



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2025 – 02:58 PM JST

PDB ID : 9KZ9 / pdb_00009kz9
EMDB ID : EMD-62656
Title : Cryo-EM structure of PSI-ACPI from Rhodomonas sp. NIES-2332 at 2.08 angstroms resolution
Authors : Zhang, W.Y.; Akita, F.; Shen, J.R.
Deposited on : 2024-12-10
Resolution : 2.08 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

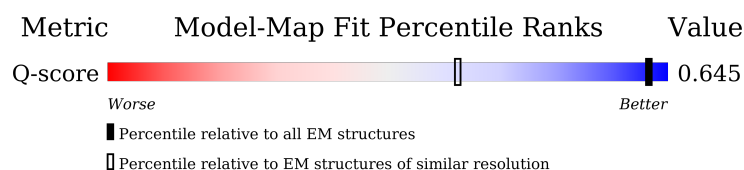
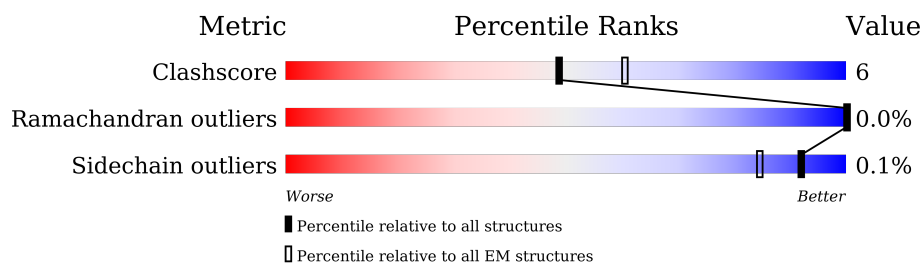
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



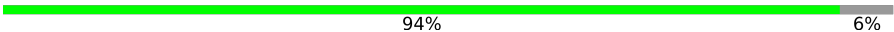











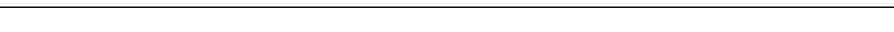

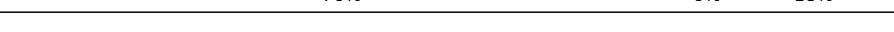

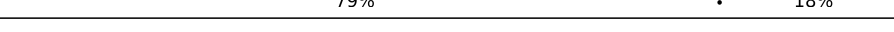








Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	1976 (1.58 - 2.58)

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	<div> <div style="width: 87%;"></div> <div style="width: 11%;"></div> <div style="width: 2%;"></div> </div> <div>87% 11% .</div>
2	B	734	<div> <div style="width: 88%;"></div> <div style="width: 11%;"></div> <div style="width: 1%;"></div> </div> <div>88% 11%</div>
3	C	81	<div> <div style="width: 91%;"></div> <div style="width: 7%;"></div> <div style="width: 2%;"></div> </div> <div>91% 7% .</div>
4	D	141	<div> <div style="width: 87%;"></div> <div style="width: 11%;"></div> <div style="width: 2%;"></div> </div> <div>87% 11% .</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	64	 94% 6%
6	F	188	 79% 7% 14%
7	I	33	 91% 9%
8	J	42	 79% 21%
9	L	153	 89% 9% ..
10	M	30	 90% 10%
11	O	153	 56% 5% • 38%
12	K	86	 70% 9% 21%
13	s	302	 49% • 49%
14	c	215	 67% 12% 21%
15	a	217	 71% 8% 21%
16	b	236	 65% 10% 25%
17	h	229	 66% • 29%
18	f	212	 76% 6% 18%
18	j	212	 70% 11% 18%
18	m	212	 79% • 18%
19	e	210	 72% 7% 21%
20	l	175	 87% 13%
21	k	232	 72% 9% 19%
22	i	200	 78% 11% 10%
23	d	219	 67% 9% 24%
24	g	216	 86% 14%
25	R	135	 61% 6% 33%
26	n	220	 70% 13% 18%
27	Q	233	 59% • 39%

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	CL0	A	801	X	-	-	-
29	CLA	A	802	X	-	-	-
29	CLA	A	803	X	-	-	-
29	CLA	A	804	X	-	-	-
29	CLA	A	805	X	-	-	-
29	CLA	A	806	X	-	-	-
29	CLA	A	807	X	-	-	-
29	CLA	A	808	X	-	-	-
29	CLA	A	809	X	-	-	-
29	CLA	A	810	X	-	-	-
29	CLA	A	811	X	-	-	-
29	CLA	A	812	X	-	-	-
29	CLA	A	813	X	-	-	-
29	CLA	A	814	X	-	-	-
29	CLA	A	815	X	-	-	-
29	CLA	A	816	X	-	-	-
29	CLA	A	817	X	-	-	-
29	CLA	A	818	X	-	-	-
29	CLA	A	819	X	-	-	-
29	CLA	A	820	X	-	-	-
29	CLA	A	821	X	-	-	-
29	CLA	A	822	X	-	-	-
29	CLA	A	823	X	-	-	-
29	CLA	A	824	X	-	-	-
29	CLA	A	825	X	-	-	-
29	CLA	A	826	X	-	-	-
29	CLA	A	827	X	-	-	-
29	CLA	A	828	X	-	-	-
29	CLA	A	829	X	-	-	-
29	CLA	A	830	X	-	-	-
29	CLA	A	831	X	-	-	-
29	CLA	A	832	X	-	-	-
29	CLA	A	833	X	-	-	-
29	CLA	A	834	X	-	-	-
29	CLA	A	835	X	-	-	-
29	CLA	A	836	X	-	-	-
29	CLA	A	837	X	-	-	-
29	CLA	A	838	X	-	-	-
29	CLA	A	839	X	-	-	-
29	CLA	A	840	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	A	850	X	-	-	-
29	CLA	A	851	X	-	-	-
29	CLA	B	801	X	-	-	-
29	CLA	B	802	X	-	-	-
29	CLA	B	803	X	-	-	-
29	CLA	B	804	X	-	-	-
29	CLA	B	805	X	-	-	-
29	CLA	B	806	X	-	-	-
29	CLA	B	807	X	-	-	-
29	CLA	B	808	X	-	-	-
29	CLA	B	809	X	-	-	-
29	CLA	B	810	X	-	-	-
29	CLA	B	811	X	-	-	-
29	CLA	B	812	X	-	-	-
29	CLA	B	813	X	-	-	-
29	CLA	B	814	X	-	-	-
29	CLA	B	815	X	-	-	-
29	CLA	B	816	X	-	-	-
29	CLA	B	817	X	-	-	-
29	CLA	B	818	X	-	-	-
29	CLA	B	819	X	-	-	-
29	CLA	B	820	X	-	-	-
29	CLA	B	821	X	-	-	-
29	CLA	B	822	X	-	-	-
29	CLA	B	823	X	-	-	-
29	CLA	B	824	X	-	-	-
29	CLA	B	825	X	-	-	-
29	CLA	B	826	X	-	-	-
29	CLA	B	827	X	-	-	-
29	CLA	B	828	X	-	-	-
29	CLA	B	829	X	-	-	-
29	CLA	B	830	X	-	-	-
29	CLA	B	831	X	-	-	-
29	CLA	B	832	X	-	-	-
29	CLA	B	833	X	-	-	-
29	CLA	B	834	X	-	-	-
29	CLA	B	835	X	-	-	-
29	CLA	B	836	X	-	-	-
29	CLA	B	837	X	-	-	-
29	CLA	B	838	X	-	-	-
29	CLA	B	839	X	-	-	-
29	CLA	B	840	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	B	841	X	-	-	-
29	CLA	B	842	X	-	-	-
29	CLA	F	201	X	-	-	-
29	CLA	F	202	X	-	-	-
29	CLA	F	203	X	-	-	-
29	CLA	J	102	X	-	-	-
29	CLA	K	101	X	-	-	-
29	CLA	K	102	X	-	-	-
29	CLA	L	202	X	-	-	-
29	CLA	L	203	X	-	-	-
29	CLA	L	204	X	-	-	-
29	CLA	L	207	X	-	-	-
29	CLA	O	201	X	-	-	-
29	CLA	O	202	X	-	-	-
29	CLA	O	206	X	-	-	-
29	CLA	Q	302	X	-	-	-
29	CLA	R	203	X	-	-	-
29	CLA	a	302	X	-	-	-
29	CLA	a	303	X	-	-	-
29	CLA	a	304	X	-	-	-
29	CLA	a	305	X	-	-	-
29	CLA	a	306	X	-	-	-
29	CLA	a	307	X	-	-	-
29	CLA	a	308	X	-	-	-
29	CLA	a	309	X	-	-	-
29	CLA	a	310	X	-	-	-
29	CLA	a	311	X	-	-	-
29	CLA	a	312	X	-	-	-
29	CLA	b	302	X	-	-	-
29	CLA	b	303	X	-	-	-
29	CLA	b	304	X	-	-	-
29	CLA	b	305	X	-	-	-
29	CLA	b	306	X	-	-	-
29	CLA	b	307	X	-	-	-
29	CLA	b	308	X	-	-	-
29	CLA	b	309	X	-	-	-
29	CLA	b	310	X	-	-	-
29	CLA	b	311	X	-	-	-
29	CLA	b	312	X	-	-	-
29	CLA	b	313	X	-	-	-
29	CLA	c	301	X	-	-	-
29	CLA	c	302	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	c	303	X	-	-	-
29	CLA	c	304	X	-	-	-
29	CLA	c	305	X	-	-	-
29	CLA	c	306	X	-	-	-
29	CLA	c	307	X	-	-	-
29	CLA	c	308	X	-	-	-
29	CLA	c	309	X	-	-	-
29	CLA	c	312	X	-	-	-
29	CLA	d	302	X	-	-	-
29	CLA	d	303	X	-	-	-
29	CLA	d	304	X	-	-	-
29	CLA	d	305	X	-	-	-
29	CLA	d	306	X	-	-	-
29	CLA	d	307	X	-	-	-
29	CLA	d	308	X	-	-	-
29	CLA	d	309	X	-	-	-
29	CLA	d	310	X	-	-	-
29	CLA	d	313	X	-	-	-
29	CLA	d	318	X	-	-	-
29	CLA	e	301	X	-	-	-
29	CLA	e	302	X	-	-	-
29	CLA	e	303	X	-	-	-
29	CLA	e	304	X	-	-	-
29	CLA	e	305	X	-	-	-
29	CLA	e	306	X	-	-	-
29	CLA	e	307	X	-	-	-
29	CLA	e	308	X	-	-	-
29	CLA	e	310	X	-	-	-
29	CLA	e	311	X	-	-	-
29	CLA	f	601	X	-	-	-
29	CLA	f	602	X	-	-	-
29	CLA	f	603	X	-	-	-
29	CLA	f	604	X	-	-	-
29	CLA	f	605	X	-	-	-
29	CLA	f	606	X	-	-	-
29	CLA	f	607	X	-	-	-
29	CLA	f	608	X	-	-	-
29	CLA	f	609	X	-	-	-
29	CLA	f	610	X	-	-	-
29	CLA	f	612	X	-	-	-
29	CLA	f	613	X	-	-	-
29	CLA	g	302	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	g	303	X	-	-	-
29	CLA	g	304	X	-	-	-
29	CLA	g	305	X	-	-	-
29	CLA	g	306	X	-	-	-
29	CLA	g	307	X	-	-	-
29	CLA	g	308	X	-	-	-
29	CLA	g	309	X	-	-	-
29	CLA	g	310	X	-	-	-
29	CLA	g	311	X	-	-	-
29	CLA	g	312	X	-	-	-
29	CLA	g	316	X	-	-	-
29	CLA	g	323	X	-	-	-
29	CLA	h	301	X	-	-	-
29	CLA	h	302	X	-	-	-
29	CLA	h	303	X	-	-	-
29	CLA	h	304	X	-	-	-
29	CLA	h	305	X	-	-	-
29	CLA	h	306	X	-	-	-
29	CLA	h	307	X	-	-	-
29	CLA	h	312	X	-	-	-
29	CLA	i	302	X	-	-	-
29	CLA	i	303	X	-	-	-
29	CLA	i	304	X	-	-	-
29	CLA	i	306	X	-	-	-
29	CLA	i	307	X	-	-	-
29	CLA	i	308	X	-	-	-
29	CLA	i	309	X	-	-	-
29	CLA	i	311	X	-	-	-
29	CLA	i	312	X	-	-	-
29	CLA	j	302	X	-	-	-
29	CLA	j	303	X	-	-	-
29	CLA	j	304	X	-	-	-
29	CLA	j	305	X	-	-	-
29	CLA	j	306	X	-	-	-
29	CLA	j	307	X	-	-	-
29	CLA	j	308	X	-	-	-
29	CLA	j	309	X	-	-	-
29	CLA	j	310	X	-	-	-
29	CLA	j	311	X	-	-	-
29	CLA	j	313	X	-	-	-
29	CLA	j	314	X	-	-	-
29	CLA	k	601	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	k	602	X	-	-	-
29	CLA	k	603	X	-	-	-
29	CLA	k	604	X	-	-	-
29	CLA	k	605	X	-	-	-
29	CLA	k	606	X	-	-	-
29	CLA	k	607	X	-	-	-
29	CLA	k	608	X	-	-	-
29	CLA	k	609	X	-	-	-
29	CLA	k	610	X	-	-	-
29	CLA	k	614	X	-	-	-
29	CLA	l	301	X	-	-	-
29	CLA	l	303	X	-	-	-
29	CLA	l	304	X	-	-	-
29	CLA	l	305	X	-	-	-
29	CLA	l	306	X	-	-	-
29	CLA	l	307	X	-	-	-
29	CLA	l	308	X	-	-	-
29	CLA	l	309	X	-	-	-
29	CLA	l	310	X	-	-	-
29	CLA	l	312	X	-	-	-
29	CLA	m	601	X	-	-	-
29	CLA	m	602	X	-	-	-
29	CLA	m	603	X	-	-	-
29	CLA	m	604	X	-	-	-
29	CLA	m	605	X	-	-	-
29	CLA	m	606	X	-	-	-
29	CLA	m	607	X	-	-	-
29	CLA	m	608	X	-	-	-
29	CLA	m	609	X	-	-	-
29	CLA	m	610	X	-	-	-
29	CLA	m	612	X	-	-	-
29	CLA	m	613	X	-	-	-
29	CLA	n	601	X	-	-	-
29	CLA	n	602	X	-	-	-
29	CLA	n	603	X	-	-	-
29	CLA	n	604	X	-	-	-
29	CLA	n	605	X	-	-	-
29	CLA	n	606	X	-	-	-
29	CLA	n	607	X	-	-	-
29	CLA	n	608	X	-	-	-
29	CLA	n	609	X	-	-	-
29	CLA	n	610	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	n	613	X	-	-	-
29	CLA	s	402	X	-	-	-
29	CLA	s	403	X	-	-	-
29	CLA	s	406	X	-	-	-
32	WVN	A	844	-	X	-	-
32	WVN	A	845	-	X	-	-
32	WVN	A	846	-	X	-	-
32	WVN	A	847	-	X	-	-
32	WVN	A	854	-	X	-	-
32	WVN	B	847	-	X	-	-
32	WVN	B	848	-	X	-	-
32	WVN	B	849	-	X	-	-
32	WVN	F	204	-	X	-	-
32	WVN	F	205	-	X	-	-
32	WVN	F	207	-	X	-	-
32	WVN	I	101	-	X	-	-
32	WVN	J	101	-	X	-	-
32	WVN	K	103	-	X	-	-
32	WVN	L	201	-	X	-	-
32	WVN	L	205	-	X	-	-
32	WVN	L	206	-	X	-	-
32	WVN	M	101	-	X	-	-
32	WVN	R	201	-	X	-	-
32	WVN	R	202	-	X	-	-
32	WVN	e	315	-	X	-	-
32	WVN	h	308	-	X	-	-
32	WVN	i	315	-	X	-	-
32	WVN	l	302	-	X	-	-
32	WVN	l	316	-	X	-	-
32	WVN	s	407	-	X	-	-
38	II0	h	309	-	X	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 61938 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
			5826	3805	994	999	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	2	0
			5832	3849	982	987	14		

- 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	138	Total	C	N	O	S	0	0
			1075	687	185	200	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
			1257	818	213	224	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	33	Total	C	N	O	S	0	0
			255	177	34	42	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	1	0
			1158	763	183	209	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	95	Total	C	N	O	S	0	0
			714	480	107	124	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	68	Total	C	N	O	S	0	0
			482	316	79	85	2		

- Molecule 13 is a protein called ACPI-s.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	s	154	Total	C	N	O	S	0	0
			1146	725	195	219	7		

- Molecule 14 is a protein called ACPI-c.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	170	Total	C	N	O	S	0	0
			1362	899	222	238	3		

- Molecule 15 is a protein called ACPI-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	172	Total	C	N	O	S	0	0
			1331	865	213	242	11		

- Molecule 16 is a protein called ACPI-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	b	178	Total	C	N	O	S	0	0
			1332	847	234	238	13		

- Molecule 17 is a protein called ACPI-h.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	h	162	Total	C	N	O	S	0	0
			1201	779	202	214	6		

- Molecule 18 is a protein called ACPI-m,f,j.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	m	174	Total	C	N	O	S	0	0
			1313	850	217	238	8		
18	f	174	Total	C	N	O	S	0	0
			1306	846	215	237	8		
18	j	173	Total	C	N	O	S	0	0
			1302	841	216	237	8		

- Molecule 19 is a protein called ACPI-e.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	166	Total	C	N	O	S	0	0
			1268	822	209	228	9		

- Molecule 20 is a protein called ACPI-l.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	175	Total	C	N	O	S	0	0
			1333	859	227	239	8		

- Molecule 21 is a protein called ACPI-k.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	k	189	Total	C	N	O	S	0	0
			1412	916	241	246	9		

- Molecule 22 is a protein called ACPI-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	i	180	Total	C	N	O	S	0	0
			1363	874	231	247	11		

- Molecule 23 is a protein called ACPI-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	166	Total	C	N	O	S	0	0
			1231	788	210	220	13		

- Molecule 24 is a protein called ACPI-g.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	g	216	Total	C	N	O	S	0	0
			1608	1047	265	285	11		

- Molecule 25 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	90	Total	C	N	O	S	0	0
			666	434	105	125	2		

- Molecule 26 is a protein called ACPI-n.

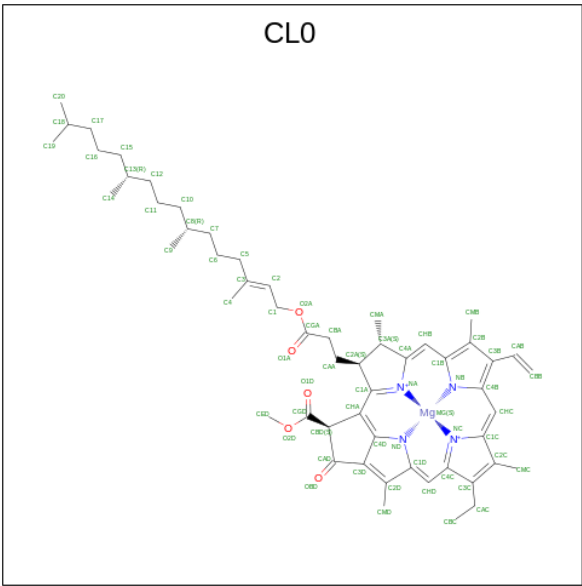
Mol	Chain	Residues	Atoms					AltConf	Trace
26	n	181	Total	C	N	O	S	0	0
			1343	862	226	245	10		

- Molecule 27 is a protein called PsaQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	143	Total	C	N	O	S	0	0
			1041	654	179	203	5		

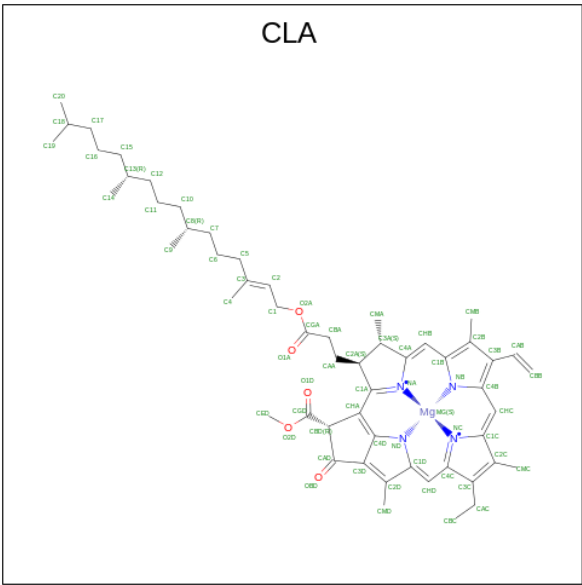
- Molecule 28 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$)

(labeled as "Ligand of Interest" by depositor).



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

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



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	F	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	L	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
29	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 61	C 51	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	h	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	m	1	Total 59	C 49	Mg 1	N 4	O 5	0
29	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	m	1	Total 51	C 41	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	m	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	m	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	l	1	Total 61	C 51	Mg 1	N 4	O 5	0
29	l	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	k	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	f	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	f	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	f	1	Total 51	C 41	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	f	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	i	1	Total 61	C 51	Mg 1	N 4	O 5	0
29	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	i	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	i	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	j	1	Total 54	C 44	Mg 1	N 4	O 5	0
29	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	j	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	j	1	Total 61	C 51	Mg 1	N 4	O 5	0
29	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	d	1	Total 62	C 52	Mg 1	N 4	O 5	0
29	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	d	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

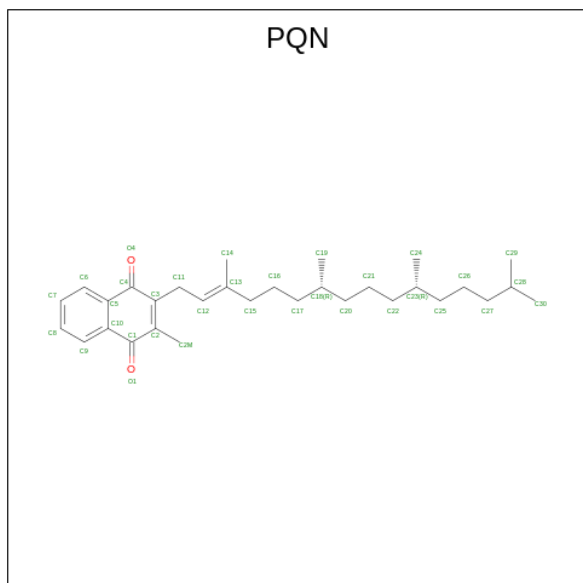
Mol	Chain	Residues	Atoms					AltConf
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 54	C 44	Mg 1	N 4	O 5	0
29	g	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	n	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	n	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	n	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 60	C 50	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

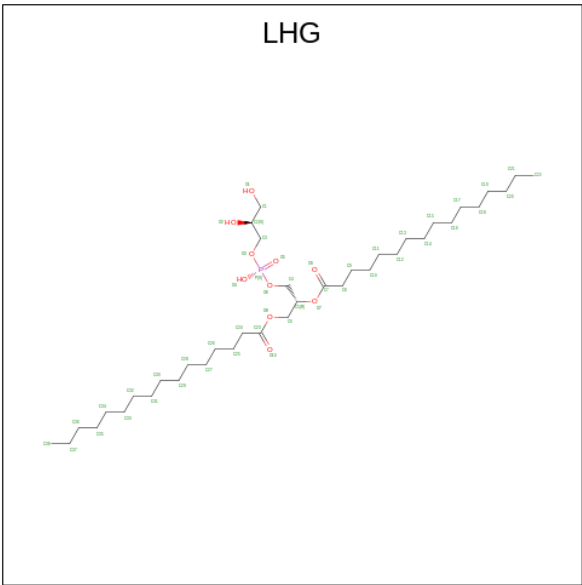
Mol	Chain	Residues	Atoms					AltConf
29	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 30 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



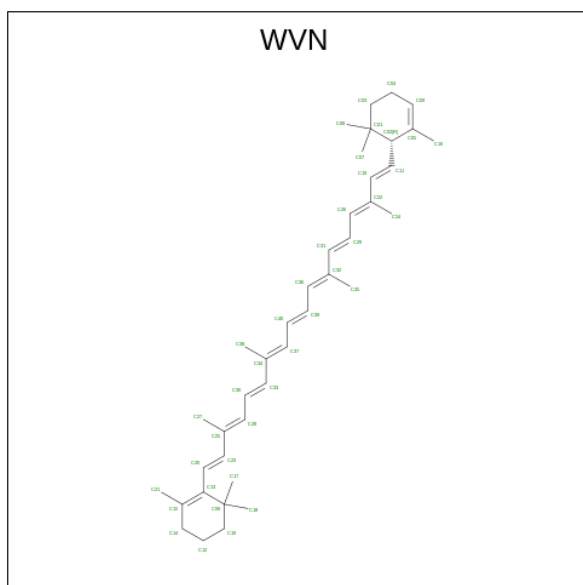
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	P	0
			48	37	10	1	
31	A	1	Total	C	O	P	0
			27	16	10	1	
31	A	1	Total	C	O	P	0
			27	20	6	1	
31	J	1	Total	C	O	P	0
			33	22	10	1	
31	L	1	Total	C	O	P	0
			47	36	10	1	
31	L	1	Total	C	O	P	0
			36	25	10	1	
31	s	1	Total	C	O	P	0
			33	24	8	1	
31	c	1	Total	C	O	P	0
			37	26	10	1	
31	c	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			49	38	10	1	
31	b	1	Total	C	O	P	0
			49	38	10	1	
31	m	1	Total	C	O	P	0
			37	26	10	1	
31	e	1	Total	C	O	P	0
			37	26	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
31	l	1	Total	C	O	P	0
			32	21	10	1	
31	f	1	Total	C	O	P	0
			49	38	10	1	
31	f	1	Total	C	O	P	0
			37	26	10	1	
31	i	1	Total	C	O	P	0
			37	26	10	1	
31	j	1	Total	C	O	P	0
			30	19	10	1	
31	g	1	Total	C	O	P	0
			45	34	10	1	
31	g	1	Total	C	O	P	0
			37	26	10	1	
31	n	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 32 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 (CCD ID: WVN) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	C	0
			40	40	
32	A	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

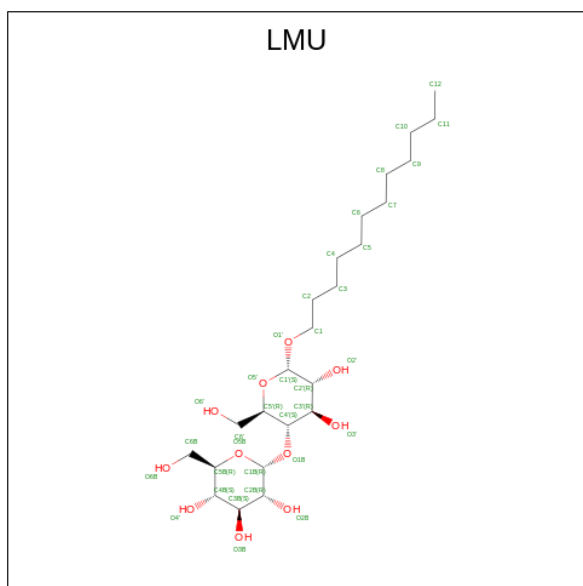
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	F	1	Total C 40 40	0
32	F	1	Total C 40 40	0
32	F	1	Total C 40 40	0
32	I	1	Total C 40 40	0
32	J	1	Total C 40 40	0
32	L	1	Total C 40 40	0
32	L	1	Total C 40 40	0
32	L	1	Total C 40 40	0
32	M	1	Total C 40 40	0
32	K	1	Total C 40 40	0
32	s	1	Total C 40 40	0
32	s	1	Total C 40 40	0
32	h	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

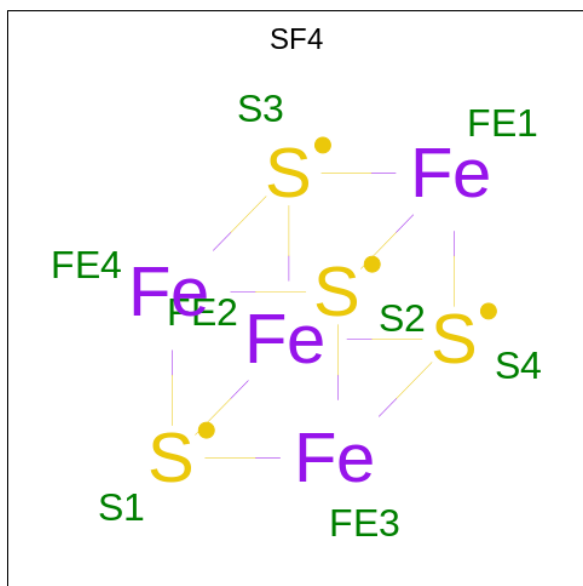
Mol	Chain	Residues	Atoms	AltConf
32	e	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	i	1	Total C 40 40	0
32	R	1	Total C 40 40	0
32	R	1	Total C 40 40	0

- Molecule 33 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



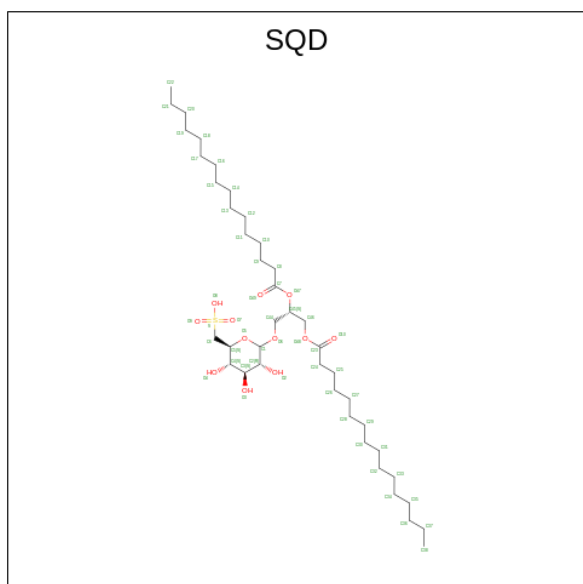
Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C O 35 24 11	0
33	A	1	Total C O 34 23 11	0
33	B	1	Total C O 35 24 11	0
33	a	1	Total C O 35 24 11	0
33	i	1	Total C O 35 24 11	0

- Molecule 34 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



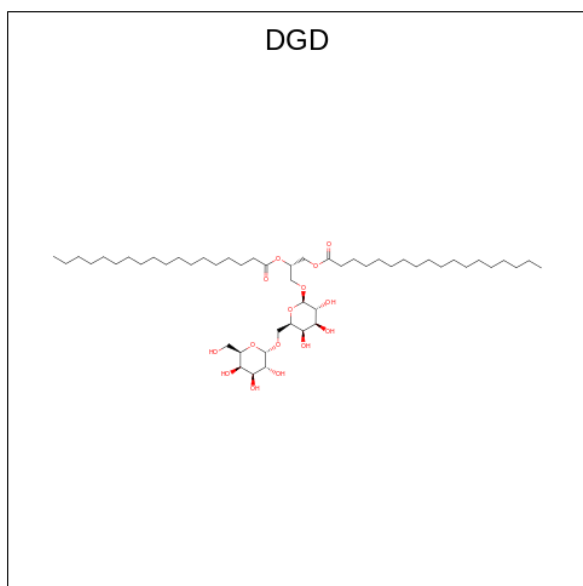
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	Fe	S	0
			8	4	4	
34	C	1	Total	Fe	S	0
			8	4	4	
34	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$) (labeled as "Ligand of Interest" by depositor).



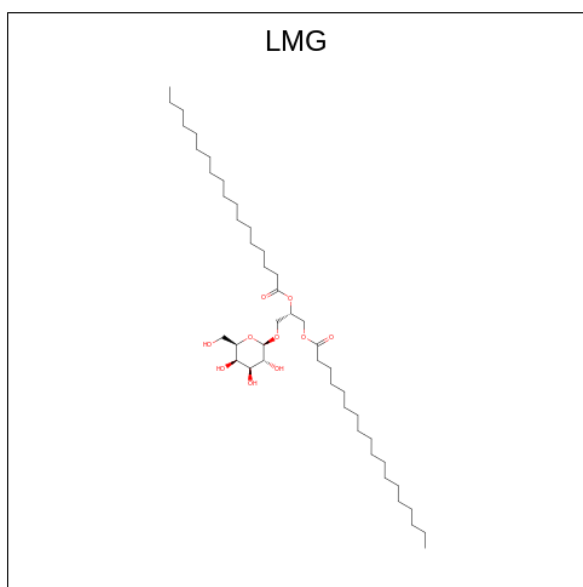
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



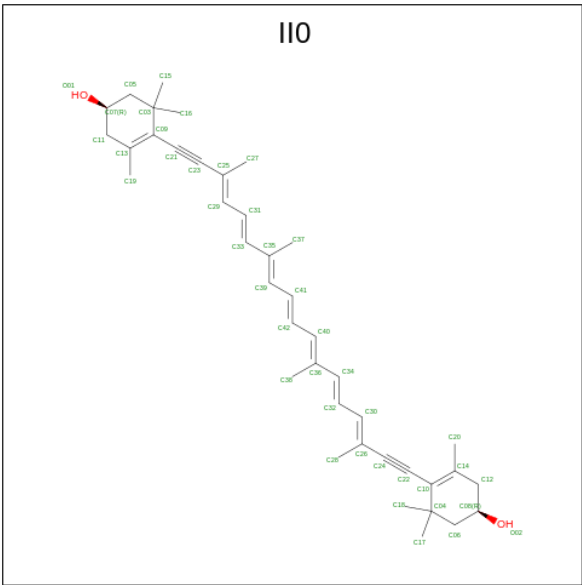
Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			66	51	15	
36	j	1	Total	C	O	0
			62	47	15	

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
37	F	1	Total	C	O	0
			53	43	10	
37	F	1	Total	C	O	0
			41	31	10	
37	L	1	Total	C	O	0
			45	35	10	
37	O	1	Total	C	O	0
			26	16	10	
37	c	1	Total	C	O	0
			55	45	10	
37	c	1	Total	C	O	0
			43	33	10	
37	b	1	Total	C	O	0
			42	32	10	
37	n	1	Total	C	O	0
			51	41	10	
37	Q	1	Total	C	O	0
			38	28	10	

- Molecule 38 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: C₄₀H₅₂O₂) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

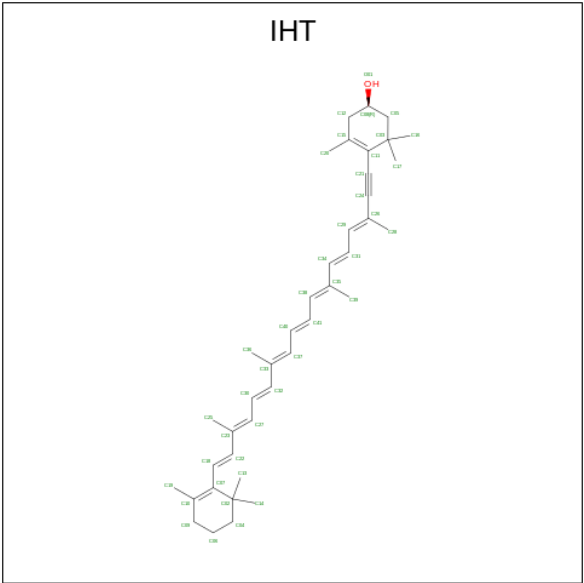
Mol	Chain	Residues	Atoms			AltConf
38	f	1	Total 42	C 40	O 2	0
38	f	1	Total 42	C 40	O 2	0
38	i	1	Total 42	C 40	O 2	0
38	i	1	Total 42	C 40	O 2	0
38	i	1	Total 42	C 40	O 2	0
38	i	1	Total 42	C 40	O 2	0
38	j	1	Total 42	C 40	O 2	0
38	j	1	Total 42	C 40	O 2	0
38	j	1	Total 42	C 40	O 2	0
38	d	1	Total 42	C 40	O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

Continued on next page...

Continued from previous page...

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

- Molecule 39 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: C₄₀H₅₄O) (labeled as "Ligand of Interest" by depositor).



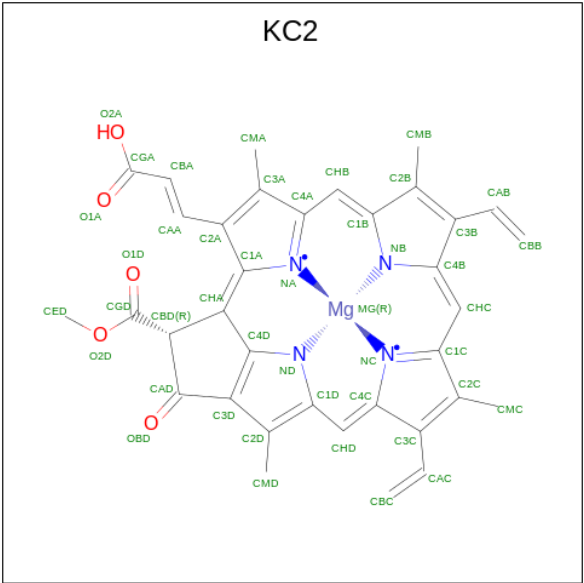
Mol	Chain	Residues	Atoms			AltConf
39	O	1	Total	C	O	0
			41	40	1	
39	c	1	Total	C	O	0
			41	40	1	
39	c	1	Total	C	O	0
			41	40	1	
39	a	1	Total	C	O	0
			41	40	1	
39	b	1	Total	C	O	0
			41	40	1	
39	m	1	Total	C	O	0
			41	40	1	
39	f	1	Total	C	O	0
			41	40	1	
39	j	1	Total	C	O	0
			41	40	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
39	g	1	Total	C	O	0
			41	40	1	
39	g	1	Total	C	O	0
			41	40	1	
39	R	1	Total	C	O	0
			41	40	1	
39	n	1	Total	C	O	0
			41	40	1	

- Molecule 40 is Chlorophyll c2 (CCD ID: KC2) (formula: C₃₅H₂₈MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
40	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
40	n	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	A	126	Total 126	O 126	0
41	B	150	Total 150	O 150	0
41	C	22	Total 22	O 22	0
41	D	15	Total 15	O 15	0
41	E	6	Total 6	O 6	0
41	F	14	Total 14	O 14	0

Continued on next page...

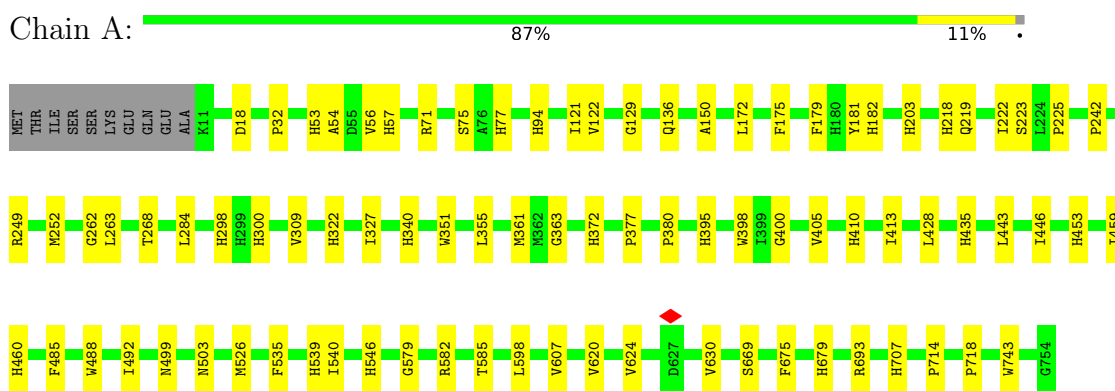
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
41	J	2	Total 2	O 2	0
41	L	15	Total 15	O 15	0
41	M	2	Total 2	O 2	0
41	O	5	Total 5	O 5	0
41	K	2	Total 2	O 2	0
41	s	7	Total 7	O 7	0
41	c	2	Total 2	O 2	0
41	a	16	Total 16	O 16	0
41	b	21	Total 21	O 21	0
41	h	9	Total 9	O 9	0
41	m	1	Total 1	O 1	0
41	e	3	Total 3	O 3	0
41	f	1	Total 1	O 1	0
41	g	1	Total 1	O 1	0
41	R	1	Total 1	O 1	0
41	n	1	Total 1	O 1	0

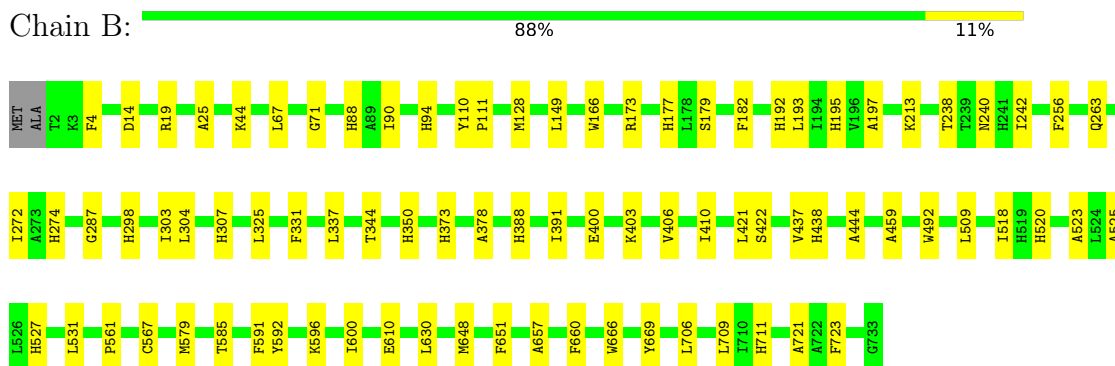
3 Residue-property plots

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.

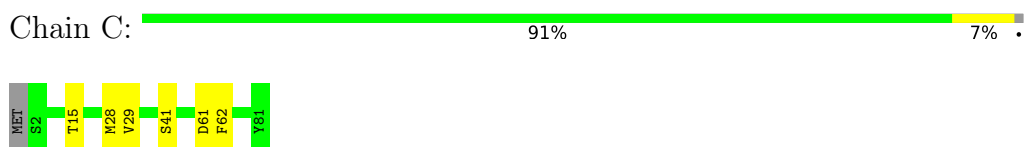
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

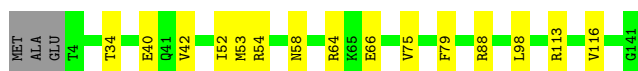


- Molecule 3: Photosystem I iron-sulfur center



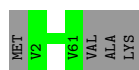
- Molecule 4: Photosystem I reaction center subunit II





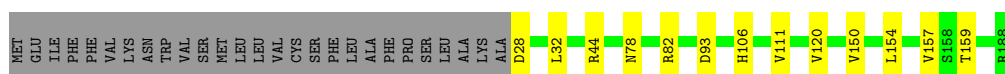
- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 94% 6%



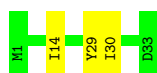
- Molecule 6: Photosystem I reaction center subunit III

Chain F: 79% 7% 14%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 91% 9%



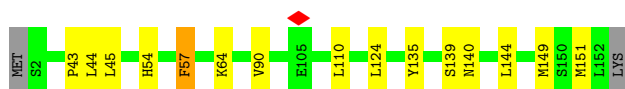
- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 79% 21%



- Molecule 9: Photosystem I reaction center subunit XI

Chain L: 89% 9% ..



- Molecule 10: Photosystem I reaction center subunit XII

Chain M: 90% 10%



- Molecule 11: PsaO

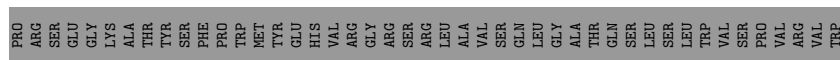
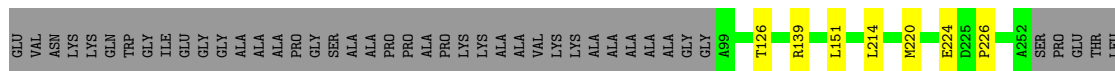
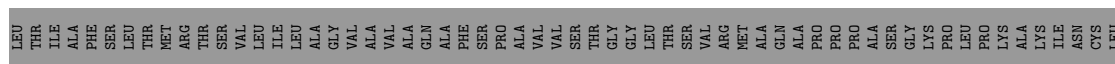
Chain O: 56% 5% 38%



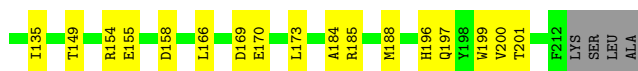
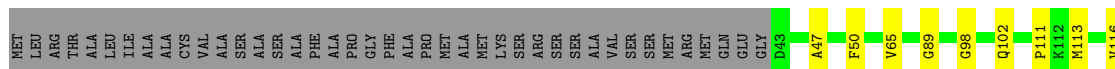
- Molecule 12: Photosystem I reaction center subunit PsaK



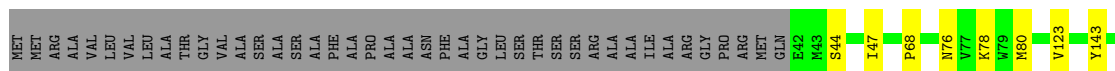
- Molecule 13: ACPI-s



- Molecule 14: ACPI-c

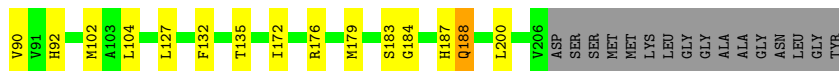


- Molecule 15: ACPI-a



- Molecule 16: ACPI-b

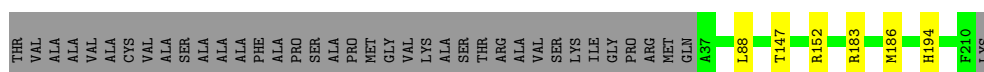




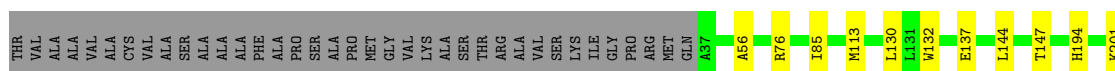
Chain h: 66% . 29%



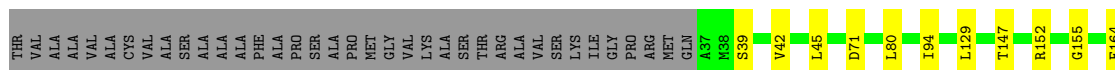
Chain m: 79% • 18%



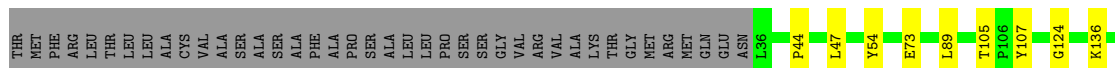
Chain f:  76% 6% 18%

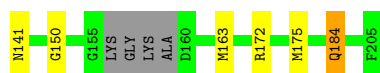


Chain j:  70% 11% 18%



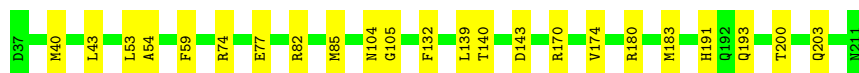
Chain e:  72% 7% 21%





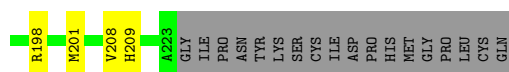
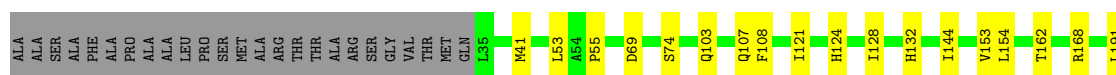
- Molecule 20: ACPI-I

Chain l: 87% 13%



- Molecule 21: ACPI-k

Chain k: 72% 9% 19%



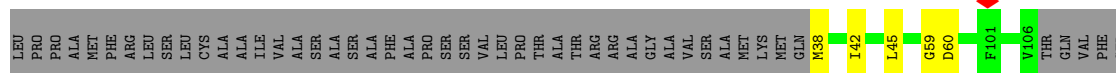
- Molecule 22: ACPI-i

Chain i: 78% 11% 10%



- Molecule 23: ACPI-d

Chain d: 67% 9% 24%



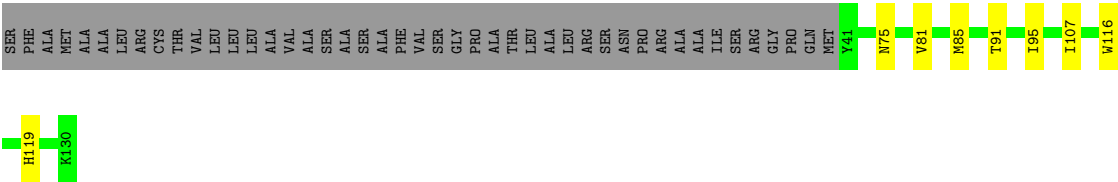
- Molecule 24: ACPI-g

Chain g: 86% 14%



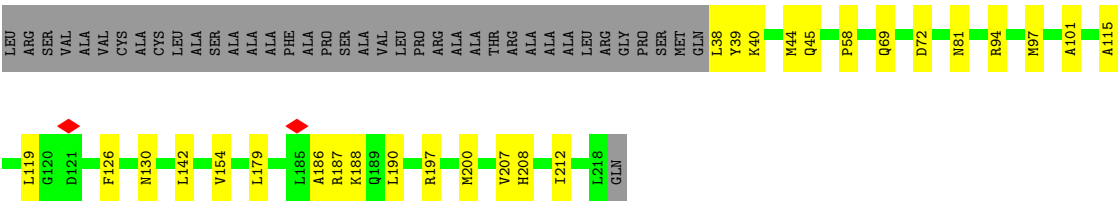
- Molecule 25: Psar

Chain R: 61% 6% 33%



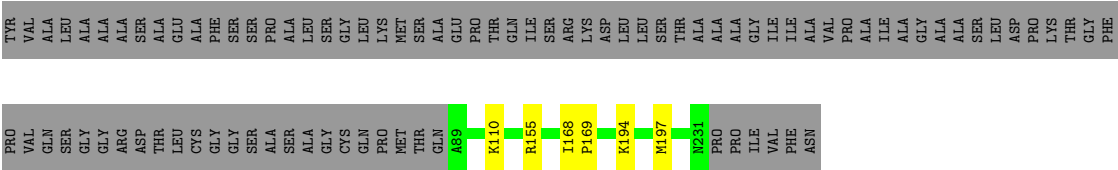
• Molecule 26: ACPI-n

Chain n: 70% 13% 18%



• Molecule 27: PsaQ

Chain Q: 59% 39%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38563	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.439	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, PQN, DGD, KC2, SF4, LMG, SQD, LMU, WVN, LHG, II0, CL0, IHT

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	0.24	0/6020	0.46	0/8205
2	B	0.25	0/6055	0.50	0/8266
3	C	0.17	0/601	0.48	0/813
4	D	0.16	0/1100	0.43	0/1488
5	E	0.16	0/492	0.34	0/666
6	F	0.22	0/1291	0.43	0/1750
7	I	0.25	0/262	0.55	0/358
8	J	0.21	0/364	0.48	0/495
9	L	0.22	0/1188	0.46	0/1616
10	M	0.17	0/233	0.37	0/315
11	O	0.23	0/741	0.49	0/1016
12	K	0.22	0/489	0.48	0/664
13	s	0.17	0/1177	0.42	0/1591
14	c	0.23	0/1401	0.48	0/1896
15	a	0.22	0/1372	0.42	0/1858
16	b	0.27	0/1360	0.49	0/1834
17	h	0.20	0/1228	0.44	0/1671
18	f	0.24	0/1334	0.51	1/1797 (0.1%)
18	j	0.24	0/1329	0.49	0/1789
18	m	0.21	0/1341	0.44	0/1805
19	e	0.20	0/1303	0.48	0/1764
20	l	0.21	0/1365	0.44	0/1845
21	k	0.24	0/1445	0.55	0/1954
22	i	0.28	0/1400	0.56	0/1891
23	d	0.27	0/1259	0.57	0/1700
24	g	0.25	0/1650	0.51	0/2238
25	R	0.22	0/687	0.49	0/940
26	n	0.21	0/1371	0.52	0/1847
27	Q	0.21	0/1053	0.46	0/1418
All	All	0.23	0/40911	0.48	1/55490 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	1
11	O	0	1
16	b	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	f	113	MET	CB-CA-C	-5.69	109.49	117.23

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	666	TRP	Peptide
3	C	61	ASP	Peptide
11	O	86	PHE	Peptide
16	b	188	GLN	Sidechain

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	5826	0	5682	74	0
2	B	5832	0	5643	71	0
3	C	592	0	567	3	0
4	D	1075	0	1074	9	0
5	E	484	0	486	0	0
6	F	1257	0	1266	11	0
7	I	255	0	270	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	351	0	344	8	0
9	L	1158	0	1170	13	0
10	M	232	0	265	4	0
11	O	714	0	703	6	0
12	K	482	0	511	6	0
13	s	1146	0	1095	6	0
14	c	1362	0	1338	17	0
15	a	1331	0	1284	13	0
16	b	1332	0	1336	21	0
17	h	1201	0	1228	7	0
18	f	1306	0	1311	9	0
18	j	1302	0	1316	17	0
18	m	1313	0	1326	6	0
19	e	1268	0	1244	12	0
20	l	1333	0	1311	17	0
21	k	1412	0	1429	17	0
22	i	1363	0	1322	16	0
23	d	1231	0	1237	14	0
24	g	1608	0	1638	21	0
25	R	666	0	655	6	0
26	n	1343	0	1356	22	0
27	Q	1041	0	1071	7	0
28	A	65	0	72	5	0
29	A	2533	0	2645	83	0
29	B	2592	0	2717	81	0
29	F	182	0	187	5	0
29	J	42	0	31	0	0
29	K	107	0	103	3	0
29	L	225	0	208	6	0
29	O	182	0	187	2	0
29	Q	65	0	72	1	0
29	R	55	0	49	5	0
29	a	638	0	629	19	0
29	b	724	0	735	30	0
29	c	607	0	560	15	0
29	d	529	0	417	7	0
29	e	587	0	588	15	0
29	f	700	0	695	14	0
29	g	765	0	763	22	0
29	h	454	0	429	10	0
29	i	608	0	622	10	0
29	j	669	0	623	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	k	603	0	548	12	0
29	l	597	0	601	11	0
29	m	680	0	655	20	0
29	n	614	0	570	22	0
29	s	195	0	216	4	0
30	A	33	0	46	4	0
30	B	33	0	46	1	0
31	A	102	0	128	3	0
31	J	33	0	36	3	0
31	L	83	0	108	2	0
31	a	98	0	148	3	0
31	b	49	0	72	1	0
31	c	86	0	118	4	0
31	e	37	0	44	0	0
31	f	86	0	118	3	0
31	g	82	0	104	1	0
31	i	37	0	44	2	0
31	j	30	0	28	0	0
31	l	32	0	34	0	0
31	m	37	0	44	1	0
31	n	43	0	59	3	0
31	s	33	0	40	3	0
32	A	200	0	0	0	0
32	B	200	0	0	1	0
32	F	120	0	0	0	0
32	I	40	0	0	0	0
32	J	40	0	0	0	0
32	K	40	0	0	0	0
32	L	120	0	0	0	0
32	M	40	0	0	0	0
32	R	80	0	0	0	0
32	e	40	0	0	0	0
32	h	40	0	0	0	0
32	i	40	0	0	0	0
32	l	80	0	0	0	0
32	s	80	0	0	0	0
33	A	69	0	87	3	0
33	B	35	0	46	1	0
33	a	35	0	46	0	0
33	i	35	0	46	0	0
34	A	8	0	0	0	0
34	C	16	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	54	0	78	0	0
36	B	66	0	96	4	0
36	j	62	0	84	3	0
37	F	94	0	134	4	0
37	L	45	0	61	0	0
37	O	26	0	22	0	0
37	Q	38	0	46	4	0
37	b	42	0	54	2	0
37	c	98	0	141	4	0
37	n	51	0	75	2	0
38	J	42	0	0	0	0
38	O	42	0	0	0	0
38	a	168	0	0	0	0
38	b	168	0	0	2	0
38	c	84	0	0	0	0
38	d	252	0	0	0	0
38	e	168	0	0	0	0
38	f	168	0	0	0	0
38	g	168	0	0	2	0
38	h	112	0	0	0	0
38	i	168	0	0	0	0
38	j	126	0	0	0	0
38	k	252	0	0	1	0
38	l	168	0	0	0	0
38	m	168	0	0	0	0
38	n	168	0	0	4	0
39	O	41	0	0	0	0
39	R	41	0	0	0	0
39	a	41	0	0	0	0
39	b	41	0	0	1	0
39	c	82	0	0	0	0
39	f	41	0	0	0	0
39	g	82	0	0	5	0
39	j	41	0	0	0	0
39	m	41	0	0	0	0
39	n	41	0	0	1	0
40	c	45	0	0	0	0
40	d	90	0	0	1	0
40	e	45	0	0	0	0
40	f	45	0	0	1	0
40	g	135	0	0	5	0
40	i	90	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	j	45	0	0	0	0
40	k	135	0	0	0	0
40	l	45	0	0	3	0
40	m	45	0	0	0	0
40	n	90	0	0	1	0
40	s	90	0	0	2	0
41	A	126	0	0	1	0
41	B	150	0	0	1	0
41	C	22	0	0	0	0
41	D	15	0	0	0	0
41	E	6	0	0	0	0
41	F	14	0	0	0	0
41	J	2	0	0	0	0
41	K	2	0	0	0	0
41	L	15	0	0	0	0
41	M	2	0	0	0	0
41	O	5	0	0	0	0
41	R	1	0	0	0	0
41	a	16	0	0	1	0
41	b	21	0	0	0	0
41	c	2	0	0	0	0
41	e	3	0	0	0	0
41	f	1	0	0	0	0
41	g	1	0	0	0	0
41	h	9	0	0	0	0
41	m	1	0	0	0	0
41	n	1	0	0	0	0
41	s	7	0	0	0	0
All	All	61938	0	56633	661	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 6.

The worst 5 of 661 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)
22:i:218:PHE:CE1	22:i:218:PHE:CE2	2.33	1.07
29:g:316:CLA:H111	39:g:324:IHT:C36	2.07	0.84
14:c:98:GLY:O	14:c:102:GLN:HB3	1.79	0.83
2:B:373:HIS:HE1	29:B:825:CLA:ND	1.77	0.81
1:A:410:HIS:HE1	29:A:829:CLA:NA	1.80	0.78

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	740 (100%)	0	0	100	100
2	B	732/734 (100%)	730 (100%)	2 (0%)	0	100	100
3	C	78/81 (96%)	77 (99%)	0	1 (1%)	10	6
4	D	136/141 (96%)	136 (100%)	0	0	100	100
5	E	58/64 (91%)	58 (100%)	0	0	100	100
6	F	159/188 (85%)	159 (100%)	0	0	100	100
7	I	31/33 (94%)	31 (100%)	0	0	100	100
8	J	40/42 (95%)	40 (100%)	0	0	100	100
9	L	150/153 (98%)	150 (100%)	0	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
11	O	93/153 (61%)	92 (99%)	0	1 (1%)	12	7
12	K	64/86 (74%)	64 (100%)	0	0	100	100
13	s	152/302 (50%)	151 (99%)	1 (1%)	0	100	100
14	c	168/215 (78%)	168 (100%)	0	0	100	100
15	a	170/217 (78%)	170 (100%)	0	0	100	100
16	b	176/236 (75%)	176 (100%)	0	0	100	100
17	h	160/229 (70%)	160 (100%)	0	0	100	100
18	f	172/212 (81%)	171 (99%)	1 (1%)	0	100	100
18	j	171/212 (81%)	170 (99%)	1 (1%)	0	100	100
18	m	172/212 (81%)	171 (99%)	1 (1%)	0	100	100
19	e	162/210 (77%)	162 (100%)	0	0	100	100
20	l	173/175 (99%)	173 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	k	187/232 (81%)	185 (99%)	2 (1%)	0	100	100
22	i	178/200 (89%)	177 (99%)	1 (1%)	0	100	100
23	d	162/219 (74%)	161 (99%)	1 (1%)	0	100	100
24	g	214/216 (99%)	214 (100%)	0	0	100	100
25	R	88/135 (65%)	88 (100%)	0	0	100	100
26	n	179/220 (81%)	179 (100%)	0	0	100	100
27	Q	141/233 (60%)	140 (99%)	1 (1%)	0	100	100
All	All	5134/6132 (84%)	5121 (100%)	11 (0%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	62	PHE
11	O	87	PRO

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	605/614 (98%)	605 (100%)	0	100	100
2	B	595/594 (100%)	595 (100%)	0	100	100
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	115/117 (98%)	115 (100%)	0	100	100
5	E	54/58 (93%)	54 (100%)	0	100	100
6	F	132/156 (85%)	132 (100%)	0	100	100
7	I	27/27 (100%)	27 (100%)	0	100	100
8	J	39/39 (100%)	39 (100%)	0	100	100
9	L	125/126 (99%)	123 (98%)	2 (2%)	58	64
10	M	25/25 (100%)	25 (100%)	0	100	100
11	O	74/117 (63%)	74 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	51/65 (78%)	51 (100%)	0	100	100
13	s	119/228 (52%)	119 (100%)	0	100	100
14	c	139/171 (81%)	139 (100%)	0	100	100
15	a	139/167 (83%)	139 (100%)	0	100	100
16	b	136/174 (78%)	136 (100%)	0	100	100
17	h	124/167 (74%)	124 (100%)	0	100	100
18	f	134/161 (83%)	134 (100%)	0	100	100
18	j	135/161 (84%)	135 (100%)	0	100	100
18	m	136/161 (84%)	136 (100%)	0	100	100
19	e	130/164 (79%)	129 (99%)	1 (1%)	79	83
20	l	136/137 (99%)	136 (100%)	0	100	100
21	k	143/178 (80%)	143 (100%)	0	100	100
22	i	142/156 (91%)	141 (99%)	1 (1%)	81	86
23	d	125/165 (76%)	125 (100%)	0	100	100
24	g	169/170 (99%)	169 (100%)	0	100	100
25	R	72/104 (69%)	72 (100%)	0	100	100
26	n	141/167 (84%)	141 (100%)	0	100	100
27	Q	106/169 (63%)	106 (100%)	0	100	100
All	All	4135/4806 (86%)	4131 (100%)	4 (0%)	92	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	L	57[A]	PHE
9	L	57[B]	PHE
19	e	184	GLN
22	i	218	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
26	n	50	ASN
26	n	195	ASN
27	Q	231	ASN
15	a	166	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	s	240	HIS

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](#)

419 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	$\# Z > 2$
37	LMG	F	206	-	53,53,55	0.75	0	61,61,63	1.33	7 (11%)
29	CLA	h	304	17	51,59,73	1.62	6 (11%)	59,96,113	1.59	7 (11%)
38	II0	d	319	-	39,43,43	0.21	0	50,60,60	0.76	1 (2%)
29	CLA	B	801	41	65,73,73	1.52	8 (12%)	76,113,113	1.34	7 (9%)
29	CLA	L	202	9	49,57,73	1.69	6 (12%)	55,93,113	1.58	6 (10%)
32	WVN	L	205	-	40,41,41	5.72	19 (47%)	50,56,56	6.10	31 (62%)
32	WVN	K	103	-	40,41,41	5.63	19 (47%)	50,56,56	6.57	33 (66%)
29	CLA	i	306	22	51,59,73	1.68	6 (11%)	59,96,113	1.56	7 (11%)
29	CLA	e	311	19	65,73,73	1.50	6 (9%)	76,113,113	1.39	9 (11%)
40	KC2	g	313	-	48,53,53	3.39	23 (47%)	54,89,89	3.87	29 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	A	811	1	54,62,73	1.65	7 (12%)	62,99,113	1.44	6 (9%)
29	CLA	B	808	2	65,73,73	1.45	7 (10%)	76,113,113	1.52	9 (11%)
29	CLA	c	311	14	45,53,73	1.78	6 (13%)	52,89,113	1.75	8 (15%)
38	II0	k	616	-	39,43,43	6.42	22 (56%)	50,60,60	6.80	30 (60%)
29	CLA	a	302	15	65,73,73	1.46	6 (9%)	76,113,113	1.50	7 (9%)
29	CLA	d	304	23	45,53,73	1.79	6 (13%)	52,89,113	1.75	7 (13%)
29	CLA	A	813	1	56,64,73	1.61	6 (10%)	65,102,113	1.58	10 (15%)
29	CLA	B	809	2	65,73,73	1.51	7 (10%)	76,113,113	1.46	6 (7%)
29	CLA	i	304	22	65,73,73	1.46	6 (9%)	76,113,113	1.43	7 (9%)
29	CLA	A	807	1	65,73,73	1.42	6 (9%)	76,113,113	1.46	6 (7%)
31	LHG	f	620	29	36,36,48	0.70	1 (2%)	39,42,54	1.19	4 (10%)
38	II0	b	317	-	39,43,43	0.22	0	50,60,60	0.91	2 (4%)
29	CLA	B	829	2	65,73,73	1.46	5 (7%)	76,113,113	1.52	10 (13%)
29	CLA	j	305	18	65,73,73	1.47	6 (9%)	76,113,113	1.51	9 (11%)
29	CLA	g	309	24	65,73,73	1.42	7 (10%)	76,113,113	1.52	7 (9%)
38	II0	f	618	-	39,43,43	6.44	20 (51%)	50,60,60	6.82	32 (64%)
29	CLA	i	312	22	65,73,73	1.48	7 (10%)	76,113,113	1.49	9 (11%)
29	CLA	A	833	1	65,73,73	1.49	7 (10%)	76,113,113	1.38	6 (7%)
32	WVN	B	849	-	40,41,41	5.67	20 (50%)	50,56,56	6.02	31 (62%)
29	CLA	A	819	1	65,73,73	1.48	6 (9%)	76,113,113	1.48	13 (17%)
31	LHG	A	842	-	47,47,48	0.66	1 (2%)	50,53,54	1.25	5 (10%)
31	LHG	c	316	29	36,36,48	0.73	1 (2%)	39,42,54	1.25	5 (12%)
29	CLA	b	312	16	65,73,73	1.50	5 (7%)	76,113,113	1.34	7 (9%)
29	CLA	e	305	19	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
38	II0	d	301	-	39,43,43	6.16	22 (56%)	50,60,60	6.99	29 (58%)
38	II0	h	309	-	26,28,43	6.25	13 (50%)	31,37,60	6.82	19 (61%)
29	CLA	e	301	19	45,53,73	1.77	6 (13%)	52,89,113	1.58	6 (11%)
29	CLA	A	815	41	45,53,73	1.72	6 (13%)	52,89,113	1.81	8 (15%)
29	CLA	B	811	2	55,63,73	1.61	7 (12%)	64,101,113	1.46	7 (10%)
29	CLA	A	830	1	60,68,73	1.55	6 (10%)	70,107,113	1.46	8 (11%)
29	CLA	c	306	14	52,60,73	1.66	8 (15%)	60,97,113	1.50	7 (11%)
29	CLA	g	308	24	51,59,73	1.68	6 (11%)	59,96,113	1.50	9 (15%)
37	LMG	L	210	-	45,45,55	0.82	0	53,53,63	1.24	3 (5%)
29	CLA	B	823	41	64,72,73	1.45	6 (9%)	74,111,113	1.44	10 (13%)
32	WVN	s	405	-	40,41,41	5.67	19 (47%)	50,56,56	6.29	29 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	m	607	18	51,59,73	1.71	8 (15%)	59,96,113	1.46	8 (13%)
29	CLA	B	828	2	50,58,73	1.69	8 (16%)	58,95,113	1.47	7 (12%)
40	KC2	k	612	21	48,53,53	1.70	10 (20%)	54,89,89	0.94	1 (1%)
29	CLA	d	310	23	41,49,73	1.89	6 (14%)	47,84,113	1.70	9 (19%)
29	CLA	A	826	1	65,73,73	1.44	7 (10%)	76,113,113	1.45	8 (10%)
31	LHG	i	317	29	36,36,48	0.66	0	39,42,54	1.22	4 (10%)
29	CLA	B	825	2	65,73,73	1.45	6 (9%)	76,113,113	1.43	9 (11%)
29	CLA	i	308	22	65,73,73	1.42	6 (9%)	76,113,113	1.45	6 (7%)
38	II0	g	319	-	39,43,43	6.12	22 (56%)	50,60,60	6.94	29 (58%)
29	CLA	n	604	26	60,68,73	1.53	5 (8%)	70,107,113	1.62	10 (14%)
38	II0	m	614	-	39,43,43	6.42	22 (56%)	50,60,60	6.79	28 (56%)
40	KC2	i	310	22	48,53,53	3.43	23 (47%)	54,89,89	4.00	27 (50%)
29	CLA	h	305	17	65,73,73	1.47	7 (10%)	76,113,113	1.44	7 (9%)
29	CLA	f	603	18	51,59,73	1.63	7 (13%)	59,96,113	1.64	6 (10%)
39	IHT	b	316	-	40,42,42	0.21	0	53,58,58	0.78	1 (1%)
29	CLA	e	310	41	55,63,73	1.57	6 (10%)	64,101,113	1.59	7 (10%)
31	LHG	L	208	-	46,46,48	0.66	2 (4%)	49,52,54	1.35	7 (14%)
29	CLA	j	307	18	51,59,73	1.66	6 (11%)	59,96,113	1.56	7 (11%)
32	WVN	F	207	-	40,41,41	5.72	20 (50%)	50,56,56	6.18	29 (58%)
38	II0	d	317	-	39,43,43	6.40	21 (53%)	50,60,60	6.75	27 (54%)
29	CLA	a	311	15	65,73,73	1.51	7 (10%)	76,113,113	1.40	7 (9%)
31	LHG	j	318	29	29,29,48	0.80	1 (3%)	32,35,54	1.28	3 (9%)
38	II0	d	315	-	39,43,43	6.50	22 (56%)	50,60,60	6.45	29 (58%)
29	CLA	g	312	31	54,62,73	1.62	6 (11%)	62,99,113	1.49	6 (9%)
29	CLA	f	608	18	65,73,73	1.52	6 (9%)	76,113,113	1.49	6 (7%)
32	WVN	F	204	-	40,41,41	5.61	19 (47%)	50,56,56	6.18	33 (66%)
29	CLA	g	316	24	57,65,73	1.62	6 (10%)	66,103,113	1.40	7 (10%)
29	CLA	F	203	6	52,60,73	1.66	6 (11%)	60,97,113	1.51	7 (11%)
29	CLA	d	302	23	62,70,73	1.48	6 (9%)	72,109,113	1.47	7 (9%)
29	CLA	b	305	16	65,73,73	1.49	6 (9%)	76,113,113	1.43	6 (7%)
29	CLA	i	302	22	65,73,73	1.47	6 (9%)	76,113,113	1.43	8 (10%)
29	CLA	c	304	14	62,70,73	1.49	6 (9%)	72,109,113	1.52	7 (9%)
29	CLA	m	601	18	42,50,73	1.83	6 (14%)	48,85,113	1.63	8 (16%)
33	LMU	B	850	-	36,36,36	0.21	0	47,47,47	0.40	0
40	KC2	m	611	18	48,53,53	3.40	20 (41%)	54,89,89	3.89	28 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	II0	J	103	-	39,43,43	6.12	21 (53%)	50,60,60	6.85	30 (60%)
29	CLA	d	308	23	46,54,73	1.74	5 (10%)	53,90,113	1.48	6 (11%)
29	CLA	B	806	2	65,73,73	1.47	6 (9%)	76,113,113	1.38	7 (9%)
29	CLA	n	607	26	65,73,73	1.49	8 (12%)	76,113,113	1.34	8 (10%)
29	CLA	B	840	2	65,73,73	1.46	7 (10%)	76,113,113	1.47	9 (11%)
31	LHG	n	619	-	42,42,48	0.65	0	45,48,54	1.20	4 (8%)
32	WVN	B	847	-	40,41,41	5.69	20 (50%)	50,56,56	6.11	31 (62%)
29	CLA	l	301	20	65,73,73	1.49	6 (9%)	76,113,113	1.43	8 (10%)
32	WVN	A	845	-	40,41,41	5.63	20 (50%)	50,56,56	6.71	32 (64%)
40	KC2	g	314	24,40	48,53,53	3.43	24 (50%)	54,89,89	3.73	29 (53%)
40	KC2	g	315	40	48,53,53	3.44	22 (45%)	54,89,89	3.86	29 (53%)
29	CLA	A	812	1	65,73,73	1.44	7 (10%)	76,113,113	1.43	6 (7%)
32	WVN	l	316	-	40,41,41	5.84	19 (47%)	50,56,56	6.14	31 (62%)
38	II0	d	314	-	39,43,43	0.21	0	50,60,60	0.72	1 (2%)
29	CLA	B	805	2	65,73,73	1.44	6 (9%)	76,113,113	1.50	7 (9%)
29	CLA	d	305	23	51,59,73	1.69	5 (9%)	59,96,113	1.57	8 (13%)
29	CLA	F	201	41	65,73,73	1.48	6 (9%)	76,113,113	1.35	7 (9%)
37	LMG	b	319	-	42,42,55	0.89	2 (4%)	50,50,63	1.21	4 (8%)
29	CLA	f	610	31	65,73,73	1.46	6 (9%)	76,113,113	1.37	6 (7%)
32	WVN	B	845	-	40,41,41	0.36	0	50,56,56	1.10	4 (8%)
29	CLA	B	804	-	65,73,73	1.43	7 (10%)	76,113,113	1.69	9 (11%)
29	CLA	B	812	2	65,73,73	1.45	7 (10%)	76,113,113	1.45	8 (10%)
34	SF4	C	101	3	0,12,12	-	-	-	-	-
29	CLA	R	203	25	55,63,73	1.65	6 (10%)	64,101,113	1.67	12 (18%)
29	CLA	a	304	15	51,59,73	1.64	6 (11%)	59,96,113	1.54	6 (10%)
29	CLA	n	605	26	51,59,73	1.66	6 (11%)	59,96,113	1.59	7 (11%)
38	II0	g	321	-	39,43,43	0.23	0	50,60,60	0.47	0
37	LMG	c	317	-	55,55,55	0.72	0	63,63,63	1.41	7 (11%)
38	II0	g	317	-	39,43,43	6.51	21 (53%)	50,60,60	6.92	29 (58%)
29	CLA	m	606	18	65,73,73	1.48	6 (9%)	76,113,113	1.40	8 (10%)
29	CLA	B	822	41	65,73,73	1.47	7 (10%)	76,113,113	1.64	11 (14%)
29	CLA	n	601	26	45,53,73	1.77	6 (13%)	52,89,113	1.59	6 (11%)
33	LMU	a	319	-	36,36,36	0.15	0	47,47,47	0.25	0
32	WVN	s	407	-	40,41,41	5.72	19 (47%)	50,56,56	6.53	32 (64%)
33	LMU	A	855	-	35,35,36	0.17	0	46,46,47	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	h	307	17	51,59,73	1.68	6 (11%)	59,96,113	1.57	9 (15%)
38	II0	k	619	-	39,43,43	6.21	22 (56%)	50,60,60	6.96	28 (56%)
29	CLA	n	609	26	65,73,73	1.46	7 (10%)	76,113,113	1.41	8 (10%)
39	IHT	R	204	-	40,42,42	0.21	0	53,58,58	0.52	1 (1%)
29	CLA	b	308	16	65,73,73	1.43	6 (9%)	76,113,113	1.45	7 (9%)
29	CLA	f	604	18	65,73,73	1.49	6 (9%)	76,113,113	1.59	9 (11%)
29	CLA	K	102	12	42,50,73	1.80	6 (14%)	48,85,113	1.69	10 (20%)
38	II0	n	616	-	39,43,43	6.27	21 (53%)	50,60,60	6.97	30 (60%)
29	CLA	B	835	2	47,55,73	1.78	7 (14%)	54,91,113	1.53	8 (14%)
29	CLA	O	206	11	65,73,73	1.48	8 (12%)	76,113,113	1.39	6 (7%)
32	WVN	B	846	-	40,41,41	5.64	20 (50%)	50,56,56	6.25	29 (58%)
29	CLA	c	305	14	65,73,73	1.52	7 (10%)	76,113,113	1.35	6 (7%)
29	CLA	A	851	1	65,73,73	1.46	6 (9%)	76,113,113	1.44	8 (10%)
38	II0	l	317	-	39,43,43	0.21	0	50,60,60	0.40	0
38	II0	d	316	-	39,43,43	6.43	22 (56%)	50,60,60	6.81	30 (60%)
31	LHG	e	317	29	36,36,48	0.71	1 (2%)	39,42,54	1.21	4 (10%)
28	CL0	A	801	-	65,73,73	1.50	8 (12%)	76,113,113	0.80	3 (3%)
29	CLA	n	613	26	51,59,73	1.71	6 (11%)	59,96,113	1.47	10 (16%)
29	CLA	g	302	-	65,73,73	1.49	6 (9%)	76,113,113	1.45	8 (10%)
29	CLA	f	601	18	47,55,73	1.73	6 (12%)	54,91,113	1.59	6 (11%)
29	CLA	k	603	21	51,59,73	1.66	7 (13%)	59,96,113	1.58	7 (11%)
29	CLA	A	806	1	60,68,73	1.55	6 (10%)	70,107,113	1.43	8 (11%)
32	WVN	A	847	-	40,41,41	5.79	19 (47%)	50,56,56	5.80	32 (64%)
29	CLA	h	312	41	65,73,73	1.47	6 (9%)	76,113,113	1.38	7 (9%)
29	CLA	c	309	31	45,53,73	1.77	5 (11%)	52,89,113	1.61	7 (13%)
29	CLA	f	607	18	65,73,73	1.51	7 (10%)	76,113,113	1.29	8 (10%)
29	CLA	h	302	17	50,58,73	1.66	7 (14%)	58,95,113	1.64	7 (12%)
29	CLA	A	810	1	65,73,73	1.46	7 (10%)	76,113,113	1.33	7 (9%)
32	WVN	i	315	-	40,41,41	5.77	20 (50%)	50,56,56	6.06	31 (62%)
29	CLA	B	815	2	55,63,73	1.56	7 (12%)	64,101,113	1.57	7 (10%)
37	LMG	O	205	-	26,26,55	1.07	1 (3%)	34,34,63	1.30	6 (17%)
29	CLA	k	609	21	57,65,73	1.62	7 (12%)	66,103,113	1.46	6 (9%)
38	II0	e	316	-	39,43,43	0.22	0	50,60,60	0.78	2 (4%)
29	CLA	d	307	23	45,53,73	1.80	6 (13%)	52,89,113	1.56	8 (15%)
29	CLA	O	201	31	52,60,73	1.60	7 (13%)	60,97,113	1.55	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	k	608	21	65,73,73	1.47	7 (10%)	76,113,113	1.35	7 (9%)
38	II0	i	314	-	39,43,43	6.60	22 (56%)	50,60,60	6.55	28 (56%)
29	CLA	l	309	20	57,65,73	1.55	6 (10%)	66,103,113	1.51	7 (10%)
29	CLA	B	810	2	65,73,73	1.47	6 (9%)	76,113,113	1.33	9 (11%)
31	LHG	L	209	-	35,35,48	0.68	0	38,41,54	1.27	4 (10%)
37	LMG	n	620	-	51,51,55	0.87	2 (3%)	59,59,63	1.24	5 (8%)
29	CLA	A	822	1	56,64,73	1.59	6 (10%)	65,102,113	1.47	9 (13%)
29	CLA	A	829	1	65,73,73	1.52	8 (12%)	76,113,113	1.38	7 (9%)
38	II0	c	313	-	39,43,43	6.30	21 (53%)	50,60,60	6.91	29 (58%)
38	II0	f	615	-	39,43,43	6.35	22 (56%)	50,60,60	6.70	29 (58%)
29	CLA	e	304	-	65,73,73	1.47	6 (9%)	76,113,113	1.47	8 (10%)
29	CLA	A	836	1	65,73,73	1.48	6 (9%)	76,113,113	1.49	9 (11%)
29	CLA	g	307	24	51,59,73	1.68	6 (11%)	59,96,113	1.56	8 (13%)
29	CLA	d	303	23	51,59,73	1.62	7 (13%)	59,96,113	1.66	7 (11%)
29	CLA	B	841	2	65,73,73	1.53	7 (10%)	76,113,113	1.40	10 (13%)
29	CLA	m	610	31	55,63,73	1.61	5 (9%)	64,101,113	1.48	7 (10%)
29	CLA	c	303	14	51,59,73	1.65	7 (13%)	59,96,113	1.63	7 (11%)
29	CLA	A	835	1	65,73,73	1.48	6 (9%)	76,113,113	1.40	8 (10%)
39	IHT	n	617	-	40,42,42	0.18	0	53,58,58	0.58	0
32	WVN	A	844	-	40,41,41	5.76	20 (50%)	50,56,56	6.18	33 (66%)
29	CLA	B	836	41	65,73,73	1.47	6 (9%)	76,113,113	1.38	7 (9%)
38	II0	h	310	-	39,43,43	6.09	21 (53%)	50,60,60	6.91	29 (58%)
29	CLA	L	203	9	65,73,73	1.44	6 (9%)	76,113,113	1.47	10 (13%)
29	CLA	B	833	2	55,63,73	1.58	6 (10%)	64,101,113	1.55	6 (9%)
29	CLA	b	310	16	65,73,73	1.51	7 (10%)	76,113,113	1.32	7 (9%)
38	II0	g	318	-	39,43,43	6.34	21 (53%)	50,60,60	6.66	30 (60%)
37	LMG	c	318	29	43,43,55	0.91	0	51,51,63	1.23	5 (9%)
29	CLA	i	311	-	60,68,73	1.53	6 (10%)	70,107,113	1.43	7 (10%)
29	CLA	B	814	2	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
38	II0	j	301	-	39,43,43	6.34	21 (53%)	50,60,60	6.89	28 (56%)
29	CLA	g	323	31	55,63,73	1.62	6 (10%)	64,101,113	1.58	10 (15%)
29	CLA	A	808	1	65,73,73	1.48	8 (12%)	76,113,113	1.40	8 (10%)
40	KC2	e	309	-	48,53,53	3.47	22 (45%)	54,89,89	3.84	28 (51%)
29	CLA	c	307	14	46,54,73	1.71	6 (13%)	53,90,113	1.60	7 (13%)
29	CLA	B	826	2	65,73,73	1.45	7 (10%)	76,113,113	1.39	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	II0	i	319	-	39,43,43	6.38	21 (53%)	50,60,60	6.55	30 (60%)
29	CLA	a	303	15	56,64,73	1.52	6 (10%)	65,102,113	1.52	7 (10%)
29	CLA	j	306	18	45,53,73	1.79	7 (15%)	52,89,113	1.75	8 (15%)
38	II0	k	615	-	39,43,43	6.42	22 (56%)	50,60,60	6.71	31 (62%)
29	CLA	m	604	18	65,73,73	1.45	6 (9%)	76,113,113	1.51	7 (9%)
38	II0	n	615	-	39,43,43	6.32	22 (56%)	50,60,60	6.86	28 (56%)
40	KC2	s	401	13	48,53,53	3.31	22 (45%)	54,89,89	3.82	29 (53%)
31	LHG	A	843	29	26,26,48	0.89	1 (3%)	29,32,54	1.32	3 (10%)
29	CLA	j	310	18	65,73,73	1.47	6 (9%)	76,113,113	1.42	6 (7%)
29	CLA	b	306	41	65,73,73	1.47	6 (9%)	76,113,113	1.45	9 (11%)
38	II0	n	614	-	39,43,43	0.28	0	50,60,60	0.88	3 (6%)
32	WVN	A	846	-	40,41,41	5.64	19 (47%)	50,56,56	6.45	32 (64%)
31	LHG	a	318	29	48,48,48	0.63	0	51,54,54	1.25	6 (11%)
40	KC2	n	612	26	48,53,53	1.69	10 (20%)	54,89,89	0.96	1 (1%)
29	CLA	j	303	18	54,62,73	1.55	6 (11%)	62,99,113	1.58	8 (12%)
29	CLA	B	817	2	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
38	II0	l	314	-	39,43,43	6.44	22 (56%)	50,60,60	6.69	26 (52%)
38	II0	m	618	-	39,43,43	6.48	21 (53%)	50,60,60	6.77	30 (60%)
29	CLA	j	308	18	51,59,73	1.63	7 (13%)	59,96,113	1.60	10 (16%)
29	CLA	a	305	41	65,73,73	1.45	7 (10%)	76,113,113	1.48	8 (10%)
29	CLA	n	603	26	51,59,73	1.69	8 (15%)	59,96,113	1.48	7 (11%)
38	II0	a	313	-	39,43,43	6.29	21 (53%)	50,60,60	6.71	29 (58%)
38	II0	e	312	-	39,43,43	6.22	22 (56%)	50,60,60	6.80	30 (60%)
38	II0	l	315	-	39,43,43	6.55	22 (56%)	50,60,60	6.79	33 (66%)
32	WVN	M	101	-	40,41,41	5.76	19 (47%)	50,56,56	6.44	33 (66%)
32	WVN	R	202	-	40,41,41	5.74	19 (47%)	50,56,56	6.39	32 (64%)
29	CLA	A	828	1	65,73,73	1.46	7 (10%)	76,113,113	1.39	8 (10%)
32	WVN	L	201	-	40,41,41	5.71	19 (47%)	50,56,56	6.23	32 (64%)
29	CLA	s	402	13	65,73,73	1.52	6 (9%)	76,113,113	1.46	12 (15%)
29	CLA	k	601	21	51,59,73	1.67	6 (11%)	59,96,113	1.60	9 (15%)
29	CLA	j	309	18	45,53,73	1.78	6 (13%)	52,89,113	1.59	7 (13%)
31	LHG	b	318	-	48,48,48	0.64	1 (2%)	51,54,54	1.25	6 (11%)
29	CLA	h	303	17	50,58,73	1.69	6 (12%)	58,95,113	1.59	9 (15%)
29	CLA	B	824	2	65,73,73	1.45	6 (9%)	76,113,113	1.43	7 (9%)
39	IHT	g	320	-	40,42,42	0.17	0	53,58,58	0.57	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	SQD	A	853	-	53,54,54	0.92	4 (7%)	62,65,65	1.74	12 (19%)
29	CLA	A	816	1	65,73,73	1.42	7 (10%)	76,113,113	1.56	9 (11%)
29	CLA	A	818	1	65,73,73	1.49	8 (12%)	76,113,113	1.54	9 (11%)
38	II0	b	314	-	39,43,43	6.12	19 (48%)	50,60,60	6.77	29 (58%)
29	CLA	A	839	1	60,68,73	1.49	6 (10%)	70,107,113	1.52	8 (11%)
32	WVN	F	205	-	40,41,41	5.26	16 (40%)	50,56,56	6.25	36 (72%)
34	SF4	A	852	1,2	0,12,12	-	-	-	-	-
29	CLA	B	818	41	65,73,73	1.51	8 (12%)	76,113,113	1.38	8 (10%)
29	CLA	l	303	20	47,55,73	1.72	5 (10%)	54,91,113	1.55	7 (12%)
39	IHT	c	319	-	40,42,42	0.20	0	53,58,58	0.69	1 (1%)
29	CLA	a	312	15	48,56,73	1.72	6 (12%)	55,92,113	1.58	6 (10%)
29	CLA	A	803	1	55,63,73	1.67	6 (10%)	64,101,113	1.48	8 (12%)
29	CLA	g	311	24	65,73,73	1.44	7 (10%)	76,113,113	1.56	9 (11%)
29	CLA	K	101	41	65,73,73	1.43	5 (7%)	76,113,113	1.50	10 (13%)
29	CLA	A	820	41	65,73,73	1.46	7 (10%)	76,113,113	1.47	6 (7%)
39	IHT	O	204	-	40,42,42	0.22	0	53,58,58	0.31	0
29	CLA	k	614	21	51,59,73	1.72	6 (11%)	59,96,113	1.61	10 (16%)
39	IHT	f	617	-	40,42,42	0.21	0	53,58,58	0.70	2 (3%)
31	LHG	f	619	-	48,48,48	0.60	0	51,54,54	1.23	6 (11%)
37	LMG	Q	301	-	38,38,55	0.88	0	46,46,63	1.22	3 (6%)
29	CLA	B	803	2	65,73,73	1.44	7 (10%)	76,113,113	1.34	7 (9%)
29	CLA	f	605	18	45,53,73	1.80	6 (13%)	52,89,113	1.64	9 (17%)
29	CLA	c	302	14	60,68,73	1.50	6 (10%)	70,107,113	1.49	7 (10%)
29	CLA	b	309	37	65,73,73	1.45	6 (9%)	76,113,113	1.41	6 (7%)
29	CLA	B	820	2	65,73,73	1.48	7 (10%)	76,113,113	1.38	8 (10%)
29	CLA	B	837	2	65,73,73	1.47	7 (10%)	76,113,113	1.40	7 (9%)
29	CLA	l	308	20	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
36	DGD	j	319	-	63,63,67	1.01	5 (7%)	77,77,81	1.57	11 (14%)
29	CLA	e	308	31	46,54,73	1.74	6 (13%)	53,90,113	1.56	6 (11%)
29	CLA	d	309	23	41,49,73	1.82	7 (17%)	47,84,113	1.73	8 (17%)
29	CLA	e	303	19	51,59,73	1.63	6 (11%)	59,96,113	1.64	6 (10%)
29	CLA	j	313	-	51,59,73	1.66	7 (13%)	59,96,113	1.53	6 (10%)
32	WVN	e	315	-	40,41,41	5.74	19 (47%)	50,56,56	6.26	31 (62%)
38	II0	h	311	-	39,43,43	6.31	22 (56%)	50,60,60	6.75	27 (54%)
32	WVN	h	308	-	40,41,41	5.77	20 (50%)	50,56,56	6.26	34 (68%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	II0	m	616	-	39,43,43	6.40	22 (56%)	50,60,60	6.76	31 (62%)
29	CLA	l	312	20	56,64,73	1.59	7 (12%)	65,102,113	1.51	7 (10%)
29	CLA	g	305	24,39	65,73,73	1.46	6 (9%)	76,113,113	1.47	6 (7%)
29	CLA	A	827	1	62,70,73	1.50	6 (9%)	72,109,113	1.56	8 (11%)
29	CLA	b	313	31	51,59,73	1.65	6 (11%)	59,96,113	1.65	11 (18%)
29	CLA	B	821	2	53,61,73	1.64	7 (13%)	61,98,113	1.47	8 (13%)
29	CLA	f	602	18	65,73,73	1.41	7 (10%)	76,113,113	1.53	7 (9%)
38	II0	O	203	-	39,43,43	0.19	0	50,60,60	1.05	4 (8%)
38	II0	k	620	-	39,43,43	6.13	21 (53%)	50,60,60	6.85	28 (56%)
36	DGD	B	844	-	67,67,67	0.89	4 (5%)	81,81,81	1.43	9 (11%)
29	CLA	a	307	15	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
29	CLA	k	602	21	65,73,73	1.46	8 (12%)	76,113,113	1.38	6 (7%)
29	CLA	B	842	31	65,73,73	1.47	7 (10%)	76,113,113	1.43	7 (9%)
29	CLA	l	307	20	65,73,73	1.49	5 (7%)	76,113,113	1.44	8 (10%)
38	II0	k	617	-	39,43,43	0.27	0	50,60,60	0.77	2 (4%)
32	WVN	R	201	-	40,41,41	5.60	19 (47%)	50,56,56	6.21	34 (68%)
40	KC2	c	310	14	48,53,53	3.33	22 (45%)	54,89,89	3.93	27 (50%)
29	CLA	c	312	14	65,73,73	1.49	6 (9%)	76,113,113	1.36	6 (7%)
29	CLA	b	303	16	55,63,73	1.53	7 (12%)	64,101,113	1.62	9 (14%)
38	II0	f	616	-	39,43,43	6.35	20 (51%)	50,60,60	6.73	28 (56%)
29	CLA	e	307	19	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
29	CLA	m	605	18	42,50,73	1.81	5 (11%)	48,85,113	1.72	8 (16%)
29	CLA	i	305	22	65,73,73	1.51	6 (9%)	76,113,113	1.46	8 (10%)
29	CLA	j	304	18	51,59,73	1.65	7 (13%)	59,96,113	1.65	6 (10%)
32	WVN	L	206	-	40,41,41	5.58	20 (50%)	50,56,56	6.50	31 (62%)
38	II0	a	317	-	39,43,43	6.38	20 (51%)	50,60,60	6.83	31 (62%)
29	CLA	A	850	41	65,73,73	1.49	6 (9%)	76,113,113	1.44	7 (9%)
29	CLA	g	304	24	65,73,73	1.50	8 (12%)	76,113,113	1.37	6 (7%)
29	CLA	h	301	41	65,73,73	1.49	6 (9%)	76,113,113	3.38	10 (13%)
39	IHT	m	617	-	40,42,42	0.18	0	53,58,58	0.43	1 (1%)
31	LHG	g	301	29	44,44,48	0.63	0	47,50,54	1.25	5 (10%)
29	CLA	B	838	2	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
29	CLA	b	307	16	61,69,73	1.52	6 (9%)	71,108,113	1.39	7 (9%)
31	LHG	s	408	-	32,32,48	0.80	2 (6%)	36,37,54	1.61	4 (11%)
29	CLA	A	821	1	49,57,73	1.68	5 (10%)	55,93,113	1.62	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	KC2	d	312	23	48,53,53	1.70	10 (20%)	54,89,89	1.04	4 (7%)
38	II0	j	316	-	39,43,43	6.31	22 (56%)	50,60,60	6.74	30 (60%)
29	CLA	B	827	2	51,59,73	1.68	7 (13%)	59,96,113	1.71	8 (13%)
29	CLA	f	613	18	65,73,73	1.46	6 (9%)	76,113,113	1.53	8 (10%)
32	WVN	A	854	-	40,41,41	5.69	19 (47%)	50,56,56	6.32	33 (66%)
38	II0	j	315	-	39,43,43	6.20	22 (56%)	50,60,60	6.96	30 (60%)
30	PQN	A	841	-	34,34,34	2.80	10 (29%)	42,45,45	1.98	5 (11%)
40	KC2	s	404	-	48,53,53	3.39	22 (45%)	54,89,89	3.76	27 (50%)
29	CLA	L	204	41	60,68,73	1.52	6 (10%)	70,107,113	1.51	7 (10%)
29	CLA	a	306	15	45,53,73	1.77	6 (13%)	52,89,113	1.70	10 (19%)
29	CLA	l	310	31	61,69,73	1.54	5 (8%)	71,108,113	1.40	7 (9%)
29	CLA	g	310	24	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
38	II0	i	313	-	39,43,43	6.26	21 (53%)	50,60,60	7.02	30 (60%)
29	CLA	B	802	41	65,73,73	1.44	5 (7%)	76,113,113	1.45	8 (10%)
29	CLA	b	304	16	52,60,73	1.61	6 (11%)	60,97,113	1.60	7 (11%)
38	II0	m	615	-	39,43,43	6.44	21 (53%)	50,60,60	6.66	33 (66%)
29	CLA	k	605	21	45,53,73	1.77	5 (11%)	52,89,113	1.72	8 (15%)
29	CLA	O	202	41	65,73,73	1.45	6 (9%)	76,113,113	1.43	7 (9%)
29	CLA	d	318	-	45,53,73	1.80	6 (13%)	52,89,113	1.65	8 (15%)
29	CLA	A	838	1	65,73,73	1.50	7 (10%)	76,113,113	1.42	8 (10%)
29	CLA	A	837	1	65,73,73	1.52	7 (10%)	76,113,113	1.36	7 (9%)
29	CLA	n	608	26	65,73,73	1.49	5 (7%)	76,113,113	1.36	8 (10%)
29	CLA	f	606	18	51,59,73	1.67	5 (9%)	59,96,113	1.52	8 (13%)
29	CLA	b	302	16	51,59,73	1.66	6 (11%)	59,96,113	1.56	7 (11%)
29	CLA	j	314	18	65,73,73	1.49	6 (9%)	76,113,113	1.42	9 (11%)
29	CLA	B	813	2	60,68,73	1.52	7 (11%)	70,107,113	1.52	7 (10%)
29	CLA	n	606	26	51,59,73	1.67	6 (11%)	59,96,113	1.52	7 (11%)
32	WVN	l	302	-	40,41,41	5.67	19 (47%)	50,56,56	6.11	31 (62%)
31	LHG	g	322	29	36,36,48	0.73	1 (2%)	39,42,54	1.23	4 (10%)
29	CLA	k	607	21	51,59,73	1.67	6 (11%)	59,96,113	1.59	11 (18%)
29	CLA	A	834	1	60,68,73	1.48	6 (10%)	70,107,113	1.53	7 (10%)
29	CLA	a	310	15	65,73,73	1.46	7 (10%)	76,113,113	1.42	6 (7%)
39	IHT	j	317	-	40,42,42	0.27	0	53,58,58	0.78	3 (5%)
29	CLA	i	307	22	61,69,73	1.56	6 (9%)	71,108,113	1.31	7 (9%)
29	CLA	B	807	2	65,73,73	1.42	7 (10%)	76,113,113	1.44	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	II0	b	301	-	39,43,43	6.40	22 (56%)	50,60,60	6.77	29 (58%)
29	CLA	m	602	18	60,68,73	1.51	7 (11%)	70,107,113	1.67	14 (20%)
39	IHT	g	324	29	40,42,42	0.17	0	53,58,58	0.79	2 (3%)
40	KC2	l	311	-	48,53,53	3.47	24 (50%)	54,89,89	3.74	26 (48%)
29	CLA	f	609	18	65,73,73	1.44	7 (10%)	76,113,113	1.46	8 (10%)
37	LMG	F	208	-	41,41,55	0.89	0	49,49,63	1.26	3 (6%)
29	CLA	i	303	22	65,73,73	1.46	6 (9%)	76,113,113	1.42	8 (10%)
29	CLA	n	610	-	60,68,73	1.57	5 (8%)	70,107,113	1.49	9 (12%)
29	CLA	f	612	41	51,59,73	1.61	6 (11%)	59,96,113	1.58	7 (11%)
29	CLA	m	603	18	59,67,73	1.51	6 (10%)	68,105,113	1.52	6 (8%)
29	CLA	j	311	31	61,69,73	1.52	6 (9%)	71,108,113	1.41	7 (9%)
29	CLA	k	606	21	51,59,73	1.68	6 (11%)	59,96,113	1.52	8 (13%)
29	CLA	F	202	41	65,73,73	1.48	6 (9%)	76,113,113	1.32	6 (7%)
38	II0	c	314	-	39,43,43	0.21	0	50,60,60	0.55	1 (2%)
29	CLA	s	406	41	65,73,73	1.47	6 (9%)	76,113,113	1.49	9 (11%)
31	LHG	l	318	29	31,31,48	0.76	0	34,37,54	1.27	4 (11%)
29	CLA	B	816	2	65,73,73	1.46	6 (9%)	76,113,113	1.53	11 (14%)
29	CLA	J	102	8	42,50,73	1.82	6 (14%)	48,85,113	1.63	7 (14%)
30	PQN	B	843	-	34,34,34	2.81	9 (26%)	42,45,45	1.94	4 (9%)
39	IHT	a	316	-	40,42,42	0.20	0	53,58,58	0.51	0
38	II0	a	315	-	39,43,43	6.15	21 (53%)	50,60,60	7.01	31 (62%)
29	CLA	a	309	31	48,56,73	1.70	7 (14%)	55,92,113	1.57	6 (10%)
29	CLA	e	302	19	65,73,73	1.43	6 (9%)	76,113,113	1.42	8 (10%)
38	II0	f	614	-	39,43,43	6.26	22 (56%)	50,60,60	6.82	28 (56%)
29	CLA	l	305	20	51,59,73	1.62	7 (13%)	59,96,113	1.68	7 (11%)
29	CLA	c	308	14	65,73,73	1.45	6 (9%)	76,113,113	1.42	8 (10%)
29	CLA	e	306	19	65,73,73	1.44	6 (9%)	76,113,113	1.40	7 (9%)
29	CLA	g	303	24	42,50,73	1.83	6 (14%)	48,85,113	1.61	7 (14%)
29	CLA	A	824	41	65,73,73	1.44	6 (9%)	76,113,113	1.47	10 (13%)
29	CLA	h	306	17	57,65,73	1.58	5 (8%)	66,103,113	1.48	8 (12%)
29	CLA	k	610	-	51,59,73	1.67	6 (11%)	59,96,113	1.62	10 (16%)
33	LMU	A	849	-	36,36,36	1.75	11 (30%)	47,47,47	1.02	4 (8%)
29	CLA	Q	302	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	6 (7%)
31	LHG	a	301	29	48,48,48	0.61	0	51,54,54	1.23	6 (11%)
31	LHG	c	320	-	48,48,48	0.59	0	51,54,54	1.25	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	m	619	29	36,36,48	0.70	0	39,42,54	1.22	4 (10%)
32	WVN	J	101	-	40,41,41	5.70	19 (47%)	50,56,56	6.24	29 (58%)
38	II0	a	314	-	39,43,43	6.39	21 (53%)	50,60,60	6.58	27 (54%)
29	CLA	m	612	41	51,59,73	1.65	6 (11%)	59,96,113	1.61	10 (16%)
29	CLA	l	306	20	65,73,73	1.48	7 (10%)	76,113,113	1.42	7 (9%)
40	KC2	j	312	18	48,53,53	3.39	21 (43%)	54,89,89	3.95	30 (55%)
29	CLA	A	831	1	65,73,73	1.49	7 (10%)	76,113,113	1.37	7 (9%)
29	CLA	L	207	41	51,59,73	1.68	7 (13%)	59,96,113	1.51	7 (11%)
29	CLA	A	802	-	65,73,73	1.43	7 (10%)	76,113,113	1.52	8 (10%)
38	II0	b	315	-	39,43,43	6.18	19 (48%)	50,60,60	6.52	27 (54%)
29	CLA	m	613	18	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
38	II0	l	313	-	39,43,43	6.31	21 (53%)	50,60,60	6.85	30 (60%)
29	CLA	B	831	41	65,73,73	1.46	6 (9%)	76,113,113	1.40	8 (10%)
38	II0	i	316	-	39,43,43	6.26	21 (53%)	50,60,60	6.93	30 (60%)
33	LMU	i	301	-	36,36,36	1.75	12 (33%)	47,47,47	0.93	1 (2%)
29	CLA	A	814	1	50,58,73	1.63	6 (12%)	58,95,113	1.62	7 (12%)
40	KC2	i	318	22	48,53,53	3.53	23 (47%)	54,89,89	3.84	28 (51%)
29	CLA	s	403	13	65,73,73	1.46	7 (10%)	76,113,113	1.50	8 (10%)
29	CLA	c	301	14	51,59,73	1.66	5 (9%)	59,96,113	1.57	6 (10%)
29	CLA	j	302	18	65,73,73	1.48	6 (9%)	76,113,113	1.40	6 (7%)
40	KC2	k	613	-	48,53,53	1.67	10 (20%)	54,89,89	1.00	1 (1%)
40	KC2	n	611	-	48,53,53	3.42	22 (45%)	54,89,89	3.91	27 (50%)
29	CLA	m	609	18	60,68,73	1.49	6 (10%)	70,107,113	1.46	7 (10%)
29	CLA	A	832	1	65,73,73	1.47	5 (7%)	76,113,113	1.39	9 (11%)
32	WVN	I	101	-	40,41,41	5.69	19 (47%)	50,56,56	6.28	32 (64%)
29	CLA	B	830	2	50,58,73	1.66	7 (14%)	58,95,113	1.58	10 (17%)
31	LHG	J	104	29	32,32,48	0.75	2 (6%)	35,38,54	1.24	3 (8%)
34	SF4	C	102	3	0,12,12	-	-	-	-	-
29	CLA	a	308	15	65,73,73	1.43	6 (9%)	76,113,113	1.46	6 (7%)
29	CLA	i	309	31	46,54,73	1.74	6 (13%)	53,90,113	1.61	6 (11%)
29	CLA	b	311	16	64,72,73	1.49	5 (7%)	74,111,113	1.64	7 (9%)
29	CLA	A	825	41	65,73,73	1.46	6 (9%)	76,113,113	1.43	10 (13%)
29	CLA	k	604	21	65,73,73	1.47	6 (9%)	76,113,113	1.46	8 (10%)
38	II0	n	618	-	39,43,43	6.47	22 (56%)	50,60,60	6.73	33 (66%)
29	CLA	B	832	41	45,53,73	1.79	7 (15%)	52,89,113	1.65	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	A	848	-	26,26,48	0.68	0	28,29,54	1.44	4 (14%)
29	CLA	m	608	18	65,73,73	1.49	7 (10%)	76,113,113	1.37	7 (9%)
29	CLA	n	602	26	50,58,73	1.64	6 (12%)	58,95,113	1.59	7 (12%)
29	CLA	A	805	1	65,73,73	1.43	6 (9%)	76,113,113	1.44	6 (7%)
29	CLA	A	823	1	55,63,73	1.61	7 (12%)	64,101,113	1.58	9 (14%)
29	CLA	A	840	1	65,73,73	1.43	6 (9%)	76,113,113	1.48	8 (10%)
38	II0	e	314	-	39,43,43	6.43	22 (56%)	50,60,60	6.92	30 (60%)
40	KC2	f	611	-	48,53,53	3.35	21 (43%)	54,89,89	3.92	29 (53%)
29	CLA	l	304	20	65,73,73	1.41	6 (9%)	76,113,113	1.53	8 (10%)
39	IHT	c	315	-	40,42,42	0.20	0	53,58,58	0.79	2 (3%)
29	CLA	B	819	2	65,73,73	1.53	7 (10%)	76,113,113	1.64	10 (13%)
38	II0	e	313	-	39,43,43	6.27	21 (53%)	50,60,60	6.65	30 (60%)
40	KC2	k	611	-	48,53,53	3.48	22 (45%)	54,89,89	3.89	29 (53%)
29	CLA	d	306	23	51,59,73	1.70	6 (11%)	59,96,113	1.53	8 (13%)
29	CLA	A	817	1	65,73,73	1.46	7 (10%)	76,113,113	1.45	8 (10%)
29	CLA	A	804	1	65,73,73	1.44	7 (10%)	76,113,113	1.56	10 (13%)
29	CLA	d	313	23	51,59,73	1.67	6 (11%)	59,96,113	1.63	12 (20%)
29	CLA	g	306	24	65,73,73	1.45	7 (10%)	76,113,113	1.71	13 (17%)
29	CLA	B	839	2	57,65,73	1.58	6 (10%)	66,103,113	1.44	7 (10%)
29	CLA	B	834	2	65,73,73	1.47	7 (10%)	76,113,113	1.49	8 (10%)
32	WVN	B	848	-	40,41,41	5.58	19 (47%)	50,56,56	6.31	34 (68%)
29	CLA	A	809	1	56,64,73	1.58	7 (12%)	65,102,113	1.42	7 (10%)
38	II0	k	618	-	39,43,43	0.27	0	50,60,60	0.76	1 (2%)
40	KC2	d	311	-	48,53,53	3.44	22 (45%)	54,89,89	3.86	30 (55%)

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
37	LMG	F	206	-	-	31/48/68/70	0/1/1/1
29	CLA	h	304	17	1/1/12/20	6/21/99/115	-
38	II0	d	319	-	-	7/21/67/67	0/2/2/2
29	CLA	B	801	41	1/1/15/20	15/37/115/115	-
29	CLA	L	202	9	1/1/11/20	6/18/96/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	WVN	L	205	-	-	16/29/63/63	0/2/2/2
32	WVN	K	103	-	-	14/29/63/63	0/2/2/2
29	CLA	i	306	22	1/1/12/20	7/21/99/115	-
29	CLA	e	311	19	1/1/15/20	16/37/115/115	-
40	KC2	g	313	-	-	8/15/71/71	-
29	CLA	A	811	1	1/1/12/20	5/24/102/115	-
29	CLA	B	808	2	1/1/15/20	5/37/115/115	-
29	CLA	c	311	14	-	7/13/91/115	-
38	II0	k	616	-	-	12/21/67/67	0/2/2/2
29	CLA	a	302	15	1/1/15/20	11/37/115/115	-
29	CLA	d	304	23	1/1/11/20	8/13/91/115	-
29	CLA	A	813	1	1/1/13/20	9/27/105/115	-
29	CLA	B	809	2	1/1/15/20	7/37/115/115	-
29	CLA	i	304	22	1/1/15/20	5/37/115/115	-
29	CLA	A	807	1	1/1/15/20	7/37/115/115	-
31	LHG	f	620	29	-	21/41/41/53	-
38	II0	b	317	-	-	9/21/67/67	0/2/2/2
29	CLA	B	829	2	1/1/15/20	8/37/115/115	-
29	CLA	j	305	18	1/1/15/20	12/37/115/115	-
29	CLA	g	309	24	1/1/15/20	12/37/115/115	-
38	II0	f	618	-	-	12/21/67/67	0/2/2/2
29	CLA	i	312	22	1/1/15/20	14/37/115/115	-
29	CLA	A	833	1	1/1/15/20	12/37/115/115	-
32	WVN	B	849	-	-	14/29/63/63	0/2/2/2
29	CLA	A	819	1	1/1/15/20	19/37/115/115	-
31	LHG	A	842	-	-	23/52/52/53	-
31	LHG	c	316	29	-	19/41/41/53	-
29	CLA	b	312	16	1/1/15/20	16/37/115/115	-
29	CLA	e	305	19	1/1/15/20	8/37/115/115	-
38	II0	d	301	-	-	14/21/67/67	0/2/2/2
38	II0	h	309	-	-	12/17/40/67	0/1/1/2
29	CLA	e	301	19	1/1/11/20	8/13/91/115	-
29	CLA	A	815	41	1/1/11/20	7/13/91/115	-
29	CLA	B	811	2	1/1/13/20	3/25/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	830	1	1/1/14/20	5/31/109/115	-
29	CLA	c	306	14	1/1/12/20	7/22/100/115	-
29	CLA	g	308	24	1/1/12/20	5/21/99/115	-
37	LMG	L	210	-	-	20/40/60/70	0/1/1/1
29	CLA	B	823	41	1/1/14/20	6/36/114/115	-
32	WVN	s	405	-	-	14/29/63/63	0/2/2/2
29	CLA	m	607	18	1/1/12/20	1/21/99/115	-
29	CLA	B	828	2	1/1/12/20	8/19/97/115	-
40	KC2	k	612	21	-	9/15/71/71	-
29	CLA	d	310	23	1/1/10/20	4/8/86/115	-
29	CLA	A	826	1	1/1/15/20	9/37/115/115	-
31	LHG	i	317	29	-	16/41/41/53	-
29	CLA	B	825	2	1/1/15/20	18/37/115/115	-
29	CLA	i	308	22	1/1/15/20	19/37/115/115	-
38	II0	g	319	-	-	13/21/67/67	0/2/2/2
29	CLA	n	604	26	1/1/14/20	11/31/109/115	-
38	II0	m	614	-	-	13/21/67/67	0/2/2/2
40	KC2	i	310	22	-	10/15/71/71	-
29	CLA	h	305	17	1/1/15/20	10/37/115/115	-
29	CLA	f	603	18	1/1/12/20	6/21/99/115	-
39	IHT	b	316	-	-	8/25/65/65	0/2/2/2
29	CLA	e	310	41	1/1/13/20	9/25/103/115	-
31	LHG	L	208	-	-	19/51/51/53	-
29	CLA	j	307	18	1/1/12/20	3/21/99/115	-
32	WVN	F	207	-	-	18/29/63/63	0/2/2/2
38	II0	d	317	-	-	13/21/67/67	0/2/2/2
29	CLA	a	311	15	1/1/15/20	11/37/115/115	-
31	LHG	j	318	29	-	13/34/34/53	-
38	II0	d	315	-	-	11/21/67/67	0/2/2/2
29	CLA	g	312	31	1/1/12/20	3/24/102/115	-
29	CLA	f	608	18	1/1/15/20	7/37/115/115	-
32	WVN	F	204	-	-	14/29/63/63	0/2/2/2
29	CLA	g	316	24	1/1/13/20	8/28/106/115	-
29	CLA	F	203	6	1/1/12/20	9/22/100/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	d	302	23	1/1/14/20	17/34/112/115	-
29	CLA	b	305	16	1/1/15/20	13/37/115/115	-
29	CLA	i	302	22	1/1/15/20	18/37/115/115	-
29	CLA	c	304	14	1/1/14/20	15/34/112/115	-
29	CLA	m	601	18	1/1/10/20	5/10/88/115	-
33	LMU	B	850	-	-	4/21/61/61	0/2/2/2
40	KC2	m	611	18	-	7/15/71/71	-
38	II0	J	103	-	-	14/21/67/67	0/2/2/2
29	CLA	d	308	23	1/1/11/20	7/15/93/115	-
29	CLA	B	806	2	1/1/15/20	14/37/115/115	-
29	CLA	n	607	26	1/1/15/20	10/37/115/115	-
29	CLA	B	840	2	1/1/15/20	5/37/115/115	-
31	LHG	n	619	-	-	20/47/47/53	-
32	WVN	B	847	-	-	14/29/63/63	0/2/2/2
29	CLA	l	301	20	1/1/15/20	11/37/115/115	-
32	WVN	A	845	-	-	17/29/63/63	0/2/2/2
40	KC2	g	314	24,40	-	10/15/71/71	-
40	KC2	g	315	40	-	7/15/71/71	-
29	CLA	A	812	1	1/1/15/20	10/37/115/115	-
32	WVN	l	316	-	-	19/29/63/63	0/2/2/2
38	II0	d	314	-	-	3/21/67/67	0/2/2/2
29	CLA	B	805	2	1/1/15/20	13/37/115/115	-
29	CLA	d	305	23	1/1/12/20	5/21/99/115	-
29	CLA	F	201	41	1/1/15/20	14/37/115/115	-
37	LMG	b	319	-	-	17/37/57/70	0/1/1/1
29	CLA	f	610	31	1/1/15/20	10/37/115/115	-
32	WVN	B	845	-	-	6/29/63/63	0/2/2/2
29	CLA	B	804	-	1/1/15/20	10/37/115/115	-
29	CLA	B	812	2	1/1/15/20	13/37/115/115	-
34	SF4	C	101	3	-	-	0/6/5/5
29	CLA	R	203	25	1/1/13/20	5/25/103/115	-
29	CLA	a	304	15	1/1/12/20	1/21/99/115	-
29	CLA	n	605	26	1/1/12/20	9/21/99/115	-
38	II0	g	321	-	-	3/21/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LMG	c	317	-	-	21/50/70/70	0/1/1/1
38	II0	g	317	-	-	9/21/67/67	0/2/2/2
29	CLA	m	606	18	1/1/15/20	15/37/115/115	-
29	CLA	B	822	41	1/1/15/20	16/37/115/115	-
29	CLA	n	601	26	1/1/11/20	5/13/91/115	-
33	LMU	a	319	-	-	13/21/61/61	0/2/2/2
32	WVN	s	407	-	-	14/29/63/63	0/2/2/2
33	LMU	A	855	-	-	17/20/60/61	0/2/2/2
29	CLA	h	307	17	1/1/12/20	5/21/99/115	-
38	II0	k	619	-	-	11/21/67/67	0/2/2/2
29	CLA	n	609	26	1/1/15/20	11/37/115/115	-
39	IHT	R	204	-	-	1/25/65/65	0/2/2/2
29	CLA	b	308	16	1/1/15/20	11/37/115/115	-
29	CLA	f	604	18	1/1/15/20	13/37/115/115	-
29	CLA	K	102	12	1/1/10/20	4/10/88/115	-
38	II0	n	616	-	-	10/21/67/67	0/2/2/2
29	CLA	B	835	2	1/1/11/20	1/16/94/115	-
29	CLA	O	206	11	1/1/15/20	9/37/115/115	-
32	WVN	B	846	-	-	15/29/63/63	0/2/2/2
29	CLA	c	305	14	1/1/15/20	5/37/115/115	-
29	CLA	A	851	1	1/1/15/20	12/37/115/115	-
38	II0	l	317	-	-	1/21/67/67	0/2/2/2
38	II0	d	316	-	-	11/21/67/67	0/2/2/2
31	LHG	e	317	29	-	21/41/41/53	-
28	CL0	A	801	-	2/2/20/25	9/37/135/135	-
29	CLA	n	613	26	1/1/12/20	8/21/99/115	-
29	CLA	g	302	-	1/1/15/20	17/37/115/115	-
29	CLA	f	601	18	1/1/11/20	4/16/94/115	-
29	CLA	k	603	21	1/1/12/20	0/21/99/115	-
29	CLA	A	806	1	1/1/14/20	5/31/109/115	-
32	WVN	A	847	-	-	18/29/63/63	0/2/2/2
29	CLA	h	312	41	1/1/15/20	6/37/115/115	-
29	CLA	c	309	31	1/1/11/20	4/13/91/115	-
29	CLA	f	607	18	1/1/15/20	13/37/115/115	-
29	CLA	h	302	17	1/1/12/20	6/19/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	810	1	1/1/15/20	17/37/115/115	-
32	WVN	i	315	-	-	18/29/63/63	0/2/2/2
29	CLA	B	815	2	1/1/13/20	3/25/103/115	-
37	LMG	O	205	-	-	10/21/41/70	0/1/1/1
29	CLA	k	609	21	1/1/13/20	9/28/106/115	-
38	II0	e	316	-	-	13/21/67/67	0/2/2/2
29	CLA	d	307	23	1/1/11/20	6/13/91/115	-
29	CLA	O	201	31	1/1/12/20	9/22/100/115	-
29	CLA	k	608	21	1/1/15/20	9/37/115/115	-
38	II0	i	314	-	-	10/21/67/67	0/2/2/2
29	CLA	l	309	20	1/1/13/20	8/28/106/115	-
29	CLA	B	810	2	1/1/15/20	8/37/115/115	-
31	LHG	L	209	-	-	23/40/40/53	-
37	LMG	n	620	-	-	18/46/66/70	0/1/1/1
29	CLA	A	822	1	1/1/13/20	13/27/105/115	-
29	CLA	A	829	1	1/1/15/20	6/37/115/115	-
38	II0	c	313	-	-	12/21/67/67	0/2/2/2
38	II0	f	615	-	-	12/21/67/67	0/2/2/2
29	CLA	e	304	-	1/1/15/20	14/37/115/115	-
29	CLA	A	836	1	1/1/15/20	9/37/115/115	-
29	CLA	g	307	24	1/1/12/20	11/21/99/115	-
29	CLA	d	303	23	1/1/12/20	7/21/99/115	-
29	CLA	B	841	2	1/1/15/20	20/37/115/115	-
29	CLA	m	610	31	1/1/13/20	16/25/103/115	-
29	CLA	c	303	14	1/1/12/20	6/21/99/115	-
29	CLA	A	835	1	1/1/15/20	12/37/115/115	-
39	IHT	n	617	-	-	6/25/65/65	0/2/2/2
32	WVN	A	844	-	-	18/29/63/63	0/2/2/2
29	CLA	B	836	41	1/1/15/20	13/37/115/115	-
38	II0	h	310	-	-	11/21/67/67	0/2/2/2
29	CLA	L	203	9	1/1/15/20	5/37/115/115	-
29	CLA	B	833	2	1/1/13/20	5/25/103/115	-
29	CLA	b	310	16	1/1/15/20	11/37/115/115	-
38	II0	g	318	-	-	13/21/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LMG	c	318	29	-	21/38/58/70	0/1/1/1
29	CLA	i	311	-	1/1/14/20	11/31/109/115	-
29	CLA	B	814	2	1/1/15/20	10/37/115/115	-
38	II0	j	301	-	-	14/21/67/67	0/2/2/2
29	CLA	g	323	31	1/1/13/20	7/25/103/115	-
29	CLA	A	808	1	1/1/15/20	8/37/115/115	-
40	KC2	e	309	-	-	9/15/71/71	-
29	CLA	c	307	14	1/1/11/20	9/15/93/115	-
29	CLA	B	826	2	1/1/15/20	9/37/115/115	-
38	II0	i	319	-	-	12/21/67/67	0/2/2/2
29	CLA	a	303	15	1/1/13/20	5/27/105/115	-
29	CLA	j	306	18	1/1/11/20	8/13/91/115	-
38	II0	k	615	-	-	14/21/67/67	0/2/2/2
29	CLA	m	604	18	1/1/15/20	12/37/115/115	-
38	II0	n	615	-	-	12/21/67/67	0/2/2/2
40	KC2	s	401	13	-	7/15/71/71	-
31	LHG	A	843	29	-	6/31/31/53	-
29	CLA	j	310	18	1/1/15/20	13/37/115/115	-
29	CLA	b	306	41	1/1/15/20	13/37/115/115	-
38	II0	n	614	-	-	10/21/67/67	0/2/2/2
32	WVN	A	846	-	-	15/29/63/63	0/2/2/2
31	LHG	a	318	29	-	27/53/53/53	-
40	KC2	n	612	26	-	12/15/71/71	-
29	CLA	j	303	18	1/1/12/20	9/24/102/115	-
29	CLA	B	817	2	1/1/15/20	12/37/115/115	-
38	II0	l	314	-	-	11/21/67/67	0/2/2/2
38	II0	m	618	-	-	13/21/67/67	0/2/2/2
29	CLA	j	308	18	1/1/12/20	9/21/99/115	-
29	CLA	a	305	41	1/1/15/20	8/37/115/115	-
29	CLA	n	603	26	1/1/12/20	9/21/99/115	-
38	II0	a	313	-	-	12/21/67/67	0/2/2/2
38	II0	e	312	-	-	14/21/67/67	0/2/2/2
38	II0	l	315	-	-	11/21/67/67	0/2/2/2
32	WVN	M	101	-	-	17/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	WVN	R	202	-	-	15/29/63/63	0/2/2/2
29	CLA	A	828	1	1/1/15/20	7/37/115/115	-
32	WVN	L	201	-	-	22/29/63/63	0/2/2/2
29	CLA	s	402	13	1/1/15/20	21/37/115/115	-
29	CLA	k	601	21	1/1/12/20	5/21/99/115	-
29	CLA	j	309	18	1/1/11/20	4/13/91/115	-
31	LHG	b	318	-	-	27/53/53/53	-
29	CLA	h	303	17	1/1/12/20	6/19/97/115	-
29	CLA	B	824	2	1/1/15/20	3/37/115/115	-
39	IHT	g	320	-	-	5/25/65/65	0/2/2/2
35	SQD	A	853	-	-	19/49/69/69	0/1/1/1
29	CLA	A	816	1	1/1/15/20	16/37/115/115	-
29	CLA	A	818	1	1/1/15/20	15/37/115/115	-
38	II0	b	314	-	-	13/21/67/67	0/2/2/2
29	CLA	A	839	1	1/1/14/20	3/31/109/115	-
32	WVN	F	205	-	-	21/29/63/63	0/2/2/2
34	SF4	A	852	1,2	-	-	0/6/5/5
29	CLA	B	818	41	1/1/15/20	12/37/115/115	-
29	CLA	l	303	20	1/1/11/20	6/16/94/115	-
39	IHT	c	319	-	-	8/25/65/65	0/2/2/2
29	CLA	a	312	15	1/1/11/20	6/17/95/115	-
29	CLA	A	803	1	1/1/13/20	7/25/103/115	-
29	CLA	g	311	24	1/1/15/20	19/37/115/115	-
29	CLA	K	101	41	1/1/15/20	17/37/115/115	-
29	CLA	A	820	41	1/1/15/20	7/37/115/115	-
39	IHT	O	204	-	-	4/25/65/65	0/2/2/2
29	CLA	k	614	21	1/1/12/20	11/21/99/115	-
39	IHT	f	617	-	-	2/25/65/65	0/2/2/2
31	LHG	f	619	-	-	18/53/53/53	-
37	LMG	Q	301	-	-	16/33/53/70	0/1/1/1
29	CLA	B	803	2	1/1/15/20	15/37/115/115	-
29	CLA	f	605	18	1/1/11/20	4/13/91/115	-
29	CLA	c	302	14	1/1/14/20	16/31/109/115	-
29	CLA	b	309	37	1/1/15/20	3/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	820	2	1/1/15/20	11/37/115/115	-
29	CLA	B	837	2	1/1/15/20	15/37/115/115	-
29	CLA	l	308	20	1/1/15/20	6/37/115/115	-
36	DGD	j	319	-	-	23/51/91/95	0/2/2/2
29	CLA	e	308	31	1/1/11/20	1/15/93/115	-
29	CLA	d	309	23	1/1/10/20	2/8/86/115	-
29	CLA	e	303	19	1/1/12/20	6/21/99/115	-
29	CLA	j	313	-	1/1/12/20	10/21/99/115	-
32	WVN	e	315	-	-	16/29/63/63	0/2/2/2
38	II0	h	311	-	-	12/21/67/67	0/2/2/2
32	WVN	h	308	-	-	18/29/63/63	0/2/2/2
38	II0	m	616	-	-	11/21/67/67	0/2/2/2
29	CLA	l	312	20	1/1/13/20	8/27/105/115	-
29	CLA	g	305	24,39	1/1/15/20	5/37/115/115	-
29	CLA	A	827	1	1/1/14/20	7/34/112/115	-
29	CLA	b	313	31	1/1/12/20	5/21/99/115	-
29	CLA	B	821	2	1/1/12/20	5/23/101/115	-
29	CLA	f	602	18	1/1/15/20	18/37/115/115	-
38	II0	O	203	-	-	4/21/67/67	0/2/2/2
38	II0	k	620	-	-	13/21/67/67	0/2/2/2
36	DGD	B	844	-	-	28/55/95/95	0/2/2/2
29	CLA	a	307	15	1/1/15/20	15/37/115/115	-
29	CLA	k	602	21	1/1/15/20	17/37/115/115	-
29	CLA	B	842	31	1/1/15/20	5/37/115/115	-
29	CLA	l	307	20	1/1/15/20	5/37/115/115	-
38	II0	k	617	-	-	4/21/67/67	0/2/2/2
32	WVN	R	201	-	-	18/29/63/63	0/2/2/2
40	KC2	c	310	14	-	10/15/71/71	-
29	CLA	c	312	14	1/1/15/20	10/37/115/115	-
29	CLA	b	303	16	1/1/13/20	11/25/103/115	-
38	II0	f	616	-	-	12/21/67/67	0/2/2/2
29	CLA	e	307	19	1/1/15/20	13/37/115/115	-
29	CLA	m	605	18	1/1/10/20	5/10/88/115	-
29	CLA	i	305	22	-	13/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	j	304	18	1/1/12/20	6/21/99/115	-
32	WVN	L	206	-	-	17/29/63/63	0/2/2/2
38	II0	a	317	-	-	13/21/67/67	0/2/2/2
29	CLA	A	850	41	1/1/15/20	3/37/115/115	-
29	CLA	g	304	24	1/1/15/20	18/37/115/115	-
29	CLA	h	301	41	1/1/15/20	9/37/115/115	-
39	IHT	m	617	-	-	2/25/65/65	0/2/2/2
31	LHG	g	301	29	-	24/49/49/53	-
29	CLA	B	838	2	1/1/15/20	13/37/115/115	-
29	CLA	b	307	16	1/1/14/20	6/33/111/115	-
31	LHG	s	408	-	-	12/34/34/53	-
29	CLA	A	821	1	1/1/11/20	6/18/96/115	-
40	KC2	d	312	23	-	12/15/71/71	-
38	II0	j	316	-	-	13/21/67/67	0/2/2/2
29	CLA	B	827	2	1/1/12/20	5/21/99/115	-
29	CLA	f	613	18	1/1/15/20	16/37/115/115	-
32	WVN	A	854	-	-	19/29/63/63	0/2/2/2
38	II0	j	315	-	-	11/21/67/67	0/2/2/2
30	PQN	A	841	-	-	10/23/43/43	0/2/2/2
40	KC2	s	404	-	-	2/15/71/71	-
29	CLA	L	204	41	1/1/14/20	4/31/109/115	-
29	CLA	a	306	15	1/1/11/20	7/13/91/115	-
29	CLA	l	310	31	1/1/14/20	12/33/111/115	-
29	CLA	g	310	24	1/1/15/20	14/37/115/115	-
38	II0	i	313	-	-	11/21/67/67	0/2/2/2
29	CLA	B	802	41	1/1/15/20	12/37/115/115	-
29	CLA	b	304	16	1/1/12/20	2/22/100/115	-
38	II0	m	615	-	-	12/21/67/67	0/2/2/2
29	CLA	k	605	21	1/1/11/20	5/13/91/115	-
29	CLA	O	202	41	1/1/15/20	8/37/115/115	-
29	CLA	d	318	-	1/1/11/20	6/13/91/115	-
29	CLA	A	838	1	1/1/15/20	9/37/115/115	-
29	CLA	A	837	1	1/1/15/20	12/37/115/115	-
29	CLA	n	608	26	1/1/15/20	16/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	f	606	18	1/1/12/20	4/21/99/115	-
29	CLA	b	302	16	1/1/12/20	4/21/99/115	-
29	CLA	j	314	18	1/1/15/20	12/37/115/115	-
29	CLA	B	813	2	1/1/14/20	13/31/109/115	-
29	CLA	n	606	26	1/1/12/20	3/21/99/115	-
32	WVN	l	302	-	-	16/29/63/63	0/2/2/2
31	LHG	g	322	29	-	17/41/41/53	-
29	CLA	k	607	21	1/1/12/20	6/21/99/115	-
29	CLA	A	834	1	1/1/14/20	8/31/109/115	-
29	CLA	a	310	15	1/1/15/20	9/37/115/115	-
39	IHT	j	317	-	-	2/25/65/65	0/2/2/2
29	CLA	i	307	22	1/1/14/20	9/33/111/115	-
29	CLA	B	807	2	1/1/15/20	8/37/115/115	-
38	II0	b	301	-	-	13/21/67/67	0/2/2/2
29	CLA	m	602	18	1/1/14/20	13/31/109/115	-
39	IHT	g	324	29	-	7/25/65/65	0/2/2/2
40	KC2	l	311	-	-	6/15/71/71	-
29	CLA	f	609	18	1/1/15/20	9/37/115/115	-
37	LMG	F	208	-	-	13/36/56/70	0/1/1/1
29	CLA	i	303	22	1/1/15/20	16/37/115/115	-
29	CLA	n	610	-	1/1/14/20	14/31/109/115	-
29	CLA	f	612	41	1/1/12/20	10/21/99/115	-
29	CLA	m	603	18	1/1/13/20	7/30/108/115	-
29	CLA	j	311	31	1/1/14/20	13/33/111/115	-
29	CLA	k	606	21	1/1/12/20	5/21/99/115	-
29	CLA	F	202	41	1/1/15/20	15/37/115/115	-
38	II0	c	314	-	-	4/21/67/67	0/2/2/2
29	CLA	s	406	41	1/1/15/20	12/37/115/115	-
31	LHG	l	318	29	-	12/36/36/53	-
29	CLA	B	816	2	1/1/15/20	17/37/115/115	-
29	CLA	J	102	8	1/1/10/20	3/10/88/115	-
30	PQN	B	843	-	-	8/23/43/43	0/2/2/2
39	IHT	a	316	-	-	5/25/65/65	0/2/2/2
38	II0	a	315	-	-	11/21/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	a	309	31	1/1/11/20	5/17/95/115	-
29	CLA	e	302	19	1/1/15/20	17/37/115/115	-
38	II0	f	614	-	-	11/21/67/67	0/2/2/2
29	CLA	l	305	20	1/1/12/20	0/21/99/115	-
29	CLA	c	308	14	1/1/15/20	15/37/115/115	-
29	CLA	e	306	19	1/1/15/20	16/37/115/115	-
29	CLA	g	303	24	1/1/10/20	5/10/88/115	-
29	CLA	A	824	41	1/1/15/20	10/37/115/115	-
29	CLA	h	306	17	1/1/13/20	10/28/106/115	-
29	CLA	k	610	-	1/1/12/20	8/21/99/115	-
33	LMU	A	849	-	-	16/21/61/61	0/2/2/2
29	CLA	Q	302	-	1/1/15/20	19/37/115/115	-
31	LHG	a	301	29	-	22/53/53/53	-
31	LHG	c	320	-	-	23/53/53/53	-
31	LHG	m	619	29	-	13/41/41/53	-
32	WVN	J	101	-	-	17/29/63/63	0/2/2/2
38	II0	a	314	-	-	10/21/67/67	0/2/2/2
29	CLA	m	612	41	1/1/12/20	9/21/99/115	-
29	CLA	l	306	20	1/1/15/20	17/37/115/115	-
40	KC2	j	312	18	-	8/15/71/71	-
29	CLA	A	831	1	1/1/15/20	13/37/115/115	-
29	CLA	L	207	41	1/1/12/20	8/21/99/115	-
29	CLA	A	802	-	1/1/15/20	10/37/115/115	-
38	II0	b	315	-	-	10/21/67/67	0/2/2/2
29	CLA	m	613	18	1/1/15/20	15/37/115/115	-
38	II0	l	313	-	-	12/21/67/67	0/2/2/2
29	CLA	B	831	41	1/1/15/20	7/37/115/115	-
38	II0	i	316	-	-	12/21/67/67	0/2/2/2
33	LMU	i	301	-	-	13/21/61/61	0/2/2/2
29	CLA	A	814	1	1/1/12/20	8/19/97/115	-
40	KC2	i	318	22	-	8/15/71/71	-
29	CLA	s	403	13	1/1/15/20	8/37/115/115	-
29	CLA	c	301	14	1/1/12/20	9/21/99/115	-
29	CLA	j	302	18	1/1/15/20	14/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	KC2	k	613	-	-	9/15/71/71	-
40	KC2	n	611	-	-	5/15/71/71	-
29	CLA	m	609	18	1/1/14/20	15/31/109/115	-
29	CLA	A	832	1	1/1/15/20	6/37/115/115	-
32	WVN	I	101	-	-	18/29/63/63	0/2/2/2
29	CLA	B	830	2	1/1/12/20	5/19/97/115	-
31	LHG	J	104	29	-	16/37/37/53	-
34	SF4	C	102	3	-	-	0/6/5/5
29	CLA	a	308	15	1/1/15/20	11/37/115/115	-
29	CLA	i	309	31	1/1/11/20	6/15/93/115	-
29	CLA	b	311	16	1/1/14/20	12/36/114/115	-
29	CLA	A	825	41	1/1/15/20	6/37/115/115	-
29	CLA	k	604	21	1/1/15/20	12/37/115/115	-
38	II0	n	618	-	-	10/21/67/67	0/2/2/2
29	CLA	B	832	41	1/1/11/20	2/13/91/115	-
31	LHG	A	848	-	-	14/27/27/53	-
29	CLA	m	608	18	1/1/15/20	10/37/115/115	-
29	CLA	n	602	26	1/1/12/20	5/19/97/115	-
29	CLA	A	805	1	1/1/15/20	10/37/115/115	-
29	CLA	A	823	1	1/1/13/20	9/25/103/115	-
29	CLA	A	840	1	1/1/15/20	16/37/115/115	-
38	II0	e	314	-	-	11/21/67/67	0/2/2/2
40	KC2	f	611	-	-	8/15/71/71	-
29	CLA	l	304	20	1/1/15/20	14/37/115/115	-
39	IHT	c	315	-	-	6/25/65/65	0/2/2/2
29	CLA	B	819	2	1/1/15/20	18/37/115/115	-
38	II0	e	313	-	-	13/21/67/67	0/2/2/2
40	KC2	k	611	-	-	8/15/71/71	-
29	CLA	d	306	23	1/1/12/20	6/21/99/115	-
29	CLA	A	817	1	1/1/15/20	11/37/115/115	-
29	CLA	A	804	1	1/1/15/20	5/37/115/115	-
29	CLA	d	313	23	1/1/12/20	8/21/99/115	-
29	CLA	g	306	24	1/1/15/20	12/37/115/115	-
29	CLA	B	839	2	1/1/13/20	8/28/106/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	834	2	1/1/15/20	9/37/115/115	-
32	WVN	B	848	-	-	15/29/63/63	0/2/2/2
29	CLA	A	809	1	1/1/13/20	9/27/105/115	-
38	II0	k	618	-	-	5/21/67/67	0/2/2/2
40	KC2	d	311	-	-	12/15/71/71	-

The worst 5 of 3619 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	k	615	II0	C14-C10	20.53	1.57	1.34
38	g	317	II0	C13-C09	20.15	1.57	1.34
38	l	315	II0	C13-C09	20.10	1.57	1.34
38	d	315	II0	C14-C10	19.87	1.57	1.34
38	e	314	II0	C13-C09	19.81	1.57	1.34

The worst 5 of 4922 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	e	314	II0	C24-C22-C10	-25.41	111.10	175.43
38	i	313	II0	C24-C22-C10	-25.20	111.61	175.43
38	m	615	II0	C23-C21-C09	-24.97	112.20	175.43
38	m	616	II0	C23-C21-C09	-24.96	112.23	175.43
38	m	615	II0	C24-C22-C10	-24.96	112.24	175.43

5 of 255 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	A	801	CL0	NA
28	A	801	CL0	ND
29	A	802	CLA	ND
29	A	803	CLA	ND
29	A	804	CLA	ND

5 of 4431 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	A	804	CLA	CHA-CBD-CGD-O1D
29	A	804	CLA	CHA-CBD-CGD-O2D
29	A	805	CLA	C1A-C2A-CAA-CBA
29	A	805	CLA	C3A-C2A-CAA-CBA
29	A	810	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

249 monomers are involved in 448 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	F	206	LMG	3	0
29	h	304	CLA	2	0
29	B	801	CLA	1	0
29	L	202	CLA	1	0
29	i	306	CLA	1	0
29	e	311	CLA	2	0
40	g	313	KC2	1	0
29	A	811	CLA	1	0
29	B	808	CLA	3	0
29	c	311	CLA	2	0
29	a	302	CLA	4	0
29	d	304	CLA	1	0
29	A	813	CLA	1	0
29	B	809	CLA	1	0
29	i	304	CLA	1	0
38	b	317	II0	1	0
29	B	829	CLA	2	0
29	g	309	CLA	1	0
29	i	312	CLA	2	0
29	A	833	CLA	3	0
29	A	819	CLA	1	0
31	A	842	LHG	1	0
31	c	316	LHG	1	0
29	b	312	CLA	6	0
29	e	305	CLA	2	0
29	e	301	CLA	1	0
29	A	830	CLA	1	0
29	c	306	CLA	1	0
29	B	823	CLA	1	0
29	m	607	CLA	4	0
29	B	828	CLA	2	0
29	A	826	CLA	2	0
31	i	317	LHG	2	0
29	B	825	CLA	5	0
29	i	308	CLA	1	0
29	n	604	CLA	2	0
29	h	305	CLA	3	0
39	b	316	IHT	1	0
31	L	208	LHG	1	0
29	a	311	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	g	312	CLA	2	0
29	f	608	CLA	3	0
29	g	316	CLA	4	0
29	F	203	CLA	1	0
29	d	302	CLA	2	0
29	b	305	CLA	5	0
29	i	302	CLA	3	0
33	B	850	LMU	1	0
29	B	806	CLA	2	0
29	n	607	CLA	4	0
29	B	840	CLA	5	0
31	n	619	LHG	3	0
29	l	301	CLA	3	0
40	g	314	KC2	2	0
40	g	315	KC2	3	0
29	A	812	CLA	1	0
29	B	805	CLA	1	0
29	F	201	CLA	2	0
37	b	319	LMG	2	0
29	f	610	CLA	2	0
32	B	845	WVN	1	0
29	B	804	CLA	2	0
29	B	812	CLA	3	0
29	R	203	CLA	5	0
29	n	605	CLA	1	0
38	g	321	II0	1	0
37	c	317	LMG	1	0
38	g	317	II0	1	0
29	B	822	CLA	3	0
33	A	855	LMU	3	0
29	h	307	CLA	1	0
29	n	609	CLA	4	0
38	n	616	II0	1	0
29	B	835	CLA	3	0
29	c	305	CLA	1	0
29	A	851	CLA	4	0
28	A	801	CL0	5	0
29	n	613	CLA	2	0
29	g	302	CLA	3	0
29	f	601	CLA	1	0
29	k	603	CLA	1	0
29	A	806	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	h	312	CLA	1	0
29	f	607	CLA	1	0
29	A	810	CLA	3	0
29	B	815	CLA	2	0
29	k	609	CLA	1	0
29	d	307	CLA	1	0
29	O	201	CLA	1	0
29	k	608	CLA	1	0
29	l	309	CLA	1	0
29	B	810	CLA	1	0
31	L	209	LHG	1	0
37	n	620	LMG	2	0
29	A	822	CLA	3	0
29	A	829	CLA	4	0
29	e	304	CLA	1	0
29	A	836	CLA	3	0
29	B	841	CLA	2	0
29	m	610	CLA	2	0
29	c	303	CLA	2	0
29	A	835	CLA	6	0
39	n	617	IHT	1	0
29	L	203	CLA	4	0
29	B	833	CLA	1	0
29	b	310	CLA	3	0
37	c	318	LMG	3	0
29	B	814	CLA	3	0
29	g	323	CLA	1	0
29	A	808	CLA	1	0
29	c	307	CLA	1	0
29	B	826	CLA	1	0
29	a	303	CLA	1	0
29	j	306	CLA	1	0
29	m	604	CLA	1	0
40	s	401	KC2	1	0
31	A	843	LHG	1	0
29	j	310	CLA	2	0
29	b	306	CLA	4	0
38	n	614	II0	3	0
29	B	817	CLA	4	0
29	j	308	CLA	1	0
29	a	305	CLA	2	0
29	n	603	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	828	CLA	1	0
29	s	402	CLA	2	0
29	j	309	CLA	3	0
31	b	318	LHG	1	0
29	B	824	CLA	2	0
39	g	320	IHT	1	0
29	A	816	CLA	3	0
29	A	818	CLA	3	0
38	b	314	II0	1	0
29	a	312	CLA	1	0
29	A	803	CLA	5	0
29	g	311	CLA	2	0
29	K	101	CLA	3	0
29	A	820	CLA	1	0
29	k	614	CLA	1	0
31	f	619	LHG	3	0
37	Q	301	LMG	4	0
29	B	803	CLA	2	0
29	c	302	CLA	1	0
29	b	309	CLA	3	0
29	B	820	CLA	3	0
29	B	837	CLA	1	0
29	l	308	CLA	2	0
36	j	319	DGD	3	0
29	j	313	CLA	1	0
29	l	312	CLA	1	0
29	g	305	CLA	3	0
29	A	827	CLA	6	0
29	b	313	CLA	3	0
29	B	821	CLA	2	0
29	f	602	CLA	2	0
36	B	844	DGD	4	0
29	a	307	CLA	6	0
29	k	602	CLA	3	0
29	B	842	CLA	3	0
29	c	312	CLA	2	0
29	b	303	CLA	1	0
29	e	307	CLA	3	0
29	i	305	CLA	1	0
29	j	304	CLA	2	0
29	A	850	CLA	2	0
29	g	304	CLA	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	h	301	CLA	3	0
31	g	301	LHG	1	0
29	B	838	CLA	2	0
29	b	307	CLA	1	0
31	s	408	LHG	3	0
40	d	312	KC2	1	0
29	B	827	CLA	2	0
29	f	613	CLA	3	0
30	A	841	PQN	4	0
40	s	404	KC2	2	0
29	L	204	CLA	1	0
29	l	310	CLA	1	0
29	g	310	CLA	1	0
29	O	202	CLA	1	0
29	A	838	CLA	4	0
29	A	837	CLA	3	0
29	n	608	CLA	4	0
29	f	606	CLA	2	0
29	b	302	CLA	2	0
29	j	314	CLA	3	0
29	B	813	CLA	3	0
29	k	607	CLA	2	0
29	A	834	CLA	1	0
29	a	310	CLA	1	0
29	i	307	CLA	2	0
29	B	807	CLA	3	0
29	m	602	CLA	6	0
39	g	324	IHT	4	0
40	l	311	KC2	3	0
37	F	208	LMG	1	0
29	n	610	CLA	4	0
29	m	603	CLA	2	0
29	j	311	CLA	1	0
29	F	202	CLA	2	0
29	s	406	CLA	1	0
29	B	816	CLA	2	0
30	B	843	PQN	1	0
29	a	309	CLA	2	0
29	e	302	CLA	4	0
29	l	305	CLA	1	0
29	c	308	CLA	5	0
29	e	306	CLA	2	0

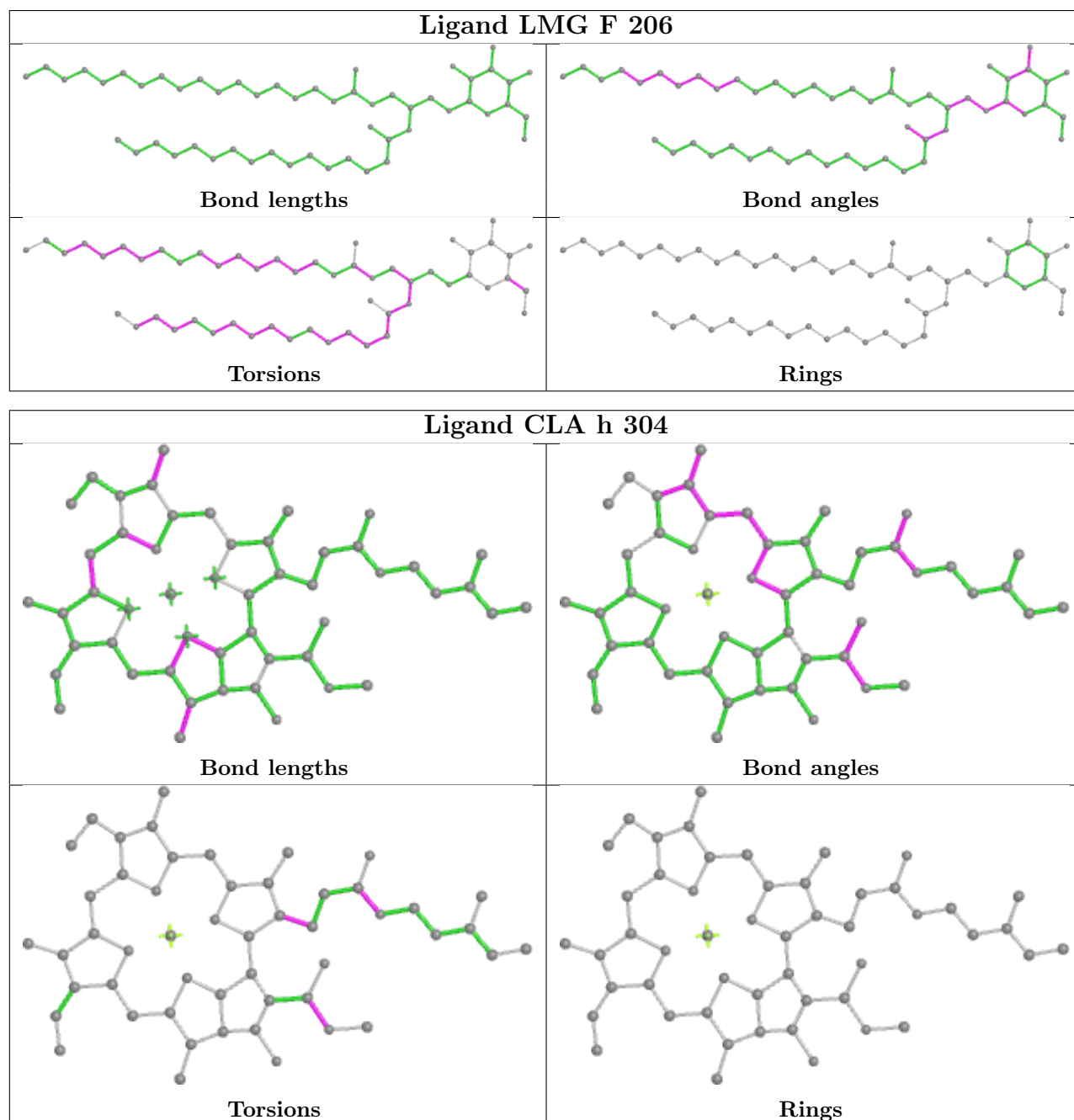
Continued on next page...

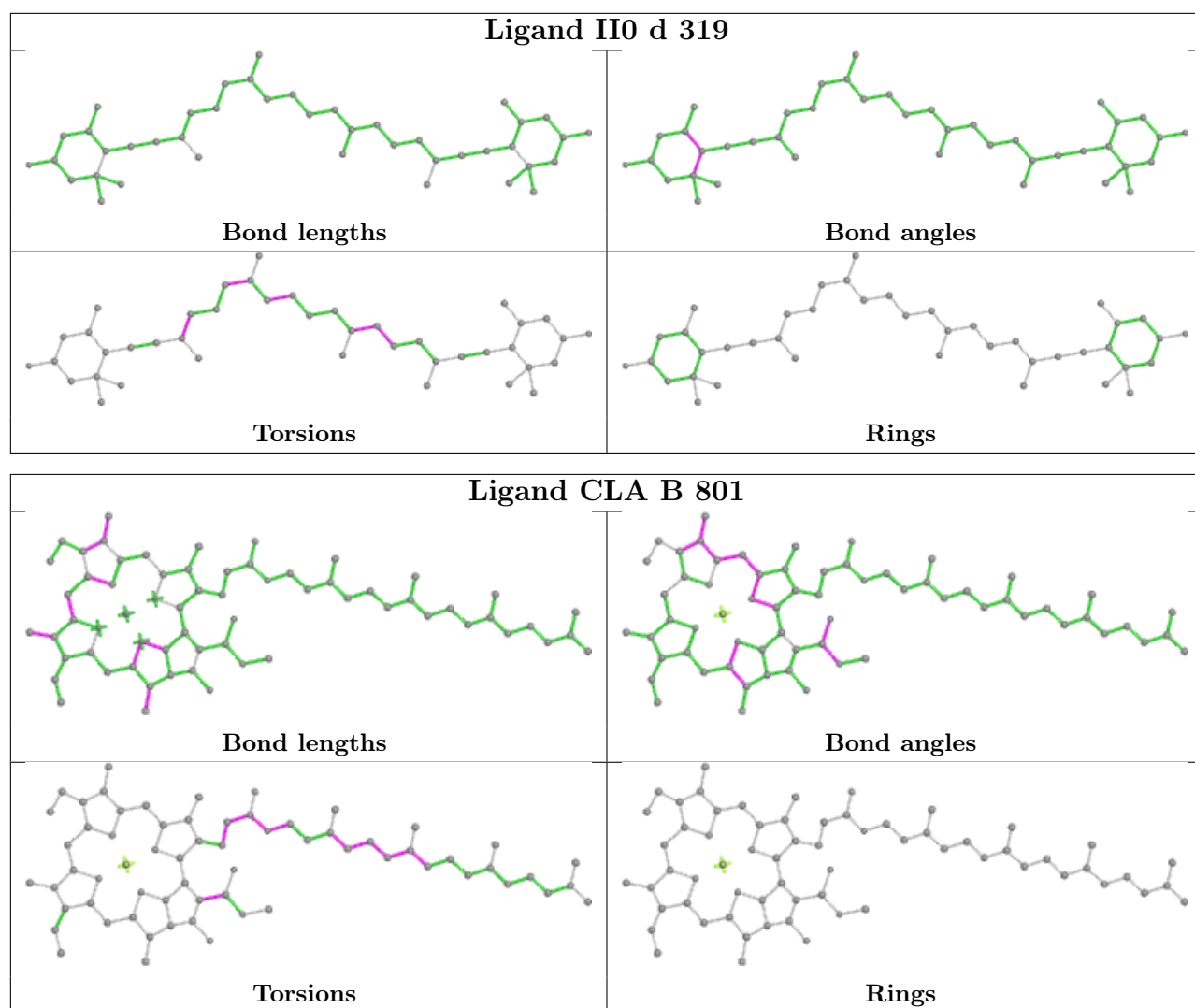
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	824	CLA	2	0
29	h	306	CLA	2	0
29	k	610	CLA	1	0
29	Q	302	CLA	1	0
31	a	301	LHG	3	0
31	c	320	LHG	3	0
31	m	619	LHG	1	0
29	l	306	CLA	1	0
29	A	831	CLA	1	0
29	L	207	CLA	1	0
29	A	802	CLA	1	0
29	m	613	CLA	4	0
29	B	831	CLA	3	0
29	A	814	CLA	3	0
40	i	318	KC2	2	0
29	s	403	CLA	1	0
29	c	301	CLA	1	0
29	j	302	CLA	1	0
40	n	611	KC2	1	0
29	A	832	CLA	4	0
29	B	830	CLA	4	0
31	J	104	LHG	3	0
29	a	308	CLA	2	0
29	b	311	CLA	4	0
29	k	604	CLA	2	0
29	B	832	CLA	1	0
31	A	848	LHG	1	0
29	m	608	CLA	1	0
29	n	602	CLA	1	0
29	A	823	CLA	4	0
29	A	840	CLA	5	0
40	f	611	KC2	1	0
29	l	304	CLA	1	0
29	B	819	CLA	5	0
29	d	306	CLA	1	0
29	A	817	CLA	2	0
29	A	804	CLA	4	0
29	d	313	CLA	3	0
29	g	306	CLA	1	0
29	B	834	CLA	4	0
38	k	618	II0	1	0

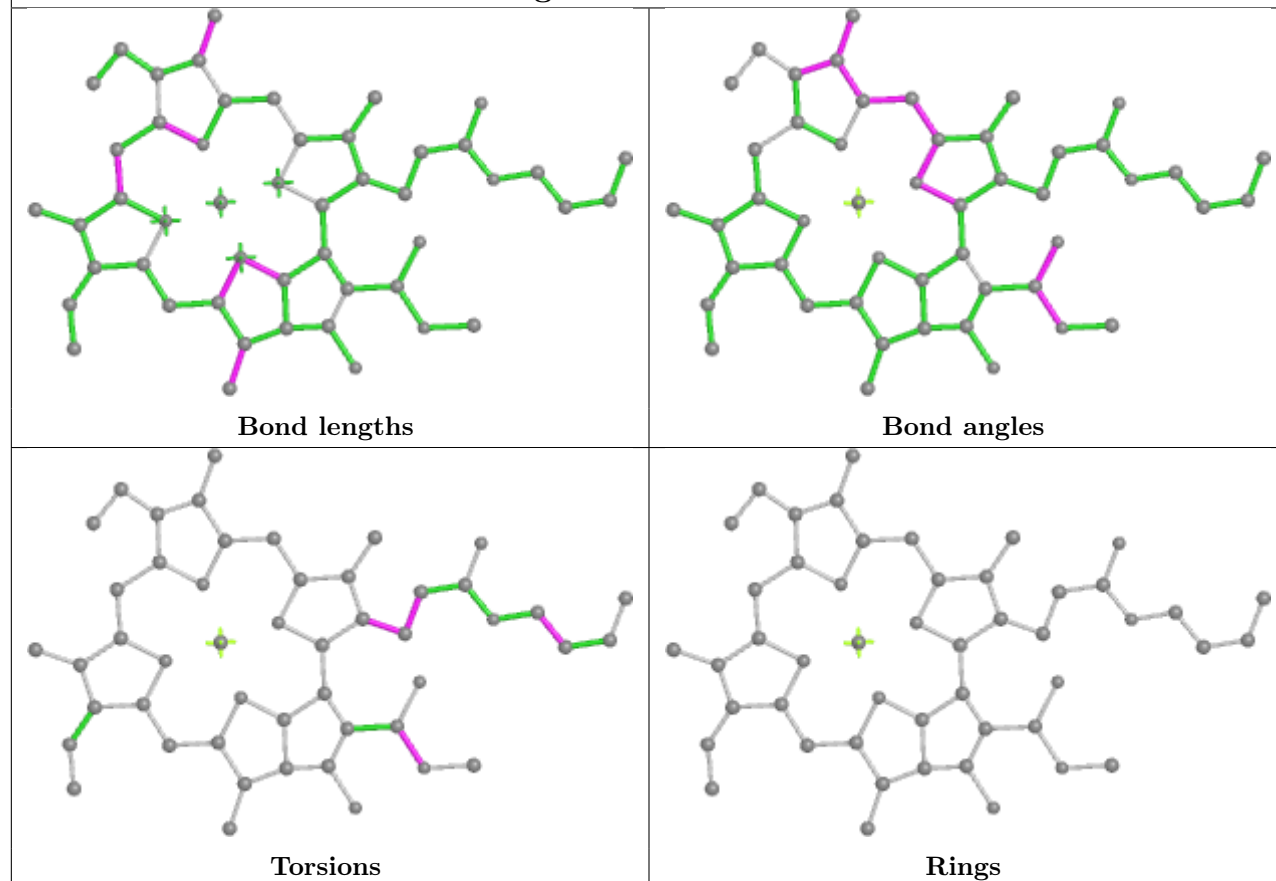
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

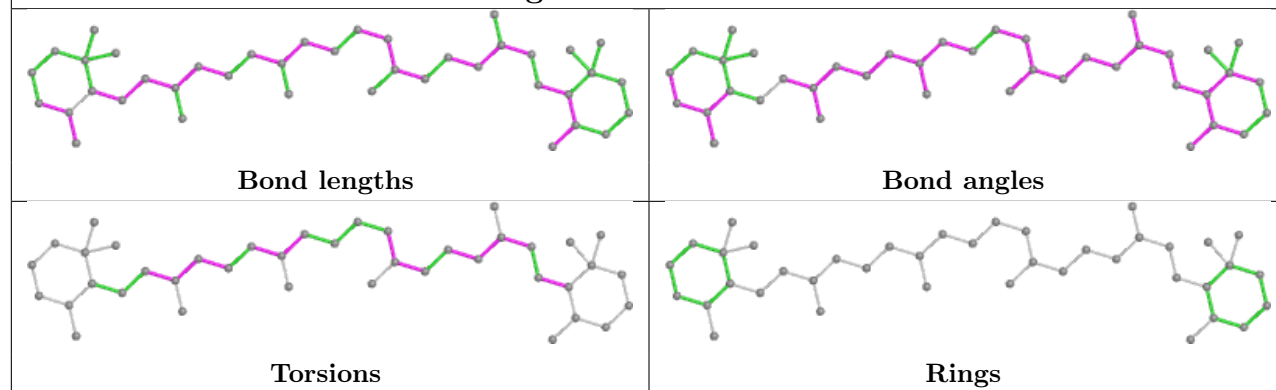


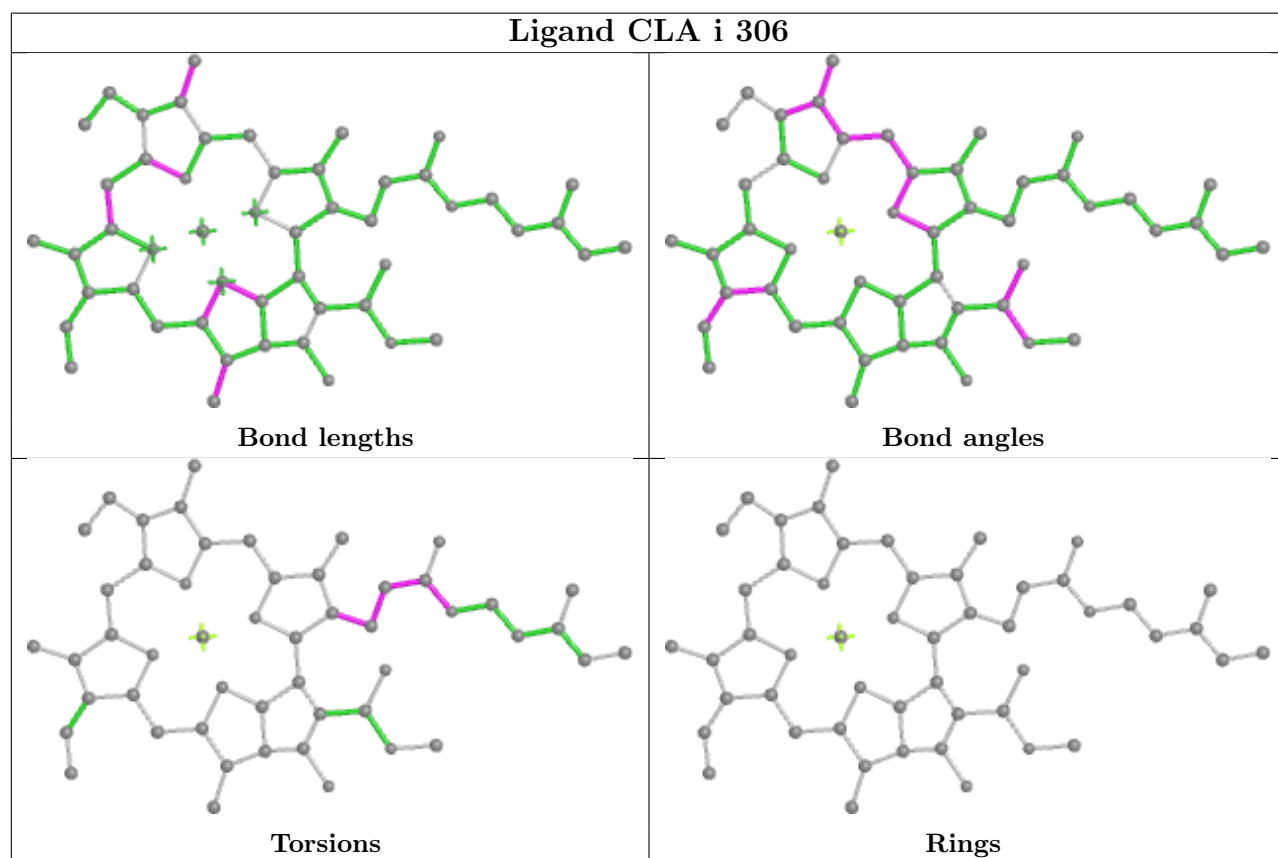
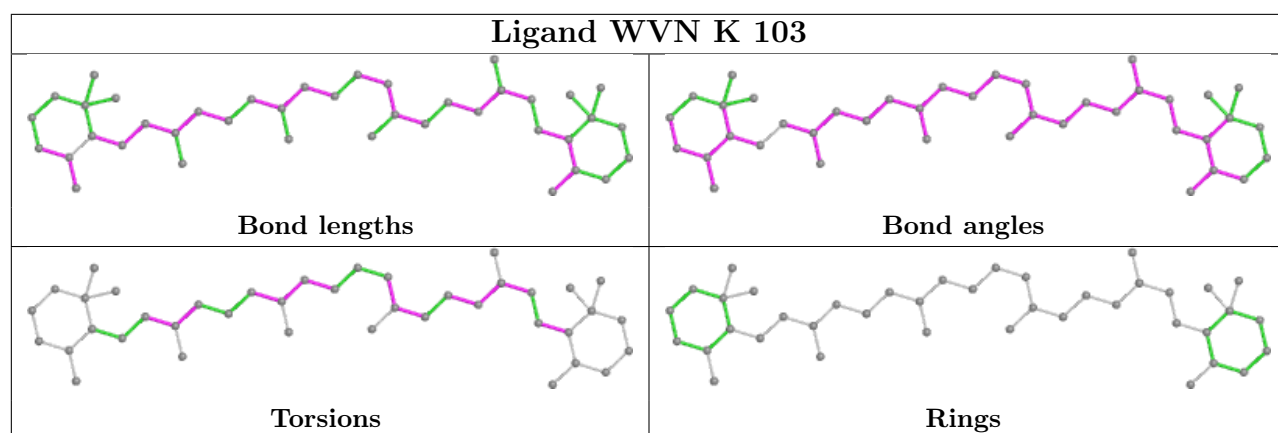


Ligand CLA L 202

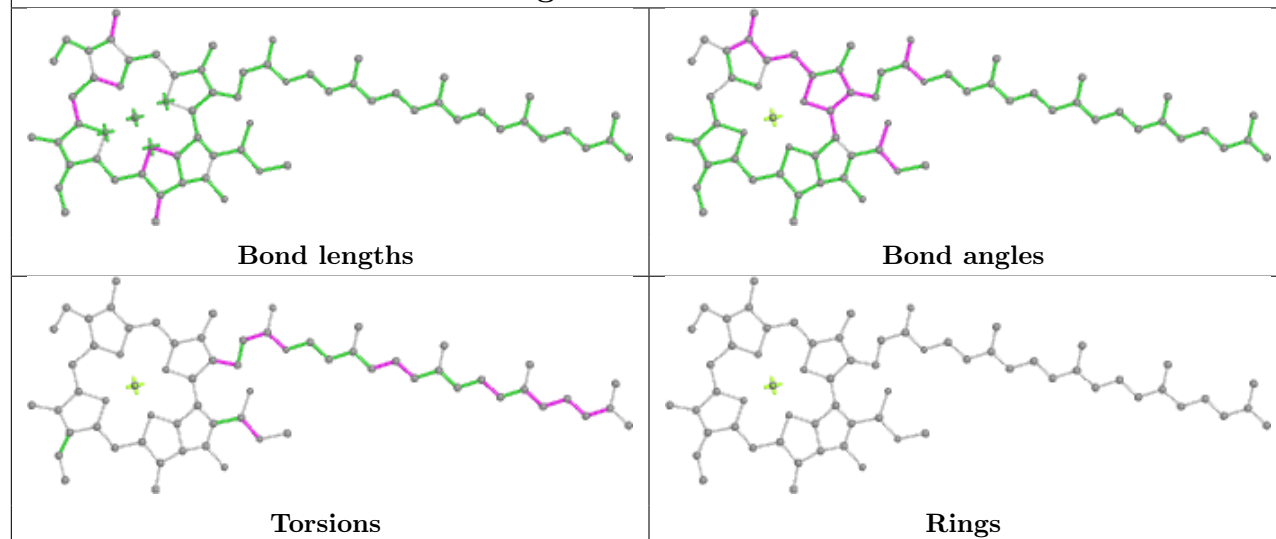


Ligand WVN L 205

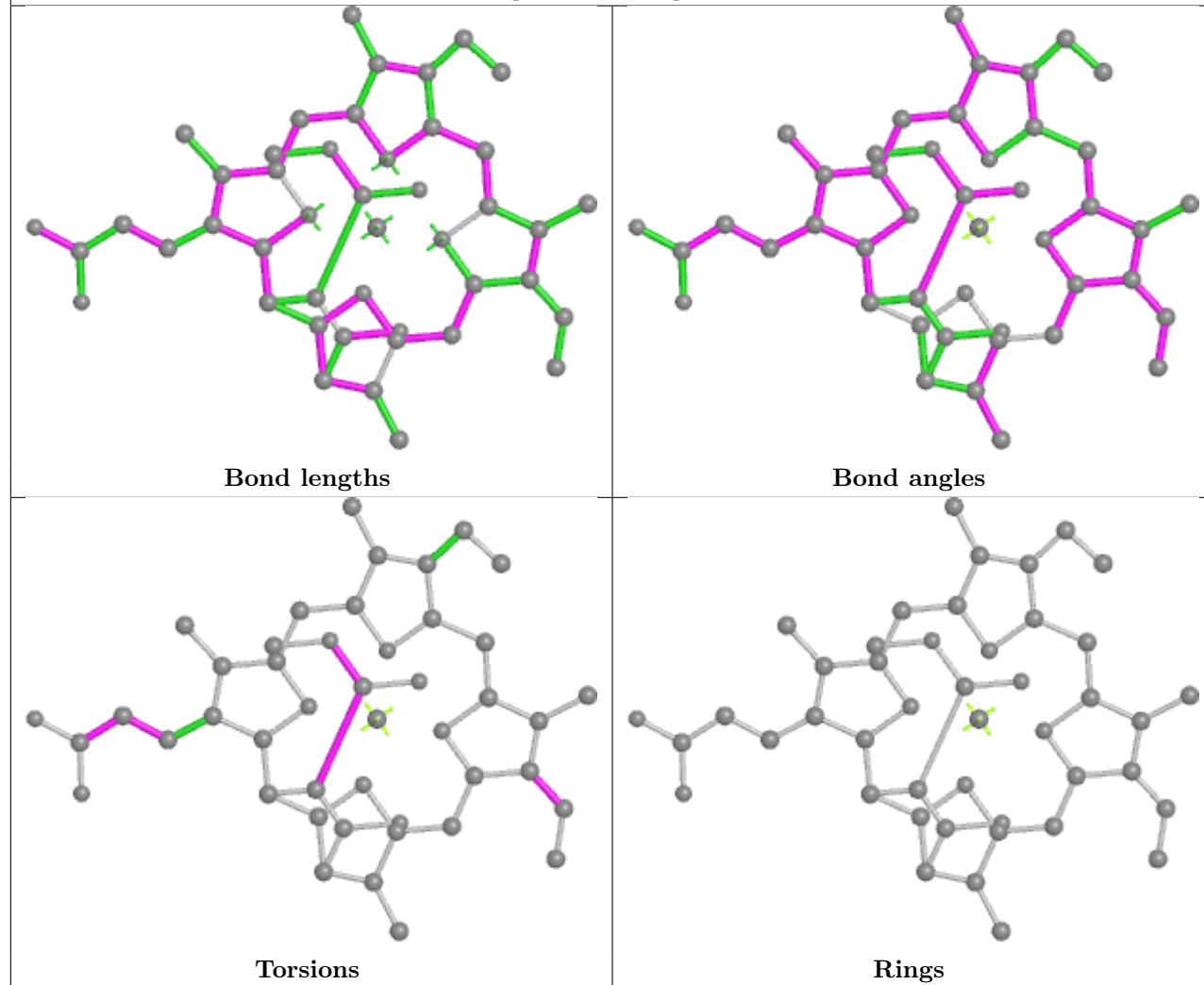




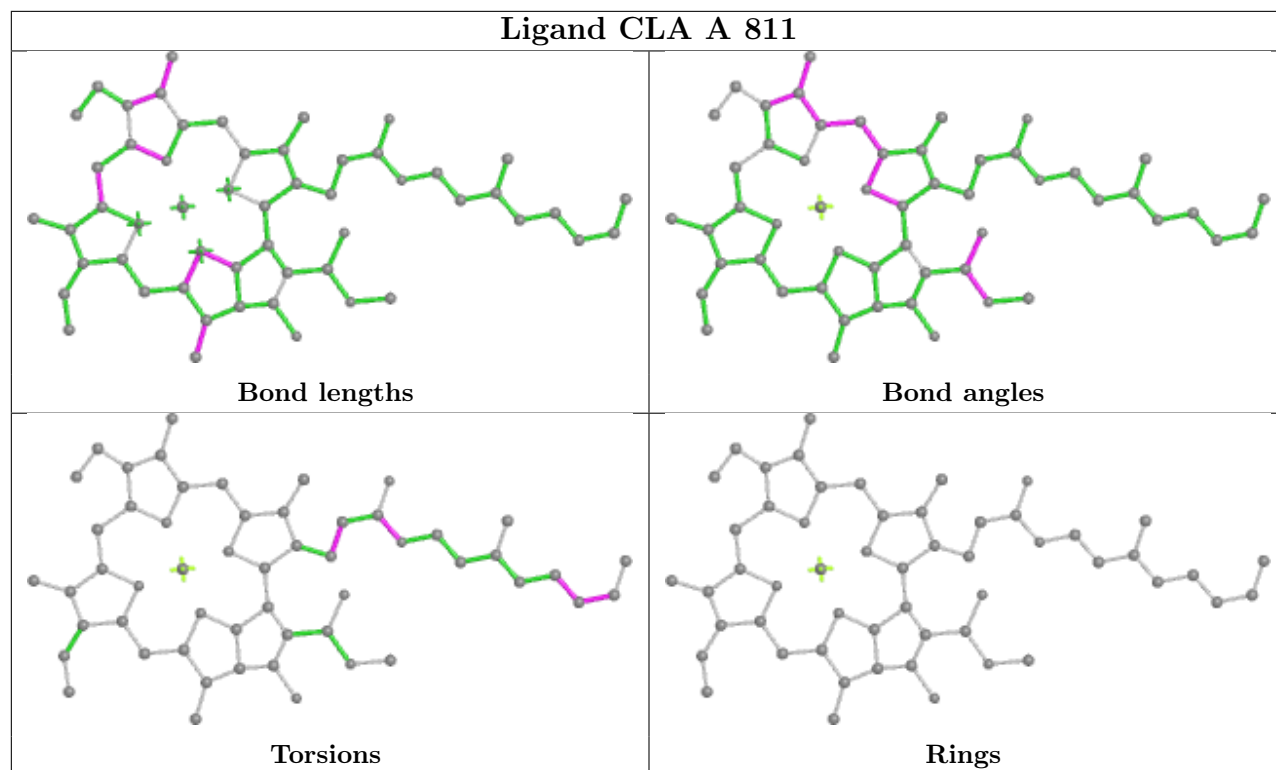
Ligand CLA e 311



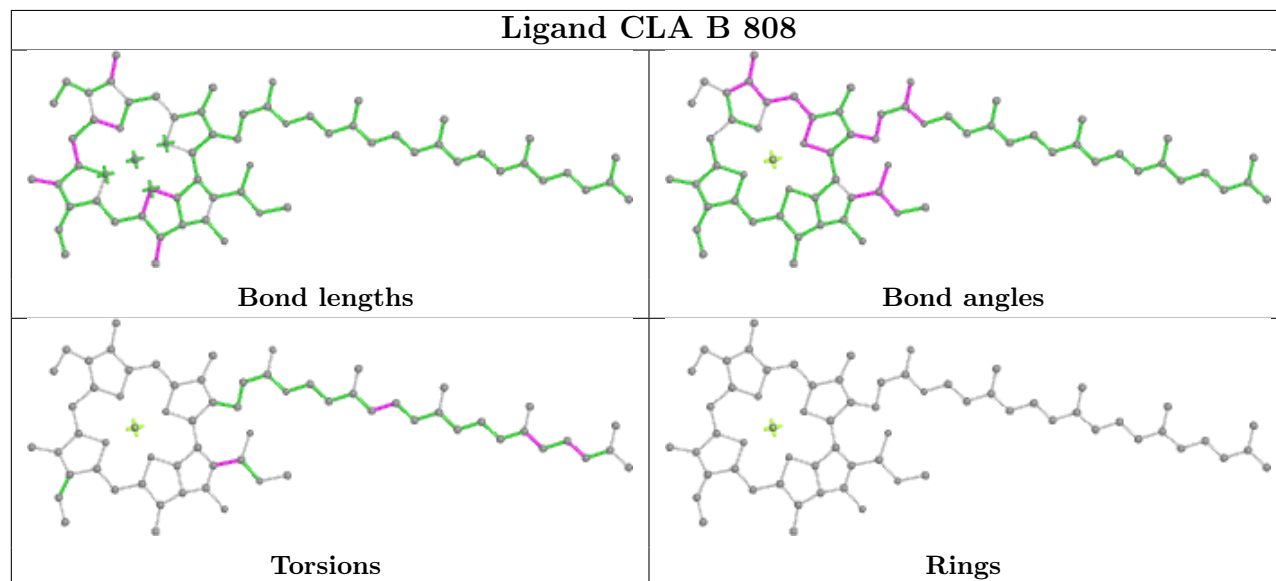
Ligand KC2 g 313



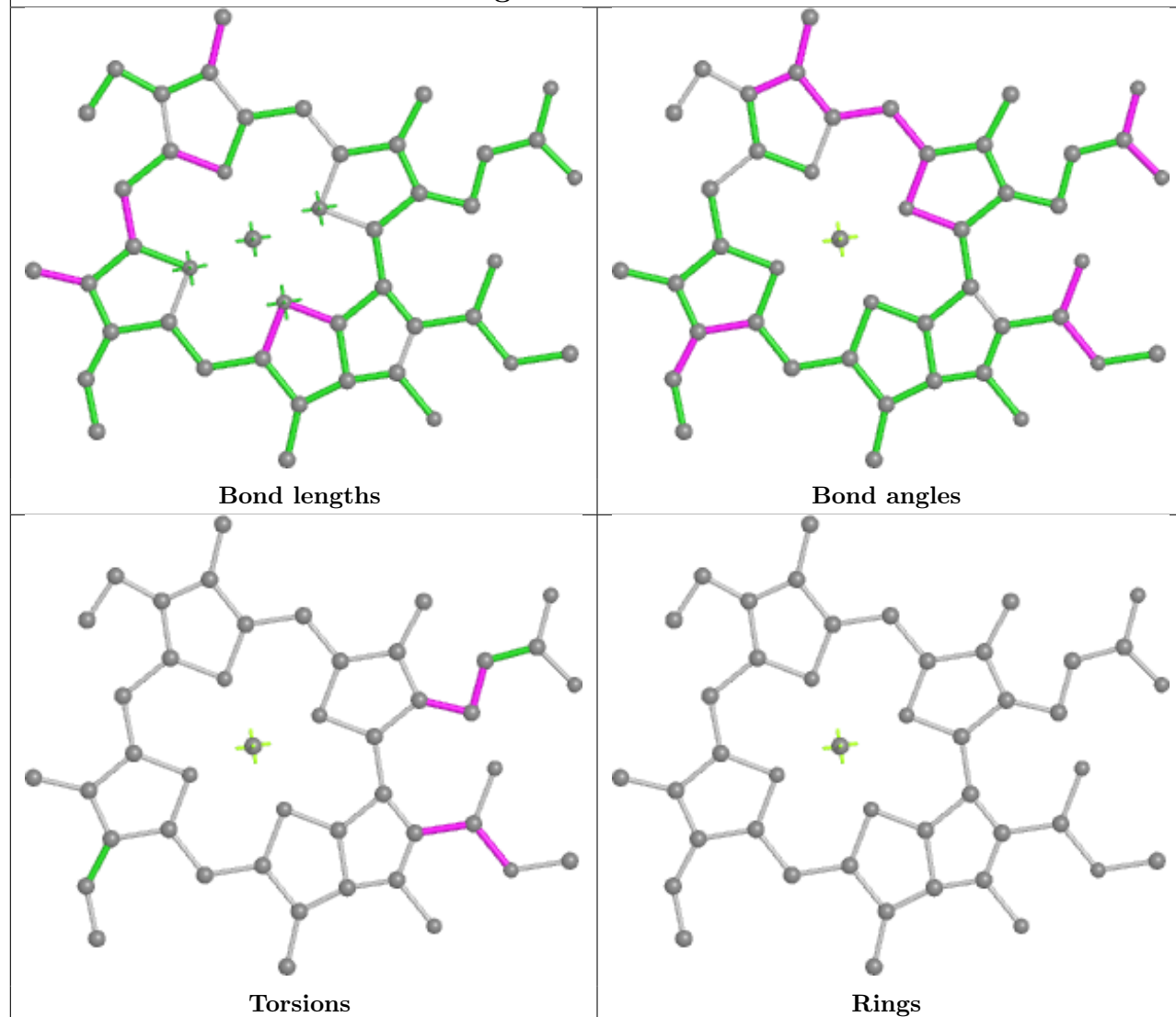
Ligand CLA A 811



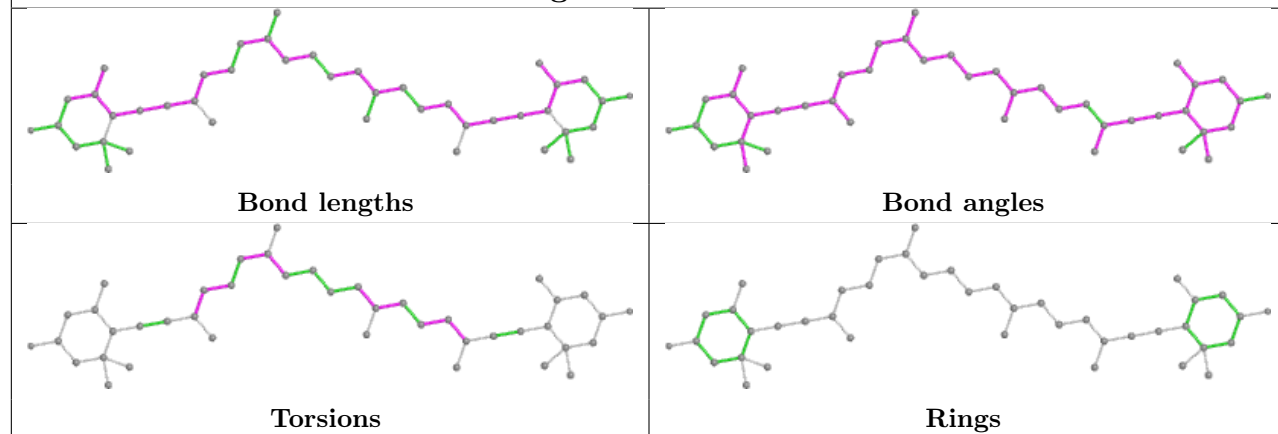
Ligand CLA B 808



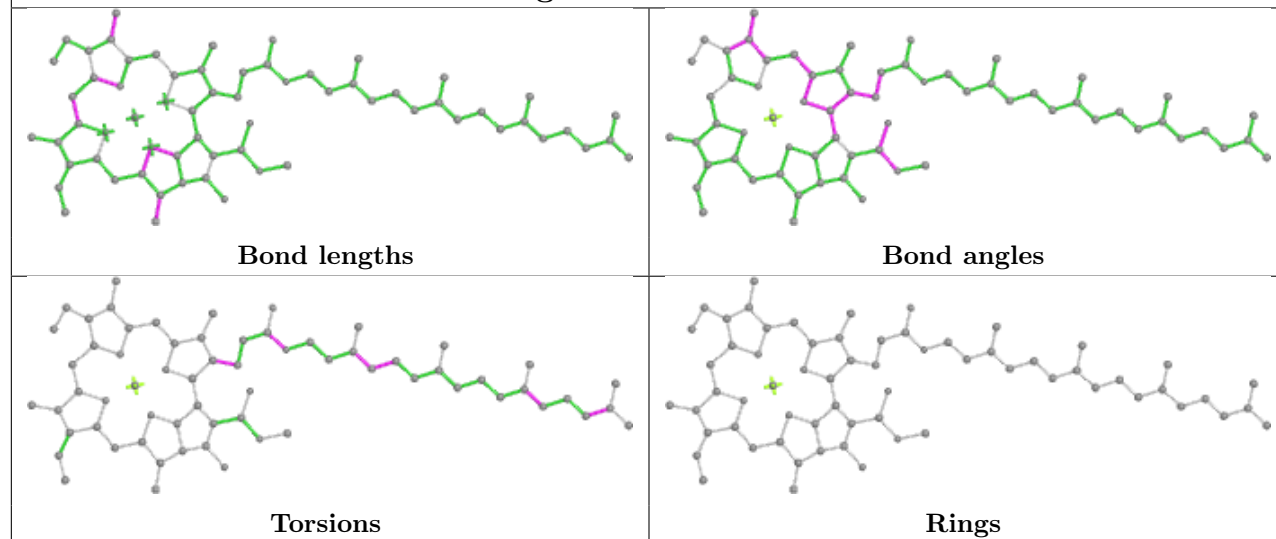
Ligand CLA c 311



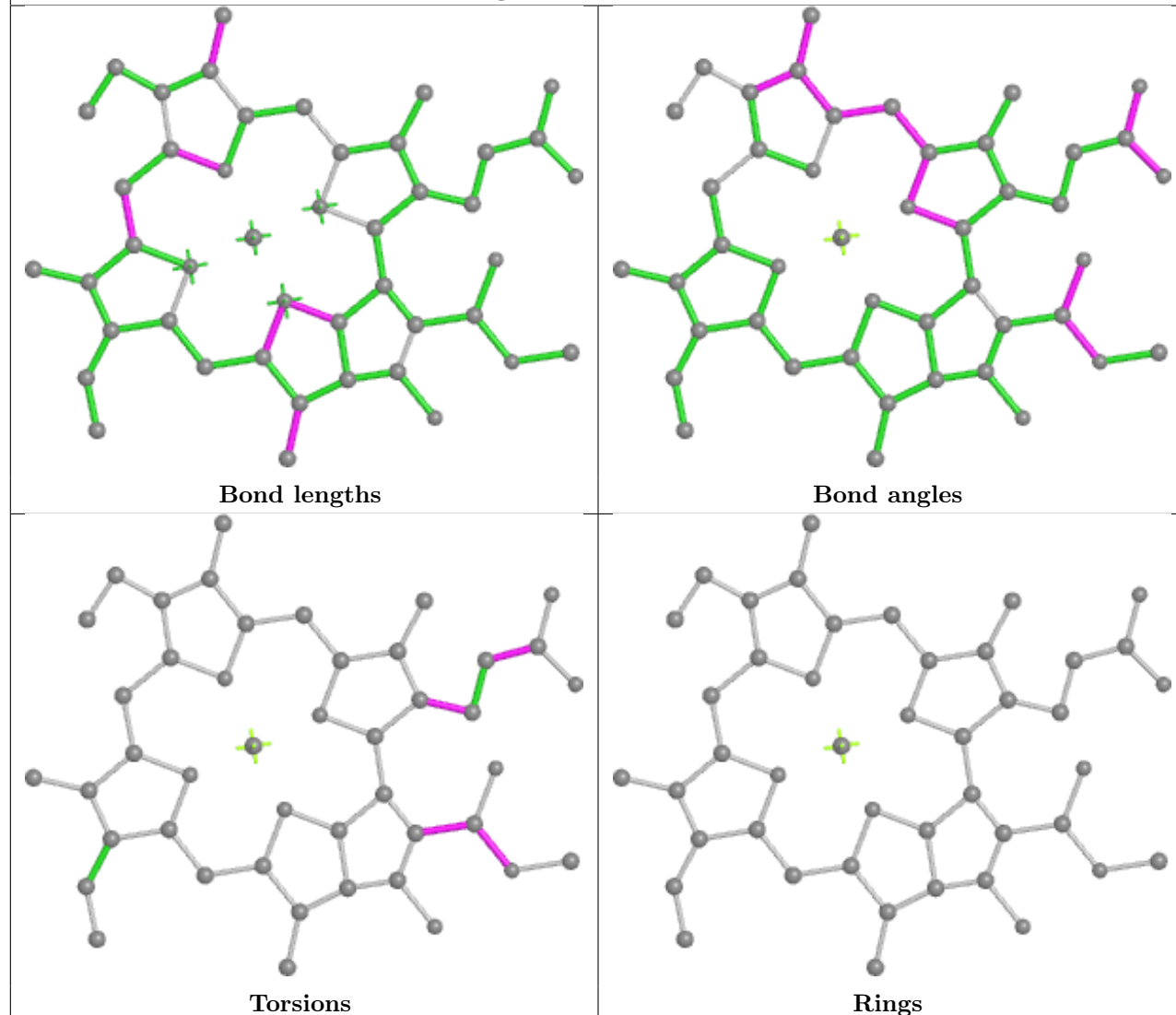
Ligand II0 k 616

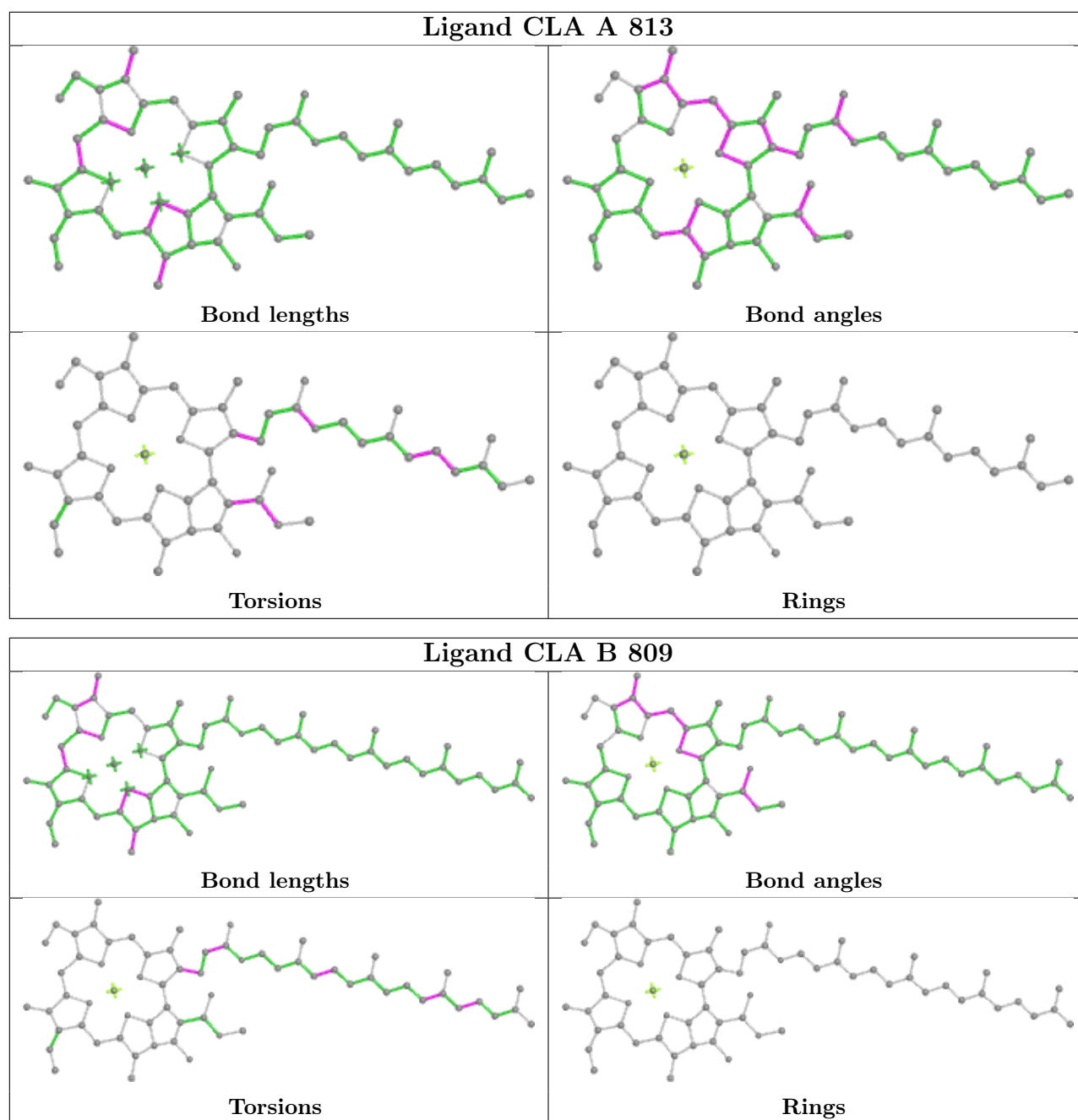


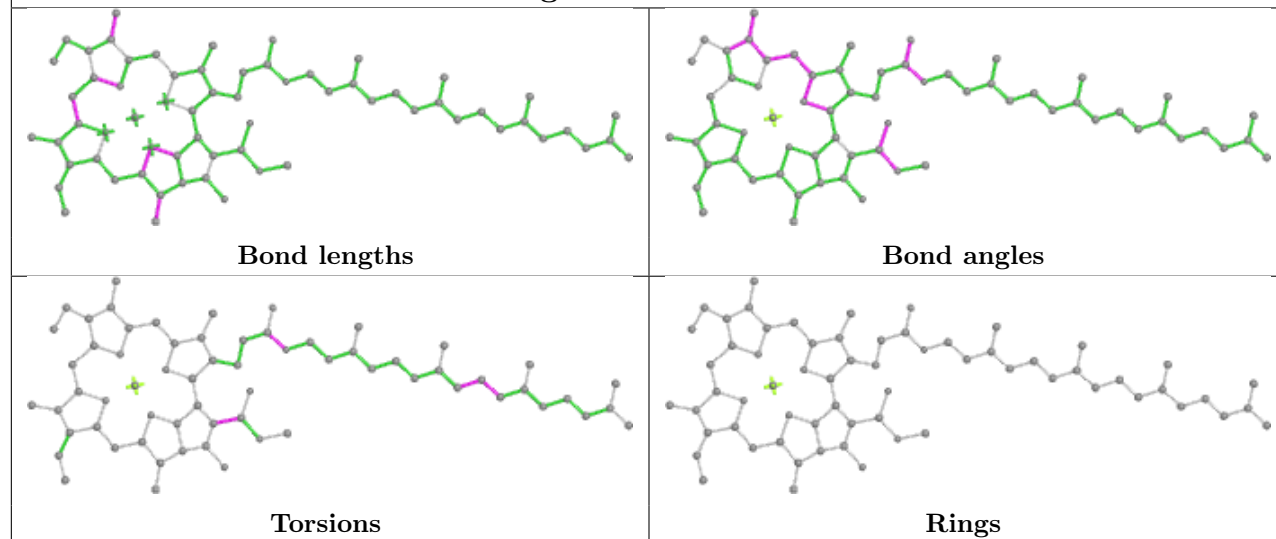
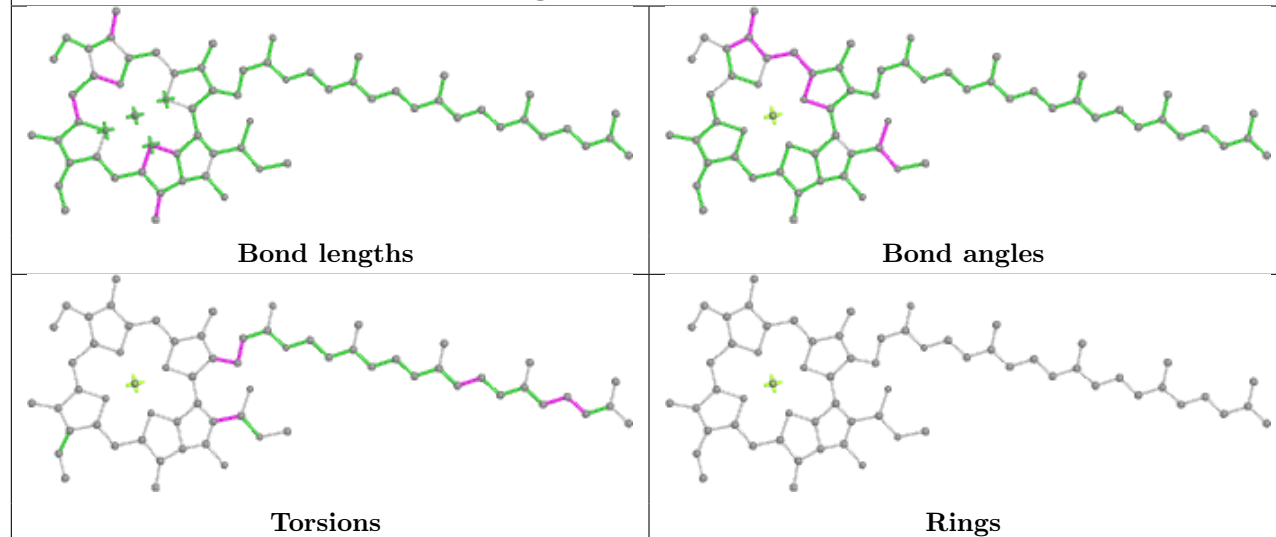
Ligand CLA a 302

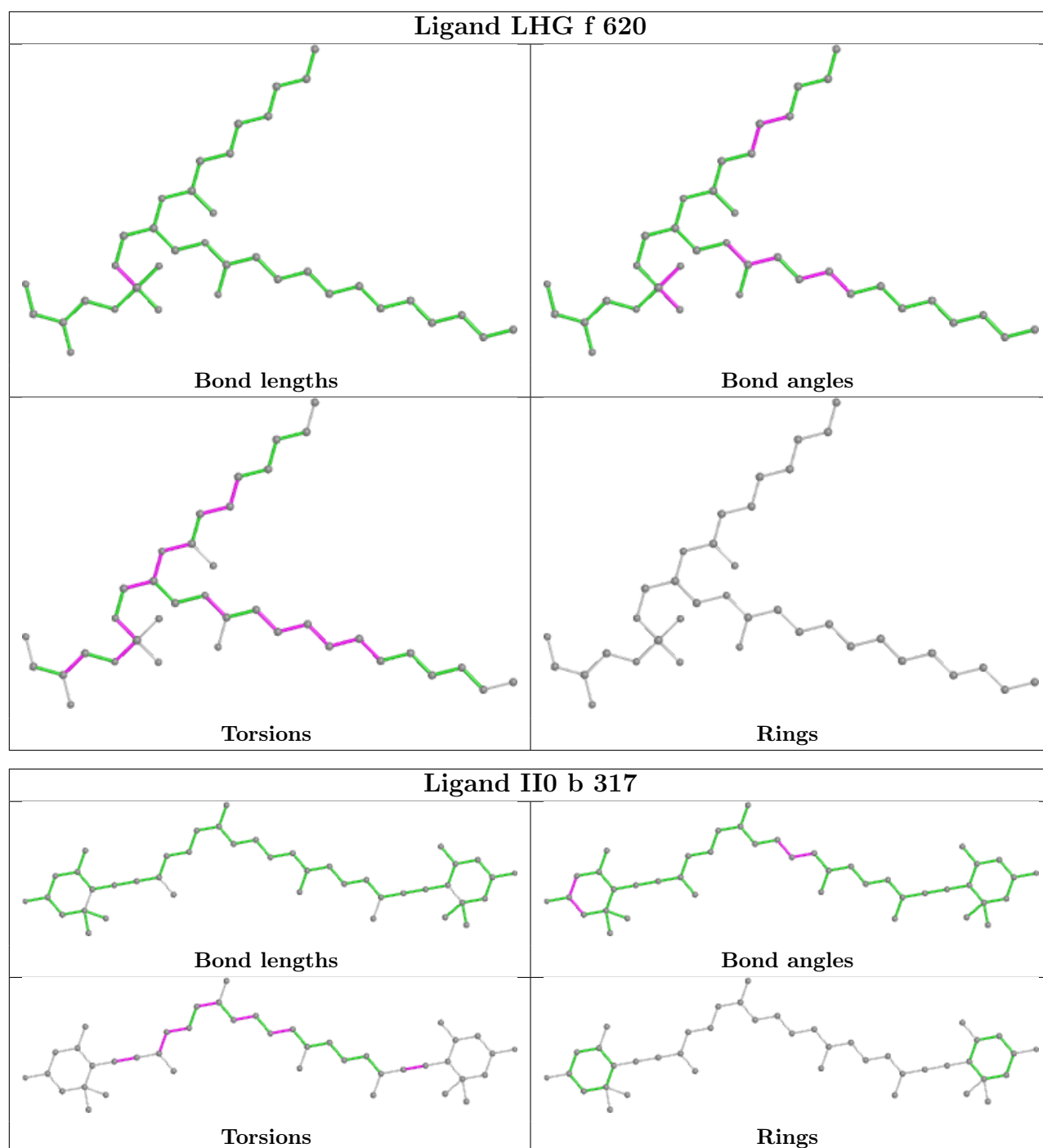


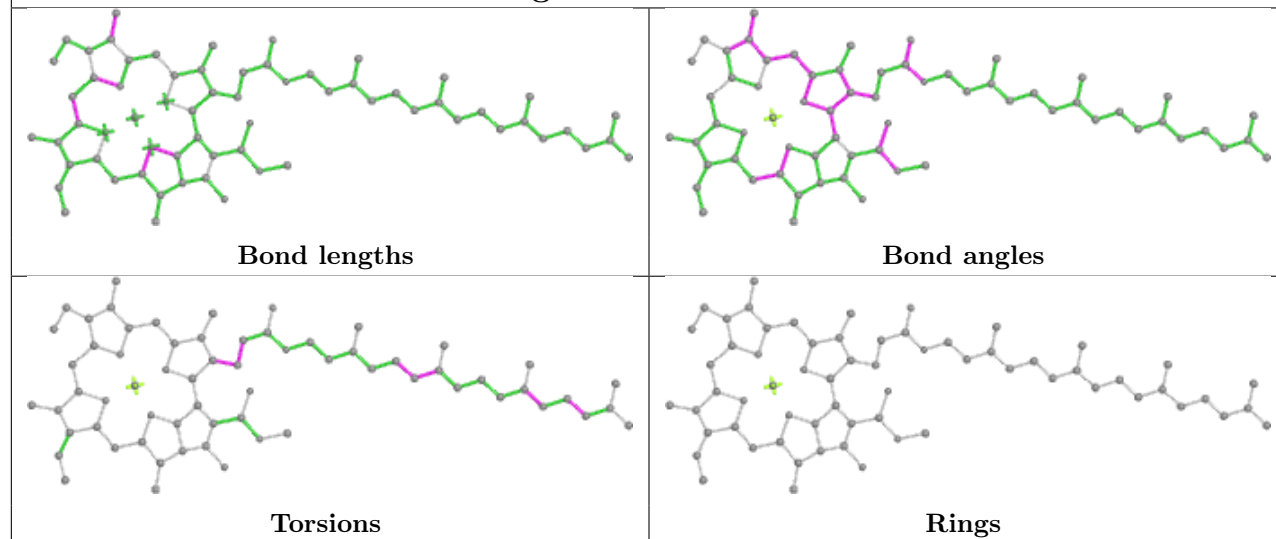
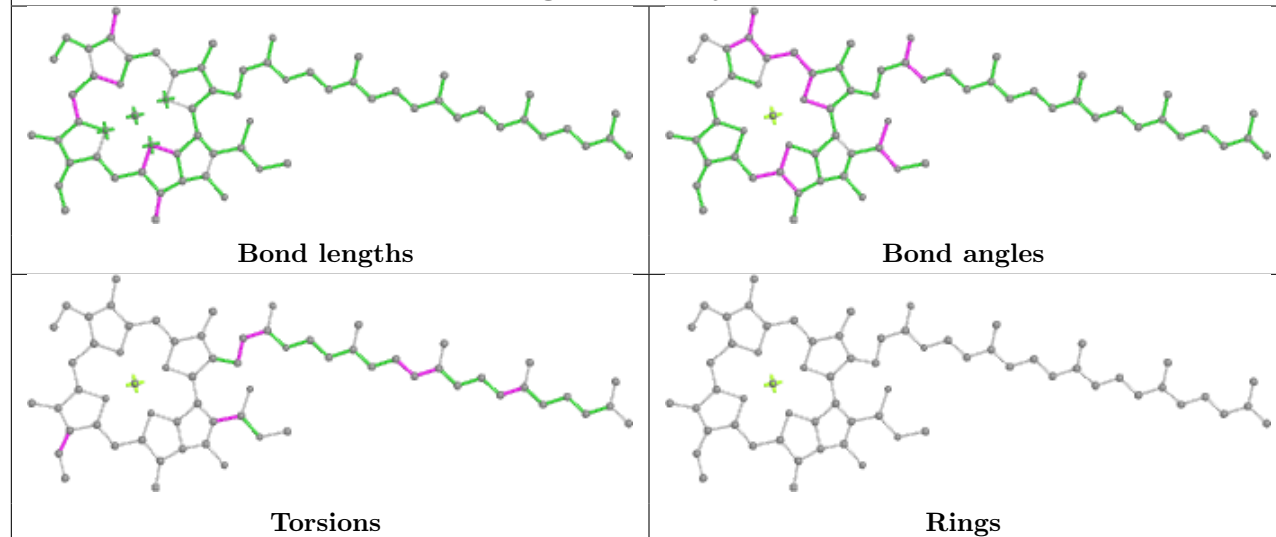
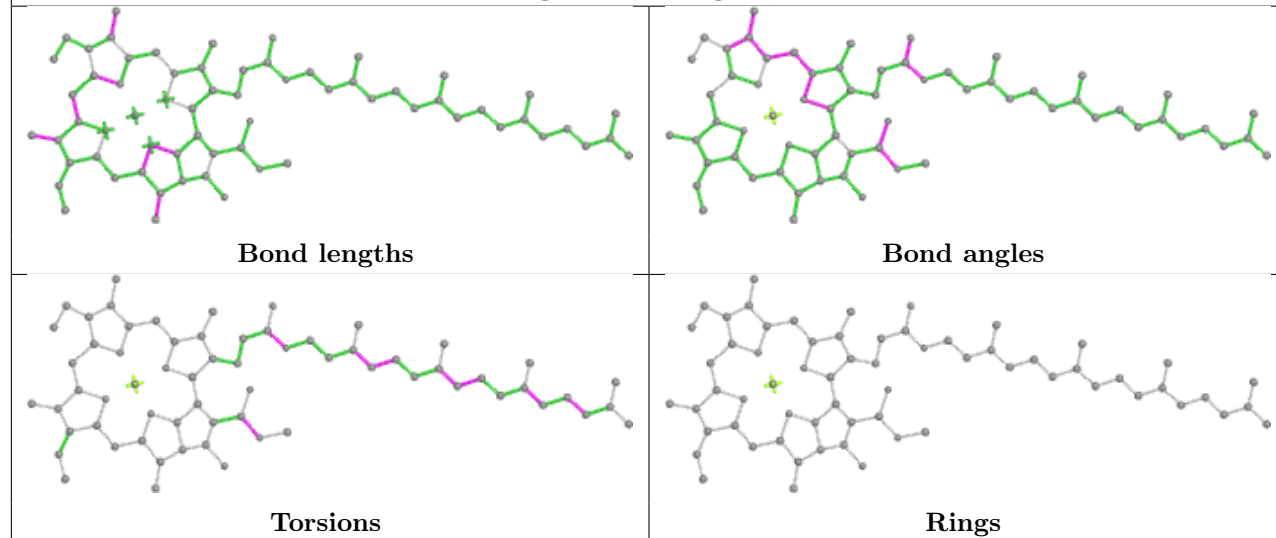
Ligand CLA d 304

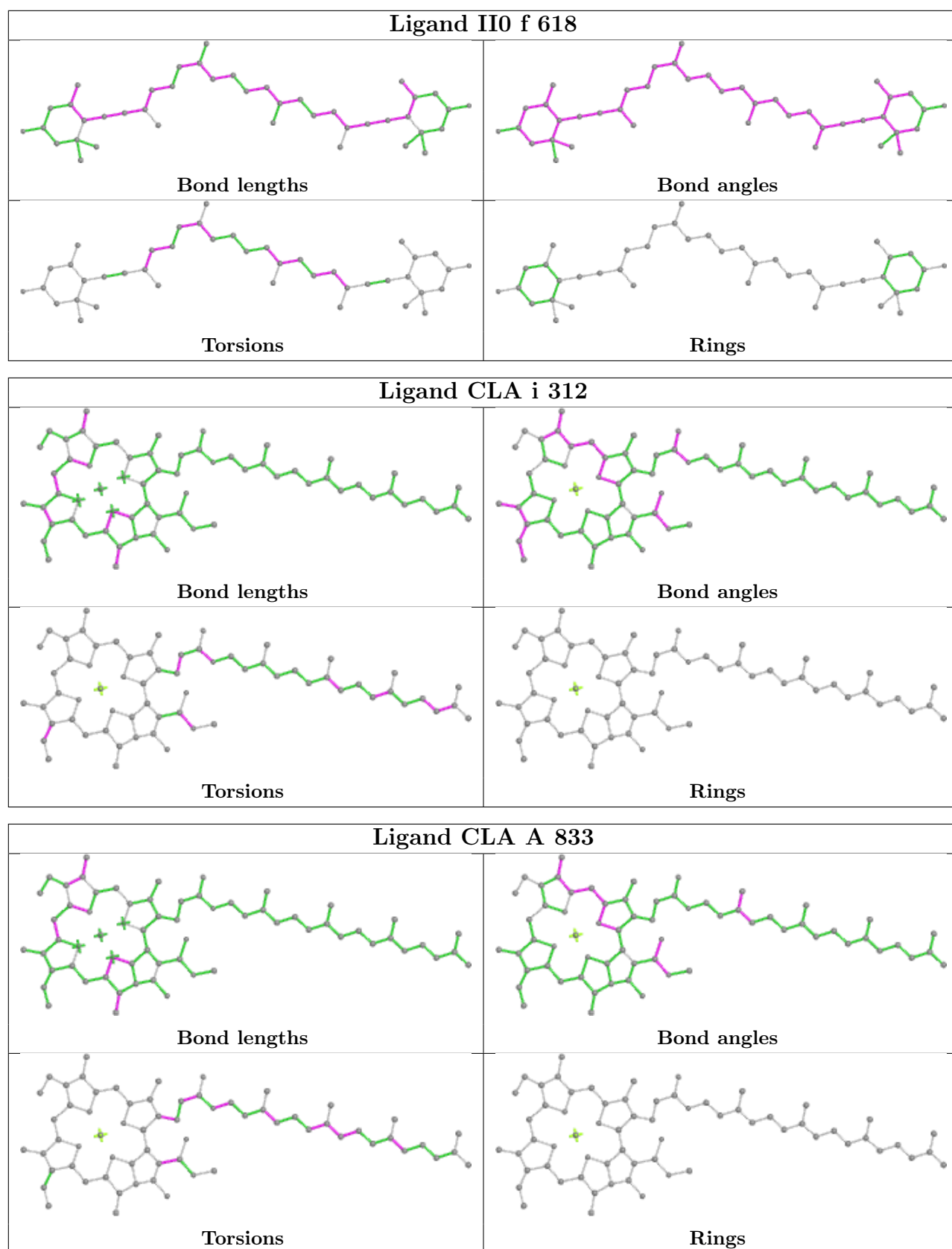


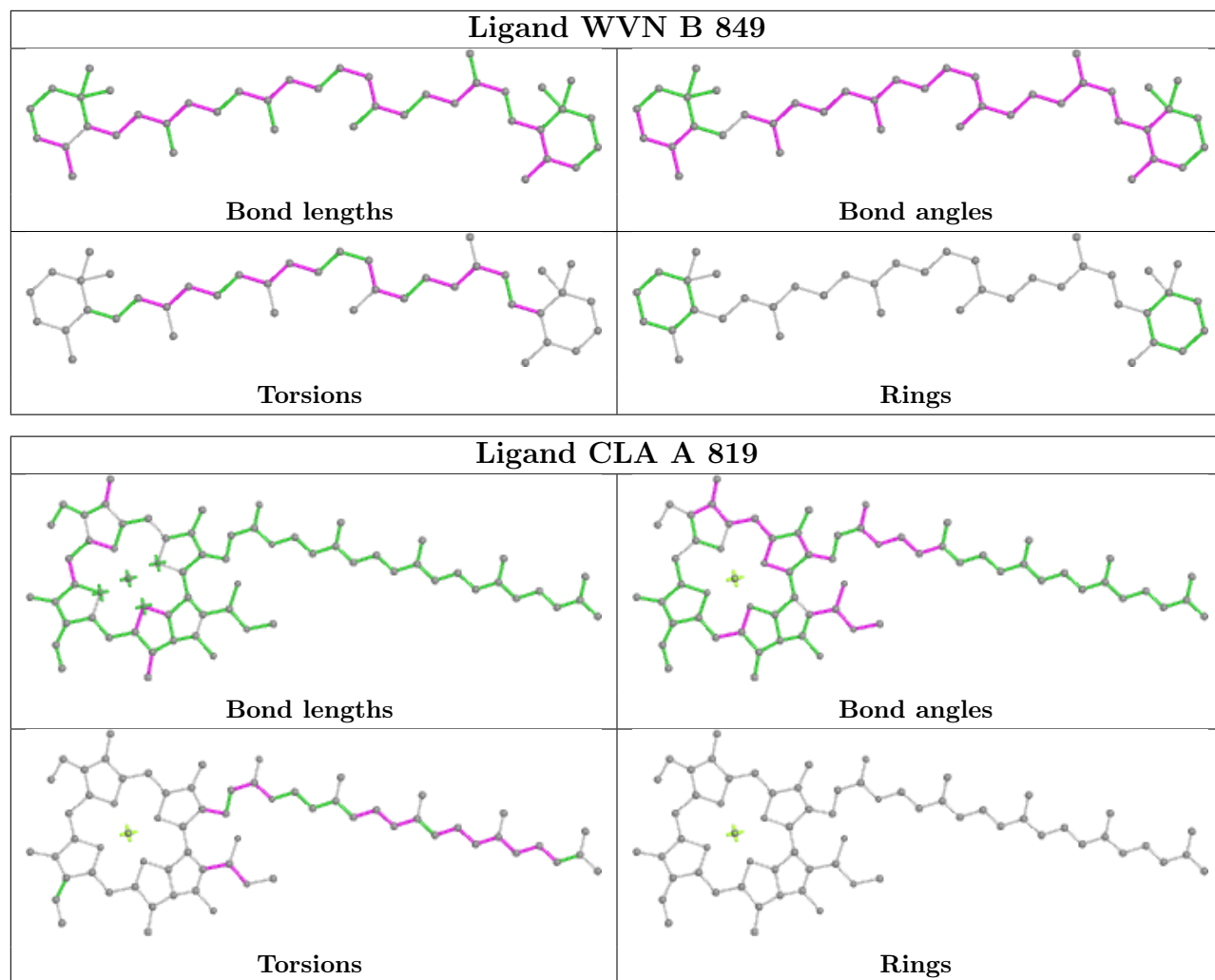


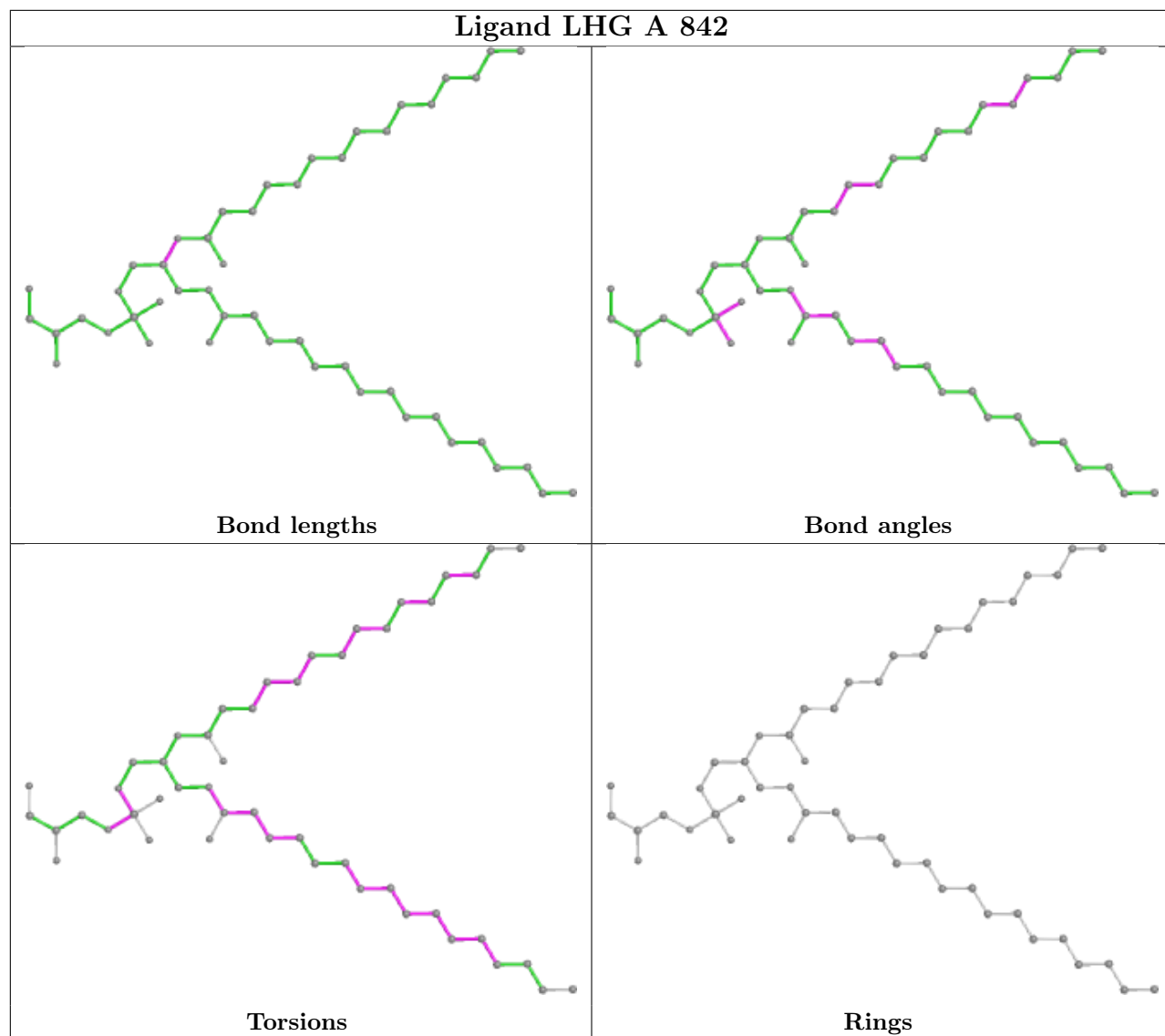
Ligand CLA i 304**Ligand CLA A 807**

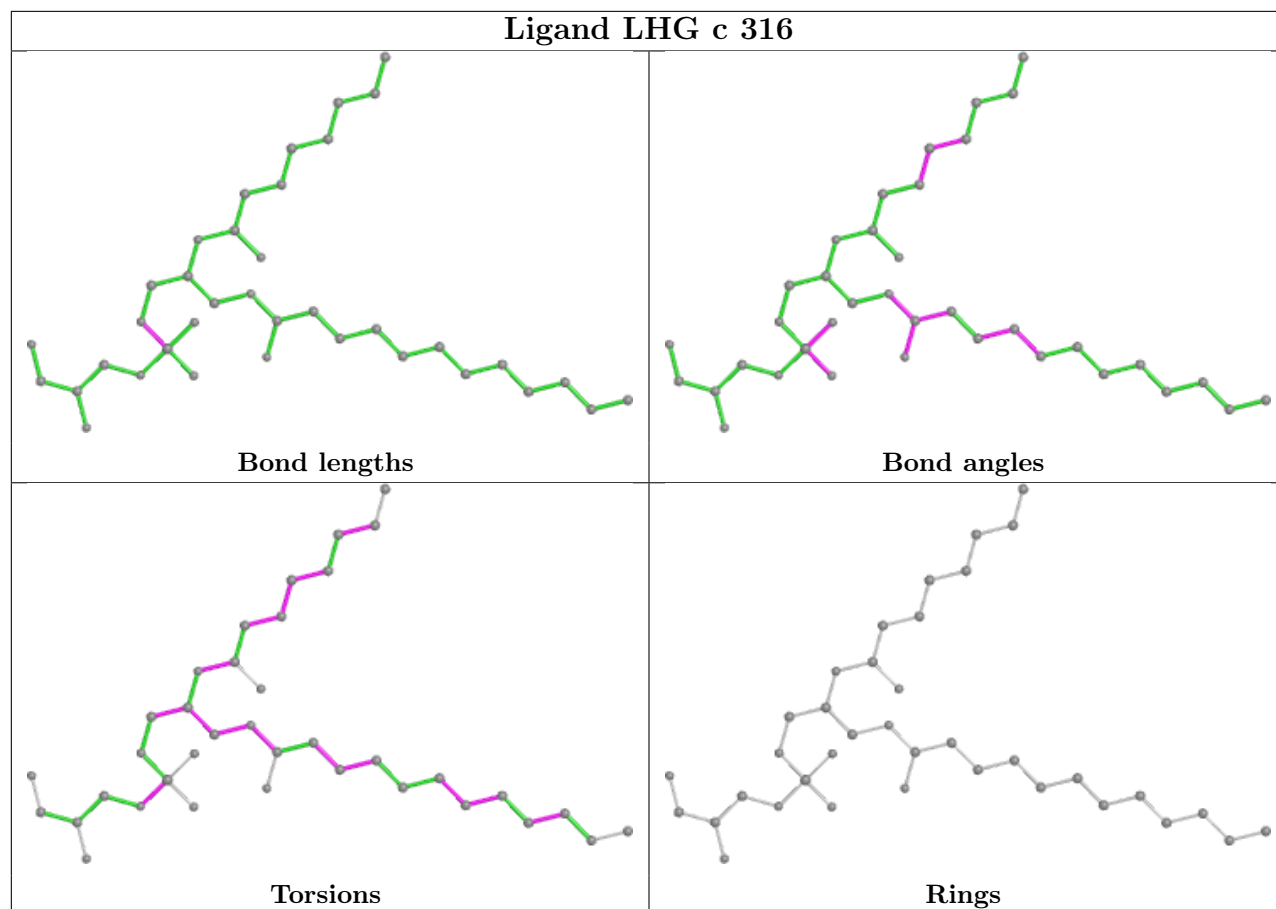
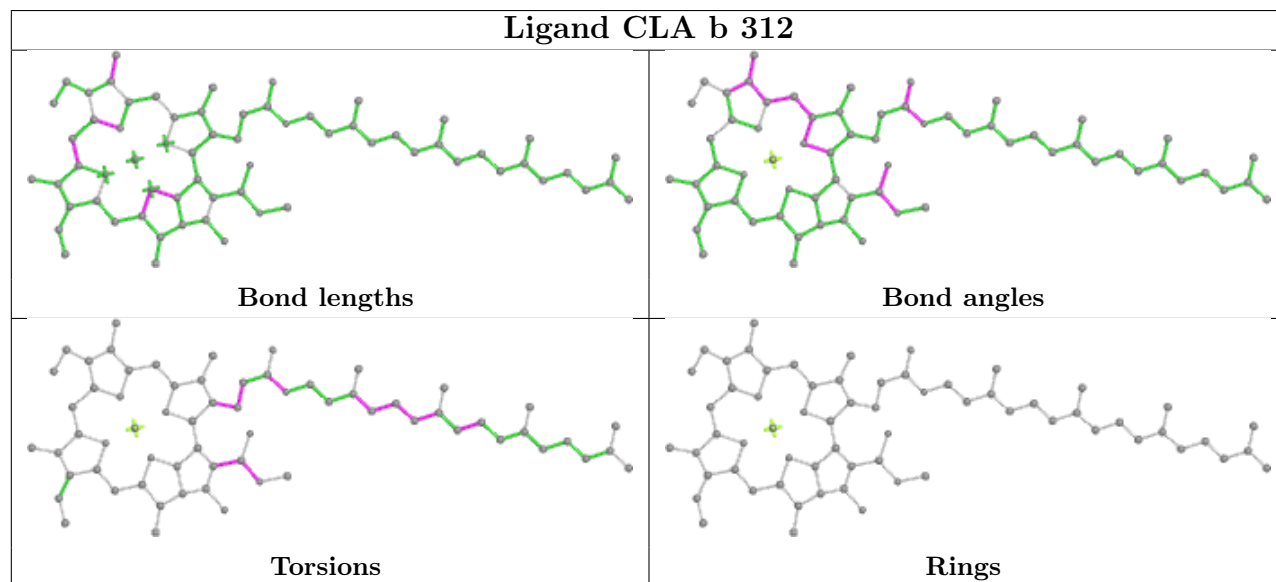


Ligand CLA B 829**Ligand CLA j 305****Ligand CLA g 309**

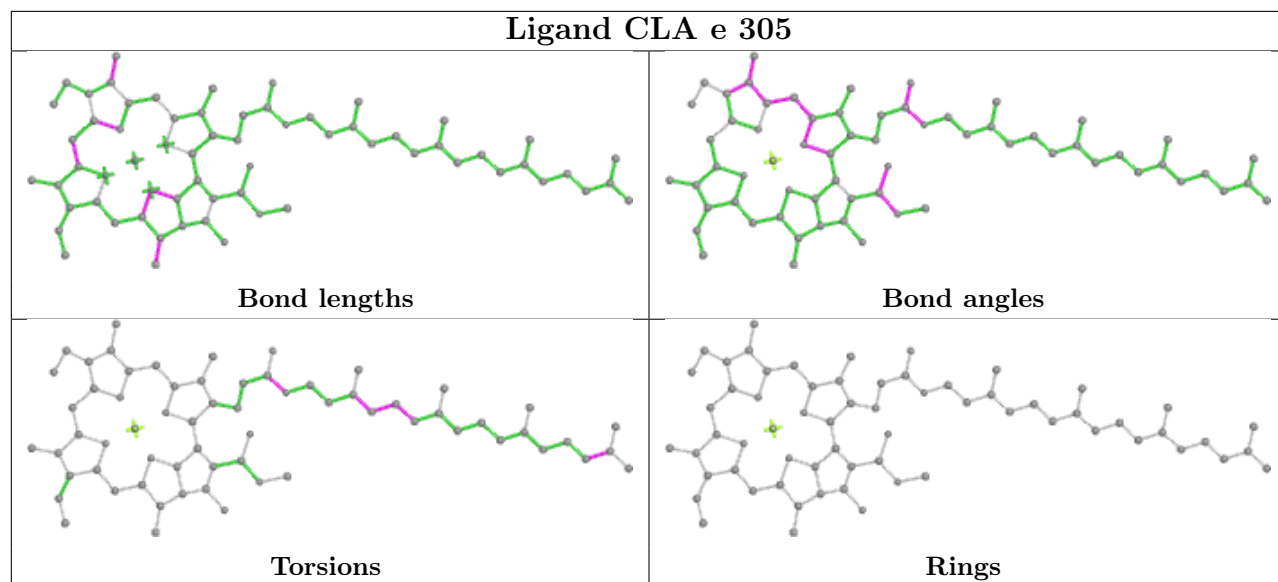




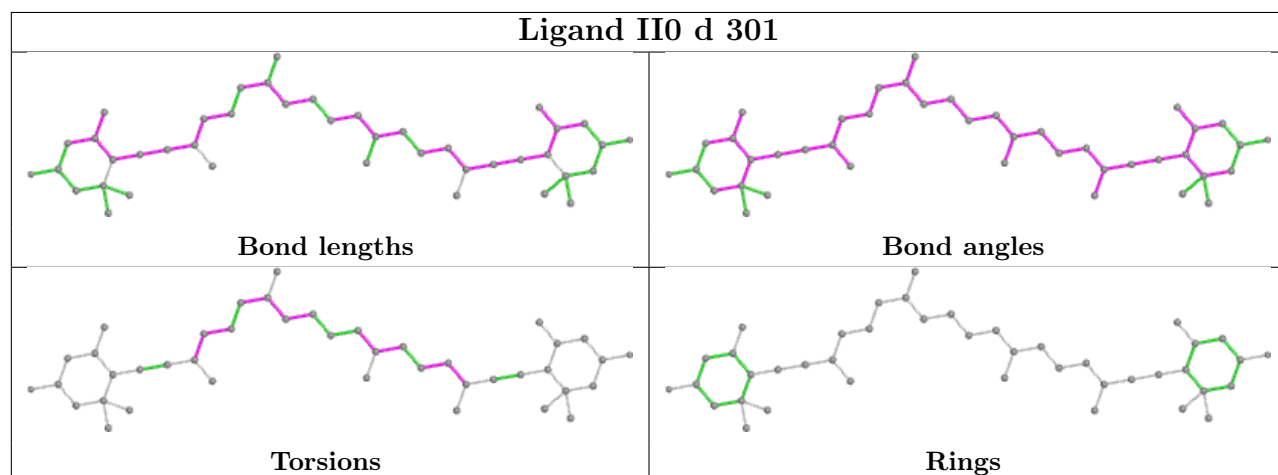


Ligand LHG c 316**Ligand CLA b 312**

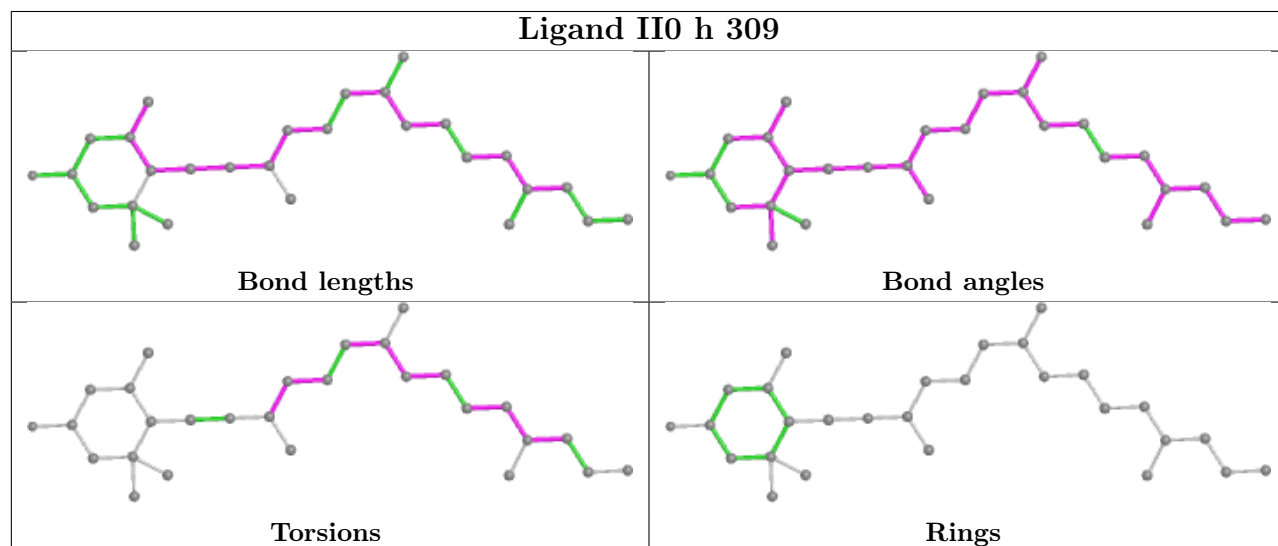
Ligand CLA e 305



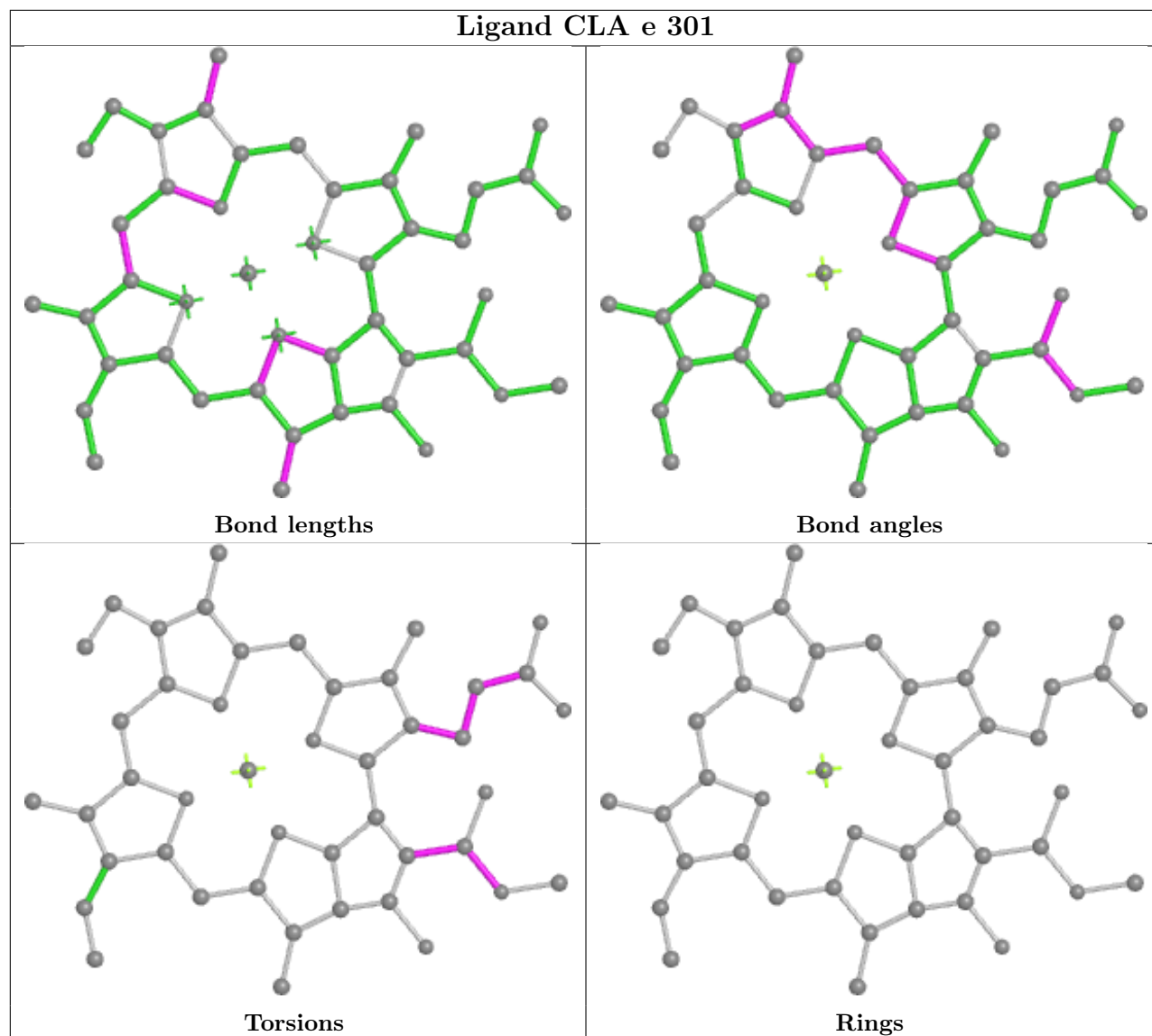
Ligand II0 d 301

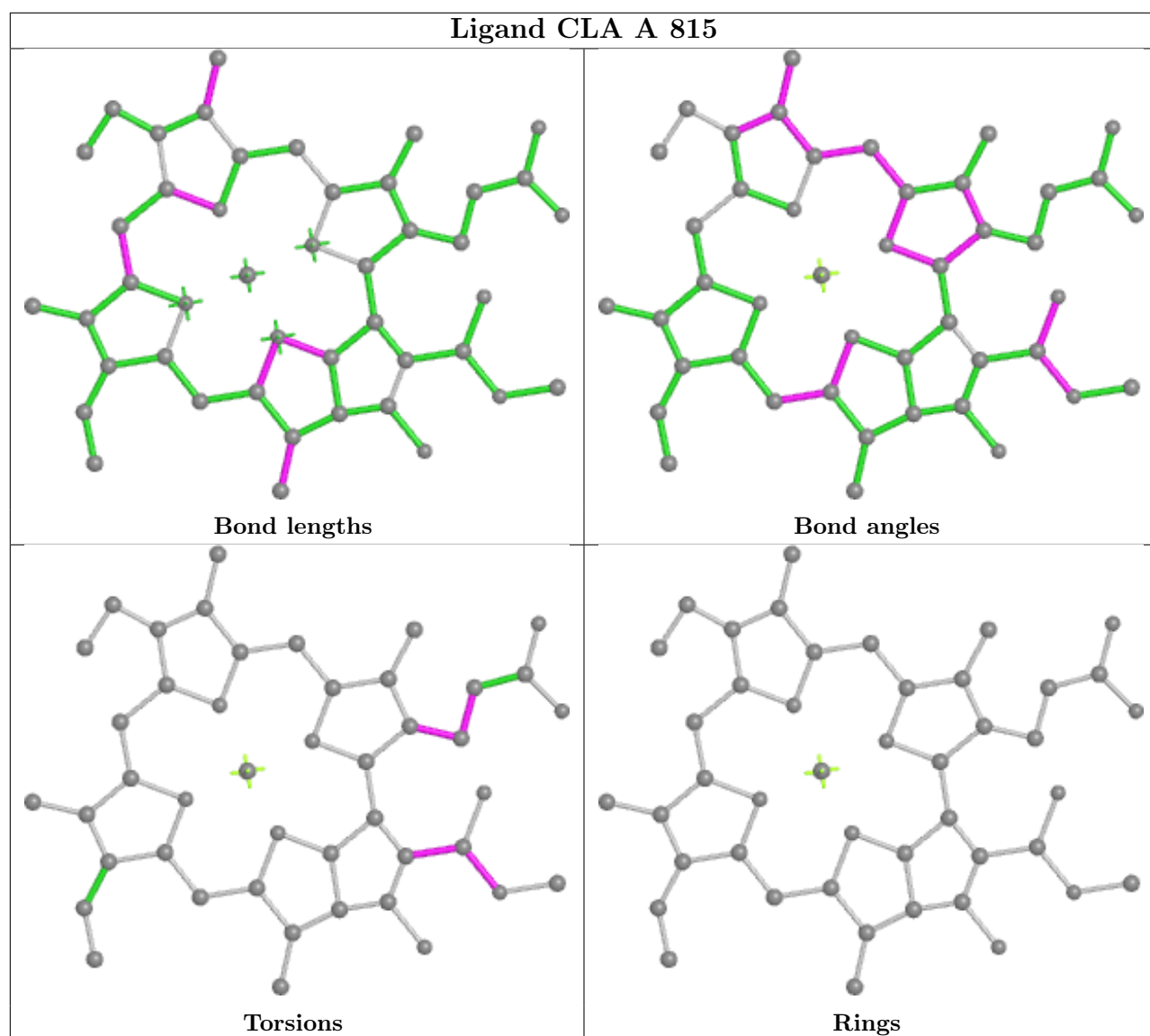


Ligand II0 h 309

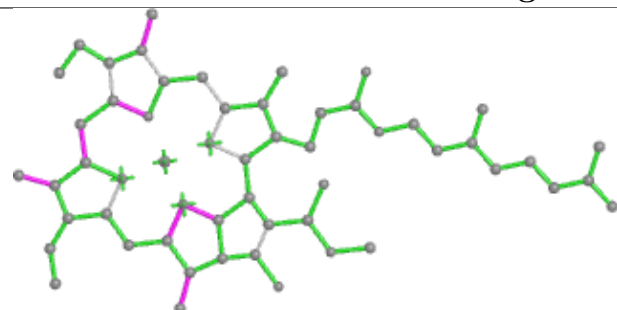


Ligand CLA e 301

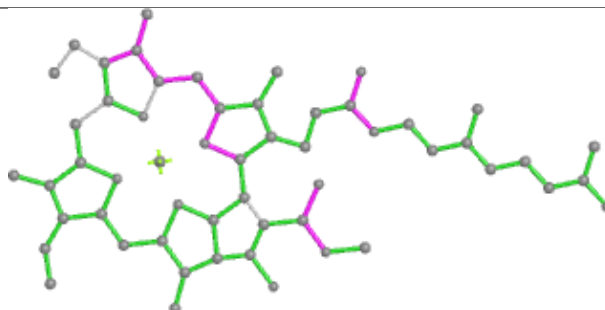




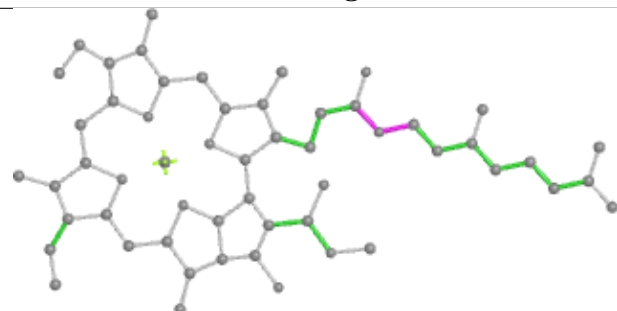
Ligand CLA B 811



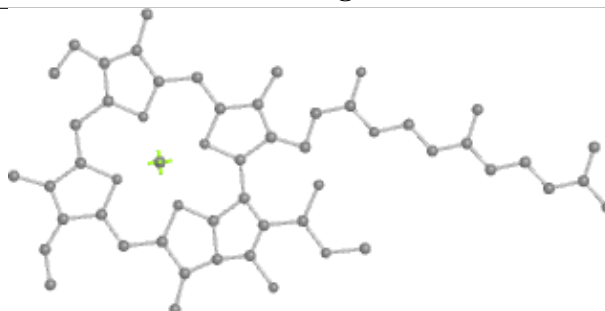
Bond lengths



Bond angles

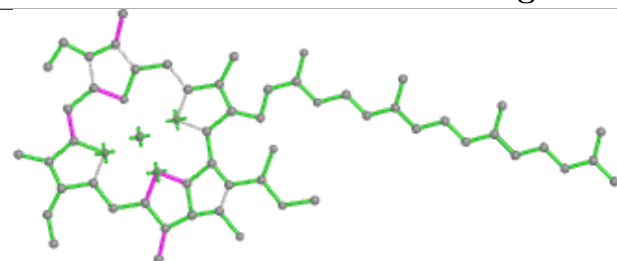


Torsions

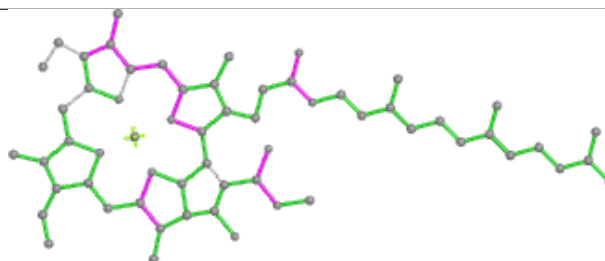


Rings

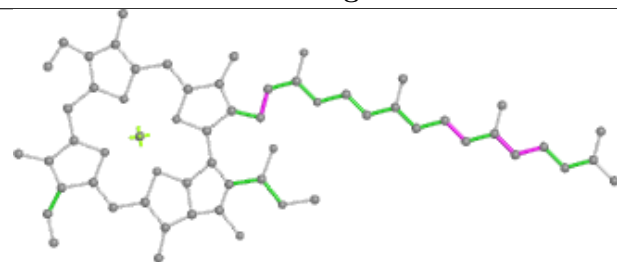
Ligand CLA A 830



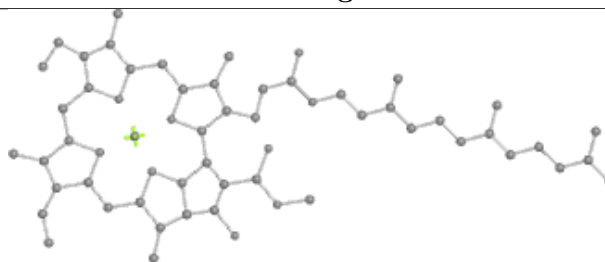
Bond lengths



Bond angles

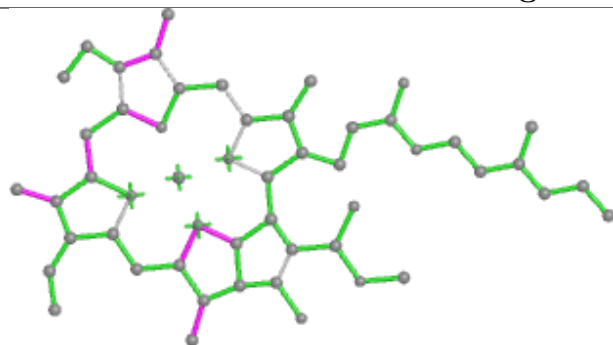


Torsions

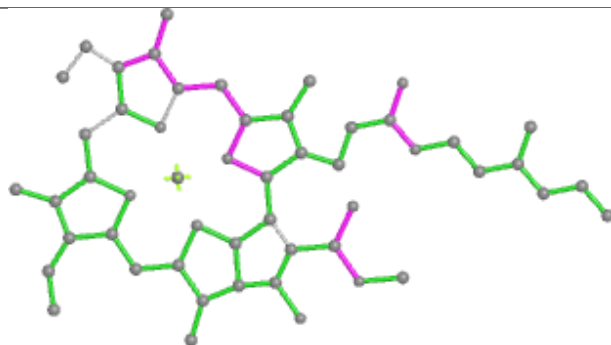


Rings

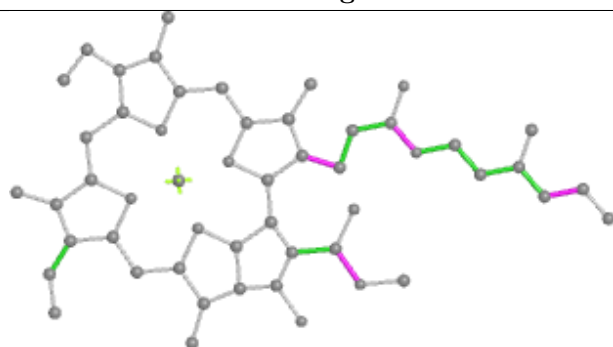
Ligand CLA c 306



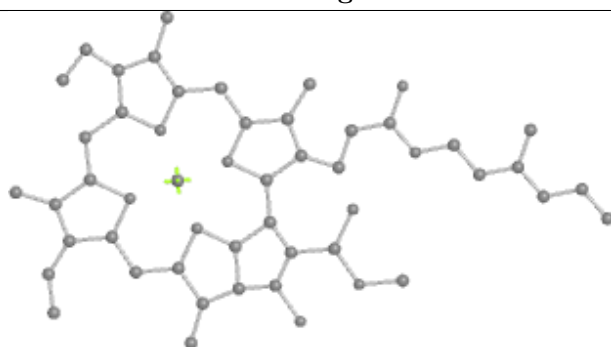
Bond lengths



Bond angles

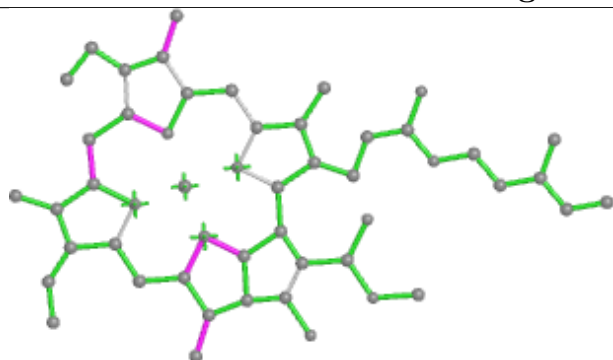


Torsions

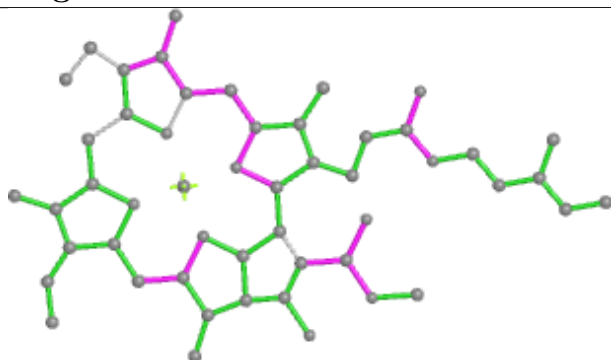


Rings

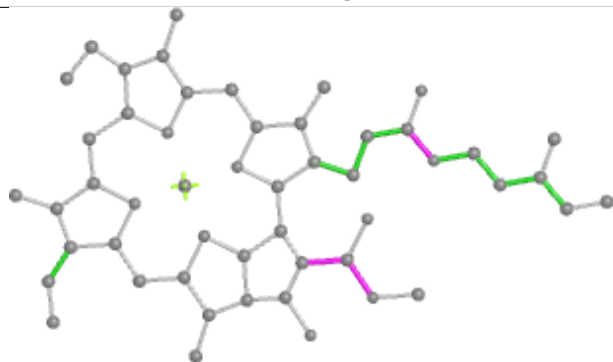
Ligand CLA g 308



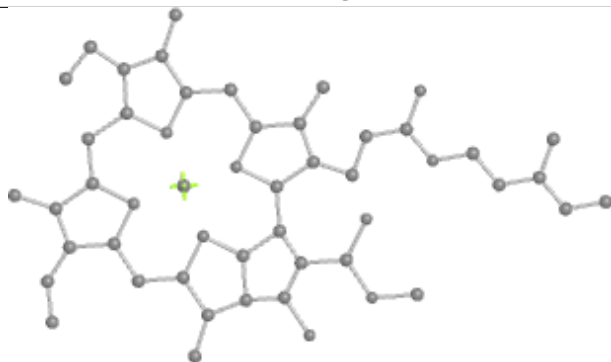
Bond lengths



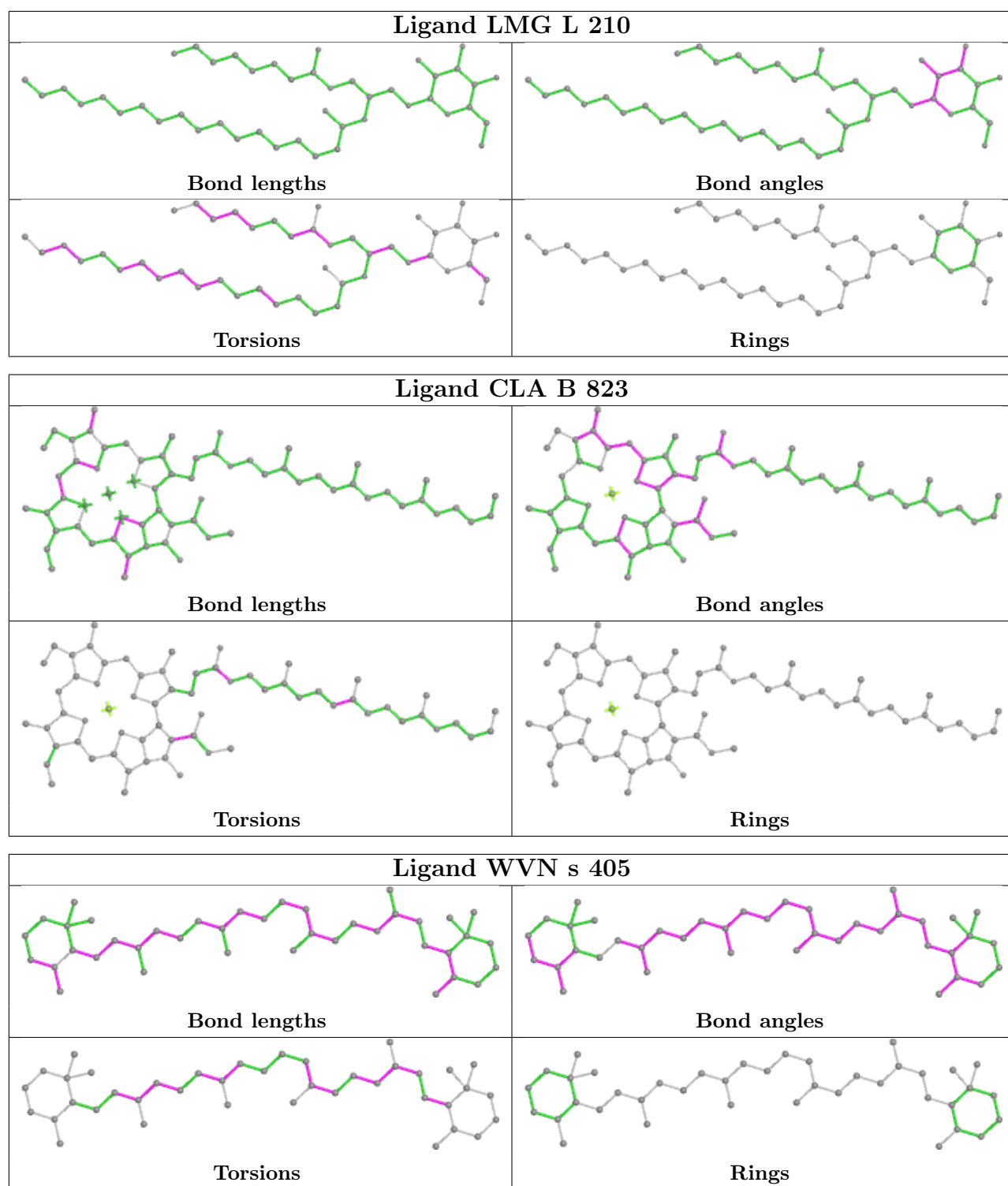
Bond angles

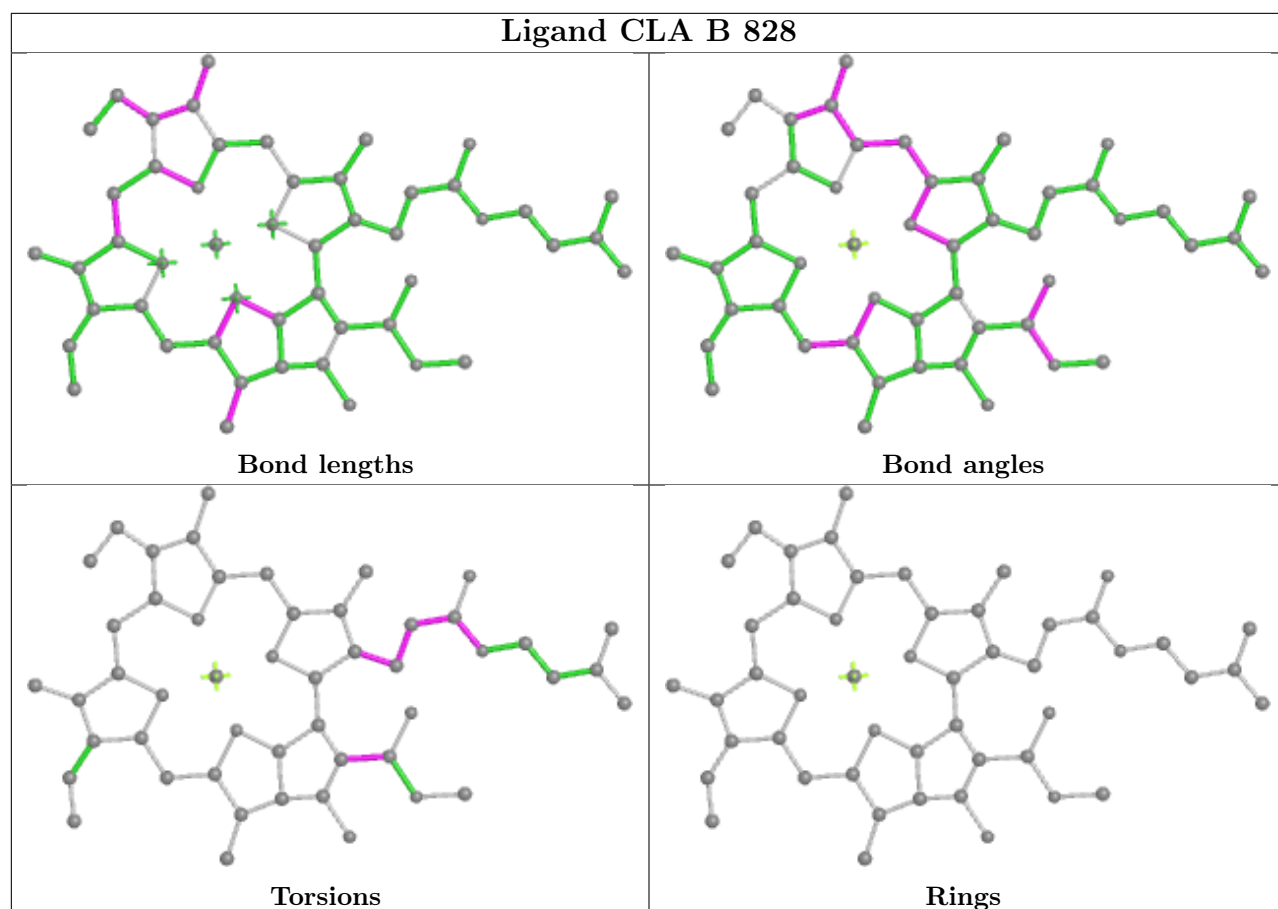
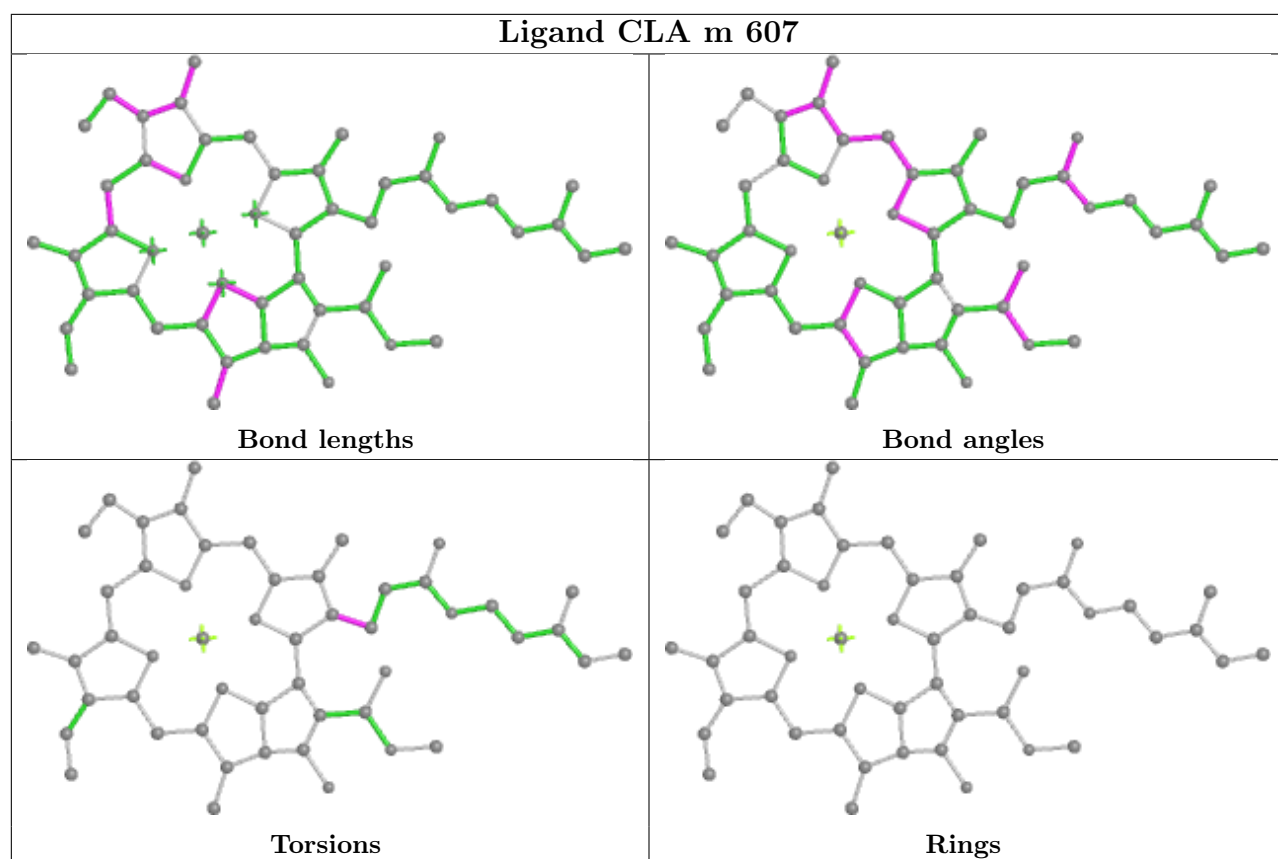


Torsions

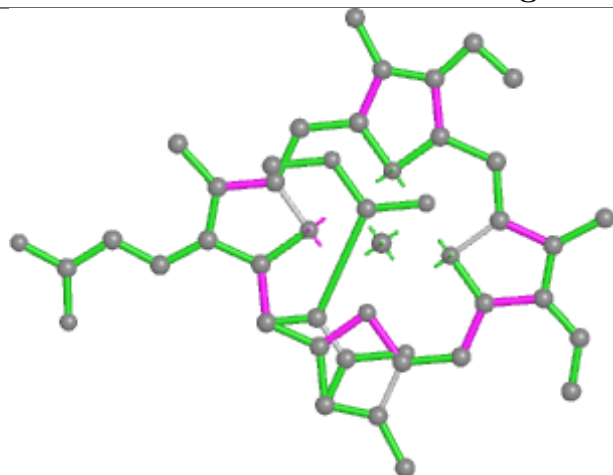


Rings

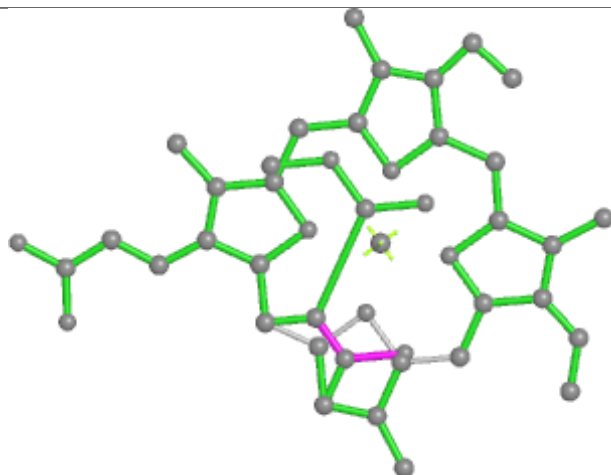




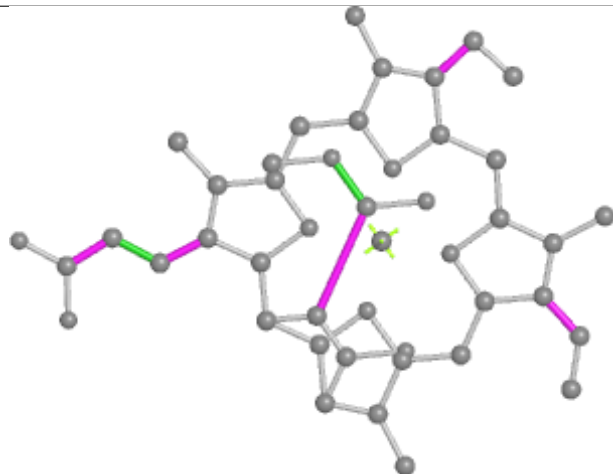
Ligand KC2 k 612



Bond lengths



Bond angles

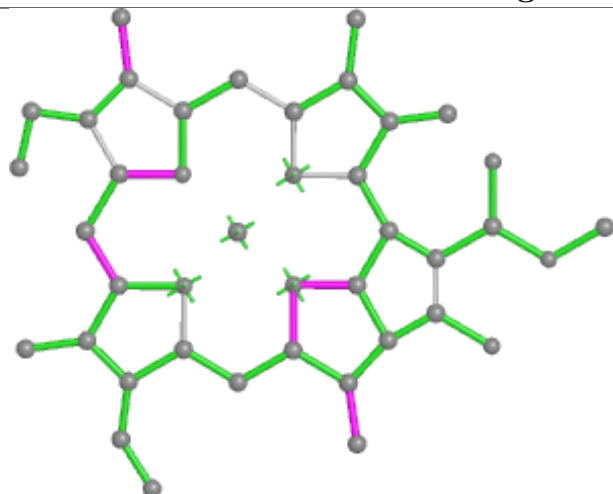


Torsions

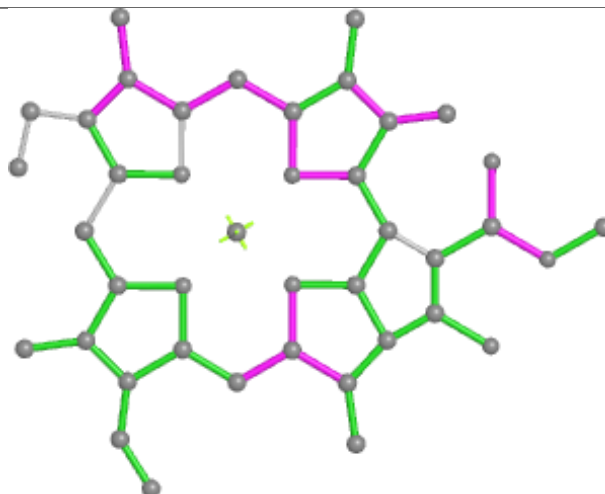


Rings

Ligand CLA d 310



Bond lengths



Bond angles

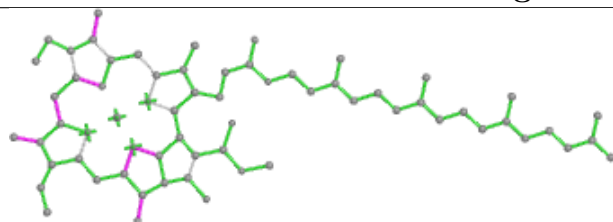


Torsions

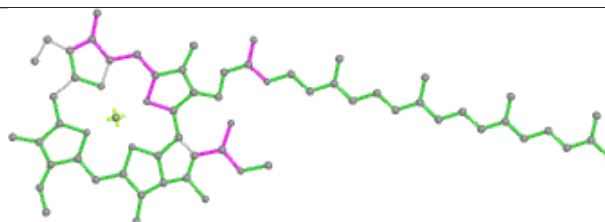


Rings

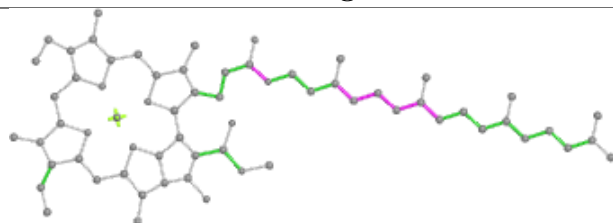
Ligand CLA A 826



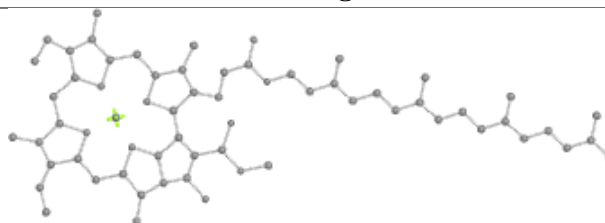
Bond lengths



Bond angles

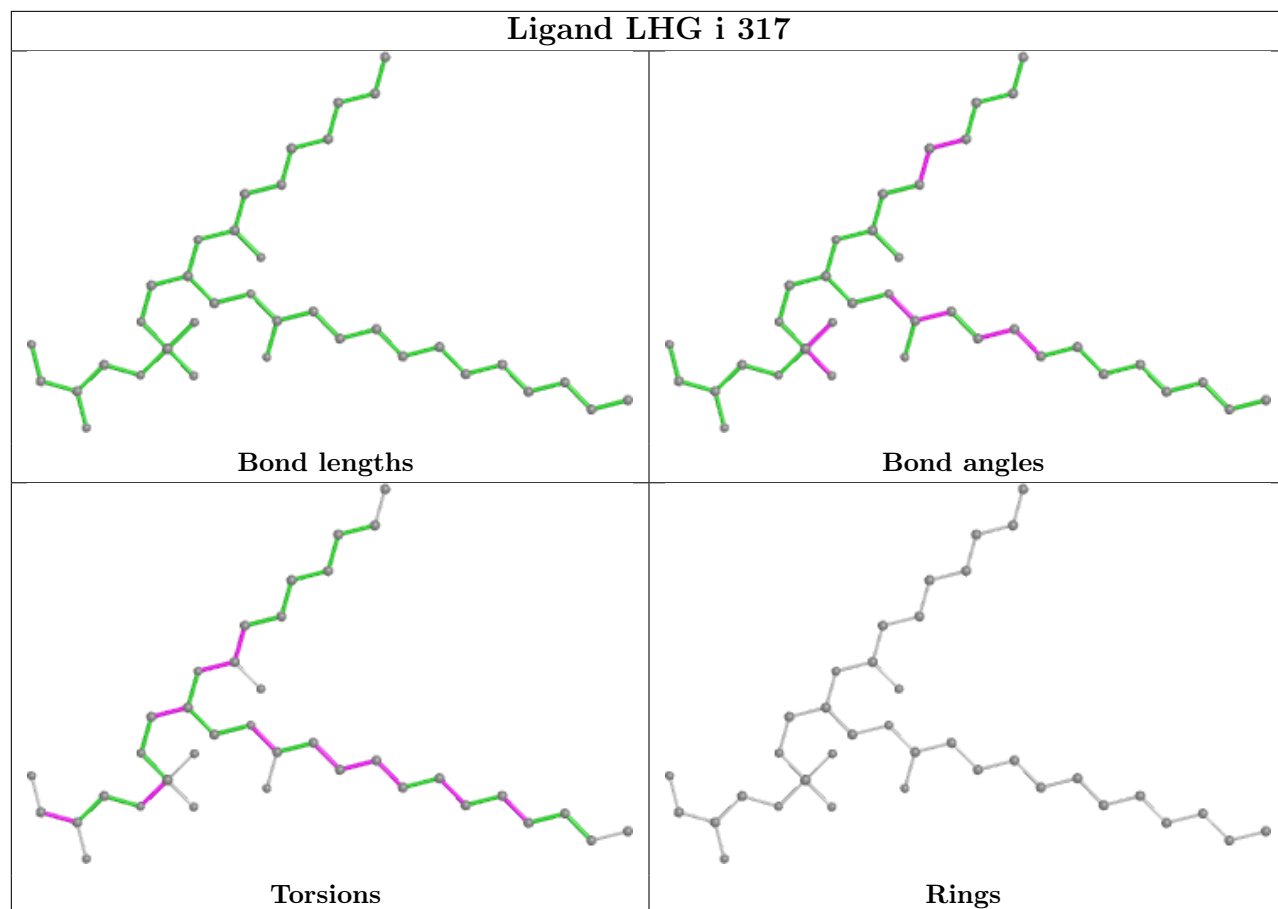


Torsions

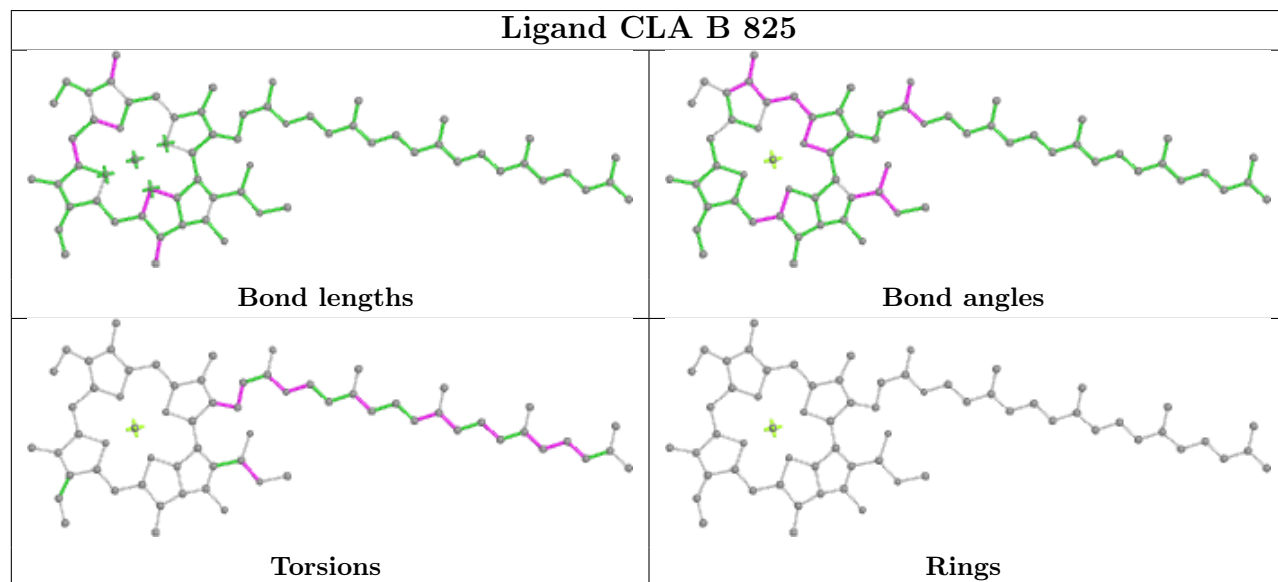


Rings

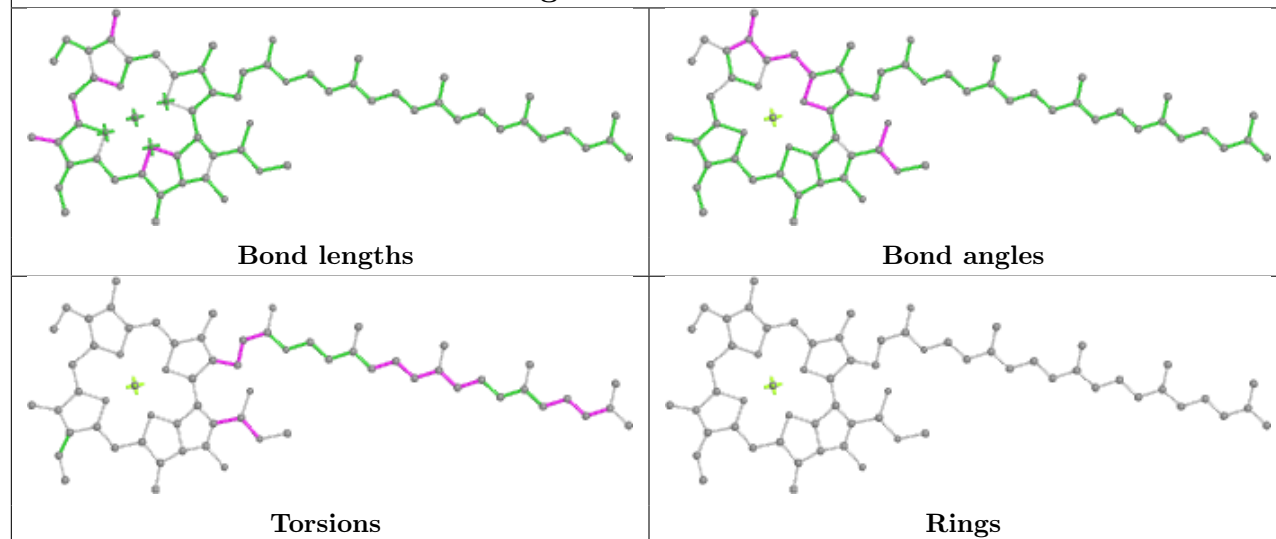
Ligand LHG i 317



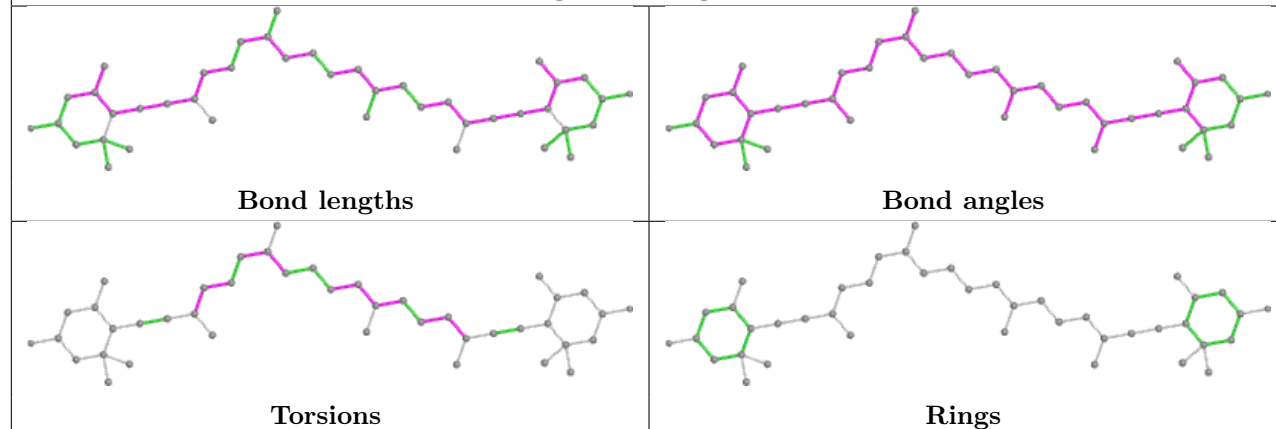
Ligand CLA B 825



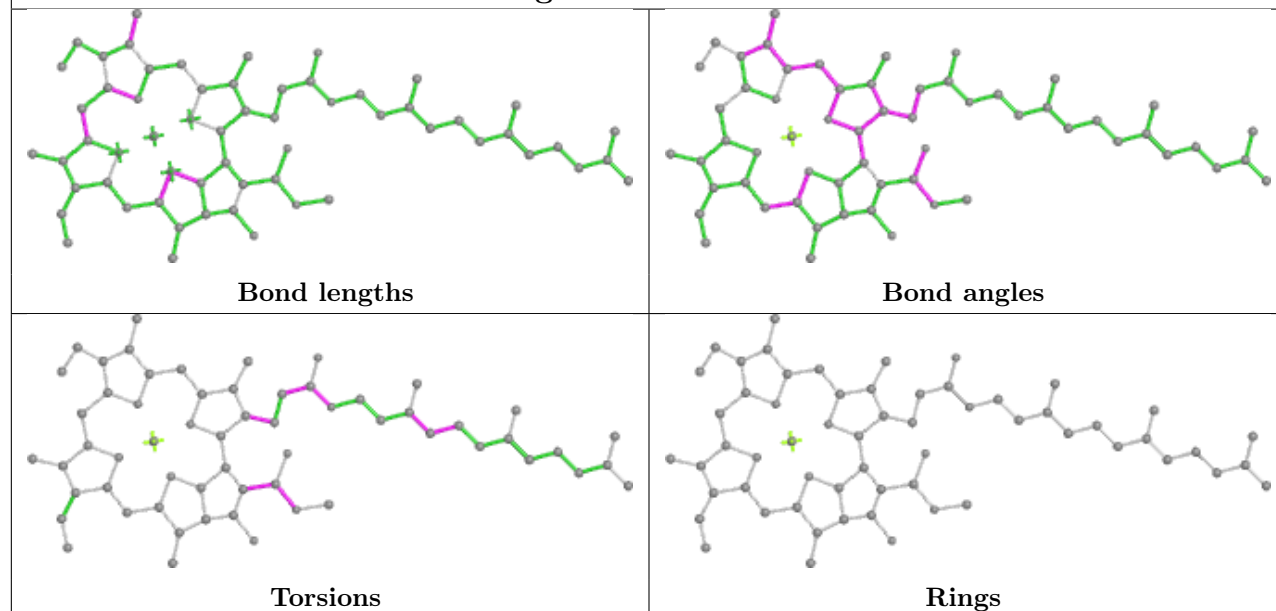
Ligand CLA i 308

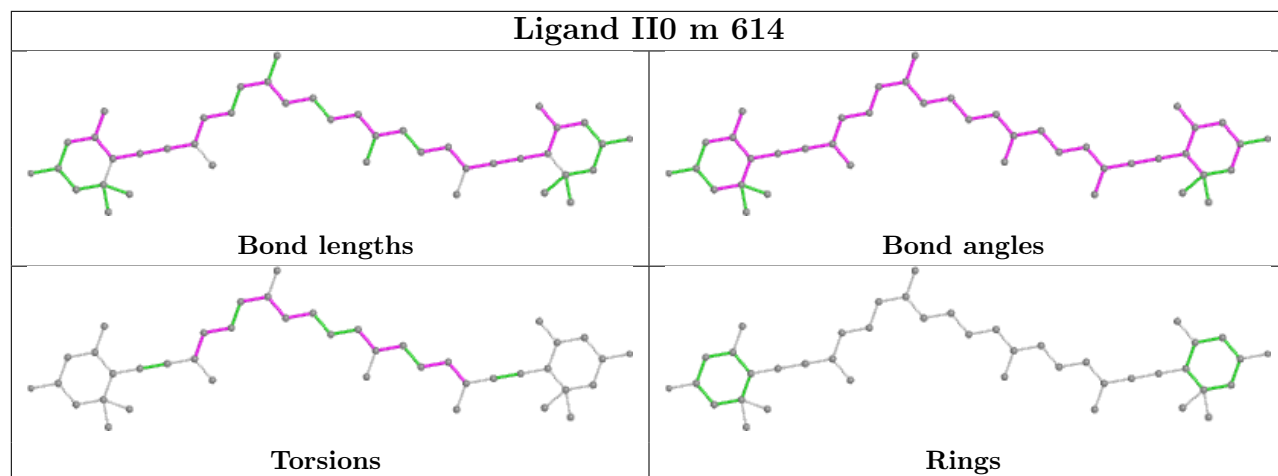
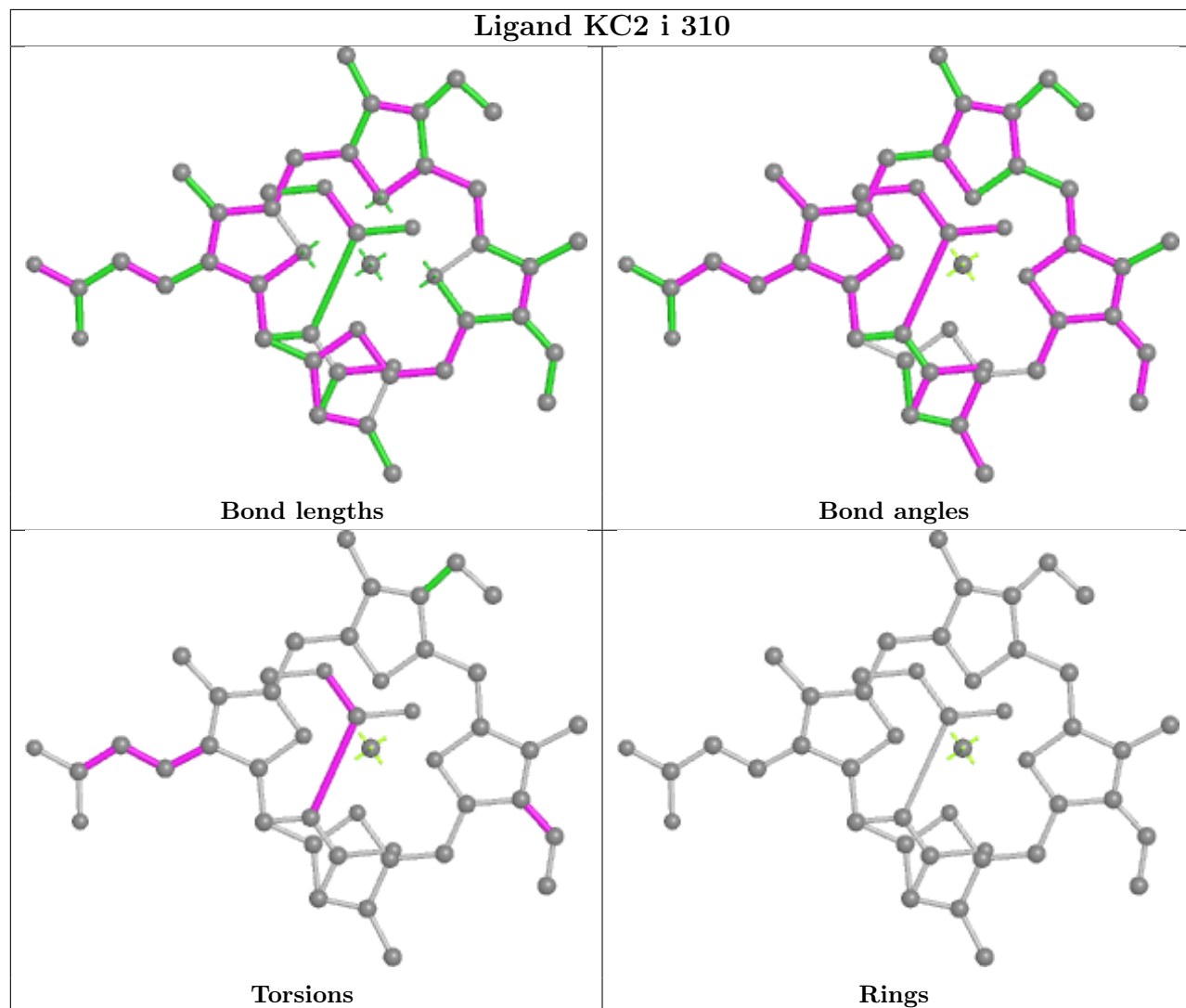


Ligand II0 g 319

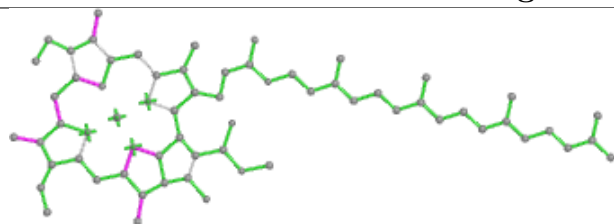


Ligand CLA n 604

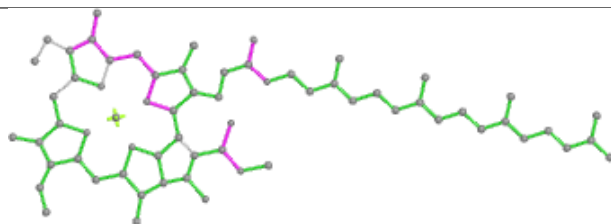


Ligand II0 m 614**Ligand KC2 i 310**

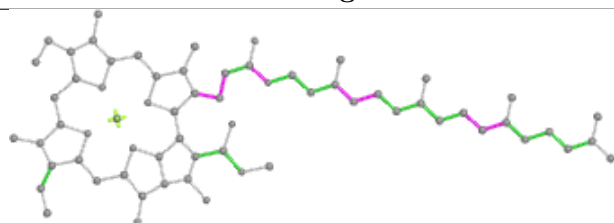
Ligand CLA h 305



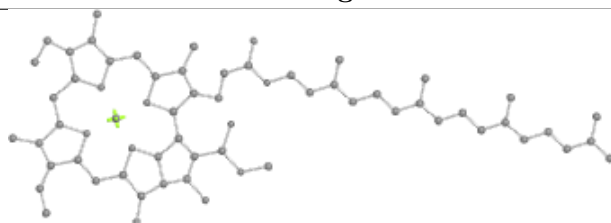
Bond lengths



Bond angles

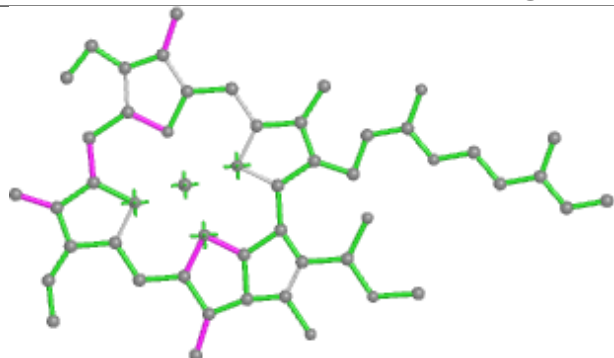


Torsions

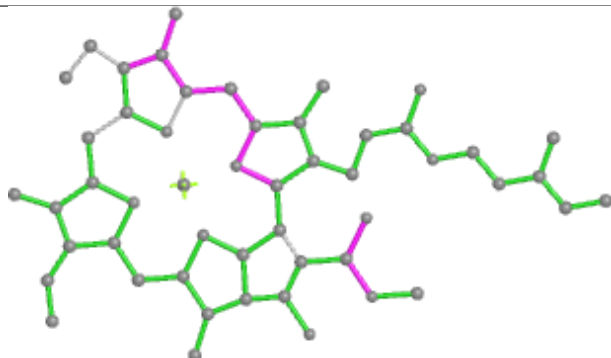


Rings

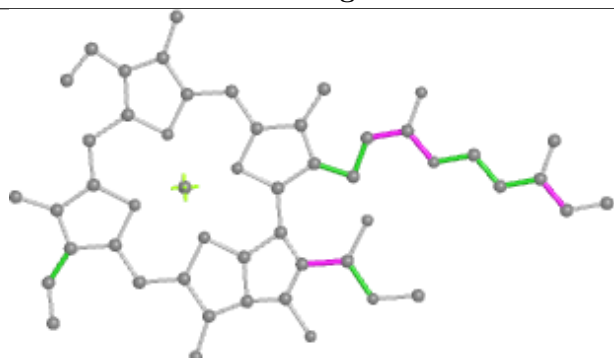
Ligand CLA f 603



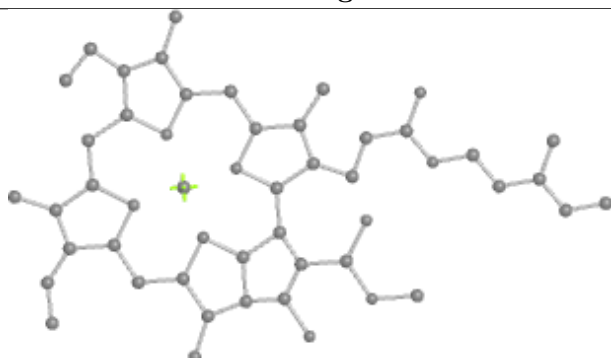
Bond lengths



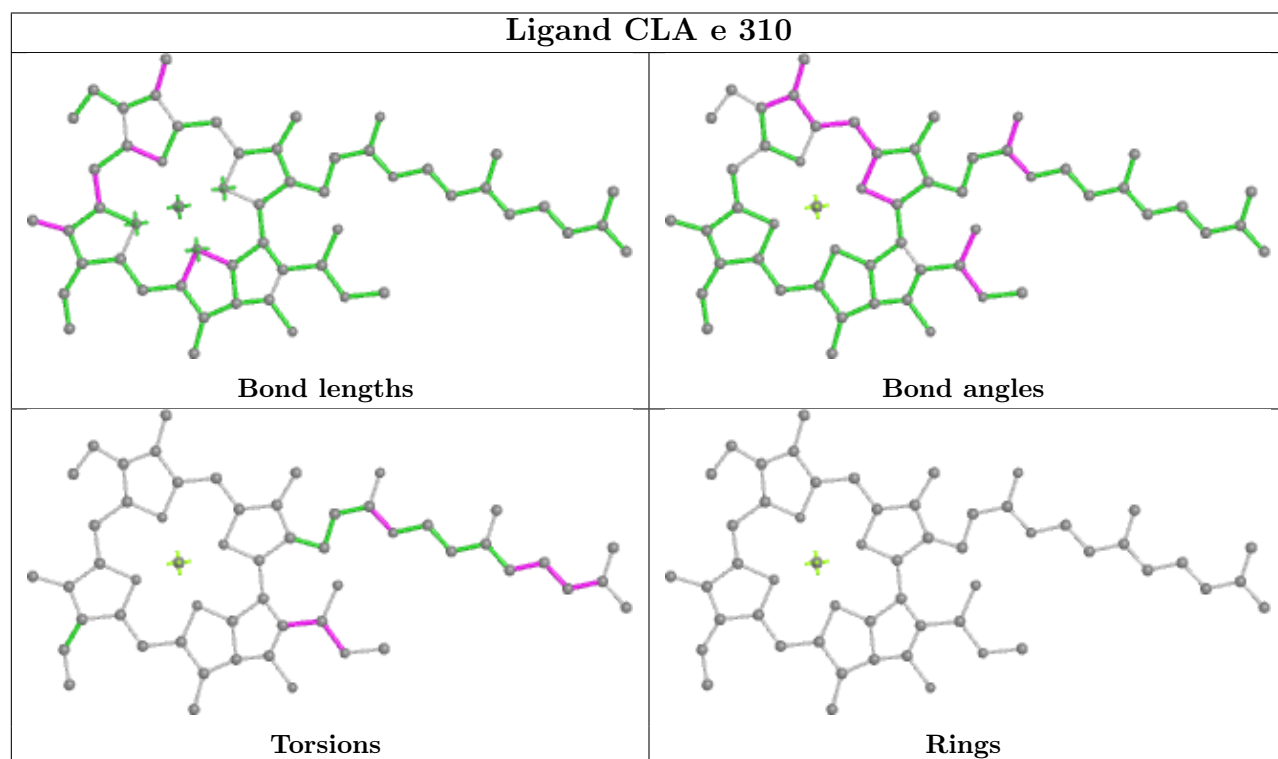
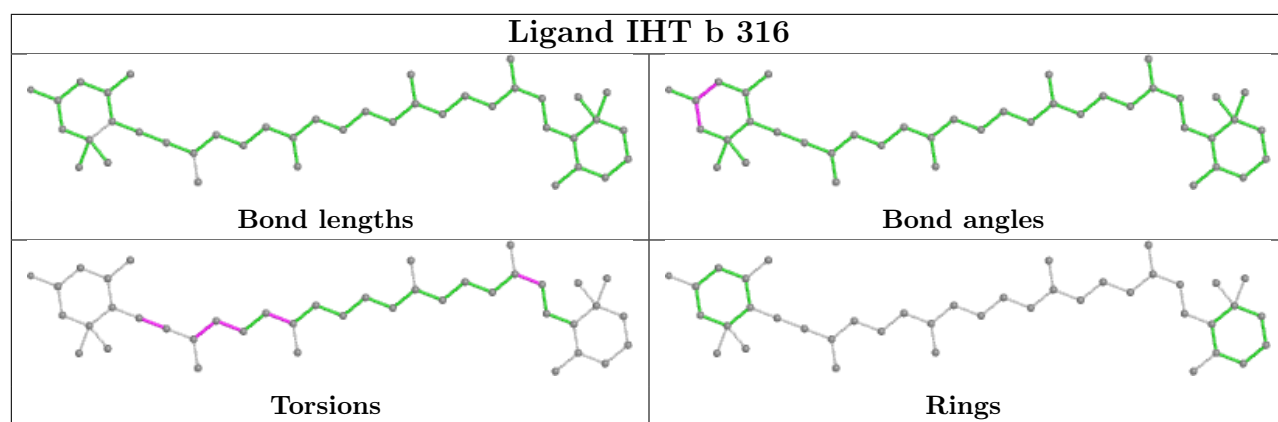
Bond angles

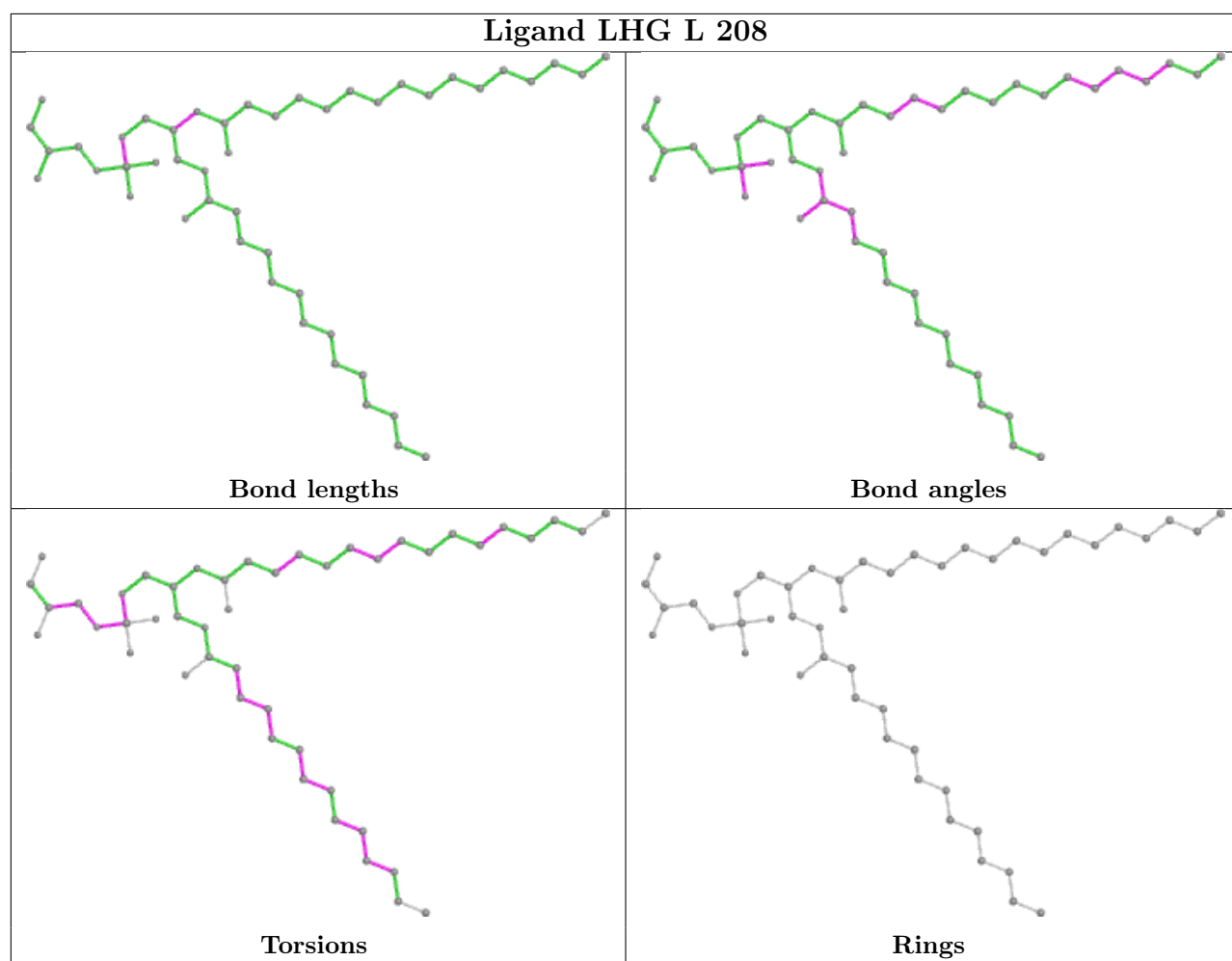


Torsions

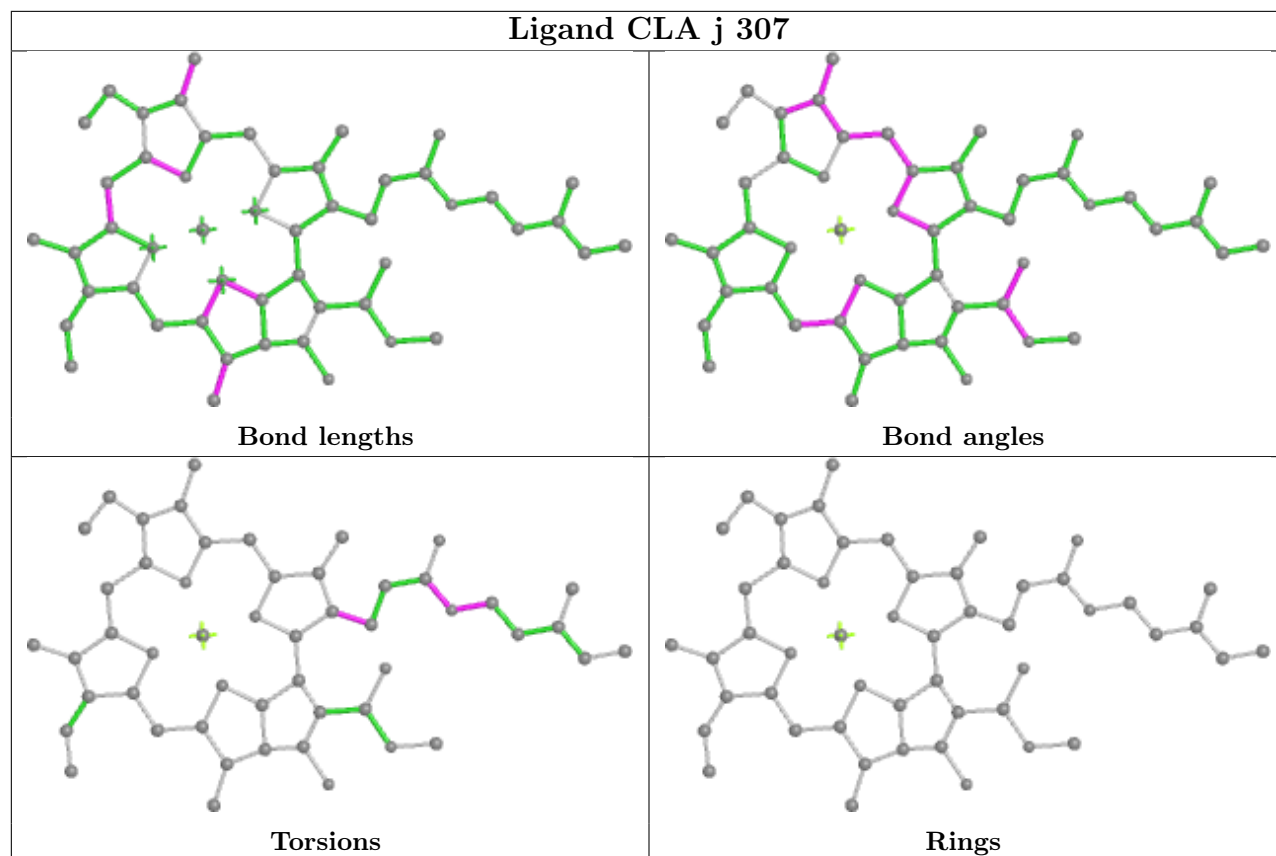


Rings

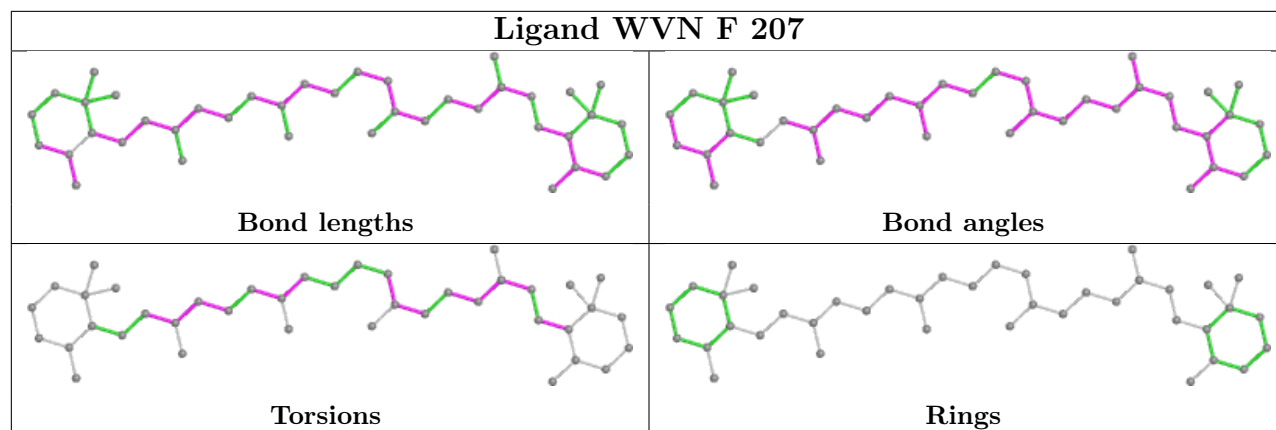




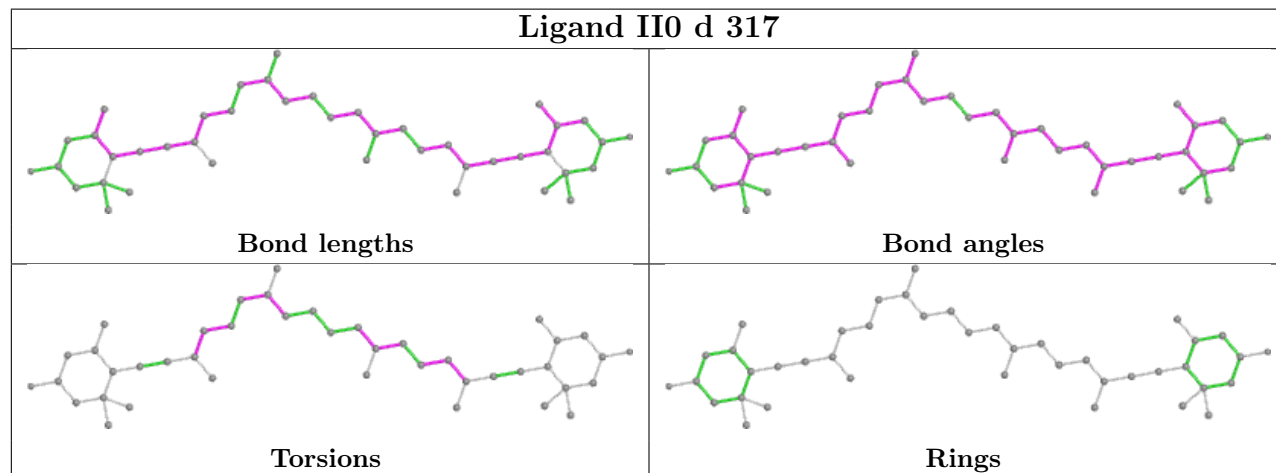
Ligand CLA j 307



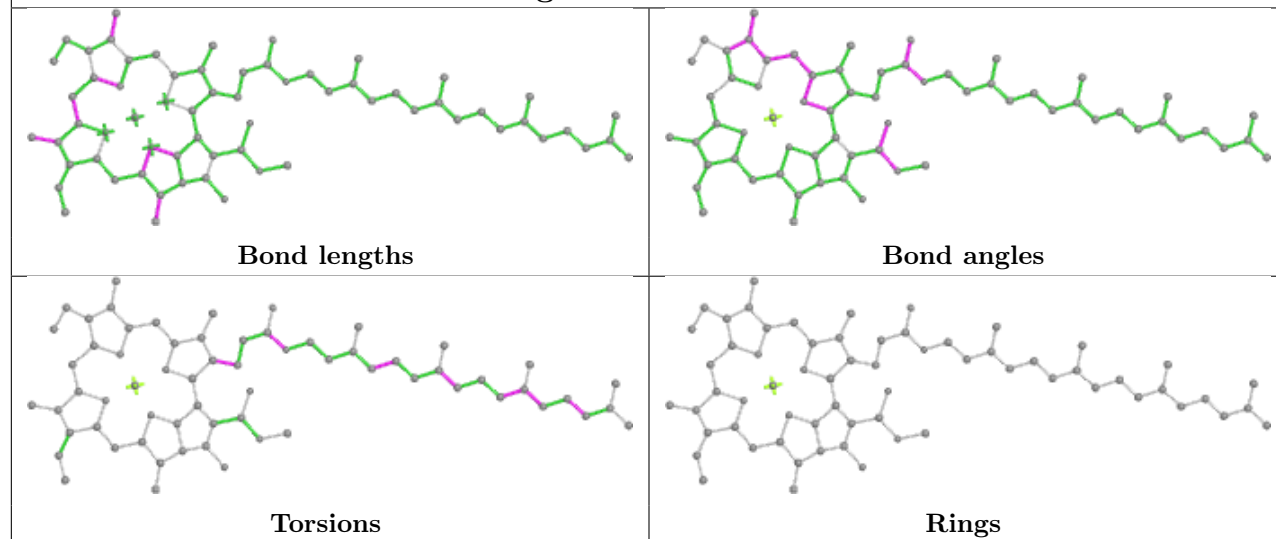
Ligand WVN F 207



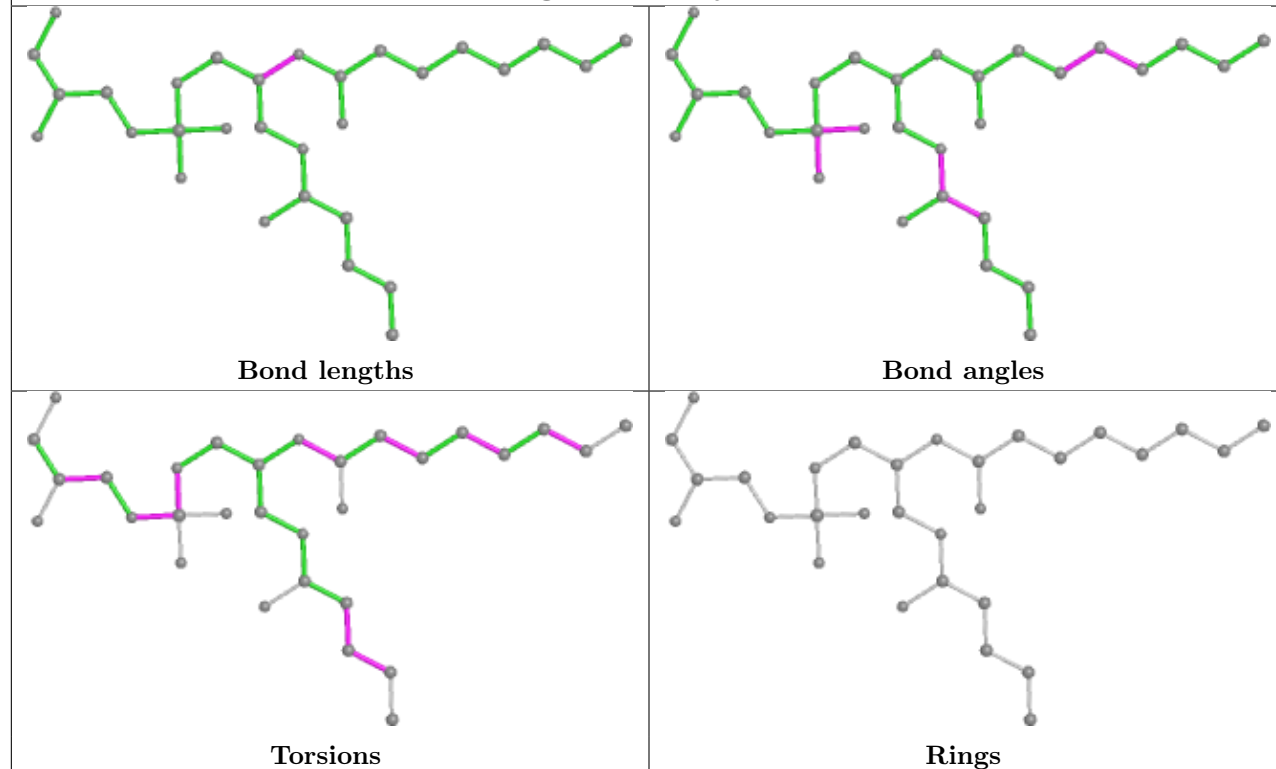
Ligand II0 d 317



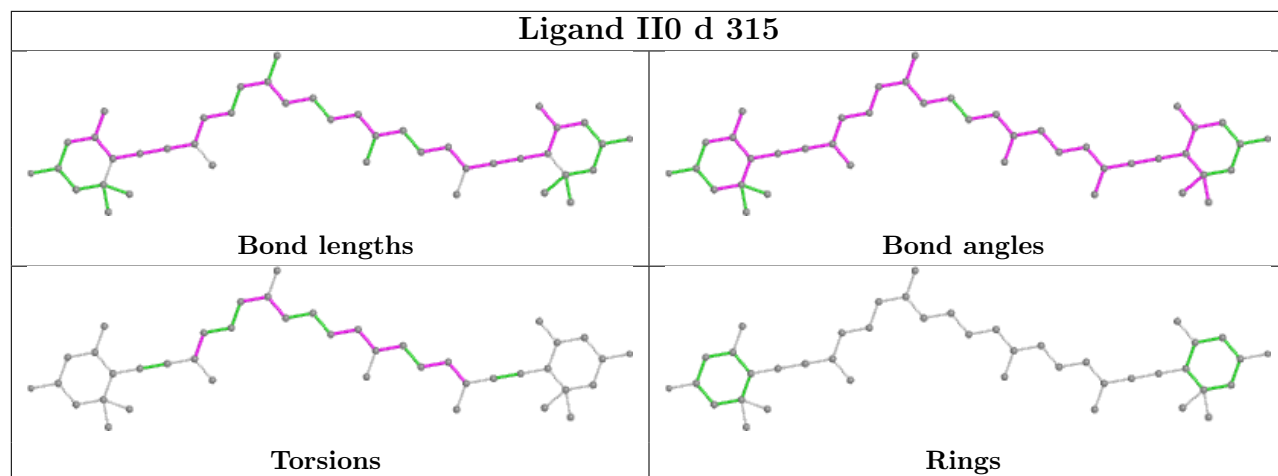
Ligand CLA a 311



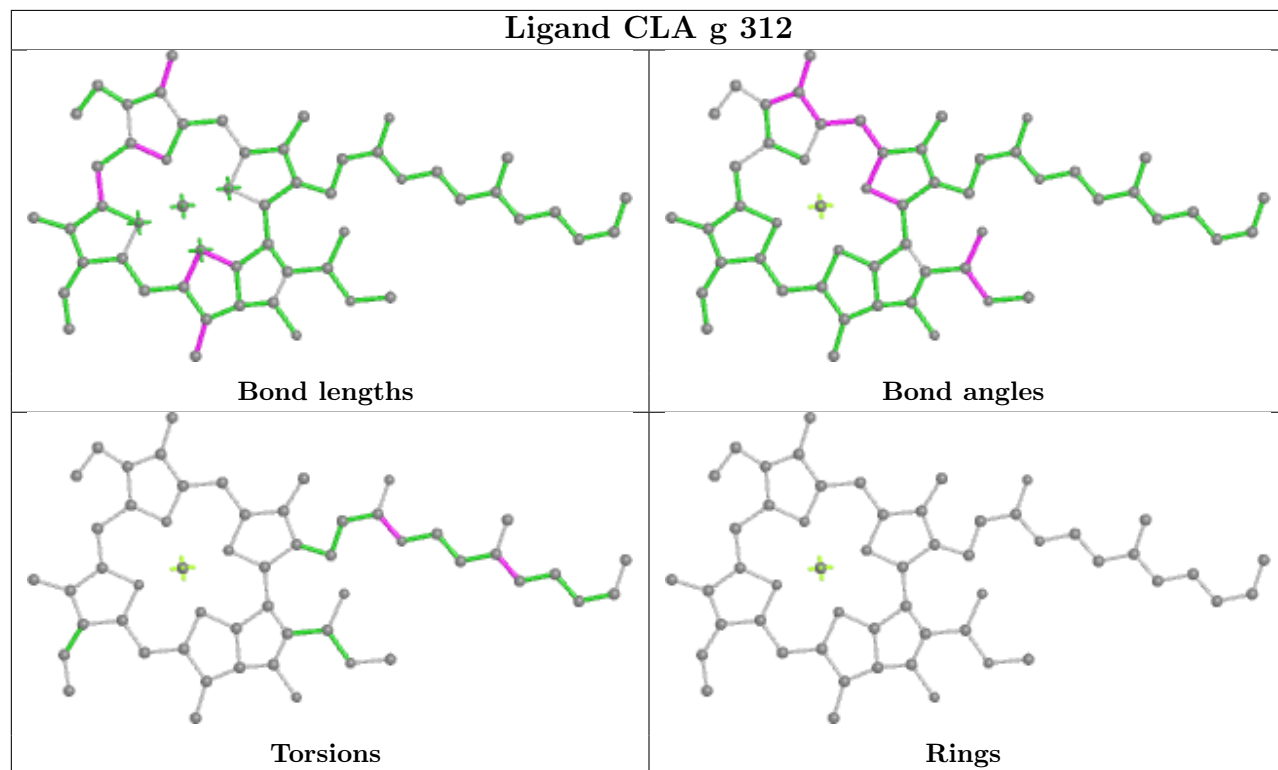
Ligand LHG j 318



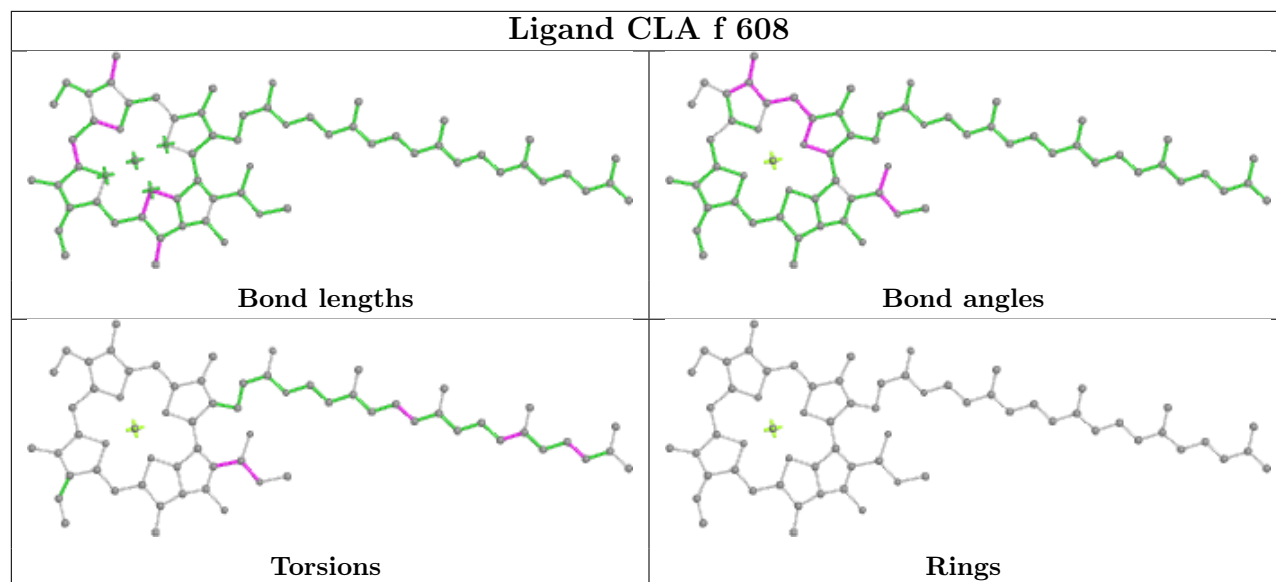
Ligand II0 d 315



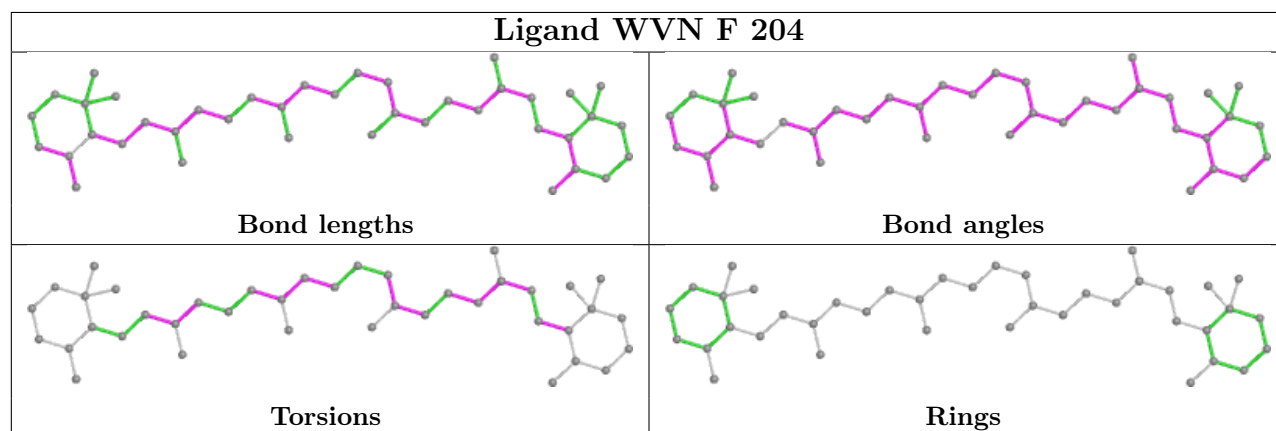
Ligand CLA g 312



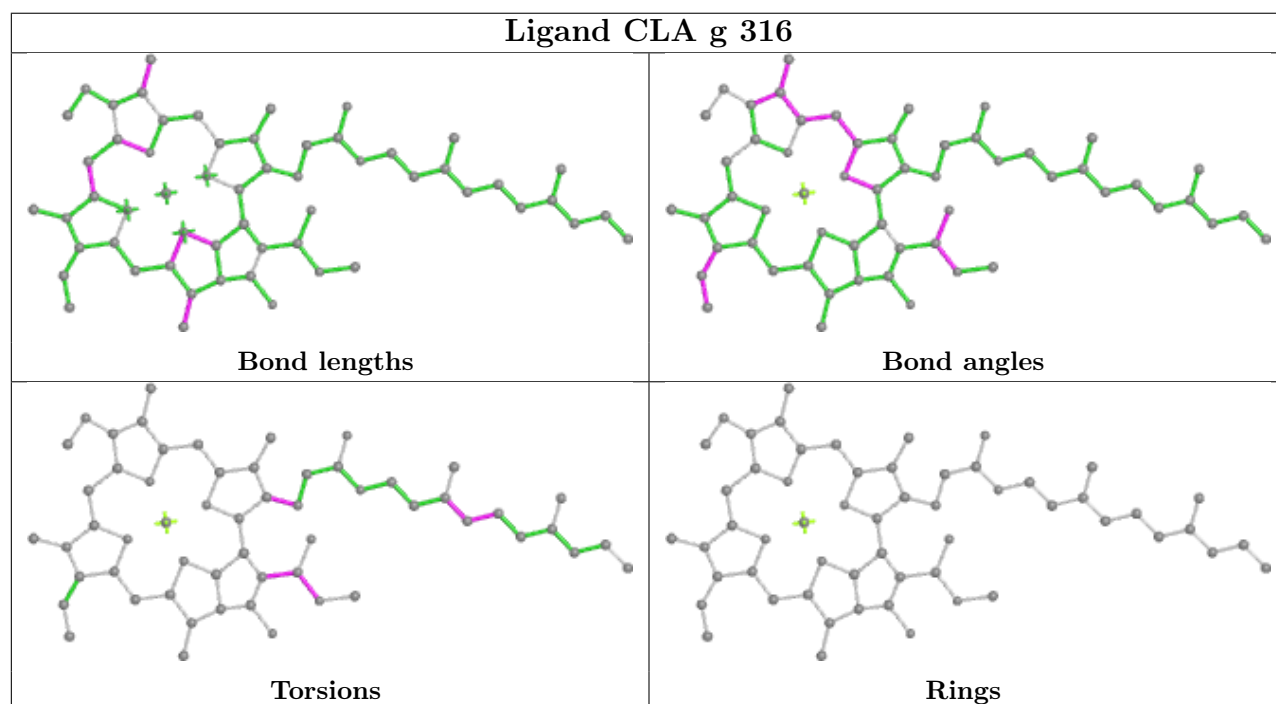
Ligand CLA f 608



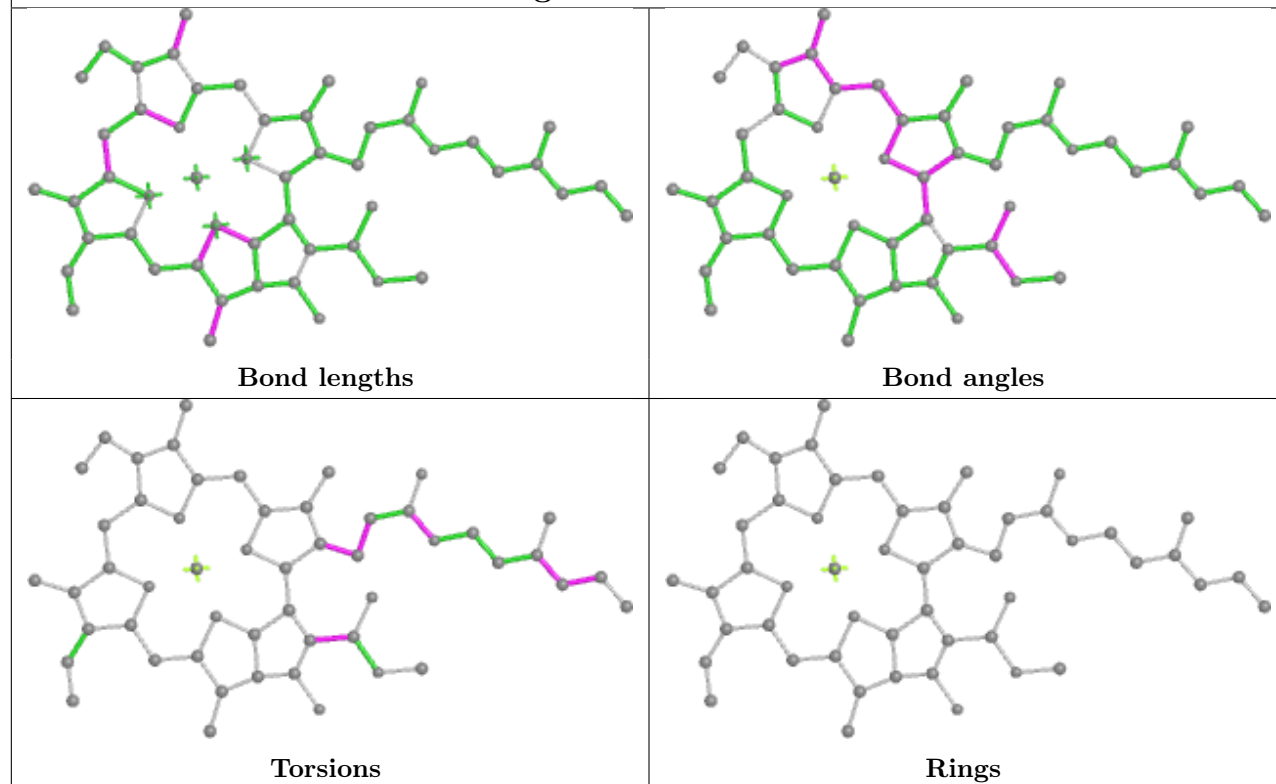
Ligand WVN F 204



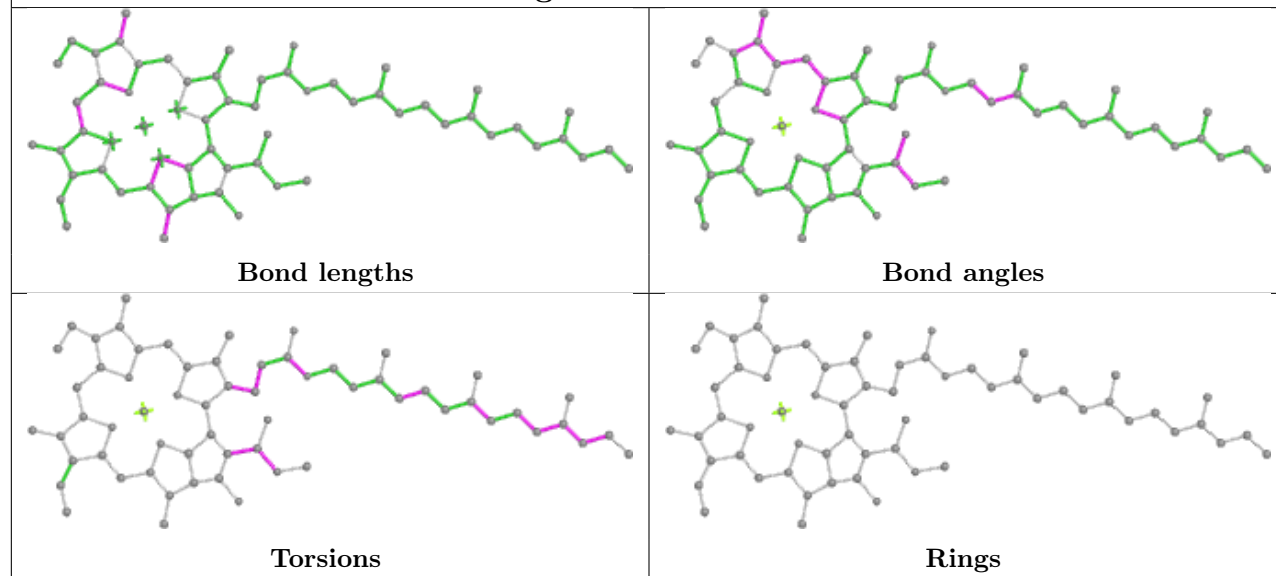
Ligand CLA g 316



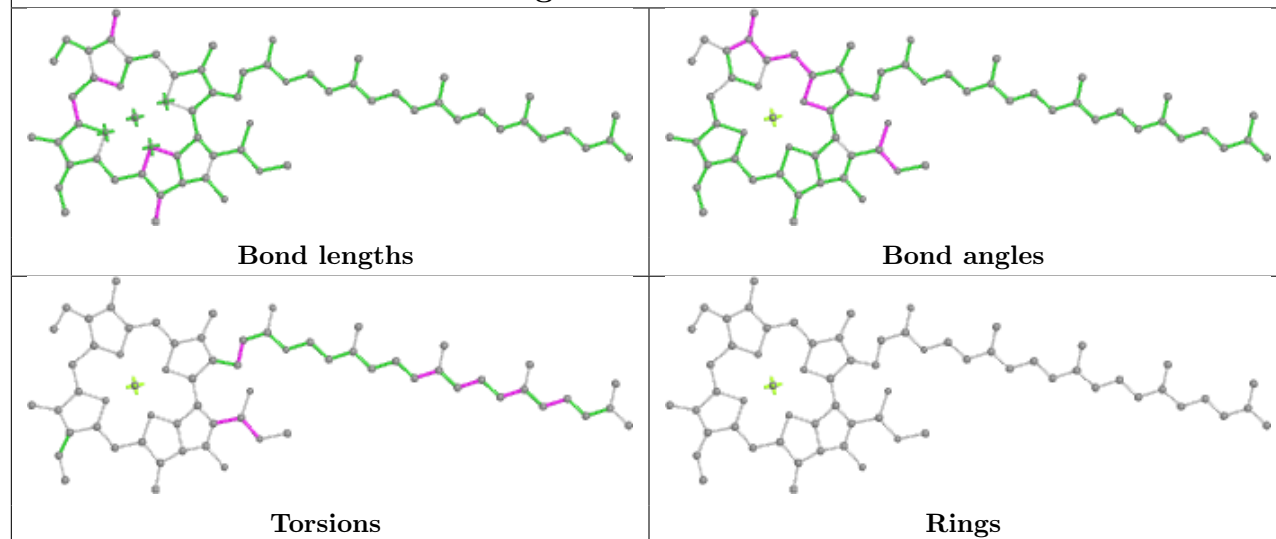
Ligand CLA F 203



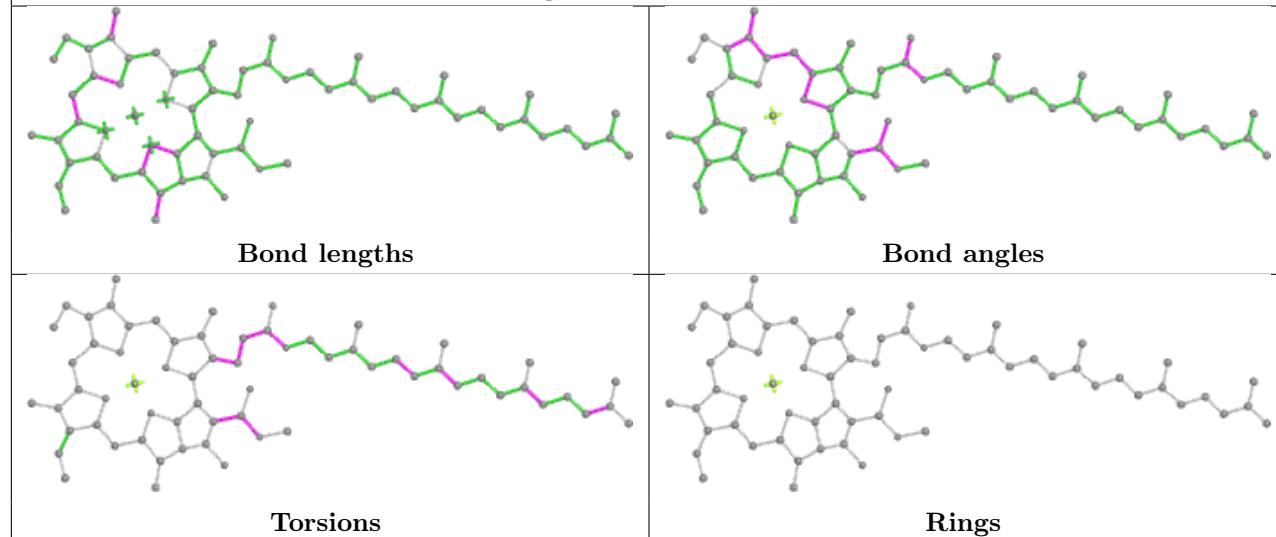
Ligand CLA d 302



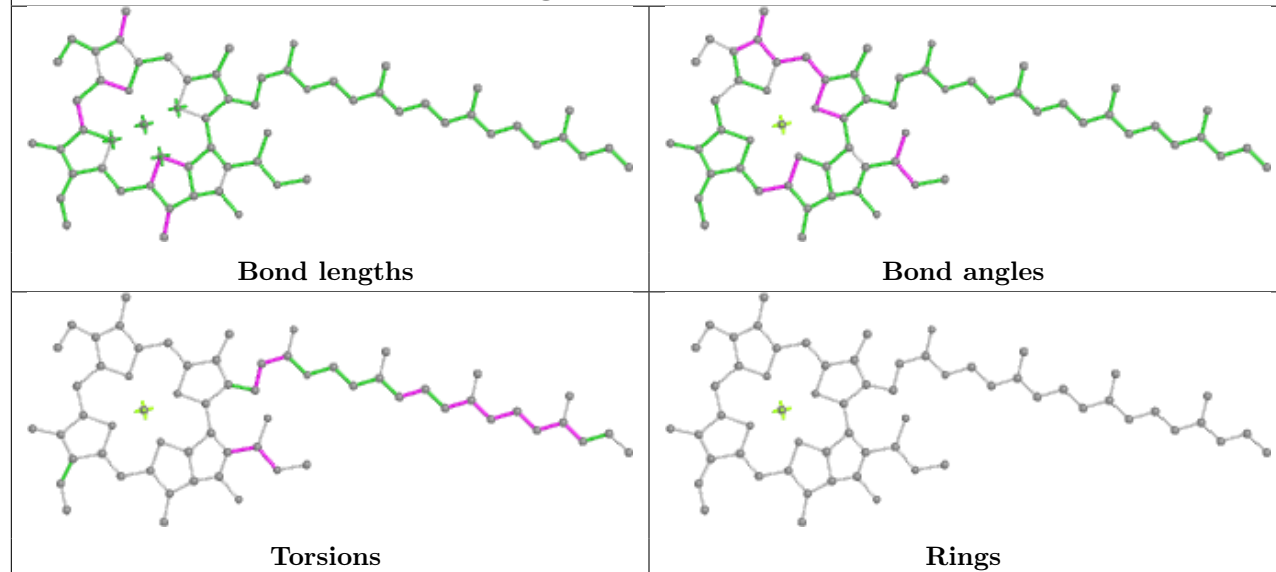
Ligand CLA b 305

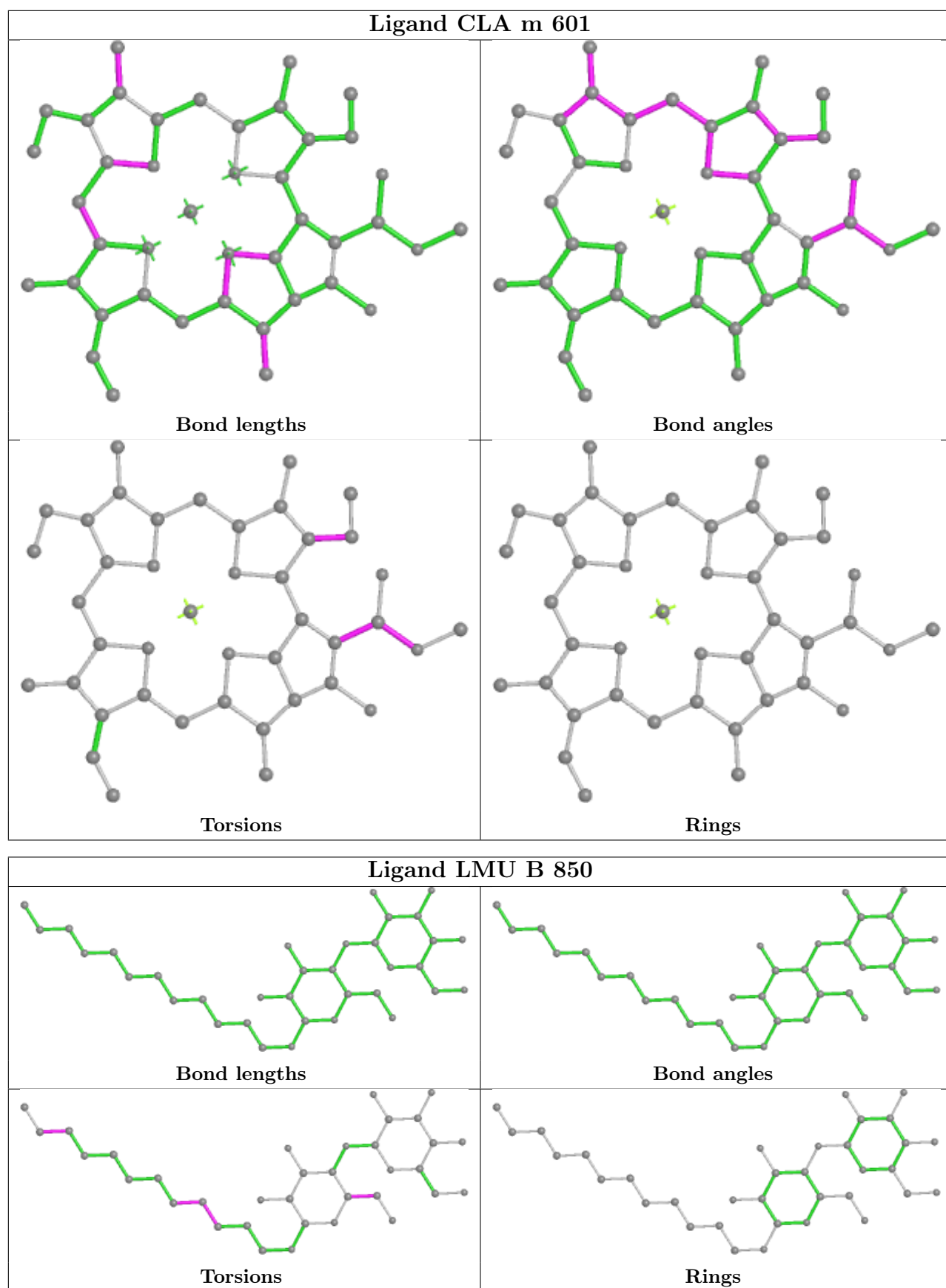


Ligand CLA i 302

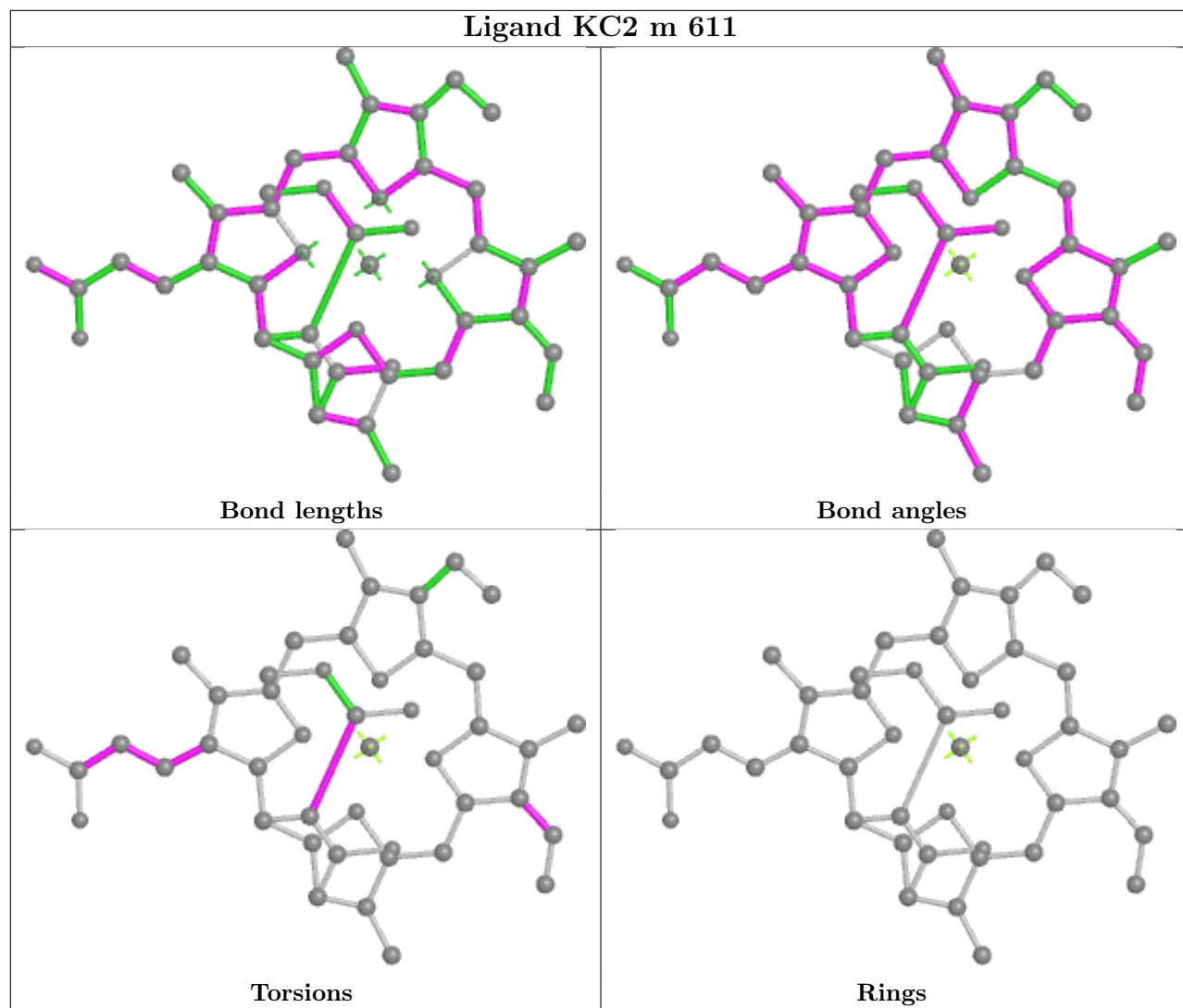


Ligand CLA c 304

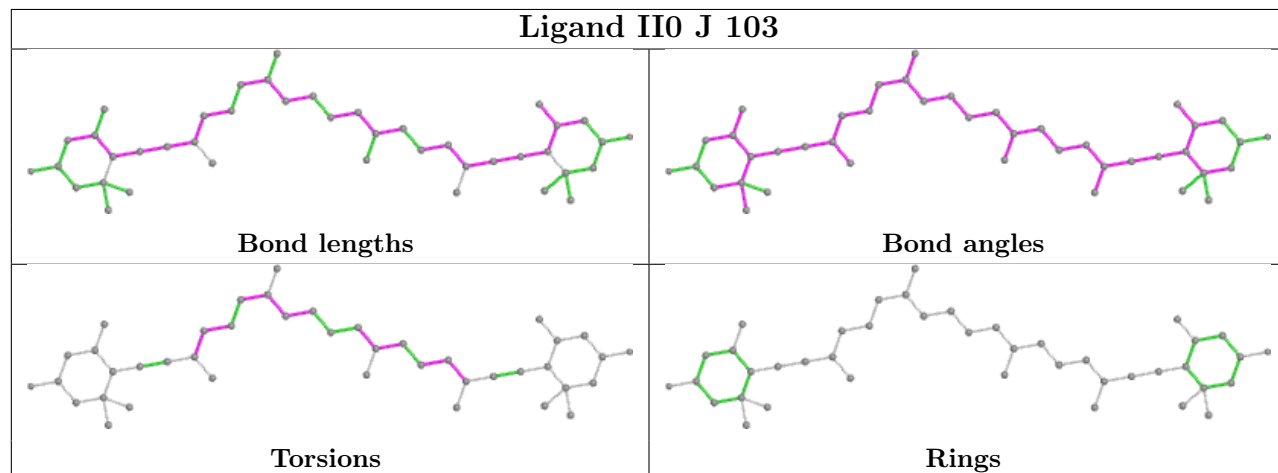




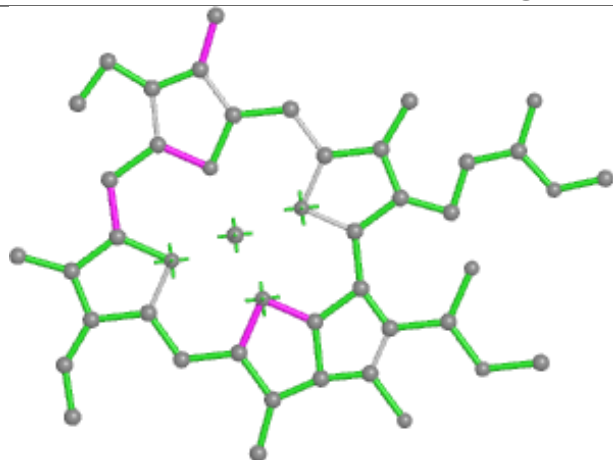
Ligand KC2 m 611



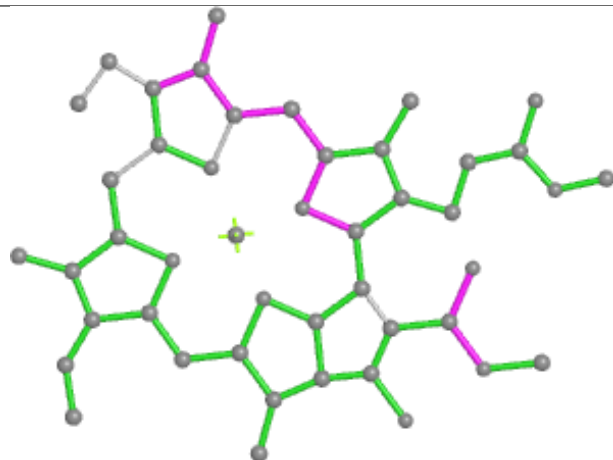
Ligand II0 J 103



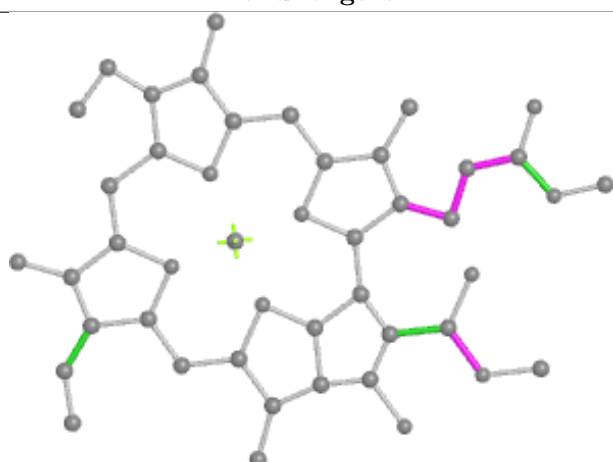
Ligand CLA d 308



Bond lengths



Bond angles

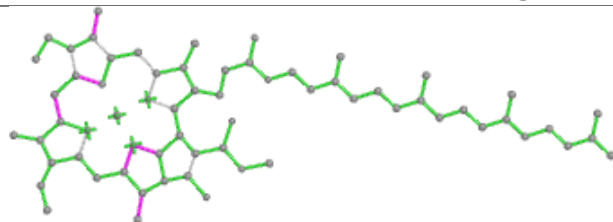


Torsions

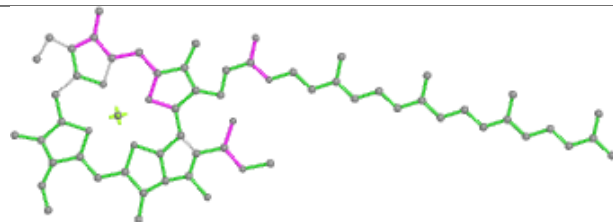


Rings

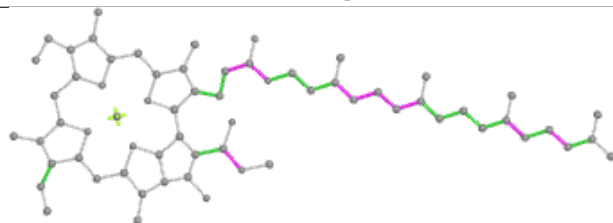
Ligand CLA B 806



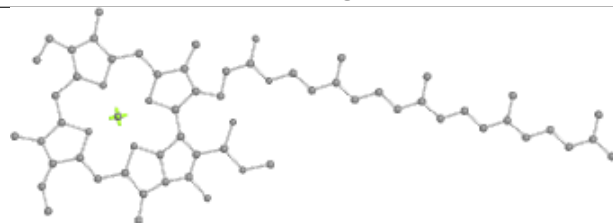
Bond lengths



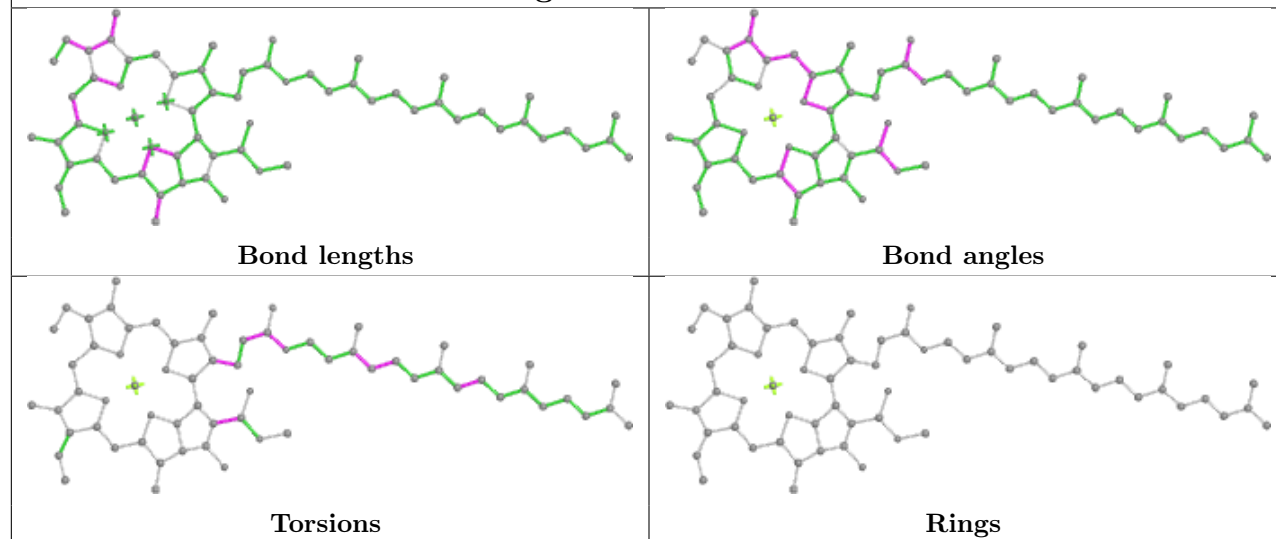
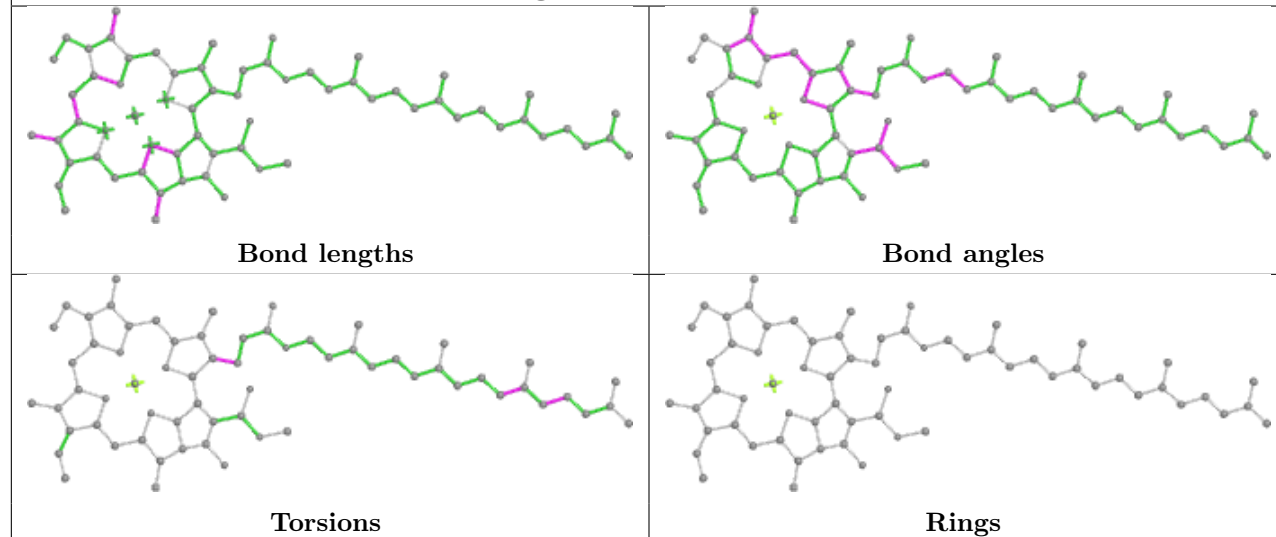
Bond angles



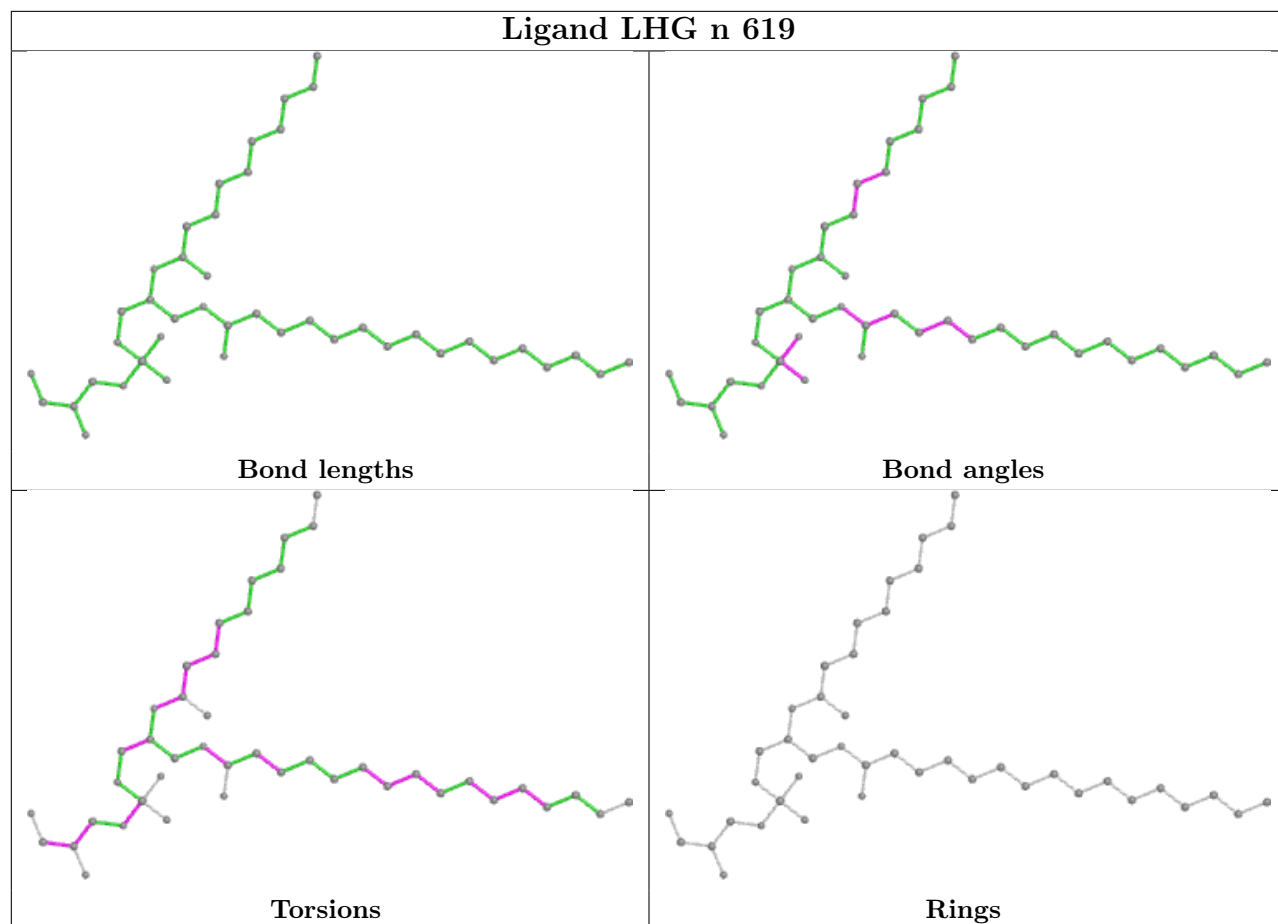
Torsions



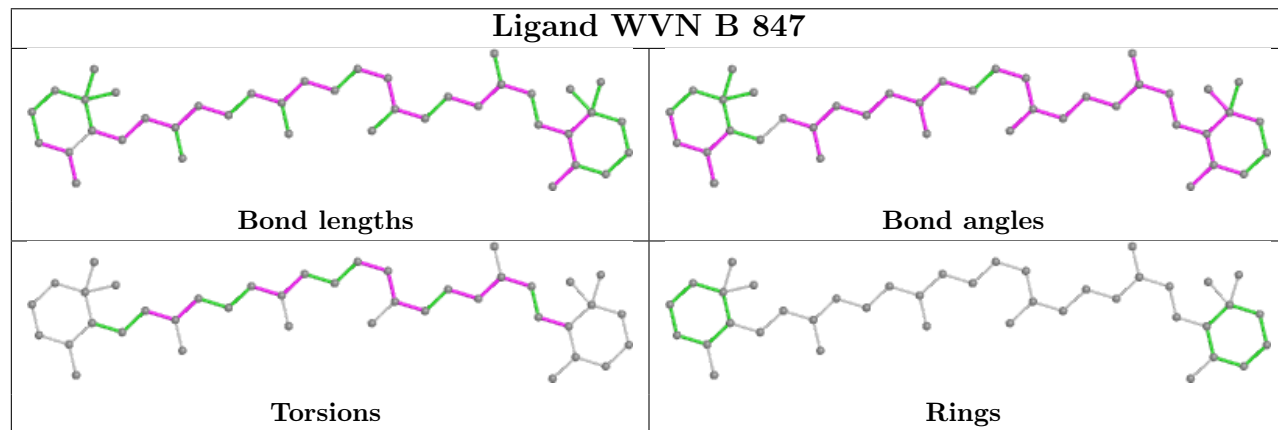
Rings

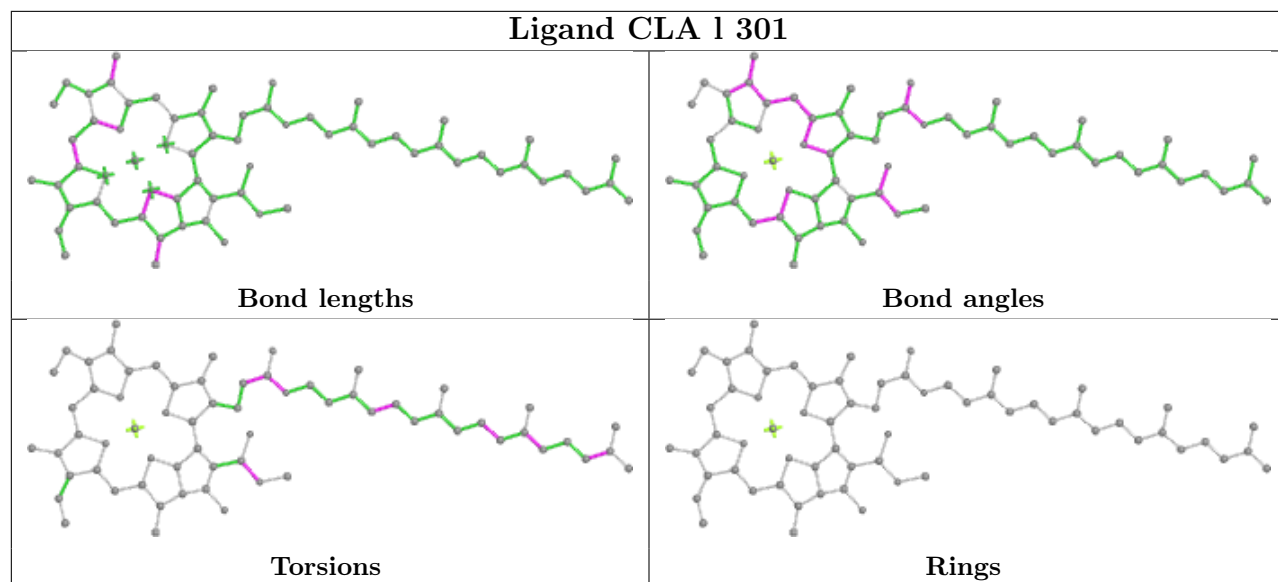
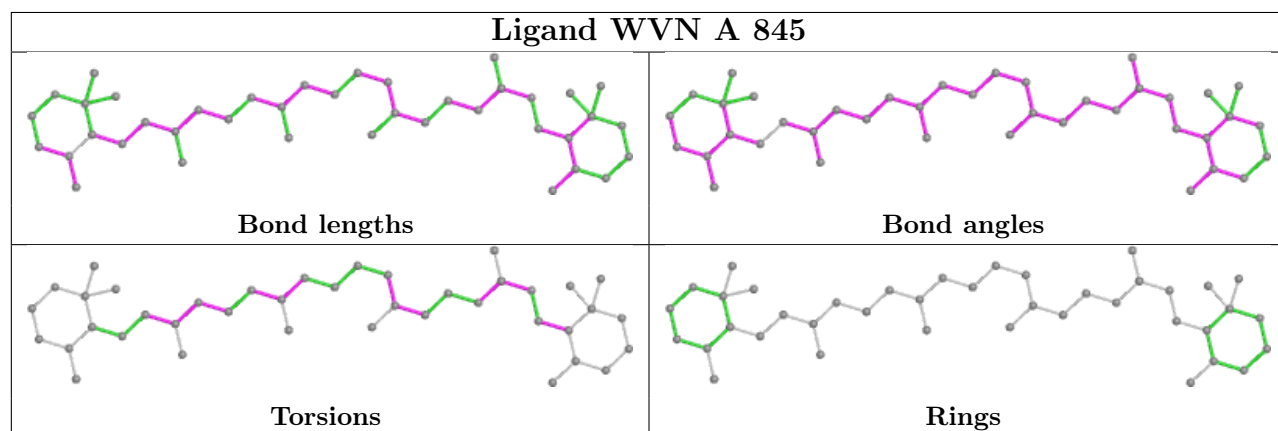
Ligand CLA n 607**Ligand CLA B 840**

Ligand LHG n 619

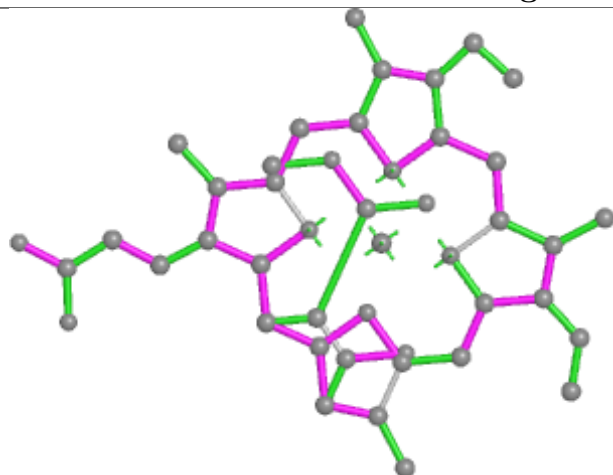


Ligand WVN B 847

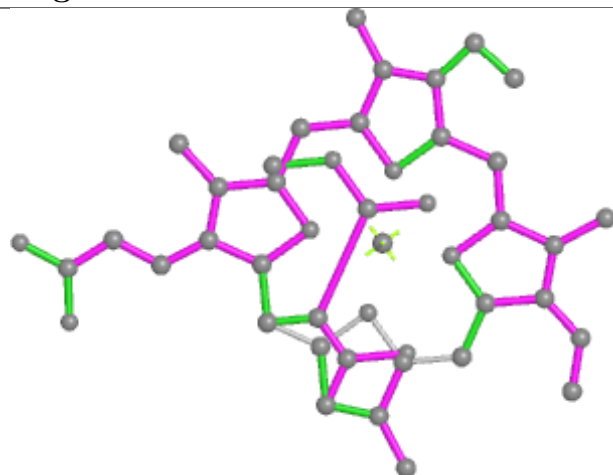


Ligand CLA 1 301**Ligand WVN A 845**

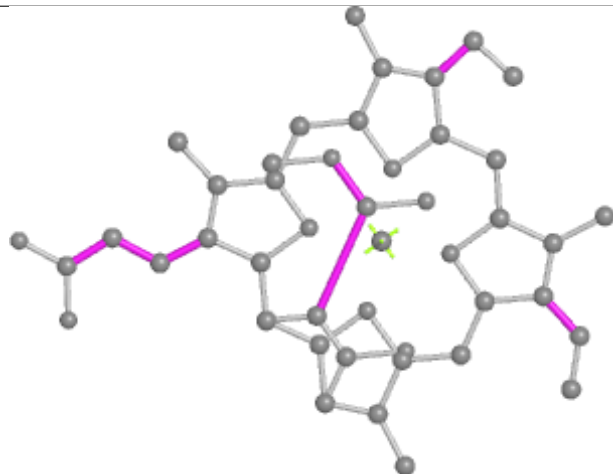
Ligand KC2 g 314



Bond lengths



Bond angles

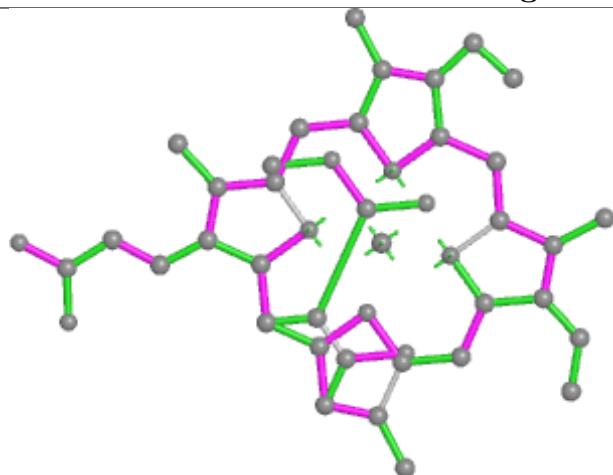


Torsions

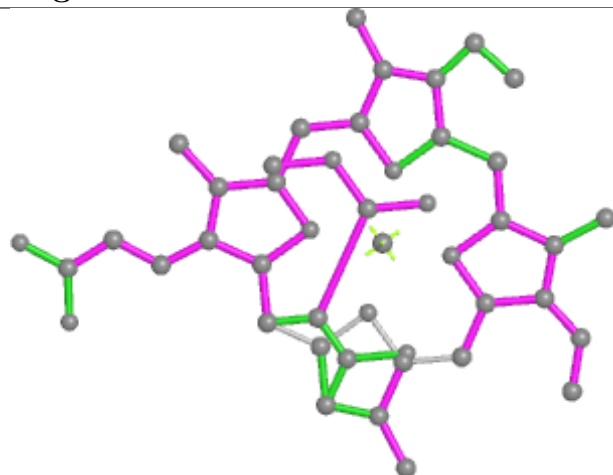


Rings

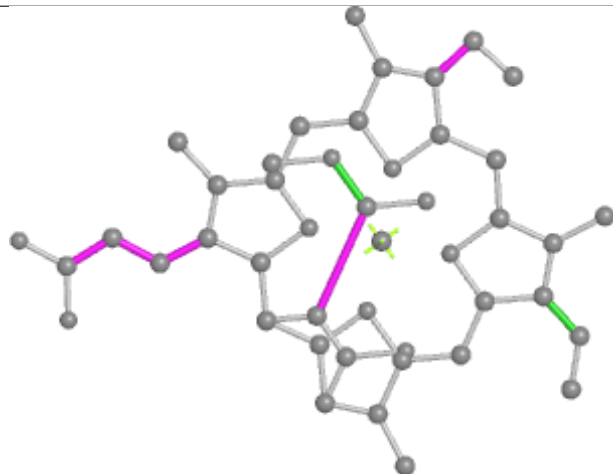
Ligand KC2 g 315



Bond lengths



Bond angles

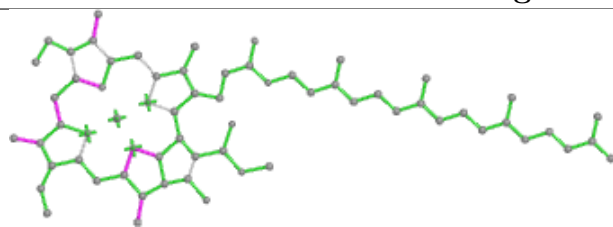


Torsions

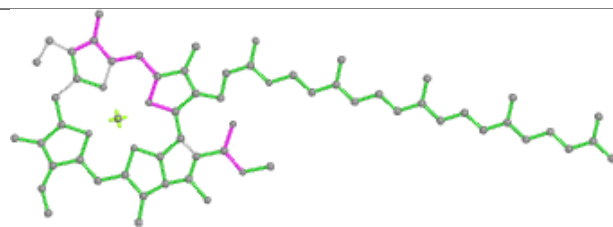


Rings

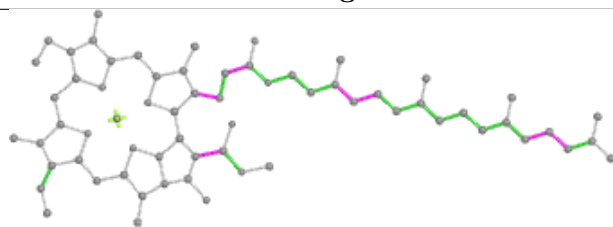
Ligand CLA A 812



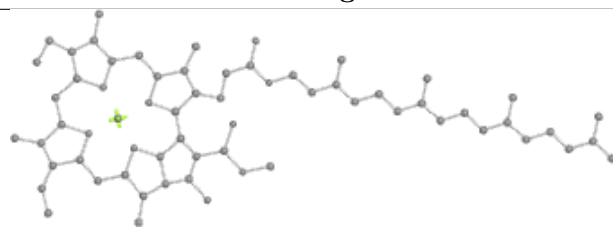
Bond lengths



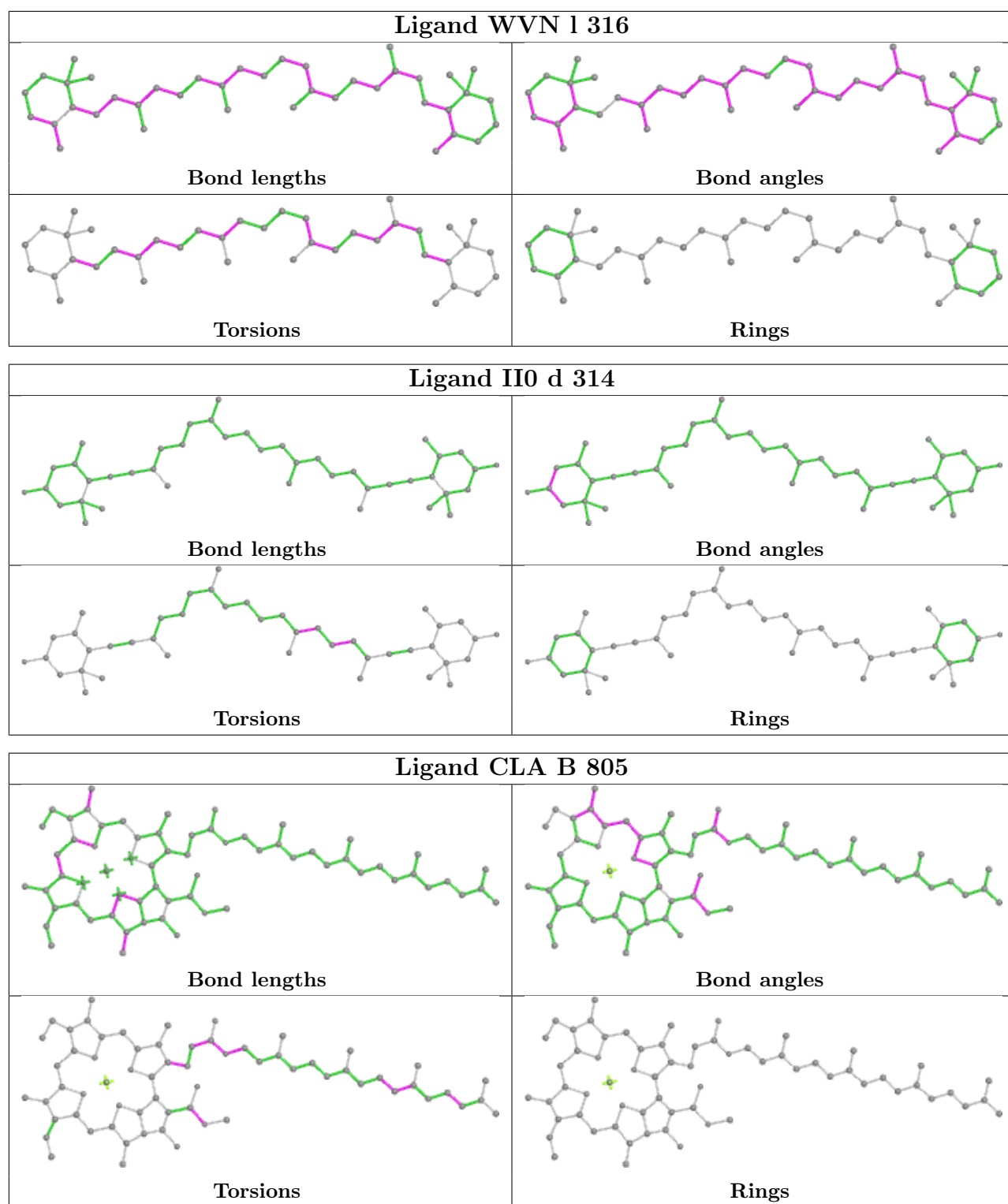
Bond angles



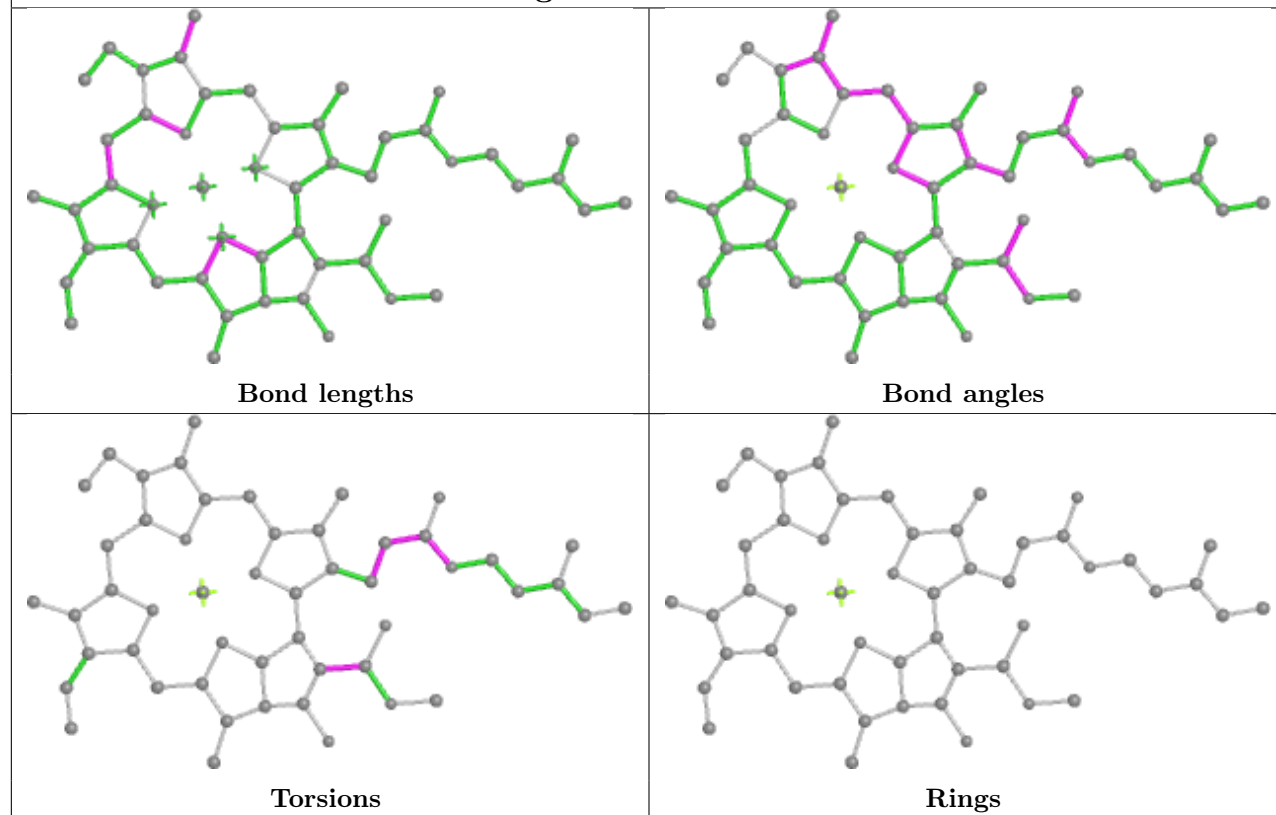
Torsions



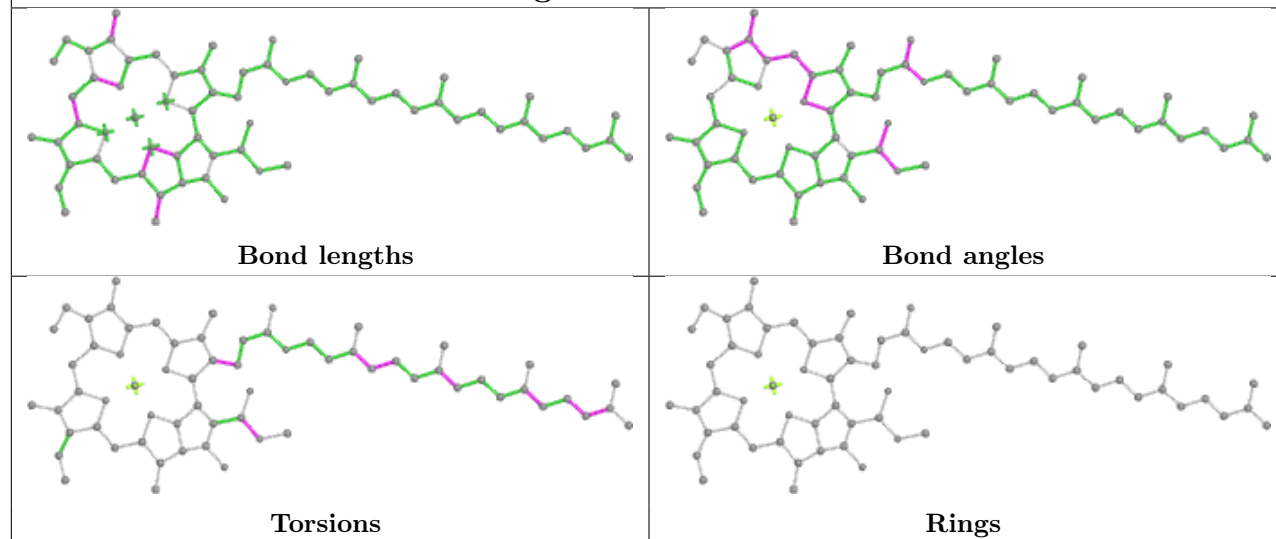
Rings

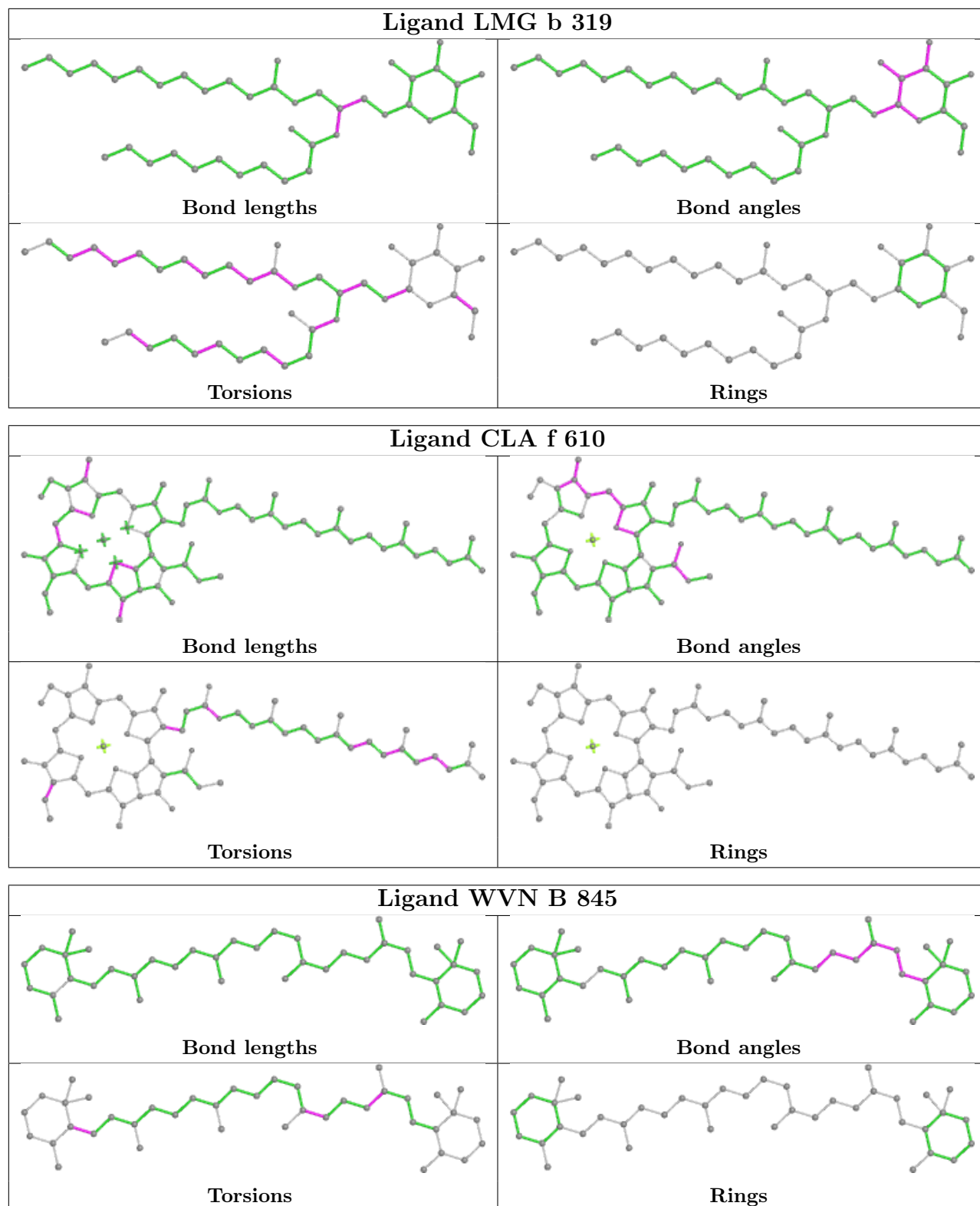


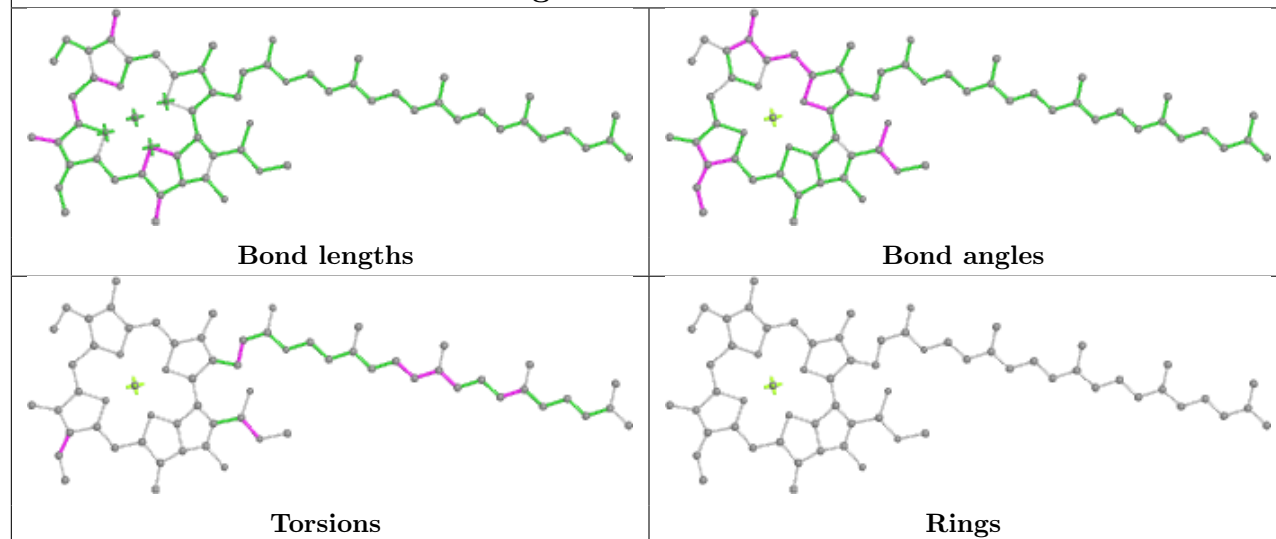
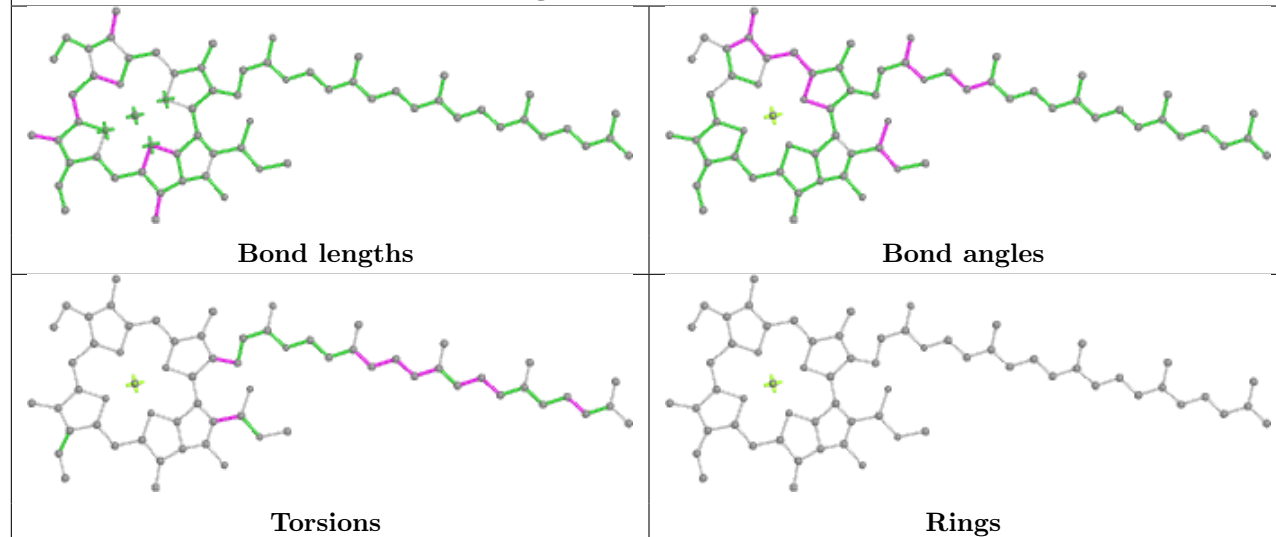
Ligand CLA d 305



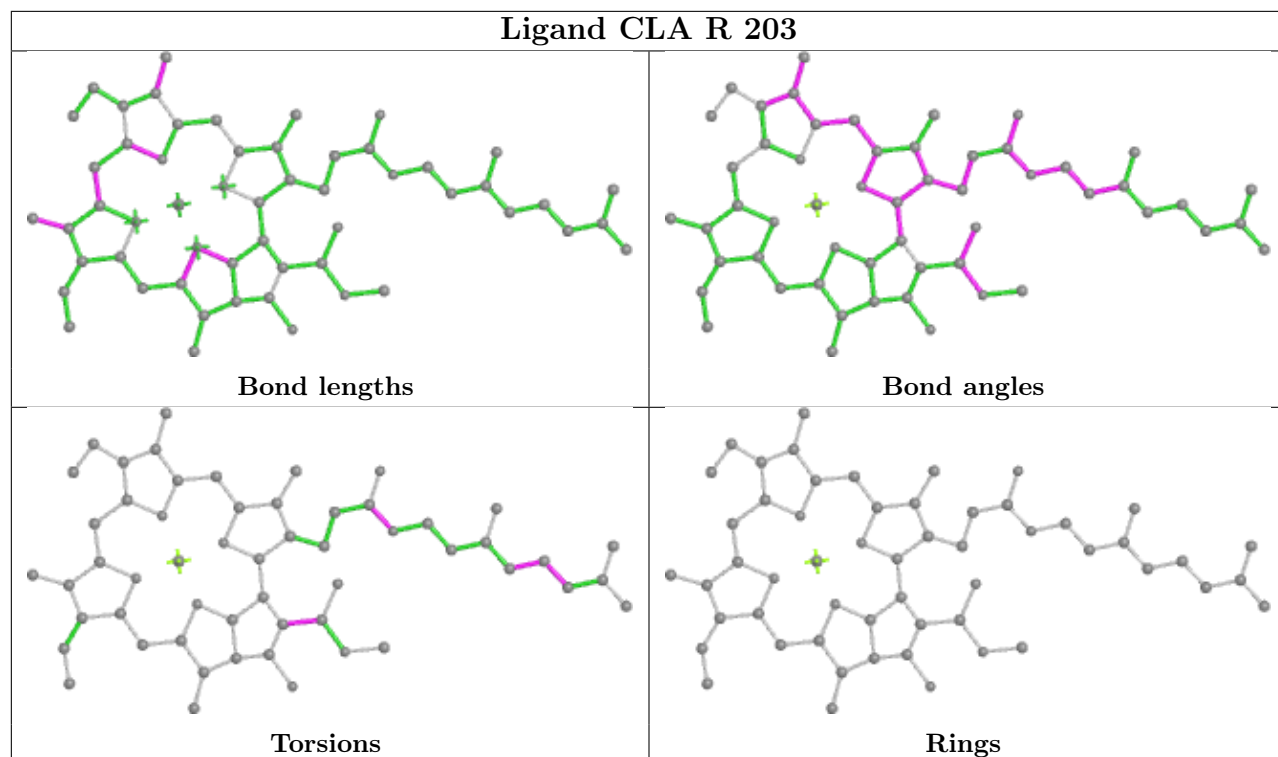
Ligand CLA F 201



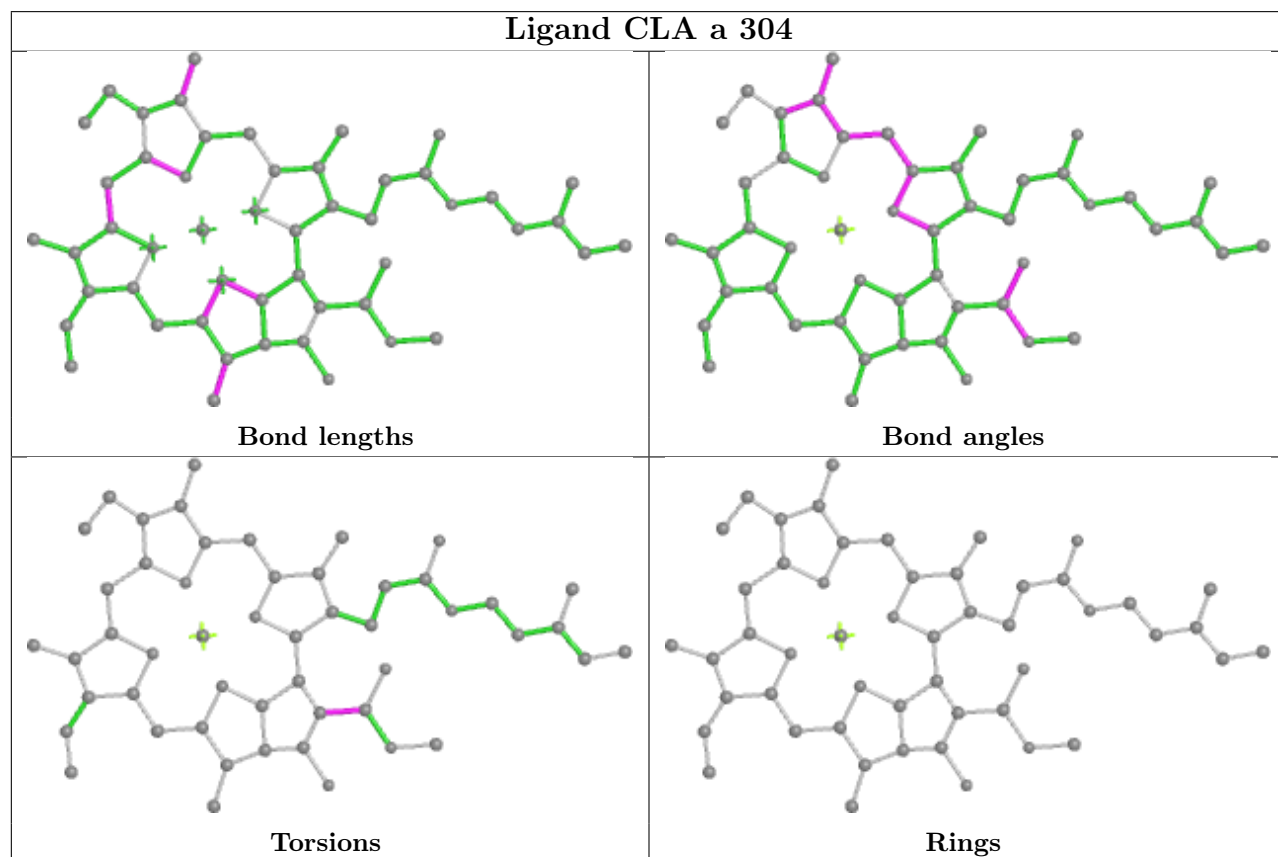


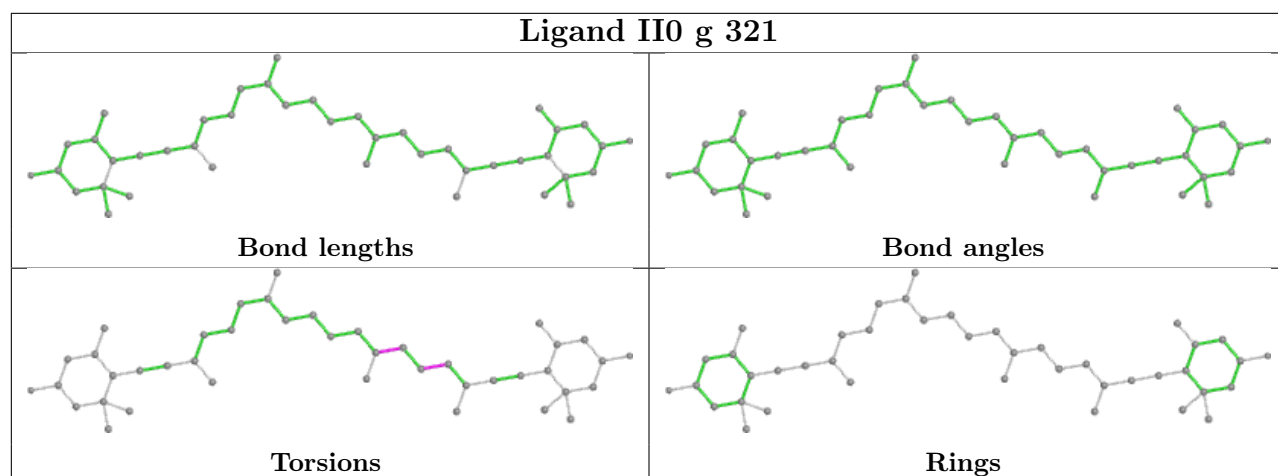
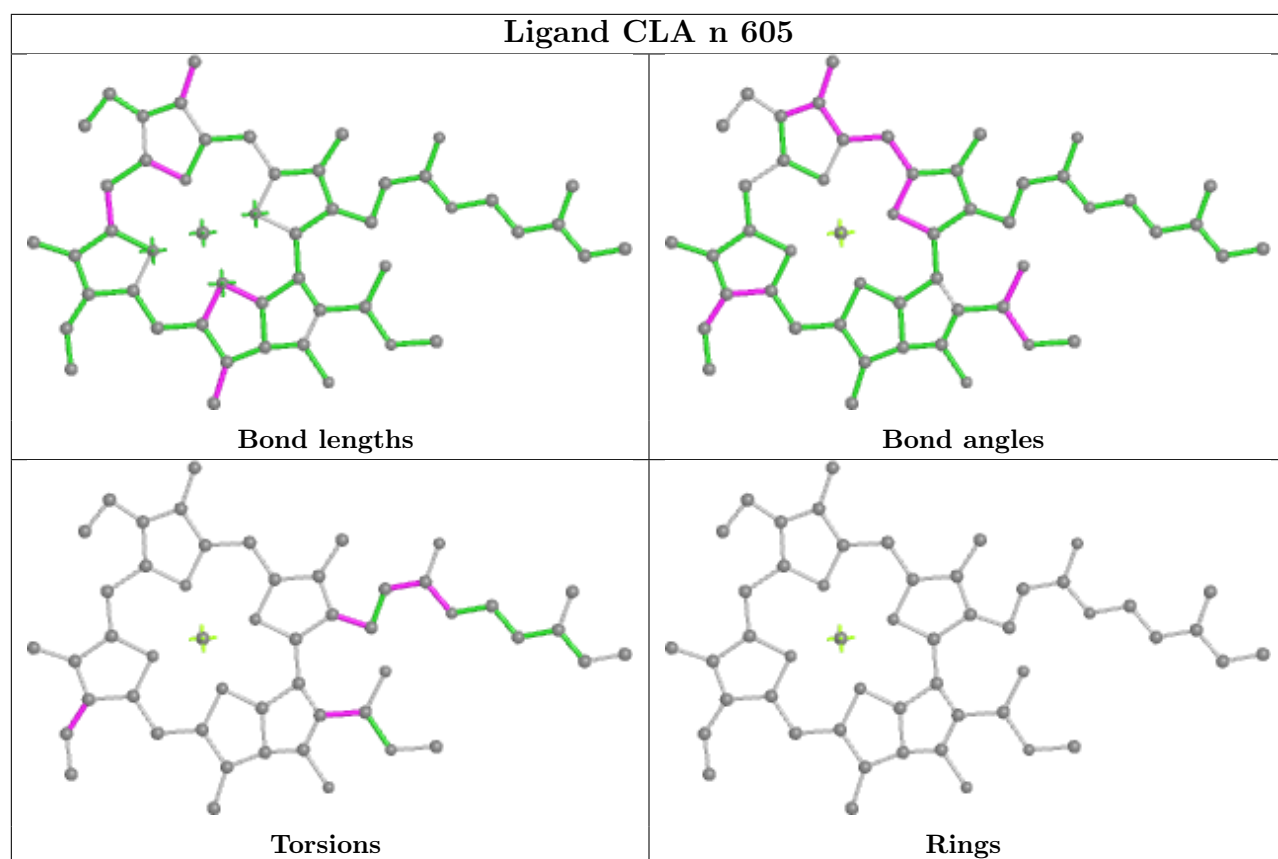
Ligand CLA B 804**Ligand CLA B 812**

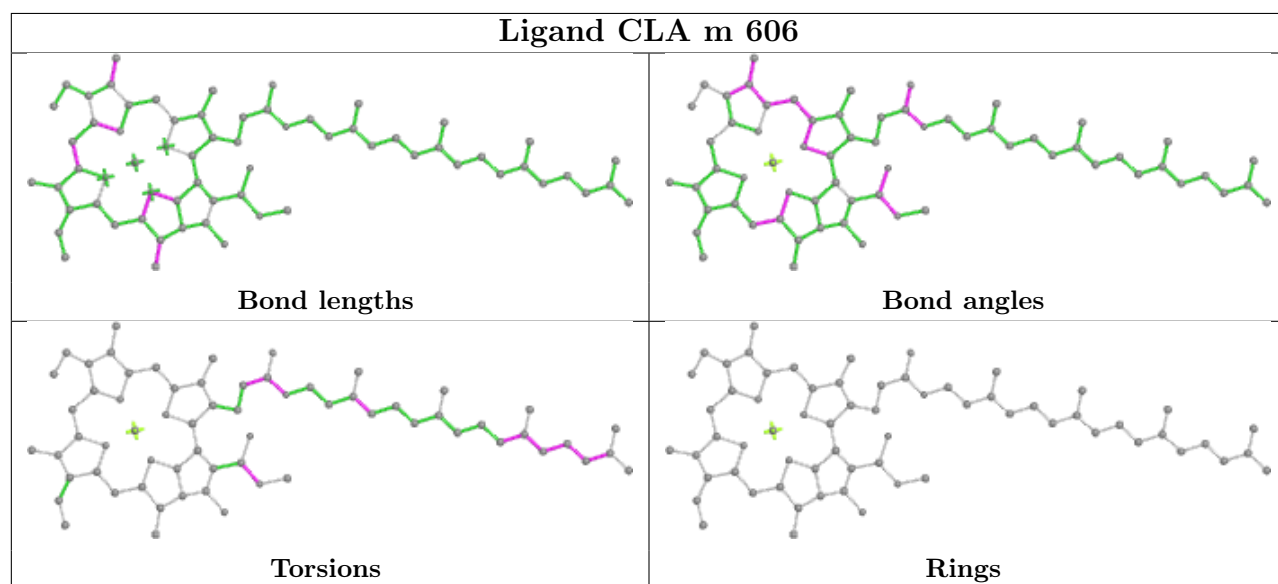
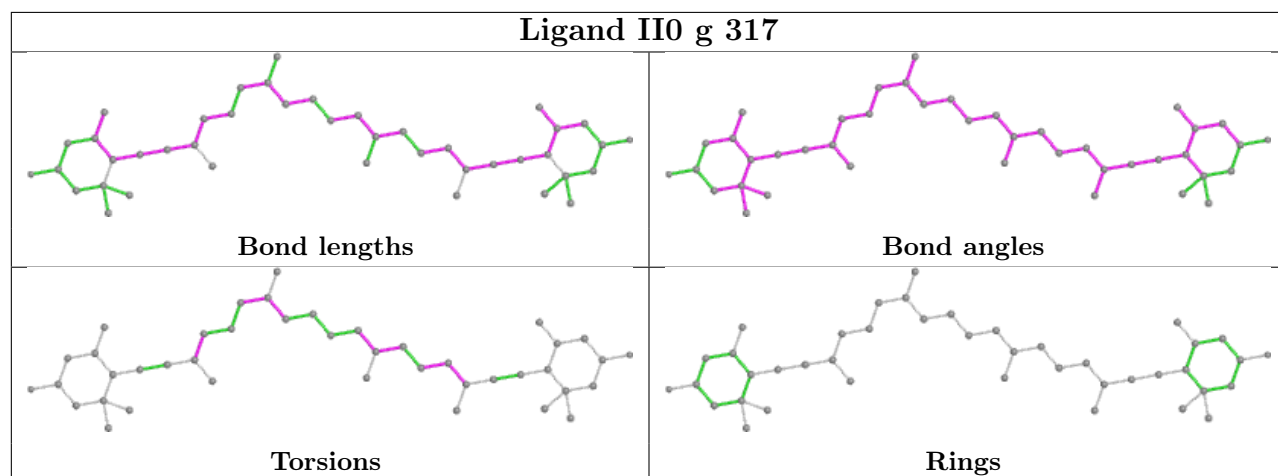
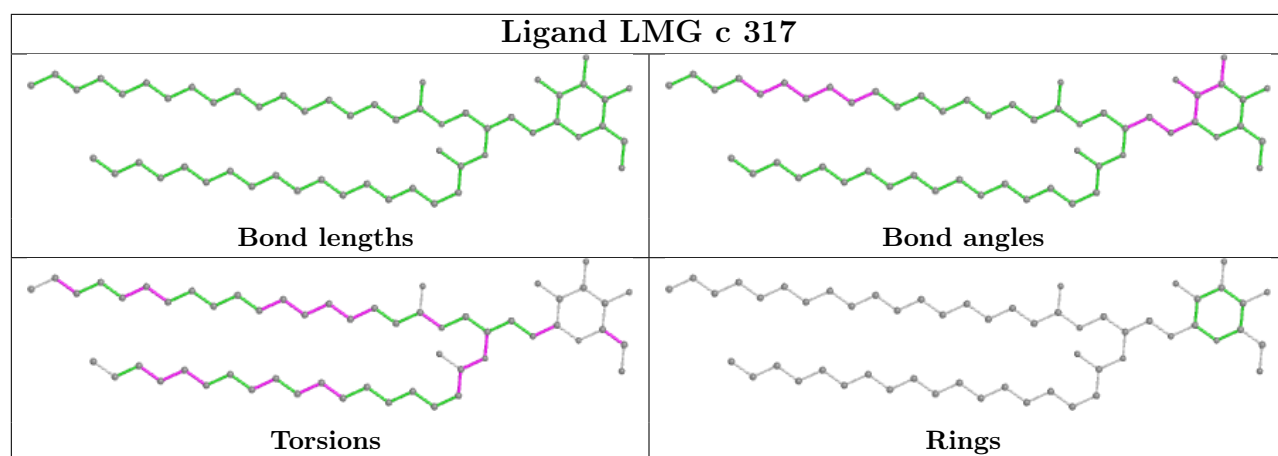
Ligand CLA R 203



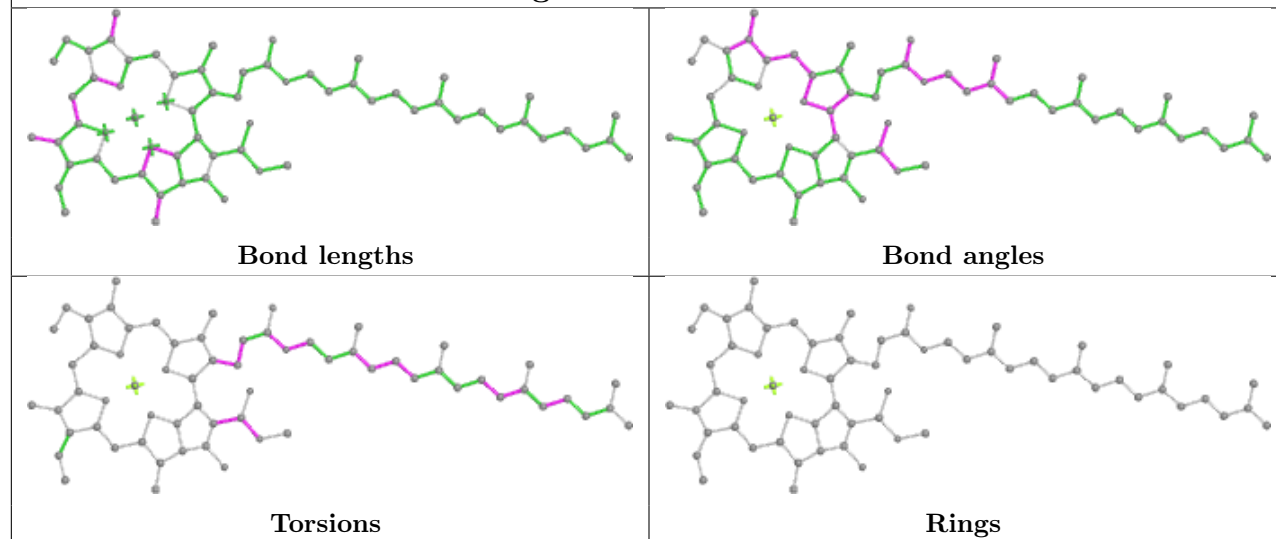
Ligand CLA a 304



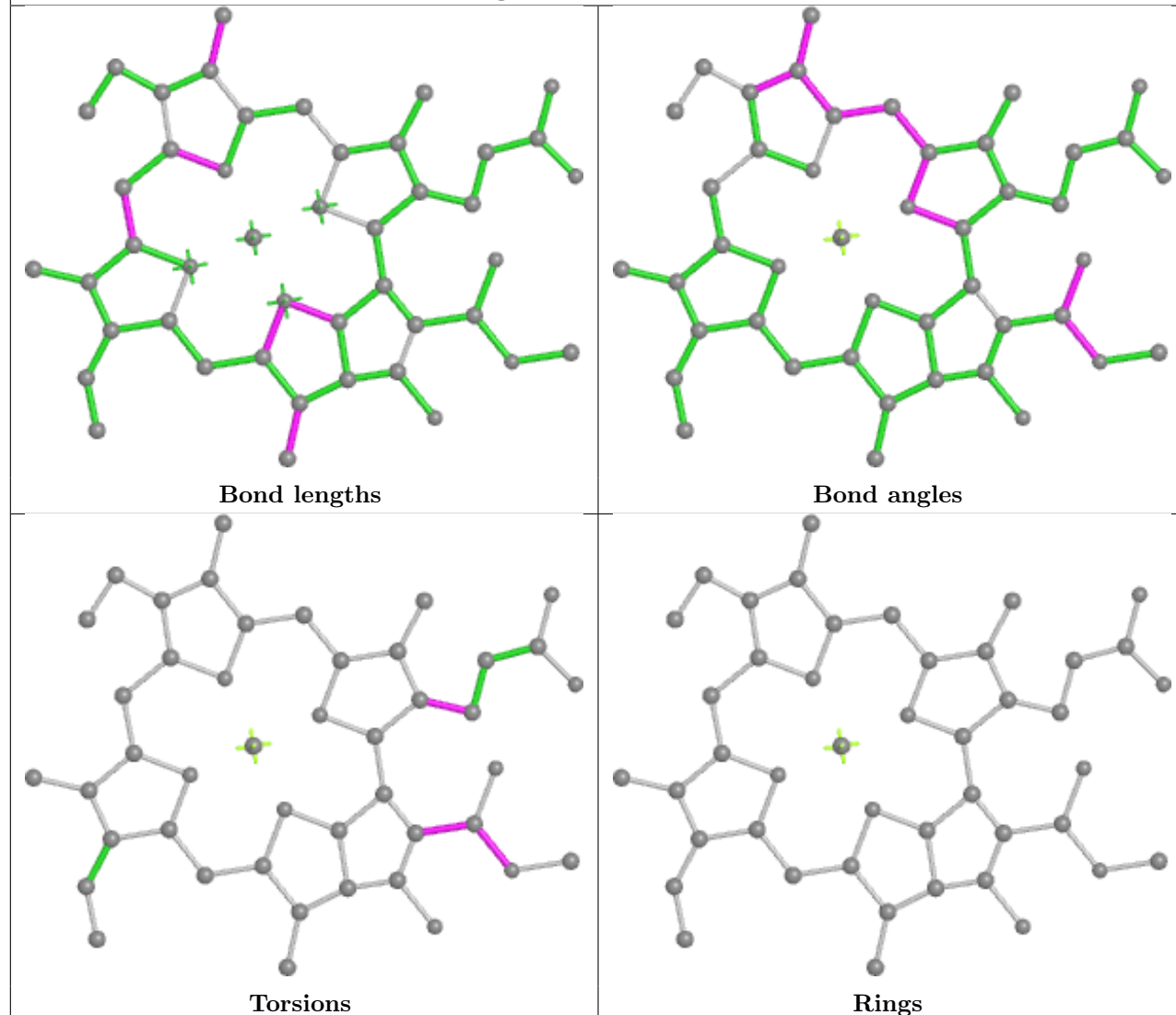


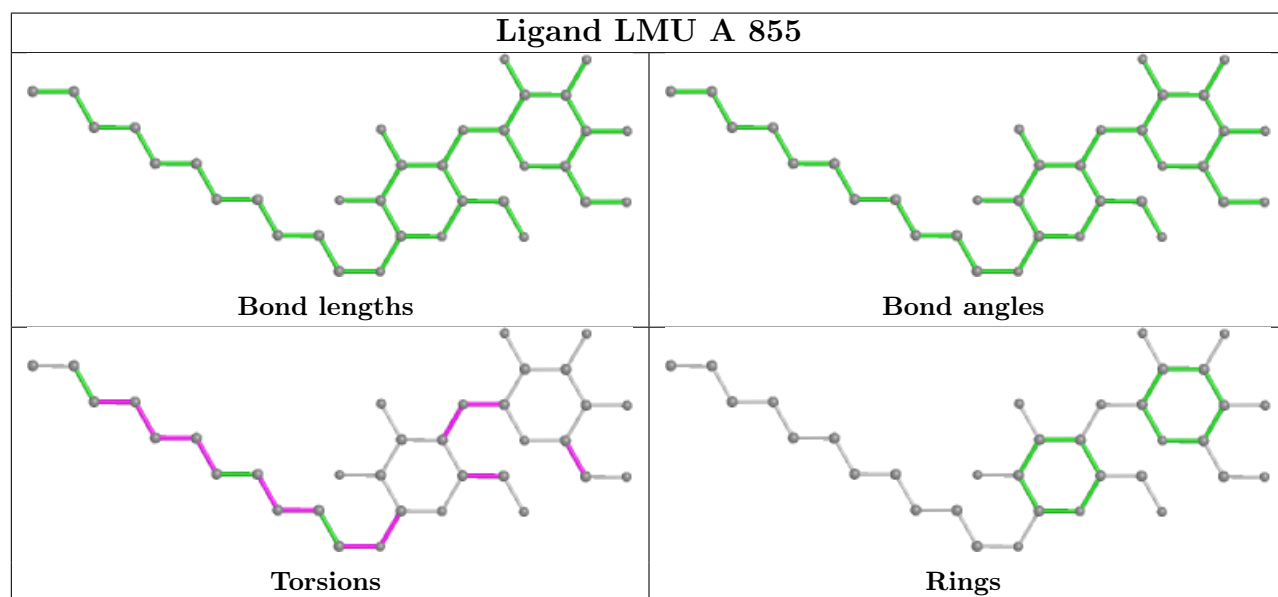
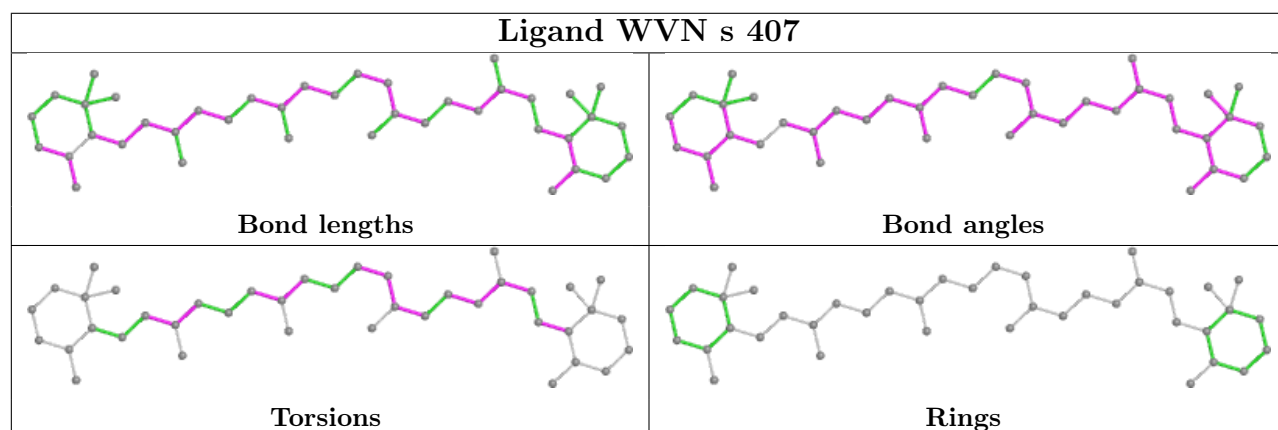
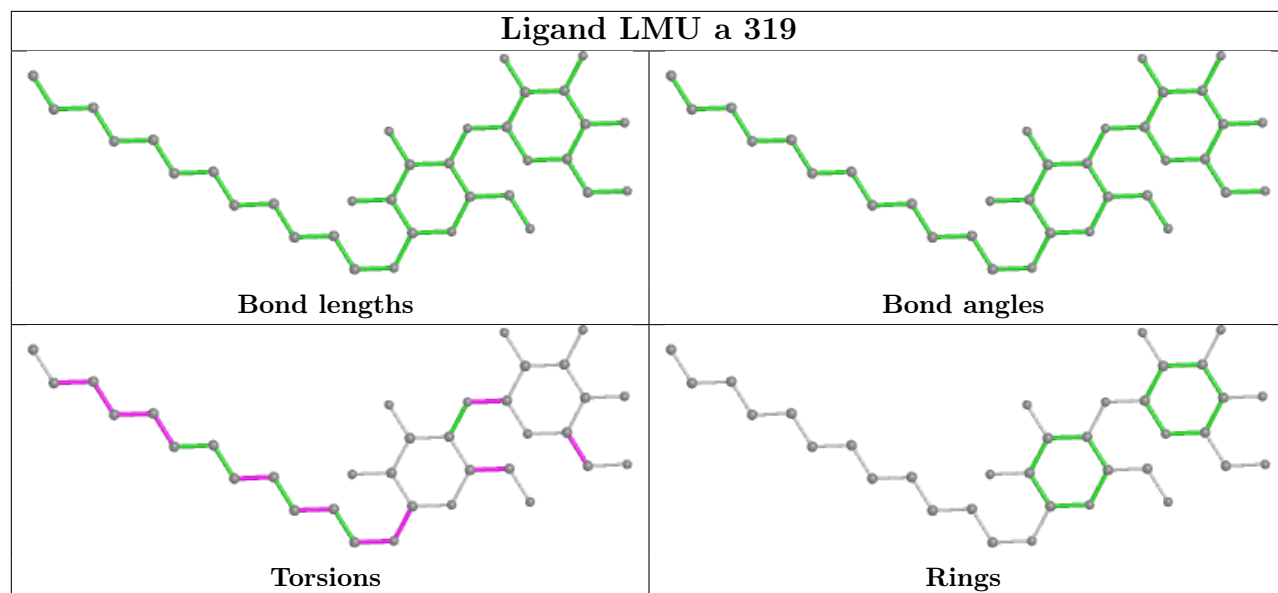


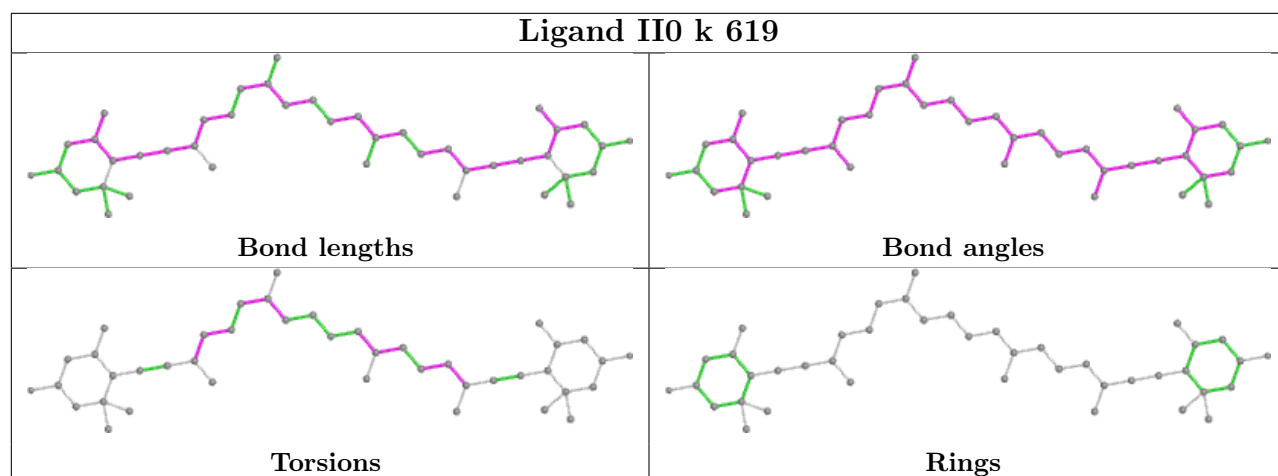
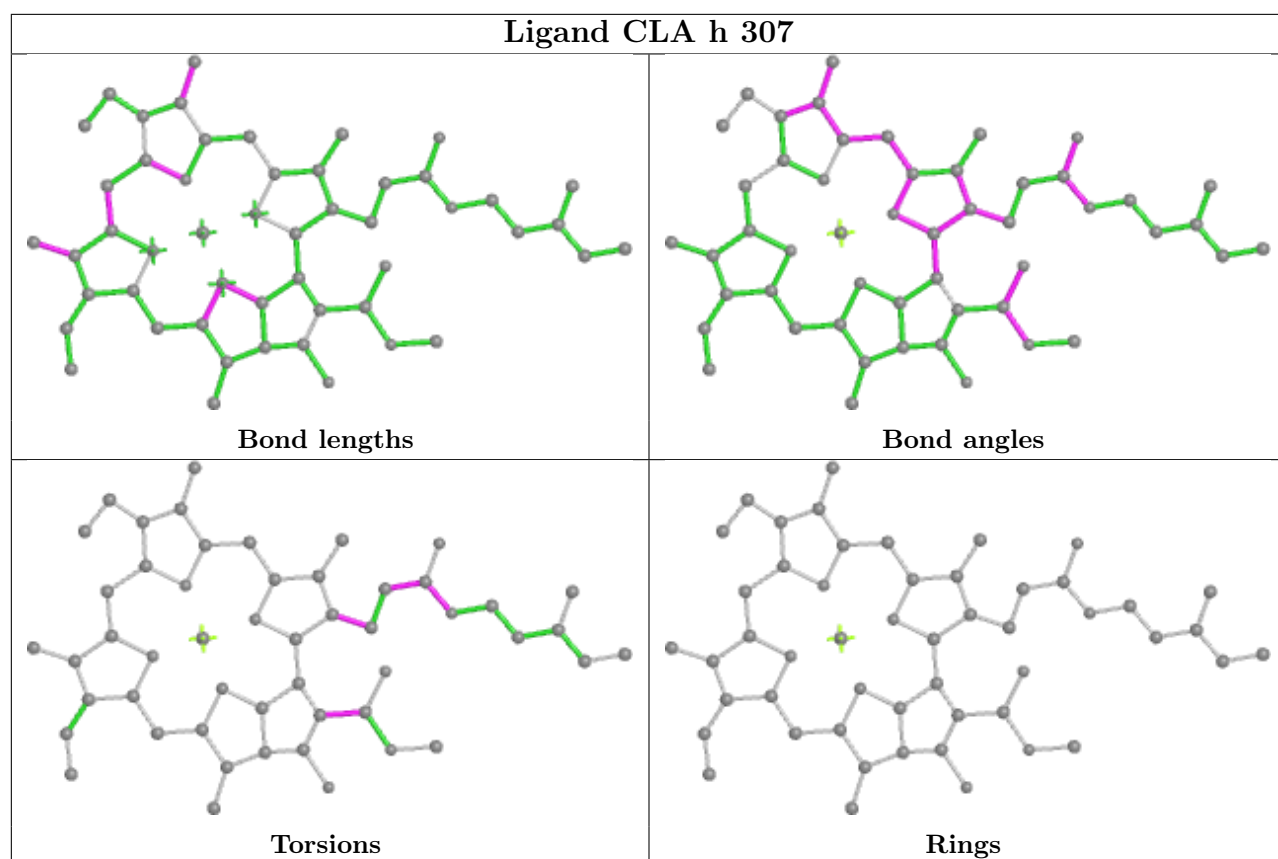
Ligand CLA B 822



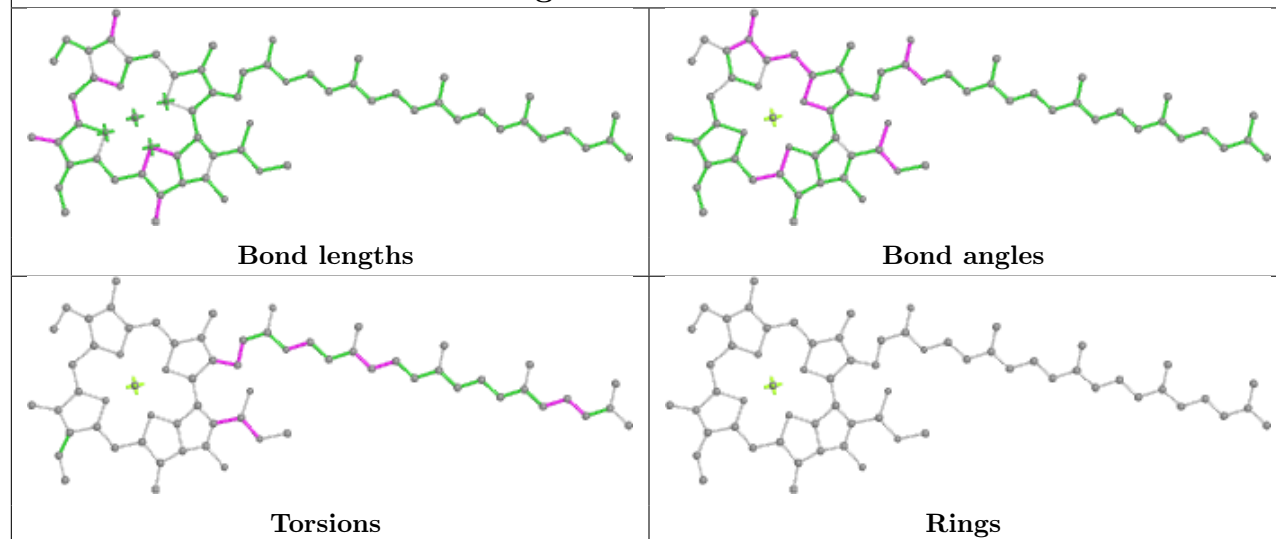
Ligand CLA n 601



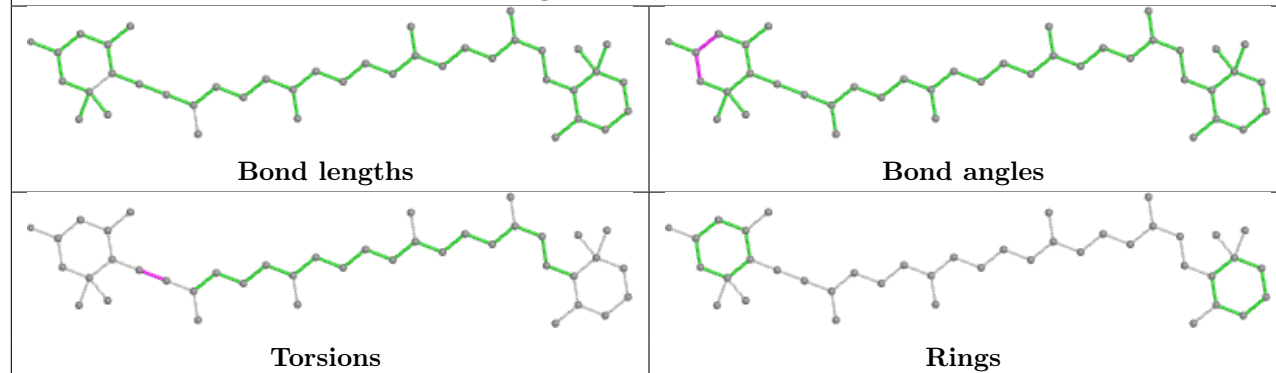




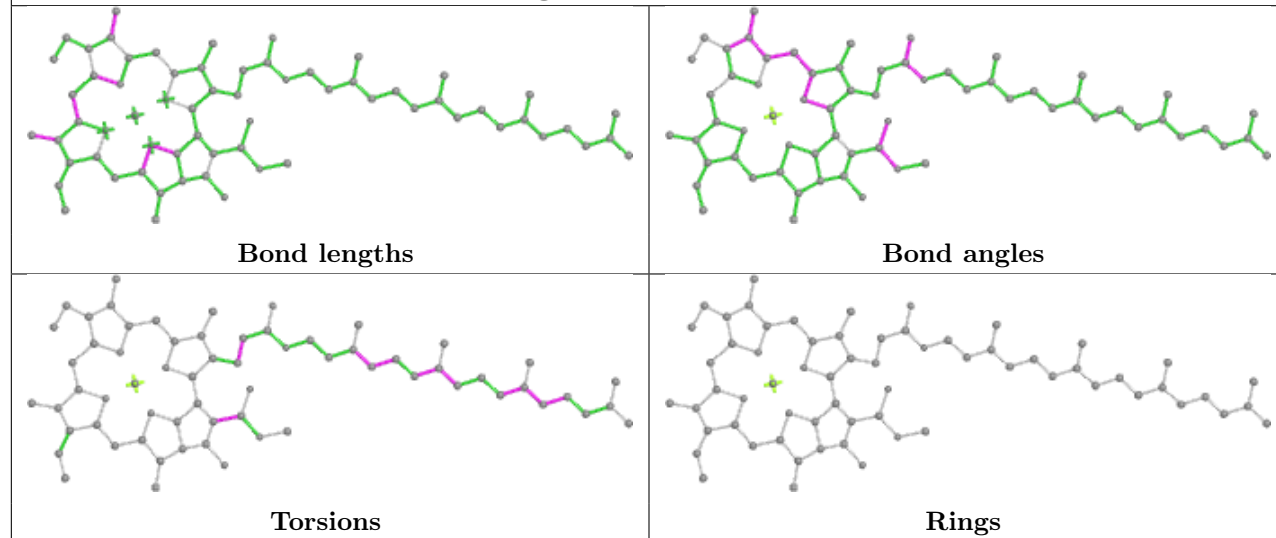
Ligand CLA n 609



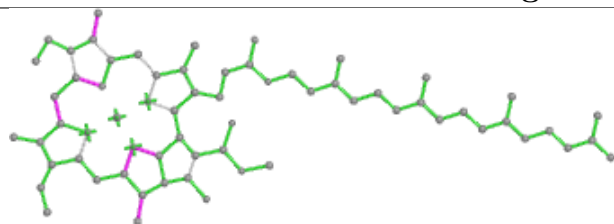
Ligand IHT R 204



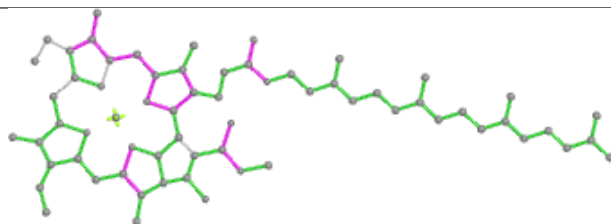
Ligand CLA b 308



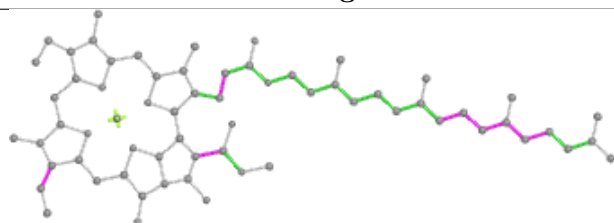
Ligand CLA f 604



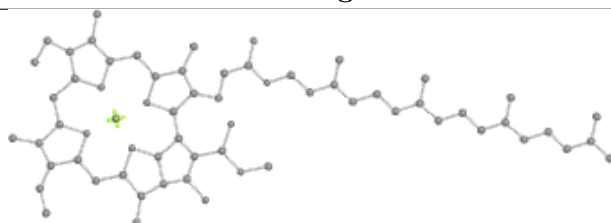
Bond lengths



Bond angles

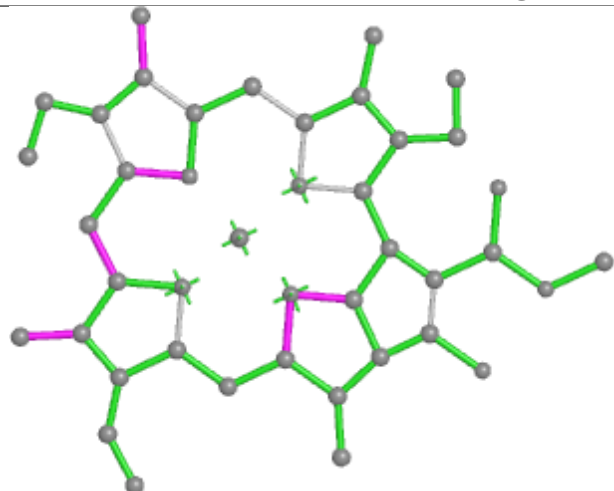


Torsions

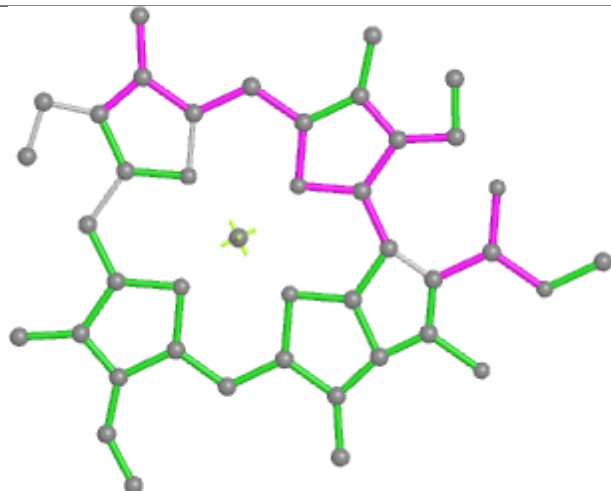


Rings

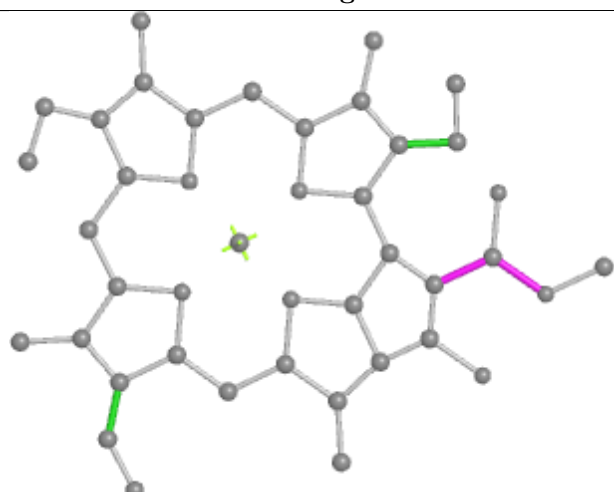
Ligand CLA K 102



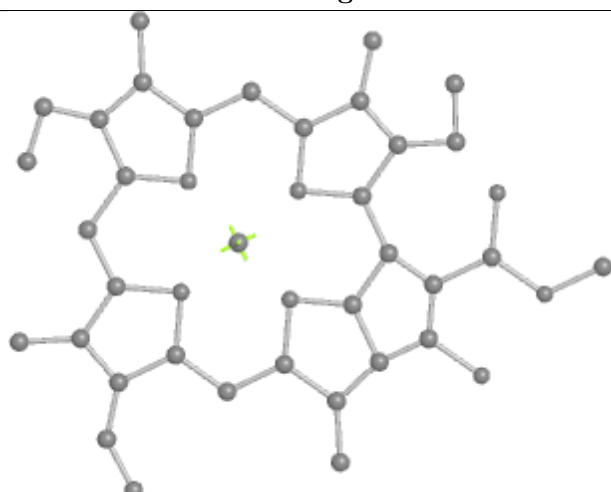
Bond lengths



Bond angles

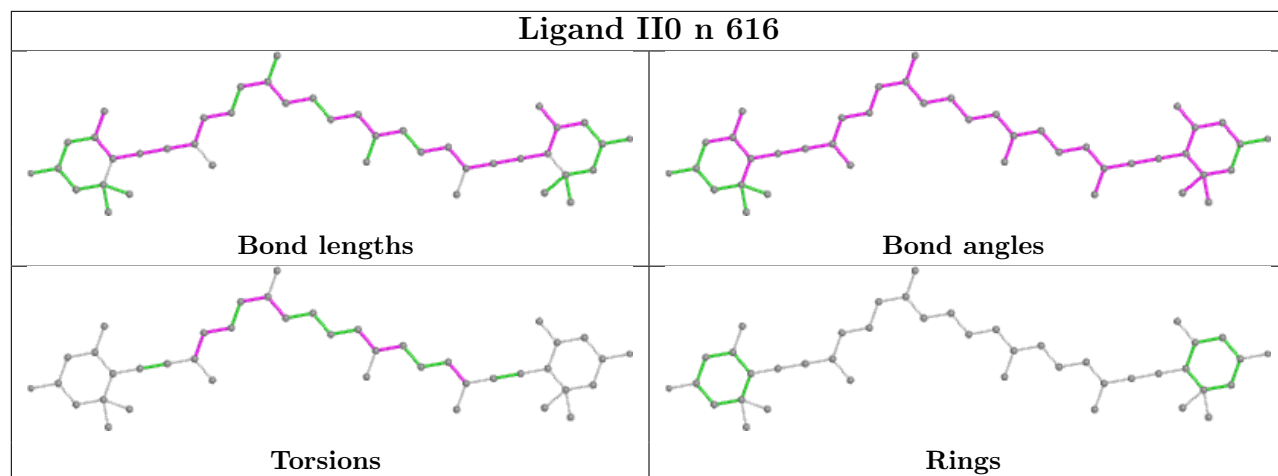


Torsions

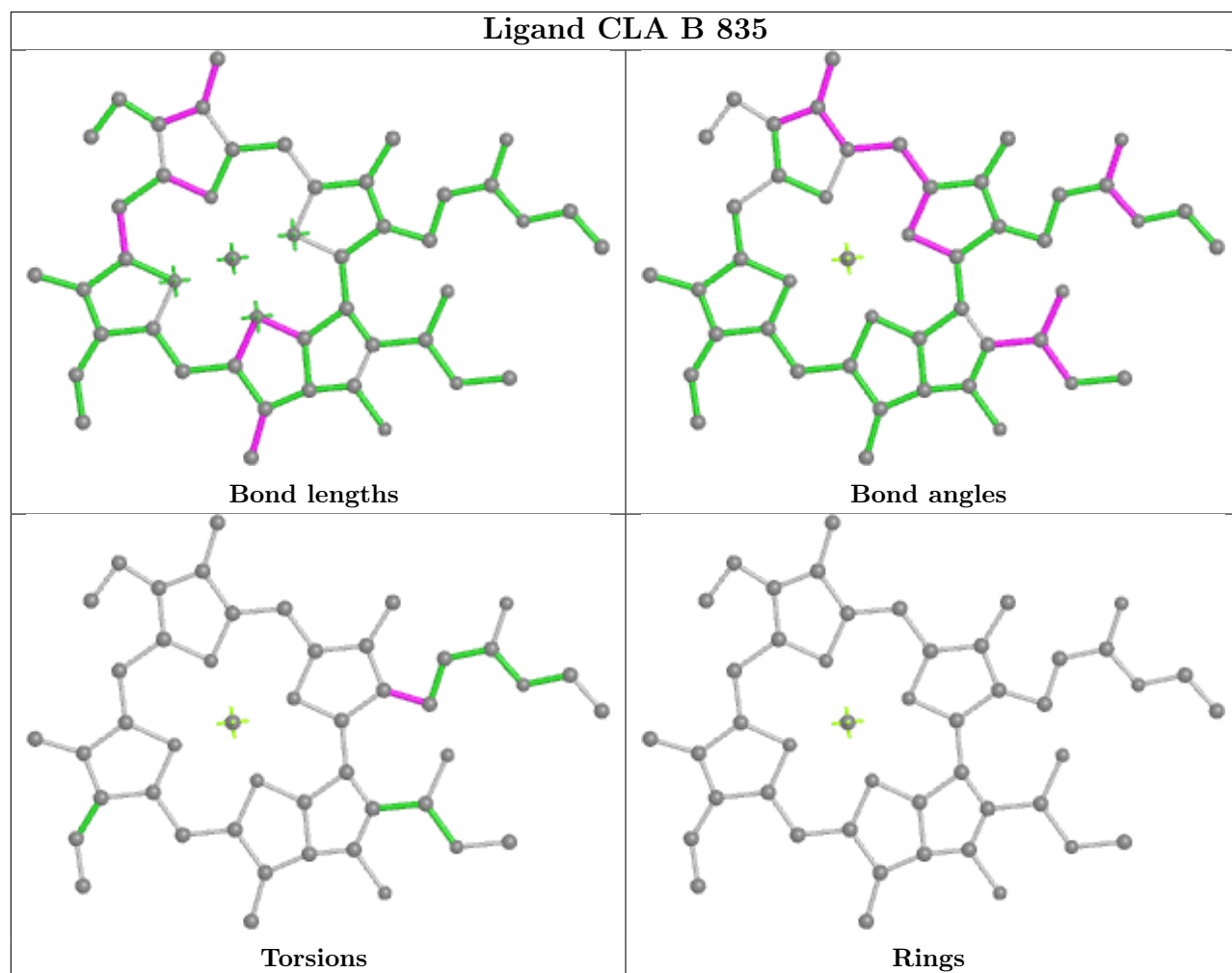


Rings

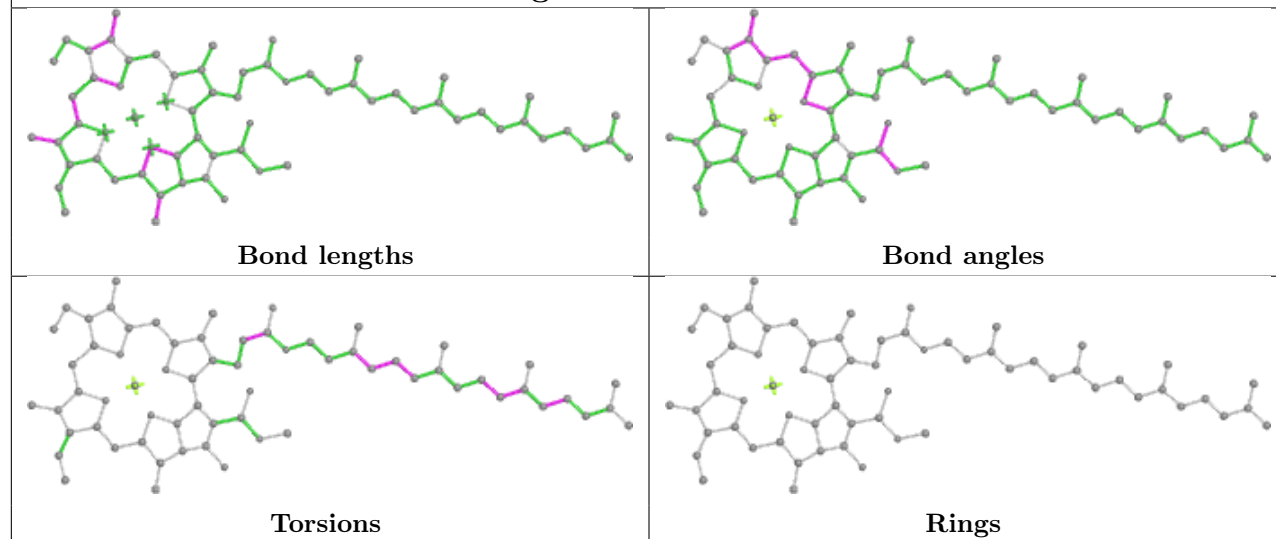
Ligand II0 n 616



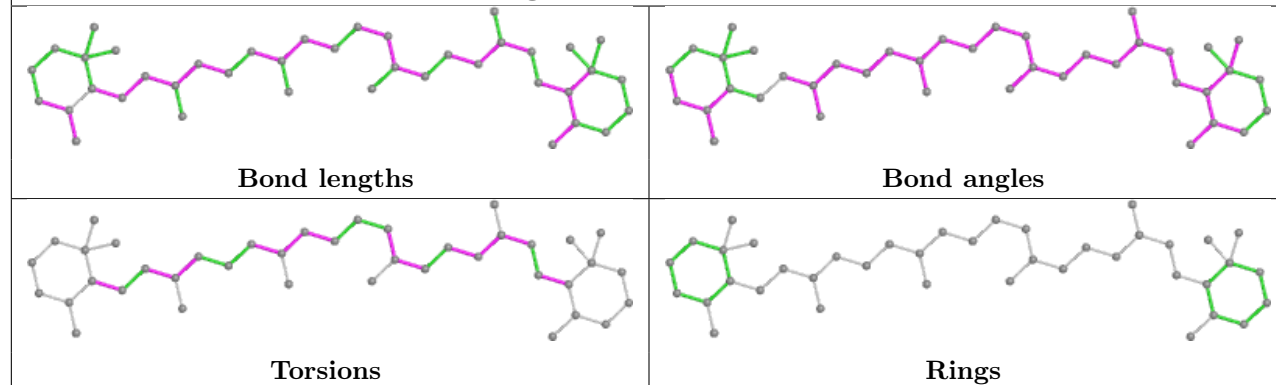
Ligand CLA B 835



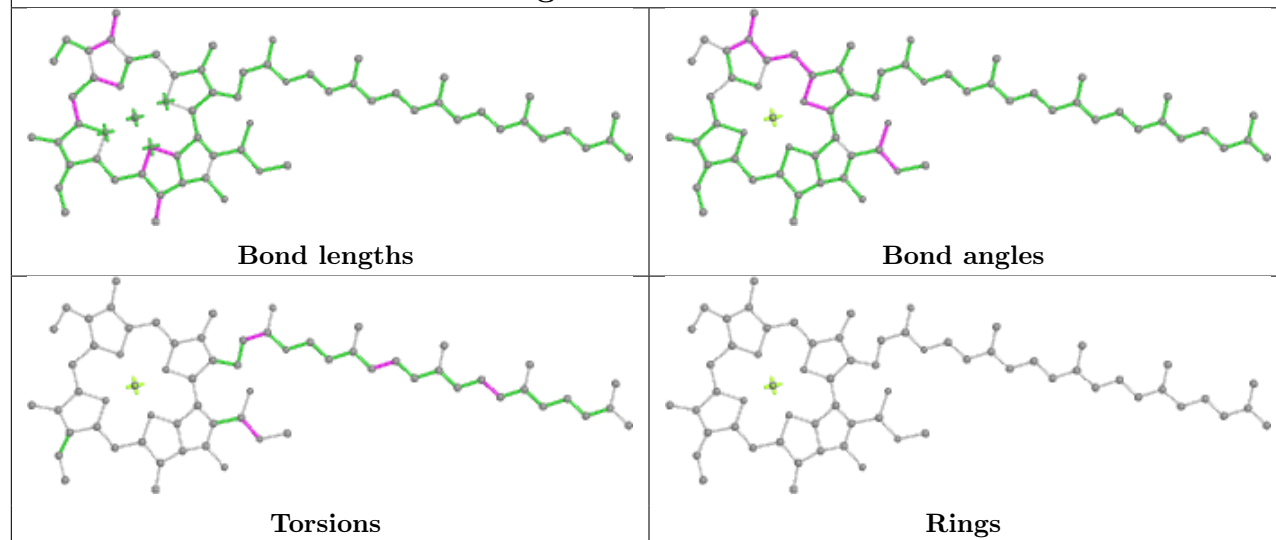
Ligand CLA O 206



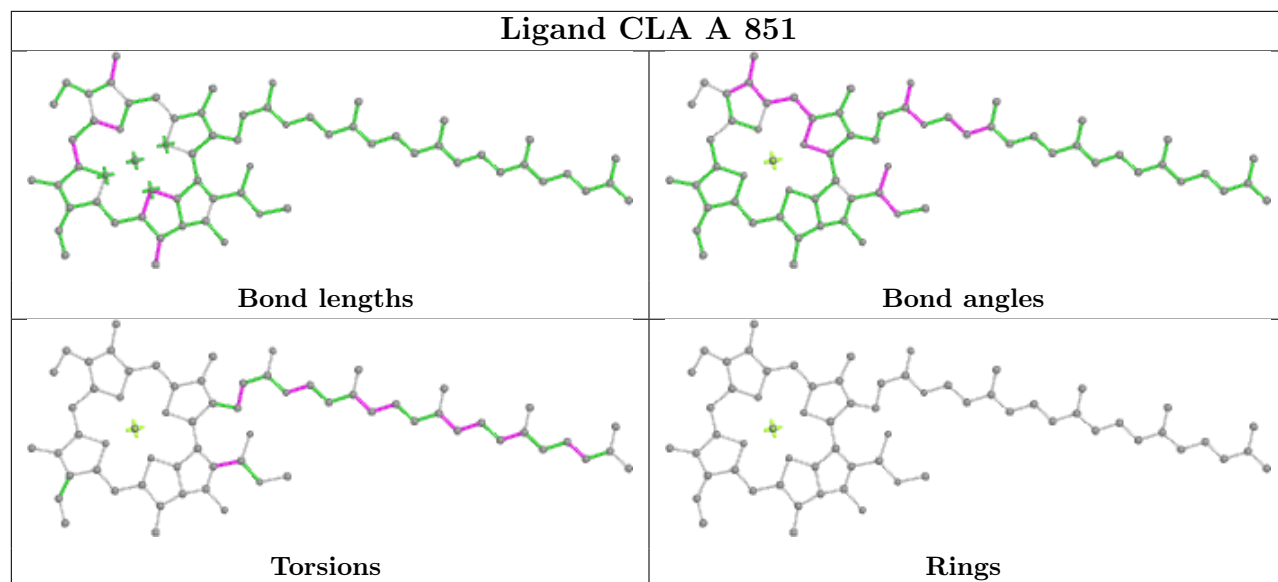
Ligand WVN B 846



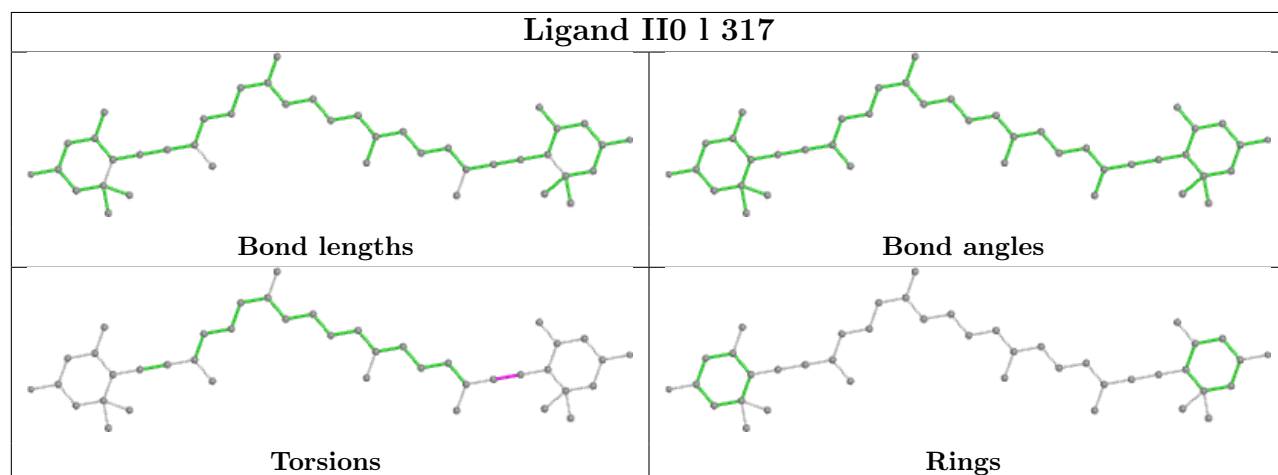
Ligand CLA c 305



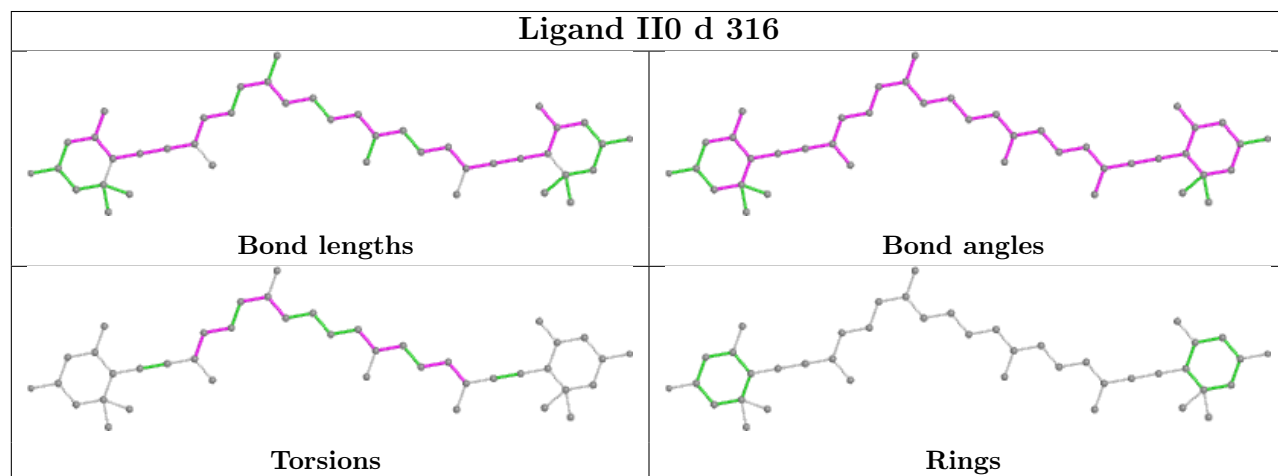
Ligand CLA A 851



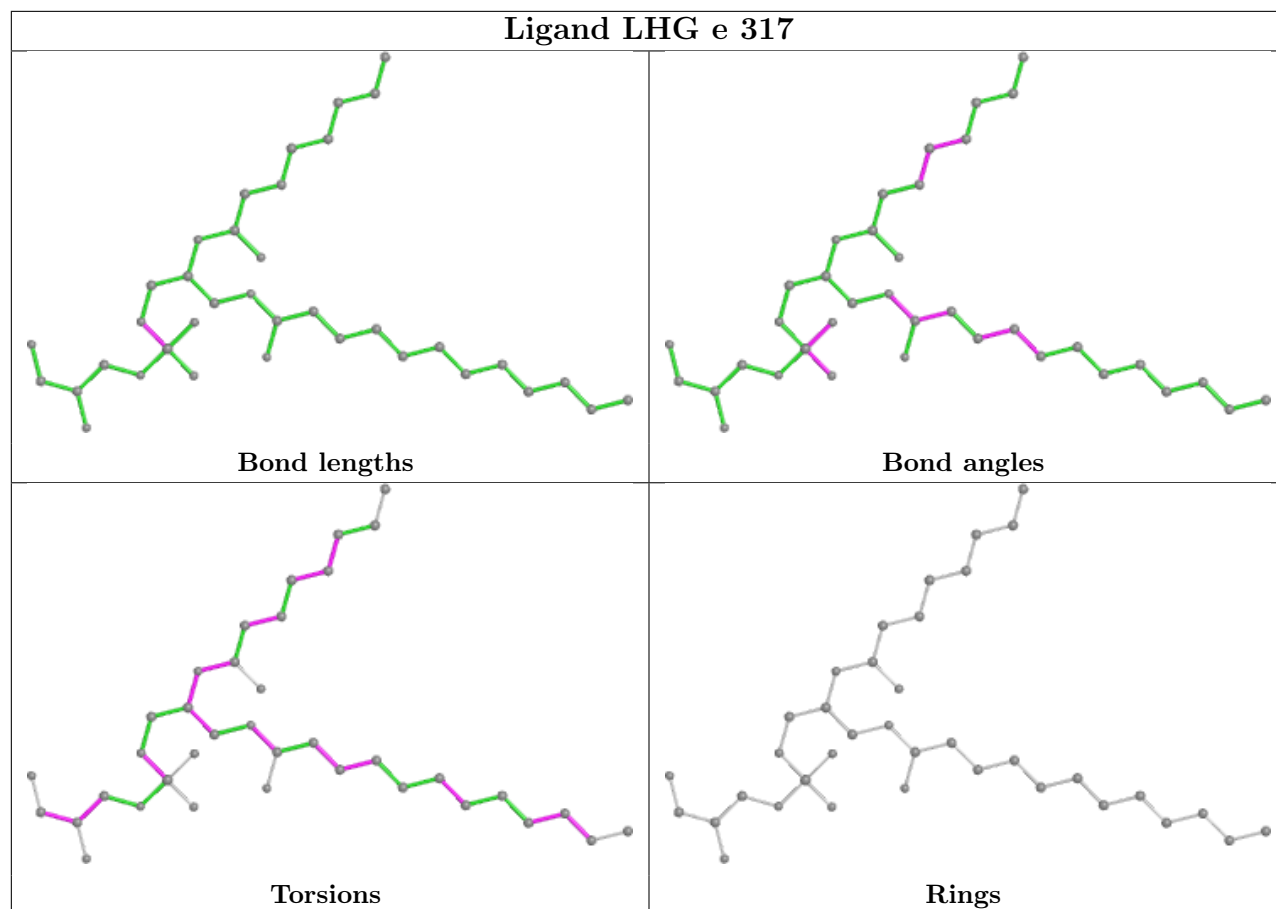
Ligand II0 l 317



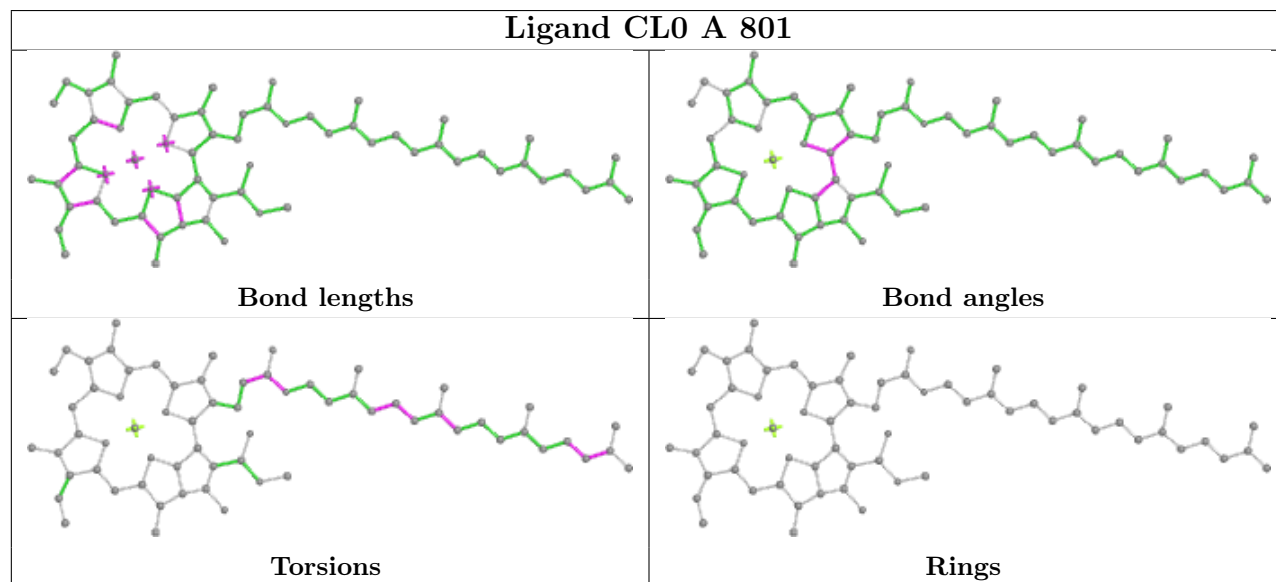
Ligand II0 d 316



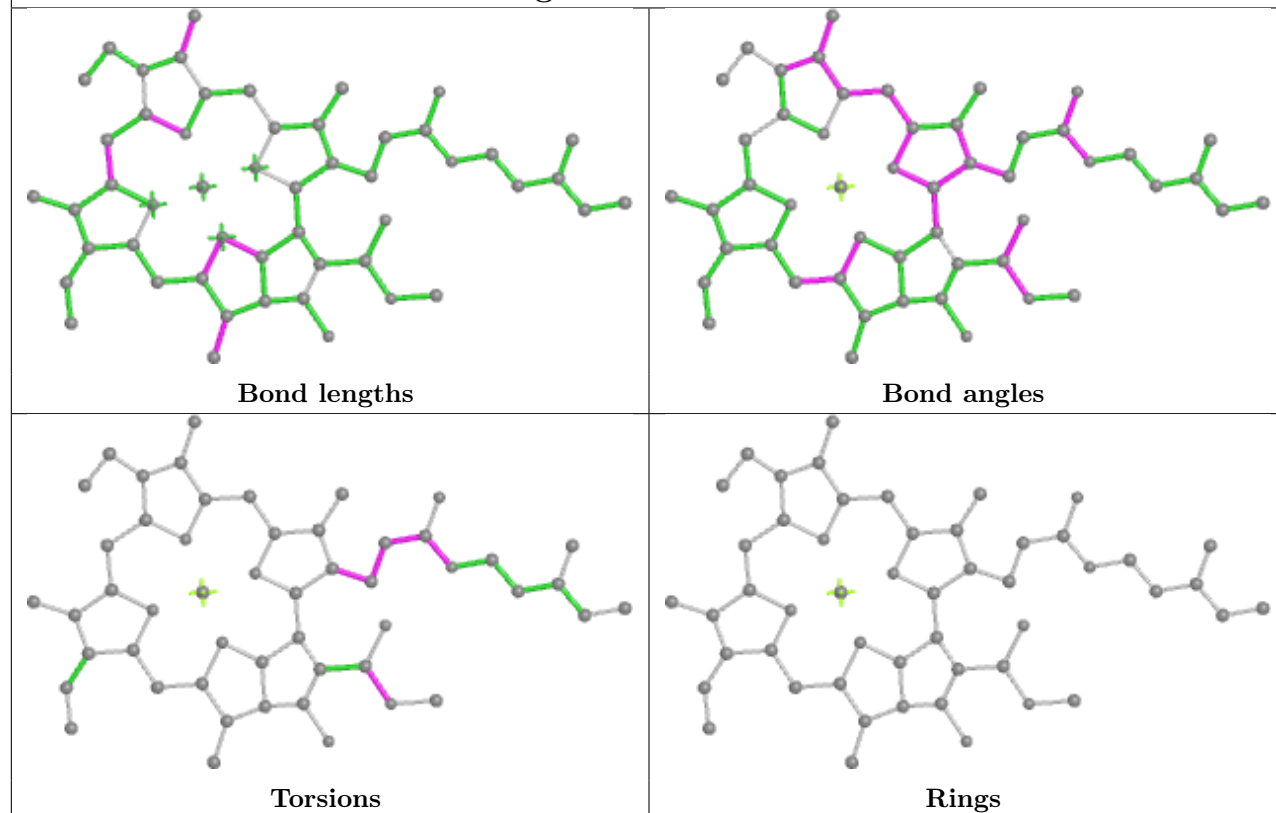
Ligand LHG e 317



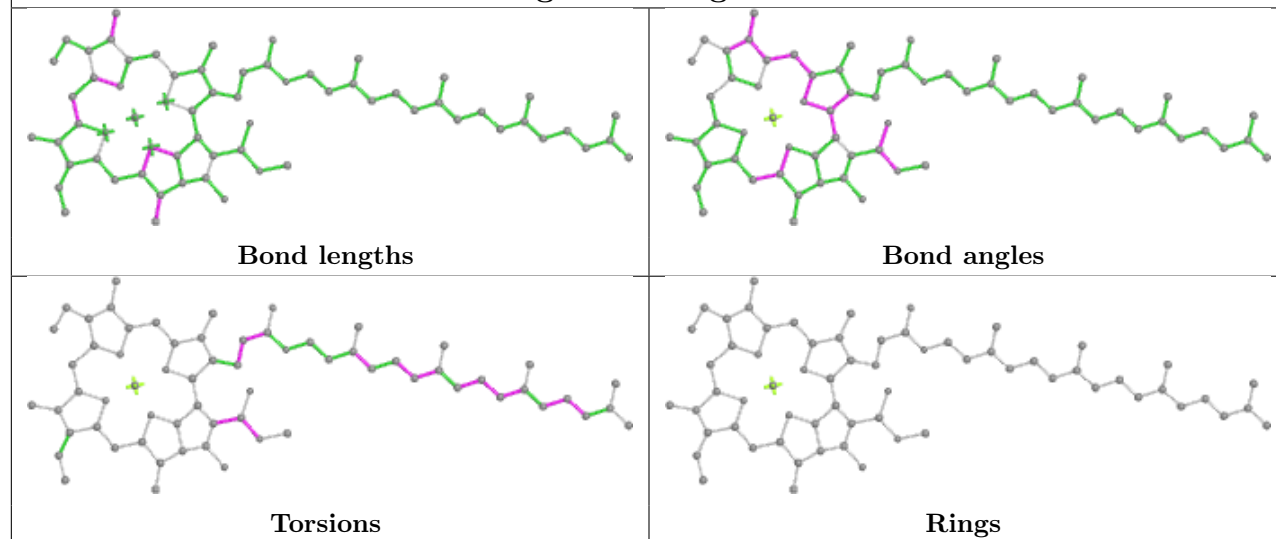
Ligand CL0 A 801



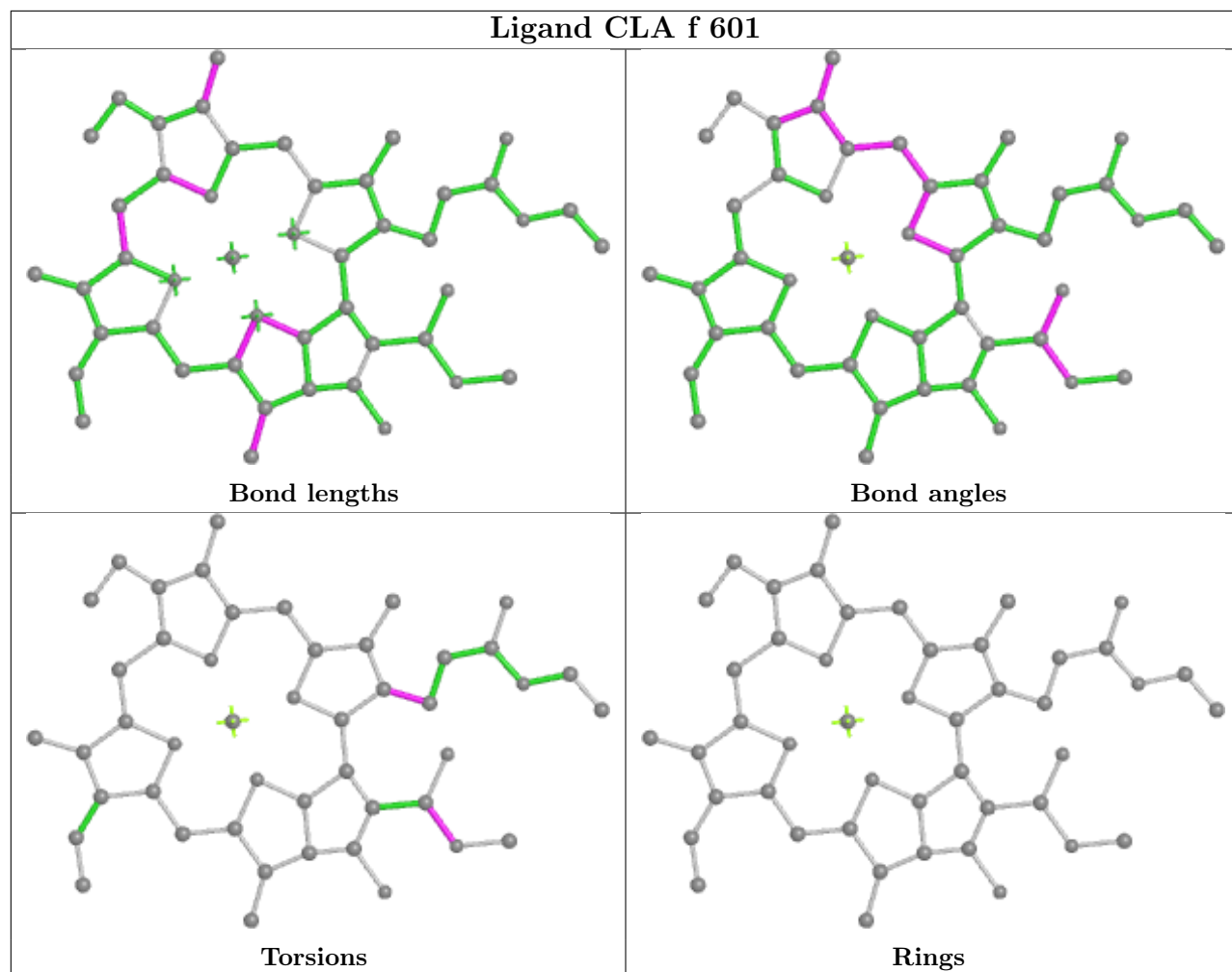
Ligand CLA n 613



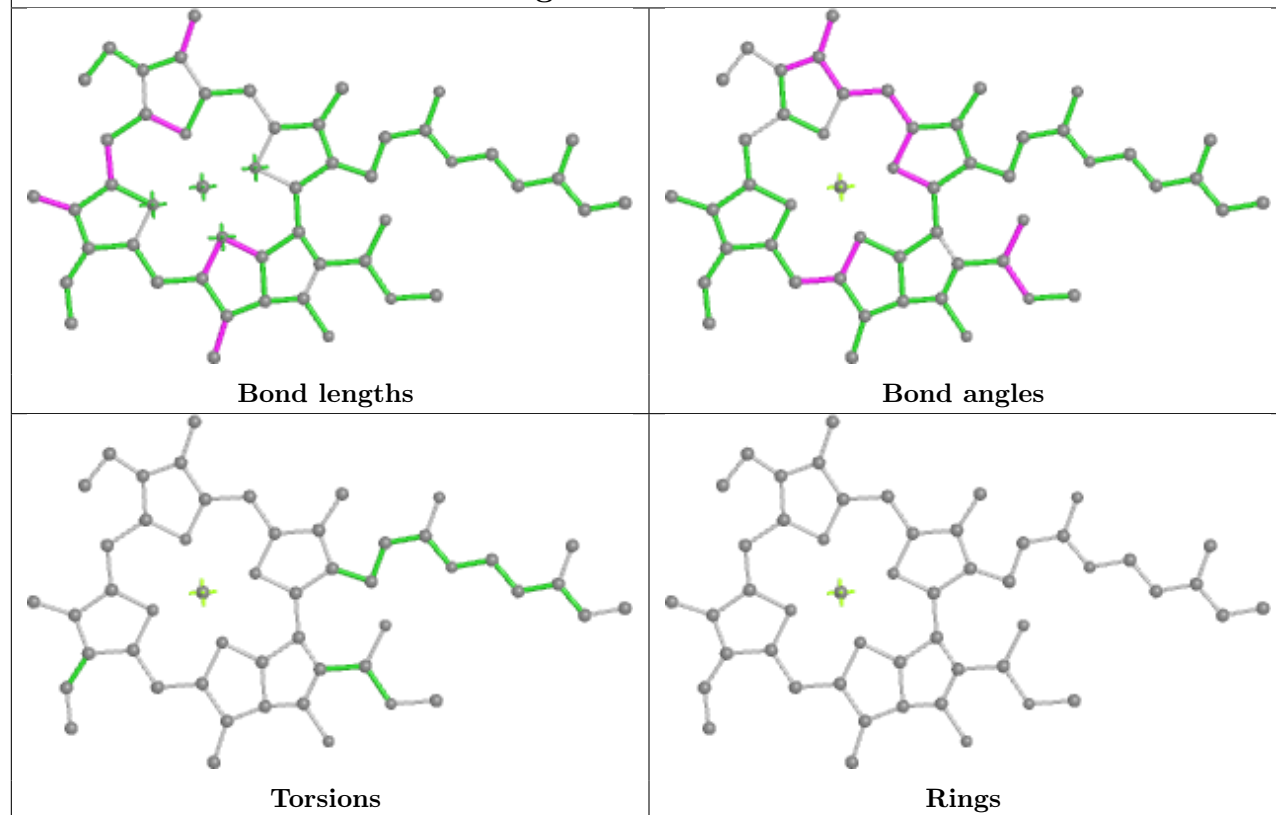
Ligand CLA g 302



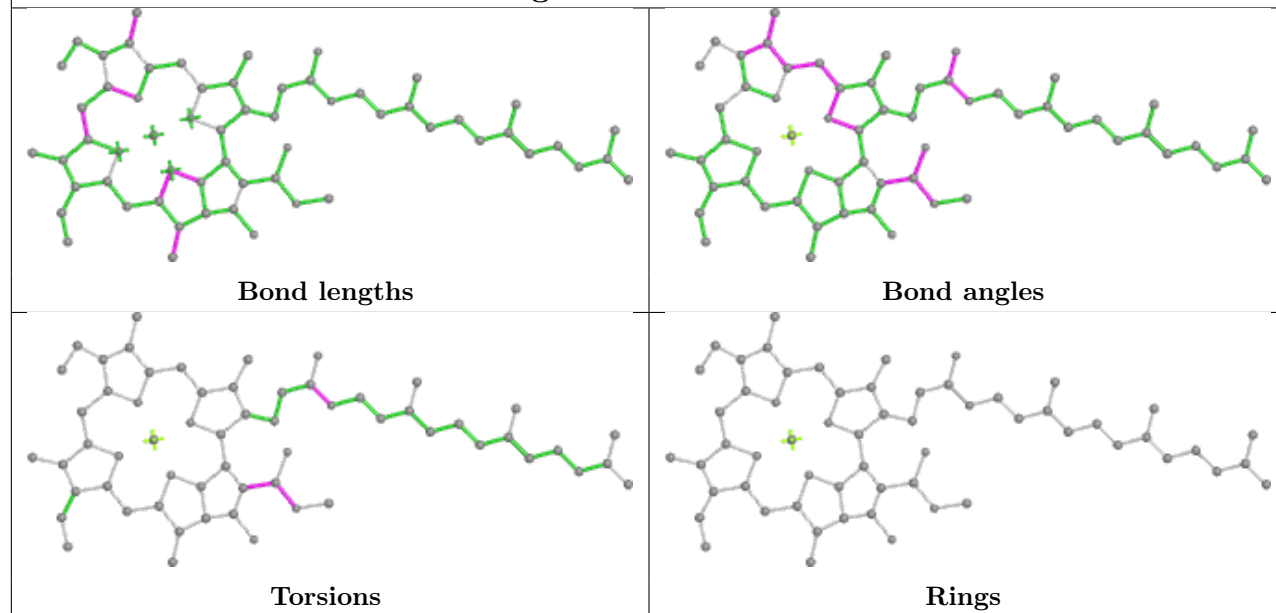
Ligand CLA f 601

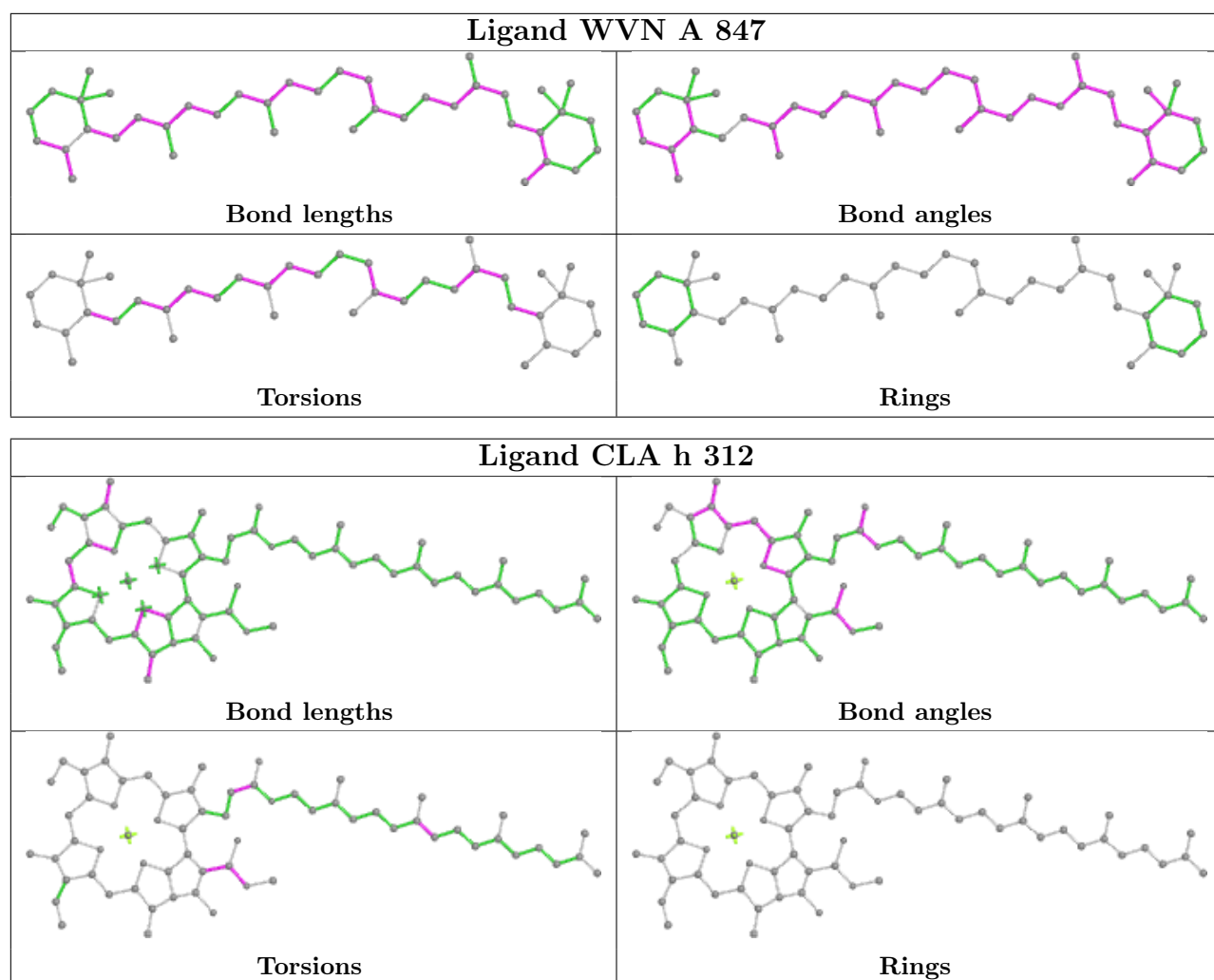


Ligand CLA k 603

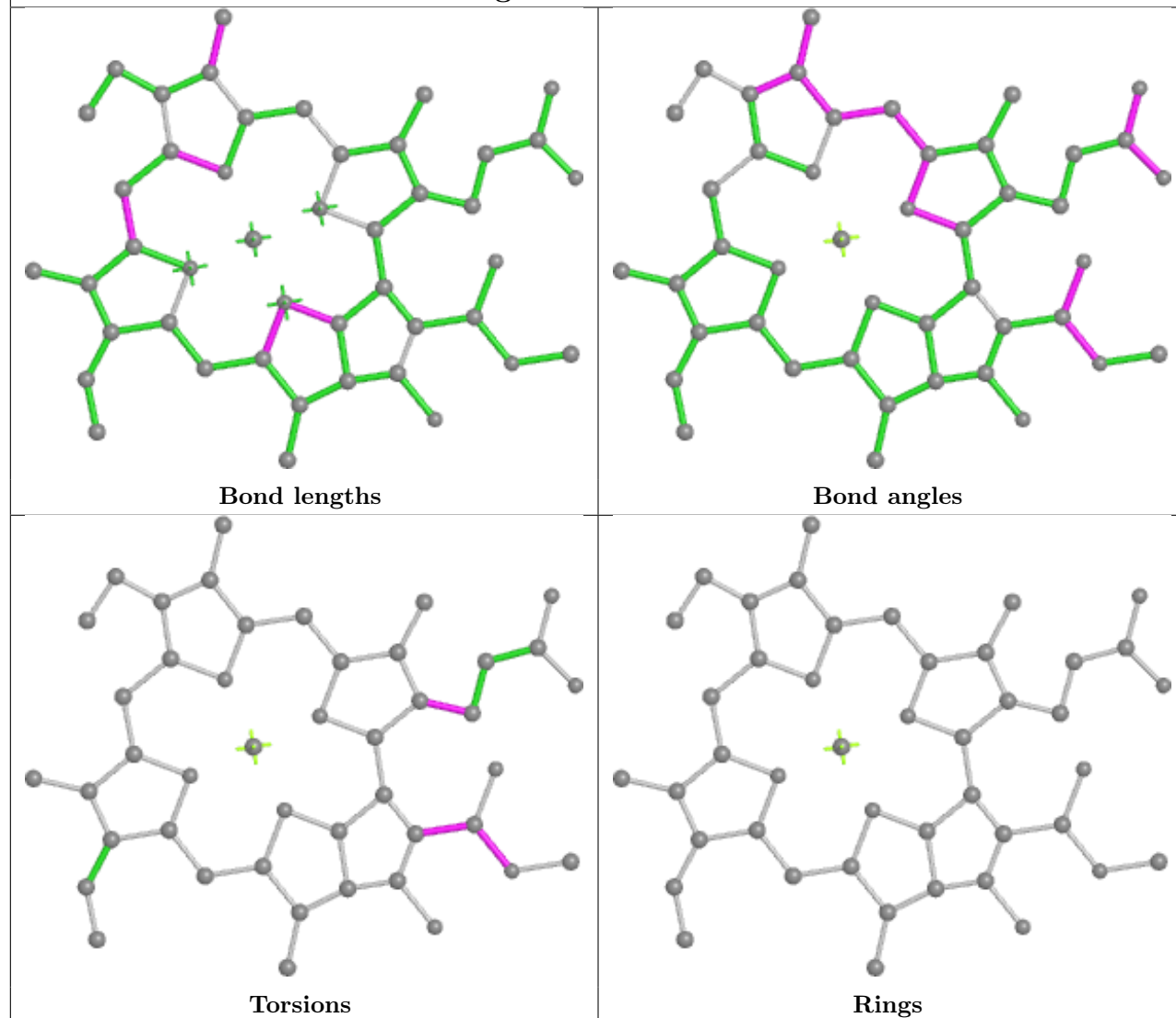


Ligand CLA A 806

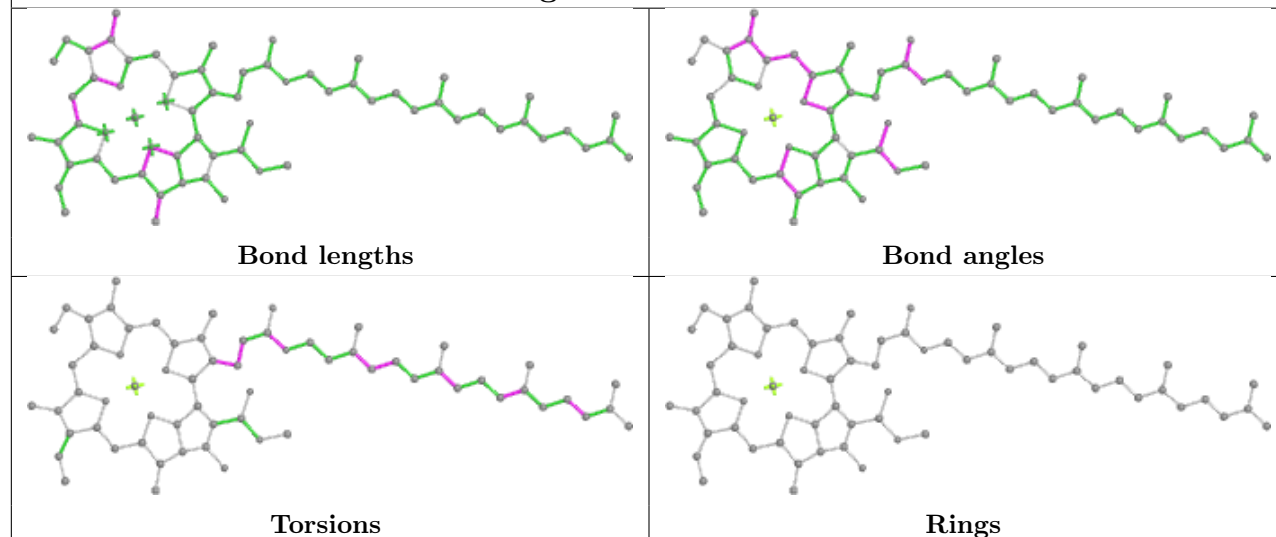




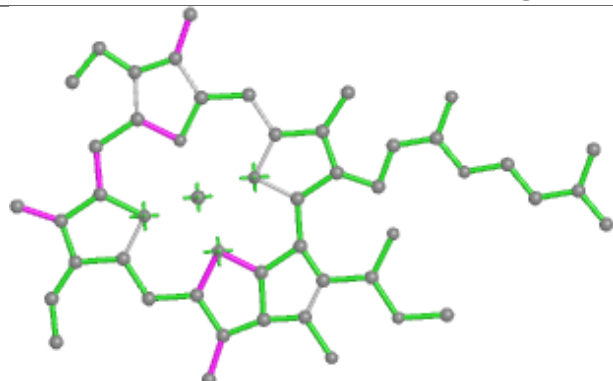
Ligand CLA c 309



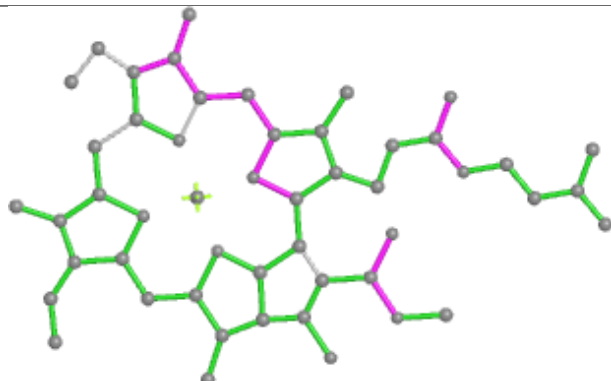
Ligand CLA f 607



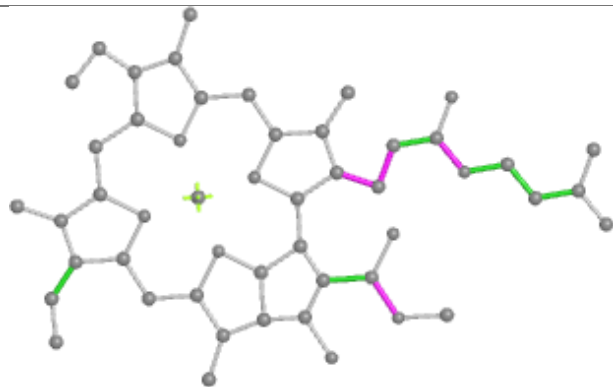
Ligand CLA h 302



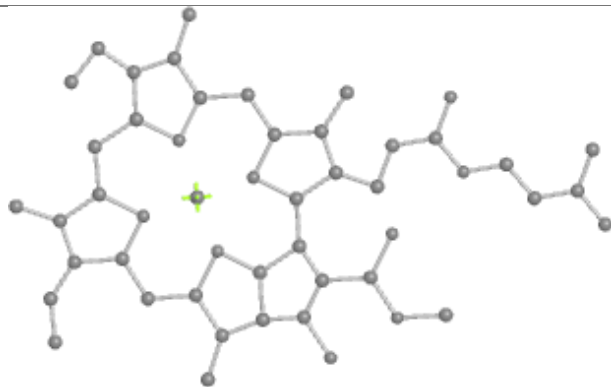
Bond lengths



Bond angles

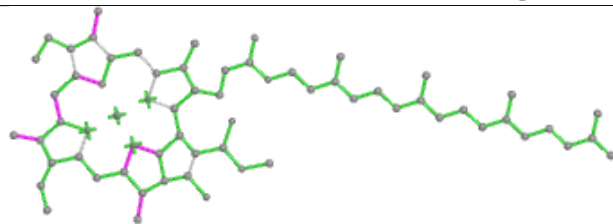


Torsions

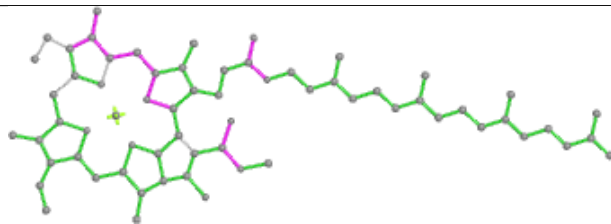


Rings

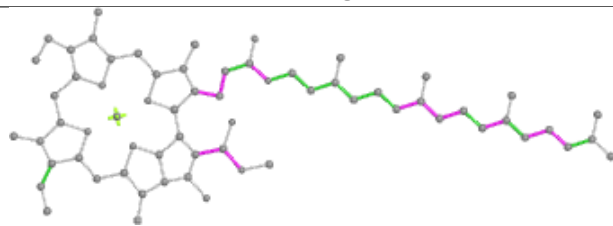
Ligand CLA A 810



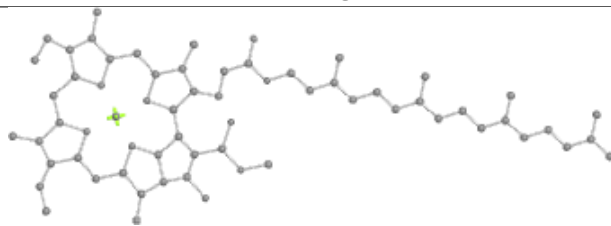
Bond lengths



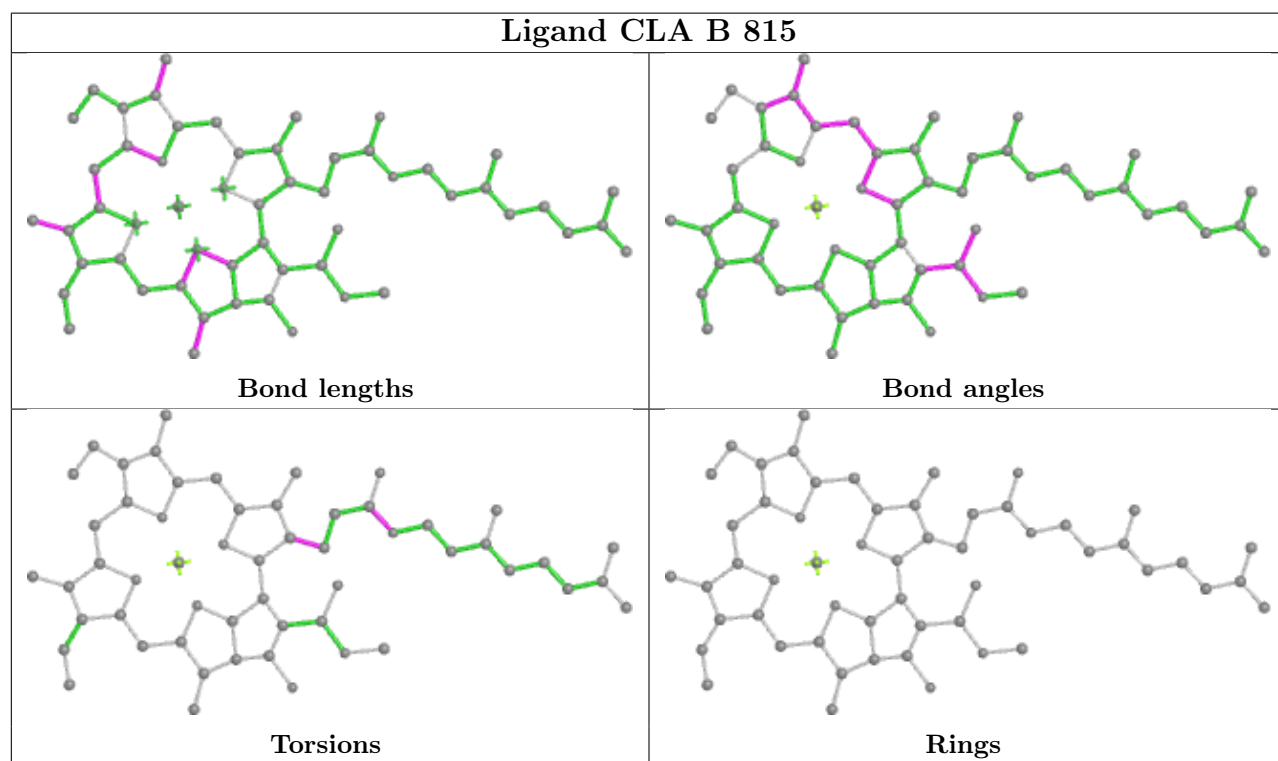
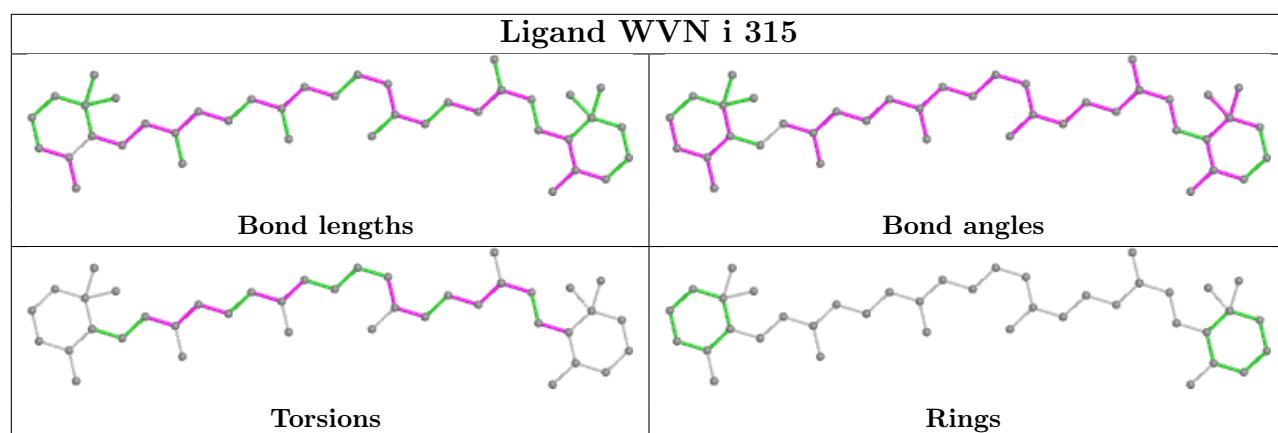
Bond angles

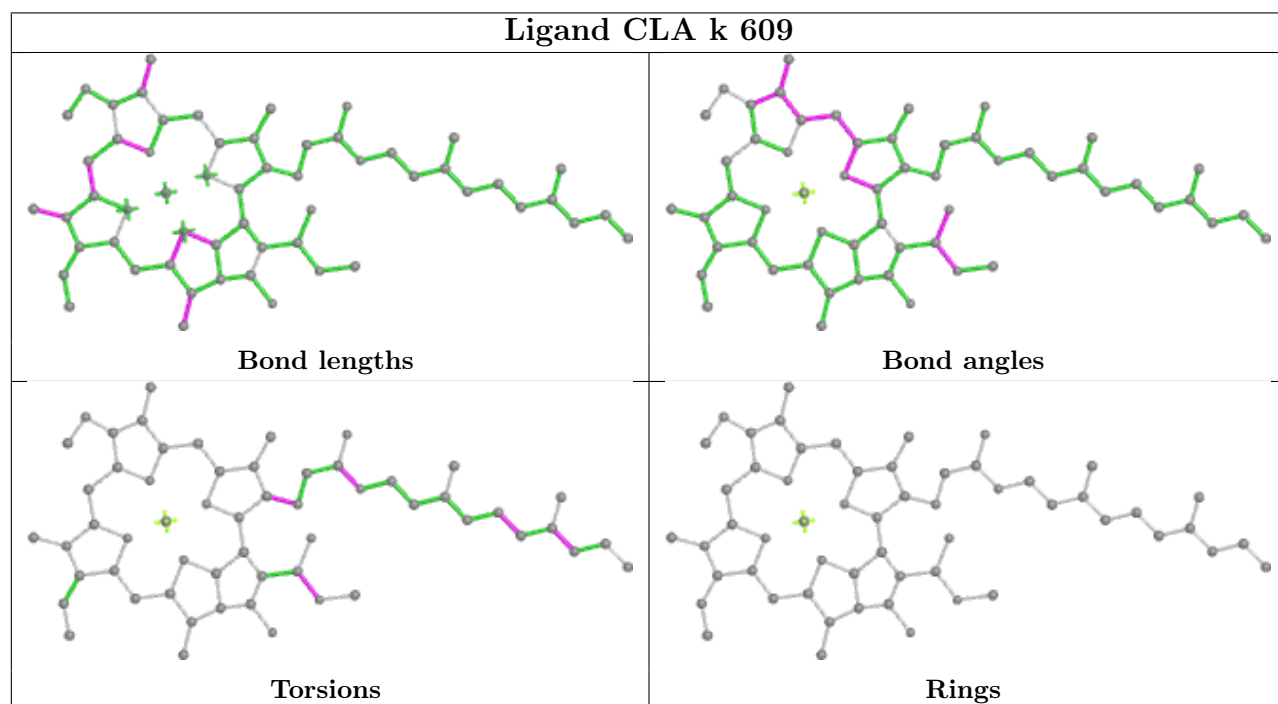
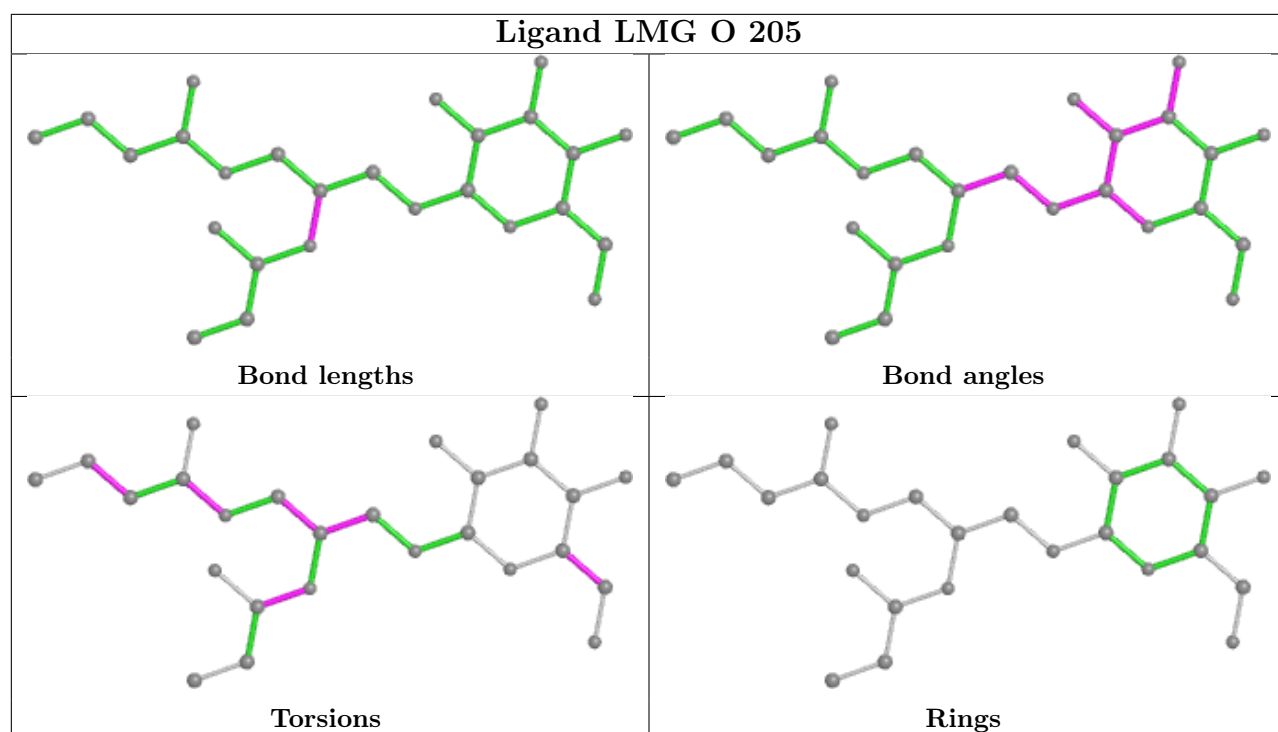


Torsions

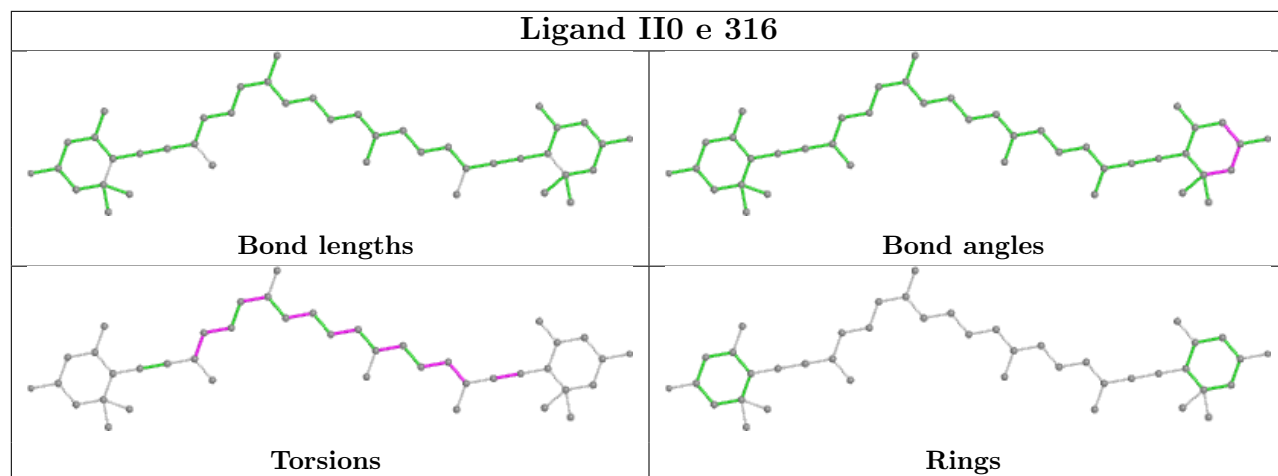


Rings

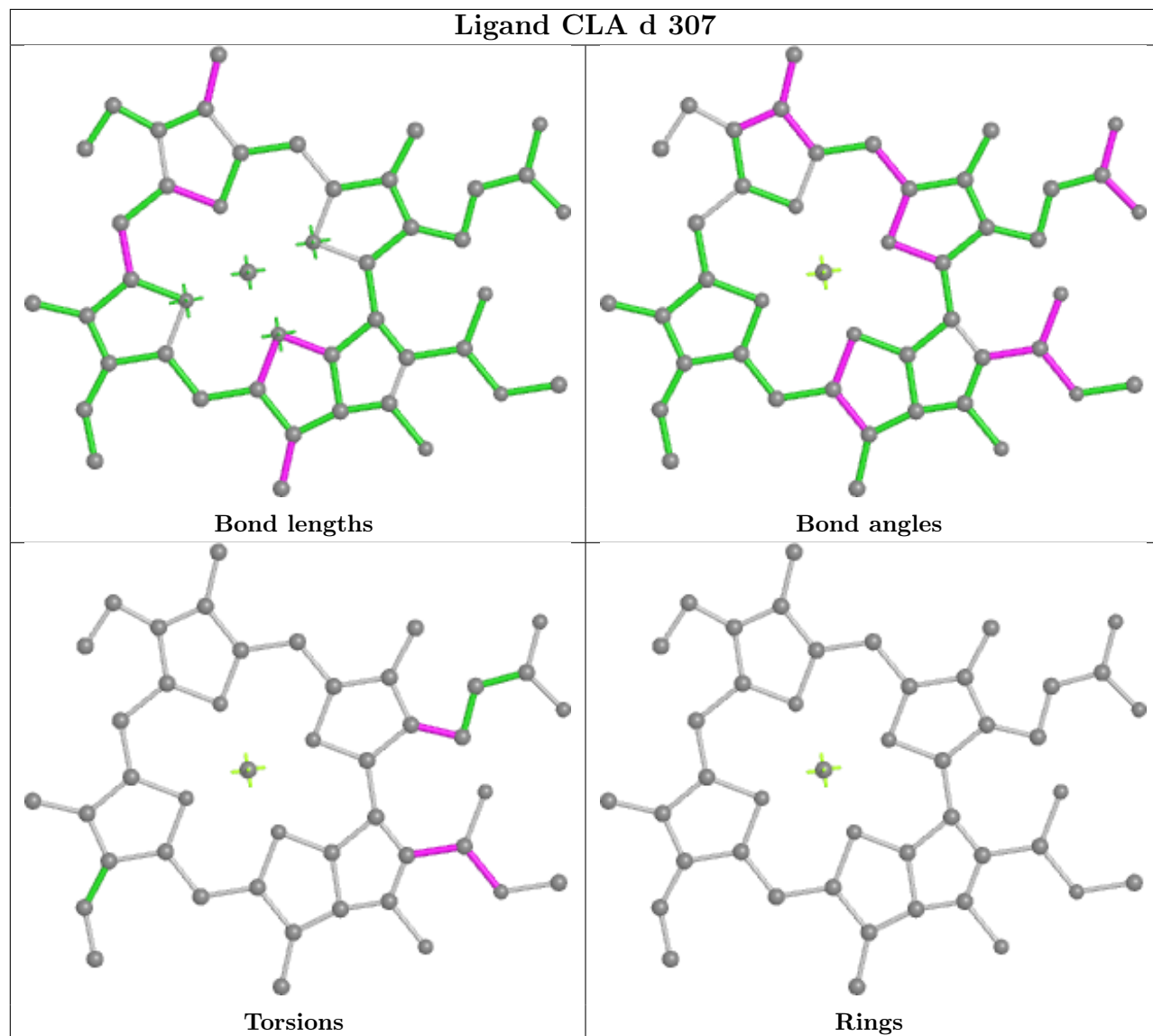


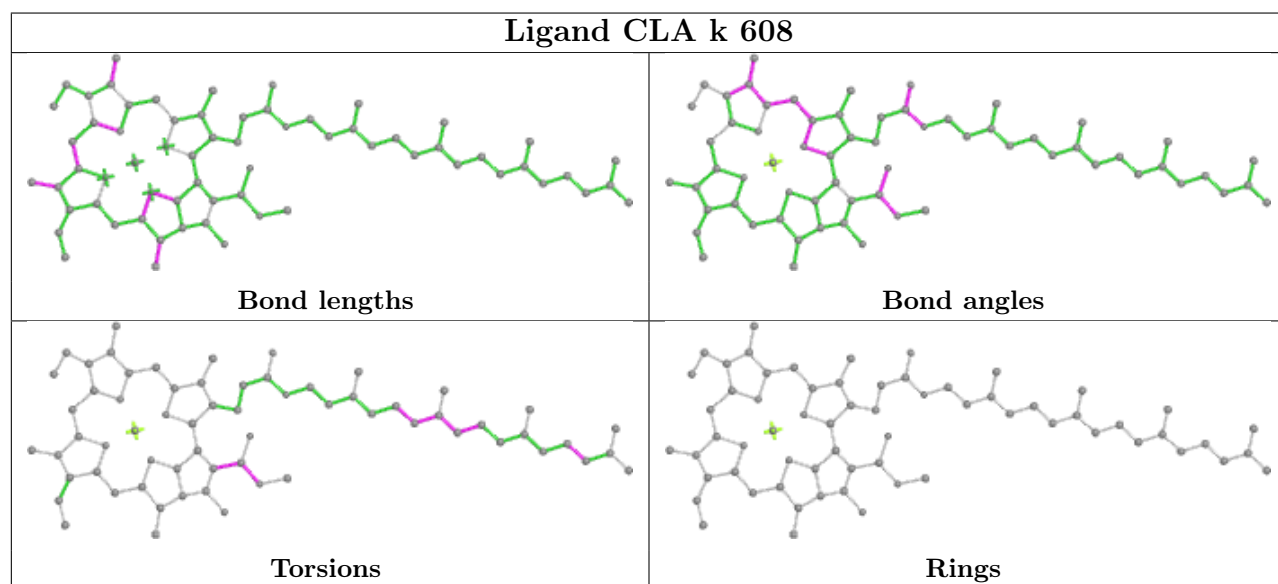
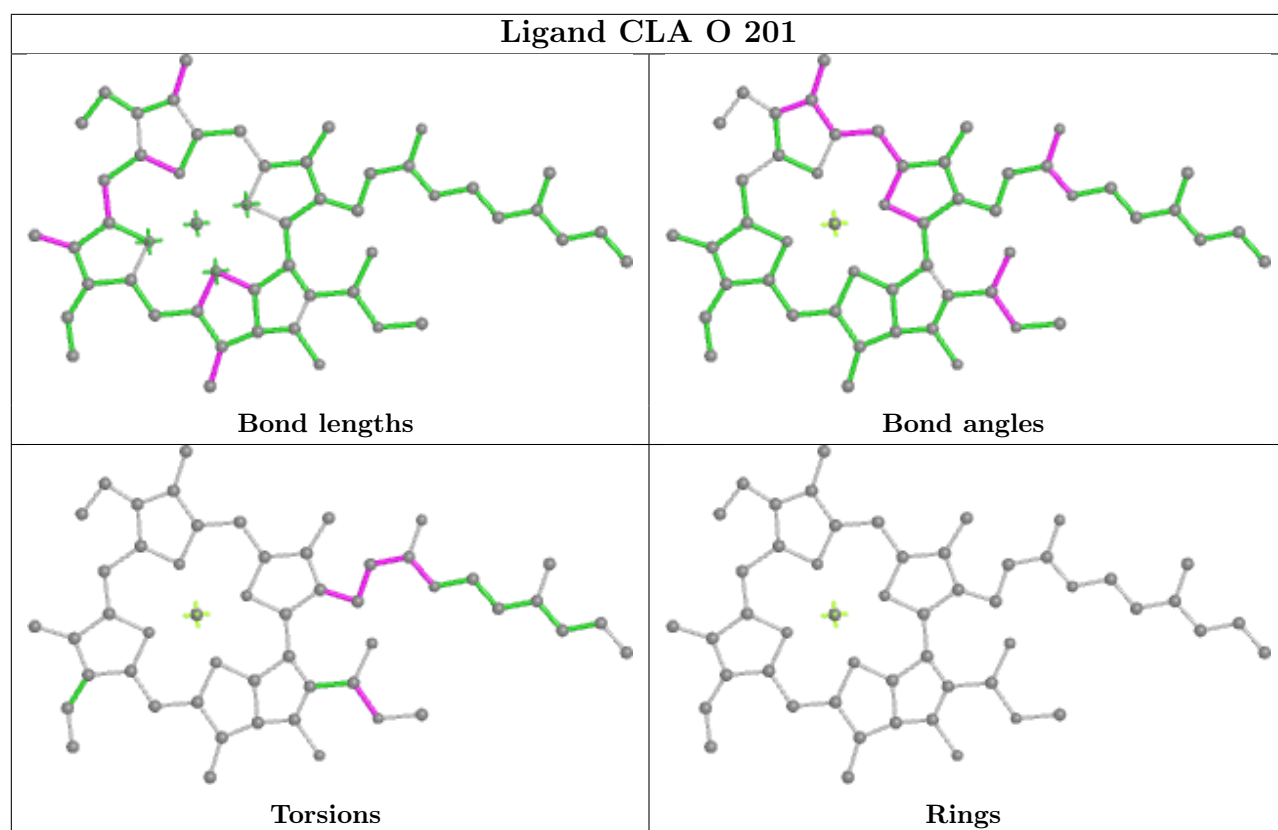


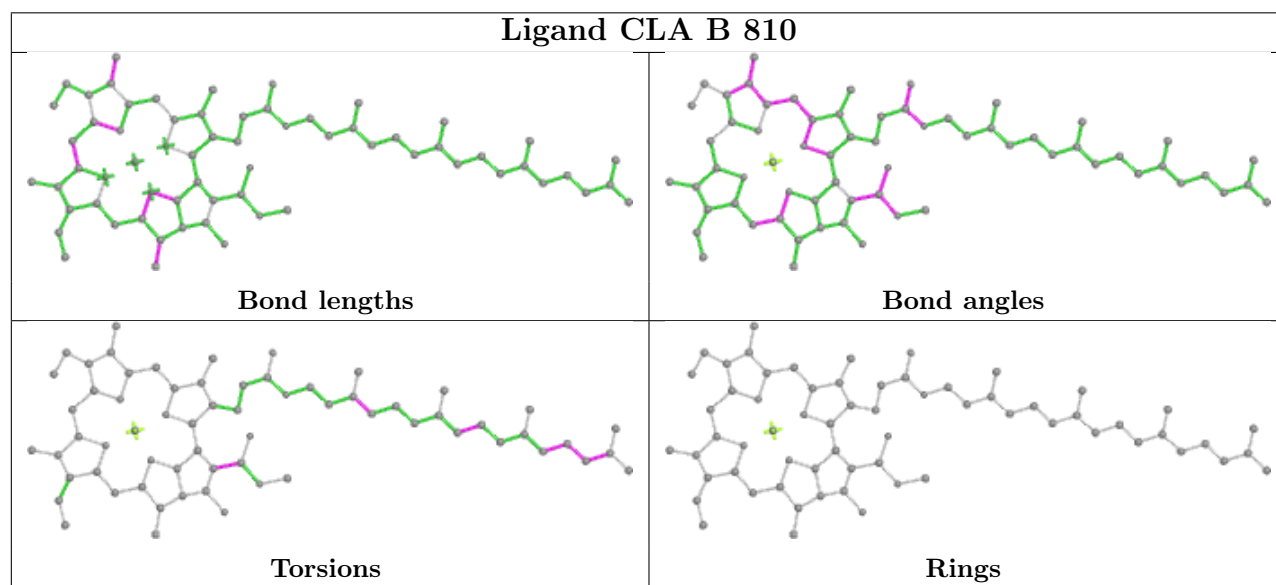
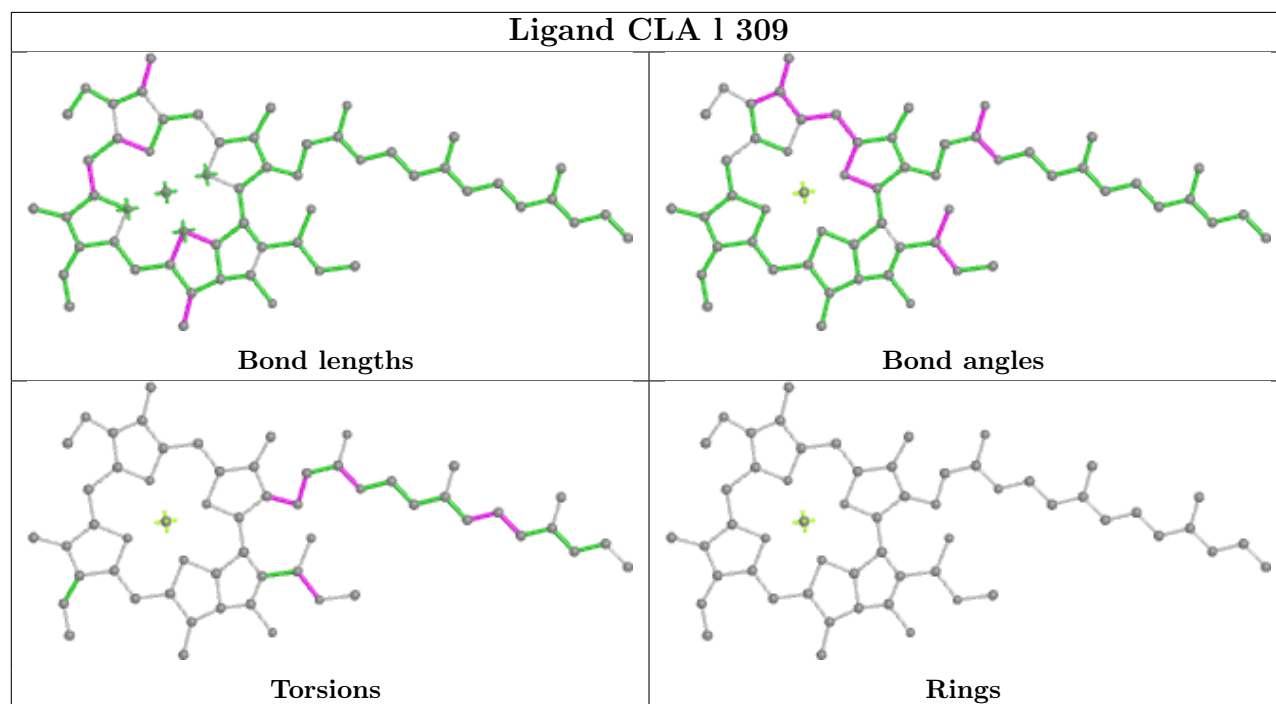
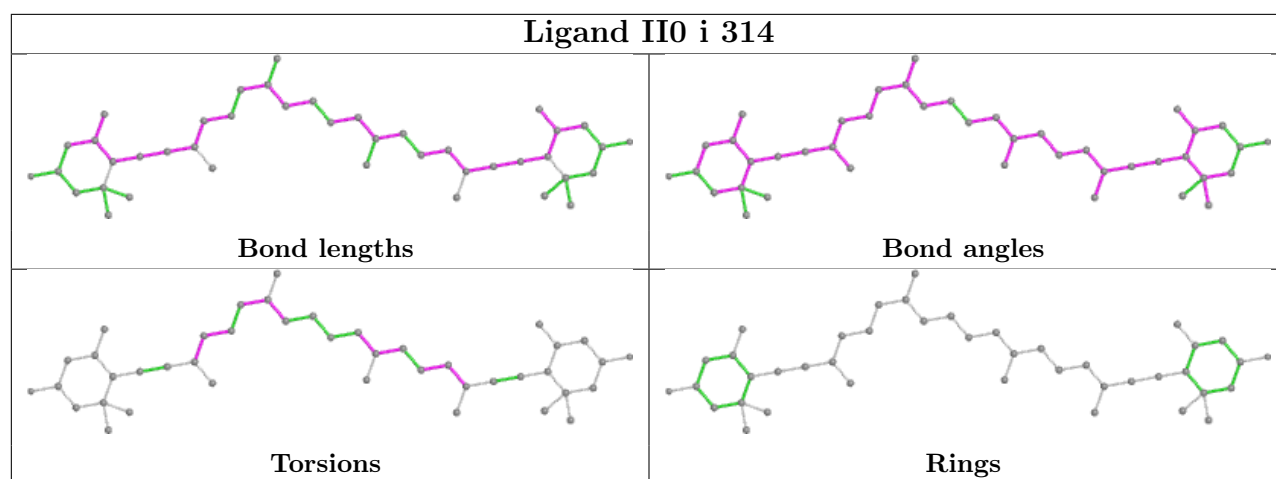
Ligand II0 e 316

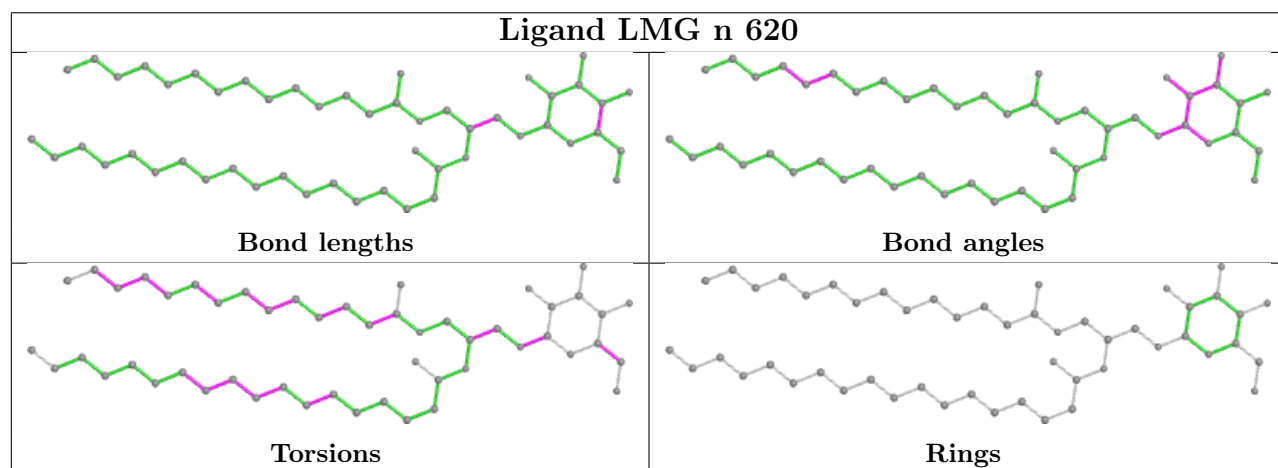
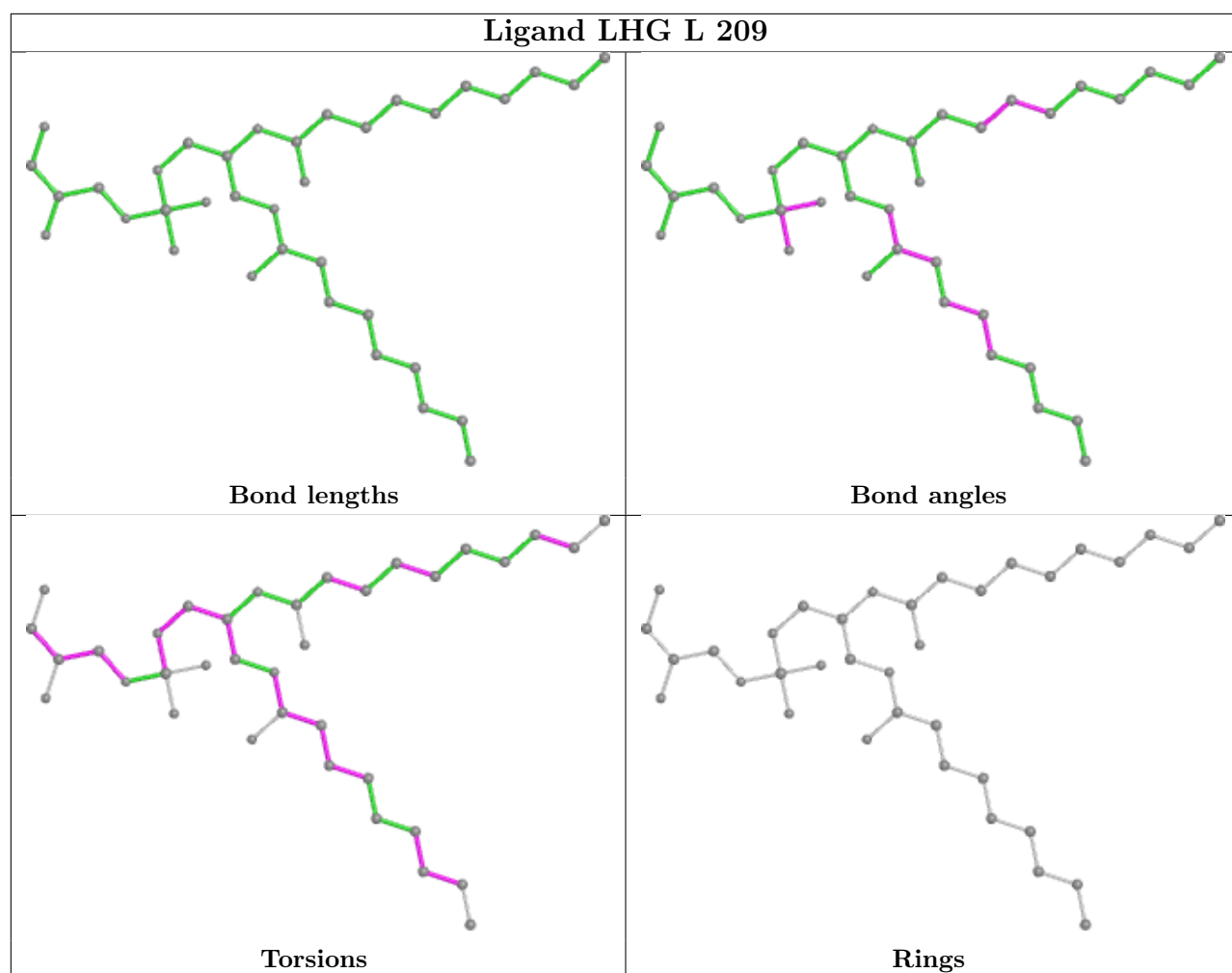


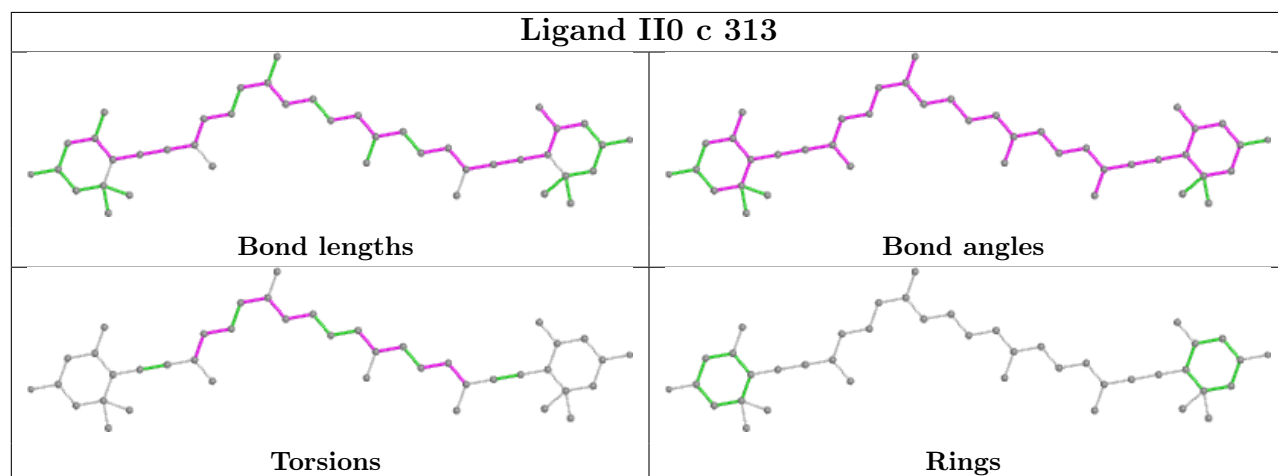
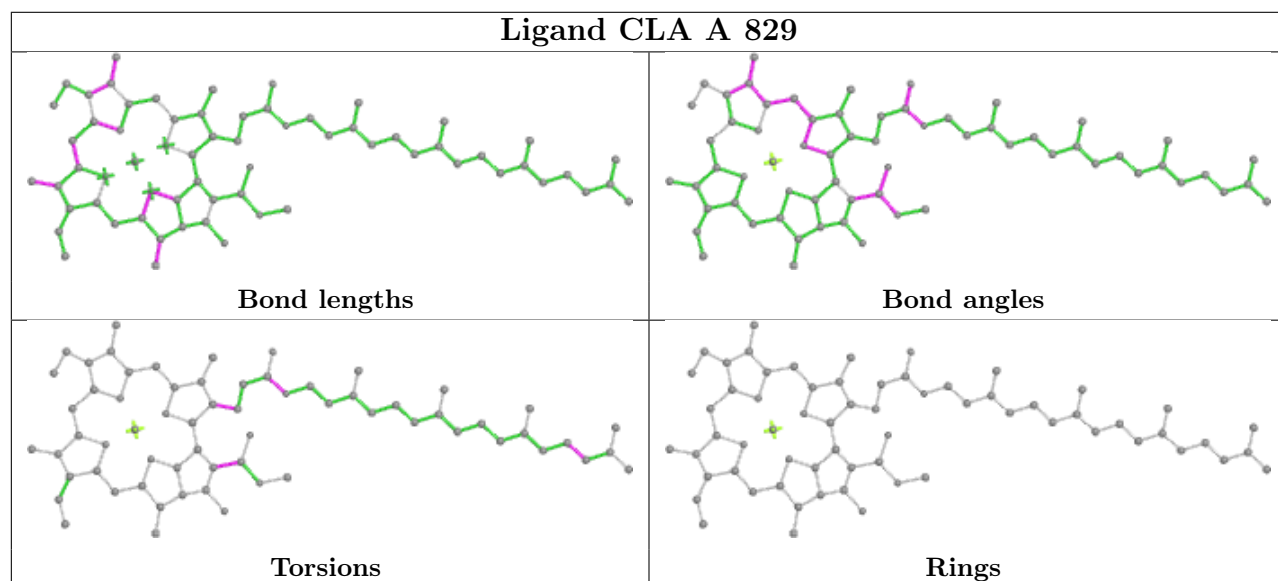
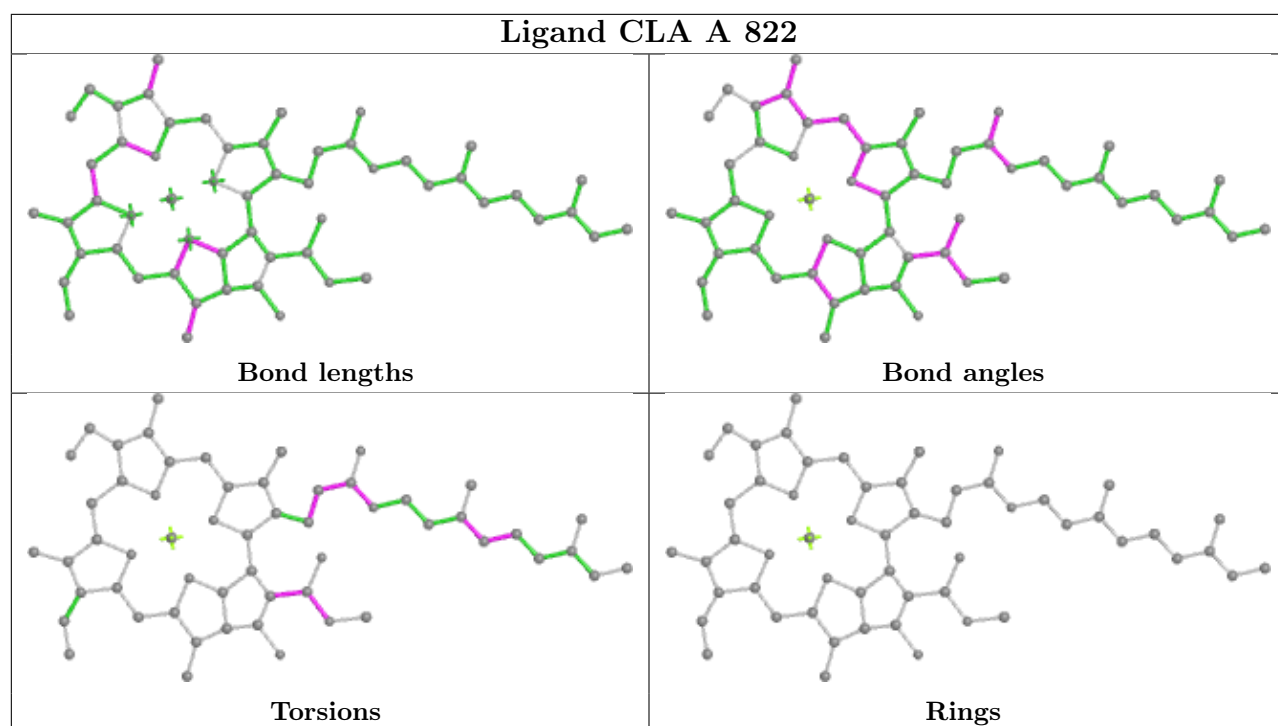
Ligand CLA d 307

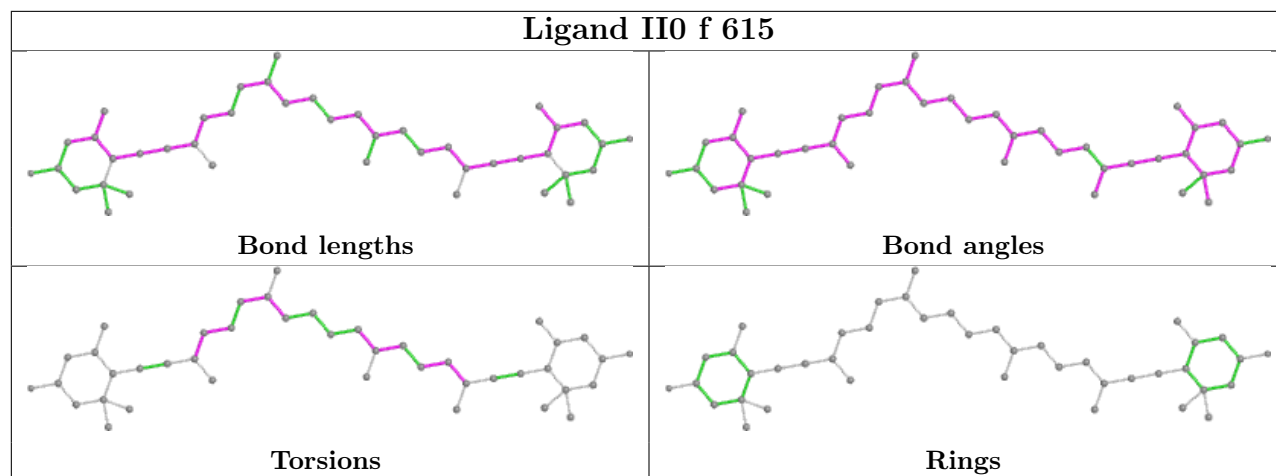
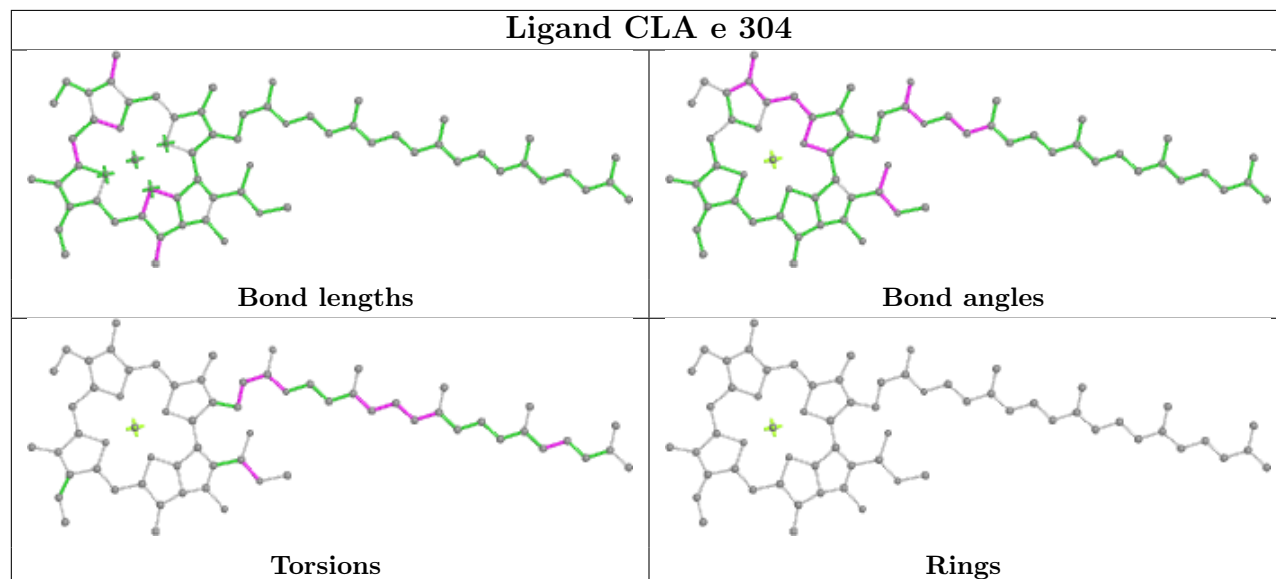
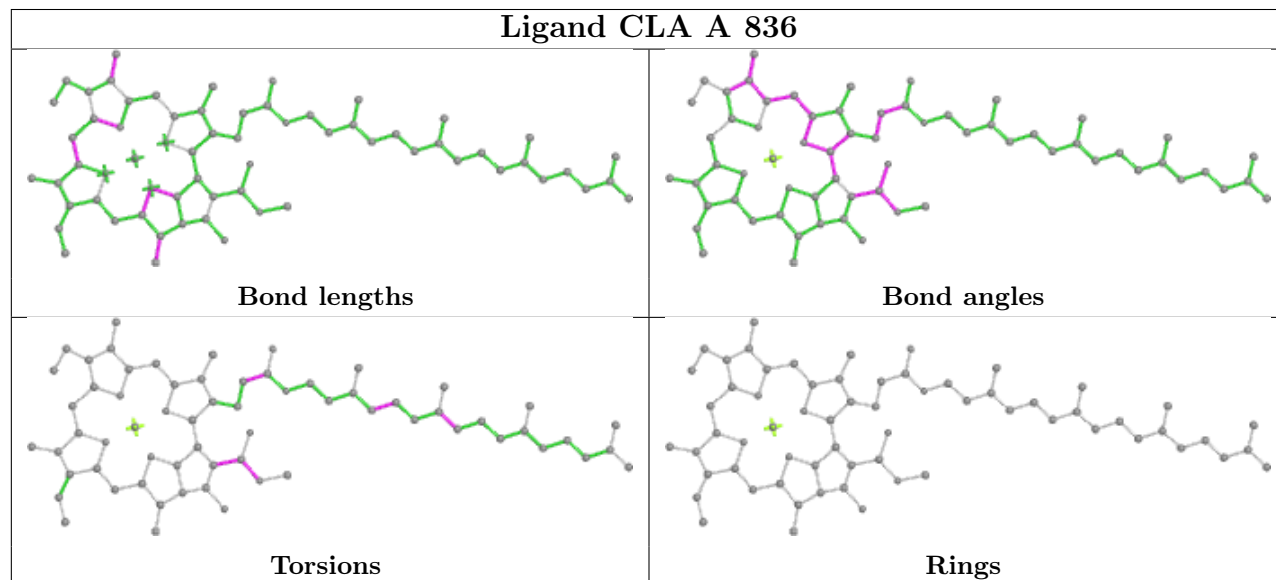




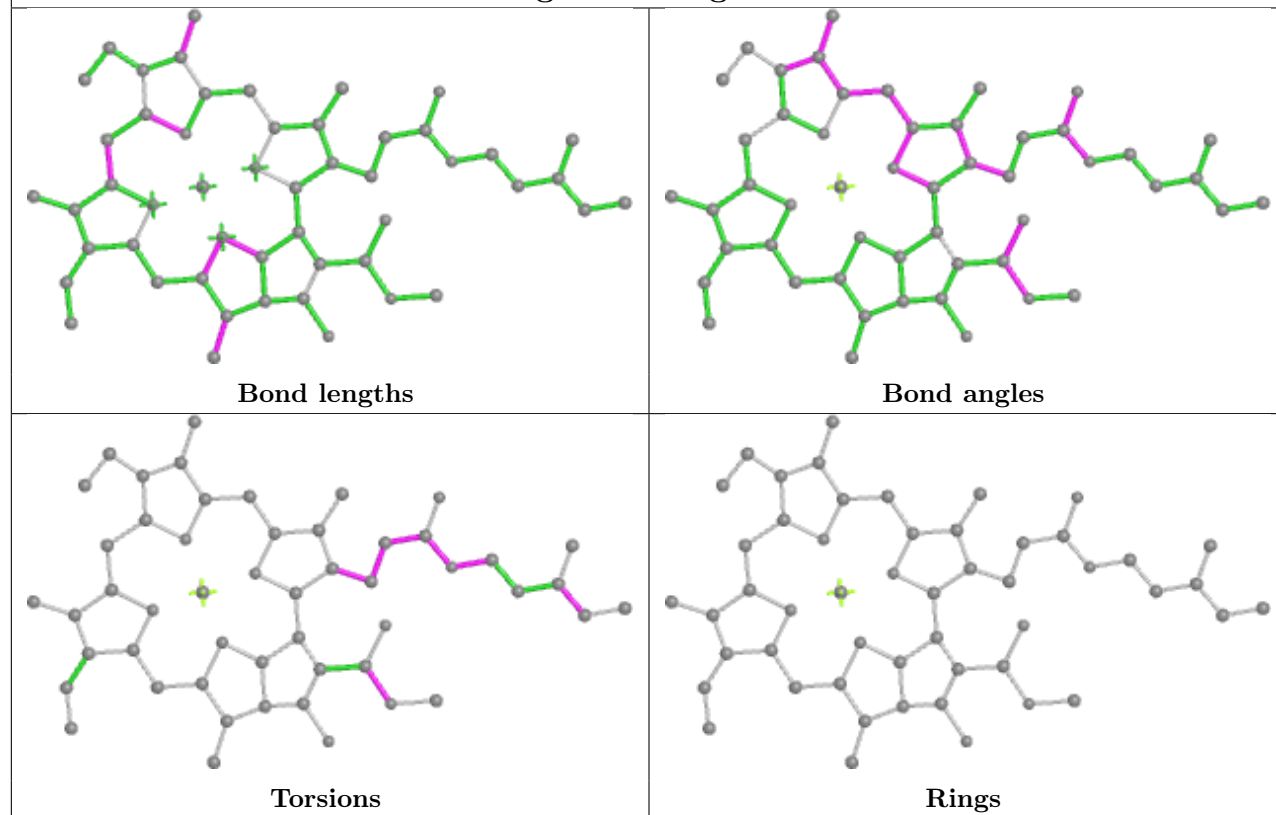




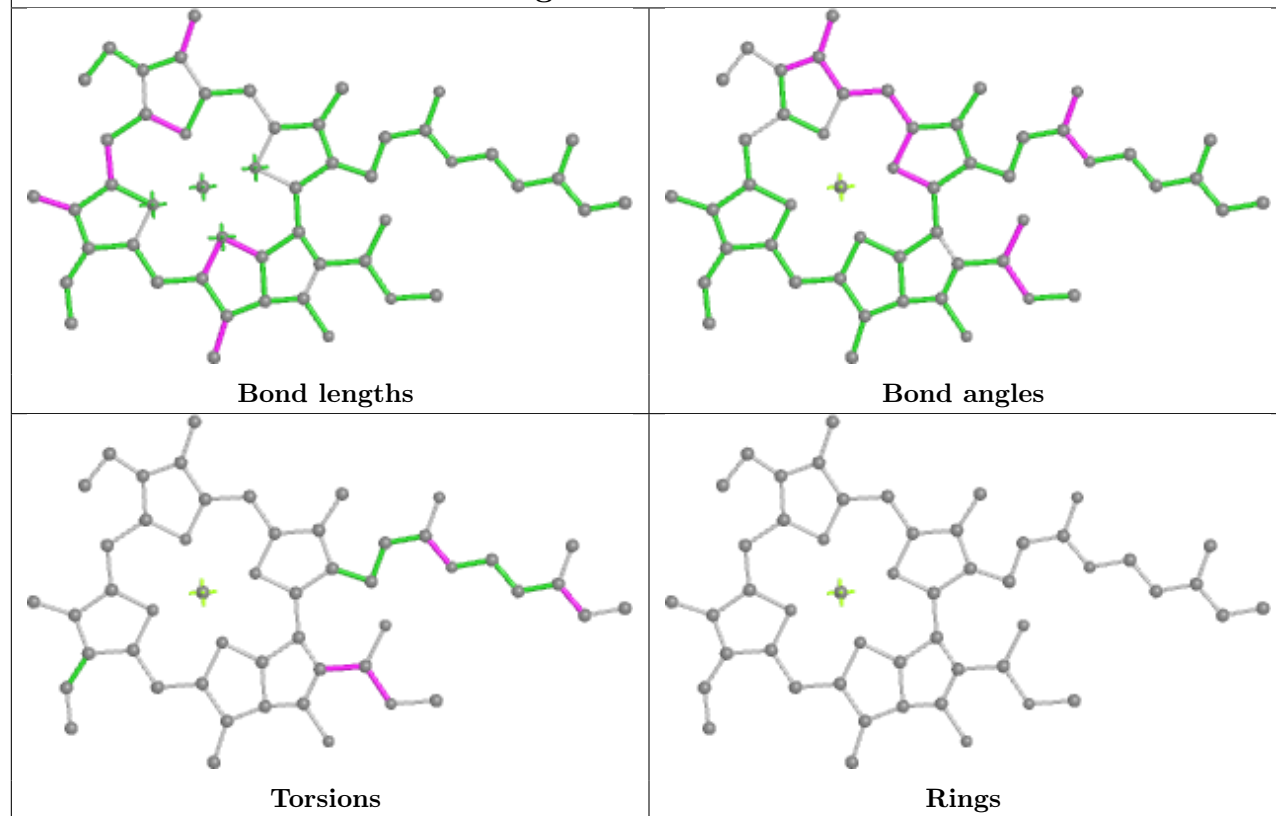


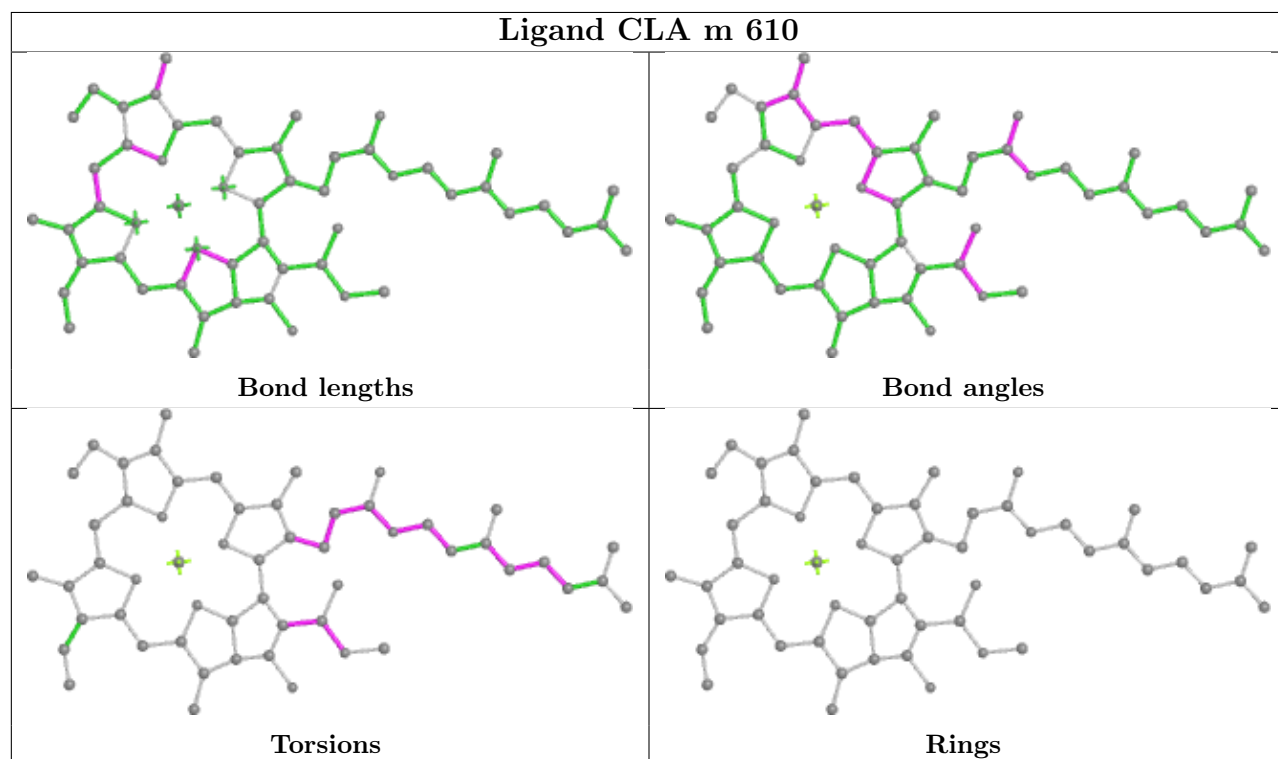
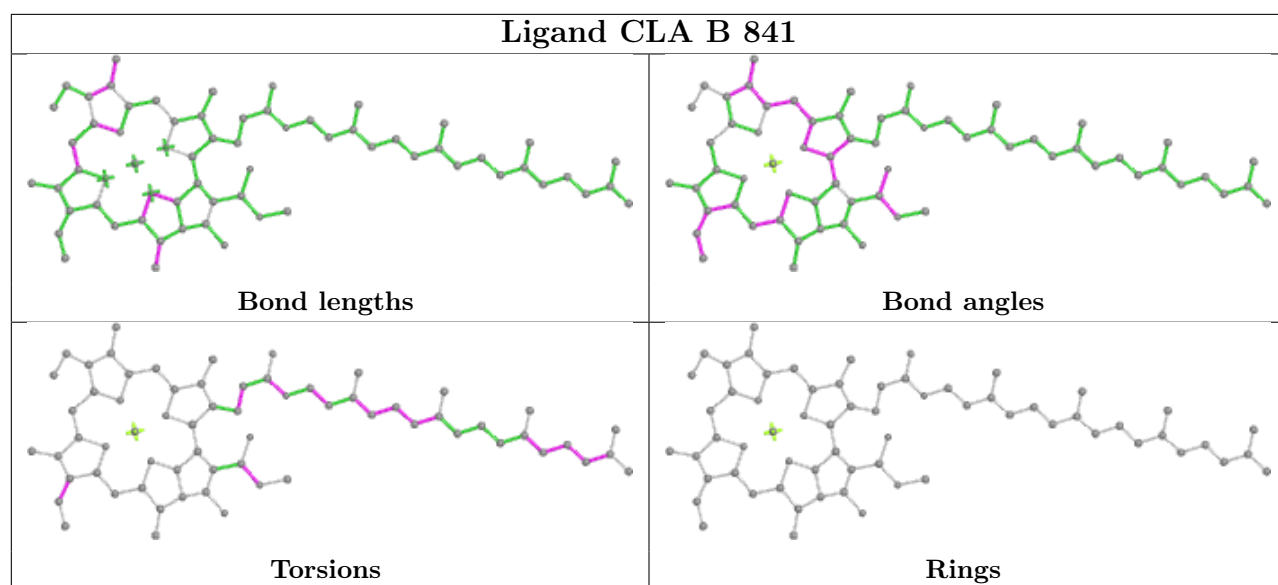
Ligand II0 f 615**Ligand CLA e 304****Ligand CLA A 836**

Ligand CLA g 307

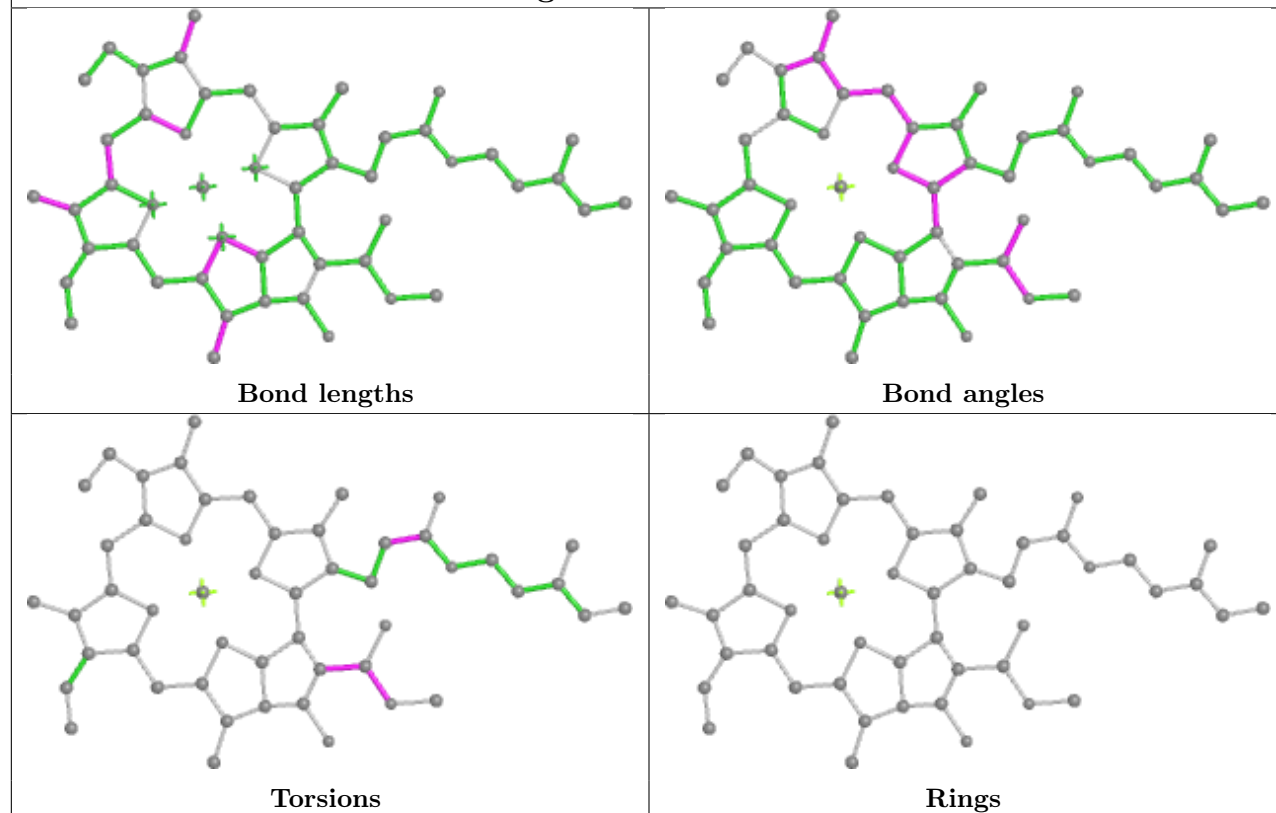


Ligand CLA d 303

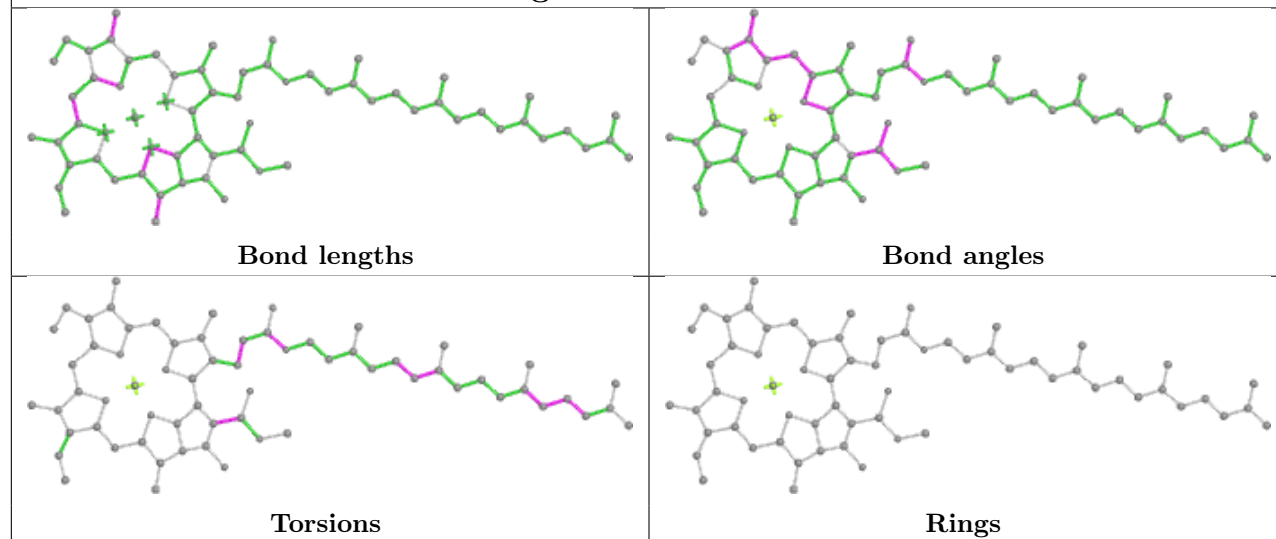


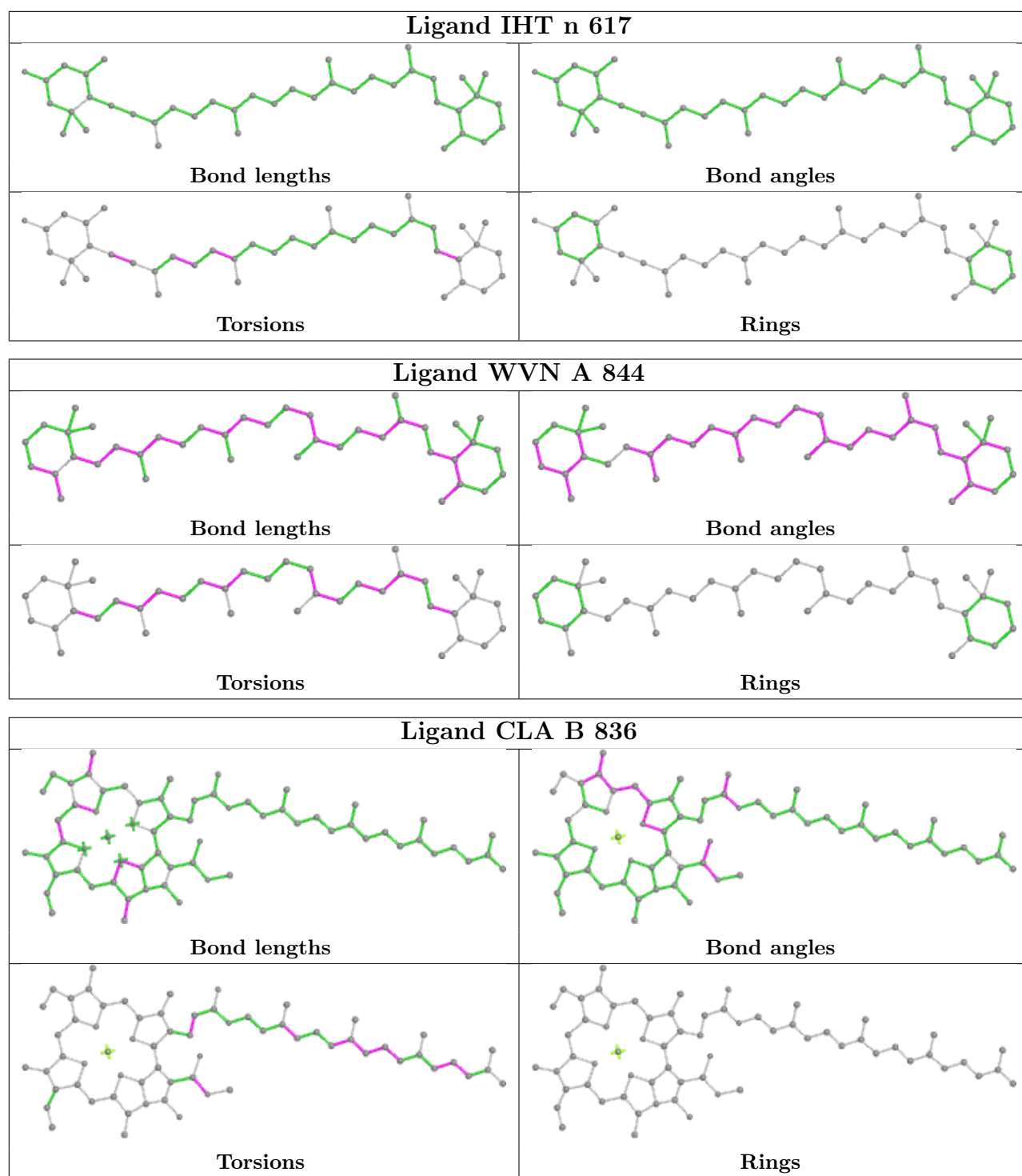


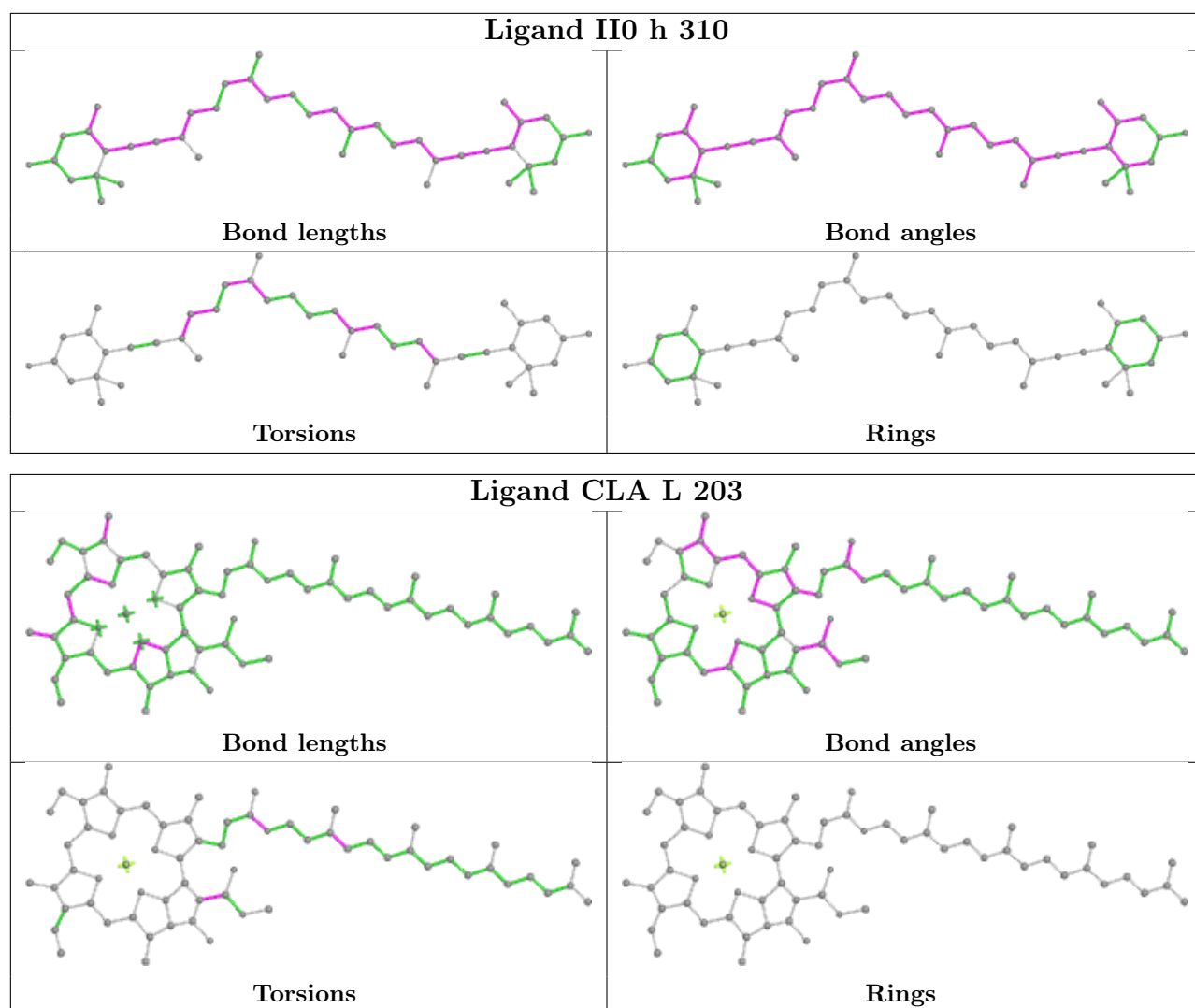
Ligand CLA c 303

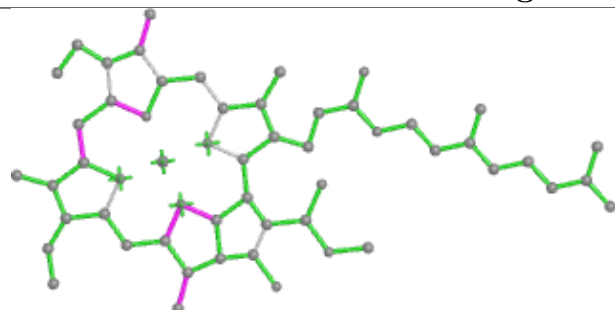
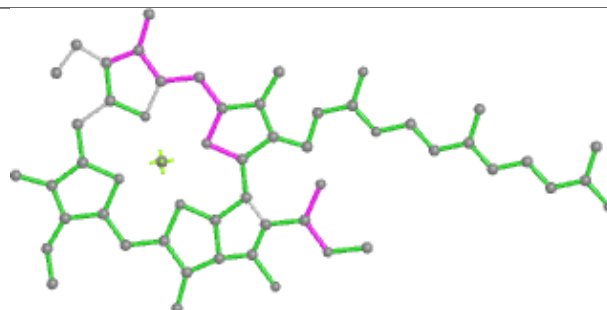
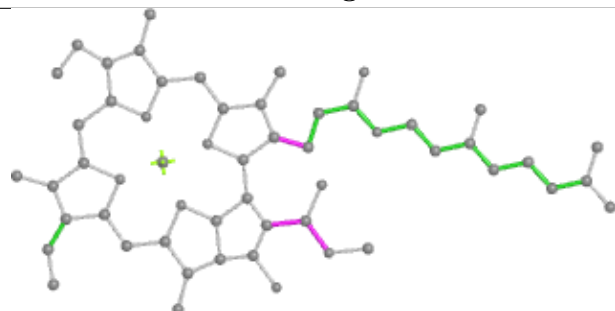
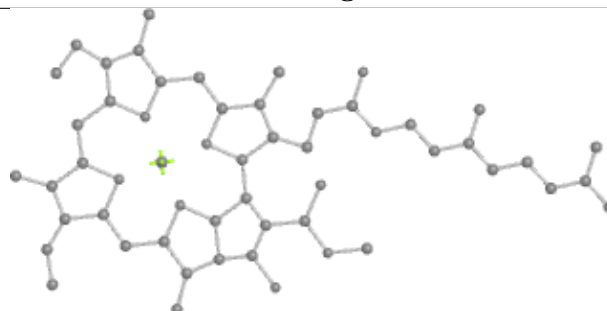
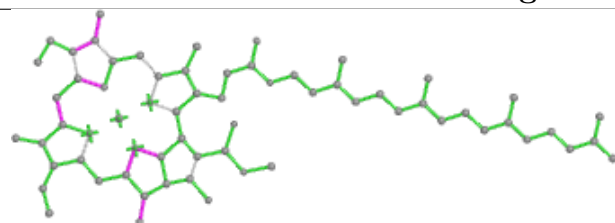
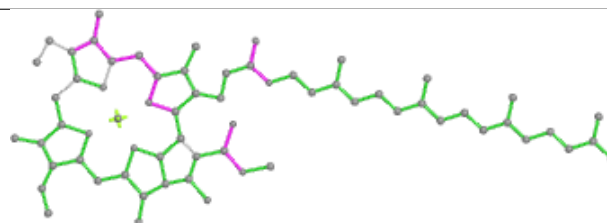
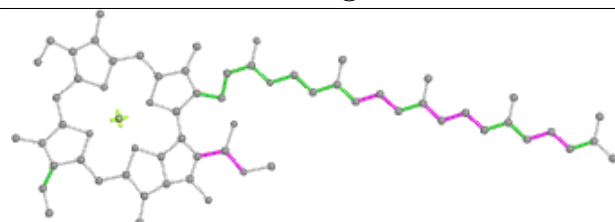
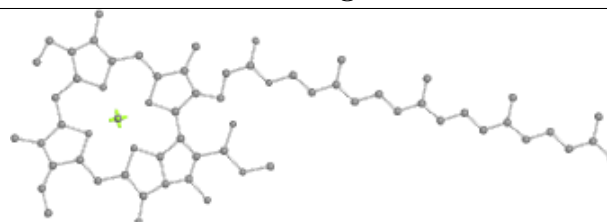


Ligand CLA A 835

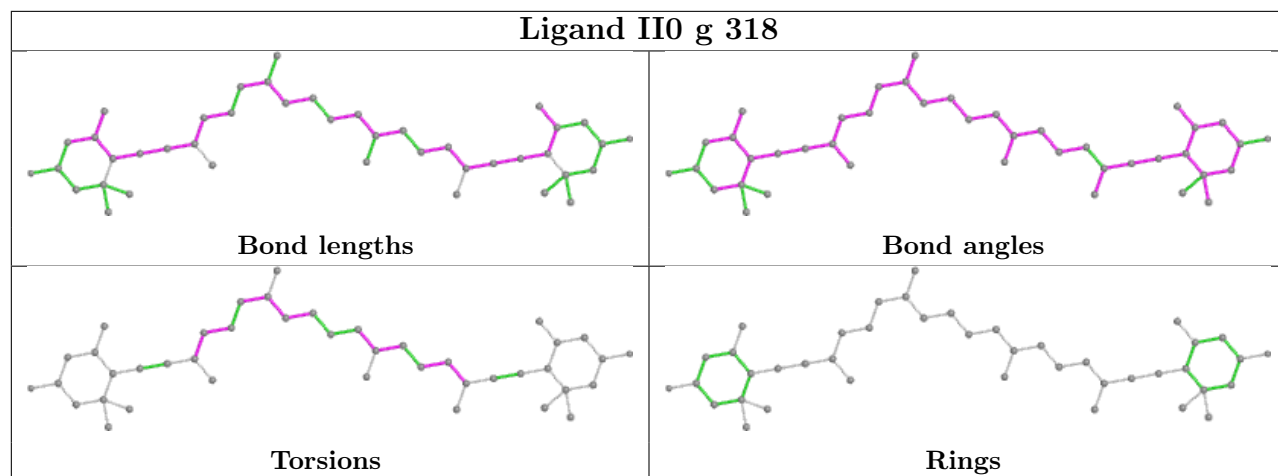




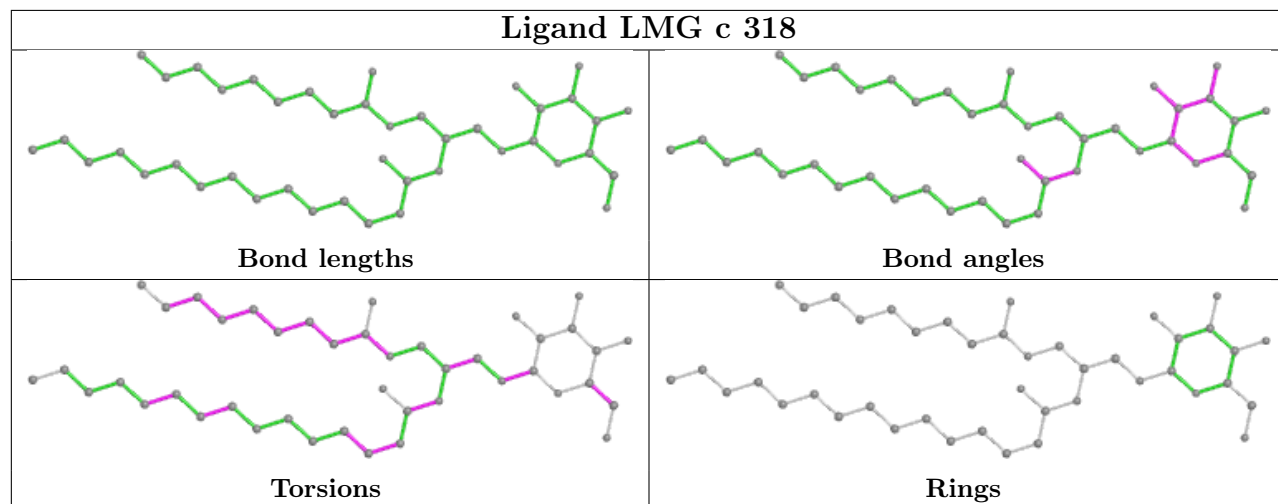


Ligand CLA B 833**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA b 310****Bond lengths****Bond angles****Torsions****Rings**

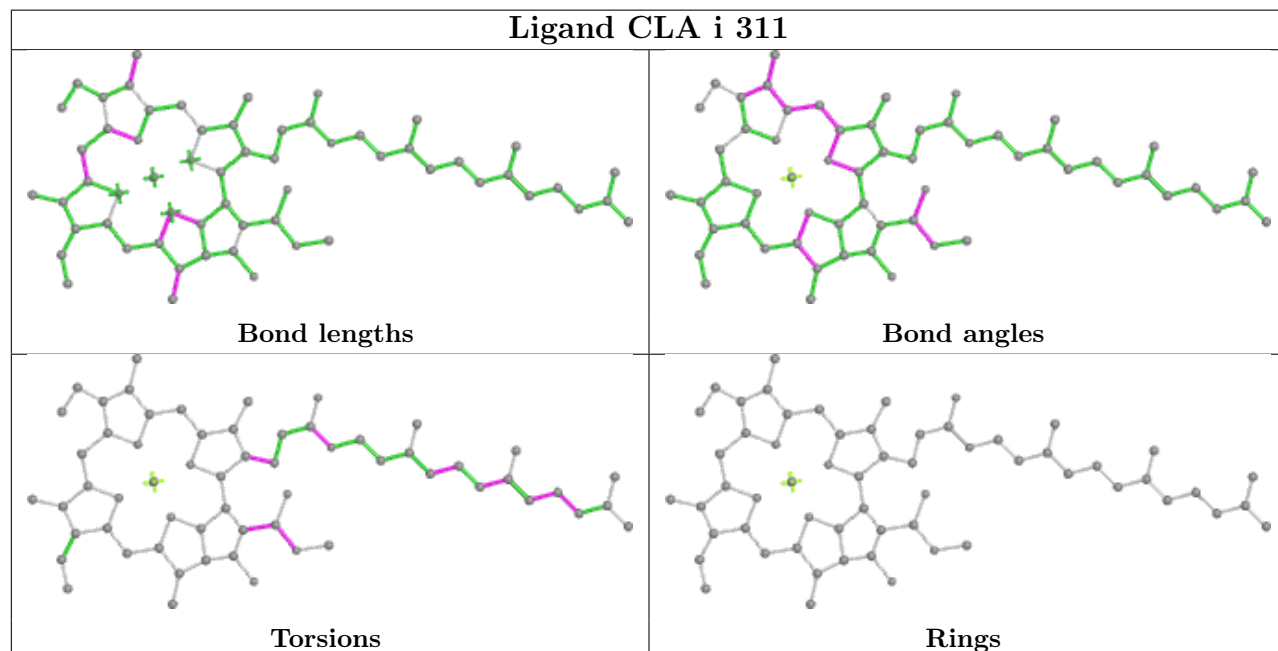
Ligand II0 g 318

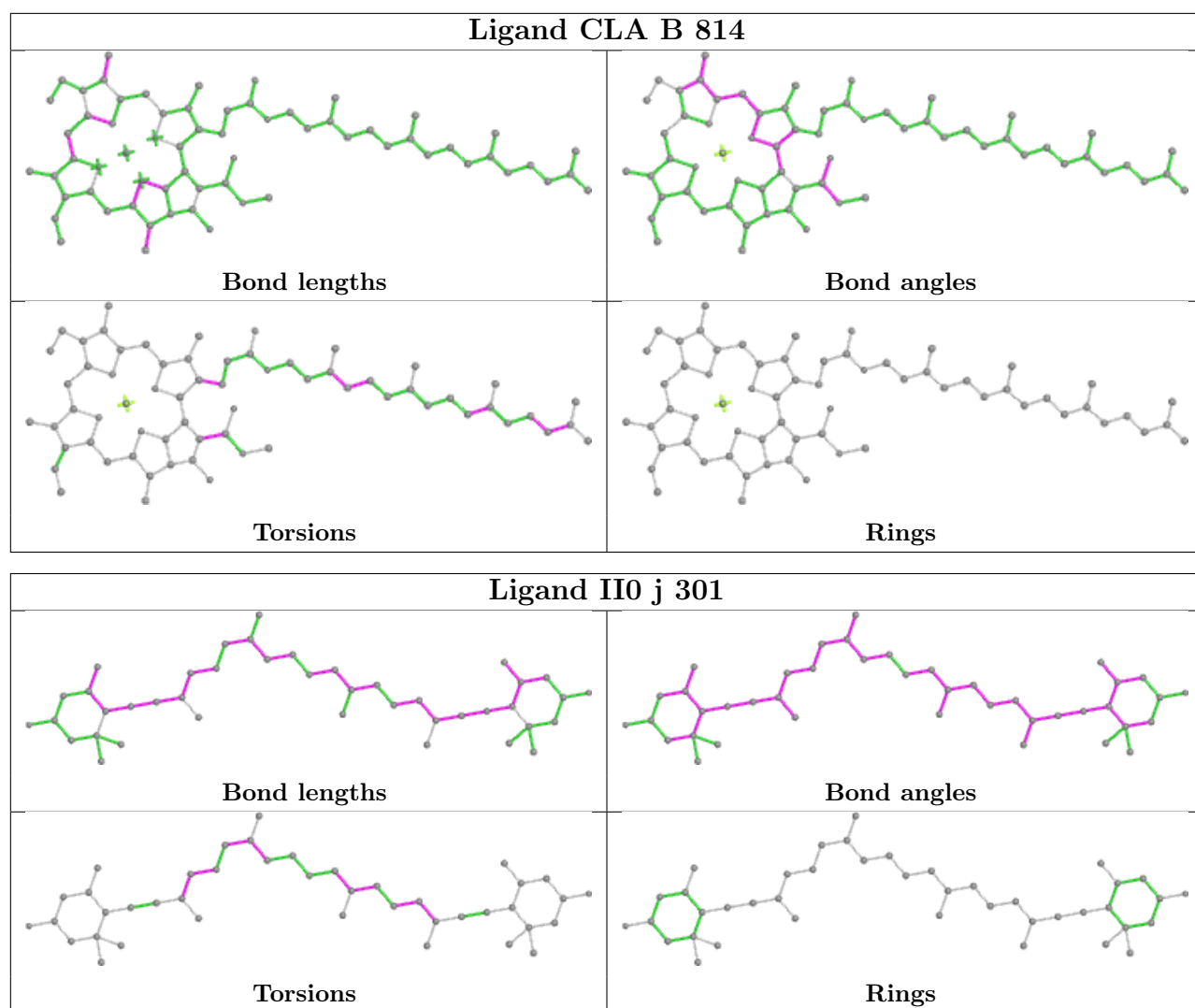


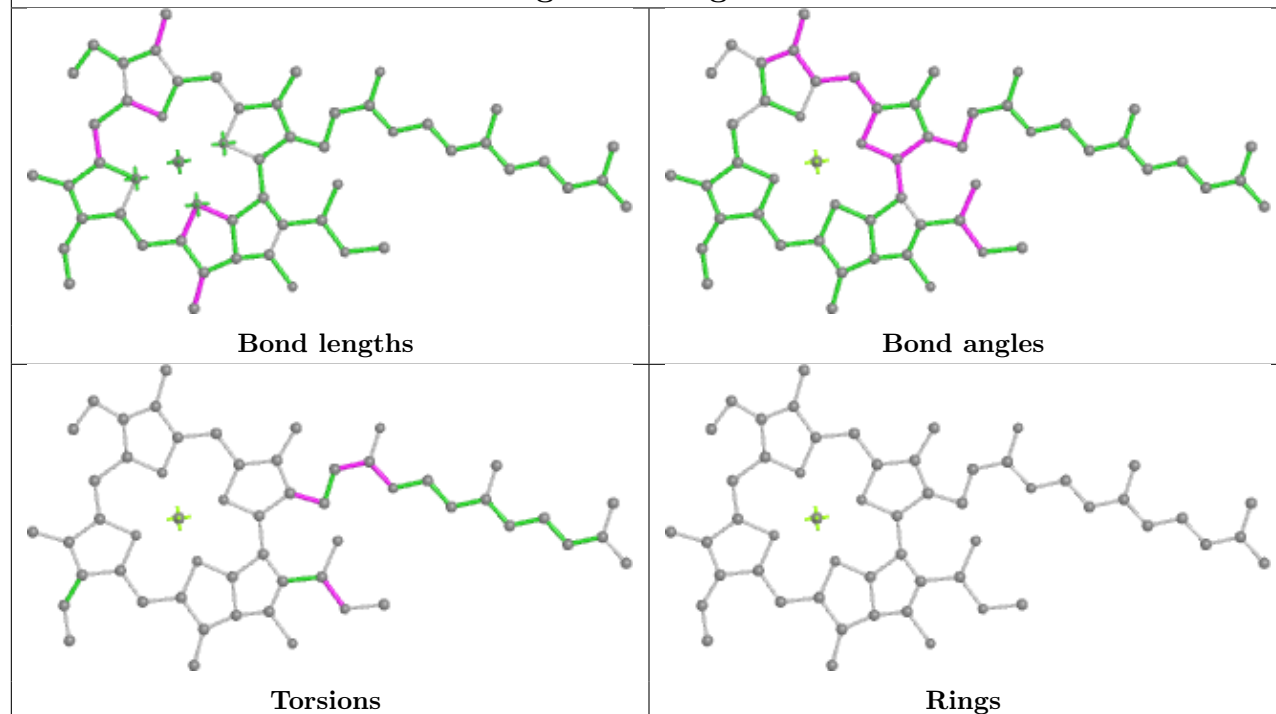
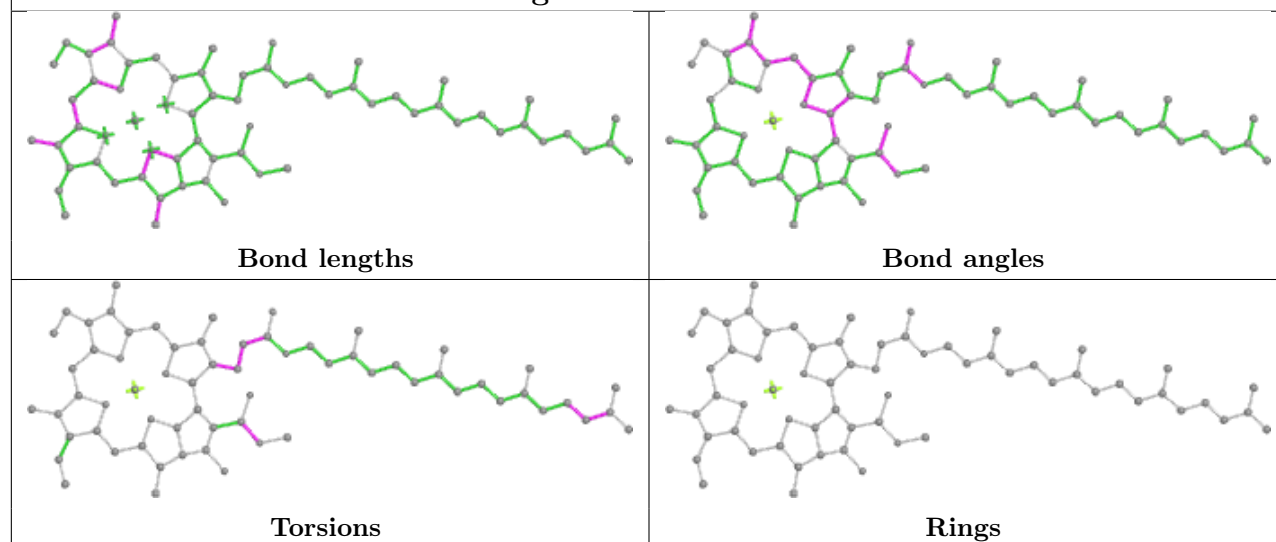
Ligand LMG c 318



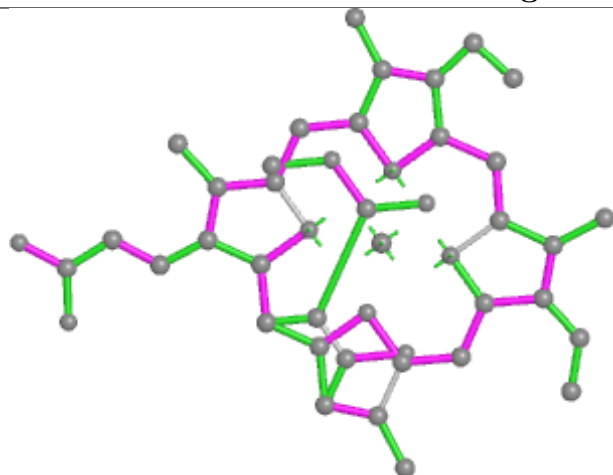
Ligand CLA i 311



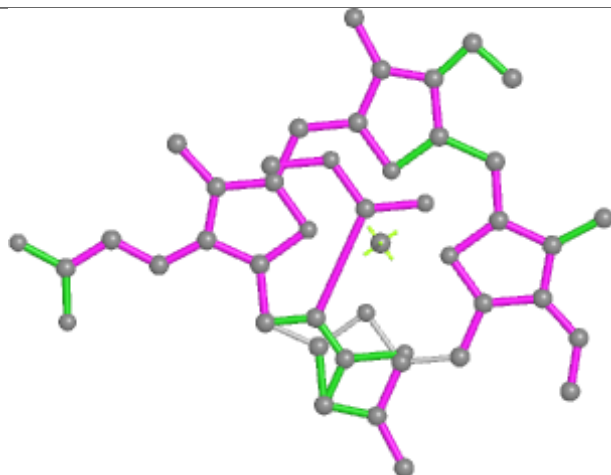


Ligand CLA g 323**Ligand CLA A 808**

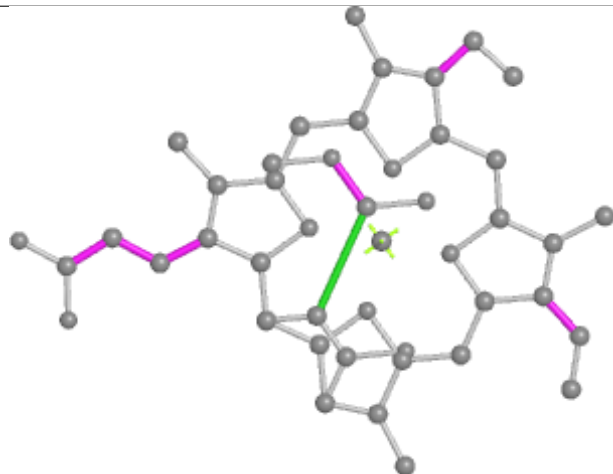
Ligand KC2 e 309



Bond lengths



Bond angles

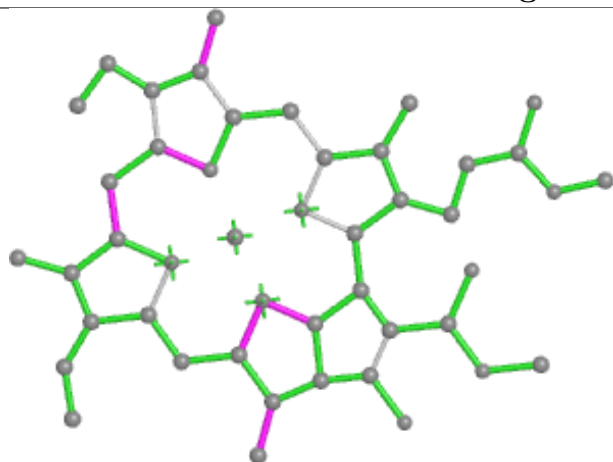


Torsions

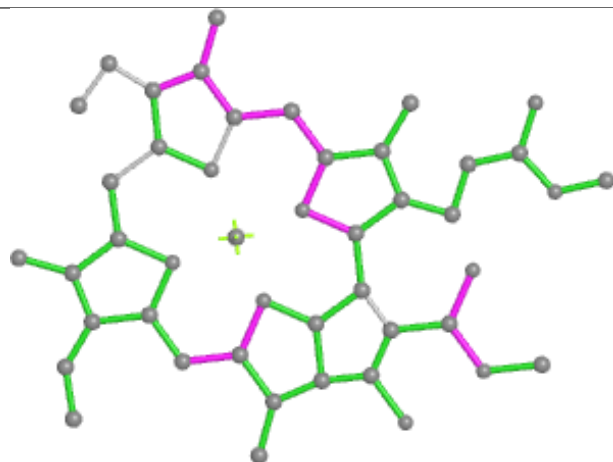


Rings

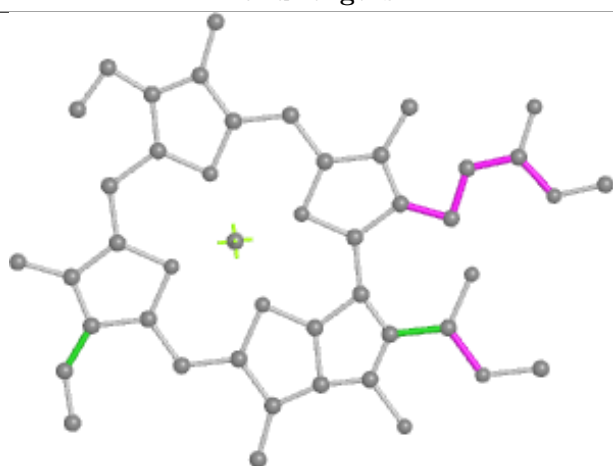
Ligand CLA c 307



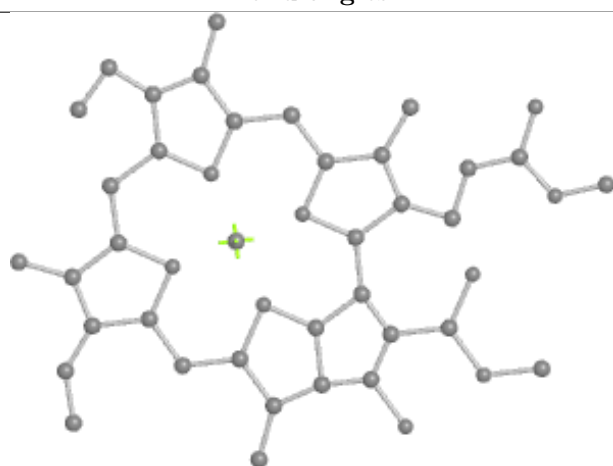
Bond lengths



Bond angles

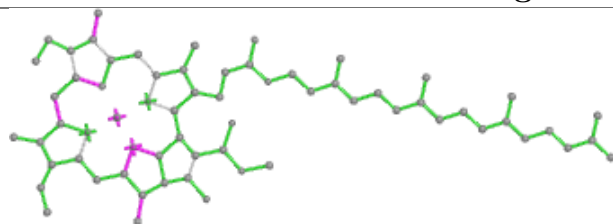


Torsions

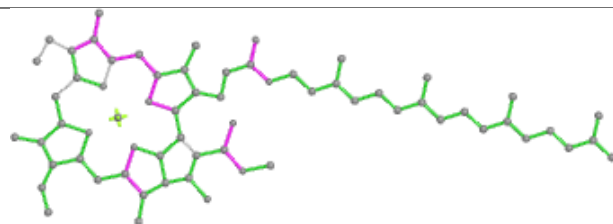


Rings

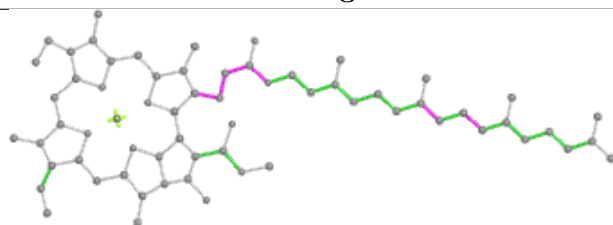
Ligand CLA B 826



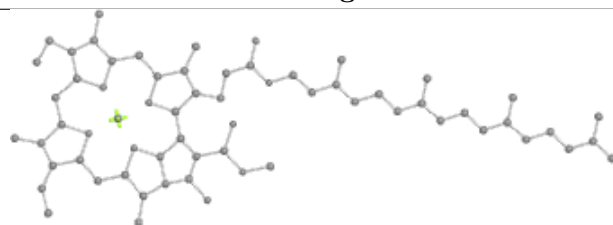
Bond lengths



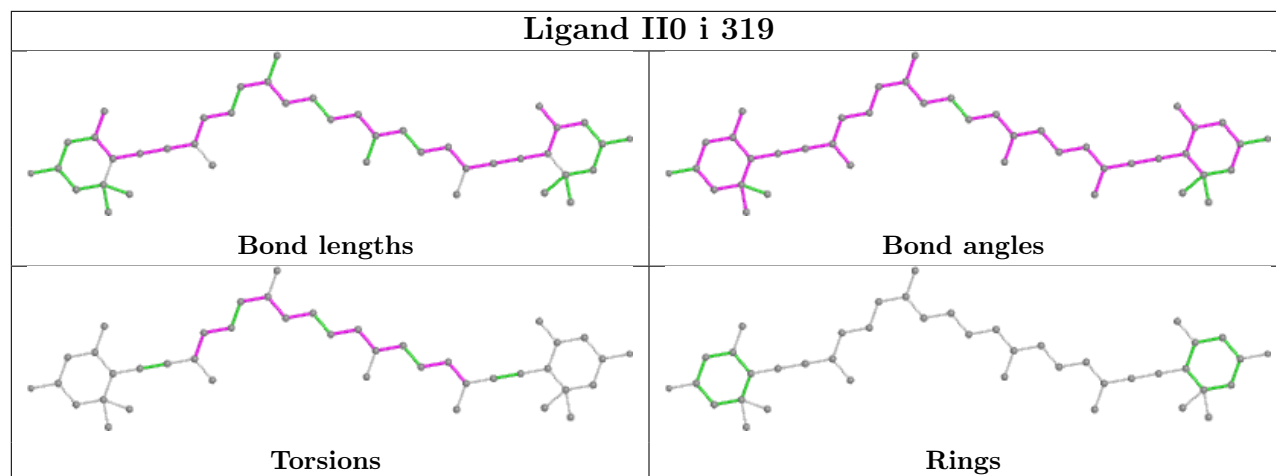
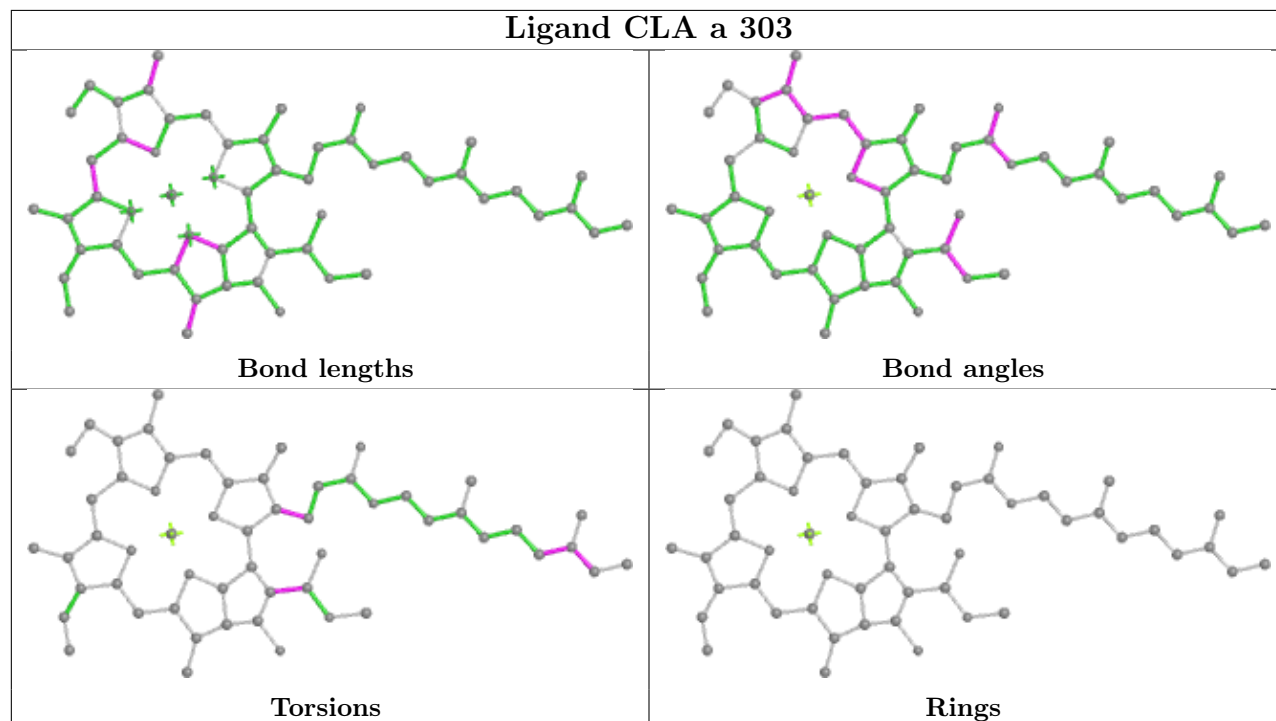
Bond angles



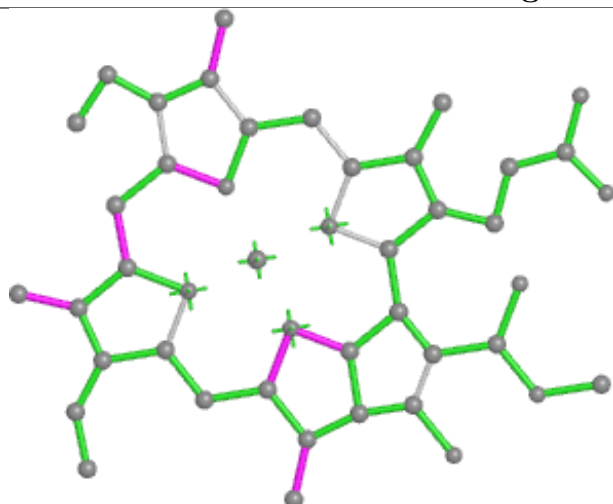
Torsions



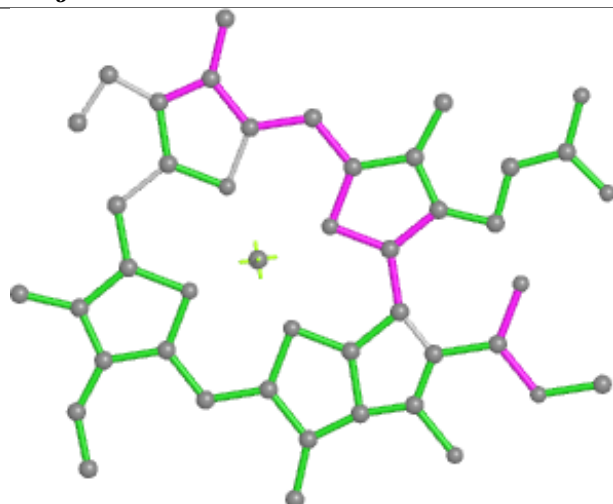
Rings

Ligand II0 i 319**Ligand CLA a 303**

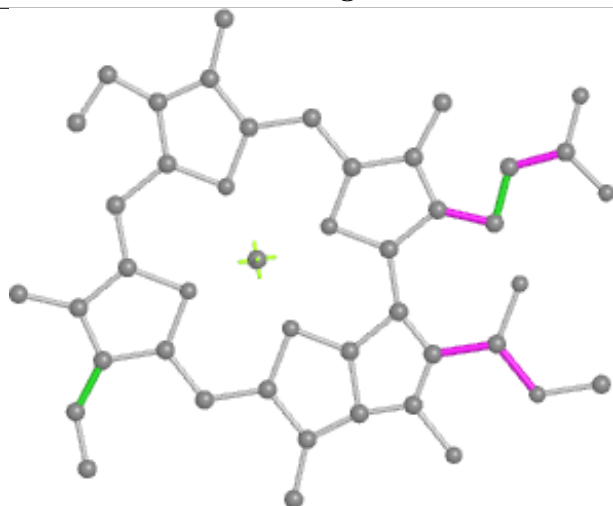
Ligand CLA j 306



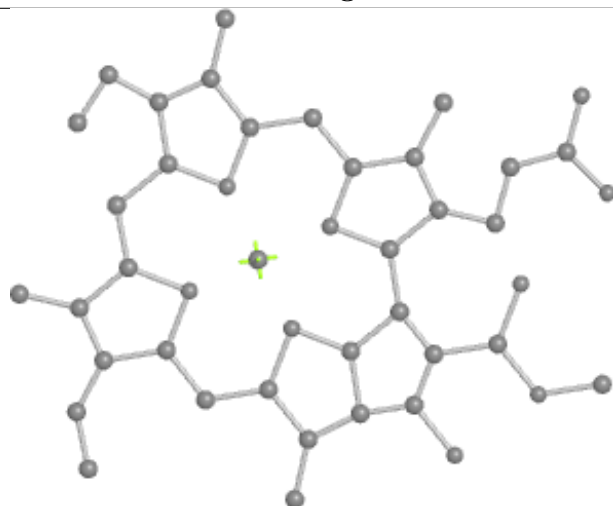
Bond lengths



Bond angles

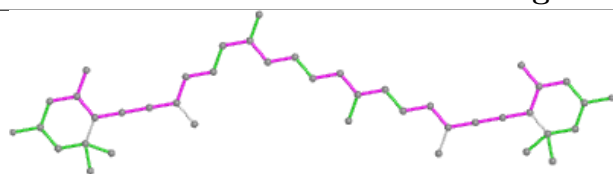


Torsions

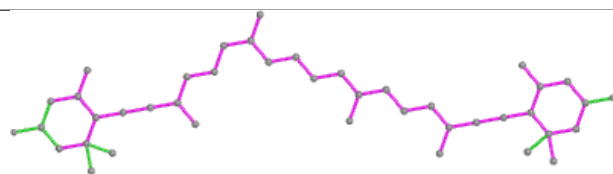


Rings

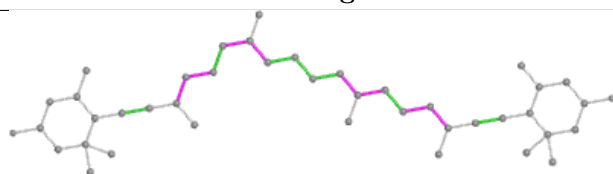
Ligand II0 k 615



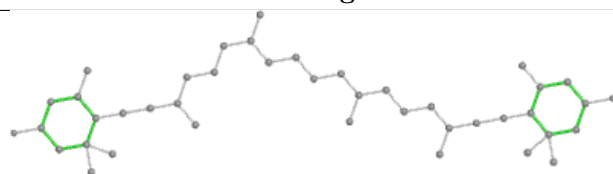
Bond lengths



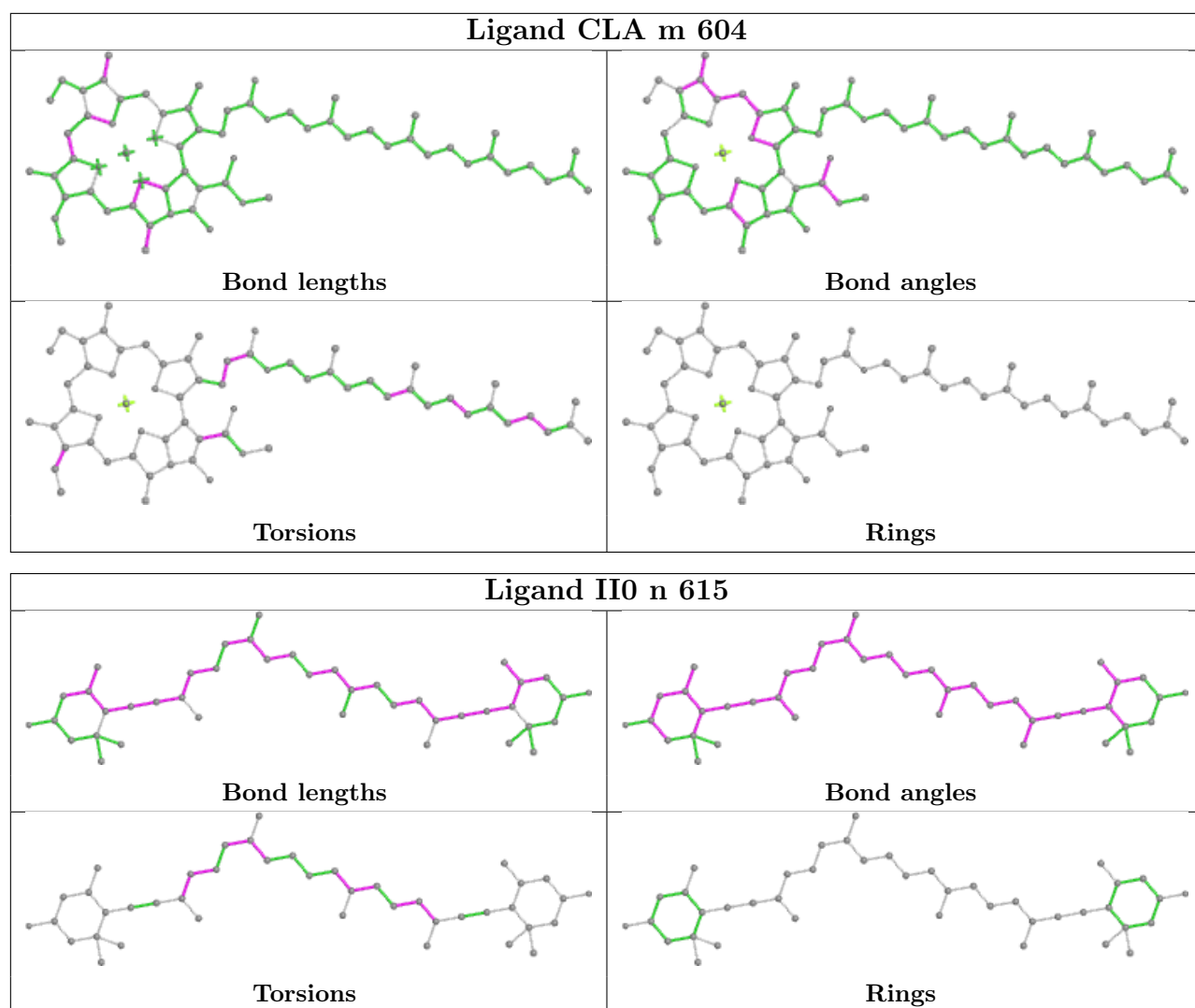
Bond angles



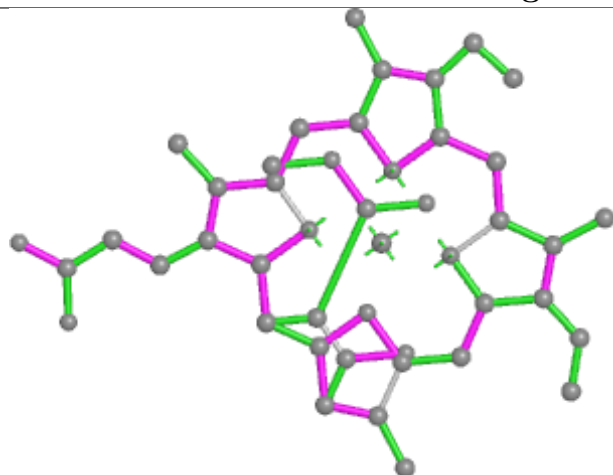
Torsions



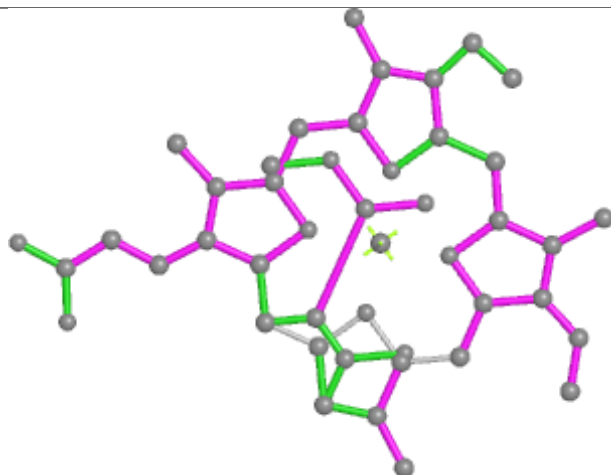
Rings



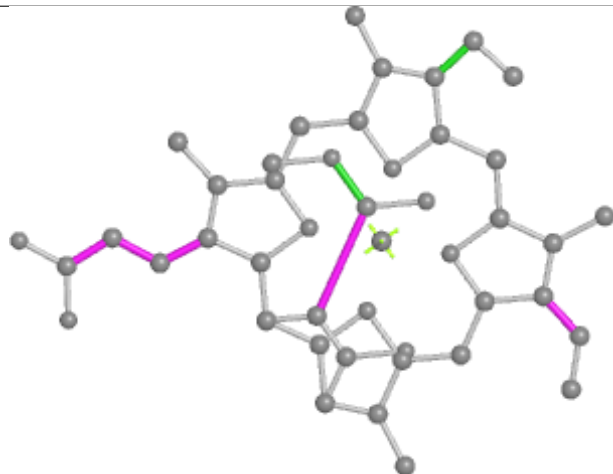
Ligand KC2 s 401



Bond lengths



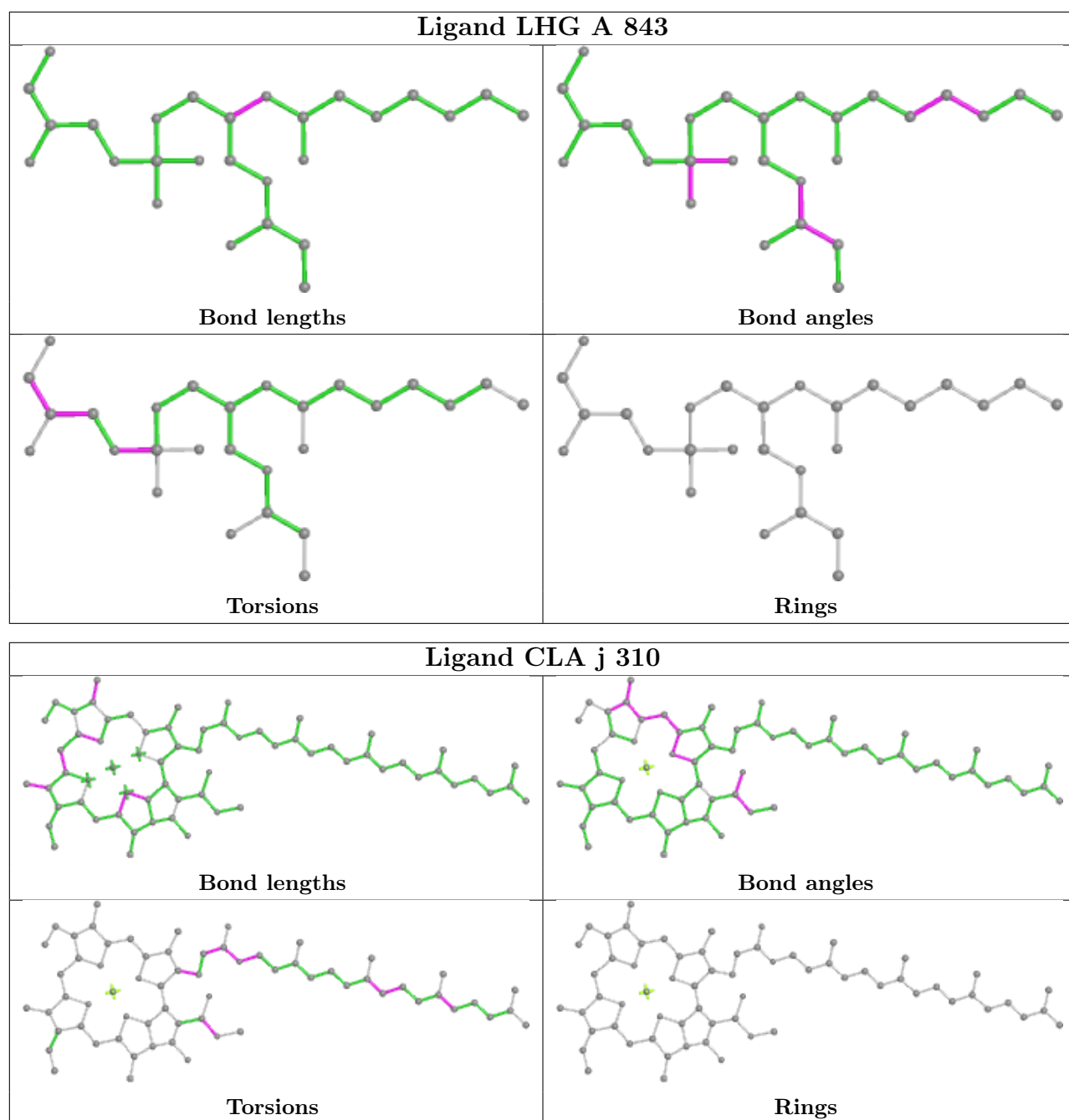
Bond angles



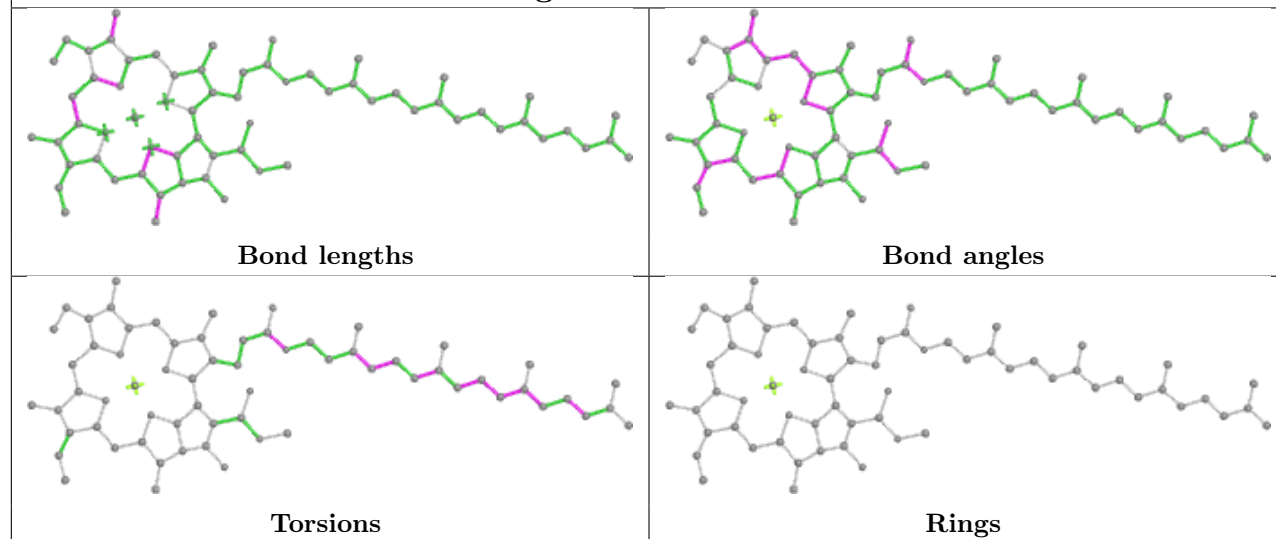
Torsions



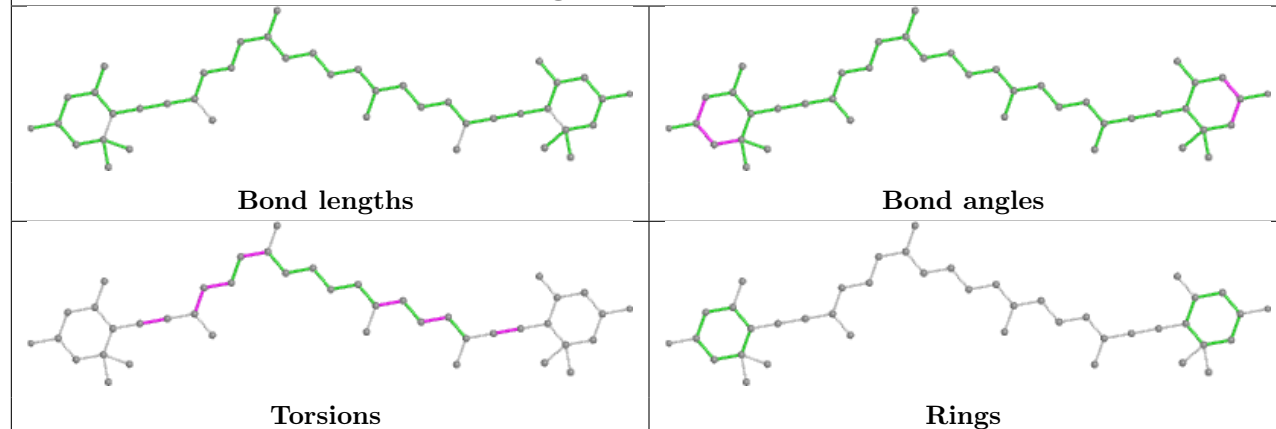
Rings



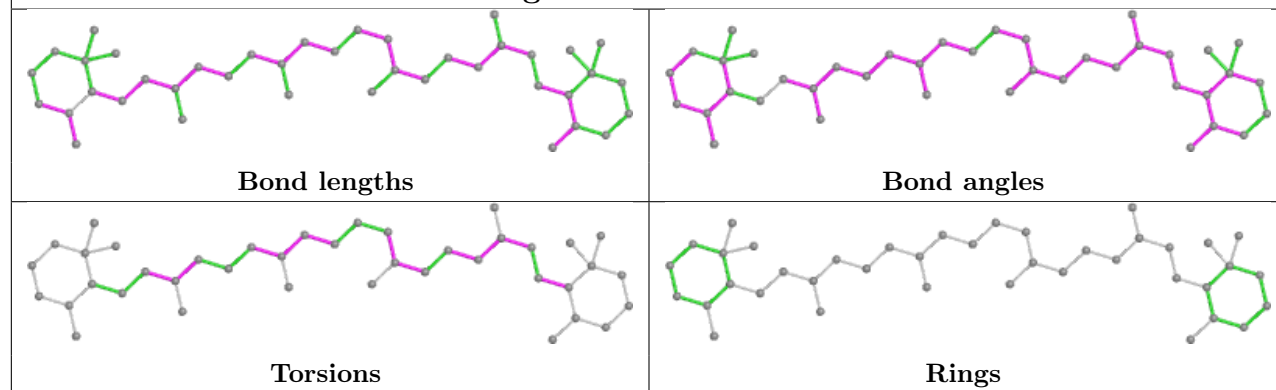
Ligand CLA b 306

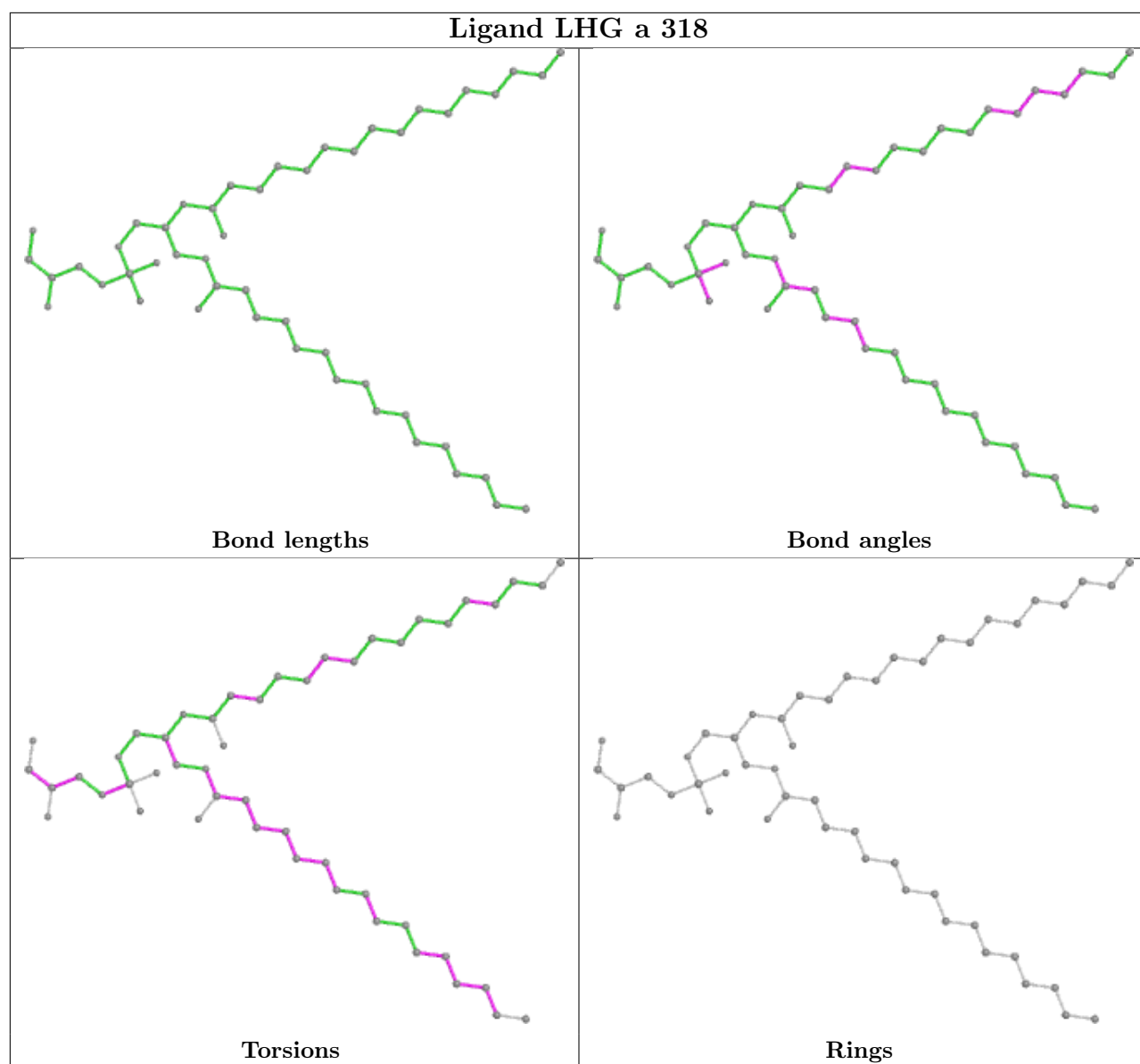


Ligand II0 n 614

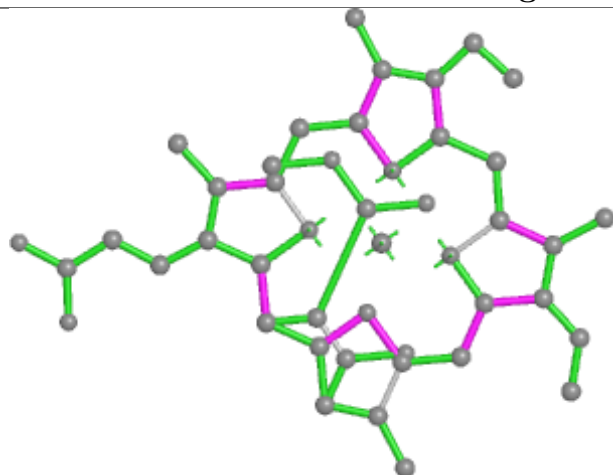


Ligand WVN A 846

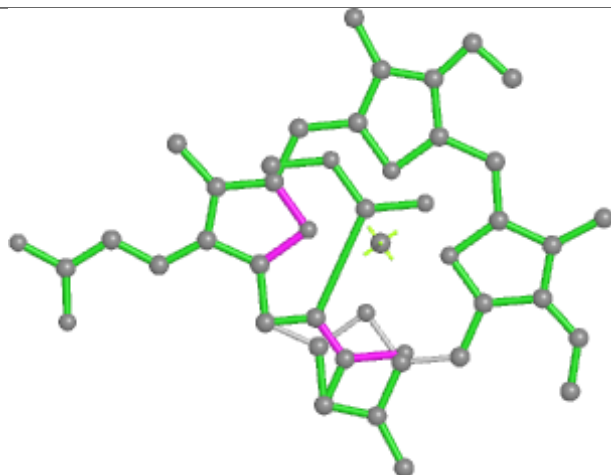




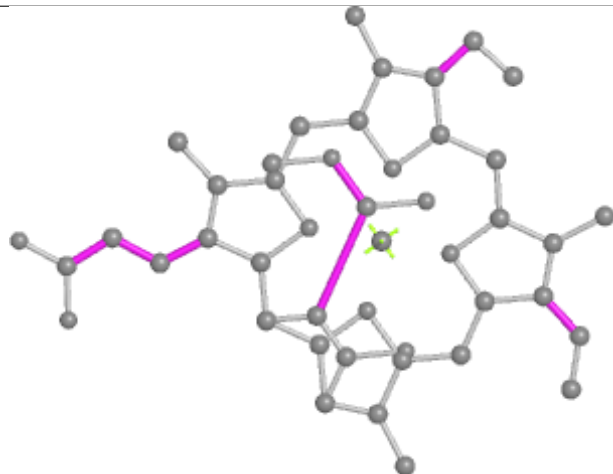
Ligand KC2 n 612



Bond lengths



Bond angles

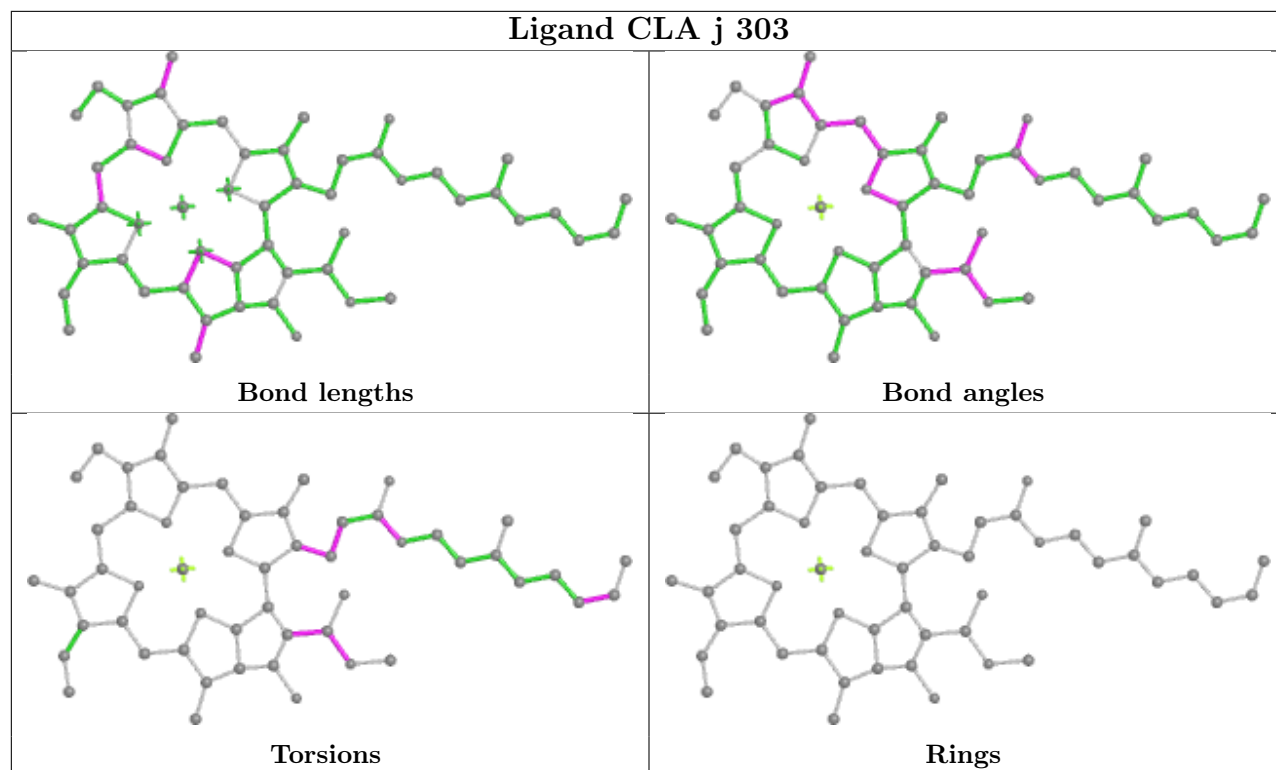


Torsions

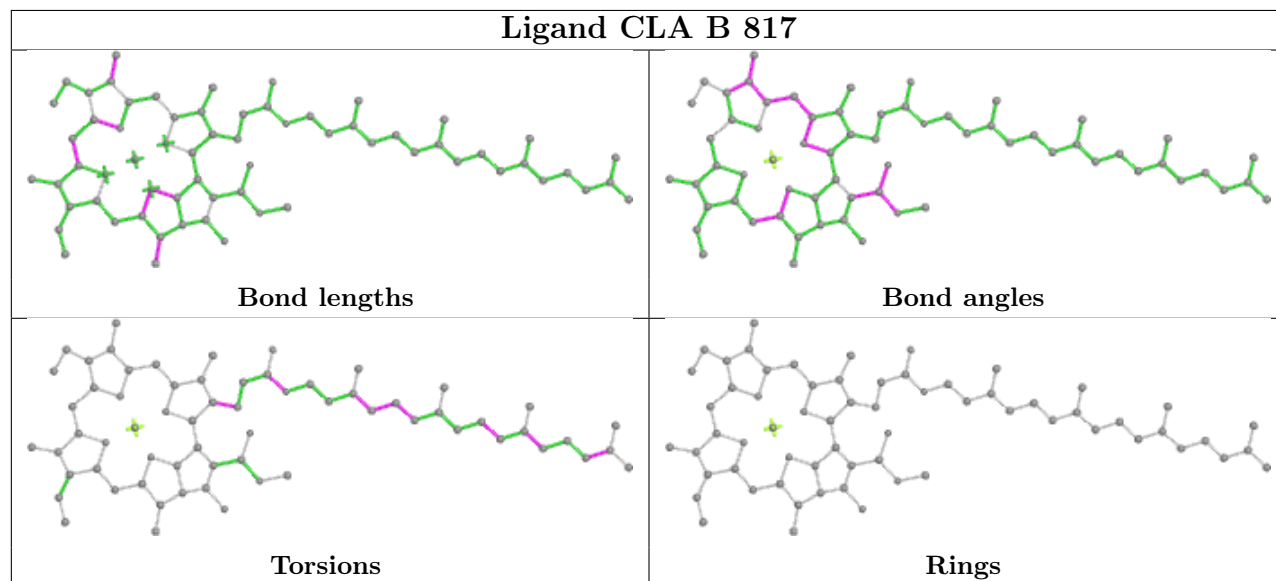


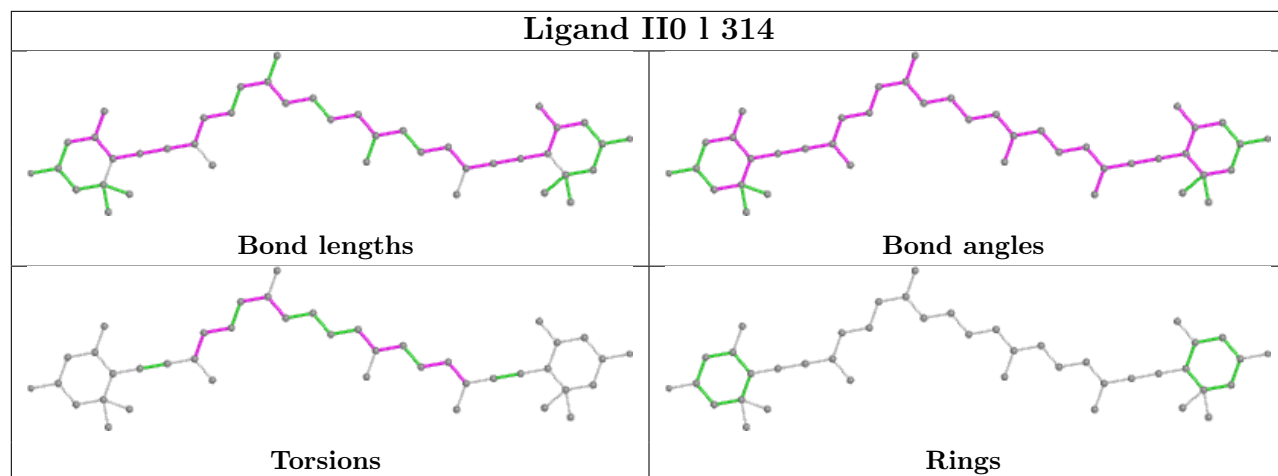
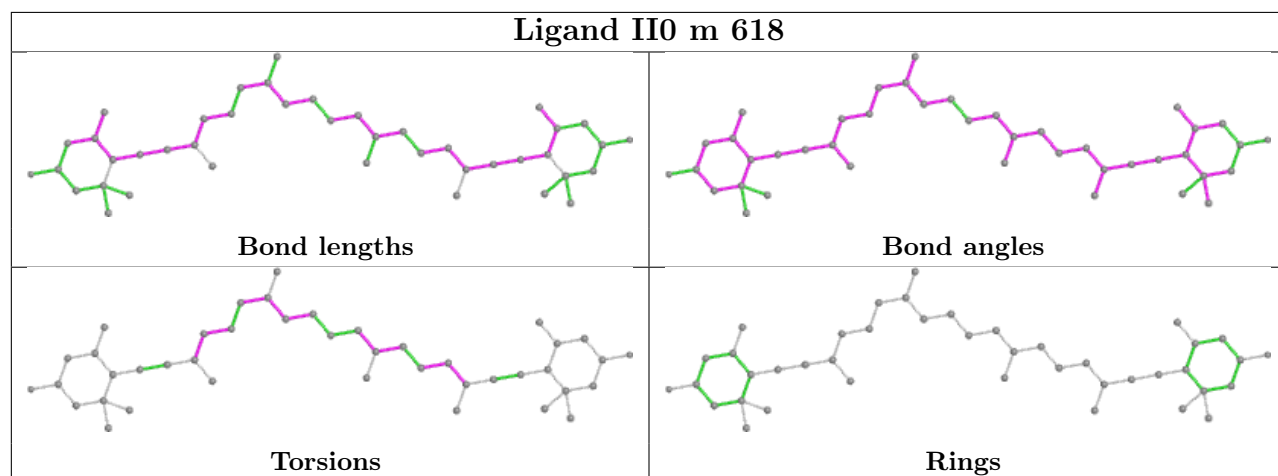
Rings

Ligand CLA j 303

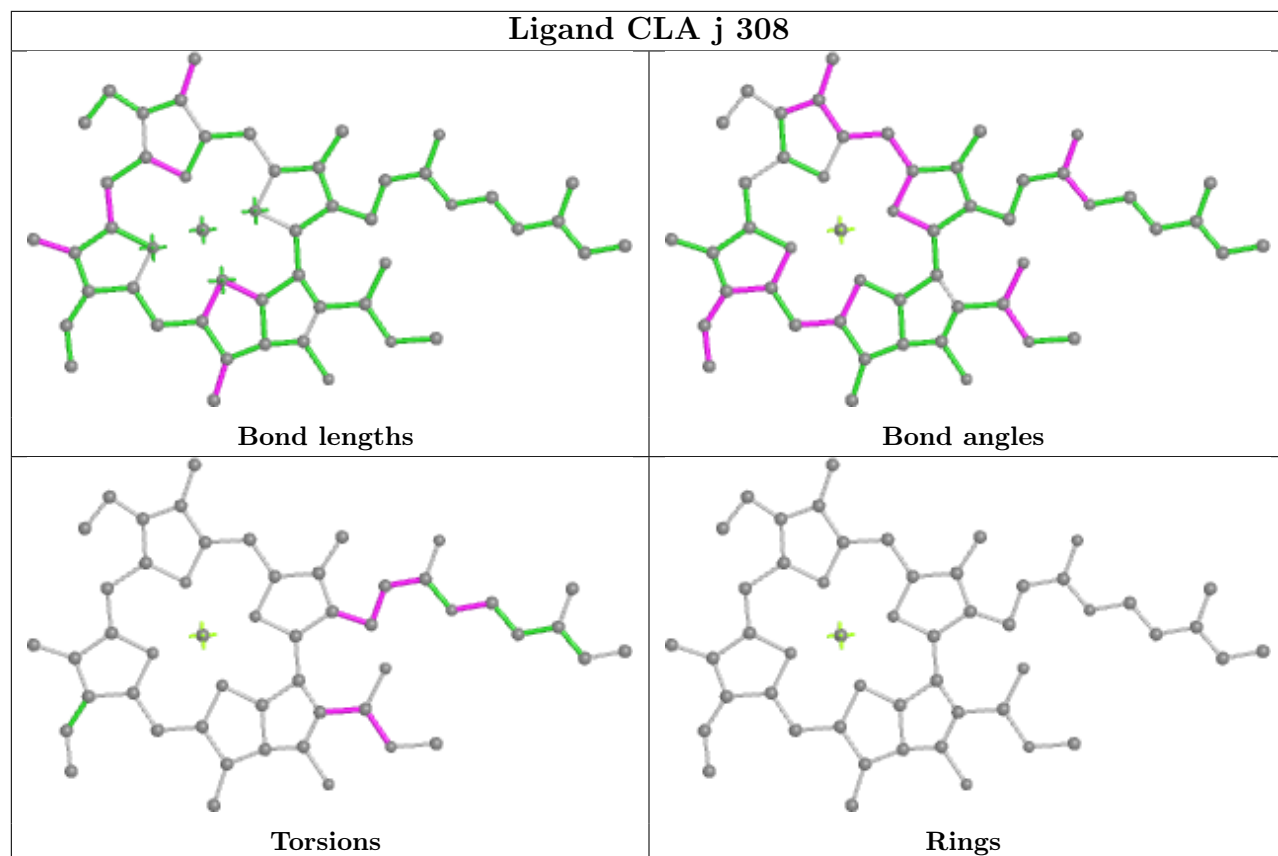


Ligand CLA B 817

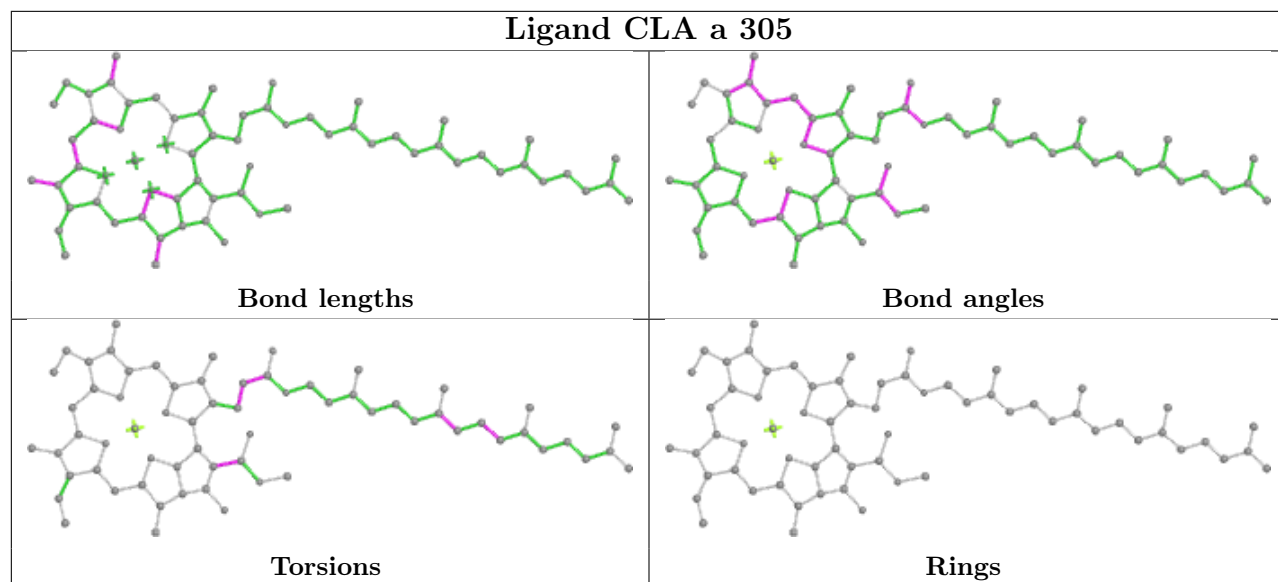


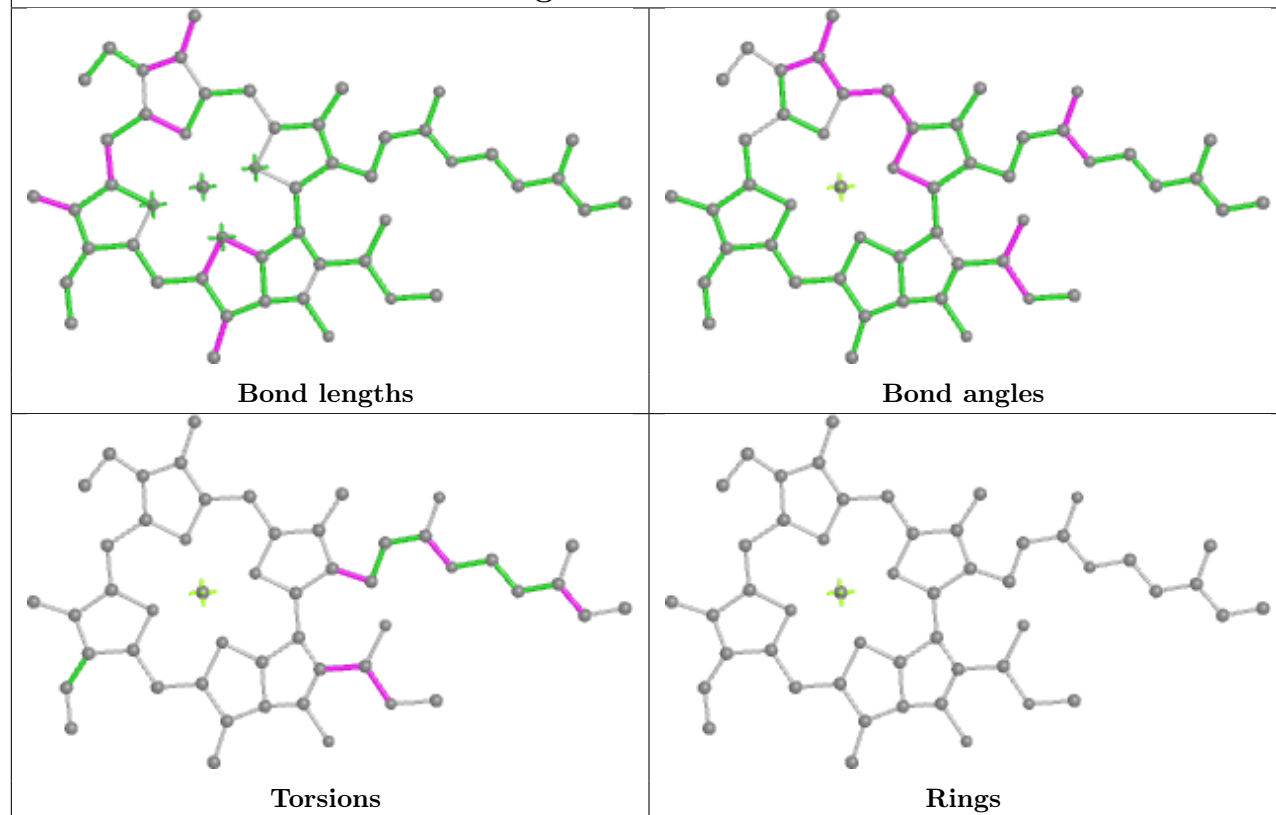
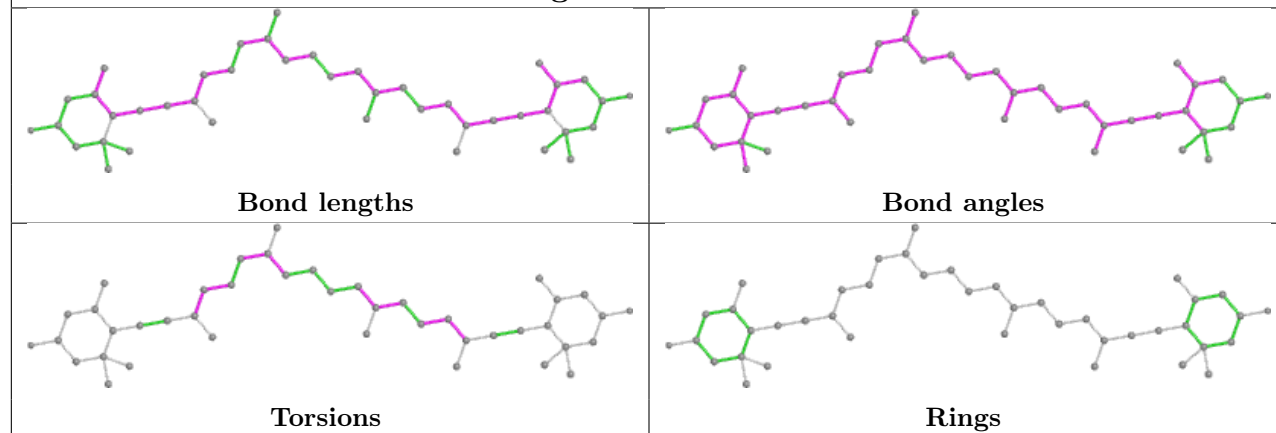
Ligand II0 l 314**Ligand II0 m 618**

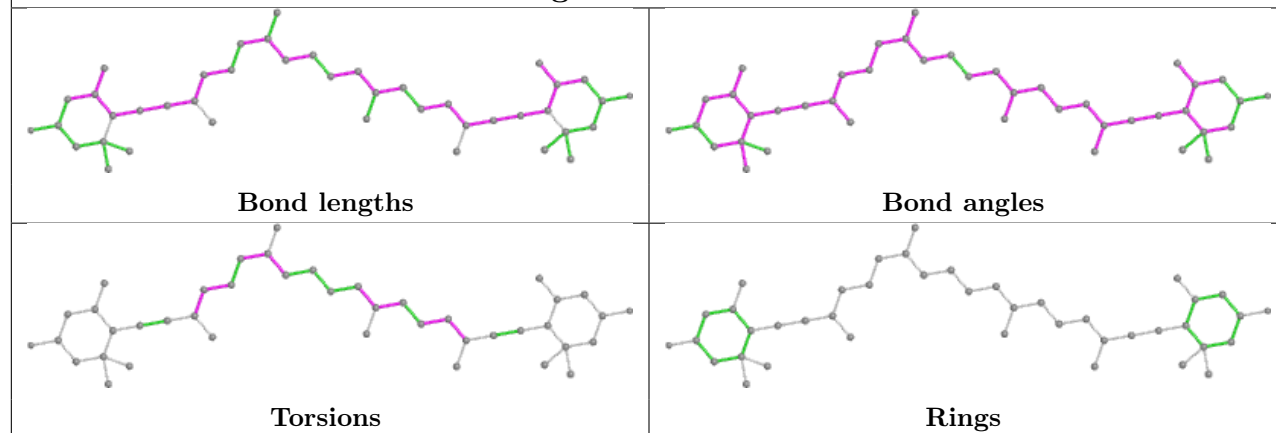
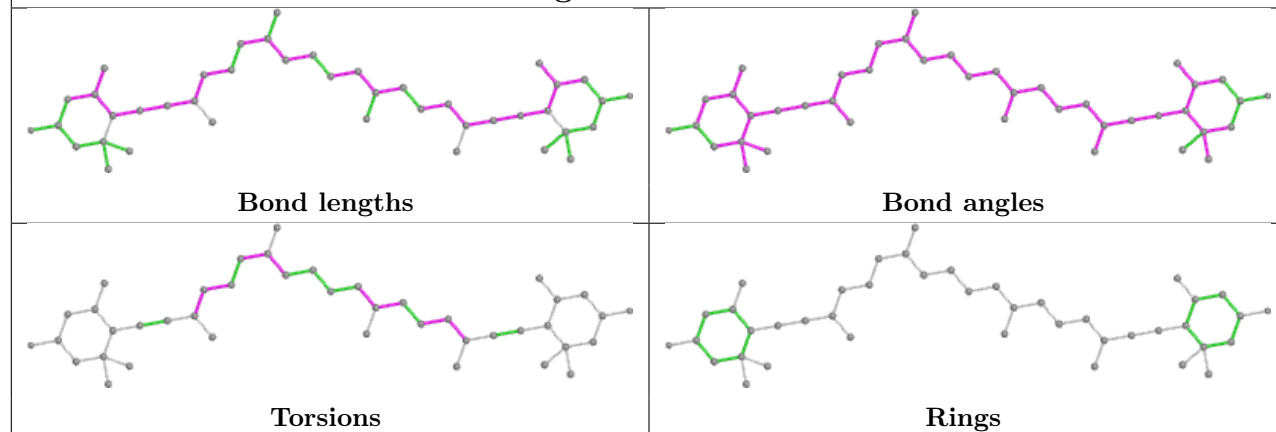
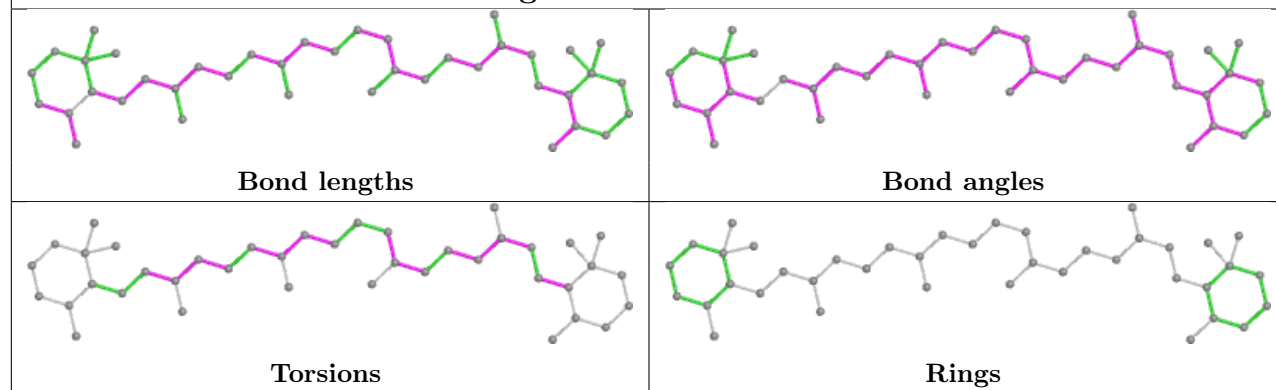
Ligand CLA j 308

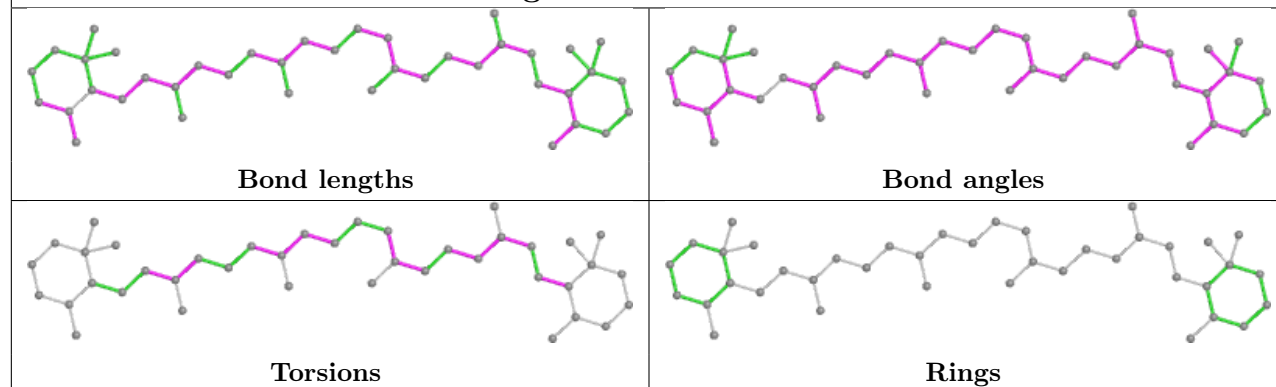
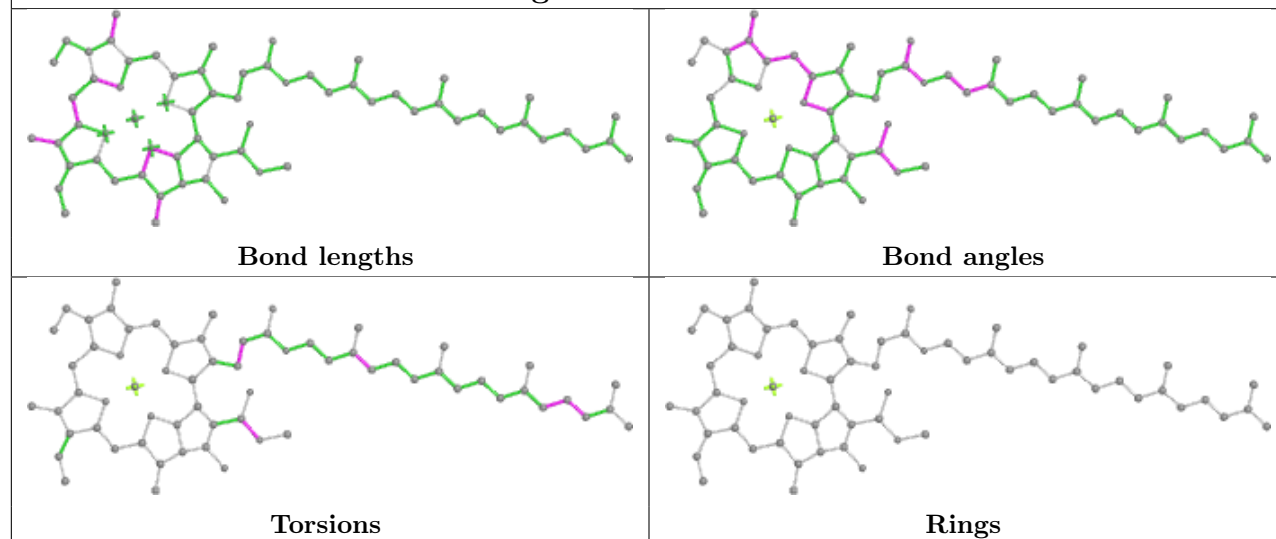
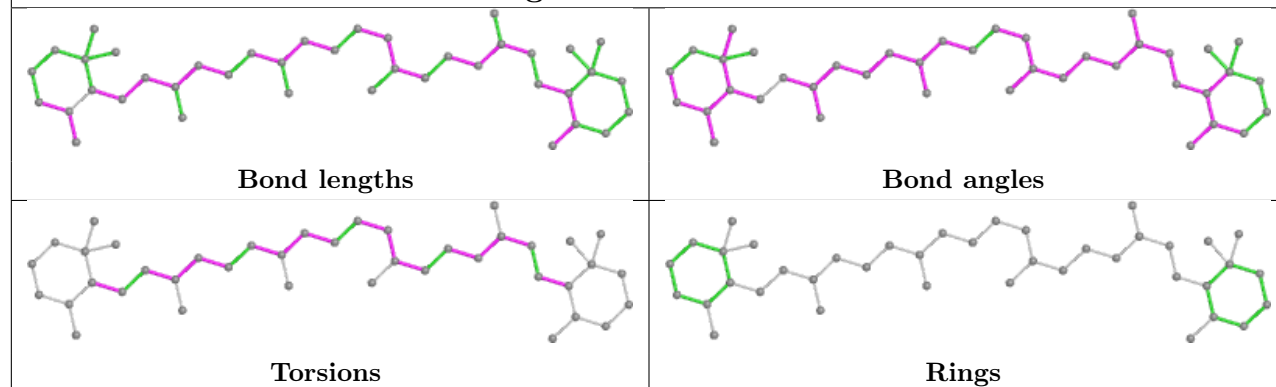


Ligand CLA a 305

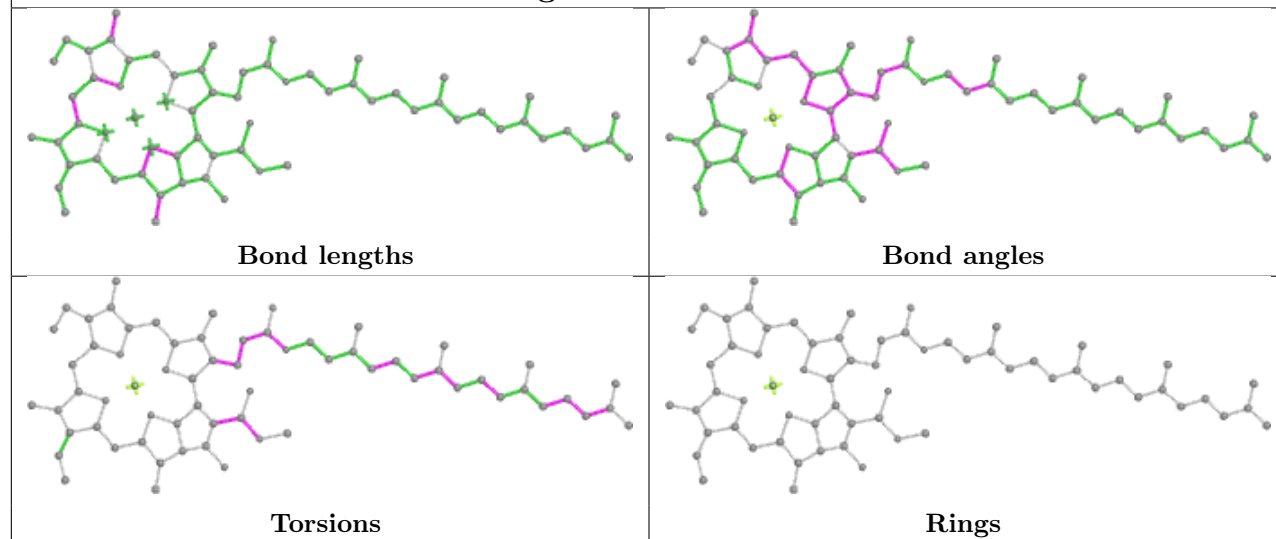


Ligand CLA n 603**Ligand II0 a 313**

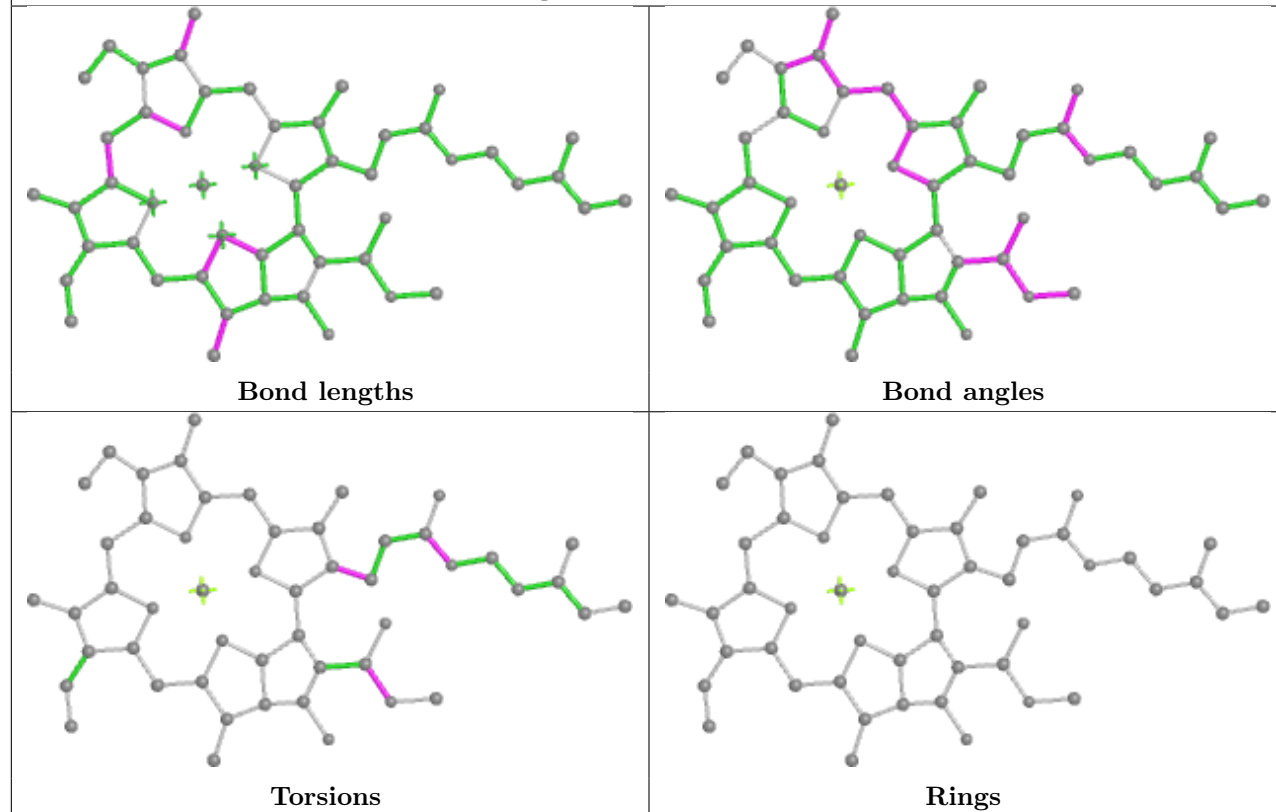
Ligand II0 e 312**Ligand II0 l 315****Ligand WVN M 101**

Ligand WVN R 202**Ligand CLA A 828****Ligand WVN L 201**

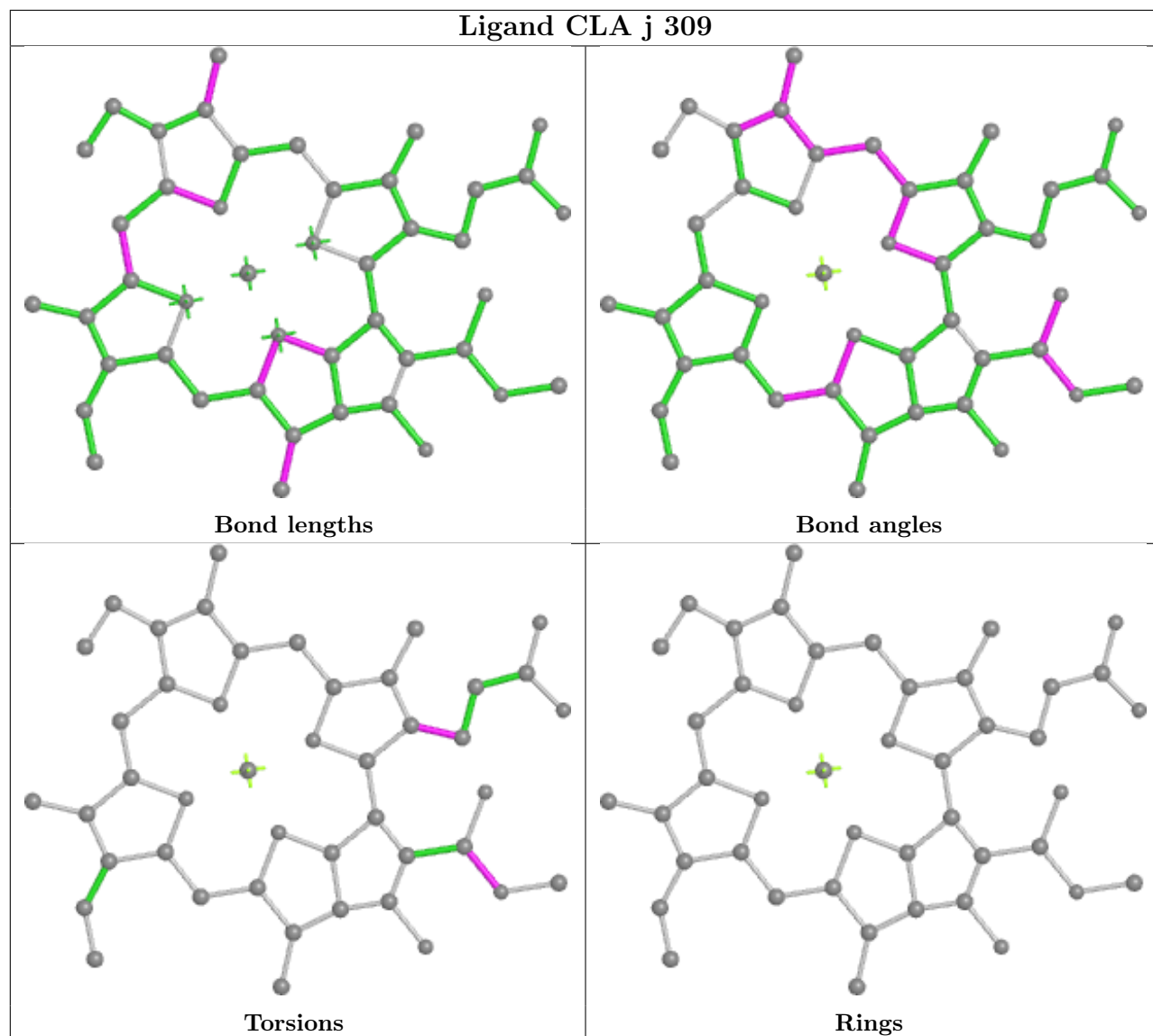
Ligand CLA s 402

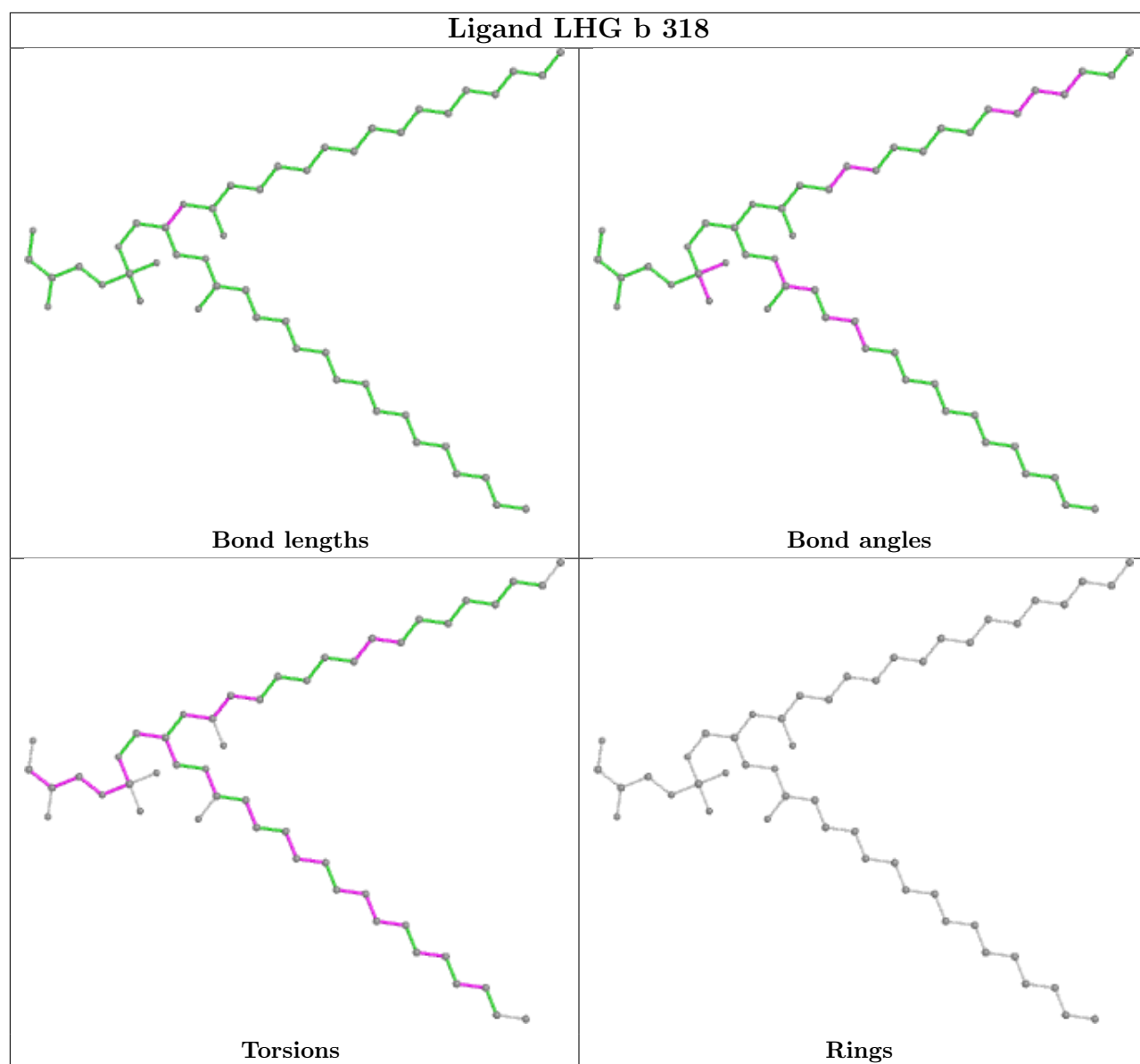


Ligand CLA k 601

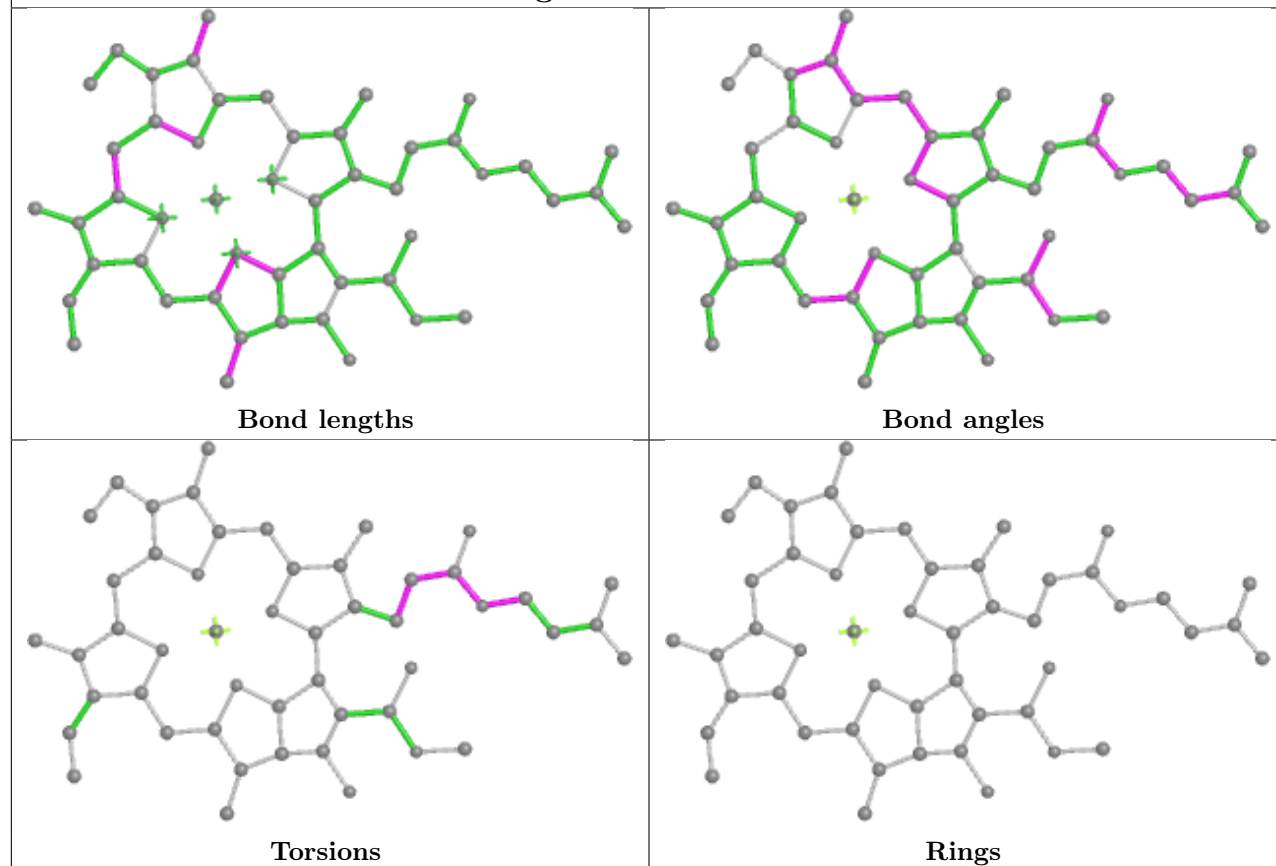


Ligand CLA j 309

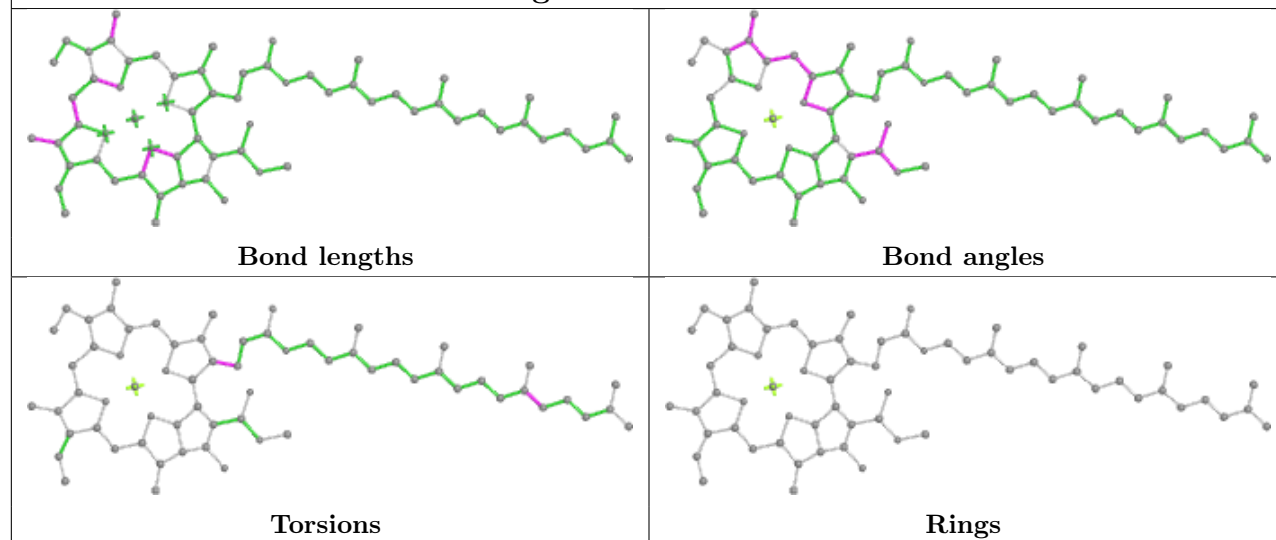


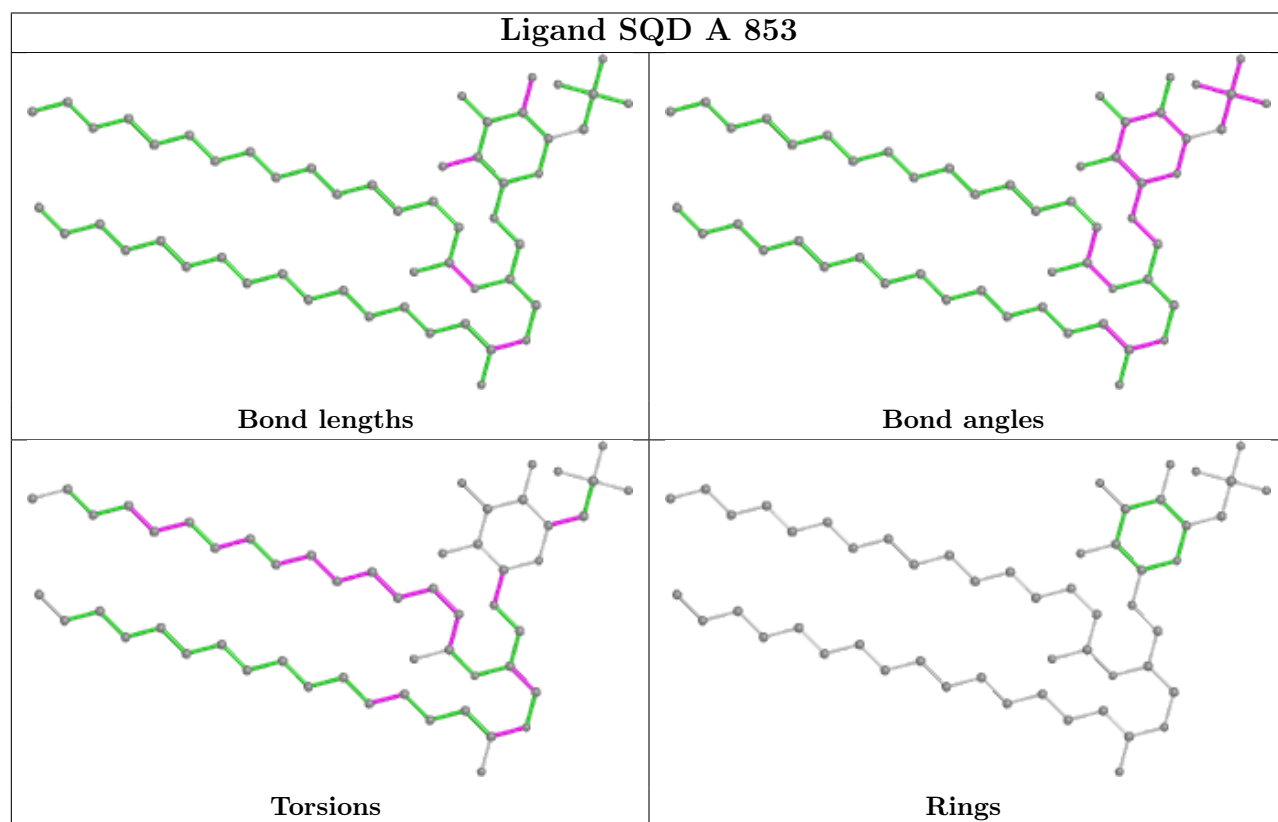
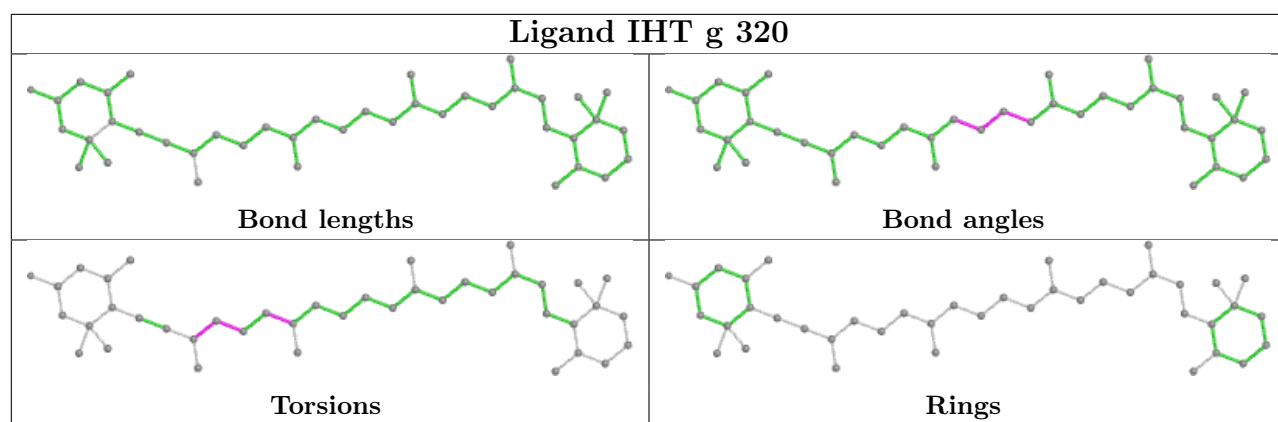


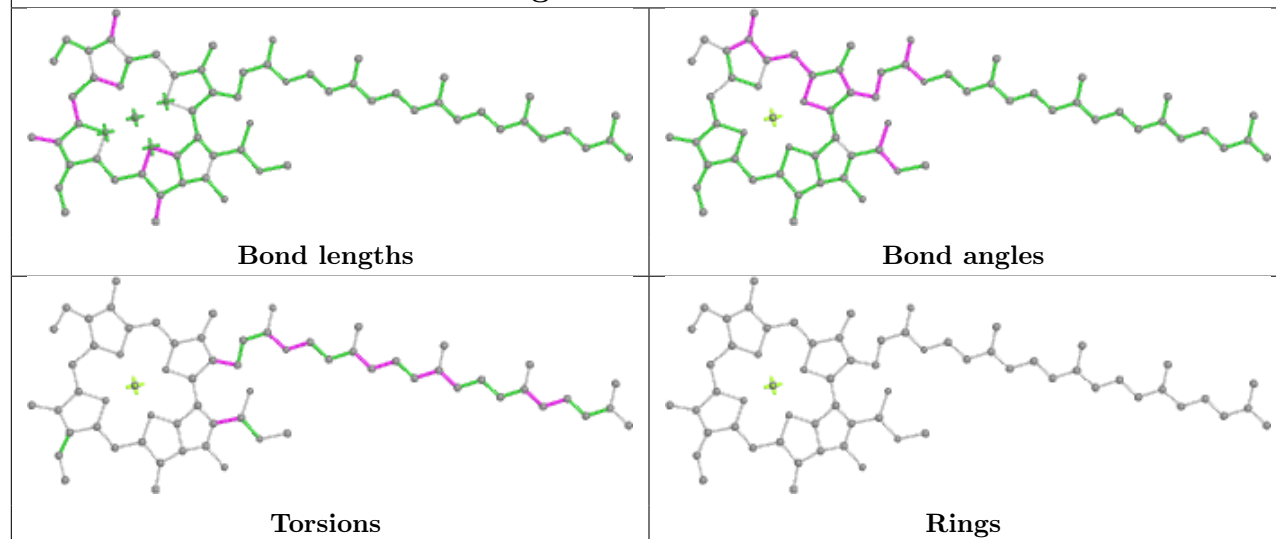
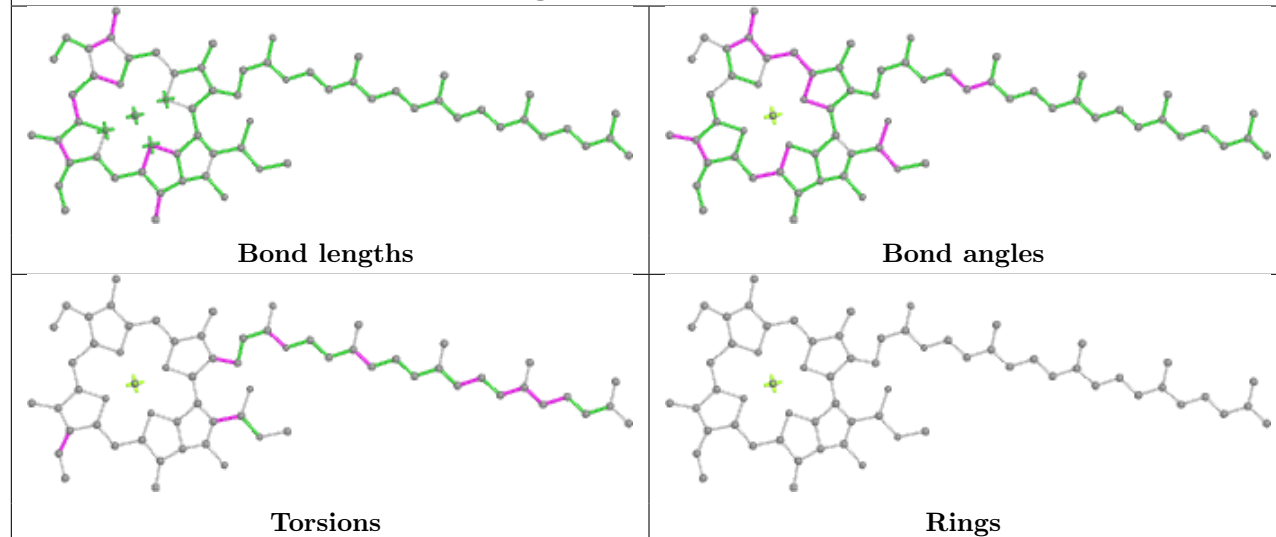
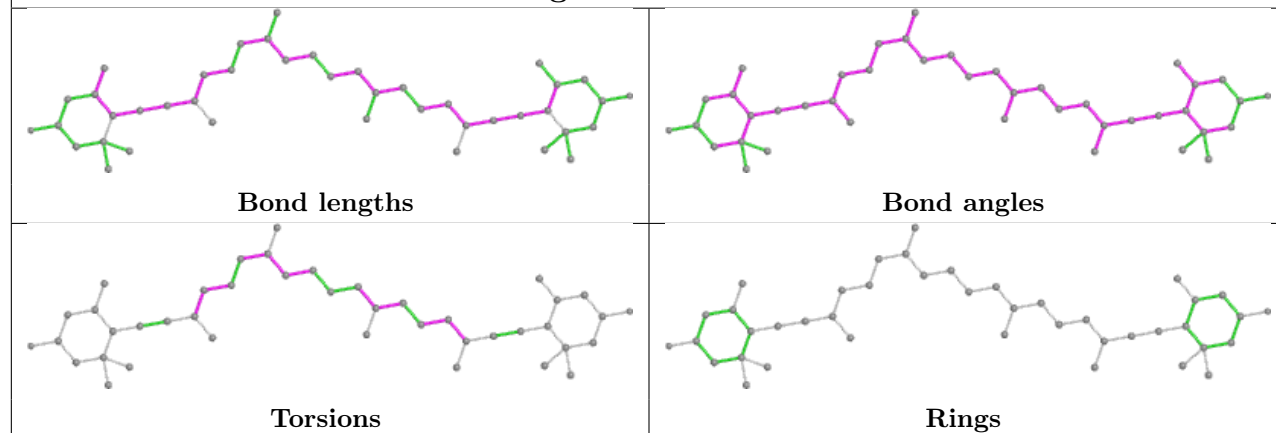
Ligand CLA h 303

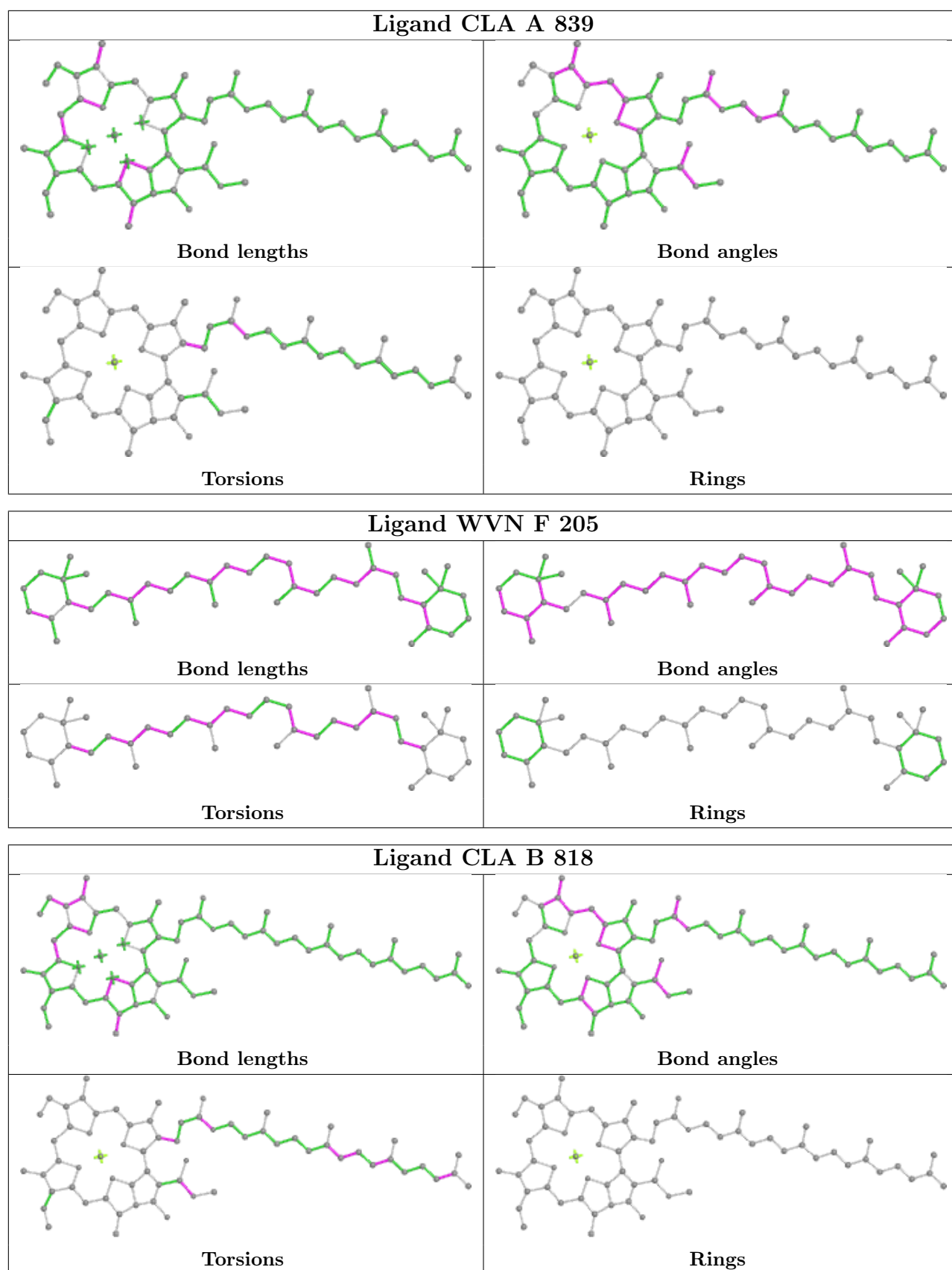


Ligand CLA B 824

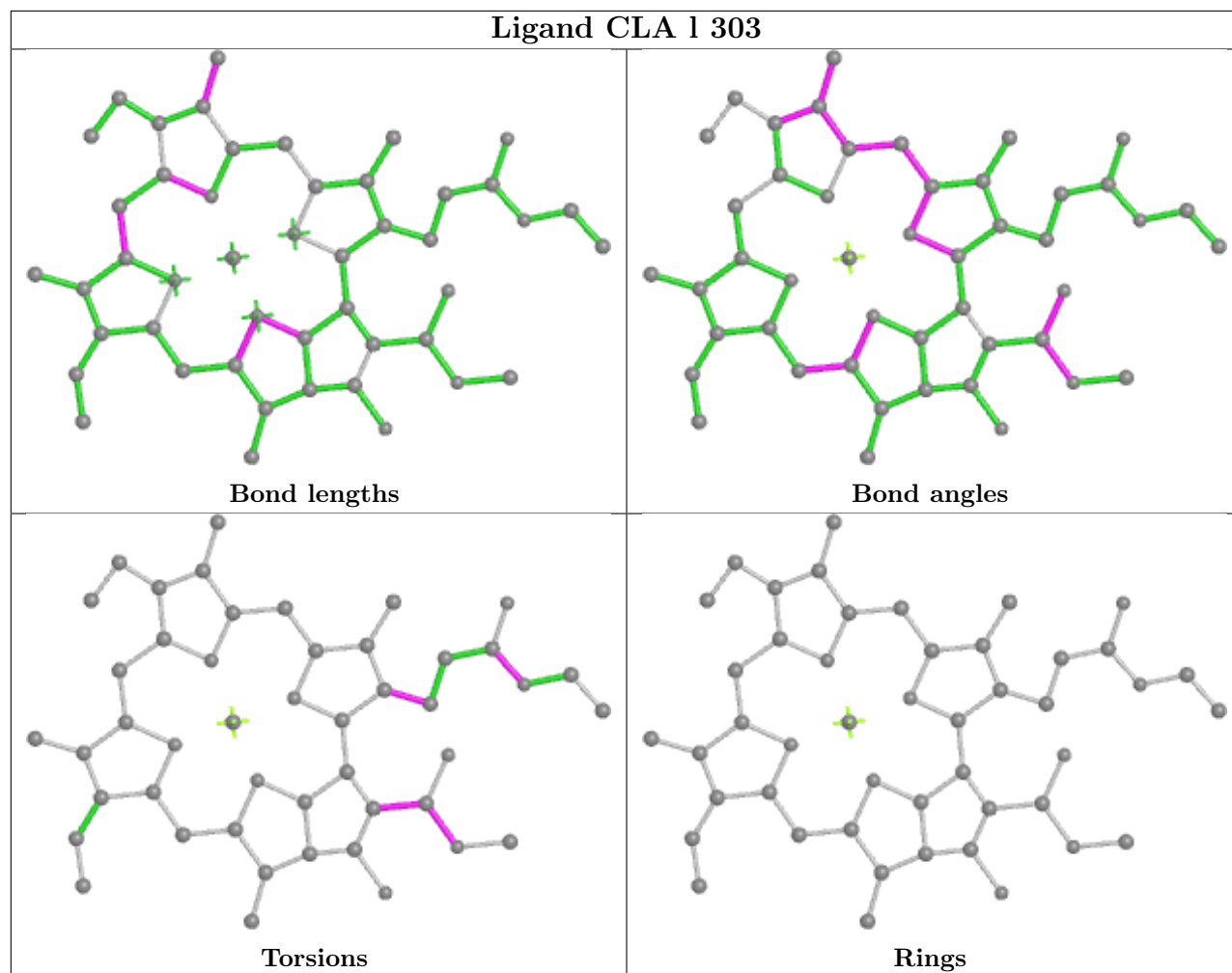




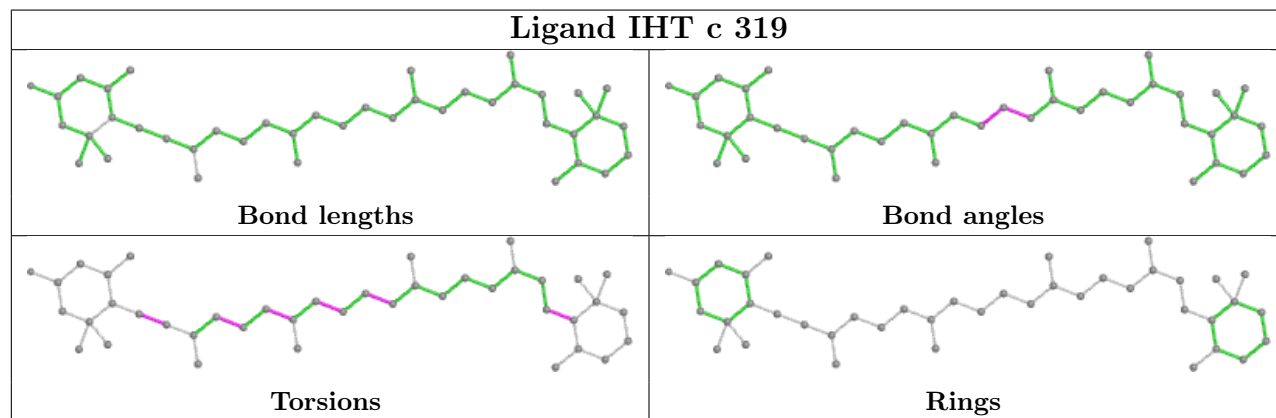
Ligand CLA A 816**Ligand CLA A 818****Ligand II0 b 314**



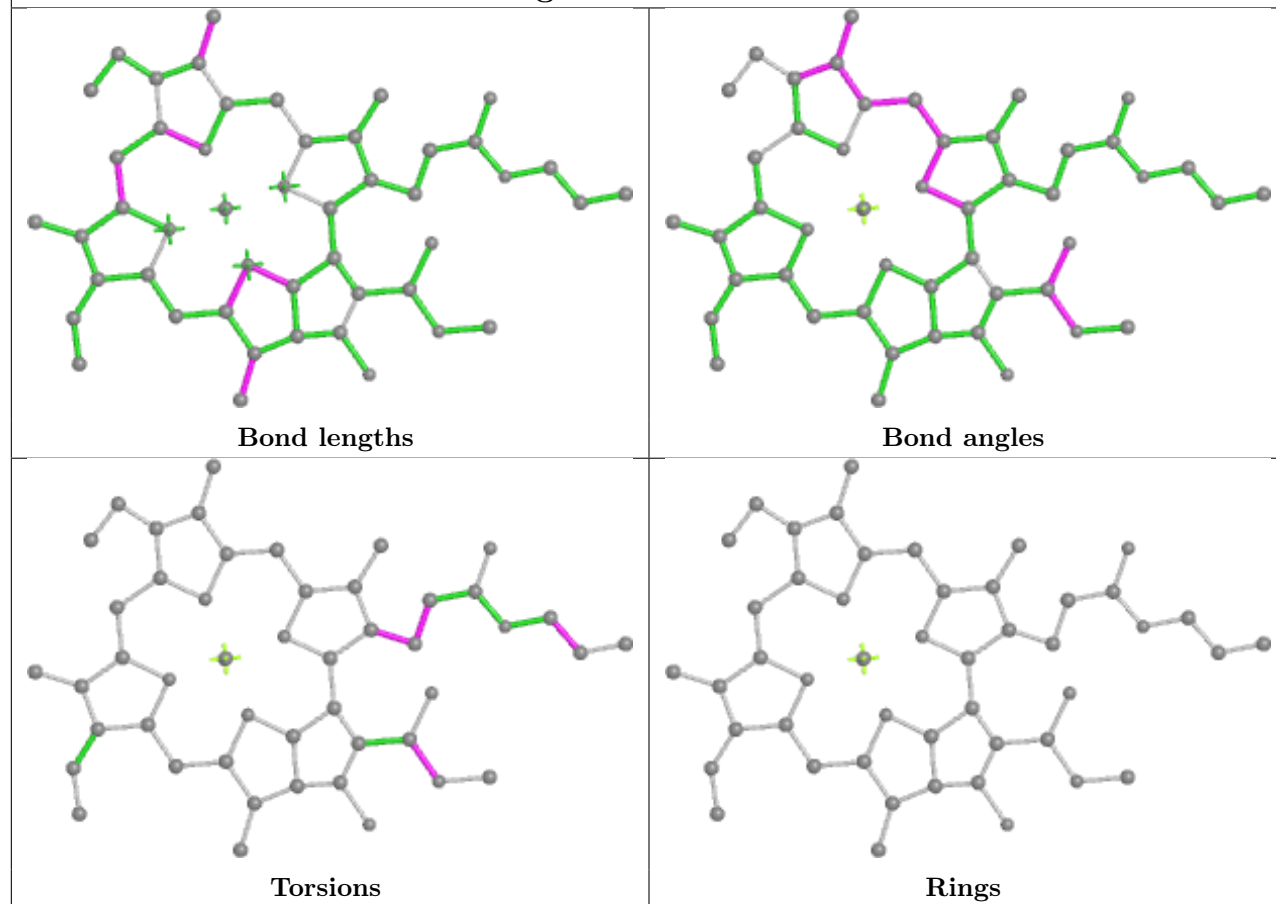
Ligand CLA l 303



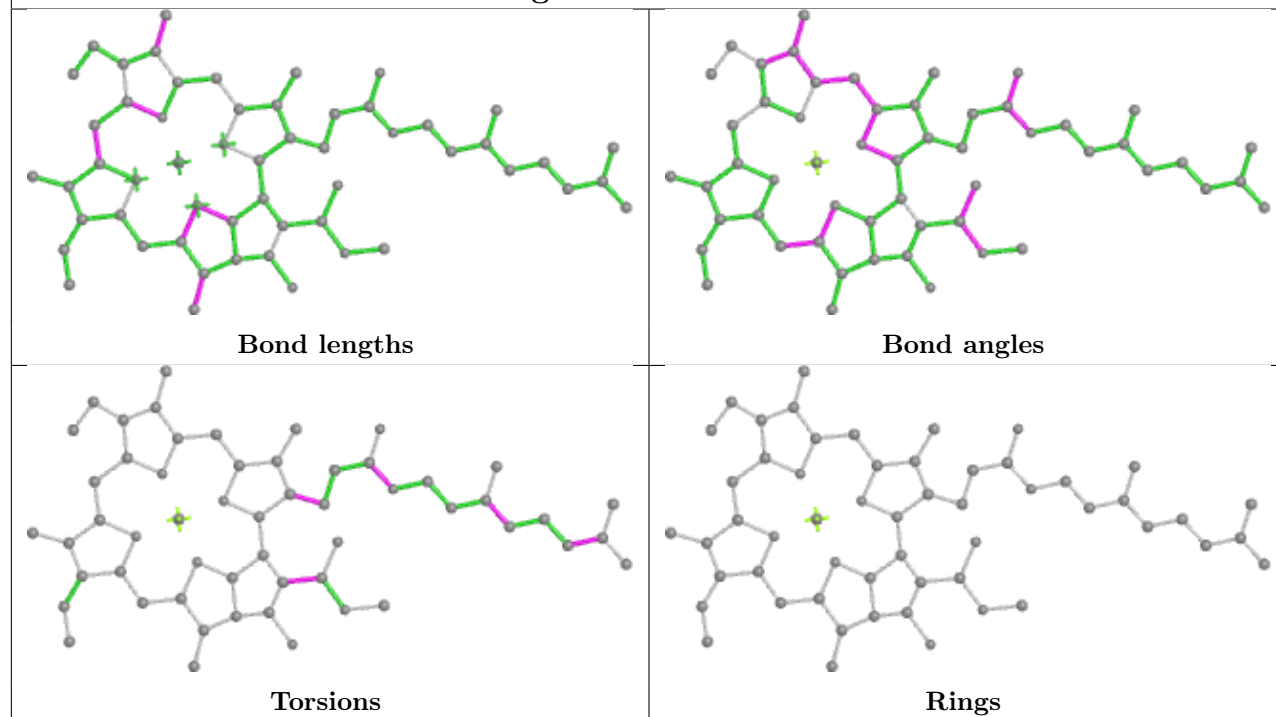
Ligand IHT c 319



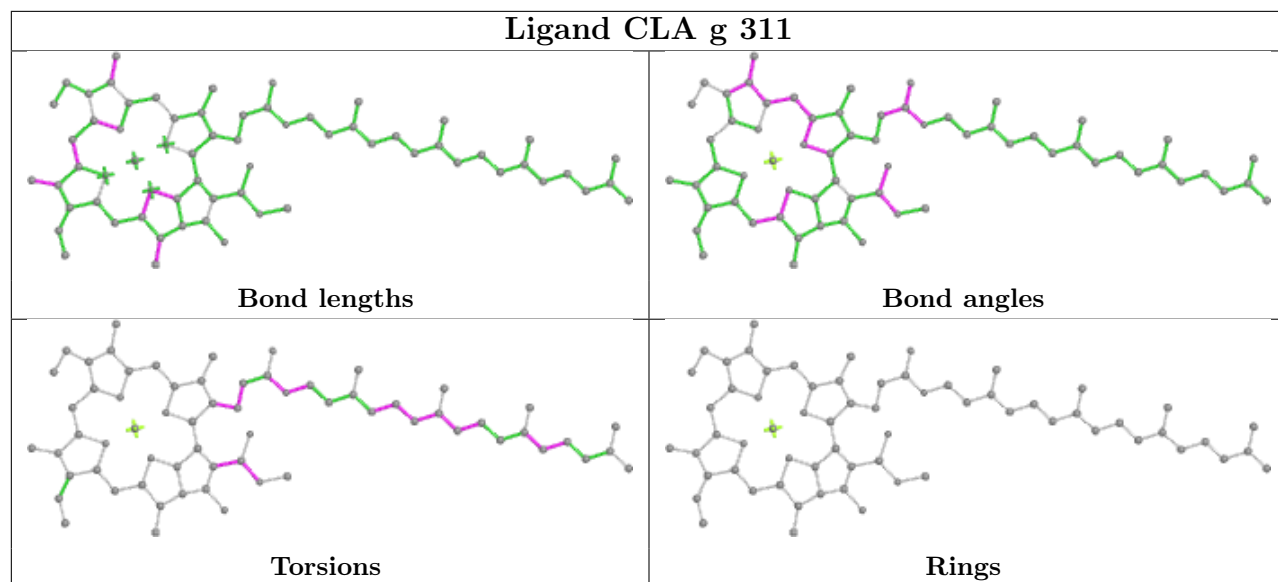
Ligand CLA a 312



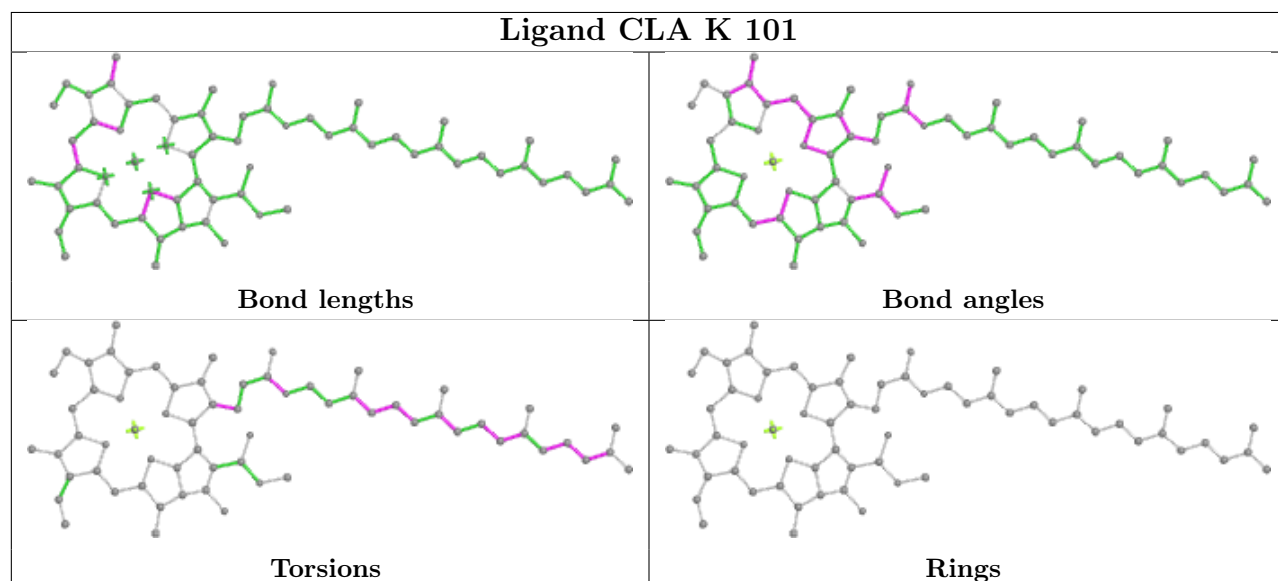
Ligand CLA A 803



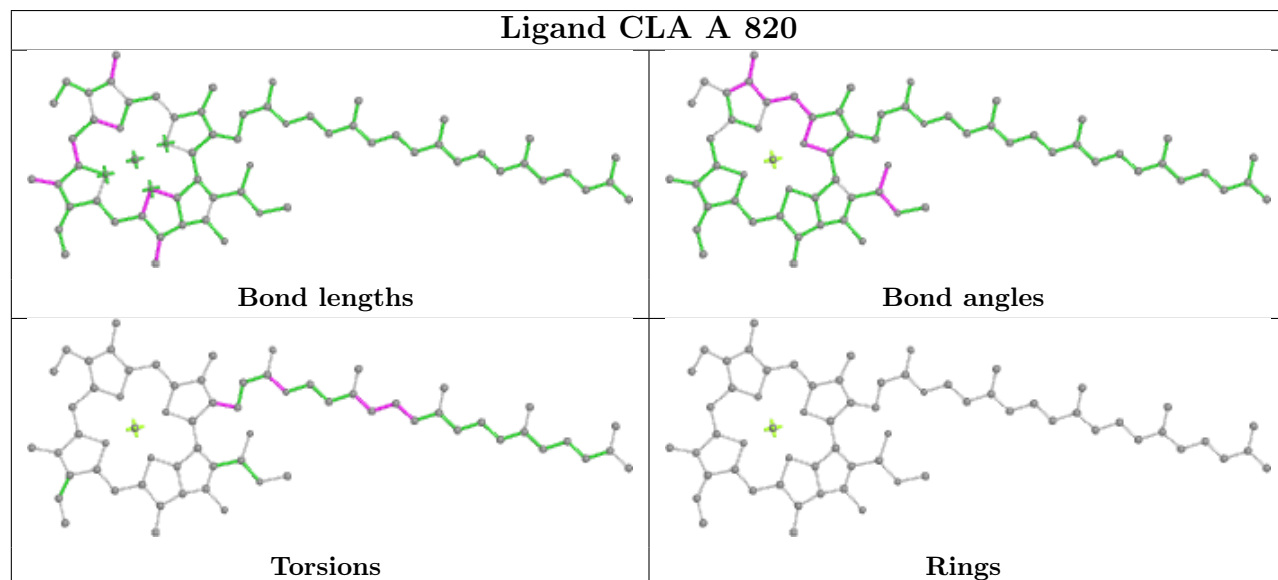
Ligand CLA g 311

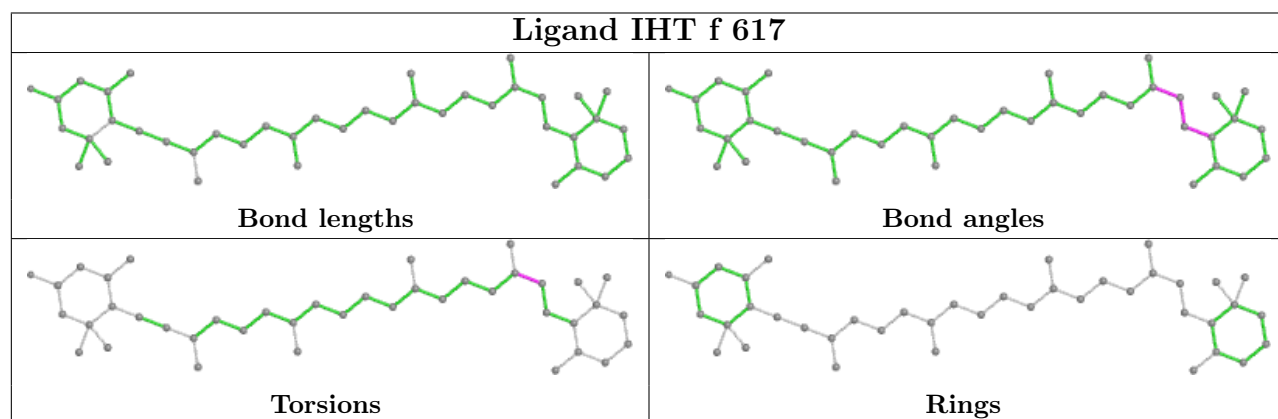
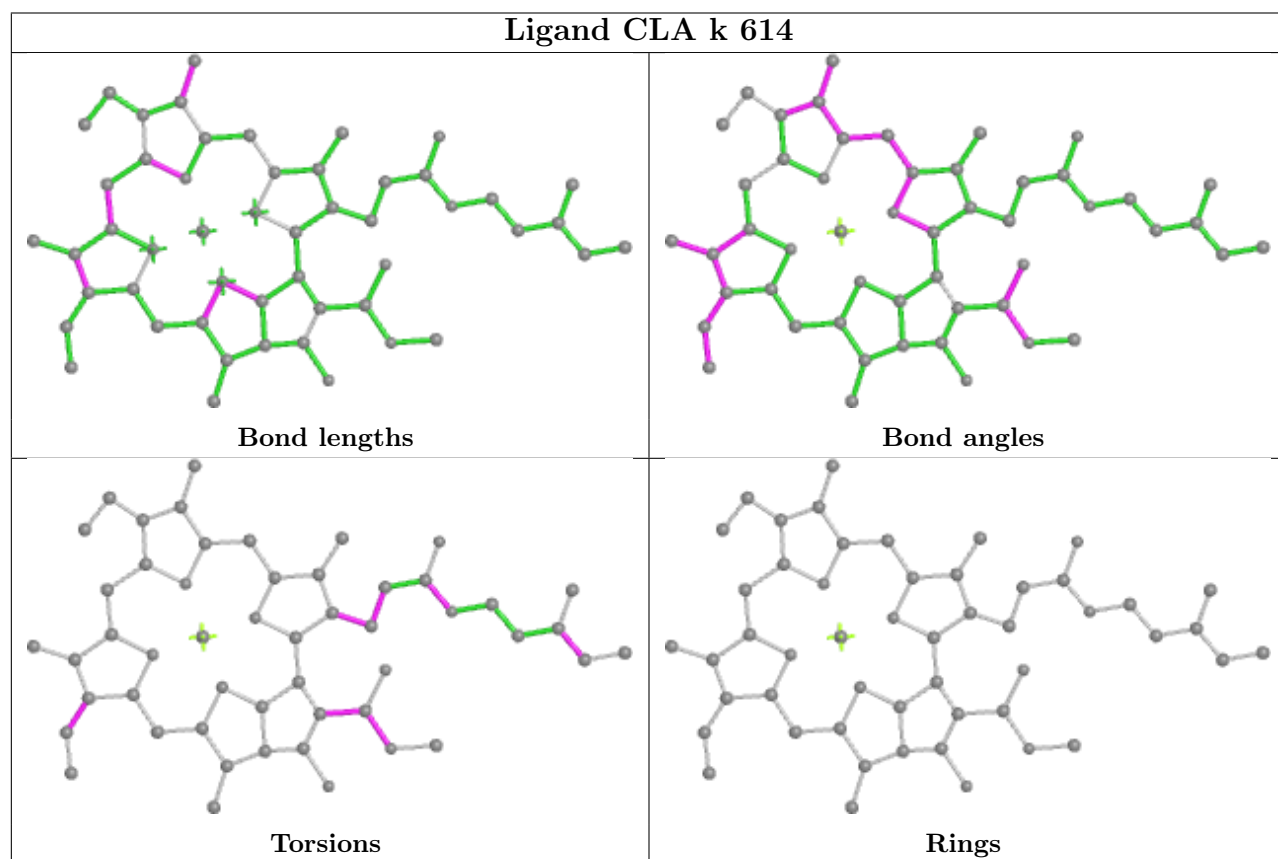
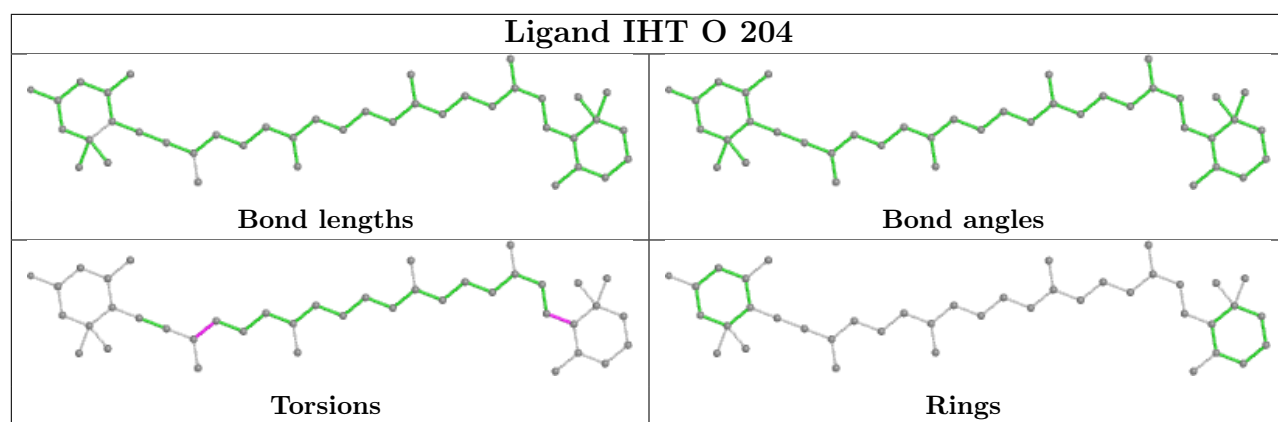


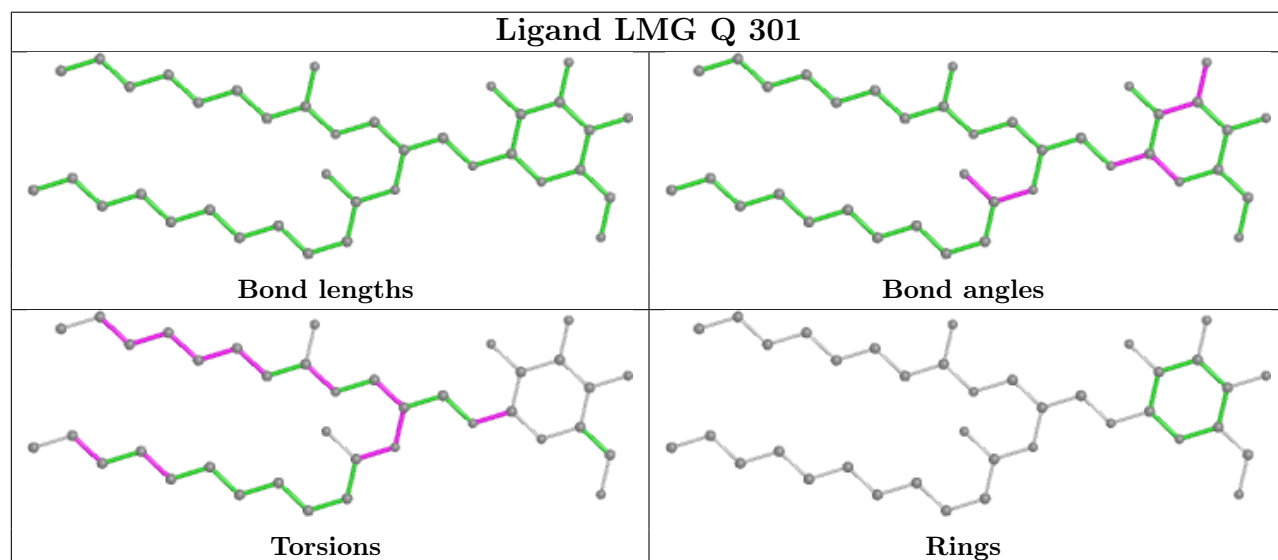
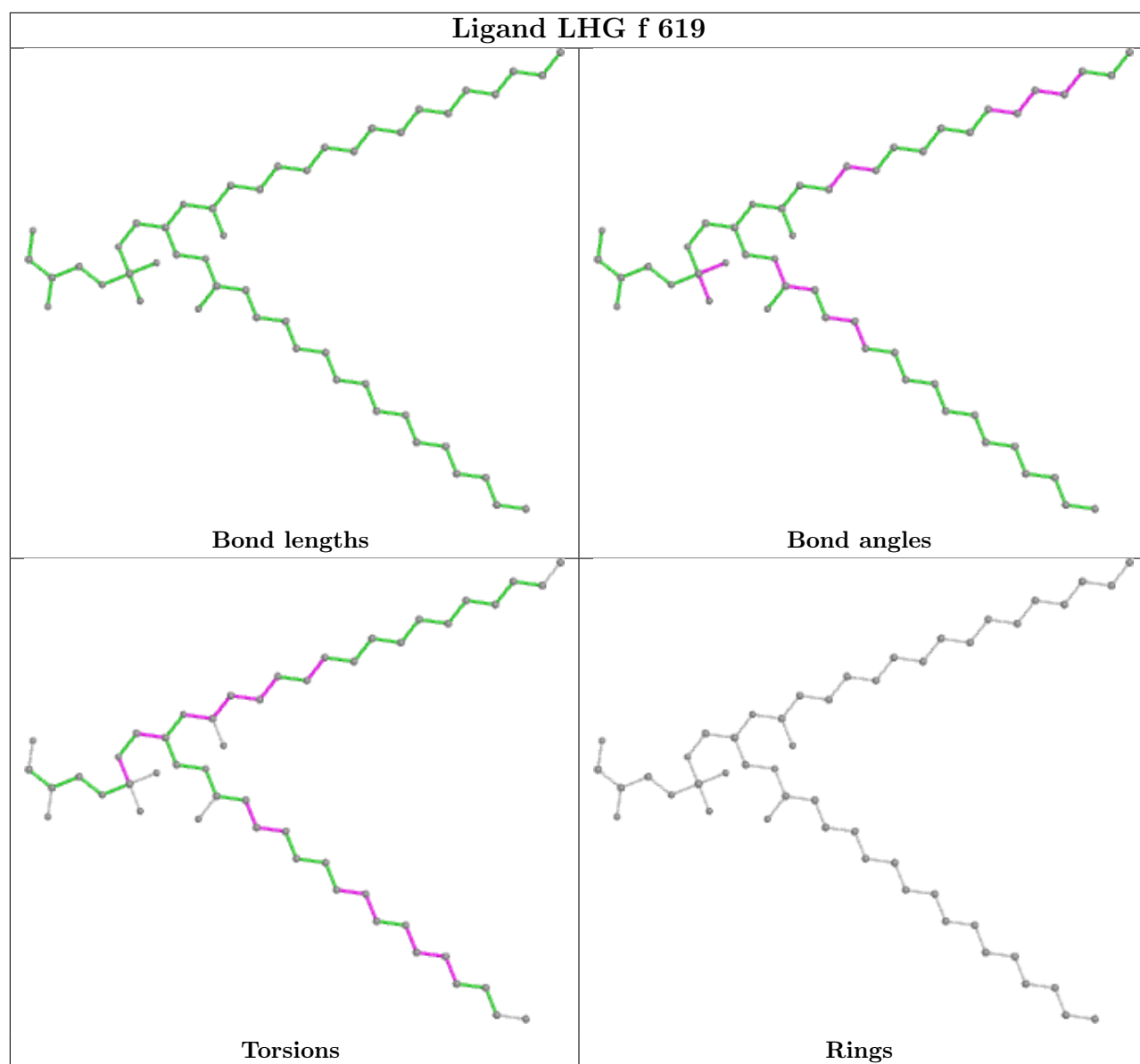
Ligand CLA K 101



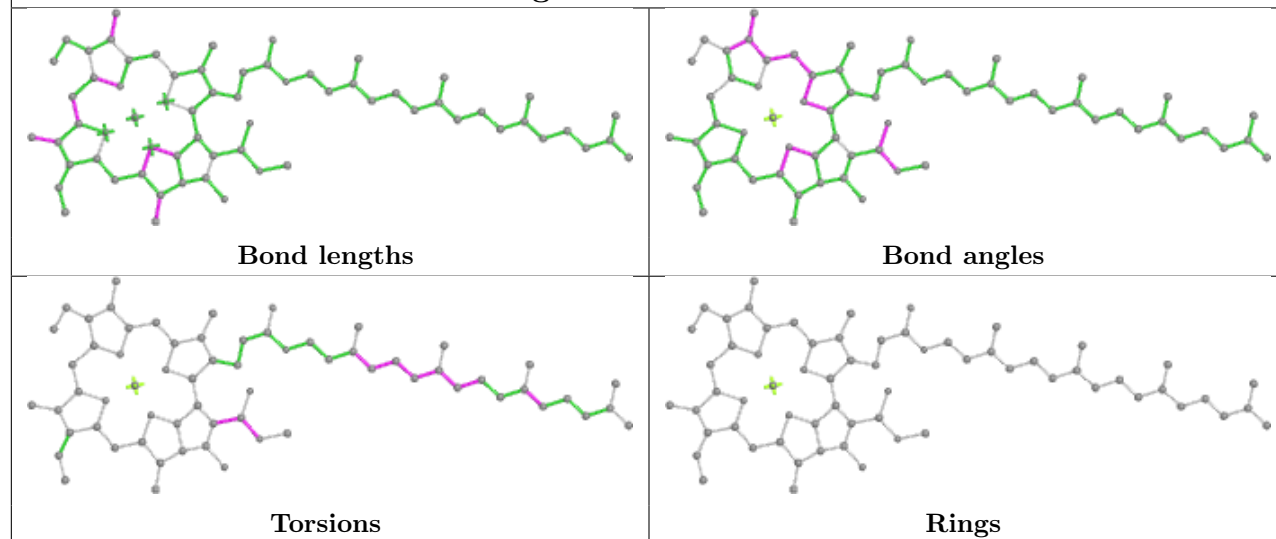
Ligand CLA A 820



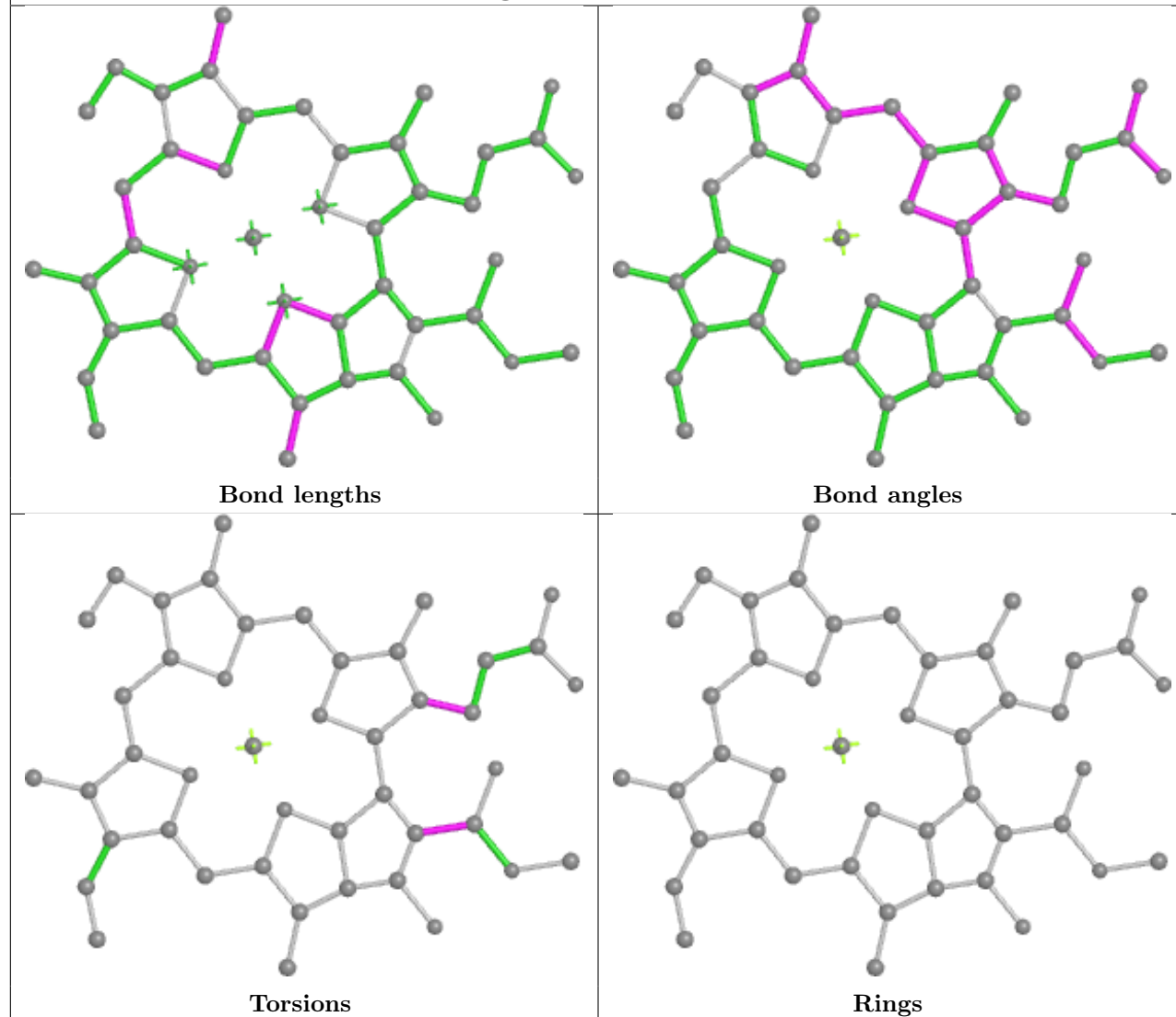


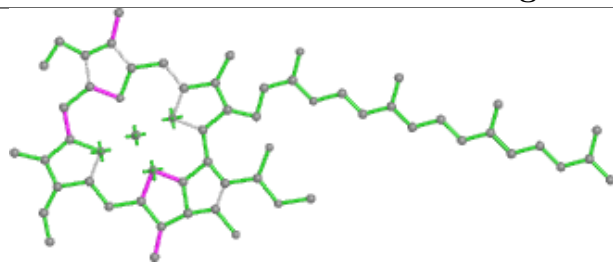


Ligand CLA B 803

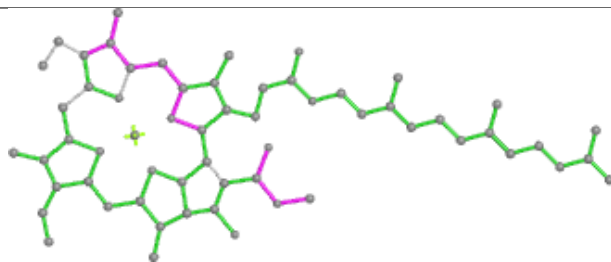


Ligand CLA f 605

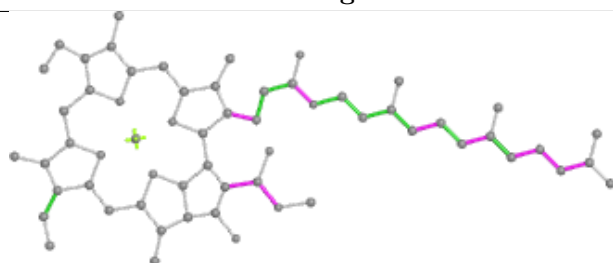


Ligand CLA c 302

Bond lengths



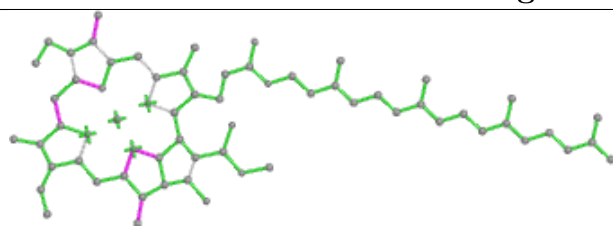
Bond angles



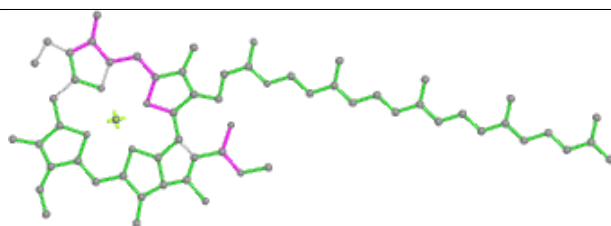
Torsions



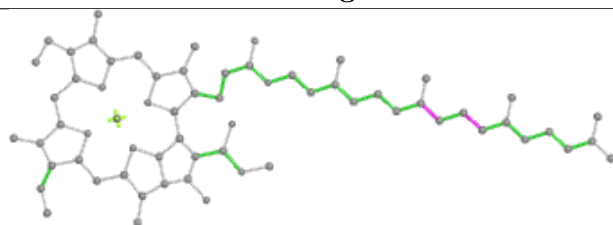
Rings

Ligand CLA b 309

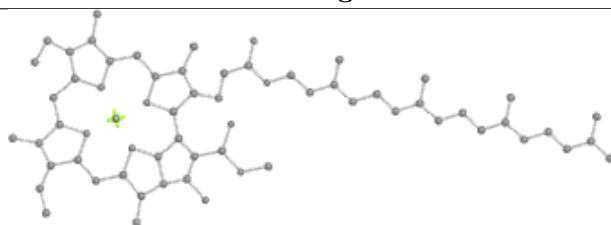
Bond lengths



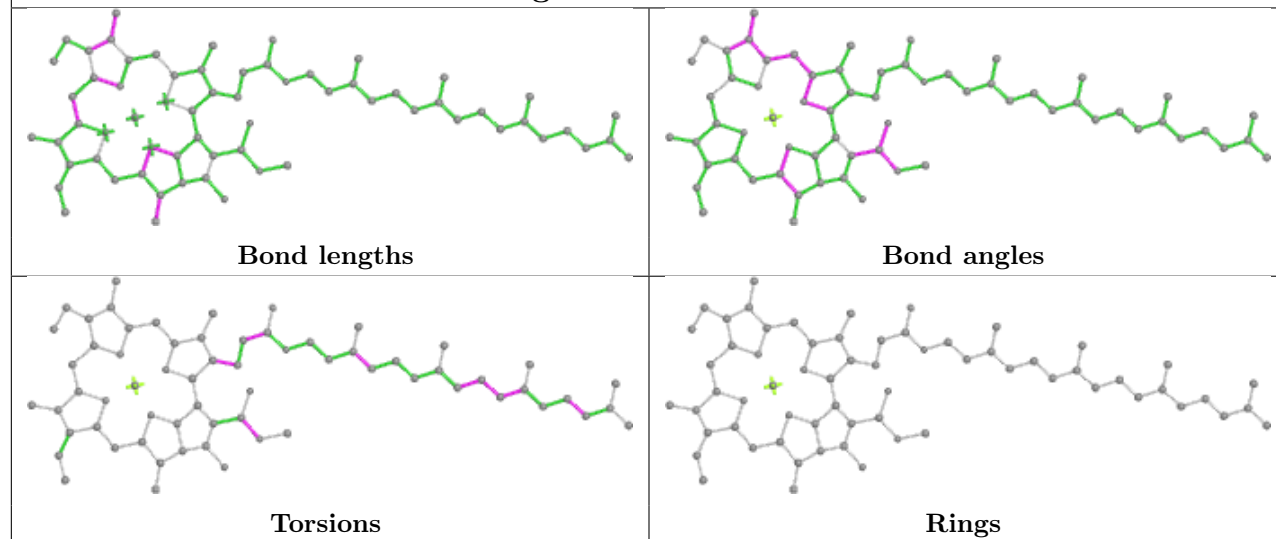
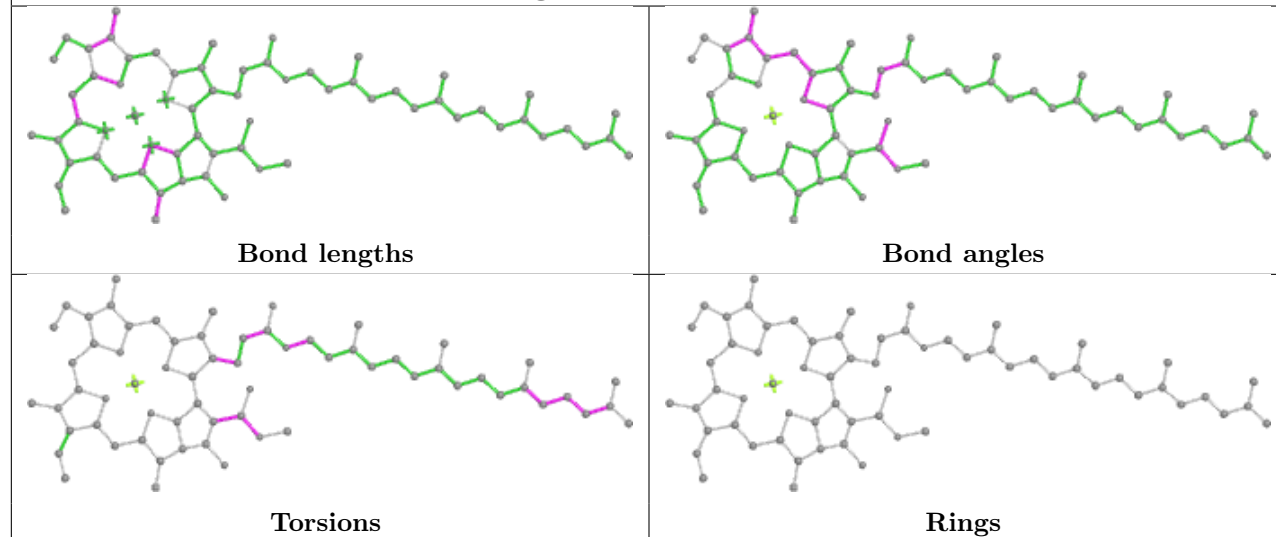
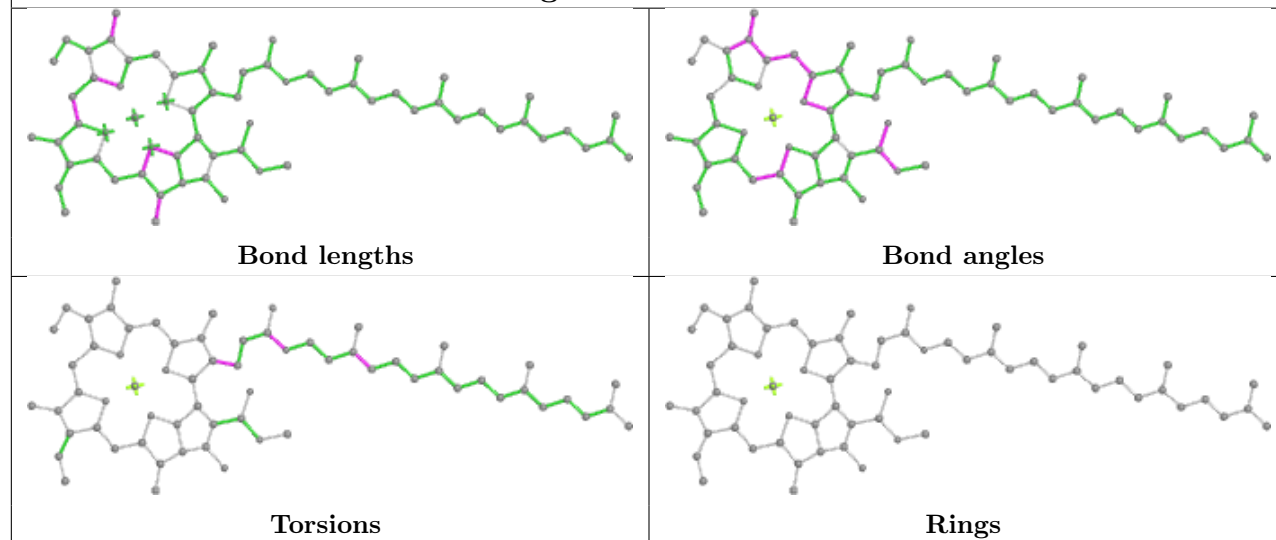
Bond angles



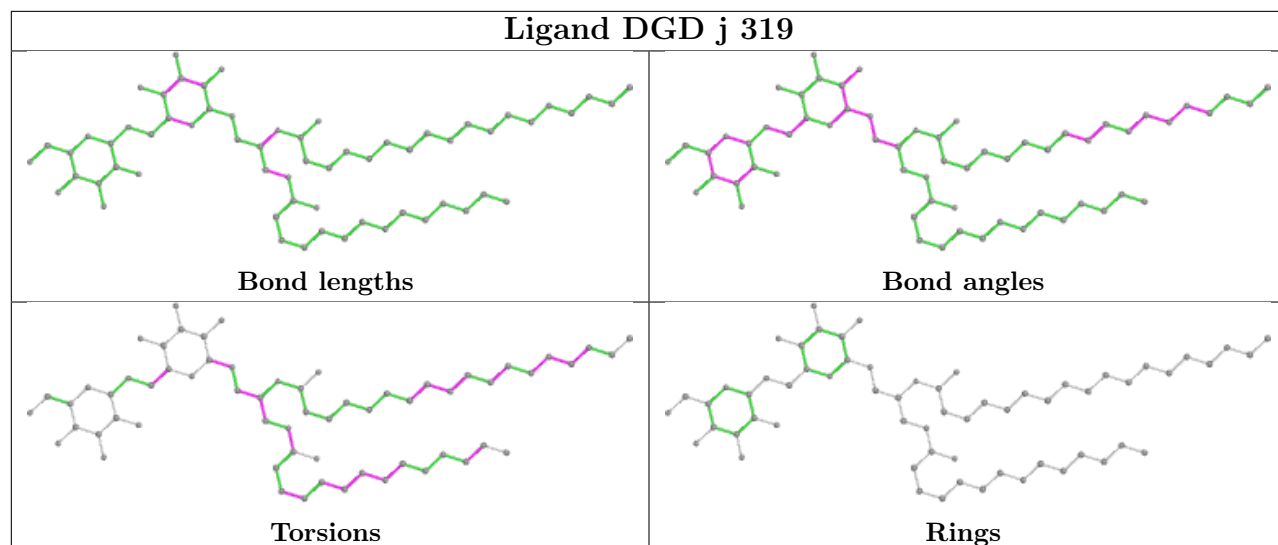
Torsions



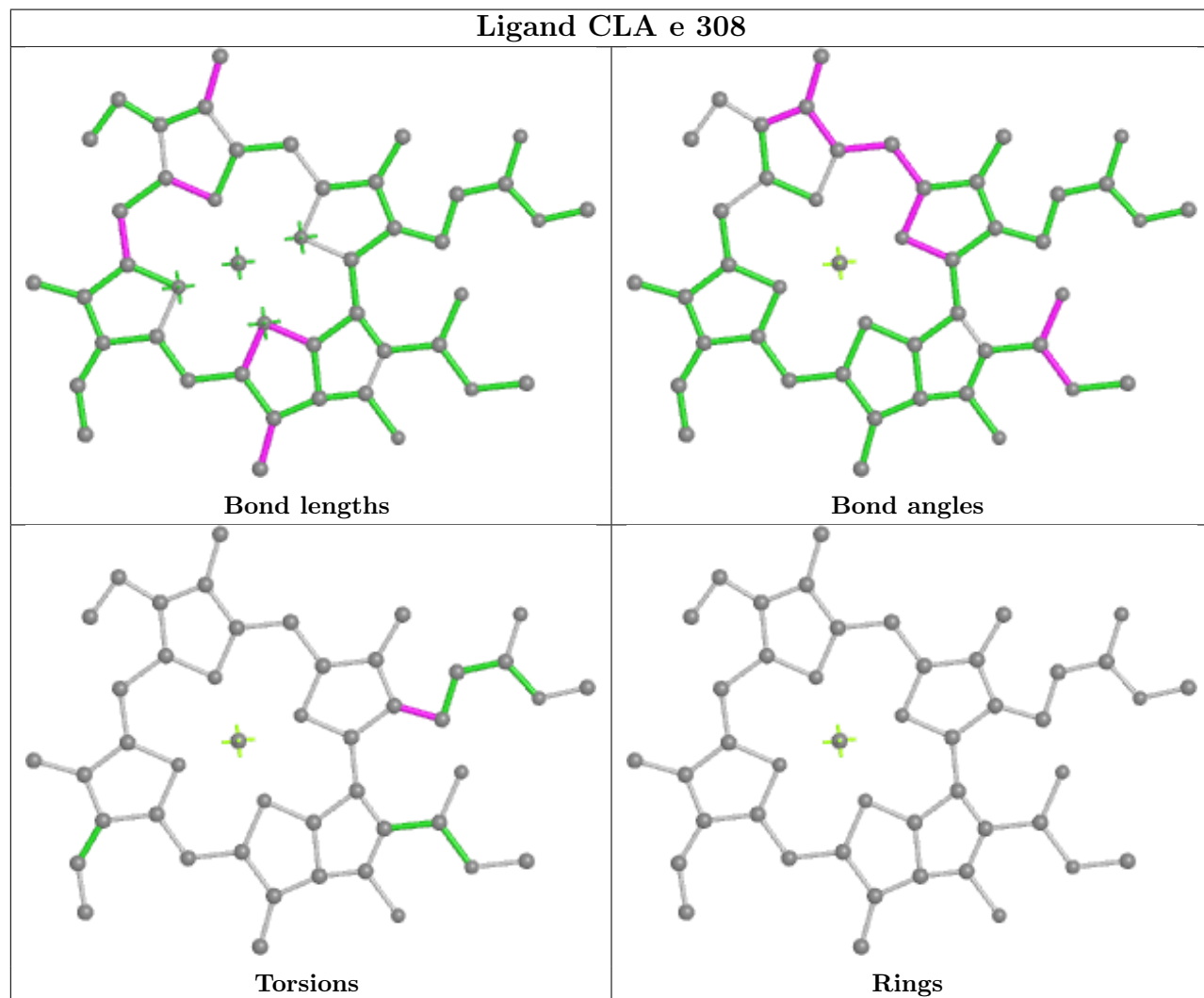
Rings

Ligand CLA B 820**Ligand CLA B 837****Ligand CLA I 308**

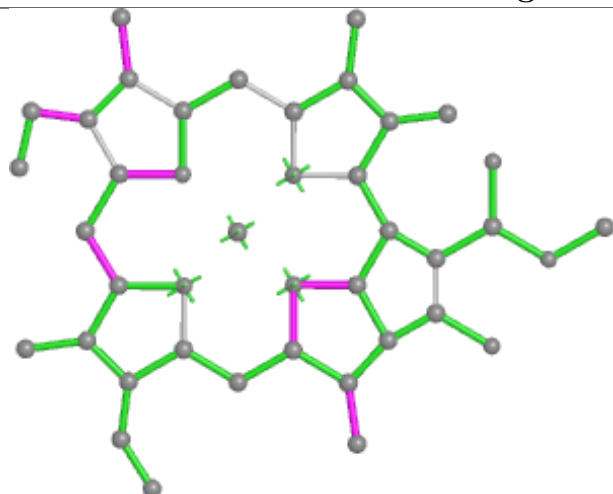
Ligand DGD j 319



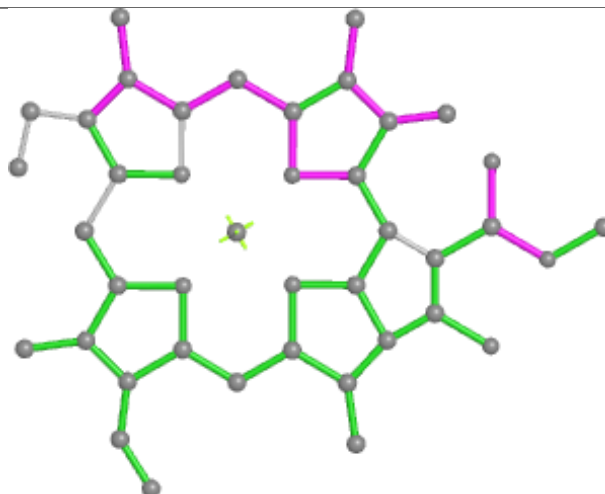
Ligand CLA e 308



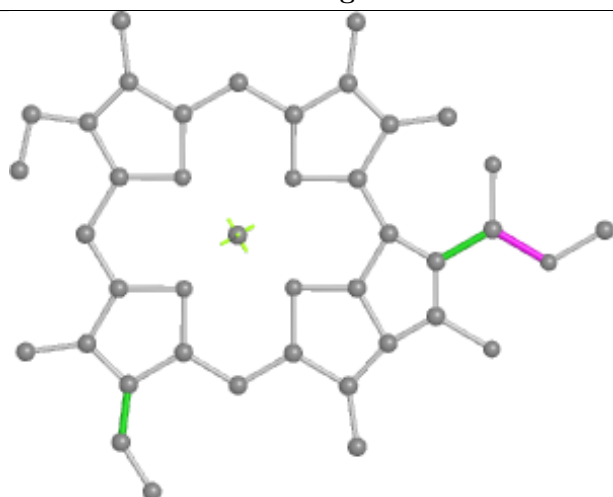
Ligand CLA d 309



Bond lengths



Bond angles

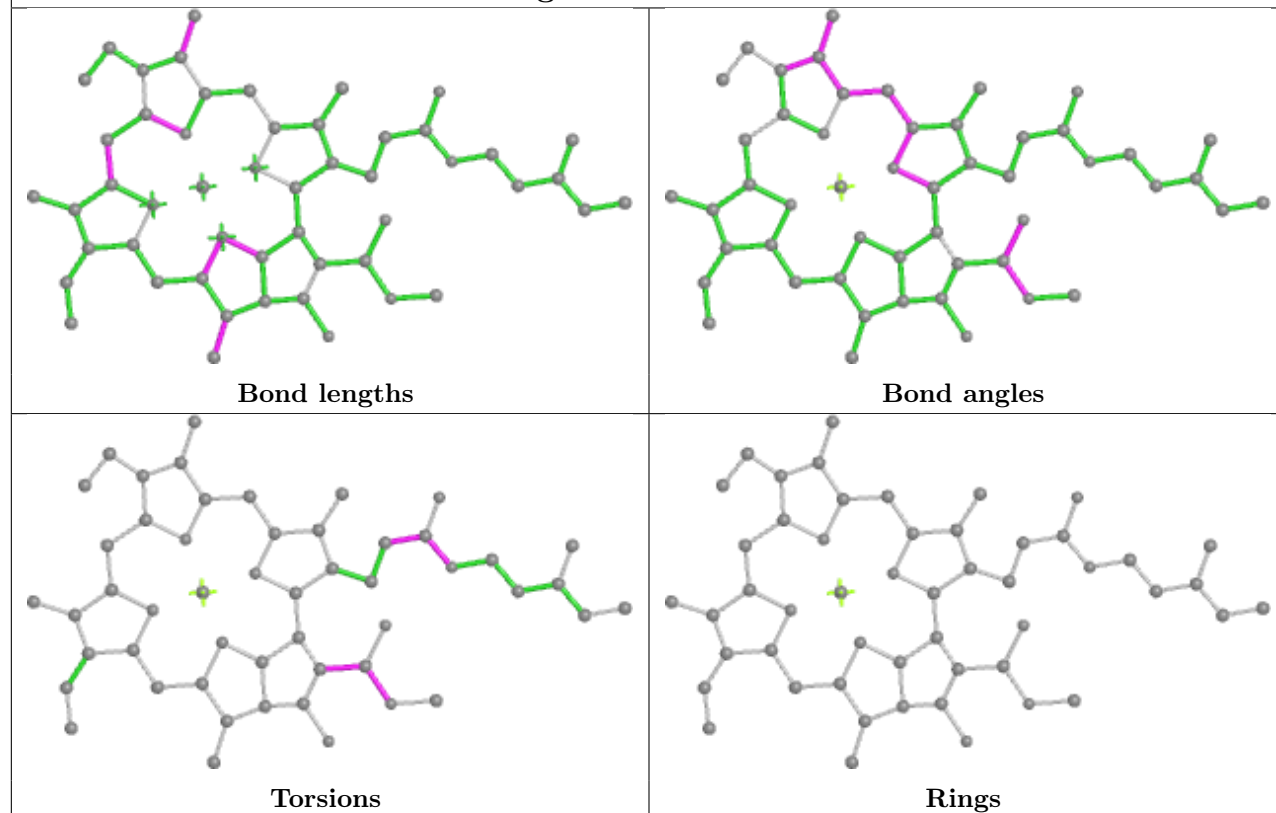


Torsions

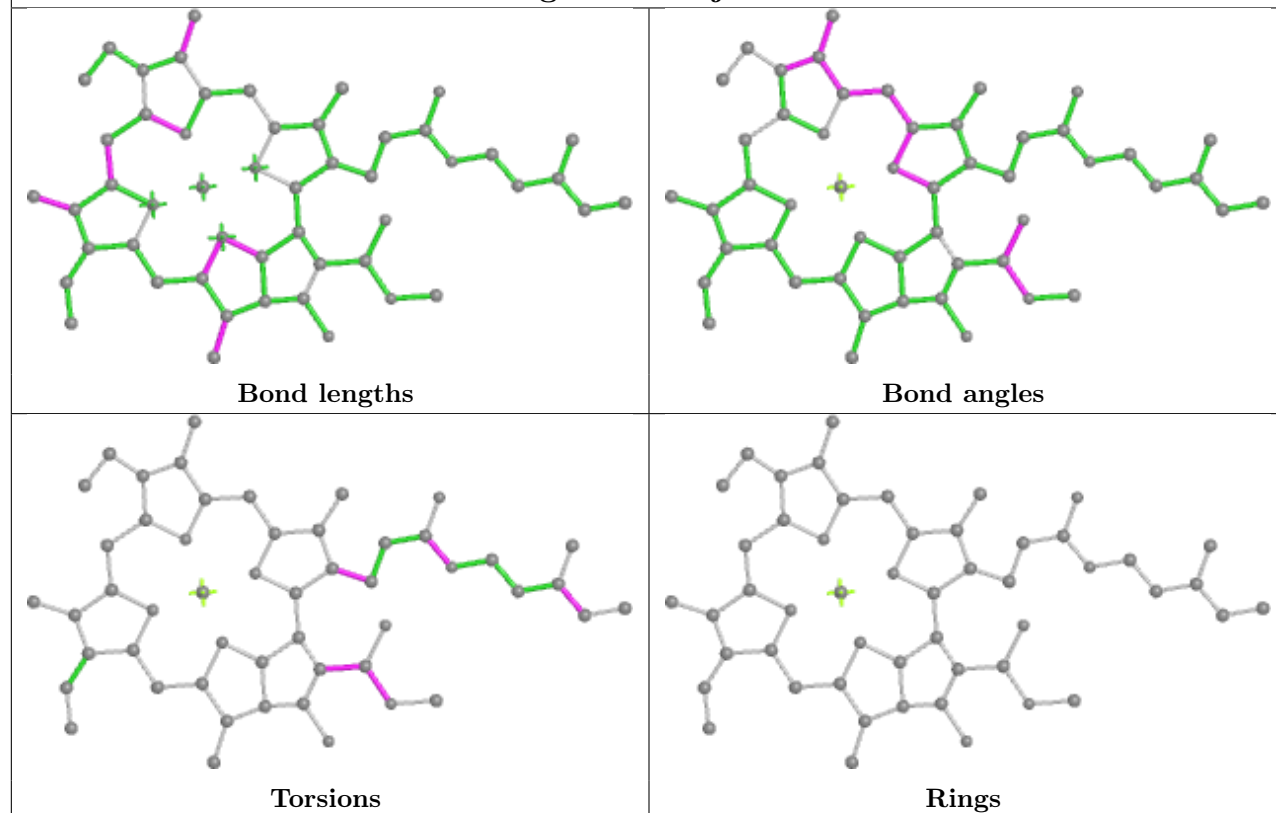


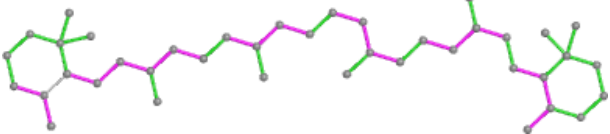
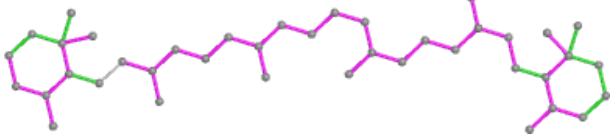
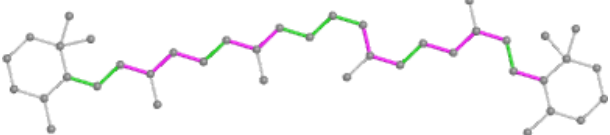
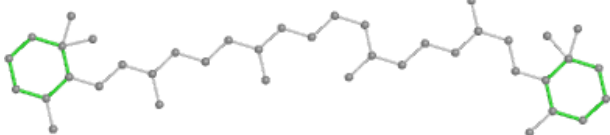
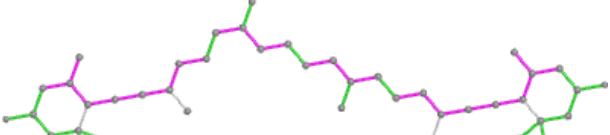
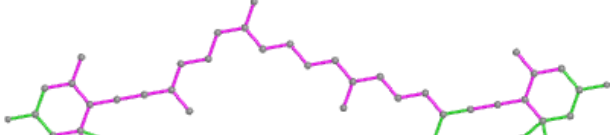
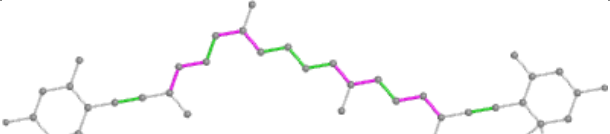
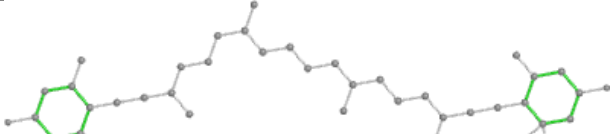
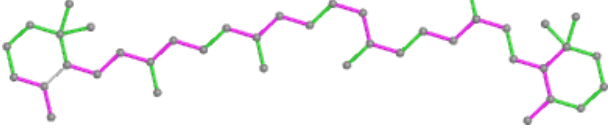
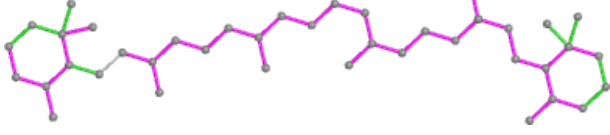
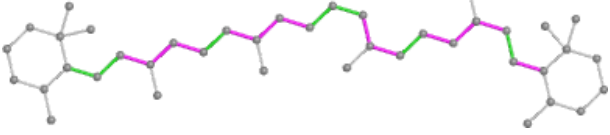
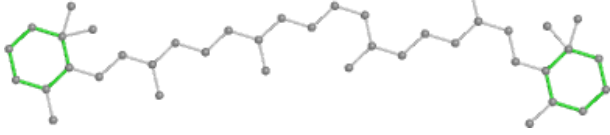
Rings

Ligand CLA e 303

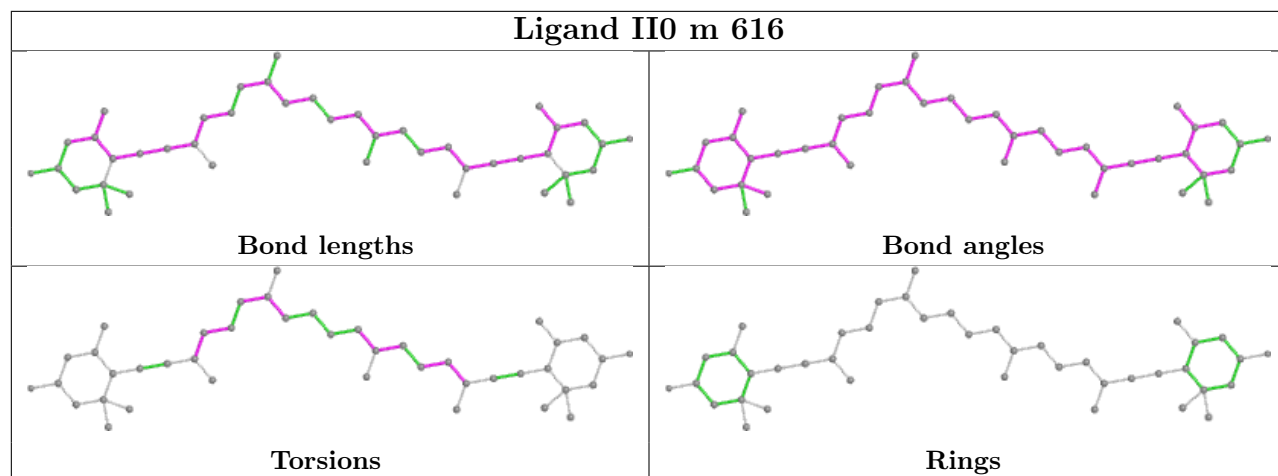


Ligand CLA j 313

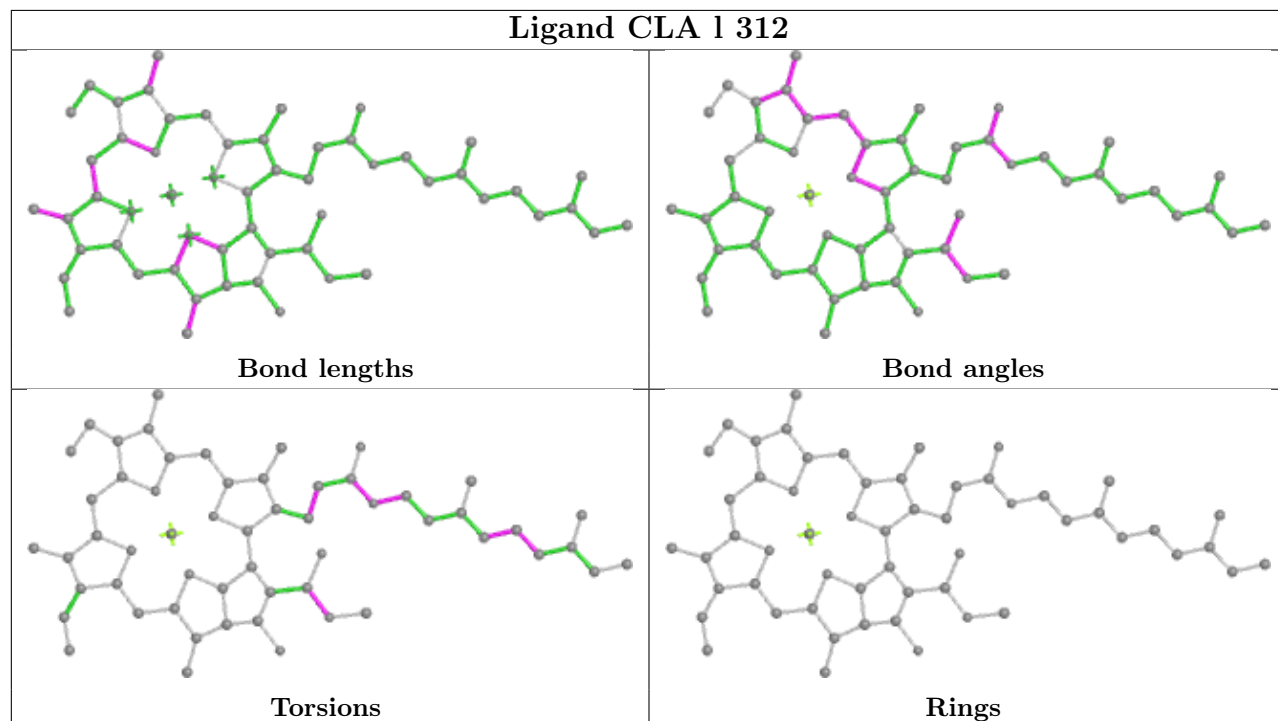


Ligand WVN e 315			
	Bond lengths		
Bond angles			
Torsions			
Rings			
Ligand II0 h 311			
	Bond lengths		
Bond angles			
Torsions			
Rings			
Ligand WVN h 308			
	Bond lengths		
Bond angles			
Torsions			
Rings			

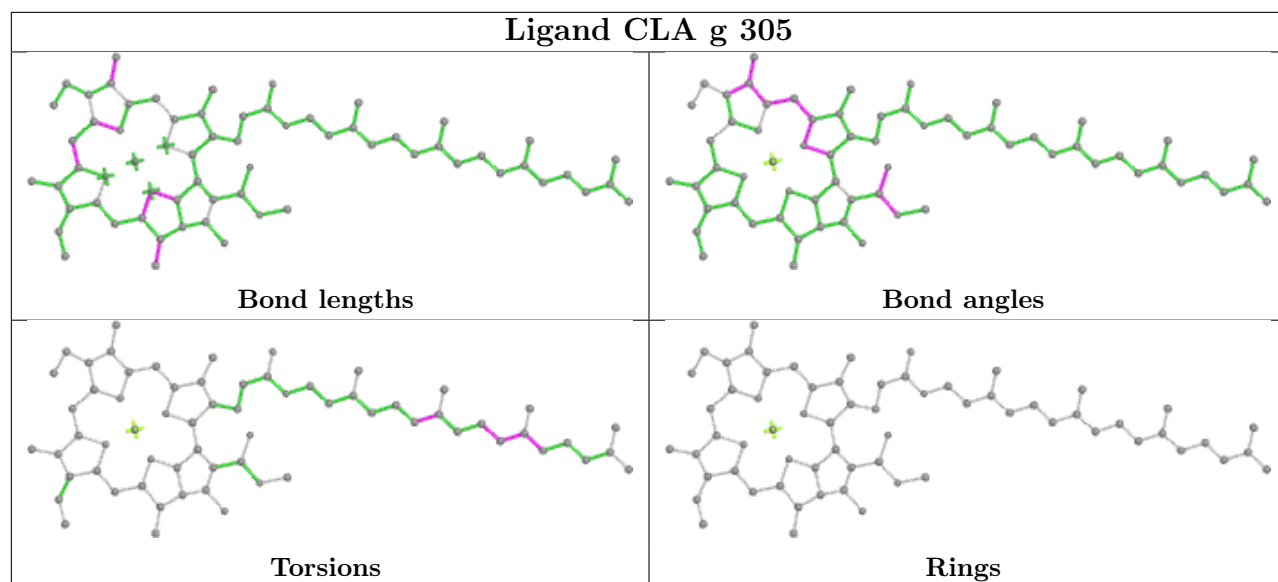
Ligand II0 m 616



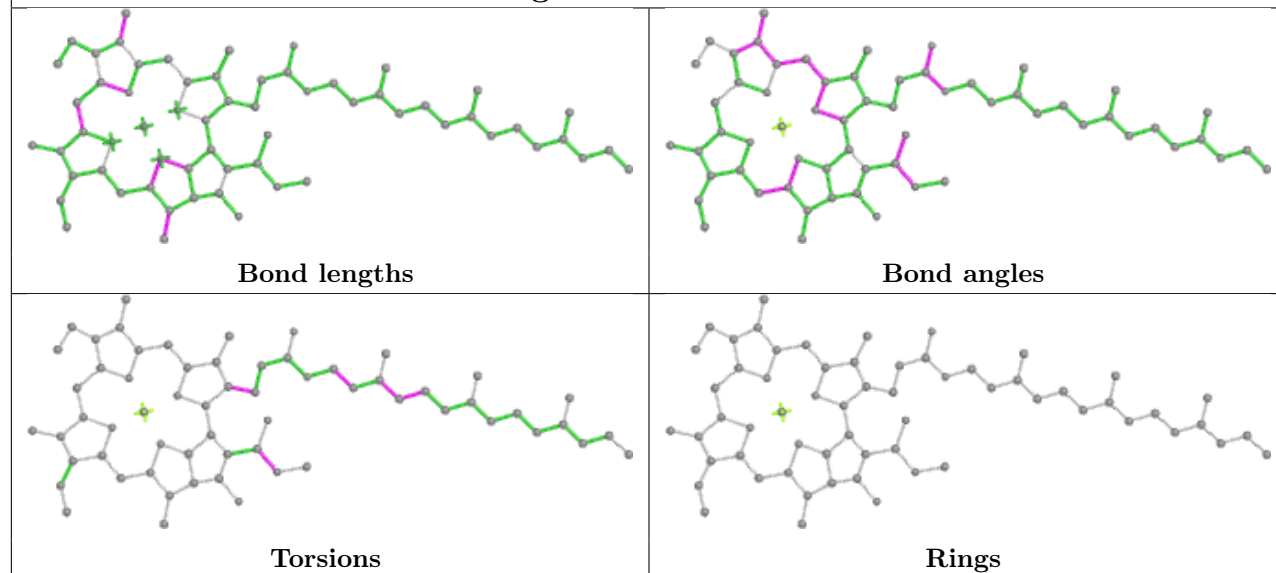
Ligand CLA l 312



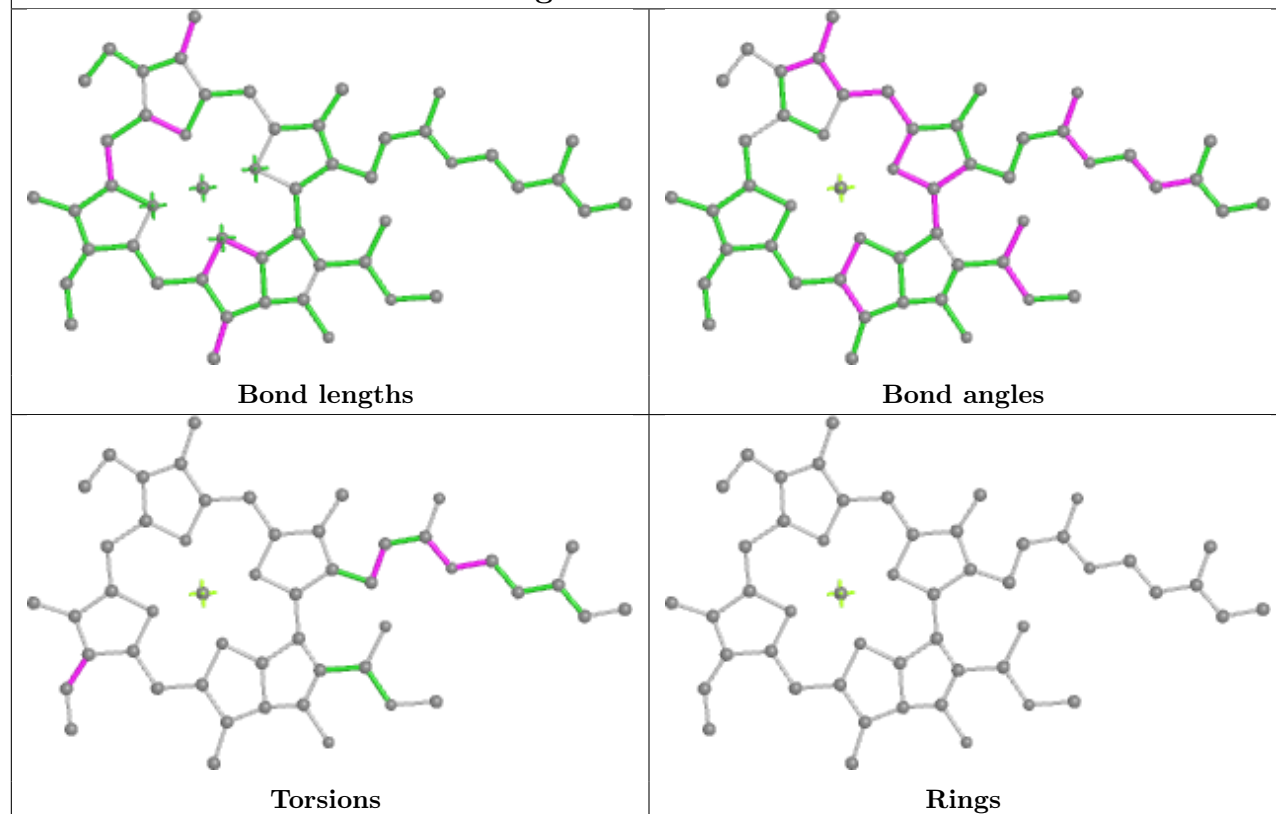
Ligand CLA g 305



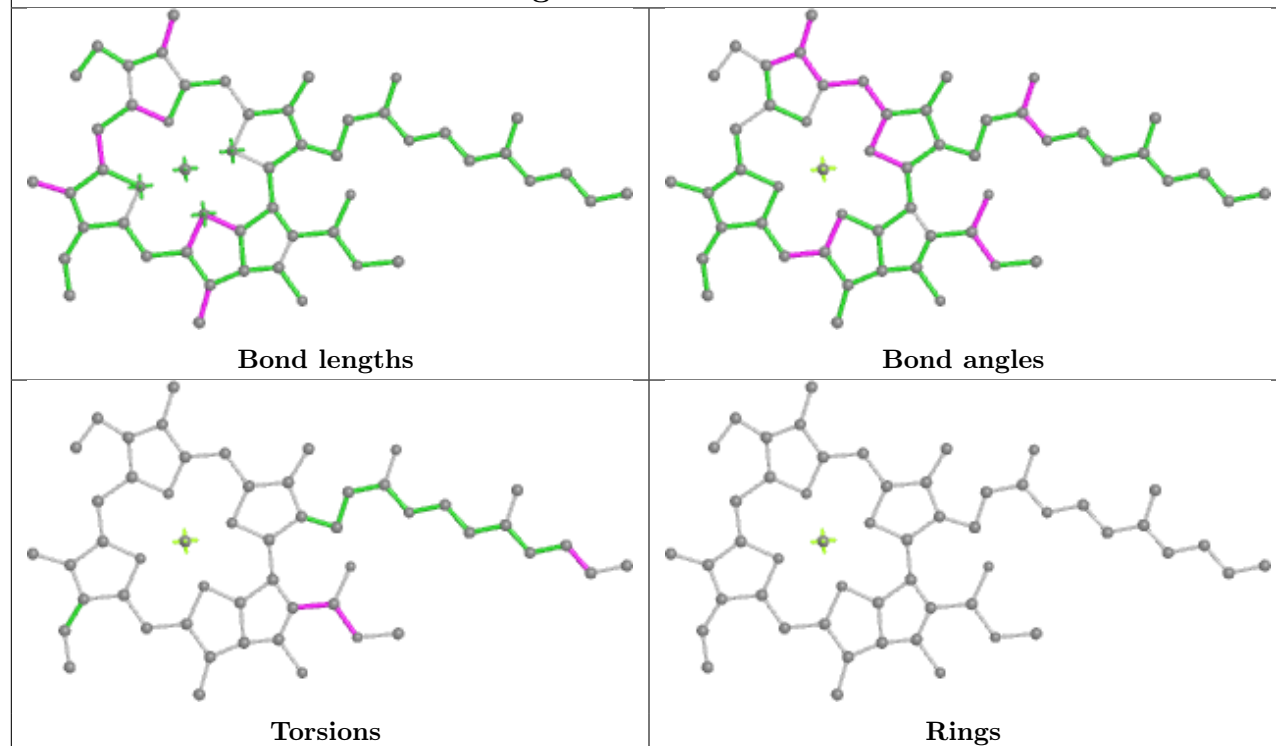
Ligand CLA A 827



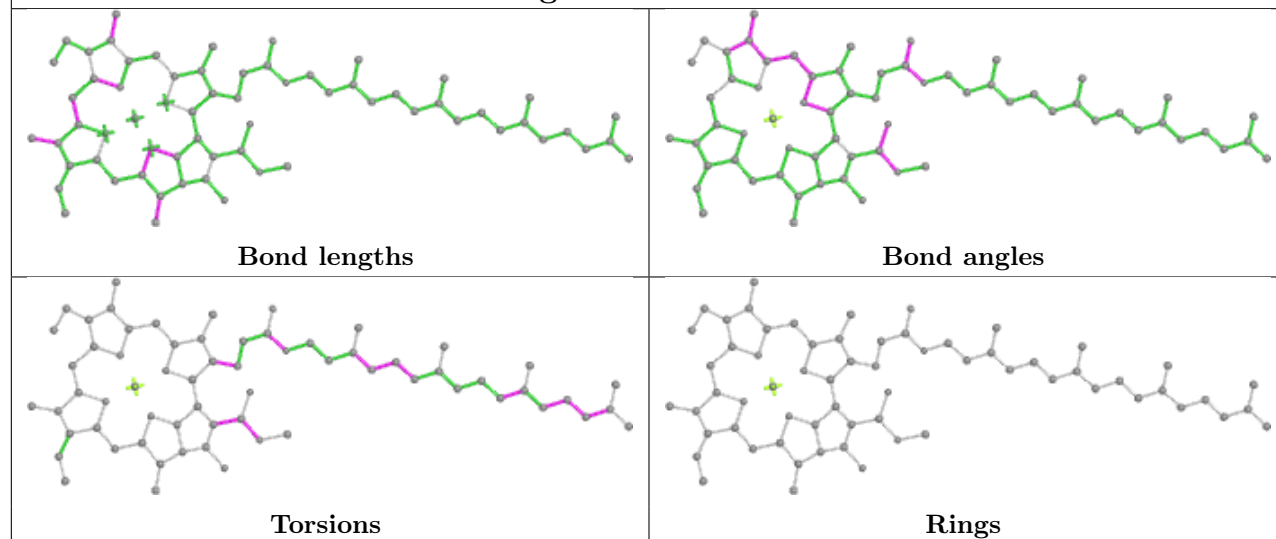
Ligand CLA b 313

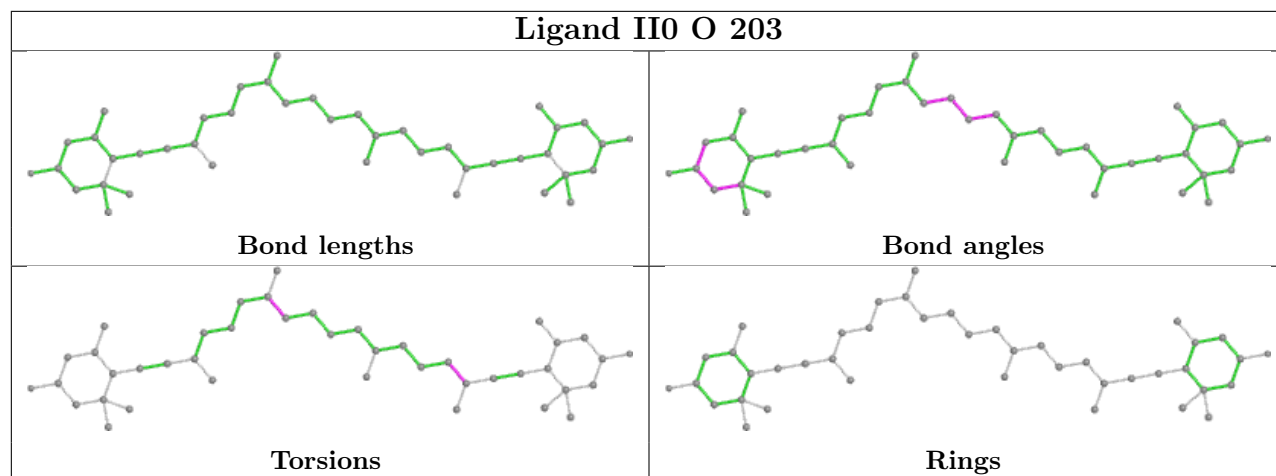
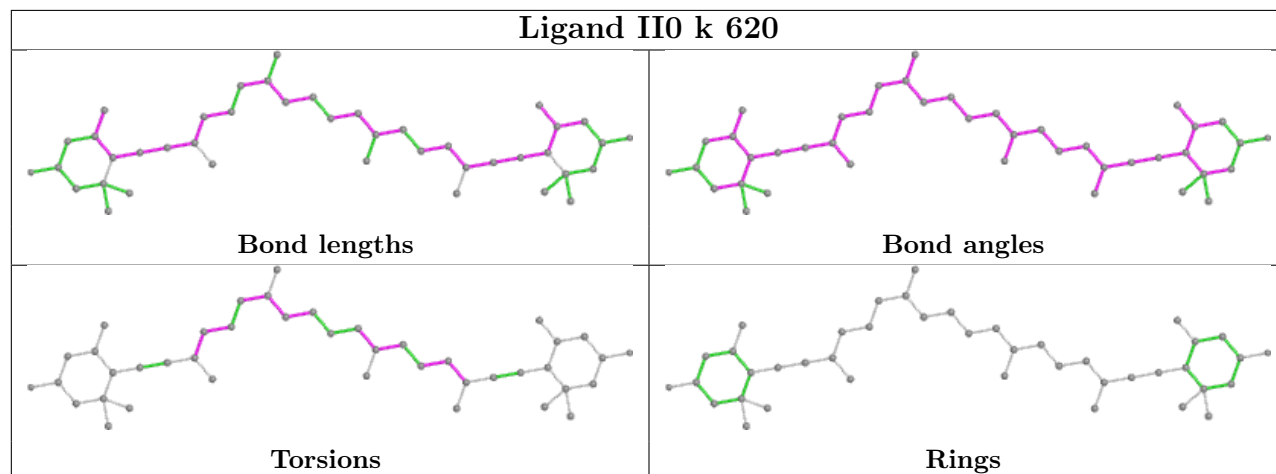
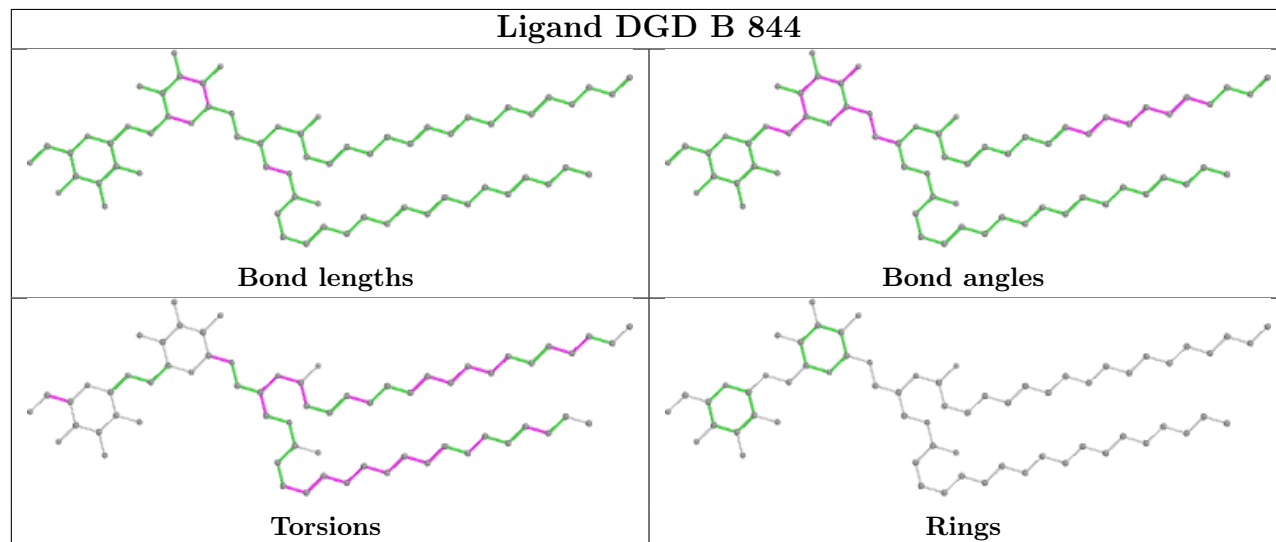


Ligand CLA B 821

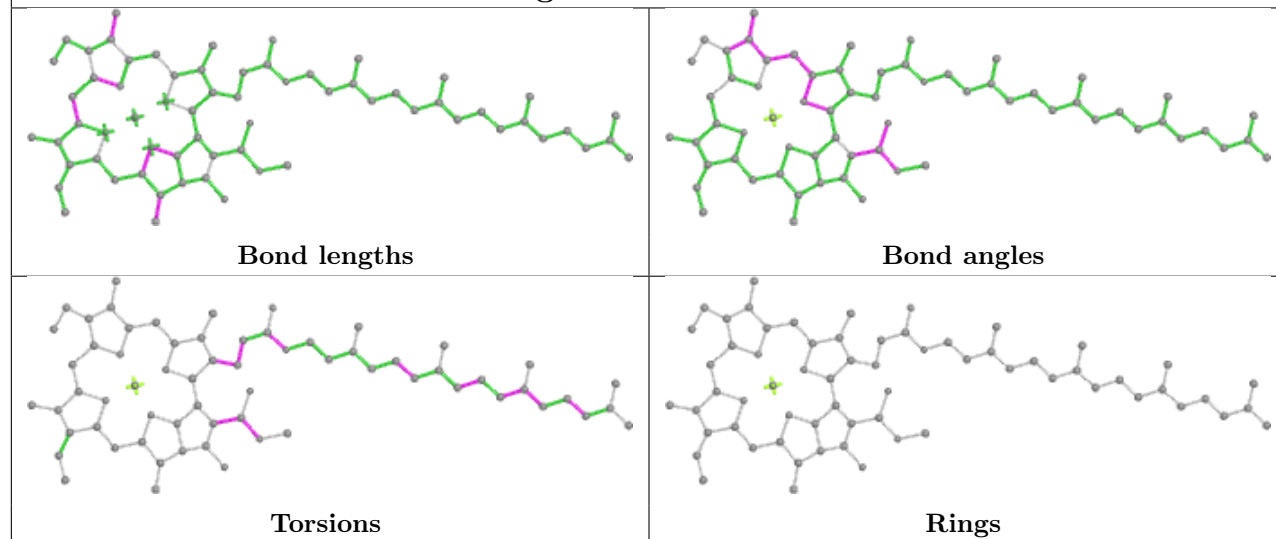


Ligand CLA f 602

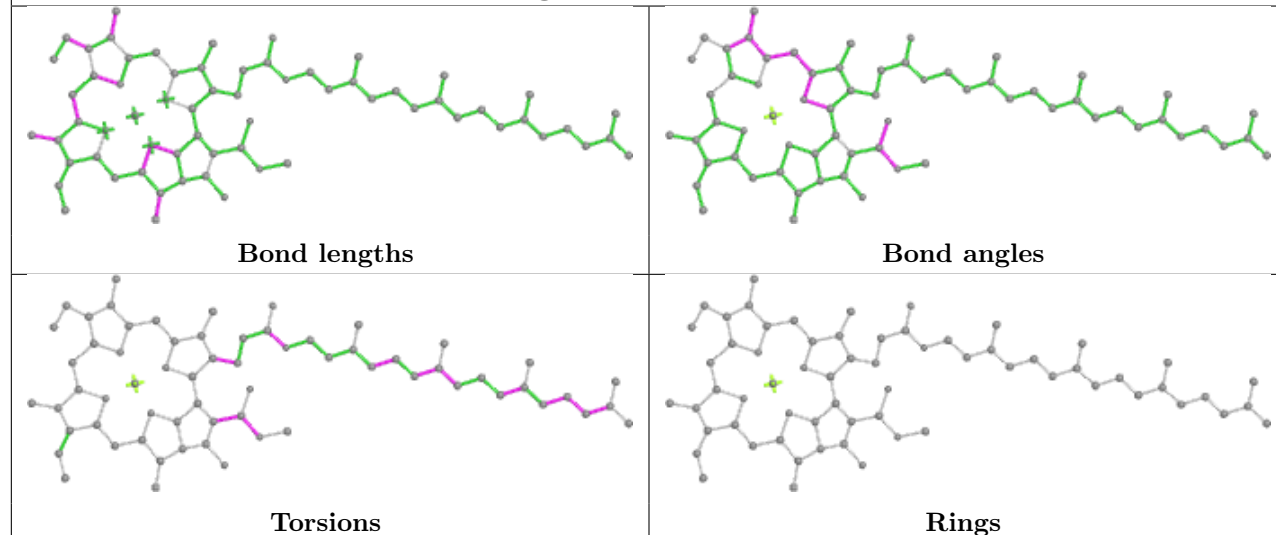


Ligand II0 O 203**Ligand II0 k 620****Ligand DGD B 844**

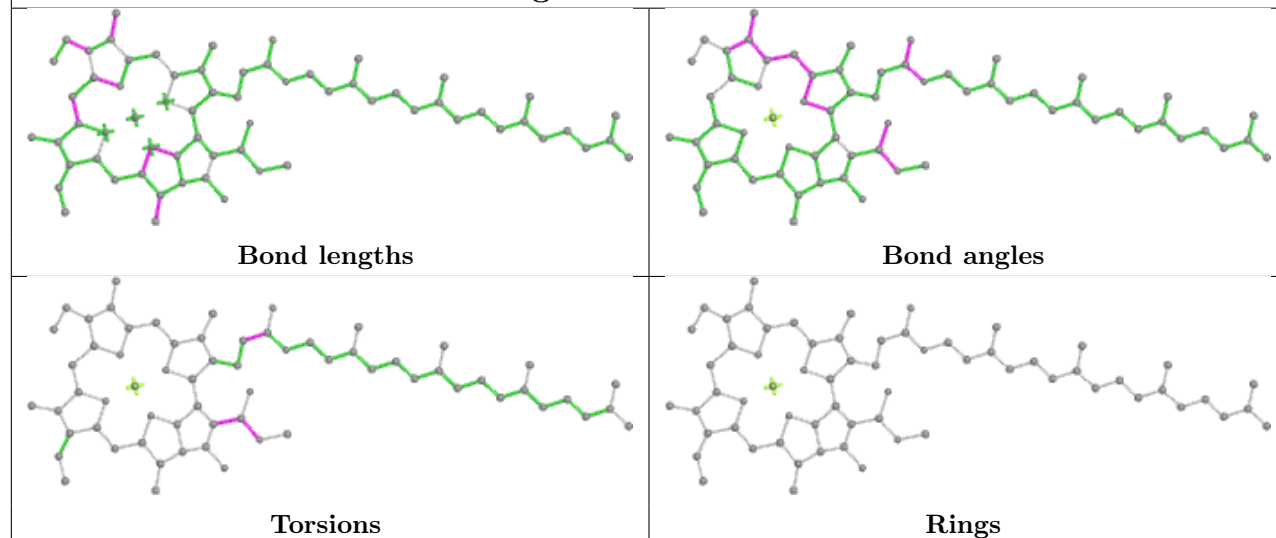
Ligand CLA a 307



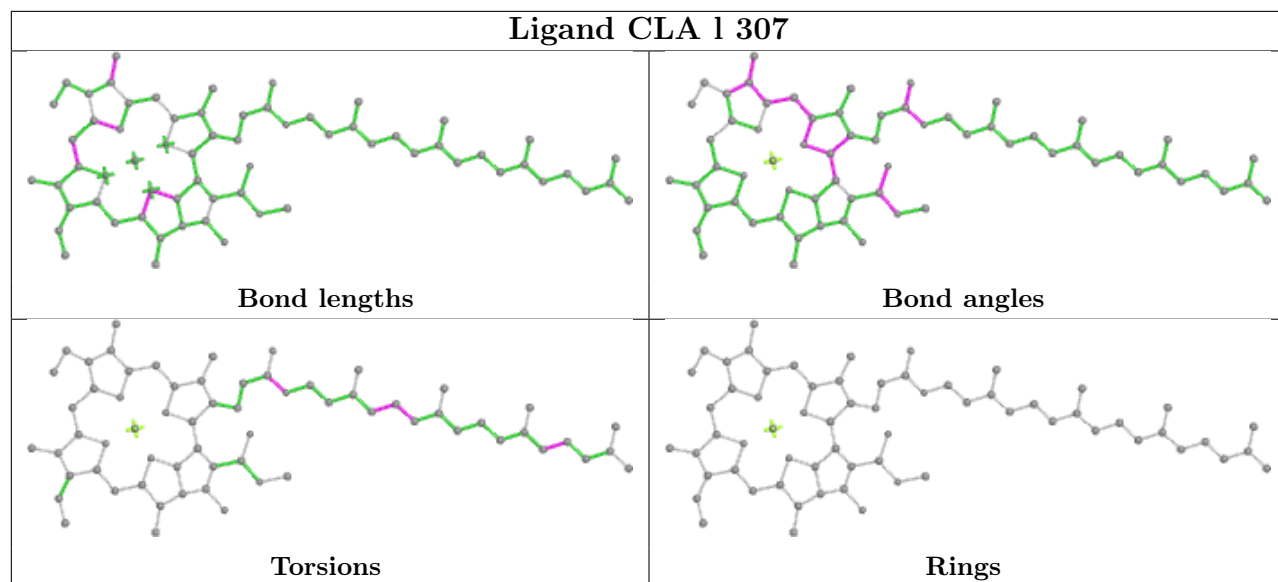
Ligand CLA k 602



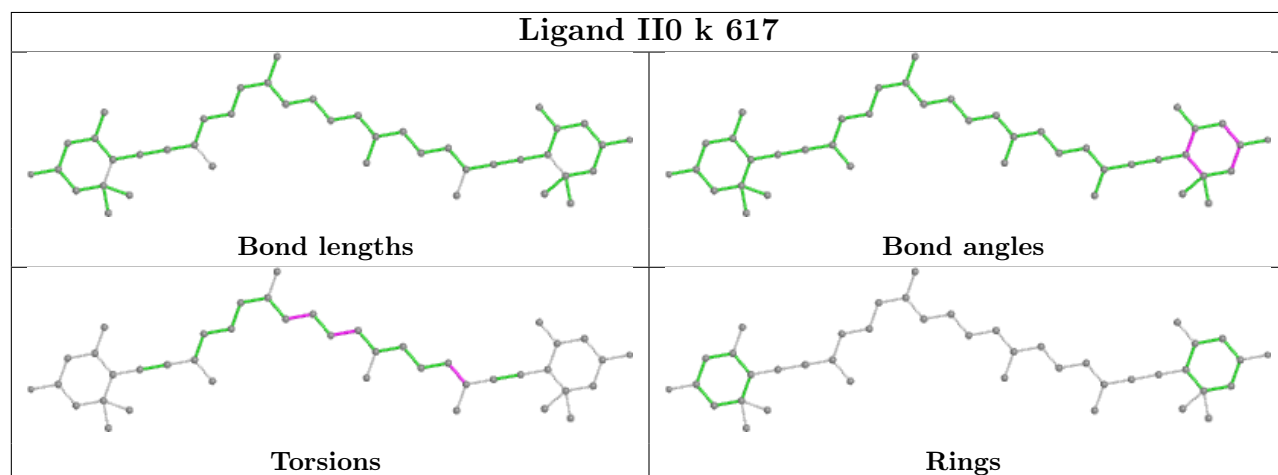
Ligand CLA B 842



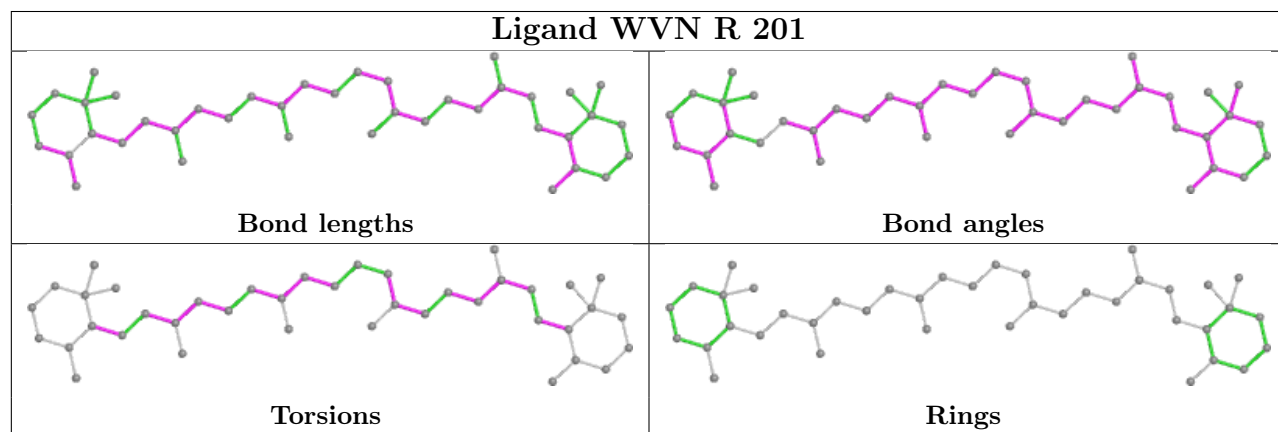
Ligand CLA l 307



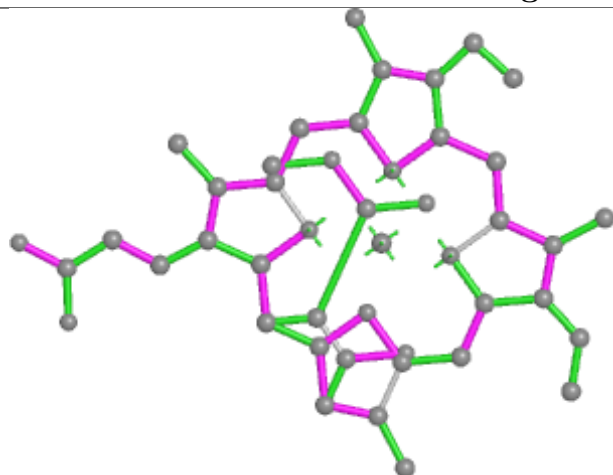
Ligand II0 k 617



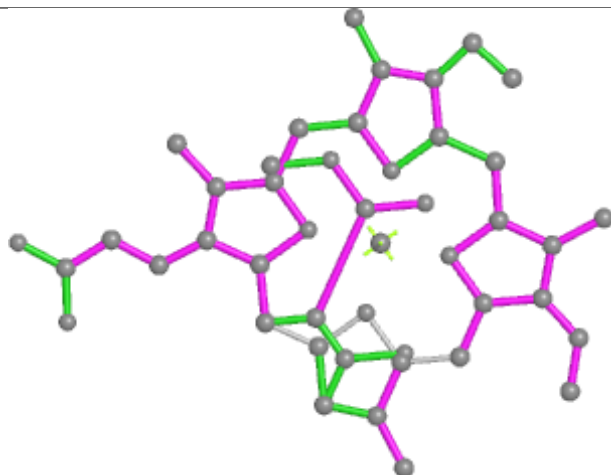
Ligand WVN R 201



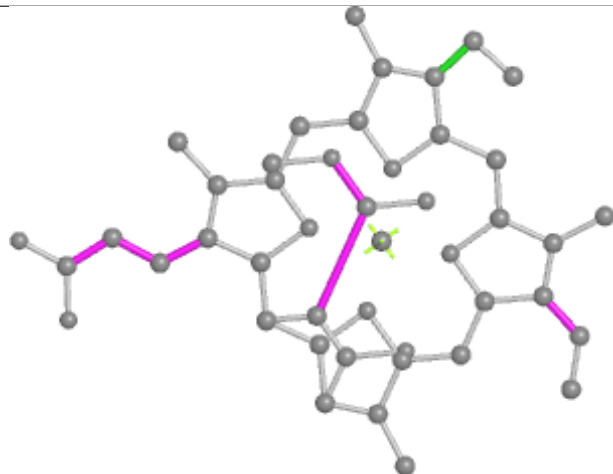
Ligand KC2 c 310



Bond lengths



Bond angles

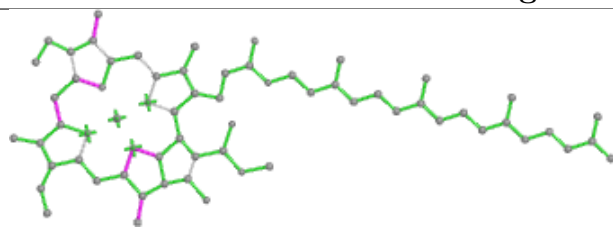


Torsions

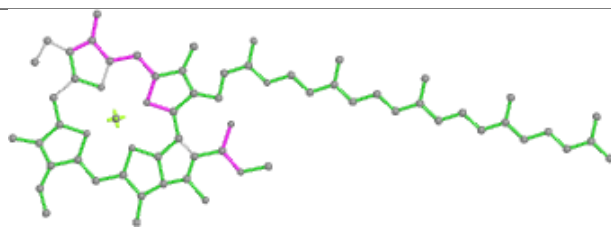


Rings

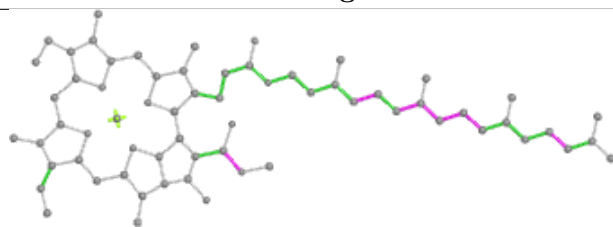
Ligand CLA c 312



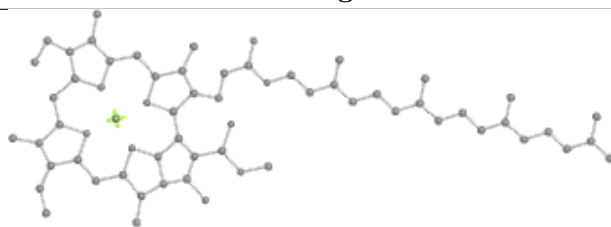
Bond lengths



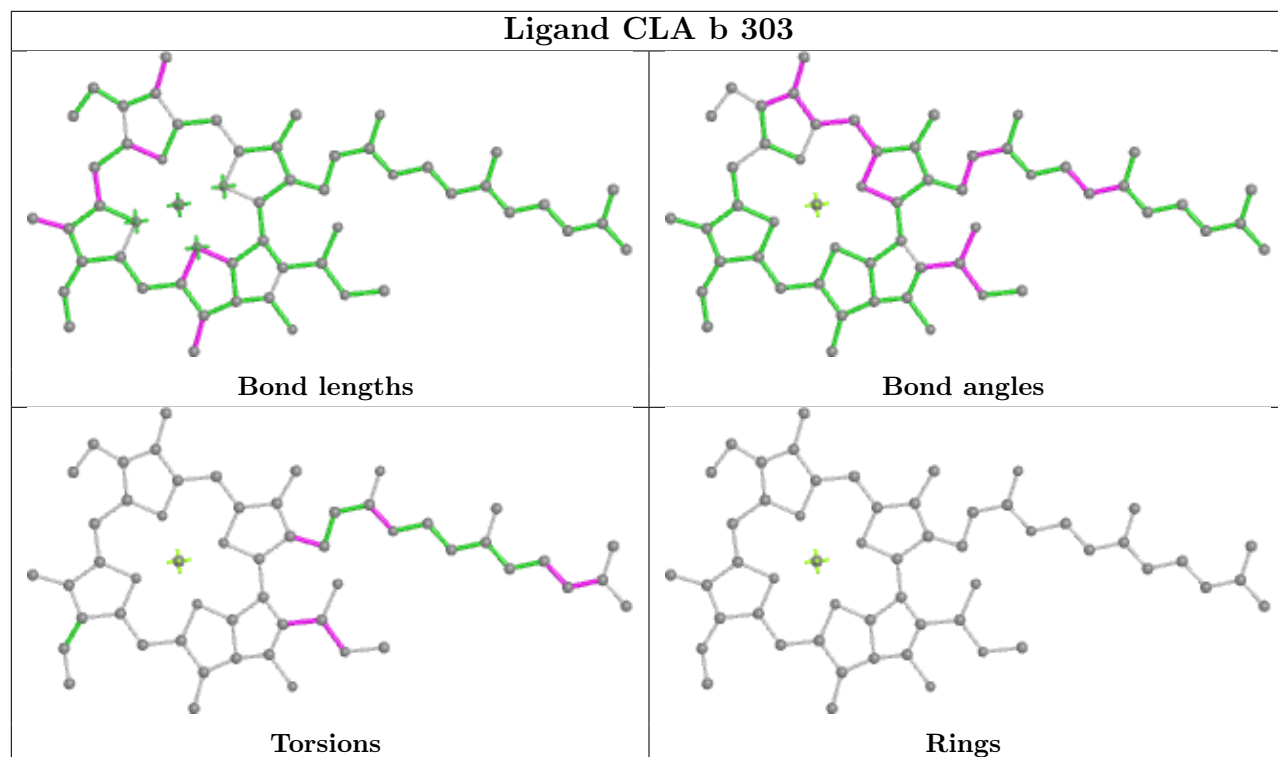
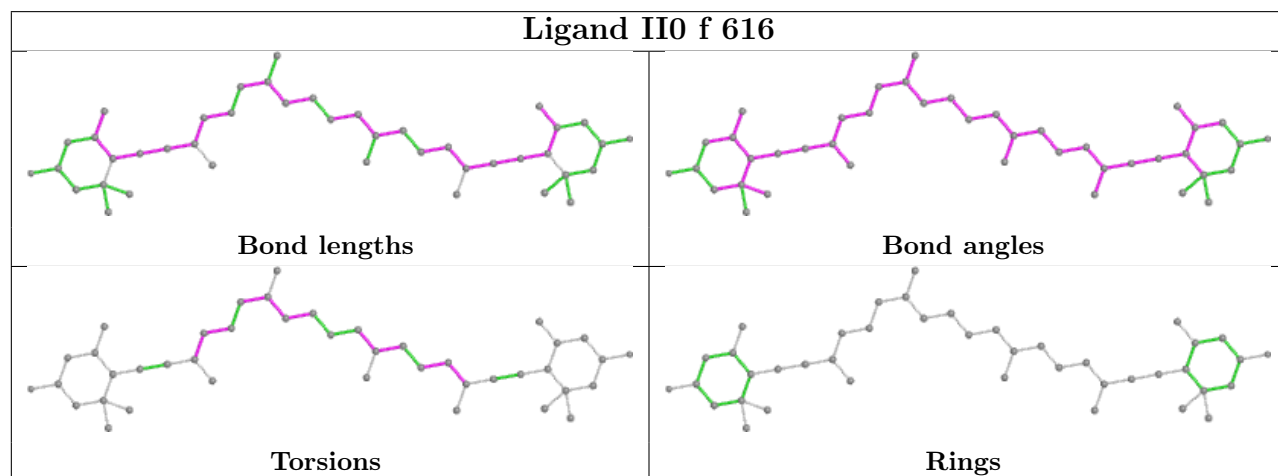
Bond angles



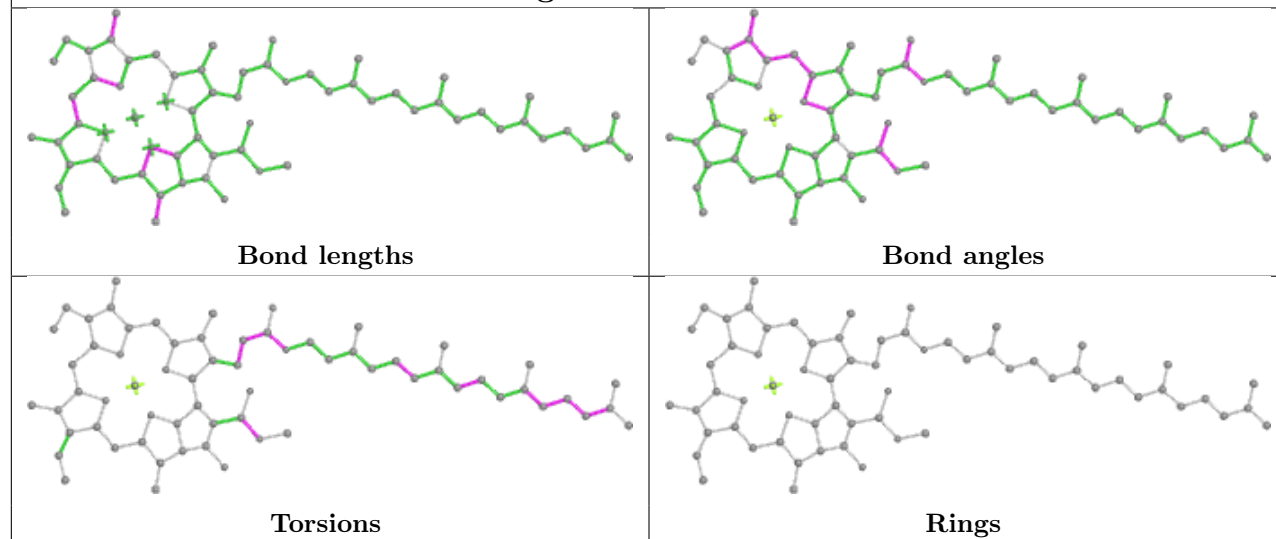
Torsions



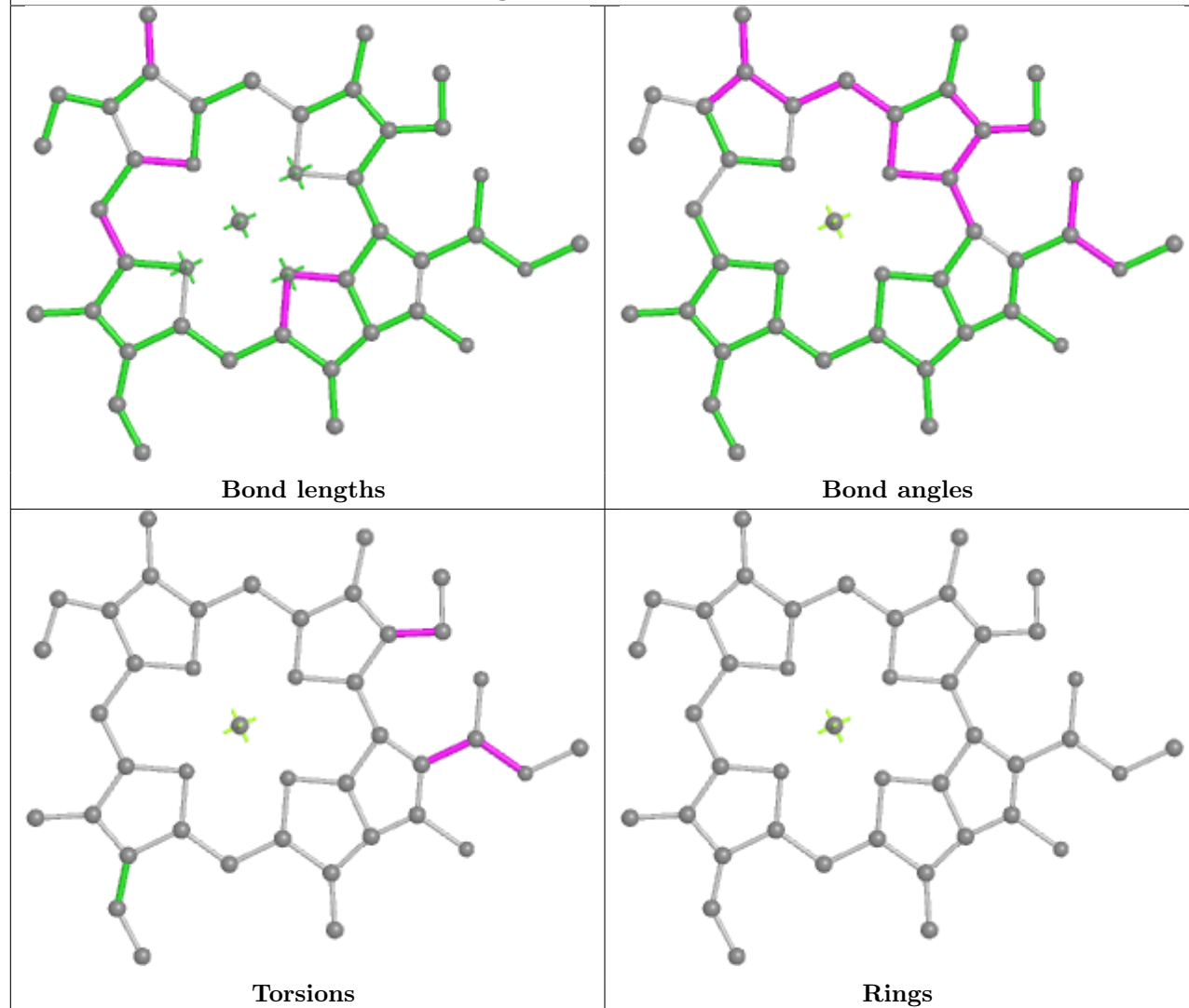
Rings

Ligand CLA b 303**Ligand II0 f 616**

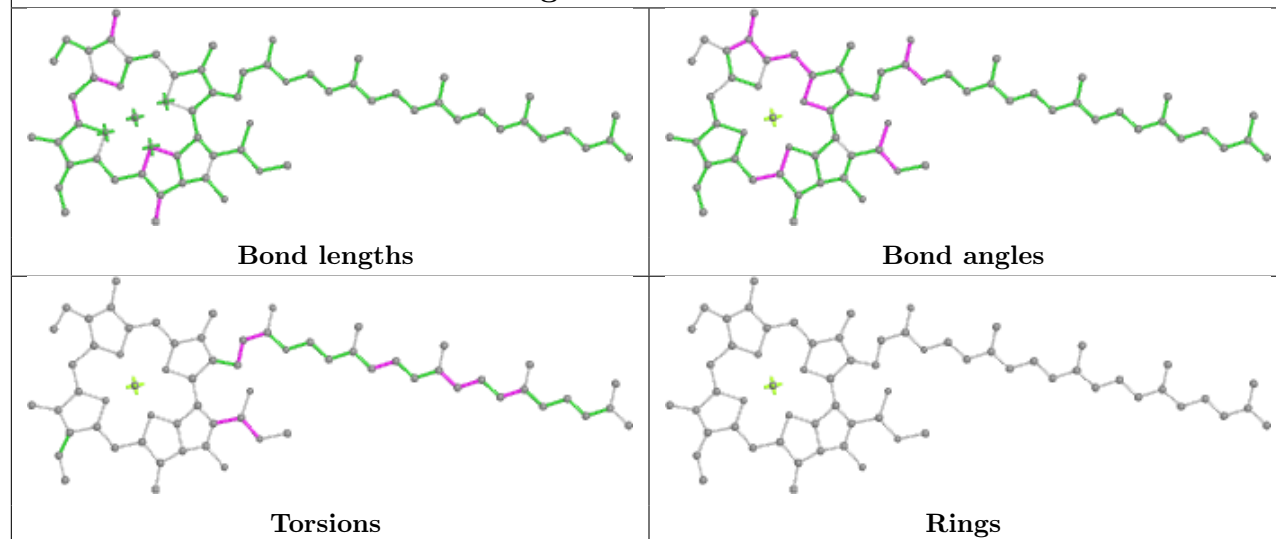
Ligand CLA e 307



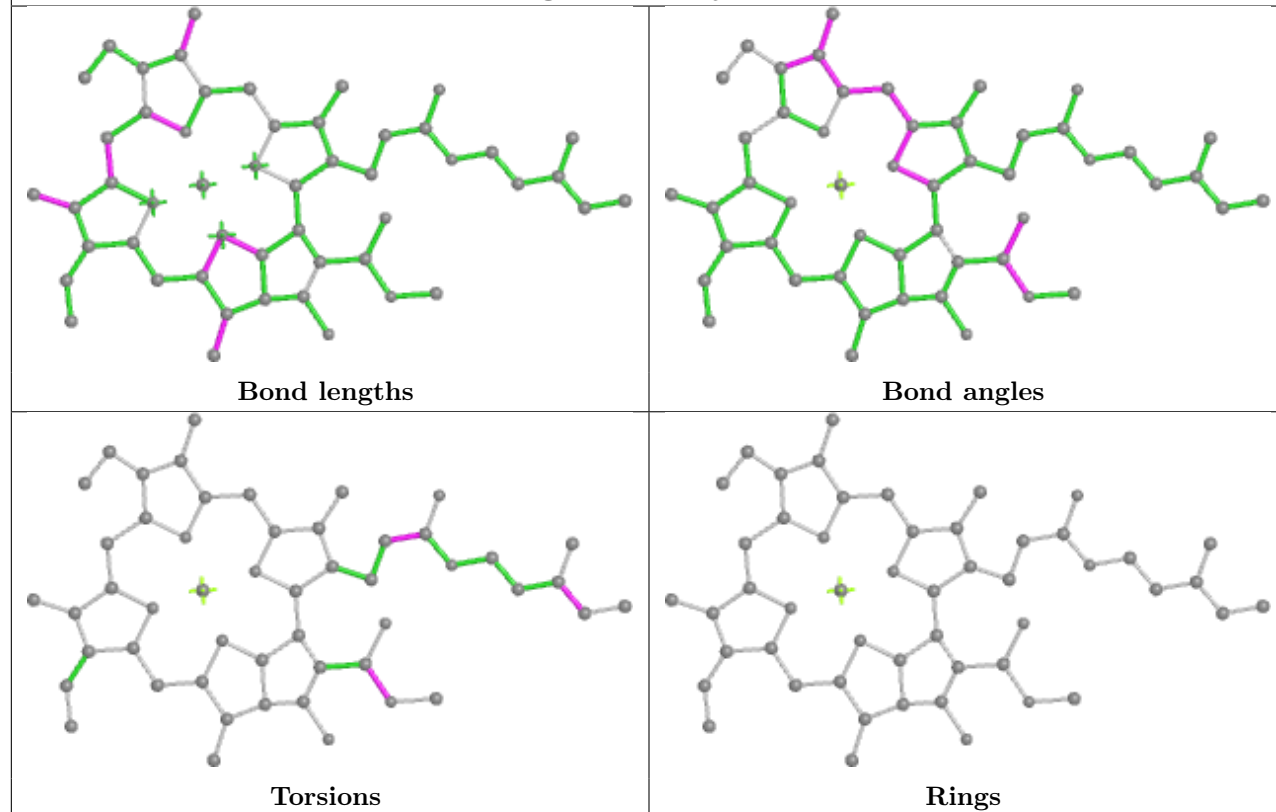
Ligand CLA m 605

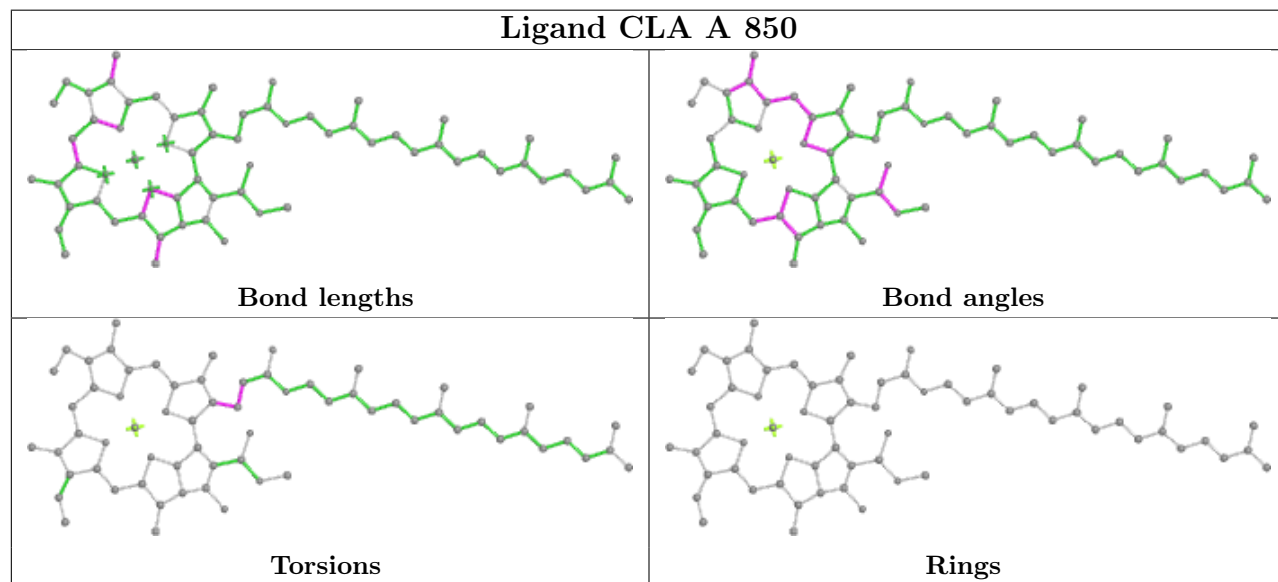
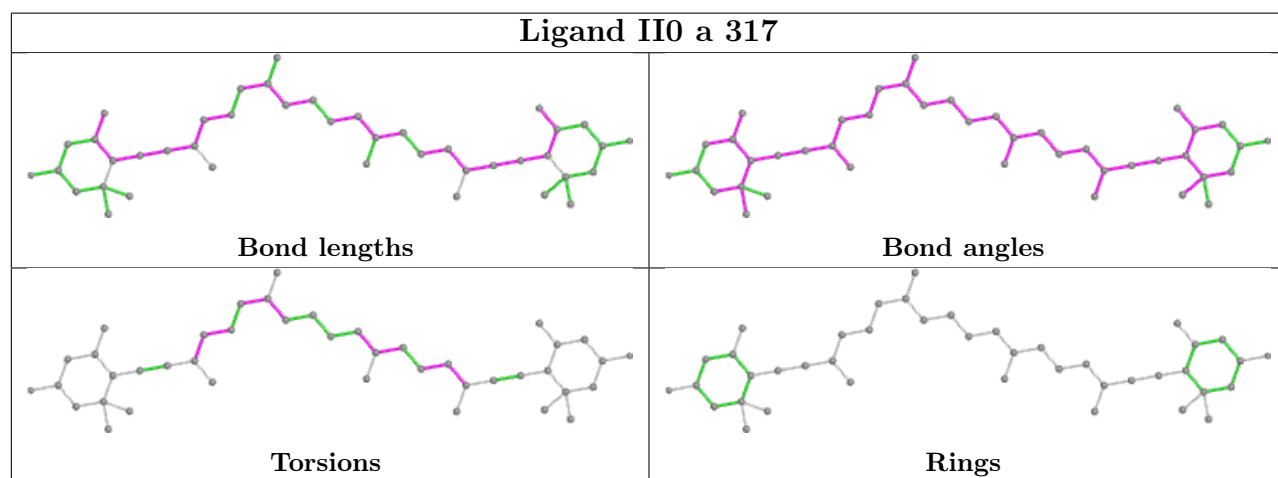
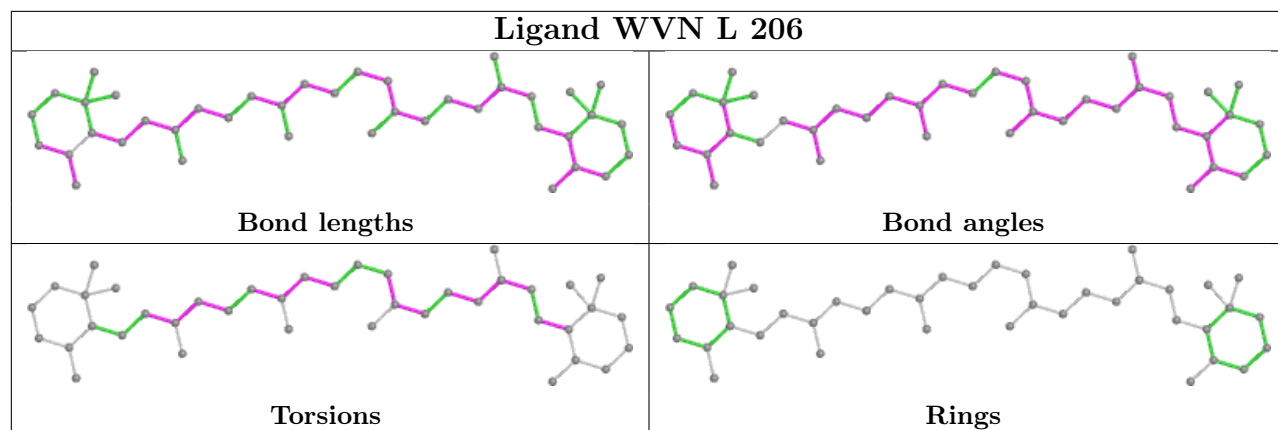


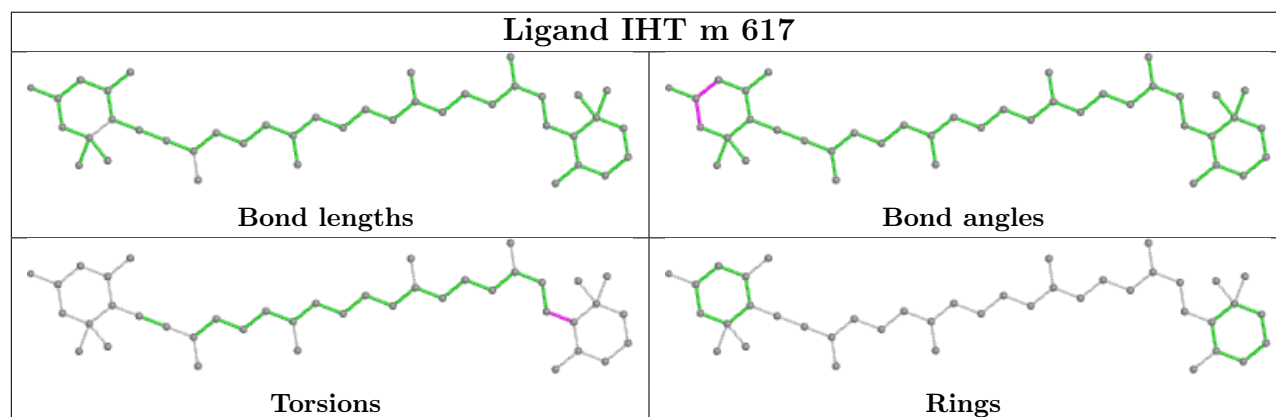
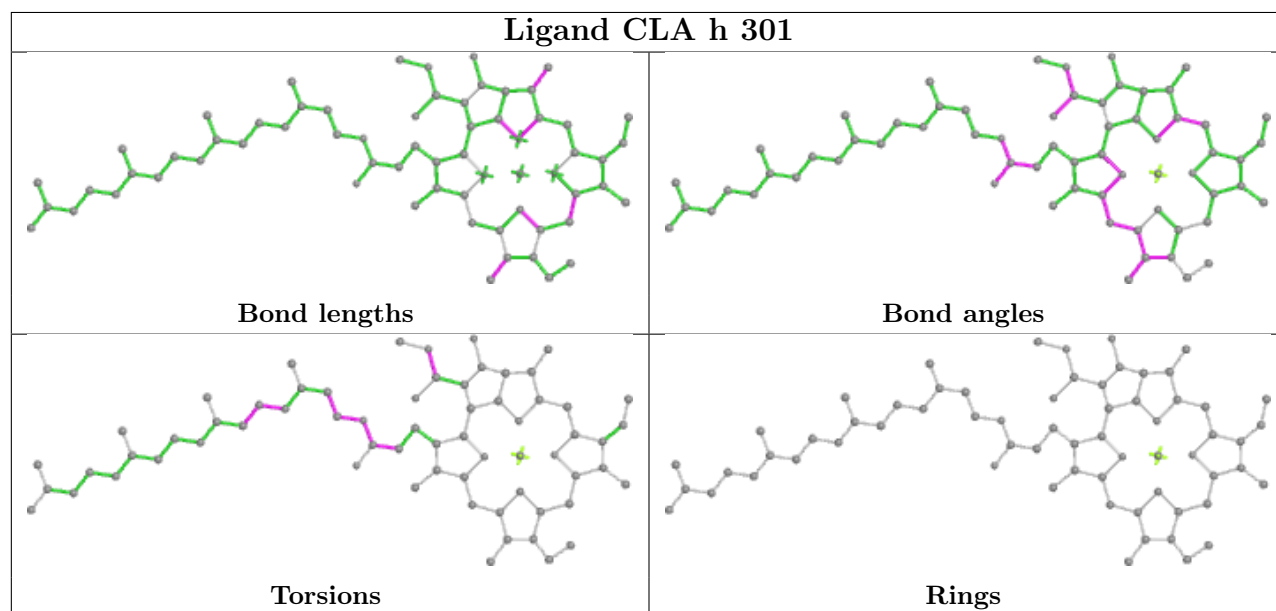
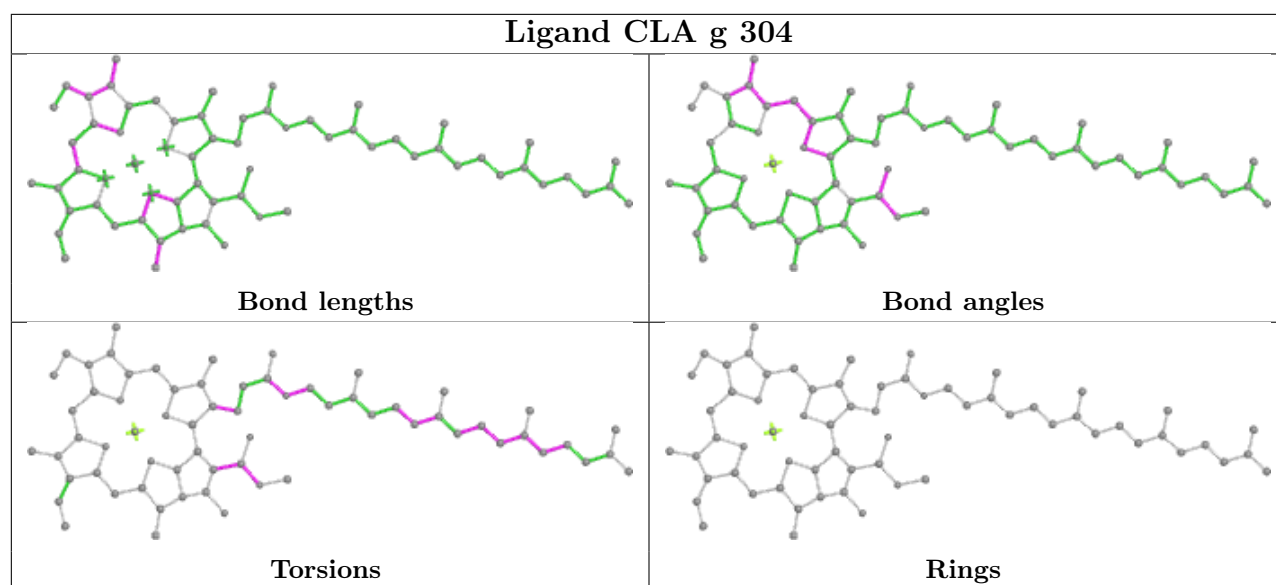
Ligand CLA i 305

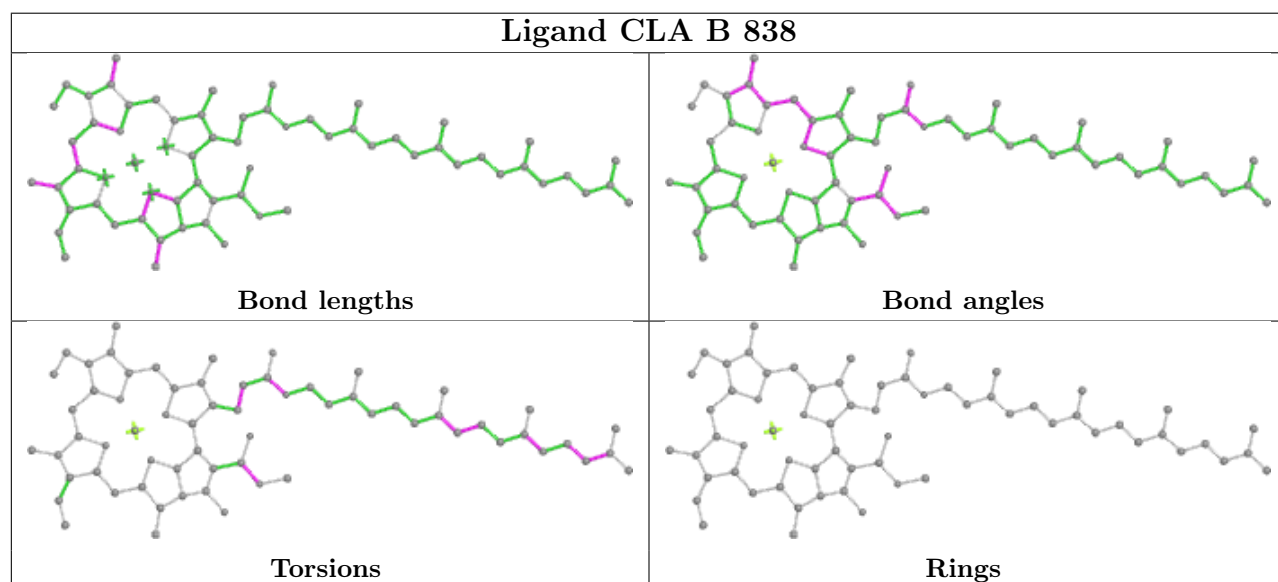
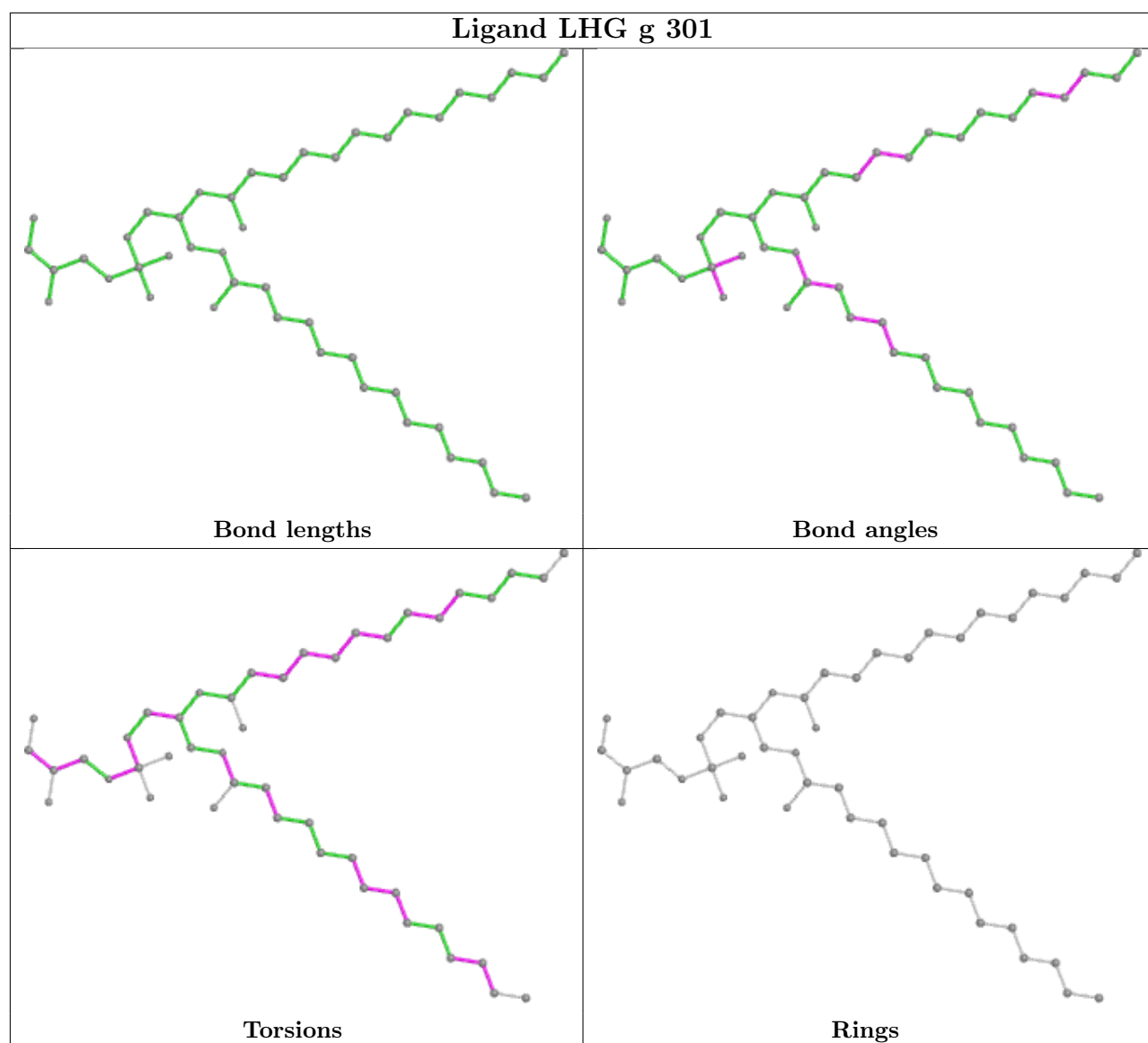


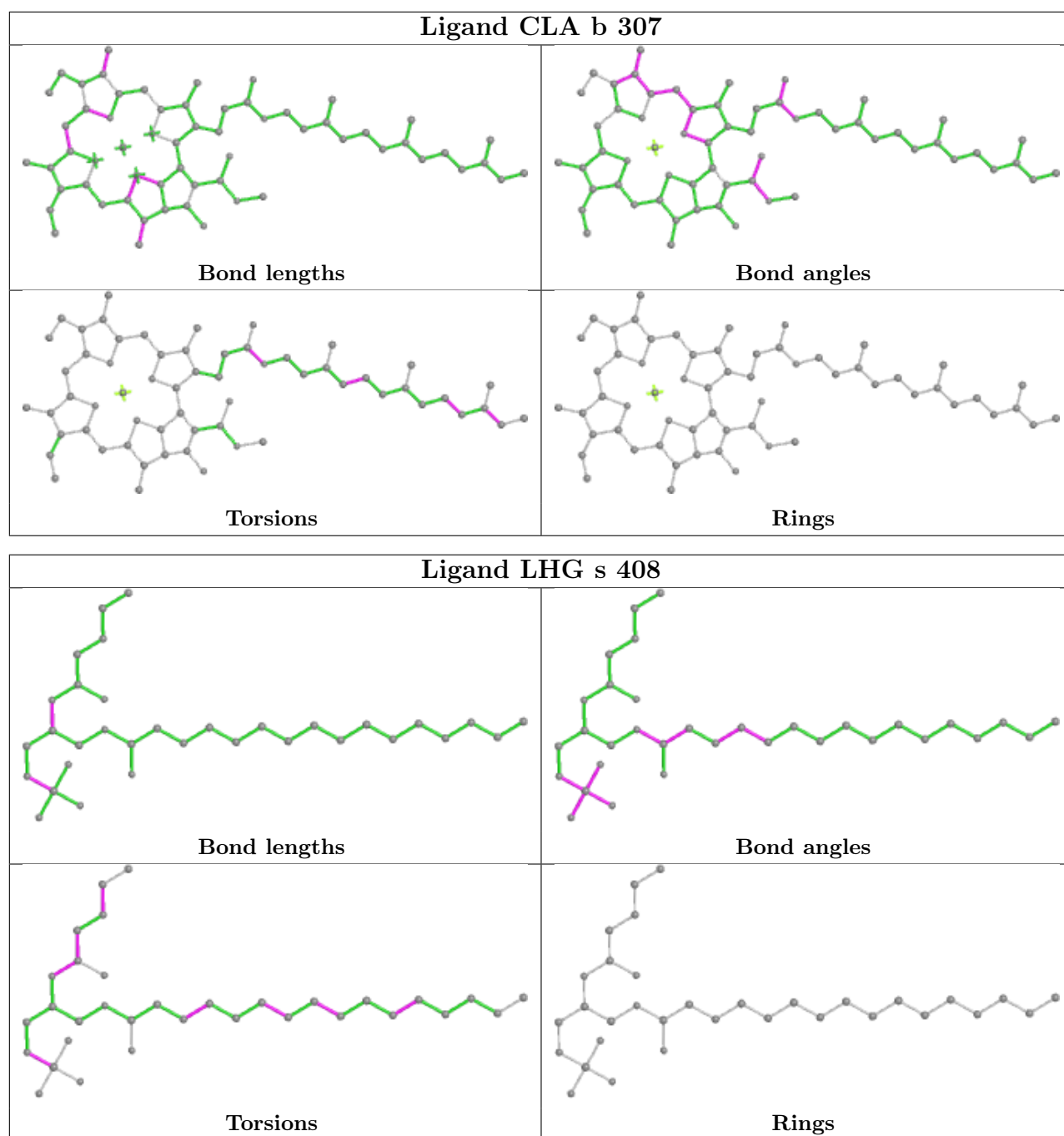
Ligand CLA j 304

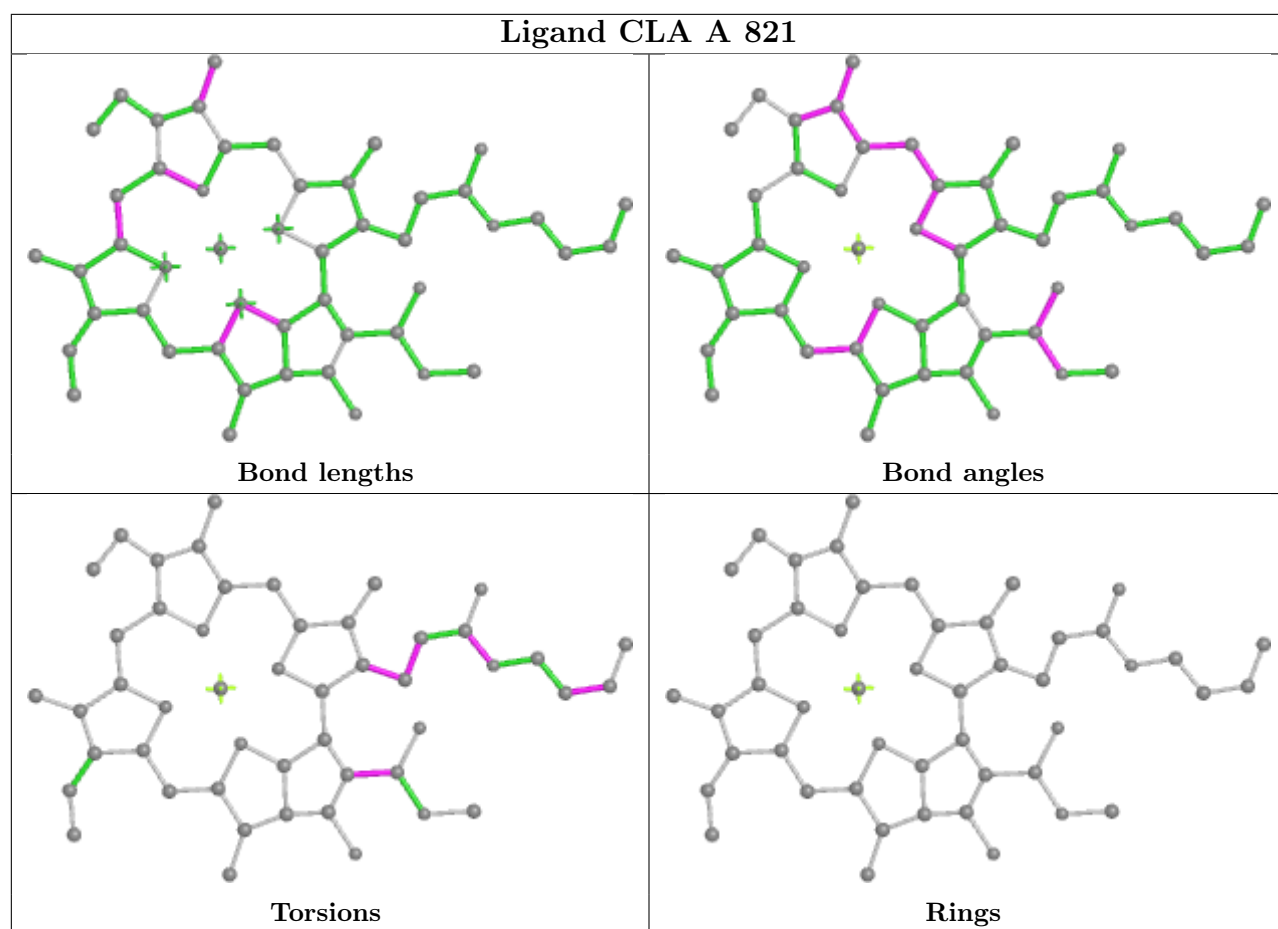




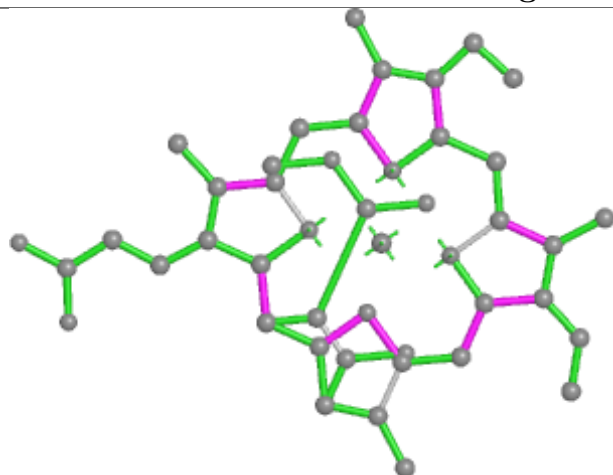




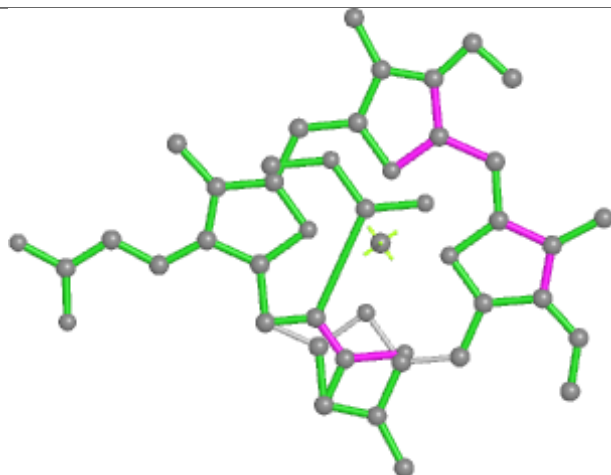




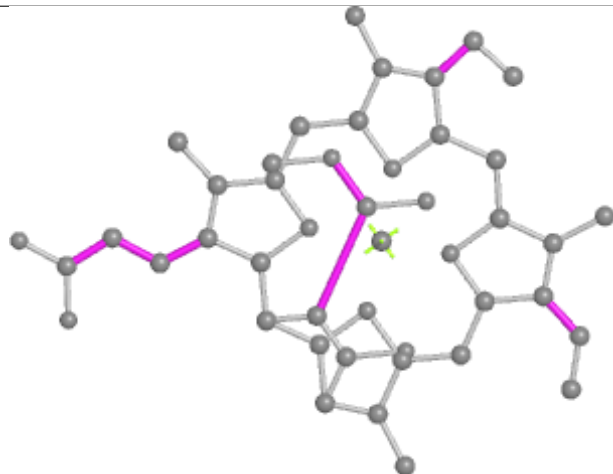
Ligand KC2 d 312



Bond lengths



Bond angles

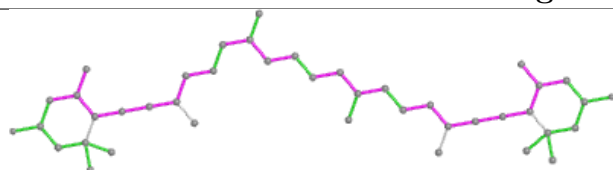


Torsions

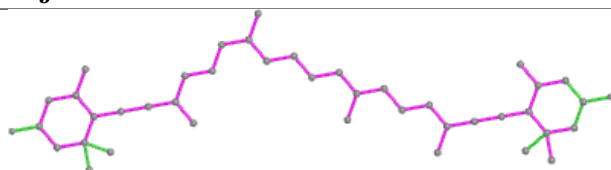


Rings

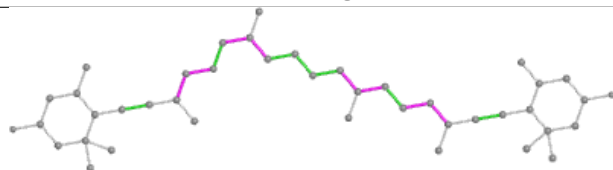
Ligand II0 j 316



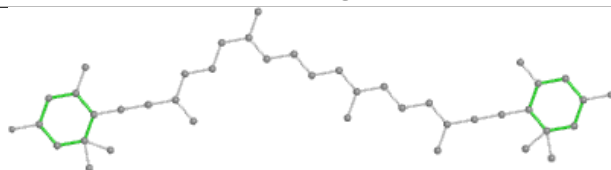
Bond lengths



Bond angles

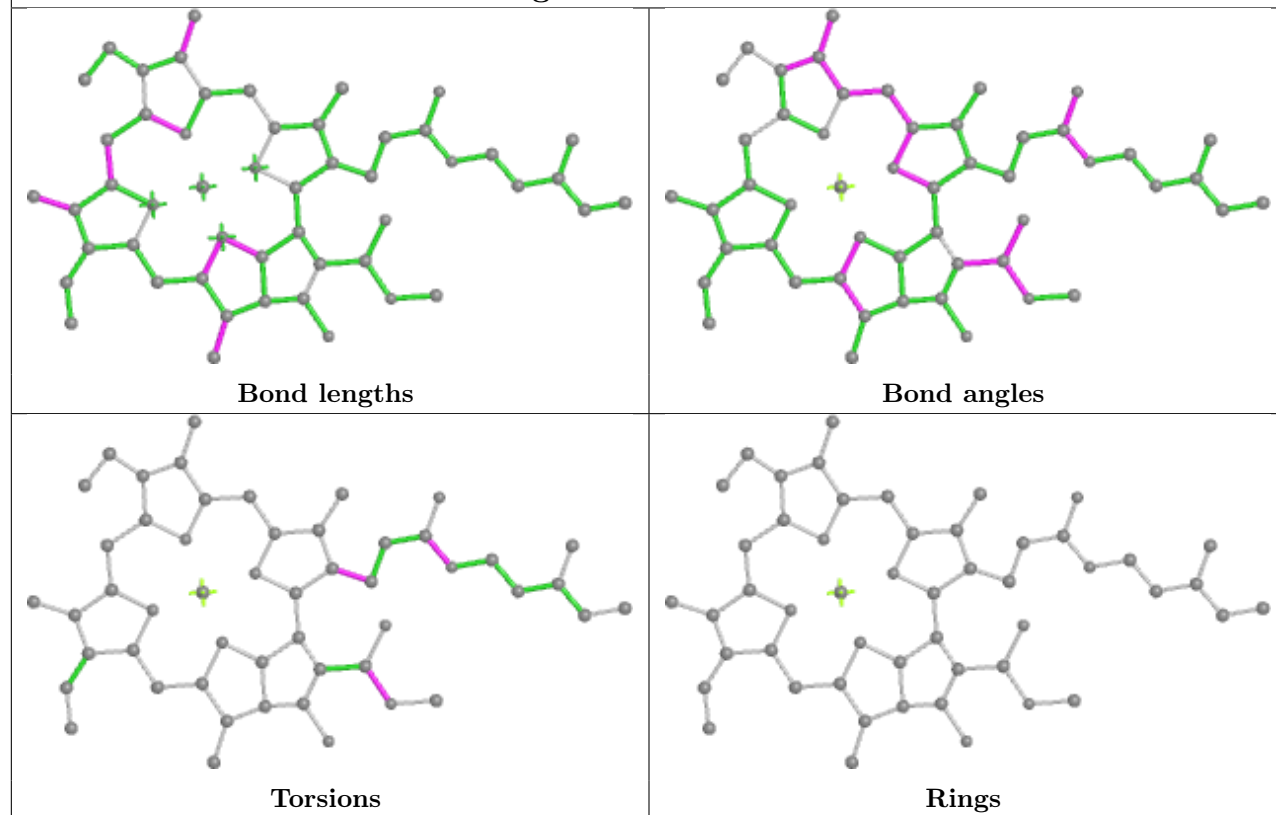


Torsions

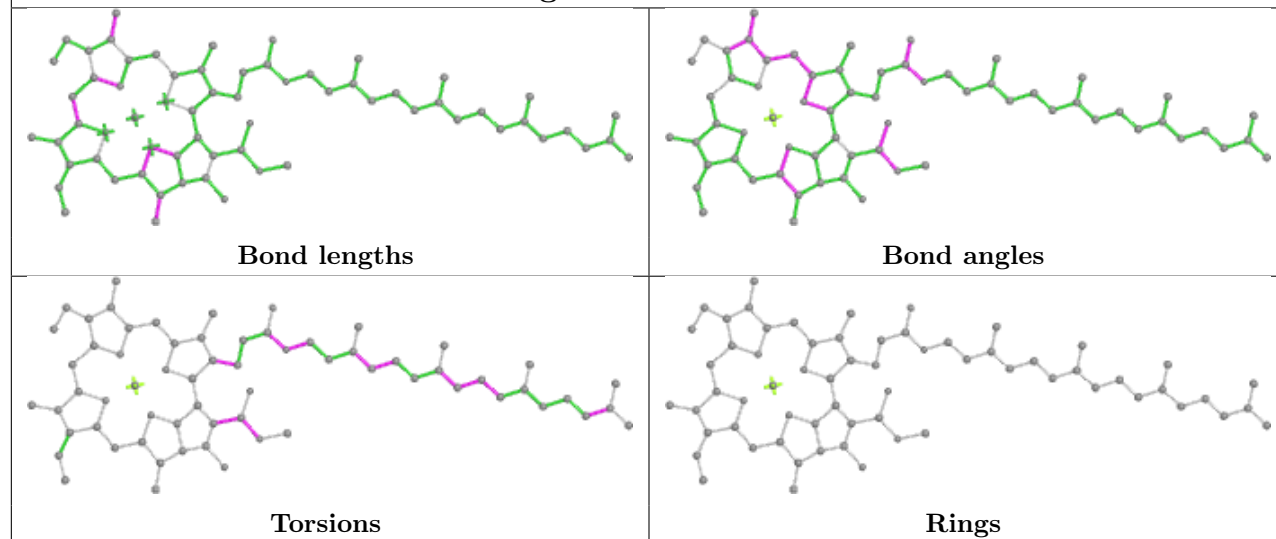


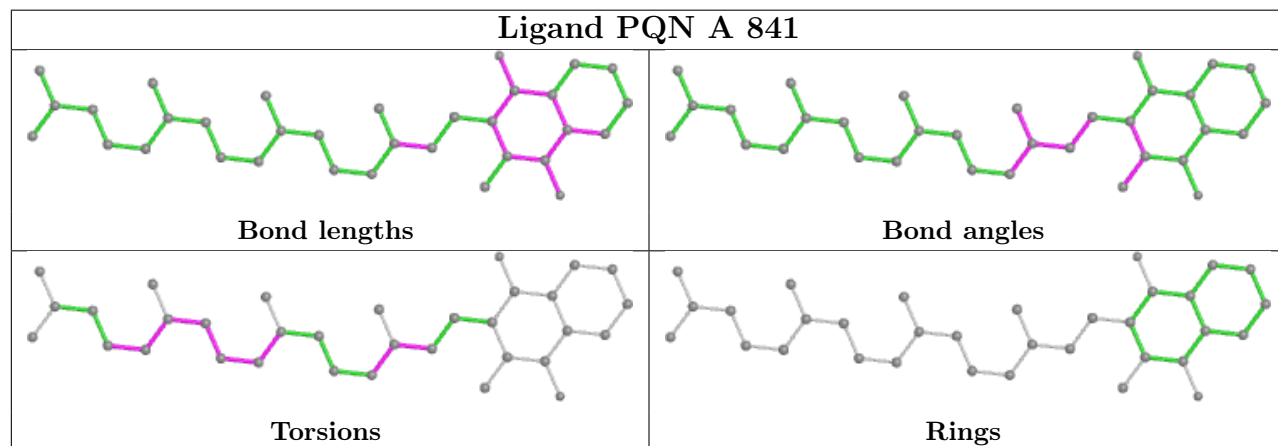
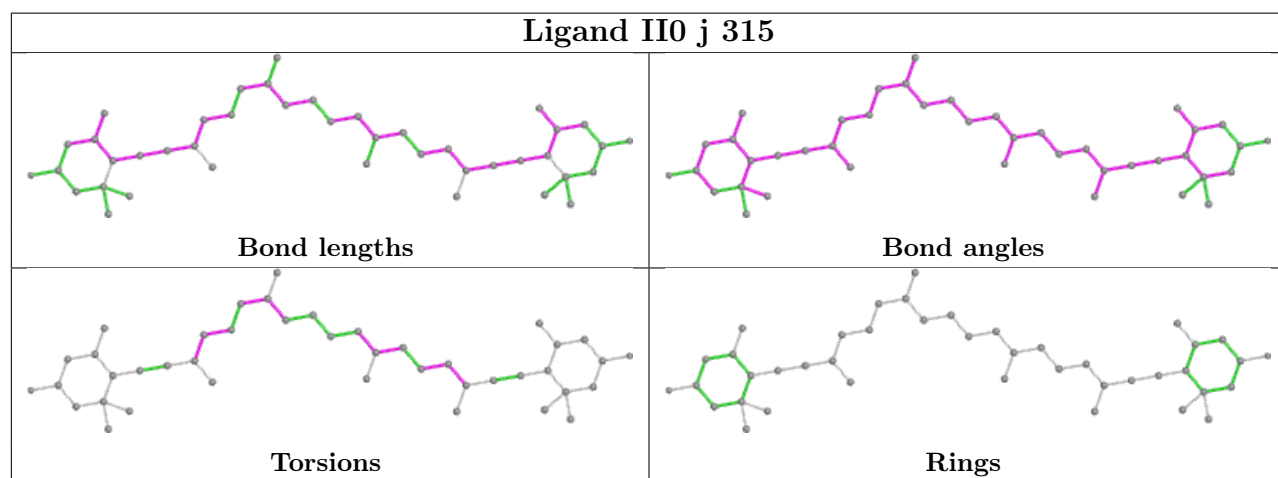
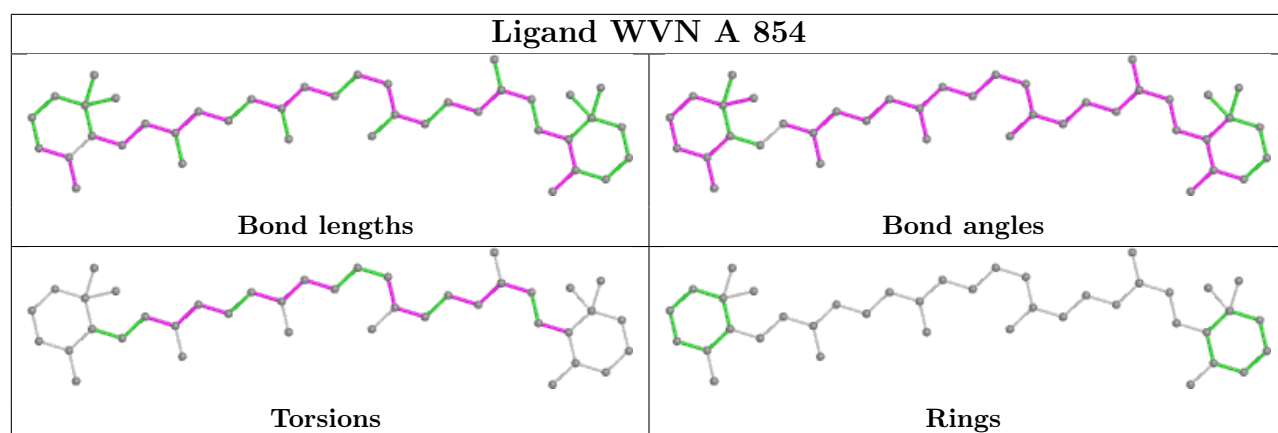
Rings

Ligand CLA B 827

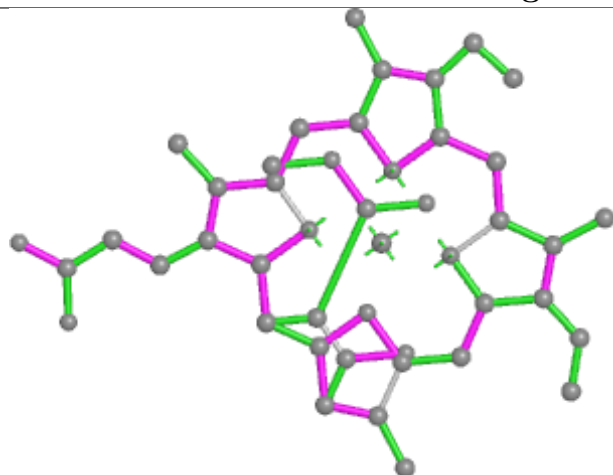


Ligand CLA f 613

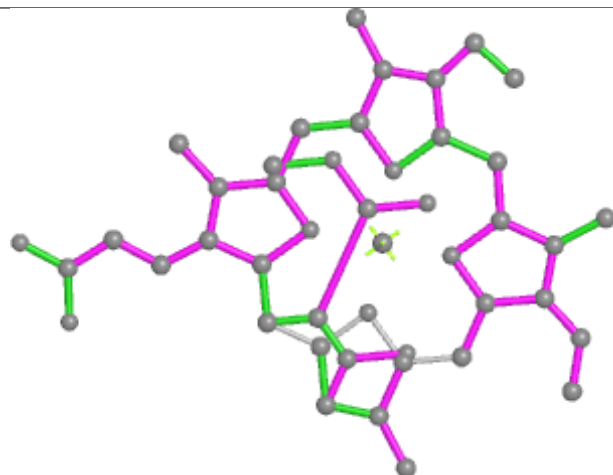




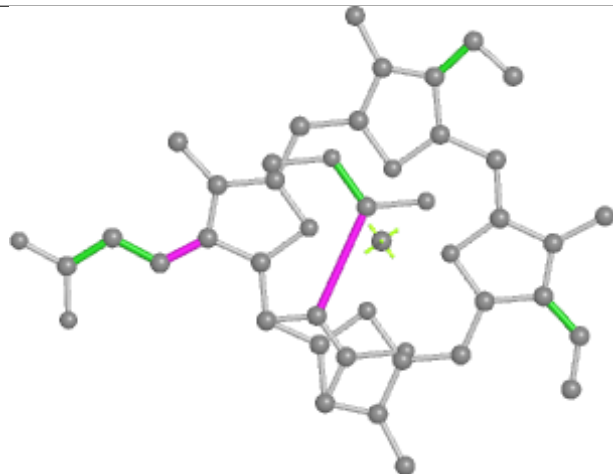
Ligand KC2 s 404



Bond lengths



Bond angles

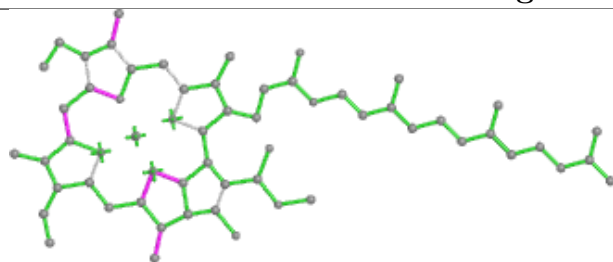


Torsions

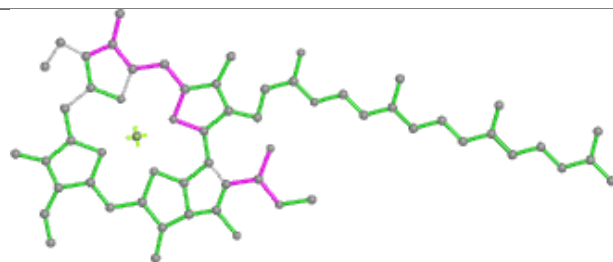


Rings

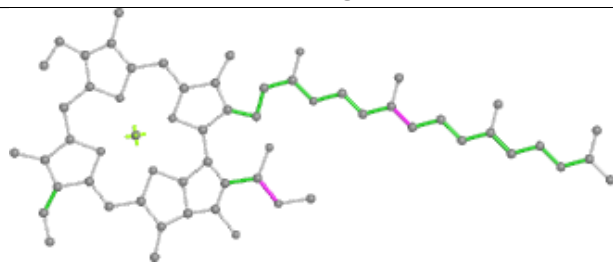
Ligand CLA L 204



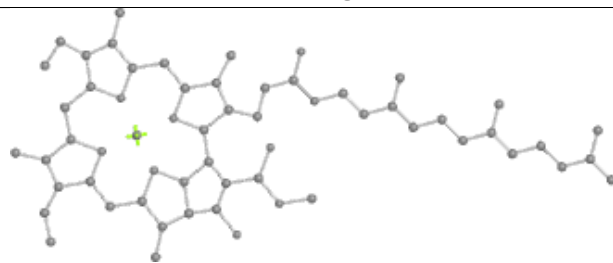
Bond lengths



Bond angles

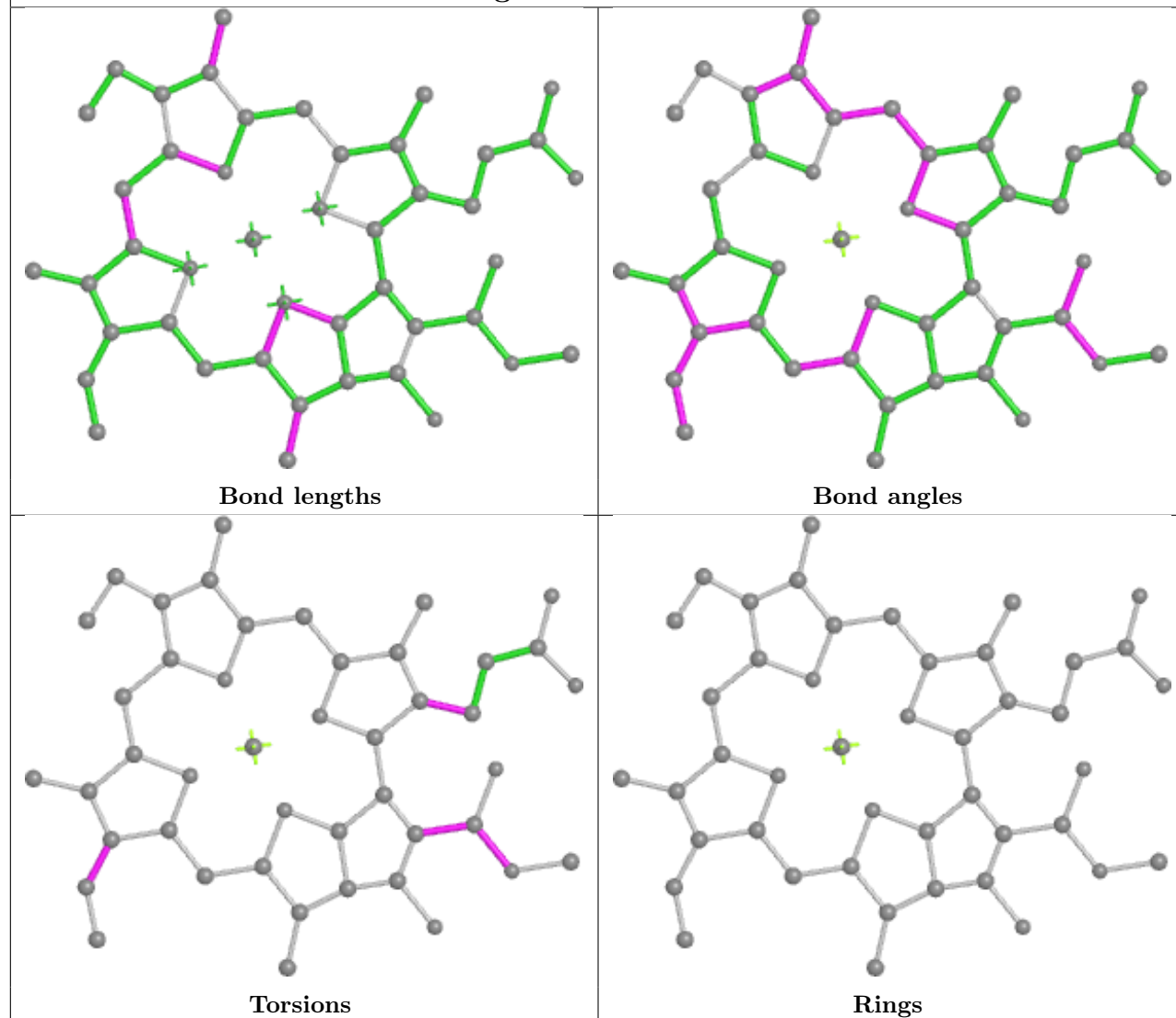


Torsions

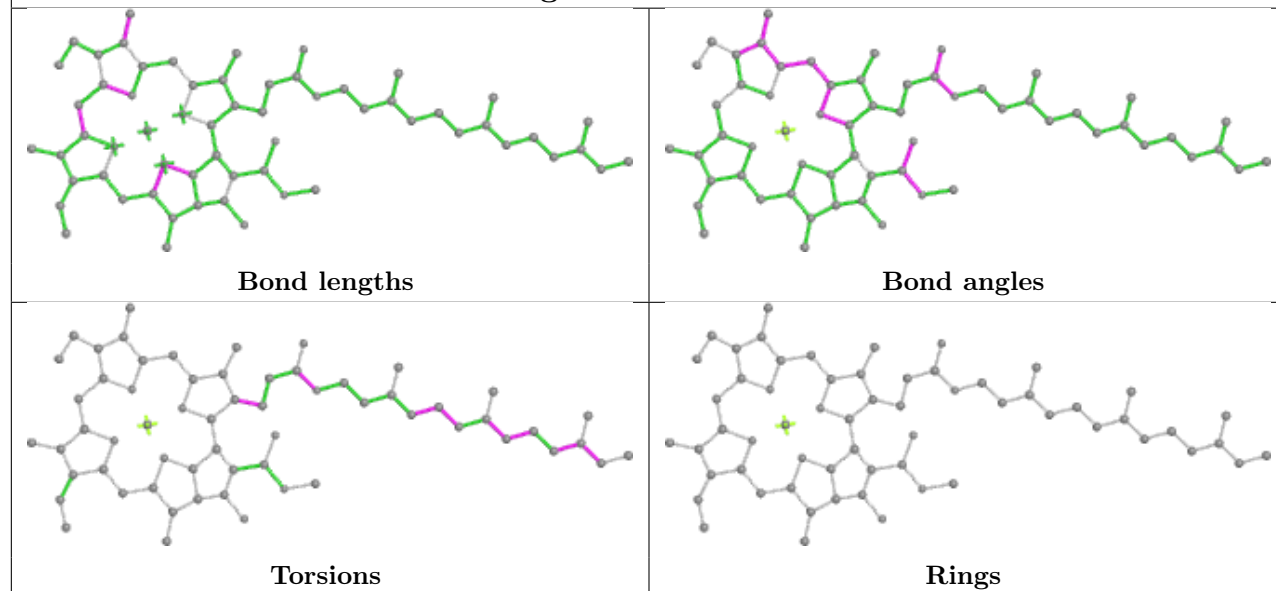


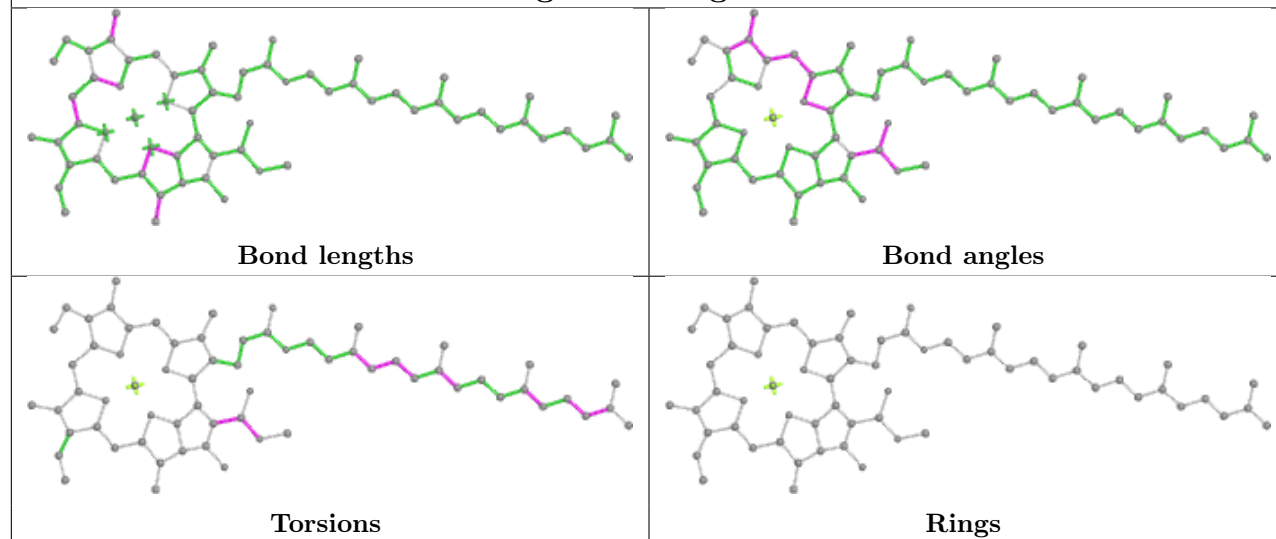
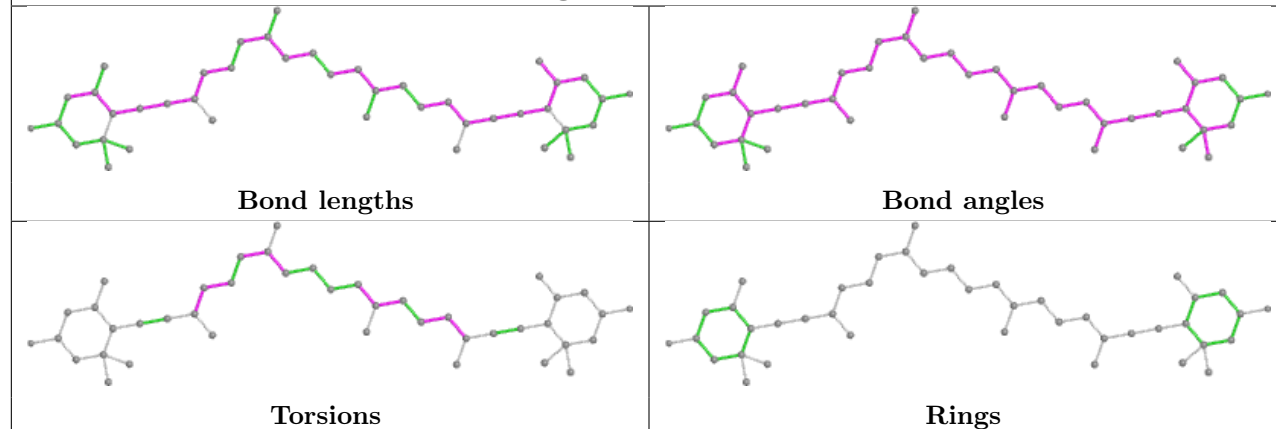
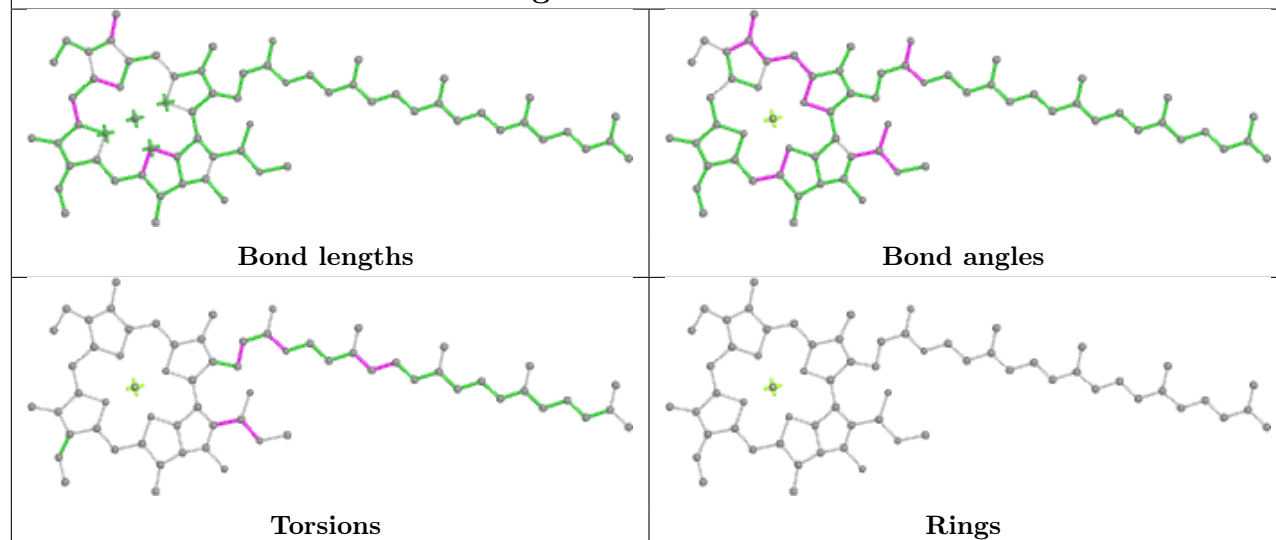
Rings

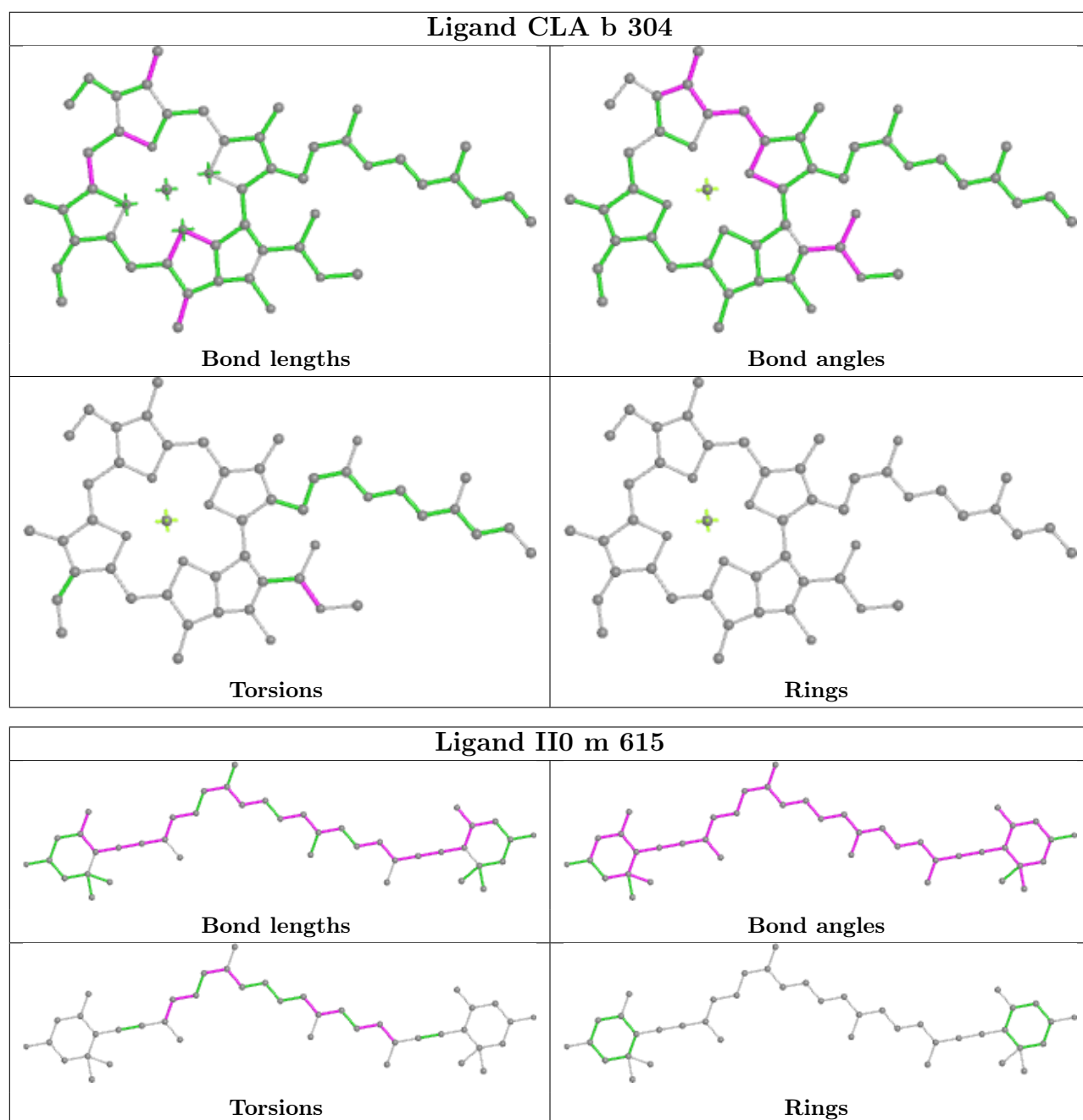
Ligand CLA a 306



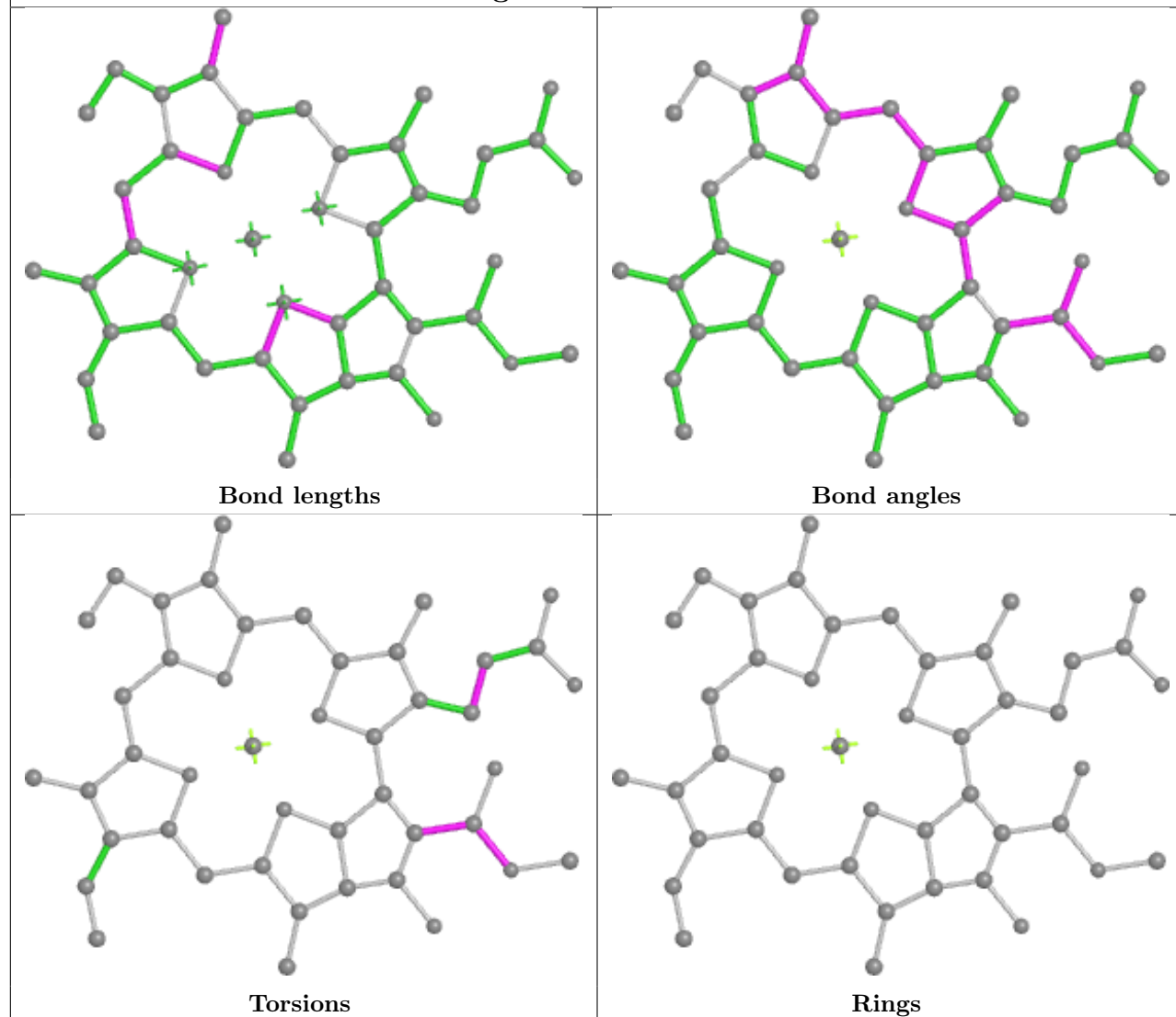
Ligand CLA l 310



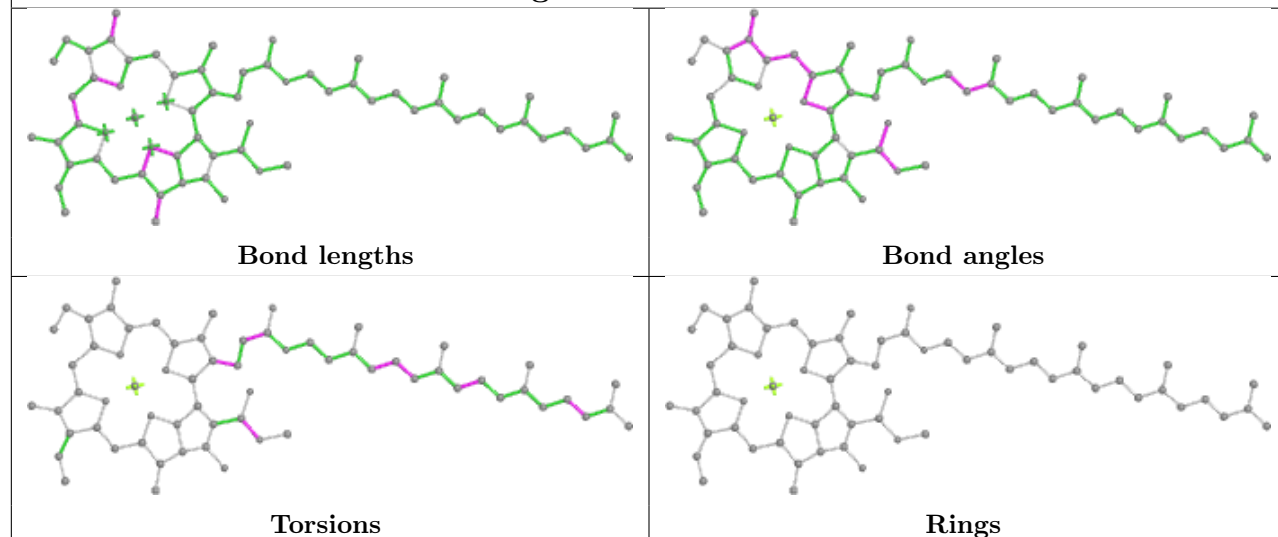
Ligand CLA g 310**Ligand II0 i 313****Ligand CLA B 802**



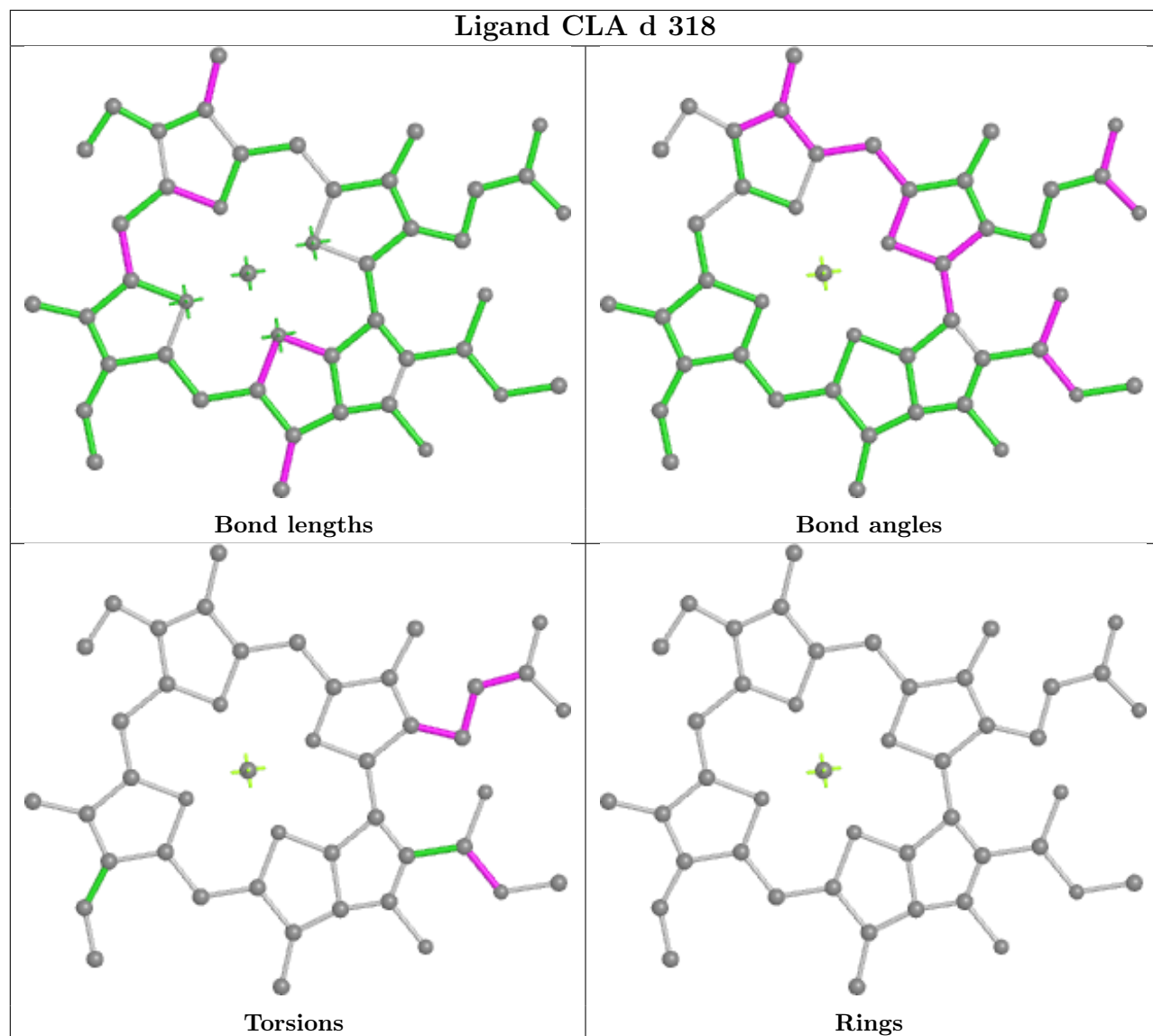
Ligand CLA k 605



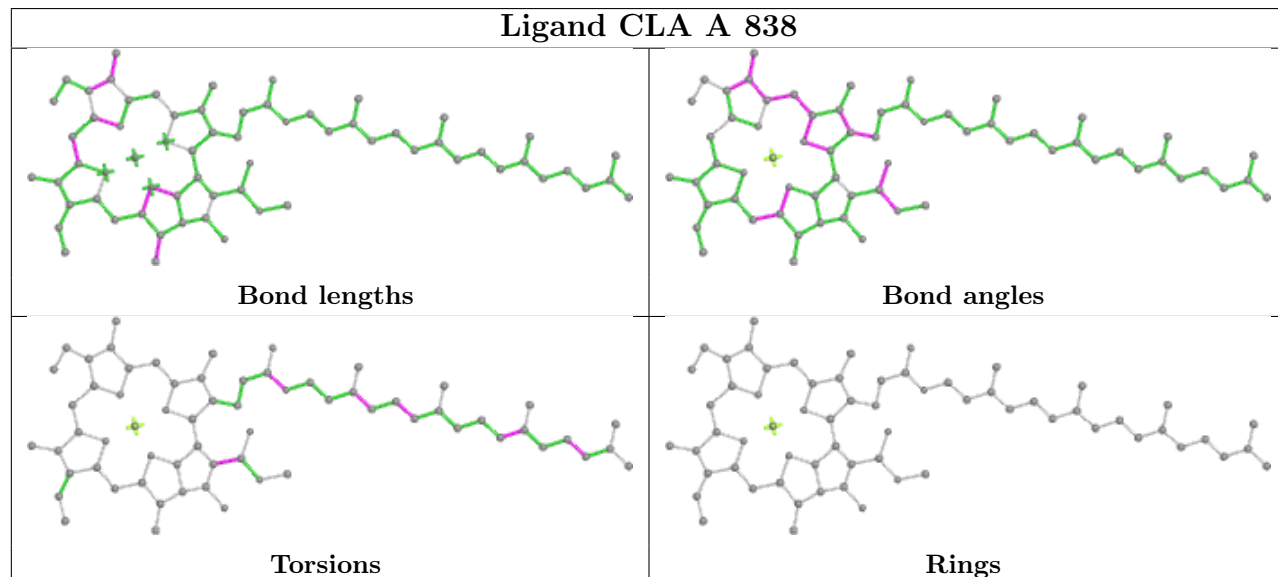
Ligand CLA O 202

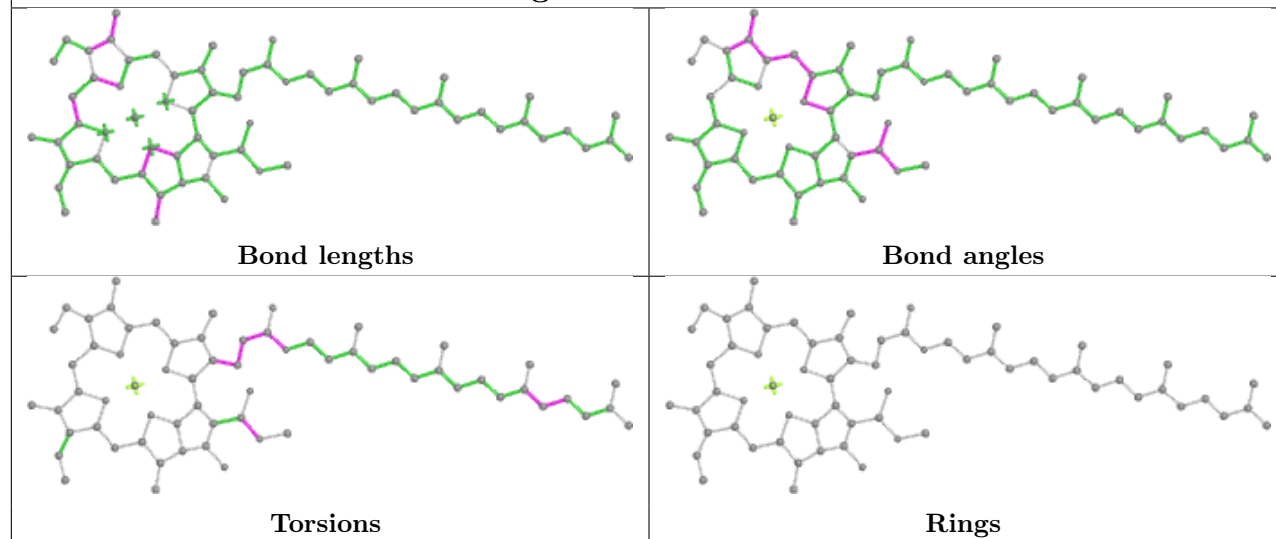
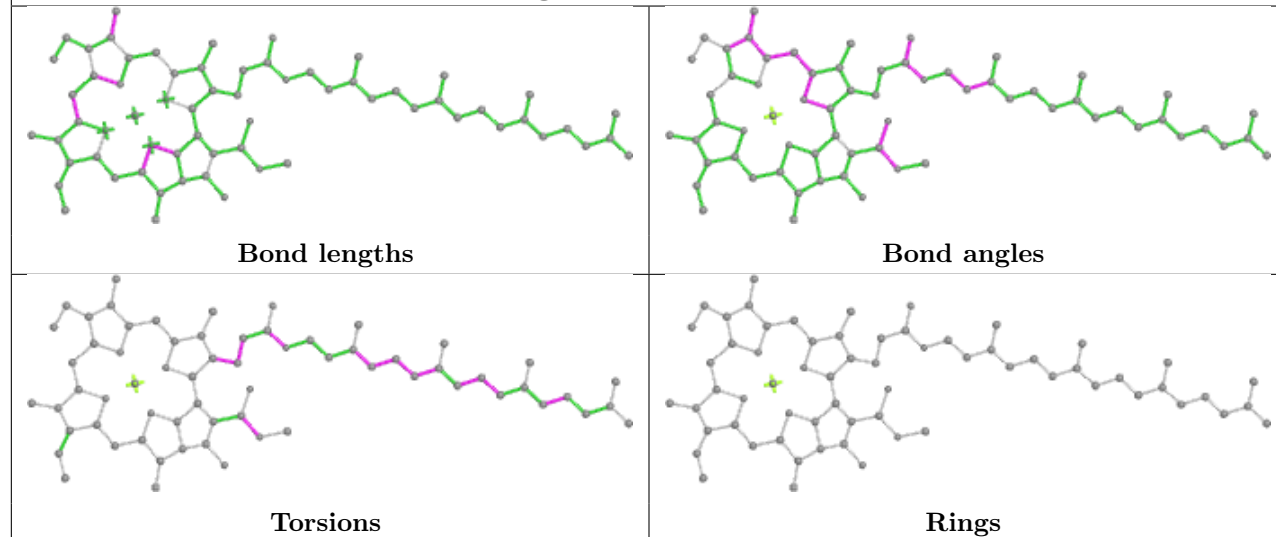


Ligand CLA d 318

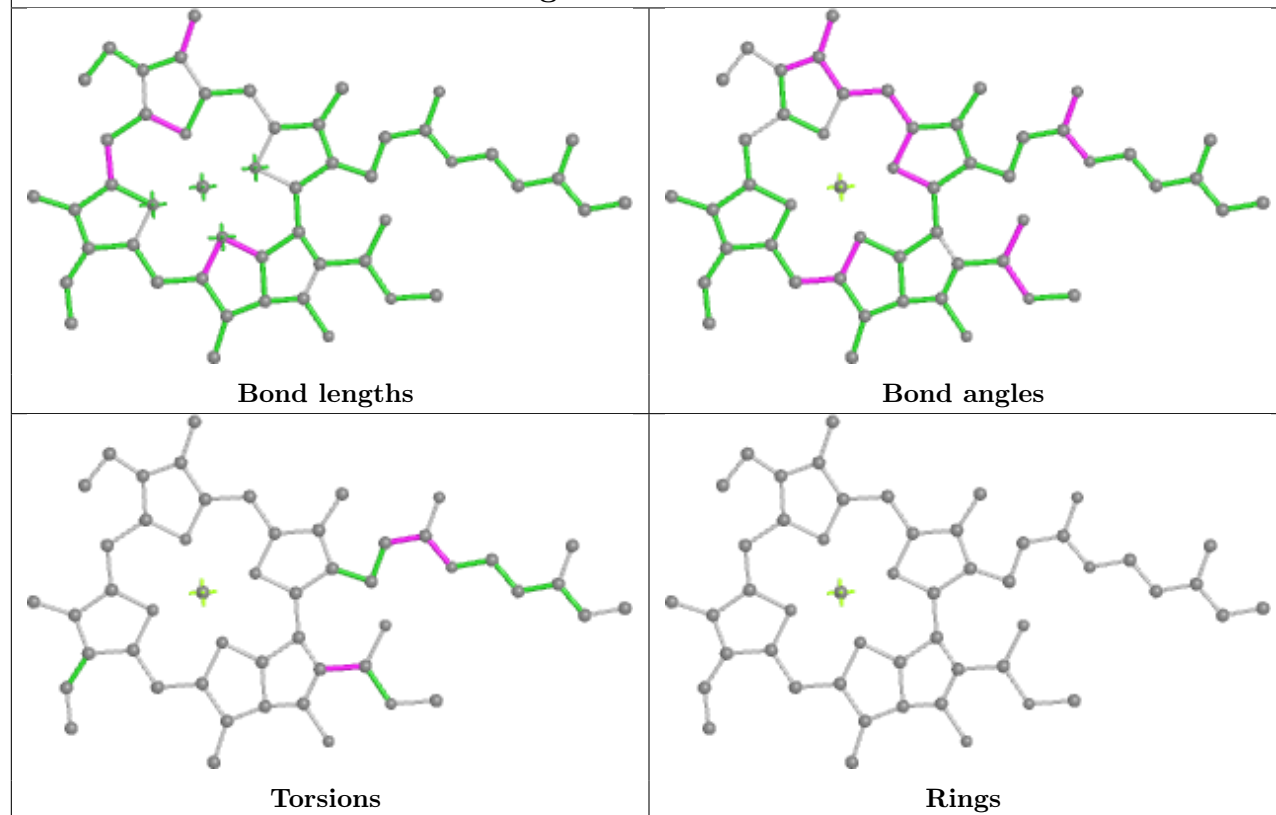


Ligand CLA A 838

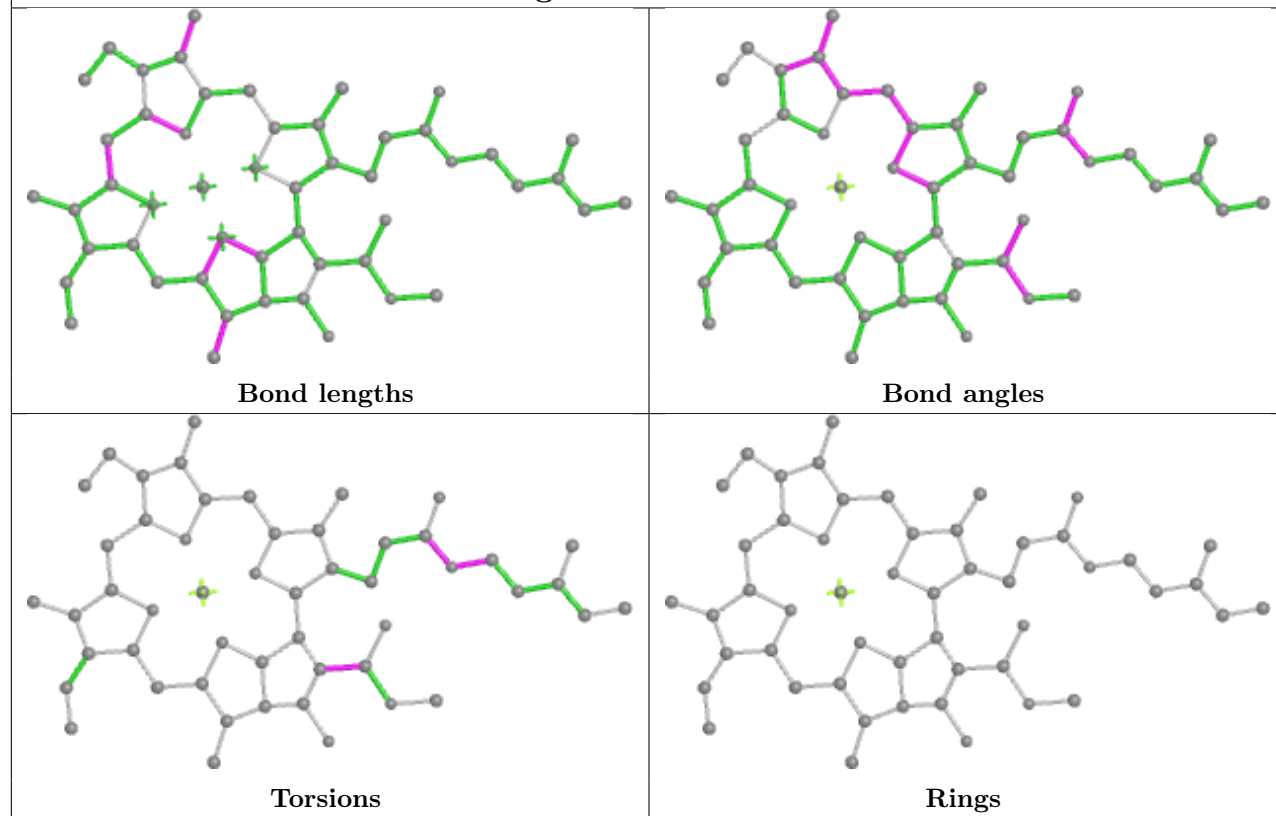


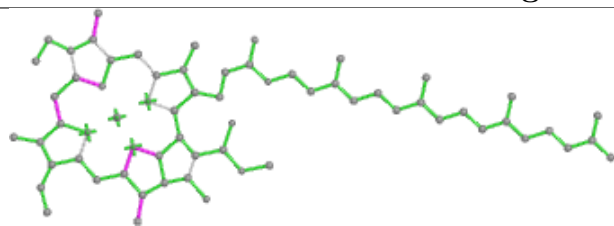
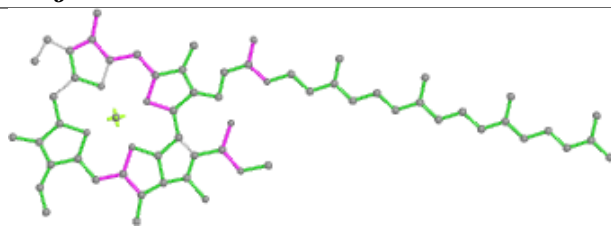
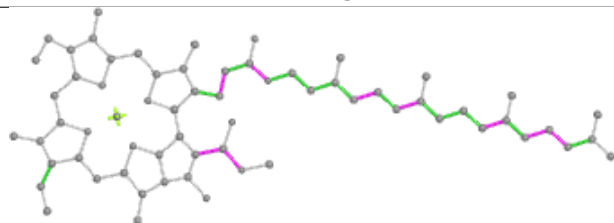
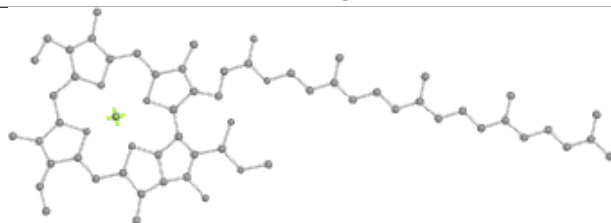
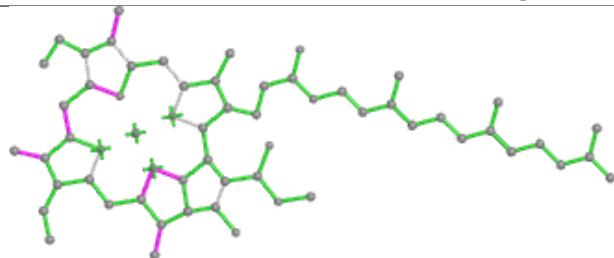
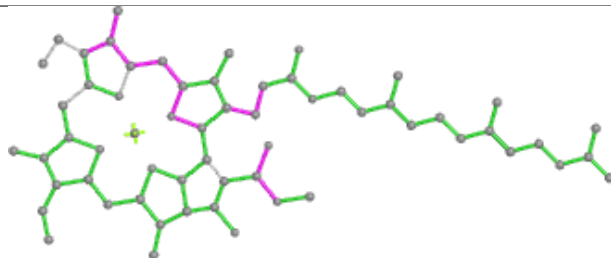
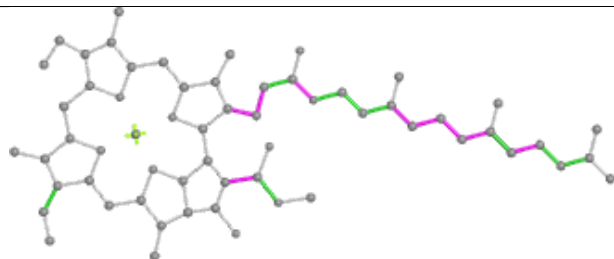
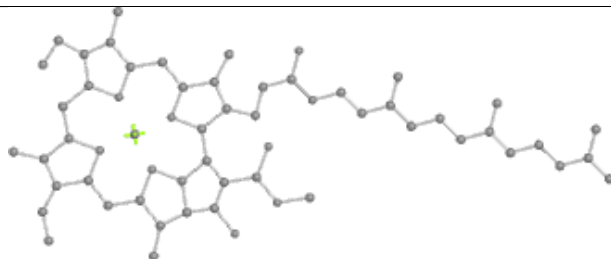
Ligand CLA A 837**Ligand CLA n 608**

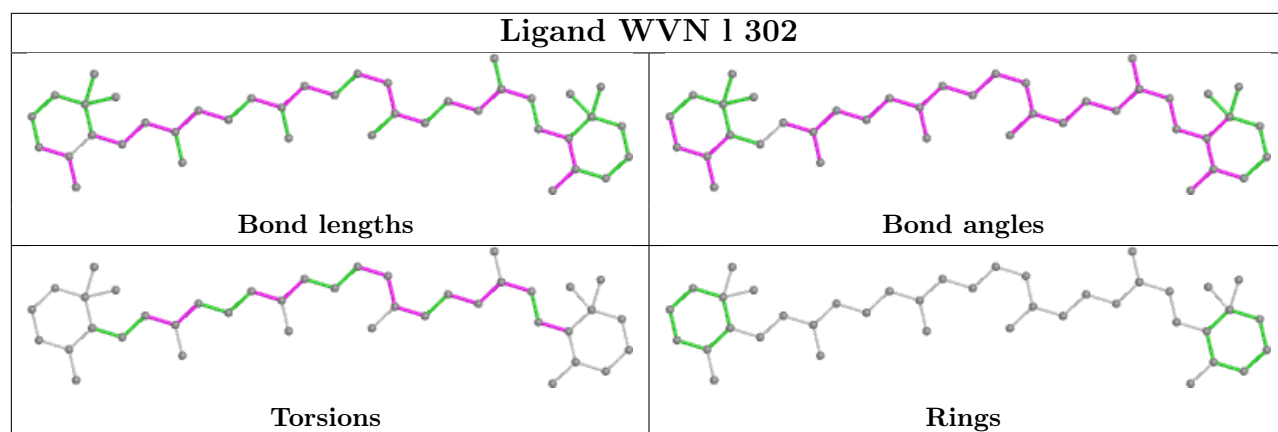
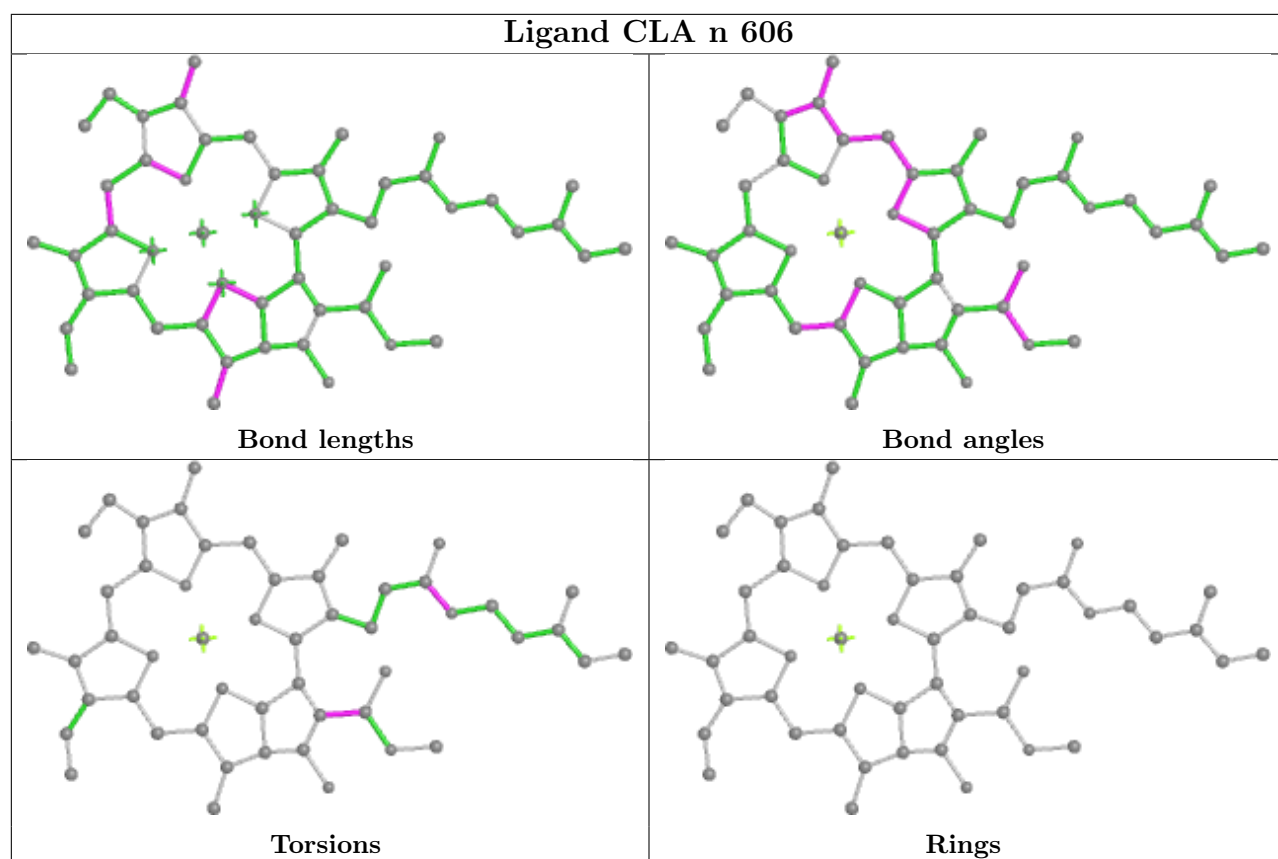
Ligand CLA f 606



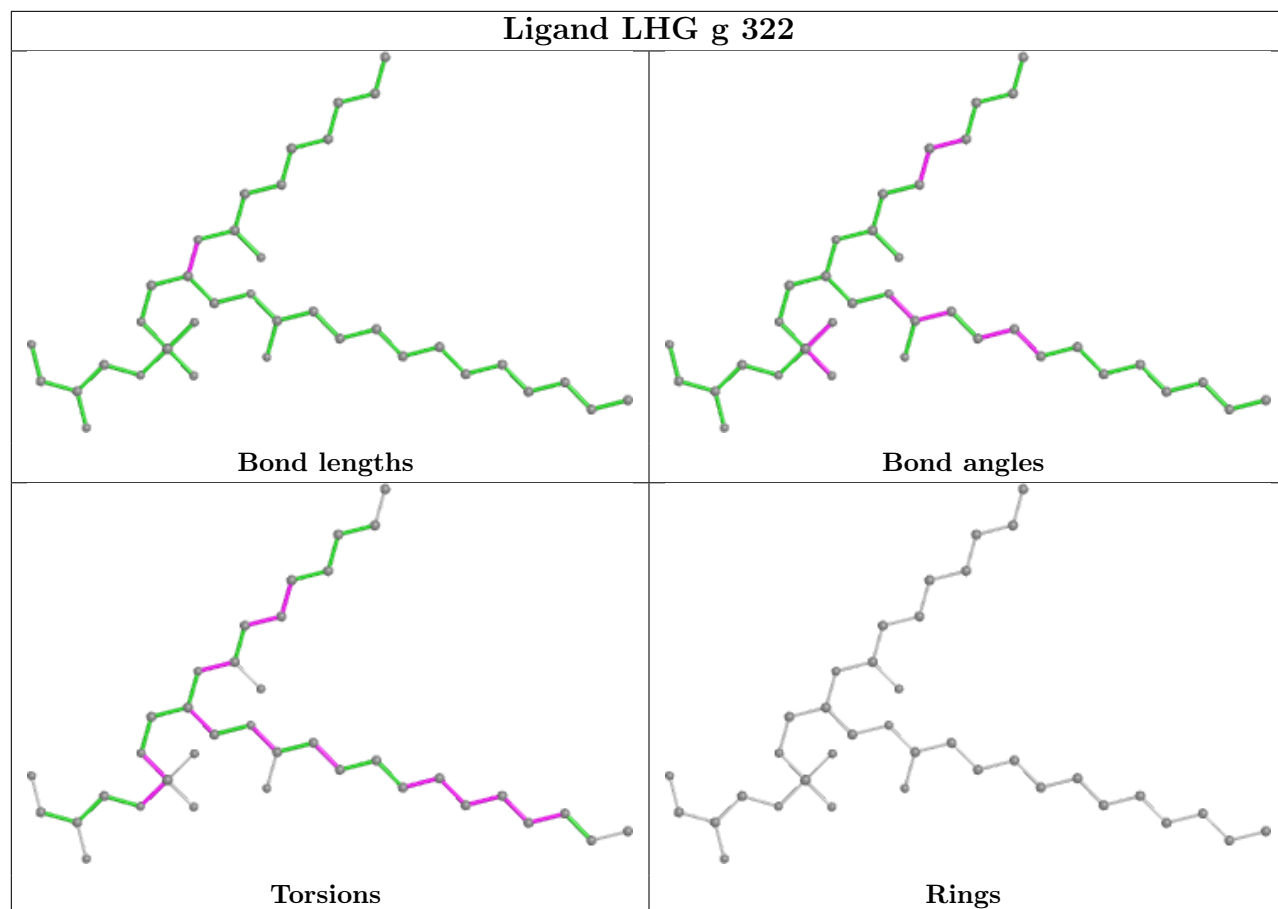
Ligand CLA b 302



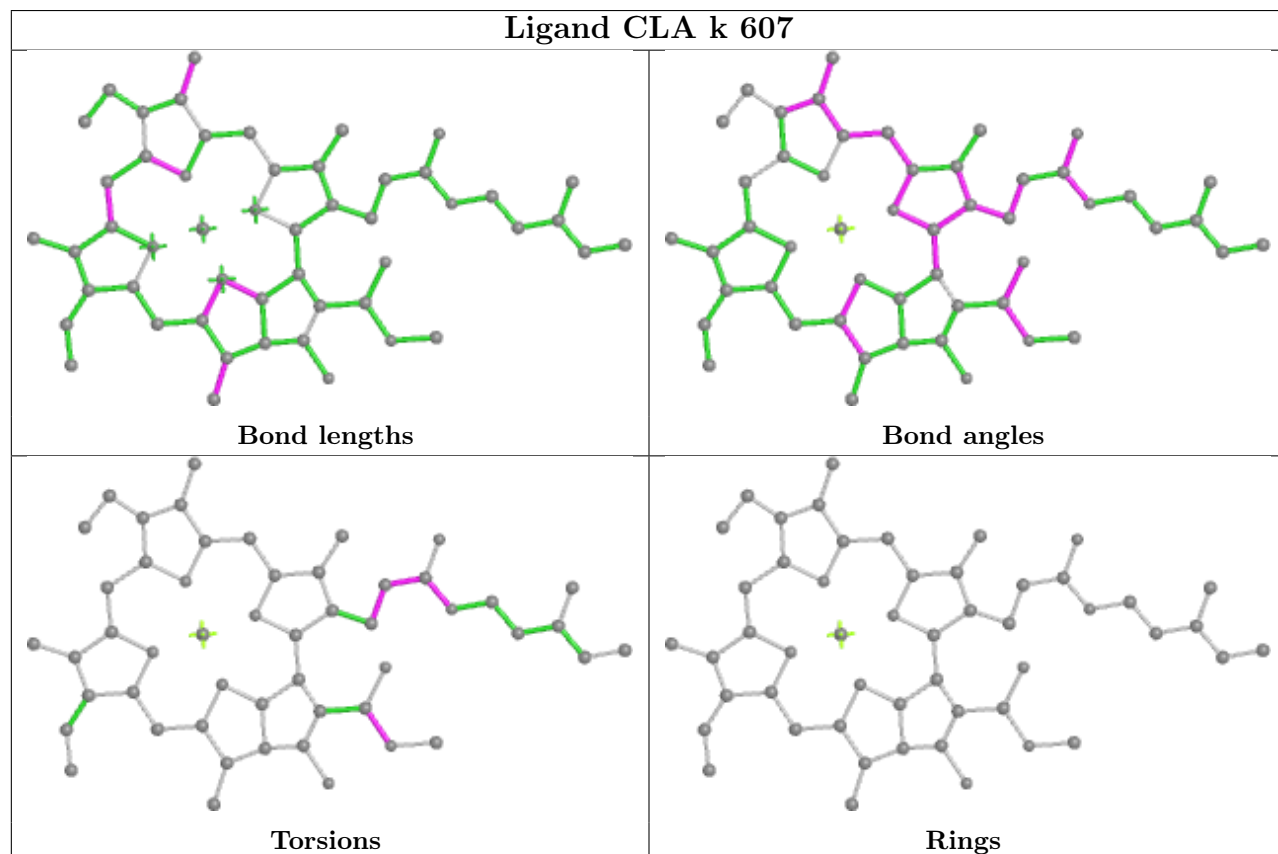
Ligand CLA j 314**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 813****Bond lengths****Bond angles****Torsions****Rings**



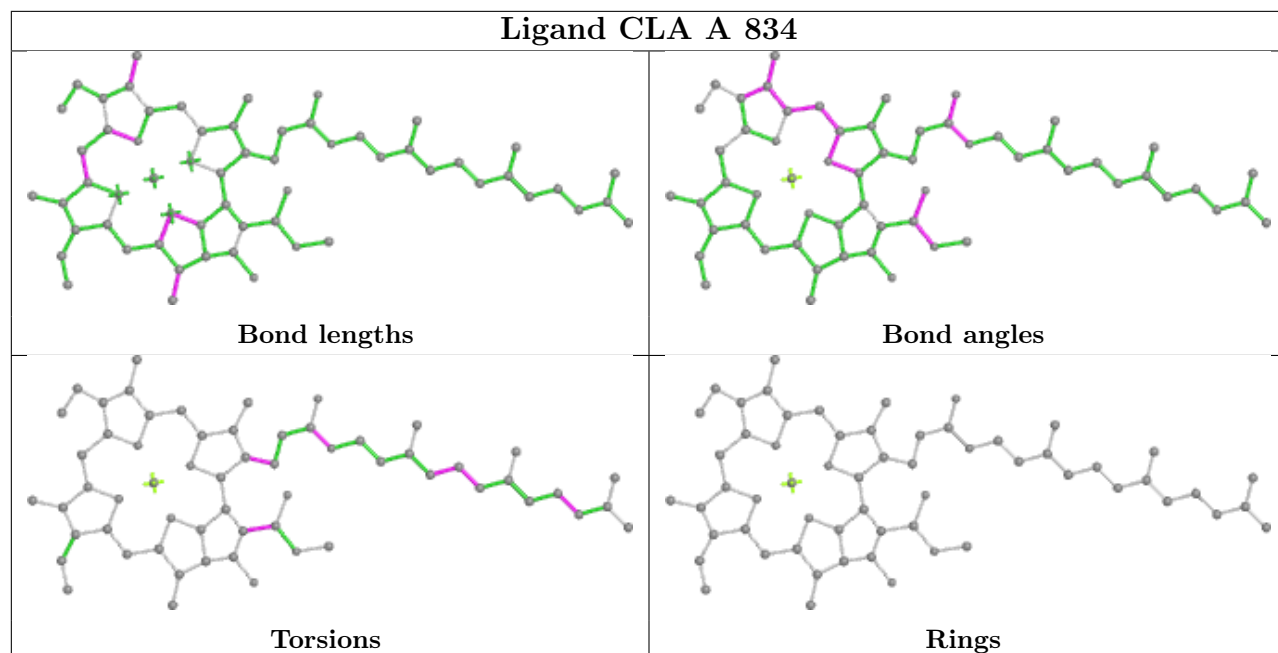
Ligand LHG g 322



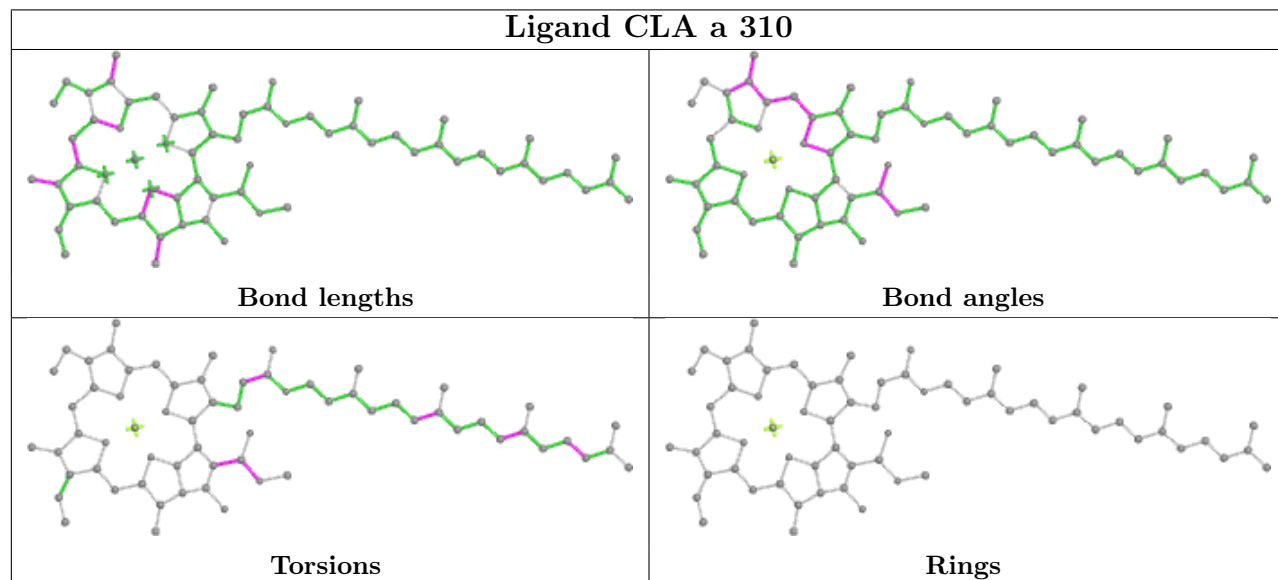
Ligand CLA k 607



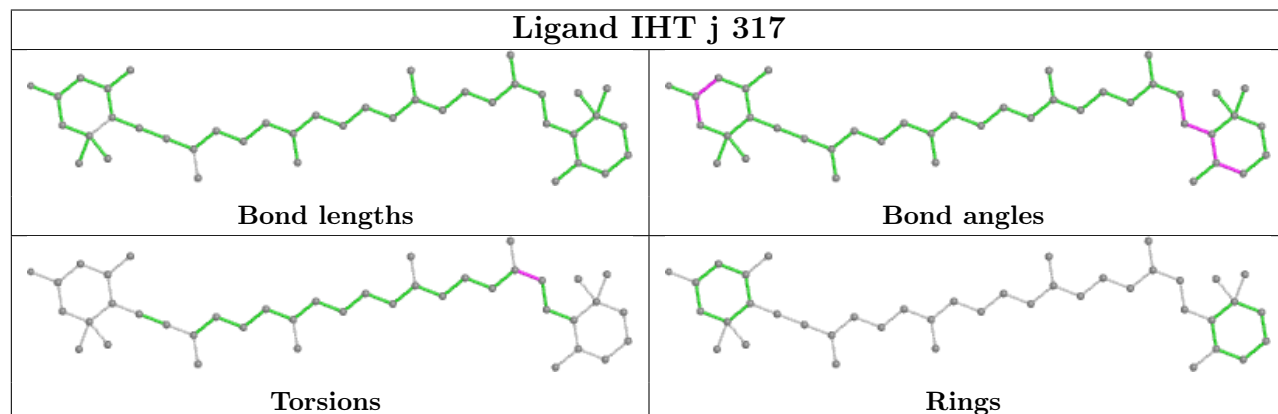
Ligand CLA A 834

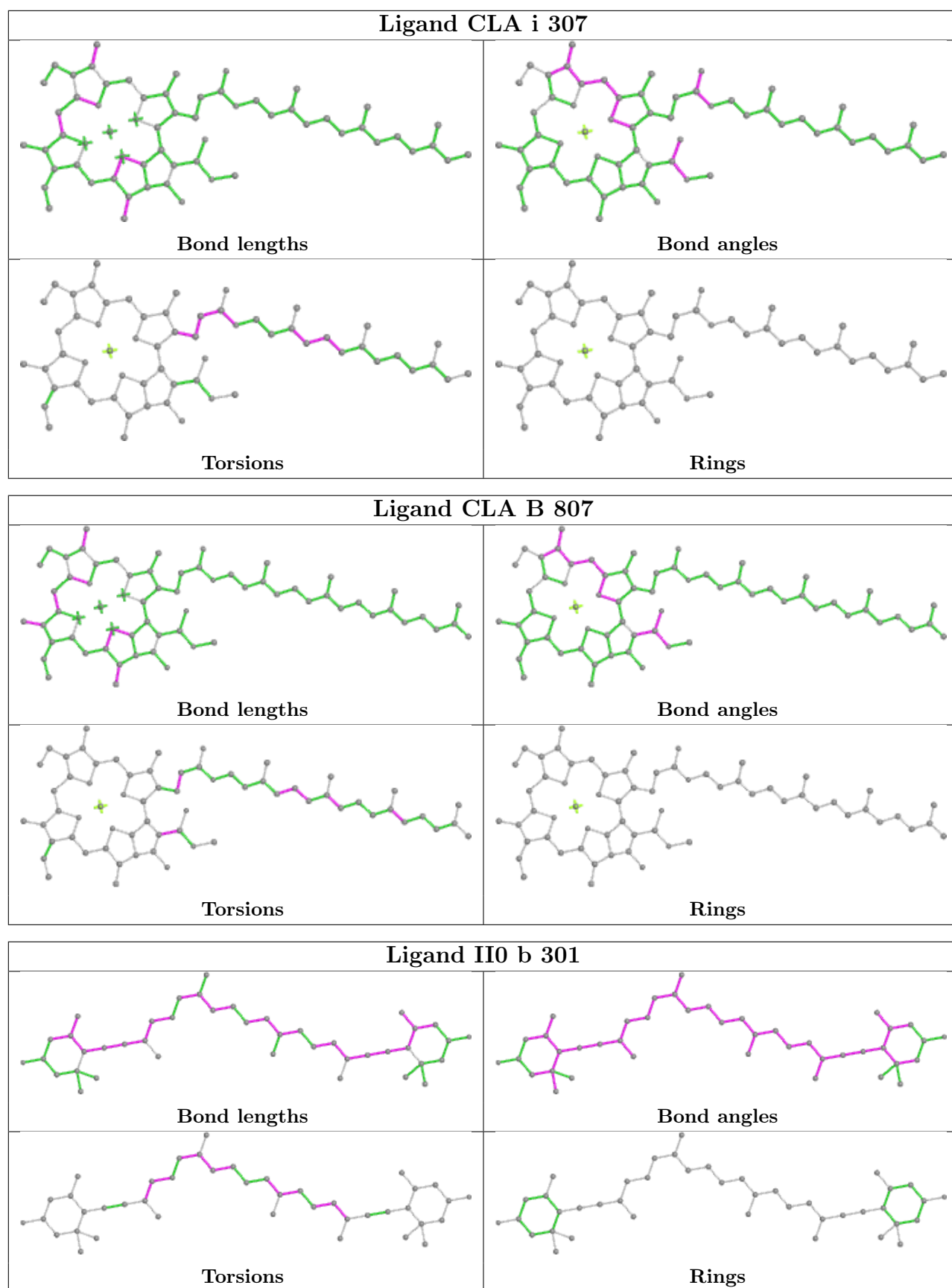


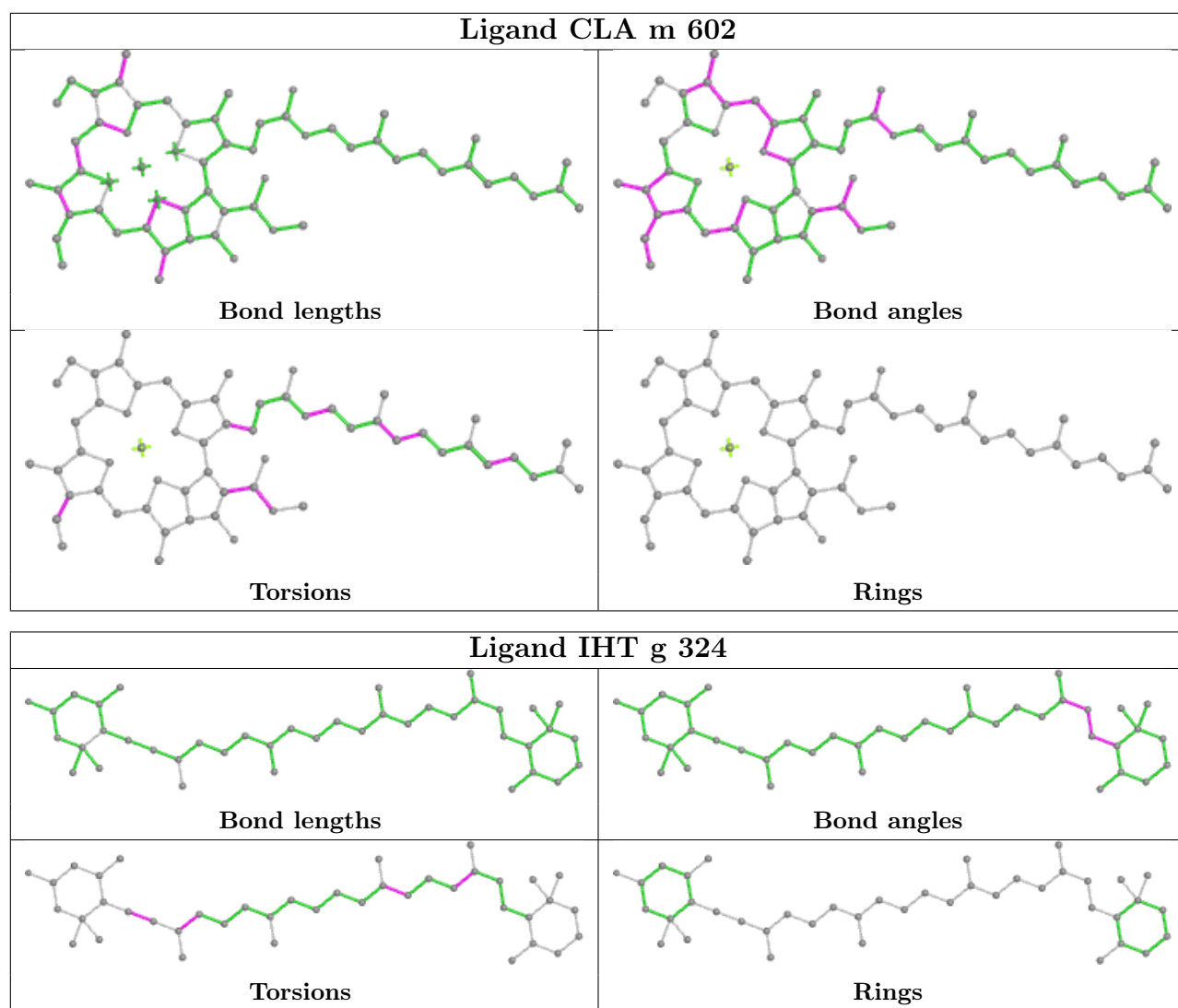
Ligand CLA a 310



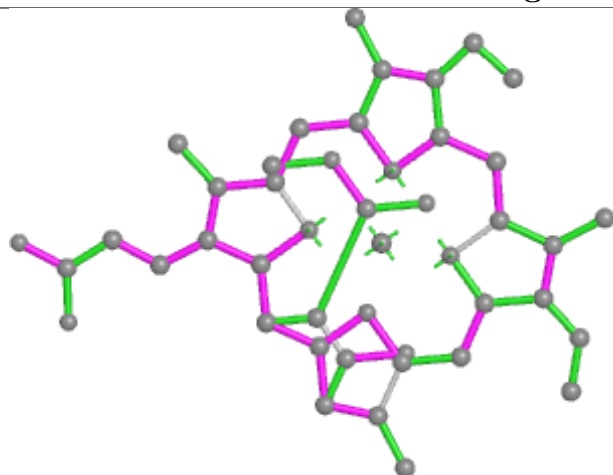
Ligand IHT j 317



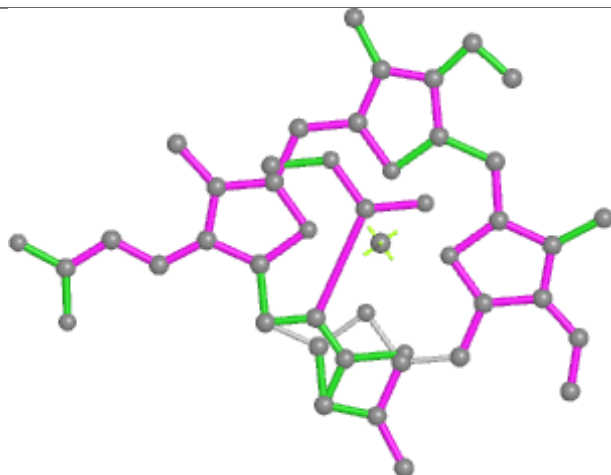




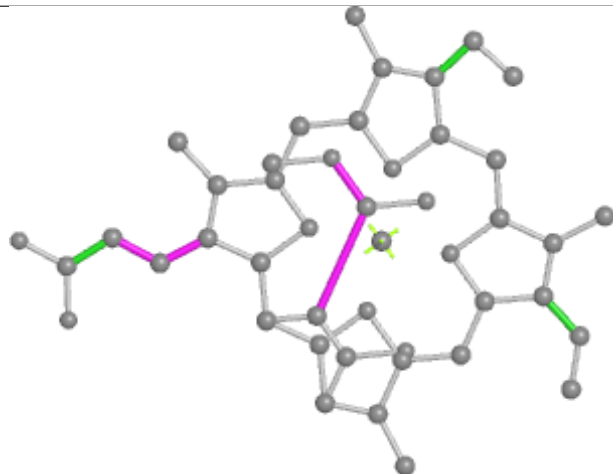
Ligand KC2 l 311



Bond lengths



Bond angles

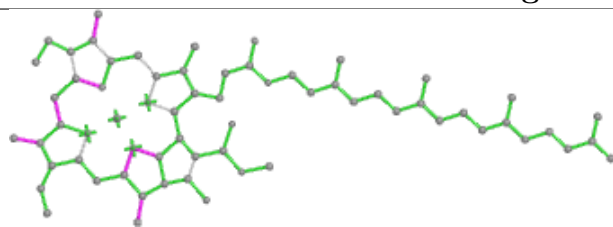


Torsions

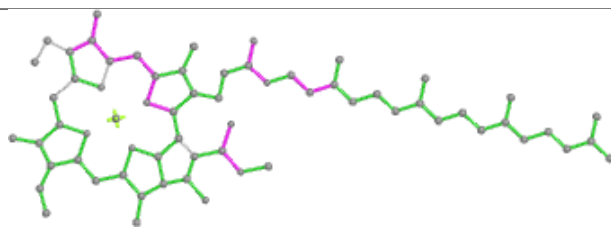


Rings

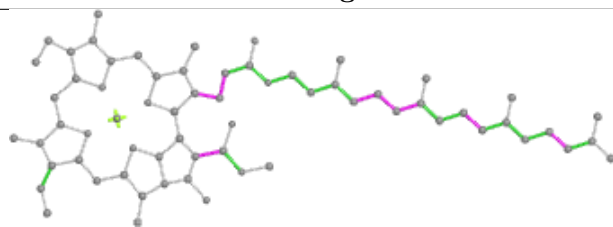
Ligand CLA f 609



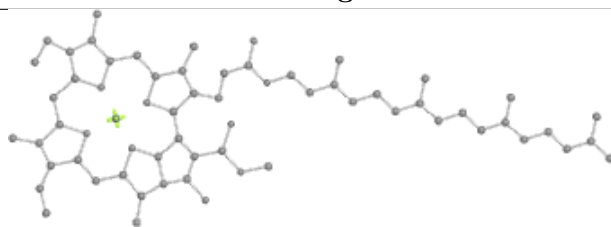
Bond lengths



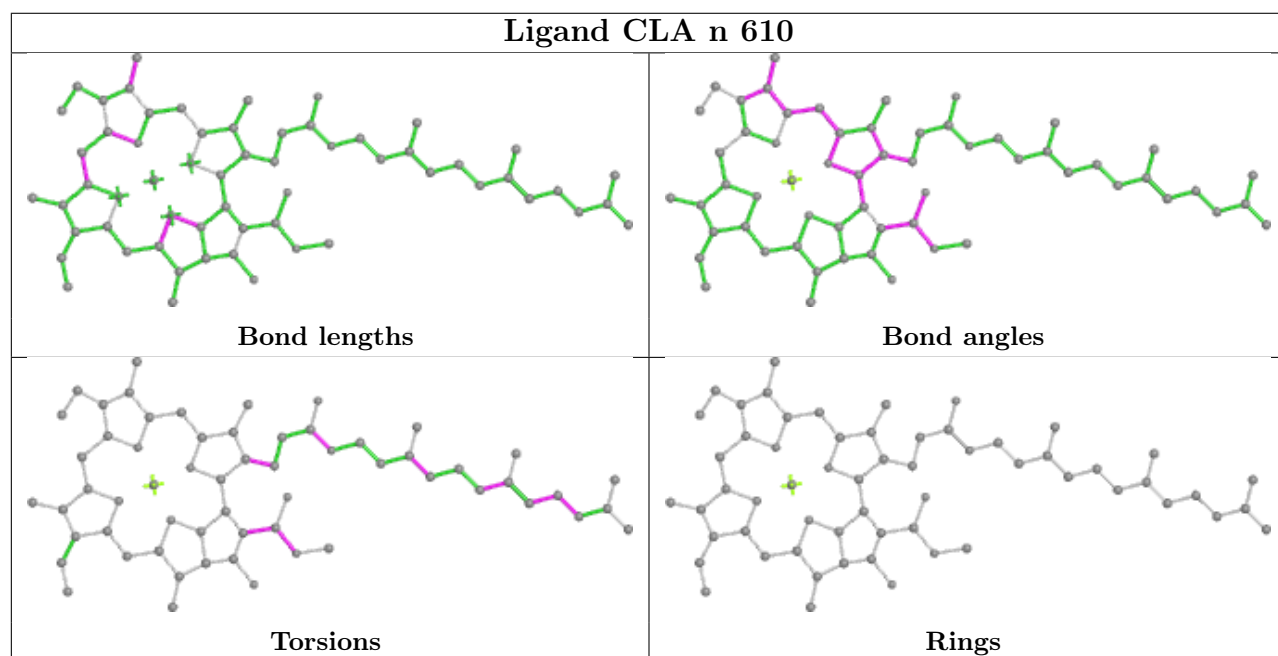
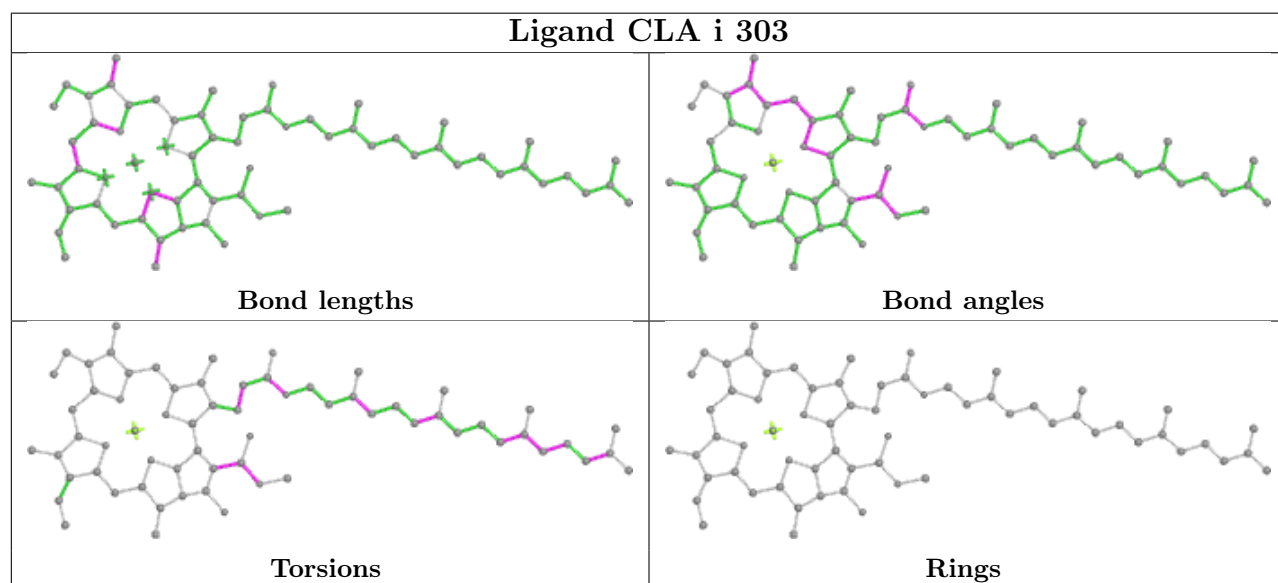
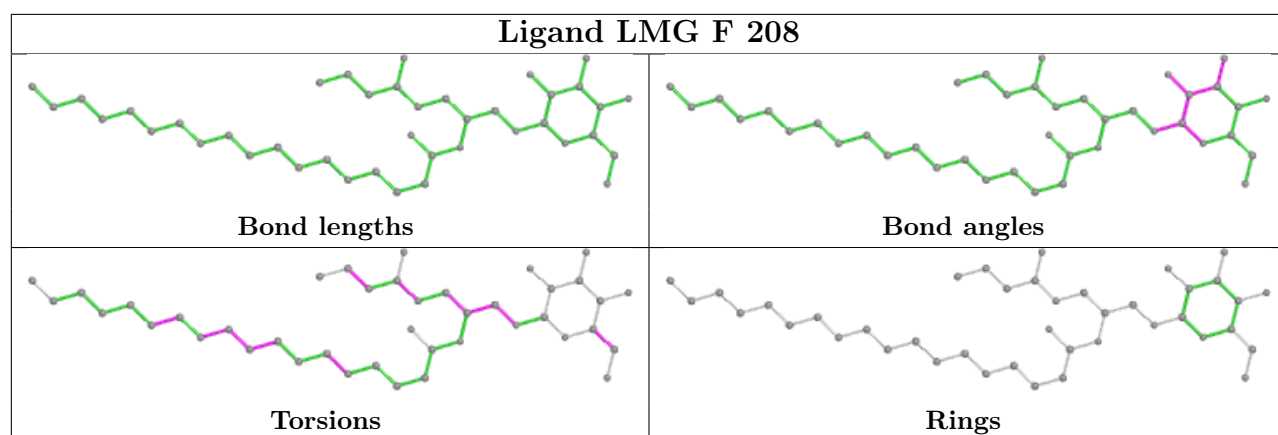
Bond angles



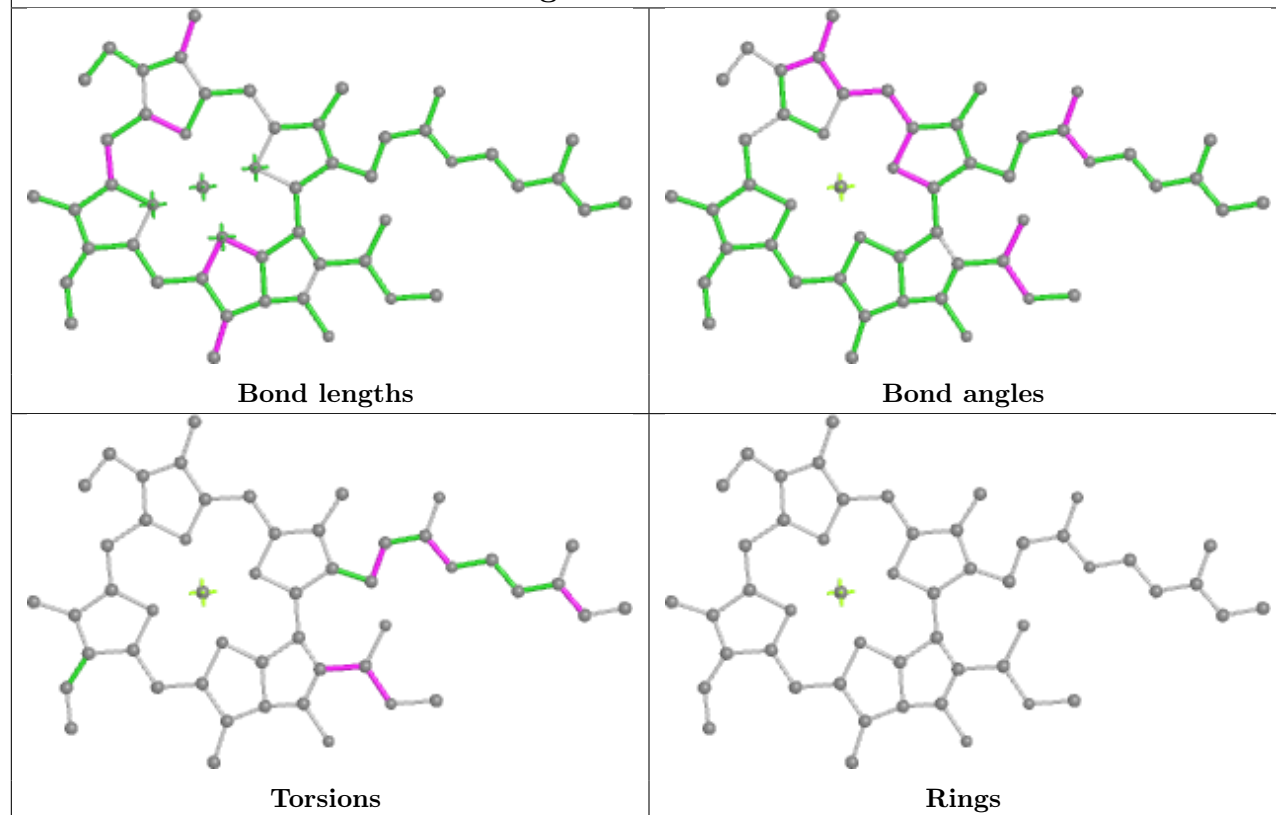
Torsions



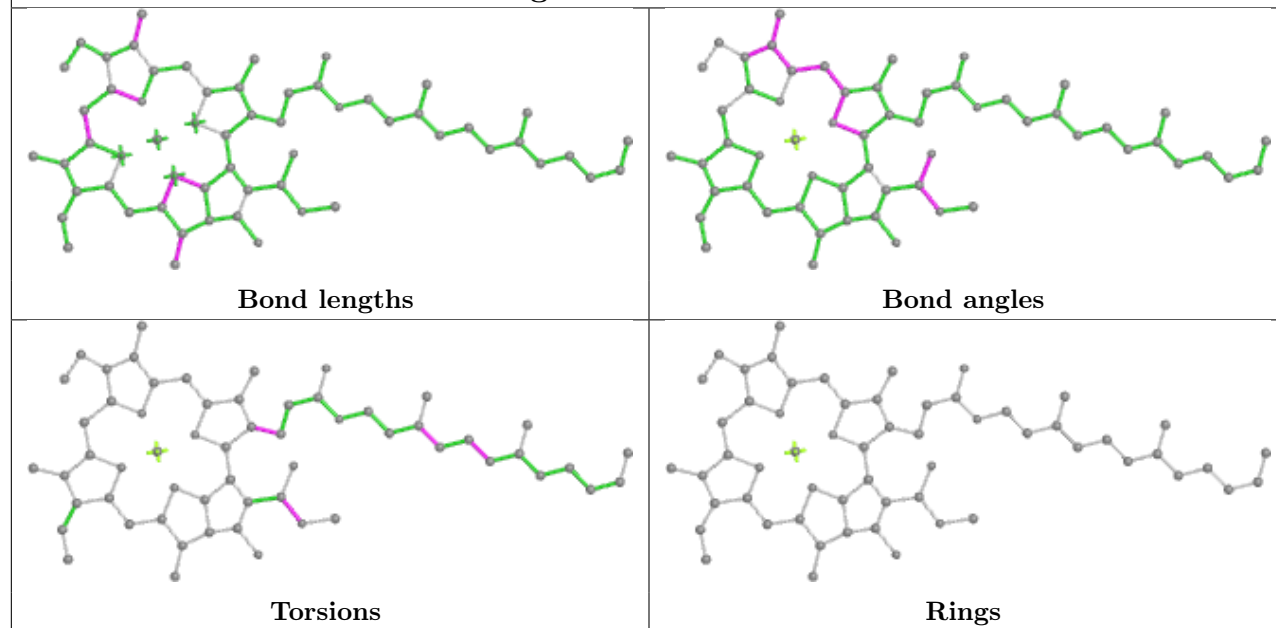
Rings



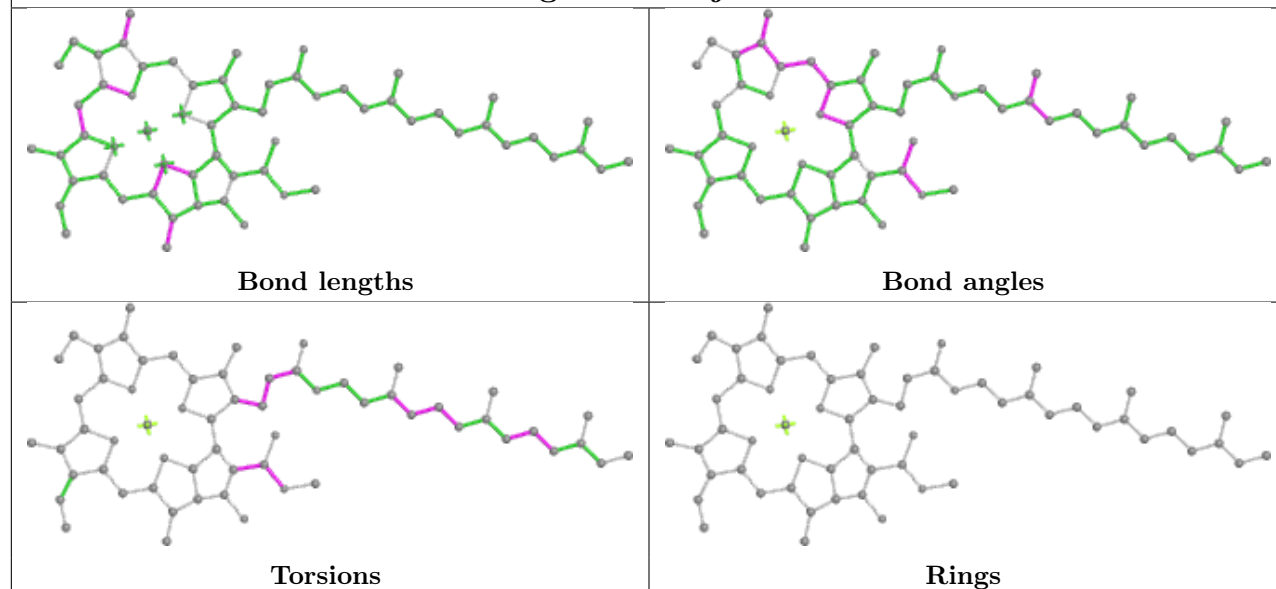
Ligand CLA f 612



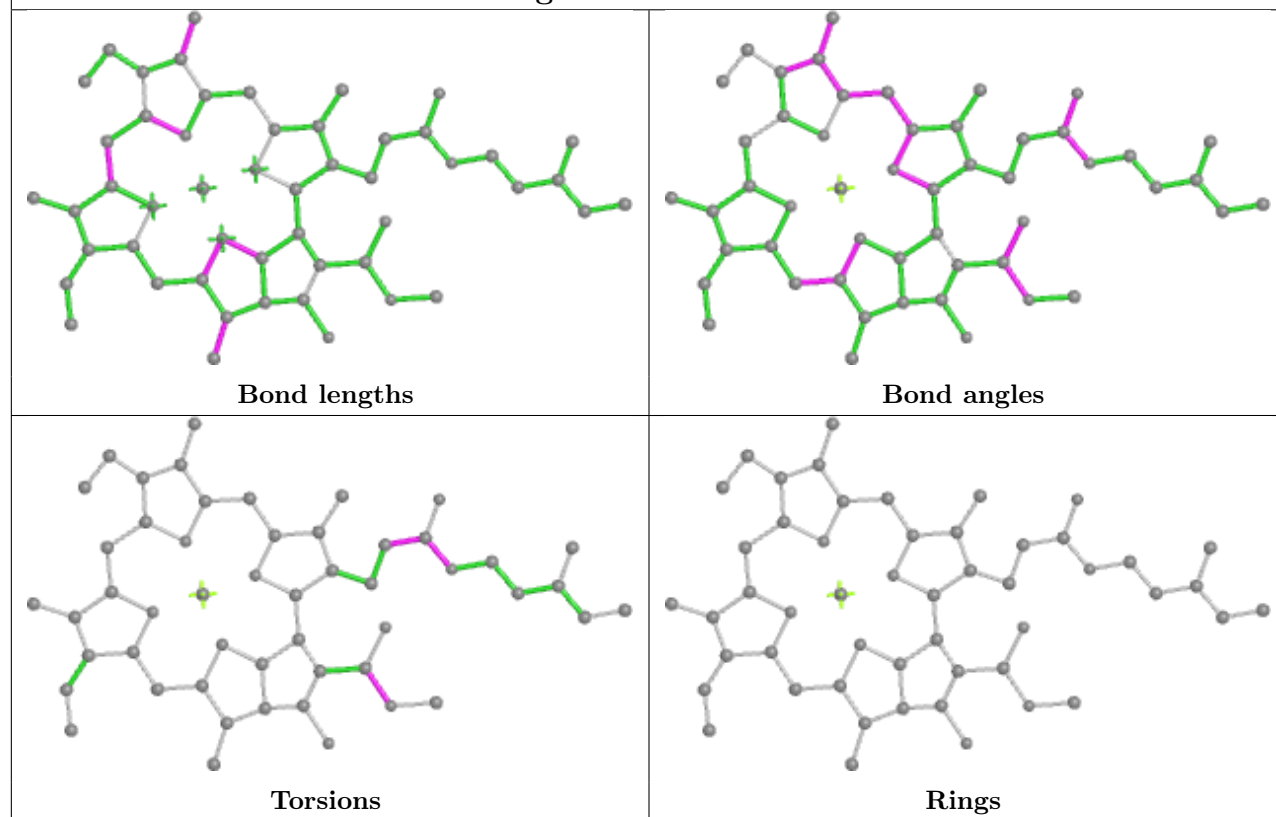
Ligand CLA m 603

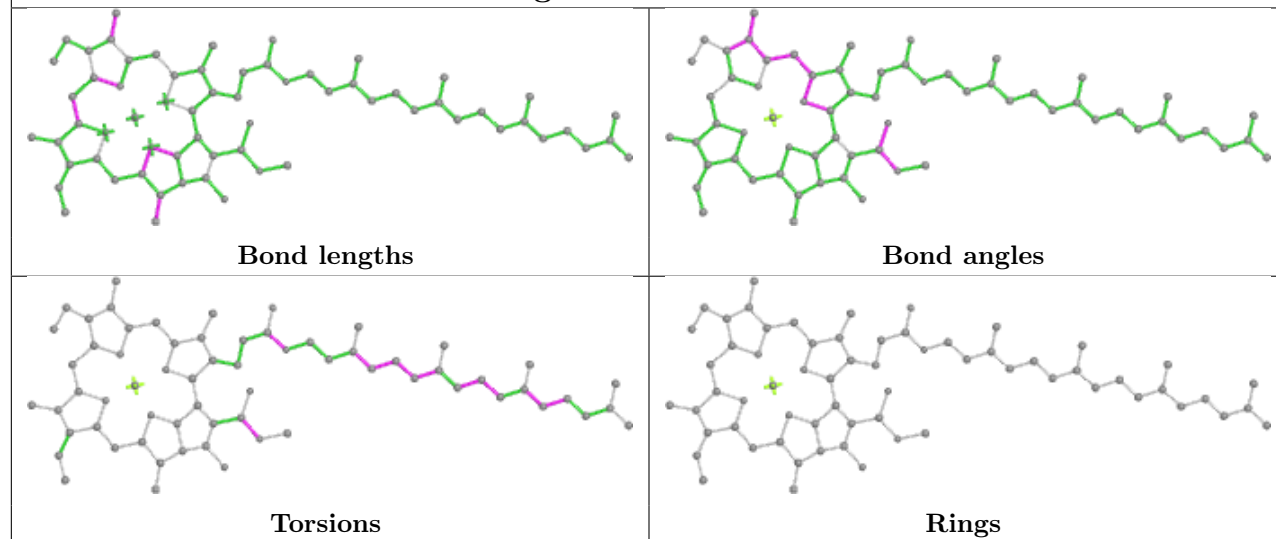
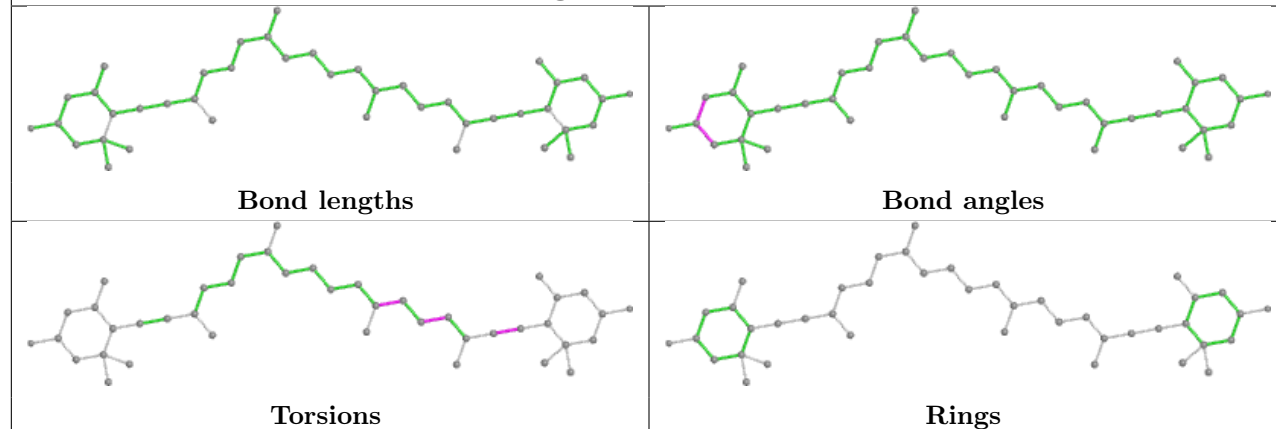
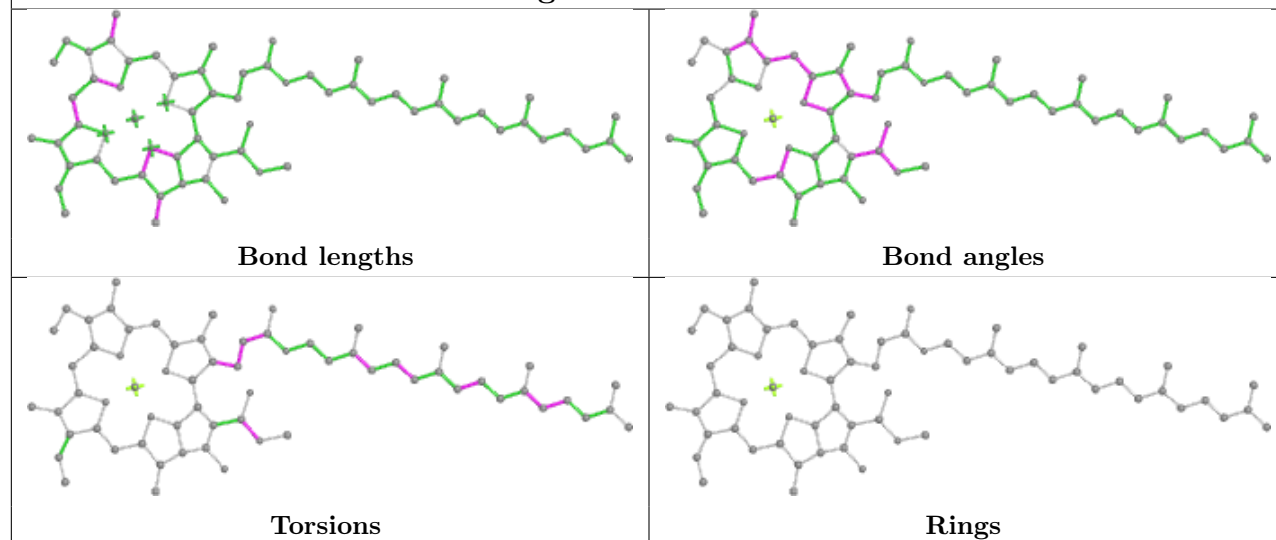


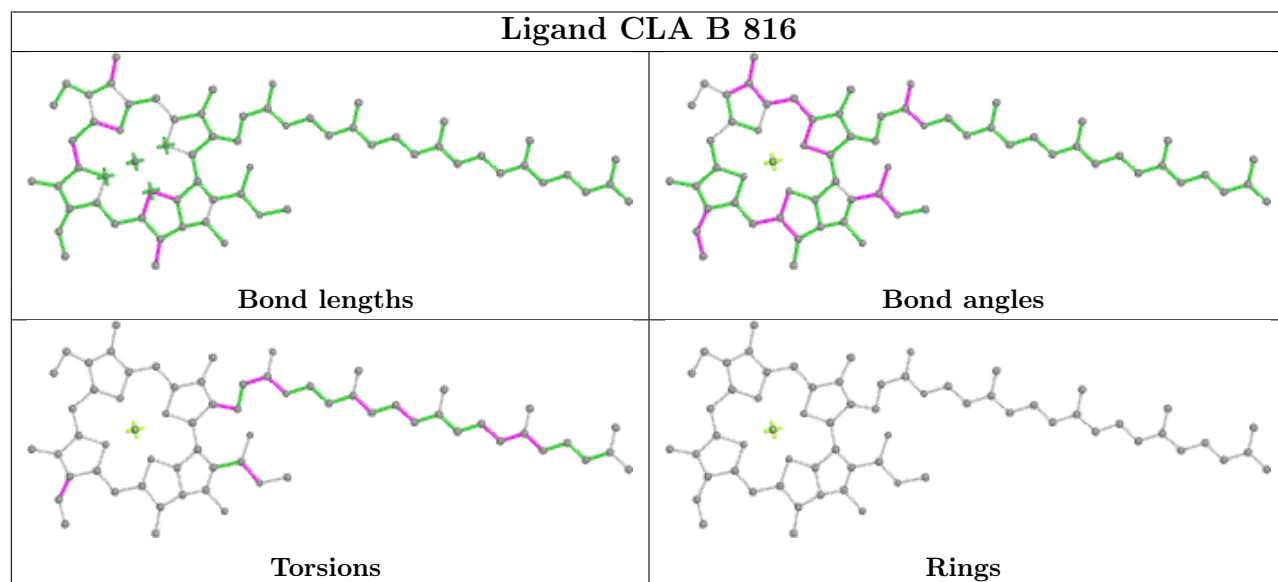
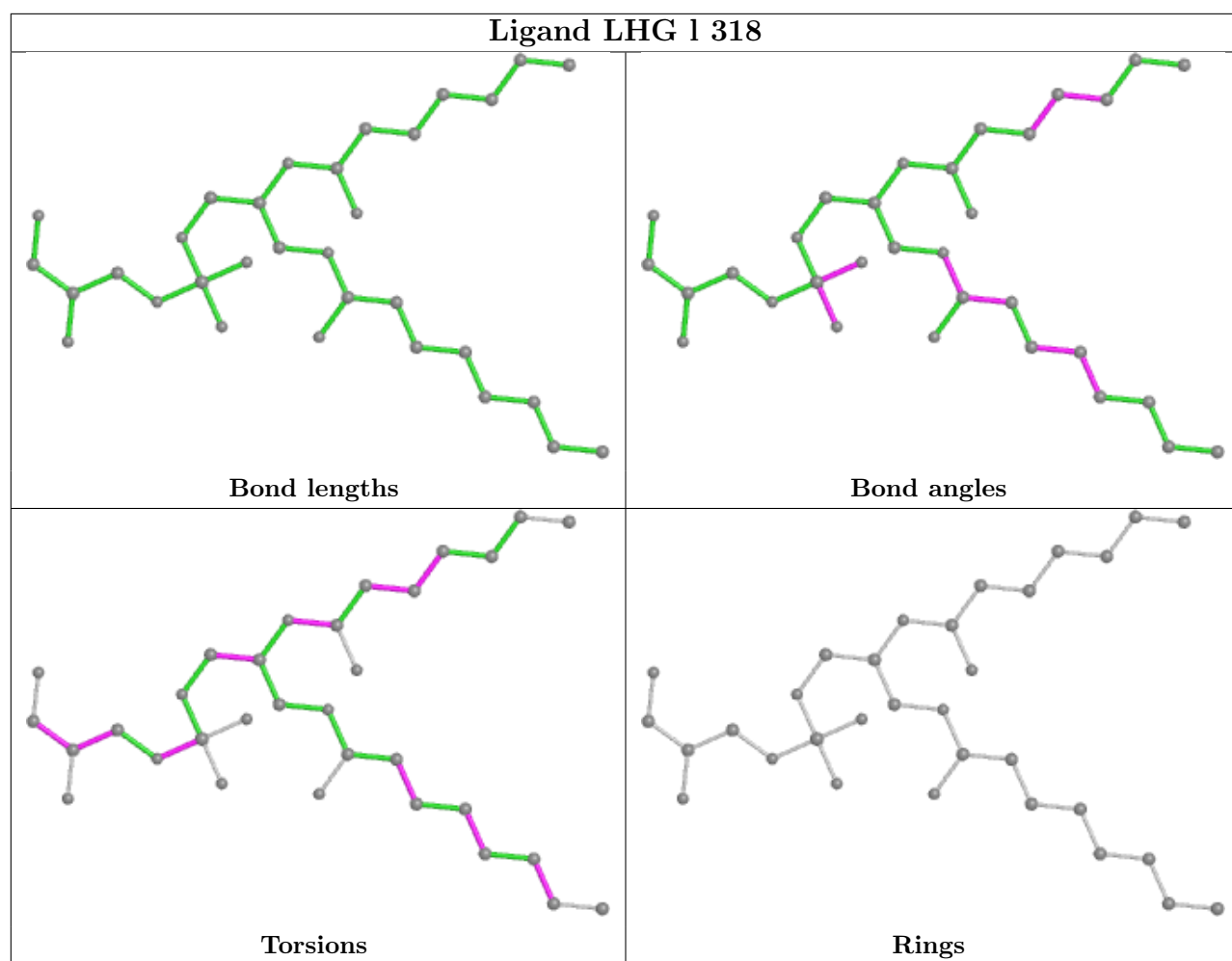
Ligand CLA j 311



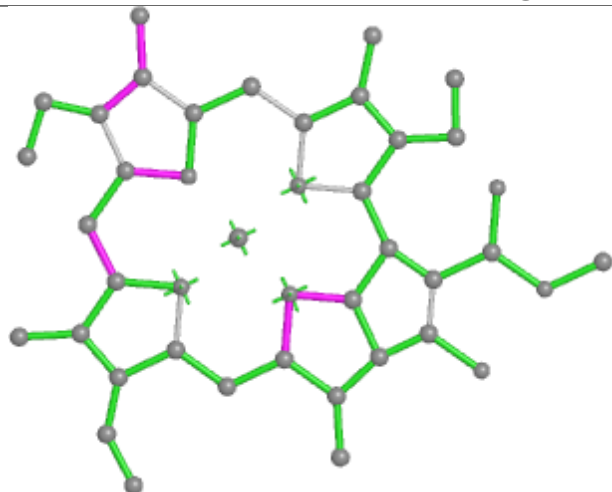
Ligand CLA k 606



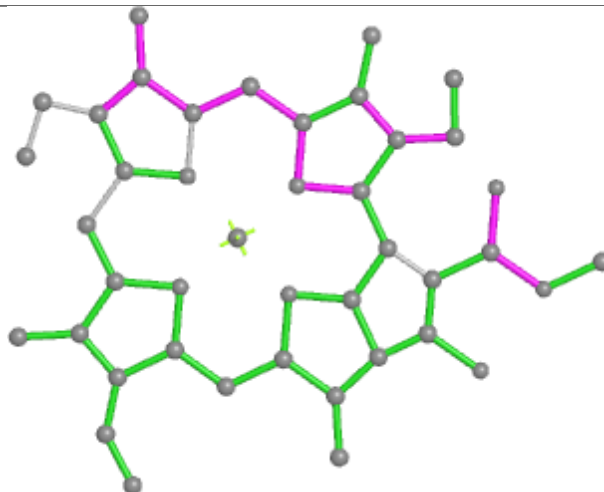
Ligand CLA F 202**Ligand II0 c 314****Ligand CLA s 406**



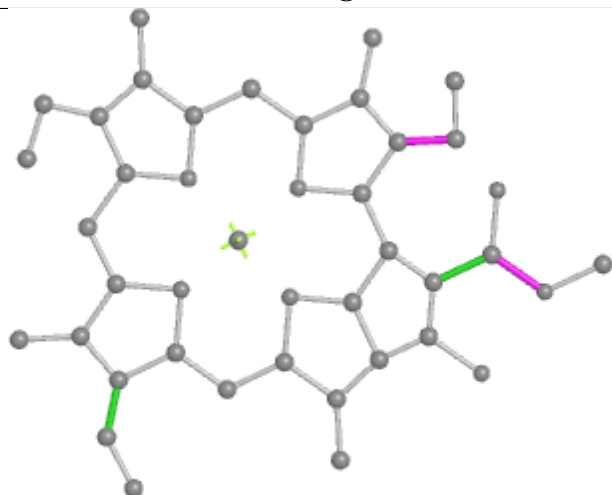
Ligand CLA J 102



Bond lengths



Bond angles

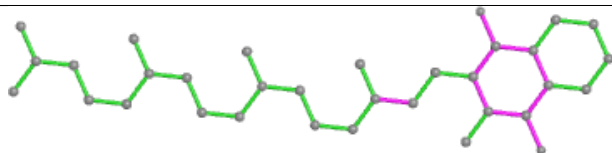


Torsions

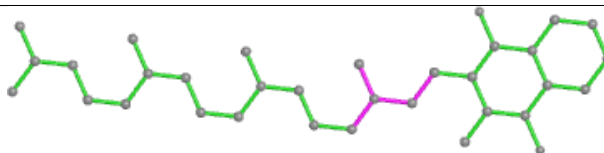


Rings

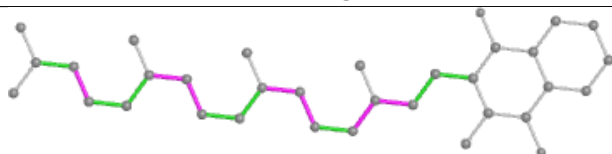
Ligand PQN B 843



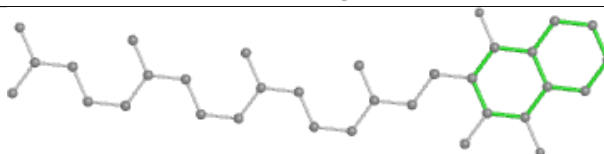
Bond lengths



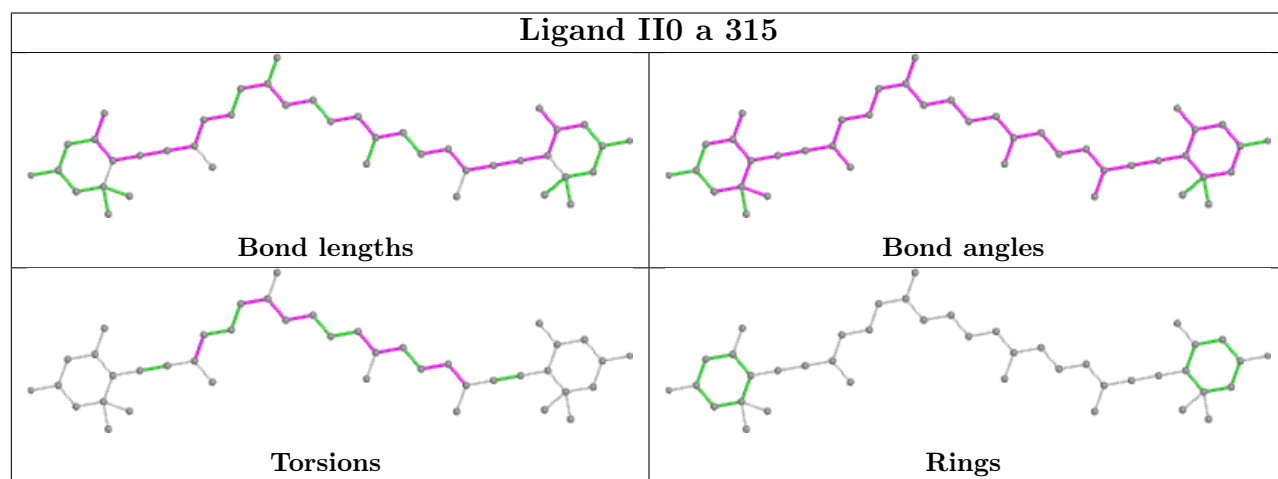
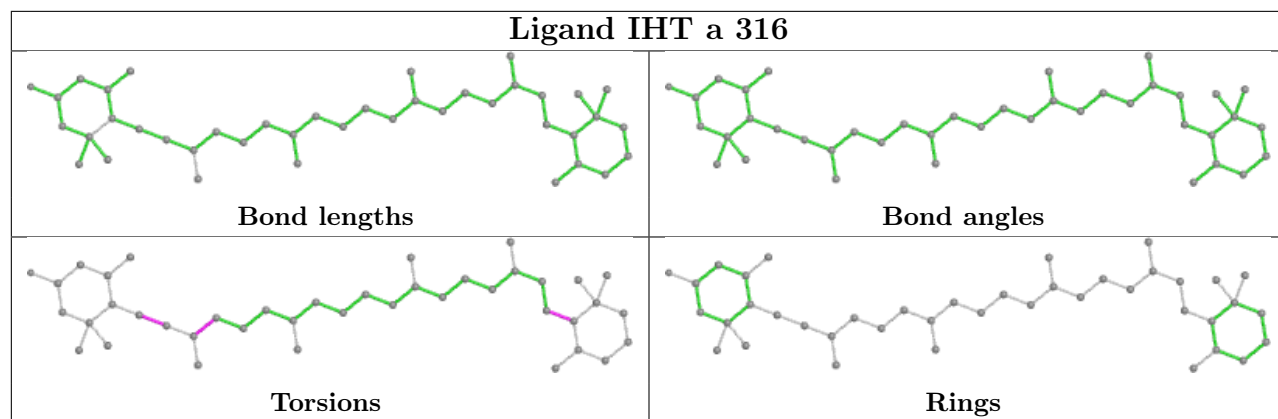
Bond angles



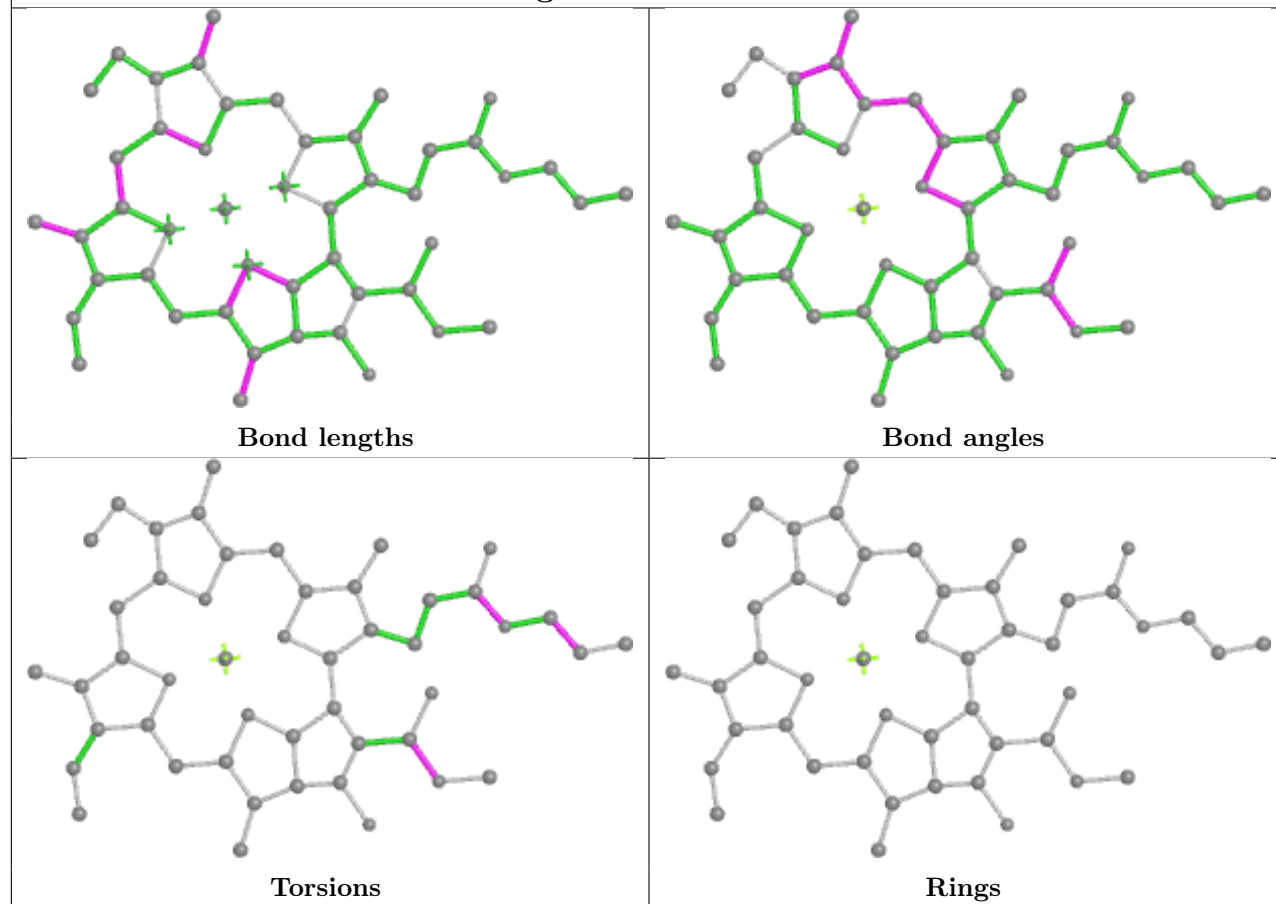
Torsions



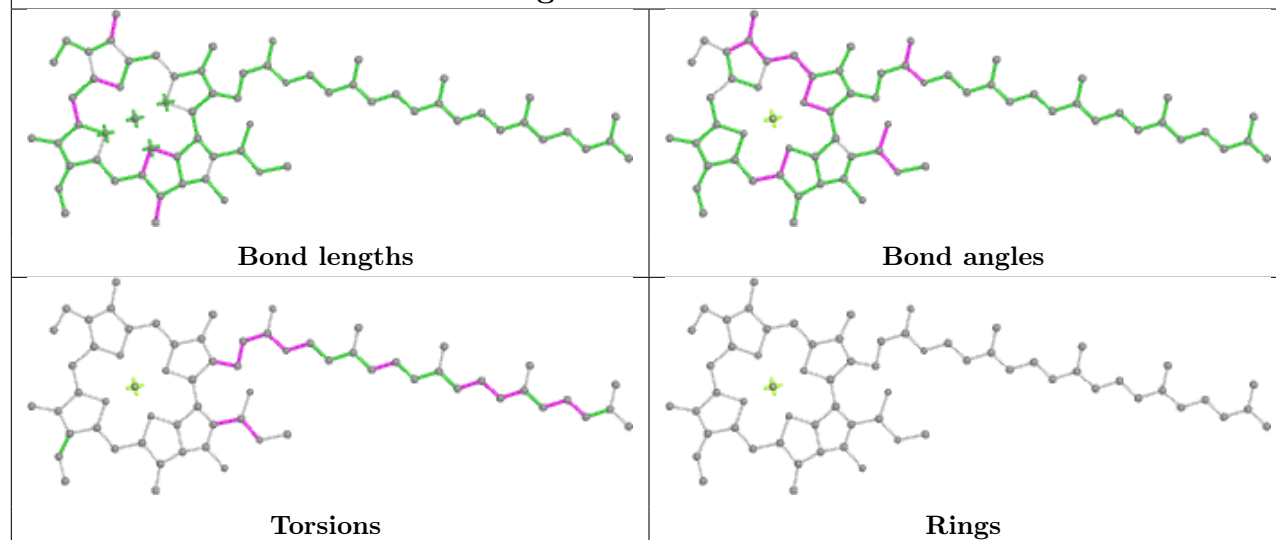
Rings

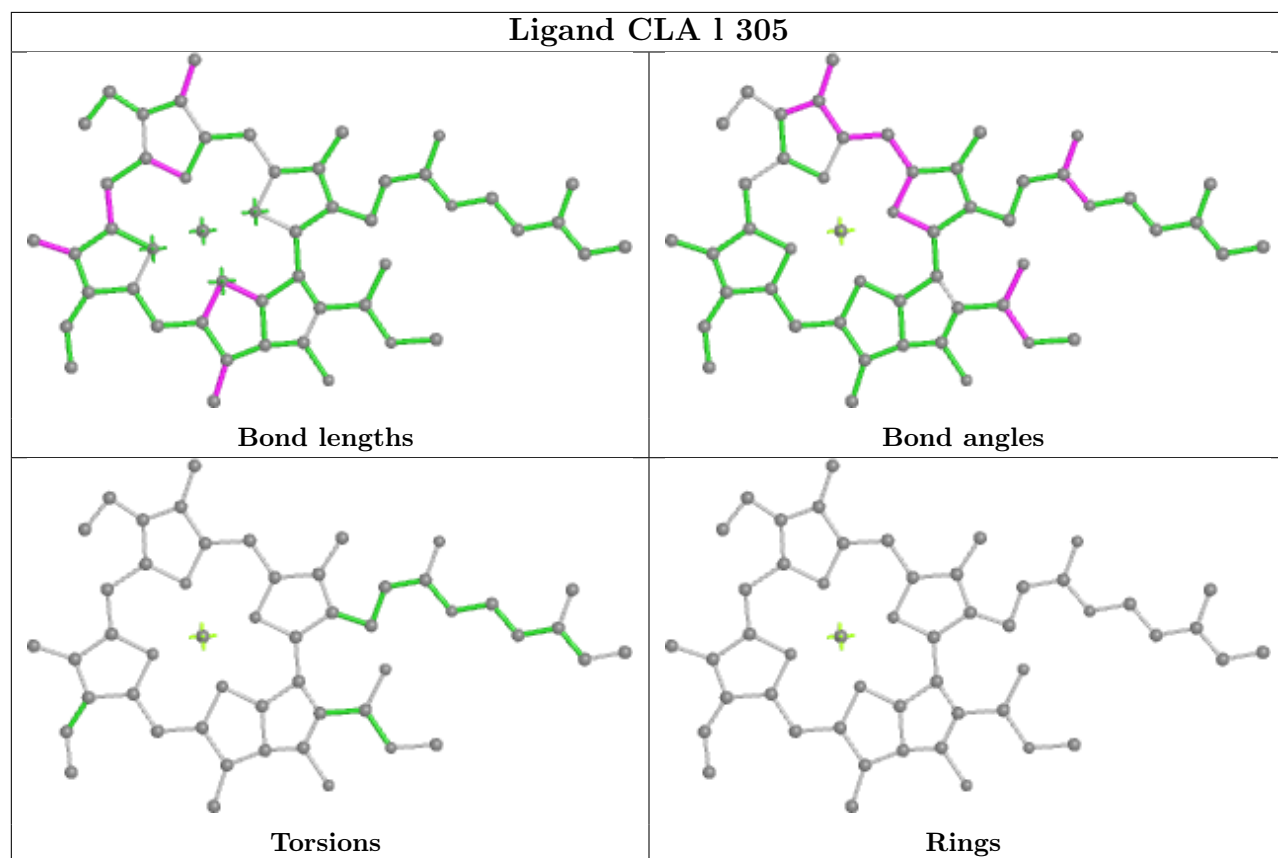
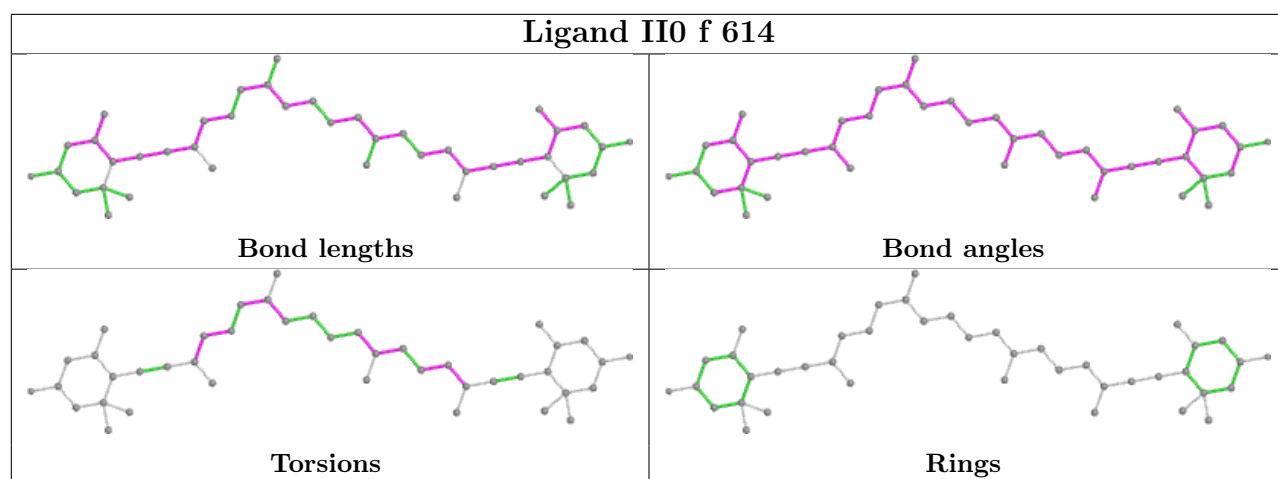


Ligand CLA a 309

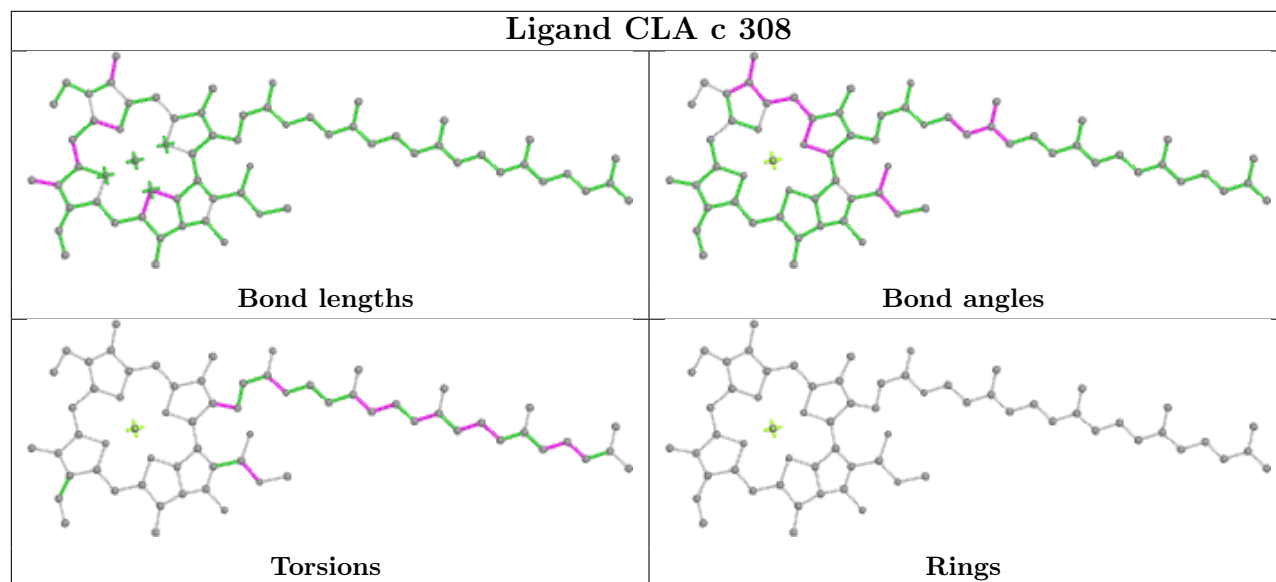


Ligand CLA e 302

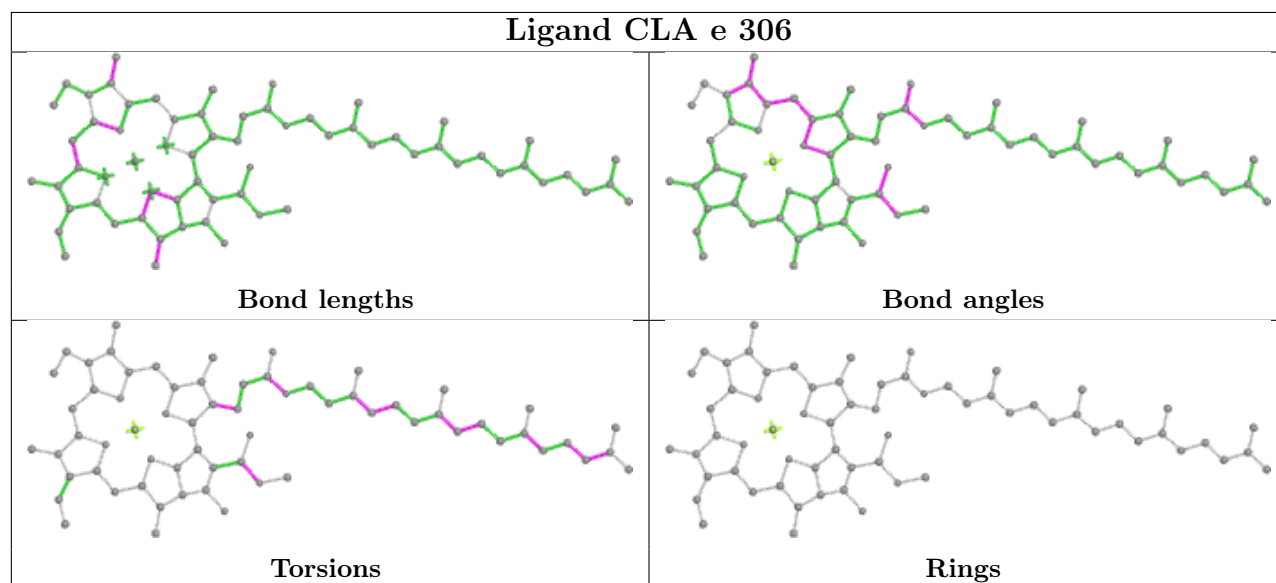




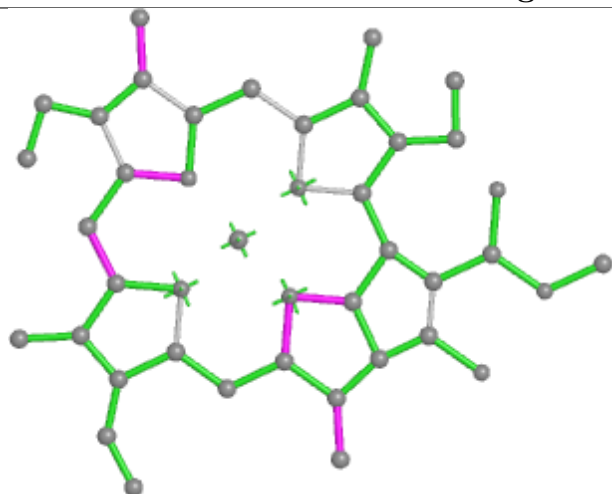
Ligand CLA c 308



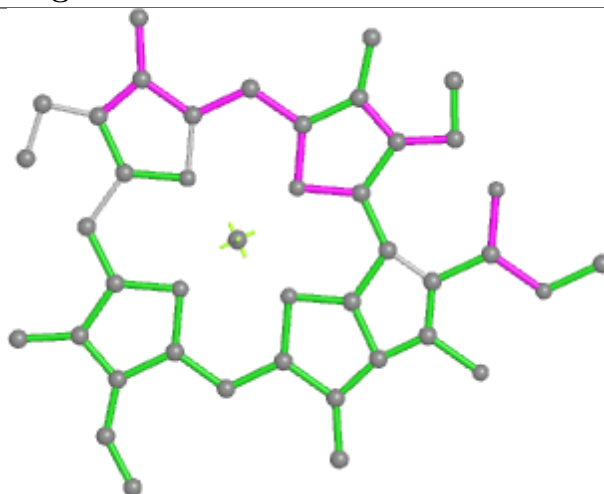
Ligand CLA e 306



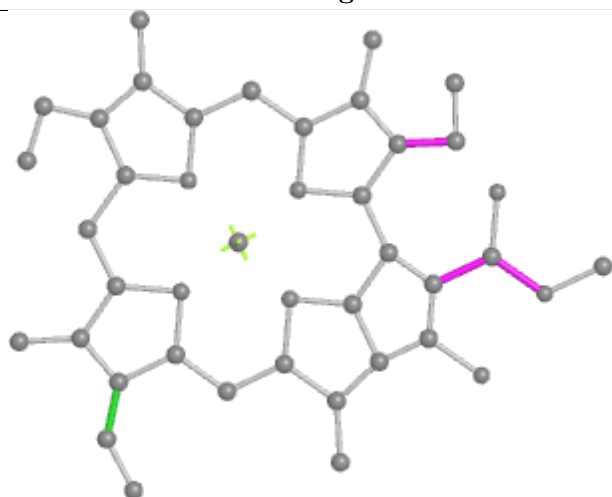
Ligand CLA g 303



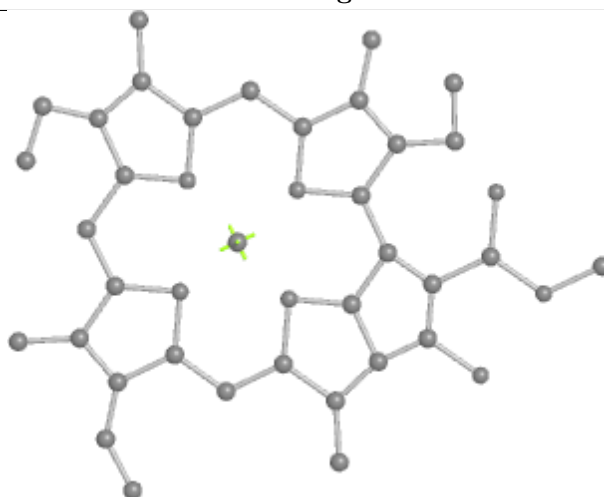
Bond lengths



Bond angles

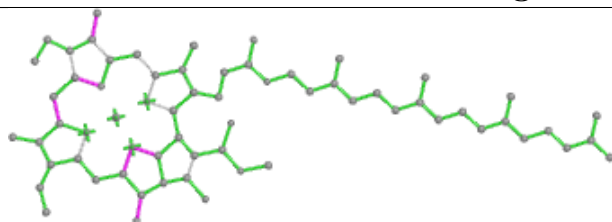


Torsions

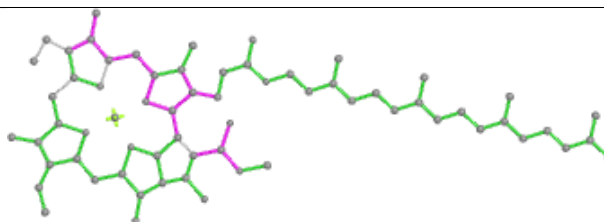


Rings

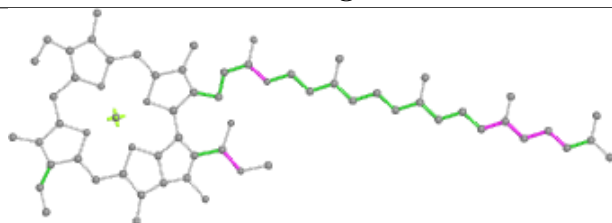
Ligand CLA A 824



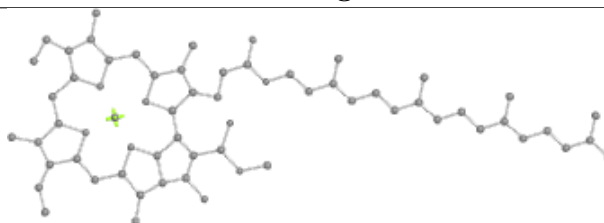
Bond lengths



Bond angles

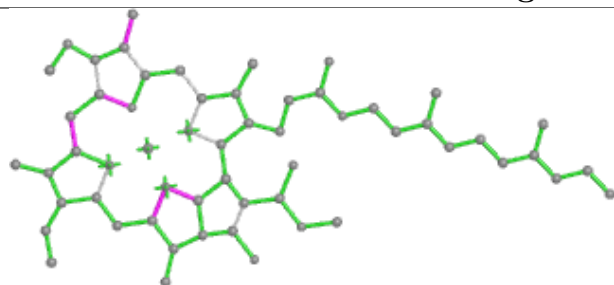


Torsions

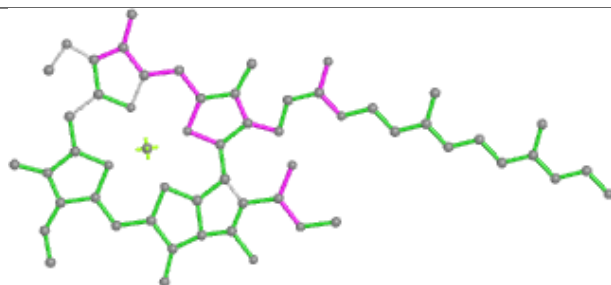


Rings

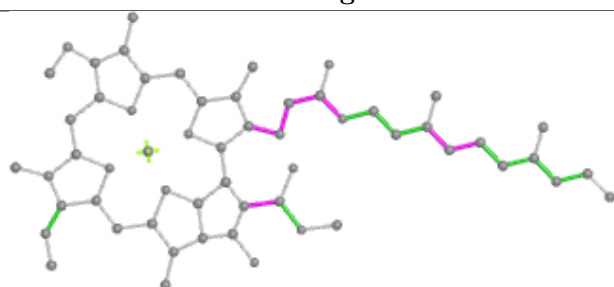
Ligand CLA h 306



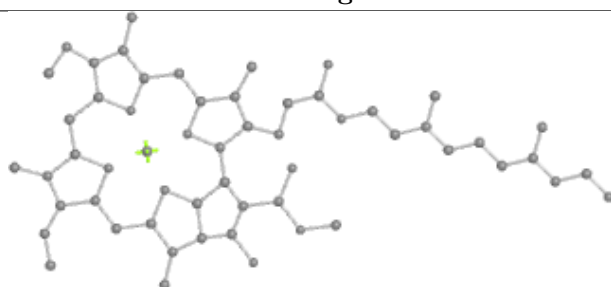
Bond lengths



Bond angles

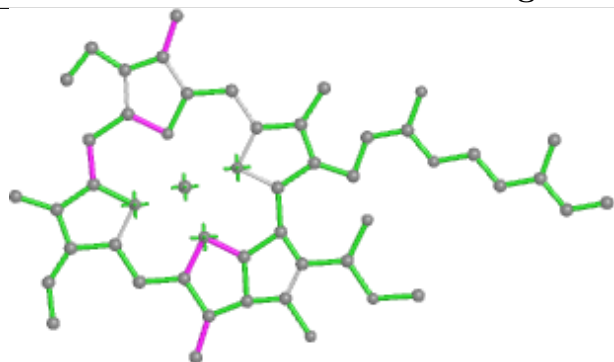


Torsions

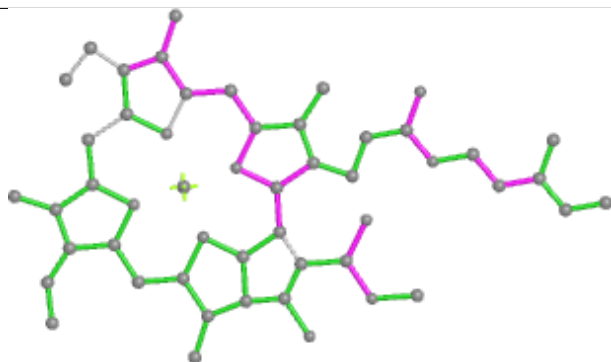


Rings

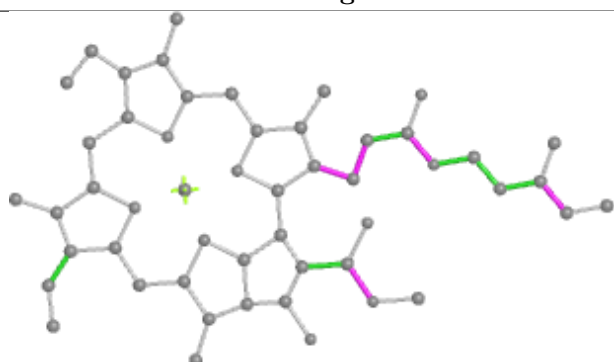
Ligand CLA k 610



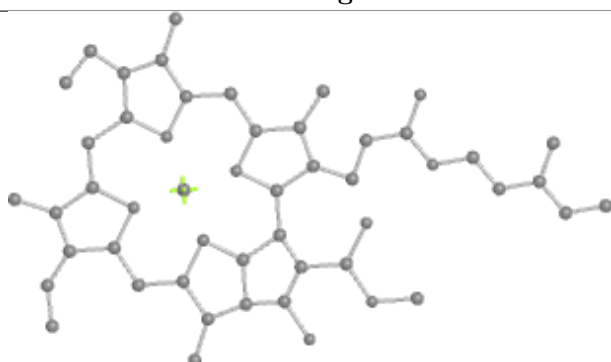
Bond lengths



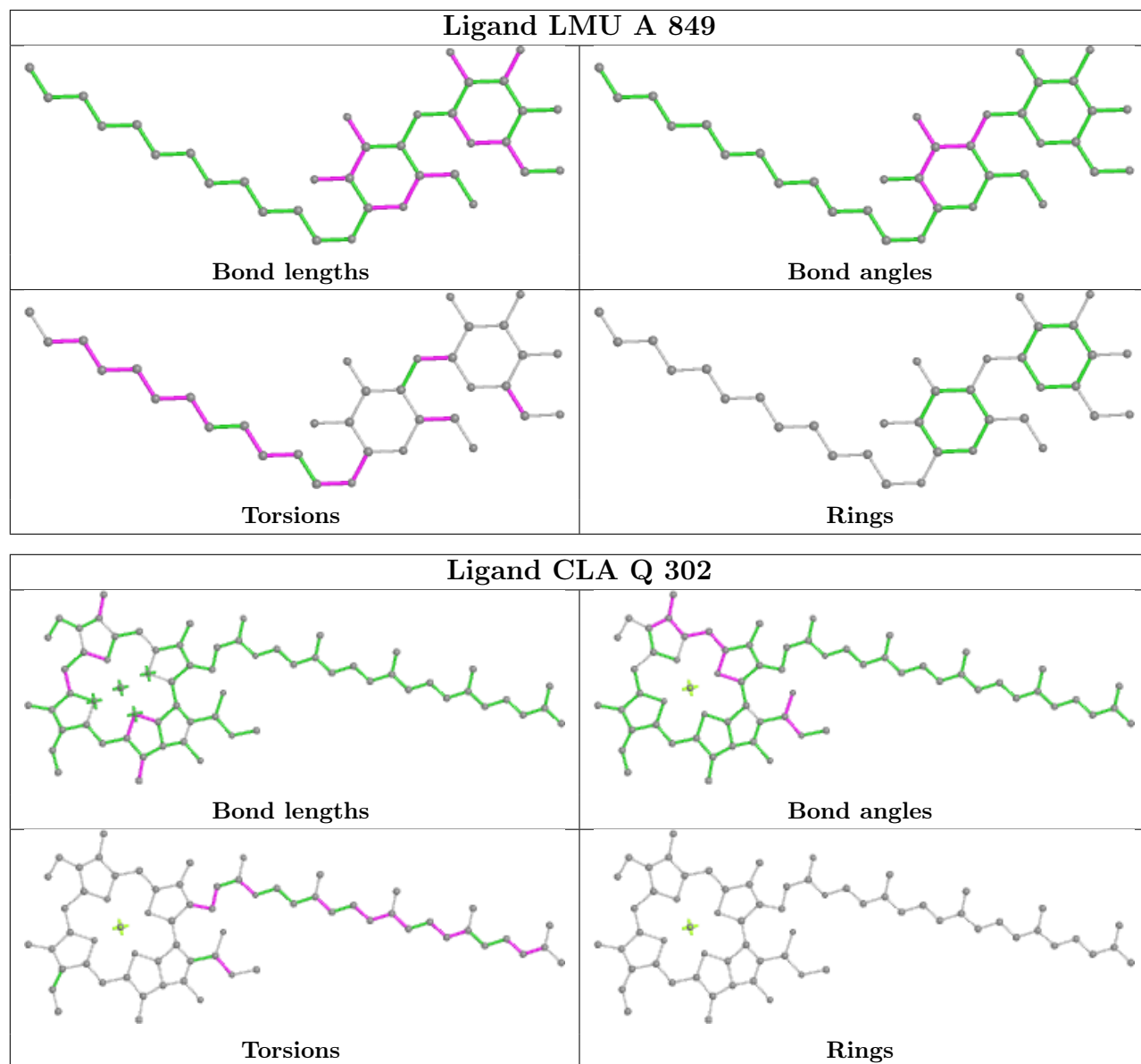
Bond angles

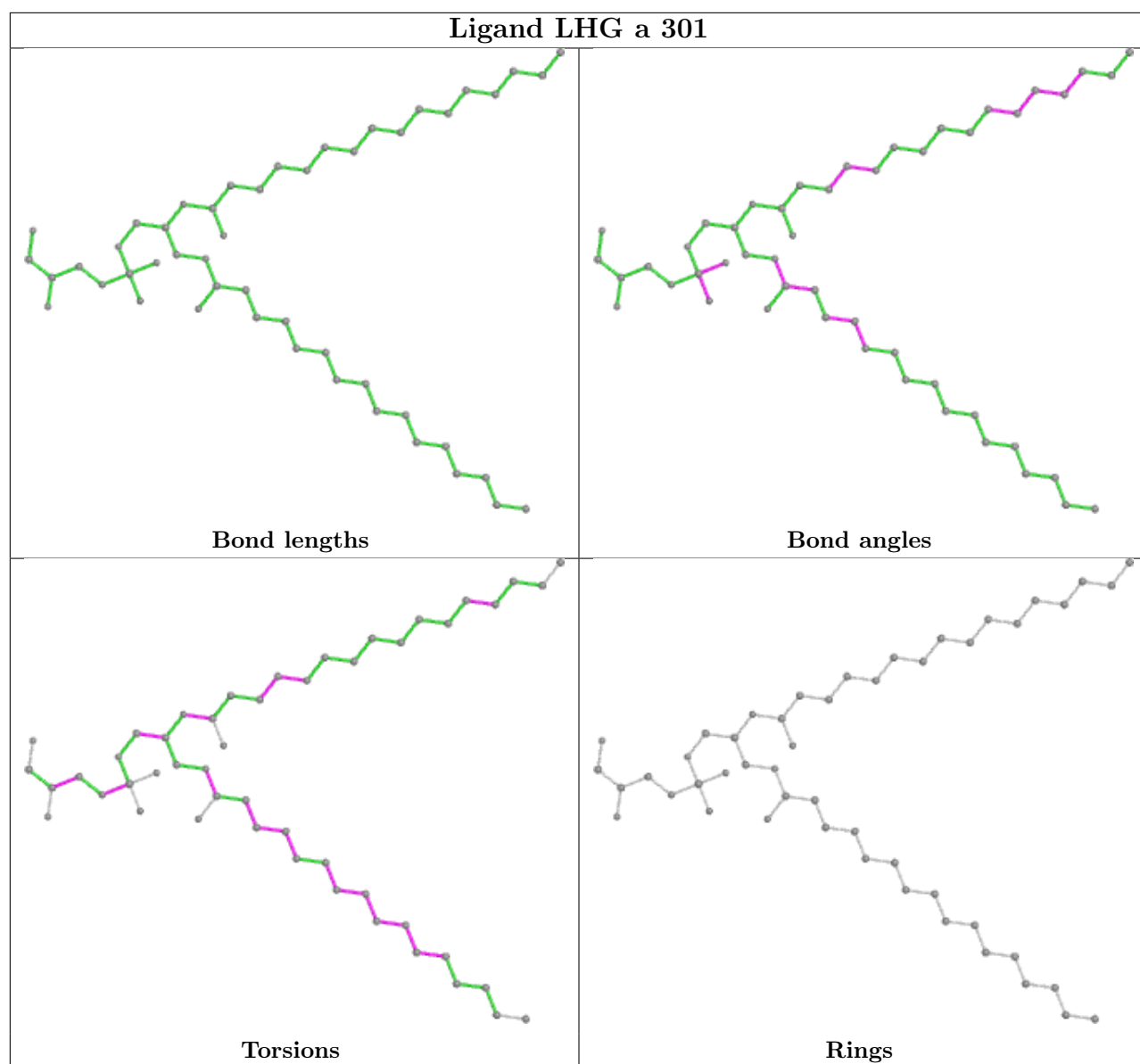


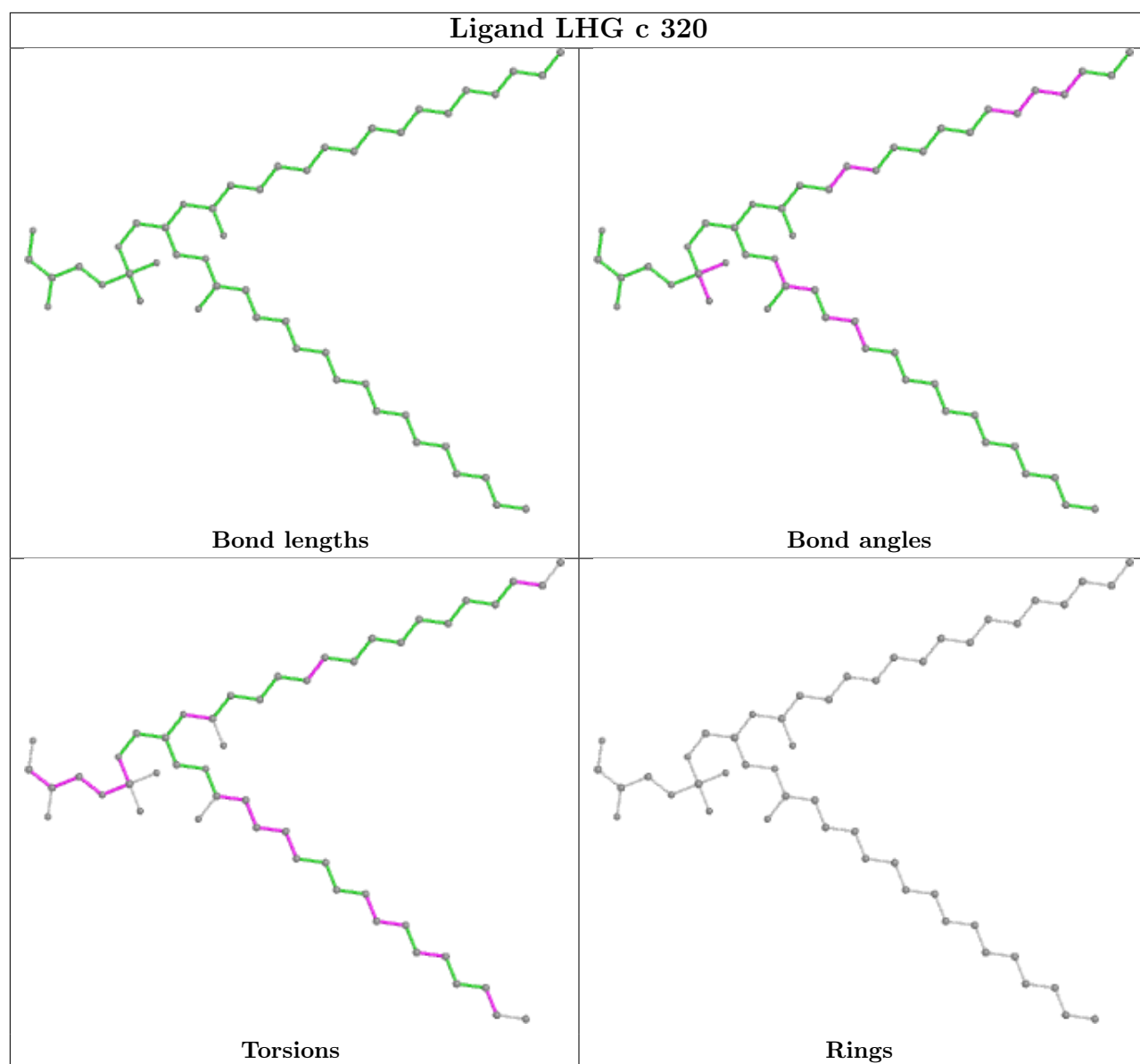
Torsions

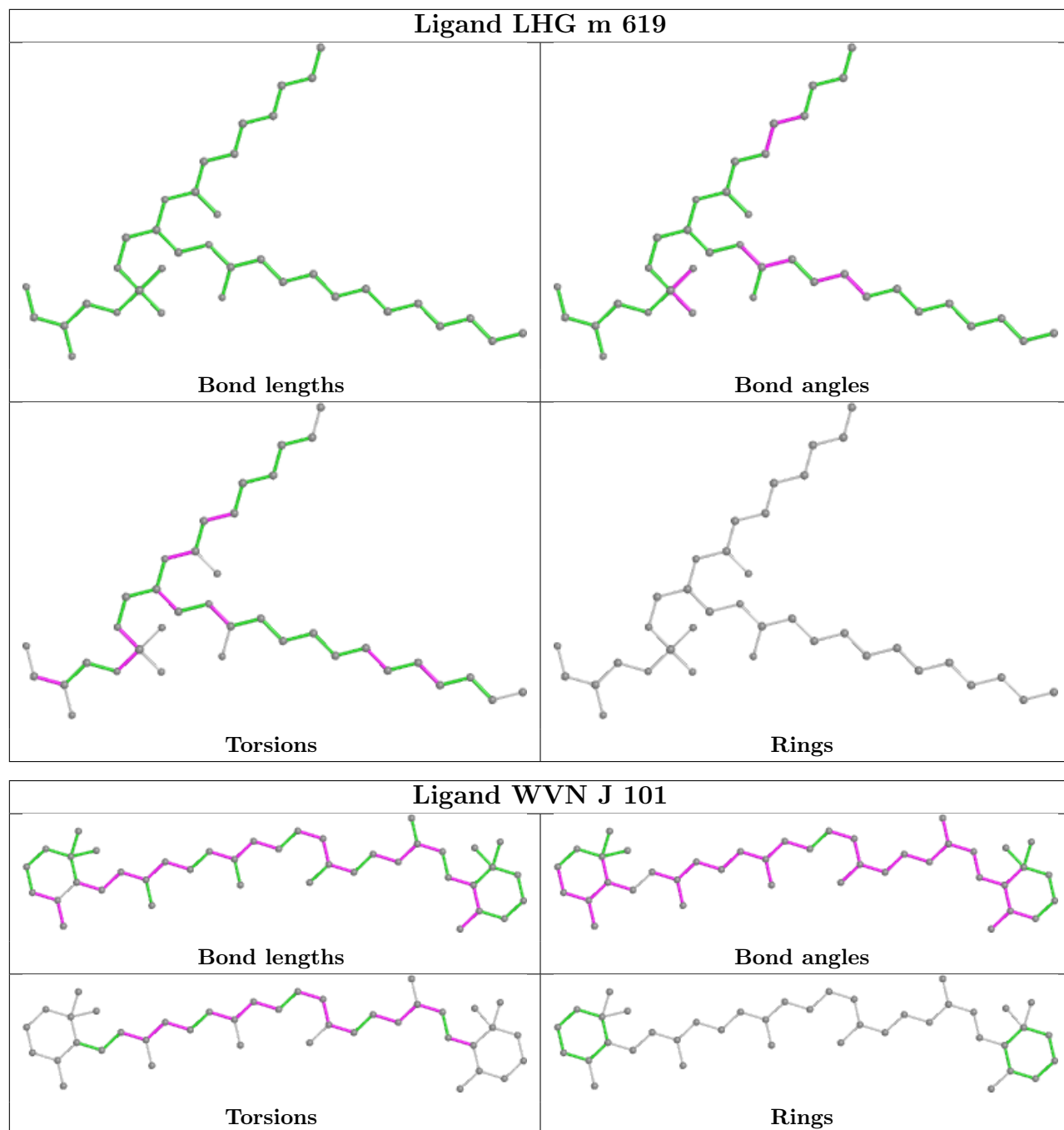


Rings

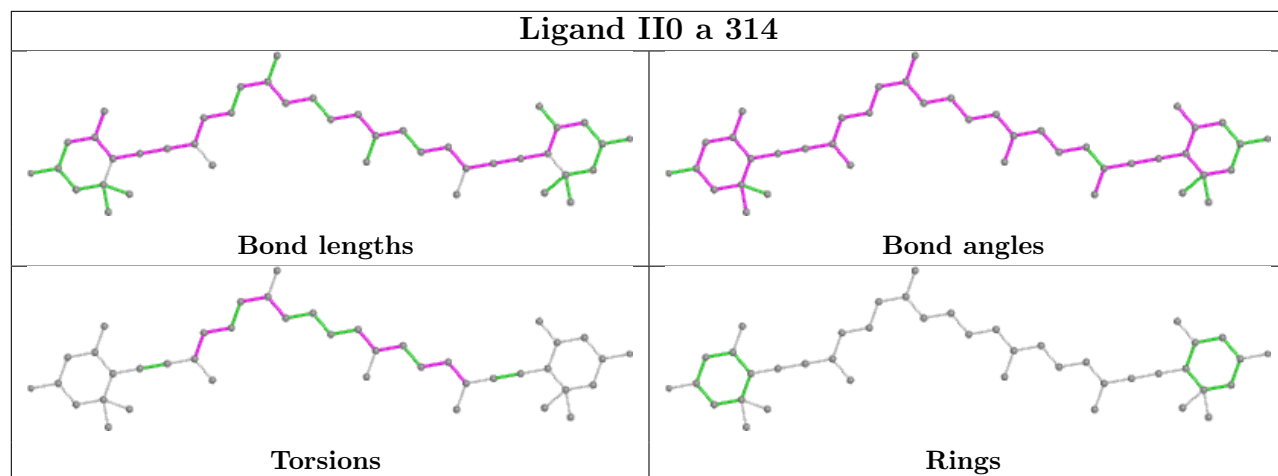




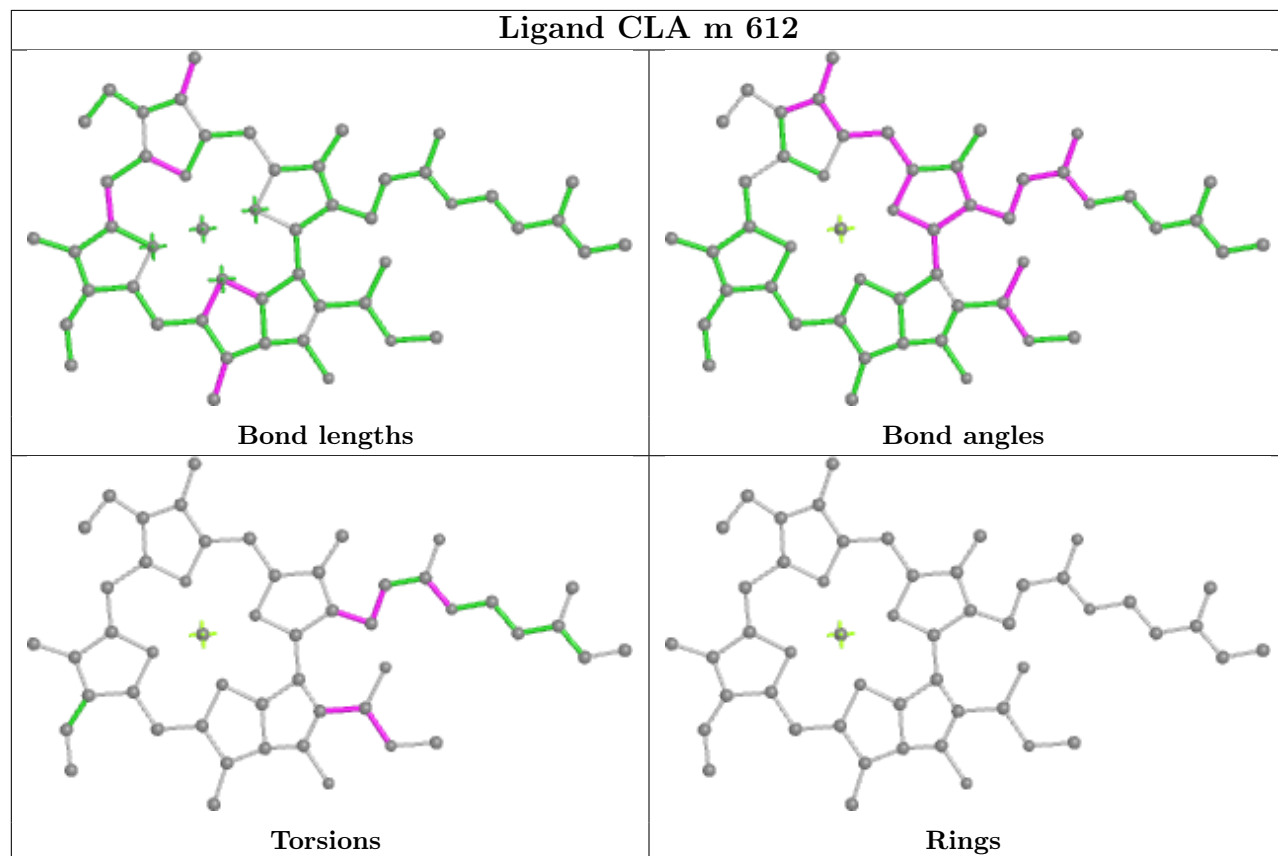




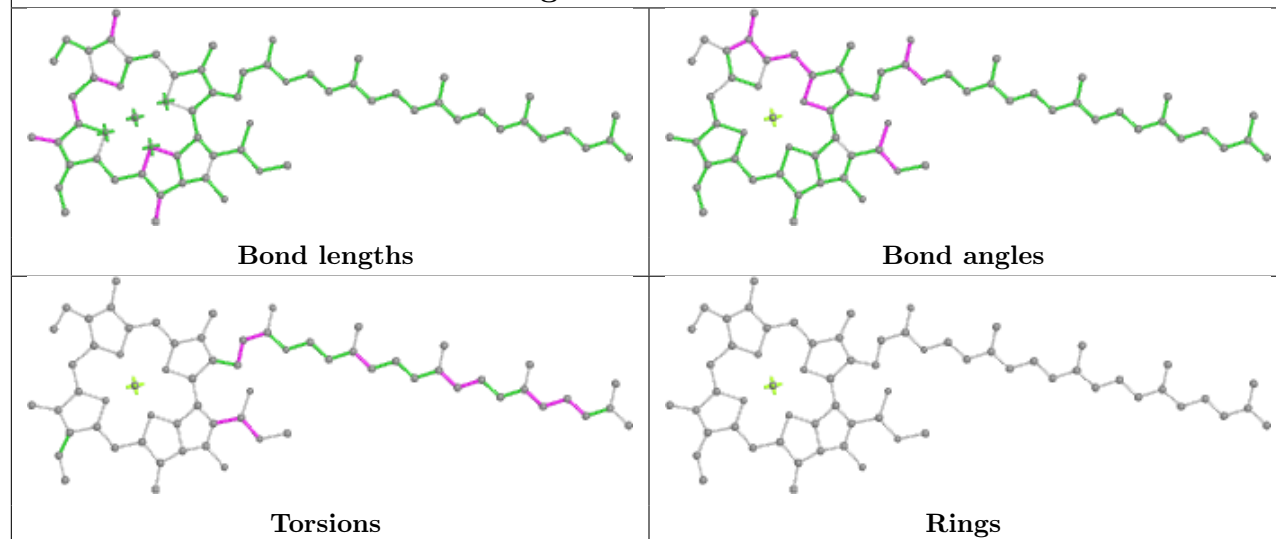
Ligand II0 a 314



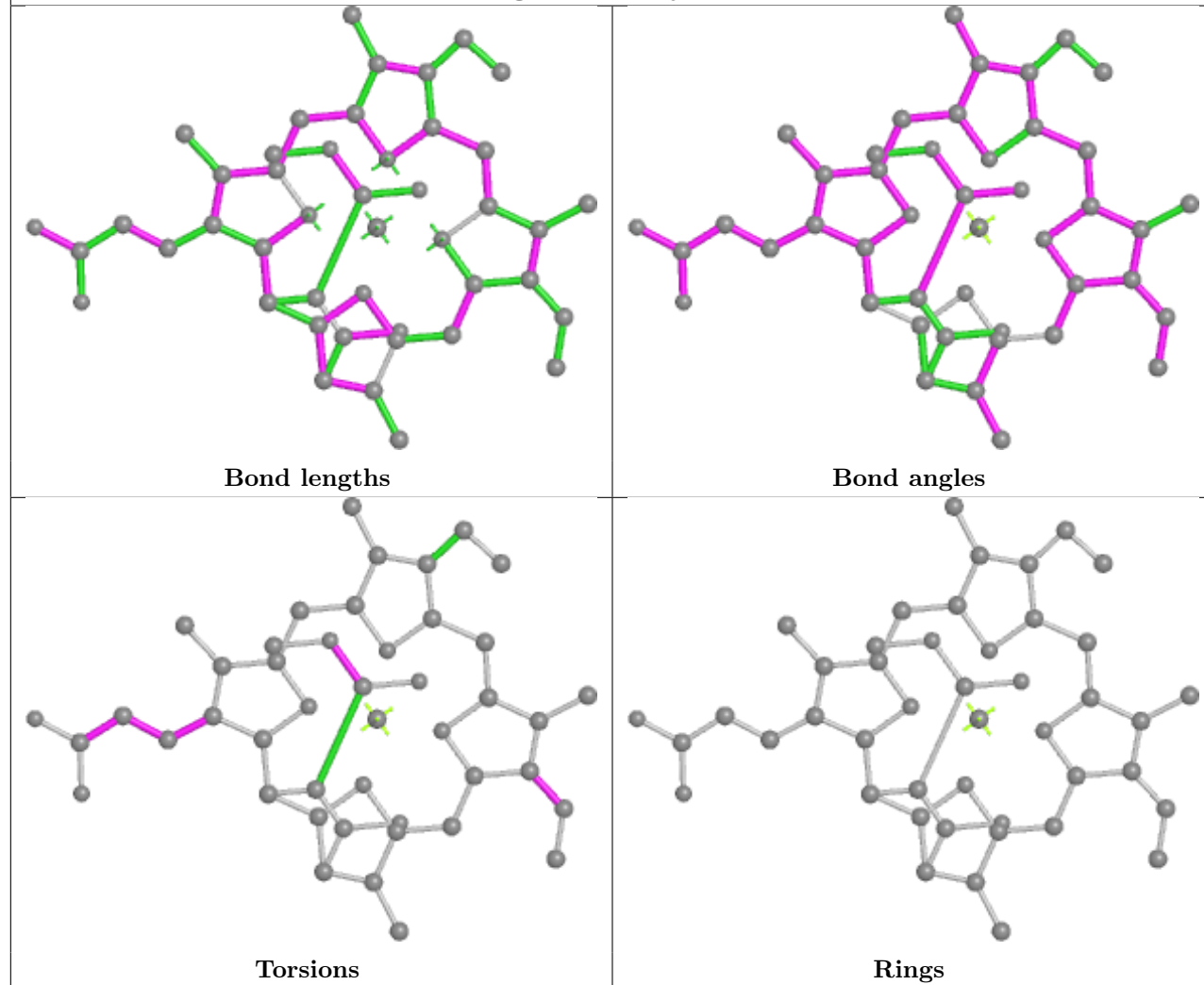
Ligand CLA m 612



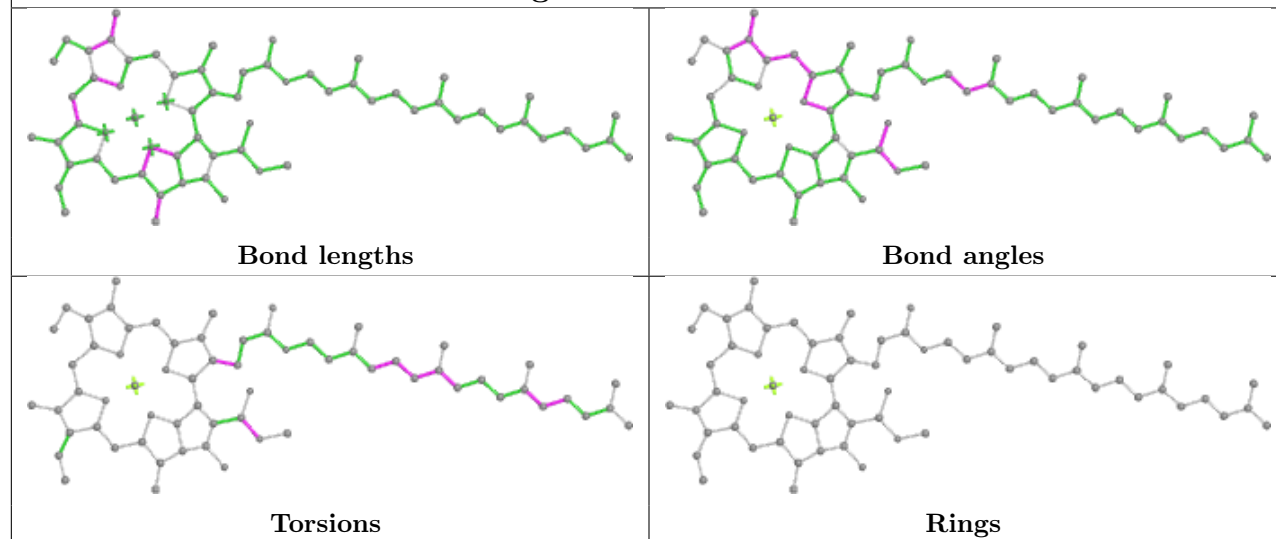
Ligand CLA l 306



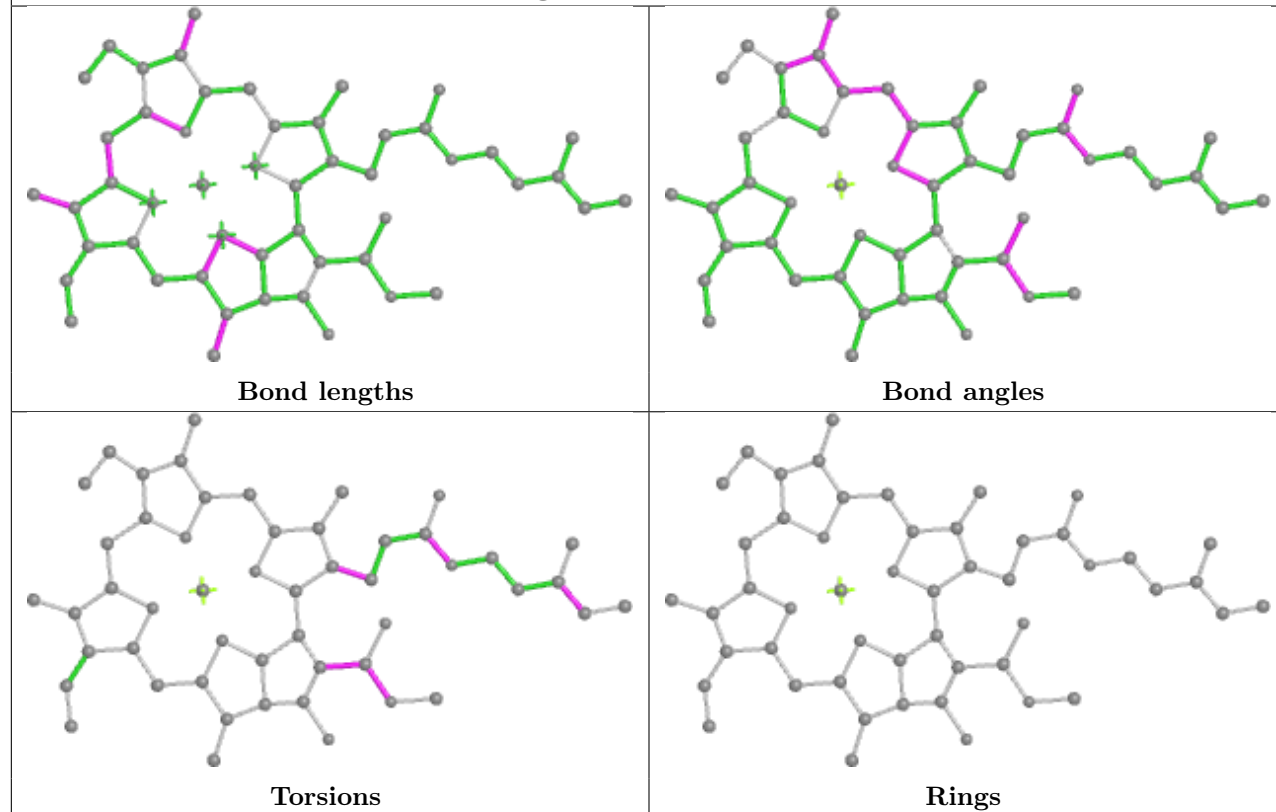
Ligand KC2 j 312

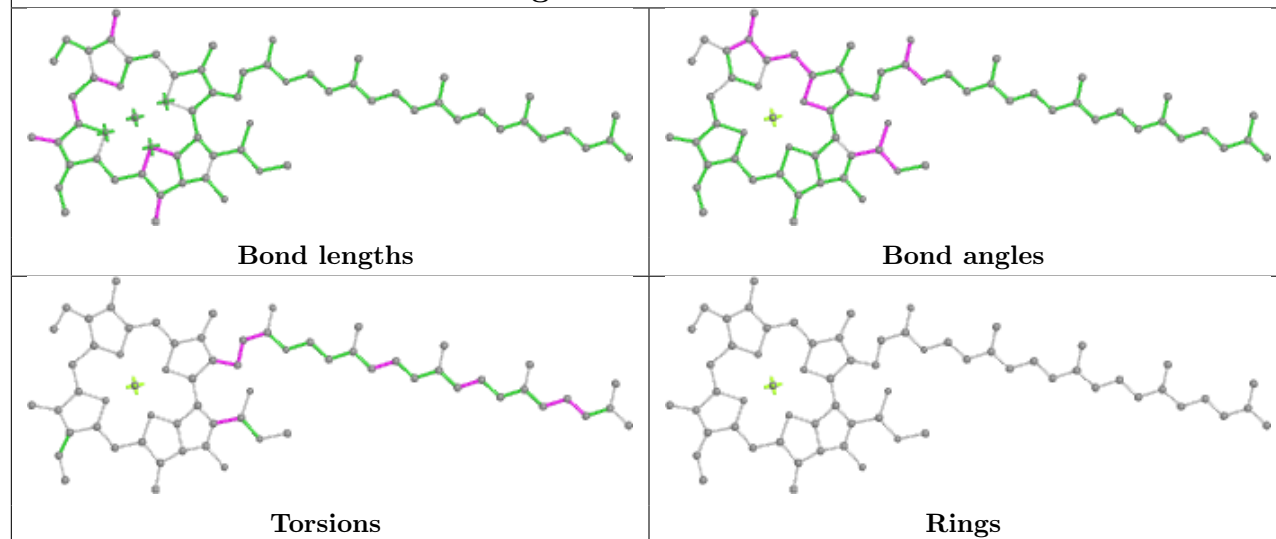
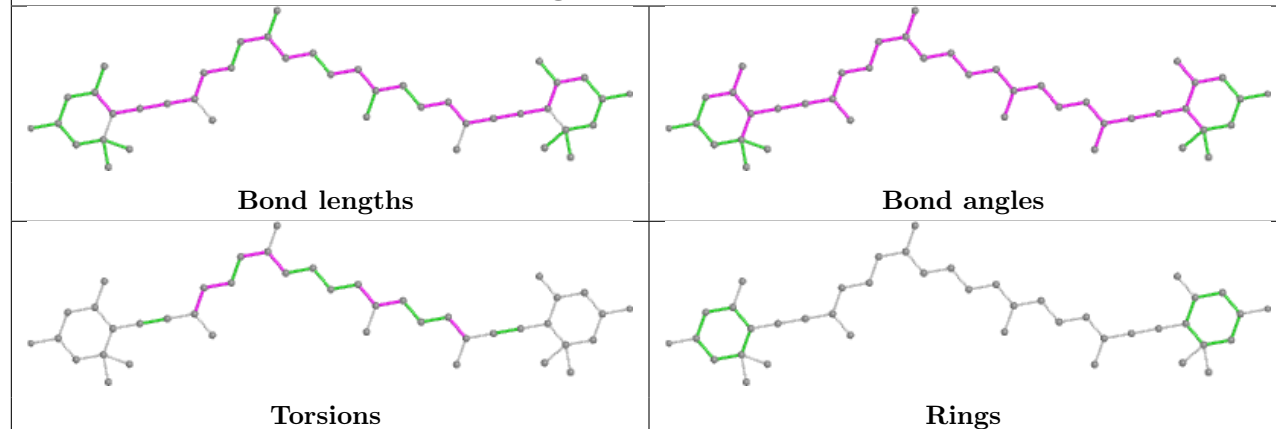
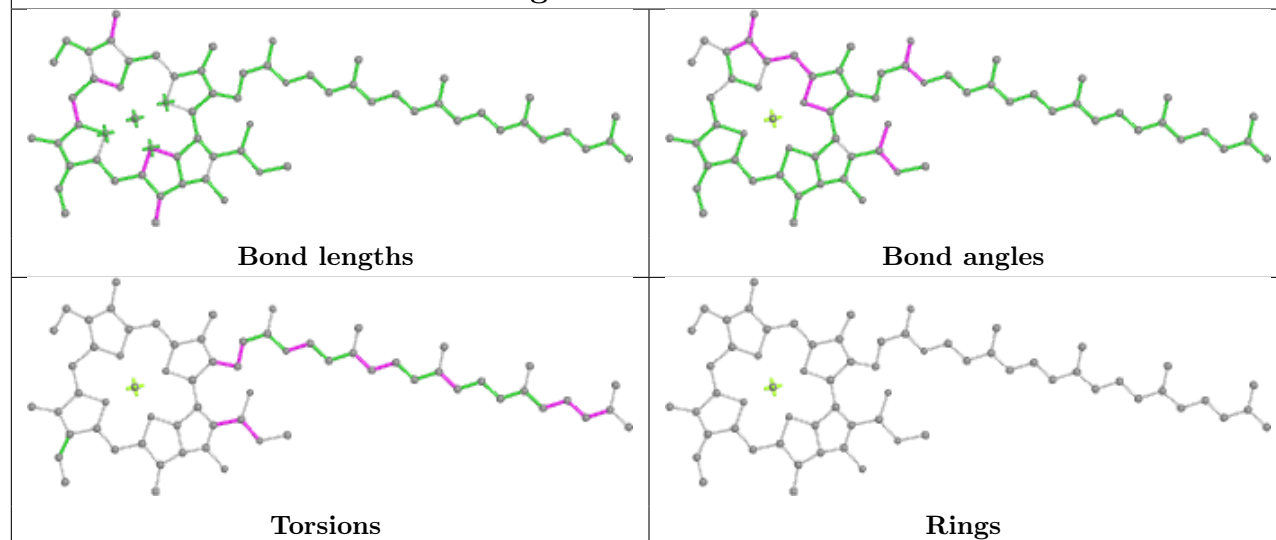


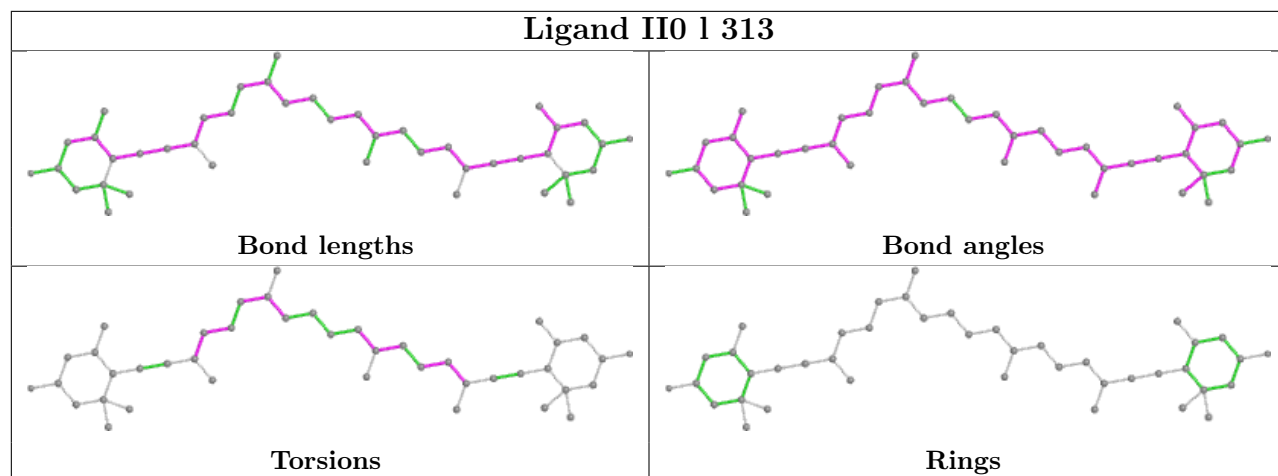
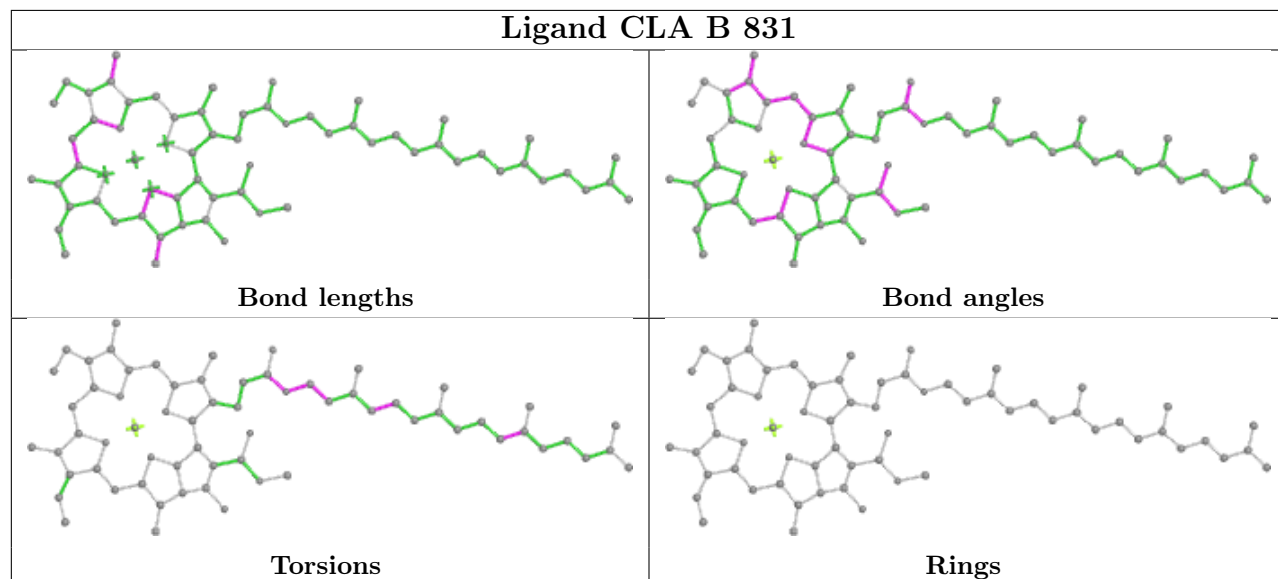
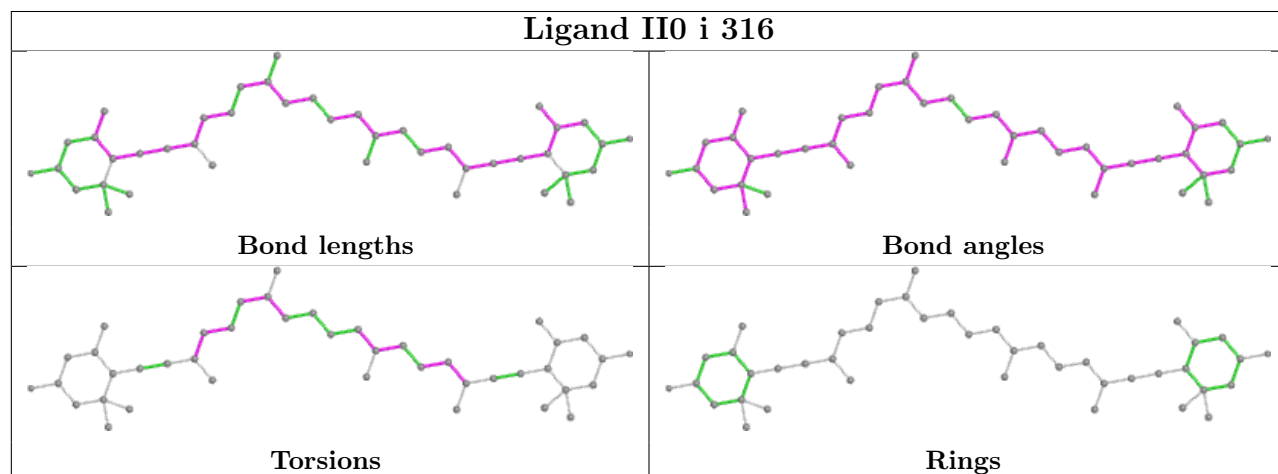
Ligand CLA A 831

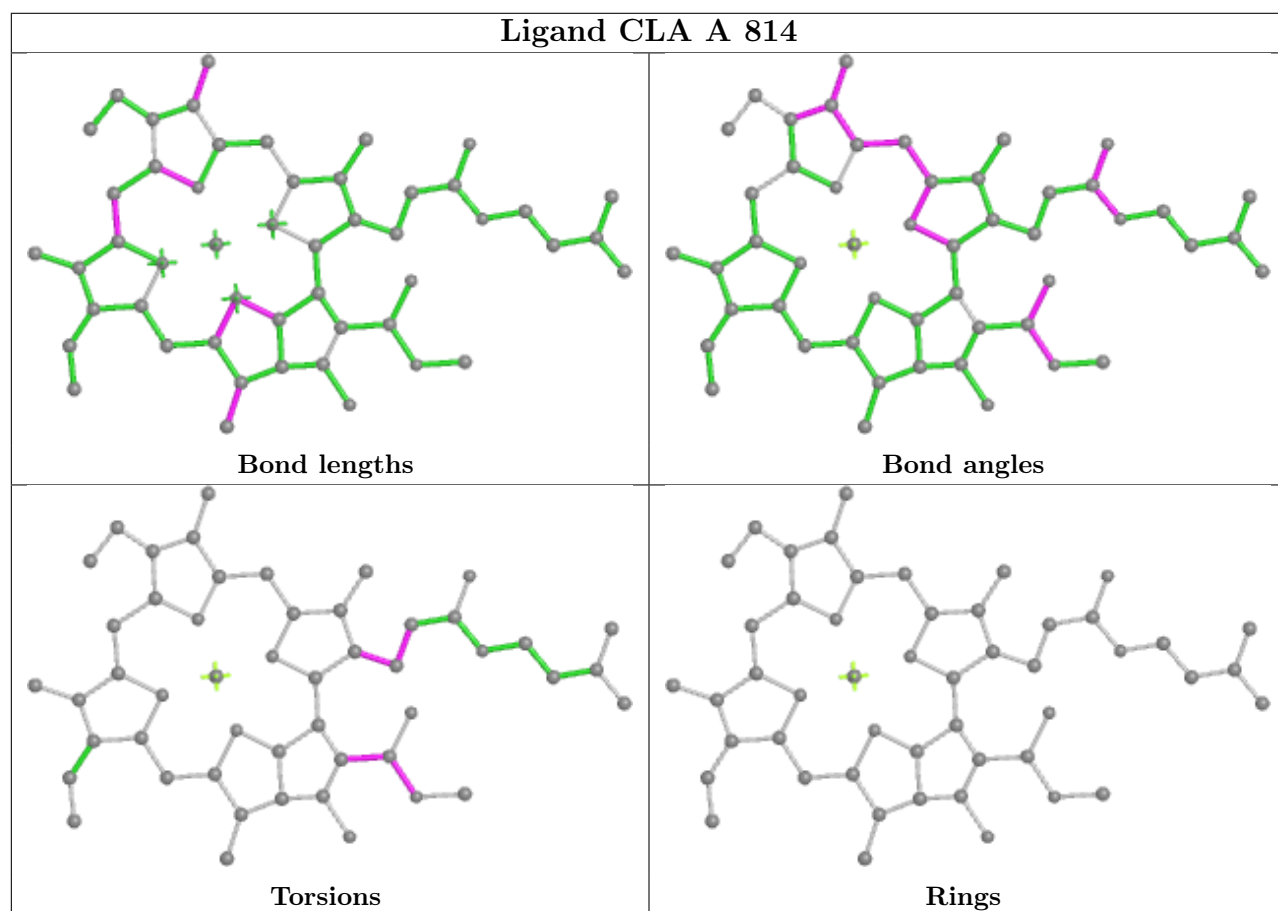
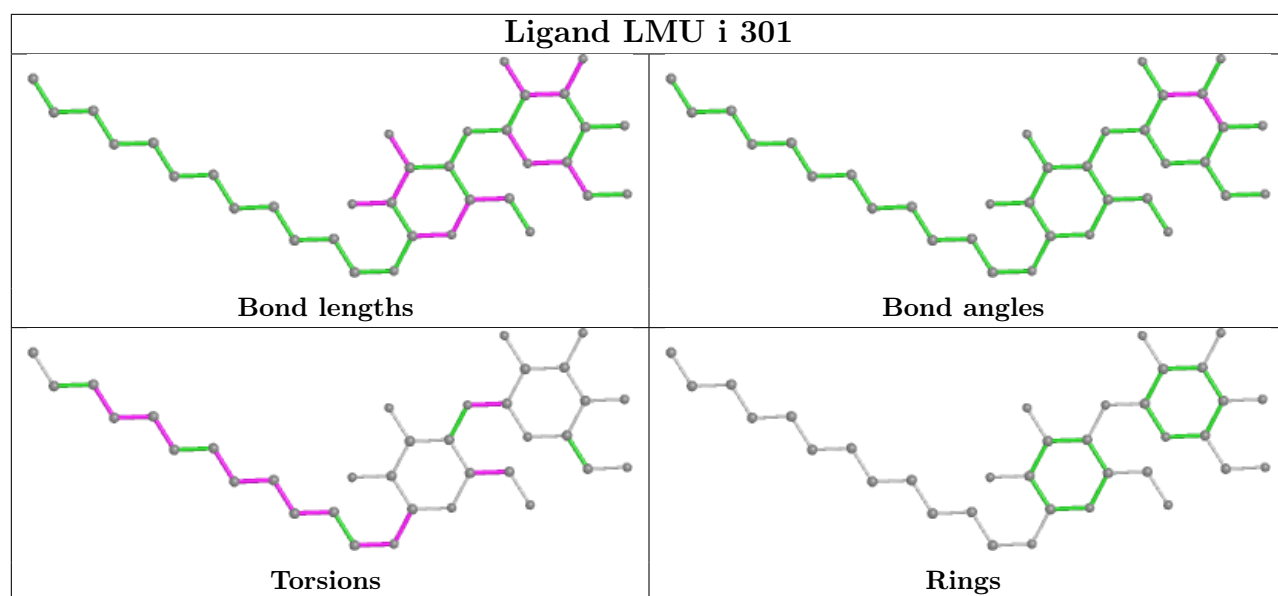


Ligand CLA L 207

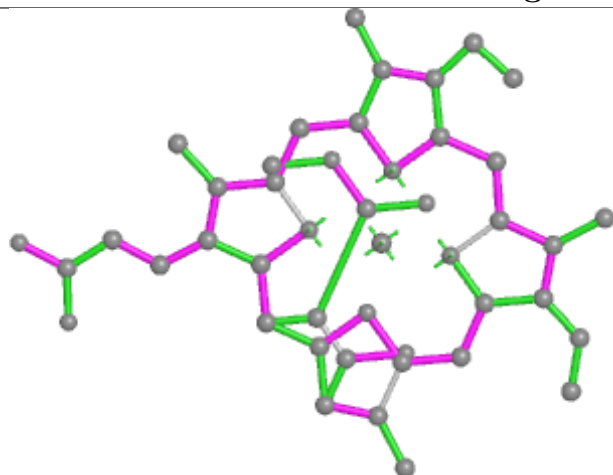


Ligand CLA A 802**Ligand II0 b 315****Ligand CLA m 613**

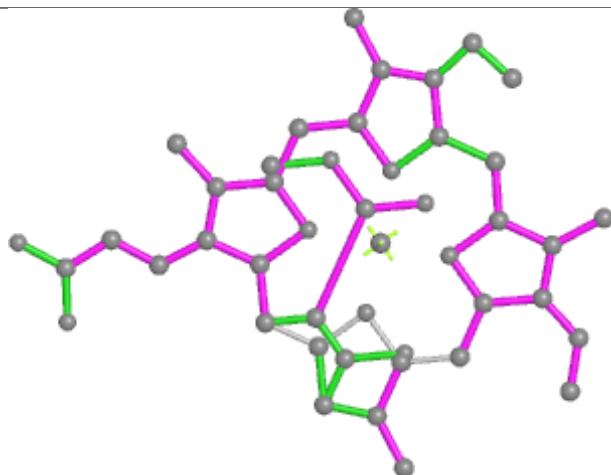
Ligand II0 I 313**Ligand CLA B 831****Ligand II0 i 316**



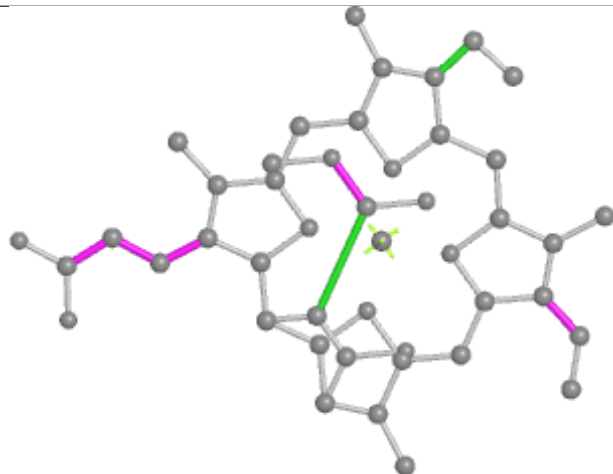
Ligand KC2 i 318



Bond lengths



Bond angles

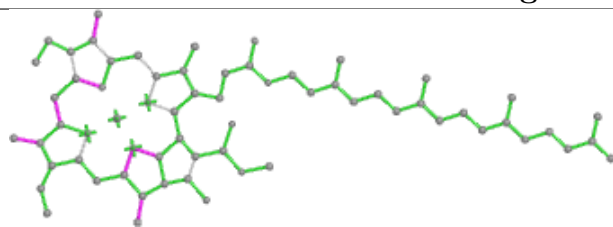


Torsions

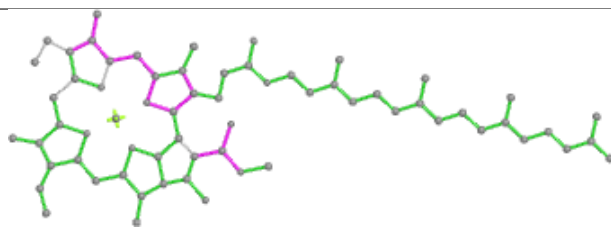


Rings

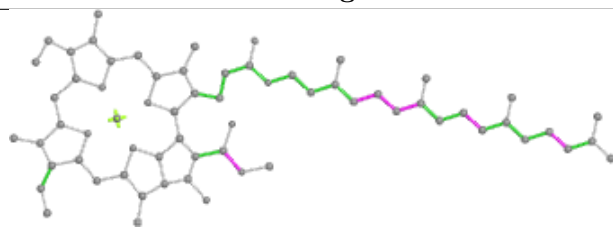
Ligand CLA s 403



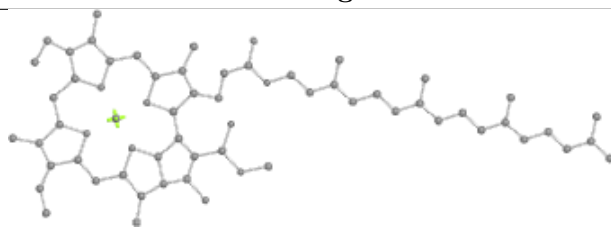
Bond lengths



Bond angles

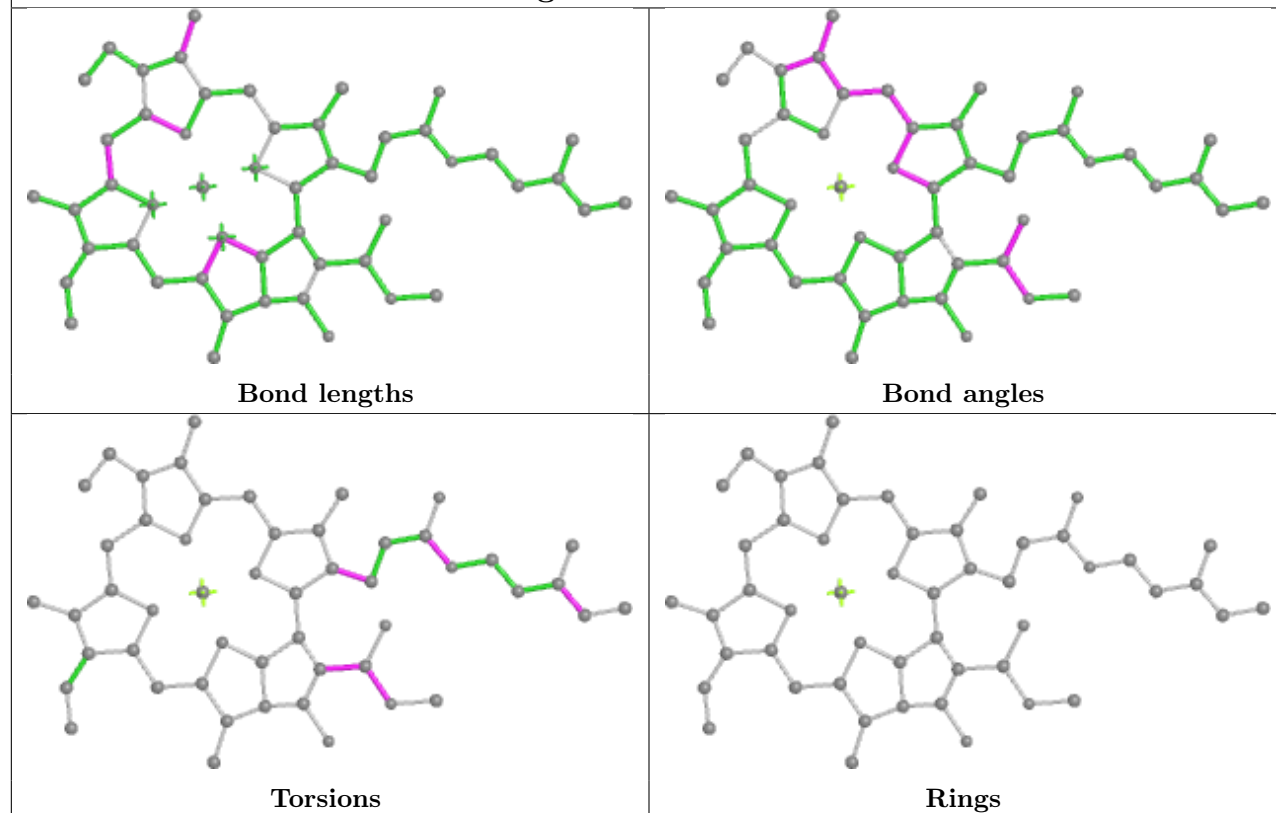


Torsions

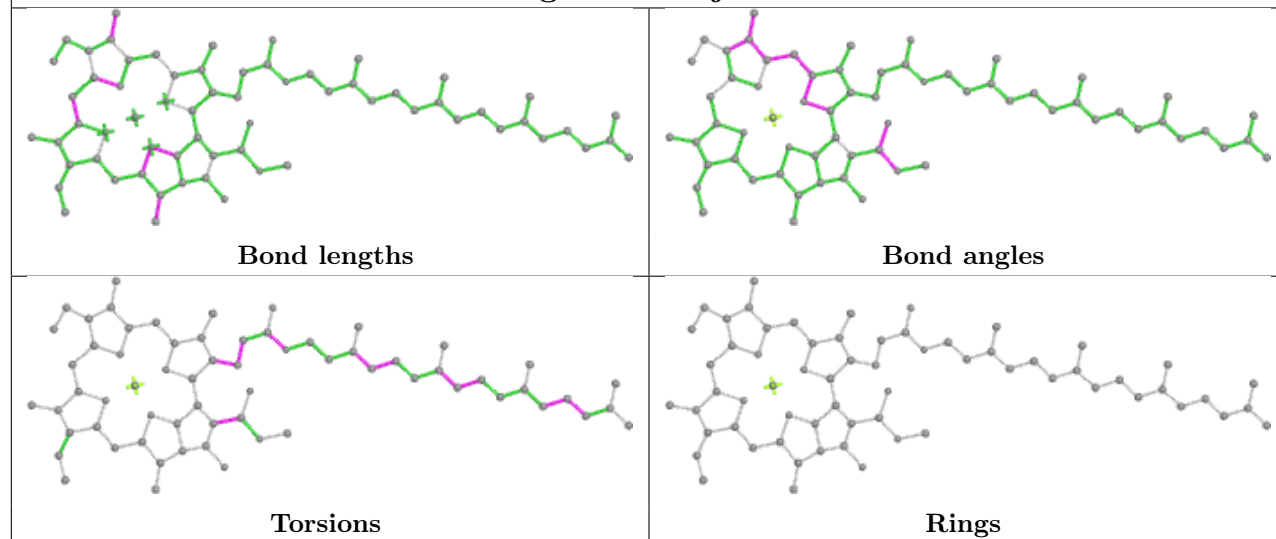


Rings

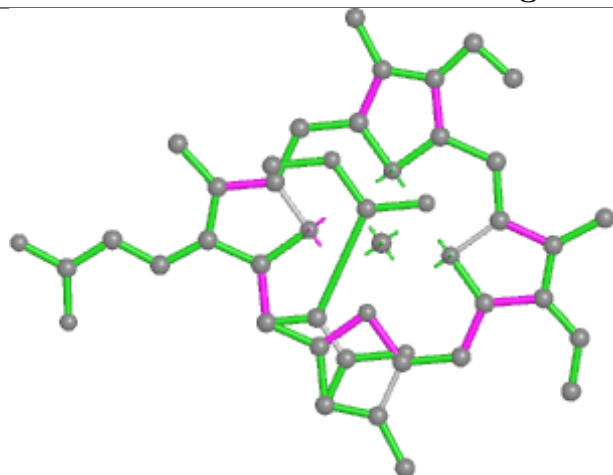
Ligand CLA c 301



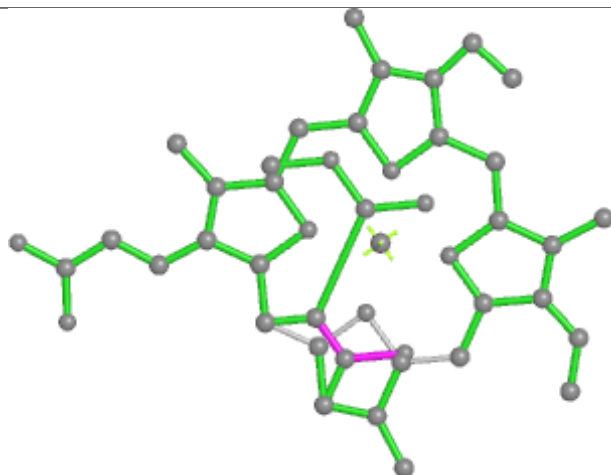
Ligand CLA j 302



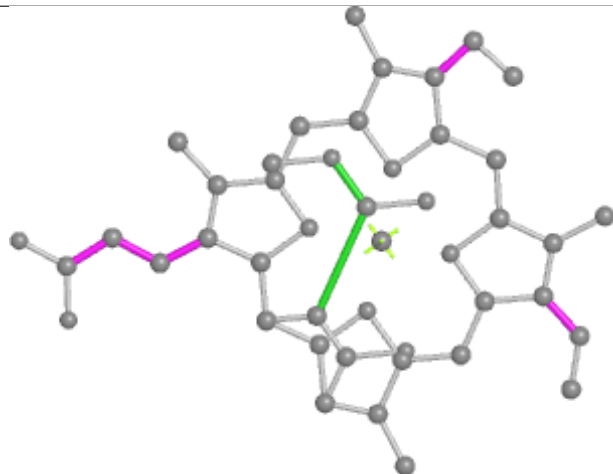
Ligand KC2 k 613



Bond lengths



Bond angles

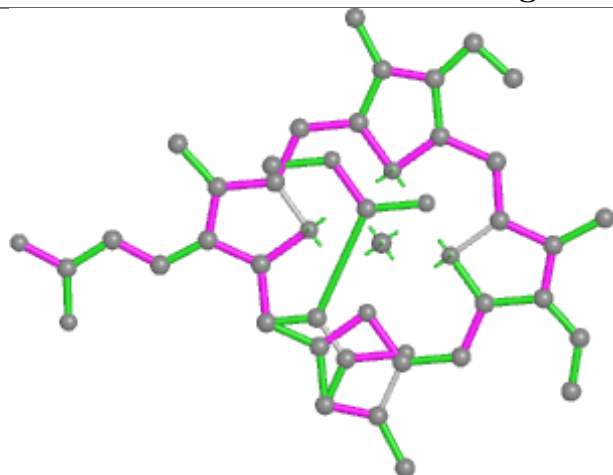


Torsions

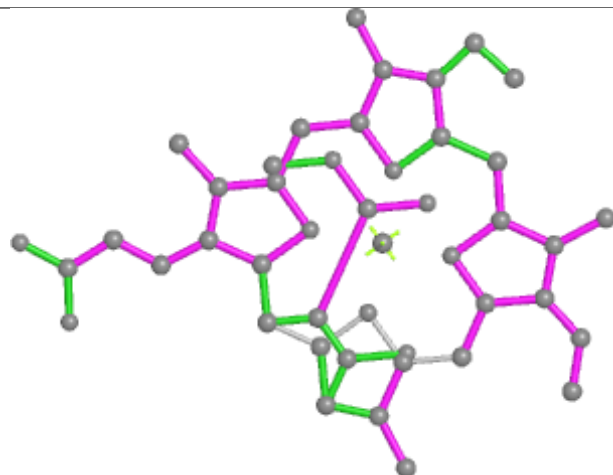


Rings

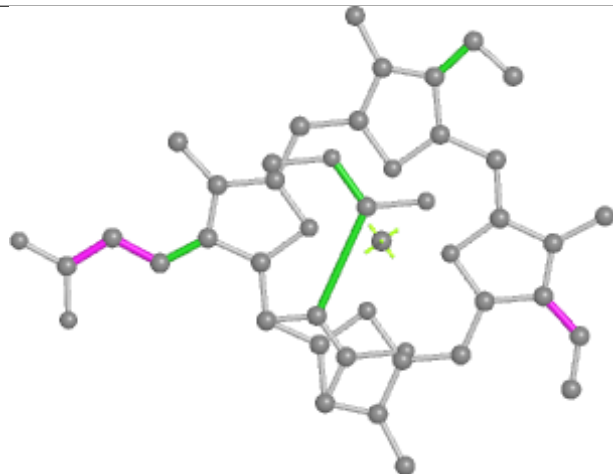
Ligand KC2 n 611



Bond lengths



Bond angles

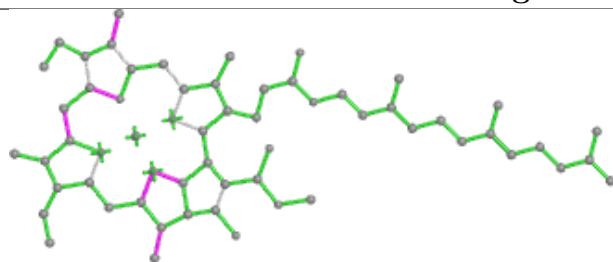


Torsions

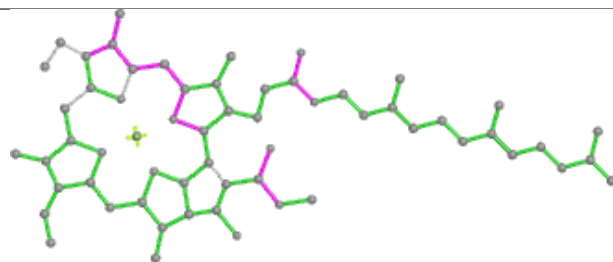


Rings

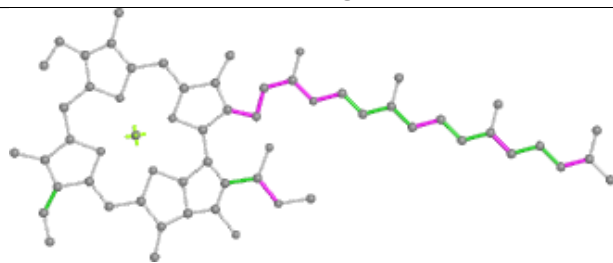
Ligand CLA m 609



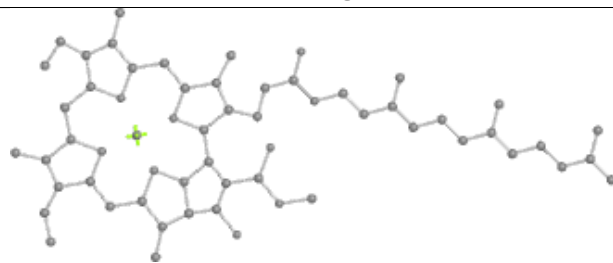
Bond lengths



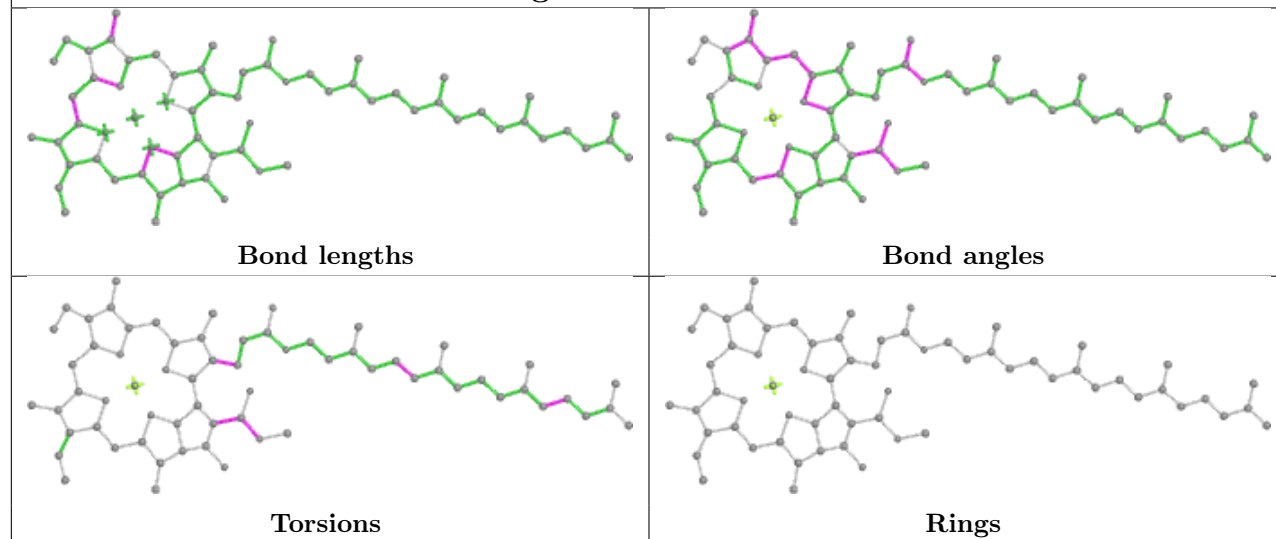
Bond angles



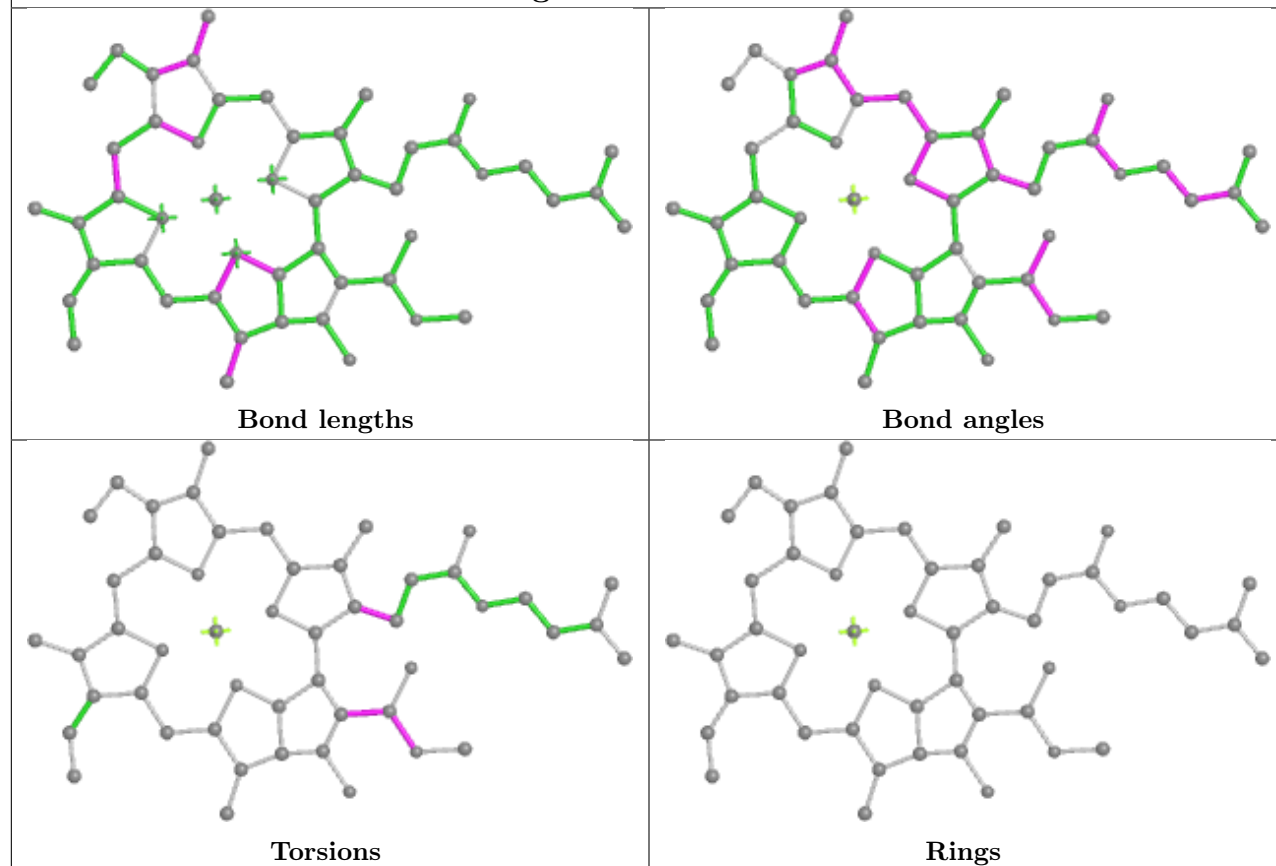
Torsions



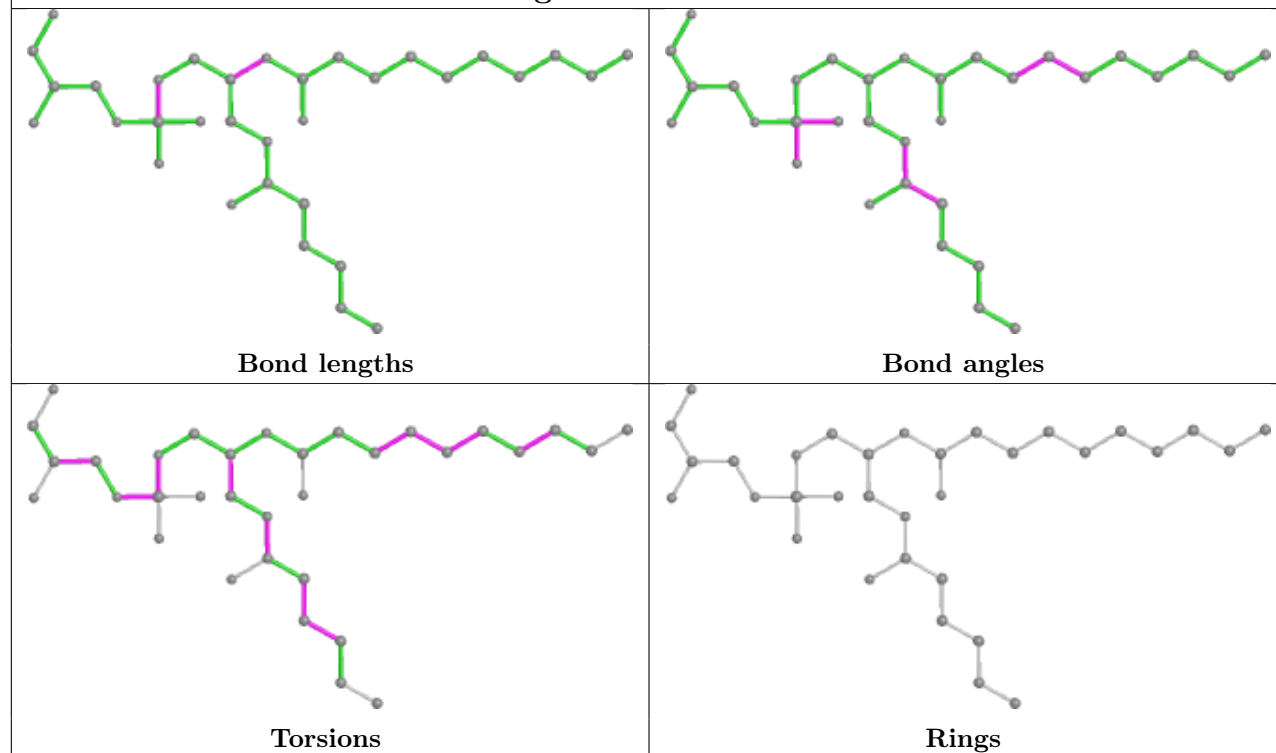
Rings

Ligand CLA A 832**Ligand WVN I 101**

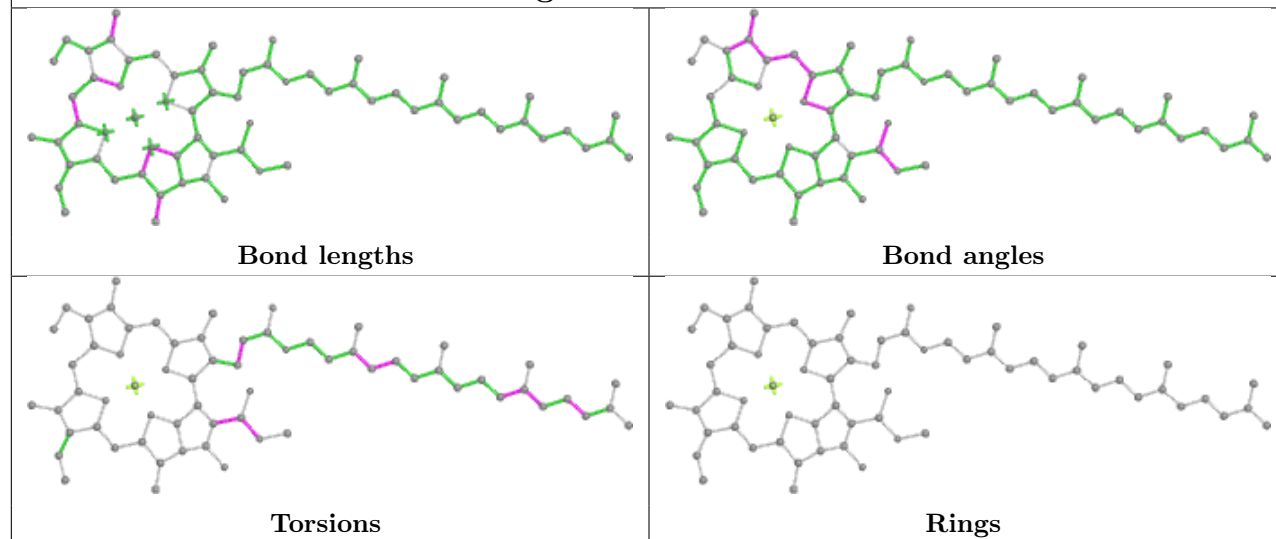
Ligand CLA B 830



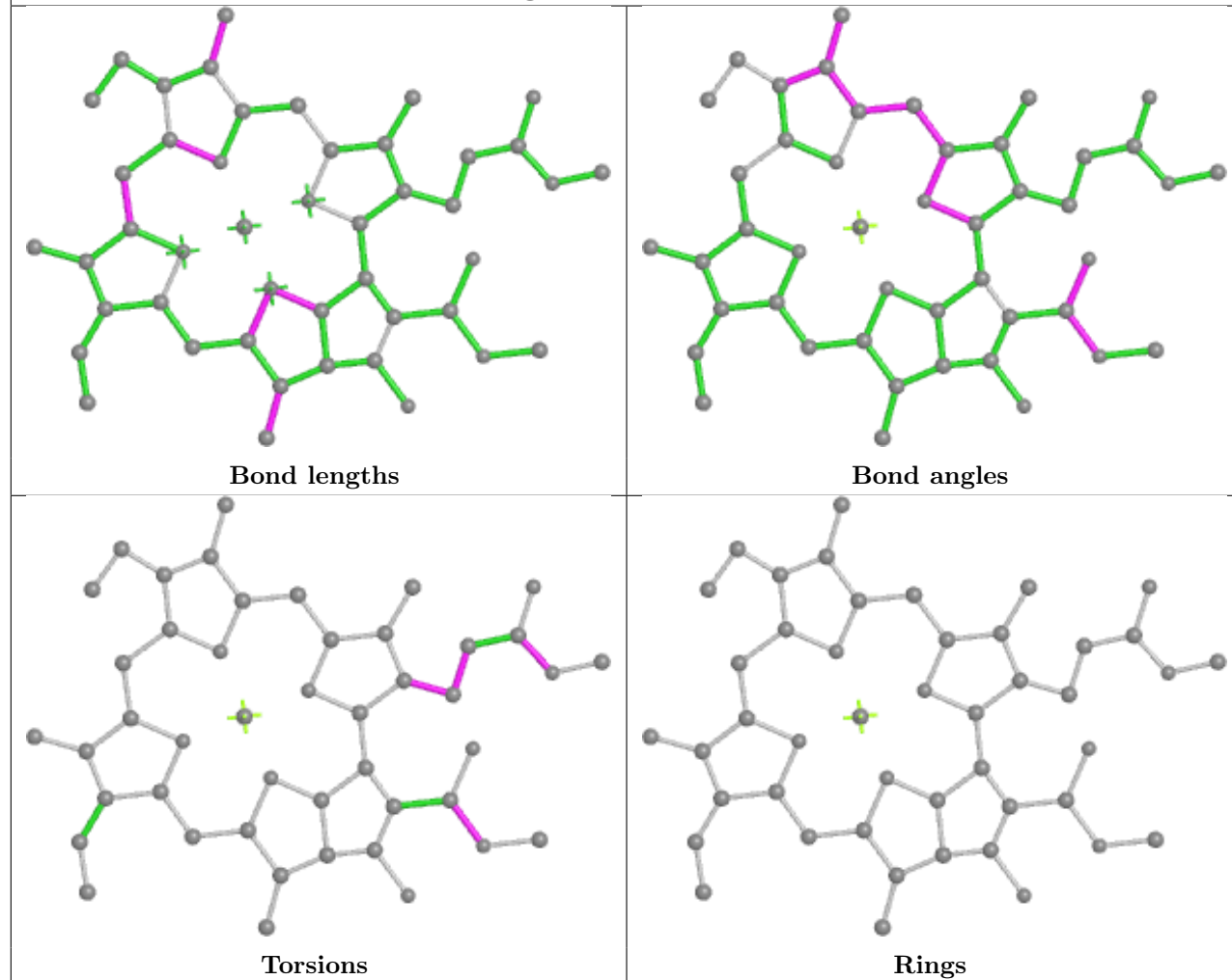
Ligand LHG J 104

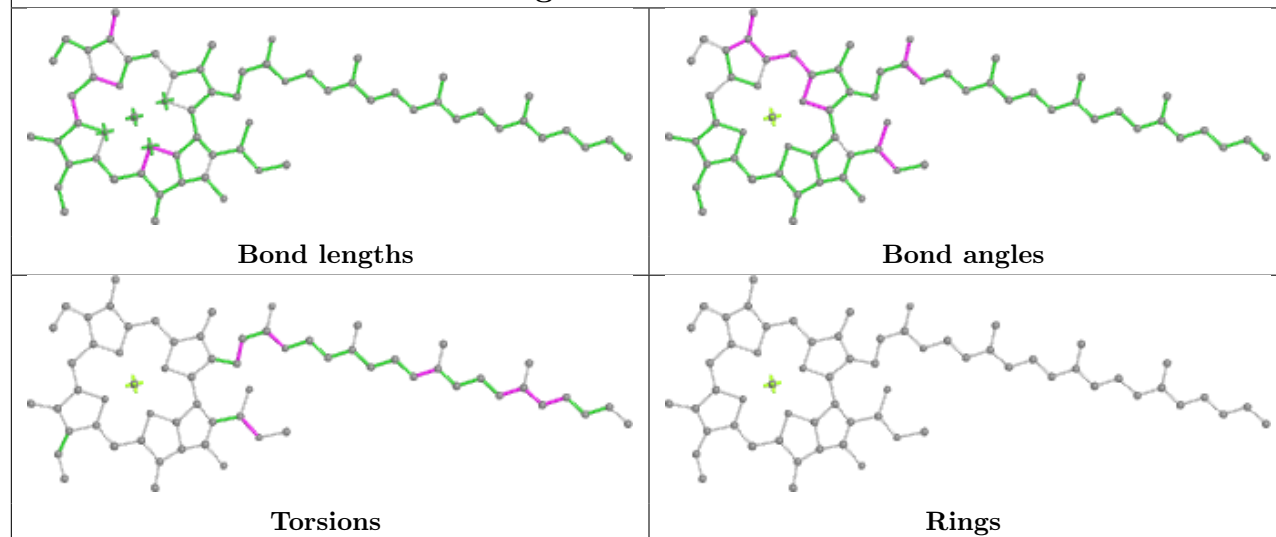
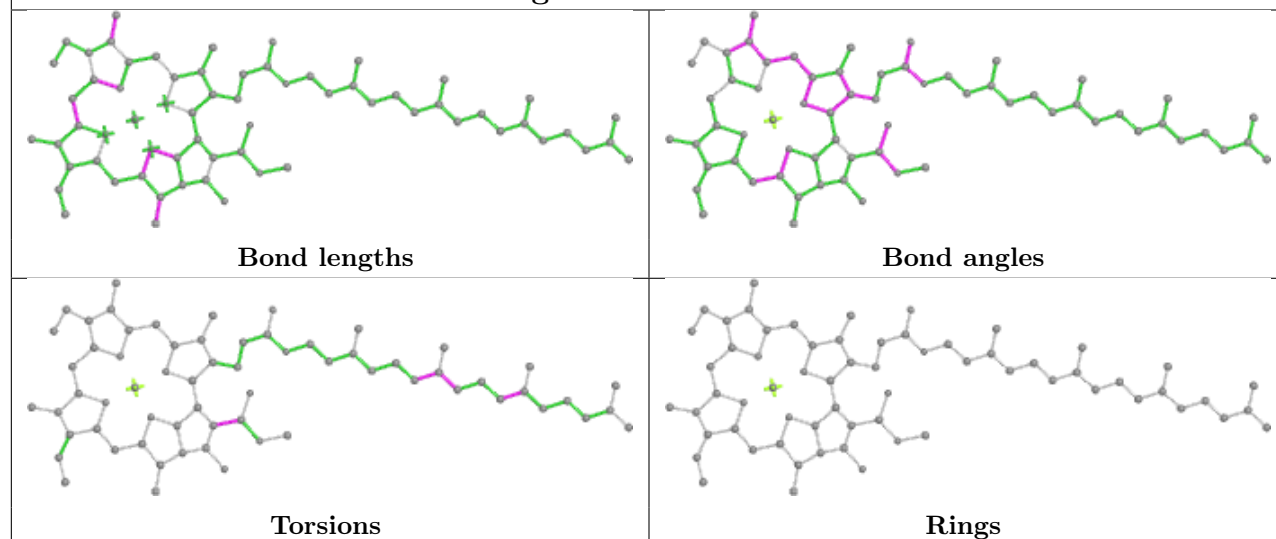
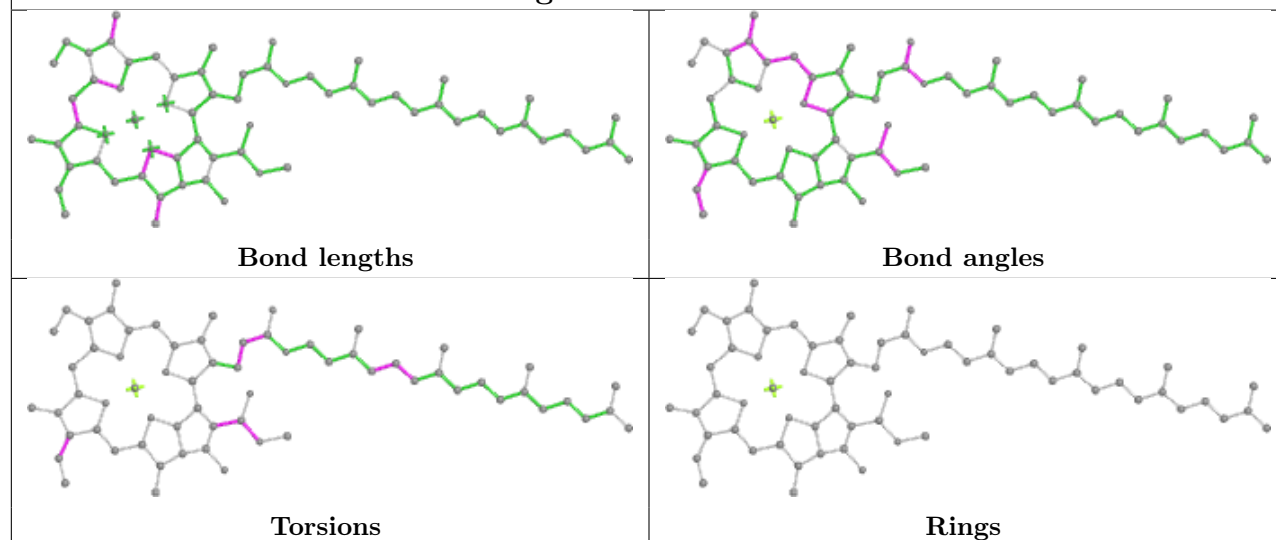


Ligand CLA a 308

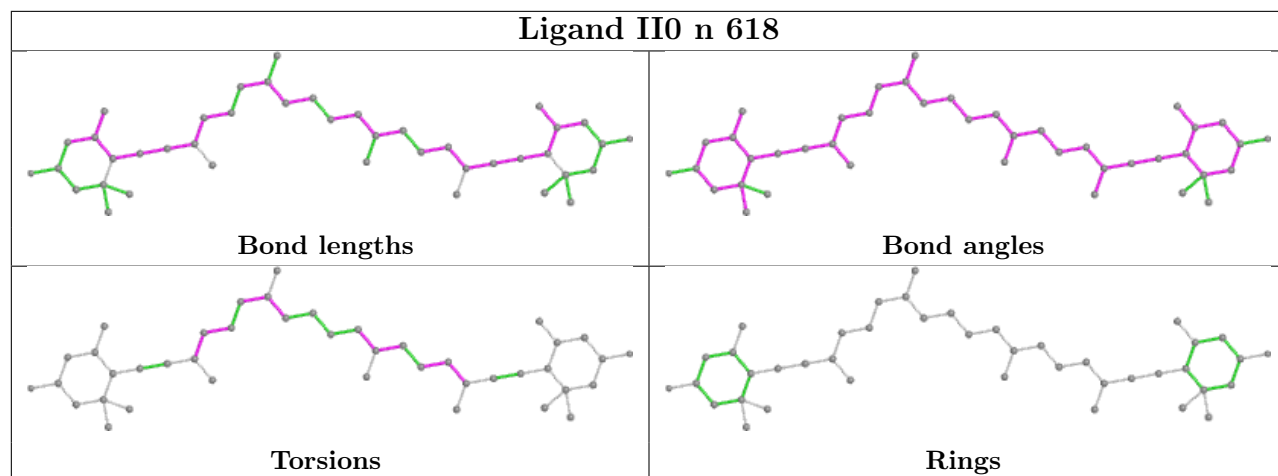


Ligand CLA i 309

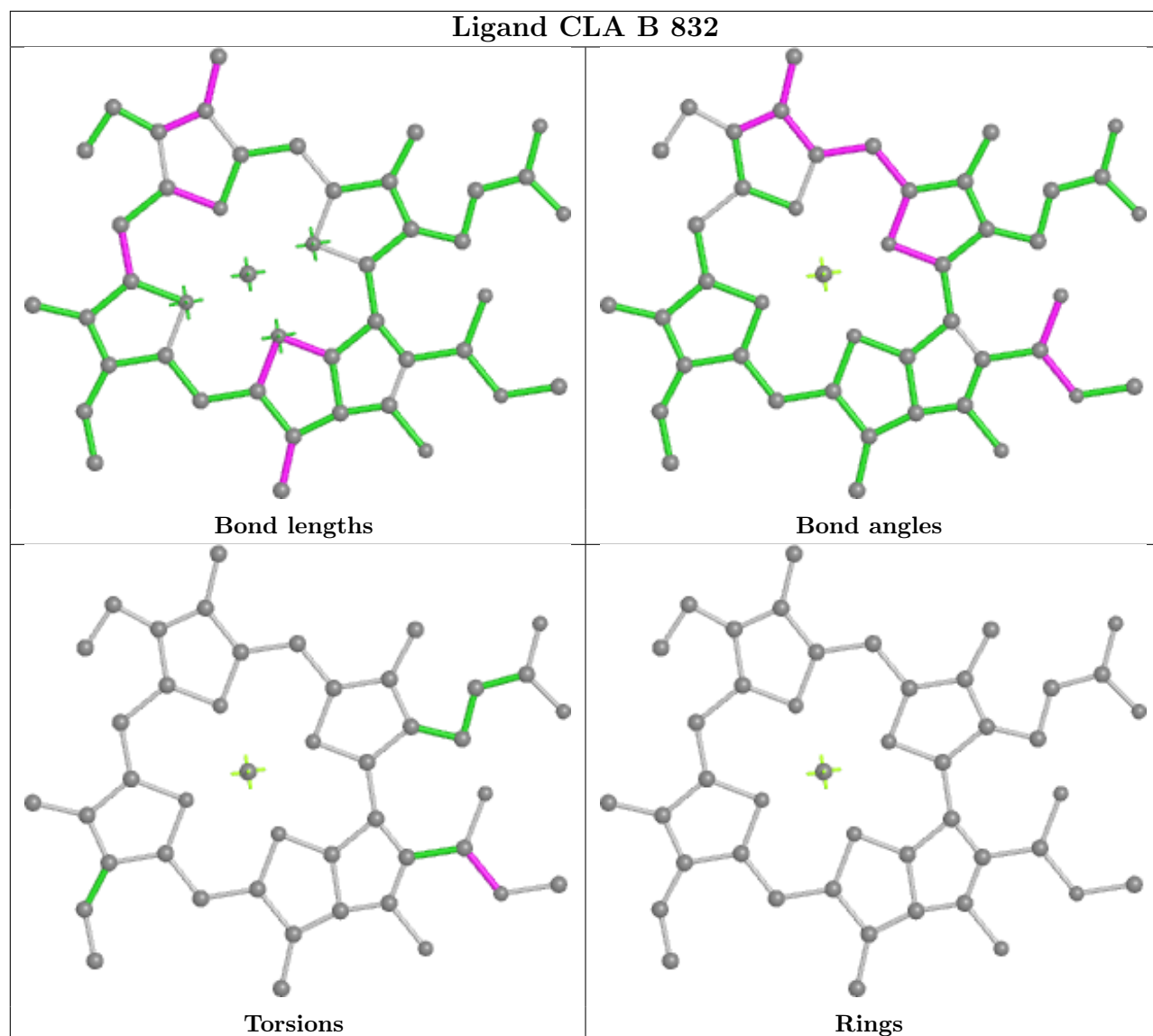


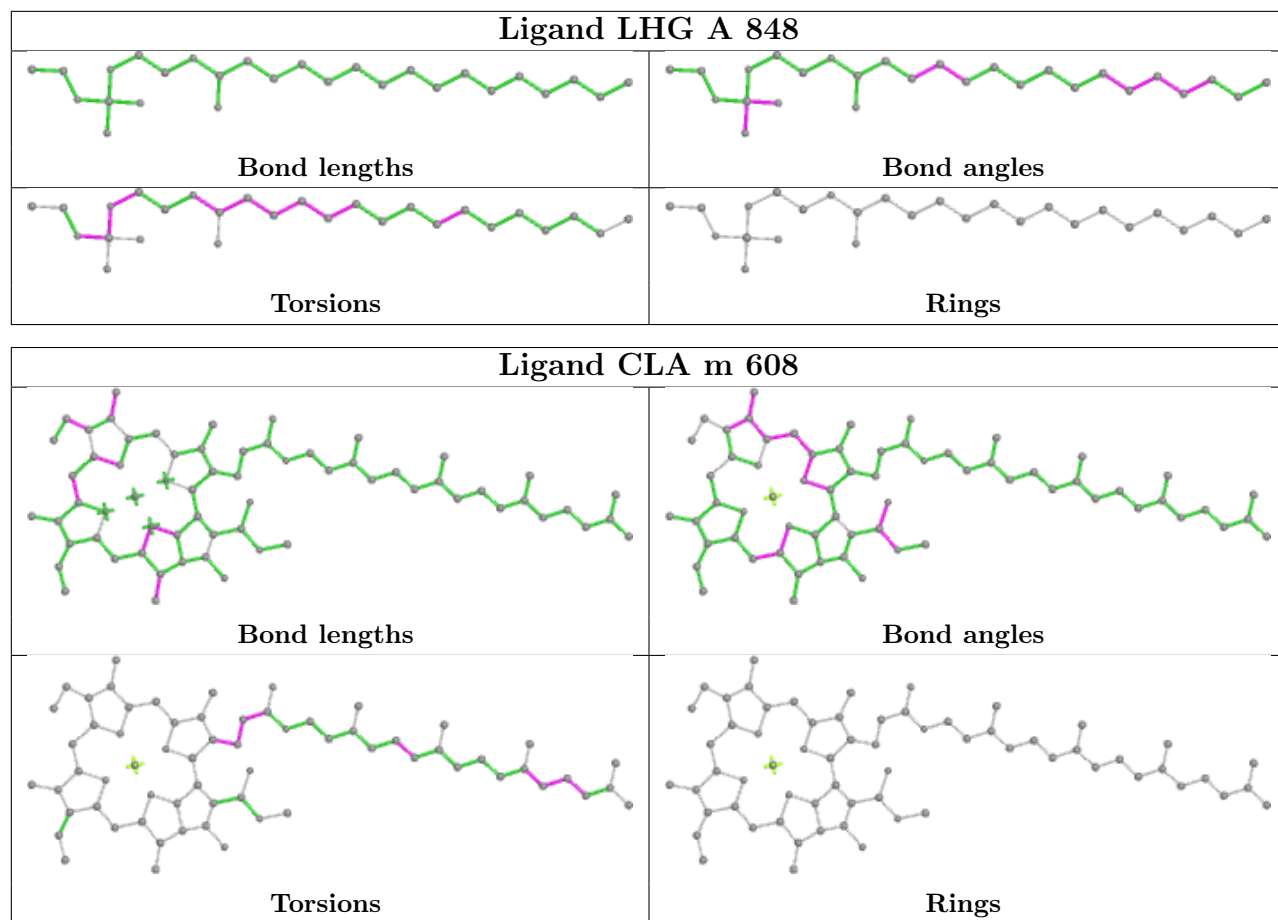
Ligand CLA b 311**Ligand CLA A 825****Ligand CLA k 604**

Ligand II0 n 618

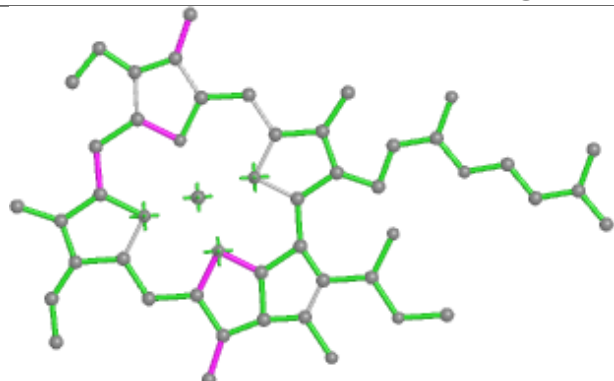


Ligand CLA B 832

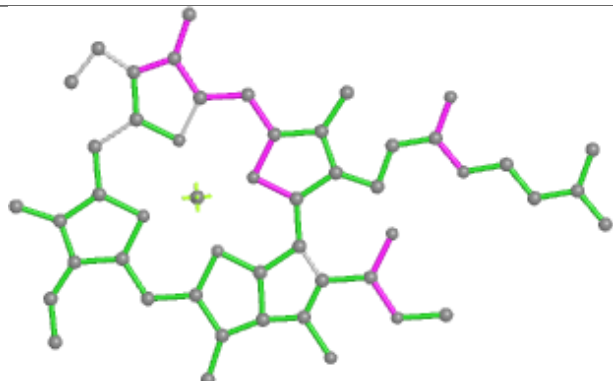




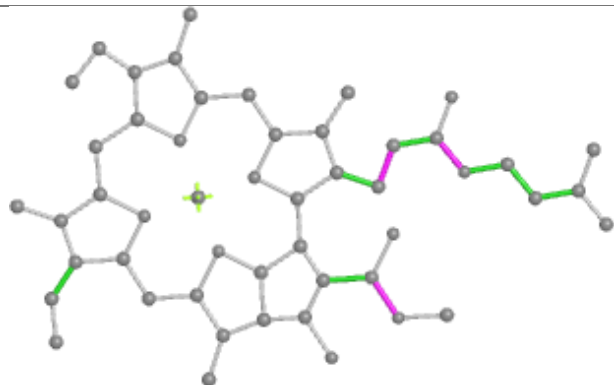
Ligand CLA n 602



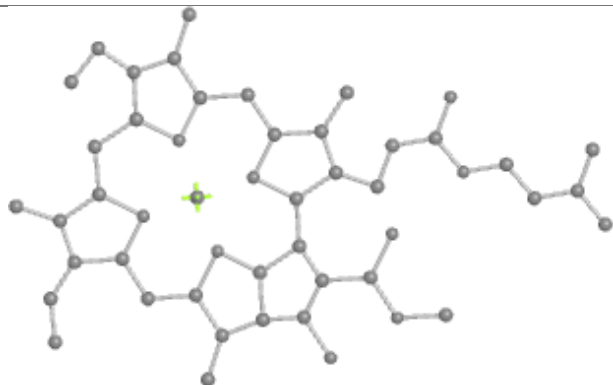
Bond lengths



Bond angles

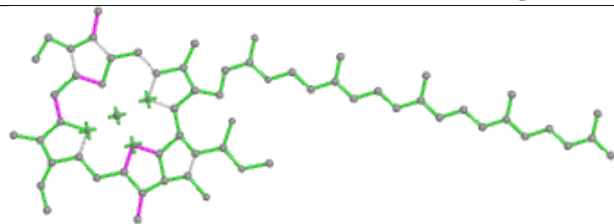


Torsions

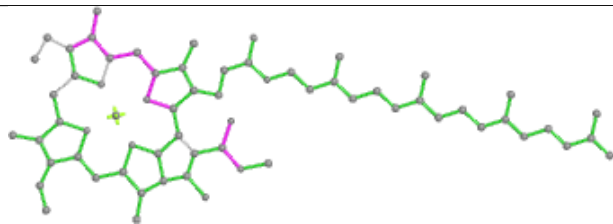


Rings

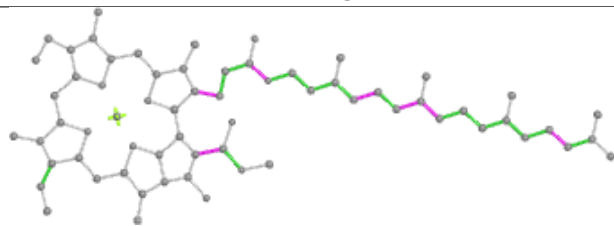
Ligand CLA A 805



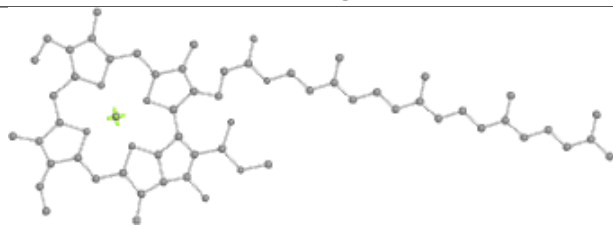
Bond lengths



Bond angles

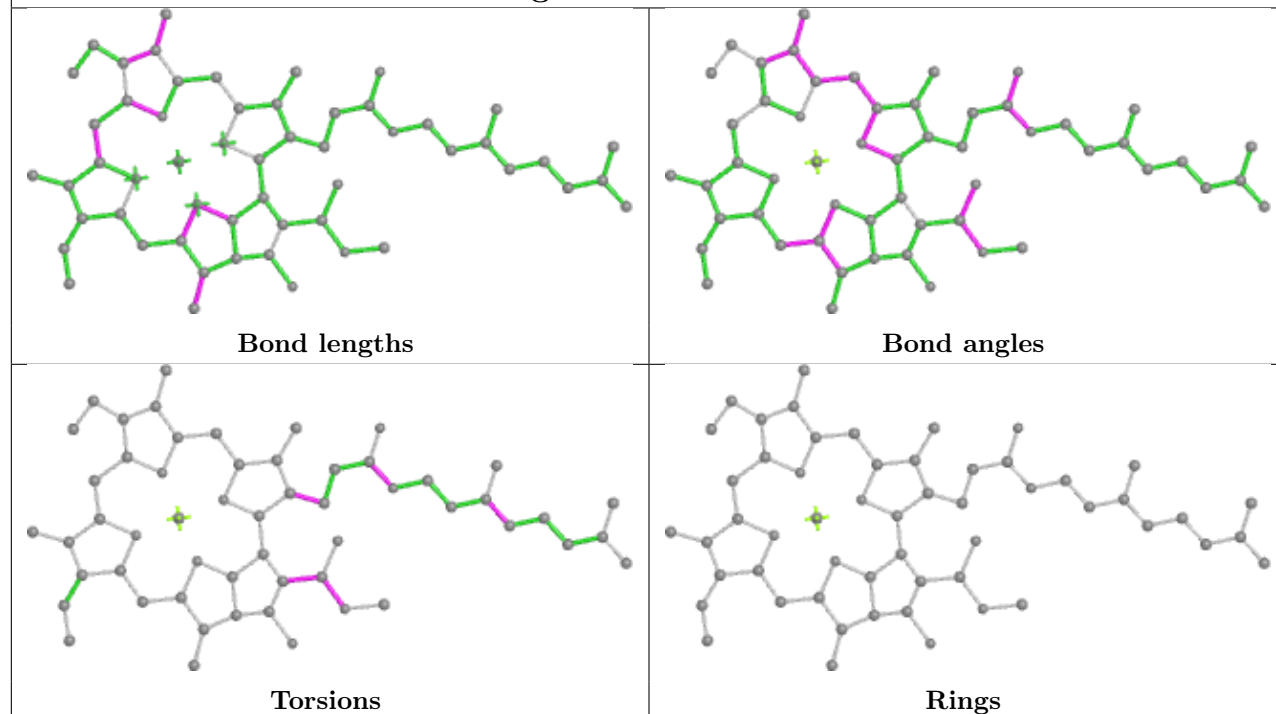


Torsions

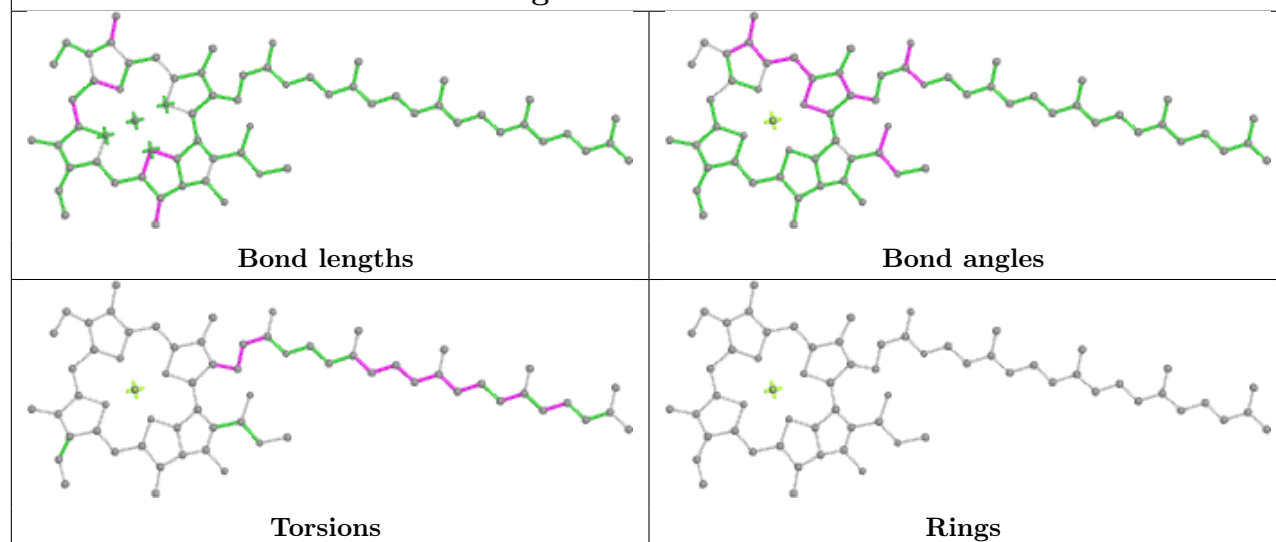


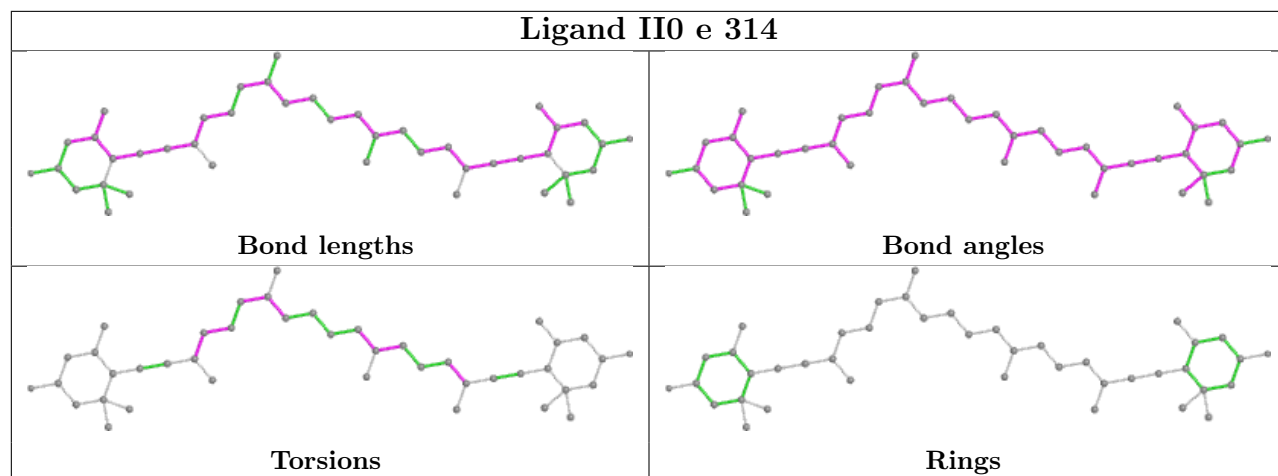
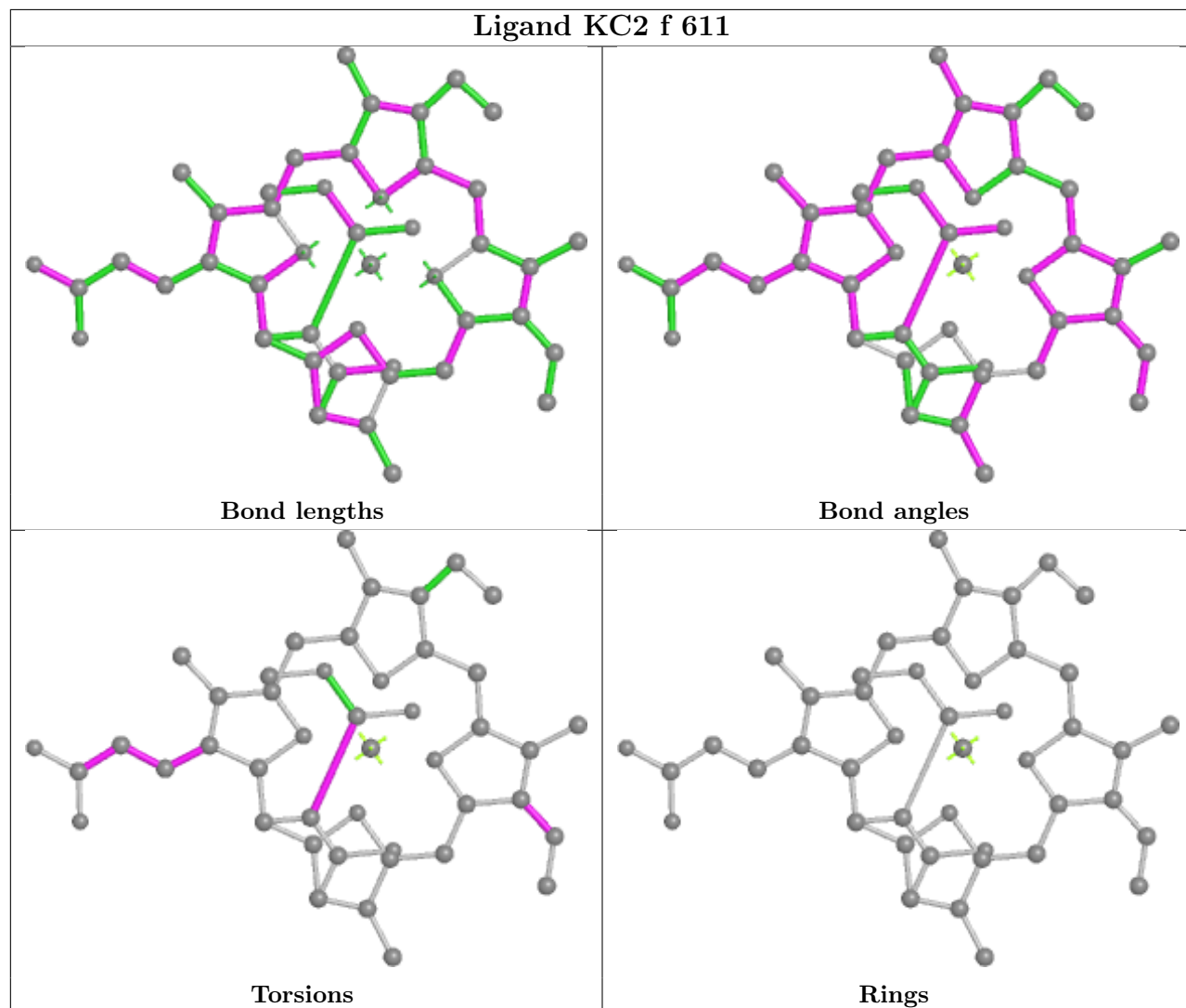
Rings

Ligand CLA A 823

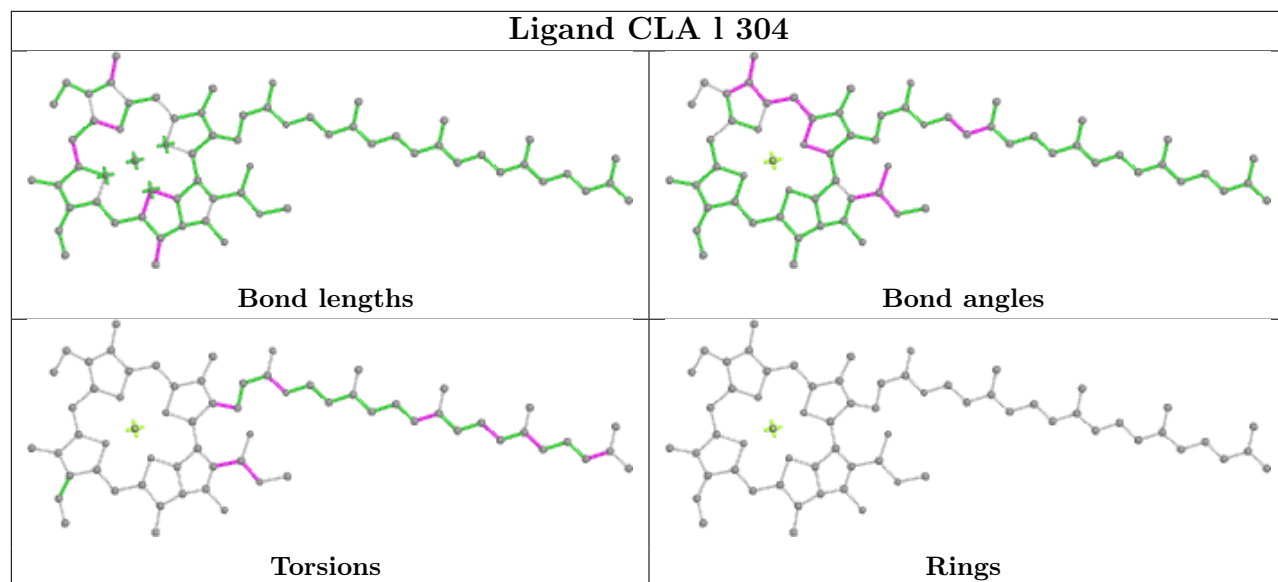


Ligand CLA A 840

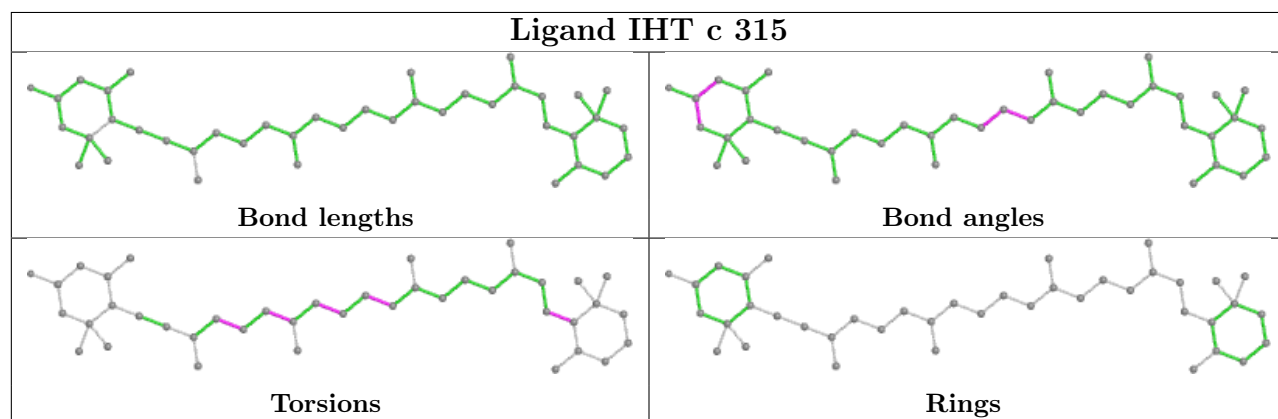


Ligand II0 e 314**Ligand KC2 f 611**

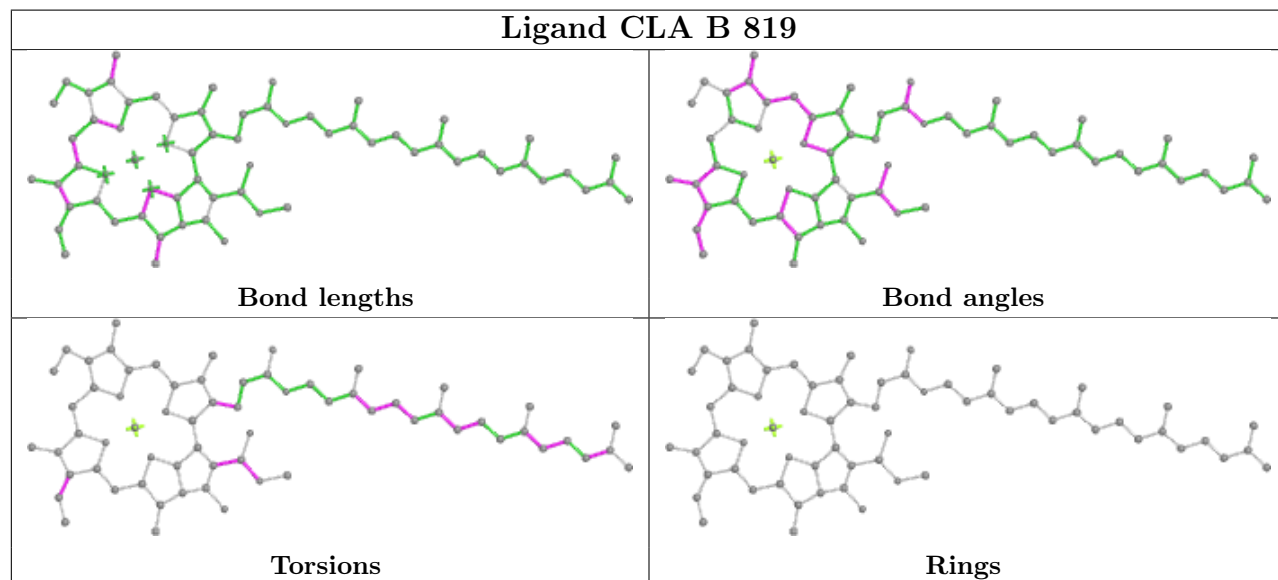
Ligand CLA l 304

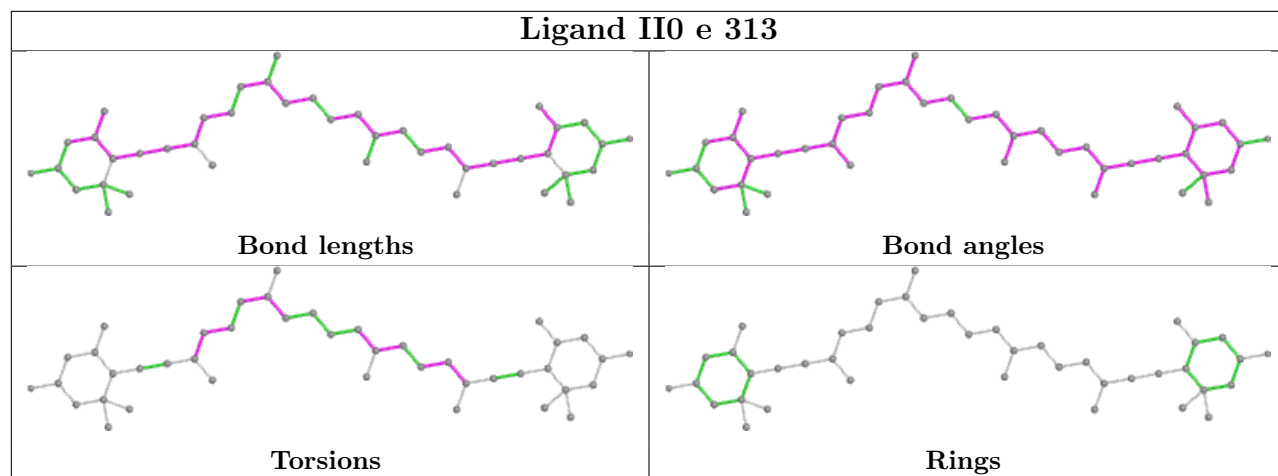
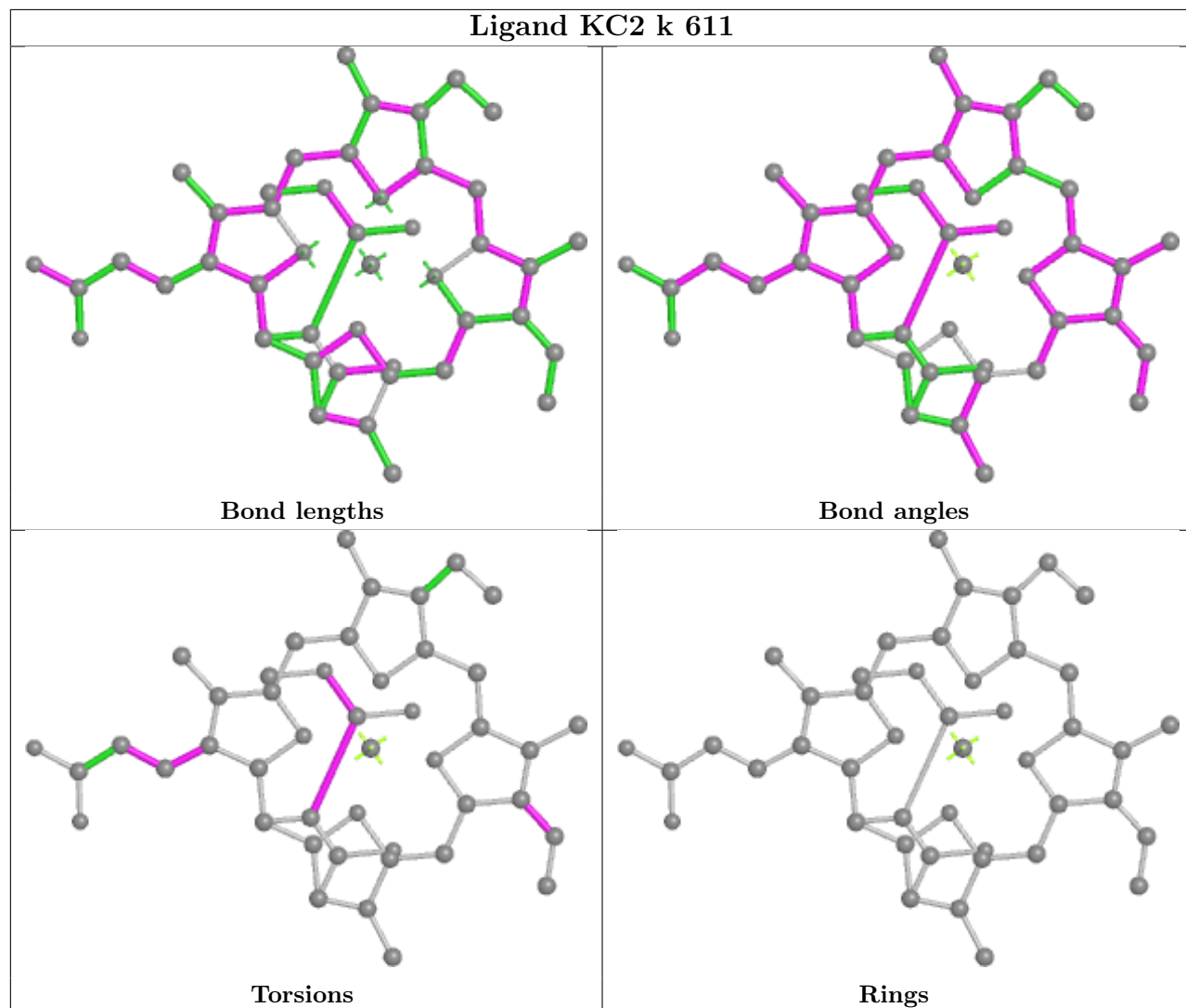


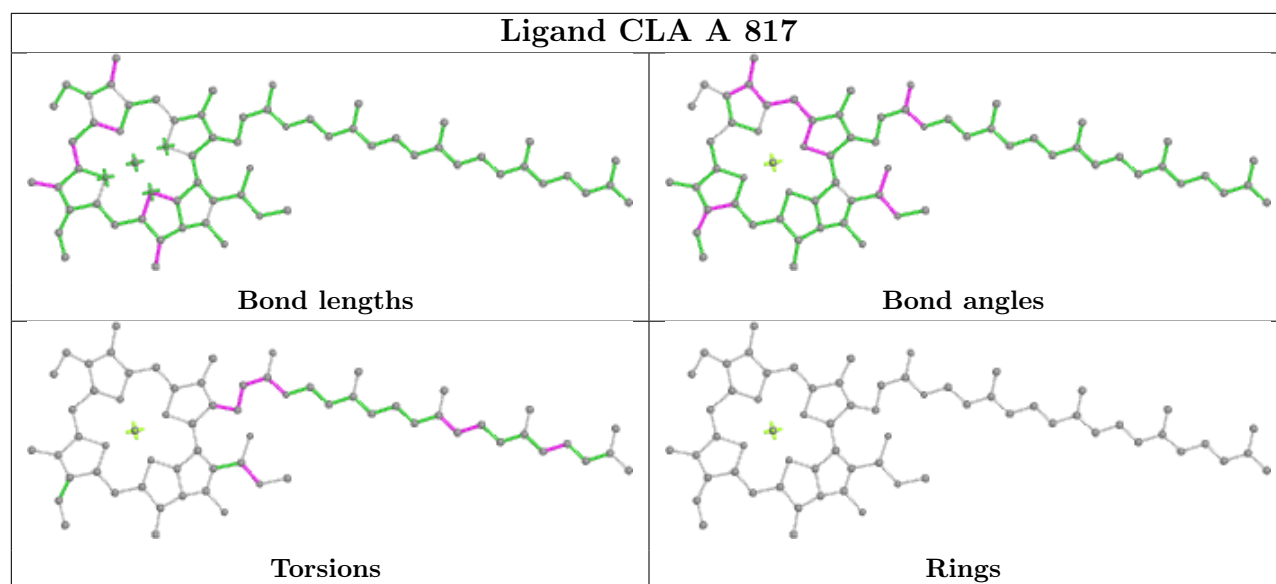
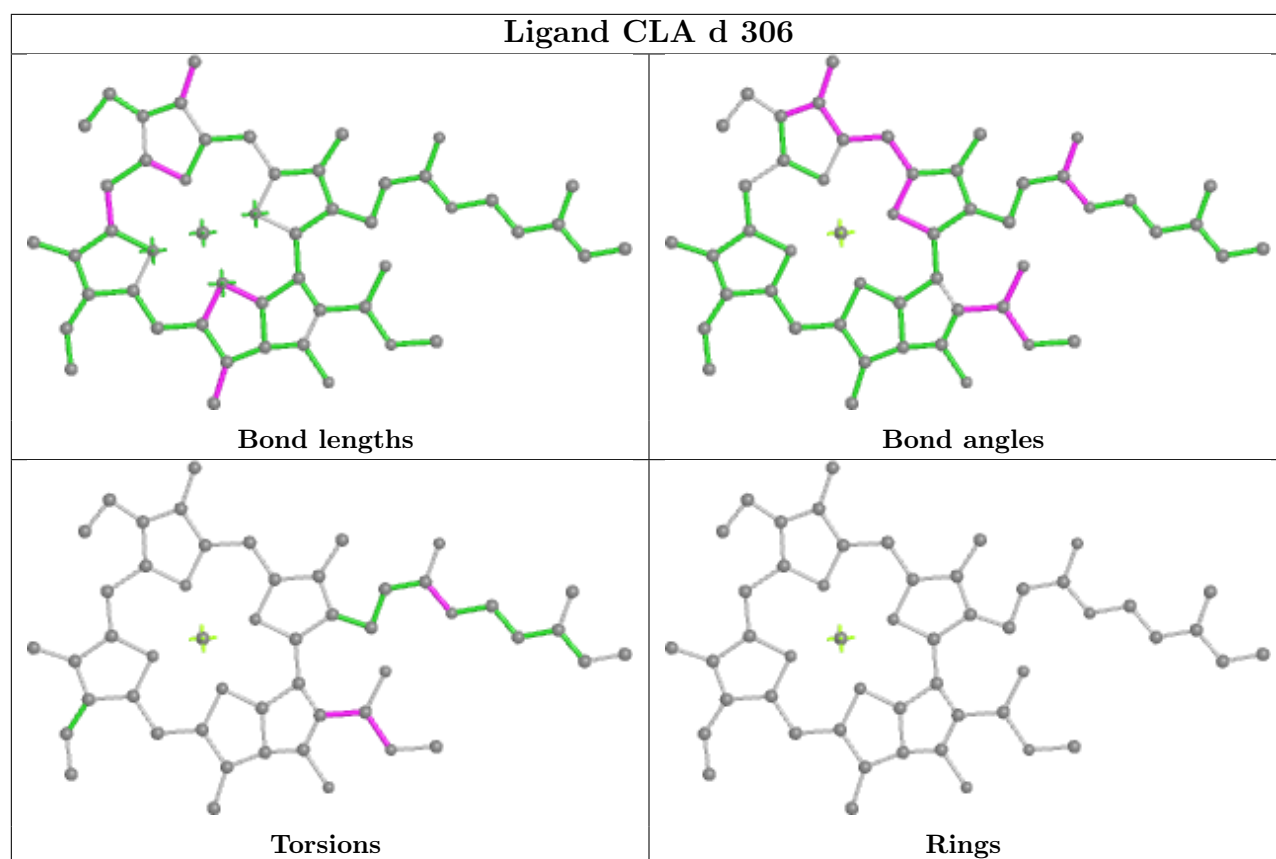
Ligand IHT c 315



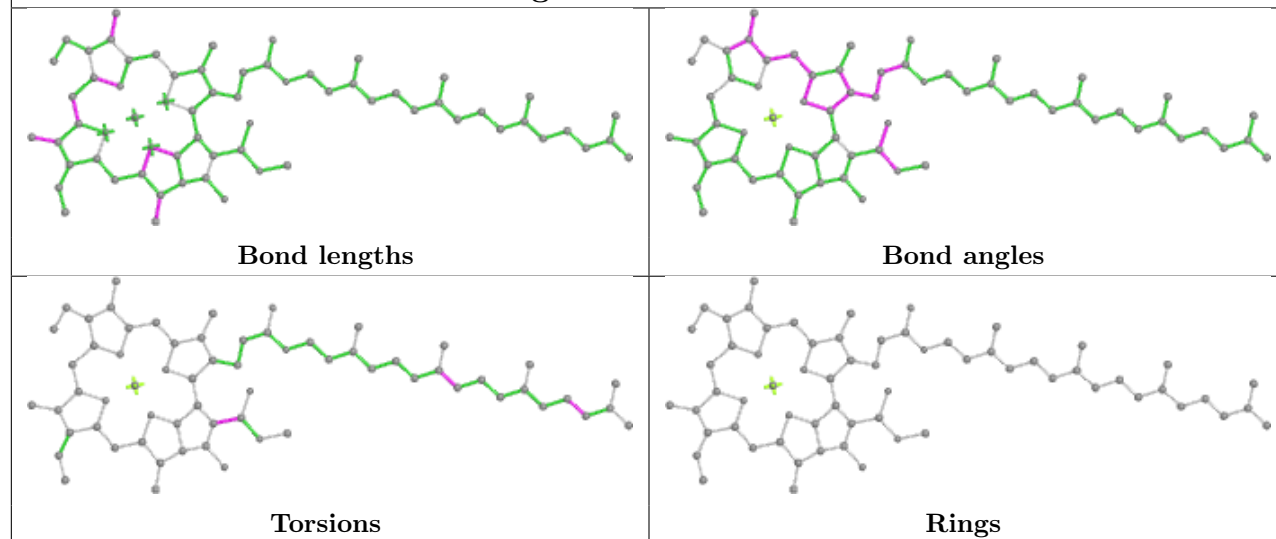
Ligand CLA B 819



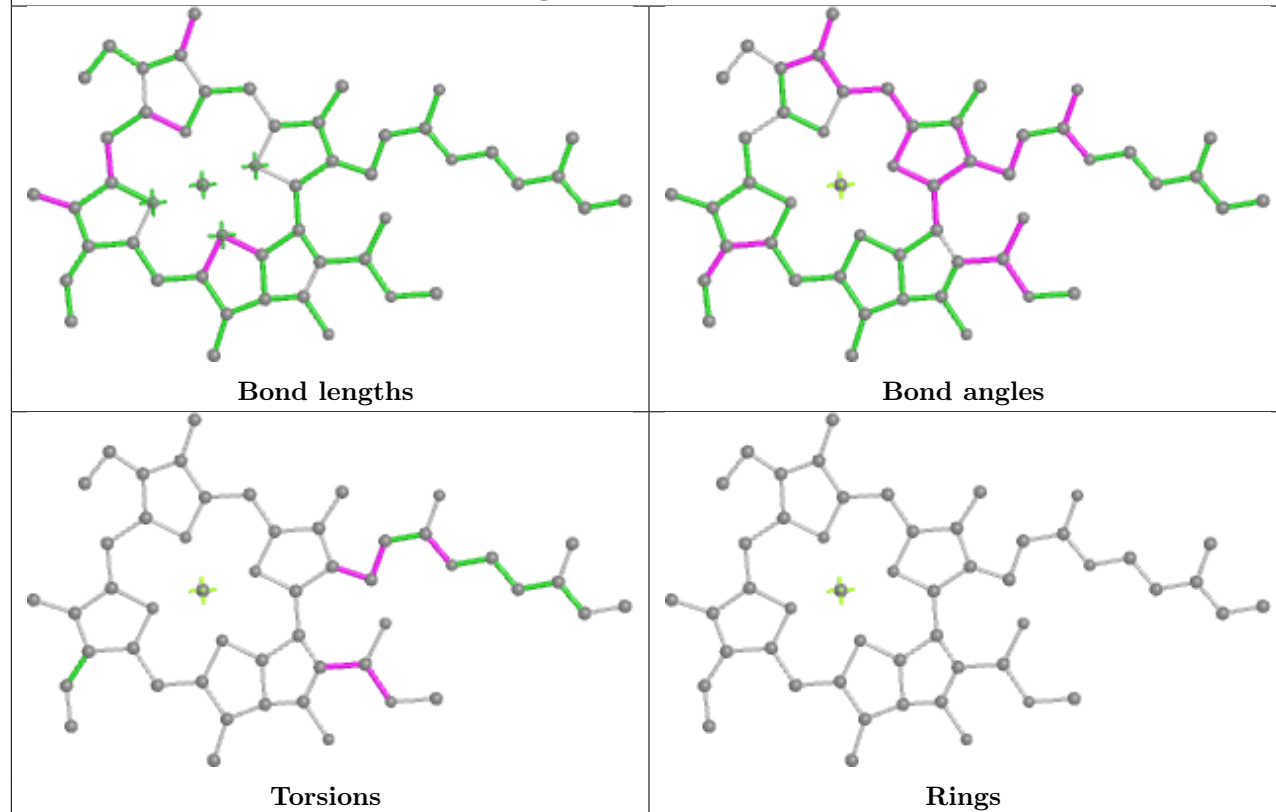
Ligand II0 e 313**Ligand KC2 k 611**

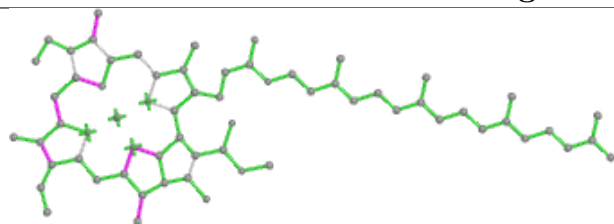
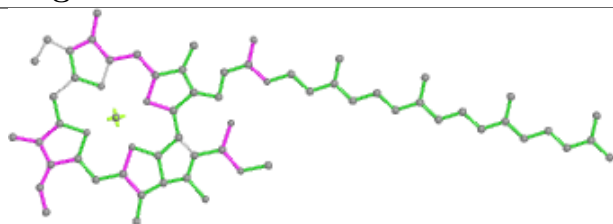
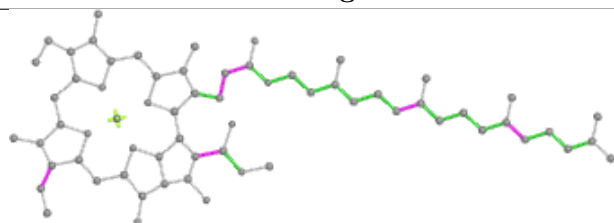
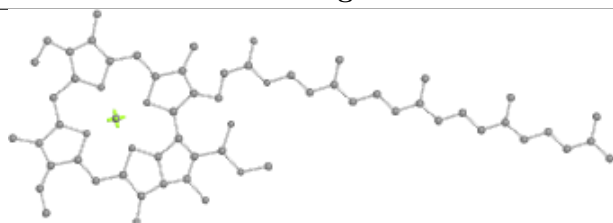
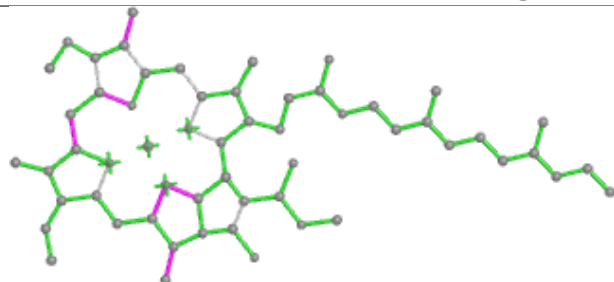
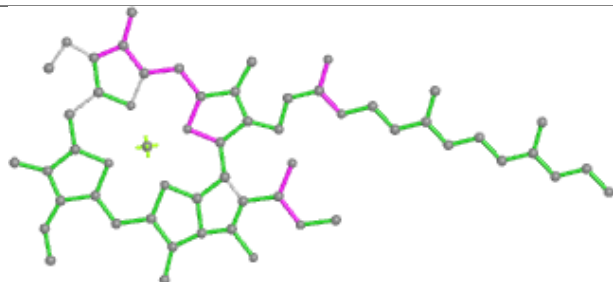
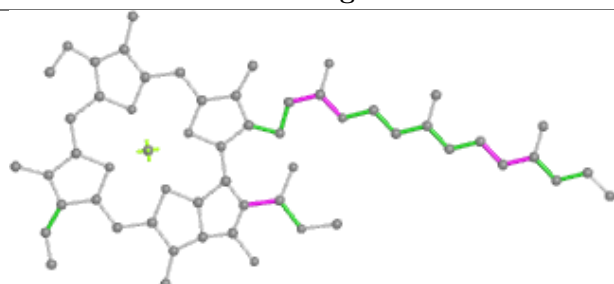
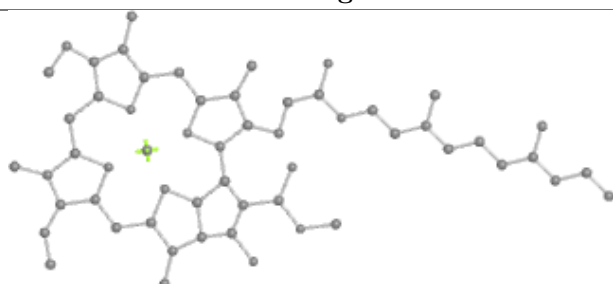


Ligand CLA A 804

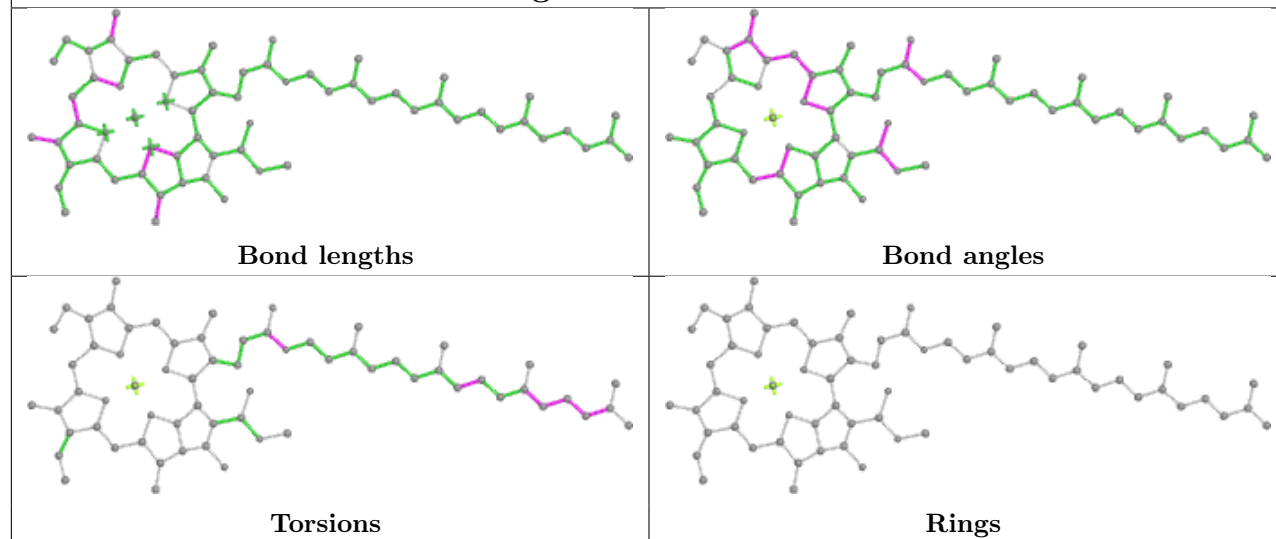


Ligand CLA d 313



Ligand CLA g 306**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 839****Bond lengths****Bond angles****Torsions****Rings**

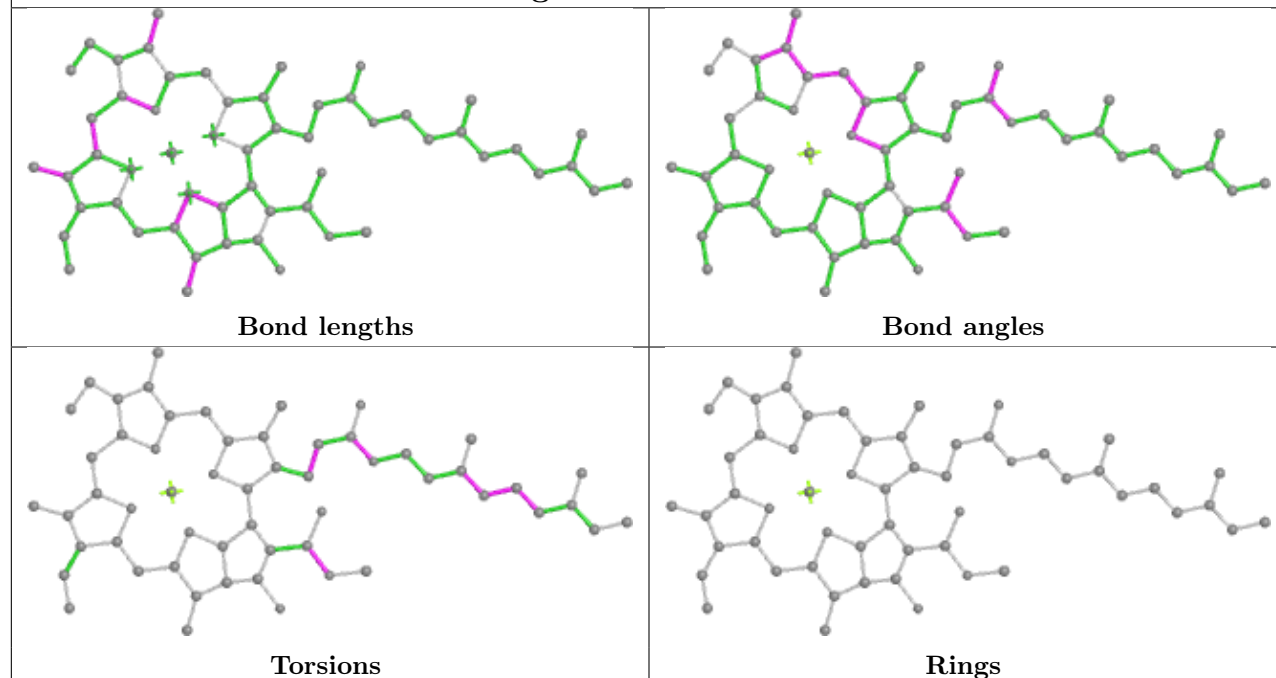
Ligand CLA B 834

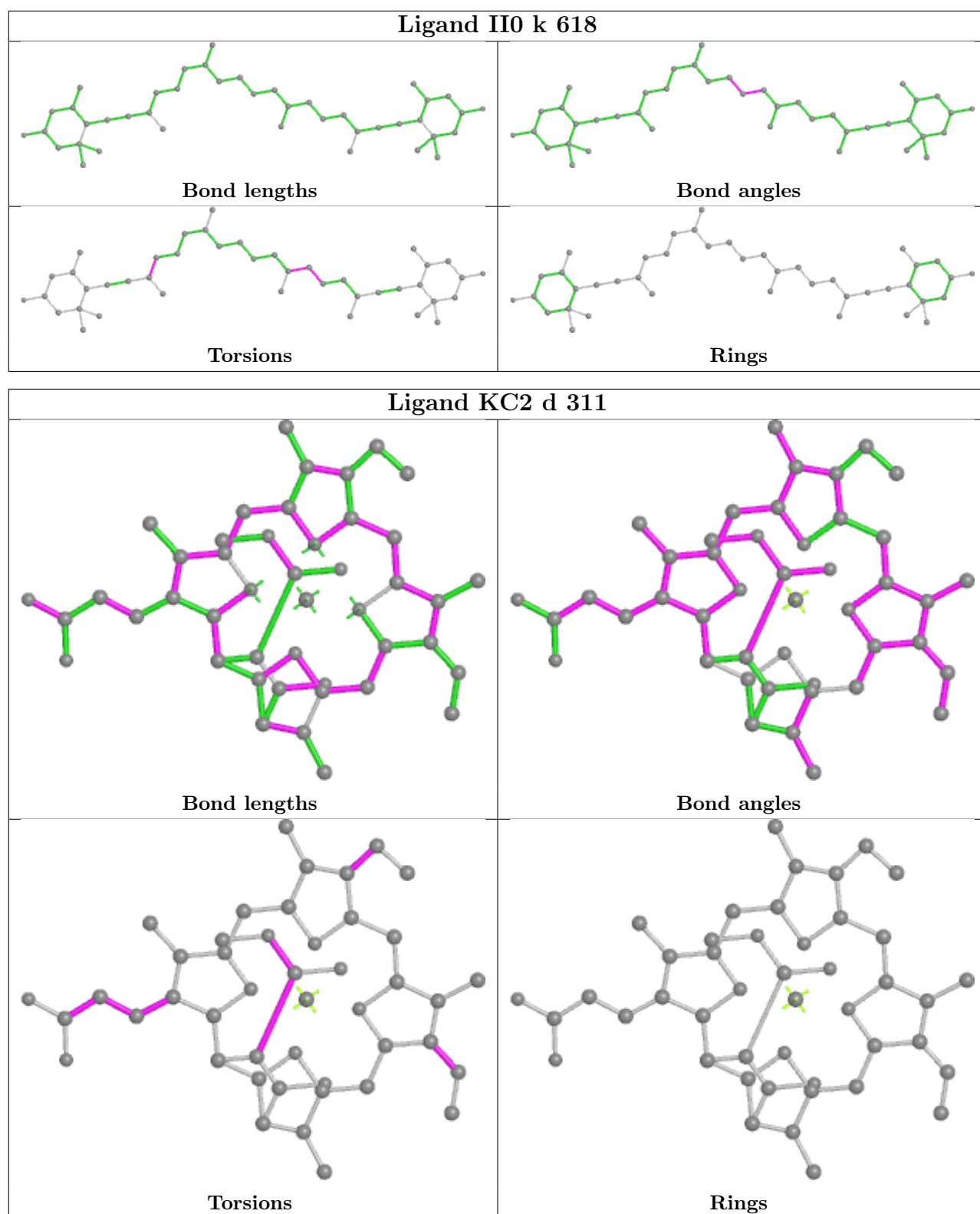


Ligand WVN B 848



Ligand CLA A 809





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

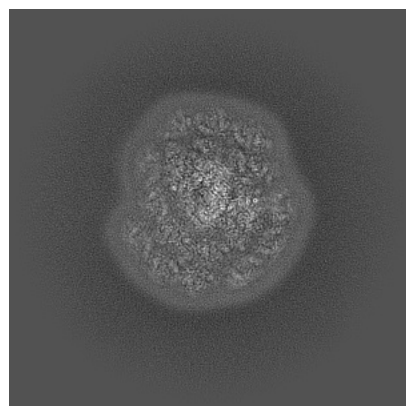
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62656. These allow visual inspection of the internal detail of the map and identification of artifacts.

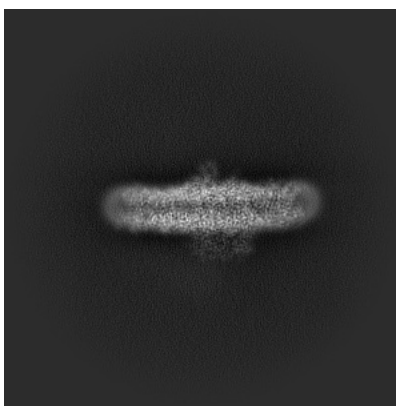
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

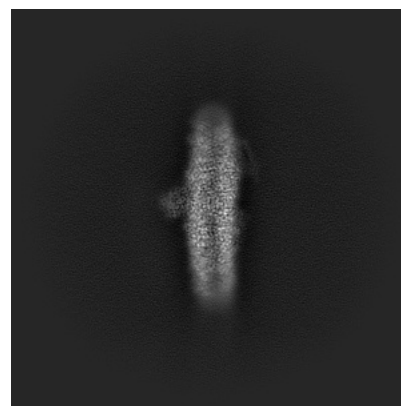
6.1.1 Primary map



X

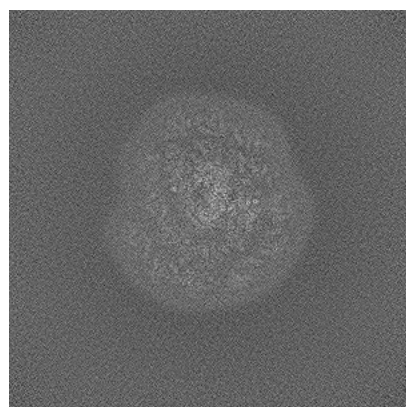


Y

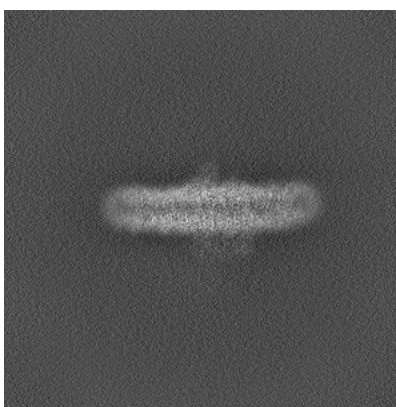


Z

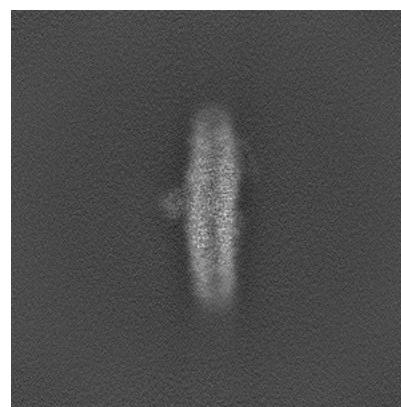
6.1.2 Raw map



X



Y

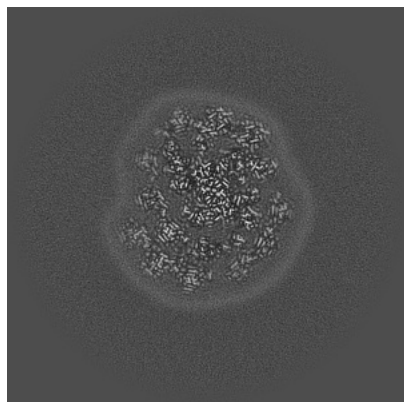


Z

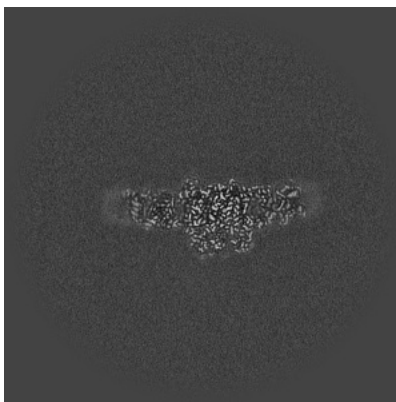
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

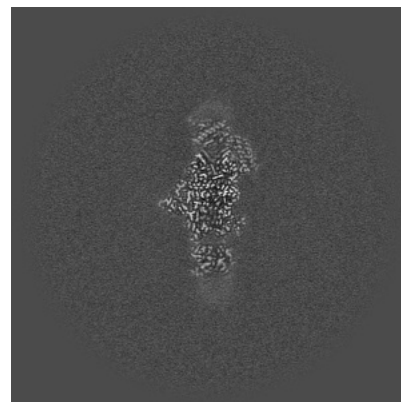
6.2.1 Primary map



X Index: 300

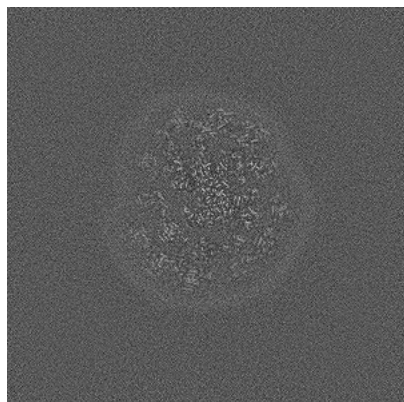


Y Index: 300

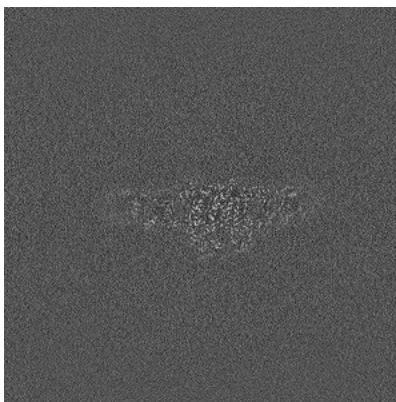


Z Index: 300

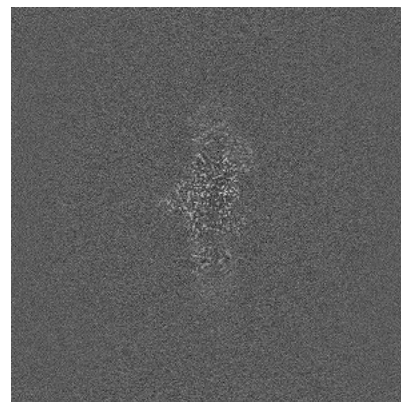
6.2.2 Raw map



X Index: 300



Y Index: 300

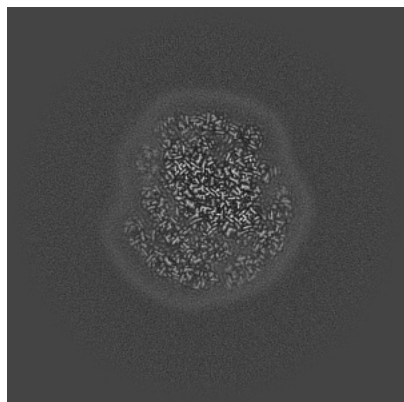


Z Index: 300

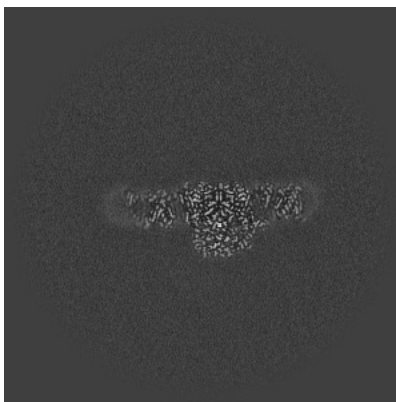
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

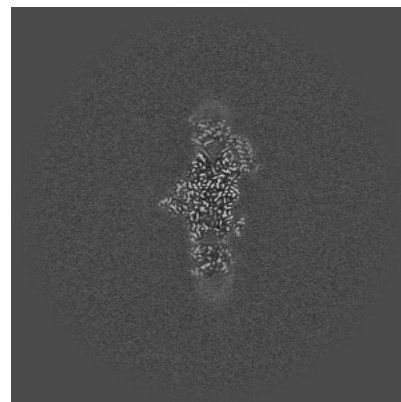
6.3.1 Primary map



X Index: 315

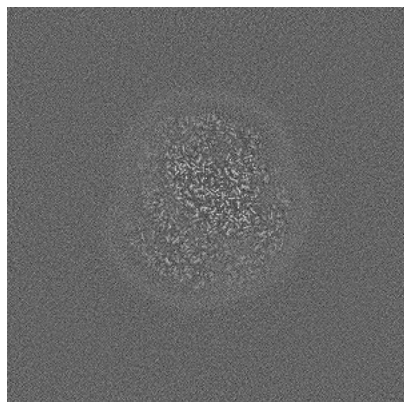


Y Index: 308

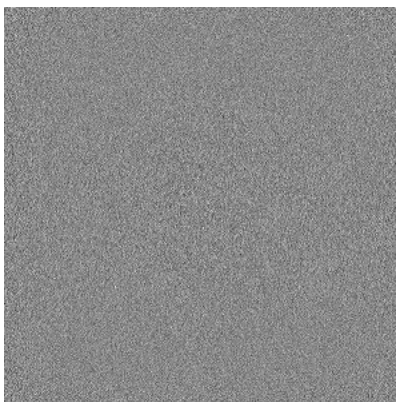


Z Index: 301

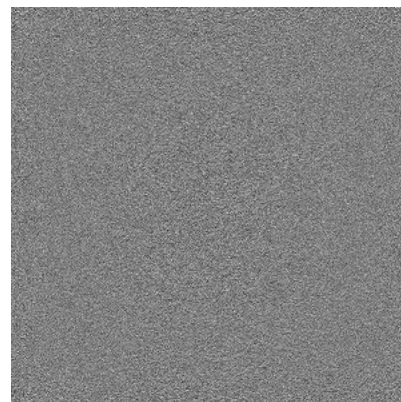
6.3.2 Raw map



X Index: 315



Y Index: 0

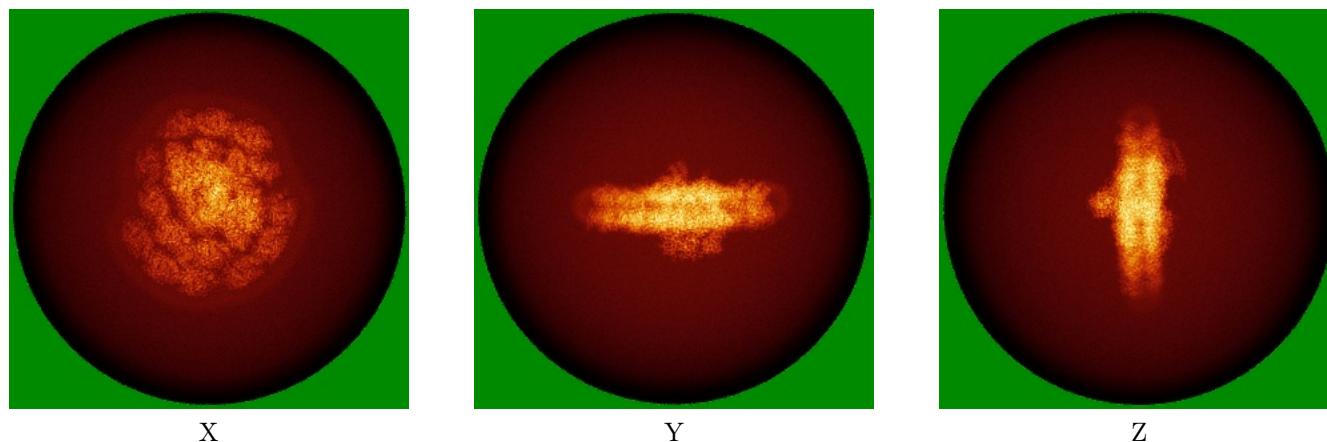


Z Index: 0

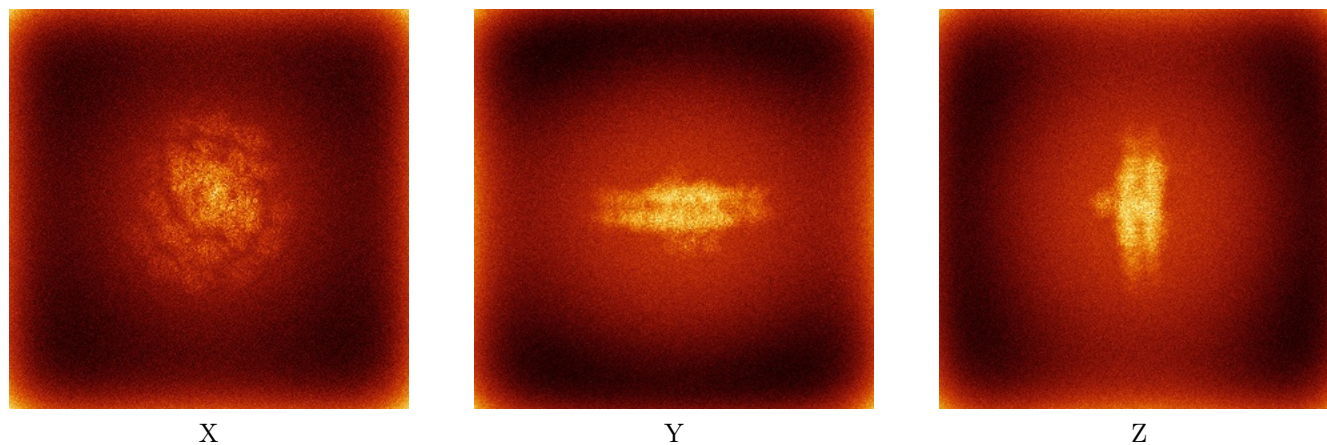
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



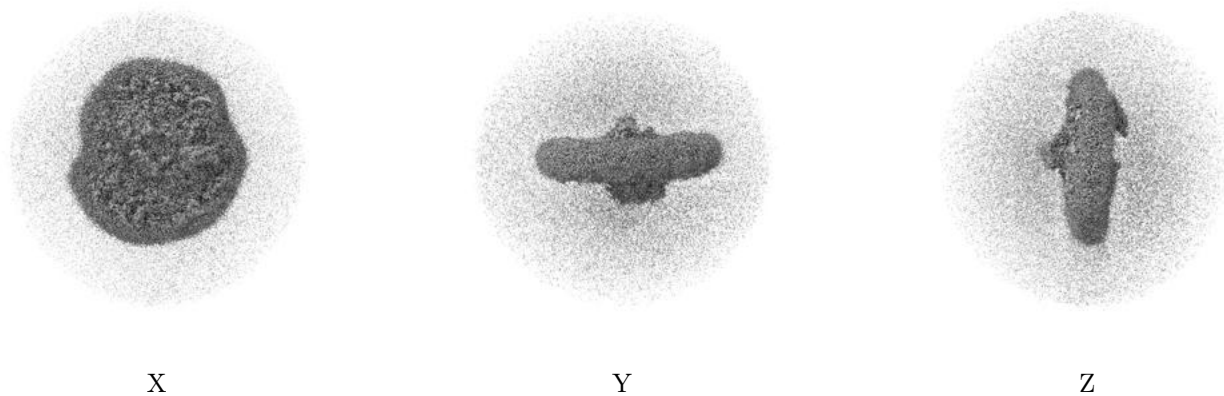
6.4.2 Raw map



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.

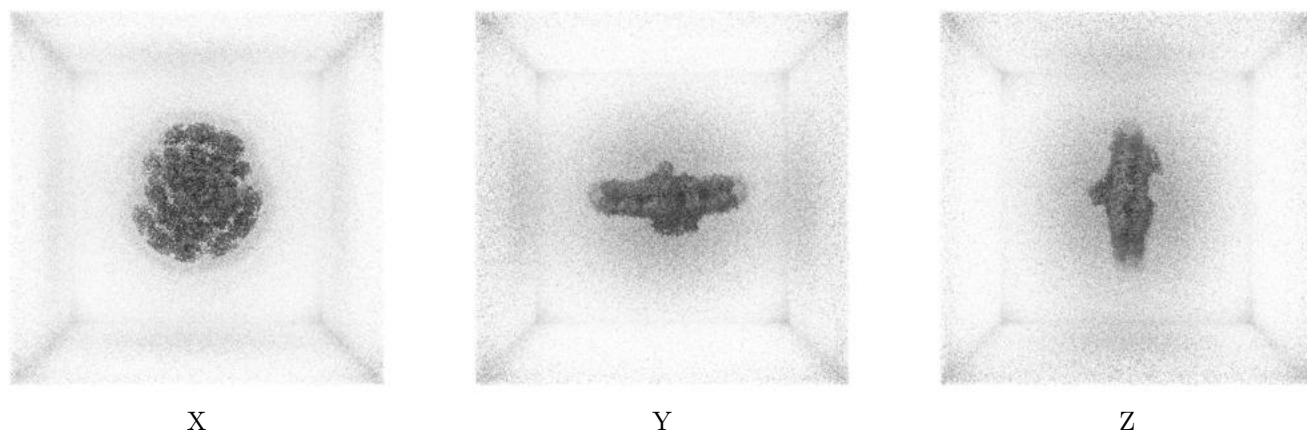
6.5 Orthogonal surface views [i](#)

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.

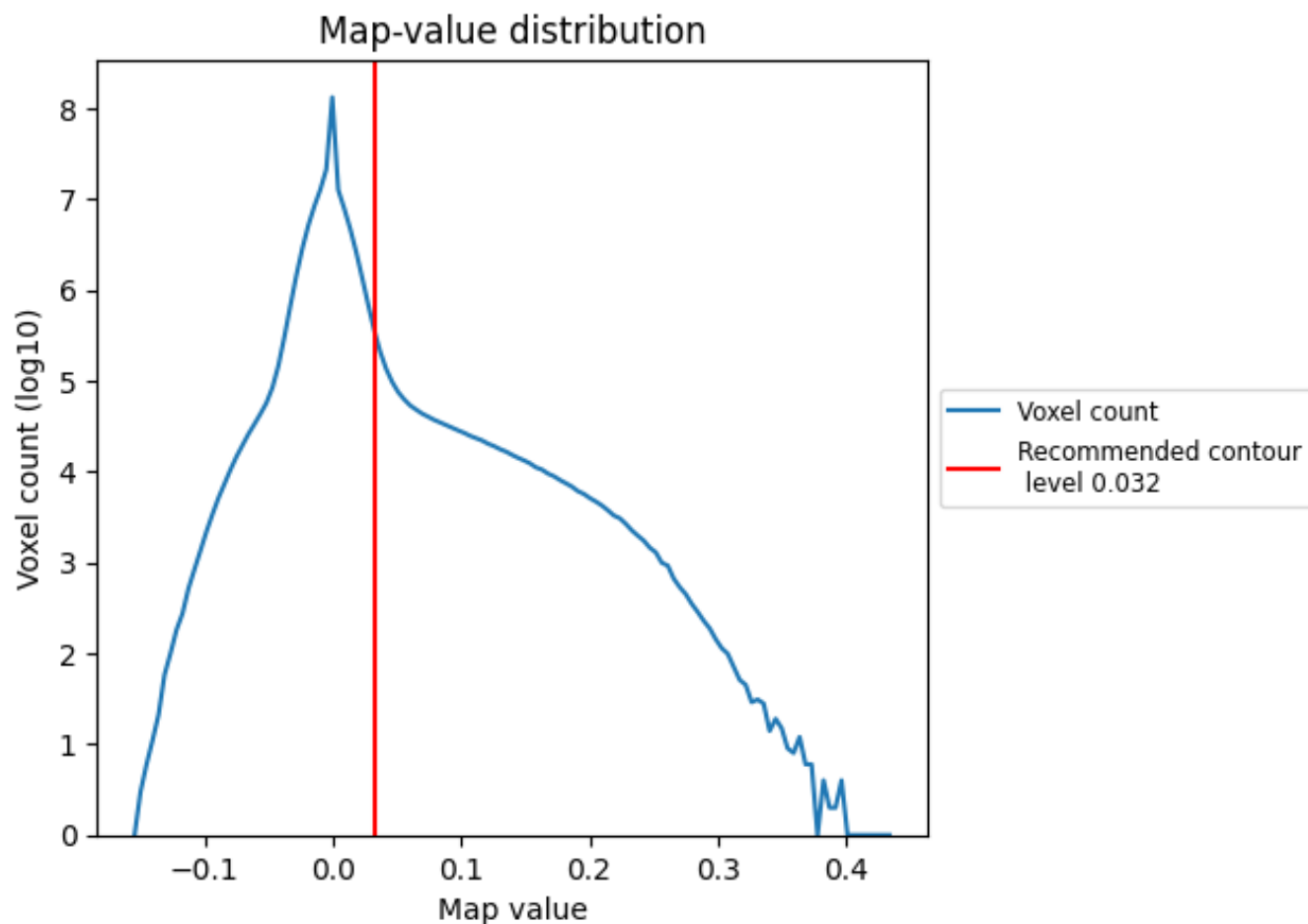
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

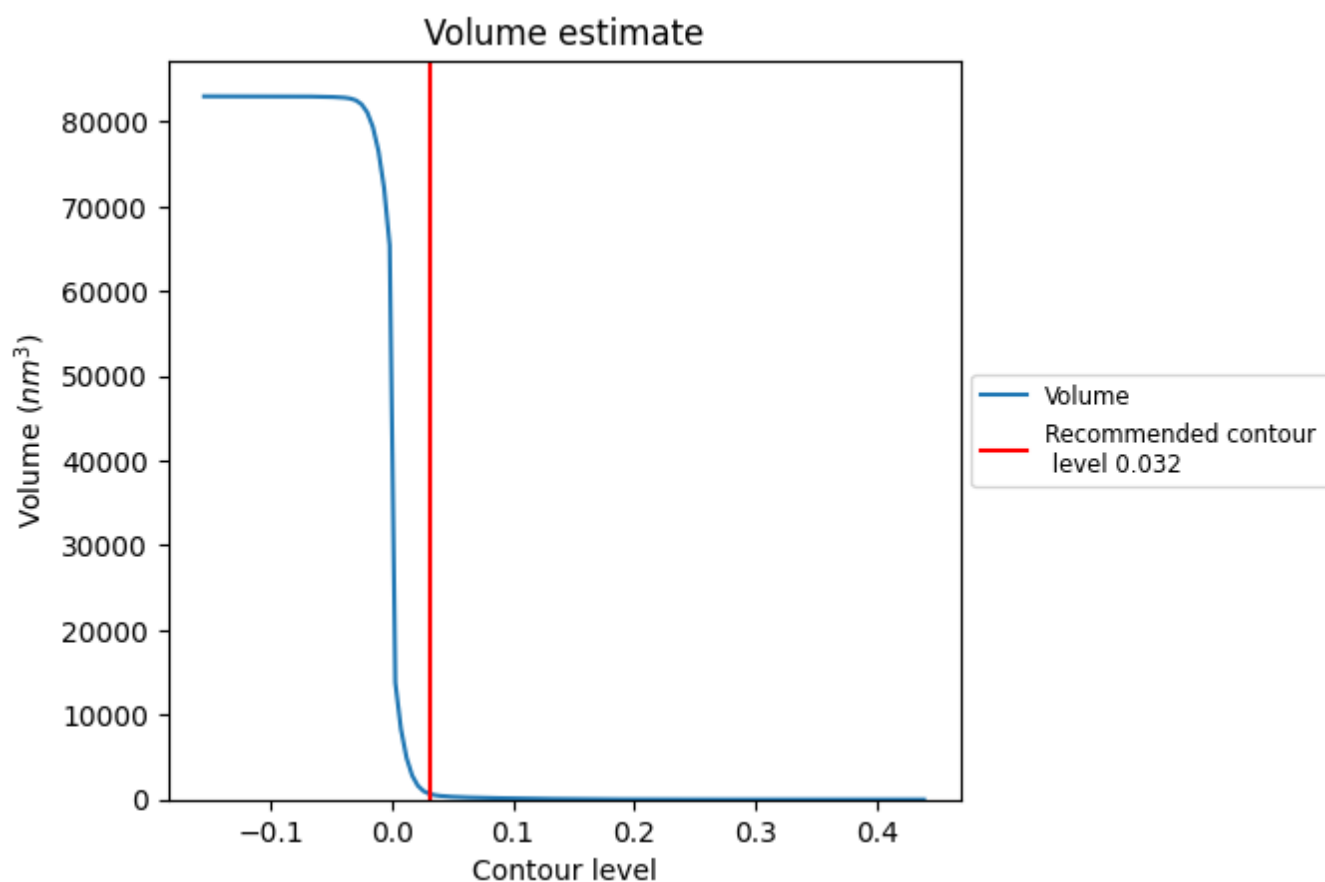
This section contains the results of statistical analysis of the map.

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.

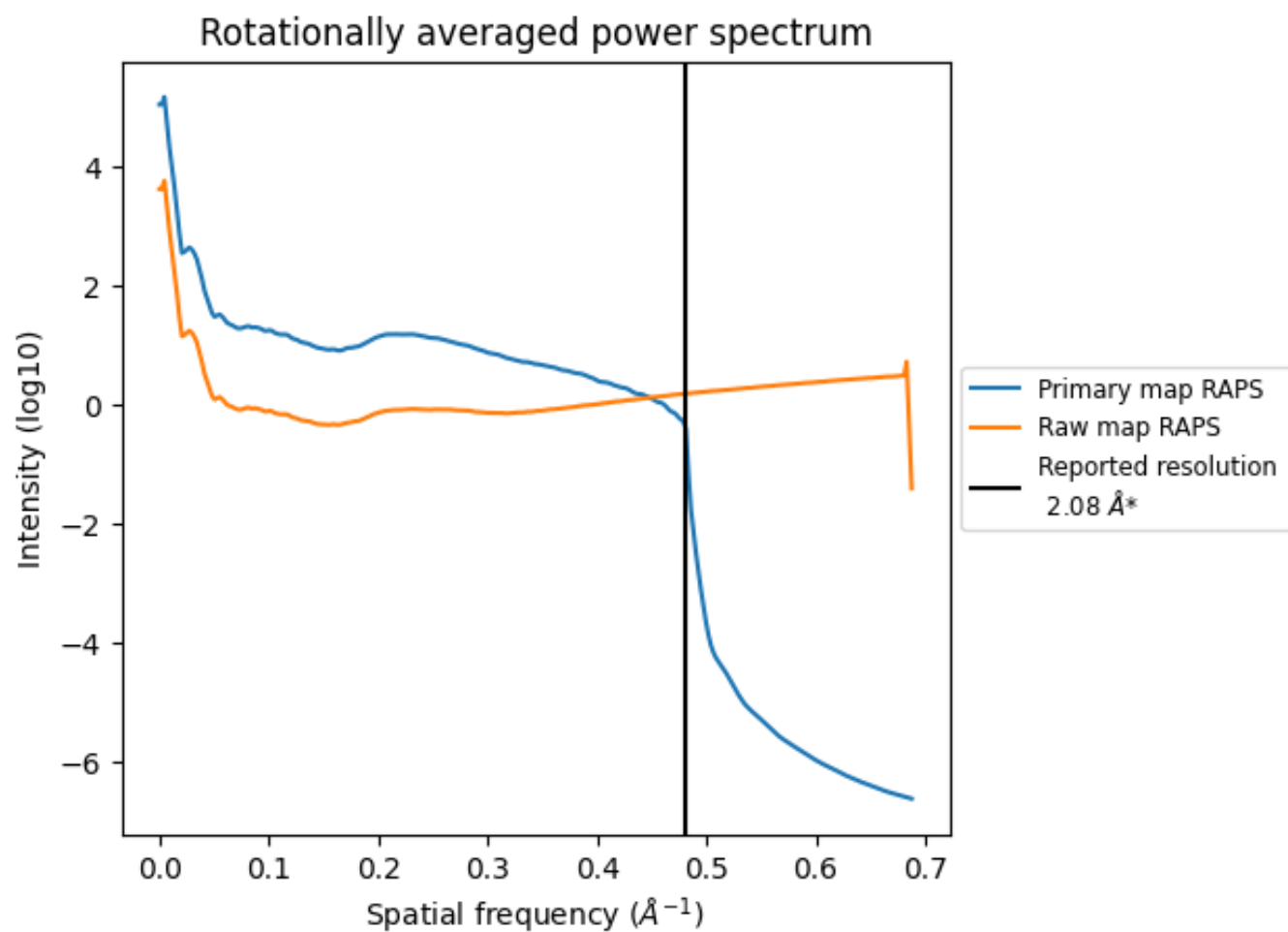
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 646 nm^3 ; this corresponds to an approximate mass of 583 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 [i](#)

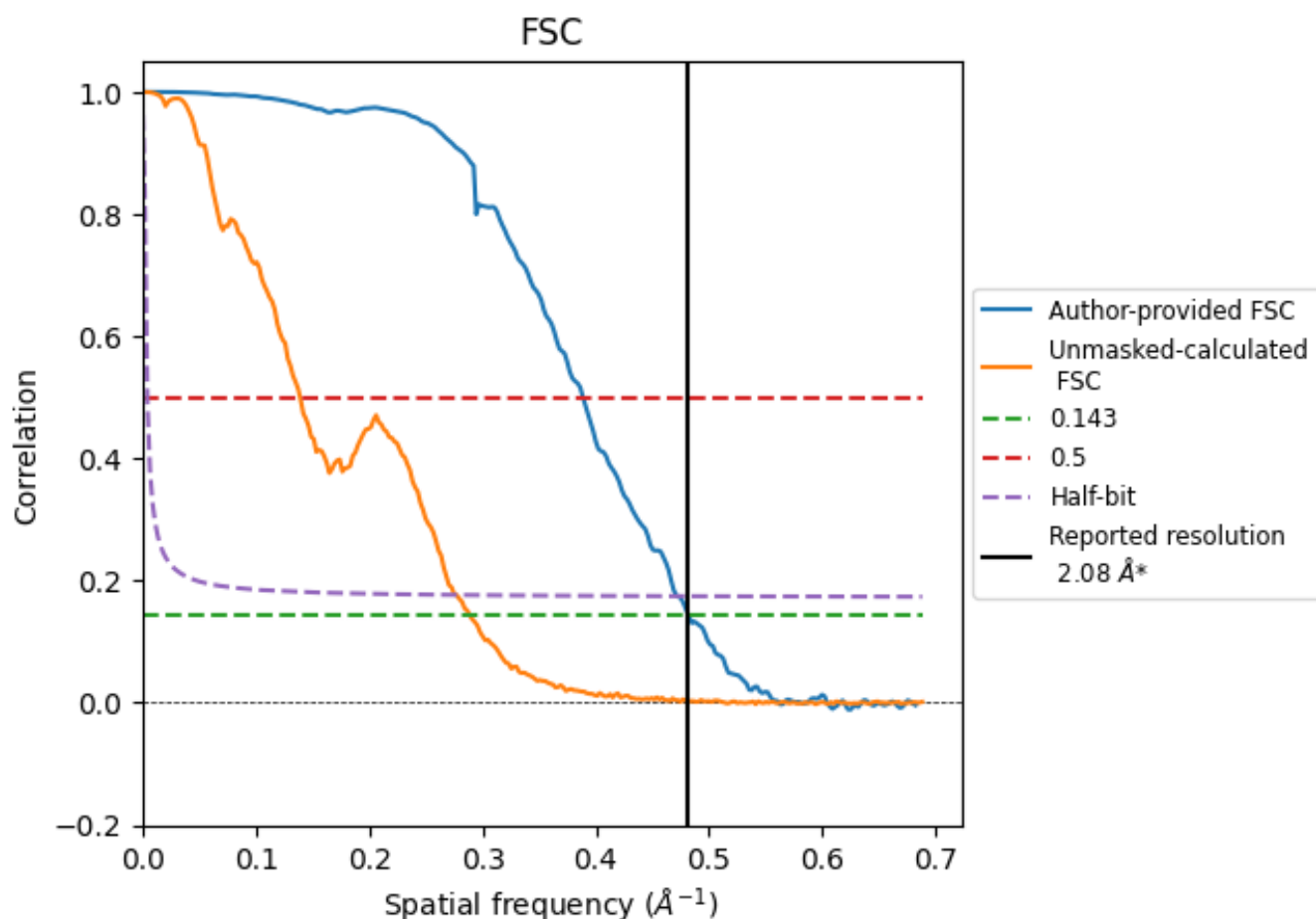


*Reported resolution corresponds to spatial frequency of 0.481 \AA^{-1}

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 0.481 Å⁻¹

8.2 Resolution estimates [i](#)

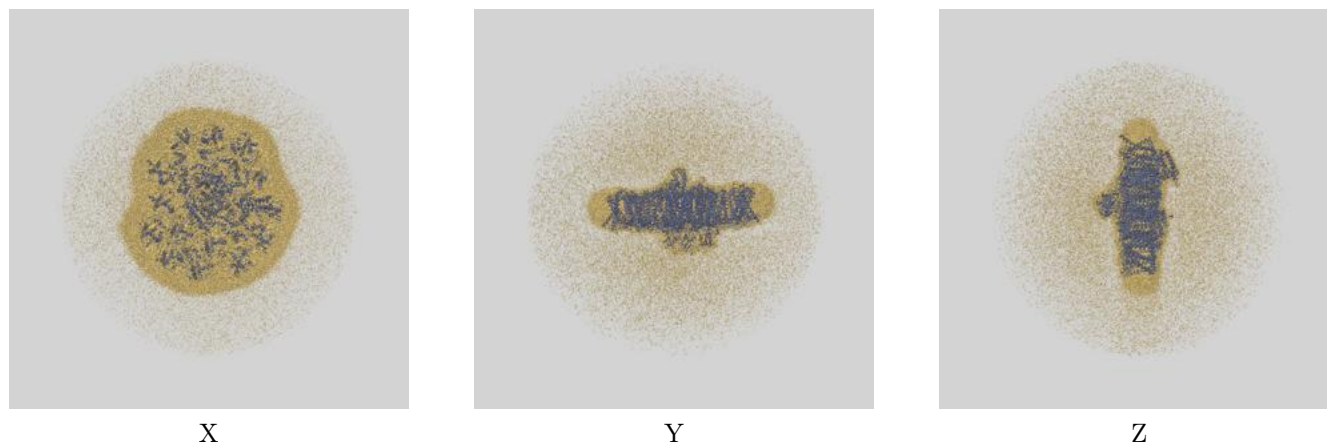
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.08	-	-
Author-provided FSC curve	2.08	2.57	2.12
Unmasked-calculated*	3.46	7.18	3.61

*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 3.46 differs from the reported value 2.08 by more than 10 %

9 Map-model fit [i](#)

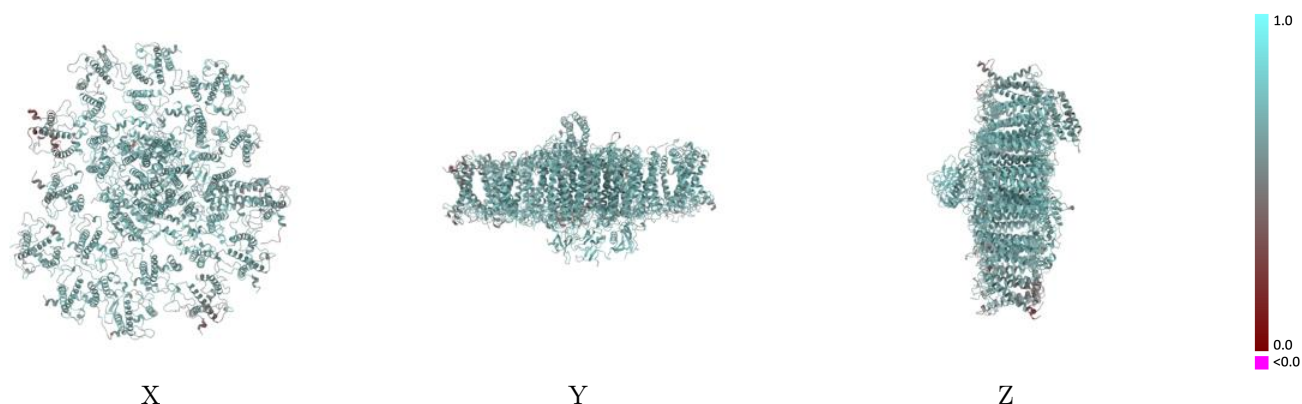
This section contains information regarding the fit between EMDB map EMD-62656 and PDB model 9KZ9. Per-residue inclusion information can be found in section [3](#) on page [43](#).

9.1 Map-model overlay [i](#)



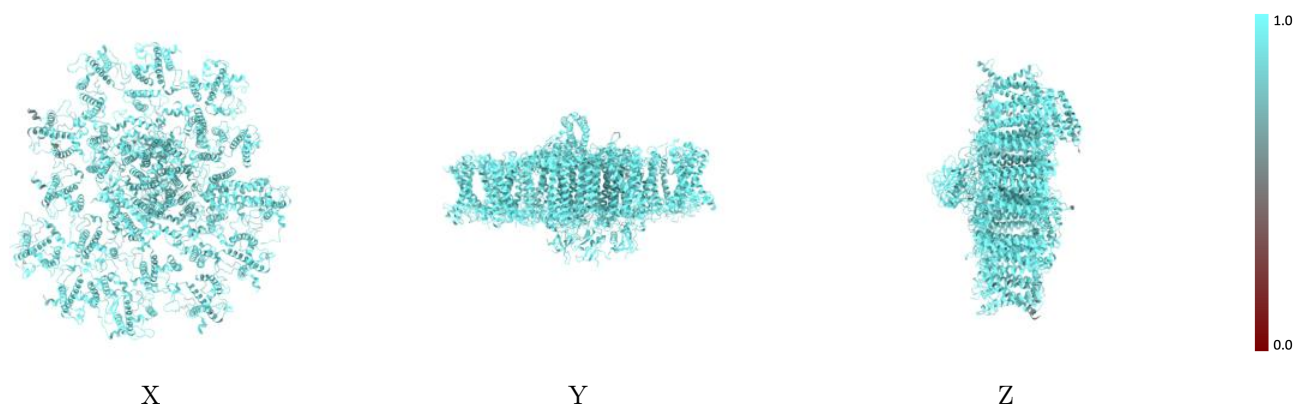
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



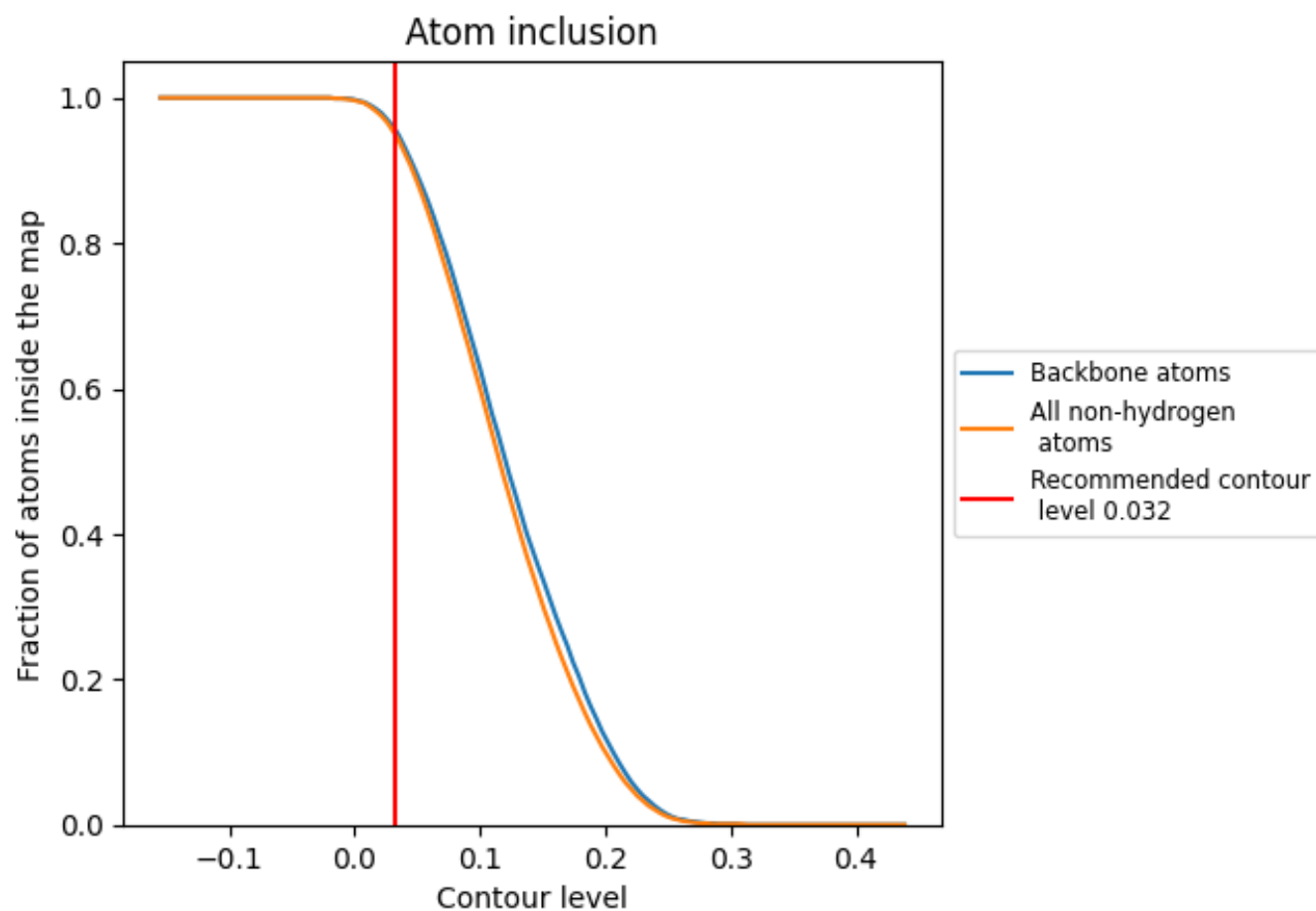
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 96% of all backbone atoms, 95% 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	 0.9510	 0.6450
A	 0.9820	 0.6990
B	 0.9830	 0.7020
C	 0.9970	 0.7120
D	 0.9870	 0.6910
E	 0.9680	 0.6680
F	 0.9680	 0.6800
I	 0.9860	 0.6850
J	 0.9720	 0.6720
K	 0.9610	 0.6620
L	 0.9650	 0.6740
M	 0.9550	 0.6570
O	 0.9670	 0.6720
Q	 0.9120	 0.6040
R	 0.9710	 0.6650
a	 0.9690	 0.6670
b	 0.9690	 0.6700
c	 0.9210	 0.6110
d	 0.8310	 0.5040
e	 0.9040	 0.5680
f	 0.9540	 0.6410
g	 0.9500	 0.6330
h	 0.9470	 0.6400
i	 0.9080	 0.5650
j	 0.9220	 0.6080
k	 0.8970	 0.5460
l	 0.9540	 0.6250
m	 0.9390	 0.6290
n	 0.8970	 0.5760
s	 0.9520	 0.6460

