73	1.65	7 (13%)	59,96,113	1.69	11 (18%)
38	KC2	l	310	20	48,53,53	3.06	22 (45%)	54,89,89	4.63	33 (61%)
28	CLA	a	307	15	45,53,73	1.77	5 (11%)	52,89,113	1.74	10 (19%)
36	II0	d	315	-	39,43,43	6.86	22 (56%)	50,60,60	2.42	20 (40%)
31	WVN	e	615	-	40,41,41	1.89	14 (35%)	50,56,56	2.03	14 (28%)
36	II0	e	614	-	39,43,43	6.86	21 (53%)	50,60,60	2.21	16 (32%)
28	CLA	g	303	24	50,58,73	1.57	7 (14%)	58,95,113	1.67	11 (18%)
36	II0	c	613	-	39,43,43	6.77	23 (58%)	50,60,60	2.14	18 (36%)
31	WVN	R	202	-	40,41,41	1.88	13 (32%)	50,56,56	2.11	17 (34%)
28	CLA	R	203	-	51,59,73	1.64	6 (11%)	59,96,113	1.82	11 (18%)
28	CLA	B	828	-	49,57,73	1.63	6 (12%)	55,93,113	1.67	9 (16%)
36	II0	a	315	-	39,43,43	6.62	23 (58%)	50,60,60	2.26	19 (38%)
28	CLA	b	606	16	61,69,73	1.53	7 (11%)	71,108,113	1.54	11 (15%)
32	LMT	A	850	-	36,36,36	1.19	6 (16%)	47,47,47	1.40	6 (12%)
28	CLA	n	602	26	50,58,73	1.65	6 (12%)	58,95,113	1.60	10 (17%)
30	LHG	b	619	28	48,48,48	0.90	2 (4%)	51,54,54	1.12	5 (9%)
37	IHT	b	616	-	40,42,42	6.31	25 (62%)	53,58,58	2.82	17 (32%)
38	KC2	n	612	-	48,53,53	3.08	21 (43%)	54,89,89	4.55	30 (55%)
30	LHG	a	319	28	48,48,48	0.89	2 (4%)	51,54,54	1.09	4 (7%)
28	CLA	a	310	30	48,56,73	1.68	9 (18%)	55,92,113	1.43	7 (12%)
28	CLA	l	307	20	65,73,73	1.41	7 (10%)	76,113,113	1.49	12 (15%)
37	IHT	R	204	-	40,42,42	6.22	25 (62%)	53,58,58	2.32	17 (32%)
33	SF4	C	101	3	0,12,12	-	-	-	-	-
28	CLA	i	309	30	46,54,73	1.74	6 (13%)	53,90,113	1.55	8 (15%)
28	CLA	g	315	-	51,59,73	1.71	7 (13%)	59,96,113	1.44	8 (13%)
28	CLA	B	810	-	55,63,73	1.65	8 (14%)	64,101,113	1.46	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	WVN	A	848	-	40,41,41	1.85	13 (32%)	50,56,56	2.65	16 (32%)
36	II0	n	615	-	39,43,43	6.74	23 (58%)	50,60,60	2.03	16 (32%)
28	CLA	A	813	-	45,53,73	1.74	6 (13%)	52,89,113	1.71	10 (19%)
28	CLA	h	305	17	51,59,73	1.62	7 (13%)	59,96,113	1.54	9 (15%)
28	CLA	f	613	-	65,73,73	1.52	7 (10%)	76,113,113	1.33	8 (10%)
28	CLA	b	611	-	65,73,73	1.48	7 (10%)	76,113,113	1.26	9 (11%)
28	CLA	g	305	24	65,73,73	1.52	5 (7%)	76,113,113	1.50	7 (9%)
28	CLA	d	308	23	41,49,73	1.85	7 (17%)	47,84,113	1.67	9 (19%)
28	CLA	B	837	-	65,73,73	1.40	6 (9%)	76,113,113	1.53	9 (11%)
31	WVN	A	847	-	40,41,41	1.91	13 (32%)	50,56,56	2.04	20 (40%)
38	KC2	k	613	-	48,53,53	3.13	22 (45%)	54,89,89	4.46	33 (61%)
28	CLA	i	302	22	51,59,73	1.71	6 (11%)	59,96,113	1.48	9 (15%)
28	CLA	A	828	-	65,73,73	1.42	8 (12%)	76,113,113	1.54	8 (10%)
30	LHG	k	620	28	36,36,48	1.15	2 (5%)	39,42,54	1.07	3 (7%)
33	SF4	C	102	3	0,12,12	-	-	-	-	-
28	CLA	Q	303	27	45,53,73	1.85	8 (17%)	52,89,113	1.86	8 (15%)
30	LHG	c	620	28	36,36,48	1.06	2 (5%)	39,42,54	1.25	3 (7%)
28	CLA	B	824	-	65,73,73	1.40	7 (10%)	76,113,113	1.62	9 (11%)
28	CLA	n	605	26	51,59,73	1.69	6 (11%)	59,96,113	1.60	10 (16%)
30	LHG	j	617	28	29,29,48	1.18	2 (6%)	32,35,54	1.34	4 (12%)
28	CLA	n	610	40	65,73,73	1.50	6 (9%)	76,113,113	1.31	7 (9%)
36	II0	J	104	-	39,43,43	6.66	22 (56%)	50,60,60	2.16	13 (26%)
36	II0	c	615	-	39,43,43	6.79	21 (53%)	50,60,60	2.40	18 (36%)
28	CLA	A	811	-	54,62,73	1.66	7 (12%)	62,99,113	1.48	10 (16%)
31	WVN	i	316	-	40,41,41	1.90	14 (35%)	50,56,56	2.22	16 (32%)
28	CLA	A	806	-	65,73,73	1.50	5 (7%)	76,113,113	1.34	12 (15%)
28	CLA	A	812	-	65,73,73	1.43	7 (10%)	76,113,113	1.65	13 (17%)
28	CLA	A	821	-	49,57,73	1.65	5 (10%)	55,93,113	1.63	9 (16%)
28	CLA	A	852	-	65,73,73	1.42	7 (10%)	76,113,113	1.46	11 (14%)
28	CLA	A	818	-	65,73,73	1.51	7 (10%)	76,113,113	1.65	13 (17%)
28	CLA	j	608	18	45,53,73	1.79	6 (13%)	52,89,113	1.64	7 (13%)
28	CLA	B	814	-	55,63,73	1.55	7 (12%)	64,101,113	1.51	7 (10%)
28	CLA	f	606	18	51,59,73	1.71	6 (11%)	59,96,113	1.49	9 (15%)
36	II0	b	614	-	39,43,43	6.78	23 (58%)	50,60,60	1.77	15 (30%)
28	CLA	A	816	-	65,73,73	1.38	7 (10%)	76,113,113	1.63	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	m	604	18	65,73,73	1.49	8 (12%)	76,113,113	1.52	7 (9%)
31	WVN	J	101	-	40,41,41	1.96	14 (35%)	50,56,56	3.41	19 (38%)
28	CLA	g	304	-	51,59,73	1.66	6 (11%)	59,96,113	1.56	6 (10%)
30	LHG	f	619	-	48,48,48	0.91	2 (4%)	51,54,54	1.02	3 (5%)
31	WVN	h	309	-	40,41,41	1.84	13 (32%)	50,56,56	2.36	20 (40%)
28	CLA	e	606	19	65,73,73	1.44	7 (10%)	76,113,113	1.41	8 (10%)
28	CLA	e	611	-	65,73,73	1.51	6 (9%)	76,113,113	1.42	9 (11%)
28	CLA	B	832	-	58,66,73	1.54	8 (13%)	67,104,113	1.60	8 (11%)
28	CLA	j	610	30	61,69,73	1.56	7 (11%)	71,108,113	1.41	9 (12%)
28	CLA	g	306	24	51,59,73	1.73	7 (13%)	59,96,113	1.47	7 (11%)
28	CLA	b	607	16	65,73,73	1.53	6 (9%)	76,113,113	1.66	14 (18%)
28	CLA	B	803	-	65,73,73	1.44	8 (12%)	76,113,113	1.84	11 (14%)
28	CLA	B	813	-	59,67,73	1.47	7 (11%)	68,105,113	1.71	9 (13%)
28	CLA	B	825	-	65,73,73	1.45	6 (9%)	76,113,113	1.33	7 (9%)
36	II0	h	310	-	26,28,43	6.09	13 (50%)	31,37,60	2.20	11 (35%)
28	CLA	d	309	30	41,49,73	1.85	6 (14%)	47,84,113	1.64	7 (14%)
36	II0	i	314	-	39,43,43	6.75	22 (56%)	50,60,60	2.01	19 (38%)
30	LHG	i	318	28	36,36,48	1.12	2 (5%)	39,42,54	1.27	4 (10%)
37	IHT	j	616	-	40,42,42	6.18	25 (62%)	53,58,58	2.24	16 (30%)
28	CLA	A	822	-	51,59,73	1.68	9 (17%)	59,96,113	1.44	9 (15%)
28	CLA	g	311	30	54,62,73	1.70	8 (14%)	62,99,113	1.42	9 (14%)
28	CLA	B	822	40	64,72,73	1.44	9 (14%)	74,111,113	1.54	10 (13%)
36	II0	d	316	-	39,43,43	6.91	22 (56%)	50,60,60	2.26	19 (38%)
28	CLA	k	606	21	51,59,73	1.68	6 (11%)	59,96,113	1.51	9 (15%)
28	CLA	c	608	14	65,73,73	1.45	7 (10%)	76,113,113	1.50	12 (15%)
28	CLA	B	807	-	65,73,73	1.52	8 (12%)	76,113,113	1.29	10 (13%)
36	II0	k	617	-	39,43,43	6.85	21 (53%)	50,60,60	2.29	20 (40%)
28	CLA	f	602	18	65,73,73	1.50	6 (9%)	76,113,113	1.40	11 (14%)
34	DGD	B	843	-	61,61,67	0.91	2 (3%)	75,75,81	1.10	5 (6%)
28	CLA	m	605	18	42,50,73	1.84	6 (14%)	48,85,113	1.69	8 (16%)
28	CLA	L	207	40	51,59,73	1.65	7 (13%)	59,96,113	1.53	7 (11%)
28	CLA	B	823	-	65,73,73	1.47	7 (10%)	76,113,113	1.55	10 (13%)
28	CLA	n	601	26	45,53,73	1.81	5 (11%)	52,89,113	1.47	8 (15%)
28	CLA	J	103	8	42,50,73	1.70	8 (19%)	48,85,113	1.64	7 (14%)
31	WVN	F	204	-	40,41,41	1.91	14 (35%)	50,56,56	2.94	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	B	834	-	47,55,73	1.74	7 (14%)	54,91,113	1.63	8 (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
28	CLA	A	851	-	1/1/15/20	4/37/115/115	-
28	CLA	k	604	21	1/1/15/20	14/37/115/115	-
28	CLA	B	831	40	1/1/11/20	4/13/91/115	-
28	CLA	l	309	30	1/1/14/20	12/33/111/115	-
31	WVN	K	102	-	-	5/29/63/63	0/2/2/2
36	II0	g	316	-	-	5/21/67/67	0/2/2/2
39	LMU	i	301	-	-	8/21/61/61	0/2/2/2
35	LMG	O	205	-	-	7/21/41/70	0/1/1/1
28	CLA	j	605	18	1/1/11/20	8/13/91/115	-
28	CLA	i	305	22	-	9/37/115/115	-
38	KC2	k	612	-	-	5/15/71/71	-
36	II0	i	313	-	-	7/21/67/67	0/2/2/2
28	CLA	A	810	28	1/1/14/20	8/34/112/115	-
35	LMG	n	620	-	-	12/50/70/70	0/1/1/1
28	CLA	m	607	-	1/1/12/20	4/21/99/115	-
37	IHT	a	317	-	-	8/25/65/65	0/2/2/2
28	CLA	b	604	-	-	16/37/115/115	-
30	LHG	A	843	-	-	7/52/52/53	-
30	LHG	g	321	28	-	12/41/41/53	-
29	PQN	A	842	-	-	8/23/43/43	0/2/2/2
28	CLA	K	103	-	1/1/10/20	5/10/88/115	-
28	CLA	A	832	-	1/1/15/20	12/37/115/115	-
28	CLA	h	303	17	1/1/12/20	6/19/97/115	-
28	CLA	a	303	15	1/1/12/20	11/22/100/115	-
38	KC2	s	201	13	-	8/15/71/71	-
28	CLA	j	601	18	1/1/12/20	6/21/99/115	-
28	CLA	A	823	-	-	6/25/103/115	-
28	CLA	b	603	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	j	609	18	1/1/12/20	2/21/99/115	-
29	PQN	B	842	-	-	5/23/43/43	0/2/2/2
28	CLA	B	818	-	-	3/15/93/115	-
28	CLA	f	603	-	1/1/12/20	7/21/99/115	-
30	LHG	A	844	28	-	6/31/31/53	-
36	II0	b	613	-	-	2/21/67/67	0/2/2/2
38	KC2	i	310	22	-	7/15/71/71	-
30	LHG	J	106	28	-	27/53/53/53	-
28	CLA	c	605	14	1/1/12/20	8/21/99/115	-
28	CLA	n	606	26	1/1/12/20	5/21/99/115	-
28	CLA	h	306	17	1/1/15/20	21/37/115/115	-
28	CLA	i	304	-	1/1/12/20	5/21/99/115	-
28	CLA	g	309	24	1/1/15/20	12/37/115/115	-
28	CLA	s	206	40	1/1/15/20	13/37/115/115	-
38	KC2	e	609	19	-	7/15/71/71	-
28	CLA	f	605	18	-	6/13/91/115	-
28	CLA	i	306	-	1/1/12/20	10/21/99/115	-
28	CLA	g	322	35	1/1/15/20	16/37/115/115	-
28	CLA	n	608	26	1/1/12/20	5/21/99/115	-
38	KC2	f	611	18	-	7/15/71/71	-
36	II0	a	314	-	-	3/21/67/67	0/2/2/2
28	CLA	A	840	40	1/1/15/20	21/37/115/115	-
28	CLA	n	604	26	1/1/14/20	12/31/109/115	-
28	CLA	a	305	-	1/1/12/20	4/21/99/115	-
35	LMG	b	621	-	-	17/44/64/70	0/1/1/1
37	IHT	g	319	-	-	8/25/65/65	0/2/2/2
36	II0	f	614	-	-	3/21/67/67	0/2/2/2
28	CLA	c	603	-	1/1/12/20	3/21/99/115	-
28	CLA	a	308	15	1/1/15/20	18/37/115/115	-
28	CLA	i	311	-	1/1/12/20	7/21/99/115	-
28	CLA	c	606	-	-	11/22/100/115	-
31	WVN	K	104	-	-	5/29/63/63	0/2/2/2
28	CLA	d	302	-	1/1/12/20	8/21/99/115	-
28	CLA	A	804	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	B	806	-	1/1/15/20	10/37/115/115	-
28	CLA	d	303	-	1/1/15/20	19/37/115/115	-
36	II0	n	616	-	-	4/21/67/67	0/2/2/2
30	LHG	l	317	28	-	14/36/36/53	-
28	CLA	A	805	1	1/1/15/20	7/37/115/115	-
31	WVN	F	203	-	-	8/29/63/63	0/2/2/2
28	CLA	d	306	-	1/1/12/20	11/21/99/115	-
28	CLA	A	807	1	1/1/15/20	10/37/115/115	-
28	CLA	b	610	16	1/1/15/20	20/37/115/115	-
28	CLA	k	607	-	1/1/12/20	8/21/99/115	-
28	CLA	B	805	-	1/1/15/20	13/37/115/115	-
28	CLA	h	304	-	1/1/12/20	6/21/99/115	-
28	CLA	m	602	18	1/1/13/20	8/27/105/115	-
28	CLA	c	604	14	-	4/37/115/115	-
36	II0	n	618	-	-	6/21/67/67	0/2/2/2
28	CLA	A	830	-	-	6/19/97/115	-
36	II0	f	615	-	-	5/21/67/67	0/2/2/2
38	KC2	d	311	-	-	5/15/71/71	-
28	CLA	F	201	40	1/1/15/20	15/37/115/115	-
38	KC2	k	611	21	-	5/15/71/71	-
36	II0	j	615	-	-	2/21/67/67	0/2/2/2
28	CLA	f	601	18	1/1/11/20	10/16/94/115	-
28	CLA	b	605	40,28	1/1/15/20	9/37/115/115	-
36	II0	k	619	-	-	5/21/67/67	0/2/2/2
28	CLA	A	809	-	1/1/13/20	10/27/105/115	-
28	CLA	a	312	-	1/1/15/20	17/37/115/115	-
28	CLA	k	602	21	1/1/12/20	8/19/97/115	-
38	KC2	g	313	38	-	2/15/71/71	-
28	CLA	e	610	40	1/1/15/20	13/37/115/115	-
28	CLA	A	854	40	1/1/15/20	16/37/115/115	-
28	CLA	c	607	14	1/1/11/20	2/15/93/115	-
28	CLA	g	307	24	1/1/12/20	6/21/99/115	-
28	CLA	A	819	-	1/1/11/20	4/13/91/115	-
28	CLA	h	302	17	1/1/12/20	7/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	A	849	-	-	16/42/42/53	-
28	CLA	n	603	-	1/1/12/20	9/21/99/115	-
28	CLA	O	206	-	1/1/15/20	16/37/115/115	-
31	WVN	A	845	-	-	7/29/63/63	0/2/2/2
35	LMG	J	105	-	-	13/50/70/70	0/1/1/1
36	II0	l	313	-	-	5/21/67/67	0/2/2/2
28	CLA	j	603	-	1/1/12/20	6/21/99/115	-
28	CLA	A	836	-	-	11/37/115/115	-
28	CLA	c	602	14	1/1/12/20	10/19/97/115	-
28	CLA	c	609	30	1/1/11/20	2/13/91/115	-
28	CLA	l	311	20	1/1/15/20	12/37/115/115	-
28	CLA	B	816	-	-	9/28/106/115	-
28	CLA	A	838	1	1/1/15/20	15/37/115/115	-
28	CLA	j	606	18	1/1/12/20	10/21/99/115	-
28	CLA	g	310	24	1/1/12/20	7/21/99/115	-
28	CLA	B	804	-	1/1/15/20	15/37/115/115	-
31	WVN	L	201	-	-	9/29/63/63	0/2/2/2
28	CLA	h	313	40	1/1/15/20	10/37/115/115	-
28	CLA	k	601	21	-	10/21/99/115	-
28	CLA	k	609	21	1/1/15/20	11/37/115/115	-
28	CLA	B	812	-	1/1/14/20	14/31/109/115	-
28	CLA	d	305	23	1/1/12/20	7/21/99/115	-
28	CLA	f	609	18	1/1/15/20	13/37/115/115	-
28	CLA	g	308	-	1/1/15/20	17/37/115/115	-
28	CLA	k	608	21	1/1/15/20	14/37/115/115	-
36	II0	h	311	-	-	7/21/67/67	0/2/2/2
36	II0	m	618	-	-	6/21/67/67	0/2/2/2
28	CLA	B	835	40	1/1/15/20	13/37/115/115	-
28	CLA	c	601	14	1/1/12/20	7/21/99/115	-
36	II0	m	615	-	-	7/21/67/67	0/2/2/2
28	CLA	l	308	20	1/1/12/20	9/21/99/115	-
31	WVN	B	845	-	-	0/29/63/63	0/2/2/2
28	CLA	h	307	17	1/1/13/20	10/28/106/115	-
28	CLA	a	304	15	1/1/12/20	7/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	l	305	20	1/1/15/20	16/37/115/115	-
28	CLA	a	311	15	1/1/15/20	12/37/115/115	-
28	CLA	j	604	18	-	13/37/115/115	-
37	IHT	m	617	-	-	9/25/65/65	0/2/2/2
28	CLA	A	802	-	1/1/15/20	15/37/115/115	-
35	LMG	L	209	28	-	19/50/70/70	0/1/1/1
28	CLA	B	820	-	1/1/12/20	6/23/101/115	-
28	CLA	i	303	22	1/1/12/20	10/19/97/115	-
28	CLA	A	827	-	1/1/14/20	9/34/112/115	-
32	LMT	b	618	-	-	9/15/35/61	0/1/1/2
28	CLA	d	301	23	1/1/12/20	4/19/97/115	-
37	IHT	b	615	-	-	6/25/65/65	0/2/2/2
28	CLA	B	802	-	1/1/15/20	21/37/115/115	-
38	KC2	i	319	-	-	6/15/71/71	-
28	CLA	e	605	19	-	17/37/115/115	-
28	CLA	d	304	23	1/1/12/20	9/21/99/115	-
28	CLA	B	827	-	-	9/19/97/115	-
28	CLA	B	817	40	1/1/15/20	10/37/115/115	-
28	CLA	b	602	16	1/1/13/20	10/25/103/115	-
28	CLA	b	609	-	1/1/12/20	6/21/99/115	-
31	WVN	B	846	-	-	6/29/63/63	0/2/2/2
28	CLA	n	607	-	1/1/15/20	13/37/115/115	-
28	CLA	B	830	40	1/1/15/20	15/37/115/115	-
38	KC2	n	611	26	-	7/15/71/71	-
33	SF4	A	853	1,2	-	-	0/6/5/5
37	IHT	f	617	-	-	7/25/65/65	0/2/2/2
28	CLA	A	808	1	1/1/15/20	12/37/115/115	-
37	IHT	k	618	-	-	11/25/65/65	0/2/2/2
36	II0	e	612	-	-	5/21/67/67	0/2/2/2
28	CLA	b	601	16	1/1/12/20	8/21/99/115	-
28	CLA	A	855	30	1/1/10/20	4/8/86/115	-
36	II0	d	313	-	-	5/21/67/67	0/2/2/2
36	II0	f	618	-	-	7/21/67/67	0/2/2/2
28	CLA	A	833	-	1/1/12/20	4/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	e	607	19	1/1/15/20	20/37/115/115	-
30	LHG	c	618	28	-	15/41/41/53	-
31	WVN	I	101	-	-	9/29/63/63	0/2/2/2
28	CLA	i	307	22	1/1/14/20	12/33/111/115	-
36	II0	d	314	-	-	3/21/67/67	0/2/2/2
28	CLA	A	803	28	1/1/13/20	7/25/103/115	-
36	II0	l	316	-	-	7/21/67/67	0/2/2/2
38	KC2	d	310	23	-	6/15/71/71	-
36	II0	g	317	-	-	5/21/67/67	0/2/2/2
36	II0	k	615	-	-	6/21/67/67	0/2/2/2
28	CLA	B	819	-	-	8/25/103/115	-
28	CLA	b	612	30	1/1/12/20	6/21/99/115	-
28	CLA	m	603	-	1/1/15/20	11/37/115/115	-
28	CLA	B	808	2	1/1/15/20	12/37/115/115	-
30	LHG	d	317	28	-	15/41/41/53	-
28	CLA	l	302	20	1/1/11/20	5/16/94/115	-
36	II0	j	614	-	-	6/21/67/67	0/2/2/2
28	CLA	L	204	40	-	7/19/97/115	-
37	IHT	n	617	-	-	8/25/65/65	0/2/2/2
38	KC2	c	610	-	-	6/15/71/71	-
28	CLA	k	603	-	1/1/12/20	3/21/99/115	-
36	II0	m	614	-	-	3/21/67/67	0/2/2/2
38	KC2	m	611	18	-	7/15/71/71	-
28	CLA	B	836	-	1/1/15/20	27/37/115/115	-
28	CLA	d	307	23	1/1/11/20	3/15/93/115	-
28	CLA	j	607	-	1/1/12/20	6/21/99/115	-
28	CLA	j	612	-	1/1/12/20	10/21/99/115	-
28	CLA	n	609	26	1/1/15/20	11/37/115/115	-
31	WVN	B	844	-	-	5/29/63/63	0/2/2/2
28	CLA	Q	302	40	1/1/15/20	18/37/115/115	-
36	II0	i	320	-	-	6/21/67/67	0/2/2/2
28	CLA	m	613	-	1/1/10/20	6/11/89/115	-
38	KC2	s	204	-	-	5/15/71/71	-
28	CLA	K	101	40	1/1/12/20	4/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	i	312	-	1/1/12/20	6/21/99/115	-
28	CLA	A	825	40	-	10/37/115/115	-
28	CLA	d	312	-	-	6/21/99/115	-
31	WVN	s	205	-	-	4/29/63/63	0/2/2/2
28	CLA	e	602	19	-	8/19/97/115	-
36	II0	b	617	-	-	1/21/67/67	0/2/2/2
28	CLA	A	835	-	1/1/15/20	11/37/115/115	-
38	KC2	g	314	38	-	5/15/71/71	-
28	CLA	A	837	-	1/1/15/20	9/37/115/115	-
28	CLA	F	202	6	1/1/12/20	11/22/100/115	-
28	CLA	s	203	28,13	-	16/37/115/115	-
28	CLA	B	829	-	-	5/19/97/115	-
28	CLA	m	601	18	1/1/10/20	2/10/88/115	-
28	CLA	k	614	-	1/1/12/20	8/21/99/115	-
28	CLA	h	301	40	-	12/37/115/115	-
28	CLA	n	613	-	1/1/12/20	10/21/99/115	-
28	CLA	B	815	-	1/1/13/20	6/30/108/115	-
28	CLA	A	831	-	1/1/15/20	8/37/115/115	-
28	CLA	m	608	18	1/1/15/20	23/37/115/115	-
28	CLA	i	308	22	1/1/12/20	4/21/99/115	-
36	II0	l	312	-	-	4/21/67/67	0/2/2/2
28	CLA	f	607	-	-	20/37/115/115	-
30	LHG	g	301	28	-	21/41/41/53	-
28	CLA	e	601	19	1/1/11/20	4/13/91/115	-
36	II0	g	320	-	-	4/21/67/67	0/2/2/2
28	CLA	a	309	15	1/1/15/20	11/37/115/115	-
31	WVN	A	846	-	-	10/29/63/63	0/2/2/2
28	CLA	A	820	40	1/1/15/20	3/37/115/115	-
35	LMG	Q	301	-	-	22/33/53/70	0/1/1/1
28	CLA	O	201	30	1/1/12/20	5/22/100/115	-
31	WVN	L	206	-	-	3/29/63/63	0/2/2/2
36	II0	m	616	-	-	3/21/67/67	0/2/2/2
28	CLA	f	608	18	1/1/15/20	17/37/115/115	-
28	CLA	m	612	40	1/1/12/20	9/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	e	603	19	1/1/12/20	5/21/99/115	-
28	CLA	l	303	20	1/1/15/20	22/37/115/115	-
36	II0	i	317	-	-	7/21/67/67	0/2/2/2
28	CLA	O	202	-	1/1/15/20	15/37/115/115	-
28	CLA	j	602	18	1/1/12/20	6/19/97/115	-
28	CLA	B	826	-	1/1/12/20	5/21/99/115	-
28	CLA	f	612	18	1/1/12/20	9/21/99/115	-
28	CLA	A	814	-	-	9/19/97/115	-
28	CLA	e	604	40	-	20/37/115/115	-
28	CLA	l	306	20	1/1/15/20	19/37/115/115	-
28	CLA	e	608	30	1/1/11/20	4/15/93/115	-
37	IHT	O	204	-	-	8/25/65/65	0/2/2/2
28	CLA	B	840	-	1/1/15/20	11/37/115/115	-
28	CLA	m	610	30	1/1/13/20	10/25/103/115	-
36	II0	c	614	-	-	1/21/67/67	0/2/2/2
31	WVN	R	201	-	-	6/29/63/63	0/2/2/2
36	II0	k	621	-	-	7/21/67/67	0/2/2/2
28	CLA	B	838	-	1/1/13/20	8/28/106/115	-
36	II0	e	613	-	-	4/21/67/67	0/2/2/2
36	II0	f	616	-	-	3/21/67/67	0/2/2/2
28	CLA	B	833	-	1/1/15/20	11/37/115/115	-
30	LHG	a	301	28	-	12/53/53/53	-
28	CLA	m	609	18	1/1/12/20	6/21/99/115	-
36	II0	g	318	-	-	2/21/67/67	0/2/2/2
32	LMT	a	320	-	-	10/21/61/61	0/2/2/2
30	LHG	b	620	-	-	17/35/35/53	-
28	CLA	f	604	18	1/1/15/20	11/37/115/115	-
30	LHG	n	619	-	-	16/47/47/53	-
28	CLA	B	811	-	1/1/15/20	17/37/115/115	-
28	CLA	a	306	40	1/1/15/20	15/37/115/115	-
36	II0	e	616	-	-	4/21/67/67	0/2/2/2
28	CLA	s	208	-	1/1/12/20	5/21/99/115	-
28	CLA	B	809	-	1/1/13/20	4/25/101/115	-
28	CLA	m	606	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	WVN	l	301	-	-	4/29/63/63	0/2/2/2
28	CLA	B	821	40	1/1/15/20	9/37/115/115	-
35	LMG	F	205	-	-	11/43/63/70	0/1/1/1
31	WVN	B	848	-	-	6/29/63/63	0/2/2/2
31	WVN	J	102	-	-	10/29/63/63	0/2/2/2
35	LMG	c	619	-	-	22/50/70/70	0/1/1/1
36	II0	n	614	-	-	1/21/67/67	0/2/2/2
36	II0	a	316	-	-	2/21/67/67	0/2/2/2
30	LHG	m	619	28	-	19/41/41/53	-
31	WVN	l	315	-	-	9/29/63/63	0/2/2/2
30	LHG	L	208	-	-	21/53/53/53	-
31	WVN	s	207	-	-	7/29/63/63	0/2/2/2
28	CLA	L	202	9	1/1/11/20	10/18/96/115	-
36	II0	O	203	-	-	3/21/67/67	0/2/2/2
28	CLA	A	824	40	1/1/15/20	12/37/115/115	-
31	WVN	B	847	-	-	2/29/63/63	0/2/2/2
36	II0	h	312	-	-	6/21/67/67	0/2/2/2
28	CLA	c	612	-	1/1/15/20	15/37/115/115	-
28	CLA	A	817	-	1/1/15/20	13/37/115/115	-
37	IHT	c	616	-	-	10/25/65/65	0/2/2/2
31	WVN	M	101	-	-	7/29/63/63	0/2/2/2
28	CLA	k	610	30	1/1/12/20	11/21/99/115	-
36	II0	a	318	-	-	7/21/67/67	0/2/2/2
36	II0	k	616	-	-	8/21/67/67	0/2/2/2
38	KC2	j	611	18	-	7/15/71/71	-
28	CLA	g	302	24	1/1/10/20	2/10/88/115	-
28	CLA	a	313	-	-	8/17/95/115	-
36	II0	i	315	-	-	4/21/67/67	0/2/2/2
28	CLA	c	611	14	-	7/13/91/115	-
28	CLA	A	834	-	1/1/12/20	3/21/99/115	-
28	CLA	A	801	-	1/1/15/20	11/37/115/115	-
32	LMT	a	302	-	-	4/15/35/61	0/1/1/2
28	CLA	j	613	-	1/1/15/20	15/37/115/115	-
36	II0	c	617	-	-	4/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	A	815	40	1/1/11/20	6/13/91/115	-
28	CLA	A	841	-	1/1/15/20	20/37/115/115	-
28	CLA	B	801	40	1/1/15/20	12/37/115/115	-
28	CLA	k	605	21	1/1/11/20	5/13/91/115	-
31	WVN	L	205	-	-	6/29/63/63	0/2/2/2
28	CLA	A	826	-	1/1/15/20	10/37/115/115	-
28	CLA	B	841	30	-	5/37/115/115	-
28	CLA	s	202	13	1/1/15/20	19/37/115/115	-
28	CLA	L	203	-	-	13/37/115/115	-
28	CLA	A	829	-	1/1/15/20	15/37/115/115	-
28	CLA	b	608	30	1/1/15/20	12/37/115/115	-
38	KC2	g	312	24	-	8/15/71/71	-
28	CLA	A	839	-	1/1/15/20	16/37/115/115	-
30	LHG	e	617	28	-	26/41/41/53	-
36	II0	l	314	-	-	4/21/67/67	0/2/2/2
28	CLA	B	839	-	1/1/15/20	15/37/115/115	-
28	CLA	f	610	30	1/1/15/20	13/37/115/115	-
28	CLA	l	304	-	1/1/12/20	6/21/99/115	-
28	CLA	h	308	17	1/1/12/20	7/21/99/115	-
38	KC2	l	310	20	-	4/15/71/71	-
28	CLA	a	307	15	1/1/11/20	2/13/91/115	-
36	II0	d	315	-	-	5/21/67/67	0/2/2/2
31	WVN	e	615	-	-	11/29/63/63	0/2/2/2
36	II0	e	614	-	-	3/21/67/67	0/2/2/2
28	CLA	g	303	24	1/1/12/20	2/19/97/115	-
36	II0	c	613	-	-	4/21/67/67	0/2/2/2
31	WVN	R	202	-	-	6/29/63/63	0/2/2/2
28	CLA	R	203	-	1/1/12/20	8/21/99/115	-
28	CLA	B	828	-	1/1/11/20	5/18/96/115	-
36	II0	a	315	-	-	2/21/67/67	0/2/2/2
28	CLA	b	606	16	1/1/14/20	13/33/111/115	-
32	LMT	A	850	-	-	11/21/61/61	0/2/2/2
28	CLA	n	602	26	-	4/19/97/115	-
30	LHG	b	619	28	-	22/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	IHT	b	616	-	-	8/25/65/65	0/2/2/2
38	KC2	n	612	-	-	7/15/71/71	-
30	LHG	a	319	28	-	15/53/53/53	-
28	CLA	a	310	30	1/1/11/20	8/17/95/115	-
28	CLA	l	307	20	1/1/15/20	12/37/115/115	-
37	IHT	R	204	-	-	3/25/65/65	0/2/2/2
33	SF4	C	101	3	-	-	0/6/5/5
28	CLA	i	309	30	1/1/11/20	5/15/93/115	-
28	CLA	g	315	-	1/1/12/20	9/21/99/115	-
28	CLA	B	810	-	1/1/13/20	6/25/103/115	-
31	WVN	A	848	-	-	9/29/63/63	0/2/2/2
36	II0	n	615	-	-	4/21/67/67	0/2/2/2
28	CLA	A	813	-	1/1/11/20	7/13/91/115	-
28	CLA	h	305	17	1/1/12/20	6/21/99/115	-
28	CLA	f	613	-	1/1/15/20	23/37/115/115	-
28	CLA	b	611	-	1/1/15/20	21/37/115/115	-
28	CLA	g	305	24	-	12/37/115/115	-
28	CLA	d	308	23	1/1/10/20	3/8/86/115	-
28	CLA	B	837	-	1/1/15/20	14/37/115/115	-
31	WVN	A	847	-	-	6/29/63/63	0/2/2/2
38	KC2	k	613	-	-	6/15/71/71	-
28	CLA	i	302	22	1/1/12/20	9/21/99/115	-
28	CLA	A	828	-	-	9/37/115/115	-
30	LHG	k	620	28	-	19/41/41/53	-
33	SF4	C	102	3	-	-	0/6/5/5
28	CLA	Q	303	27	1/1/11/20	6/13/91/115	-
30	LHG	c	620	28	-	25/41/41/53	-
28	CLA	B	824	-	1/1/15/20	9/37/115/115	-
28	CLA	n	605	26	1/1/12/20	8/21/99/115	-
30	LHG	j	617	28	-	5/34/34/53	-
28	CLA	n	610	40	1/1/15/20	16/37/115/115	-
36	II0	J	104	-	-	6/21/67/67	0/2/2/2
36	II0	c	615	-	-	2/21/67/67	0/2/2/2
28	CLA	A	811	-	-	5/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	WVN	i	316	-	-	9/29/63/63	0/2/2/2
28	CLA	A	806	-	1/1/15/20	10/37/115/115	-
28	CLA	A	812	-	1/1/15/20	23/37/115/115	-
28	CLA	A	821	-	-	6/18/96/115	-
28	CLA	A	852	-	1/1/15/20	12/37/115/115	-
28	CLA	A	818	-	1/1/15/20	19/37/115/115	-
28	CLA	j	608	18	1/1/11/20	6/13/91/115	-
28	CLA	B	814	-	-	9/25/103/115	-
28	CLA	f	606	18	-	5/21/99/115	-
36	II0	b	614	-	-	8/21/67/67	0/2/2/2
28	CLA	A	816	-	1/1/15/20	17/37/115/115	-
28	CLA	m	604	18	-	13/37/115/115	-
31	WVN	J	101	-	-	11/29/63/63	0/2/2/2
28	CLA	g	304	-	1/1/12/20	4/21/99/115	-
30	LHG	f	619	-	-	38/53/53/53	-
31	WVN	h	309	-	-	8/29/63/63	0/2/2/2
28	CLA	e	606	19	1/1/15/20	22/37/115/115	-
28	CLA	e	611	-	1/1/15/20	21/37/115/115	-
28	CLA	B	832	-	1/1/13/20	5/29/107/115	-
28	CLA	j	610	30	1/1/14/20	15/33/111/115	-
28	CLA	g	306	24	1/1/12/20	8/21/99/115	-
28	CLA	b	607	16	1/1/15/20	17/37/115/115	-
28	CLA	B	803	-	1/1/15/20	9/37/115/115	-
28	CLA	B	813	-	1/1/13/20	14/30/108/115	-
28	CLA	B	825	-	1/1/15/20	9/37/115/115	-
36	II0	h	310	-	-	3/17/40/67	0/1/1/2
28	CLA	d	309	30	1/1/10/20	3/8/86/115	-
36	II0	i	314	-	-	5/21/67/67	0/2/2/2
30	LHG	i	318	28	-	13/41/41/53	-
37	IHT	j	616	-	-	5/25/65/65	0/2/2/2
28	CLA	A	822	-	1/1/12/20	6/21/99/115	-
28	CLA	g	311	30	1/1/12/20	4/24/102/115	-
28	CLA	B	822	40	-	11/36/114/115	-
36	II0	d	316	-	-	8/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	k	606	21	-	10/21/99/115	-
28	CLA	c	608	14	1/1/15/20	15/37/115/115	-
28	CLA	B	807	-	1/1/15/20	13/37/115/115	-
36	II0	k	617	-	-	2/21/67/67	0/2/2/2
28	CLA	f	602	18	1/1/15/20	14/37/115/115	-
34	DGD	B	843	-	-	5/49/89/95	0/2/2/2
28	CLA	m	605	18	-	4/10/88/115	-
28	CLA	L	207	40	1/1/12/20	6/21/99/115	-
28	CLA	B	823	-	1/1/15/20	2/37/115/115	-
28	CLA	n	601	26	1/1/11/20	4/13/91/115	-
28	CLA	J	103	8	1/1/10/20	5/10/88/115	-
31	WVN	F	204	-	-	12/29/63/63	0/2/2/2
28	CLA	B	834	-	1/1/11/20	2/16/94/115	-

The worst 5 of 4219 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	b	616	IHT	C15-C11	25.61	1.63	1.34
37	g	319	IHT	C15-C11	25.50	1.63	1.34
37	a	317	IHT	C15-C11	25.34	1.63	1.34
37	R	204	IHT	C15-C11	25.21	1.63	1.34
37	O	204	IHT	C15-C11	25.16	1.63	1.34

The worst 5 of 4792 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	J	101	WVN	C29-C26-C22	13.31	146.31	127.31
38	g	312	KC2	C1A-NA-C4A	-12.33	101.16	106.71
38	i	319	KC2	C1A-NA-C4A	-12.21	101.22	106.71
38	l	310	KC2	C1A-NA-C4A	-12.16	101.24	106.71
38	j	611	KC2	C1A-NA-C4A	-11.84	101.39	106.71

5 of 217 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	A	801	CLA	ND
28	A	802	CLA	ND
28	A	803	CLA	ND
28	A	804	CLA	ND

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Mol	Chain	Res	Type	Atom
28	A	805	CLA	ND

5 of 3777 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	801	CLA	CHA-CBD-CGD-O1D
28	A	801	CLA	CHA-CBD-CGD-O2D
28	A	801	CLA	CBD-CGD-O2D-CED
28	A	802	CLA	C1A-C2A-CAA-CBA
28	A	802	CLA	CBA-CGA-O2A-C1

There are no ring outliers.

108 monomers are involved in 236 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	851	CLA	3	0
28	B	831	CLA	2	0
31	K	102	WVN	1	0
28	A	810	CLA	2	0
30	A	843	LHG	1	0
29	A	842	PQN	1	0
28	A	832	CLA	2	0
28	A	823	CLA	3	0
29	B	842	PQN	1	0
30	A	844	LHG	1	0
30	J	106	LHG	6	0
28	A	840	CLA	2	0
28	A	804	CLA	2	0
28	B	806	CLA	1	0
28	A	807	CLA	5	0
28	B	805	CLA	3	0
28	A	830	CLA	1	0
28	F	201	CLA	3	0
28	A	809	CLA	3	0
28	A	854	CLA	6	0
28	A	819	CLA	1	0
30	A	849	LHG	3	0
28	O	206	CLA	8	0
35	J	105	LMG	2	0
28	A	836	CLA	6	0
28	A	838	CLA	4	0
28	B	804	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B	835	CLA	6	0
28	A	802	CLA	8	0
35	L	209	LMG	4	0
28	B	820	CLA	1	0
28	A	827	CLA	2	0
28	B	802	CLA	3	0
28	B	827	CLA	2	0
28	B	817	CLA	3	0
31	B	846	WVN	1	0
28	B	830	CLA	4	0
28	A	808	CLA	1	0
31	I	101	WVN	2	0
28	A	803	CLA	2	0
28	B	819	CLA	1	0
28	B	808	CLA	1	0
28	L	204	CLA	3	0
28	B	836	CLA	3	0
28	Q	302	CLA	7	0
28	K	101	CLA	1	0
28	A	835	CLA	4	0
28	A	837	CLA	3	0
28	F	202	CLA	1	0
28	B	815	CLA	5	0
28	A	831	CLA	3	0
31	A	846	WVN	1	0
28	A	820	CLA	4	0
35	Q	301	LMG	4	0
28	O	201	CLA	1	0
31	L	206	WVN	1	0
28	O	202	CLA	4	0
28	A	814	CLA	1	0
28	B	840	CLA	2	0
28	B	833	CLA	3	0
28	B	811	CLA	3	0
28	B	821	CLA	4	0
35	F	205	LMG	3	0
30	L	208	LHG	2	0
28	L	202	CLA	2	0
28	A	824	CLA	4	0
28	A	817	CLA	3	0
28	A	834	CLA	2	0
28	A	801	CLA	5	0

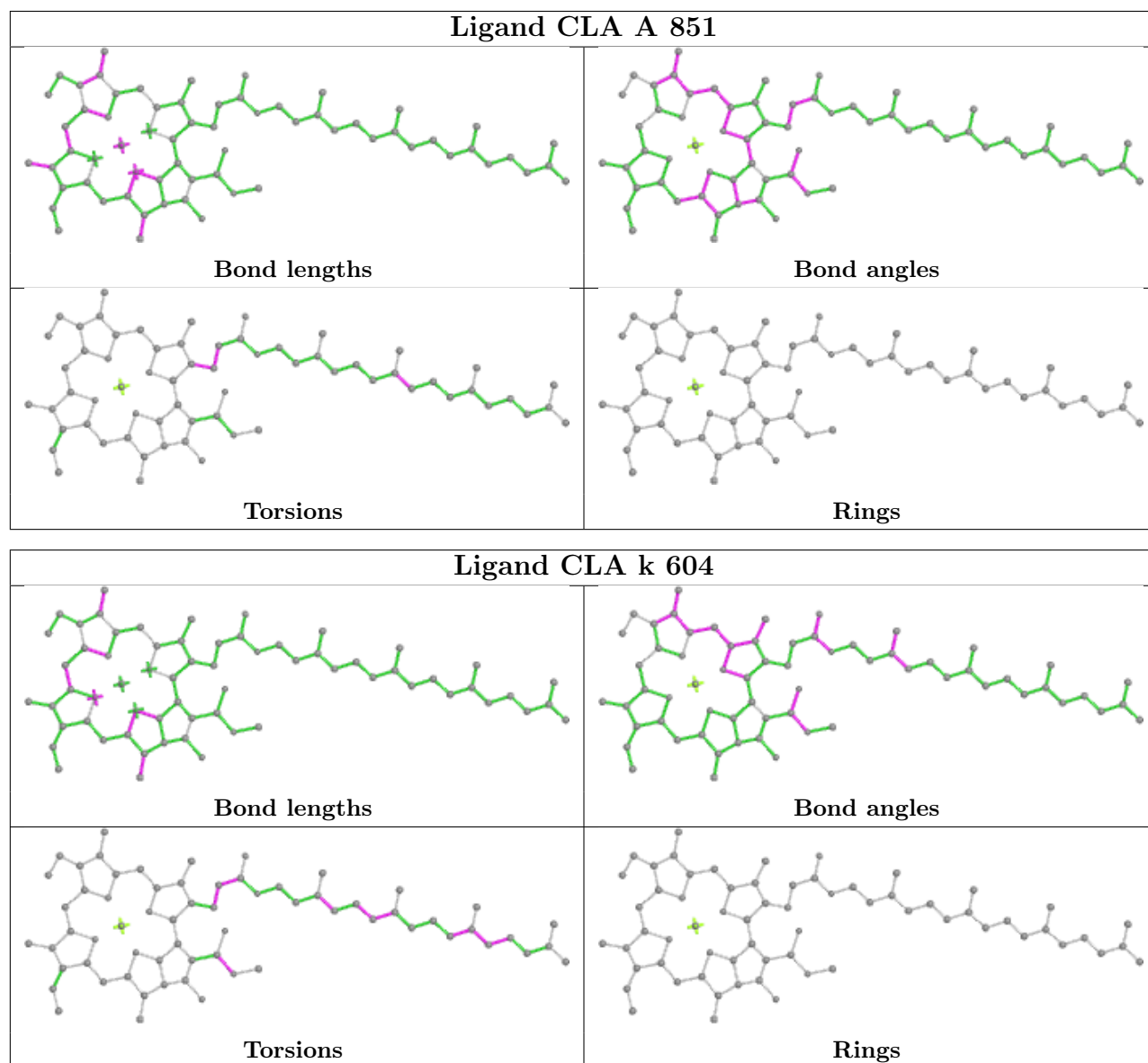
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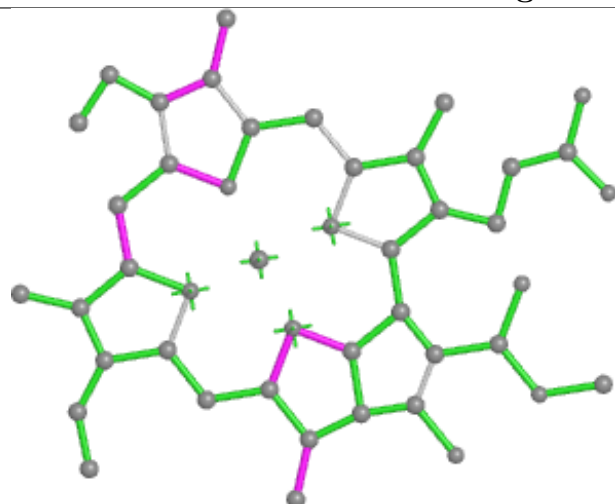
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	815	CLA	1	0
28	A	841	CLA	5	0
28	B	801	CLA	5	0
28	A	826	CLA	3	0
28	B	841	CLA	3	0
28	L	203	CLA	5	0
28	A	829	CLA	2	0
28	A	839	CLA	5	0
28	B	839	CLA	3	0
31	R	202	WVN	7	0
28	R	203	CLA	1	0
32	A	850	LMT	2	0
28	B	810	CLA	1	0
31	A	848	WVN	1	0
28	A	813	CLA	1	0
28	B	837	CLA	4	0
31	A	847	WVN	3	0
28	A	828	CLA	4	0
28	B	824	CLA	3	0
28	A	811	CLA	2	0
28	A	806	CLA	4	0
28	A	812	CLA	1	0
28	A	821	CLA	3	0
28	A	852	CLA	2	0
28	A	818	CLA	3	0
28	B	814	CLA	1	0
28	A	816	CLA	3	0
31	J	101	WVN	1	0
28	B	832	CLA	4	0
28	B	803	CLA	5	0
28	B	813	CLA	8	0
28	B	825	CLA	2	0
28	A	822	CLA	2	0
28	B	822	CLA	5	0
28	B	807	CLA	2	0
34	B	843	DGD	2	0
28	L	207	CLA	2	0
28	B	823	CLA	2	0
28	B	834	CLA	2	0

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

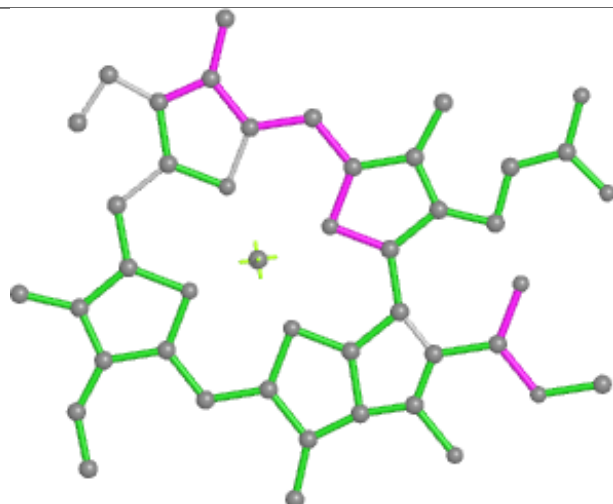
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



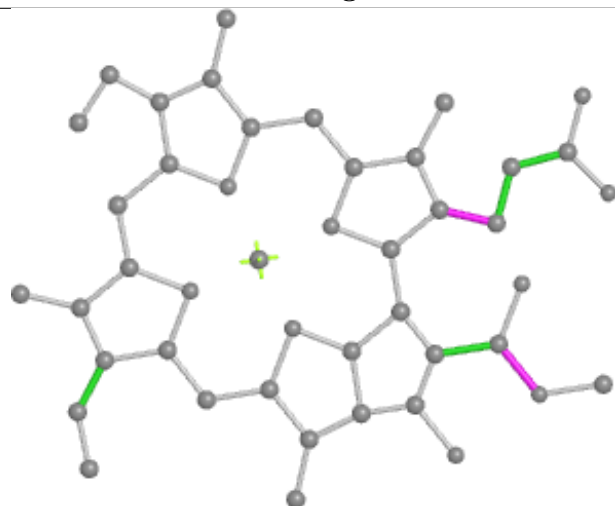
Ligand CLA B 831



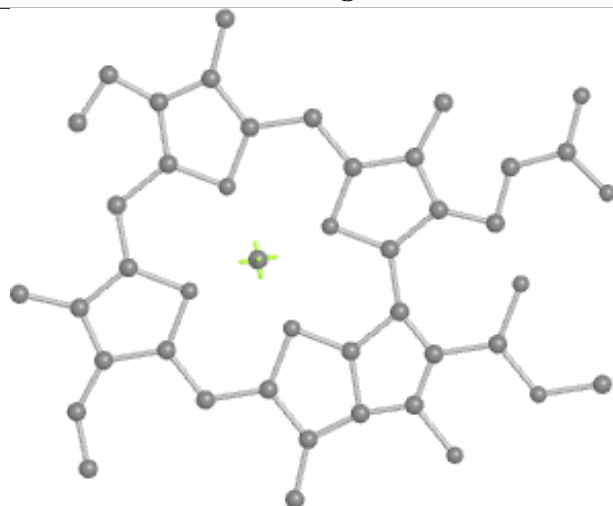
Bond lengths



Bond angles

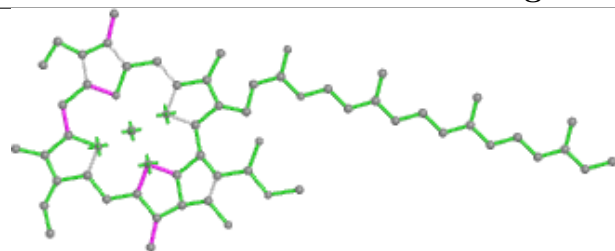


Torsions

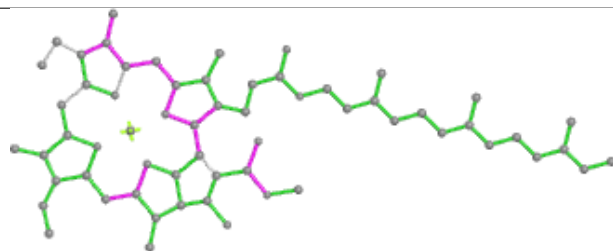


Rings

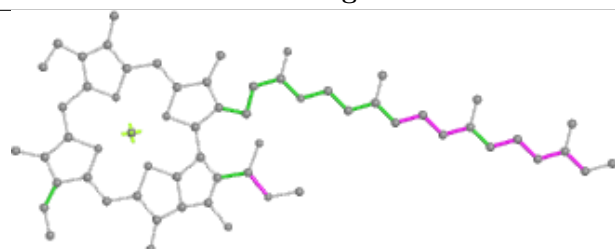
Ligand CLA 1 309



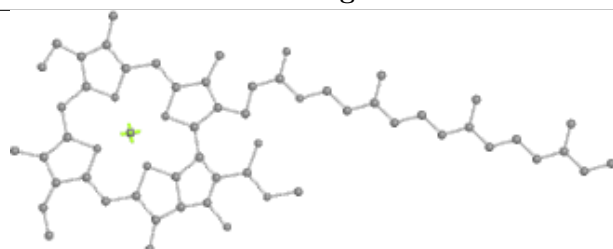
Bond lengths



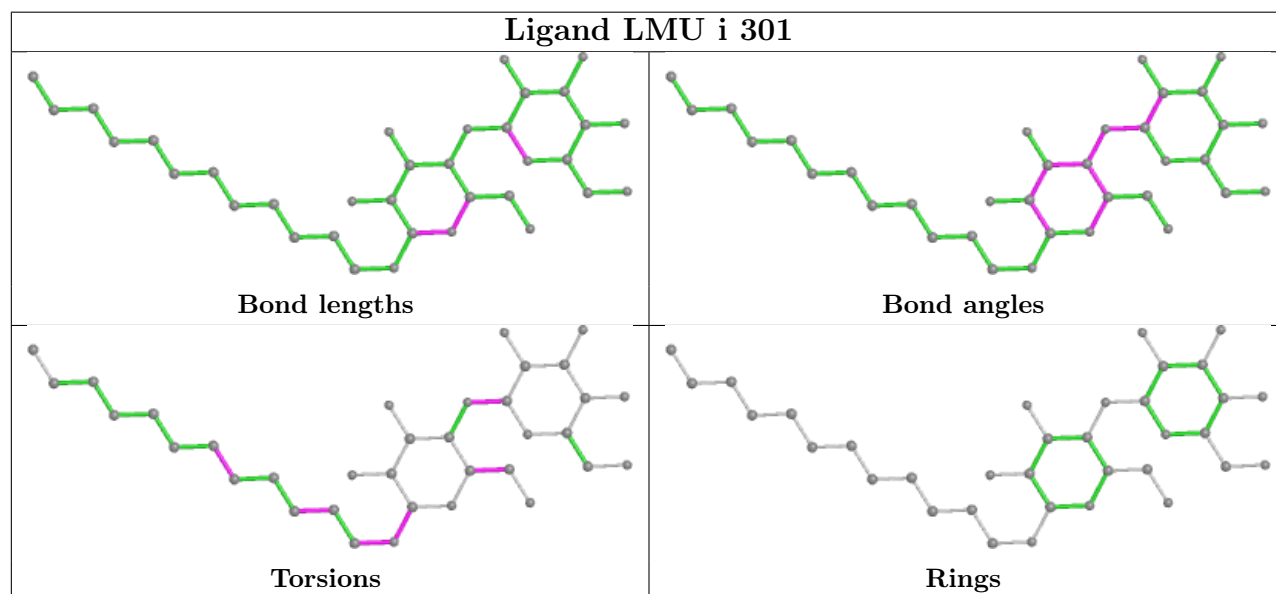
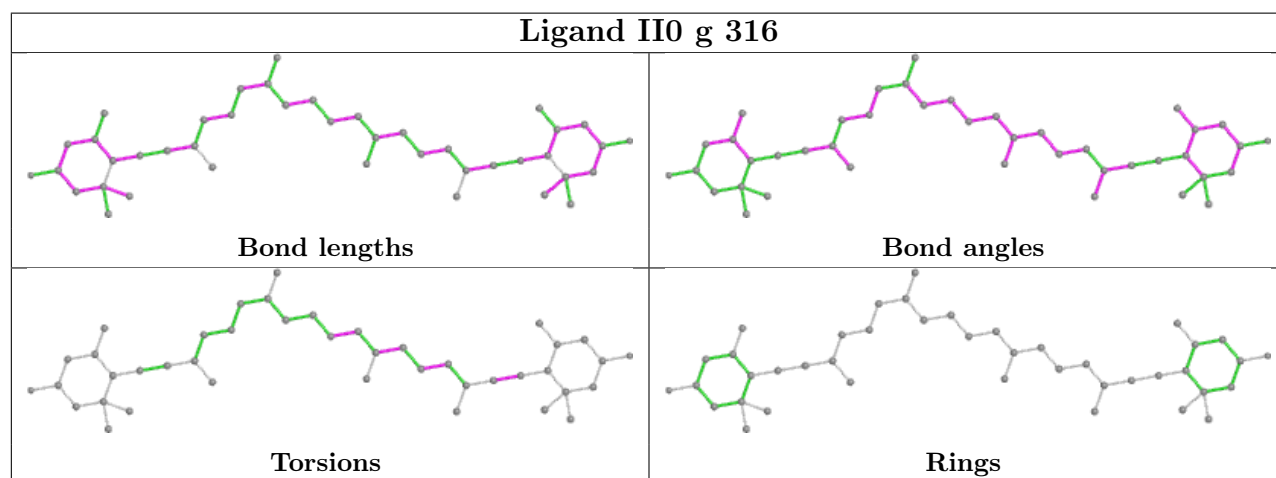
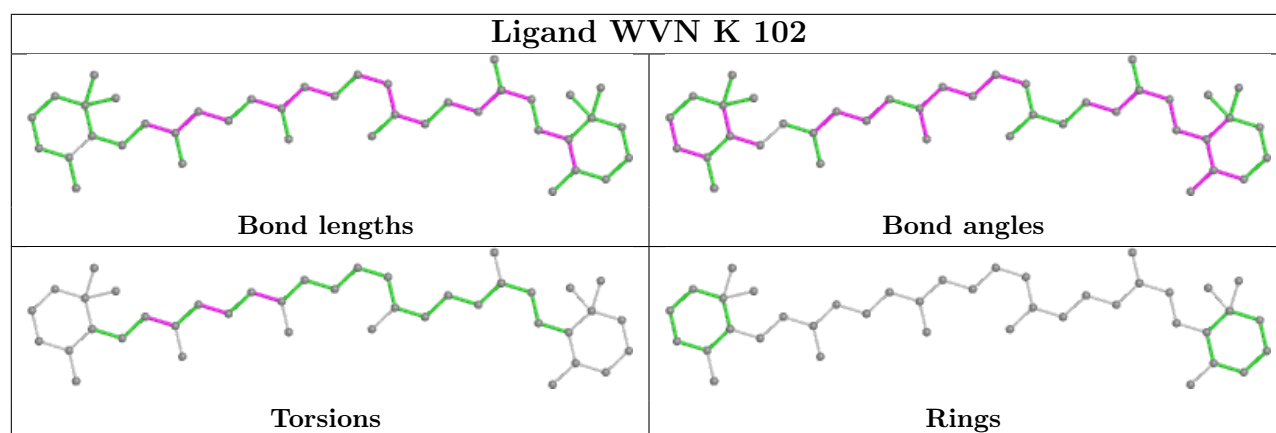
Bond angles

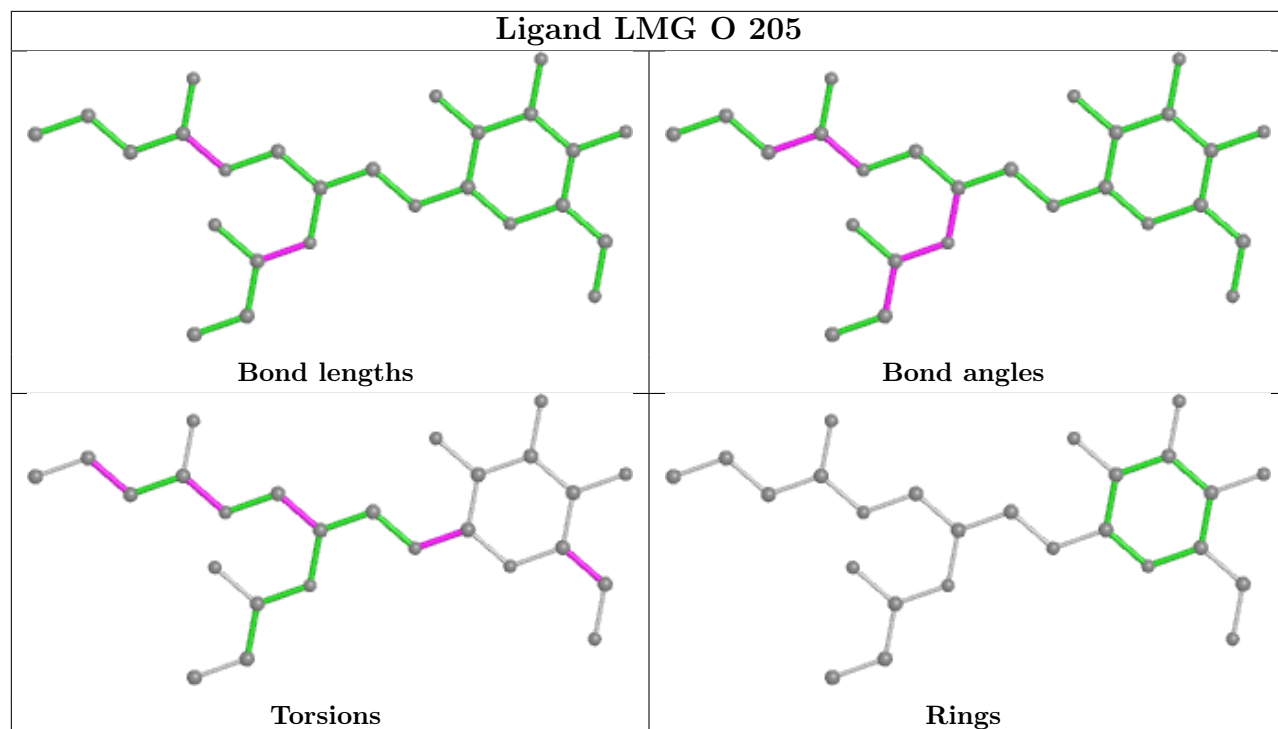


Torsions

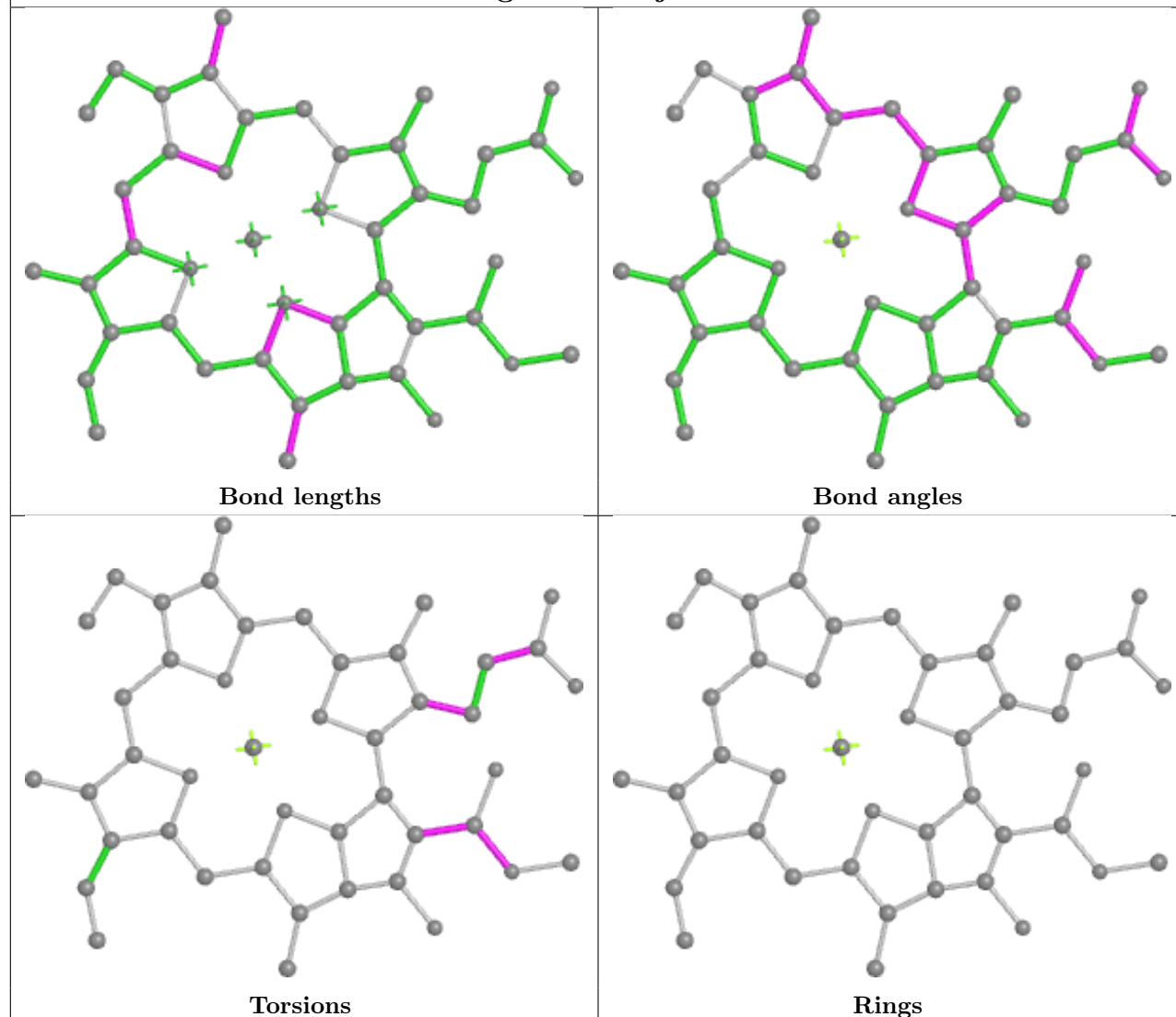


Rings

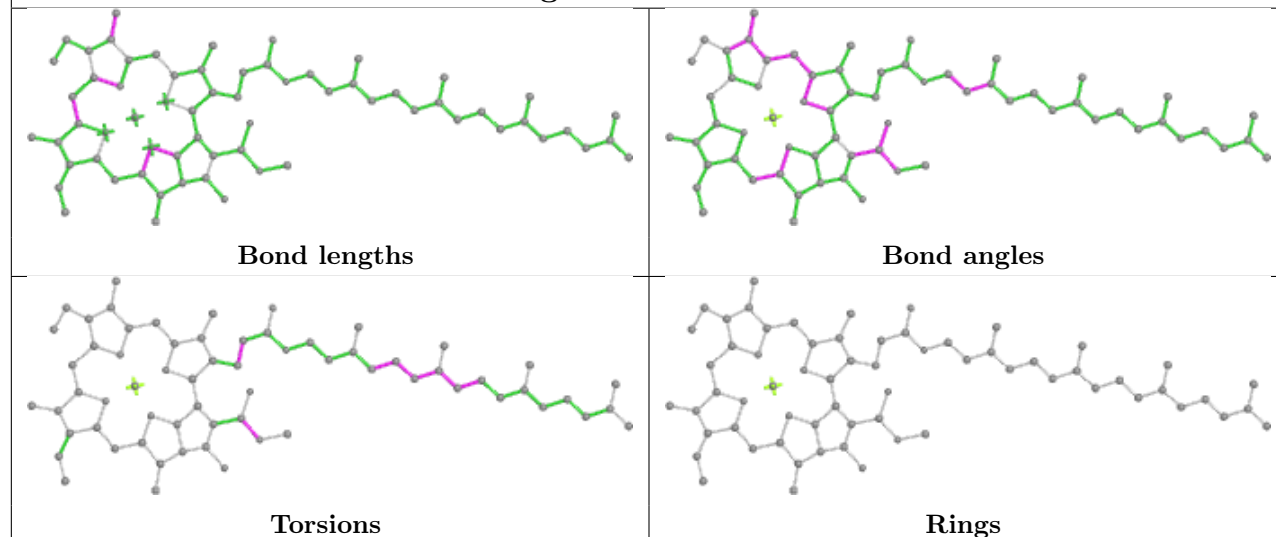




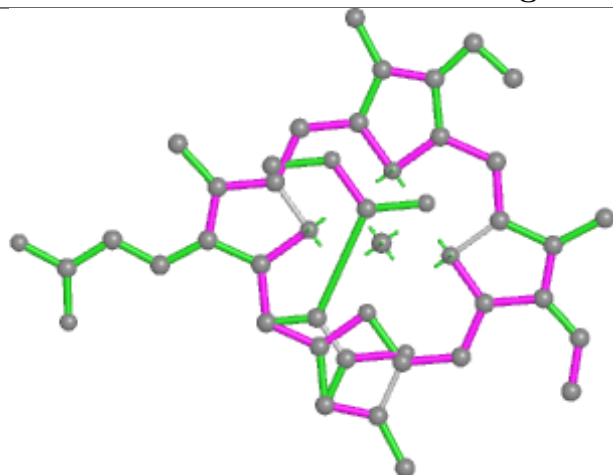
Ligand CLA j 605



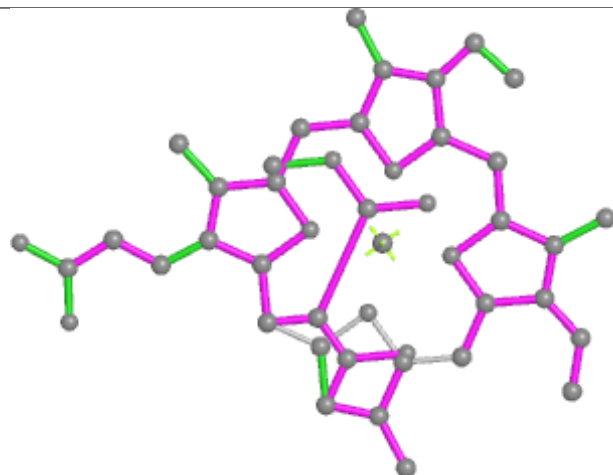
Ligand CLA i 305



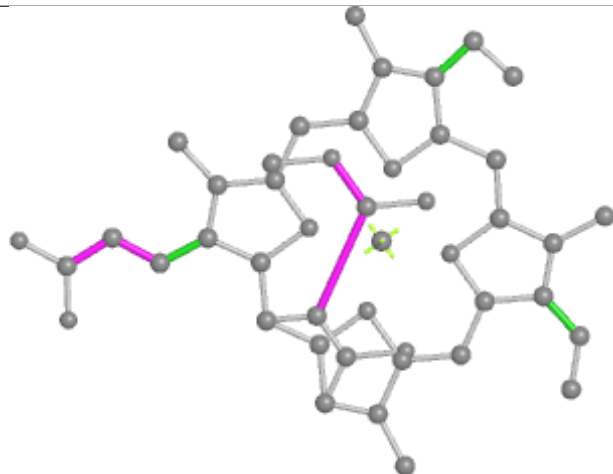
Ligand KC2 k 612



Bond lengths



Bond angles

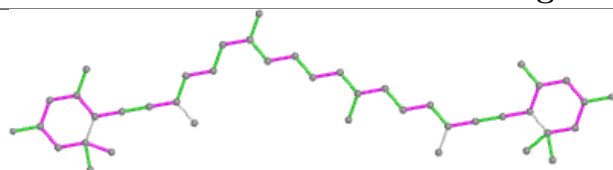


Torsions

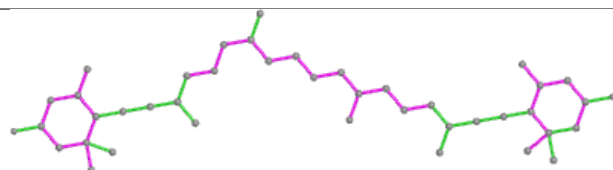


Rings

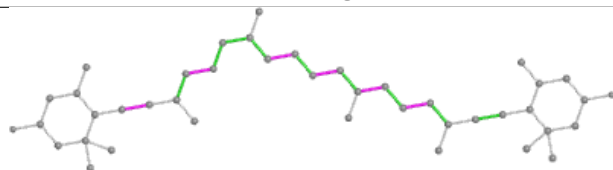
Ligand II0 i 313



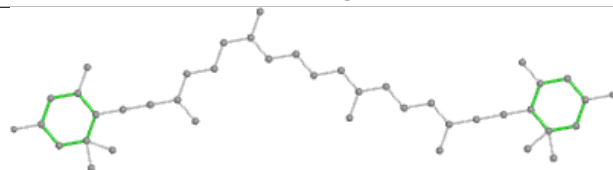
Bond lengths



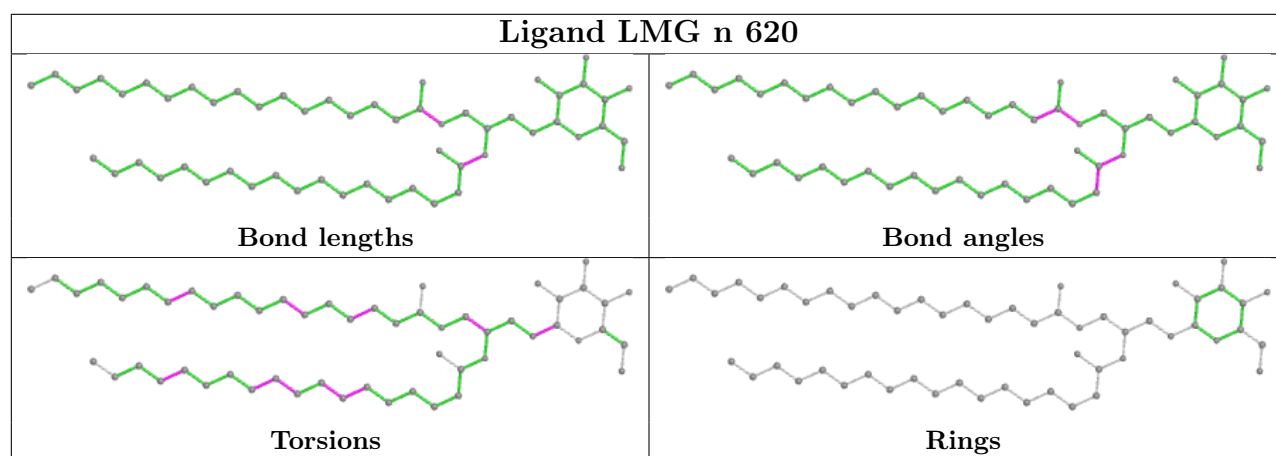
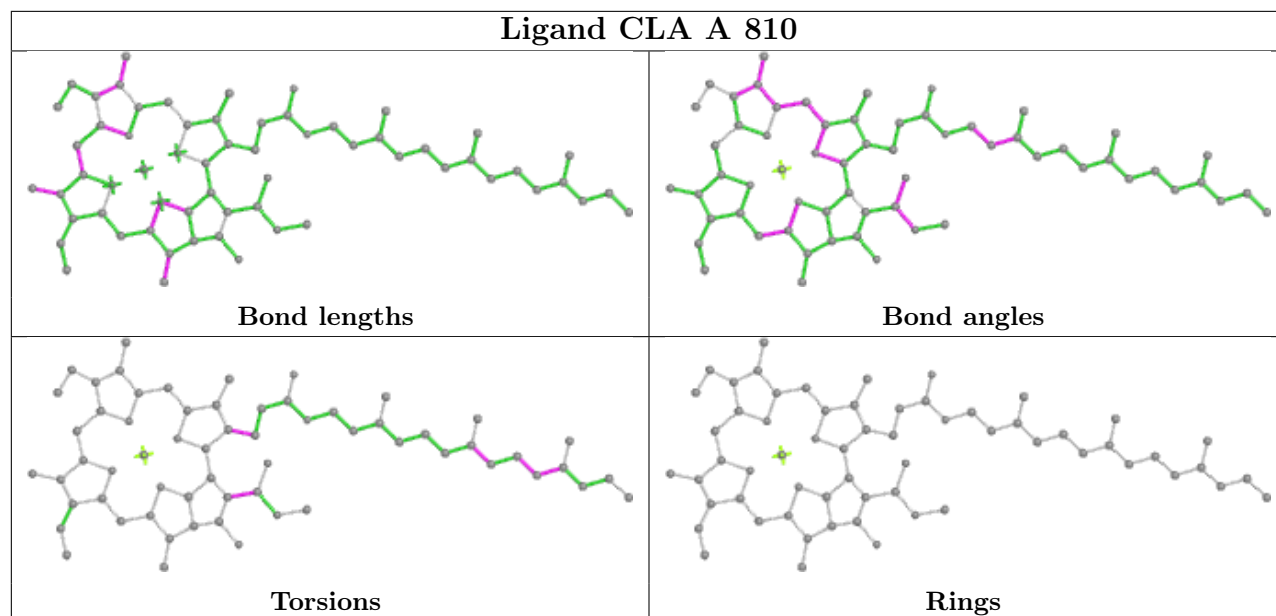
Bond angles

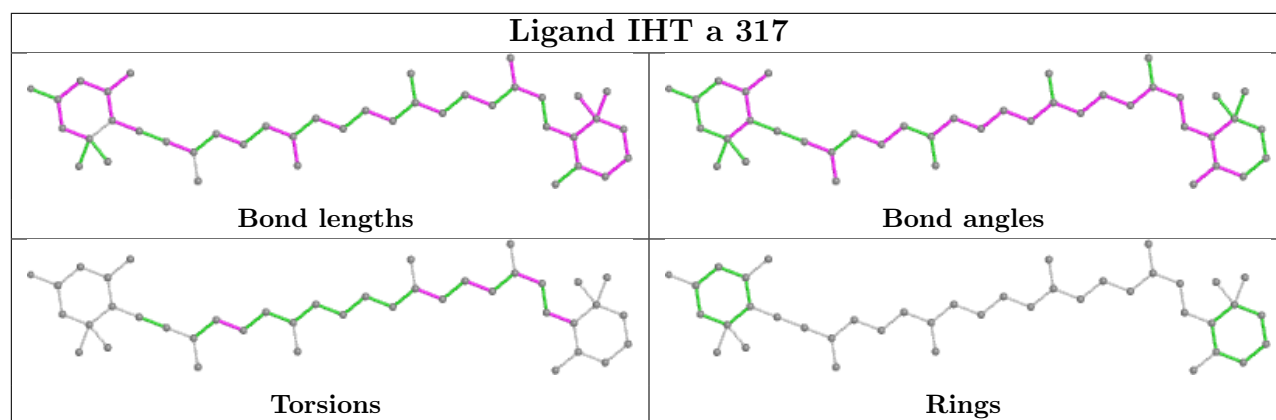
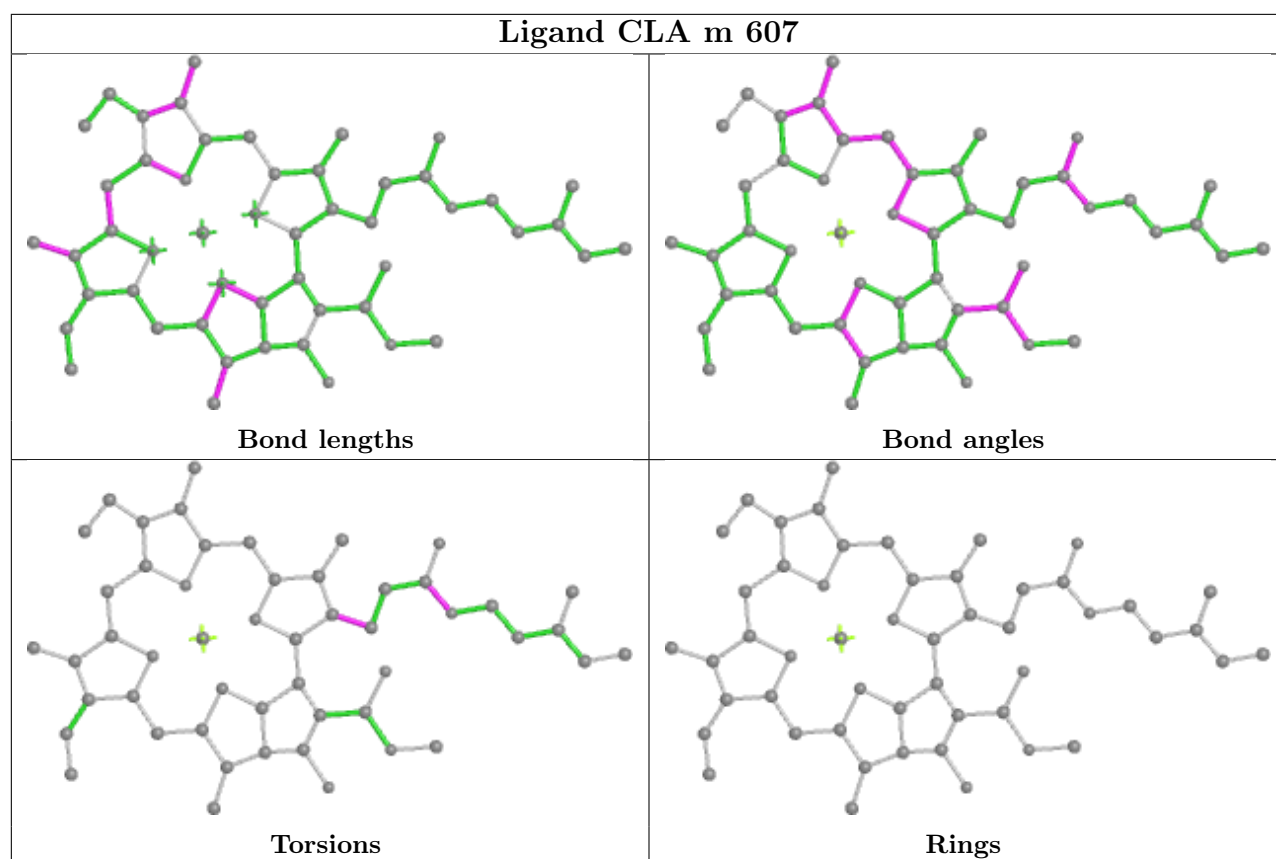


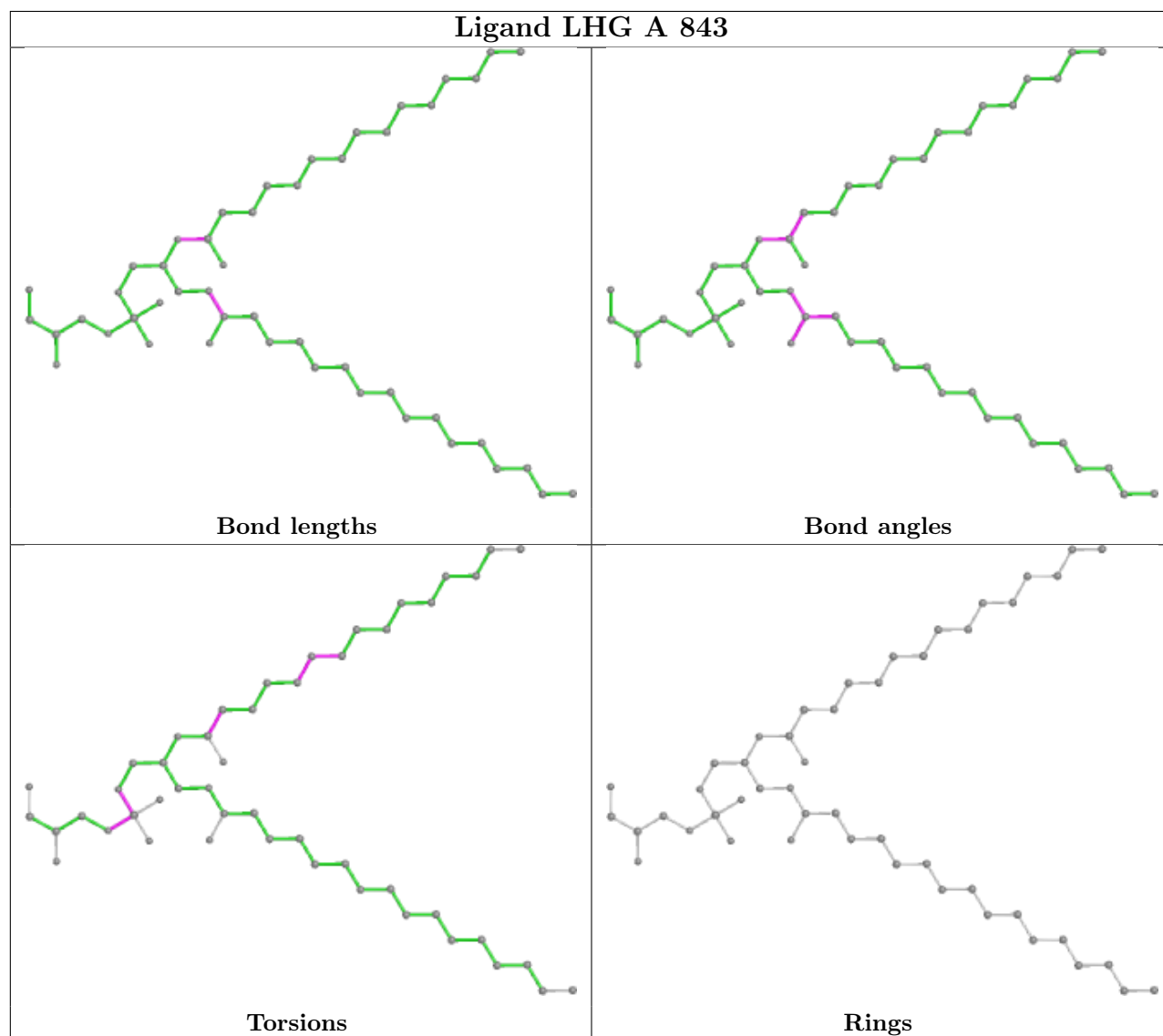
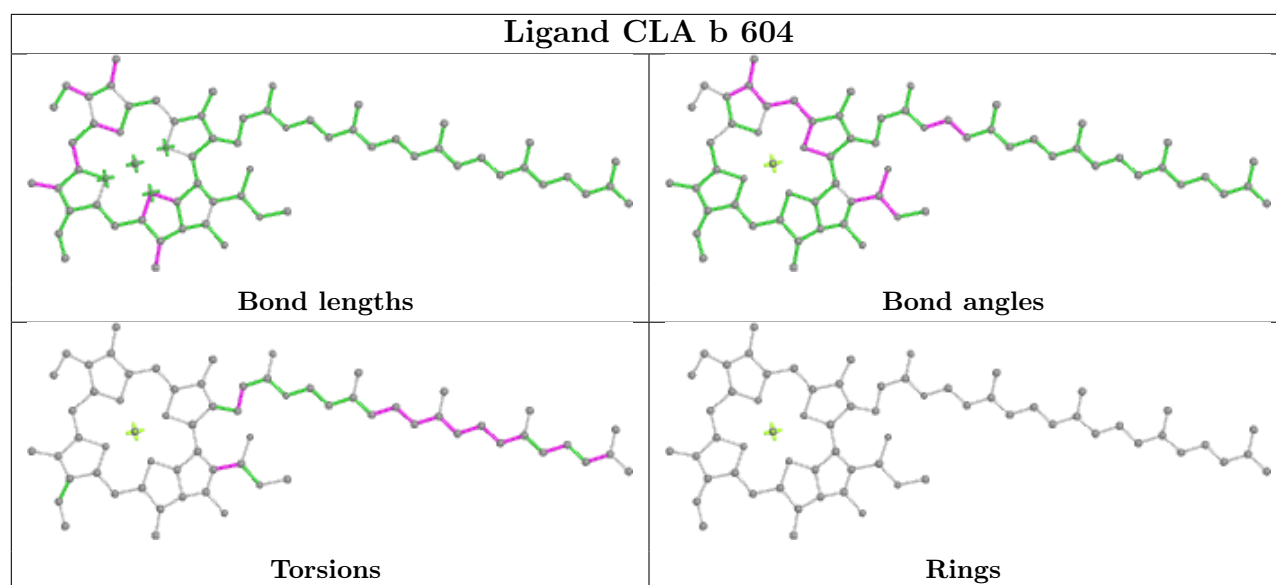
Torsions

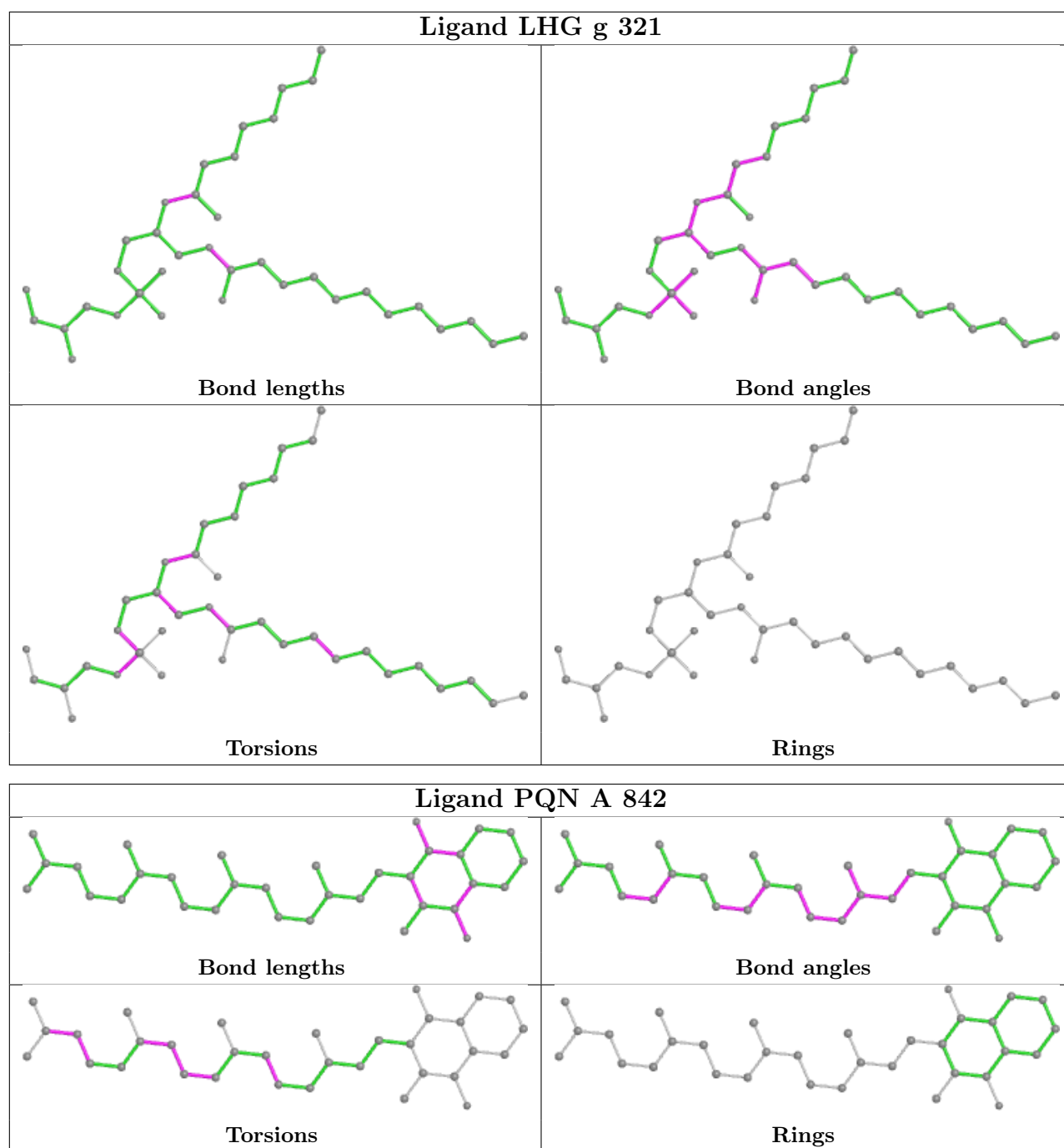


Rings

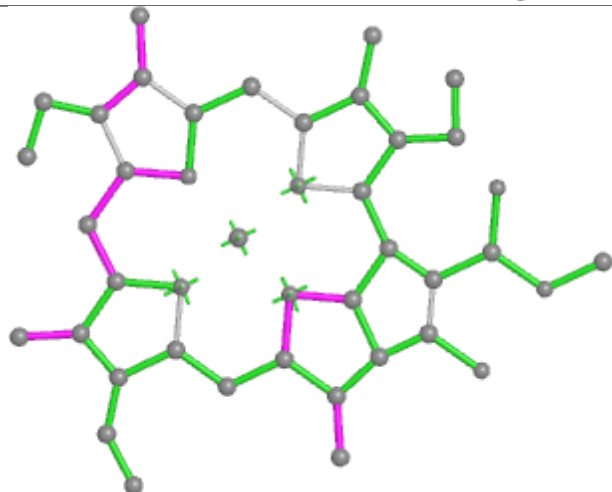




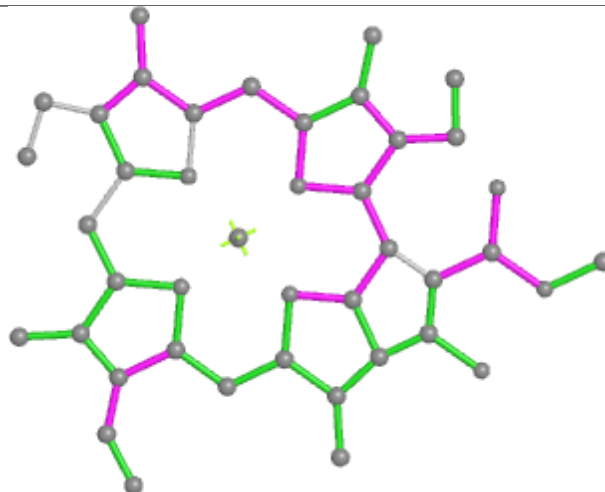




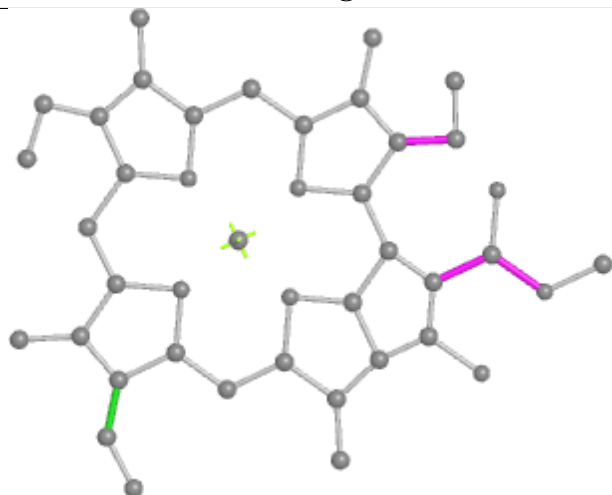
Ligand CLA K 103



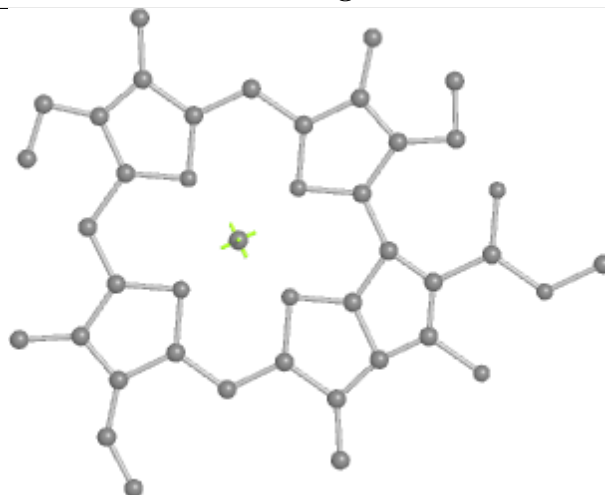
Bond lengths



Bond angles

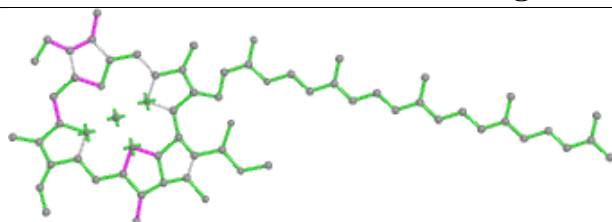


Torsions

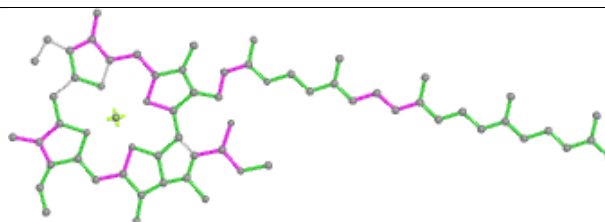


Rings

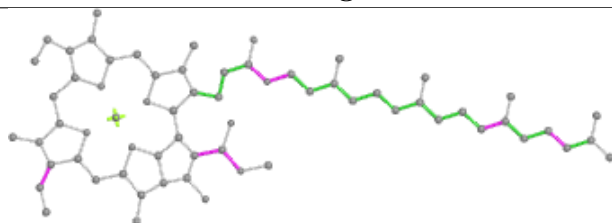
Ligand CLA A 832



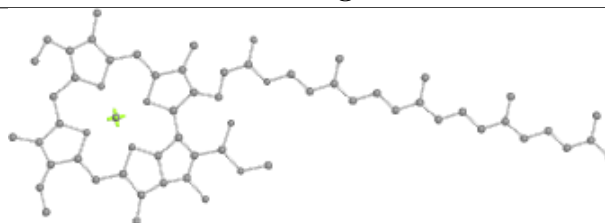
Bond lengths



Bond angles

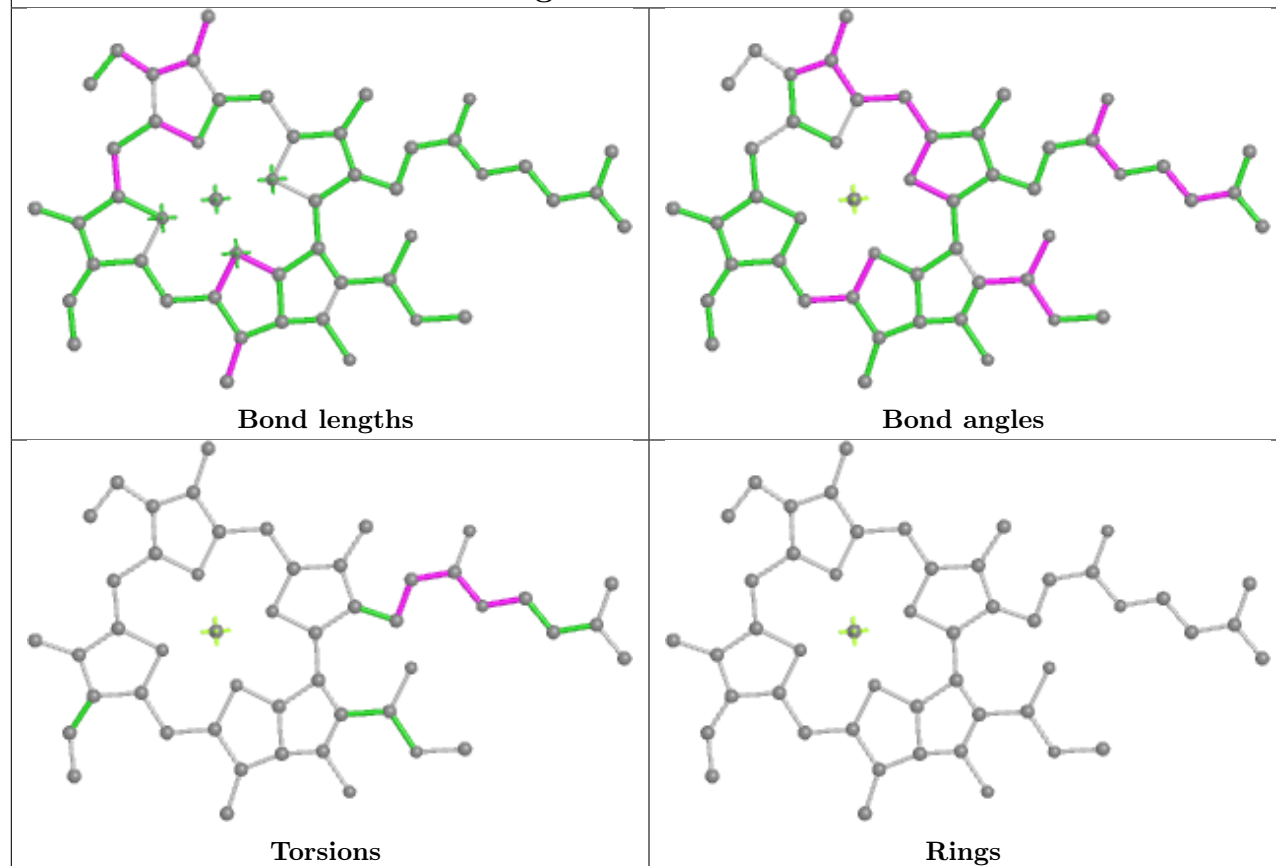


Torsions

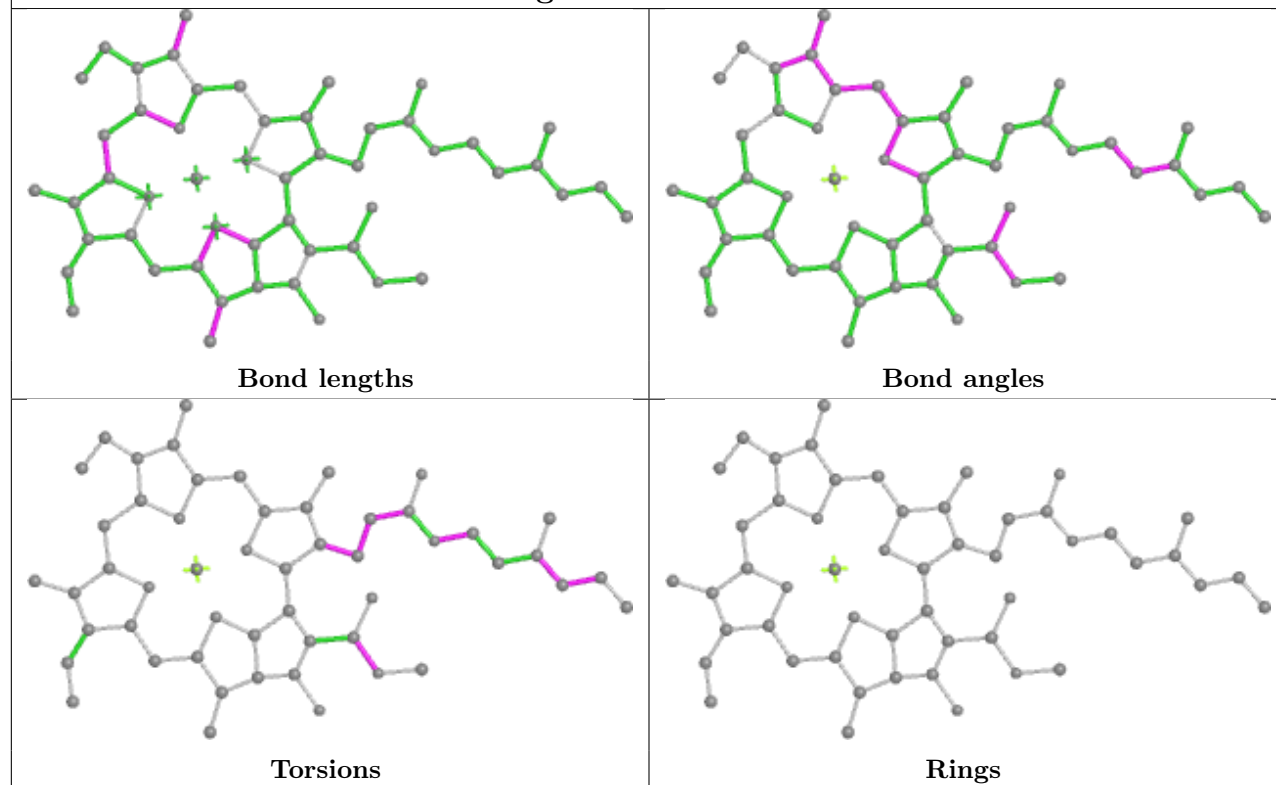


Rings

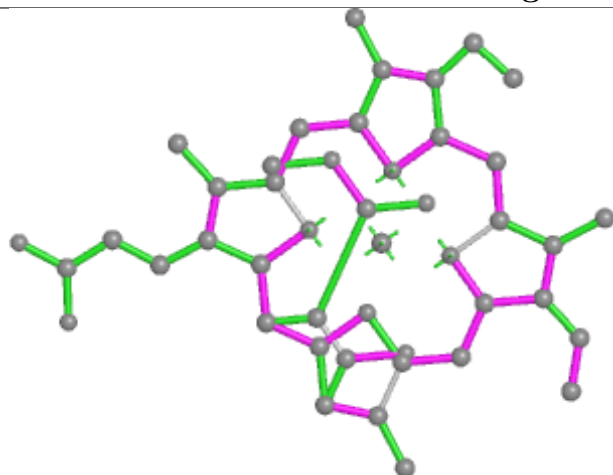
Ligand CLA h 303



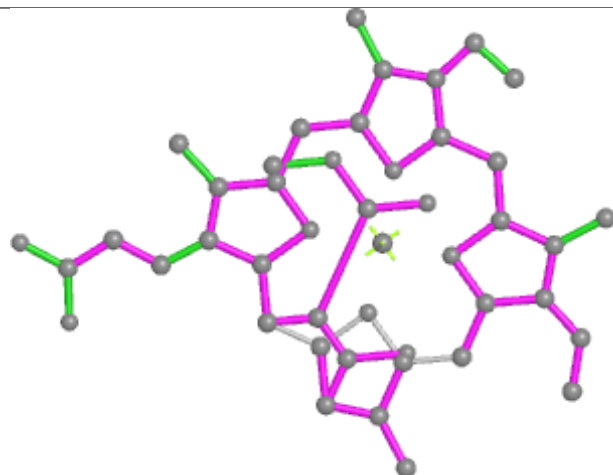
Ligand CLA a 303



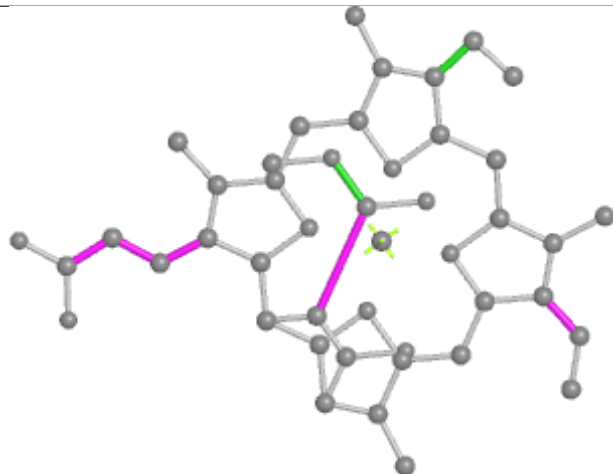
Ligand KC2 s 201



Bond lengths



Bond angles

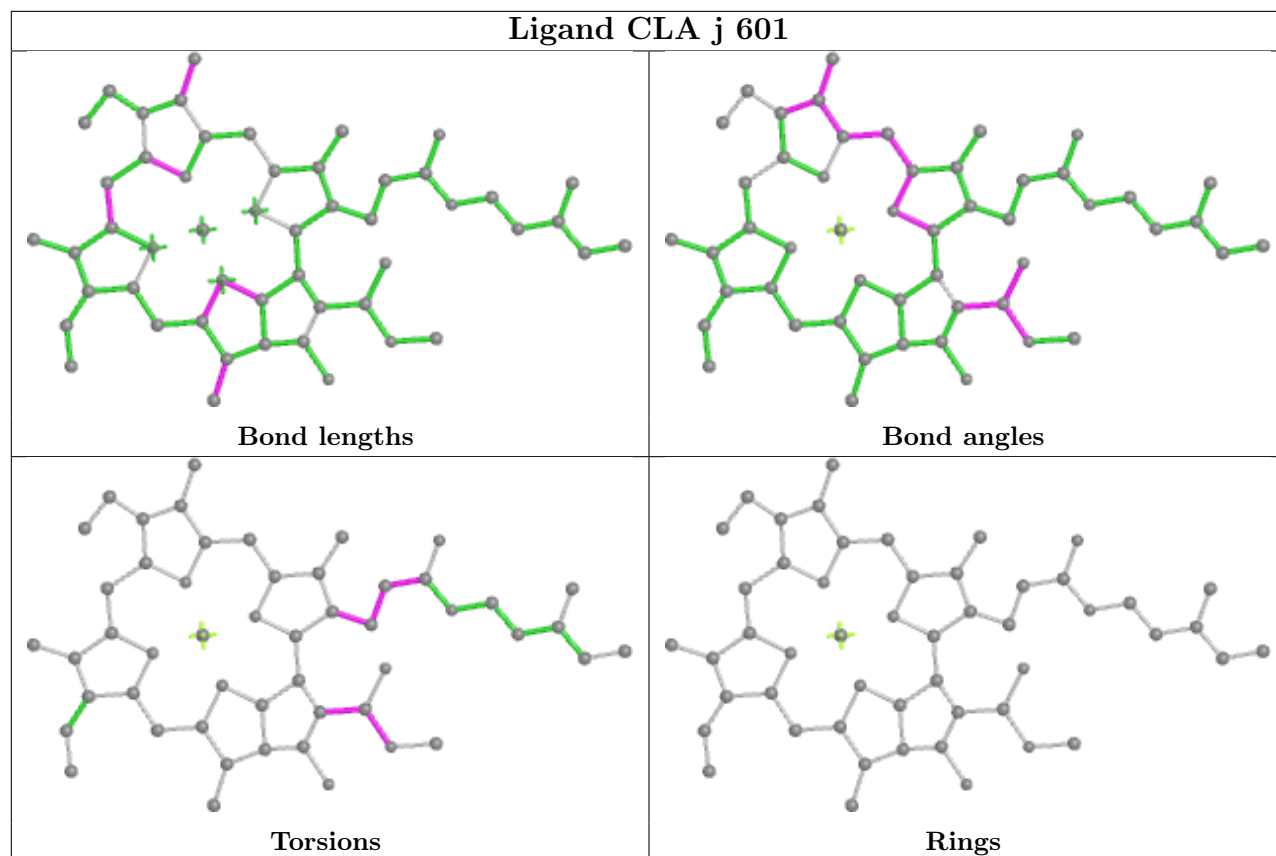


Torsions

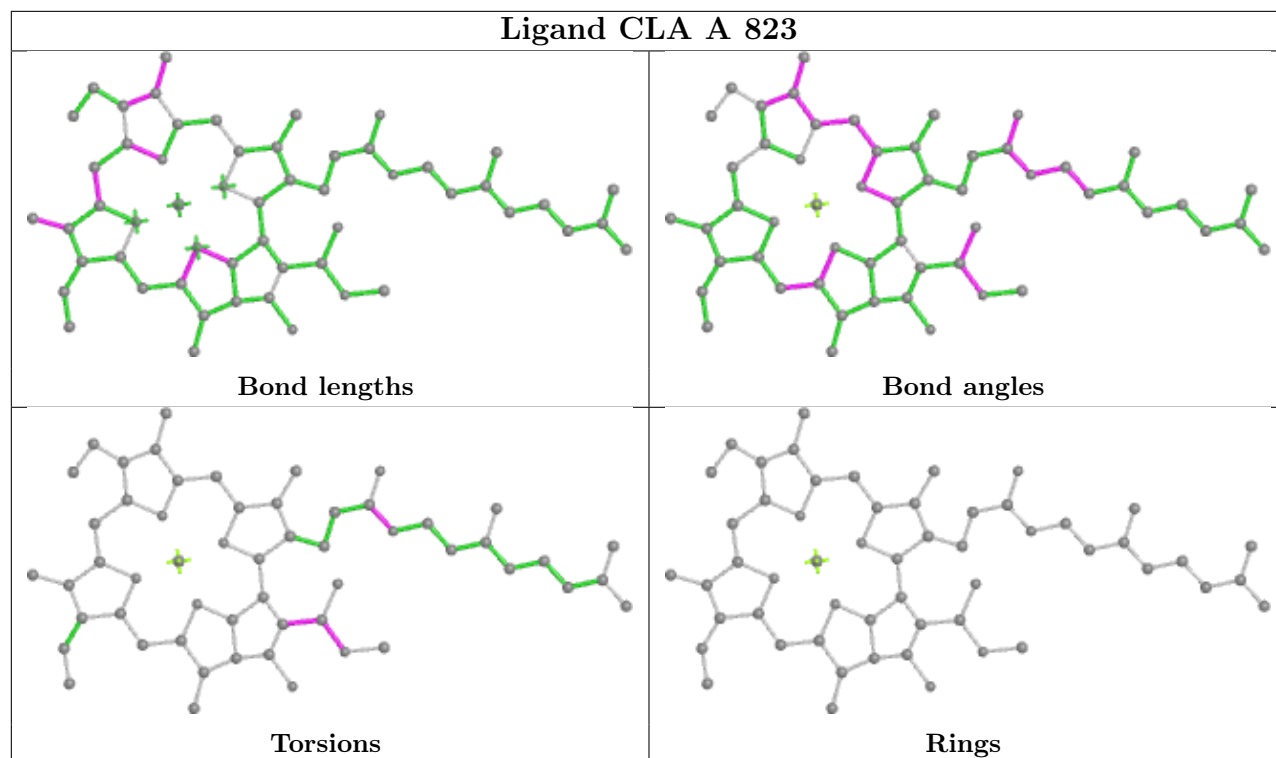


Rings

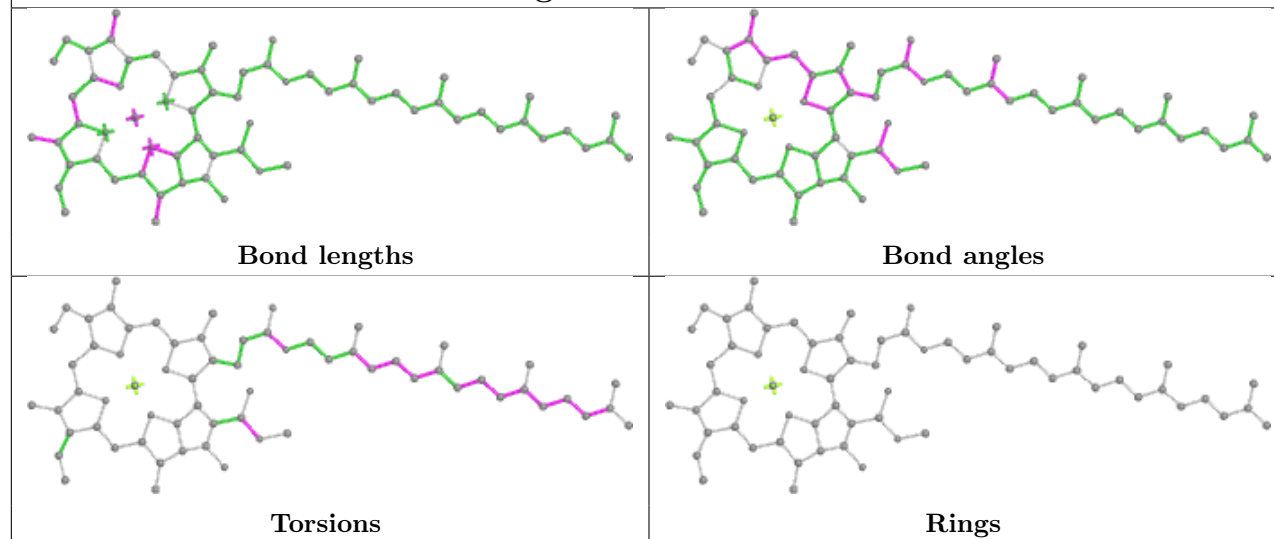
Ligand CLA j 601



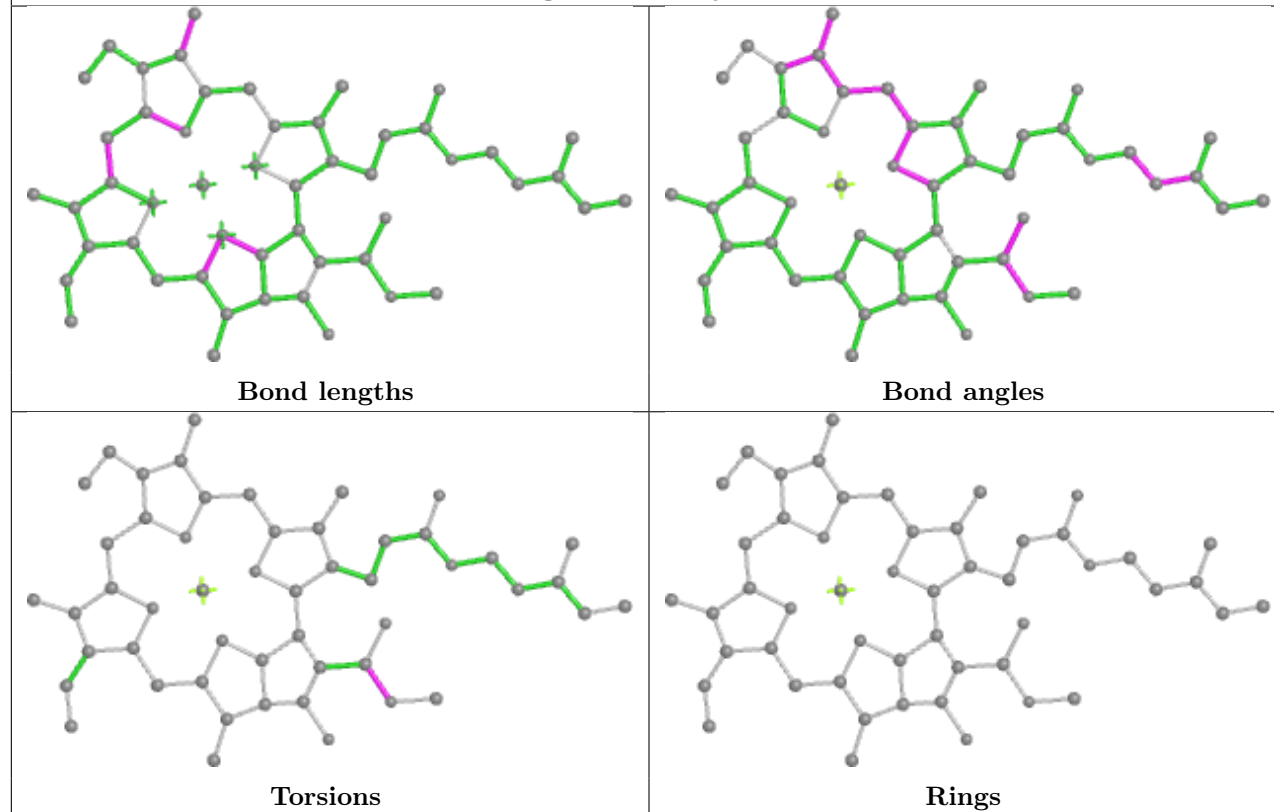
Ligand CLA A 823

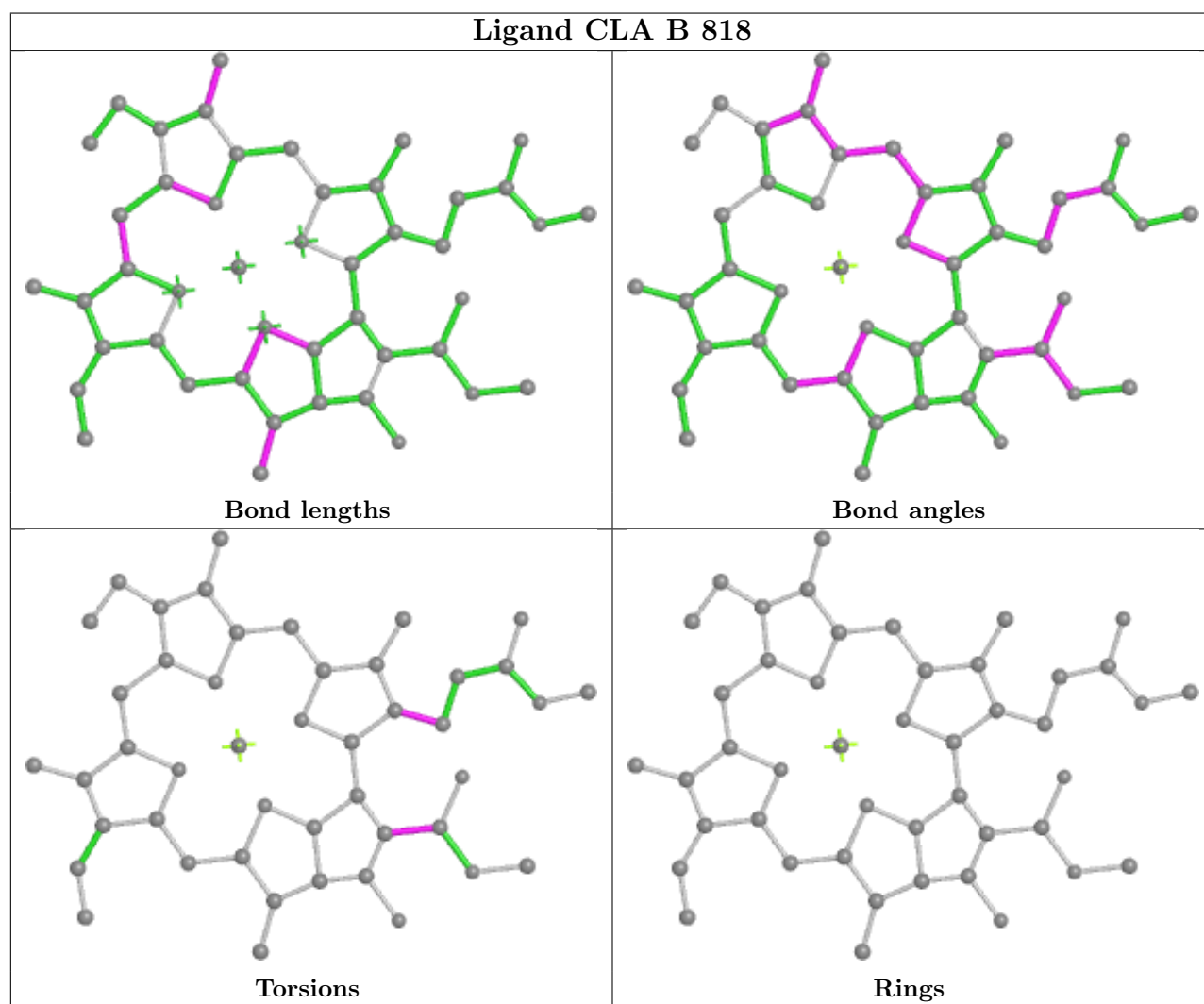
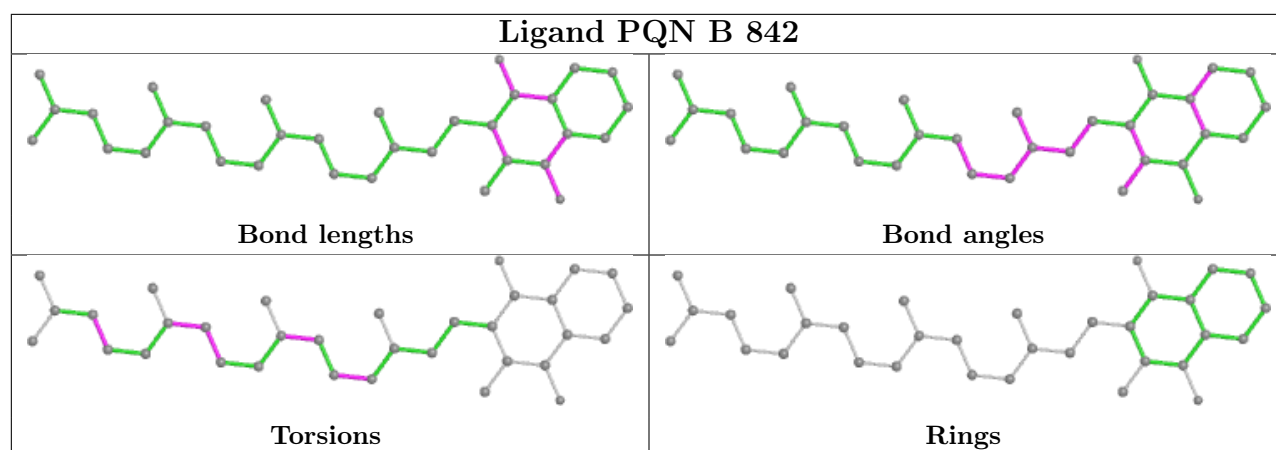


Ligand CLA b 603

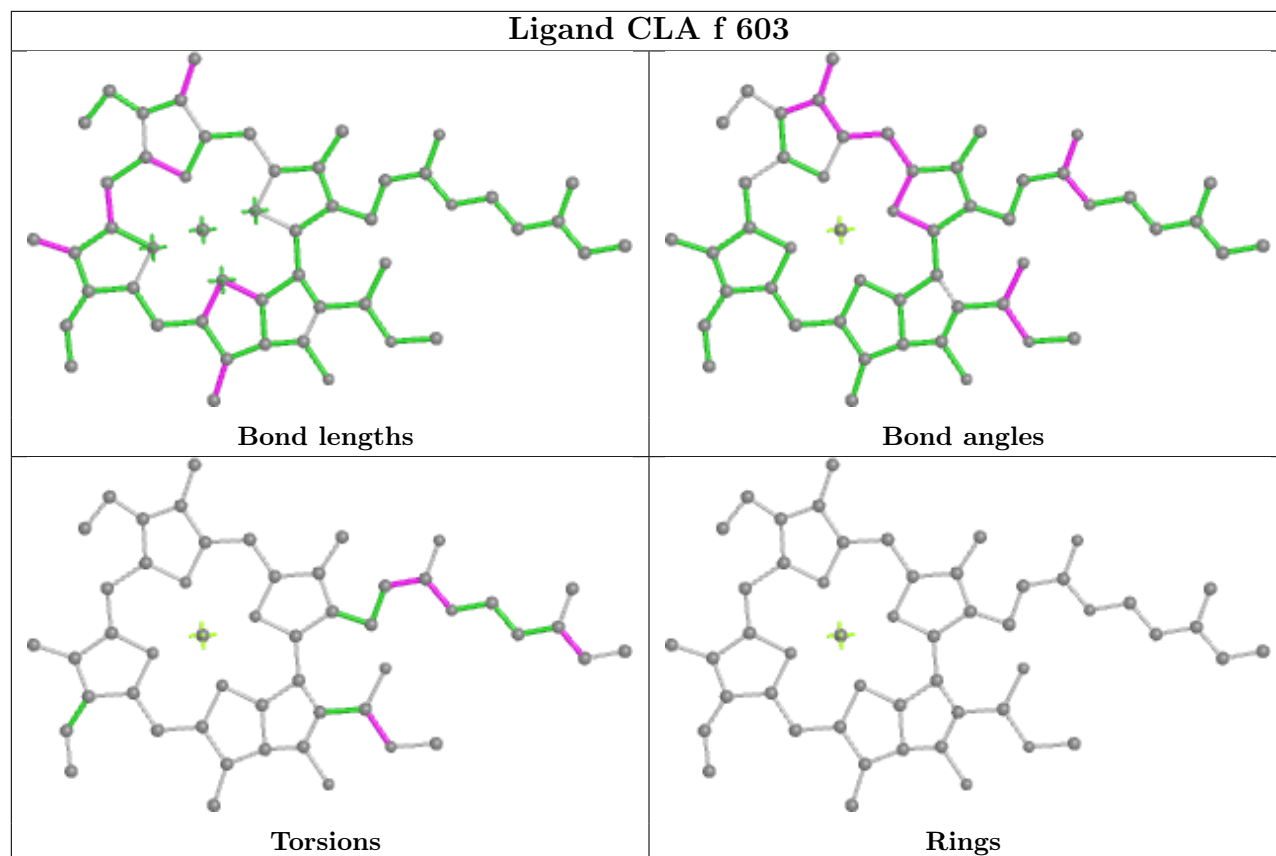


Ligand CLA j 609

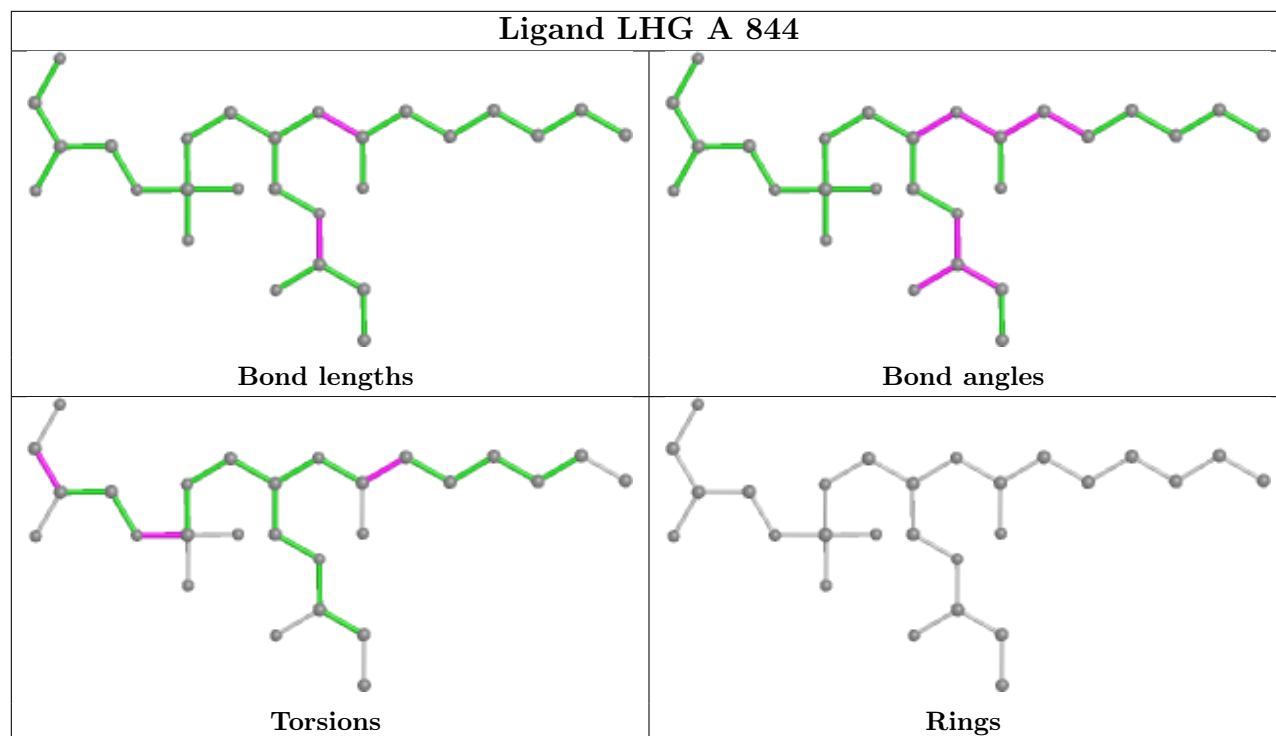


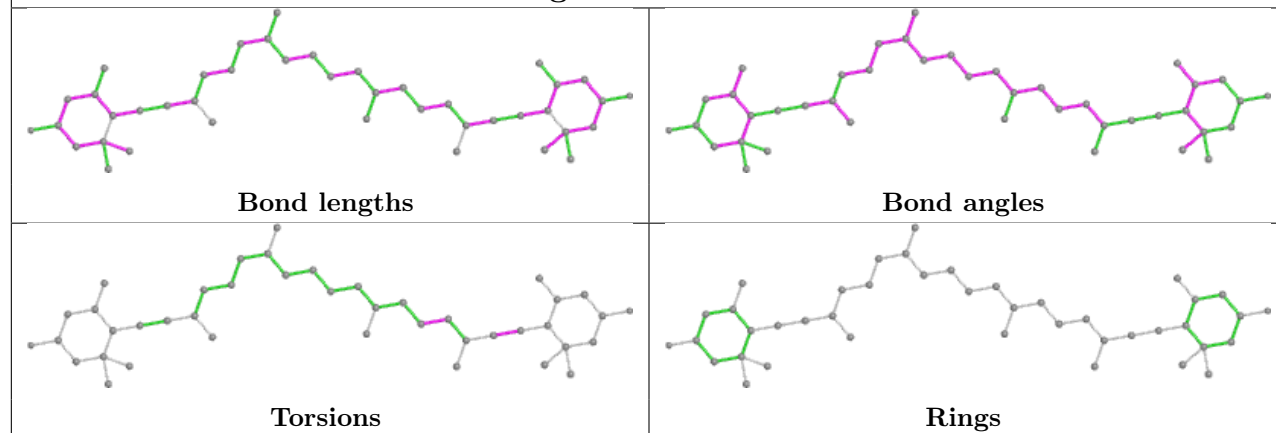
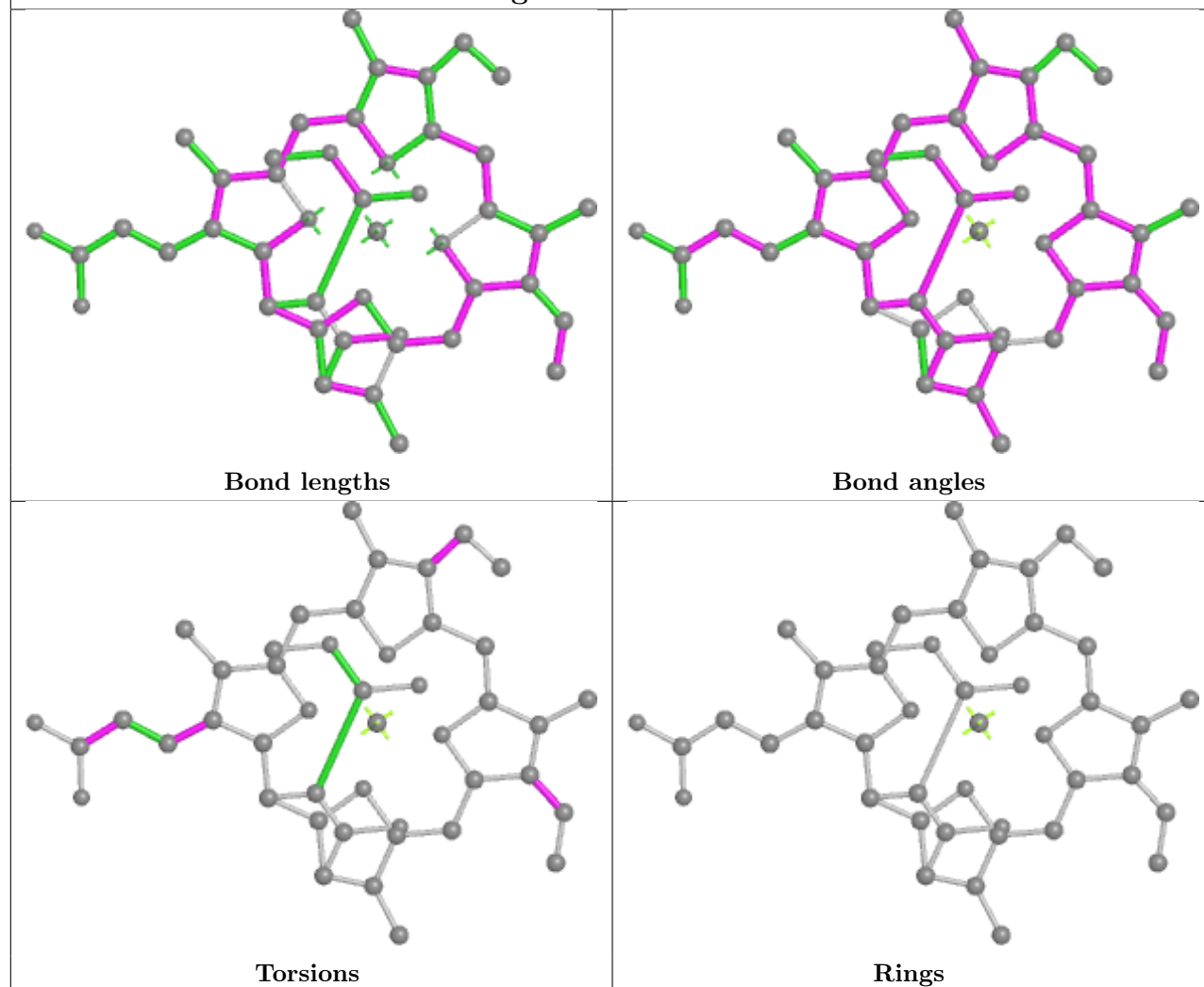


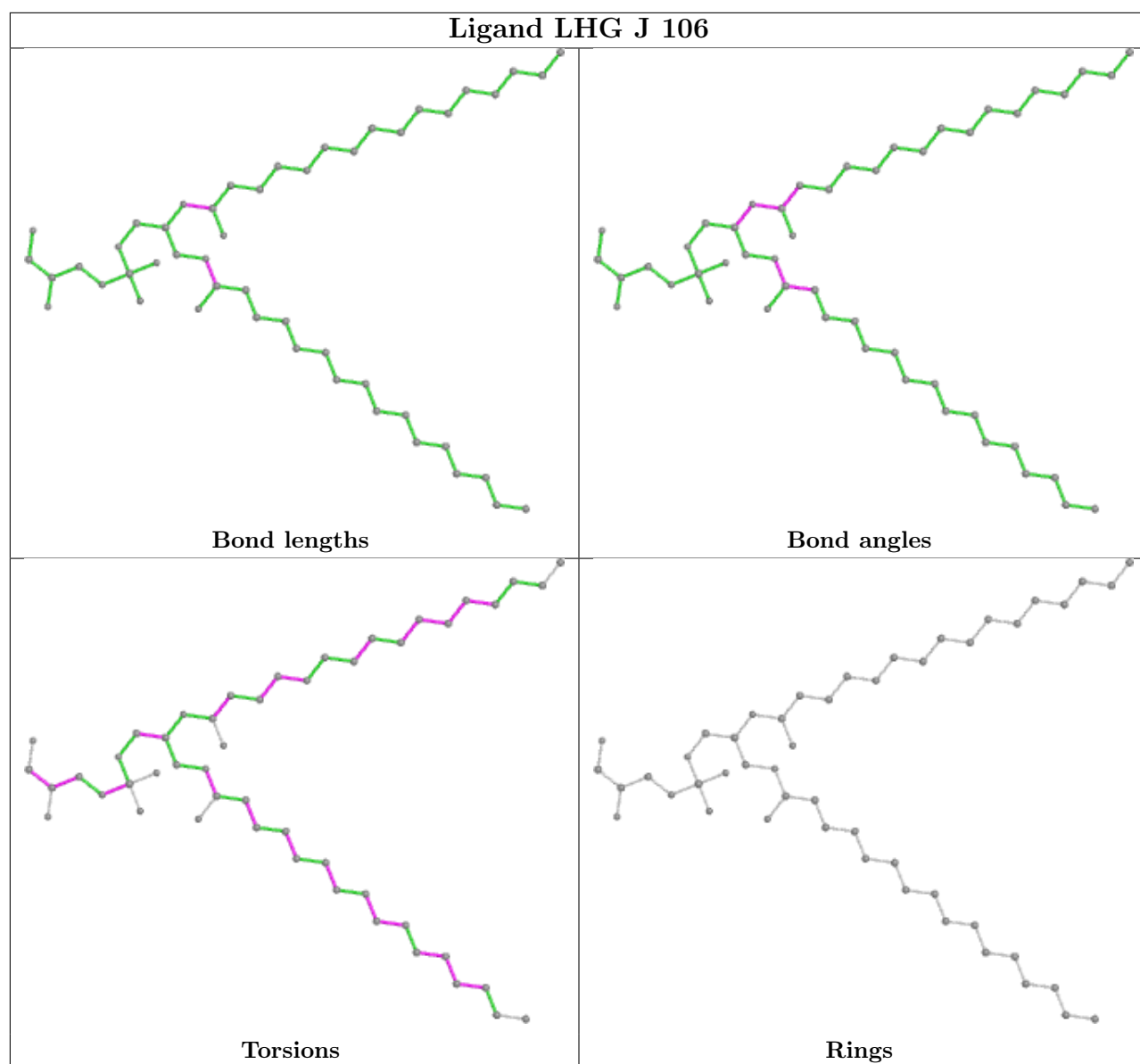
Ligand CLA f 603



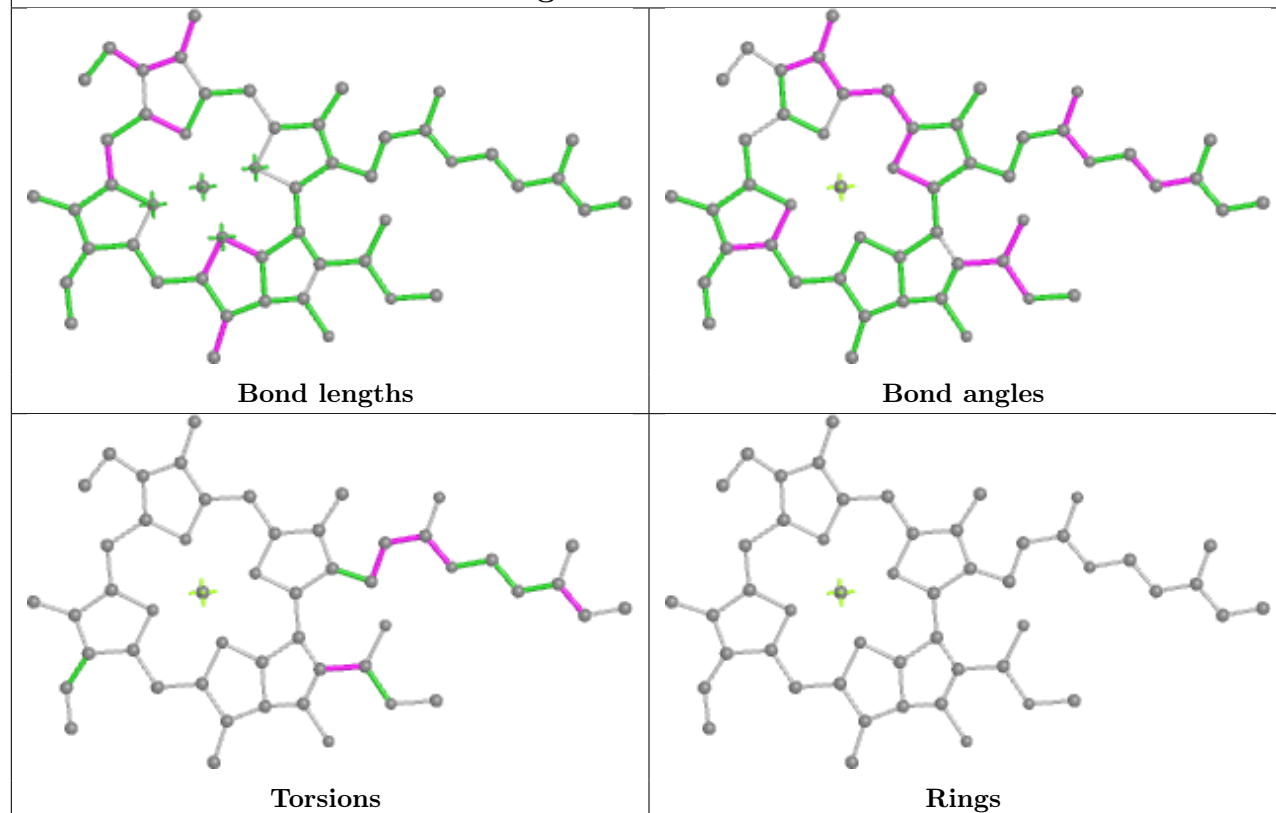
Ligand LHG A 844



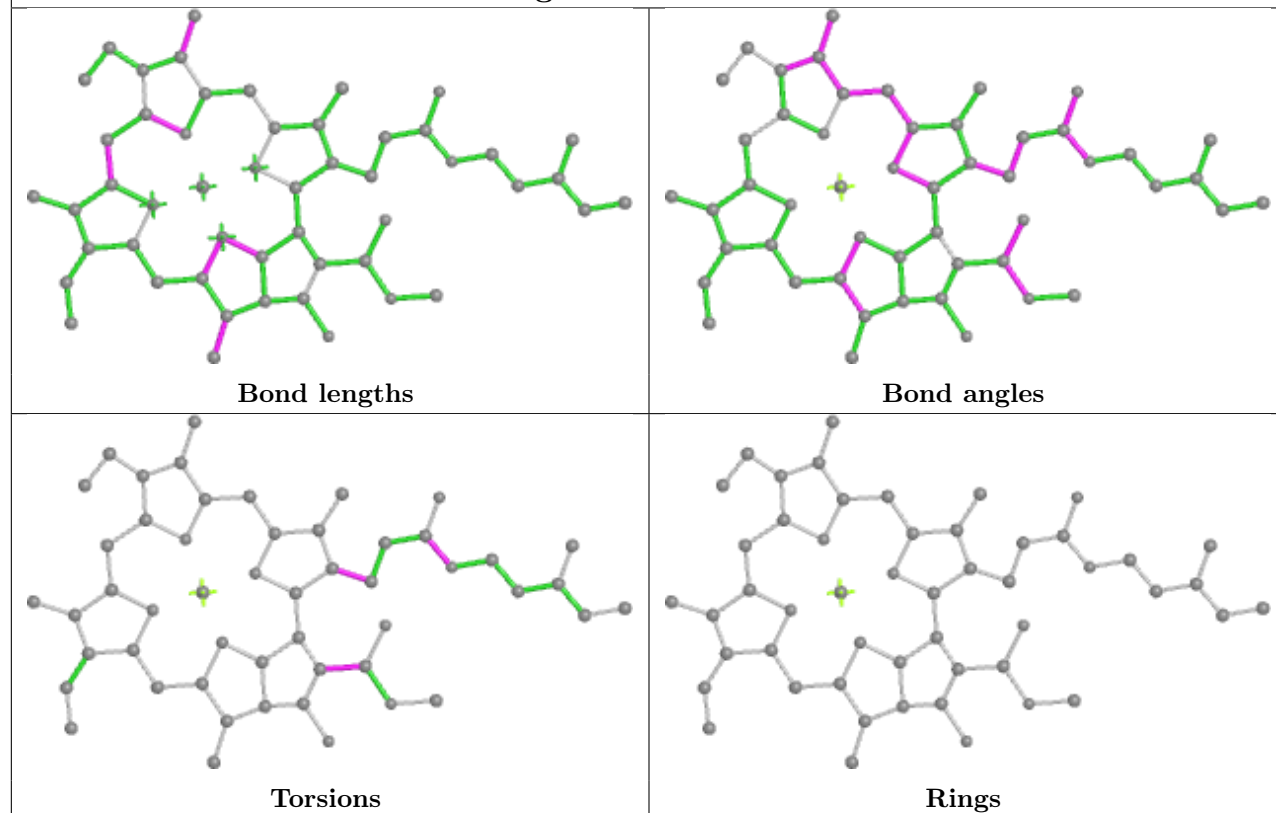
Ligand II0 b 613**Ligand KC2 i 310**



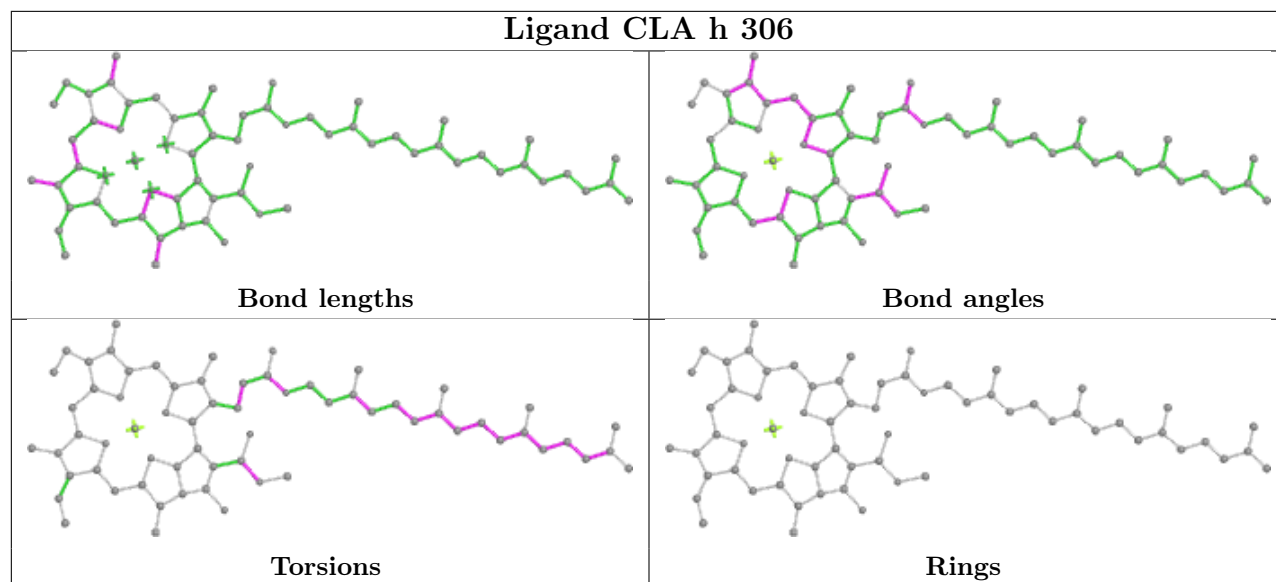
Ligand CLA c 605



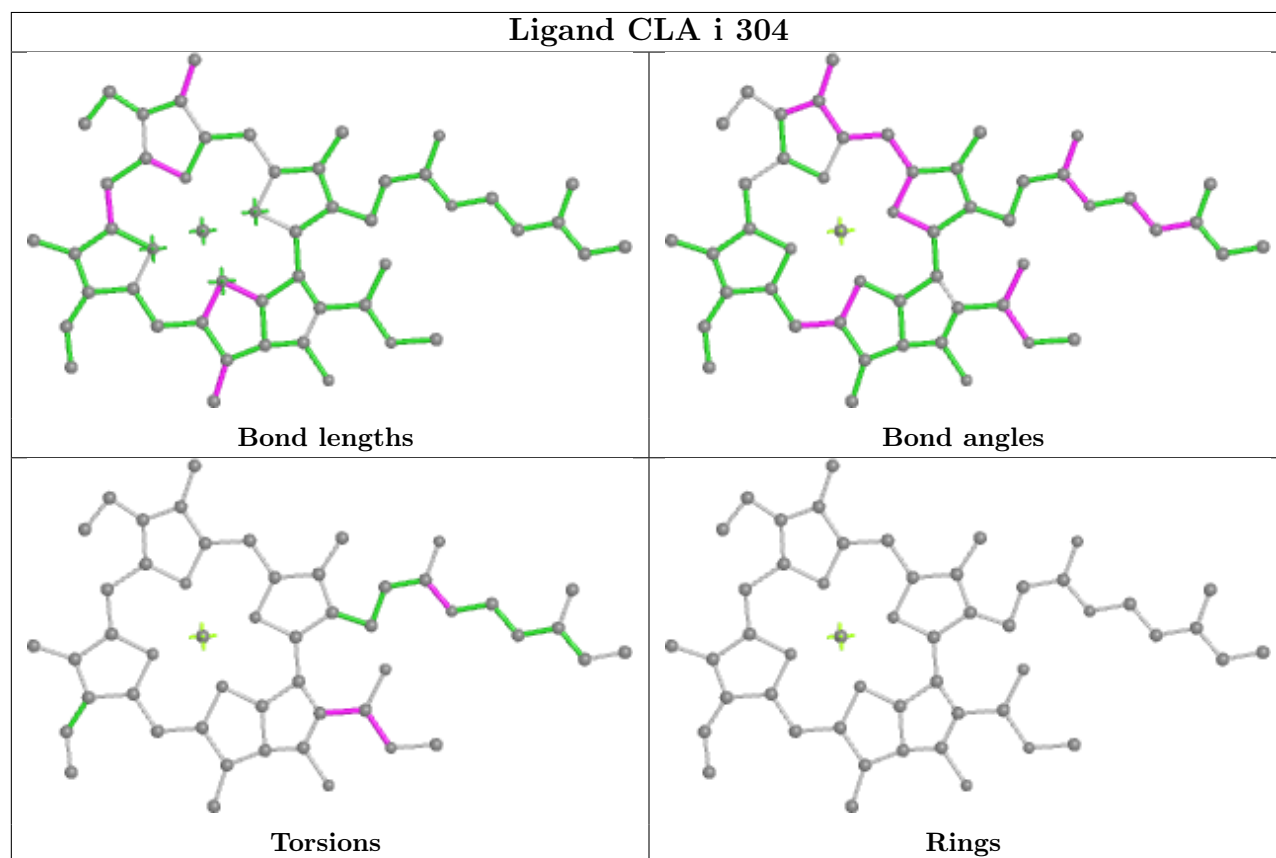
Ligand CLA n 606

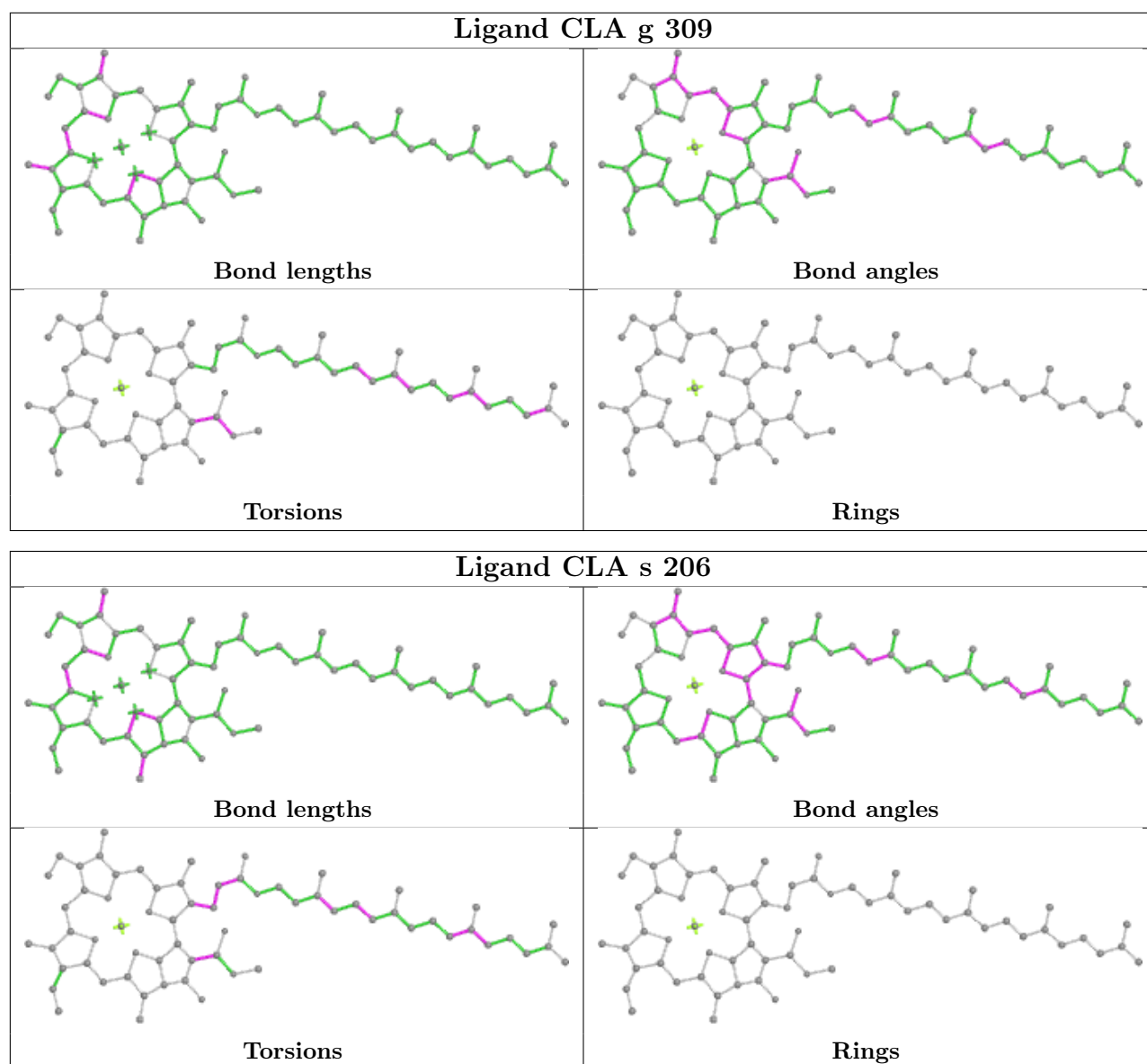


Ligand CLA h 306

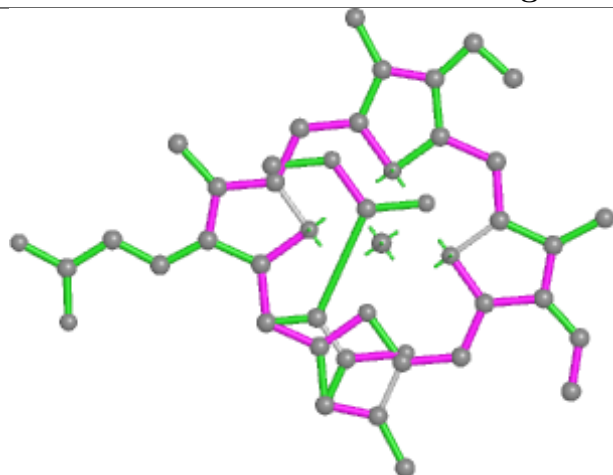


Ligand CLA i 304

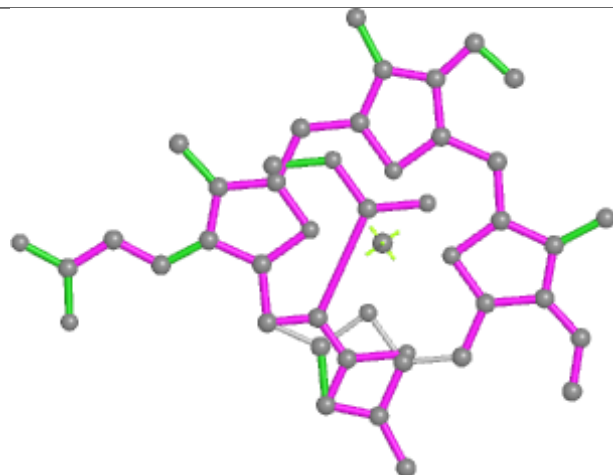




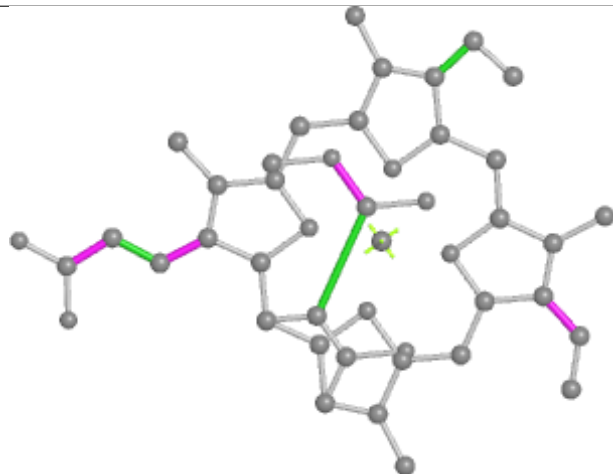
Ligand KC2 e 609



Bond lengths



Bond angles

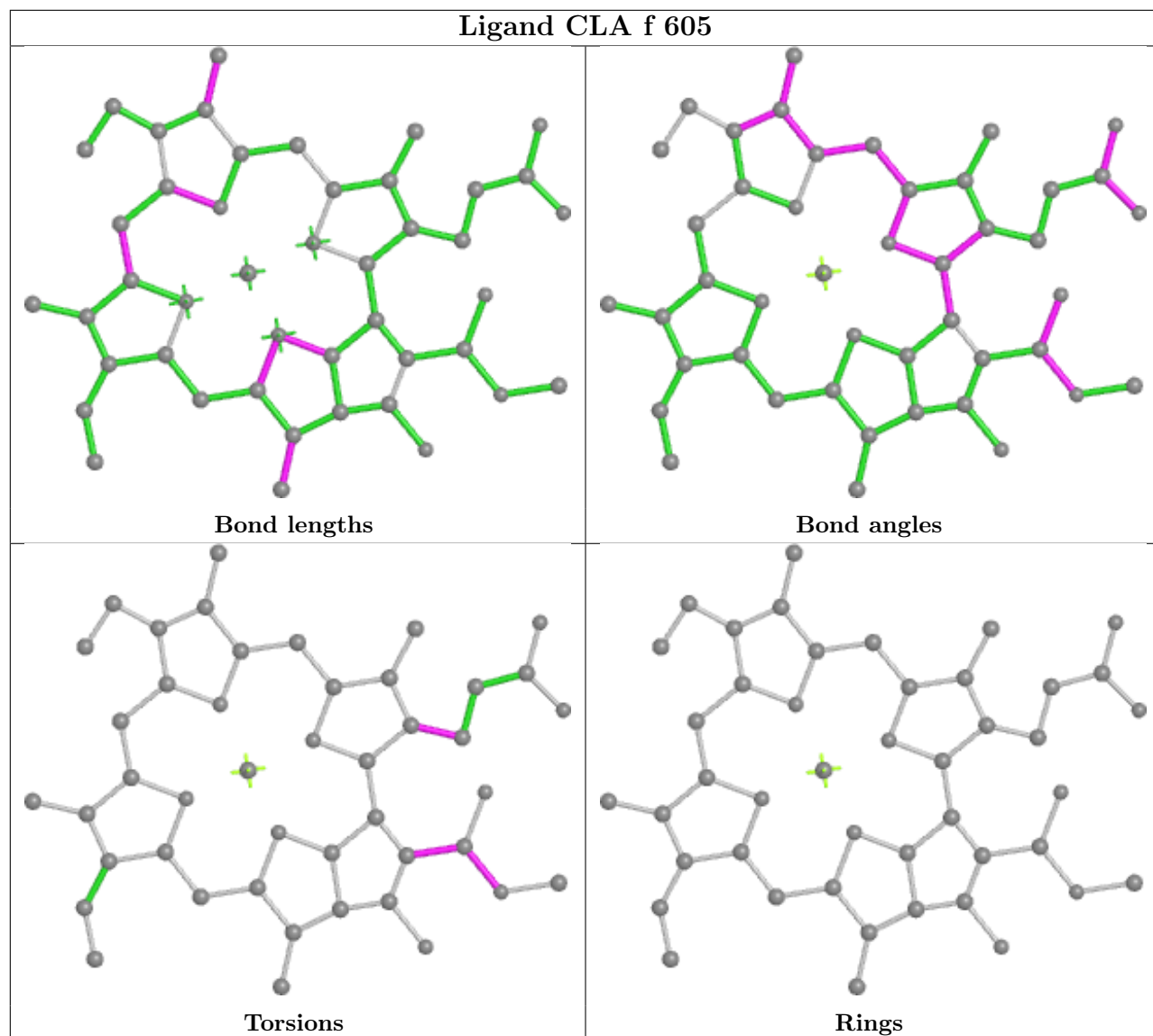


Torsions

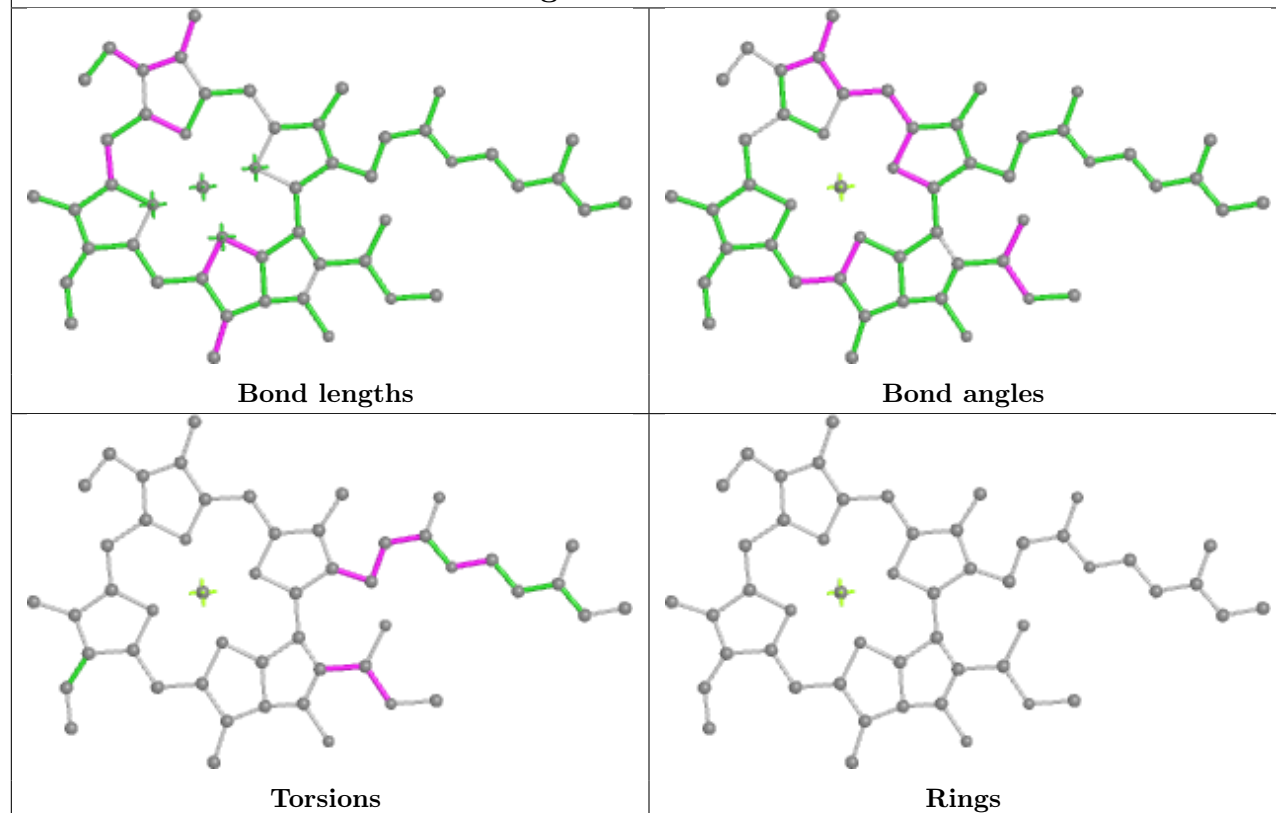


Rings

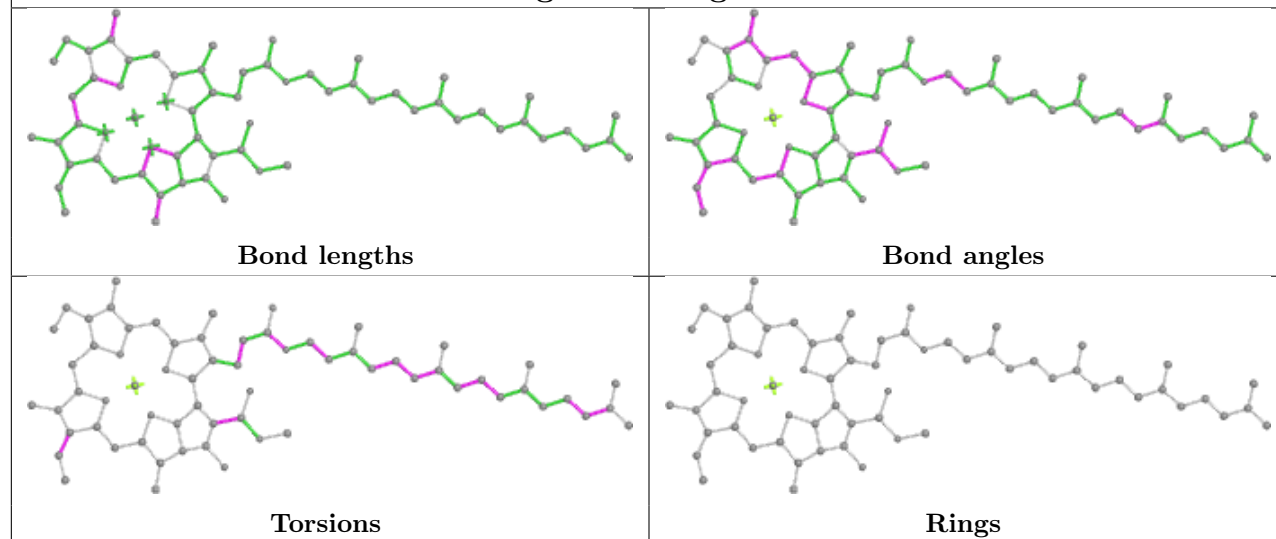
Ligand CLA f 605

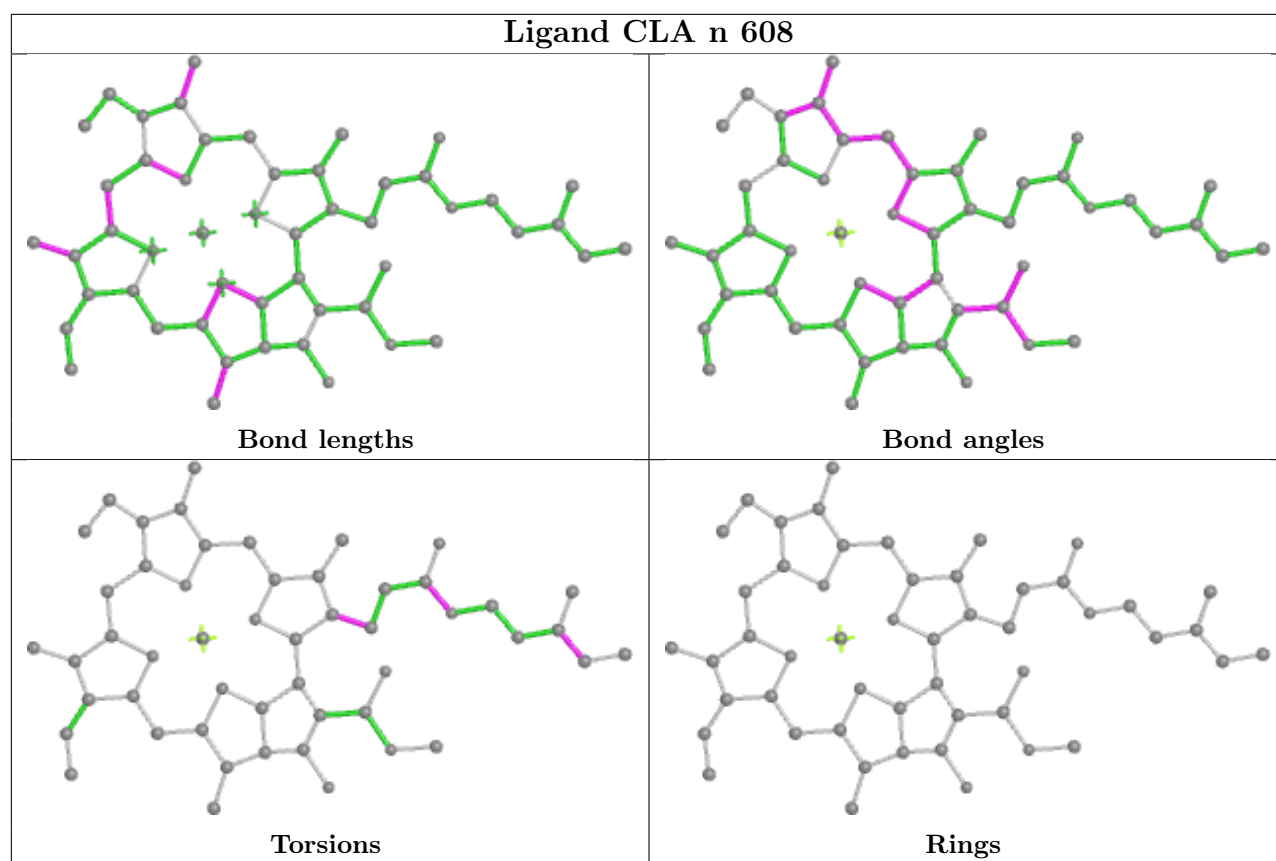


Ligand CLA i 306

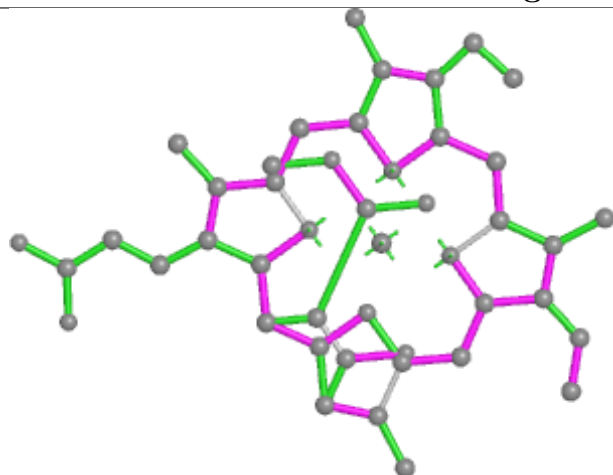


Ligand CLA g 322

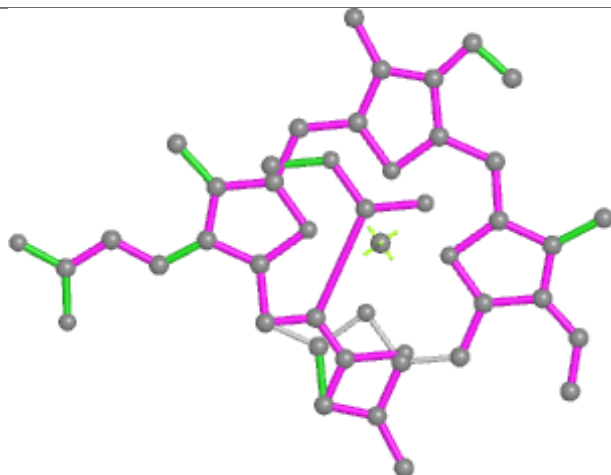




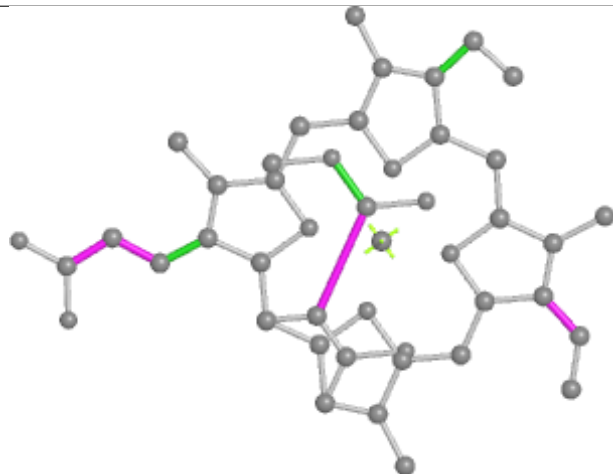
Ligand KC2 f 611



Bond lengths



Bond angles

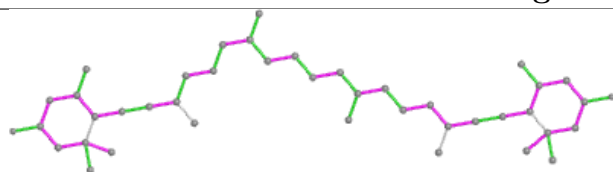


Torsions

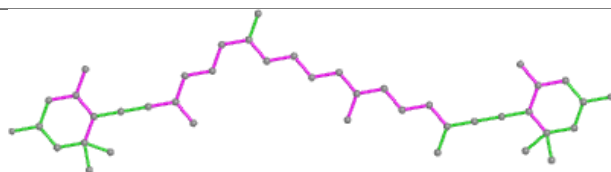


Rings

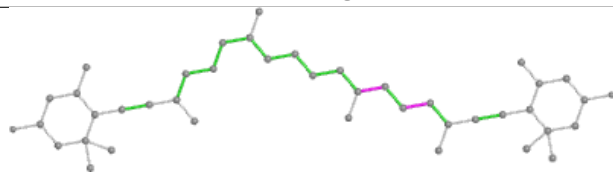
Ligand II0 a 314



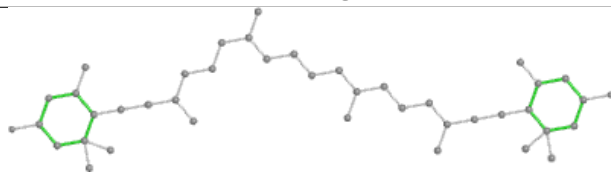
Bond lengths



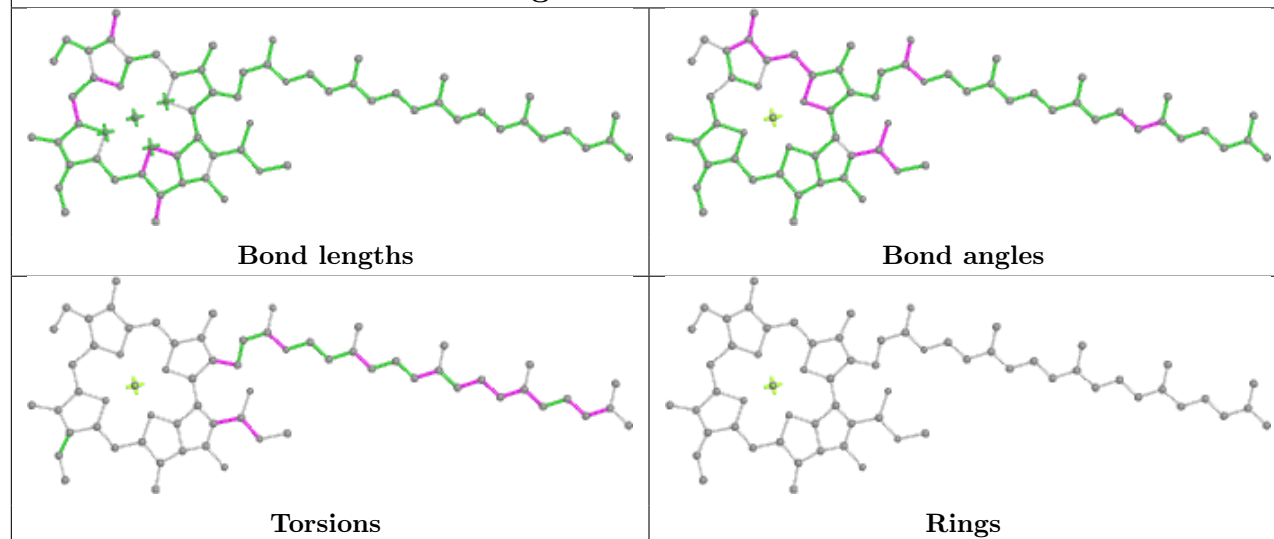
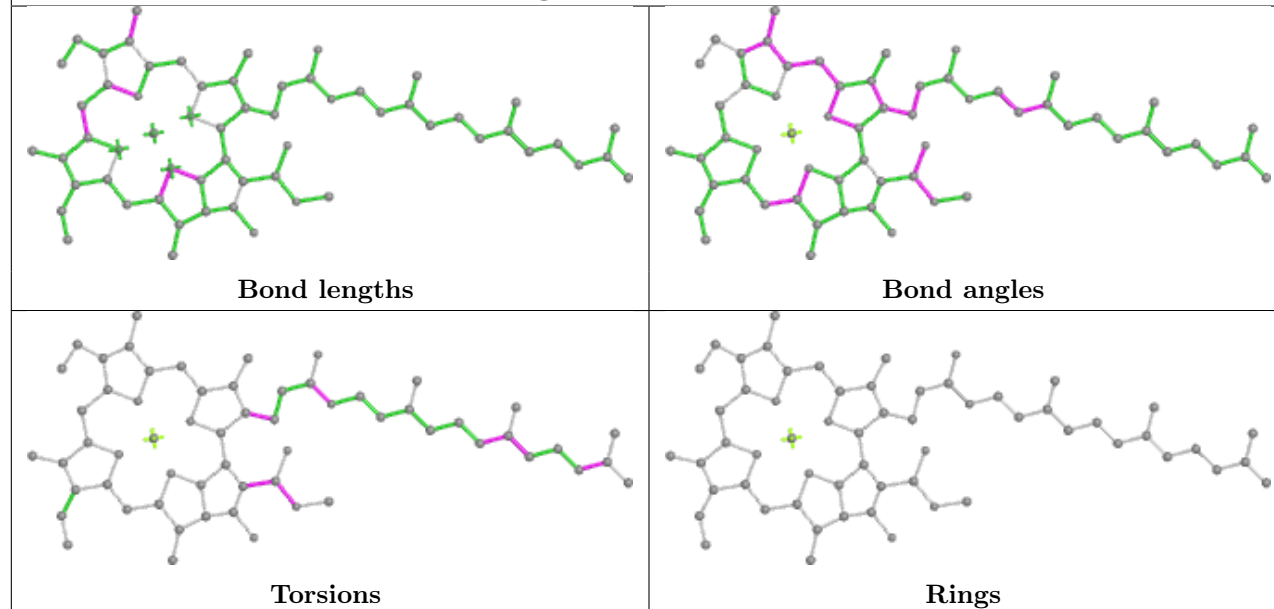
Bond angles

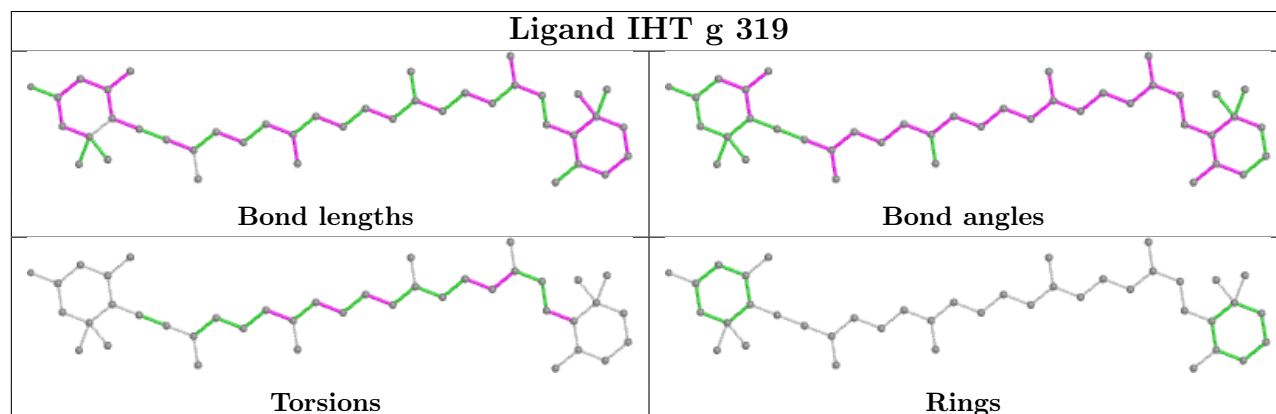
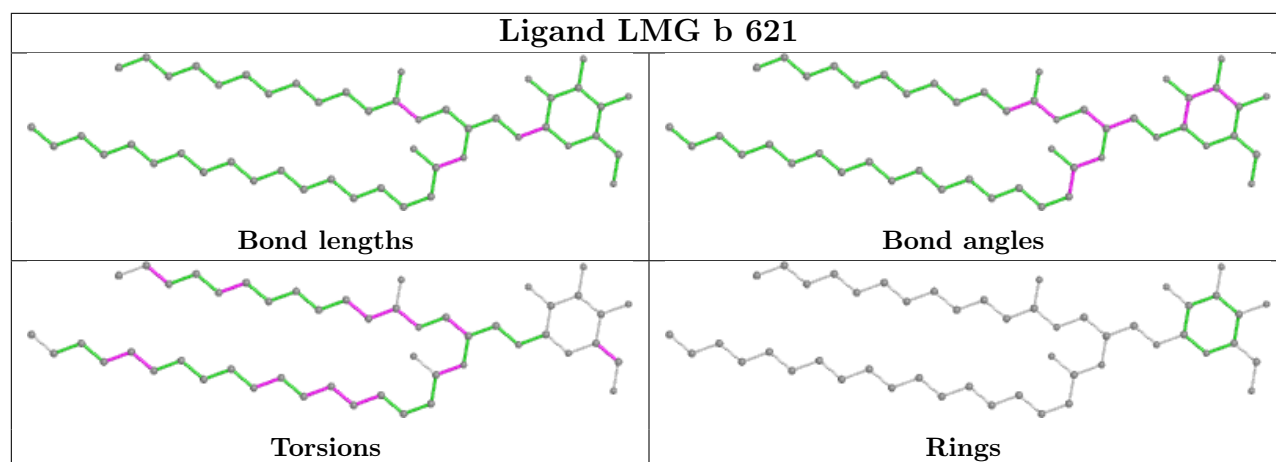
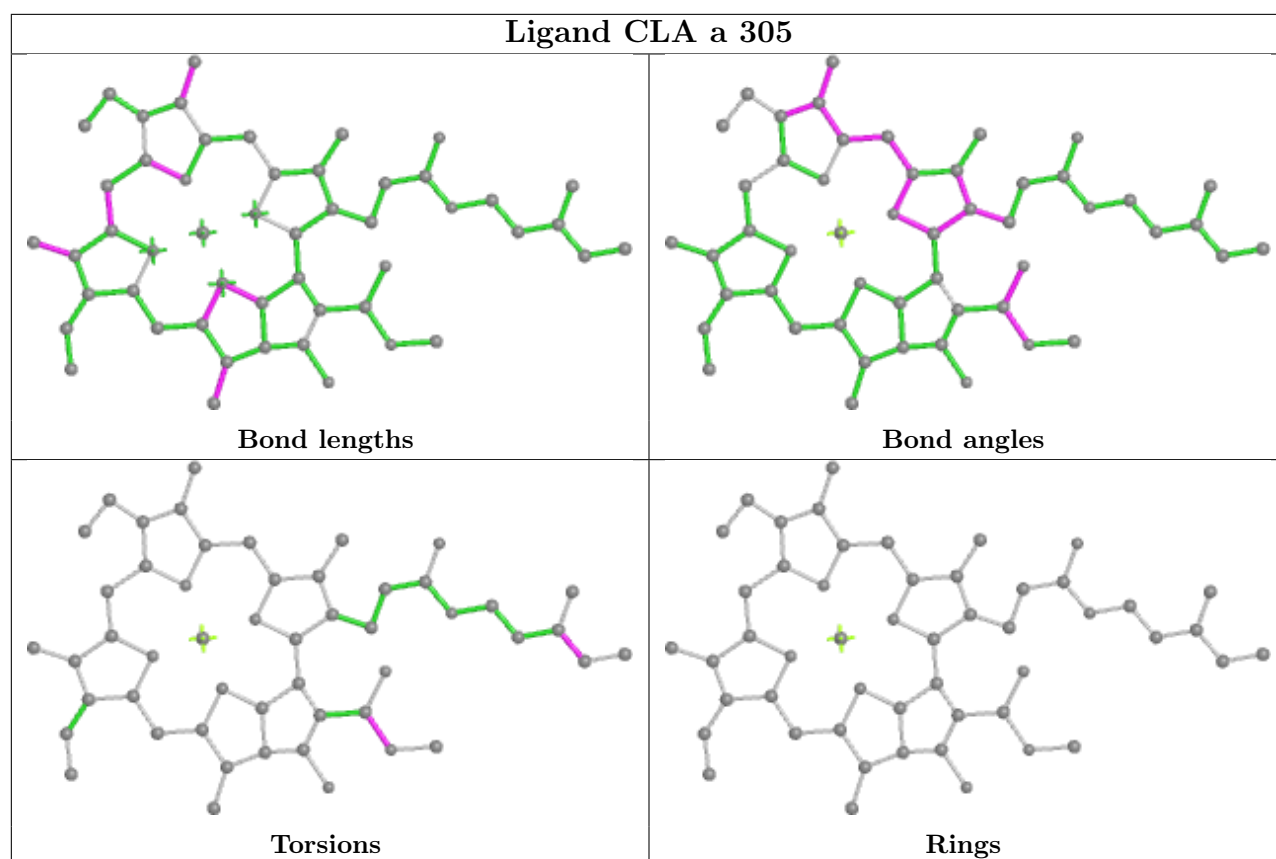


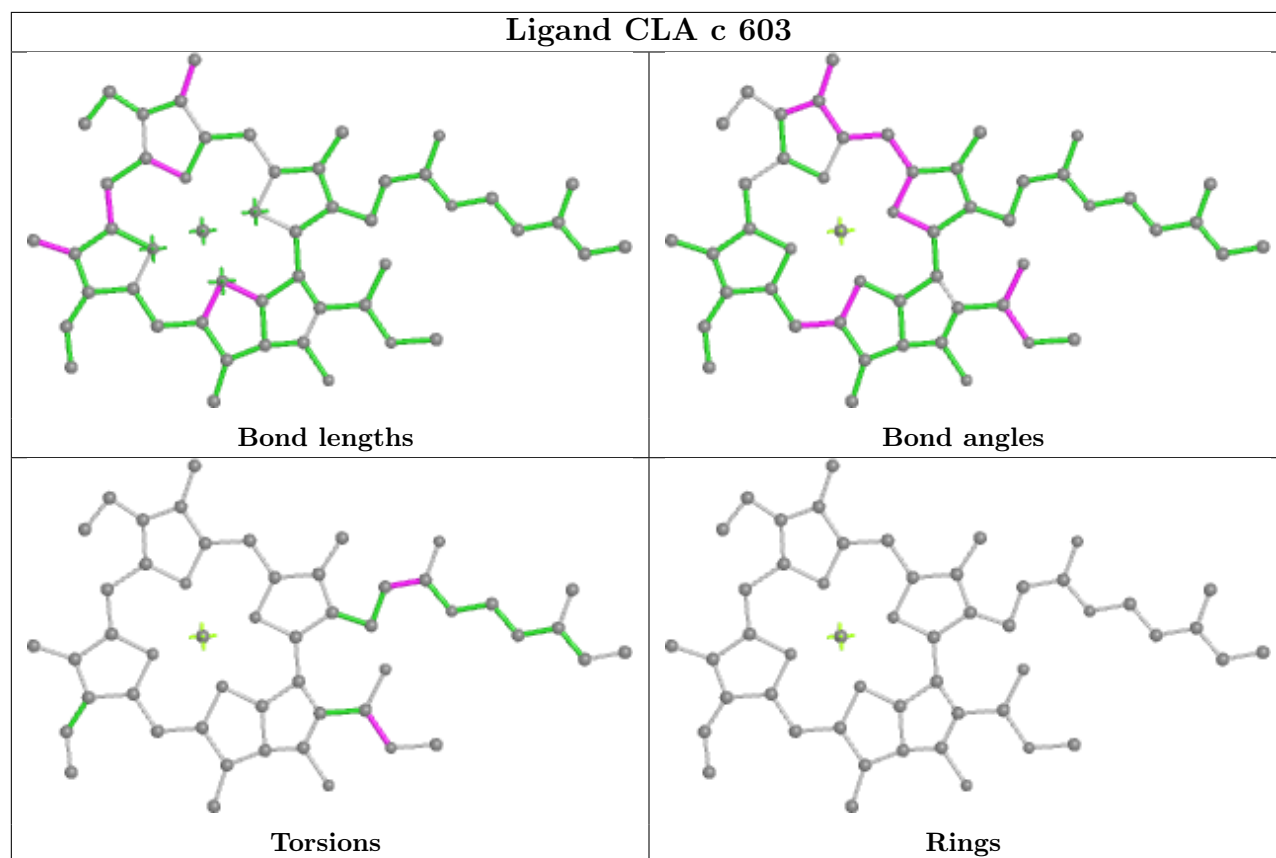
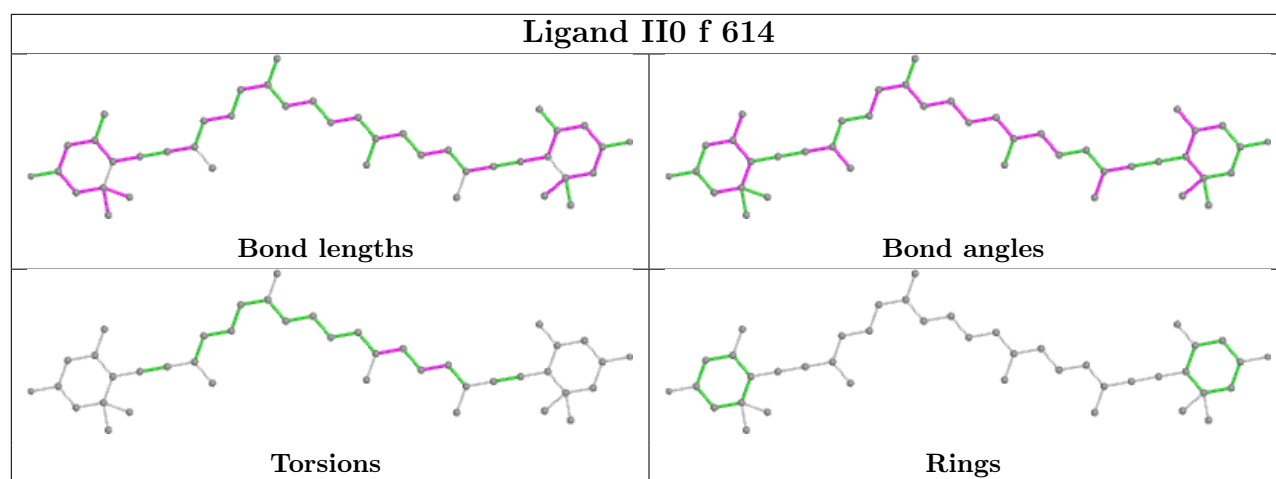
Torsions



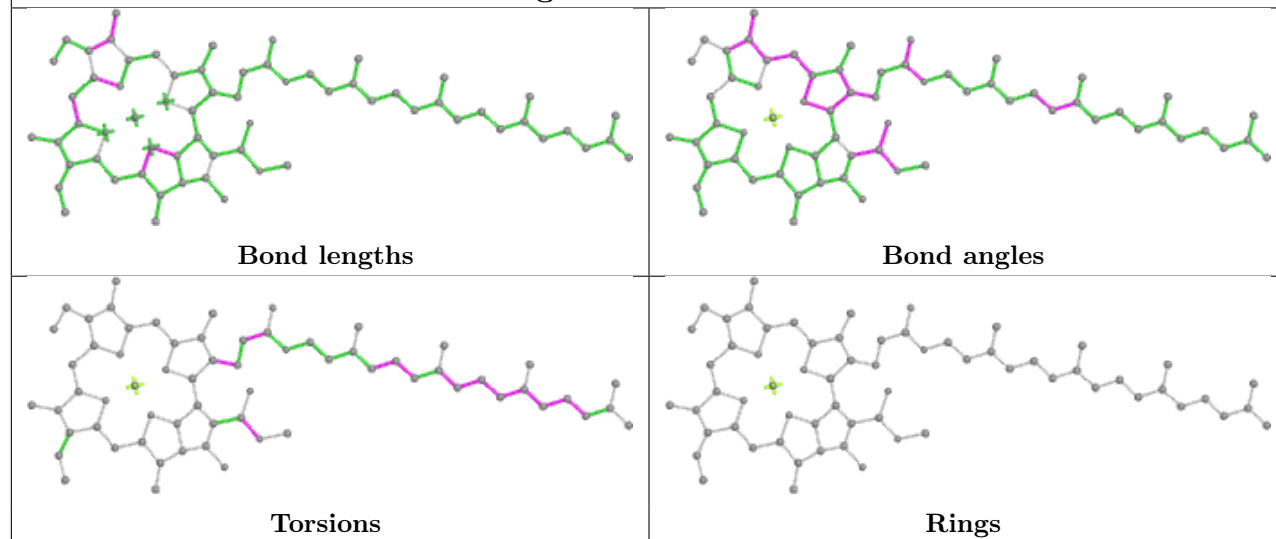
Rings

Ligand CLA A 840**Ligand CLA n 604**

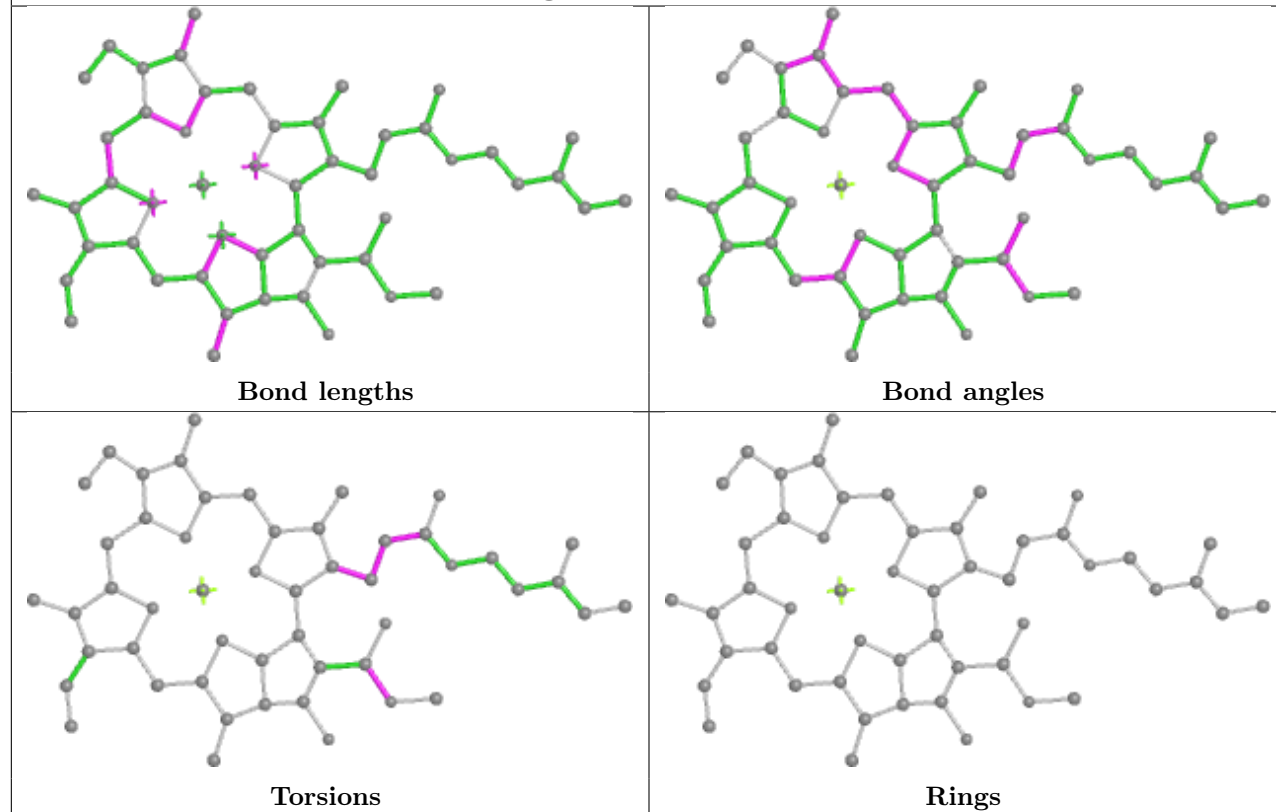


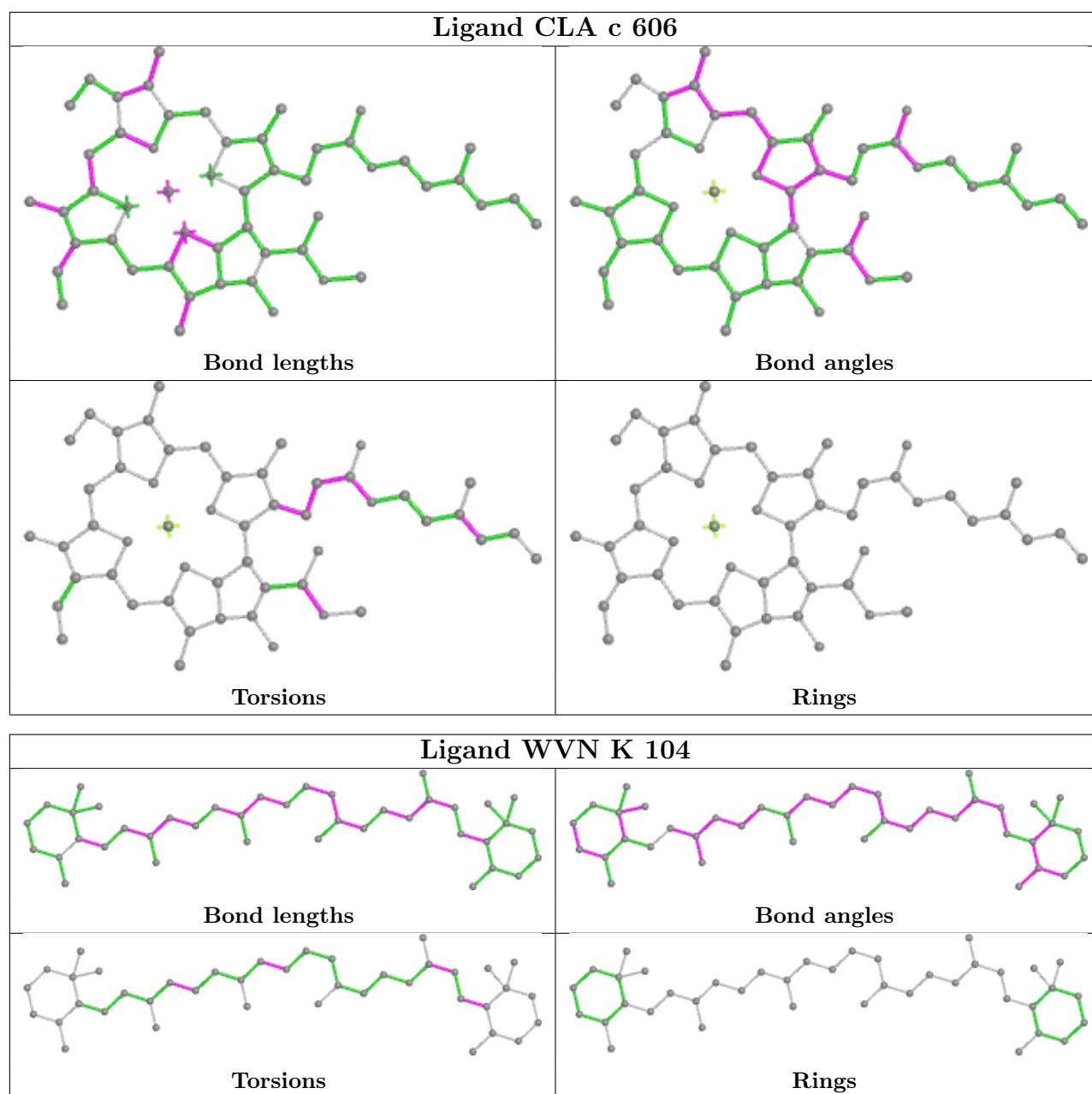


Ligand CLA a 308

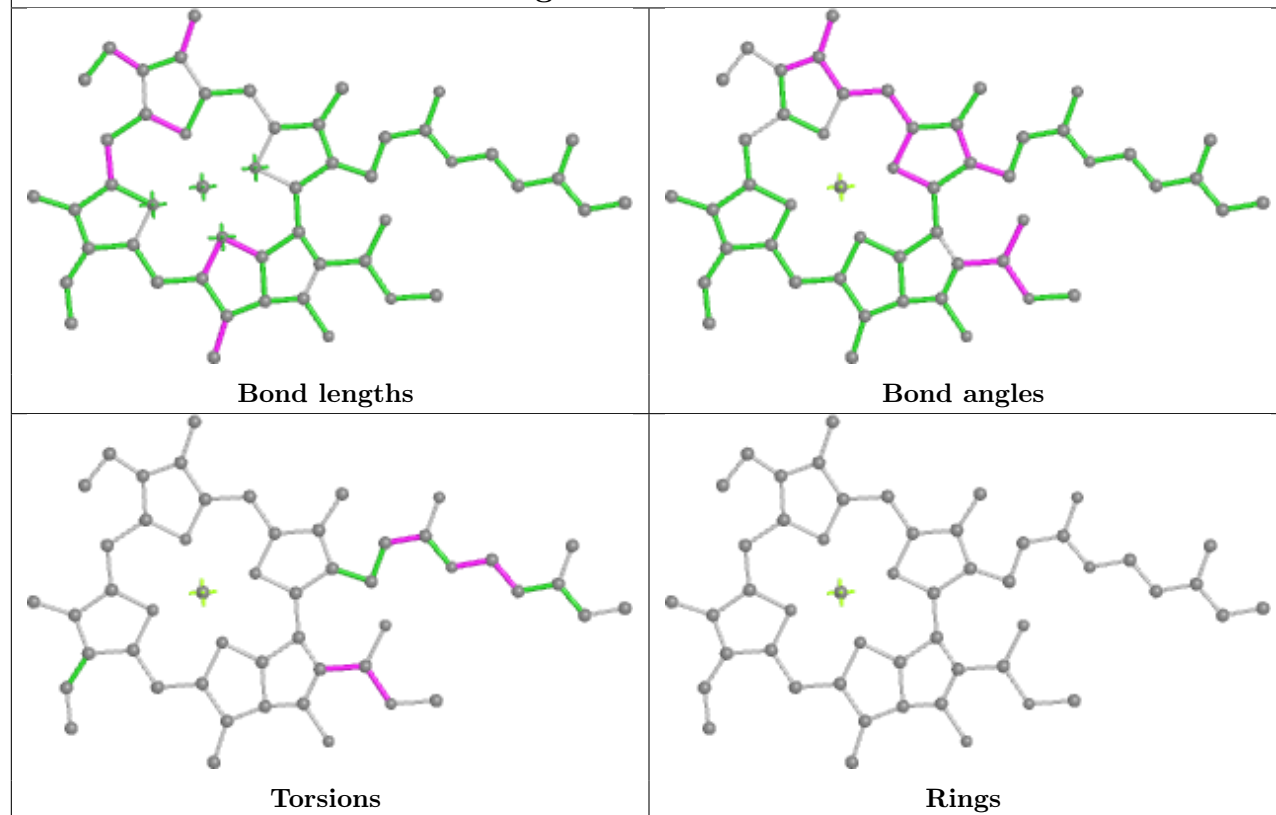


Ligand CLA i 311

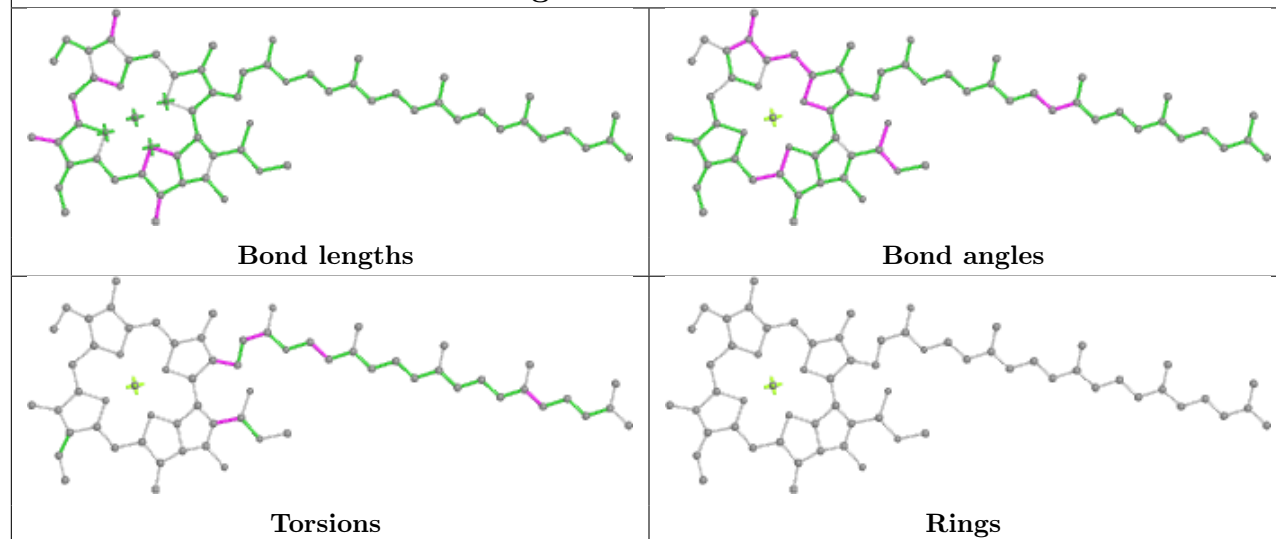


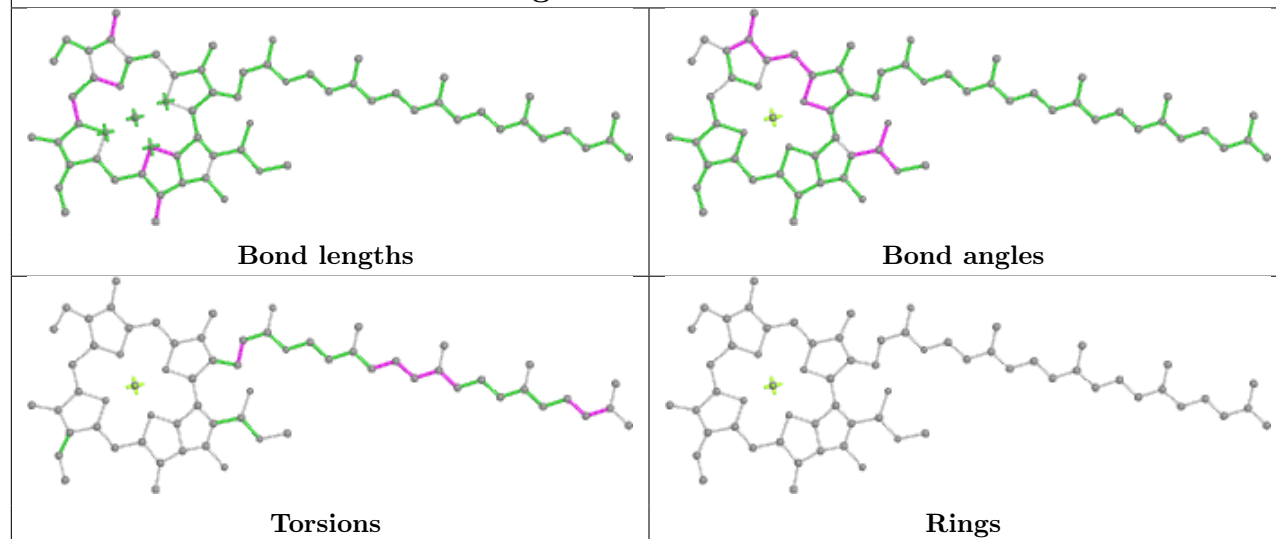
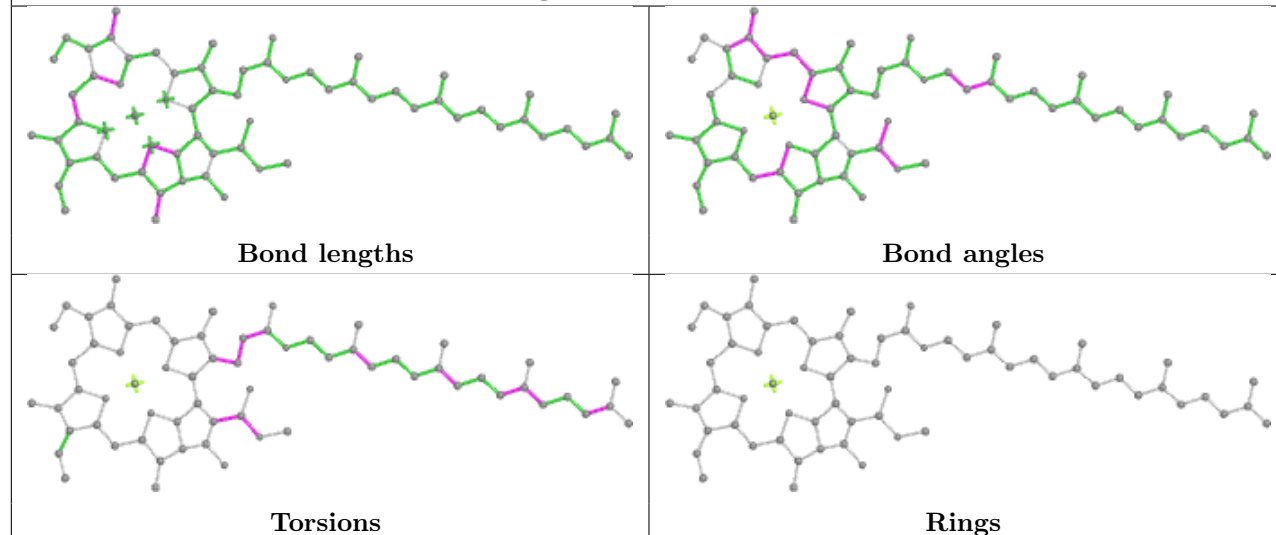
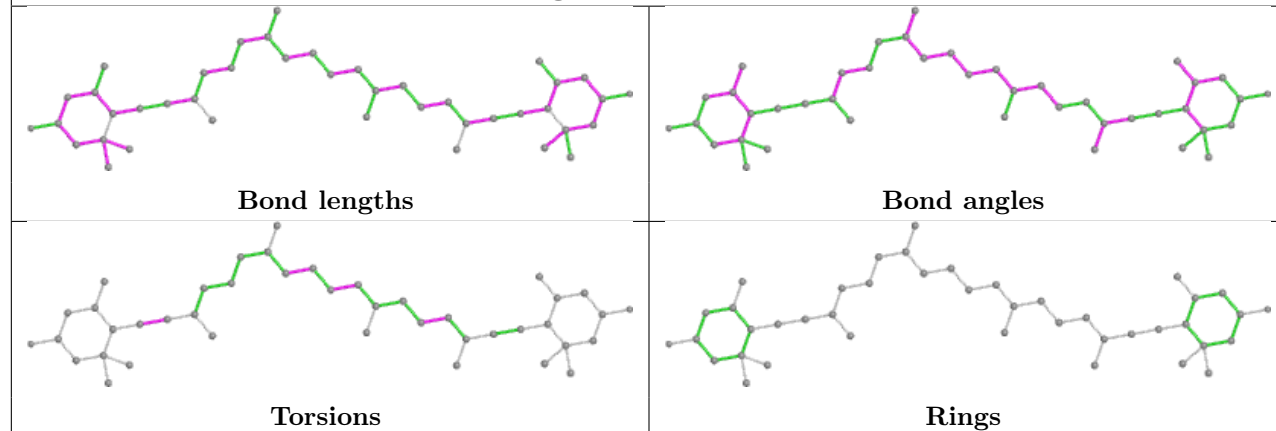


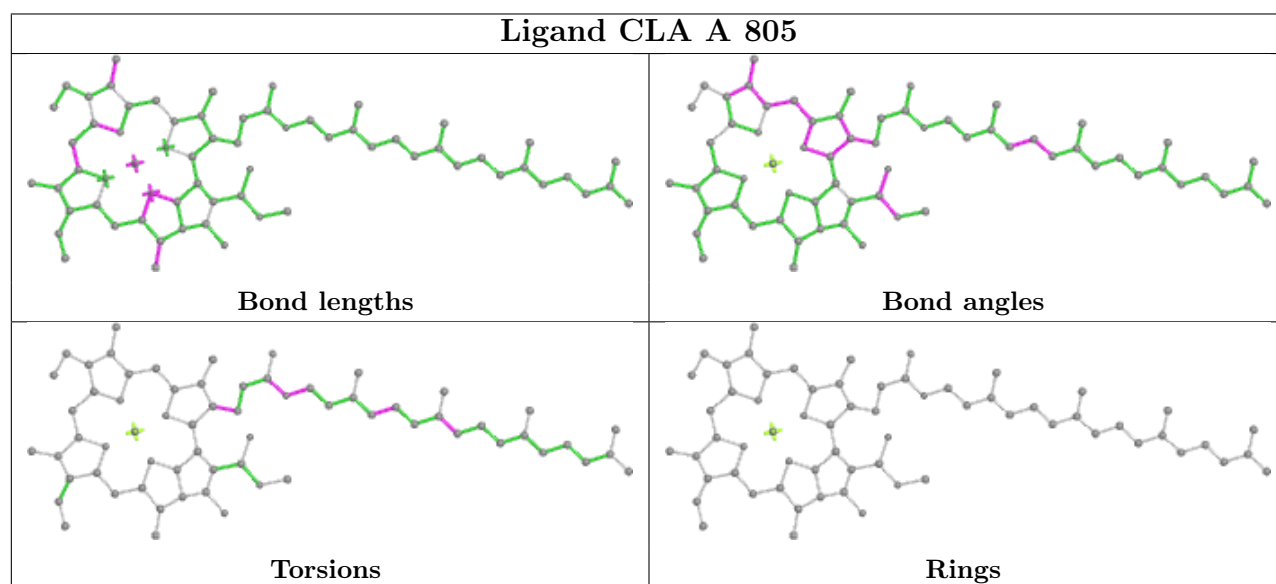
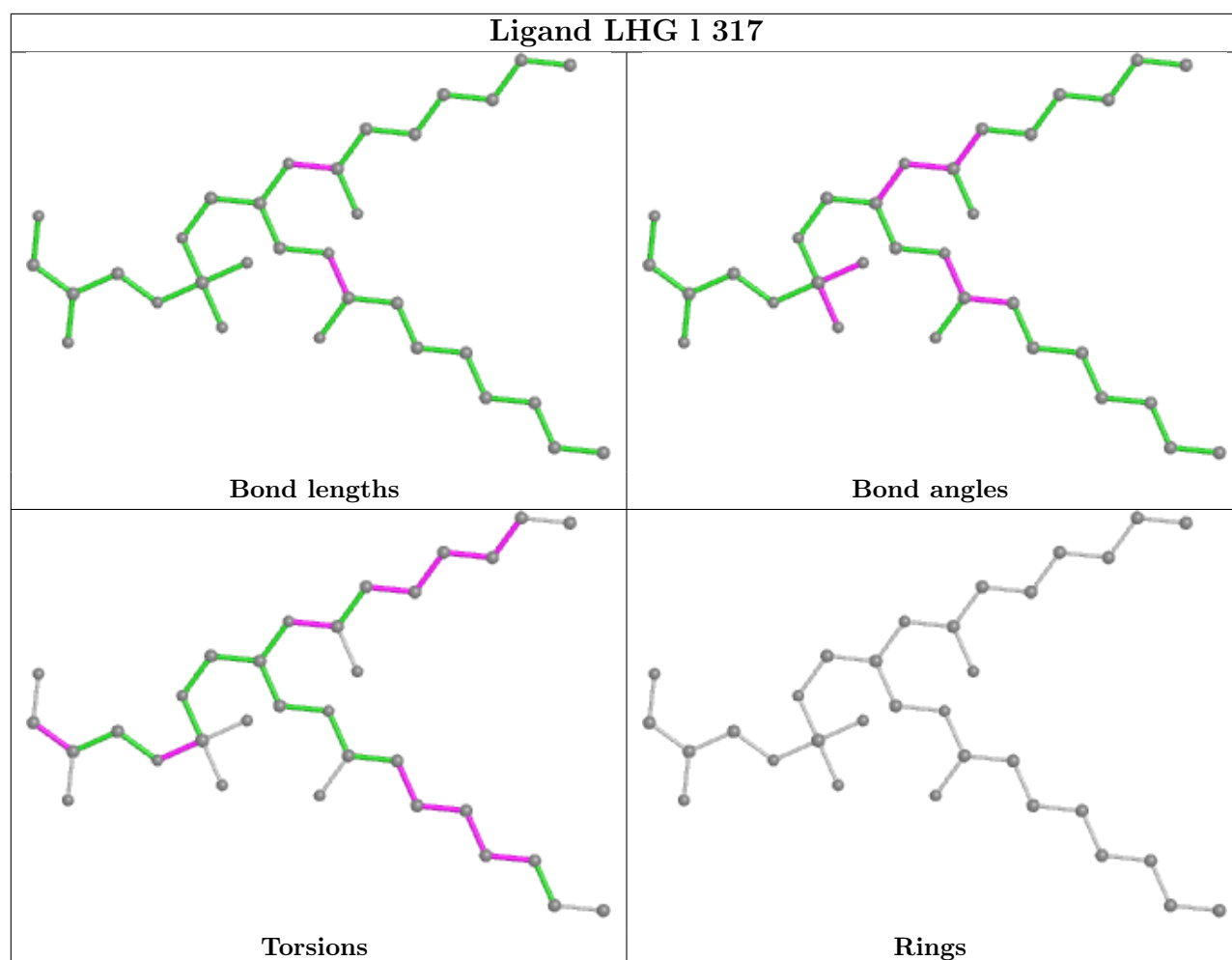
Ligand CLA d 302

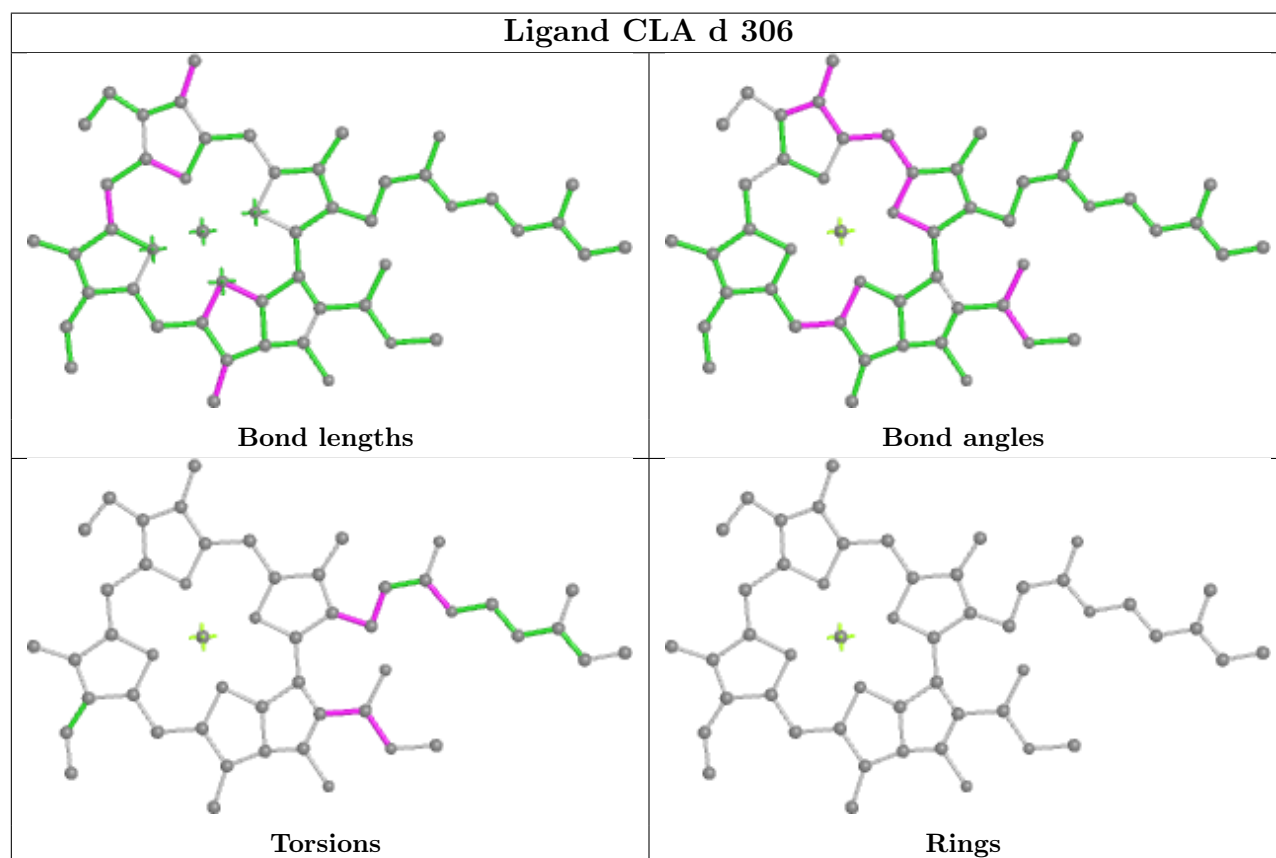
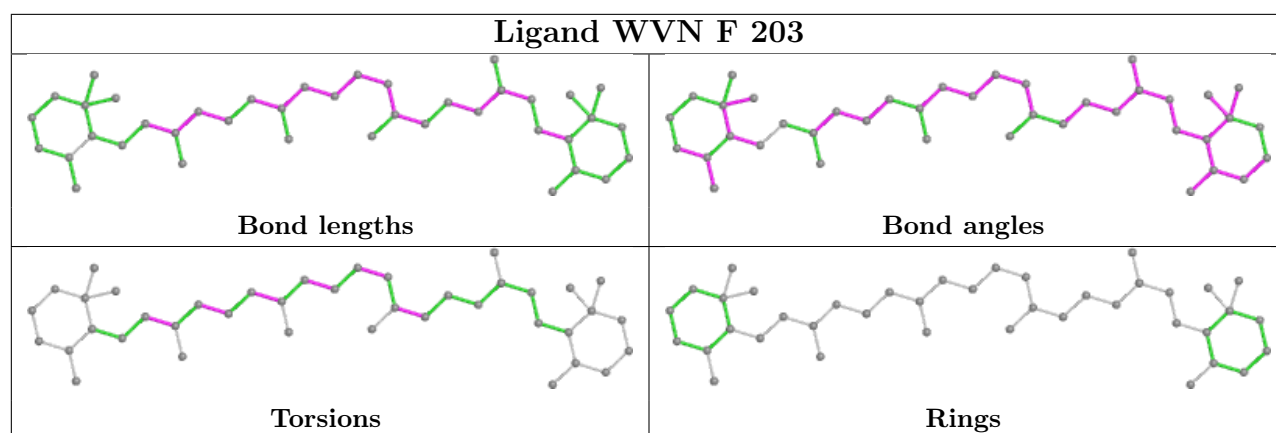


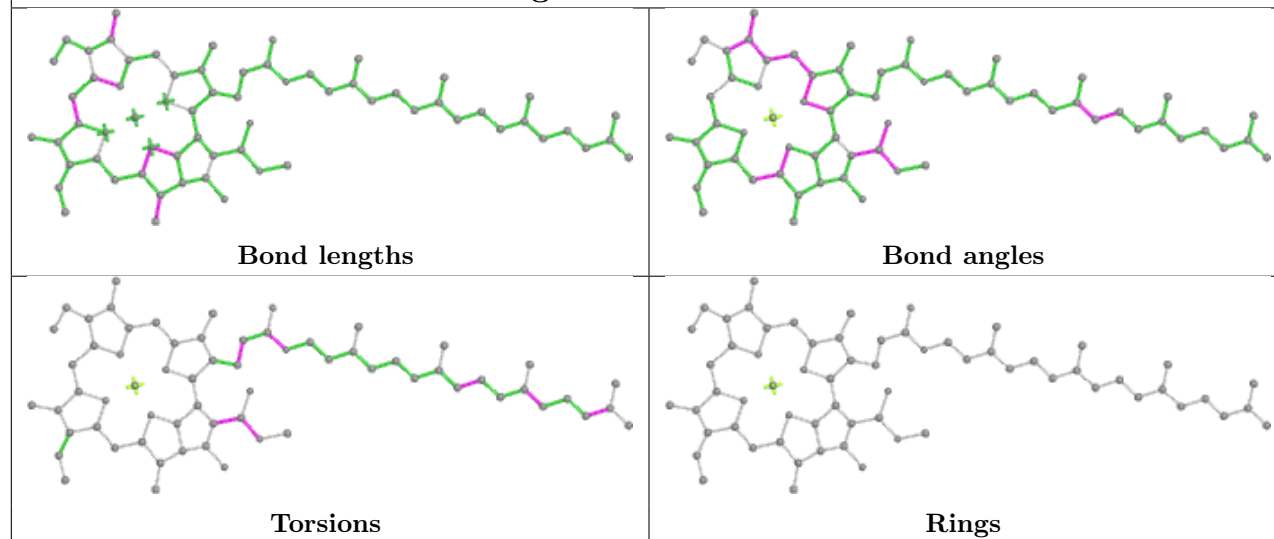
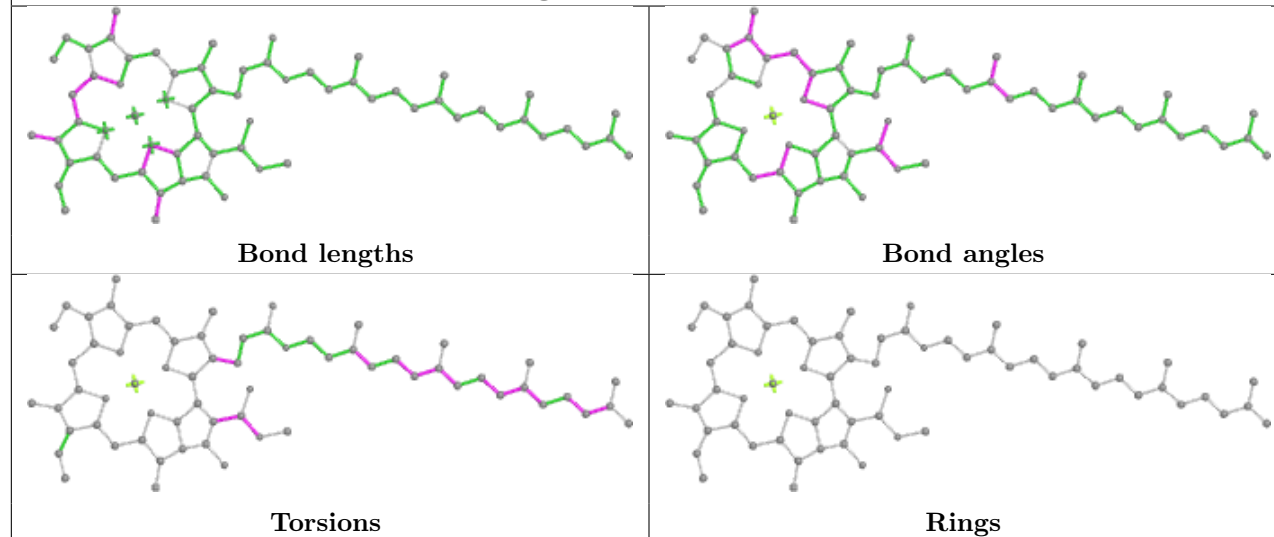
Ligand CLA A 804



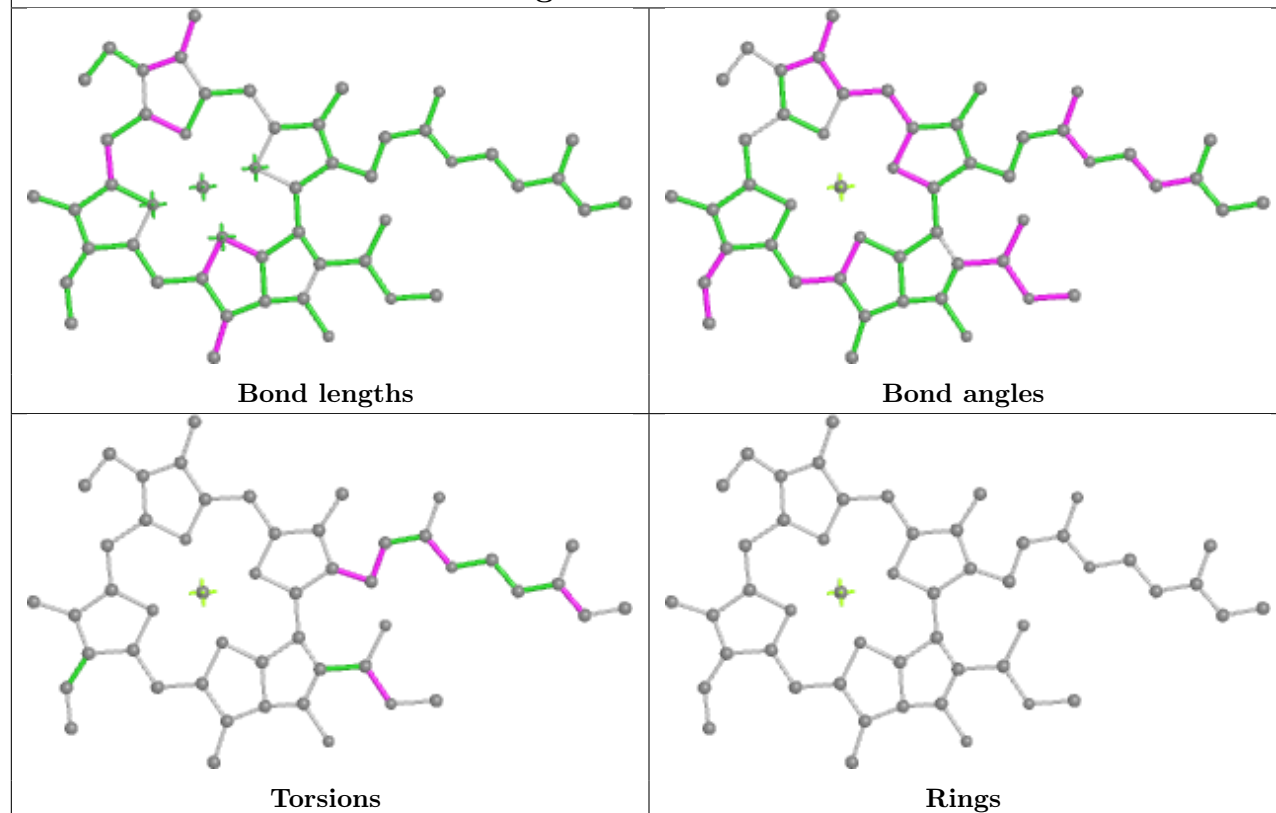
Ligand CLA B 806**Ligand CLA d 303****Ligand II0 n 616**



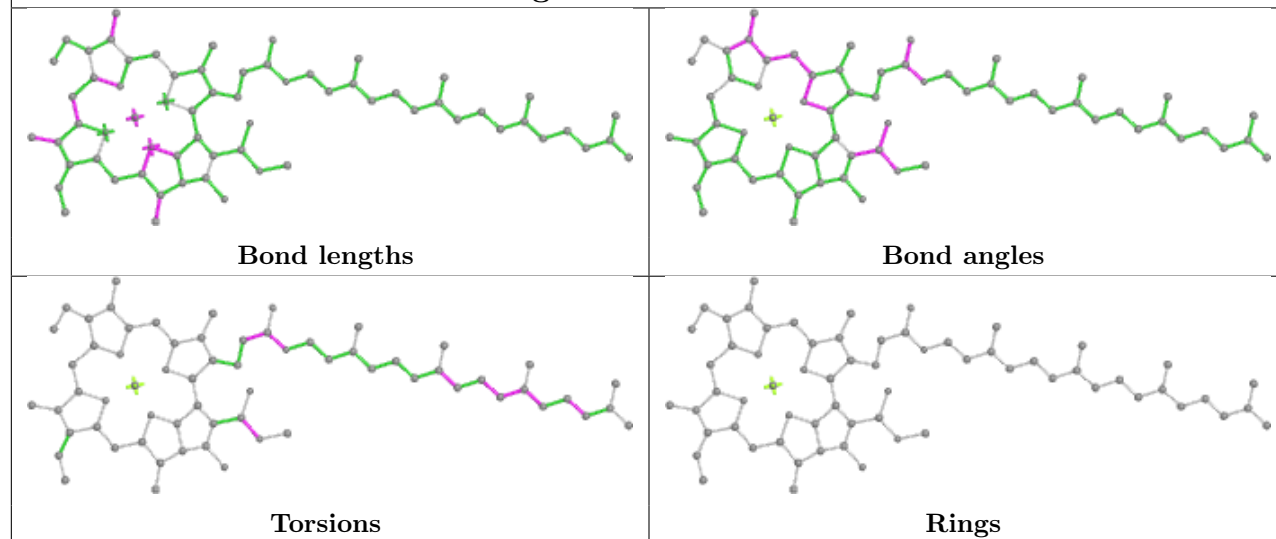


Ligand CLA A 807**Ligand CLA b 610**

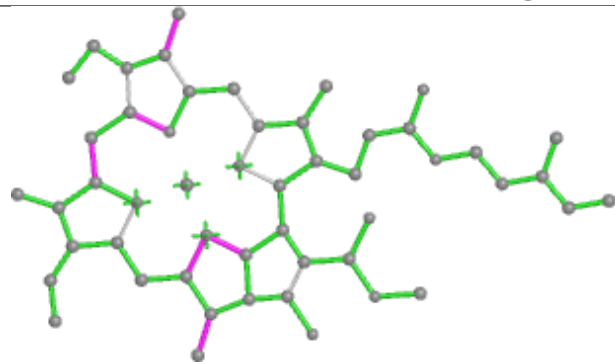
Ligand CLA k 607



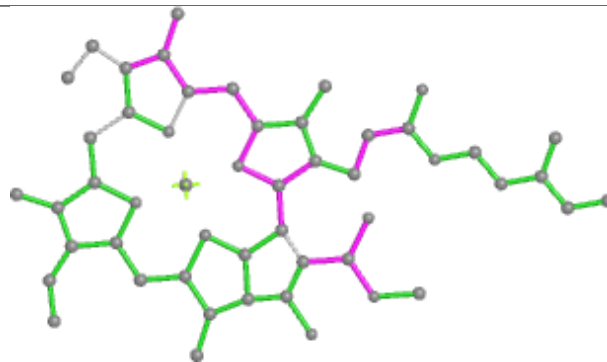
Ligand CLA B 805



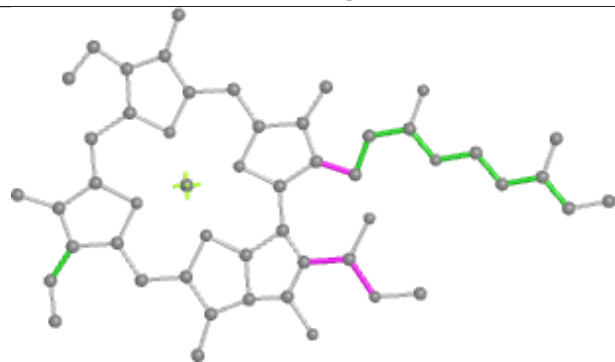
Ligand CLA h 304



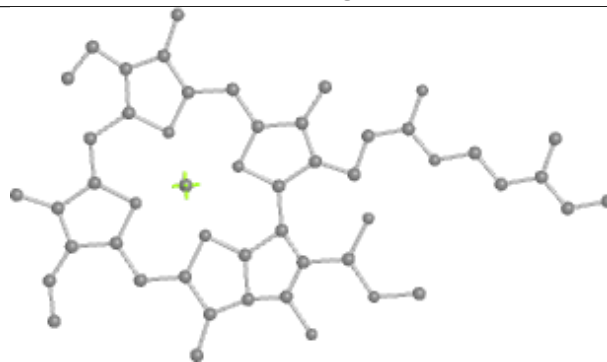
Bond lengths



Bond angles

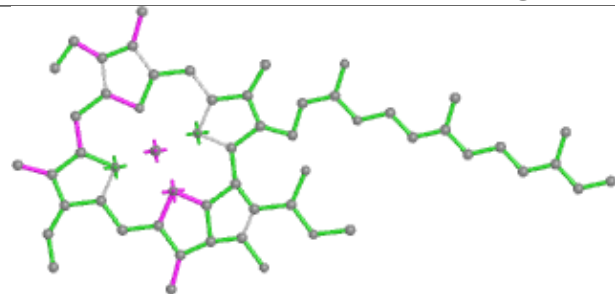


Torsions

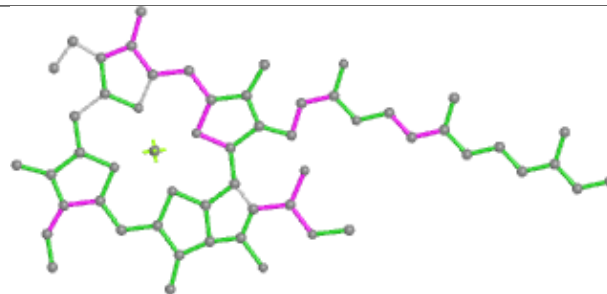


Rings

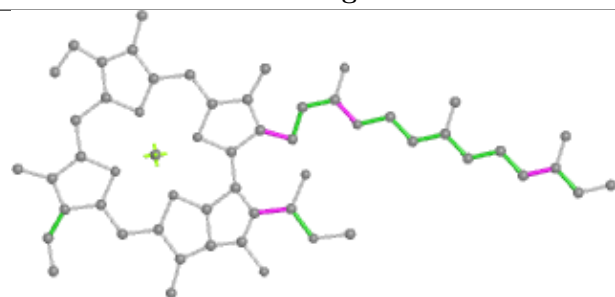
Ligand CLA m 602



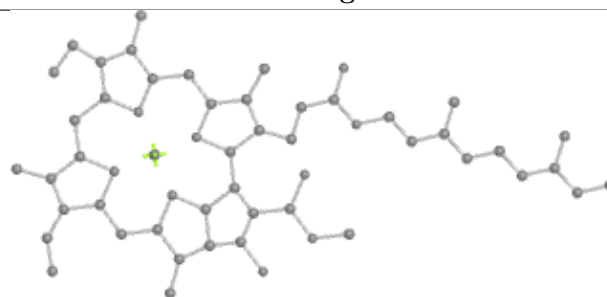
Bond lengths



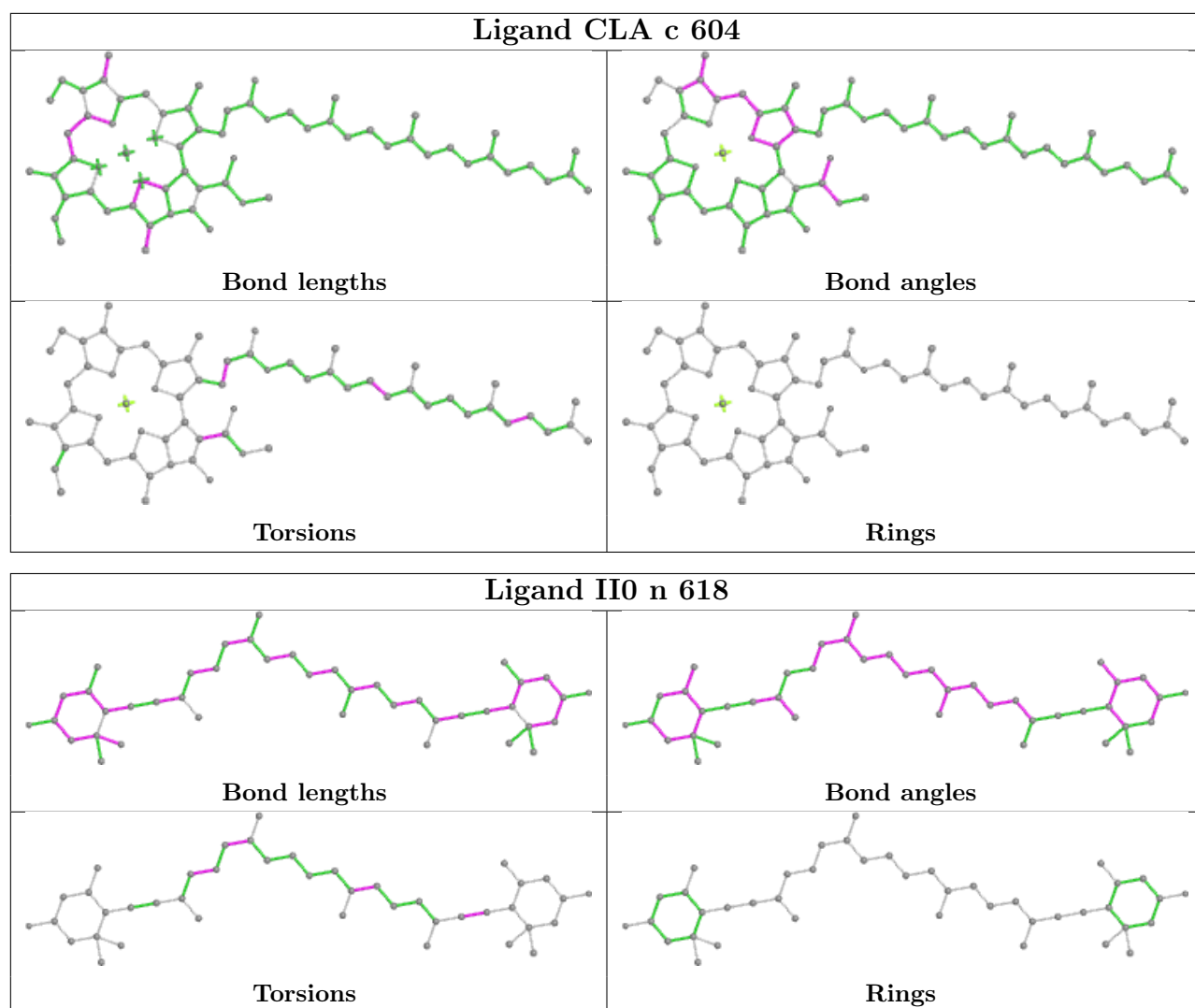
Bond angles

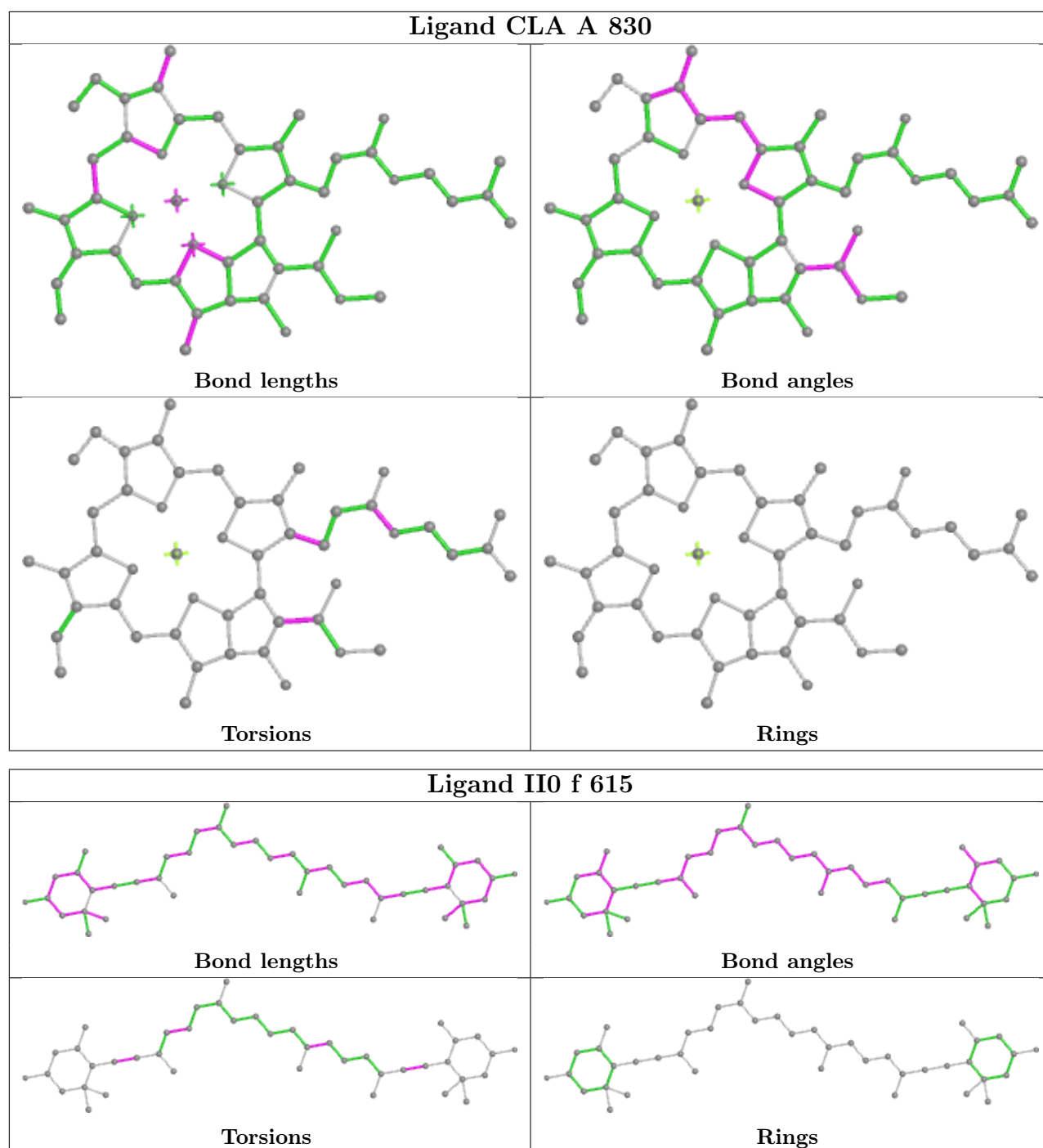


Torsions

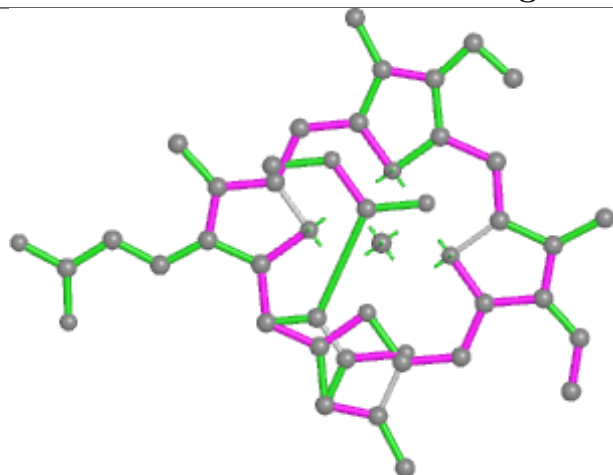


Rings

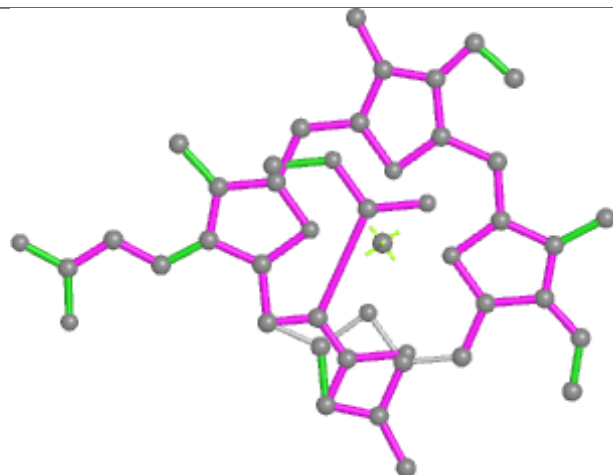




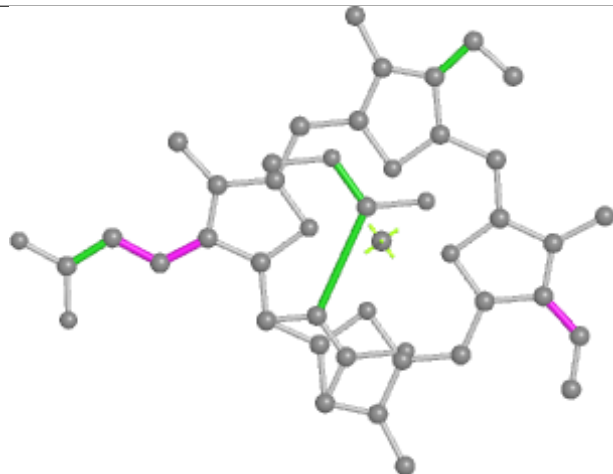
Ligand KC2 d 311



Bond lengths



Bond angles

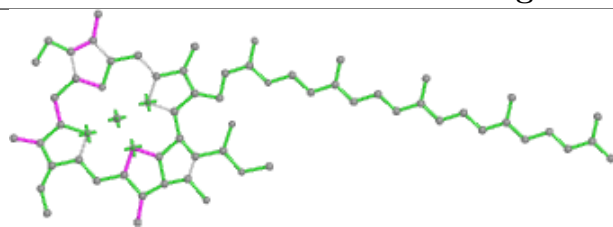


Torsions

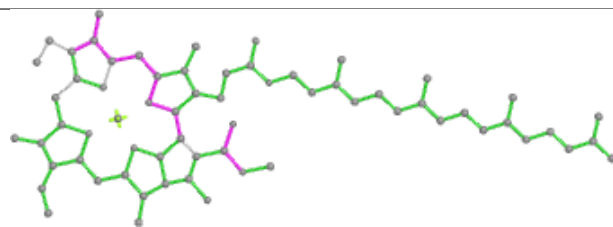


Rings

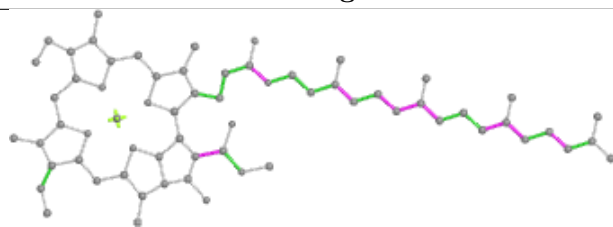
Ligand CLA F 201



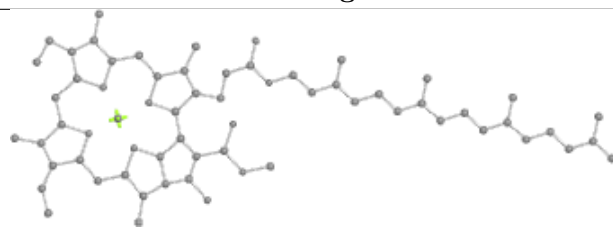
Bond lengths



Bond angles

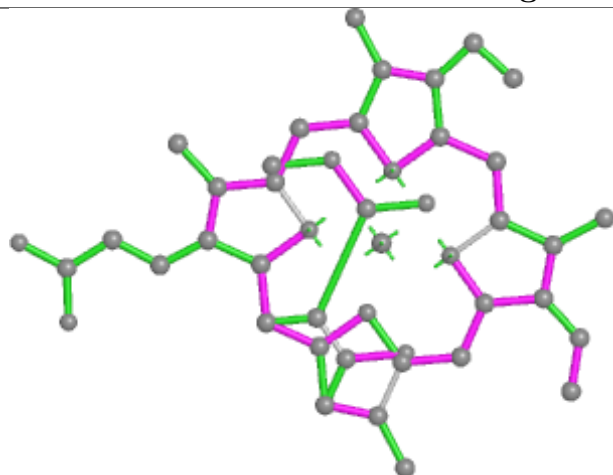


Torsions

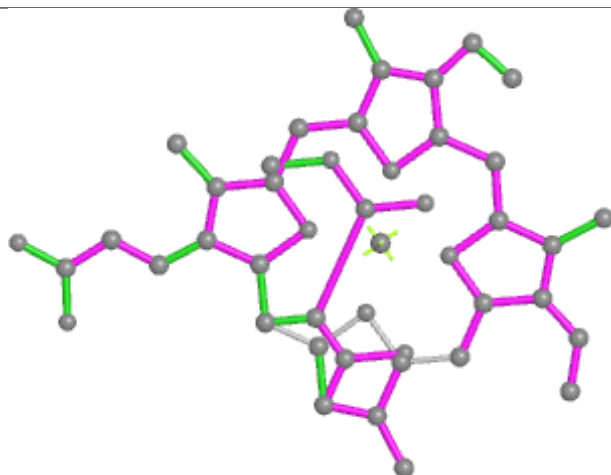


Rings

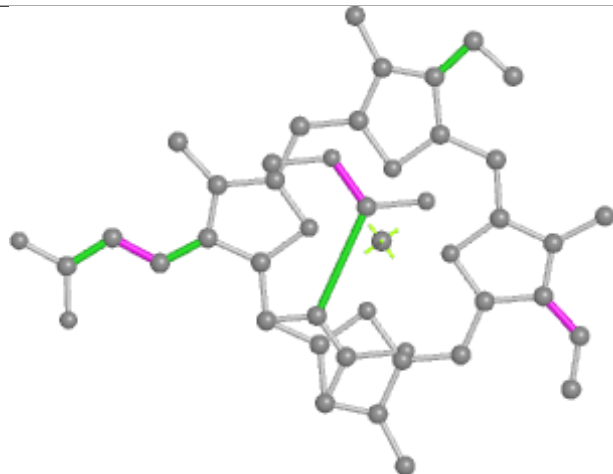
Ligand KC2 k 611



Bond lengths



Bond angles

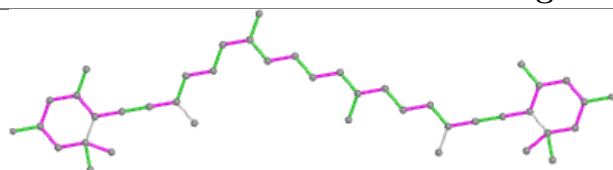


Torsions

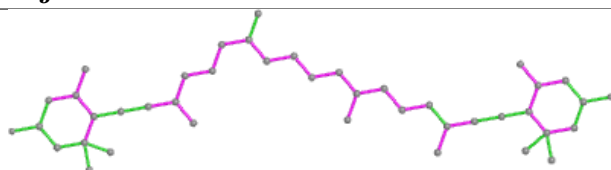


Rings

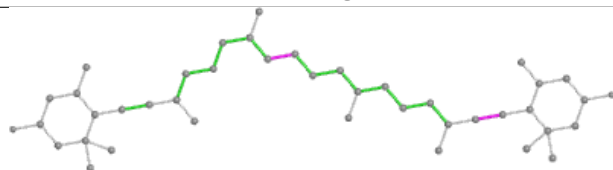
Ligand II0 j 615



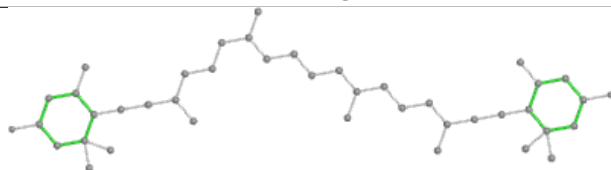
Bond lengths



Bond angles

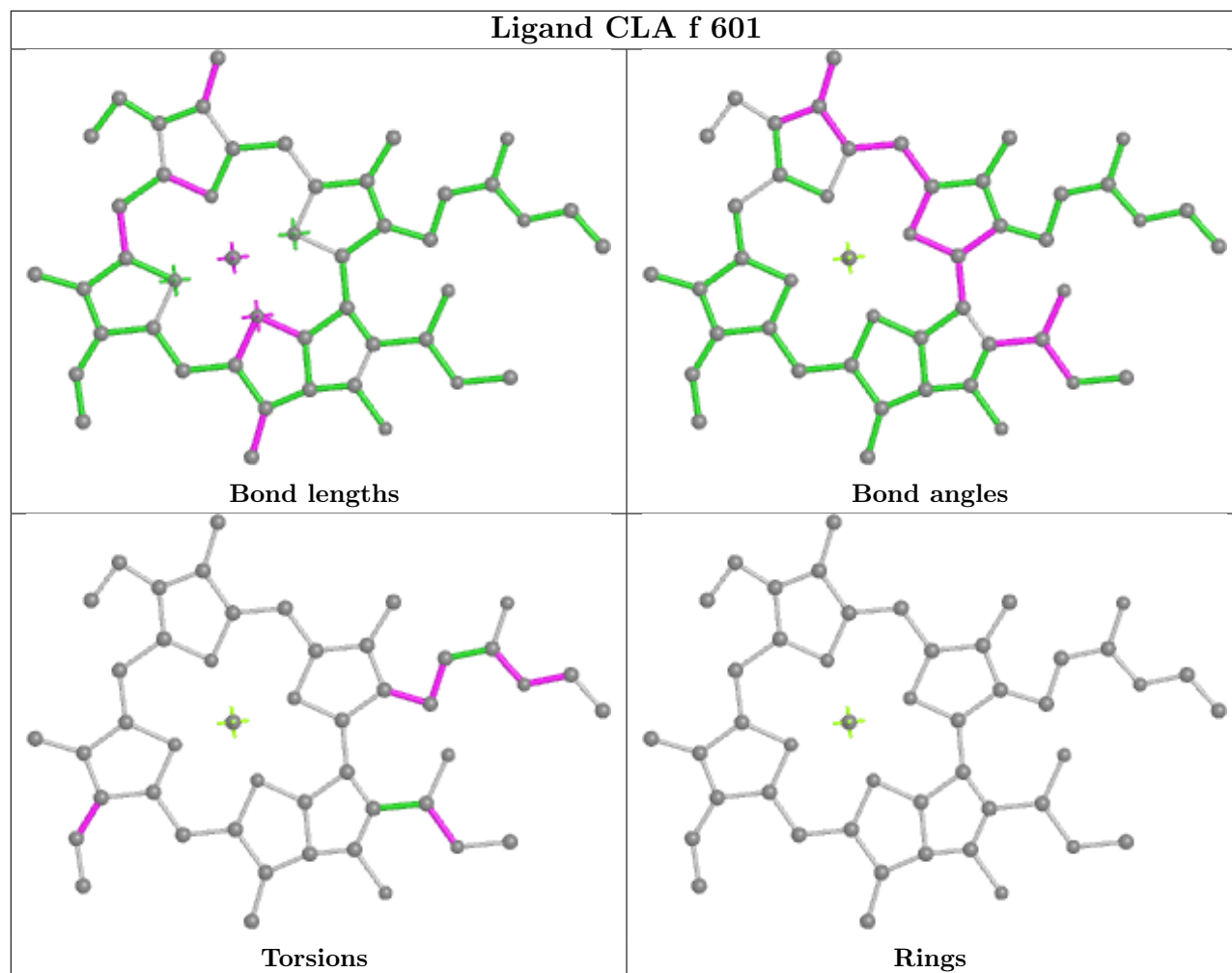


Torsions

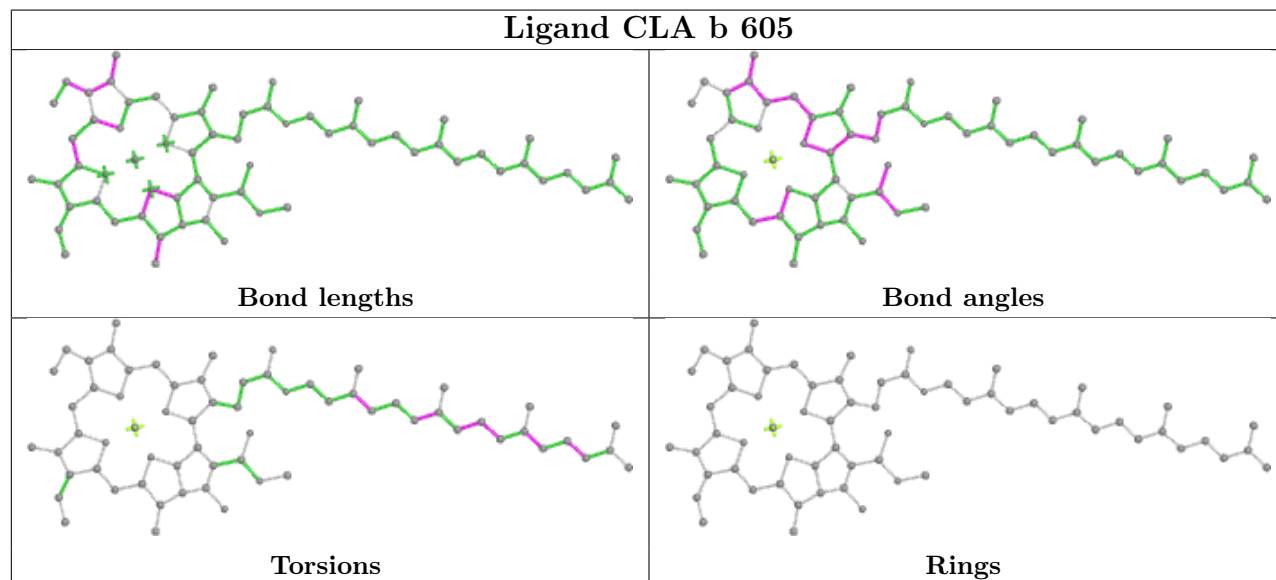


Rings

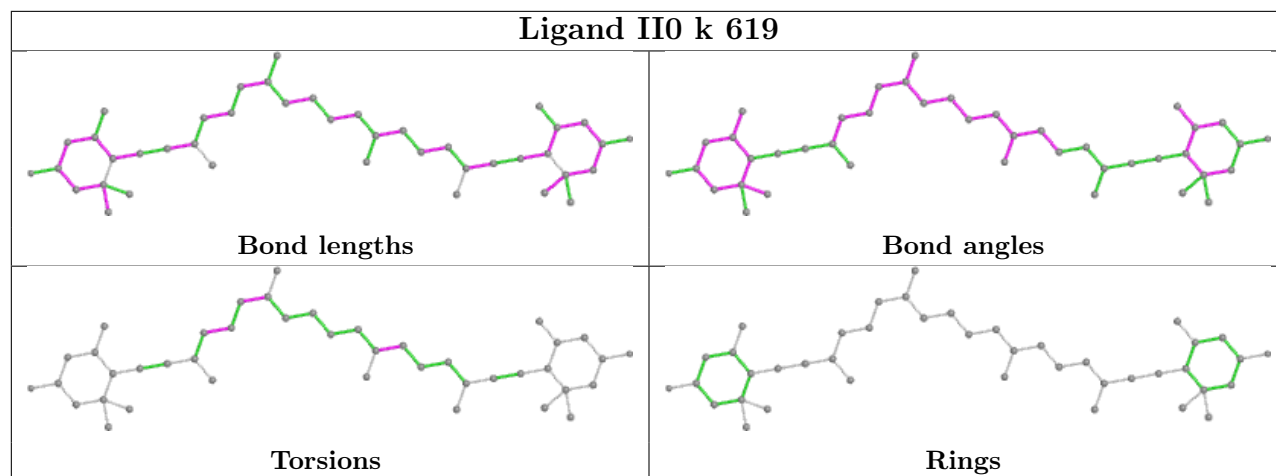
Ligand CLA f 601



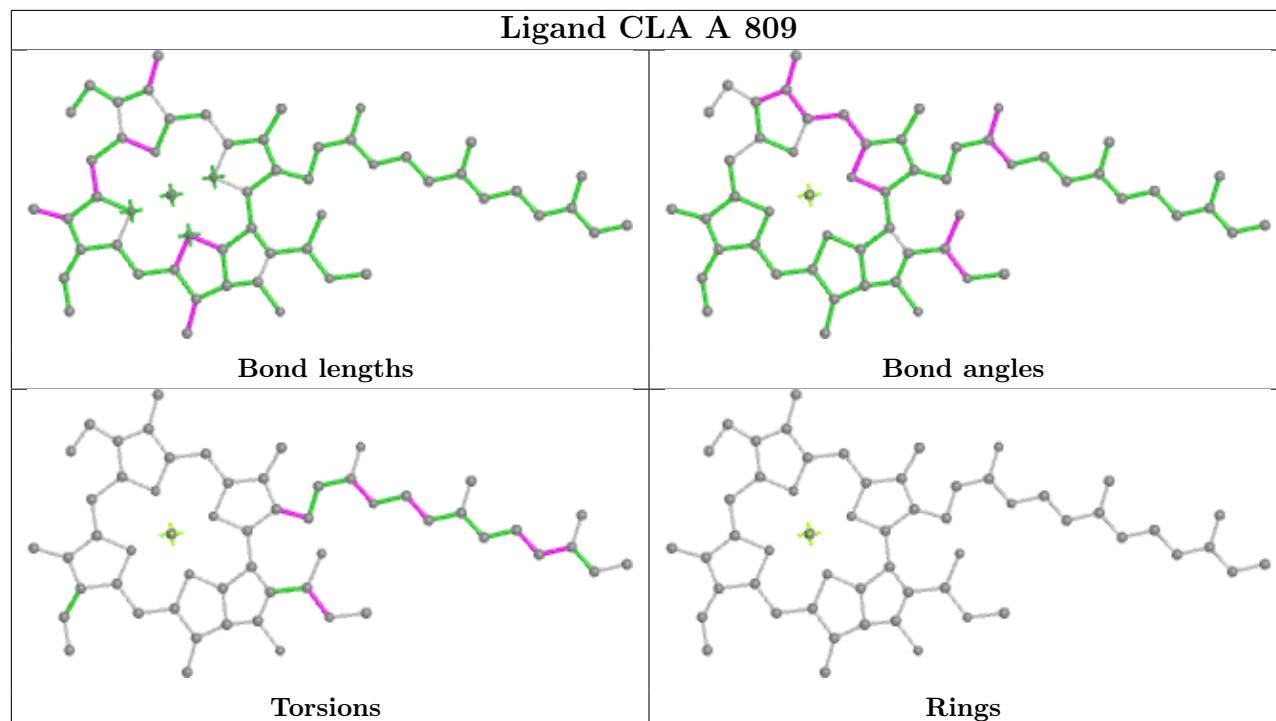
Ligand CLA b 605



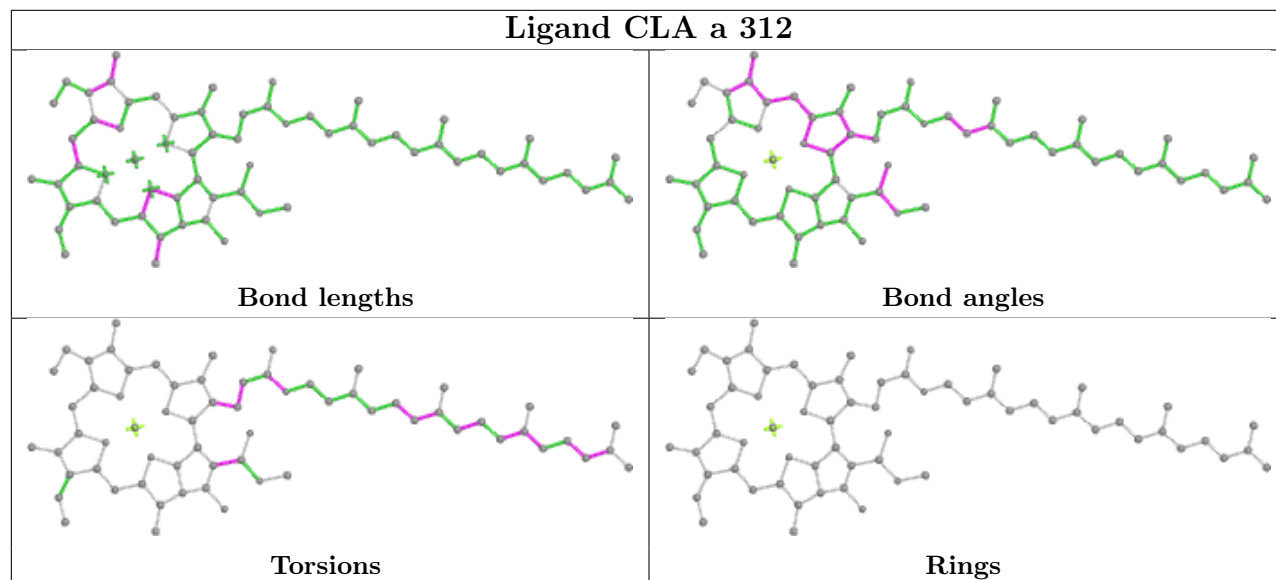
Ligand II0 k 619



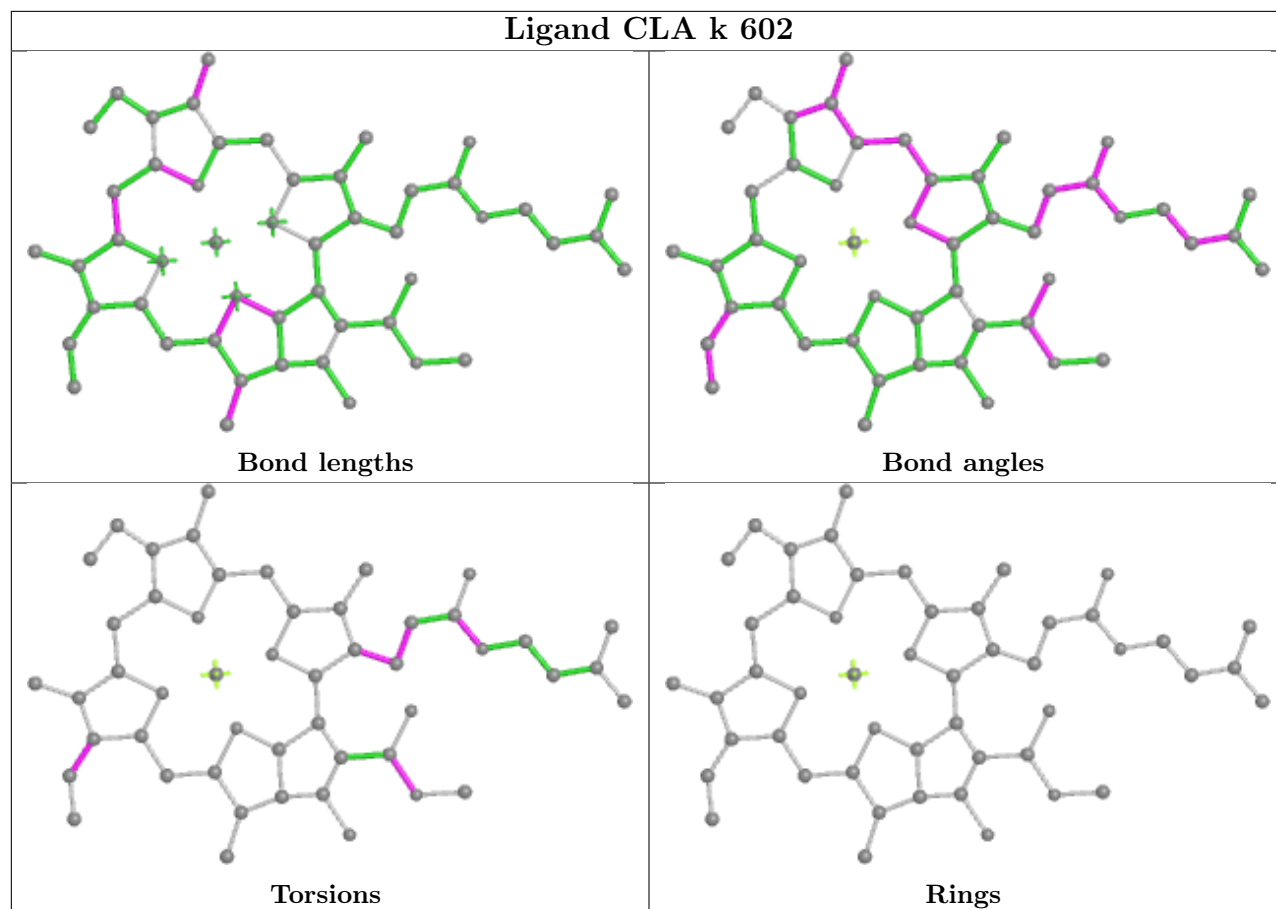
Ligand CLA A 809

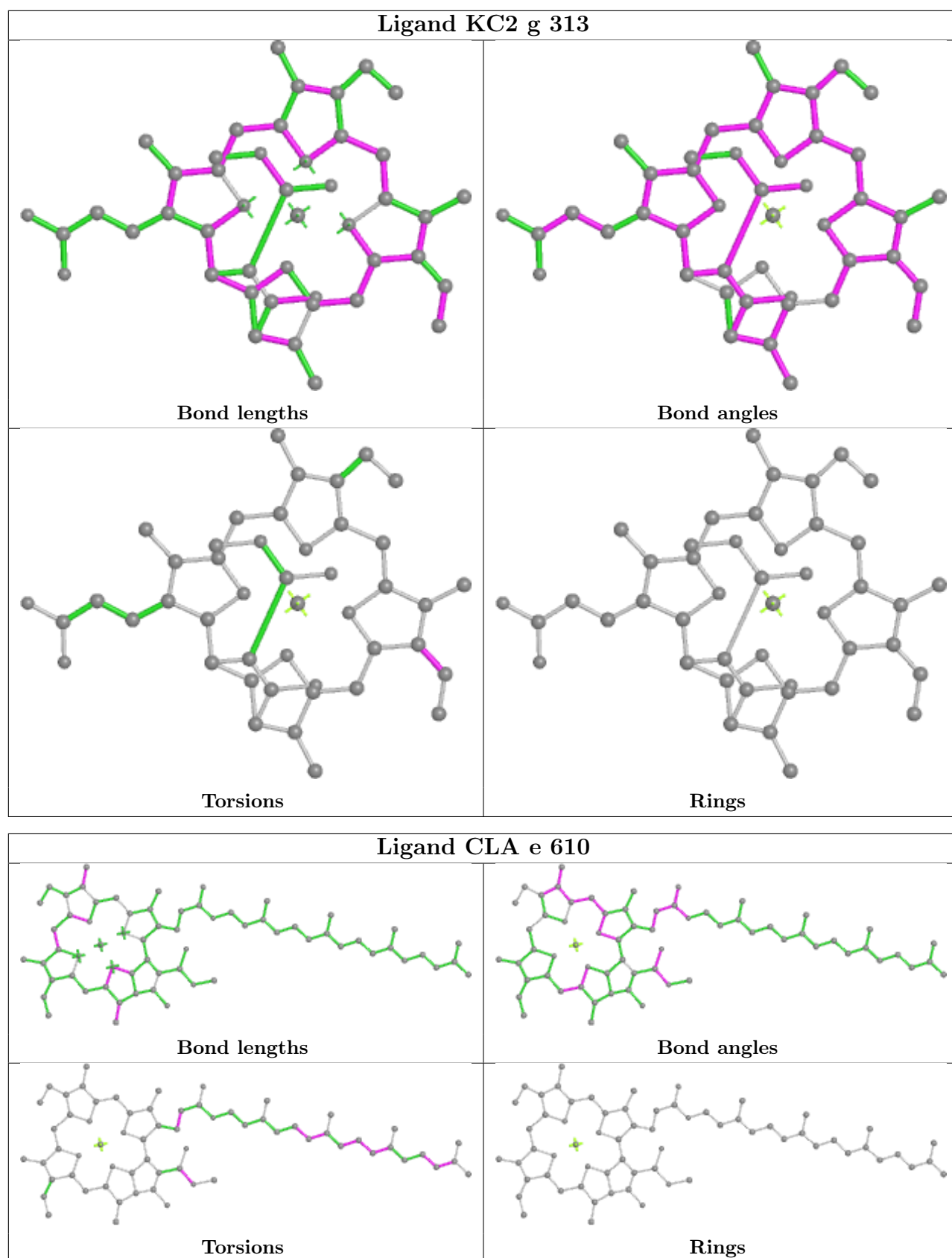


Ligand CLA a 312

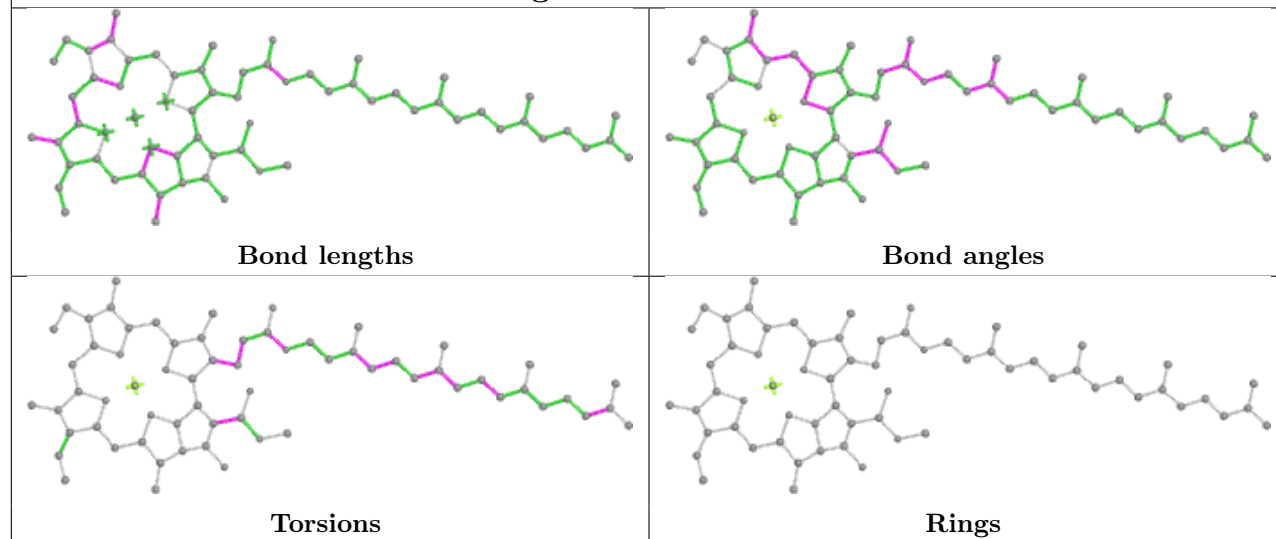


Ligand CLA k 602

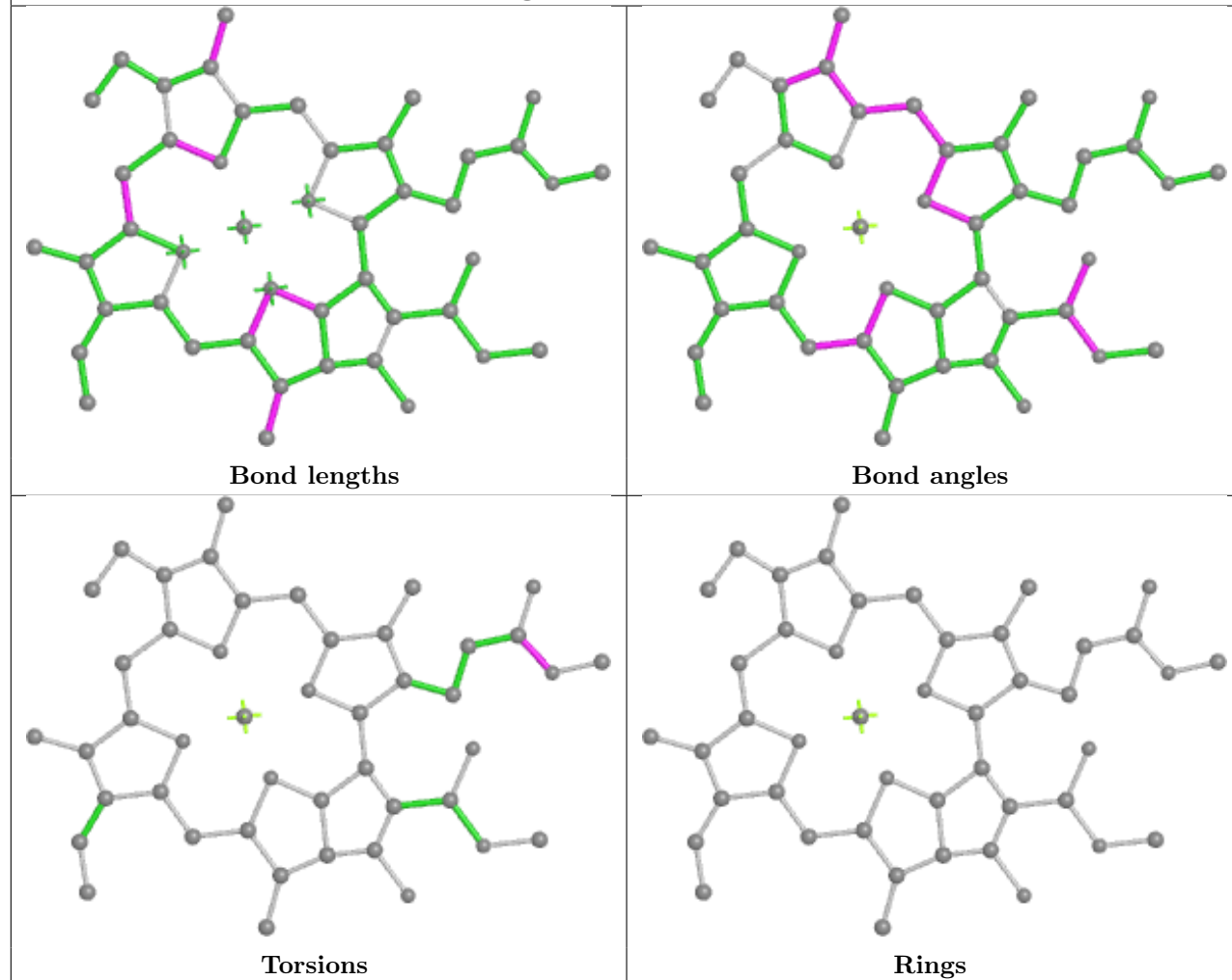


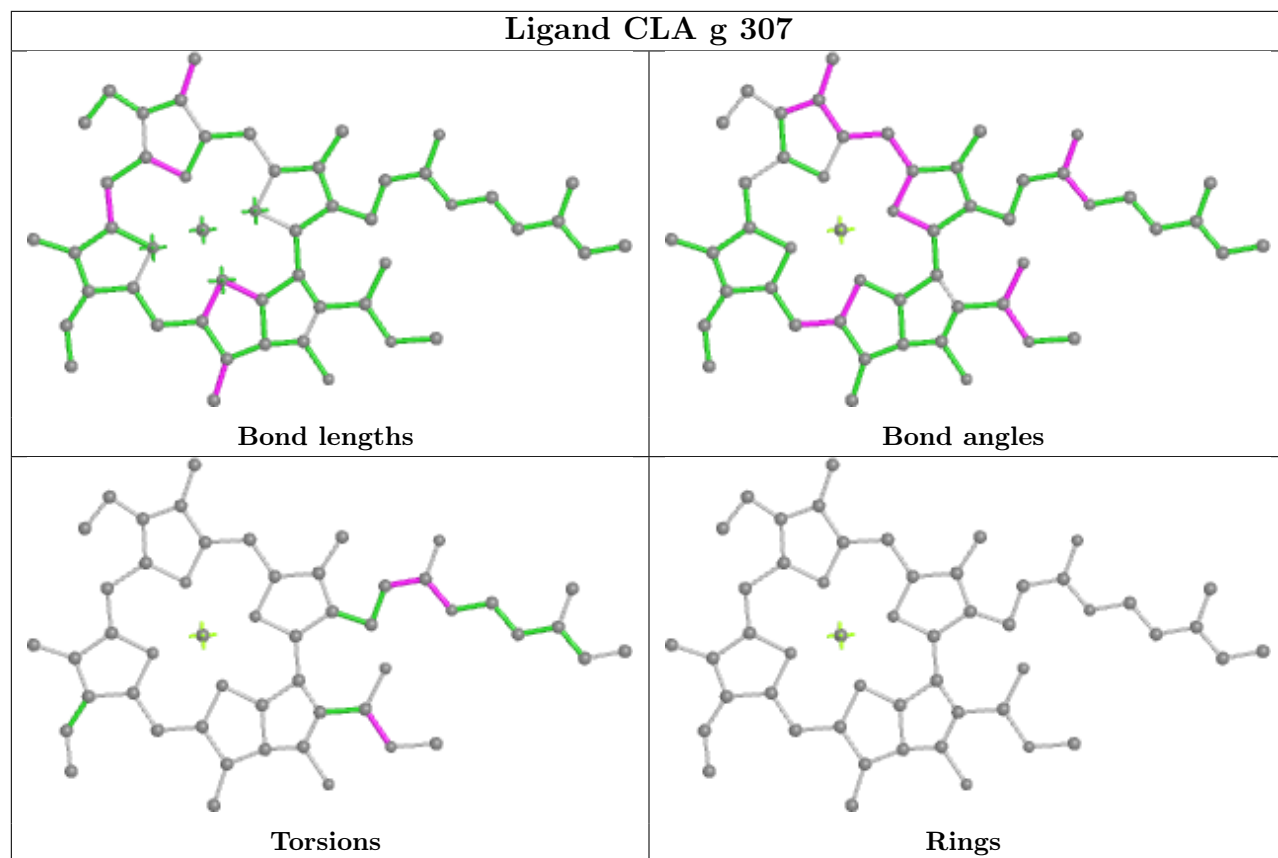


Ligand CLA A 854

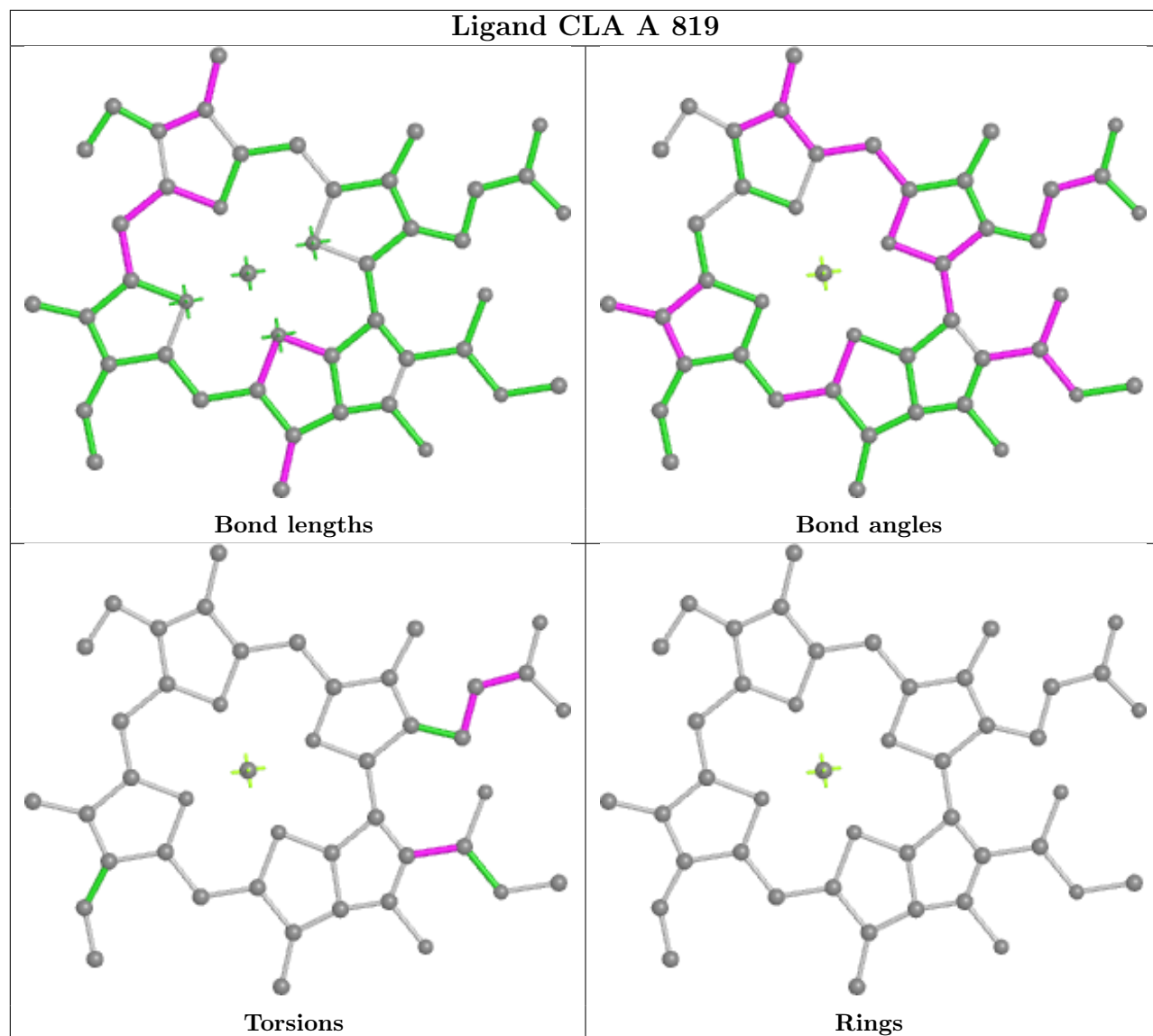


Ligand CLA c 607

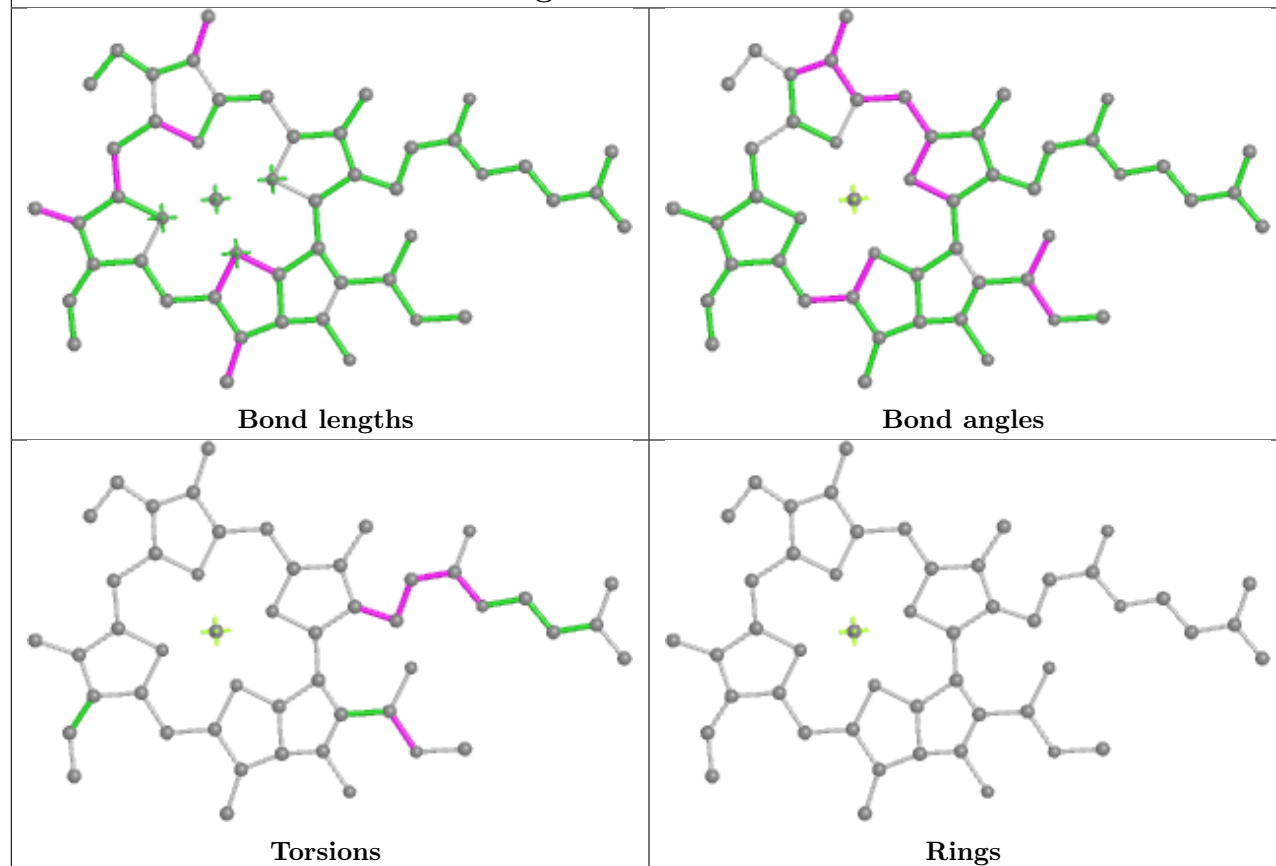




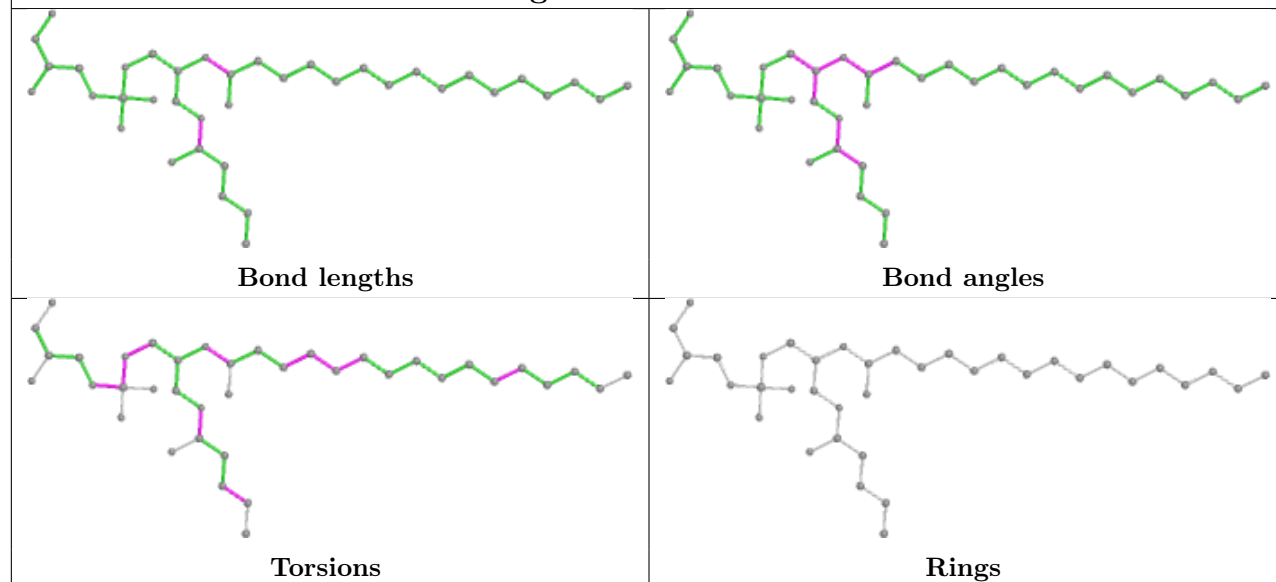
Ligand CLA A 819

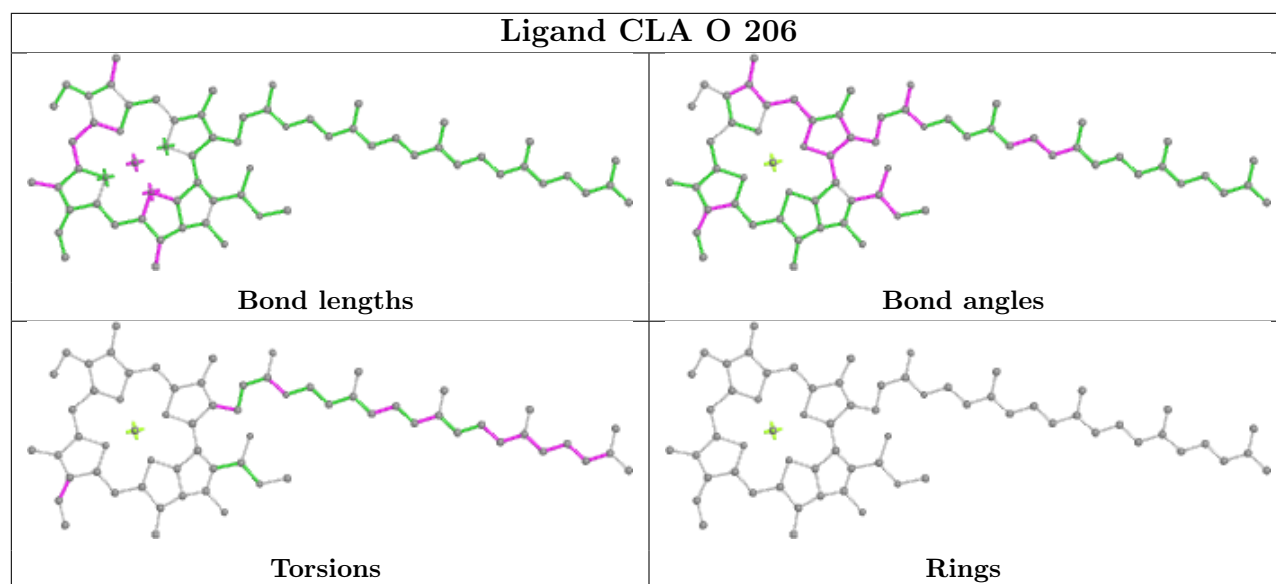
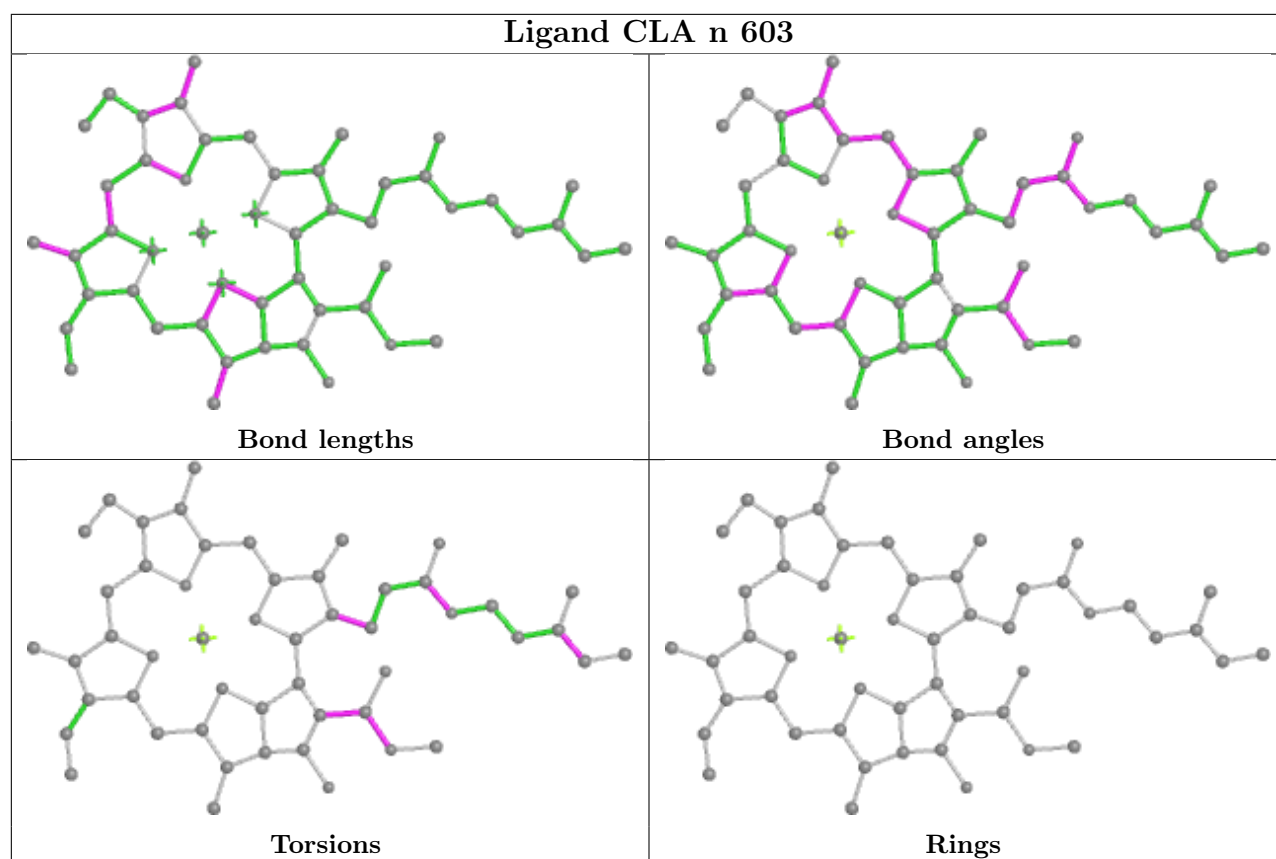


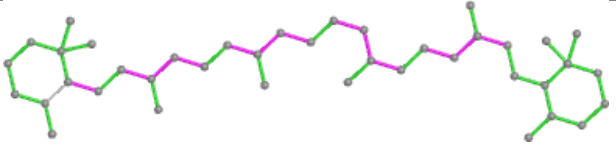
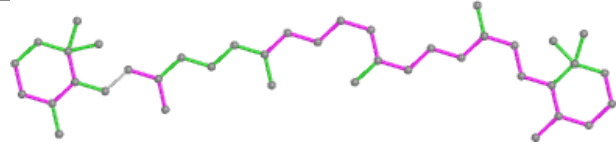
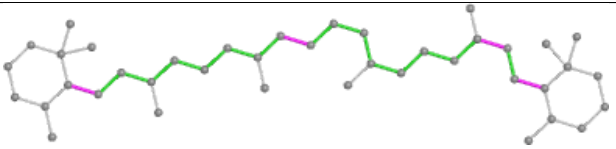
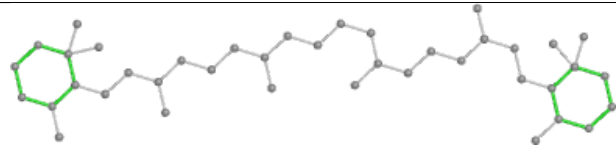
Ligand CLA h 302

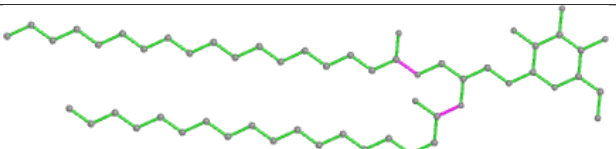
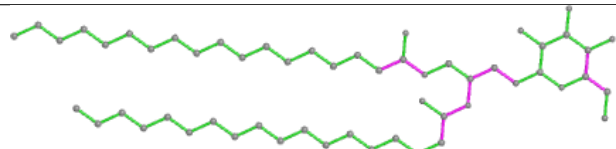
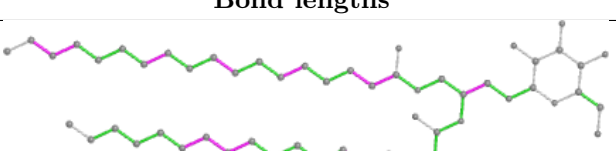
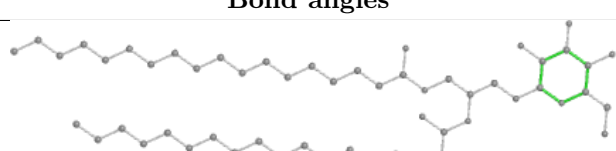


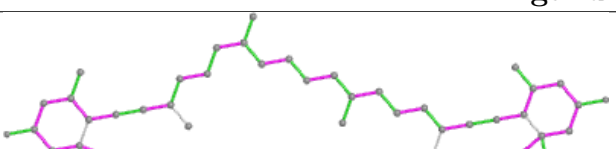
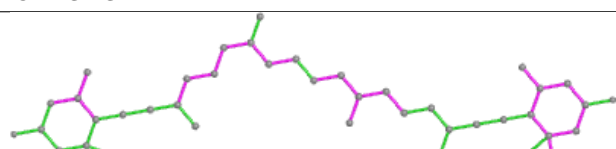
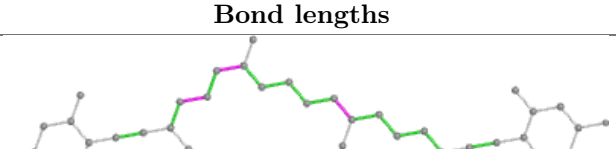
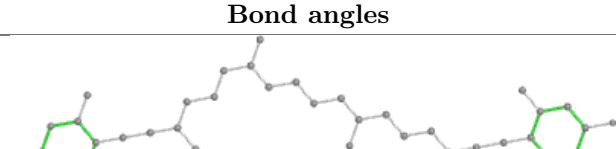
Ligand LHG A 849



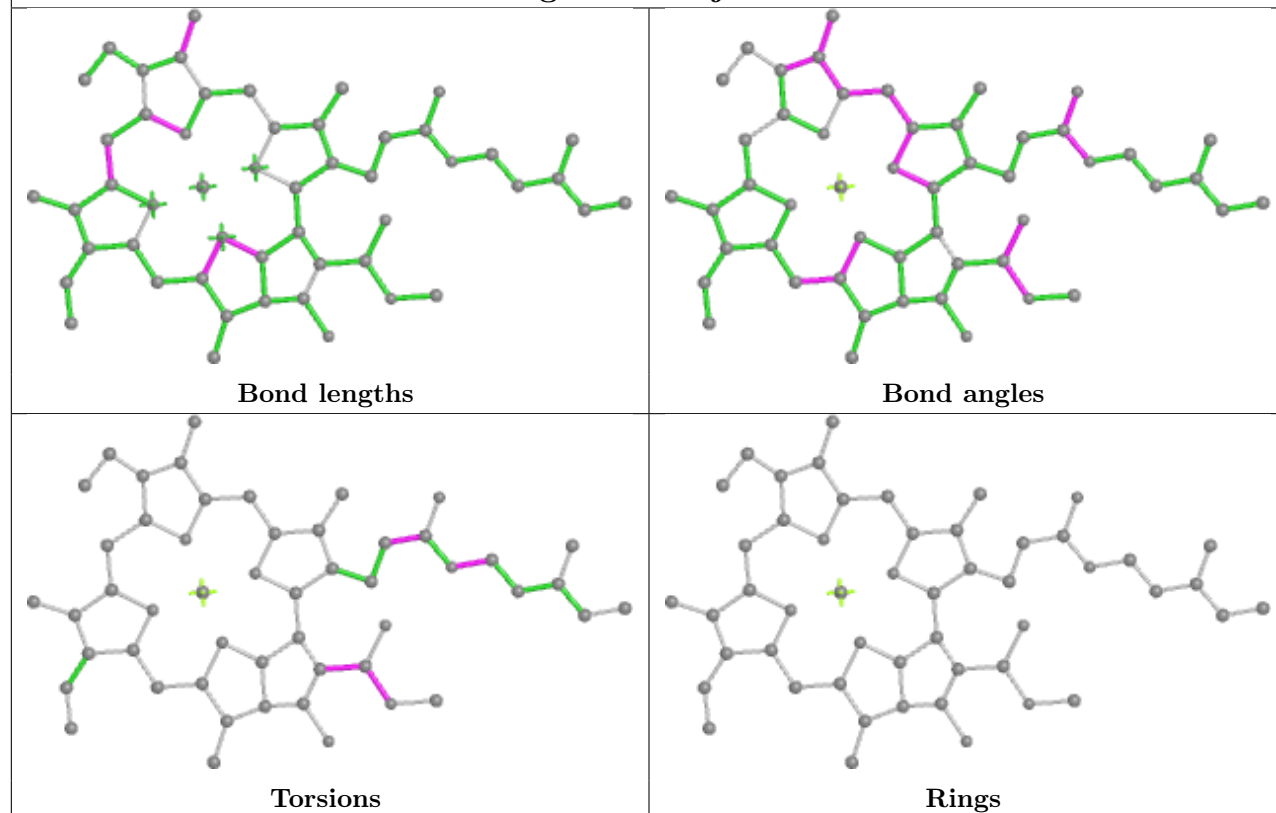


Ligand WVN A 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

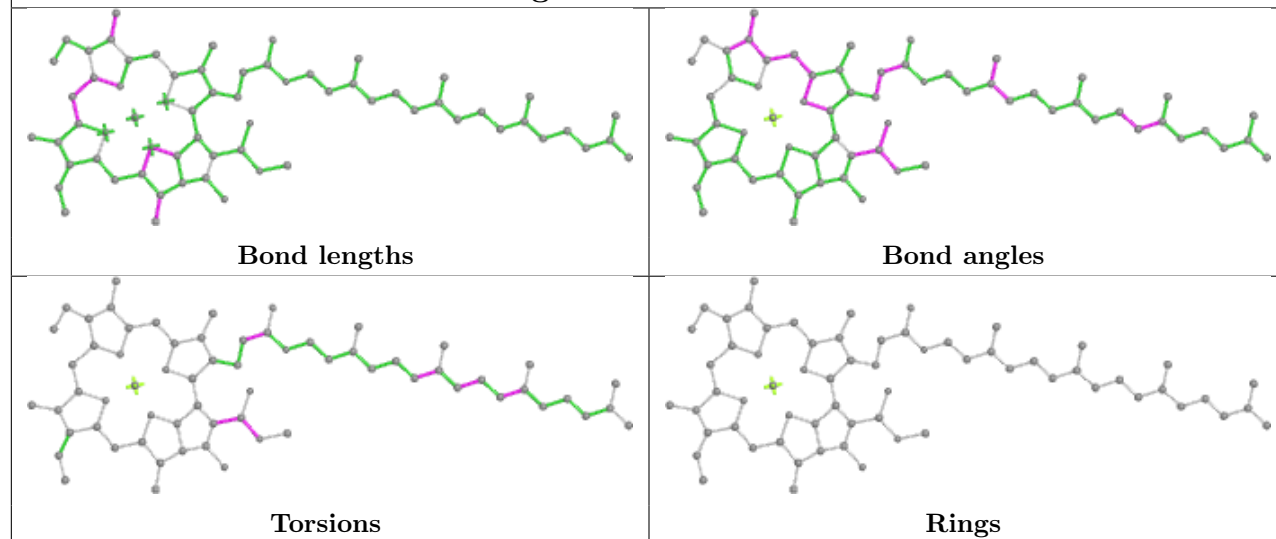
Ligand LMG J 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 I 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

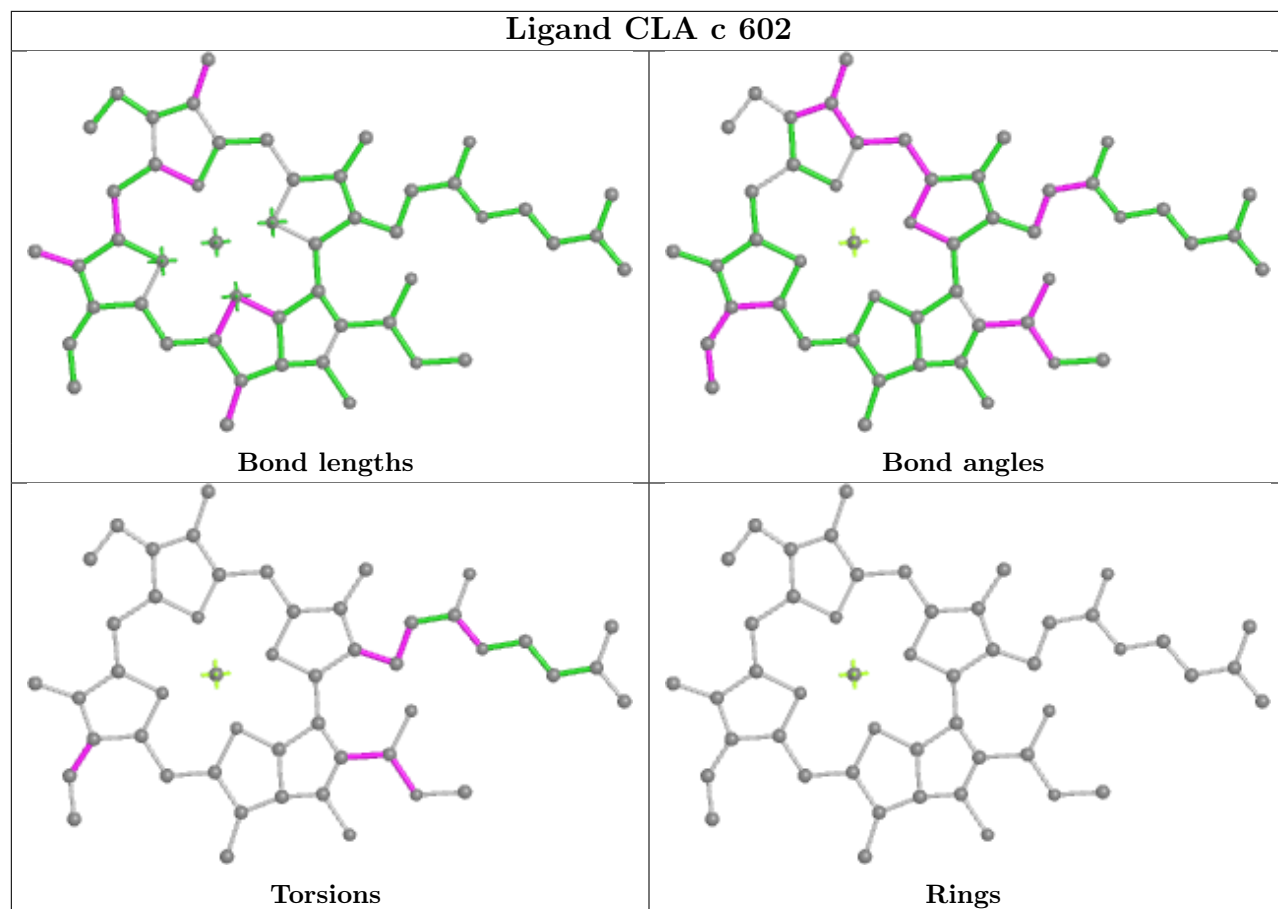
Ligand CLA j 603



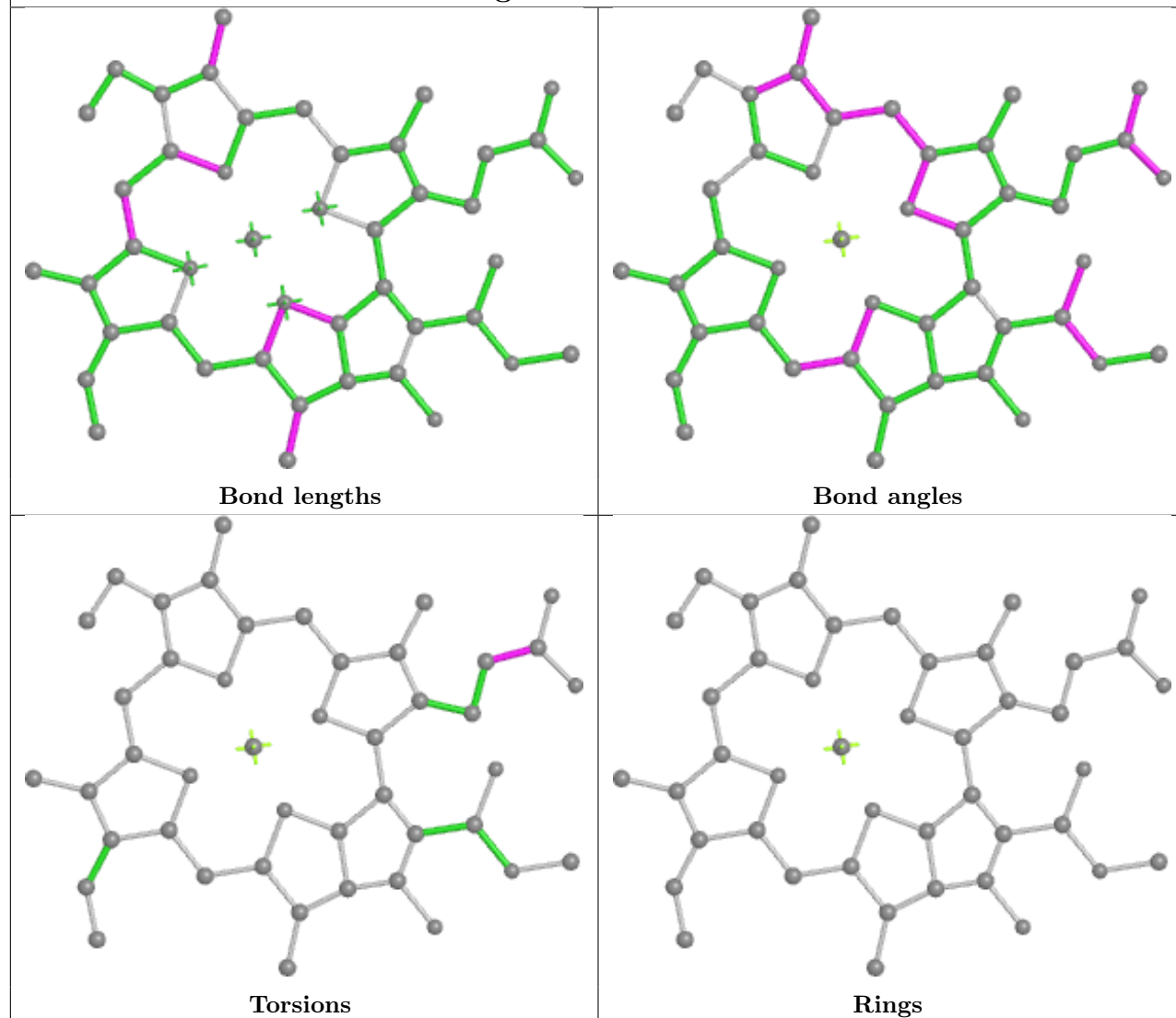
Ligand CLA A 836



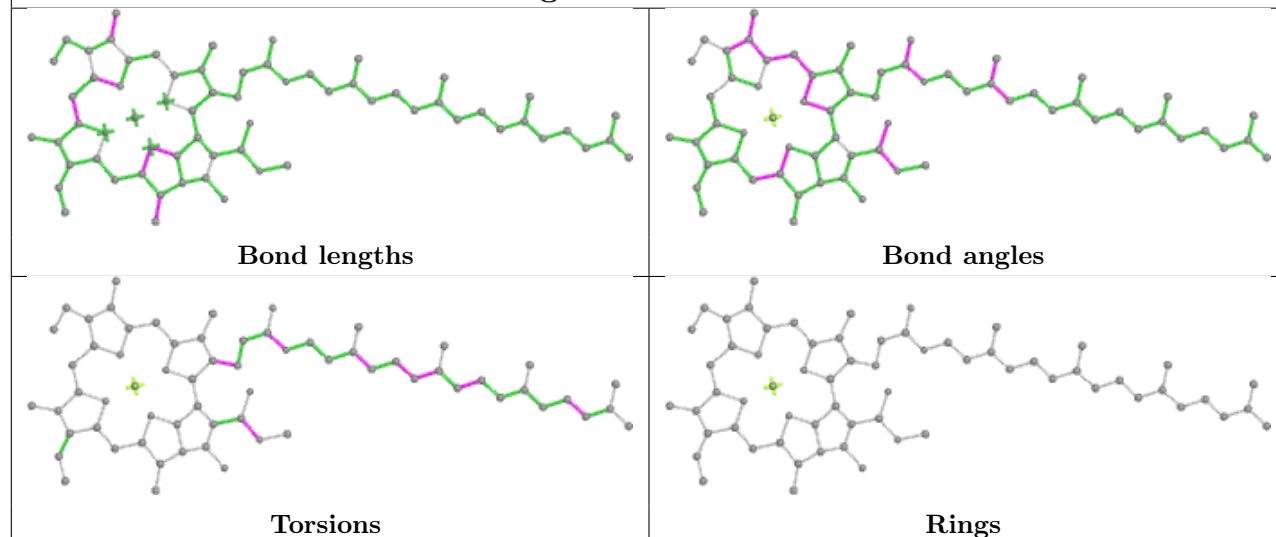
Ligand CLA c 602



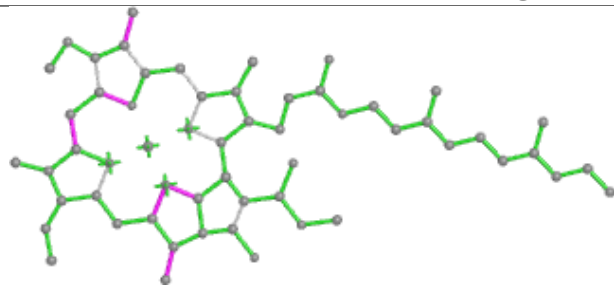
Ligand CLA c 609



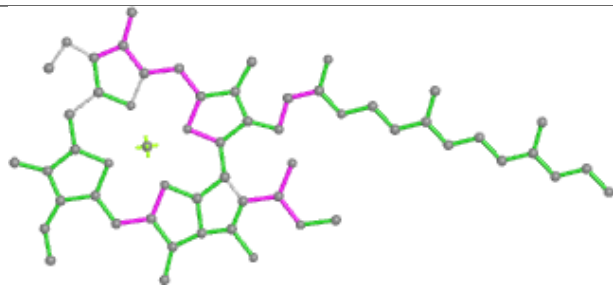
Ligand CLA l 311



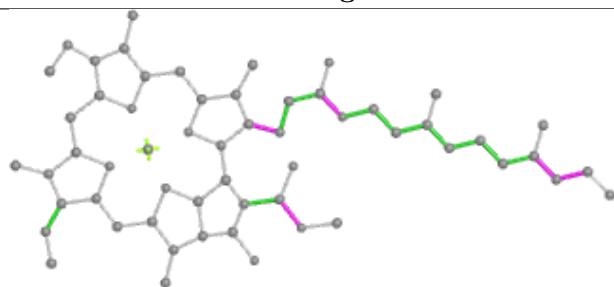
Ligand CLA B 816



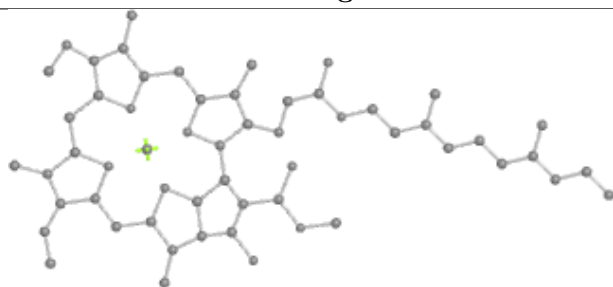
Bond lengths



Bond angles

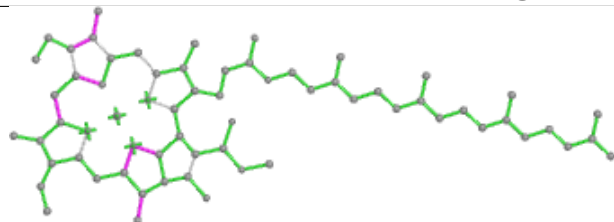


Torsions

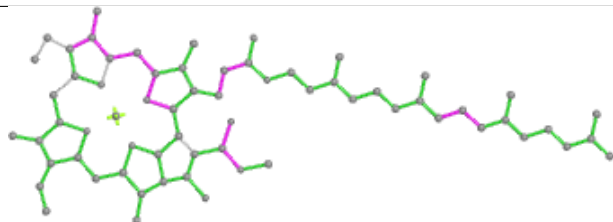


Rings

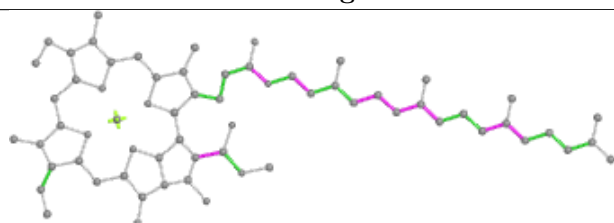
Ligand CLA A 838



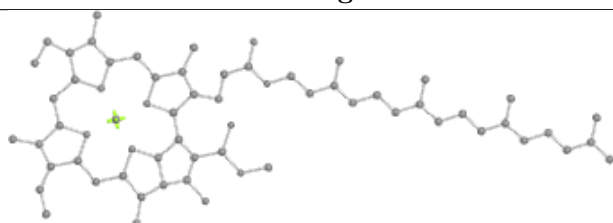
Bond lengths



Bond angles

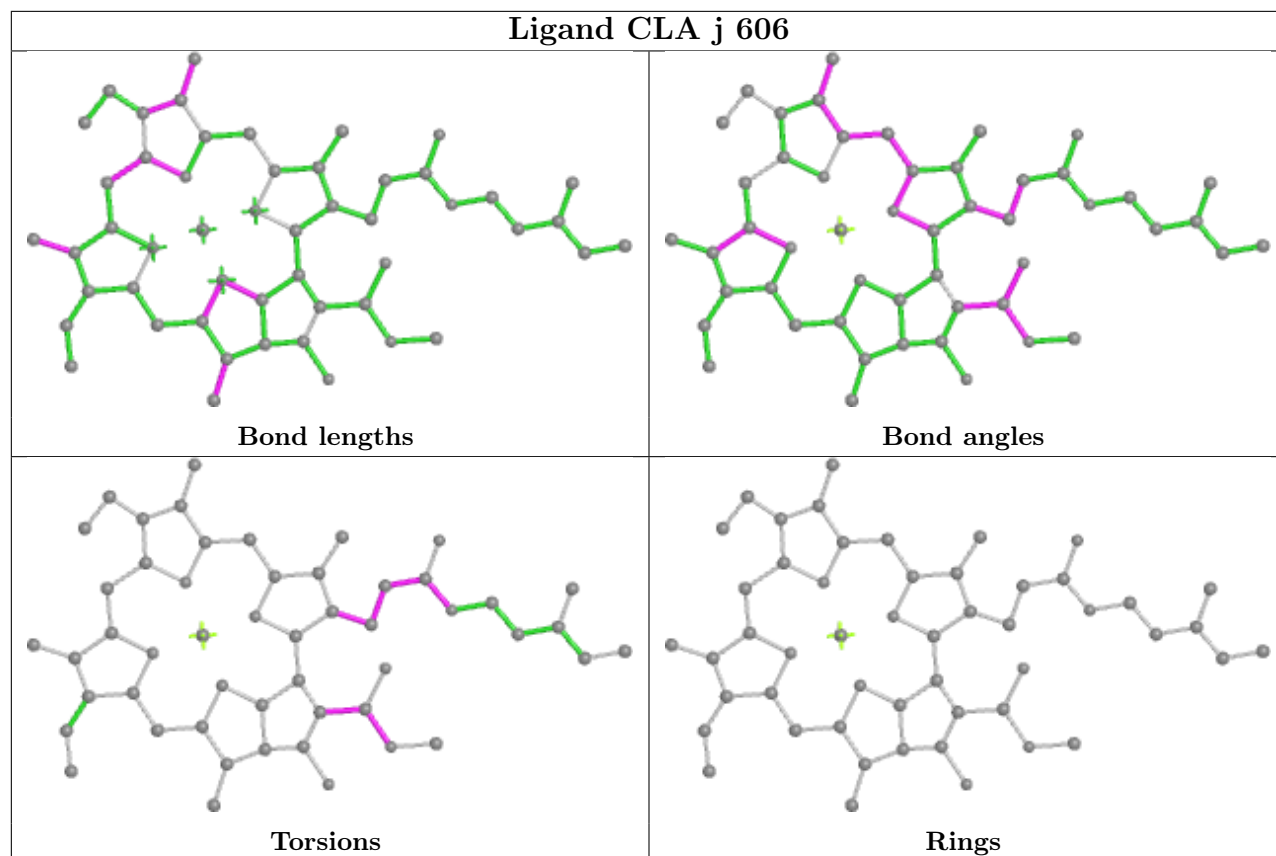


Torsions

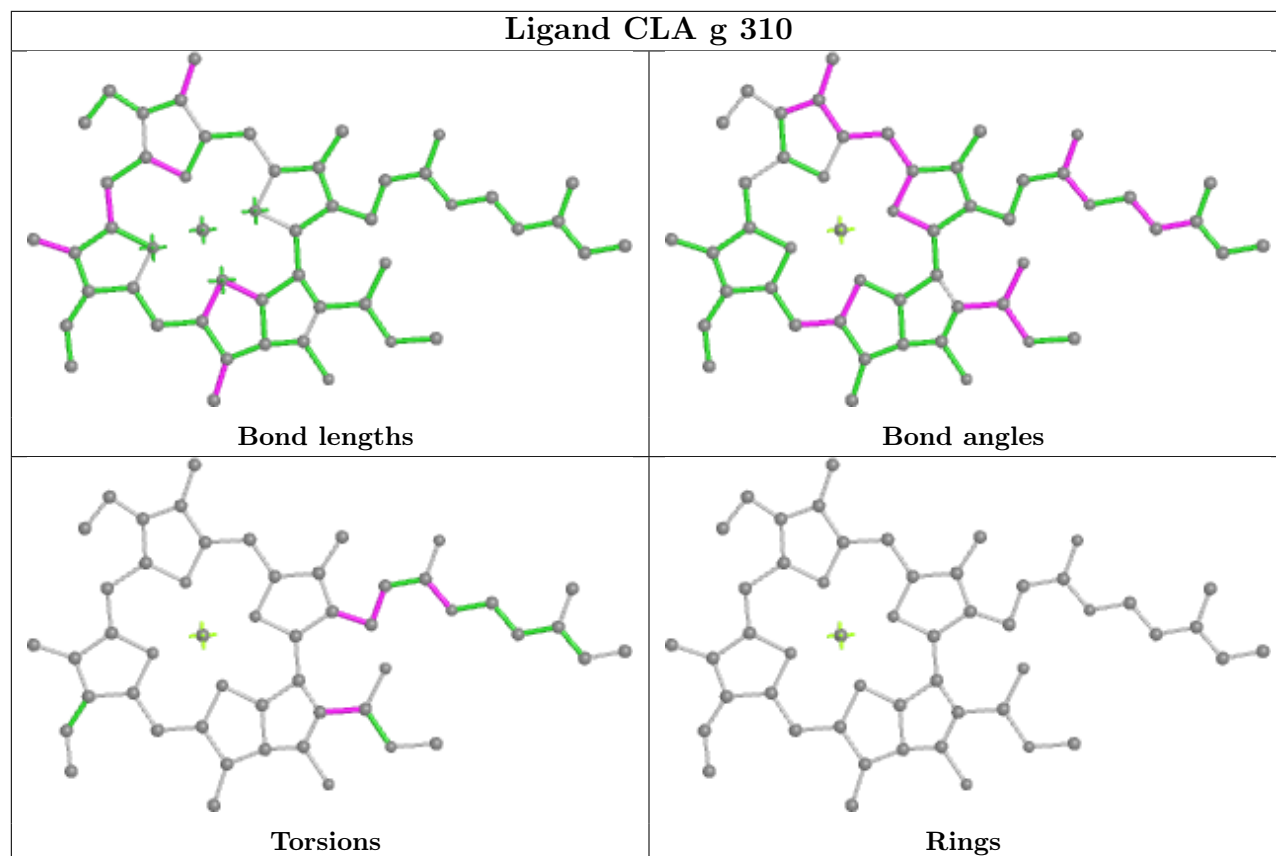


Rings

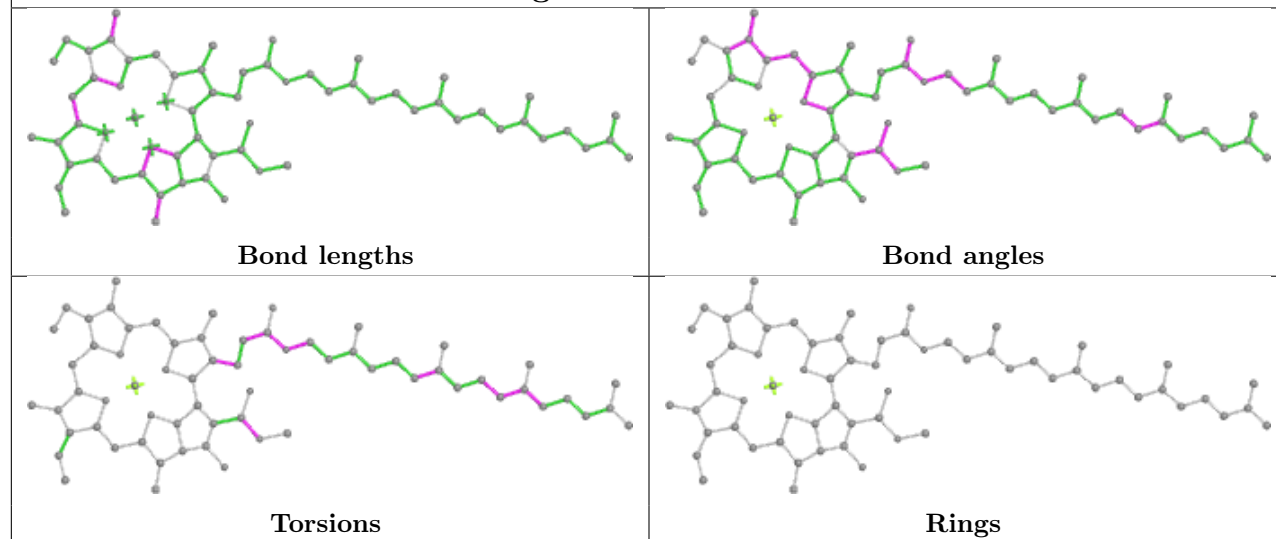
Ligand CLA j 606



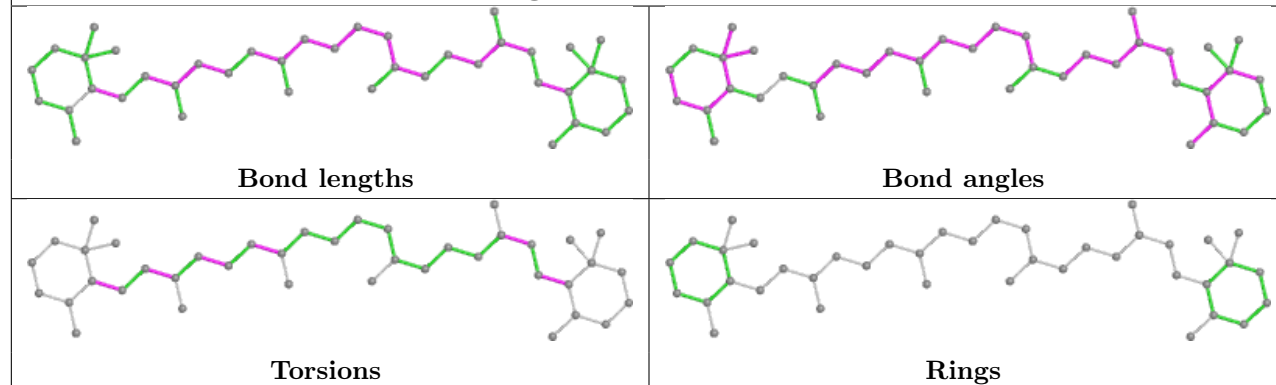
Ligand CLA g 310



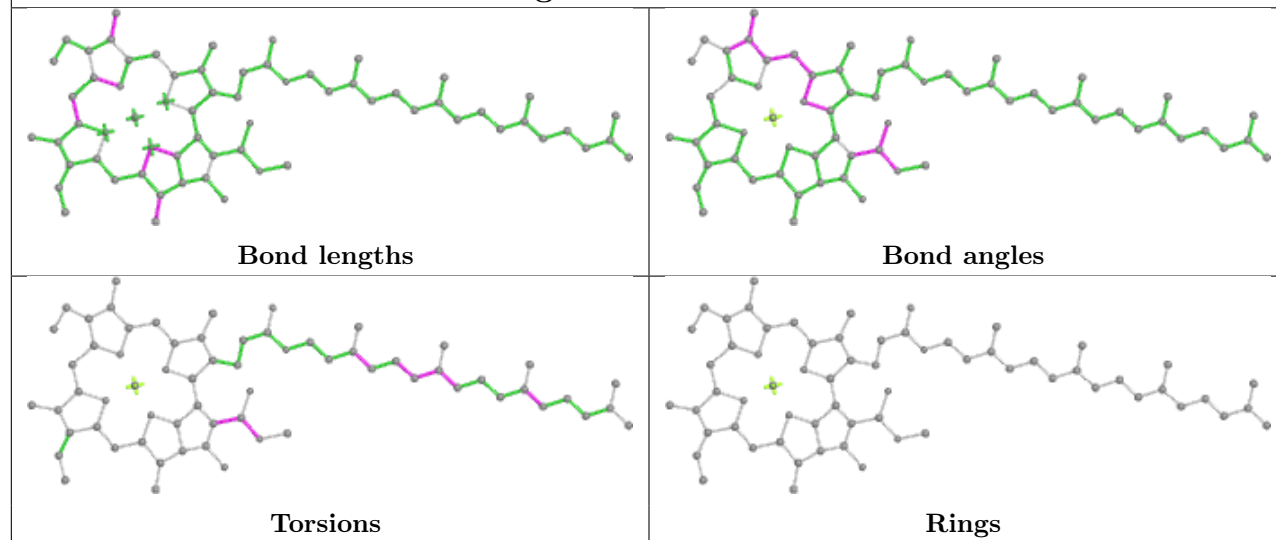
Ligand CLA B 804



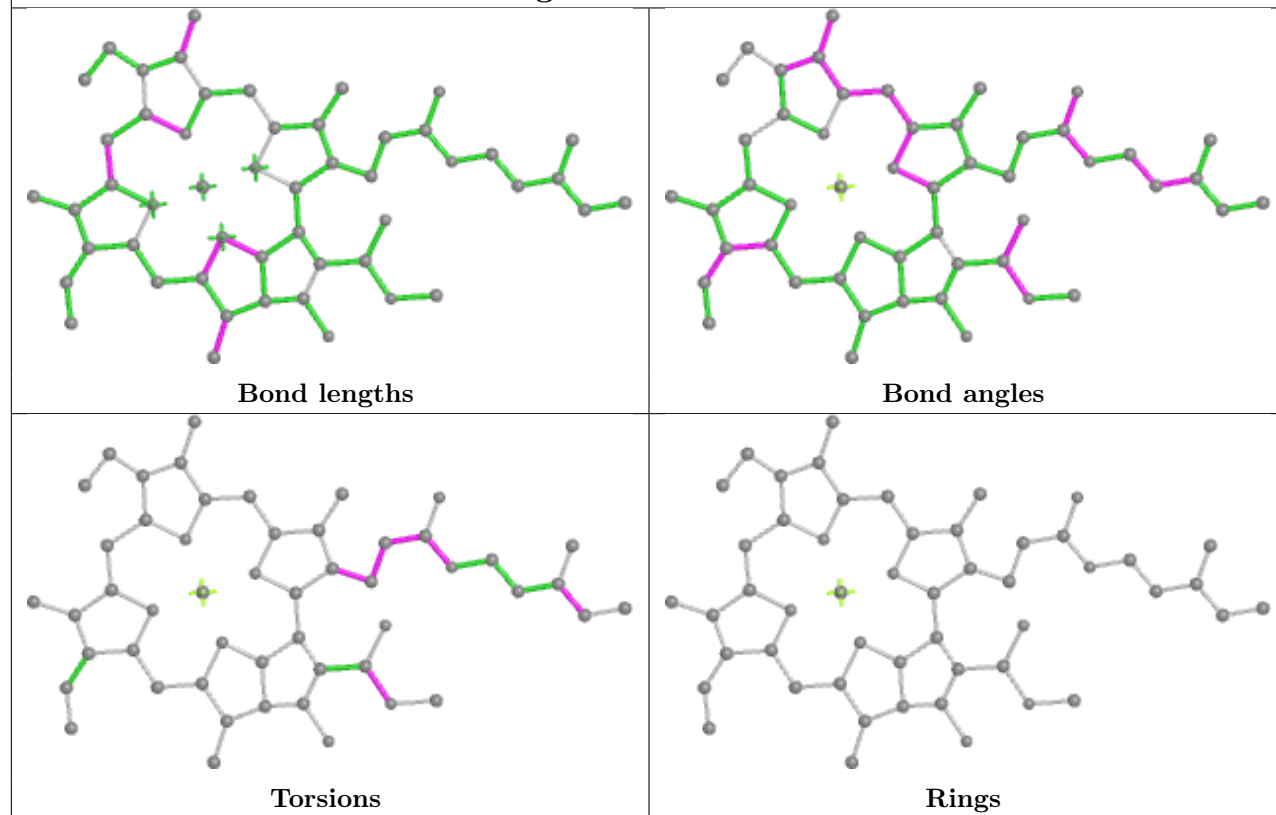
Ligand WVN L 201



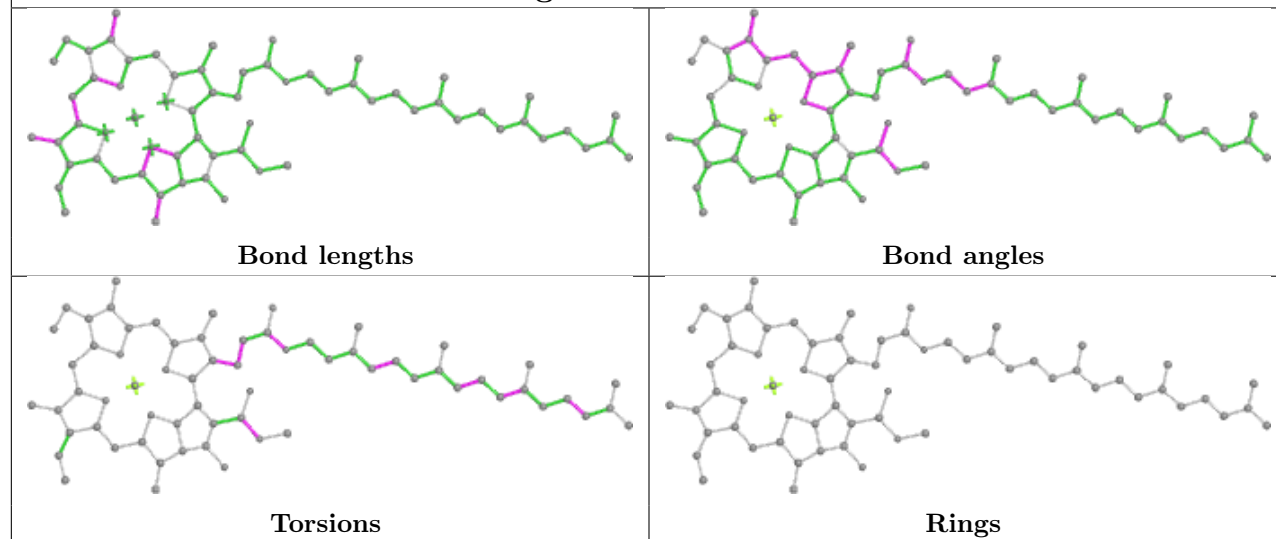
Ligand CLA h 313



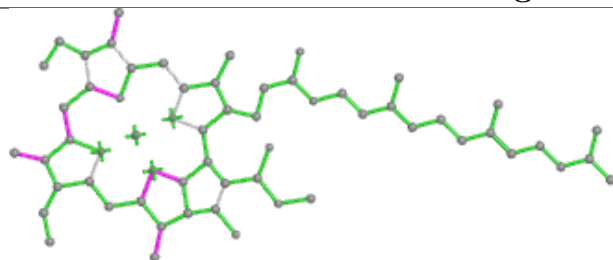
Ligand CLA k 601



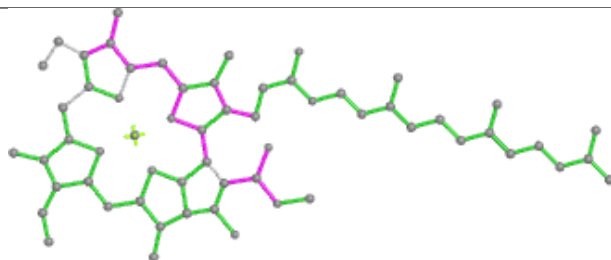
Ligand CLA k 609



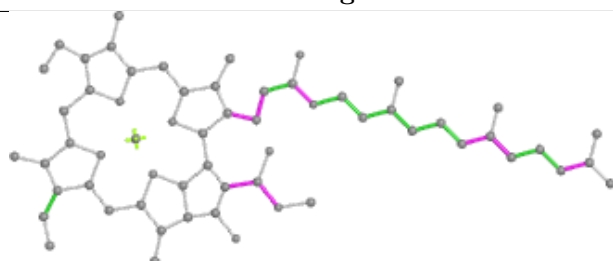
Ligand CLA B 812



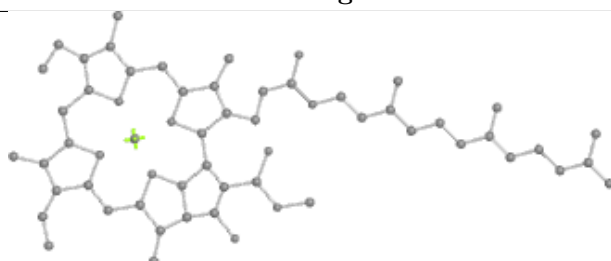
Bond lengths



Bond angles

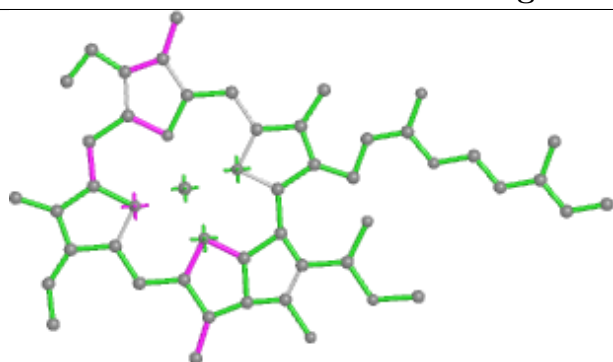


Torsions

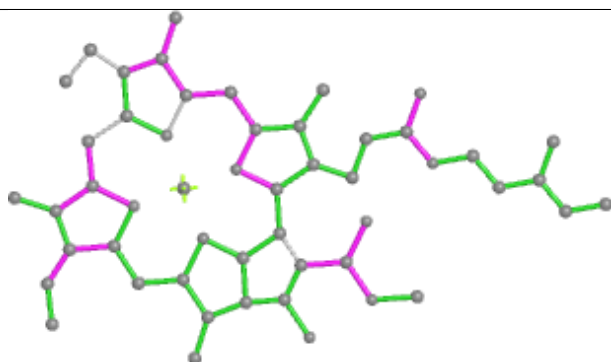


Rings

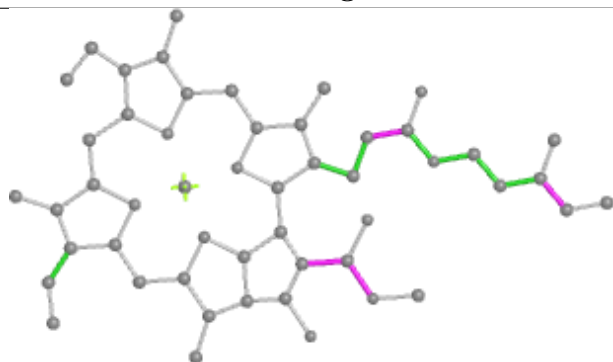
Ligand CLA d 305



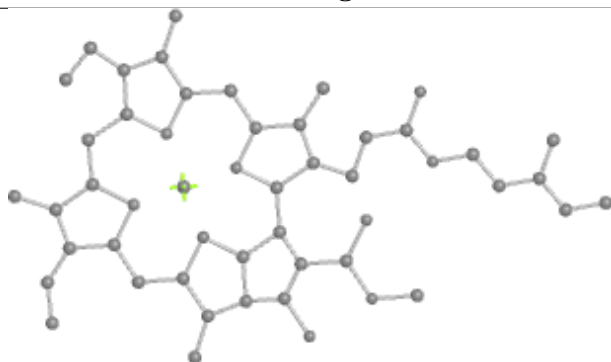
Bond lengths



Bond angles

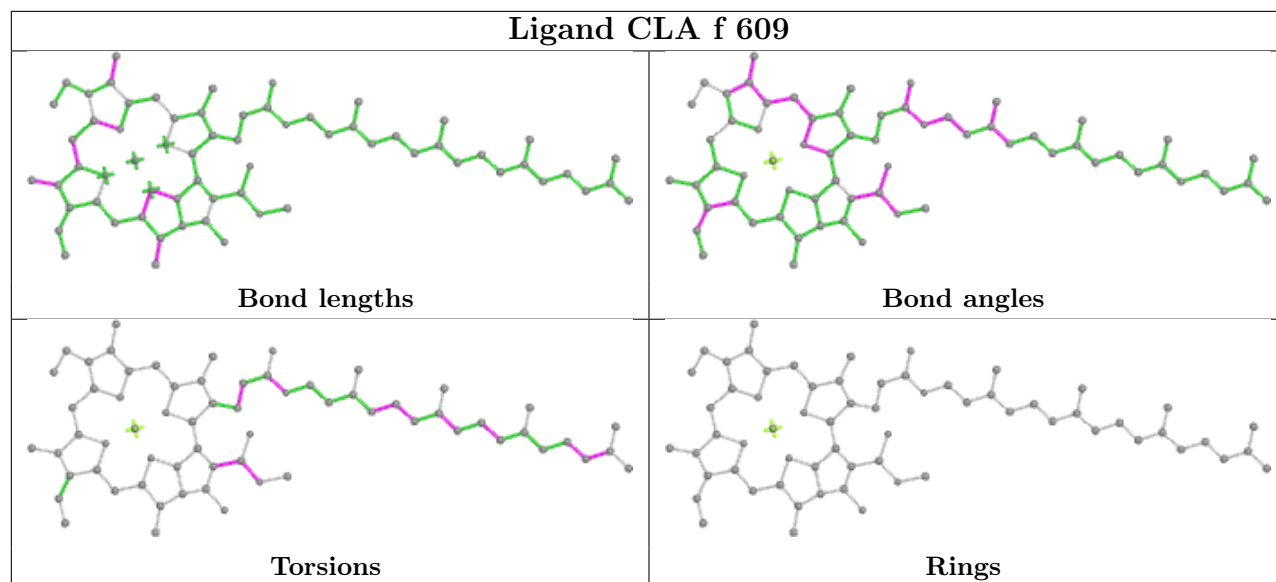


Torsions

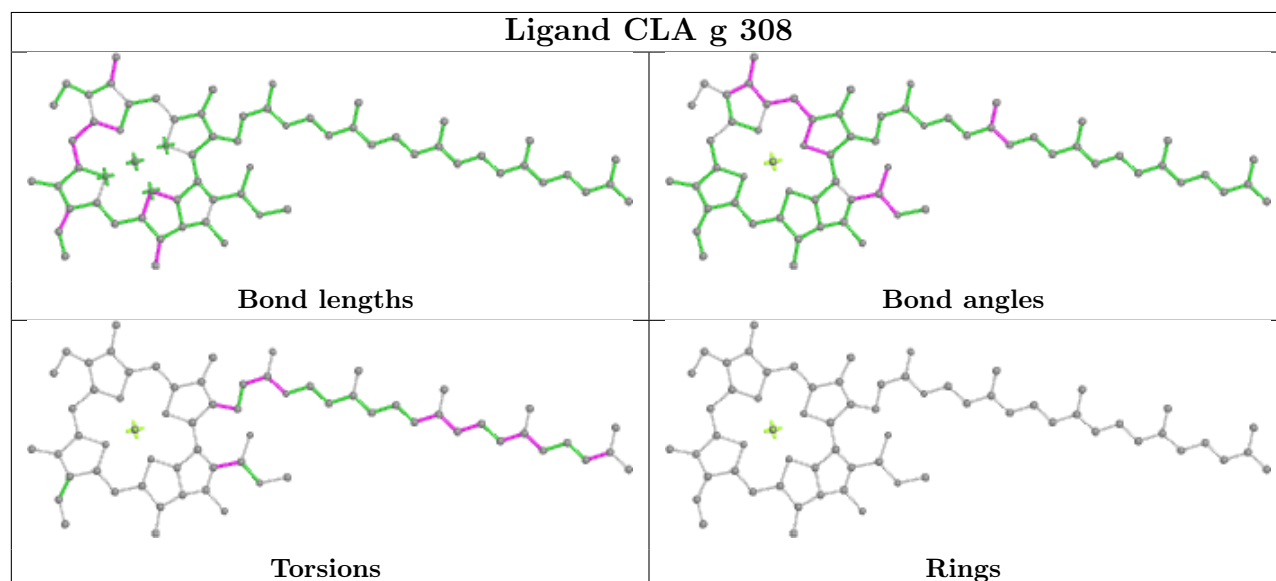


Rings

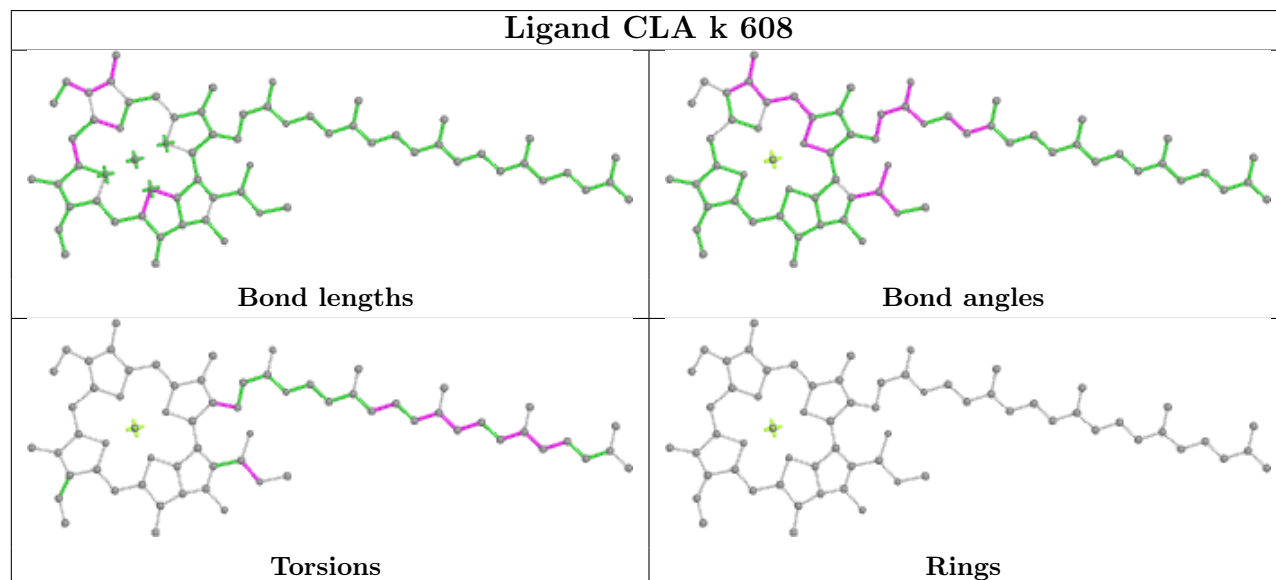
Ligand CLA f 609

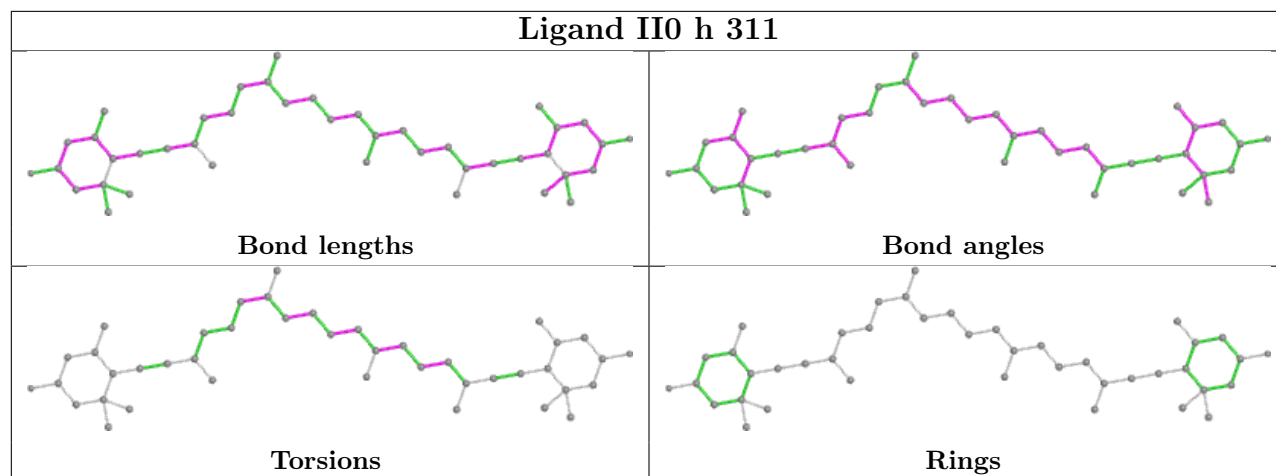
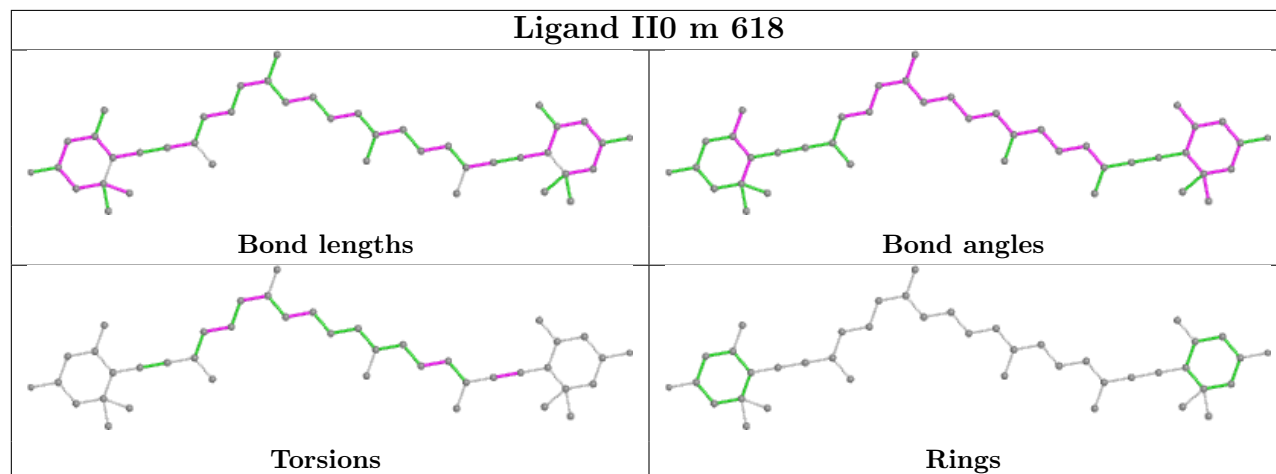
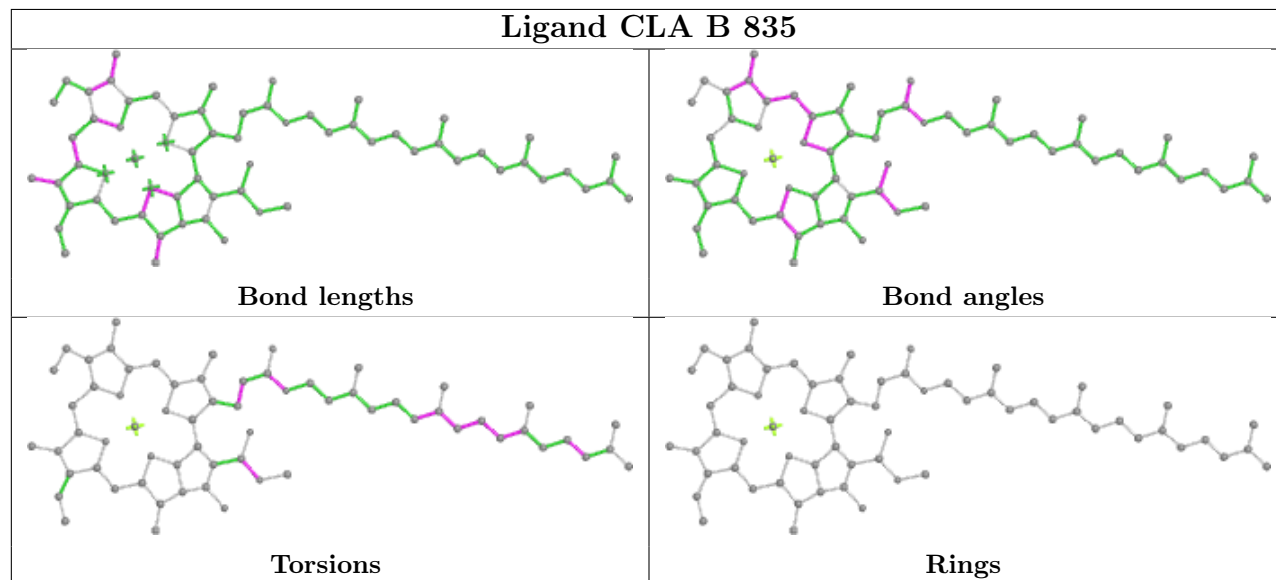


Ligand CLA g 308

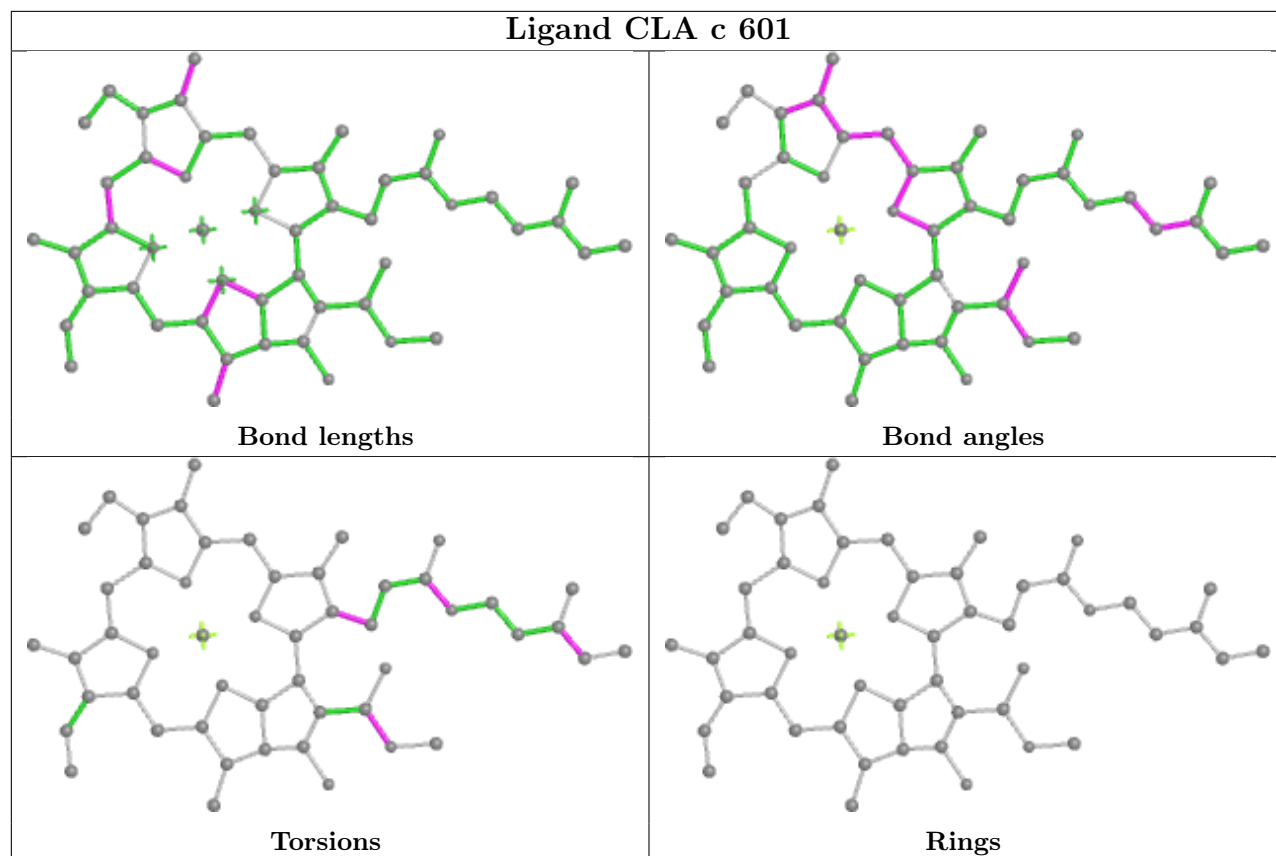


Ligand CLA k 608

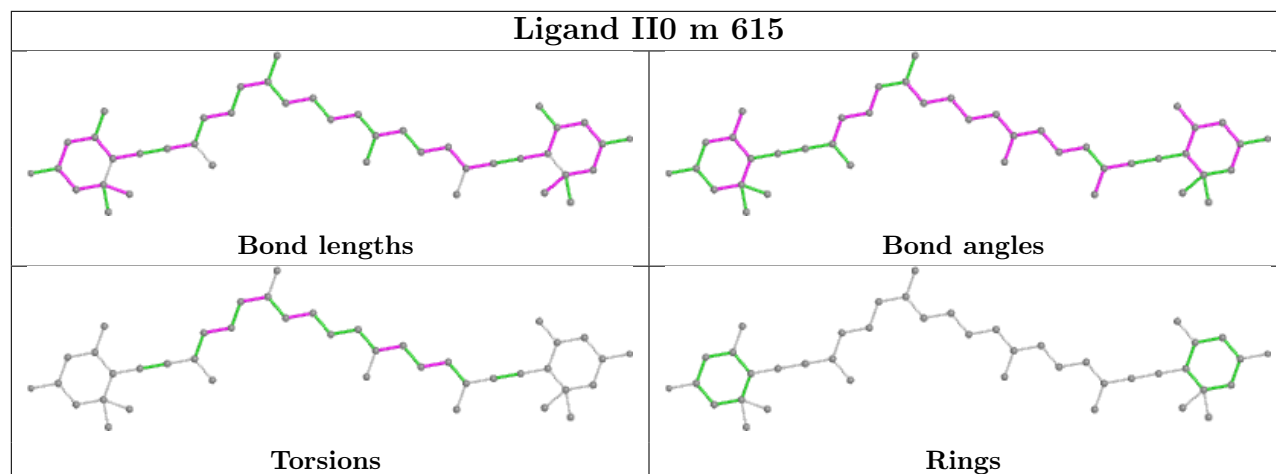


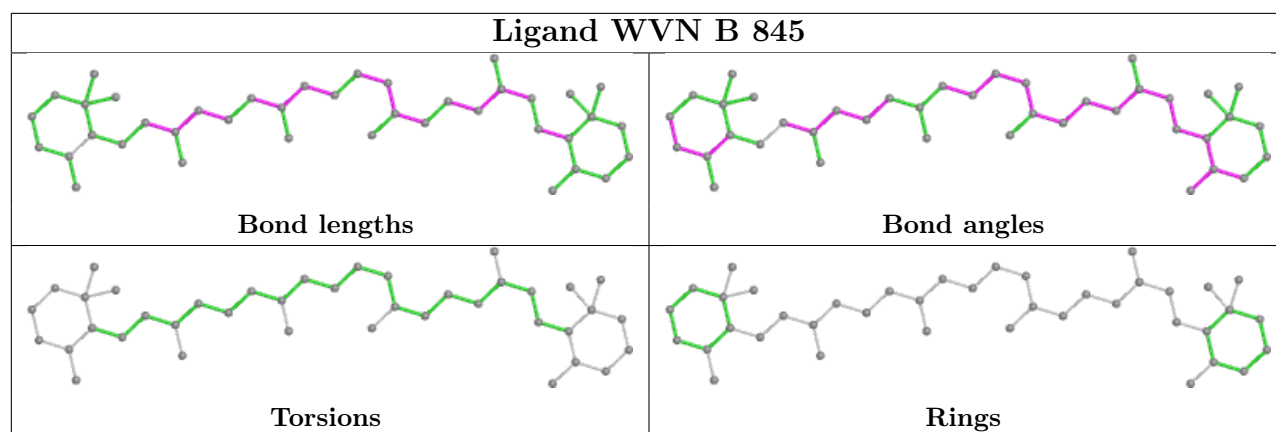
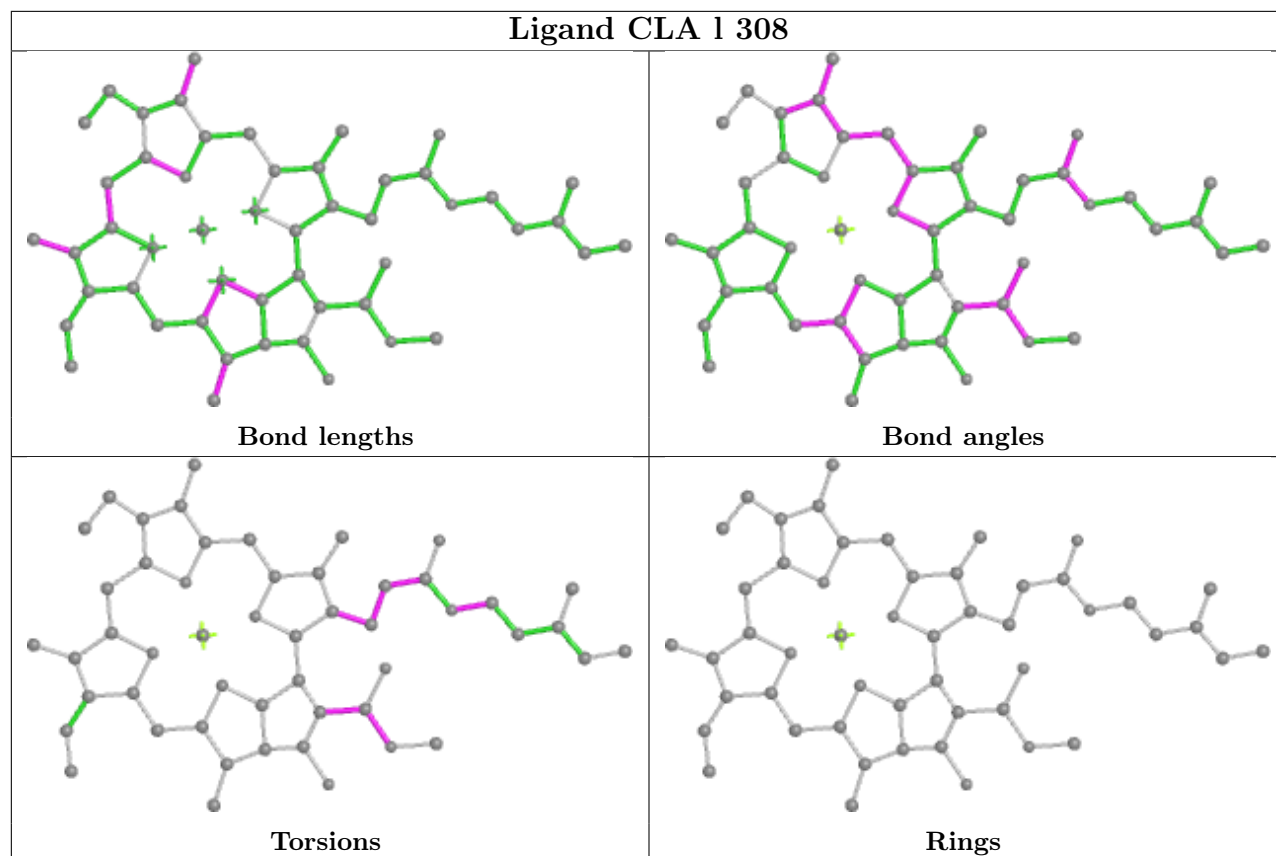
Ligand II0 h 311**Ligand II0 m 618****Ligand CLA B 835**

Ligand CLA c 601

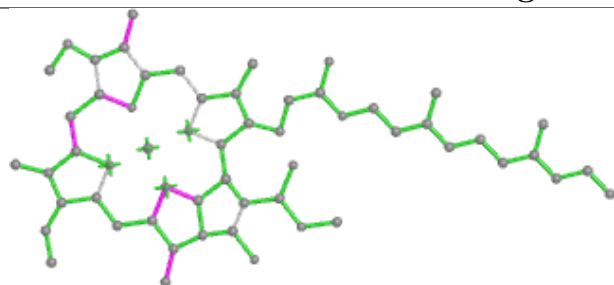


Ligand II0 m 615

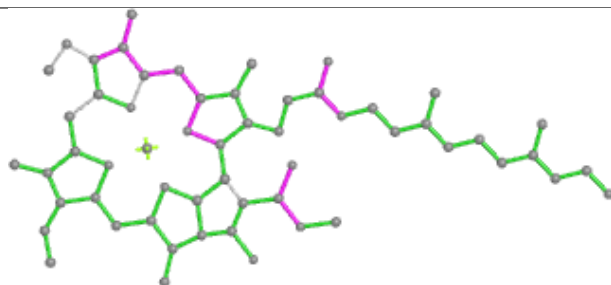




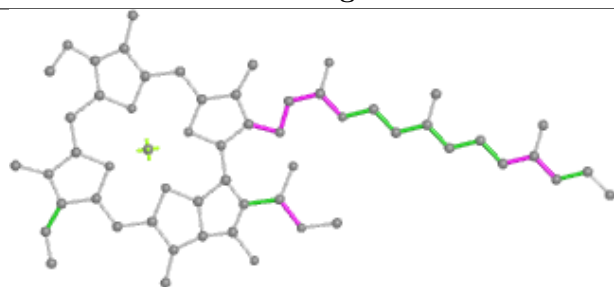
Ligand CLA h 307



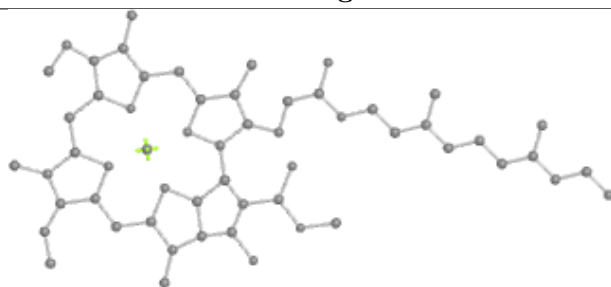
Bond lengths



Bond angles

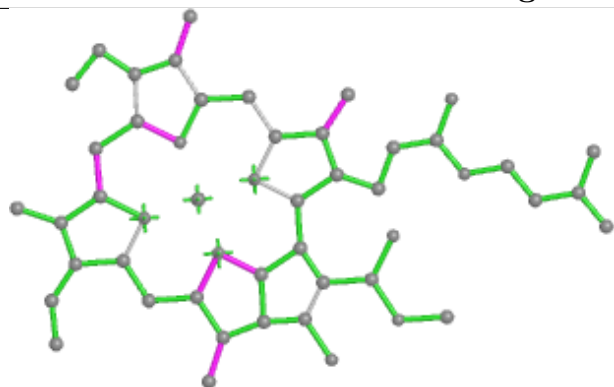


Torsions

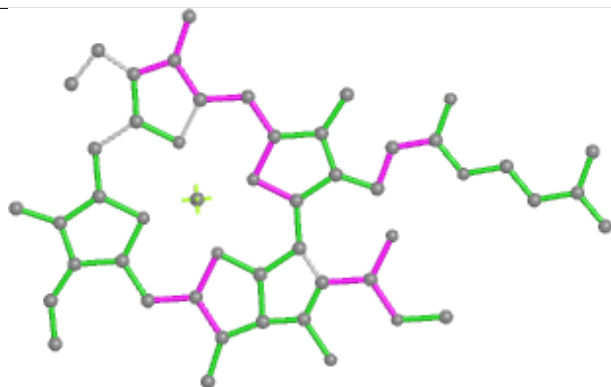


Rings

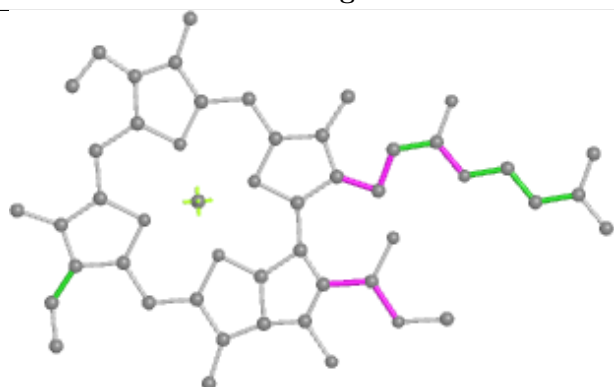
Ligand CLA a 304



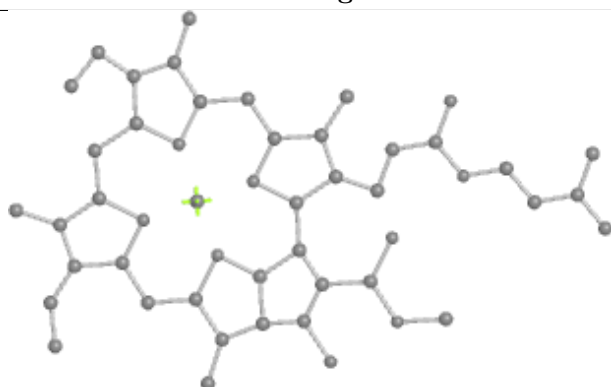
Bond lengths



Bond angles

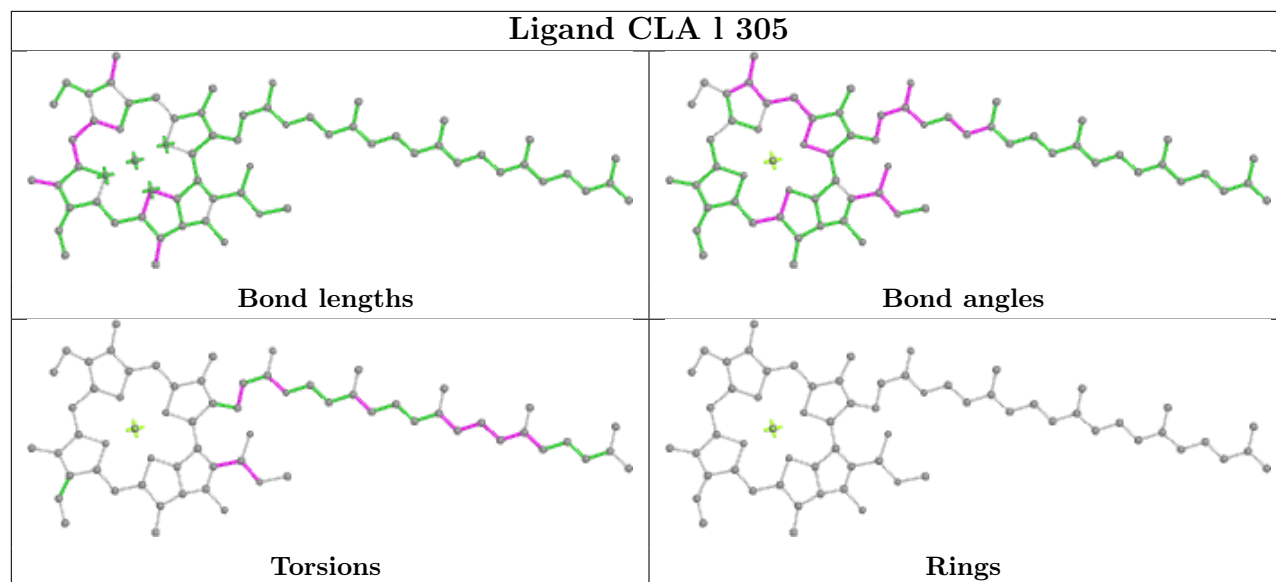


Torsions

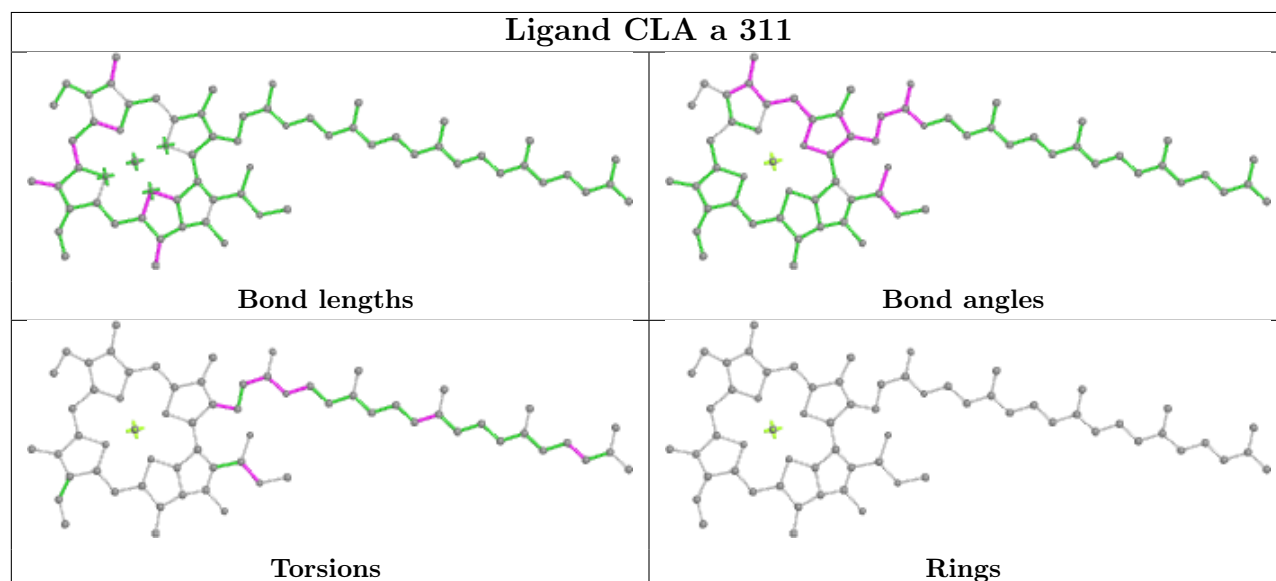


Rings

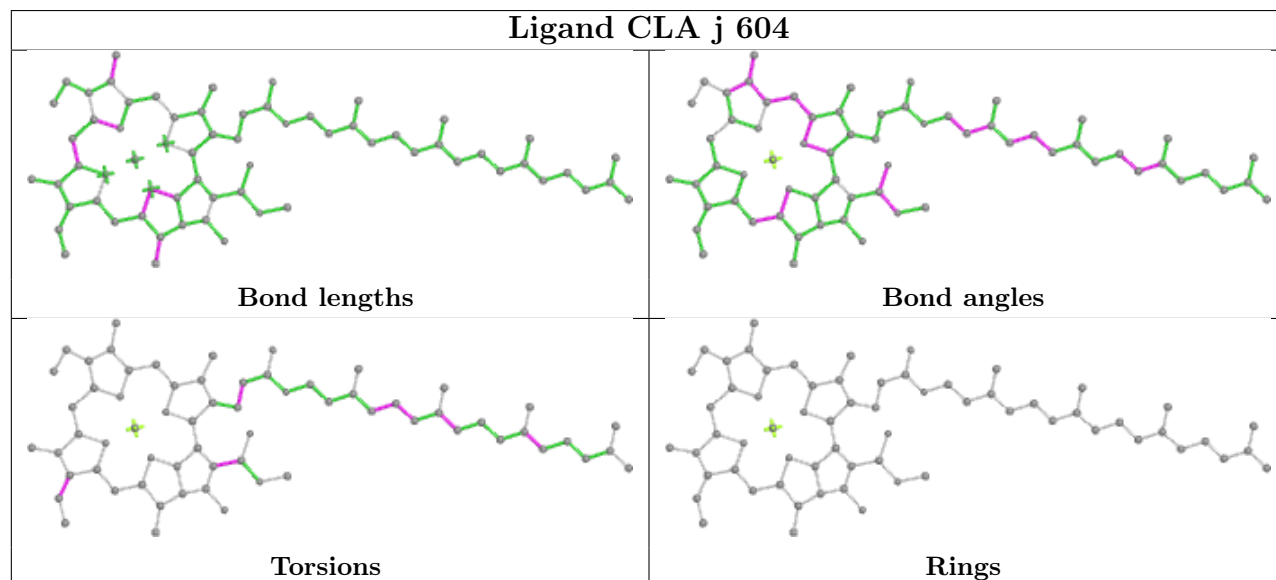
Ligand CLA l 305

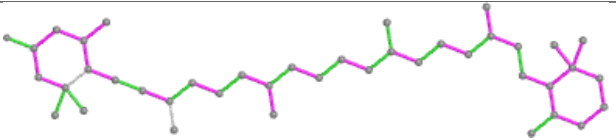
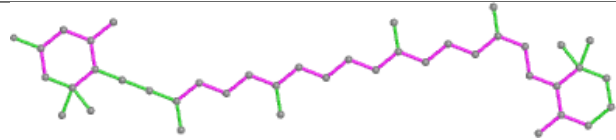
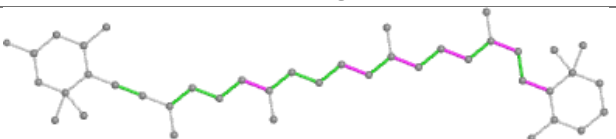



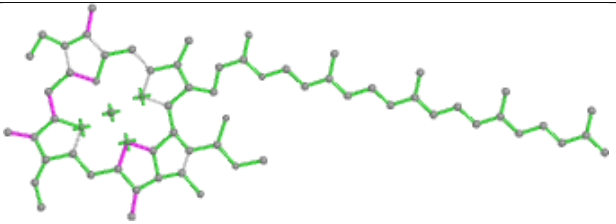
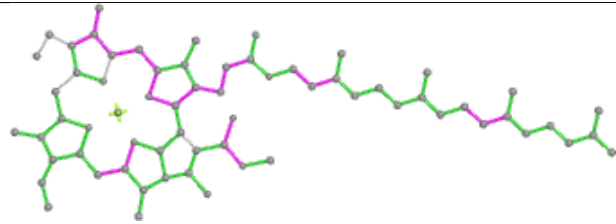
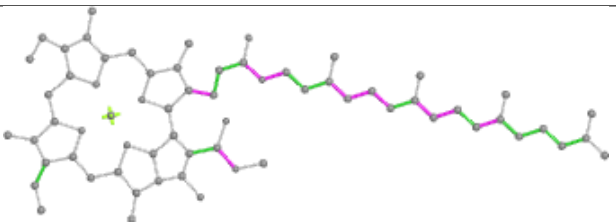
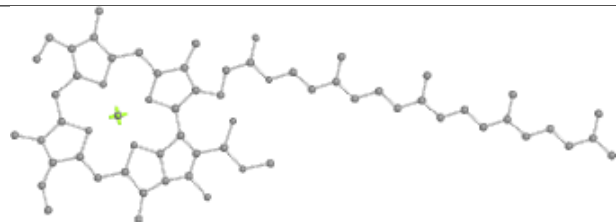
Ligand CLA a 311

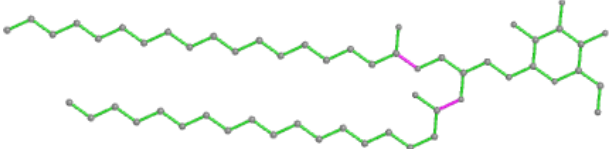
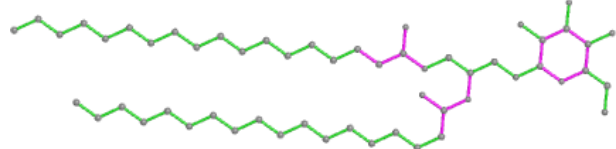
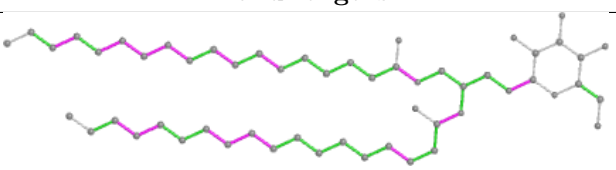



Ligand CLA j 604

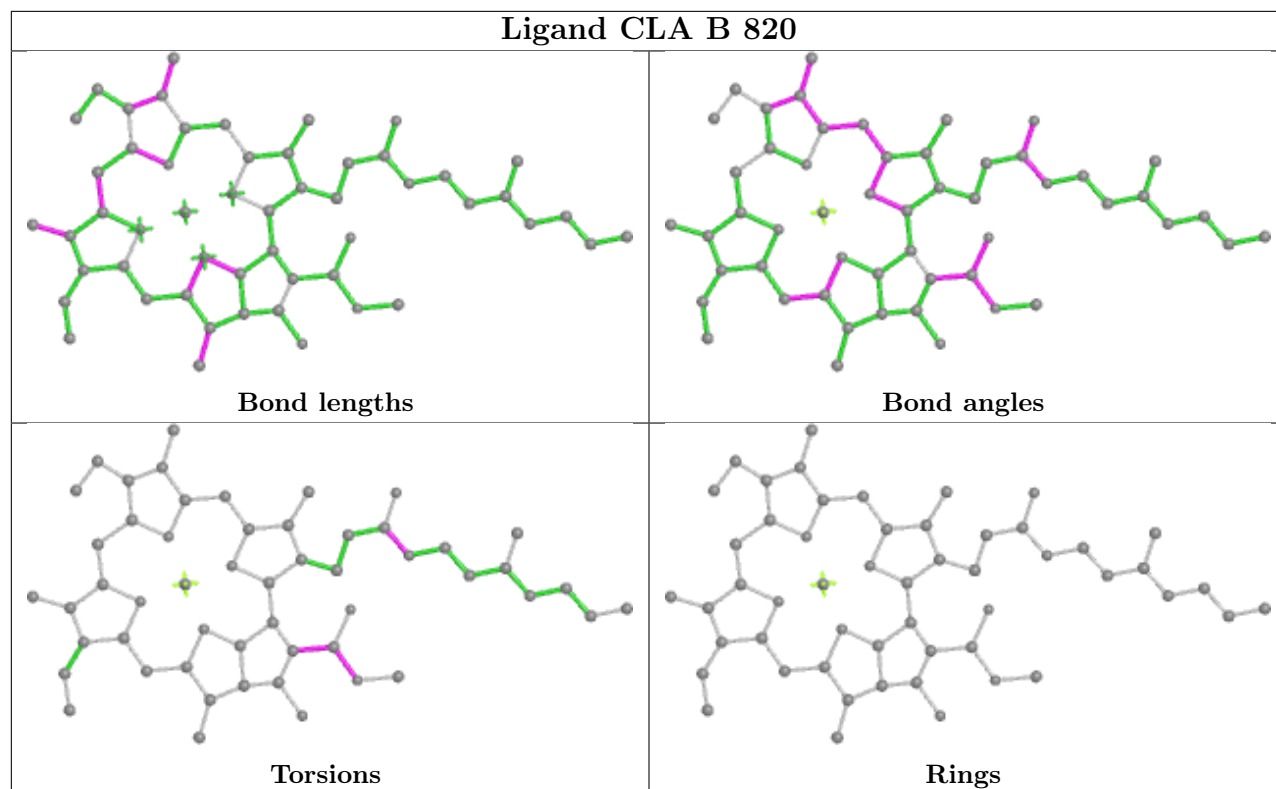


Ligand IHT m 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

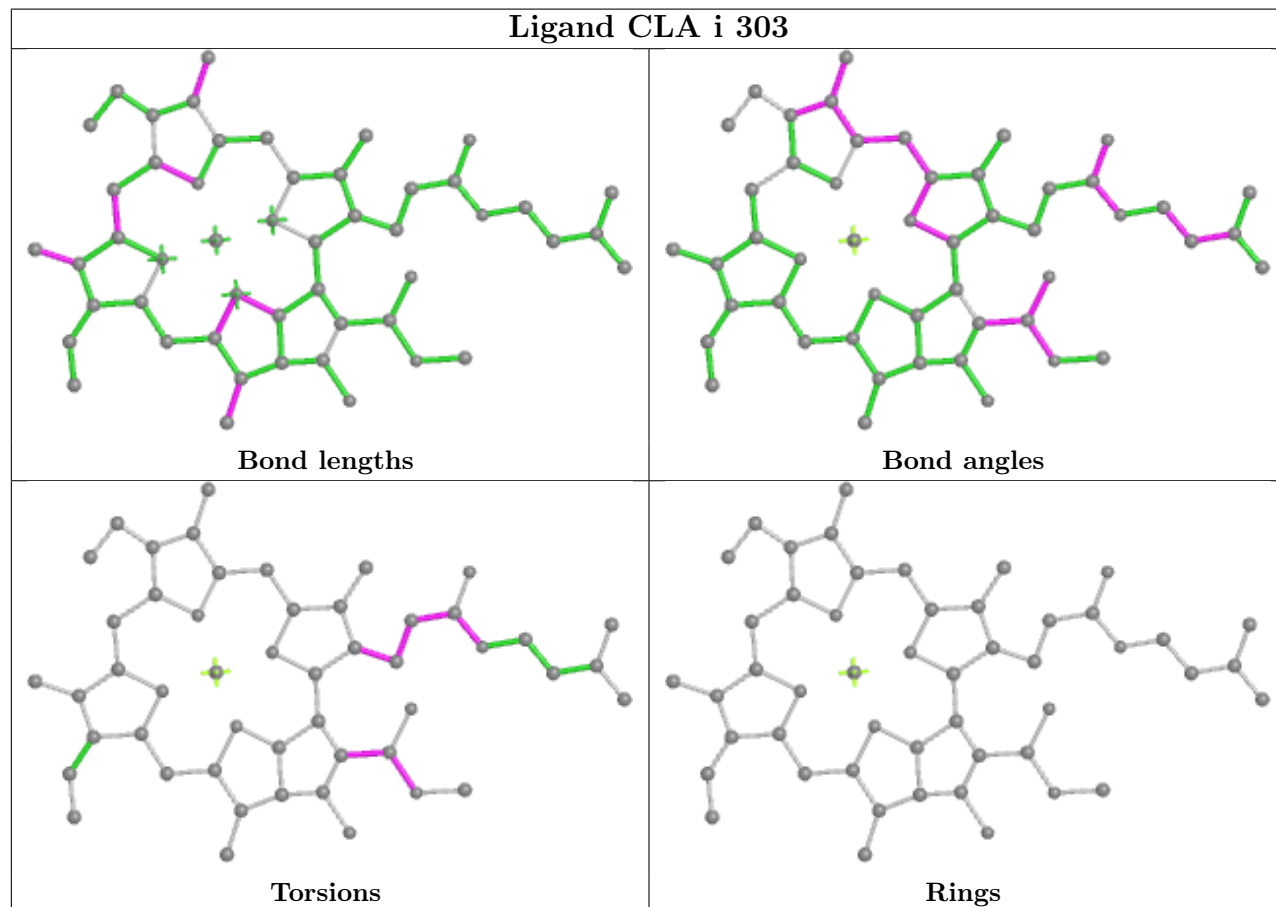
Ligand CLA A 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

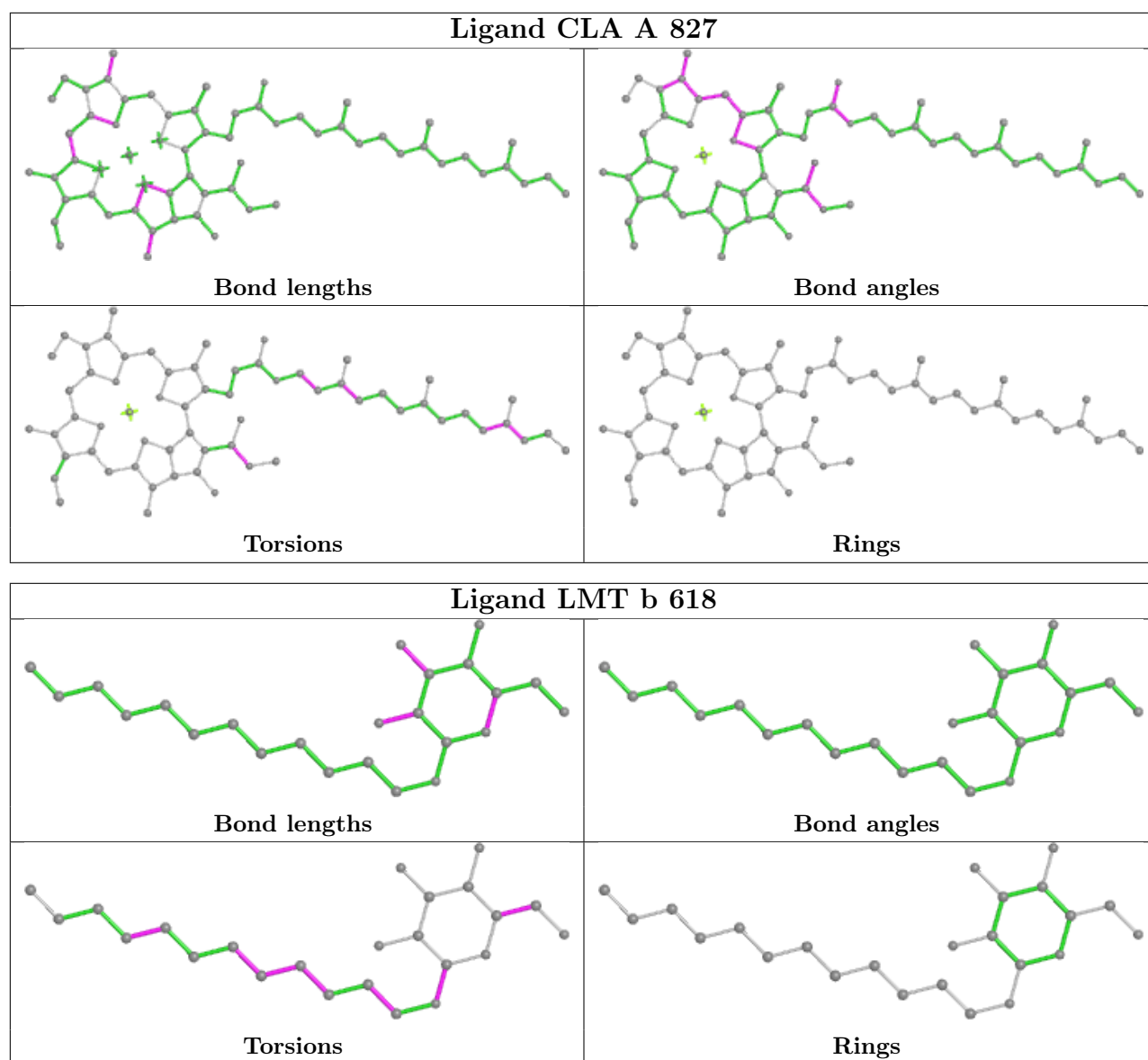
Ligand LMG L 209	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 820

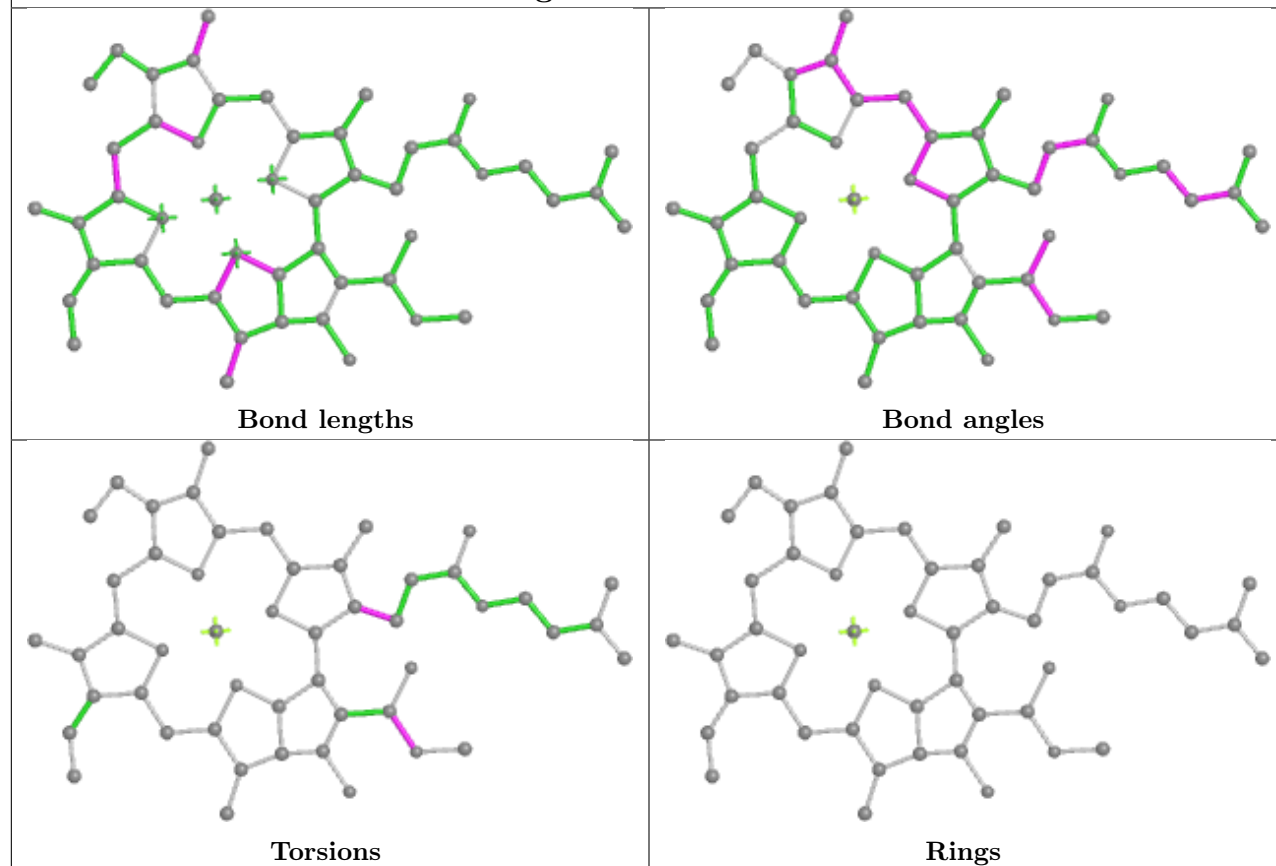


Ligand CLA i 303

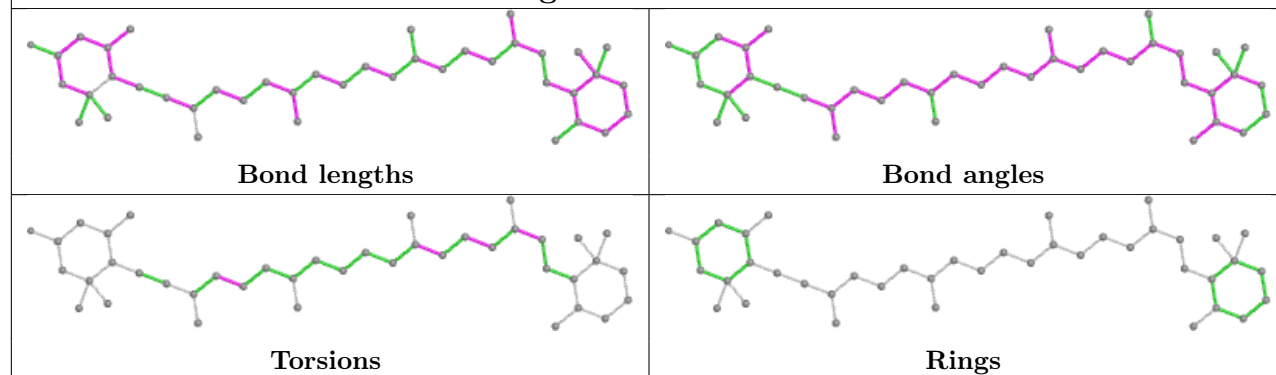




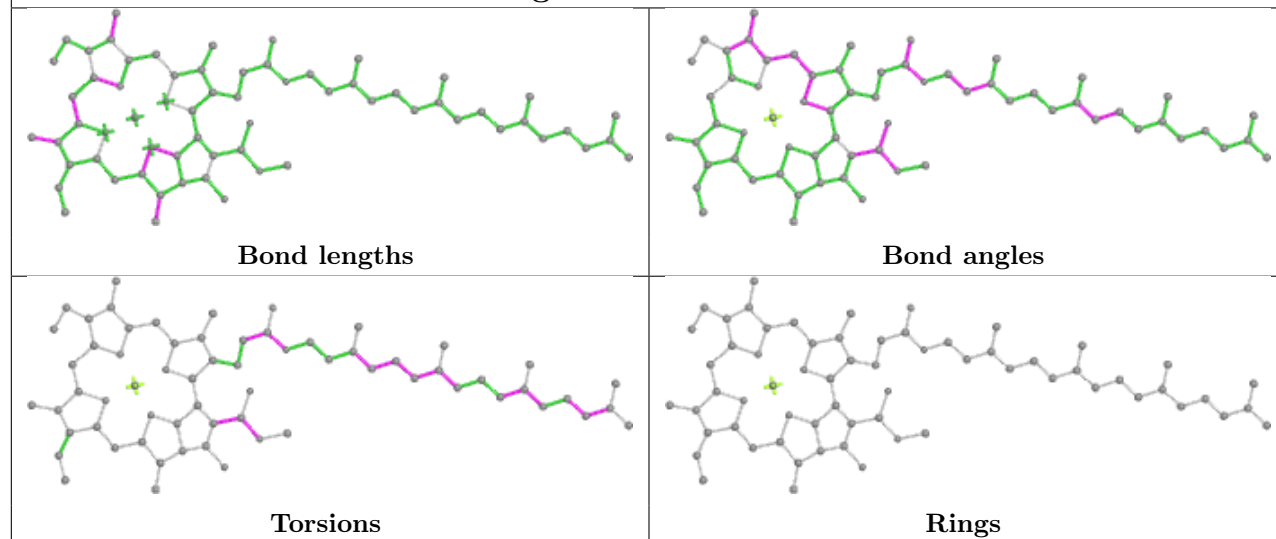
Ligand CLA d 301



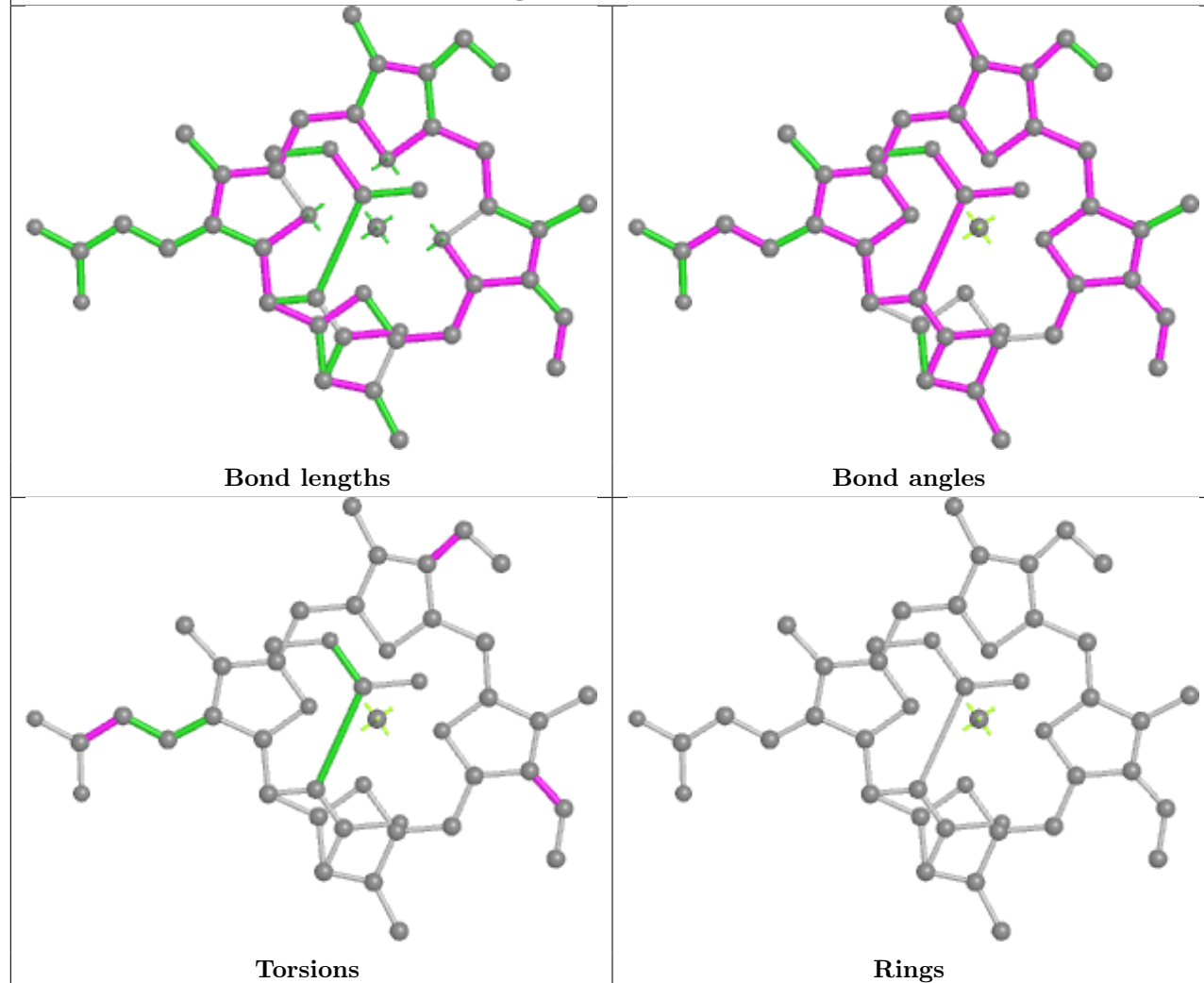
Ligand IHT b 615



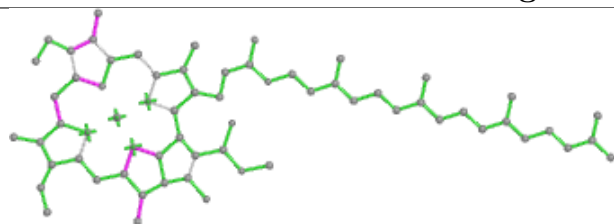
Ligand CLA B 802



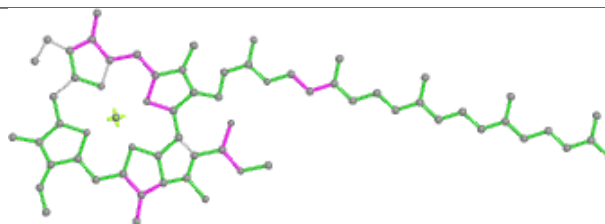
Ligand KC2 i 319



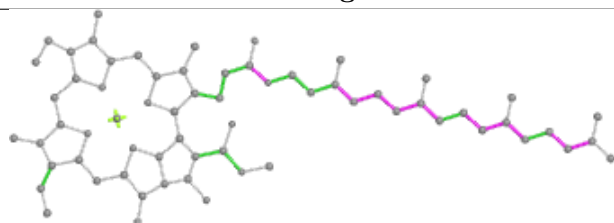
Ligand CLA e 605



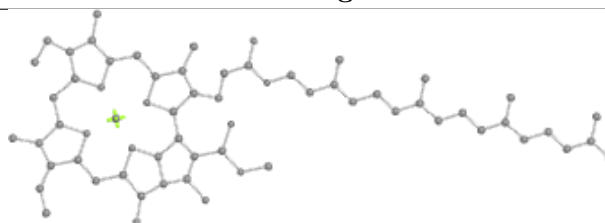
Bond lengths



Bond angles

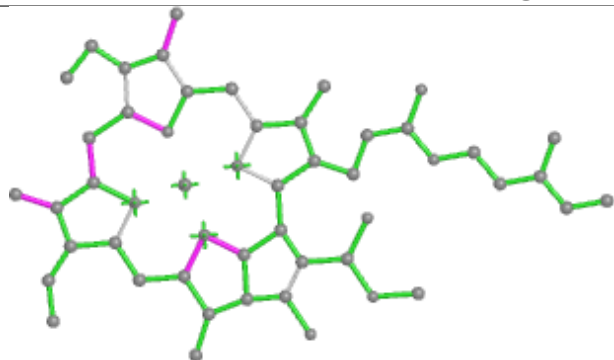


Torsions

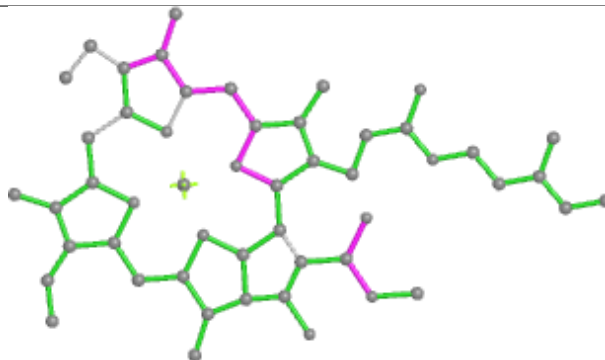


Rings

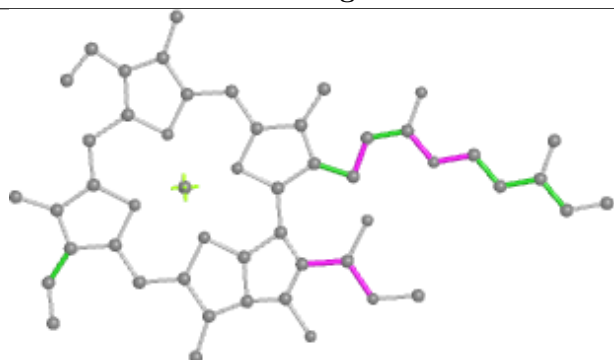
Ligand CLA d 304



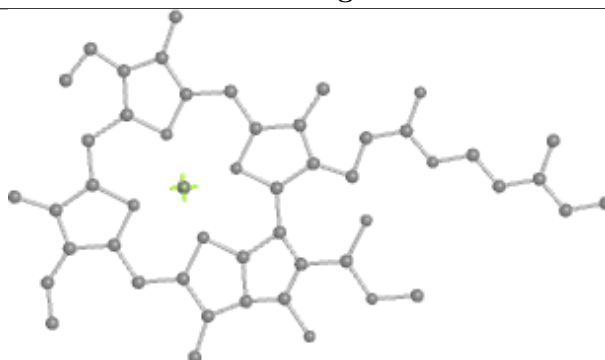
Bond lengths



Bond angles

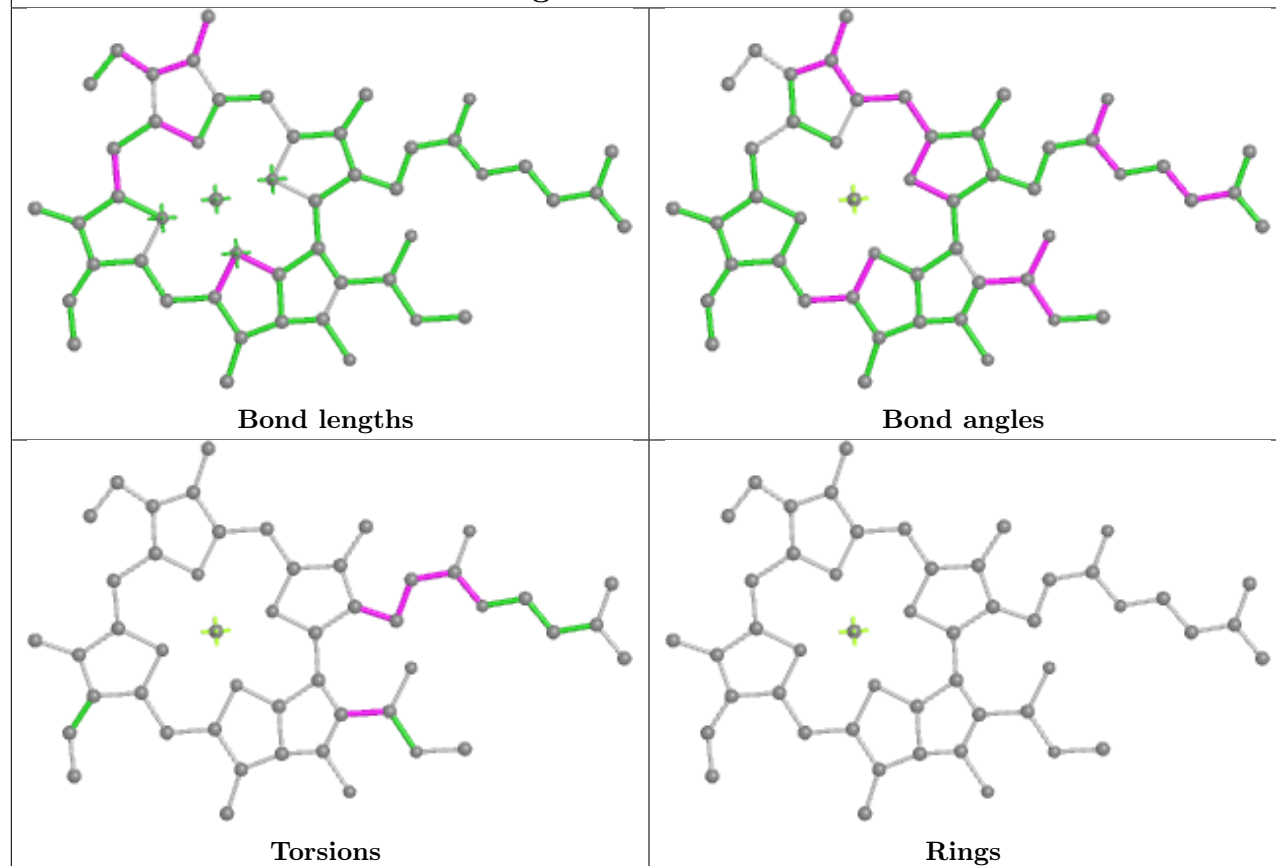


Torsions

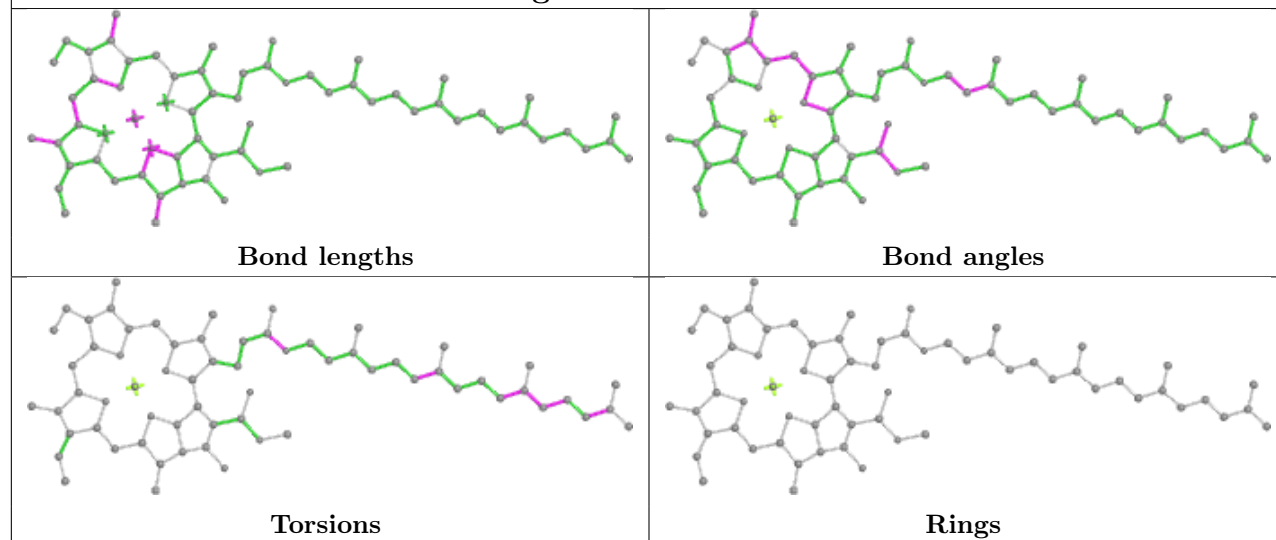


Rings

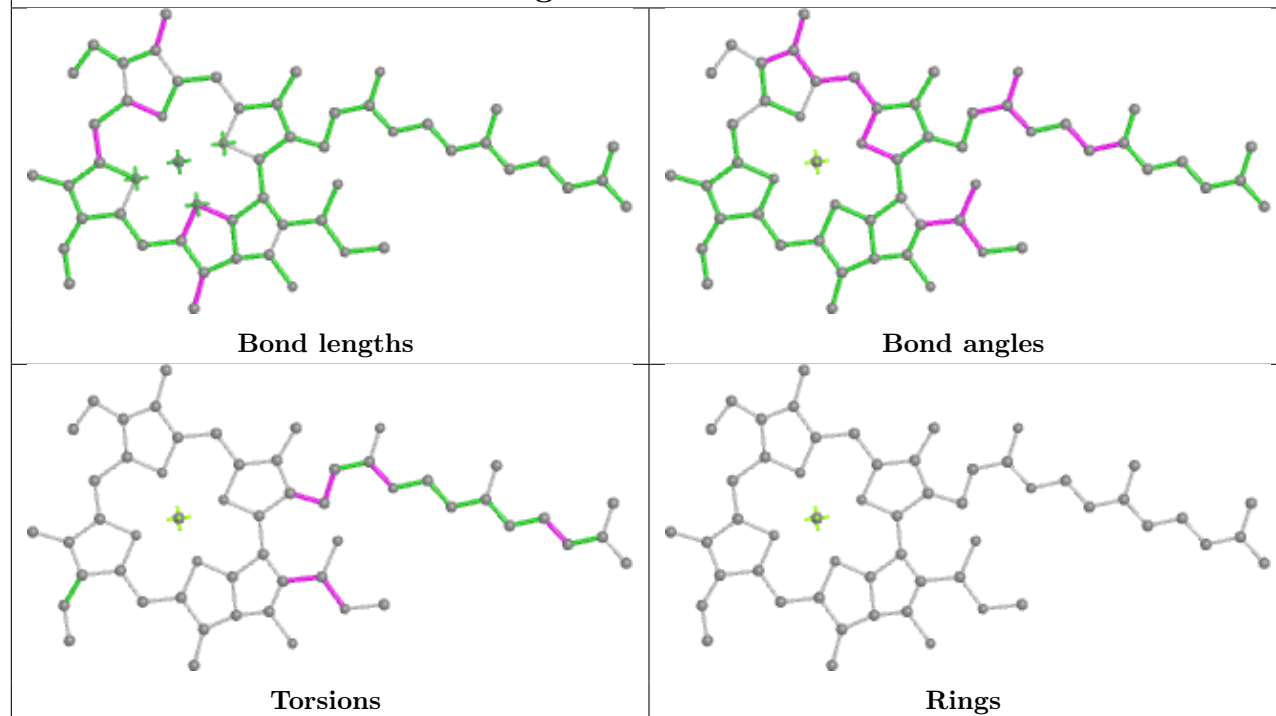
Ligand CLA B 827



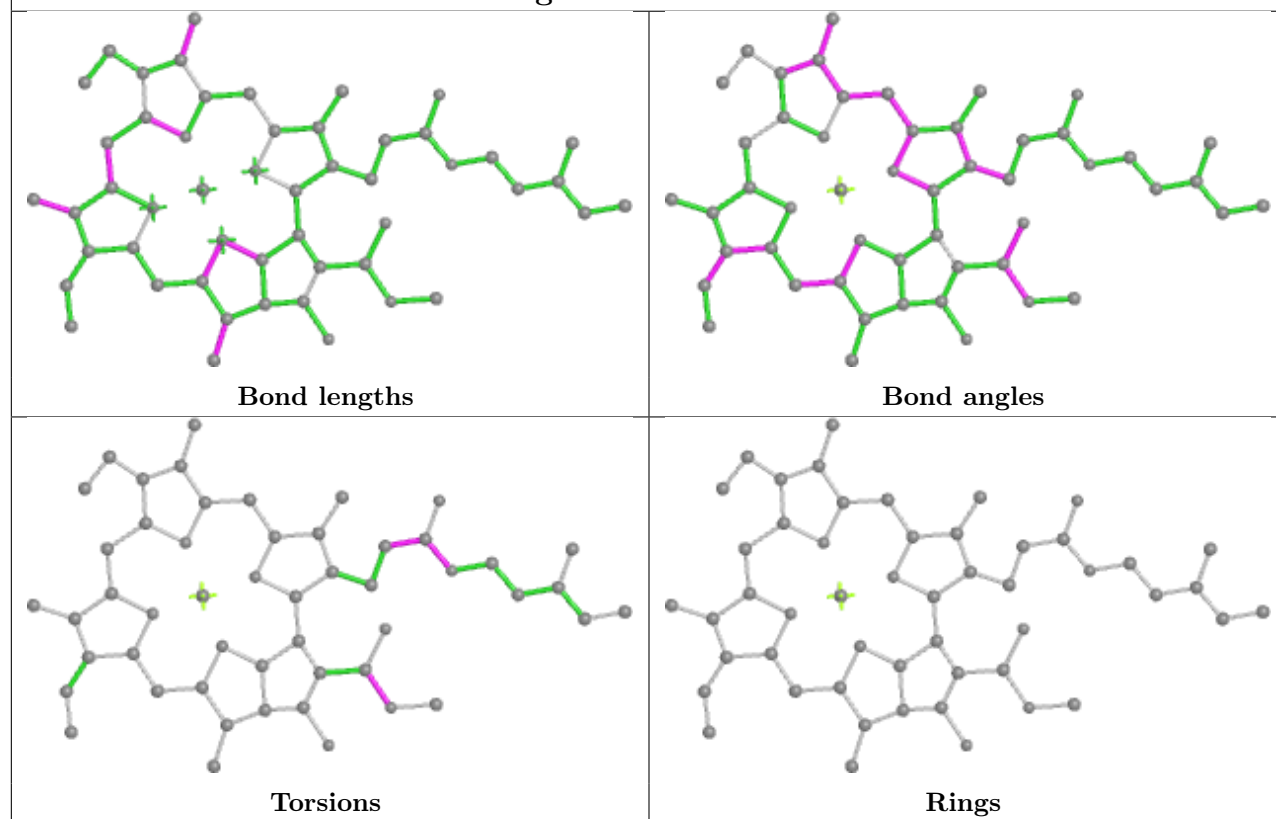
Ligand CLA B 817

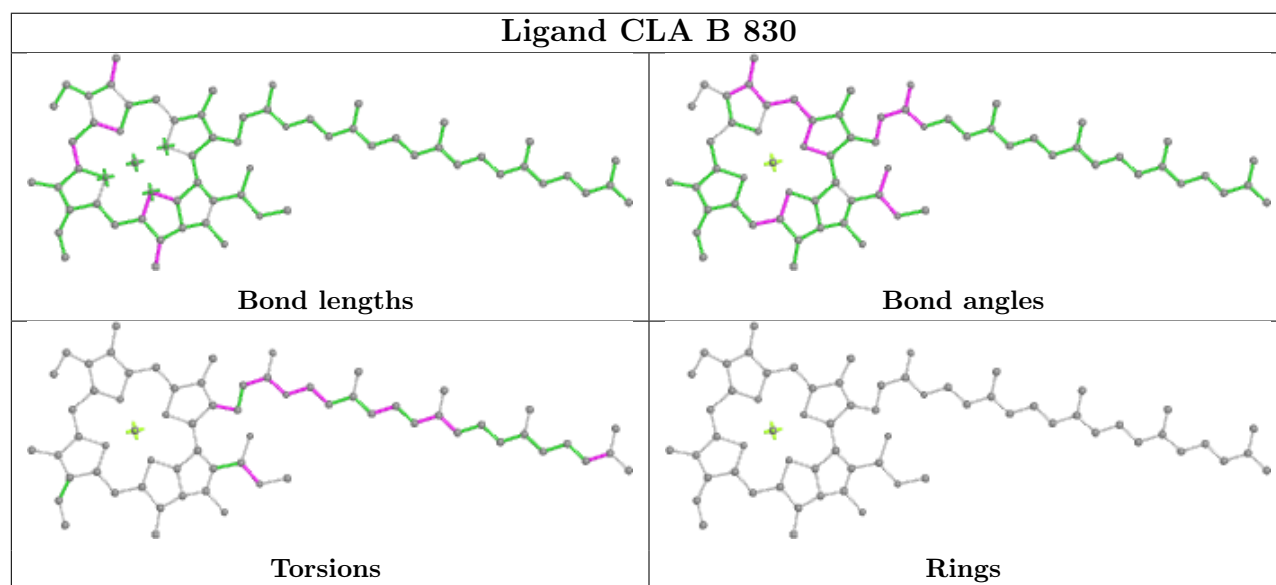
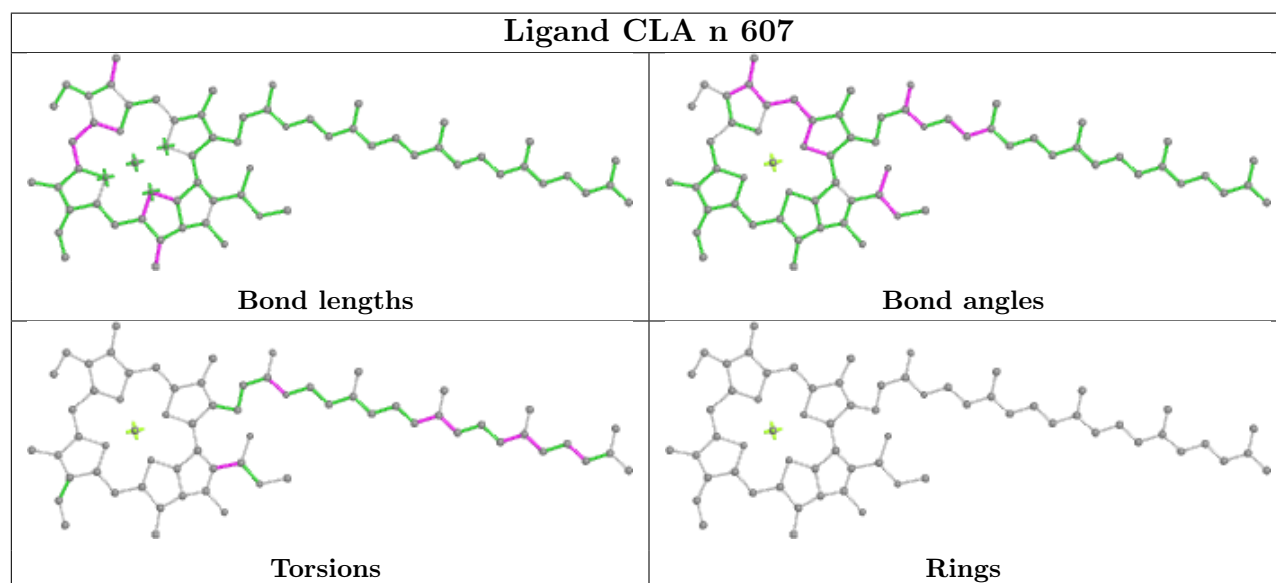
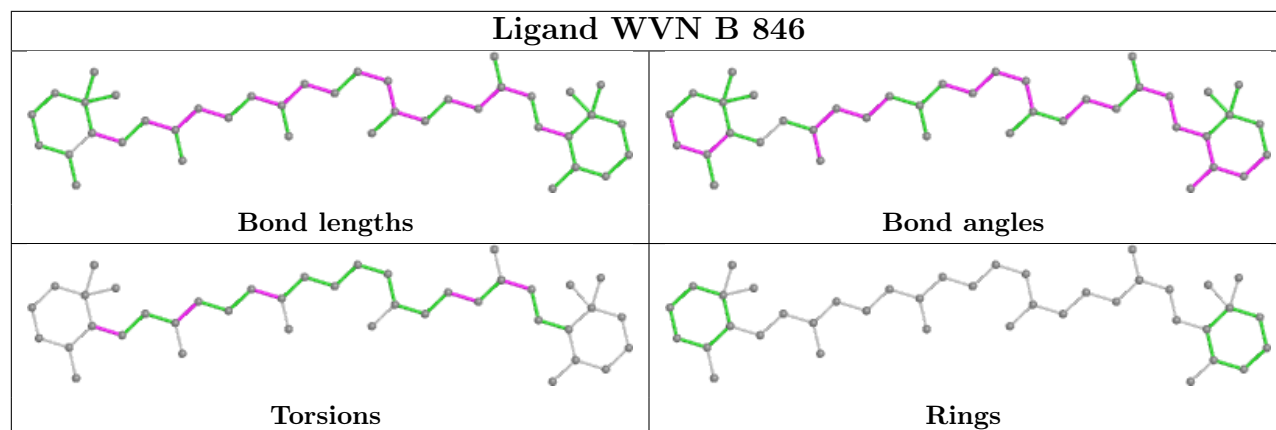


Ligand CLA b 602

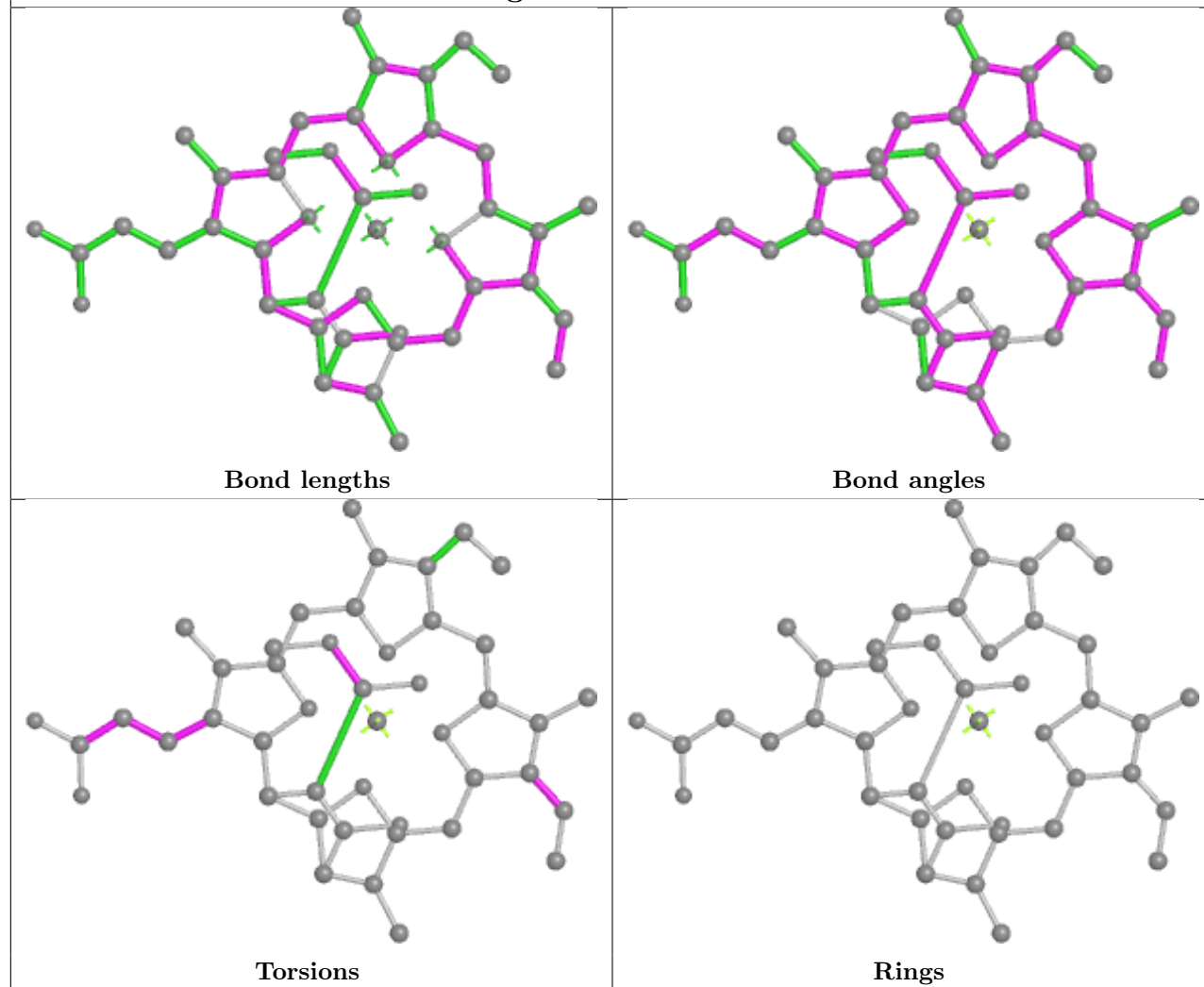


Ligand CLA b 609

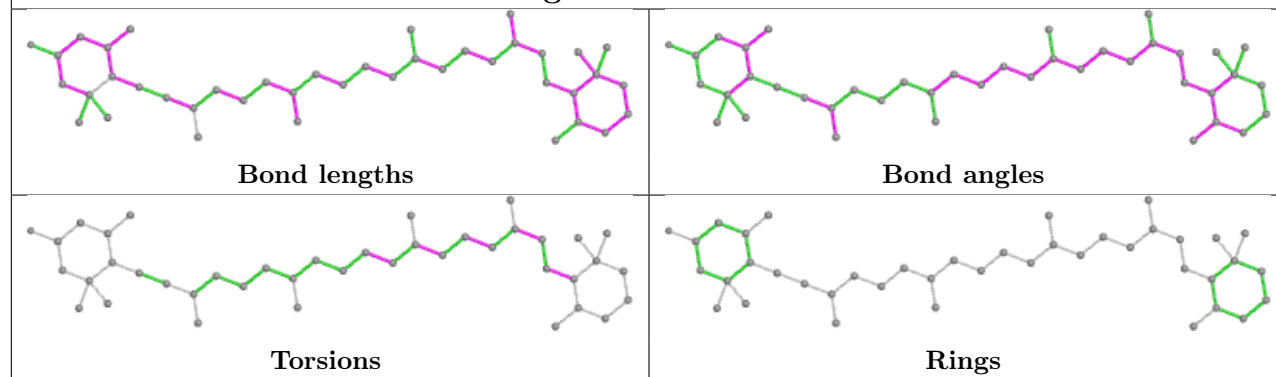


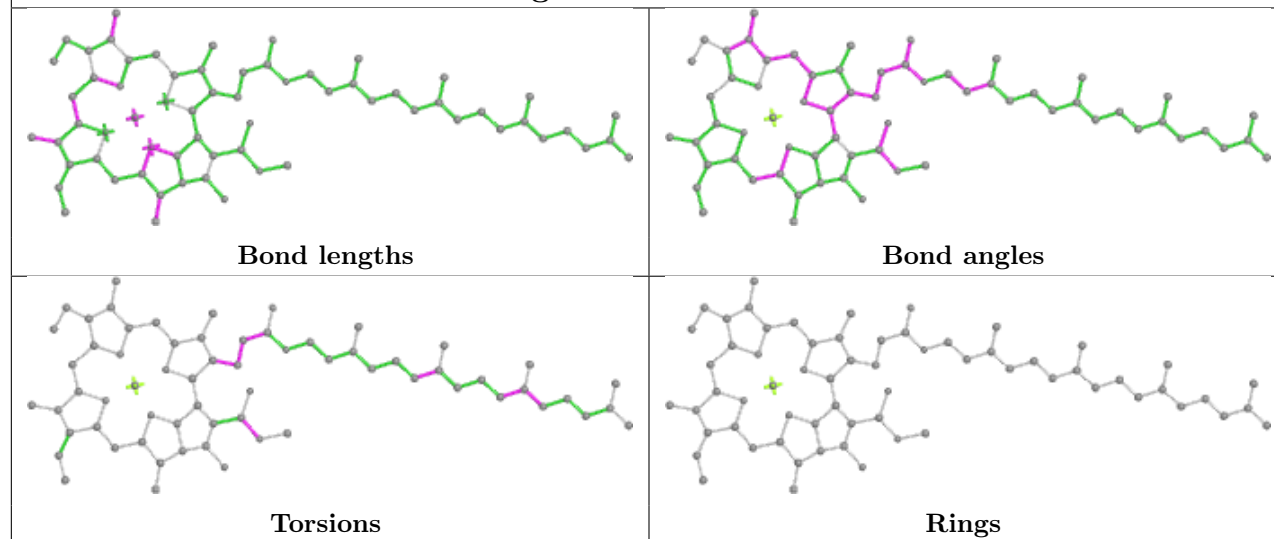
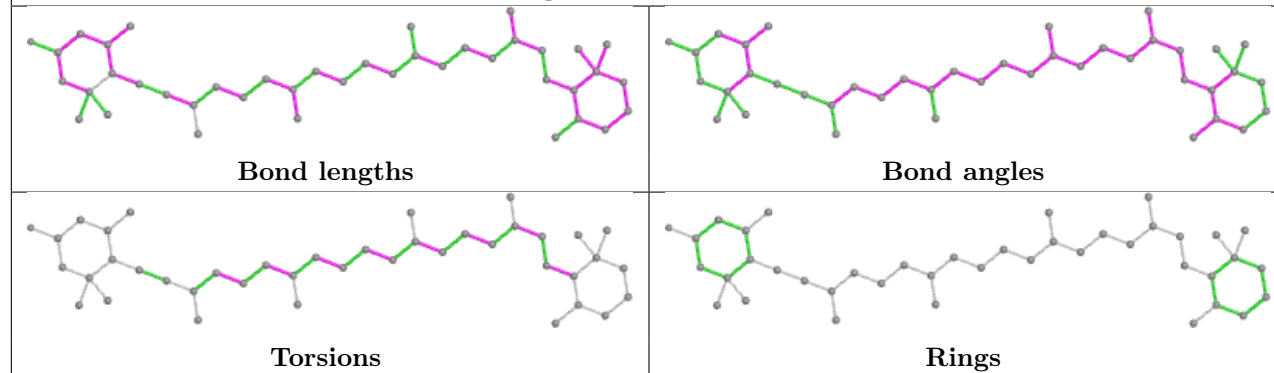
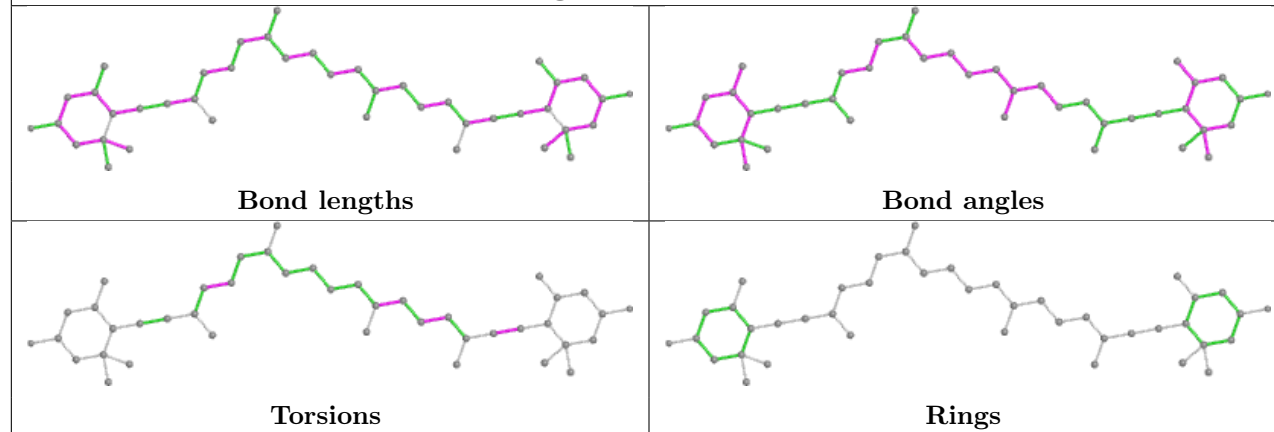


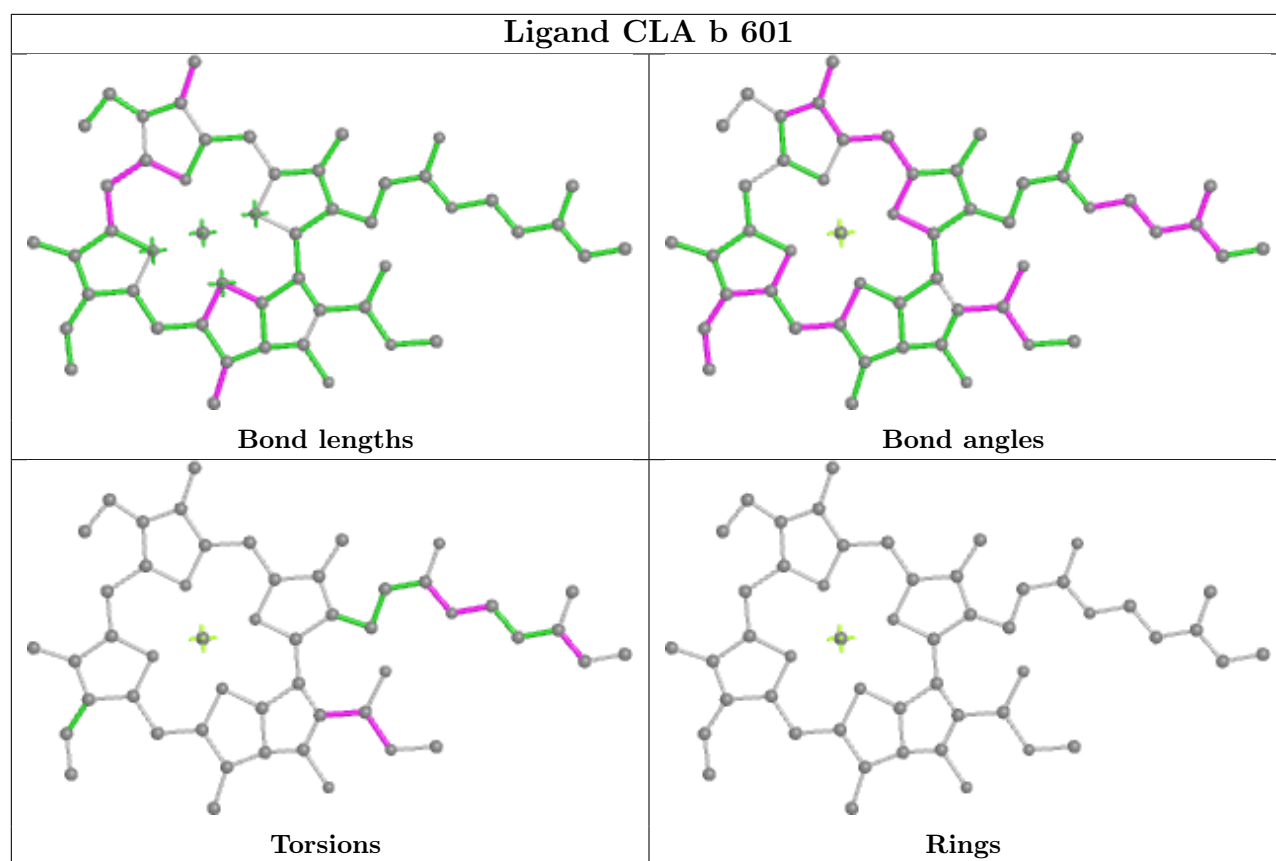
Ligand KC2 n 611



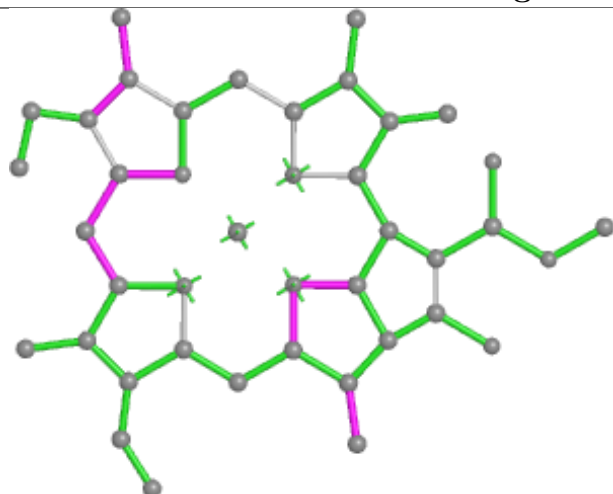
Ligand IHT f 617



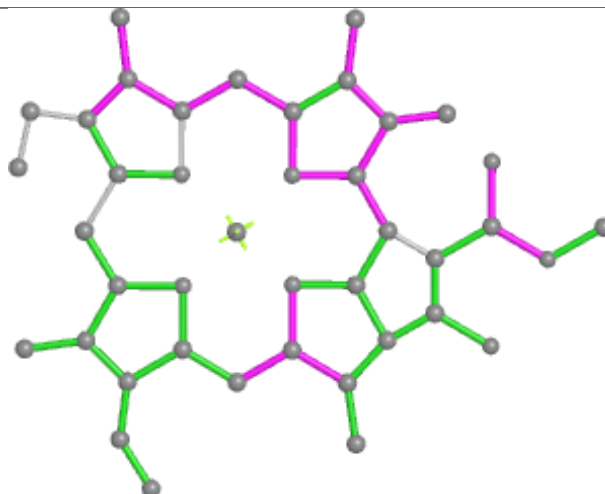
Ligand CLA A 808**Ligand IHT k 618****Ligand II0 e 612**



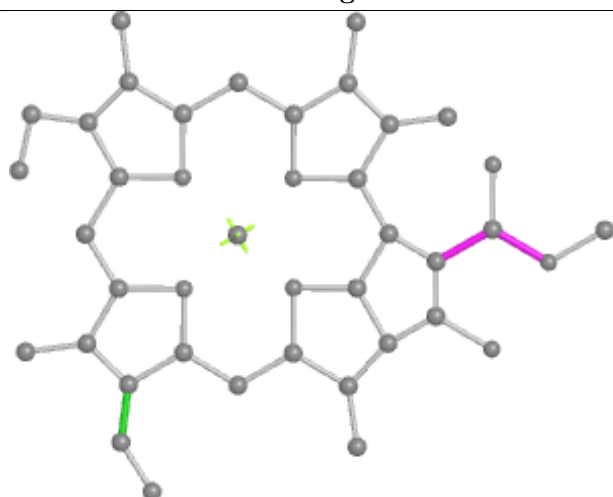
Ligand CLA A 855



Bond lengths



Bond angles

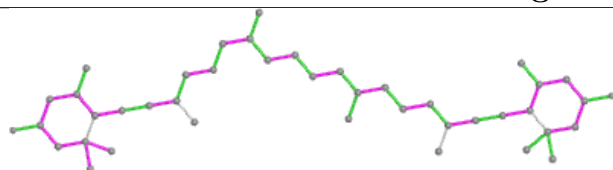


Torsions

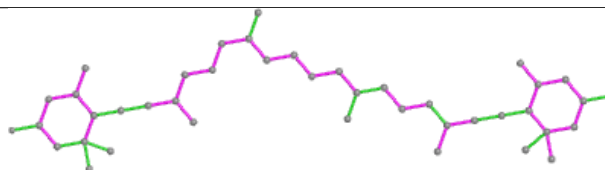


Rings

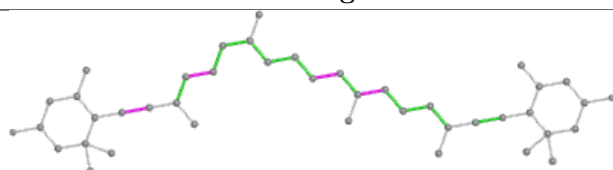
Ligand II0 d 313



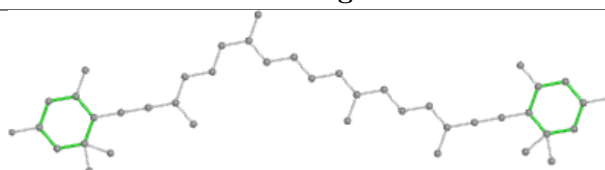
Bond lengths



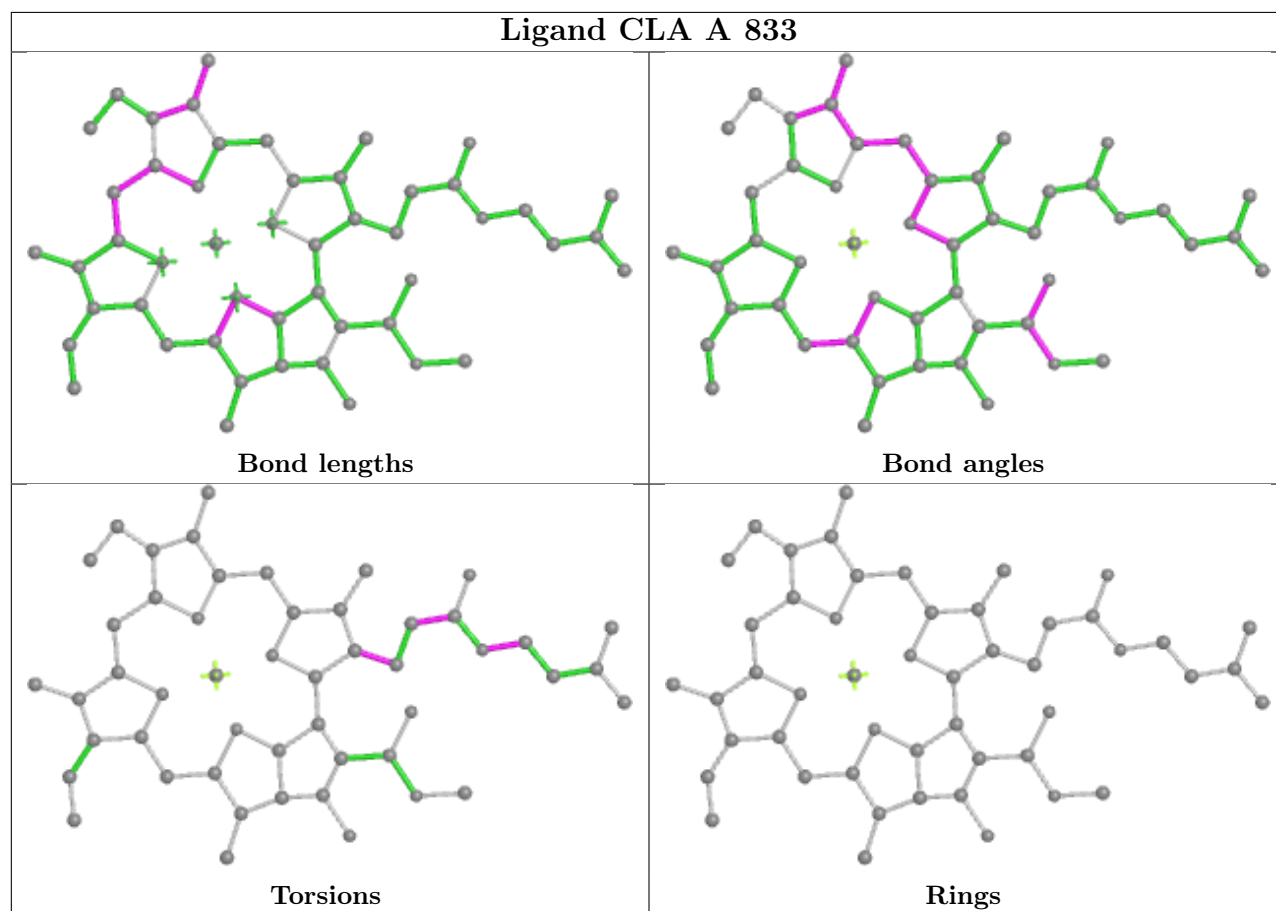
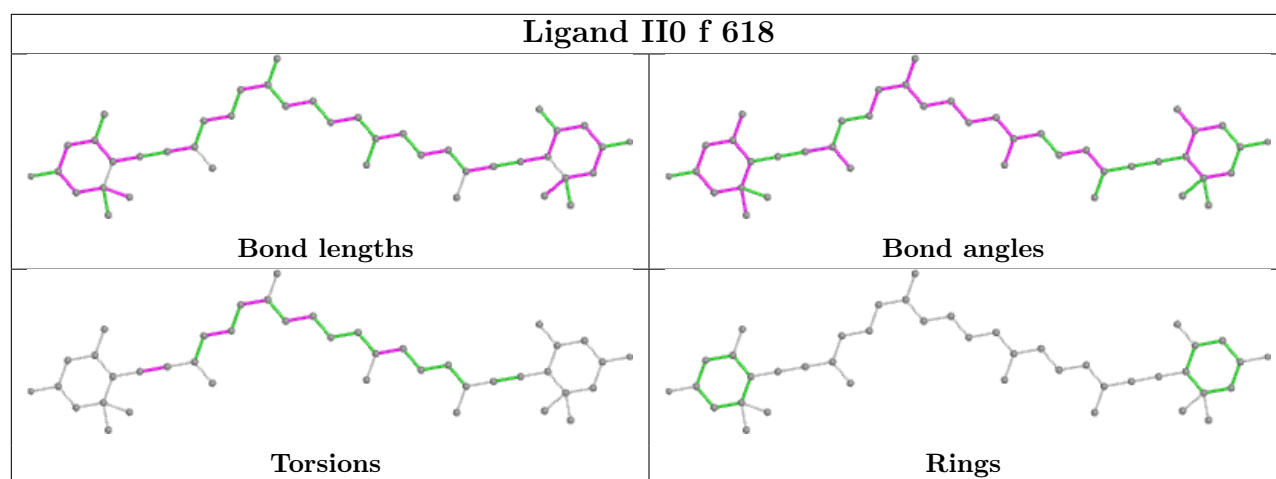
Bond angles



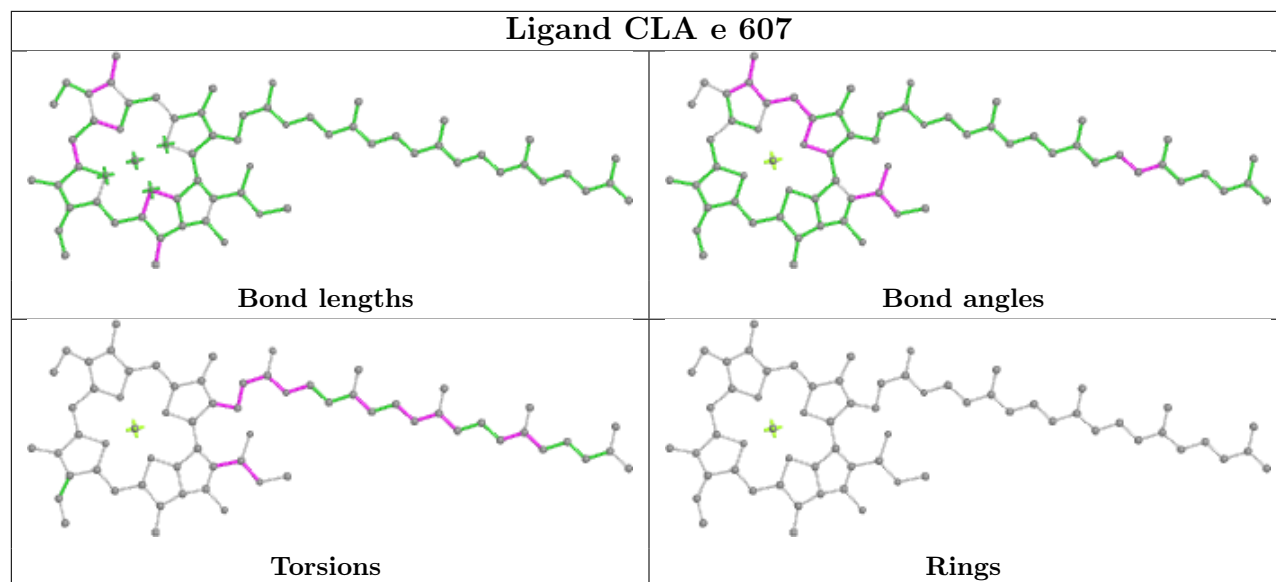
Torsions



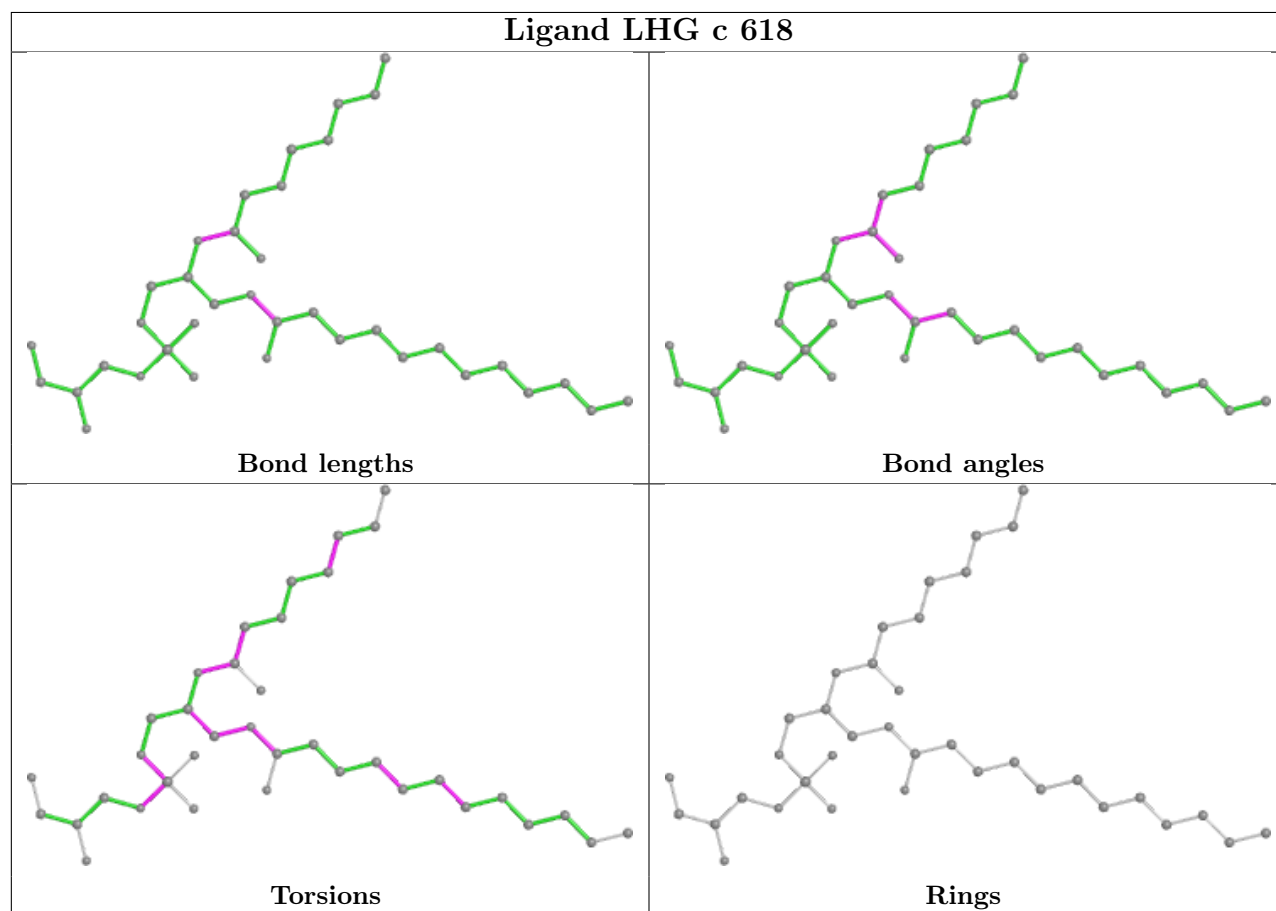
Rings

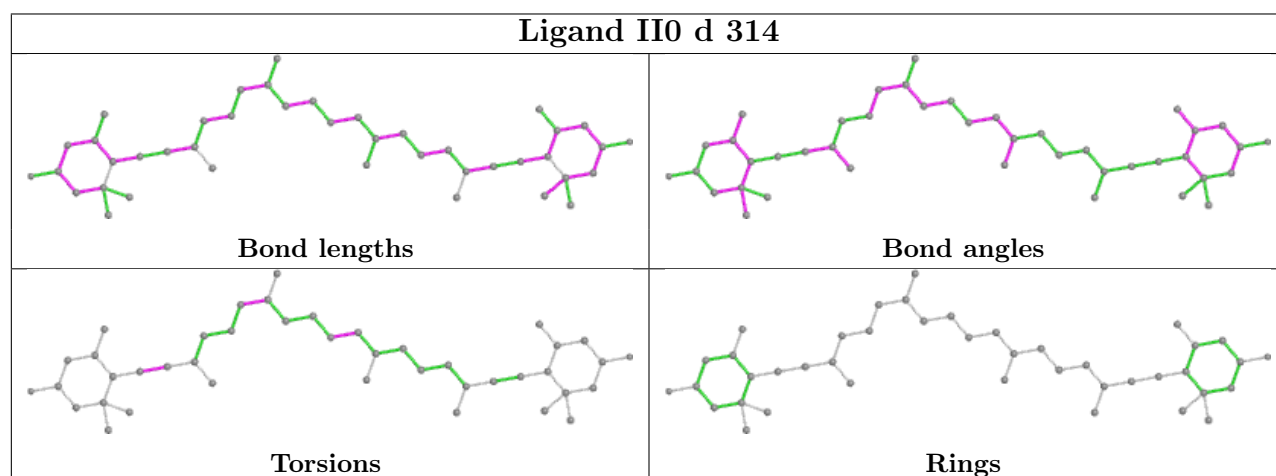
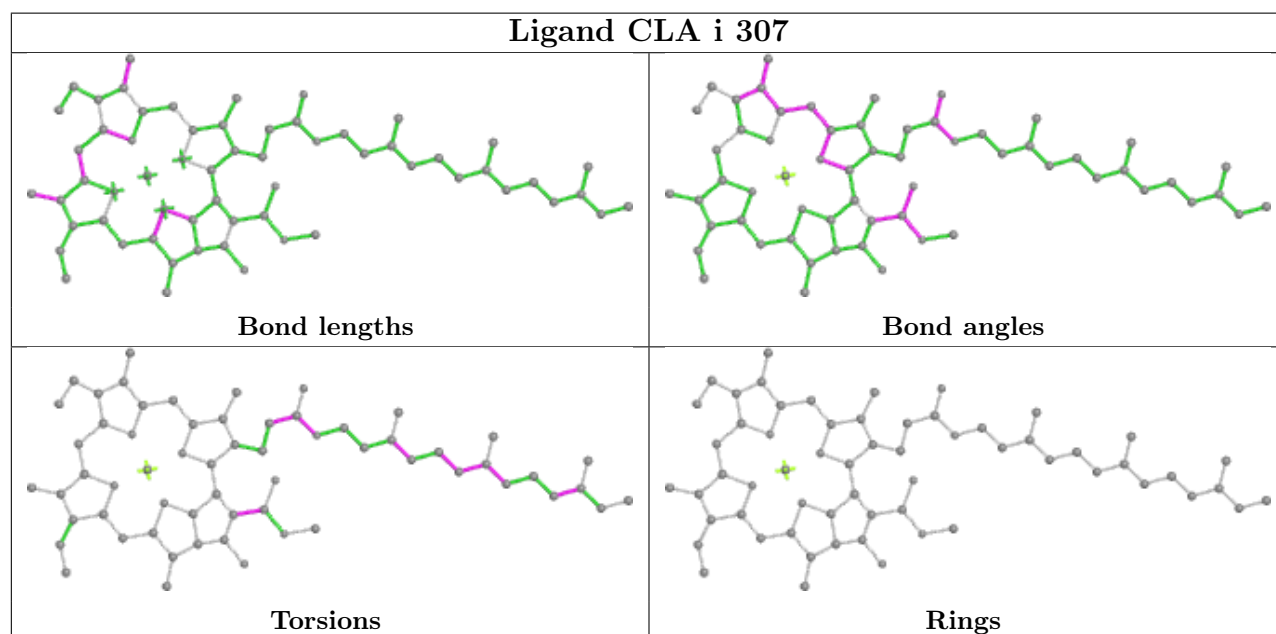
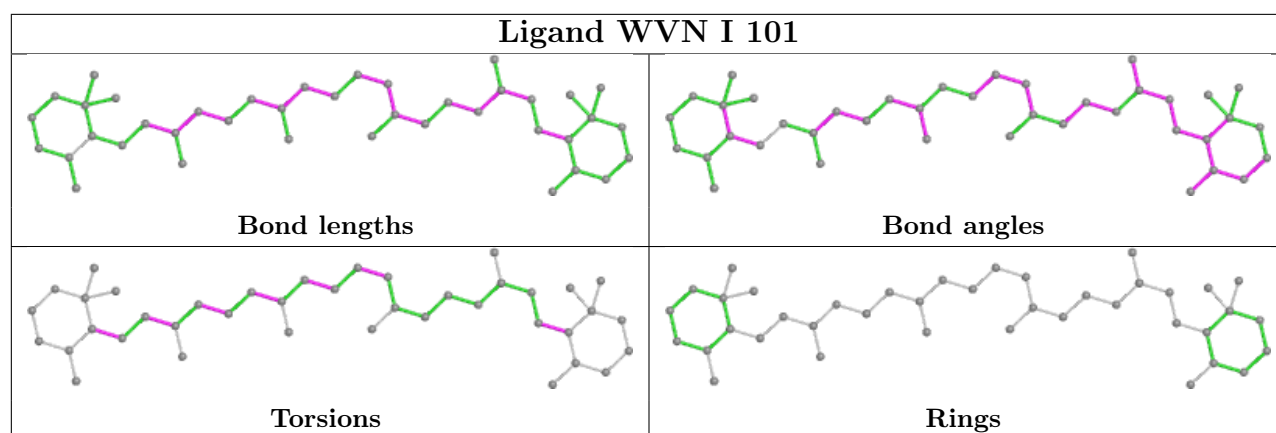


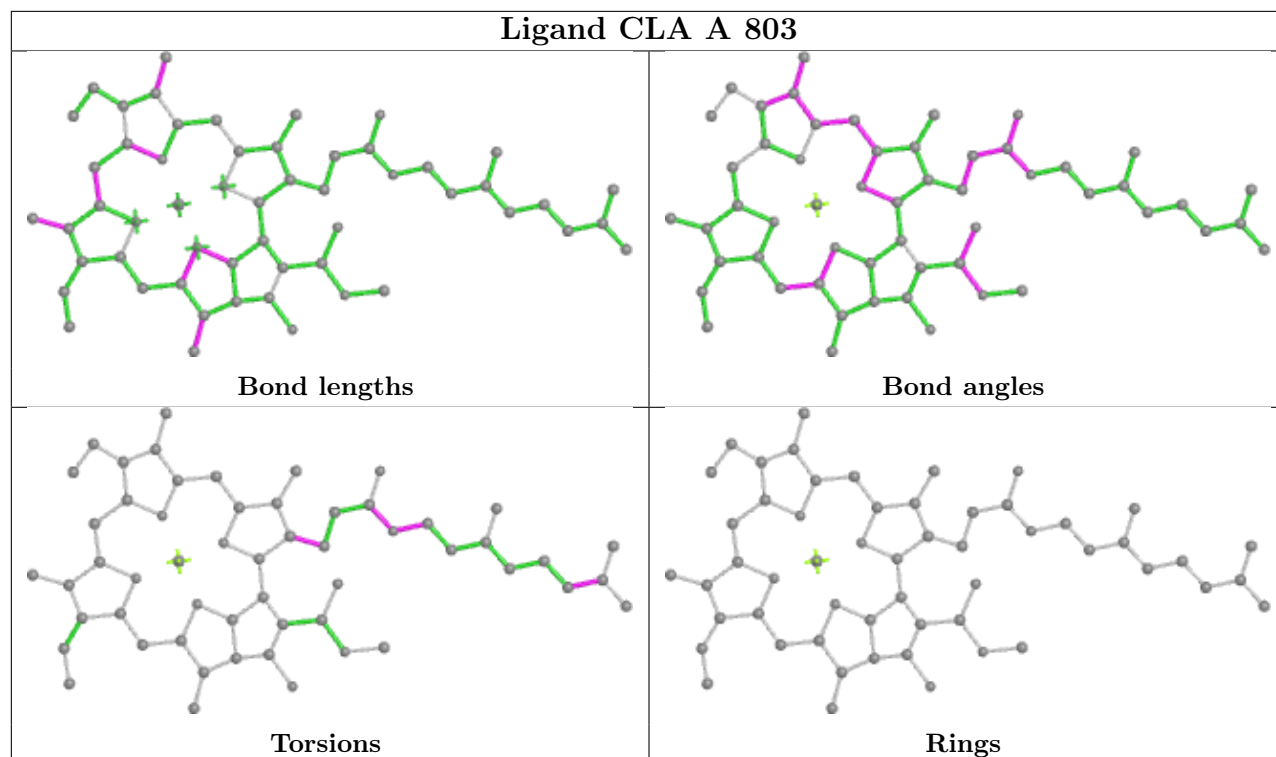
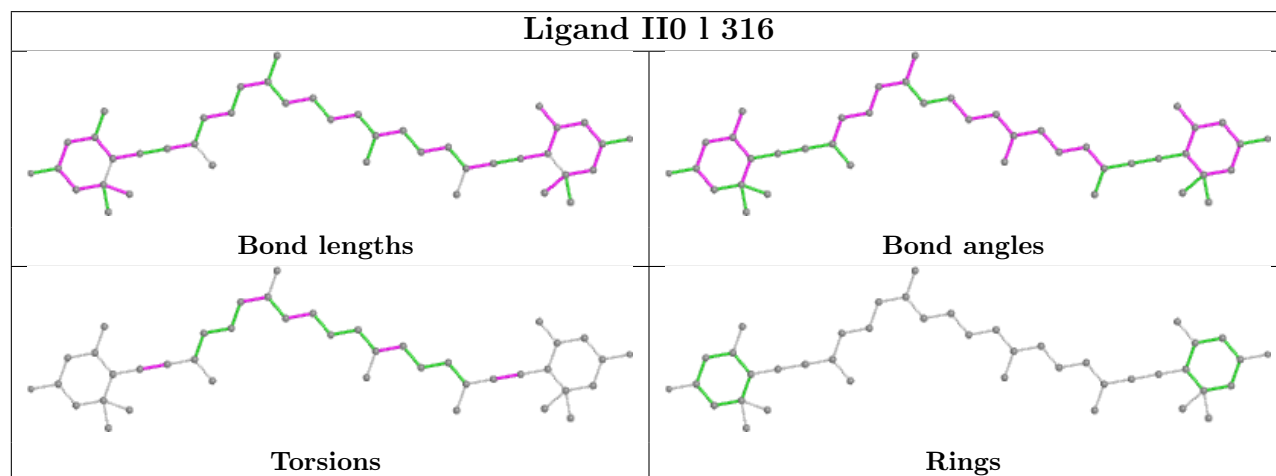
Ligand CLA e 607



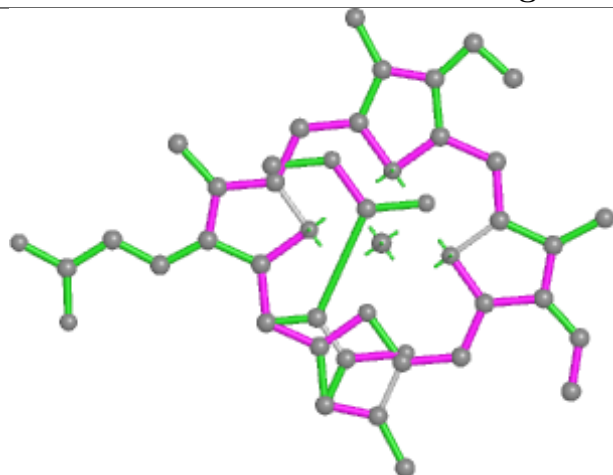
Ligand LHG c 618



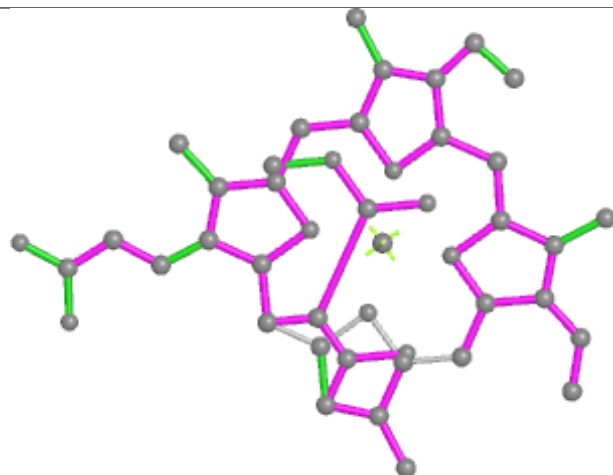


Ligand CLA A 803**Ligand II0 1 316**

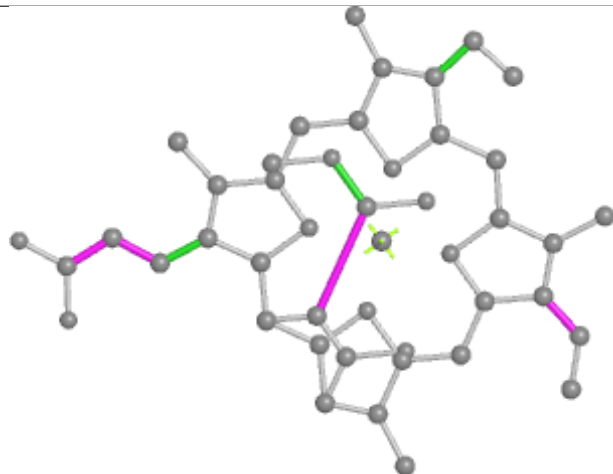
Ligand KC2 d 310



Bond lengths



Bond angles

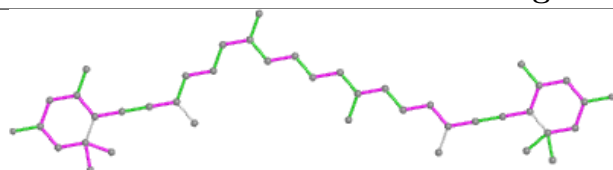


Torsions

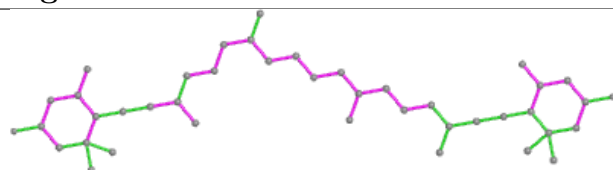


Rings

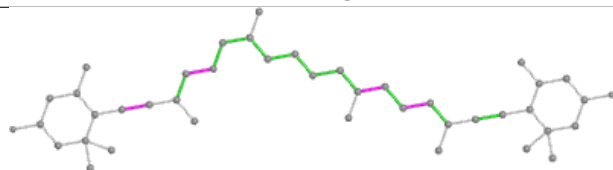
Ligand II0 g 317



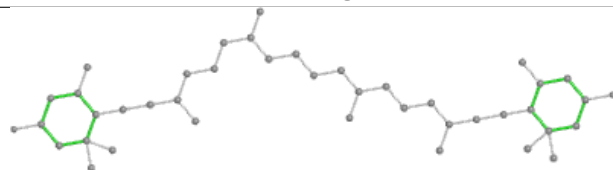
Bond lengths



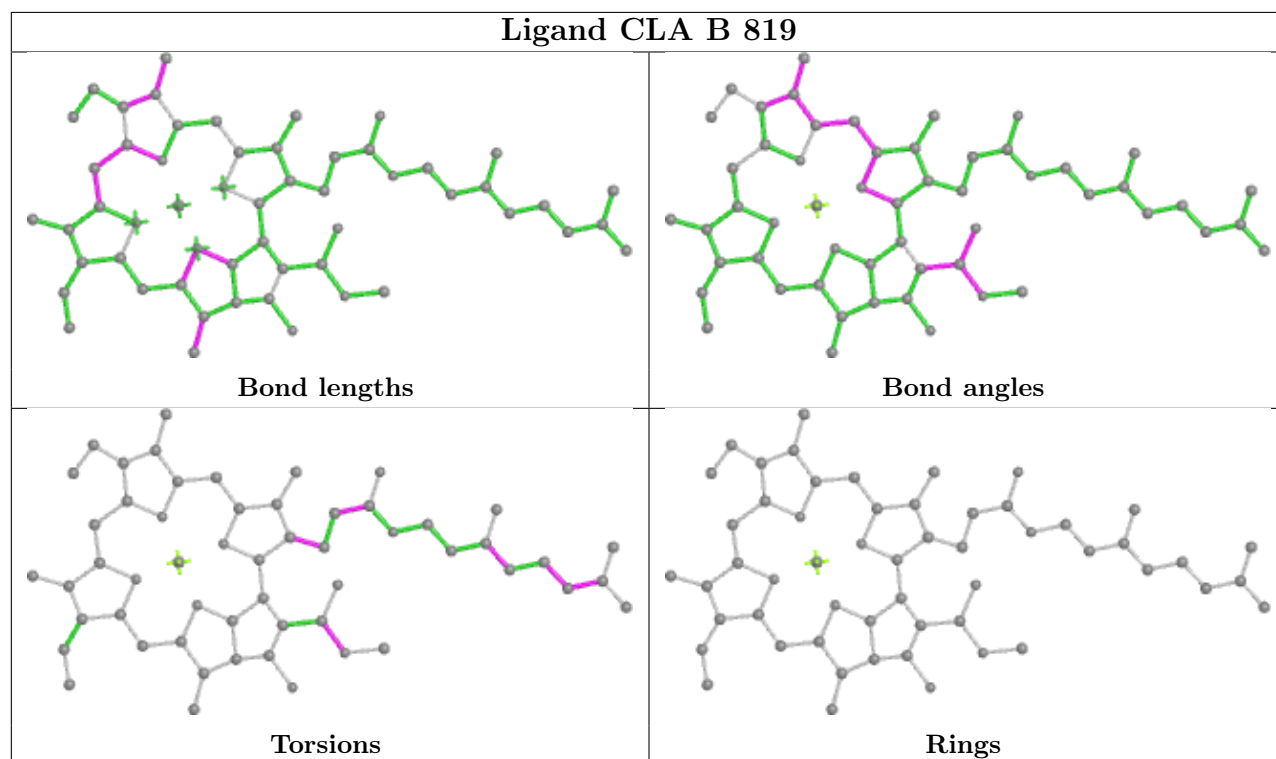
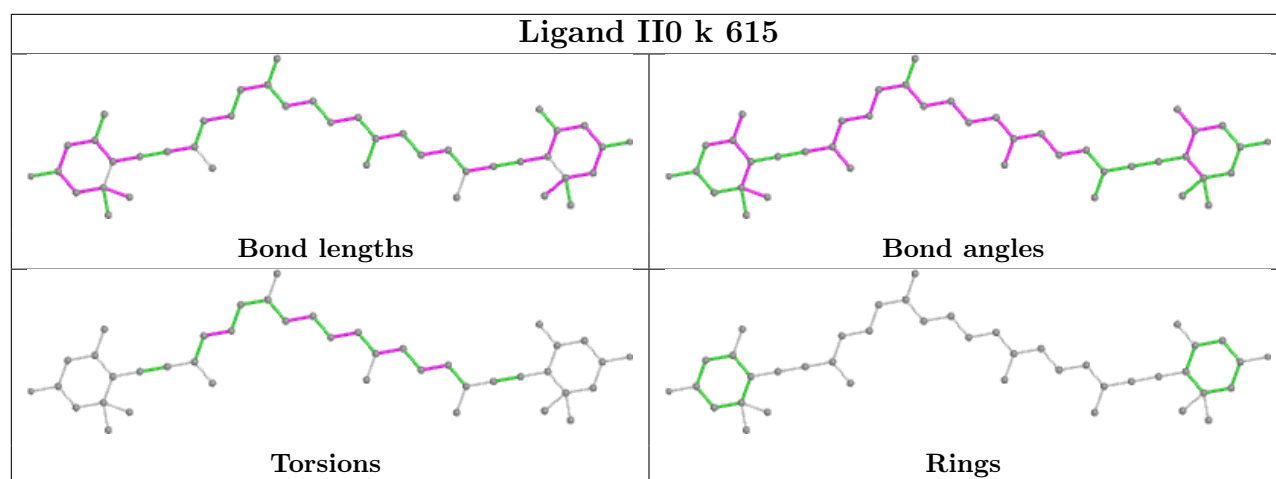
Bond angles



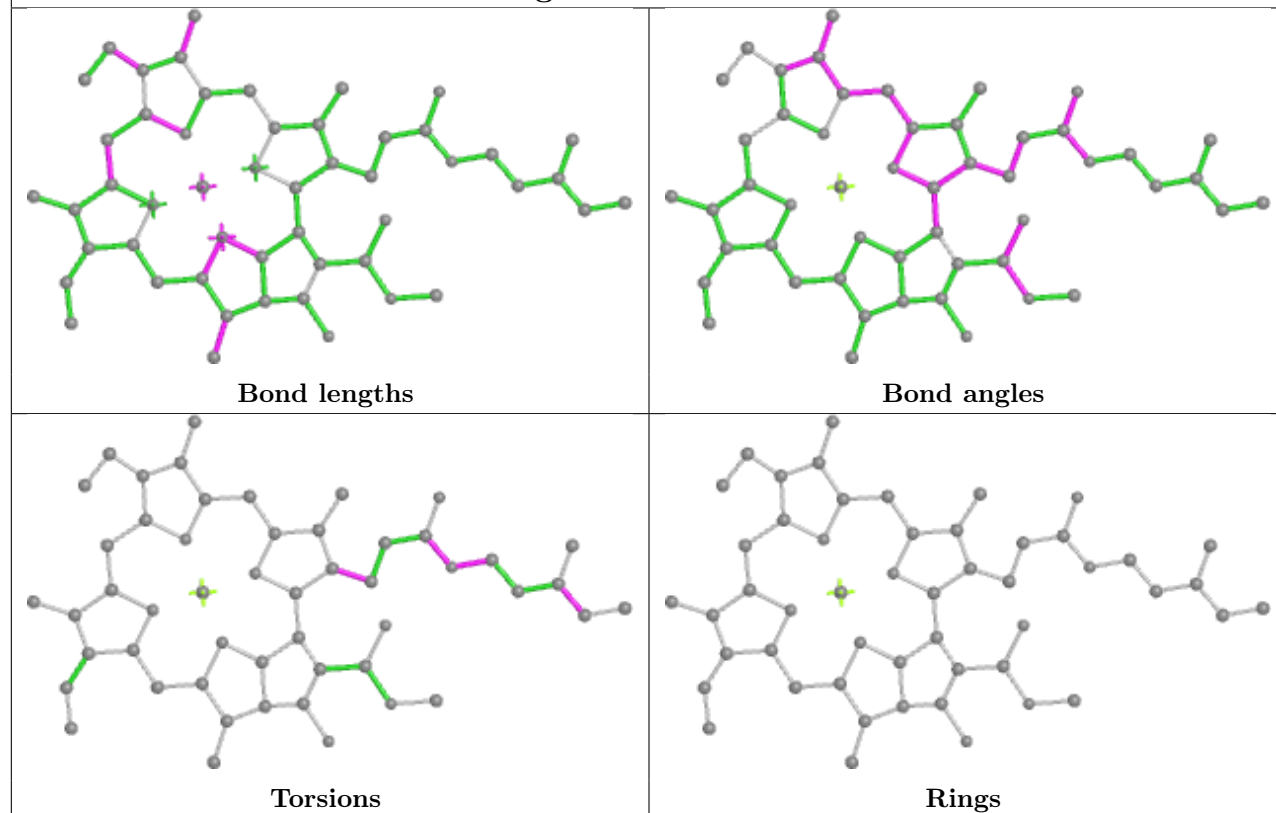
Torsions



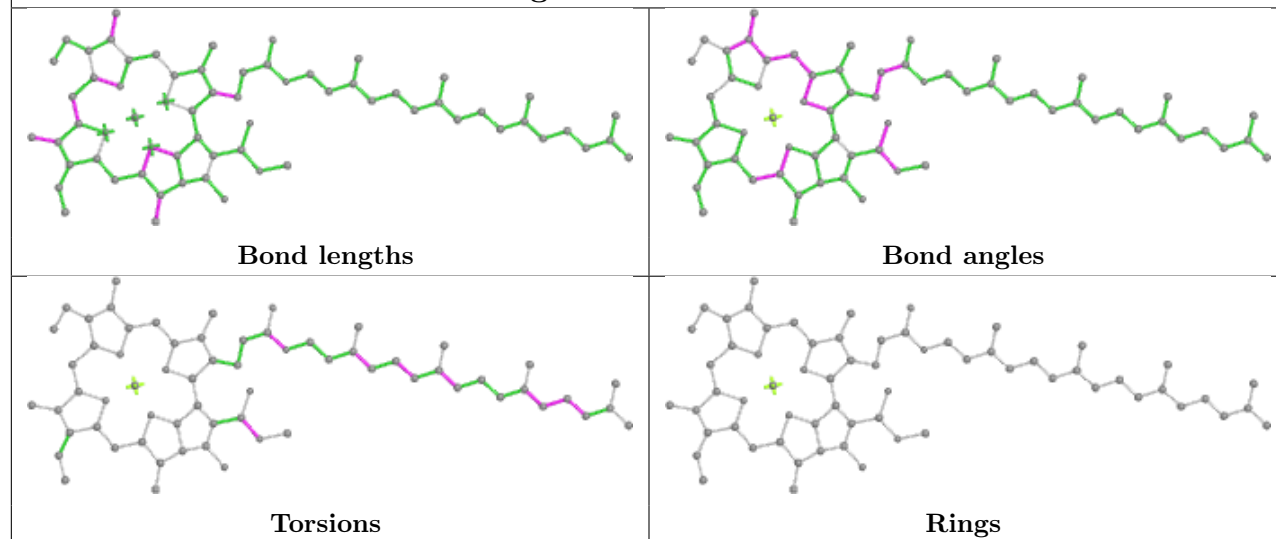
Rings



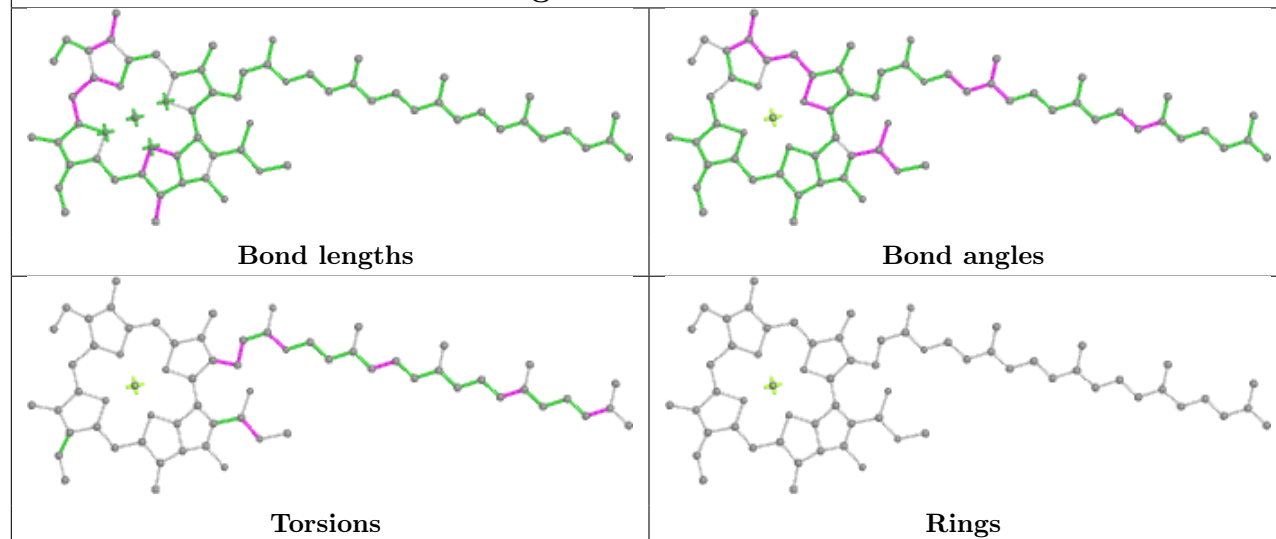
Ligand CLA b 612



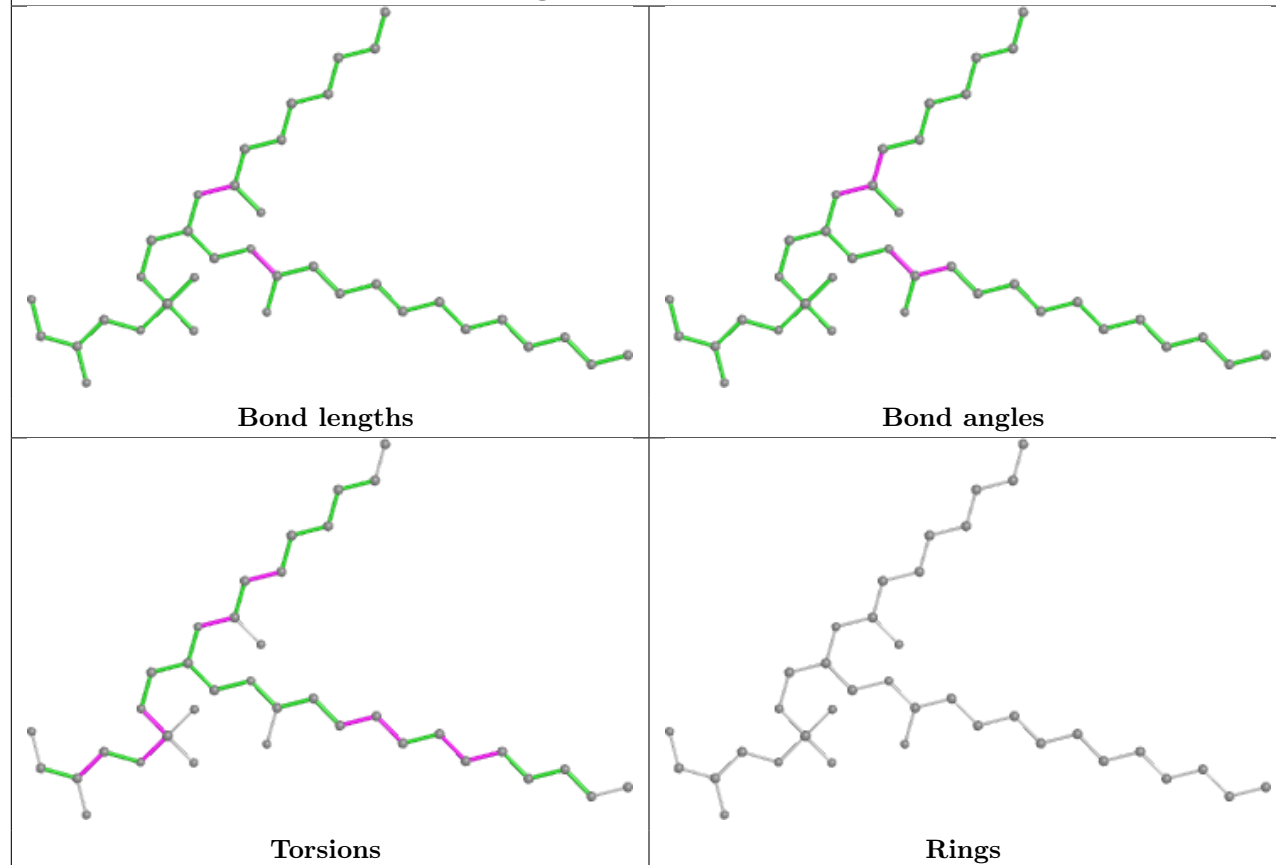
Ligand CLA m 603



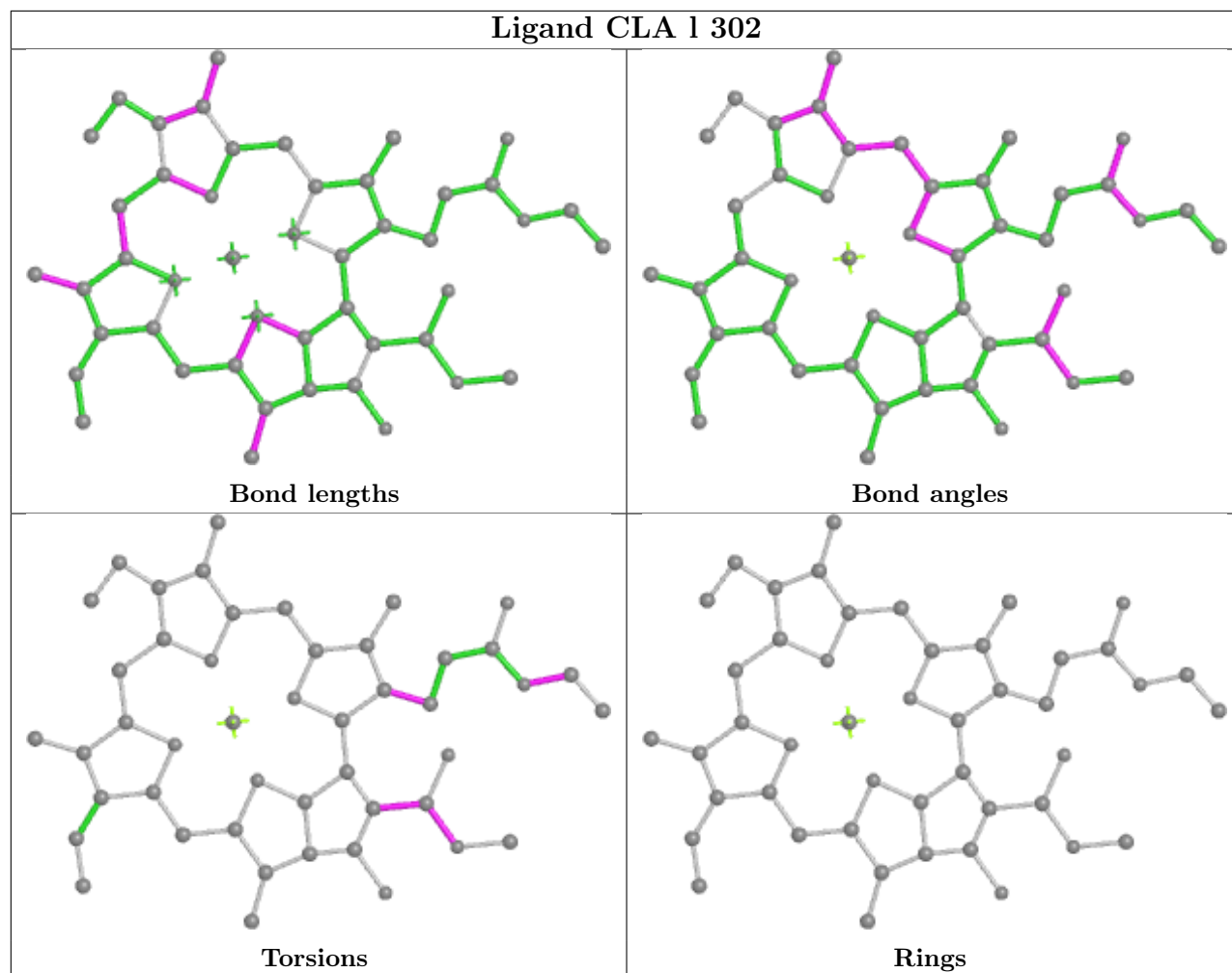
Ligand CLA B 808



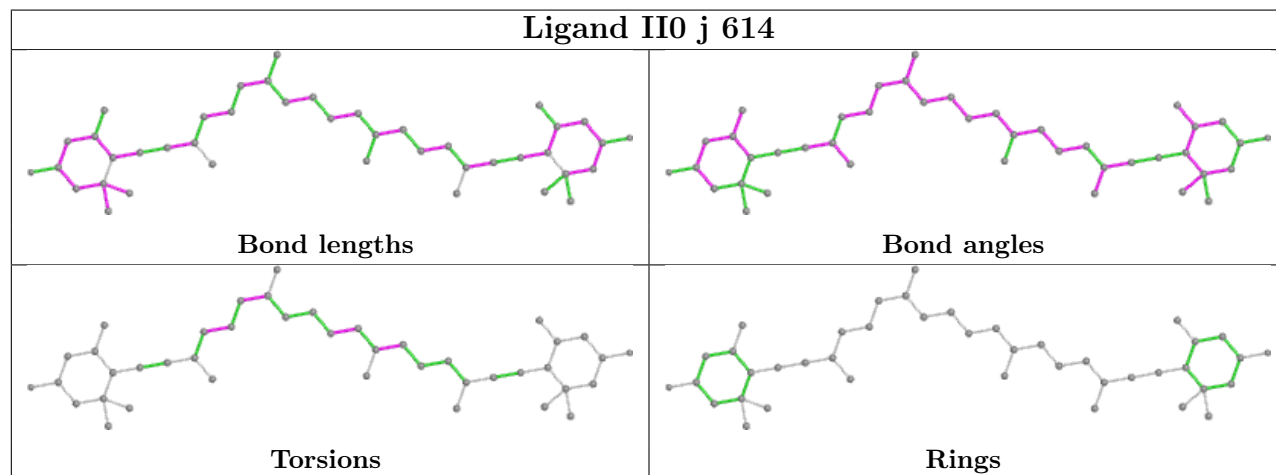
Ligand LHG d 317



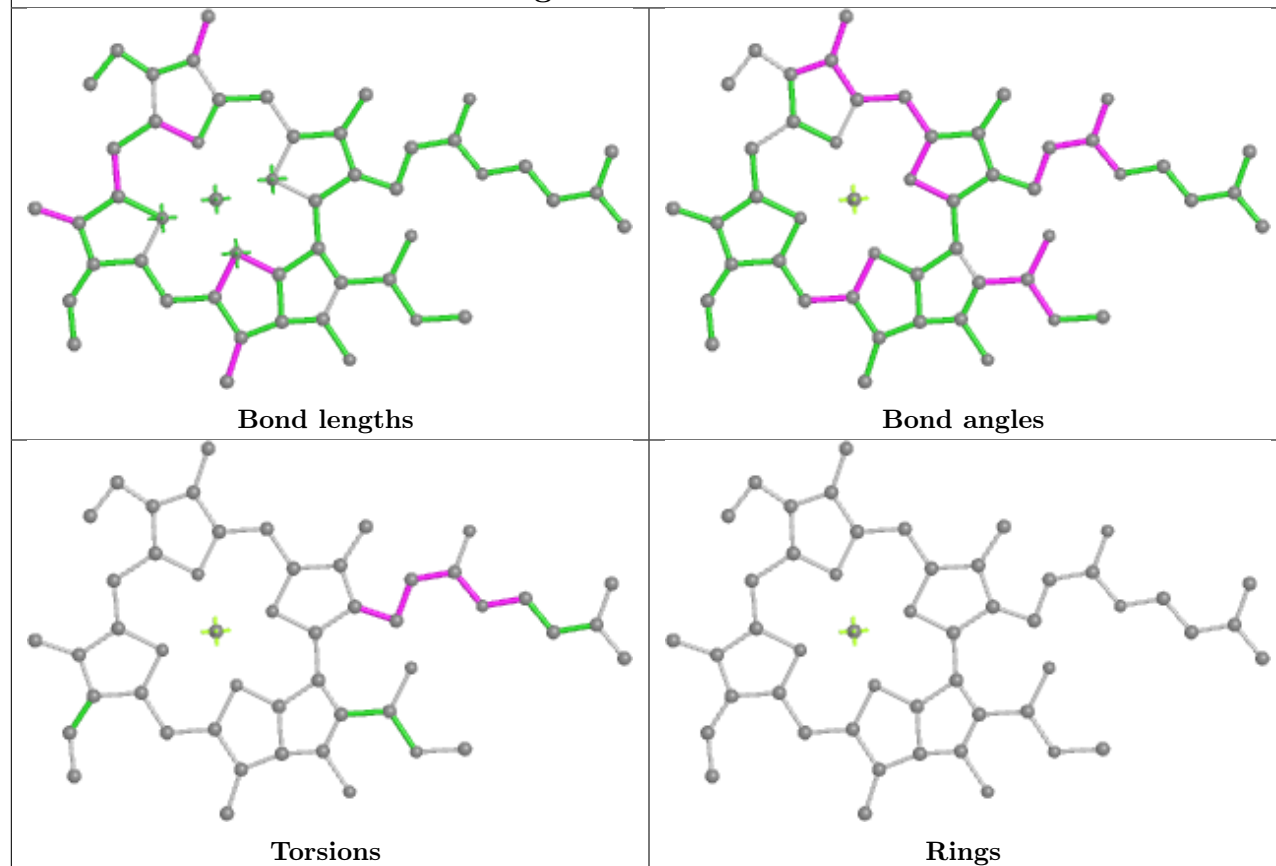
Ligand CLA l 302



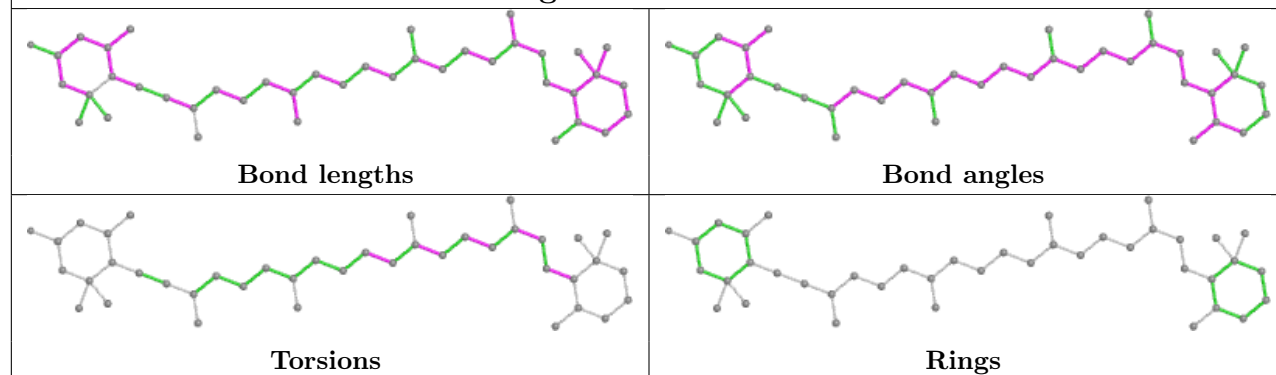
Ligand II0 j 614



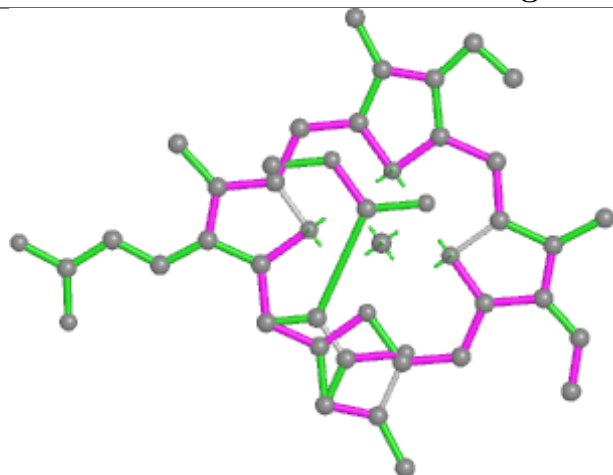
Ligand CLA L 204



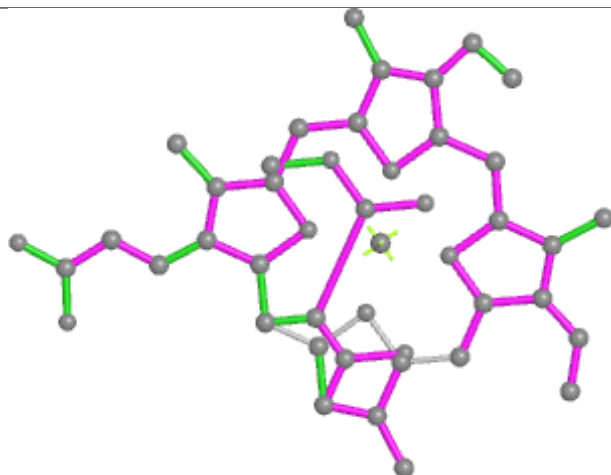
Ligand IHT n 617



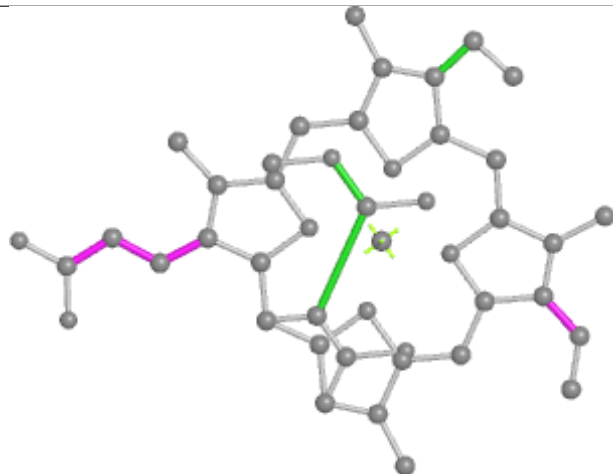
Ligand KC2 c 610



Bond lengths



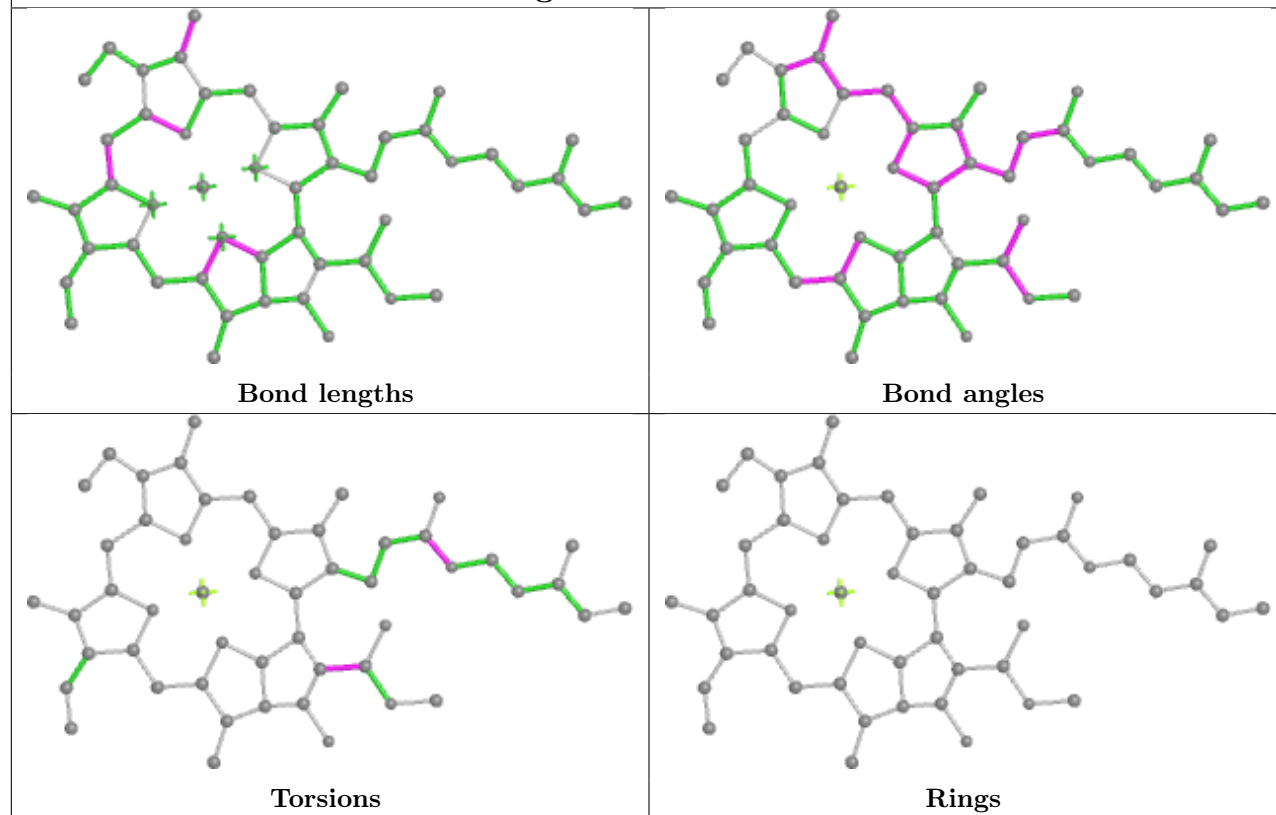
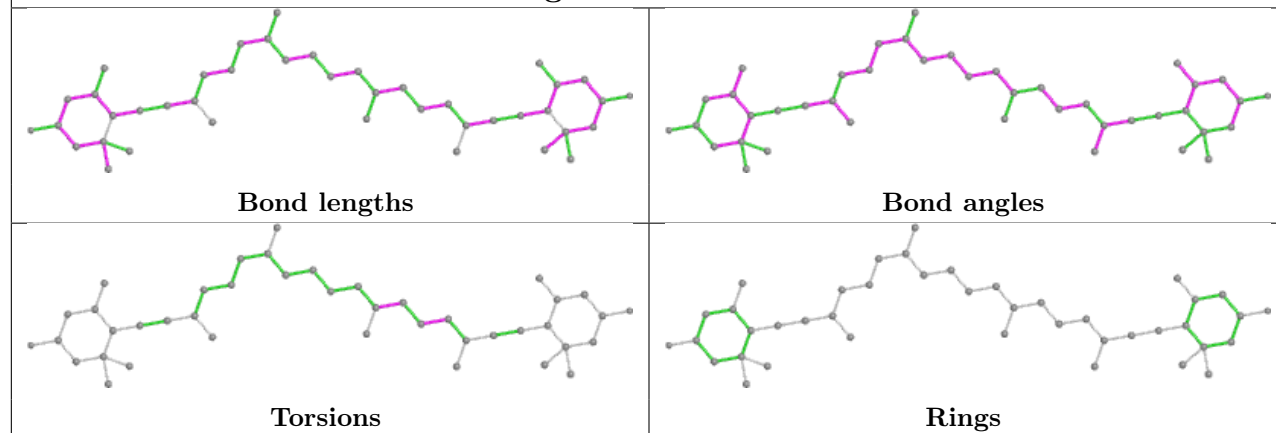
Bond angles

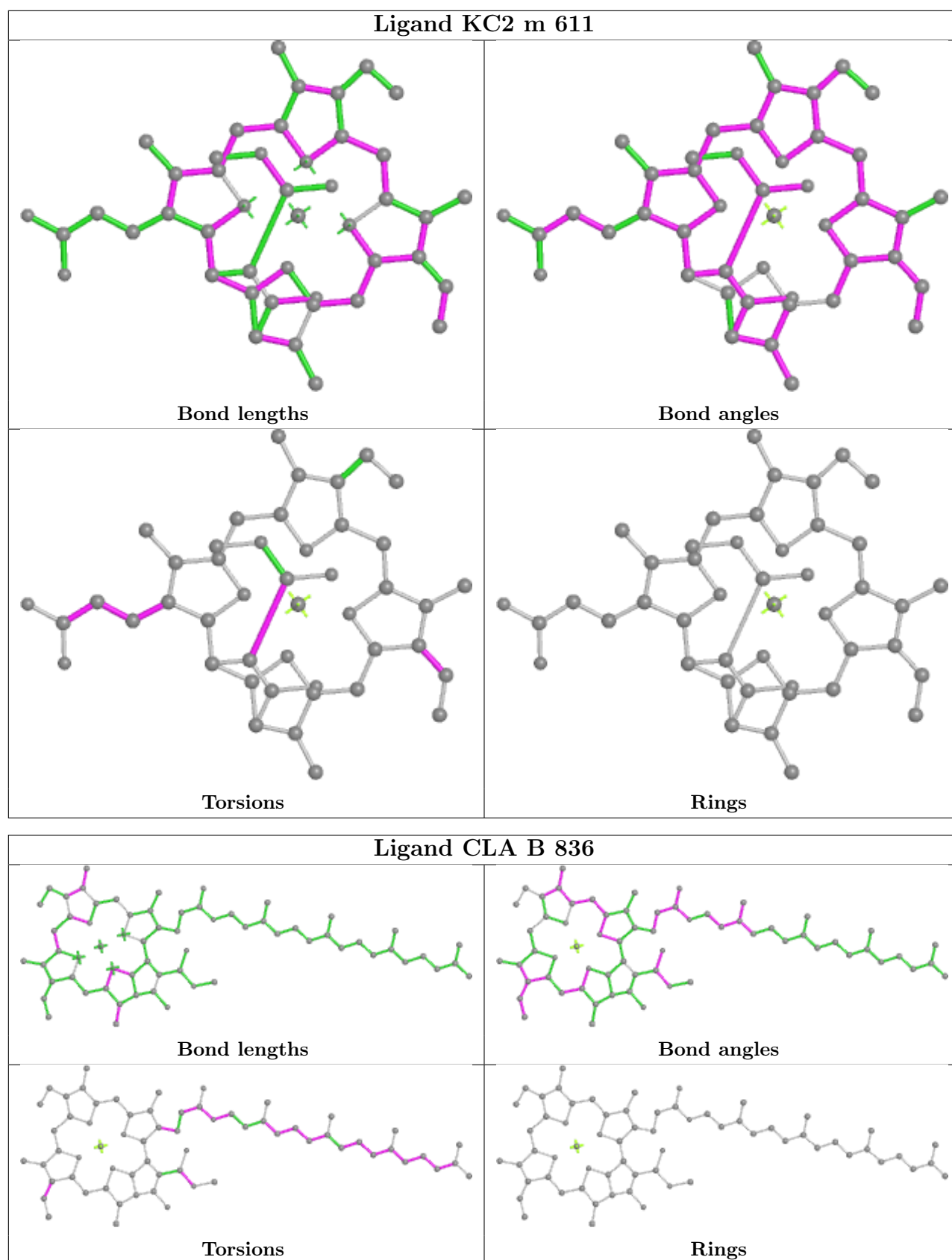


Torsions

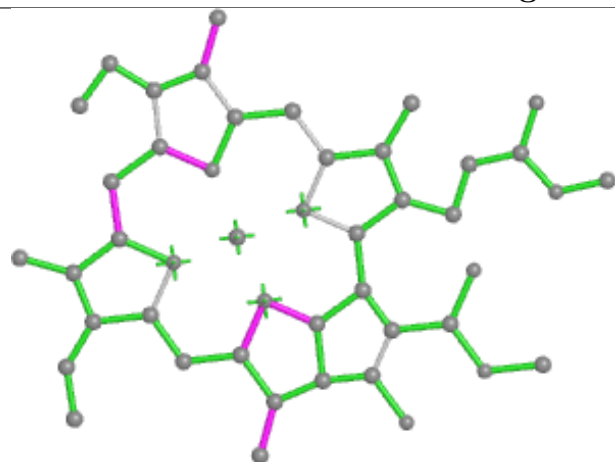


Rings

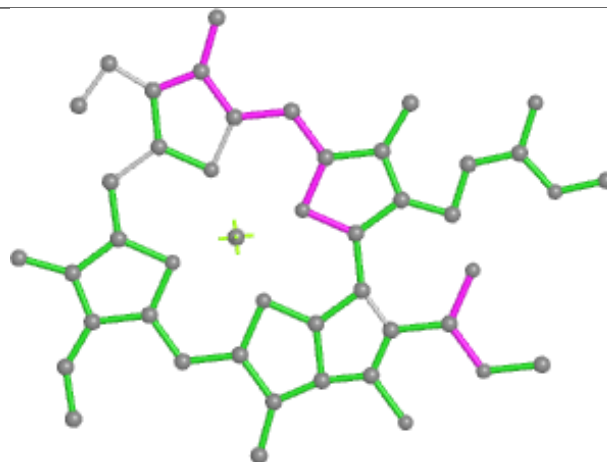
Ligand CLA k 603**Ligand II0 m 614**



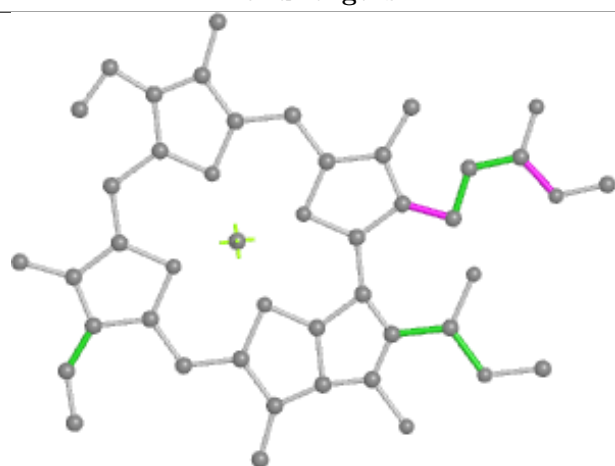
Ligand CLA d 307



Bond lengths



Bond angles

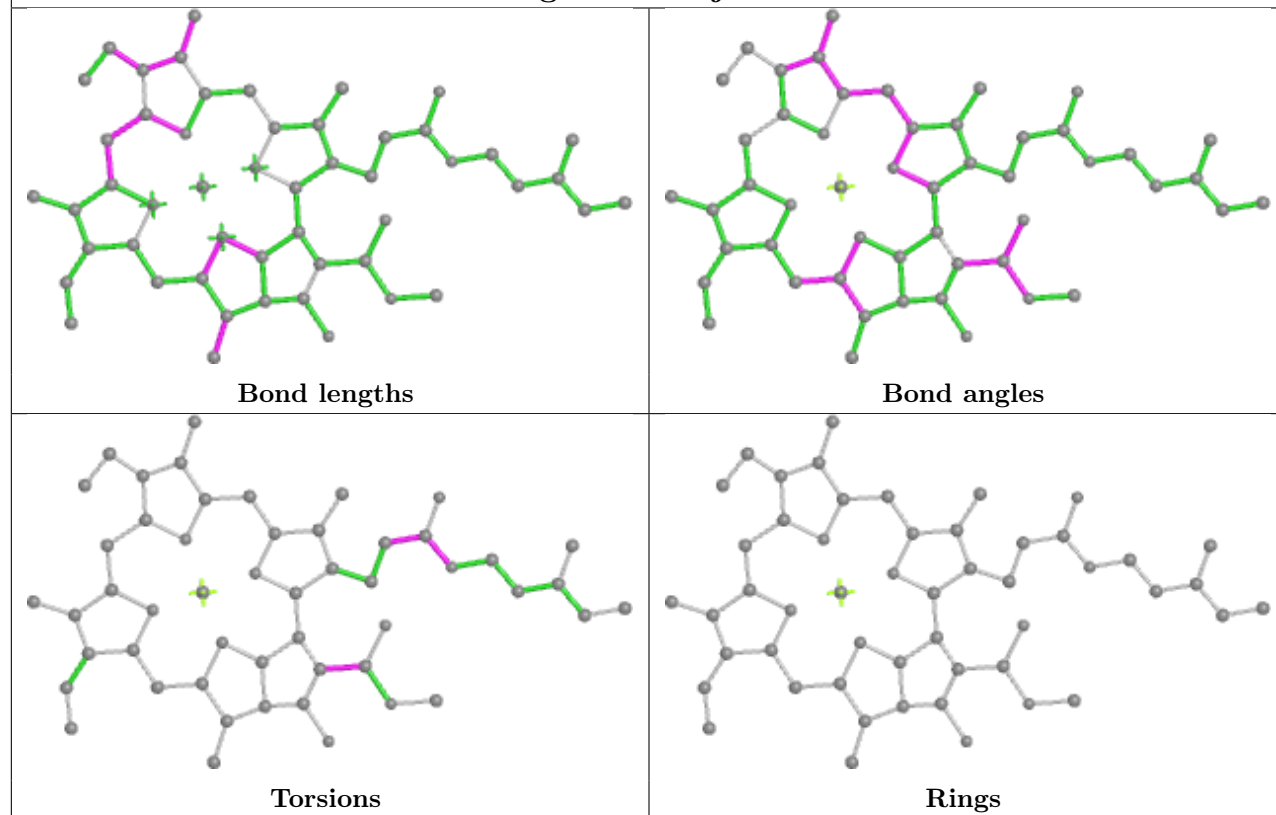


Torsions

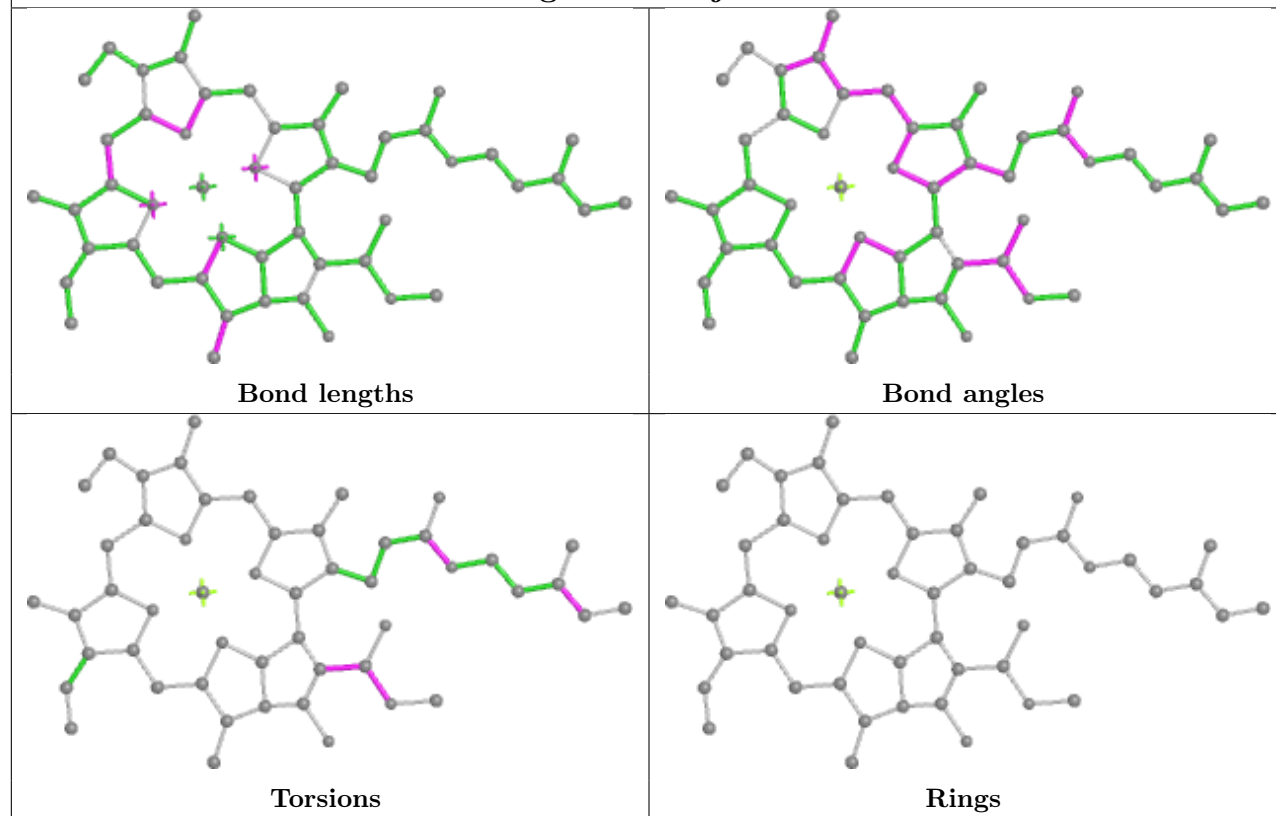


Rings

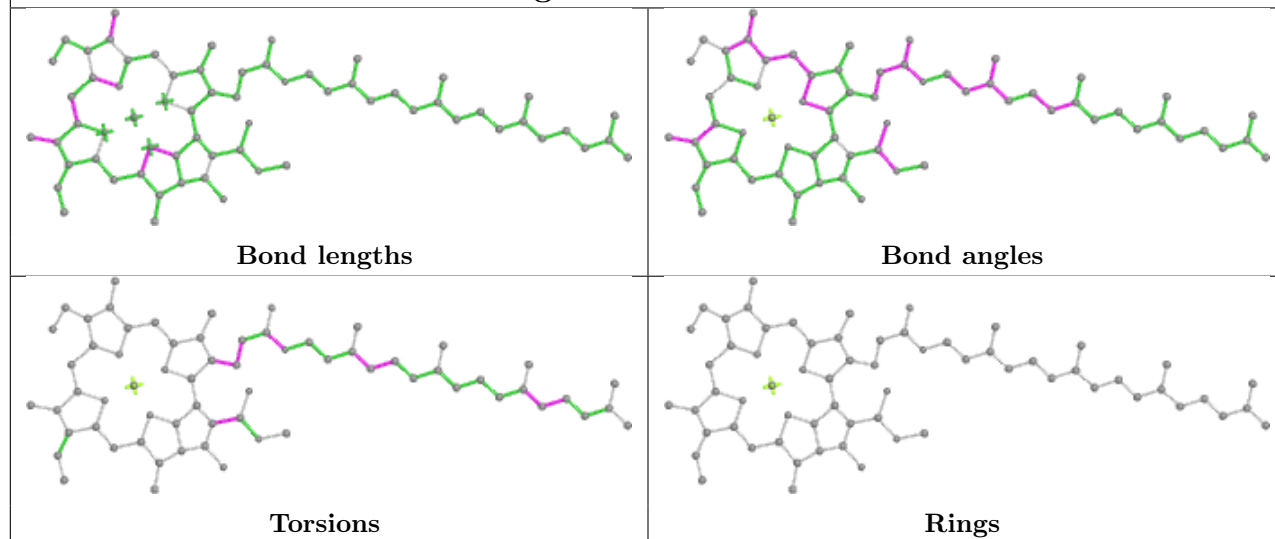
Ligand CLA j 607



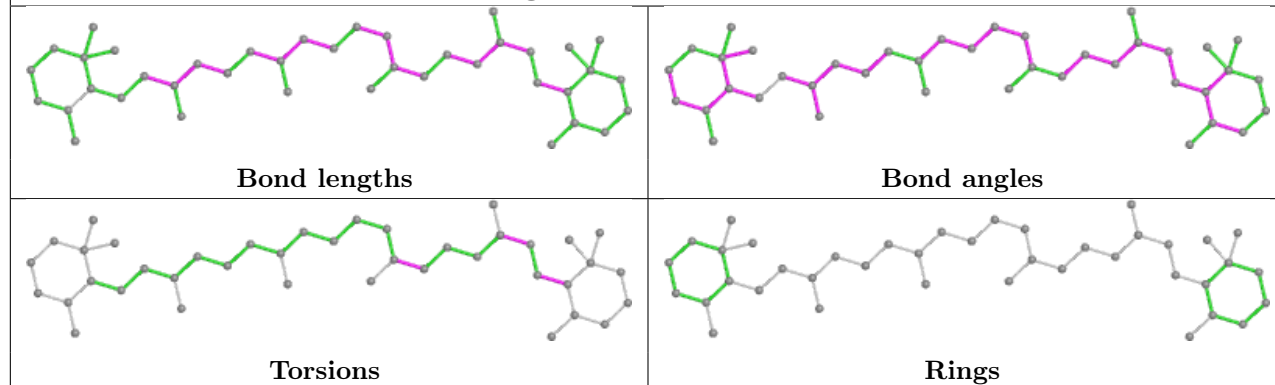
Ligand CLA j 612



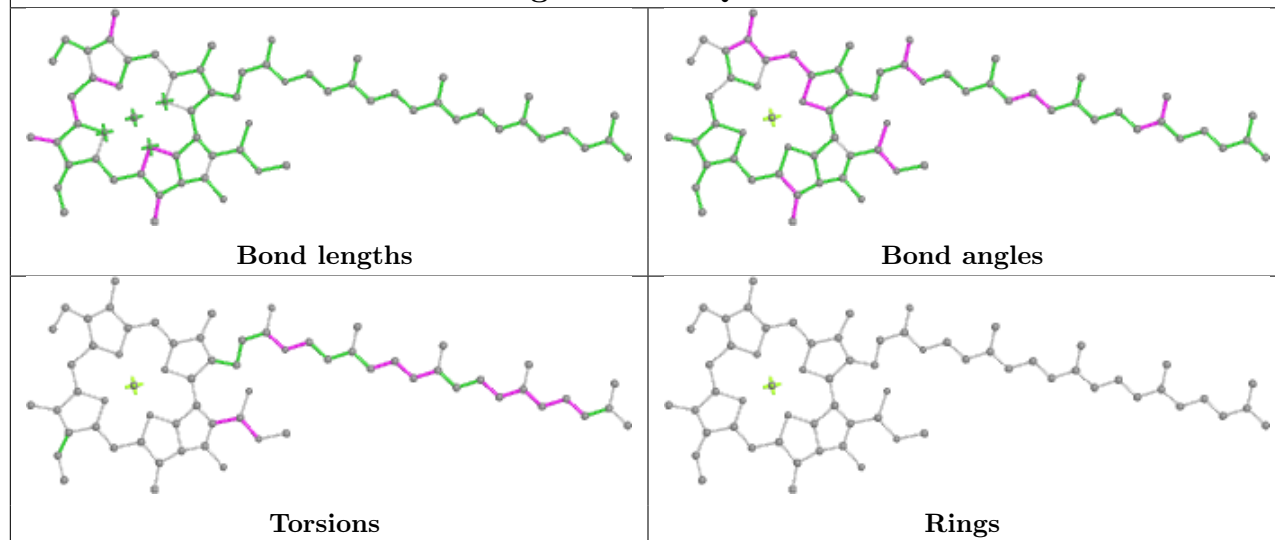
Ligand CLA n 609



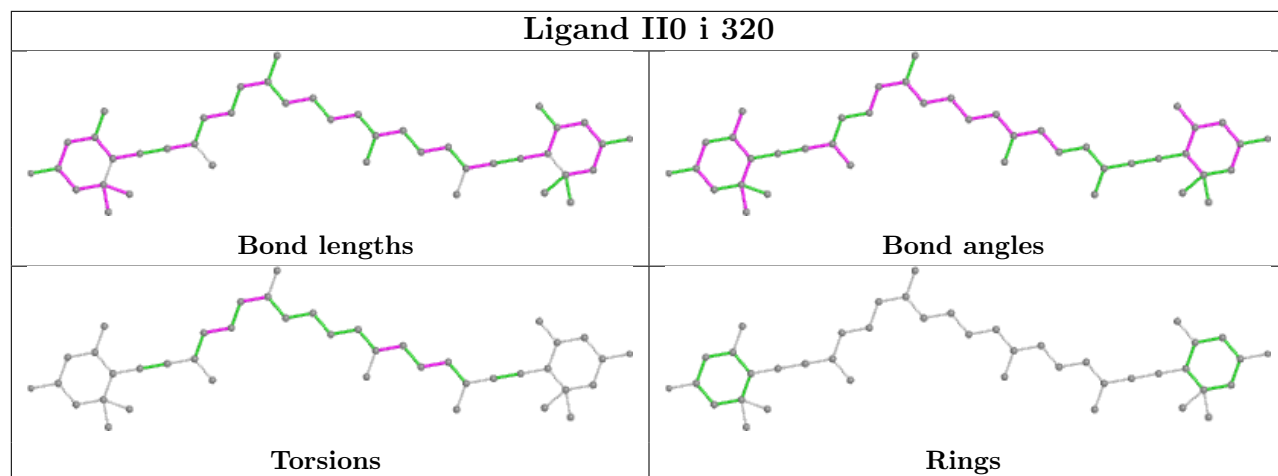
Ligand WVN B 844



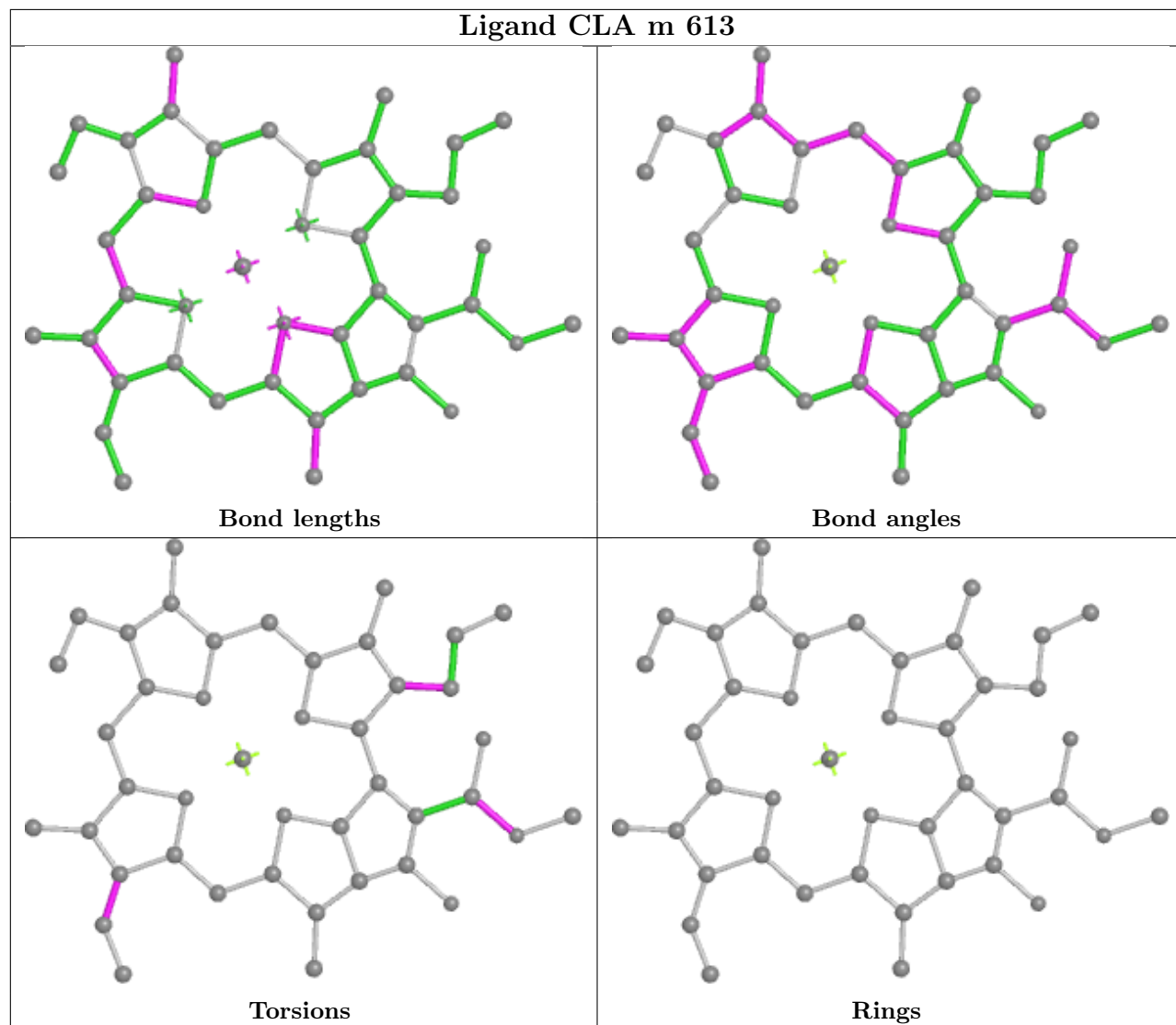
Ligand CLA Q 302



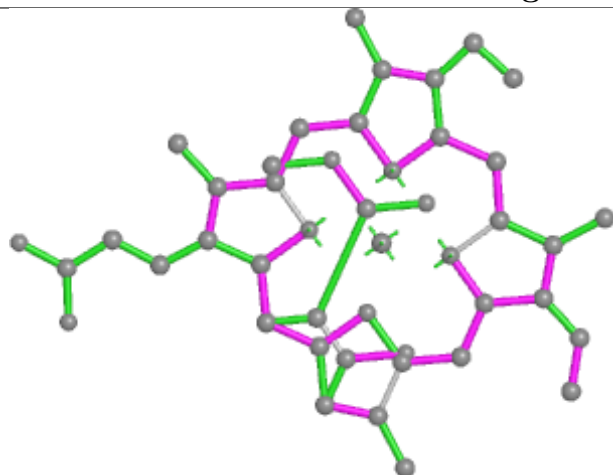
Ligand II0 i 320



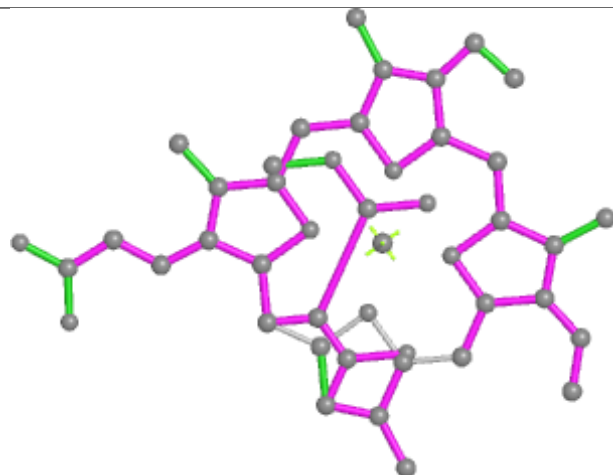
Ligand CLA m 613



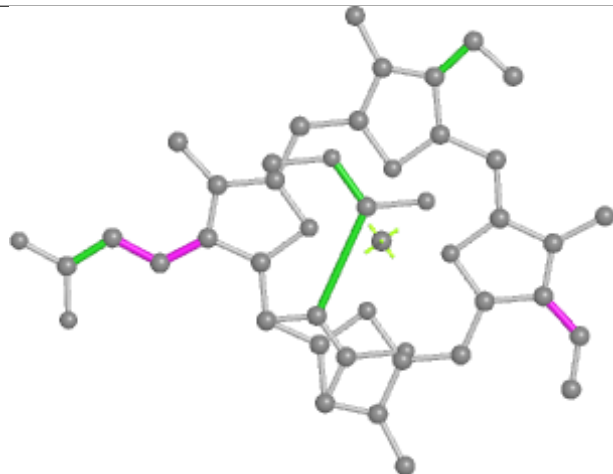
Ligand KC2 s 204



Bond lengths



Bond angles

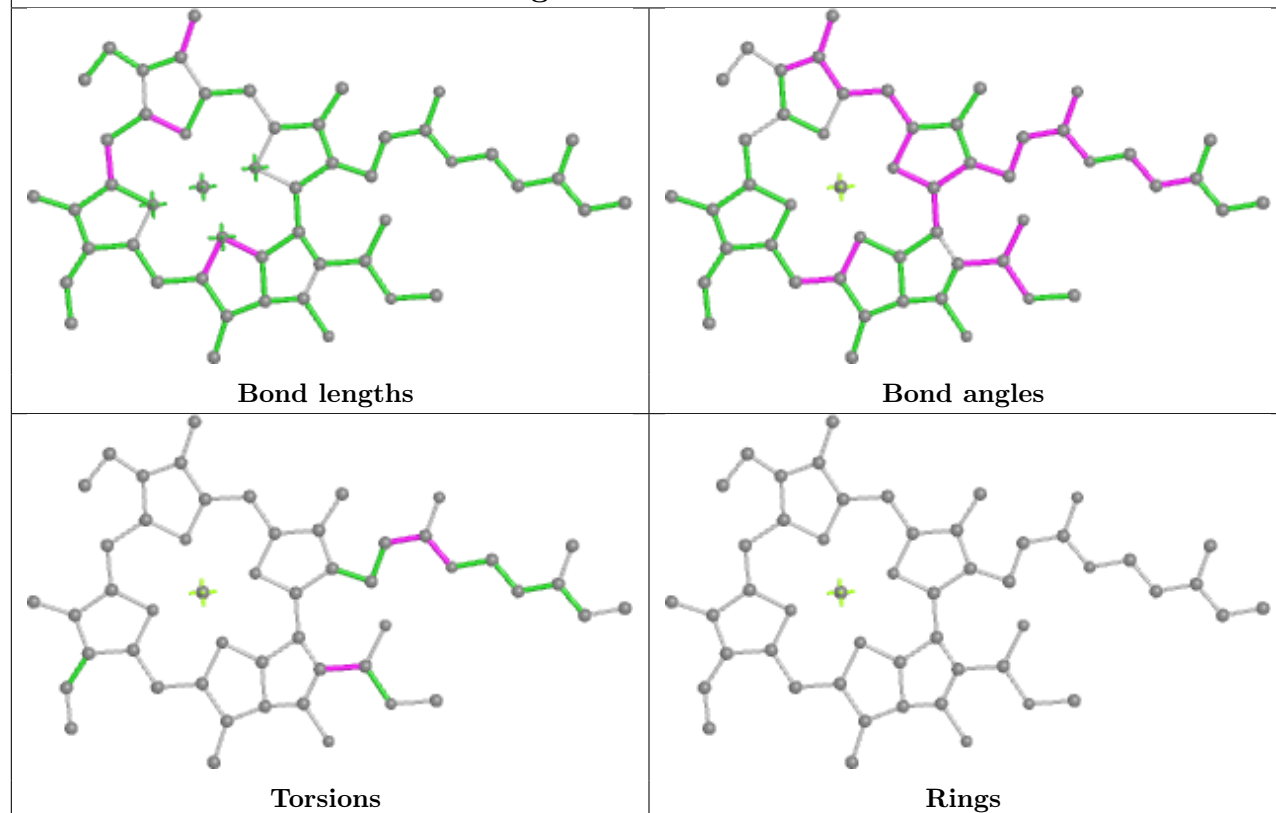


Torsions

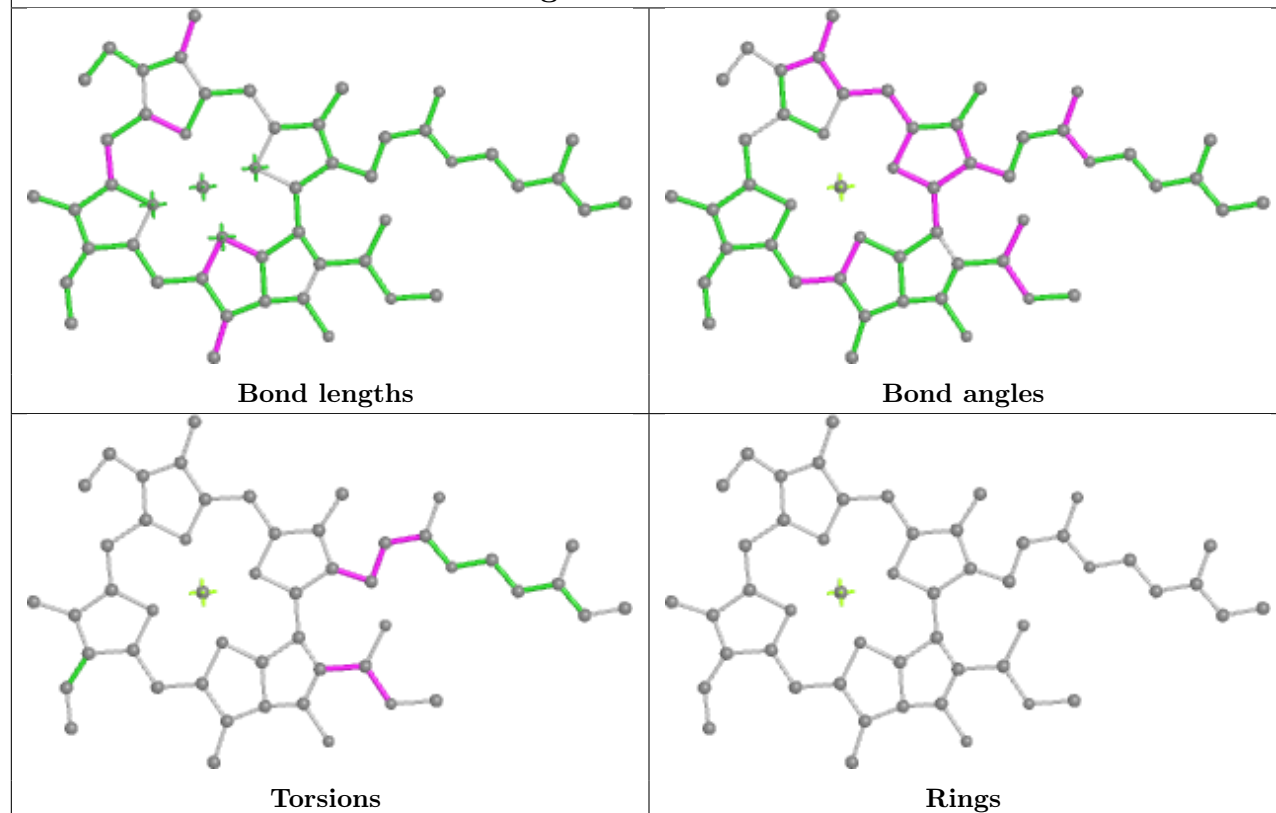


Rings

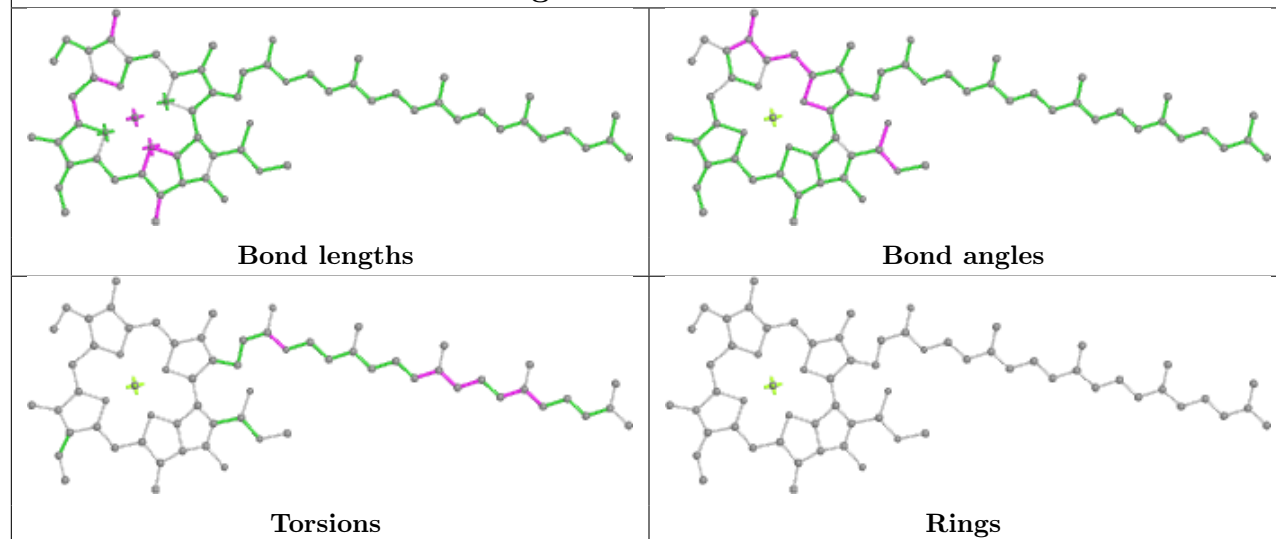
Ligand CLA K 101



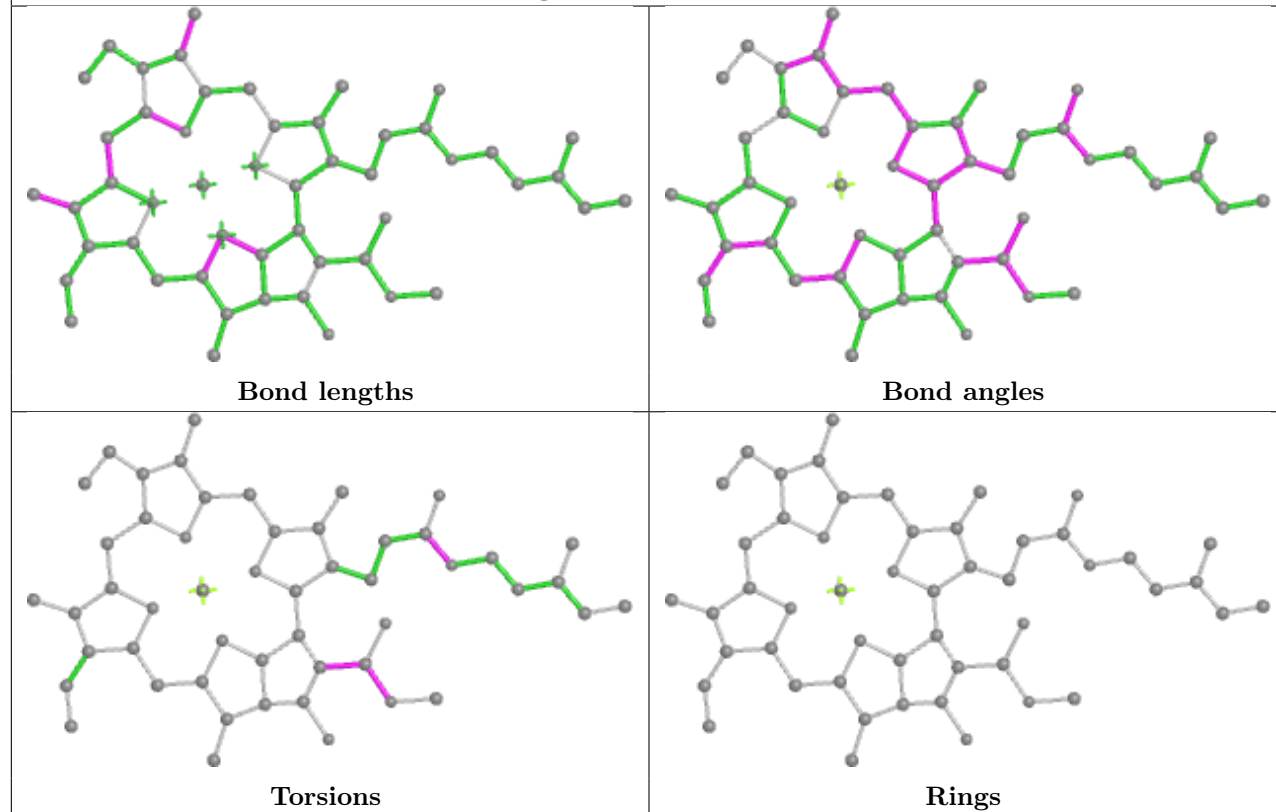
Ligand CLA i 312

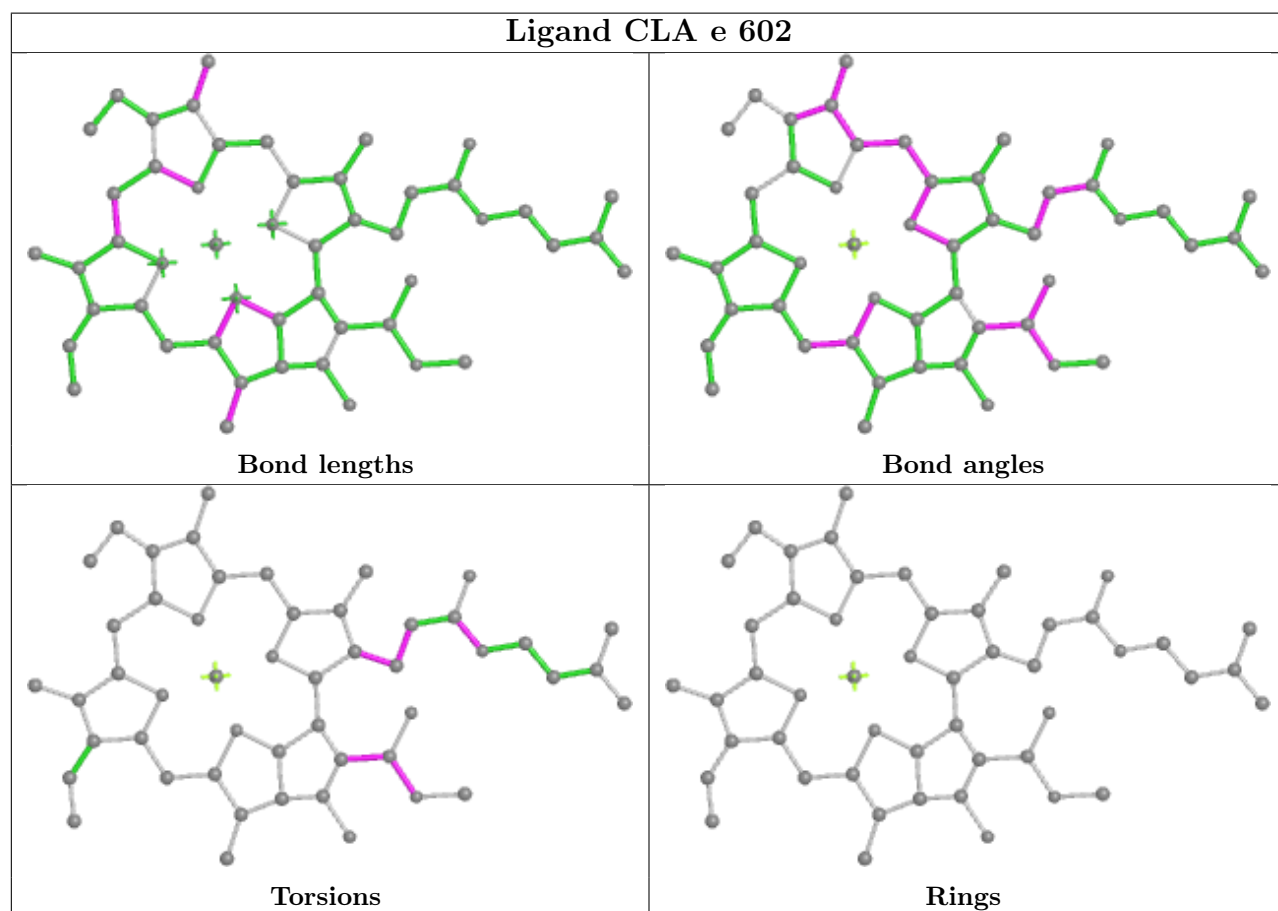
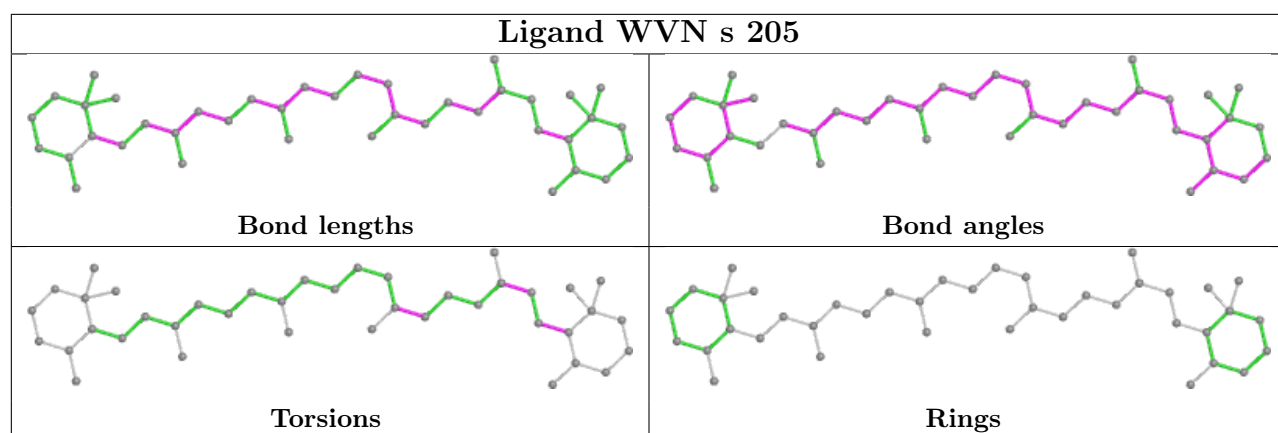


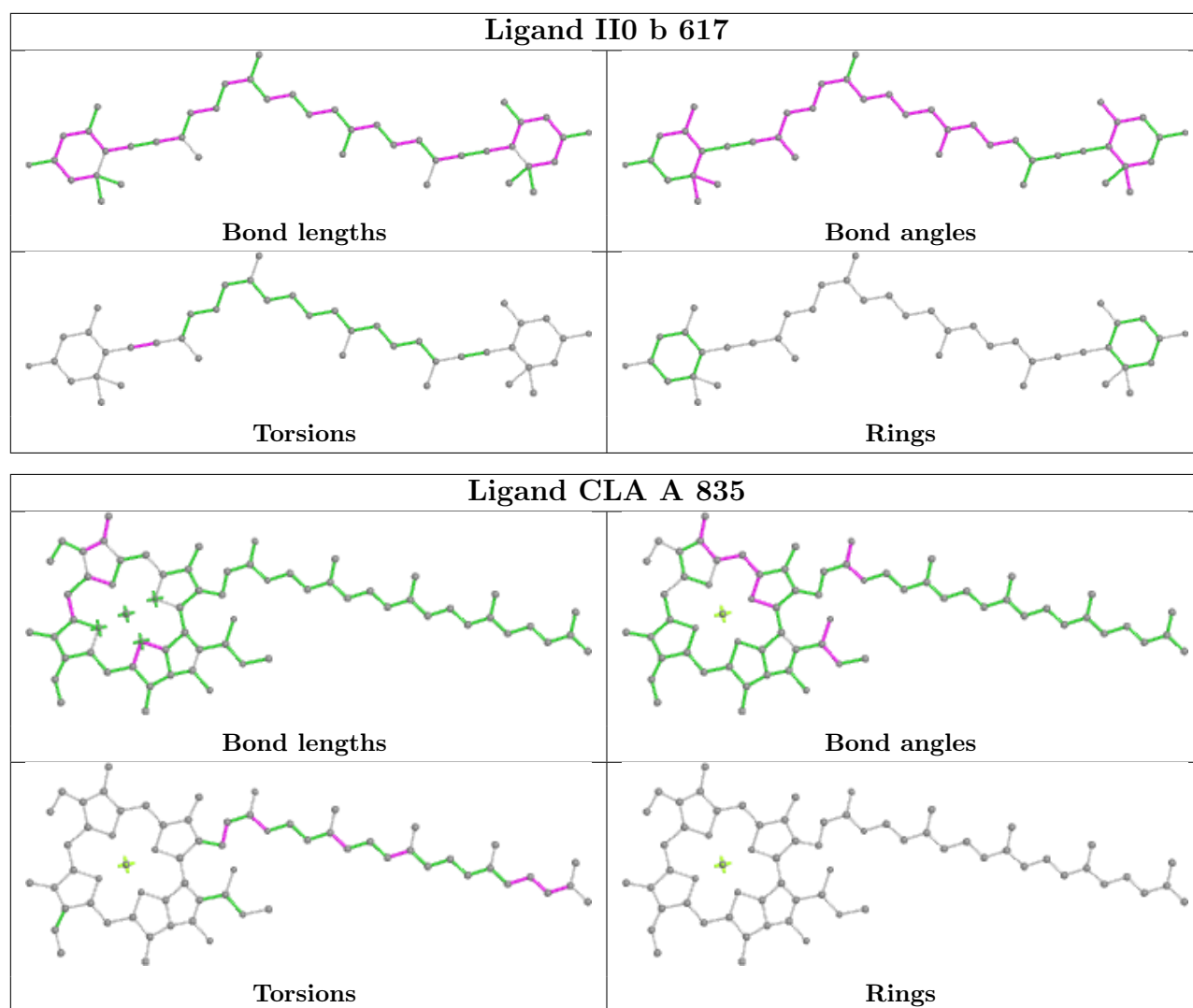
Ligand CLA A 825



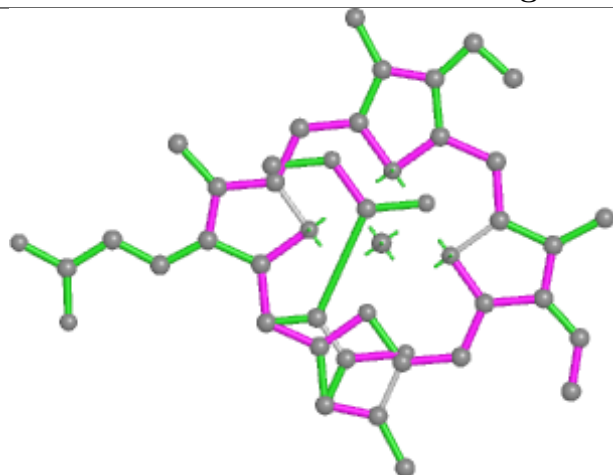
Ligand CLA d 312



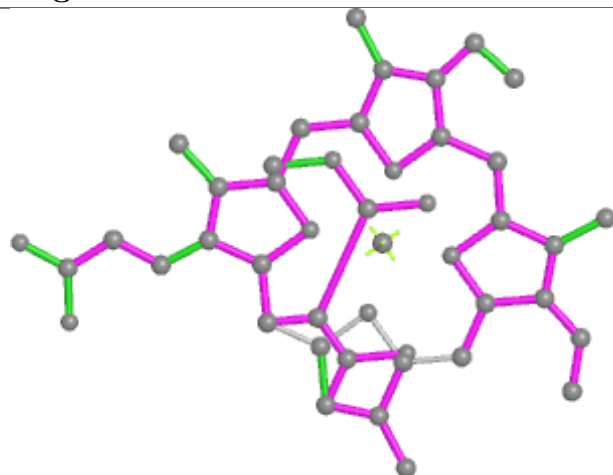




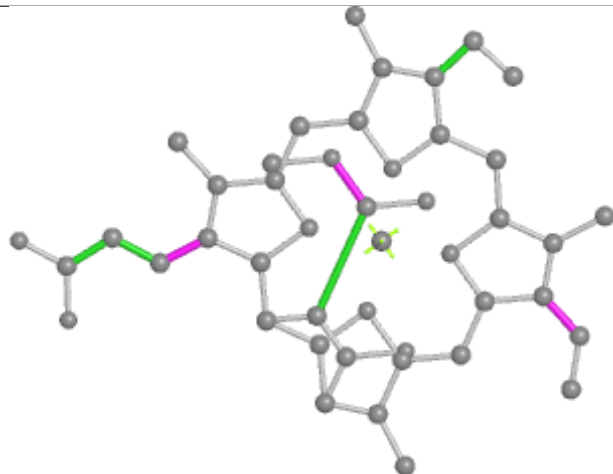
Ligand KC2 g 314



Bond lengths



Bond angles

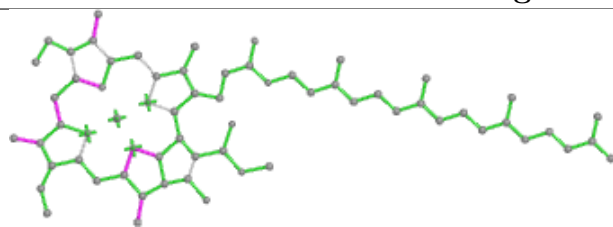


Torsions

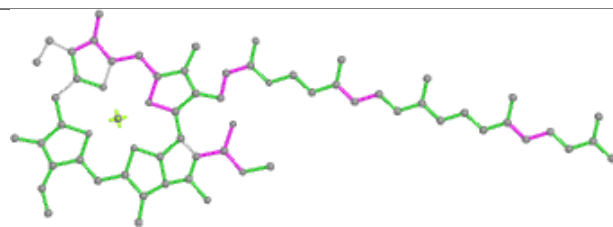


Rings

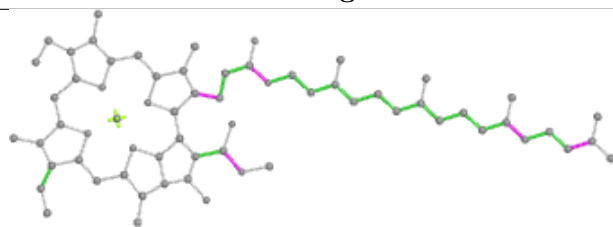
Ligand CLA A 837



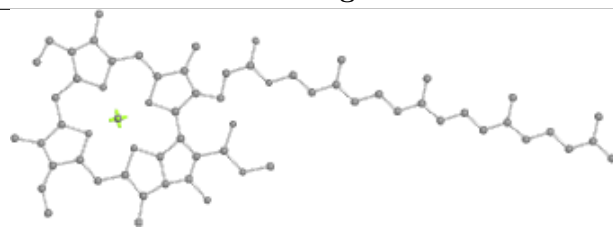
Bond lengths



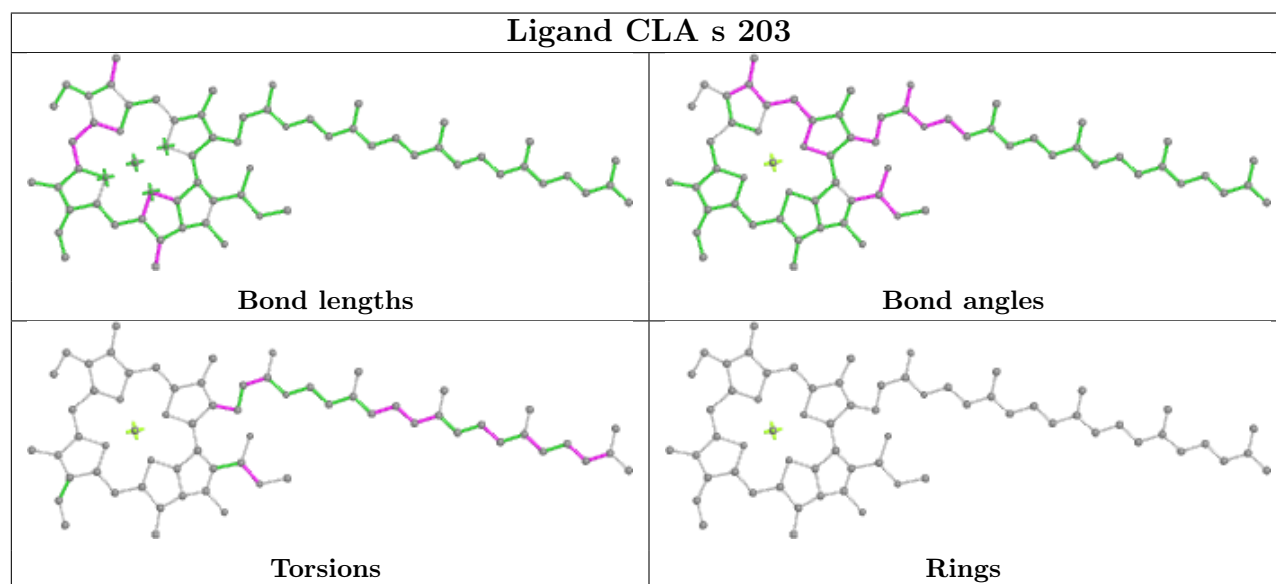
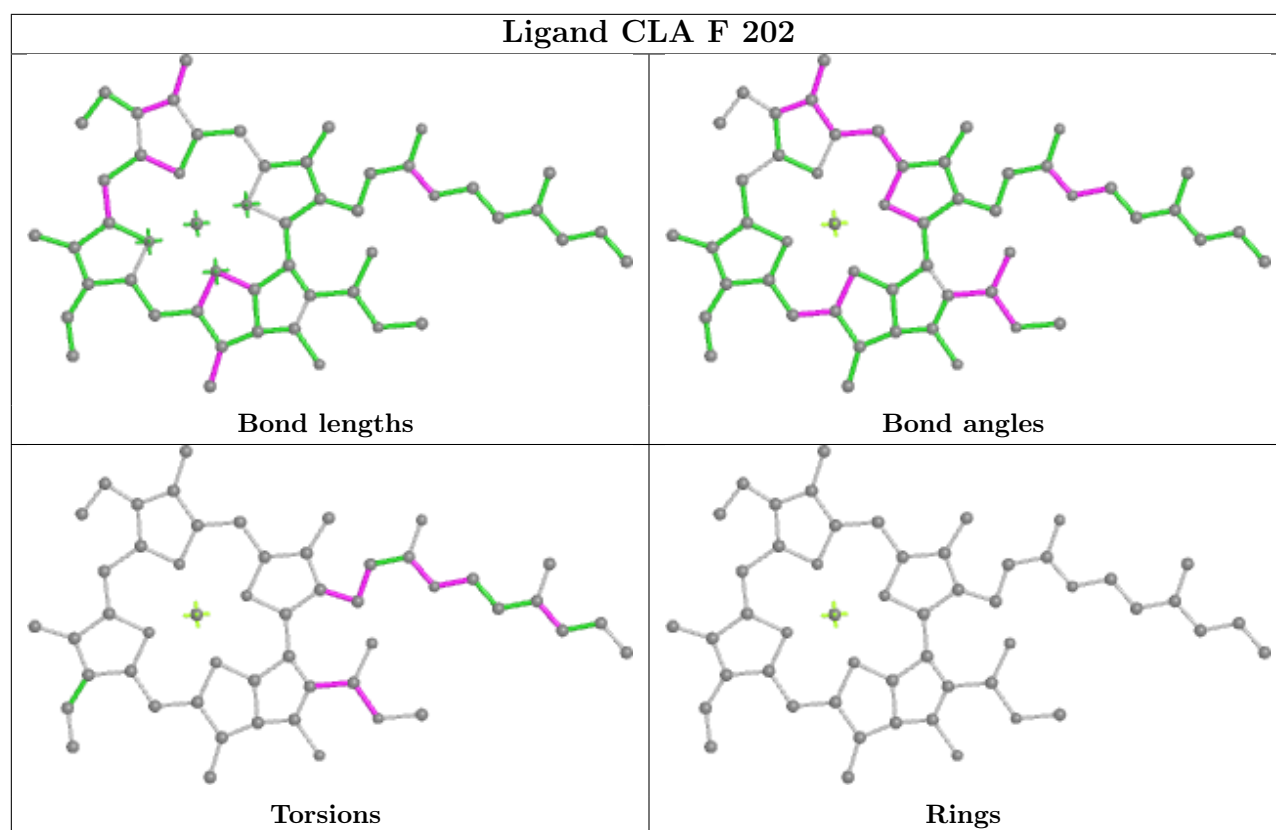
Bond angles

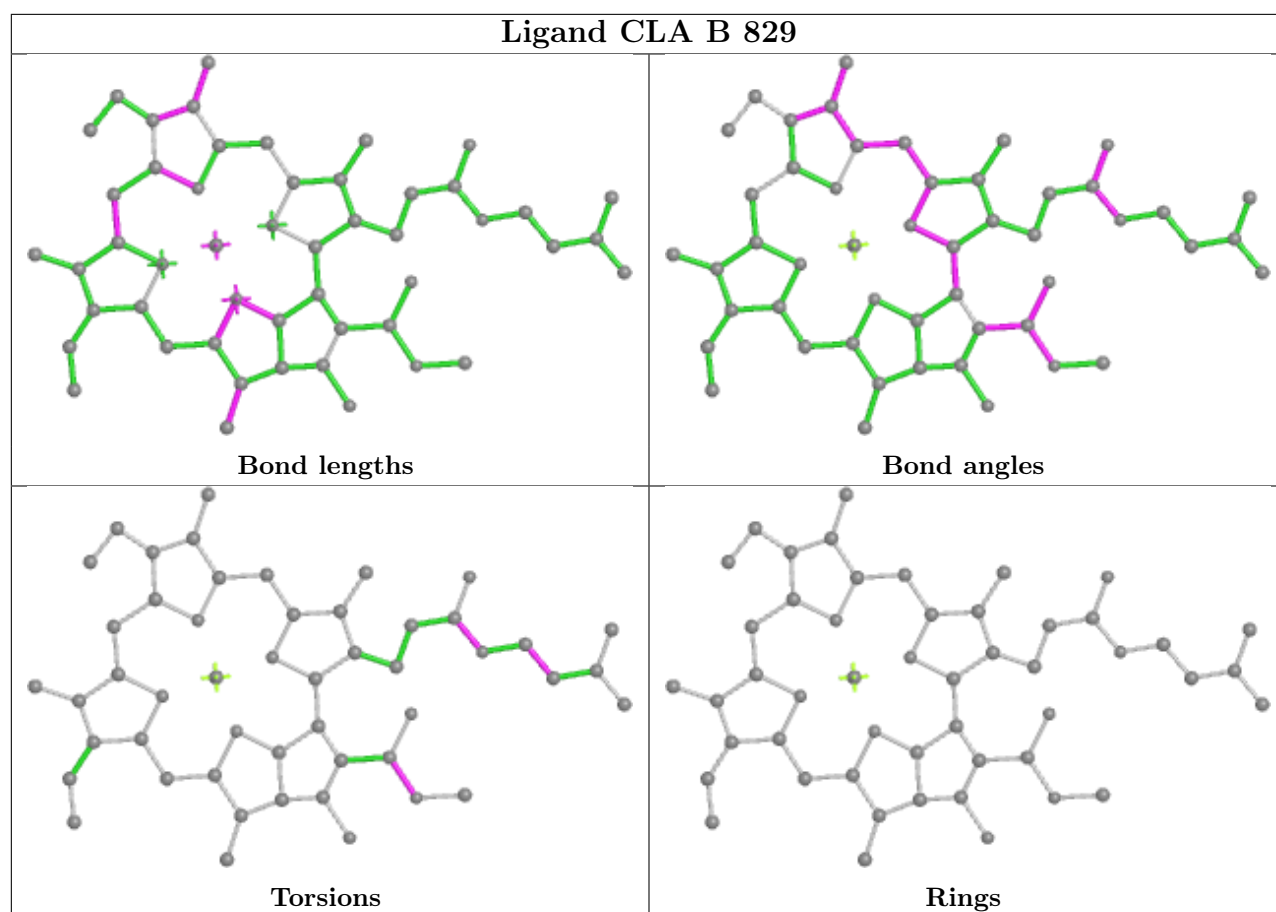


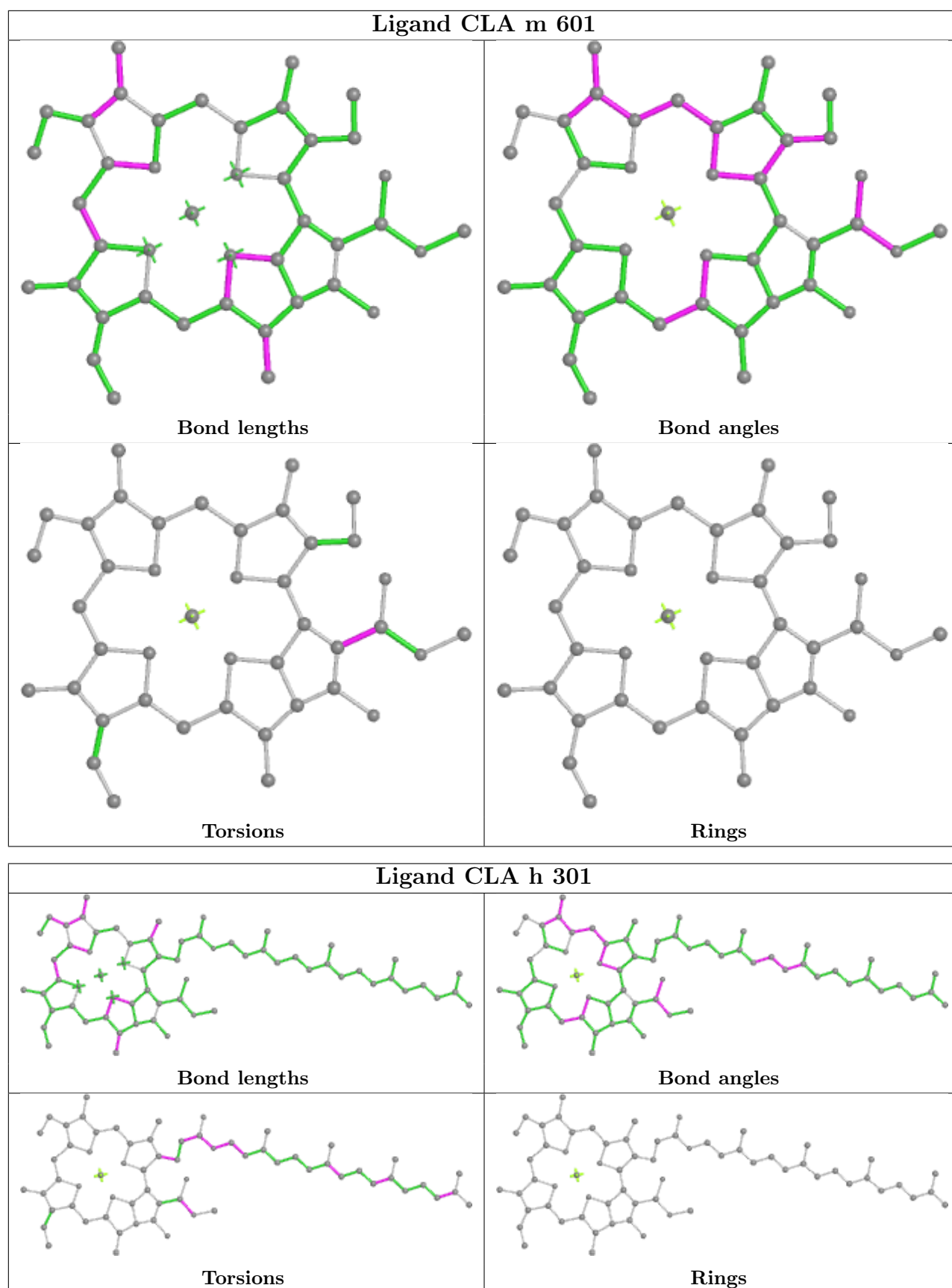
Torsions



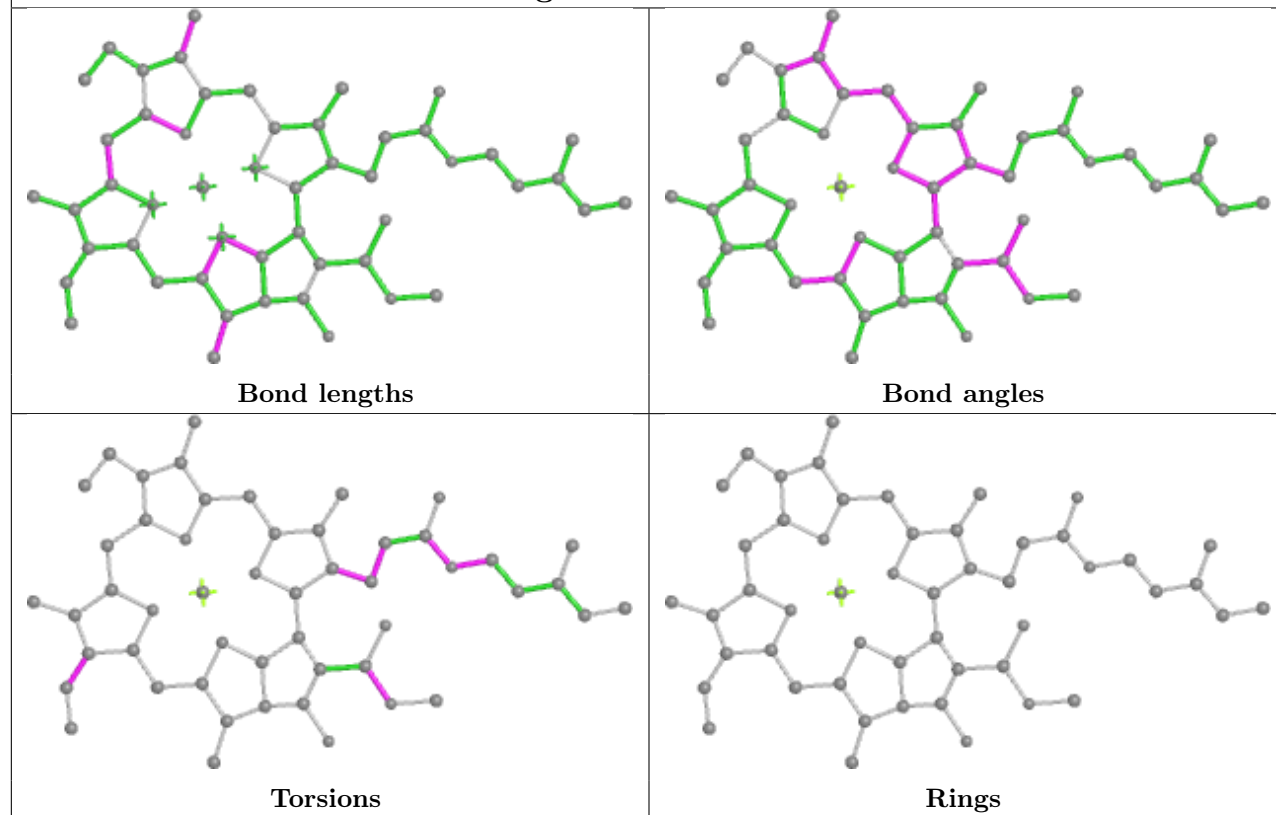
Rings



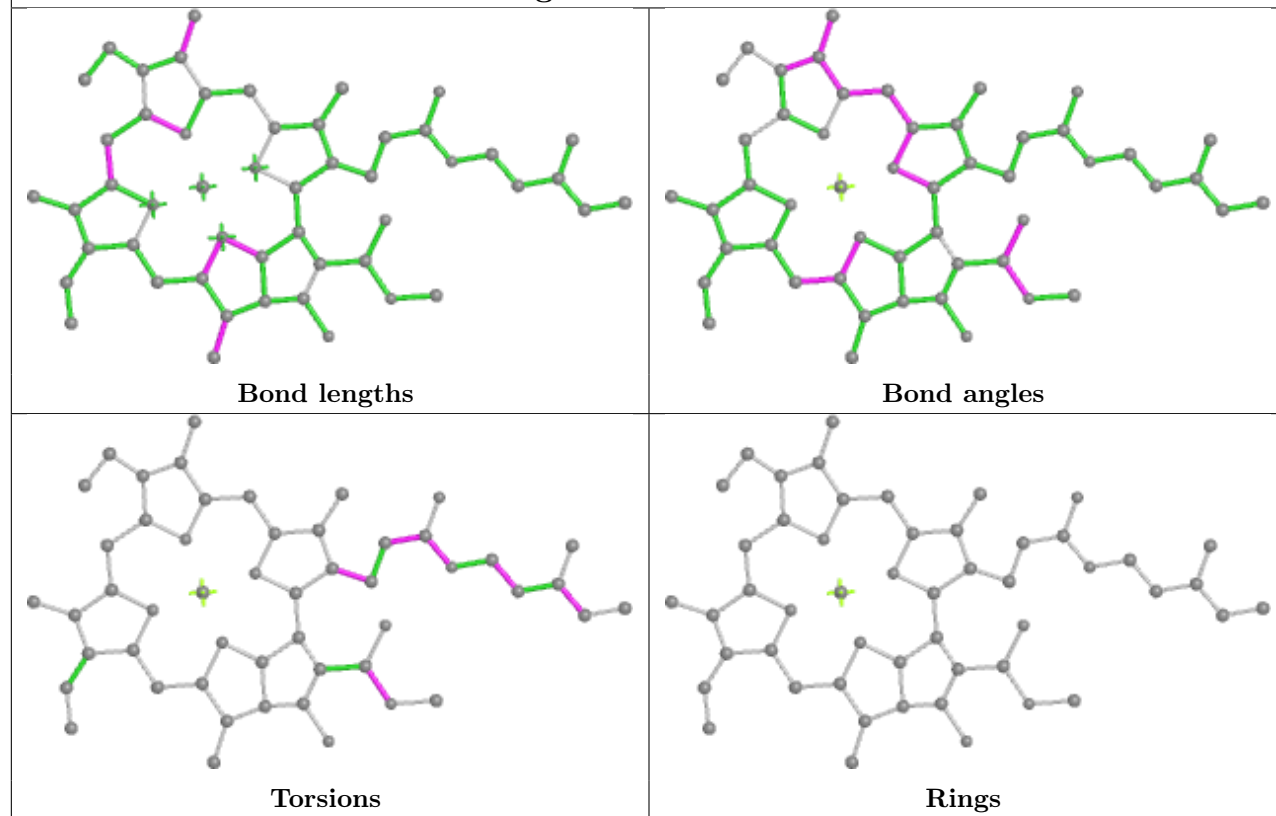




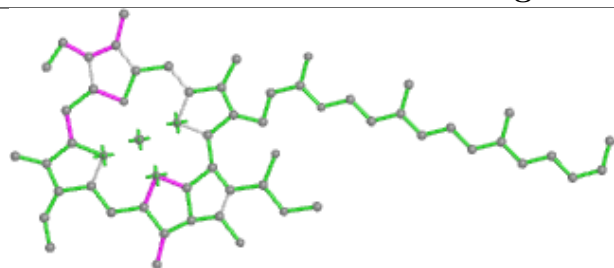
Ligand CLA k 614



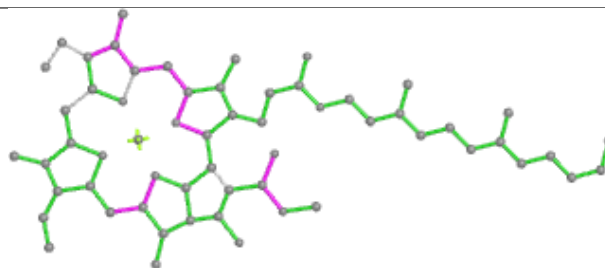
Ligand CLA n 613



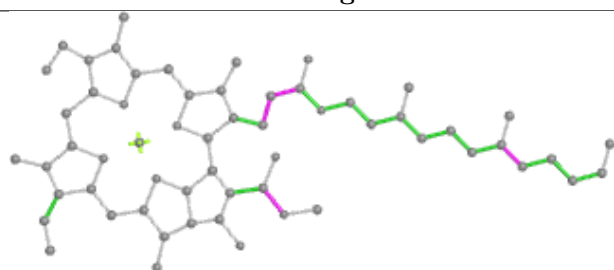
Ligand CLA B 815



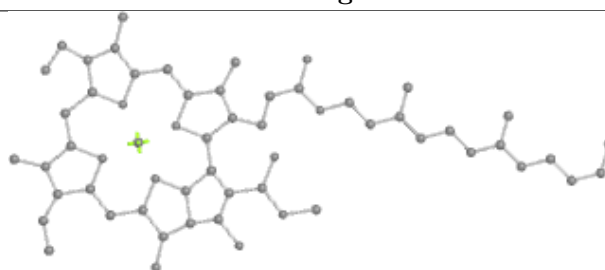
Bond lengths



Bond angles

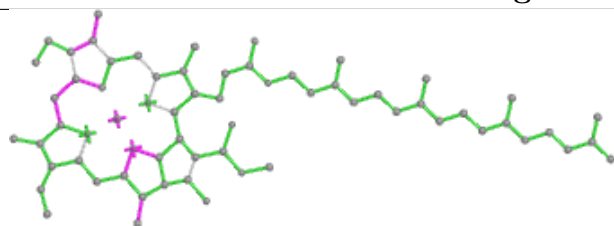


Torsions

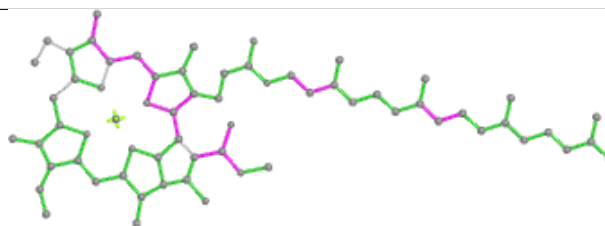


Rings

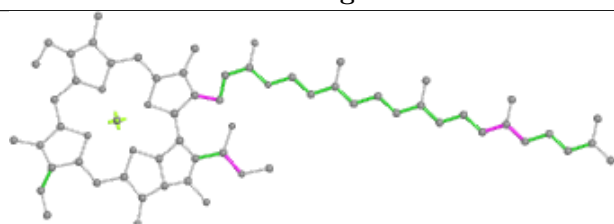
Ligand CLA A 831



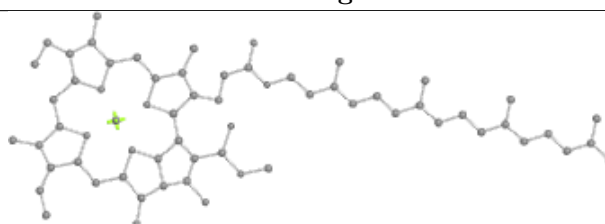
Bond lengths



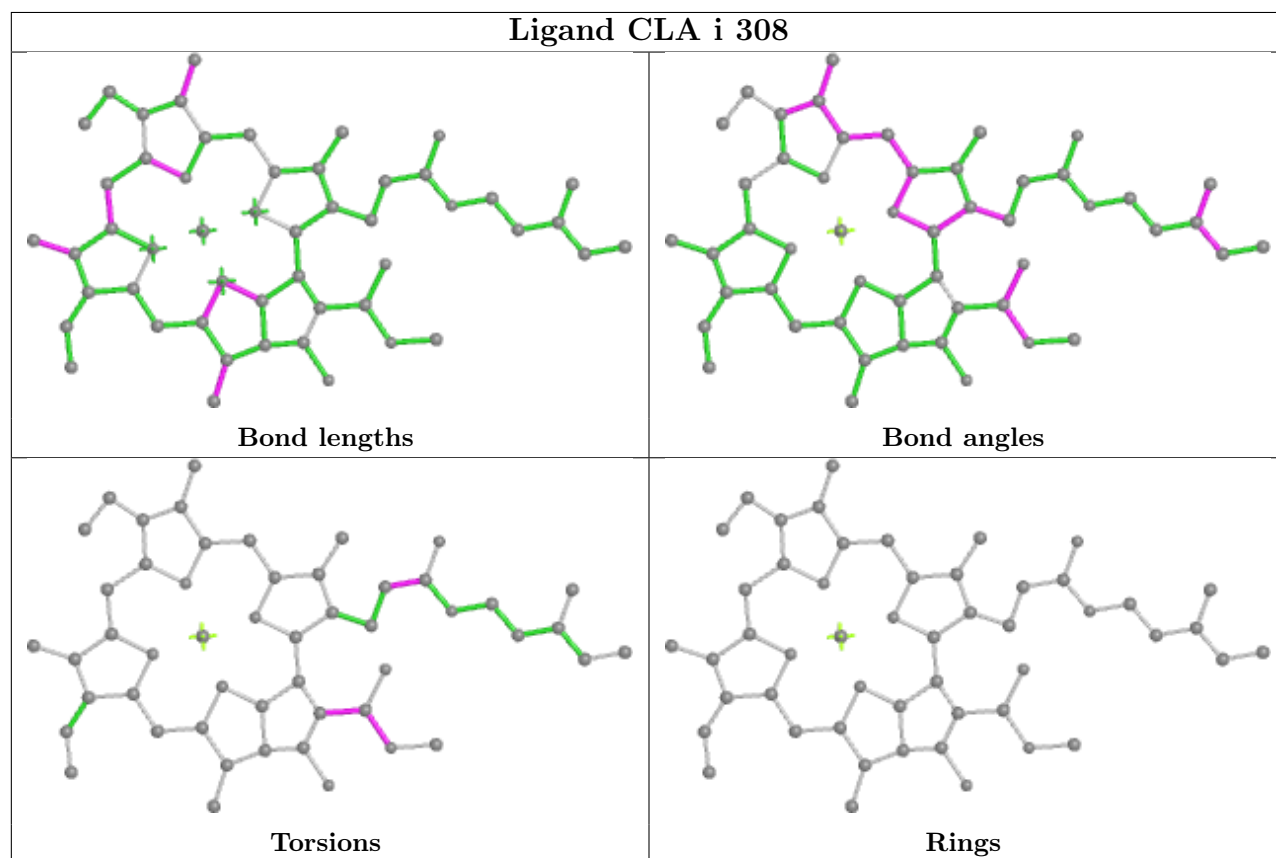
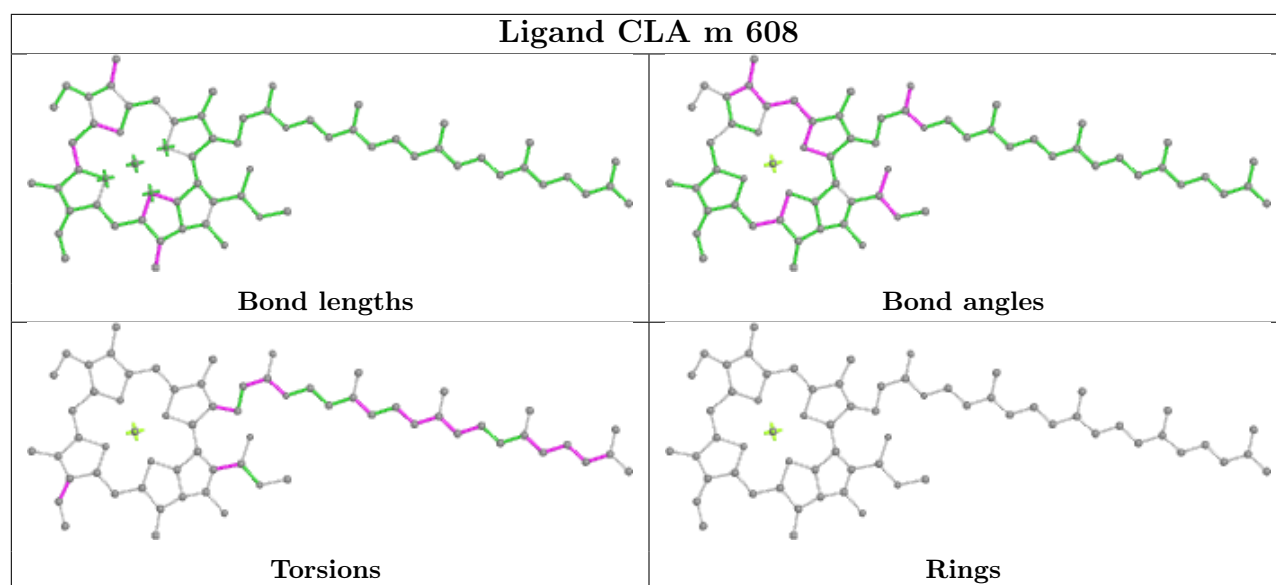
Bond angles

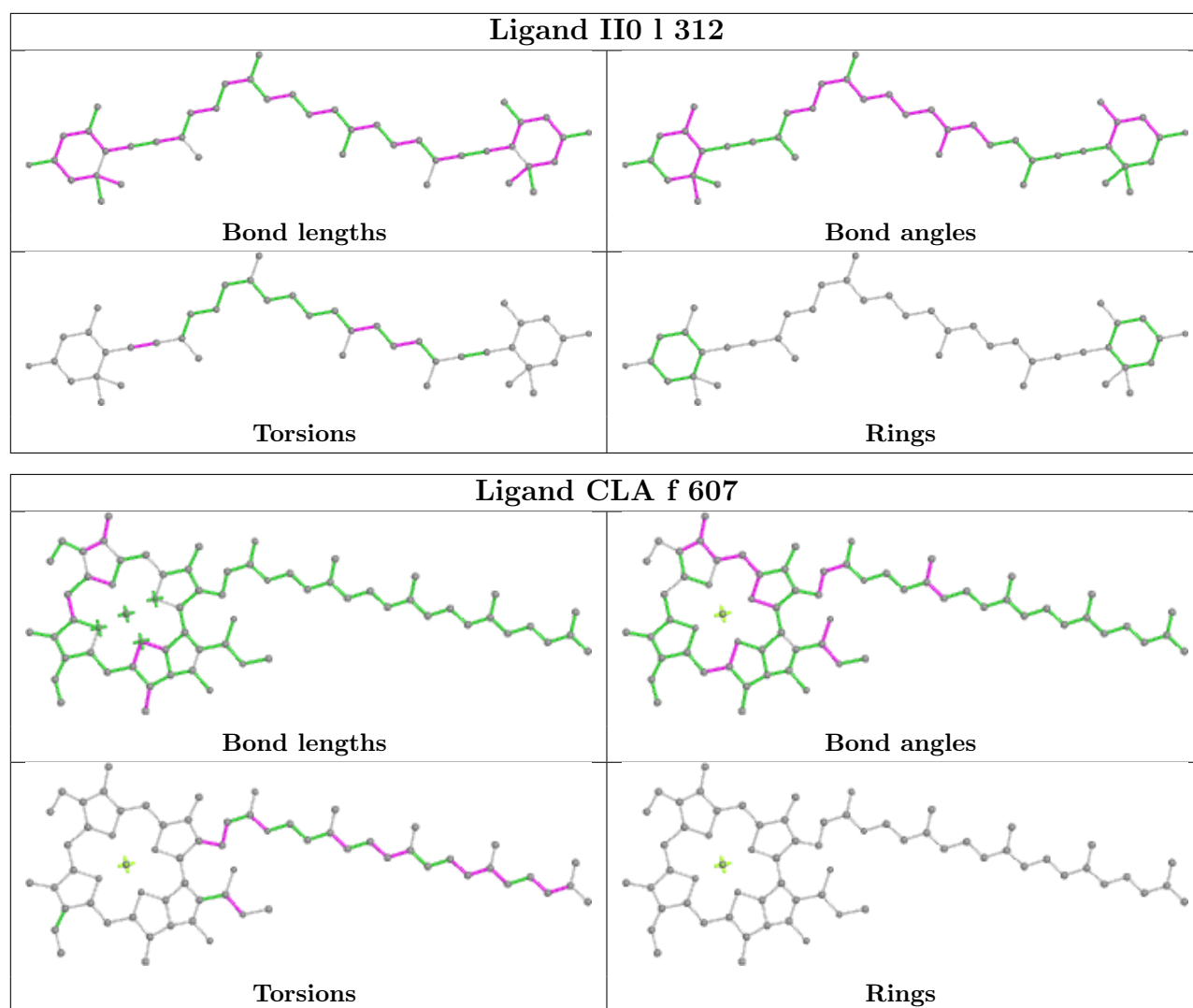


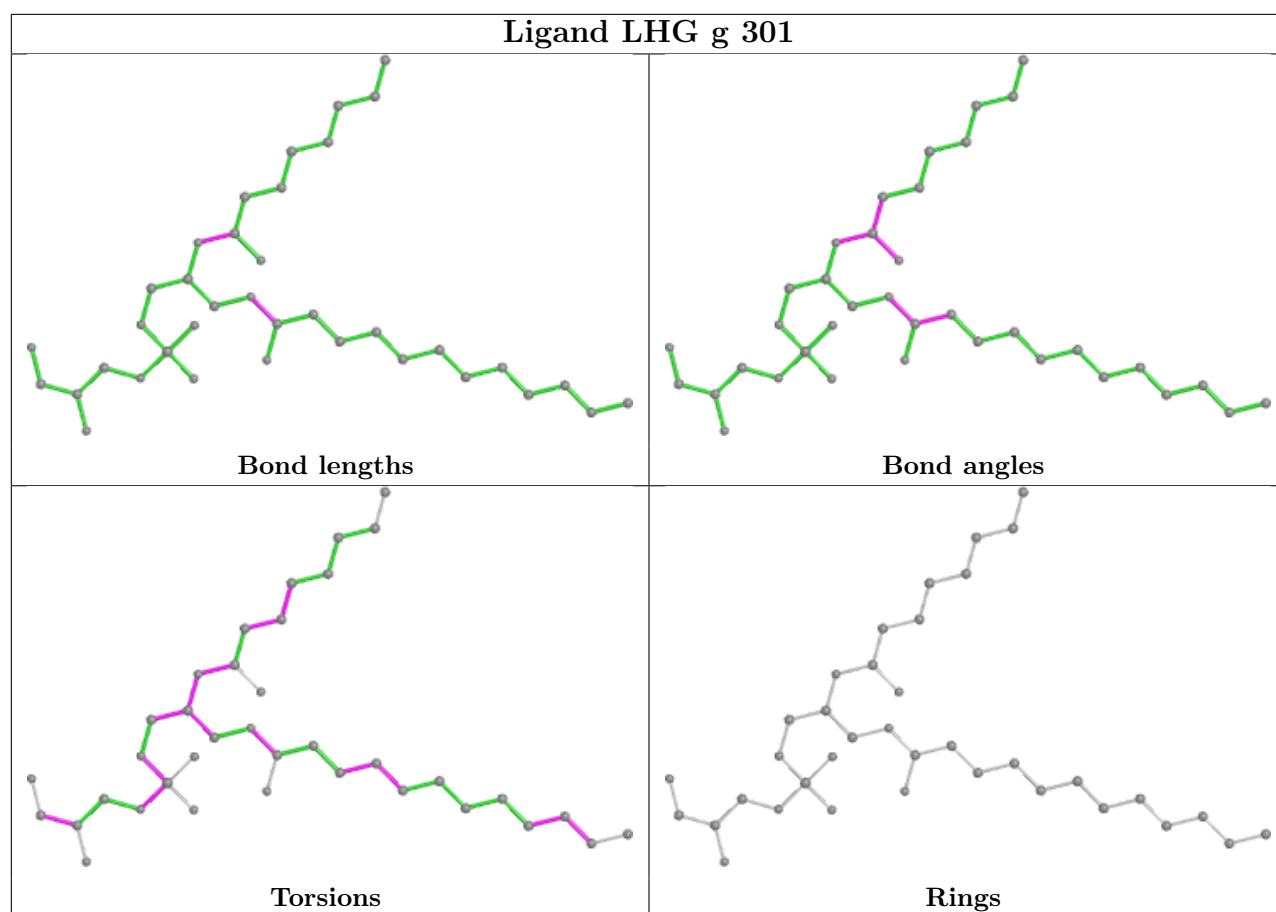
Torsions



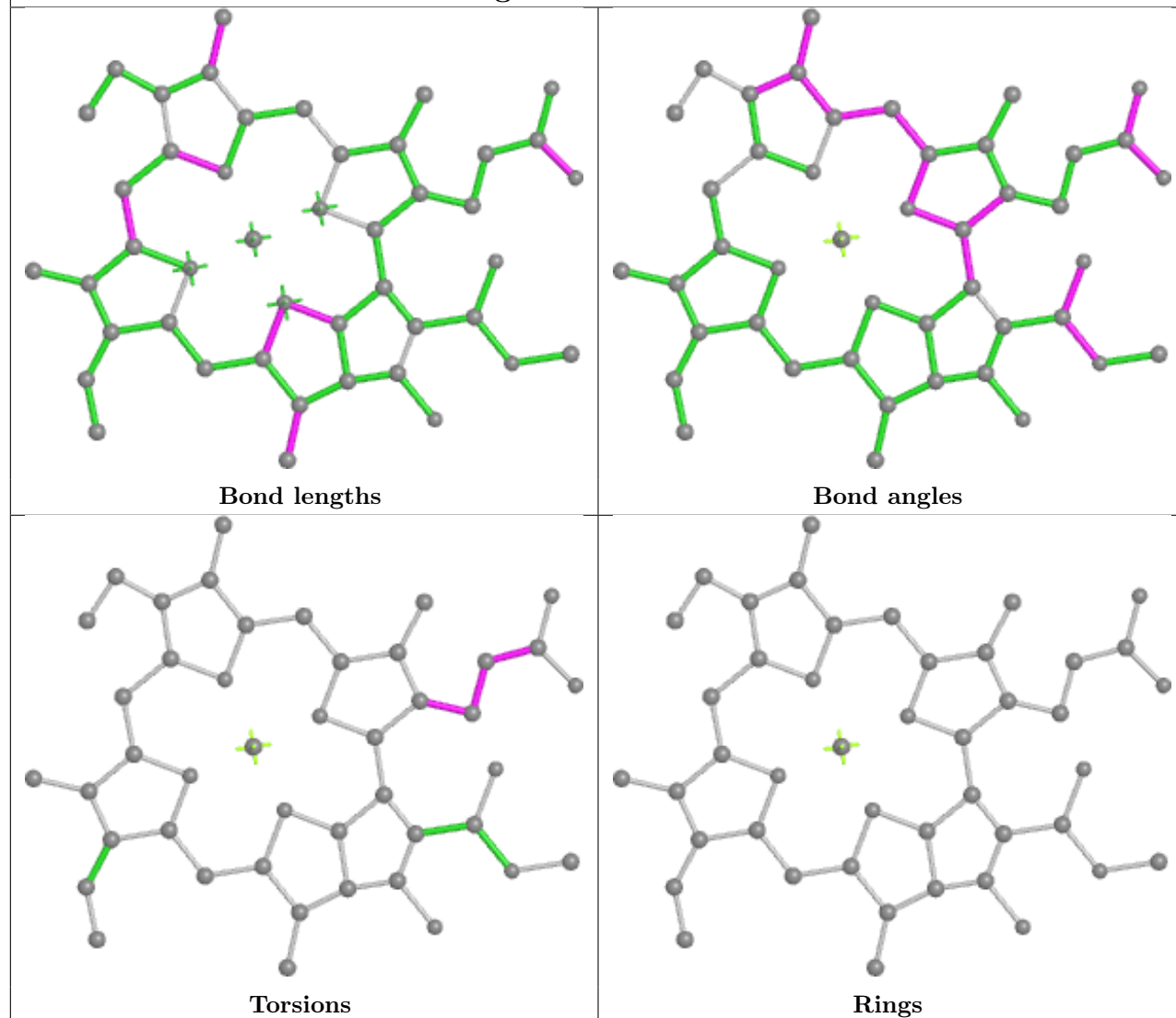
Rings



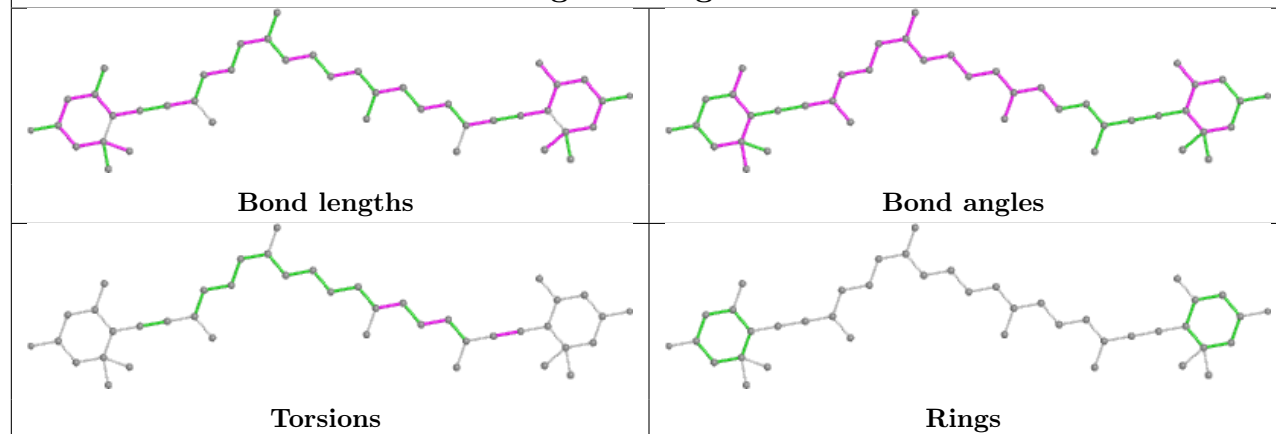




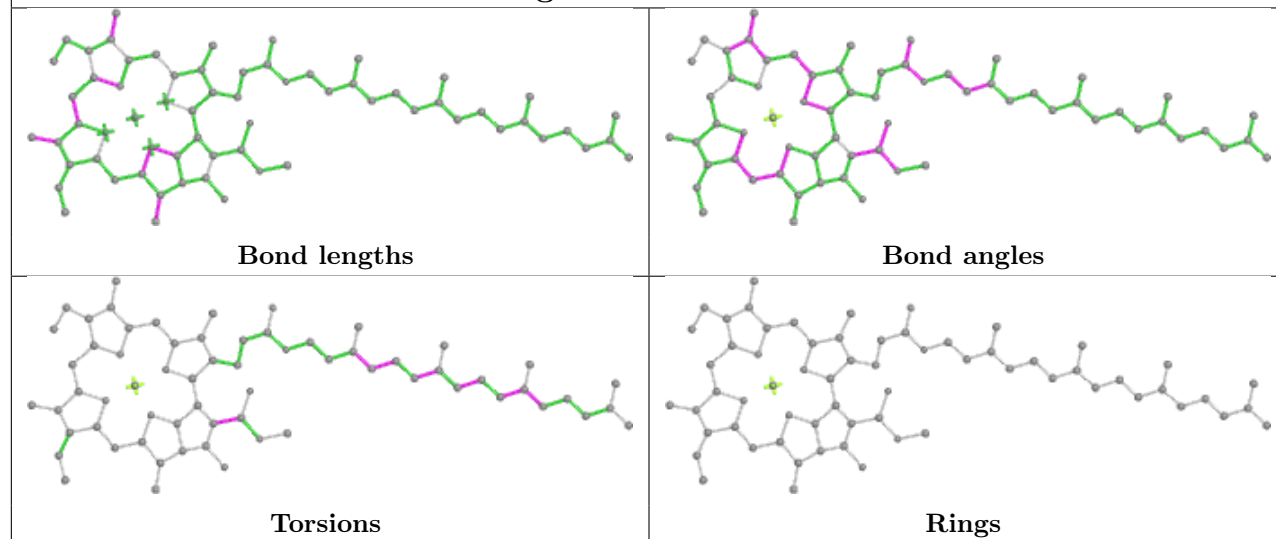
Ligand CLA e 601



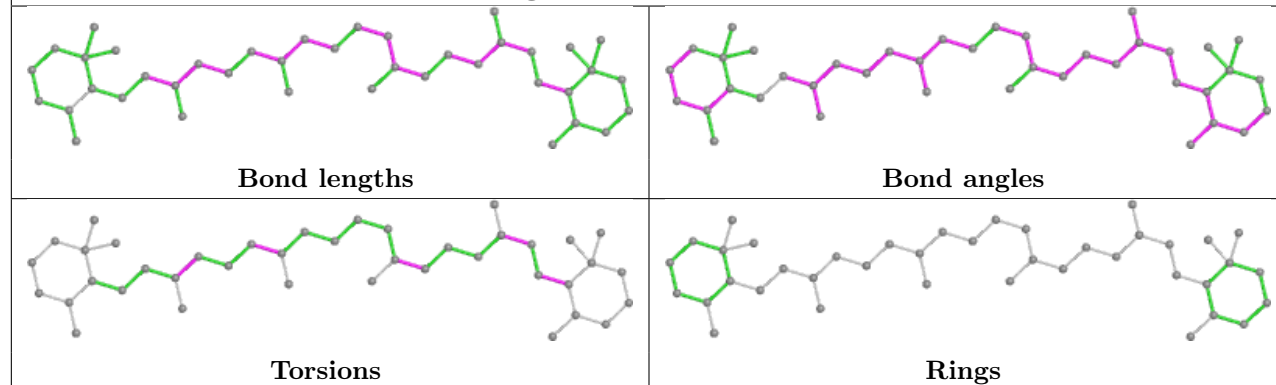
Ligand II0 g 320



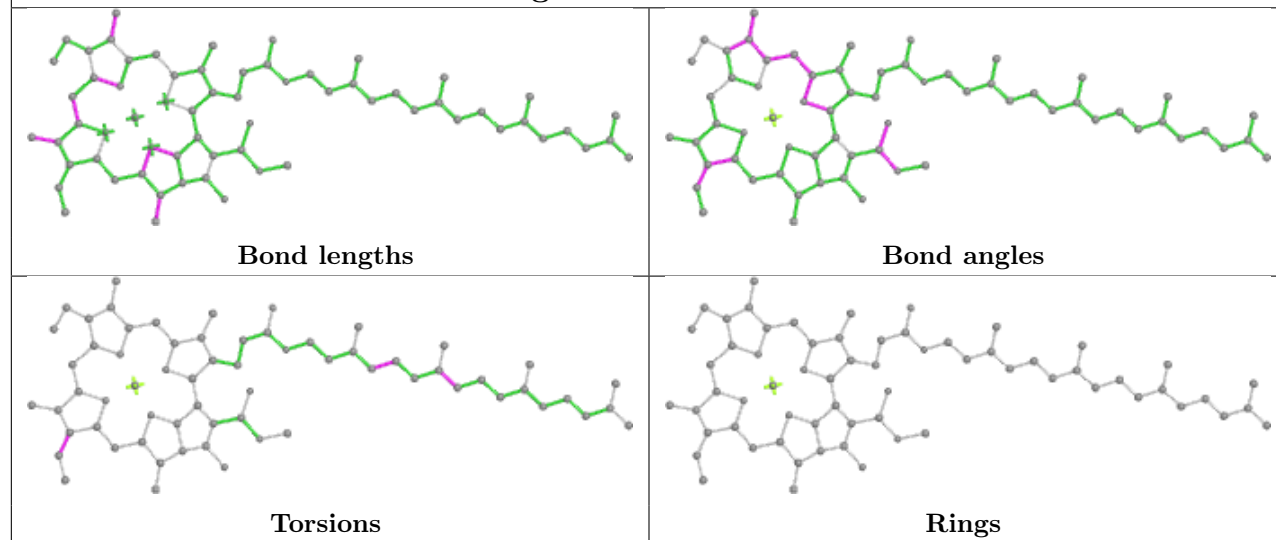
Ligand CLA a 309

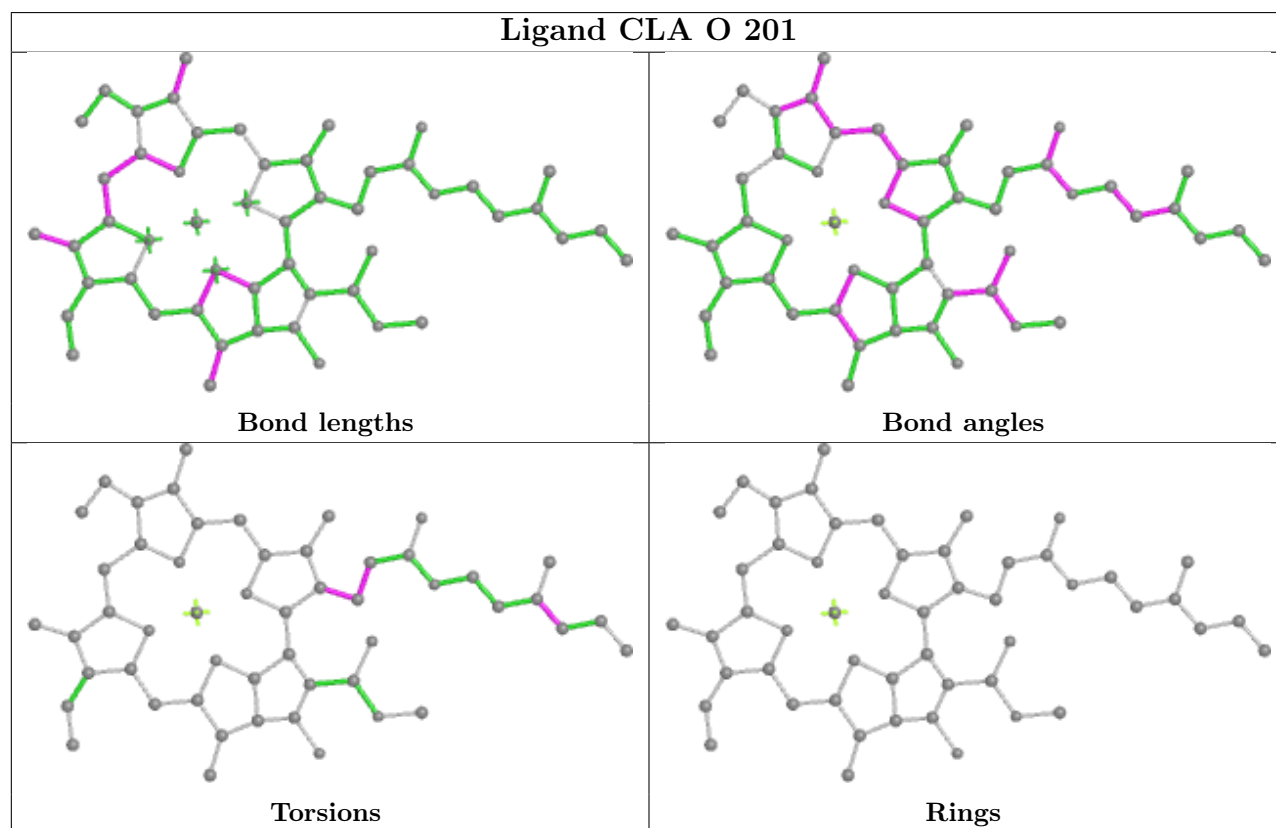
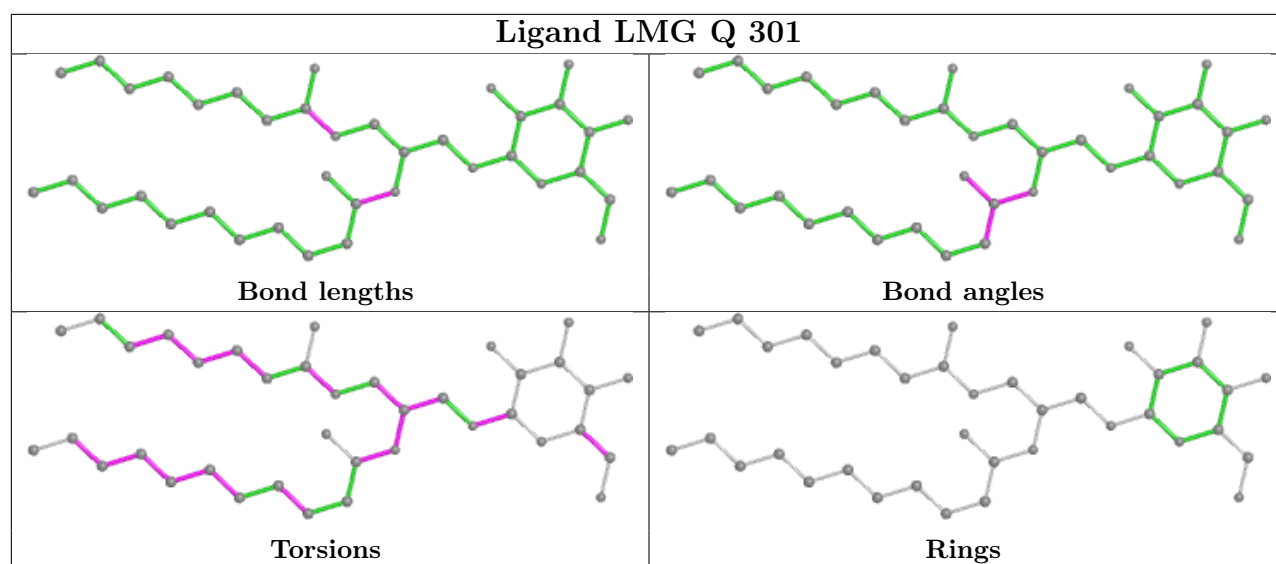


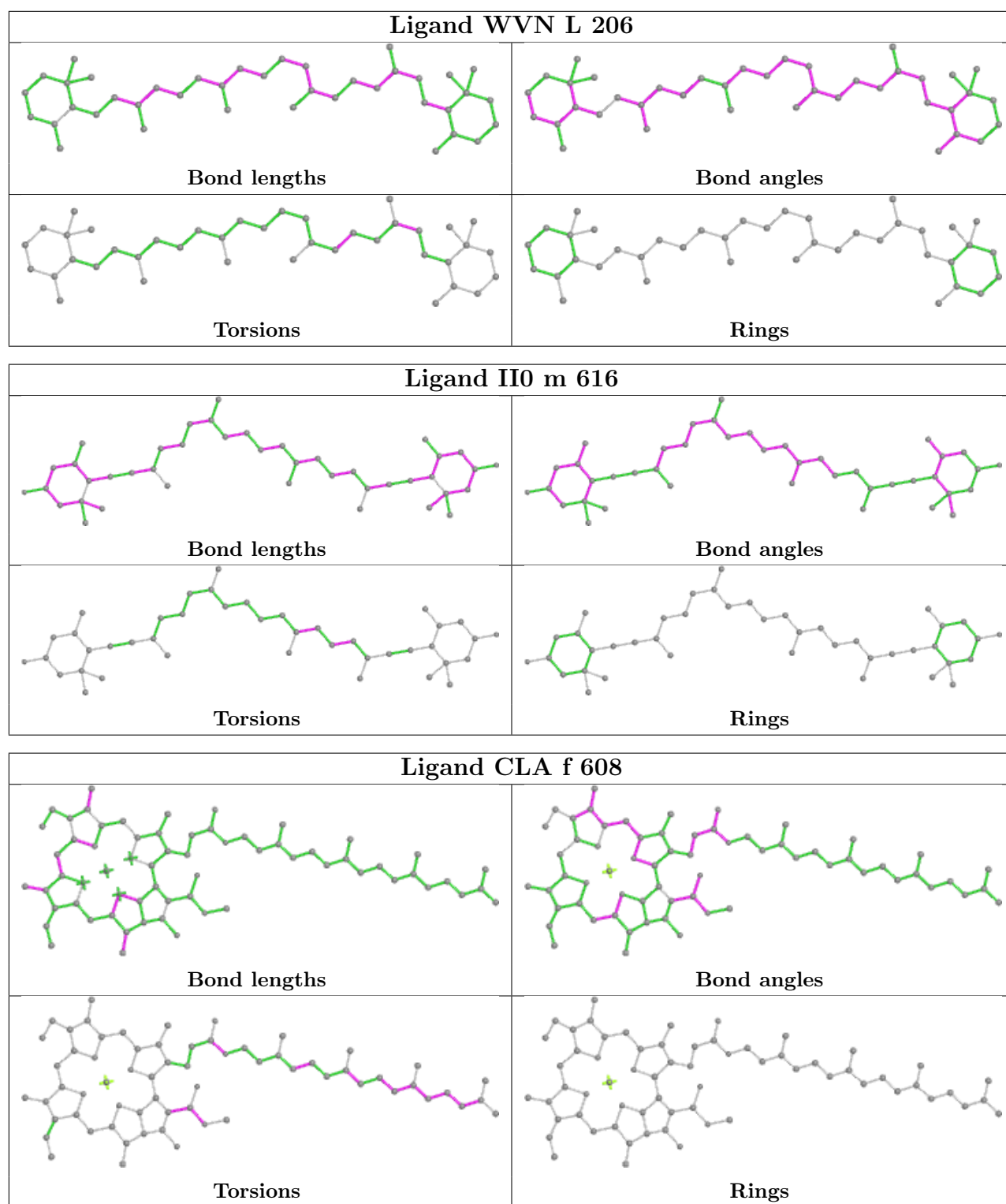
Ligand WVN A 846

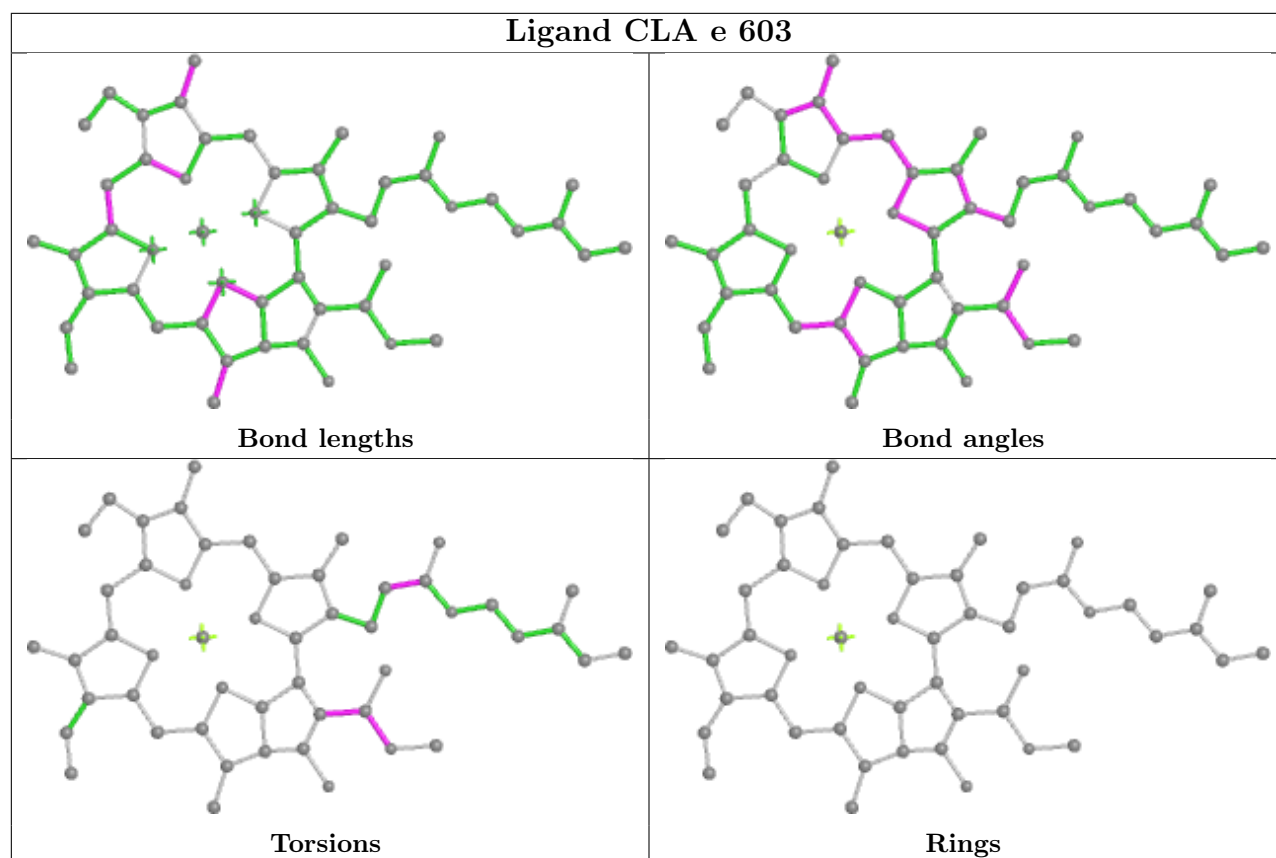
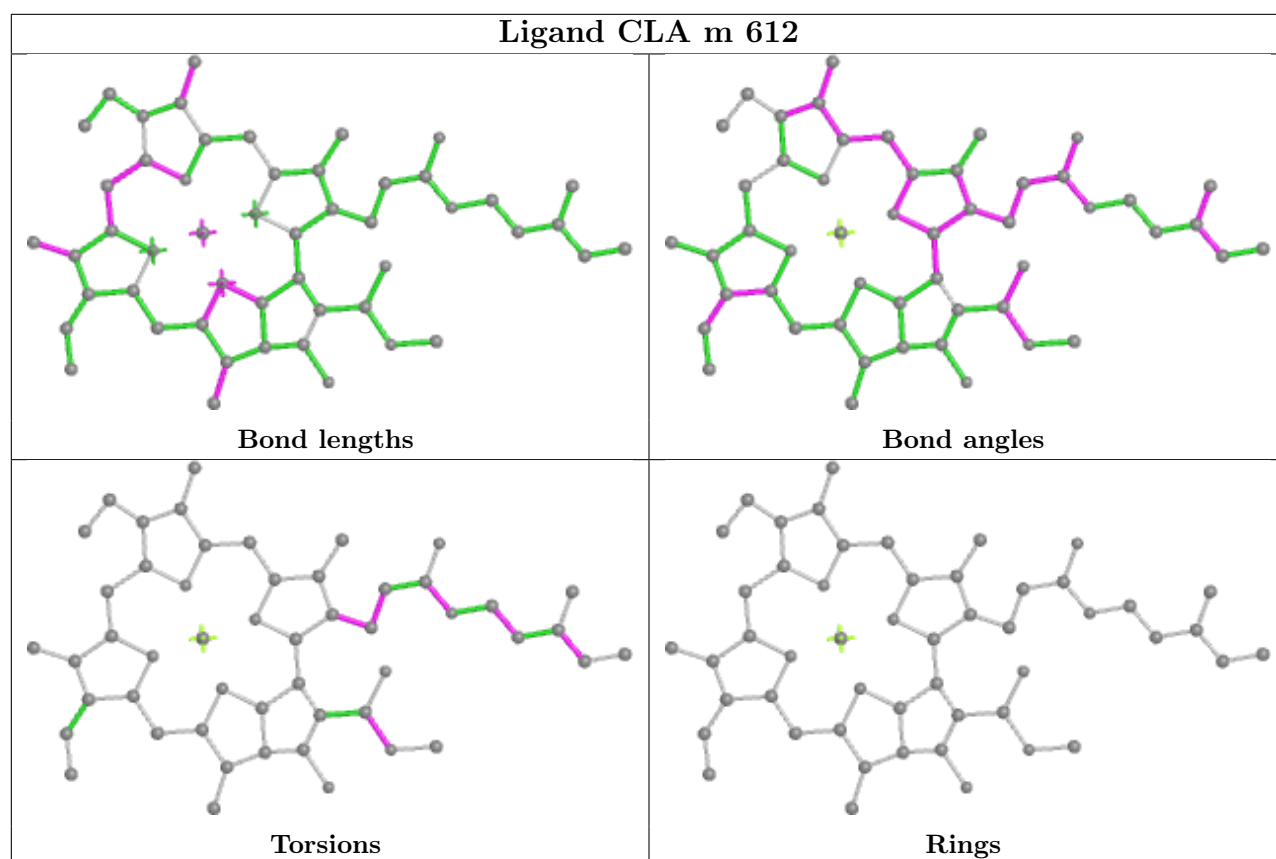


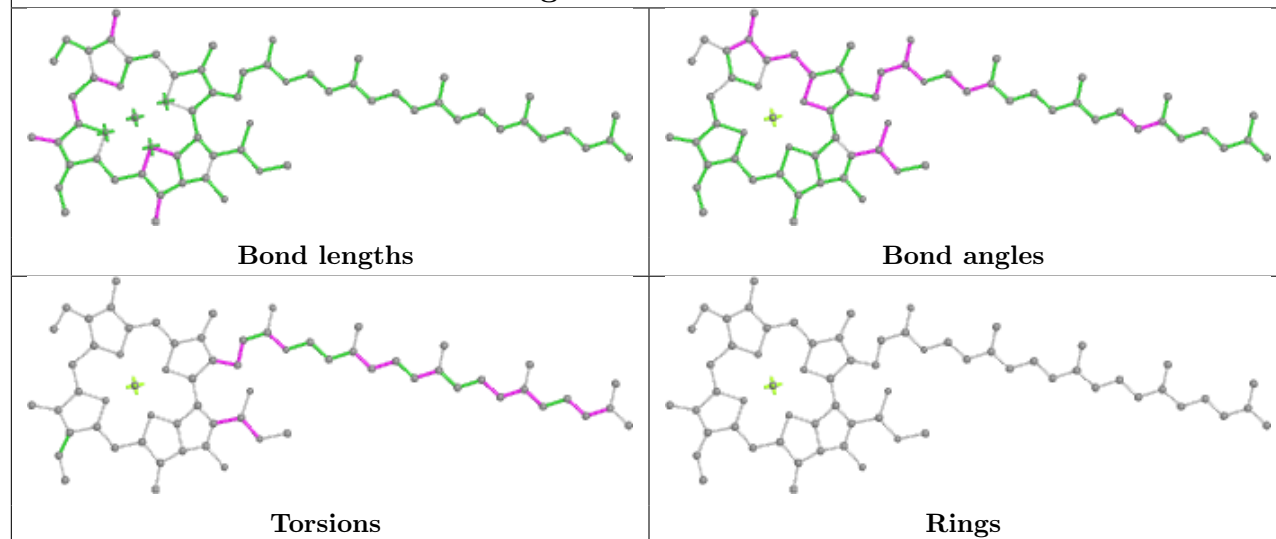
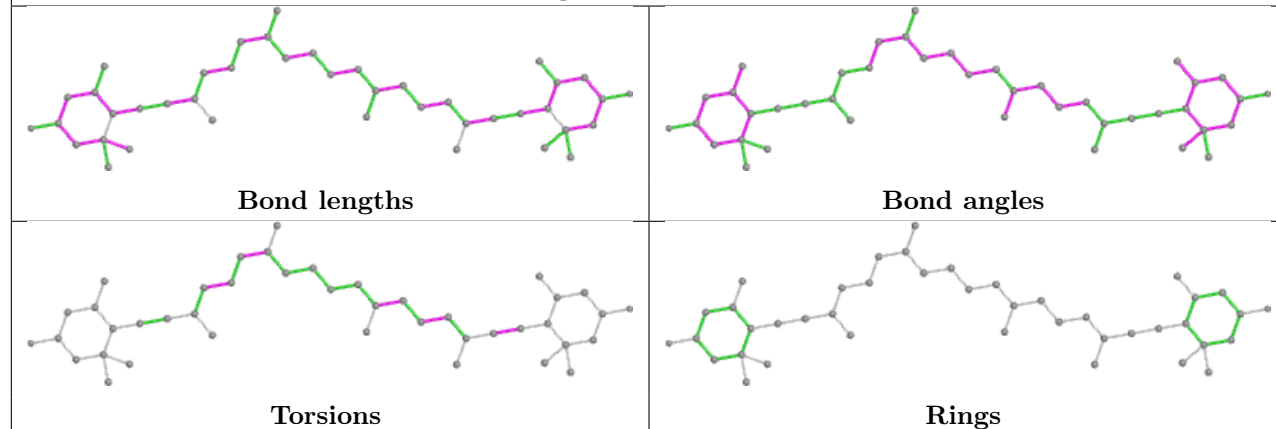
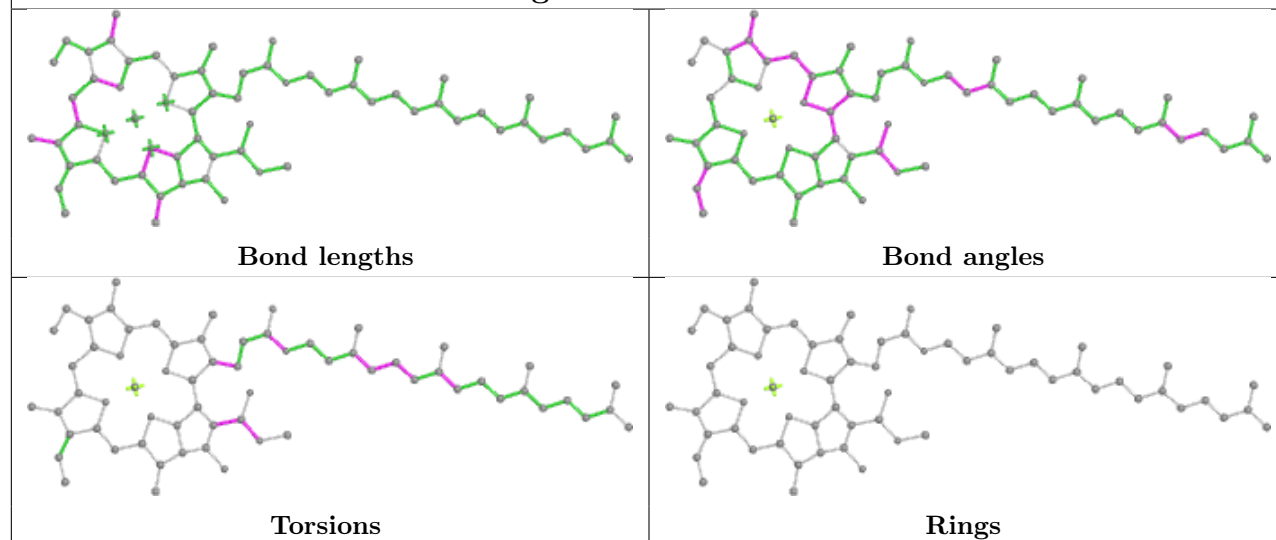
Ligand CLA A 820



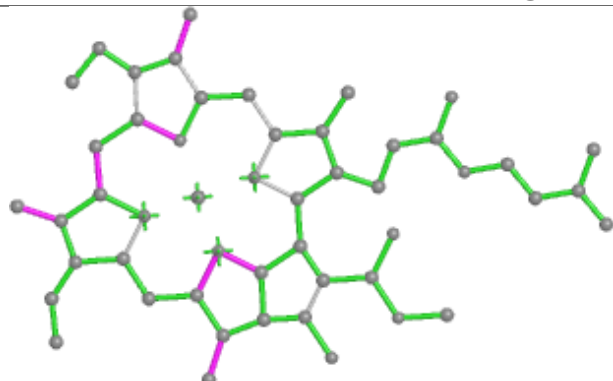




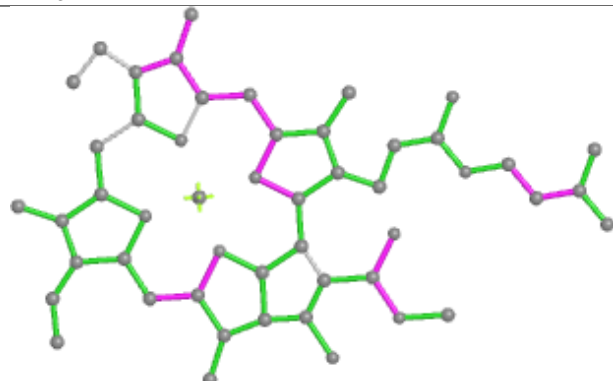


Ligand CLA l 303**Ligand II0 i 317****Ligand CLA O 202**

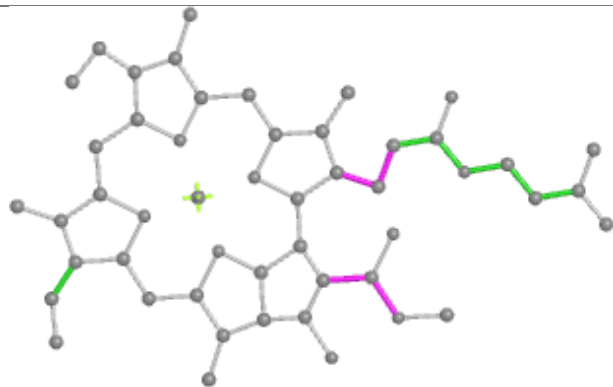
Ligand CLA j 602



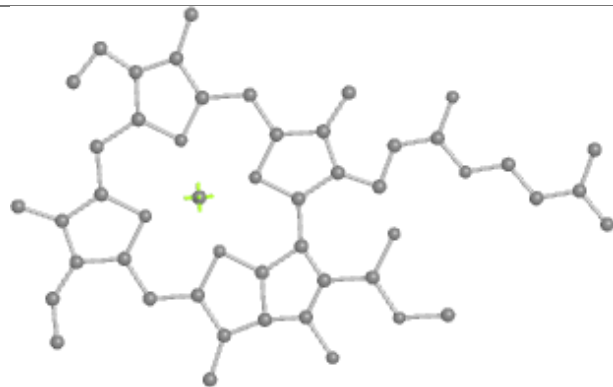
Bond lengths



Bond angles

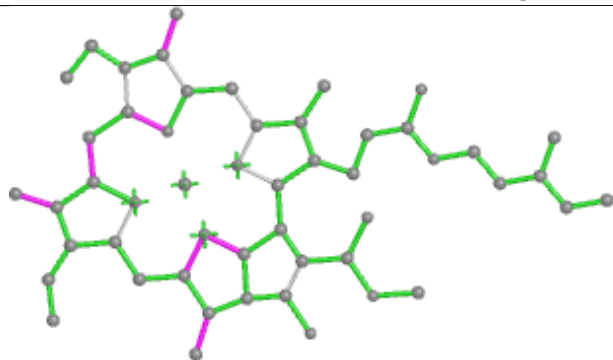


Torsions

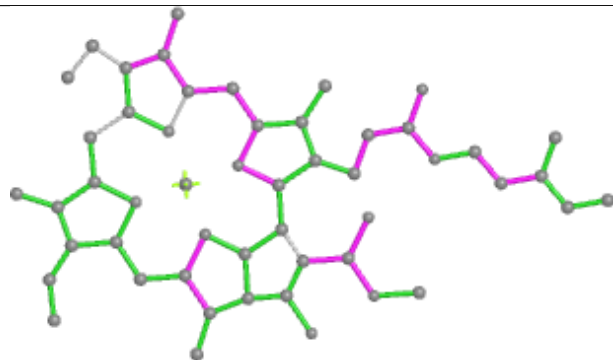


Rings

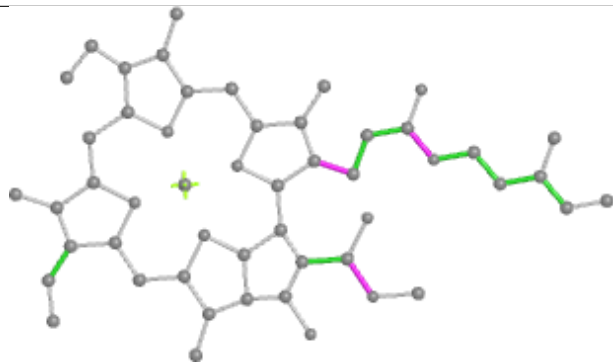
Ligand CLA B 826



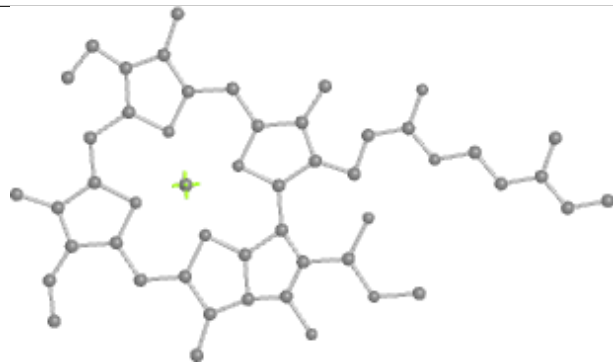
Bond lengths



Bond angles

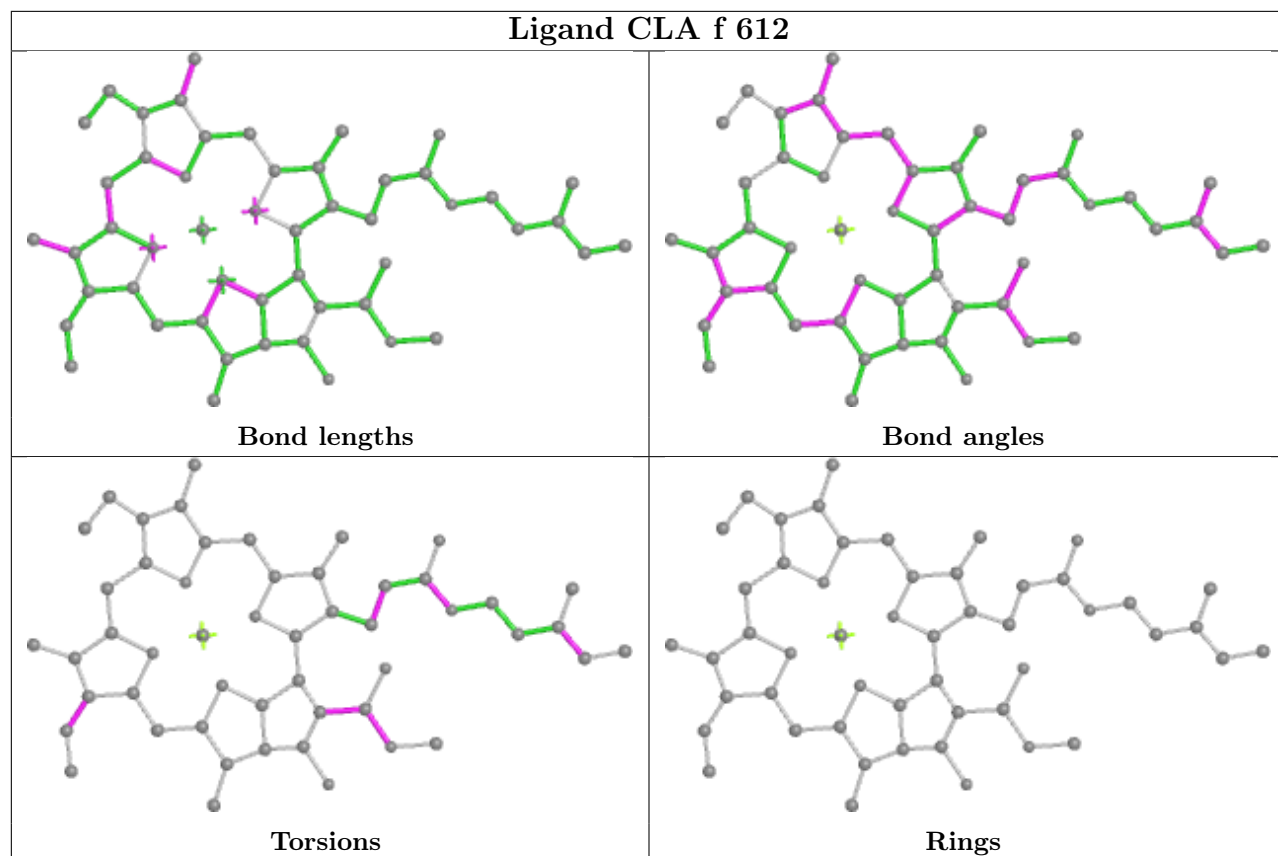


Torsions

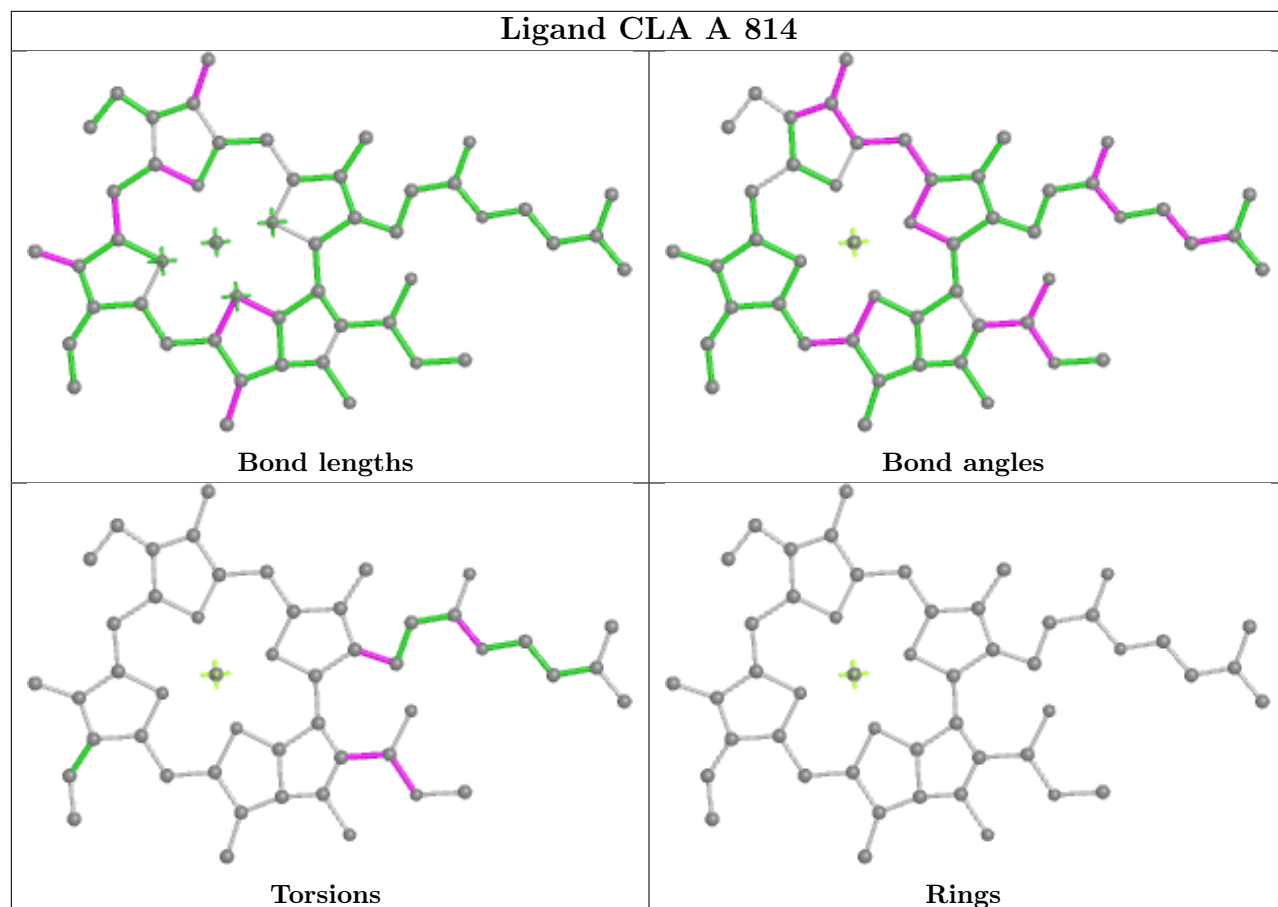


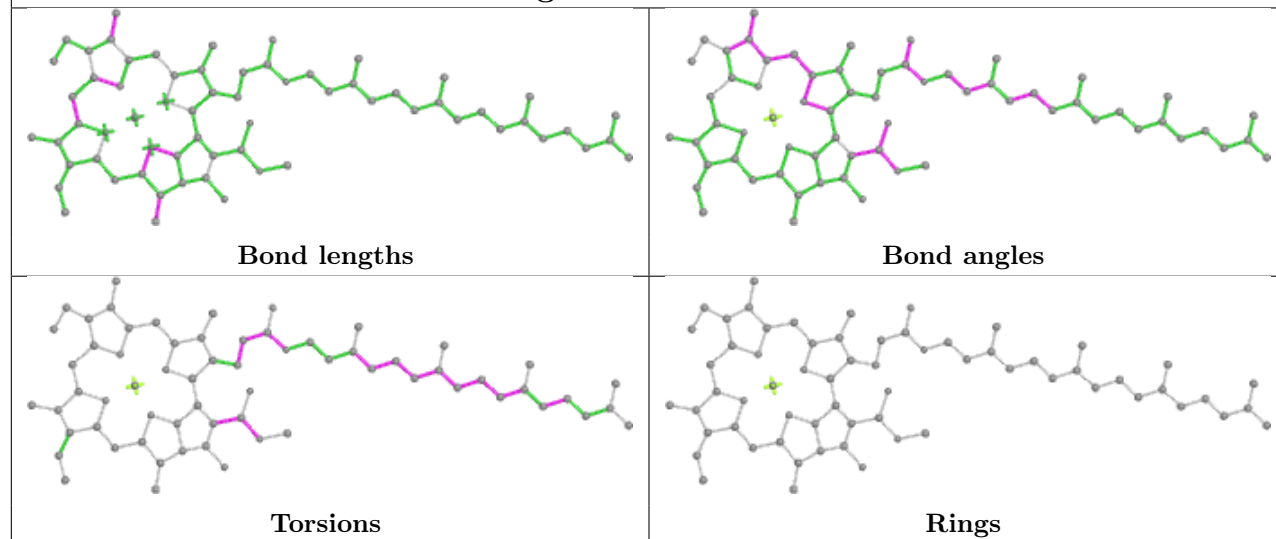
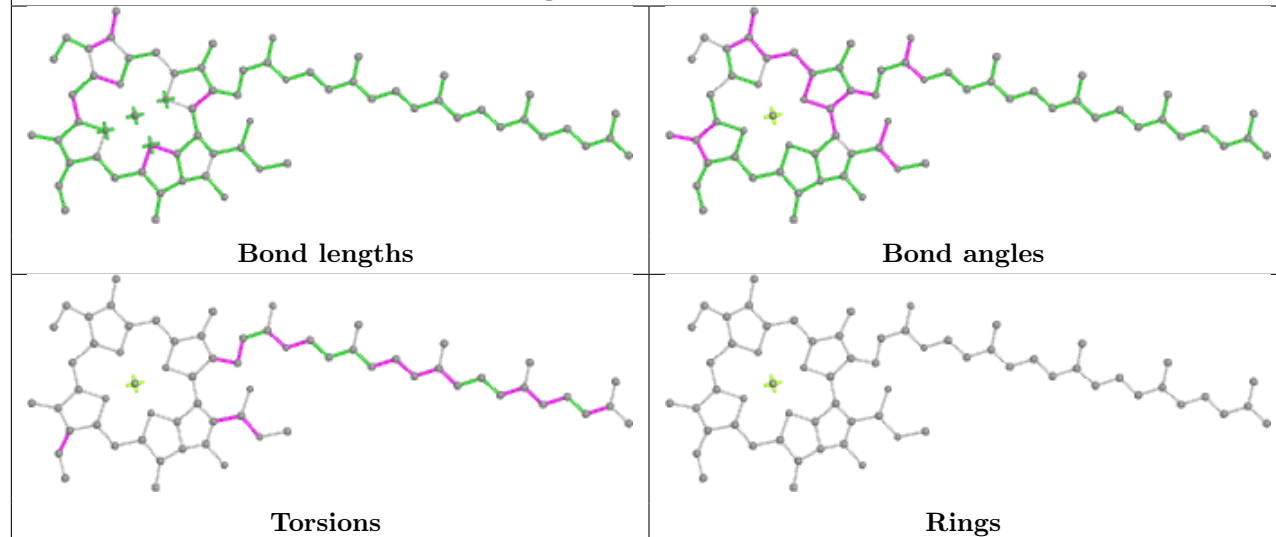
Rings

Ligand CLA f 612

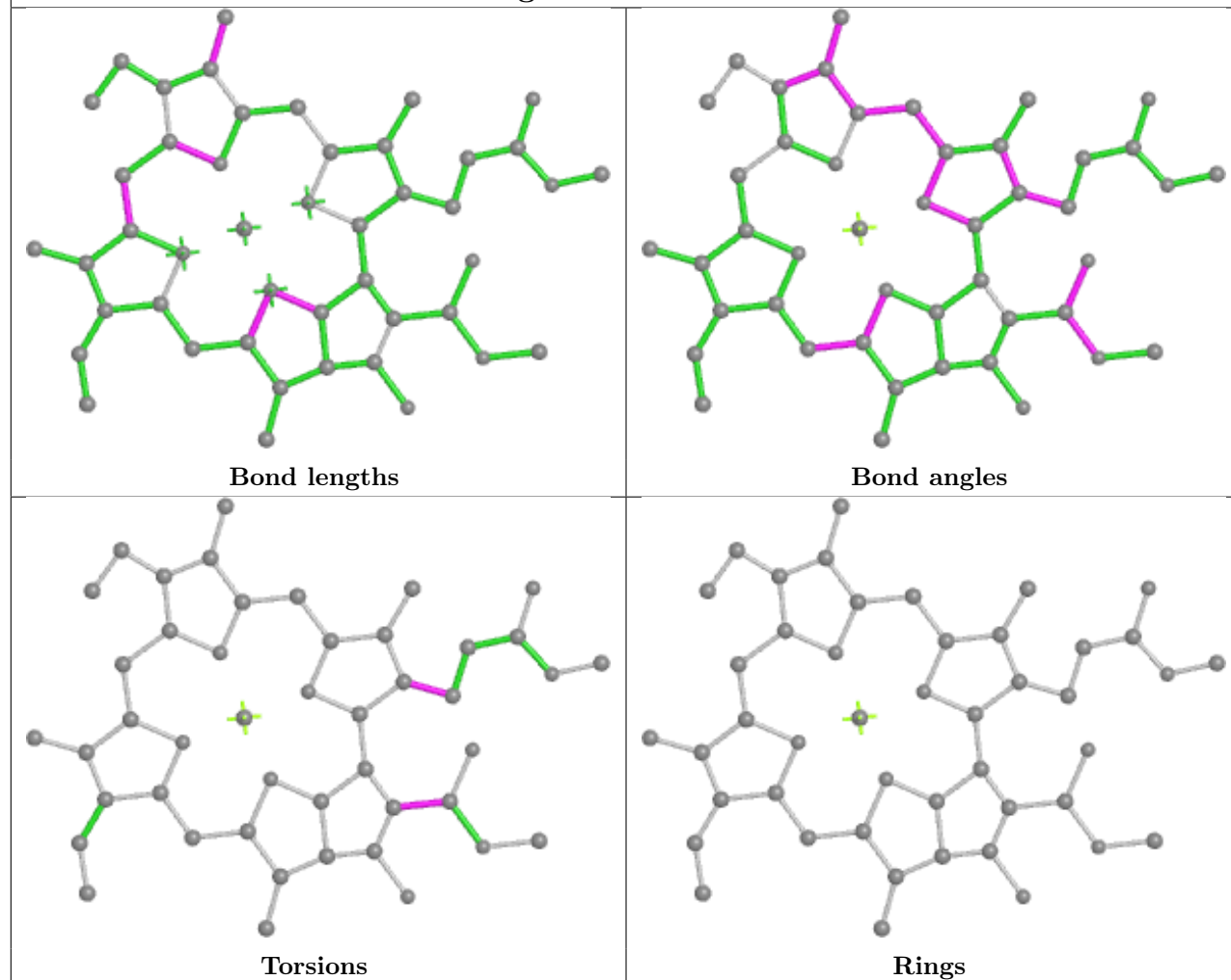


Ligand CLA A 814

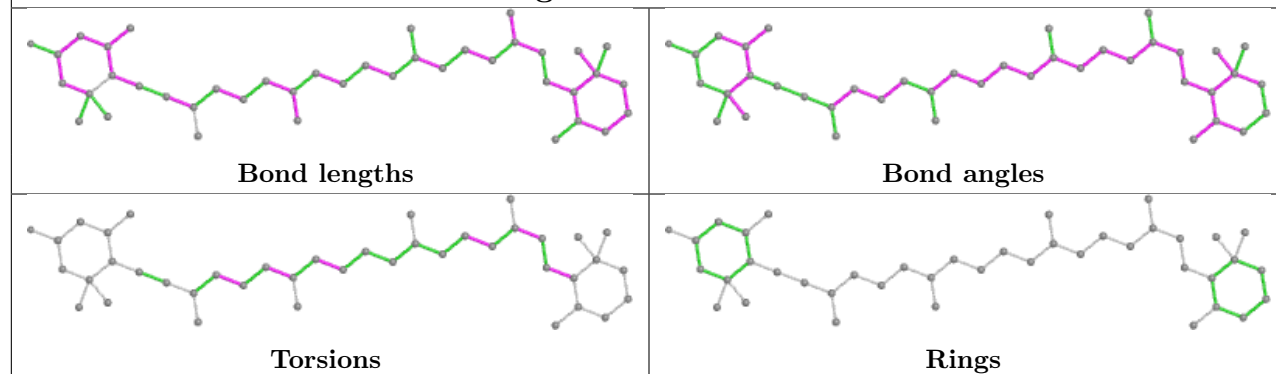


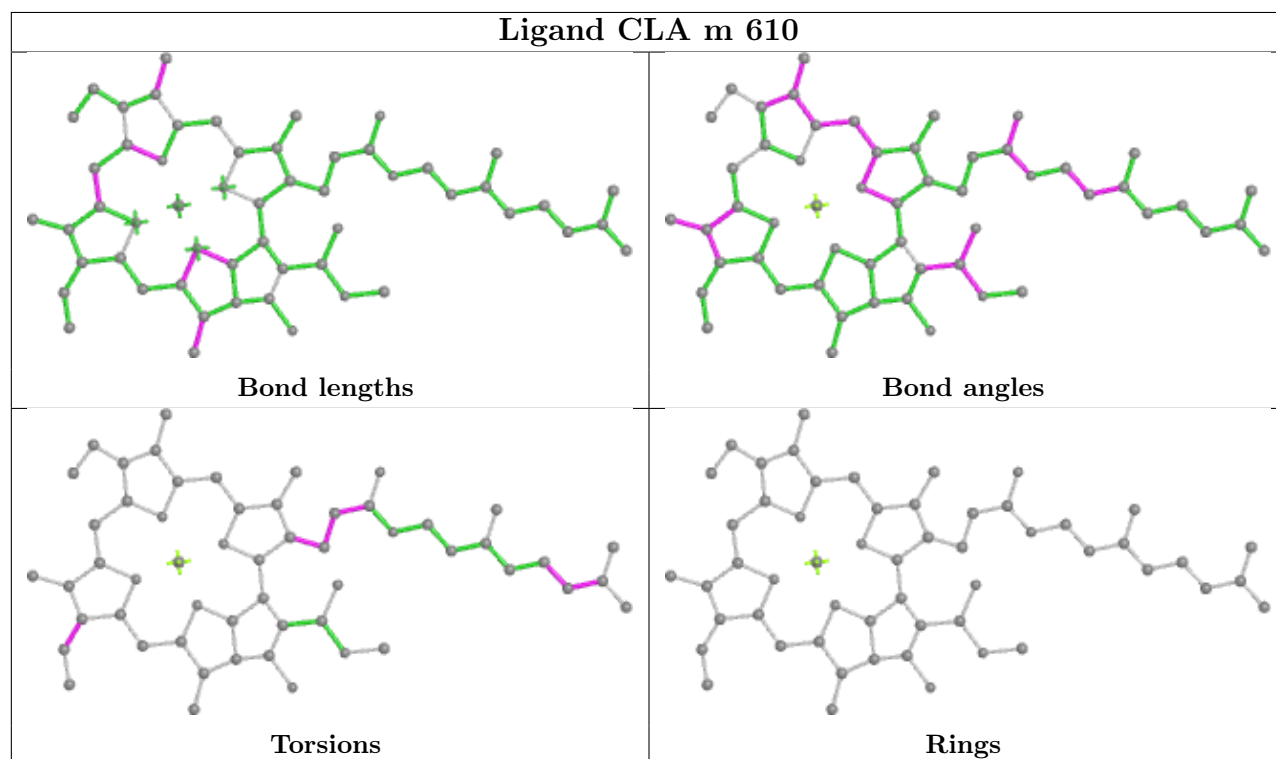
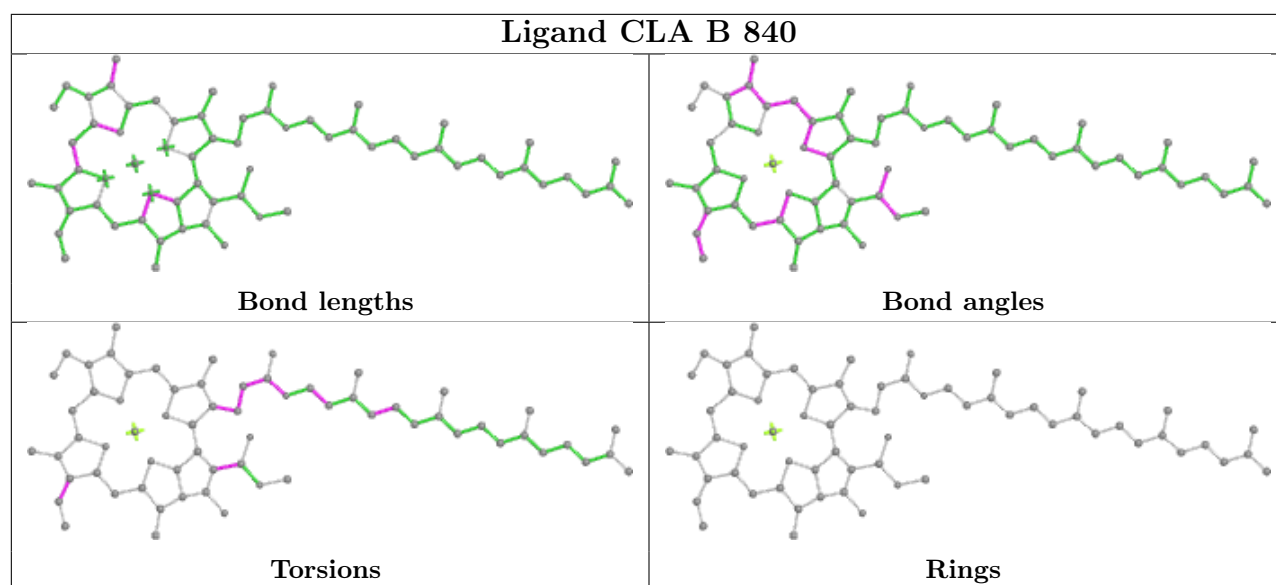
Ligand CLA e 604**Ligand CLA l 306**

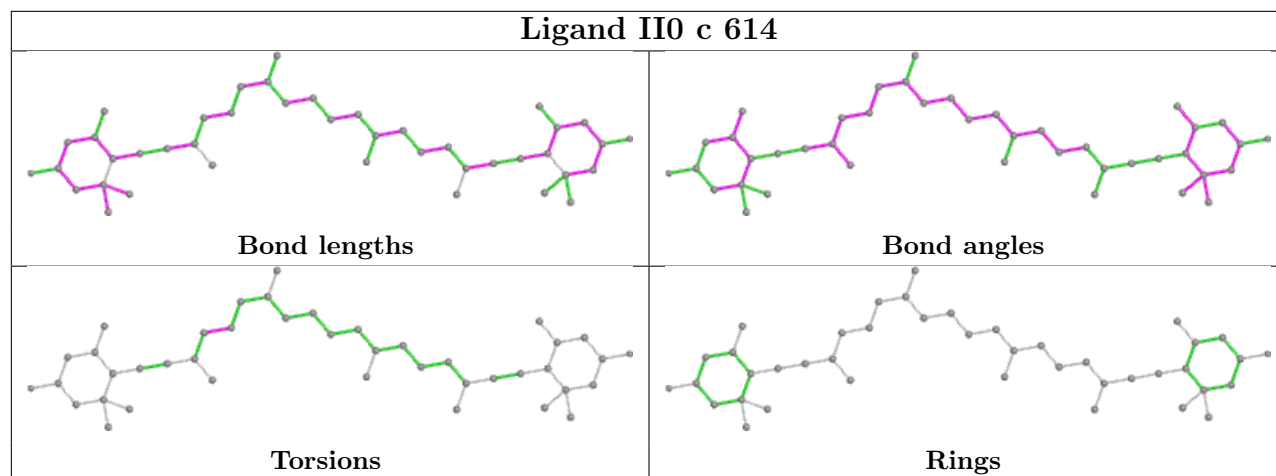
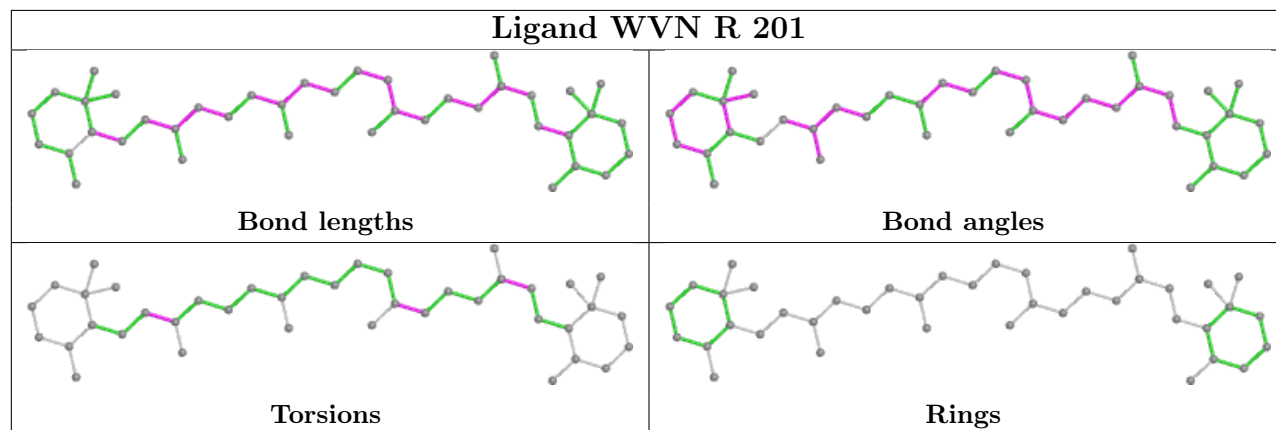
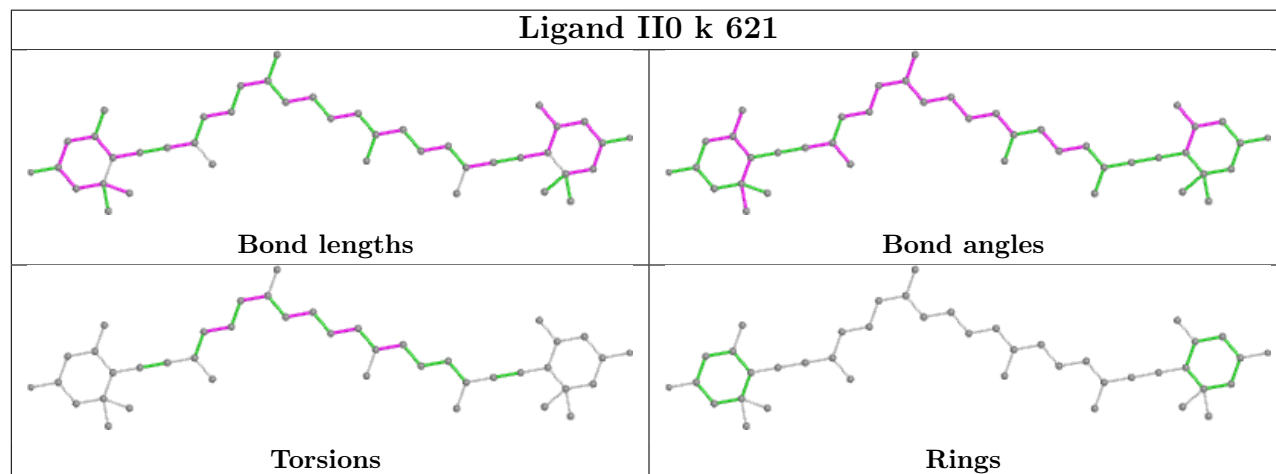
Ligand CLA e 608

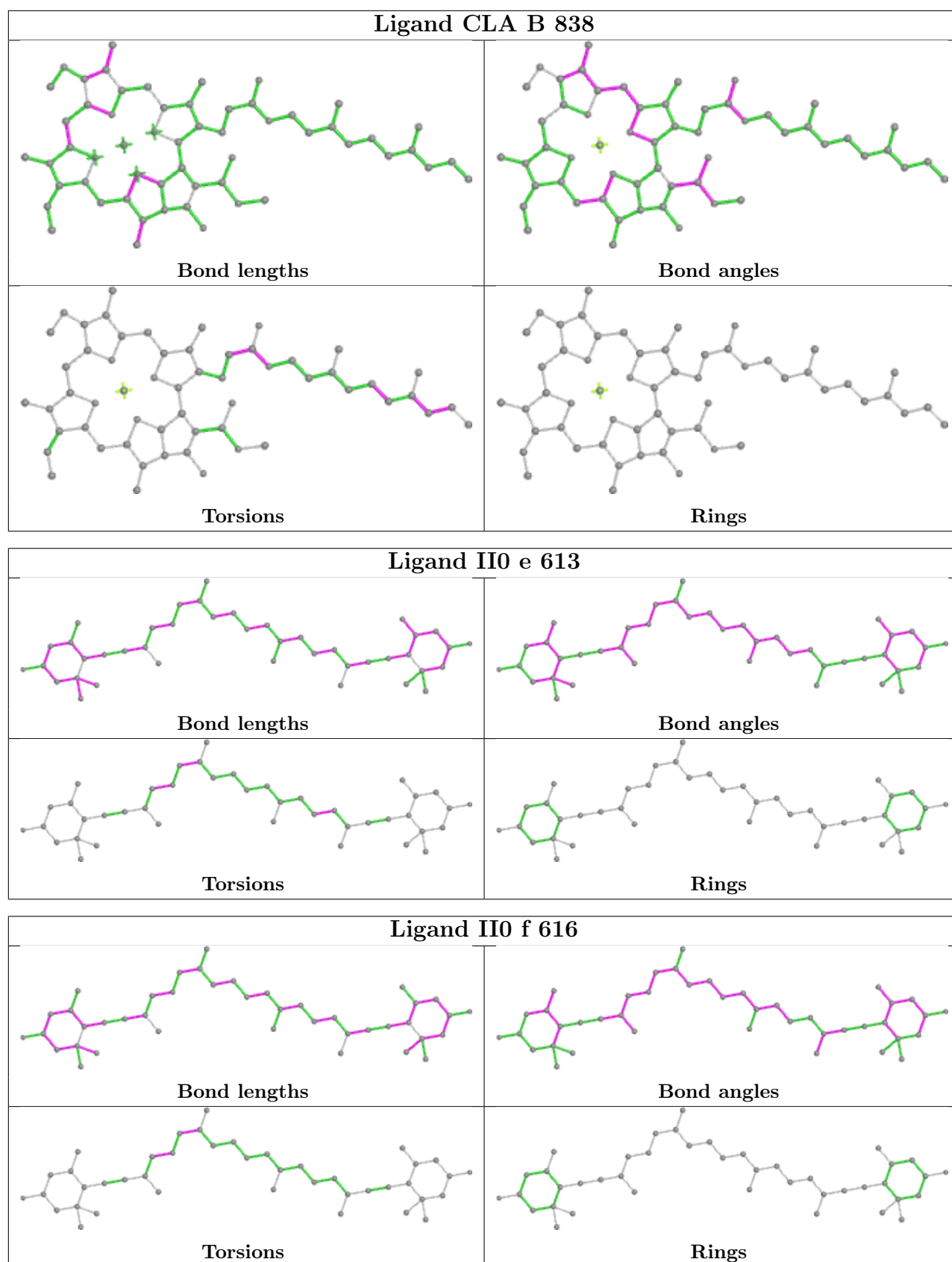


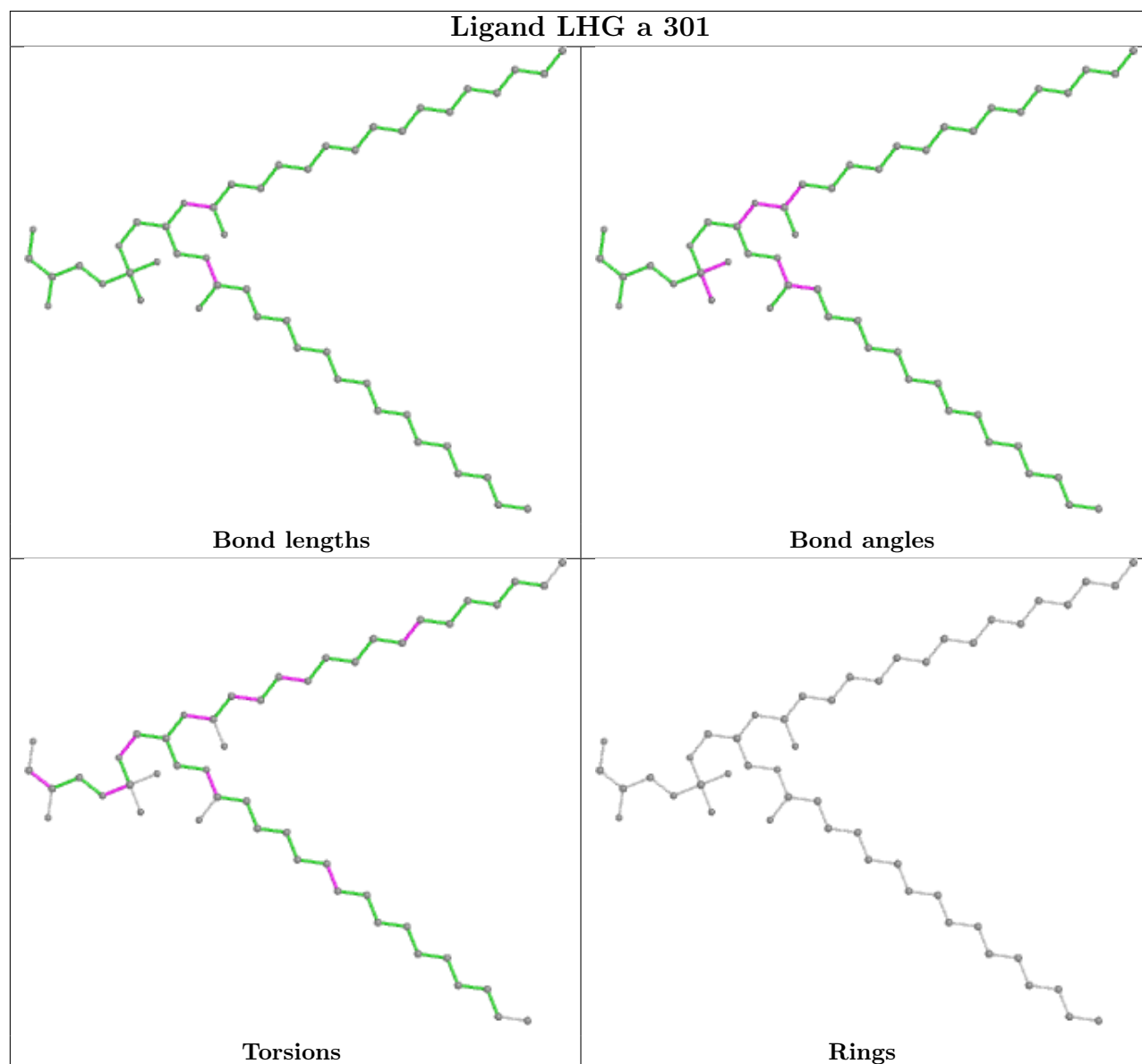
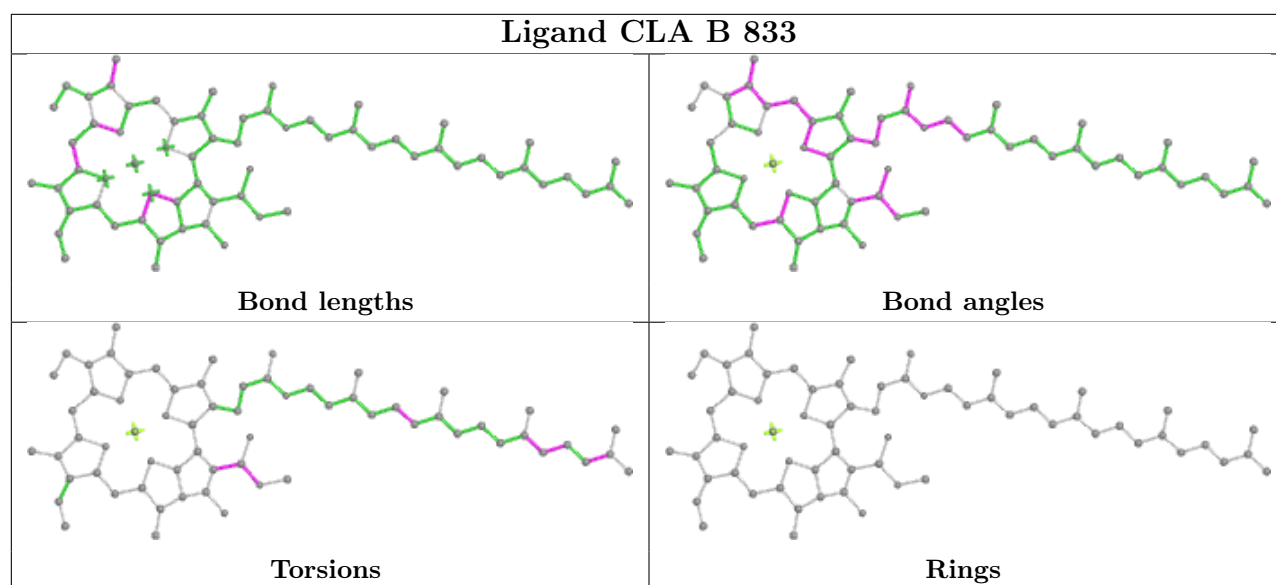
Ligand IHT O 204

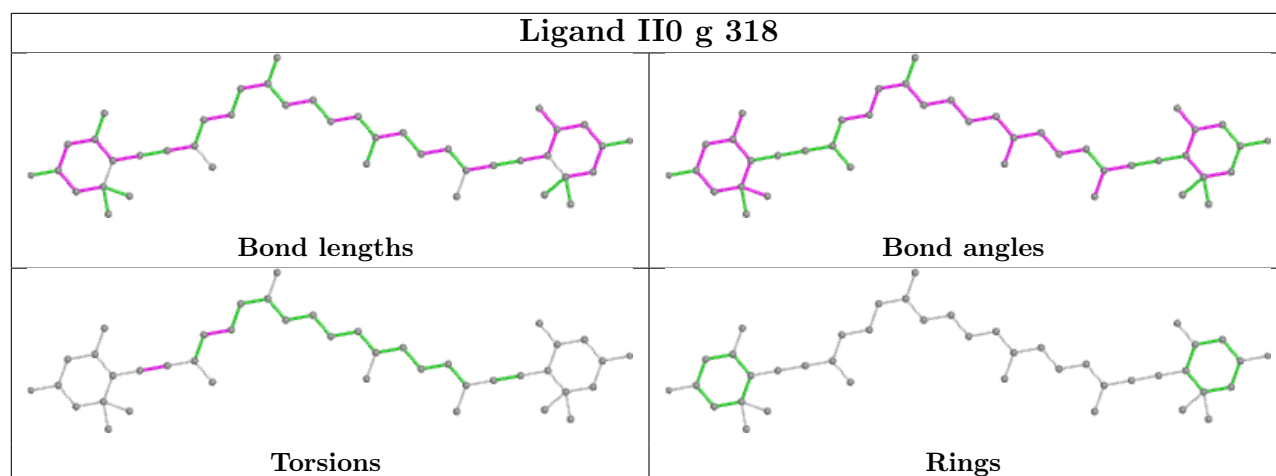
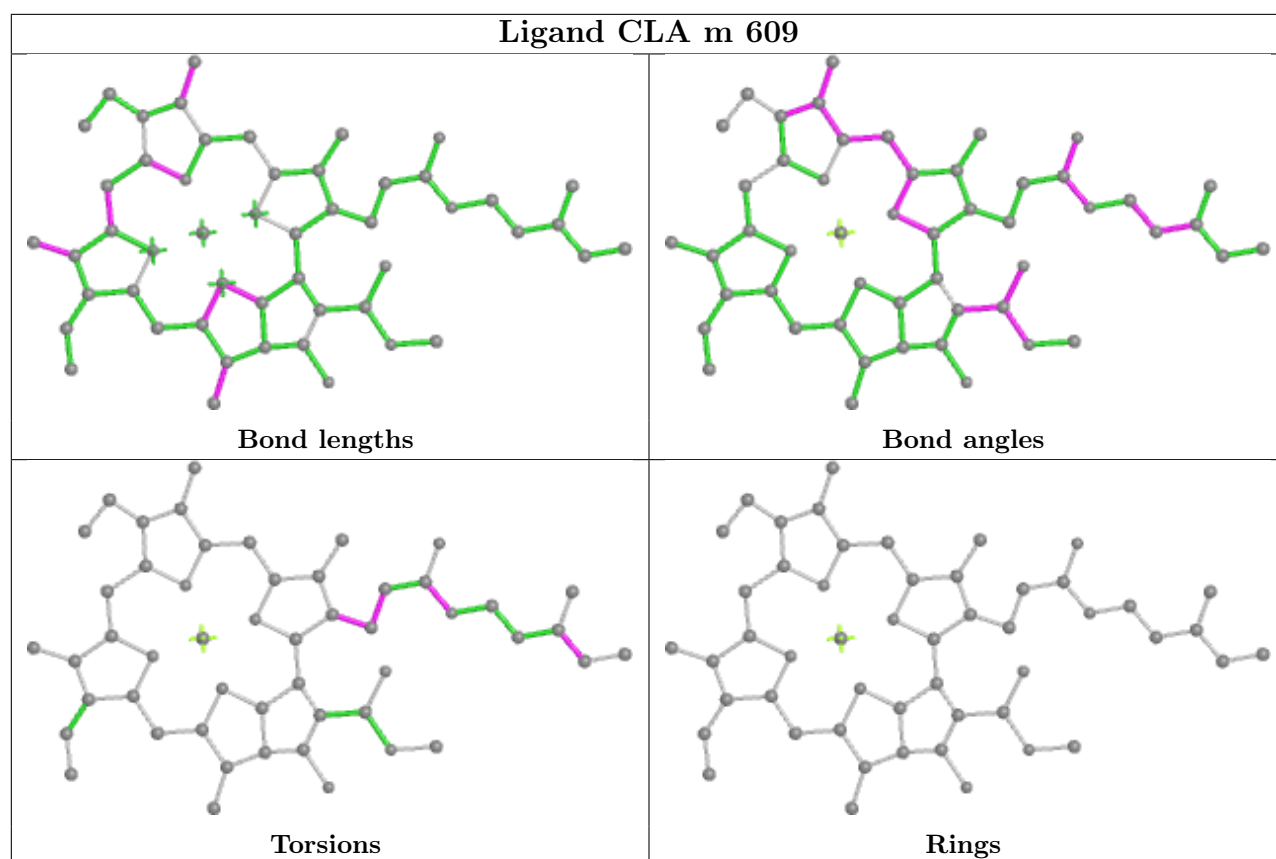


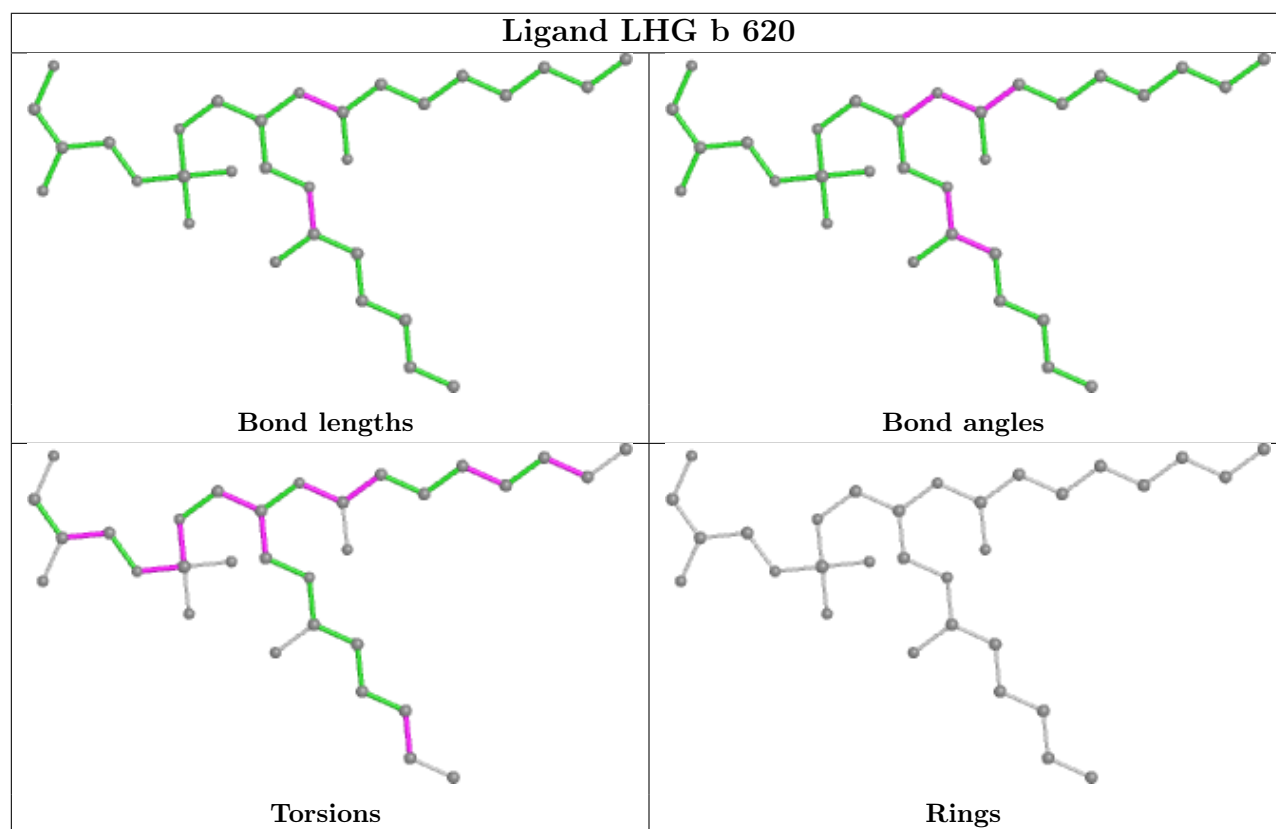
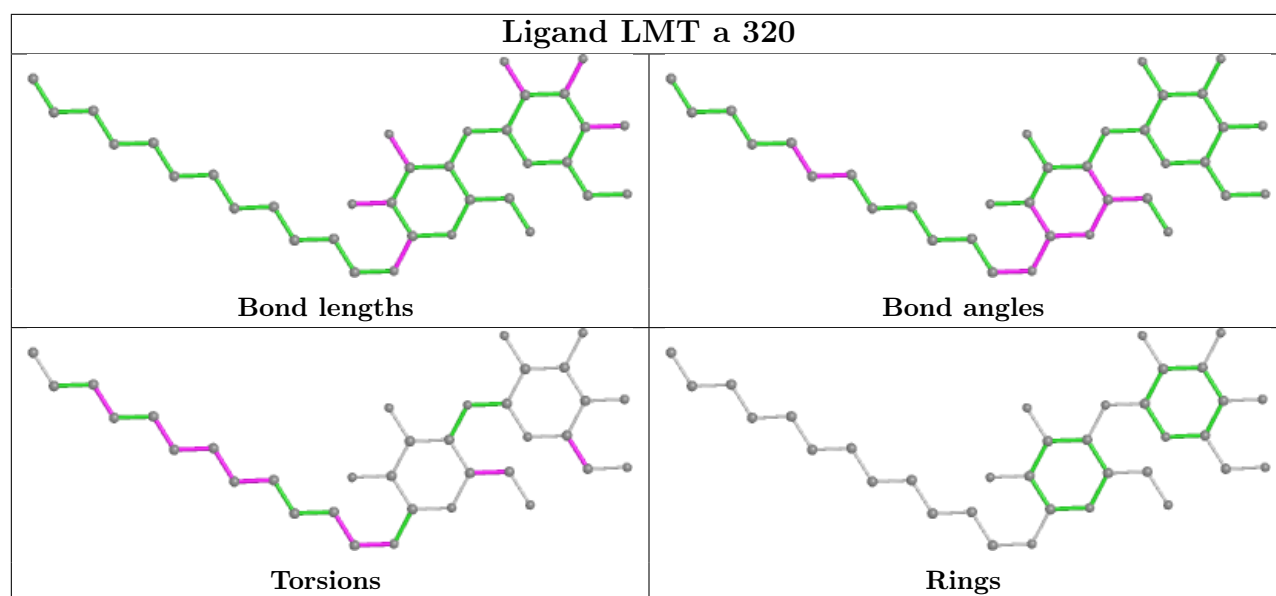


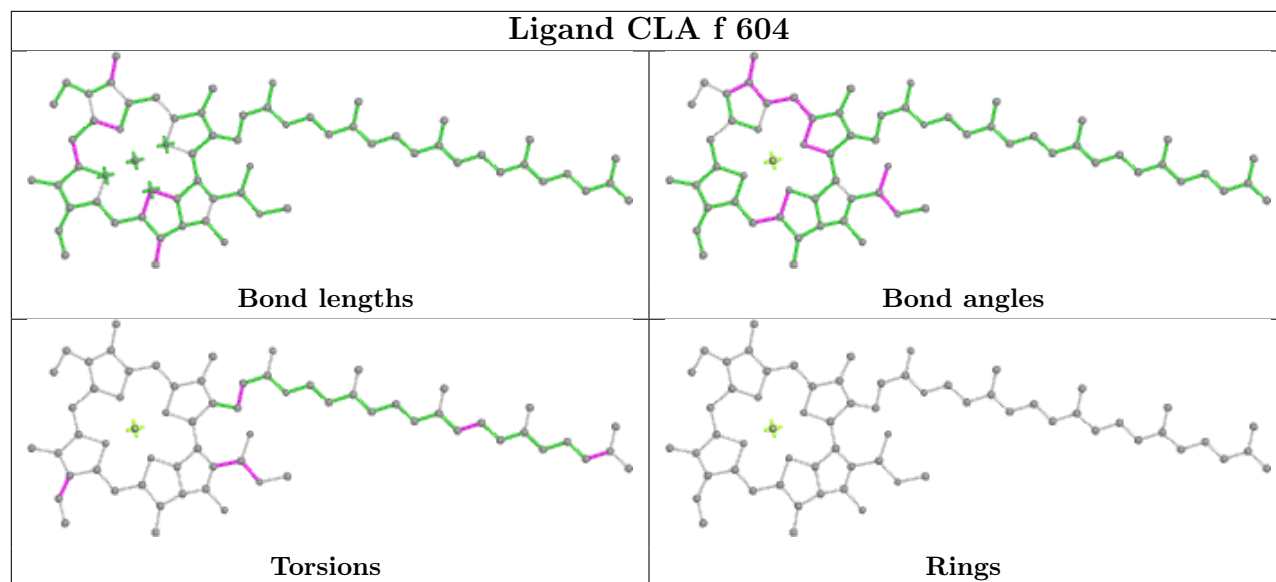
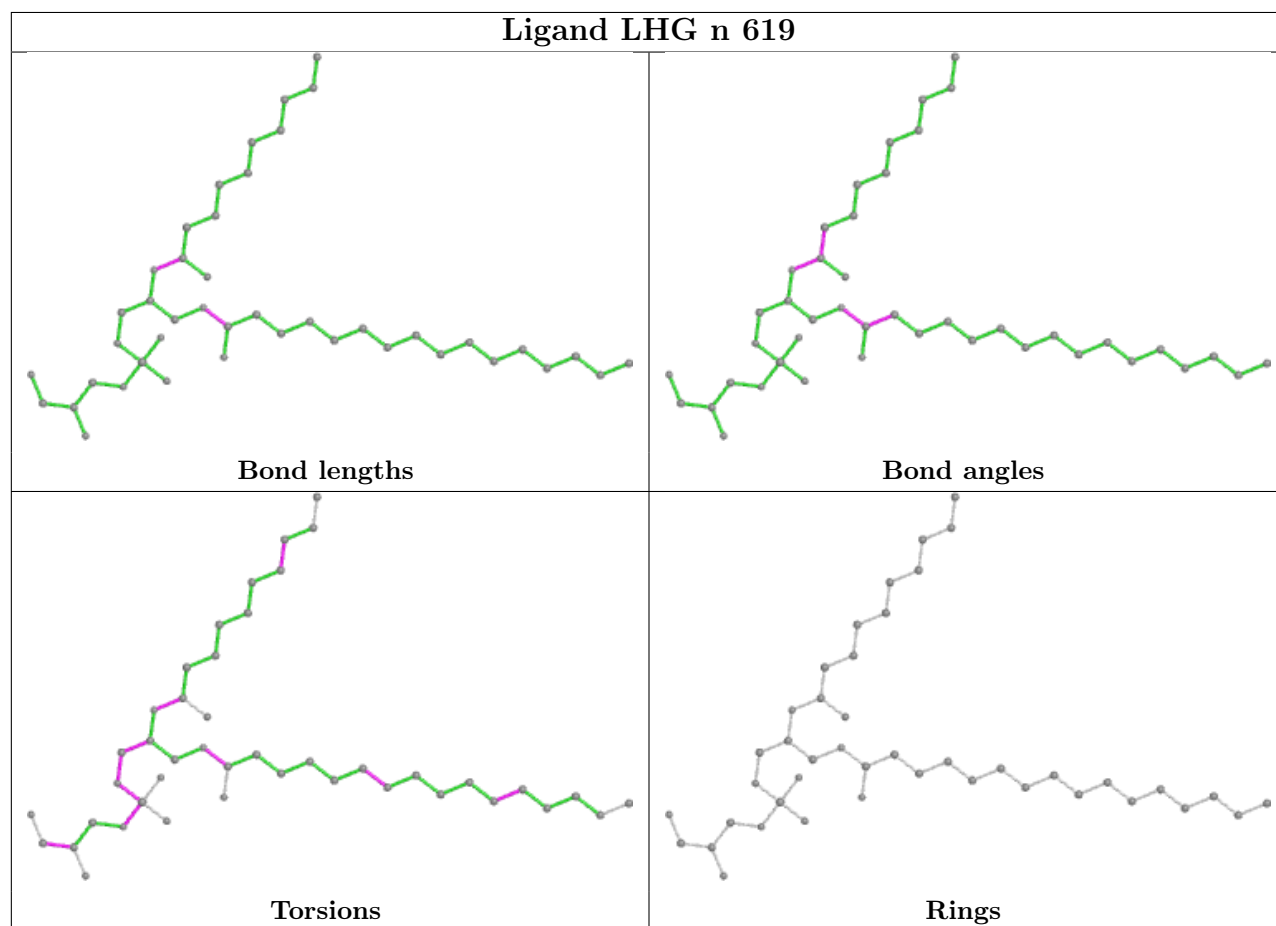
Ligand II0 c 614**Ligand WVN R 201****Ligand II0 k 621**

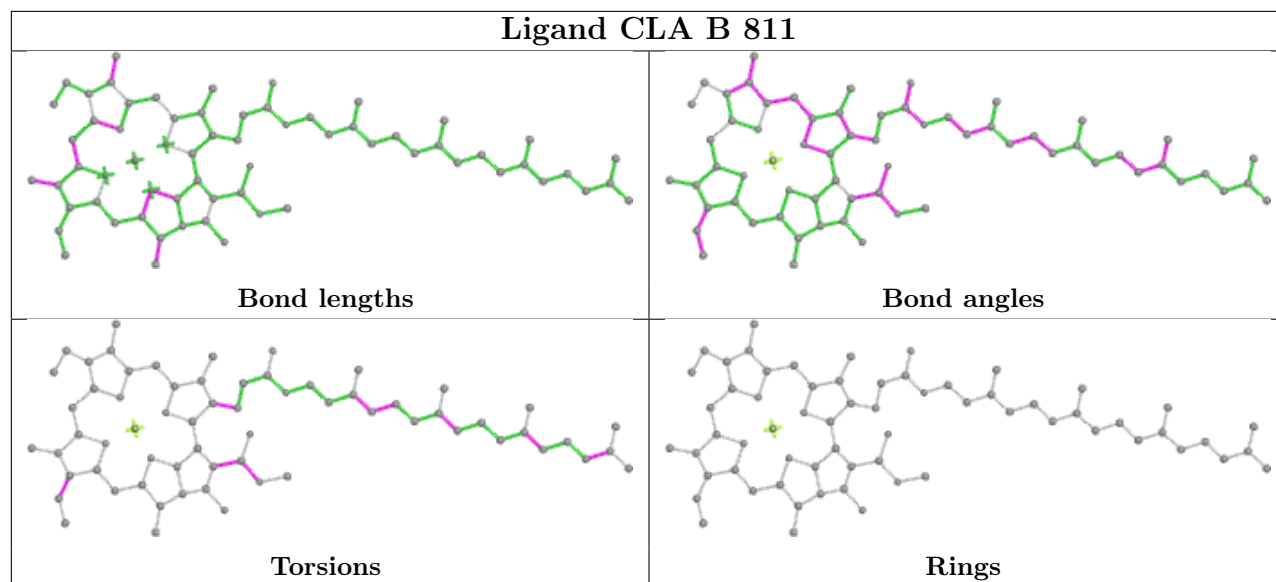
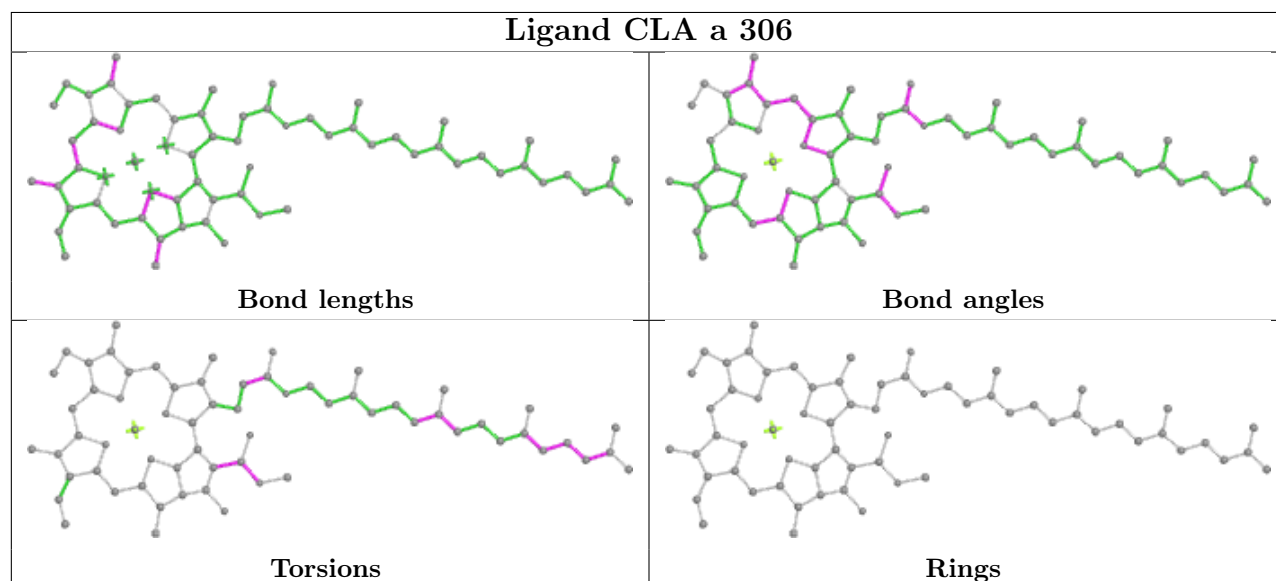
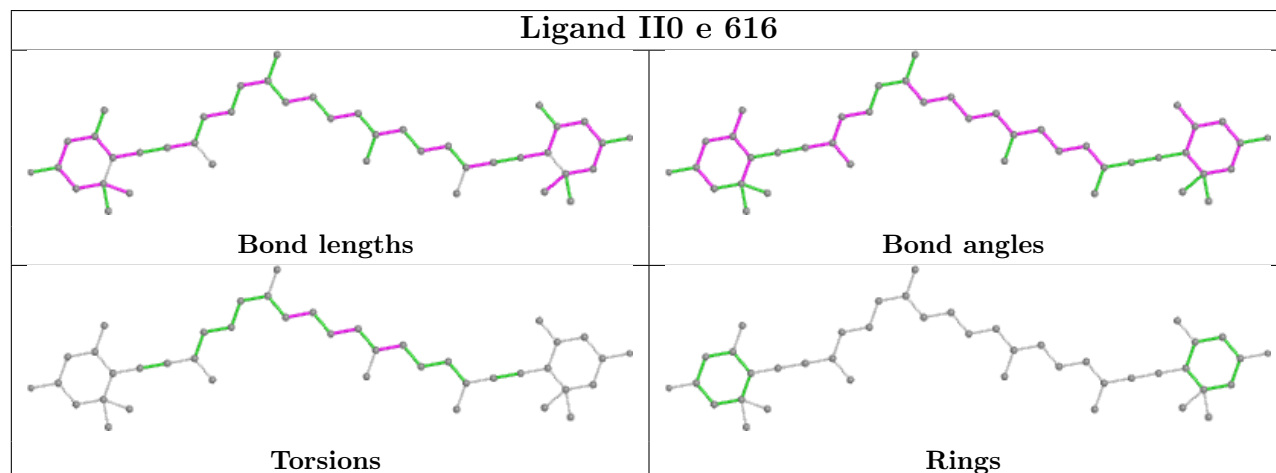




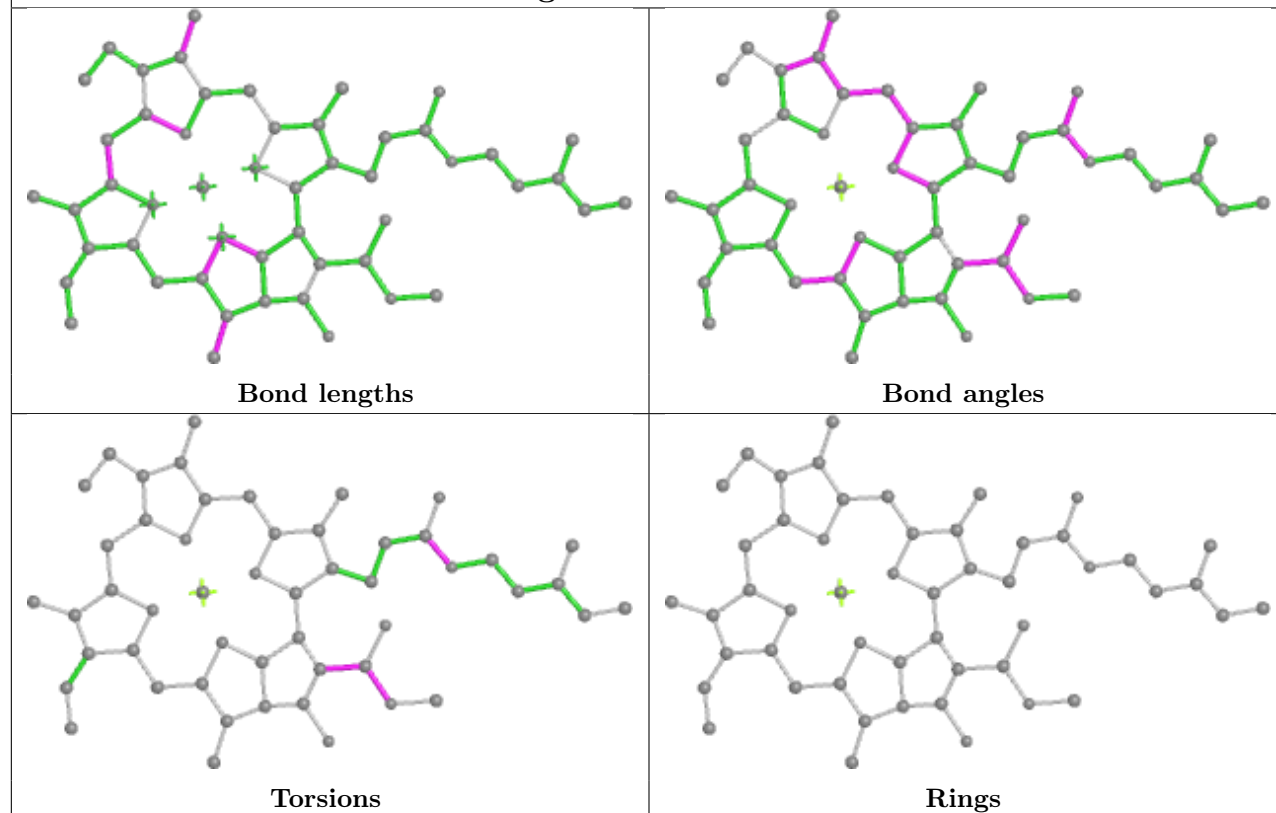




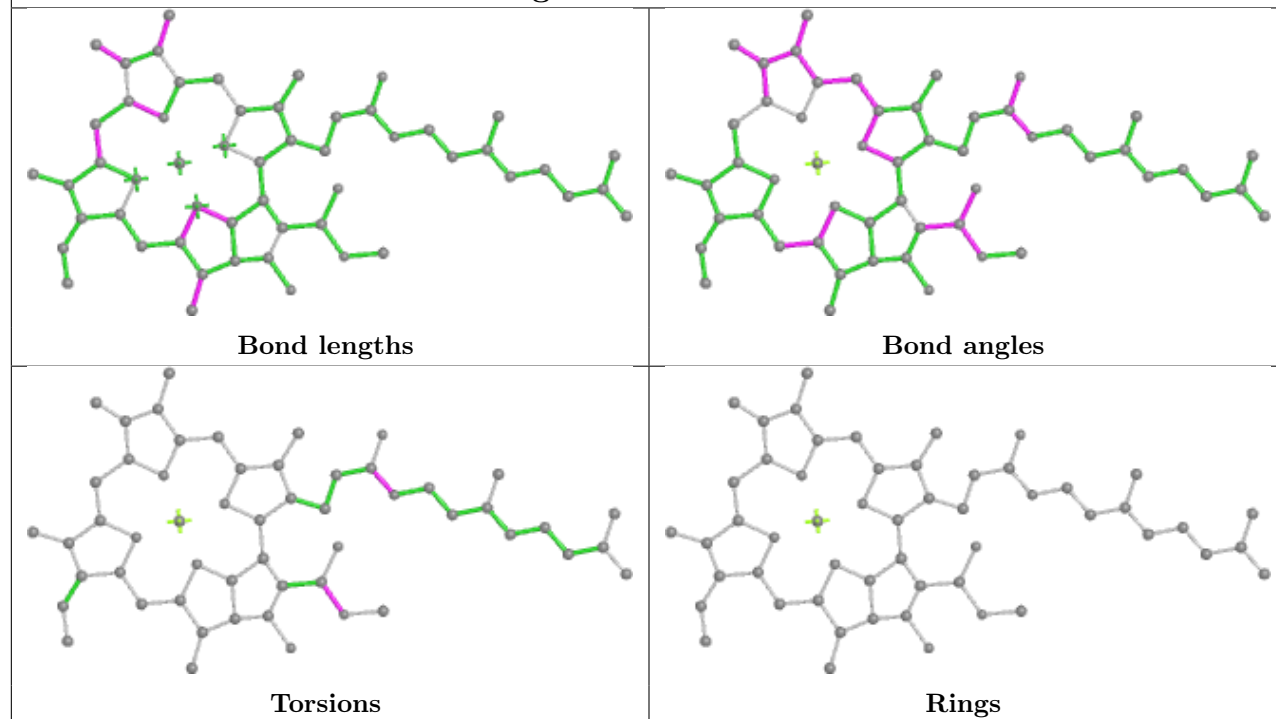
Ligand CLA f 604**Ligand LHG n 619**

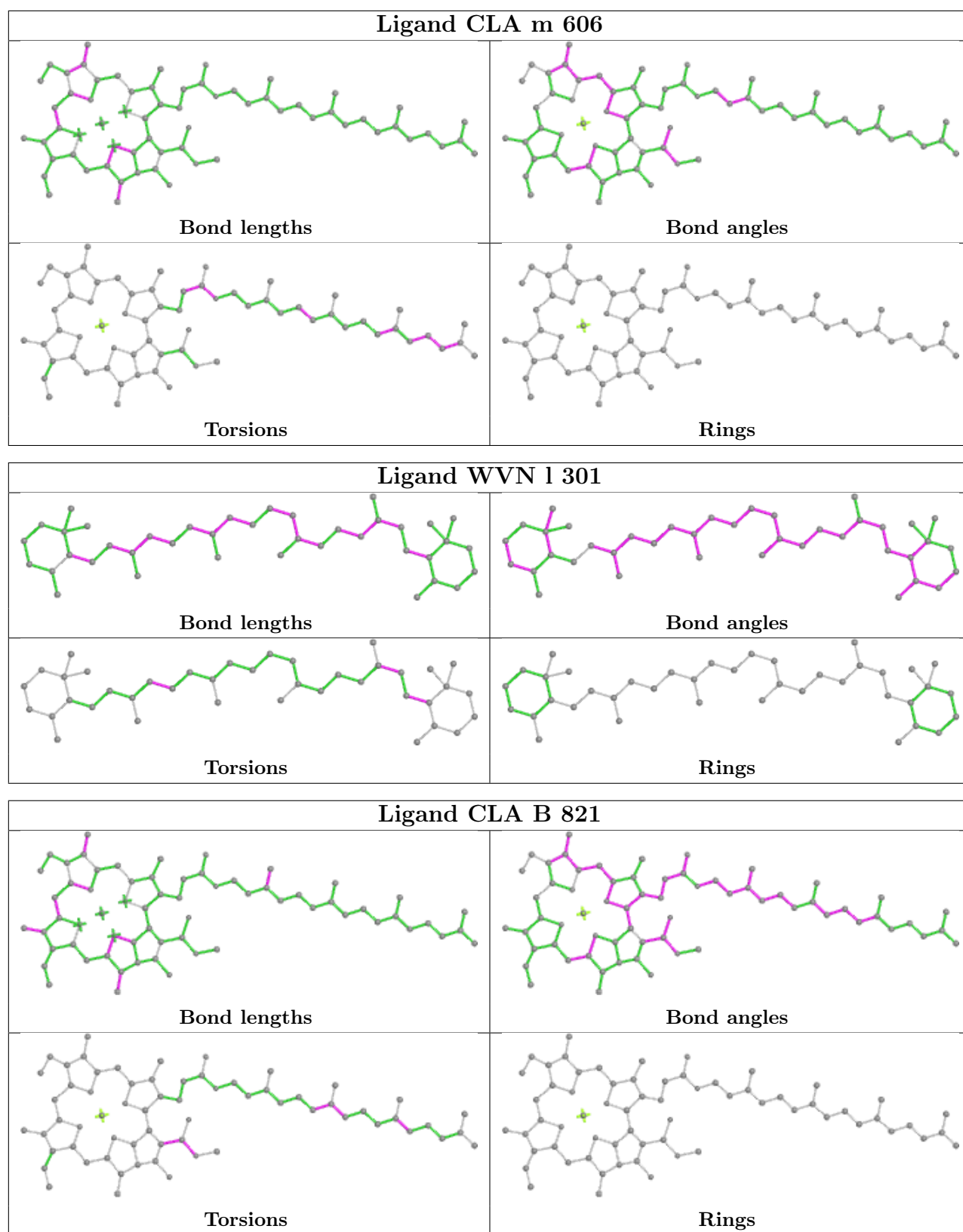
Ligand CLA B 811**Ligand CLA a 306****Ligand II0 e 616**

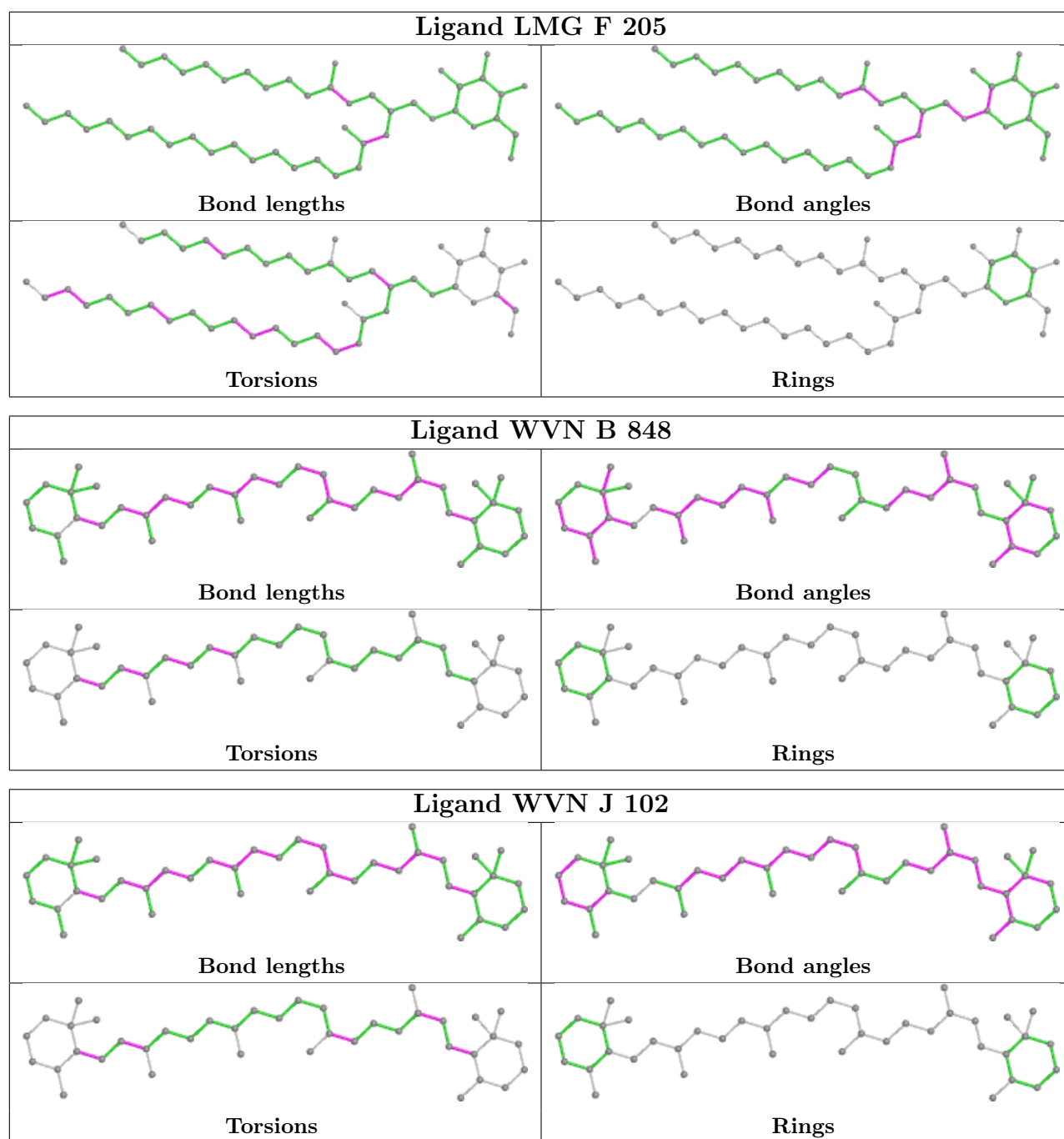
Ligand CLA s 208

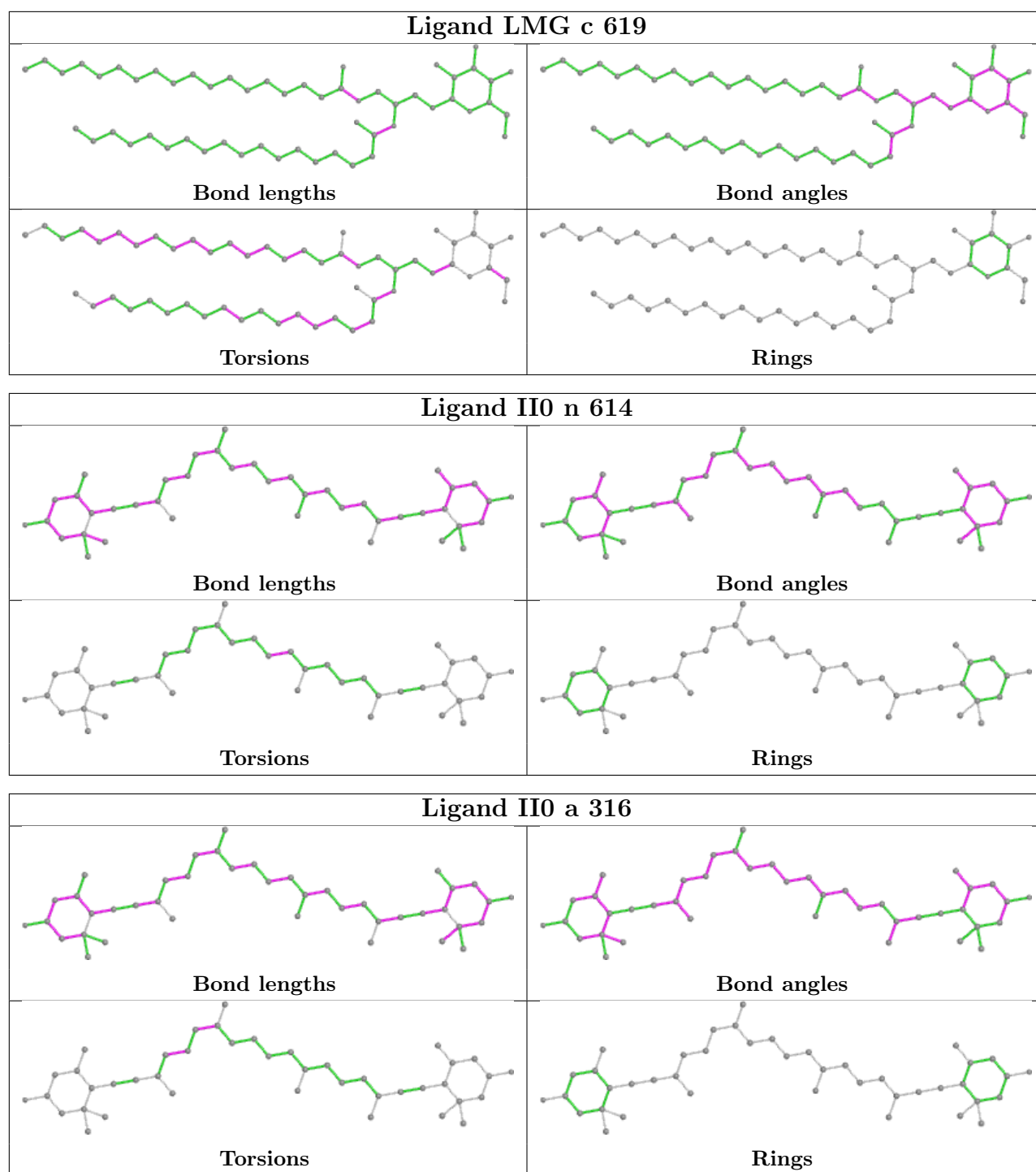


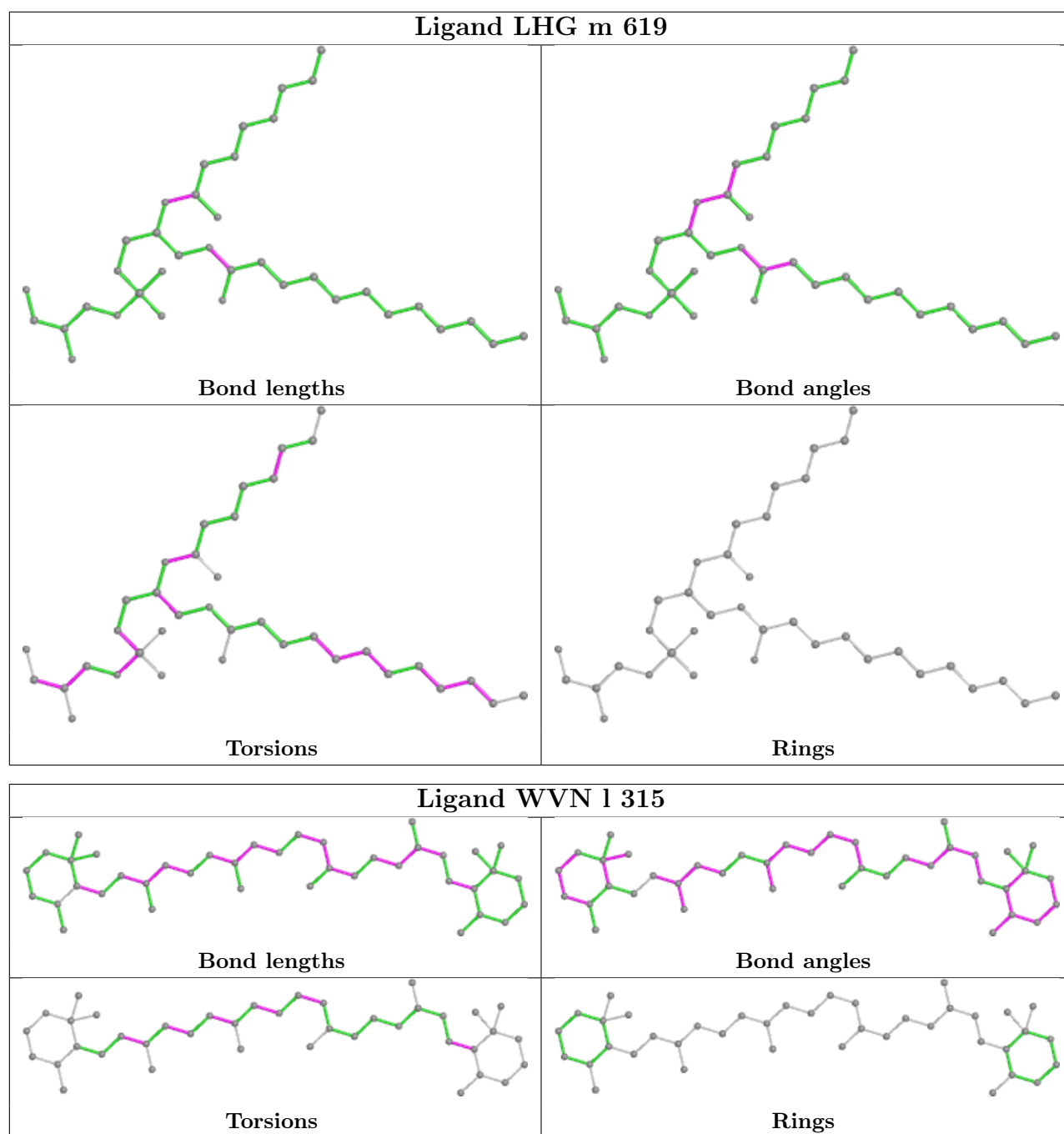
Ligand CLA B 809



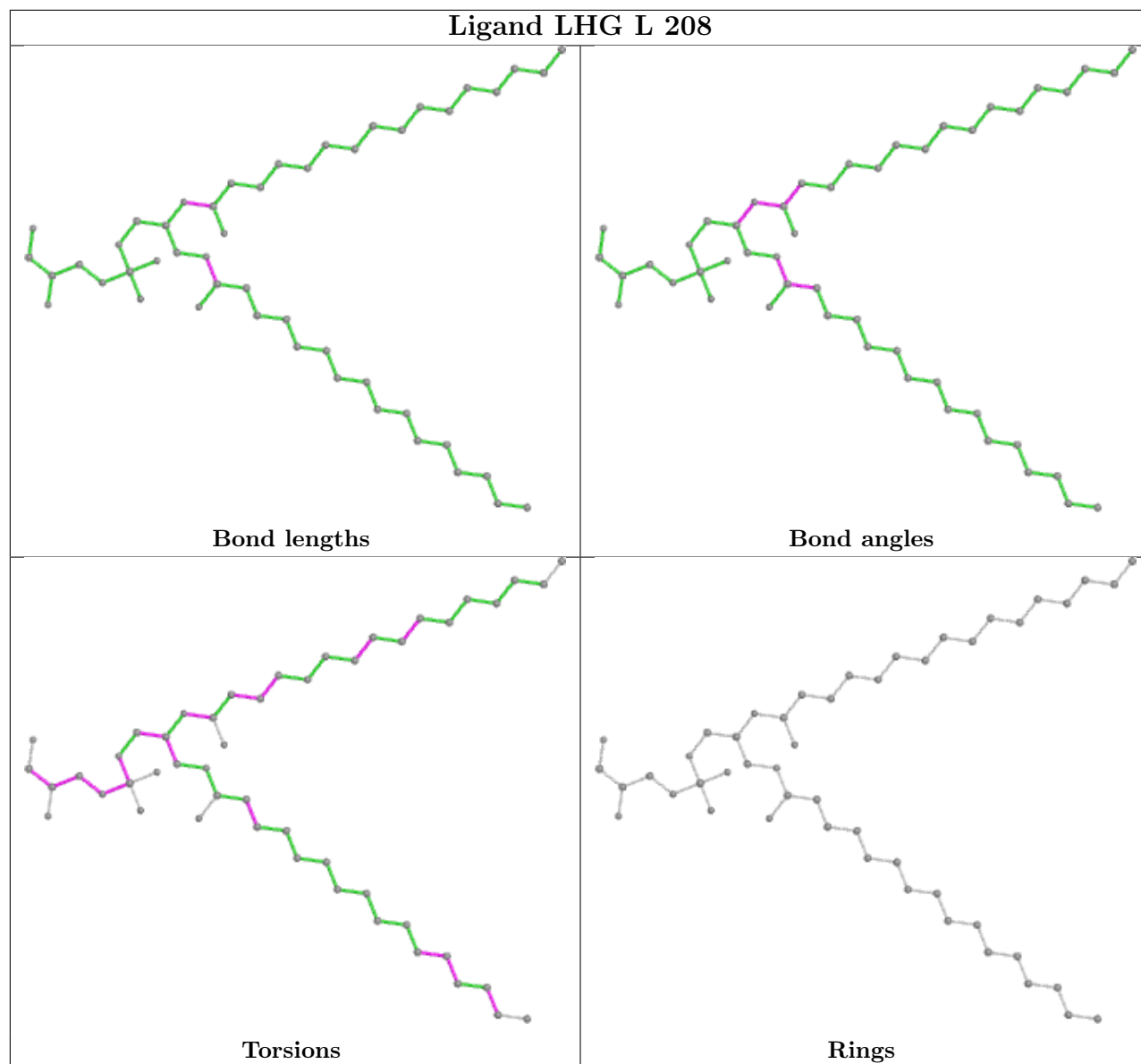




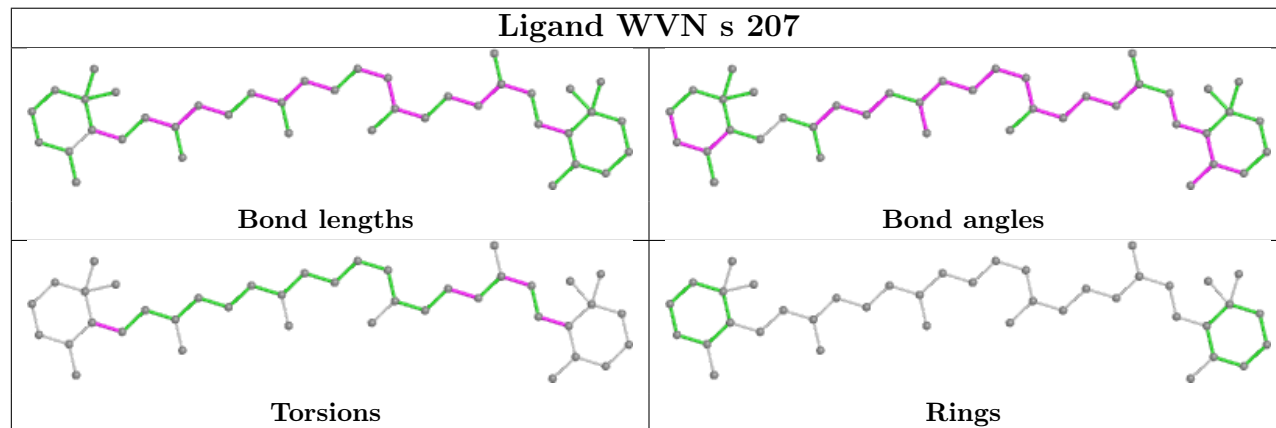




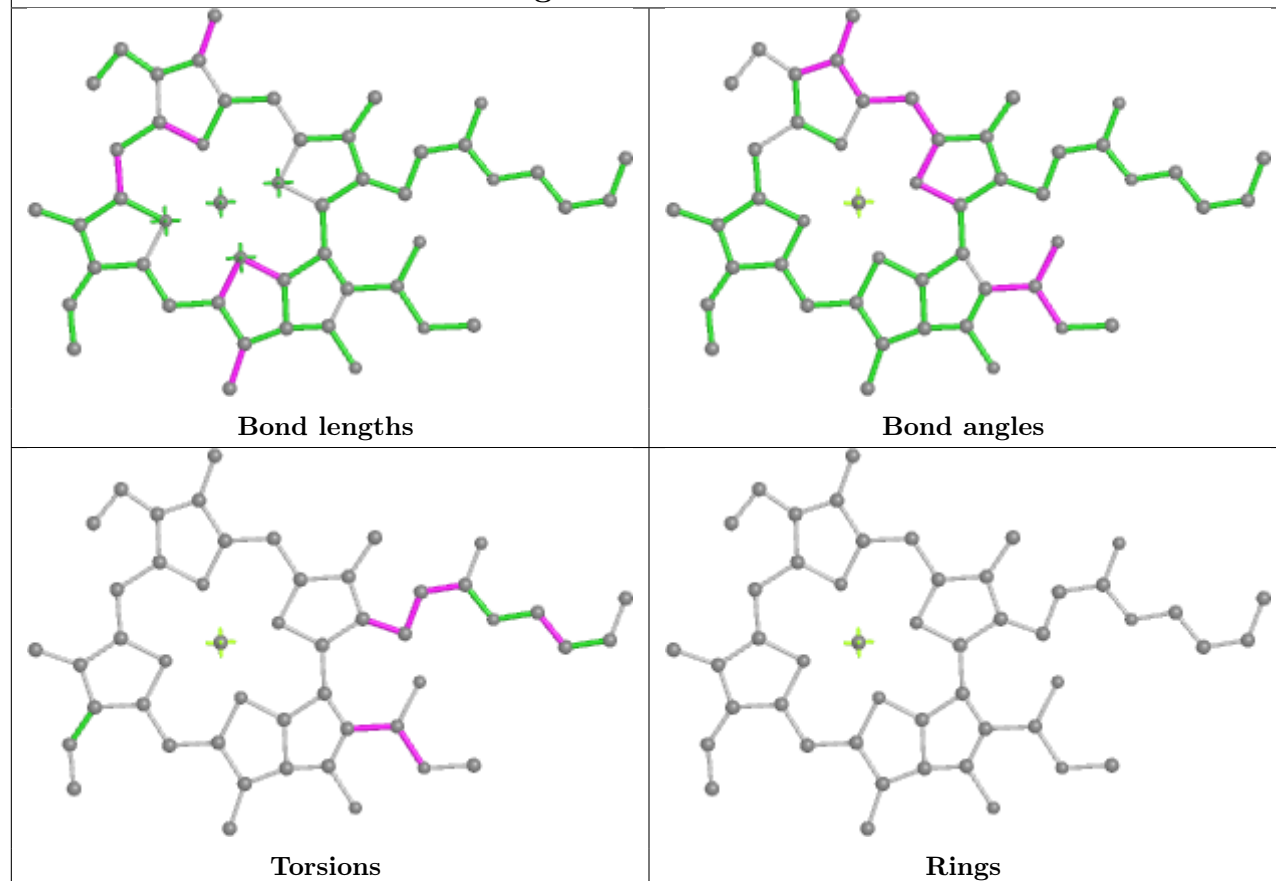
Ligand LHG L 208



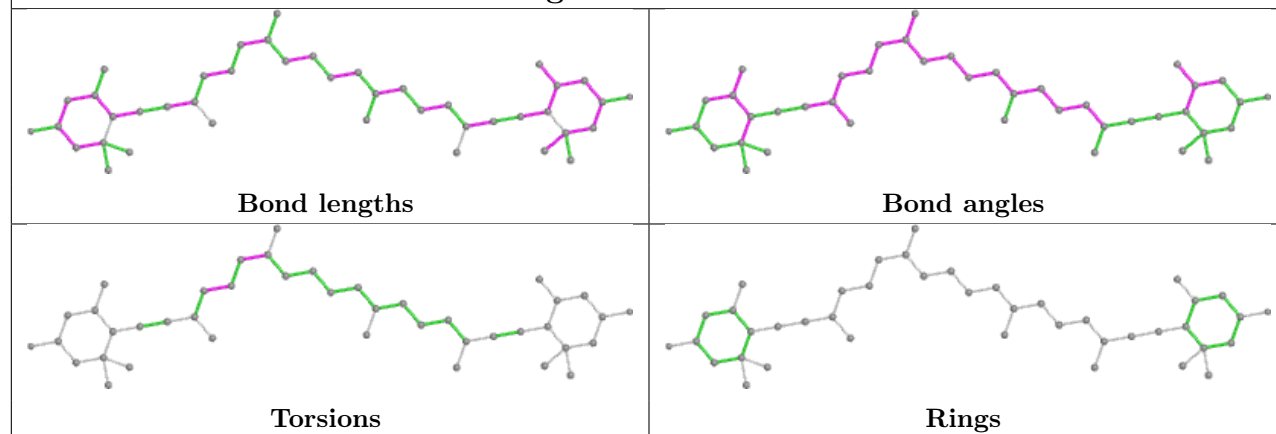
Ligand WVN s 207



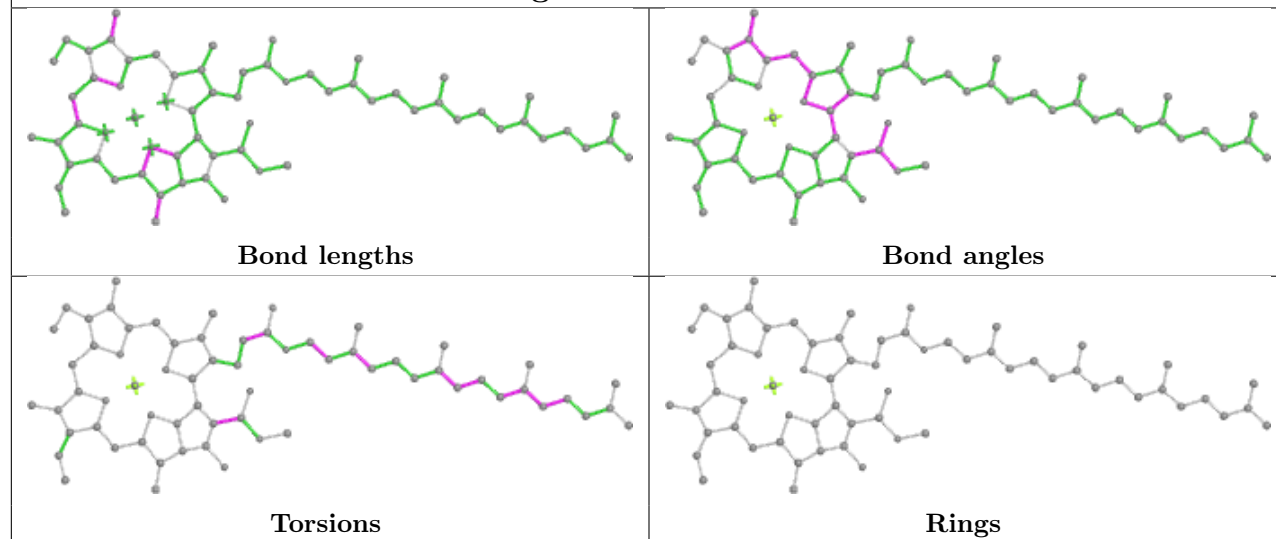
Ligand CLA L 202



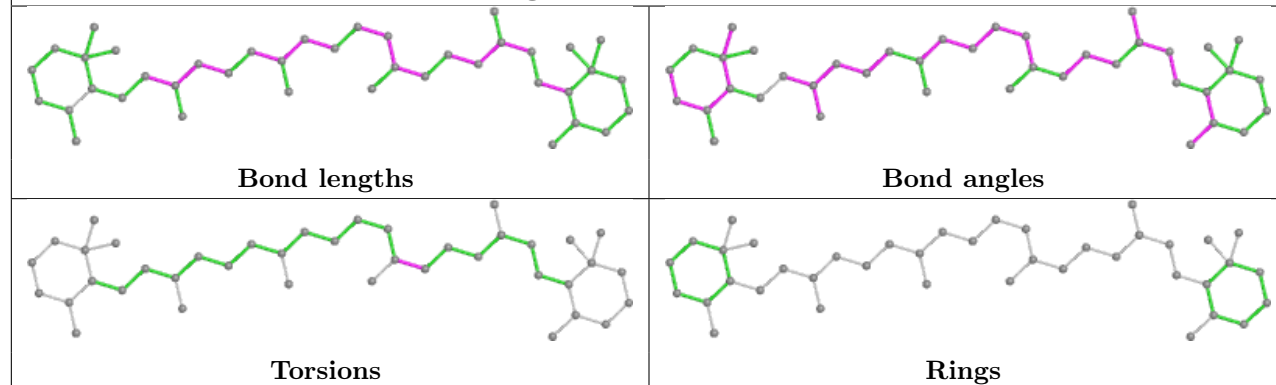
Ligand II0 O 203



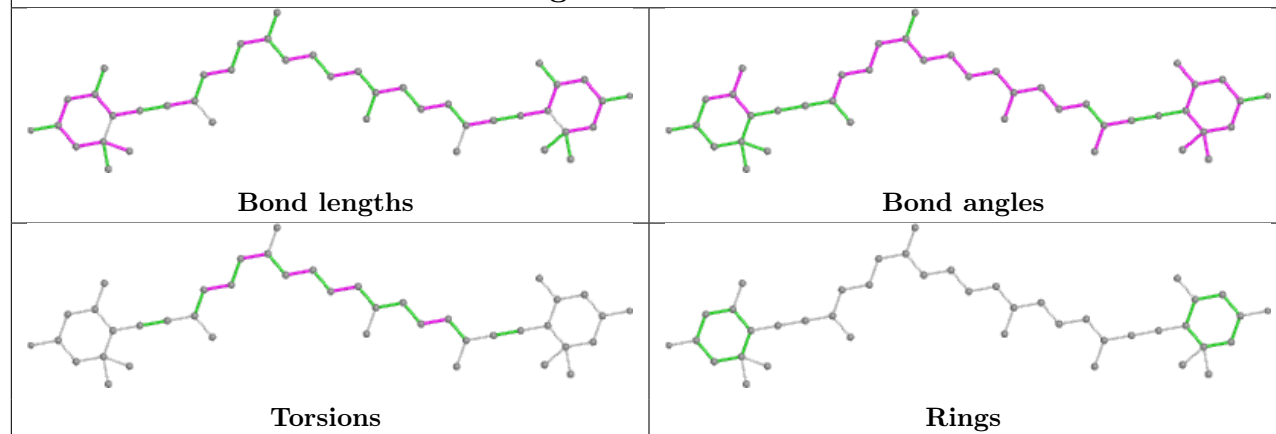
Ligand CLA A 824

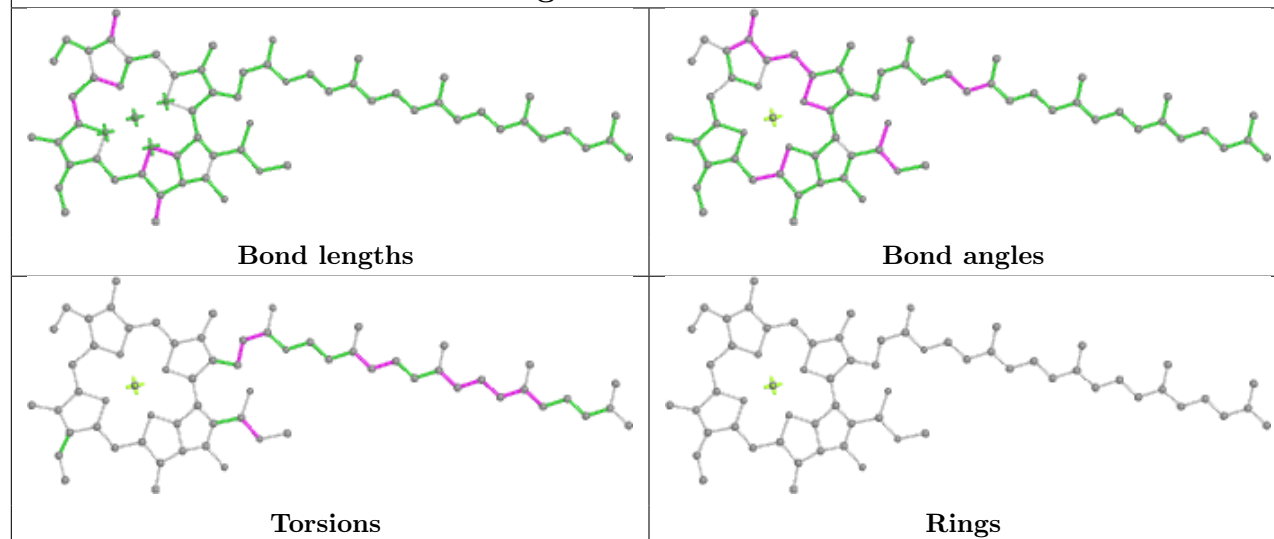
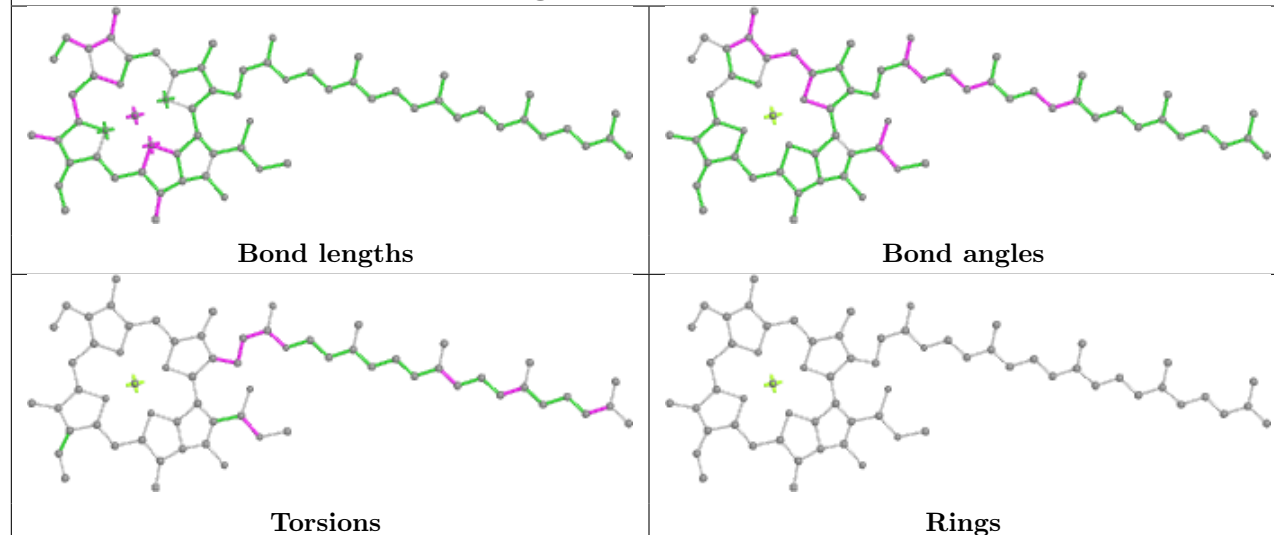
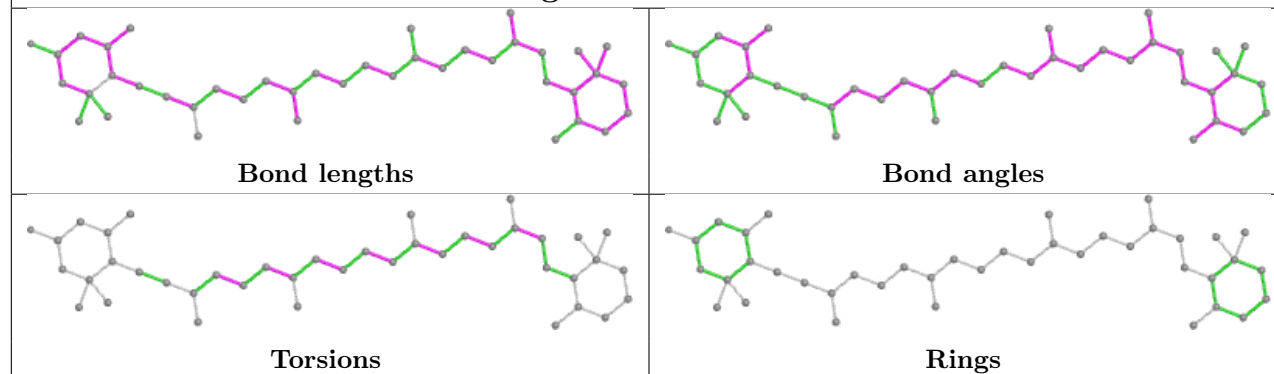


Ligand WVN B 847

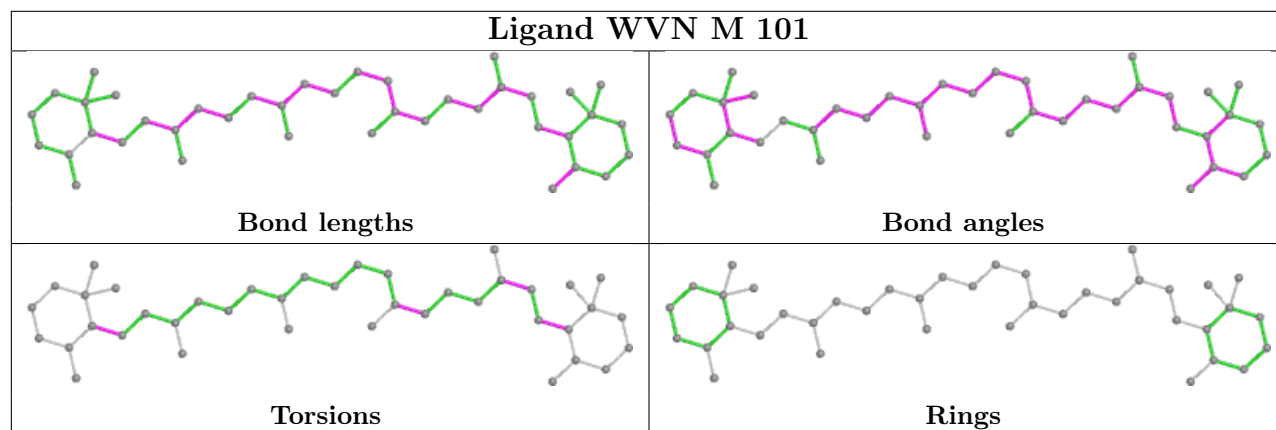


Ligand II0 h 312

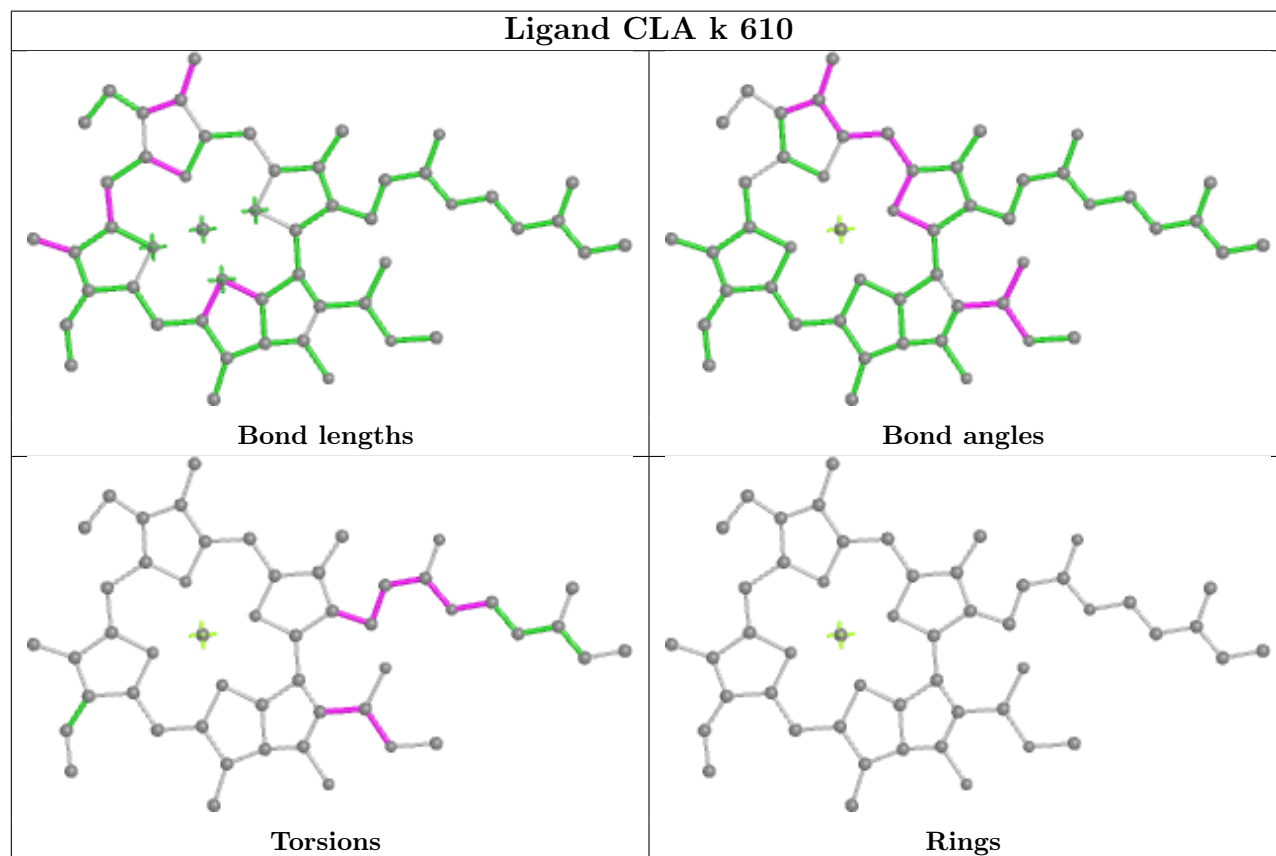


Ligand CLA c 612**Ligand CLA A 817****Ligand IHT c 616**

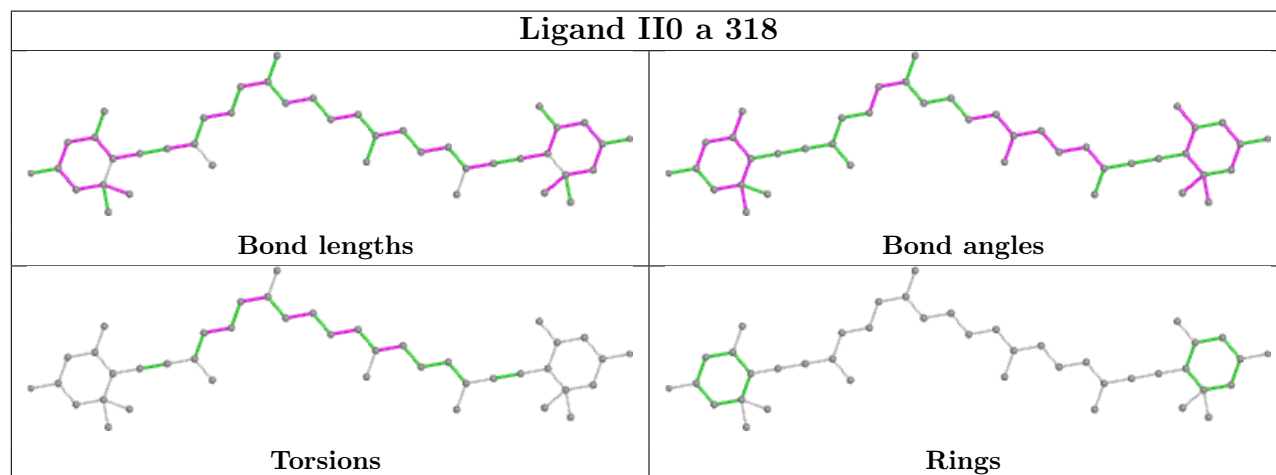
Ligand WVN M 101

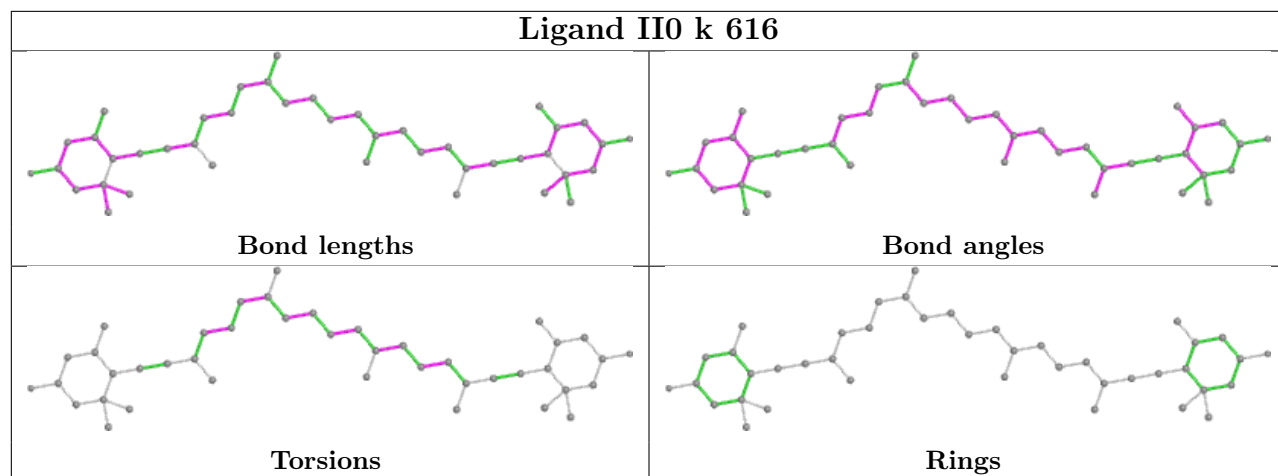
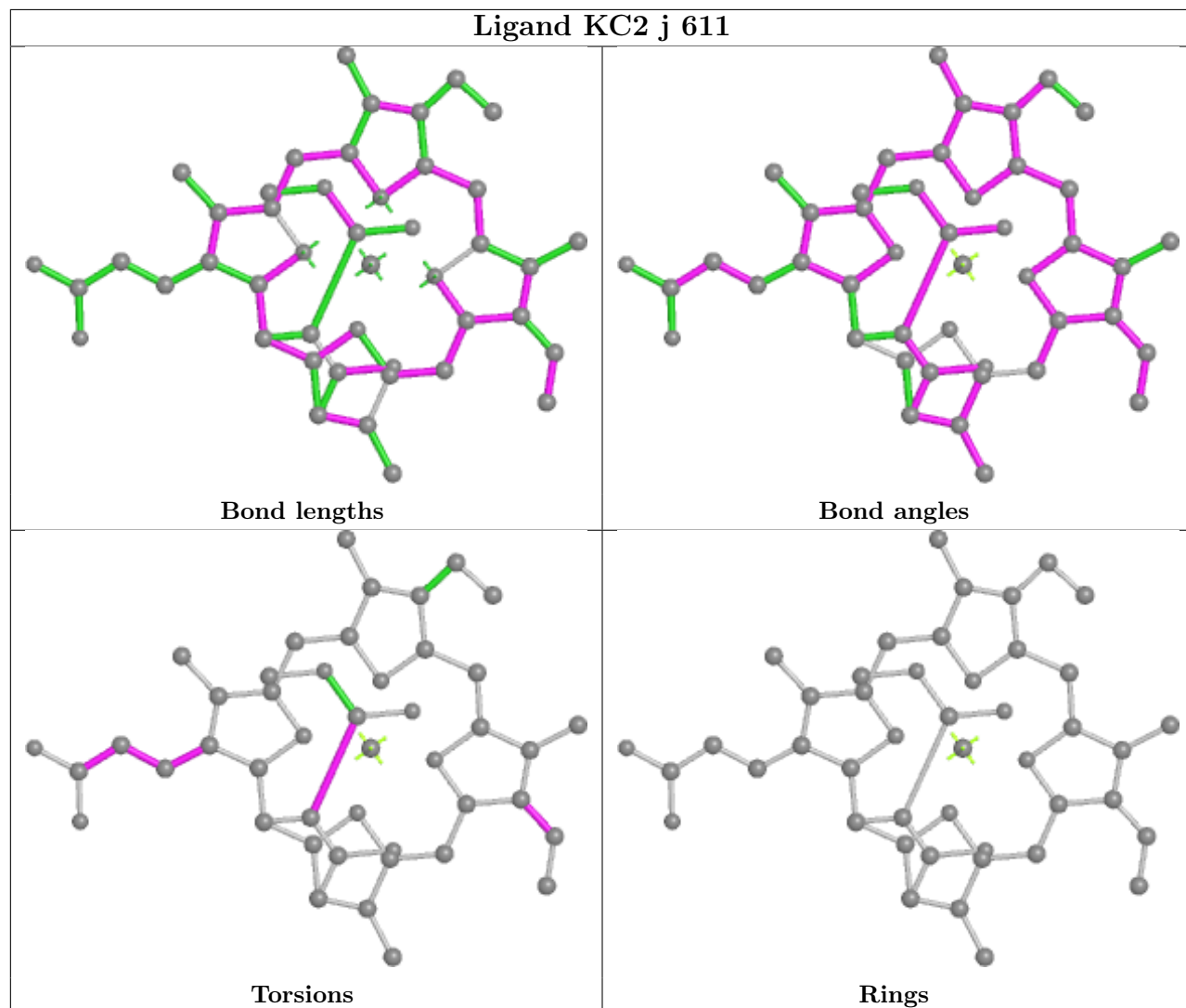


Ligand CLA k 610

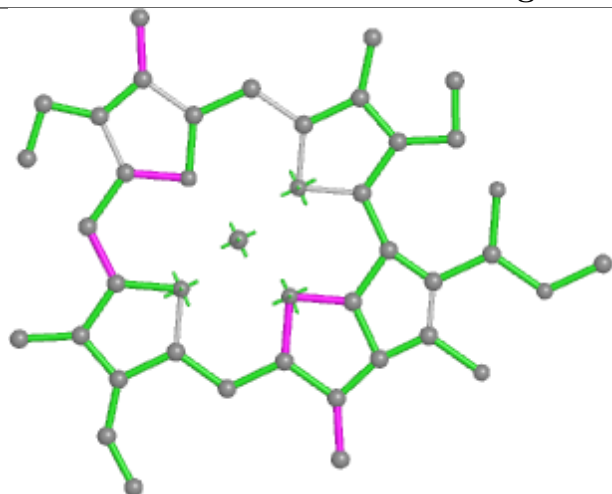


Ligand II0 a 318

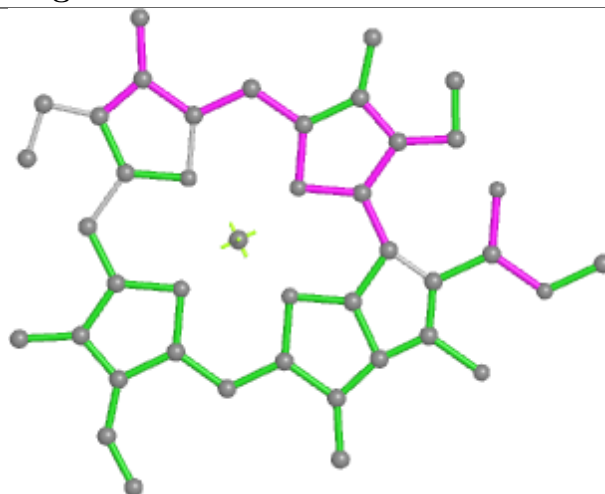


Ligand II0 k 616**Ligand KC2 j 611**

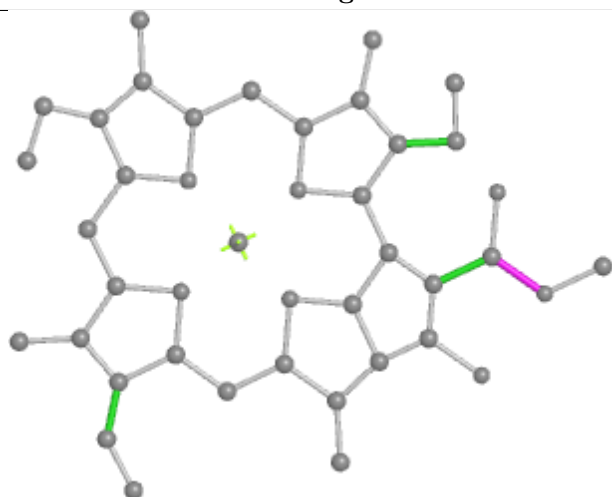
Ligand CLA g 302



Bond lengths



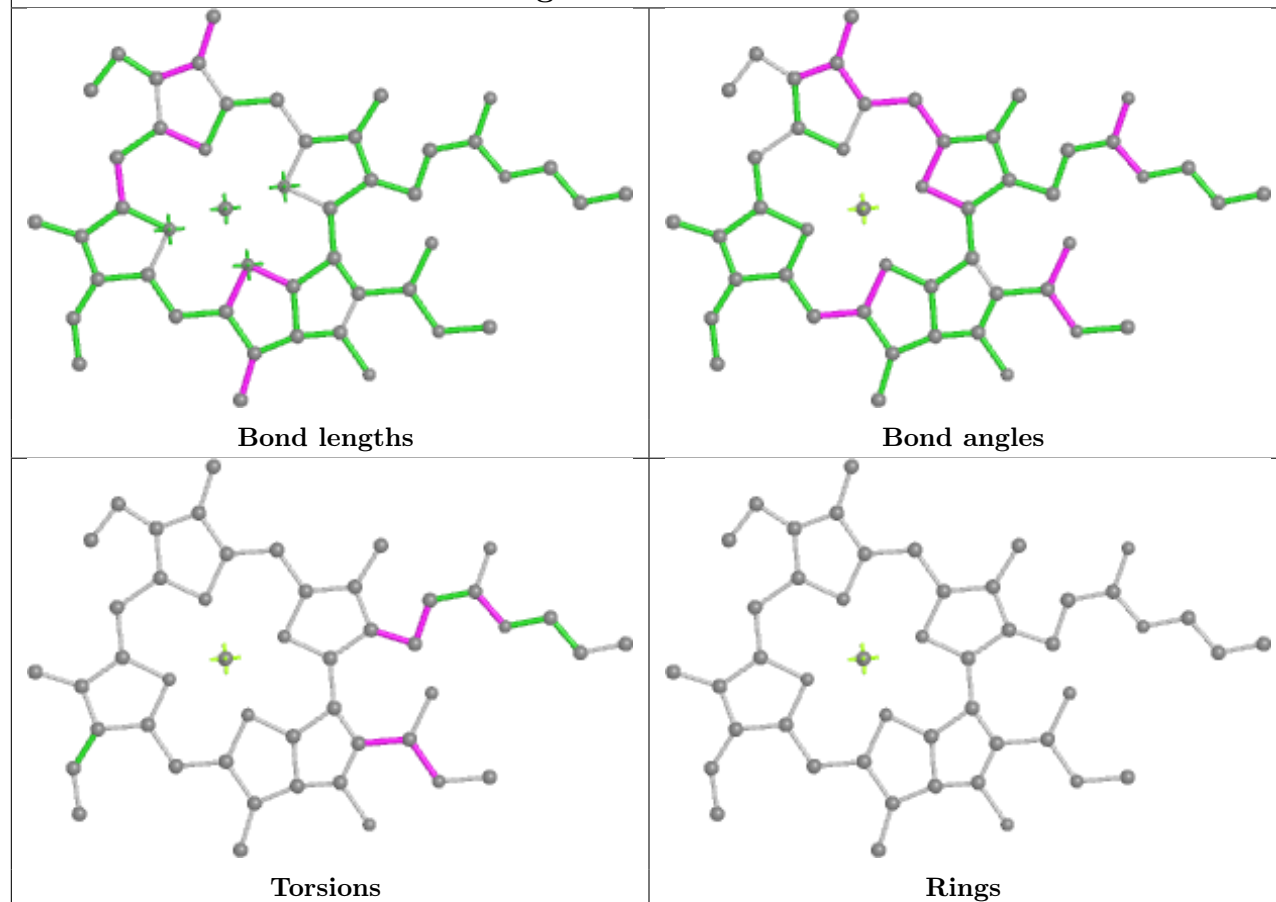
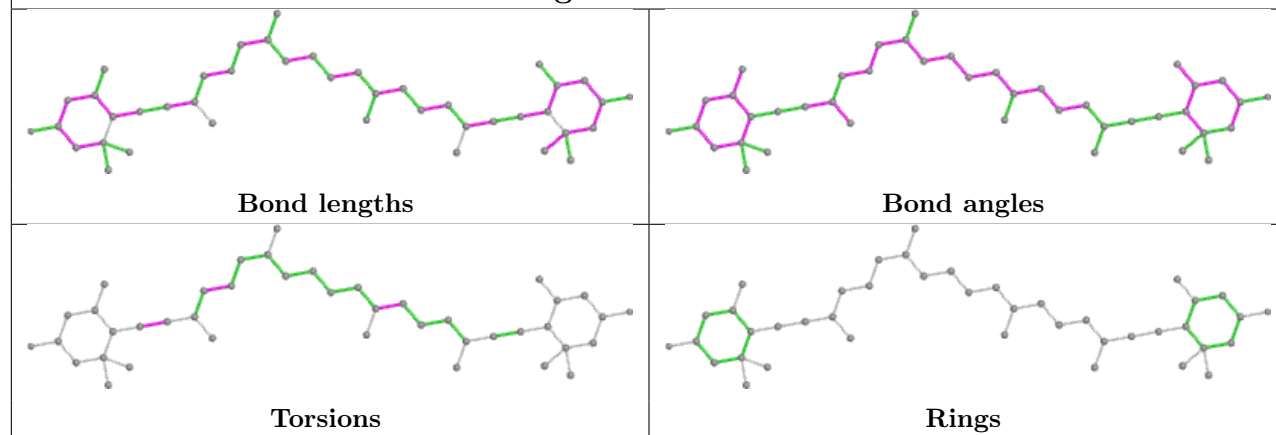
Bond angles



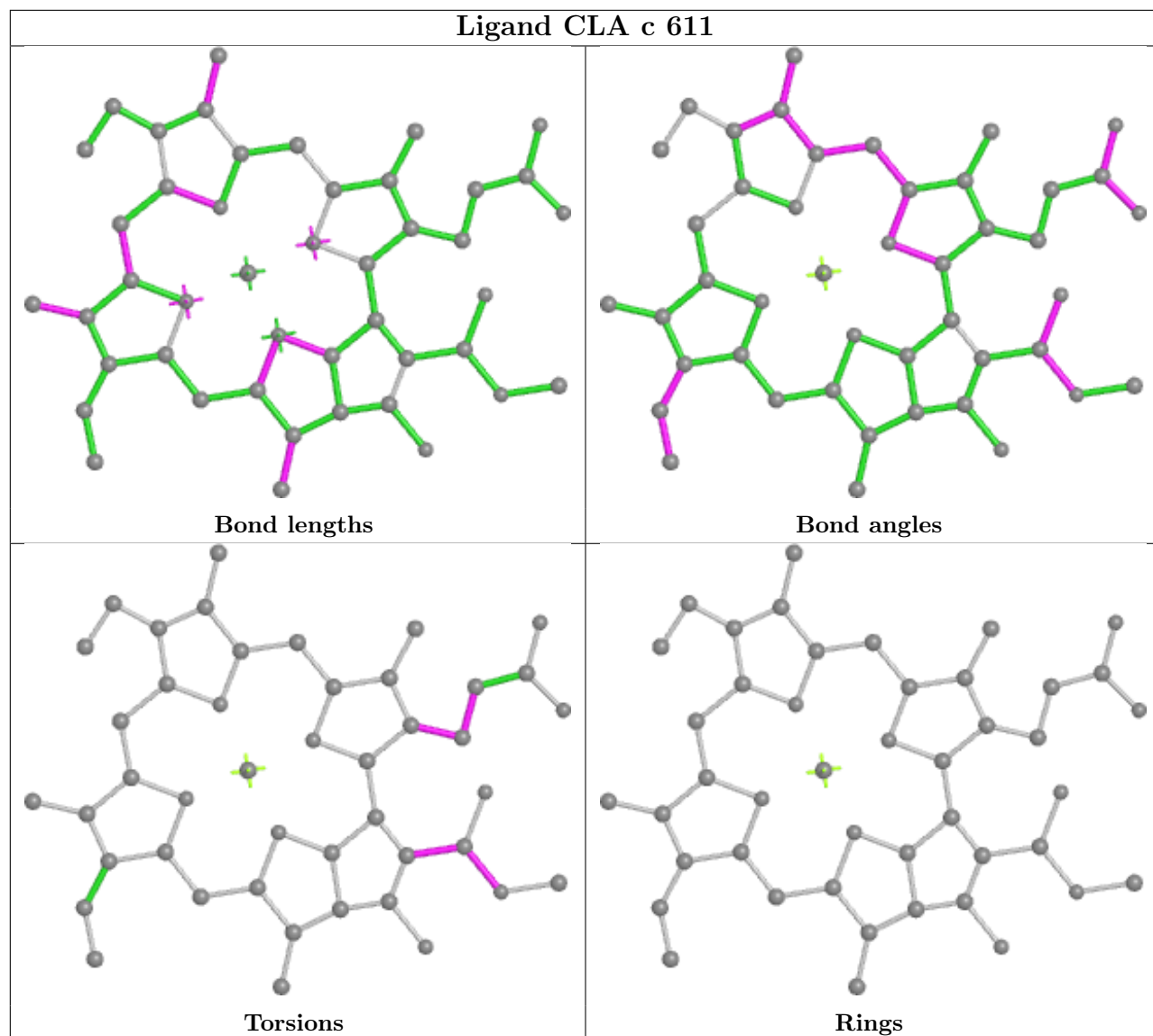
Torsions

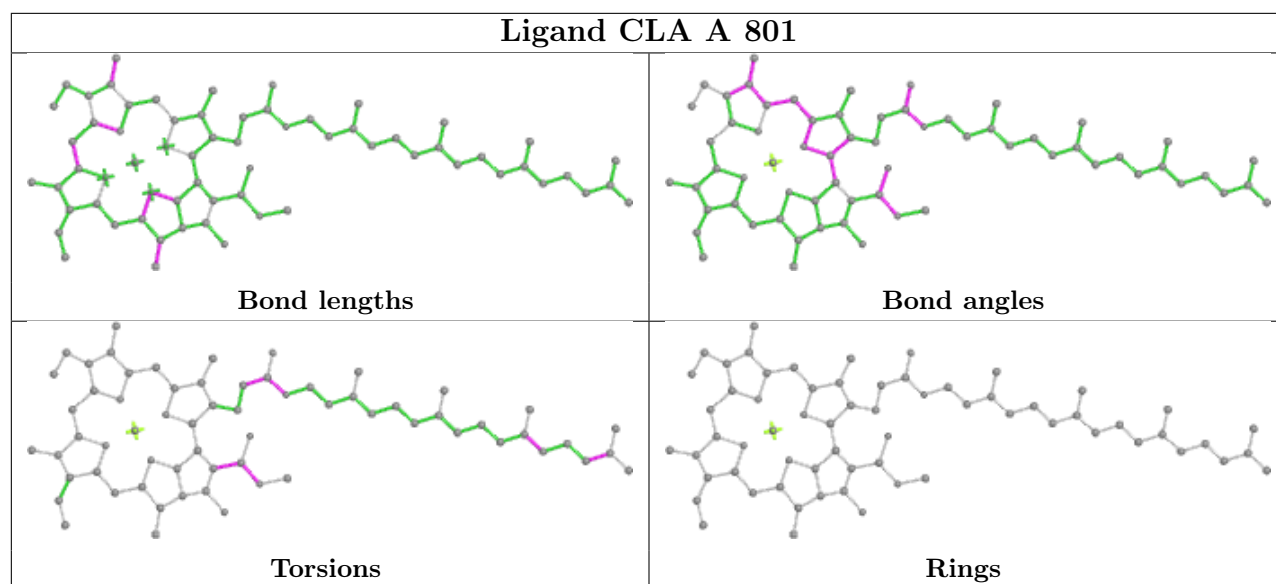
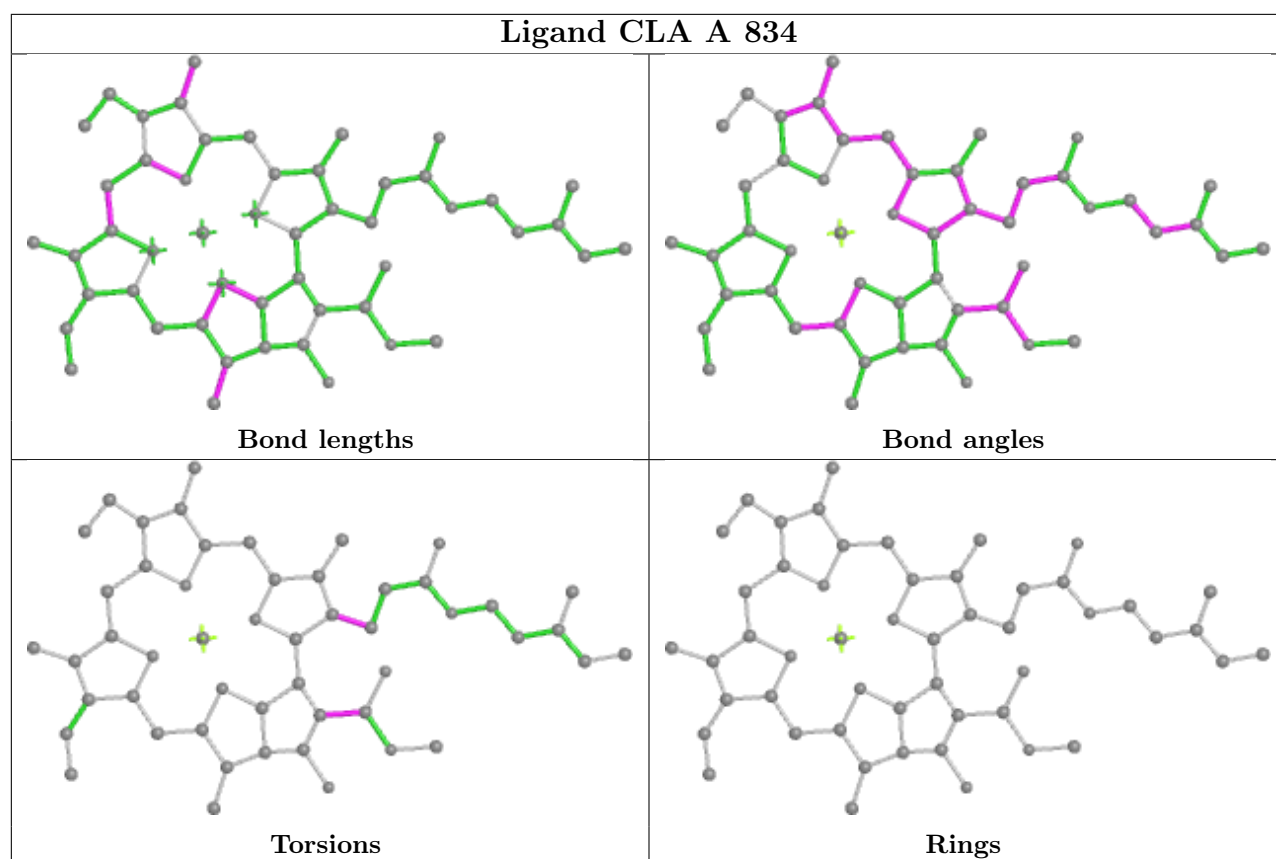


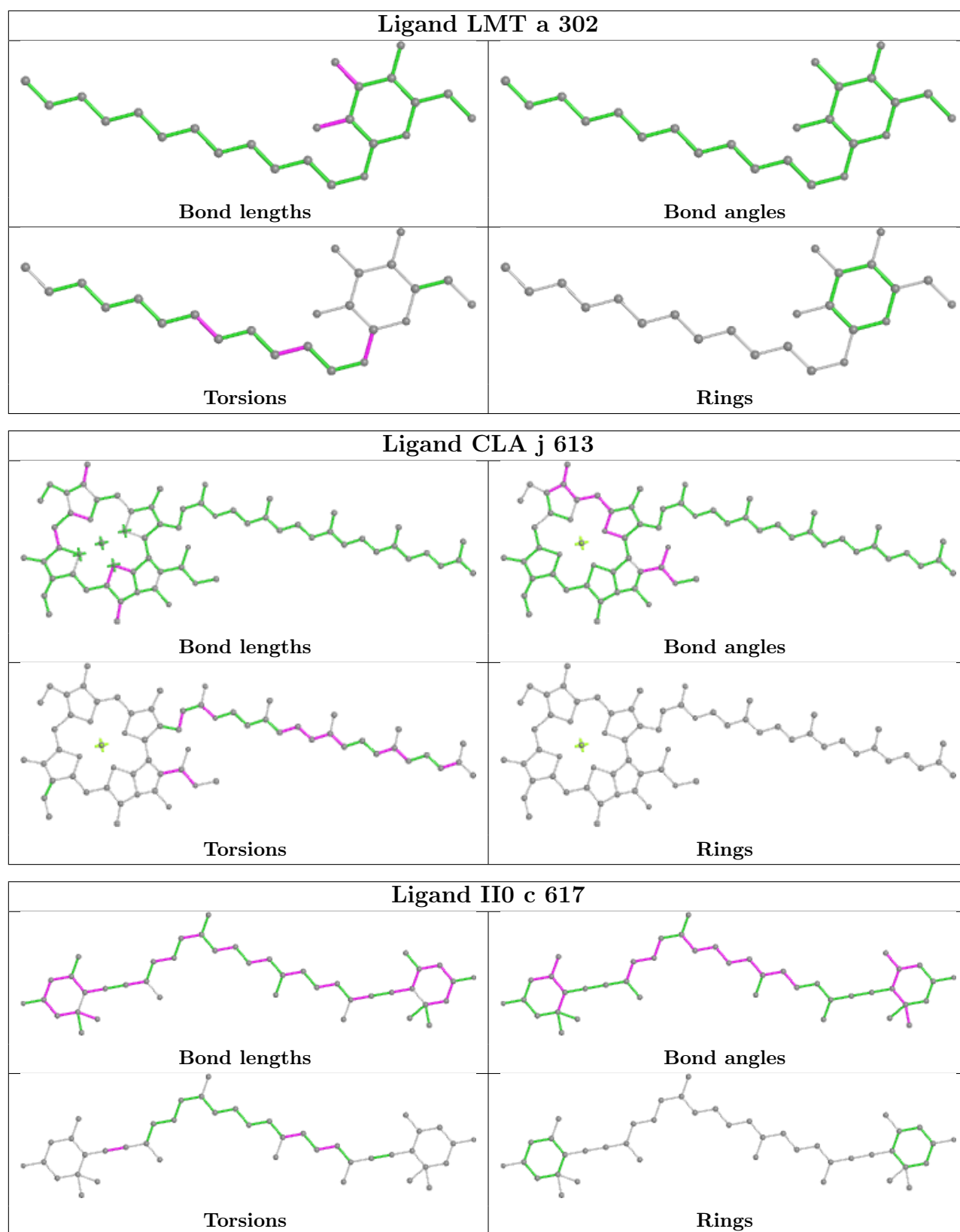
Rings

Ligand CLA a 313**Ligand II0 i 315**

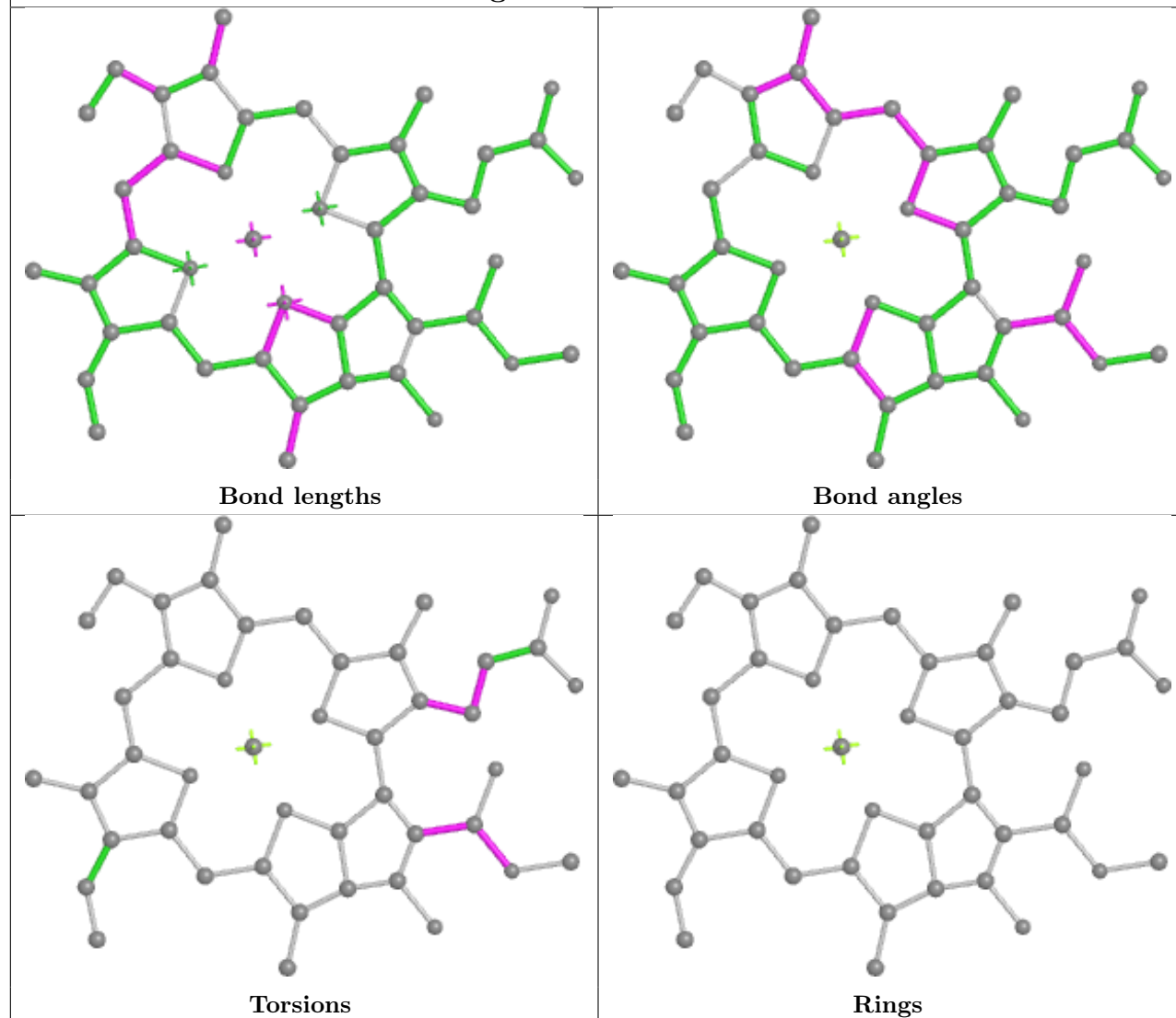
Ligand CLA c 611



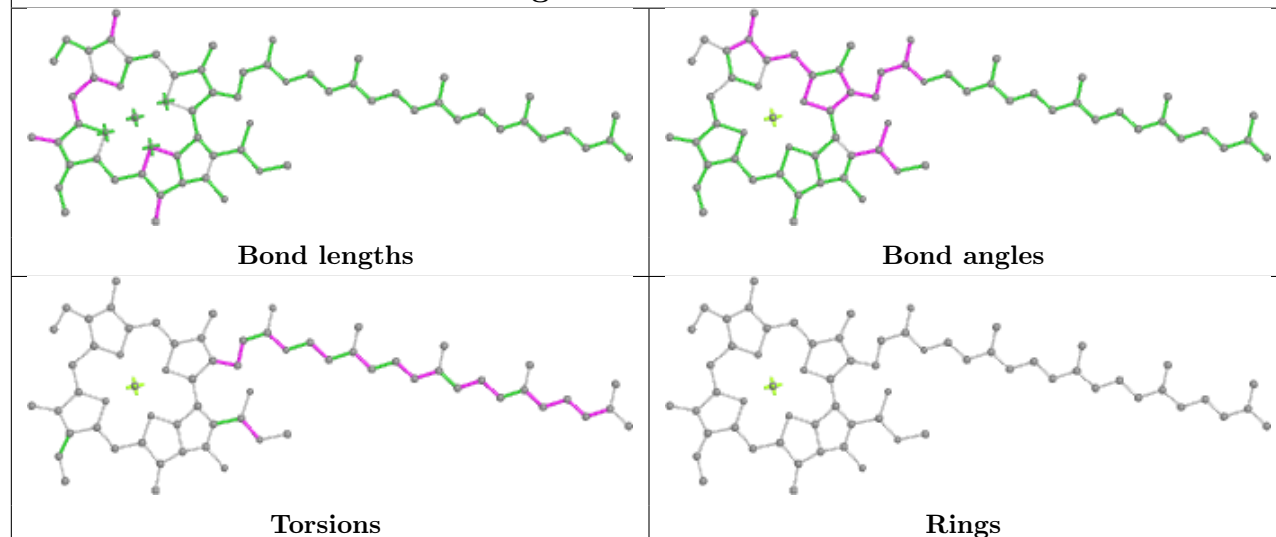




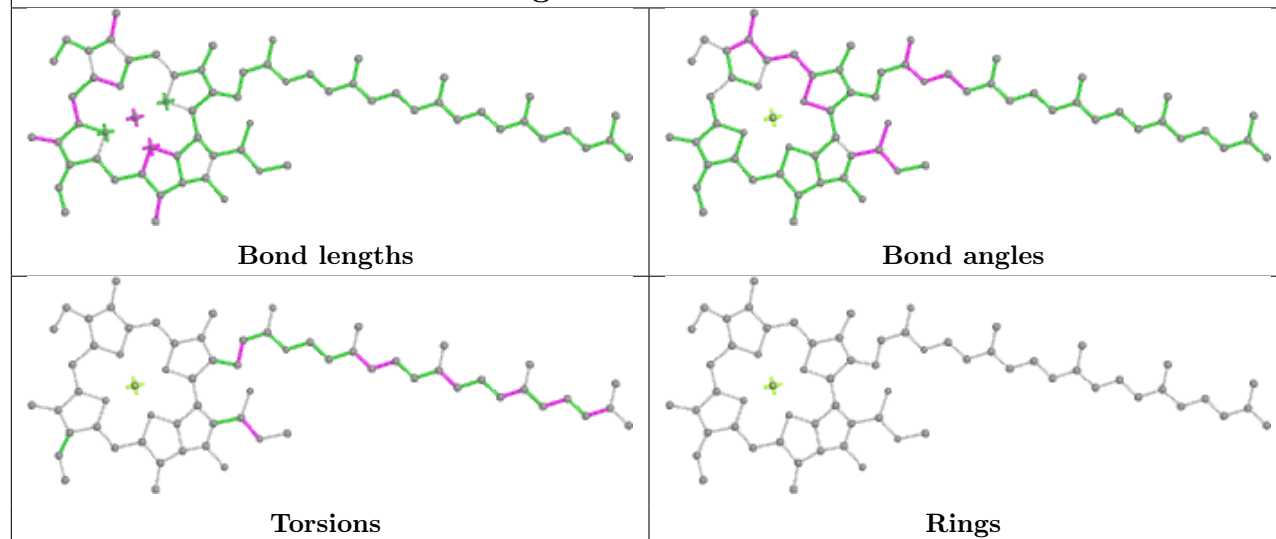
Ligand CLA A 815



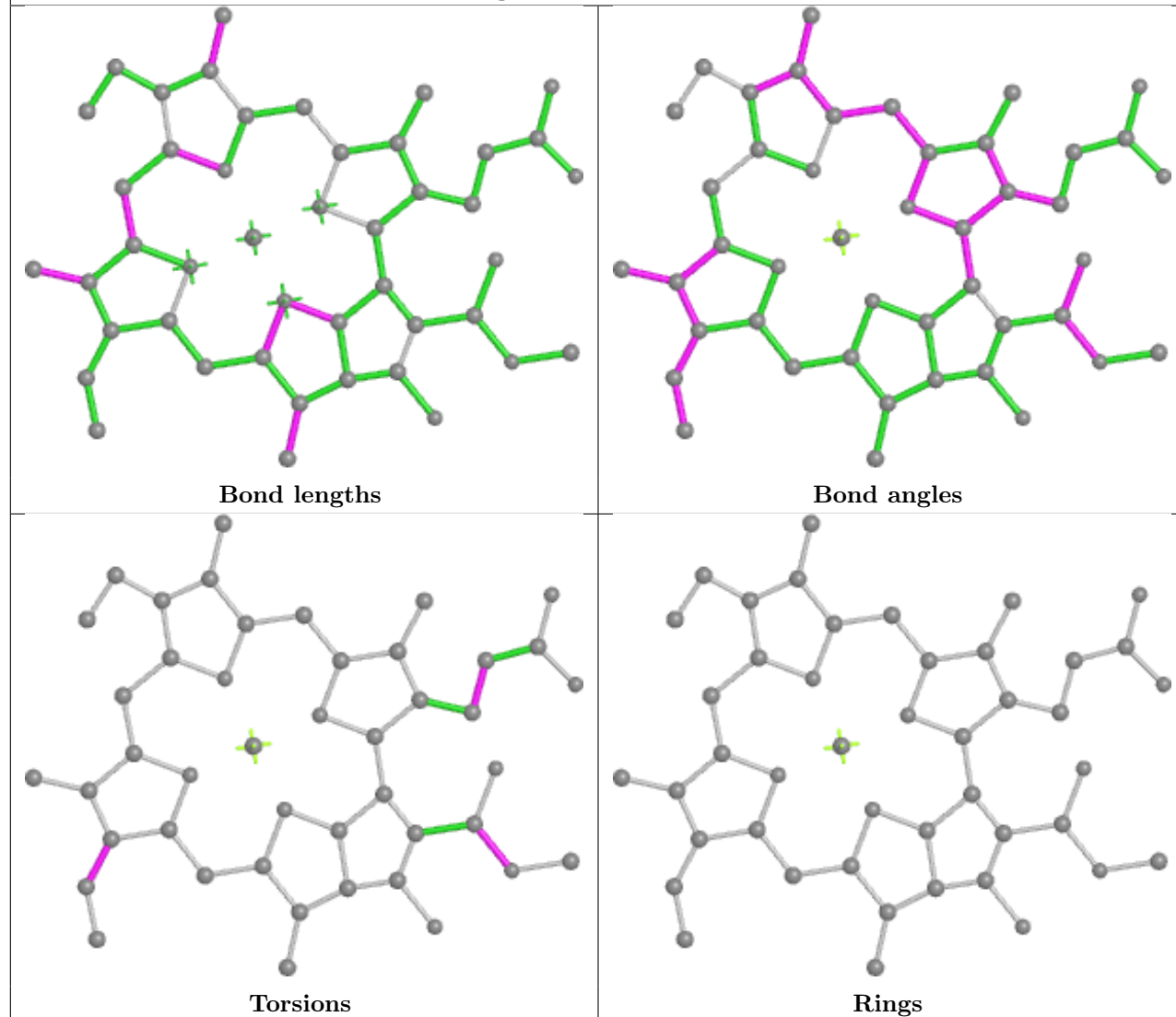
Ligand CLA A 841

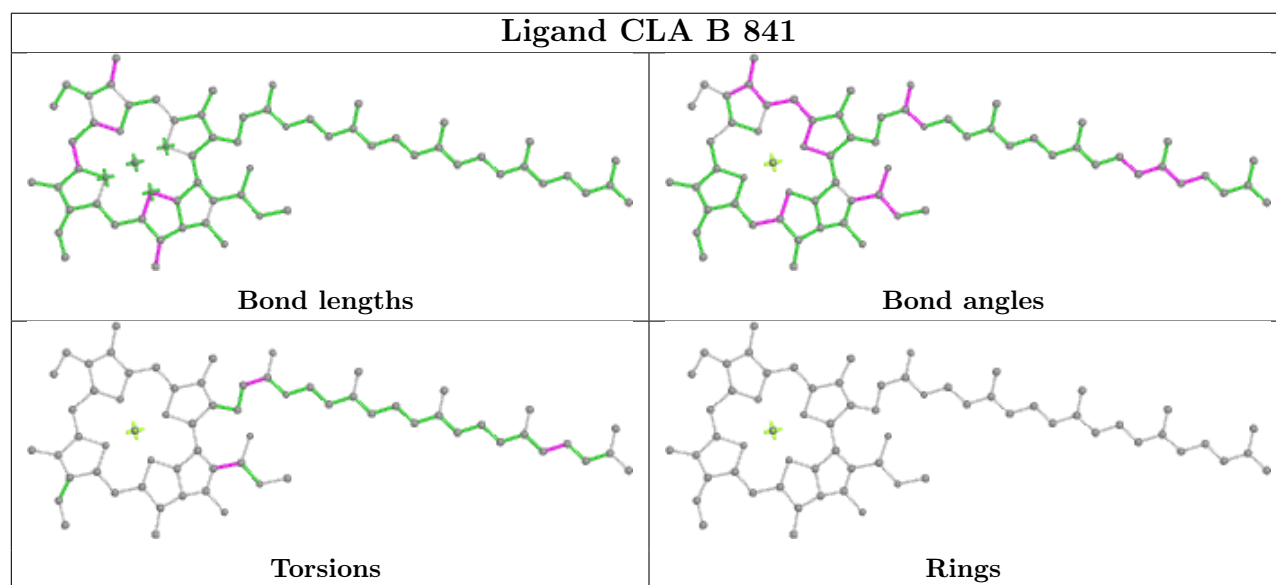
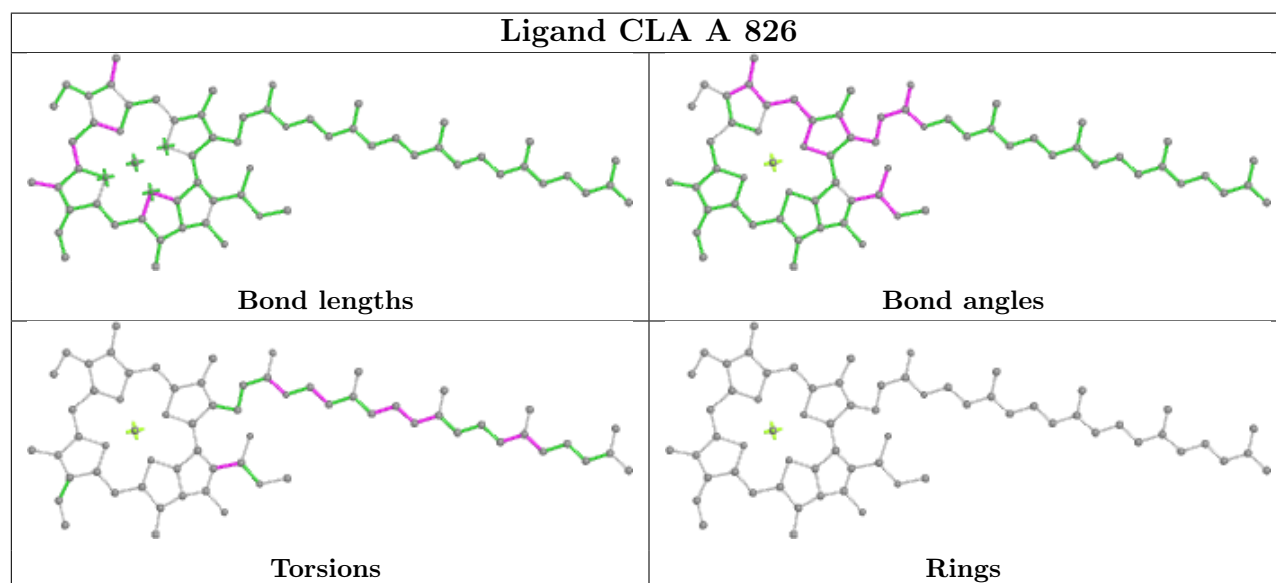
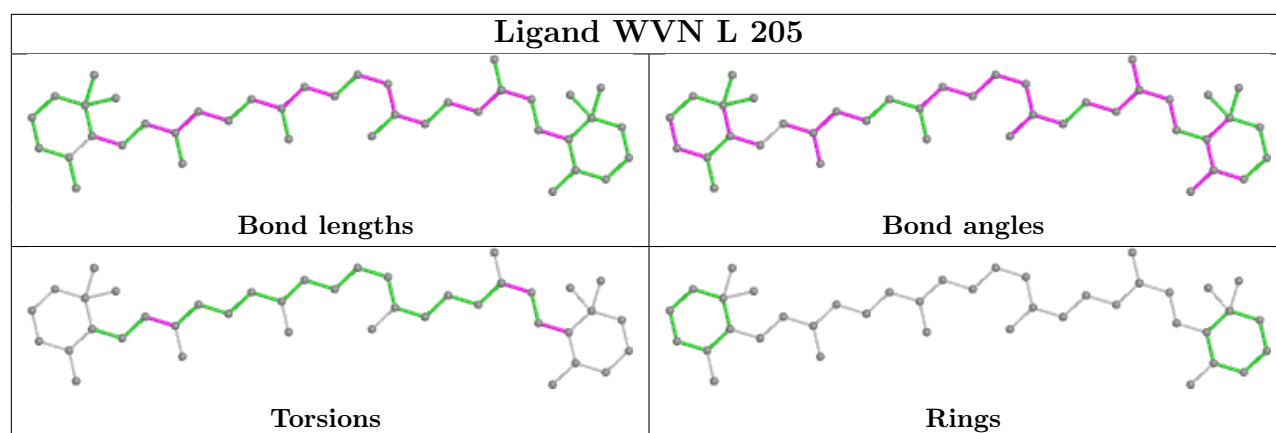


Ligand CLA B 801

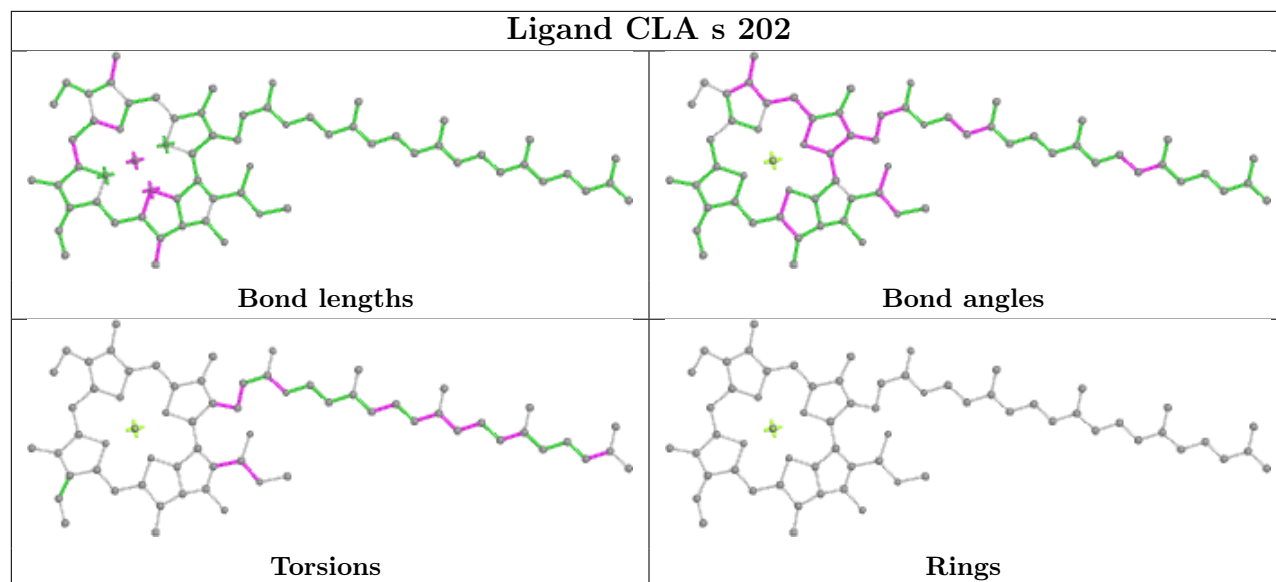


Ligand CLA k 605

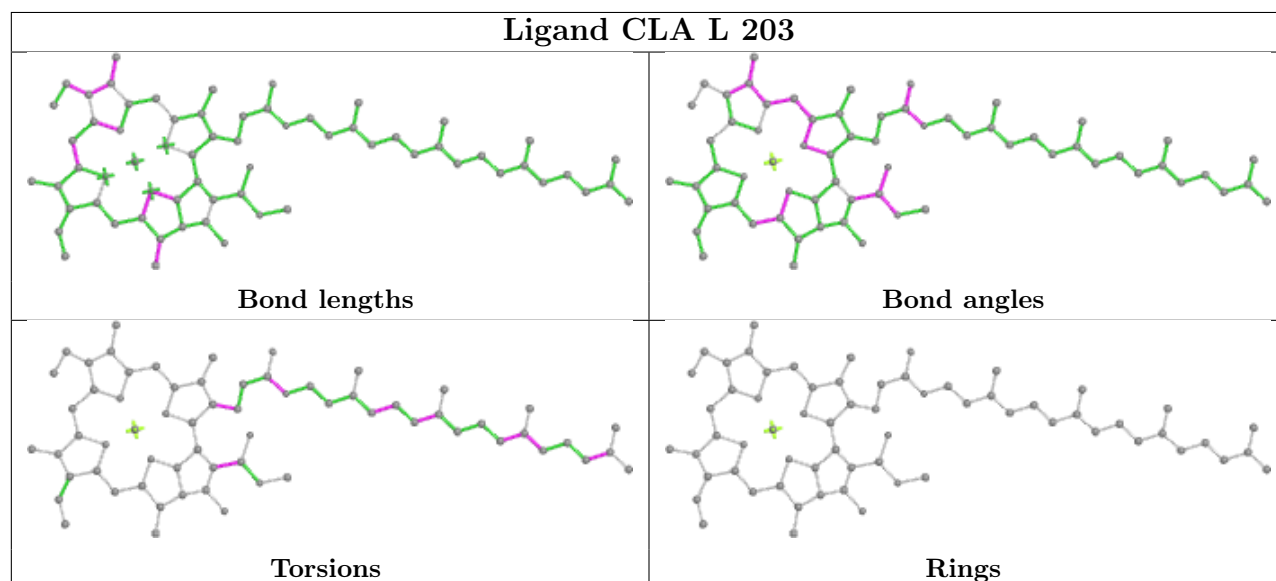




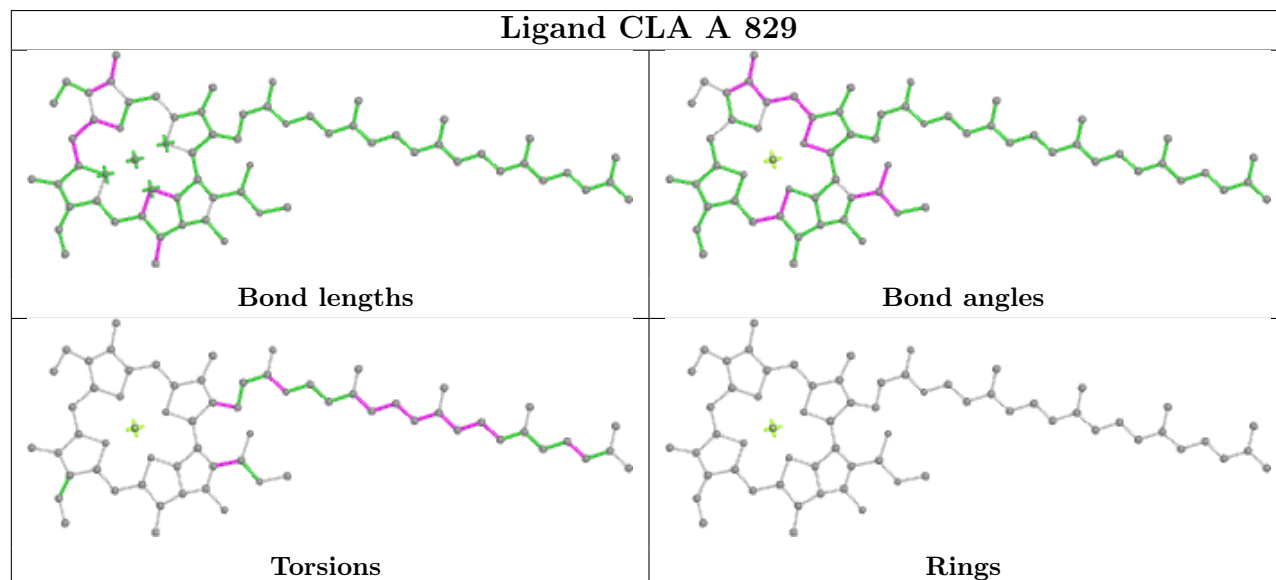
Ligand CLA s 202



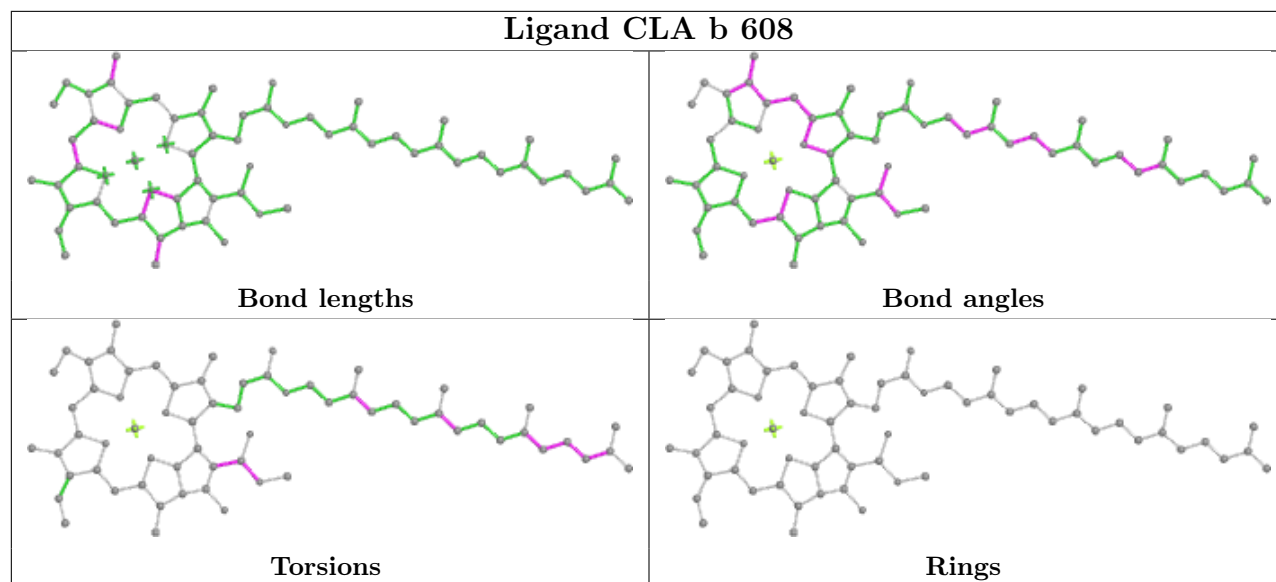
Ligand CLA L 203



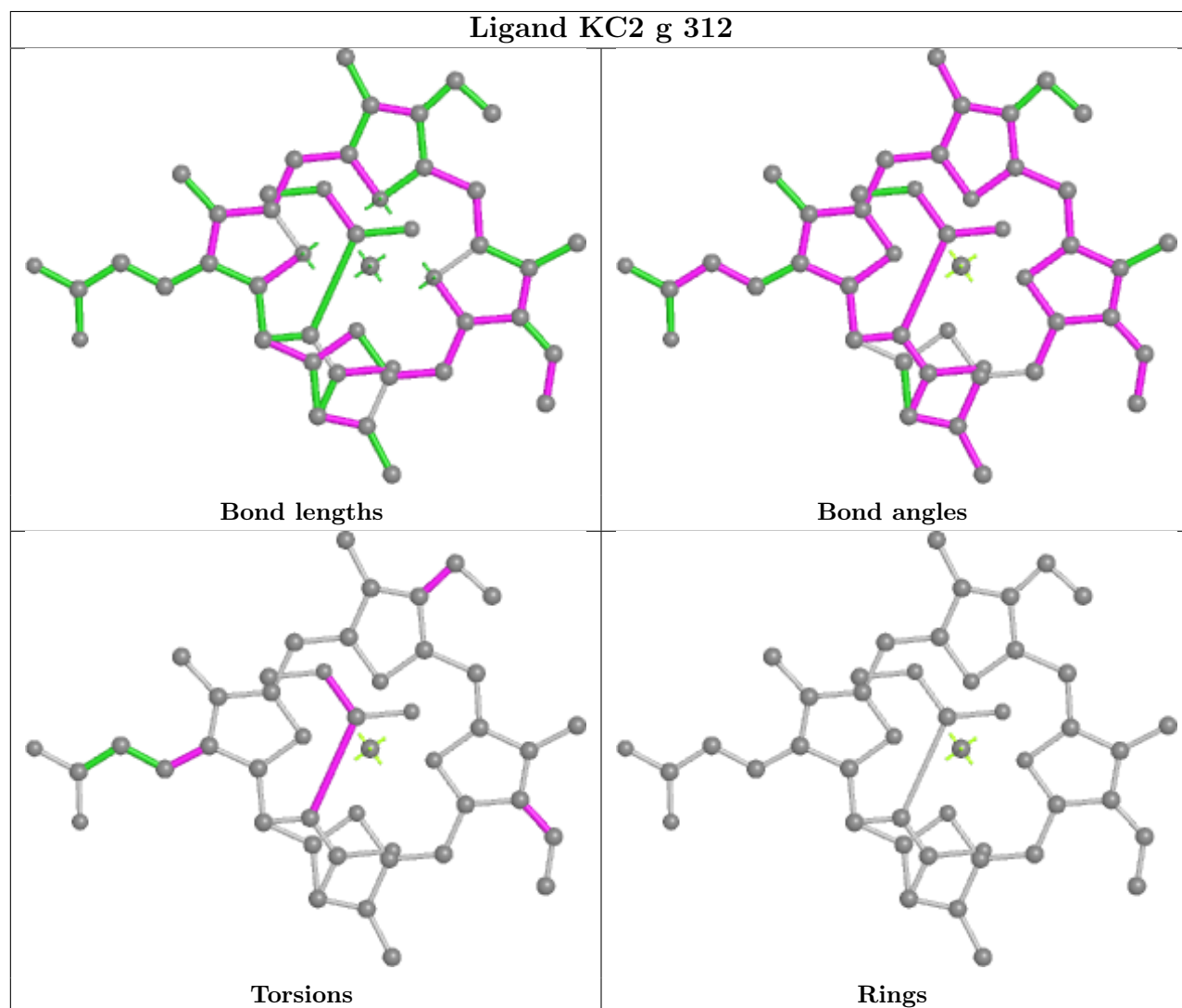
Ligand CLA A 829



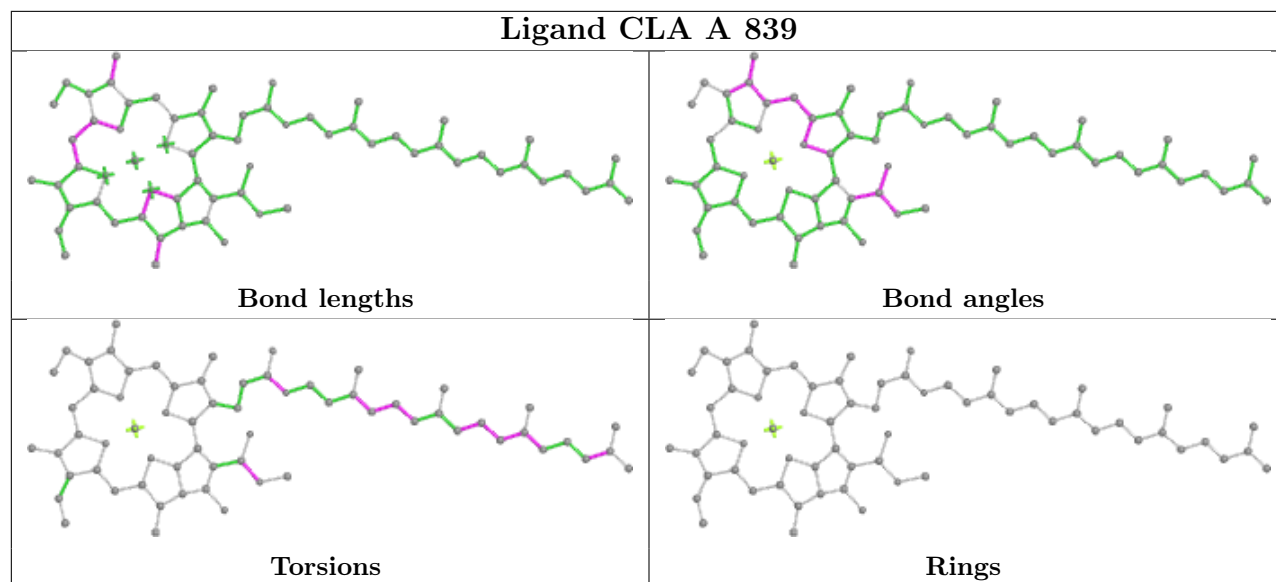
Ligand CLA b 608



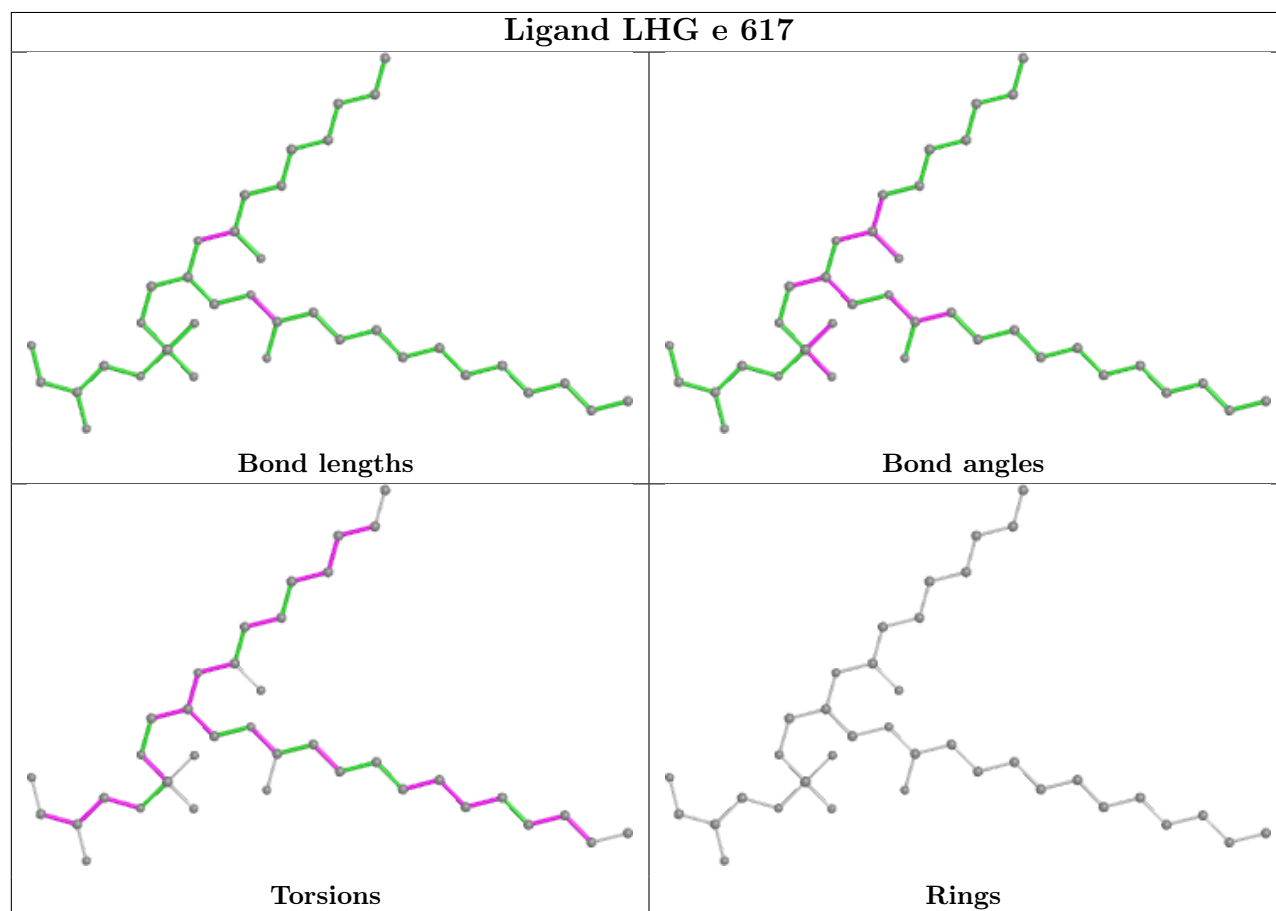
Ligand KC2 g 312

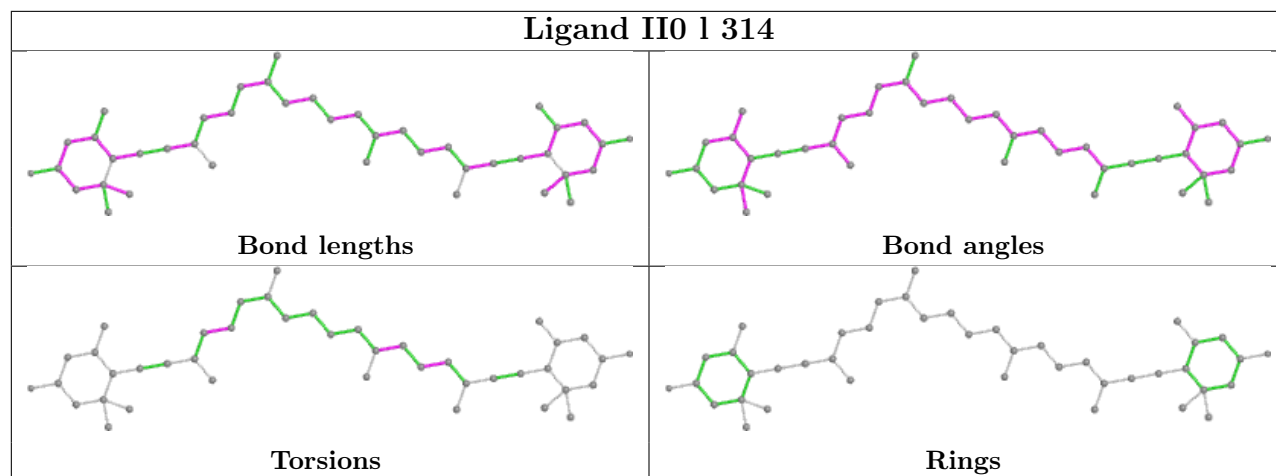
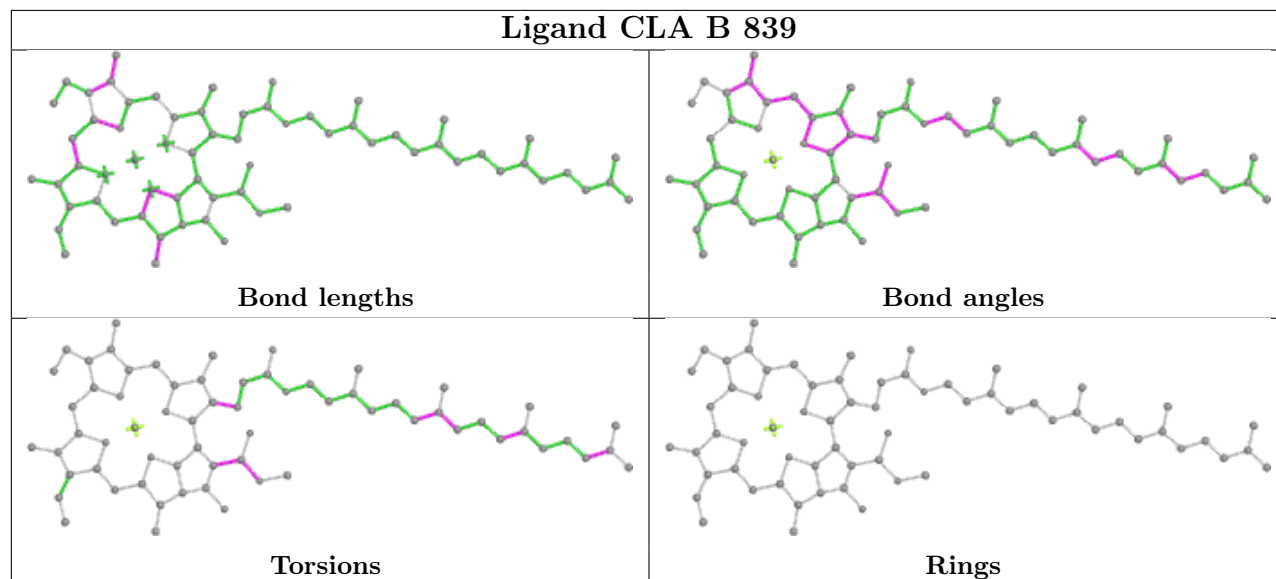
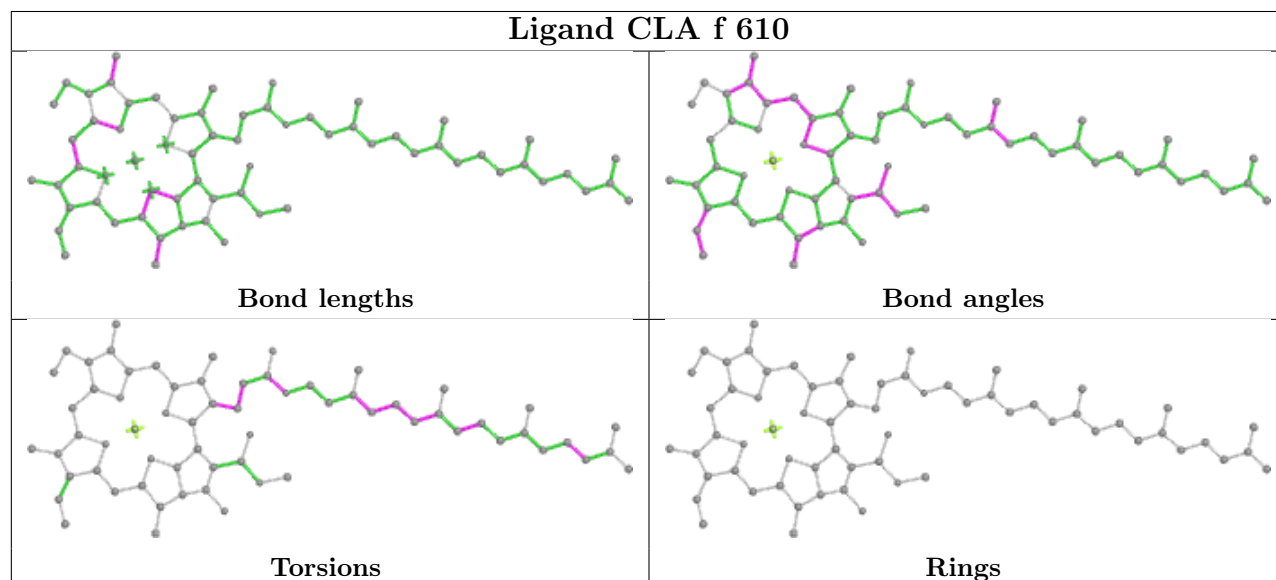


Ligand CLA A 839

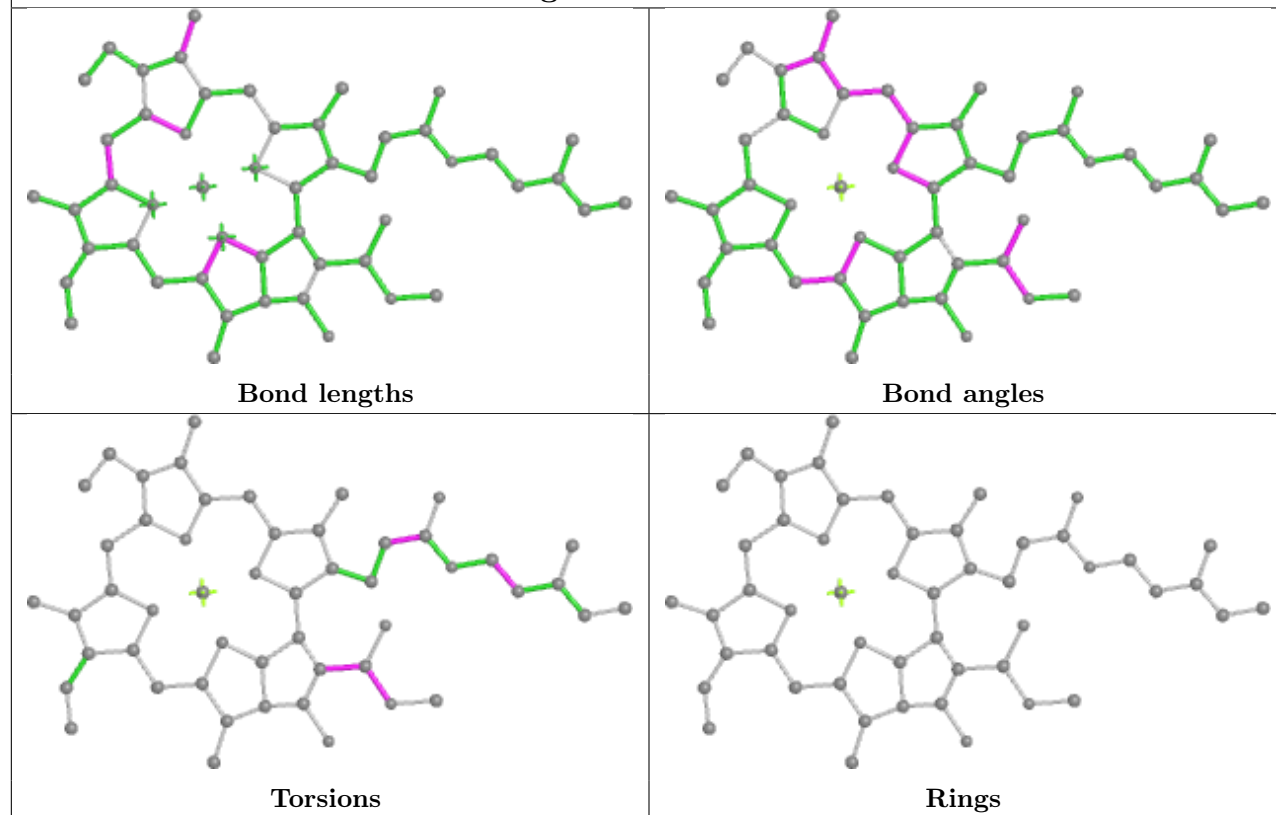


Ligand LHG e 617

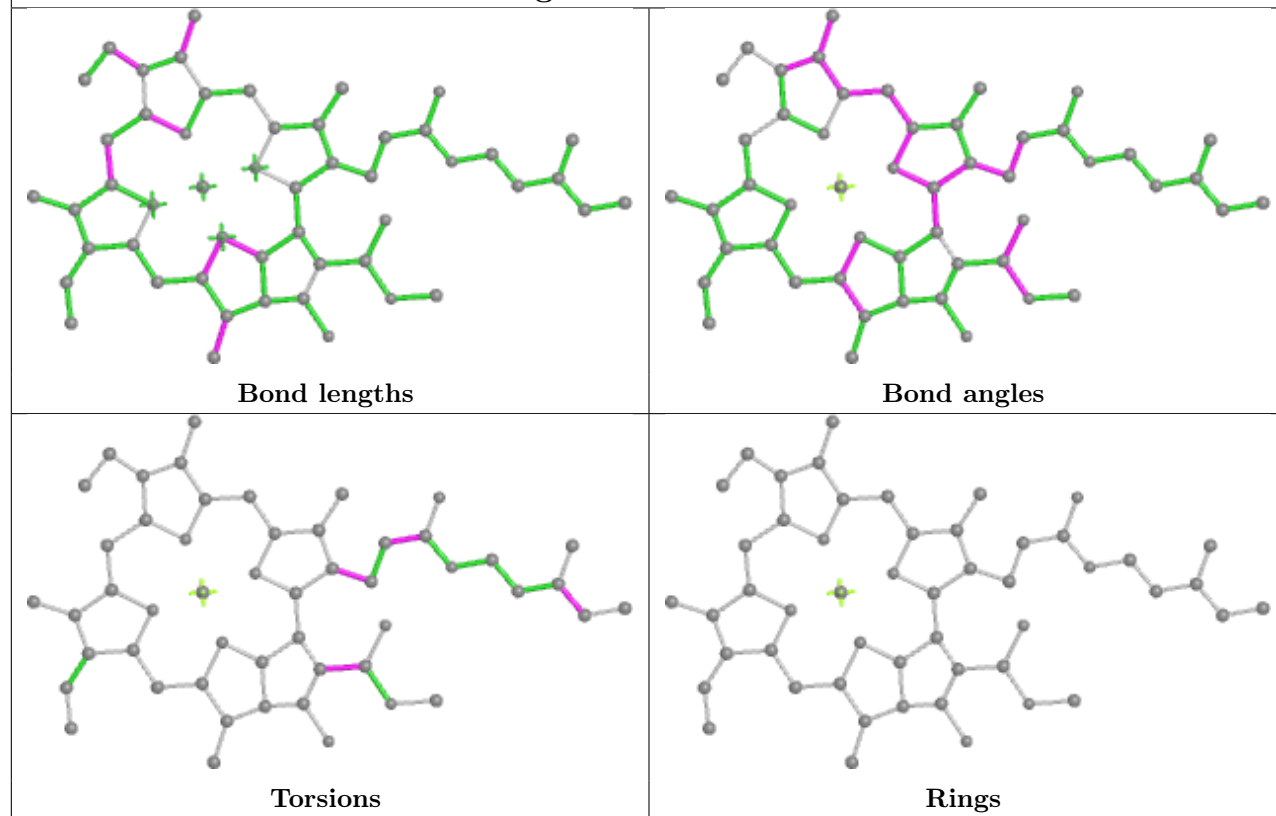


Ligand II0 l 314**Ligand CLA B 839****Ligand CLA f 610**

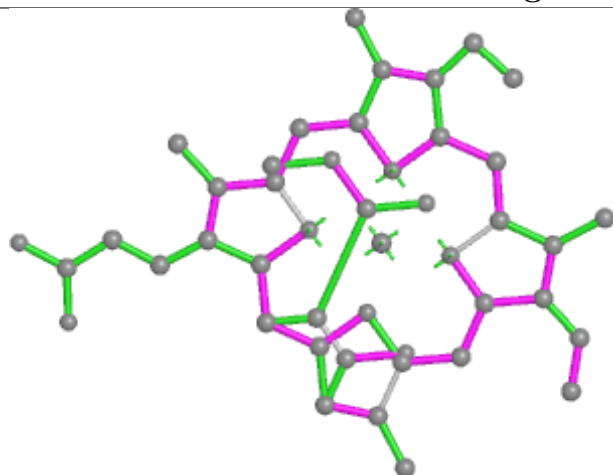
Ligand CLA l 304



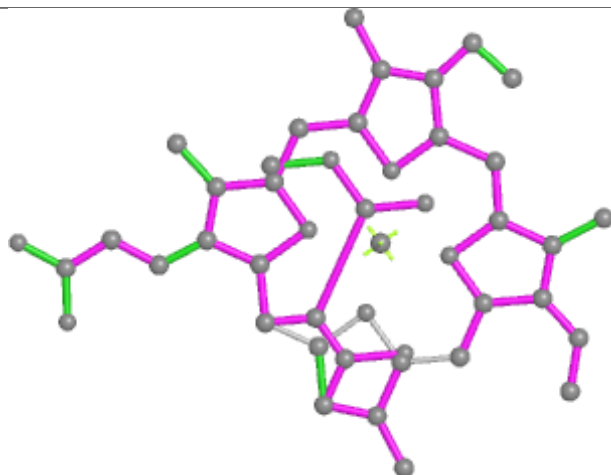
Ligand CLA h 308



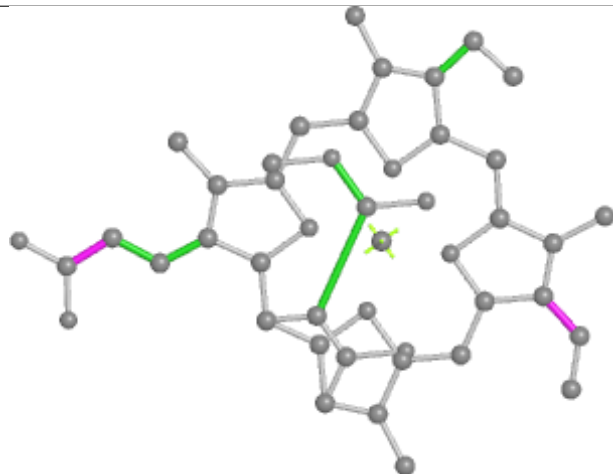
Ligand KC2 I 310



Bond lengths



Bond angles

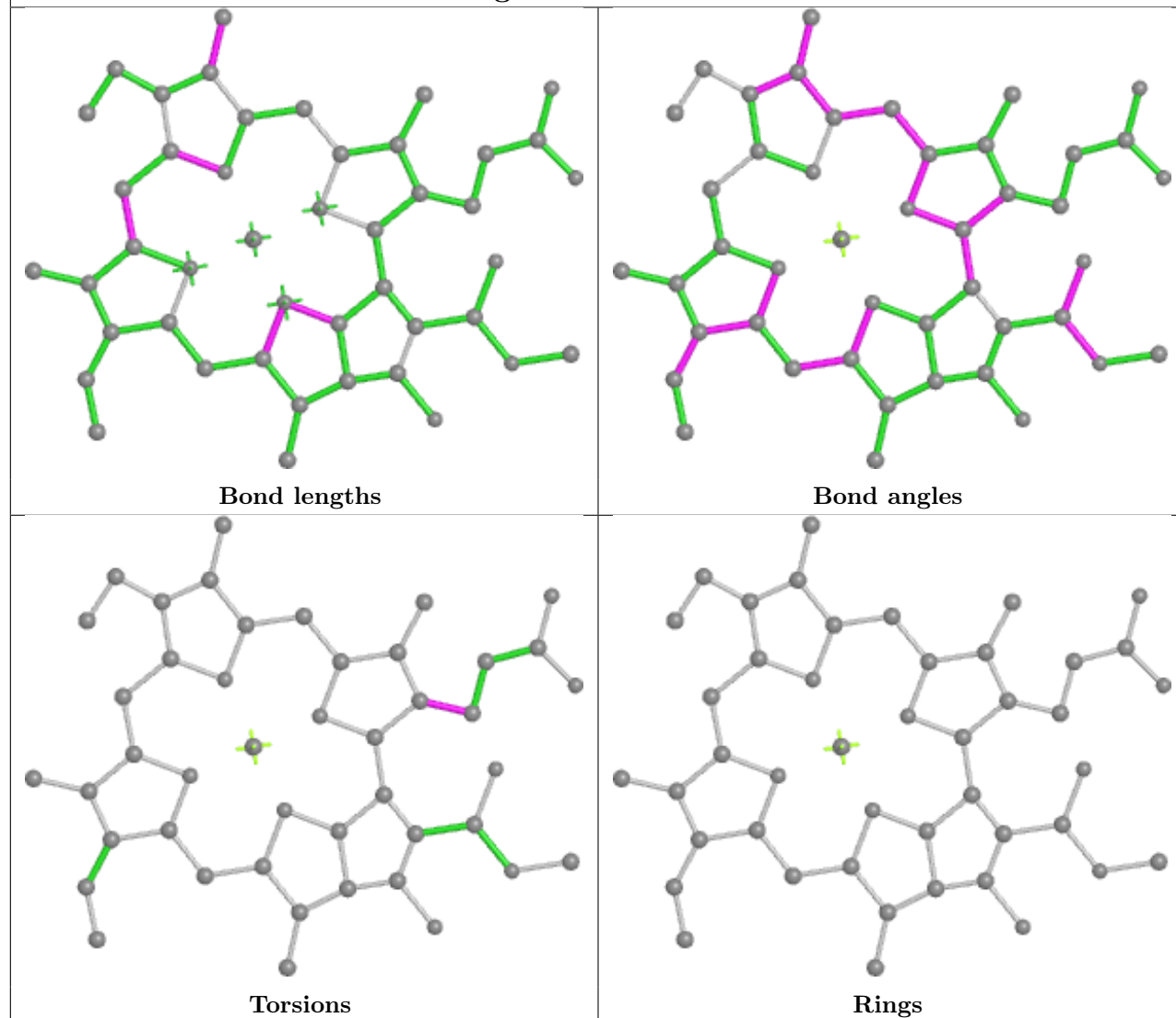


Torsions

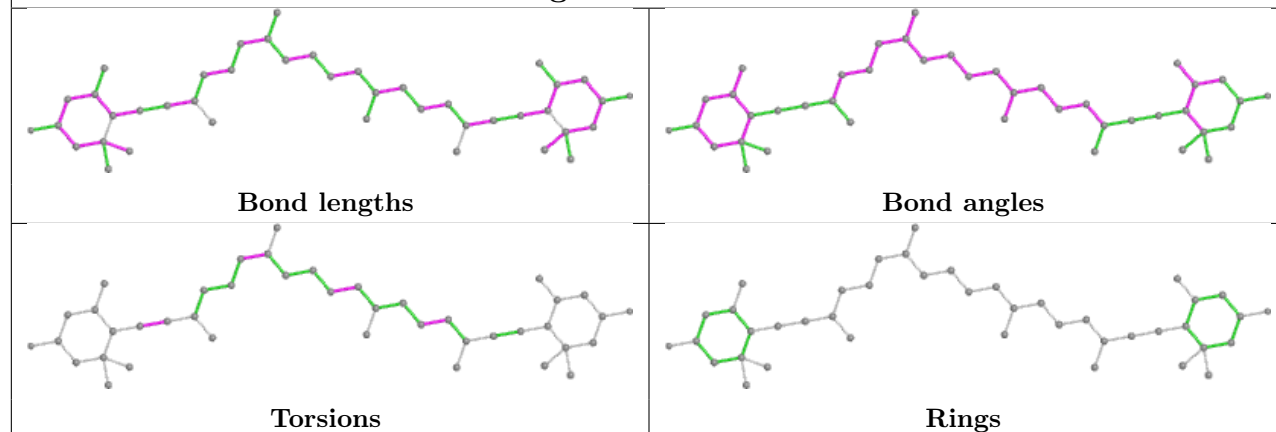


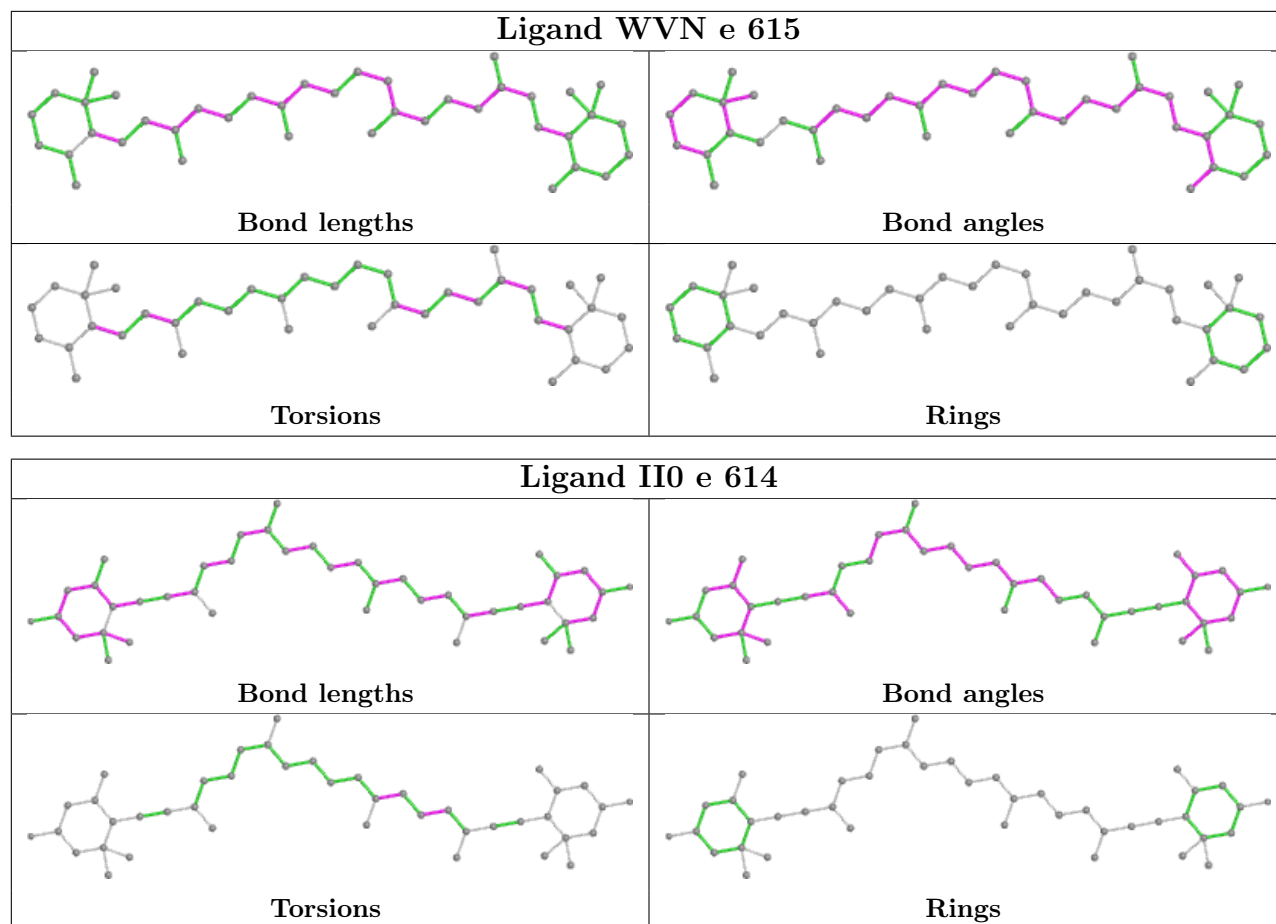
Rings

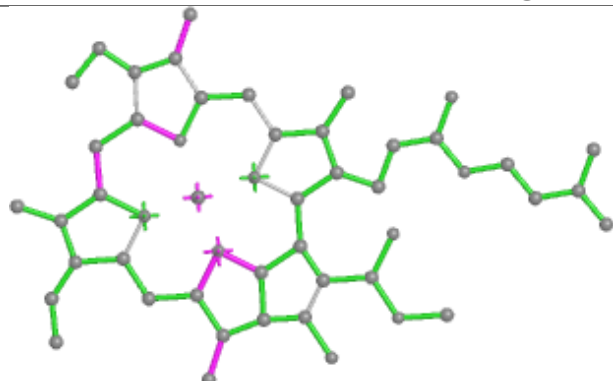
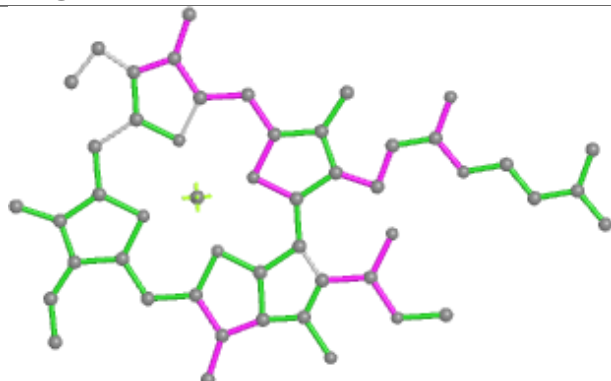
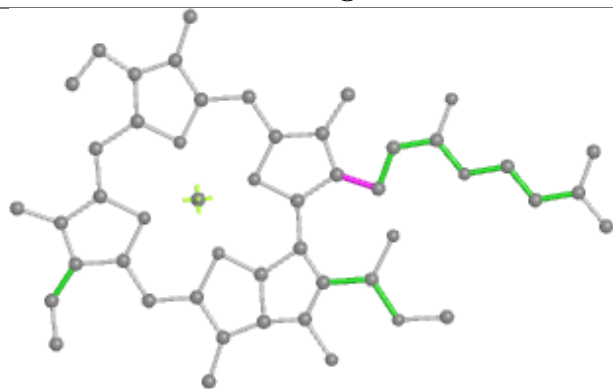
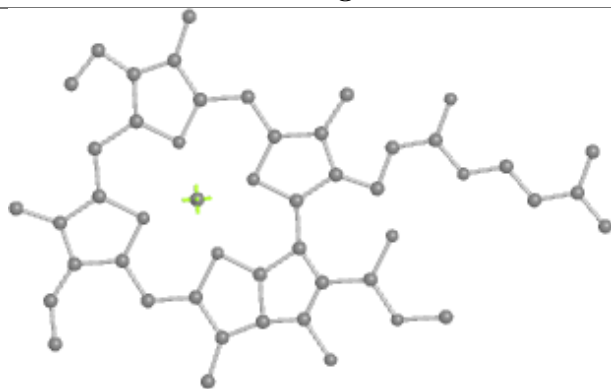
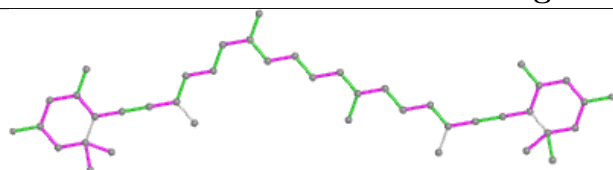
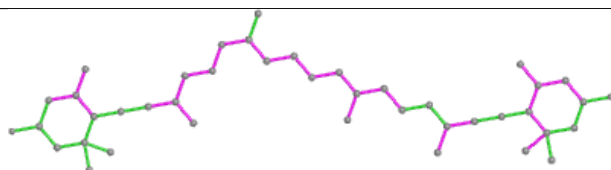
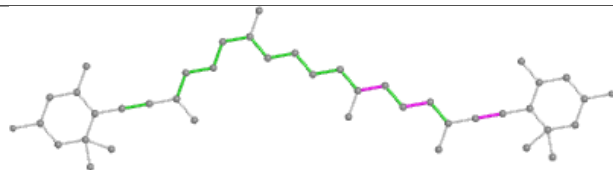
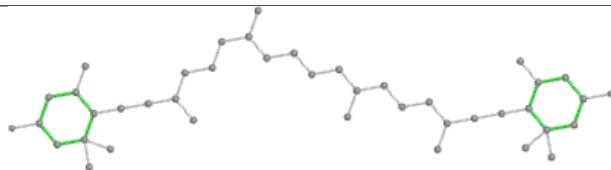
Ligand CLA a 307

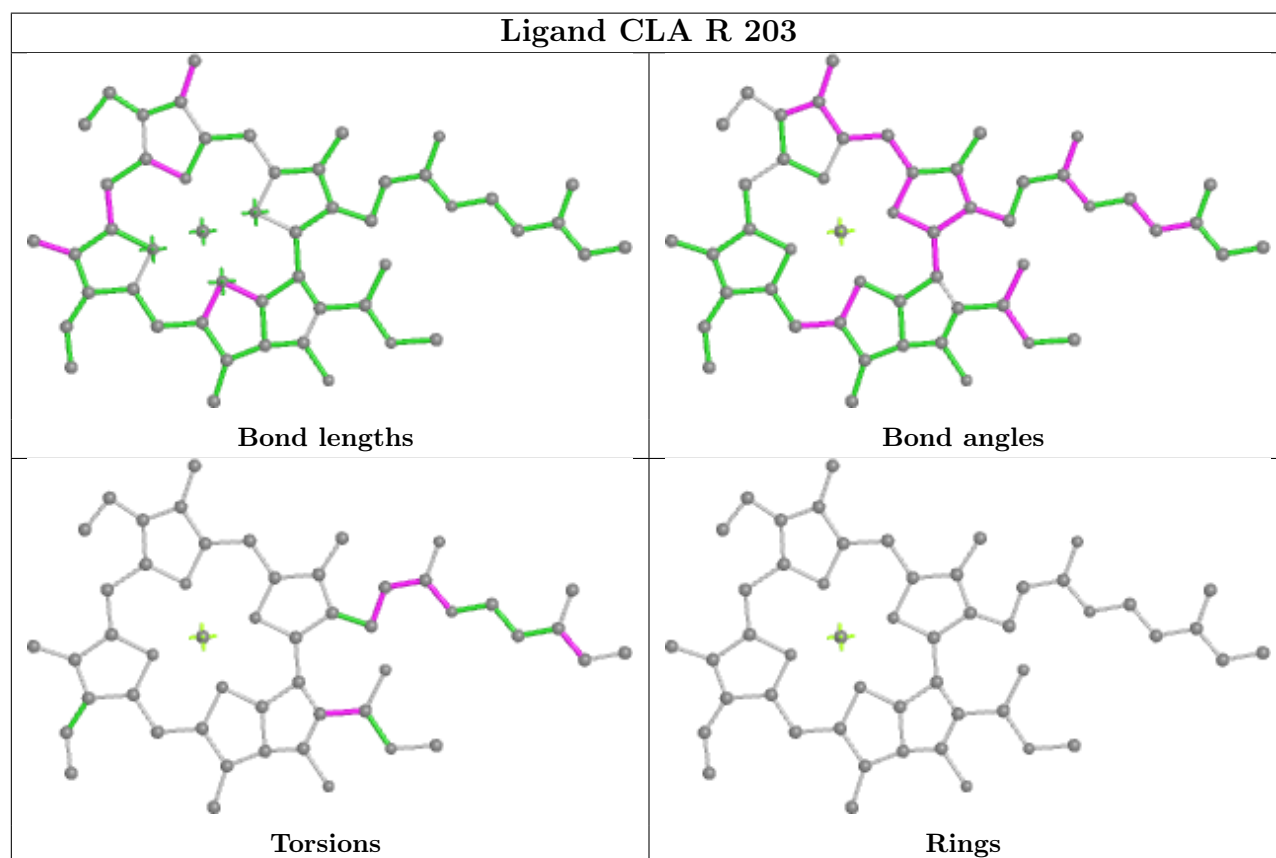
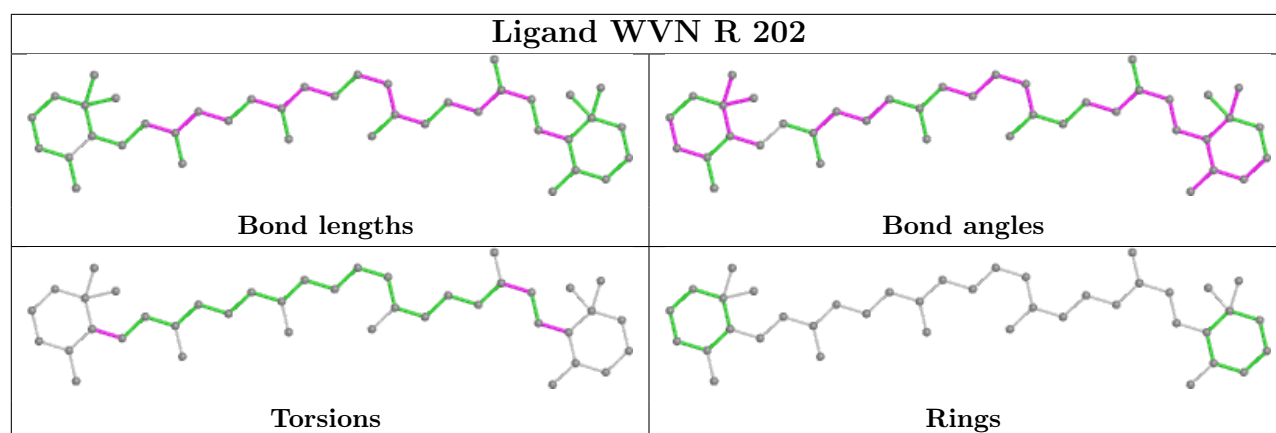


Ligand II0 d 315

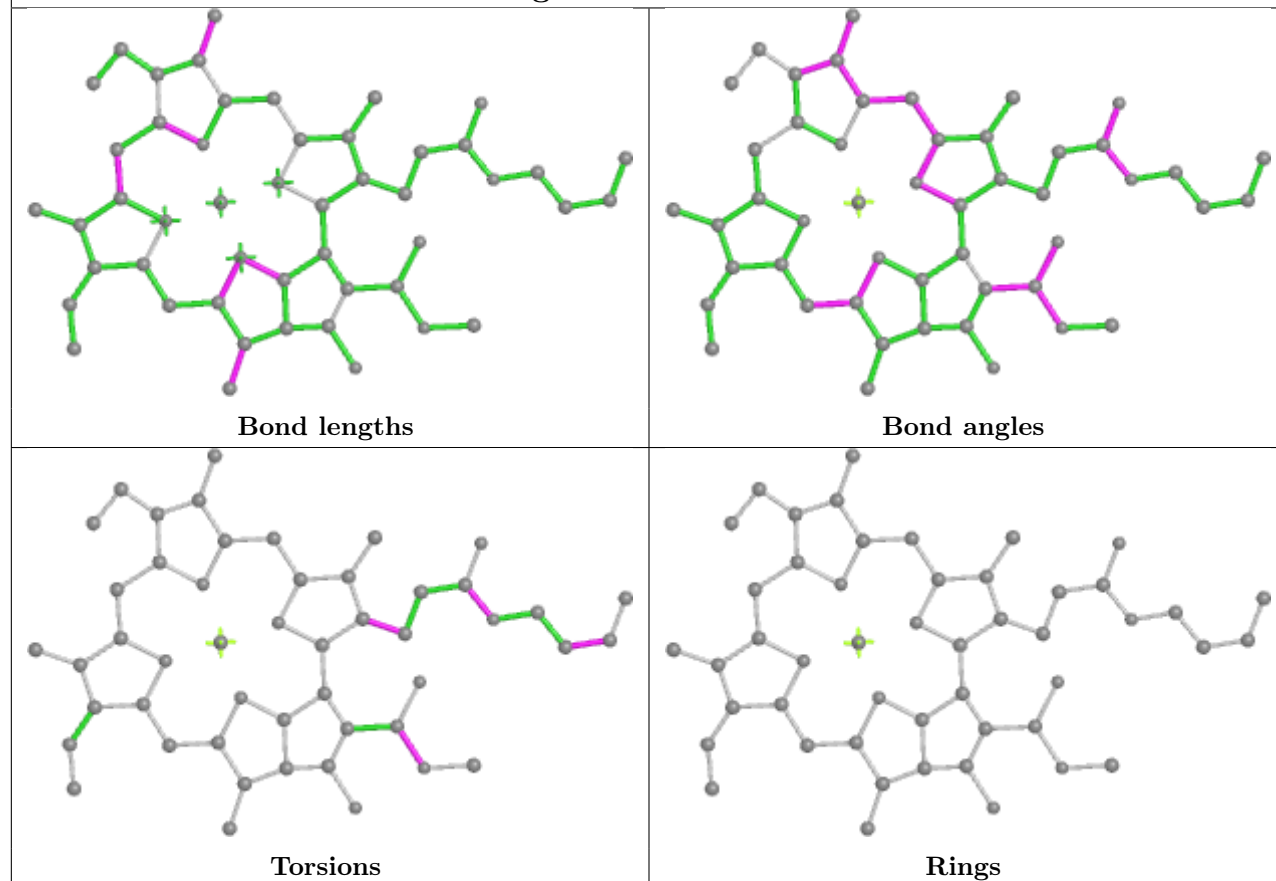




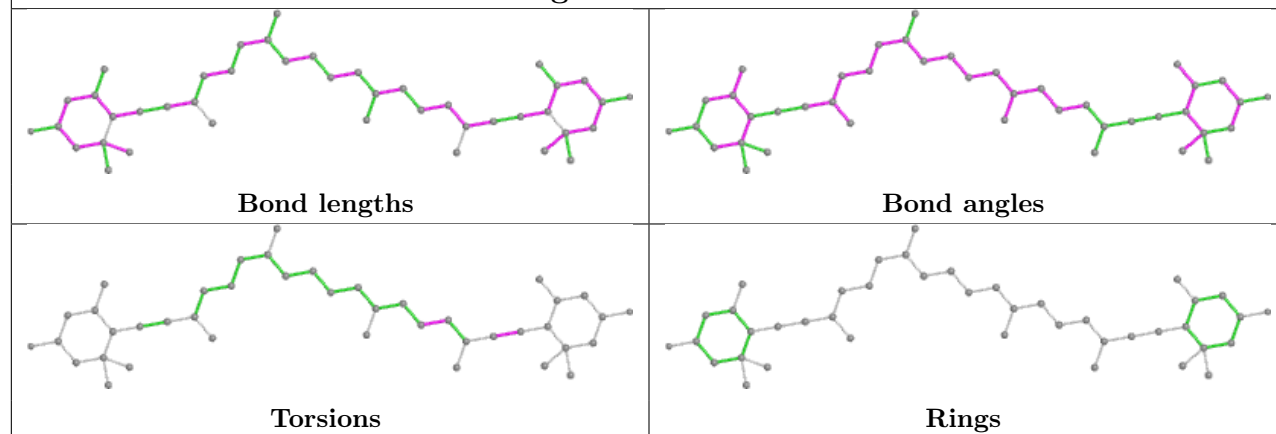
Ligand CLA g 303**Bond lengths****Bond angles****Torsions****Rings****Ligand II0 c 613****Bond lengths****Bond angles****Torsions****Rings**

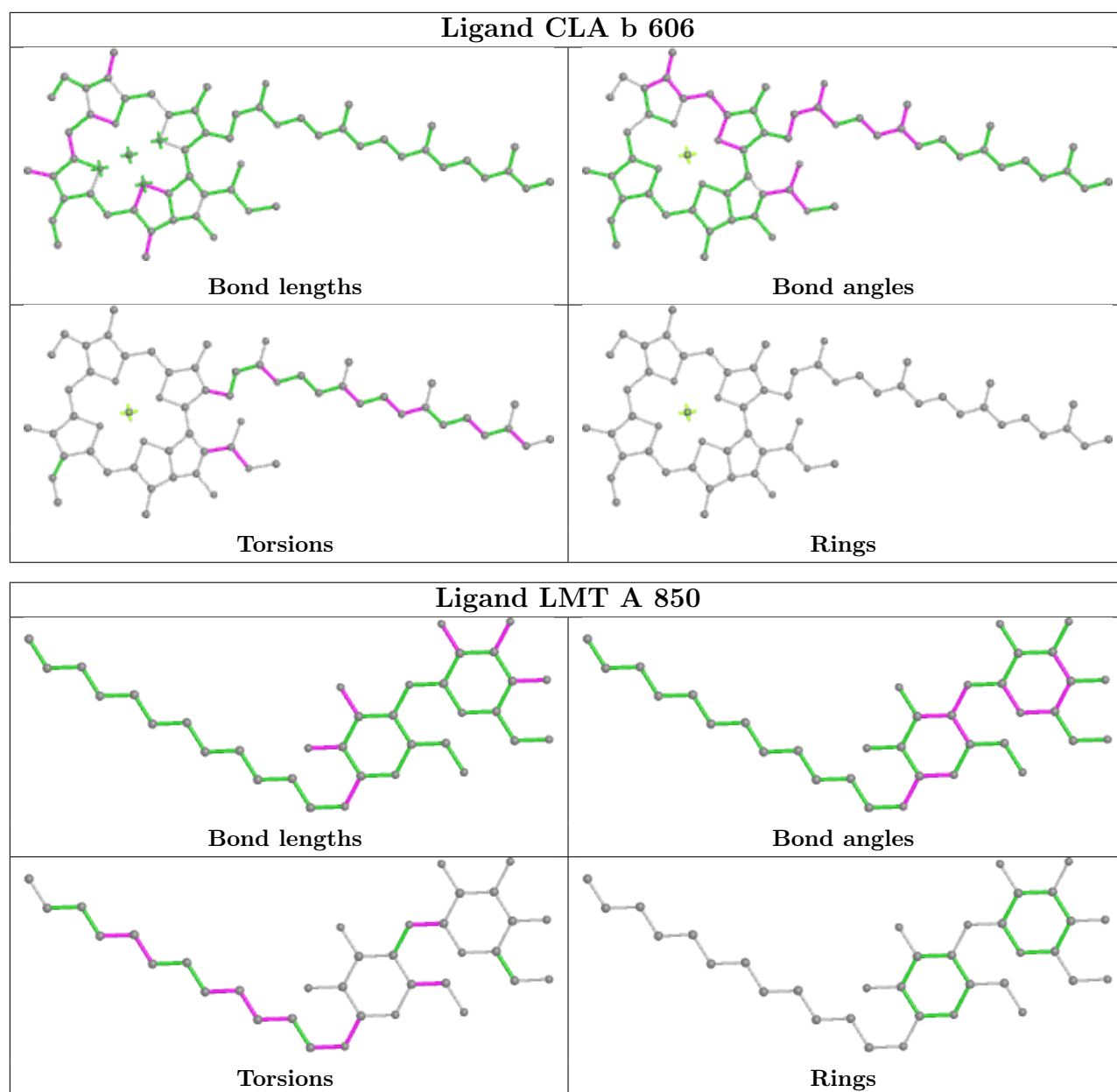


Ligand CLA B 828

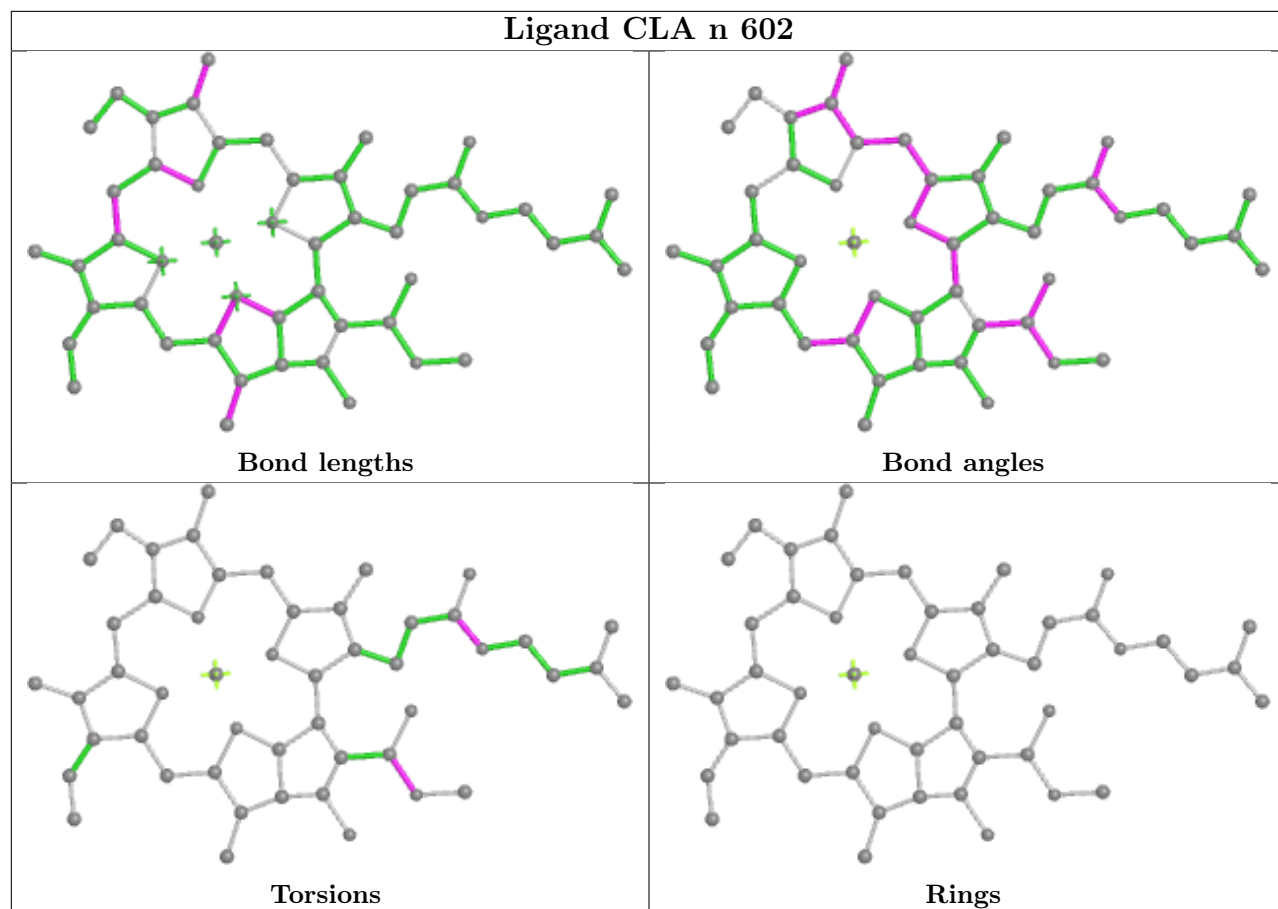


Ligand II0 a 315

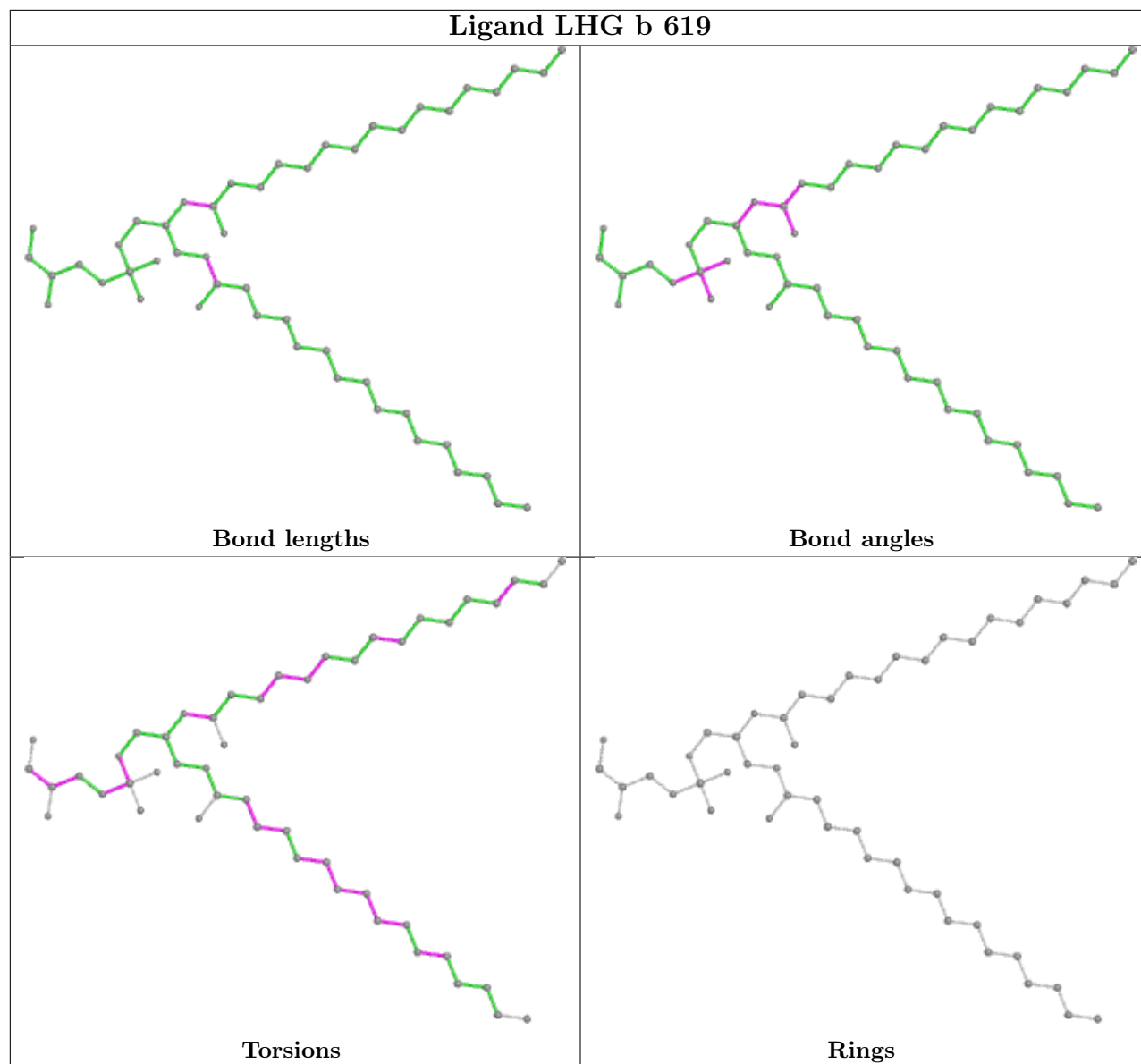




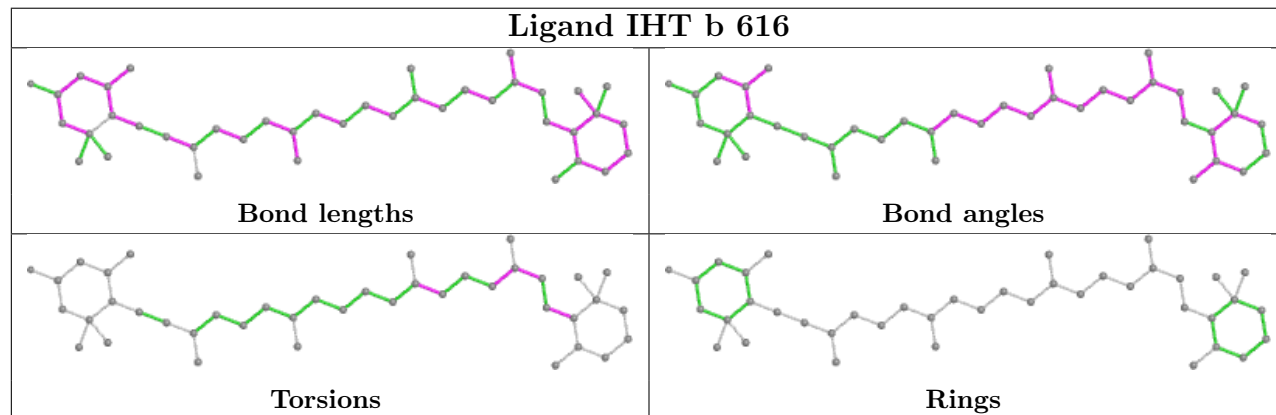
Ligand CLA n 602



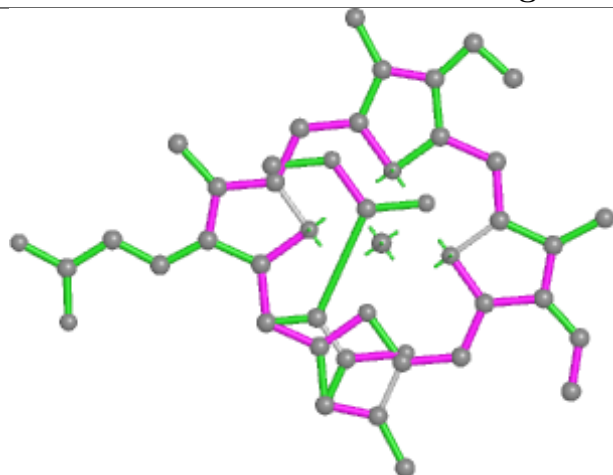
Ligand LHG b 619



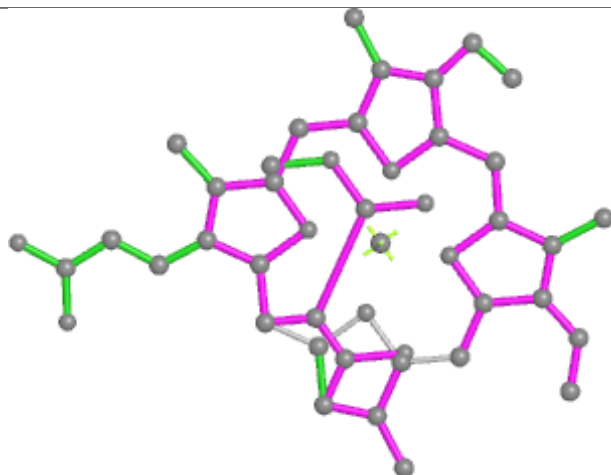
Ligand IHT b 616



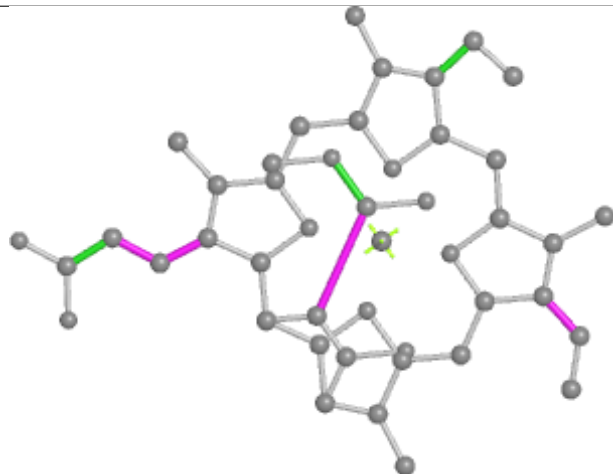
Ligand KC2 n 612



Bond lengths



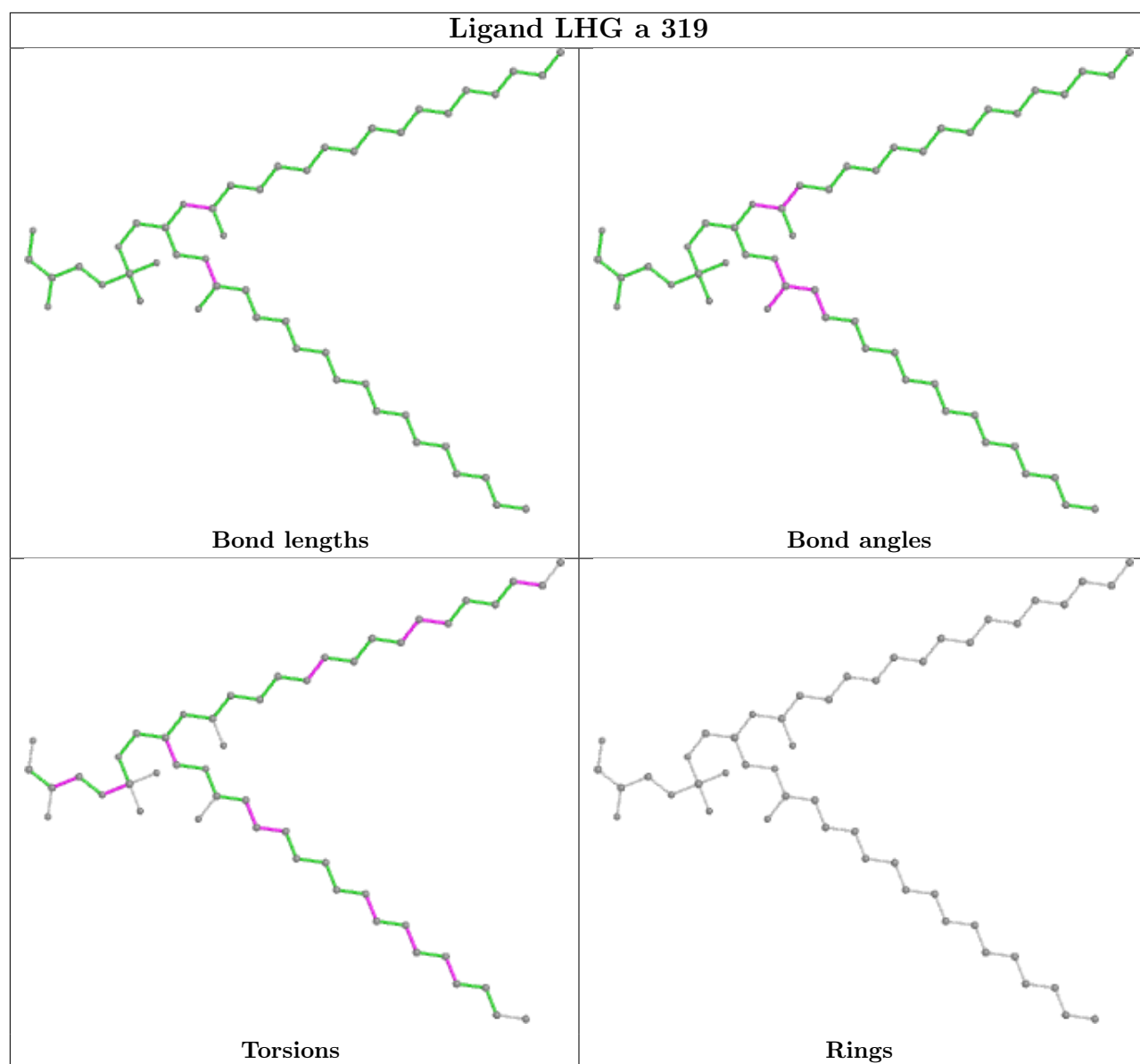
Bond angles



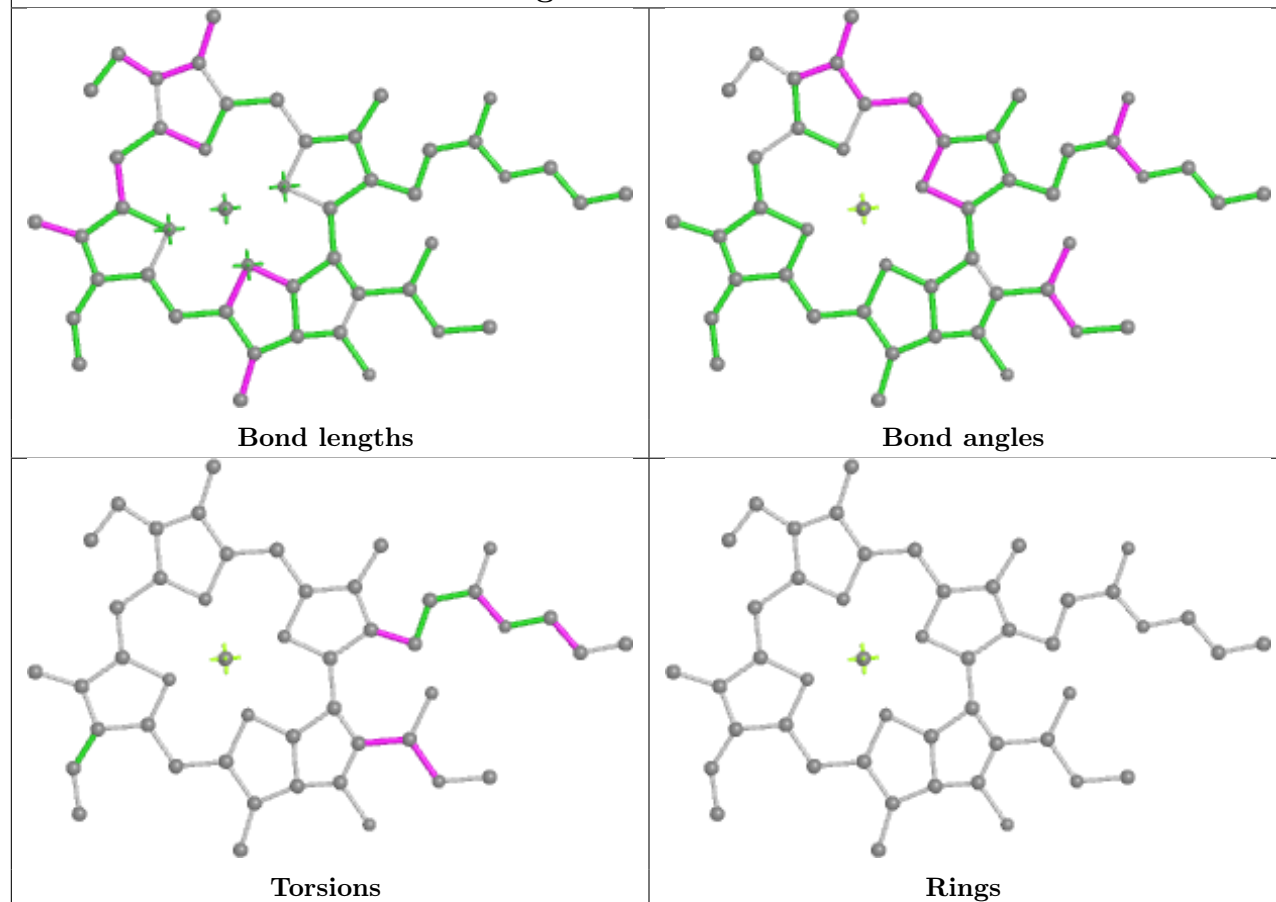
Torsions



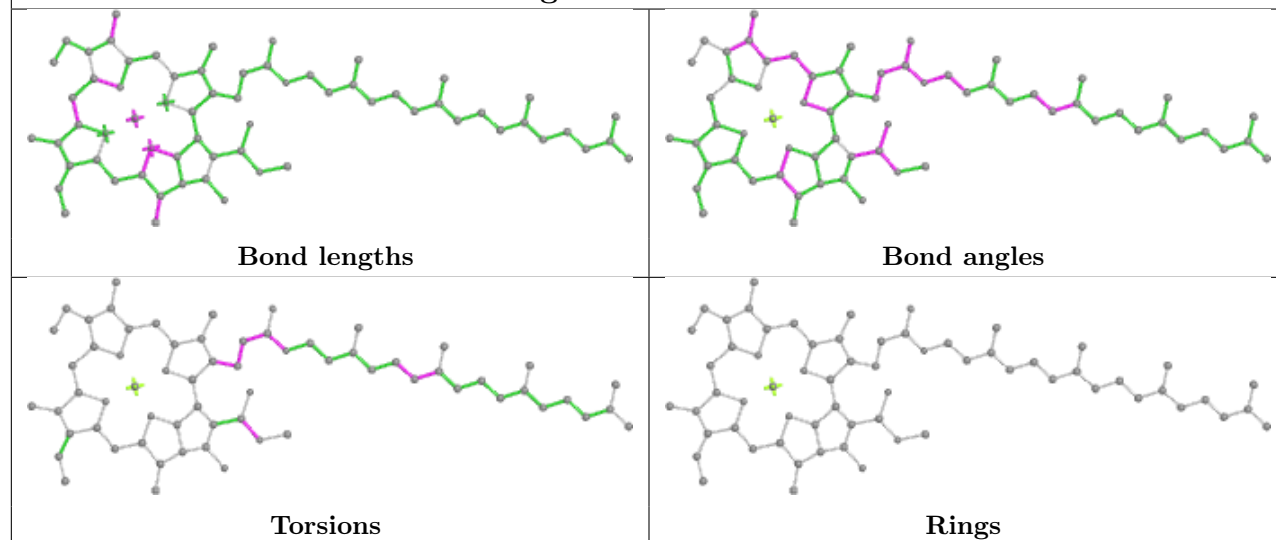
Rings



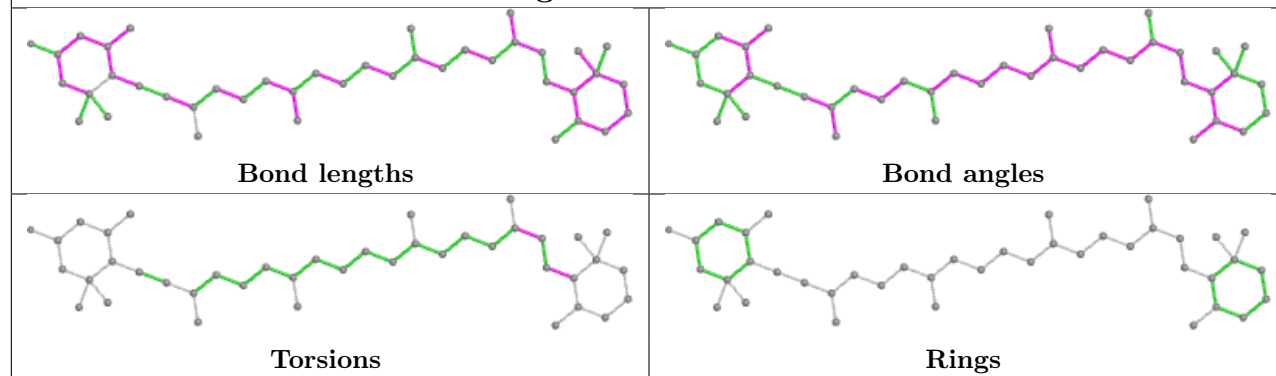
Ligand CLA a 310



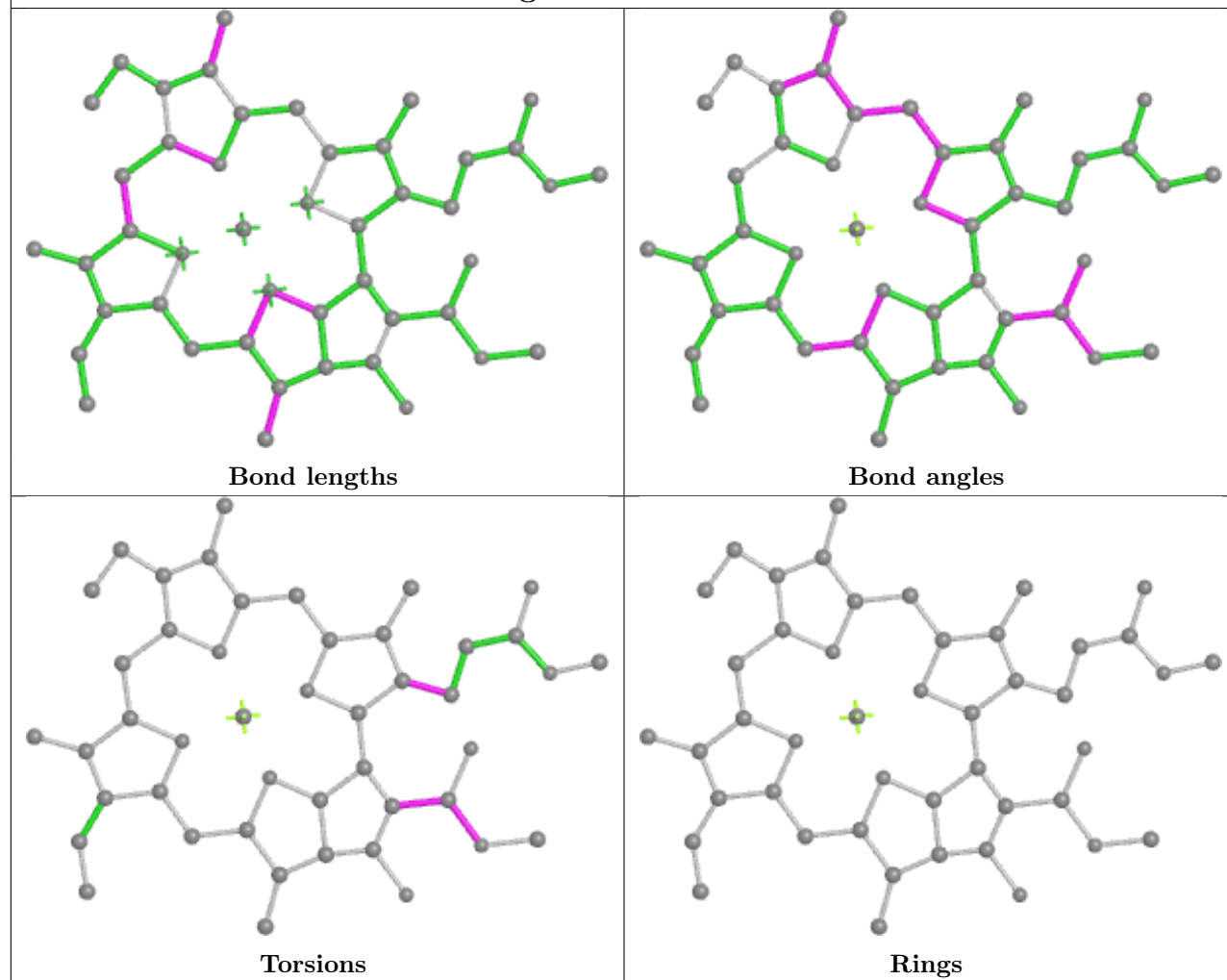
Ligand CLA l 307



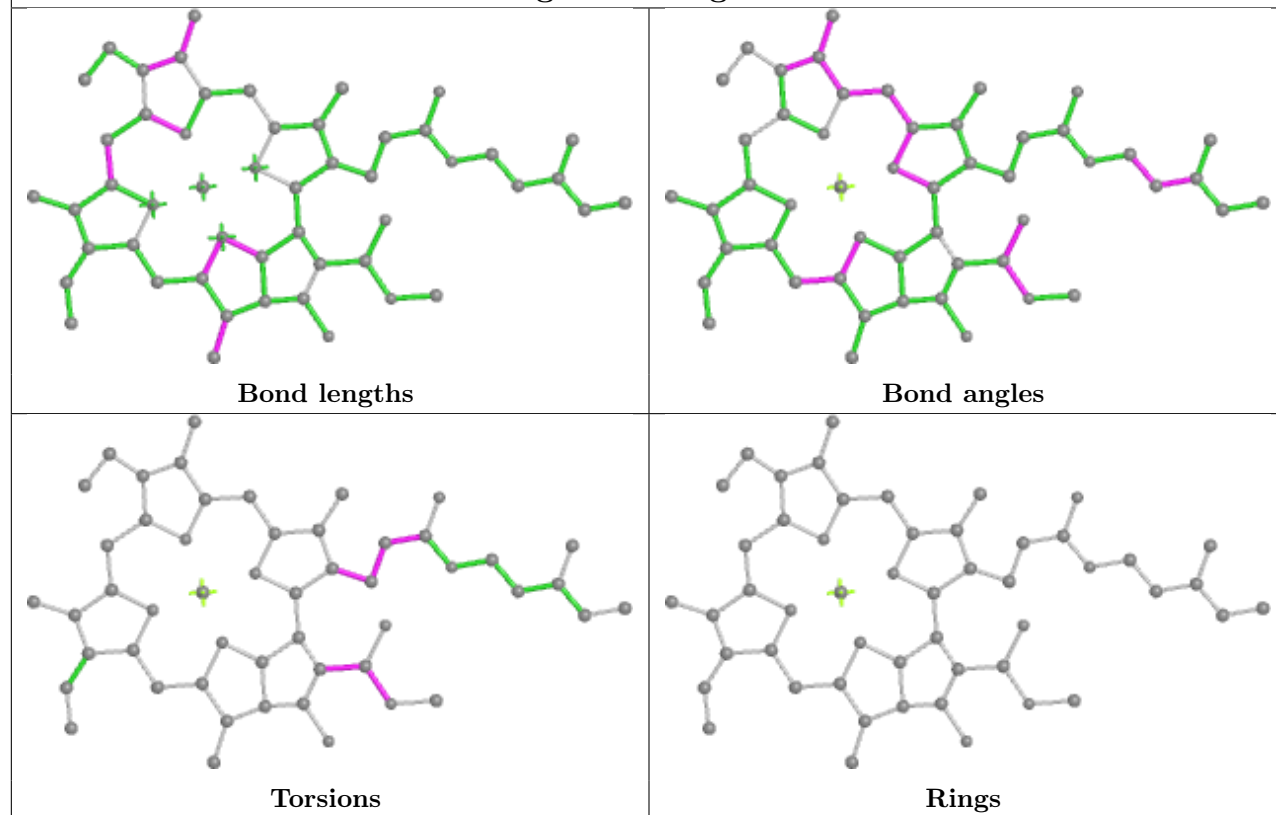
Ligand IHT R 204



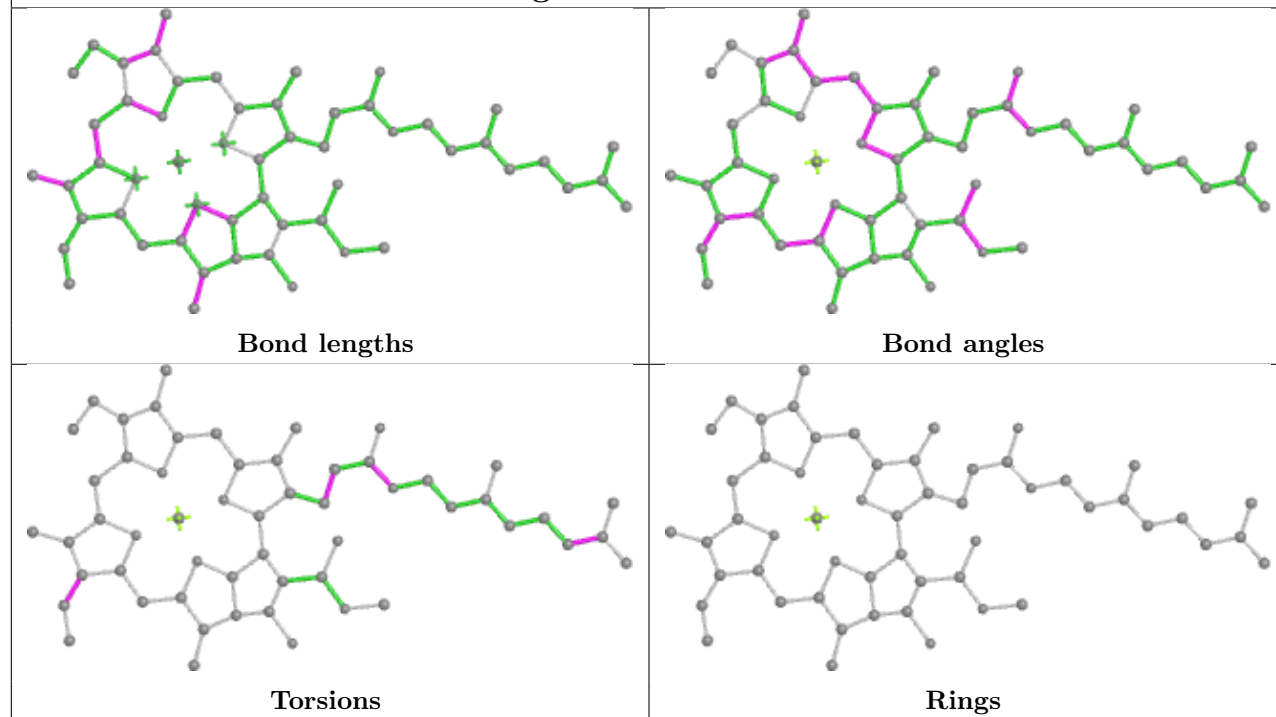
Ligand CLA i 309

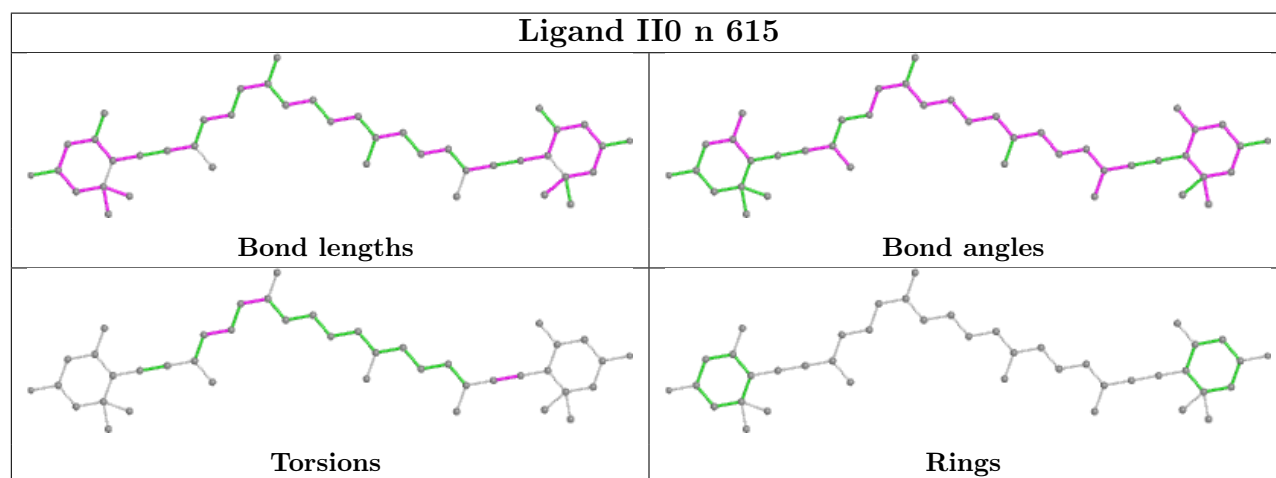
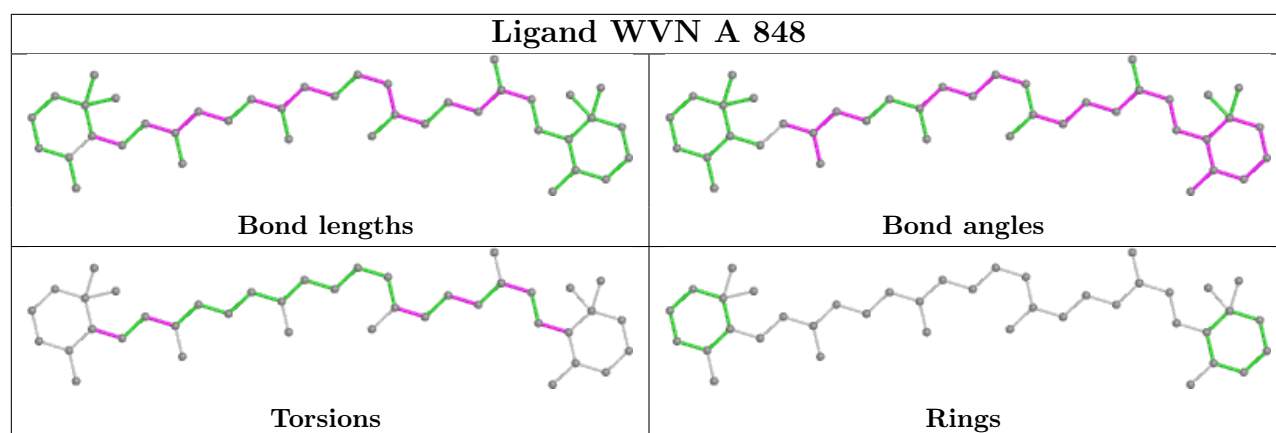


Ligand CLA g 315

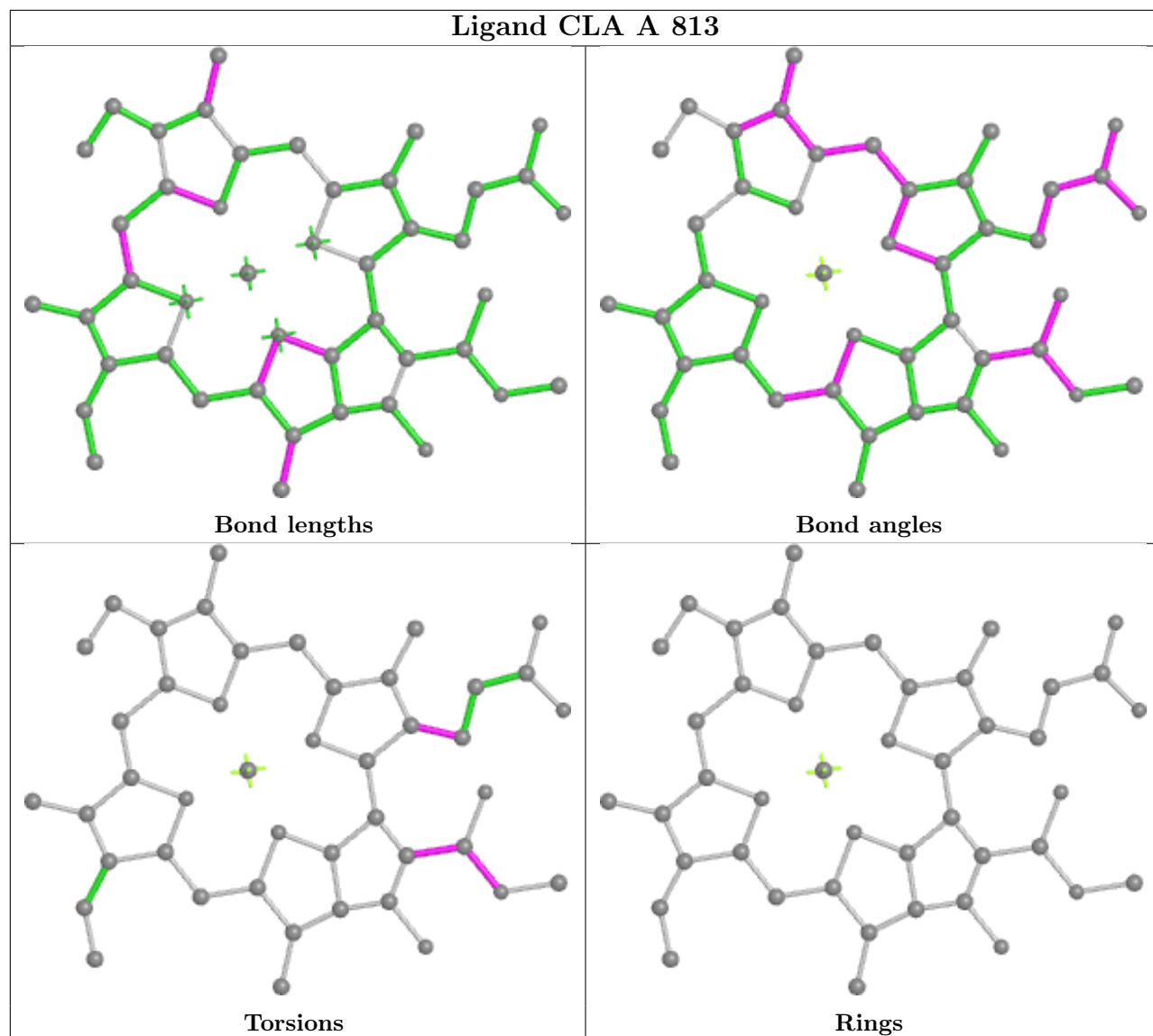


Ligand CLA B 810

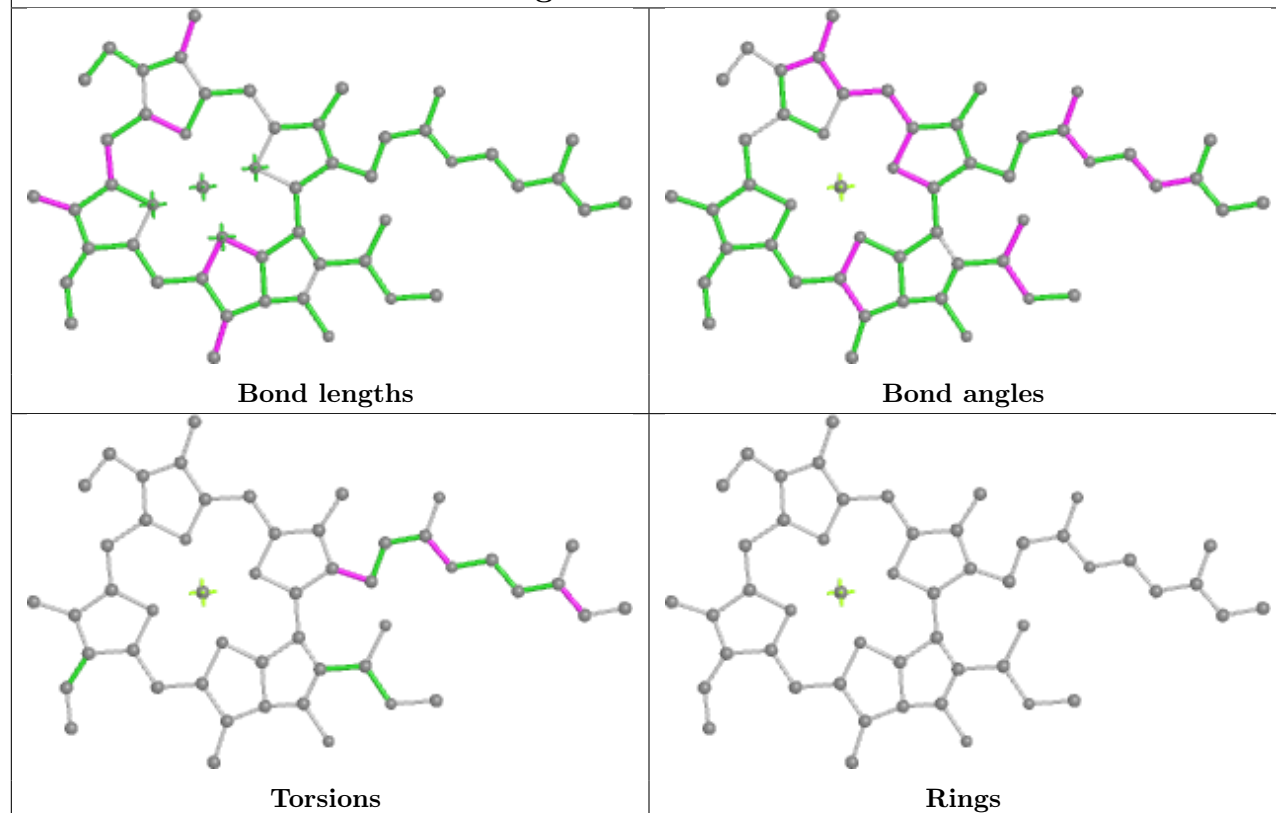




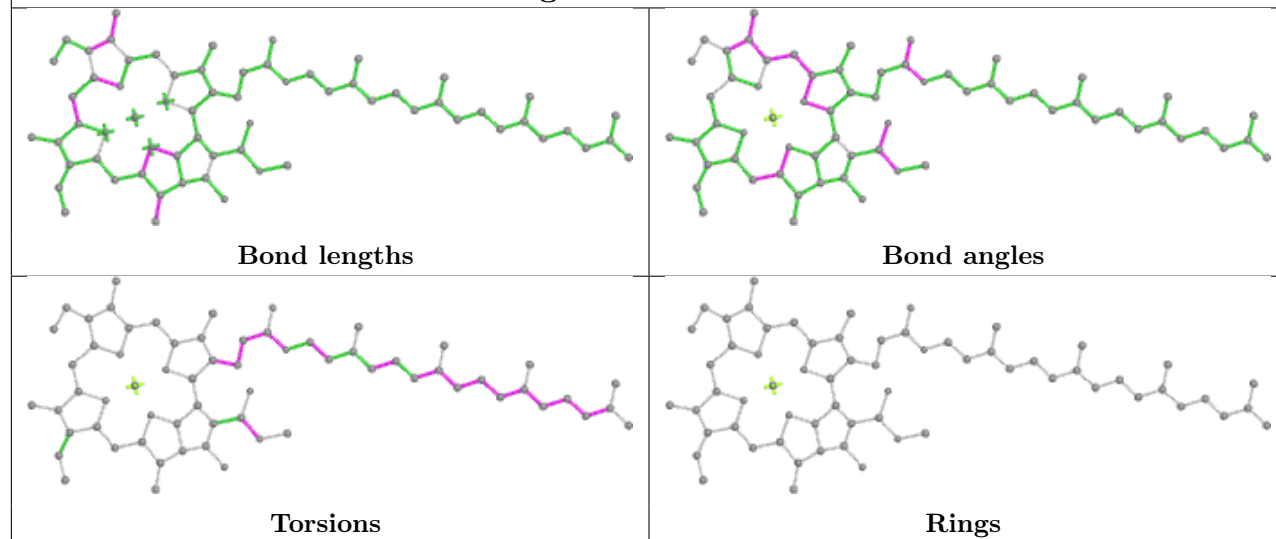
Ligand CLA A 813



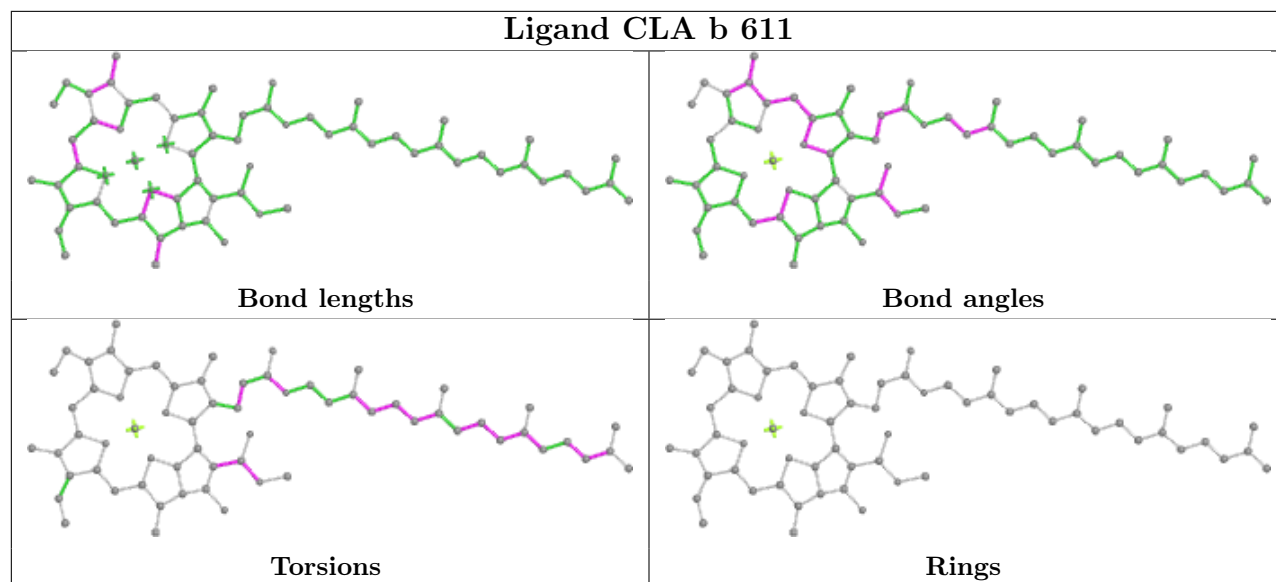
Ligand CLA h 305



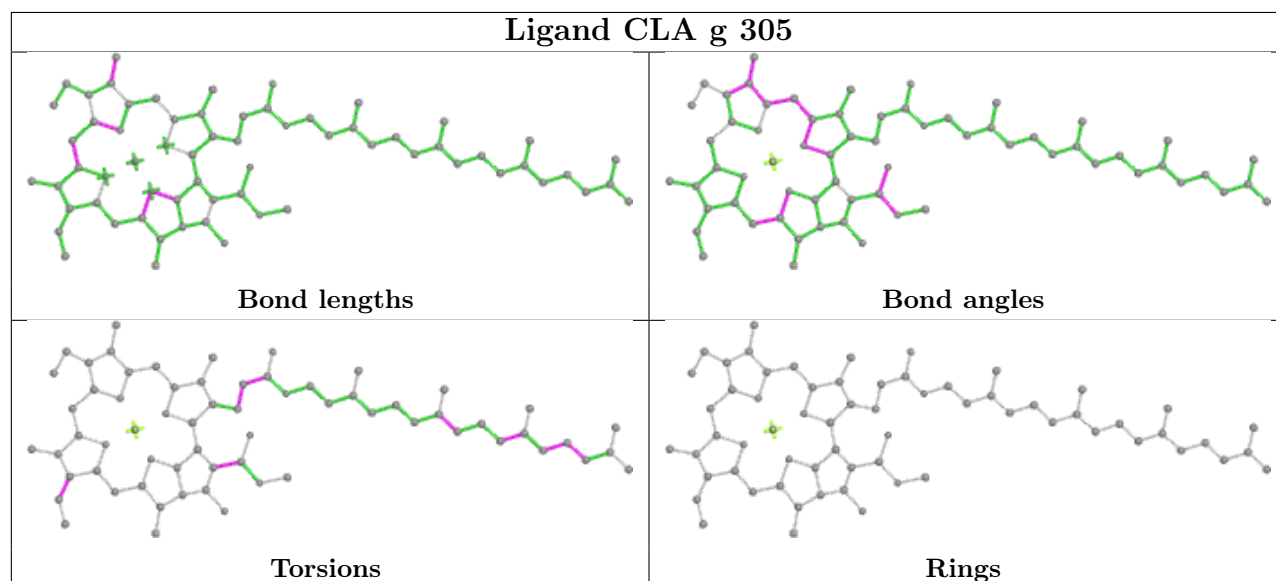
Ligand CLA f 613



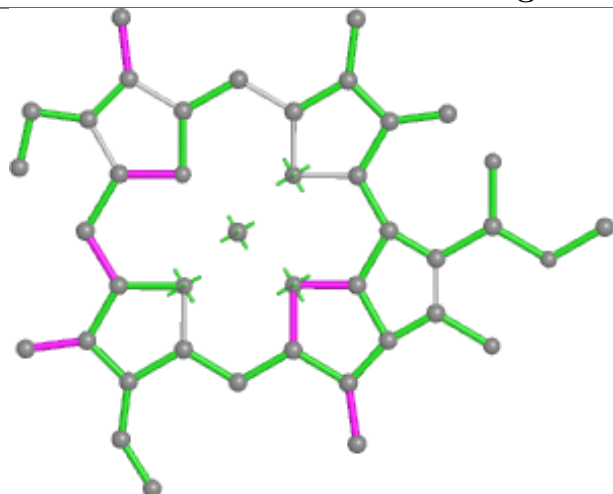
Ligand CLA b 611



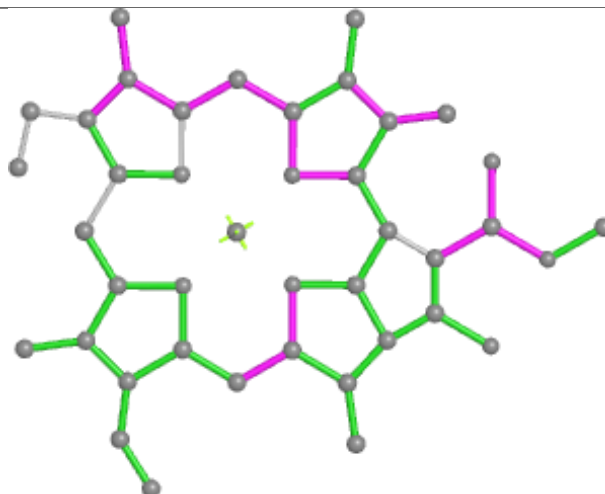
Ligand CLA g 305



Ligand CLA d 308



Bond lengths



Bond angles

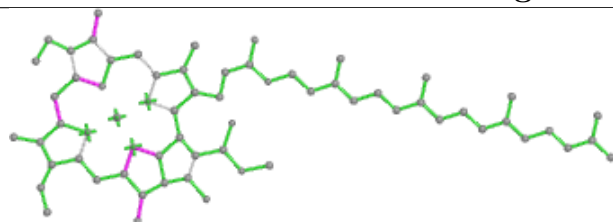


Torsions

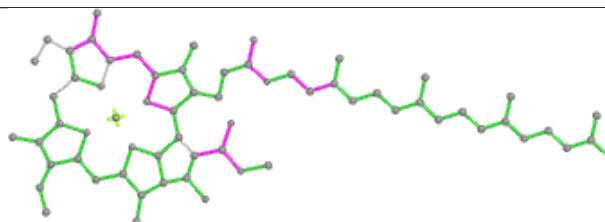


Rings

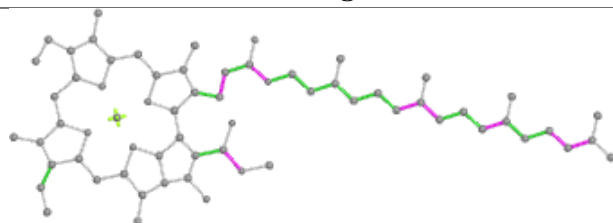
Ligand CLA B 837



Bond lengths



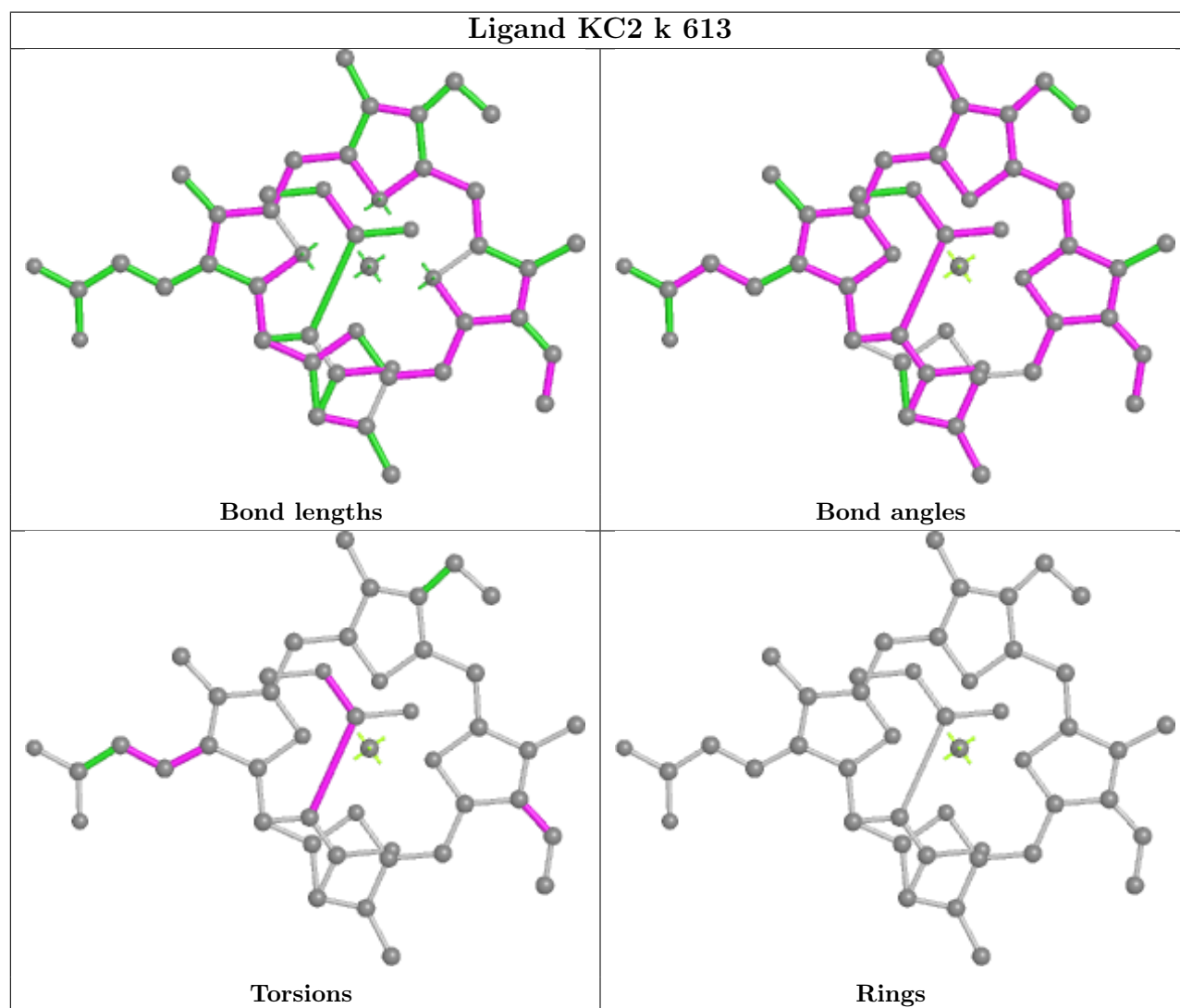
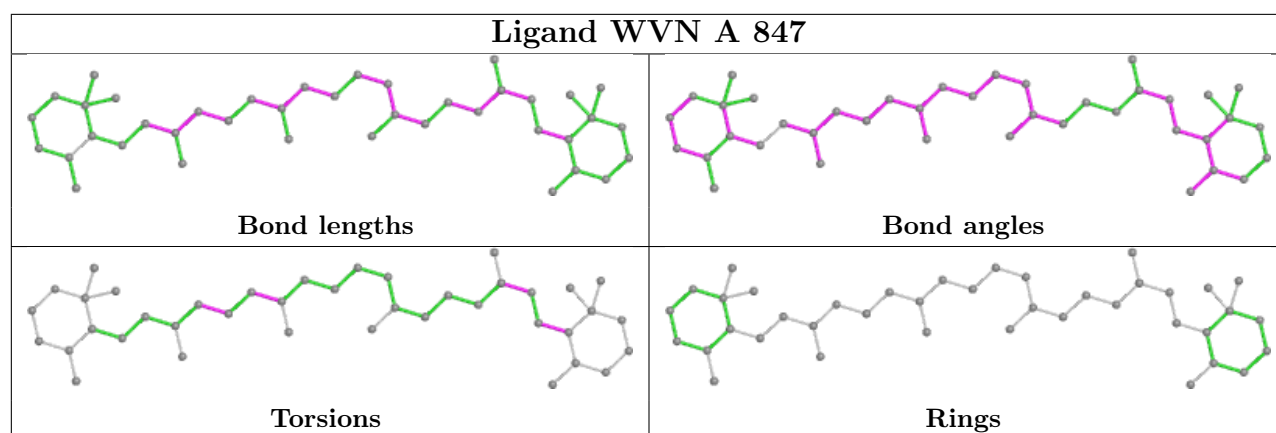
Bond angles



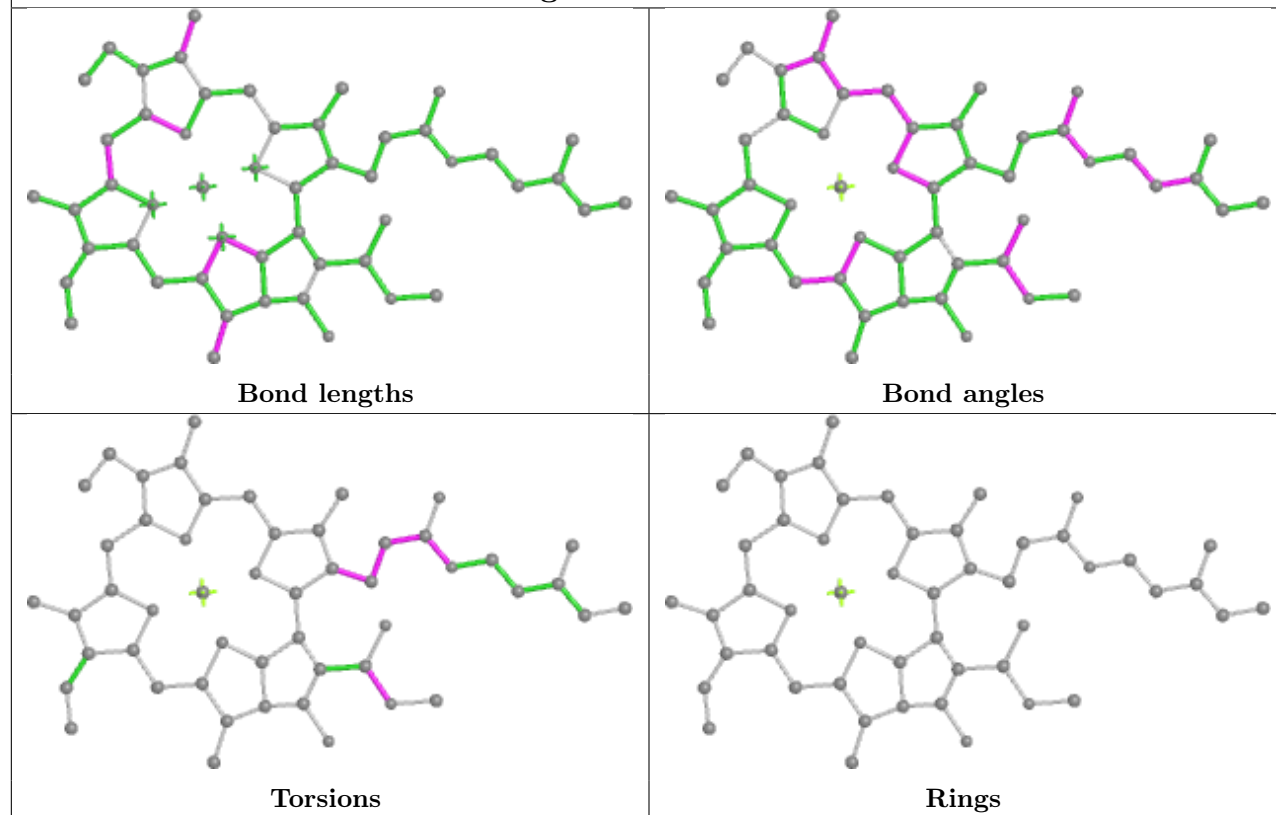
Torsions



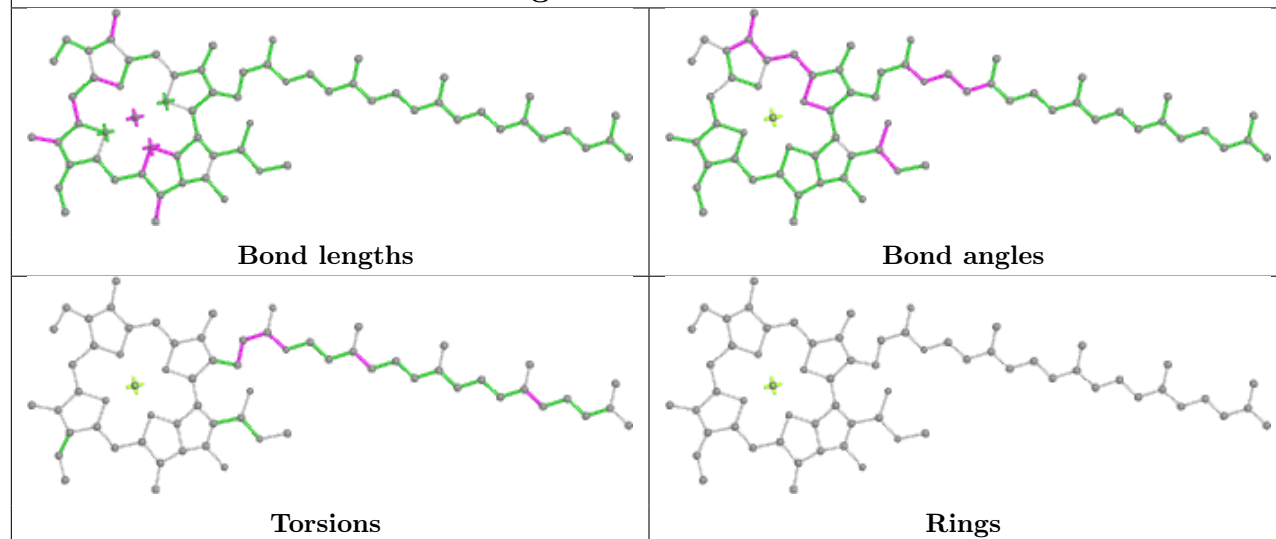
Rings

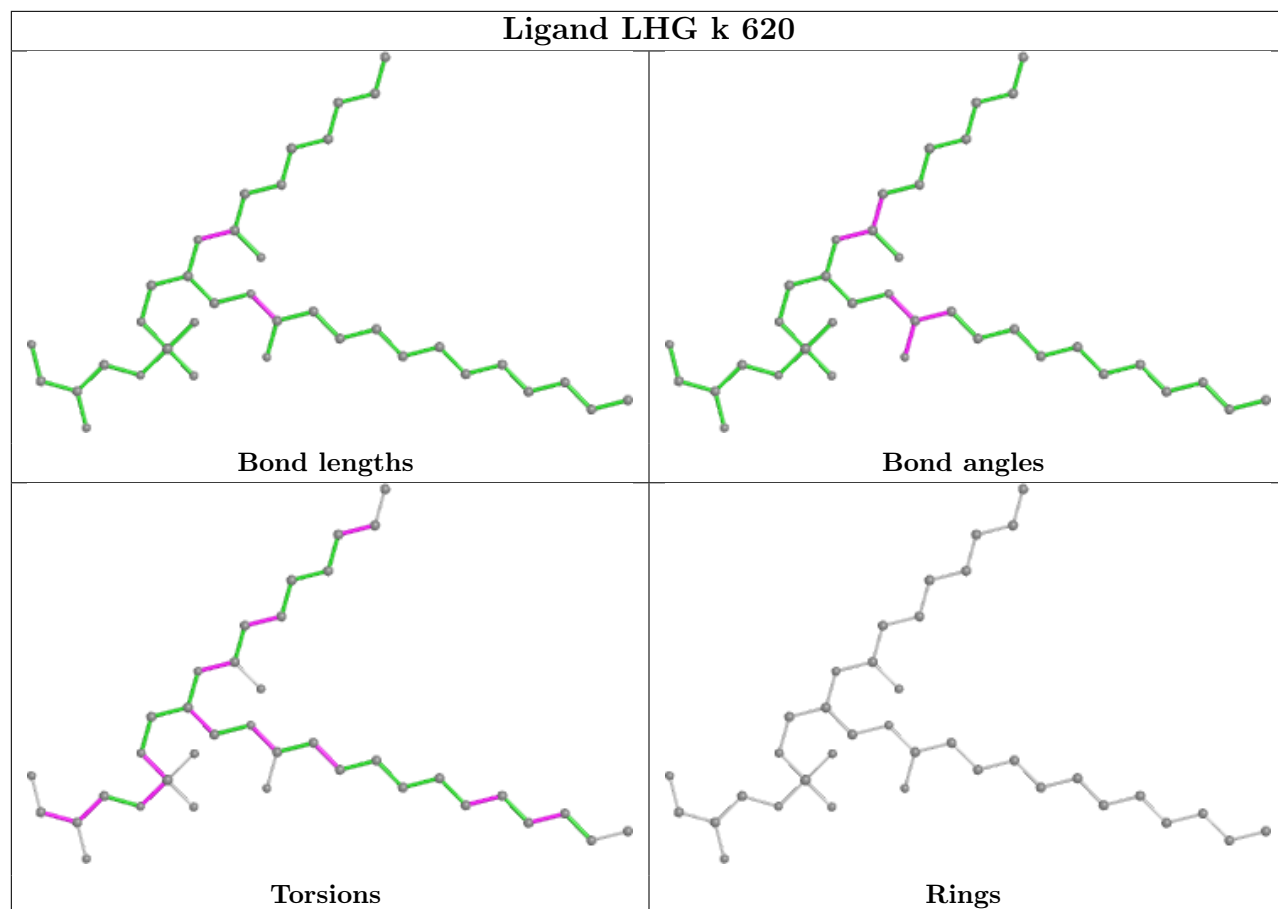


Ligand CLA i 302

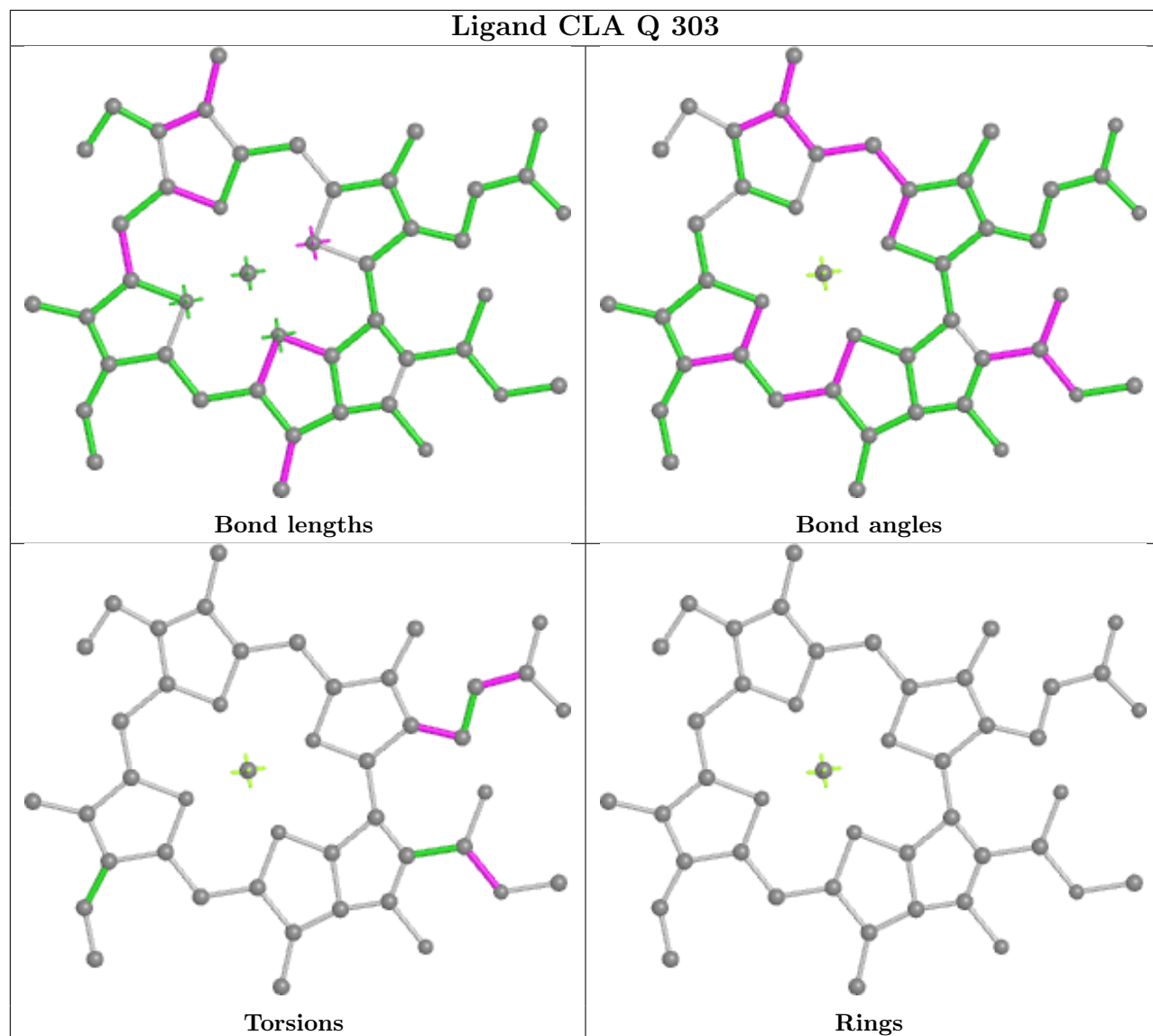


Ligand CLA A 828

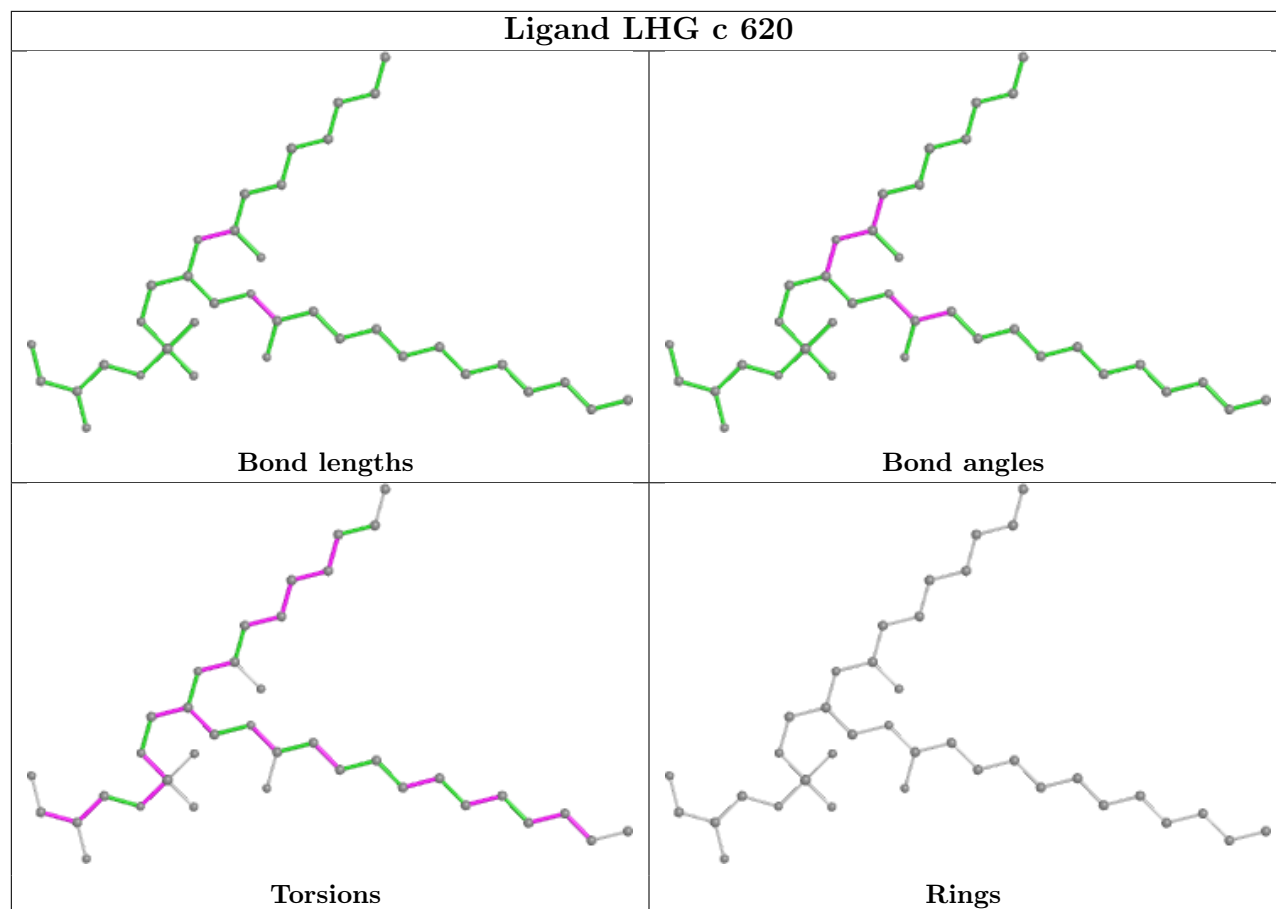




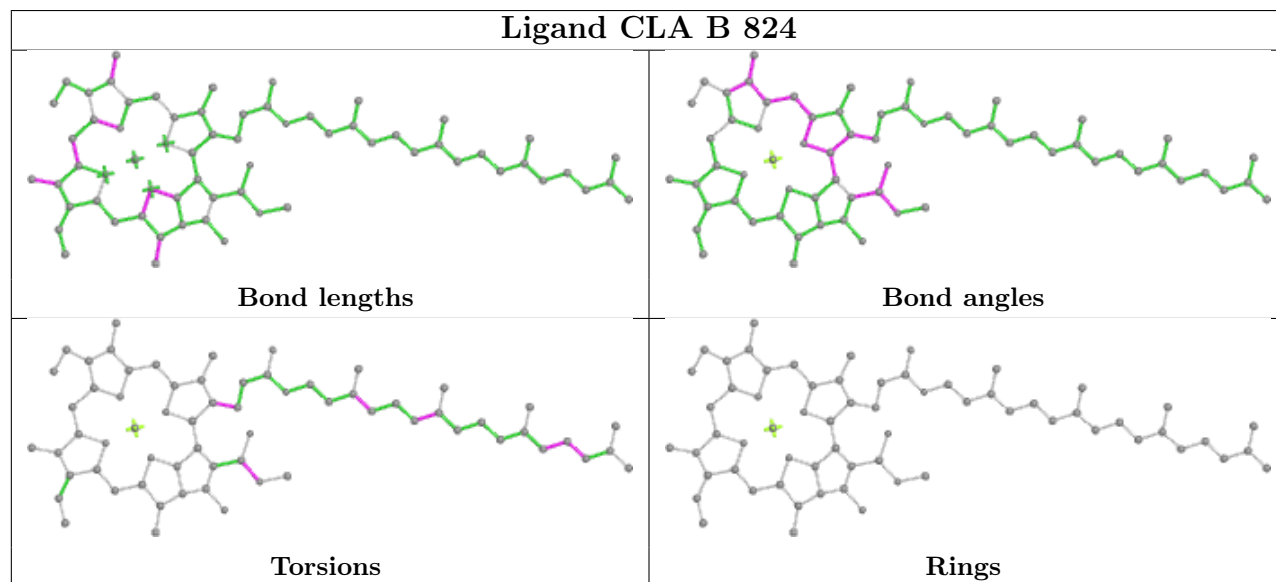
Ligand CLA Q 303

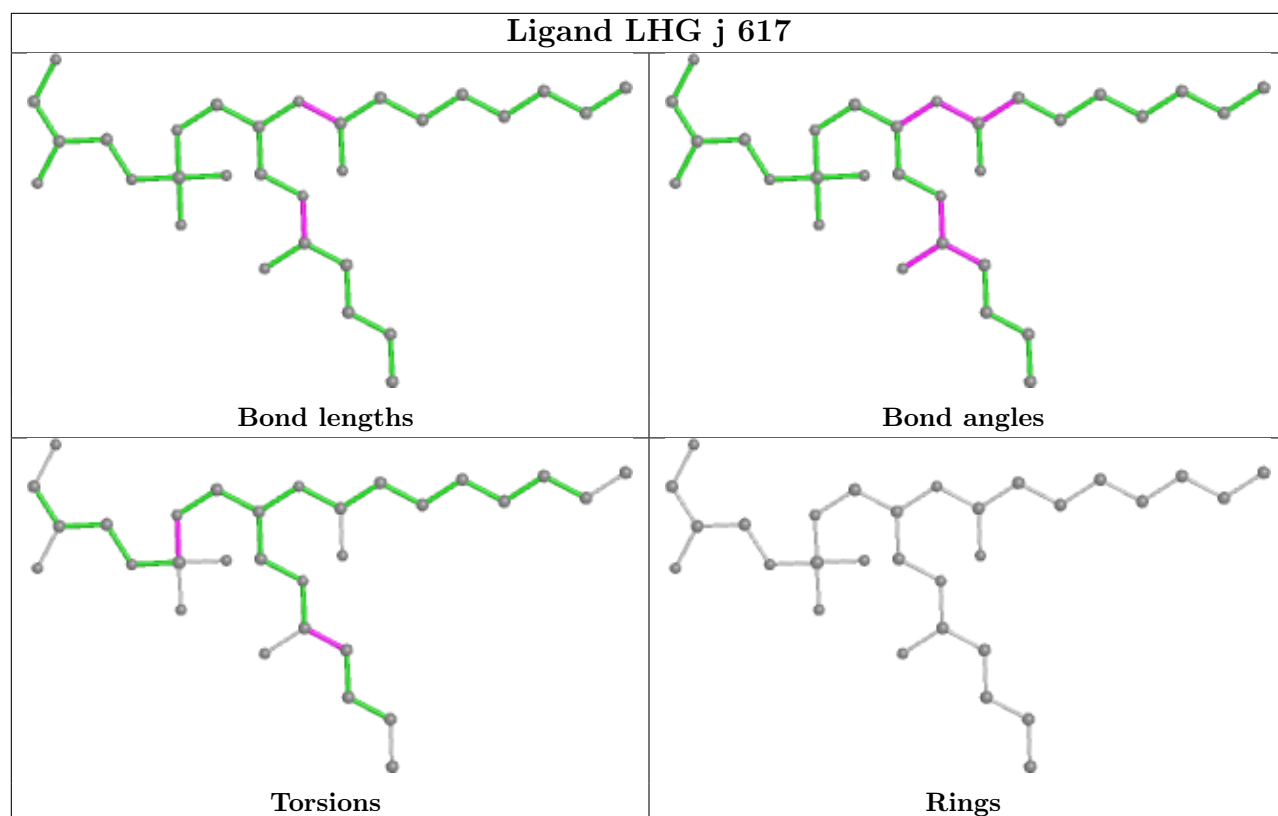
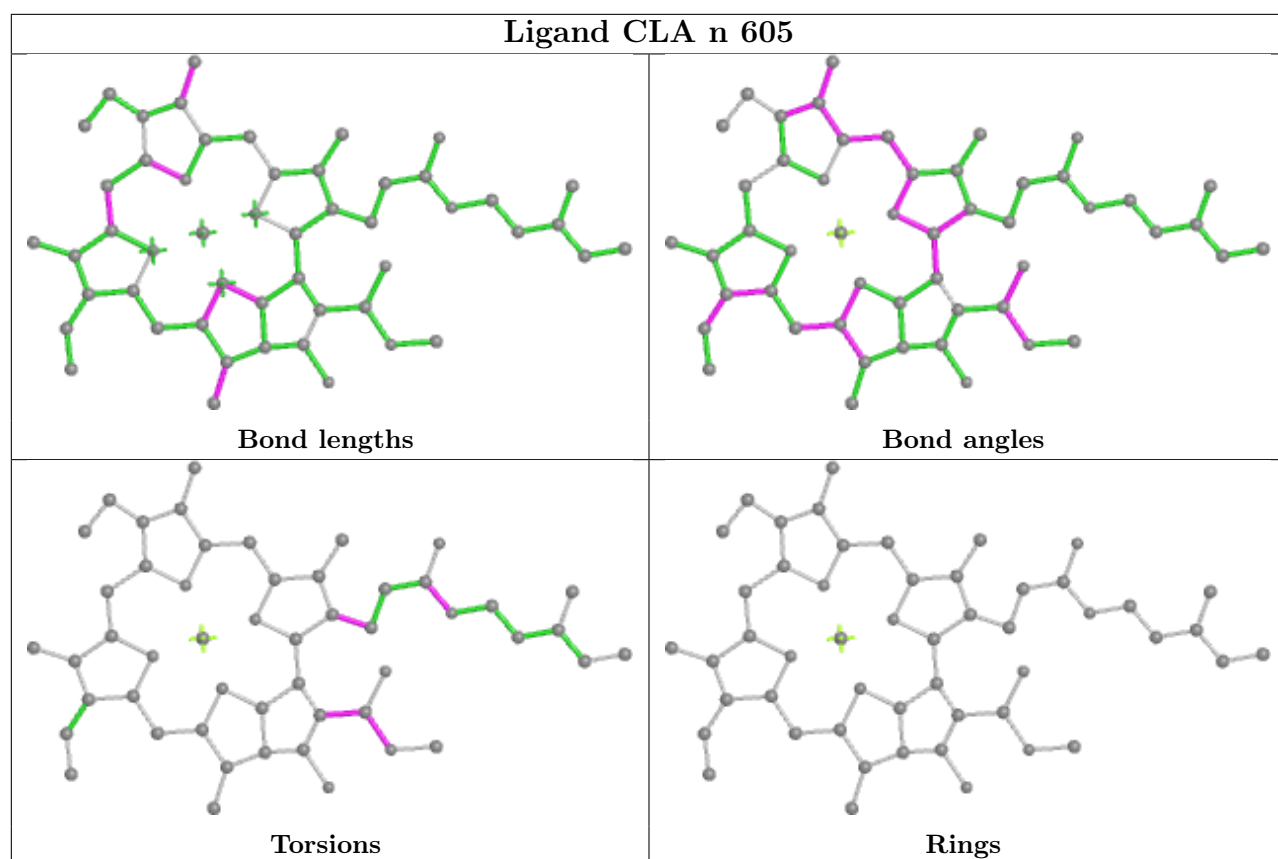


Ligand LHG c 620

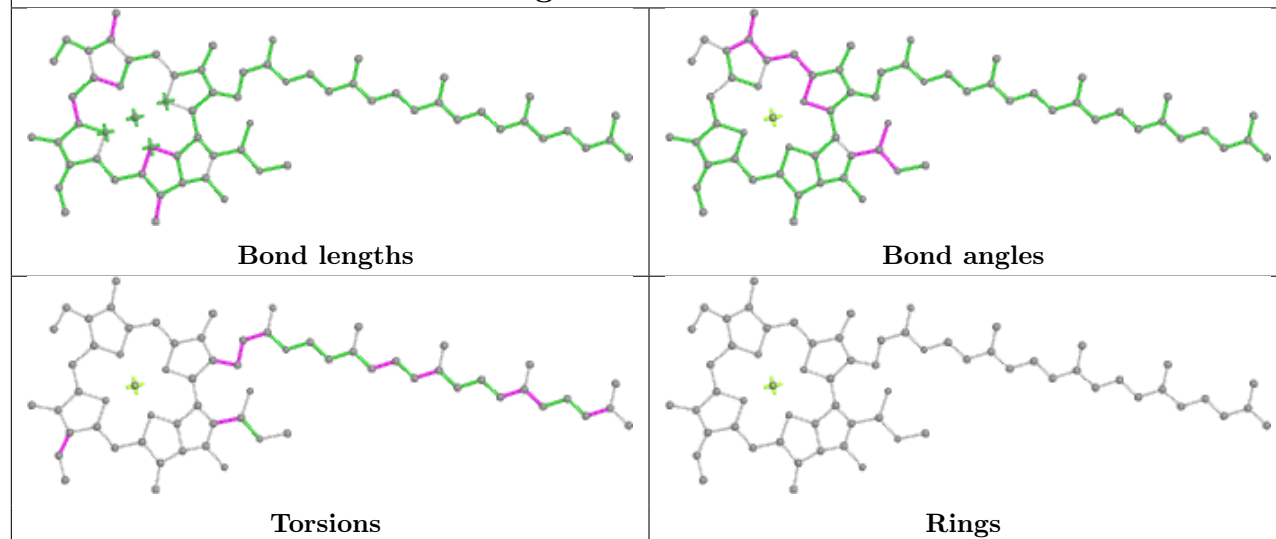


Ligand CLA B 824

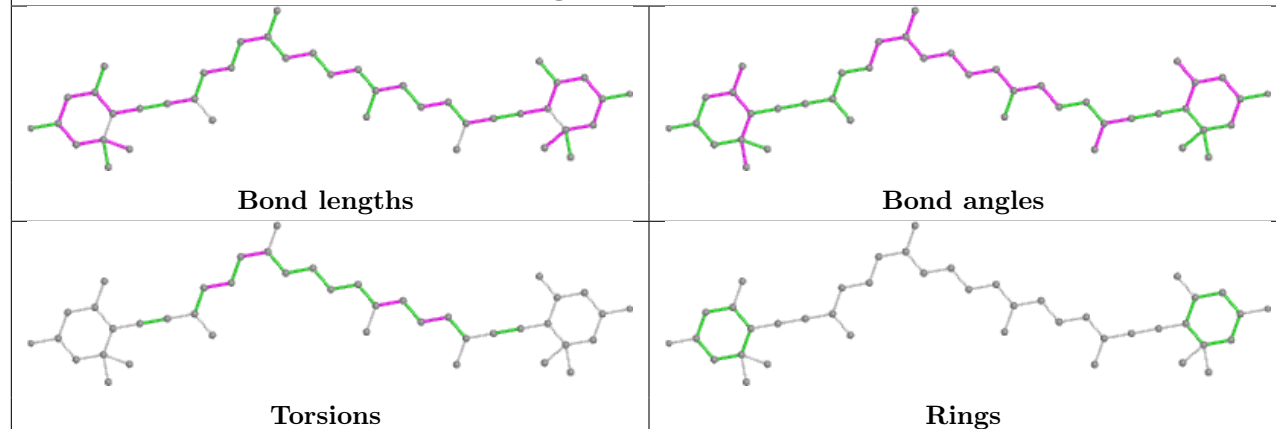




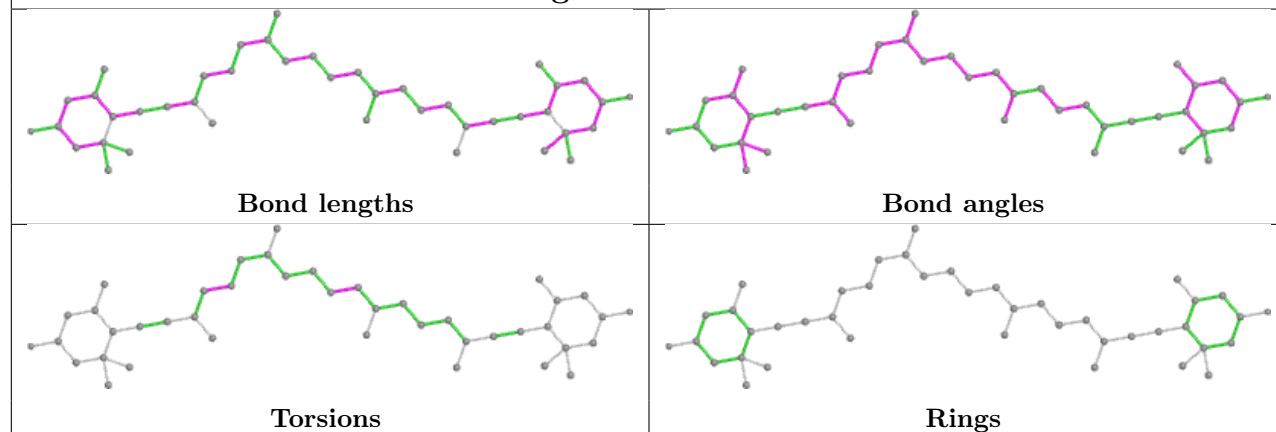
Ligand CLA n 610



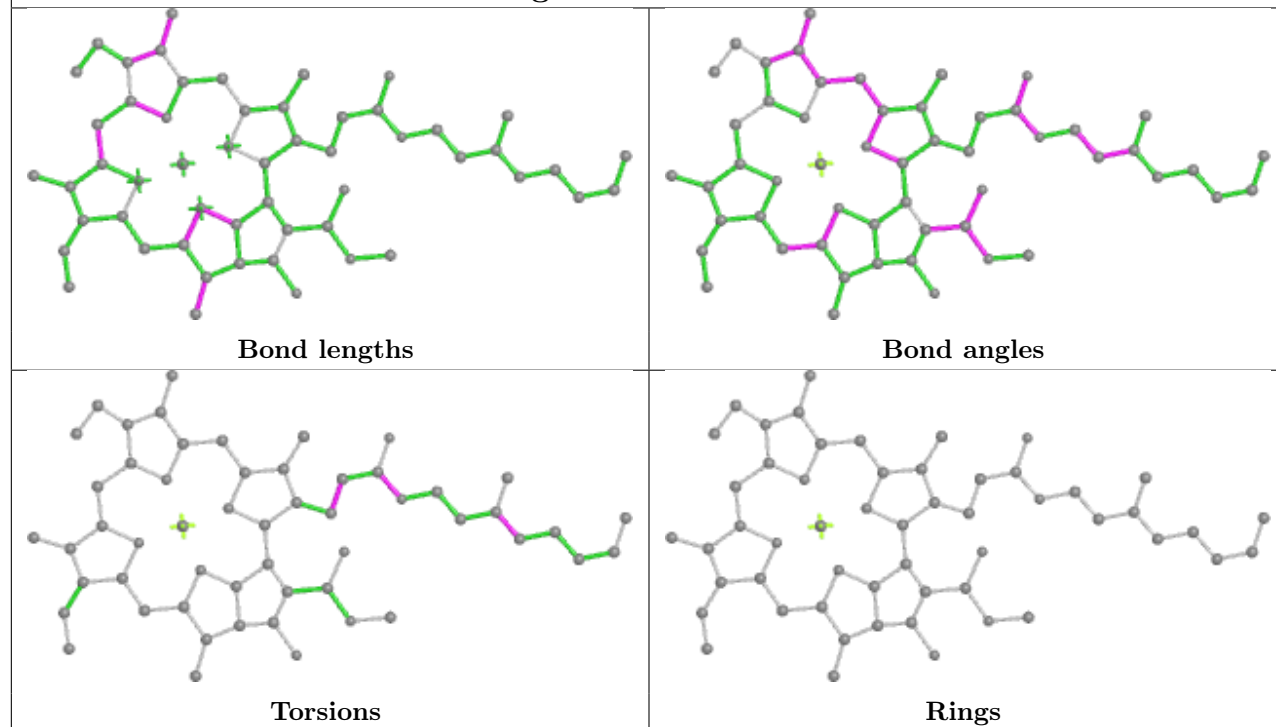
Ligand II0 J 104



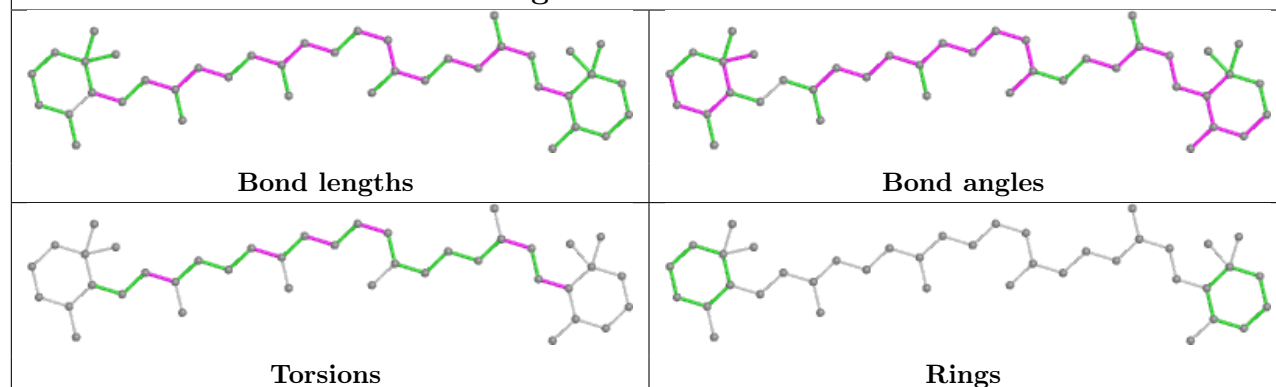
Ligand II0 c 615



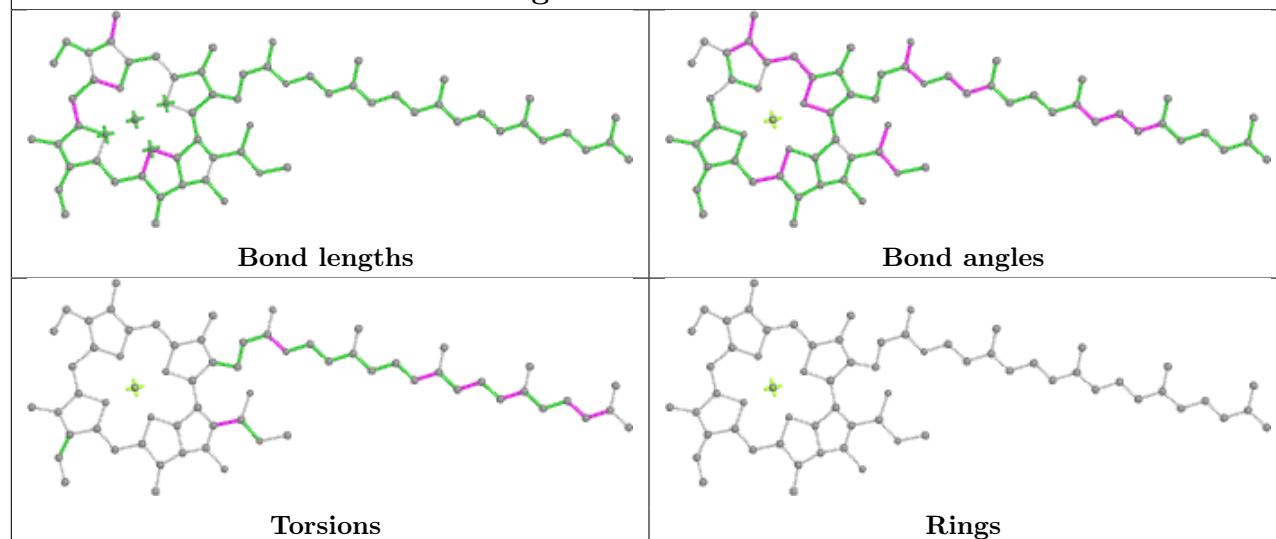
Ligand CLA A 811



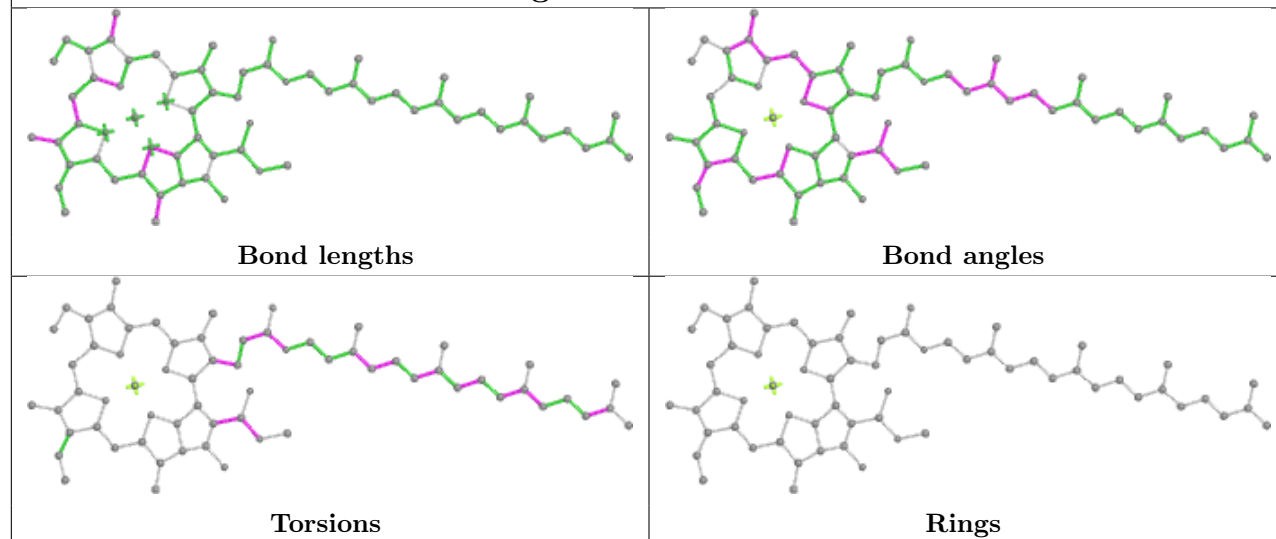
Ligand WVN i 316



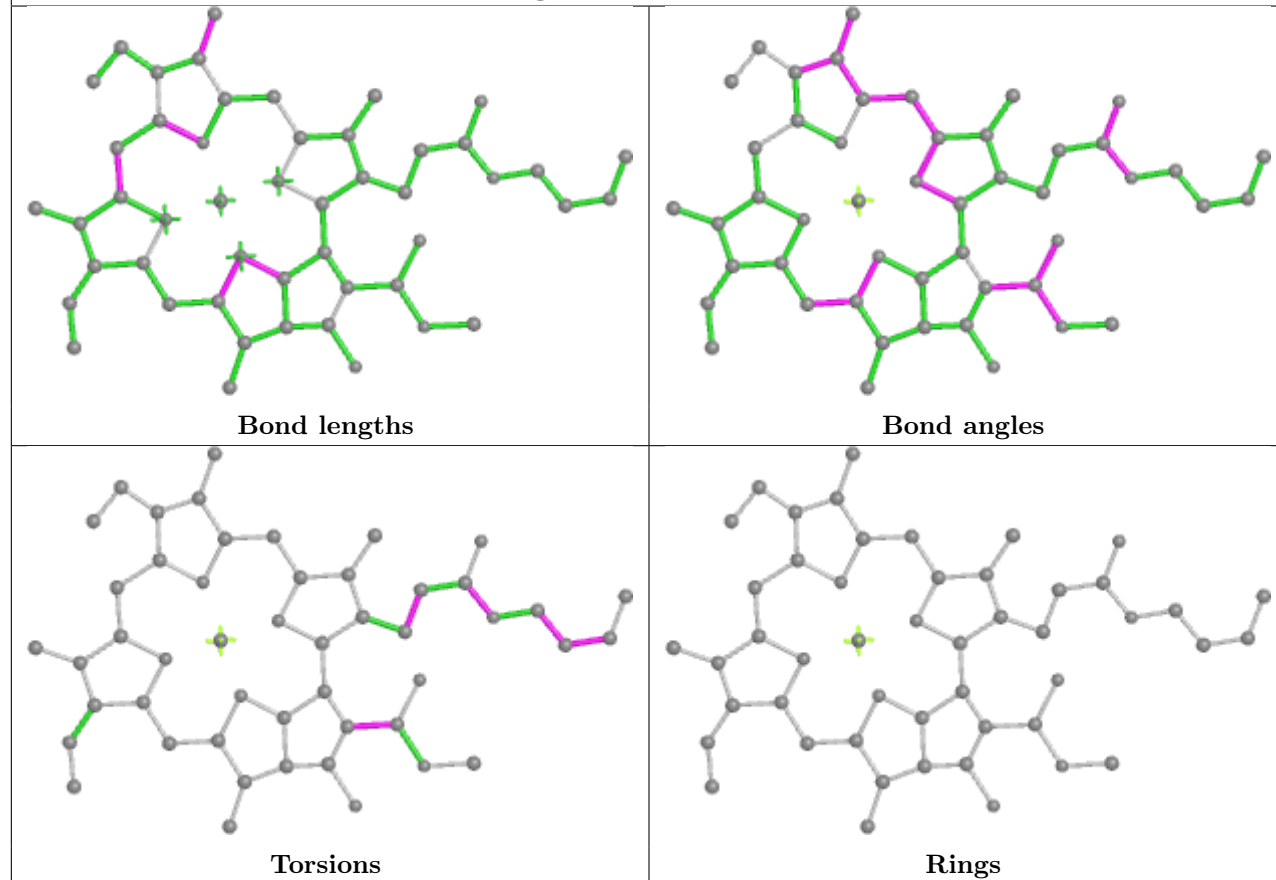
Ligand CLA A 806

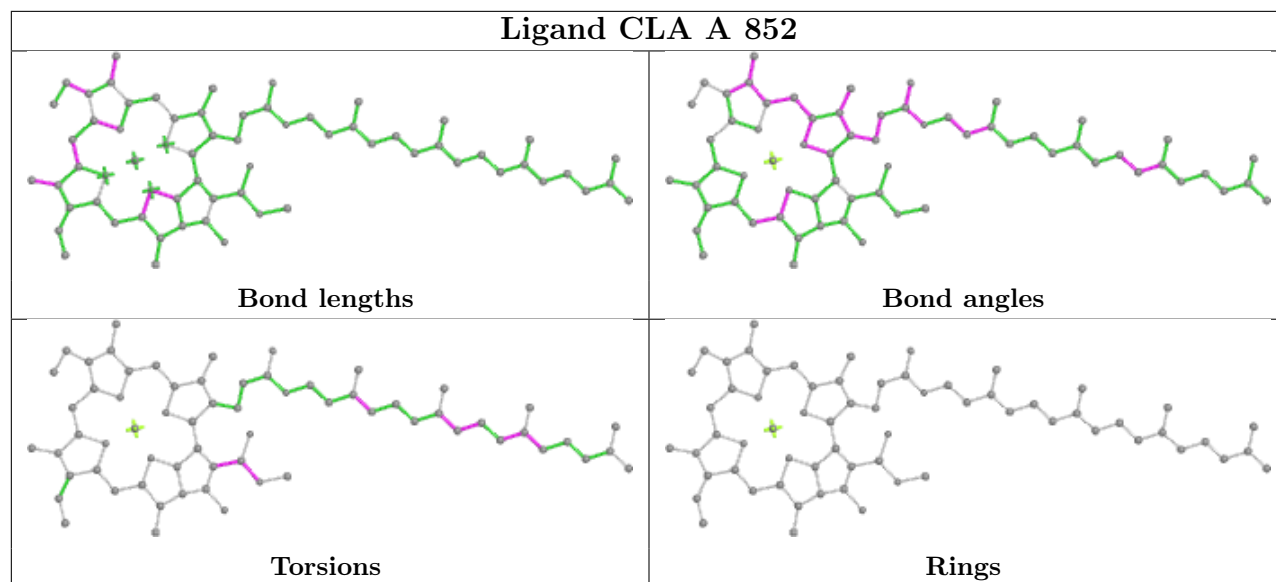
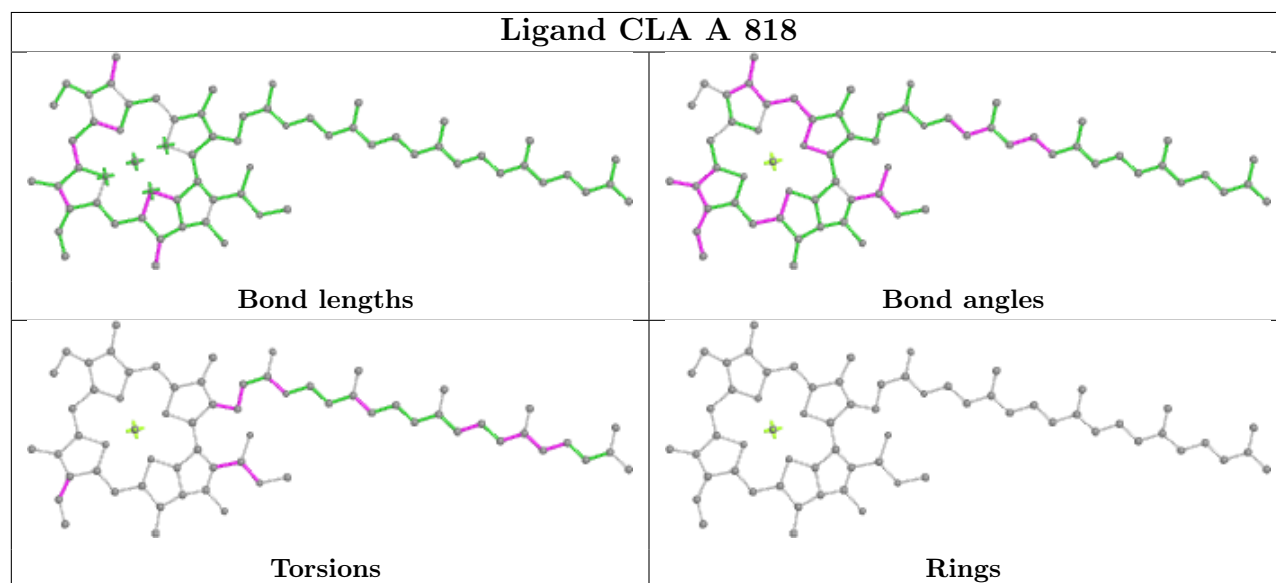


Ligand CLA A 812

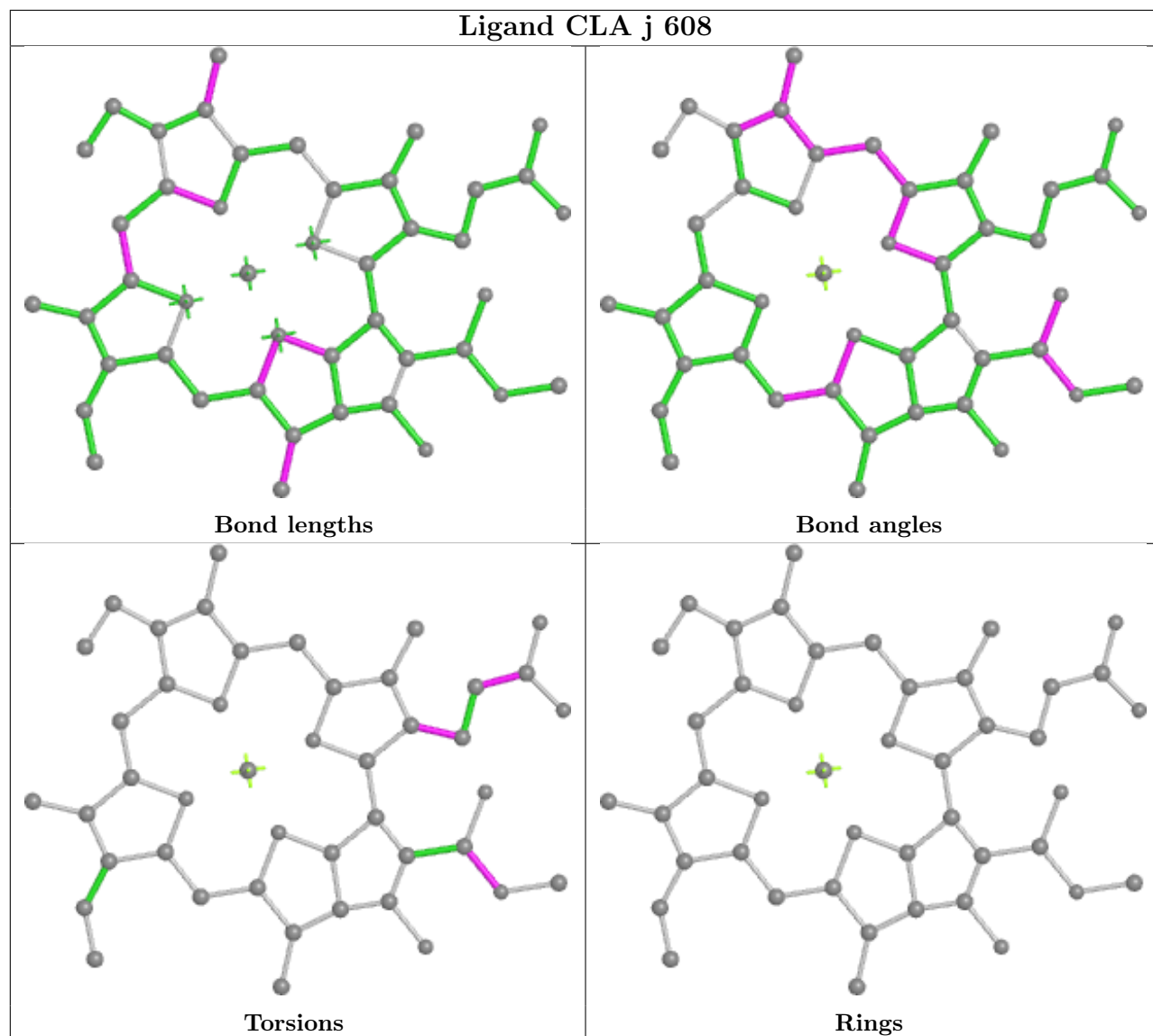


Ligand CLA A 821

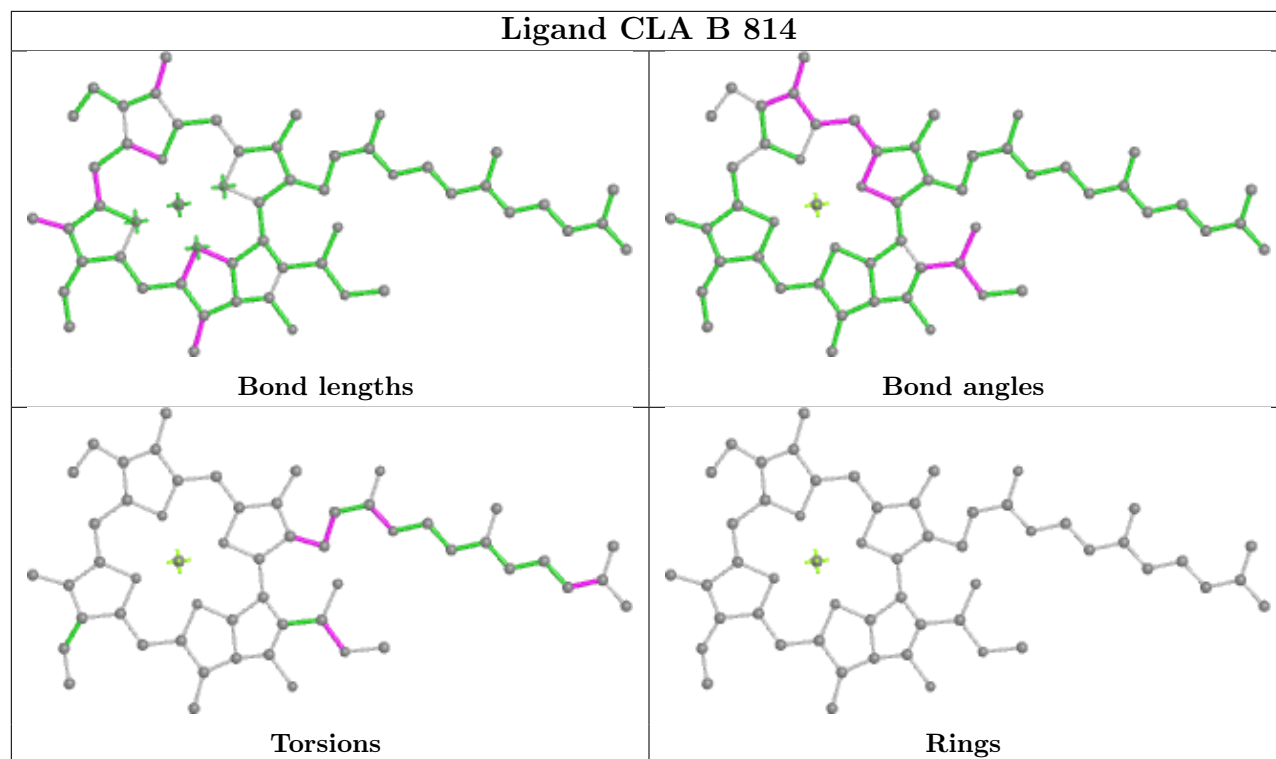


Ligand CLA A 852**Ligand CLA A 818**

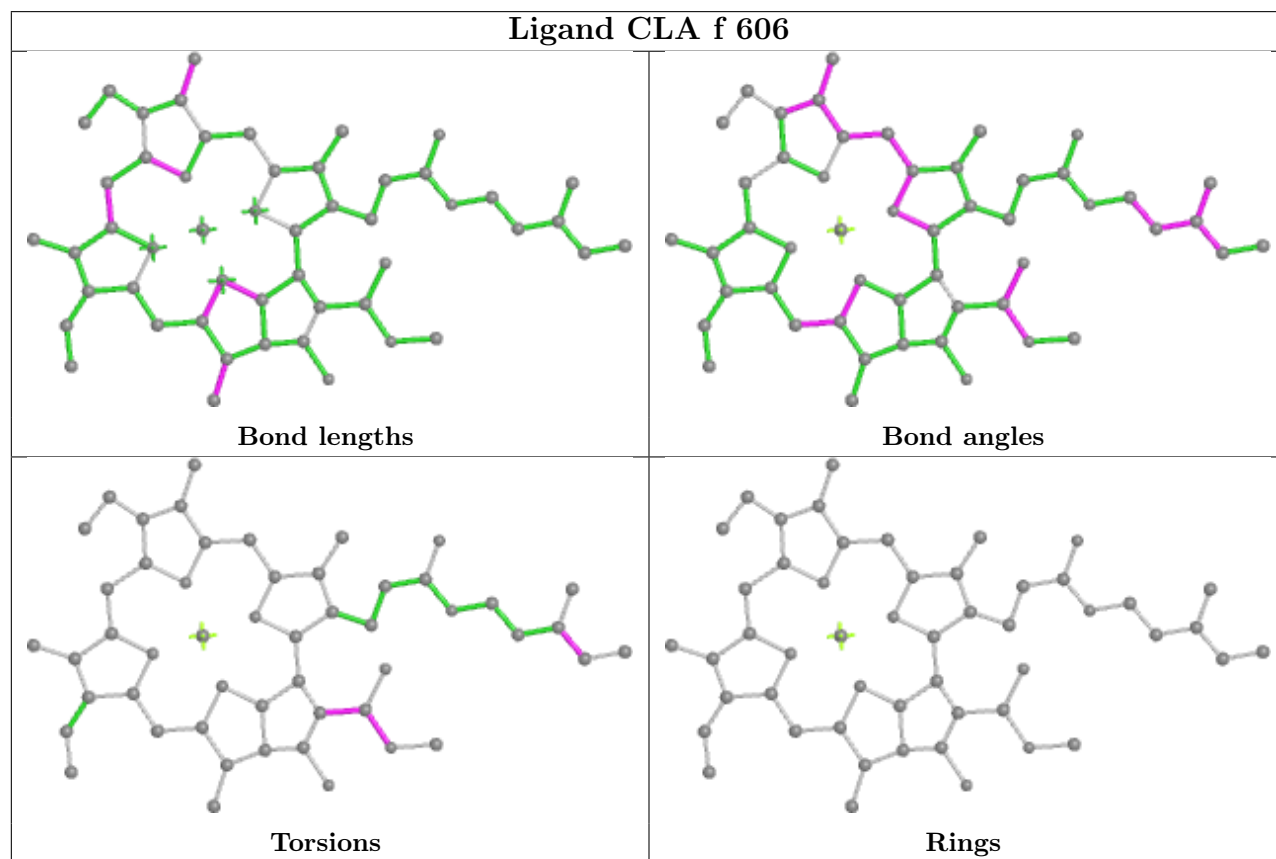
Ligand CLA j 608

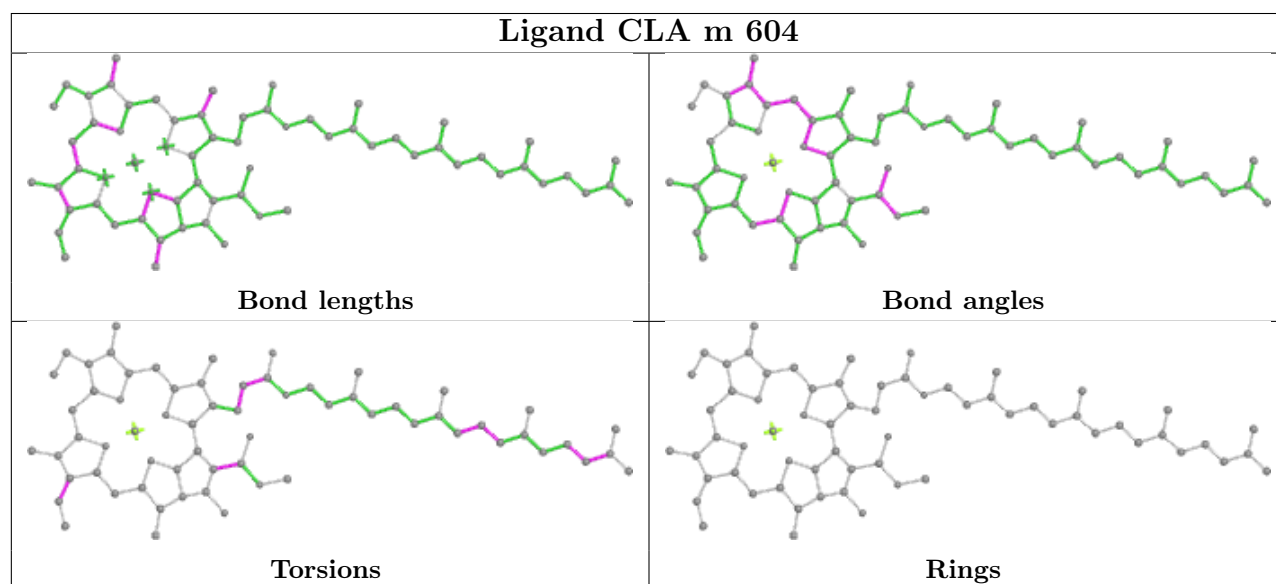
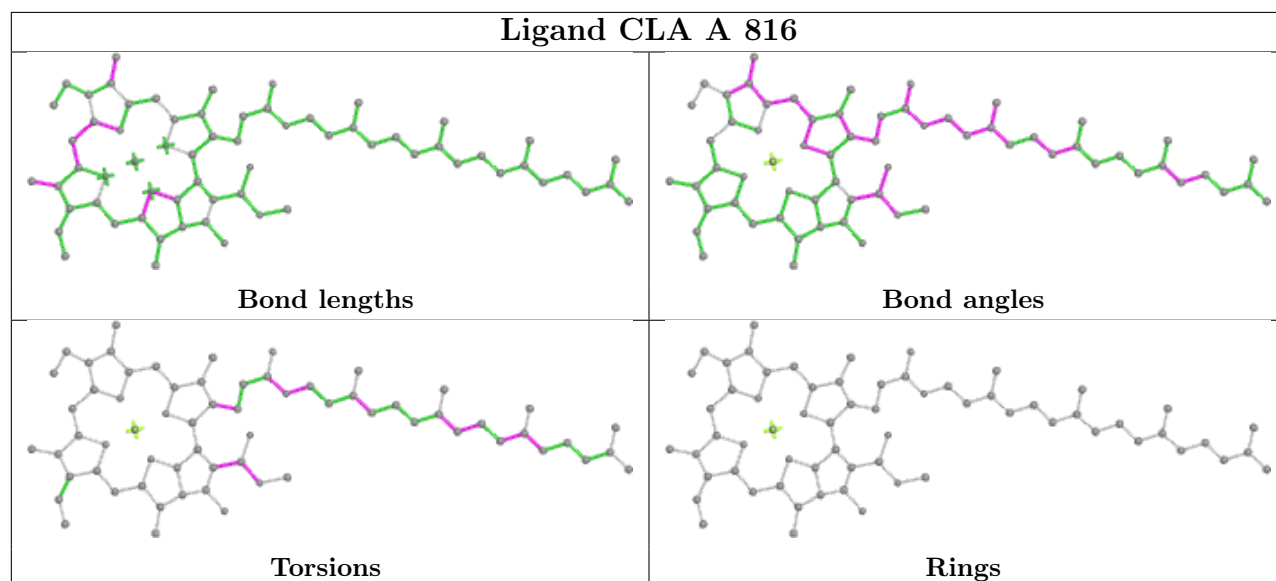
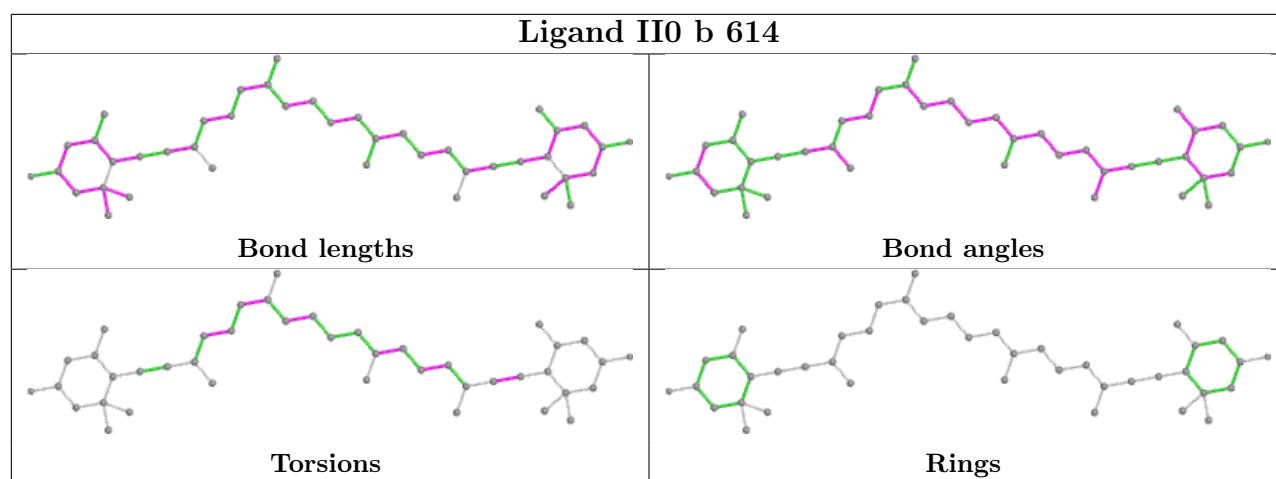


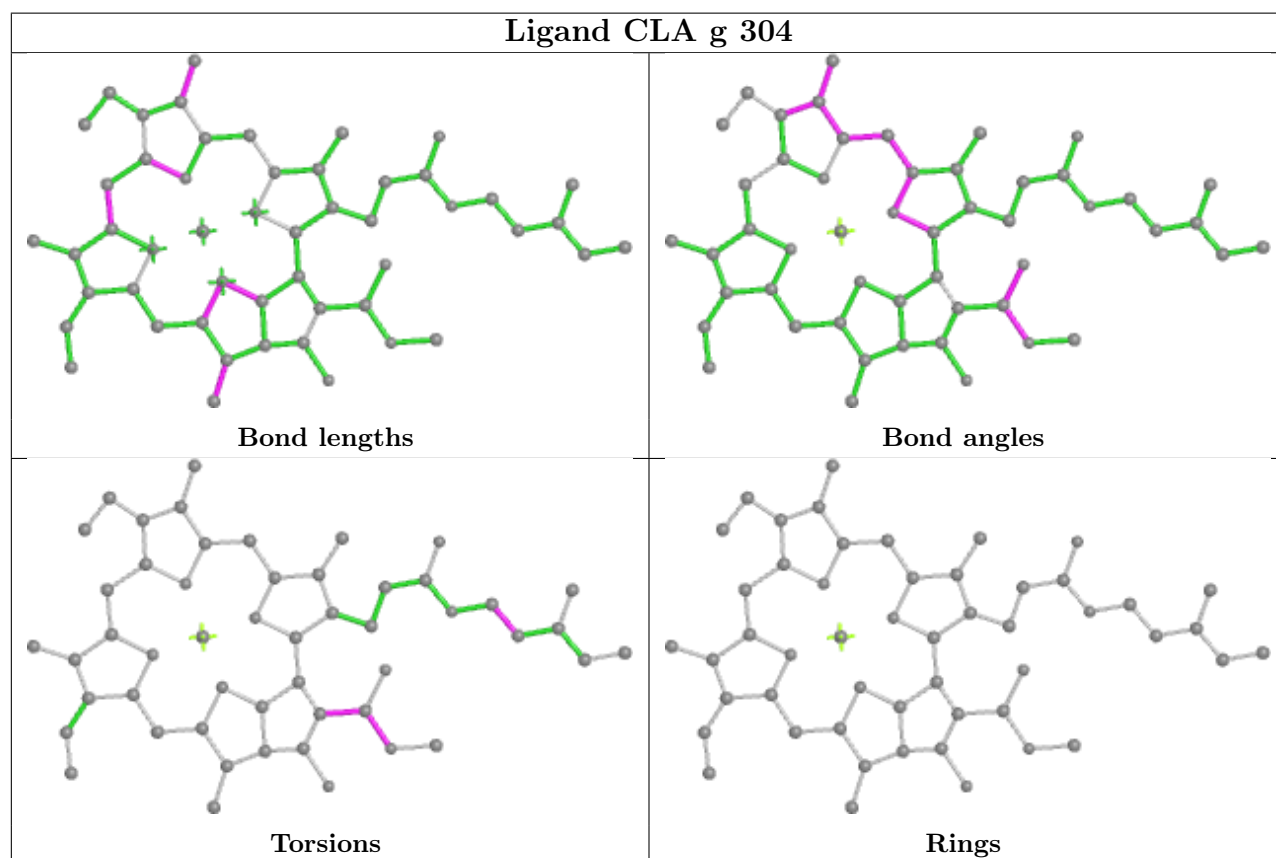
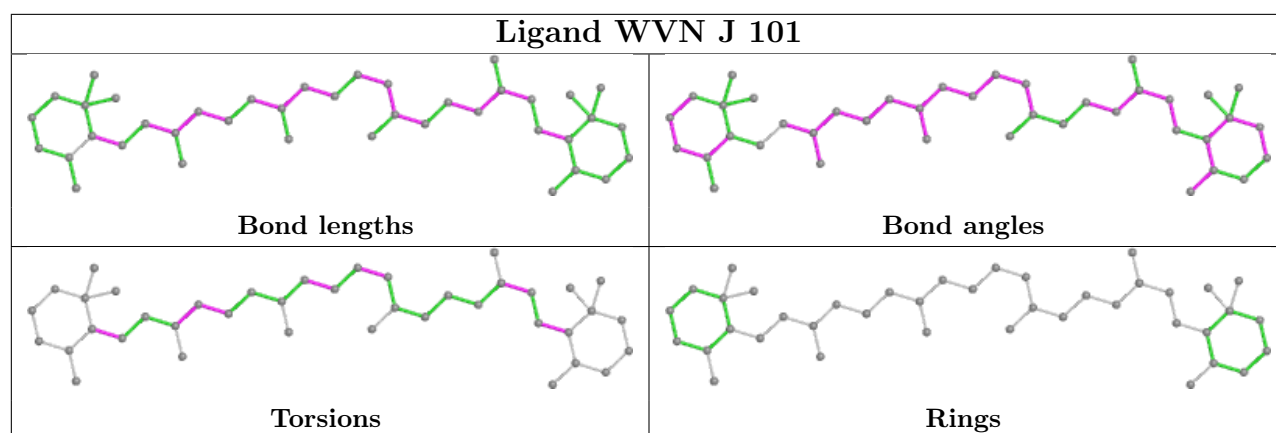
Ligand CLA B 814

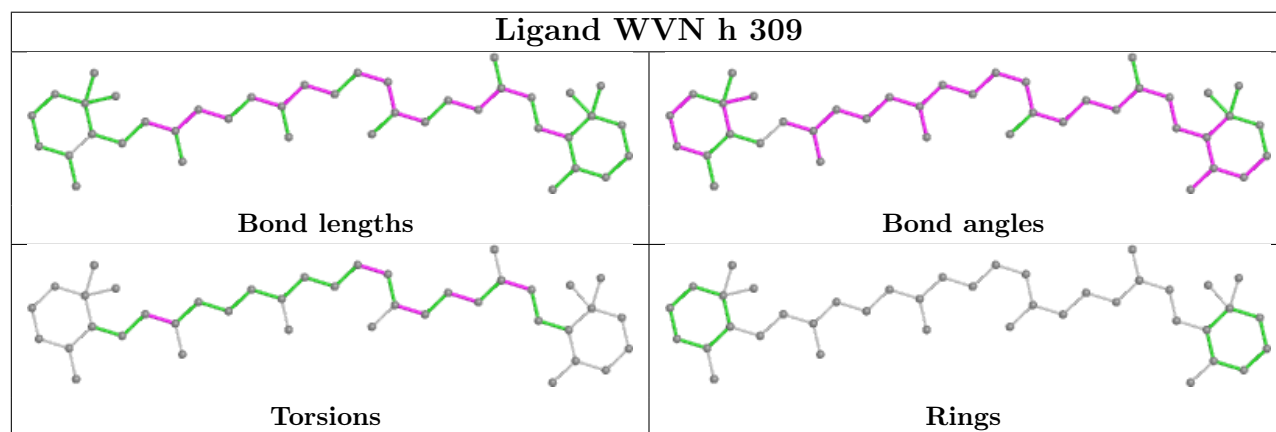
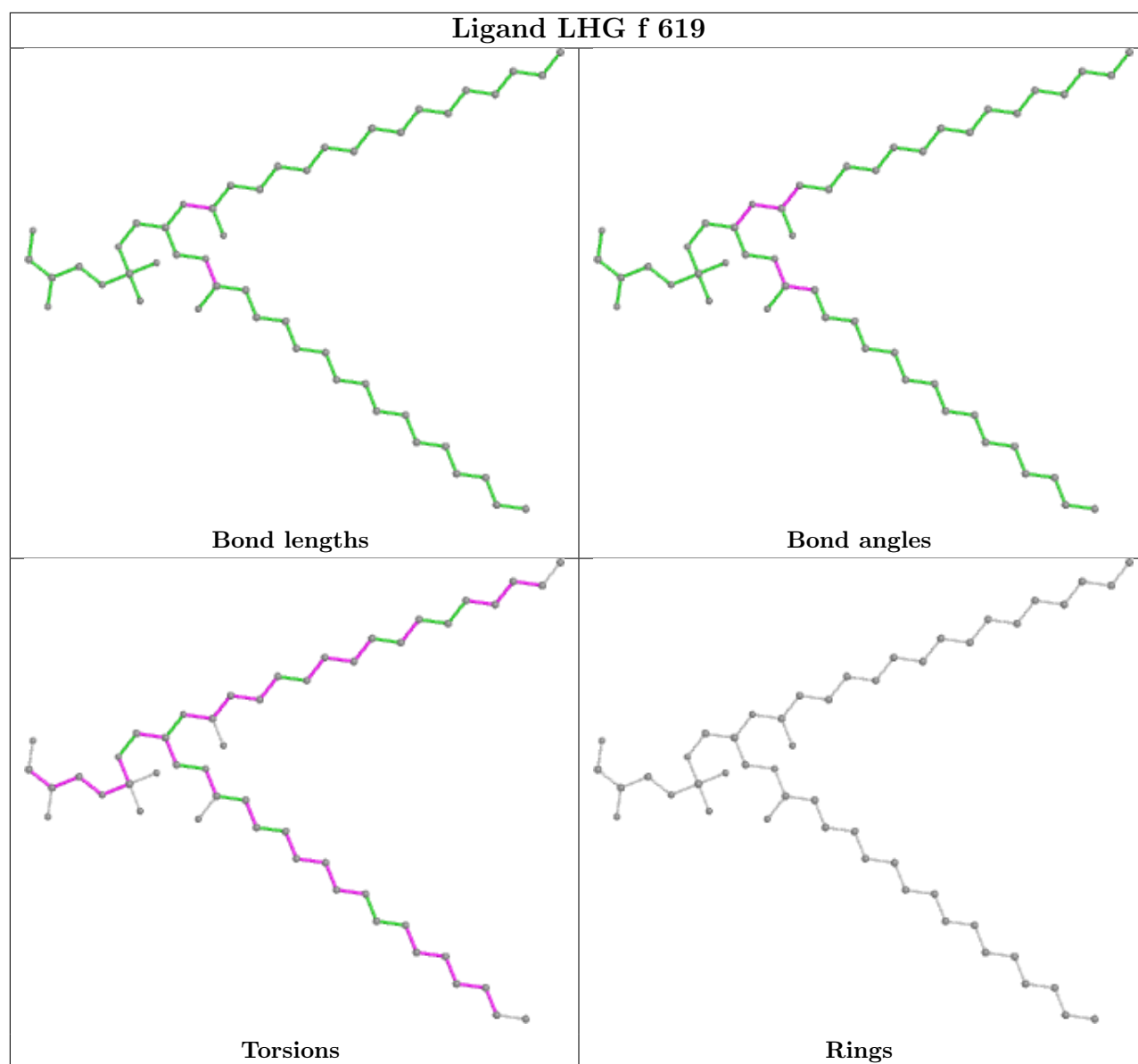


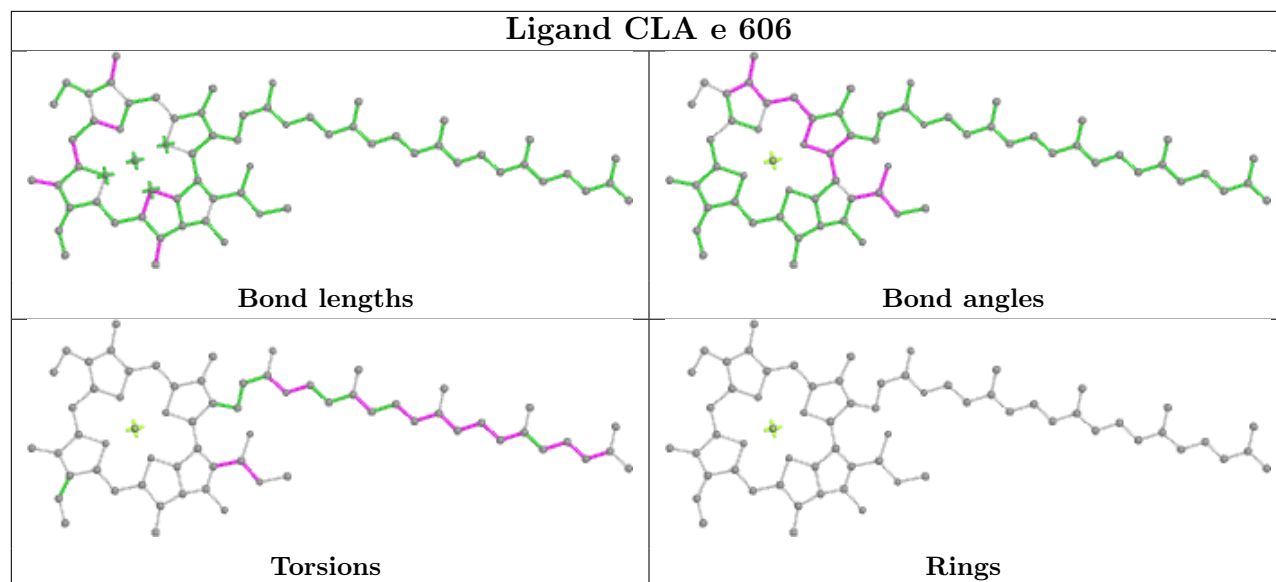
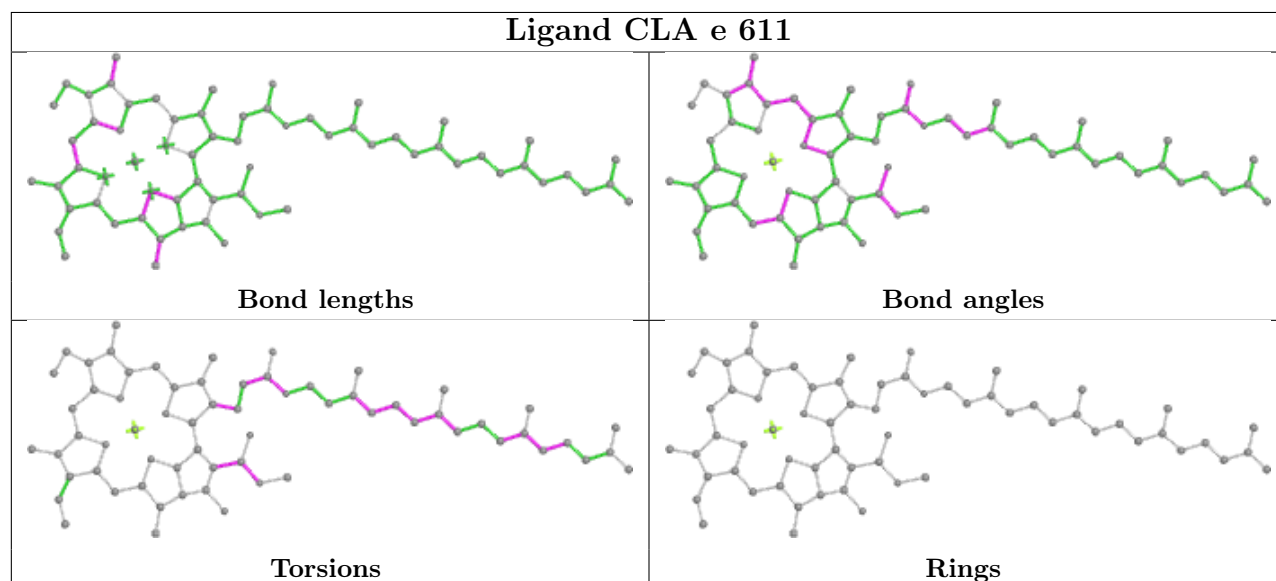
Ligand CLA f 606

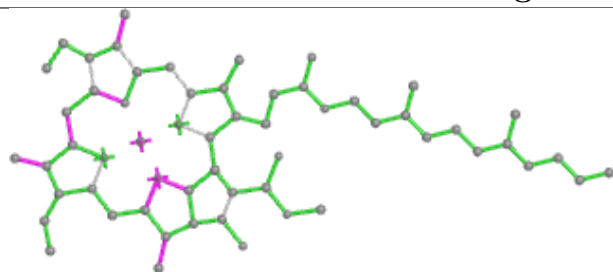




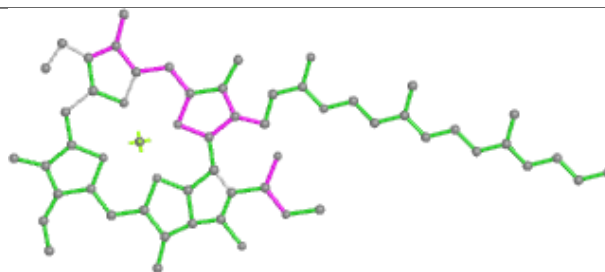




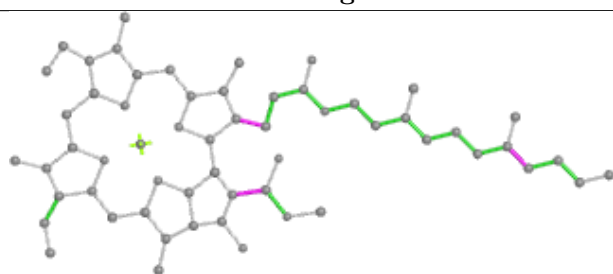
Ligand CLA e 606**Ligand CLA e 611**

Ligand CLA B 832

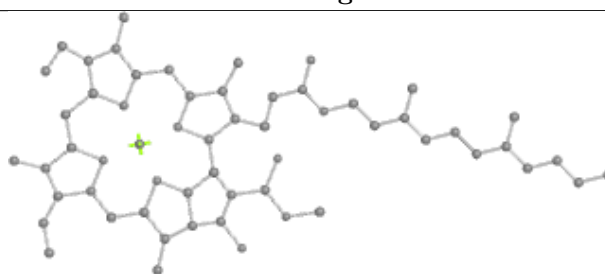
Bond lengths



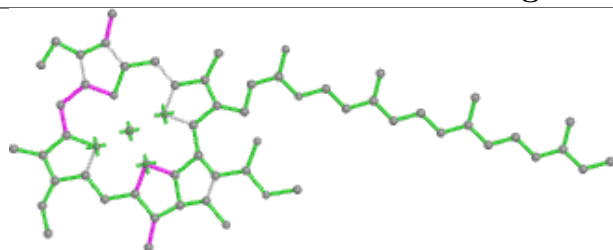
Bond angles



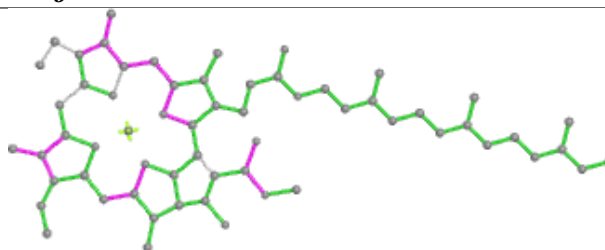
Torsions



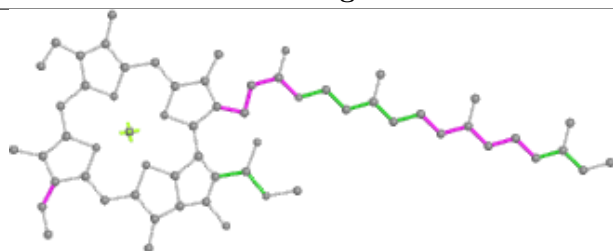
Rings

Ligand CLA j 610

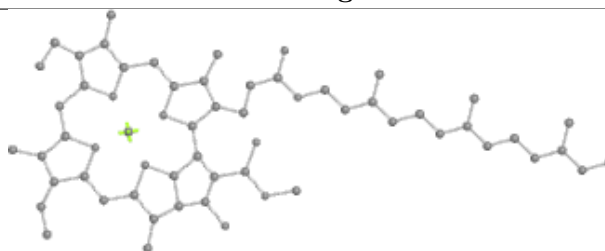
Bond lengths



Bond angles

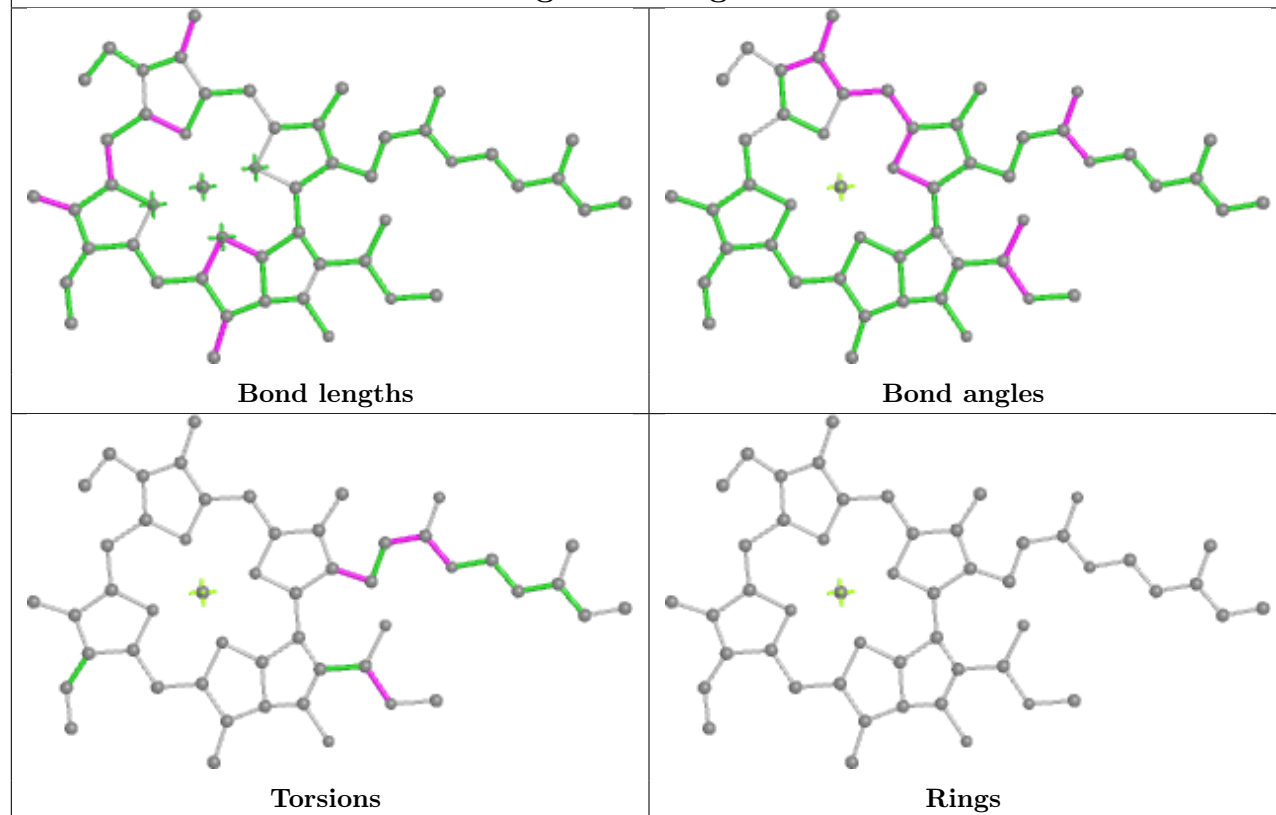


Torsions

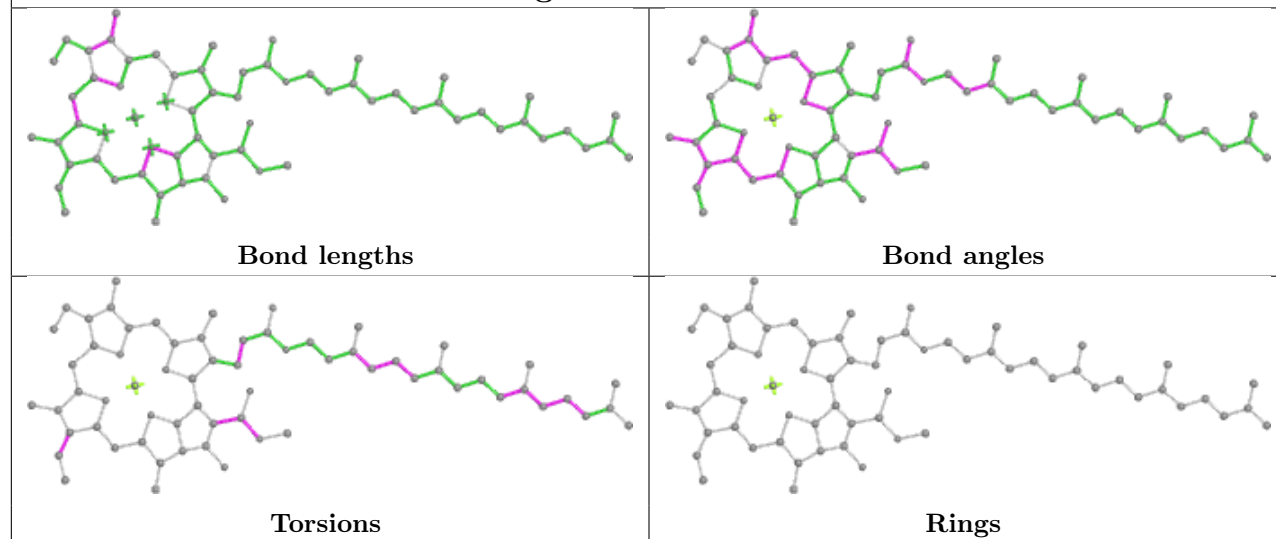


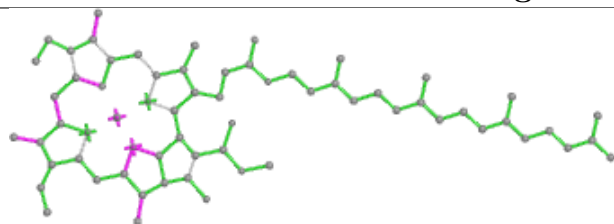
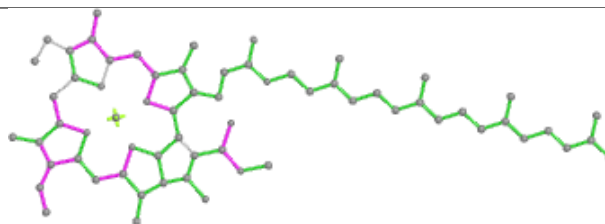
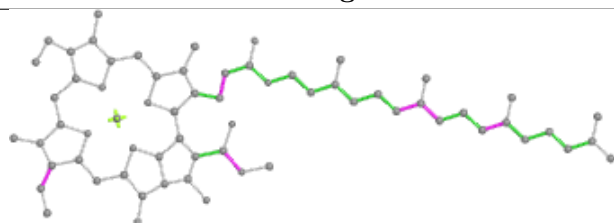
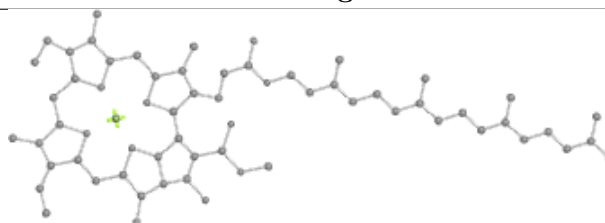
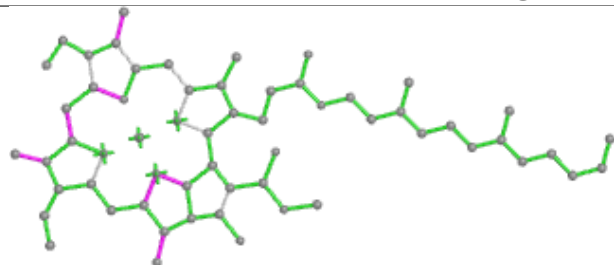
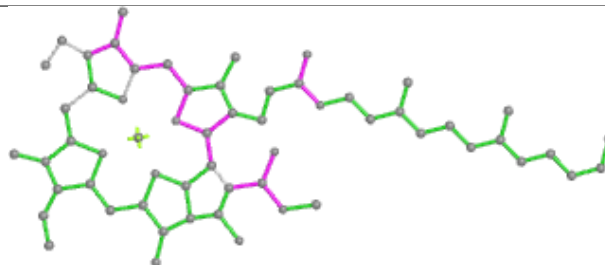
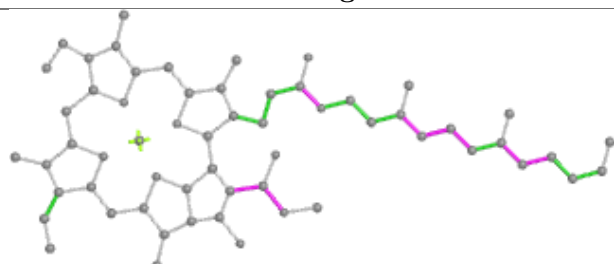
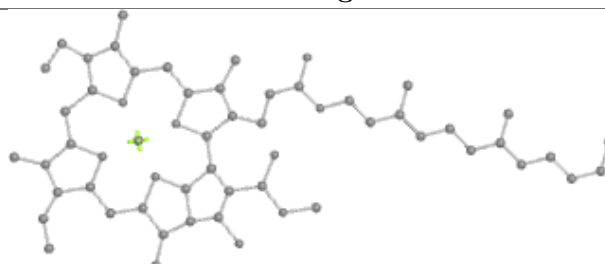
Rings

Ligand CLA g 306

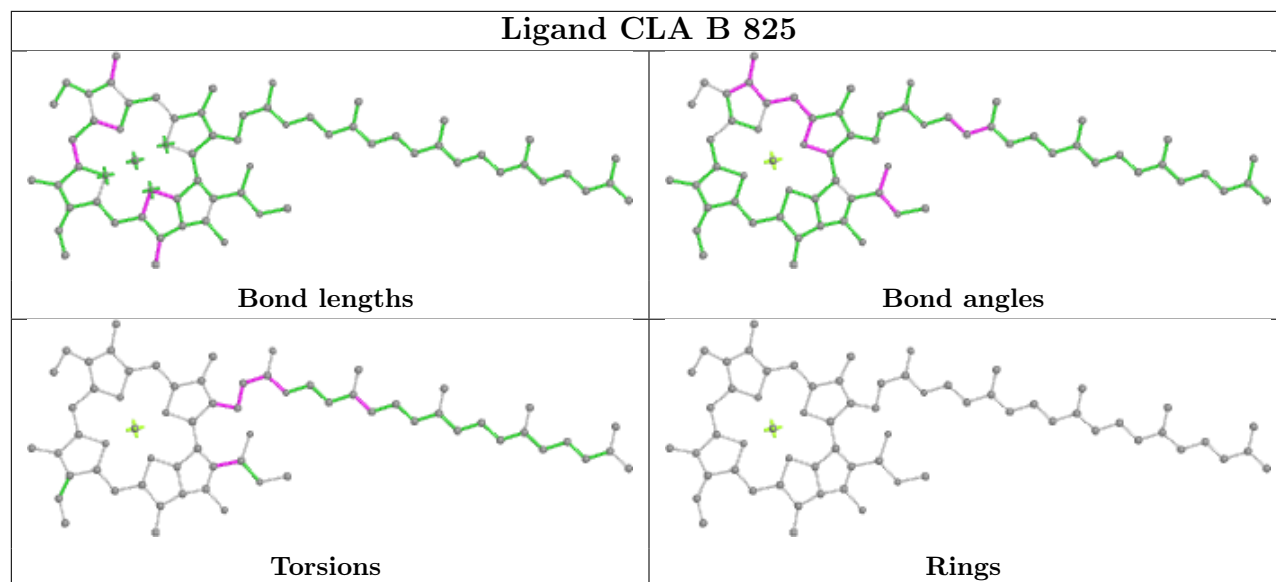


Ligand CLA b 607

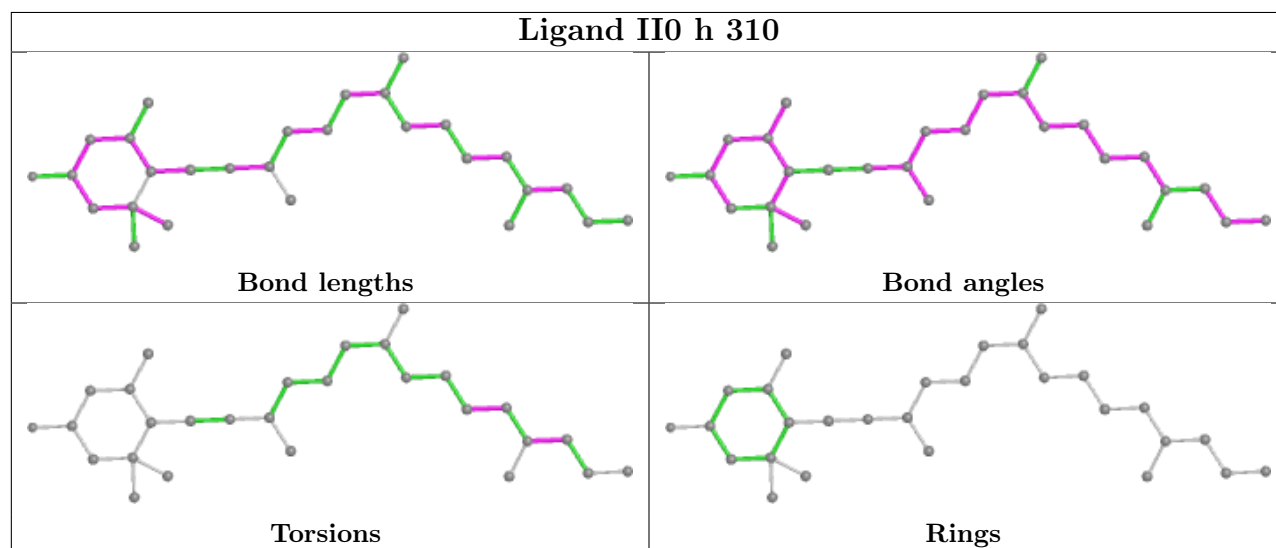


Ligand CLA B 803**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 813****Bond lengths****Bond angles****Torsions****Rings**

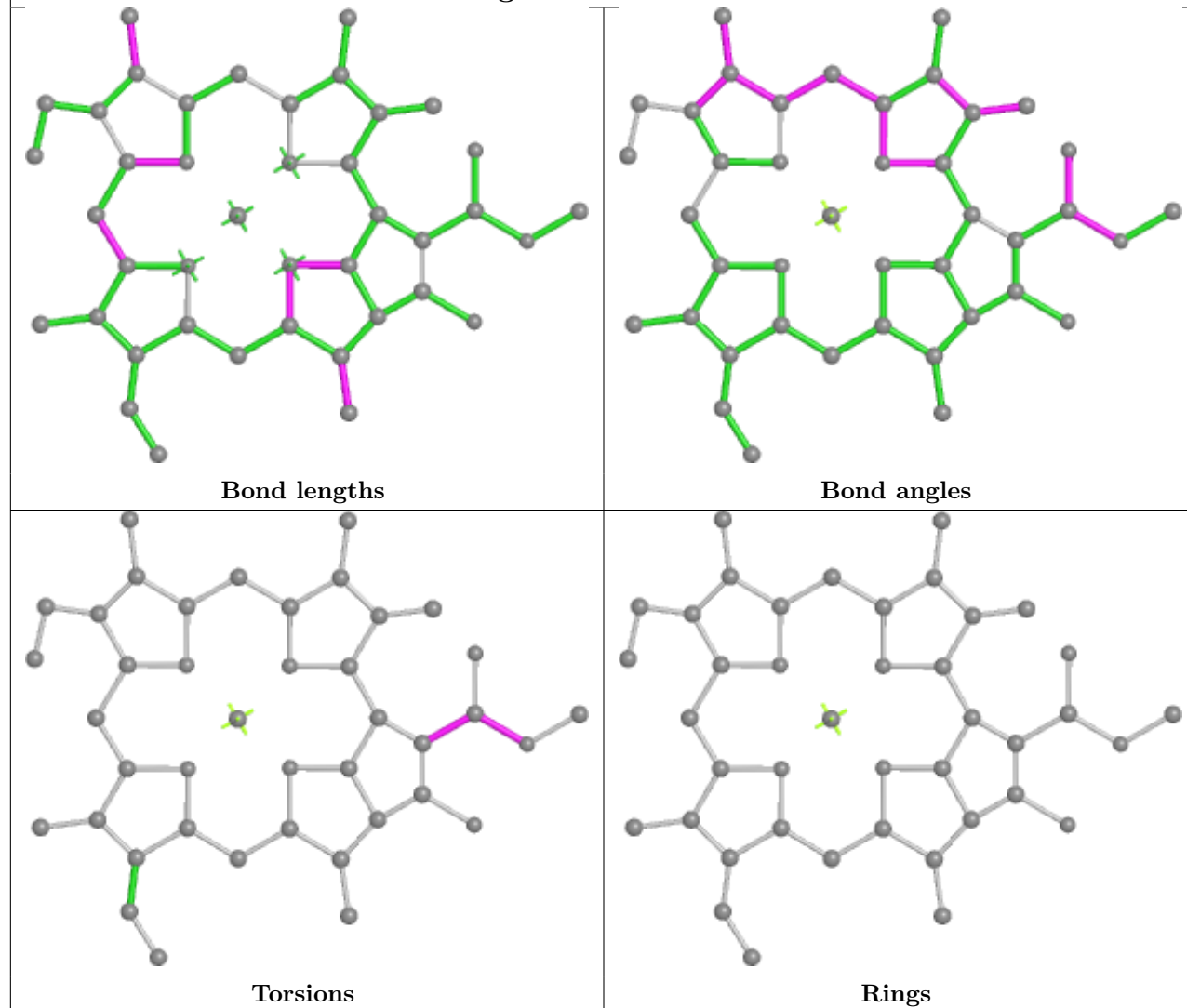
Ligand CLA B 825



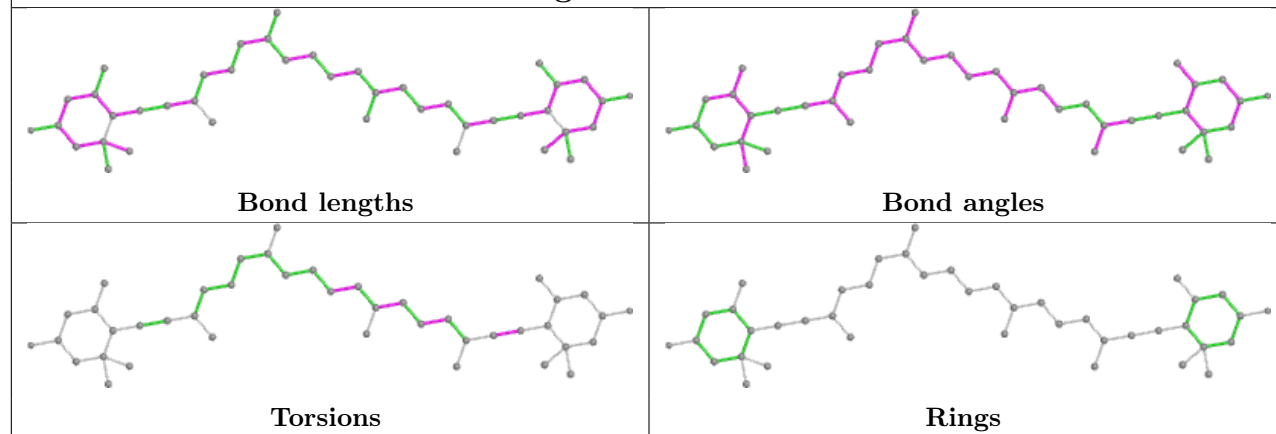
Ligand II0 h 310



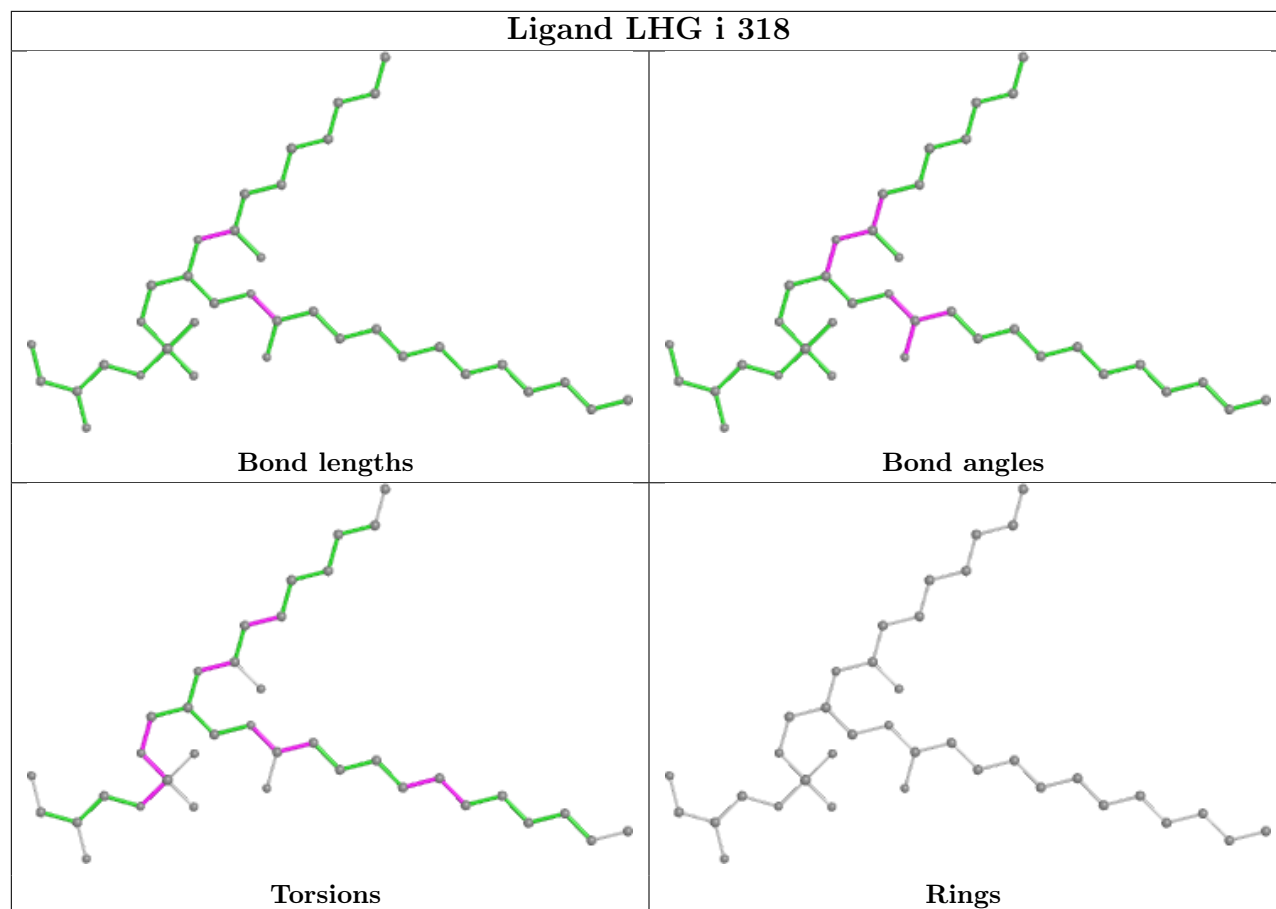
Ligand CLA d 309



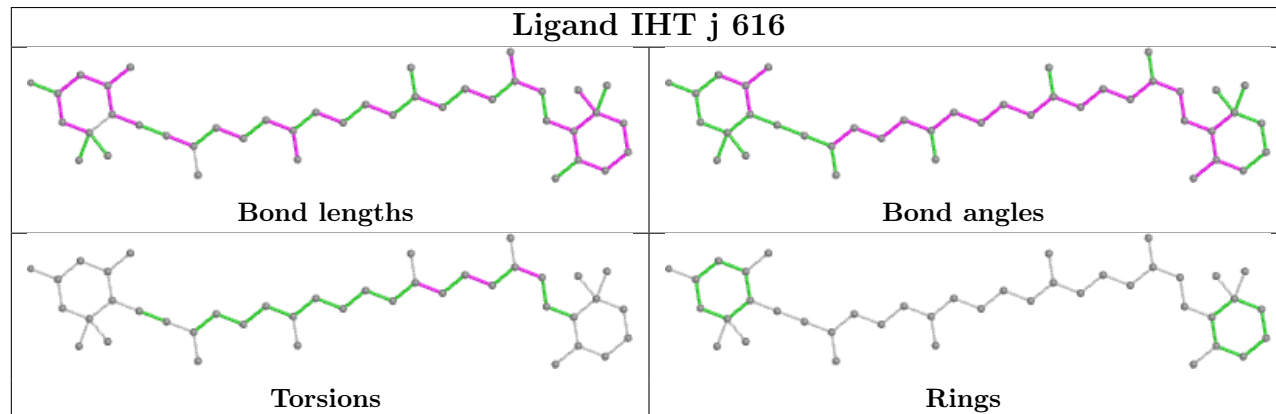
Ligand II0 i 314



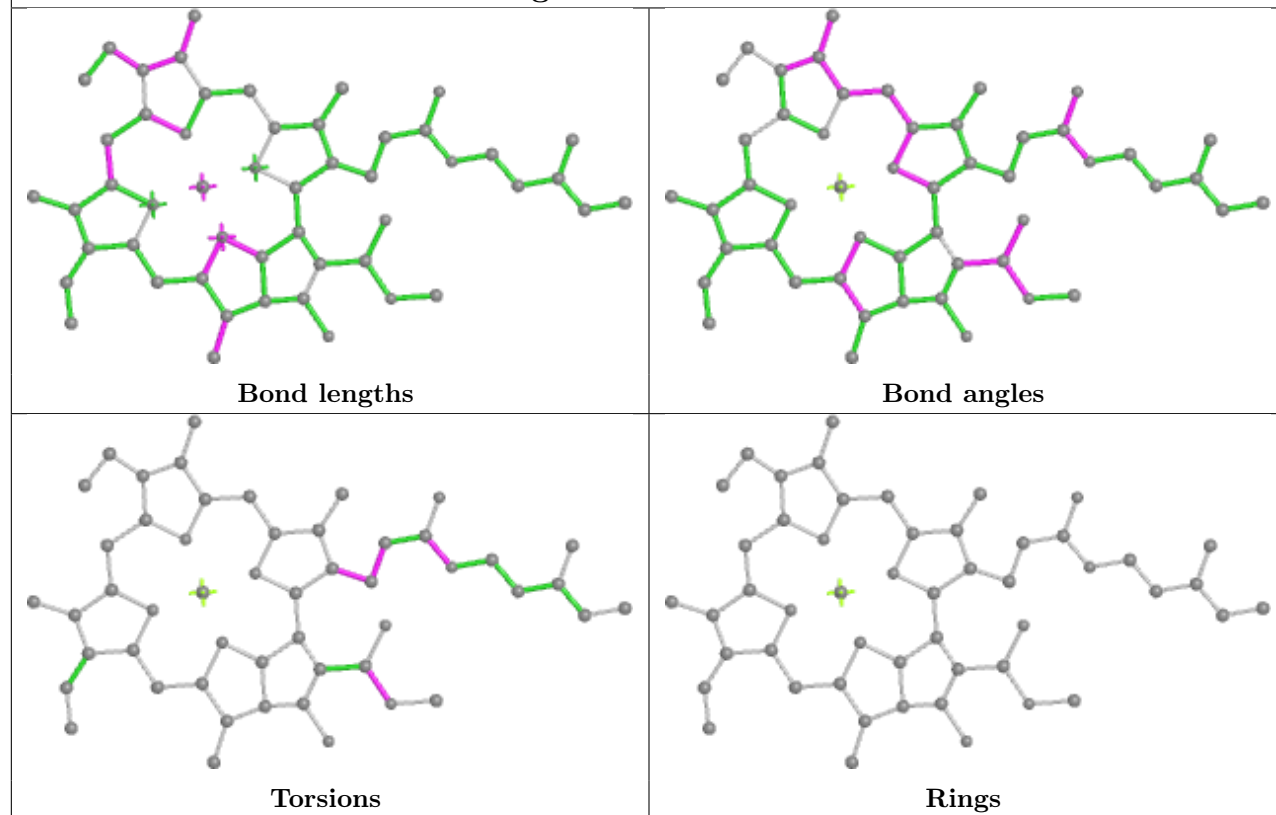
Ligand LHG i 318



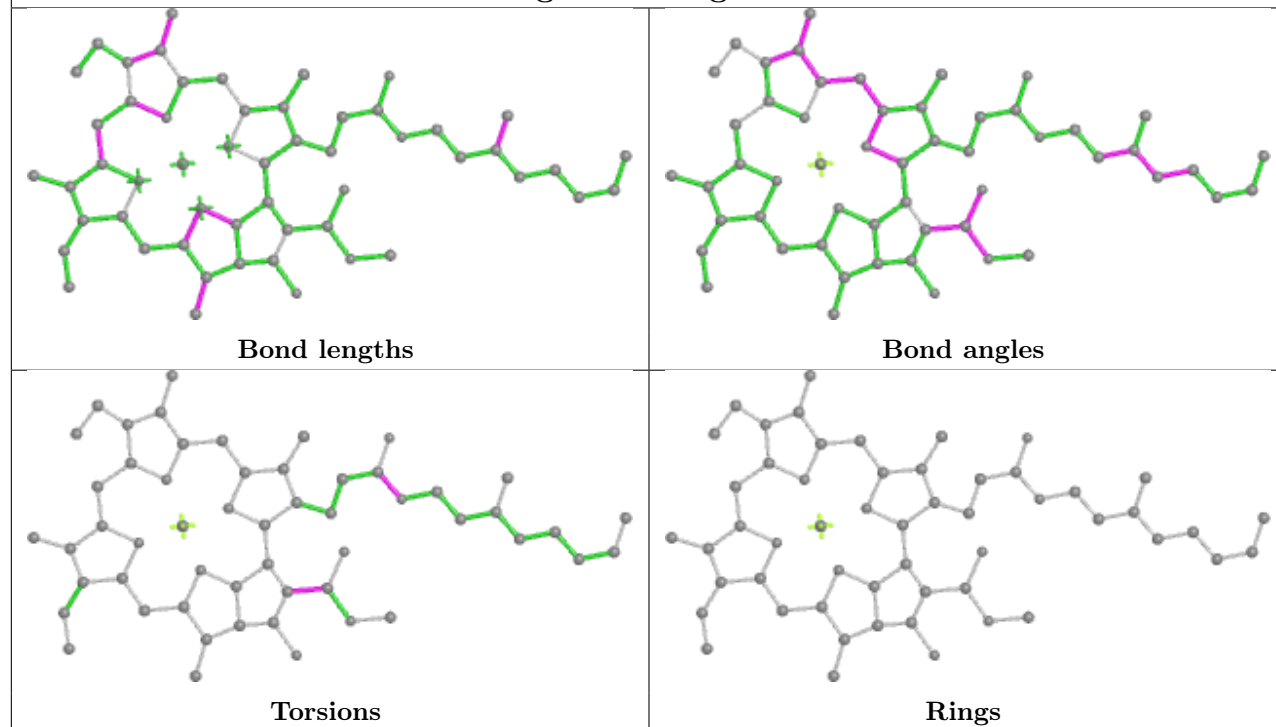
Ligand IHT j 616

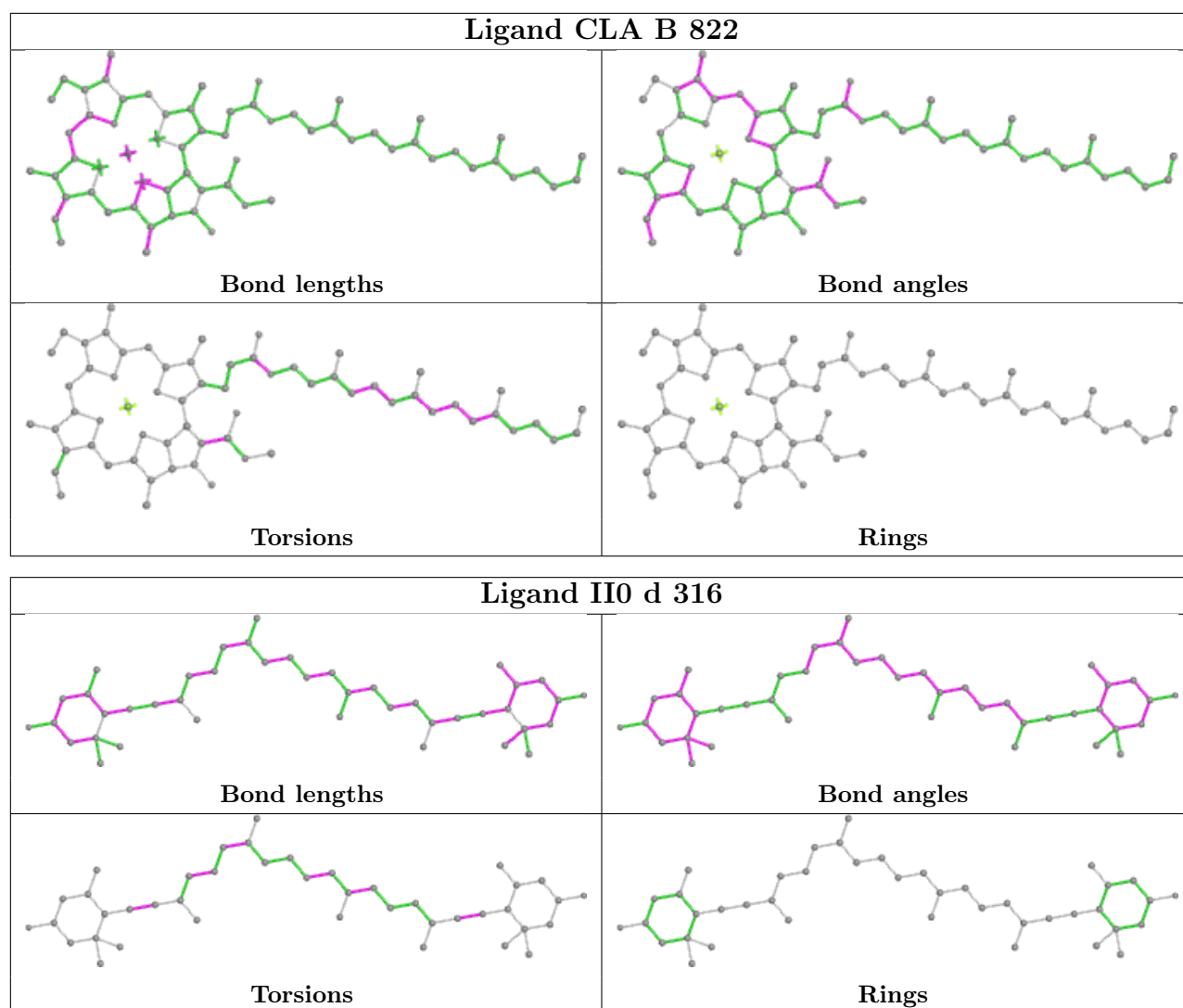


Ligand CLA A 822

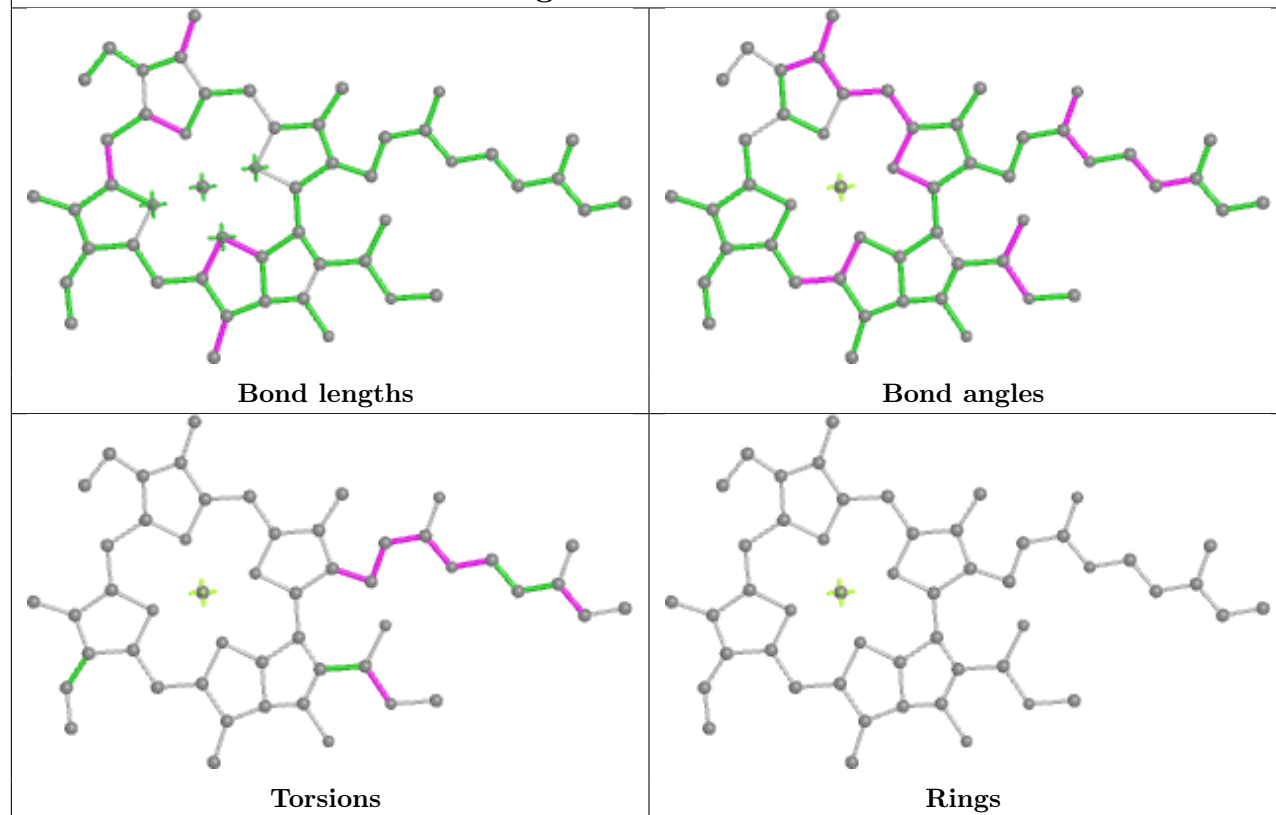


Ligand CLA g 311

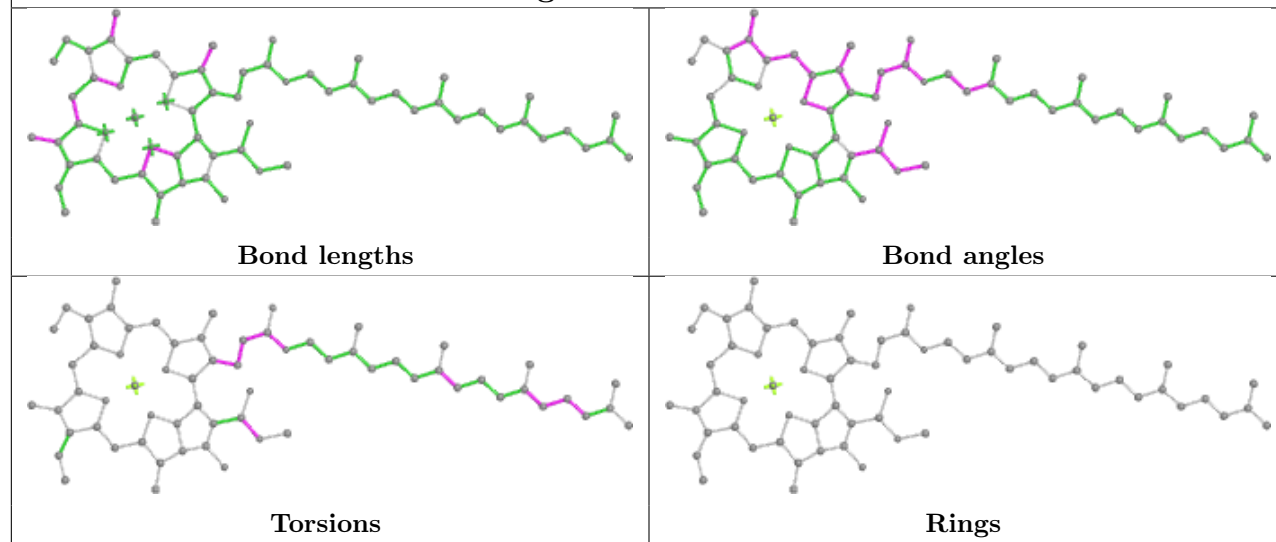




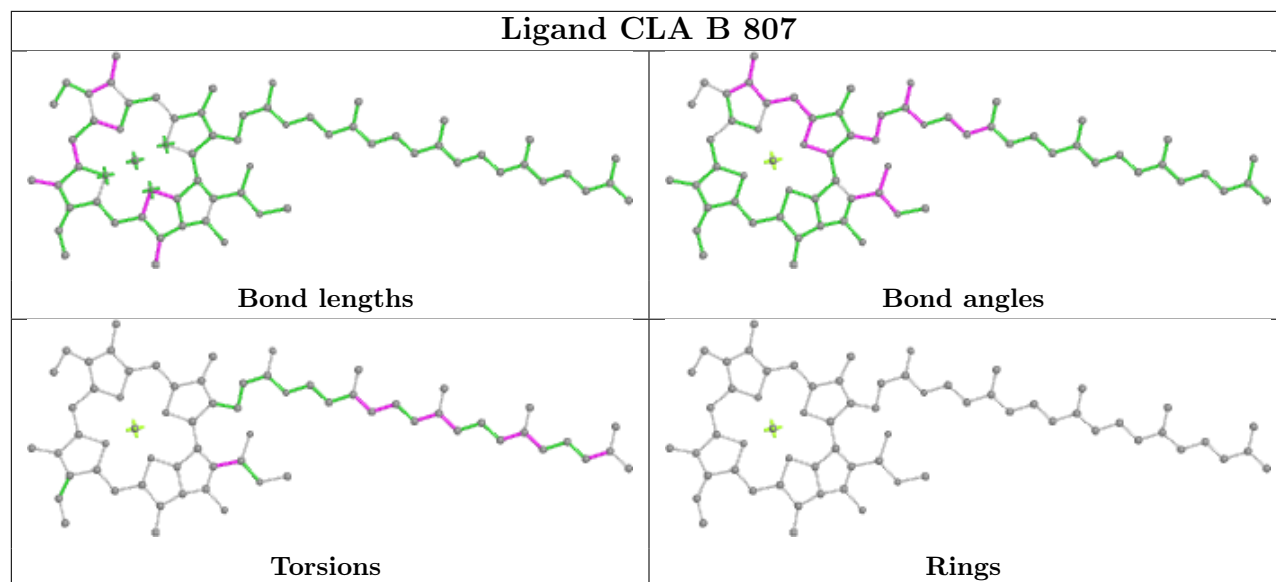
Ligand CLA k 606



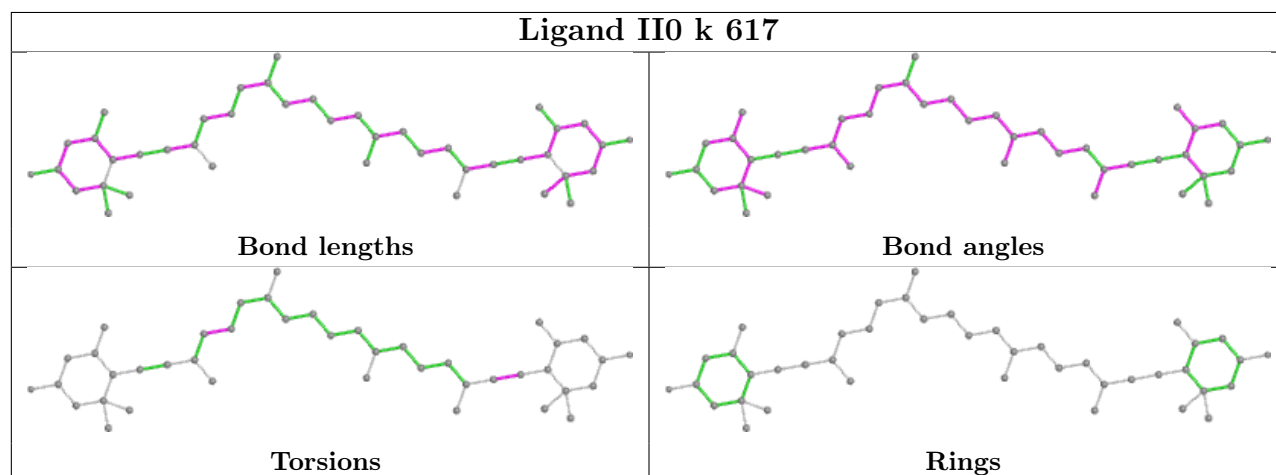
Ligand CLA c 608



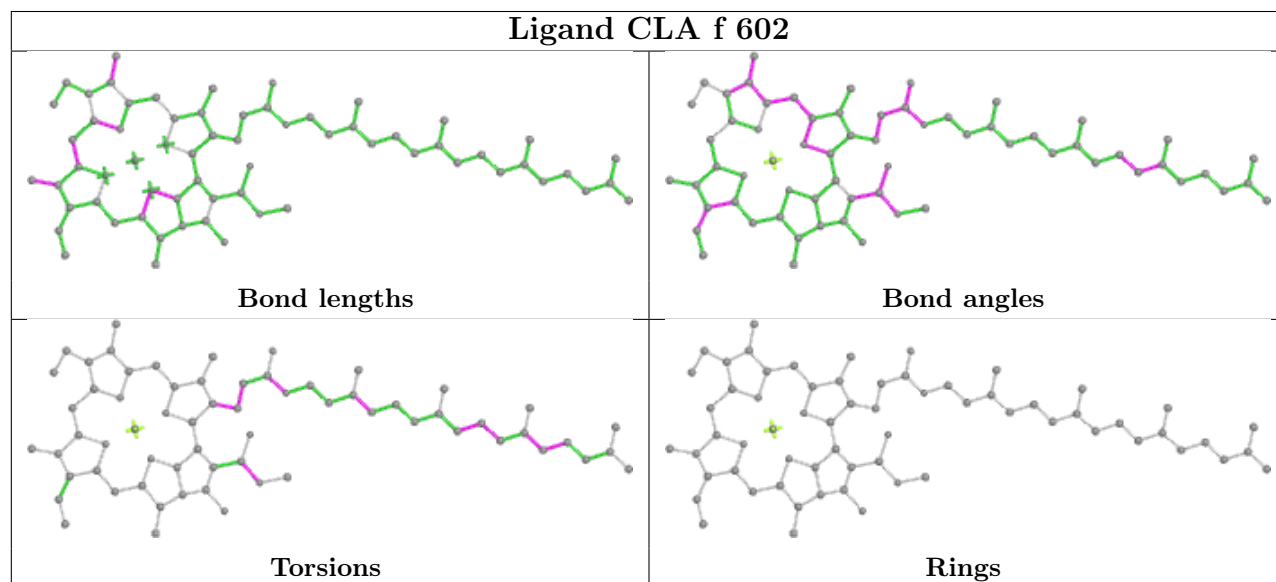
Ligand CLA B 807

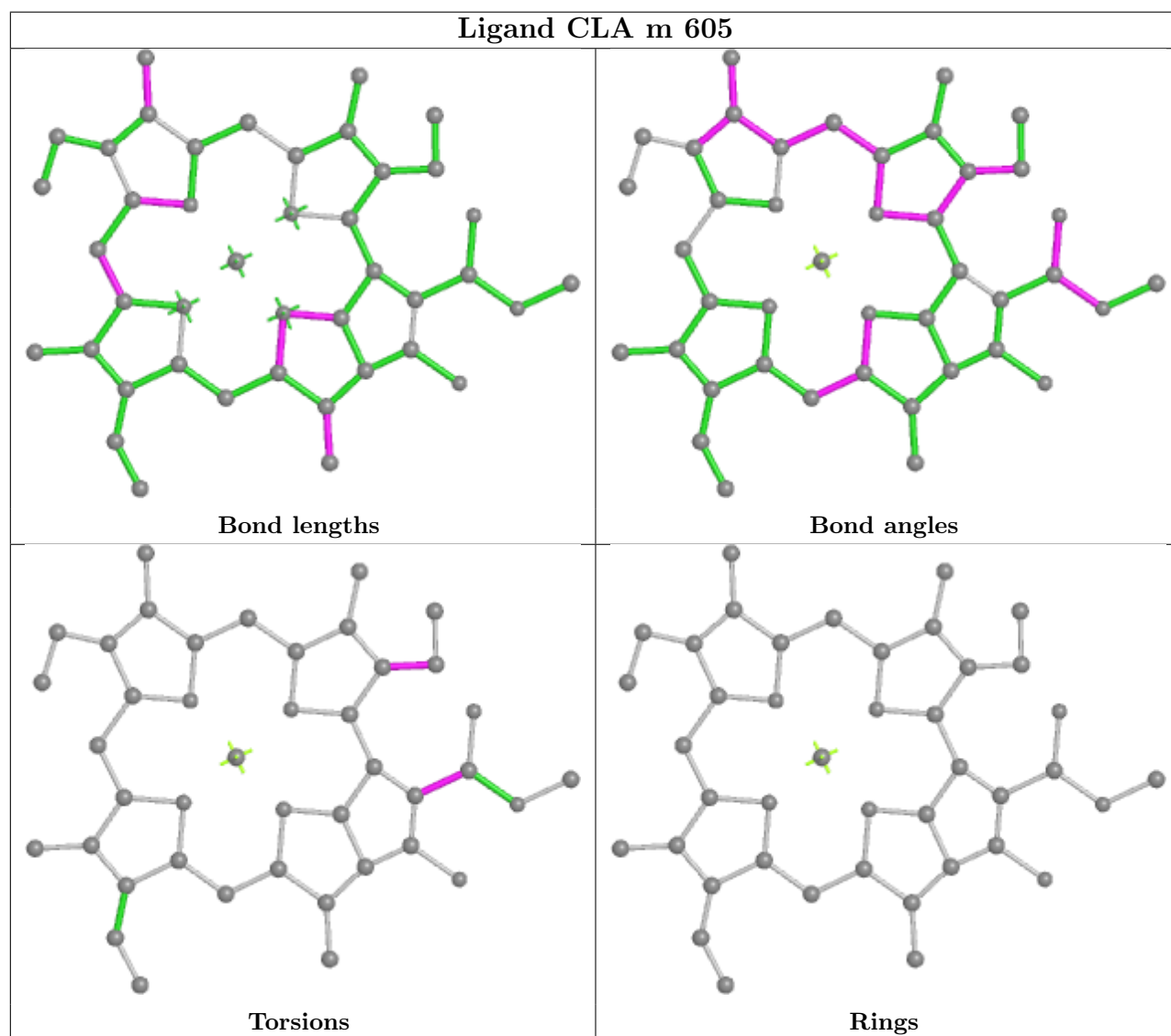
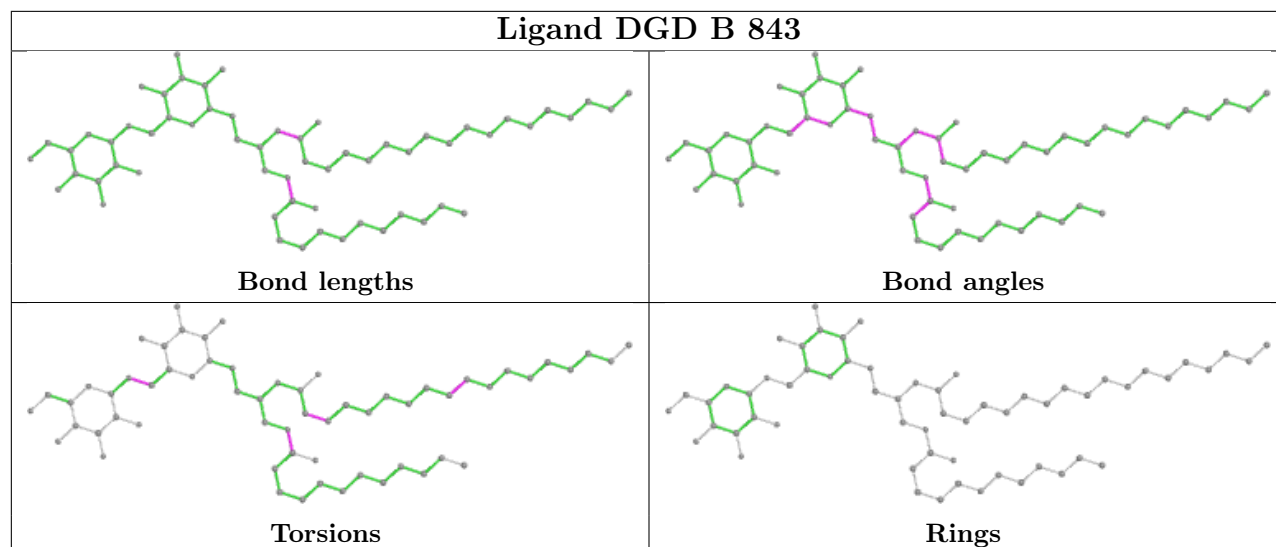


Ligand II0 k 617

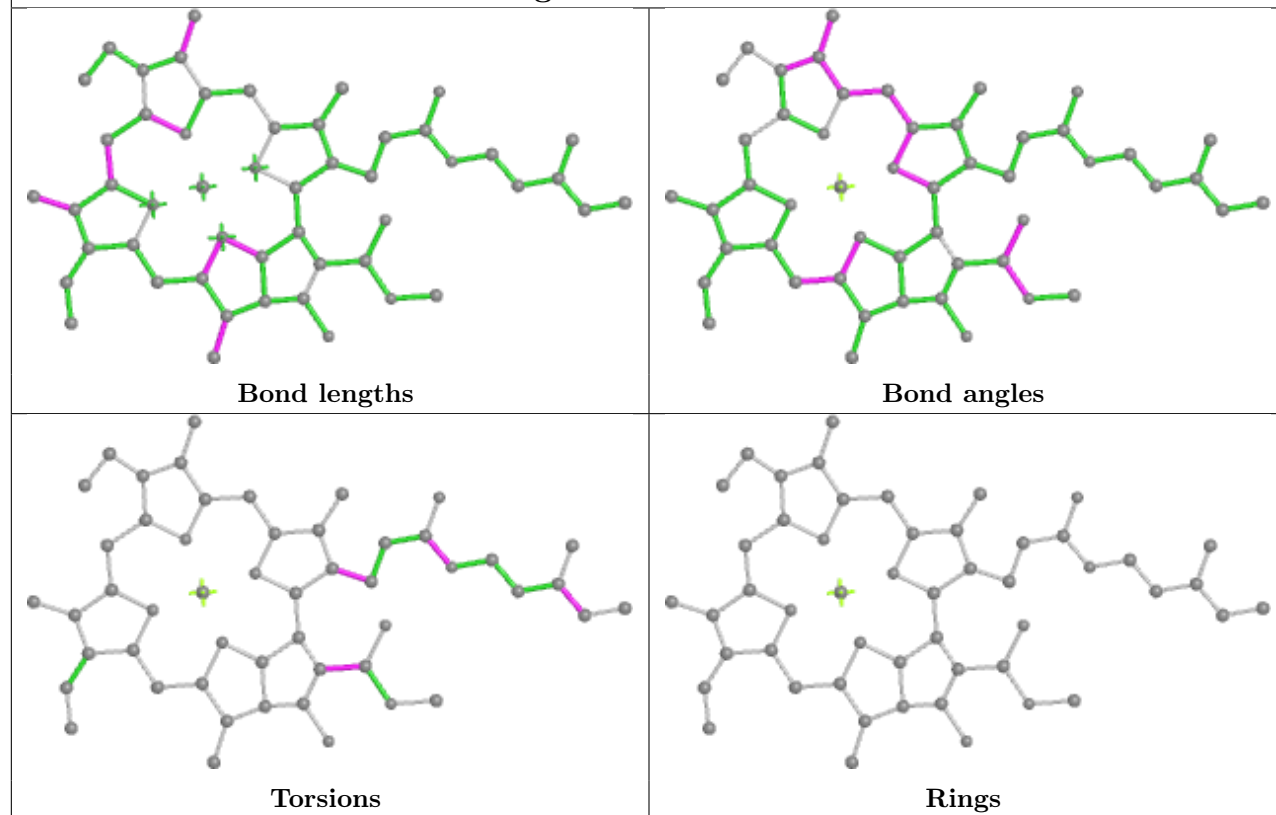


Ligand CLA f 602

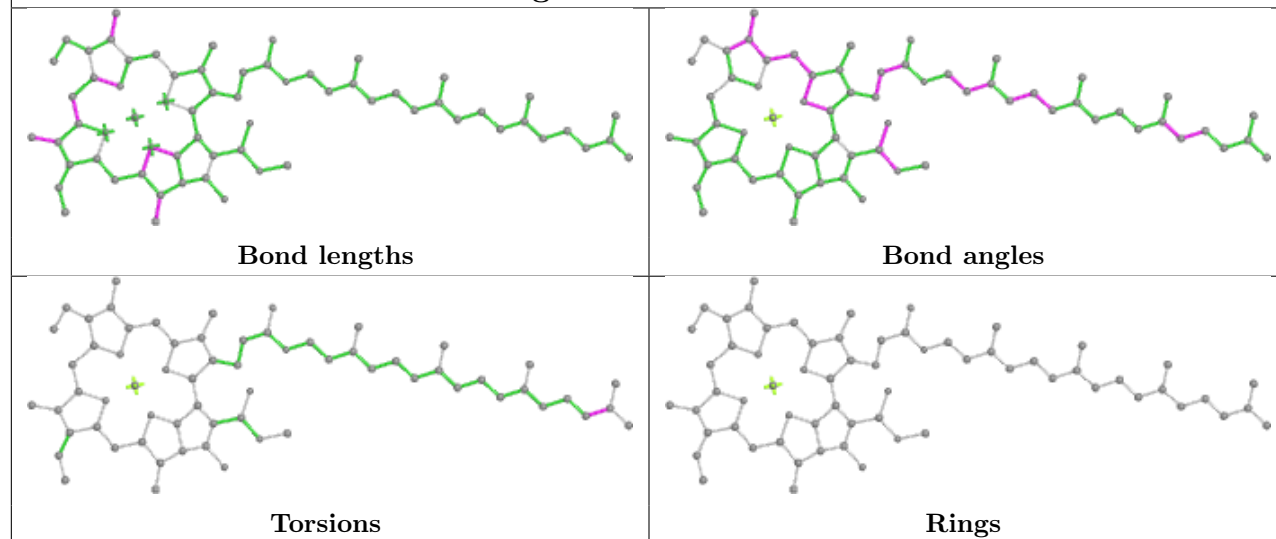




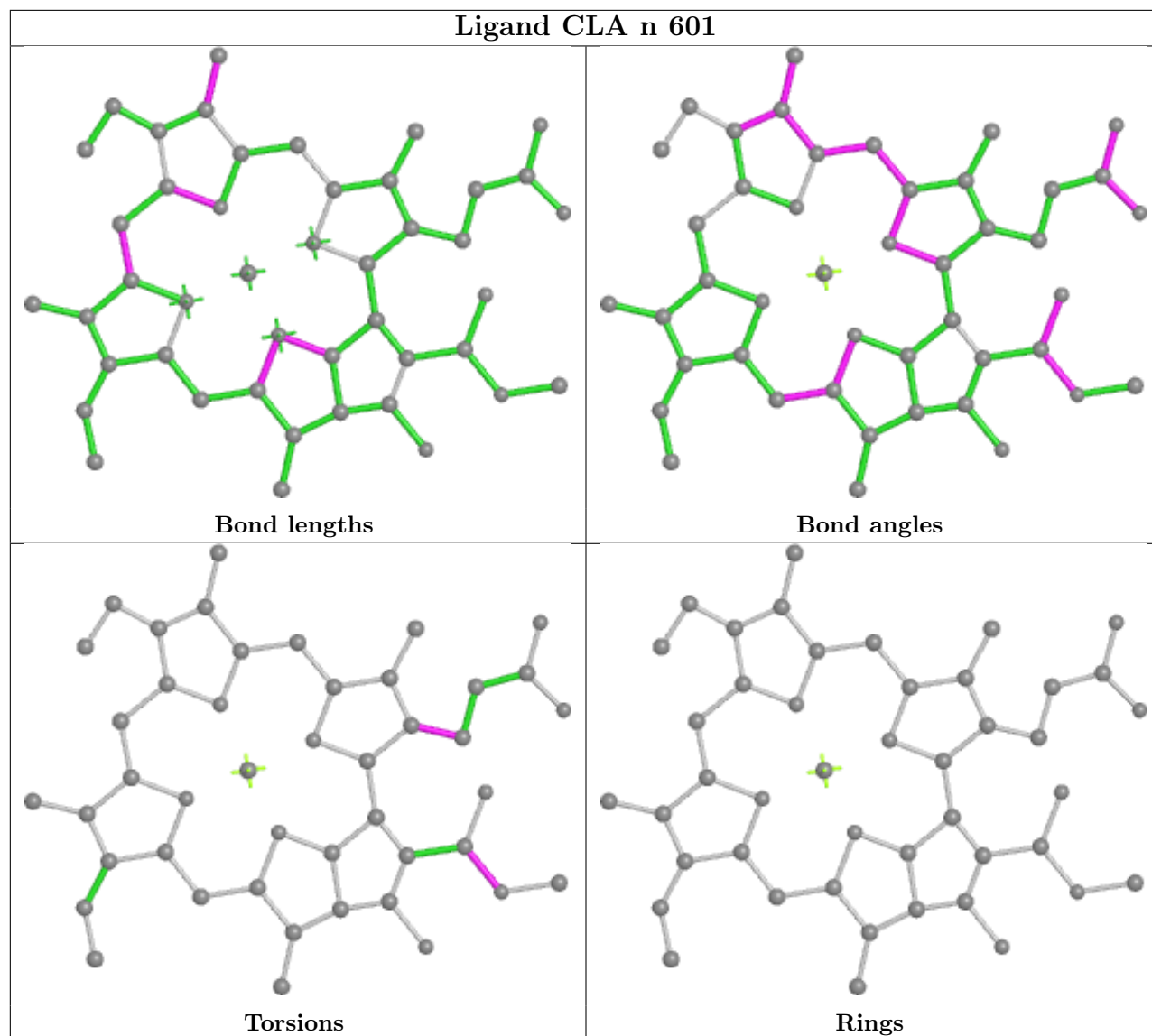
Ligand CLA L 207



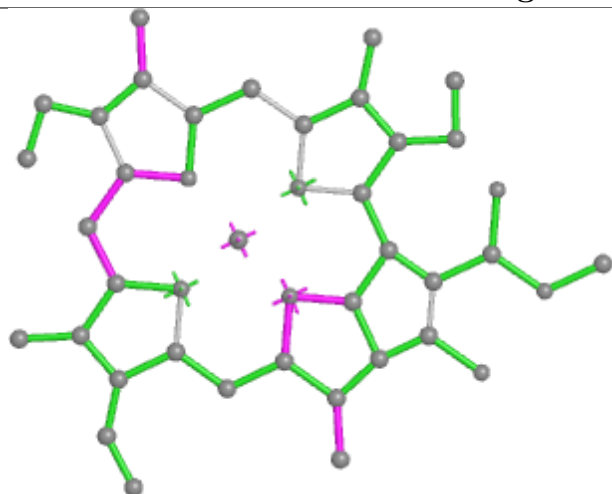
Ligand CLA B 823



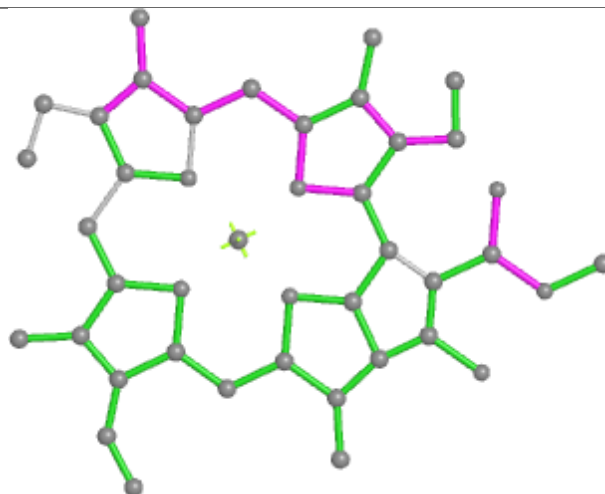
Ligand CLA n 601



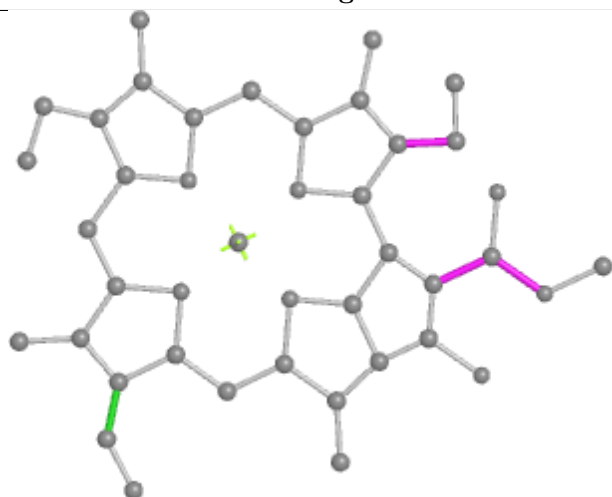
Ligand CLA J 103



Bond lengths



Bond angles

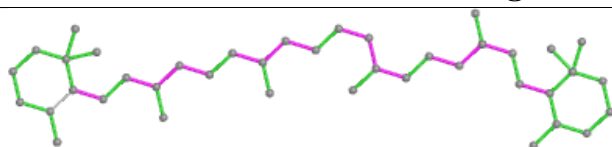


Torsions

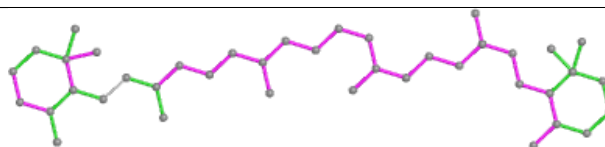


Rings

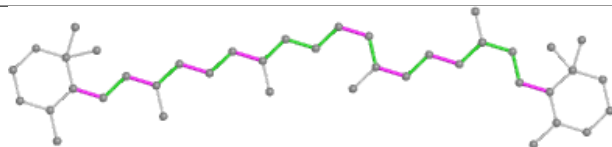
Ligand WVN F 204



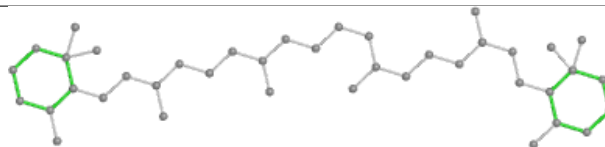
Bond lengths



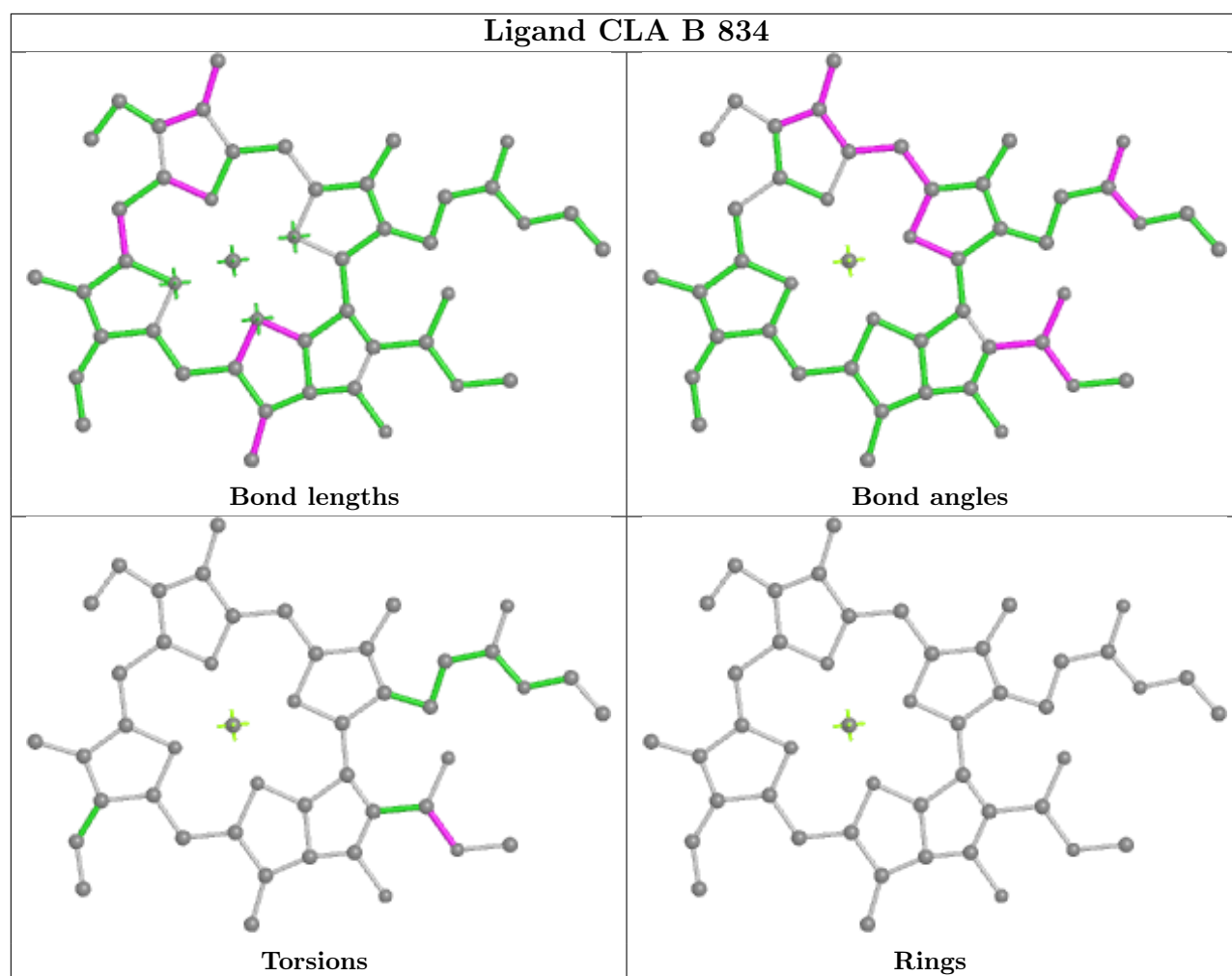
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

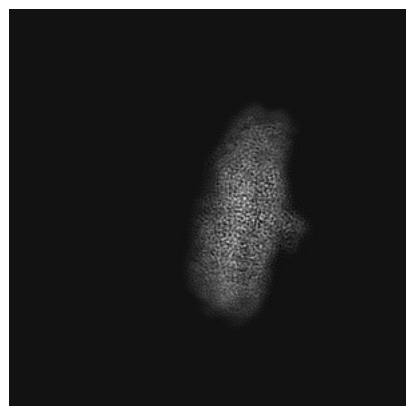
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37642. These allow visual inspection of the internal detail of the map and identification of artifacts.

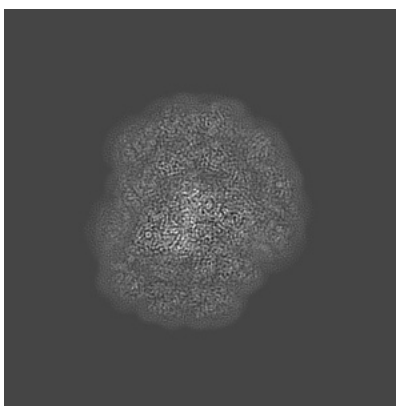
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

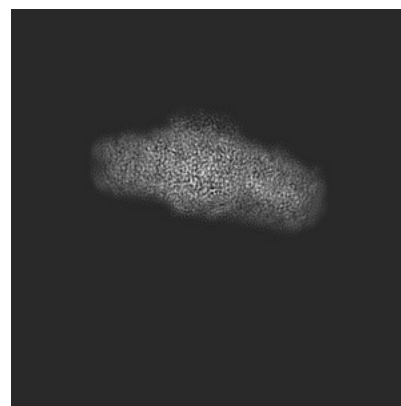
6.1.1 Primary map



X

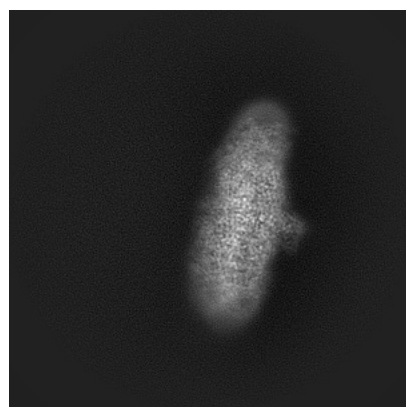


Y

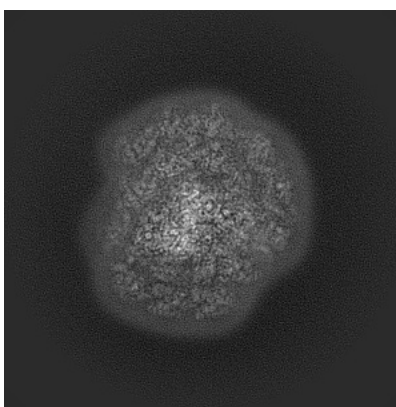


Z

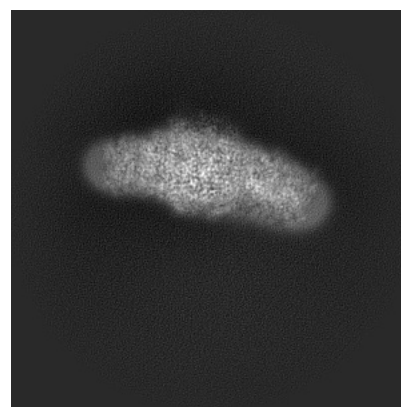
6.1.2 Raw map



X



Y

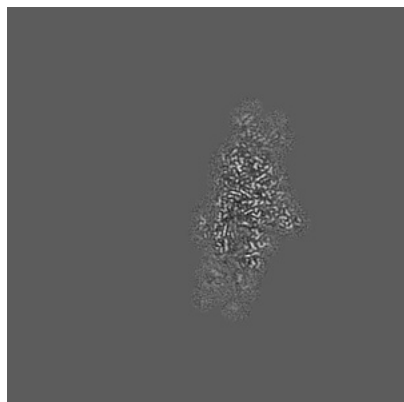


Z

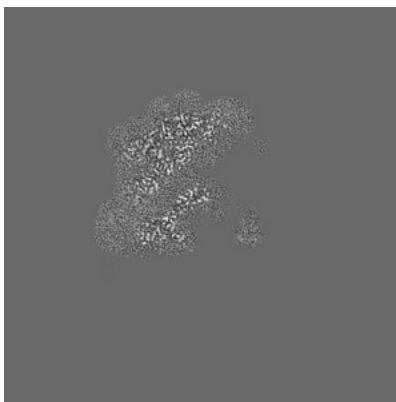
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

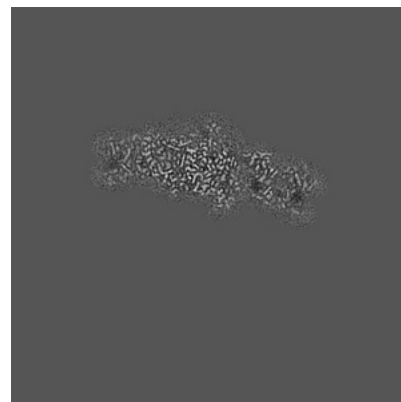
6.2.1 Primary map



X Index: 180

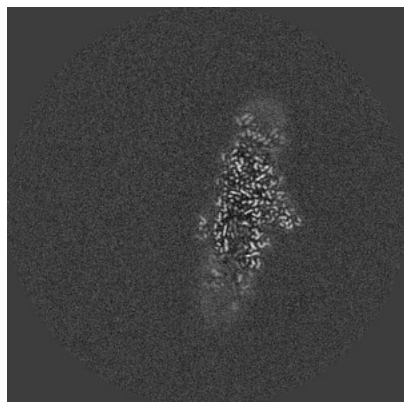


Y Index: 180

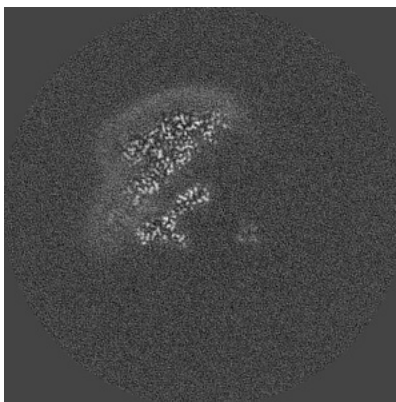


Z Index: 180

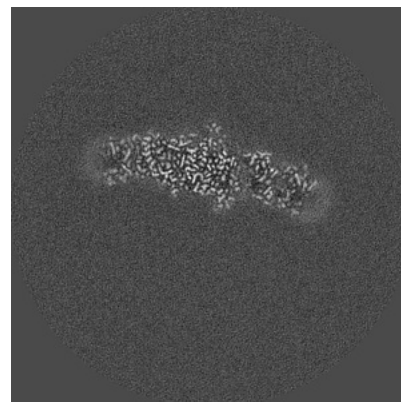
6.2.2 Raw map



X Index: 180



Y Index: 180

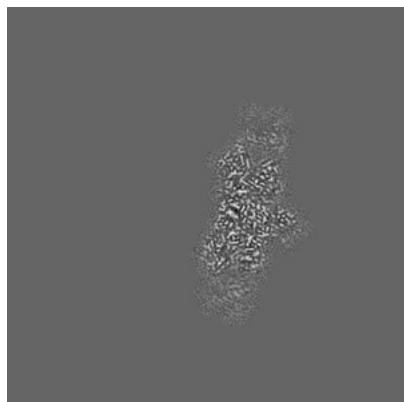


Z Index: 180

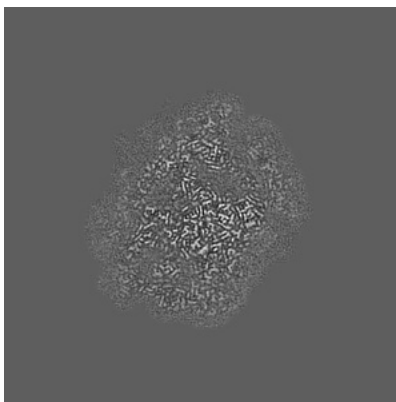
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

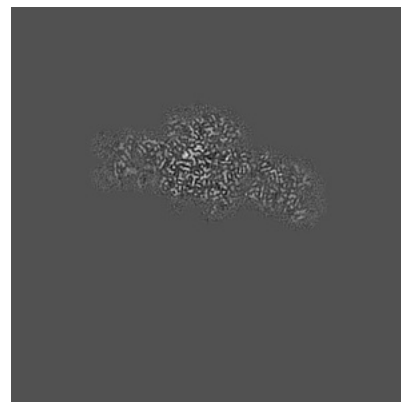
6.3.1 Primary map



X Index: 165

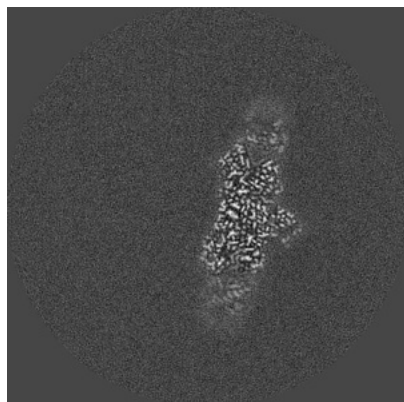


Y Index: 211

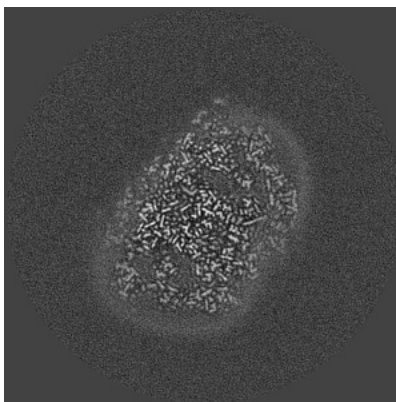


Z Index: 170

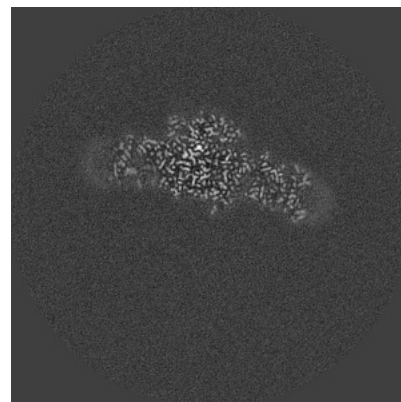
6.3.2 Raw map



X Index: 165



Y Index: 216

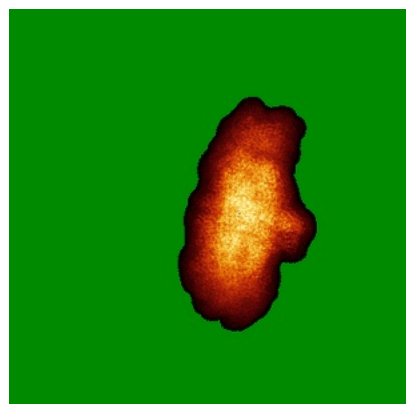


Z Index: 170

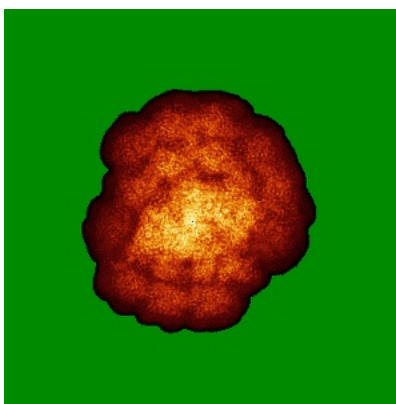
The images above show the largest variance slices of the map in three orthogonal directions.

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

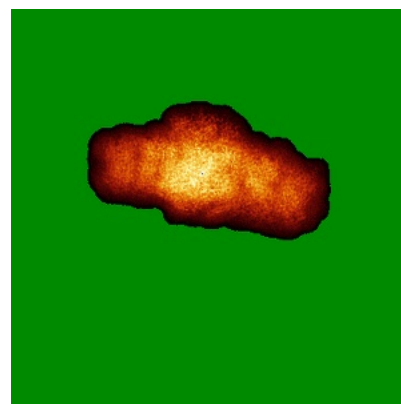
6.4.1 Primary map



X

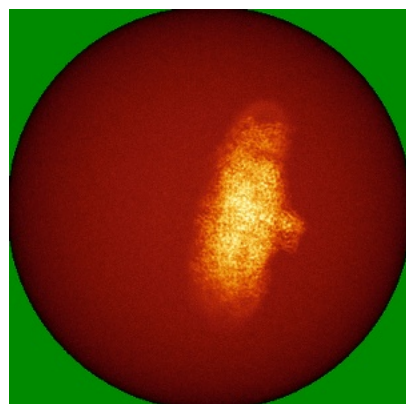


Y

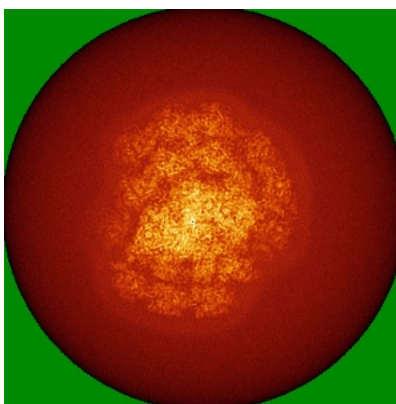


Z

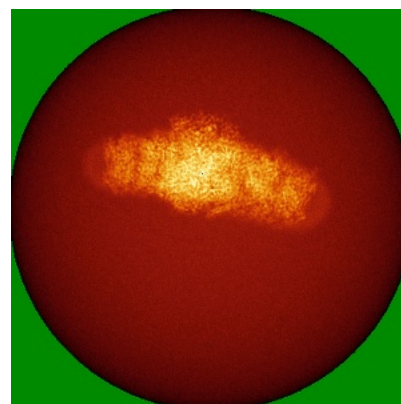
6.4.2 Raw map



X



Y

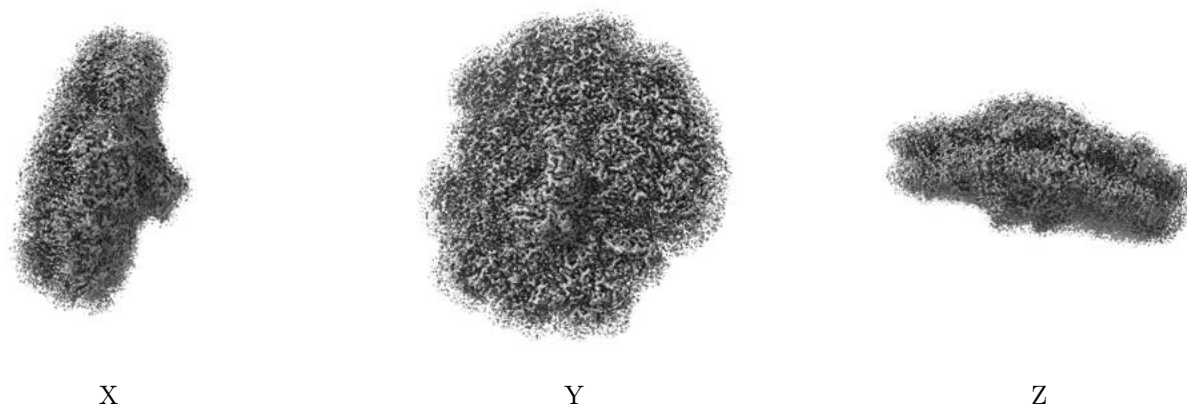


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

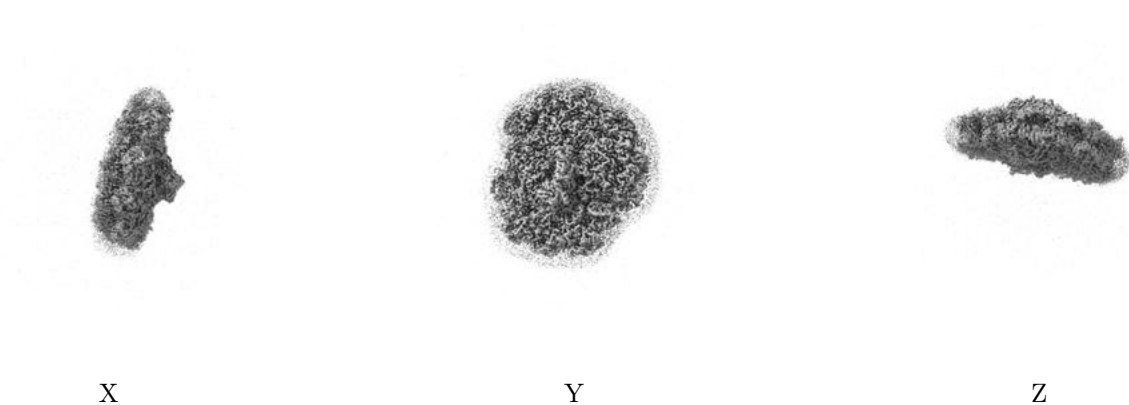
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

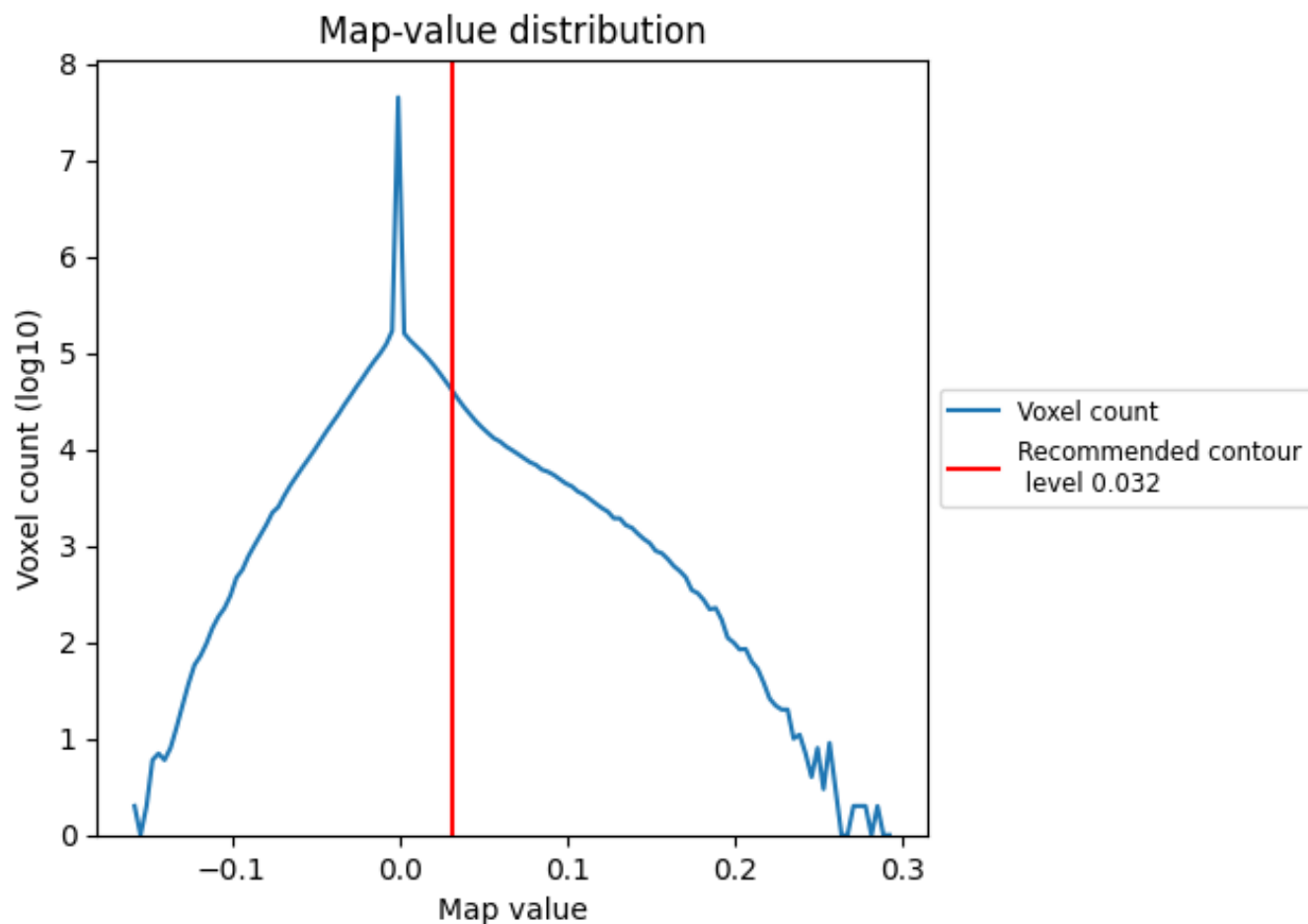
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

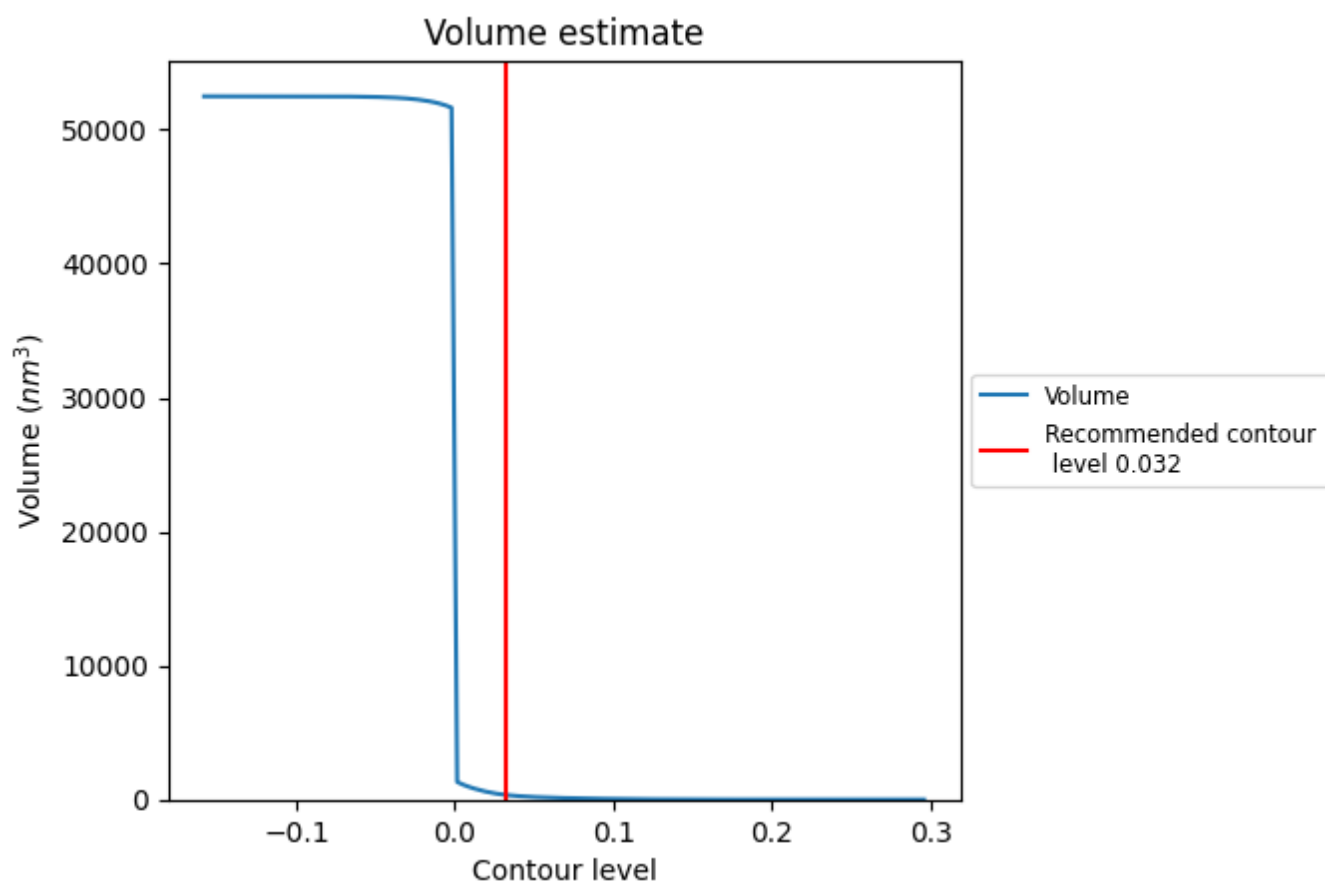
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

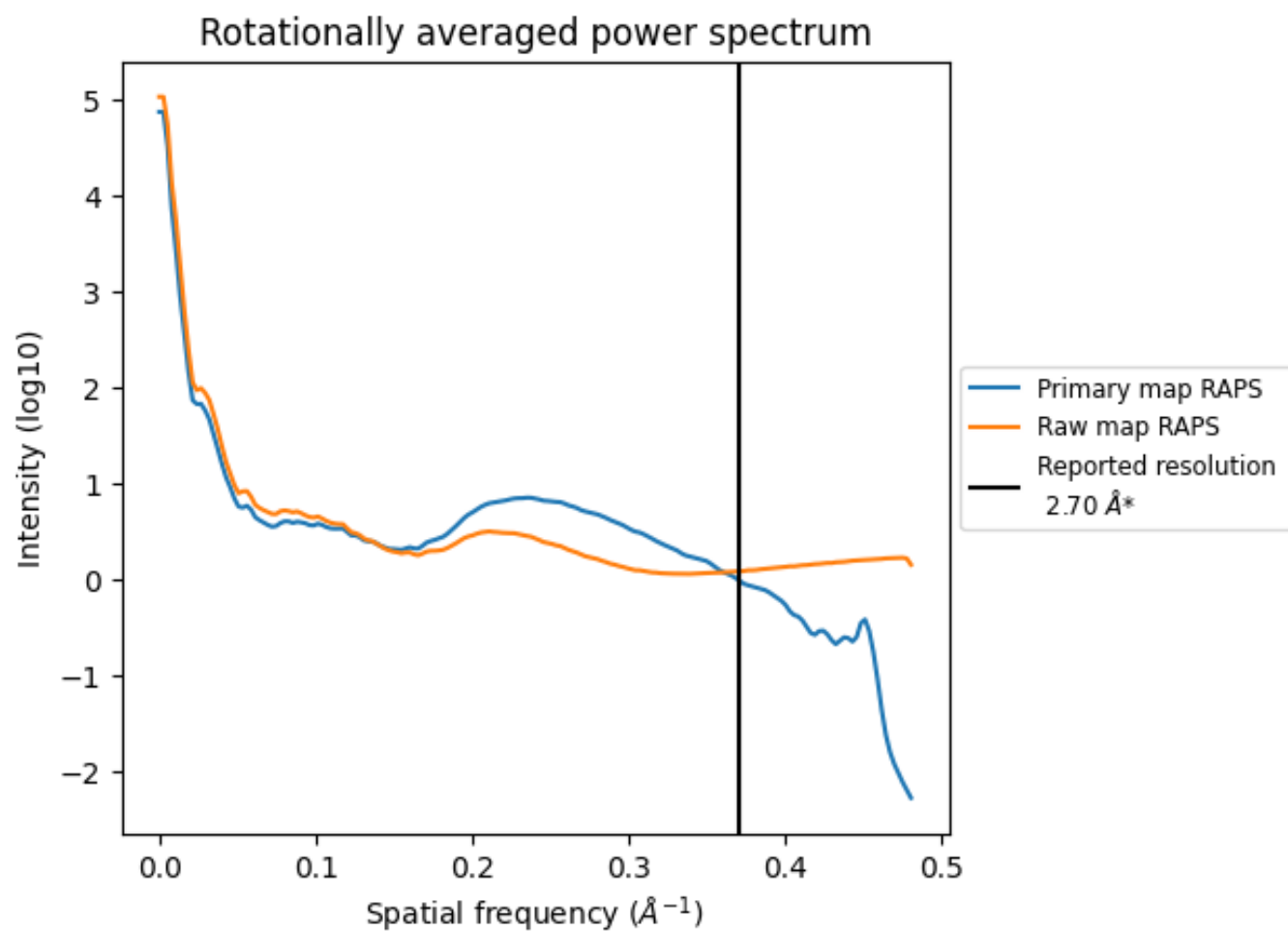
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 349 nm³; this corresponds to an approximate mass of 315 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 ⓘ

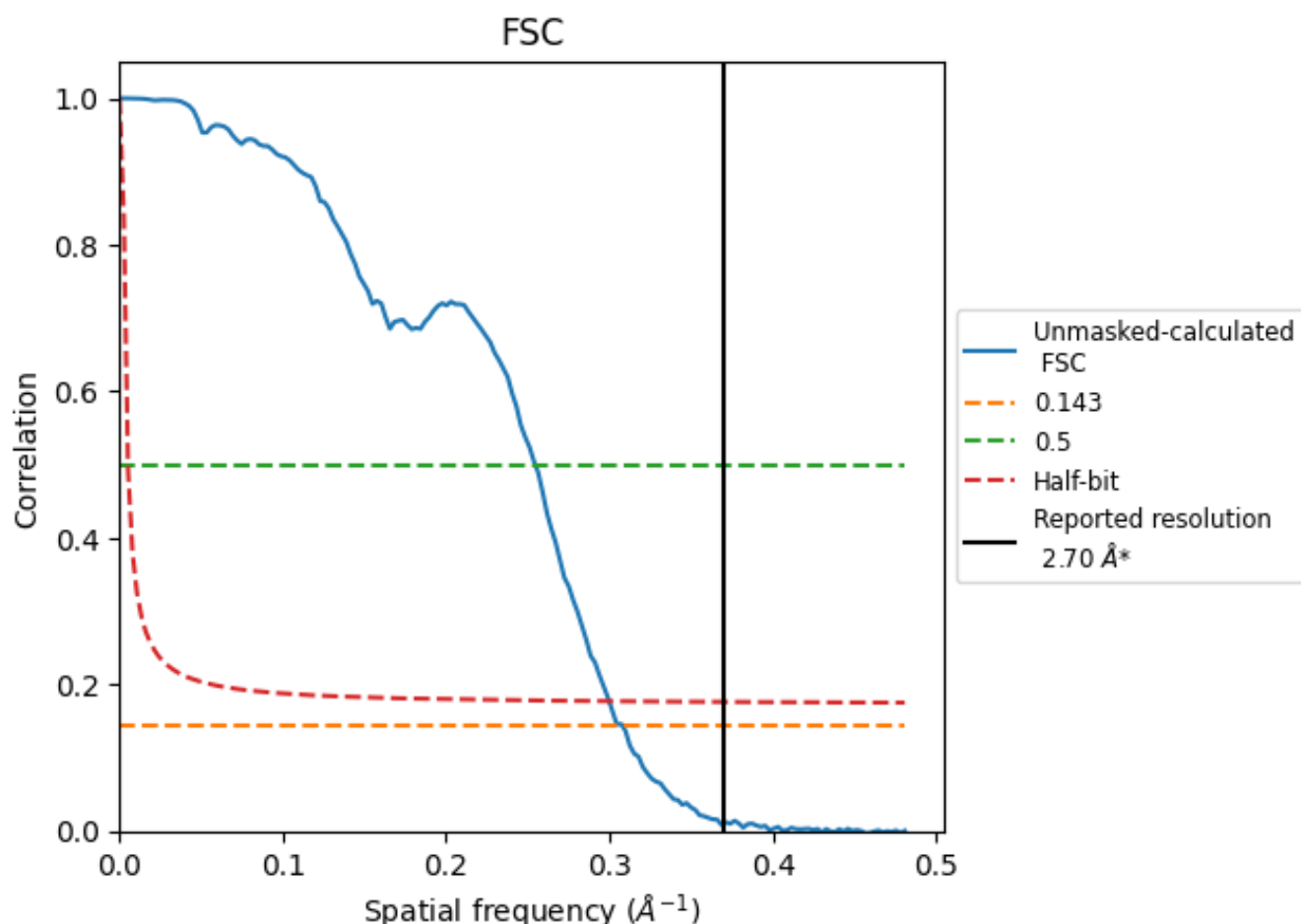


*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

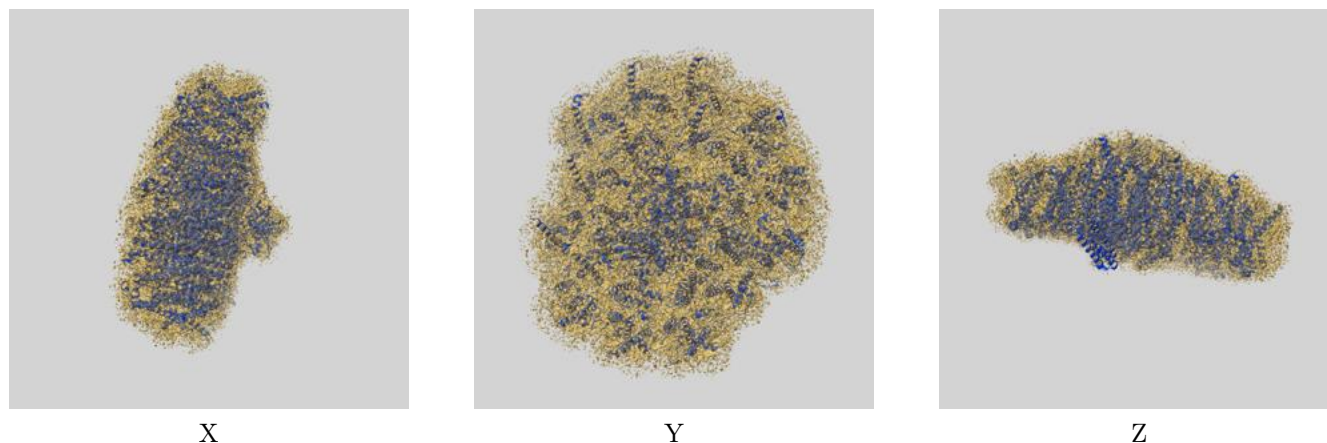
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.25	3.93	3.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

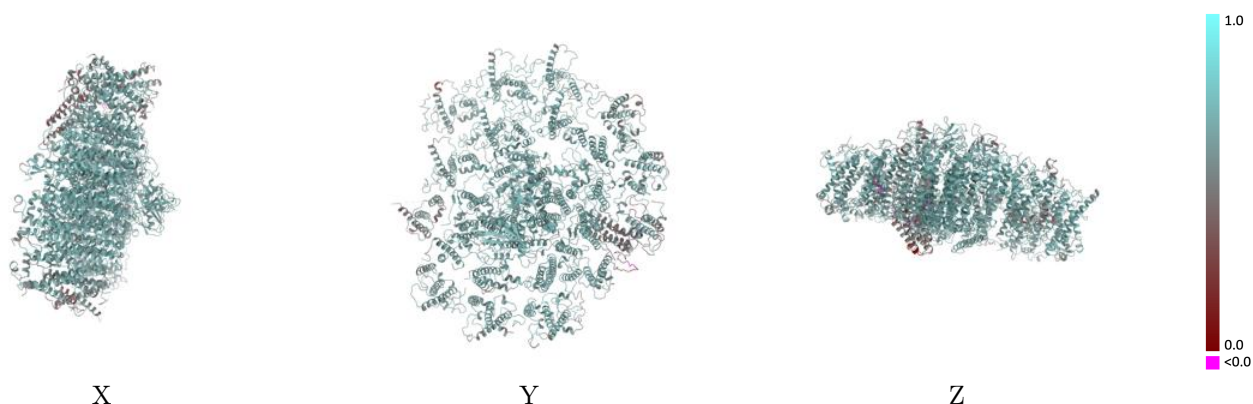
This section contains information regarding the fit between EMDB map EMD-37642 and PDB model 8WM6. Per-residue inclusion information can be found in section [3](#) on page [41](#).

9.1 Map-model overlay [i](#)



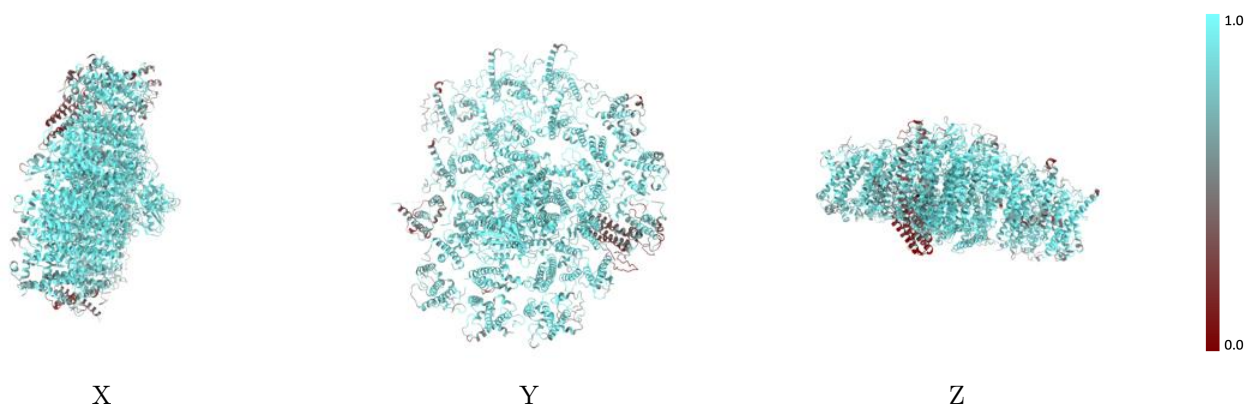
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



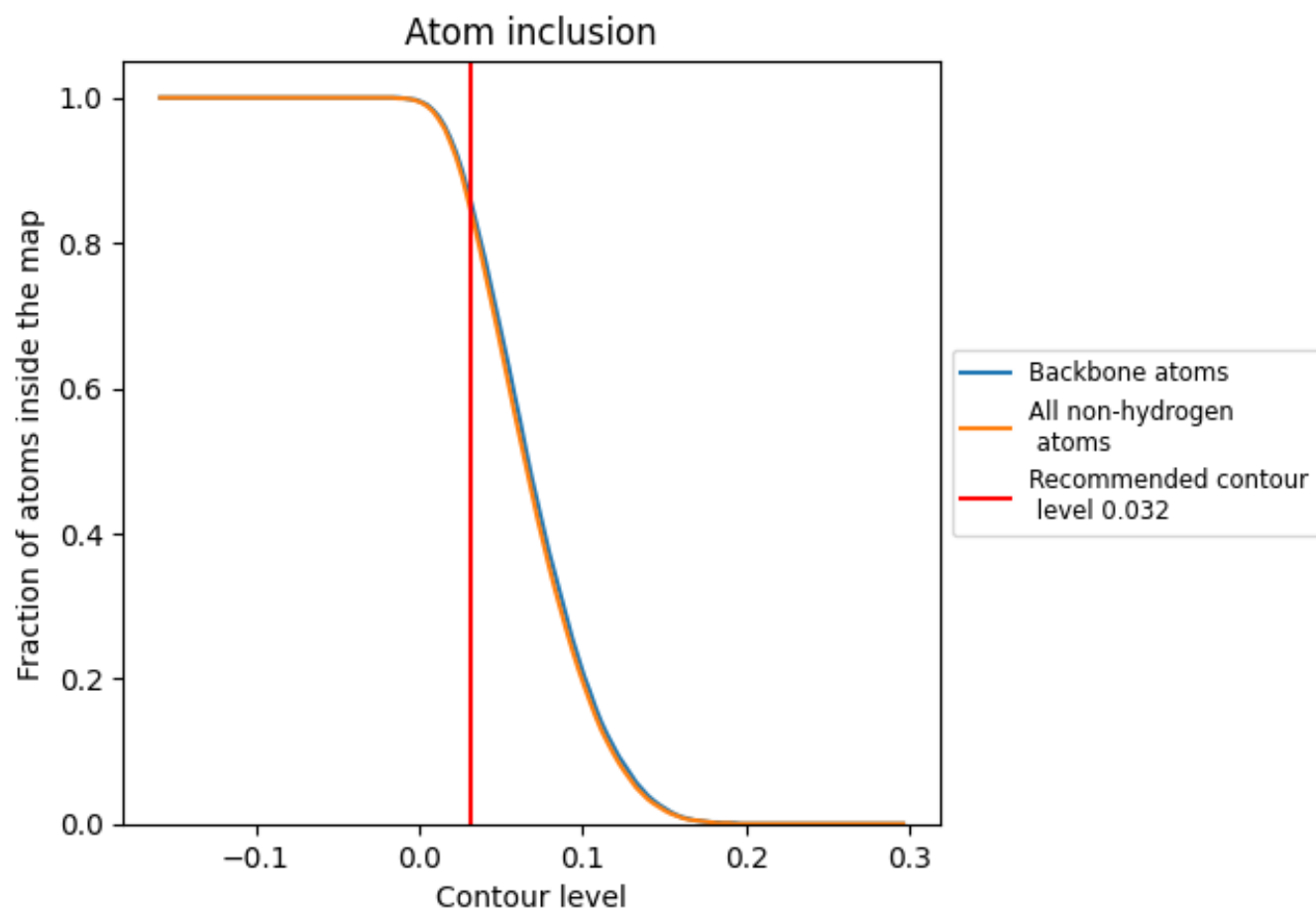
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.032).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.6190
A	 0.9560	 0.6740
B	 0.9620	 0.6780
C	 0.9610	 0.6650
D	 0.8910	 0.6380
E	 0.8590	 0.6300
F	 0.9250	 0.6600
I	 0.9570	 0.6610
J	 0.9210	 0.6630
K	 0.8700	 0.6330
L	 0.9100	 0.6530
M	 0.9480	 0.6580
O	 0.8770	 0.6260
Q	 0.2720	 0.3930
R	 0.9240	 0.6520
a	 0.9190	 0.6430
b	 0.8960	 0.6360
c	 0.7960	 0.5960
d	 0.5010	 0.4930
e	 0.7280	 0.5650
f	 0.8040	 0.6020
g	 0.7870	 0.6040
h	 0.8440	 0.6090
i	 0.6260	 0.5310
j	 0.8130	 0.6040
k	 0.7010	 0.5440
l	 0.8460	 0.6150
m	 0.8580	 0.6220
n	 0.7180	 0.5690
s	 0.8770	 0.6320

