



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2025 – 04:55 PM JST

PDB ID : 9L0K / pdb_00009l0k
EMDB ID : EMD-62717
Title : Cryo-EM structure of PSI-11ACPIs from Rhodomonas sp. NIES-2332 at 2.14 angstrom resolution
Authors : Zhang, W.Y.; Akita, F.; Shen, J.R.
Deposited on : 2024-12-12
Resolution : 2.14 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

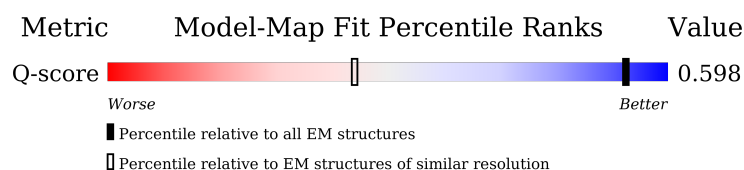
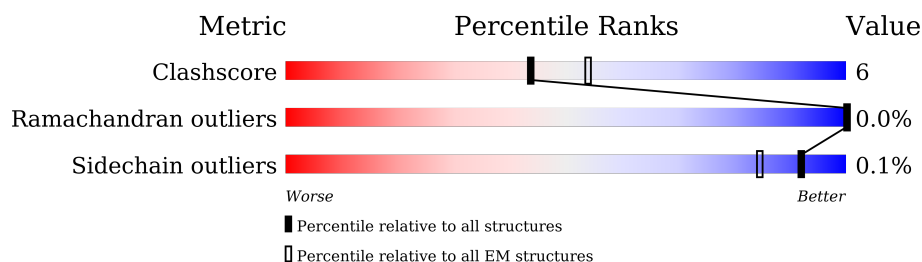
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.14 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.











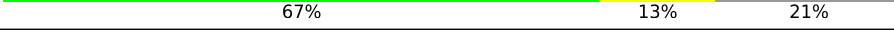
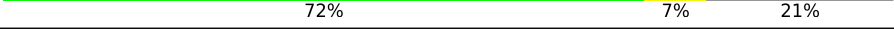
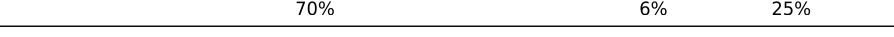

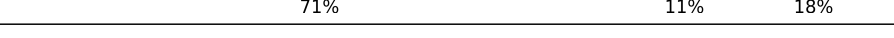
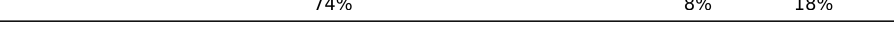
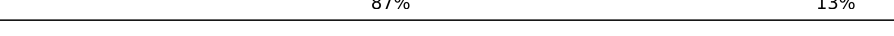


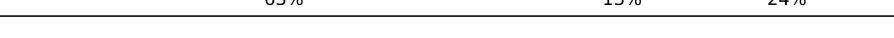
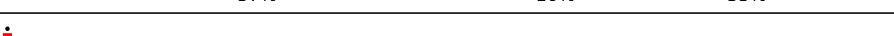


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	2493 (1.66 - 2.64)

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	
2	B	734	
3	C	81	
4	D	141	

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Mol	Chain	Length	Quality of chain
5	E	64	
6	F	188	
7	I	36	
8	J	42	
9	L	153	
10	M	30	
11	K	87	
12	s	302	
13	c	215	
14	a	217	
15	b	236	
16	h	229	
17	j	212	
17	m	212	
18	l	175	
19	k	232	
20	i	200	
21	d	219	
22	R	135	
23	n	220	
24	Q	233	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CL0	A	801	X	-	-	-
26	CLA	A	802	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	A	803	X	-	-	-
26	CLA	A	804	X	-	-	-
26	CLA	A	805	X	-	-	-
26	CLA	A	806	X	-	-	-
26	CLA	A	807	X	-	-	-
26	CLA	A	808	X	-	-	-
26	CLA	A	809	X	-	-	-
26	CLA	A	810	X	-	-	-
26	CLA	A	811	X	-	-	-
26	CLA	A	812	X	-	-	-
26	CLA	A	813	X	-	-	-
26	CLA	A	814	X	-	-	-
26	CLA	A	815	X	-	-	-
26	CLA	A	816	X	-	-	-
26	CLA	A	817	X	-	-	-
26	CLA	A	818	X	-	-	-
26	CLA	A	819	X	-	-	-
26	CLA	A	820	X	-	-	-
26	CLA	A	821	X	-	-	-
26	CLA	A	822	X	-	-	-
26	CLA	A	823	X	-	-	-
26	CLA	A	824	X	-	-	-
26	CLA	A	825	X	-	-	-
26	CLA	A	826	X	-	-	-
26	CLA	A	827	X	-	-	-
26	CLA	A	828	X	-	-	-
26	CLA	A	829	X	-	-	-
26	CLA	A	830	X	-	-	-
26	CLA	A	831	X	-	-	-
26	CLA	A	832	X	-	-	-
26	CLA	A	833	X	-	-	-
26	CLA	A	834	X	-	-	-
26	CLA	A	835	X	-	-	-
26	CLA	A	836	X	-	-	-
26	CLA	A	837	X	-	-	-
26	CLA	A	838	X	-	-	-
26	CLA	A	839	X	-	-	-
26	CLA	A	840	X	-	-	-
26	CLA	A	841	X	-	-	-
26	CLA	A	851	X	-	-	-
26	CLA	A	852	X	-	-	-
26	CLA	A	856	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	B	801	X	-	-	-
26	CLA	B	802	X	-	-	-
26	CLA	B	803	X	-	-	-
26	CLA	B	804	X	-	-	-
26	CLA	B	805	X	-	-	-
26	CLA	B	806	X	-	-	-
26	CLA	B	807	X	-	-	-
26	CLA	B	808	X	-	-	-
26	CLA	B	809	X	-	-	-
26	CLA	B	810	X	-	-	-
26	CLA	B	811	X	-	-	-
26	CLA	B	812	X	-	-	-
26	CLA	B	813	X	-	-	-
26	CLA	B	814	X	-	-	-
26	CLA	B	815	X	-	-	-
26	CLA	B	816	X	-	-	-
26	CLA	B	817	X	-	-	-
26	CLA	B	818	X	-	-	-
26	CLA	B	819	X	-	-	-
26	CLA	B	820	X	-	-	-
26	CLA	B	821	X	-	-	-
26	CLA	B	822	X	-	-	-
26	CLA	B	823	X	-	-	-
26	CLA	B	824	X	-	-	-
26	CLA	B	825	X	-	-	-
26	CLA	B	826	X	-	-	-
26	CLA	B	827	X	-	-	-
26	CLA	B	828	X	-	-	-
26	CLA	B	829	X	-	-	-
26	CLA	B	830	X	-	-	-
26	CLA	B	831	X	-	-	-
26	CLA	B	832	X	-	-	-
26	CLA	B	833	X	-	-	-
26	CLA	B	834	X	-	-	-
26	CLA	B	836	X	-	-	-
26	CLA	B	837	X	-	-	-
26	CLA	B	838	X	-	-	-
26	CLA	B	839	X	-	-	-
26	CLA	B	840	X	-	-	-
26	CLA	B	841	X	-	-	-
26	CLA	B	842	X	-	-	-
26	CLA	F	201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	F	202	X	-	-	-
26	CLA	J	103	X	-	-	-
26	CLA	K	101	X	-	-	-
26	CLA	L	202	X	-	-	-
26	CLA	L	203	X	-	-	-
26	CLA	L	204	X	-	-	-
26	CLA	L	206	X	-	-	-
26	CLA	Q	302	X	-	-	-
26	CLA	R	201	X	-	-	-
26	CLA	a	301	X	-	-	-
26	CLA	a	302	X	-	-	-
26	CLA	a	303	X	-	-	-
26	CLA	a	304	X	-	-	-
26	CLA	a	305	X	-	-	-
26	CLA	a	306	X	-	-	-
26	CLA	a	307	X	-	-	-
26	CLA	a	308	X	-	-	-
26	CLA	a	309	X	-	-	-
26	CLA	a	311	X	-	-	-
26	CLA	b	303	X	-	-	-
26	CLA	b	304	X	-	-	-
26	CLA	b	305	X	-	-	-
26	CLA	b	306	X	-	-	-
26	CLA	b	307	X	-	-	-
26	CLA	b	308	X	-	-	-
26	CLA	b	309	X	-	-	-
26	CLA	b	310	X	-	-	-
26	CLA	b	311	X	-	-	-
26	CLA	b	312	X	-	-	-
26	CLA	b	313	X	-	-	-
26	CLA	c	301	X	-	-	-
26	CLA	c	303	X	-	-	-
26	CLA	c	304	X	-	-	-
26	CLA	c	305	X	-	-	-
26	CLA	c	306	X	-	-	-
26	CLA	c	307	X	-	-	-
26	CLA	c	308	X	-	-	-
26	CLA	c	311	X	-	-	-
26	CLA	c	312	X	-	-	-
26	CLA	d	302	X	-	-	-
26	CLA	d	303	X	-	-	-
26	CLA	d	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	d	305	X	-	-	-
26	CLA	d	306	X	-	-	-
26	CLA	d	307	X	-	-	-
26	CLA	d	308	X	-	-	-
26	CLA	d	309	X	-	-	-
26	CLA	d	310	X	-	-	-
26	CLA	d	313	X	-	-	-
26	CLA	d	318	X	-	-	-
26	CLA	h	301	X	-	-	-
26	CLA	h	302	X	-	-	-
26	CLA	h	303	X	-	-	-
26	CLA	h	304	X	-	-	-
26	CLA	h	305	X	-	-	-
26	CLA	h	306	X	-	-	-
26	CLA	h	307	X	-	-	-
26	CLA	h	308	X	-	-	-
26	CLA	h	313	X	-	-	-
26	CLA	i	301	X	-	-	-
26	CLA	i	302	X	-	-	-
26	CLA	i	303	X	-	-	-
26	CLA	i	304	X	-	-	-
26	CLA	i	305	X	-	-	-
26	CLA	i	306	X	-	-	-
26	CLA	i	307	X	-	-	-
26	CLA	i	308	X	-	-	-
26	CLA	i	310	X	-	-	-
26	CLA	i	311	X	-	-	-
26	CLA	j	601	X	-	-	-
26	CLA	j	602	X	-	-	-
26	CLA	j	603	X	-	-	-
26	CLA	j	604	X	-	-	-
26	CLA	j	605	X	-	-	-
26	CLA	j	606	X	-	-	-
26	CLA	j	607	X	-	-	-
26	CLA	j	608	X	-	-	-
26	CLA	j	609	X	-	-	-
26	CLA	j	610	X	-	-	-
26	CLA	j	612	X	-	-	-
26	CLA	j	613	X	-	-	-
26	CLA	k	601	X	-	-	-
26	CLA	k	602	X	-	-	-
26	CLA	k	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	k	605	X	-	-	-
26	CLA	k	606	X	-	-	-
26	CLA	k	607	X	-	-	-
26	CLA	k	608	X	-	-	-
26	CLA	k	609	X	-	-	-
26	CLA	k	610	X	-	-	-
26	CLA	k	614	X	-	-	-
26	CLA	l	301	X	-	-	-
26	CLA	l	304	X	-	-	-
26	CLA	l	305	X	-	-	-
26	CLA	l	306	X	-	-	-
26	CLA	l	307	X	-	-	-
26	CLA	l	308	X	-	-	-
26	CLA	l	309	X	-	-	-
26	CLA	l	310	X	-	-	-
26	CLA	l	311	X	-	-	-
26	CLA	l	313	X	-	-	-
26	CLA	m	601	X	-	-	-
26	CLA	m	602	X	-	-	-
26	CLA	m	603	X	-	-	-
26	CLA	m	604	X	-	-	-
26	CLA	m	605	X	-	-	-
26	CLA	m	606	X	-	-	-
26	CLA	m	607	X	-	-	-
26	CLA	m	608	X	-	-	-
26	CLA	m	609	X	-	-	-
26	CLA	m	610	X	-	-	-
26	CLA	m	612	X	-	-	-
26	CLA	m	613	X	-	-	-
26	CLA	n	601	X	-	-	-
26	CLA	n	602	X	-	-	-
26	CLA	n	603	X	-	-	-
26	CLA	n	604	X	-	-	-
26	CLA	n	605	X	-	-	-
26	CLA	n	607	X	-	-	-
26	CLA	n	608	X	-	-	-
26	CLA	n	609	X	-	-	-
26	CLA	n	610	X	-	-	-
26	CLA	n	613	X	-	-	-
26	CLA	s	402	X	-	-	-
26	CLA	s	403	X	-	-	-
26	CLA	s	406	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	s	408	X	-	-	-
29	WVN	A	845	-	X	-	-
29	WVN	A	846	-	X	-	-
29	WVN	A	847	-	X	-	-
29	WVN	A	848	-	X	-	-
29	WVN	A	857	-	X	-	-
29	WVN	B	846	-	X	-	-
29	WVN	B	847	-	X	-	-
29	WVN	B	848	-	X	-	-
29	WVN	B	849	-	X	-	-
29	WVN	B	850	-	X	-	-
29	WVN	B	853	-	X	-	-
29	WVN	F	203	-	X	-	-
29	WVN	I	101	-	X	-	-
29	WVN	J	101	-	X	-	-
29	WVN	J	102	-	X	-	-
29	WVN	K	102	-	X	-	-
29	WVN	L	201	-	X	-	-
29	WVN	L	205	-	X	-	-
29	WVN	M	101	-	X	-	-
29	WVN	R	200	-	X	-	-
29	WVN	h	309	-	X	-	-
29	WVN	i	315	-	X	-	-
29	WVN	l	303	-	X	-	-
29	WVN	l	316	-	X	-	-
29	WVN	s	407	-	X	-	-
35	II0	h	310	-	X	-	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 53701 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 Photosystem I reaction center subunit PsaK.

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

- Molecule 12 is a protein called ACPI-s.

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

- Molecule 13 is a protein called ACPI-c.

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

- Molecule 14 is a protein called ACPI-a.

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

- Molecule 15 is a protein called ACPI-b.

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

- Molecule 16 is a protein called ACPI-h.

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

- Molecule 17 is a protein called ACPI-m.

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

- Molecule 18 is a protein called ACPI-l.

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

- Molecule 19 is a protein called ACPI-k.

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

- Molecule 20 is a protein called ACPI-i.

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

- Molecule 21 is a protein called ACPI-d.

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

- Molecule 22 is a protein called PsaR.

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

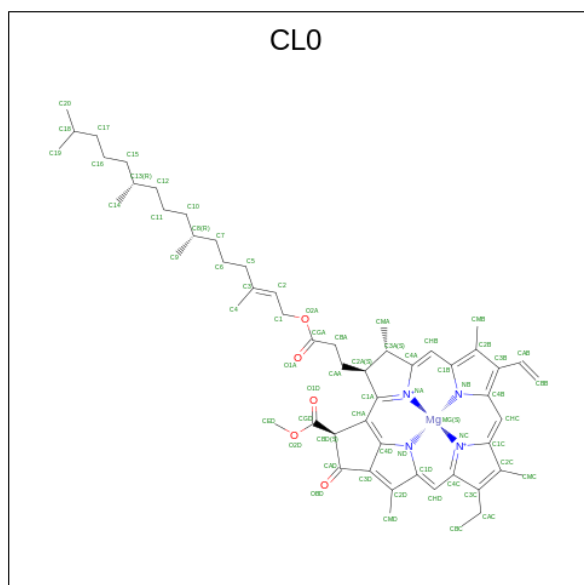
- Molecule 23 is a protein called ACPI-n.

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

- Molecule 24 is a protein called PsaQ.

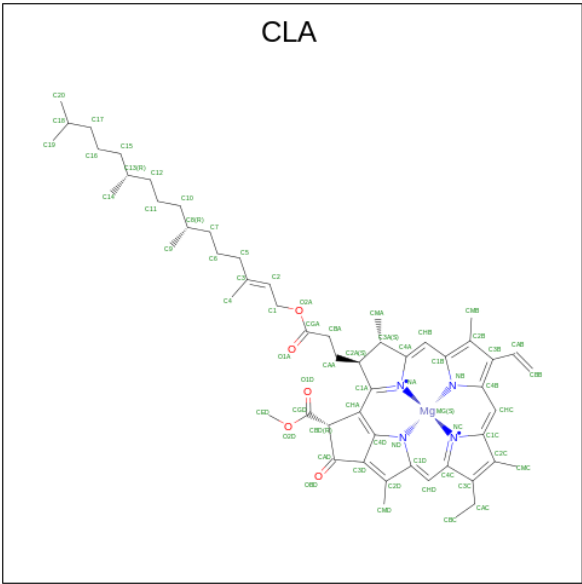
Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	143	Total	C	N	O	S	0	0
			1041	654	179	203	5		

- Molecule 25 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
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	F	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	L	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	L	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	K	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	s	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	c	1	Total 62	C 52	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
26	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
26	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	h	1	Total 57	C 47	Mg 1	N 4	O 5	0
26	h	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	m	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	m	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	m	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	m	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	l	1	Total 47	C 37	Mg 1	N 4	O 5	0
26	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	l	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	l	1	Total 57	C 47	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	l	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	l	1	Total 56	C 46	Mg 1	N 4	O 5	0
26	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	k	1	Total 57	C 47	Mg 1	N 4	O 5	0
26	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	i	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	i	1	Total 46	C 36	Mg 1	N 4	O 5	0

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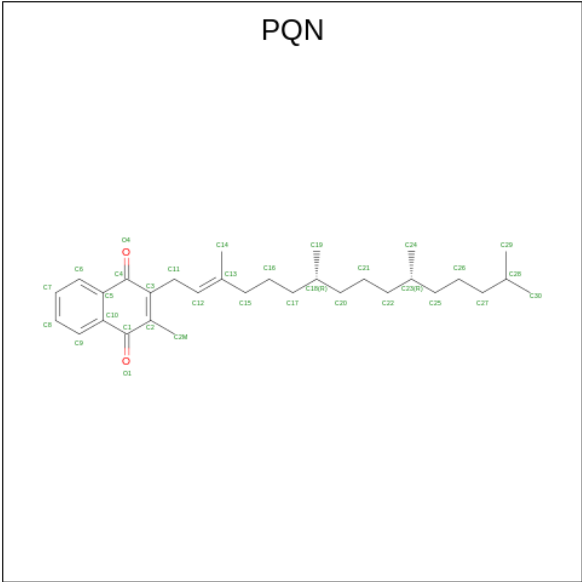
Mol	Chain	Residues	Atoms					AltConf
26	i	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	j	1	Total 54	C 44	Mg 1	N 4	O 5	0
26	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	j	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	d	1	Total 62	C 52	Mg 1	N 4	O 5	0
26	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	d	1	Total 46	C 36	Mg 1	N 4	O 5	0

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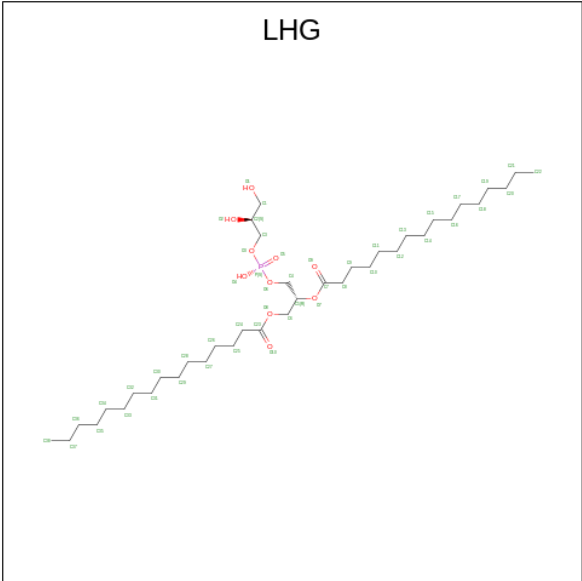
Mol	Chain	Residues	Atoms					AltConf
26	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
26	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
26	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	n	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	n	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	n	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	n	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 27 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



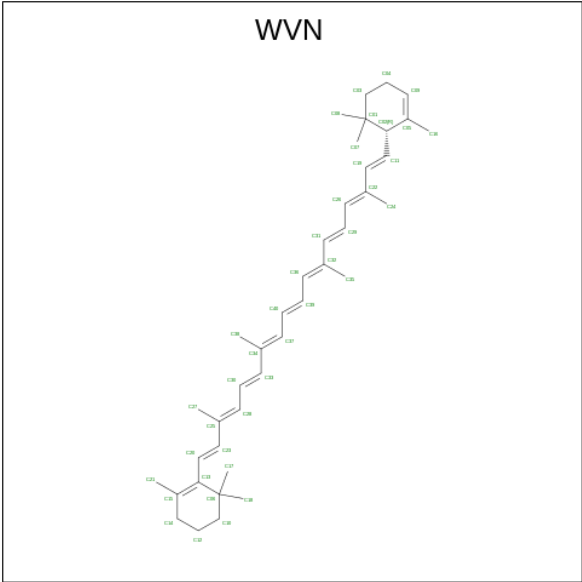
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			48	37	10	1	

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Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			27	16	10	1	
28	A	1	Total	C	O	P	0
			27	20	6	1	
28	A	1	Total	C	O	P	0
			36	25	10	1	
28	B	1	Total	C	O	P	0
			49	38	10	1	
28	J	1	Total	C	O	P	0
			33	22	10	1	
28	L	1	Total	C	O	P	0
			47	36	10	1	
28	L	1	Total	C	O	P	0
			45	34	10	1	
28	s	1	Total	C	O	P	0
			33	24	8	1	
28	c	1	Total	C	O	P	0
			37	26	10	1	
28	c	1	Total	C	O	P	0
			49	38	10	1	
28	b	1	Total	C	O	P	0
			49	38	10	1	
28	b	1	Total	C	O	P	0
			49	38	10	1	
28	m	1	Total	C	O	P	0
			37	26	10	1	
28	l	1	Total	C	O	P	0
			32	21	10	1	
28	i	1	Total	C	O	P	0
			37	26	10	1	
28	j	1	Total	C	O	P	0
			30	19	10	1	
28	n	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 29 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).



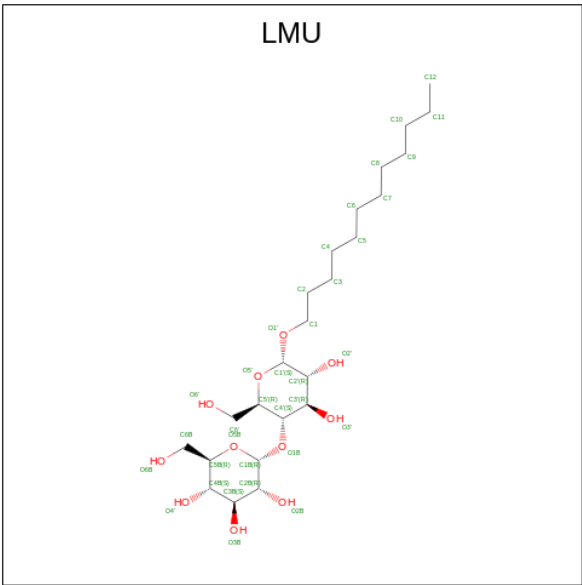
Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total	C	0
			40	40	
29	A	1	Total	C	0
			40	40	
29	A	1	Total	C	0
			40	40	
29	A	1	Total	C	0
			40	40	
29	A	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	F	1	Total	C	0
			40	40	
29	F	1	Total	C	0
			40	40	

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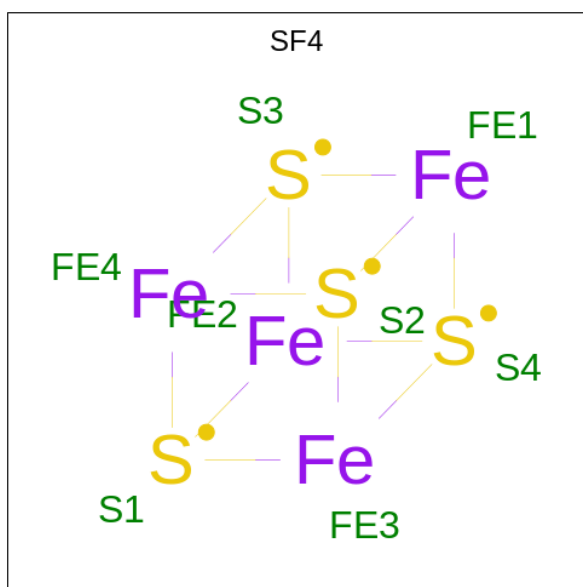
Mol	Chain	Residues	Atoms	AltConf
29	I	1	Total C 40 40	0
29	J	1	Total C 40 40	0
29	J	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	M	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	s	1	Total C 40 40	0
29	s	1	Total C 40 40	0
29	h	1	Total C 40 40	0
29	l	1	Total C 40 40	0
29	l	1	Total C 40 40	0
29	i	1	Total C 40 40	0
29	R	1	Total C 40 40	0

- Molecule 30 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



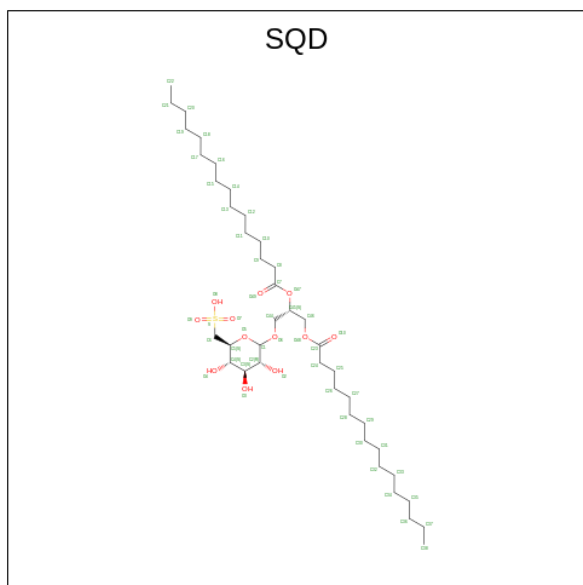
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			35	24	11	
30	A	1	Total	C	O	0
			34	23	11	
30	B	1	Total	C	O	0
			35	24	11	
30	a	1	Total	C	O	0
			35	24	11	
30	i	1	Total	C	O	0
			35	24	11	

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



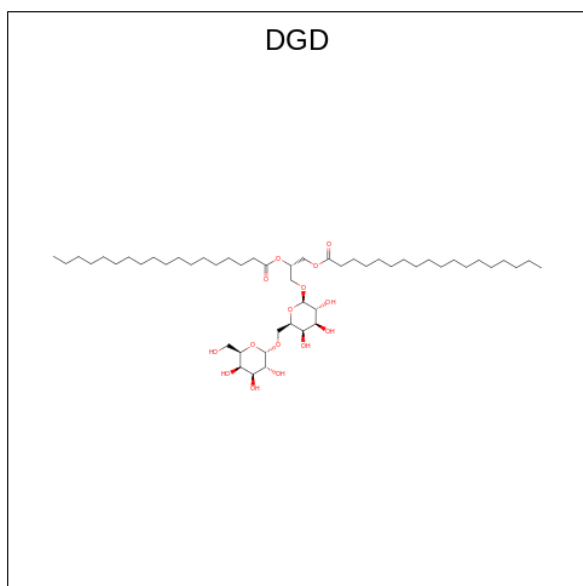
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	Fe	S	0
			8	4	4	
31	C	1	Total	Fe	S	0
			8	4	4	
31	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



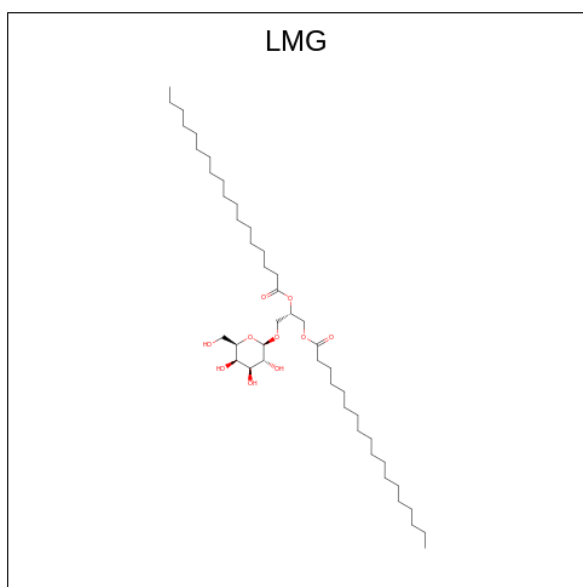
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



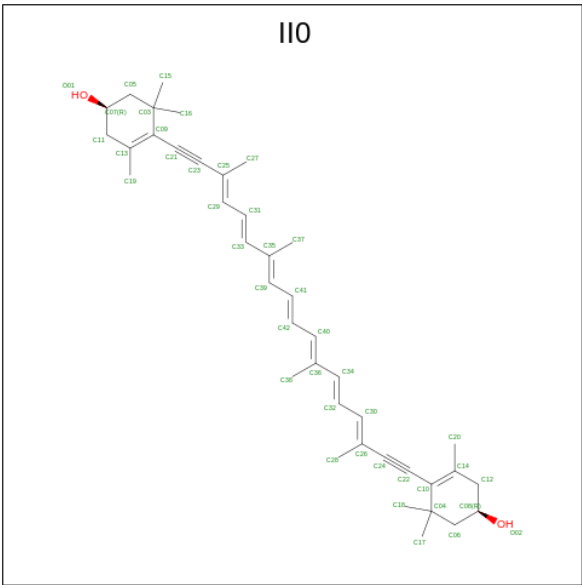
Mol	Chain	Residues	Atoms				AltConf
33	B	1	Total	C	O		0
			66	51	15		
33	j	1	Total	C	O		0
			62	47	15		

- Molecule 34 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
34	F	1	Total	C	O	0
			53	43	10	
34	F	1	Total	C	O	0
			41	31	10	
34	L	1	Total	C	O	0
			45	35	10	
34	c	1	Total	C	O	0
			55	45	10	
34	c	1	Total	C	O	0
			43	33	10	
34	b	1	Total	C	O	0
			42	32	10	
34	n	1	Total	C	O	0
			51	41	10	
34	Q	1	Total	C	O	0
			38	28	10	

- Molecule 35 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
35	J	1	Total	C	O	0
			42	40	2	
35	c	1	Total	C	O	0
			42	40	2	
35	c	1	Total	C	O	0
			42	40	2	
35	c	1	Total	C	O	0
			42	40	2	
35	a	1	Total	C	O	0
			42	40	2	
35	a	1	Total	C	O	0
			42	40	2	
35	a	1	Total	C	O	0
			42	40	2	
35	a	1	Total	C	O	0
			42	40	2	
35	b	1	Total	C	O	0
			42	40	2	
35	b	1	Total	C	O	0
			42	40	2	
35	b	1	Total	C	O	0
			42	40	2	
35	h	1	Total	C	O	0
			28	27	1	
35	h	1	Total	C	O	0
			42	40	2	
35	h	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
35	m	1	Total 42	C 40	O 2	0
35	m	1	Total 42	C 40	O 2	0
35	m	1	Total 42	C 40	O 2	0
35	m	1	Total 42	C 40	O 2	0
35	l	1	Total 42	C 40	O 2	0
35	l	1	Total 42	C 40	O 2	0
35	l	1	Total 42	C 40	O 2	0
35	l	1	Total 42	C 40	O 2	0
35	k	1	Total 42	C 40	O 2	0
35	k	1	Total 42	C 40	O 2	0
35	k	1	Total 42	C 40	O 2	0
35	k	1	Total 42	C 40	O 2	0
35	k	1	Total 42	C 40	O 2	0
35	k	1	Total 42	C 40	O 2	0
35	k	1	Total 42	C 40	O 2	0
35	i	1	Total 42	C 40	O 2	0
35	i	1	Total 42	C 40	O 2	0
35	i	1	Total 42	C 40	O 2	0
35	i	1	Total 42	C 40	O 2	0
35	i	1	Total 42	C 40	O 2	0
35	j	1	Total 42	C 40	O 2	0
35	j	1	Total 42	C 40	O 2	0

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

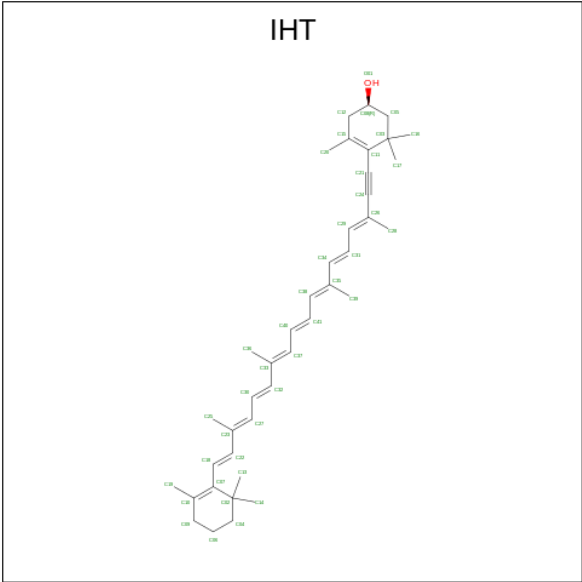
- ## KC2

WORLDWIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					AltConf
36	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	m	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	l	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	n	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 37 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: C₄₀H₅₄O) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	A	130	Total	O	0
			130	130	
38	B	147	Total	O	0
			147	147	
38	C	25	Total	O	0
			25	25	
38	D	15	Total	O	0
			15	15	

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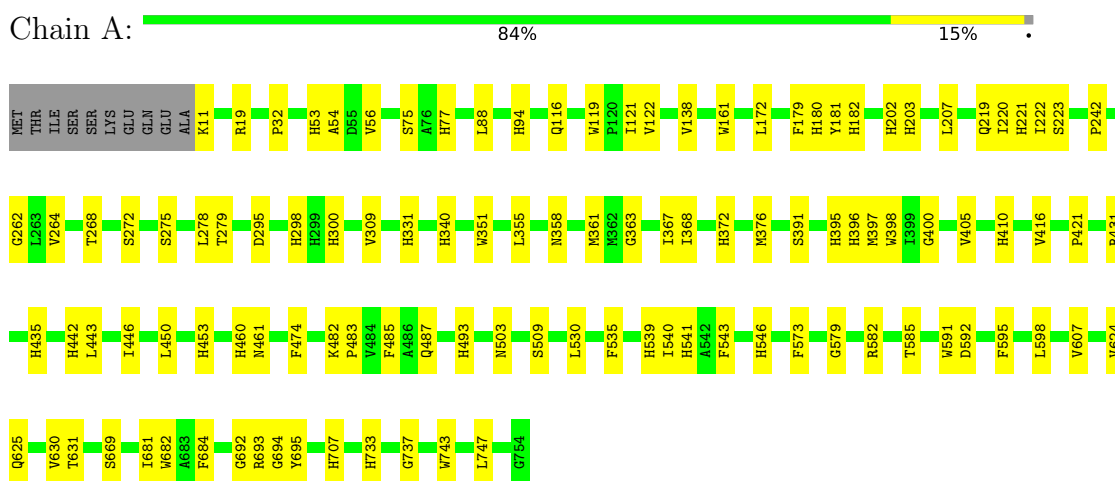
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Mol	Chain	Residues	Atoms		AltConf
38	E	6	Total 6	O 6	0
38	F	15	Total 15	O 15	0
38	J	2	Total 2	O 2	0
38	L	12	Total 12	O 12	0
38	M	2	Total 2	O 2	0
38	s	10	Total 10	O 10	0
38	c	2	Total 2	O 2	0
38	a	16	Total 16	O 16	0
38	b	18	Total 18	O 18	0
38	h	9	Total 9	O 9	0
38	m	1	Total 1	O 1	0
38	R	1	Total 1	O 1	0

3 Residue-property plots

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

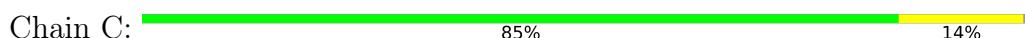
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center





- Molecule 4: Photosystem I reaction center subunit II

Chain D: 91% 7%



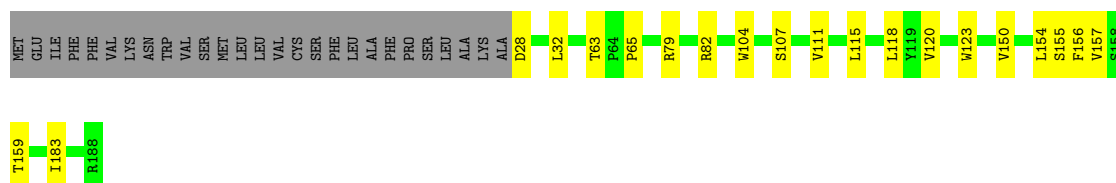
- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 92% 6%



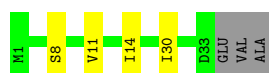
- Molecule 6: Photosystem I reaction center subunit III

Chain F: 75% 11% 14%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 81% 11% 8%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 88% 12%



- Molecule 9: Photosystem I reaction center subunit XI

Chain L: 6% 90% 8%



- Molecule 10: Photosystem I reaction center subunit XII

Diagram illustrating a 100% stacked bar chart with categories M1, I7, L13, A21, L28, Y29, and Q30. The segments are stacked vertically, with M1 at the bottom and Q30 at the top.

- Chain K: 

MET	ASN	ALA	ASP	LEU	LEU	ILE	ALA	LEU	V10	P11	Q12	T13	W16	I32	K42	GLY	THR	GLY	PRO	SER	LEU	PRO	ILE	SER	G52	S53	S54	A55	G56	F57	L62	S65	L80	S81	Y82	V83	L86	SER
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- Chain s:  47% 0 49%

[illegible]

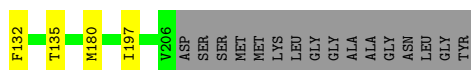
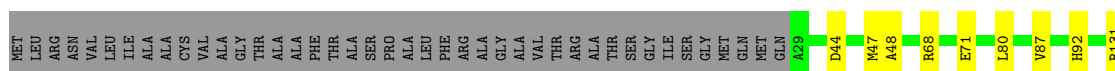
- Chain c:  67% 13% 21%

M113	MET
Q125	LEU
T149	THR
R154	ALA
E155	LEU
D158	ILE
L166	ALA
H183	CYS
A184	VAL
R185	ALA
M188	SER
H196	ALA
V200	PRO
T201	PHE
K202	GLY
Q203	GLY
L206	PHE
E207	PRO
Q208	MET
L209	ALA
F212	MET
LVS	LVS
SER	SER
LEU	SER
ALA	SER
	ARG
	SER
	SER
	ARG
	MET
	MET
	GLN
	GLY
	D13
	F44
	S45
	A46
	A47
	V48
	F49
	F50
	V65
	G83
	G88
	Q102
	P111
	F113

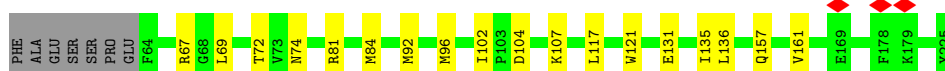
- Chain a:  72% 7% 21%

Met	Met	Arg	Ala	Val	Leu	Val	Leu	Ala	Thr	Gly	Val	Ala	Ser	Ala	Ser	Phe	Pro	Ala	Ala	Asn	Phe	Gly	Leu	Ser	Thr	Ser	Ser	Arg	Ala	Ala	Ile	Ala	Arg	Gly	Pro	Arg	Met	Gln	E42	M43	S44	E45	A46	I47	P53	I56	K78	M99	Y143	S141
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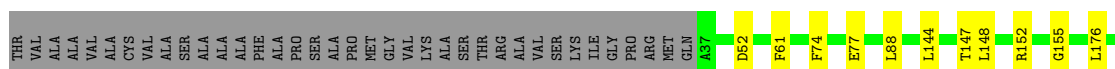
- Chain b:  70% 6% 25%



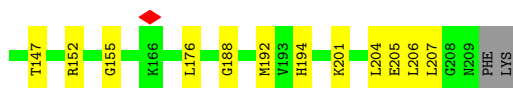
• Molecule 16: ACPI-h



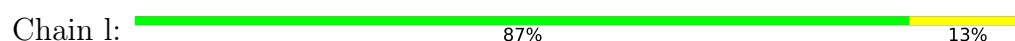
• Molecule 17: ACPI-m



• Molecule 17: ACPI-m

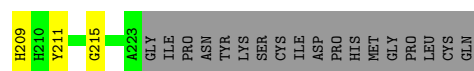


• Molecule 18: ACPI-l



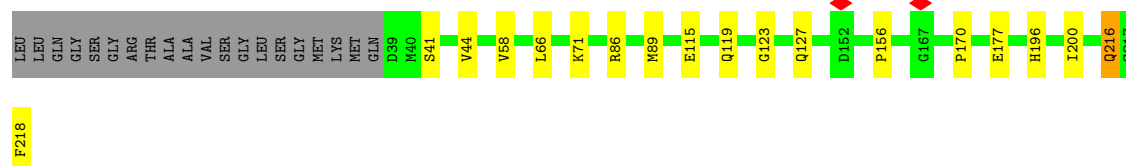
• Molecule 19: ACPI-k





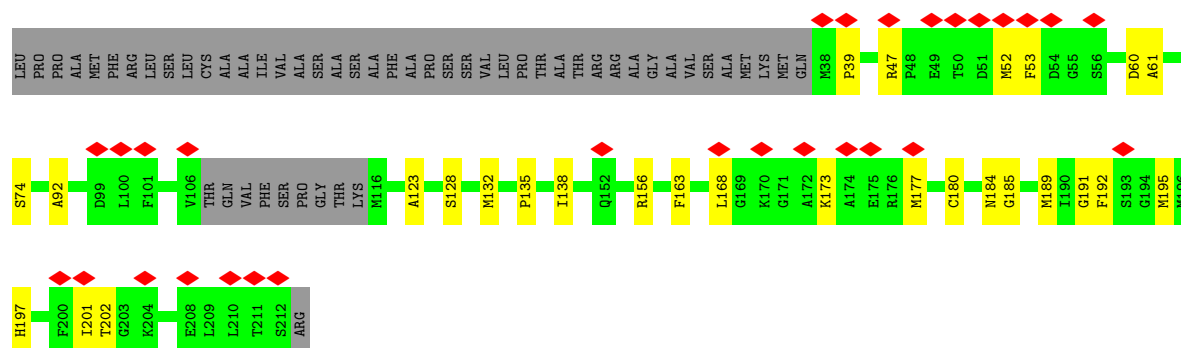
- Molecule 20: ACPI-i

Chain i: 81% 8% 10%



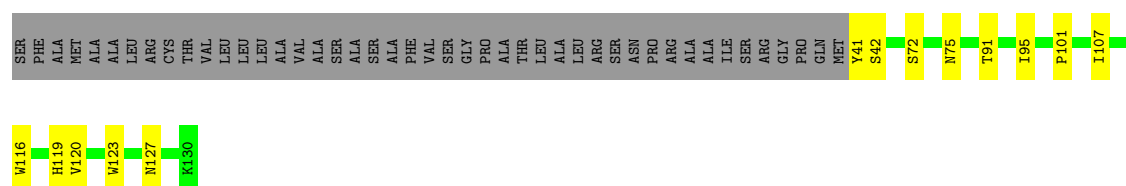
- Molecule 21: ACPI-d

Chain d: 13% 63% 13% 24%



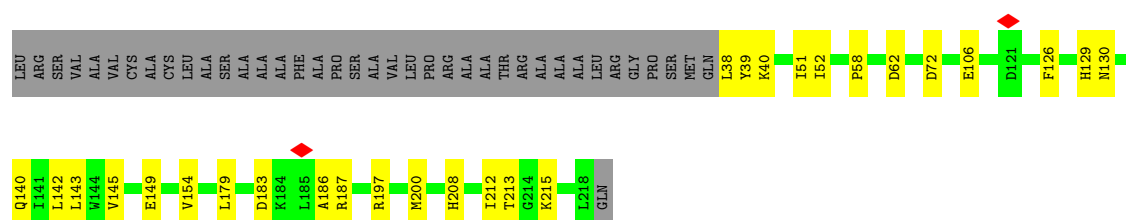
- Molecule 22: PsaR

Chain R: 57% 10% 33%



- Molecule 23: ACPI-n

Chain n: 70% 13% 18%



- Molecule 24: PsaQ



TYR	VAL	ALA	LEU	ALA	ALA	ALA	SER	ALA	GLU	ALA	PHE	SER	SER	PRO	ALA	LEU	SER	GLY	LEU	LYS	MET	SER	THR	ALA	GLU	PRO	THR	GLN	ILE	SER	ARG	LYS	ASP	LEU	LEU	SER	THR	ALA	ALA	ALA	GLY	ILE	ILE	ALA	VAL	PRO	ALA	ALA	GLY	ALA	SER	LEU	ASP	PRO	LYS	THR	GLY	PHE
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PRO	VAL	GLN	SER	GLY	GLY	ARG	ASP	THR	LEU	CYS	GLY	GLY	SER	SER	ALA	ALA	GLY	CYS	GLN	PRO	LYS	MET	THR	GLN	K189	K107	V118	K126	K126	L142	L145	K160	K161	G165	I168	P169	G172	K176	S176	T177	I193	K194	M197	V212	K231	PRO
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PRO	ILE	VAL	PHE	ASN
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33179	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	0.363	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.20	0/6020	0.44	0/8205
2	B	0.21	0/6055	0.48	0/8266
3	C	0.15	0/601	0.50	0/813
4	D	0.16	0/1100	0.44	0/1488
5	E	0.14	0/492	0.41	0/666
6	F	0.23	0/1291	0.49	0/1750
7	I	0.25	0/262	0.54	0/358
8	J	0.20	0/364	0.51	0/495
9	L	0.20	0/1188	0.47	0/1616
10	M	0.18	0/233	0.40	0/315
11	K	0.22	0/489	0.52	0/664
12	s	0.18	0/1177	0.50	0/1591
13	c	0.21	0/1401	0.50	0/1896
14	a	0.20	0/1372	0.45	0/1858
15	b	0.21	0/1360	0.51	0/1834
16	h	0.21	0/1228	0.50	0/1671
17	j	0.22	0/1329	0.50	0/1789
17	m	0.23	0/1341	0.51	0/1805
18	l	0.21	0/1365	0.45	0/1845
19	k	0.33	0/1445	0.69	0/1954
20	i	0.35	1/1400 (0.1%)	0.66	3/1891 (0.2%)
21	d	0.25	0/1259	0.58	0/1700
22	R	0.20	0/687	0.46	0/940
23	n	0.22	0/1371	0.60	2/1847 (0.1%)
24	Q	0.22	0/1053	0.51	0/1418
All	All	0.22	1/35883 (0.0%)	0.51	5/48675 (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
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	i	156	PRO	CG-CD	-6.83	1.27	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	i	156	PRO	N-CD-CG	-9.02	89.67	103.20
20	i	156	PRO	CA-N-CD	-7.29	101.79	112.00
23	n	140	GLN	CA-CB-CG	7.03	128.16	114.10
20	i	170	PRO	CA-N-CD	-5.17	104.76	112.00
23	n	140	GLN	CB-CG-CD	5.01	121.12	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	666	TRP	Peptide
3	C	61	ASP	Peptide

5.2 Too-close contacts [i](#)

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	99	0
2	B	5832	0	5643	94	0
3	C	592	0	567	6	0
4	D	1075	0	1074	7	0
5	E	484	0	486	1	0
6	F	1257	0	1266	15	0
7	I	255	0	270	4	0
8	J	351	0	344	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	1158	0	1170	10	0
10	M	232	0	265	4	0
11	K	482	0	511	7	0
12	s	1146	0	1095	10	0
13	c	1362	0	1338	17	0
14	a	1331	0	1284	11	0
15	b	1332	0	1336	12	0
16	h	1201	0	1228	13	0
17	j	1302	0	1316	17	0
17	m	1313	0	1326	15	0
18	l	1333	0	1311	16	0
19	k	1412	0	1429	17	0
20	i	1363	0	1322	13	0
21	d	1231	0	1237	23	0
22	R	666	0	655	9	0
23	n	1343	0	1356	22	0
24	Q	1041	0	1071	11	0
25	A	65	0	72	4	0
26	A	2663	0	2789	112	0
26	B	2592	0	2717	108	0
26	F	117	0	115	4	0
26	J	42	0	31	1	0
26	K	42	0	31	0	0
26	L	225	0	209	8	0
26	Q	65	0	72	0	0
26	R	55	0	49	4	0
26	a	638	0	629	13	0
26	b	659	0	663	22	0
26	c	607	0	560	14	0
26	d	529	0	417	9	0
26	h	519	0	501	15	0
26	i	608	0	621	7	0
26	j	669	0	622	14	0
26	k	603	0	548	13	0
26	l	597	0	601	17	0
26	m	680	0	655	21	0
26	n	614	0	570	16	0
26	s	260	0	288	5	0
27	A	33	0	46	4	0
27	B	33	0	46	2	0
28	A	138	0	170	7	0
28	B	49	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	J	33	0	36	0	0
28	L	92	0	126	0	0
28	b	98	0	147	3	0
28	c	86	0	118	4	0
28	i	37	0	44	0	0
28	j	30	0	29	0	0
28	l	32	0	34	0	0
28	m	37	0	44	0	0
28	n	43	0	59	1	0
28	s	33	0	40	3	0
29	A	200	0	0	0	0
29	B	280	0	0	0	0
29	F	80	0	0	0	0
29	I	40	0	0	0	0
29	J	80	0	0	0	0
29	K	40	0	0	0	0
29	L	80	0	0	0	0
29	M	40	0	0	0	0
29	R	40	0	0	0	0
29	h	40	0	0	0	0
29	i	40	0	0	0	0
29	l	80	0	0	0	0
29	s	80	0	0	0	0
30	A	69	0	87	2	0
30	B	35	0	46	1	0
30	a	35	0	46	0	0
30	i	35	0	46	2	0
31	A	8	0	0	0	0
31	C	16	0	0	1	0
32	A	54	0	78	0	0
33	B	66	0	96	6	0
33	j	62	0	84	3	0
34	F	94	0	134	2	0
34	L	45	0	61	2	0
34	Q	38	0	46	3	0
34	b	42	0	54	1	0
34	c	98	0	141	1	0
34	n	51	0	75	3	0
35	J	42	0	0	0	0
35	a	168	0	0	0	0
35	b	126	0	0	1	0
35	c	126	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	d	252	0	0	1	0
35	h	112	0	0	0	0
35	i	210	0	0	1	0
35	j	84	0	0	0	0
35	k	252	0	0	0	0
35	l	168	0	0	0	0
35	m	168	0	0	0	0
35	n	168	0	0	1	0
36	c	45	0	0	0	0
36	d	90	0	0	3	0
36	i	90	0	0	0	0
36	j	45	0	0	0	0
36	k	135	0	0	0	0
36	l	45	0	0	0	0
36	m	45	0	0	0	0
36	n	90	0	0	1	0
36	s	90	0	0	2	0
37	R	41	0	0	0	0
37	a	41	0	0	0	0
37	b	82	0	0	1	0
37	c	41	0	0	0	0
37	j	41	0	0	0	0
37	m	41	0	0	0	0
37	n	41	0	0	0	0
38	A	130	0	0	0	0
38	B	147	0	0	2	0
38	C	25	0	0	0	0
38	D	15	0	0	0	0
38	E	6	0	0	0	0
38	F	15	0	0	0	0
38	J	2	0	0	0	0
38	L	12	0	0	0	0
38	M	2	0	0	0	0
38	R	1	0	0	0	0
38	a	16	0	0	0	0
38	b	18	0	0	0	0
38	c	2	0	0	0	0
38	h	9	0	0	0	0
38	m	1	0	0	0	0
38	s	10	0	0	0	0
All	All	53701	0	49349	641	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 641 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)
20:i:218:PHE:CE1	20:i:218:PHE:CE2	2.35	1.02
21:d:201:ILE:CD1	36:d:312:KC2:CED	2.38	0.99
1:A:410:HIS:HE1	26:A:829:CLA:NA	1.74	0.86
2:B:388:HIS:HE1	26:B:827:CLA:NA	1.80	0.80
21:d:201:ILE:HD13	36:d:312:KC2:CED	2.12	0.79

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/752 (98%)	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	4
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	31/36 (86%)	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	K	64/87 (74%)	64 (100%)	0	0	100	100
12	s	152/302 (50%)	151 (99%)	1 (1%)	0	100	100
13	c	168/215 (78%)	168 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	a	170/217 (78%)	170 (100%)	0	0	100	100
15	b	176/236 (75%)	176 (100%)	0	0	100	100
16	h	160/229 (70%)	160 (100%)	0	0	100	100
17	j	171/212 (81%)	170 (99%)	1 (1%)	0	100	100
17	m	172/212 (81%)	171 (99%)	1 (1%)	0	100	100
18	l	173/175 (99%)	173 (100%)	0	0	100	100
19	k	187/232 (81%)	185 (99%)	2 (1%)	0	100	100
20	i	178/200 (89%)	178 (100%)	0	0	100	100
21	d	162/219 (74%)	161 (99%)	1 (1%)	0	100	100
22	R	88/135 (65%)	88 (100%)	0	0	100	100
23	n	179/220 (81%)	179 (100%)	0	0	100	100
24	Q	141/233 (60%)	140 (99%)	1 (1%)	0	100	100
All	All	4493/5345 (84%)	4483 (100%)	9 (0%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	62	PHE

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	I	27/29 (93%)	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	63
10	M	25/25 (100%)	25 (100%)	0	100	100
11	K	51/66 (77%)	51 (100%)	0	100	100
12	s	119/228 (52%)	119 (100%)	0	100	100
13	c	139/171 (81%)	139 (100%)	0	100	100
14	a	139/167 (83%)	139 (100%)	0	100	100
15	b	136/174 (78%)	136 (100%)	0	100	100
16	h	124/167 (74%)	124 (100%)	0	100	100
17	j	135/161 (84%)	135 (100%)	0	100	100
17	m	136/161 (84%)	136 (100%)	0	100	100
18	l	136/137 (99%)	136 (100%)	0	100	100
19	k	143/178 (80%)	142 (99%)	1 (1%)	81	85
20	i	142/156 (91%)	141 (99%)	1 (1%)	81	85
21	d	125/165 (76%)	125 (100%)	0	100	100
22	R	72/104 (69%)	72 (100%)	0	100	100
23	n	141/167 (84%)	141 (100%)	0	100	100
24	Q	106/169 (63%)	106 (100%)	0	100	100
All	All	3628/4197 (86%)	3624 (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	k	101	LEU
20	i	216	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
23	n	50	ASN
23	n	195	ASN

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Mol	Chain	Res	Type
12	s	170	GLN
6	F	106	HIS
24	Q	229	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

354 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	$\# Z > 2$
35	II0	h	310	-	26,28,43	6.56	14 (53%)	31,37,60	7.02	20 (64%)
35	II0	n	614	-	39,43,43	0.21	0	50,60,60	0.45	0
29	WVN	A	848	-	40,41,41	5.60	20 (50%)	50,56,56	6.48	33 (66%)
35	II0	m	615	-	39,43,43	6.59	22 (56%)	50,60,60	6.80	30 (60%)
34	LMG	Q	301	-	38,38,55	0.87	0	46,46,63	1.23	3 (6%)
29	WVN	B	846	-	40,41,41	5.55	20 (50%)	50,56,56	6.45	33 (66%)
29	WVN	s	405	-	40,41,41	5.69	19 (47%)	50,56,56	6.21	29 (58%)
26	CLA	m	613	17	65,73,73	1.51	6 (9%)	76,113,113	1.39	6 (7%)
35	II0	j	614	-	39,43,43	6.52	22 (56%)	50,60,60	6.99	29 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	d	304	-	45,53,73	1.79	5 (11%)	52,89,113	1.62	6 (11%)
29	WVN	K	102	-	40,41,41	5.62	18 (45%)	50,56,56	6.49	32 (64%)
36	KC2	m	611	17	48,53,53	1.73	9 (18%)	54,89,89	0.97	3 (5%)
26	CLA	A	824	38	65,73,73	1.47	6 (9%)	76,113,113	1.50	7 (9%)
26	CLA	c	307	13	46,54,73	1.74	6 (13%)	53,90,113	1.58	6 (11%)
26	CLA	B	829	2	65,73,73	1.49	5 (7%)	76,113,113	1.45	9 (11%)
26	CLA	A	813	1	56,64,73	1.64	6 (10%)	65,102,113	1.52	10 (15%)
26	CLA	d	307	21	45,53,73	1.81	6 (13%)	52,89,113	1.55	7 (13%)
26	CLA	j	609	17	65,73,73	1.50	5 (7%)	76,113,113	1.36	7 (9%)
26	CLA	A	817	1	65,73,73	1.51	6 (9%)	76,113,113	1.37	7 (9%)
29	WVN	B	848	-	40,41,41	5.69	18 (45%)	50,56,56	6.31	32 (64%)
26	CLA	c	308	13	65,73,73	1.47	6 (9%)	76,113,113	1.37	7 (9%)
29	WVN	l	316	-	40,41,41	5.72	19 (47%)	50,56,56	6.40	32 (64%)
26	CLA	j	608	17	45,53,73	1.79	5 (11%)	52,89,113	1.58	7 (13%)
26	CLA	B	809	2	65,73,73	1.51	7 (10%)	76,113,113	1.41	6 (7%)
35	II0	h	312	-	39,43,43	6.55	22 (56%)	50,60,60	6.85	28 (56%)
29	WVN	A	845	-	40,41,41	5.80	20 (50%)	50,56,56	6.07	32 (64%)
35	II0	l	315	-	39,43,43	6.57	22 (56%)	50,60,60	6.72	26 (52%)
26	CLA	i	303	20	65,73,73	1.51	5 (7%)	76,113,113	1.39	8 (10%)
26	CLA	A	804	1	65,73,73	1.47	6 (9%)	76,113,113	1.48	6 (7%)
27	PQN	B	843	-	34,34,34	3.07	12 (35%)	42,45,45	2.01	5 (11%)
34	LMG	n	620	-	51,51,55	0.83	2 (3%)	59,59,63	1.24	5 (8%)
26	CLA	n	603	23	51,59,73	1.76	7 (13%)	59,96,113	1.51	10 (16%)
26	CLA	h	307	16	57,65,73	1.64	5 (8%)	66,103,113	1.51	8 (12%)
26	CLA	k	601	19	51,59,73	1.68	5 (9%)	59,96,113	1.56	7 (11%)
29	WVN	L	201	-	40,41,41	5.59	20 (50%)	50,56,56	6.45	34 (68%)
28	LHG	L	207	-	46,46,48	0.65	1 (2%)	49,52,54	1.28	6 (12%)
35	II0	c	316	-	39,43,43	6.63	22 (56%)	50,60,60	7.02	28 (56%)
36	KC2	k	612	19	48,53,53	1.71	10 (20%)	54,89,89	0.81	0
26	CLA	d	306	21	51,59,73	1.72	7 (13%)	59,96,113	1.53	8 (13%)
26	CLA	F	201	38	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
26	CLA	a	309	14	65,73,73	1.51	5 (7%)	76,113,113	1.42	7 (9%)
25	CL0	A	801	-	65,73,73	1.49	8 (12%)	76,113,113	0.87	4 (5%)
26	CLA	A	812	1	65,73,73	1.48	5 (7%)	76,113,113	1.41	6 (7%)
26	CLA	n	607	23	65,73,73	1.50	6 (9%)	76,113,113	1.35	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	a	305	14	45,53,73	1.80	5 (11%)	52,89,113	1.60	7 (13%)
35	II0	k	620	-	39,43,43	6.39	22 (56%)	50,60,60	6.93	27 (54%)
26	CLA	j	612	-	51,59,73	1.69	6 (11%)	59,96,113	1.53	6 (10%)
26	CLA	B	802	38	65,73,73	1.50	5 (7%)	76,113,113	1.45	8 (10%)
27	PQN	A	842	-	34,34,34	3.06	13 (38%)	42,45,45	2.08	6 (14%)
28	LHG	A	849	-	26,26,48	0.68	0	28,29,54	1.42	4 (14%)
35	II0	a	314	-	39,43,43	6.41	21 (53%)	50,60,60	6.95	29 (58%)
35	II0	k	618	-	39,43,43	0.22	0	50,60,60	0.51	1 (2%)
26	CLA	A	803	1	55,63,73	1.70	6 (10%)	64,101,113	1.48	7 (10%)
35	II0	d	315	-	39,43,43	6.54	22 (56%)	50,60,60	6.83	28 (56%)
26	CLA	s	408	38	65,73,73	1.51	5 (7%)	76,113,113	1.35	7 (9%)
26	CLA	B	842	28	65,73,73	1.48	7 (10%)	76,113,113	1.42	7 (9%)
35	II0	n	615	-	39,43,43	6.48	21 (53%)	50,60,60	6.90	27 (54%)
34	LMG	F	206	-	41,41,55	0.86	0	49,49,63	1.25	3 (6%)
28	LHG	s	409	-	32,32,48	0.80	1 (3%)	36,37,54	1.61	4 (11%)
32	SQD	A	854	-	53,54,54	0.93	3 (5%)	62,65,65	1.70	12 (19%)
36	KC2	s	404	-	48,53,53	1.82	11 (22%)	54,89,89	0.86	1 (1%)
26	CLA	i	307	20	65,73,73	1.49	6 (9%)	76,113,113	1.37	6 (7%)
36	KC2	i	318	20	48,53,53	1.67	10 (20%)	54,89,89	0.93	1 (1%)
26	CLA	A	834	1	60,68,73	1.50	5 (8%)	70,107,113	1.51	7 (10%)
26	CLA	d	303	21	51,59,73	1.69	5 (9%)	59,96,113	1.60	7 (11%)
26	CLA	A	852	1	65,73,73	1.50	6 (9%)	76,113,113	1.41	6 (7%)
26	CLA	b	307	15	61,69,73	1.54	6 (9%)	71,108,113	1.40	8 (11%)
26	CLA	d	313	21	51,59,73	1.70	6 (11%)	59,96,113	1.63	9 (15%)
26	CLA	h	302	16	50,58,73	1.69	7 (14%)	58,95,113	1.59	8 (13%)
26	CLA	k	610	-	51,59,73	1.71	5 (9%)	59,96,113	1.55	8 (13%)
26	CLA	h	308	16	51,59,73	1.70	5 (9%)	59,96,113	1.54	8 (13%)
26	CLA	A	808	1	65,73,73	1.51	6 (9%)	76,113,113	1.43	8 (10%)
29	WVN	B	853	-	40,41,41	5.63	21 (52%)	50,56,56	6.38	33 (66%)
29	WVN	J	102	-	40,41,41	5.71	19 (47%)	50,56,56	6.32	29 (58%)
28	LHG	n	619	-	42,42,48	0.65	1 (2%)	45,48,54	1.20	4 (8%)
30	LMU	A	850	-	36,36,36	1.78	11 (30%)	47,47,47	1.03	2 (4%)
26	CLA	B	841	2	65,73,73	1.52	5 (7%)	76,113,113	1.40	7 (9%)
26	CLA	B	831	38	65,73,73	1.49	5 (7%)	76,113,113	1.35	7 (9%)
28	LHG	A	844	-	26,26,48	0.82	0	29,32,54	1.32	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	A	831	1	65,73,73	1.50	6 (9%)	76,113,113	1.39	7 (9%)
26	CLA	A	856	38	65,73,73	1.48	5 (7%)	76,113,113	1.44	9 (11%)
26	CLA	A	826	1	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
26	CLA	B	820	2	65,73,73	1.51	6 (9%)	76,113,113	1.38	7 (9%)
35	II0	i	312	-	39,43,43	6.60	22 (56%)	50,60,60	6.93	30 (60%)
26	CLA	a	303	14	51,59,73	1.71	6 (11%)	59,96,113	1.58	9 (15%)
35	II0	a	316	-	39,43,43	6.63	22 (56%)	50,60,60	6.88	30 (60%)
36	KC2	i	309	20	48,53,53	1.68	10 (20%)	54,89,89	1.11	5 (9%)
26	CLA	j	606	17	51,59,73	1.70	5 (9%)	59,96,113	1.57	7 (11%)
26	CLA	A	841	1	65,73,73	1.49	5 (7%)	76,113,113	1.50	10 (13%)
26	CLA	B	807	2	65,73,73	1.45	5 (7%)	76,113,113	1.40	6 (7%)
29	WVN	A	846	-	40,41,41	5.66	20 (50%)	50,56,56	6.50	32 (64%)
26	CLA	l	305	18	65,73,73	1.41	5 (7%)	76,113,113	1.50	8 (10%)
29	WVN	B	847	-	40,41,41	5.69	20 (50%)	50,56,56	6.18	31 (62%)
26	CLA	b	310	15	65,73,73	1.50	7 (10%)	76,113,113	1.36	8 (10%)
26	CLA	B	818	38	65,73,73	1.50	8 (12%)	76,113,113	1.40	7 (9%)
26	CLA	B	810	2	65,73,73	1.52	5 (7%)	76,113,113	1.33	8 (10%)
26	CLA	h	313	38	65,73,73	1.50	6 (9%)	76,113,113	1.39	7 (9%)
26	CLA	A	830	1	60,68,73	1.58	6 (10%)	70,107,113	1.40	6 (8%)
26	CLA	i	302	20	65,73,73	1.47	7 (10%)	76,113,113	1.42	8 (10%)
26	CLA	B	825	2	65,73,73	1.49	6 (9%)	76,113,113	1.40	8 (10%)
26	CLA	A	806	1	60,68,73	1.56	5 (8%)	70,107,113	1.41	7 (10%)
26	CLA	s	402	12	65,73,73	1.53	6 (9%)	76,113,113	1.42	11 (14%)
26	CLA	A	816	1	65,73,73	1.46	6 (9%)	76,113,113	1.58	9 (11%)
26	CLA	l	309	18	65,73,73	1.49	6 (9%)	76,113,113	1.40	8 (10%)
34	LMG	c	319	26	43,43,55	0.83	0	51,51,63	1.24	4 (7%)
26	CLA	n	605	23	51,59,73	1.69	5 (9%)	59,96,113	1.54	8 (13%)
26	CLA	A	809	1	56,64,73	1.62	6 (10%)	65,102,113	1.45	7 (10%)
35	II0	a	312	-	39,43,43	6.44	22 (56%)	50,60,60	6.74	28 (56%)
26	CLA	A	805	1	65,73,73	1.48	6 (9%)	76,113,113	1.43	7 (9%)
26	CLA	m	602	17	60,68,73	1.53	7 (11%)	70,107,113	1.53	10 (14%)
26	CLA	a	307	14	65,73,73	1.49	5 (7%)	76,113,113	1.35	6 (7%)
26	CLA	k	602	19	65,73,73	1.44	6 (9%)	76,113,113	1.46	6 (7%)
35	II0	d	317	-	39,43,43	6.52	22 (56%)	50,60,60	6.98	27 (54%)
26	CLA	h	301	38	65,73,73	1.50	6 (9%)	76,113,113	3.33	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	WVN	F	204	-	40,41,41	0.17	0	50,56,56	0.51	0
26	CLA	n	604	23	60,68,73	1.54	5 (8%)	70,107,113	1.58	10 (14%)
26	CLA	d	309	21	41,49,73	1.86	5 (12%)	47,84,113	1.69	9 (19%)
26	CLA	d	308	21	46,54,73	1.78	5 (10%)	53,90,113	1.46	6 (11%)
28	LHG	c	317	-	36,36,48	0.71	1 (2%)	39,42,54	1.26	5 (12%)
26	CLA	j	605	17	45,53,73	1.82	5 (11%)	52,89,113	1.70	7 (13%)
26	CLA	B	836	38	65,73,73	1.49	6 (9%)	76,113,113	1.42	8 (10%)
26	CLA	m	605	17	42,50,73	1.84	5 (11%)	48,85,113	1.66	7 (14%)
26	CLA	A	811	1	54,62,73	1.67	5 (9%)	62,99,113	1.46	7 (11%)
26	CLA	m	603	17	59,67,73	1.58	6 (10%)	68,105,113	1.39	6 (8%)
36	KC2	d	311	-	48,53,53	1.70	9 (18%)	54,89,89	1.01	1 (1%)
26	CLA	a	302	14	56,64,73	1.54	6 (10%)	65,102,113	1.54	7 (10%)
36	KC2	d	312	-	48,53,53	1.72	11 (22%)	54,89,89	1.13	6 (11%)
26	CLA	a	304	38	65,73,73	1.49	6 (9%)	76,113,113	1.42	8 (10%)
36	KC2	k	611	19	48,53,53	1.71	10 (20%)	54,89,89	1.01	3 (5%)
30	LMU	B	852	-	36,36,36	0.23	0	47,47,47	0.37	0
29	WVN	M	101	-	40,41,41	5.64	19 (47%)	50,56,56	6.43	34 (68%)
26	CLA	c	302	13	60,68,73	1.59	6 (10%)	70,107,113	1.41	9 (12%)
26	CLA	A	833	1	65,73,73	1.52	5 (7%)	76,113,113	1.33	6 (7%)
35	II0	m	616	-	39,43,43	6.75	22 (56%)	50,60,60	6.61	26 (52%)
26	CLA	A	838	1	65,73,73	1.53	5 (7%)	76,113,113	1.37	7 (9%)
29	WVN	R	200	-	40,41,41	5.70	20 (50%)	50,56,56	6.42	29 (58%)
26	CLA	l	307	18	65,73,73	1.47	5 (7%)	76,113,113	1.48	7 (9%)
35	II0	k	619	-	39,43,43	6.38	21 (53%)	50,60,60	6.92	28 (56%)
26	CLA	A	819	1	65,73,73	1.50	6 (9%)	76,113,113	1.43	8 (10%)
26	CLA	c	304	13	62,70,73	1.52	5 (8%)	72,109,113	1.51	6 (8%)
26	CLA	L	204	38	60,68,73	1.57	6 (10%)	70,107,113	1.45	7 (10%)
35	II0	b	314	-	39,43,43	6.39	21 (53%)	50,60,60	6.91	29 (58%)
28	LHG	m	618	26	36,36,48	0.70	0	39,42,54	1.23	4 (10%)
26	CLA	A	827	1	62,70,73	1.55	6 (9%)	72,109,113	1.50	8 (11%)
26	CLA	A	832	1	65,73,73	1.52	5 (7%)	76,113,113	1.37	7 (9%)
26	CLA	Q	302	-	65,73,73	1.49	5 (7%)	76,113,113	1.38	7 (9%)
36	KC2	n	612	-	48,53,53	1.69	10 (20%)	54,89,89	1.03	4 (7%)
26	CLA	a	310	14	65,73,73	1.53	6 (9%)	76,113,113	1.38	7 (9%)
26	CLA	i	304	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	k	607	19	51,59,73	1.69	7 (13%)	59,96,113	1.60	10 (16%)
28	LHG	c	320	-	48,48,48	0.60	0	51,54,54	1.25	6 (11%)
26	CLA	b	308	15	65,73,73	1.48	5 (7%)	76,113,113	1.39	6 (7%)
26	CLA	B	808	2	65,73,73	1.49	7 (10%)	76,113,113	1.52	9 (11%)
26	CLA	A	829	1	65,73,73	1.53	7 (10%)	76,113,113	1.37	5 (6%)
26	CLA	a	306	14	65,73,73	1.51	6 (9%)	76,113,113	1.33	7 (9%)
26	CLA	j	603	17	51,59,73	1.66	6 (11%)	59,96,113	1.60	6 (10%)
26	CLA	i	311	20	65,73,73	1.52	6 (9%)	76,113,113	1.41	8 (10%)
35	II0	j	615	-	39,43,43	6.53	22 (56%)	50,60,60	6.88	29 (58%)
26	CLA	B	826	2	65,73,73	1.51	6 (9%)	76,113,113	1.34	7 (9%)
26	CLA	A	818	1	65,73,73	1.50	6 (9%)	76,113,113	1.48	9 (11%)
26	CLA	m	601	17	42,50,73	1.85	5 (11%)	48,85,113	1.62	7 (14%)
35	II0	d	301	-	39,43,43	6.42	21 (53%)	50,60,60	6.82	29 (58%)
26	CLA	s	406	38	65,73,73	1.49	6 (9%)	76,113,113	1.47	10 (13%)
26	CLA	A	820	38	65,73,73	1.50	6 (9%)	76,113,113	1.42	7 (9%)
26	CLA	l	310	18	57,65,73	1.58	6 (10%)	66,103,113	1.48	7 (10%)
34	LMG	b	319	-	42,42,55	0.88	2 (4%)	50,50,63	1.19	4 (8%)
35	II0	k	615	-	39,43,43	6.70	22 (56%)	50,60,60	6.57	30 (60%)
26	CLA	m	604	17	65,73,73	1.47	6 (9%)	76,113,113	1.52	7 (9%)
35	II0	d	316	-	39,43,43	6.59	22 (56%)	50,60,60	6.69	28 (56%)
26	CLA	K	101	11	42,50,73	1.86	6 (14%)	48,85,113	1.67	8 (16%)
35	II0	m	619	-	39,43,43	6.64	22 (56%)	50,60,60	6.80	29 (58%)
26	CLA	j	607	17	51,59,73	1.68	8 (15%)	59,96,113	1.67	12 (20%)
28	LHG	i	317	26	36,36,48	0.70	1 (2%)	39,42,54	1.24	4 (10%)
26	CLA	j	610	28	61,69,73	1.55	5 (8%)	71,108,113	1.42	6 (8%)
29	WVN	B	849	-	40,41,41	5.75	19 (47%)	50,56,56	6.16	30 (60%)
29	WVN	h	309	-	40,41,41	5.65	20 (50%)	50,56,56	6.21	33 (66%)
30	LMU	i	300	-	36,36,36	1.79	10 (27%)	47,47,47	0.88	0
26	CLA	B	840	2	65,73,73	1.51	6 (9%)	76,113,113	1.43	8 (10%)
26	CLA	c	309	-	45,53,73	2.42	12 (26%)	52,89,113	4.77	25 (48%)
26	CLA	A	802	-	65,73,73	1.45	6 (9%)	76,113,113	1.50	8 (10%)
26	CLA	B	830	2	50,58,73	1.70	6 (12%)	58,95,113	1.51	9 (15%)
26	CLA	h	303	16	50,58,73	1.71	5 (10%)	58,95,113	1.55	8 (13%)
35	II0	l	317	-	39,43,43	0.21	0	50,60,60	0.27	0
26	CLA	m	608	17	65,73,73	1.51	5 (7%)	76,113,113	1.34	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	F	202	6	52,60,73	1.69	5 (9%)	60,97,113	1.46	6 (10%)
28	LHG	b	302	26	48,48,48	0.60	0	51,54,54	1.23	5 (9%)
28	LHG	j	617	26	29,29,48	0.78	1 (3%)	32,35,54	1.28	3 (9%)
26	CLA	i	306	20	61,69,73	1.57	5 (8%)	71,108,113	1.38	7 (9%)
26	CLA	m	610	28	55,63,73	1.63	5 (9%)	64,101,113	1.49	7 (10%)
35	II0	k	617	-	39,43,43	0.23	0	50,60,60	0.52	1 (2%)
26	CLA	A	825	38	65,73,73	1.47	6 (9%)	76,113,113	1.44	9 (11%)
26	CLA	B	812	2	65,73,73	1.48	5 (7%)	76,113,113	1.46	7 (9%)
26	CLA	k	605	19	45,53,73	1.81	5 (11%)	52,89,113	1.62	7 (13%)
35	II0	h	311	-	39,43,43	6.30	21 (53%)	50,60,60	7.04	28 (56%)
35	II0	n	616	-	39,43,43	6.59	22 (56%)	50,60,60	6.93	27 (54%)
26	CLA	B	814	2	65,73,73	1.47	6 (9%)	76,113,113	1.38	6 (7%)
35	II0	m	614	-	39,43,43	6.57	21 (53%)	50,60,60	6.89	30 (60%)
26	CLA	b	304	15	55,63,73	1.56	5 (9%)	64,101,113	1.60	8 (12%)
26	CLA	l	311	28	61,69,73	1.55	5 (8%)	71,108,113	1.43	7 (9%)
26	CLA	B	839	2	57,65,73	1.60	6 (10%)	66,103,113	1.42	7 (10%)
26	CLA	B	828	2	50,58,73	1.74	6 (12%)	58,95,113	1.48	9 (15%)
35	II0	a	313	-	39,43,43	6.53	22 (56%)	50,60,60	6.68	29 (58%)
29	WVN	A	847	-	40,41,41	5.59	19 (47%)	50,56,56	6.69	33 (66%)
26	CLA	B	823	38	64,72,73	1.49	7 (10%)	74,111,113	1.38	8 (10%)
33	DGD	j	618	-	63,63,67	0.97	2 (3%)	77,77,81	1.53	12 (15%)
26	CLA	B	805	2	65,73,73	1.46	5 (7%)	76,113,113	1.56	7 (9%)
26	CLA	B	813	2	60,68,73	1.56	6 (10%)	70,107,113	1.51	10 (14%)
26	CLA	b	306	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	7 (9%)
29	WVN	B	850	-	40,41,41	5.68	19 (47%)	50,56,56	6.14	32 (64%)
31	SF4	A	853	2,1	0,12,12	-	-	-	-	-
30	LMU	a	317	-	36,36,36	0.17	0	47,47,47	0.46	0
26	CLA	A	815	38	45,53,73	1.80	6 (13%)	52,89,113	1.68	6 (11%)
35	II0	c	314	-	39,43,43	0.30	0	50,60,60	0.53	1 (2%)
26	CLA	k	603	19	51,59,73	1.74	6 (11%)	59,96,113	1.44	6 (10%)
35	II0	i	314	-	39,43,43	6.59	22 (56%)	50,60,60	6.89	29 (58%)
26	CLA	l	306	18	51,59,73	1.66	5 (9%)	59,96,113	1.65	7 (11%)
26	CLA	s	403	12	65,73,73	1.49	6 (9%)	76,113,113	1.44	8 (10%)
28	LHG	B	851	26	48,48,48	0.60	0	51,54,54	1.23	6 (11%)
26	CLA	c	312	13	65,73,73	1.52	5 (7%)	76,113,113	1.35	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMG	F	205	-	53,53,55	0.75	0	61,61,63	1.33	8 (13%)
26	CLA	L	206	-	51,59,73	1.71	5 (9%)	59,96,113	1.48	6 (10%)
26	CLA	B	804	-	65,73,73	1.49	8 (12%)	76,113,113	1.73	13 (17%)
35	II0	i	313	-	39,43,43	6.60	22 (56%)	50,60,60	6.71	28 (56%)
26	CLA	A	807	1	65,73,73	1.47	5 (7%)	76,113,113	1.41	7 (9%)
26	CLA	c	311	-	45,53,73	1.78	6 (13%)	52,89,113	1.66	7 (13%)
26	CLA	k	609	19	57,65,73	1.63	5 (8%)	66,103,113	1.48	7 (10%)
36	KC2	k	613	-	48,53,53	1.69	10 (20%)	54,89,89	0.89	1 (1%)
26	CLA	n	608	-	65,73,73	1.54	6 (9%)	76,113,113	1.30	9 (11%)
26	CLA	B	801	38	65,73,73	1.50	6 (9%)	76,113,113	1.34	6 (7%)
26	CLA	a	311	14	48,56,73	1.75	5 (10%)	55,92,113	1.54	6 (10%)
26	CLA	n	609	23	65,73,73	1.48	5 (7%)	76,113,113	1.33	7 (9%)
26	CLA	n	610	-	60,68,73	1.57	5 (8%)	70,107,113	1.45	8 (11%)
35	II0	J	104	-	39,43,43	6.41	22 (56%)	50,60,60	7.04	29 (58%)
26	CLA	A	810	1	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
26	CLA	j	604	17	65,73,73	1.47	6 (9%)	76,113,113	1.51	8 (10%)
26	CLA	i	301	20	65,73,73	1.51	5 (7%)	76,113,113	1.40	7 (9%)
26	CLA	b	313	28	51,59,73	1.69	6 (11%)	59,96,113	1.57	10 (16%)
37	IHT	m	617	-	40,42,42	0.25	0	53,58,58	0.58	1 (1%)
26	CLA	m	606	17	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
30	LMU	A	858	-	35,35,36	0.20	0	46,46,47	0.50	0
26	CLA	b	312	15	65,73,73	1.51	5 (7%)	76,113,113	1.38	6 (7%)
37	IHT	b	316	-	40,42,42	0.27	0	53,58,58	0.88	3 (5%)
28	LHG	A	843	-	47,47,48	0.62	1 (2%)	50,53,54	1.23	5 (10%)
35	II0	k	616	-	39,43,43	6.65	22 (56%)	50,60,60	6.66	26 (52%)
26	CLA	l	313	18	56,64,73	1.64	5 (8%)	65,102,113	1.55	7 (10%)
29	WVN	J	101	-	40,41,41	5.63	18 (45%)	50,56,56	6.31	32 (64%)
26	CLA	B	816	2	65,73,73	1.52	5 (7%)	76,113,113	1.33	7 (9%)
29	WVN	B	845	-	40,41,41	0.15	0	50,56,56	0.41	0
26	CLA	A	840	38	65,73,73	1.52	6 (9%)	76,113,113	1.45	8 (10%)
31	SF4	C	102	3	0,12,12	-	-	-	-	-
26	CLA	B	803	2	65,73,73	1.48	8 (12%)	76,113,113	1.28	7 (9%)
28	LHG	A	855	-	35,35,48	0.69	0	38,41,54	1.25	4 (10%)
26	CLA	d	302	21	62,70,73	1.54	6 (9%)	72,109,113	1.40	7 (9%)
26	CLA	A	836	1	65,73,73	1.53	6 (9%)	76,113,113	1.43	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	B	834	2	65,73,73	1.49	5 (7%)	76,113,113	1.46	8 (10%)
26	CLA	d	310	21	41,49,73	1.89	6 (14%)	47,84,113	1.65	8 (17%)
31	SF4	C	101	3	0,12,12	-	-	-		
26	CLA	l	301	18	65,73,73	1.51	6 (9%)	76,113,113	1.39	7 (9%)
26	CLA	j	602	17	54,62,73	1.60	6 (11%)	62,99,113	1.56	7 (11%)
26	CLA	B	822	38	65,73,73	1.50	7 (10%)	76,113,113	1.51	8 (10%)
26	CLA	h	306	16	65,73,73	1.51	6 (9%)	76,113,113	1.40	9 (11%)
28	LHG	J	105	26	32,32,48	0.75	1 (3%)	35,38,54	1.26	3 (8%)
26	CLA	n	602	23	50,58,73	1.63	6 (12%)	58,95,113	1.65	7 (12%)
28	LHG	b	318	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	6 (11%)
29	WVN	A	857	-	40,41,41	5.69	20 (50%)	50,56,56	6.42	31 (62%)
26	CLA	c	306	13	52,60,73	1.70	7 (13%)	60,97,113	1.45	8 (13%)
26	CLA	c	303	13	51,59,73	1.70	5 (9%)	59,96,113	1.55	6 (10%)
35	II0	d	319	-	39,43,43	0.29	0	50,60,60	0.80	2 (4%)
26	CLA	b	303	15	51,59,73	1.68	5 (9%)	59,96,113	1.55	7 (11%)
37	IHT	R	202	-	40,42,42	0.23	0	53,58,58	0.36	0
34	LMG	c	318	-	55,55,55	0.71	0	63,63,63	1.38	9 (14%)
26	CLA	n	606	23	51,59,73	1.75	7 (13%)	59,96,113	1.48	7 (11%)
26	CLA	j	613	17	65,73,73	1.52	6 (9%)	76,113,113	1.39	8 (10%)
26	CLA	d	305	-	51,59,73	1.69	5 (9%)	59,96,113	1.56	7 (11%)
26	CLA	B	824	2	65,73,73	1.49	6 (9%)	76,113,113	1.39	6 (7%)
26	CLA	A	839	1	60,68,73	1.55	5 (8%)	70,107,113	1.45	6 (8%)
35	II0	l	314	-	39,43,43	6.42	22 (56%)	50,60,60	7.01	30 (60%)
29	WVN	I	101	-	40,41,41	5.50	19 (47%)	50,56,56	6.42	33 (66%)
26	CLA	h	304	-	65,73,73	1.51	5 (7%)	76,113,113	1.39	7 (9%)
37	IHT	j	616	-	40,42,42	0.23	0	53,58,58	0.84	3 (5%)
26	CLA	L	202	9	49,57,73	1.72	5 (10%)	55,93,113	1.56	7 (12%)
26	CLA	L	203	9	65,73,73	1.48	5 (7%)	76,113,113	1.46	8 (10%)
28	LHG	l	318	26	31,31,48	0.77	1 (3%)	34,37,54	1.28	4 (11%)
26	CLA	i	308	28	46,54,73	1.77	5 (10%)	53,90,113	1.58	6 (11%)
26	CLA	A	823	1	55,63,73	1.64	5 (9%)	64,101,113	1.52	8 (12%)
26	CLA	k	608	19	65,73,73	1.49	7 (10%)	76,113,113	1.32	7 (9%)
37	IHT	n	617	-	40,42,42	0.22	0	53,58,58	0.60	0
36	KC2	s	401	12	48,53,53	3.26	22 (45%)	54,89,89	3.94	30 (55%)
37	IHT	c	315	-	40,42,42	0.54	0	53,58,58	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	B	817	2	65,73,73	1.52	5 (7%)	76,113,113	1.38	6 (7%)
26	CLA	k	604	-	65,73,73	1.61	7 (10%)	76,113,113	1.35	8 (10%)
35	II0	b	315	-	39,43,43	6.51	21 (53%)	50,60,60	6.77	24 (48%)
26	CLA	A	822	1	56,64,73	1.61	6 (10%)	65,102,113	1.48	7 (10%)
26	CLA	k	606	19	51,59,73	1.67	6 (11%)	59,96,113	1.54	8 (13%)
36	KC2	n	611	23	48,53,53	1.70	10 (20%)	54,89,89	1.11	4 (7%)
33	DGD	B	844	-	67,67,67	0.87	1 (1%)	81,81,81	1.44	9 (11%)
35	II0	b	317	-	39,43,43	0.41	0	50,60,60	0.51	0
26	CLA	h	305	16	51,59,73	1.69	6 (11%)	59,96,113	1.55	8 (13%)
29	WVN	i	315	-	40,41,41	5.71	21 (52%)	50,56,56	6.49	30 (60%)
26	CLA	B	819	2	65,73,73	1.53	7 (10%)	76,113,113	1.54	11 (14%)
36	KC2	l	312	18	48,53,53	1.71	11 (22%)	54,89,89	1.01	2 (3%)
26	CLA	B	806	2	65,73,73	1.50	5 (7%)	76,113,113	1.36	8 (10%)
26	CLA	m	609	17	60,68,73	1.56	5 (8%)	70,107,113	1.42	7 (10%)
26	CLA	b	309	34	65,73,73	1.49	5 (7%)	76,113,113	1.38	6 (7%)
26	CLA	c	305	13	65,73,73	1.52	6 (9%)	76,113,113	1.36	6 (7%)
35	II0	i	319	-	39,43,43	6.56	21 (53%)	50,60,60	6.72	29 (58%)
26	CLA	A	814	1	50,58,73	1.68	6 (12%)	58,95,113	1.59	8 (13%)
26	CLA	b	305	15	52,60,73	1.67	6 (11%)	60,97,113	1.60	7 (11%)
26	CLA	l	304	18	47,55,73	1.76	5 (10%)	54,91,113	1.56	7 (12%)
26	CLA	B	827	2	51,59,73	1.69	6 (11%)	59,96,113	1.69	9 (15%)
26	CLA	b	311	15	64,72,73	1.52	6 (9%)	74,111,113	1.42	7 (9%)
26	CLA	B	832	38	45,53,73	1.83	5 (11%)	52,89,113	1.64	6 (11%)
36	KC2	j	611	17	48,53,53	1.69	9 (18%)	54,89,89	0.92	2 (3%)
26	CLA	R	201	22	55,63,73	1.70	5 (9%)	64,101,113	1.62	10 (15%)
26	CLA	B	835	2	47,55,73	1.83	7 (14%)	54,91,113	1.53	9 (16%)
29	WVN	s	407	-	40,41,41	5.65	19 (47%)	50,56,56	6.62	32 (64%)
35	II0	d	314	-	39,43,43	0.19	0	50,60,60	0.62	2 (4%)
35	II0	n	618	-	39,43,43	6.58	22 (56%)	50,60,60	6.87	29 (58%)
26	CLA	B	821	2	53,61,73	1.66	6 (11%)	61,98,113	1.46	9 (14%)
29	WVN	L	205	-	40,41,41	5.69	19 (47%)	50,56,56	6.21	30 (60%)
26	CLA	n	601	23	45,53,73	1.80	5 (11%)	52,89,113	1.61	7 (13%)
26	CLA	A	821	1	49,57,73	1.72	5 (10%)	55,93,113	1.65	8 (14%)
34	LMG	L	209	-	45,45,55	0.83	1 (2%)	53,53,63	1.23	3 (5%)
26	CLA	B	811	2	55,63,73	1.65	6 (10%)	64,101,113	1.44	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	l	308	18	65,73,73	1.49	5 (7%)	76,113,113	1.37	6 (7%)
26	CLA	d	318	-	45,53,73	1.79	5 (11%)	52,89,113	1.63	6 (11%)
26	CLA	B	837	2	65,73,73	1.51	6 (9%)	76,113,113	1.32	5 (6%)
37	IHT	a	315	-	40,42,42	0.24	0	53,58,58	0.59	1 (1%)
26	CLA	i	310	-	60,68,73	1.55	6 (10%)	70,107,113	1.48	6 (8%)
26	CLA	c	301	13	51,59,73	1.68	5 (9%)	59,96,113	1.54	6 (10%)
26	CLA	a	308	28	48,56,73	1.74	5 (10%)	55,92,113	1.57	7 (12%)
26	CLA	J	103	8	42,50,73	1.86	5 (11%)	48,85,113	1.66	7 (14%)
35	II0	l	302	-	39,43,43	6.71	21 (53%)	50,60,60	6.91	28 (56%)
26	CLA	A	835	1	65,73,73	1.50	5 (7%)	76,113,113	1.38	7 (9%)
26	CLA	k	614	19	51,59,73	1.72	6 (11%)	59,96,113	1.57	7 (11%)
26	CLA	A	851	38	65,73,73	1.53	6 (9%)	76,113,113	1.43	6 (7%)
26	CLA	j	601	17	65,73,73	1.51	6 (9%)	76,113,113	1.41	7 (9%)
35	II0	c	313	-	39,43,43	6.50	22 (56%)	50,60,60	6.90	29 (58%)
26	CLA	B	833	2	55,63,73	1.64	5 (9%)	64,101,113	1.57	8 (12%)
26	CLA	m	607	17	51,59,73	1.71	5 (9%)	59,96,113	1.46	7 (11%)
37	IHT	b	301	-	40,42,42	0.30	0	53,58,58	0.54	0
26	CLA	B	838	2	65,73,73	1.48	6 (9%)	76,113,113	1.43	8 (10%)
26	CLA	n	613	23	51,59,73	1.72	5 (9%)	59,96,113	1.51	9 (15%)
35	II0	i	316	-	39,43,43	6.50	21 (53%)	50,60,60	6.98	33 (66%)
29	WVN	F	203	-	40,41,41	5.66	18 (45%)	50,56,56	6.17	32 (64%)
26	CLA	m	612	38	51,59,73	1.68	6 (11%)	59,96,113	1.57	9 (15%)
26	CLA	a	301	14	65,73,73	1.50	7 (10%)	76,113,113	1.46	8 (10%)
26	CLA	B	815	2	55,63,73	1.62	5 (9%)	64,101,113	1.47	6 (9%)
36	KC2	c	310	13	48,53,53	3.32	20 (41%)	54,89,89	3.83	29 (53%)
26	CLA	A	837	1	65,73,73	1.52	6 (9%)	76,113,113	1.36	6 (7%)
26	CLA	i	305	20	51,59,73	1.70	8 (15%)	59,96,113	1.67	8 (13%)
28	LHG	L	208	-	44,44,48	0.64	0	47,50,54	1.25	5 (10%)
26	CLA	A	828	1	65,73,73	1.51	6 (9%)	76,113,113	1.37	7 (9%)
29	WVN	l	303	-	40,41,41	5.63	19 (47%)	50,56,56	6.28	32 (64%)

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
35	II0	h	310	-	-	11/17/40/67	0/1/1/2
35	II0	n	614	-	-	1/21/67/67	0/2/2/2
29	WVN	A	848	-	-	18/29/63/63	0/2/2/2
35	II0	m	615	-	-	11/21/67/67	0/2/2/2
34	LMG	Q	301	-	-	15/33/53/70	0/1/1/1
29	WVN	B	846	-	-	15/29/63/63	0/2/2/2
29	WVN	s	405	-	-	16/29/63/63	0/2/2/2
26	CLA	m	613	17	1/1/15/20	12/37/115/115	-
35	II0	j	614	-	-	13/21/67/67	0/2/2/2
26	CLA	d	304	-	1/1/11/20	8/13/91/115	-
29	WVN	K	102	-	-	17/29/63/63	0/2/2/2
36	KC2	m	611	17	-	10/15/71/71	-
26	CLA	A	824	38	1/1/15/20	10/37/115/115	-
26	CLA	c	307	13	1/1/11/20	7/15/93/115	-
26	CLA	B	829	2	1/1/15/20	11/37/115/115	-
26	CLA	A	813	1	1/1/13/20	10/27/105/115	-
26	CLA	d	307	21	1/1/11/20	7/13/91/115	-
26	CLA	j	609	17	1/1/15/20	15/37/115/115	-
26	CLA	A	817	1	1/1/15/20	11/37/115/115	-
29	WVN	B	848	-	-	17/29/63/63	0/2/2/2
26	CLA	c	308	13	1/1/15/20	17/37/115/115	-
29	WVN	l	316	-	-	17/29/63/63	0/2/2/2
26	CLA	j	608	17	1/1/11/20	5/13/91/115	-
26	CLA	B	809	2	1/1/15/20	7/37/115/115	-
35	II0	h	312	-	-	11/21/67/67	0/2/2/2
29	WVN	A	845	-	-	16/29/63/63	0/2/2/2
35	II0	l	315	-	-	11/21/67/67	0/2/2/2
26	CLA	i	303	20	1/1/15/20	6/37/115/115	-
26	CLA	A	804	1	1/1/15/20	9/37/115/115	-
27	PQN	B	843	-	-	7/23/43/43	0/2/2/2
34	LMG	n	620	-	-	17/46/66/70	0/1/1/1
26	CLA	n	603	23	1/1/12/20	6/21/99/115	-
26	CLA	h	307	16	1/1/13/20	7/28/106/115	-
26	CLA	k	601	19	1/1/12/20	5/21/99/115	-
29	WVN	L	201	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	L	207	-	-	19/51/51/53	-
35	II0	c	316	-	-	13/21/67/67	0/2/2/2
36	KC2	k	612	19	-	9/15/71/71	-
26	CLA	d	306	21	1/1/12/20	5/21/99/115	-
26	CLA	F	201	38	1/1/15/20	15/37/115/115	-
26	CLA	a	309	14	1/1/15/20	10/37/115/115	-
25	CL0	A	801	-	2/2/20/25	16/37/135/135	-
26	CLA	A	812	1	1/1/15/20	12/37/115/115	-
26	CLA	n	607	23	1/1/15/20	11/37/115/115	-
26	CLA	a	305	14	1/1/11/20	5/13/91/115	-
35	II0	k	620	-	-	13/21/67/67	0/2/2/2
26	CLA	j	612	-	1/1/12/20	9/21/99/115	-
26	CLA	B	802	38	1/1/15/20	13/37/115/115	-
27	PQN	A	842	-	-	10/23/43/43	0/2/2/2
28	LHG	A	849	-	-	14/27/27/53	-
35	II0	a	314	-	-	14/21/67/67	0/2/2/2
35	II0	k	618	-	-	1/21/67/67	0/2/2/2
26	CLA	A	803	1	1/1/13/20	4/25/103/115	-
35	II0	d	315	-	-	12/21/67/67	0/2/2/2
26	CLA	s	408	38	1/1/15/20	9/37/115/115	-
26	CLA	B	842	28	1/1/15/20	11/37/115/115	-
35	II0	n	615	-	-	11/21/67/67	0/2/2/2
34	LMG	F	206	-	-	12/36/56/70	0/1/1/1
28	LHG	s	409	-	-	15/34/34/53	-
32	SQD	A	854	-	-	19/49/69/69	0/1/1/1
36	KC2	s	404	-	-	1/15/71/71	-
26	CLA	i	307	20	1/1/15/20	10/37/115/115	-
36	KC2	i	318	20	-	11/15/71/71	-
26	CLA	A	834	1	1/1/14/20	7/31/109/115	-
26	CLA	d	303	21	1/1/12/20	7/21/99/115	-
26	CLA	A	852	1	1/1/15/20	12/37/115/115	-
26	CLA	b	307	15	1/1/14/20	9/33/111/115	-
26	CLA	d	313	21	1/1/12/20	7/21/99/115	-
26	CLA	h	302	16	1/1/12/20	6/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	k	610	-	1/1/12/20	10/21/99/115	-
26	CLA	h	308	16	1/1/12/20	6/21/99/115	-
26	CLA	A	808	1	1/1/15/20	7/37/115/115	-
29	WVN	B	853	-	-	20/29/63/63	0/2/2/2
29	WVN	J	102	-	-	19/29/63/63	0/2/2/2
28	LHG	n	619	-	-	23/47/47/53	-
30	LMU	A	850	-	-	13/21/61/61	0/2/2/2
26	CLA	B	841	2	1/1/15/20	15/37/115/115	-
26	CLA	B	831	38	1/1/15/20	12/37/115/115	-
28	LHG	A	844	-	-	8/31/31/53	-
26	CLA	A	831	1	1/1/15/20	13/37/115/115	-
26	CLA	A	856	38	1/1/15/20	11/37/115/115	-
26	CLA	A	826	1	1/1/15/20	11/37/115/115	-
26	CLA	B	820	2	1/1/15/20	9/37/115/115	-
35	II0	i	312	-	-	12/21/67/67	0/2/2/2
26	CLA	a	303	14	1/1/12/20	0/21/99/115	-
35	II0	a	316	-	-	10/21/67/67	0/2/2/2
36	KC2	i	309	20	-	11/15/71/71	-
26	CLA	j	606	17	1/1/12/20	6/21/99/115	-
26	CLA	A	841	1	1/1/15/20	13/37/115/115	-
26	CLA	B	807	2	1/1/15/20	11/37/115/115	-
29	WVN	A	846	-	-	16/29/63/63	0/2/2/2
26	CLA	l	305	18	1/1/15/20	14/37/115/115	-
29	WVN	B	847	-	-	16/29/63/63	0/2/2/2
26	CLA	b	310	15	1/1/15/20	13/37/115/115	-
26	CLA	B	818	38	1/1/15/20	10/37/115/115	-
26	CLA	B	810	2	1/1/15/20	13/37/115/115	-
26	CLA	h	313	38	1/1/15/20	4/37/115/115	-
26	CLA	A	830	1	1/1/14/20	8/31/109/115	-
26	CLA	i	302	20	1/1/15/20	16/37/115/115	-
26	CLA	B	825	2	1/1/15/20	19/37/115/115	-
26	CLA	A	806	1	1/1/14/20	5/31/109/115	-
26	CLA	s	402	12	1/1/15/20	21/37/115/115	-
26	CLA	A	816	1	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	l	309	18	1/1/15/20	6/37/115/115	-
34	LMG	c	319	26	-	21/38/58/70	0/1/1/1
26	CLA	n	605	23	1/1/12/20	7/21/99/115	-
26	CLA	A	809	1	1/1/13/20	11/27/105/115	-
35	II0	a	312	-	-	11/21/67/67	0/2/2/2
26	CLA	A	805	1	1/1/15/20	14/37/115/115	-
26	CLA	m	602	17	1/1/14/20	15/31/109/115	-
26	CLA	a	307	14	1/1/15/20	13/37/115/115	-
26	CLA	k	602	19	1/1/15/20	15/37/115/115	-
35	II0	d	317	-	-	13/21/67/67	0/2/2/2
26	CLA	h	301	38	1/1/15/20	10/37/115/115	-
29	WVN	F	204	-	-	6/29/63/63	0/2/2/2
26	CLA	n	604	23	1/1/14/20	11/31/109/115	-
26	CLA	d	309	21	1/1/10/20	2/8/86/115	-
26	CLA	d	308	21	1/1/11/20	9/15/93/115	-
28	LHG	c	317	-	-	19/41/41/53	-
26	CLA	j	605	17	1/1/11/20	8/13/91/115	-
26	CLA	B	836	38	1/1/15/20	15/37/115/115	-
26	CLA	m	605	17	1/1/10/20	5/10/88/115	-
26	CLA	A	811	1	1/1/12/20	8/24/102/115	-
26	CLA	m	603	17	1/1/13/20	7/30/108/115	-
36	KC2	d	311	-	-	13/15/71/71	-
26	CLA	a	302	14	1/1/13/20	5/27/105/115	-
36	KC2	d	312	-	-	11/15/71/71	-
26	CLA	a	304	38	1/1/15/20	8/37/115/115	-
36	KC2	k	611	19	-	13/15/71/71	-
30	LMU	B	852	-	-	2/21/61/61	0/2/2/2
29	WVN	M	101	-	-	18/29/63/63	0/2/2/2
26	CLA	c	302	13	-	15/31/109/115	-
26	CLA	A	833	1	1/1/15/20	16/37/115/115	-
35	II0	m	616	-	-	12/21/67/67	0/2/2/2
26	CLA	A	838	1	1/1/15/20	10/37/115/115	-
29	WVN	R	200	-	-	17/29/63/63	0/2/2/2
26	CLA	l	307	18	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	II0	k	619	-	-	10/21/67/67	0/2/2/2
26	CLA	A	819	1	1/1/15/20	19/37/115/115	-
26	CLA	c	304	13	1/1/14/20	13/34/112/115	-
26	CLA	L	204	38	1/1/14/20	6/31/109/115	-
35	II0	b	314	-	-	11/21/67/67	0/2/2/2
28	LHG	m	618	26	-	11/41/41/53	-
26	CLA	A	827	1	1/1/14/20	8/34/112/115	-
26	CLA	A	832	1	1/1/15/20	6/37/115/115	-
26	CLA	Q	302	-	1/1/15/20	13/37/115/115	-
36	KC2	n	612	-	-	11/15/71/71	-
26	CLA	a	310	14	-	12/37/115/115	-
26	CLA	i	304	-	1/1/15/20	15/37/115/115	-
26	CLA	k	607	19	1/1/12/20	11/21/99/115	-
28	LHG	c	320	-	-	21/53/53/53	-
26	CLA	b	308	15	1/1/15/20	13/37/115/115	-
26	CLA	B	808	2	1/1/15/20	8/37/115/115	-
26	CLA	A	829	1	1/1/15/20	5/37/115/115	-
26	CLA	a	306	14	1/1/15/20	12/37/115/115	-
26	CLA	j	603	17	1/1/12/20	5/21/99/115	-
26	CLA	i	311	20	1/1/15/20	12/37/115/115	-
35	II0	j	615	-	-	10/21/67/67	0/2/2/2
26	CLA	B	826	2	1/1/15/20	16/37/115/115	-
26	CLA	A	818	1	1/1/15/20	16/37/115/115	-
26	CLA	m	601	17	1/1/10/20	4/10/88/115	-
35	II0	d	301	-	-	10/21/67/67	0/2/2/2
26	CLA	s	406	38	1/1/15/20	10/37/115/115	-
26	CLA	A	820	38	1/1/15/20	8/37/115/115	-
26	CLA	l	310	18	1/1/13/20	9/28/106/115	-
34	LMG	b	319	-	-	15/37/57/70	0/1/1/1
35	II0	k	615	-	-	13/21/67/67	0/2/2/2
26	CLA	m	604	17	1/1/15/20	12/37/115/115	-
35	II0	d	316	-	-	13/21/67/67	0/2/2/2
26	CLA	K	101	11	1/1/10/20	4/10/88/115	-
35	II0	m	619	-	-	11/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	j	607	17	1/1/12/20	11/21/99/115	-
28	LHG	i	317	26	-	17/41/41/53	-
26	CLA	j	610	28	1/1/14/20	8/33/111/115	-
29	WVN	B	849	-	-	17/29/63/63	0/2/2/2
29	WVN	h	309	-	-	19/29/63/63	0/2/2/2
30	LMU	i	300	-	-	13/21/61/61	0/2/2/2
26	CLA	B	840	2	1/1/15/20	8/37/115/115	-
26	CLA	h	303	16	1/1/12/20	7/19/97/115	-
26	CLA	A	802	-	1/1/15/20	7/37/115/115	-
26	CLA	B	830	2	1/1/12/20	9/19/97/115	-
26	CLA	c	309	-	-	4/13/91/115	-
35	II0	l	317	-	-	3/21/67/67	0/2/2/2
26	CLA	m	608	17	1/1/15/20	12/37/115/115	-
26	CLA	F	202	6	1/1/12/20	11/22/100/115	-
28	LHG	b	302	26	-	22/53/53/53	-
28	LHG	j	617	26	-	16/34/34/53	-
26	CLA	i	306	20	1/1/14/20	15/33/111/115	-
26	CLA	m	610	28	1/1/13/20	12/25/103/115	-
35	II0	k	617	-	-	2/21/67/67	0/2/2/2
26	CLA	A	825	38	1/1/15/20	5/37/115/115	-
26	CLA	B	812	2	1/1/15/20	14/37/115/115	-
26	CLA	k	605	19	1/1/11/20	5/13/91/115	-
35	II0	h	311	-	-	14/21/67/67	0/2/2/2
35	II0	n	616	-	-	13/21/67/67	0/2/2/2
26	CLA	B	814	2	1/1/15/20	12/37/115/115	-
35	II0	m	614	-	-	13/21/67/67	0/2/2/2
26	CLA	b	304	15	1/1/13/20	11/25/103/115	-
26	CLA	l	311	28	1/1/14/20	11/33/111/115	-
26	CLA	B	839	2	1/1/13/20	9/28/106/115	-
26	CLA	B	828	2	1/1/12/20	10/19/97/115	-
35	II0	a	313	-	-	11/21/67/67	0/2/2/2
29	WVN	A	847	-	-	17/29/63/63	0/2/2/2
26	CLA	B	823	38	1/1/14/20	10/36/114/115	-
33	DGD	j	618	-	-	23/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	805	2	1/1/15/20	13/37/115/115	-
26	CLA	B	813	2	1/1/14/20	13/31/109/115	-
26	CLA	b	306	-	1/1/15/20	17/37/115/115	-
29	WVN	B	850	-	-	17/29/63/63	0/2/2/2
31	SF4	A	853	2,1	-	-	0/6/5/5
30	LMU	a	317	-	-	15/21/61/61	0/2/2/2
26	CLA	A	815	38	1/1/11/20	5/13/91/115	-
35	II0	c	314	-	-	1/21/67/67	0/2/2/2
26	CLA	k	603	19	1/1/12/20	5/21/99/115	-
35	II0	i	314	-	-	13/21/67/67	0/2/2/2
26	CLA	l	306	18	1/1/12/20	1/21/99/115	-
26	CLA	s	403	12	1/1/15/20	10/37/115/115	-
28	LHG	B	851	26	-	32/53/53/53	-
26	CLA	c	312	13	1/1/15/20	14/37/115/115	-
34	LMG	F	205	-	-	29/48/68/70	0/1/1/1
26	CLA	L	206	-	1/1/12/20	4/21/99/115	-
26	CLA	B	804	-	1/1/15/20	10/37/115/115	-
35	II0	i	313	-	-	13/21/67/67	0/2/2/2
26	CLA	A	807	1	1/1/15/20	11/37/115/115	-
26	CLA	c	311	-	1/1/11/20	6/13/91/115	-
26	CLA	k	609	19	1/1/13/20	9/28/106/115	-
36	KC2	k	613	-	-	12/15/71/71	-
26	CLA	n	608	-	1/1/15/20	16/37/115/115	-
26	CLA	B	801	38	1/1/15/20	17/37/115/115	-
26	CLA	a	311	14	1/1/11/20	8/17/95/115	-
26	CLA	n	609	23	1/1/15/20	11/37/115/115	-
26	CLA	n	610	-	1/1/14/20	11/31/109/115	-
35	II0	J	104	-	-	12/21/67/67	0/2/2/2
26	CLA	A	810	1	1/1/15/20	12/37/115/115	-
26	CLA	j	604	17	1/1/15/20	11/37/115/115	-
26	CLA	i	301	20	1/1/15/20	20/37/115/115	-
26	CLA	b	313	28	1/1/12/20	6/21/99/115	-
37	IHT	m	617	-	-	4/25/65/65	0/2/2/2
26	CLA	m	606	17	1/1/15/20	17/37/115/115	-
30	LMU	A	858	-	-	6/20/60/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	b	312	15	1/1/15/20	13/37/115/115	-
37	IHT	b	316	-	-	5/25/65/65	0/2/2/2
28	LHG	A	843	-	-	19/52/52/53	-
35	II0	k	616	-	-	10/21/67/67	0/2/2/2
26	CLA	l	313	18	1/1/13/20	9/27/105/115	-
29	WVN	J	101	-	-	19/29/63/63	0/2/2/2
26	CLA	B	816	2	1/1/15/20	16/37/115/115	-
29	WVN	B	845	-	-	2/29/63/63	0/2/2/2
26	CLA	A	840	38	1/1/15/20	10/37/115/115	-
31	SF4	C	102	3	-	-	0/6/5/5
26	CLA	B	803	2	1/1/15/20	16/37/115/115	-
28	LHG	A	855	-	-	23/40/40/53	-
26	CLA	d	302	21	1/1/14/20	17/34/112/115	-
26	CLA	A	836	1	1/1/15/20	10/37/115/115	-
26	CLA	B	834	2	1/1/15/20	11/37/115/115	-
26	CLA	d	310	21	1/1/10/20	4/8/86/115	-
31	SF4	C	101	3	-	-	0/6/5/5
26	CLA	l	301	18	1/1/15/20	12/37/115/115	-
26	CLA	j	602	17	1/1/12/20	9/24/102/115	-
26	CLA	B	822	38	1/1/15/20	19/37/115/115	-
26	CLA	h	306	16	1/1/15/20	9/37/115/115	-
28	LHG	J	105	26	-	14/37/37/53	-
26	CLA	n	602	23	1/1/12/20	5/19/97/115	-
28	LHG	b	318	-	-	32/53/53/53	-
29	WVN	A	857	-	-	18/29/63/63	0/2/2/2
26	CLA	c	306	13	1/1/12/20	6/22/100/115	-
26	CLA	c	303	13	1/1/12/20	6/21/99/115	-
35	II0	d	319	-	-	11/21/67/67	0/2/2/2
26	CLA	b	303	15	1/1/12/20	5/21/99/115	-
37	IHT	R	202	-	-	2/25/65/65	0/2/2/2
34	LMG	c	318	-	-	24/50/70/70	0/1/1/1
26	CLA	n	606	23	-	4/21/99/115	-
26	CLA	j	613	17	1/1/15/20	13/37/115/115	-
26	CLA	d	305	-	1/1/12/20	6/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	824	2	1/1/15/20	8/37/115/115	-
26	CLA	A	839	1	1/1/14/20	2/31/109/115	-
35	II0	l	314	-	-	12/21/67/67	0/2/2/2
29	WVN	I	101	-	-	17/29/63/63	0/2/2/2
26	CLA	h	304	-	1/1/15/20	16/37/115/115	-
37	IHT	j	616	-	-	3/25/65/65	0/2/2/2
26	CLA	L	202	9	1/1/11/20	8/18/96/115	-
26	CLA	L	203	9	1/1/15/20	4/37/115/115	-
28	LHG	l	318	26	-	9/36/36/53	-
26	CLA	i	308	28	1/1/11/20	7/15/93/115	-
26	CLA	A	823	1	1/1/13/20	9/25/103/115	-
26	CLA	k	608	19	1/1/15/20	14/37/115/115	-
37	IHT	n	617	-	-	3/25/65/65	0/2/2/2
36	KC2	s	401	12	-	5/15/71/71	-
37	IHT	c	315	-	-	0/25/65/65	0/2/2/2
26	CLA	B	817	2	1/1/15/20	10/37/115/115	-
26	CLA	k	604	-	-	9/37/115/115	-
35	II0	b	315	-	-	13/21/67/67	0/2/2/2
26	CLA	A	822	1	1/1/13/20	16/27/105/115	-
26	CLA	k	606	19	1/1/12/20	5/21/99/115	-
36	KC2	n	611	23	-	12/15/71/71	-
33	DGD	B	844	-	-	27/55/95/95	0/2/2/2
35	II0	b	317	-	-	0/21/67/67	0/2/2/2
26	CLA	h	305	16	1/1/12/20	6/21/99/115	-
29	WVN	i	315	-	-	15/29/63/63	0/2/2/2
26	CLA	B	819	2	1/1/15/20	19/37/115/115	-
36	KC2	l	312	18	-	5/15/71/71	-
26	CLA	B	806	2	1/1/15/20	12/37/115/115	-
26	CLA	m	609	17	1/1/14/20	12/31/109/115	-
26	CLA	b	309	34	1/1/15/20	6/37/115/115	-
26	CLA	c	305	13	1/1/15/20	4/37/115/115	-
35	II0	i	319	-	-	12/21/67/67	0/2/2/2
26	CLA	A	814	1	1/1/12/20	9/19/97/115	-
26	CLA	b	305	15	1/1/12/20	4/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	l	304	18	1/1/11/20	5/16/94/115	-
26	CLA	B	827	2	1/1/12/20	4/21/99/115	-
26	CLA	b	311	15	1/1/14/20	12/36/114/115	-
26	CLA	B	832	38	1/1/11/20	2/13/91/115	-
36	KC2	j	611	17	-	11/15/71/71	-
26	CLA	R	201	22	1/1/13/20	5/25/103/115	-
26	CLA	B	835	2	-	2/16/94/115	-
29	WVN	s	407	-	-	18/29/63/63	0/2/2/2
35	II0	d	314	-	-	0/21/67/67	0/2/2/2
35	II0	n	618	-	-	11/21/67/67	0/2/2/2
26	CLA	B	821	2	1/1/12/20	7/23/101/115	-
29	WVN	L	205	-	-	16/29/63/63	0/2/2/2
26	CLA	n	601	23	1/1/11/20	5/13/91/115	-
26	CLA	A	821	1	1/1/11/20	7/18/96/115	-
34	LMG	L	209	-	-	18/40/60/70	0/1/1/1
26	CLA	B	811	2	1/1/13/20	3/25/103/115	-
26	CLA	l	308	18	1/1/15/20	5/37/115/115	-
26	CLA	d	318	-	1/1/11/20	5/13/91/115	-
26	CLA	B	837	2	1/1/15/20	15/37/115/115	-
37	IHT	a	315	-	-	5/25/65/65	0/2/2/2
26	CLA	i	310	-	1/1/14/20	10/31/109/115	-
26	CLA	c	301	13	1/1/12/20	9/21/99/115	-
26	CLA	a	308	28	1/1/11/20	3/17/95/115	-
26	CLA	J	103	8	1/1/10/20	3/10/88/115	-
35	II0	l	302	-	-	12/21/67/67	0/2/2/2
26	CLA	A	835	1	1/1/15/20	11/37/115/115	-
26	CLA	k	614	19	1/1/12/20	10/21/99/115	-
26	CLA	A	851	38	1/1/15/20	3/37/115/115	-
26	CLA	j	601	17	1/1/15/20	14/37/115/115	-
35	II0	c	313	-	-	12/21/67/67	0/2/2/2
26	CLA	B	833	2	1/1/13/20	5/25/103/115	-
26	CLA	m	607	17	1/1/12/20	5/21/99/115	-
37	IHT	b	301	-	-	4/25/65/65	0/2/2/2
26	CLA	B	838	2	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	n	613	23	1/1/12/20	8/21/99/115	-
35	II0	i	316	-	-	13/21/67/67	0/2/2/2
29	WVN	F	203	-	-	17/29/63/63	0/2/2/2
26	CLA	m	612	38	1/1/12/20	7/21/99/115	-
26	CLA	a	301	14	1/1/15/20	16/37/115/115	-
26	CLA	B	815	2	1/1/13/20	8/25/103/115	-
36	KC2	c	310	13	-	7/15/71/71	-
26	CLA	A	837	1	1/1/15/20	14/37/115/115	-
26	CLA	i	305	20	1/1/12/20	7/21/99/115	-
28	LHG	L	208	-	-	23/49/49/53	-
26	CLA	A	828	1	1/1/15/20	11/37/115/115	-
29	WVN	l	303	-	-	16/29/63/63	0/2/2/2

The worst 5 of 2797 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	k	615	II0	C14-C10	20.87	1.58	1.34
35	m	616	II0	C13-C09	19.92	1.57	1.34
35	h	310	II0	C13-C09	19.86	1.57	1.34
35	h	312	II0	C13-C09	19.71	1.56	1.34
35	c	316	II0	C14-C10	19.66	1.56	1.34

The worst 5 of 3776 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	312	II0	C23-C21-C09	-26.03	109.52	175.43
35	c	316	II0	C23-C21-C09	-26.02	109.55	175.43
35	n	618	II0	C23-C21-C09	-25.82	110.04	175.43
35	h	310	II0	C23-C21-C09	-25.69	110.38	175.43
35	j	614	II0	C23-C21-C09	-25.41	111.10	175.43

5 of 214 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	801	CL0	NA
25	A	801	CL0	ND
26	A	802	CLA	ND
26	A	803	CLA	ND
26	A	804	CLA	ND

5 of 3811 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	801	CL0	C1-C2-C3-C4
26	A	804	CLA	CHA-CBD-CGD-O1D
26	A	804	CLA	CHA-CBD-CGD-O2D
26	A	804	CLA	CAD-CBD-CGD-O1D
26	A	809	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

208 monomers are involved in 424 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	n	614	II0	1	0
34	Q	301	LMG	3	0
26	m	613	CLA	5	0
26	d	304	CLA	1	0
26	A	824	CLA	2	0
26	c	307	CLA	1	0
26	B	829	CLA	1	0
26	j	609	CLA	1	0
26	A	817	CLA	2	0
26	c	308	CLA	3	0
26	j	608	CLA	2	0
26	B	809	CLA	1	0
26	A	804	CLA	4	0
27	B	843	PQN	2	0
34	n	620	LMG	3	0
26	h	307	CLA	2	0
26	d	306	CLA	1	0
26	F	201	CLA	2	0
25	A	801	CL0	4	0
26	A	812	CLA	4	0
26	n	607	CLA	3	0
26	B	802	CLA	3	0
27	A	842	PQN	4	0
28	A	849	LHG	2	0
26	A	803	CLA	4	0
26	B	842	CLA	4	0
34	F	206	LMG	1	0
28	s	409	LHG	3	0
36	s	404	KC2	1	0
26	i	307	CLA	1	0
26	A	834	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	852	CLA	3	0
26	b	307	CLA	1	0
26	d	313	CLA	4	0
26	k	610	CLA	1	0
26	h	308	CLA	1	0
26	A	808	CLA	1	0
28	n	619	LHG	1	0
26	B	841	CLA	2	0
26	B	831	CLA	3	0
28	A	844	LHG	2	0
26	A	831	CLA	4	0
26	A	856	CLA	1	0
26	A	826	CLA	2	0
26	B	820	CLA	2	0
26	a	303	CLA	1	0
26	A	841	CLA	7	0
26	B	807	CLA	4	0
26	l	305	CLA	3	0
26	b	310	CLA	5	0
26	B	818	CLA	2	0
26	B	810	CLA	3	0
26	h	313	CLA	3	0
26	A	830	CLA	3	0
26	B	825	CLA	5	0
26	A	806	CLA	1	0
26	s	402	CLA	2	0
26	A	816	CLA	4	0
26	l	309	CLA	4	0
34	c	319	LMG	1	0
26	A	809	CLA	1	0
26	A	805	CLA	6	0
26	m	602	CLA	5	0
26	a	307	CLA	1	0
26	k	602	CLA	2	0
26	h	301	CLA	6	0
26	n	604	CLA	1	0
26	d	308	CLA	1	0
26	B	836	CLA	4	0
26	A	811	CLA	1	0
26	m	603	CLA	1	0
36	d	312	KC2	3	0
26	a	304	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	852	LMU	1	0
26	c	302	CLA	1	0
26	A	833	CLA	3	0
26	A	838	CLA	2	0
26	A	819	CLA	1	0
26	c	304	CLA	2	0
26	L	204	CLA	3	0
35	b	314	II0	1	0
26	A	827	CLA	7	0
26	A	832	CLA	4	0
26	a	310	CLA	1	0
26	i	304	CLA	1	0
26	k	607	CLA	1	0
28	c	320	LHG	4	0
26	B	808	CLA	4	0
26	A	829	CLA	7	0
26	a	306	CLA	1	0
26	j	603	CLA	3	0
26	i	311	CLA	3	0
26	B	826	CLA	3	0
26	A	818	CLA	5	0
26	m	601	CLA	2	0
26	s	406	CLA	3	0
34	b	319	LMG	1	0
26	m	604	CLA	1	0
26	j	607	CLA	1	0
26	j	610	CLA	3	0
30	i	300	LMU	2	0
26	B	840	CLA	4	0
26	c	309	CLA	1	0
26	A	802	CLA	4	0
26	B	830	CLA	4	0
26	m	608	CLA	2	0
26	F	202	CLA	2	0
28	b	302	LHG	2	0
26	i	306	CLA	1	0
26	m	610	CLA	2	0
26	A	825	CLA	2	0
26	B	812	CLA	3	0
26	k	605	CLA	1	0
26	B	814	CLA	5	0
26	b	304	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	839	CLA	1	0
26	B	828	CLA	4	0
26	B	823	CLA	4	0
33	j	618	DGD	3	0
26	B	805	CLA	1	0
26	B	813	CLA	1	0
26	b	306	CLA	3	0
26	A	815	CLA	1	0
26	k	603	CLA	1	0
26	l	306	CLA	3	0
28	B	851	LHG	2	0
26	c	312	CLA	2	0
34	F	205	LMG	1	0
26	L	206	CLA	1	0
26	B	804	CLA	3	0
26	A	807	CLA	1	0
26	k	609	CLA	3	0
26	n	608	CLA	6	0
26	B	801	CLA	3	0
26	a	311	CLA	1	0
26	n	609	CLA	2	0
26	n	610	CLA	2	0
26	A	810	CLA	2	0
26	j	604	CLA	2	0
26	i	301	CLA	1	0
26	b	313	CLA	1	0
30	A	858	LMU	2	0
26	b	312	CLA	4	0
28	A	843	LHG	1	0
26	l	313	CLA	3	0
26	B	816	CLA	2	0
26	A	840	CLA	2	0
31	C	102	SF4	1	0
26	B	803	CLA	4	0
28	A	855	LHG	2	0
26	d	302	CLA	3	0
26	A	836	CLA	6	0
26	B	834	CLA	3	0
26	l	301	CLA	3	0
26	B	822	CLA	5	0
26	h	306	CLA	1	0
28	b	318	LHG	1	0

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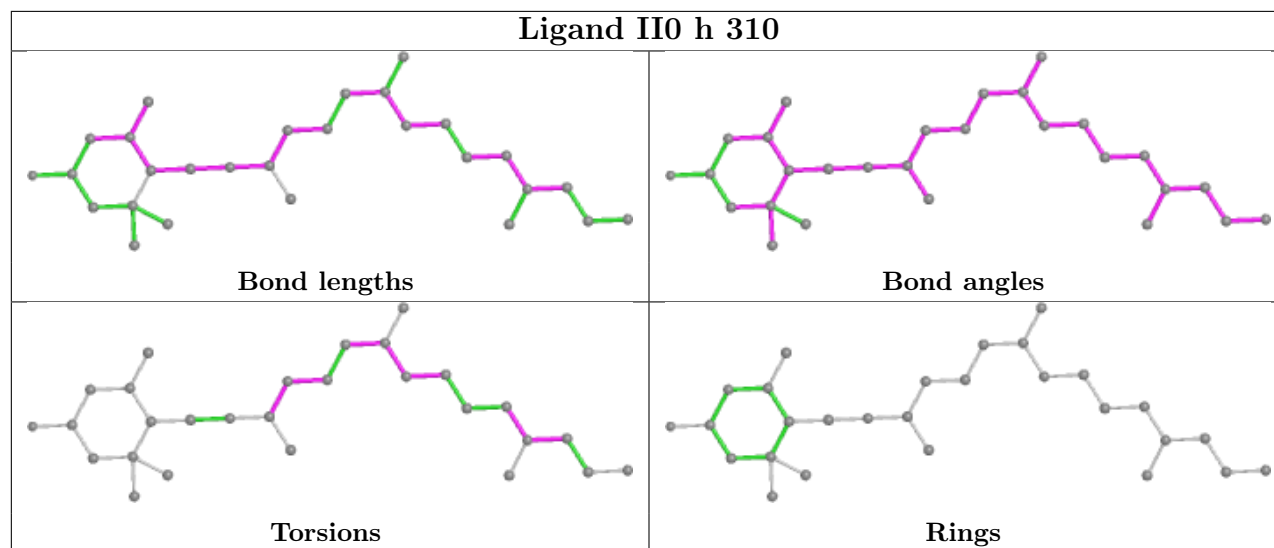
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	306	CLA	1	0
26	c	303	CLA	1	0
35	d	319	II0	1	0
26	j	613	CLA	2	0
26	B	824	CLA	2	0
26	A	839	CLA	2	0
26	h	304	CLA	2	0
26	L	202	CLA	1	0
26	L	203	CLA	4	0
26	A	823	CLA	4	0
26	k	608	CLA	1	0
36	s	401	KC2	1	0
26	B	817	CLA	6	0
26	k	604	CLA	2	0
26	A	822	CLA	4	0
36	n	611	KC2	1	0
33	B	844	DGD	6	0
26	h	305	CLA	2	0
26	B	819	CLA	3	0
26	B	806	CLA	2	0
26	m	609	CLA	1	0
26	b	309	CLA	6	0
26	c	305	CLA	1	0
35	i	319	II0	1	0
26	A	814	CLA	2	0
26	l	304	CLA	1	0
26	B	827	CLA	3	0
26	b	311	CLA	1	0
26	B	832	CLA	1	0
26	R	201	CLA	4	0
26	B	835	CLA	3	0
26	B	821	CLA	3	0
34	L	209	LMG	2	0
26	B	811	CLA	2	0
26	l	308	CLA	2	0
26	B	837	CLA	5	0
26	c	301	CLA	2	0
26	a	308	CLA	1	0
26	J	103	CLA	1	0
26	A	835	CLA	4	0
26	k	614	CLA	1	0
26	A	851	CLA	2	0

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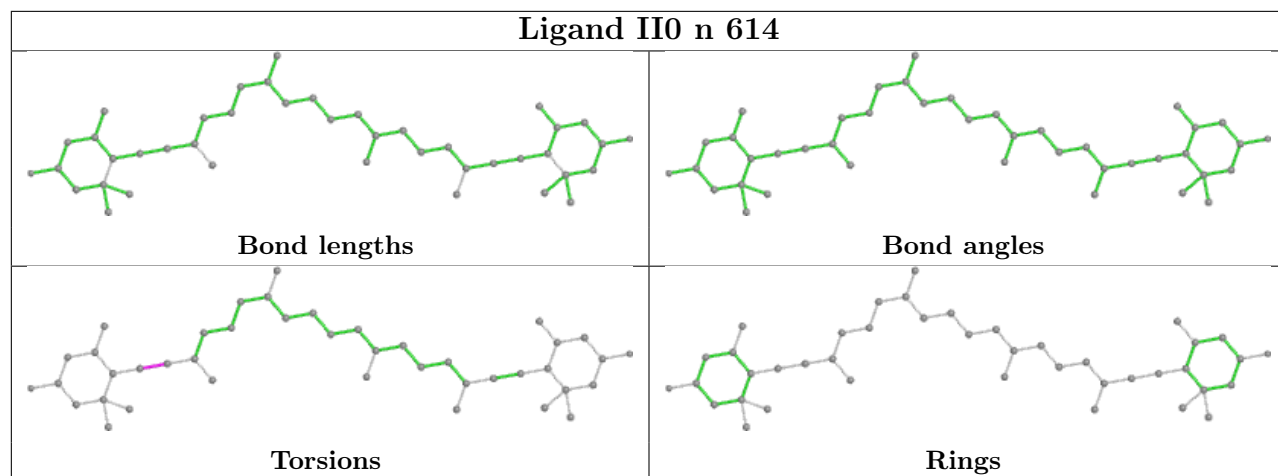
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	833	CLA	3	0
26	m	607	CLA	2	0
37	b	301	IHT	1	0
26	B	838	CLA	2	0
26	n	613	CLA	2	0
26	a	301	CLA	7	0
26	B	815	CLA	3	0
26	A	837	CLA	7	0
26	A	828	CLA	3	0

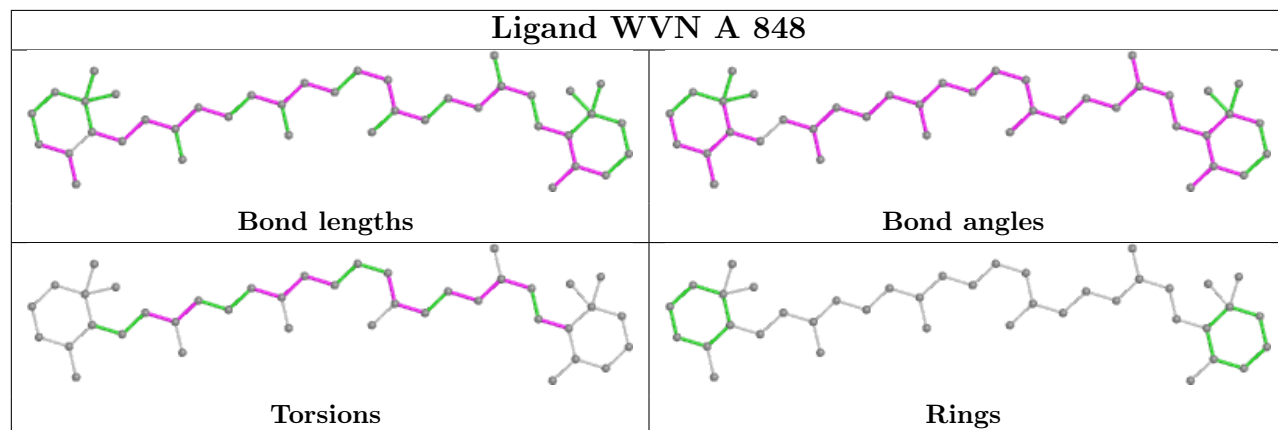
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



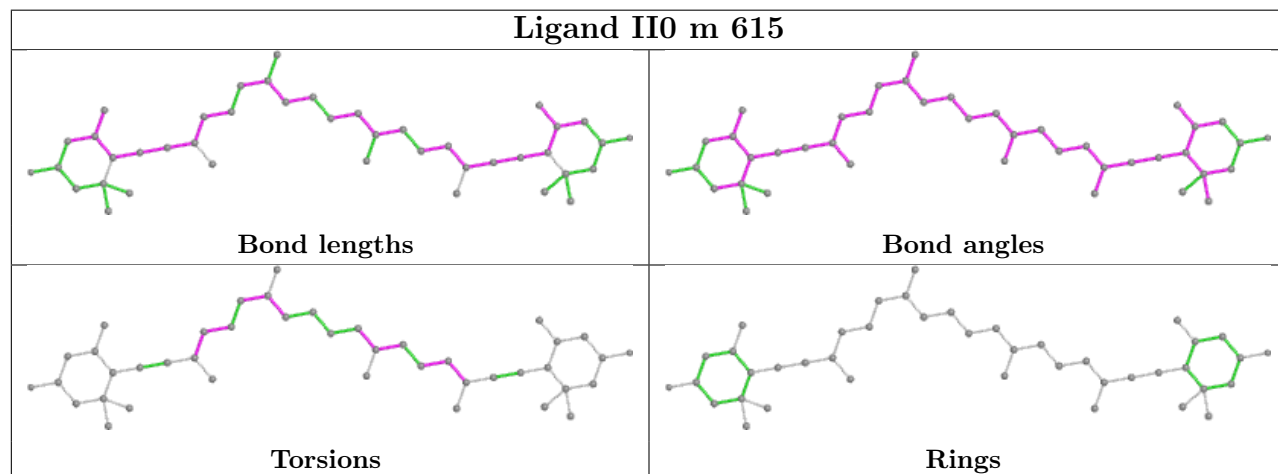
Ligand II0 n 614

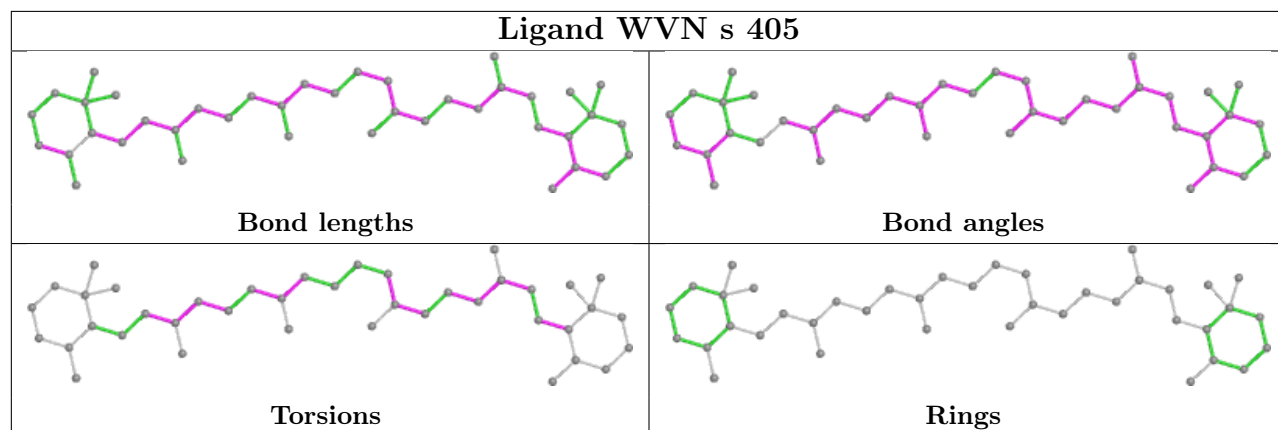
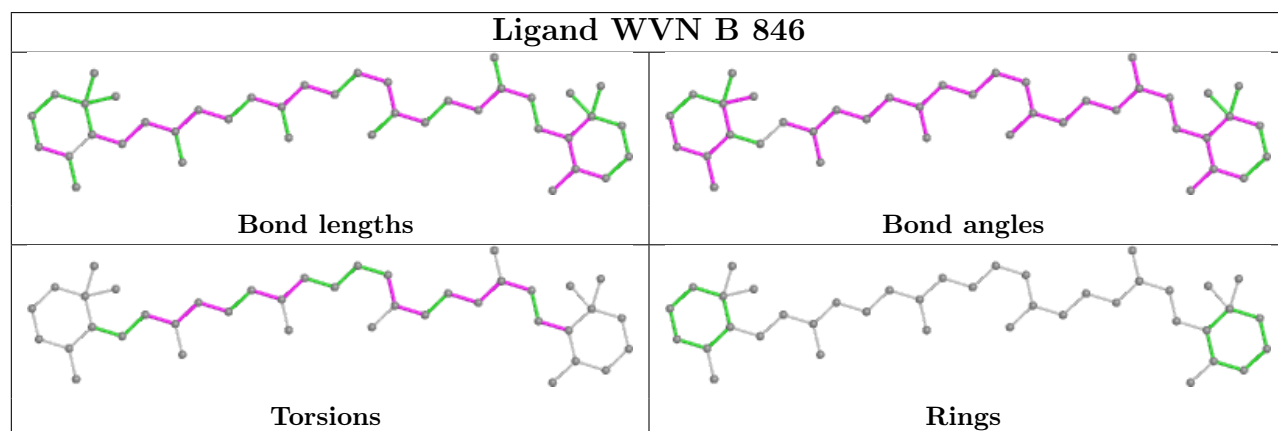
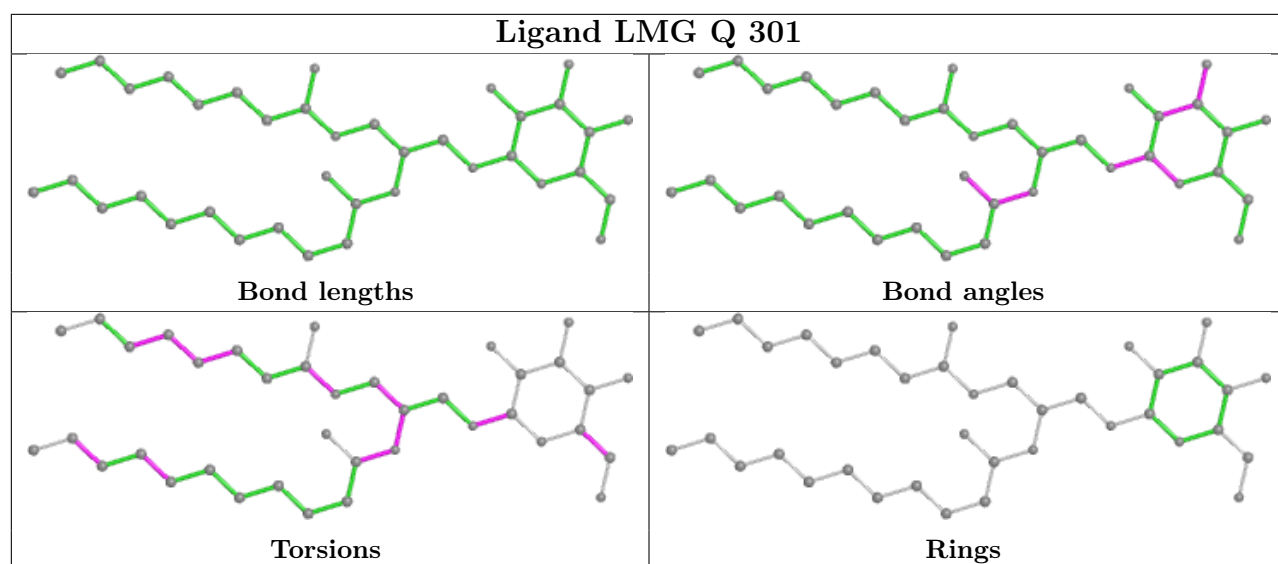


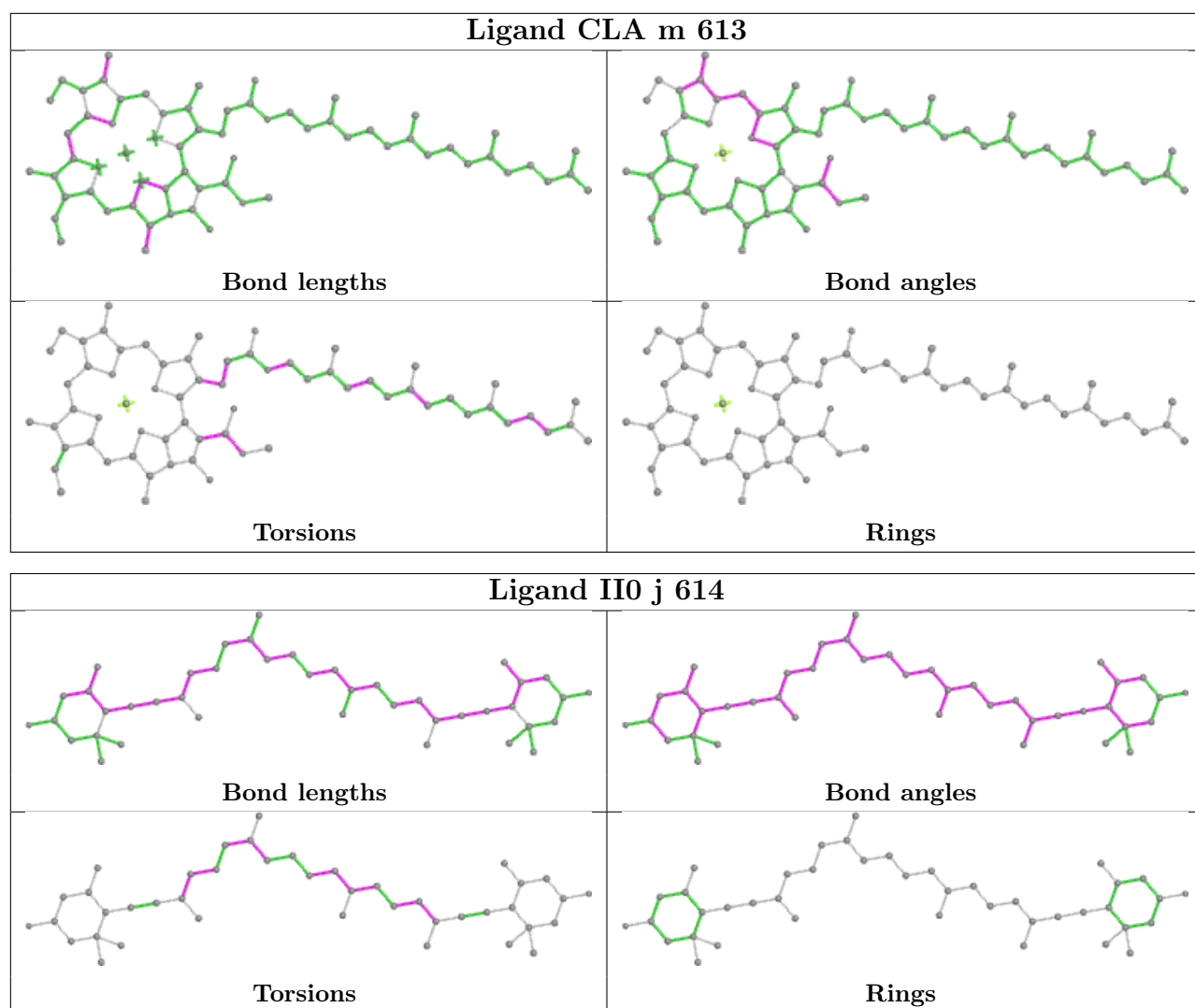
Ligand WVN A 848



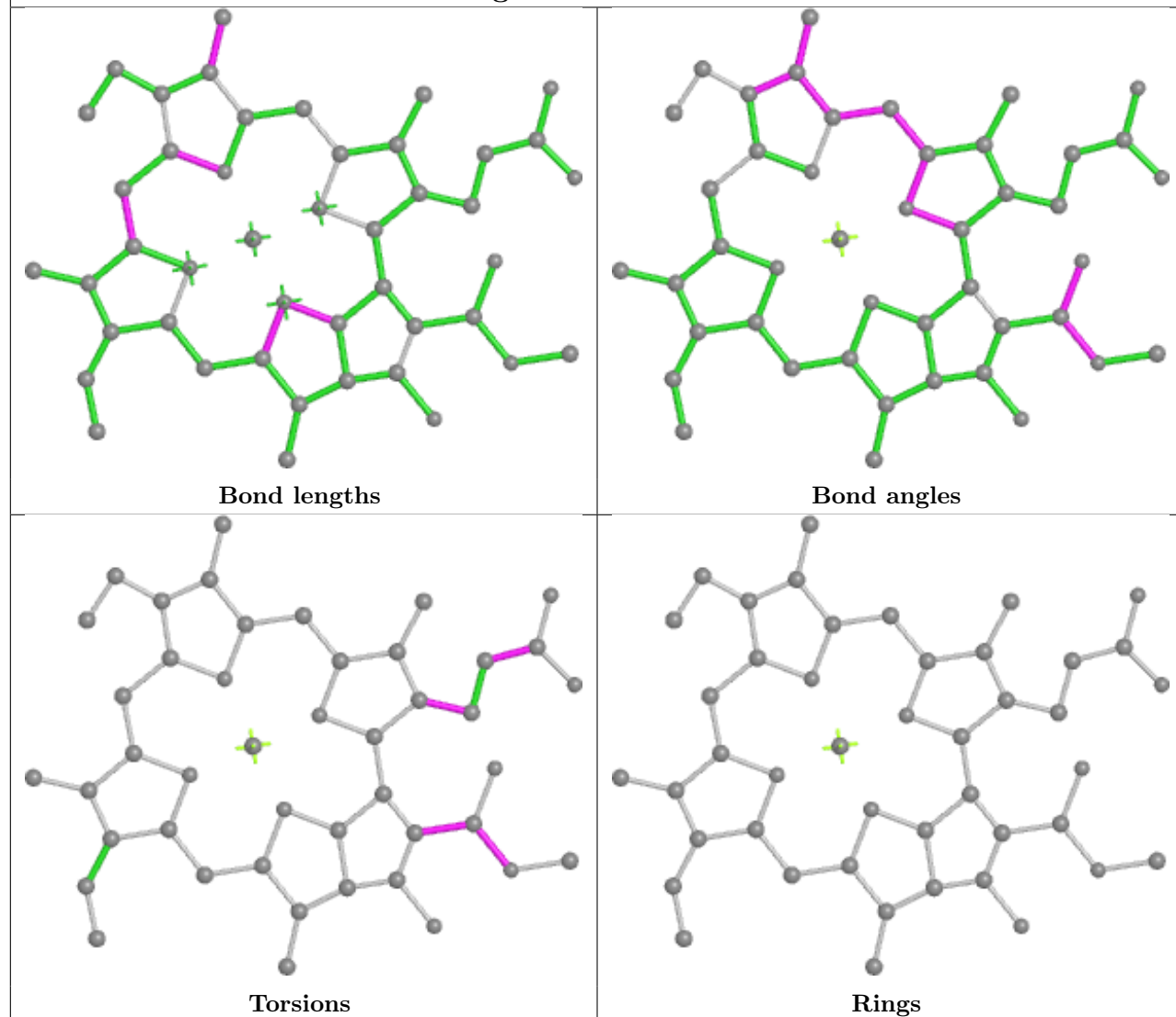
Ligand II0 m 615



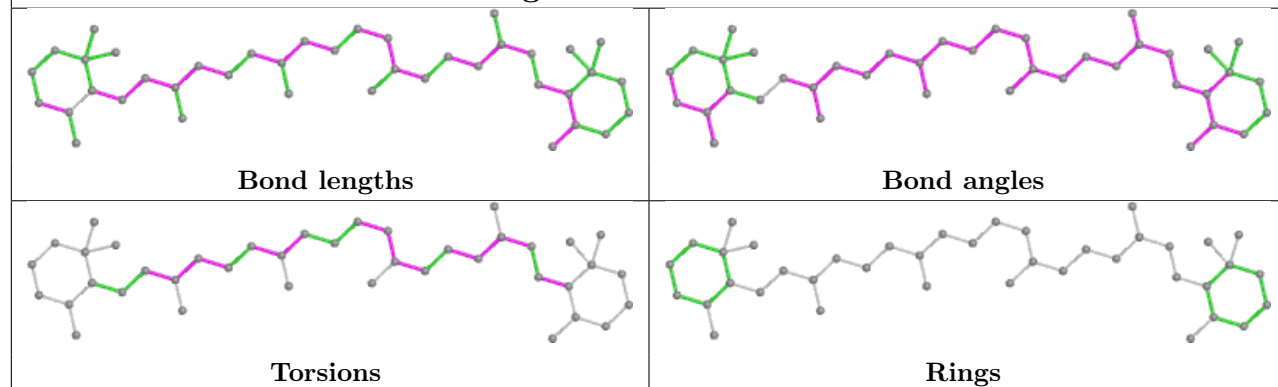


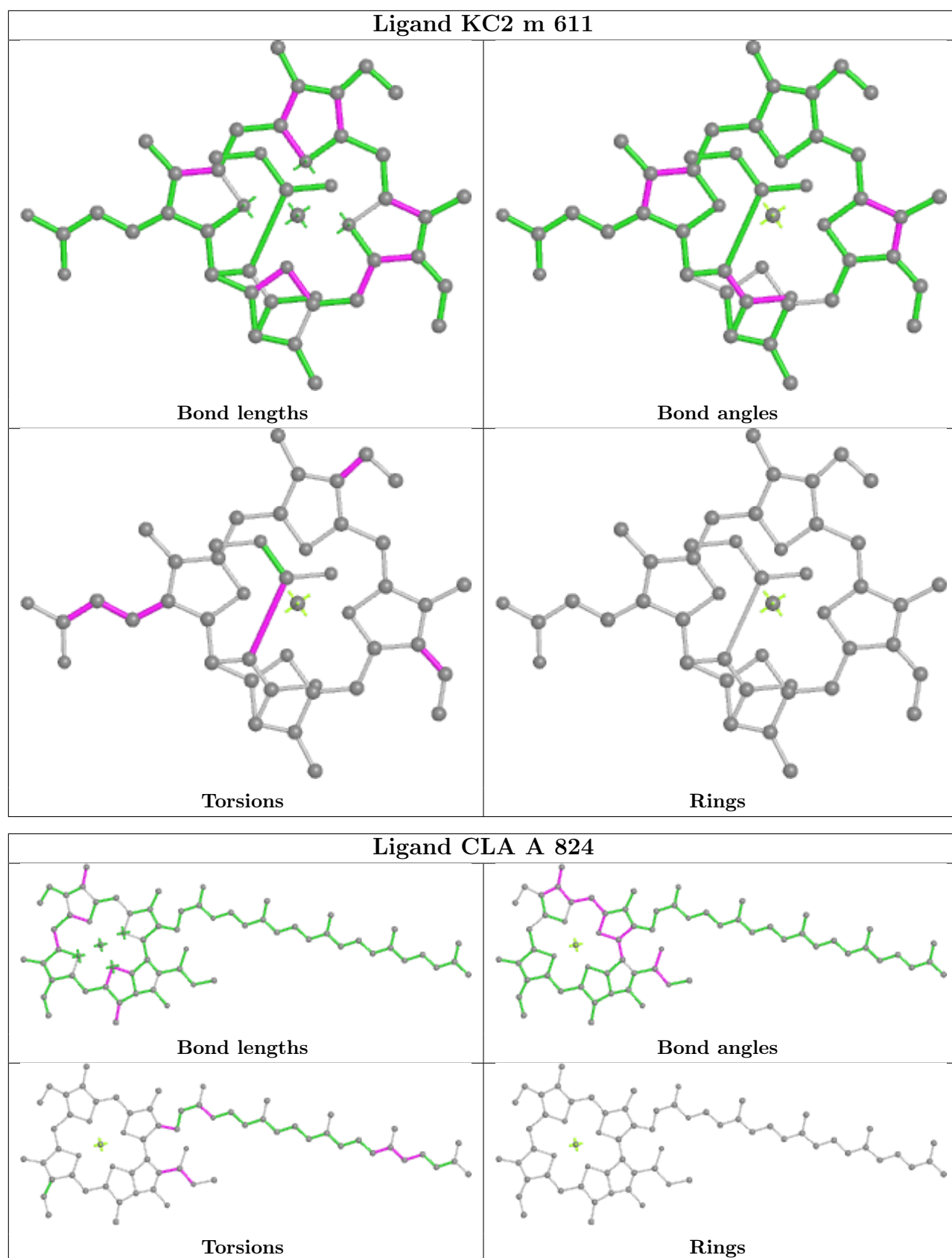


Ligand CLA d 304

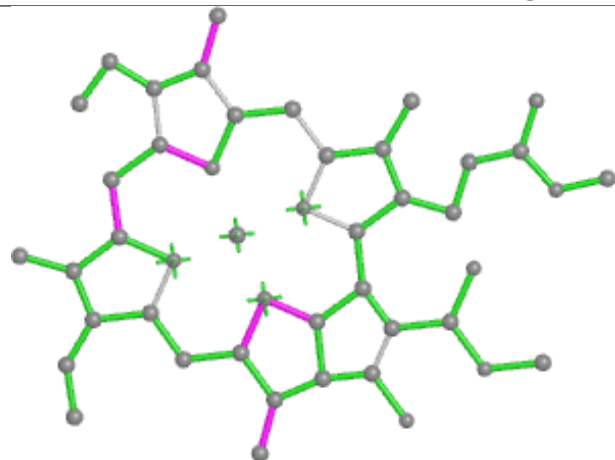


Ligand WVN K 102

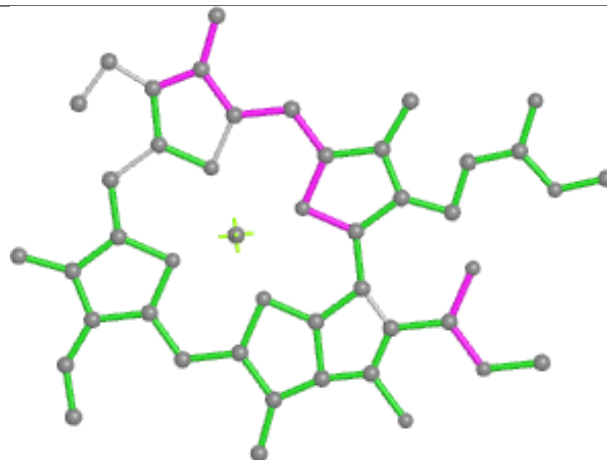




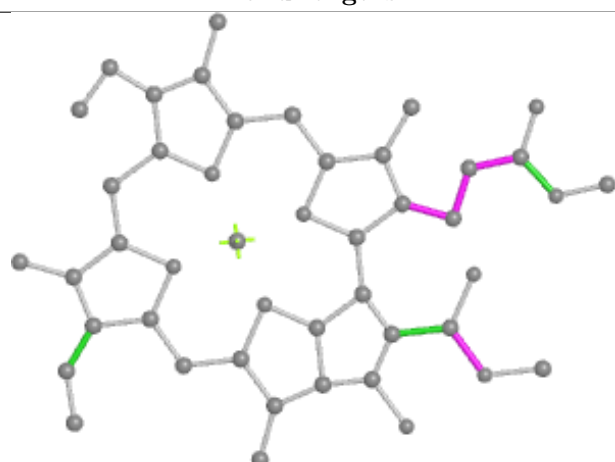
Ligand CLA c 307



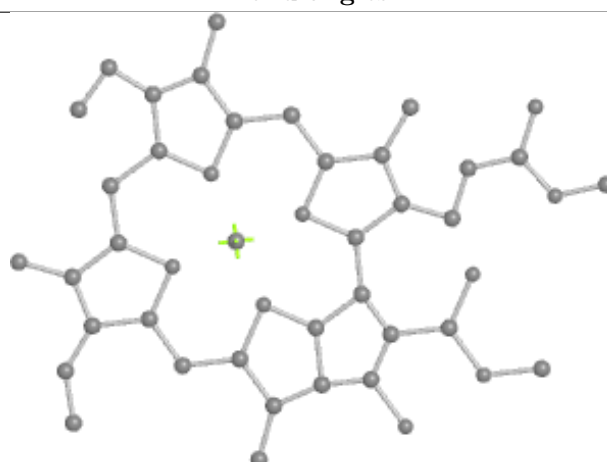
Bond lengths



Bond angles

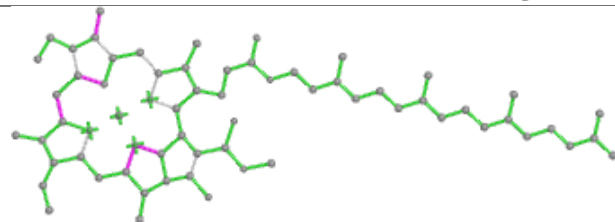


Torsions

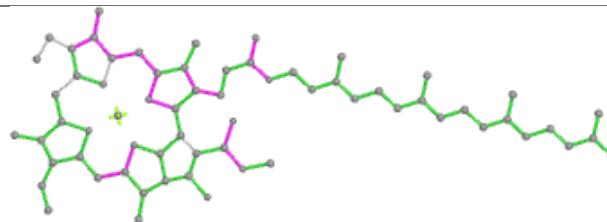


Rings

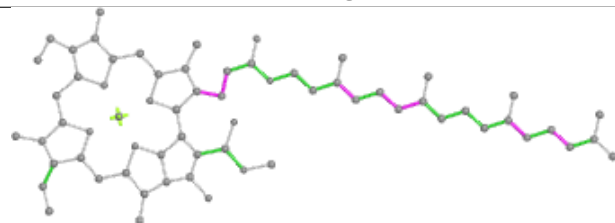
Ligand CLA B 829



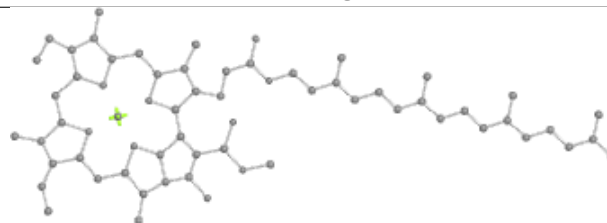
Bond lengths



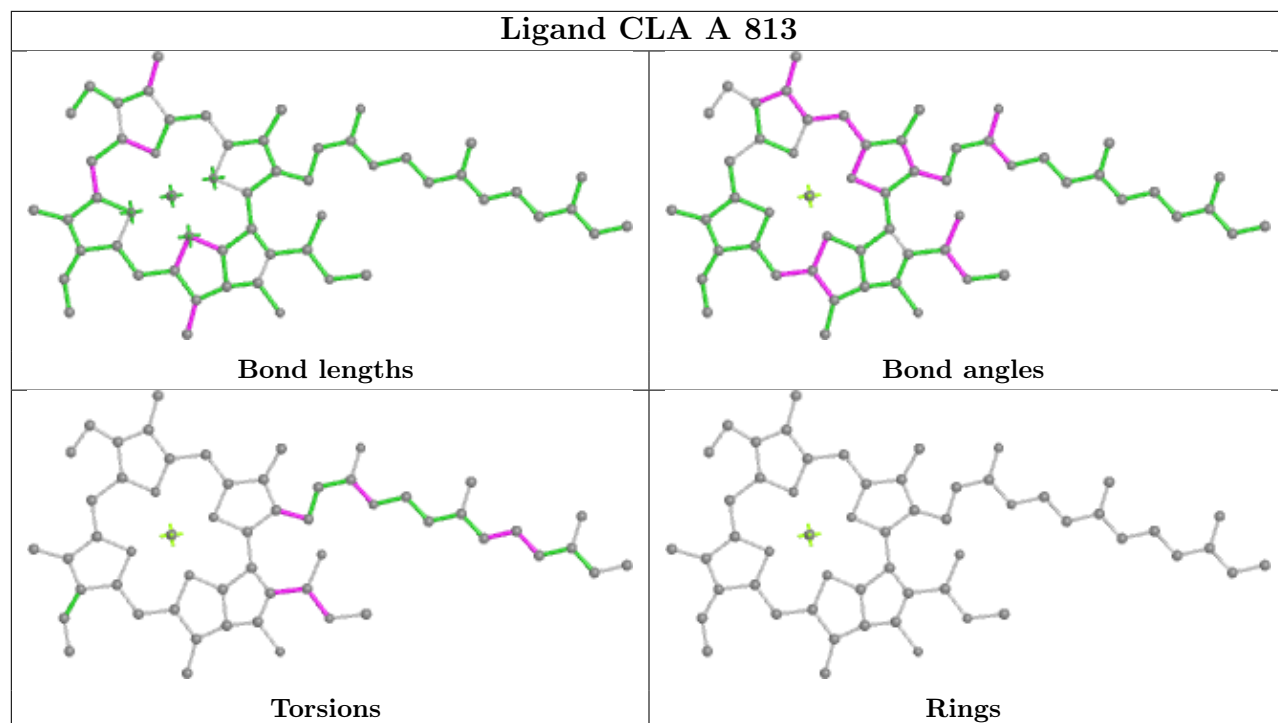
Bond angles



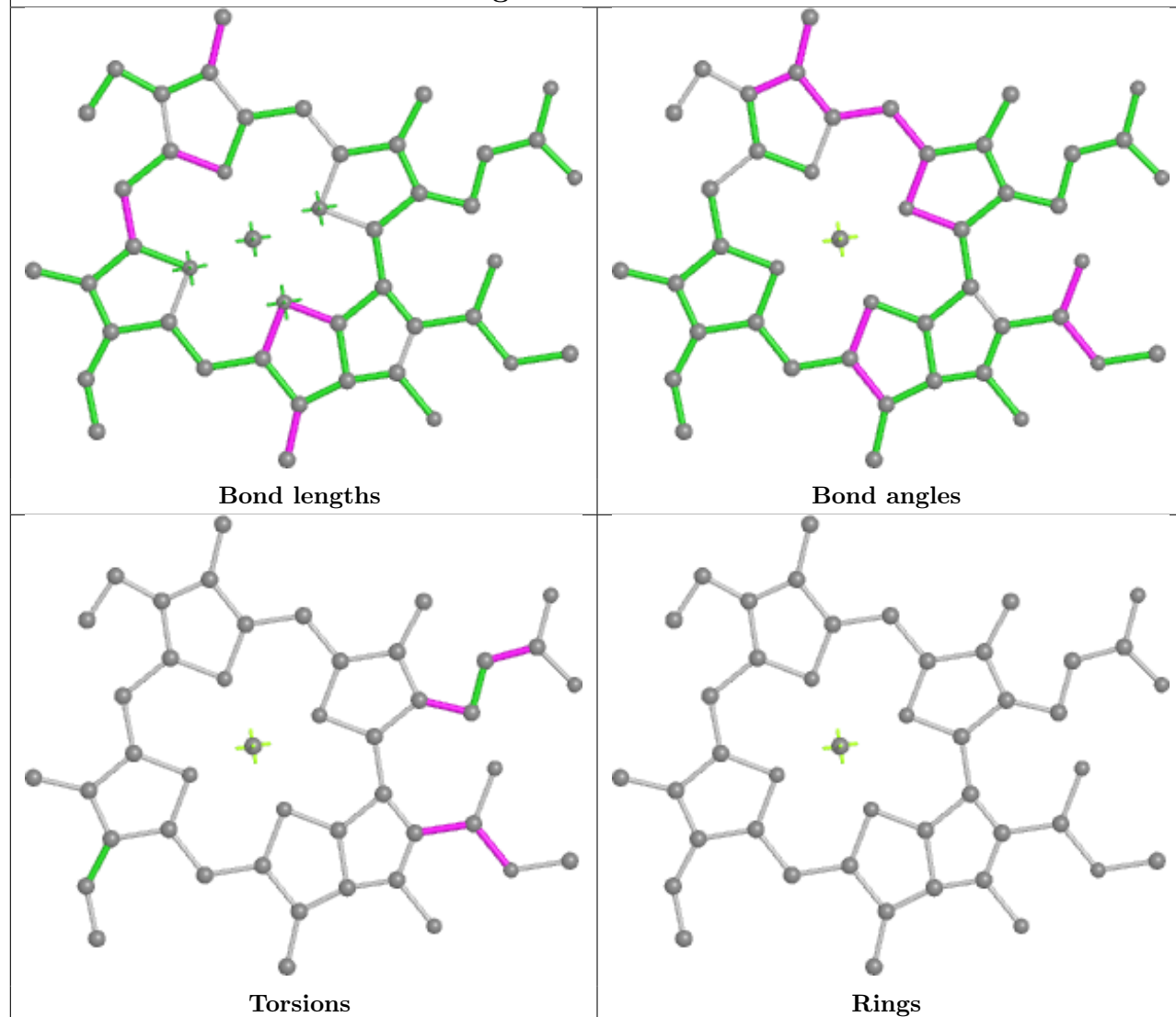
Torsions



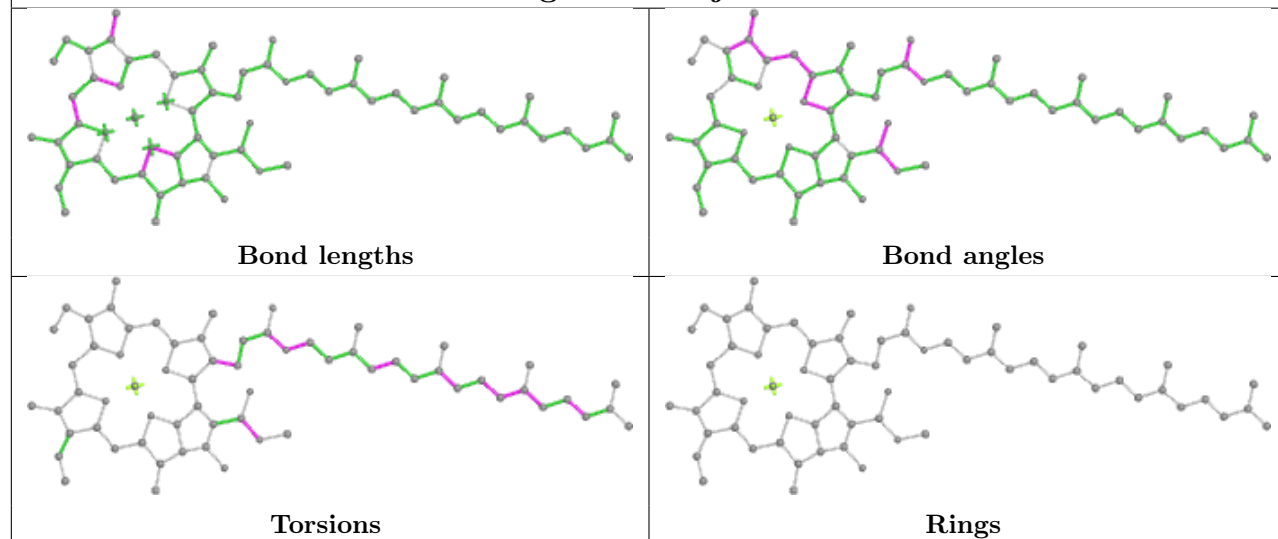
Rings



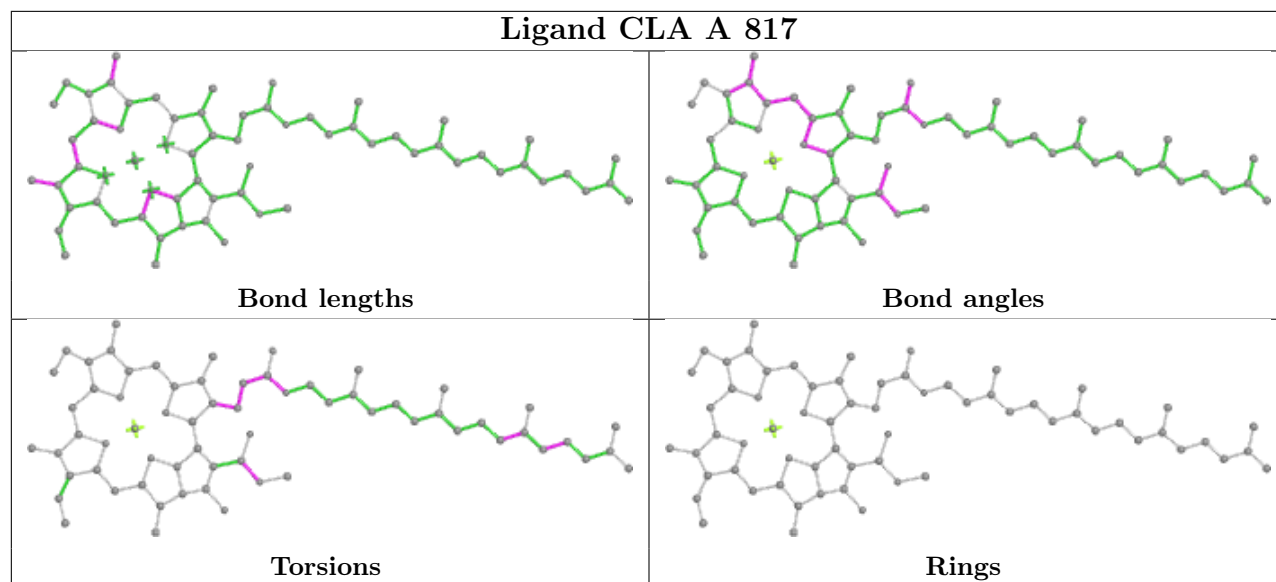
Ligand CLA d 307



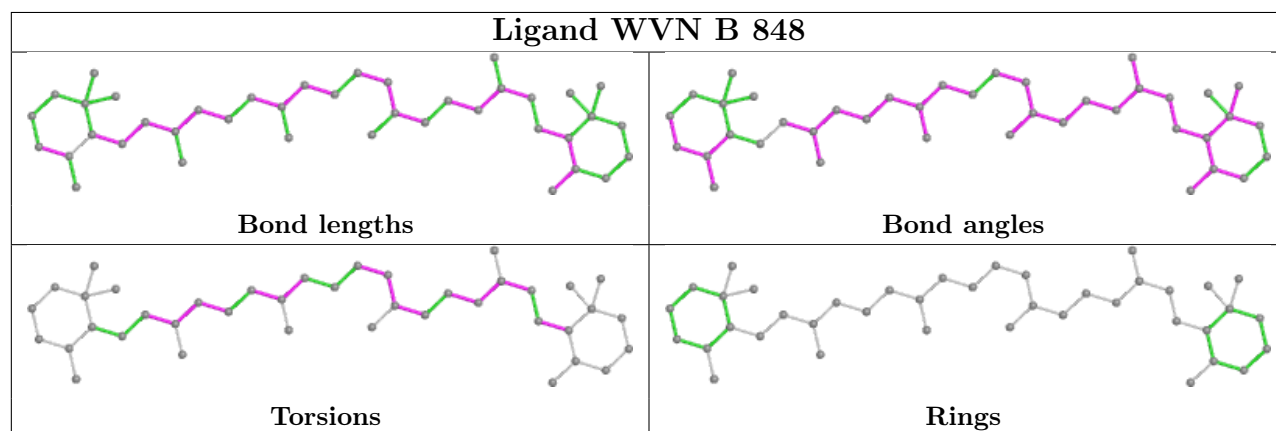
Ligand CLA j 609



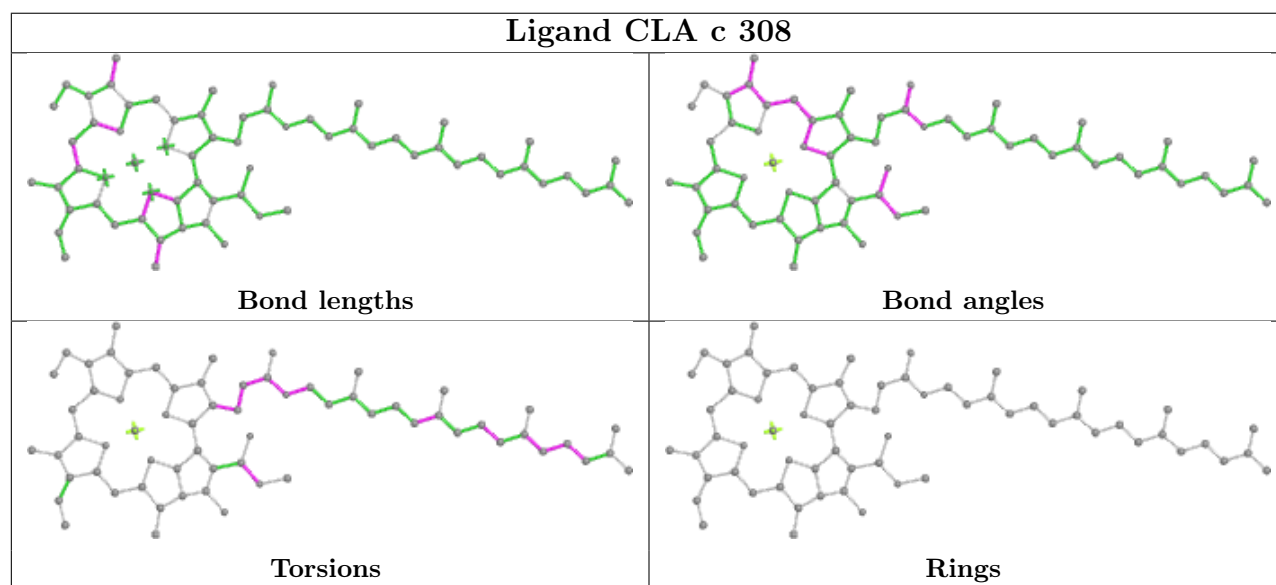
Ligand CLA A 817

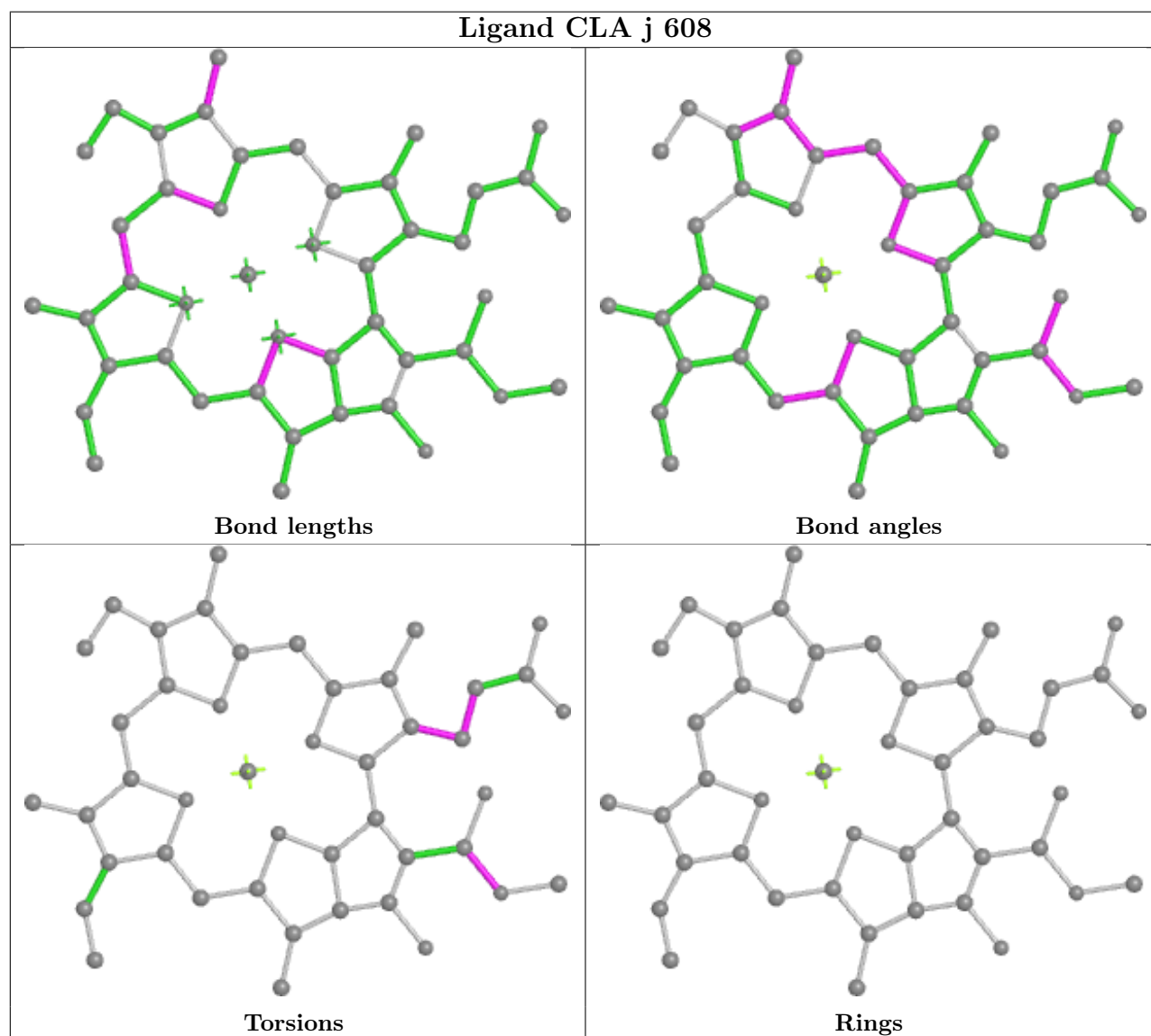
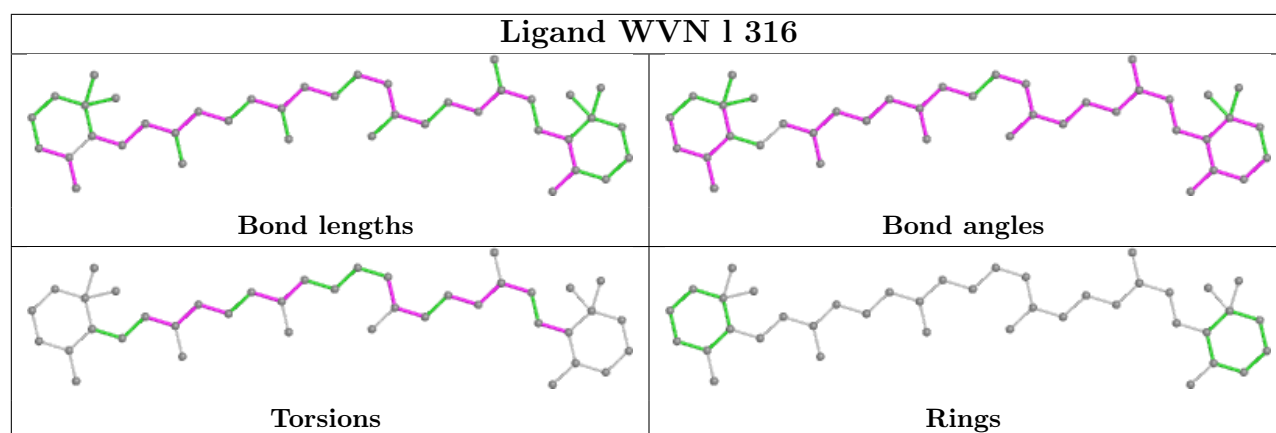


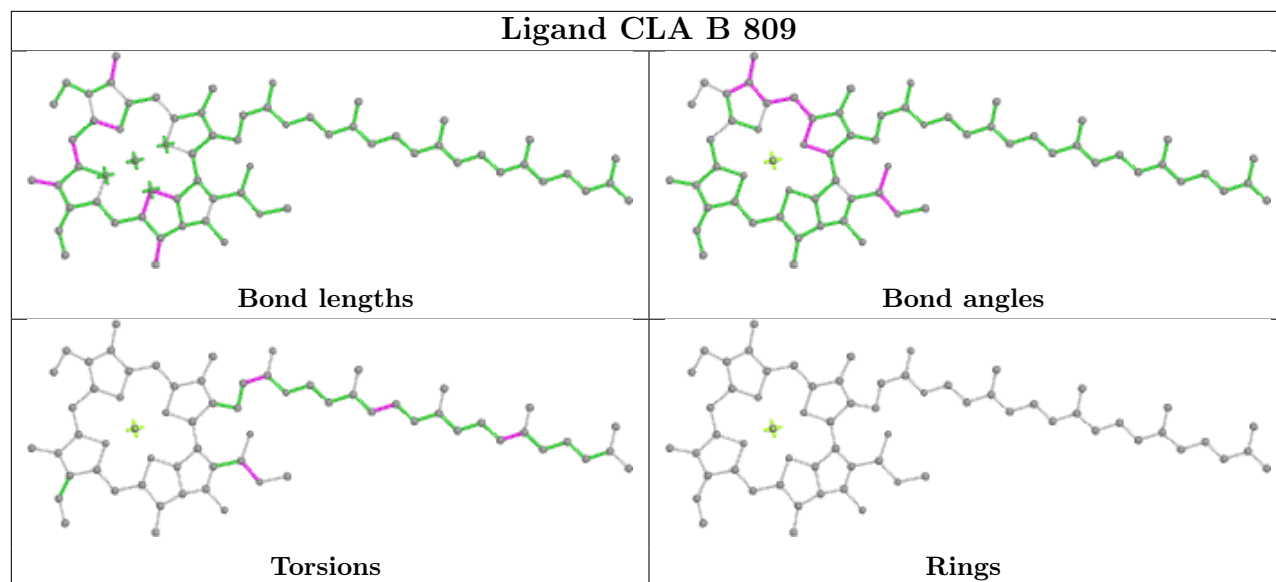
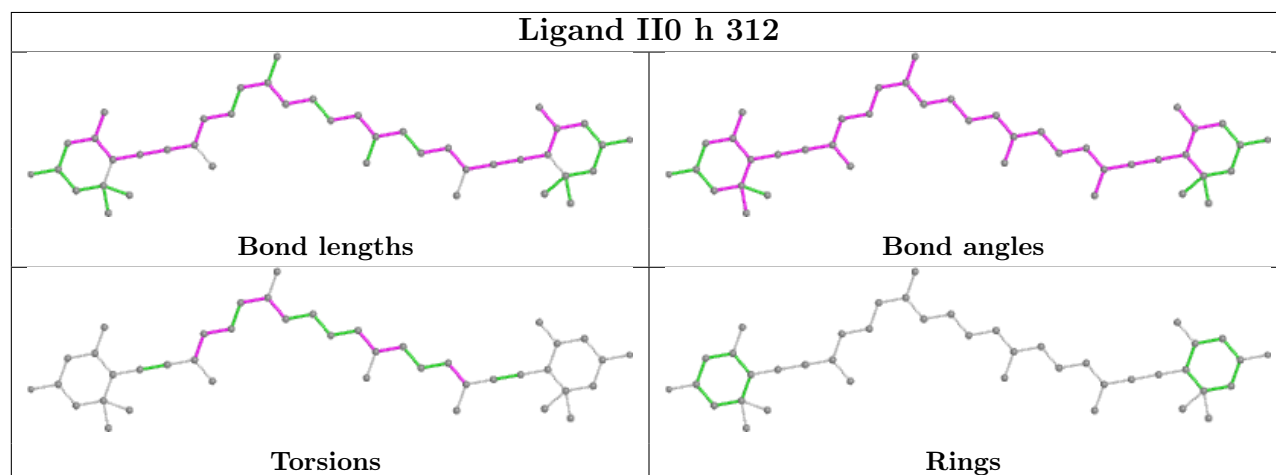
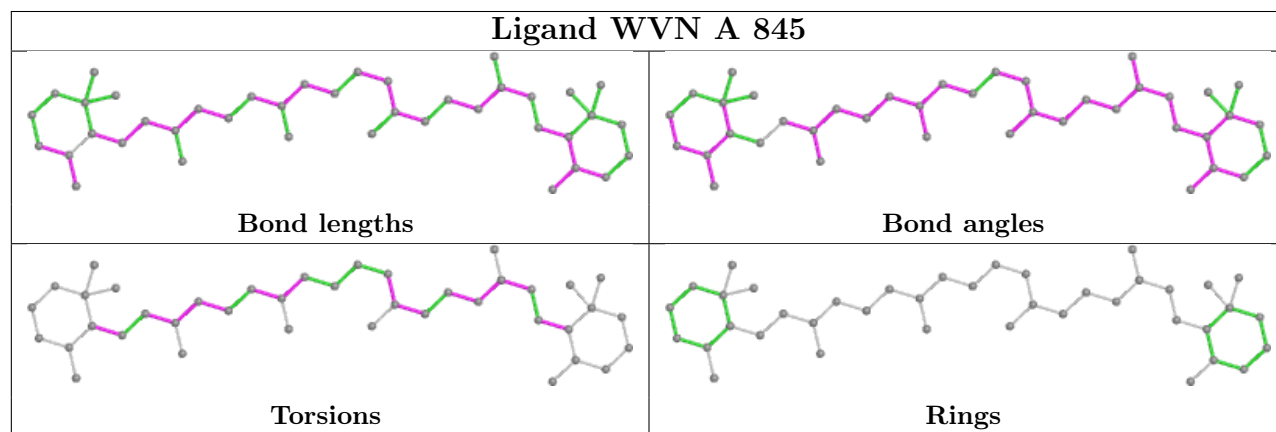
Ligand WVN B 848

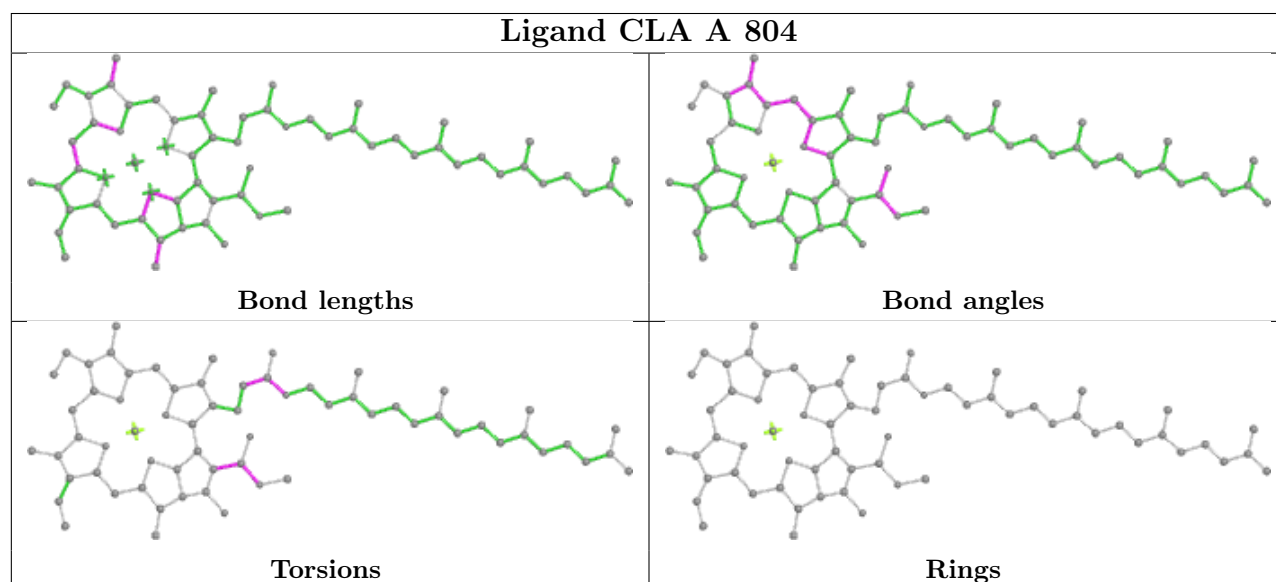
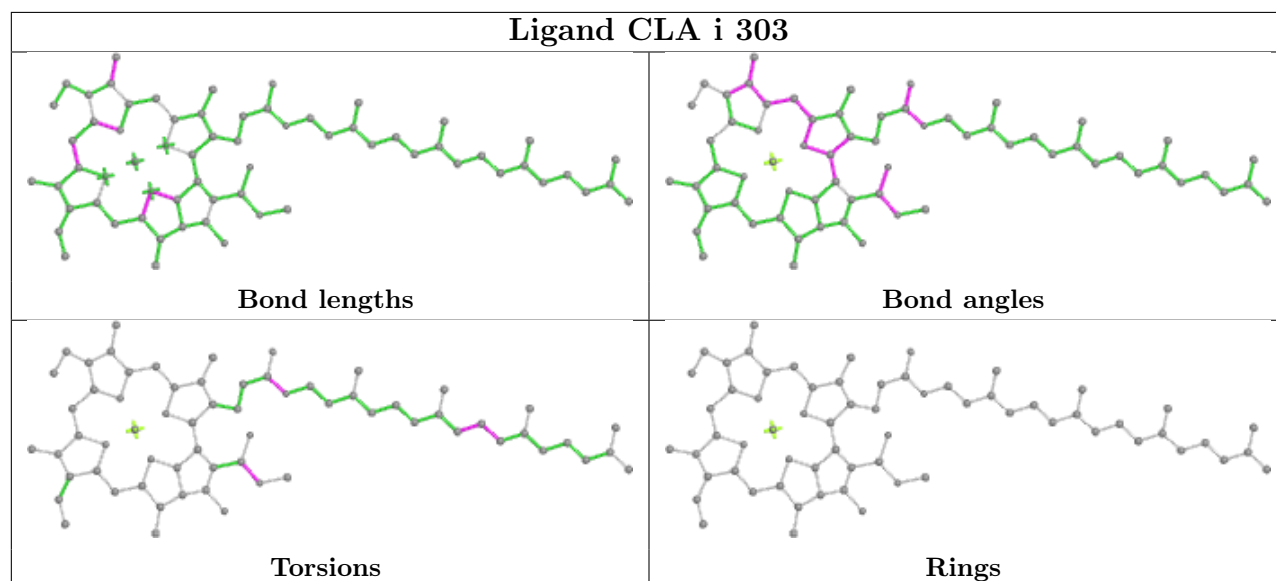
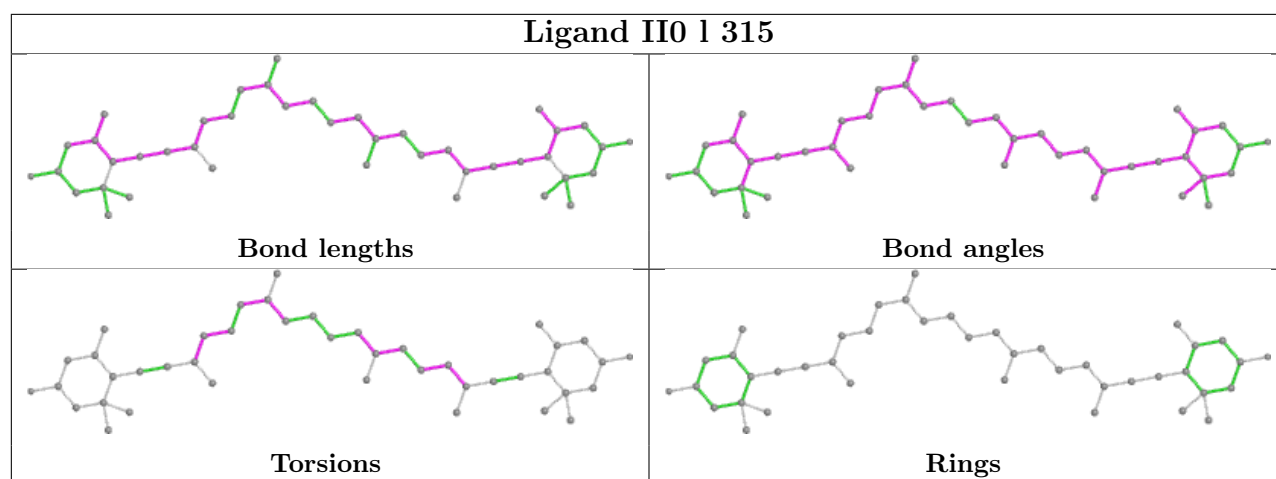


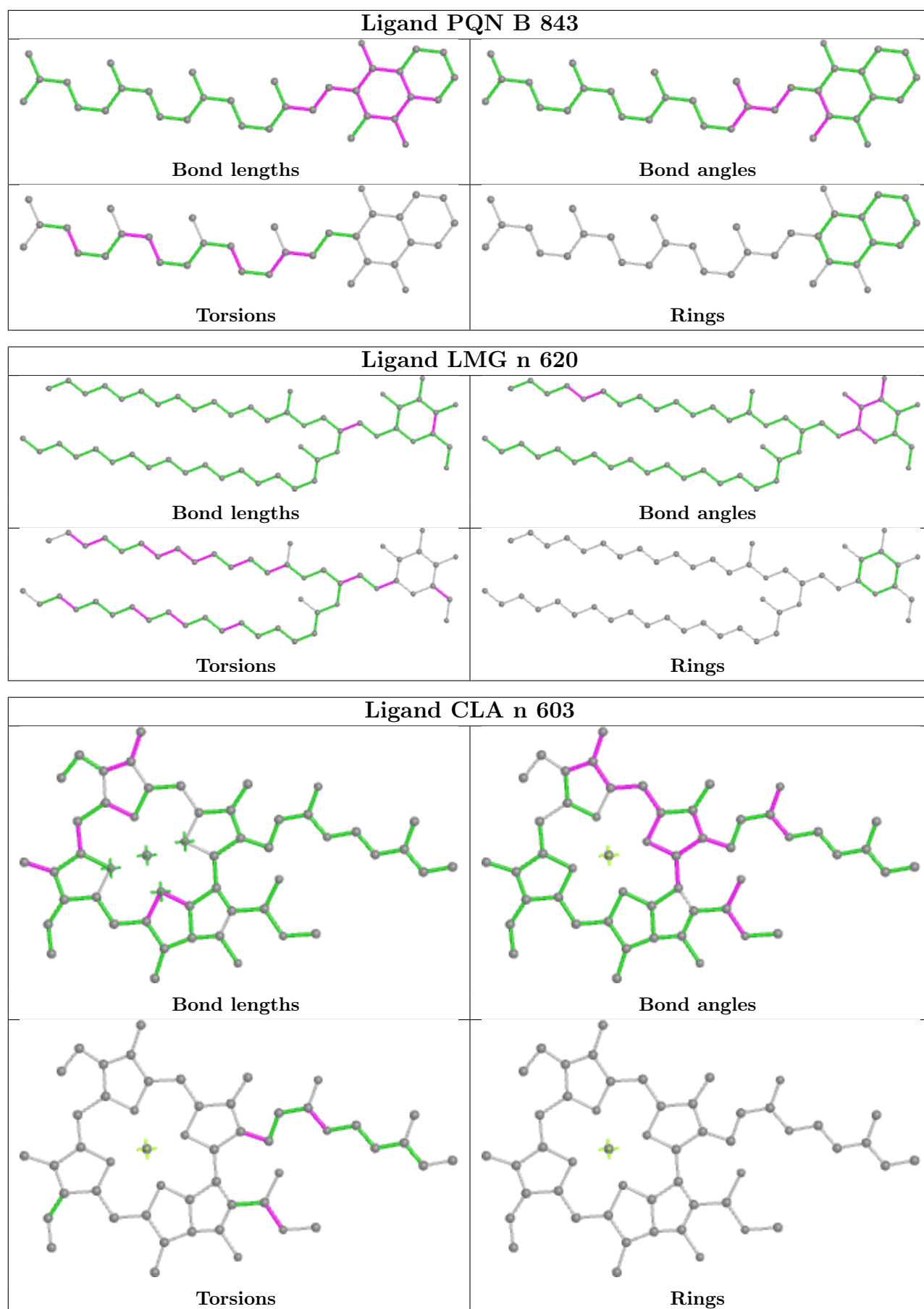
Ligand CLA c 308



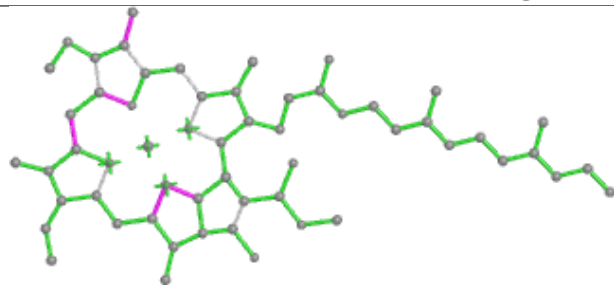


Ligand CLA B 809**Ligand II0 h 312****Ligand WVN A 845**

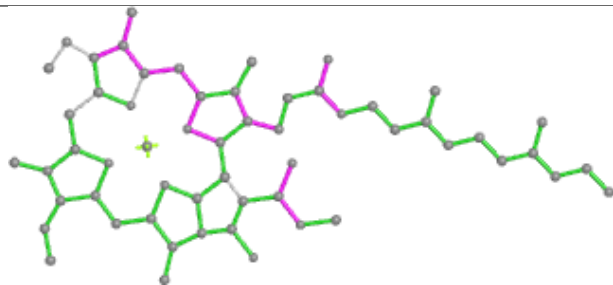




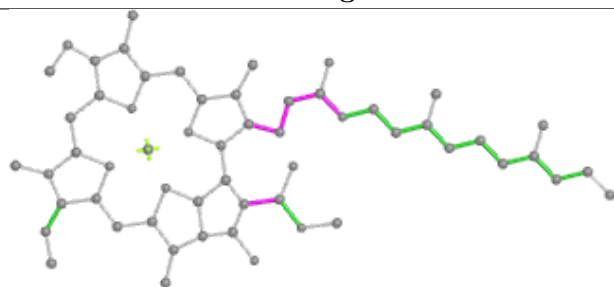
Ligand CLA h 307



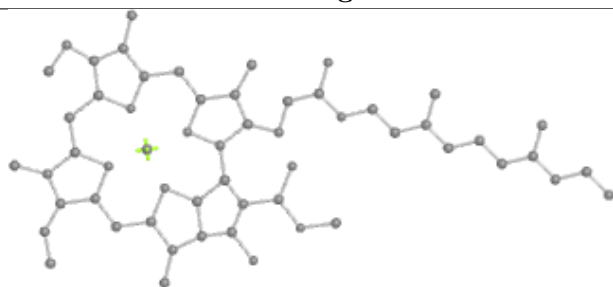
Bond lengths



Bond angles

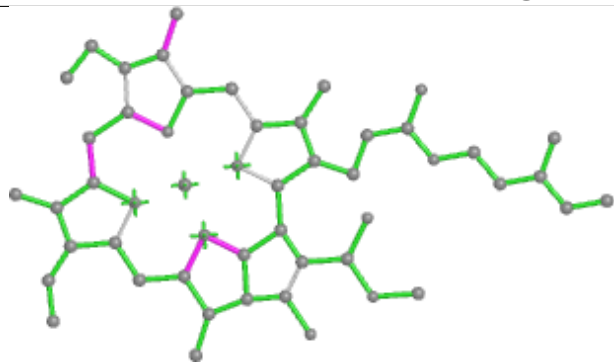


Torsions

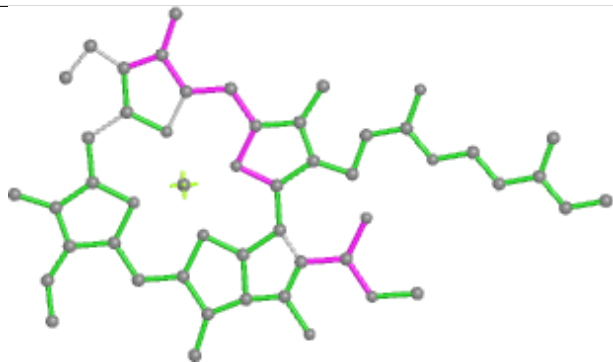


Rings

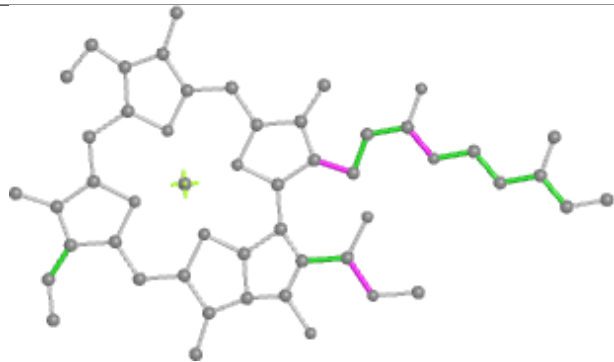
Ligand CLA k 601



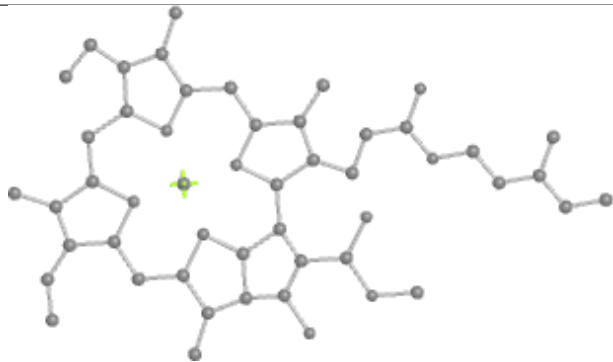
Bond lengths



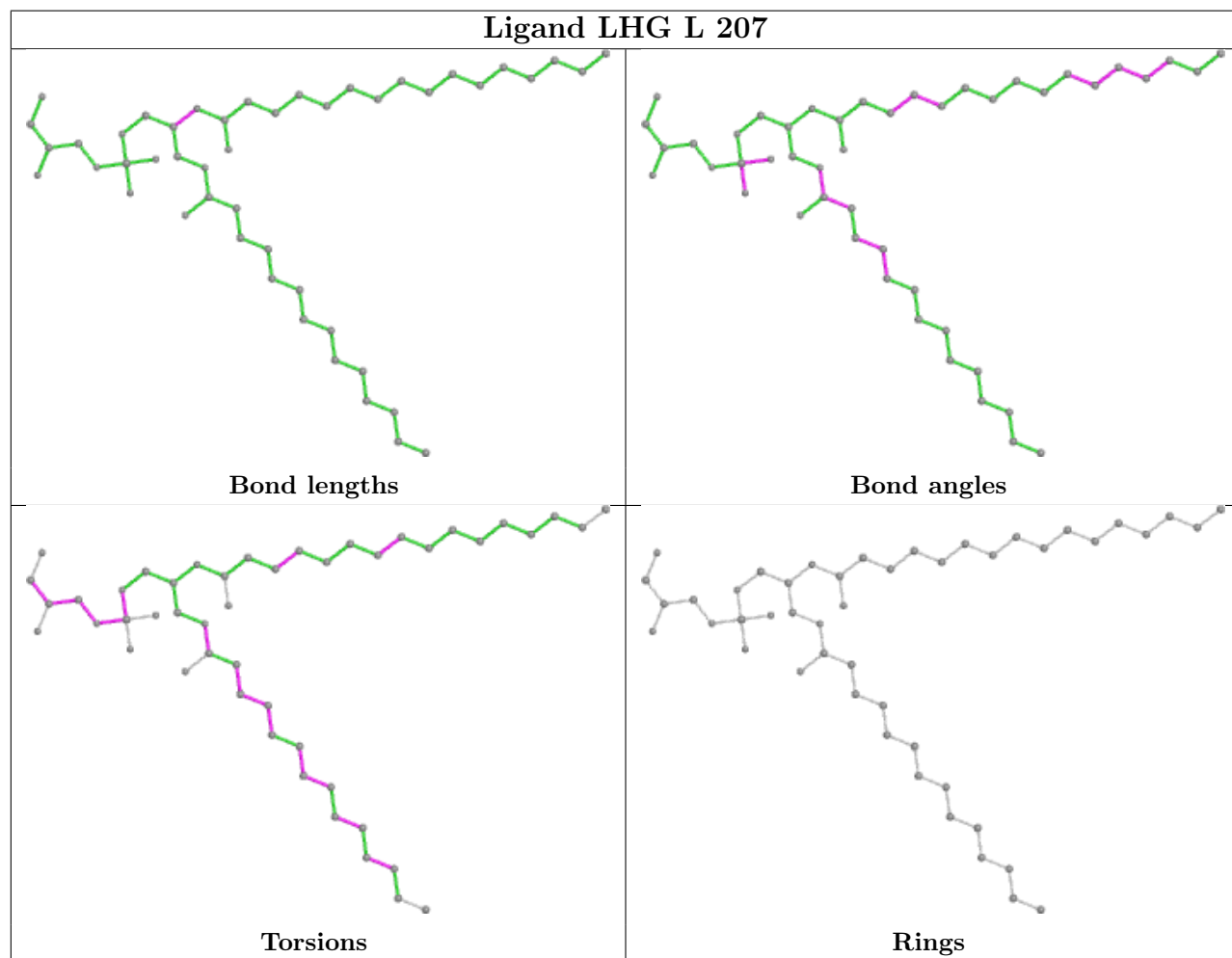
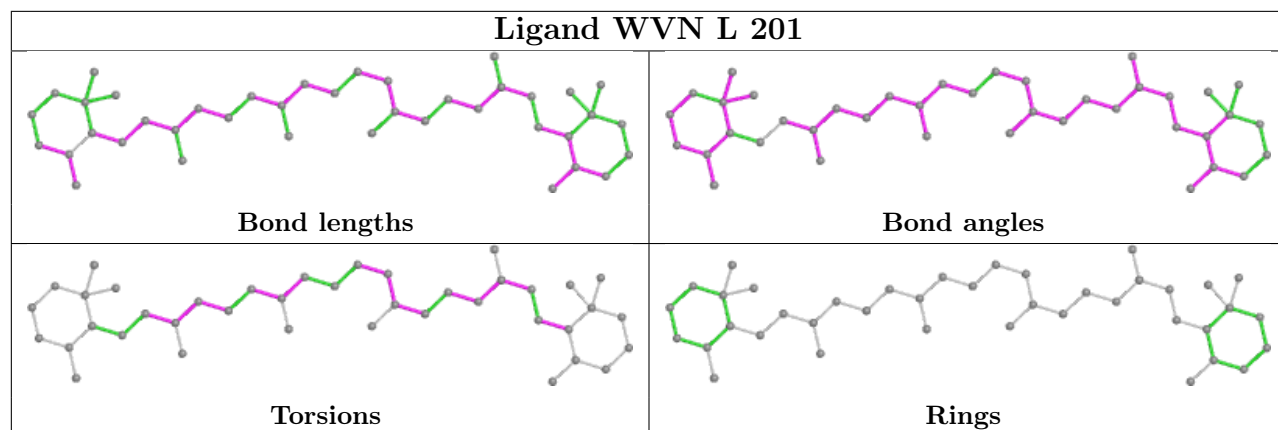
Bond angles

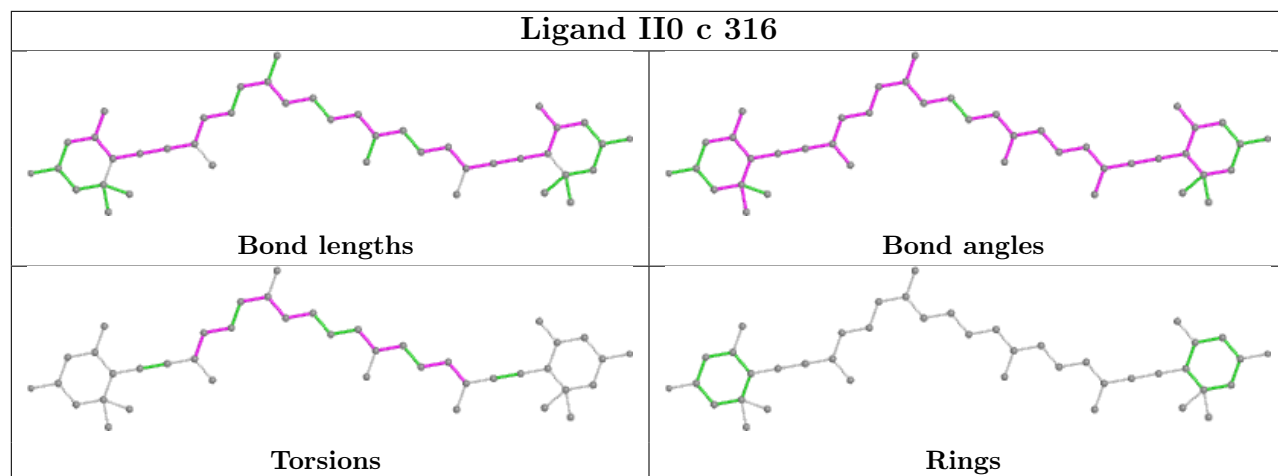
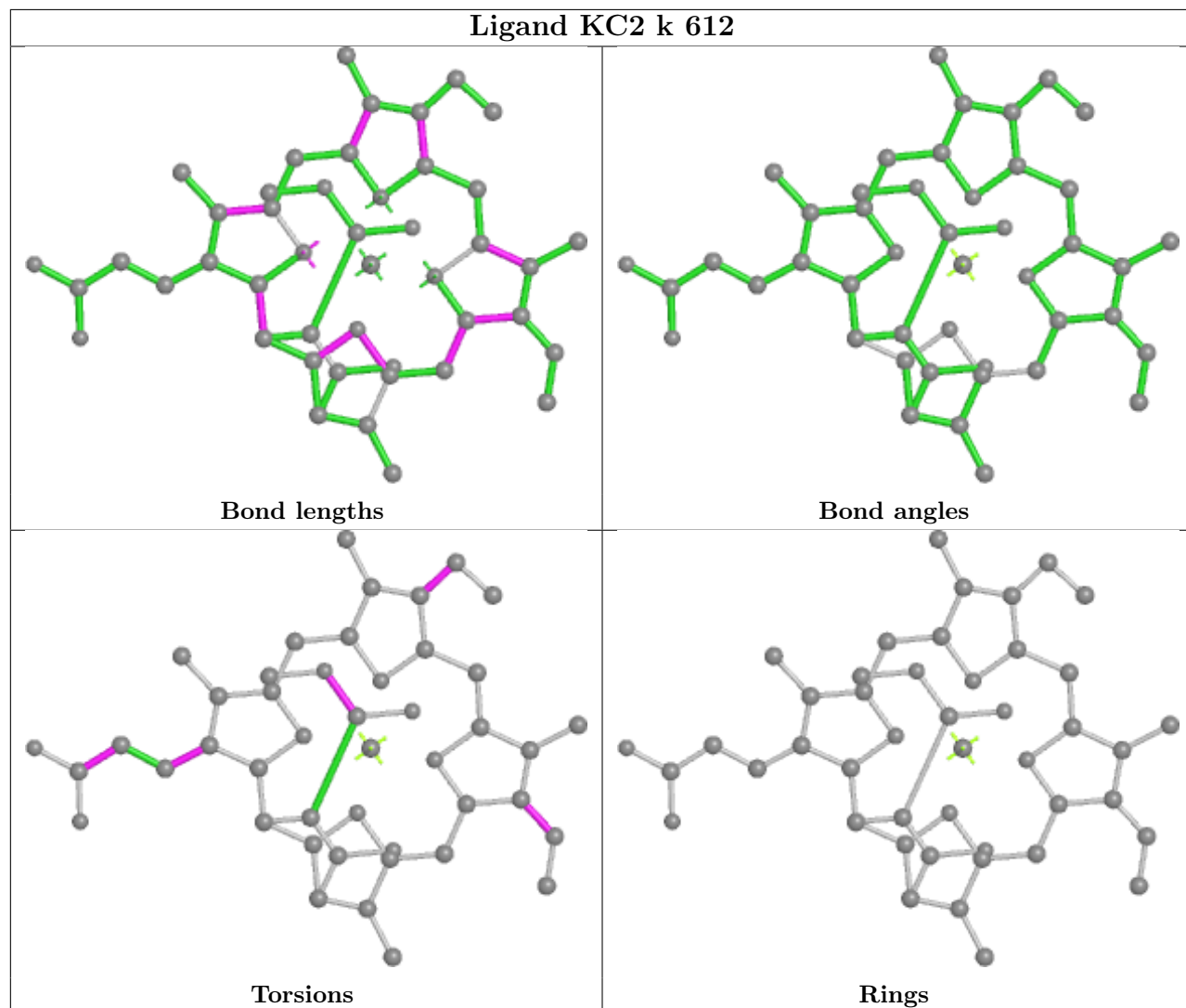


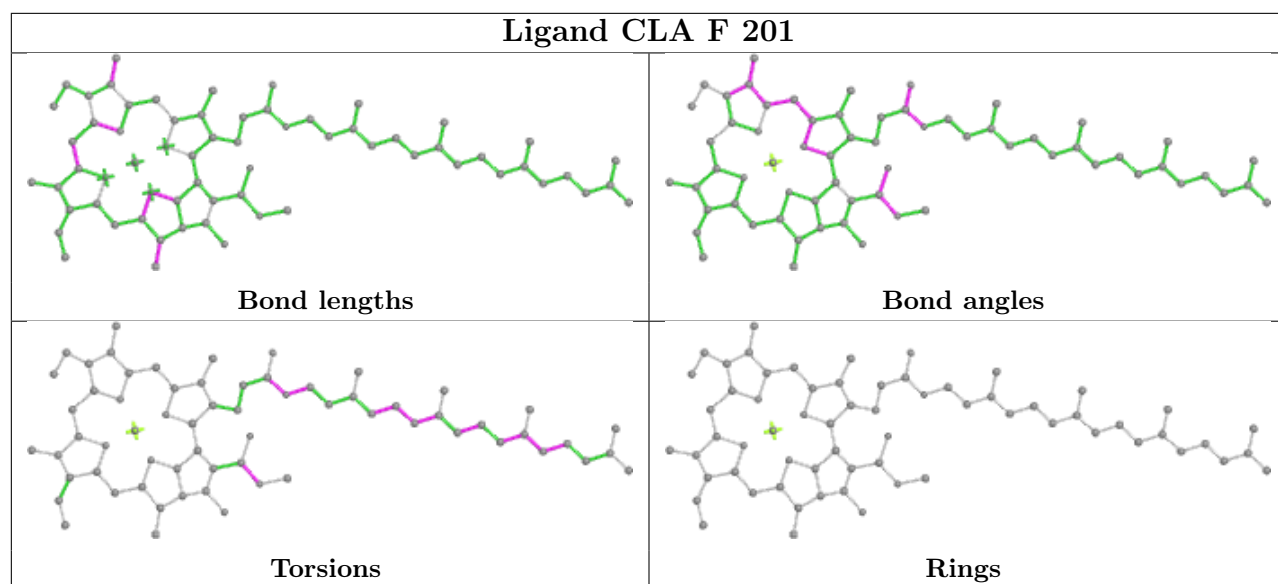
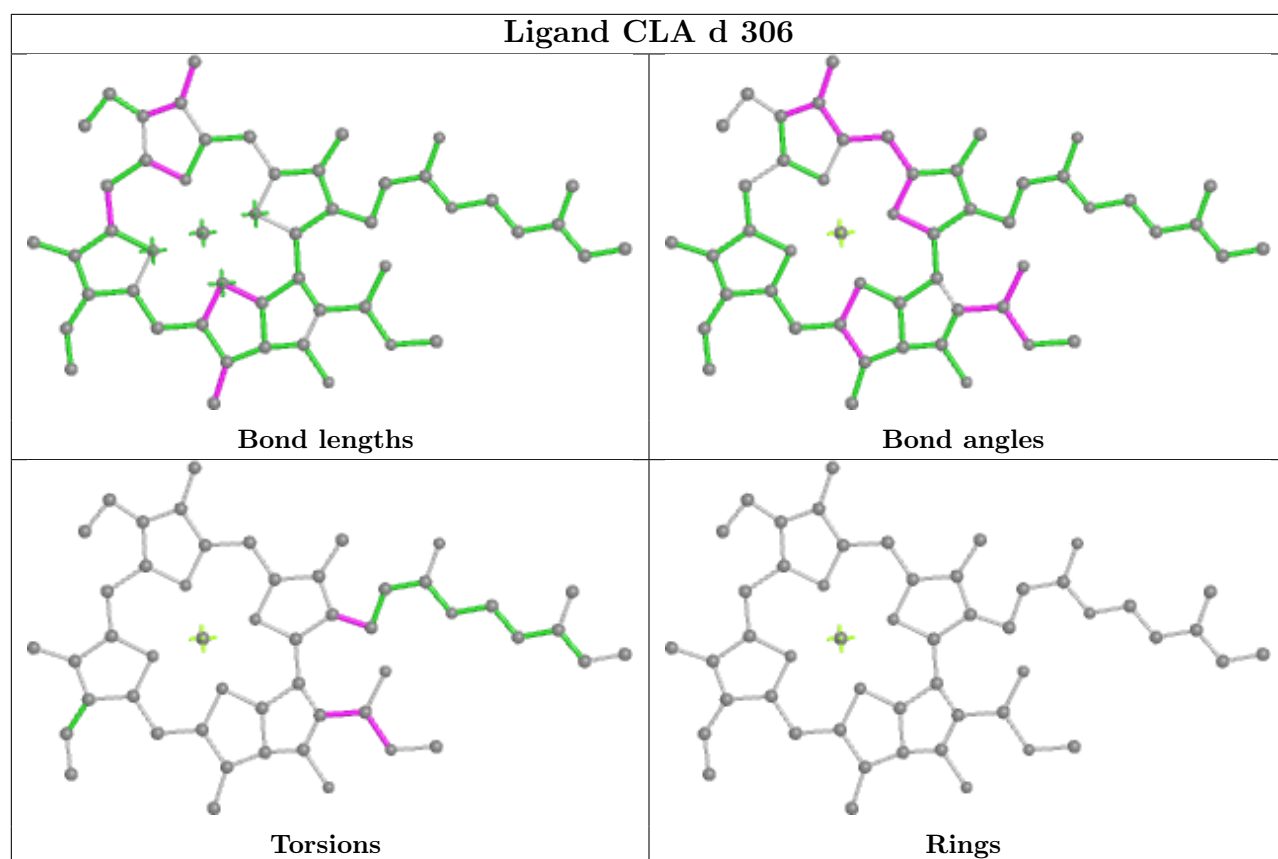
Torsions



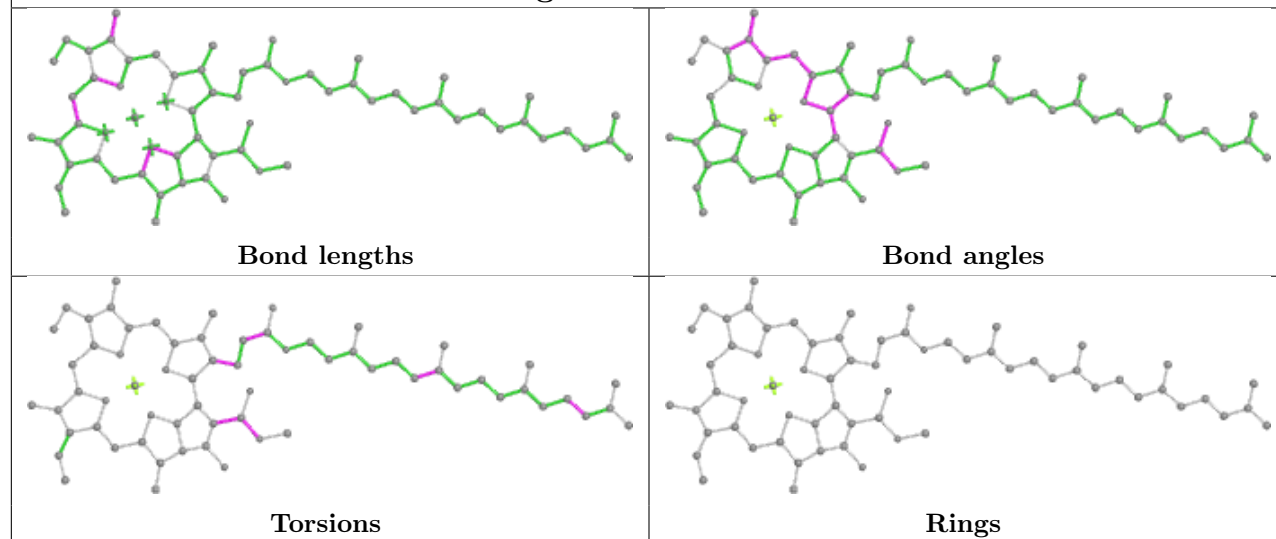
Rings



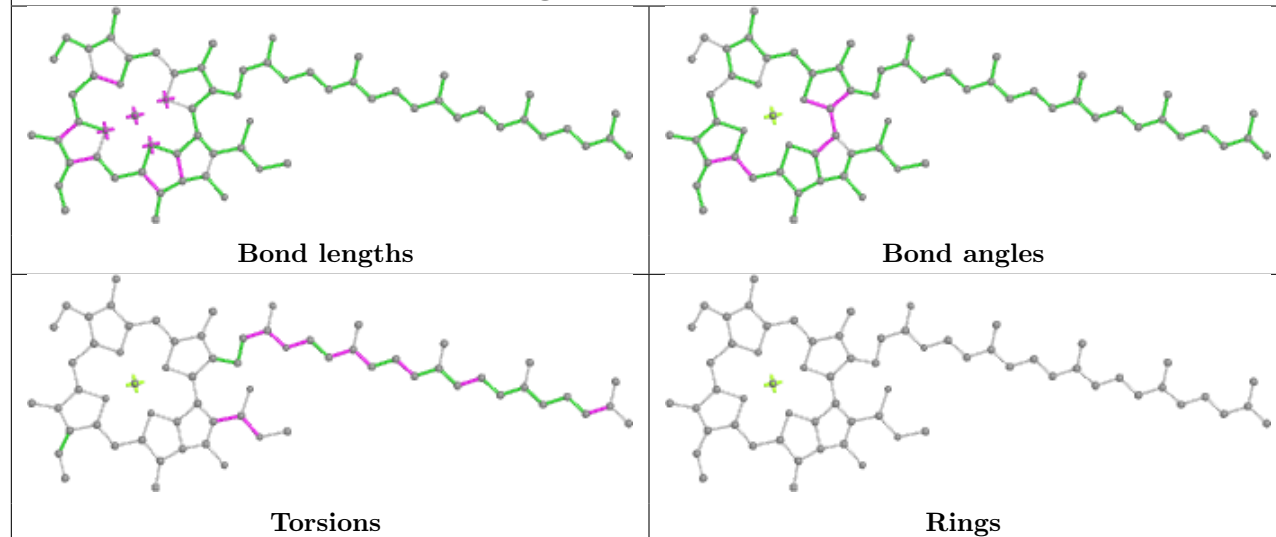
Ligand II0 c 316**Ligand KC2 k 612**



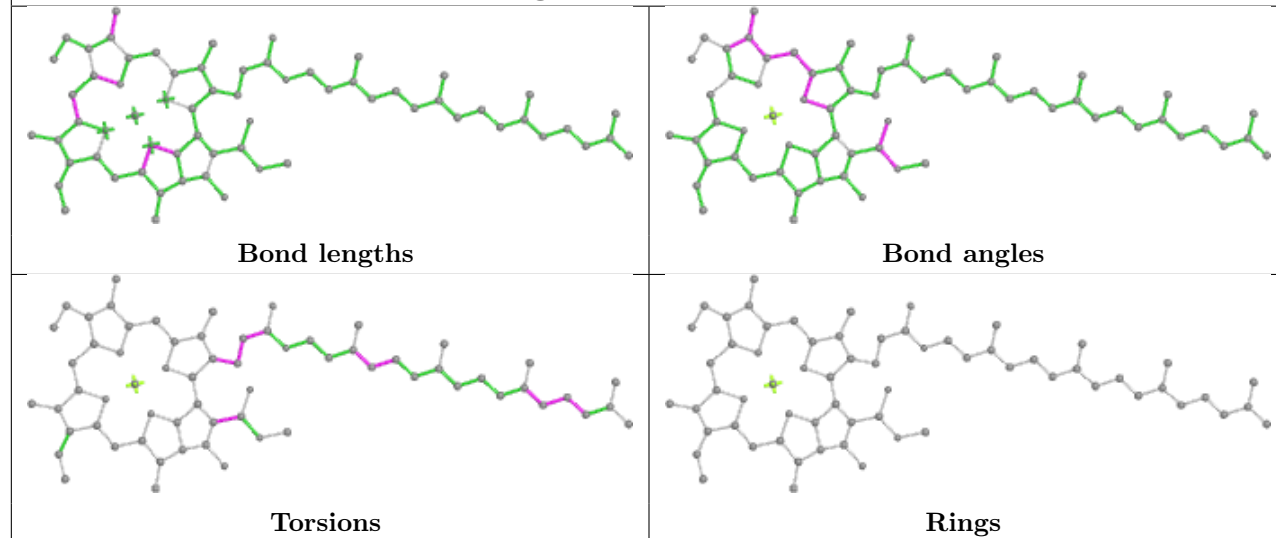
Ligand CLA a 309



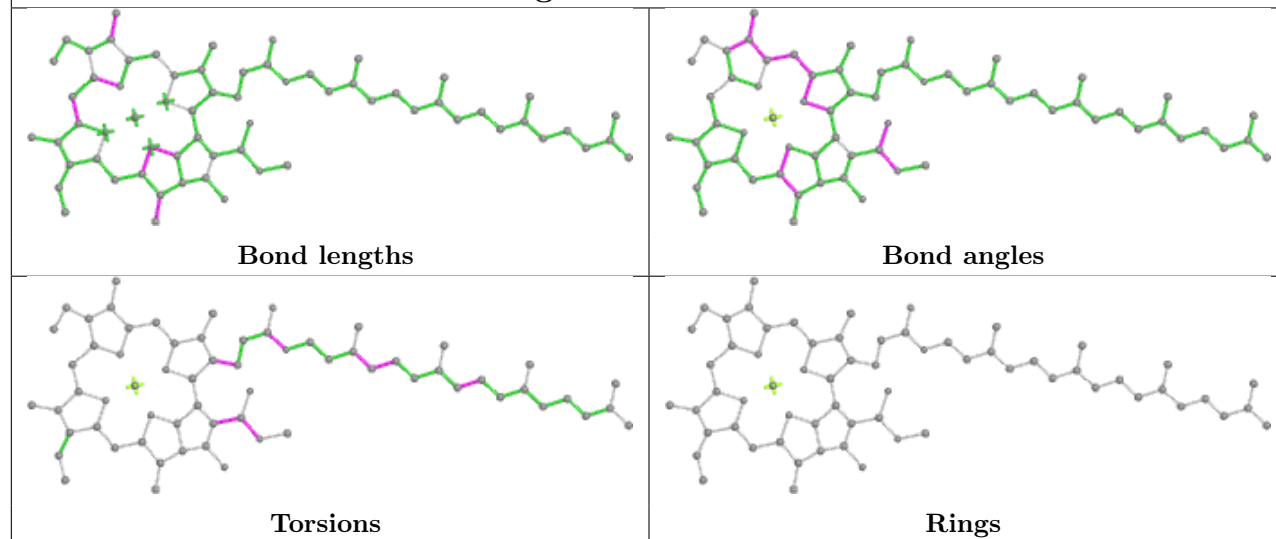
Ligand CL0 A 801



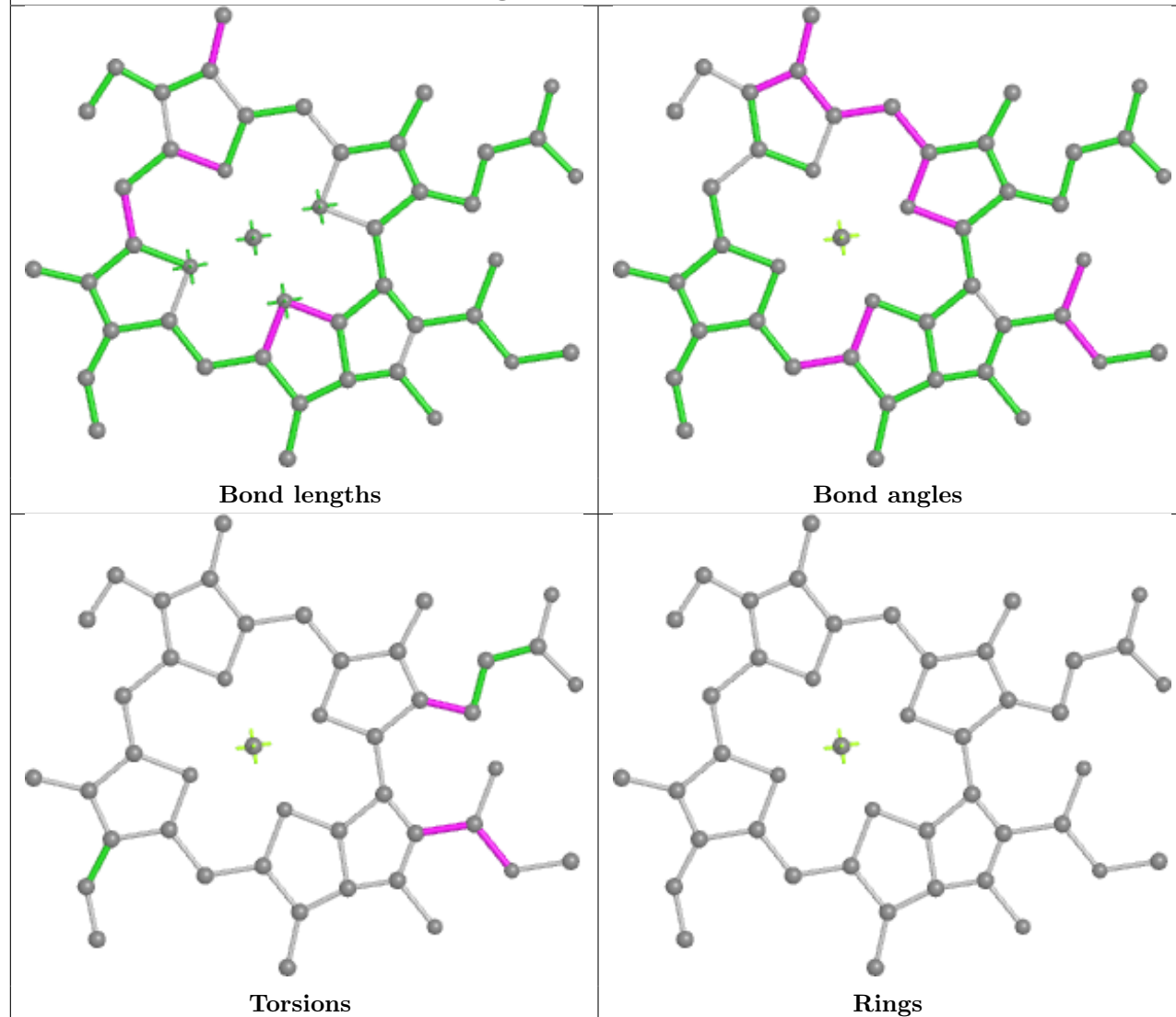
Ligand CLA A 812

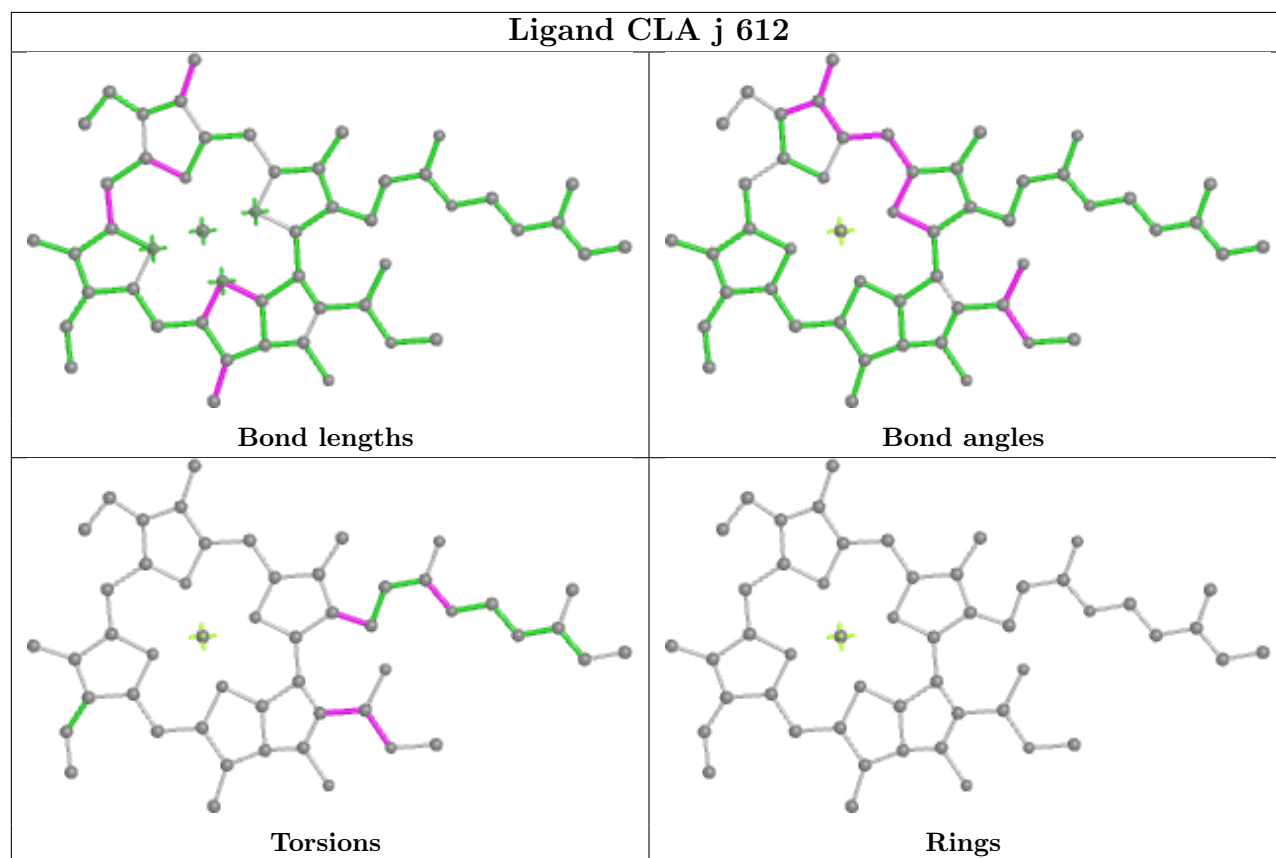
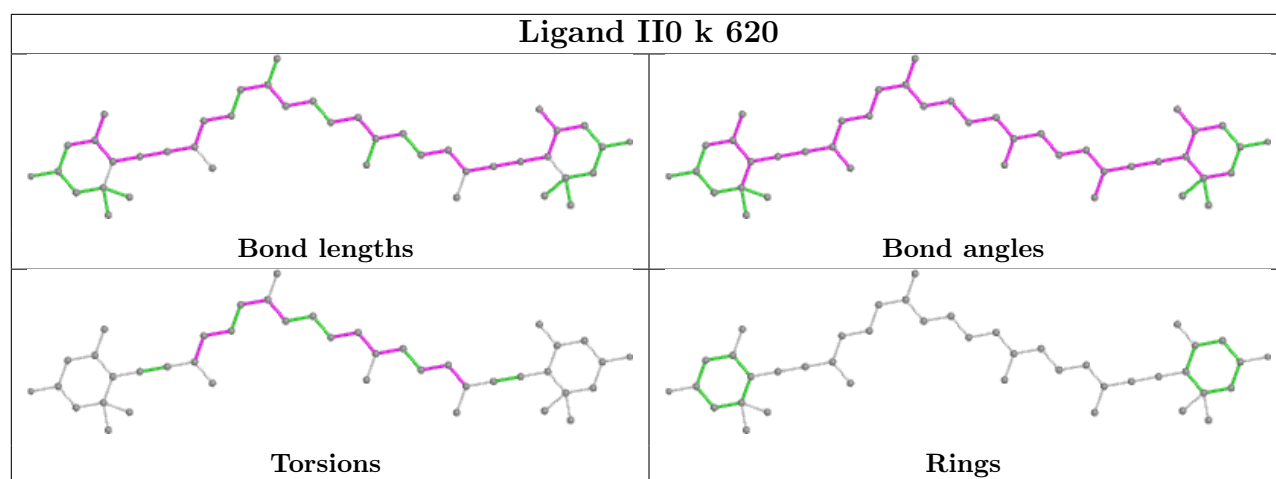


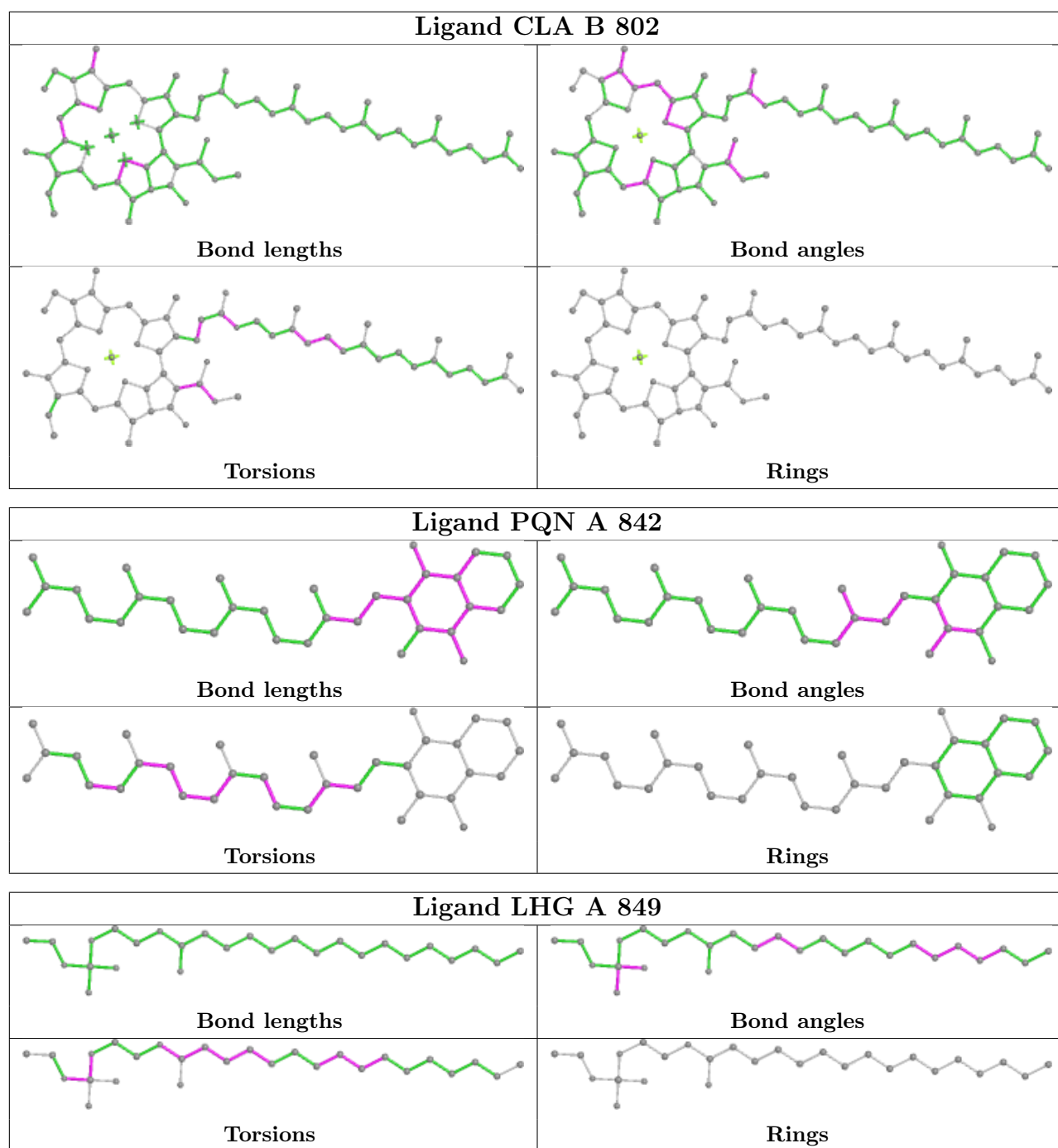
Ligand CLA n 607



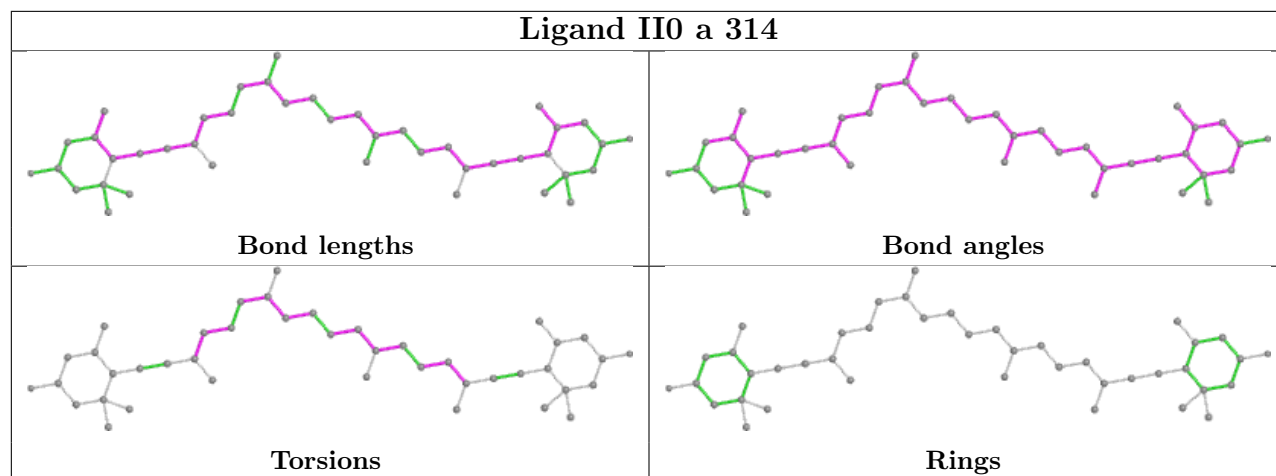
Ligand CLA a 305



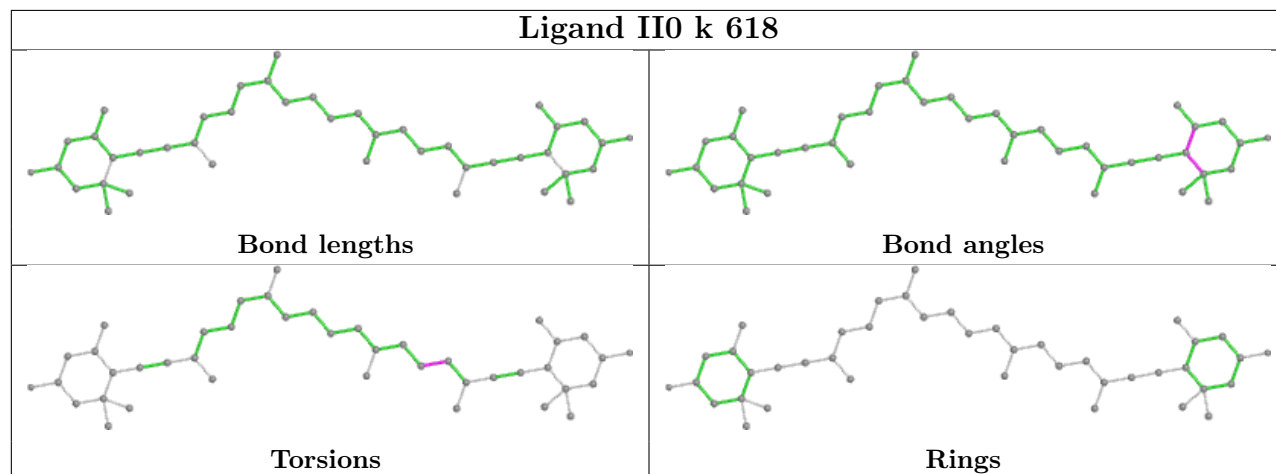




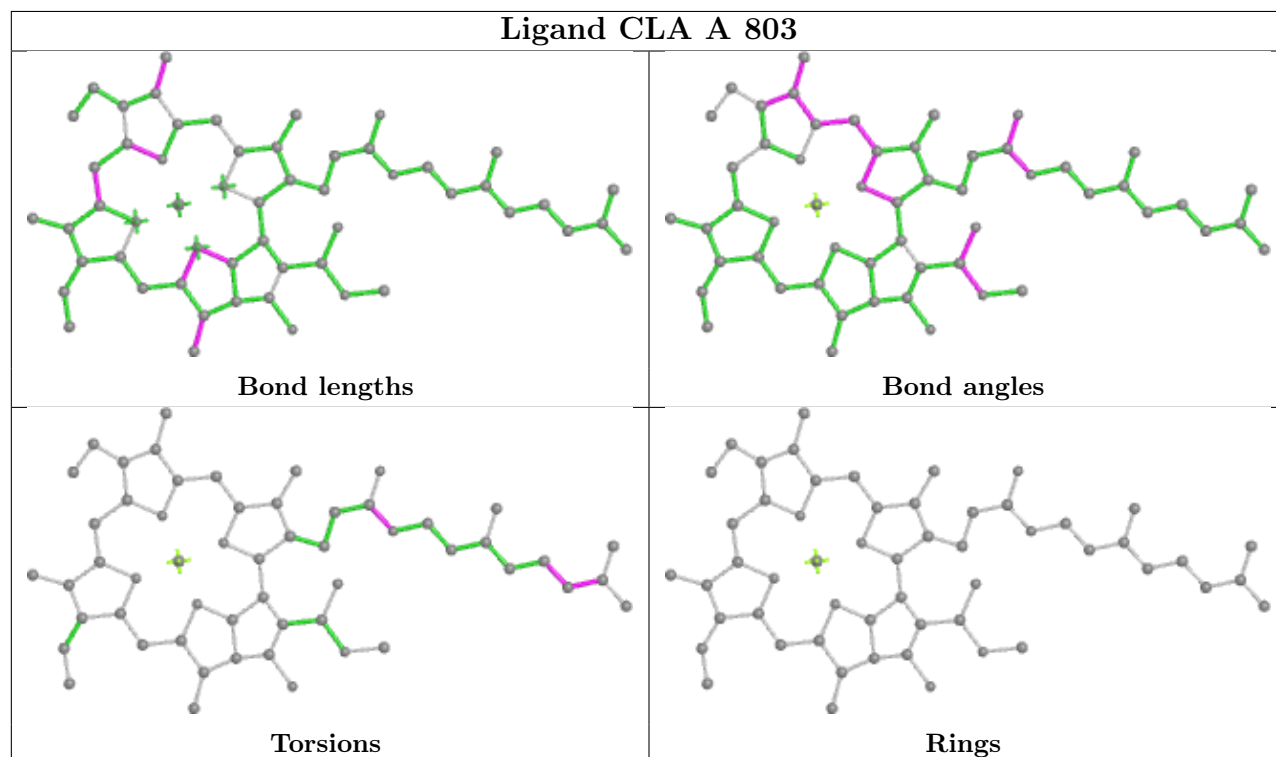
Ligand II0 a 314

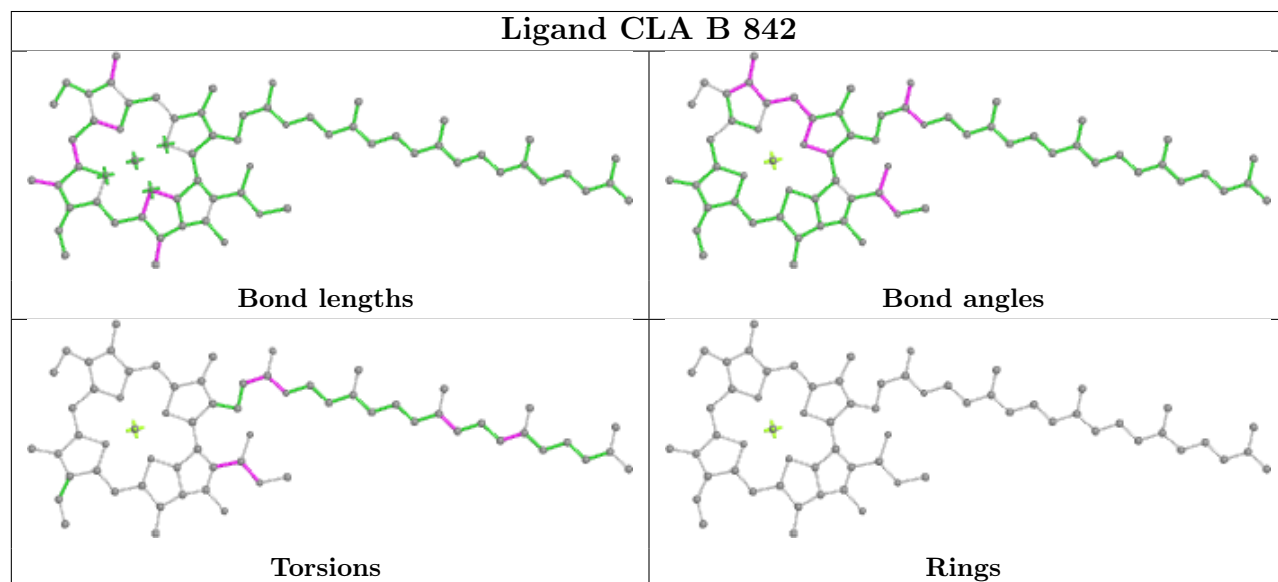
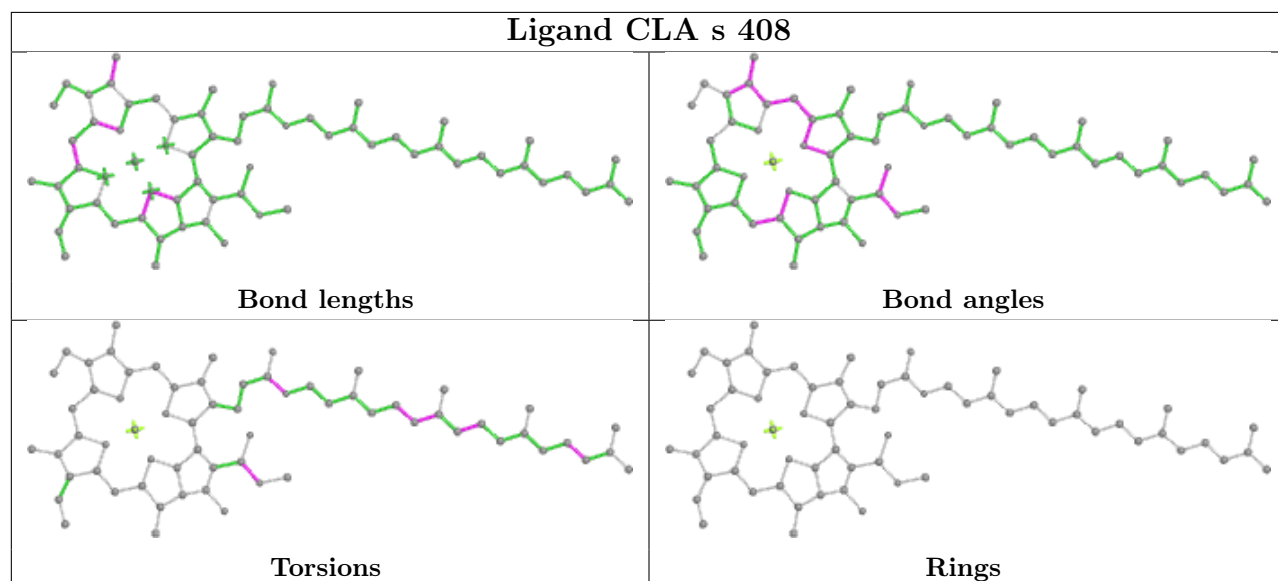
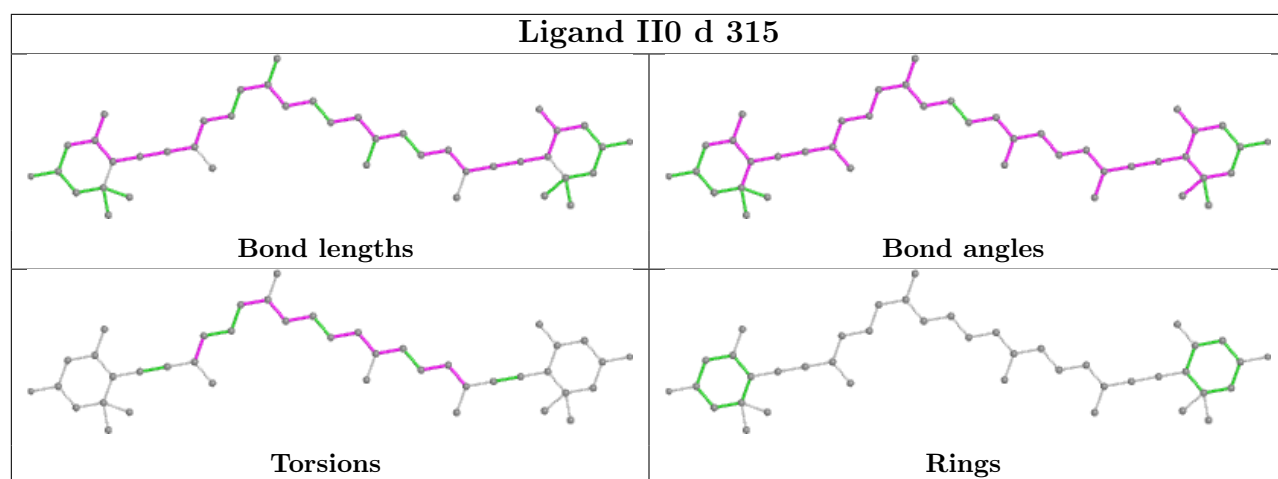


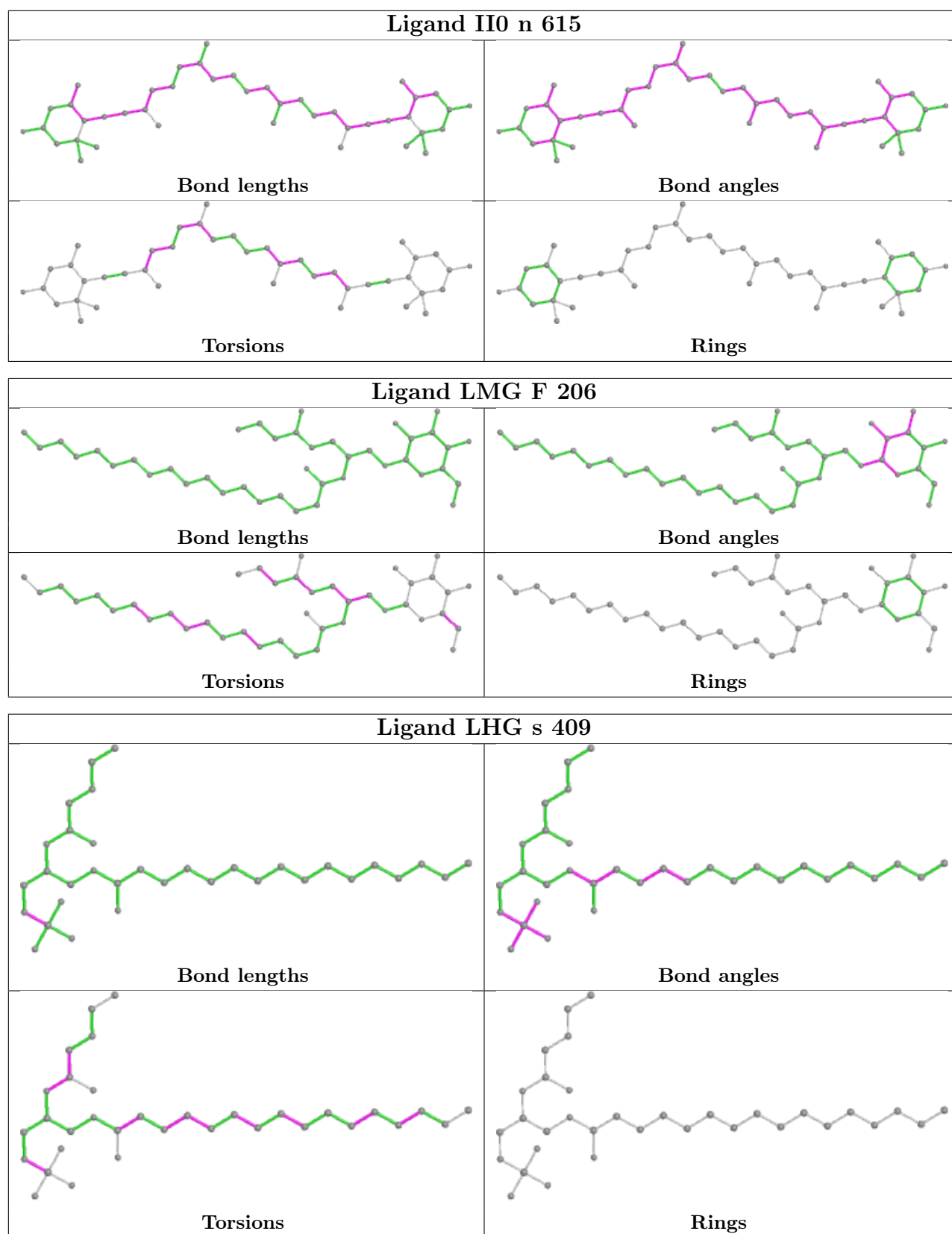
Ligand II0 k 618

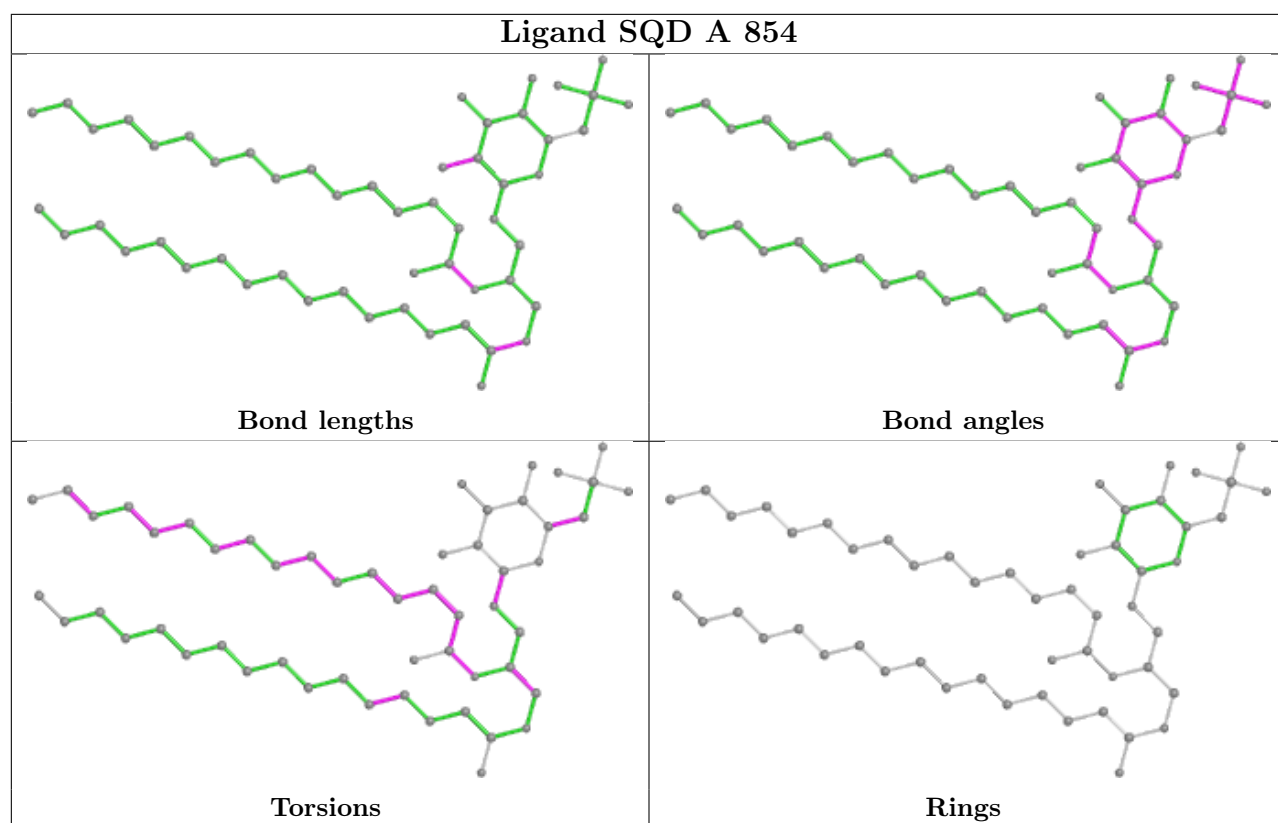


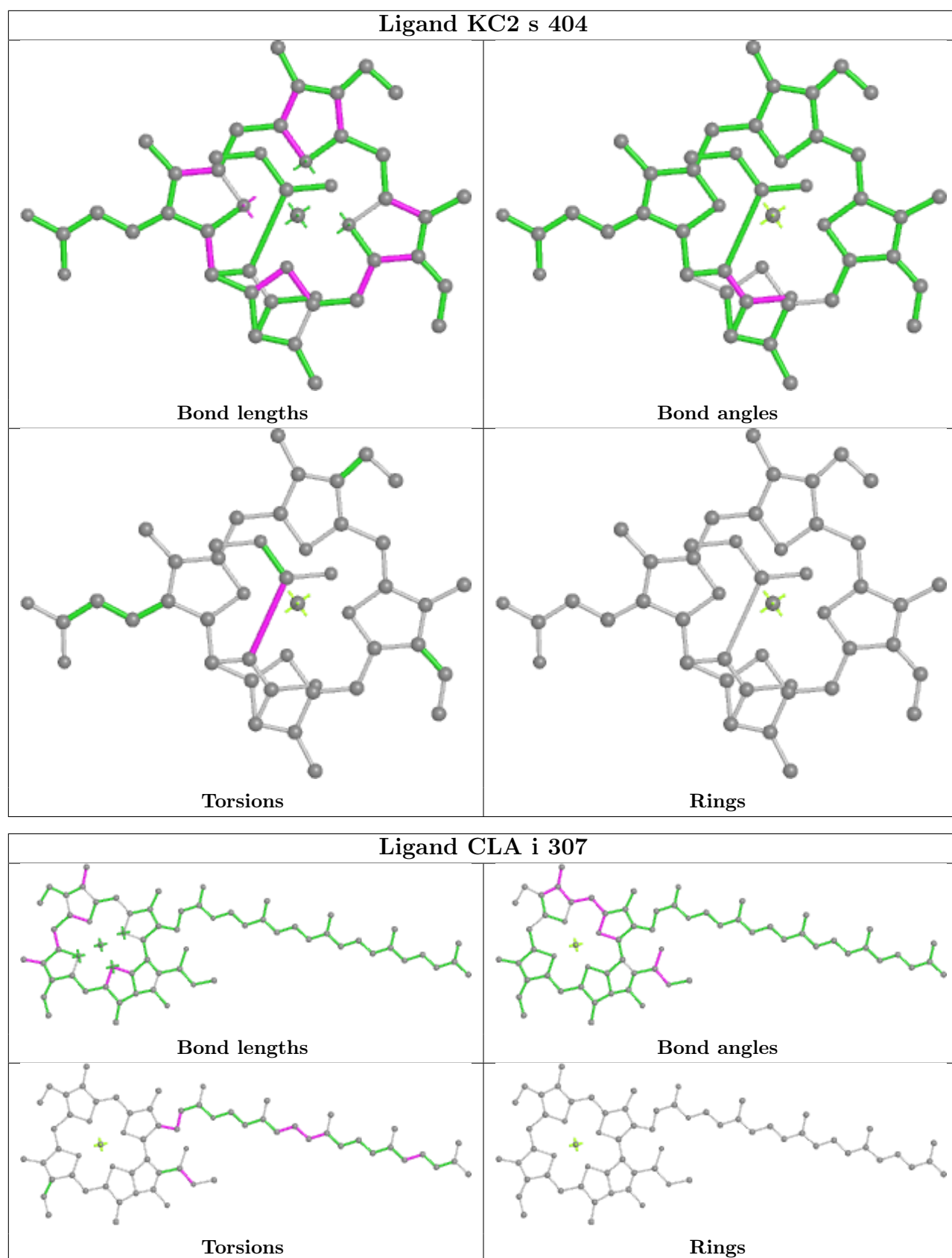
Ligand CLA A 803



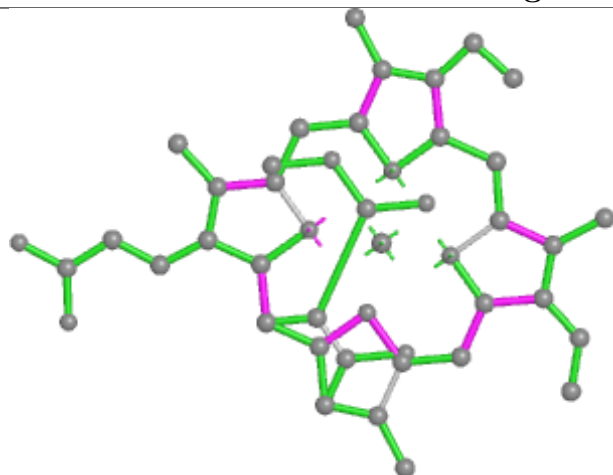




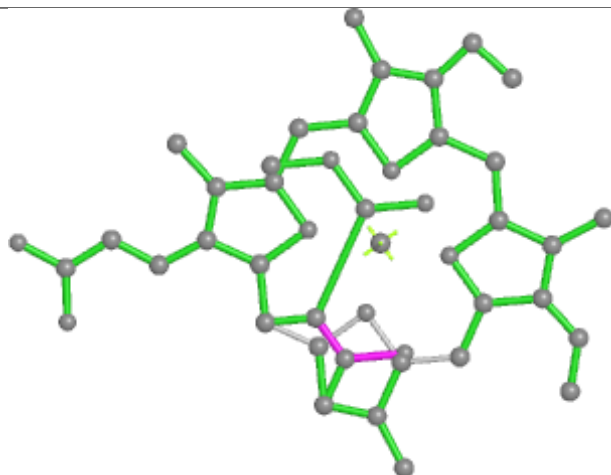




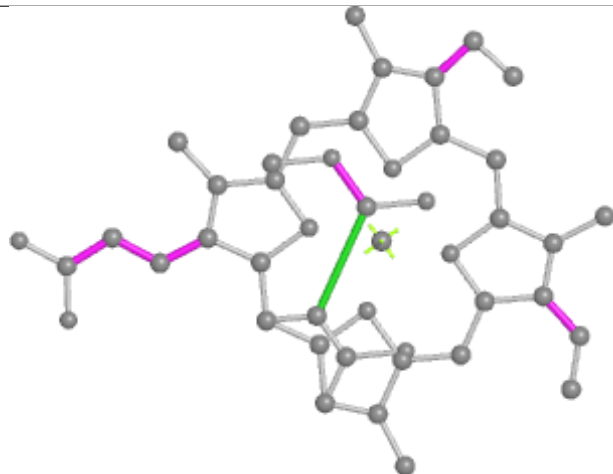
Ligand KC2 i 318



Bond lengths



Bond angles

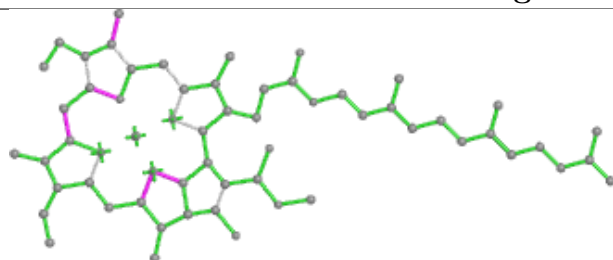


Torsions

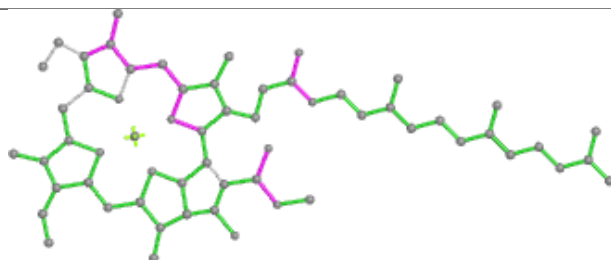


Rings

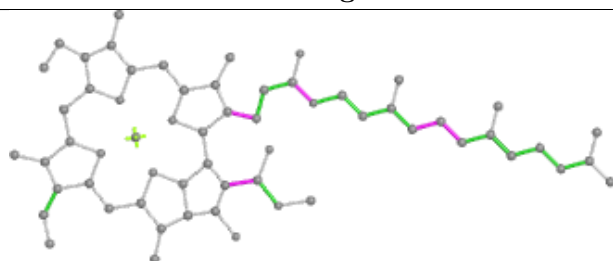
Ligand CLA A 834



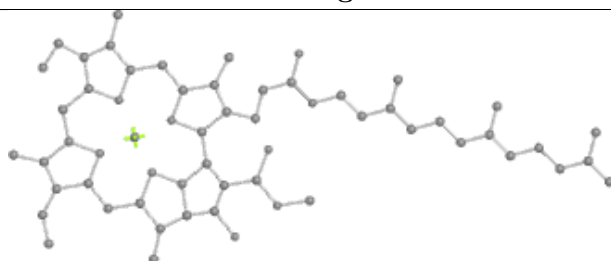
Bond lengths



Bond angles

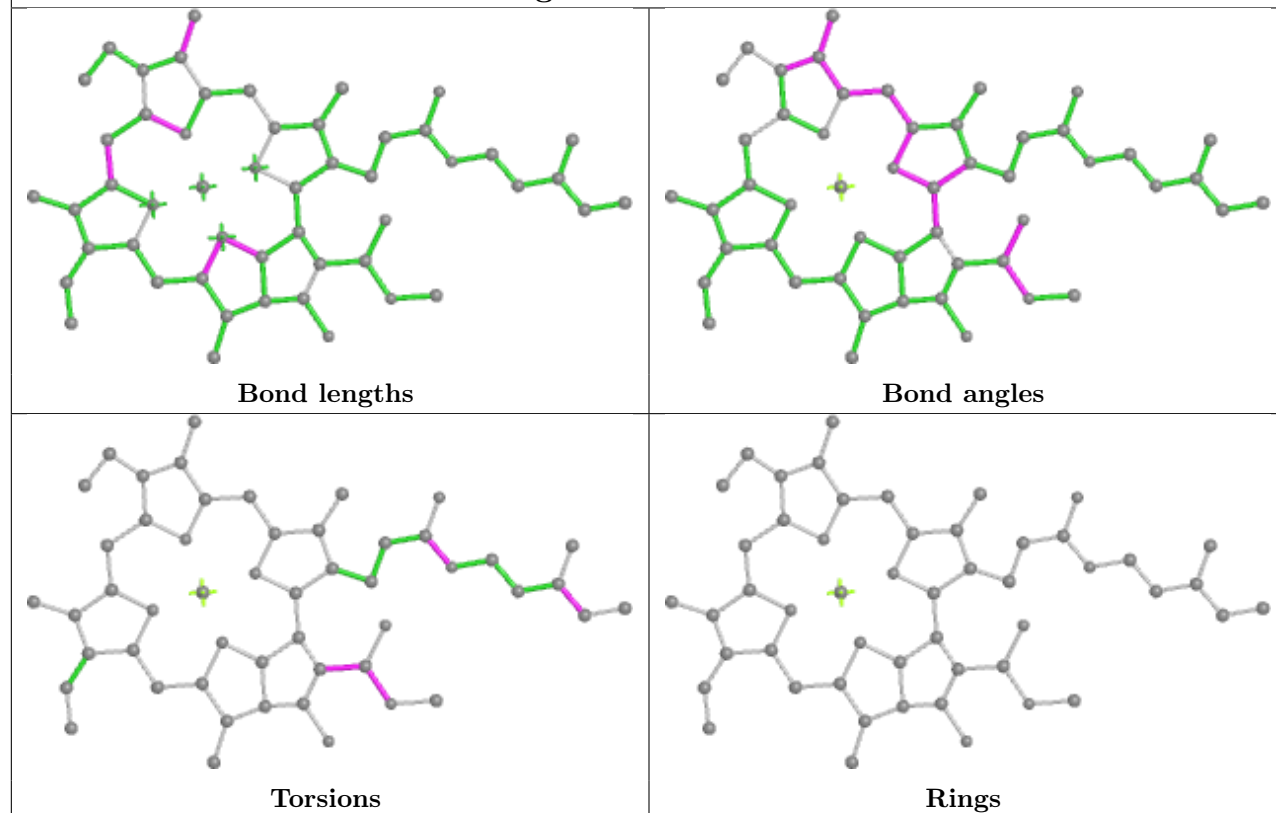


Torsions

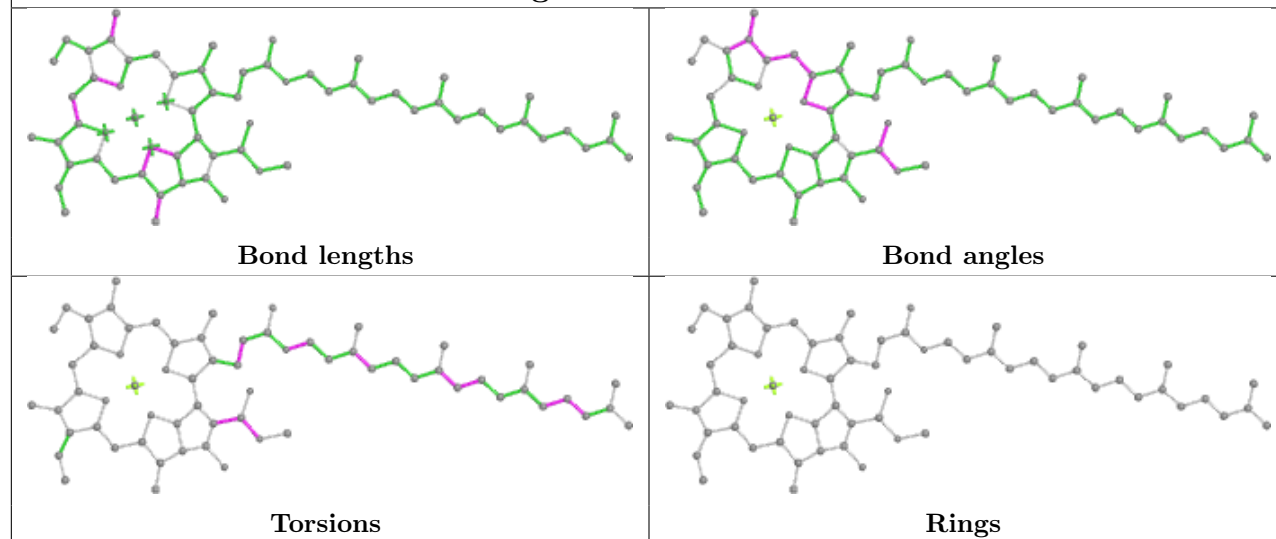


Rings

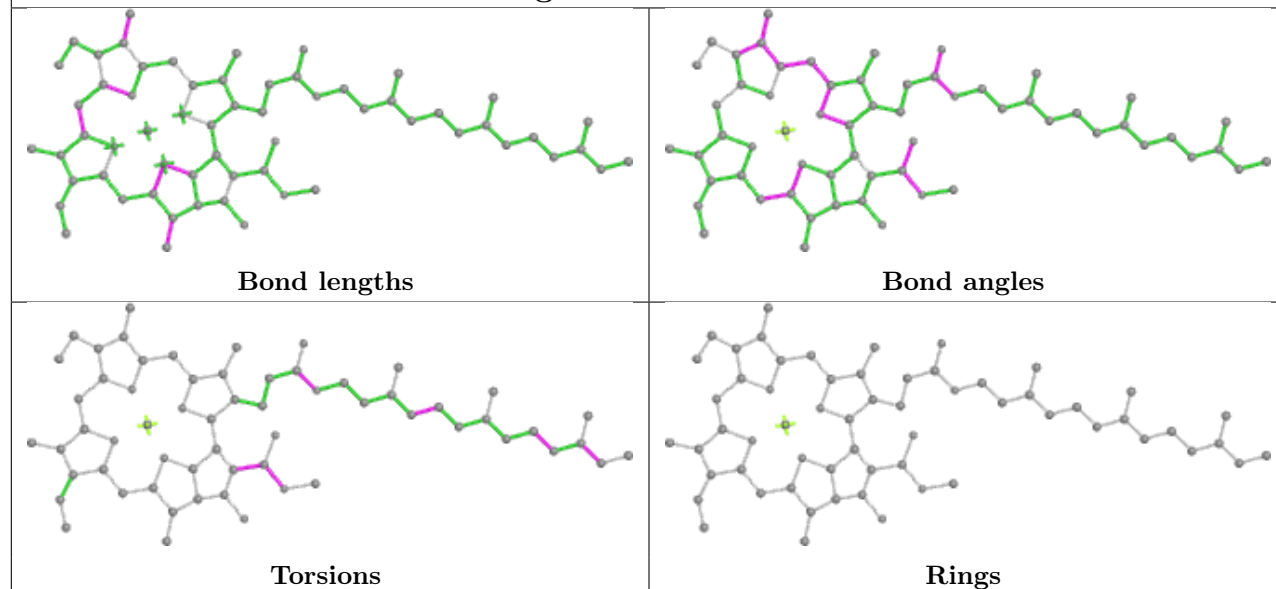
Ligand CLA d 303



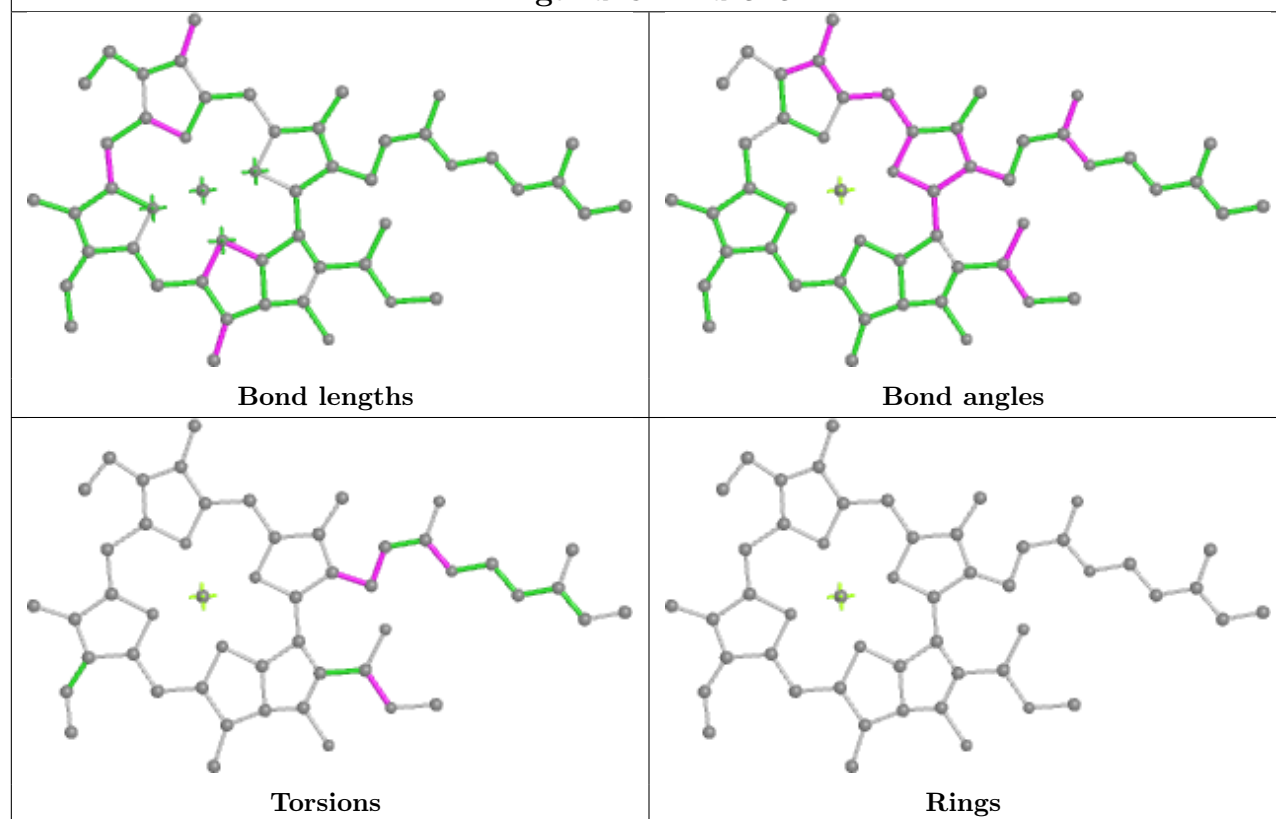
Ligand CLA A 852



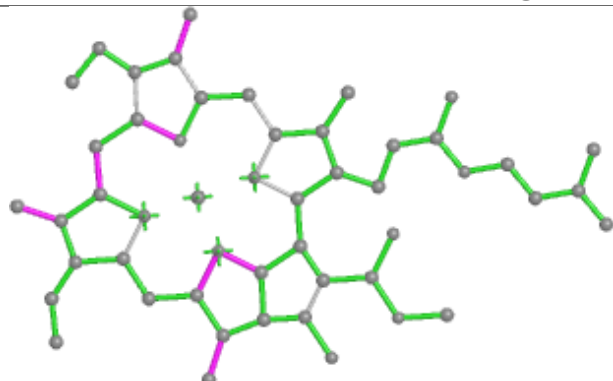
Ligand CLA b 307



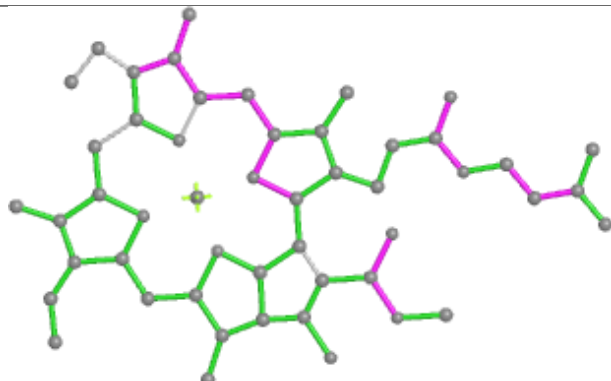
Ligand CLA d 313



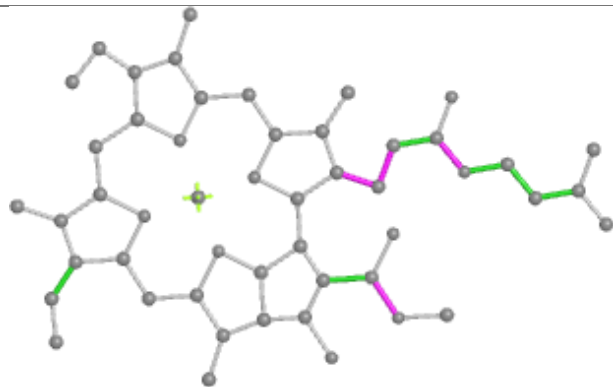
Ligand CLA h 302



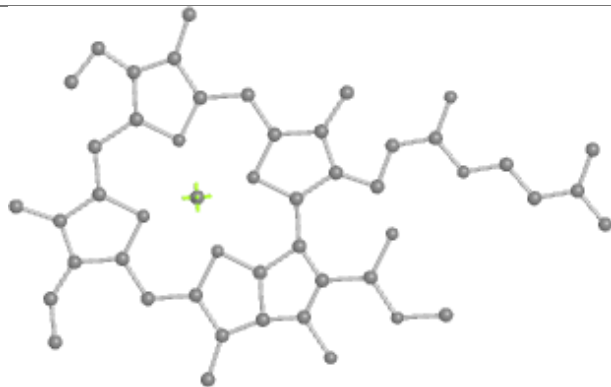
Bond lengths



Bond angles

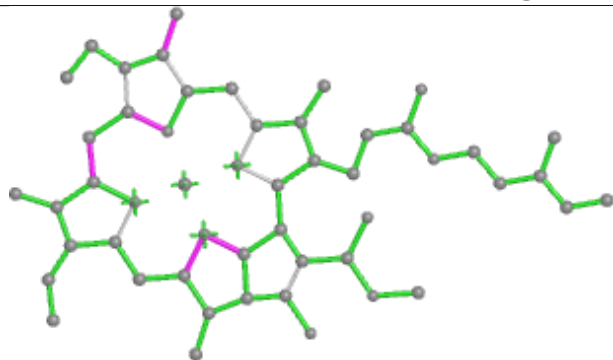


Torsions

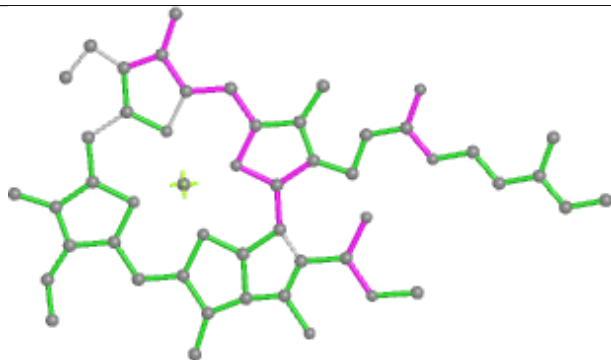


Rings

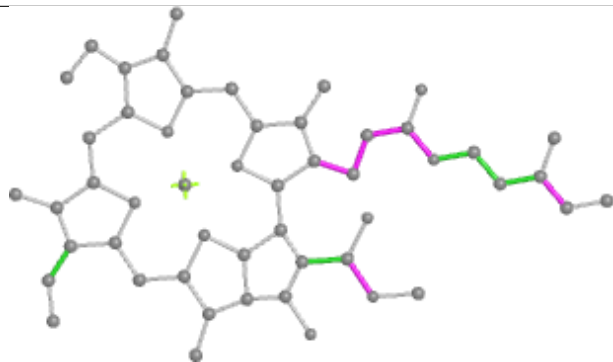
Ligand CLA k 610



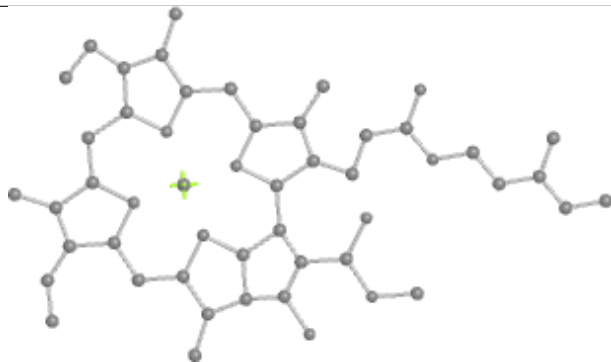
Bond lengths



Bond angles

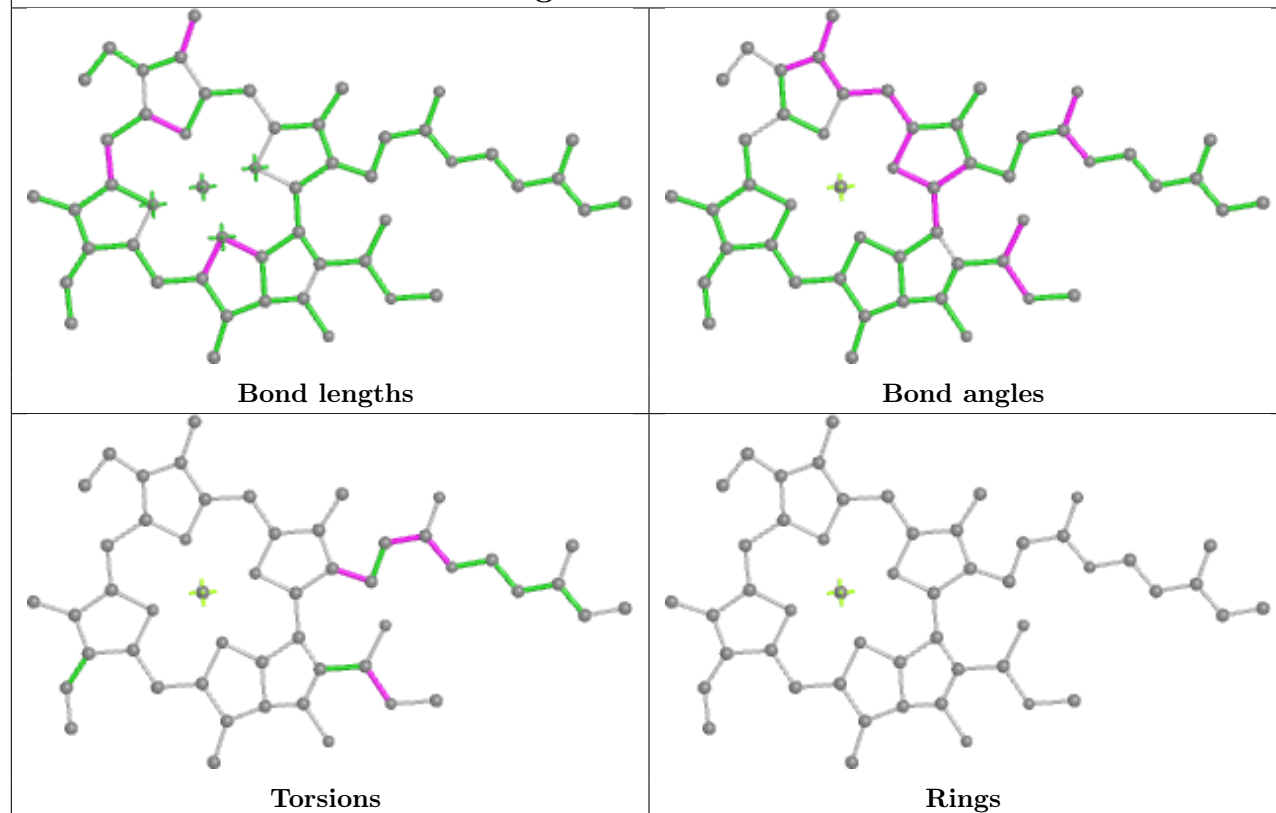


Torsions

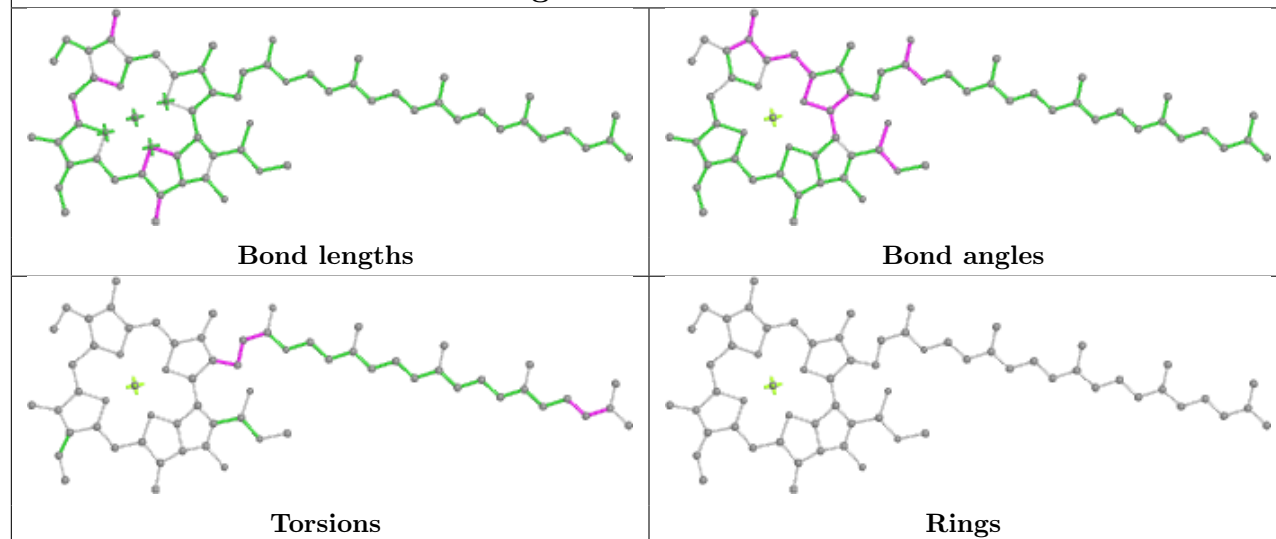


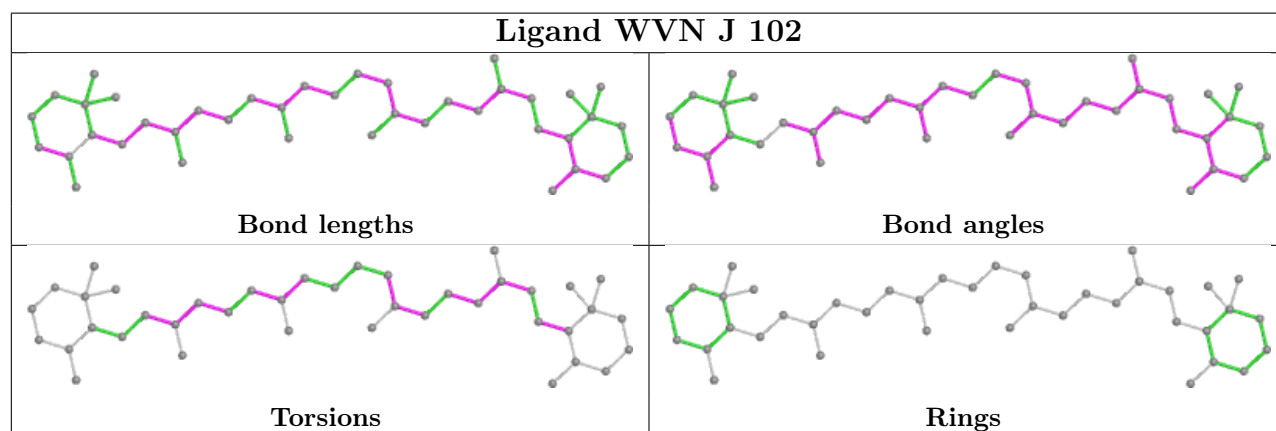
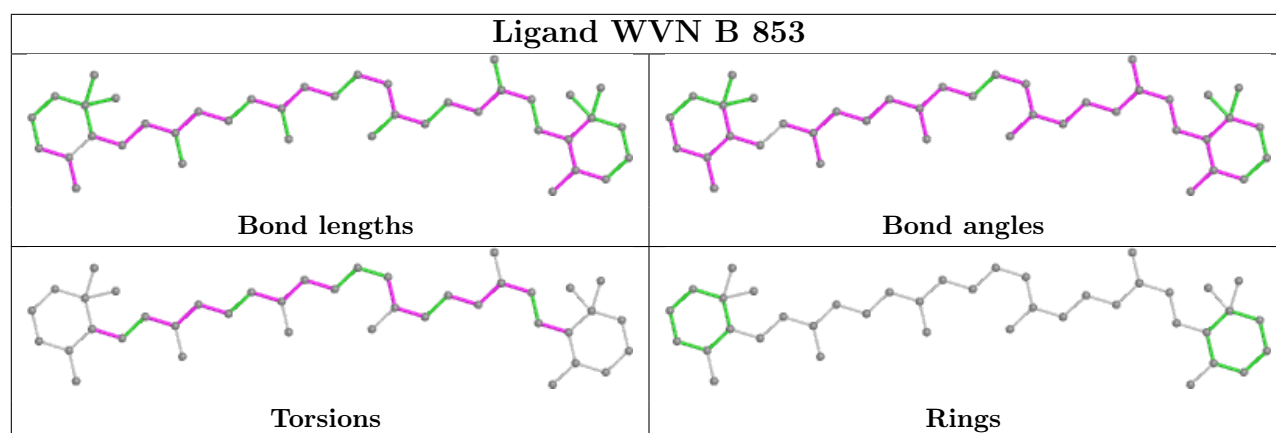
Rings

Ligand CLA h 308

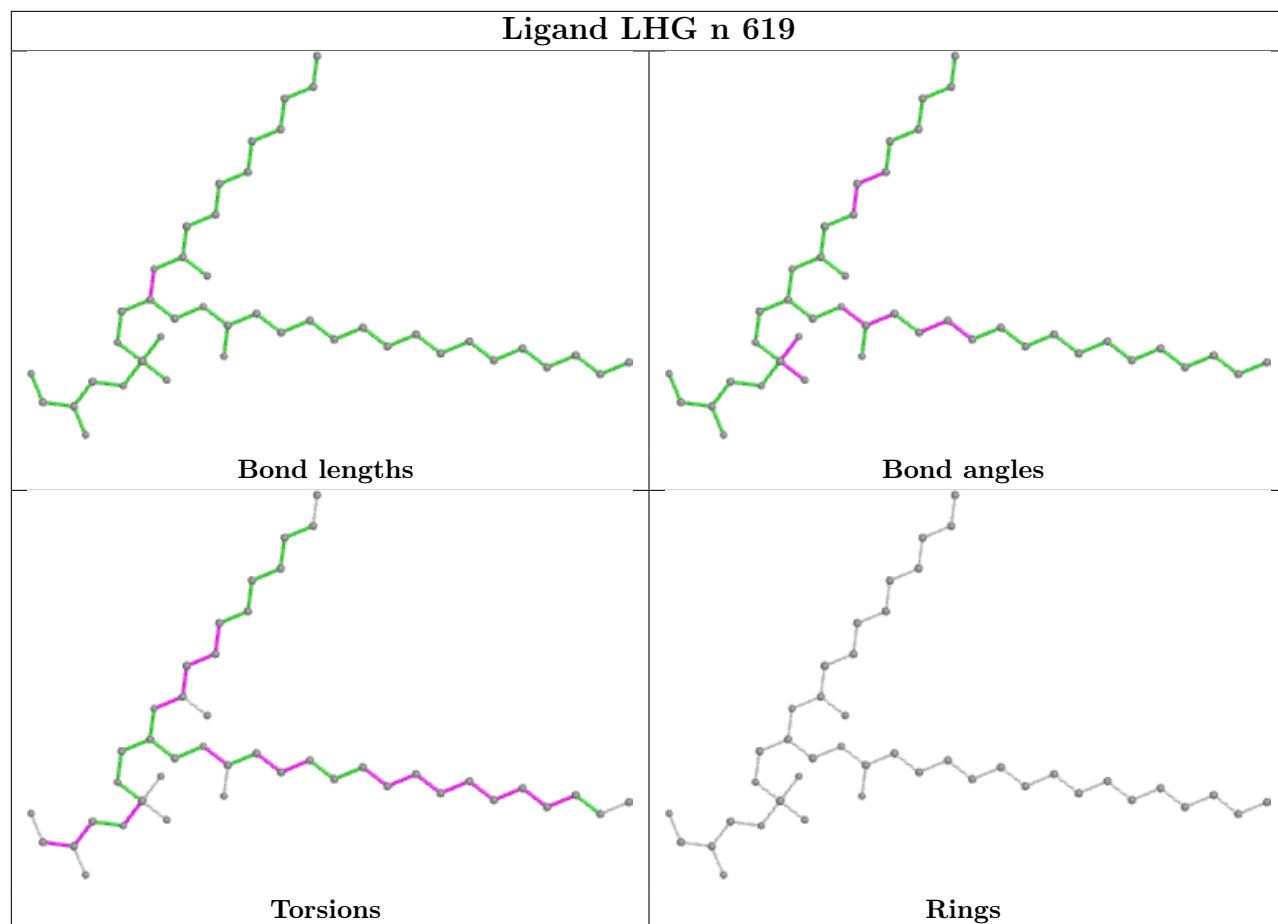


Ligand CLA A 808

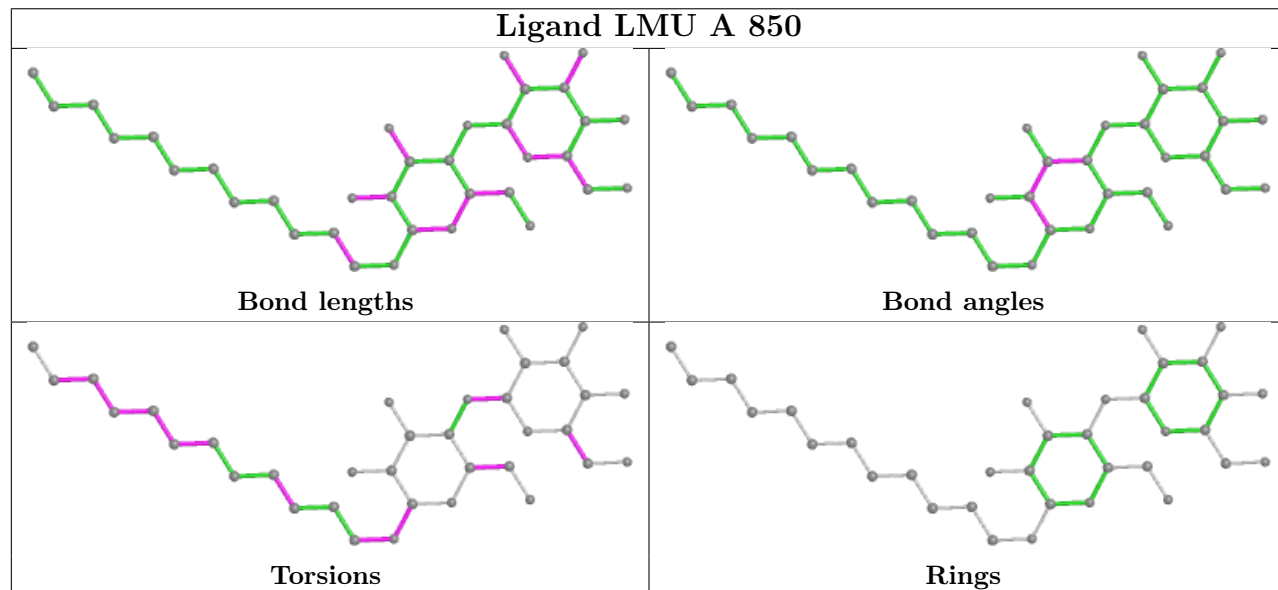


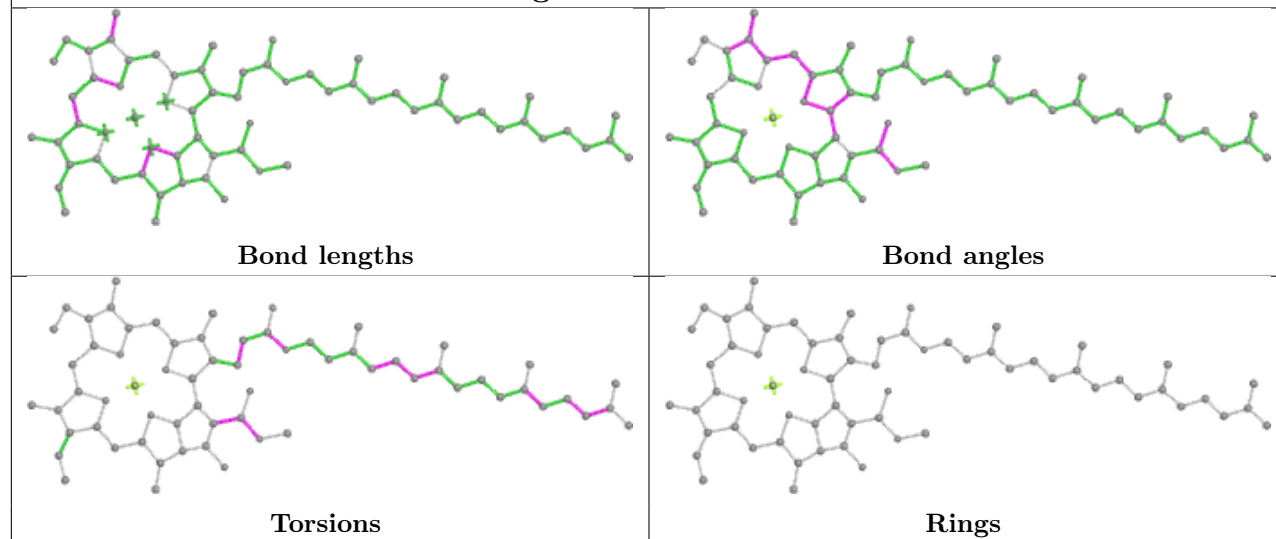
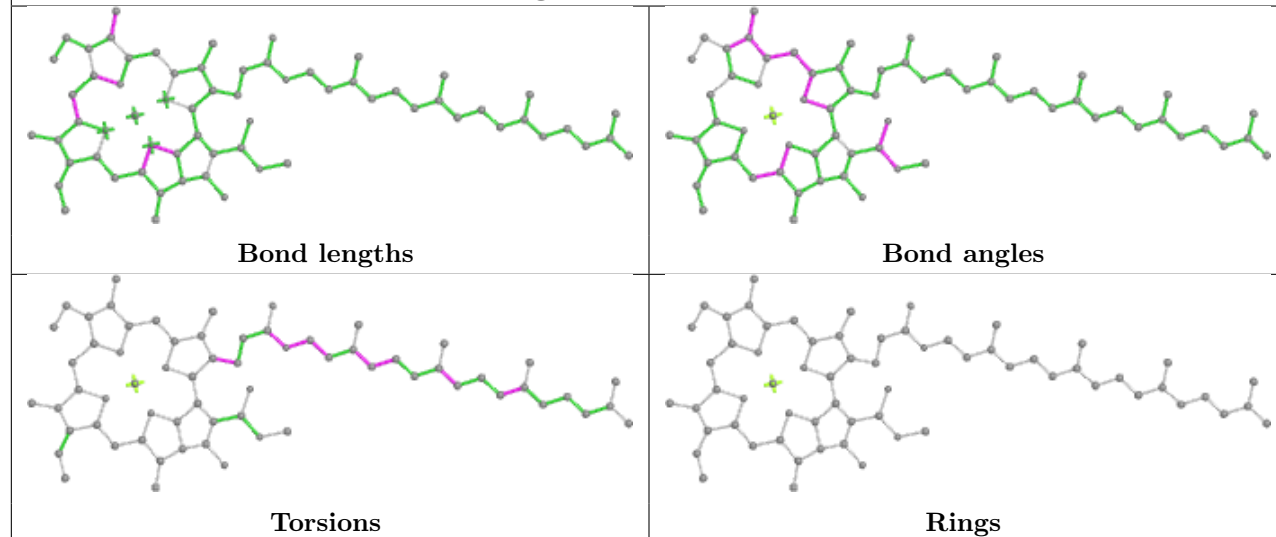


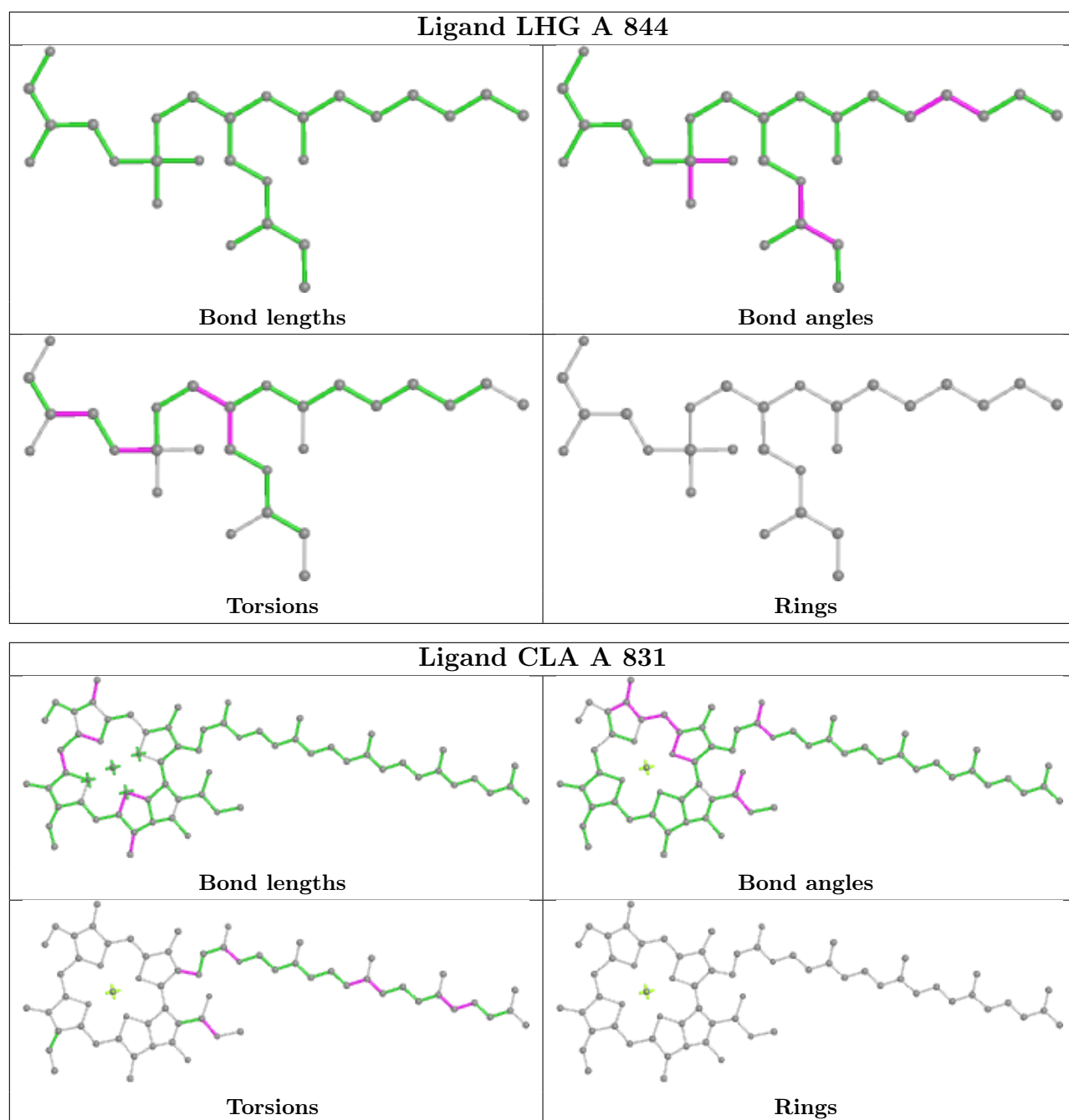
Ligand LHG n 619

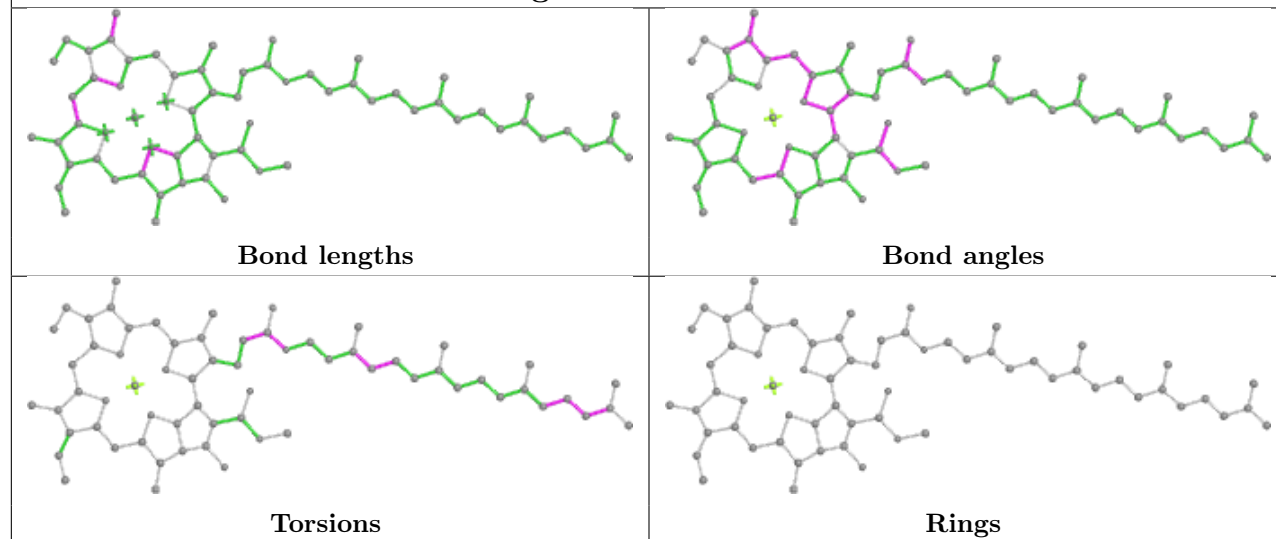
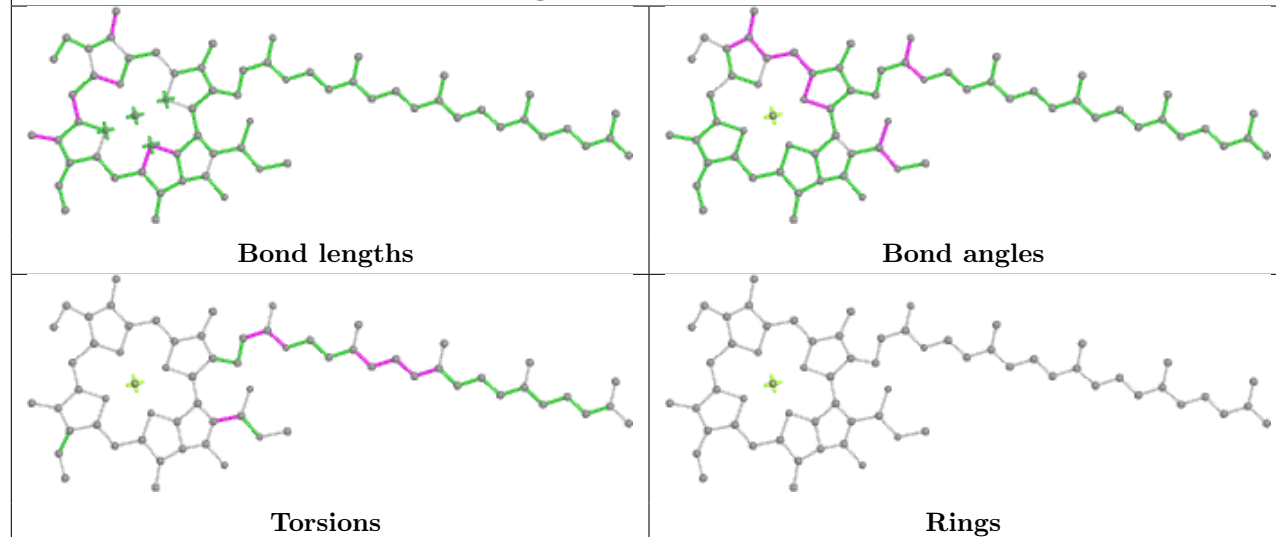
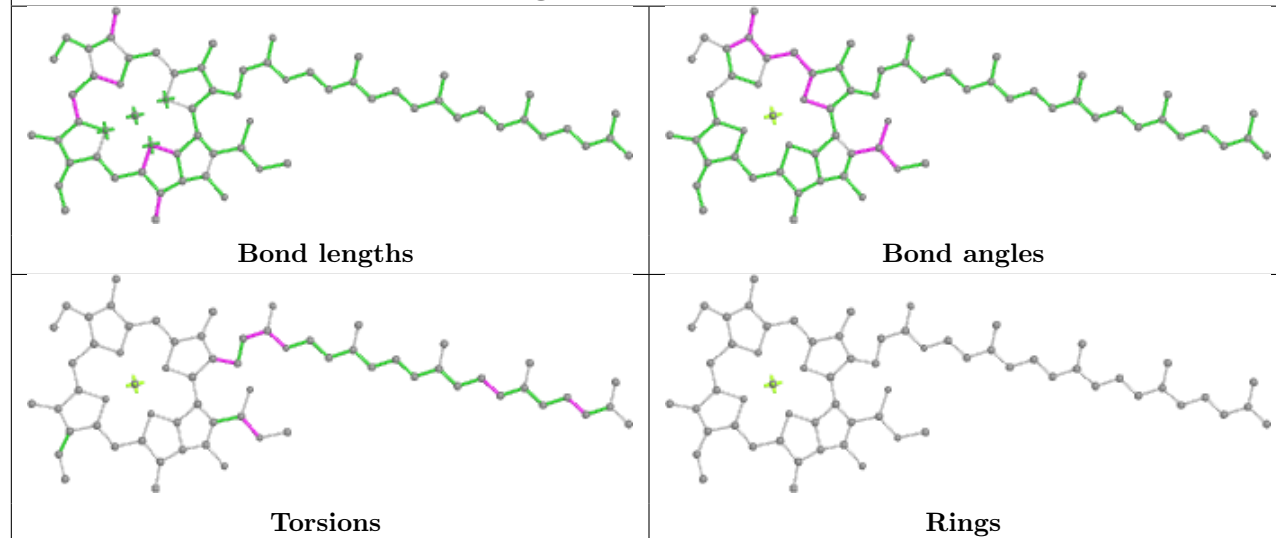


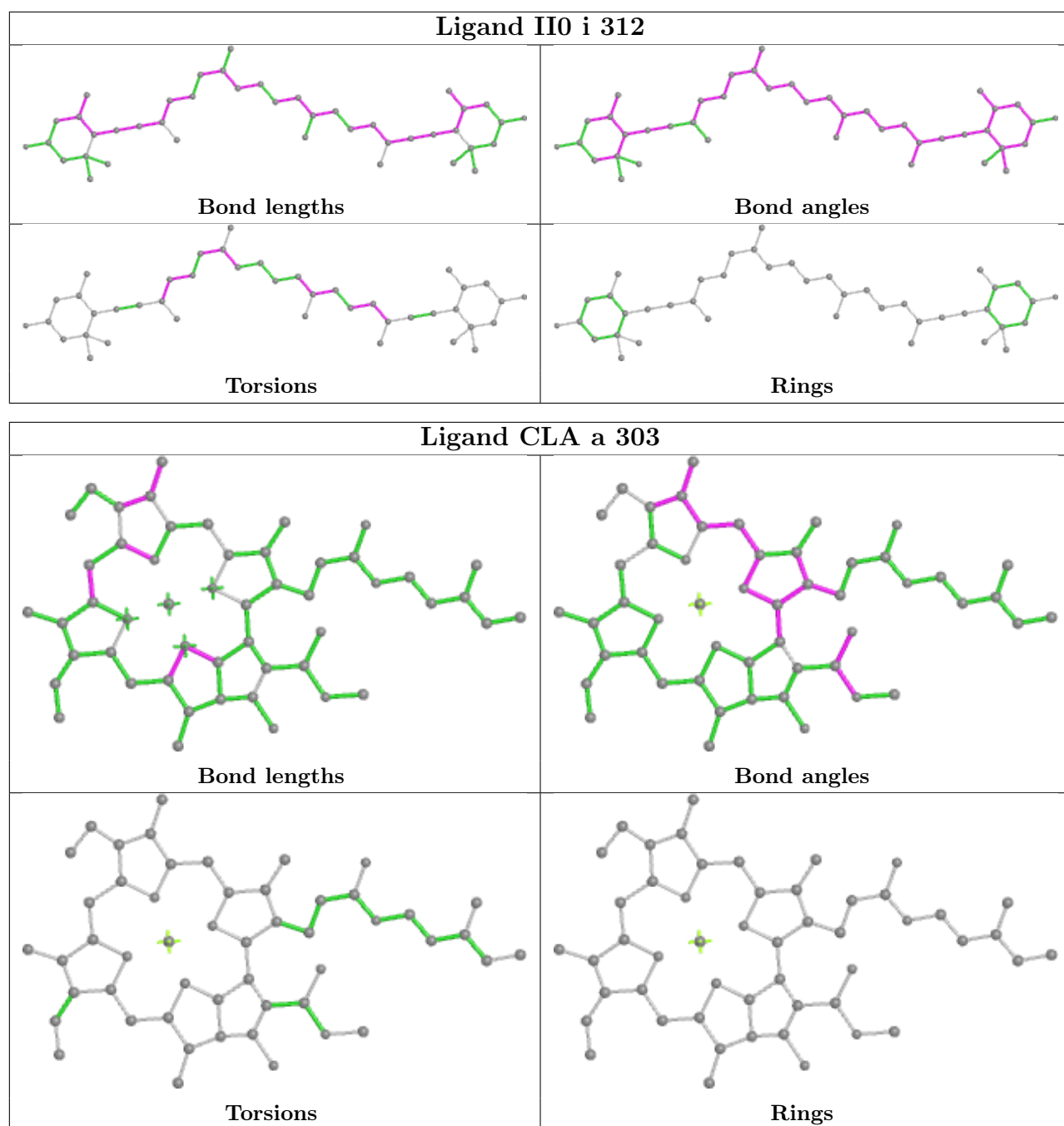
Ligand LMU A 850

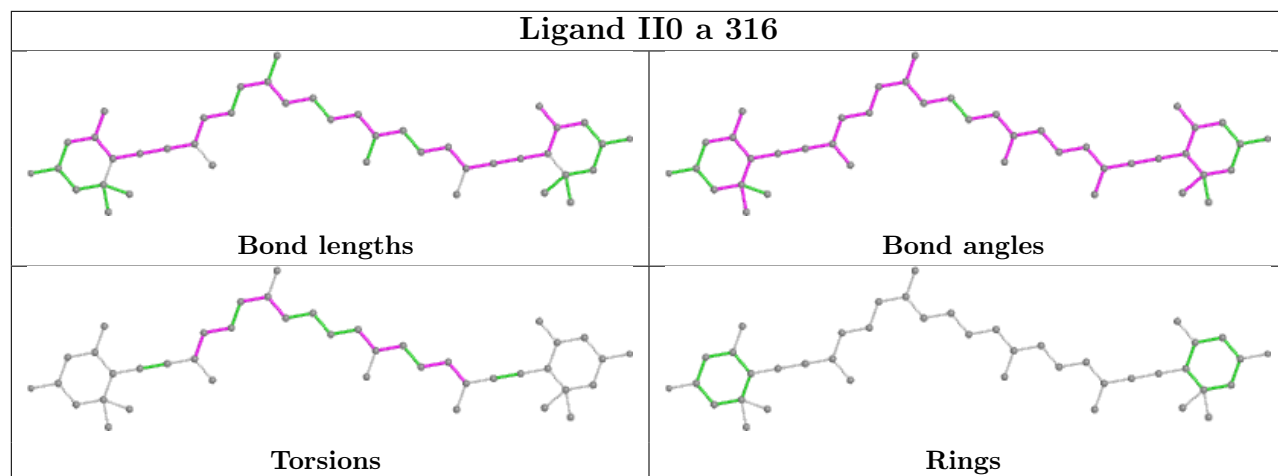
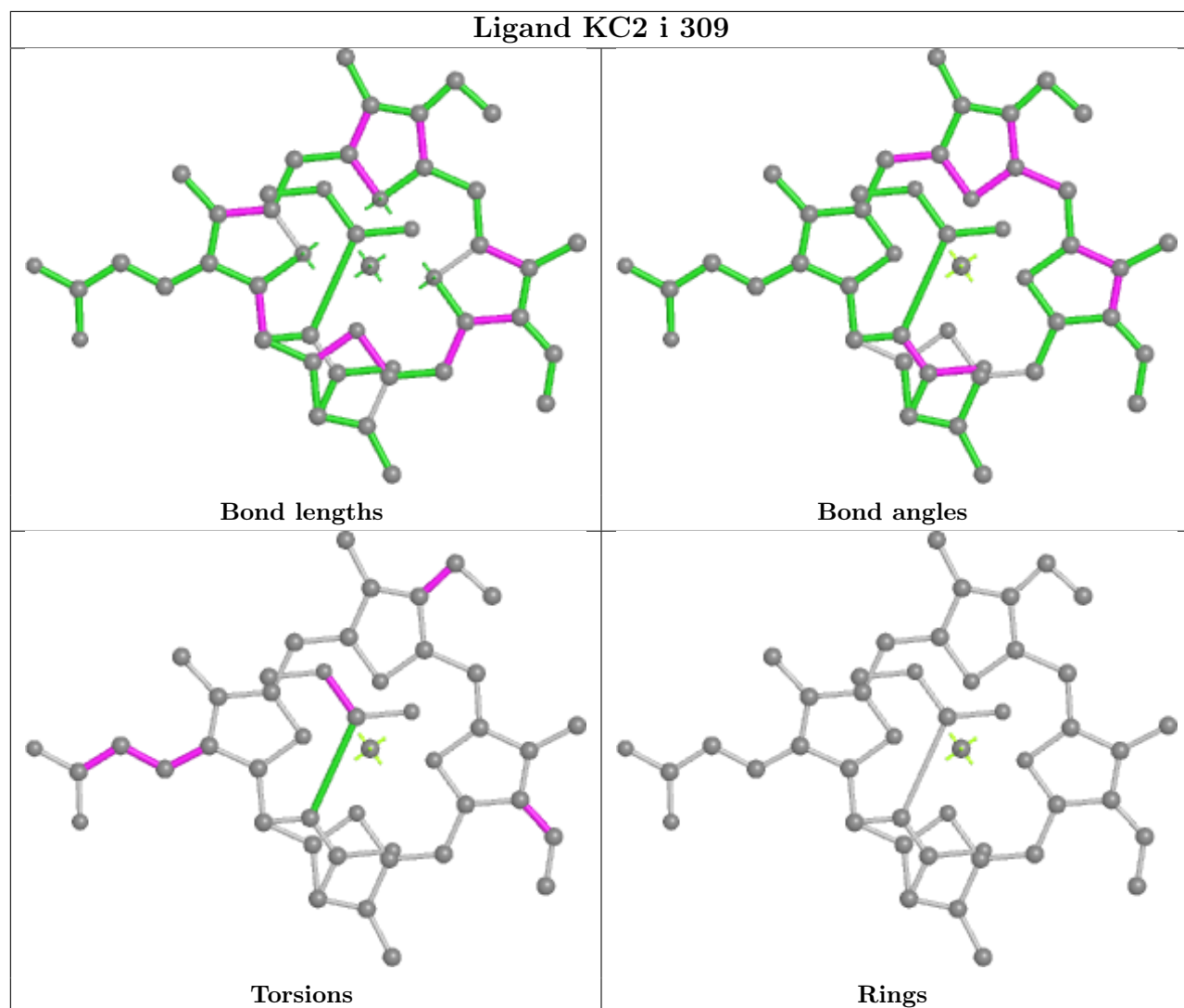


Ligand CLA B 841**Ligand CLA B 831**

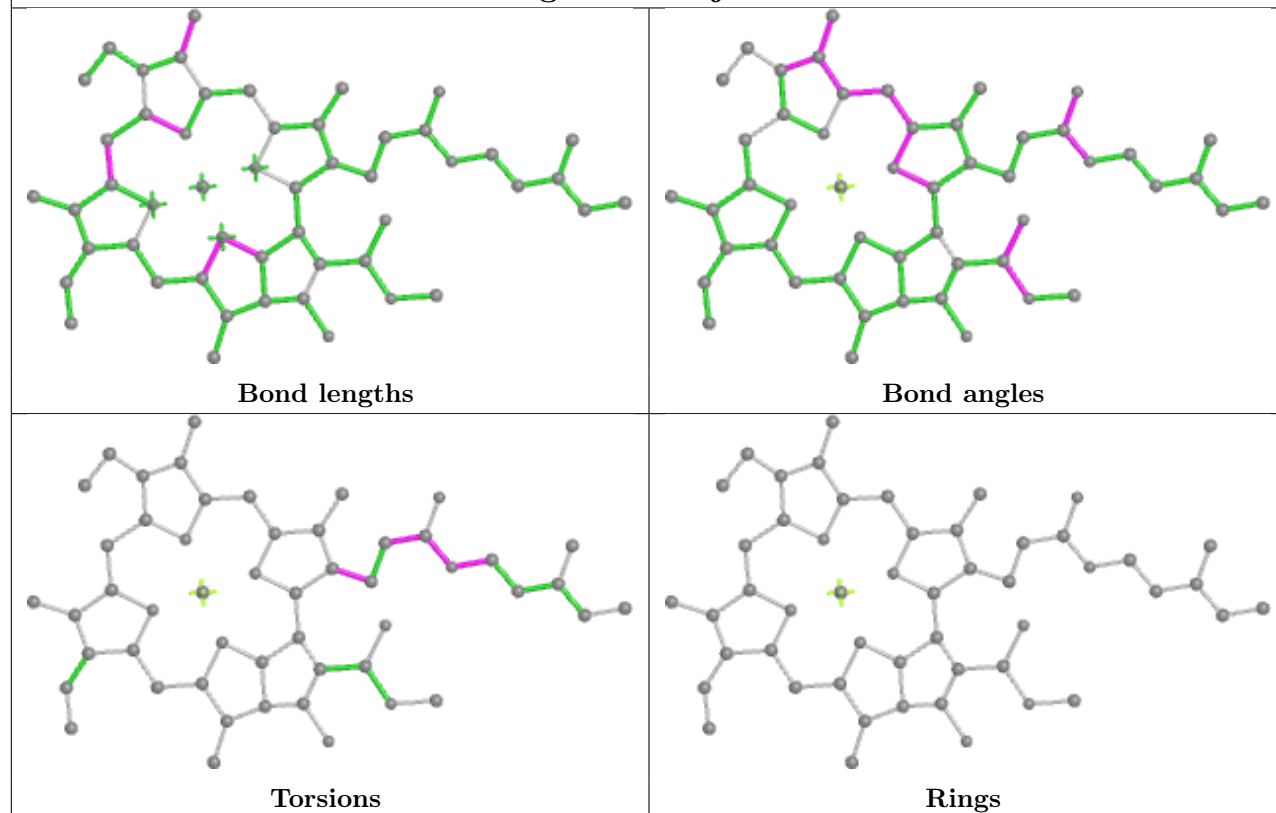


Ligand CLA A 856**Ligand CLA A 826****Ligand CLA B 820**

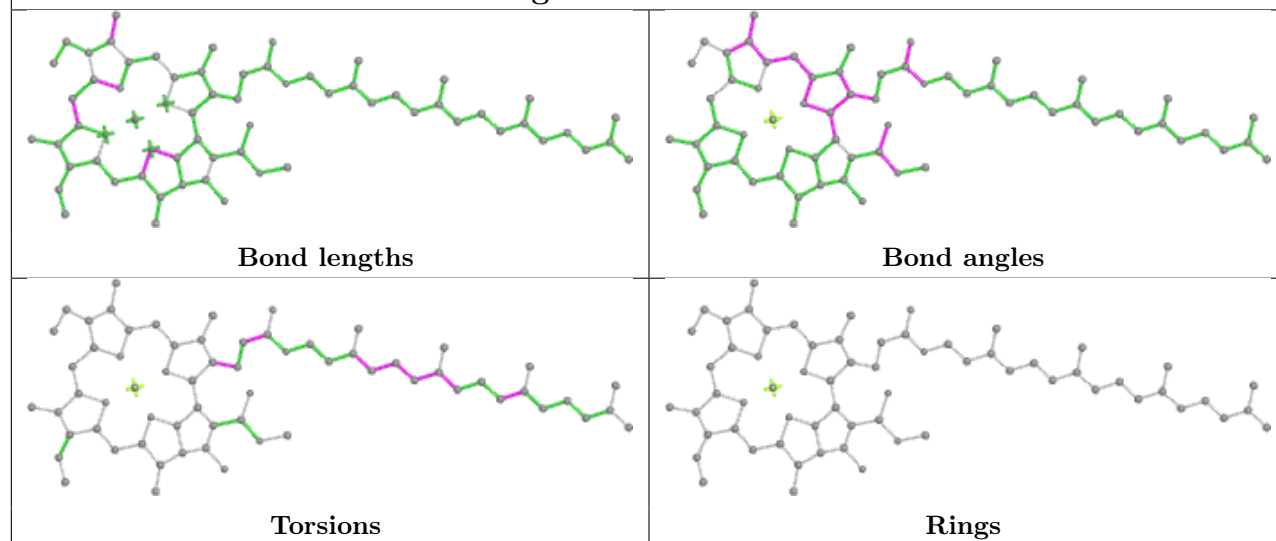


Ligand II0 a 316**Ligand KC2 i 309**

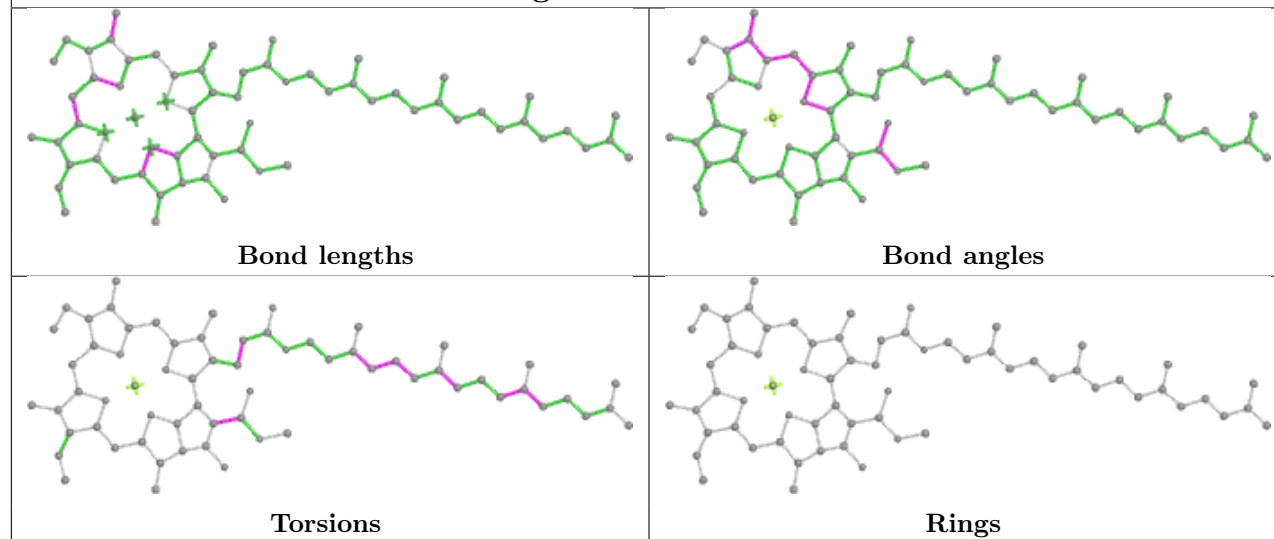
Ligand CLA j 606



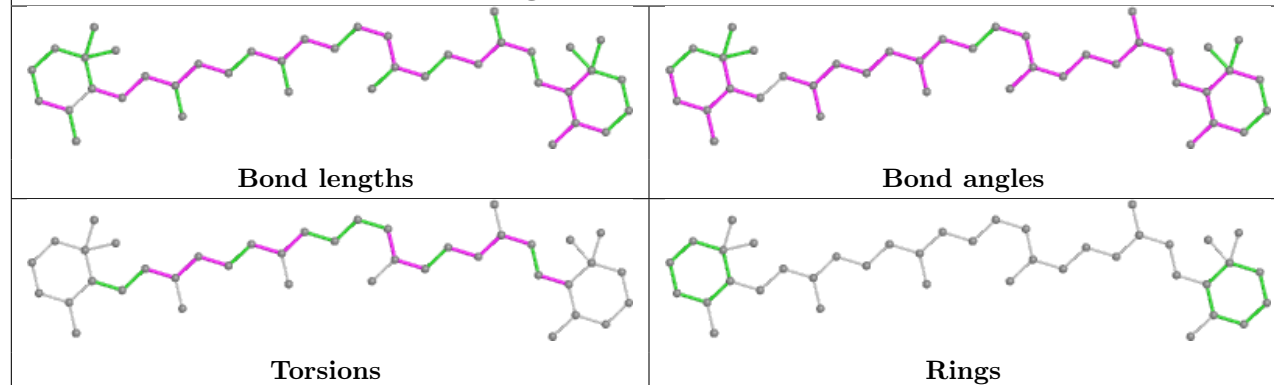
Ligand CLA A 841



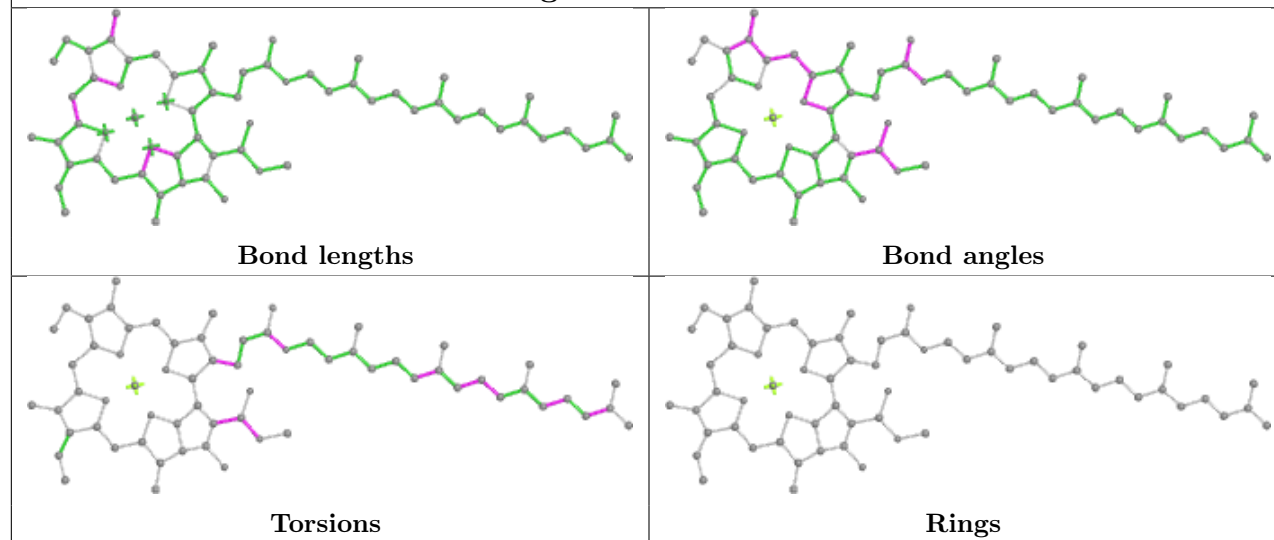
Ligand CLA B 807

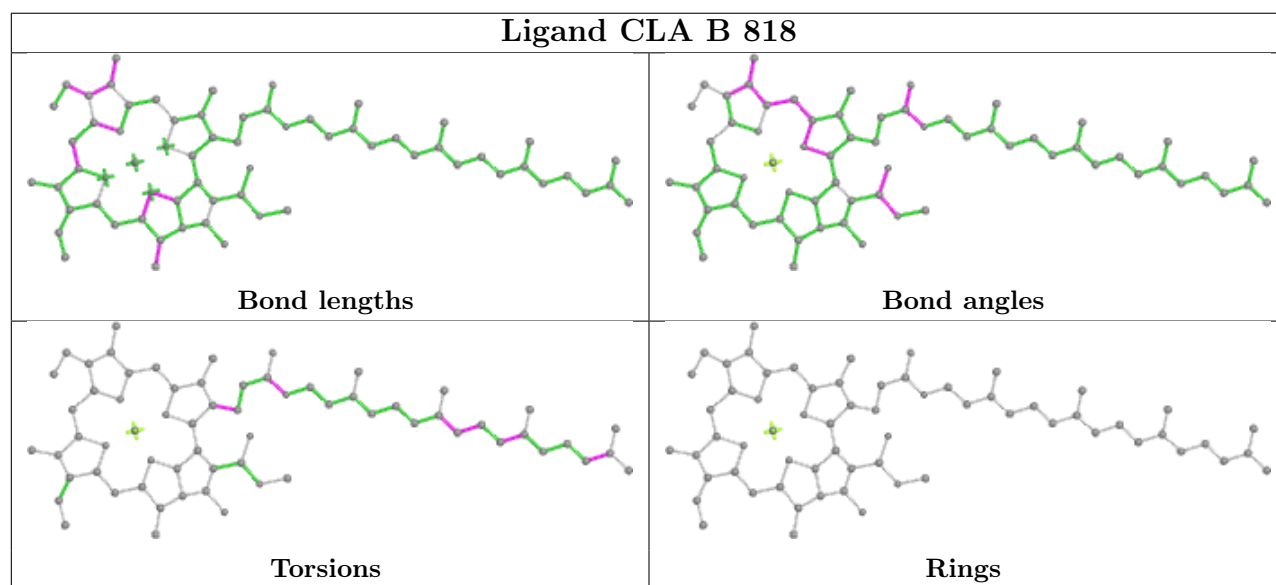
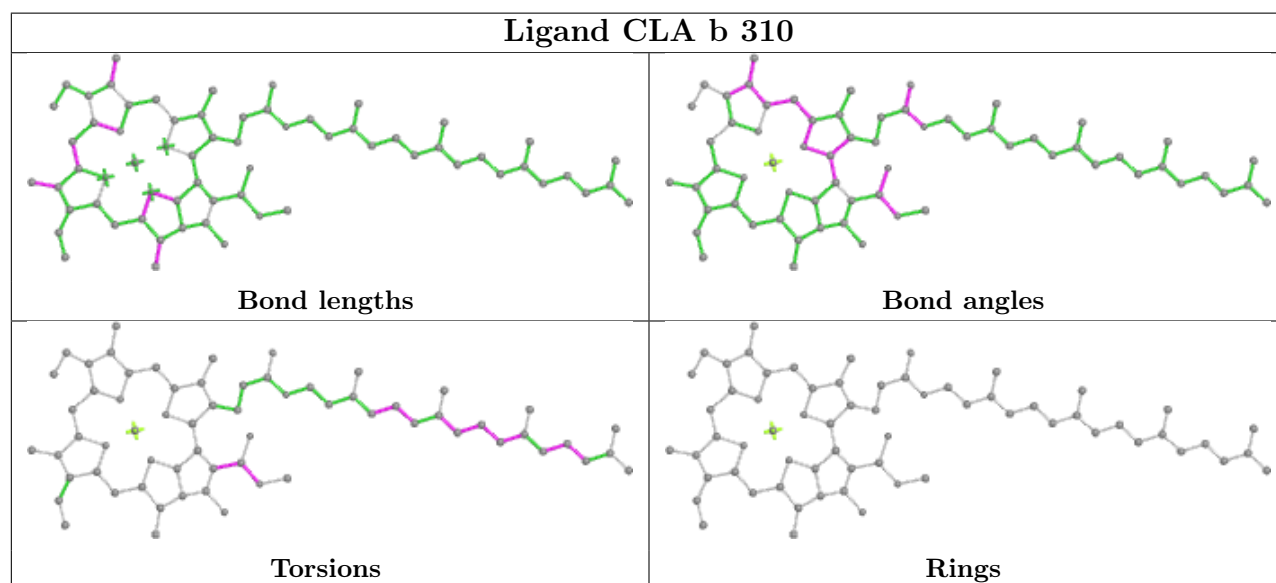
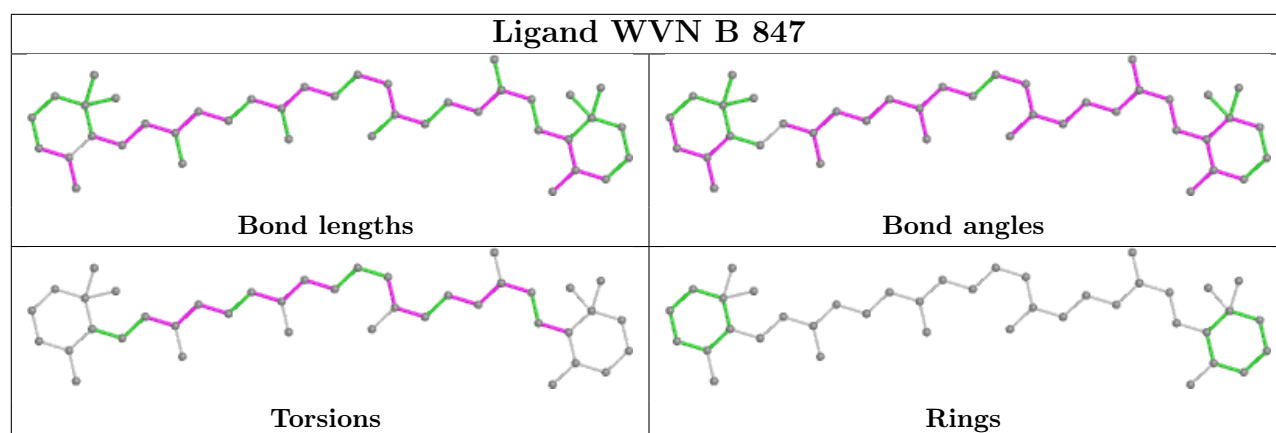


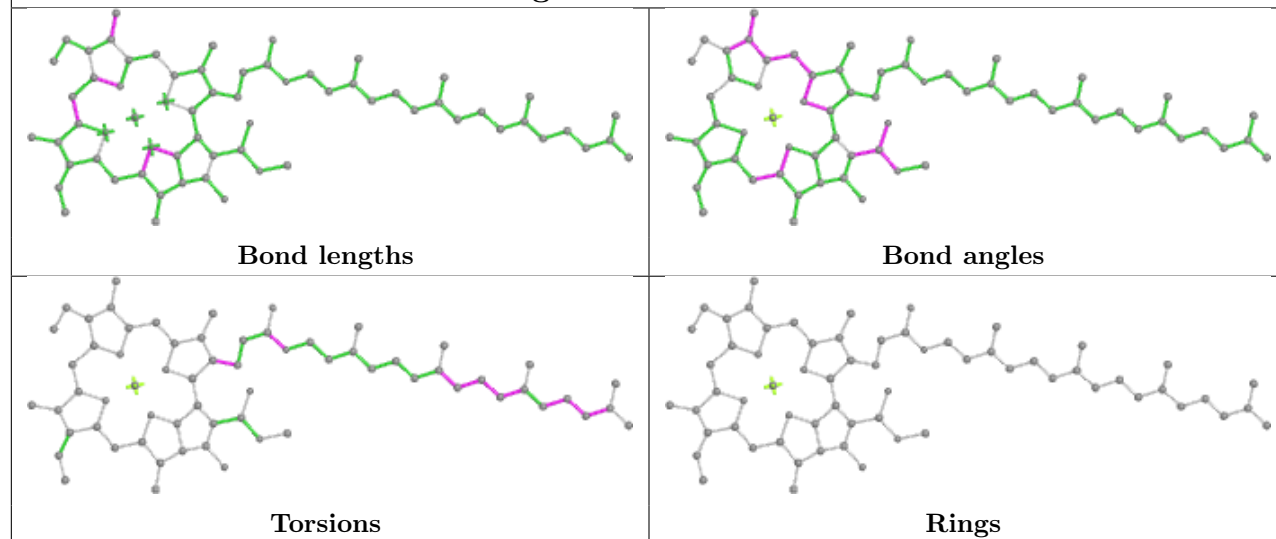
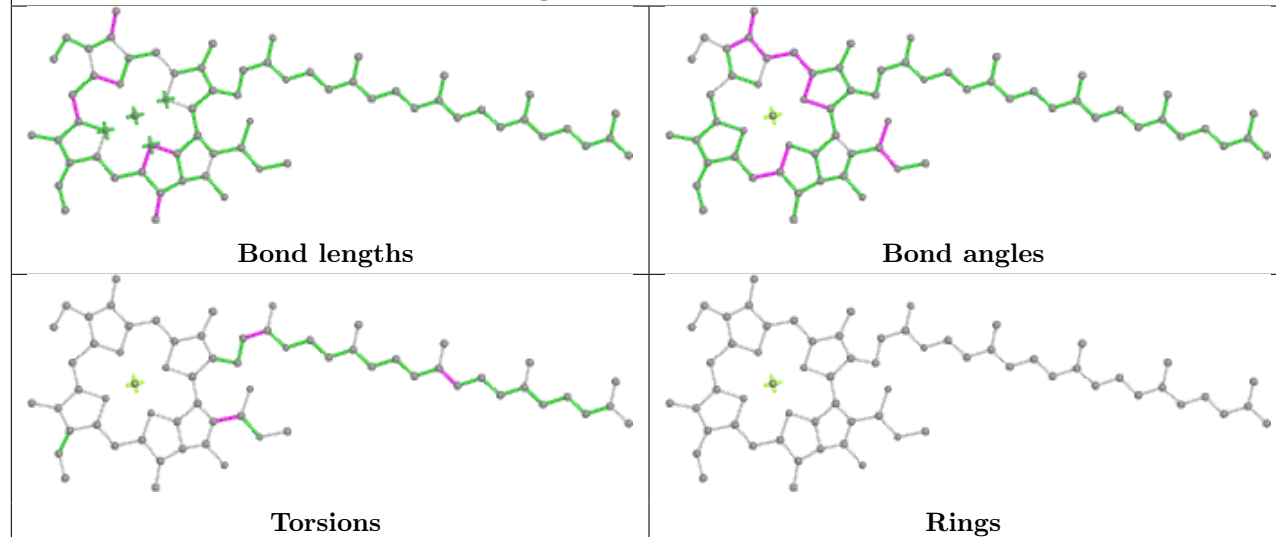
Ligand WVN A 846



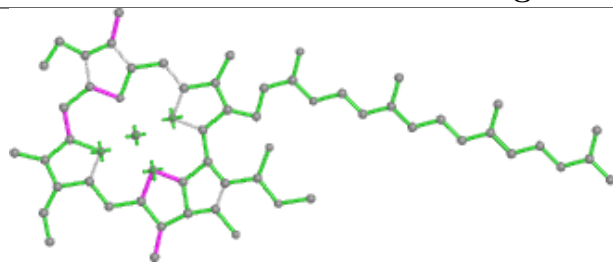
Ligand CLA I 305



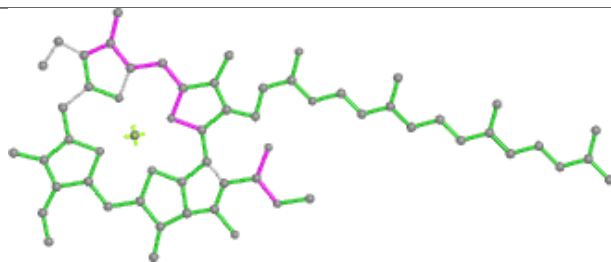


Ligand CLA B 810**Ligand CLA h 313**

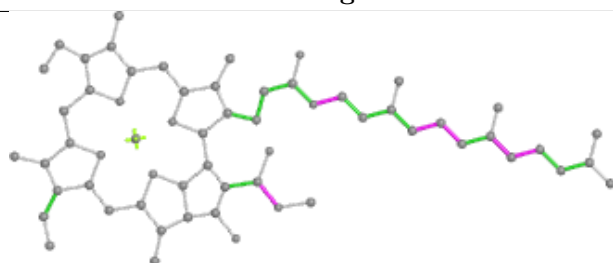
Ligand CLA A 830



Bond lengths



Bond angles

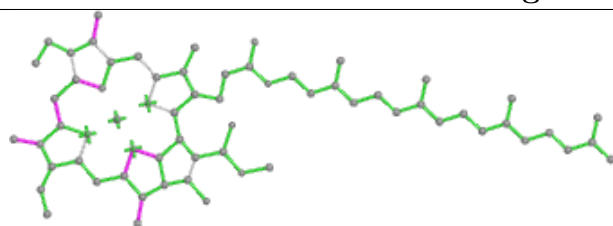


Torsions

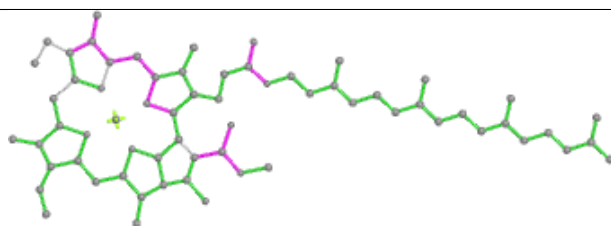


Rings

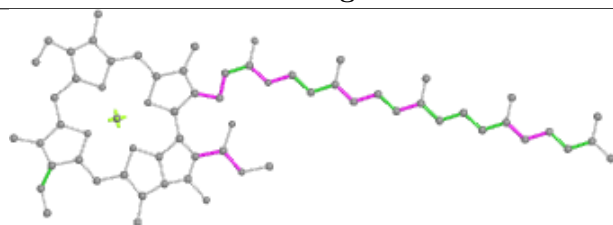
Ligand CLA i 302



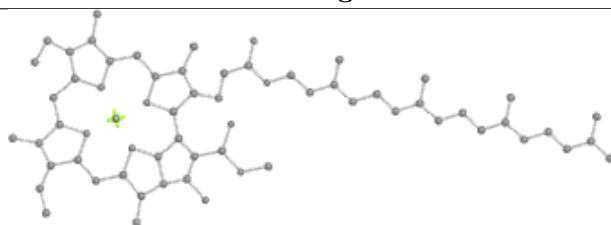
Bond lengths



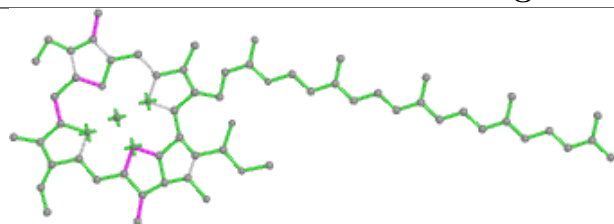
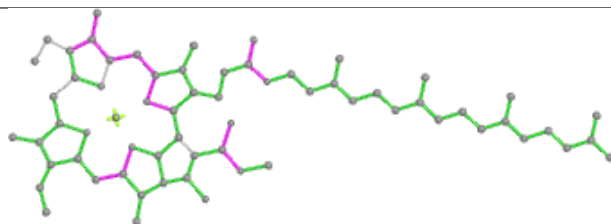
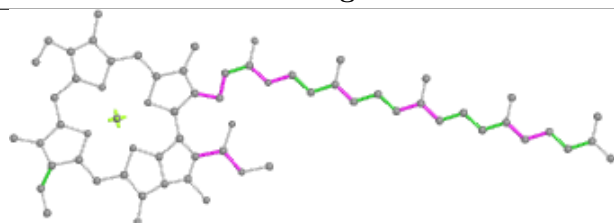
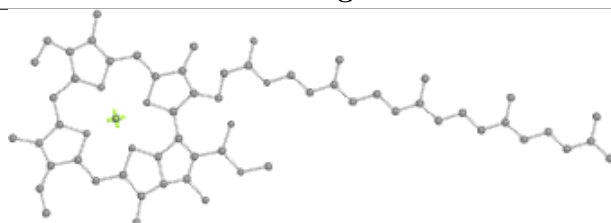
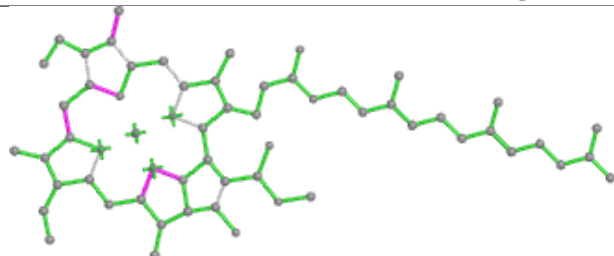
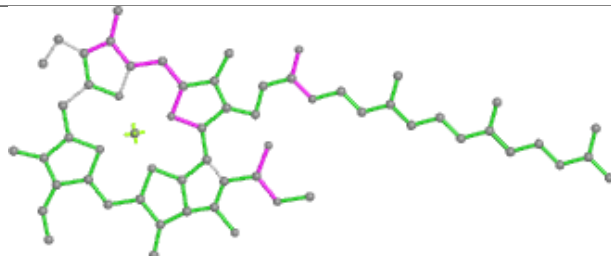
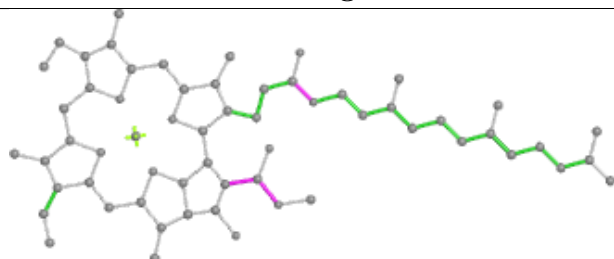
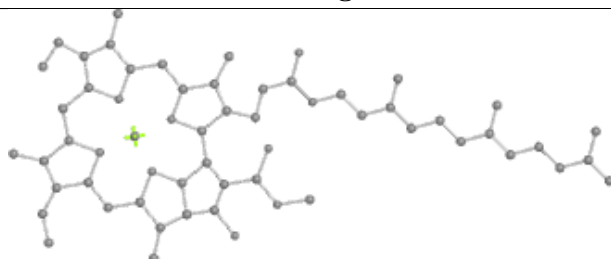
Bond angles



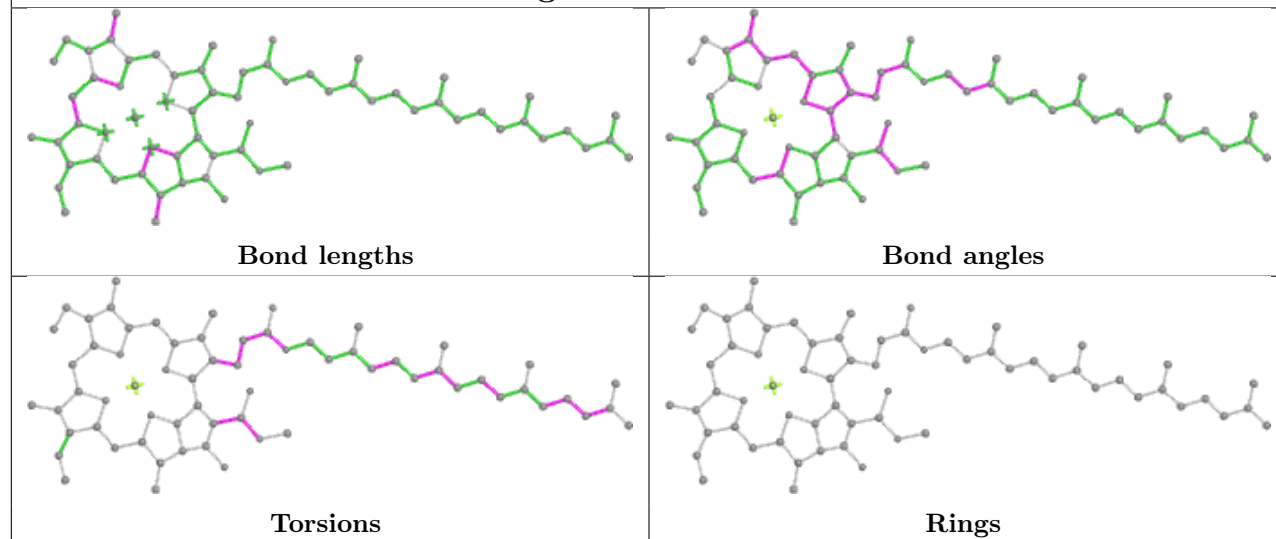
Torsions



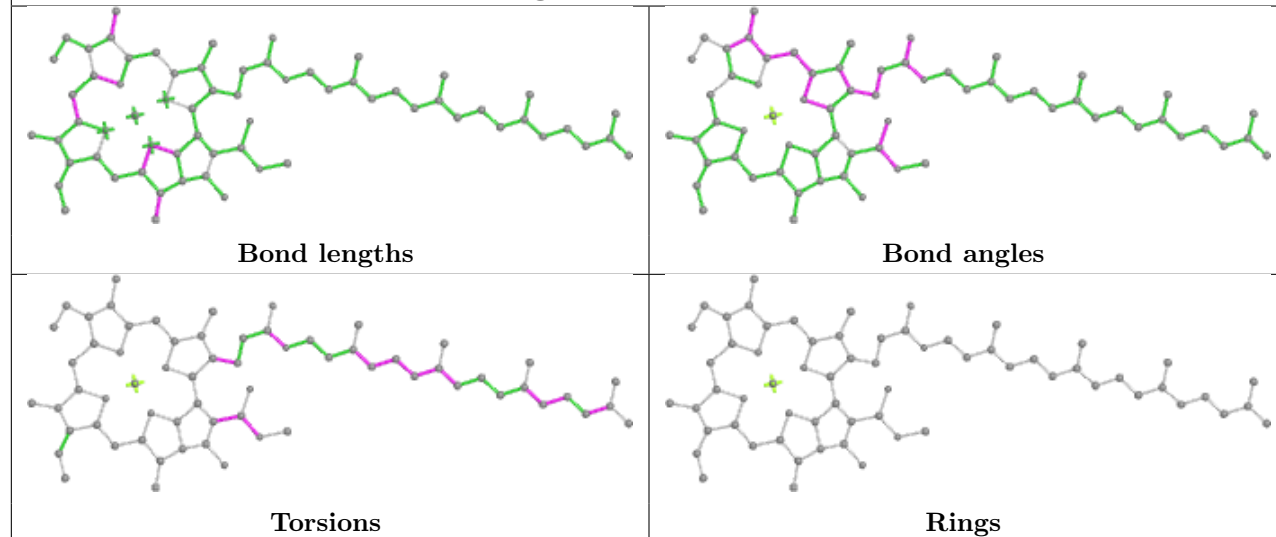
Rings

Ligand CLA B 825**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 806****Bond lengths****Bond angles****Torsions****Rings**

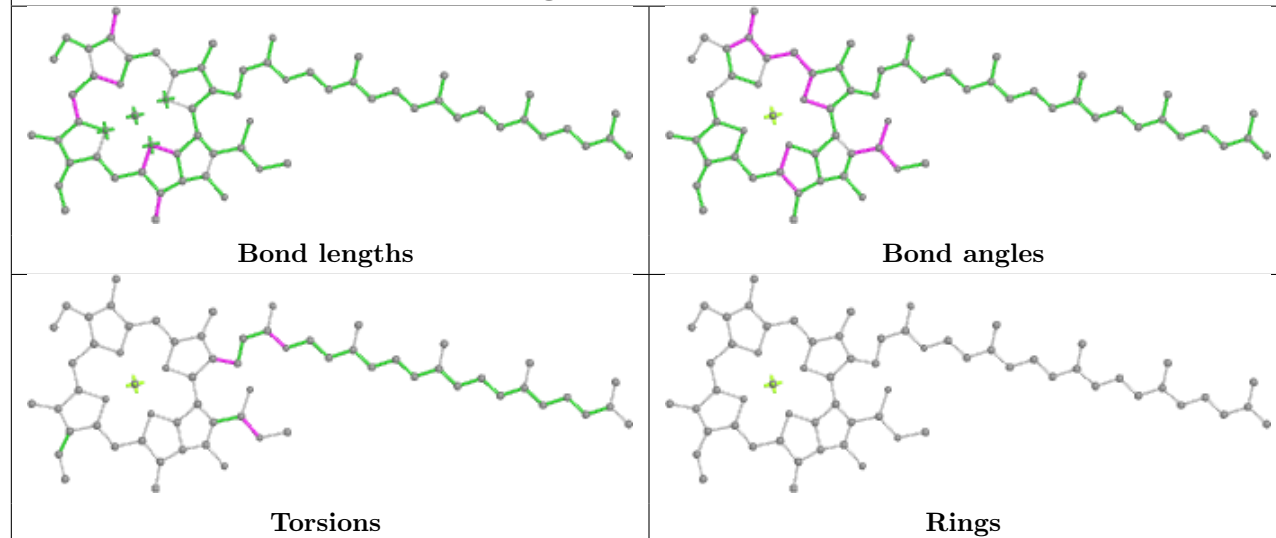
Ligand CLA s 402

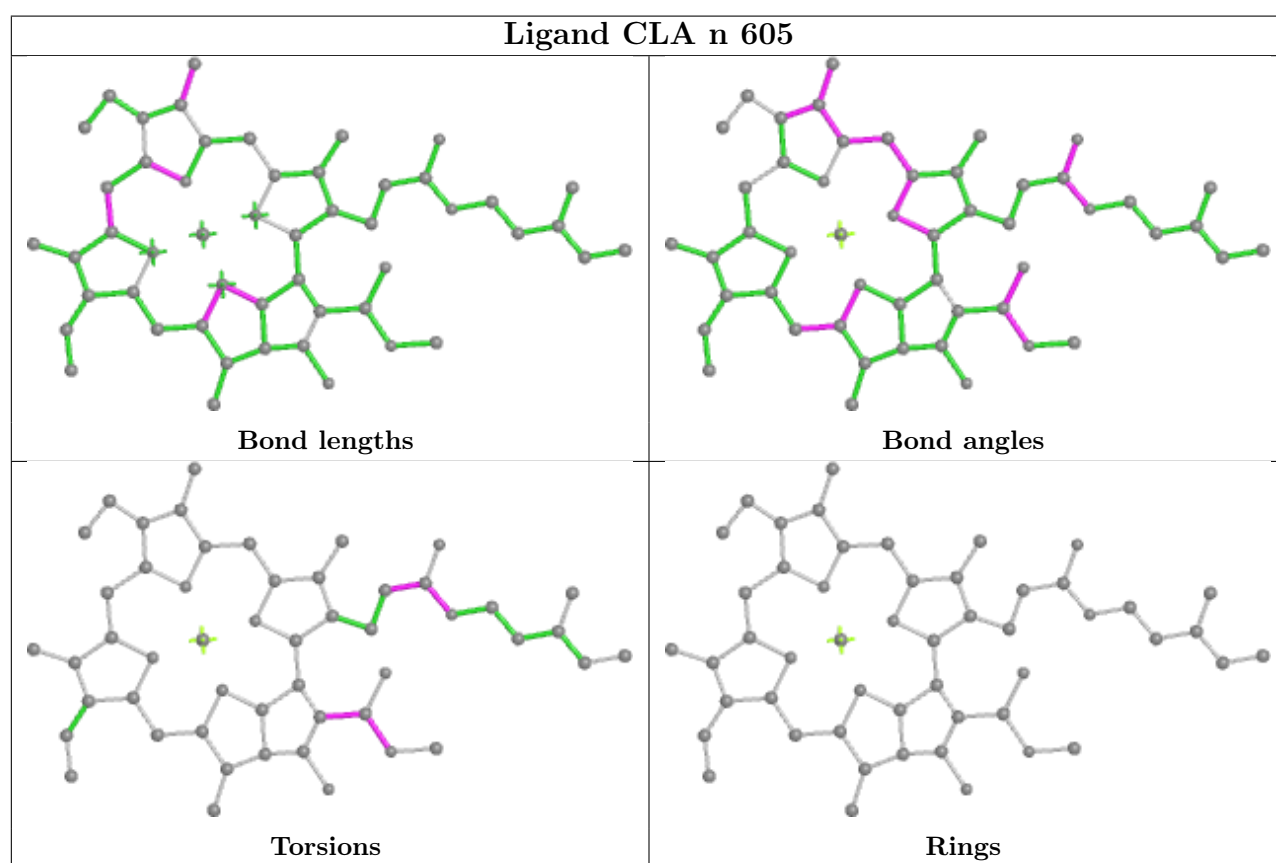
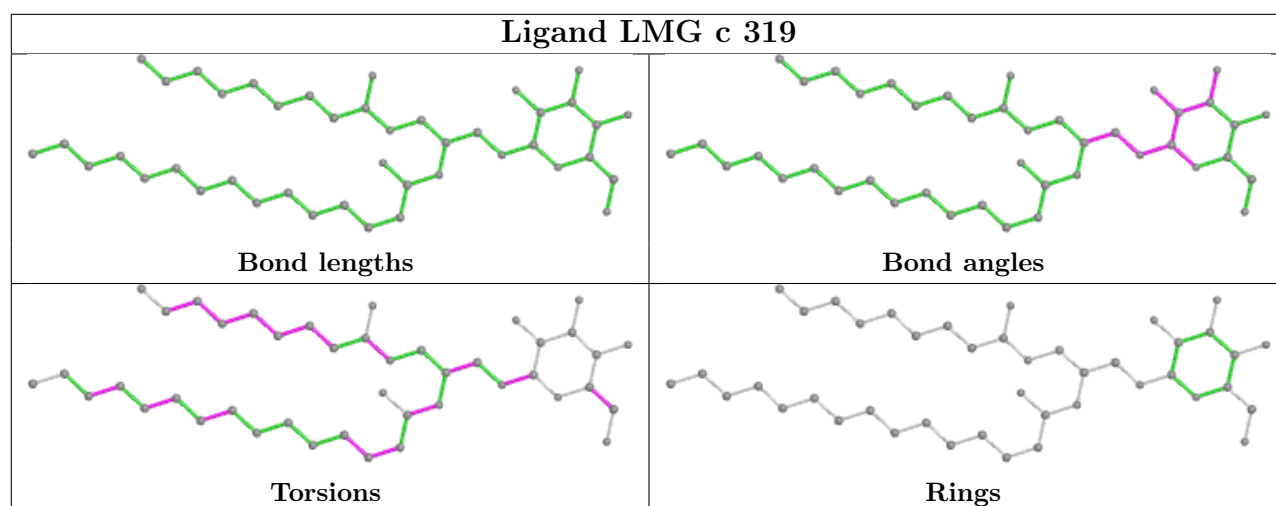


Ligand CLA A 816

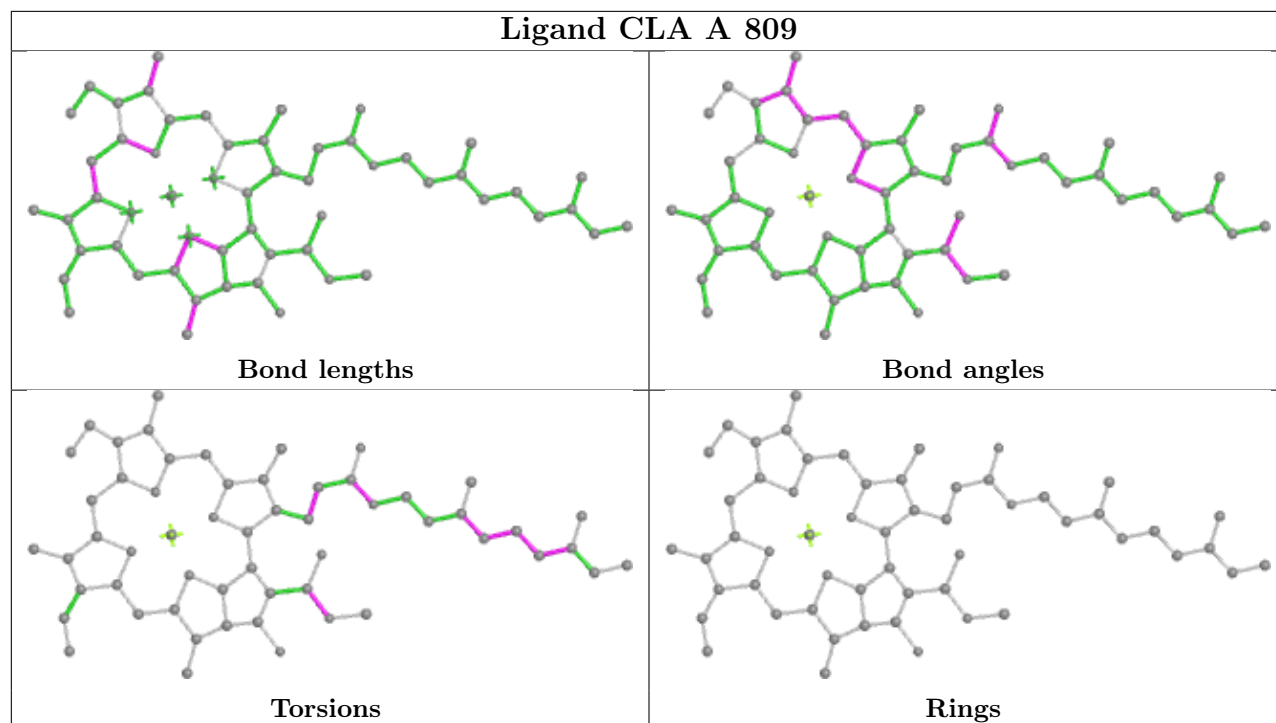


Ligand CLA l 309

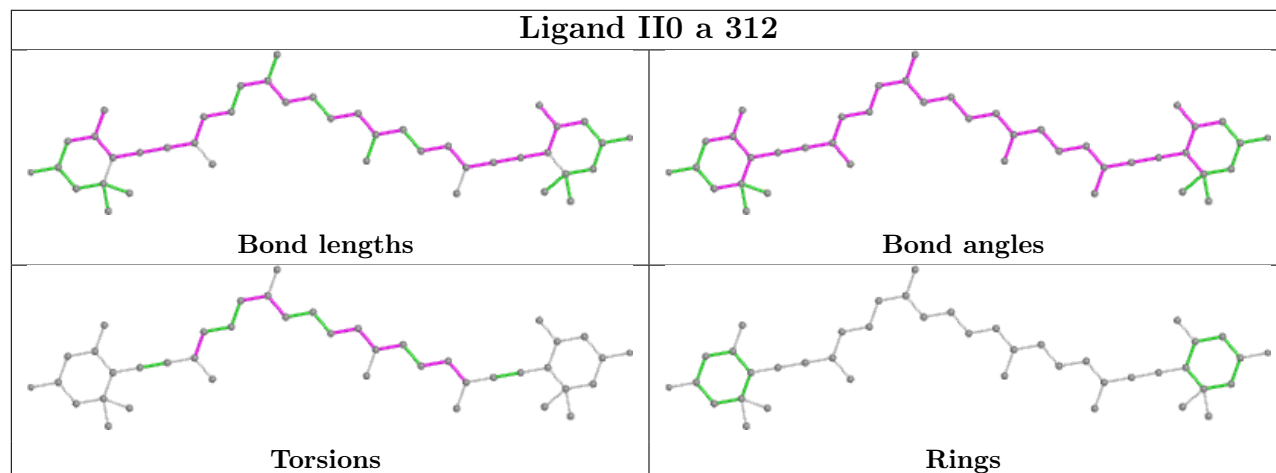




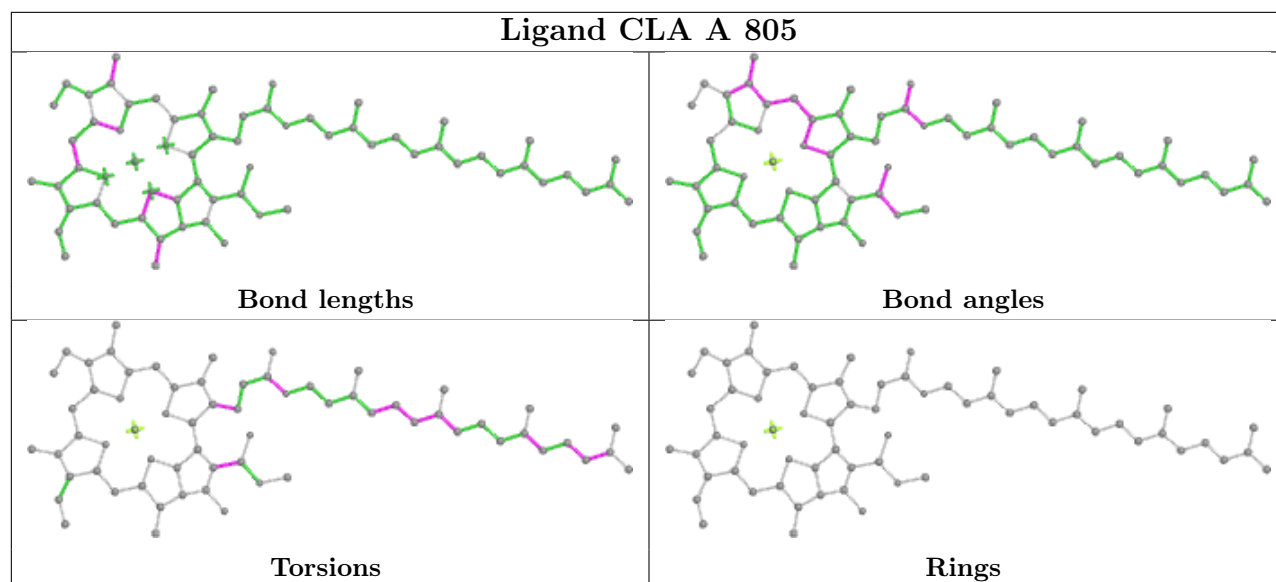
Ligand CLA A 809

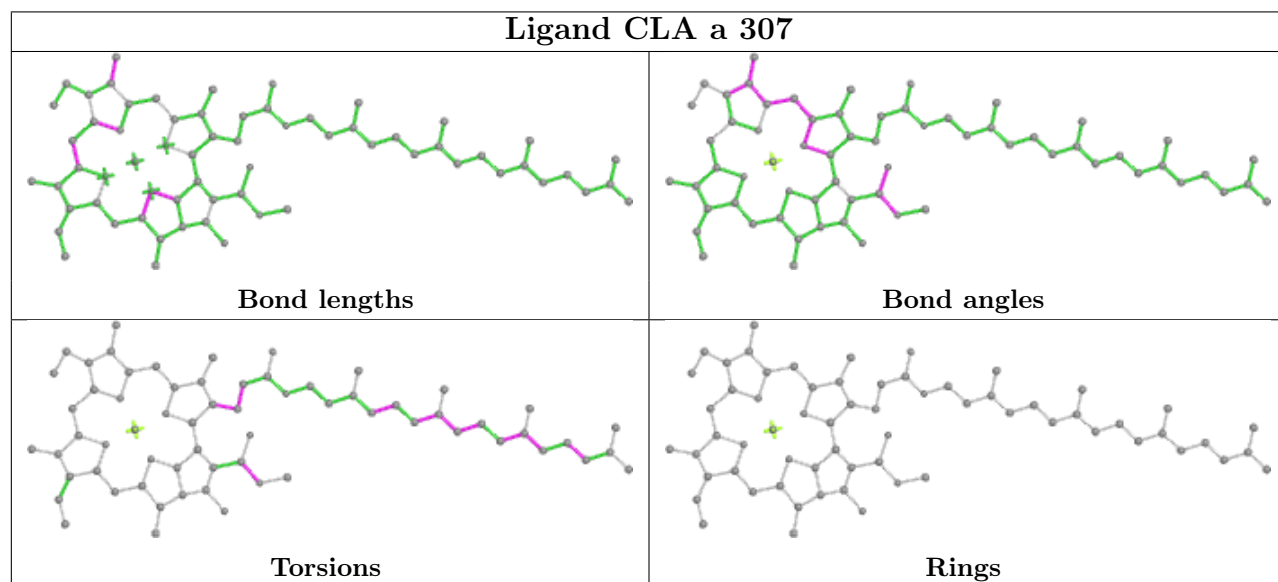
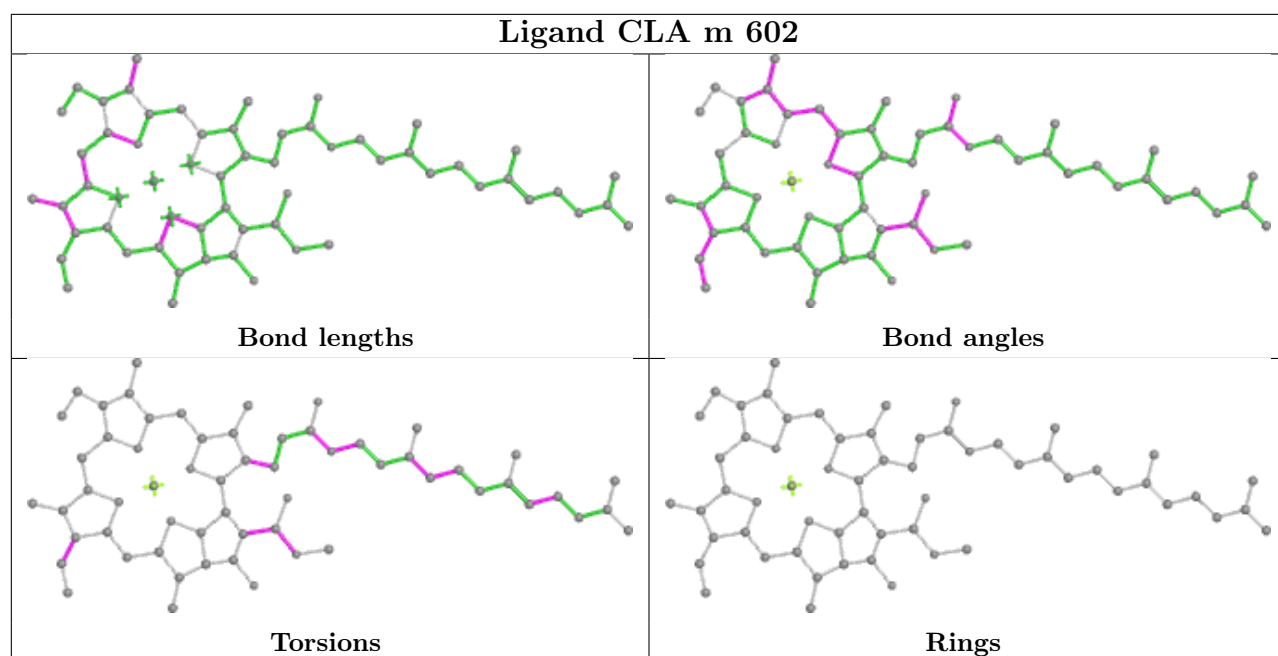


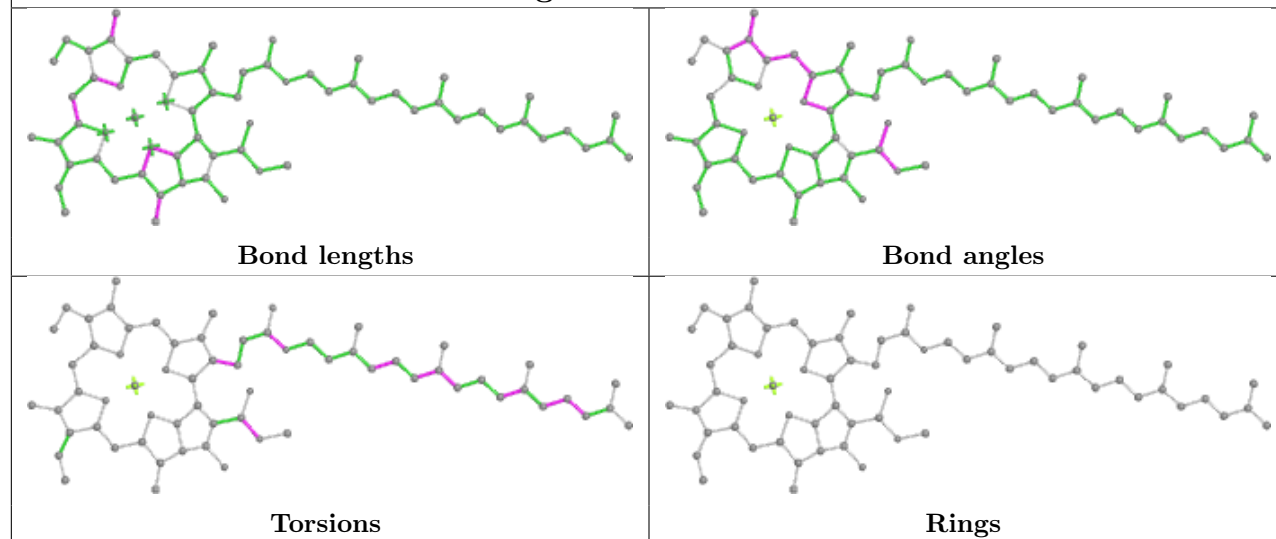
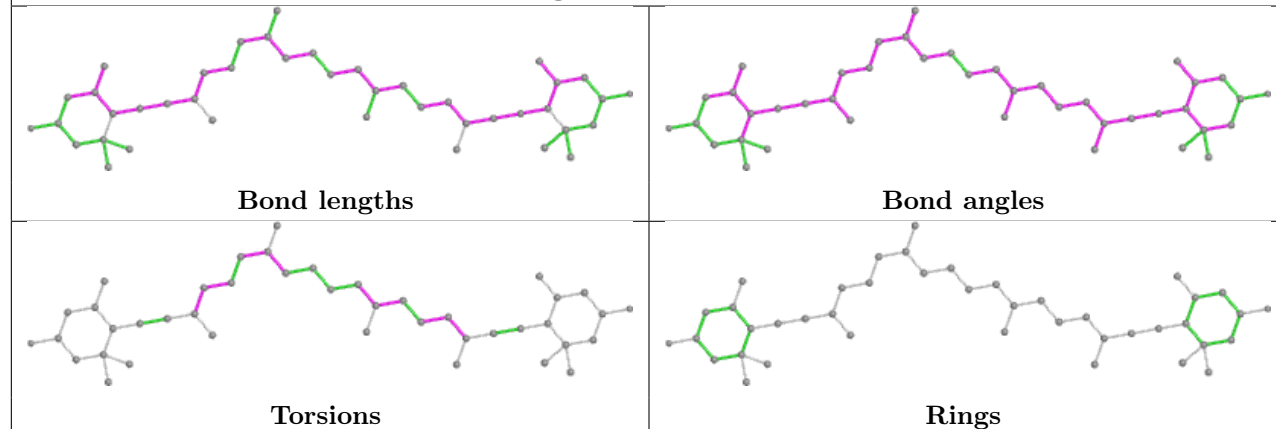
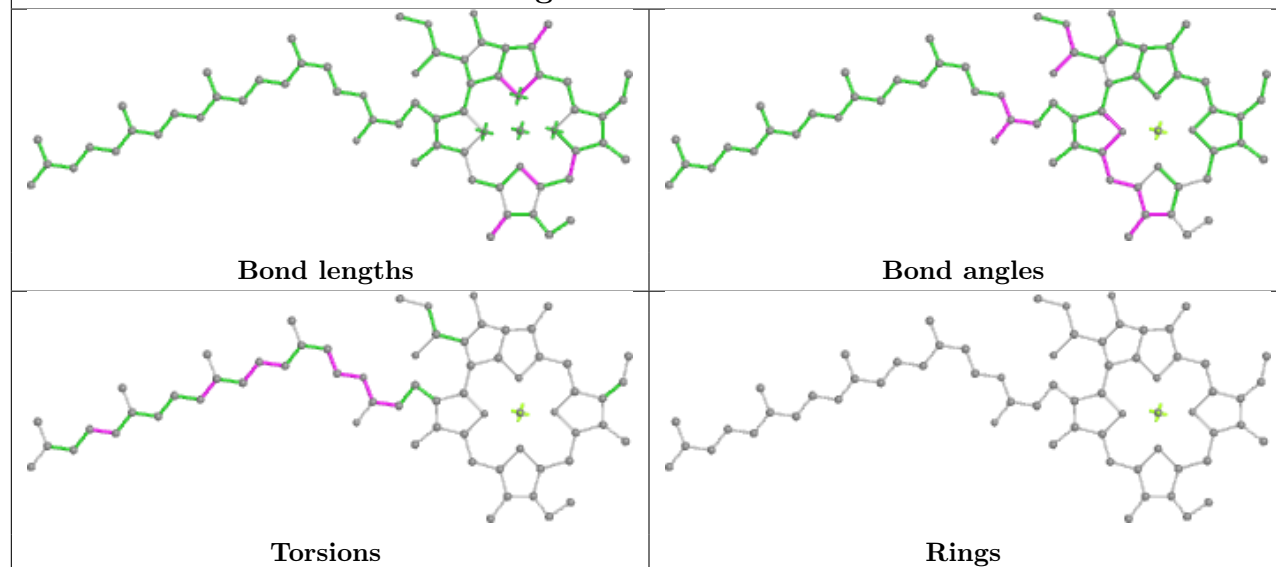
Ligand II0 a 312

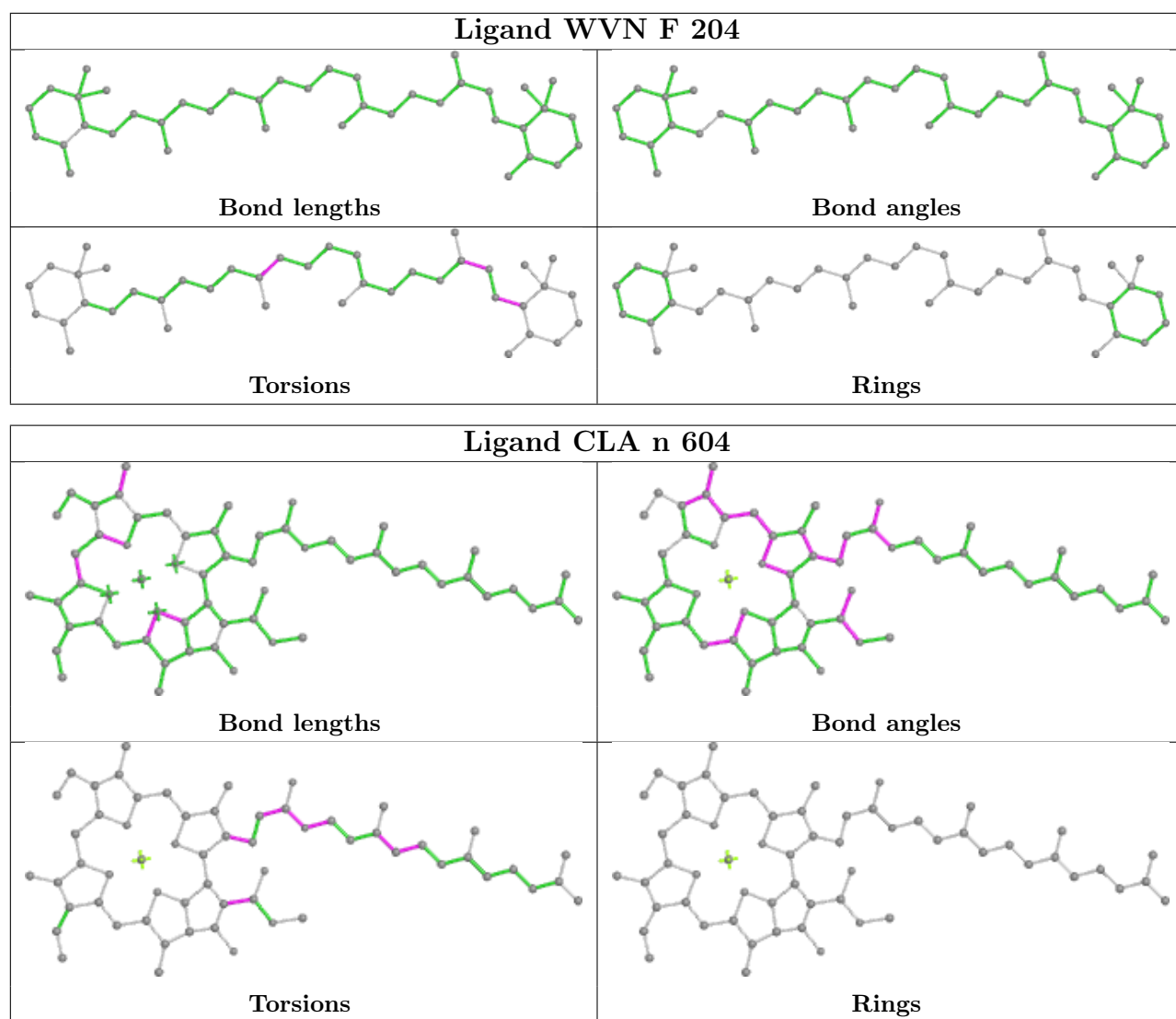


Ligand CLA A 805

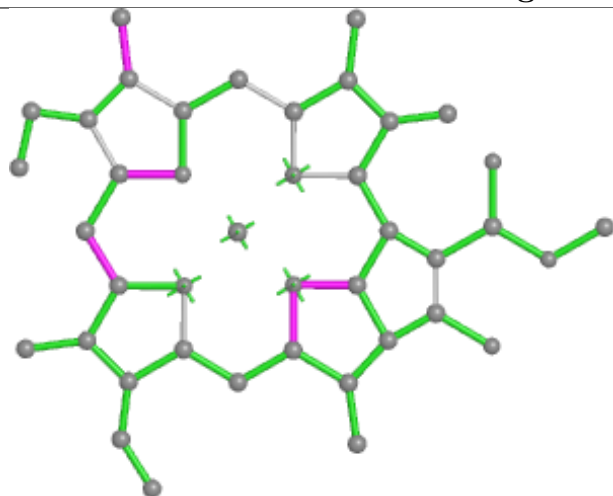




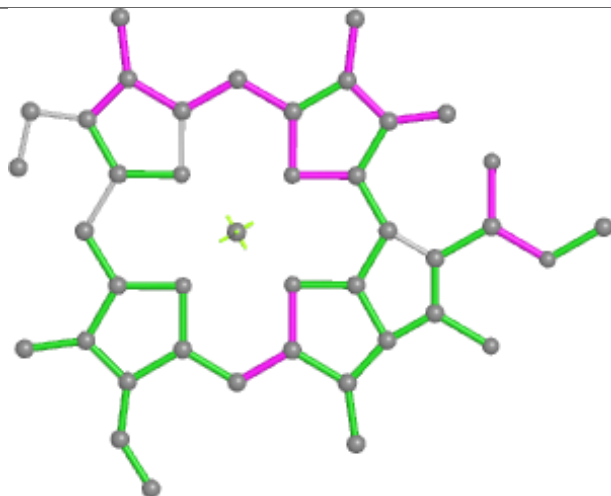
Ligand CLA k 602**Ligand II0 d 317****Ligand CLA h 301**



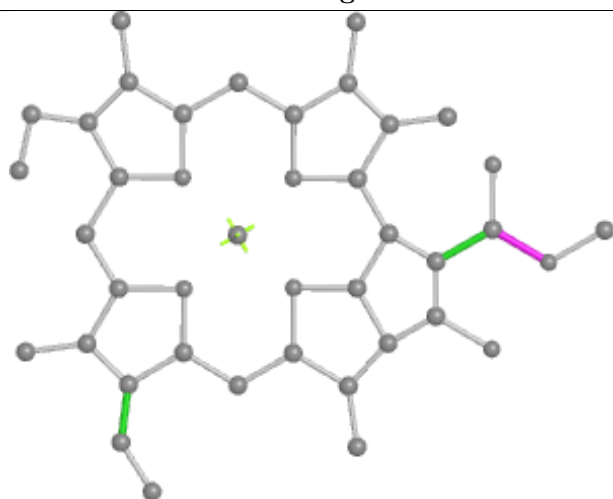
Ligand CLA d 309



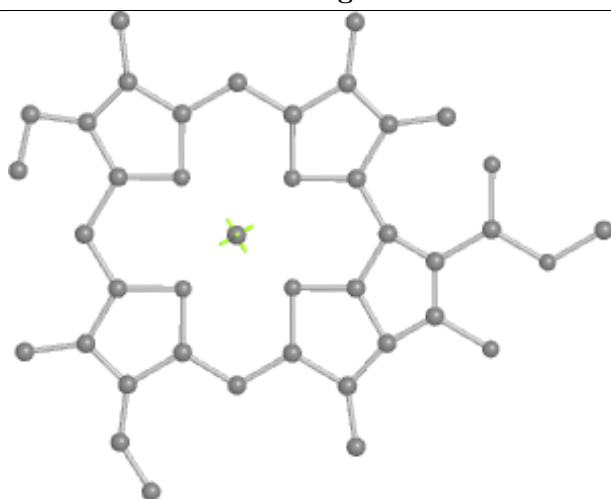
Bond lengths



Bond angles

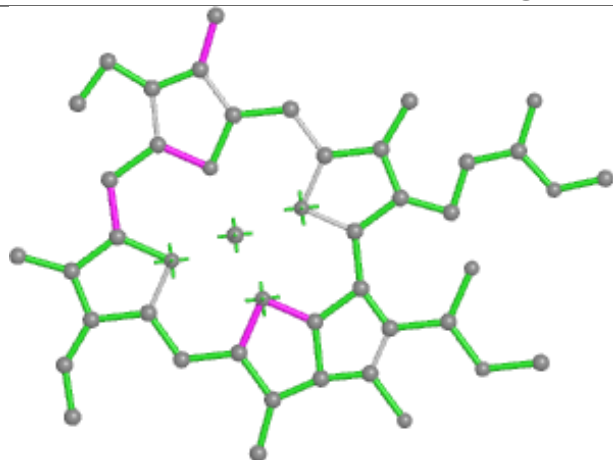


Torsions

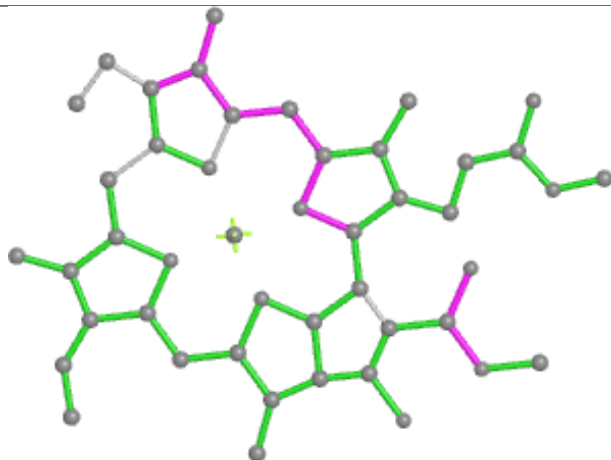


Rings

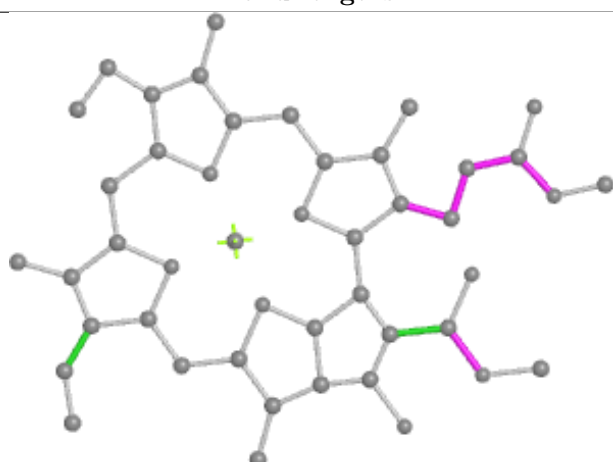
Ligand CLA d 308



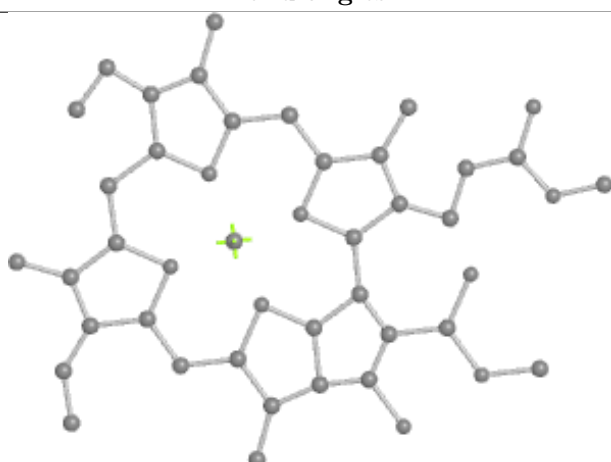
Bond lengths



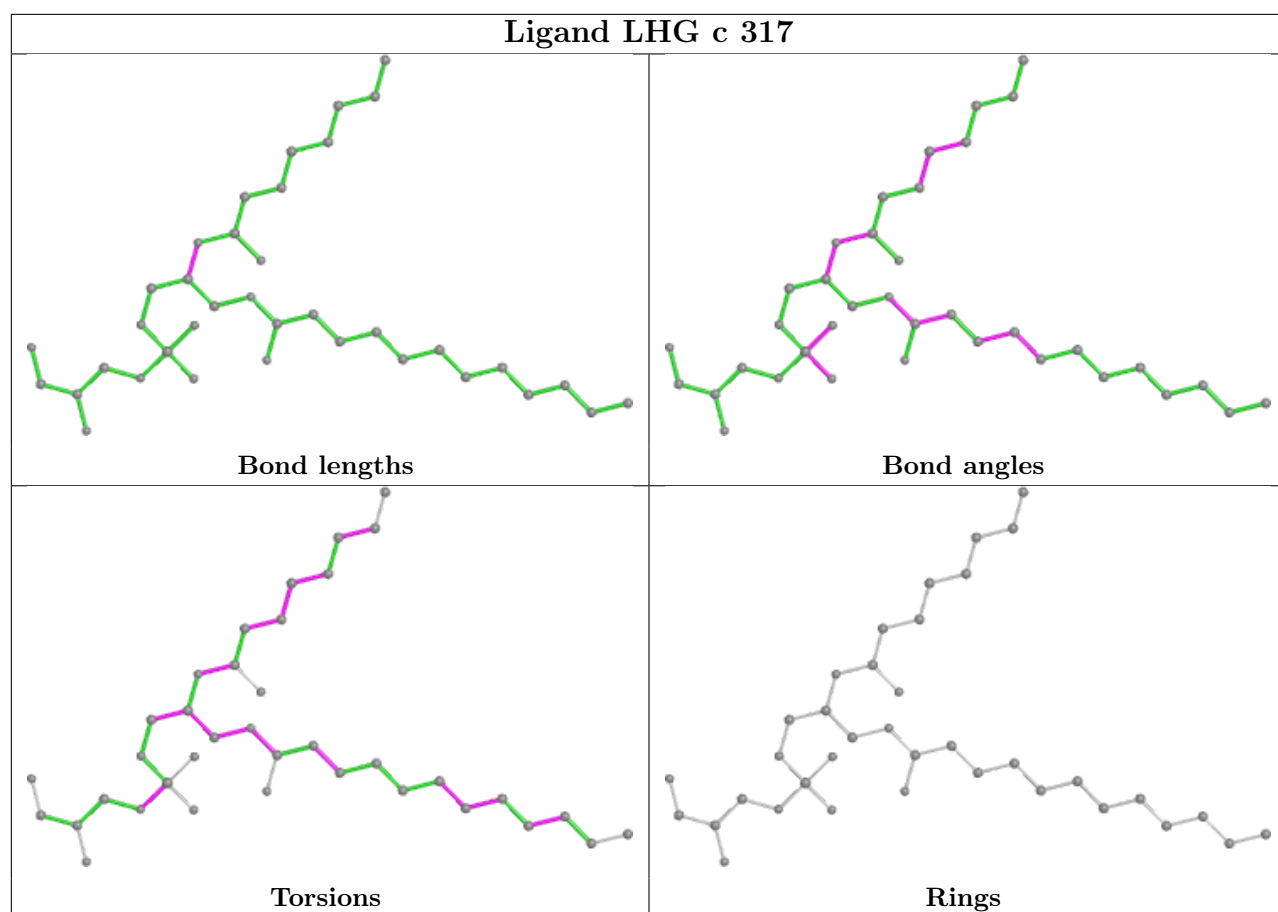
Bond angles



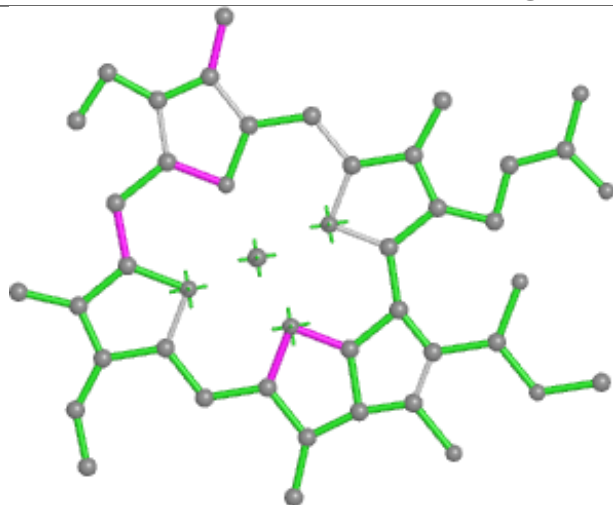
Torsions



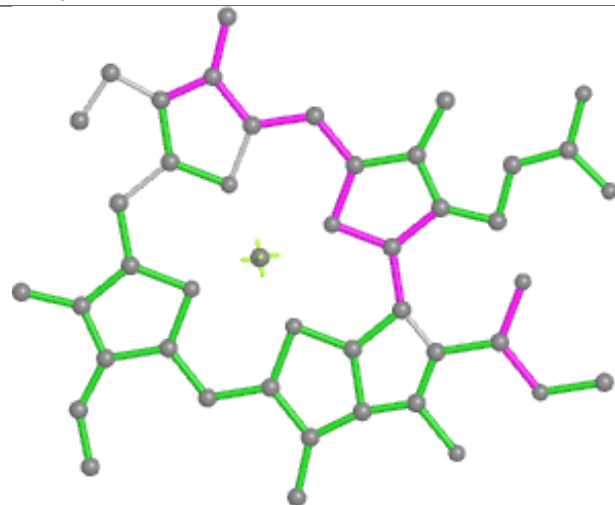
Rings



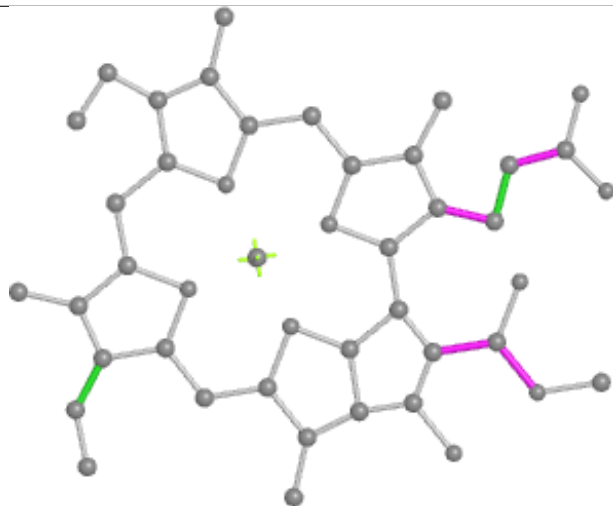
Ligand CLA j 605



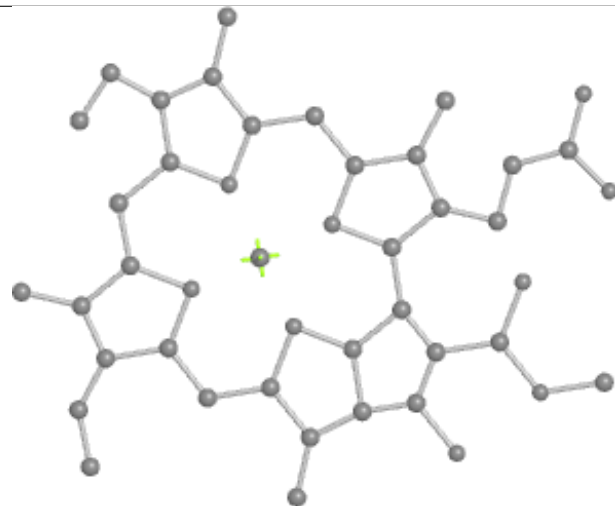
Bond lengths



Bond angles

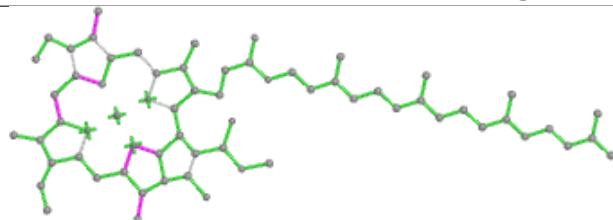


Torsions

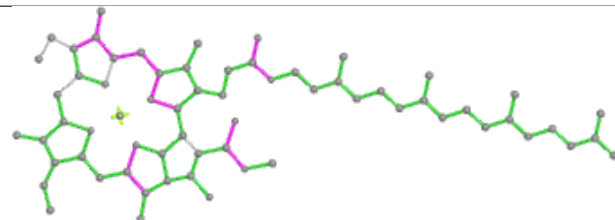


Rings

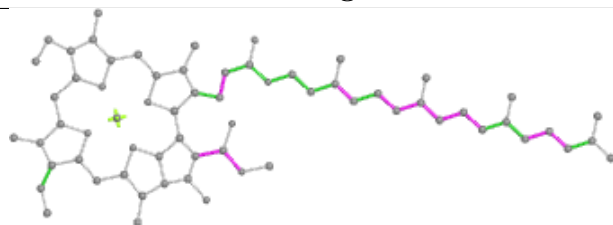
Ligand CLA B 836



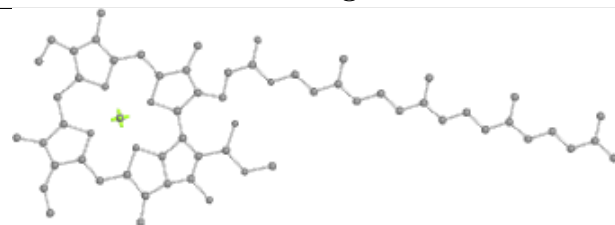
Bond lengths



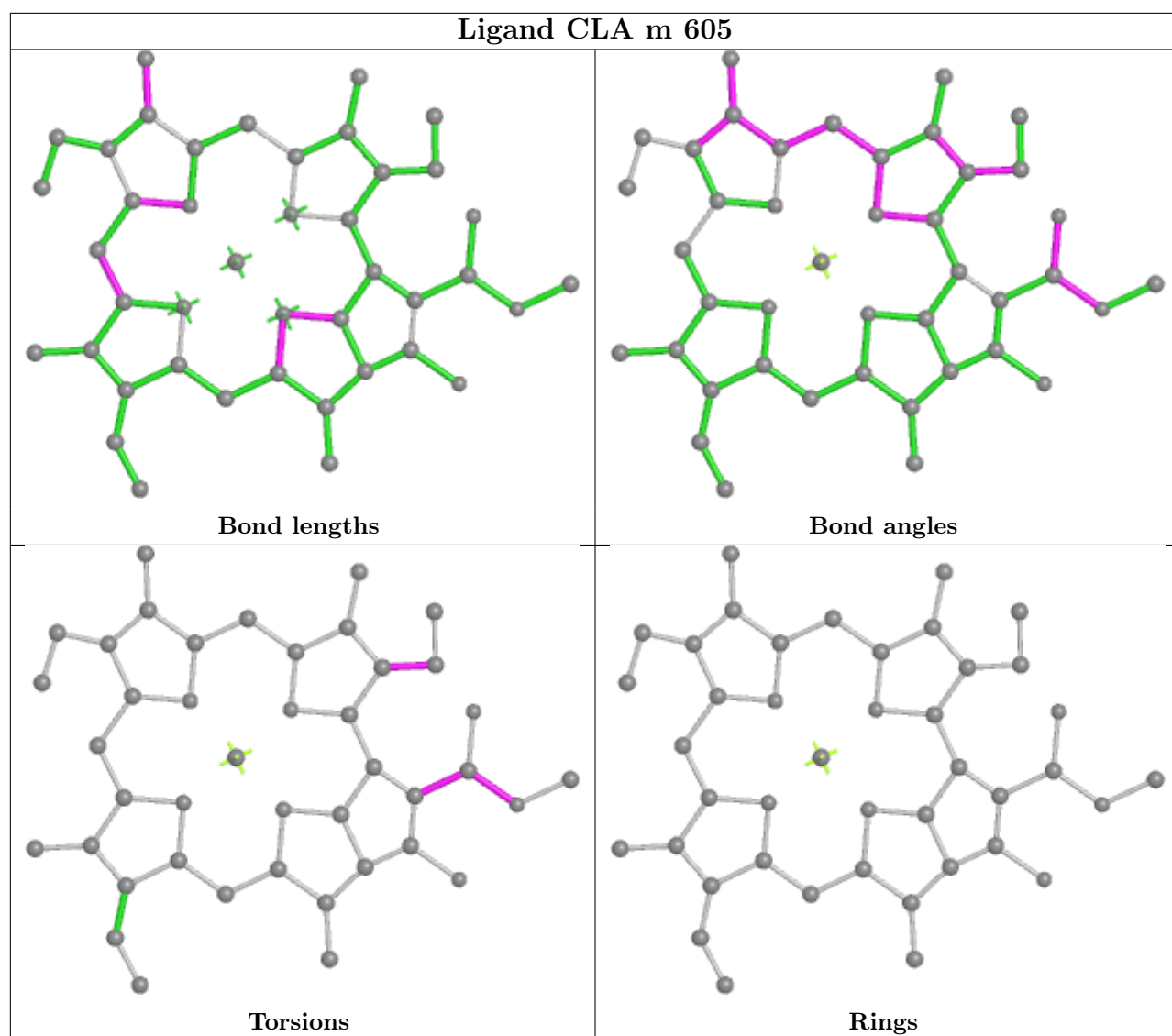
Bond angles



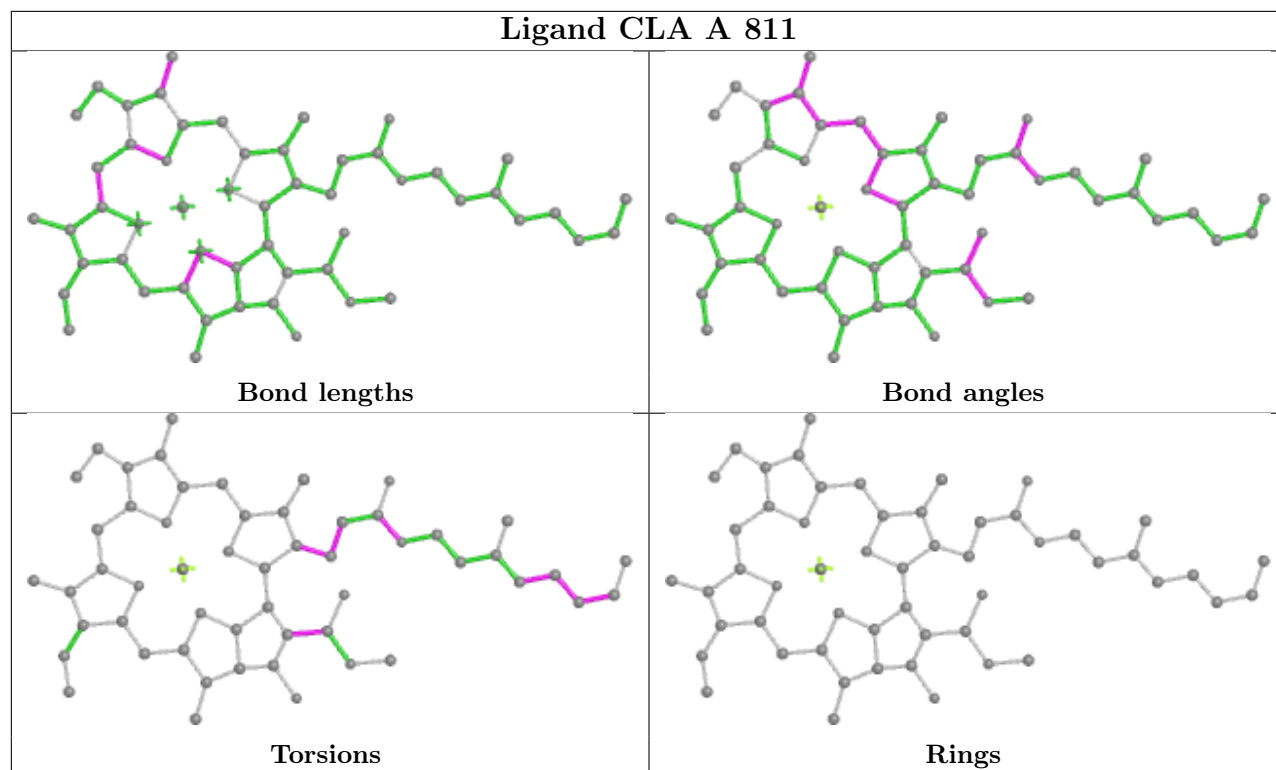
Torsions



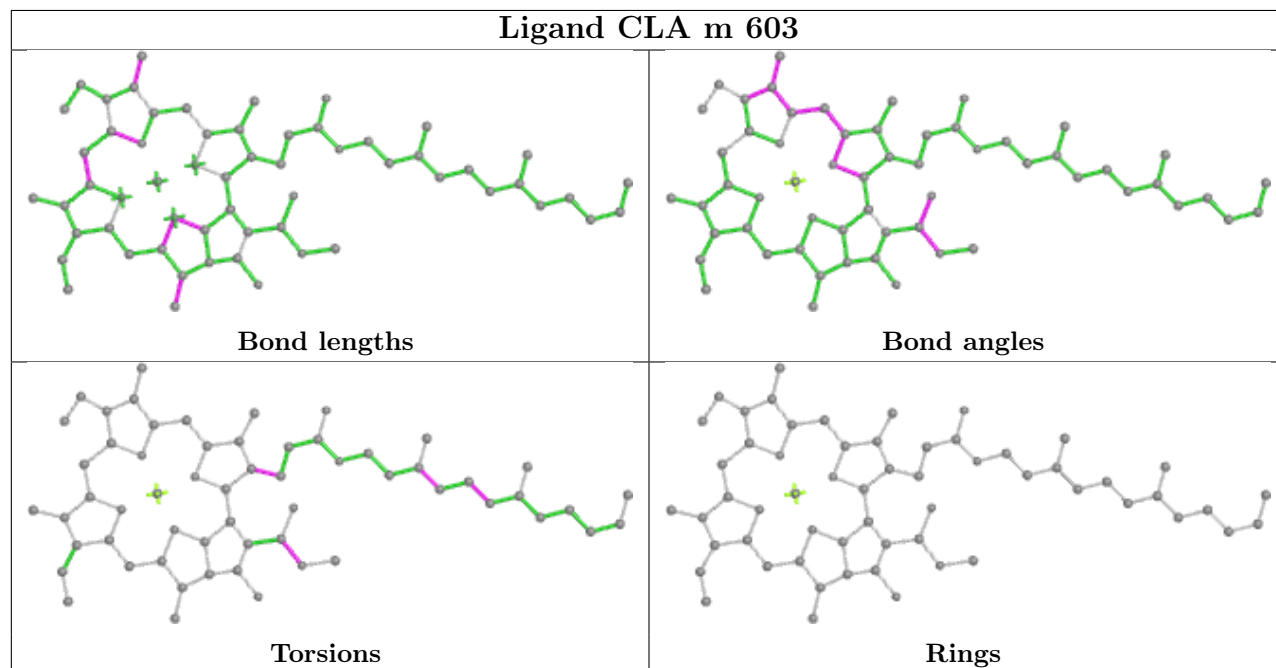
Rings



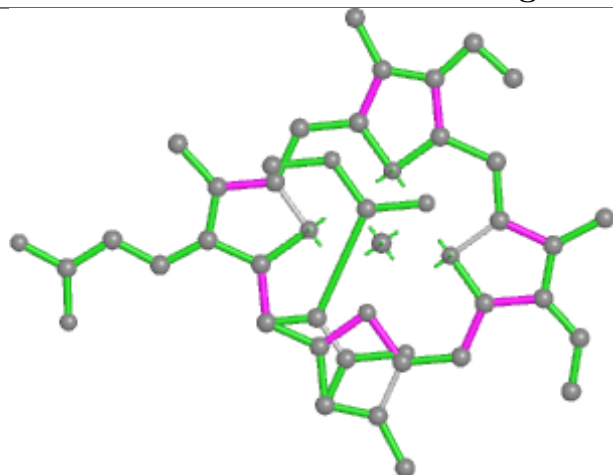
Ligand CLA A 811



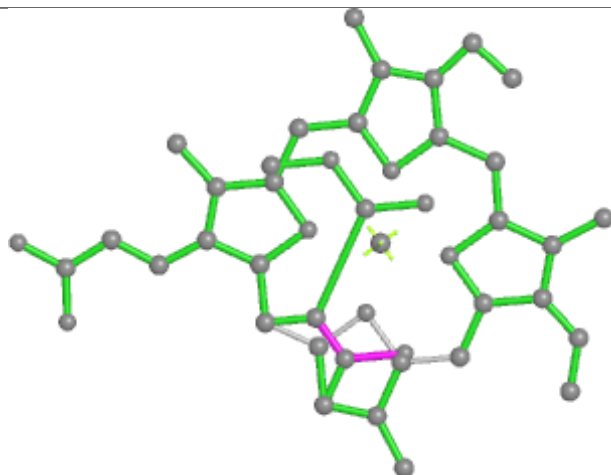
Ligand CLA m 603



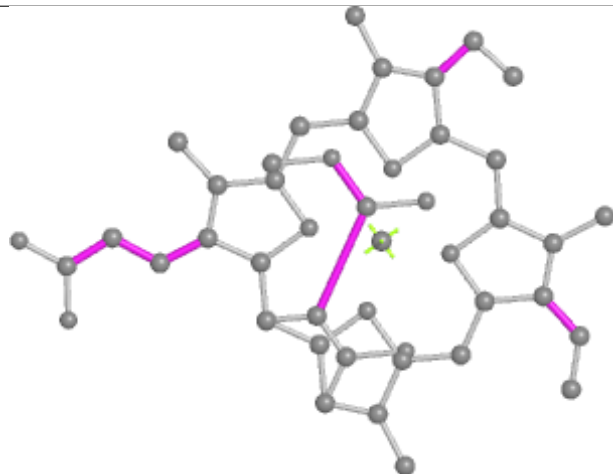
Ligand KC2 d 311



Bond lengths



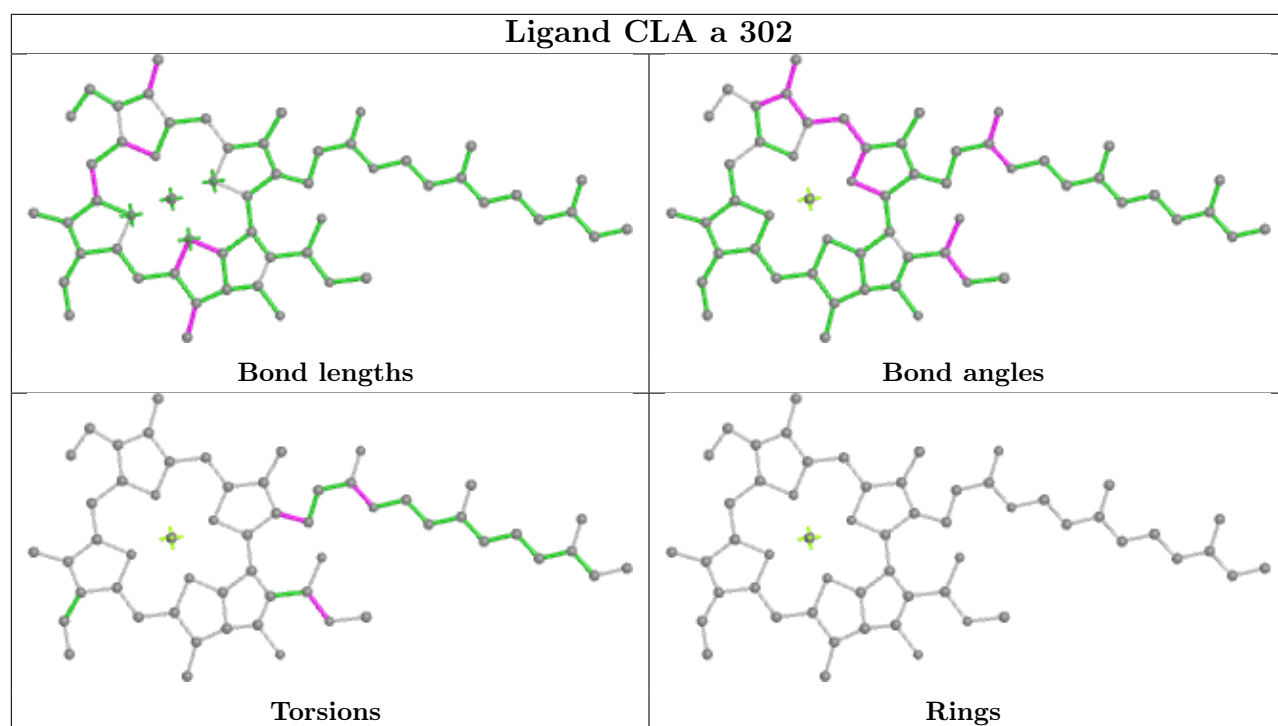
Bond angles



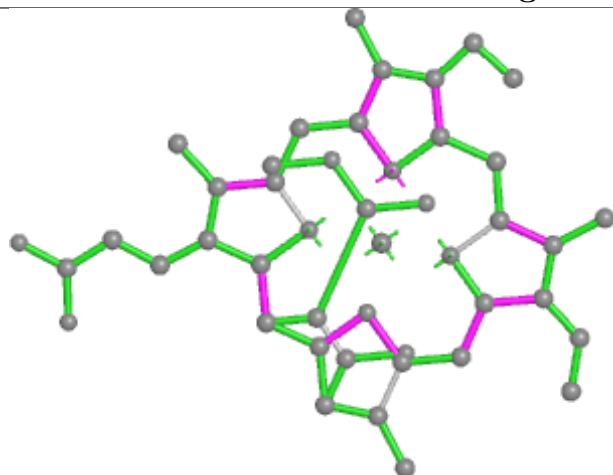
Torsions



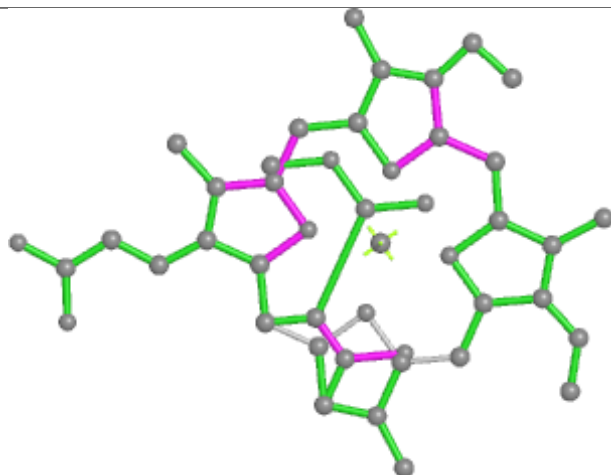
Rings



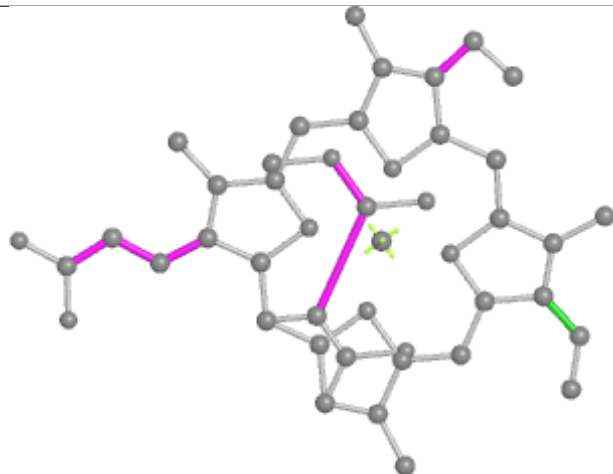
Ligand KC2 d 312



Bond lengths



Bond angles

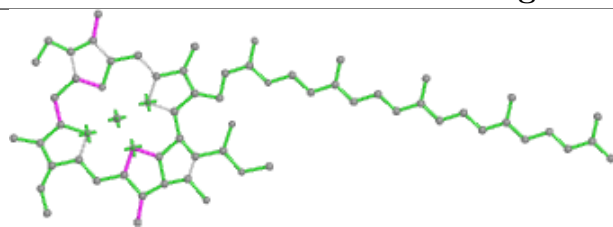


Torsions

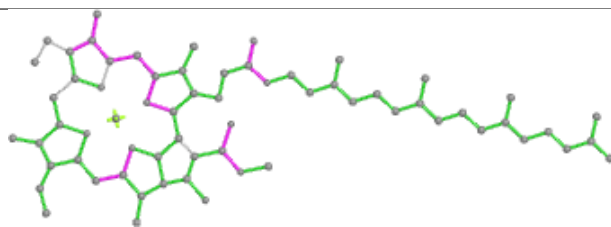


Rings

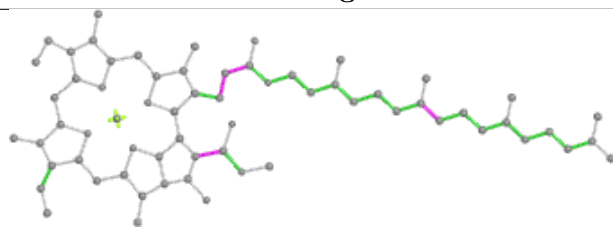
Ligand CLA a 304



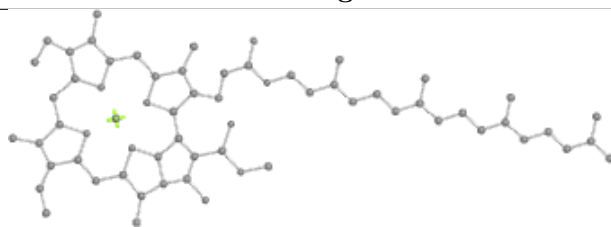
Bond lengths



Bond angles

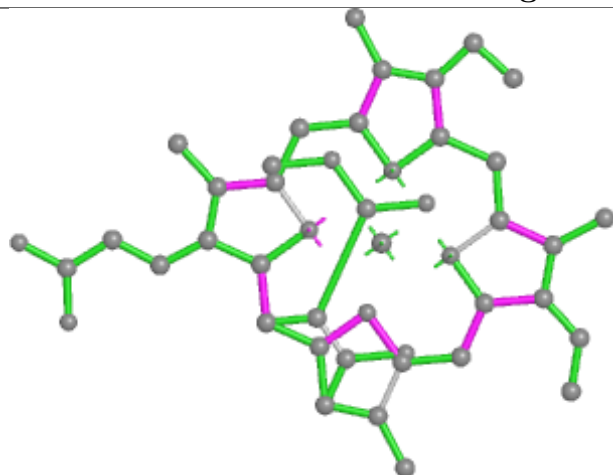


Torsions

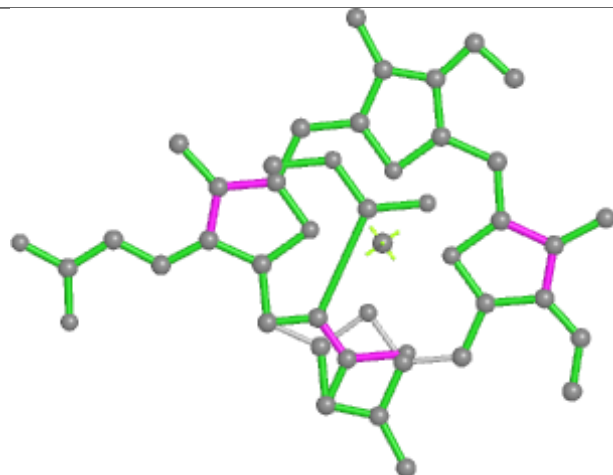


Rings

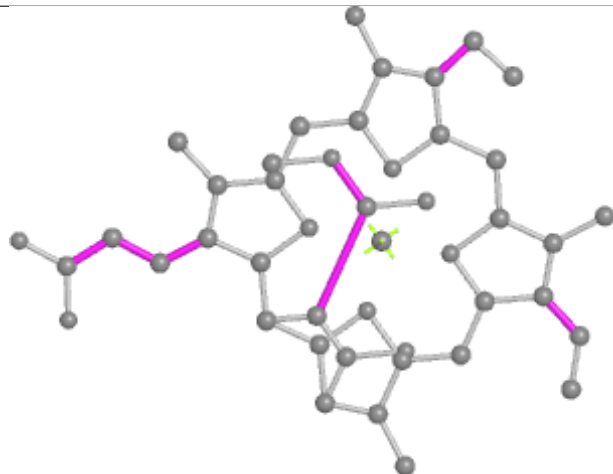
Ligand KC2 k 611



Bond lengths



Bond angles

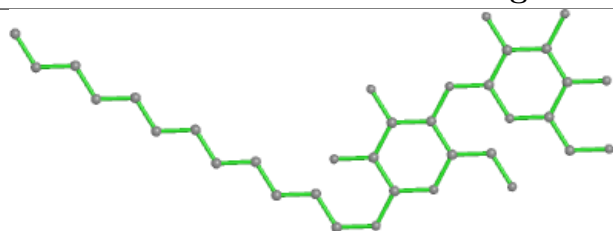


Torsions

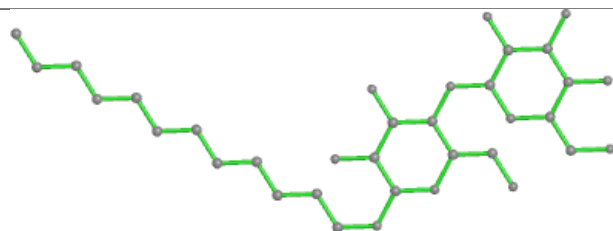


Rings

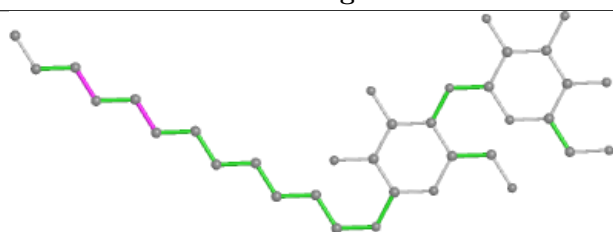
Ligand LMU B 852



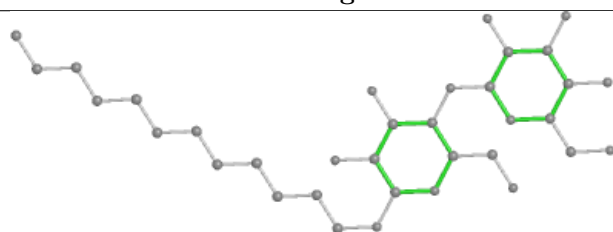
Bond lengths



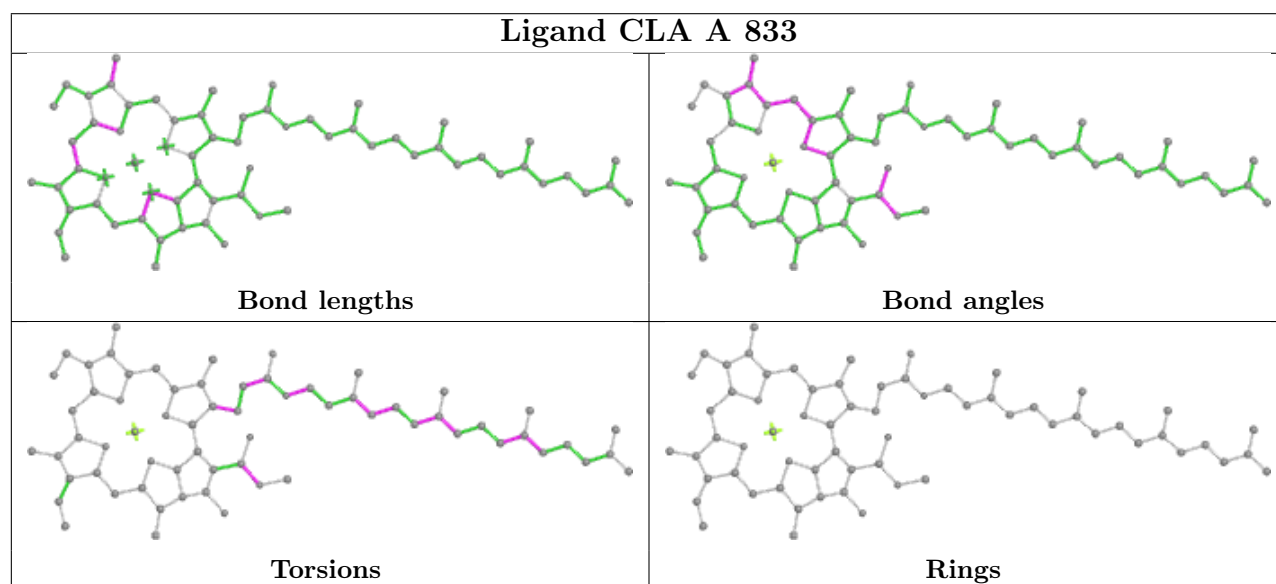
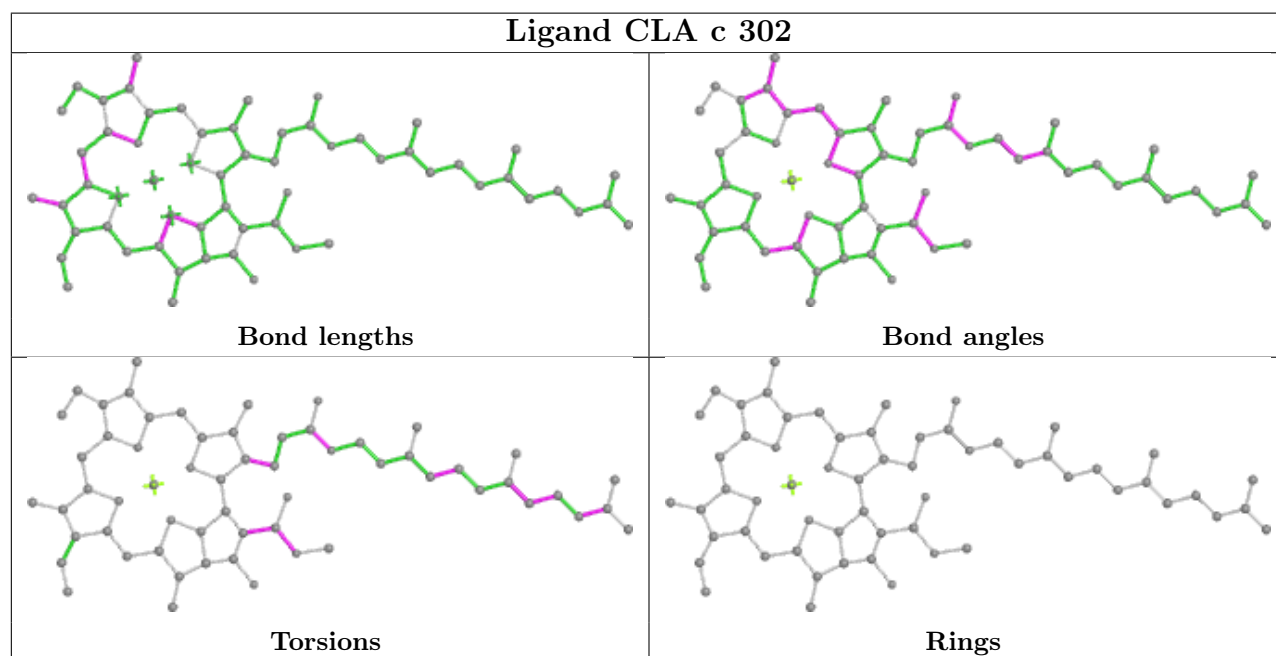
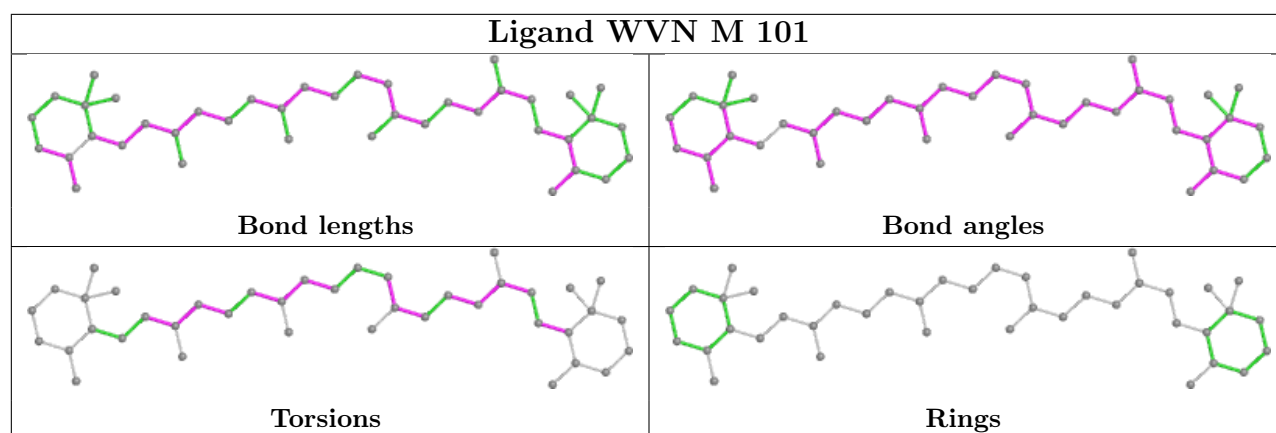
Bond angles

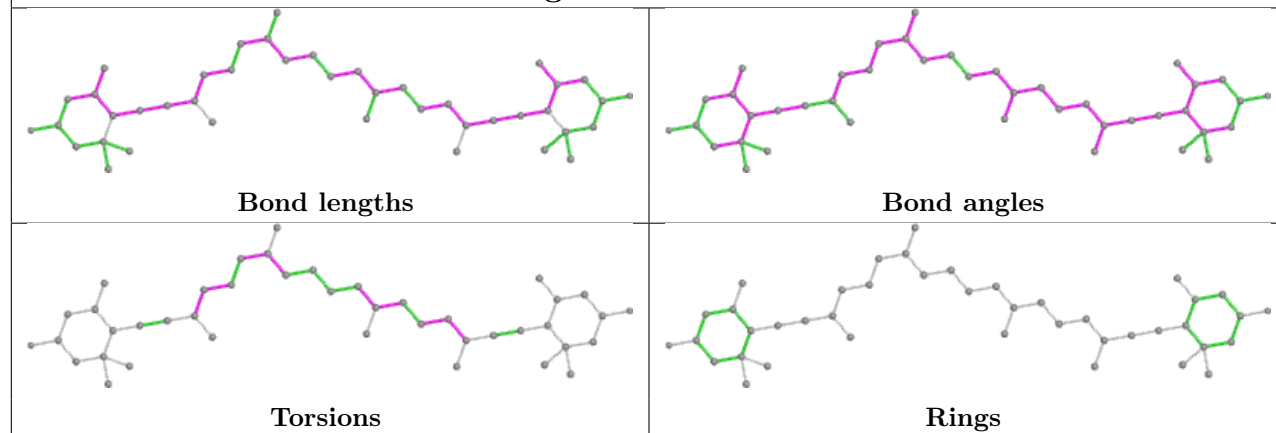
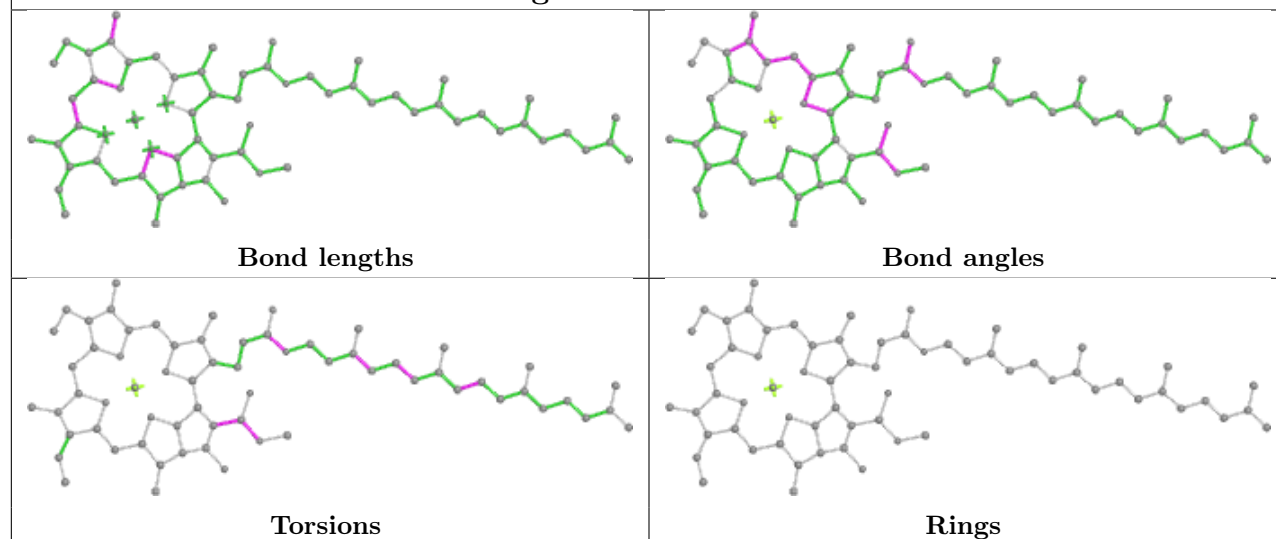
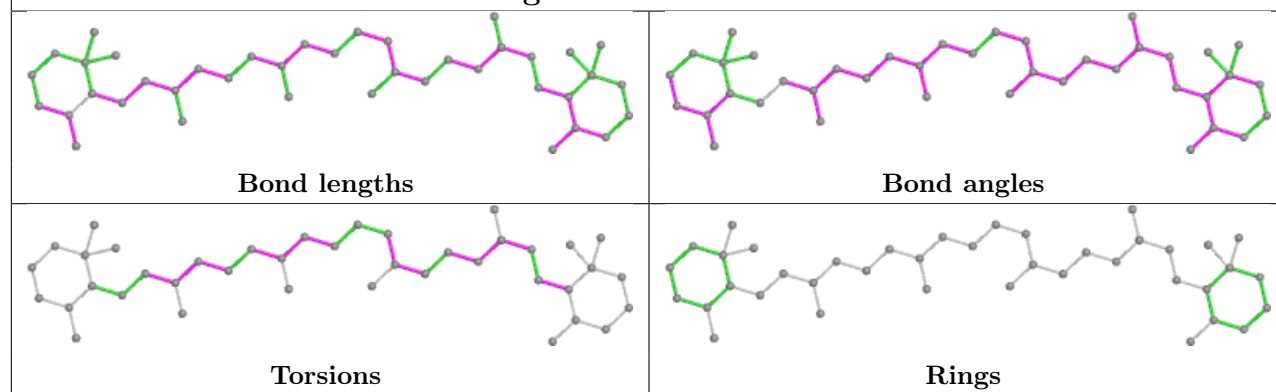


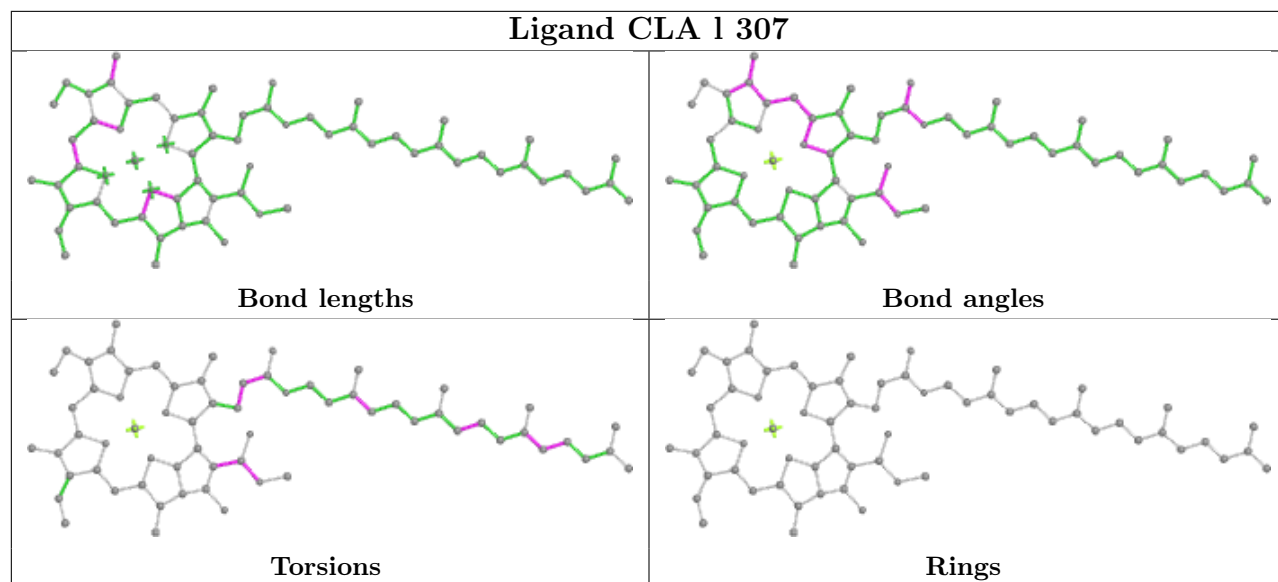
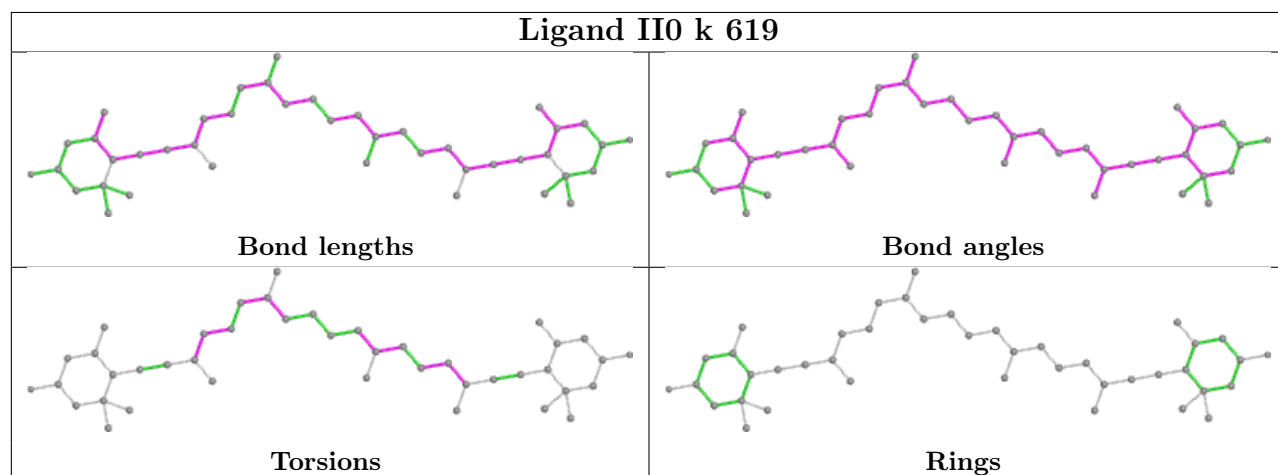
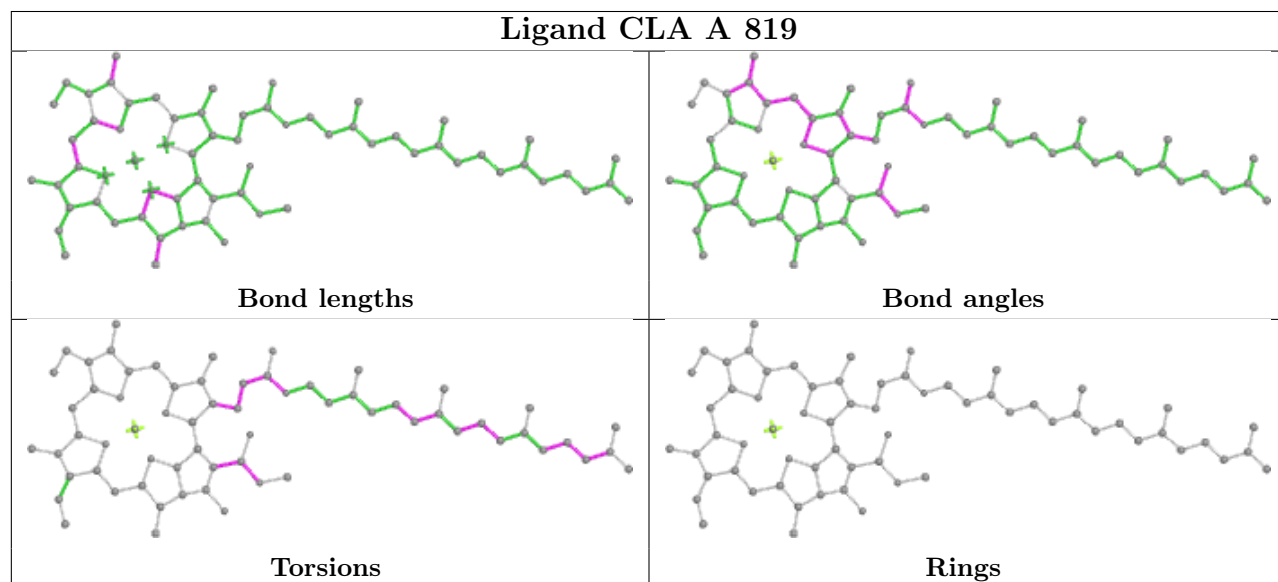
Torsions



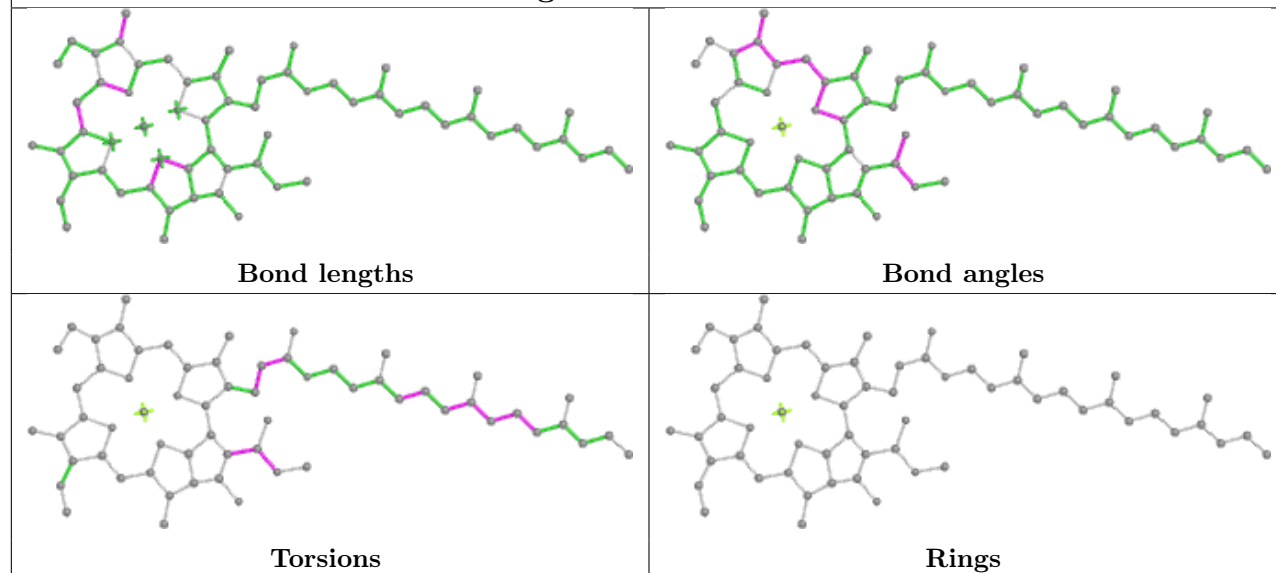
Rings



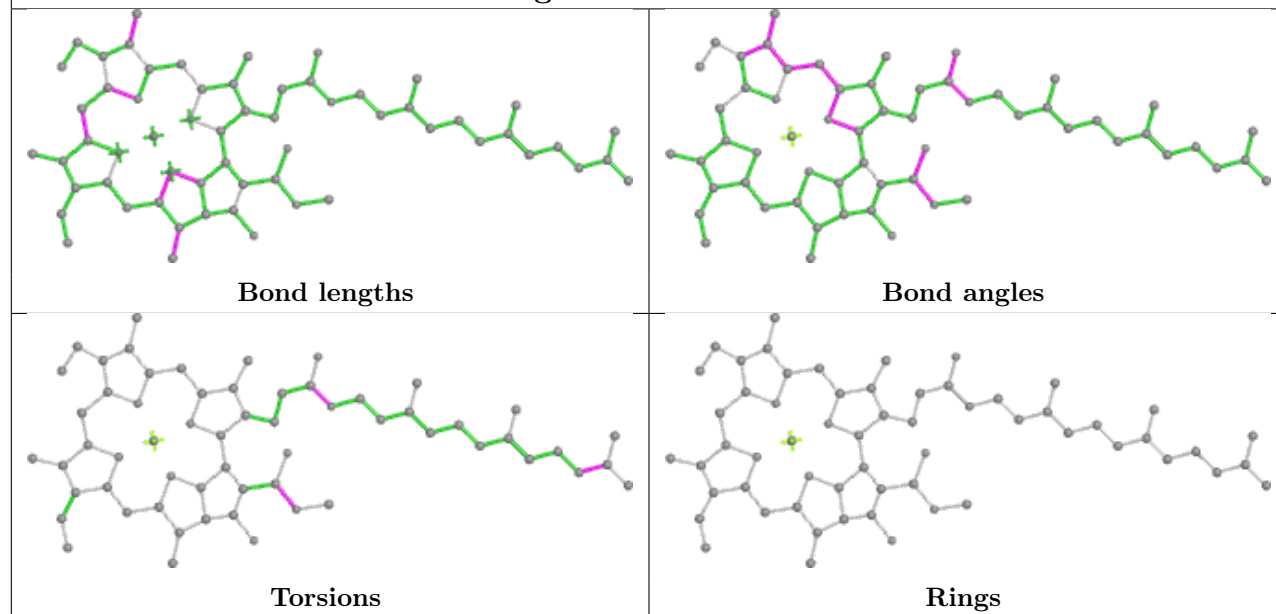
Ligand II0 m 616**Ligand CLA A 838****Ligand WVN R 200**

Ligand CLA I 307**Ligand II0 k 619****Ligand CLA A 819**

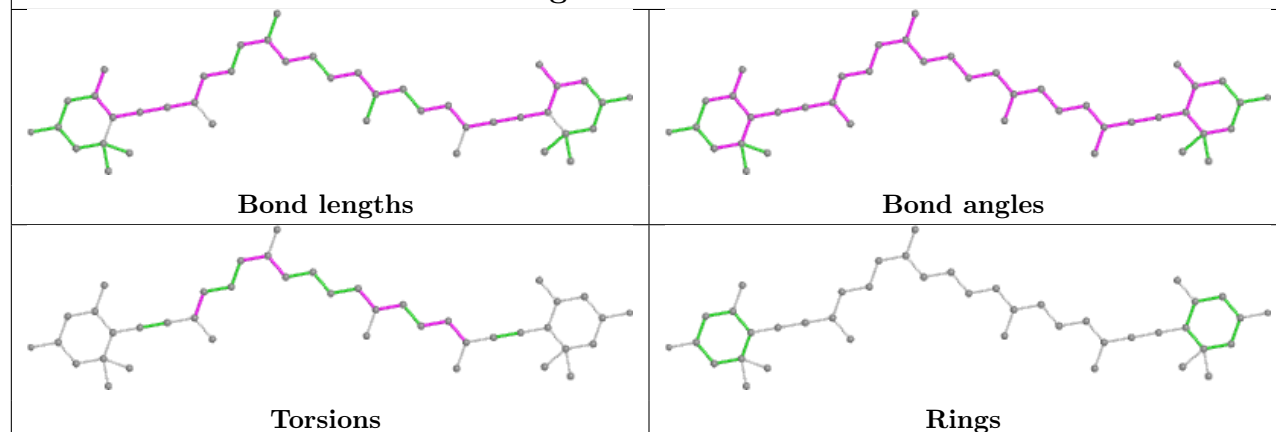
Ligand CLA c 304

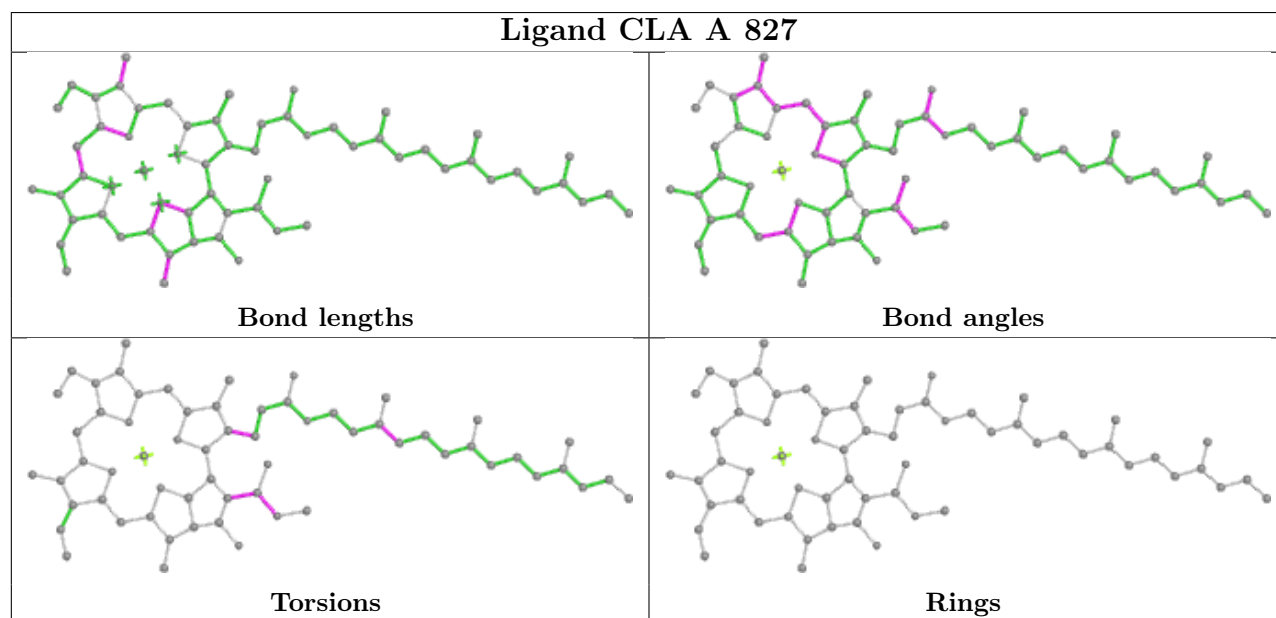
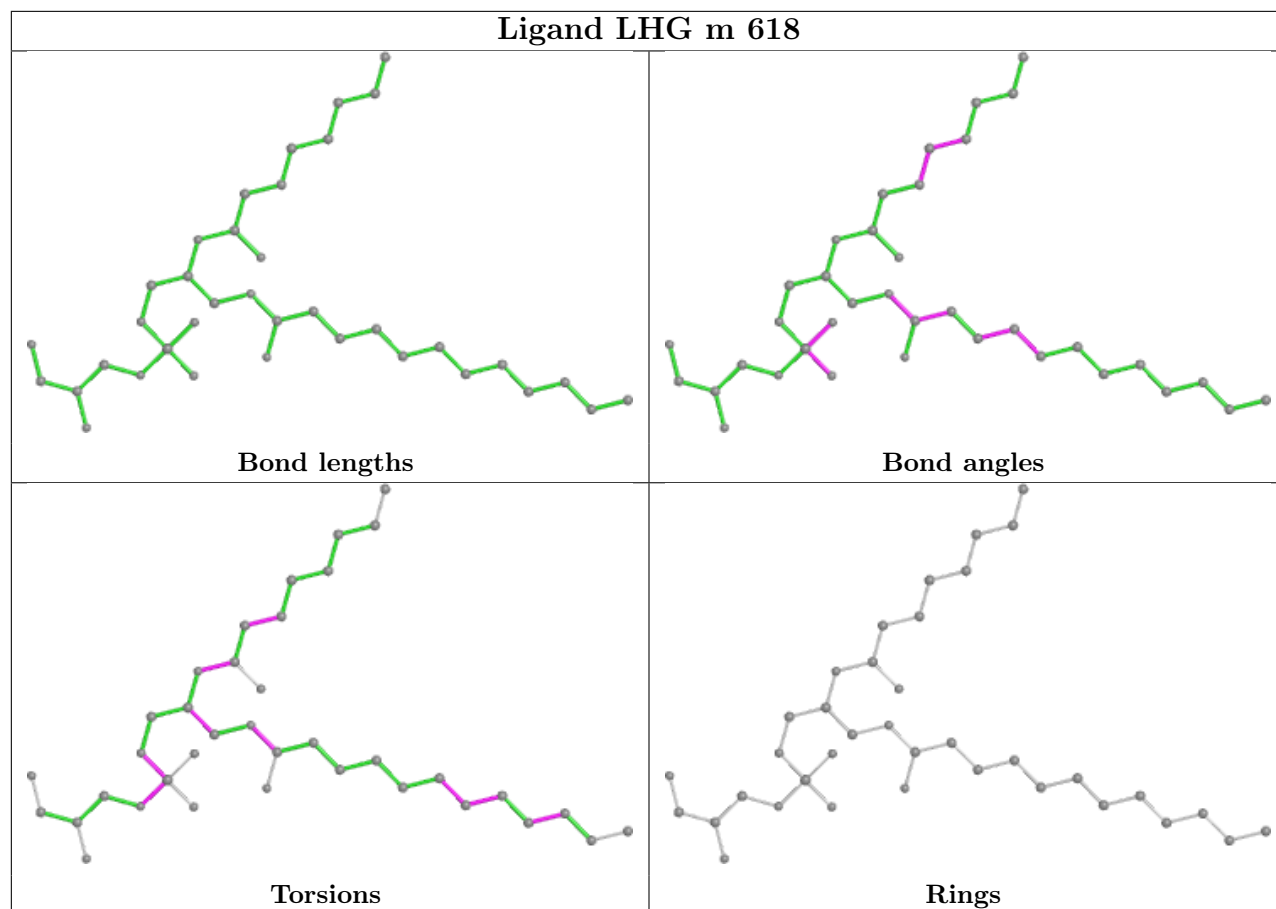


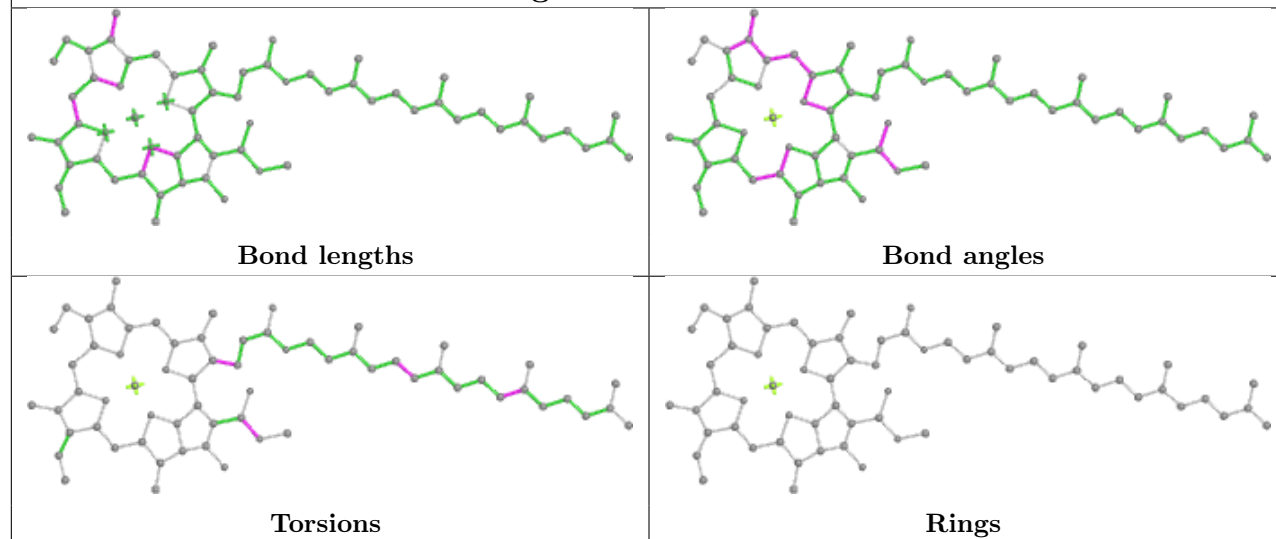
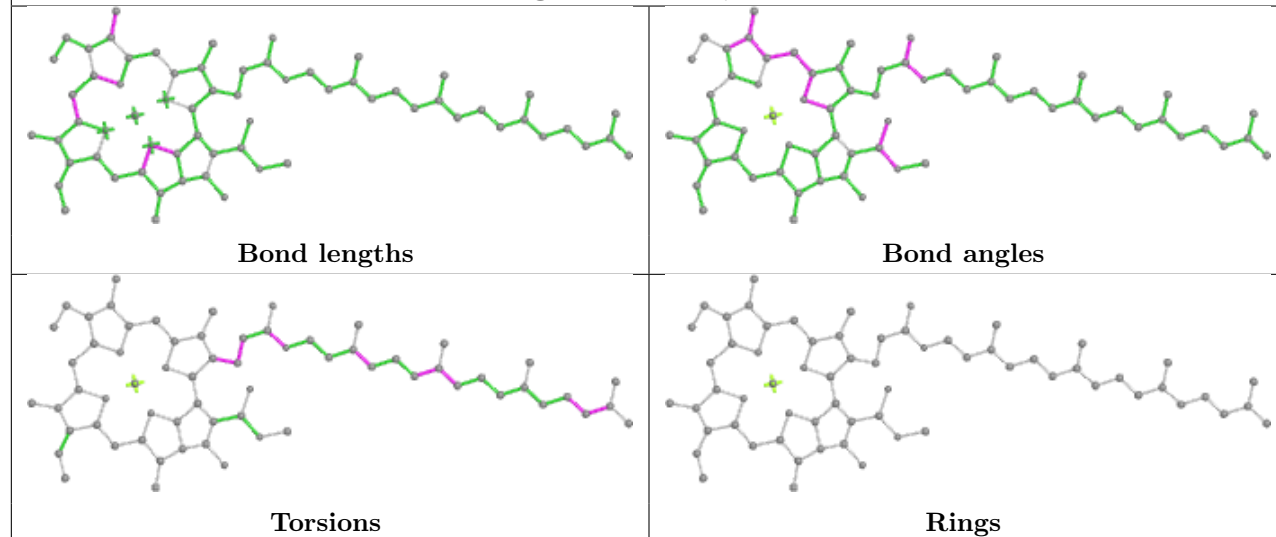
Ligand CLA L 204



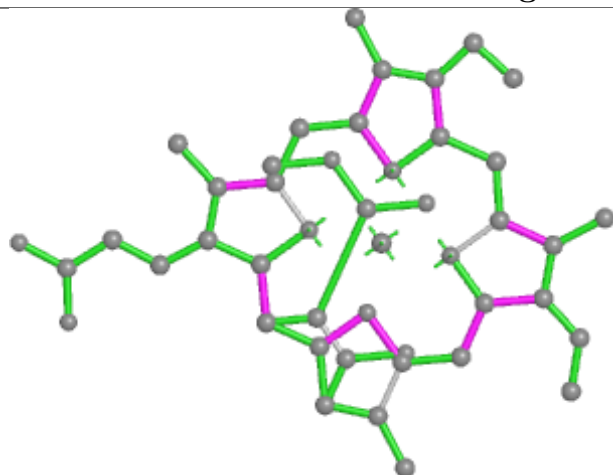
Ligand II0 b 314



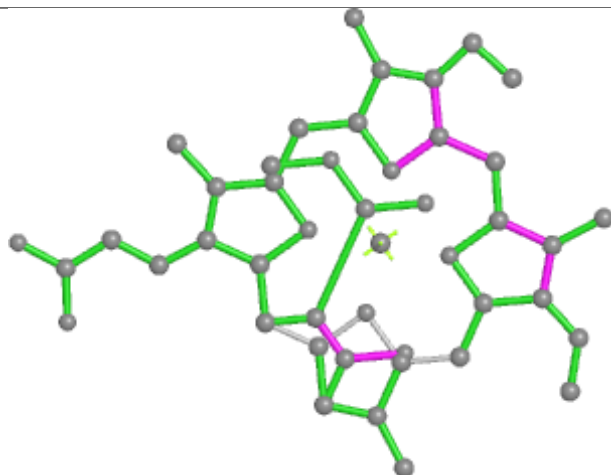


Ligand CLA A 832**Ligand CLA Q 302**

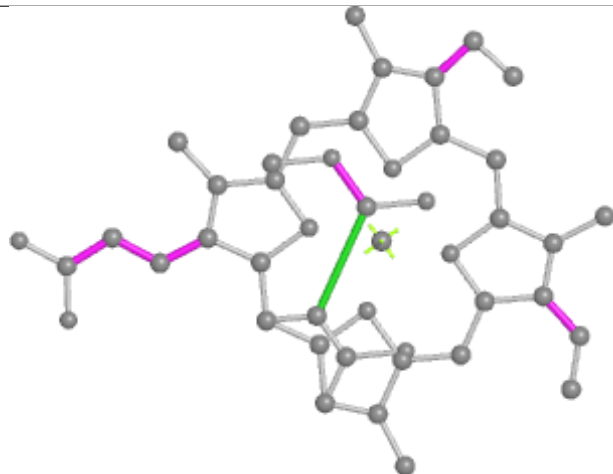
Ligand KC2 n 612



Bond lengths



Bond angles

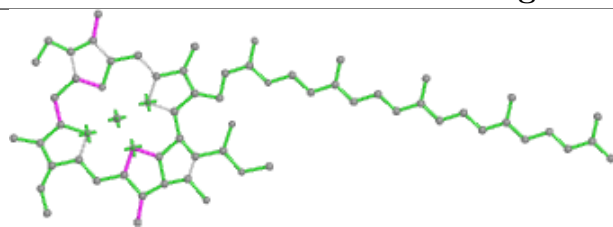


Torsions

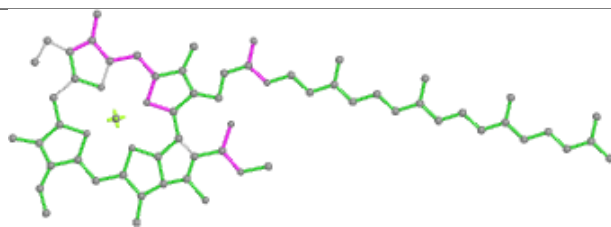


Rings

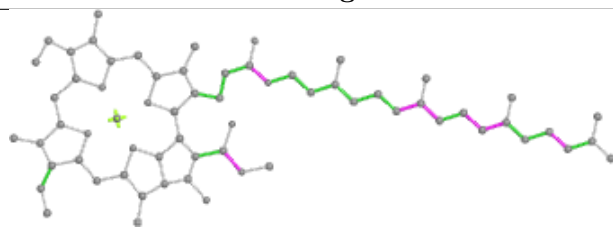
Ligand CLA a 310



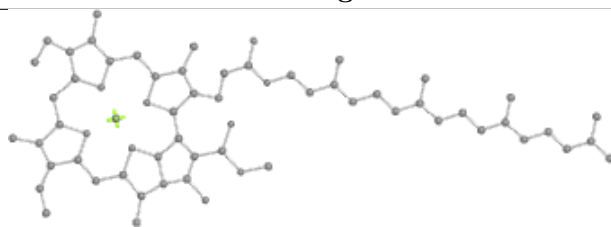
Bond lengths



Bond angles

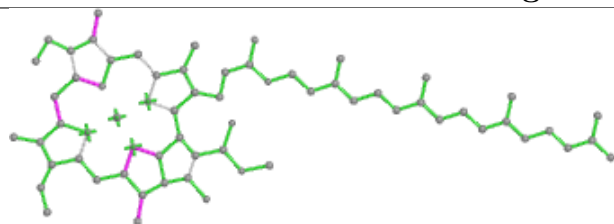


Torsions

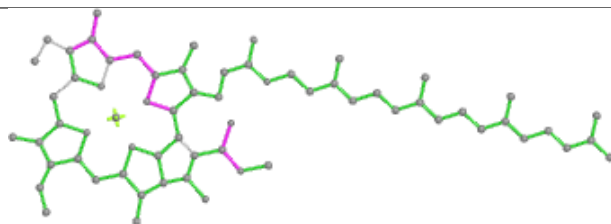


Rings

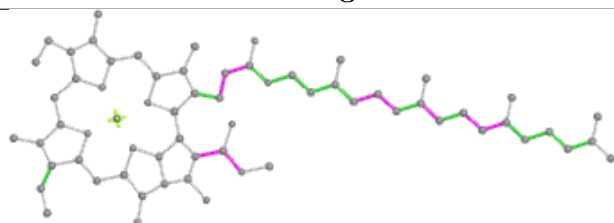
Ligand CLA i 304



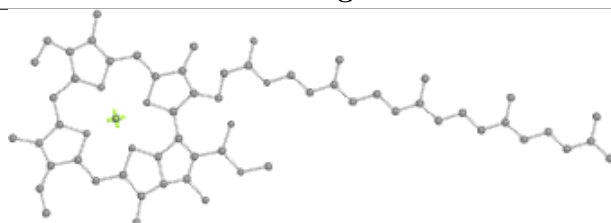
Bond lengths



Bond angles

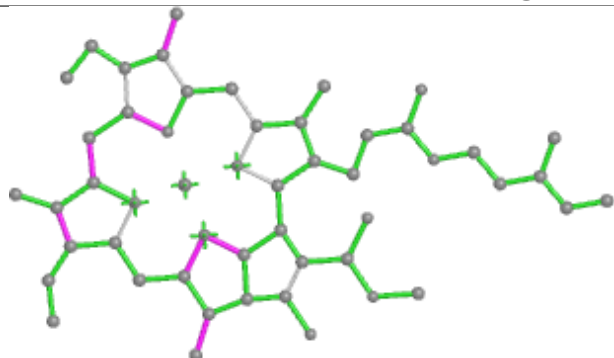


Torsions

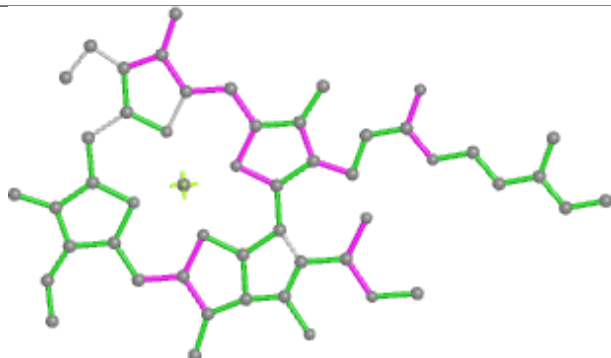


Rings

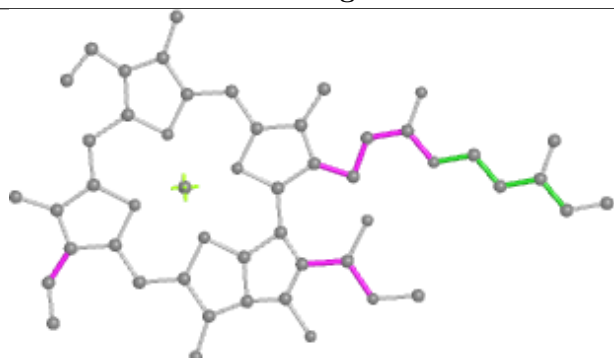
Ligand CLA k 607



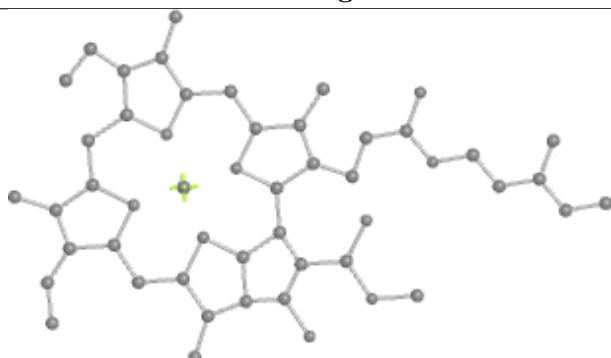
Bond lengths



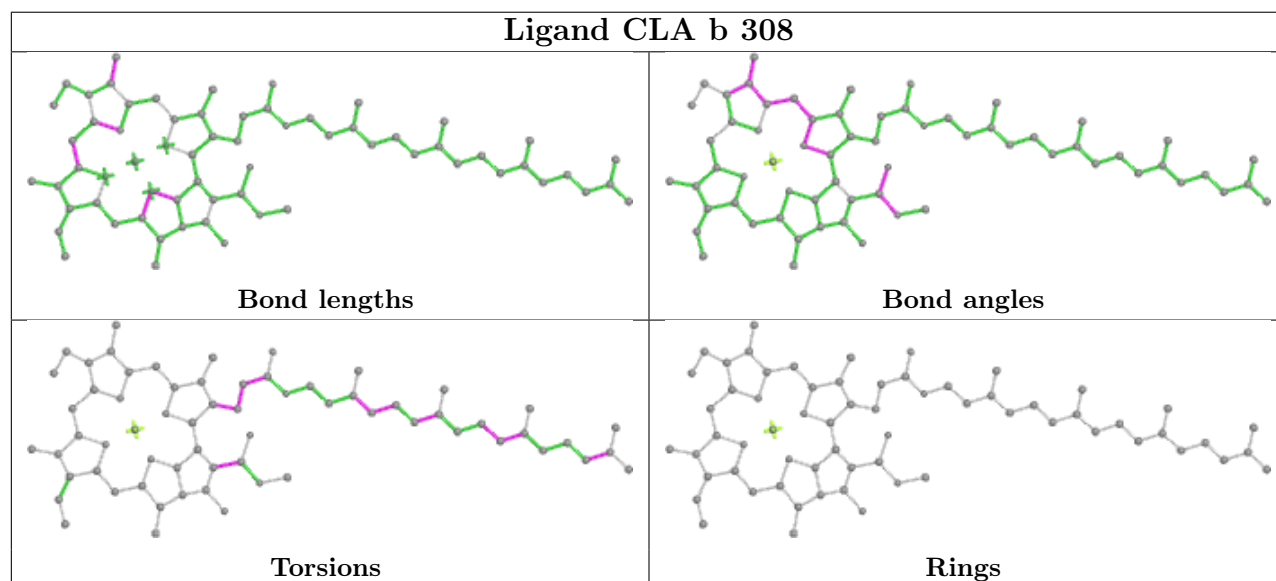
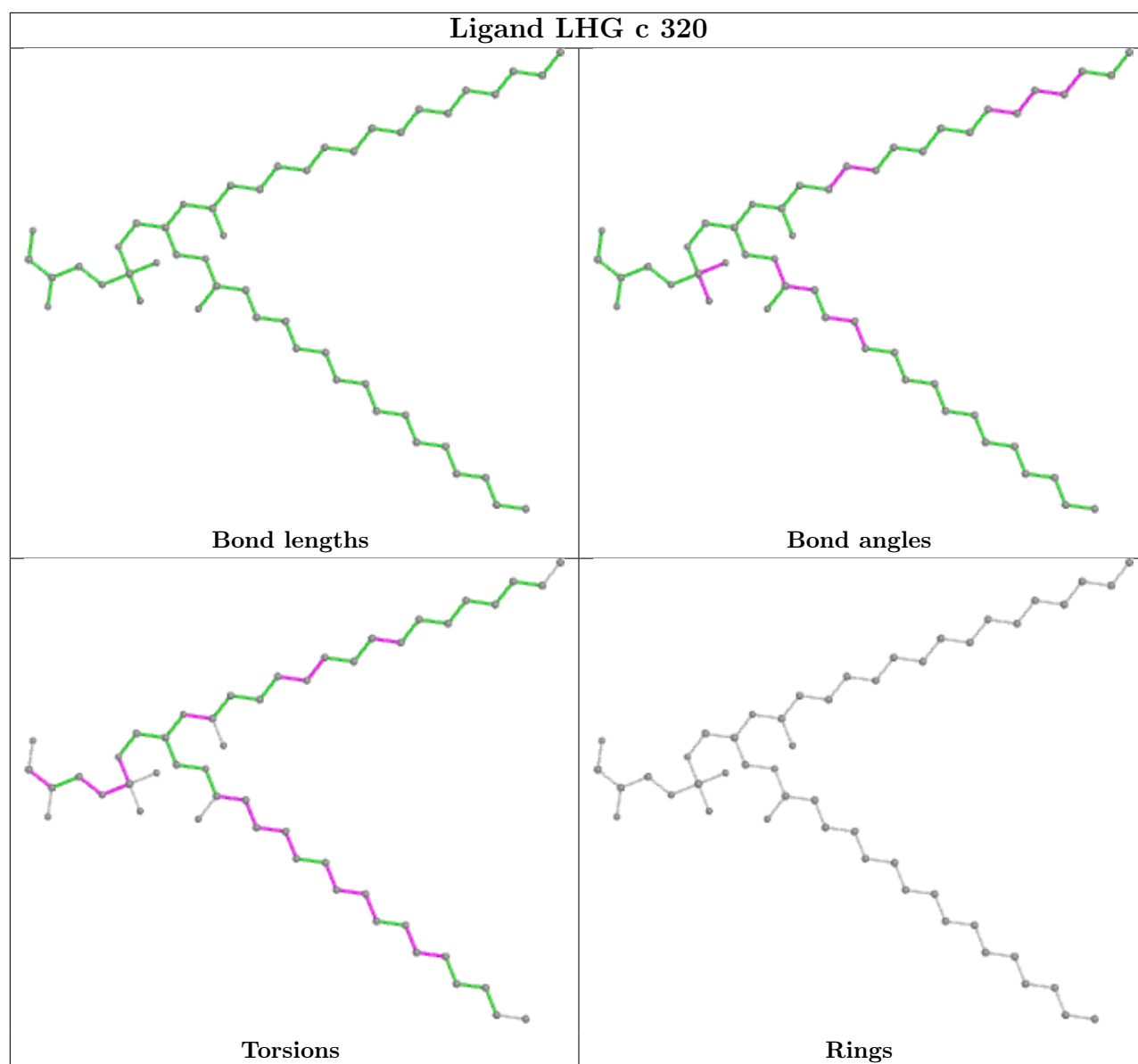
Bond angles

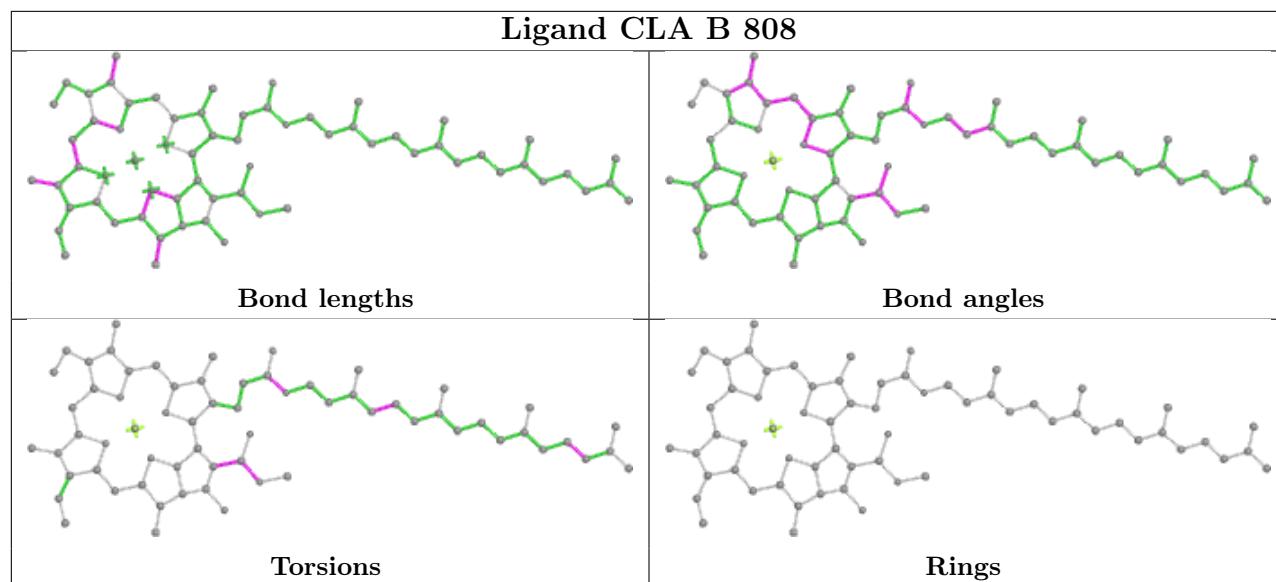
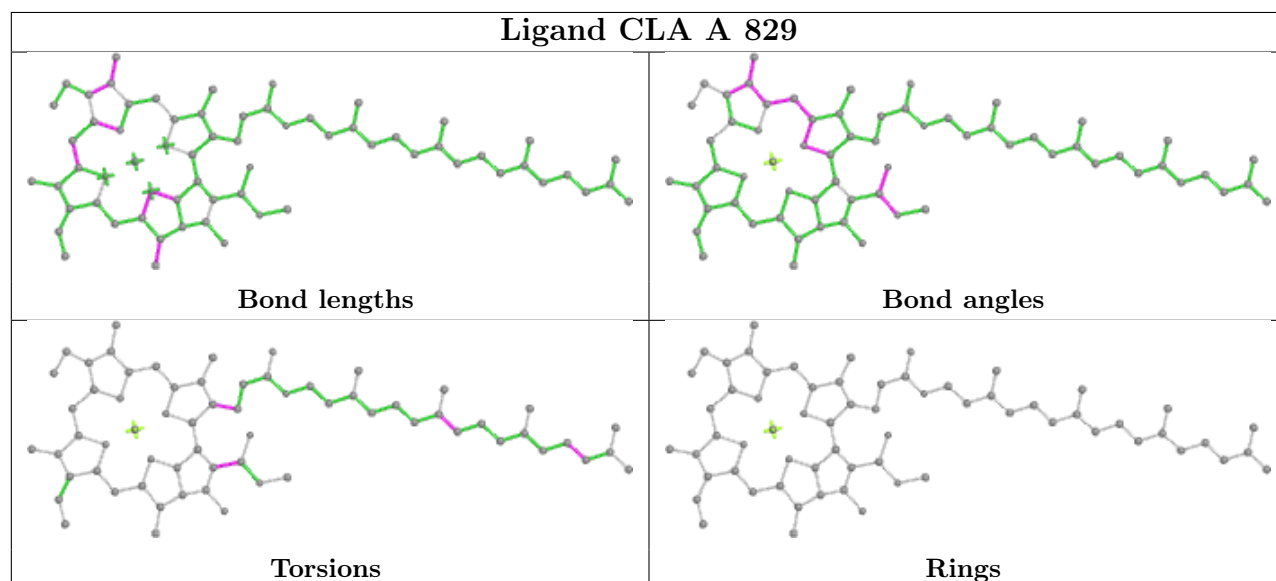
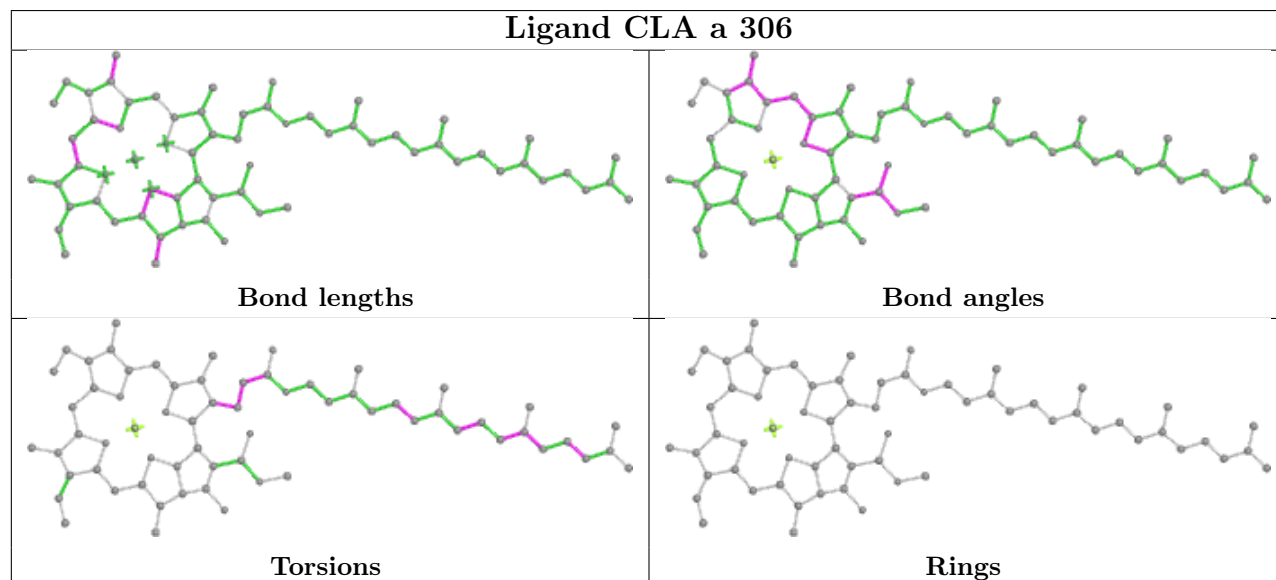


Torsions

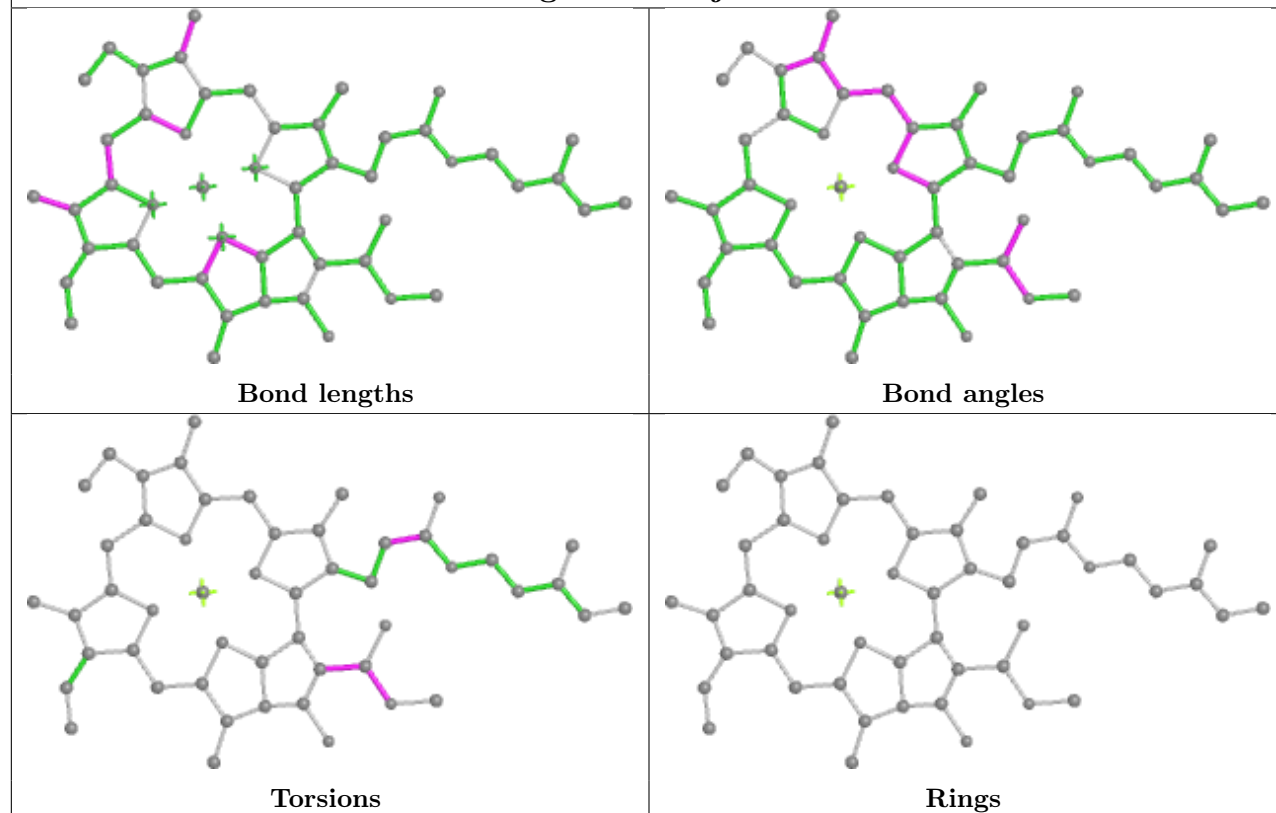


Rings

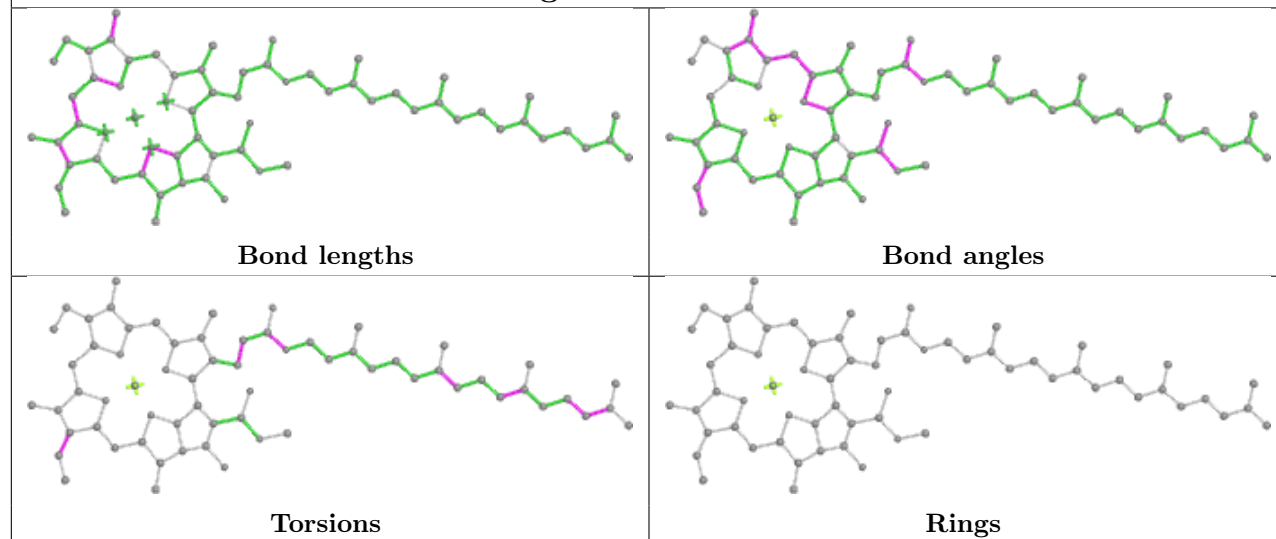


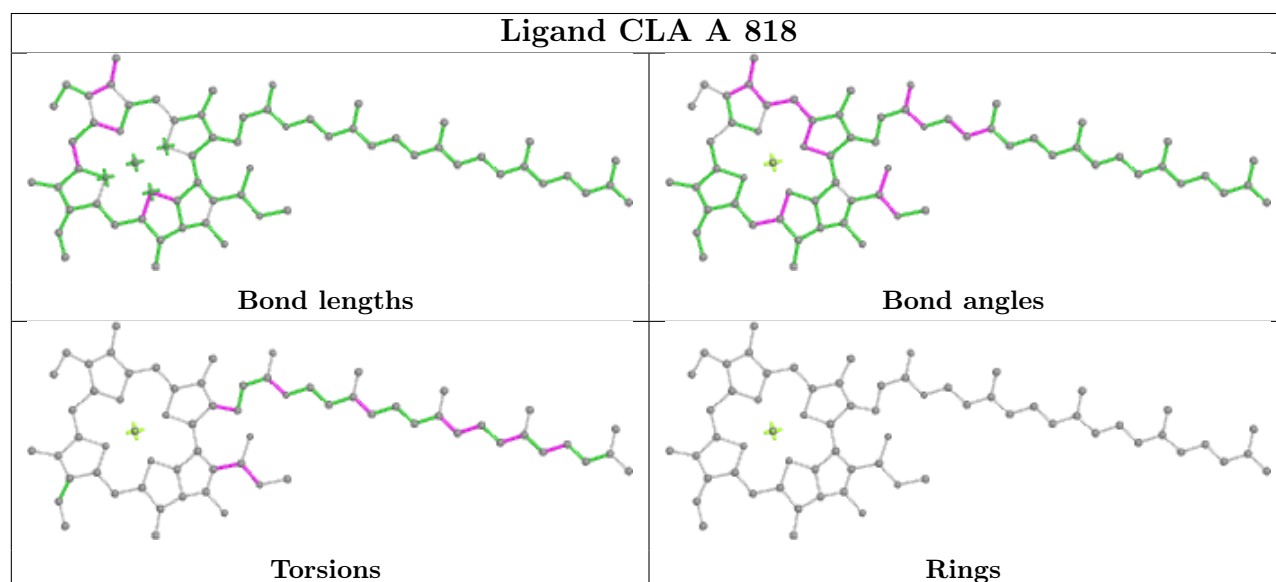
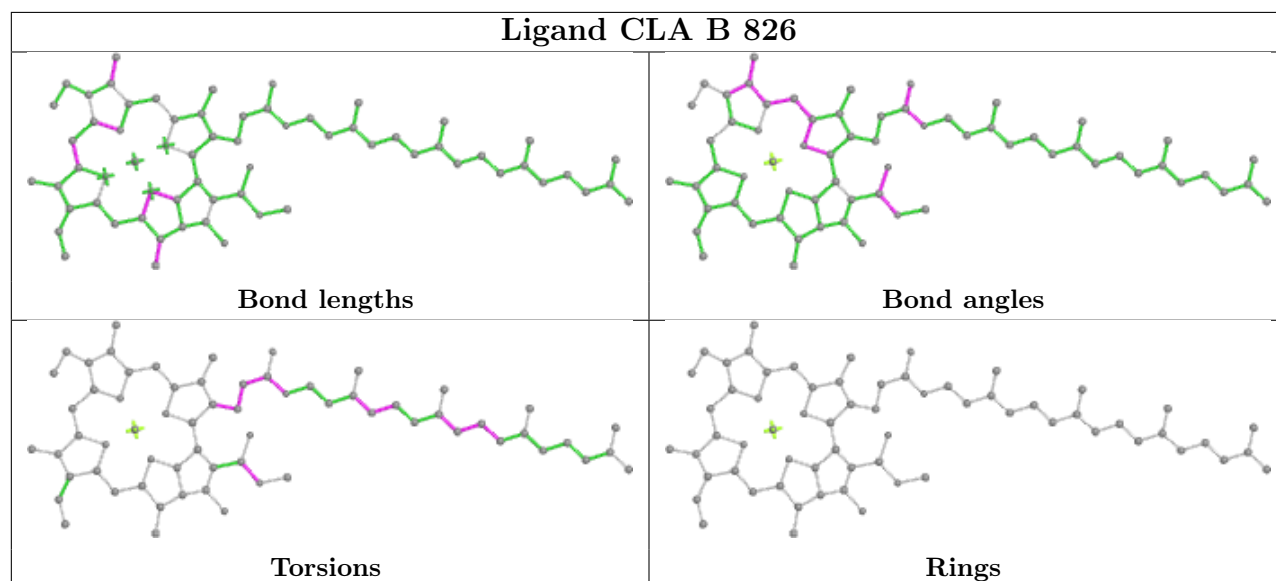
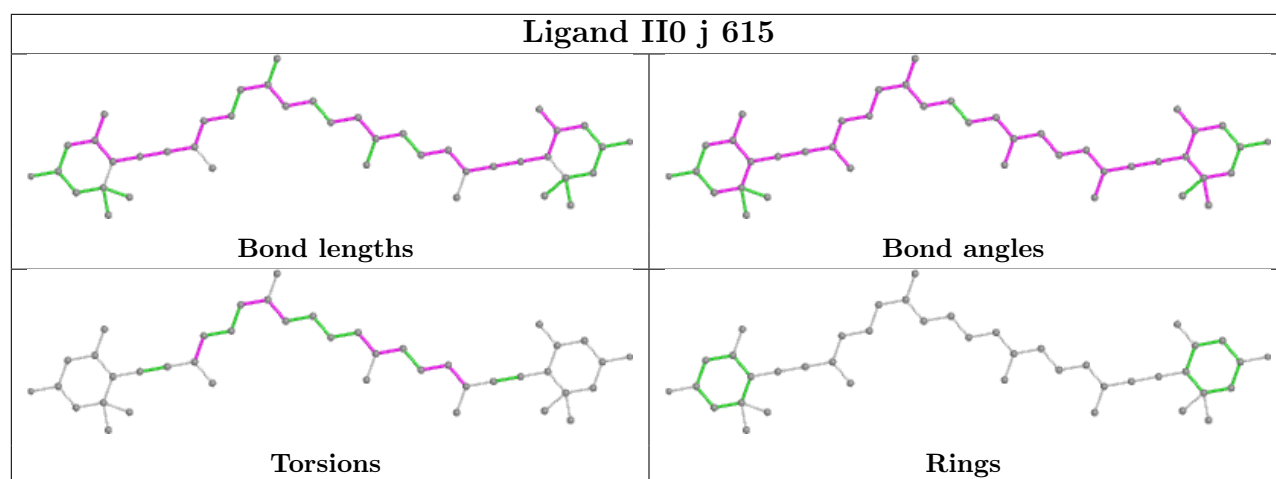
Ligand CLA B 808**Ligand CLA A 829****Ligand CLA a 306**

Ligand CLA j 603

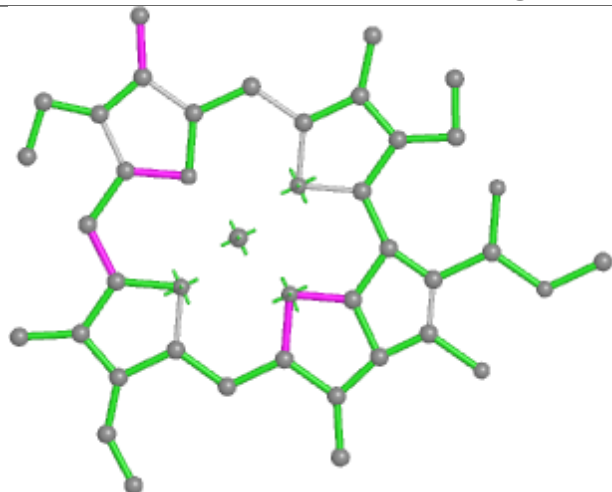


Ligand CLA i 311

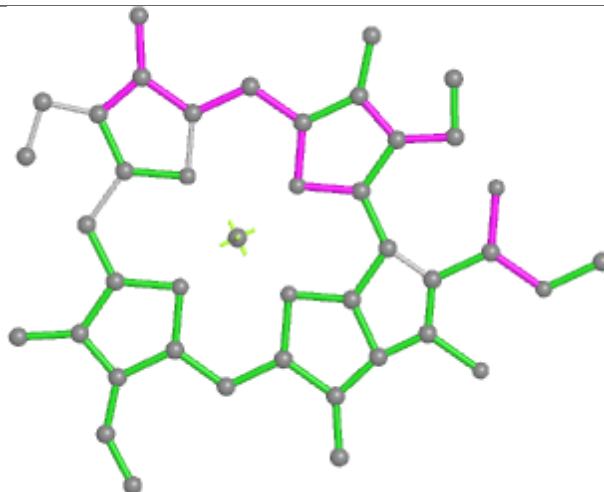




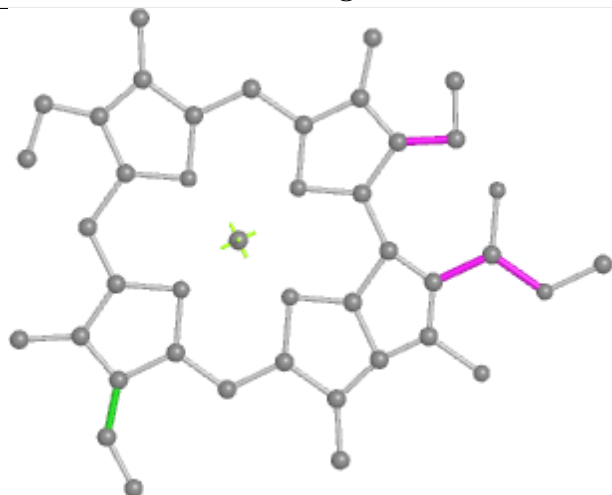
Ligand CLA m 601



Bond lengths



Bond angles

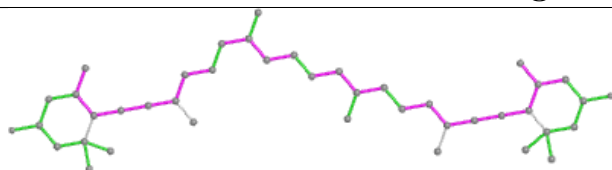


Torsions

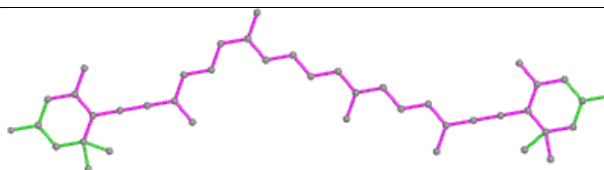


Rings

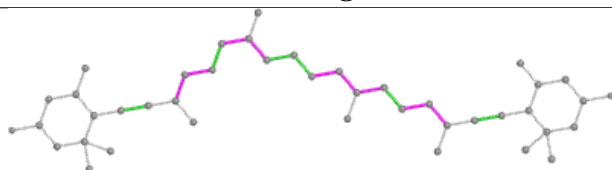
Ligand II0 d 301



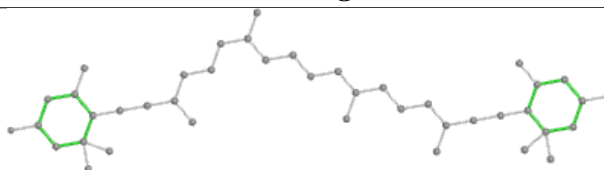
Bond lengths



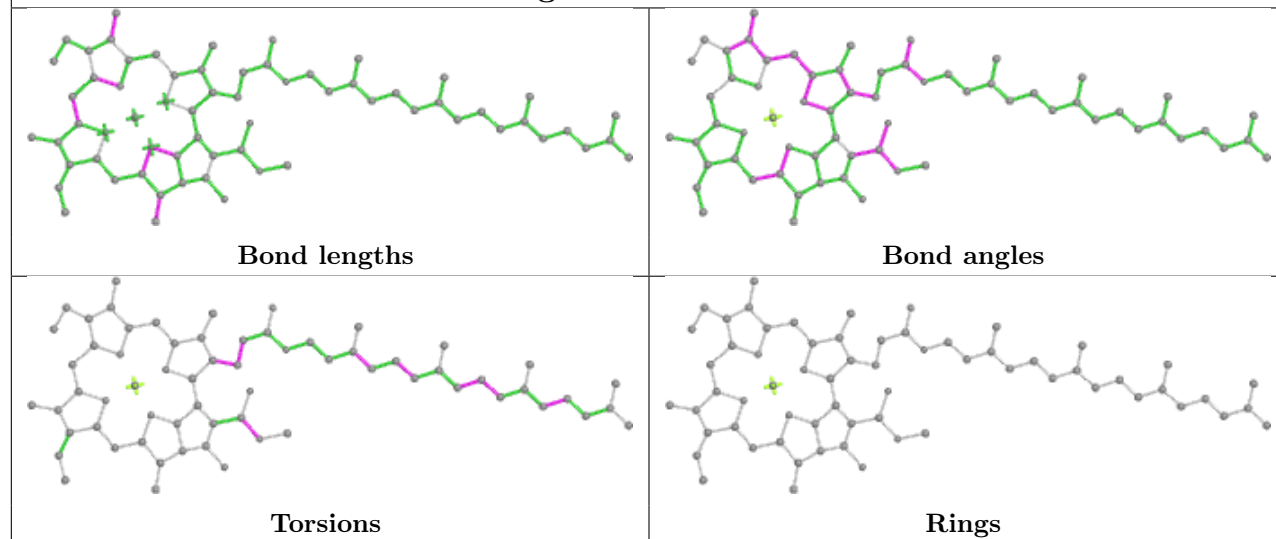
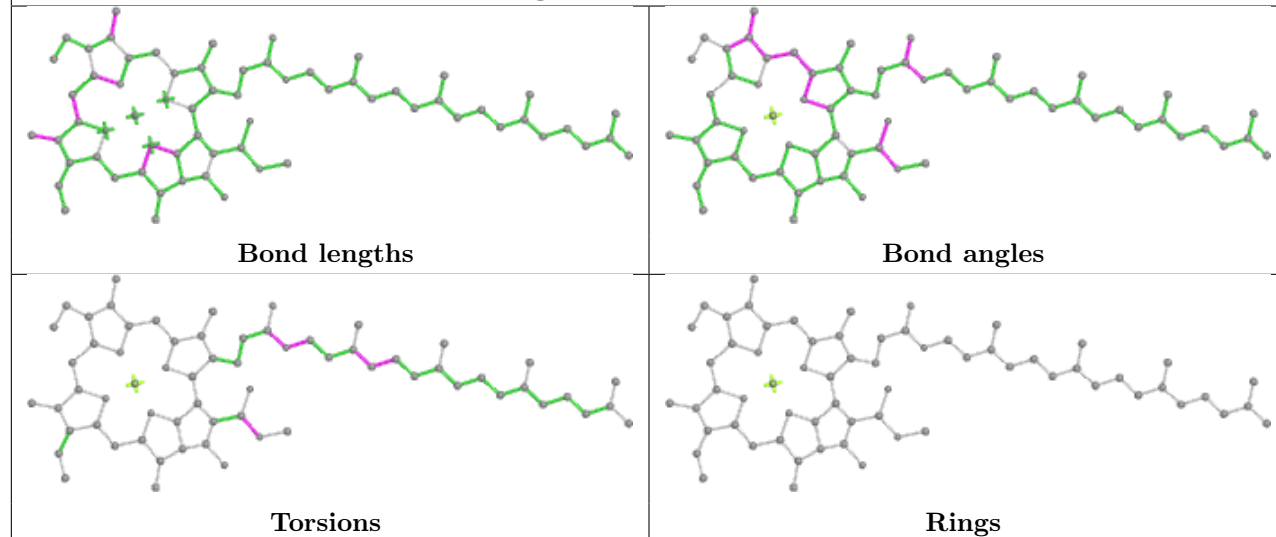
Bond angles

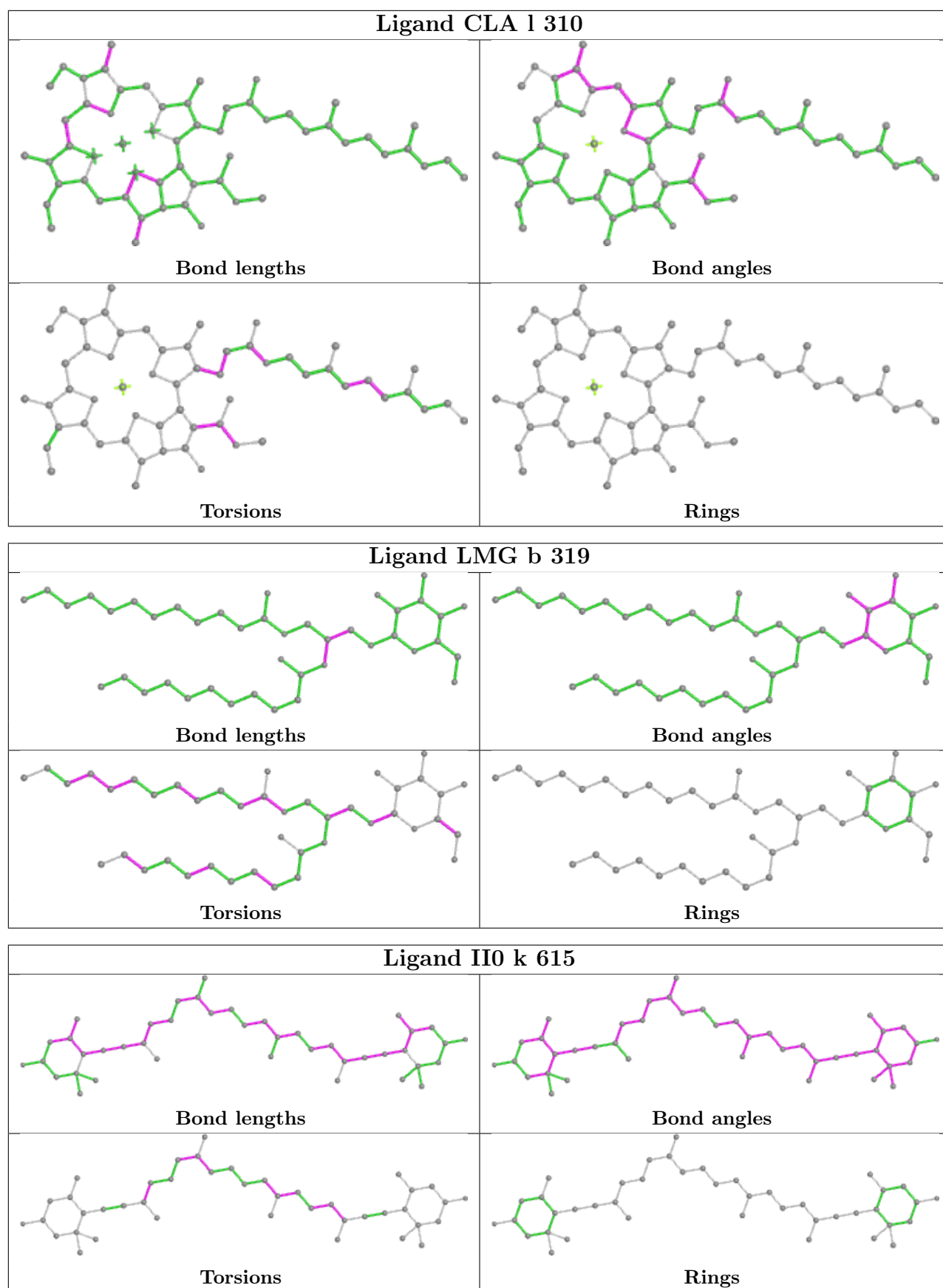


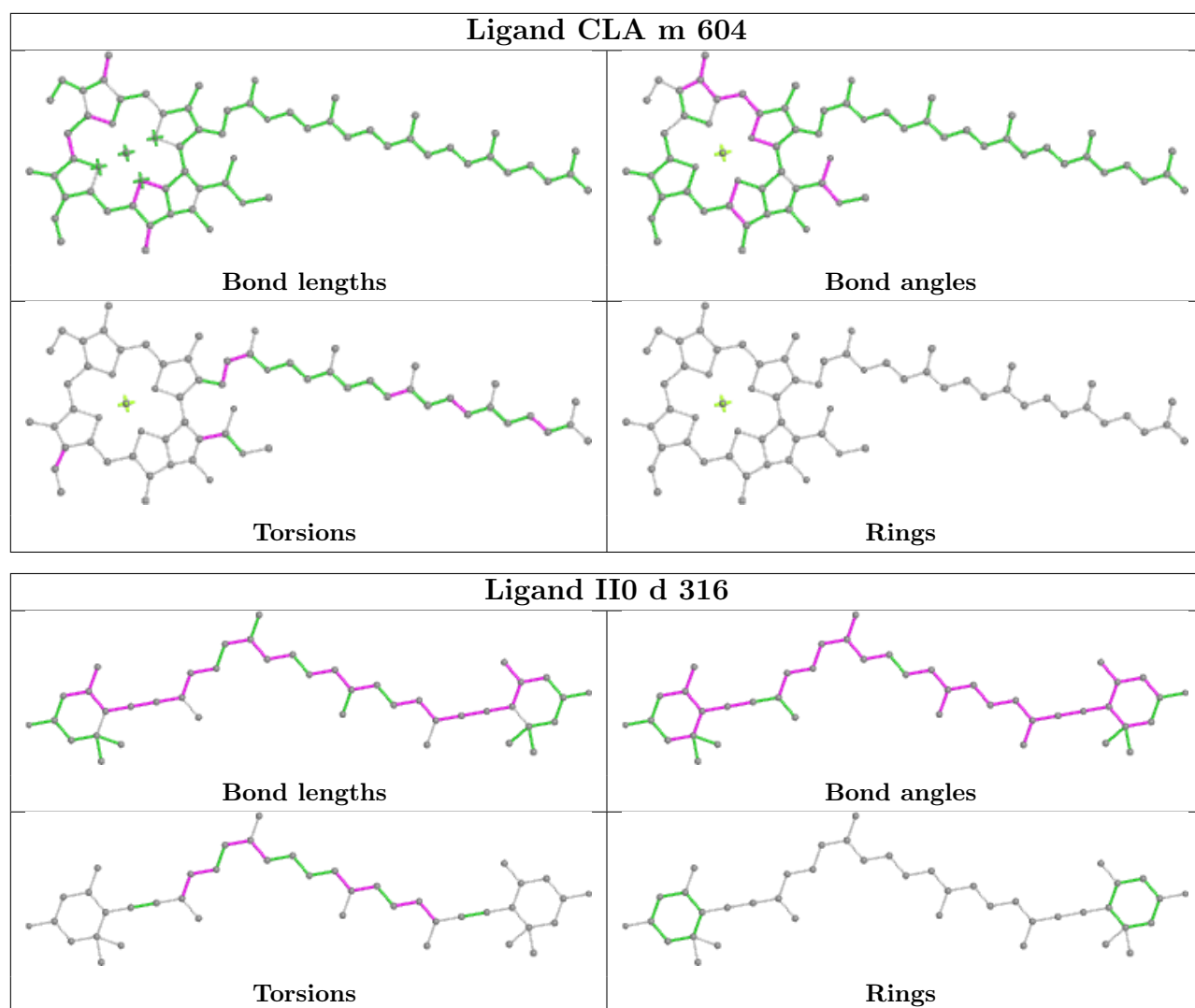
Torsions



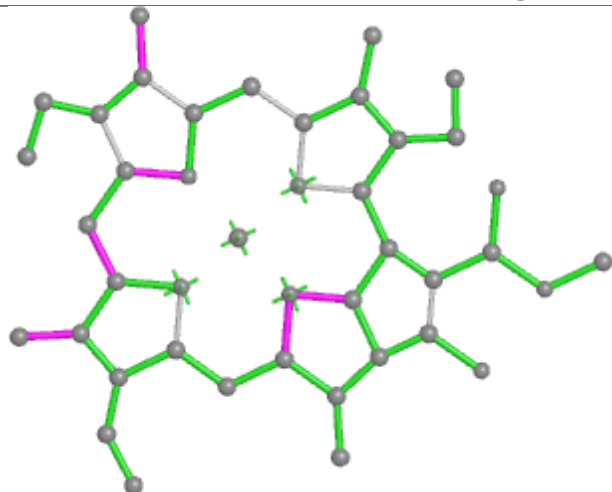
Rings

Ligand CLA s 406**Ligand CLA A 820**

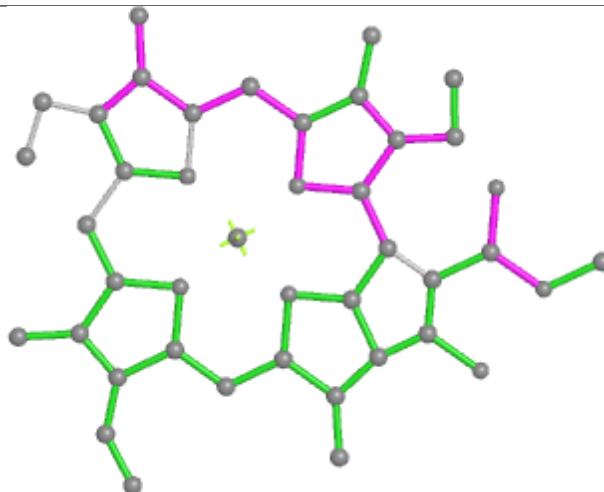




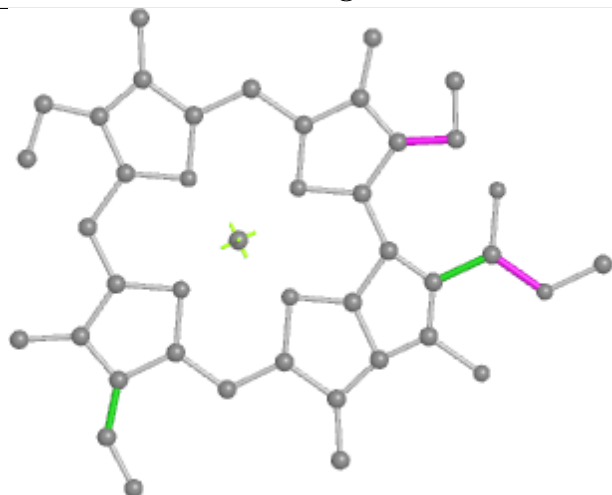
Ligand CLA K 101



Bond lengths



Bond angles

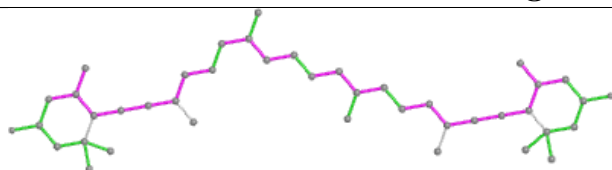


Torsions

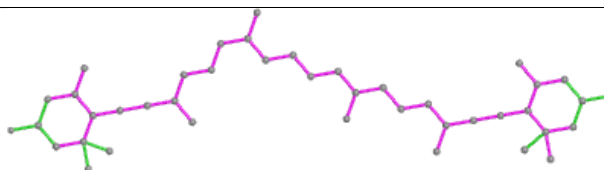


Rings

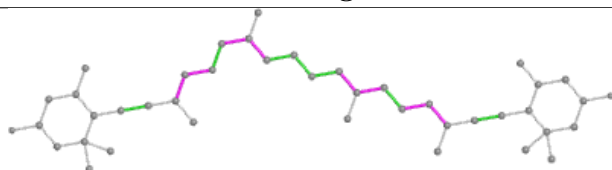
Ligand II0 m 619



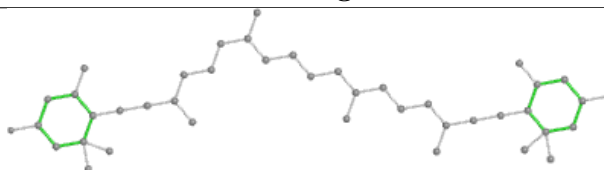
Bond lengths



Bond angles

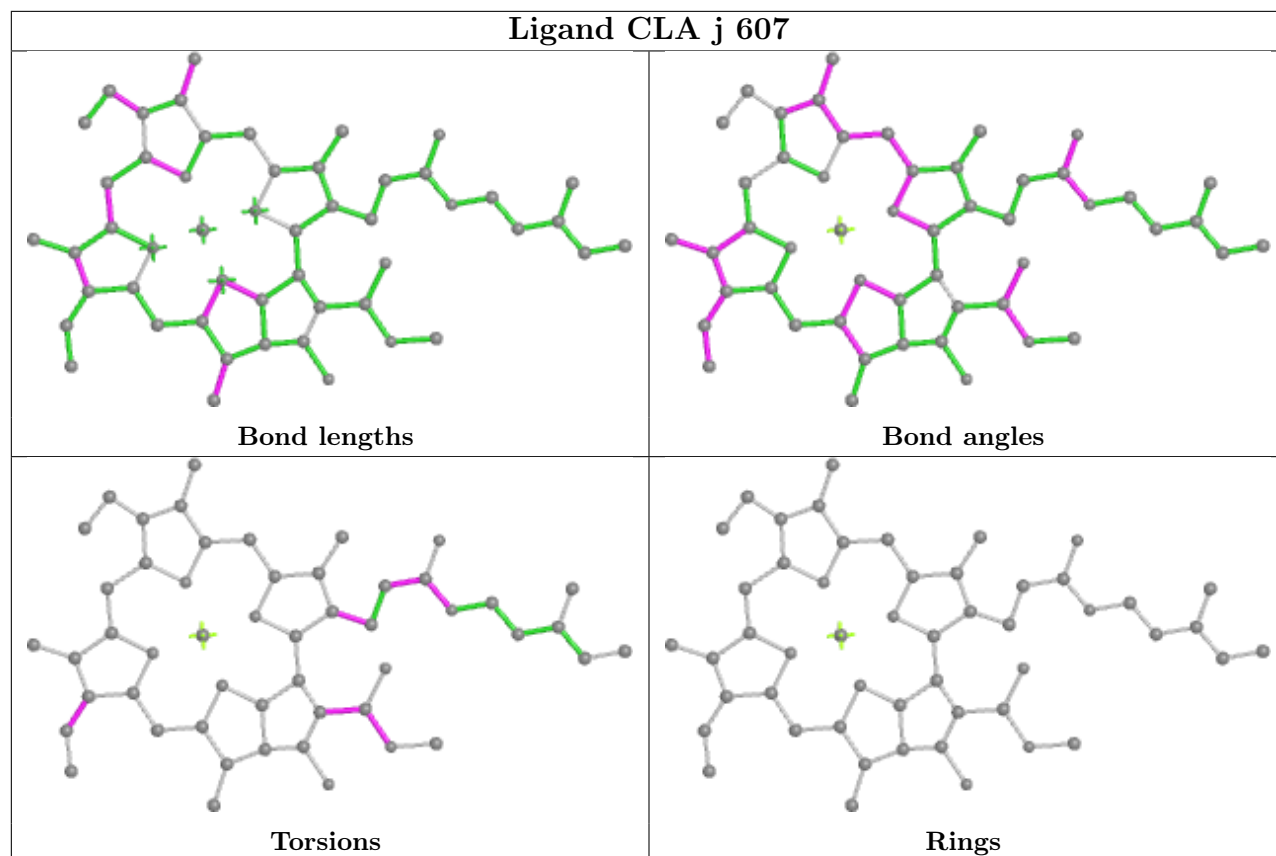


Torsions

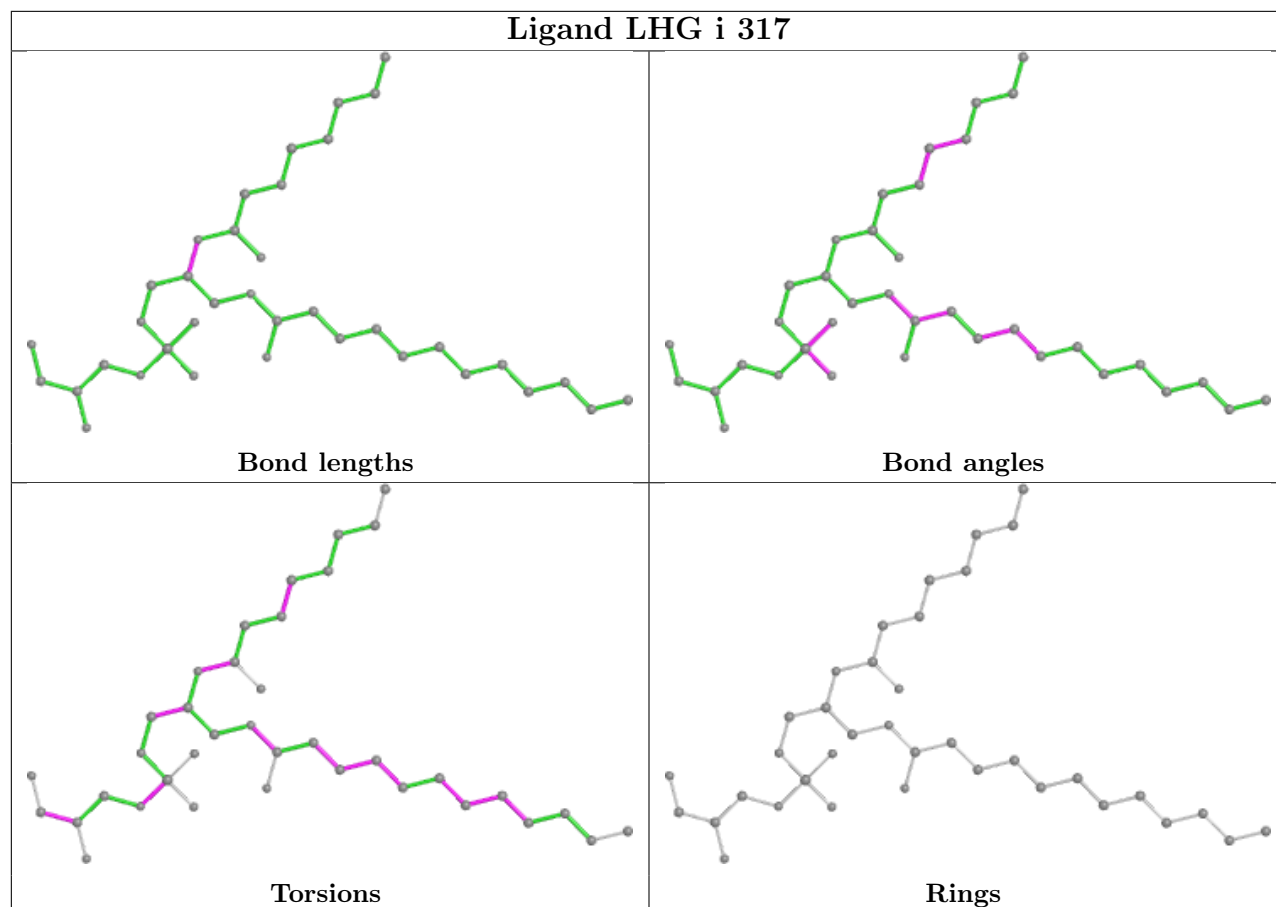


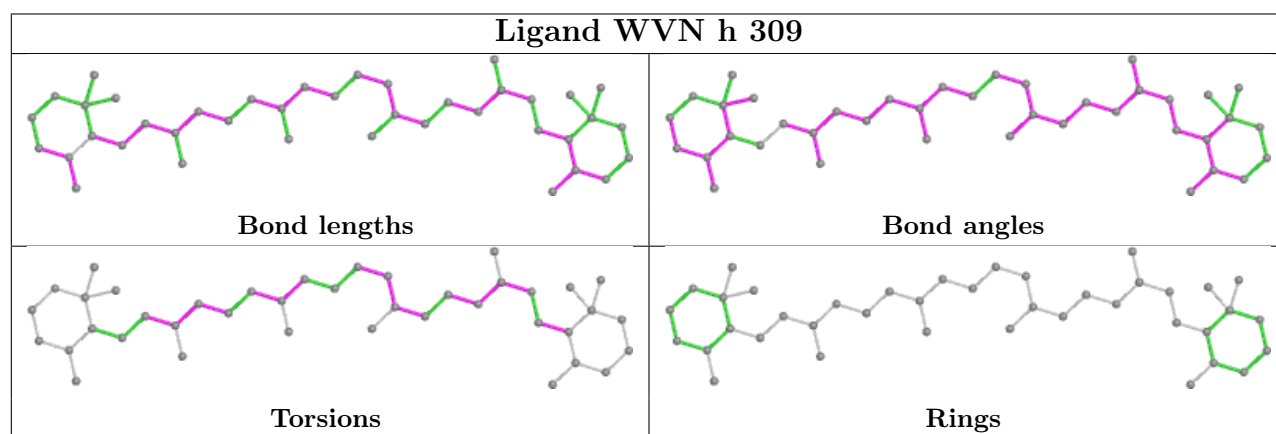
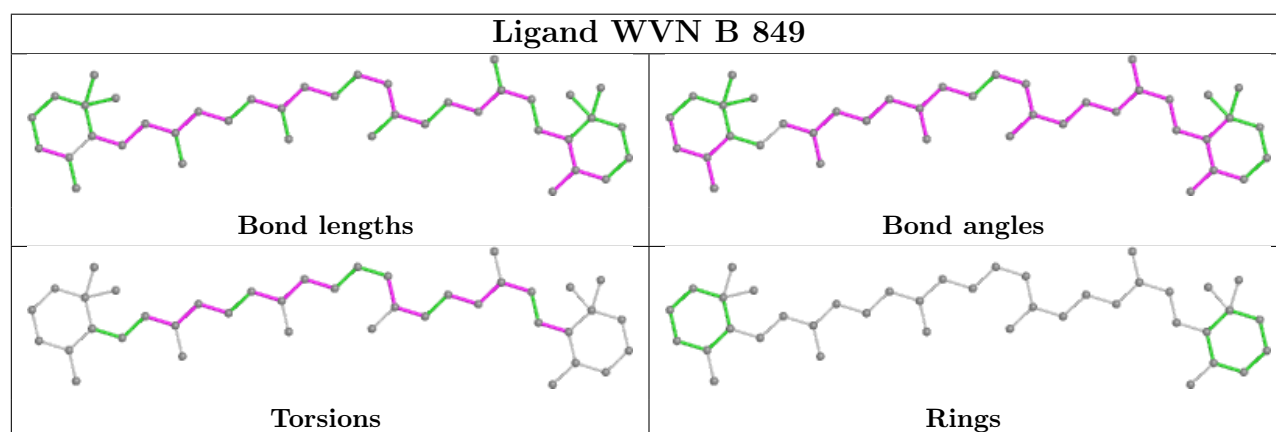
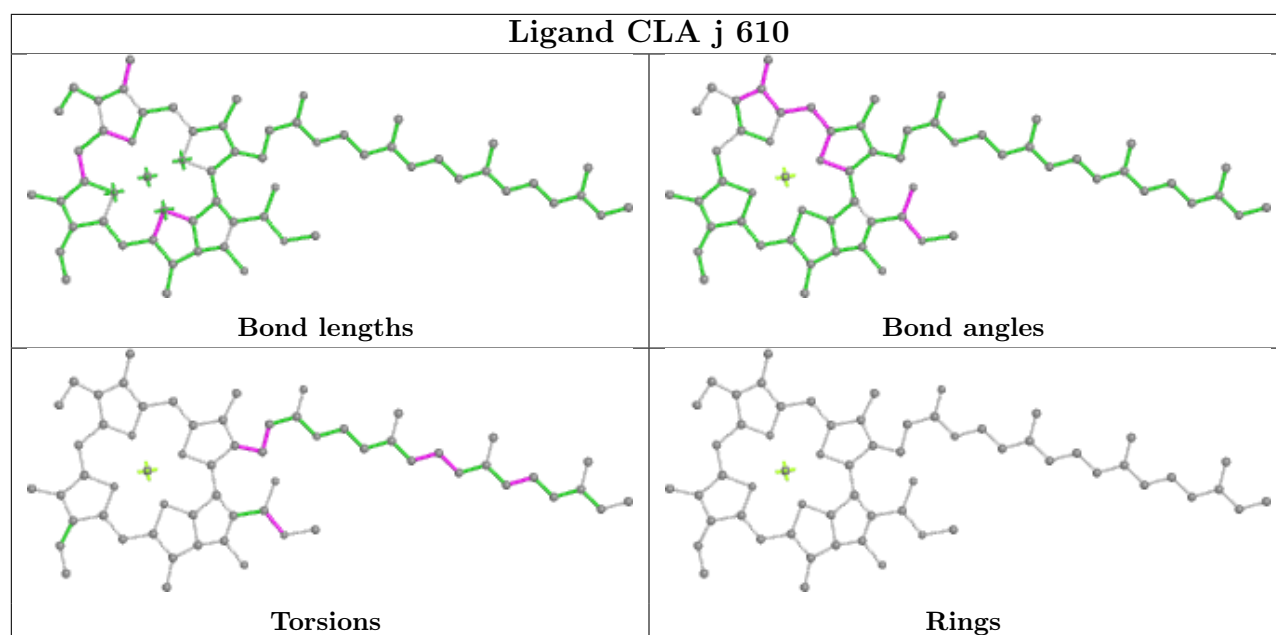
Rings

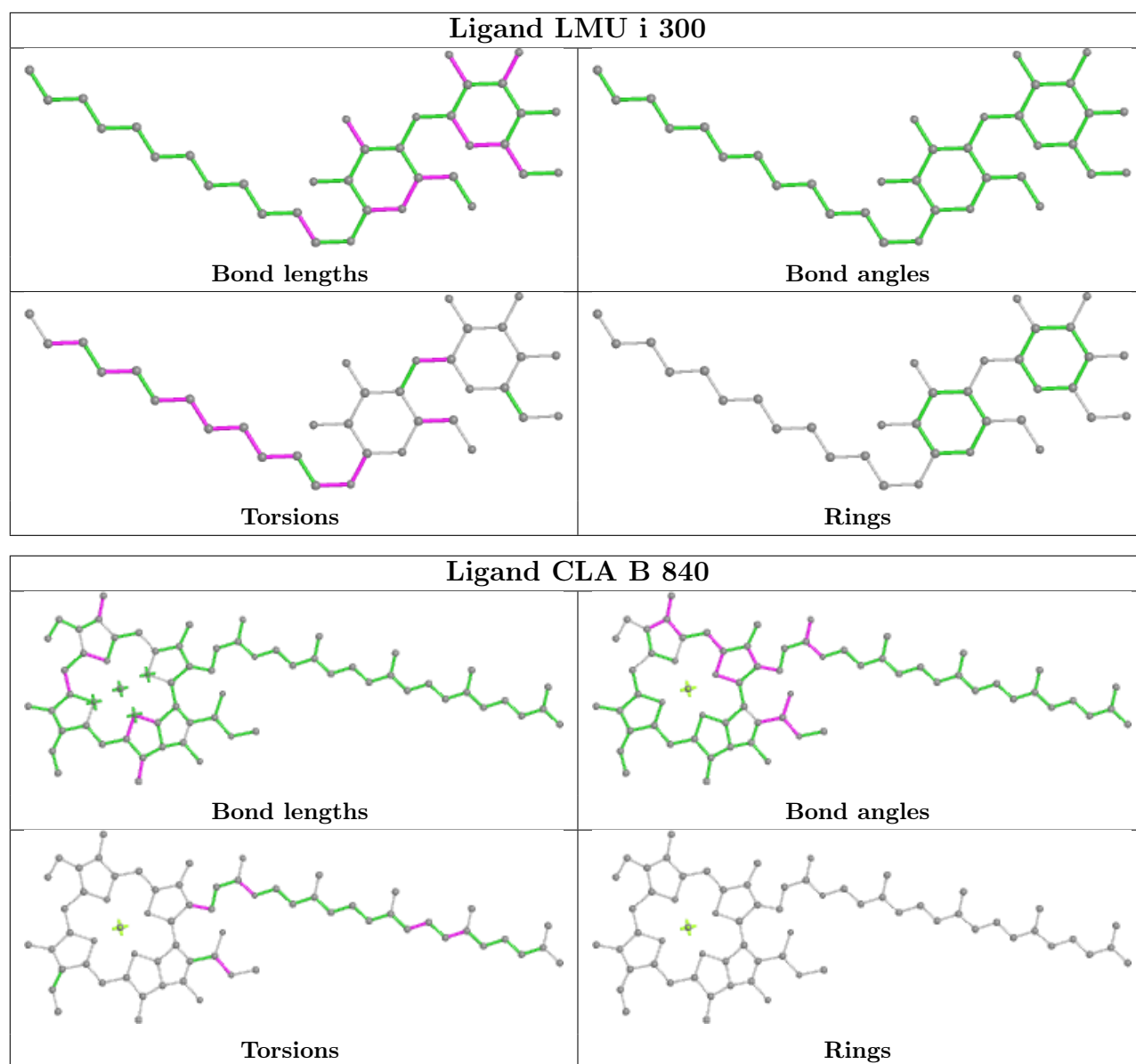
Ligand CLA j 607



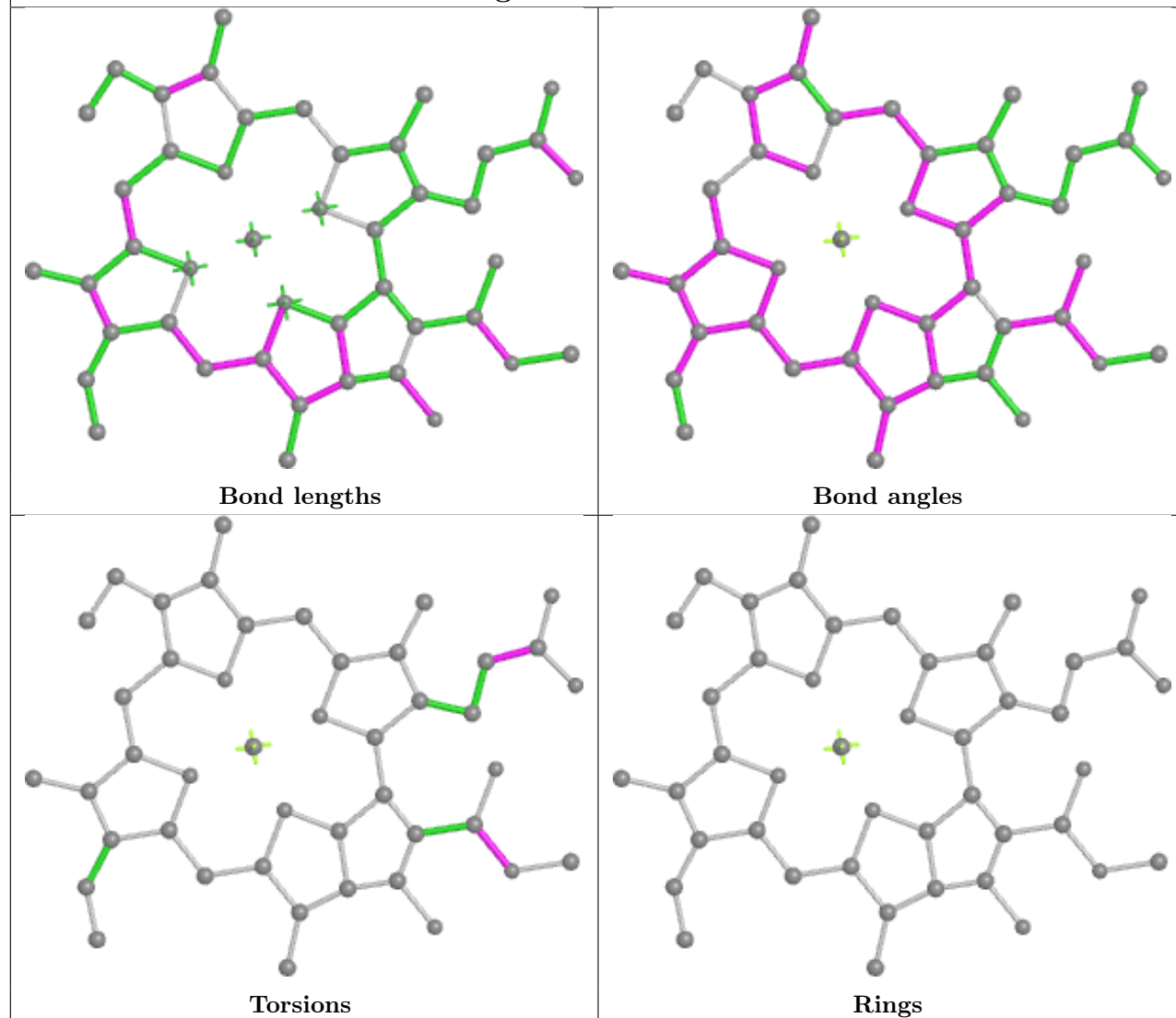
Ligand LHG i 317



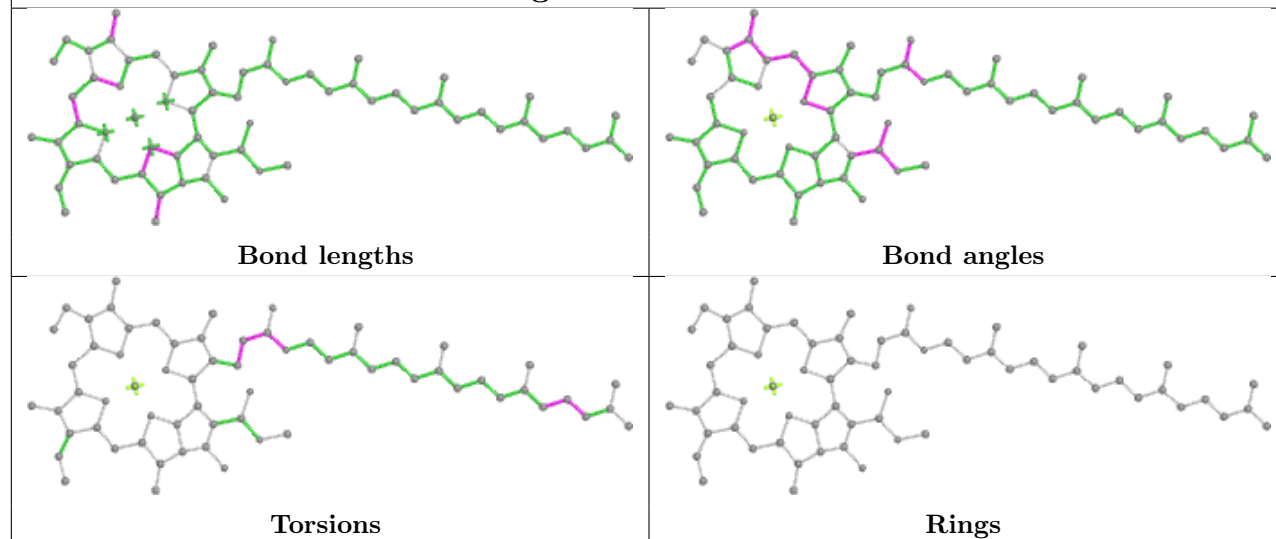


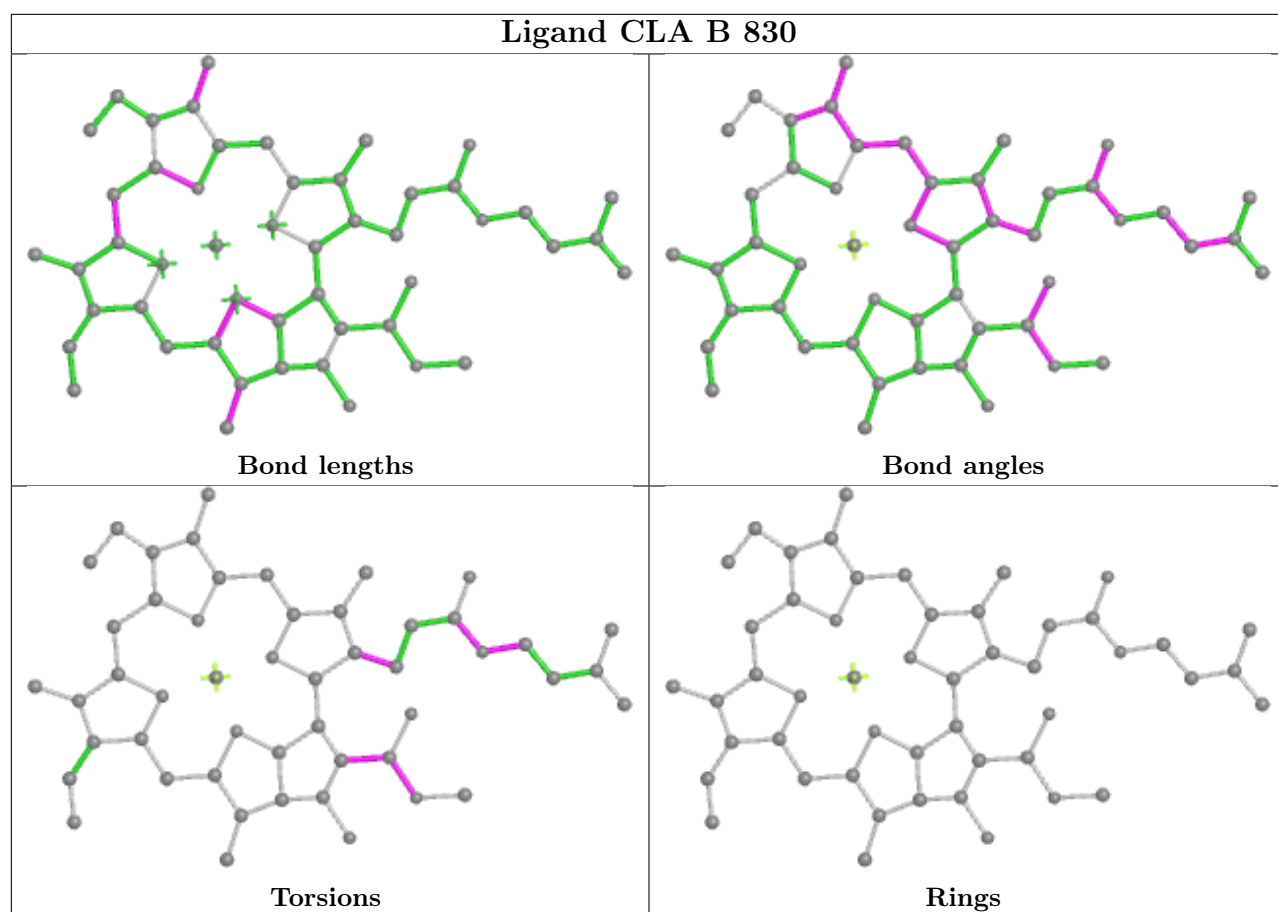


Ligand CLA c 309

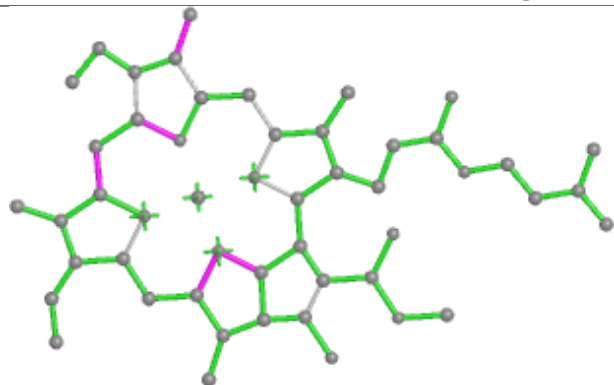


Ligand CLA A 802

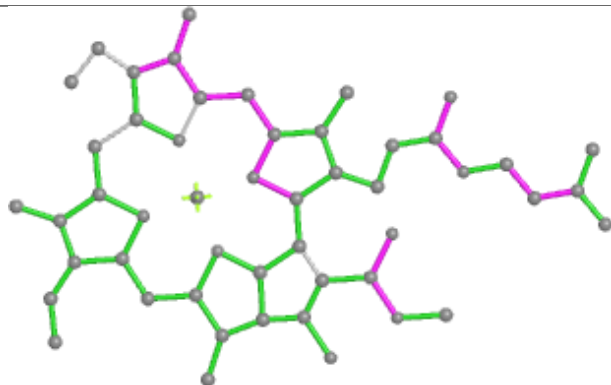




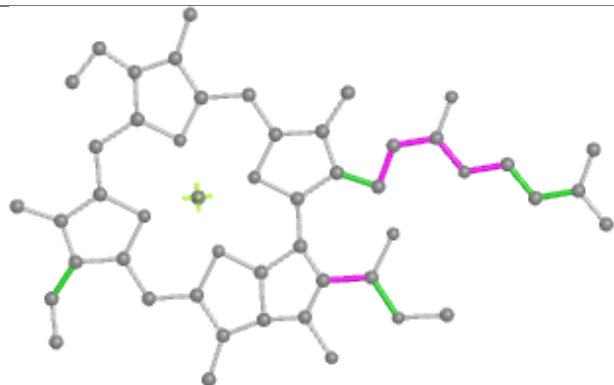
Ligand CLA h 303



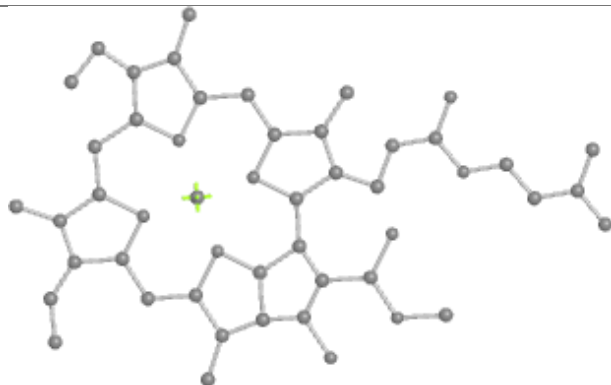
Bond lengths



Bond angles

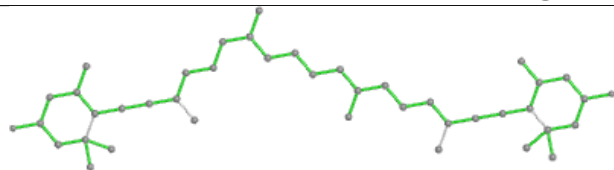


Torsions

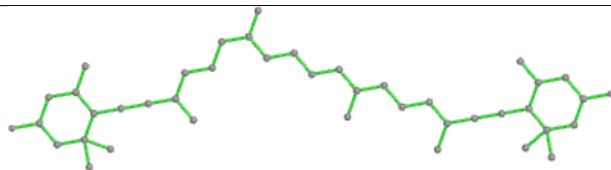


Rings

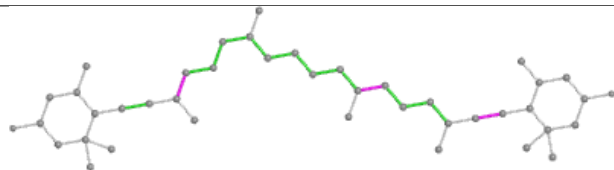
Ligand II0 l 317



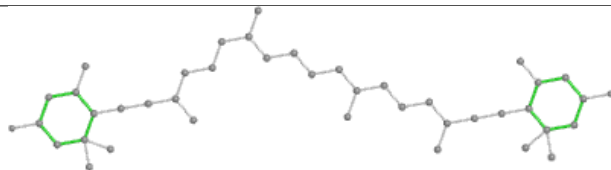
Bond lengths



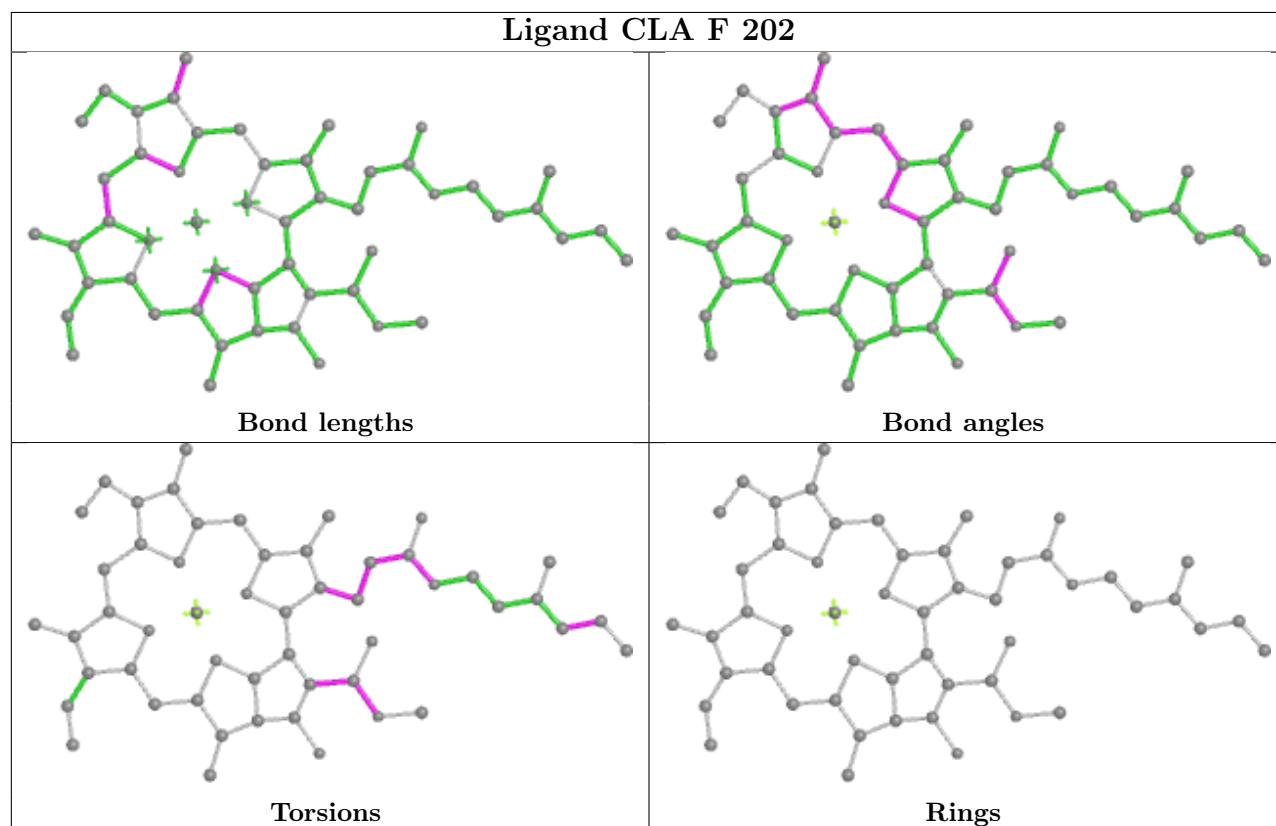
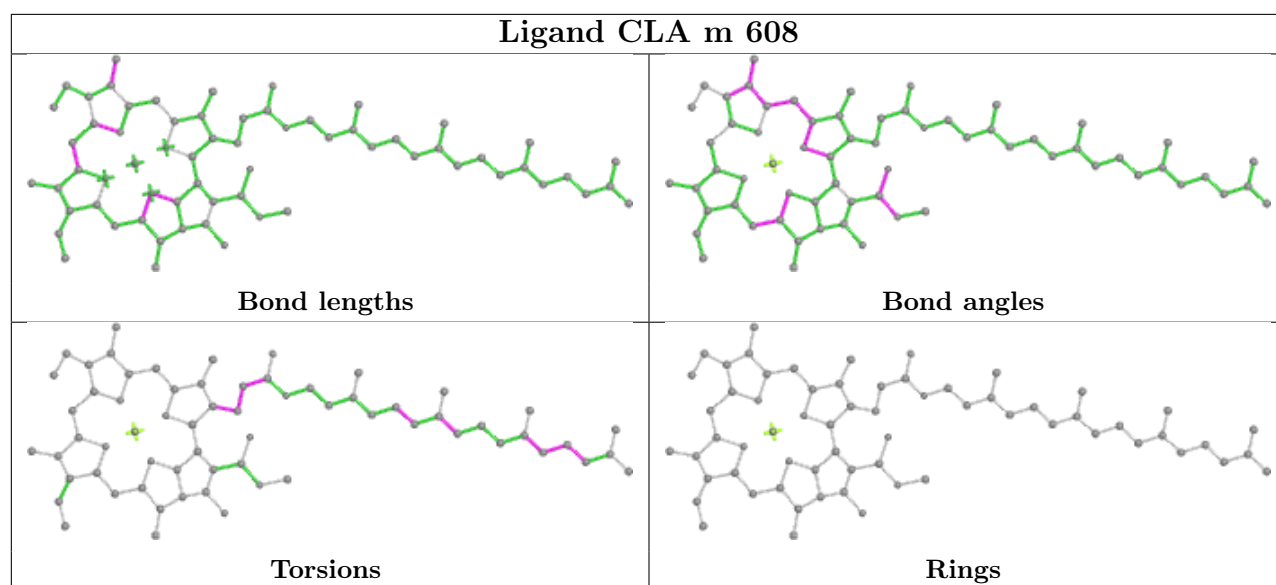
Bond angles

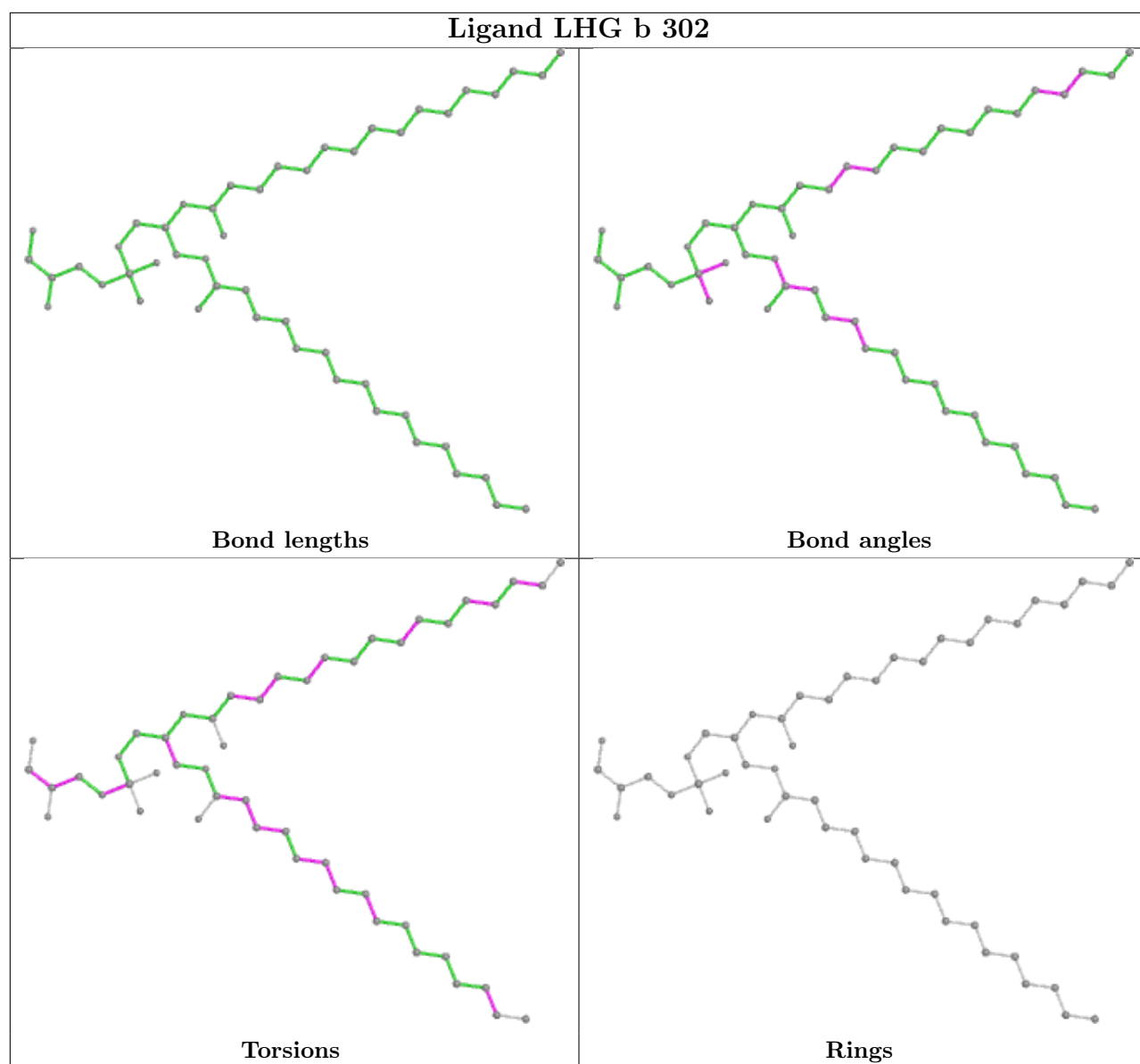


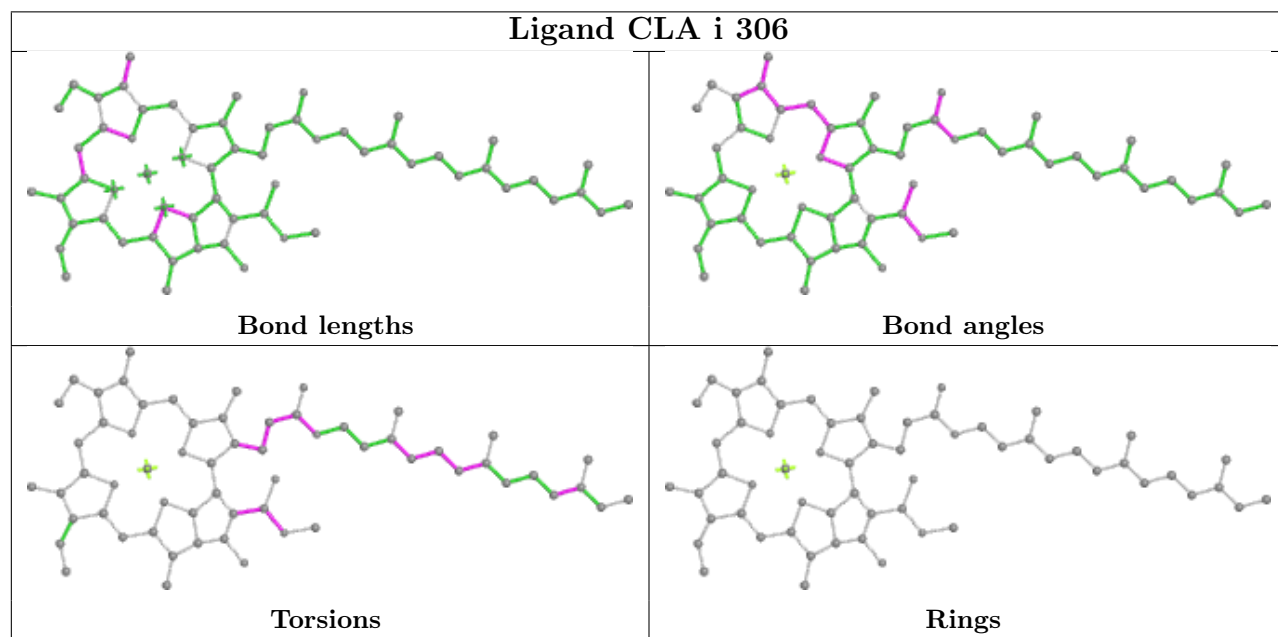
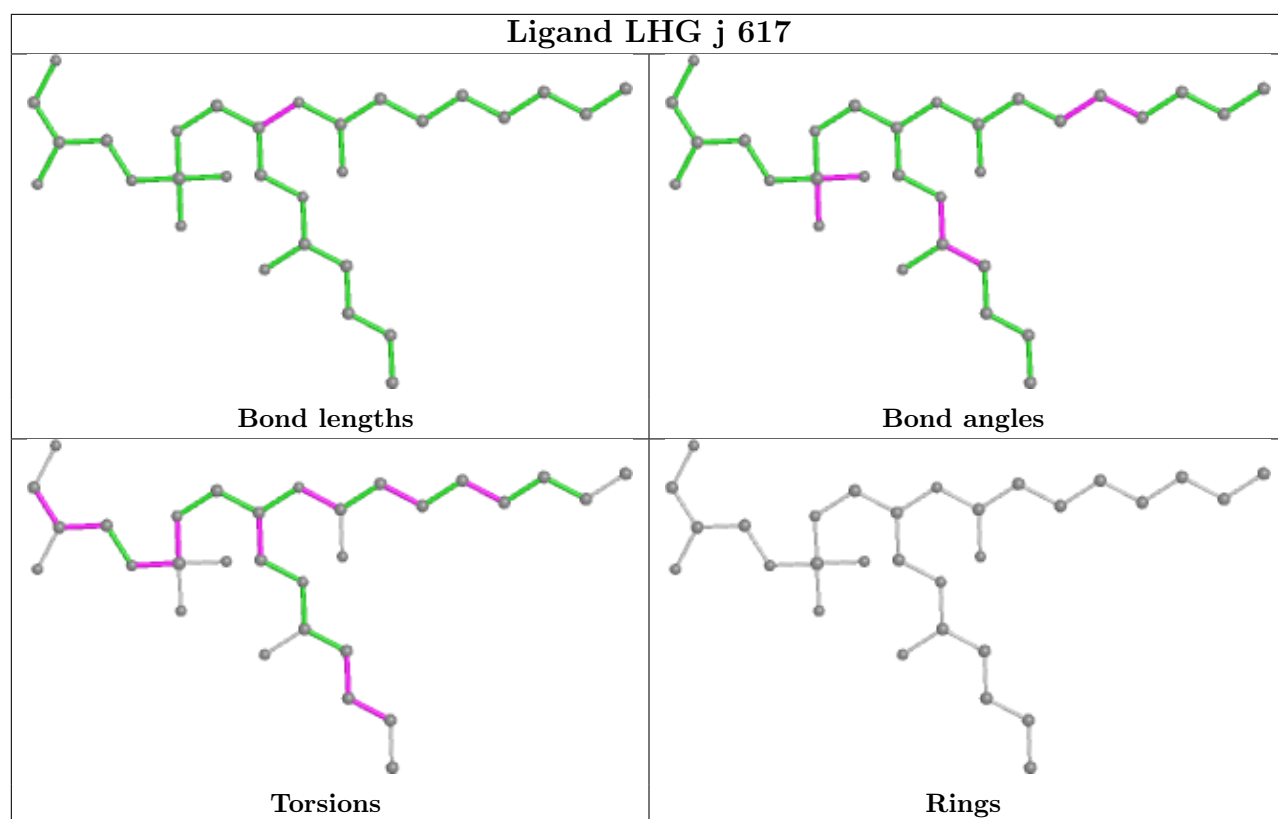
Torsions

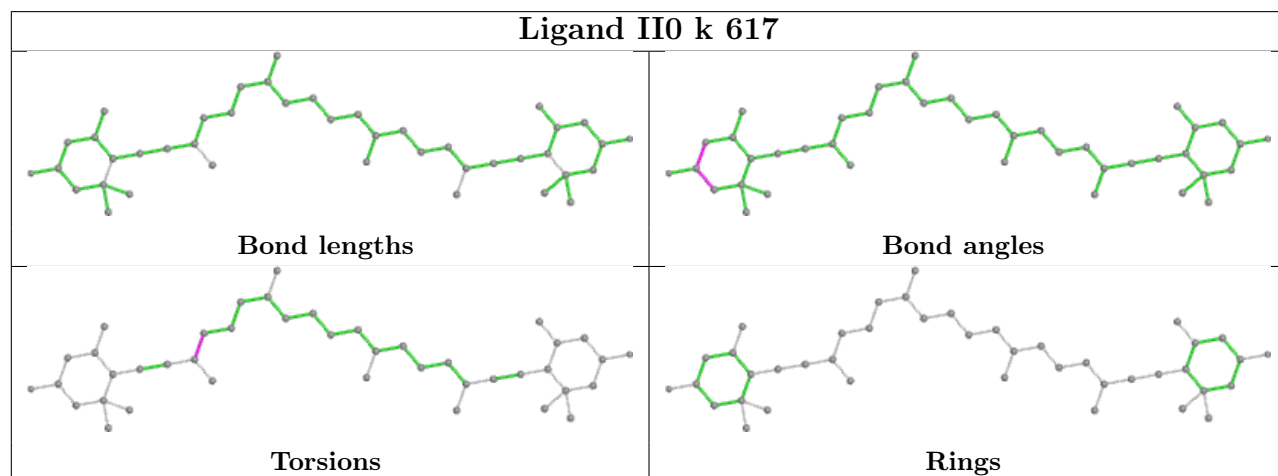
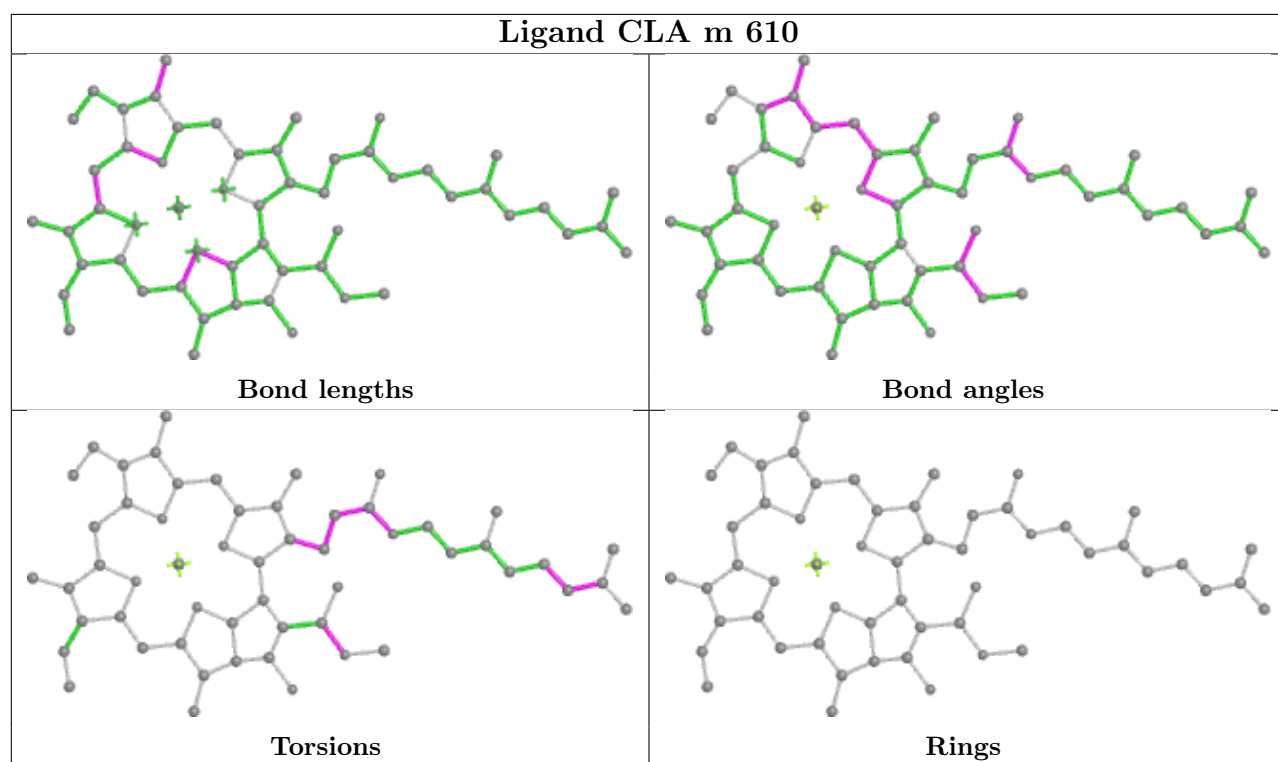


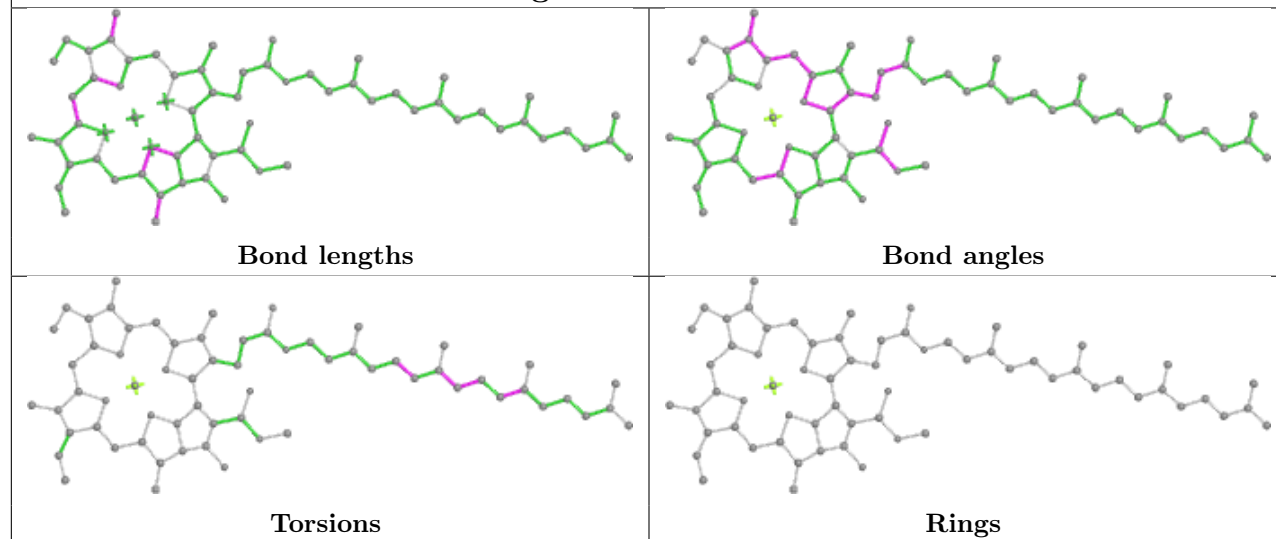
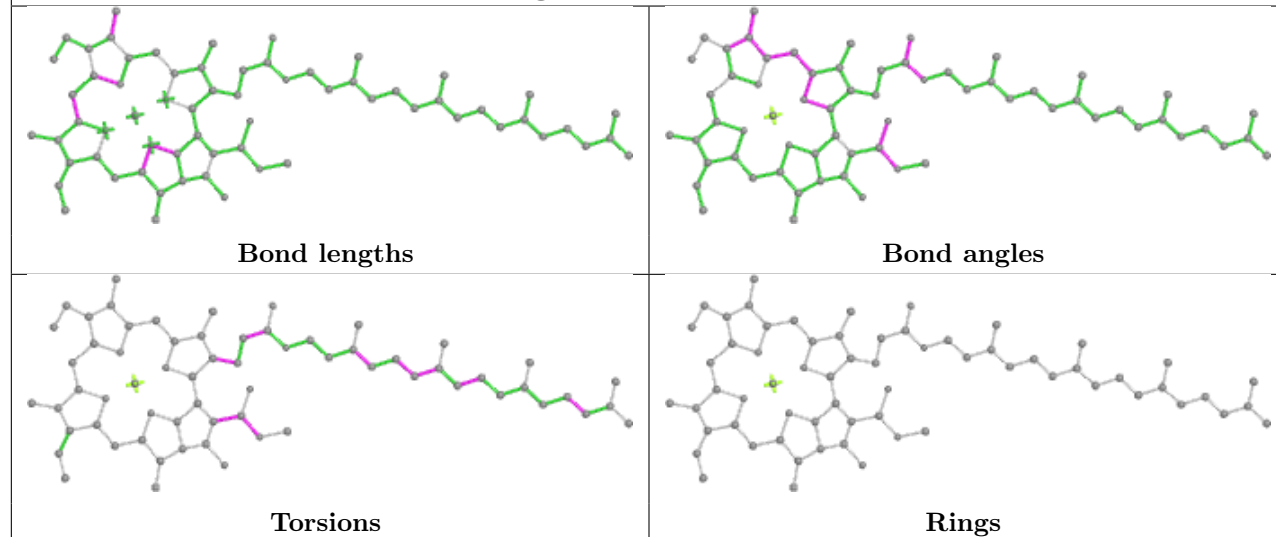
Rings



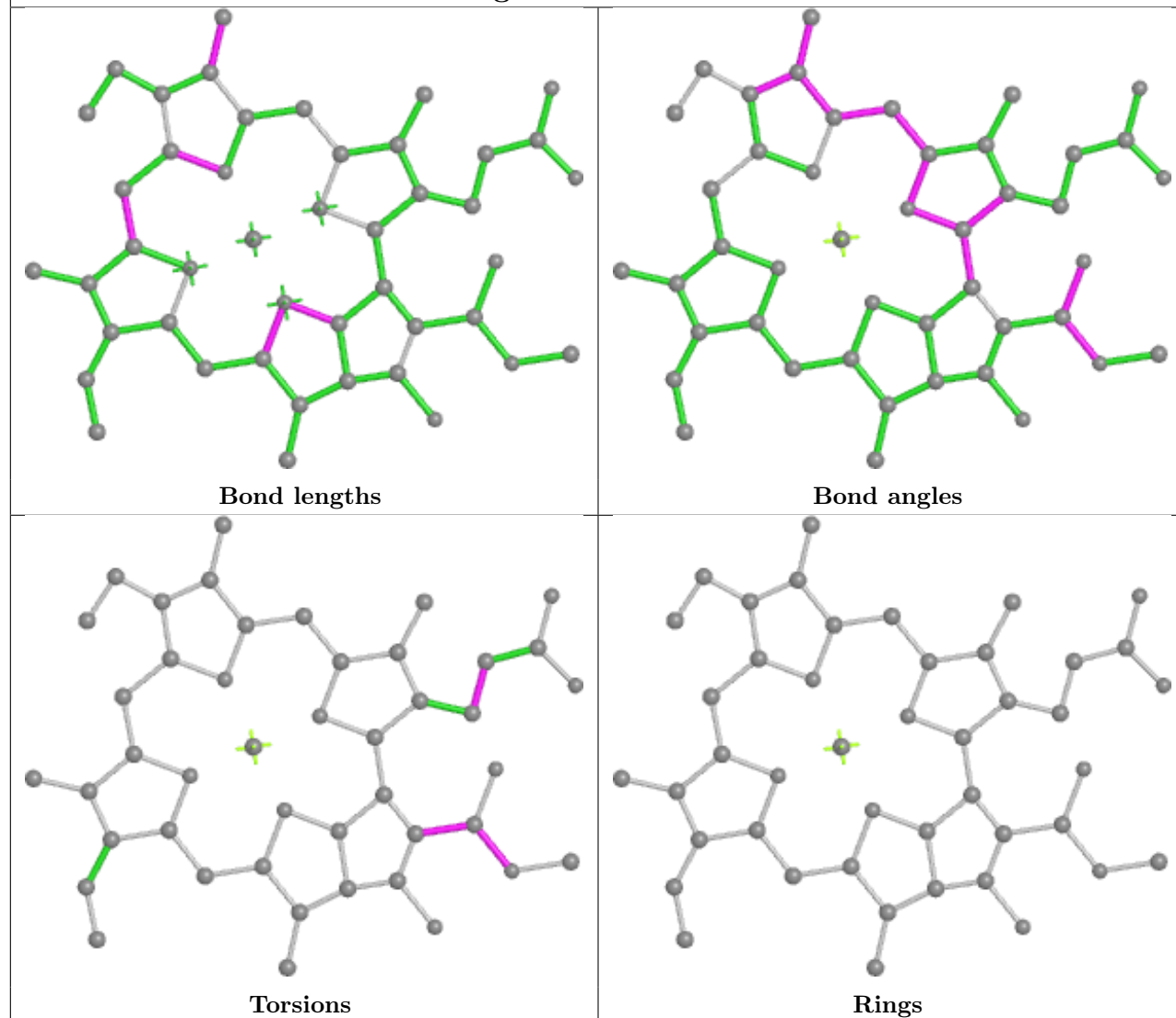




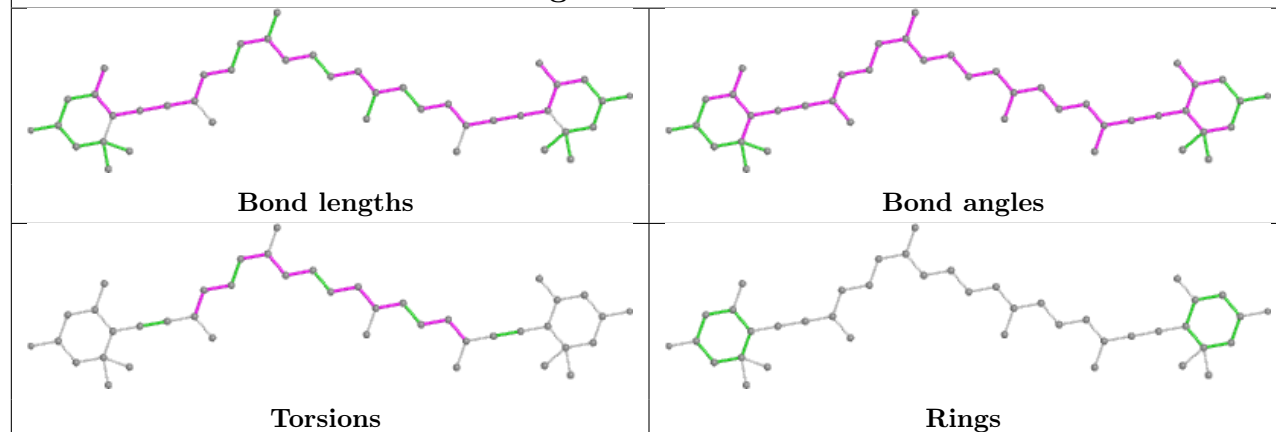


Ligand CLA A 825**Ligand CLA B 812**

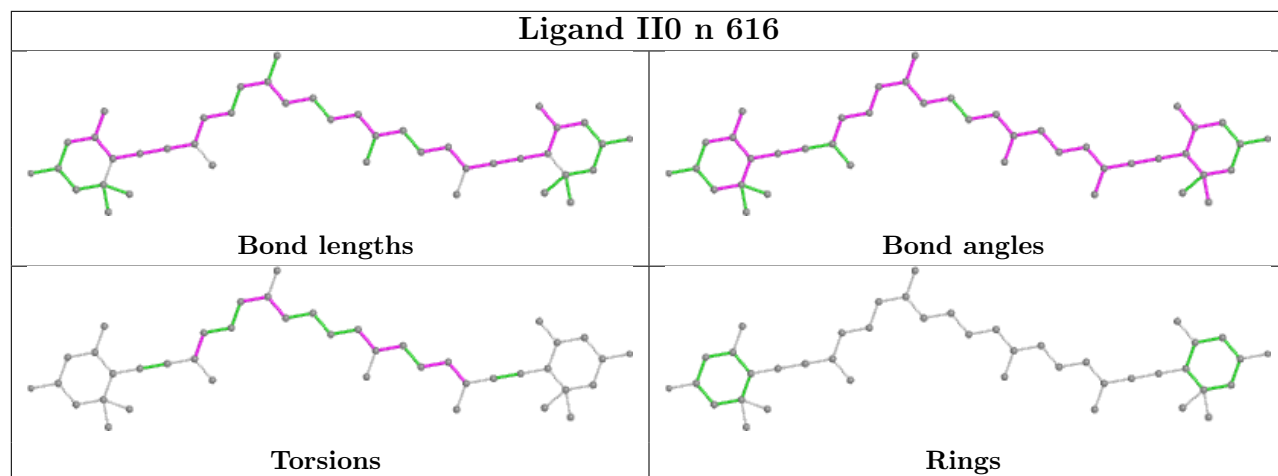
Ligand CLA k 605



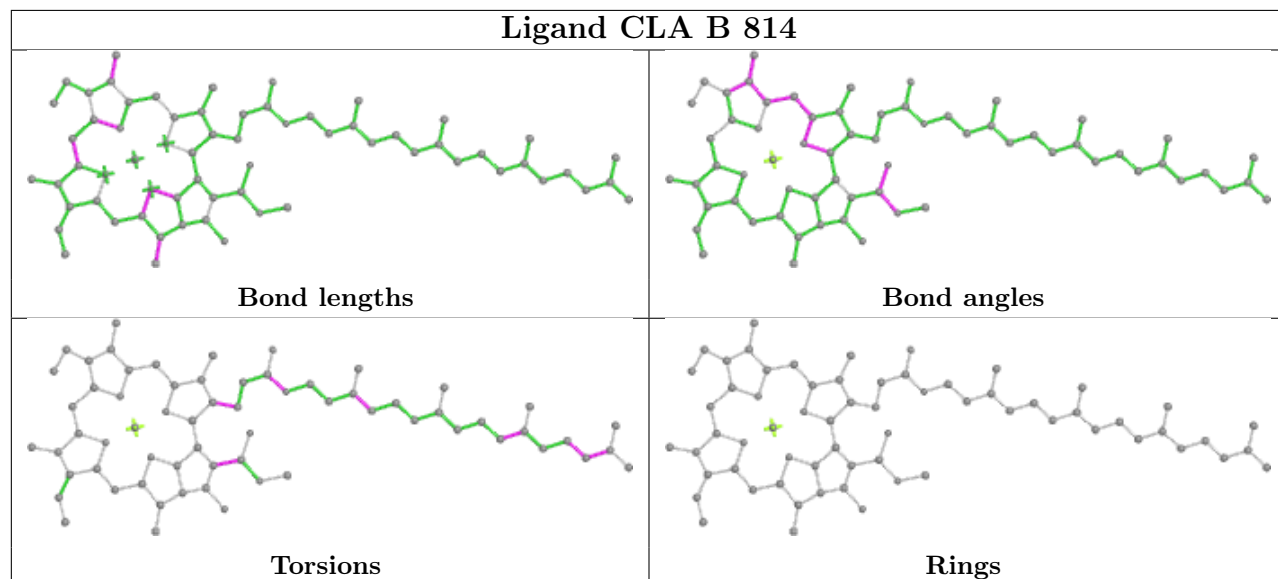
Ligand II0 h 311



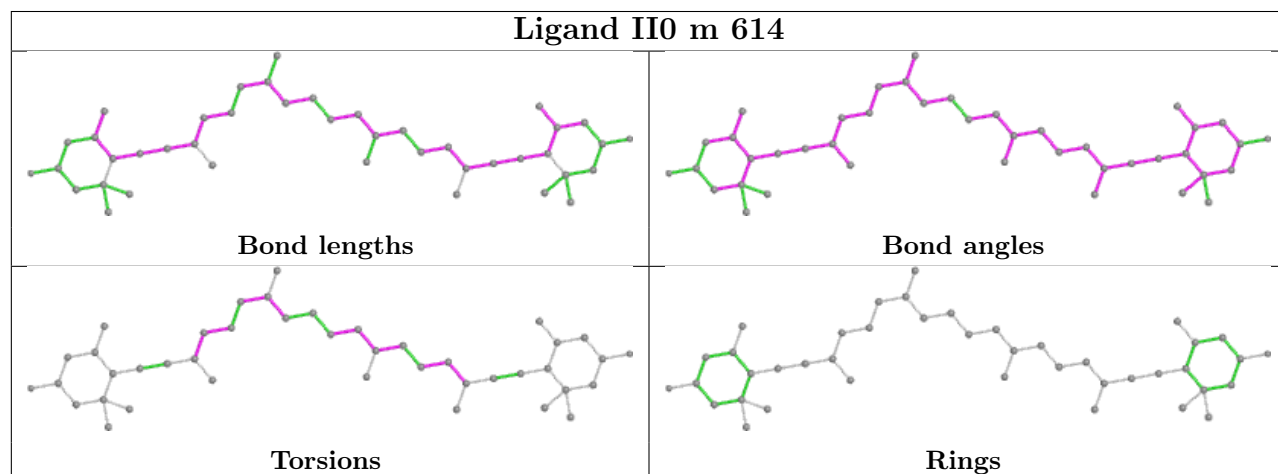
Ligand II0 n 616



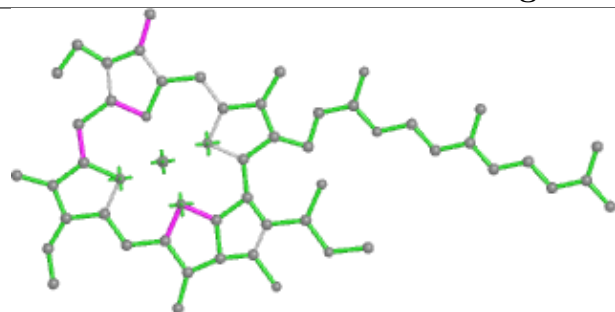
Ligand CLA B 814



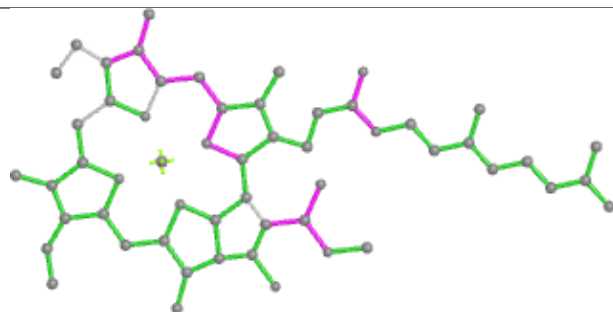
Ligand II0 m 614



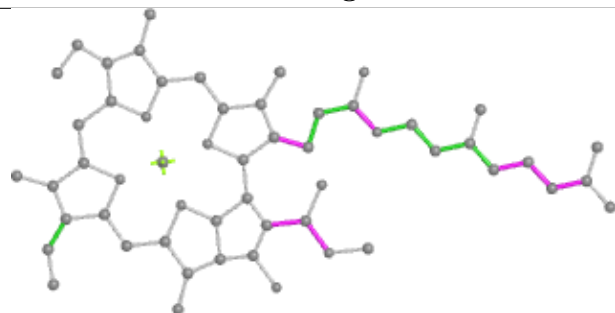
Ligand CLA b 304



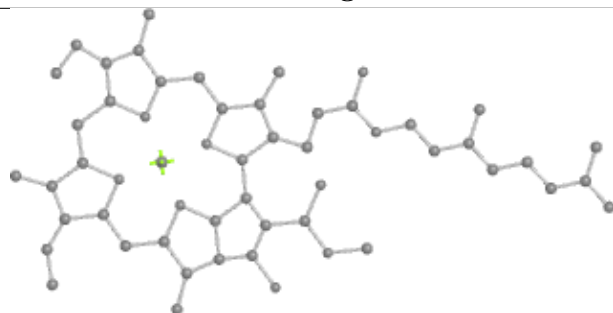
Bond lengths



Bond angles

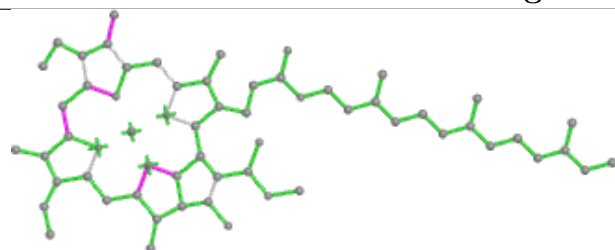


Torsions

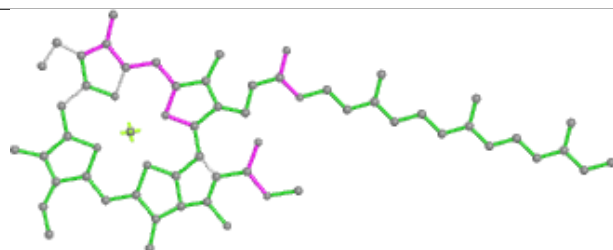


Rings

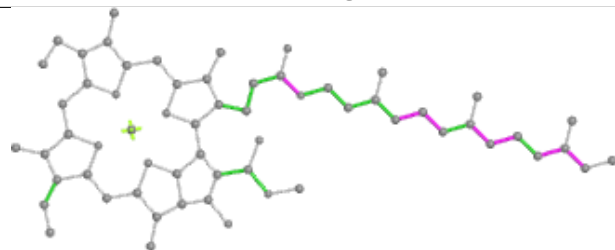
Ligand CLA l 311



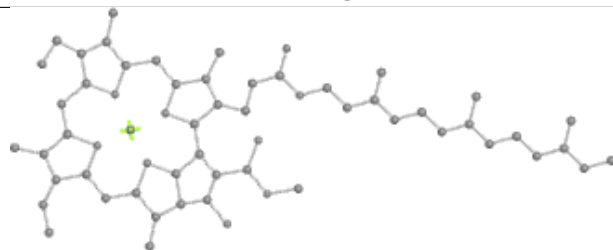
Bond lengths



Bond angles

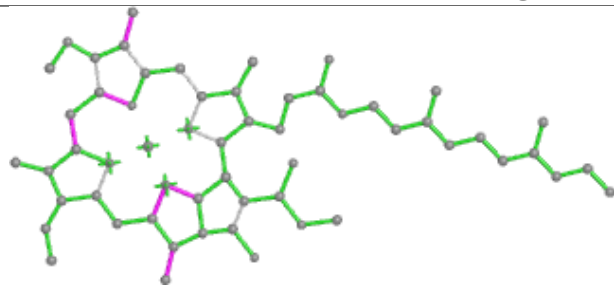


Torsions

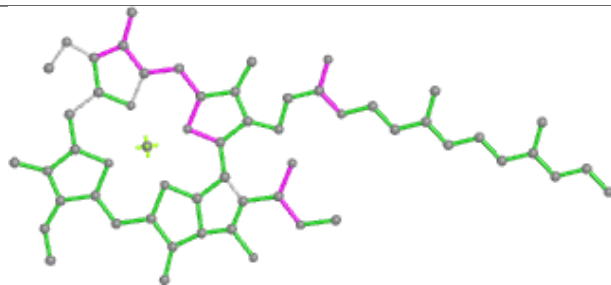


Rings

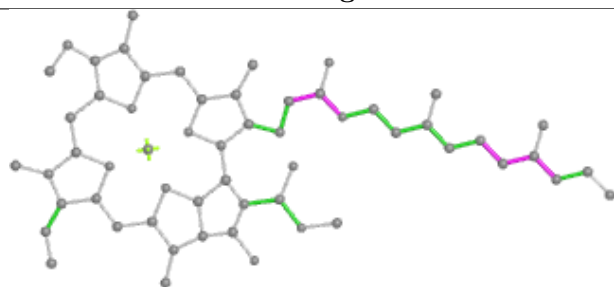
Ligand CLA B 839



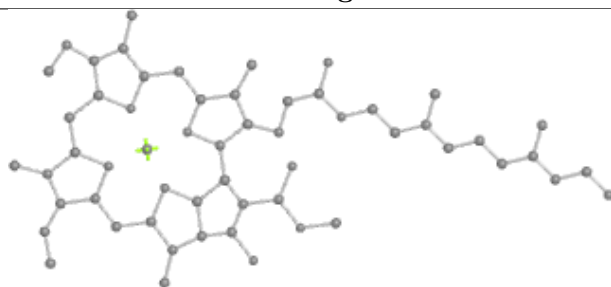
Bond lengths



Bond angles

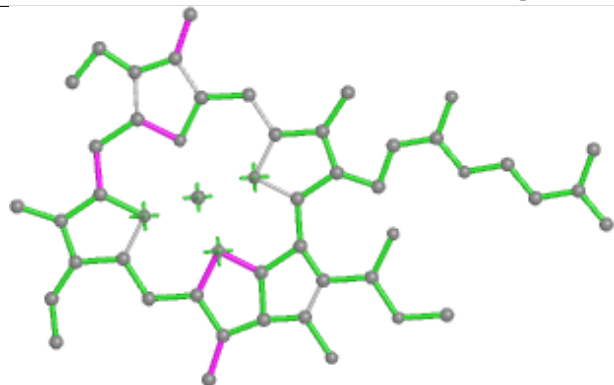


Torsions

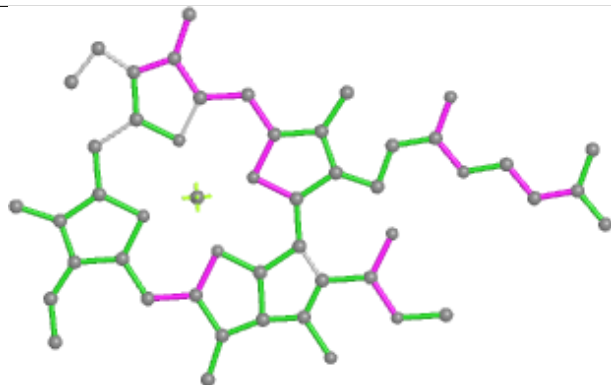


Rings

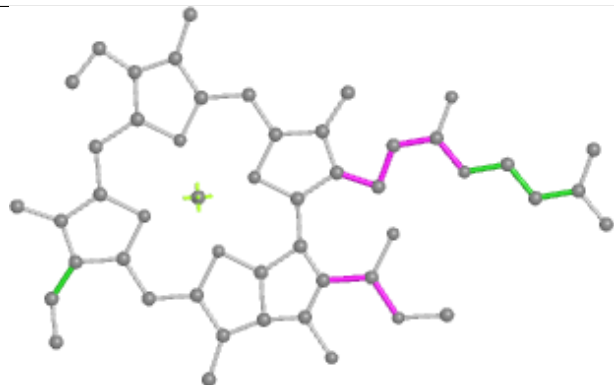
Ligand CLA B 828



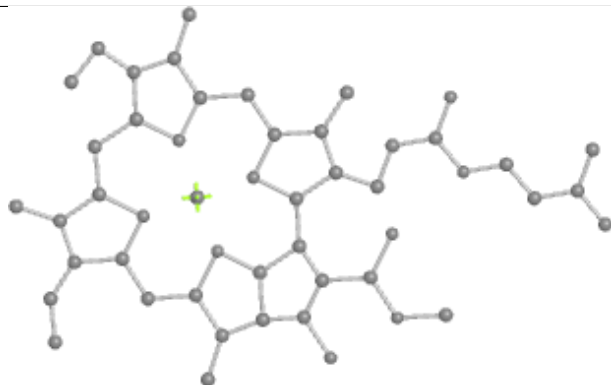
Bond lengths



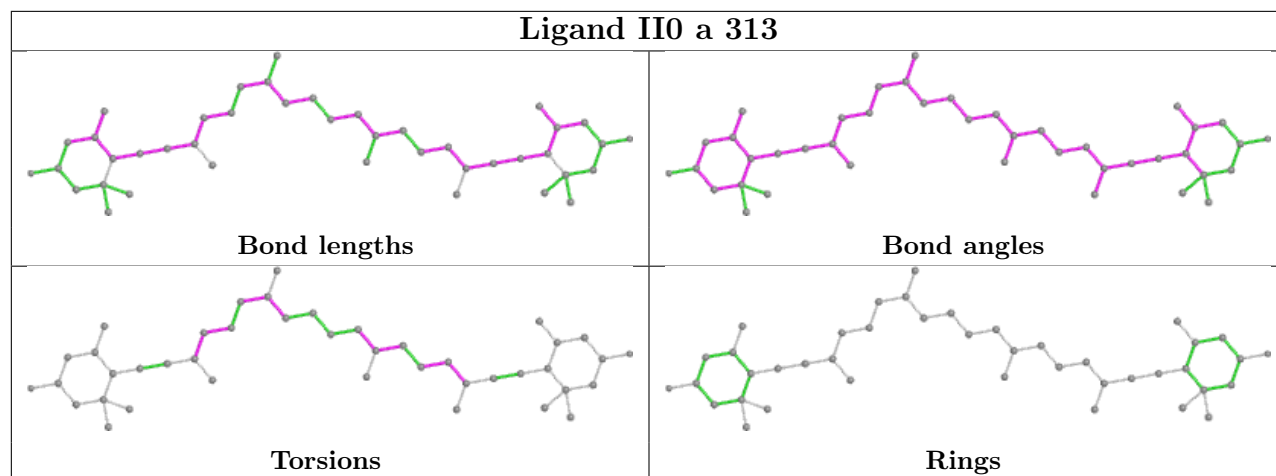
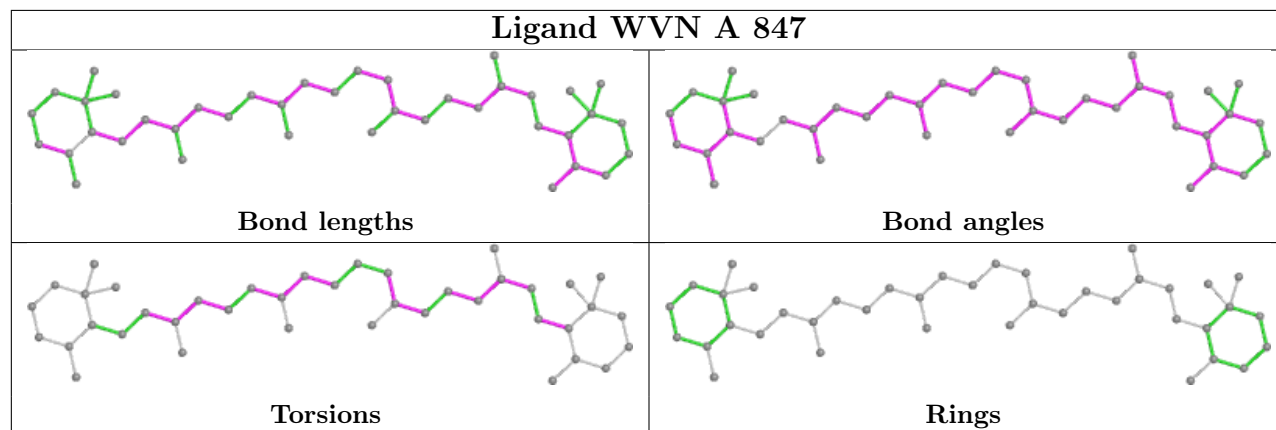
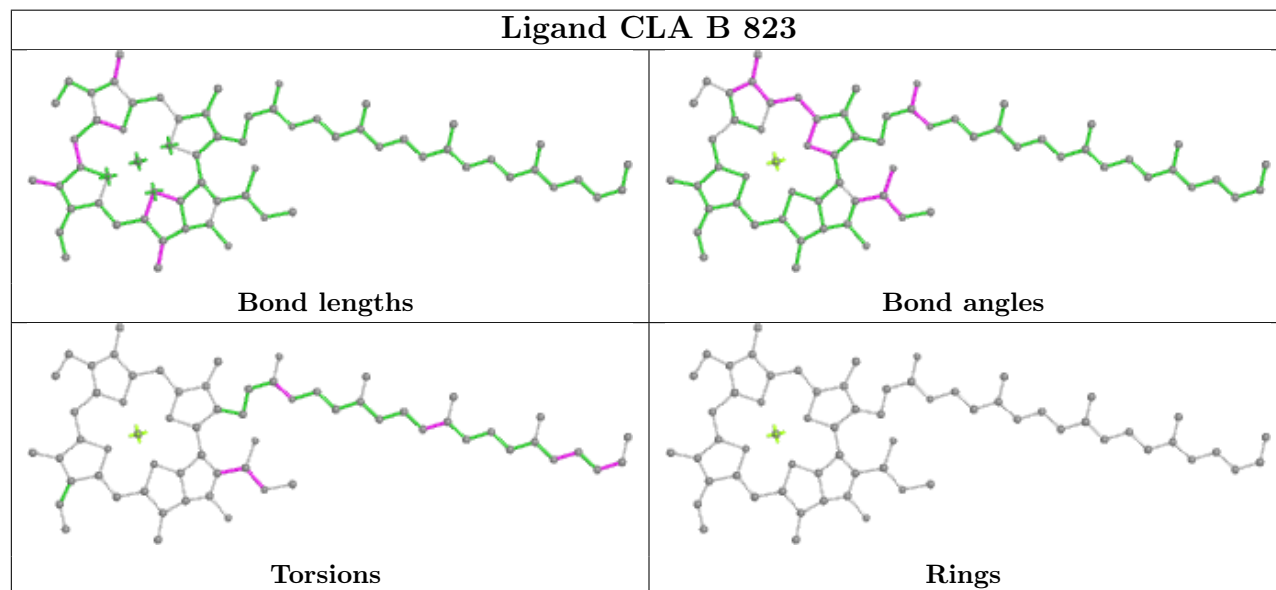
Bond angles



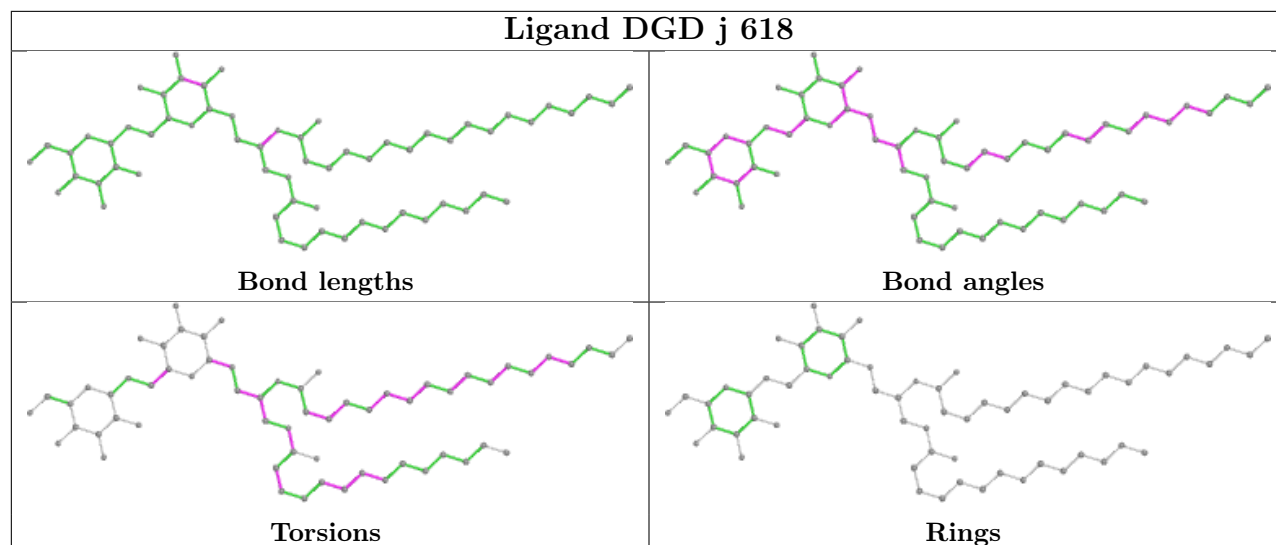
Torsions



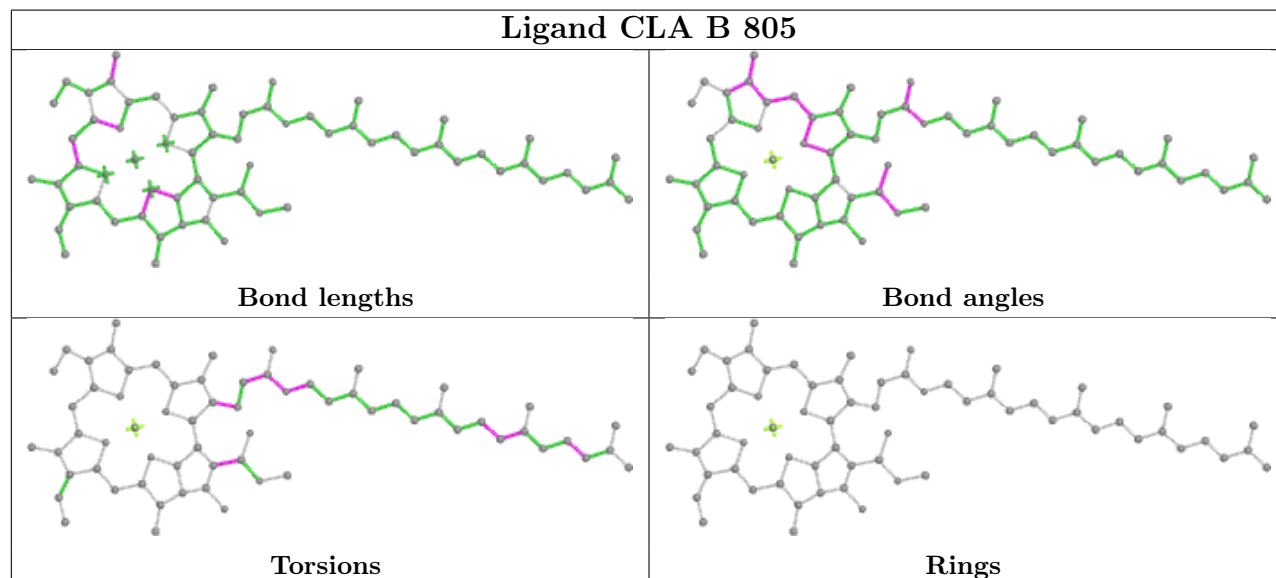
Rings

Ligand II0 a 313**Ligand WVN A 847****Ligand CLA B 823**

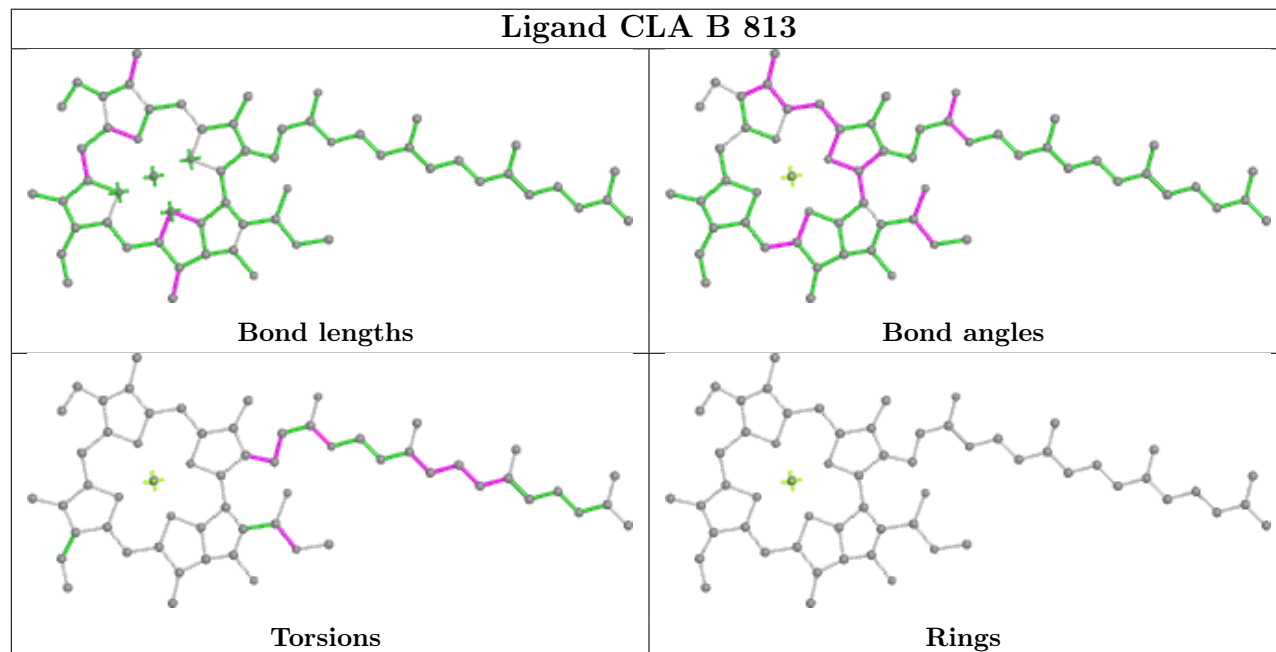
Ligand DGD j 618

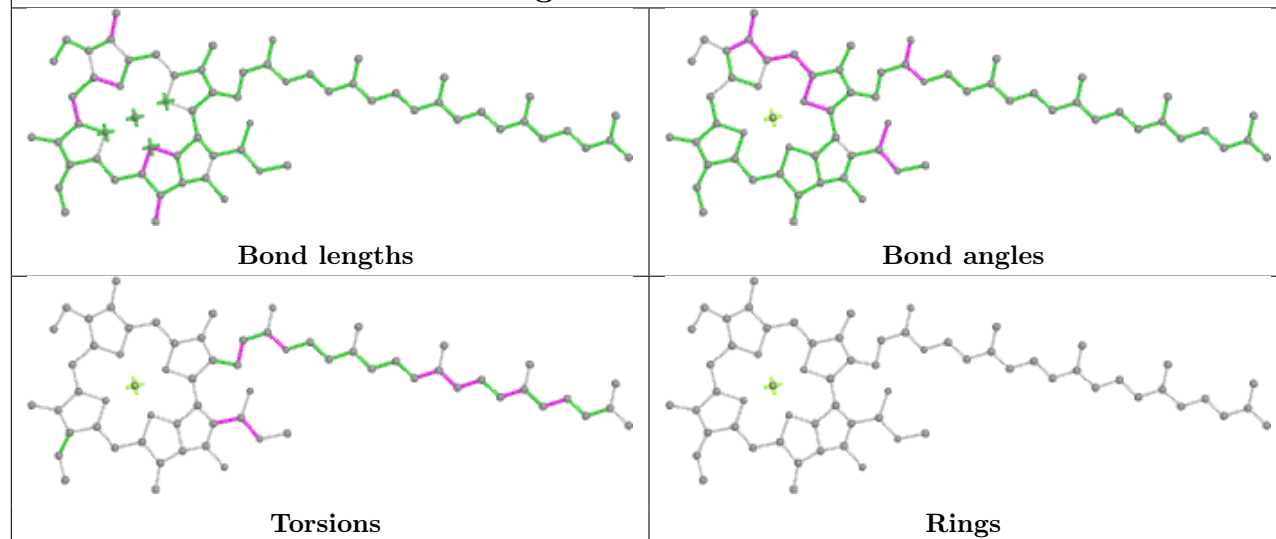
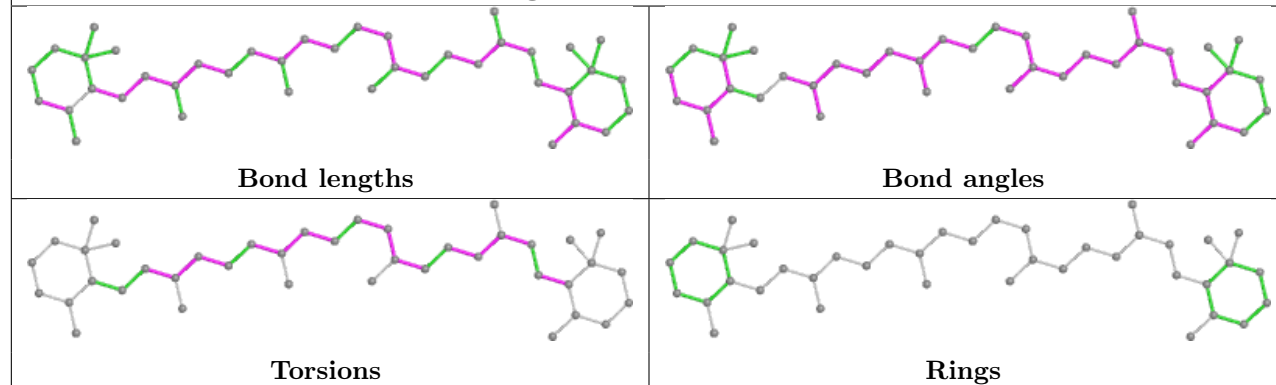


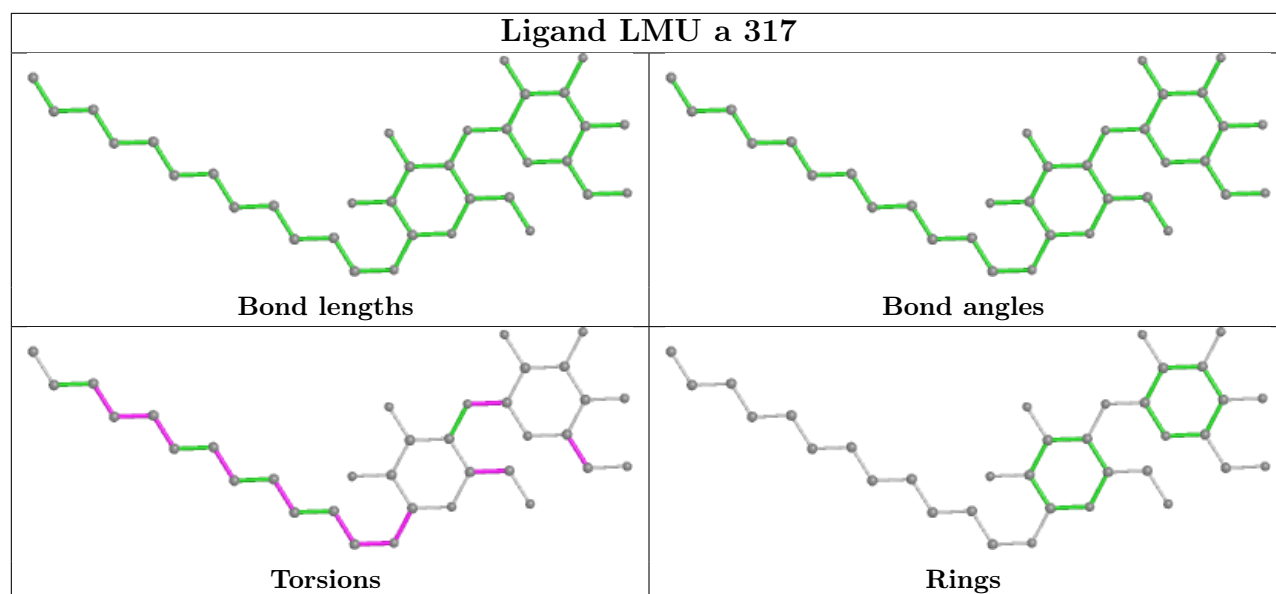
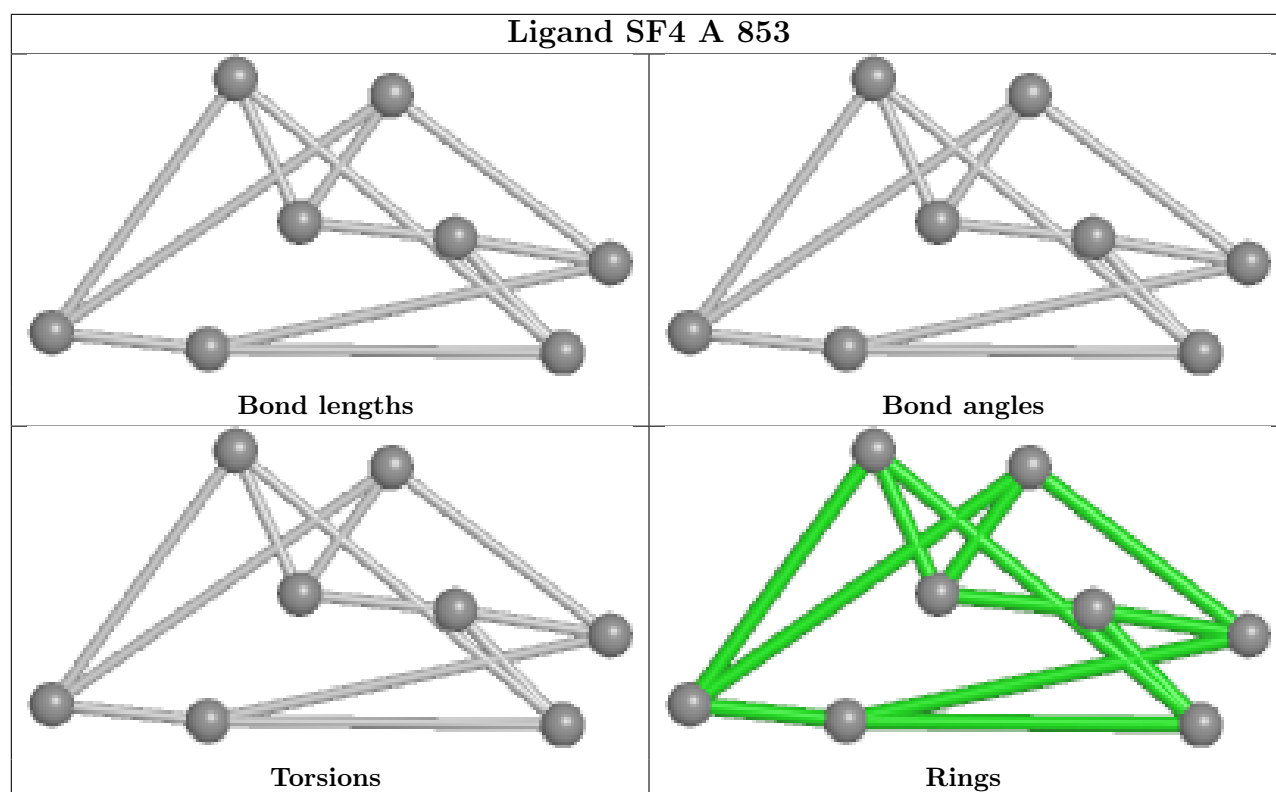
Ligand CLA B 805



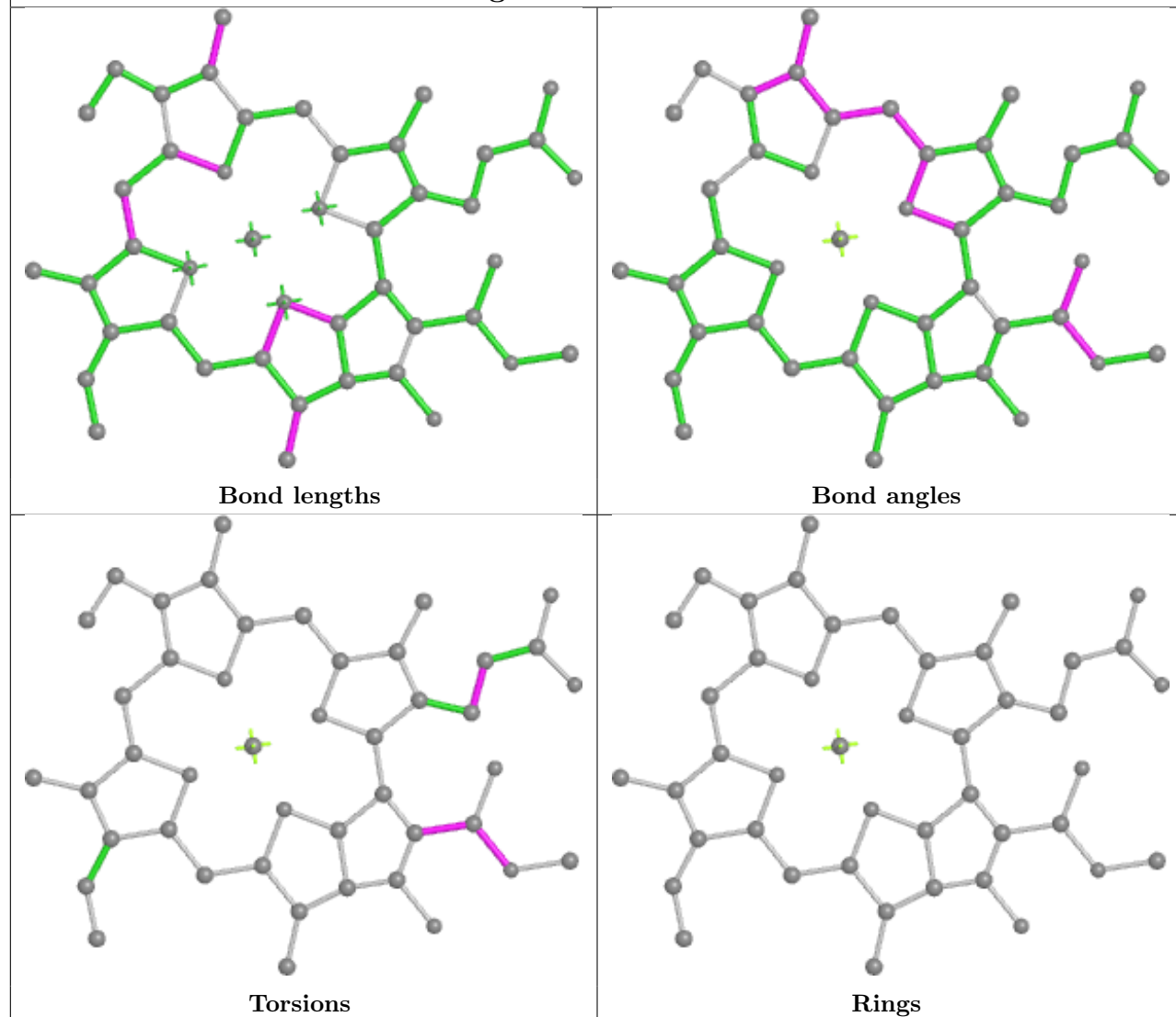
Ligand CLA B 813



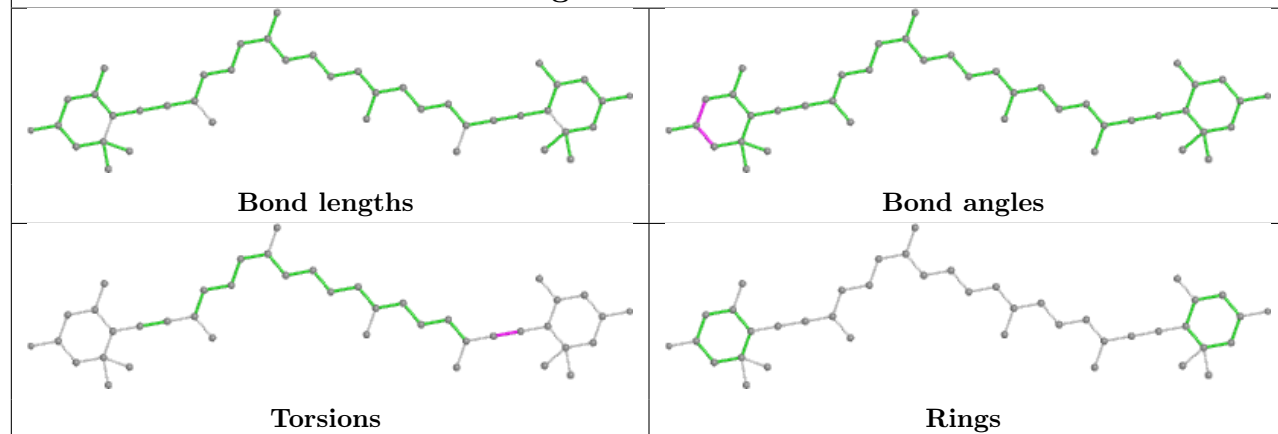
Ligand CLA b 306**Ligand WVN B 850**

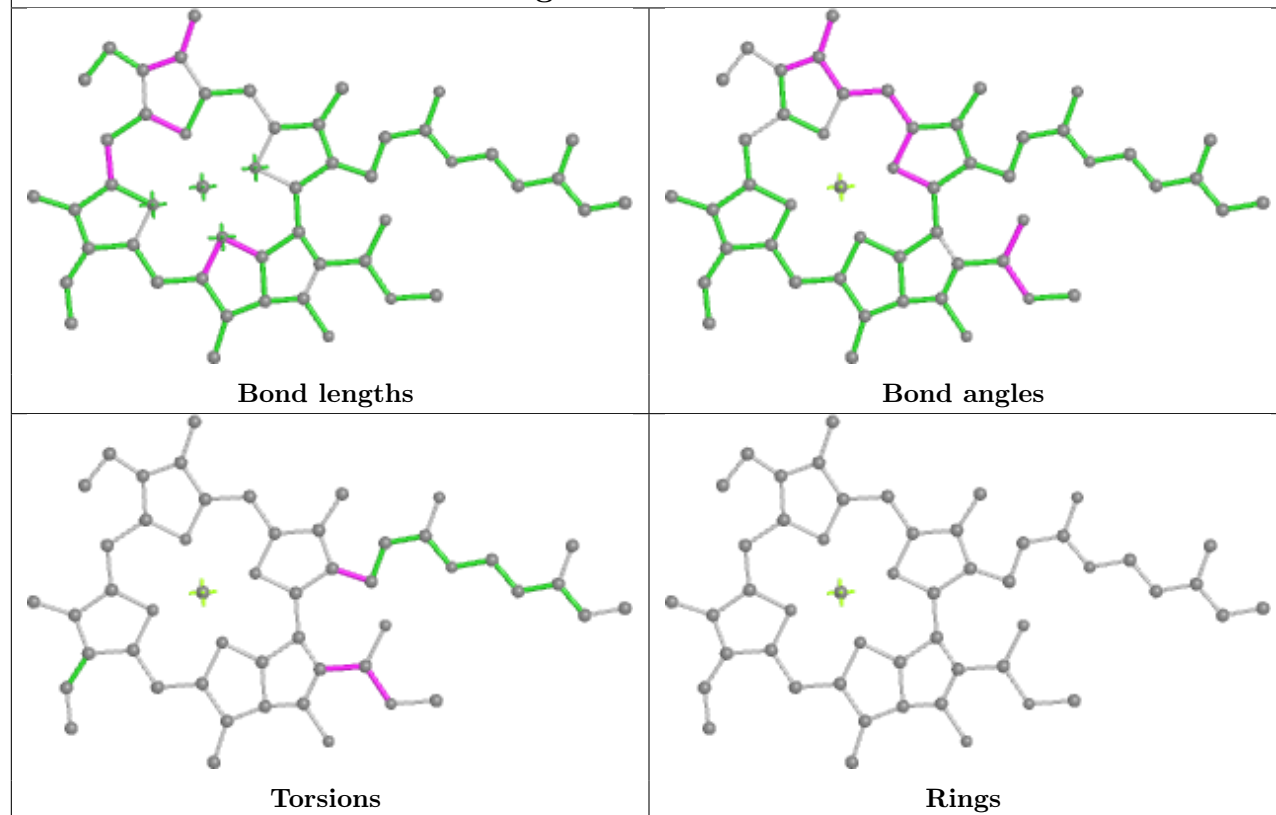
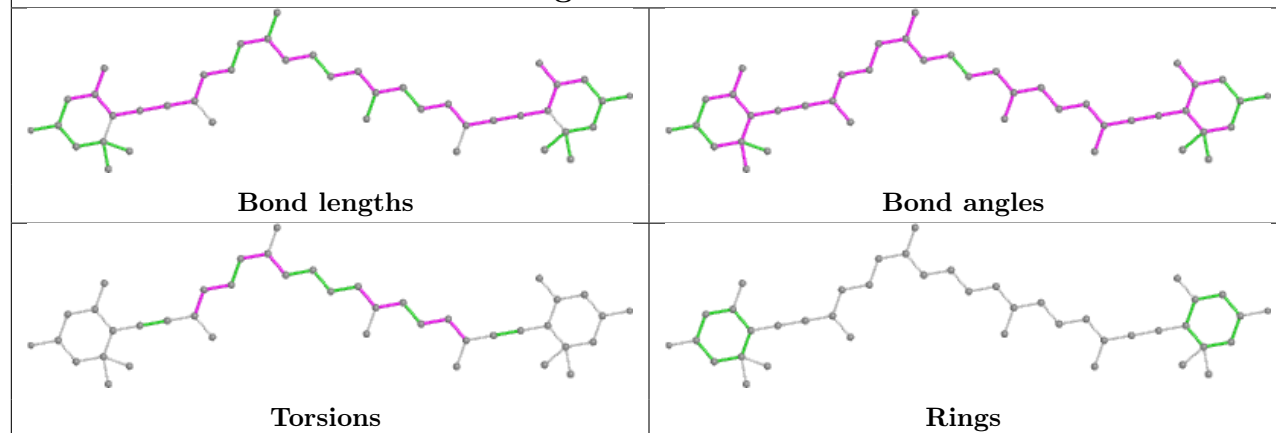


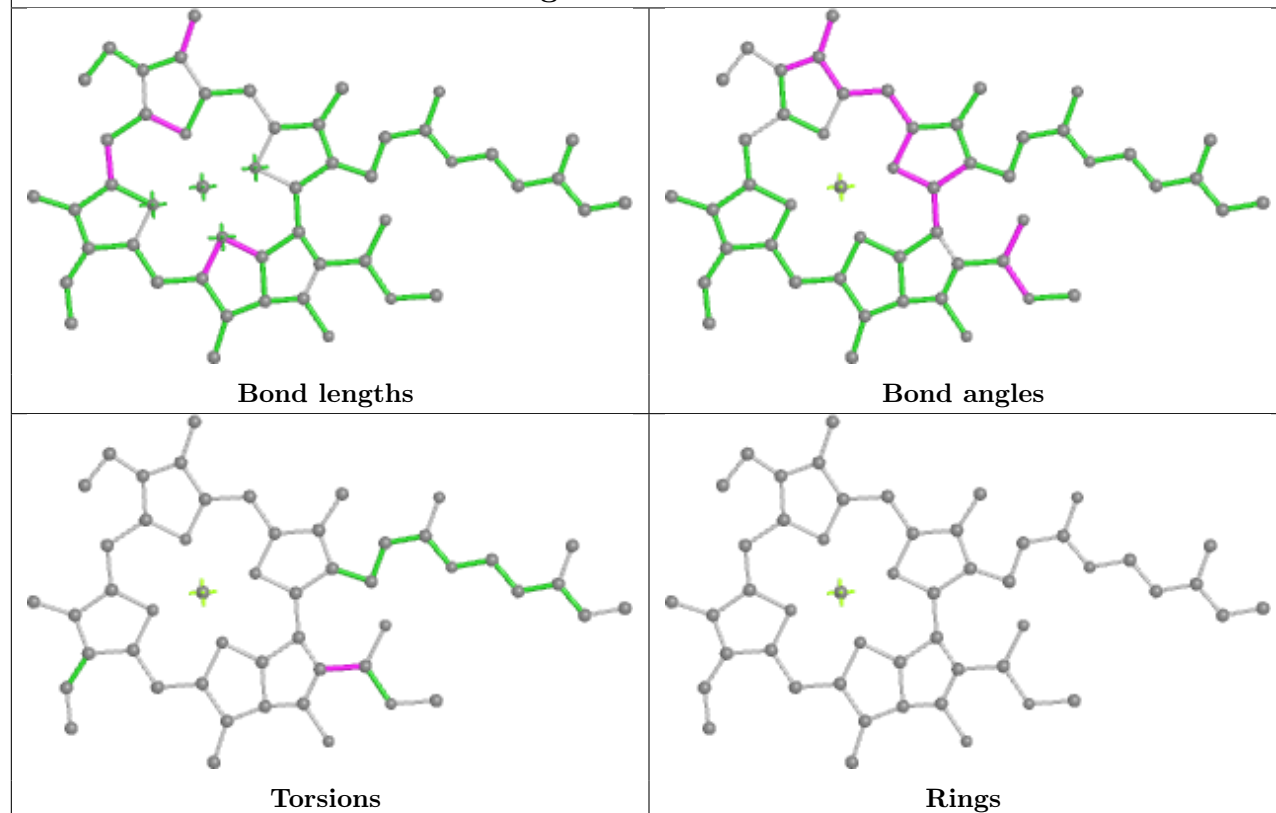
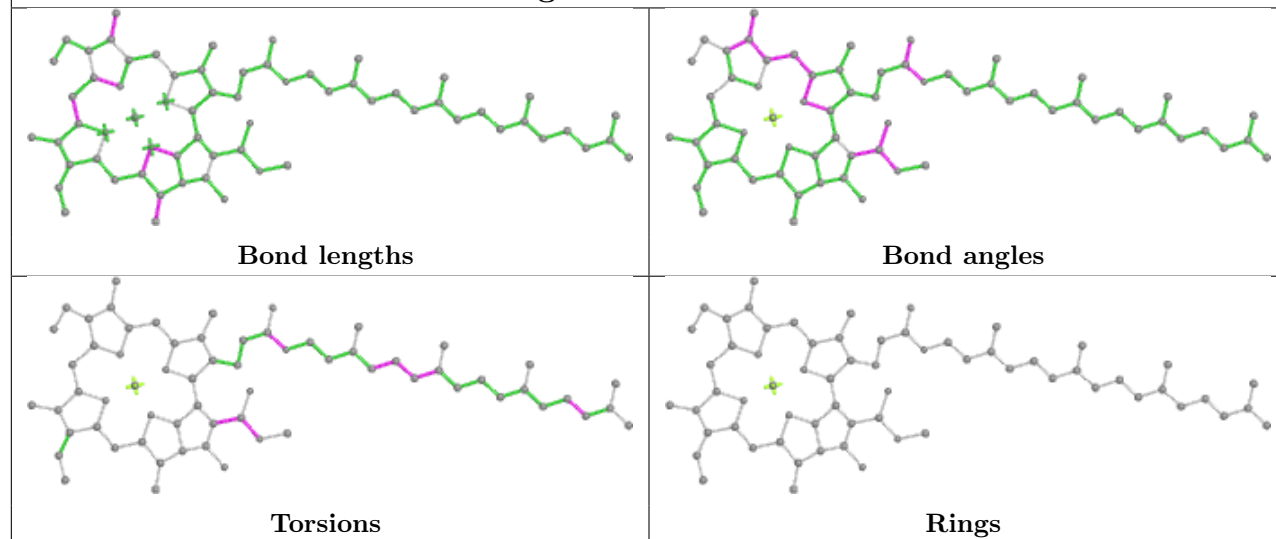
Ligand CLA A 815

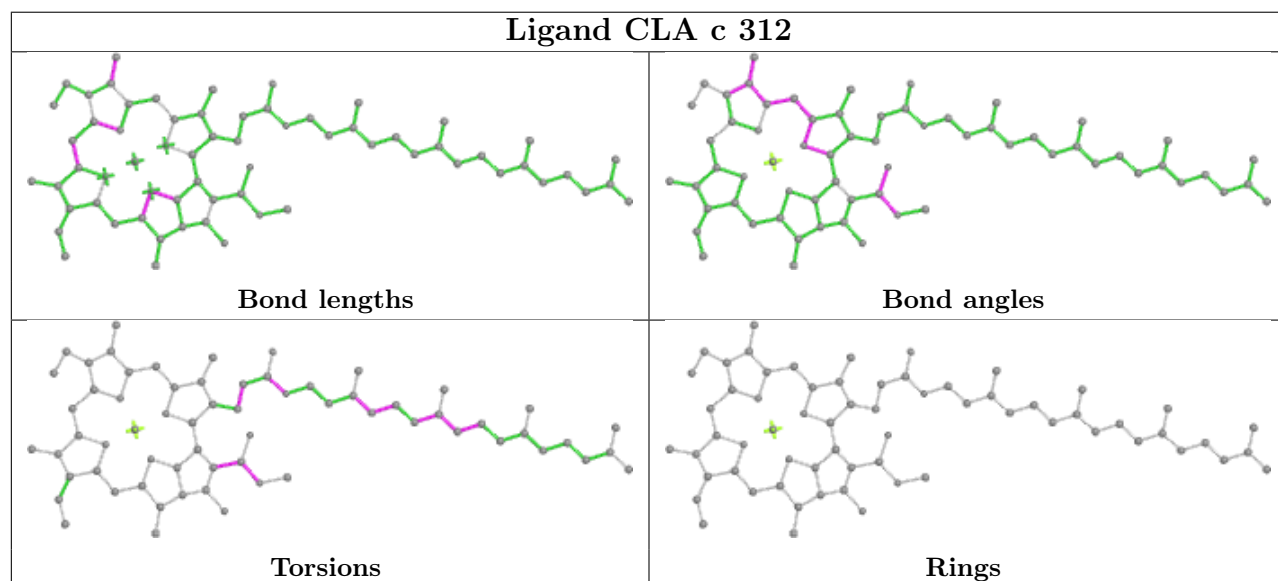
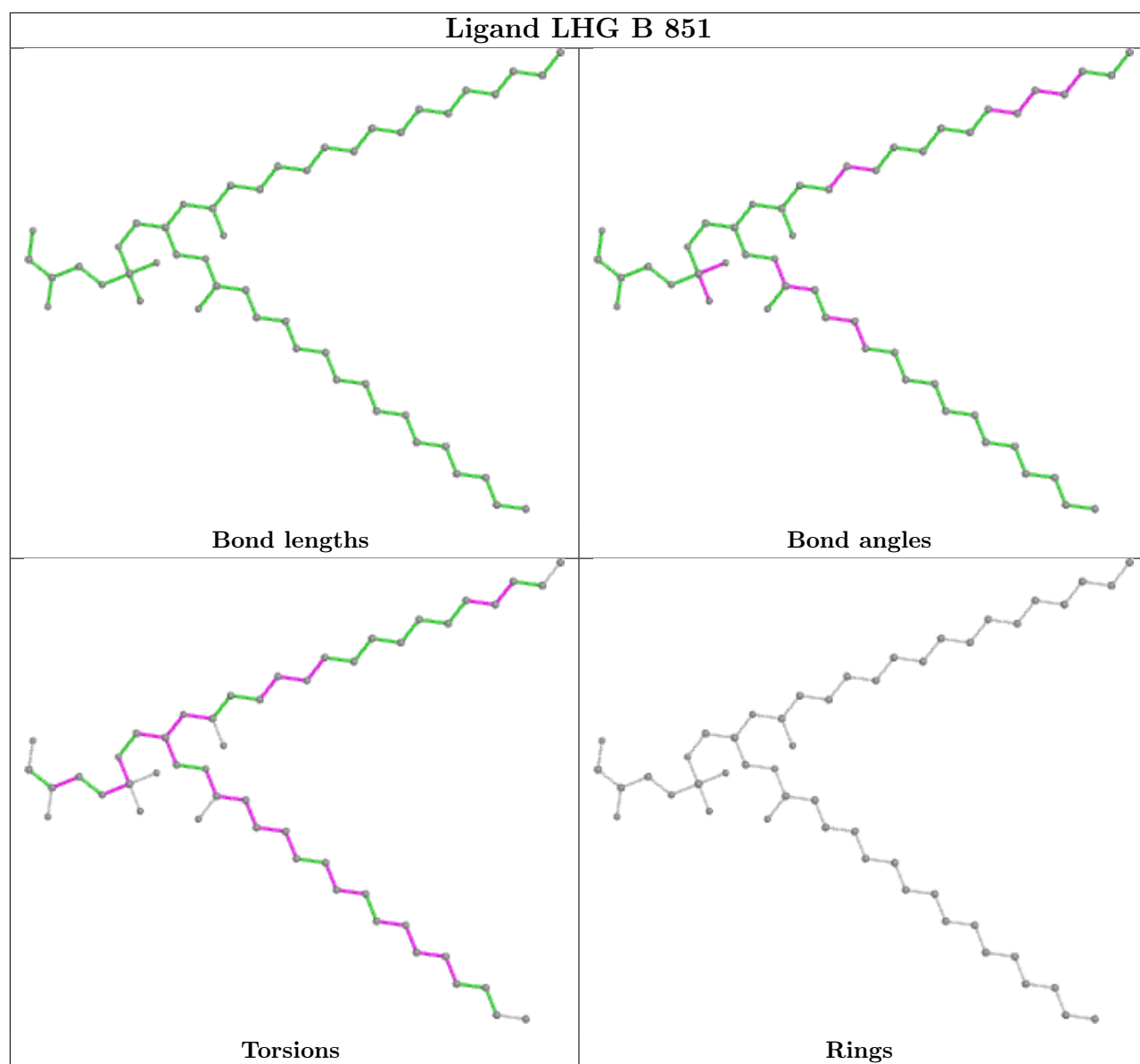


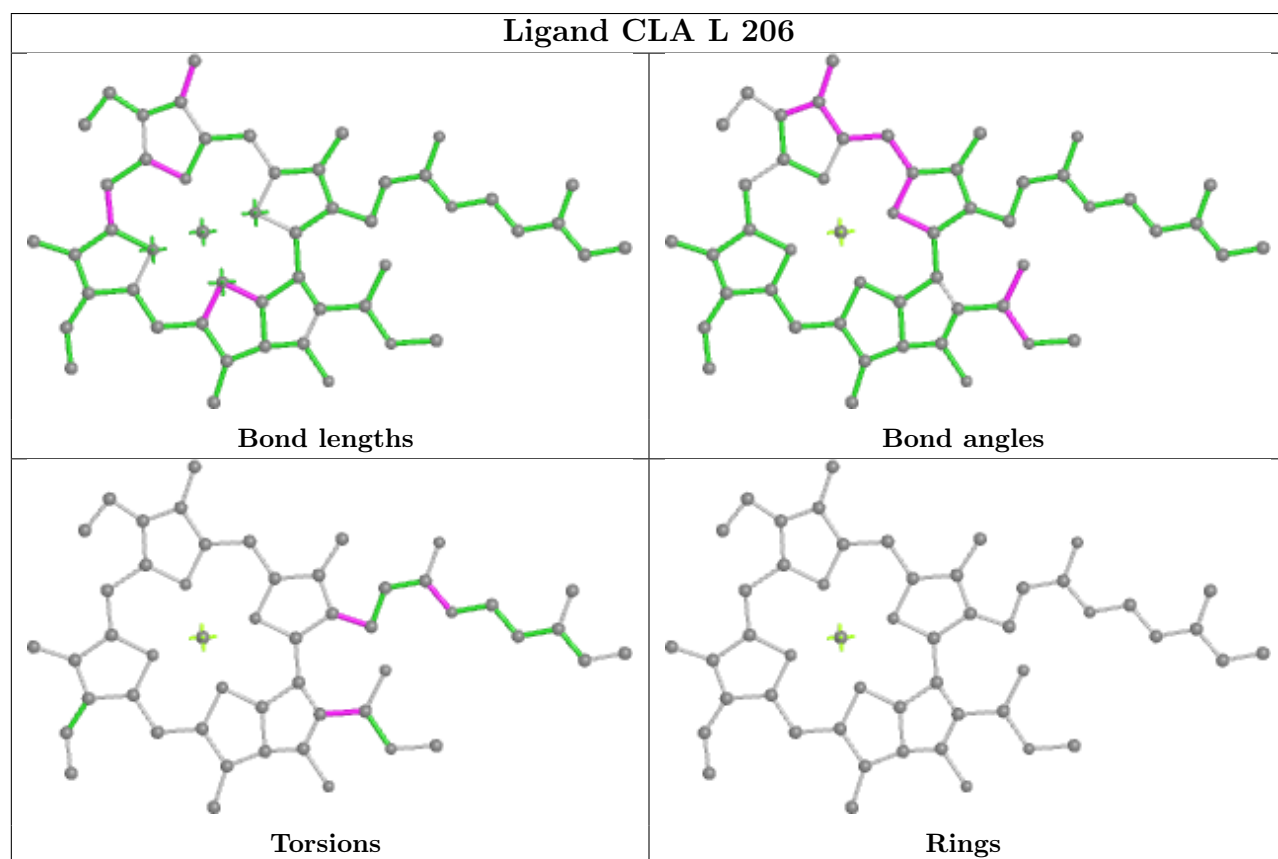
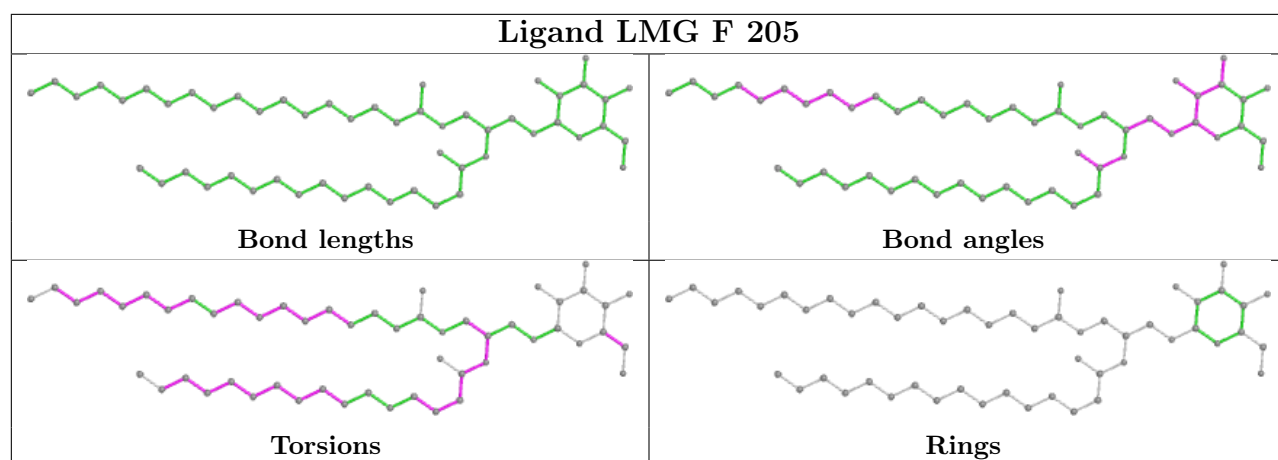
Ligand II0 c 314

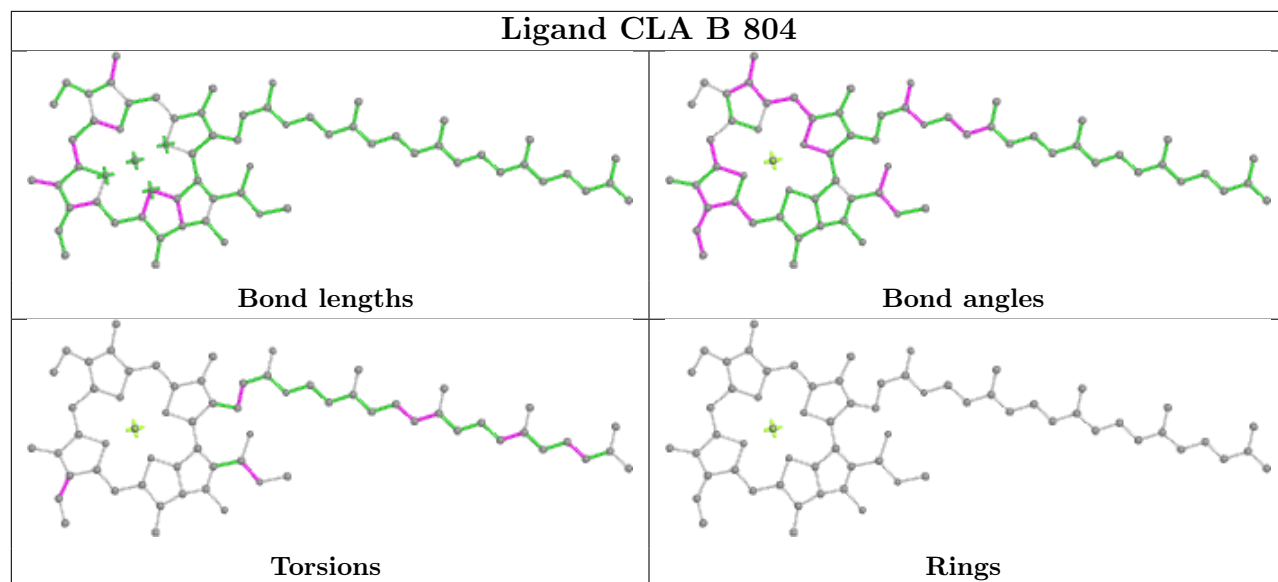
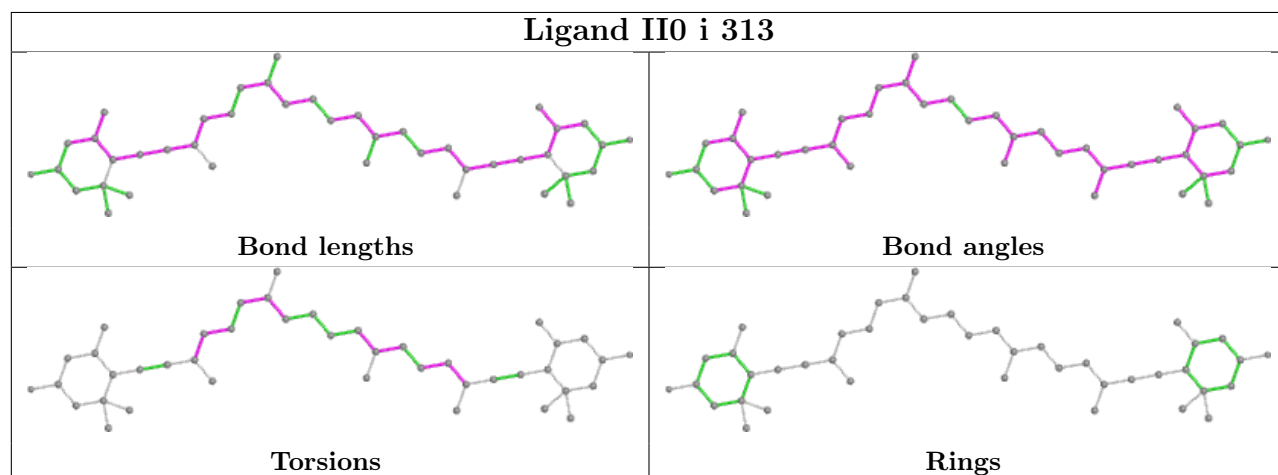
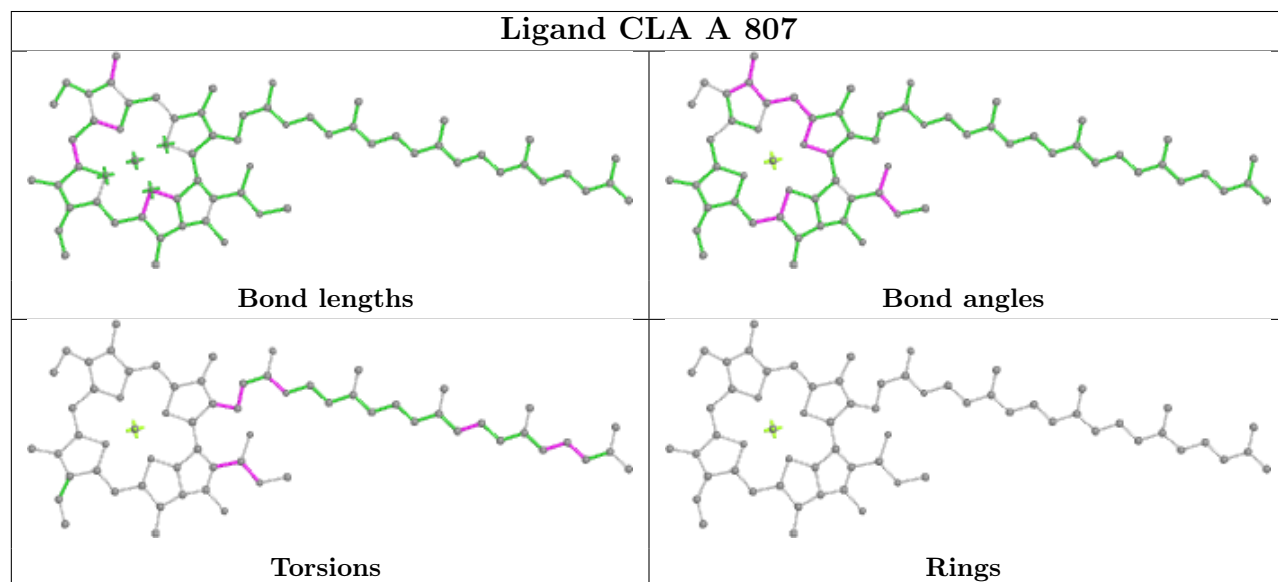


Ligand CLA k 603**Ligand II0 i 314**

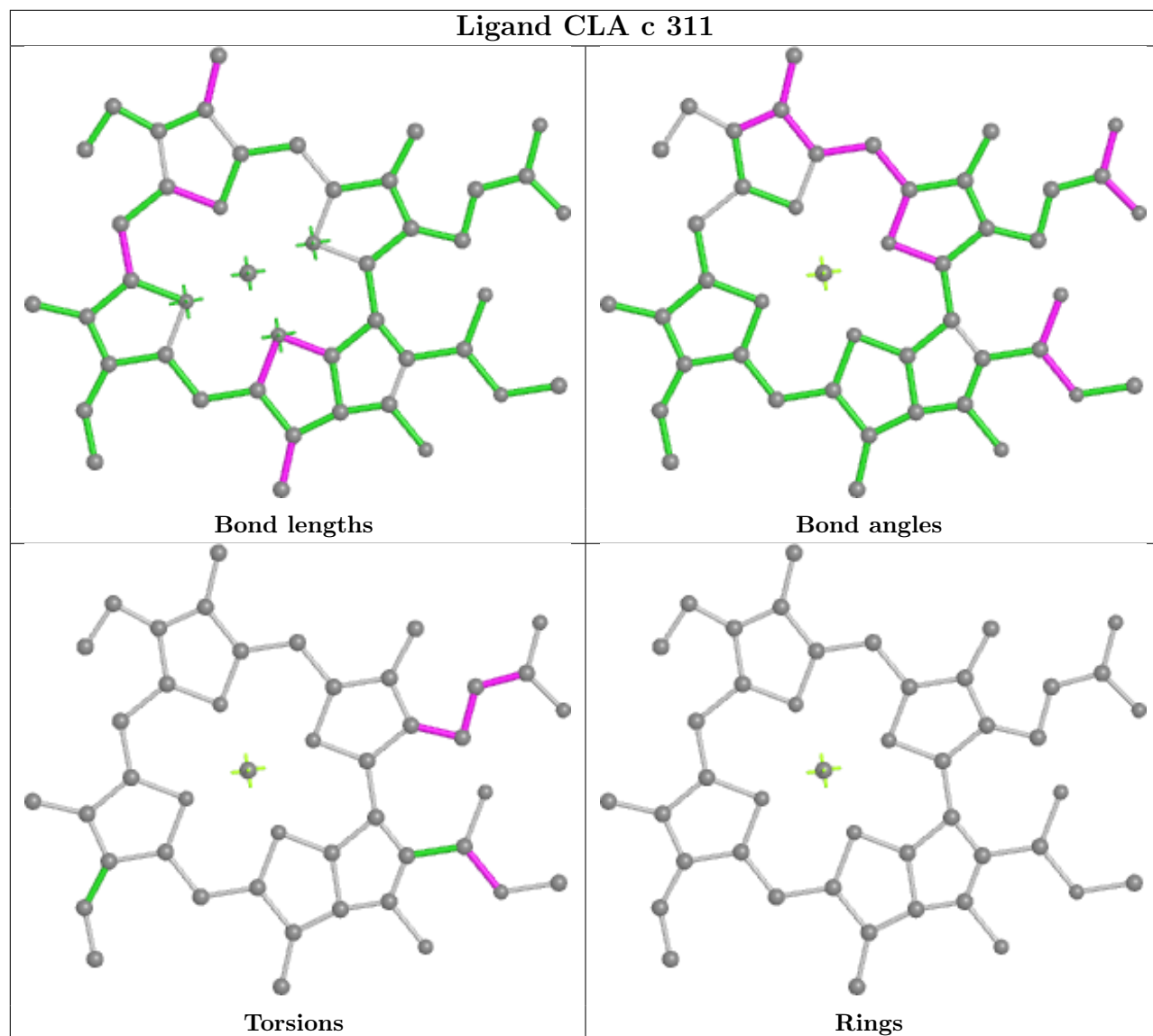
Ligand CLA l 306**Ligand CLA s 403**



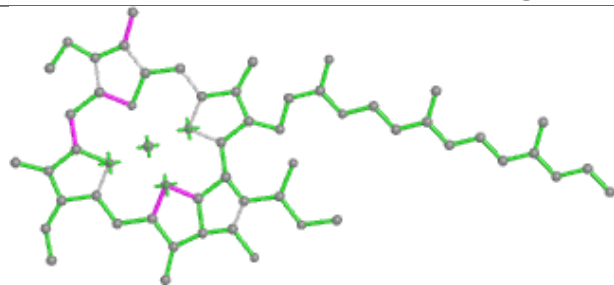


Ligand CLA B 804**Ligand II0 i 313****Ligand CLA A 807**

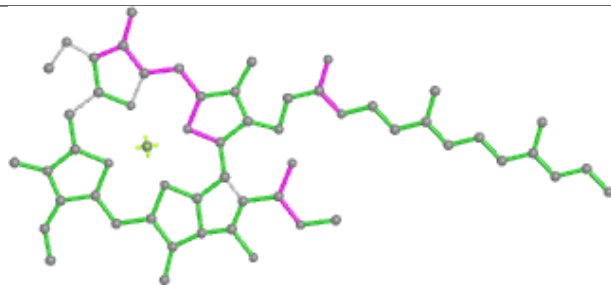
Ligand CLA c 311



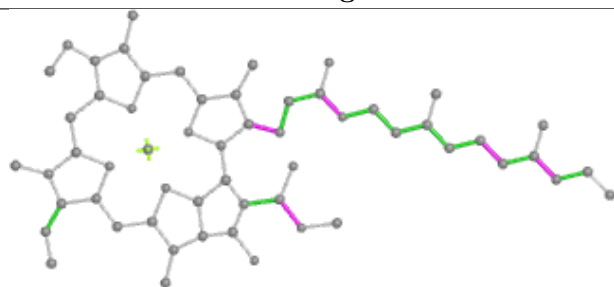
Ligand CLA k 609



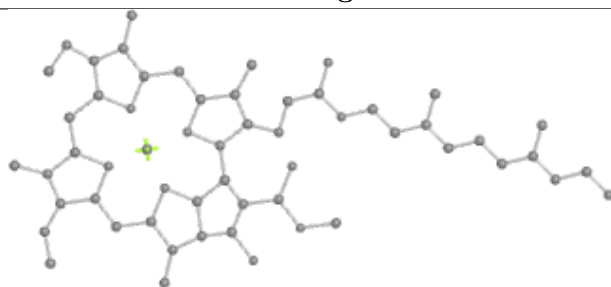
Bond lengths



Bond angles

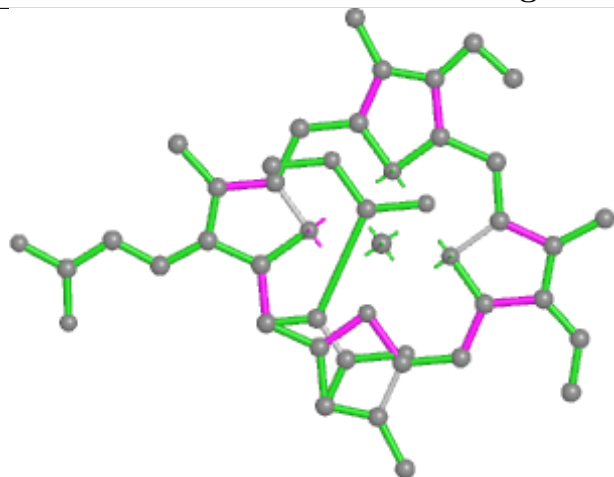


Torsions

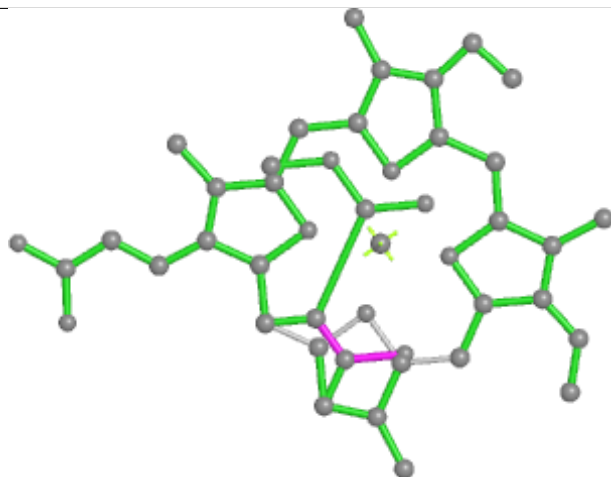


Rings

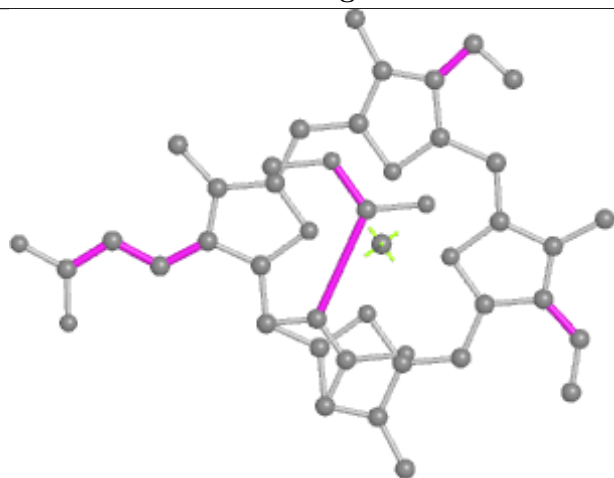
Ligand KC2 k 613



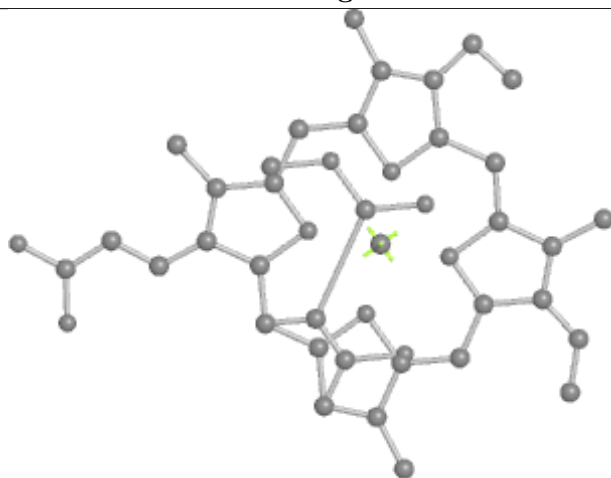
Bond lengths



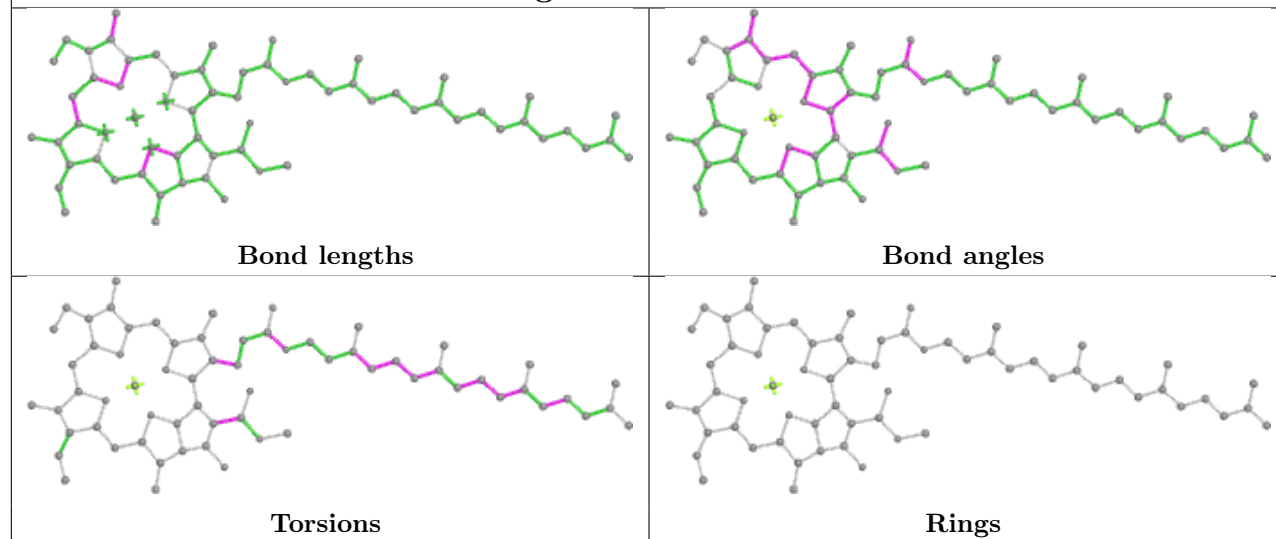
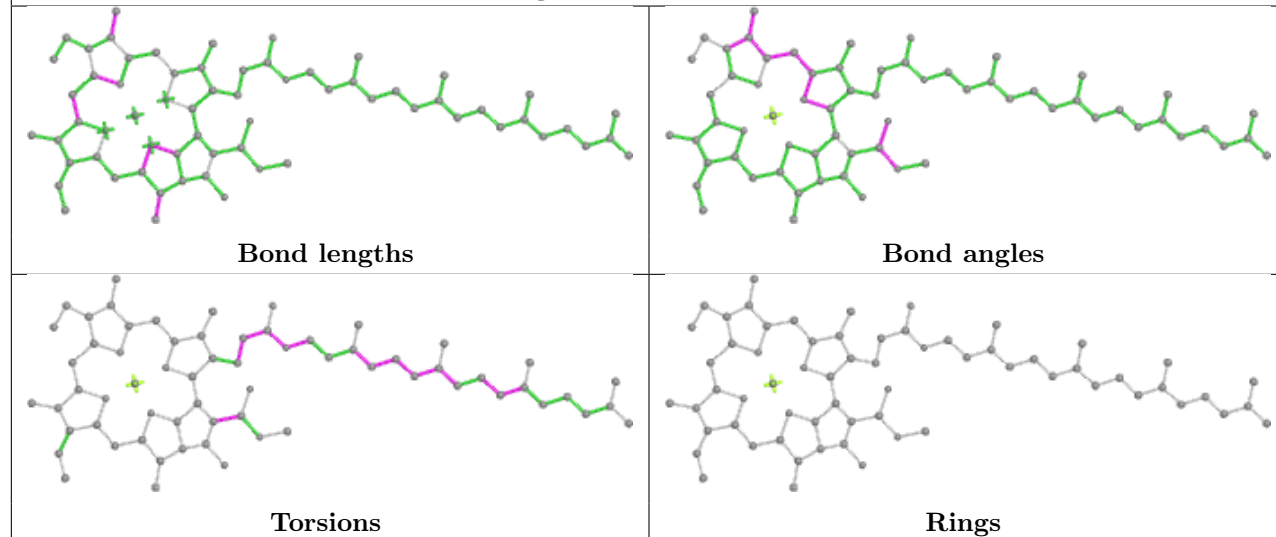
Bond angles



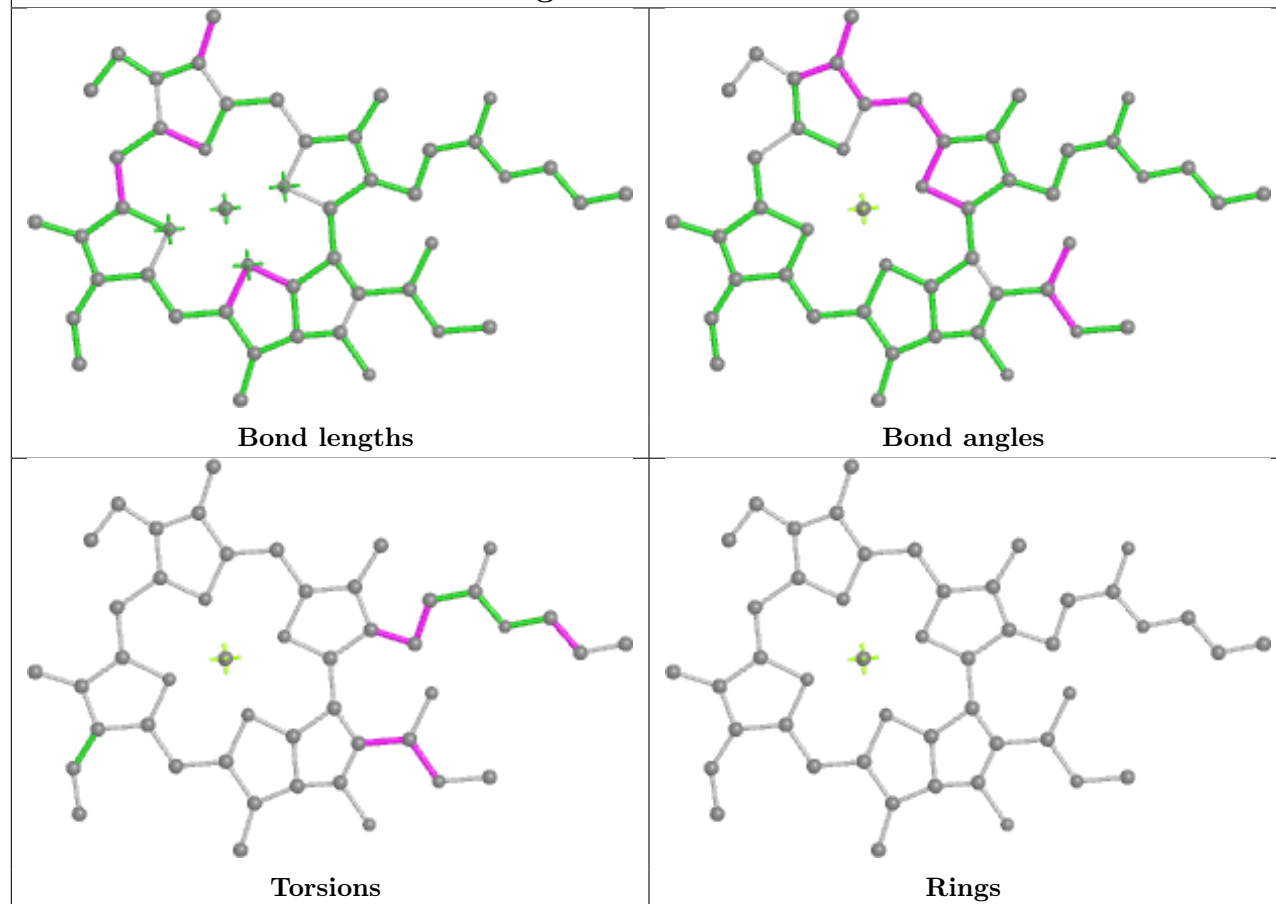
Torsions



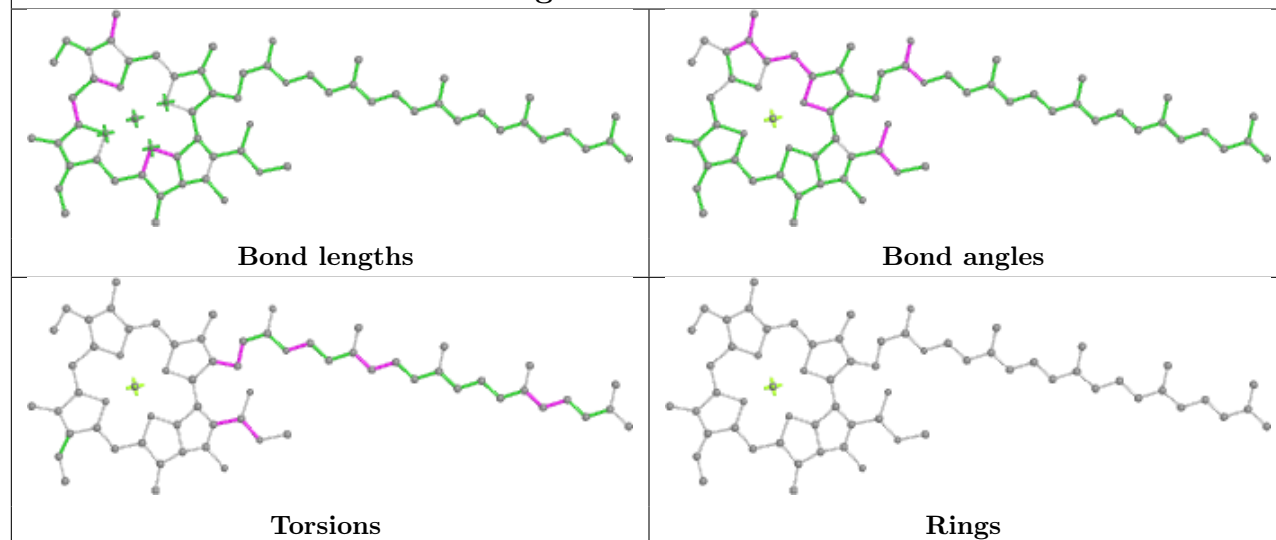
Rings

Ligand CLA n 608**Ligand CLA B 801**

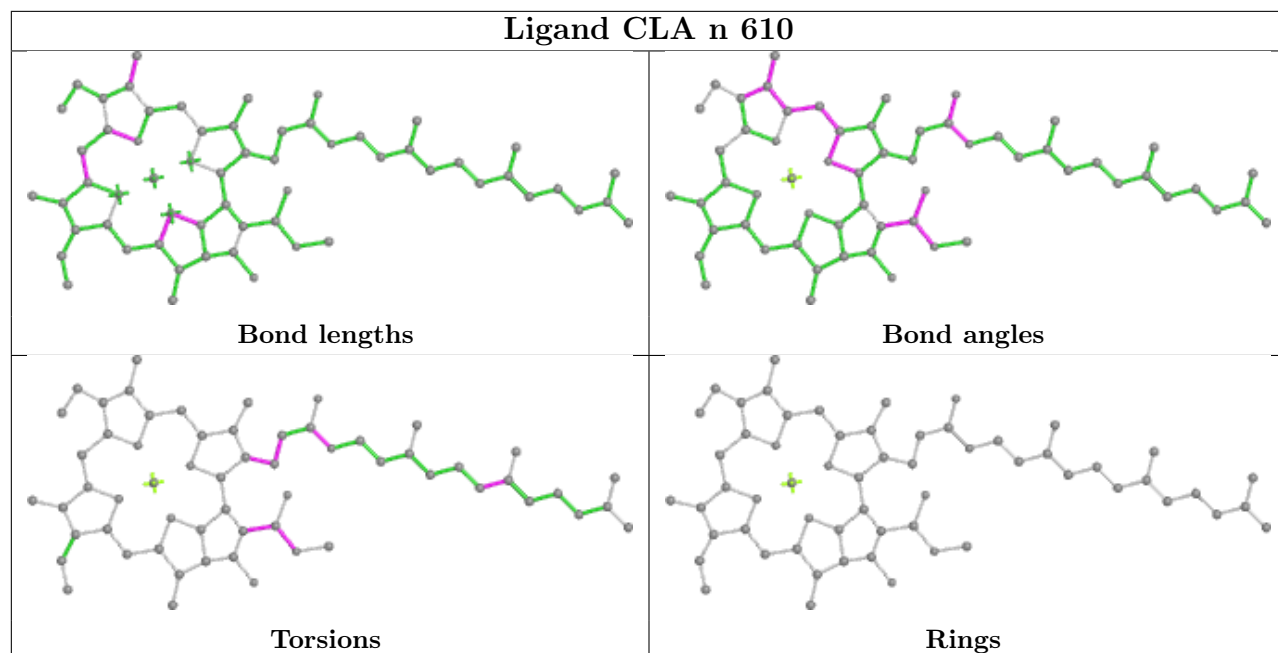
Ligand CLA a 311



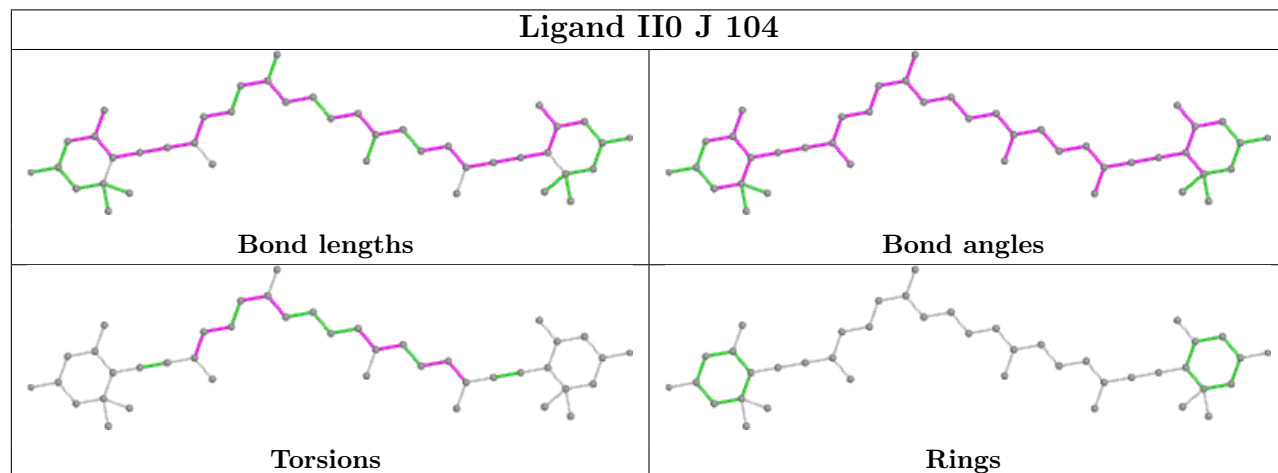
Ligand CLA n 609



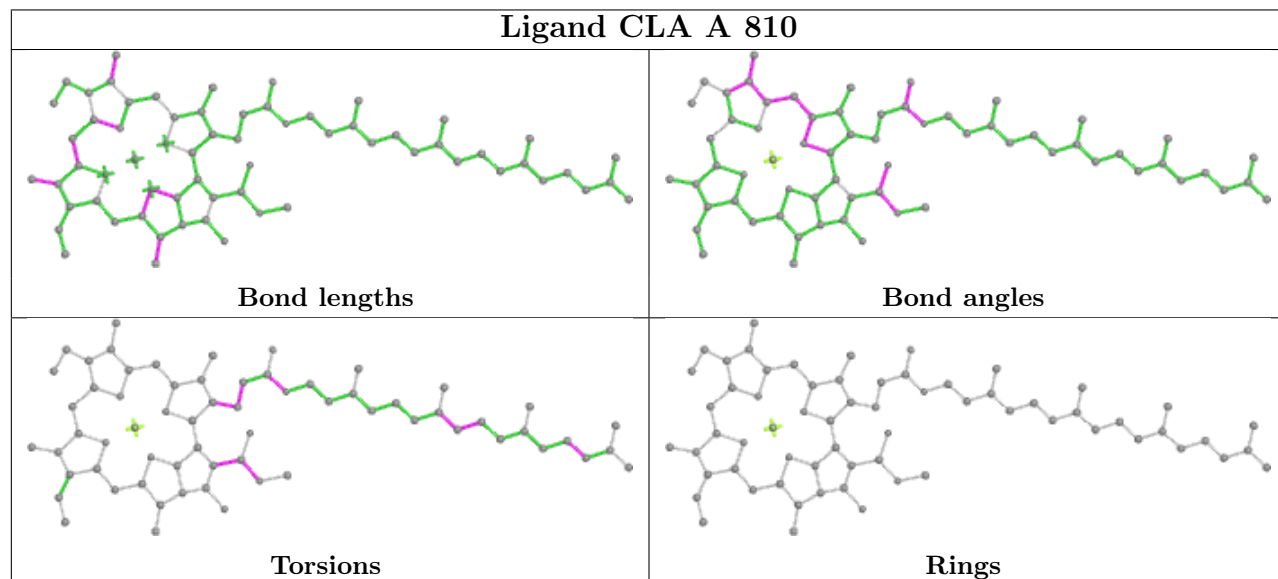
Ligand CLA n 610

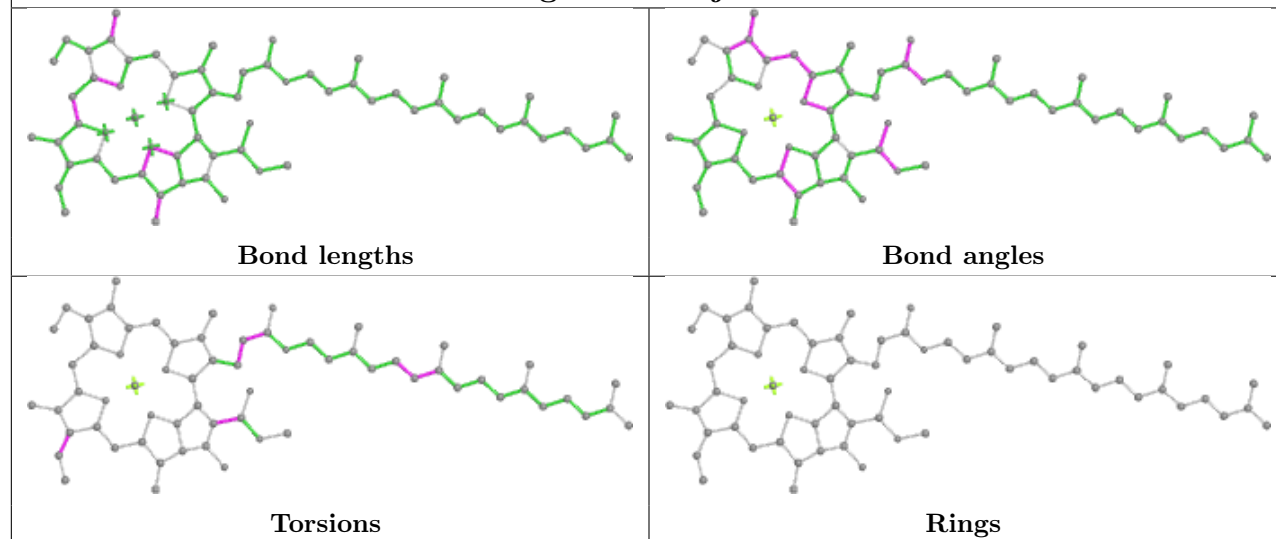
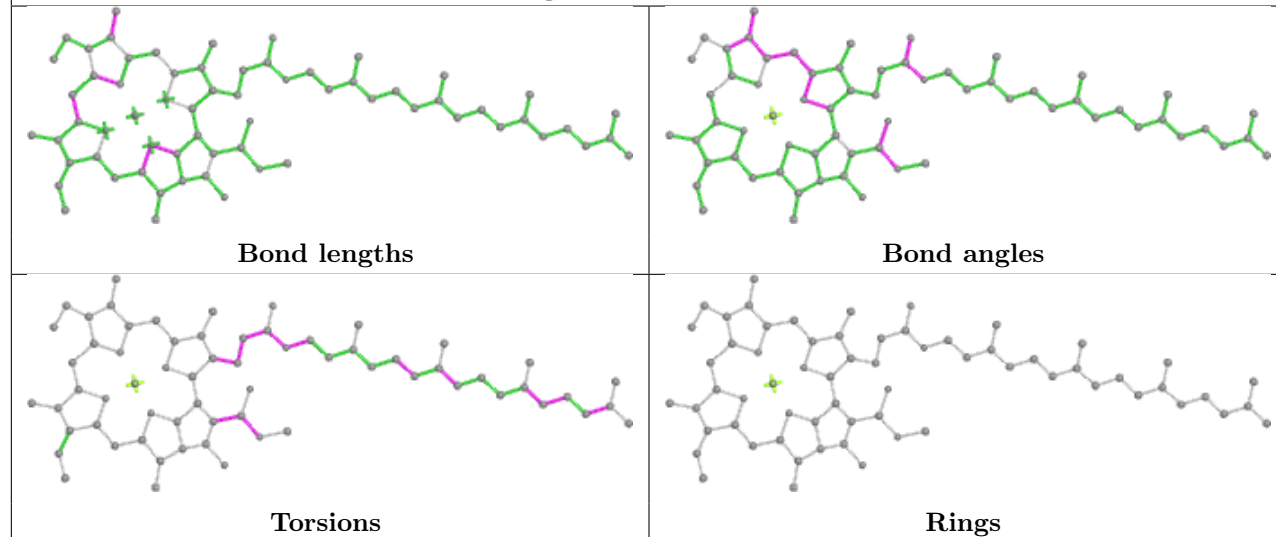


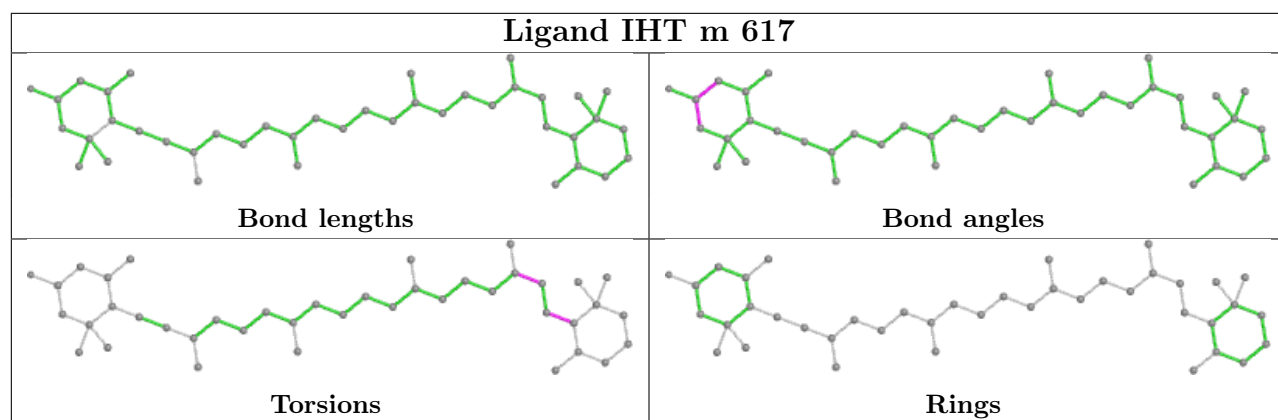
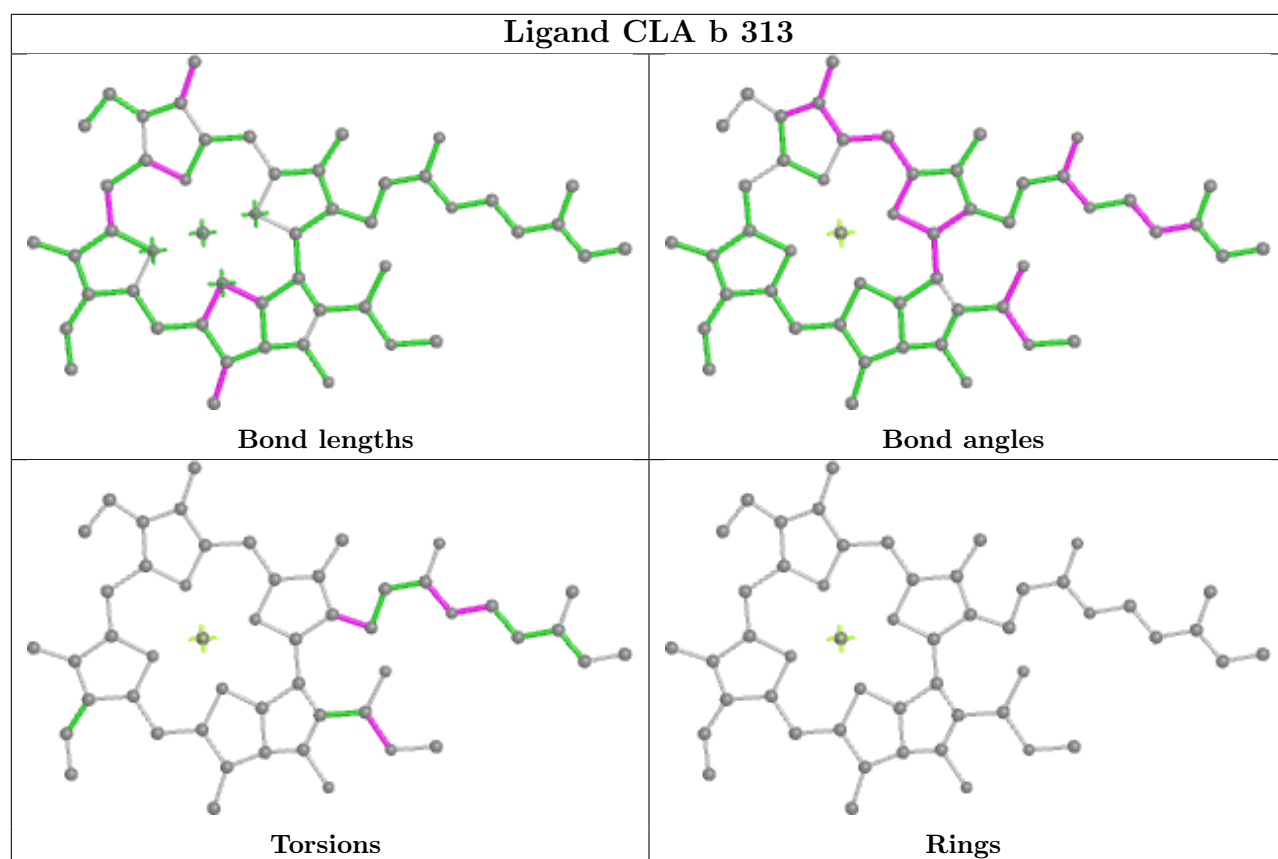
Ligand II0 J 104

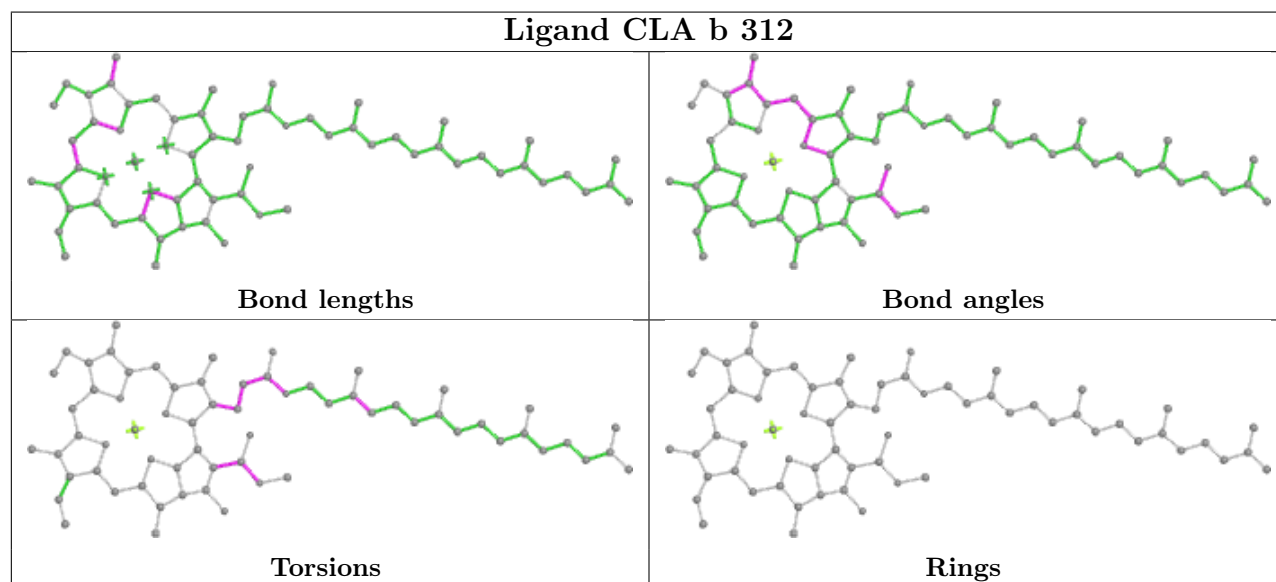
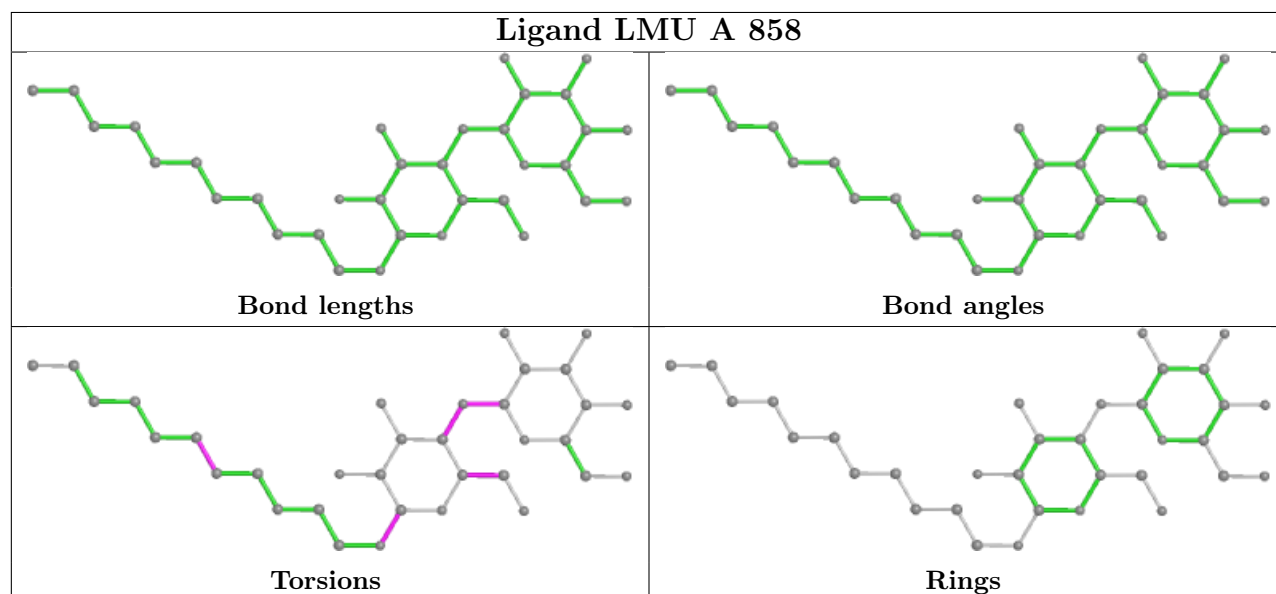
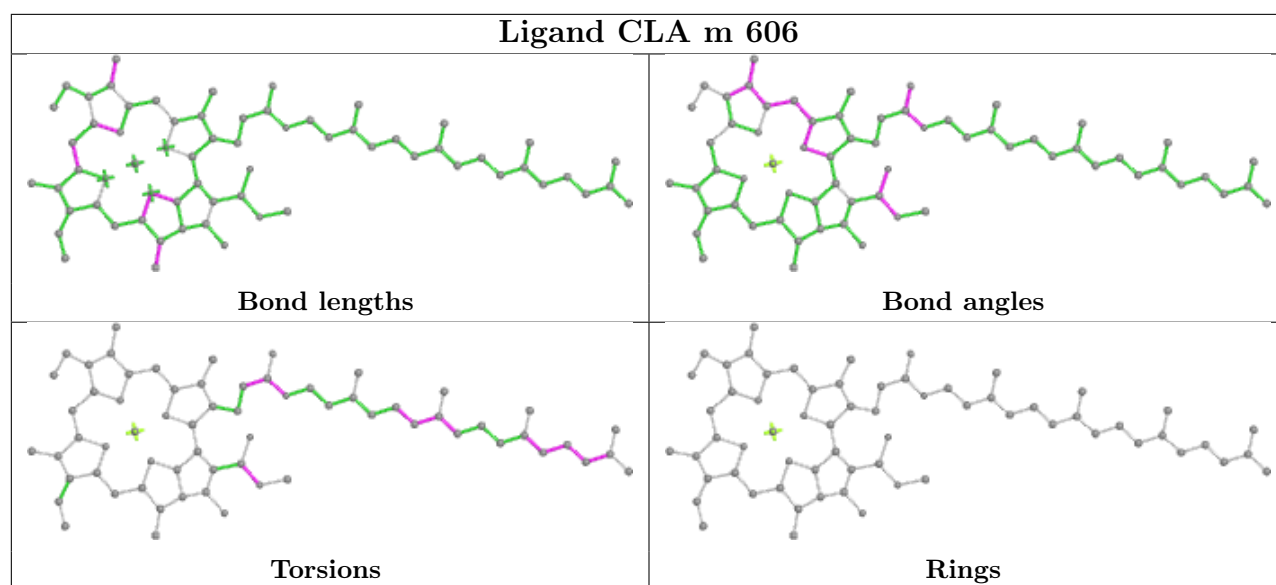


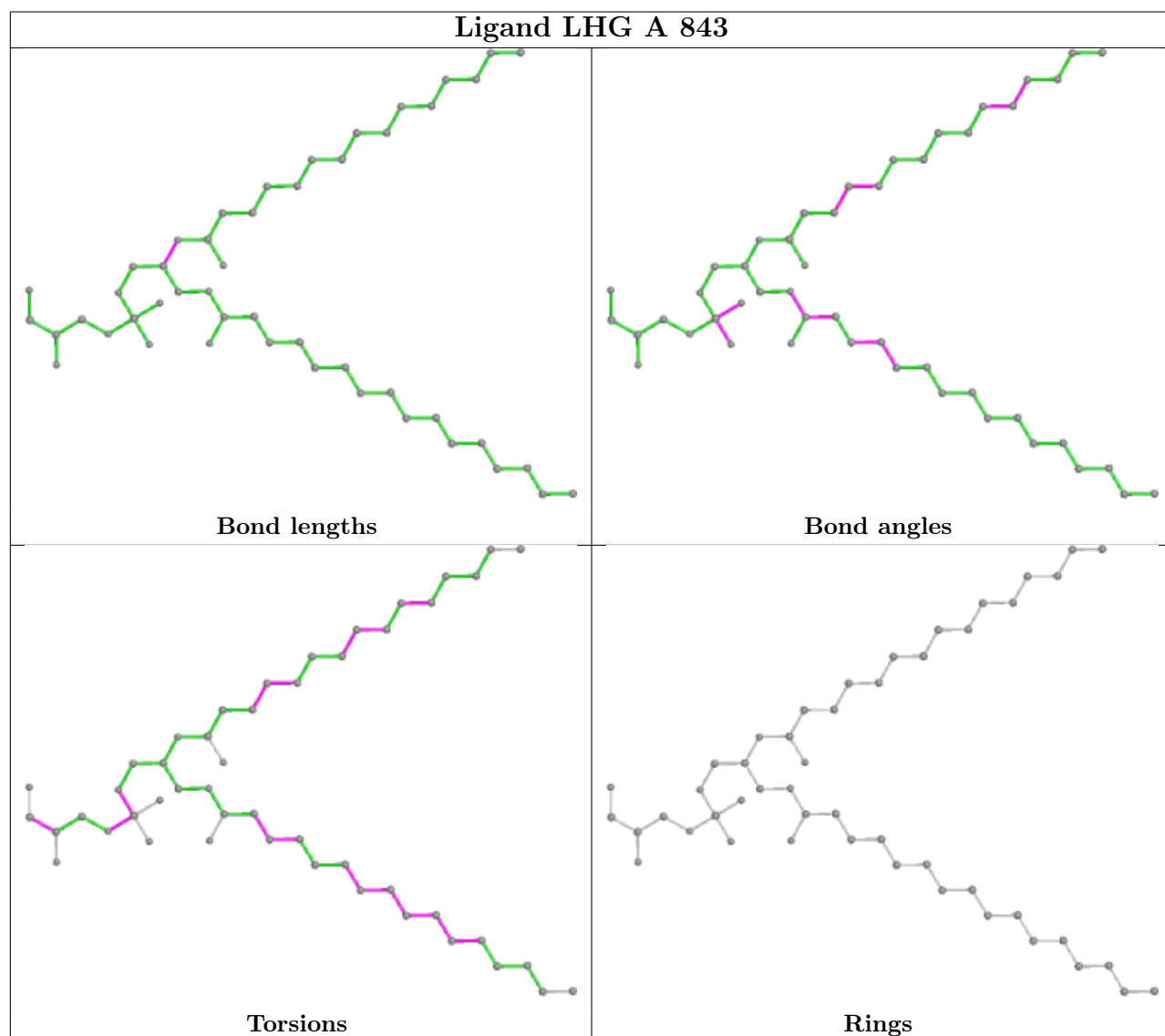
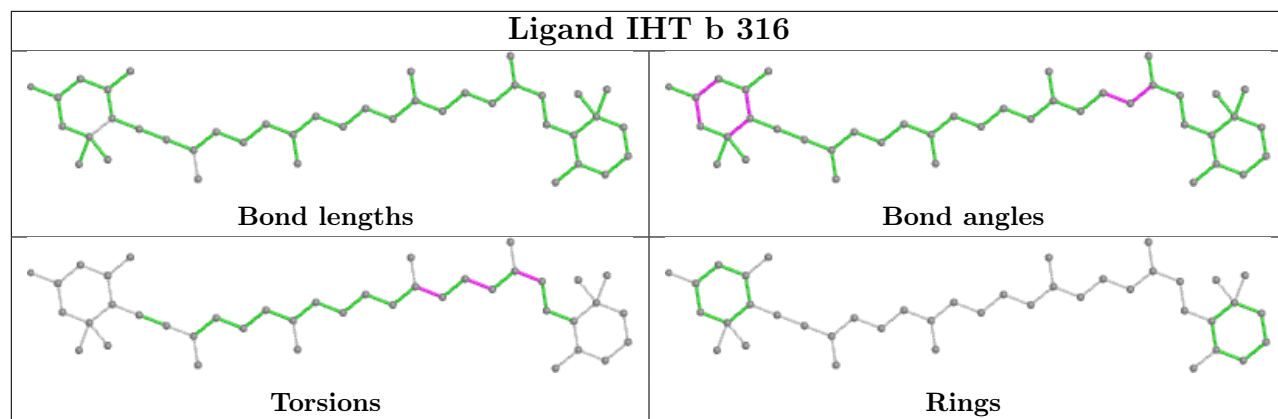
Ligand CLA A 810



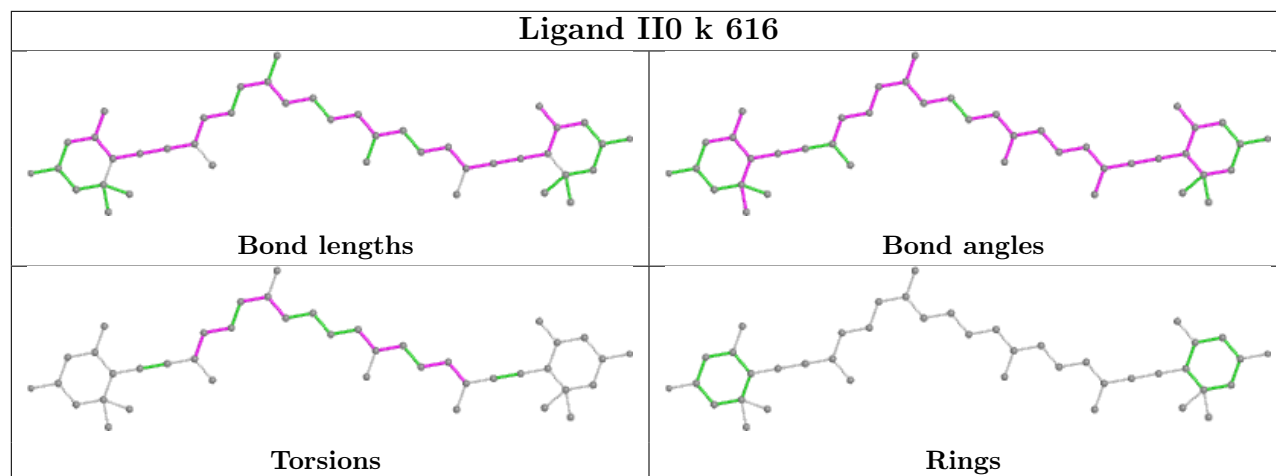
Ligand CLA j 604**Ligand CLA i 301**



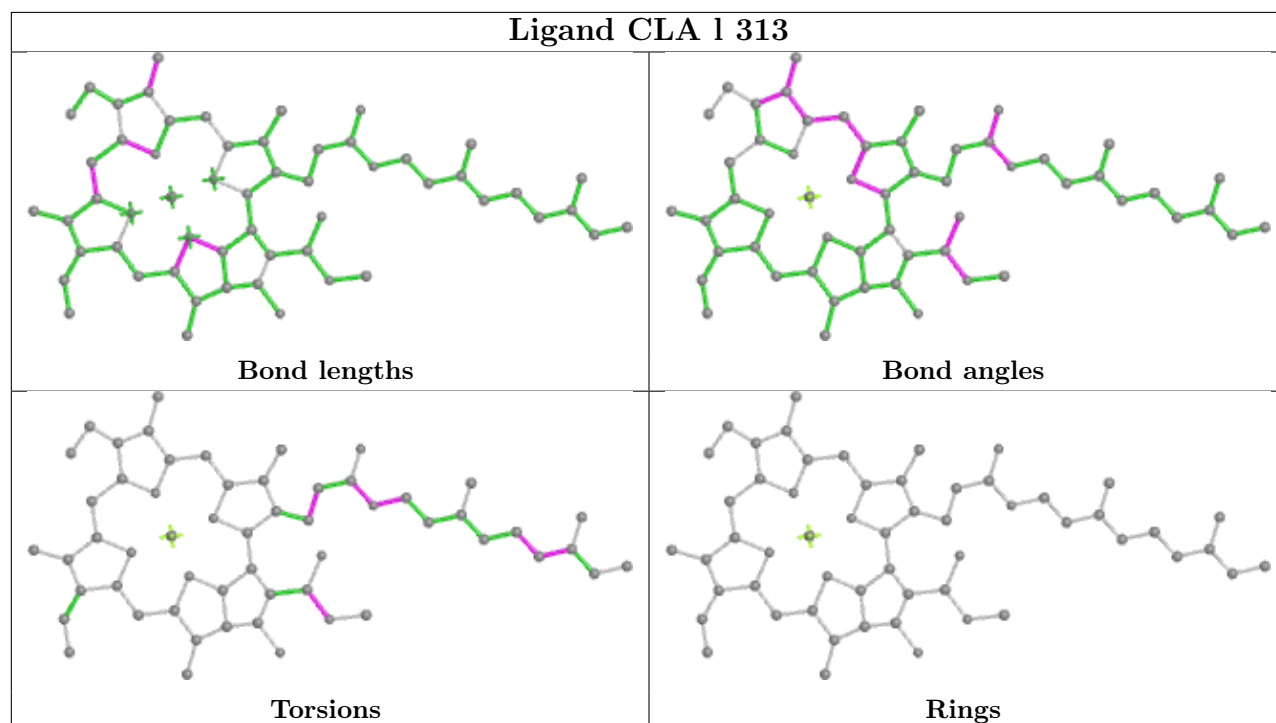




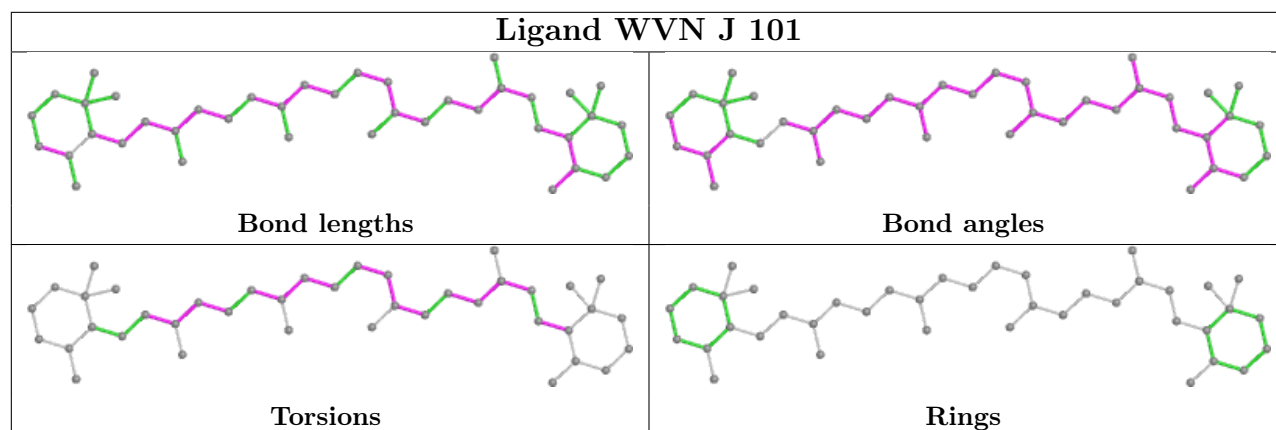
Ligand II0 k 616



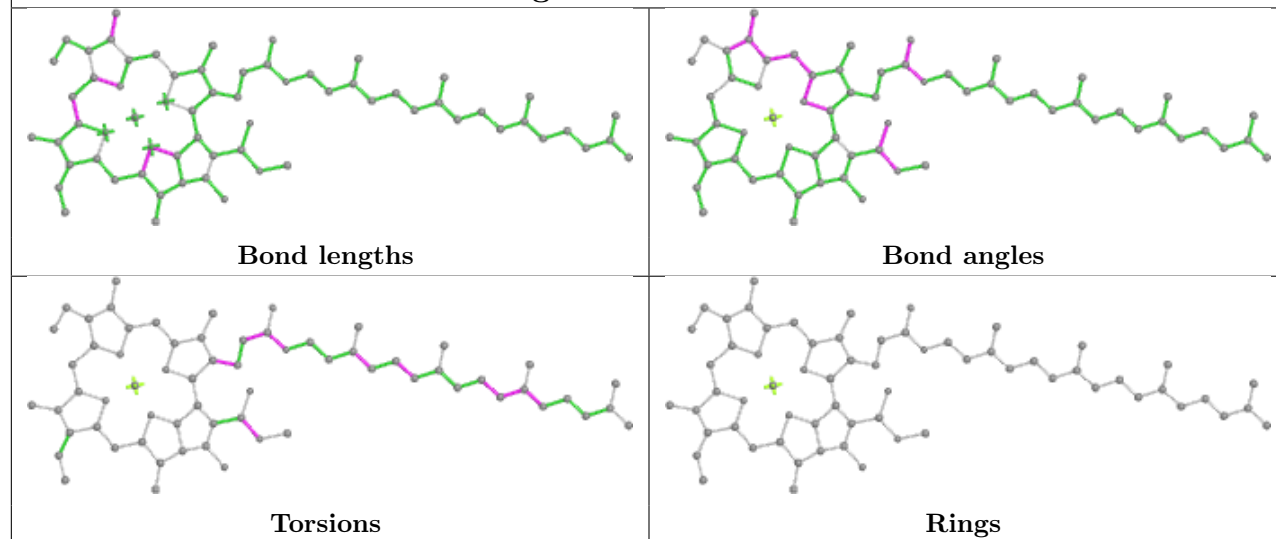
Ligand CLA l 313



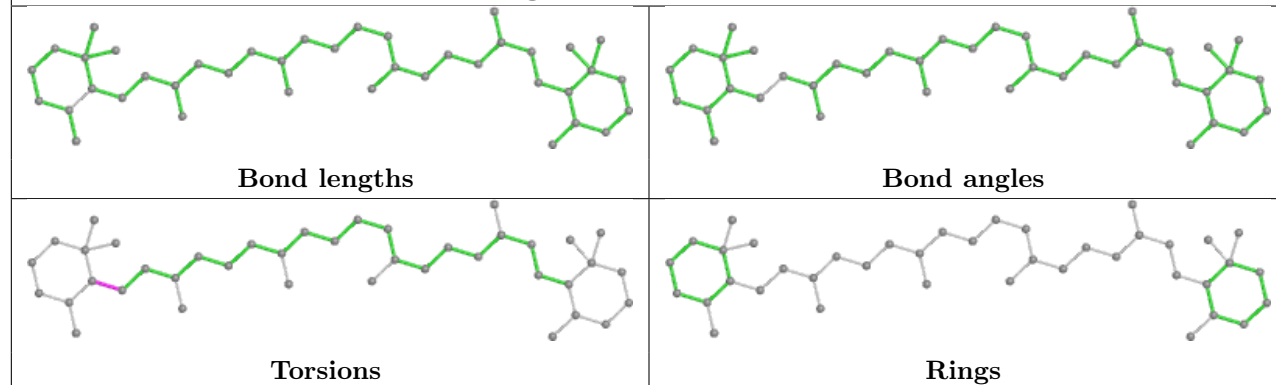
Ligand WVN J 101



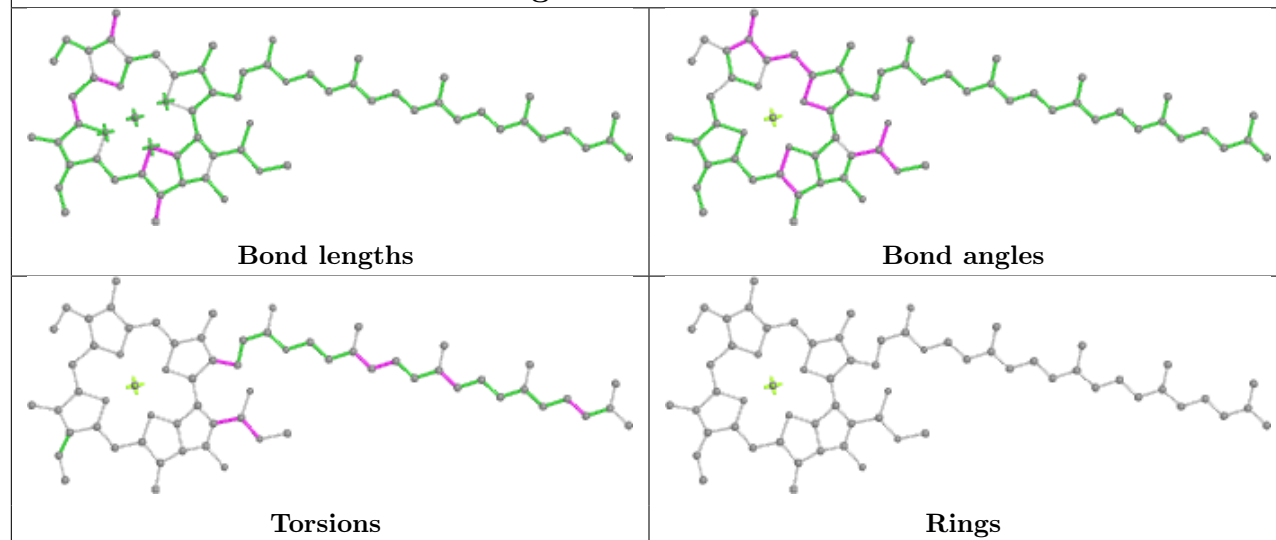
Ligand CLA B 816

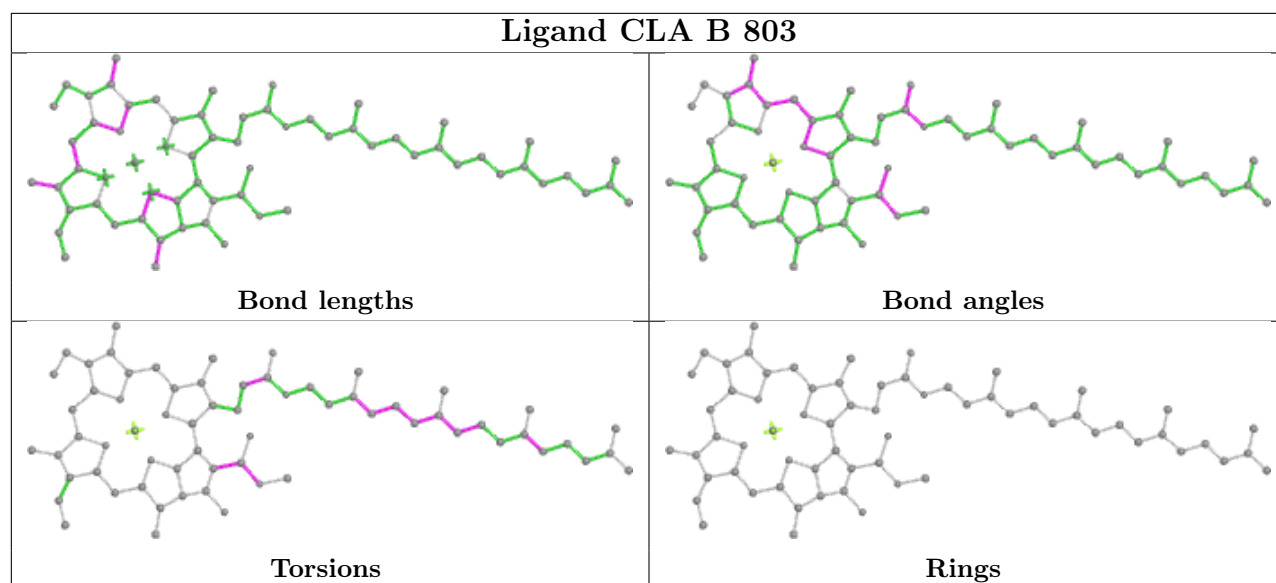
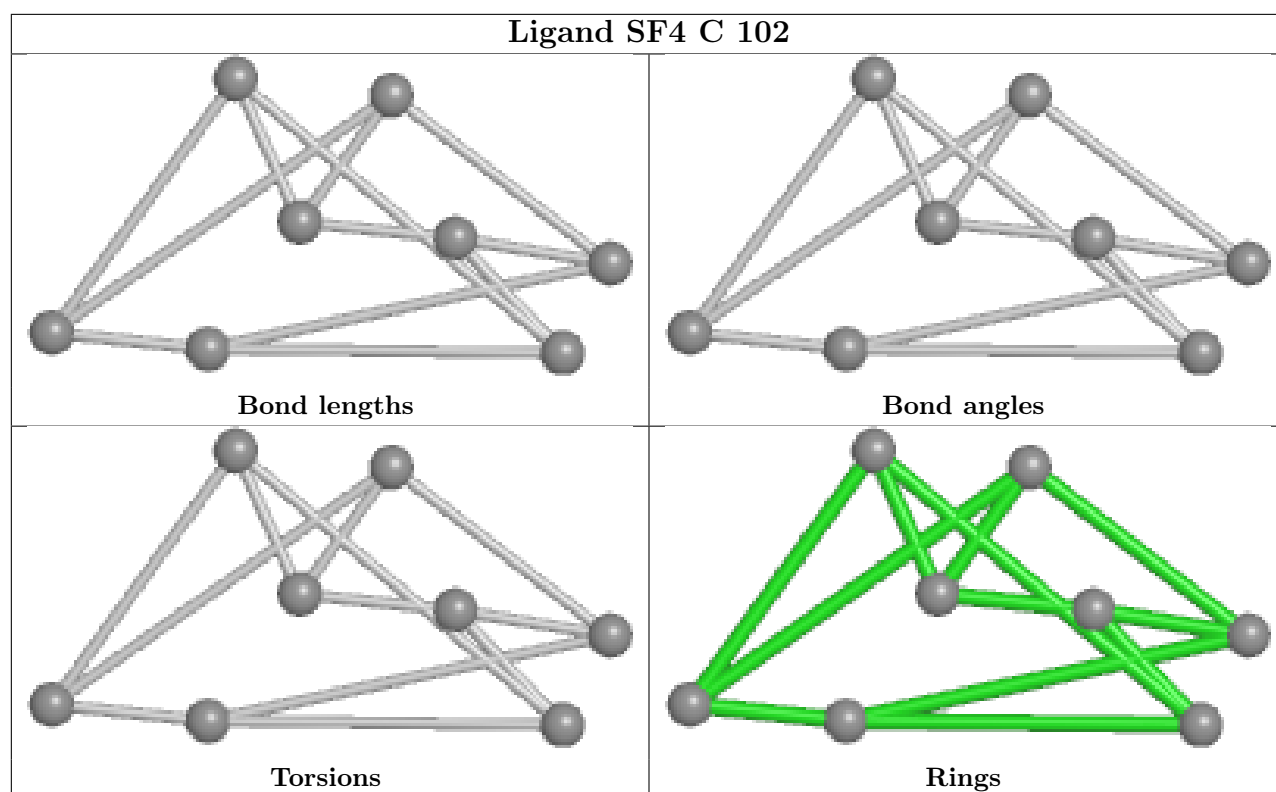


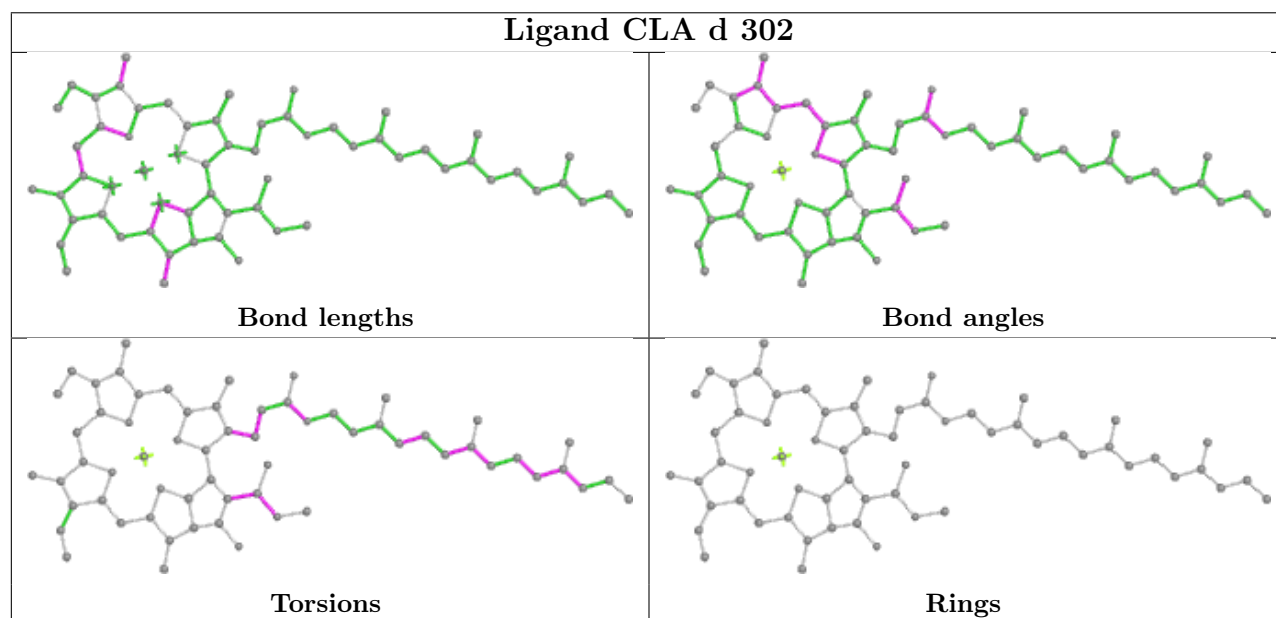
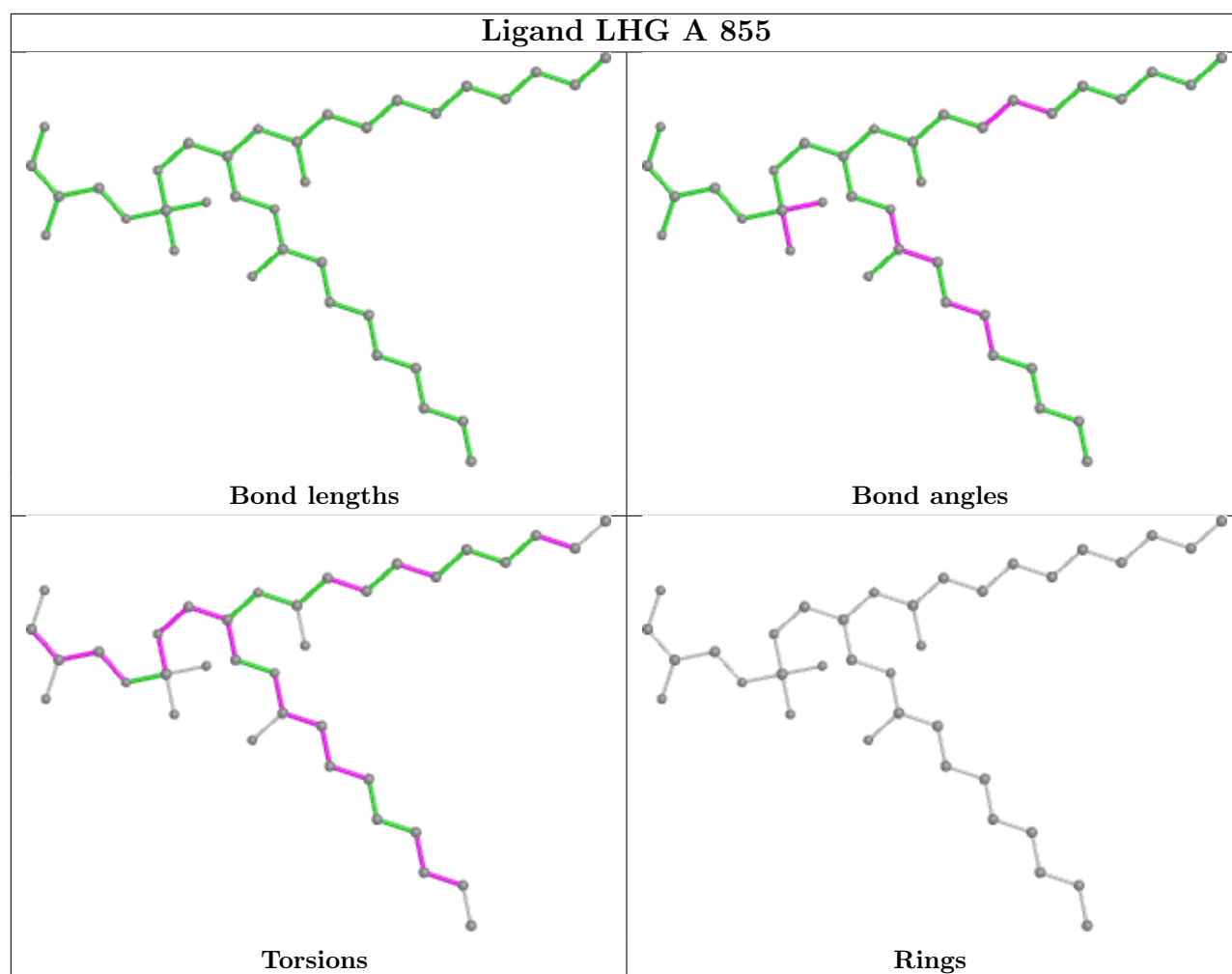
Ligand WVN B 845

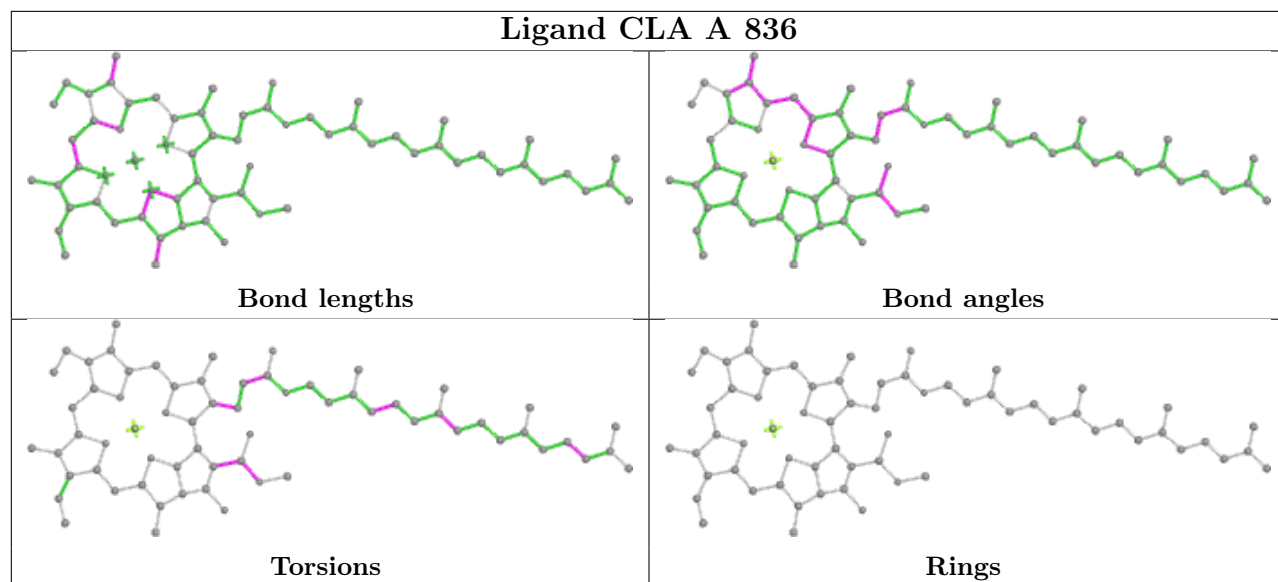
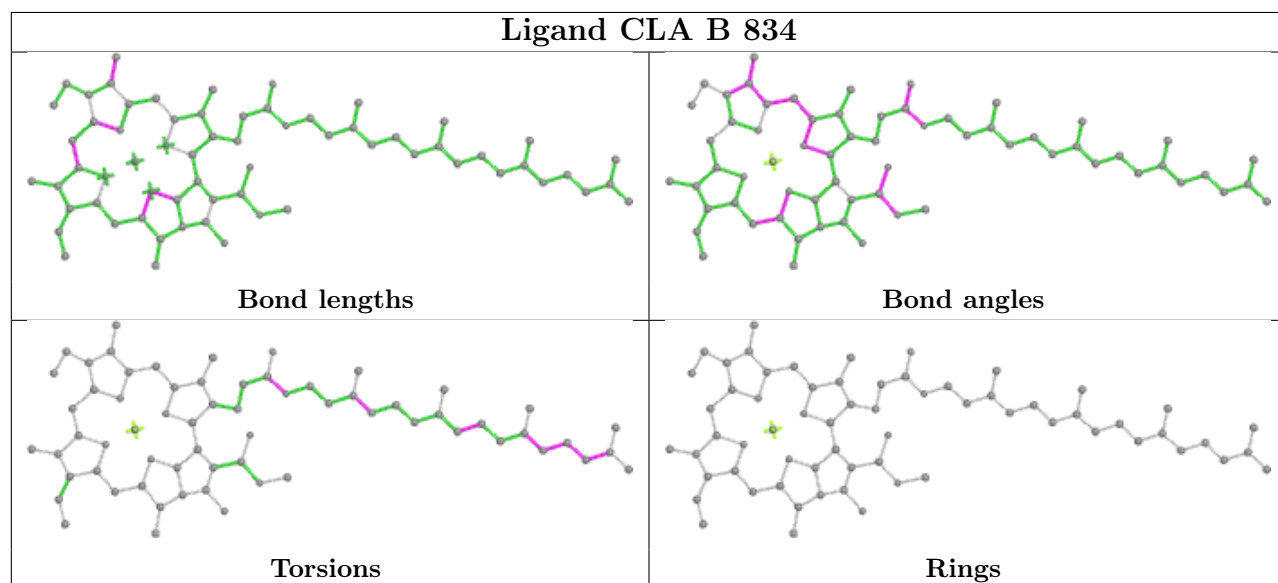


Ligand CLA A 840

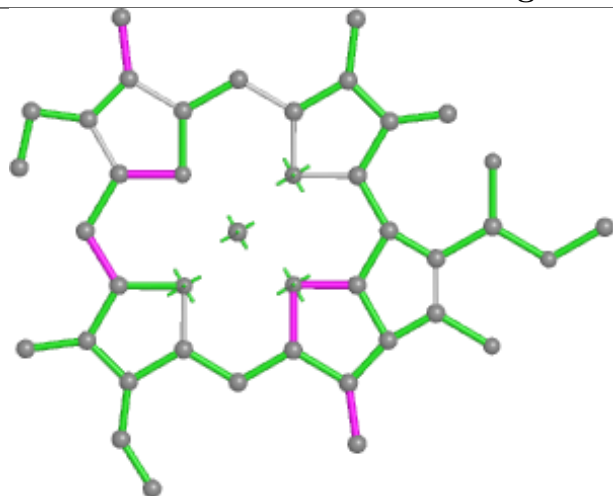




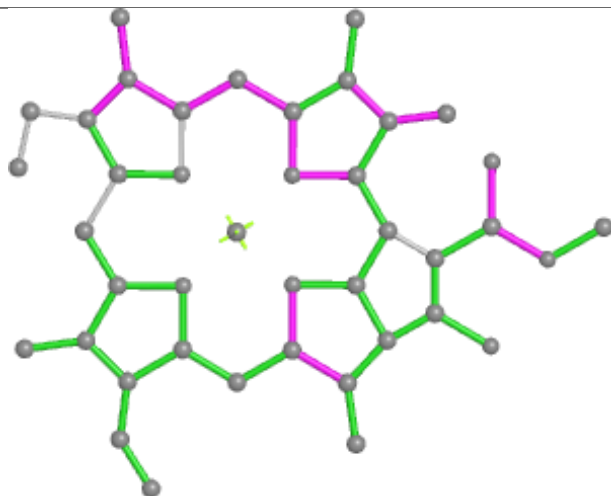


Ligand CLA A 836**Ligand CLA B 834**

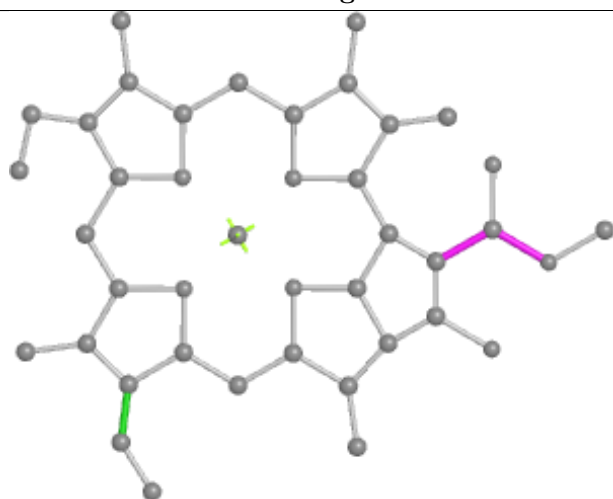
Ligand CLA d 310



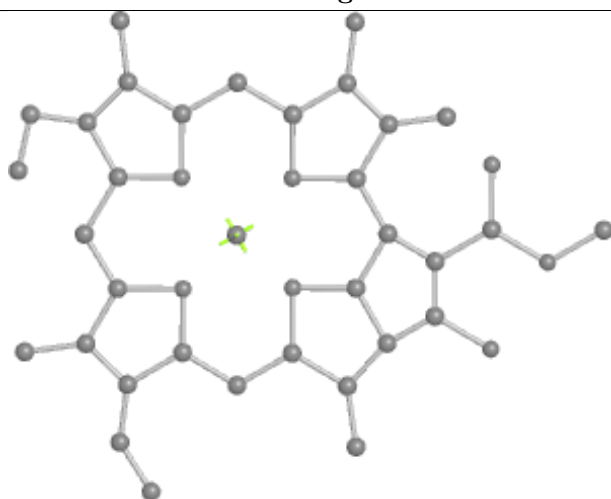
Bond lengths



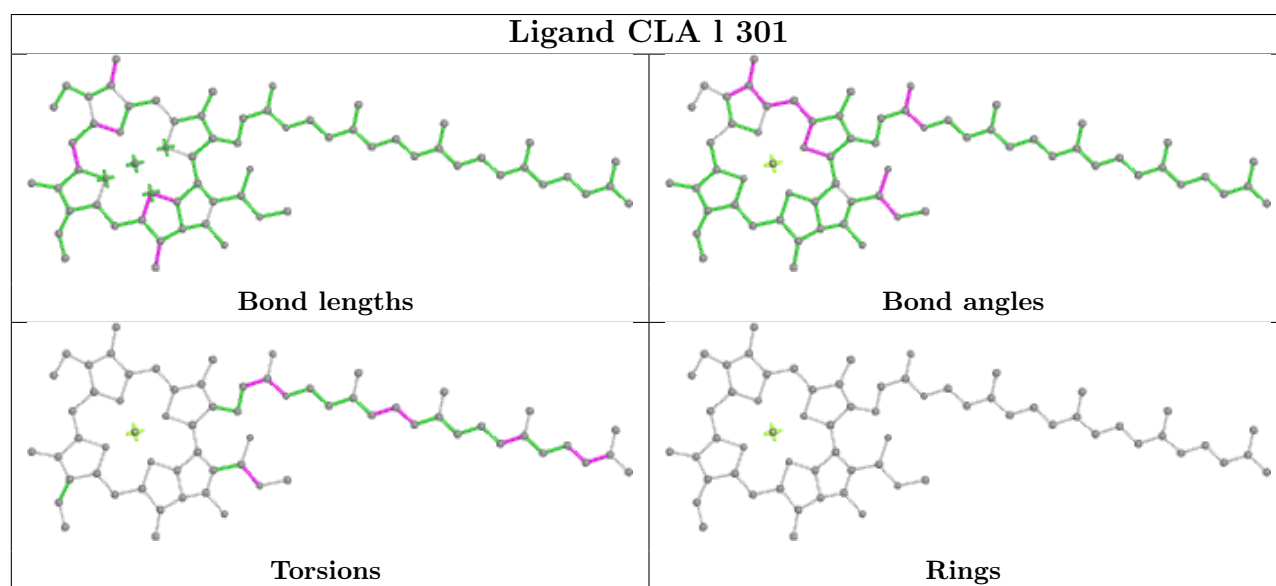
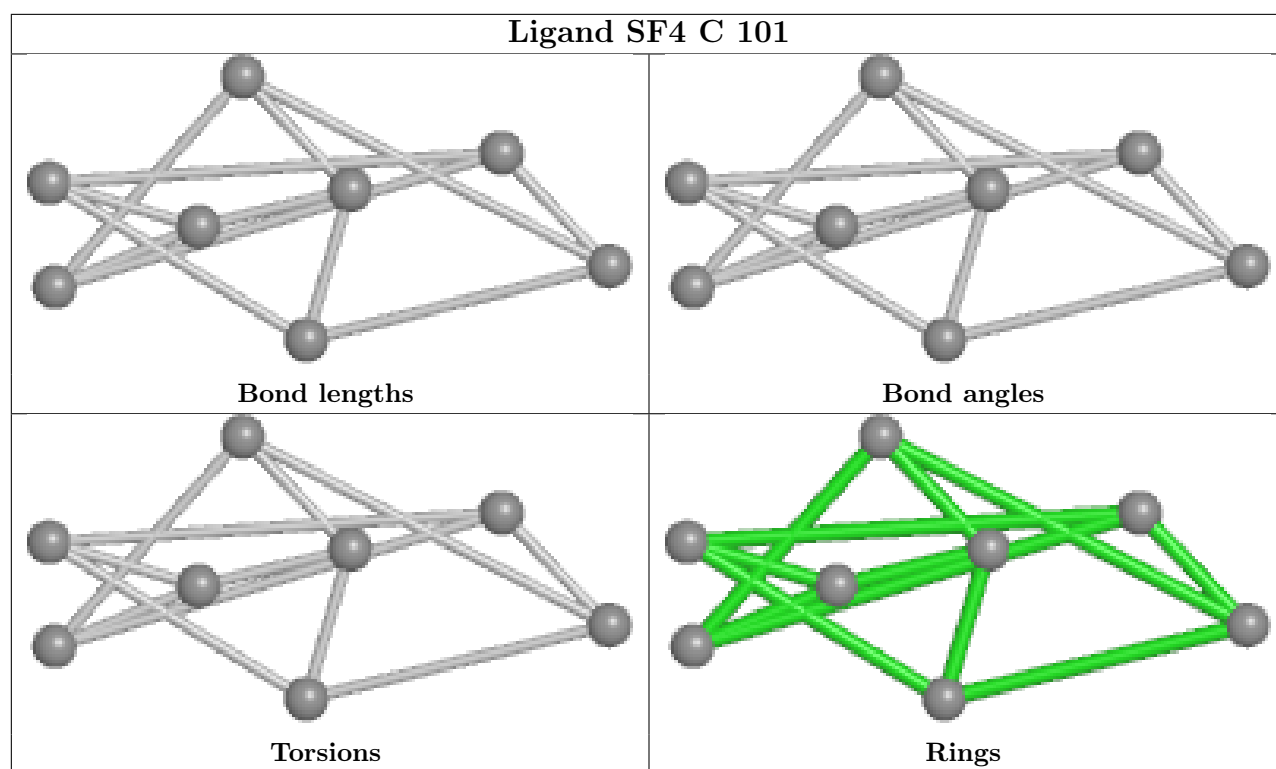
Bond angles



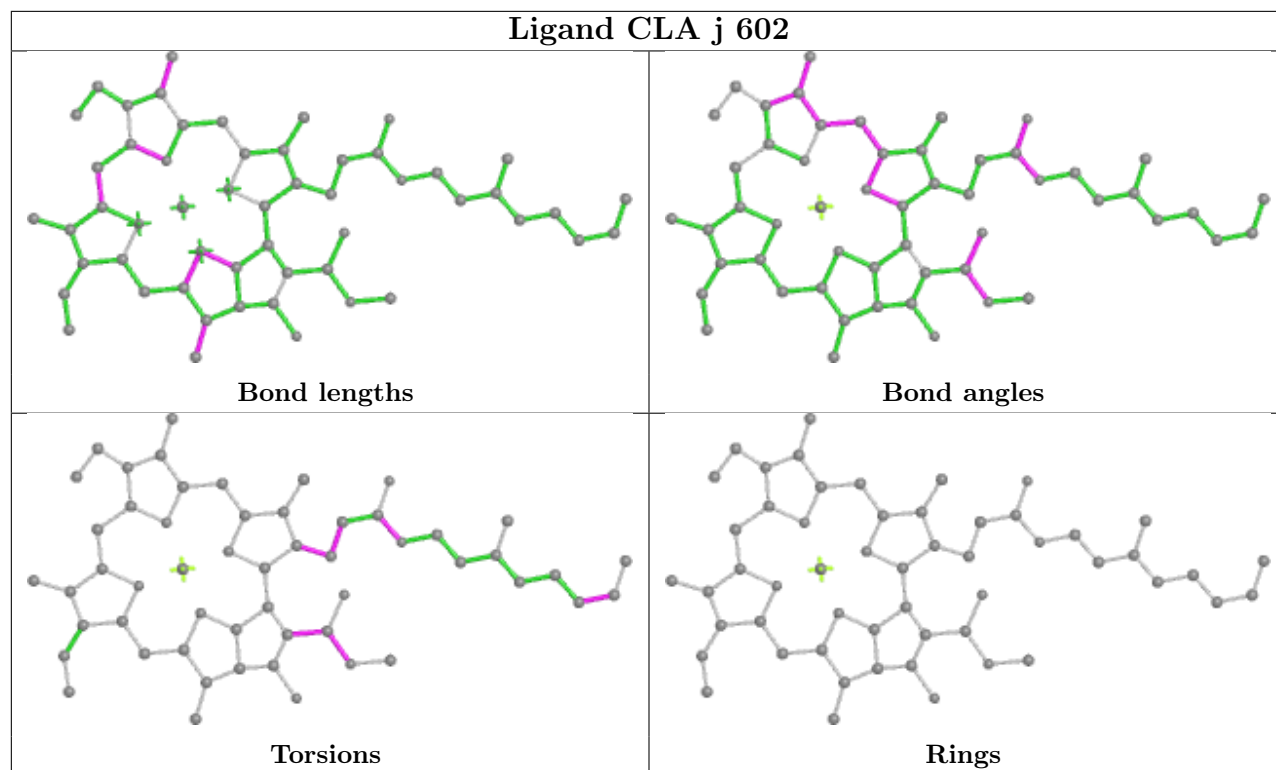
Torsions



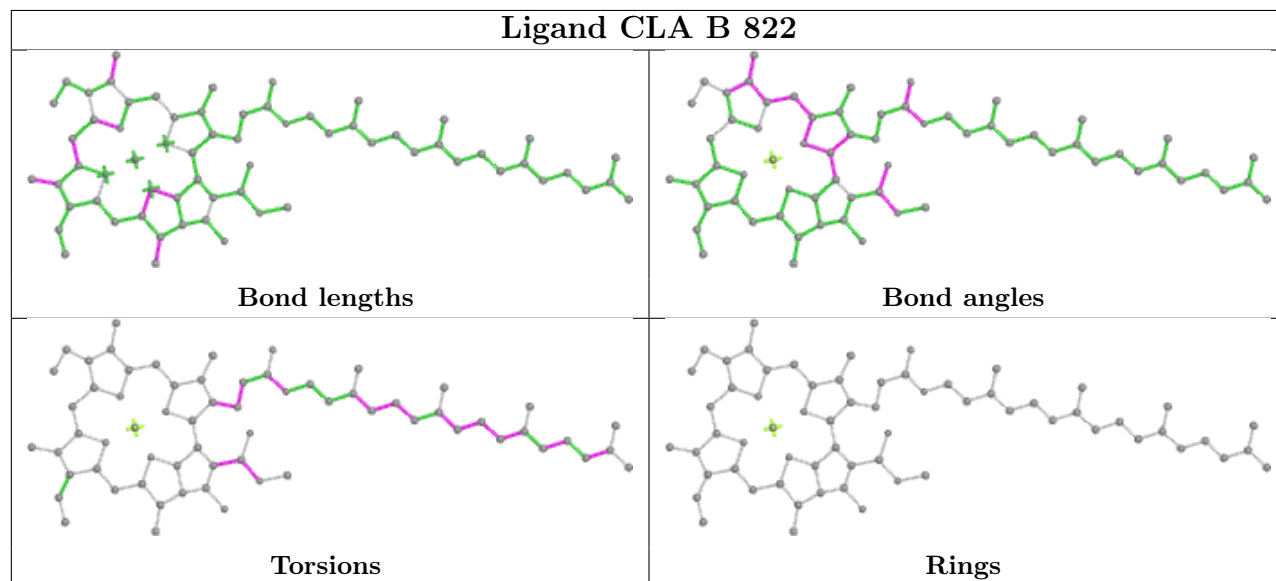
Rings



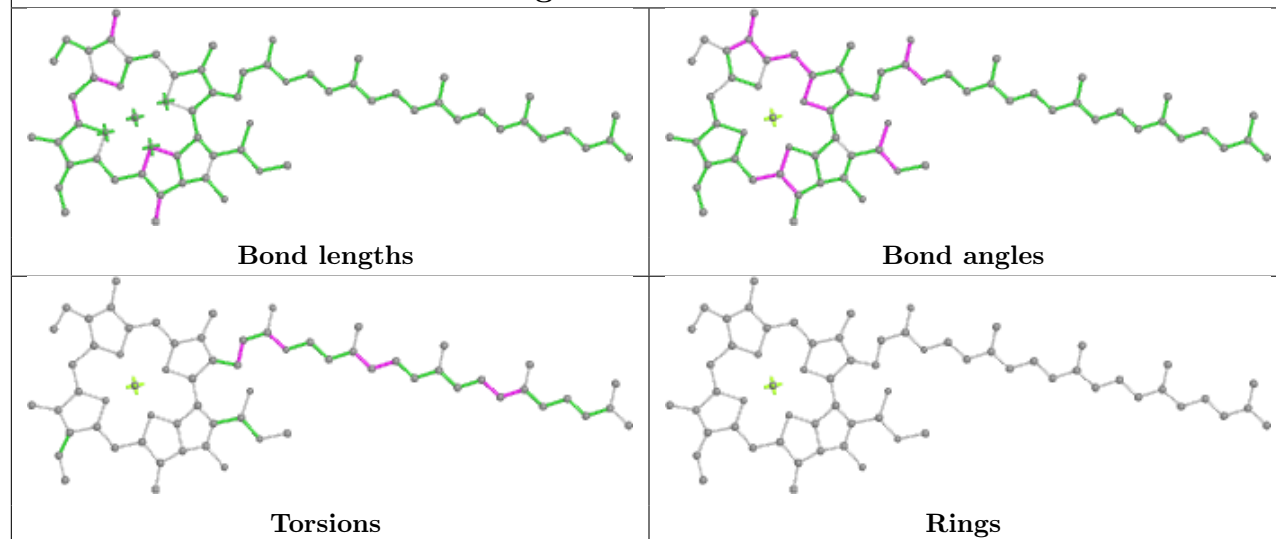
Ligand CLA j 602



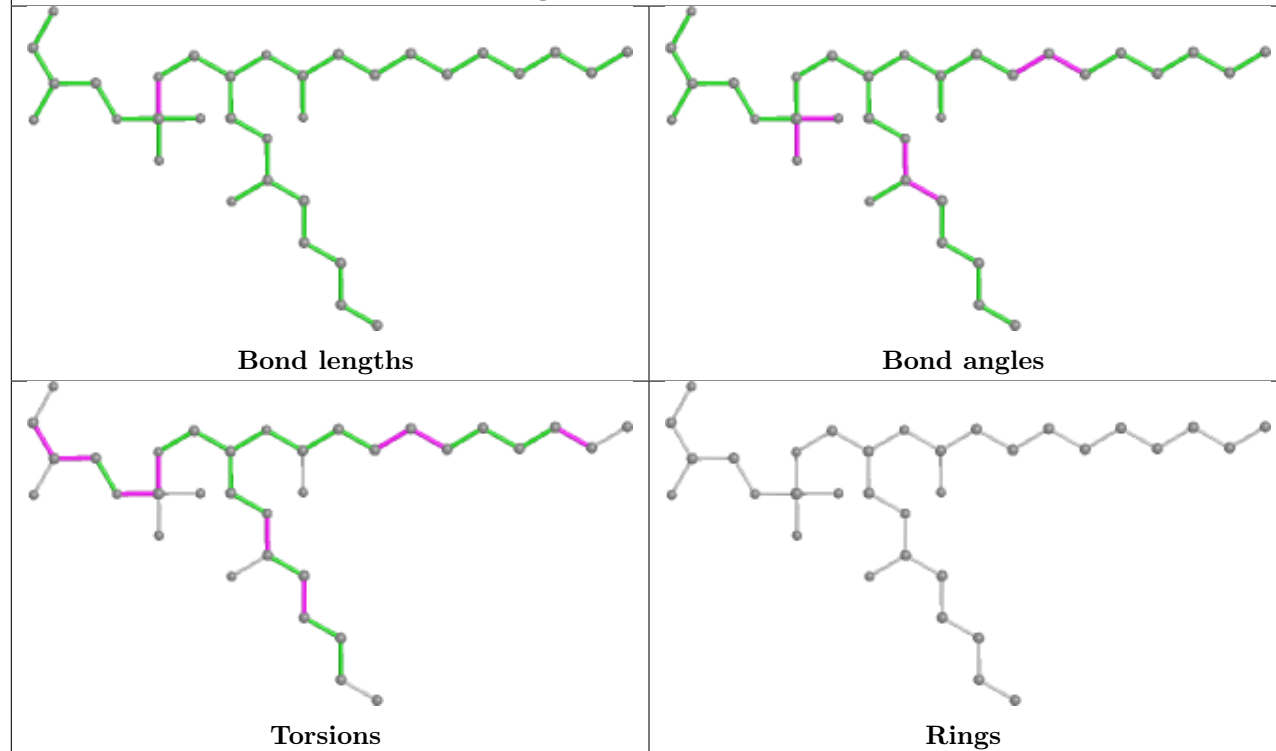
Ligand CLA B 822



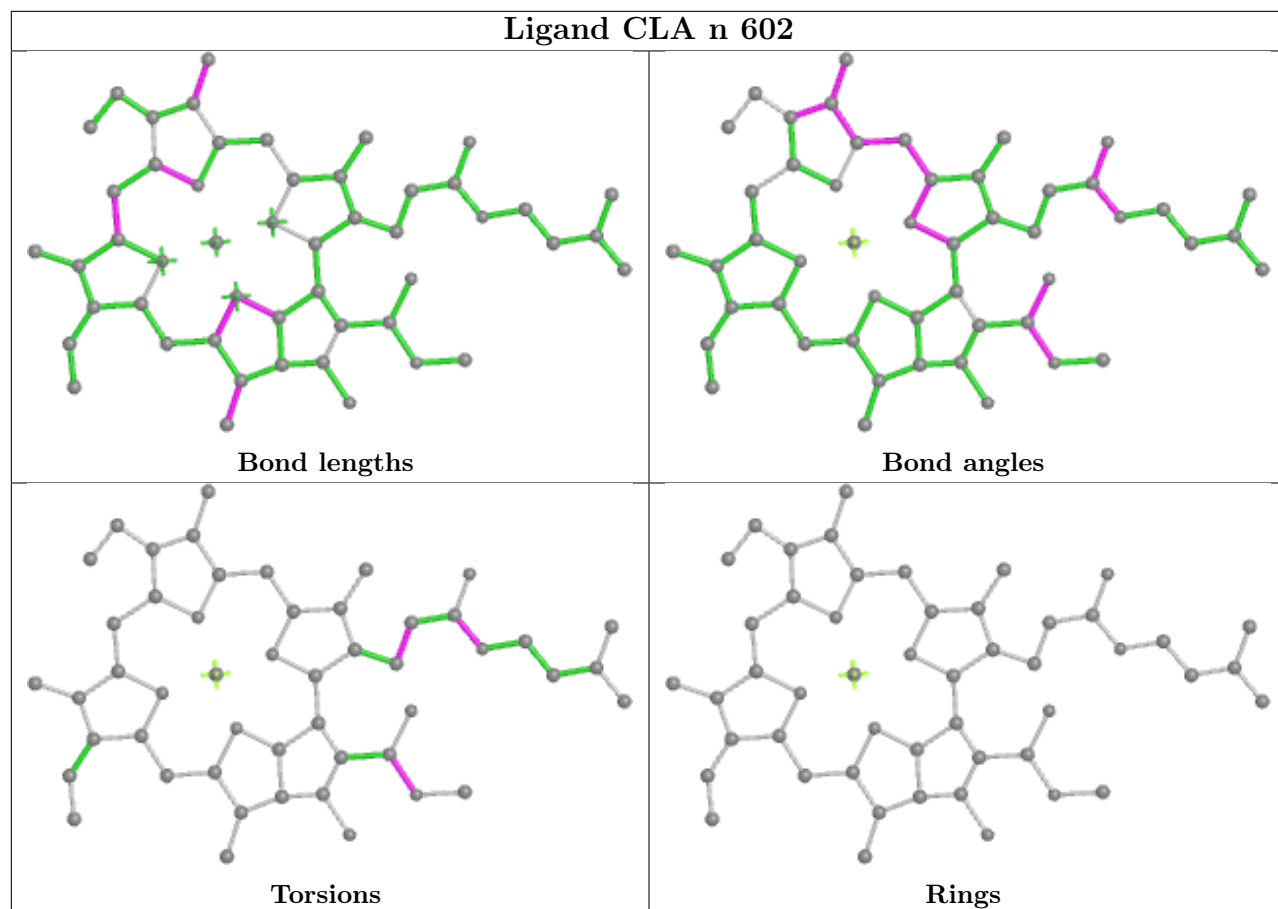
Ligand CLA h 306

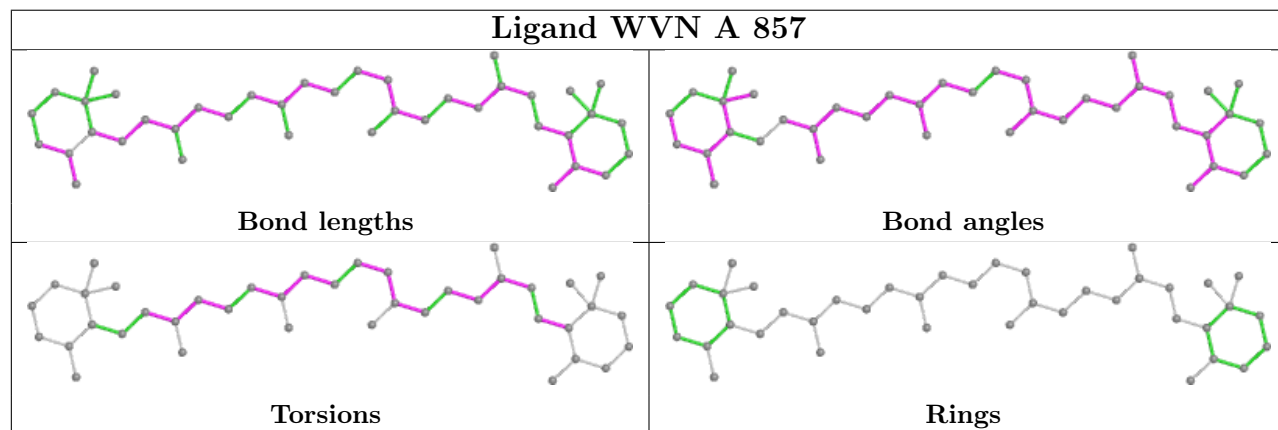
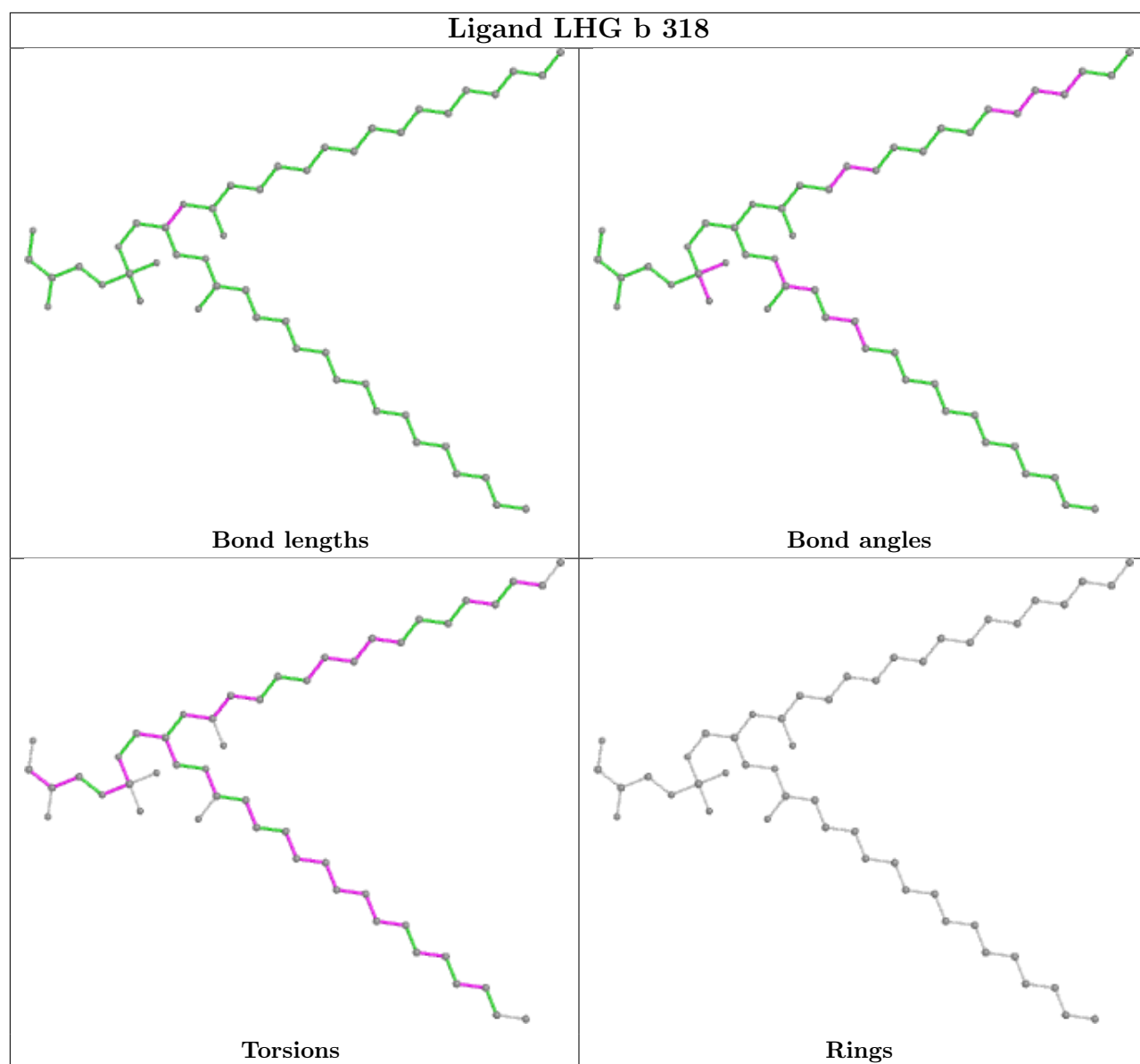


Ligand LHG J 105

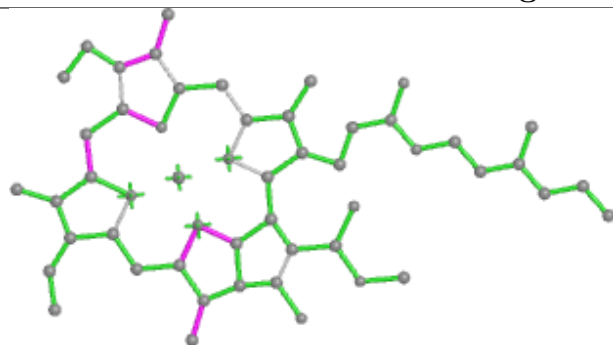


Ligand CLA n 602

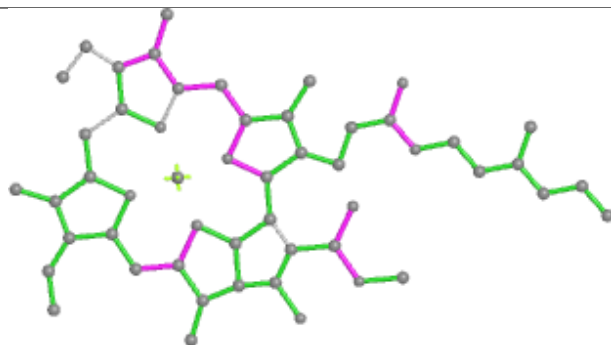




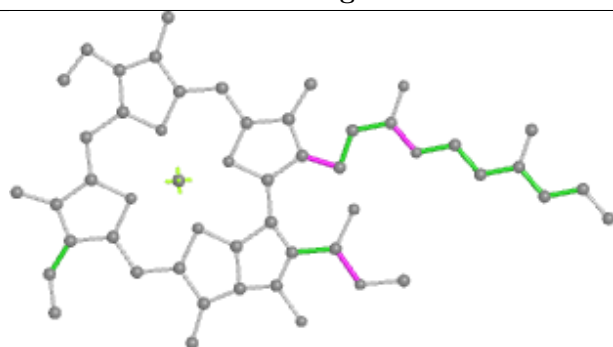
Ligand CLA c 306



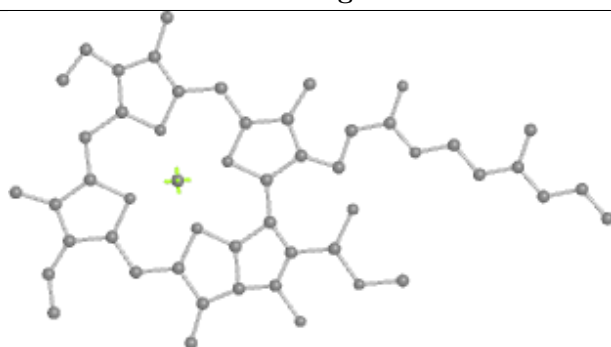
Bond lengths



Bond angles

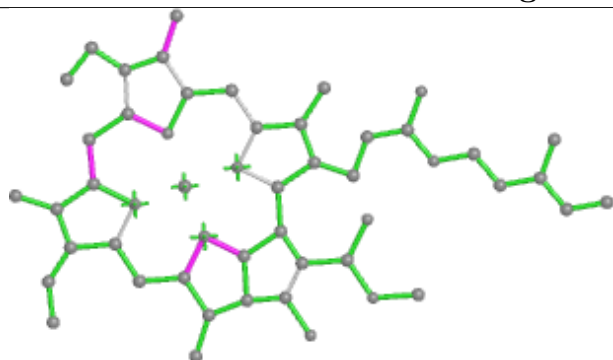


Torsions

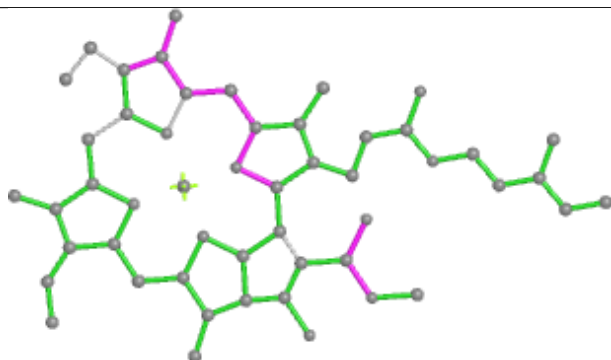


Rings

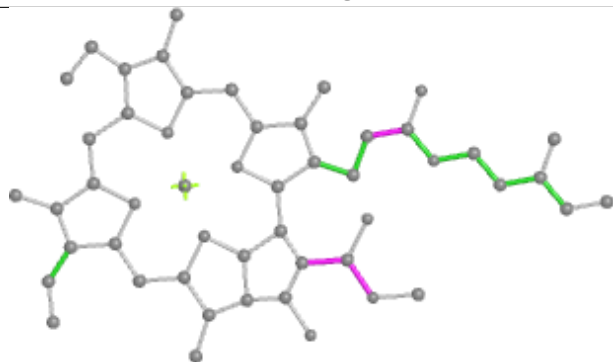
Ligand CLA c 303



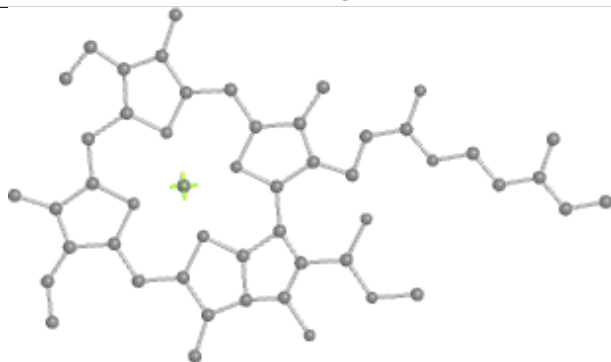
Bond lengths



Bond angles

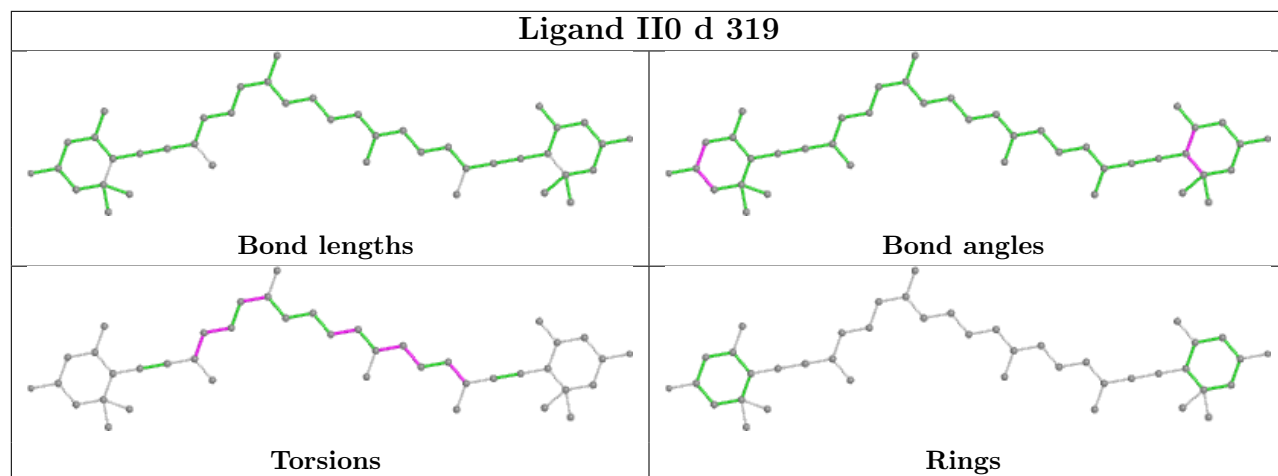


Torsions

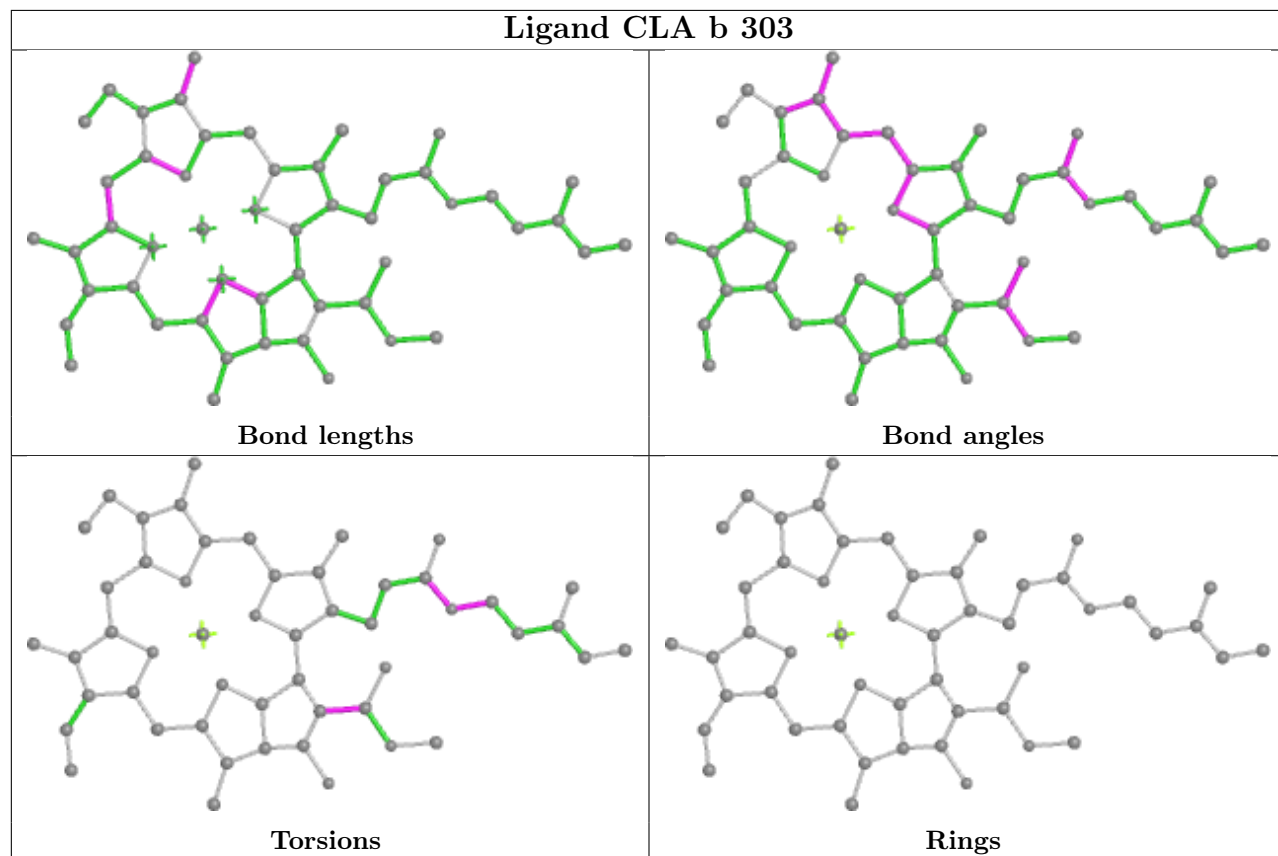


Rings

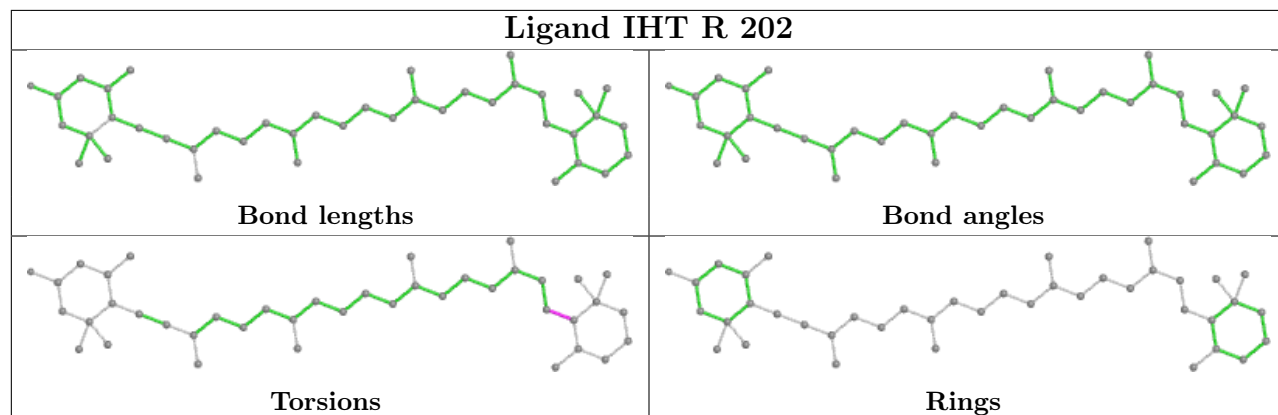
Ligand II0 d 319

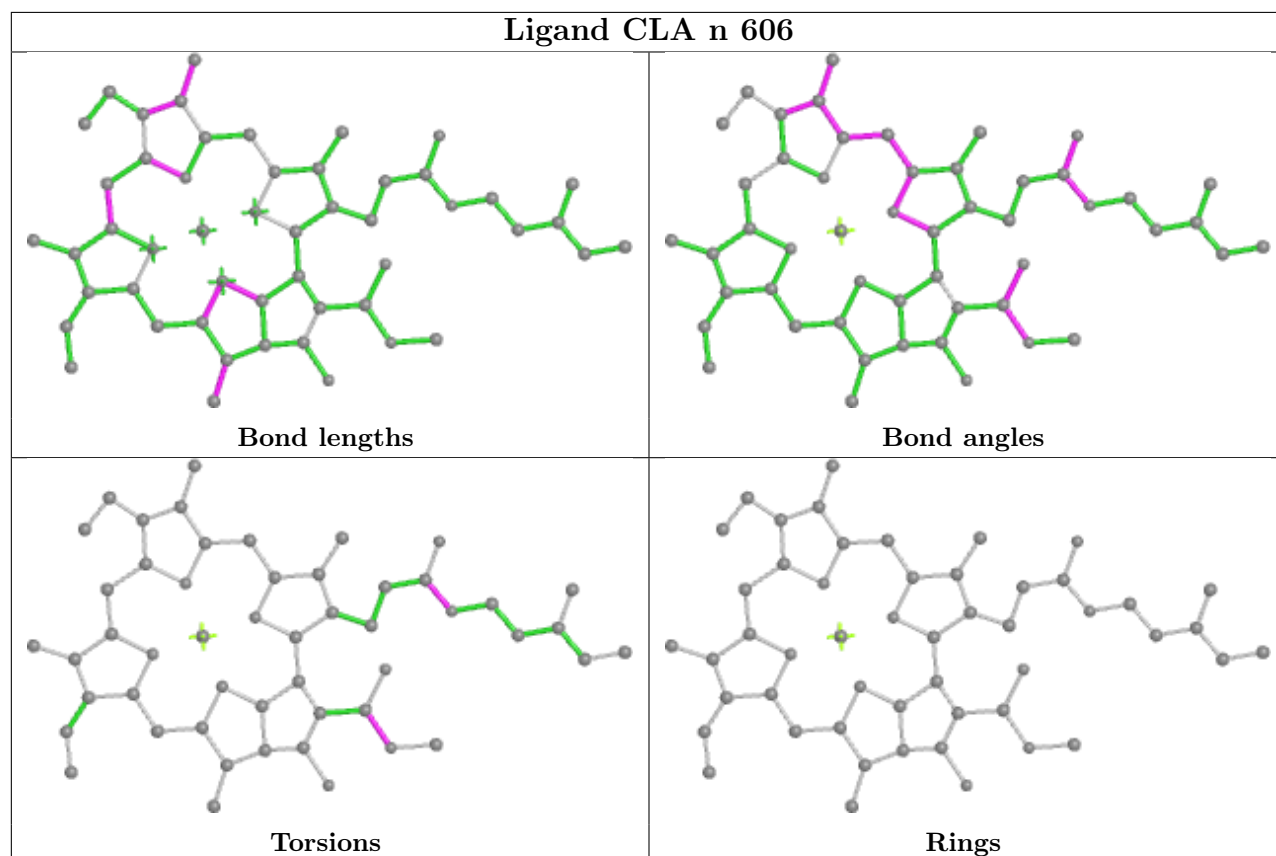
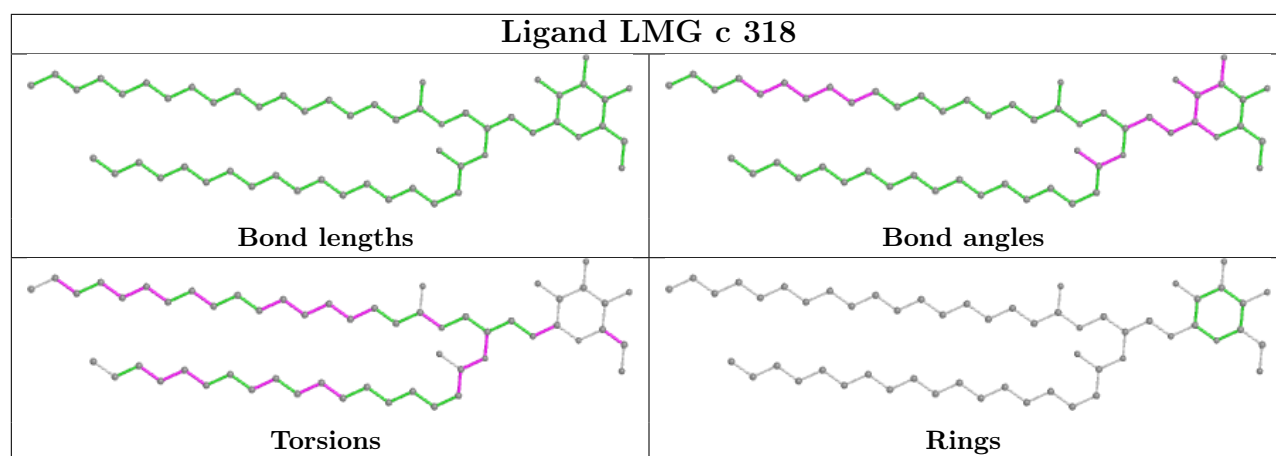


Ligand CLA b 303

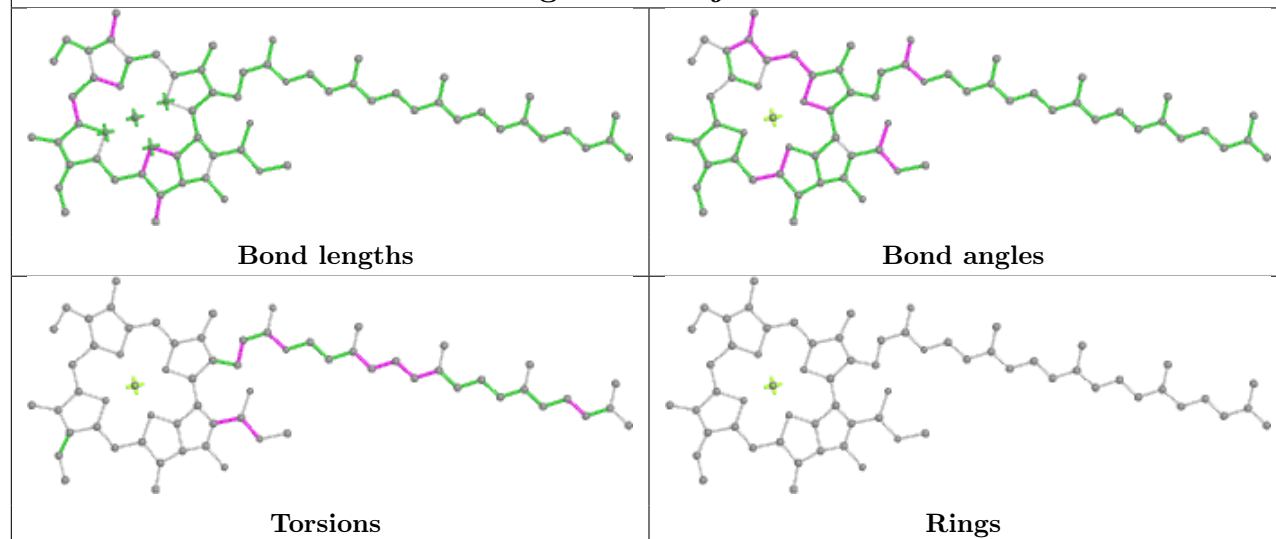


Ligand IHT R 202

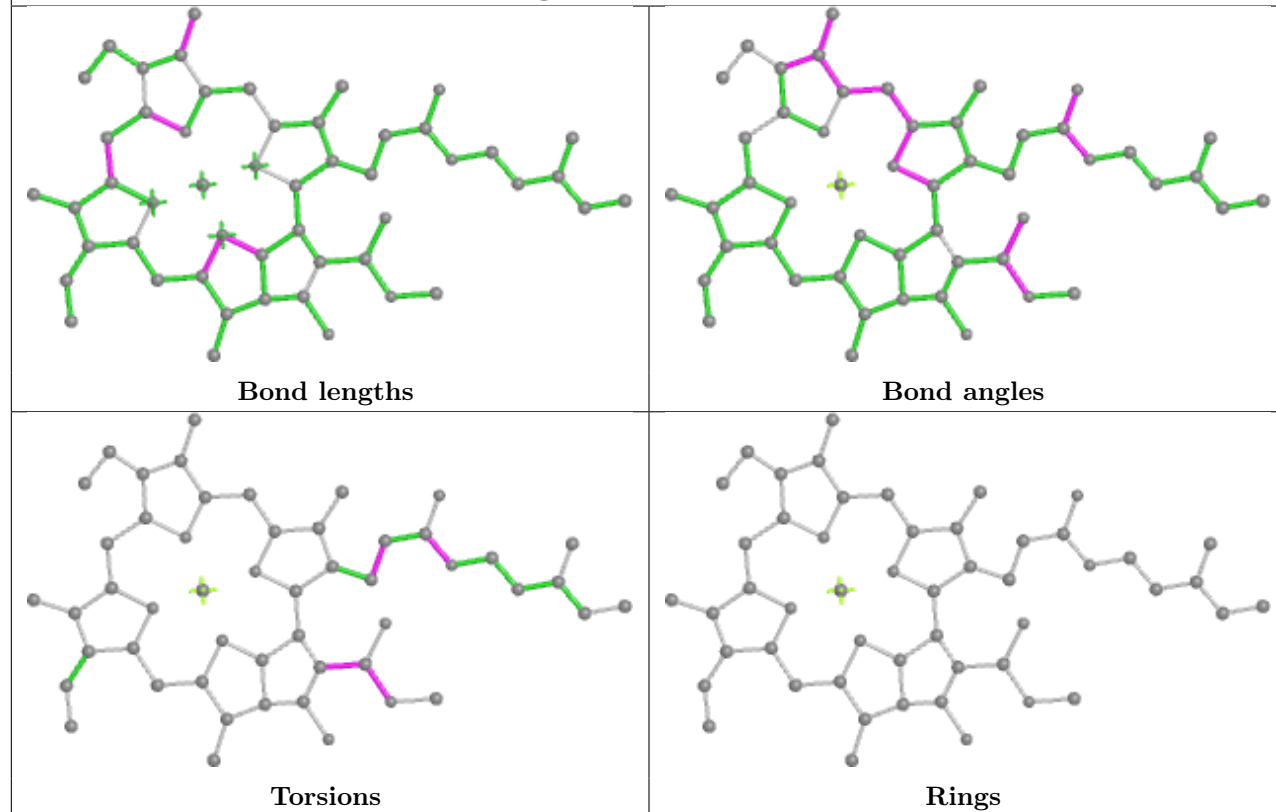




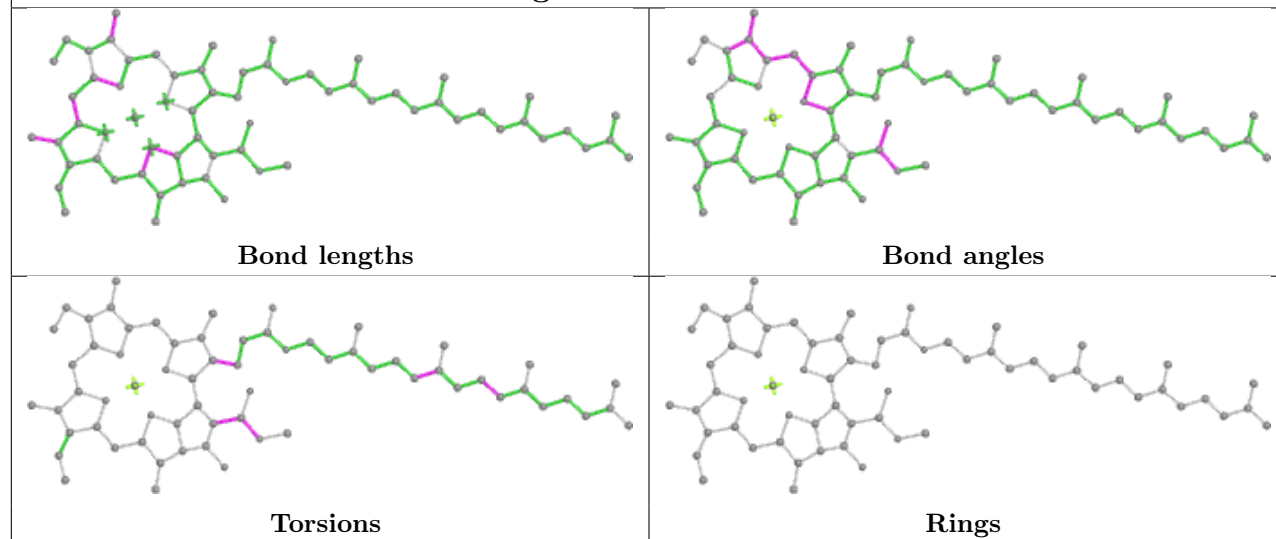
Ligand CLA j 613



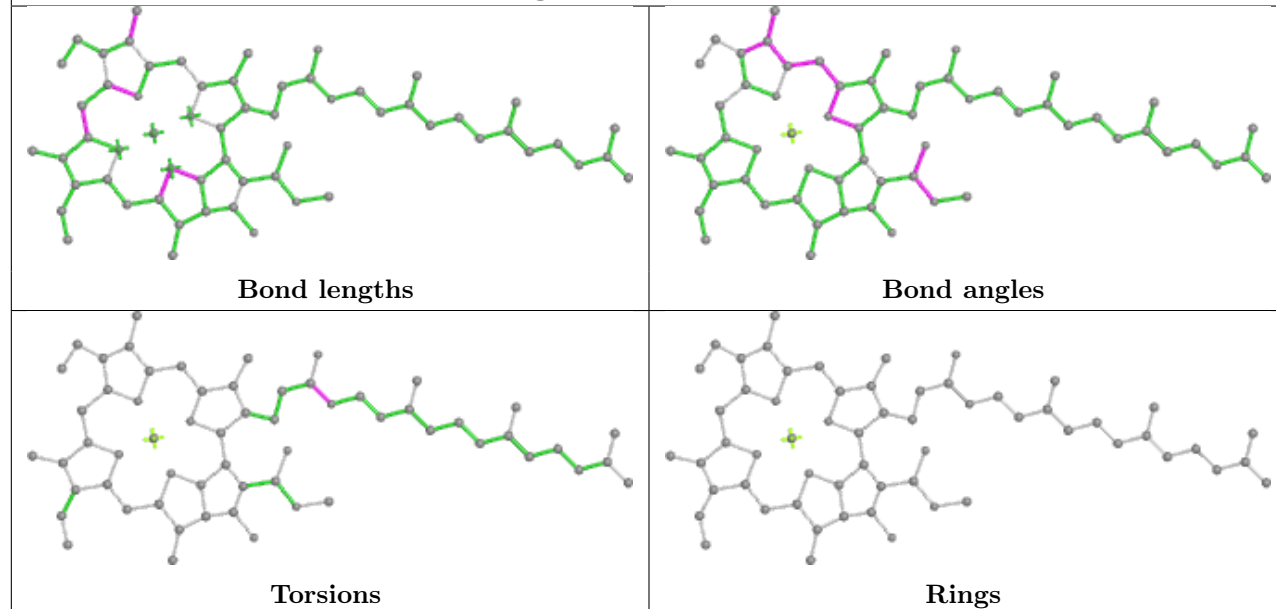
Ligand CLA d 305



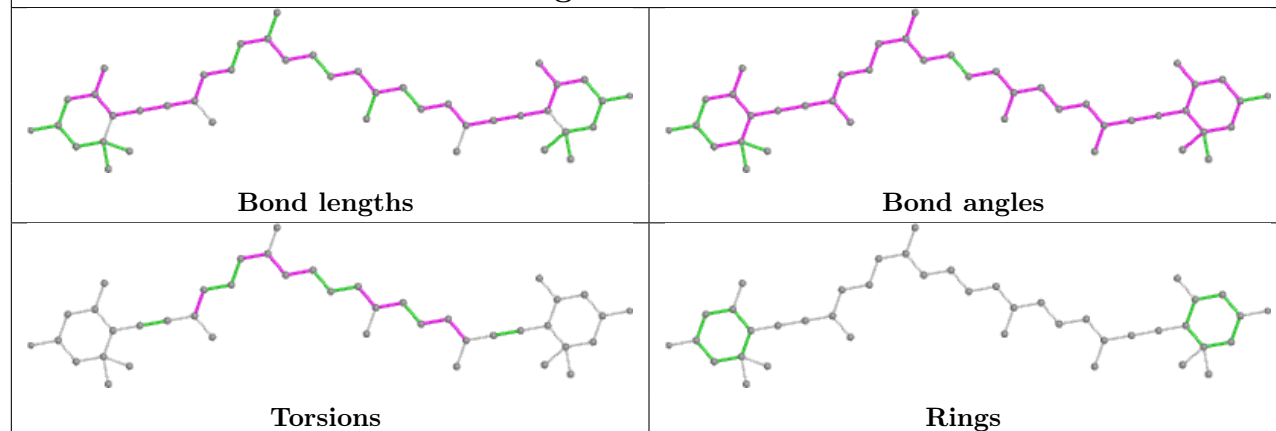
Ligand CLA B 824

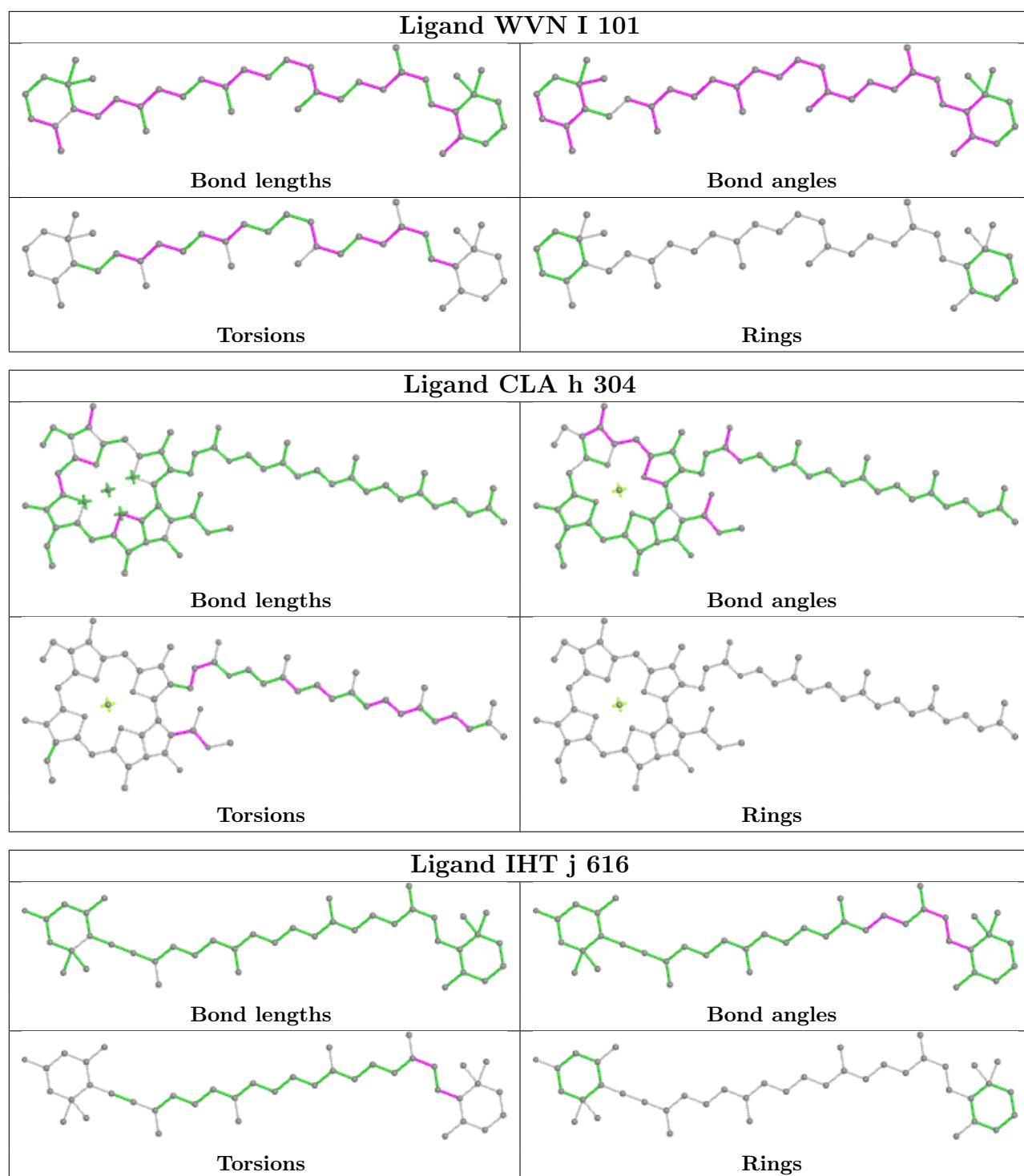


Ligand CLA A 839

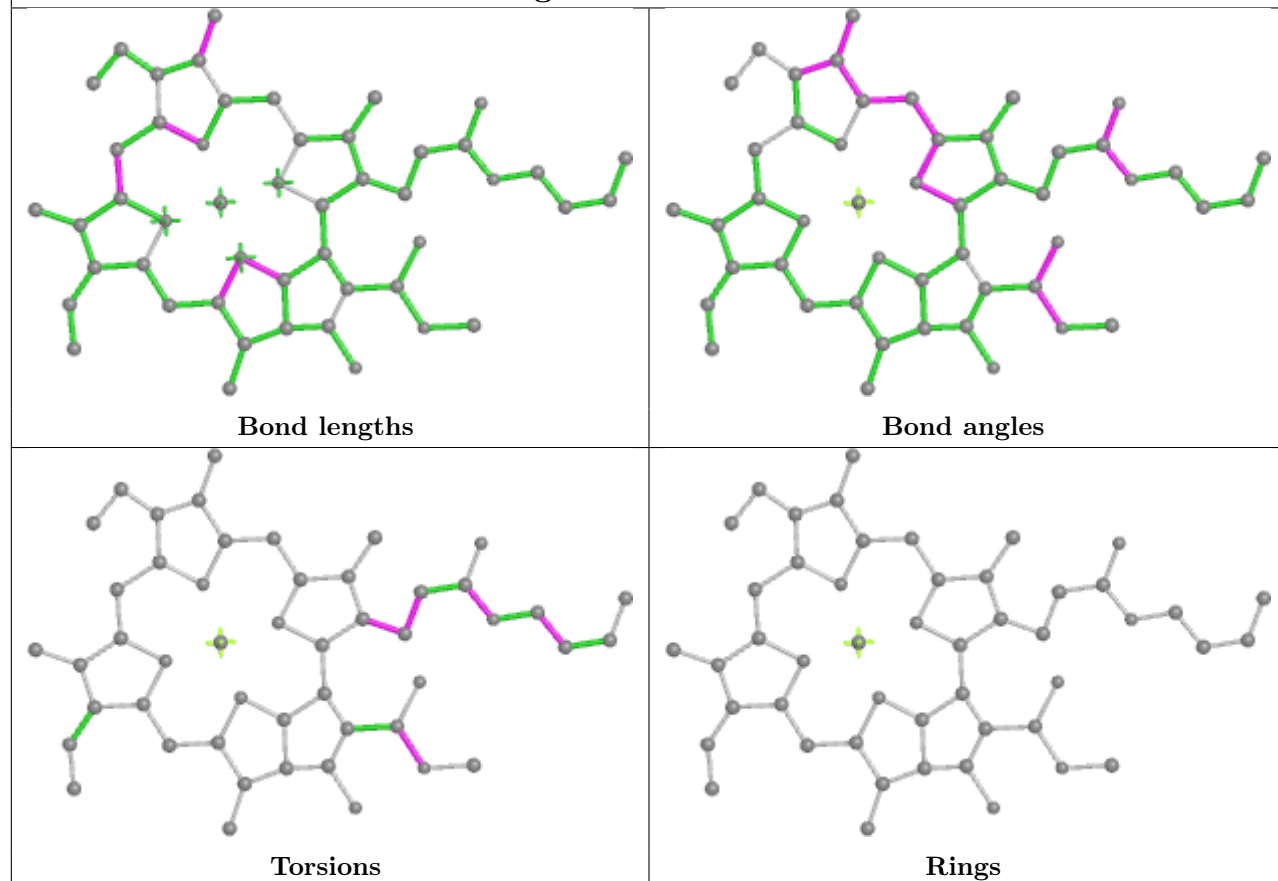


Ligand II0 I 314

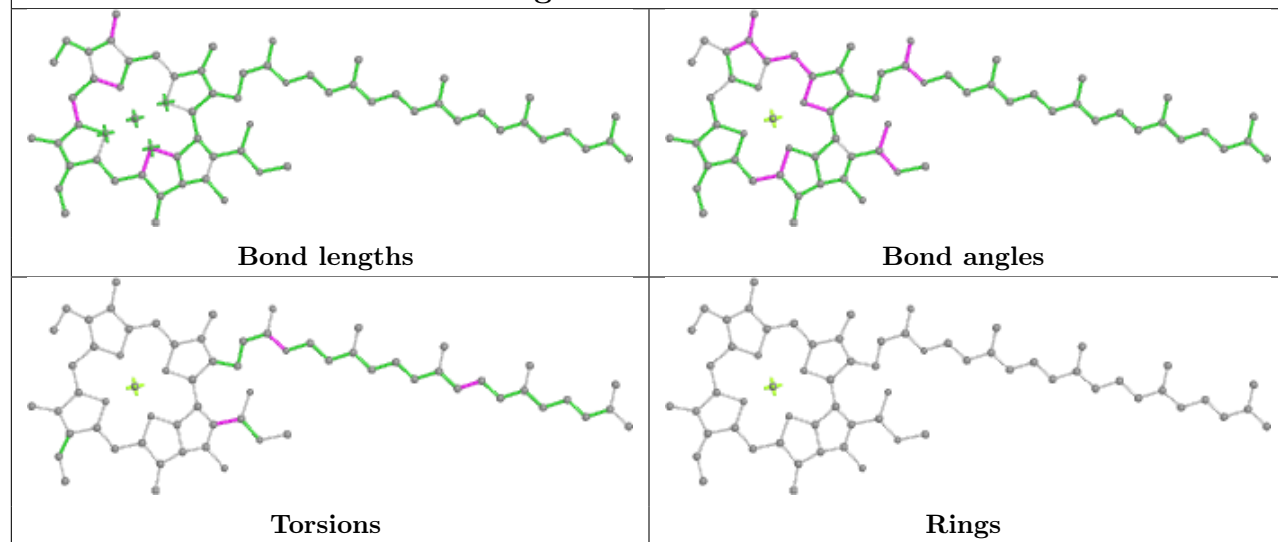


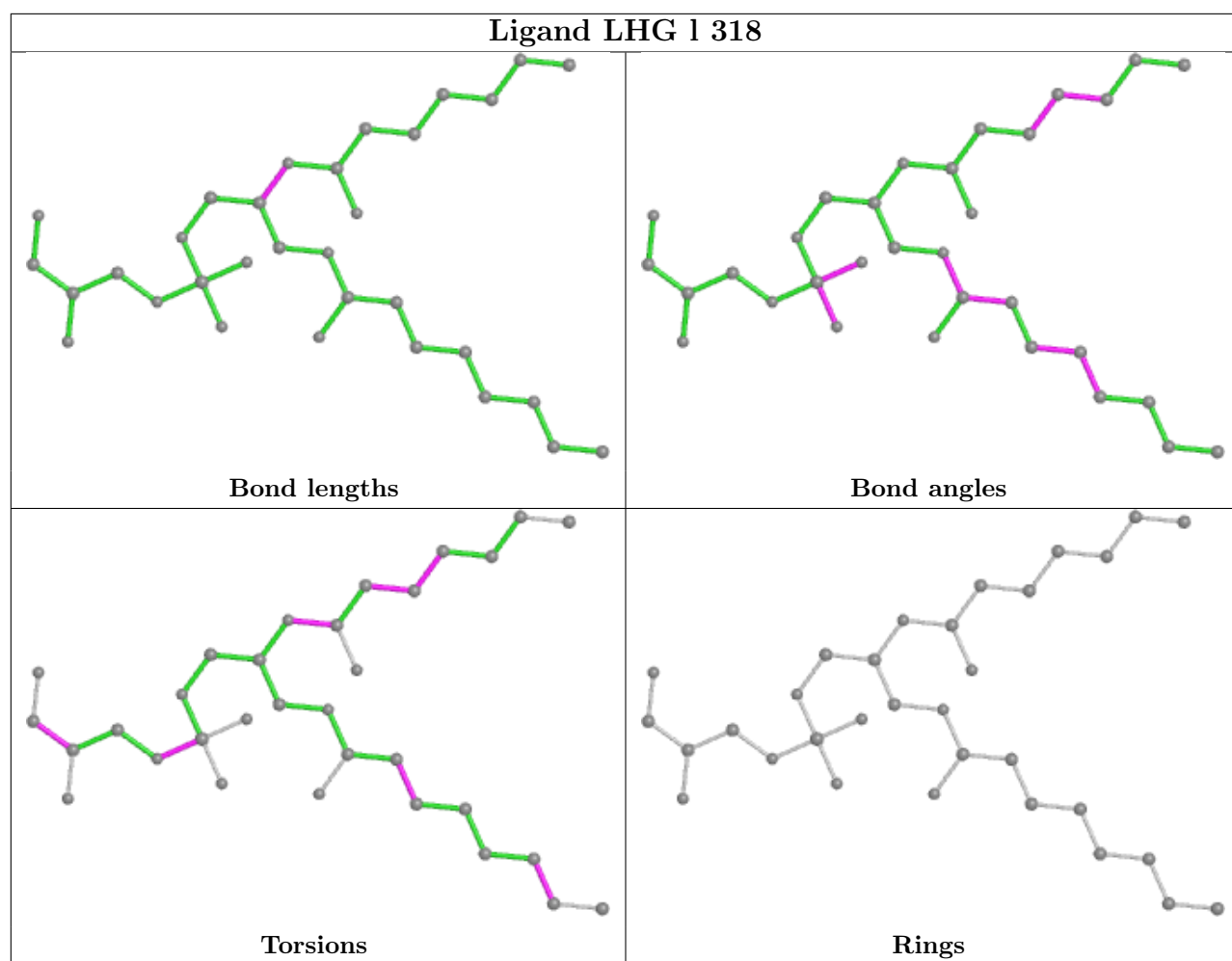


Ligand CLA L 202

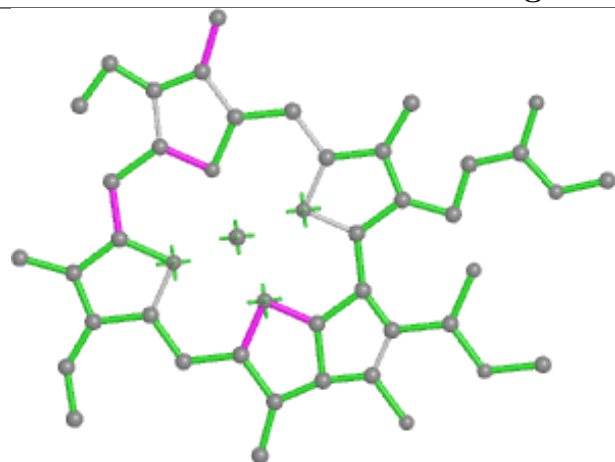


Ligand CLA L 203

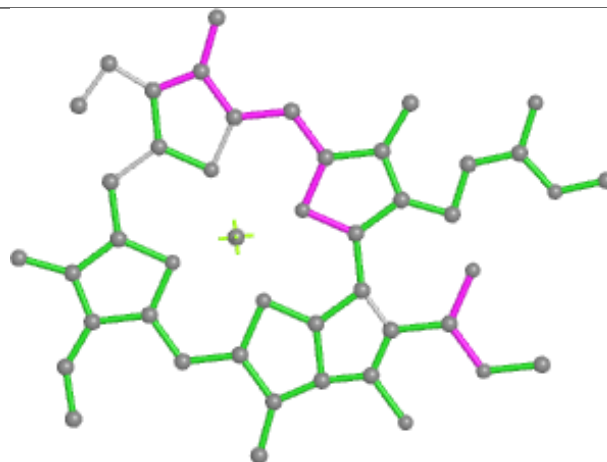




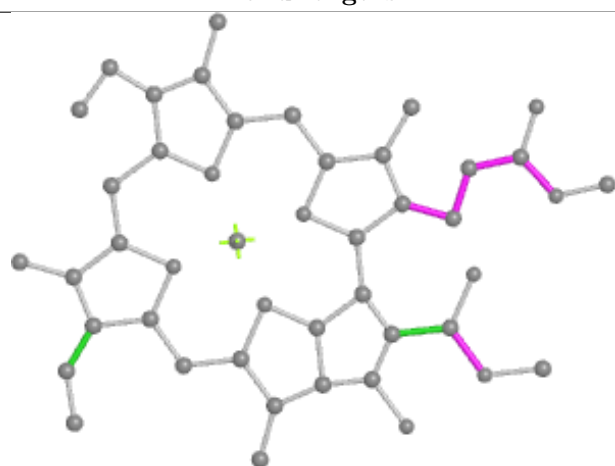
Ligand CLA i 308



Bond lengths



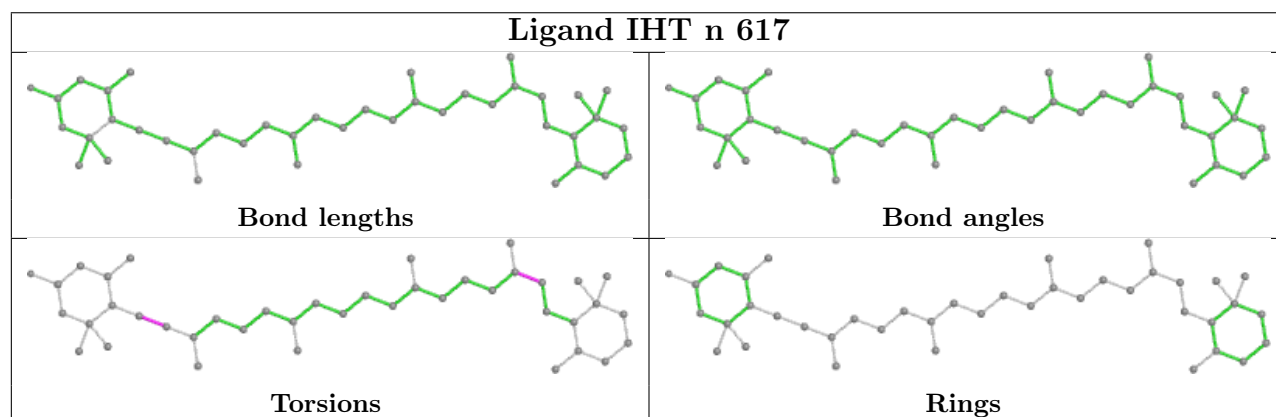
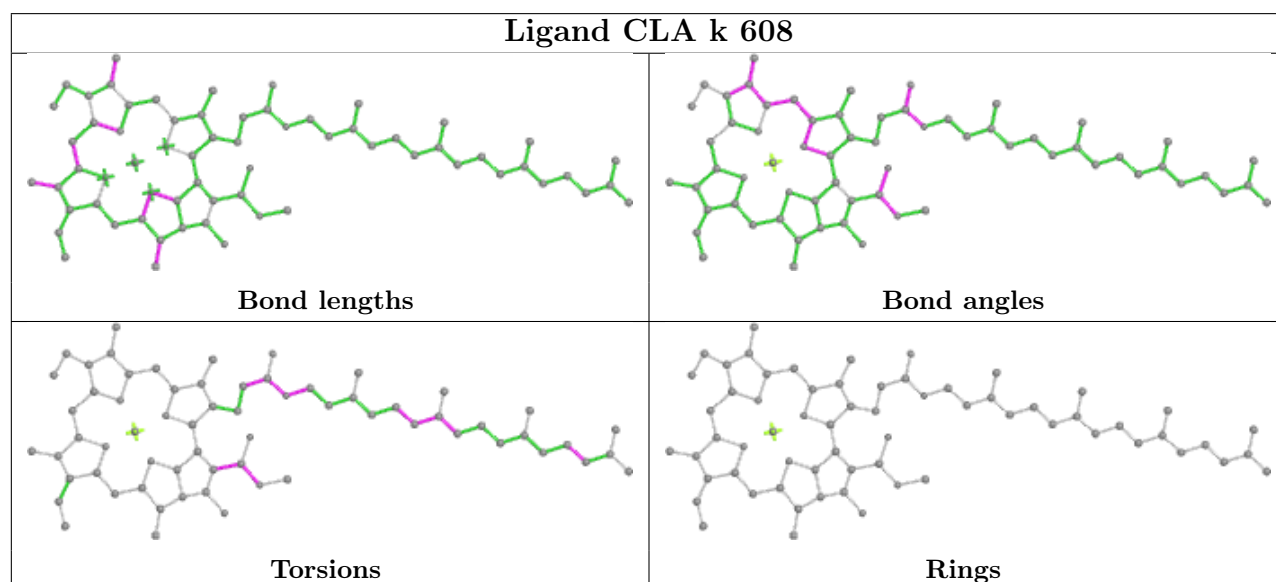
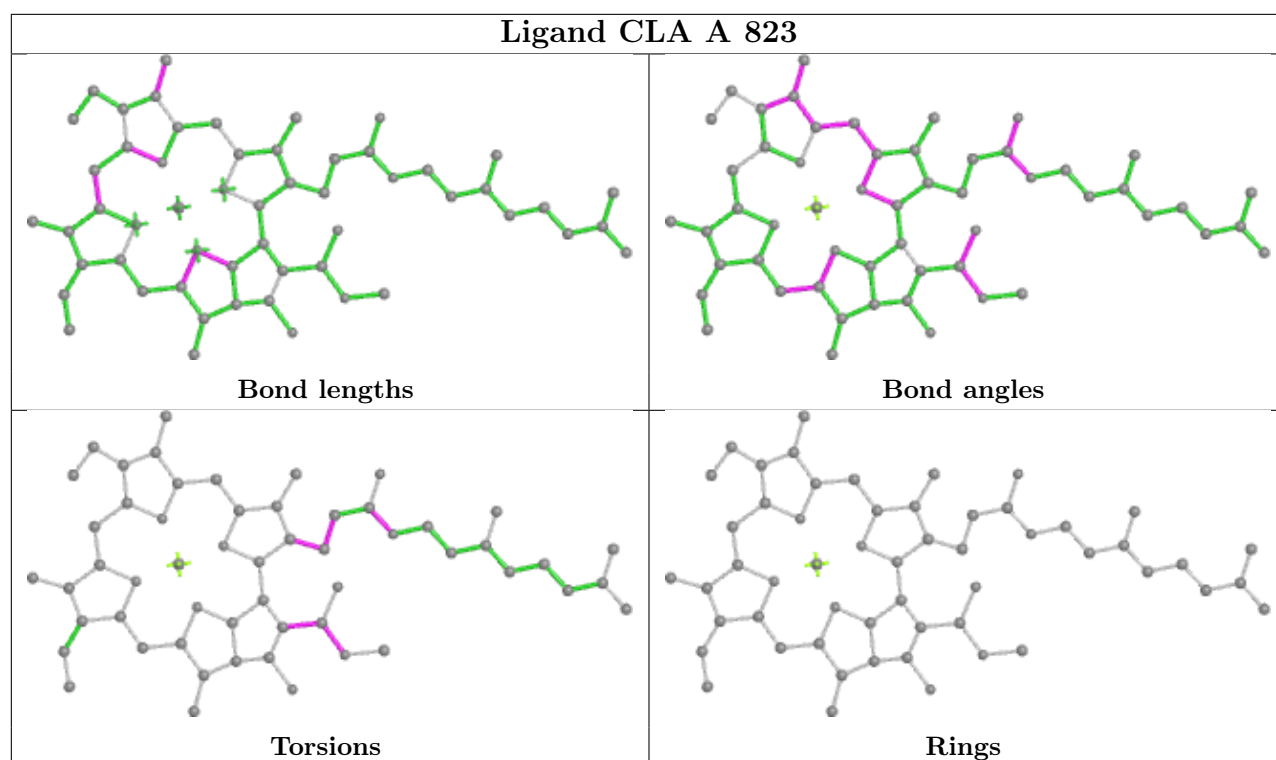
Bond angles



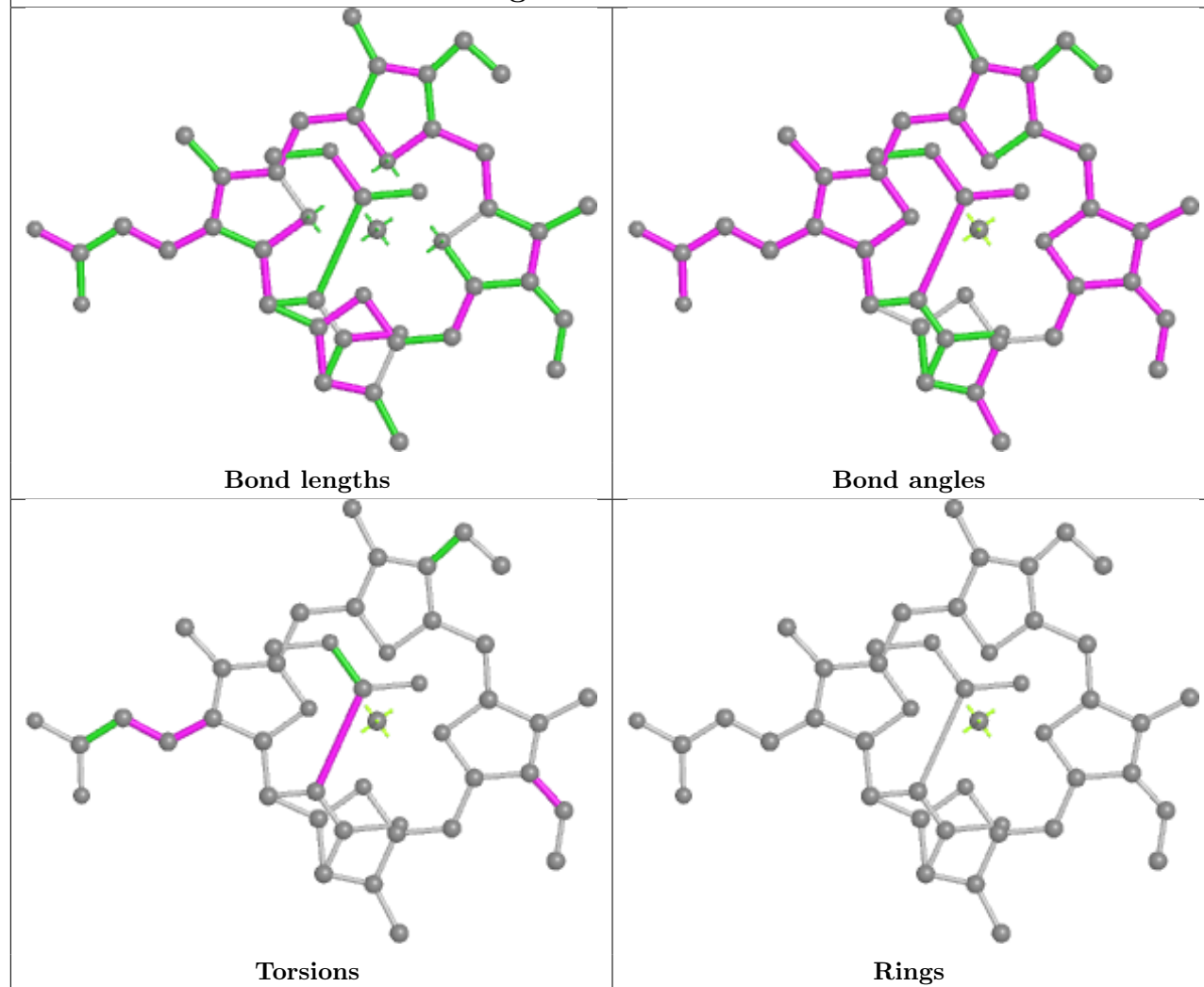
Torsions



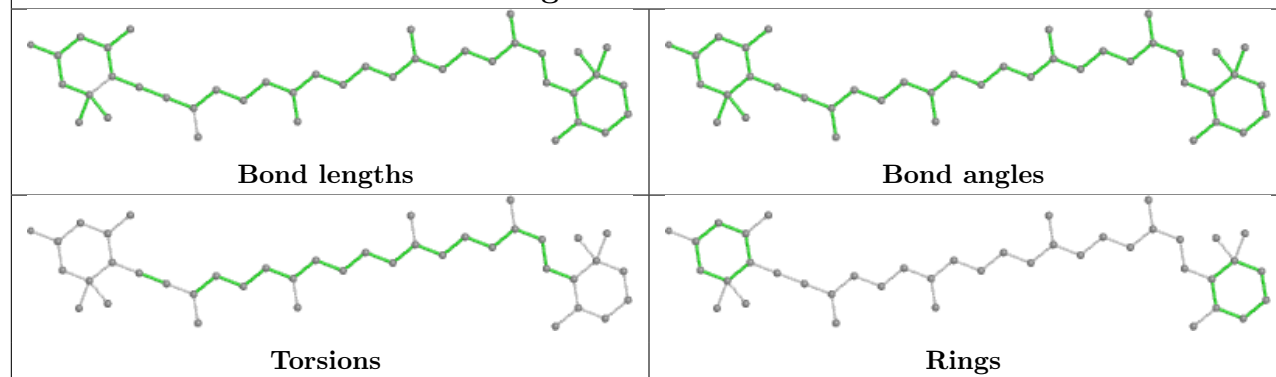
Rings

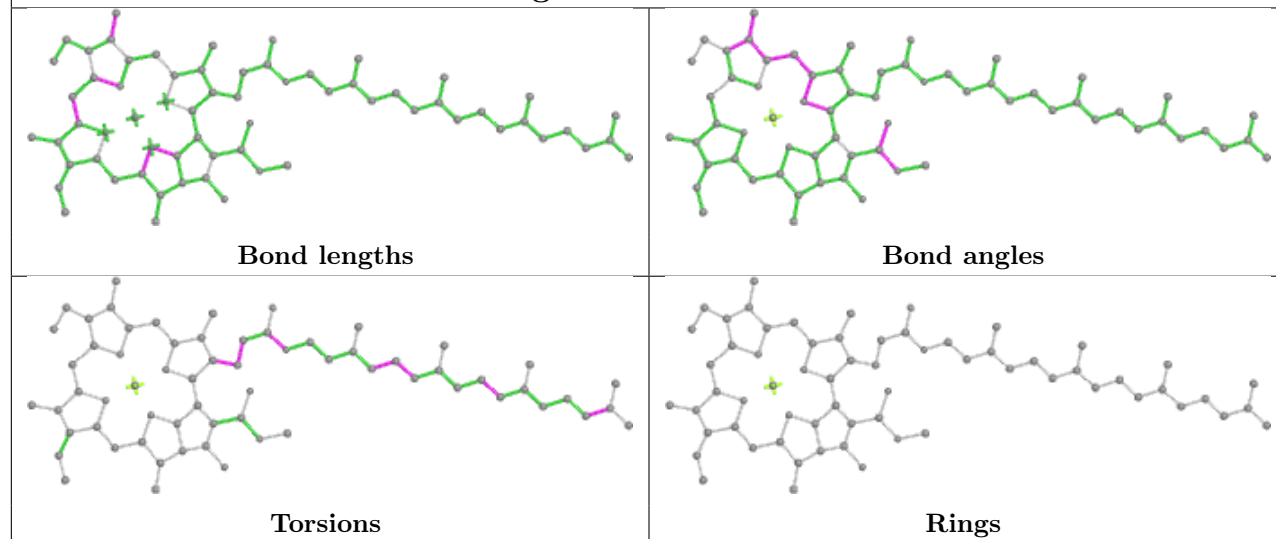
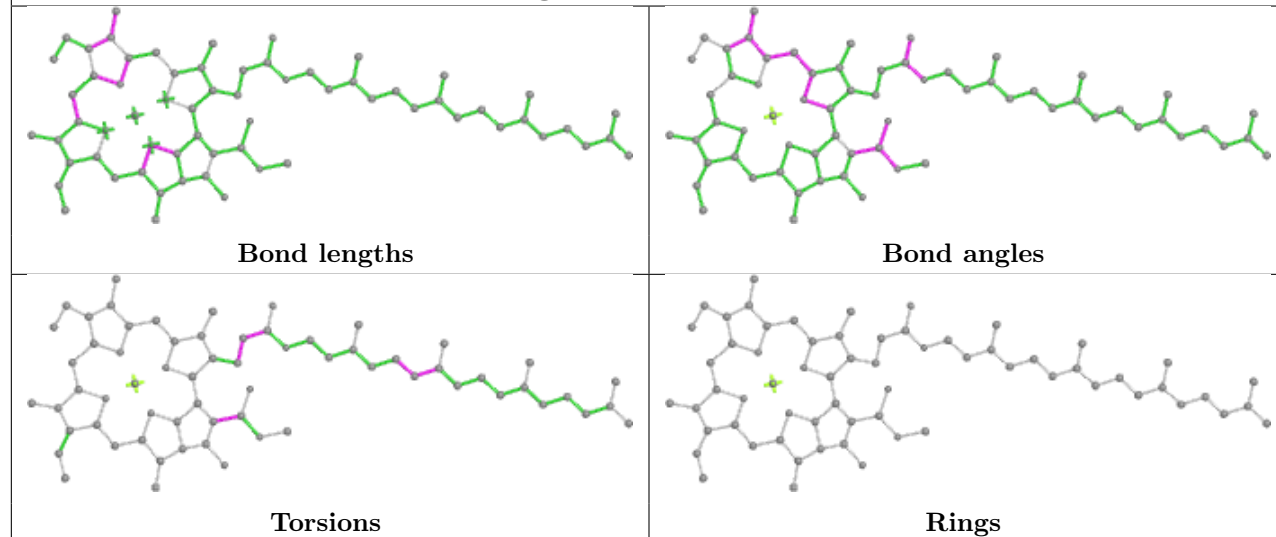
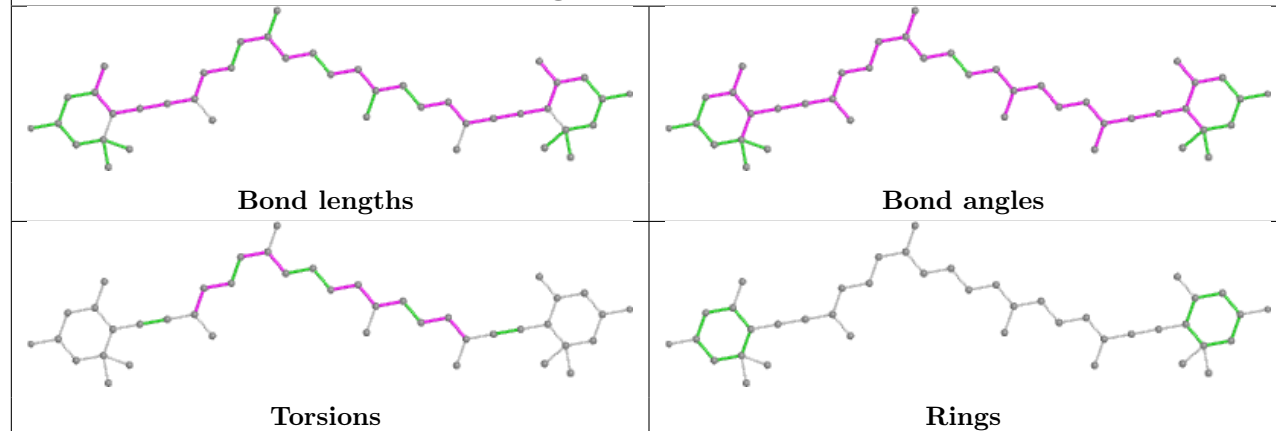


Ligand KC2 s 401

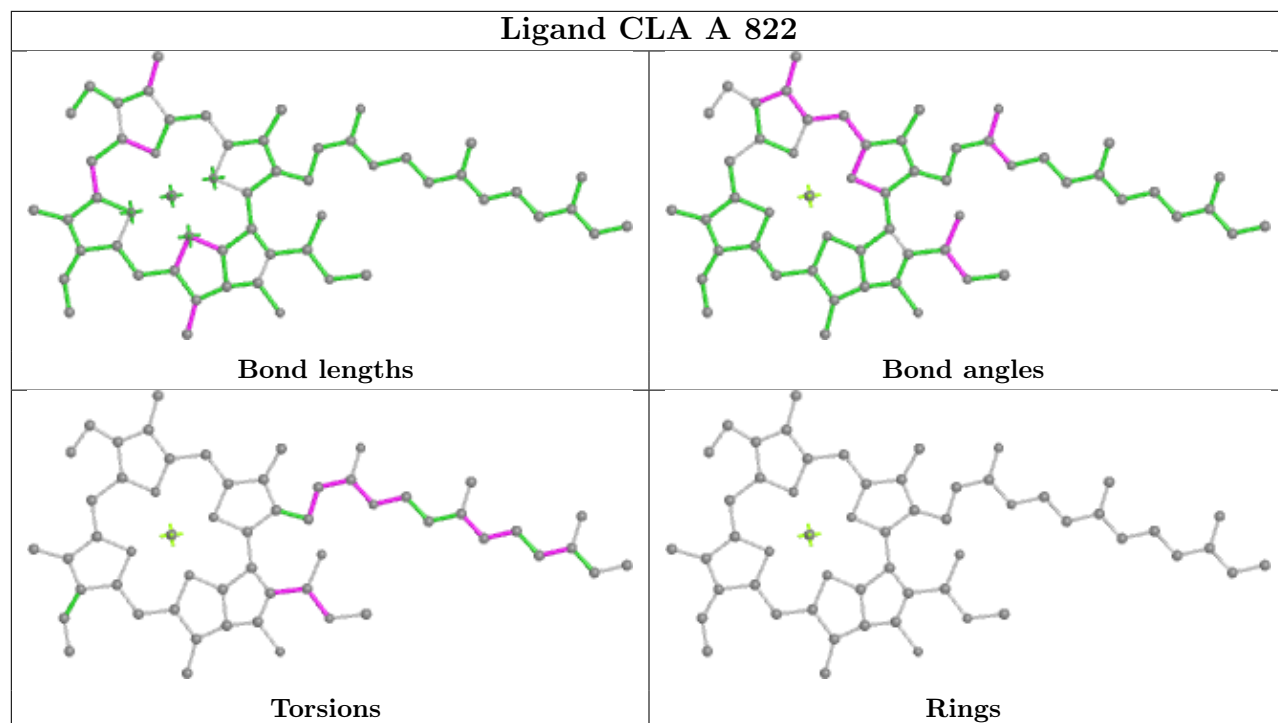


Ligand IHT c 315

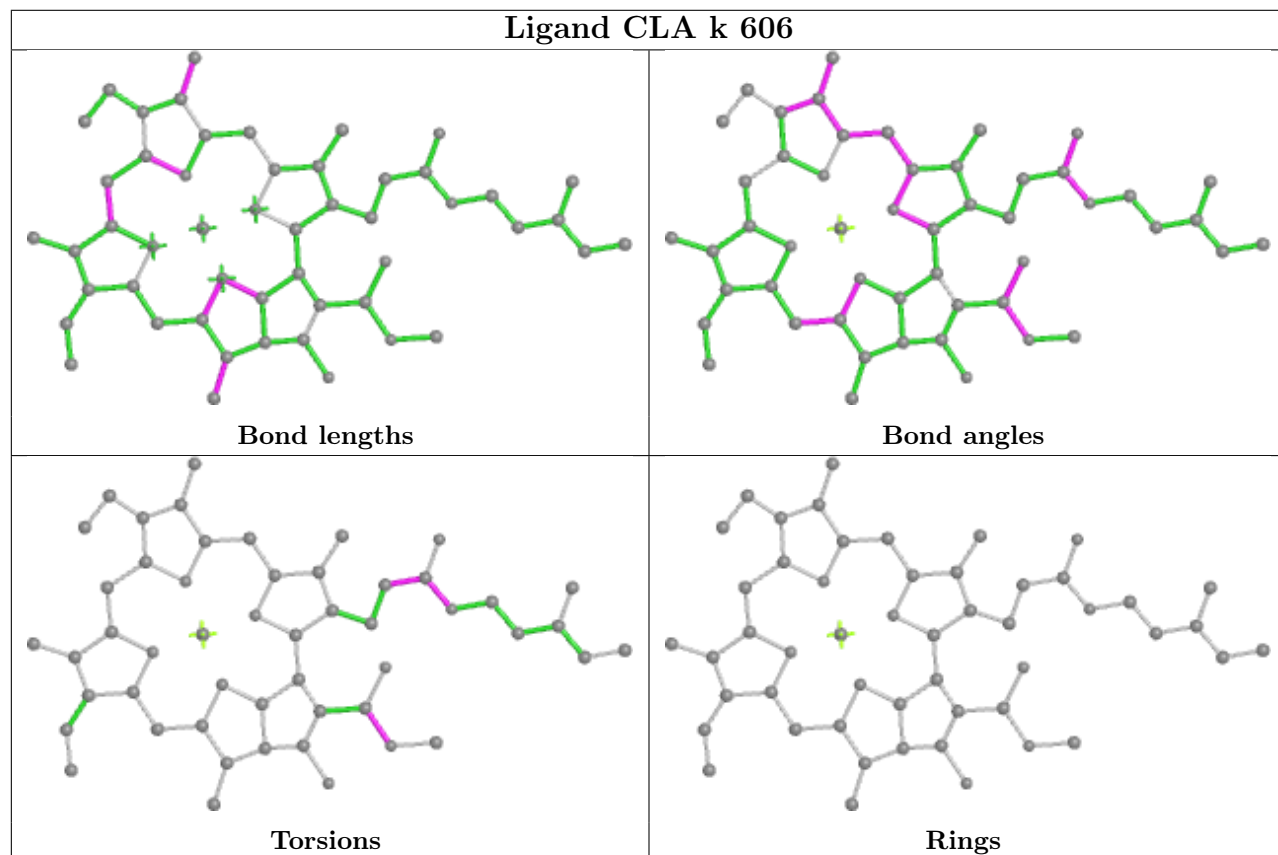


Ligand CLA B 817**Ligand CLA k 604****Ligand II0 b 315**

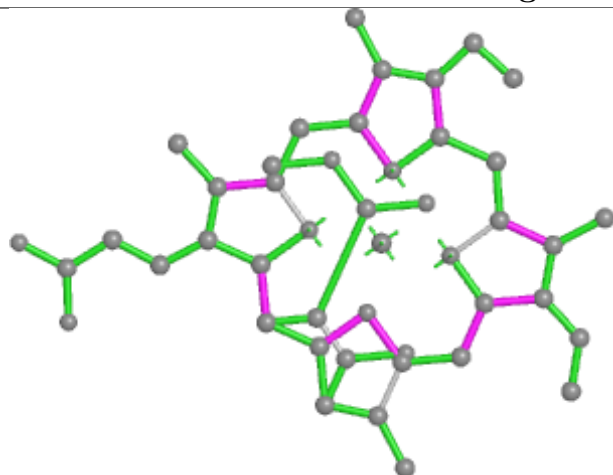
Ligand CLA A 822



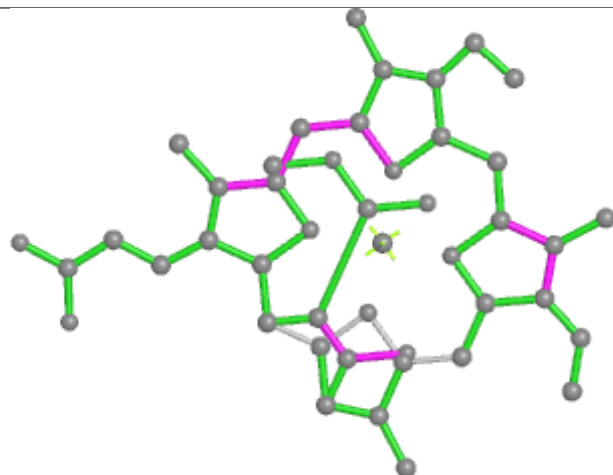
Ligand CLA k 606



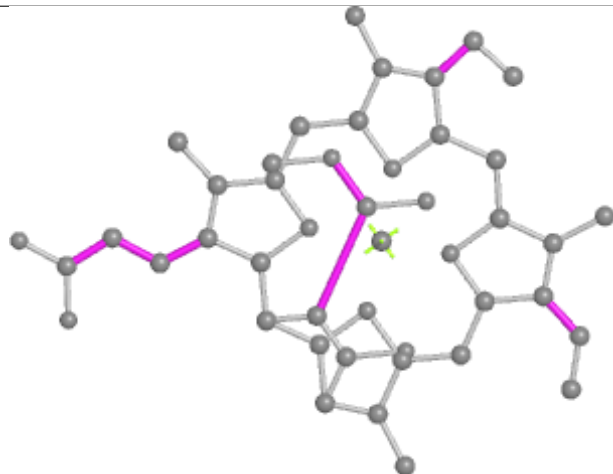
Ligand KC2 n 611



Bond lengths



Bond angles

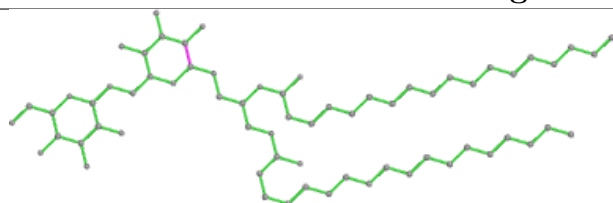


Torsions

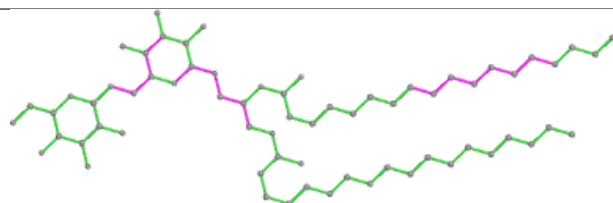


Rings

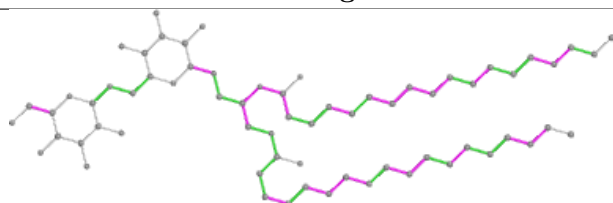
Ligand DGD B 844



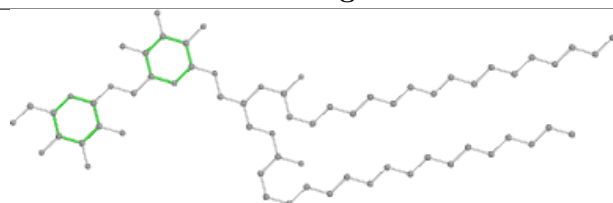
Bond lengths



Bond angles

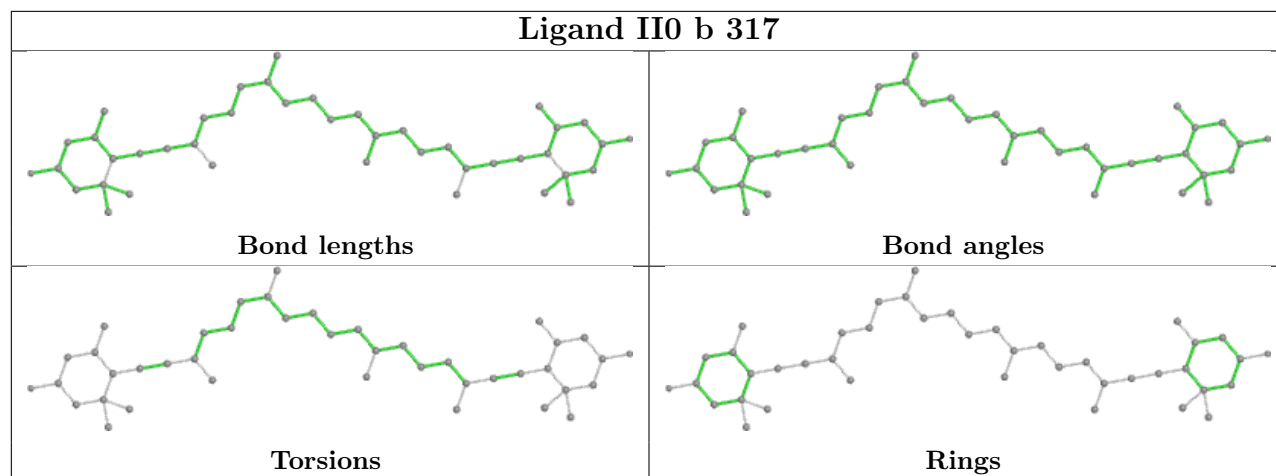


Torsions

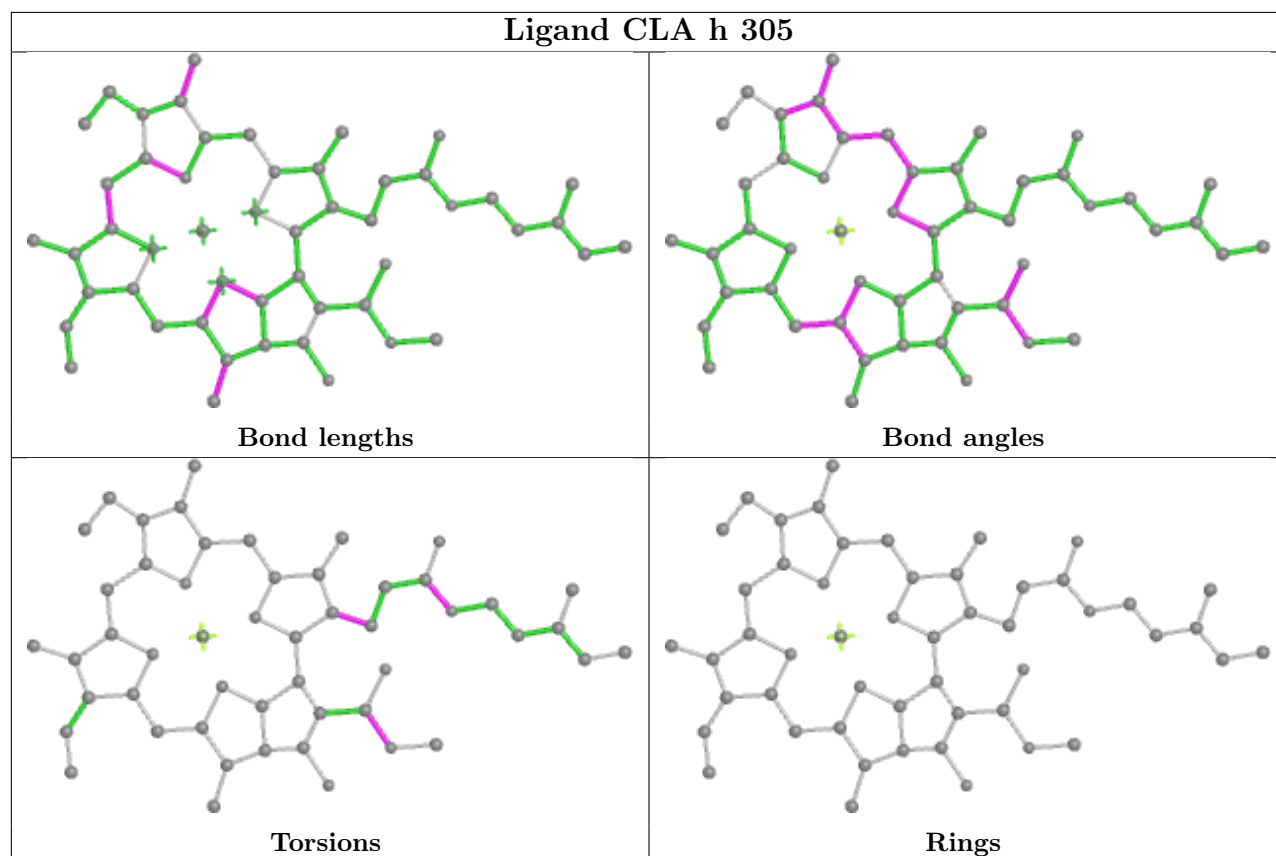


Rings

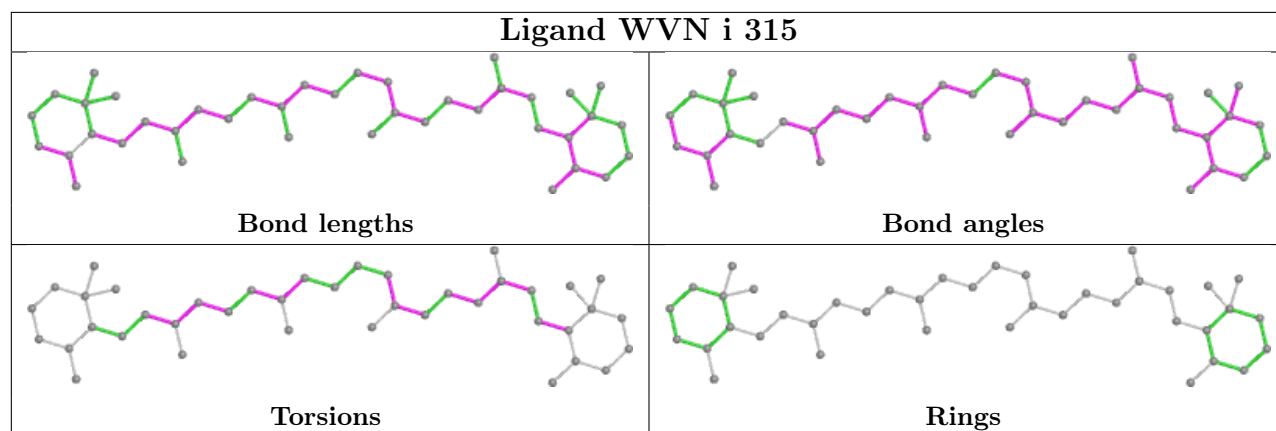
Ligand II0 b 317

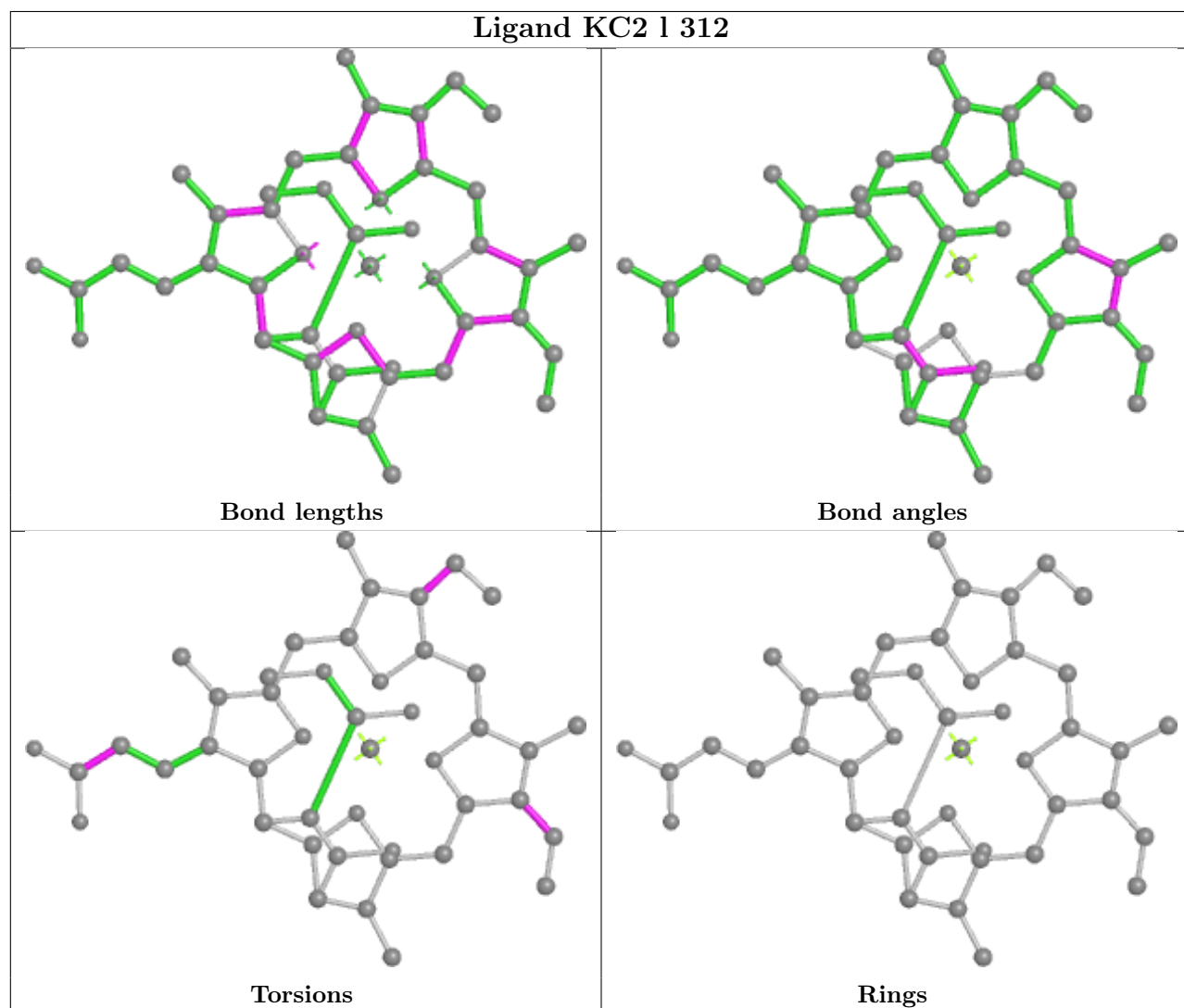
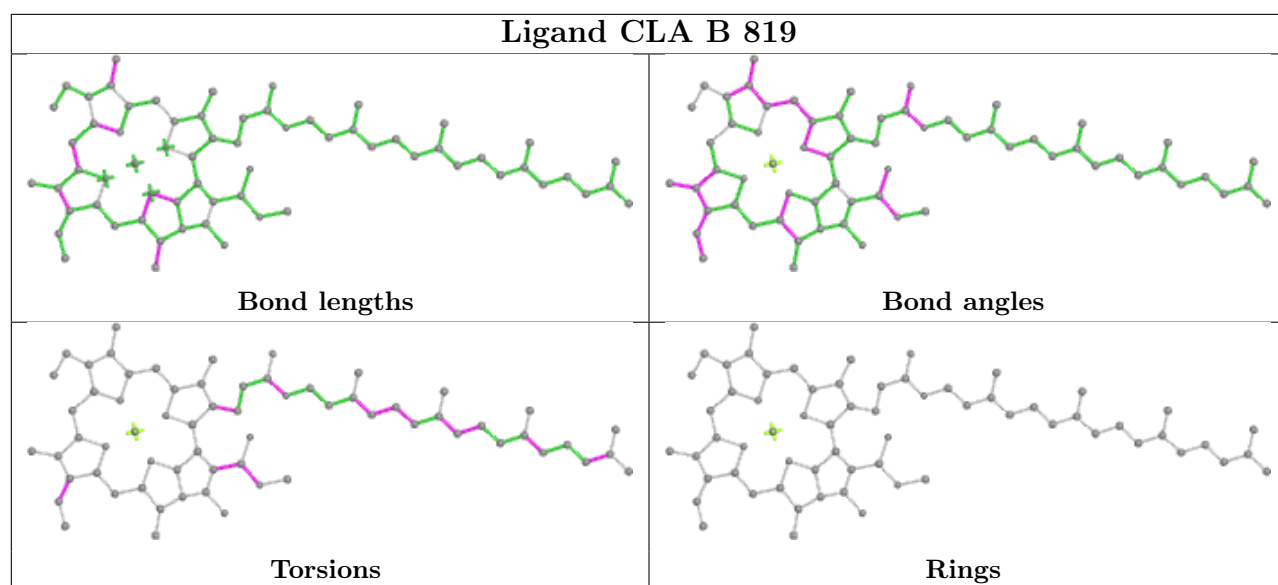


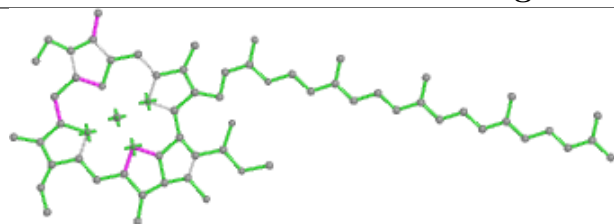
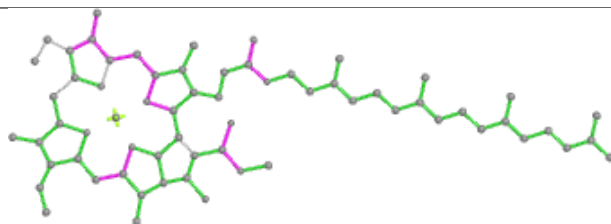
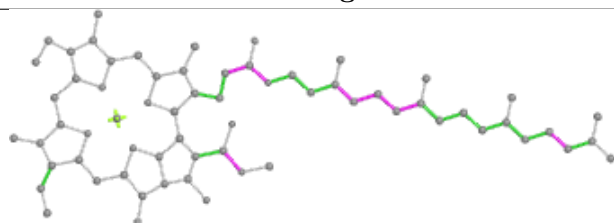
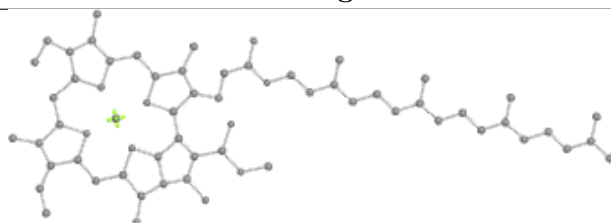
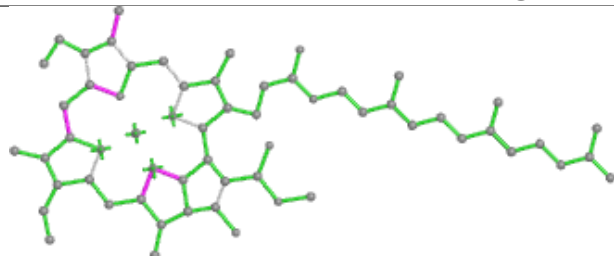
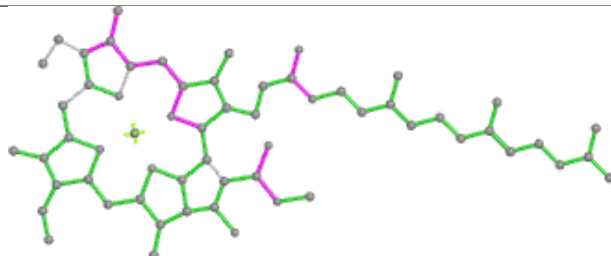
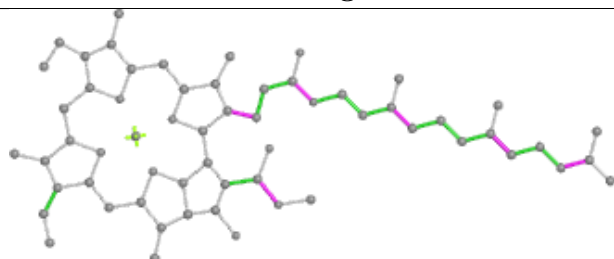
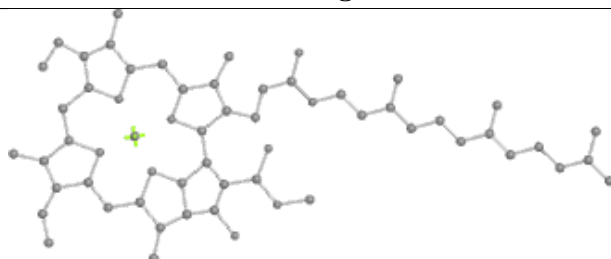
Ligand CLA h 305



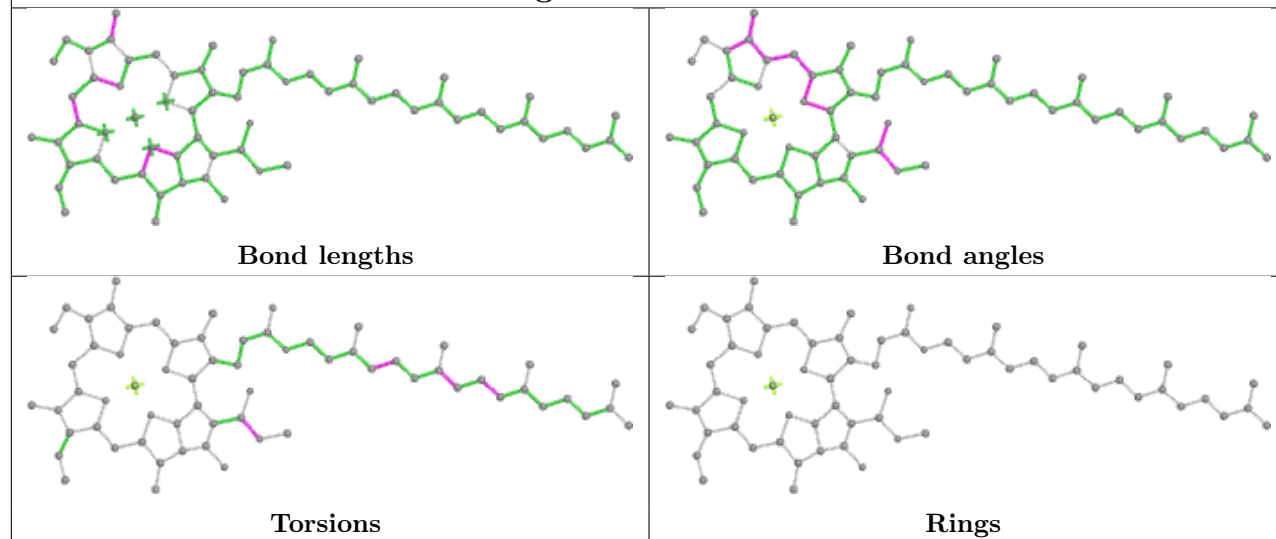
Ligand WVN i 315



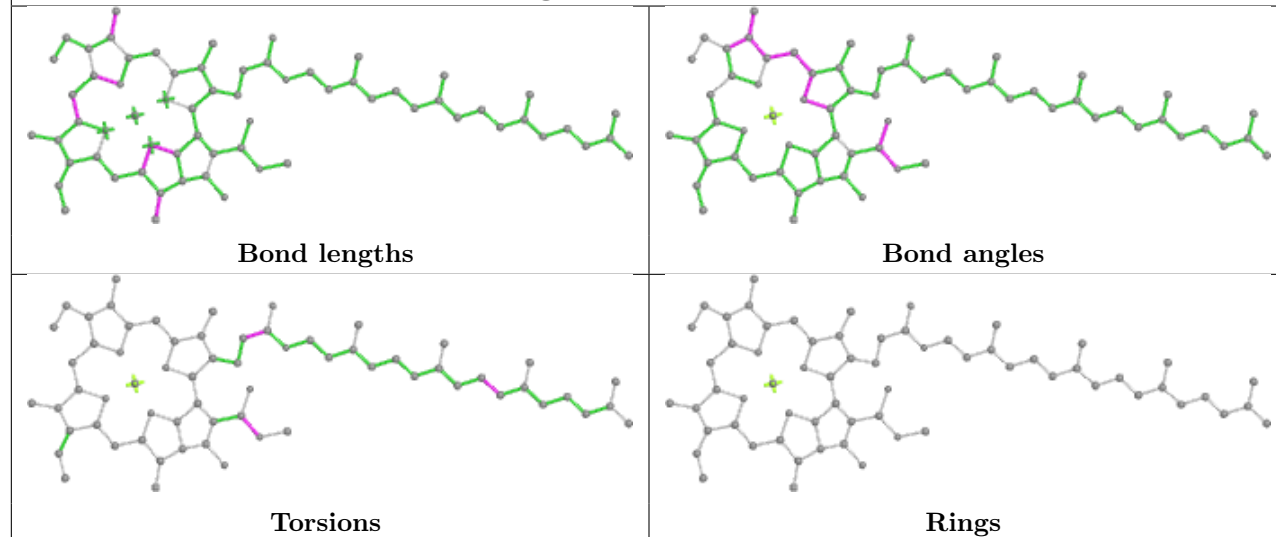


Ligand CLA B 806**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA m 609****Bond lengths****Bond angles****Torsions****Rings**

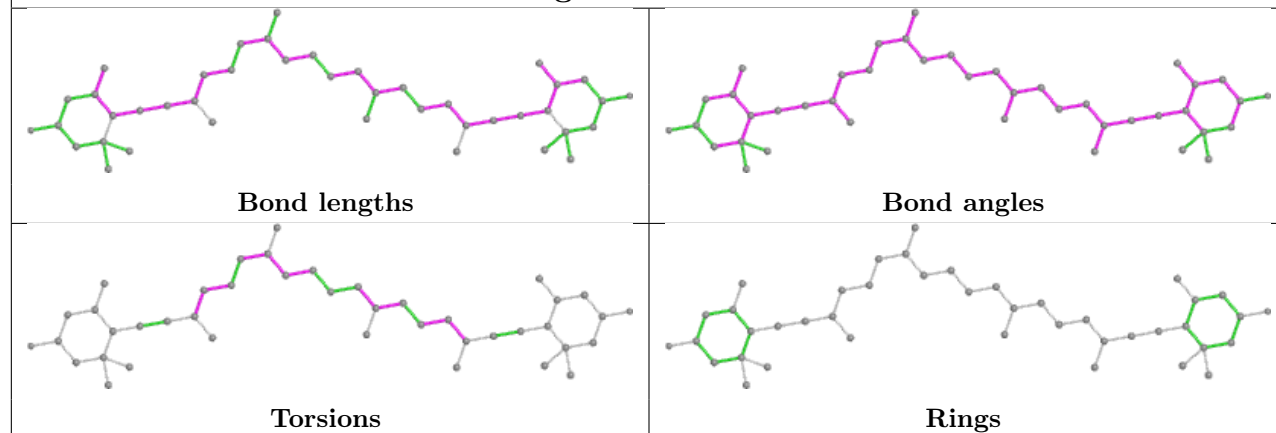
Ligand CLA b 309



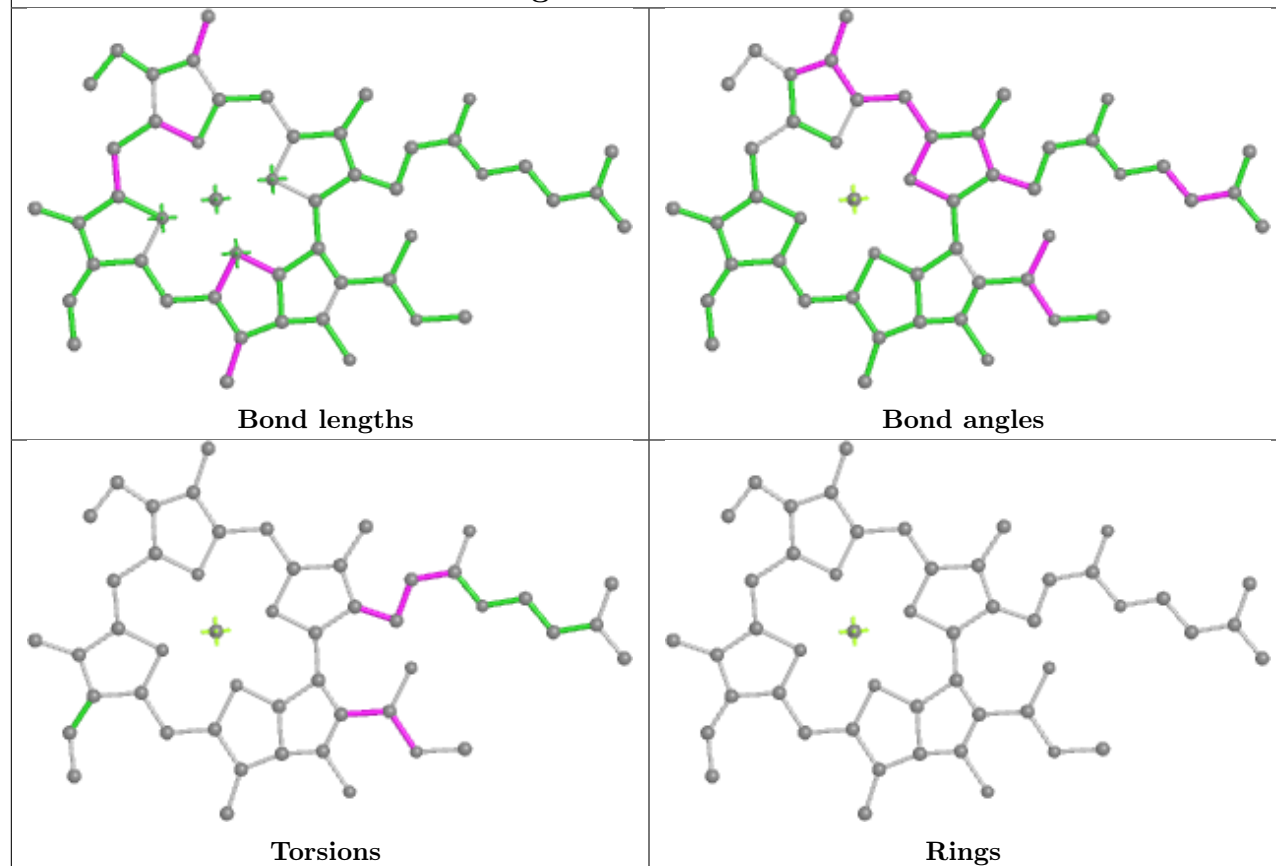
Ligand CLA c 305



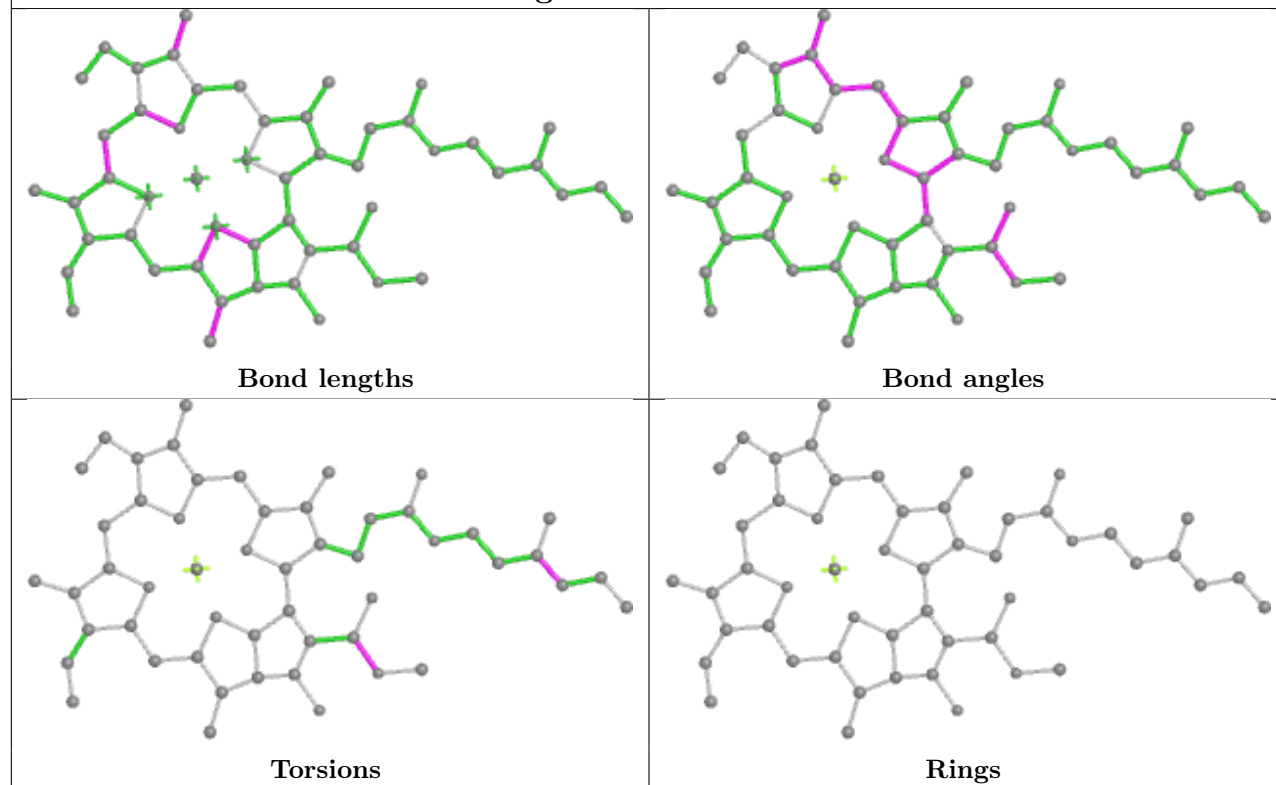
Ligand II0 i 319



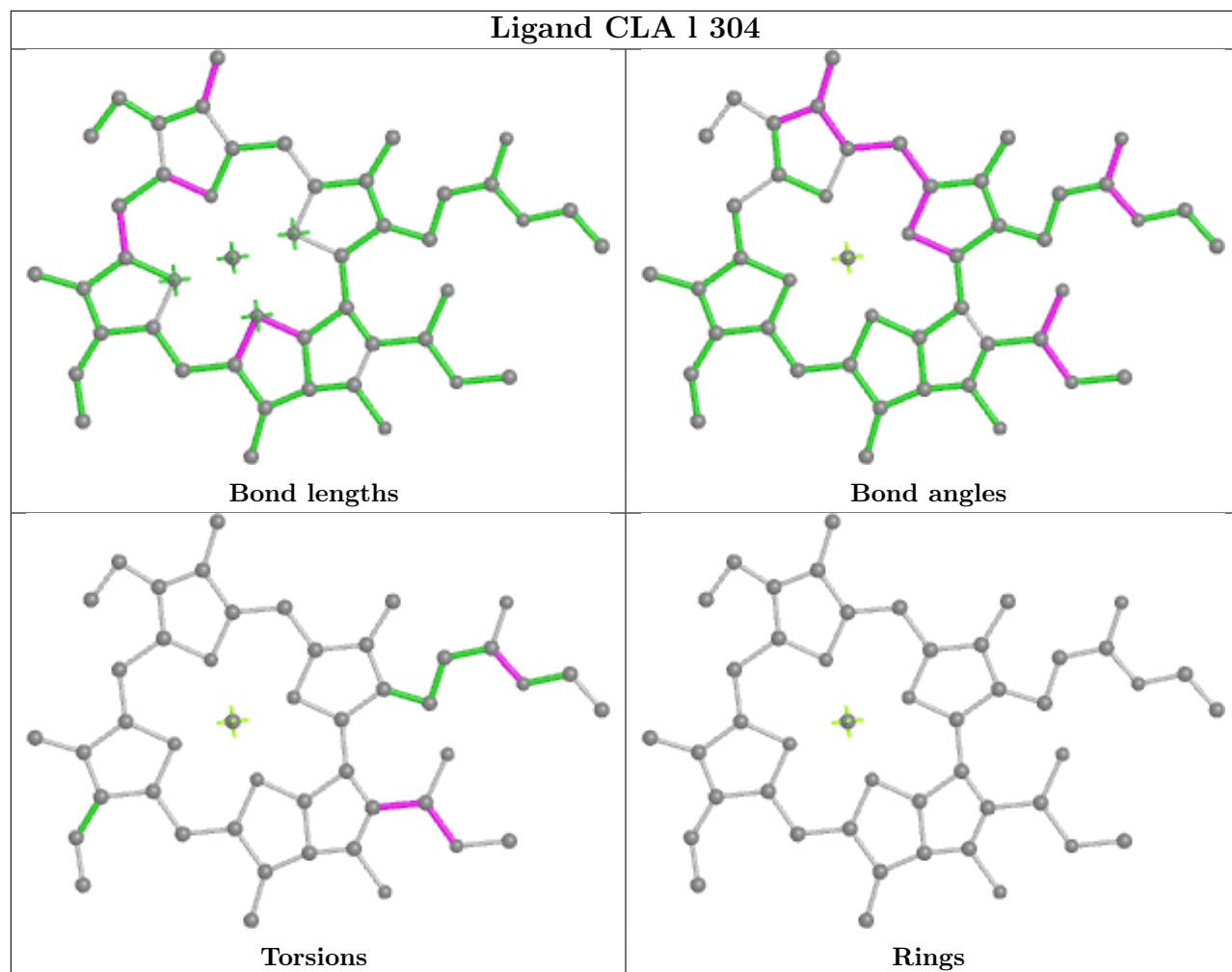
Ligand CLA A 814

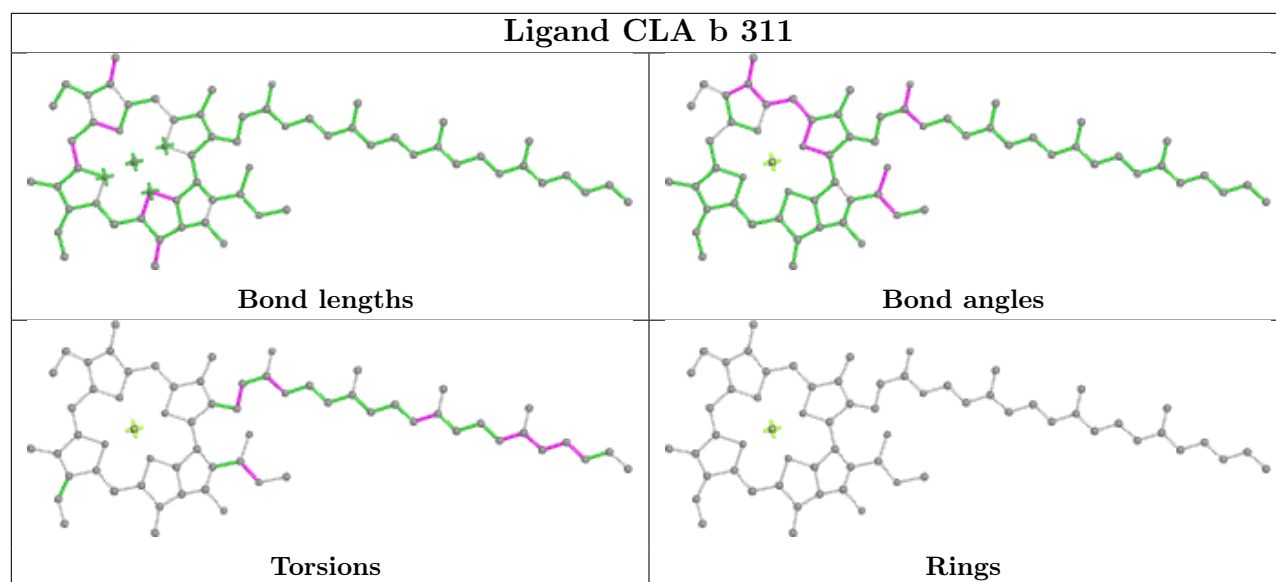
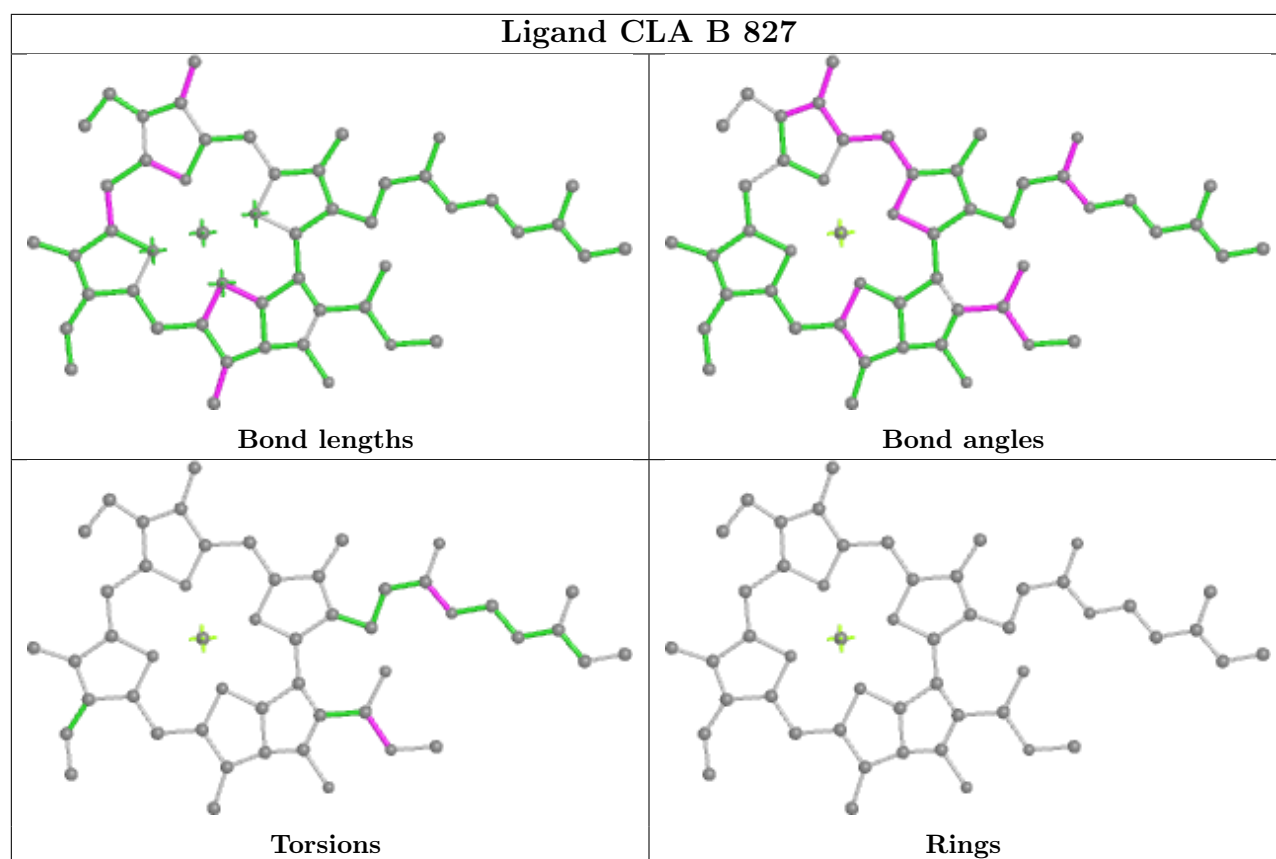


Ligand CLA b 305

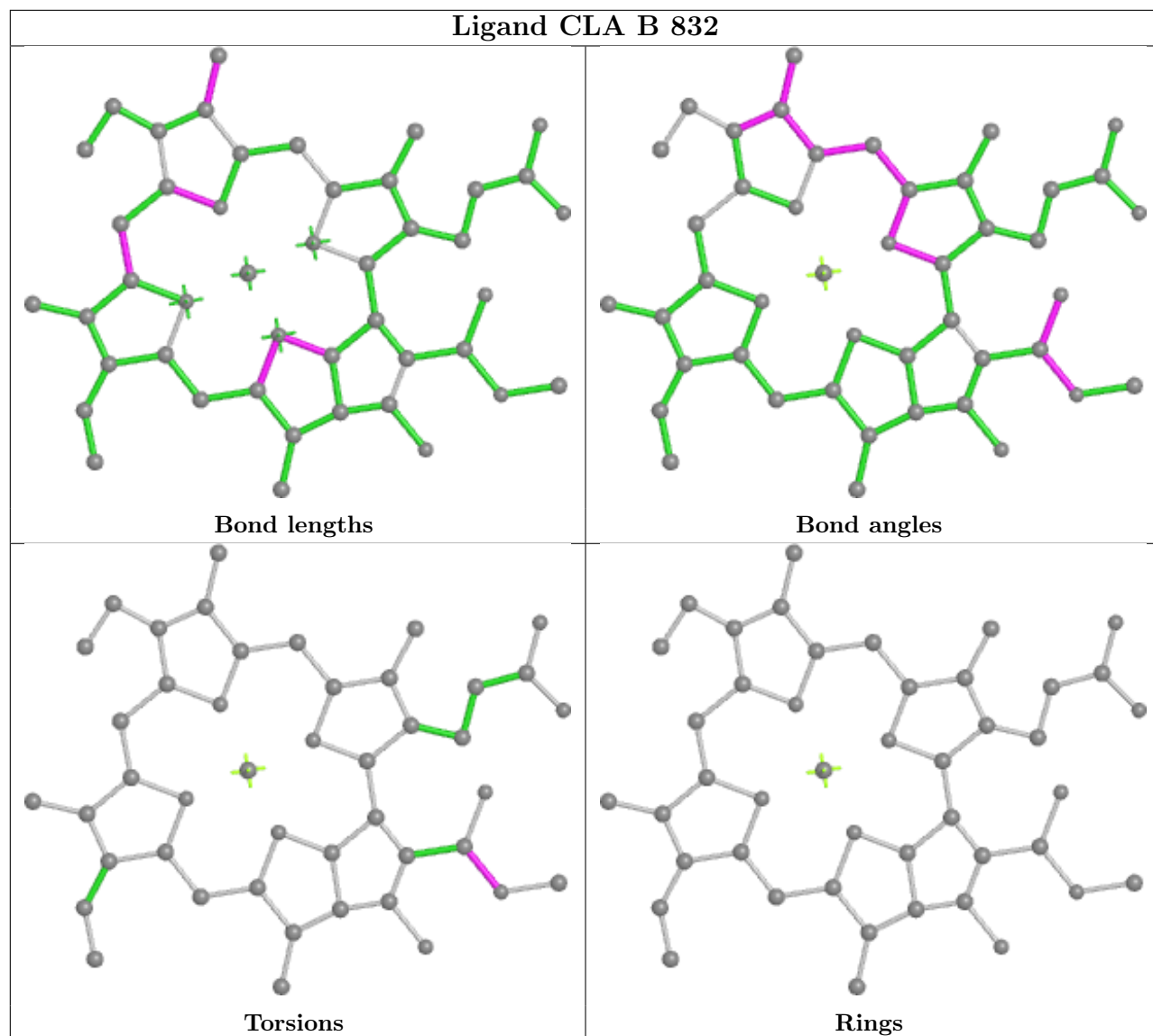


Ligand CLA 1 304

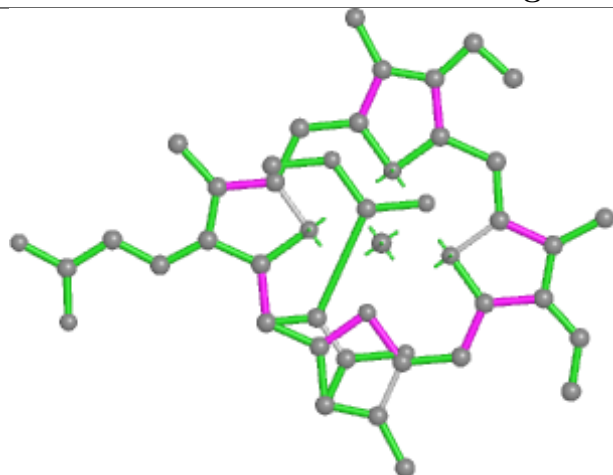




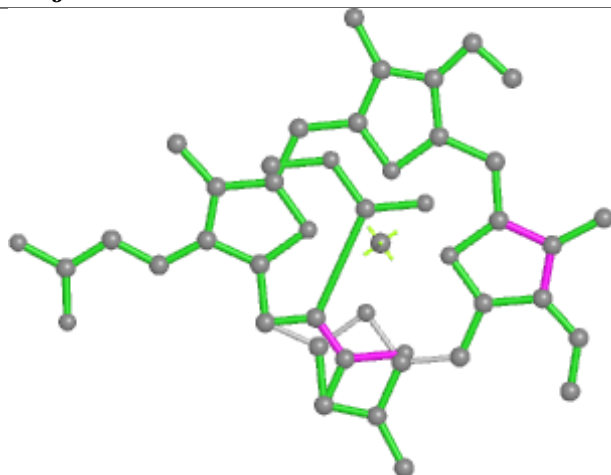
Ligand CLA B 832



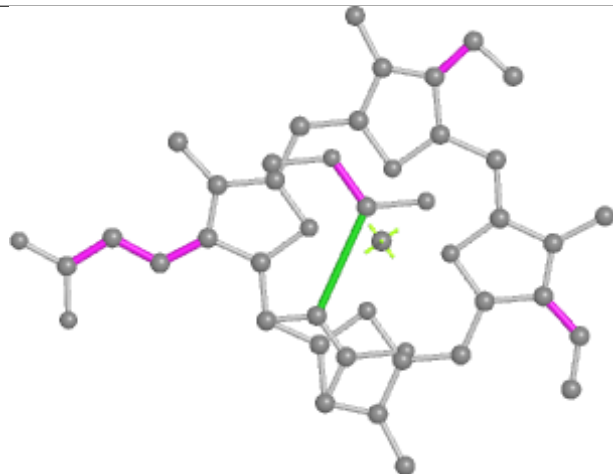
Ligand KC2 j 611



Bond lengths



Bond angles

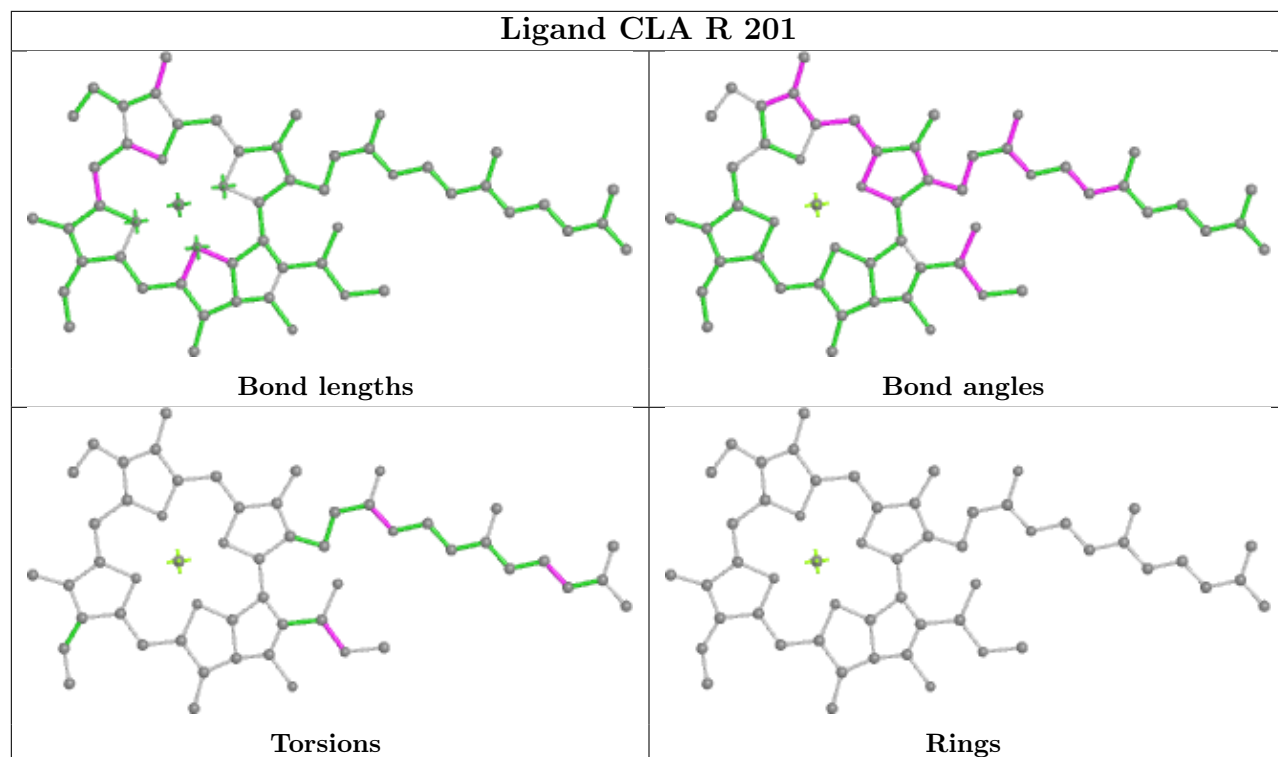


Torsions

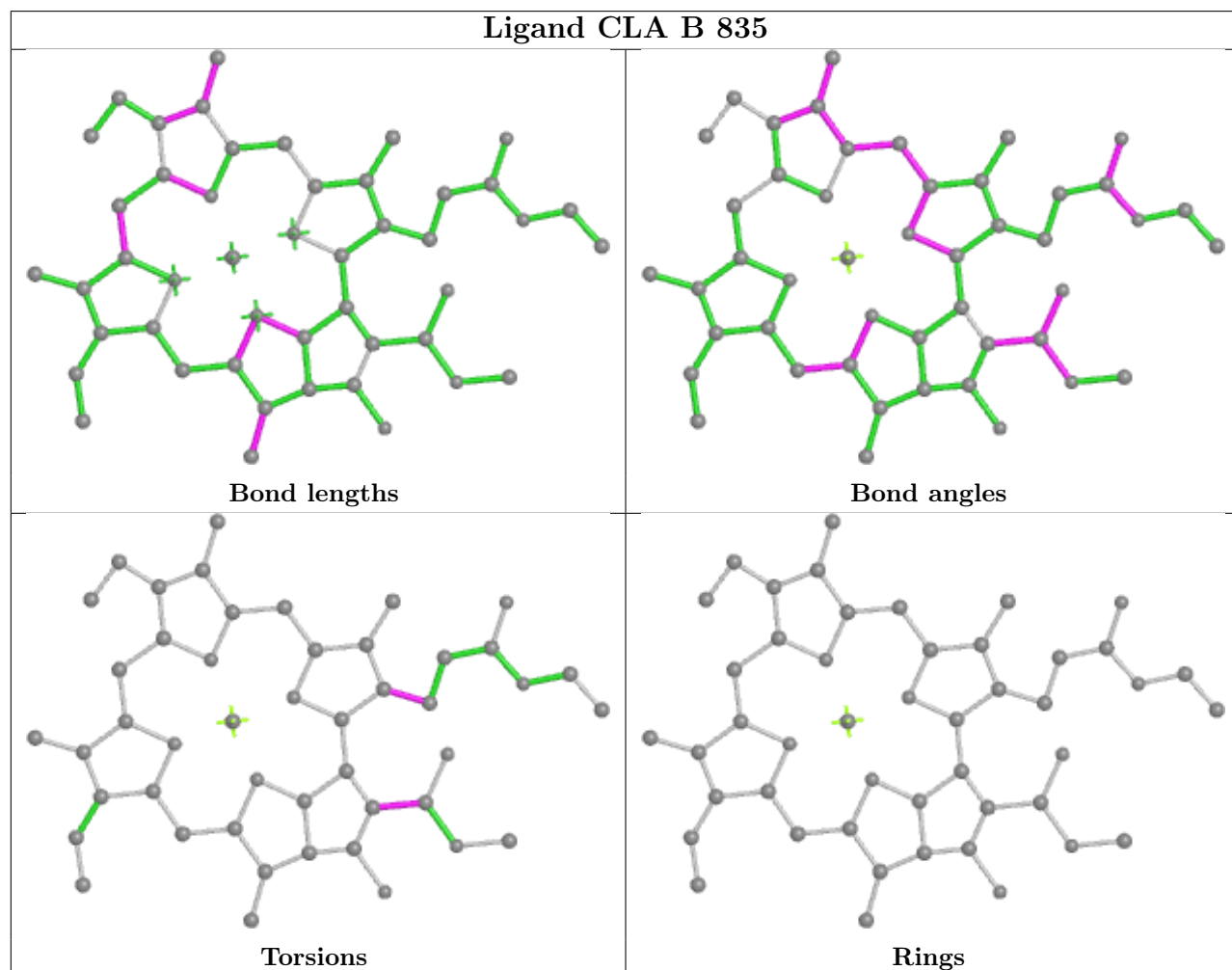


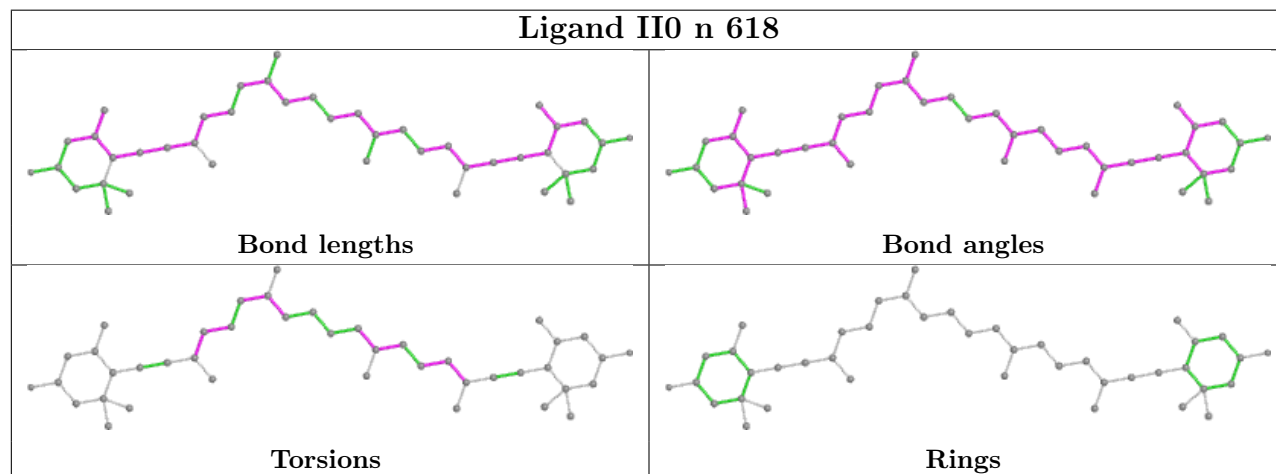
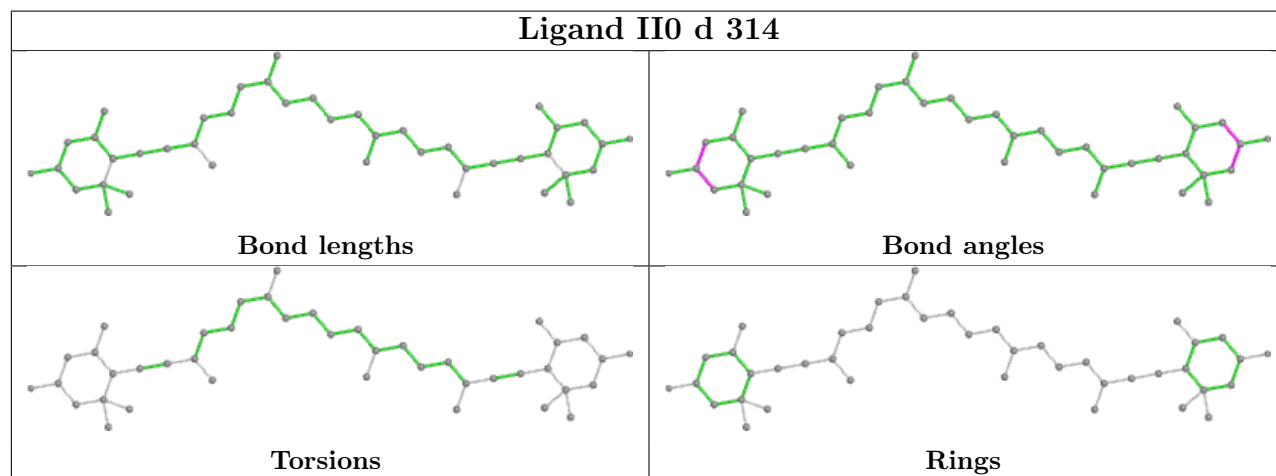
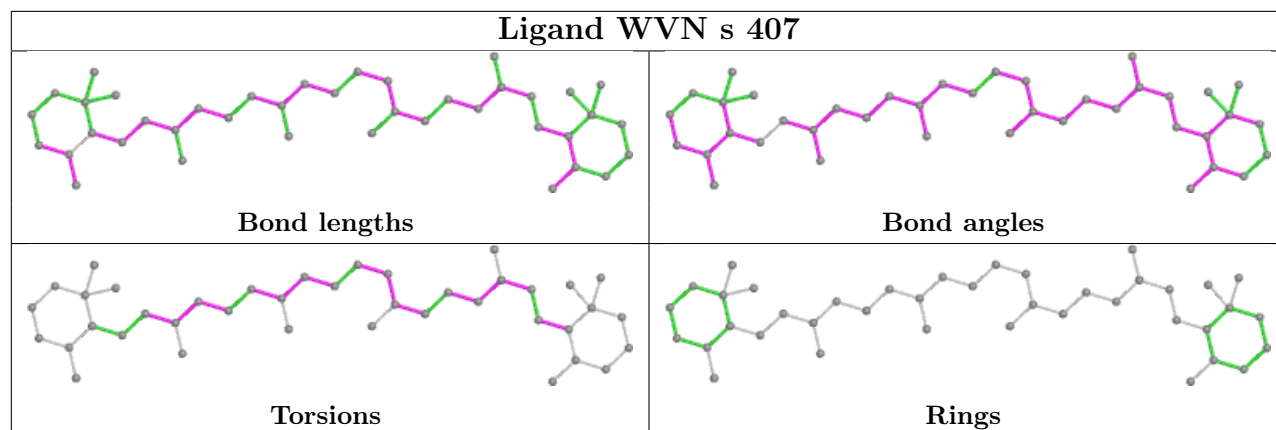
Rings

Ligand CLA R 201

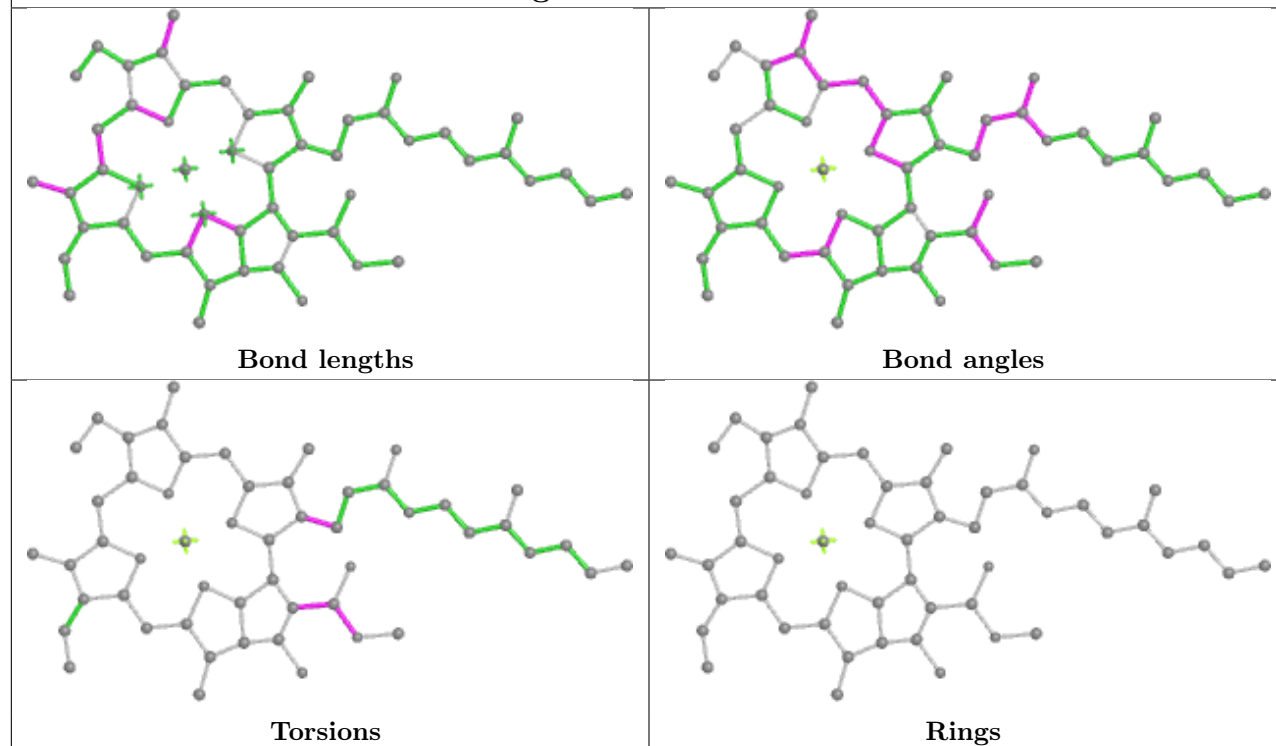


Ligand CLA B 835

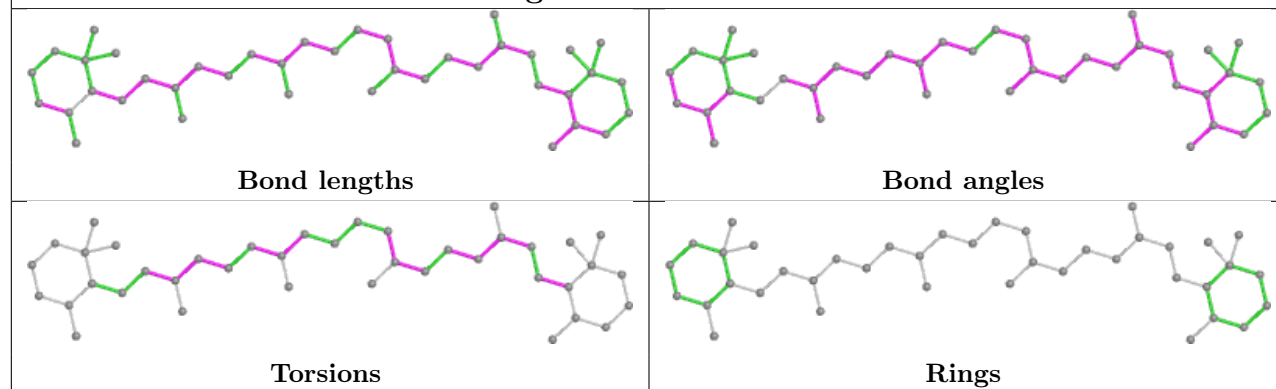




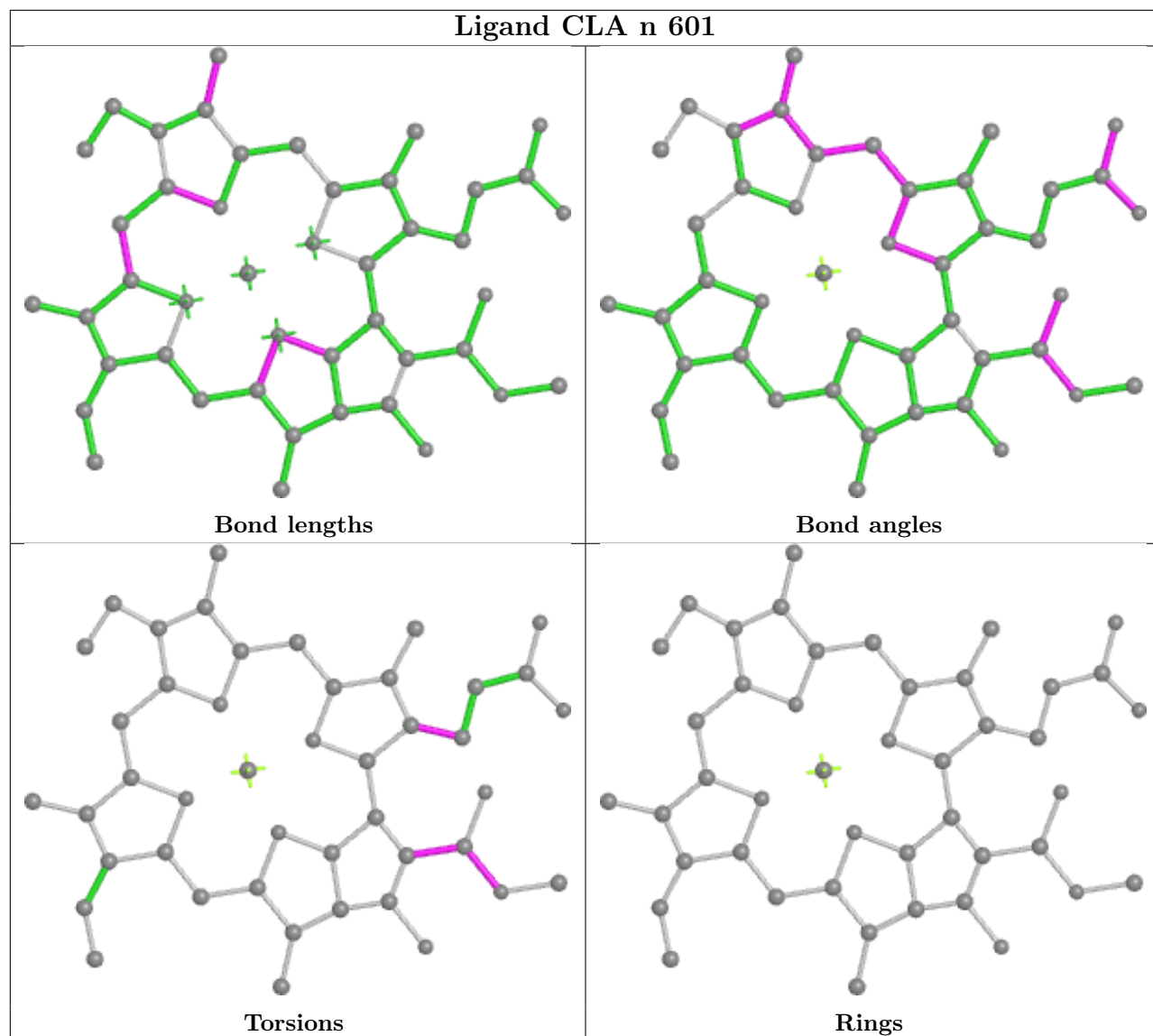
Ligand CLA B 821



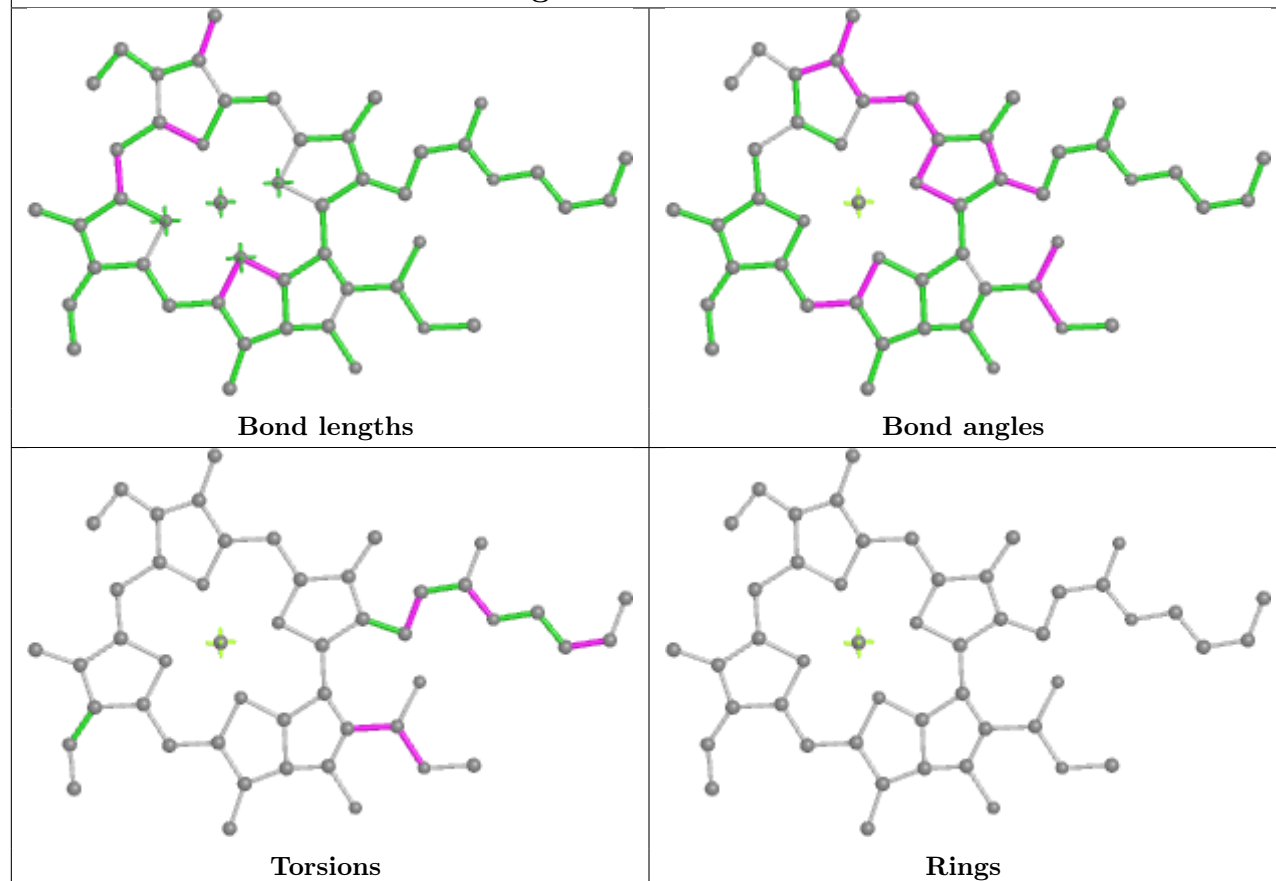
Ligand WVN L 205



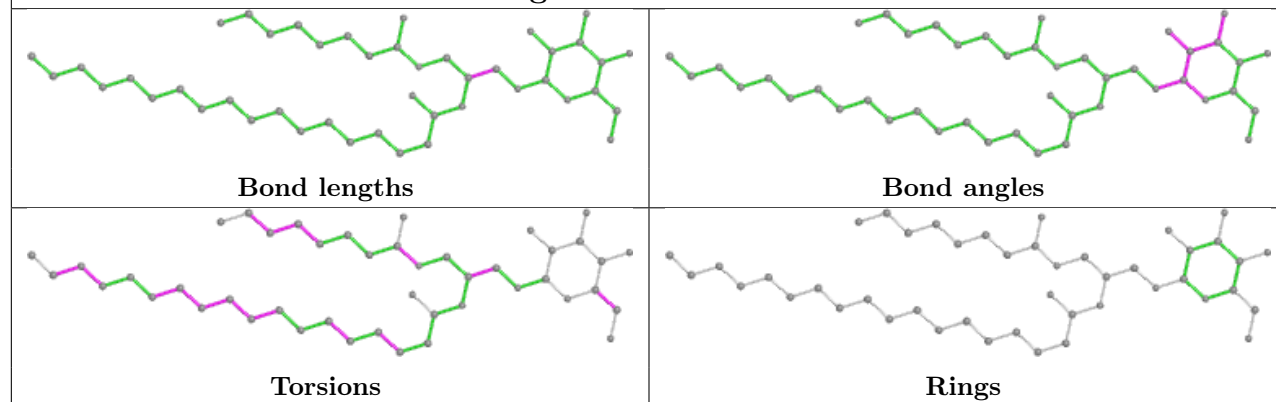
Ligand CLA n 601



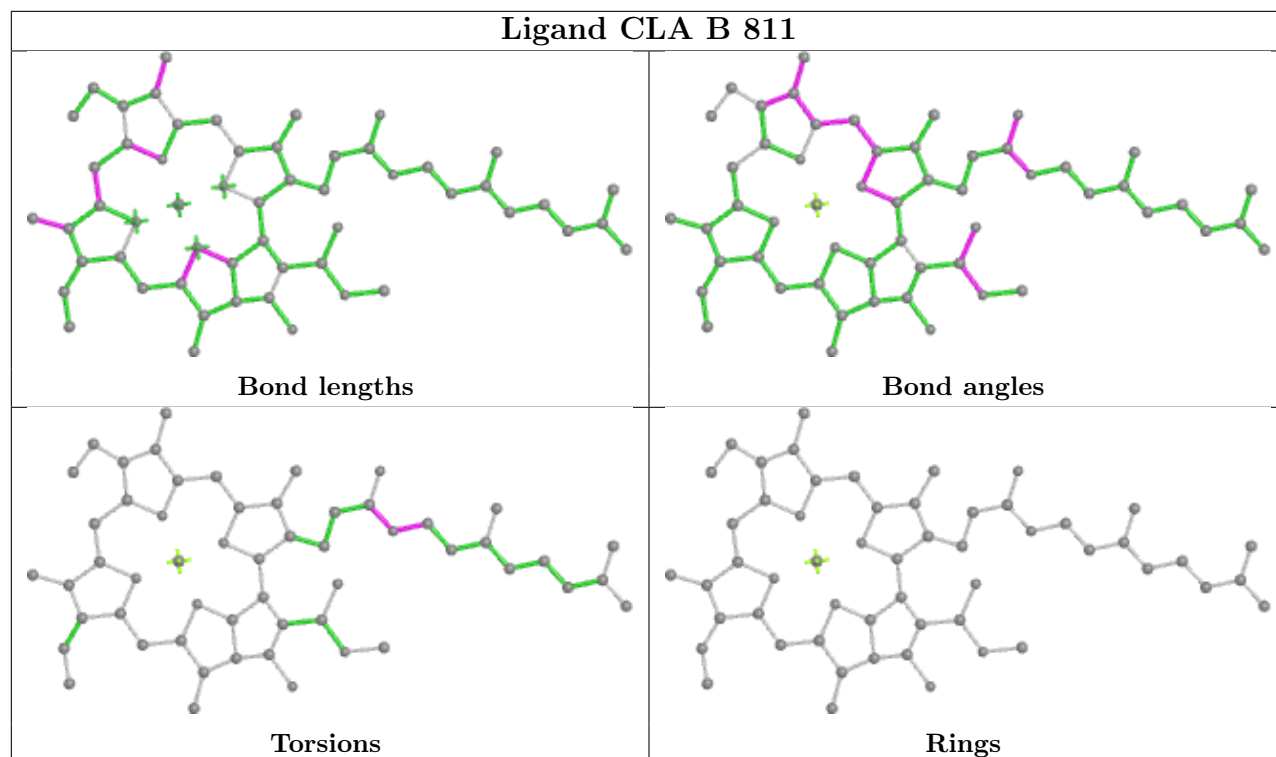
Ligand CLA A 821



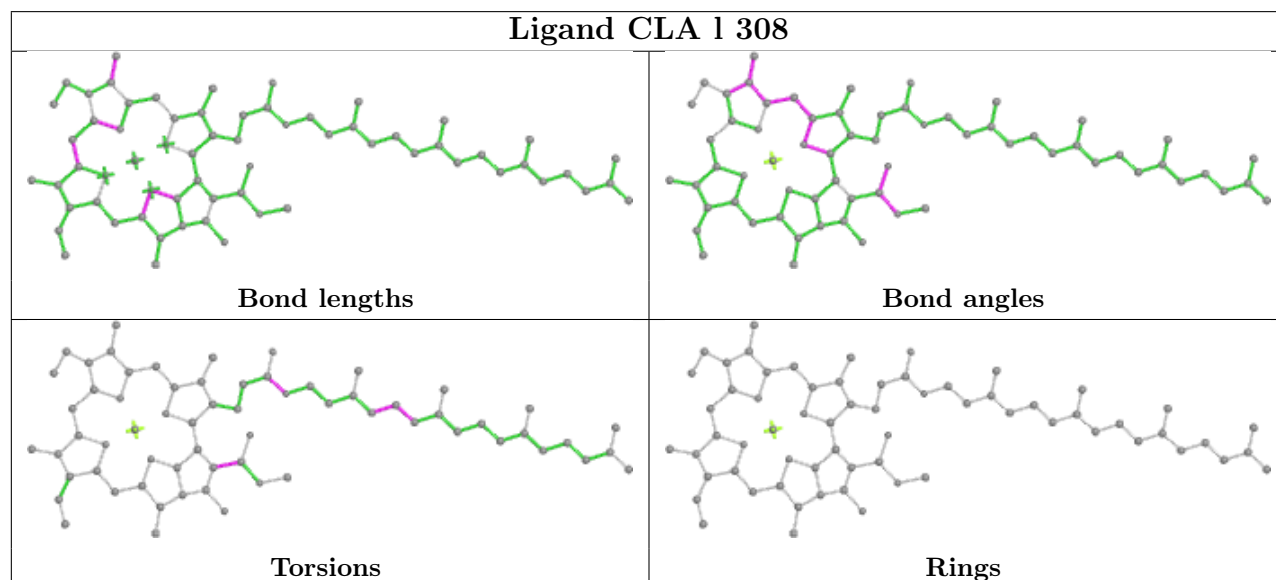
Ligand LMG L 209



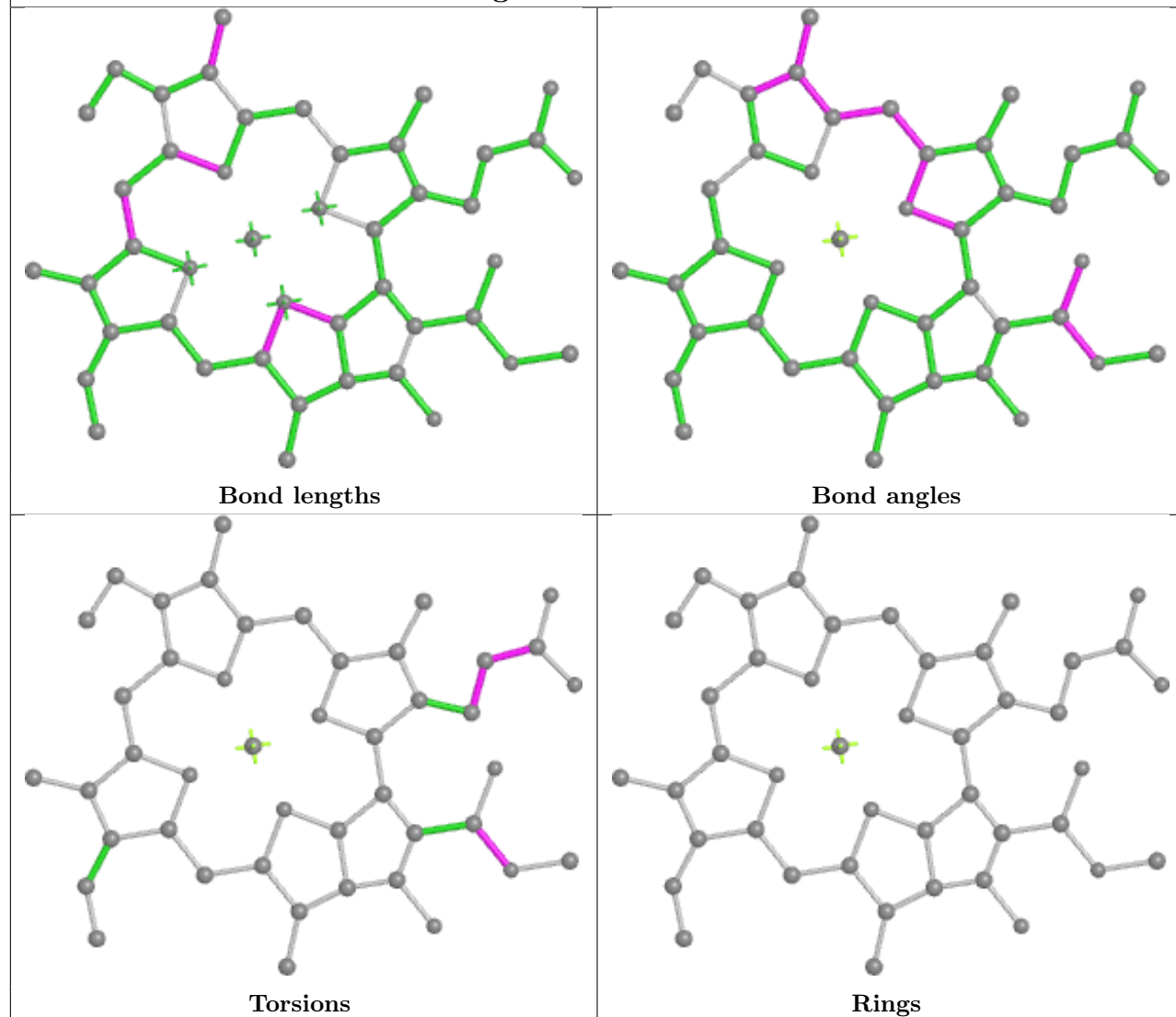
Ligand CLA B 811



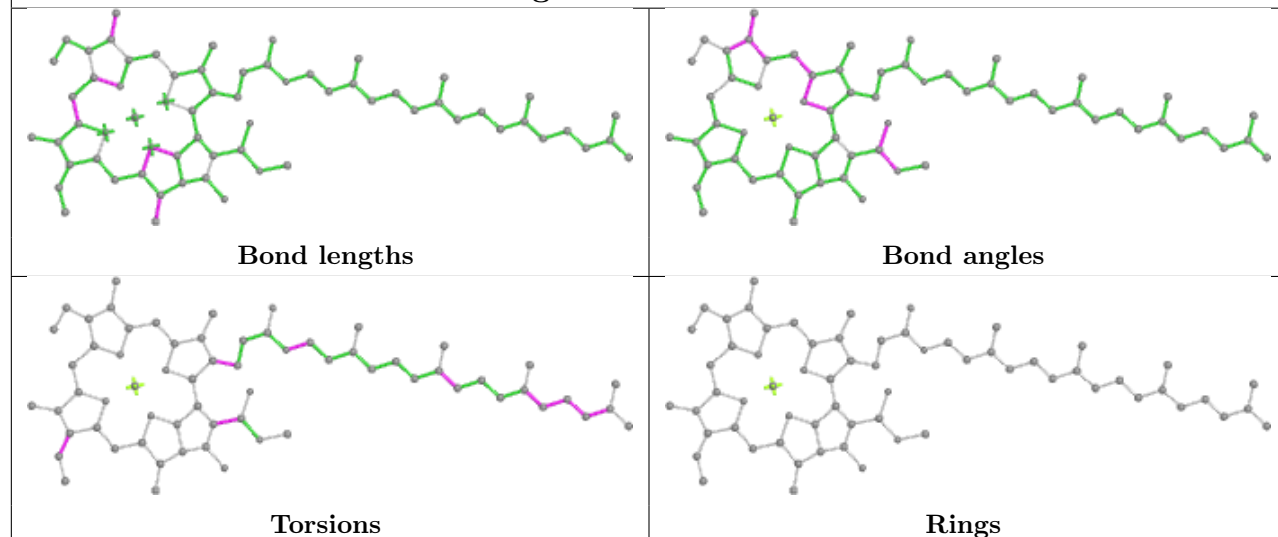
Ligand CLA I 308

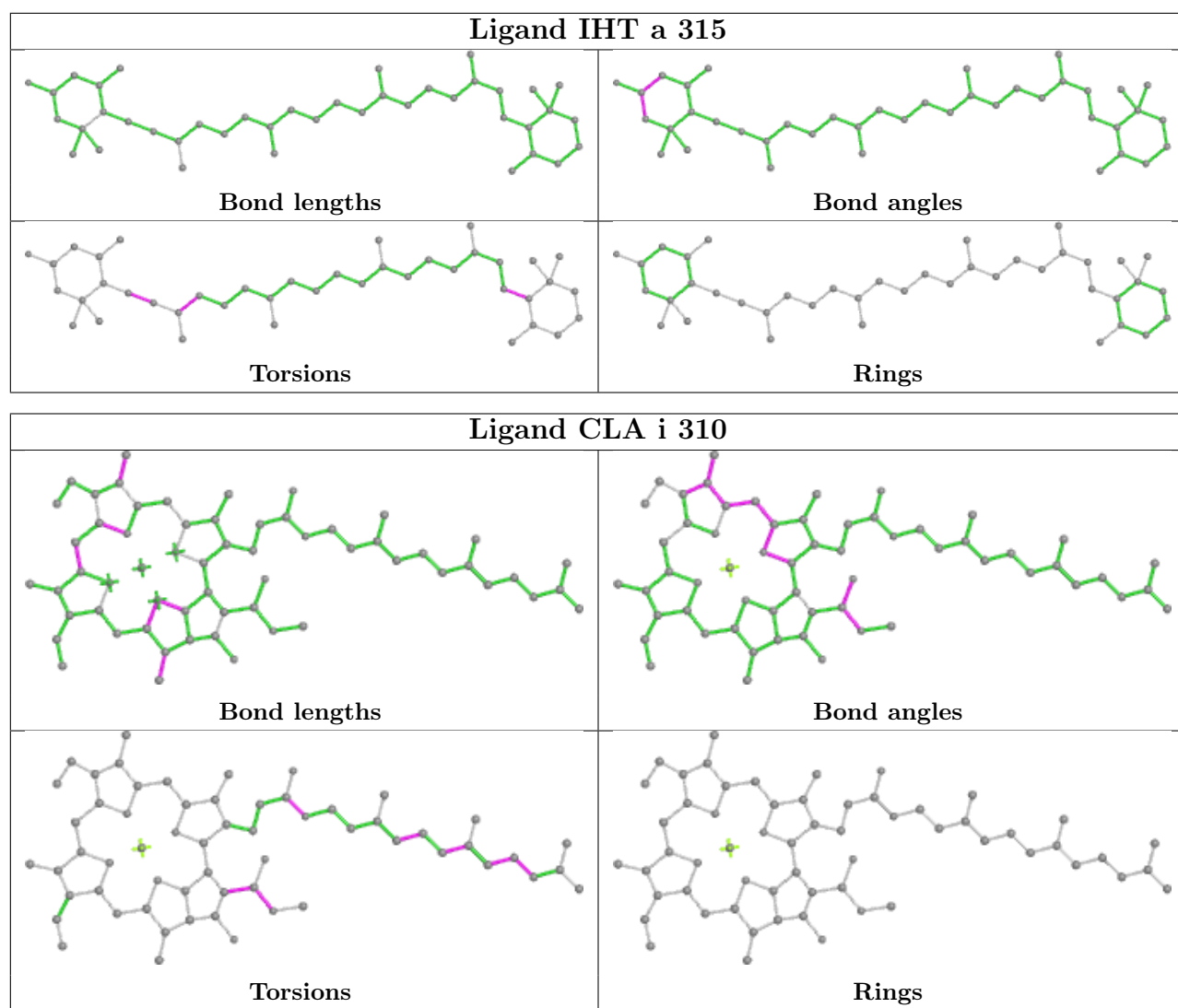


Ligand CLA d 318

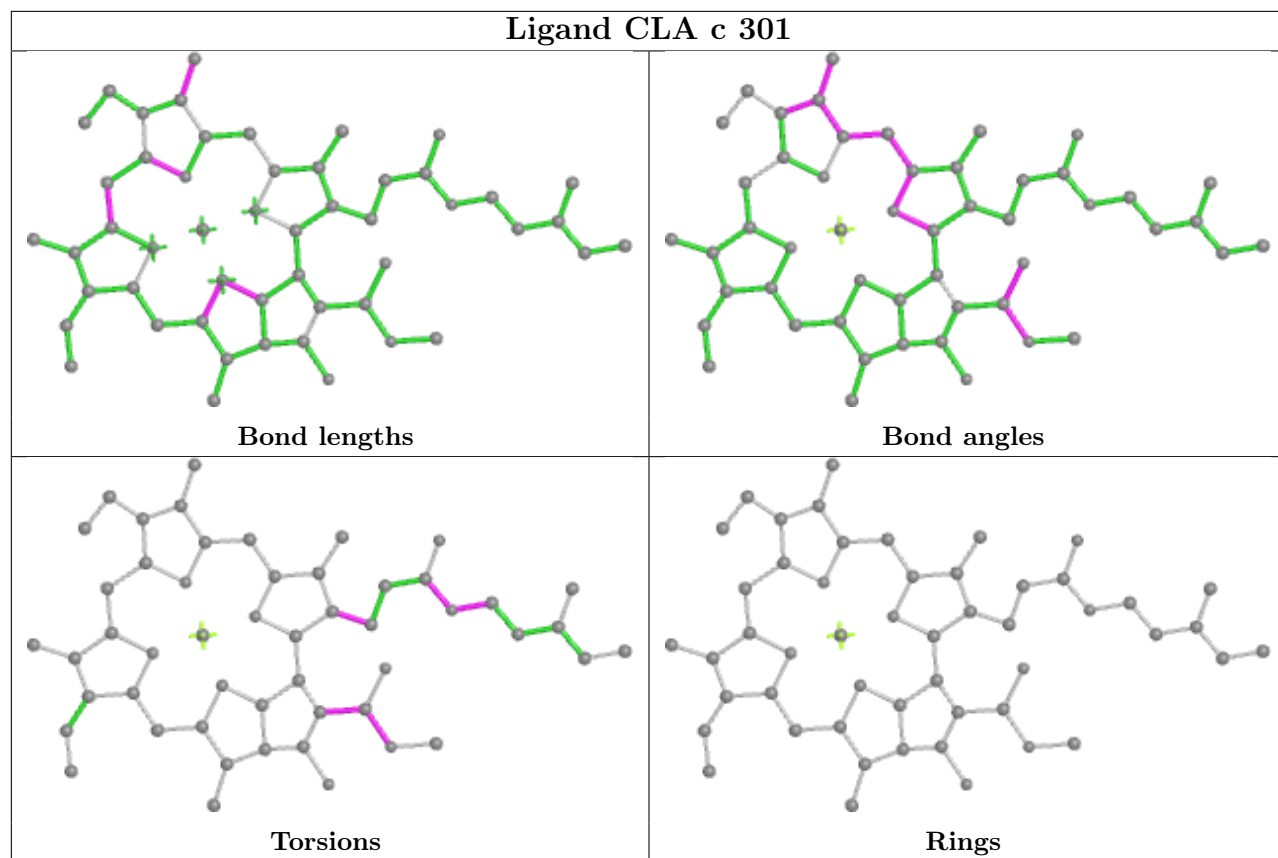


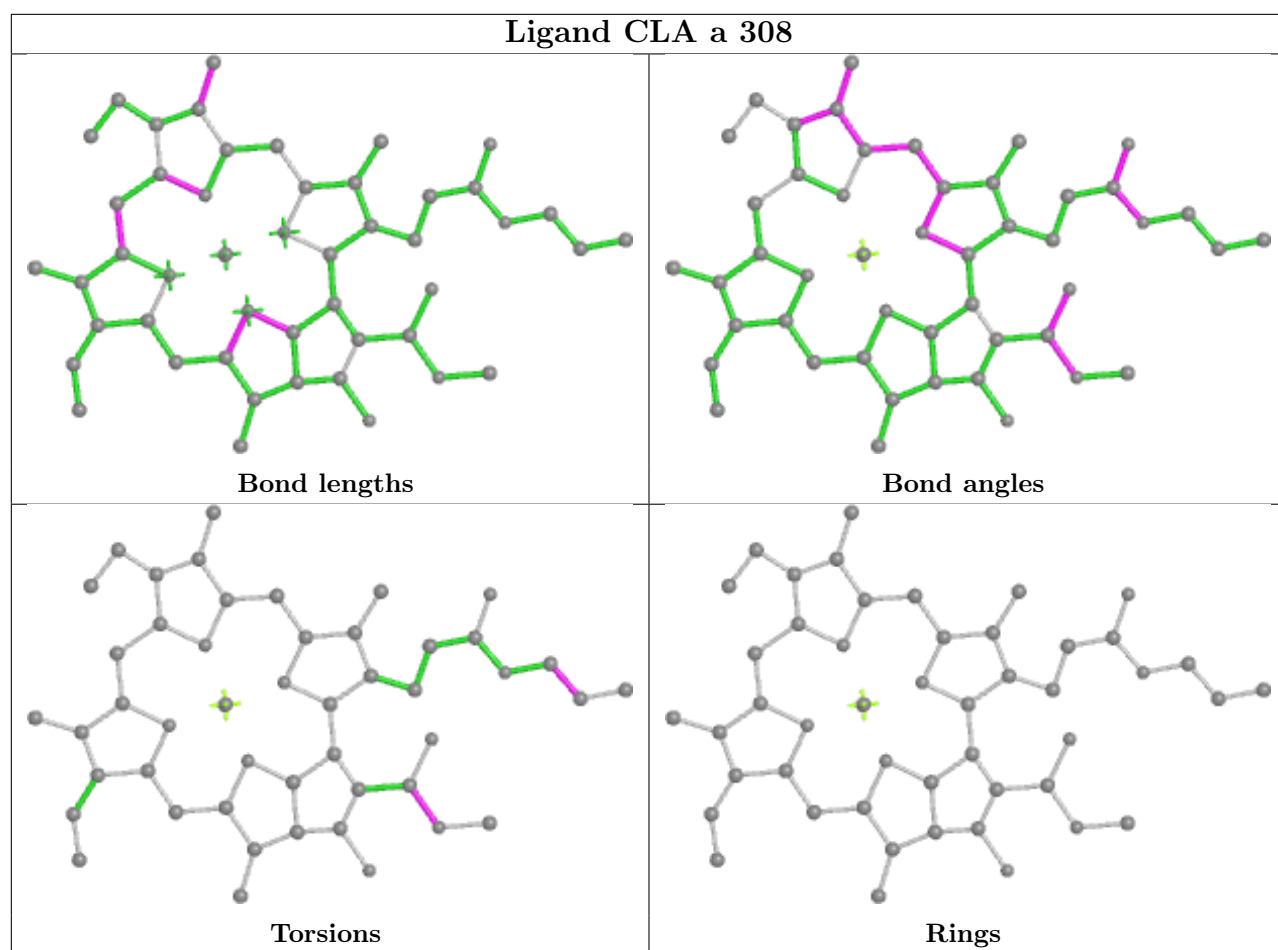
Ligand CLA B 837



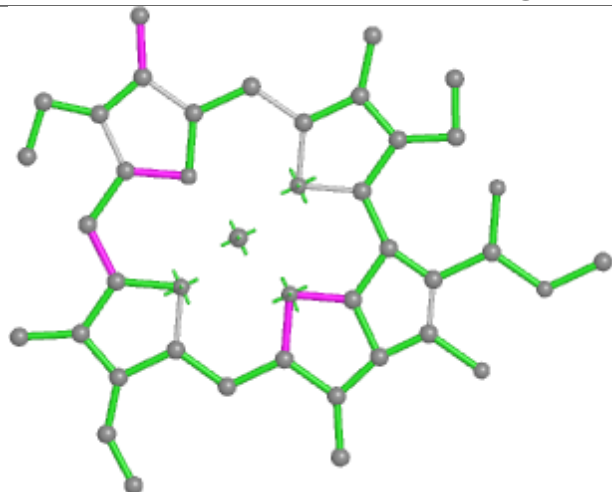


Ligand CLA c 301

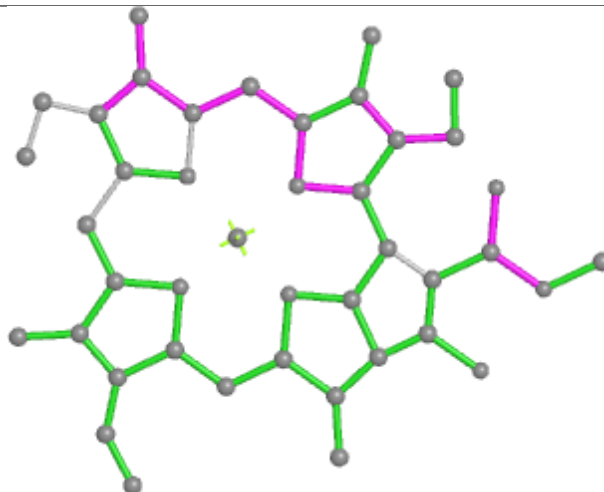




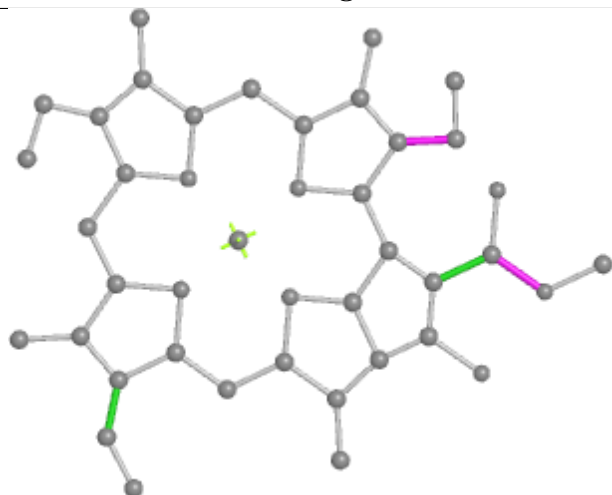
Ligand CLA J 103



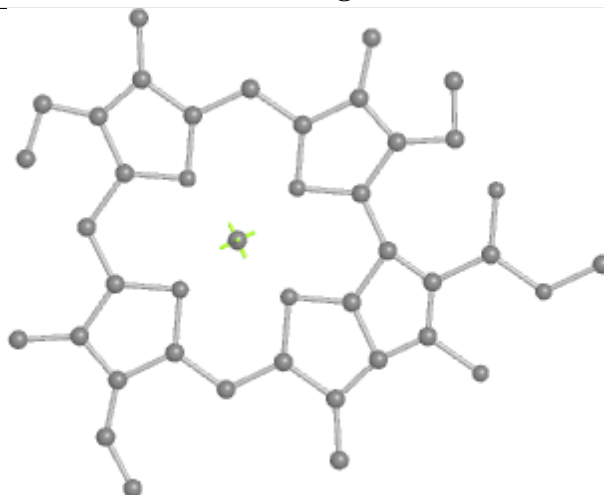
Bond lengths



Bond angles

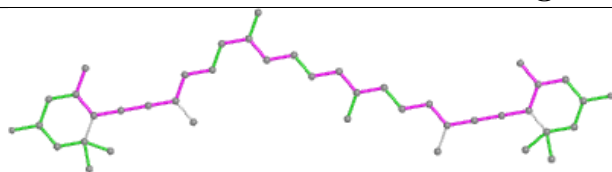


Torsions

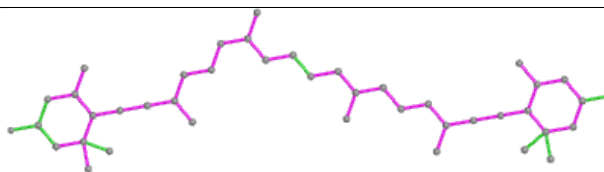


Rings

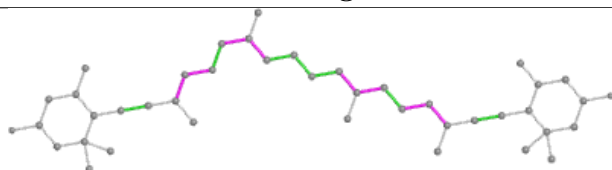
Ligand II0 1 302



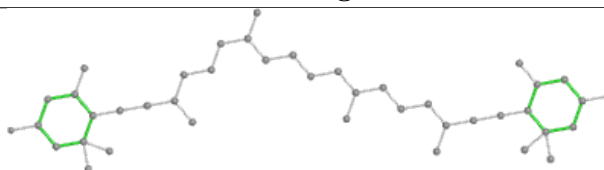
Bond lengths



Bond angles

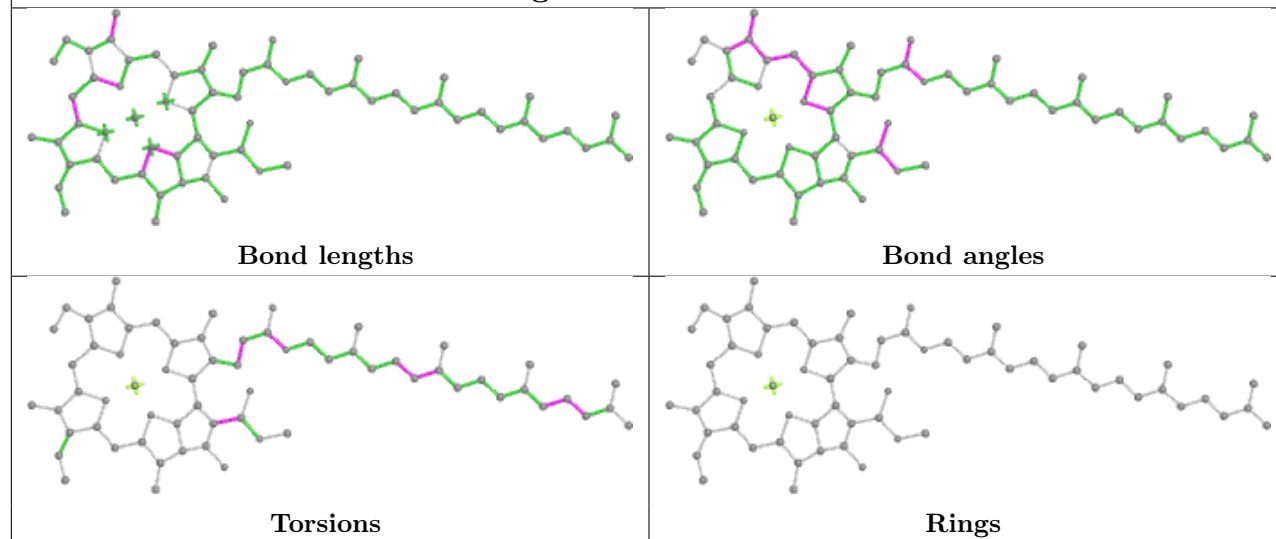


Torsions

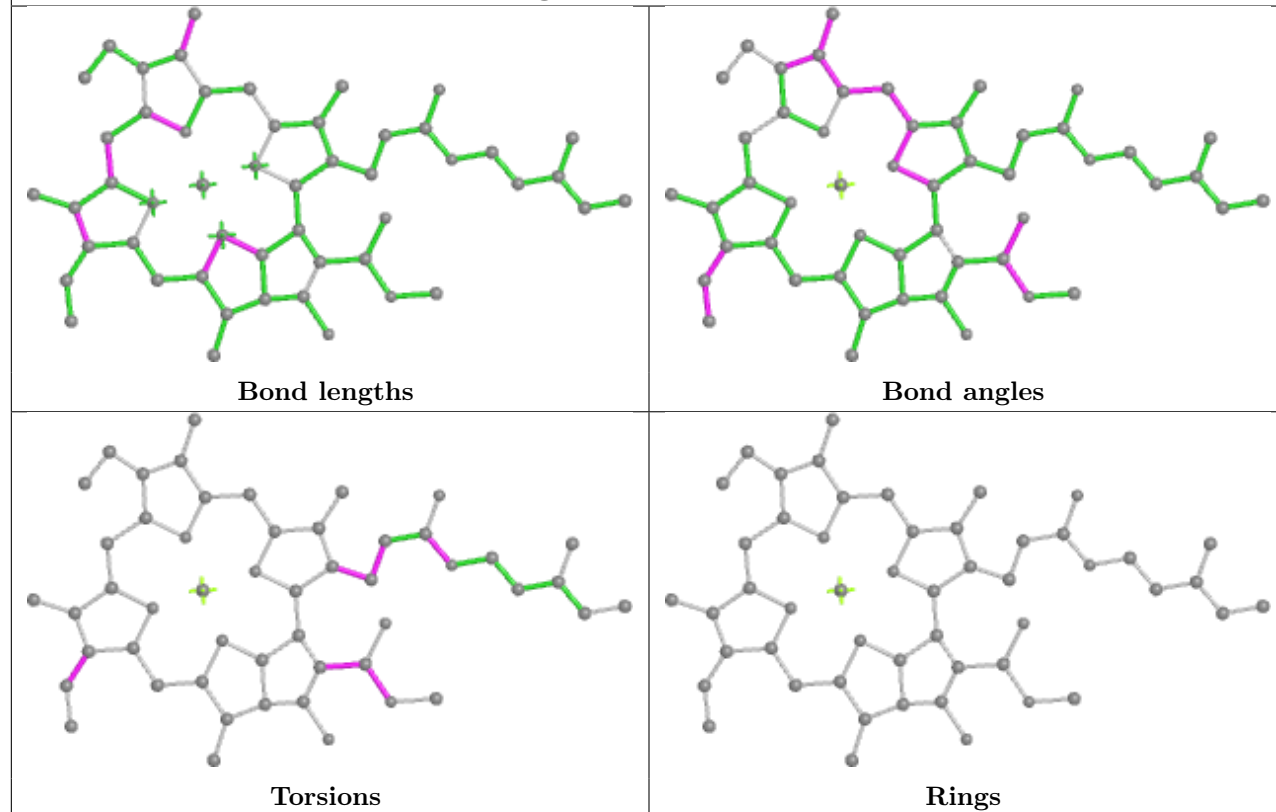


Rings

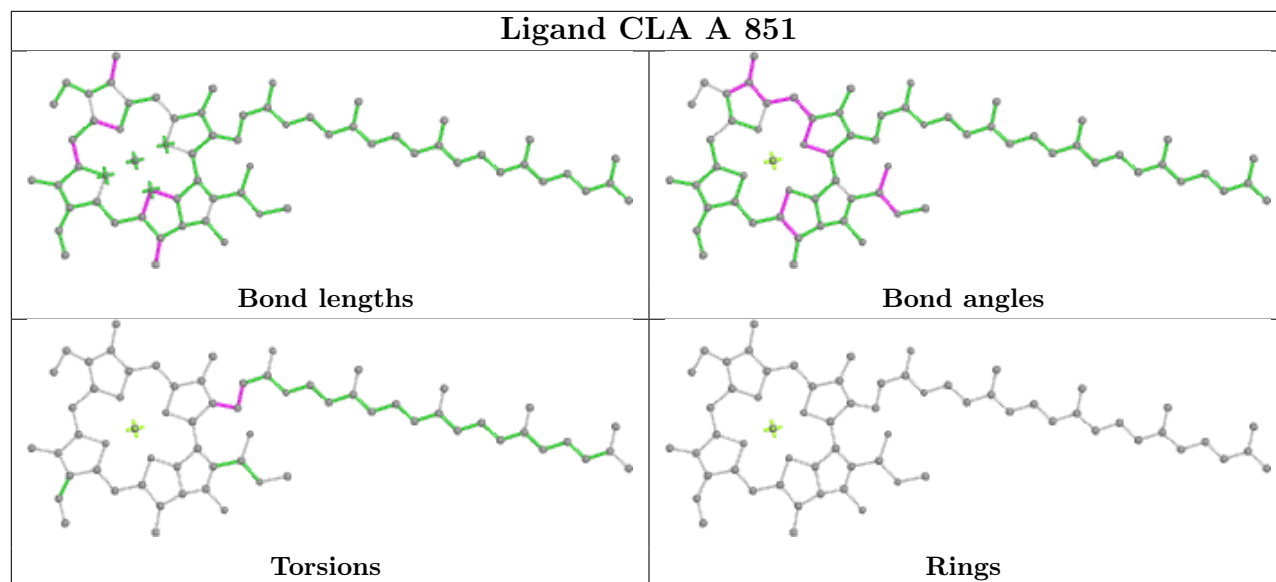
Ligand CLA A 835



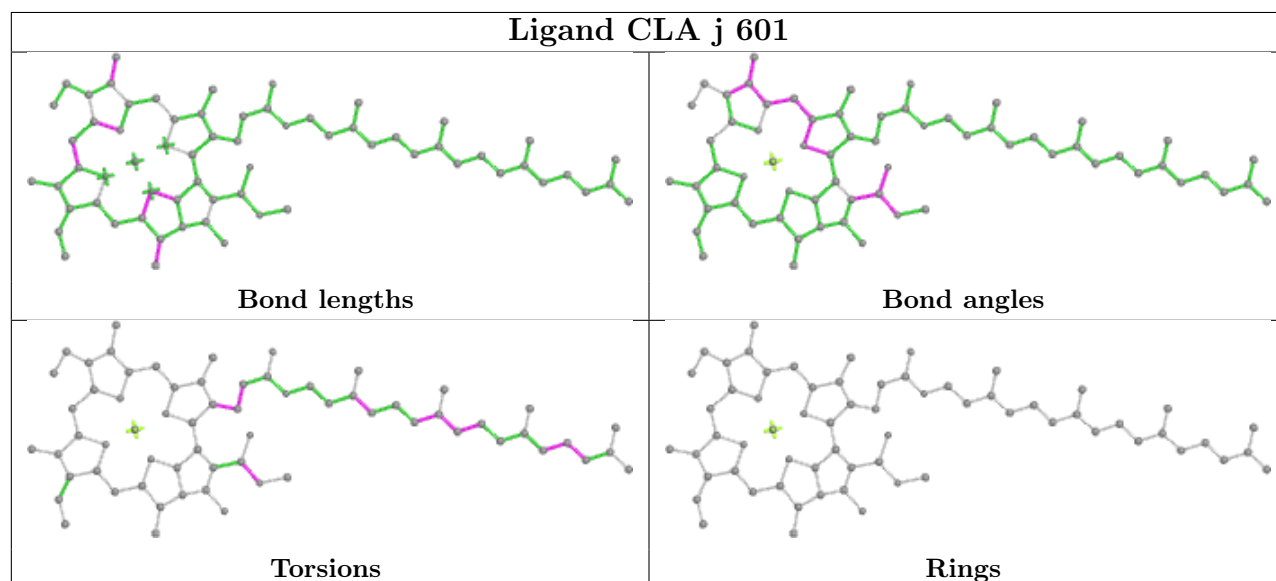
Ligand CLA k 614



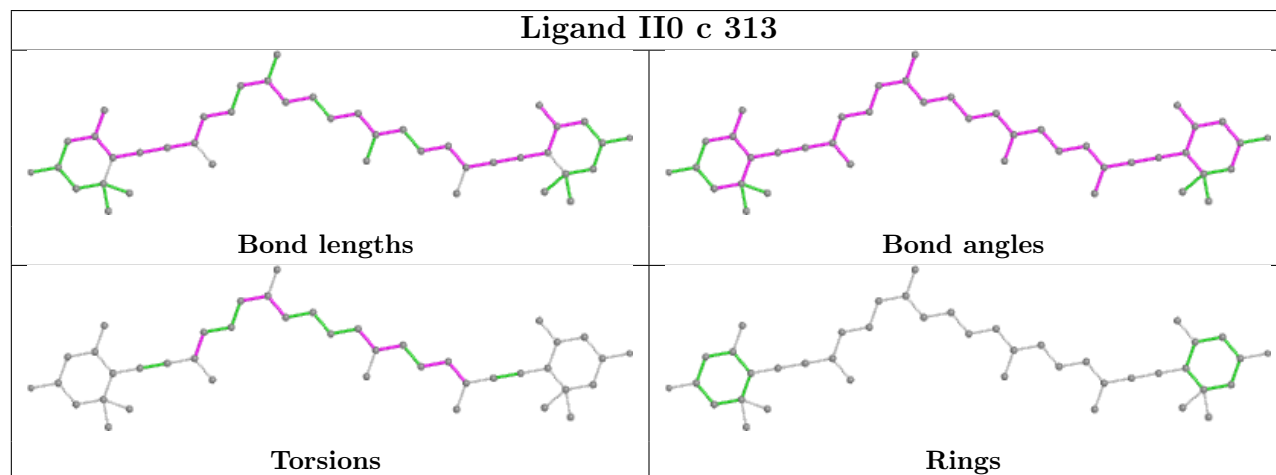
Ligand CLA A 851

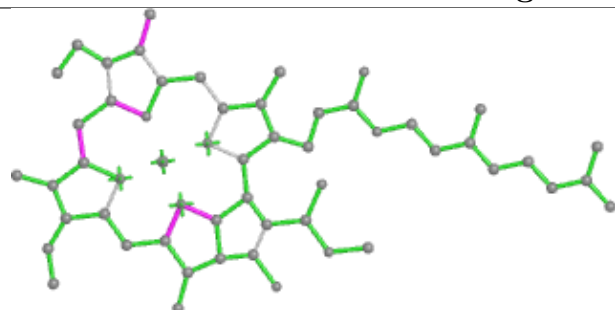


Ligand CLA j 601

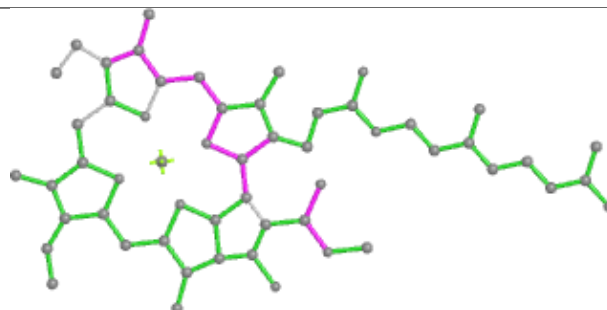


Ligand II0 c 313

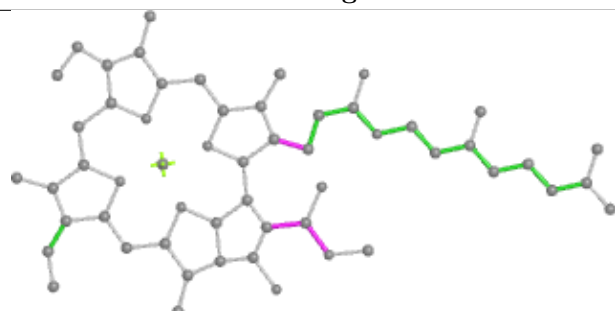


Ligand CLA B 833

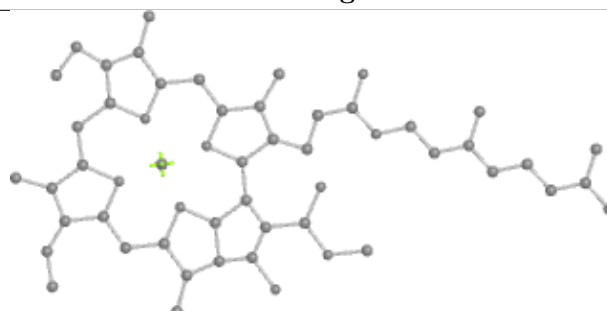
Bond lengths



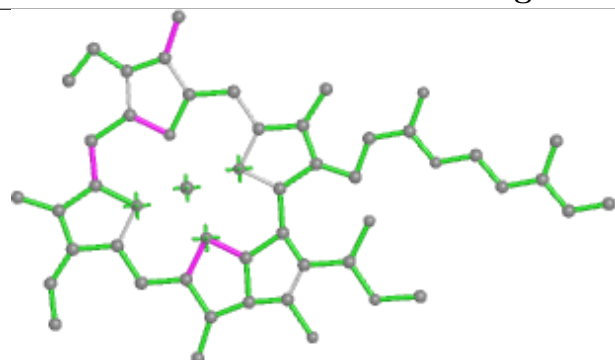
Bond angles



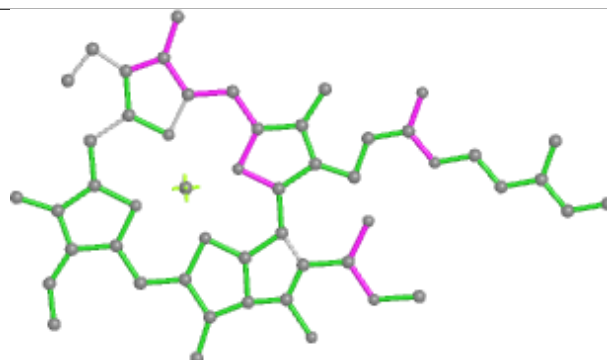
Torsions



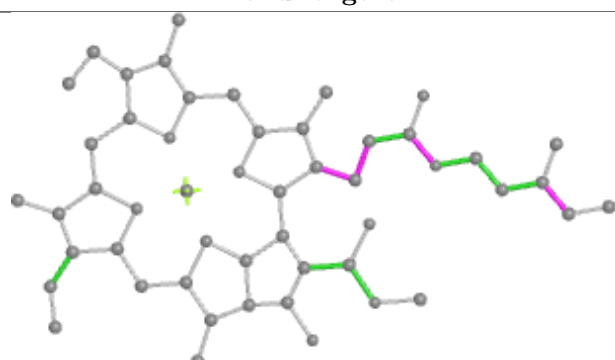
Rings

Ligand CLA m 607

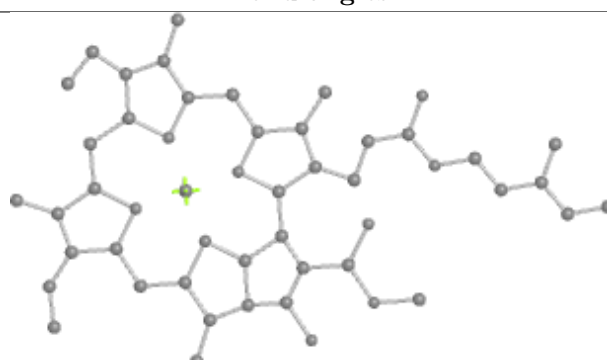
Bond lengths



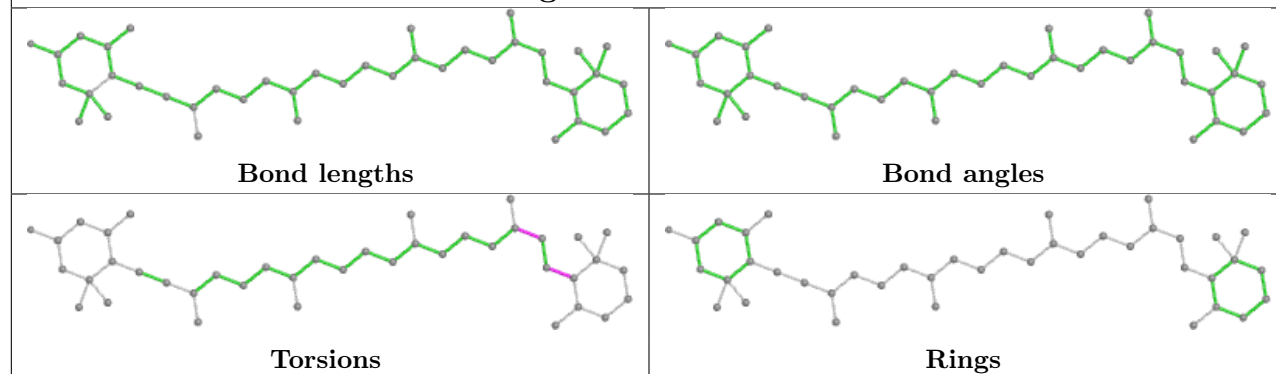
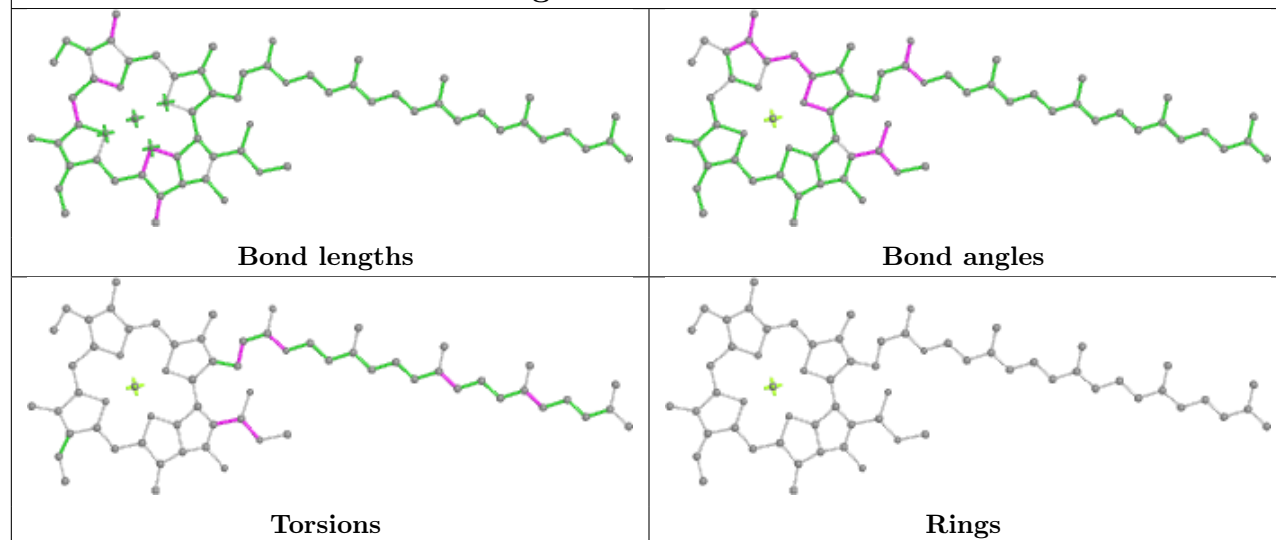
Bond angles



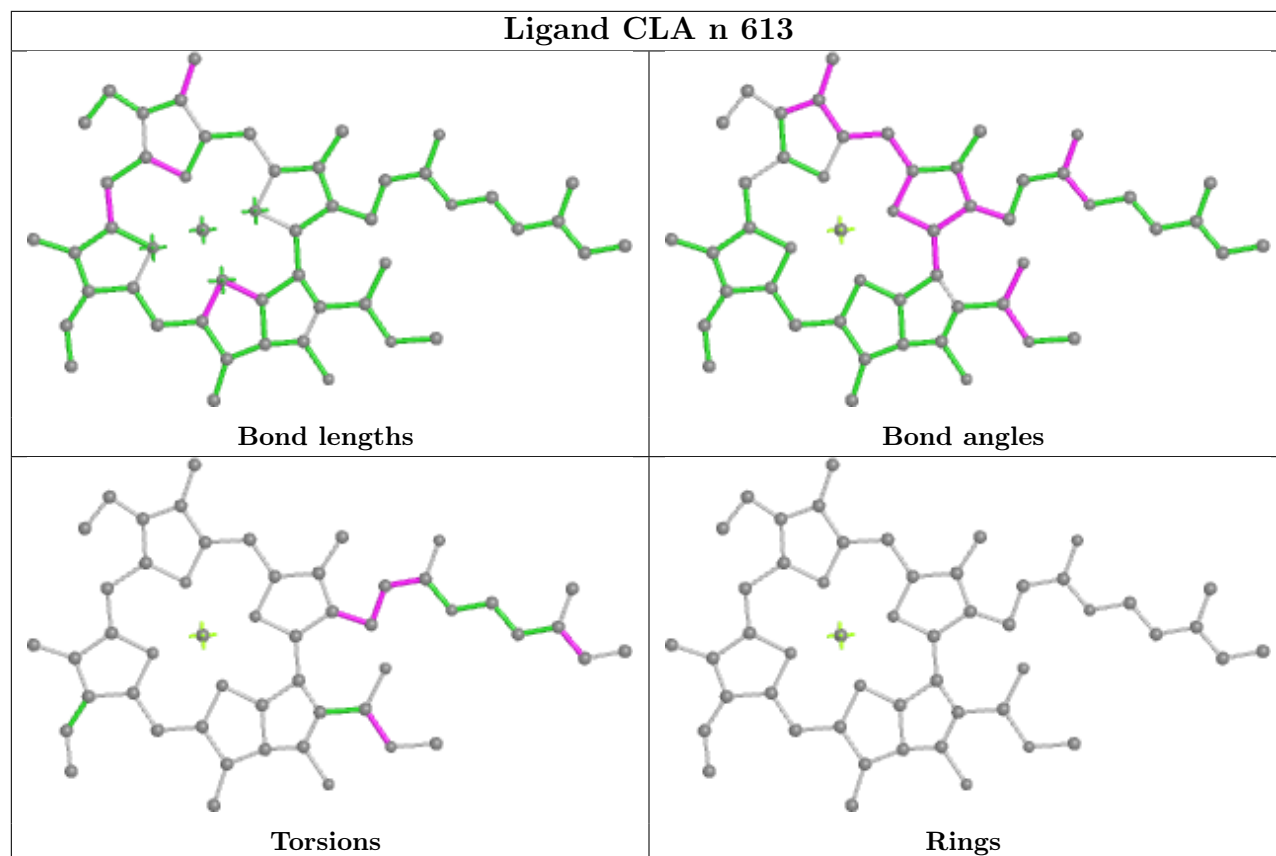
Torsions



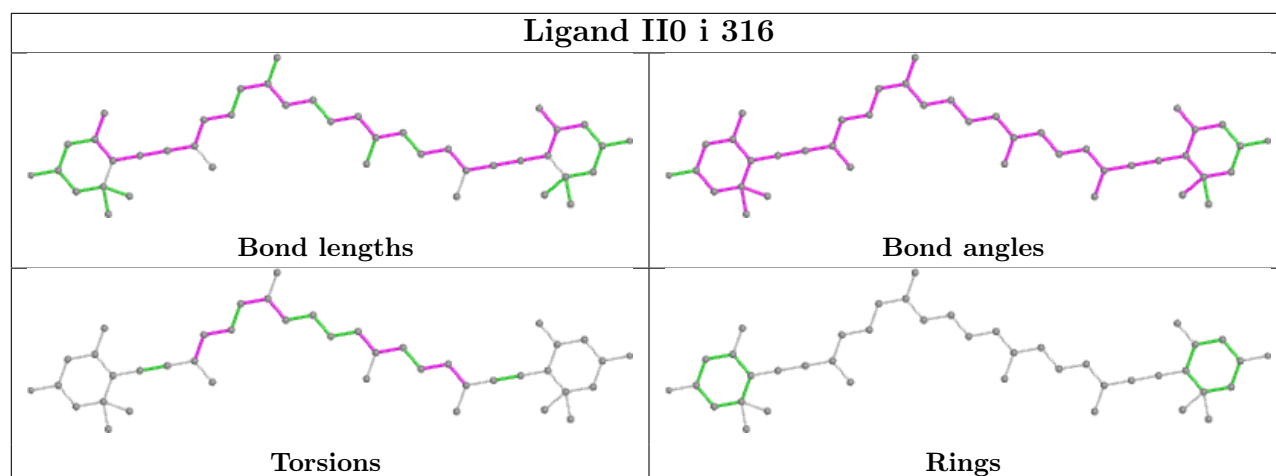
Rings

Ligand IHT b 301**Ligand CLA B 838**

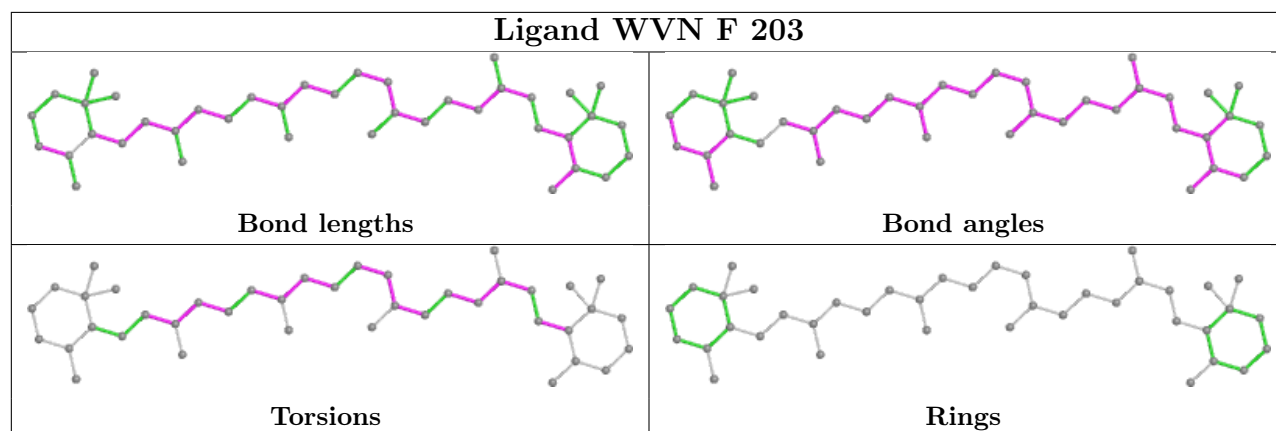
Ligand CLA n 613

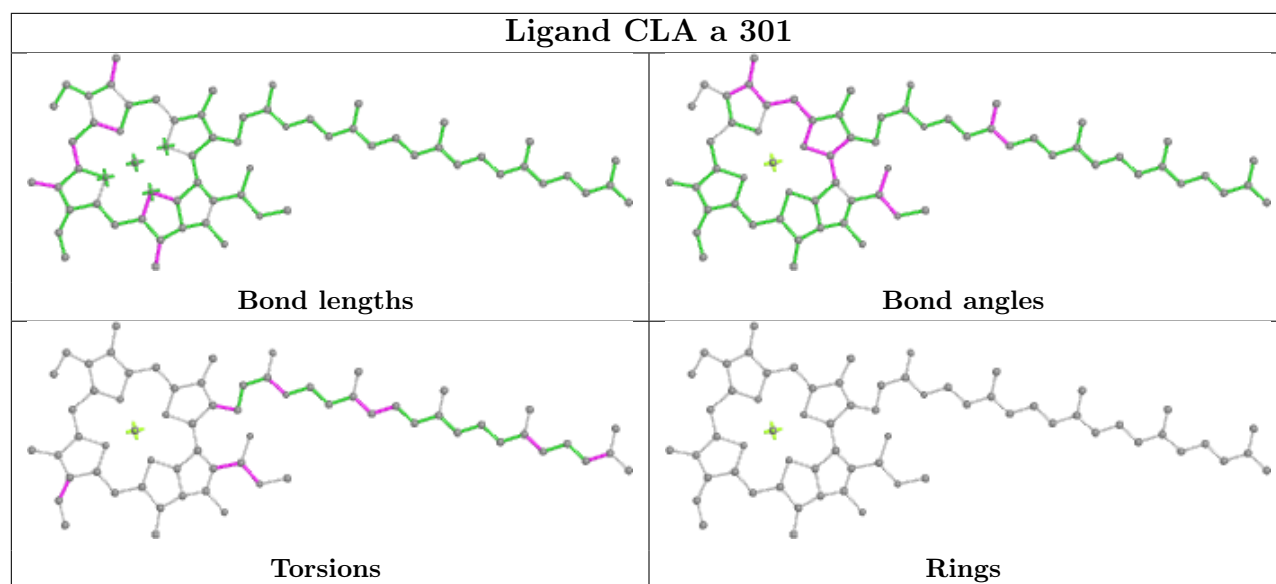
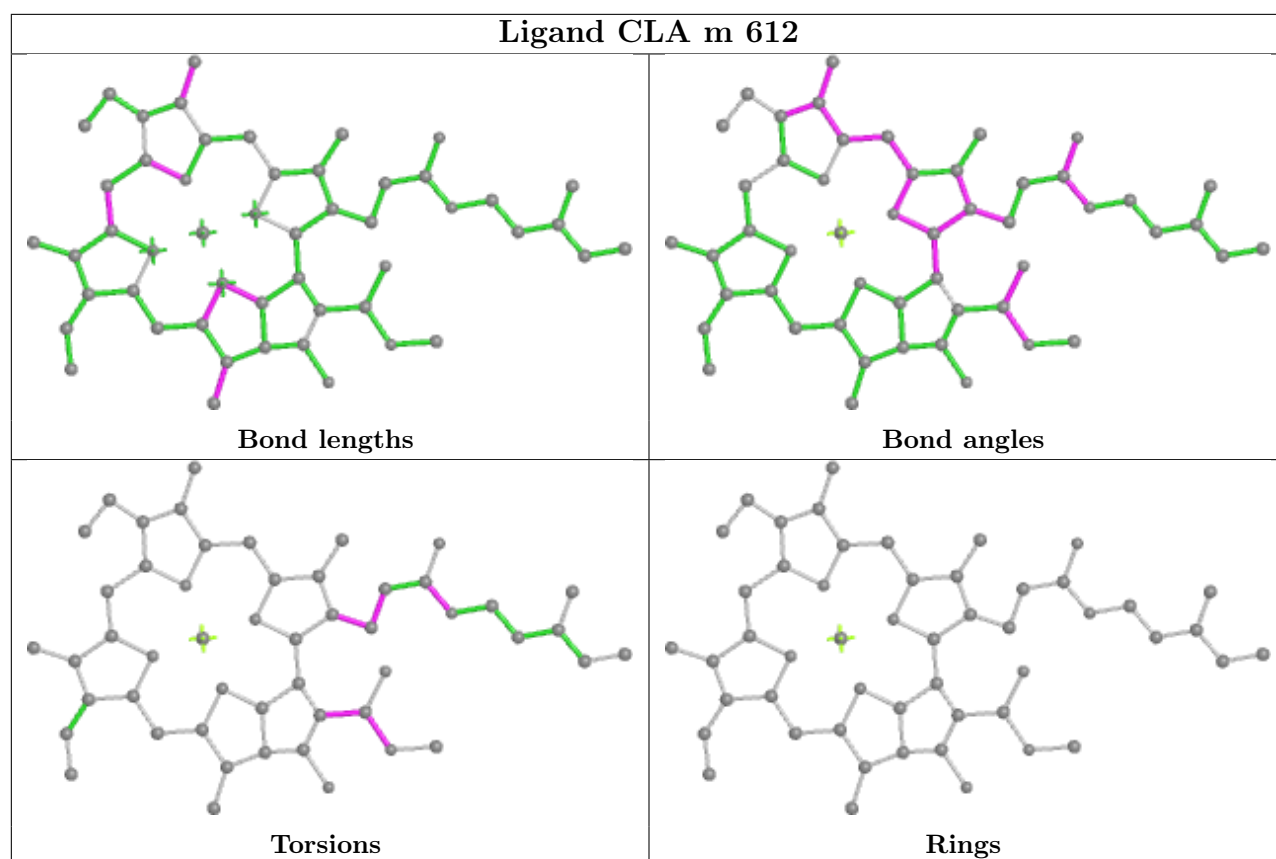


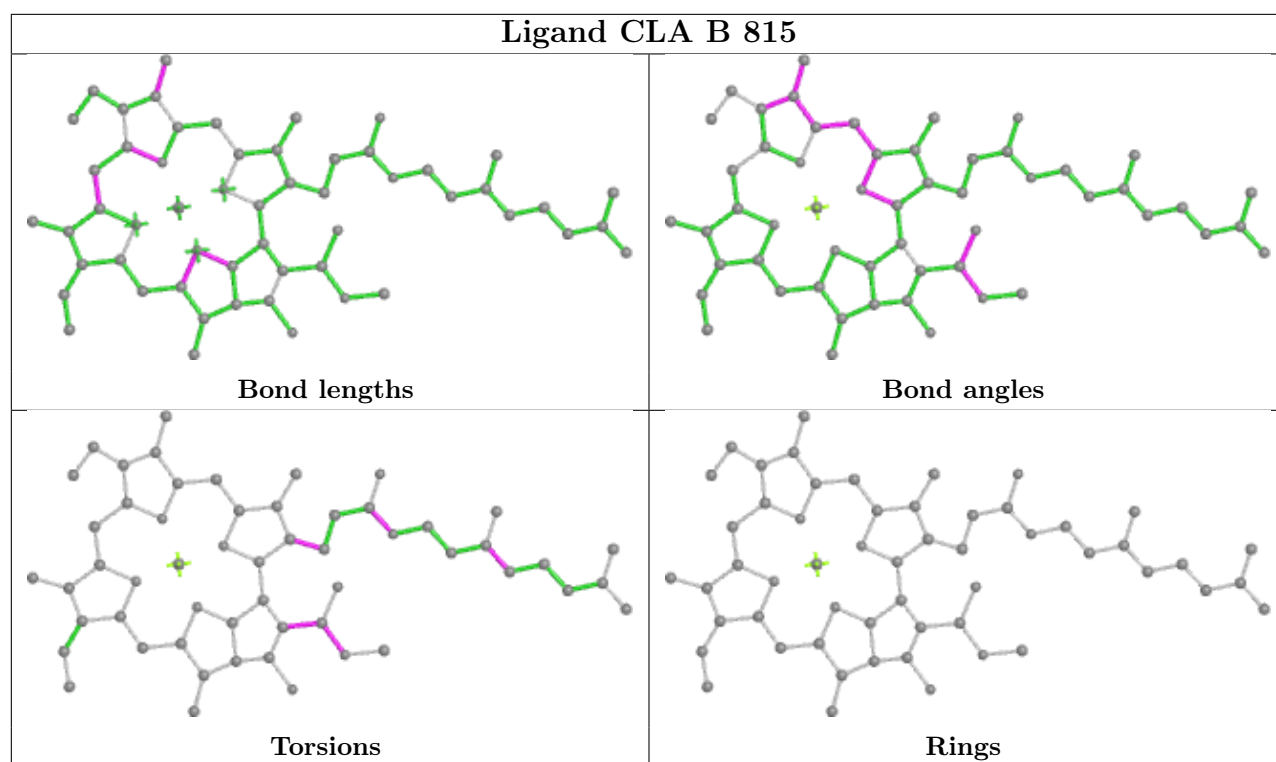
Ligand II0 i 316



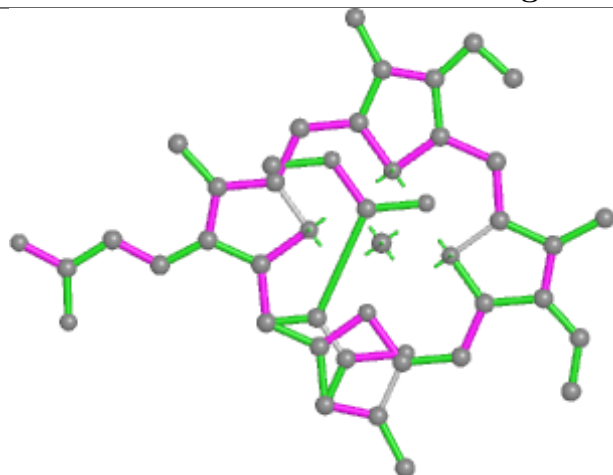
Ligand WVN F 203



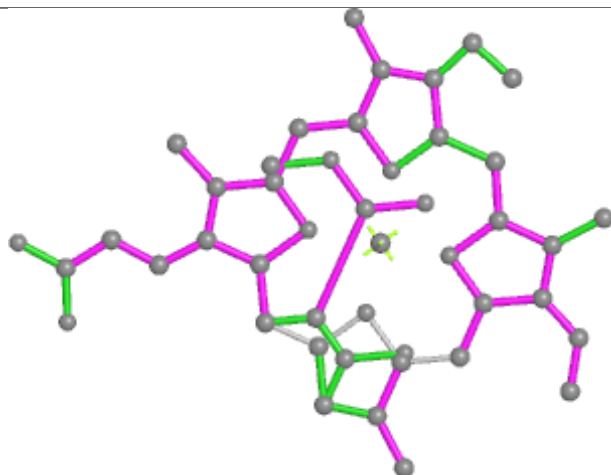




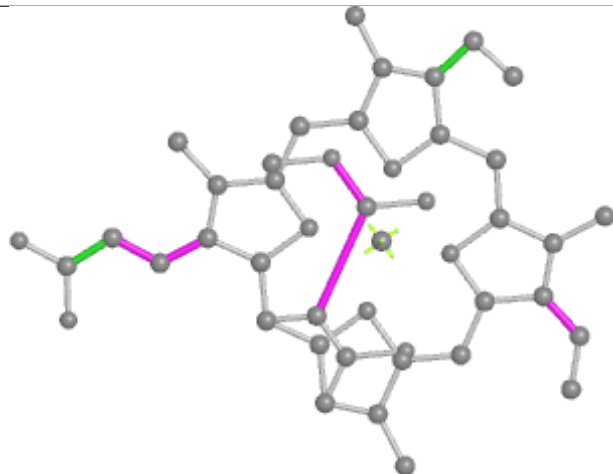
Ligand KC2 c 310



Bond lengths



Bond angles

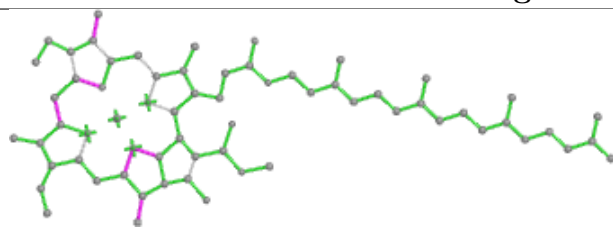


Torsions

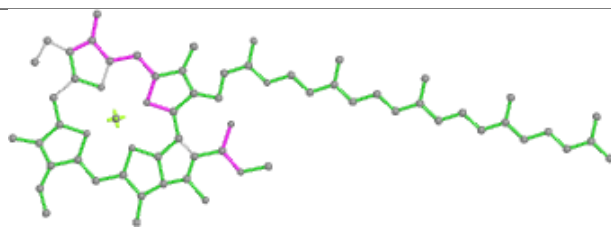


Rings

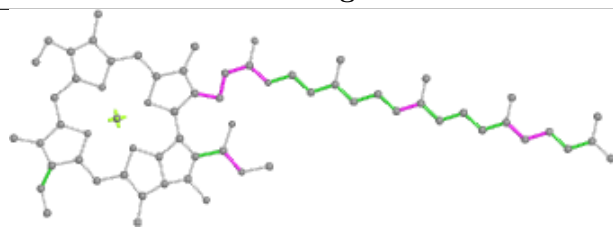
Ligand CLA A 837



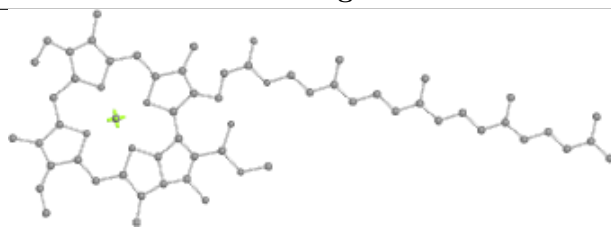
Bond lengths



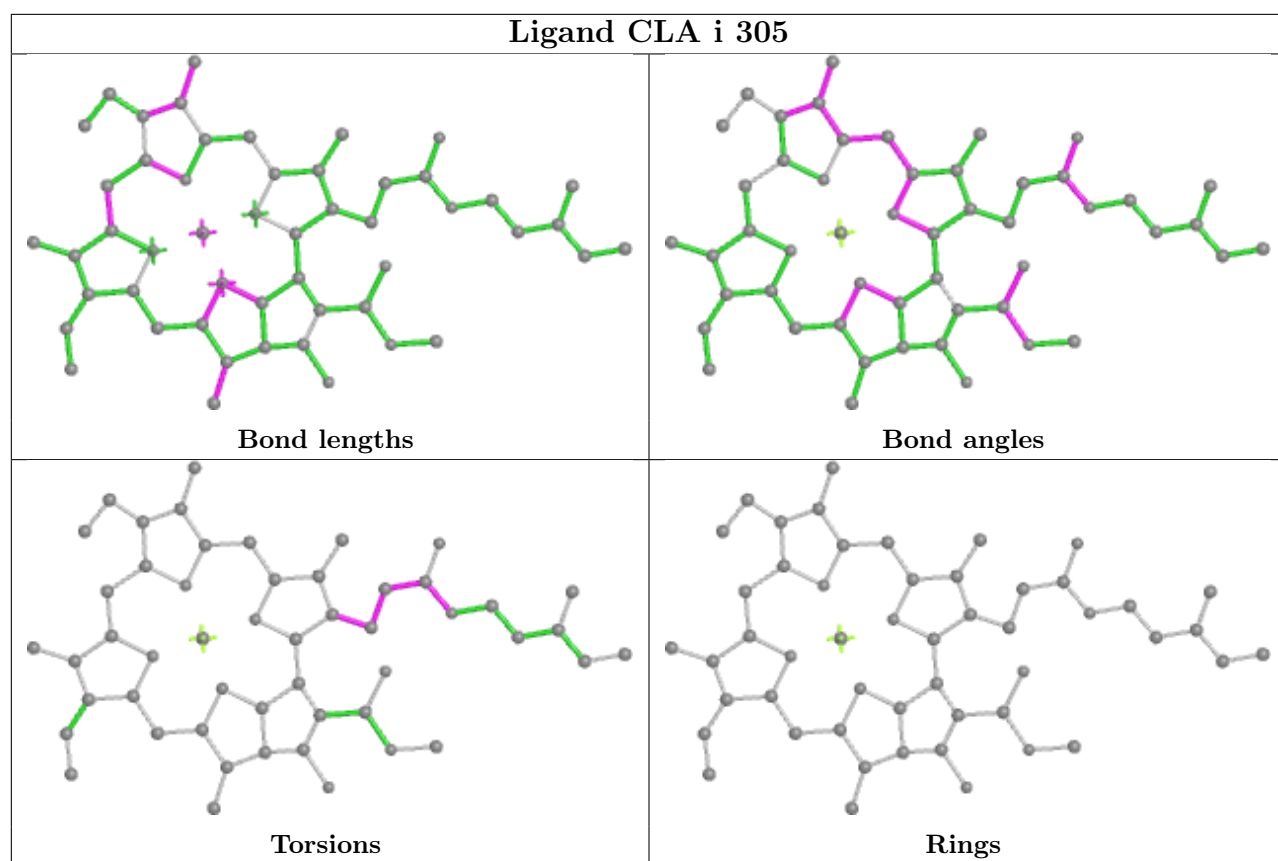
Bond angles

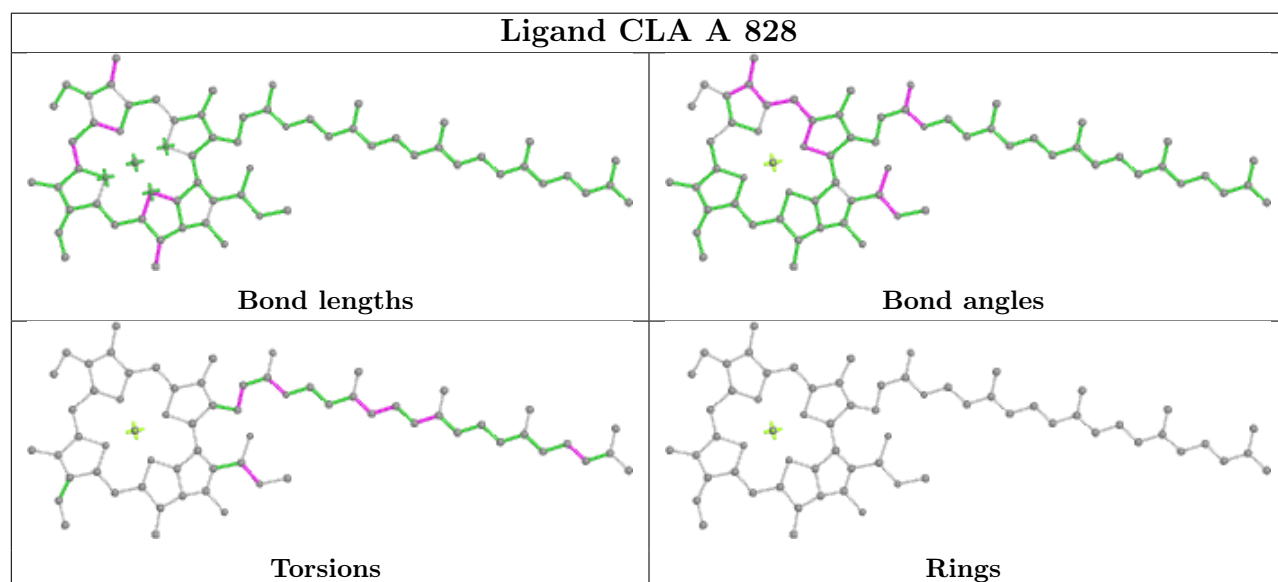
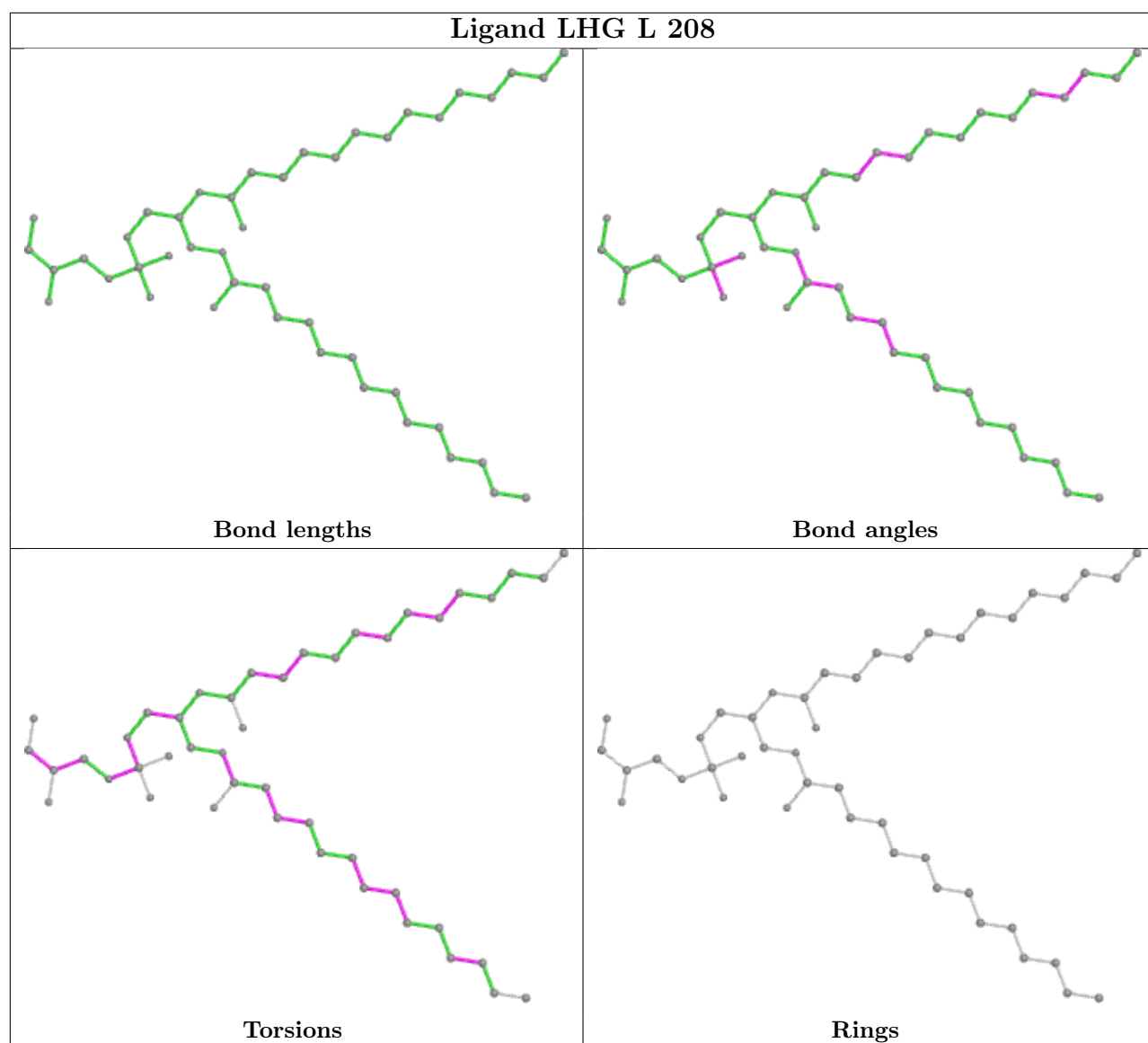


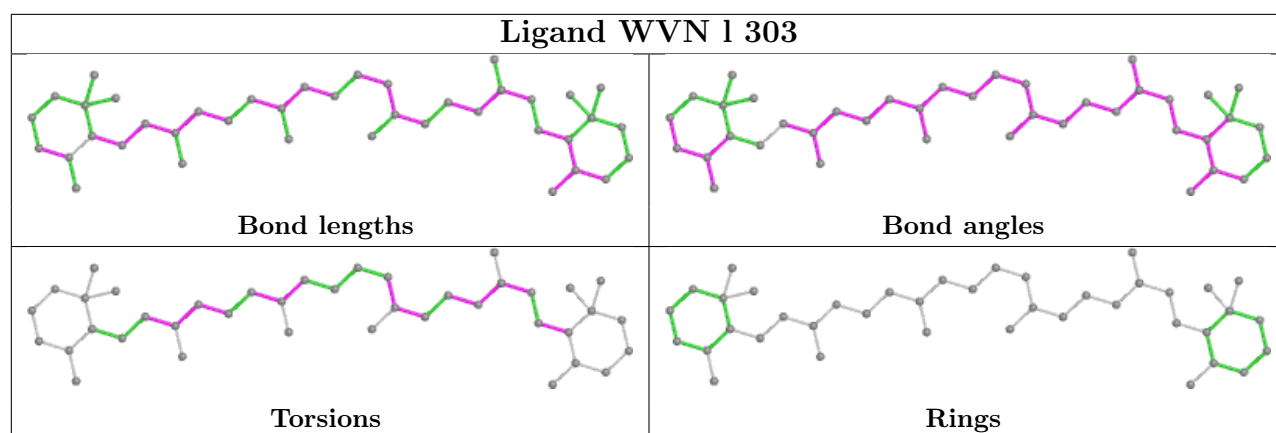
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

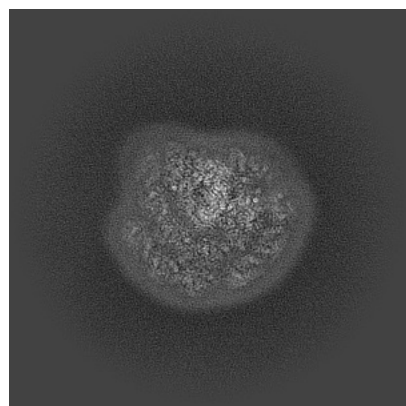
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62717. These allow visual inspection of the internal detail of the map and identification of artifacts.

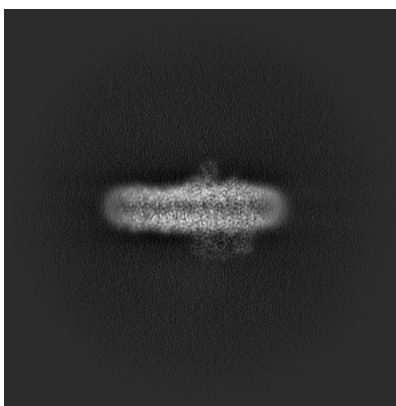
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

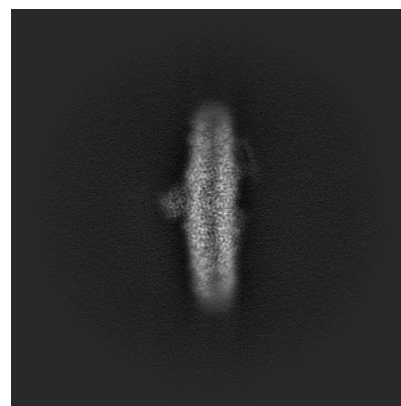
6.1.1 Primary map



X

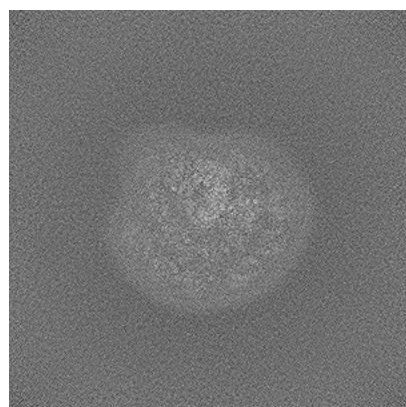


Y

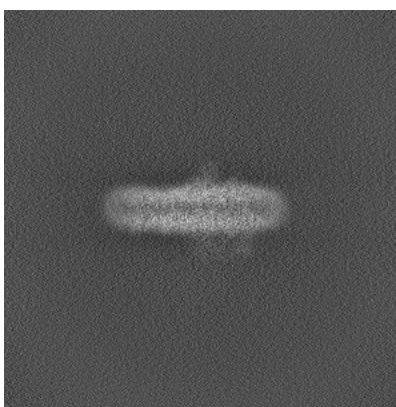


Z

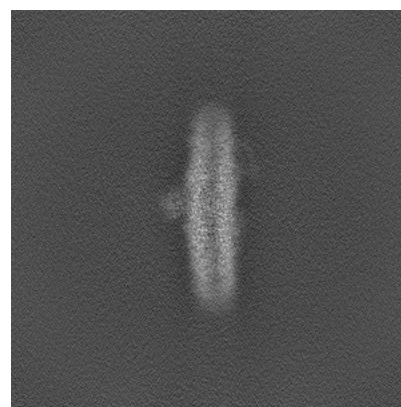
6.1.2 Raw map



X



Y

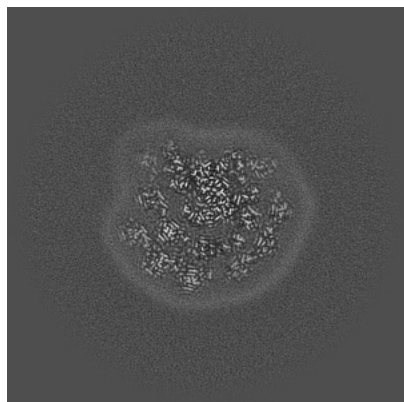


Z

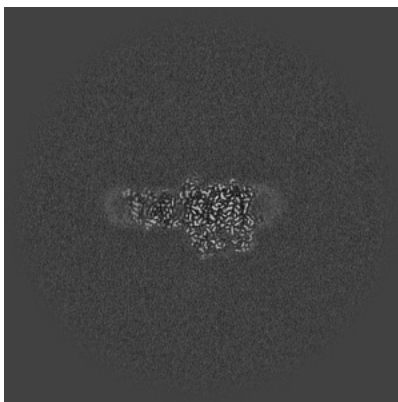
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

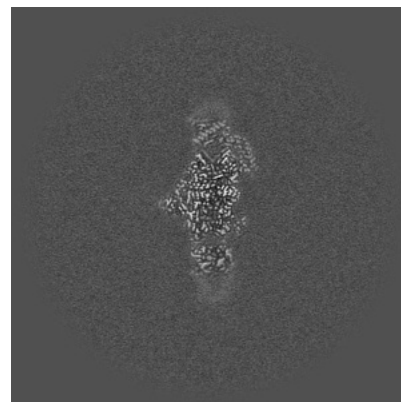
6.2.1 Primary map



X Index: 300

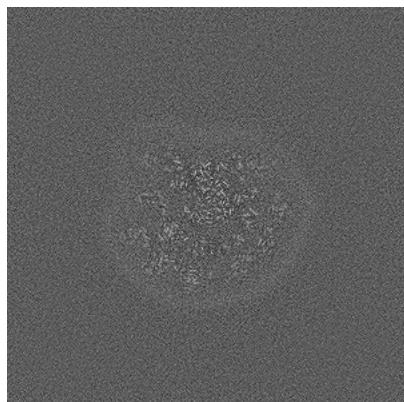


Y Index: 300

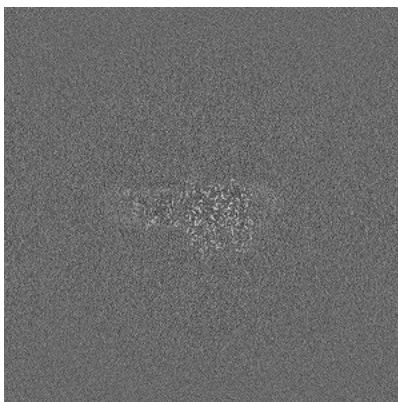


Z Index: 300

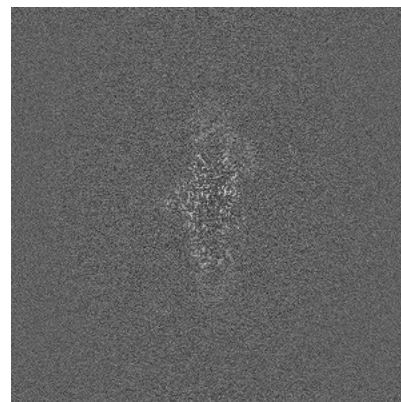
6.2.2 Raw map



X Index: 300



Y Index: 300

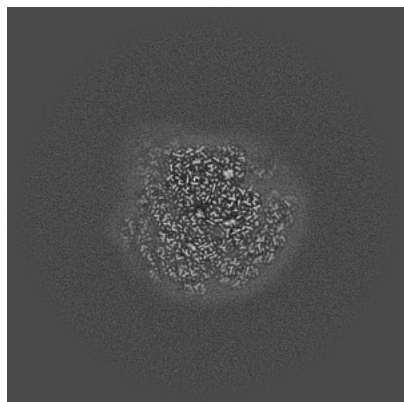


Z Index: 300

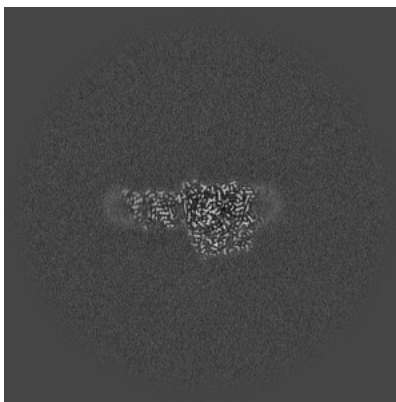
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

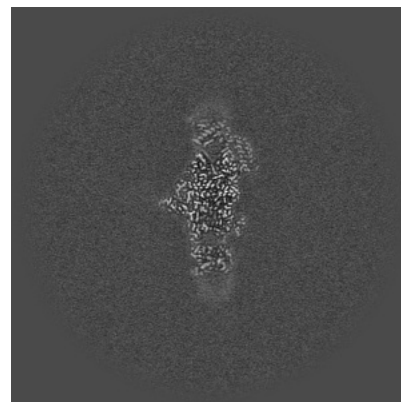
6.3.1 Primary map



X Index: 282

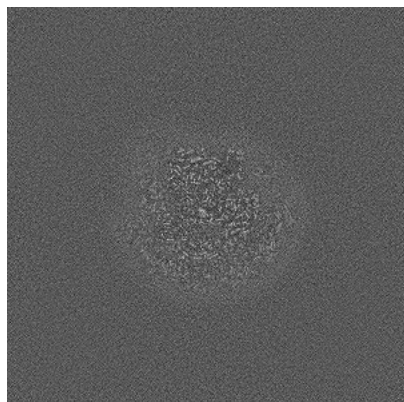


Y Index: 304

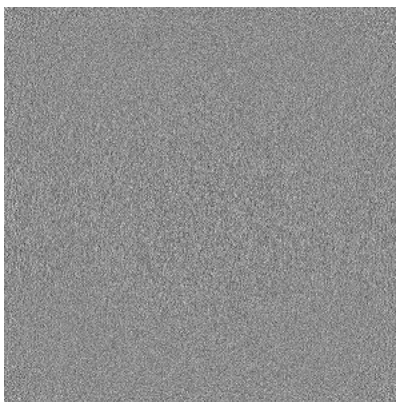


Z Index: 301

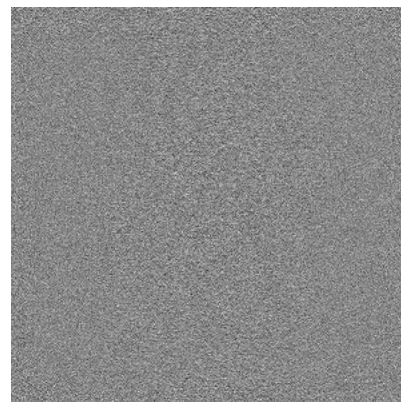
6.3.2 Raw map



X Index: 284



Y Index: 0

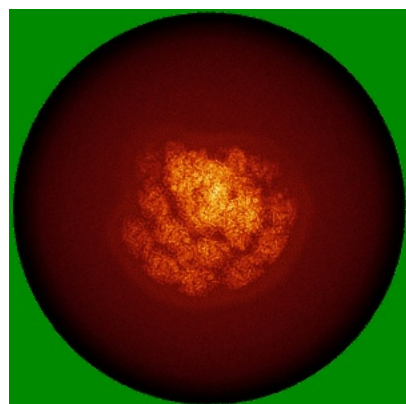


Z Index: 0

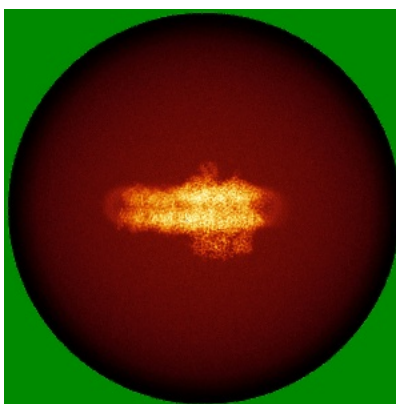
The images above show the largest variance slices of the map in three orthogonal directions.

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

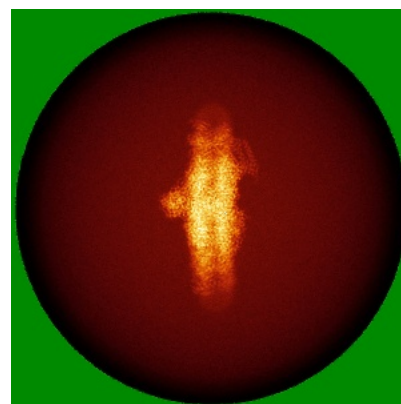
6.4.1 Primary map



X

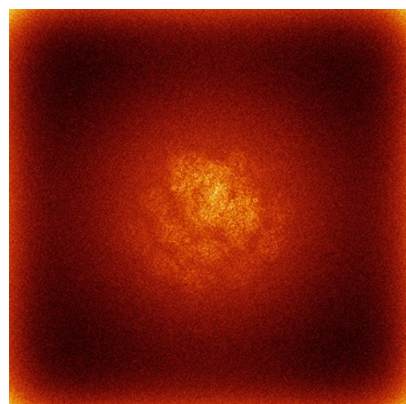


Y

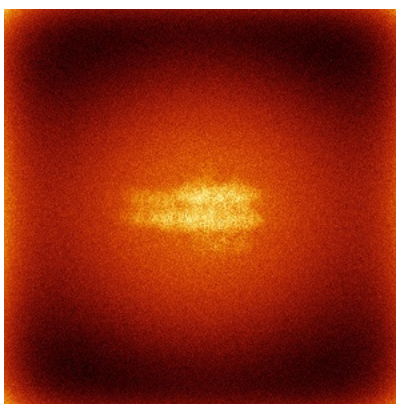


Z

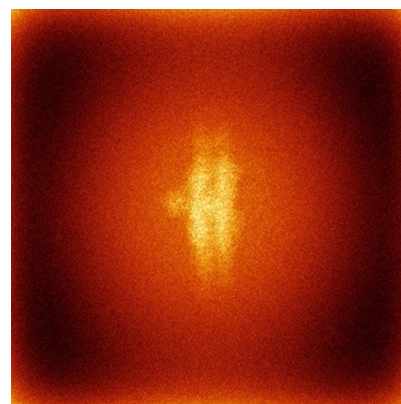
6.4.2 Raw map



X



Y

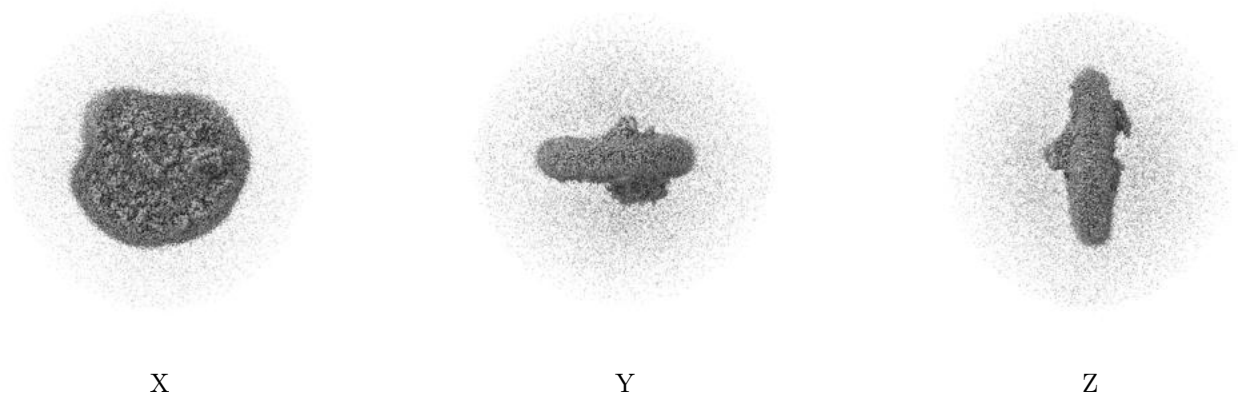


Z

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

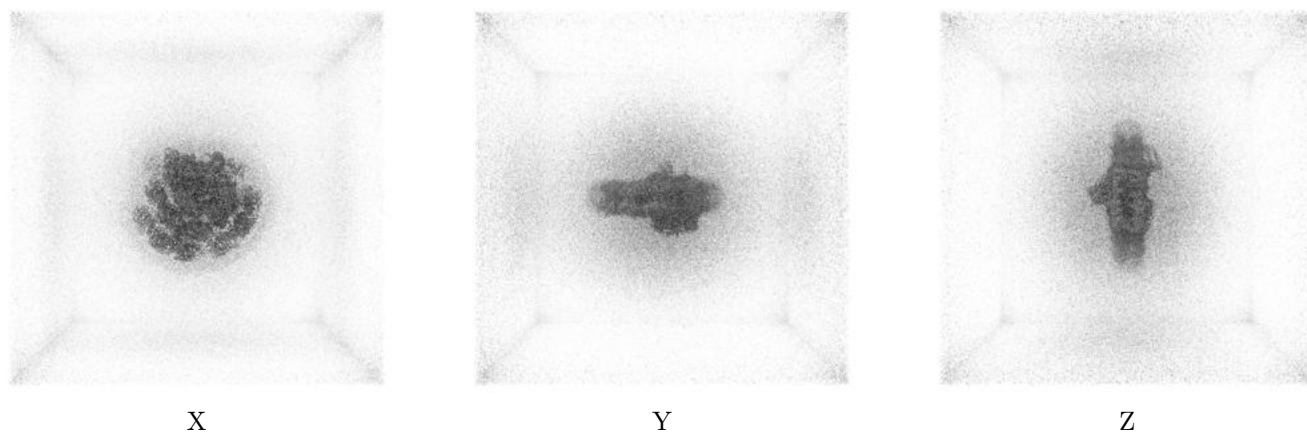
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

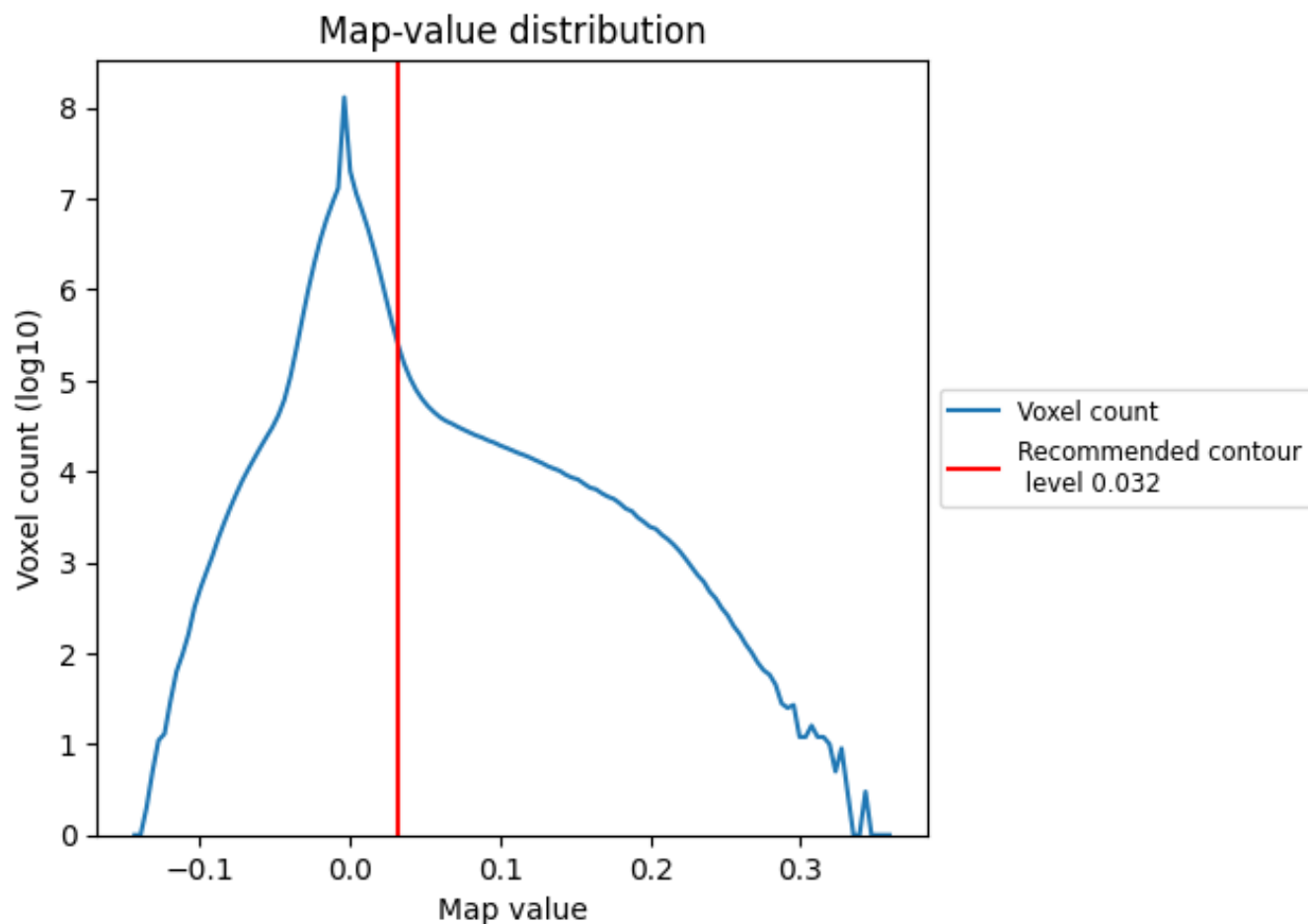
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

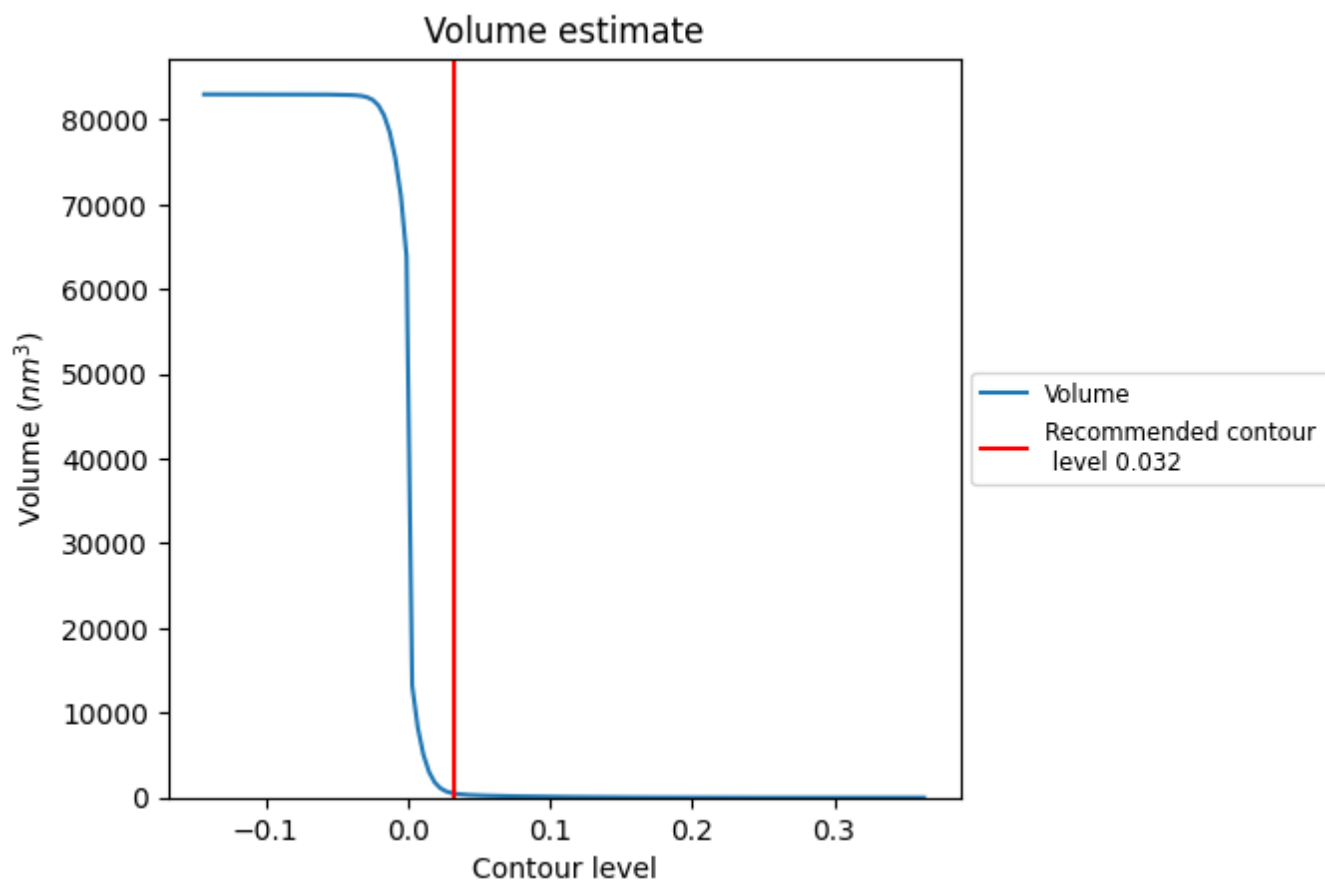
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

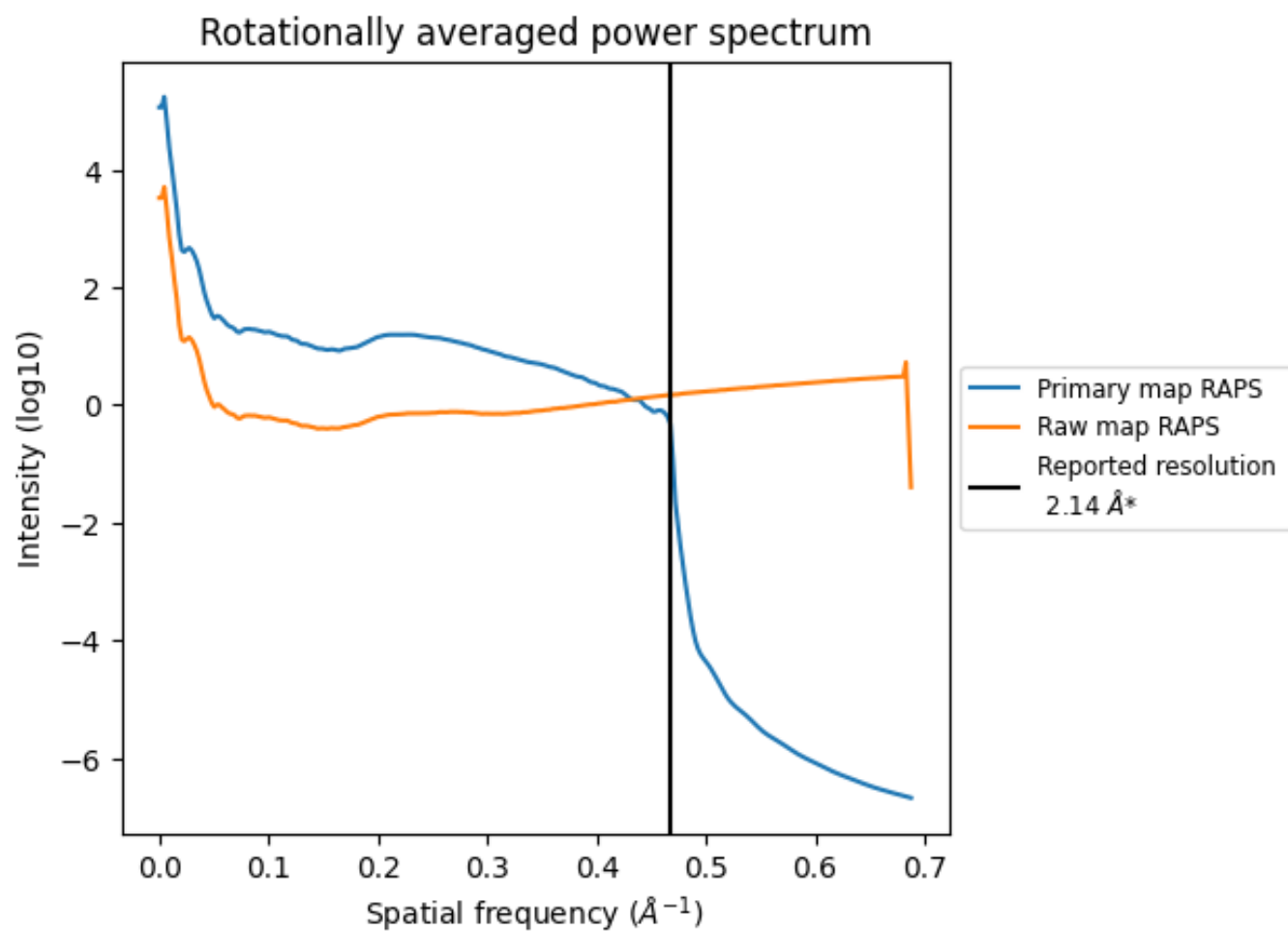
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 505 nm³; this corresponds to an approximate mass of 456 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](#)

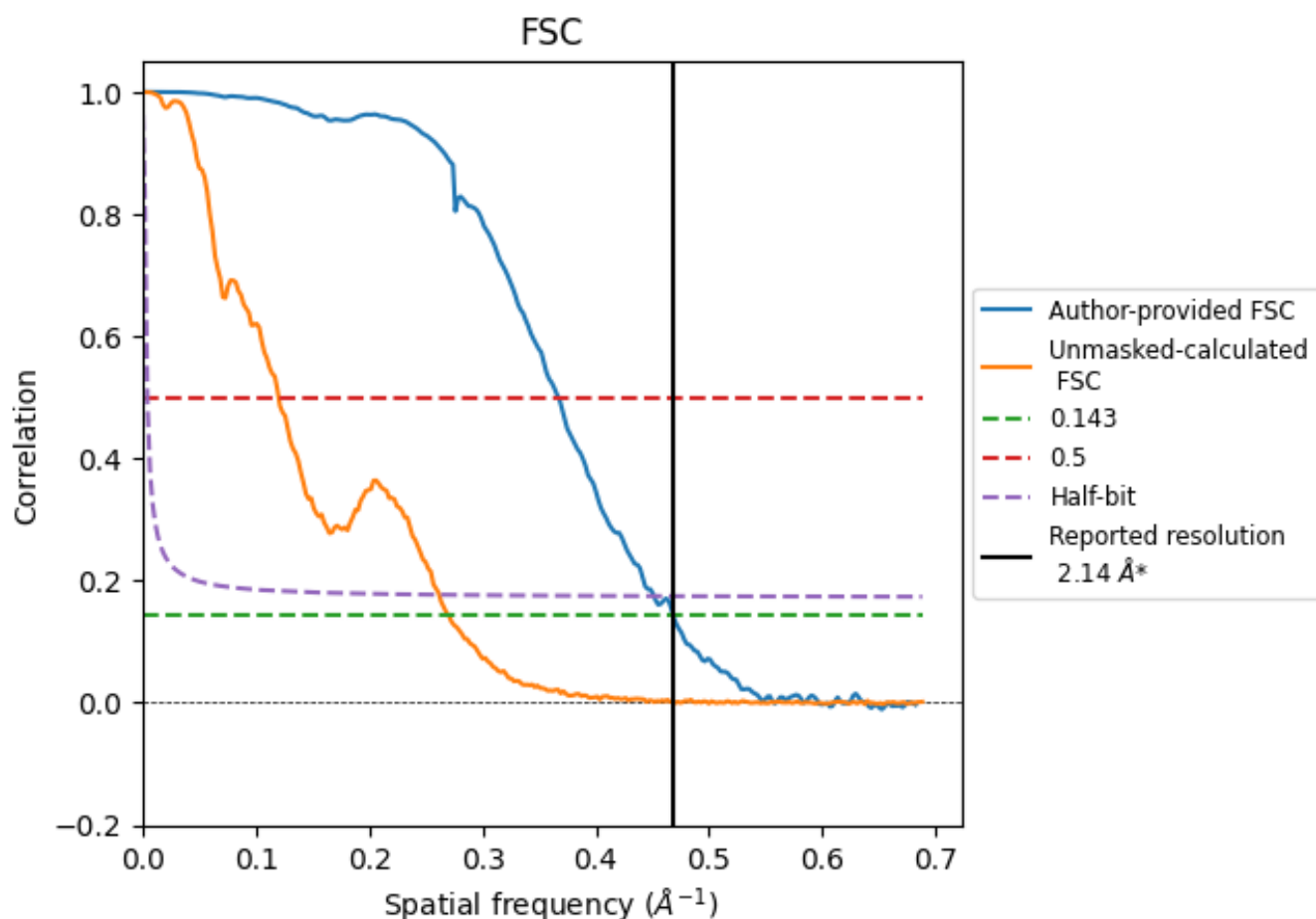


*Reported resolution corresponds to spatial frequency of 0.467 \AA^{-1}

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 0.467 Å⁻¹

8.2 Resolution estimates [i](#)

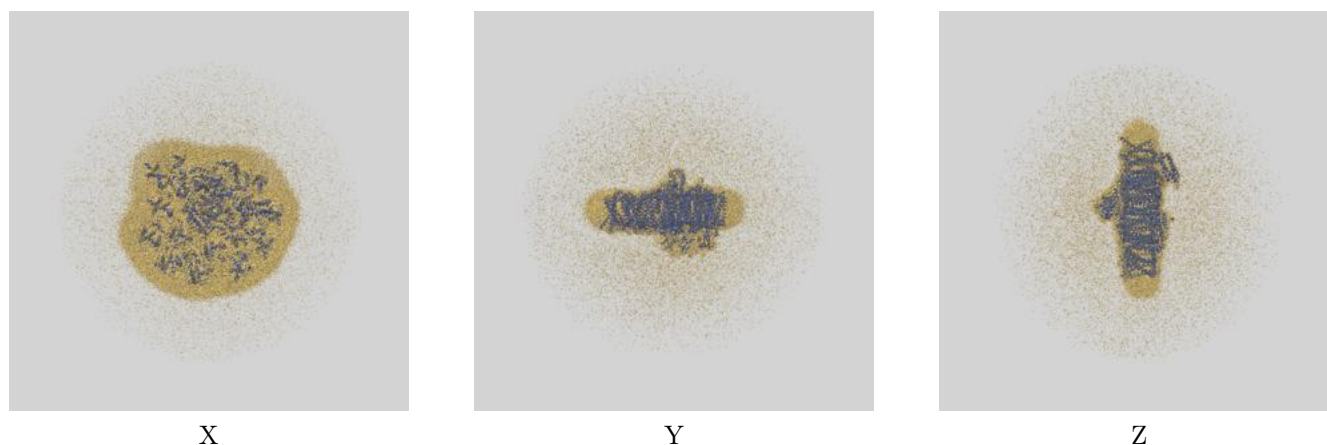
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	2.14	2.72	2.22
Unmasked-calculated*	3.70	8.31	3.82

*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 3.70 differs from the reported value 2.14 by more than 10 %

9 Map-model fit [i](#)

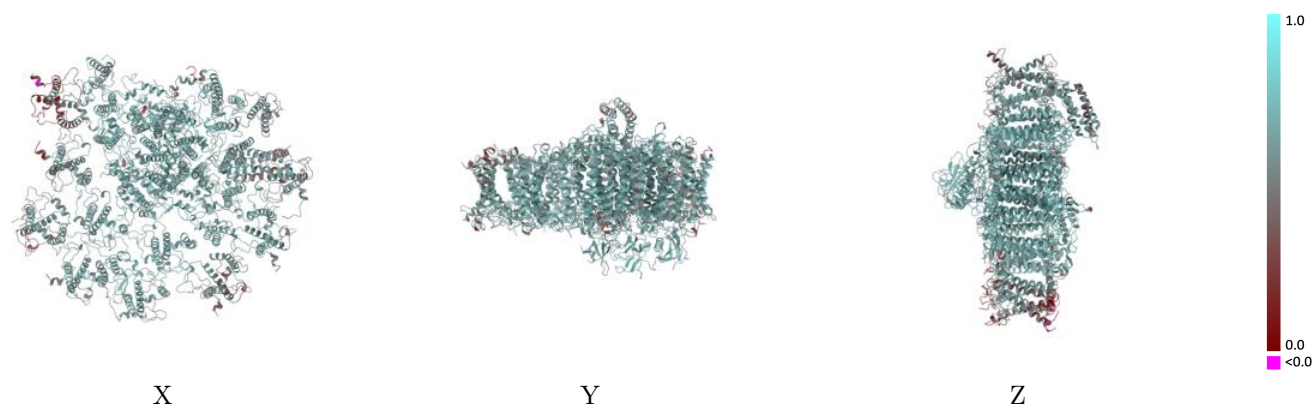
This section contains information regarding the fit between EMDB map EMD-62717 and PDB model 9L0K. Per-residue inclusion information can be found in section [3](#) on page [39](#).

9.1 Map-model overlay [i](#)



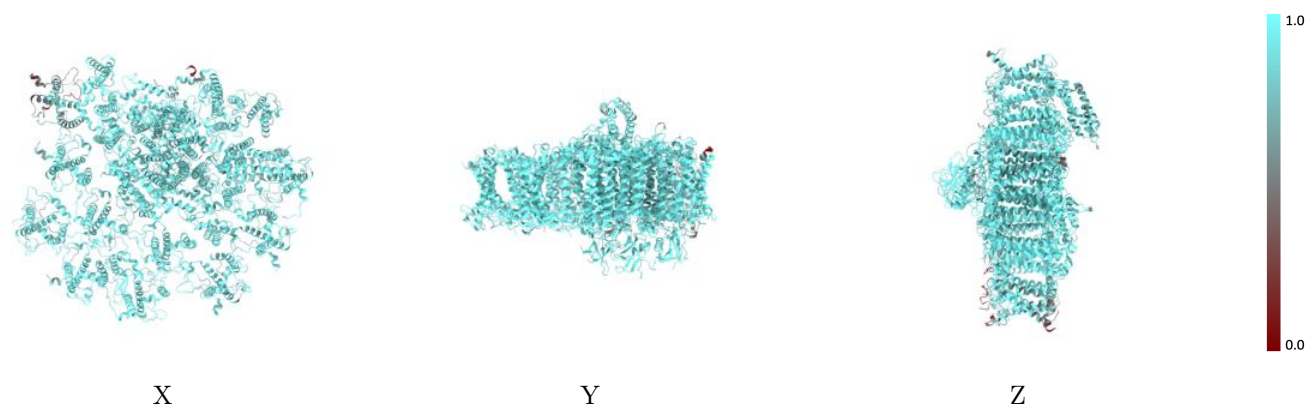
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



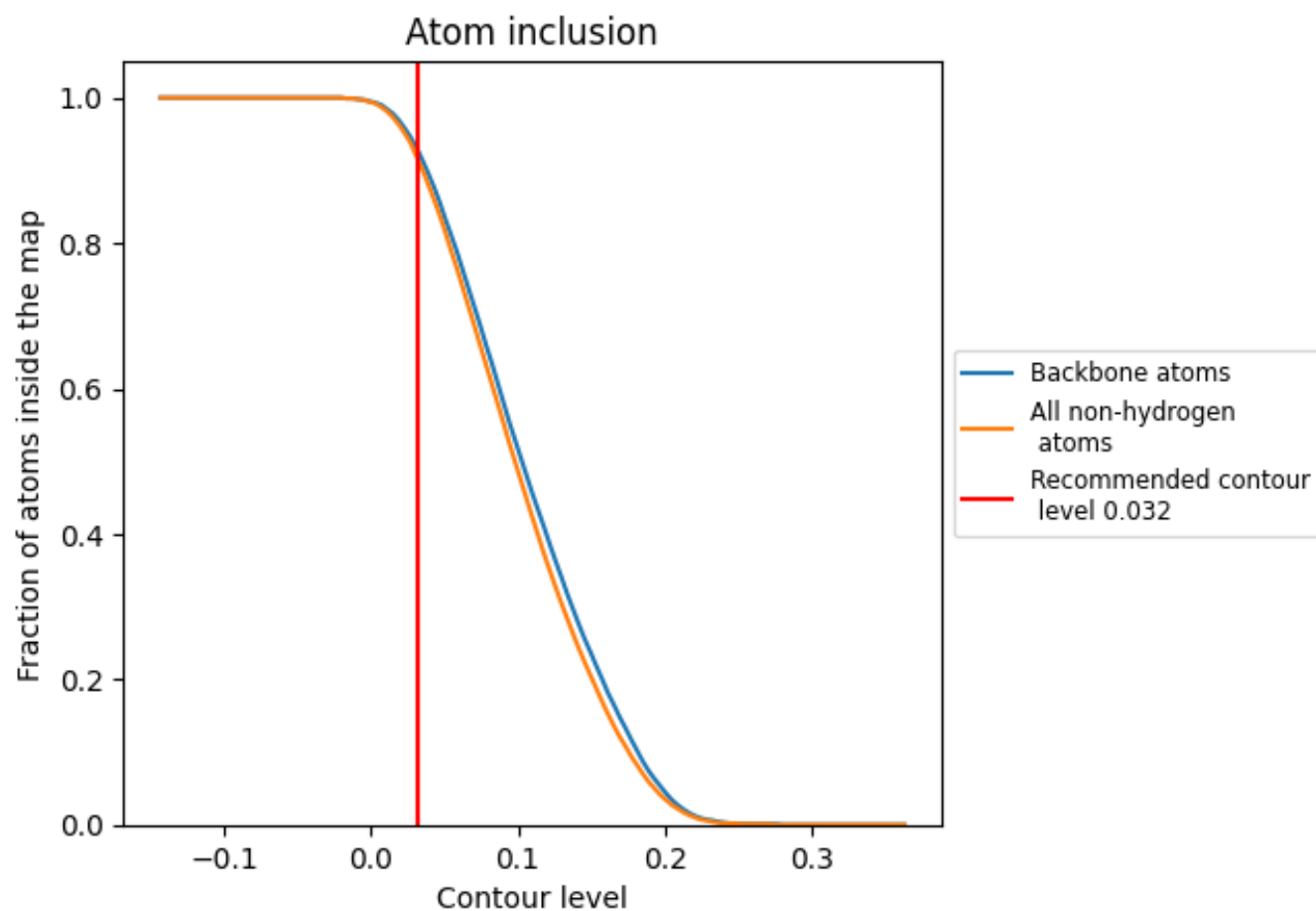
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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	 0.9150	 0.5980
A	 0.9610	 0.6550
B	 0.9750	 0.6640
C	 0.9950	 0.6790
D	 0.9640	 0.6460
E	 0.9450	 0.6280
F	 0.9520	 0.6390
I	 0.9660	 0.6490
J	 0.9700	 0.6370
K	 0.8450	 0.5340
L	 0.8130	 0.5460
M	 0.9400	 0.6280
Q	 0.8540	 0.5510
R	 0.9550	 0.6290
a	 0.9590	 0.6410
b	 0.9530	 0.6350
c	 0.8870	 0.5640
d	 0.6340	 0.3600
h	 0.8380	 0.5340
i	 0.8560	 0.5200
j	 0.8970	 0.5690
k	 0.8590	 0.4960
l	 0.9280	 0.5910
m	 0.9200	 0.5910
n	 0.8520	 0.5260
s	 0.9320	 0.6120

