



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:10 PM UTC

PDB ID : 8WMV / pdb_00008wmv
EMDB ID : EMD-37659
Title : The structure of PSI-14CAC complex at stationary growth phase
Authors : Zhang, S.M.; Si, L.; Li, M.
Deposited on : 2023-10-04
Resolution : 2.94 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

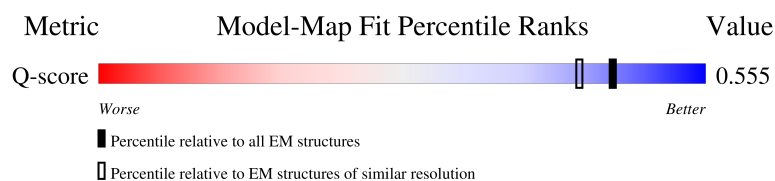
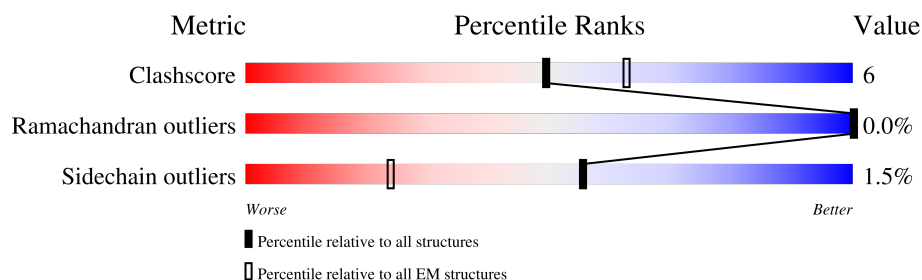
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 Å.

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



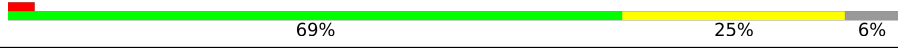
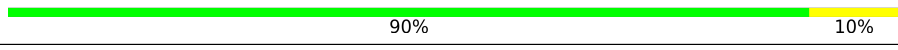
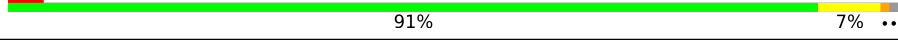
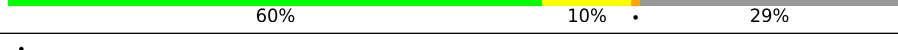
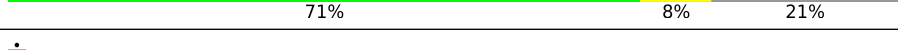
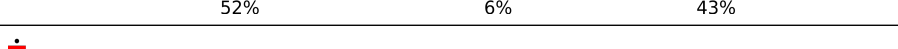
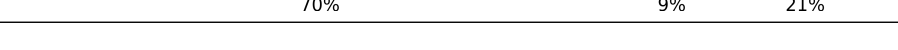
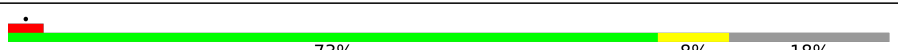
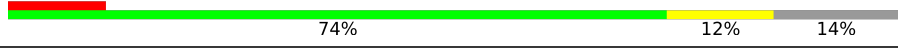
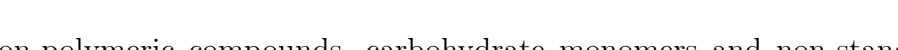
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13068 (2.44 - 3.44)

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	O	146	
12	K	87	
13	s	269	
14	c	216	
15	a	216	
16	b	223	
17	h	225	
18	f	212	
18	j	212	
18	m	212	
19	e	203	
20	l	238	
21	k	241	
22	i	218	
23	d	213	
24	g	255	
25	R	129	
26	n	219	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	A	801	X	-	-	-
27	CLA	A	802	X	-	-	-
27	CLA	A	803	X	-	-	-
27	CLA	A	804	X	-	-	-
27	CLA	A	805	X	-	-	-
27	CLA	A	807	X	-	-	-
27	CLA	A	808	X	-	-	-
27	CLA	A	809	X	-	-	-
27	CLA	A	810	X	-	-	-
27	CLA	A	812	X	-	-	-
27	CLA	A	813	X	-	-	-
27	CLA	A	814	X	-	-	-
27	CLA	A	815	X	-	-	-
27	CLA	A	816	X	-	-	-
27	CLA	A	817	X	-	-	-
27	CLA	A	818	X	-	-	-
27	CLA	A	819	X	-	-	-
27	CLA	A	820	X	-	-	-
27	CLA	A	822	X	-	-	-
27	CLA	A	823	X	-	-	-
27	CLA	A	824	X	-	-	-
27	CLA	A	826	X	-	-	-
27	CLA	A	827	X	-	-	-
27	CLA	A	828	X	-	-	-
27	CLA	A	829	X	-	-	-
27	CLA	A	831	X	-	-	-
27	CLA	A	832	X	-	-	-
27	CLA	A	833	X	-	-	-
27	CLA	A	834	X	-	-	-
27	CLA	A	835	X	-	-	-
27	CLA	A	837	X	-	-	-
27	CLA	A	838	X	-	-	-
27	CLA	A	839	X	-	-	-
27	CLA	A	841	X	-	-	-
27	CLA	A	842	X	-	-	-
27	CLA	A	852	X	-	-	-
27	CLA	A	853	X	-	-	-
27	CLA	A	855	X	-	-	-
27	CLA	A	856	X	-	-	-
27	CLA	B	801	X	-	-	-
27	CLA	B	802	X	-	-	-
27	CLA	B	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	B	804	X	-	-	-
27	CLA	B	805	X	-	-	-
27	CLA	B	806	X	-	-	-
27	CLA	B	807	X	-	-	-
27	CLA	B	808	X	-	-	-
27	CLA	B	809	X	-	-	-
27	CLA	B	810	X	-	-	-
27	CLA	B	811	X	-	-	-
27	CLA	B	812	X	-	-	-
27	CLA	B	813	X	-	-	-
27	CLA	B	814	X	-	-	-
27	CLA	B	816	X	-	-	-
27	CLA	B	818	X	-	-	-
27	CLA	B	819	X	-	-	-
27	CLA	B	820	X	-	-	-
27	CLA	B	821	X	-	-	-
27	CLA	B	822	X	-	-	-
27	CLA	B	823	X	-	-	-
27	CLA	B	824	X	-	-	-
27	CLA	B	825	X	-	-	-
27	CLA	B	826	X	-	-	-
27	CLA	B	827	X	-	-	-
27	CLA	B	828	X	-	-	-
27	CLA	B	829	X	-	-	-
27	CLA	B	830	X	-	-	-
27	CLA	B	831	X	-	-	-
27	CLA	B	832	X	-	-	-
27	CLA	B	833	X	-	-	-
27	CLA	B	834	X	-	-	-
27	CLA	B	835	X	-	-	-
27	CLA	B	836	X	-	-	-
27	CLA	B	837	X	-	-	-
27	CLA	B	838	X	-	-	-
27	CLA	B	839	X	-	-	-
27	CLA	B	840	X	-	-	-
27	CLA	F	201	X	-	-	-
27	CLA	F	202	X	-	-	-
27	CLA	F	203	X	-	-	-
27	CLA	J	103	X	-	-	-
27	CLA	J	105	X	-	-	-
27	CLA	K	101	X	-	-	-
27	CLA	K	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	L	202	X	-	-	-
27	CLA	L	204	X	-	-	-
27	CLA	L	206	X	-	-	-
27	CLA	O	202	X	-	-	-
27	CLA	O	206	X	-	-	-
27	CLA	R	203	X	-	-	-
27	CLA	a	303	X	-	-	-
27	CLA	a	304	X	-	-	-
27	CLA	a	305	X	-	-	-
27	CLA	a	306	X	-	-	-
27	CLA	a	308	X	-	-	-
27	CLA	a	309	X	-	-	-
27	CLA	a	310	X	-	-	-
27	CLA	a	311	X	-	-	-
27	CLA	a	313	X	-	-	-
27	CLA	b	601	X	-	-	-
27	CLA	b	602	X	-	-	-
27	CLA	b	603	X	-	-	-
27	CLA	b	605	X	-	-	-
27	CLA	b	606	X	-	-	-
27	CLA	b	607	X	-	-	-
27	CLA	b	608	X	-	-	-
27	CLA	b	610	X	-	-	-
27	CLA	b	611	X	-	-	-
27	CLA	c	601	X	-	-	-
27	CLA	c	602	X	-	-	-
27	CLA	c	603	X	-	-	-
27	CLA	c	605	X	-	-	-
27	CLA	c	607	X	-	-	-
27	CLA	c	608	X	-	-	-
27	CLA	c	609	X	-	-	-
27	CLA	c	612	X	-	-	-
27	CLA	d	301	X	-	-	-
27	CLA	d	302	X	-	-	-
27	CLA	d	303	X	-	-	-
27	CLA	d	305	X	-	-	-
27	CLA	d	306	X	-	-	-
27	CLA	d	308	X	-	-	-
27	CLA	e	601	X	-	-	-
27	CLA	e	602	X	-	-	-
27	CLA	e	603	X	-	-	-
27	CLA	e	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	e	607	X	-	-	-
27	CLA	e	608	X	-	-	-
27	CLA	e	610	X	-	-	-
27	CLA	f	601	X	-	-	-
27	CLA	f	602	X	-	-	-
27	CLA	f	603	X	-	-	-
27	CLA	f	604	X	-	-	-
27	CLA	f	607	X	-	-	-
27	CLA	f	608	X	-	-	-
27	CLA	f	609	X	-	-	-
27	CLA	f	610	X	-	-	-
27	CLA	f	612	X	-	-	-
27	CLA	g	302	X	-	-	-
27	CLA	g	303	X	-	-	-
27	CLA	g	304	X	-	-	-
27	CLA	g	305	X	-	-	-
27	CLA	g	306	X	-	-	-
27	CLA	g	308	X	-	-	-
27	CLA	g	309	X	-	-	-
27	CLA	g	310	X	-	-	-
27	CLA	g	311	X	-	-	-
27	CLA	g	322	X	-	-	-
27	CLA	h	301	X	-	-	-
27	CLA	h	302	X	-	-	-
27	CLA	h	303	X	-	-	-
27	CLA	h	304	X	-	-	-
27	CLA	h	305	X	-	-	-
27	CLA	h	306	X	-	-	-
27	CLA	h	307	X	-	-	-
27	CLA	h	308	X	-	-	-
27	CLA	h	313	X	-	-	-
27	CLA	i	302	X	-	-	-
27	CLA	i	303	X	-	-	-
27	CLA	i	304	X	-	-	-
27	CLA	i	305	X	-	-	-
27	CLA	i	306	X	-	-	-
27	CLA	i	307	X	-	-	-
27	CLA	i	308	X	-	-	-
27	CLA	i	309	X	-	-	-
27	CLA	i	311	X	-	-	-
27	CLA	i	312	X	-	-	-
27	CLA	j	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	j	602	X	-	-	-
27	CLA	j	603	X	-	-	-
27	CLA	j	604	X	-	-	-
27	CLA	j	607	X	-	-	-
27	CLA	j	608	X	-	-	-
27	CLA	j	609	X	-	-	-
27	CLA	j	611	X	-	-	-
27	CLA	j	612	X	-	-	-
27	CLA	k	301	X	-	-	-
27	CLA	k	302	X	-	-	-
27	CLA	k	303	X	-	-	-
27	CLA	k	304	X	-	-	-
27	CLA	k	305	X	-	-	-
27	CLA	k	306	X	-	-	-
27	CLA	k	307	X	-	-	-
27	CLA	k	308	X	-	-	-
27	CLA	k	309	X	-	-	-
27	CLA	k	313	X	-	-	-
27	CLA	l	303	X	-	-	-
27	CLA	l	304	X	-	-	-
27	CLA	l	305	X	-	-	-
27	CLA	l	307	X	-	-	-
27	CLA	l	308	X	-	-	-
27	CLA	l	309	X	-	-	-
27	CLA	l	310	X	-	-	-
27	CLA	l	312	X	-	-	-
27	CLA	m	601	X	-	-	-
27	CLA	m	602	X	-	-	-
27	CLA	m	603	X	-	-	-
27	CLA	m	605	X	-	-	-
27	CLA	m	606	X	-	-	-
27	CLA	m	607	X	-	-	-
27	CLA	m	608	X	-	-	-
27	CLA	m	609	X	-	-	-
27	CLA	m	611	X	-	-	-
27	CLA	m	612	X	-	-	-
27	CLA	n	601	X	-	-	-
27	CLA	n	602	X	-	-	-
27	CLA	n	603	X	-	-	-
27	CLA	n	604	X	-	-	-
27	CLA	n	605	X	-	-	-
27	CLA	n	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	n	607	X	-	-	-
27	CLA	n	608	X	-	-	-
27	CLA	n	609	X	-	-	-
27	CLA	n	610	X	-	-	-
27	CLA	n	613	X	-	-	-
27	CLA	s	202	X	-	-	-
27	CLA	s	206	X	-	-	-
27	CLA	s	209	X	-	-	-
32	SF4	A	854	-	-	X	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 59342 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1083	692	186	202	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
			485	309	84	92		

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called PsaO.

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

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

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

- Molecule 13 is a protein called chain s.

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

- Molecule 14 is a protein called CAC-c.

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

- Molecule 15 is a protein called CAC-a.

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

- Molecule 16 is a protein called CAC-b.

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

- Molecule 17 is a protein called CAC-h.

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

- Molecule 18 is a protein called CAC-m, CAC-f.

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

- Molecule 19 is a protein called CAC-e.

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

- Molecule 20 is a protein called CAC-l.

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

- Molecule 21 is a protein called CAC-k.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	k	160	Total	C	N	O	S	0	0
			1196	774	199	213	10		

- Molecule 22 is a protein called CAC-i.

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

- Molecule 23 is a protein called CAC-d.

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

- Molecule 24 is a protein called CAC-g.

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

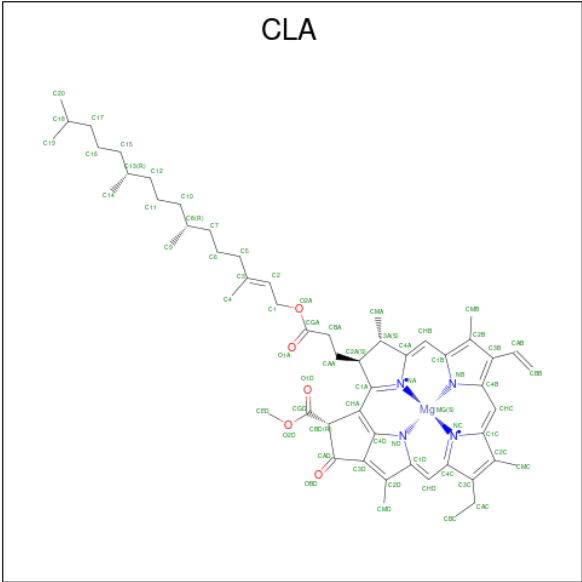
- Molecule 25 is a protein called PsaR.

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

- Molecule 26 is a protein called CAC-n.

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

- Molecule 27 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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

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Mol	Chain	Residues	Atoms					AltConf
27	K	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	s	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	s	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
27	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	h	1	Total 50	C 40	Mg 1	N 4	O 5	0

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

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

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

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

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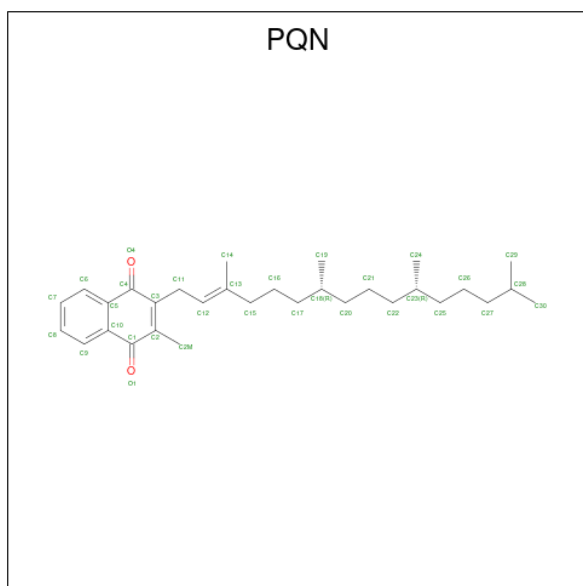
Mol	Chain	Residues	Atoms					AltConf
27	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
27	d	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
27	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	g	1	Total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

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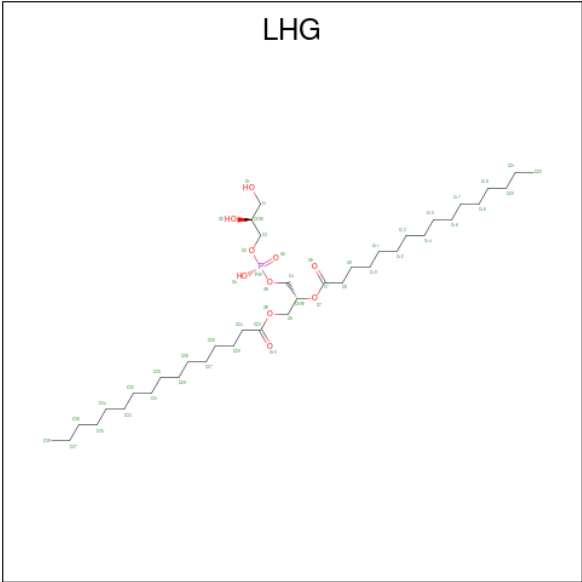
Mol	Chain	Residues	Atoms					AltConf
27	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



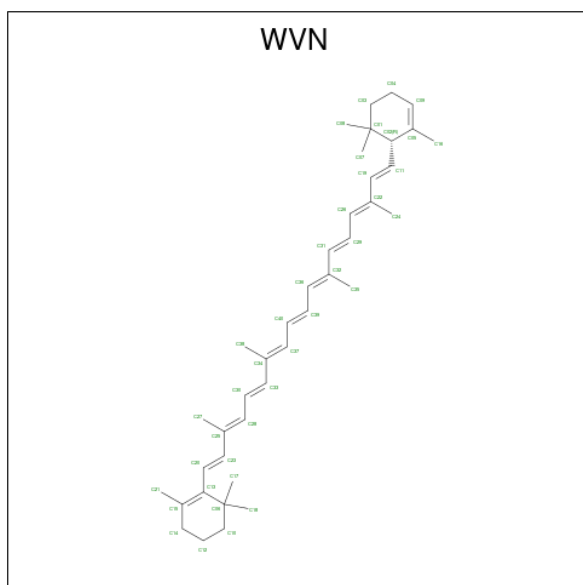
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O	P	0
			48	37	10	1	
29	A	1	Total	C	O	P	0
			27	16	10	1	
29	A	1	Total	C	O	P	0
			38	27	10	1	
29	J	1	Total	C	O	P	0
			49	38	10	1	
29	L	1	Total	C	O	P	0
			49	38	10	1	
29	c	1	Total	C	O	P	0
			37	26	10	1	
29	c	1	Total	C	O	P	0
			37	26	10	1	
29	a	1	Total	C	O	P	0
			49	38	10	1	
29	a	1	Total	C	O	P	0
			49	38	10	1	
29	b	1	Total	C	O	P	0
			49	38	10	1	
29	b	1	Total	C	O	P	0
			31	20	10	1	
29	m	1	Total	C	O	P	0
			37	26	10	1	
29	e	1	Total	C	O	P	0
			37	26	10	1	
29	l	1	Total	C	O	P	0
			32	21	10	1	

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Mol	Chain	Residues	Atoms				AltConf
29	k	1	Total	C	O	P	0
			37	26	10	1	
29	f	1	Total	C	O	P	0
			49	38	10	1	
29	i	1	Total	C	O	P	0
			37	26	10	1	
29	j	1	Total	C	O	P	0
			30	19	10	1	
29	d	1	Total	C	O	P	0
			37	26	10	1	
29	g	1	Total	C	O	P	0
			37	26	10	1	
29	g	1	Total	C	O	P	0
			37	26	10	1	
29	n	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 30 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
30	A	1	Total	C	0
			40	40	
30	A	1	Total	C	0
			40	40	

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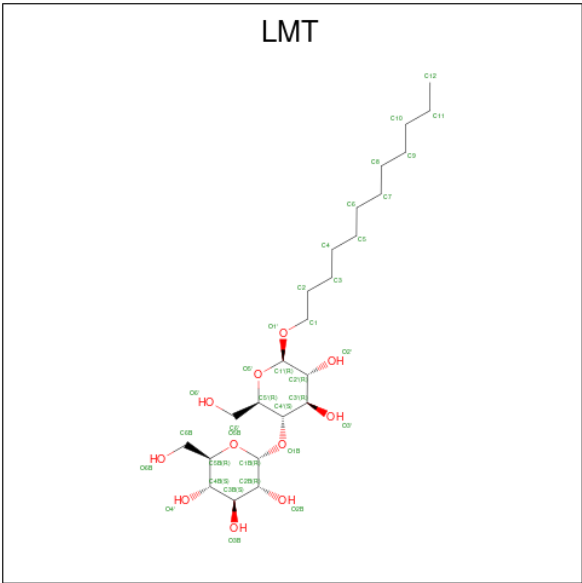
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	I	1	Total C 40 40	0
30	J	1	Total C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

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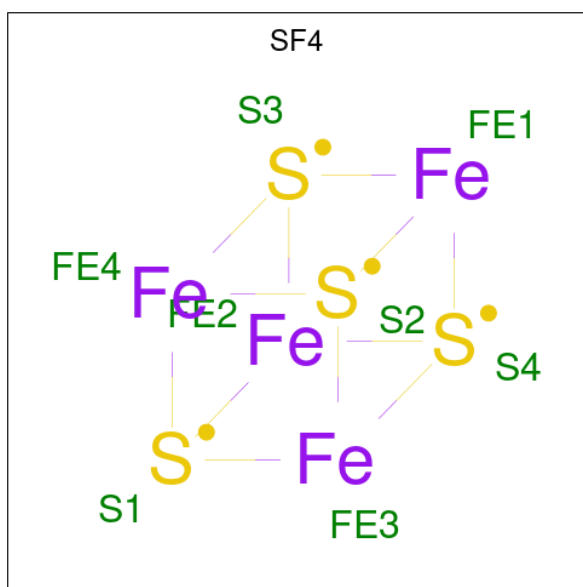
Mol	Chain	Residues	Atoms	AltConf
30	e	1	Total C 40 40	0
30	l	1	Total C 40 40	0
30	l	1	Total C 40 40	0
30	i	1	Total C 40 40	0
30	R	1	Total C 40 40	0
30	R	1	Total C 40 40	0

- Molecule 31 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



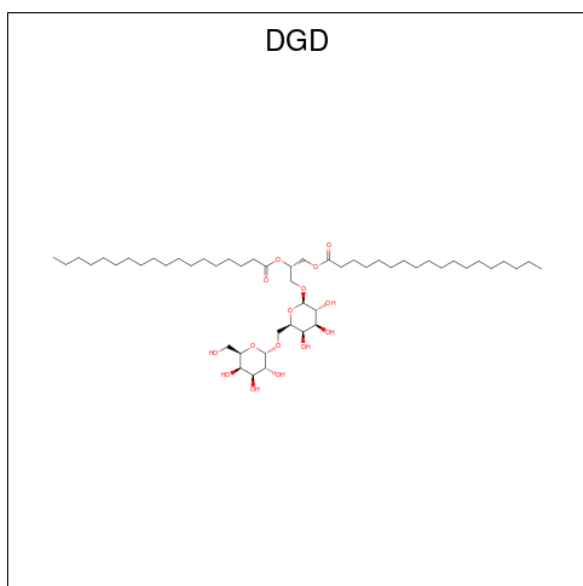
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C O 35 24 11	0
31	a	1	Total C O 24 18 6	0
31	a	1	Total C O 35 24 11	0
31	b	1	Total C O 24 18 6	0

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



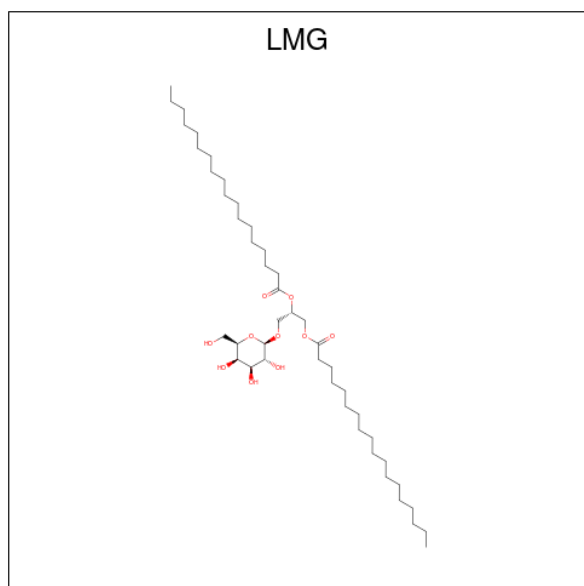
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	Fe	S	0
			8	4	4	
32	C	1	Total	Fe	S	0
			8	4	4	
32	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



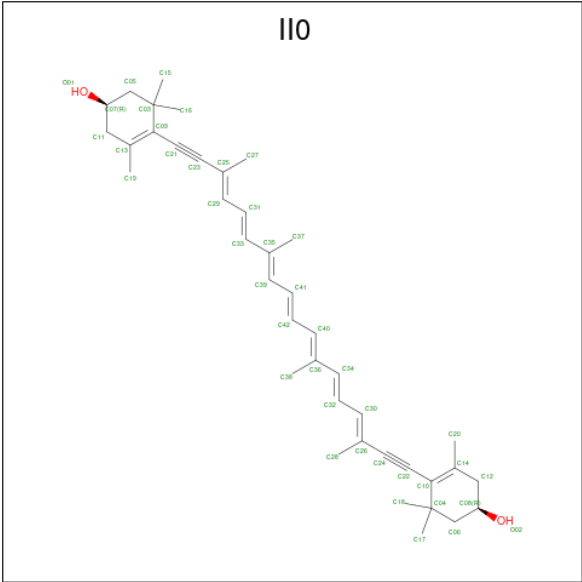
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			60	45	15	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
34	F	1	Total	C	O	0
			48	38	10	
34	J	1	Total	C	O	0
			55	45	10	
34	L	1	Total	C	O	0
			55	45	10	
34	O	1	Total	C	O	0
			26	16	10	
34	s	1	Total	C	O	0
			55	45	10	
34	c	1	Total	C	O	0
			55	45	10	
34	b	1	Total	C	O	0
			49	39	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: $C_{40}H_{52}O_2$).



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

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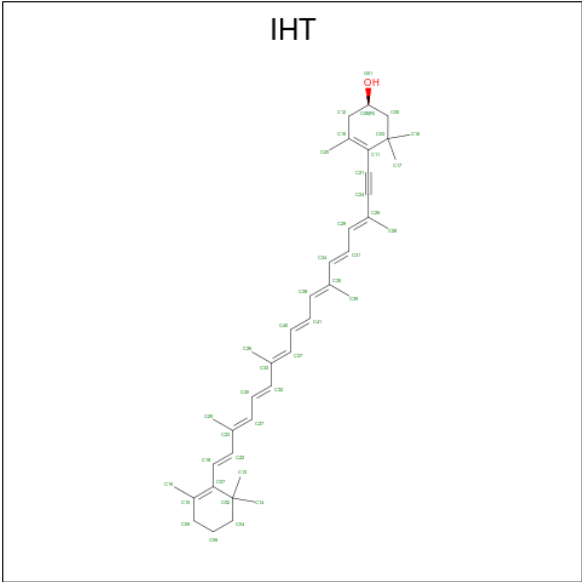
Mol	Chain	Residues	Atoms			AltConf
35	h	1	Total	C	O	0
			42	40	2	
35	h	1	Total	C	O	0
			42	40	2	
35	m	1	Total	C	O	0
			42	40	2	
35	m	1	Total	C	O	0
			42	40	2	
35	m	1	Total	C	O	0
			42	40	2	
35	e	1	Total	C	O	0
			42	40	2	
35	e	1	Total	C	O	0
			42	40	2	
35	e	1	Total	C	O	0
			42	40	2	
35	e	1	Total	C	O	0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

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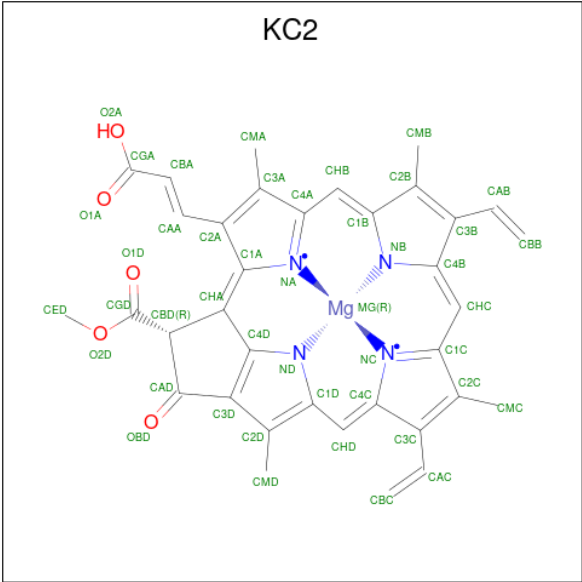
Mol	Chain	Residues	Atoms			AltConf
35	f	1	Total	C	O	0
			42	40	2	
35	i	1	Total	C	O	0
			42	40	2	
35	i	1	Total	C	O	0
			42	40	2	
35	i	1	Total	C	O	0
			42	40	2	
35	j	1	Total	C	O	0
			42	40	2	
35	j	1	Total	C	O	0
			42	40	2	
35	j	1	Total	C	O	0
			42	40	2	
35	d	1	Total	C	O	0
			42	40	2	
35	d	1	Total	C	O	0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

- Molecule 36 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).



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

- Molecule 37 is Chlorophyll c2 (CCD ID: KC2) (formula: C₃₅H₂₈MgN₄O₅).



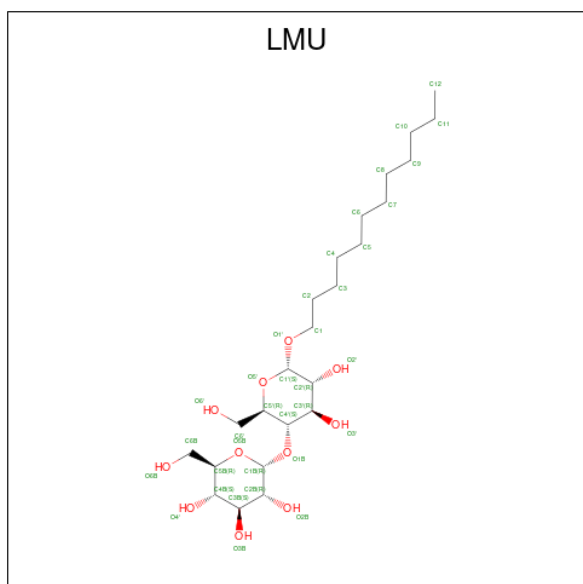
Mol	Chain	Residues	Atoms					AltConf
37	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	k	1	Total	C	Mg	N	O	0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

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

- Molecule 38 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	49	Total	O	0
			49	49	
39	B	58	Total	O	0
			58	58	

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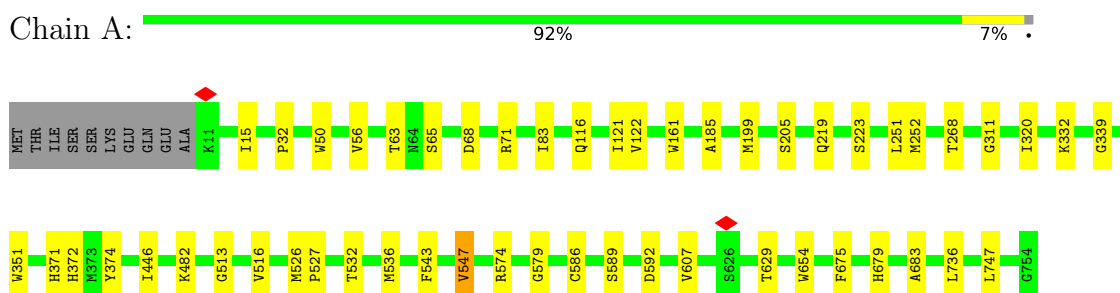
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Mol	Chain	Residues	Atoms		AltConf
39	C	7	Total 7	O 7	0
39	D	1	Total 1	O 1	0
39	F	4	Total 4	O 4	0
39	I	1	Total 1	O 1	0
39	J	1	Total 1	O 1	0
39	L	1	Total 1	O 1	0
39	O	1	Total 1	O 1	0
39	K	1	Total 1	O 1	0
39	a	3	Total 3	O 3	0
39	b	2	Total 2	O 2	0
39	h	1	Total 1	O 1	0
39	m	1	Total 1	O 1	0
39	e	4	Total 4	O 4	0
39	n	2	Total 2	O 2	0

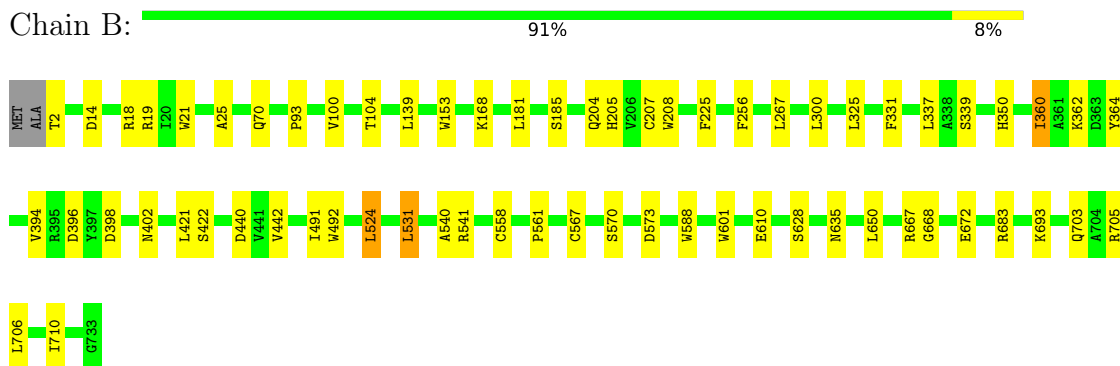
3 Residue-property plots

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

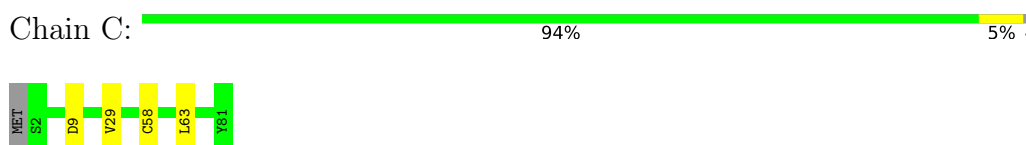
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



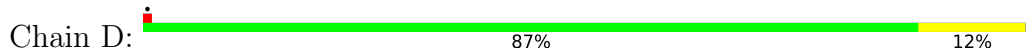
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center

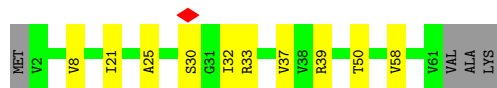
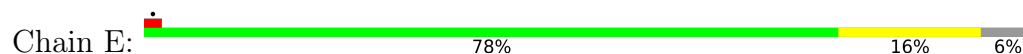


- Molecule 4: Photosystem I reaction center subunit II

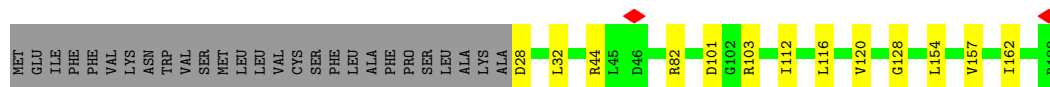
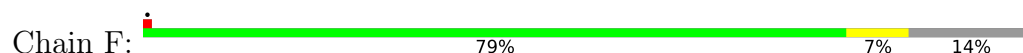




- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 6: Photosystem I reaction center subunit III



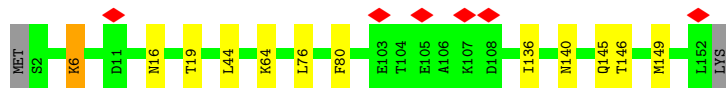
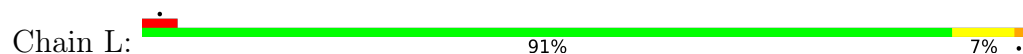
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 9: Photosystem I reaction center subunit XI

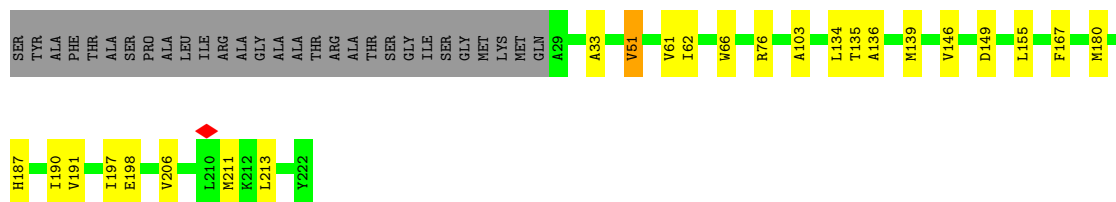


- Molecule 10: Photosystem I reaction center subunit XII



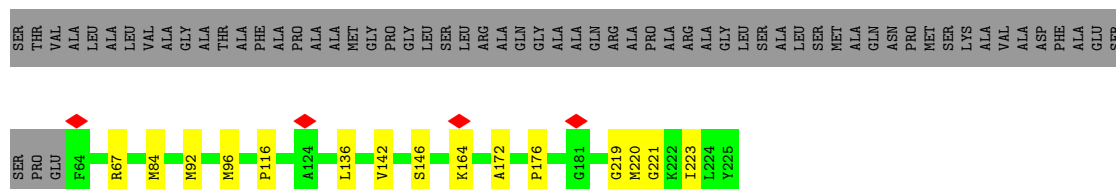
- Molecule 11: PsaO

Chain b:  76% 10% 13%



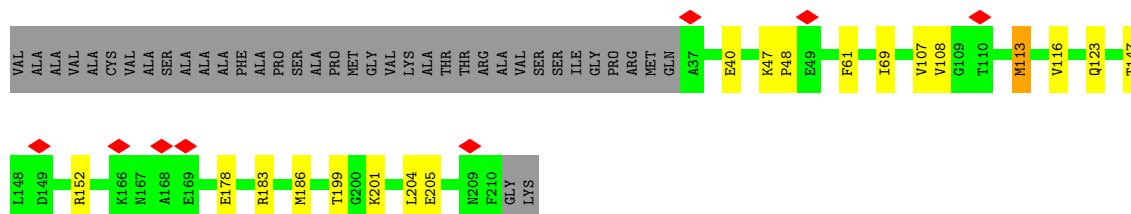
• Molecule 17: CAC-h

Chain h:  65% 7% 28%



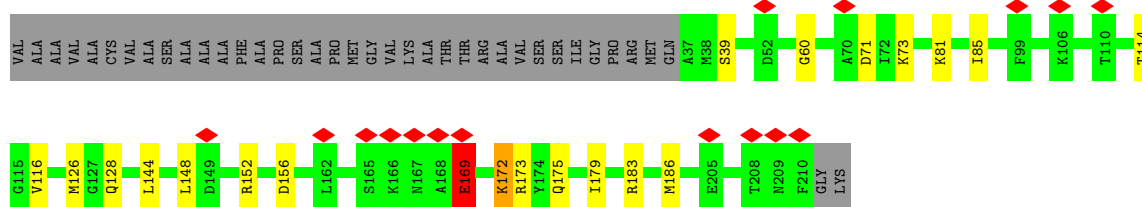
• Molecule 18: CAC-m, CAC-f

Chain m:  73% 8% 18%



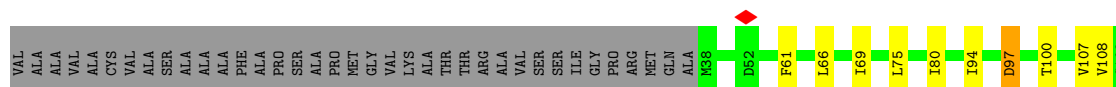
• Molecule 18: CAC-m, CAC-f

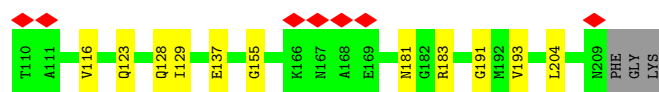
Chain f:  8% 72% 9% 18%



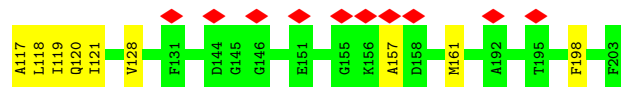
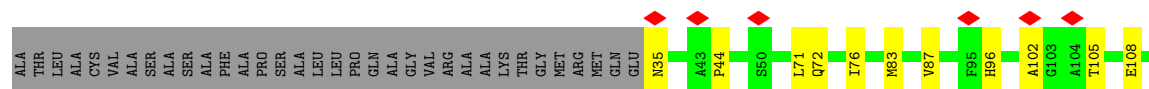
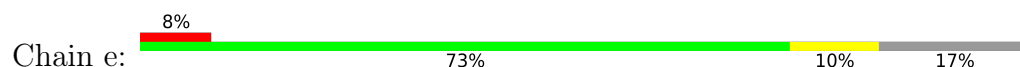
• Molecule 18: CAC-m, CAC-f

Chain j:  71% 9% 19%

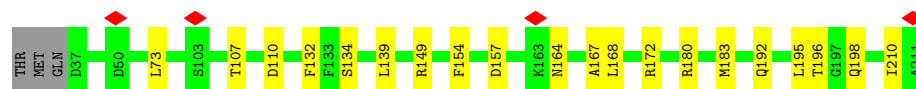
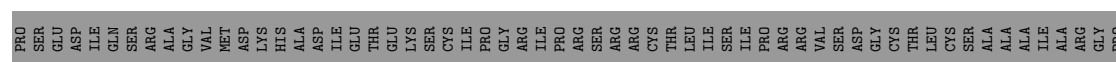




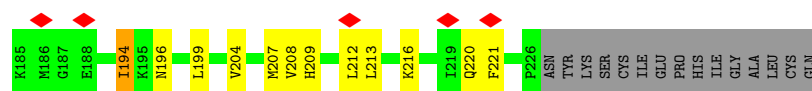
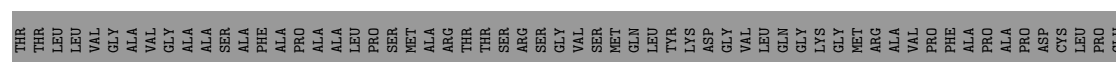
- Molecule 19: CAC-e



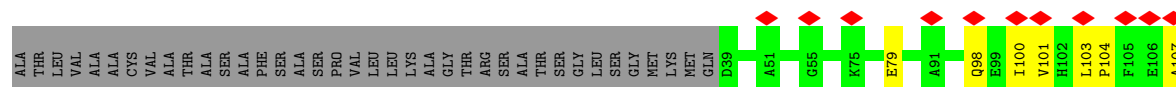
- Molecule 20: CAC-l

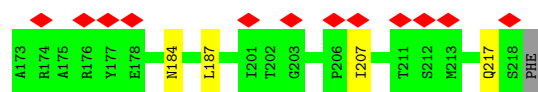


- Molecule 21: CAC-k

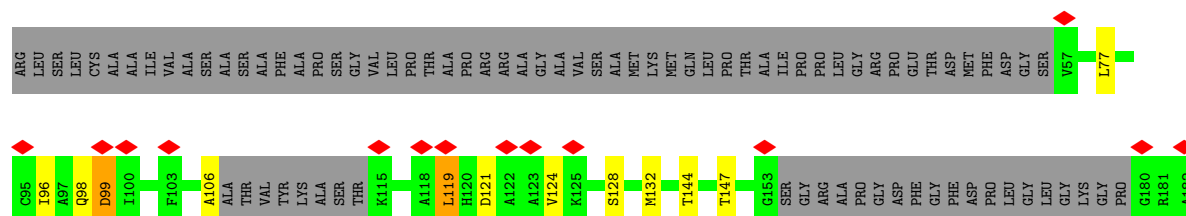


- Molecule 22: CAC-i

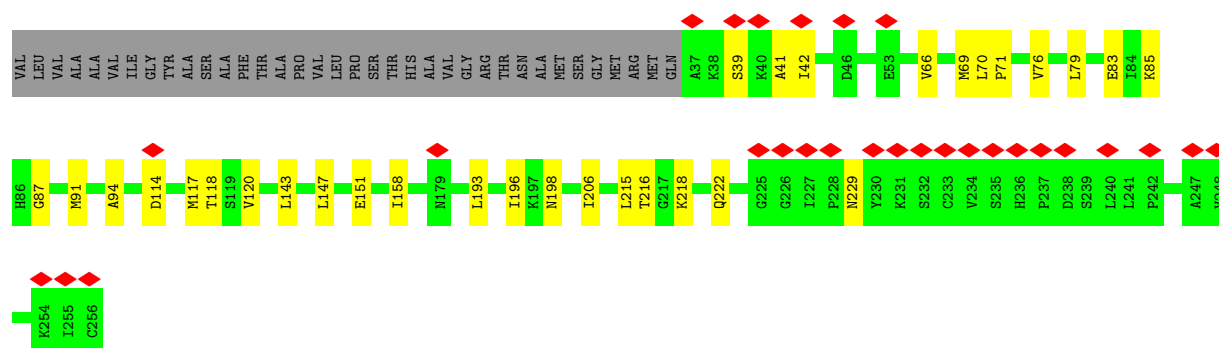
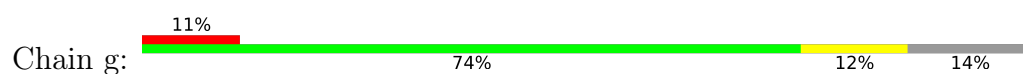




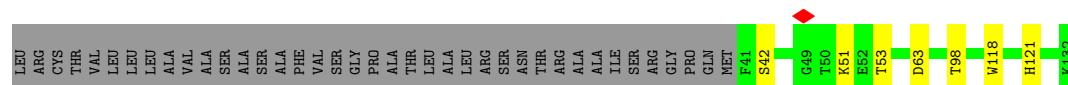
• Molecule 23: CAC-d



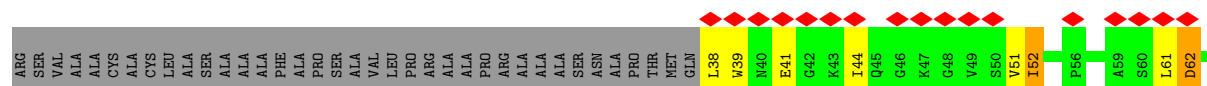
• Molecule 24: CAC-g

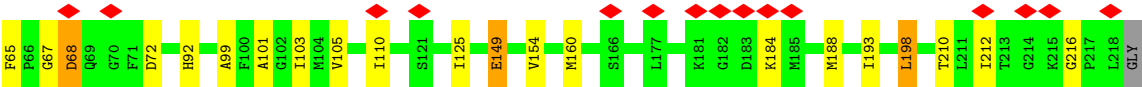


• Molecule 25: PsaR



• Molecule 26: CAC-n





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42423	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.206	Depositor
Minimum map value	-0.100	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.023	Depositor
Map size ($\text{\AA}$)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.52	0/6019	0.76	0/8204
2	B	0.54	1/6045 (0.0%)	0.80	3/8254 (0.0%)
3	C	0.43	0/601	0.82	0/813
4	D	0.50	0/1108	0.79	0/1499
5	E	0.48	0/493	0.77	0/667
6	F	0.55	0/1287	0.83	0/1747
7	I	0.60	0/271	0.81	0/370
8	J	0.45	0/364	0.77	0/495
9	L	0.48	0/1175	0.80	0/1599
10	M	0.48	0/233	0.90	2/315 (0.6%)
11	O	0.59	0/799	0.85	0/1094
12	K	0.48	0/495	0.86	0/672
13	s	0.55	0/1170	0.85	0/1580
14	c	0.57	0/1396	0.88	0/1889
15	a	0.50	0/1406	0.81	0/1903
16	b	0.57	0/1469	0.91	0/1983
17	h	0.56	0/1226	0.94	0/1667
18	f	0.51	0/1328	0.87	1/1790 (0.1%)
18	j	0.61	0/1318	0.94	2/1775 (0.1%)
18	m	0.52	0/1335	0.85	1/1798 (0.1%)
19	e	0.54	0/1324	0.88	0/1795
20	l	0.52	0/1379	0.83	0/1863
21	k	0.61	0/1223	0.95	0/1651
22	i	0.55	0/1359	0.91	0/1835
23	d	0.50	0/993	0.87	1/1335 (0.1%)
24	g	0.57	0/1673	0.90	0/2264
25	R	0.45	0/686	0.79	1/940 (0.1%)
26	n	0.63	0/1383	0.94	1/1867 (0.1%)
All	All	0.54	1/39558 (0.0%)	0.84	12/53664 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	635	ASN	C-N	5.04	1.39	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	362	LYS	N-CA-C	-7.16	104.69	113.50
18	m	113	MET	CB-CA-C	-5.95	109.72	116.63
2	B	667	ARG	N-CA-C	5.81	117.61	111.28
18	j	191	GLY	CA-C-N	5.80	128.33	120.44
18	j	191	GLY	C-N-CA	5.80	128.33	120.44

There are no chirality outliers.

There are no planarity outliers.

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	5825	0	5678	37	0
2	B	5826	0	5642	50	0
3	C	592	0	567	3	0
4	D	1083	0	1077	11	0
5	E	485	0	489	5	0
6	F	1254	0	1264	13	0
7	I	264	0	276	7	0
8	J	351	0	344	4	0
9	L	1146	0	1160	14	0
10	M	232	0	265	4	0
11	O	773	0	765	31	0
12	K	488	0	516	6	0
13	s	1140	0	1099	9	0
14	c	1357	0	1337	14	0
15	a	1361	0	1305	4	0
16	b	1439	0	1456	18	0
17	h	1200	0	1228	10	0
18	f	1302	0	1320	30	0
18	j	1293	0	1321	17	0
18	m	1309	0	1335	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	e	1286	0	1262	15	0
20	l	1344	0	1315	14	0
21	k	1196	0	1204	26	0
22	i	1324	0	1297	18	0
23	d	974	0	978	10	0
24	g	1630	0	1644	20	0
25	R	664	0	647	3	0
26	n	1350	0	1348	22	0
27	A	2758	0	2820	78	0
27	B	2440	0	2452	46	0
27	F	182	0	187	7	0
27	J	93	0	72	2	0
27	K	93	0	72	0	0
27	L	215	0	191	5	0
27	O	130	0	144	2	0
27	R	51	0	41	0	0
27	a	619	0	588	11	0
27	b	673	0	696	22	0
27	c	586	0	520	9	0
27	d	447	0	366	6	0
27	e	582	0	578	23	0
27	f	700	0	695	25	0
27	g	661	0	611	14	0
27	h	505	0	470	11	0
27	i	528	0	451	11	0
27	j	586	0	515	16	0
27	k	545	0	493	14	0
27	l	535	0	538	12	0
27	m	600	0	565	21	0
27	n	605	0	552	14	0
27	s	297	0	298	8	0
28	A	33	0	46	2	0
28	B	33	0	46	1	0
29	A	113	0	142	4	0
29	J	49	0	74	6	0
29	L	49	0	74	2	0
29	a	98	0	148	2	0
29	b	80	0	106	6	0
29	c	74	0	88	6	0
29	d	37	0	44	0	0
29	e	37	0	44	1	0
29	f	49	0	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	g	74	0	88	4	0
29	i	37	0	44	1	0
29	j	30	0	30	2	0
29	k	37	0	44	0	0
29	l	32	0	34	2	0
29	m	37	0	44	0	0
29	n	43	0	59	1	0
30	A	160	0	0	0	0
30	B	240	0	0	0	0
30	F	80	0	0	0	0
30	I	40	0	0	0	0
30	J	80	0	0	0	0
30	K	40	0	0	0	0
30	L	80	0	0	0	0
30	M	40	0	0	0	0
30	O	40	0	0	0	0
30	R	80	0	0	0	0
30	e	40	0	0	0	0
30	h	40	0	0	0	0
30	i	40	0	0	0	0
30	l	80	0	0	0	0
30	s	80	0	0	1	0
31	A	35	0	44	1	0
31	a	59	0	79	1	0
31	b	24	0	34	1	0
32	A	8	0	0	5	0
32	C	16	0	0	0	0
33	B	60	0	81	2	0
34	F	48	0	69	1	0
34	J	55	0	86	3	0
34	L	55	0	86	2	0
34	O	26	0	22	0	0
34	b	49	0	71	2	0
34	c	55	0	86	3	0
34	s	55	0	86	3	0
35	J	42	0	0	0	0
35	O	42	0	0	0	0
35	a	168	0	0	0	0
35	b	126	0	0	1	0
35	c	168	0	0	0	0
35	d	126	0	0	0	0
35	e	168	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	f	168	0	0	1	0
35	g	168	0	0	0	0
35	h	112	0	0	1	0
35	i	126	0	0	1	0
35	j	126	0	0	1	0
35	k	168	0	0	1	0
35	l	210	0	0	2	0
35	m	126	0	0	1	0
35	n	168	0	0	1	0
36	O	41	0	0	0	0
36	R	41	0	0	0	0
36	a	41	0	0	0	0
36	b	41	0	0	3	0
36	c	82	0	0	1	0
36	f	41	0	0	2	0
36	g	41	0	0	1	0
36	j	41	0	0	2	0
36	k	41	0	0	0	0
36	m	41	0	0	0	0
36	n	41	0	0	0	0
37	c	45	0	0	0	0
37	d	90	0	0	0	0
37	e	45	0	0	0	0
37	f	45	0	0	2	0
37	g	135	0	0	0	0
37	i	90	0	0	1	0
37	j	45	0	0	1	0
37	k	135	0	0	4	0
37	l	45	0	0	1	0
37	m	45	0	0	7	0
37	n	90	0	0	0	0
37	s	90	0	0	0	0
38	i	35	0	46	1	0
39	A	49	0	0	0	0
39	B	58	0	0	1	0
39	C	7	0	0	0	0
39	D	1	0	0	0	0
39	F	4	0	0	0	0
39	I	1	0	0	0	0
39	J	1	0	0	0	0
39	K	1	0	0	0	0
39	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	O	1	0	0	0	0
39	a	3	0	0	0	0
39	b	2	0	0	0	0
39	e	4	0	0	0	0
39	h	1	0	0	0	0
39	m	1	0	0	0	0
39	n	2	0	0	0	0
All	All	59342	0	54073	645	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 645 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)
11:O:27:GLN:HB2	18:f:148:LEU:O	1.49	1.12
11:O:27:GLN:OE1	18:f:148:LEU:O	1.63	1.11
11:O:27:GLN:CB	18:f:148:LEU:O	2.05	1.04
21:k:221:PHE:HE2	37:k:311:KC2:CED	1.71	1.02
26:n:67:GLY:HA3	26:n:193:ILE:HG21	1.37	1.02

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%)	720 (97%)	20 (3%)	0	100	100
2	B	731/734 (100%)	705 (96%)	26 (4%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	137/141 (97%)	133 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	58/64 (91%)	56 (97%)	2 (3%)	0	100	100
6	F	159/188 (85%)	156 (98%)	3 (2%)	0	100	100
7	I	32/36 (89%)	32 (100%)	0	0	100	100
8	J	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
9	L	149/153 (97%)	148 (99%)	1 (1%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
11	O	102/146 (70%)	94 (92%)	8 (8%)	0	100	100
12	K	65/87 (75%)	65 (100%)	0	0	100	100
13	s	152/269 (56%)	145 (95%)	7 (5%)	0	100	100
14	c	168/216 (78%)	162 (96%)	6 (4%)	0	100	100
15	a	173/216 (80%)	166 (96%)	7 (4%)	0	100	100
16	b	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
17	h	160/225 (71%)	156 (98%)	4 (2%)	0	100	100
18	f	172/212 (81%)	166 (96%)	6 (4%)	0	100	100
18	j	170/212 (80%)	163 (96%)	7 (4%)	0	100	100
18	m	172/212 (81%)	164 (95%)	8 (5%)	0	100	100
19	e	167/203 (82%)	164 (98%)	3 (2%)	0	100	100
20	l	173/238 (73%)	169 (98%)	4 (2%)	0	100	100
21	k	158/241 (66%)	151 (96%)	7 (4%)	0	100	100
22	i	171/218 (78%)	161 (94%)	9 (5%)	1 (1%)	21	45
23	d	123/213 (58%)	122 (99%)	1 (1%)	0	100	100
24	g	217/255 (85%)	202 (93%)	15 (7%)	0	100	100
25	R	88/129 (68%)	85 (97%)	3 (3%)	0	100	100
26	n	179/219 (82%)	172 (96%)	7 (4%)	0	100	100
All	All	4954/5955 (83%)	4788 (97%)	165 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	i	142	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	607/616 (98%)	604 (100%)	3 (0%)	81	90
2	B	593/593 (100%)	587 (99%)	6 (1%)	68	81
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	115/117 (98%)	115 (100%)	0	100	100
5	E	55/58 (95%)	54 (98%)	1 (2%)	51	72
6	F	133/157 (85%)	133 (100%)	0	100	100
7	I	28/29 (97%)	28 (100%)	0	100	100
8	J	39/39 (100%)	39 (100%)	0	100	100
9	L	124/126 (98%)	123 (99%)	1 (1%)	73	84
10	M	25/25 (100%)	24 (96%)	1 (4%)	28	53
11	O	81/110 (74%)	78 (96%)	3 (4%)	30	55
12	K	52/66 (79%)	51 (98%)	1 (2%)	50	71
13	s	116/195 (60%)	114 (98%)	2 (2%)	53	73
14	c	138/171 (81%)	138 (100%)	0	100	100
15	a	139/165 (84%)	139 (100%)	0	100	100
16	b	149/168 (89%)	144 (97%)	5 (3%)	32	58
17	h	123/162 (76%)	123 (100%)	0	100	100
18	f	135/161 (84%)	131 (97%)	4 (3%)	36	61
18	j	136/161 (84%)	133 (98%)	3 (2%)	45	69
18	m	137/161 (85%)	131 (96%)	6 (4%)	25	50
19	e	130/155 (84%)	130 (100%)	0	100	100
20	l	137/191 (72%)	136 (99%)	1 (1%)	76	86
21	k	122/186 (66%)	119 (98%)	3 (2%)	42	66
22	i	138/168 (82%)	135 (98%)	3 (2%)	45	69
23	d	97/157 (62%)	94 (97%)	3 (3%)	35	60
24	g	171/199 (86%)	166 (97%)	5 (3%)	37	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	R	69/98 (70%)	68 (99%)	1 (1%)	59	76
26	n	140/163 (86%)	134 (96%)	6 (4%)	26	51
All	All	3996/4665 (86%)	3938 (98%)	58 (2%)	55	75

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	m	204	LEU
26	n	62	ASP
18	f	172	LYS
26	n	52	ILE
24	g	118	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
18	f	76	GLN
26	n	129	HIS
26	n	208	HIS
26	n	179	GLN
24	g	100	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](#)

407 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	n	614	-	39,43,43	6.72	21 (53%)	48,60,60	2.20	14 (29%)
27	CLA	e	603	19	55,59,73	1.31	6 (10%)	64,96,113	1.44	8 (12%)
37	KC2	f	611	18	49,53,53	2.75	19 (38%)	60,89,89	3.79	32 (53%)
30	WVN	B	843	-	40,41,41	1.73	11 (27%)	51,56,56	2.49	21 (41%)
27	CLA	B	813	-	59,63,73	1.20	7 (11%)	70,101,113	1.39	9 (12%)
35	II0	j	614	-	39,43,43	6.77	22 (56%)	48,60,60	2.07	15 (31%)
27	CLA	A	819	-	49,53,73	1.41	7 (14%)	58,89,113	1.72	10 (17%)
27	CLA	B	806	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	9 (10%)
27	CLA	f	604	18	69,73,73	1.13	7 (10%)	82,113,113	1.36	8 (9%)
27	CLA	g	306	24	55,59,73	1.31	5 (9%)	64,96,113	1.39	7 (10%)
30	WVN	F	205	-	40,41,41	1.79	13 (32%)	51,56,56	2.90	18 (35%)
27	CLA	B	824	-	69,73,73	1.17	7 (10%)	82,113,113	1.31	8 (9%)
27	CLA	g	305	24	69,73,73	1.18	8 (11%)	82,113,113	1.43	10 (12%)
27	CLA	B	833	-	51,55,73	1.29	7 (13%)	60,91,113	1.85	7 (11%)
27	CLA	l	310	29	65,69,73	1.19	7 (10%)	77,108,113	1.24	4 (5%)
27	CLA	a	310	29	52,56,73	1.27	6 (11%)	61,92,113	1.42	8 (13%)
30	WVN	l	316	-	40,41,41	1.79	10 (25%)	51,56,56	2.51	19 (37%)
36	IHT	f	617	-	40,42,42	6.23	26 (65%)	52,58,58	2.21	14 (26%)
27	CLA	A	856	29	45,49,73	1.48	11 (24%)	54,84,113	2.24	9 (16%)
30	WVN	J	101	-	40,41,41	1.68	10 (25%)	51,56,56	2.26	18 (35%)
27	CLA	a	313	-	52,56,73	1.30	7 (13%)	61,92,113	1.20	7 (11%)
27	CLA	A	821	-	53,57,73	1.28	9 (16%)	61,93,113	1.53	8 (13%)
27	CLA	c	611	14	49,53,73	1.40	8 (16%)	58,89,113	1.45	10 (17%)
30	WVN	i	315	-	40,41,41	1.78	10 (25%)	51,56,56	2.39	16 (31%)
27	CLA	B	826	-	54,58,73	1.27	7 (12%)	64,95,113	1.35	6 (9%)
27	CLA	m	605	18	46,50,73	1.37	8 (17%)	53,85,113	1.62	13 (24%)
36	IHT	c	620	-	40,42,42	6.21	25 (62%)	52,58,58	2.21	20 (38%)
35	II0	m	615	-	39,43,43	6.66	22 (56%)	48,60,60	1.78	10 (20%)
27	CLA	B	810	-	69,73,73	1.17	8 (11%)	82,113,113	1.54	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	KC2	d	309	23	49,53,53	2.77	20 (40%)	60,89,89	3.78	33 (55%)
27	CLA	g	309	-	69,73,73	1.19	8 (11%)	82,113,113	1.60	10 (12%)
27	CLA	g	302	24	46,50,73	1.37	7 (15%)	53,85,113	1.83	8 (15%)
27	CLA	B	822	-	69,73,73	1.19	8 (11%)	82,113,113	1.50	16 (19%)
30	WVN	s	207	-	40,41,41	1.74	11 (27%)	51,56,56	2.40	15 (29%)
27	CLA	A	832	-	69,73,73	1.15	5 (7%)	82,113,113	1.62	13 (15%)
27	CLA	B	825	-	55,59,73	1.32	8 (14%)	64,96,113	1.40	9 (14%)
27	CLA	n	603	-	55,59,73	1.34	7 (12%)	64,96,113	1.45	10 (15%)
27	CLA	g	308	-	69,73,73	1.18	7 (10%)	82,113,113	1.54	11 (13%)
37	KC2	l	311	20	49,53,53	2.74	20 (40%)	60,89,89	3.85	33 (55%)
30	WVN	F	204	-	40,41,41	1.67	11 (27%)	51,56,56	2.54	20 (39%)
27	CLA	f	610	29	69,73,73	1.16	7 (10%)	82,113,113	1.26	8 (9%)
27	CLA	B	827	-	53,57,73	1.27	7 (13%)	61,93,113	1.45	9 (14%)
35	II0	b	613	-	39,43,43	6.69	24 (61%)	48,60,60	1.90	11 (22%)
32	SF4	C	102	3	0,12,12	-	-	-	-	-
35	II0	m	613	-	39,43,43	6.61	20 (51%)	48,60,60	1.77	13 (27%)
35	II0	f	616	-	39,43,43	6.58	20 (51%)	48,60,60	1.98	14 (29%)
37	KC2	e	609	19	49,53,53	2.77	20 (40%)	60,89,89	3.78	33 (55%)
29	LHG	g	301	27	36,36,48	1.14	2 (5%)	39,42,54	1.45	6 (15%)
35	II0	c	614	-	39,43,43	6.68	21 (53%)	48,60,60	2.18	16 (33%)
38	LMU	i	301	-	36,36,36	1.22	3 (8%)	47,47,47	1.47	7 (14%)
27	CLA	i	304	-	55,59,73	1.30	7 (12%)	64,96,113	1.38	9 (14%)
35	II0	a	318	-	39,43,43	6.87	21 (53%)	48,60,60	2.60	16 (33%)
27	CLA	A	812	-	69,73,73	1.16	9 (13%)	82,113,113	1.51	13 (15%)
35	II0	d	313	-	39,43,43	6.86	21 (53%)	48,60,60	1.66	14 (29%)
33	DGD	B	842	-	61,61,67	0.90	2 (3%)	75,75,81	1.10	3 (4%)
37	KC2	c	610	-	49,53,53	2.76	20 (40%)	60,89,89	3.72	31 (51%)
27	CLA	L	202	9	53,57,73	1.32	8 (15%)	61,93,113	1.44	7 (11%)
29	LHG	c	621	27	36,36,48	1.09	2 (5%)	39,42,54	1.27	3 (7%)
27	CLA	d	302	-	55,59,73	1.26	6 (10%)	64,96,113	1.34	9 (14%)
27	CLA	A	833	-	54,58,73	1.27	6 (11%)	64,95,113	1.33	6 (9%)
35	II0	c	613	-	39,43,43	6.71	22 (56%)	48,60,60	2.08	14 (29%)
27	CLA	A	825	39	69,73,73	1.16	9 (13%)	82,113,113	1.26	8 (9%)
35	II0	i	318	-	39,43,43	6.60	22 (56%)	48,60,60	1.78	8 (16%)
30	WVN	K	103	-	40,41,41	1.71	10 (25%)	51,56,56	1.99	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	SF4	C	101	3	0,12,12	-	-	-		
29	LHG	A	850	-	37,37,48	1.05	2 (5%)	40,43,54	1.20	3 (7%)
27	CLA	A	838	29	56,60,73	1.26	7 (12%)	65,97,113	1.50	7 (10%)
35	II0	i	314	-	39,43,43	6.61	22 (56%)	48,60,60	1.92	14 (29%)
30	WVN	B	844	-	40,41,41	1.58	13 (32%)	51,56,56	2.56	24 (47%)
27	CLA	A	824	39	69,73,73	1.16	8 (11%)	82,113,113	1.45	11 (13%)
27	CLA	A	828	-	69,73,73	1.17	10 (14%)	82,113,113	1.38	10 (12%)
27	CLA	L	204	39	54,58,73	1.40	10 (18%)	64,95,113	1.44	9 (14%)
35	II0	c	617	-	39,43,43	6.66	21 (53%)	48,60,60	2.12	15 (31%)
35	II0	a	316	-	39,43,43	6.79	21 (53%)	48,60,60	1.90	13 (27%)
27	CLA	m	609	29	59,63,73	1.28	5 (8%)	70,101,113	1.52	11 (15%)
35	II0	n	615	-	39,43,43	6.74	23 (58%)	48,60,60	1.92	13 (27%)
27	CLA	d	306	23	50,54,73	1.34	7 (14%)	59,90,113	1.35	6 (10%)
35	II0	g	318	-	39,43,43	6.54	19 (48%)	48,60,60	2.06	15 (31%)
27	CLA	d	305	-	55,59,73	1.28	6 (10%)	64,96,113	1.54	9 (14%)
37	KC2	n	611	26	49,53,53	2.71	19 (38%)	60,89,89	3.87	33 (55%)
27	CLA	h	306	17	69,73,73	1.17	7 (10%)	82,113,113	1.28	11 (13%)
36	IHT	g	319	-	40,42,42	6.20	25 (62%)	52,58,58	2.25	17 (32%)
27	CLA	h	305	-	55,59,73	1.26	8 (14%)	64,96,113	1.40	8 (12%)
27	CLA	B	840	29	69,73,73	1.16	8 (11%)	82,113,113	1.33	10 (12%)
36	IHT	R	204	-	40,42,42	6.31	26 (65%)	52,58,58	2.23	16 (30%)
27	CLA	f	612	18	55,59,73	1.34	8 (14%)	64,96,113	1.51	15 (23%)
27	CLA	A	807	1	69,73,73	1.15	7 (10%)	82,113,113	1.31	5 (6%)
27	CLA	A	822	-	55,59,73	1.31	8 (14%)	64,96,113	1.43	6 (9%)
27	CLA	i	312	-	55,59,73	1.28	5 (9%)	64,96,113	1.43	9 (14%)
27	CLA	j	606	18	55,59,73	1.32	6 (10%)	64,96,113	1.73	10 (15%)
27	CLA	g	303	24	54,58,73	1.23	6 (11%)	64,95,113	1.44	8 (12%)
27	CLA	A	808	1	69,73,73	1.12	5 (7%)	82,113,113	1.38	12 (14%)
27	CLA	d	311	-	55,59,73	1.29	6 (10%)	64,96,113	1.50	11 (17%)
37	KC2	g	312	24	49,53,53	2.75	20 (40%)	60,89,89	3.74	33 (55%)
27	CLA	j	608	18	55,59,73	1.28	6 (10%)	64,96,113	1.41	12 (18%)
31	LMT	a	320	-	36,36,36	0.40	0	47,47,47	1.06	4 (8%)
36	IHT	n	617	-	40,42,42	6.28	26 (65%)	52,58,58	2.36	16 (30%)
27	CLA	k	307	21	69,73,73	1.19	7 (10%)	82,113,113	1.30	5 (6%)
27	CLA	i	302	22	55,59,73	1.30	5 (9%)	64,96,113	1.35	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	KC2	i	310	22	49,53,53	2.76	20 (40%)	60,89,89	3.69	32 (53%)
35	II0	l	317	-	39,43,43	6.84	21 (53%)	48,60,60	1.86	12 (25%)
27	CLA	A	801	-	69,73,73	1.16	6 (8%)	82,113,113	1.15	8 (9%)
27	CLA	d	301	23	54,58,73	1.28	8 (14%)	64,95,113	1.43	9 (14%)
35	II0	e	616	-	39,43,43	6.73	21 (53%)	48,60,60	1.72	11 (22%)
27	CLA	a	311	15	69,73,73	1.13	7 (10%)	82,113,113	1.52	10 (12%)
27	CLA	A	815	39	49,53,73	1.39	7 (14%)	58,89,113	1.77	8 (13%)
35	II0	l	314	-	39,43,43	6.70	23 (58%)	48,60,60	2.18	13 (27%)
29	LHG	a	319	27	48,48,48	0.91	2 (4%)	51,54,54	1.25	5 (9%)
27	CLA	m	601	18	46,50,73	1.41	6 (13%)	53,85,113	1.24	4 (7%)
27	CLA	m	606	18	69,73,73	1.15	8 (11%)	82,113,113	1.33	7 (8%)
27	CLA	a	309	15	69,73,73	1.17	9 (13%)	82,113,113	1.38	7 (8%)
27	CLA	k	302	-	55,59,73	1.28	7 (12%)	64,96,113	1.47	12 (18%)
27	CLA	F	201	39	69,73,73	1.15	7 (10%)	82,113,113	1.30	6 (7%)
27	CLA	B	821	39	68,72,73	1.14	8 (11%)	80,111,113	1.26	8 (10%)
35	II0	k	316	-	39,43,43	6.89	20 (51%)	48,60,60	1.86	12 (25%)
35	II0	j	613	-	39,43,43	6.69	21 (53%)	48,60,60	2.50	20 (41%)
27	CLA	b	608	29	69,73,73	1.13	6 (8%)	82,113,113	1.31	10 (12%)
27	CLA	a	308	15	69,73,73	1.15	6 (8%)	82,113,113	1.30	10 (12%)
27	CLA	c	605	-	55,59,73	1.32	5 (9%)	64,96,113	1.27	7 (10%)
27	CLA	k	304	21	49,53,73	1.39	8 (16%)	58,89,113	1.84	16 (27%)
27	CLA	i	306	-	55,59,73	1.29	6 (10%)	64,96,113	1.37	7 (10%)
27	CLA	s	206	-	69,73,73	1.17	7 (10%)	82,113,113	1.36	10 (12%)
35	II0	l	313	-	39,43,43	6.77	20 (51%)	48,60,60	1.82	13 (27%)
27	CLA	c	609	29	49,53,73	1.36	8 (16%)	58,89,113	1.39	10 (17%)
27	CLA	c	604	14	69,73,73	1.17	7 (10%)	82,113,113	1.35	5 (6%)
36	IHT	m	616	-	40,42,42	6.22	25 (62%)	52,58,58	2.08	16 (30%)
27	CLA	j	607	18	49,53,73	1.38	6 (12%)	58,89,113	1.27	5 (8%)
27	CLA	A	826	-	69,73,73	1.21	8 (11%)	82,113,113	1.62	15 (18%)
27	CLA	c	608	14	69,73,73	1.18	7 (10%)	82,113,113	1.52	10 (12%)
27	CLA	B	802	-	69,73,73	1.13	7 (10%)	82,113,113	1.75	12 (14%)
27	CLA	i	311	22	55,59,73	1.37	9 (16%)	64,96,113	1.59	12 (18%)
35	II0	f	618	-	39,43,43	6.70	20 (51%)	48,60,60	2.08	17 (35%)
34	LMG	s	210	-	55,55,55	0.87	2 (3%)	63,63,63	0.99	3 (4%)
27	CLA	l	312	20	69,73,73	1.16	7 (10%)	82,113,113	1.41	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	KC2	d	310	-	49,53,53	2.73	20 (40%)	60,89,89	3.63	32 (53%)
27	CLA	B	811	-	64,68,73	1.20	8 (12%)	76,107,113	1.37	9 (11%)
27	CLA	b	606	16	65,69,73	1.20	8 (12%)	77,108,113	1.38	11 (14%)
30	WVN	A	849	-	40,41,41	1.68	11 (27%)	51,56,56	2.06	13 (25%)
27	CLA	A	841	-	69,73,73	1.13	9 (13%)	82,113,113	1.29	9 (10%)
27	CLA	n	601	26	49,53,73	1.38	7 (14%)	58,89,113	1.32	5 (8%)
27	CLA	e	605	19	69,73,73	1.14	7 (10%)	82,113,113	1.43	9 (10%)
30	WVN	L	201	-	40,41,41	1.69	14 (35%)	51,56,56	2.61	17 (33%)
27	CLA	f	607	-	69,73,73	1.21	7 (10%)	82,113,113	1.37	10 (12%)
29	LHG	k	319	27	36,36,48	1.13	2 (5%)	39,42,54	1.18	5 (12%)
30	WVN	J	102	-	40,41,41	1.78	11 (27%)	51,56,56	2.08	17 (33%)
27	CLA	k	309	29	55,59,73	1.40	6 (10%)	64,96,113	1.88	18 (28%)
27	CLA	e	604	39	69,73,73	1.15	7 (10%)	82,113,113	1.59	11 (13%)
27	CLA	e	610	39	69,73,73	1.19	8 (11%)	82,113,113	1.18	7 (8%)
34	LMG	O	205	-	26,26,55	1.30	2 (7%)	34,34,63	1.28	4 (11%)
27	CLA	A	811	-	58,62,73	1.26	7 (12%)	68,99,113	1.41	8 (11%)
27	CLA	g	310	24	55,59,73	1.32	7 (12%)	64,96,113	1.58	14 (21%)
27	CLA	F	203	6	56,60,73	1.26	8 (14%)	65,97,113	1.46	6 (9%)
27	CLA	A	820	39	69,73,73	1.18	9 (13%)	82,113,113	1.41	11 (13%)
27	CLA	B	803	-	69,73,73	1.12	8 (11%)	82,113,113	1.47	9 (10%)
27	CLA	b	603	-	69,73,73	1.17	9 (13%)	82,113,113	1.35	9 (10%)
35	II0	e	613	-	39,43,43	6.81	23 (58%)	48,60,60	1.85	13 (27%)
27	CLA	h	303	17	54,58,73	1.28	8 (14%)	64,95,113	1.49	9 (14%)
27	CLA	n	610	39	69,73,73	1.23	9 (13%)	82,113,113	1.25	8 (9%)
27	CLA	R	203	-	55,59,73	1.30	7 (12%)	64,96,113	1.57	11 (17%)
27	CLA	B	818	-	59,63,73	1.30	9 (15%)	70,101,113	1.35	9 (12%)
27	CLA	h	301	39	69,73,73	1.20	9 (13%)	82,113,113	1.44	14 (17%)
27	CLA	h	304	-	55,59,73	1.31	10 (18%)	64,96,113	1.64	11 (17%)
29	LHG	f	619	-	48,48,48	0.91	2 (4%)	51,54,54	1.04	3 (5%)
27	CLA	s	208	-	55,59,73	1.31	8 (14%)	64,96,113	1.67	18 (28%)
27	CLA	b	610	16	69,73,73	1.13	6 (8%)	82,113,113	1.31	7 (8%)
27	CLA	g	304	-	55,59,73	1.32	10 (18%)	64,96,113	1.47	14 (21%)
27	CLA	a	304	15	54,58,73	1.29	7 (12%)	64,95,113	1.40	8 (12%)
27	CLA	B	838	-	69,73,73	1.17	7 (10%)	82,113,113	1.41	7 (8%)
27	CLA	O	206	-	69,73,73	1.17	7 (10%)	82,113,113	1.34	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	b	604	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	5 (6%)
27	CLA	A	827	-	66,70,73	1.16	7 (10%)	78,109,113	1.35	13 (16%)
28	PQN	B	841	-	34,34,34	1.88	5 (14%)	43,45,45	1.30	4 (9%)
27	CLA	f	613	-	69,73,73	1.20	6 (8%)	82,113,113	1.42	10 (12%)
27	CLA	a	303	15	56,60,73	1.36	10 (17%)	65,97,113	1.63	13 (20%)
37	KC2	k	312	-	49,53,53	2.79	20 (40%)	60,89,89	3.73	33 (55%)
29	LHG	a	301	27	48,48,48	0.91	2 (4%)	51,54,54	1.15	5 (9%)
27	CLA	m	611	39	55,59,73	1.31	10 (18%)	64,96,113	1.53	13 (20%)
35	II0	b	612	-	39,43,43	6.44	21 (53%)	48,60,60	2.17	16 (33%)
27	CLA	B	849	-	55,59,73	1.24	7 (12%)	64,96,113	1.43	9 (14%)
35	II0	n	618	-	39,43,43	6.83	21 (53%)	48,60,60	1.85	15 (31%)
31	LMT	b	616	-	24,24,36	1.14	3 (12%)	29,29,47	1.24	3 (10%)
27	CLA	B	804	-	69,73,73	1.19	8 (11%)	82,113,113	1.31	8 (9%)
27	CLA	B	839	-	69,73,73	1.22	10 (14%)	82,113,113	1.44	14 (17%)
27	CLA	A	830	-	54,58,73	1.28	10 (18%)	64,95,113	1.49	10 (15%)
27	CLA	K	101	39	55,59,73	1.31	8 (14%)	64,96,113	1.59	10 (15%)
34	LMG	L	208	-	55,55,55	0.88	2 (3%)	63,63,63	1.55	9 (14%)
35	II0	n	616	-	39,43,43	6.86	21 (53%)	48,60,60	1.79	13 (27%)
30	WVN	B	846	-	40,41,41	1.75	10 (25%)	51,56,56	2.51	19 (37%)
27	CLA	A	853	-	69,73,73	1.12	6 (8%)	82,113,113	1.33	8 (9%)
27	CLA	m	607	18	69,73,73	1.17	8 (11%)	82,113,113	1.26	10 (12%)
27	CLA	B	837	-	61,65,73	1.23	7 (11%)	72,103,113	1.46	11 (15%)
27	CLA	f	601	18	51,55,73	1.35	7 (13%)	60,91,113	1.29	6 (10%)
29	LHG	J	107	27	48,48,48	0.93	2 (4%)	51,54,54	0.92	3 (5%)
27	CLA	h	307	17	61,65,73	1.23	6 (9%)	72,103,113	1.17	4 (5%)
27	CLA	s	209	-	55,59,73	1.30	6 (10%)	64,96,113	1.29	5 (7%)
30	WVN	h	309	-	40,41,41	1.73	9 (22%)	51,56,56	2.62	22 (43%)
35	II0	k	315	-	39,43,43	6.50	23 (58%)	48,60,60	2.15	16 (33%)
35	II0	a	314	-	39,43,43	6.49	22 (56%)	48,60,60	2.08	19 (39%)
27	CLA	A	809	-	60,64,73	1.26	8 (13%)	71,102,113	1.39	7 (9%)
35	II0	m	614	-	39,43,43	6.64	22 (56%)	48,60,60	2.03	14 (29%)
27	CLA	A	803	-	59,63,73	1.24	8 (13%)	70,101,113	1.50	9 (12%)
27	CLA	e	607	19	69,73,73	1.14	7 (10%)	82,113,113	1.29	9 (10%)
27	CLA	d	308	29	45,49,73	1.42	5 (11%)	54,84,113	1.54	9 (16%)
27	CLA	j	604	18	69,73,73	1.18	7 (10%)	82,113,113	1.62	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	f	605	18	49,53,73	1.41	7 (14%)	58,89,113	1.46	6 (10%)
30	WVN	A	846	-	40,41,41	1.74	10 (25%)	51,56,56	2.39	13 (25%)
27	CLA	B	816	39	69,73,73	1.25	8 (11%)	82,113,113	1.53	8 (9%)
27	CLA	A	842	-	69,73,73	1.16	9 (13%)	82,113,113	1.45	11 (13%)
37	KC2	s	204	-	49,53,53	2.70	21 (42%)	60,89,89	3.78	35 (58%)
27	CLA	B	807	2	69,73,73	1.17	7 (10%)	82,113,113	1.31	8 (9%)
36	IHT	j	616	-	40,42,42	6.23	26 (65%)	52,58,58	2.26	16 (30%)
35	II0	f	614	-	39,43,43	6.68	21 (53%)	48,60,60	1.94	15 (31%)
27	CLA	B	801	-	69,73,73	1.15	7 (10%)	82,113,113	1.21	7 (8%)
27	CLA	h	308	17	55,59,73	1.34	8 (14%)	64,96,113	1.71	9 (14%)
29	LHG	b	617	27	48,48,48	0.89	4 (8%)	51,54,54	1.20	4 (7%)
37	KC2	k	311	-	49,53,53	2.73	20 (40%)	60,89,89	3.77	36 (60%)
27	CLA	b	601	16	55,59,73	1.30	7 (12%)	64,96,113	1.43	7 (10%)
27	CLA	A	814	-	54,58,73	1.28	7 (12%)	64,95,113	1.37	7 (10%)
37	KC2	j	610	18	49,53,53	2.75	19 (38%)	60,89,89	3.76	31 (51%)
27	CLA	B	817	-	50,54,73	1.34	7 (14%)	59,90,113	1.59	8 (13%)
30	WVN	e	615	-	40,41,41	1.72	10 (25%)	51,56,56	2.25	15 (29%)
27	CLA	L	203	-	69,73,73	1.13	8 (11%)	82,113,113	1.19	7 (8%)
35	II0	i	313	-	39,43,43	6.81	23 (58%)	48,60,60	1.77	11 (22%)
27	CLA	A	806	-	69,73,73	1.18	7 (10%)	82,113,113	1.36	9 (10%)
27	CLA	A	834	-	55,59,73	1.33	7 (12%)	64,96,113	1.55	12 (18%)
27	CLA	j	603	-	55,59,73	1.31	8 (14%)	64,96,113	1.51	11 (17%)
27	CLA	e	608	29	50,54,73	1.34	7 (14%)	59,90,113	1.59	8 (13%)
37	KC2	n	612	-	49,53,53	2.71	19 (38%)	60,89,89	3.86	32 (53%)
27	CLA	A	829	-	69,73,73	1.17	7 (10%)	82,113,113	1.37	10 (12%)
27	CLA	B	815	-	61,65,73	1.20	6 (9%)	72,103,113	1.37	9 (12%)
27	CLA	c	601	14	55,59,73	1.27	6 (10%)	64,96,113	1.40	9 (14%)
35	II0	k	314	-	39,43,43	6.67	20 (51%)	48,60,60	1.79	12 (25%)
27	CLA	b	611	-	69,73,73	1.14	7 (10%)	82,113,113	1.16	6 (7%)
30	WVN	O	201	-	40,41,41	1.64	9 (22%)	51,56,56	2.02	14 (27%)
34	LMG	b	619	-	49,49,55	1.01	3 (6%)	57,57,63	1.17	5 (8%)
27	CLA	l	309	20	55,59,73	1.34	9 (16%)	64,96,113	1.44	11 (17%)
27	CLA	g	322	-	69,73,73	1.20	6 (8%)	82,113,113	1.43	9 (10%)
27	CLA	j	602	18	54,58,73	1.25	8 (14%)	64,95,113	1.55	10 (15%)
27	CLA	n	609	26	69,73,73	1.18	8 (11%)	82,113,113	1.49	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	WVN	A	847	-	40,41,41	1.73	10 (25%)	51,56,56	2.63	18 (35%)
27	CLA	n	605	26	55,59,73	1.35	7 (12%)	64,96,113	1.81	14 (21%)
27	CLA	s	202	13	69,73,73	1.21	8 (11%)	82,113,113	1.40	13 (15%)
30	WVN	l	301	-	40,41,41	1.68	10 (25%)	51,56,56	2.24	15 (29%)
34	LMG	c	619	-	55,55,55	0.99	2 (3%)	63,63,63	1.50	12 (19%)
27	CLA	n	608	26	55,59,73	1.28	8 (14%)	64,96,113	1.32	7 (10%)
27	CLA	j	612	-	69,73,73	1.14	6 (8%)	82,113,113	1.18	8 (9%)
35	II0	l	315	-	39,43,43	6.60	21 (53%)	48,60,60	2.02	14 (29%)
27	CLA	i	305	22	69,73,73	1.16	7 (10%)	82,113,113	1.19	7 (8%)
27	CLA	A	835	-	69,73,73	1.14	7 (10%)	82,113,113	1.30	9 (10%)
27	CLA	A	855	39	69,73,73	1.22	10 (14%)	82,113,113	1.64	18 (21%)
27	CLA	f	609	18	69,73,73	1.14	8 (11%)	82,113,113	1.22	8 (9%)
27	CLA	b	602	16	59,63,73	1.22	7 (11%)	70,101,113	1.49	11 (15%)
27	CLA	F	202	39	69,73,73	1.18	6 (8%)	82,113,113	1.18	7 (8%)
30	WVN	L	205	-	40,41,41	1.77	10 (25%)	51,56,56	2.06	14 (27%)
27	CLA	c	603	-	55,59,73	1.27	8 (14%)	64,96,113	1.56	8 (12%)
27	CLA	k	305	21	55,59,73	1.31	11 (20%)	64,96,113	1.52	9 (14%)
27	CLA	f	608	18	69,73,73	1.17	7 (10%)	82,113,113	1.14	5 (6%)
27	CLA	k	303	-	69,73,73	1.17	7 (10%)	82,113,113	1.34	10 (12%)
27	CLA	n	613	-	55,59,73	1.28	6 (10%)	64,96,113	1.21	8 (12%)
27	CLA	A	831	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	6 (7%)
27	CLA	k	301	21	54,58,73	1.33	7 (12%)	64,95,113	1.29	6 (9%)
27	CLA	j	611	-	55,59,73	1.28	6 (10%)	64,96,113	1.43	8 (12%)
27	CLA	m	604	18	69,73,73	1.22	7 (10%)	82,113,113	1.52	14 (17%)
37	KC2	i	317	-	49,53,53	2.91	22 (44%)	60,89,89	3.41	32 (53%)
30	WVN	I	101	-	40,41,41	1.70	11 (27%)	51,56,56	2.06	14 (27%)
27	CLA	b	607	16	69,73,73	1.15	5 (7%)	82,113,113	1.62	14 (17%)
27	CLA	B	812	-	63,67,73	1.20	8 (12%)	74,105,113	1.47	9 (12%)
27	CLA	c	602	14	54,58,73	1.31	9 (16%)	64,95,113	1.75	13 (20%)
35	II0	g	316	-	39,43,43	6.66	22 (56%)	48,60,60	2.02	13 (27%)
29	LHG	b	618	-	30,30,48	1.22	2 (6%)	33,36,54	1.24	3 (9%)
27	CLA	m	608	18	55,59,73	1.29	6 (10%)	64,96,113	1.32	8 (12%)
27	CLA	d	307	23	45,49,73	1.44	7 (15%)	54,84,113	1.56	8 (14%)
30	WVN	s	205	-	40,41,41	1.70	12 (30%)	51,56,56	2.45	20 (39%)
27	CLA	f	606	18	55,59,73	1.31	7 (12%)	64,96,113	1.49	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	g	307	24	55,59,73	1.28	6 (10%)	64,96,113	1.41	7 (10%)
27	CLA	g	315	-	55,59,73	1.31	5 (9%)	64,96,113	1.39	11 (17%)
27	CLA	a	312	-	69,73,73	1.16	9 (13%)	82,113,113	1.48	8 (9%)
27	CLA	a	306	39	69,73,73	1.13	7 (10%)	82,113,113	1.40	9 (10%)
27	CLA	a	305	-	55,59,73	1.31	9 (16%)	64,96,113	1.40	7 (10%)
27	CLA	c	607	14	50,54,73	1.35	6 (12%)	59,90,113	1.24	7 (11%)
27	CLA	O	202	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
35	II0	b	615	-	39,43,43	6.48	20 (51%)	48,60,60	2.32	17 (35%)
27	CLA	A	805	1	69,73,73	1.16	9 (13%)	82,113,113	1.47	10 (12%)
35	II0	d	312	-	39,43,43	6.69	23 (58%)	48,60,60	1.99	14 (29%)
29	LHG	c	618	27	36,36,48	1.14	2 (5%)	39,42,54	1.32	3 (7%)
27	CLA	i	303	22	54,58,73	1.30	8 (14%)	64,95,113	1.52	12 (18%)
27	CLA	l	303	20	51,55,73	1.34	7 (13%)	60,91,113	1.43	4 (6%)
27	CLA	e	601	19	49,53,73	1.37	8 (16%)	58,89,113	1.68	5 (8%)
30	WVN	R	202	-	40,41,41	1.67	12 (30%)	51,56,56	2.72	22 (43%)
27	CLA	B	831	-	62,66,73	1.23	8 (12%)	73,104,113	1.48	14 (19%)
27	CLA	n	607	-	69,73,73	1.17	9 (13%)	82,113,113	1.35	13 (15%)
27	CLA	A	816	-	69,73,73	1.10	6 (8%)	82,113,113	1.47	14 (17%)
27	CLA	B	814	-	63,67,73	1.21	8 (12%)	74,105,113	1.30	6 (8%)
27	CLA	B	830	39	49,53,73	1.39	9 (18%)	58,89,113	1.57	5 (8%)
35	II0	k	318	-	39,43,43	6.51	19 (48%)	48,60,60	2.17	20 (41%)
27	CLA	l	304	20	69,73,73	1.14	8 (11%)	82,113,113	1.48	11 (13%)
32	SF4	A	854	1,2	0,12,12	-	-	-	-	-
27	CLA	j	605	18	49,53,73	1.40	6 (12%)	58,89,113	1.59	8 (13%)
27	CLA	A	852	-	69,73,73	1.16	7 (10%)	82,113,113	1.10	4 (4%)
27	CLA	A	837	-	69,73,73	1.13	6 (8%)	82,113,113	1.45	10 (12%)
35	II0	d	314	-	39,43,43	6.86	22 (56%)	48,60,60	2.18	13 (27%)
35	II0	j	615	-	39,43,43	6.78	20 (51%)	48,60,60	1.85	11 (22%)
27	CLA	B	834	39	69,73,73	1.20	8 (11%)	82,113,113	1.21	10 (12%)
27	CLA	A	802	-	69,73,73	1.14	9 (13%)	82,113,113	1.49	14 (17%)
27	CLA	B	836	-	69,73,73	1.09	4 (5%)	82,113,113	1.47	11 (13%)
27	CLA	B	808	-	58,62,73	1.37	8 (13%)	71,100,113	1.18	4 (5%)
35	II0	O	203	-	39,43,43	6.68	20 (51%)	48,60,60	1.97	11 (22%)
37	KC2	k	310	21	49,53,53	2.77	19 (38%)	60,89,89	3.83	33 (55%)
27	CLA	l	307	20	69,73,73	1.20	9 (13%)	82,113,113	1.60	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	PQN	A	843	-	34,34,34	1.89	5 (14%)	43,45,45	1.31	4 (9%)
29	LHG	A	845	27	26,26,48	1.25	3 (11%)	29,32,54	1.51	5 (17%)
27	CLA	B	809	-	59,63,73	1.24	8 (13%)	70,101,113	1.48	14 (20%)
27	CLA	s	203	13,27	69,73,73	1.16	6 (8%)	82,113,113	1.44	7 (8%)
27	CLA	b	605	39,27	69,73,73	1.16	9 (13%)	82,113,113	1.39	7 (8%)
35	II0	e	612	-	39,43,43	6.93	23 (58%)	48,60,60	1.84	11 (22%)
27	CLA	m	612	-	47,51,73	1.39	8 (17%)	55,86,113	1.60	14 (25%)
27	CLA	B	829	39	69,73,73	1.14	7 (10%)	82,113,113	1.35	13 (15%)
27	CLA	k	306	-	55,59,73	1.34	6 (10%)	64,96,113	1.44	11 (17%)
29	LHG	A	844	-	47,47,48	0.97	2 (4%)	50,53,54	1.17	3 (6%)
30	WVN	M	101	-	40,41,41	1.68	11 (27%)	51,56,56	2.34	19 (37%)
30	WVN	B	847	-	40,41,41	1.72	11 (27%)	51,56,56	2.07	13 (25%)
30	WVN	R	201	-	40,41,41	1.69	10 (25%)	51,56,56	2.32	19 (37%)
27	CLA	J	105	29	55,59,73	1.35	8 (14%)	64,96,113	1.74	13 (20%)
35	II0	h	311	-	39,43,43	6.51	22 (56%)	48,60,60	2.18	18 (37%)
36	IHT	a	317	-	40,42,42	6.24	26 (65%)	52,58,58	2.08	14 (26%)
27	CLA	B	823	-	69,73,73	1.16	9 (13%)	82,113,113	1.38	11 (13%)
34	LMG	F	206	-	48,48,55	0.98	2 (4%)	56,56,63	1.25	5 (8%)
30	WVN	B	845	-	40,41,41	1.70	11 (27%)	51,56,56	2.52	19 (37%)
29	LHG	d	315	27	36,36,48	1.11	2 (5%)	39,42,54	1.09	2 (5%)
35	II0	e	614	-	39,43,43	6.69	20 (51%)	48,60,60	2.03	14 (29%)
37	KC2	s	201	13	49,53,53	2.59	20 (40%)	60,89,89	3.77	34 (56%)
27	CLA	d	304	-	55,59,73	1.31	7 (12%)	64,96,113	1.35	7 (10%)
27	CLA	A	813	-	49,53,73	1.44	7 (14%)	58,89,113	2.29	12 (20%)
29	LHG	g	321	27	36,36,48	1.12	2 (5%)	39,42,54	1.52	8 (20%)
29	LHG	l	318	27	31,31,48	1.17	2 (6%)	34,37,54	1.27	4 (11%)
27	CLA	A	818	-	69,73,73	1.19	7 (10%)	82,113,113	1.57	12 (14%)
27	CLA	a	307	15	49,53,73	1.39	9 (18%)	58,89,113	1.74	12 (20%)
36	IHT	O	204	-	40,42,42	6.17	26 (65%)	52,58,58	2.27	20 (38%)
27	CLA	e	611	-	69,73,73	1.18	9 (13%)	82,113,113	1.46	12 (14%)
27	CLA	d	303	23	69,73,73	1.17	6 (8%)	82,113,113	1.18	4 (4%)
29	LHG	j	617	27	29,29,48	1.22	2 (6%)	32,35,54	1.52	6 (18%)
37	KC2	m	610	18	49,53,53	2.78	20 (40%)	60,89,89	3.78	33 (55%)
37	KC2	g	314	37	49,53,53	2.77	20 (40%)	60,89,89	3.74	33 (55%)
27	CLA	A	810	-	66,70,73	1.15	7 (10%)	78,109,113	1.15	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LHG	L	207	-	48,48,48	0.90	2 (4%)	51,54,54	1.06	2 (3%)
27	CLA	L	206	39	55,59,73	1.26	7 (12%)	64,96,113	1.37	6 (9%)
36	IHT	c	616	-	40,42,42	6.30	25 (62%)	52,58,58	2.57	14 (26%)
27	CLA	A	840	1	69,73,73	1.23	9 (13%)	82,113,113	1.49	8 (9%)
27	CLA	A	836	-	69,73,73	1.18	7 (10%)	82,113,113	1.51	12 (14%)
27	CLA	B	805	-	69,73,73	1.11	6 (8%)	82,113,113	1.45	6 (7%)
29	LHG	i	316	27	36,36,48	1.16	2 (5%)	39,42,54	1.56	6 (15%)
27	CLA	j	609	29	65,69,73	1.22	9 (13%)	77,108,113	1.58	13 (16%)
27	CLA	m	603	-	69,73,73	1.13	7 (10%)	82,113,113	1.46	11 (13%)
27	CLA	A	804	-	69,73,73	1.17	9 (13%)	82,113,113	1.58	9 (10%)
27	CLA	m	602	18	60,64,73	1.22	8 (13%)	71,102,113	1.43	10 (14%)
27	CLA	A	839	39	69,73,73	1.17	7 (10%)	82,113,113	1.12	8 (9%)
27	CLA	c	612	-	69,73,73	1.13	5 (7%)	82,113,113	1.33	8 (9%)
35	II0	J	104	-	39,43,43	6.69	22 (56%)	48,60,60	1.92	11 (22%)
27	CLA	n	604	26	64,68,73	1.28	10 (15%)	76,107,113	1.38	9 (11%)
27	CLA	B	835	-	69,73,73	1.16	7 (10%)	82,113,113	1.57	11 (13%)
37	KC2	g	313	37	49,53,53	2.76	20 (40%)	60,89,89	3.78	32 (53%)
36	IHT	k	317	-	40,42,42	6.20	26 (65%)	52,58,58	2.18	18 (34%)
27	CLA	c	606	-	56,60,73	1.34	7 (12%)	65,97,113	1.61	12 (18%)
31	LMT	A	851	-	36,36,36	1.23	5 (13%)	47,47,47	1.43	7 (14%)
27	CLA	i	308	22	55,59,73	1.28	6 (10%)	64,96,113	1.66	17 (26%)
27	CLA	e	602	19	54,58,73	1.32	8 (14%)	64,95,113	1.57	9 (14%)
29	LHG	n	619	-	42,42,48	0.96	2 (4%)	45,48,54	1.38	4 (8%)
30	WVN	B	848	-	40,41,41	1.68	11 (27%)	51,56,56	2.71	23 (45%)
35	II0	h	312	-	39,43,43	6.76	22 (56%)	48,60,60	2.31	16 (33%)
27	CLA	k	313	-	55,59,73	1.33	6 (10%)	64,96,113	1.35	10 (15%)
35	II0	g	317	-	39,43,43	6.67	22 (56%)	48,60,60	2.15	13 (27%)
27	CLA	A	823	-	59,63,73	1.25	7 (11%)	70,101,113	1.34	8 (11%)
27	CLA	f	602	18	69,73,73	1.14	6 (8%)	82,113,113	1.39	12 (14%)
29	LHG	m	617	27	36,36,48	1.07	2 (5%)	39,42,54	1.26	4 (10%)
27	CLA	B	819	-	57,61,73	1.29	9 (15%)	67,98,113	1.27	6 (8%)
27	CLA	n	606	26	55,59,73	1.32	7 (12%)	64,96,113	1.52	8 (12%)
35	II0	a	315	-	39,43,43	6.76	24 (61%)	48,60,60	1.88	17 (35%)
35	II0	g	320	-	39,43,43	6.68	22 (56%)	48,60,60	1.97	13 (27%)
27	CLA	h	302	17	54,58,73	1.28	7 (12%)	64,95,113	1.41	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	IHT	b	614	-	40,42,42	6.35	25 (62%)	52,58,58	2.24	16 (30%)
27	CLA	B	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.44	10 (12%)
27	CLA	j	601	18	55,59,73	1.32	6 (10%)	64,96,113	1.28	5 (7%)
27	CLA	b	609	-	55,59,73	1.29	9 (16%)	64,96,113	1.59	9 (14%)
30	WVN	A	848	-	40,41,41	1.71	12 (30%)	51,56,56	2.61	22 (43%)
27	CLA	i	307	22	65,69,73	1.22	7 (10%)	77,108,113	1.24	6 (7%)
34	LMG	J	106	-	55,55,55	0.86	3 (5%)	63,63,63	0.99	3 (4%)
29	LHG	e	617	27	36,36,48	1.10	2 (5%)	39,42,54	1.43	4 (10%)
35	II0	f	615	-	39,43,43	6.63	23 (58%)	48,60,60	2.21	18 (37%)
27	CLA	f	603	-	55,59,73	1.28	6 (10%)	64,96,113	1.40	9 (14%)
27	CLA	n	602	26	54,58,73	1.29	7 (12%)	64,95,113	1.52	10 (15%)
27	CLA	i	309	29	50,54,73	1.35	8 (16%)	59,90,113	1.59	11 (18%)
27	CLA	k	308	21	69,73,73	1.23	6 (8%)	82,113,113	1.49	17 (20%)
27	CLA	l	305	-	55,59,73	1.27	9 (16%)	64,96,113	1.40	8 (12%)
35	II0	l	302	-	39,43,43	6.78	21 (53%)	48,60,60	2.23	16 (33%)
35	II0	h	310	-	26,28,43	6.04	12 (46%)	30,37,60	2.33	11 (36%)
27	CLA	A	817	-	69,73,73	1.18	10 (14%)	82,113,113	1.33	11 (13%)
27	CLA	J	103	8	46,50,73	1.33	7 (15%)	53,85,113	1.47	6 (11%)
27	CLA	B	828	-	54,58,73	1.32	8 (14%)	64,95,113	1.48	10 (15%)
27	CLA	K	102	-	46,50,73	1.38	7 (15%)	53,85,113	1.53	8 (15%)
27	CLA	g	311	29	58,62,73	1.28	8 (13%)	68,99,113	1.45	6 (8%)
31	LMT	a	302	-	24,24,36	1.18	3 (12%)	29,29,47	0.97	0
27	CLA	l	308	20	69,73,73	1.14	6 (8%)	82,113,113	1.27	7 (8%)
27	CLA	e	606	19	69,73,73	1.18	9 (13%)	82,113,113	1.25	7 (8%)
27	CLA	B	820	39	69,73,73	1.19	8 (11%)	82,113,113	1.41	10 (12%)
27	CLA	h	313	39	69,73,73	1.14	7 (10%)	82,113,113	1.29	6 (7%)
35	II0	c	615	-	39,43,43	6.75	20 (51%)	48,60,60	2.24	17 (35%)
27	CLA	l	306	20	69,73,73	1.16	8 (11%)	82,113,113	1.56	13 (15%)

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	n	614	-	-	1/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	e	603	19	1/1/12/20	2/23/99/115	-
37	KC2	f	611	18	-	5/15/71/71	-
30	WVN	B	843	-	-	10/29/63/63	0/2/2/2
27	CLA	B	813	-	1/1/13/20	5/27/103/115	-
35	II0	j	614	-	-	2/21/67/67	0/2/2/2
27	CLA	A	819	-	1/1/11/20	3/15/91/115	-
27	CLA	B	806	-	1/1/15/20	9/39/115/115	-
27	CLA	f	604	18	1/1/15/20	10/39/115/115	-
27	CLA	g	306	24	1/1/12/20	8/23/99/115	-
30	WVN	F	205	-	-	12/29/63/63	0/2/2/2
27	CLA	B	824	-	1/1/15/20	7/39/115/115	-
27	CLA	g	305	24	1/1/15/20	13/39/115/115	-
27	CLA	B	833	-	1/1/11/20	2/18/94/115	-
27	CLA	l	310	29	1/1/14/20	13/35/111/115	-
27	CLA	a	310	29	1/1/11/20	6/19/95/115	-
30	WVN	l	316	-	-	9/29/63/63	0/2/2/2
36	IHT	f	617	-	-	7/25/65/65	0/2/2/2
27	CLA	A	856	29	1/1/10/20	4/10/86/115	-
30	WVN	J	101	-	-	8/29/63/63	0/2/2/2
27	CLA	a	313	-	1/1/11/20	11/19/95/115	-
27	CLA	A	821	-	-	5/20/96/115	-
27	CLA	c	611	14	-	5/15/91/115	-
30	WVN	i	315	-	-	9/29/63/63	0/2/2/2
27	CLA	B	826	-	1/1/12/20	9/21/97/115	-
27	CLA	m	605	18	1/1/10/20	6/12/88/115	-
36	IHT	c	620	-	-	11/25/65/65	0/2/2/2
35	II0	m	615	-	-	3/21/67/67	0/2/2/2
27	CLA	B	810	-	1/1/15/20	12/39/115/115	-
37	KC2	d	309	23	-	7/15/71/71	-
27	CLA	g	309	-	1/1/15/20	10/39/115/115	-
27	CLA	g	302	24	1/1/10/20	4/12/88/115	-
27	CLA	B	822	-	1/1/15/20	4/39/115/115	-
30	WVN	s	207	-	-	6/29/63/63	0/2/2/2
27	CLA	A	832	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	825	-	1/1/12/20	3/23/99/115	-
27	CLA	n	603	-	1/1/12/20	9/23/99/115	-
27	CLA	g	308	-	1/1/15/20	16/39/115/115	-
37	KC2	l	311	20	-	5/15/71/71	-
30	WVN	F	204	-	-	9/29/63/63	0/2/2/2
27	CLA	f	610	29	1/1/15/20	16/39/115/115	-
27	CLA	B	827	-	1/1/11/20	5/20/96/115	-
35	II0	b	613	-	-	8/21/67/67	0/2/2/2
32	SF4	C	102	3	-	-	0/6/5/5
35	II0	m	613	-	-	4/21/67/67	0/2/2/2
35	II0	f	616	-	-	3/21/67/67	0/2/2/2
37	KC2	e	609	19	-	7/15/71/71	-
29	LHG	g	301	27	-	20/41/41/53	-
35	II0	c	614	-	-	1/21/67/67	0/2/2/2
38	LMU	i	301	-	-	8/21/61/61	0/2/2/2
27	CLA	i	304	-	1/1/12/20	3/23/99/115	-
35	II0	a	318	-	-	8/21/67/67	0/2/2/2
27	CLA	A	812	-	1/1/15/20	20/39/115/115	-
35	II0	d	313	-	-	6/21/67/67	0/2/2/2
33	DGD	B	842	-	-	5/49/89/95	0/2/2/2
37	KC2	c	610	-	-	8/15/71/71	-
27	CLA	L	202	9	1/1/11/20	9/20/96/115	-
29	LHG	c	621	27	-	23/41/41/53	-
27	CLA	d	302	-	1/1/12/20	7/23/99/115	-
27	CLA	A	833	-	1/1/12/20	5/21/97/115	-
35	II0	c	613	-	-	4/21/67/67	0/2/2/2
27	CLA	A	825	39	-	7/39/115/115	-
35	II0	i	318	-	-	5/21/67/67	0/2/2/2
30	WVN	K	103	-	-	5/29/63/63	0/2/2/2
32	SF4	C	101	3	-	-	0/6/5/5
29	LHG	A	850	-	-	15/42/42/53	-
27	CLA	A	838	29	1/1/12/20	7/24/100/115	-
35	II0	i	314	-	-	3/21/67/67	0/2/2/2
30	WVN	B	844	-	-	0/29/63/63	0/2/2/2
27	CLA	A	824	39	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	828	-	1/1/15/20	9/39/115/115	-
27	CLA	L	204	39	1/1/12/20	5/21/97/115	-
35	II0	c	617	-	-	5/21/67/67	0/2/2/2
35	II0	a	316	-	-	2/21/67/67	0/2/2/2
27	CLA	m	609	29	1/1/13/20	13/27/103/115	-
35	II0	n	615	-	-	3/21/67/67	0/2/2/2
27	CLA	d	306	23	1/1/11/20	5/17/93/115	-
35	II0	g	318	-	-	3/21/67/67	0/2/2/2
27	CLA	d	305	-	1/1/12/20	9/23/99/115	-
37	KC2	n	611	26	-	4/15/71/71	-
27	CLA	h	306	17	1/1/15/20	19/39/115/115	-
36	IHT	g	319	-	-	5/25/65/65	0/2/2/2
27	CLA	h	305	-	1/1/12/20	6/23/99/115	-
27	CLA	B	840	29	1/1/15/20	4/39/115/115	-
36	IHT	R	204	-	-	2/25/65/65	0/2/2/2
27	CLA	f	612	18	1/1/12/20	8/23/99/115	-
27	CLA	A	807	1	1/1/15/20	7/39/115/115	-
27	CLA	A	822	-	1/1/12/20	8/23/99/115	-
27	CLA	i	312	-	1/1/12/20	5/23/99/115	-
27	CLA	j	606	18	-	10/23/99/115	-
27	CLA	g	303	24	1/1/12/20	4/21/97/115	-
27	CLA	A	808	1	1/1/15/20	8/39/115/115	-
27	CLA	d	311	-	-	7/23/99/115	-
37	KC2	g	312	24	-	10/15/71/71	-
27	CLA	j	608	18	1/1/12/20	2/23/99/115	-
31	LMT	a	320	-	-	13/21/61/61	0/2/2/2
36	IHT	n	617	-	-	8/25/65/65	0/2/2/2
27	CLA	k	307	21	1/1/15/20	16/39/115/115	-
27	CLA	i	302	22	1/1/12/20	7/23/99/115	-
37	KC2	i	310	22	-	9/15/71/71	-
35	II0	l	317	-	-	4/21/67/67	0/2/2/2
27	CLA	A	801	-	1/1/15/20	9/39/115/115	-
27	CLA	d	301	23	1/1/12/20	4/21/97/115	-
35	II0	e	616	-	-	4/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	311	15	1/1/15/20	13/39/115/115	-
27	CLA	A	815	39	1/1/11/20	4/15/91/115	-
35	II0	l	314	-	-	5/21/67/67	0/2/2/2
29	LHG	a	319	27	-	14/53/53/53	-
27	CLA	m	601	18	1/1/10/20	1/12/88/115	-
27	CLA	m	606	18	1/1/15/20	13/39/115/115	-
27	CLA	a	309	15	1/1/15/20	10/39/115/115	-
27	CLA	k	302	-	1/1/12/20	2/23/99/115	-
27	CLA	F	201	39	1/1/15/20	16/39/115/115	-
27	CLA	B	821	39	1/1/14/20	8/38/114/115	-
35	II0	k	316	-	-	1/21/67/67	0/2/2/2
35	II0	j	613	-	-	5/21/67/67	0/2/2/2
27	CLA	b	608	29	1/1/15/20	10/39/115/115	-
27	CLA	a	308	15	1/1/15/20	20/39/115/115	-
27	CLA	c	605	-	1/1/12/20	9/23/99/115	-
27	CLA	k	304	21	1/1/11/20	4/15/91/115	-
27	CLA	i	306	-	1/1/12/20	2/23/99/115	-
27	CLA	s	206	-	1/1/15/20	11/39/115/115	-
35	II0	l	313	-	-	3/21/67/67	0/2/2/2
27	CLA	c	609	29	1/1/11/20	5/15/91/115	-
27	CLA	c	604	14	-	9/39/115/115	-
36	IHT	m	616	-	-	4/25/65/65	0/2/2/2
27	CLA	j	607	18	1/1/11/20	4/15/91/115	-
27	CLA	A	826	-	1/1/15/20	8/39/115/115	-
27	CLA	c	608	14	1/1/15/20	16/39/115/115	-
27	CLA	B	802	-	1/1/15/20	7/39/115/115	-
27	CLA	i	311	22	1/1/12/20	7/23/99/115	-
35	II0	f	618	-	-	7/21/67/67	0/2/2/2
34	LMG	s	210	-	-	12/50/70/70	0/1/1/1
27	CLA	l	312	20	1/1/15/20	14/39/115/115	-
37	KC2	d	310	-	-	6/15/71/71	-
27	CLA	B	811	-	1/1/14/20	11/33/109/115	-
27	CLA	b	606	16	1/1/14/20	14/35/111/115	-
30	WVN	A	849	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	841	-	1/1/15/20	15/39/115/115	-
27	CLA	n	601	26	1/1/11/20	9/15/91/115	-
27	CLA	e	605	19	-	17/39/115/115	-
30	WVN	L	201	-	-	9/29/63/63	0/2/2/2
27	CLA	f	607	-	1/1/15/20	18/39/115/115	-
29	LHG	k	319	27	-	12/41/41/53	-
30	WVN	J	102	-	-	8/29/63/63	0/2/2/2
27	CLA	k	309	29	1/1/12/20	11/23/99/115	-
27	CLA	e	604	39	-	21/39/115/115	-
27	CLA	e	610	39	1/1/15/20	14/39/115/115	-
34	LMG	O	205	-	-	6/21/41/70	0/1/1/1
27	CLA	A	811	-	-	7/26/102/115	-
27	CLA	g	310	24	1/1/12/20	6/23/99/115	-
27	CLA	F	203	6	1/1/12/20	13/24/100/115	-
27	CLA	A	820	39	1/1/15/20	3/39/115/115	-
27	CLA	B	803	-	1/1/15/20	12/39/115/115	-
27	CLA	b	603	-	1/1/15/20	15/39/115/115	-
35	II0	e	613	-	-	5/21/67/67	0/2/2/2
27	CLA	h	303	17	1/1/12/20	10/21/97/115	-
27	CLA	n	610	39	1/1/15/20	16/39/115/115	-
27	CLA	R	203	-	1/1/12/20	5/23/99/115	-
27	CLA	B	818	-	1/1/13/20	10/27/103/115	-
27	CLA	h	301	39	1/1/15/20	13/39/115/115	-
27	CLA	h	304	-	1/1/12/20	4/23/99/115	-
29	LHG	f	619	-	-	35/53/53/53	-
27	CLA	b	610	16	1/1/15/20	20/39/115/115	-
27	CLA	s	208	-	-	5/23/99/115	-
27	CLA	g	304	-	1/1/12/20	3/23/99/115	-
27	CLA	a	304	15	1/1/12/20	5/21/97/115	-
27	CLA	B	838	-	1/1/15/20	18/39/115/115	-
27	CLA	O	206	-	1/1/15/20	17/39/115/115	-
27	CLA	b	604	-	-	15/39/115/115	-
27	CLA	A	827	-	1/1/14/20	7/36/112/115	-
28	PQN	B	841	-	-	10/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	f	613	-	-	20/39/115/115	-
27	CLA	a	303	15	1/1/12/20	7/24/100/115	-
37	KC2	k	312	-	-	9/15/71/71	-
29	LHG	a	301	27	-	13/53/53/53	-
27	CLA	m	611	39	1/1/12/20	12/23/99/115	-
35	II0	b	612	-	-	1/21/67/67	0/2/2/2
27	CLA	B	849	-	-	10/23/99/115	-
35	II0	n	618	-	-	5/21/67/67	0/2/2/2
31	LMT	b	616	-	-	9/15/35/61	0/1/1/2
27	CLA	B	804	-	1/1/15/20	14/39/115/115	-
27	CLA	B	839	-	1/1/15/20	8/39/115/115	-
27	CLA	A	830	-	-	5/21/97/115	-
27	CLA	K	101	39	1/1/12/20	8/23/99/115	-
34	LMG	L	208	-	-	19/50/70/70	0/1/1/1
35	II0	n	616	-	-	3/21/67/67	0/2/2/2
30	WVN	B	846	-	-	7/29/63/63	0/2/2/2
27	CLA	A	853	-	1/1/15/20	9/39/115/115	-
27	CLA	m	607	18	1/1/15/20	9/39/115/115	-
27	CLA	B	837	-	1/1/13/20	8/30/106/115	-
27	CLA	f	601	18	1/1/11/20	5/18/94/115	-
29	LHG	J	107	27	-	28/53/53/53	-
27	CLA	h	307	17	1/1/13/20	14/30/106/115	-
27	CLA	s	209	-	1/1/12/20	6/23/99/115	-
30	WVN	h	309	-	-	8/29/63/63	0/2/2/2
35	II0	k	315	-	-	8/21/67/67	0/2/2/2
35	II0	a	314	-	-	5/21/67/67	0/2/2/2
27	CLA	A	809	-	1/1/13/20	9/29/105/115	-
35	II0	m	614	-	-	8/21/67/67	0/2/2/2
27	CLA	A	803	-	1/1/13/20	6/27/103/115	-
27	CLA	e	607	19	1/1/15/20	22/39/115/115	-
27	CLA	d	308	29	1/1/10/20	2/10/86/115	-
27	CLA	j	604	18	1/1/15/20	16/39/115/115	-
27	CLA	f	605	18	-	6/15/91/115	-
30	WVN	A	846	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	816	39	1/1/15/20	9/39/115/115	-
27	CLA	A	842	-	1/1/15/20	15/39/115/115	-
37	KC2	s	204	-	-	6/15/71/71	-
27	CLA	B	807	2	1/1/15/20	11/39/115/115	-
36	IHT	j	616	-	-	6/25/65/65	0/2/2/2
35	II0	f	614	-	-	5/21/67/67	0/2/2/2
27	CLA	B	801	-	1/1/15/20	20/39/115/115	-
27	CLA	h	308	17	1/1/12/20	10/23/99/115	-
29	LHG	b	617	27	-	20/53/53/53	-
37	KC2	k	311	-	-	8/15/71/71	-
27	CLA	b	601	16	1/1/12/20	10/23/99/115	-
27	CLA	A	814	-	1/1/12/20	8/21/97/115	-
37	KC2	j	610	18	-	5/15/71/71	-
27	CLA	B	817	-	-	4/17/93/115	-
30	WVN	e	615	-	-	11/29/63/63	0/2/2/2
27	CLA	L	203	-	-	14/39/115/115	-
35	II0	i	313	-	-	4/21/67/67	0/2/2/2
27	CLA	A	806	-	-	10/39/115/115	-
27	CLA	A	834	-	1/1/12/20	2/23/99/115	-
27	CLA	j	603	-	1/1/12/20	3/23/99/115	-
27	CLA	e	608	29	1/1/11/20	6/17/93/115	-
37	KC2	n	612	-	-	7/15/71/71	-
27	CLA	A	829	-	1/1/15/20	14/39/115/115	-
27	CLA	B	815	-	-	8/30/106/115	-
27	CLA	c	601	14	1/1/12/20	10/23/99/115	-
35	II0	k	314	-	-	3/21/67/67	0/2/2/2
27	CLA	b	611	-	1/1/15/20	22/39/115/115	-
30	WVN	O	201	-	-	9/29/63/63	0/2/2/2
34	LMG	b	619	-	-	16/44/64/70	0/1/1/1
27	CLA	l	309	20	1/1/12/20	6/23/99/115	-
27	CLA	g	322	-	1/1/15/20	19/39/115/115	-
27	CLA	j	602	18	1/1/12/20	4/21/97/115	-
27	CLA	n	609	26	1/1/15/20	10/39/115/115	-
30	WVN	A	847	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	n	605	26	1/1/12/20	7/23/99/115	-
27	CLA	s	202	13	1/1/15/20	14/39/115/115	-
30	WVN	l	301	-	-	3/29/63/63	0/2/2/2
34	LMG	c	619	-	-	21/50/70/70	0/1/1/1
27	CLA	n	608	26	1/1/12/20	7/23/99/115	-
27	CLA	j	612	-	1/1/15/20	16/39/115/115	-
35	II0	l	315	-	-	5/21/67/67	0/2/2/2
27	CLA	i	305	22	1/1/15/20	10/39/115/115	-
27	CLA	A	835	-	1/1/15/20	14/39/115/115	-
27	CLA	A	855	39	1/1/15/20	15/39/115/115	-
27	CLA	f	609	18	1/1/15/20	7/39/115/115	-
27	CLA	b	602	16	1/1/13/20	10/27/103/115	-
27	CLA	F	202	39	1/1/15/20	13/39/115/115	-
30	WVN	L	205	-	-	6/29/63/63	0/2/2/2
27	CLA	c	603	-	1/1/12/20	2/23/99/115	-
27	CLA	k	305	21	1/1/12/20	12/23/99/115	-
27	CLA	f	608	18	1/1/15/20	6/39/115/115	-
27	CLA	k	303	-	1/1/15/20	11/39/115/115	-
27	CLA	n	613	-	1/1/12/20	9/23/99/115	-
27	CLA	A	831	-	1/1/15/20	8/39/115/115	-
27	CLA	k	301	21	1/1/12/20	5/21/97/115	-
27	CLA	j	611	-	1/1/12/20	8/23/99/115	-
27	CLA	m	604	18	-	14/39/115/115	-
37	KC2	i	317	-	-	8/15/71/71	-
30	WVN	I	101	-	-	9/29/63/63	0/2/2/2
27	CLA	b	607	16	1/1/15/20	17/39/115/115	-
27	CLA	B	812	-	1/1/13/20	11/32/108/115	-
27	CLA	c	602	14	1/1/12/20	10/21/97/115	-
35	II0	g	316	-	-	4/21/67/67	0/2/2/2
29	LHG	b	618	-	-	15/35/35/53	-
27	CLA	m	608	18	1/1/12/20	4/23/99/115	-
27	CLA	d	307	23	-	2/10/86/115	-
30	WVN	s	205	-	-	4/29/63/63	0/2/2/2
27	CLA	f	606	18	-	4/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	g	307	24	-	8/23/99/115	-
27	CLA	g	315	-	-	9/23/99/115	-
27	CLA	a	312	-	-	19/39/115/115	-
27	CLA	a	306	39	1/1/15/20	14/39/115/115	-
27	CLA	a	305	-	1/1/12/20	6/23/99/115	-
27	CLA	c	607	14	1/1/11/20	5/17/93/115	-
27	CLA	O	202	-	1/1/15/20	14/39/115/115	-
35	II0	b	615	-	-	2/21/67/67	0/2/2/2
27	CLA	A	805	1	1/1/15/20	9/39/115/115	-
35	II0	d	312	-	-	5/21/67/67	0/2/2/2
29	LHG	c	618	27	-	13/41/41/53	-
27	CLA	i	303	22	1/1/12/20	9/21/97/115	-
27	CLA	l	303	20	1/1/11/20	5/18/94/115	-
27	CLA	e	601	19	1/1/11/20	7/15/91/115	-
30	WVN	R	202	-	-	10/29/63/63	0/2/2/2
27	CLA	B	831	-	1/1/13/20	6/31/107/115	-
27	CLA	n	607	-	1/1/15/20	13/39/115/115	-
27	CLA	A	816	-	1/1/15/20	17/39/115/115	-
27	CLA	B	814	-	1/1/13/20	5/32/108/115	-
27	CLA	B	830	39	1/1/11/20	6/15/91/115	-
35	II0	k	318	-	-	6/21/67/67	0/2/2/2
27	CLA	l	304	20	1/1/15/20	21/39/115/115	-
32	SF4	A	854	1,2	-	-	0/6/5/5
27	CLA	j	605	18	-	5/15/91/115	-
27	CLA	A	852	-	1/1/15/20	7/39/115/115	-
27	CLA	A	837	-	1/1/15/20	10/39/115/115	-
35	II0	d	314	-	-	5/21/67/67	0/2/2/2
35	II0	j	615	-	-	9/21/67/67	0/2/2/2
27	CLA	B	834	39	1/1/15/20	15/39/115/115	-
27	CLA	A	802	-	1/1/15/20	14/39/115/115	-
27	CLA	B	836	-	1/1/15/20	12/39/115/115	-
27	CLA	B	808	-	1/1/13/20	2/25/101/115	-
35	II0	O	203	-	-	4/21/67/67	0/2/2/2
37	KC2	k	310	21	-	8/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	l	307	20	1/1/15/20	15/39/115/115	-
28	PQN	A	843	-	-	12/23/43/43	0/2/2/2
29	LHG	A	845	27	-	5/31/31/53	-
27	CLA	B	809	-	1/1/13/20	5/27/103/115	-
27	CLA	s	203	13,27	-	19/39/115/115	-
27	CLA	b	605	39,27	1/1/15/20	13/39/115/115	-
35	II0	e	612	-	-	4/21/67/67	0/2/2/2
27	CLA	m	612	-	1/1/10/20	8/13/89/115	-
27	CLA	B	829	39	1/1/15/20	11/39/115/115	-
27	CLA	k	306	-	1/1/12/20	11/23/99/115	-
29	LHG	A	844	-	-	4/52/52/53	-
30	WVN	M	101	-	-	7/29/63/63	0/2/2/2
30	WVN	B	847	-	-	12/29/63/63	0/2/2/2
30	WVN	R	201	-	-	6/29/63/63	0/2/2/2
27	CLA	J	105	29	1/1/12/20	9/23/99/115	-
35	II0	h	311	-	-	8/21/67/67	0/2/2/2
36	IHT	a	317	-	-	4/25/65/65	0/2/2/2
27	CLA	B	823	-	1/1/15/20	13/39/115/115	-
34	LMG	F	206	-	-	11/43/63/70	0/1/1/1
30	WVN	B	845	-	-	10/29/63/63	0/2/2/2
29	LHG	d	315	27	-	15/41/41/53	-
35	II0	e	614	-	-	5/21/67/67	0/2/2/2
37	KC2	s	201	13	-	7/15/71/71	-
27	CLA	d	304	-	-	7/23/99/115	-
27	CLA	A	813	-	1/1/11/20	6/15/91/115	-
29	LHG	g	321	27	-	13/41/41/53	-
29	LHG	l	318	27	-	14/36/36/53	-
27	CLA	A	818	-	1/1/15/20	16/39/115/115	-
27	CLA	a	307	15	-	6/15/91/115	-
36	IHT	O	204	-	-	10/25/65/65	0/2/2/2
27	CLA	e	611	-	-	14/39/115/115	-
27	CLA	d	303	23	1/1/15/20	23/39/115/115	-
29	LHG	j	617	27	-	4/34/34/53	-
37	KC2	m	610	18	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	KC2	g	314	37	-	5/15/71/71	-
27	CLA	A	810	-	1/1/14/20	11/36/112/115	-
29	LHG	L	207	-	-	20/53/53/53	-
27	CLA	L	206	39	1/1/12/20	5/23/99/115	-
36	IHT	c	616	-	-	8/25/65/65	0/2/2/2
27	CLA	A	840	1	-	15/39/115/115	-
27	CLA	A	836	-	-	6/39/115/115	-
27	CLA	B	805	-	1/1/15/20	10/39/115/115	-
29	LHG	i	316	27	-	11/41/41/53	-
27	CLA	j	609	29	1/1/14/20	18/35/111/115	-
27	CLA	m	603	-	1/1/15/20	9/39/115/115	-
27	CLA	A	804	-	1/1/15/20	6/39/115/115	-
27	CLA	m	602	18	1/1/13/20	10/29/105/115	-
27	CLA	A	839	39	1/1/15/20	13/39/115/115	-
27	CLA	c	612	-	1/1/15/20	14/39/115/115	-
35	II0	J	104	-	-	7/21/67/67	0/2/2/2
27	CLA	n	604	26	1/1/14/20	10/33/109/115	-
27	CLA	B	835	-	1/1/15/20	23/39/115/115	-
37	KC2	g	313	37	-	3/15/71/71	-
36	IHT	k	317	-	-	7/25/65/65	0/2/2/2
27	CLA	c	606	-	-	11/24/100/115	-
31	LMT	A	851	-	-	13/21/61/61	0/2/2/2
27	CLA	i	308	22	1/1/12/20	4/23/99/115	-
27	CLA	e	602	19	1/1/12/20	11/21/97/115	-
29	LHG	n	619	-	-	16/47/47/53	-
30	WVN	B	848	-	-	7/29/63/63	0/2/2/2
35	II0	h	312	-	-	5/21/67/67	0/2/2/2
27	CLA	k	313	-	1/1/12/20	11/23/99/115	-
35	II0	g	317	-	-	3/21/67/67	0/2/2/2
27	CLA	A	823	-	1/1/13/20	4/27/103/115	-
27	CLA	f	602	18	1/1/15/20	15/39/115/115	-
29	LHG	m	617	27	-	16/41/41/53	-
27	CLA	B	819	-	1/1/12/20	6/25/101/115	-
27	CLA	n	606	26	1/1/12/20	6/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	II0	a	315	-	-	4/21/67/67	0/2/2/2
35	II0	g	320	-	-	3/21/67/67	0/2/2/2
27	CLA	h	302	17	1/1/12/20	7/21/97/115	-
36	IHT	b	614	-	-	5/25/65/65	0/2/2/2
27	CLA	B	832	-	1/1/15/20	8/39/115/115	-
27	CLA	j	601	18	1/1/12/20	5/23/99/115	-
27	CLA	b	609	-	-	5/23/99/115	-
30	WVN	A	848	-	-	8/29/63/63	0/2/2/2
27	CLA	i	307	22	1/1/14/20	11/35/111/115	-
34	LMG	J	106	-	-	14/50/70/70	0/1/1/1
29	LHG	e	617	27	-	26/41/41/53	-
35	II0	f	615	-	-	5/21/67/67	0/2/2/2
27	CLA	f	603	-	1/1/12/20	7/23/99/115	-
27	CLA	n	602	26	1/1/12/20	2/21/97/115	-
27	CLA	i	309	29	1/1/11/20	5/17/93/115	-
27	CLA	k	308	21	1/1/15/20	12/39/115/115	-
27	CLA	l	305	-	1/1/12/20	4/23/99/115	-
35	II0	l	302	-	-	6/21/67/67	0/2/2/2
35	II0	h	310	-	-	3/17/40/67	0/1/1/2
27	CLA	A	817	-	1/1/15/20	15/39/115/115	-
27	CLA	J	103	8	1/1/10/20	4/12/88/115	-
27	CLA	B	828	-	1/1/12/20	5/21/97/115	-
27	CLA	K	102	-	1/1/10/20	5/12/88/115	-
27	CLA	g	311	29	1/1/12/20	8/26/102/115	-
31	LMT	a	302	-	-	6/15/35/61	0/1/1/2
27	CLA	l	308	20	1/1/15/20	10/39/115/115	-
27	CLA	e	606	19	1/1/15/20	20/39/115/115	-
27	CLA	B	820	39	1/1/15/20	13/39/115/115	-
27	CLA	h	313	39	1/1/15/20	7/39/115/115	-
35	II0	c	615	-	-	2/21/67/67	0/2/2/2
27	CLA	l	306	20	-	15/39/115/115	-

The worst 5 of 4103 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	R	204	IHT	C15-C11	25.57	1.63	1.35
36	c	616	IHT	C15-C11	25.37	1.63	1.35
36	n	617	IHT	C15-C11	25.20	1.62	1.35
36	j	616	IHT	C15-C11	25.05	1.62	1.35
36	m	616	IHT	C15-C11	25.02	1.62	1.35

The worst 5 of 4638 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	813	CLA	C4A-NA-C1A	13.35	112.77	106.68
37	n	612	KC2	C1A-NA-C4A	-12.43	101.01	106.68
37	l	311	KC2	C1A-NA-C4A	-12.02	101.20	106.68
37	n	611	KC2	C1A-NA-C4A	-11.76	101.31	106.68
37	m	610	KC2	C1A-NA-C4A	-11.65	101.36	106.68

5 of 218 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	801	CLA	ND
27	A	802	CLA	ND
27	A	803	CLA	ND
27	A	804	CLA	ND
27	A	805	CLA	ND

5 of 3615 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	801	CLA	CBD-CGD-O2D-CED
27	A	802	CLA	C1A-C2A-CAA-CBA
27	A	802	CLA	CBA-CGA-O2A-C1
27	A	802	CLA	O1A-CGA-O2A-C1
27	A	803	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

227 monomers are involved in 408 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	n	614	II0	1	0
37	f	611	KC2	2	0
27	f	604	CLA	4	0
27	B	824	CLA	1	0
27	l	310	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	310	CLA	1	0
36	f	617	IHT	2	0
27	A	856	CLA	3	0
27	A	821	CLA	2	0
27	B	826	CLA	1	0
36	c	620	IHT	1	0
35	m	615	II0	1	0
27	B	810	CLA	1	0
27	g	309	CLA	1	0
27	g	302	CLA	2	0
27	B	822	CLA	1	0
27	A	832	CLA	1	0
27	B	825	CLA	1	0
27	n	603	CLA	2	0
27	g	308	CLA	3	0
37	l	311	KC2	1	0
27	f	610	CLA	4	0
35	b	613	II0	1	0
35	f	616	II0	1	0
29	g	301	LHG	4	0
38	i	301	LMU	1	0
27	A	812	CLA	1	0
33	B	842	DGD	2	0
27	L	202	CLA	2	0
29	c	621	LHG	6	0
35	i	318	II0	1	0
29	A	850	LHG	4	0
27	A	838	CLA	2	0
27	A	824	CLA	3	0
27	A	828	CLA	2	0
27	m	609	CLA	6	0
27	d	305	CLA	2	0
27	h	306	CLA	6	0
36	g	319	IHT	1	0
27	h	305	CLA	1	0
27	B	840	CLA	1	0
27	A	807	CLA	1	0
27	A	822	CLA	2	0
27	j	606	CLA	2	0
27	g	303	CLA	2	0
27	A	808	CLA	2	0
31	a	320	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	k	307	CLA	2	0
27	i	302	CLA	2	0
27	A	801	CLA	2	0
27	d	301	CLA	1	0
27	a	311	CLA	1	0
27	A	815	CLA	1	0
29	a	319	LHG	1	0
27	m	601	CLA	2	0
27	m	606	CLA	2	0
27	F	201	CLA	1	0
27	B	821	CLA	1	0
27	b	608	CLA	5	0
27	a	308	CLA	2	0
27	k	304	CLA	3	0
27	i	306	CLA	1	0
27	s	206	CLA	2	0
35	l	313	II0	2	0
27	c	604	CLA	1	0
27	j	607	CLA	3	0
27	A	826	CLA	2	0
27	c	608	CLA	3	0
27	B	802	CLA	2	0
27	i	311	CLA	1	0
34	s	210	LMG	3	0
27	l	312	CLA	1	0
27	b	606	CLA	3	0
27	A	841	CLA	1	0
27	e	605	CLA	2	0
27	f	607	CLA	2	0
27	k	309	CLA	2	0
27	e	604	CLA	4	0
27	e	610	CLA	3	0
27	A	811	CLA	2	0
27	F	203	CLA	1	0
27	A	820	CLA	2	0
27	B	803	CLA	2	0
27	b	603	CLA	3	0
27	n	610	CLA	4	0
27	h	301	CLA	2	0
29	f	619	LHG	3	0
27	s	208	CLA	2	0
27	b	610	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	304	CLA	1	0
27	B	838	CLA	5	0
27	A	827	CLA	2	0
28	B	841	PQN	1	0
27	a	303	CLA	2	0
29	a	301	LHG	1	0
27	B	849	CLA	2	0
31	b	616	LMT	1	0
27	B	804	CLA	3	0
27	A	830	CLA	2	0
34	L	208	LMG	2	0
27	A	853	CLA	2	0
27	B	837	CLA	1	0
27	f	601	CLA	2	0
29	J	107	LHG	6	0
27	h	307	CLA	1	0
35	k	315	II0	1	0
27	A	809	CLA	3	0
27	A	803	CLA	1	0
27	e	607	CLA	5	0
27	j	604	CLA	1	0
27	B	816	CLA	2	0
27	A	842	CLA	4	0
36	j	616	IHT	2	0
27	B	801	CLA	2	0
27	h	308	CLA	2	0
29	b	617	LHG	5	0
37	k	311	KC2	3	0
27	b	601	CLA	1	0
27	A	814	CLA	2	0
37	j	610	KC2	1	0
27	L	203	CLA	2	0
27	A	806	CLA	1	0
27	j	603	CLA	1	0
27	A	829	CLA	2	0
27	B	815	CLA	1	0
27	c	601	CLA	1	0
27	b	611	CLA	3	0
34	b	619	LMG	2	0
27	l	309	CLA	1	0
27	g	322	CLA	4	0
27	j	602	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	n	609	CLA	2	0
27	s	202	CLA	3	0
34	c	619	LMG	3	0
27	n	608	CLA	1	0
27	i	305	CLA	1	0
27	A	835	CLA	1	0
27	A	855	CLA	4	0
27	f	609	CLA	1	0
27	F	202	CLA	5	0
27	c	603	CLA	1	0
27	k	305	CLA	1	0
27	f	608	CLA	7	0
27	n	613	CLA	1	0
27	A	831	CLA	2	0
27	k	301	CLA	2	0
27	m	604	CLA	1	0
37	i	317	KC2	1	0
27	b	607	CLA	1	0
27	B	812	CLA	1	0
27	c	602	CLA	2	0
29	b	618	LHG	1	0
30	s	205	WVN	1	0
27	f	606	CLA	2	0
27	a	312	CLA	3	0
27	a	306	CLA	1	0
27	c	607	CLA	1	0
27	O	202	CLA	2	0
27	i	303	CLA	2	0
27	l	303	CLA	1	0
27	e	601	CLA	1	0
27	B	831	CLA	1	0
27	n	607	CLA	1	0
27	A	816	CLA	1	0
27	B	814	CLA	2	0
27	B	830	CLA	1	0
27	l	304	CLA	3	0
32	A	854	SF4	5	0
27	j	605	CLA	1	0
27	A	852	CLA	4	0
27	A	837	CLA	4	0
35	j	615	II0	1	0
27	B	834	CLA	3	0

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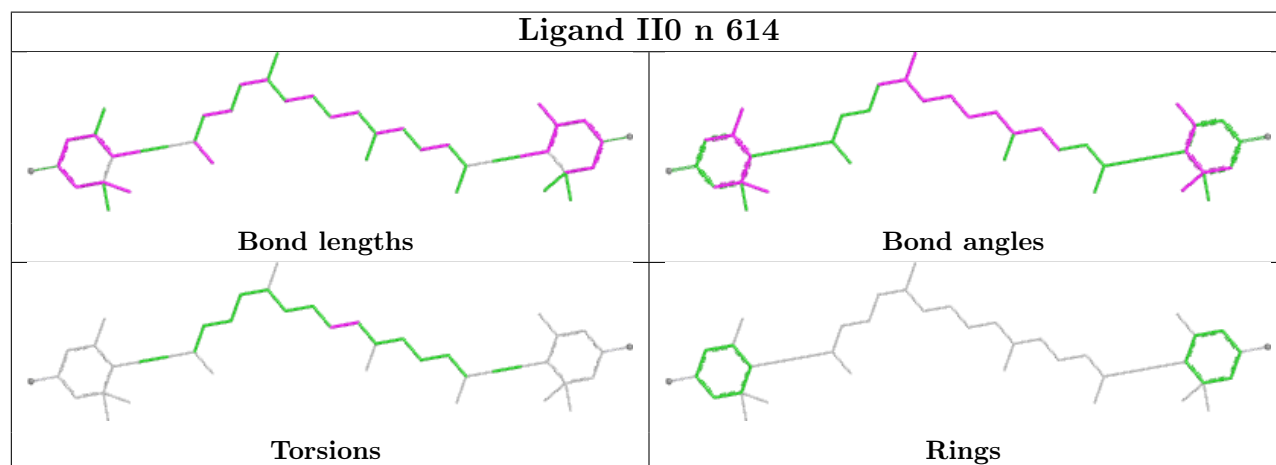
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	802	CLA	7	0
27	B	836	CLA	4	0
27	B	808	CLA	1	0
37	k	310	KC2	1	0
27	l	307	CLA	2	0
28	A	843	PQN	2	0
27	B	809	CLA	2	0
27	s	203	CLA	1	0
27	b	605	CLA	1	0
27	m	612	CLA	1	0
27	B	829	CLA	1	0
27	k	306	CLA	1	0
27	J	105	CLA	2	0
34	F	206	LMG	1	0
27	d	304	CLA	1	0
29	l	318	LHG	2	0
27	A	818	CLA	3	0
27	e	611	CLA	4	0
27	d	303	CLA	2	0
29	j	617	LHG	2	0
37	m	610	KC2	7	0
29	L	207	LHG	2	0
27	L	206	CLA	1	0
27	A	840	CLA	2	0
27	A	836	CLA	2	0
27	B	805	CLA	1	0
29	i	316	LHG	1	0
27	j	609	CLA	4	0
27	m	603	CLA	6	0
27	A	804	CLA	2	0
27	m	602	CLA	4	0
27	A	839	CLA	8	0
27	n	604	CLA	2	0
27	B	835	CLA	5	0
27	c	606	CLA	1	0
31	A	851	LMT	1	0
27	i	308	CLA	2	0
27	e	602	CLA	1	0
29	n	619	LHG	1	0
35	h	312	II0	1	0
27	A	823	CLA	1	0
27	f	602	CLA	3	0

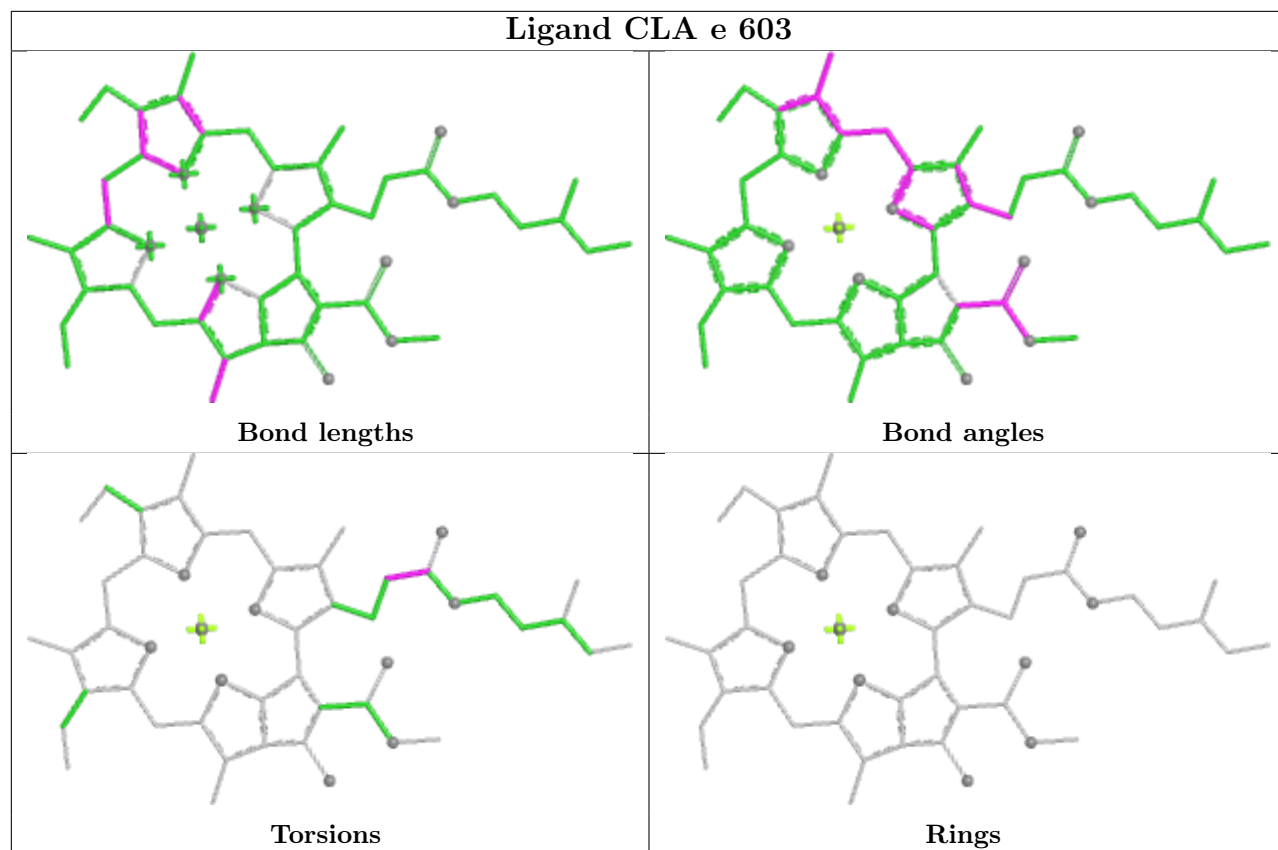
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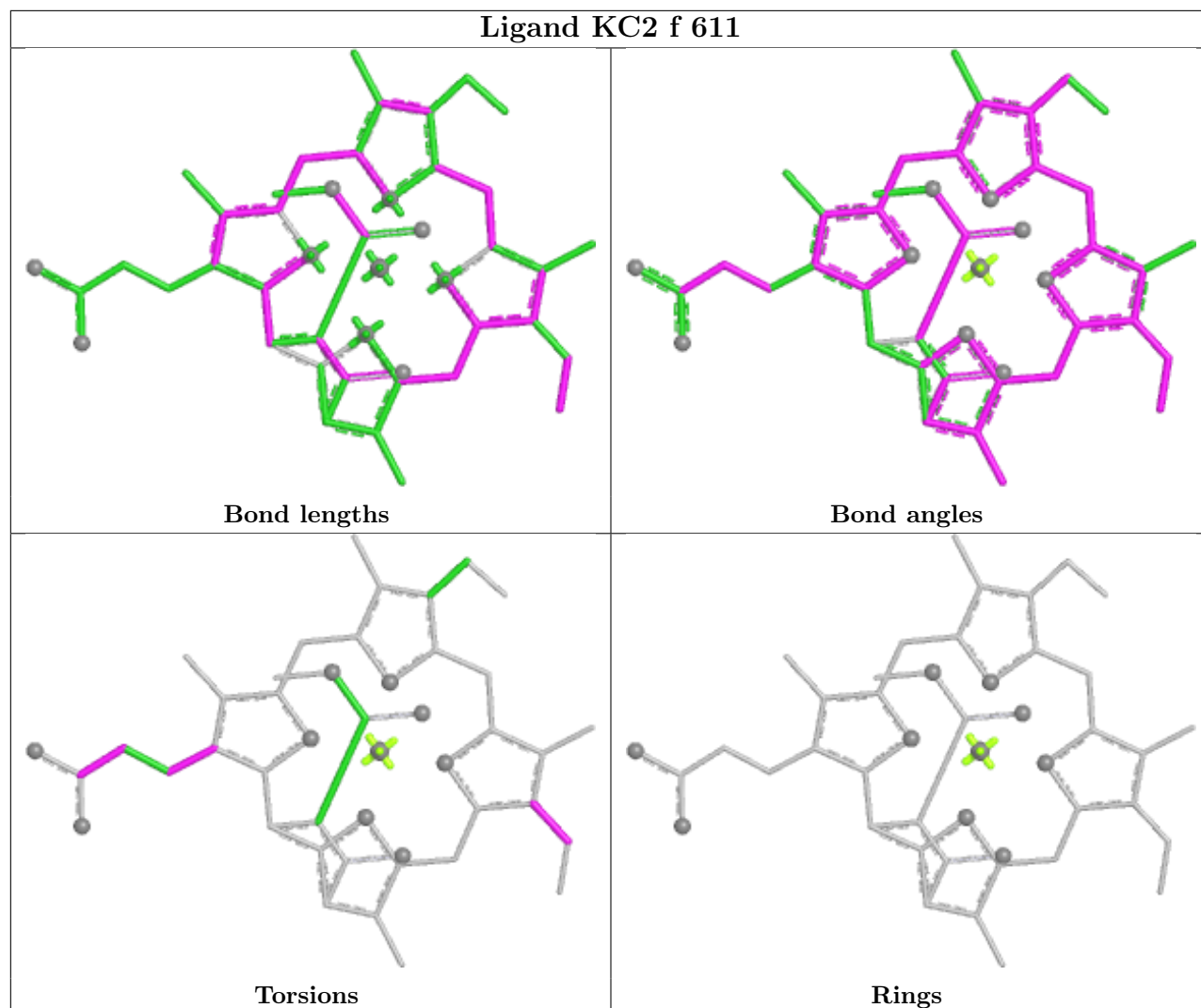
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	b	614	IHT	3	0
27	j	601	CLA	2	0
34	J	106	LMG	3	0
29	e	617	LHG	1	0
27	n	602	CLA	1	0
27	i	309	CLA	2	0
27	k	308	CLA	3	0
27	A	817	CLA	2	0
27	g	311	CLA	2	0
27	l	308	CLA	3	0
27	e	606	CLA	4	0
27	B	820	CLA	3	0

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.

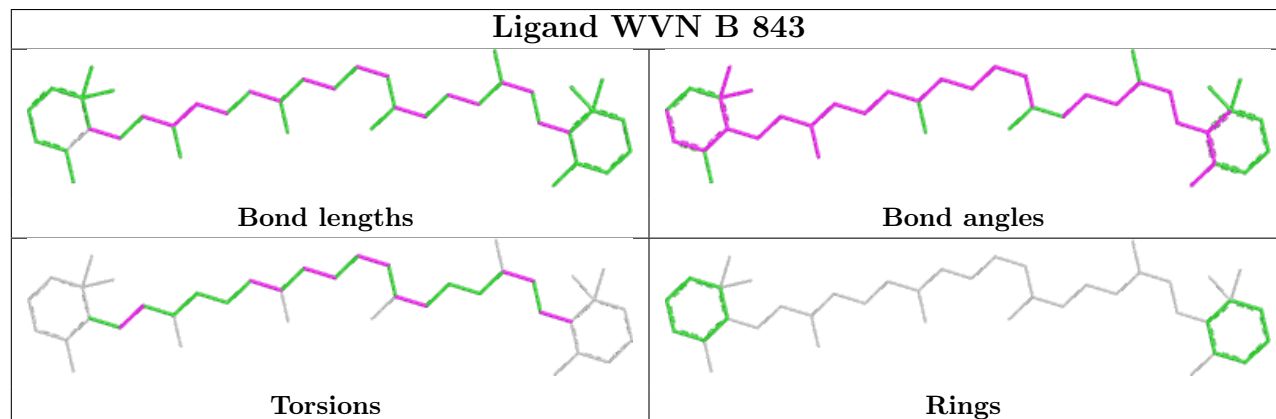


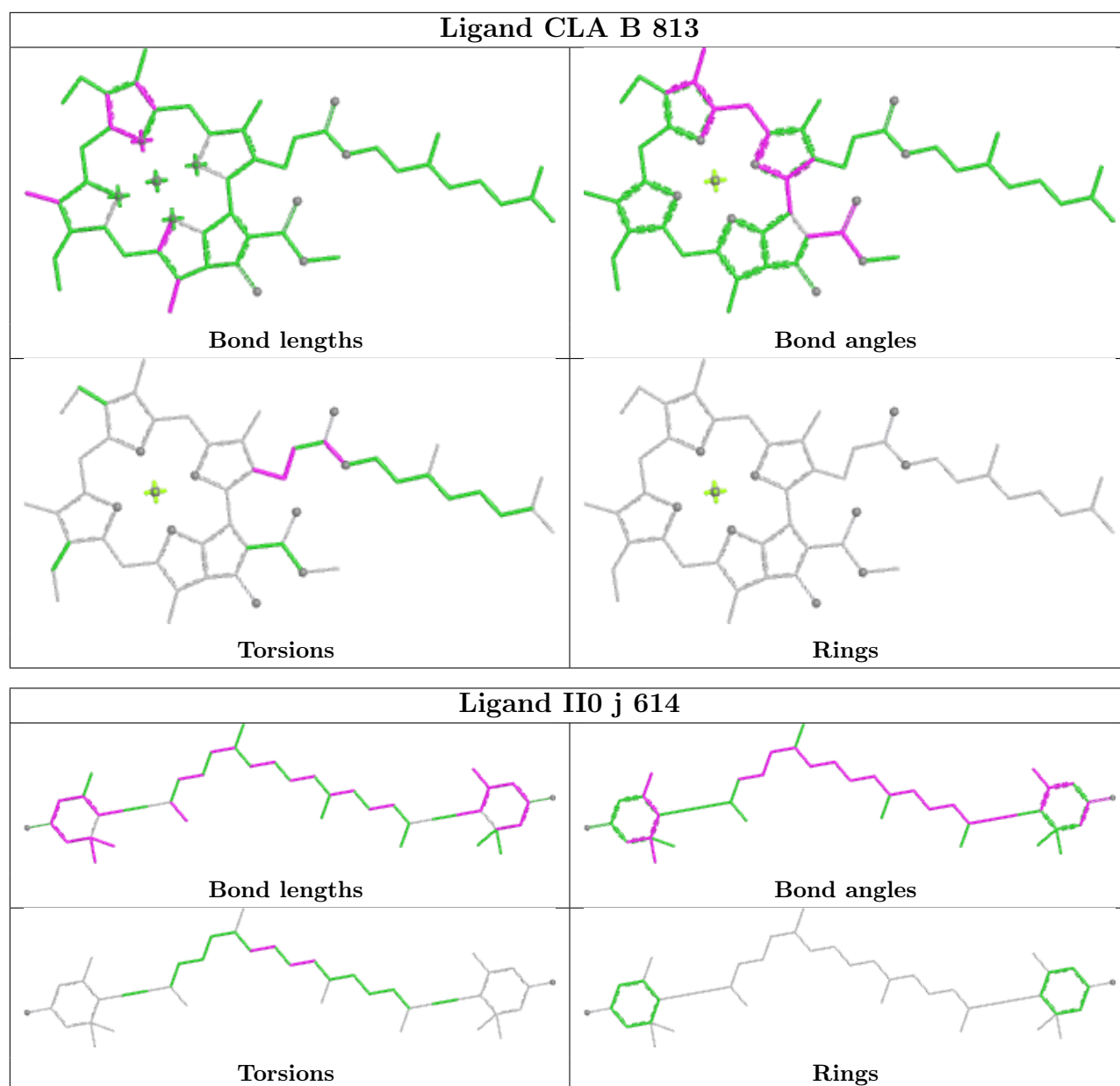


Ligand KC2 f 611

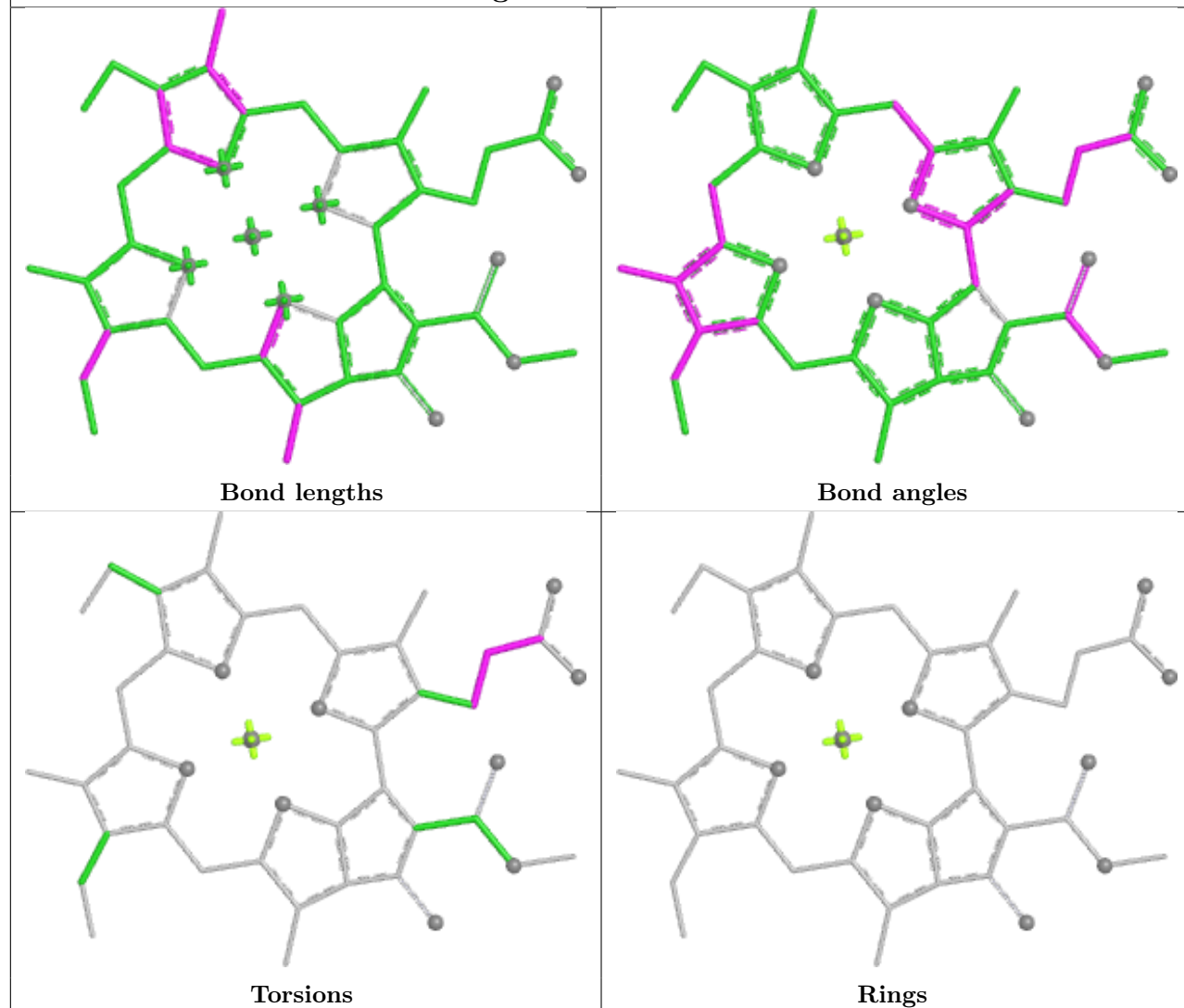


Ligand WVN B 843

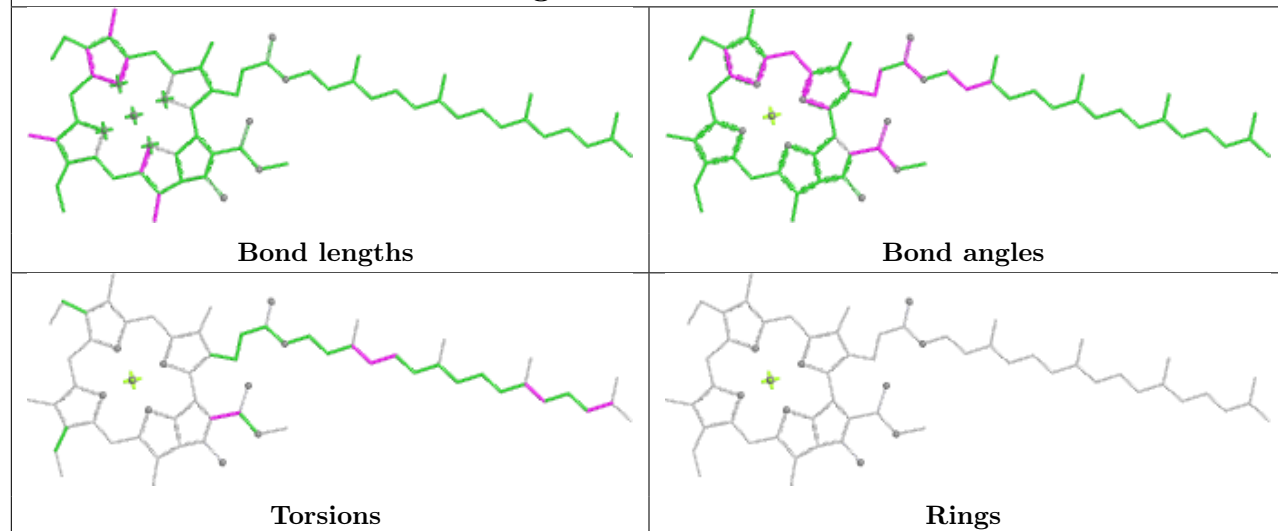


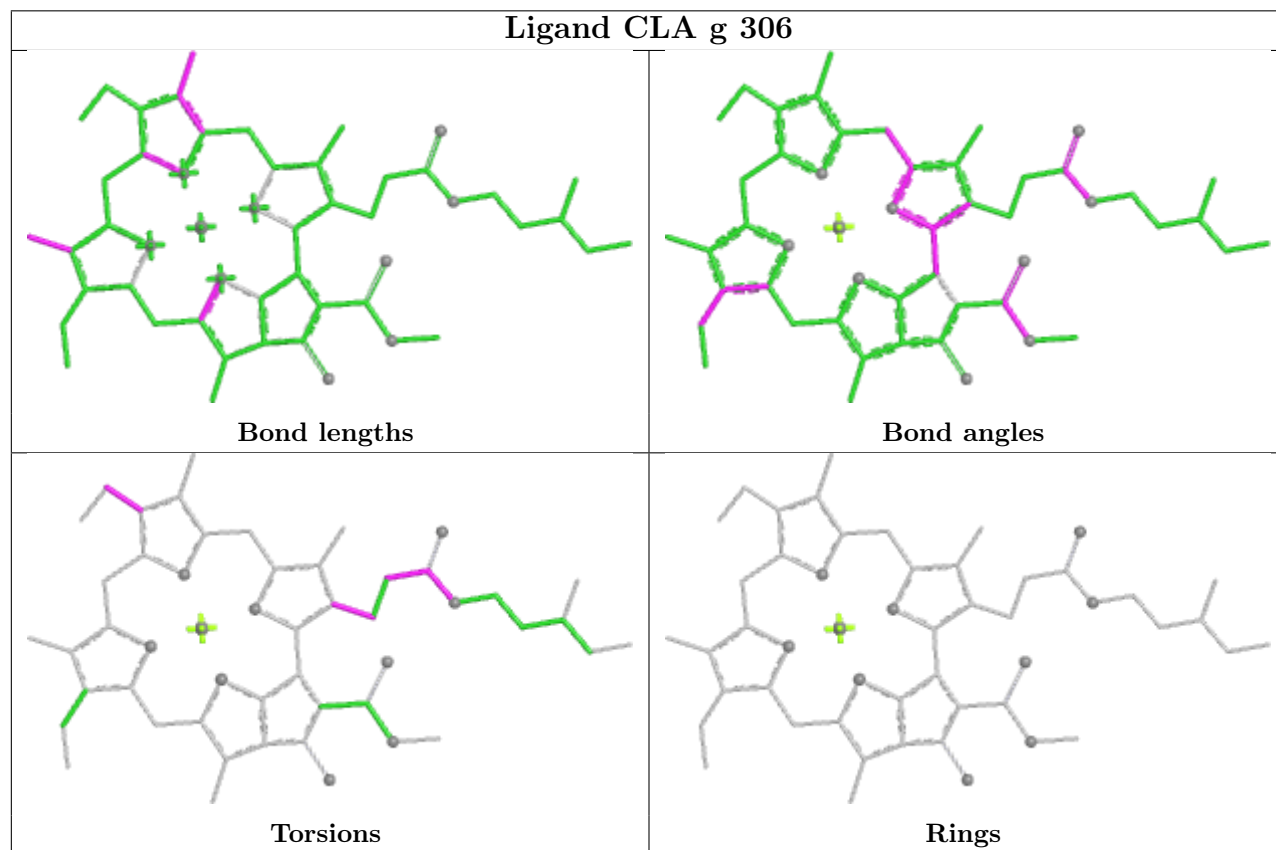
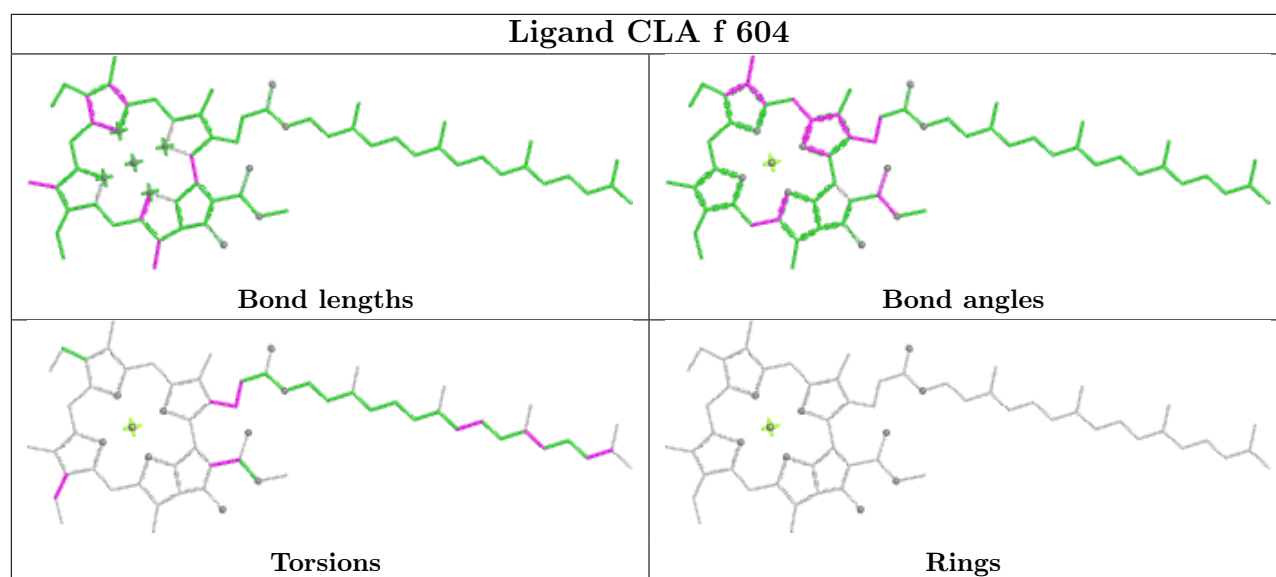


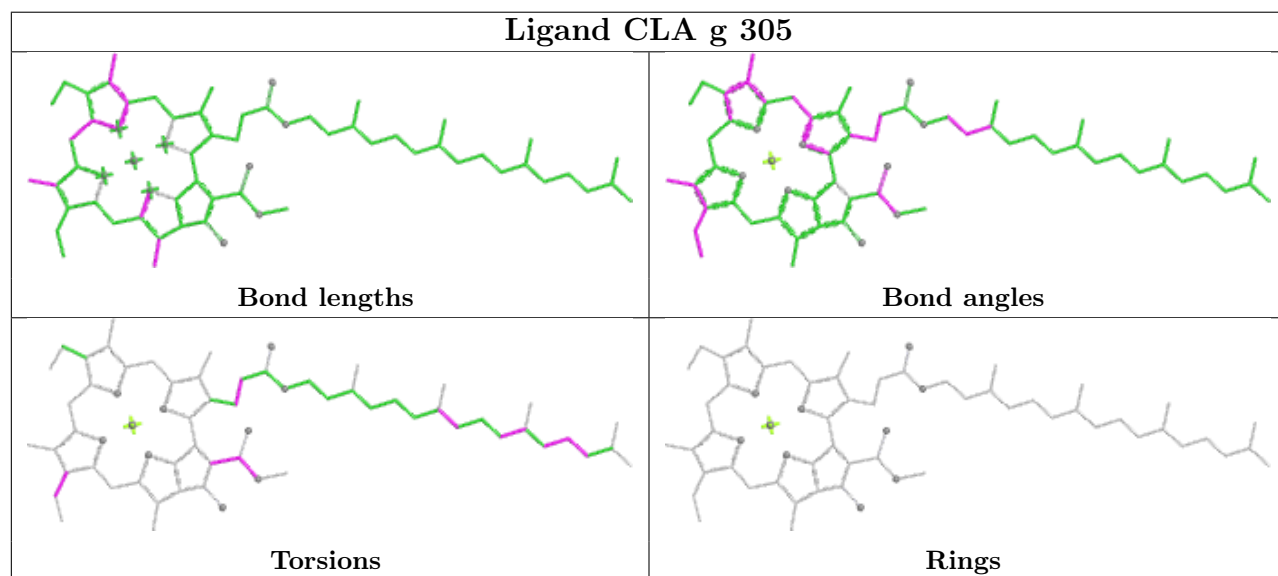
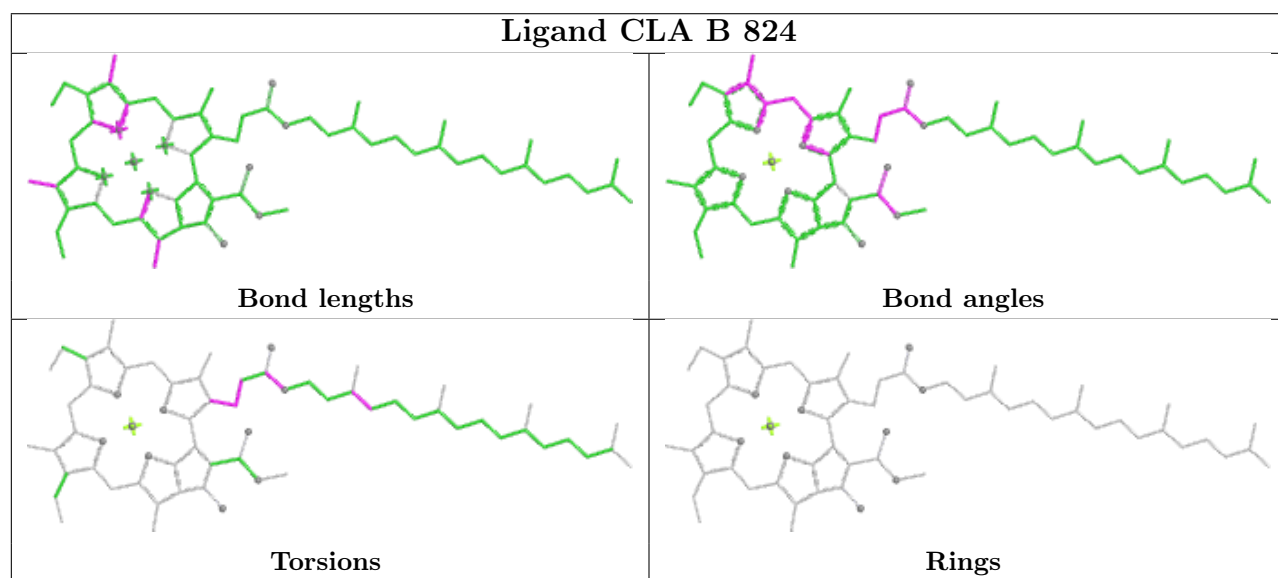
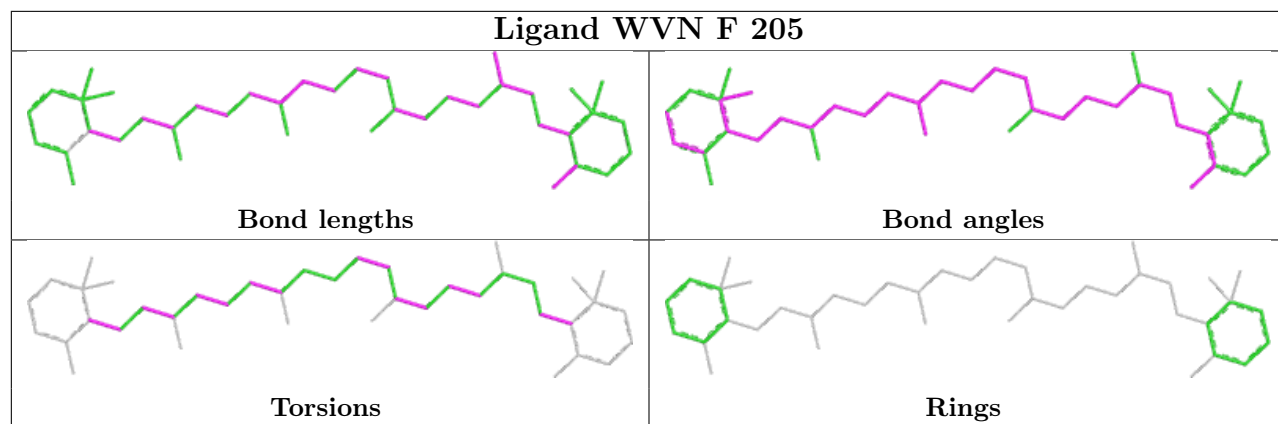
Ligand CLA A 819



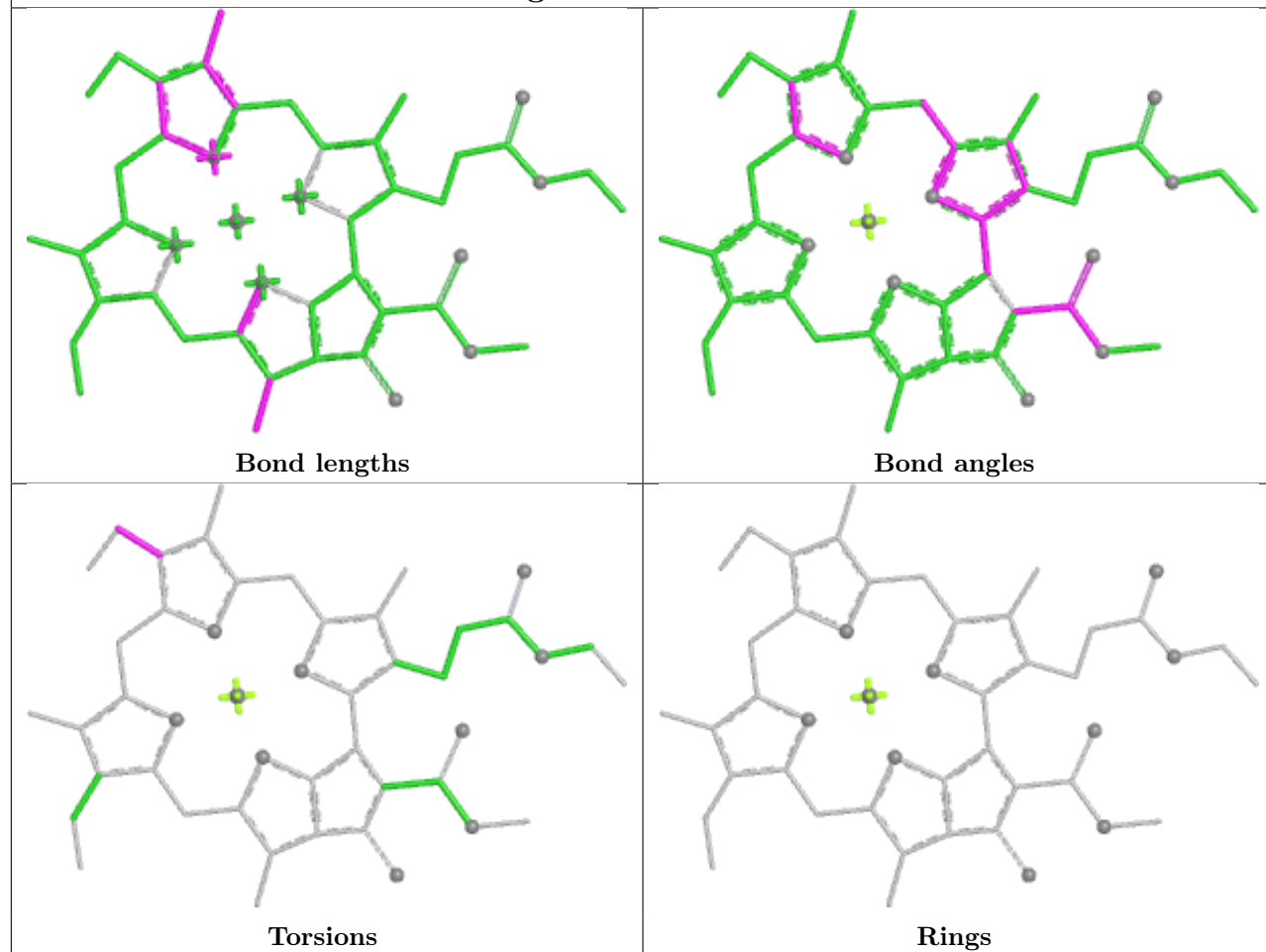
Ligand CLA B 806



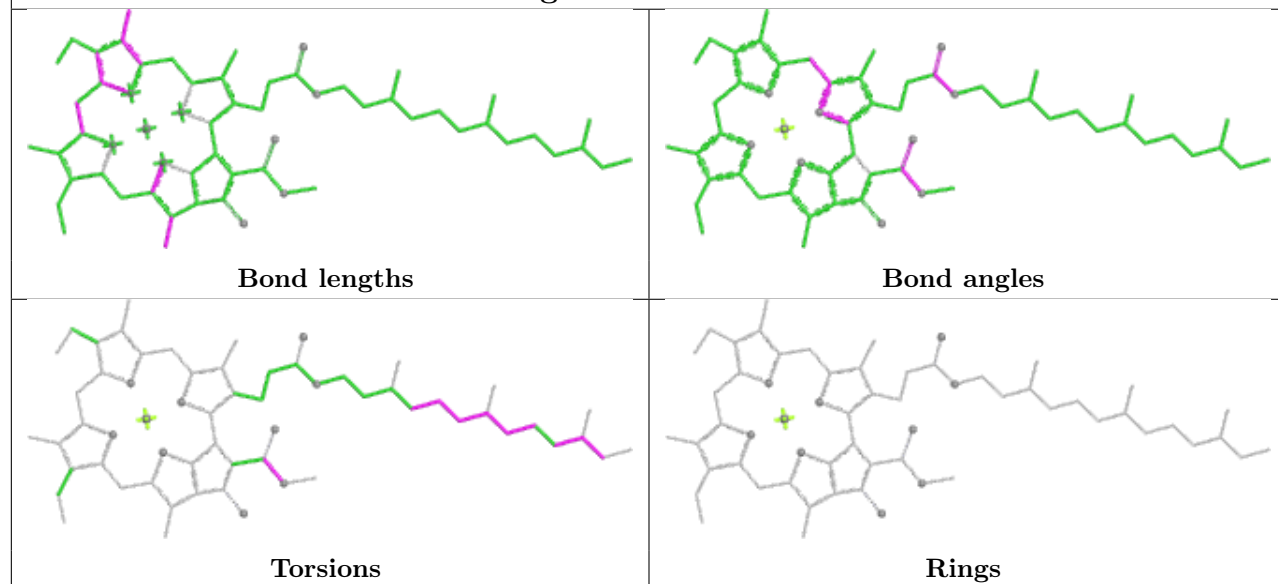


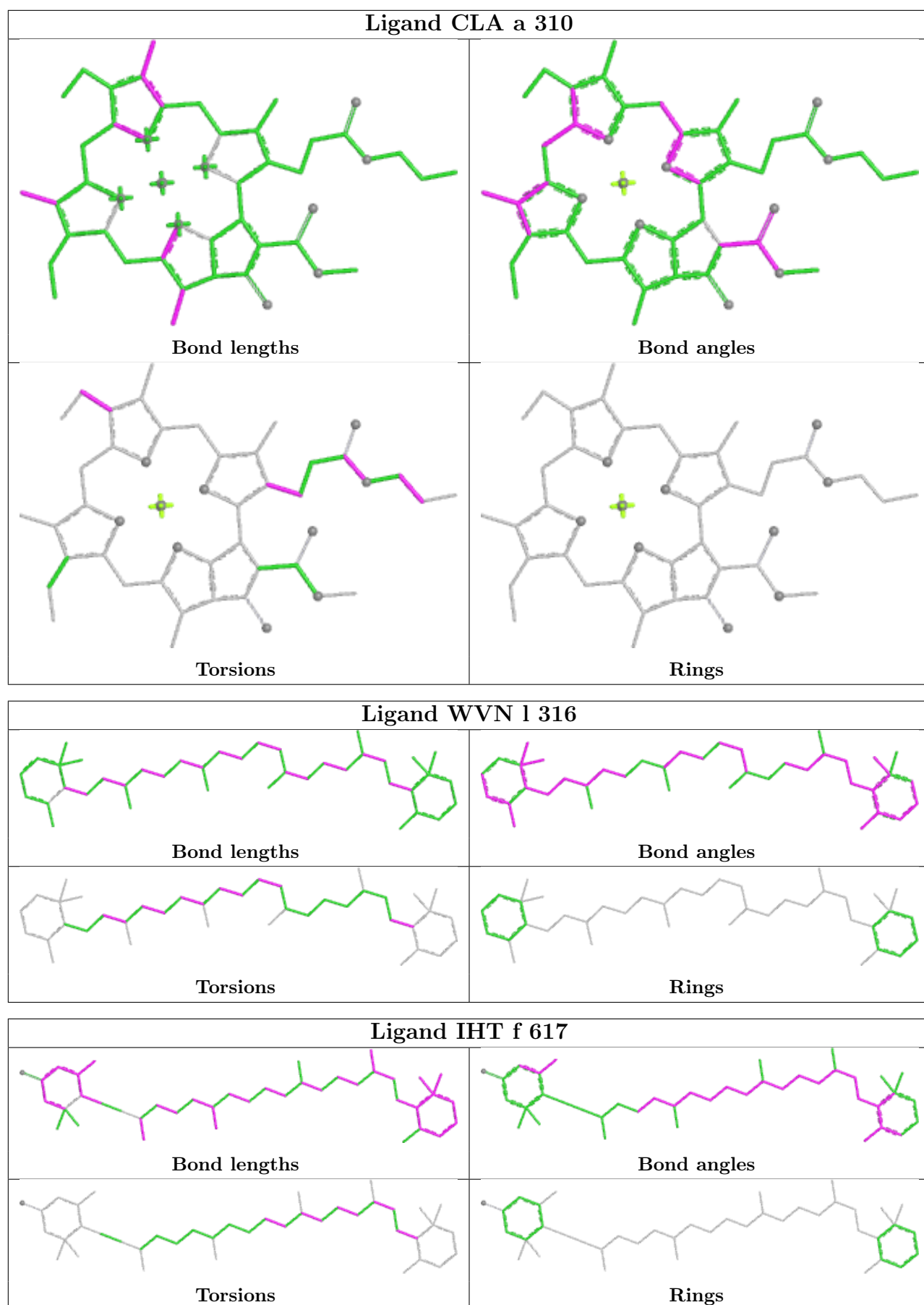


Ligand CLA B 833

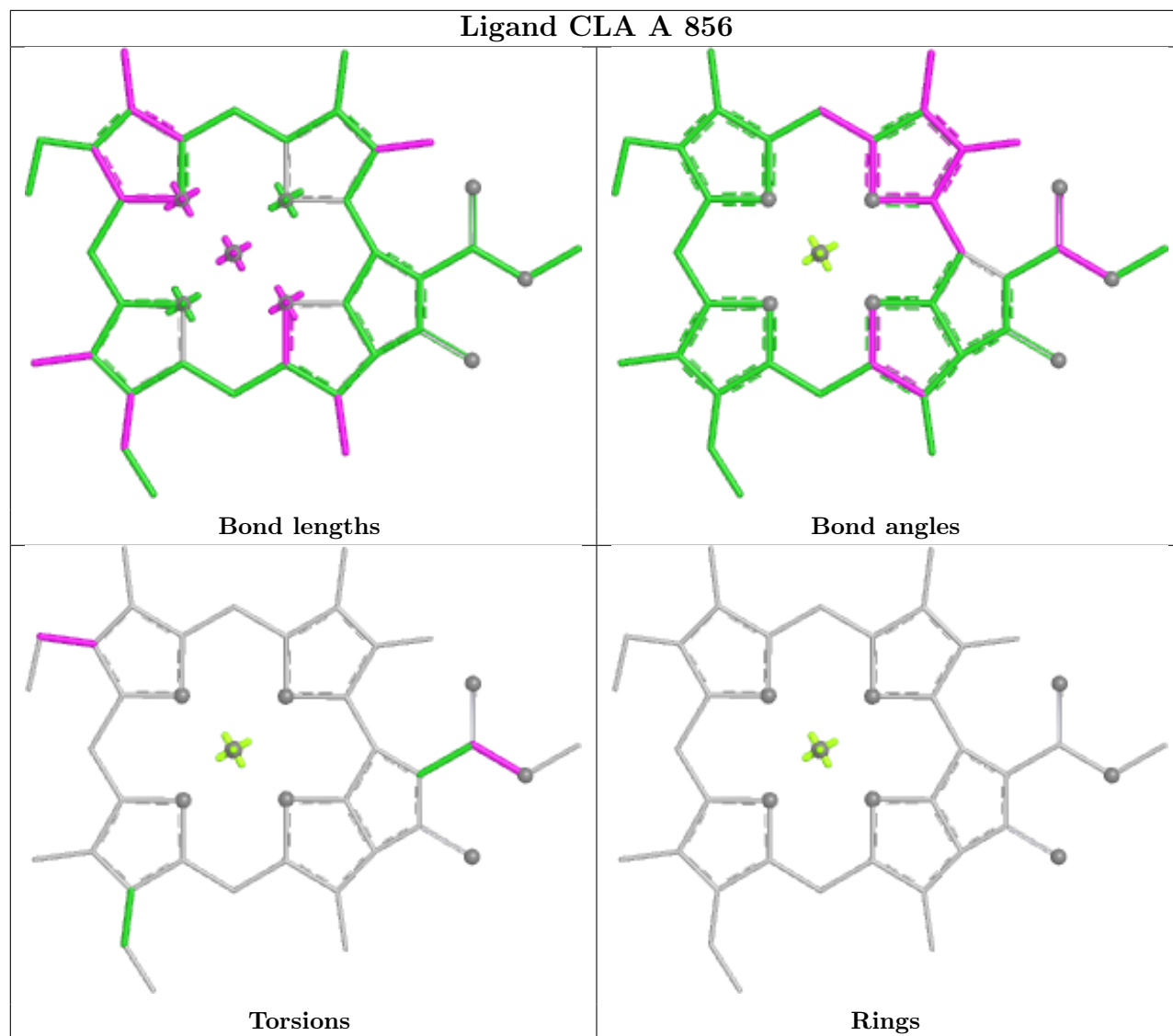


Ligand CLA I 310

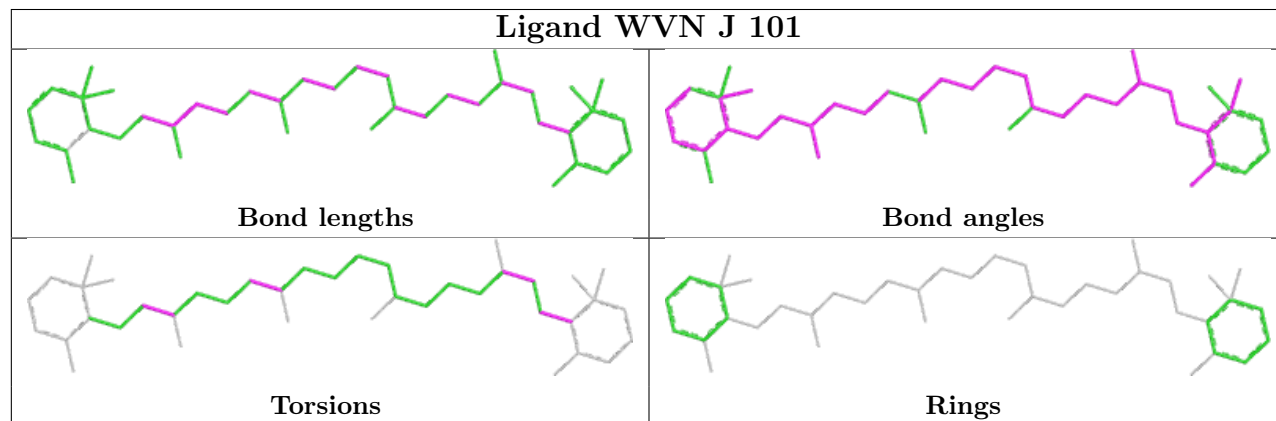




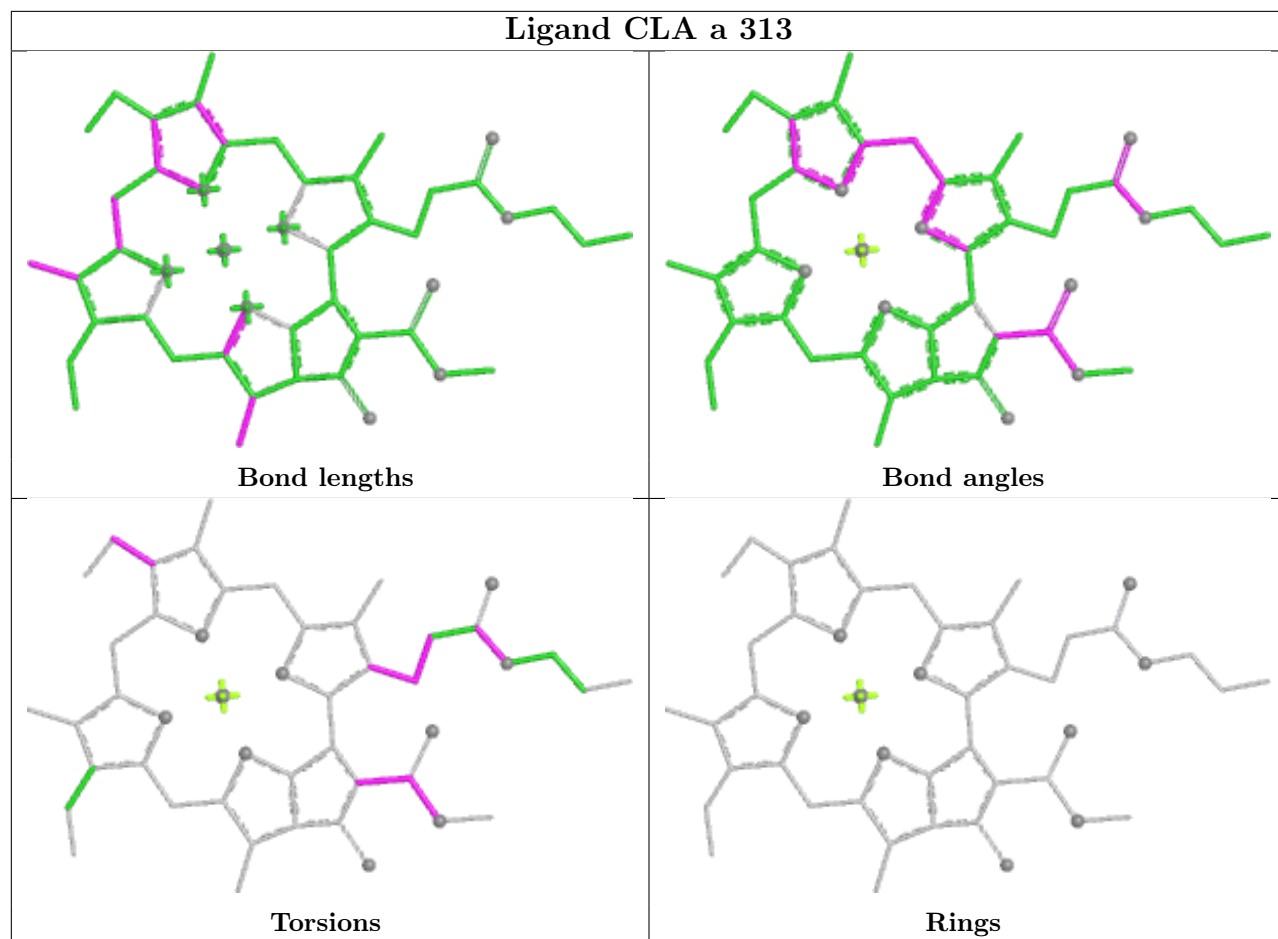
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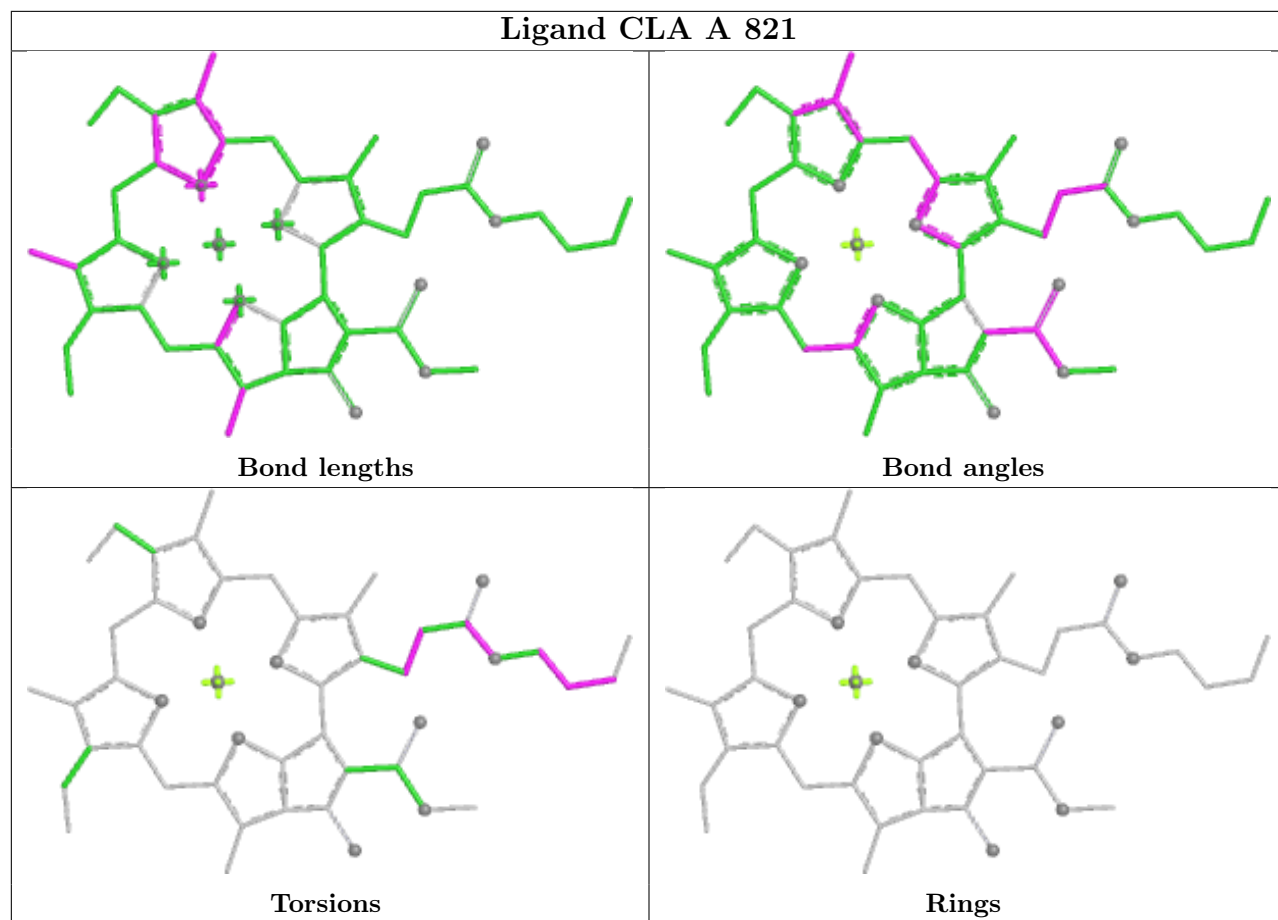
Ligand WVN J 101



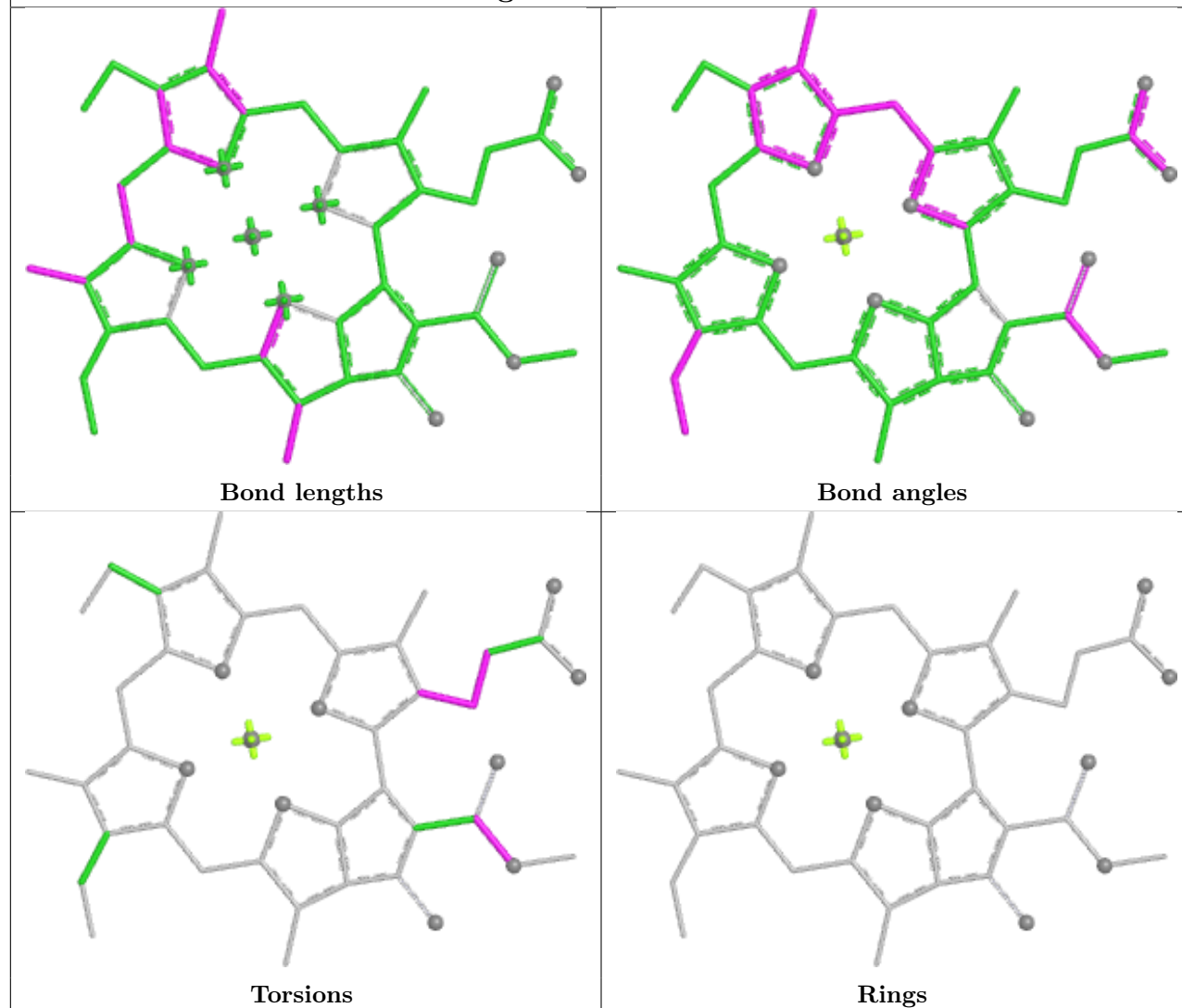
Ligand CLA a 313



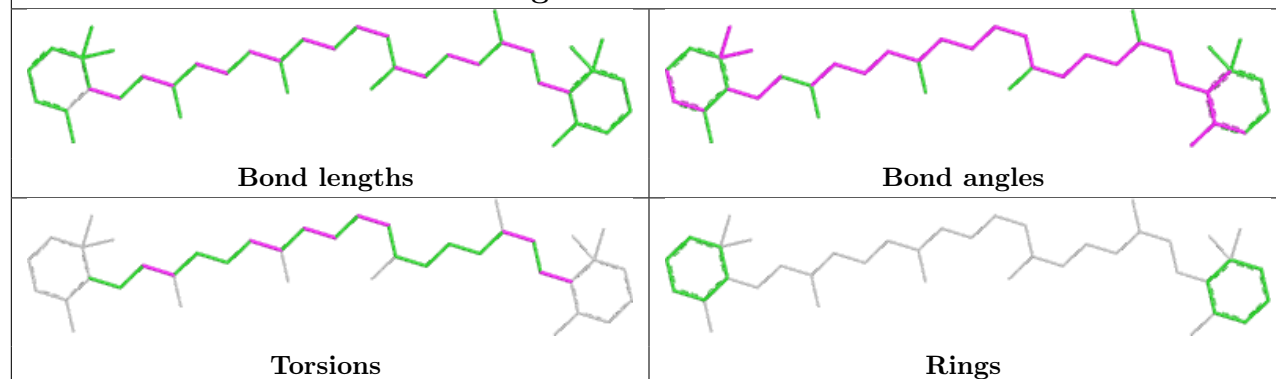
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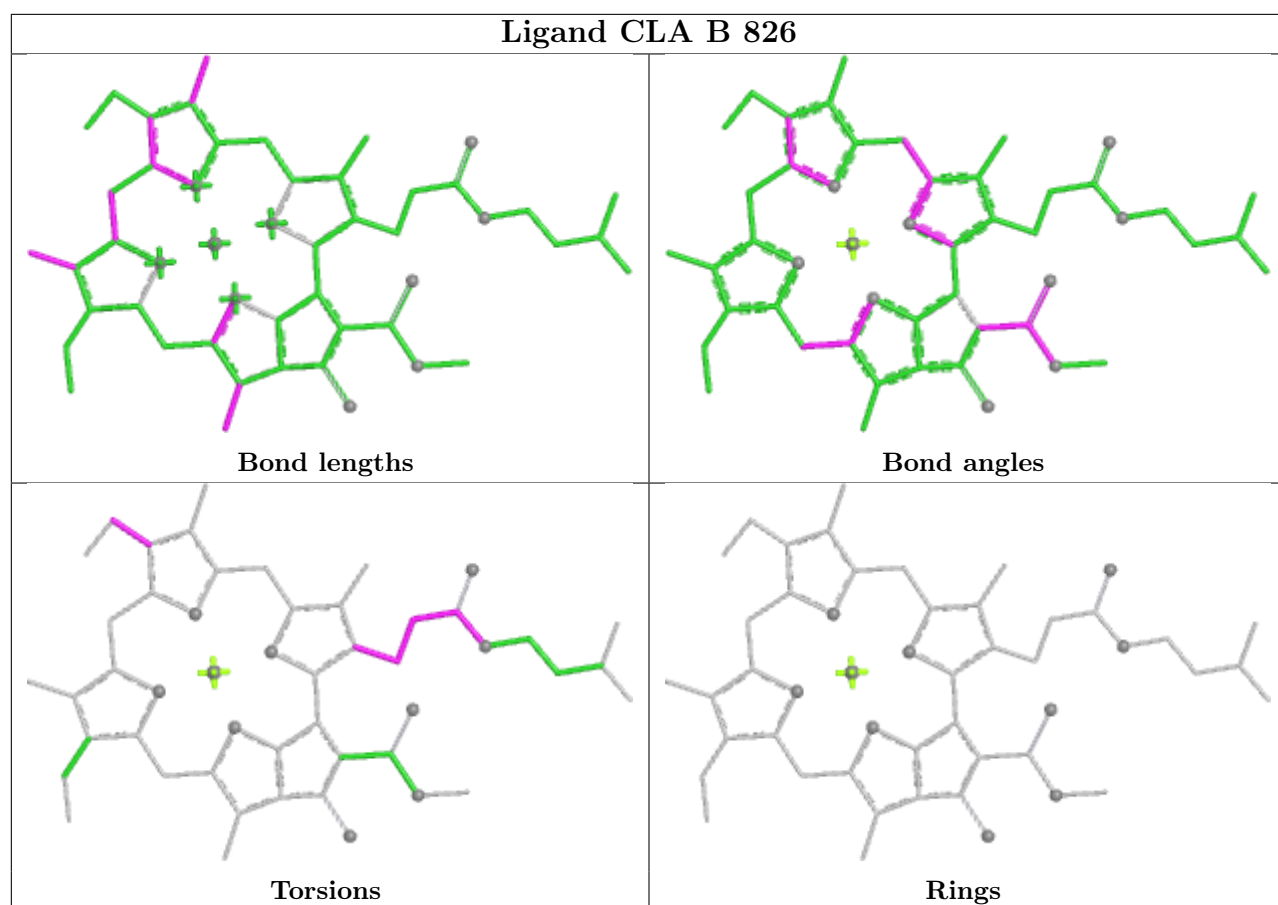


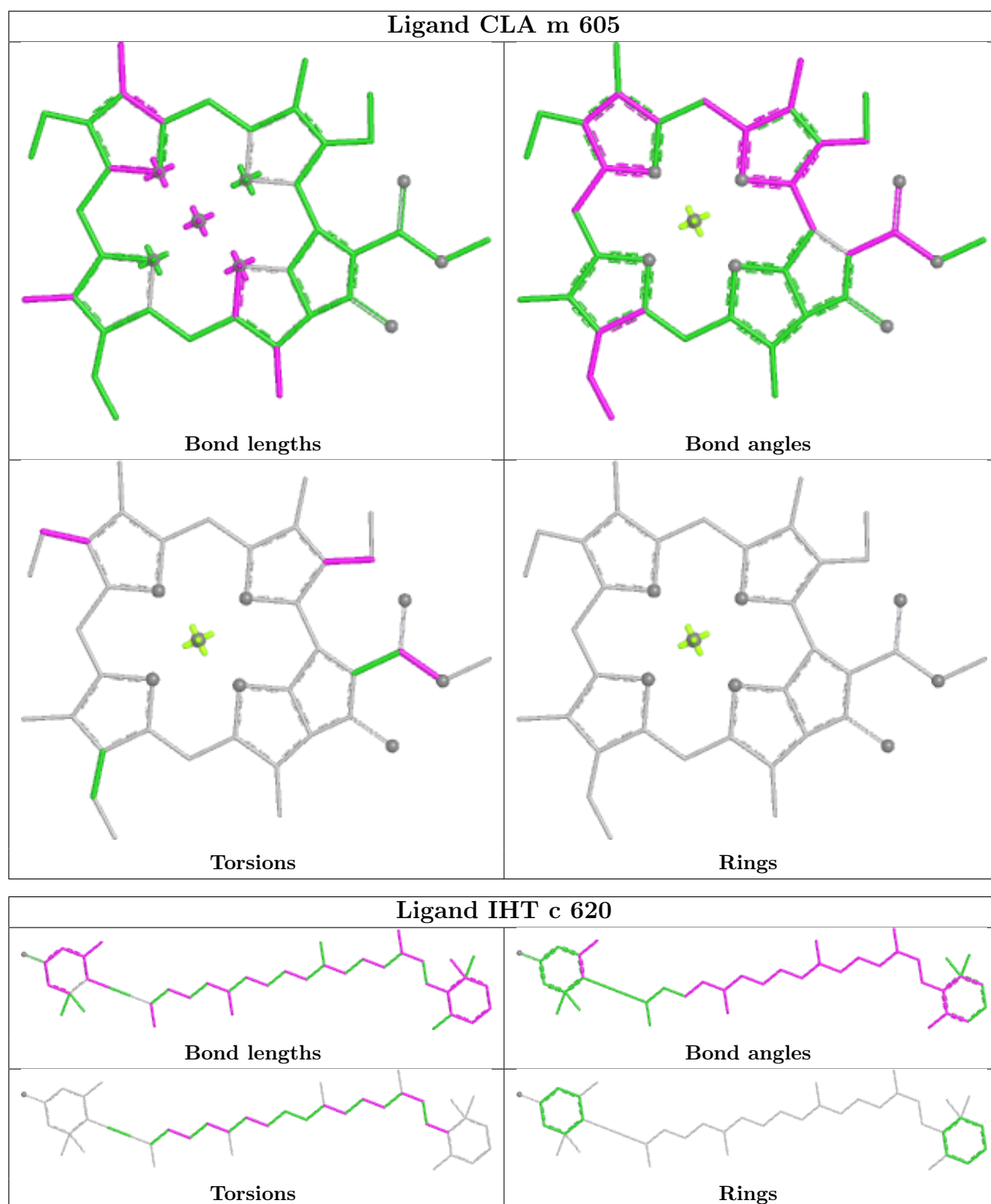
Ligand CLA c 611

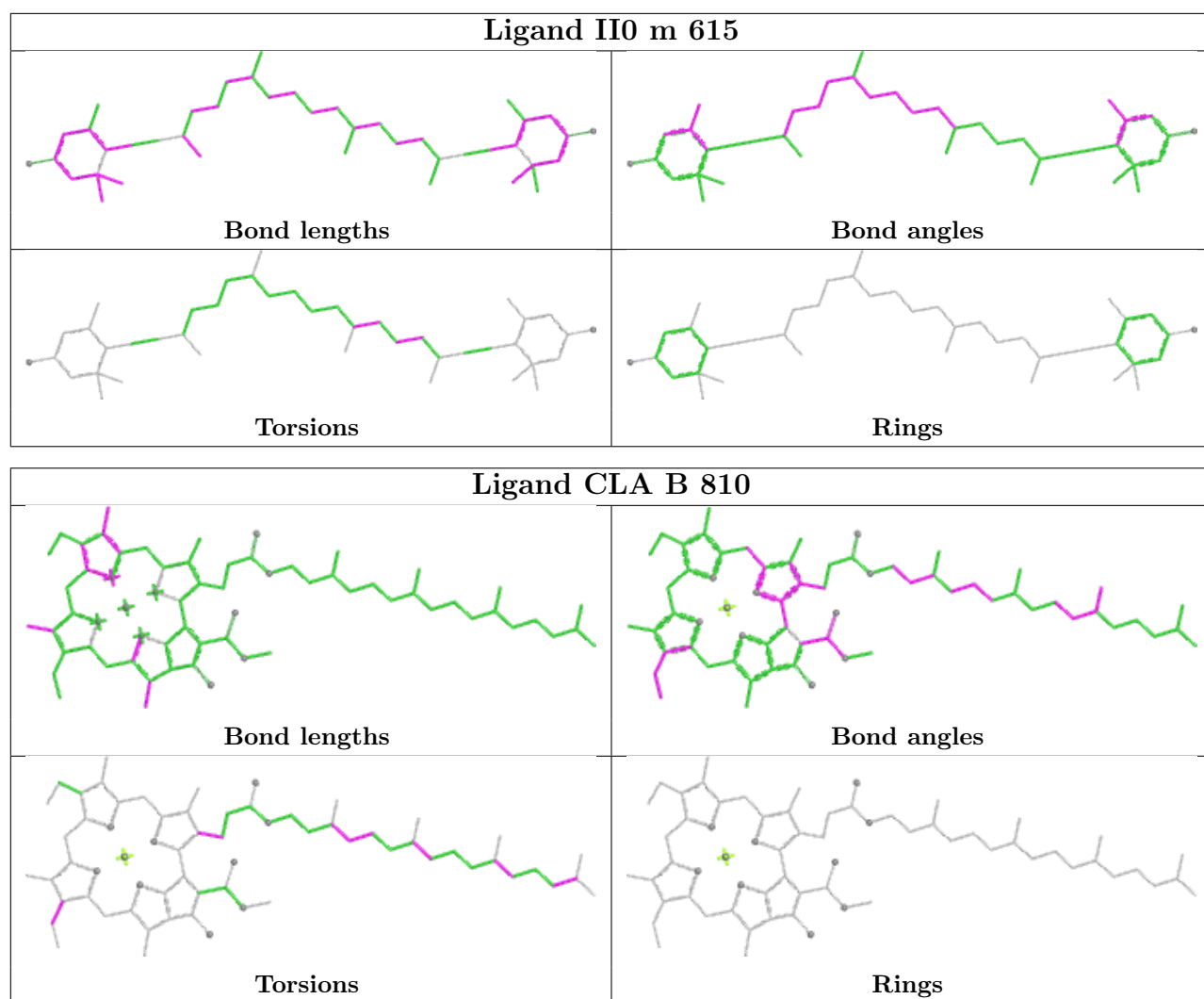


Ligand WVN i 315

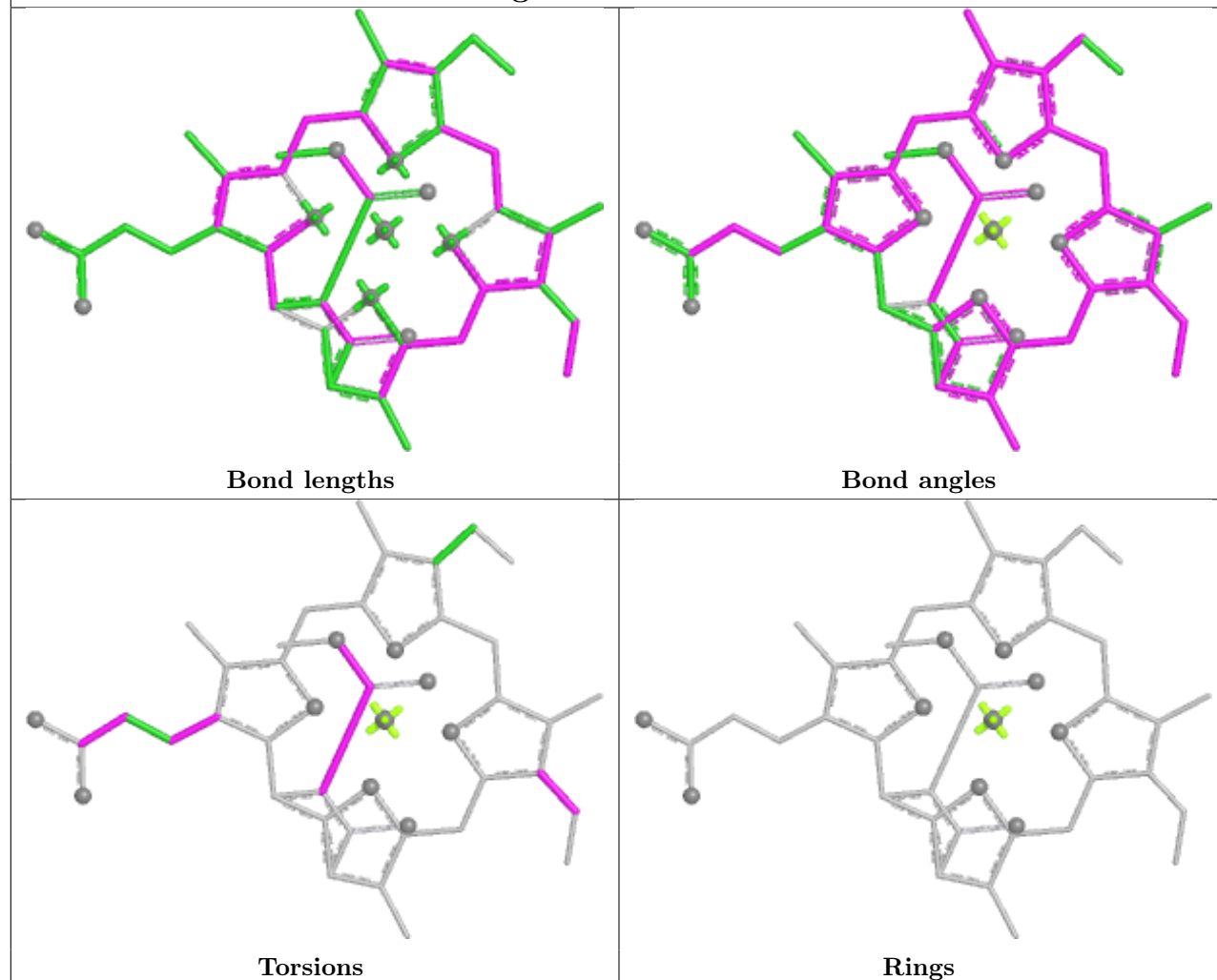




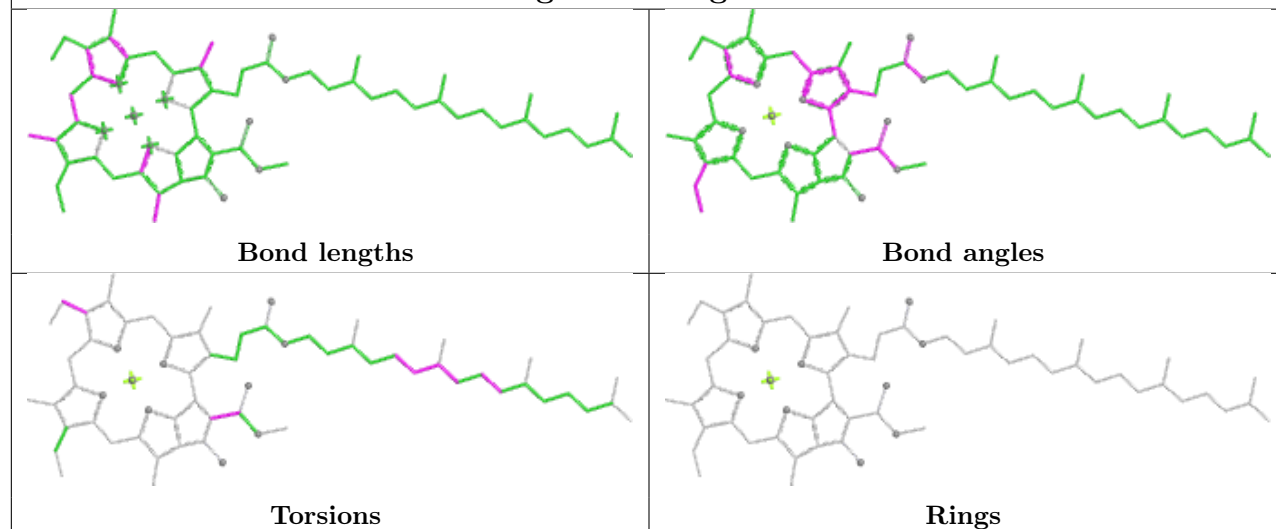




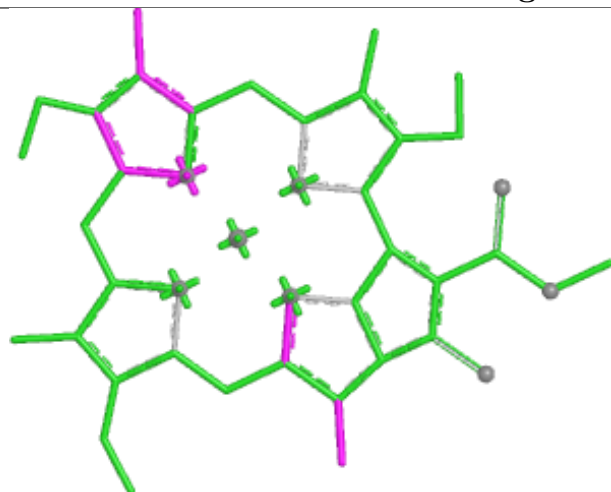
Ligand KC2 d 309



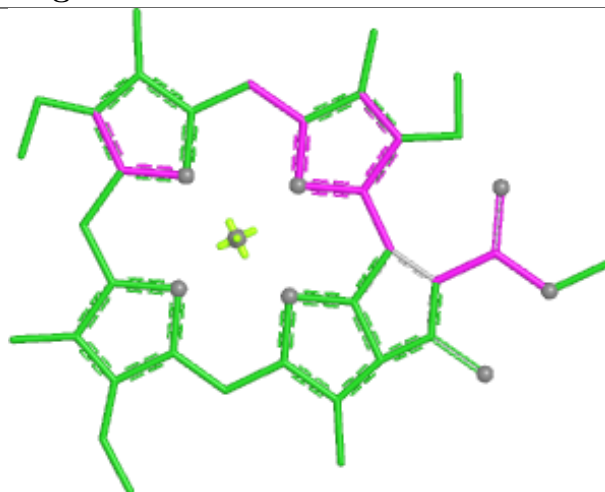
Ligand CLA g 309



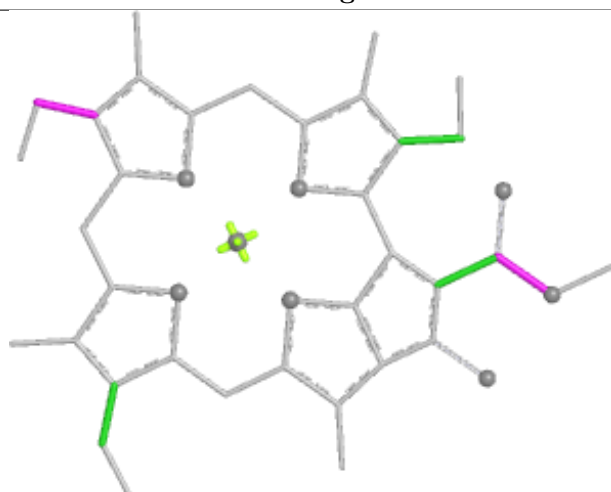
Ligand CLA g 302



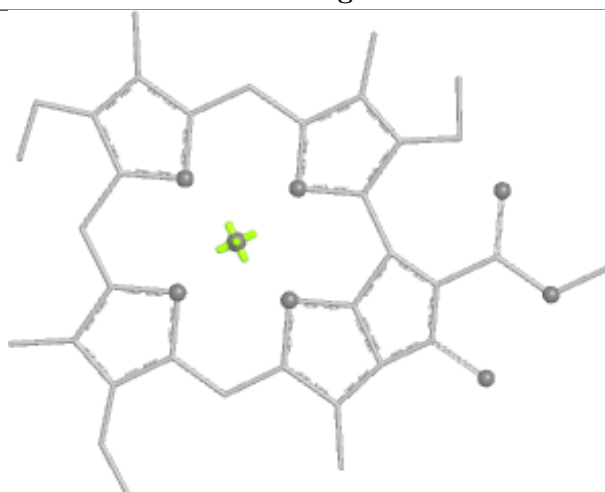
Bond lengths



Bond angles

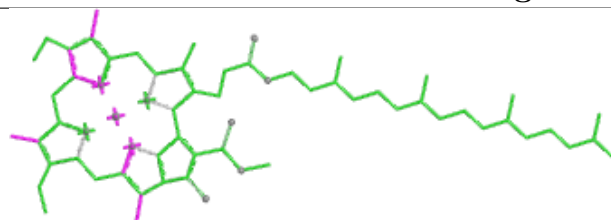


Torsions

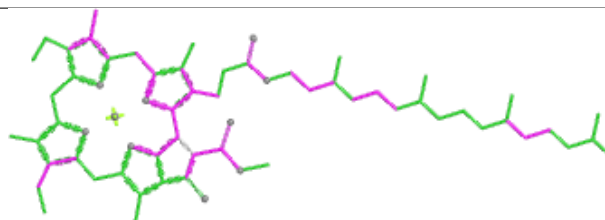


Rings

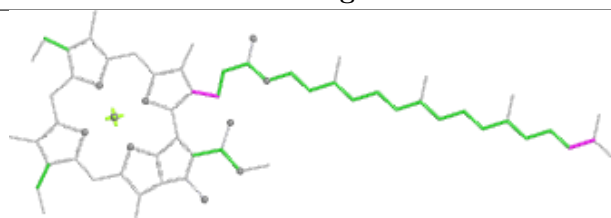
Ligand CLA B 822



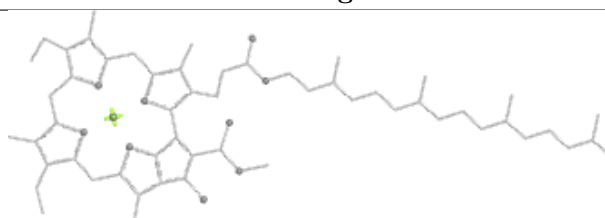
Bond lengths



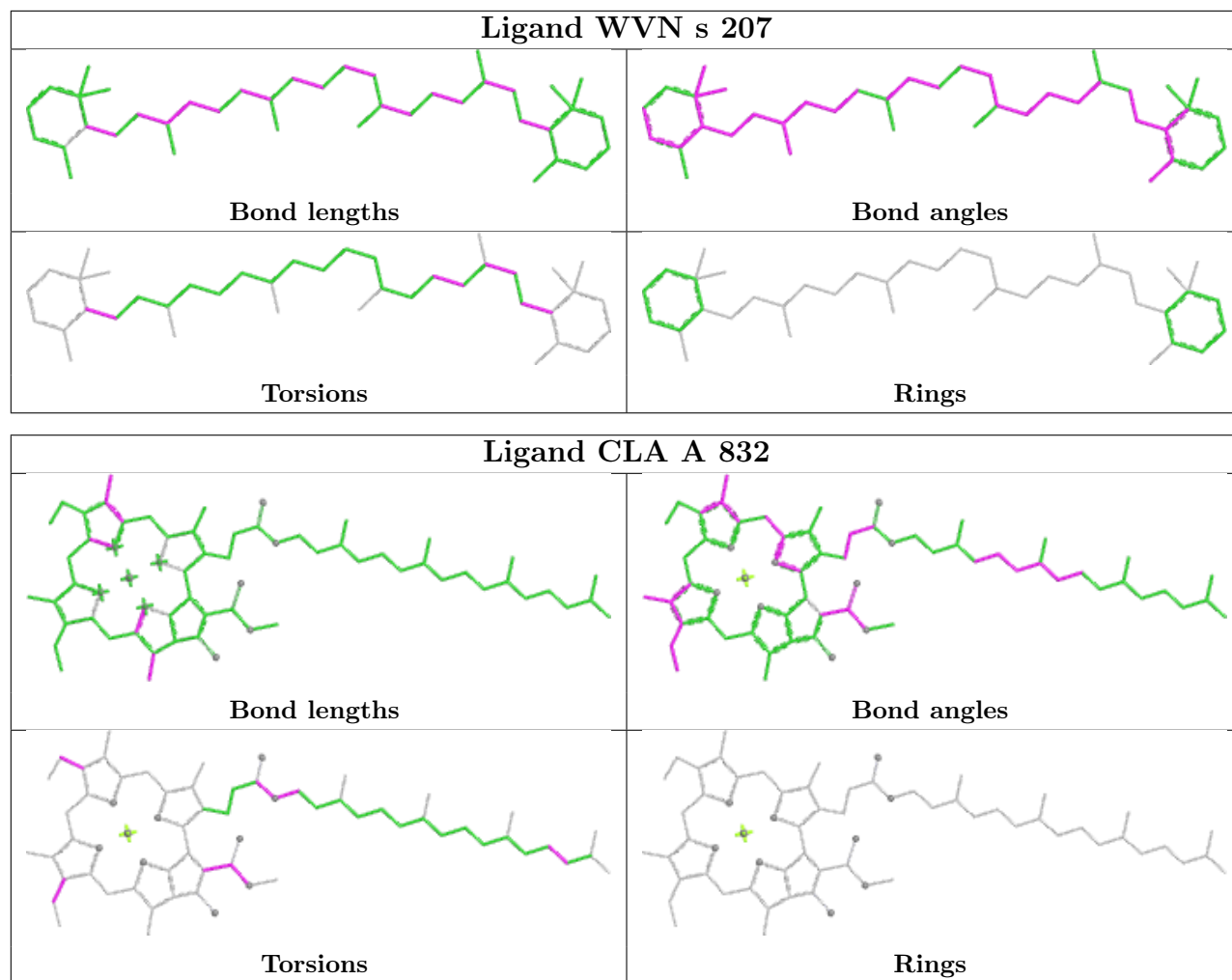
Bond angles



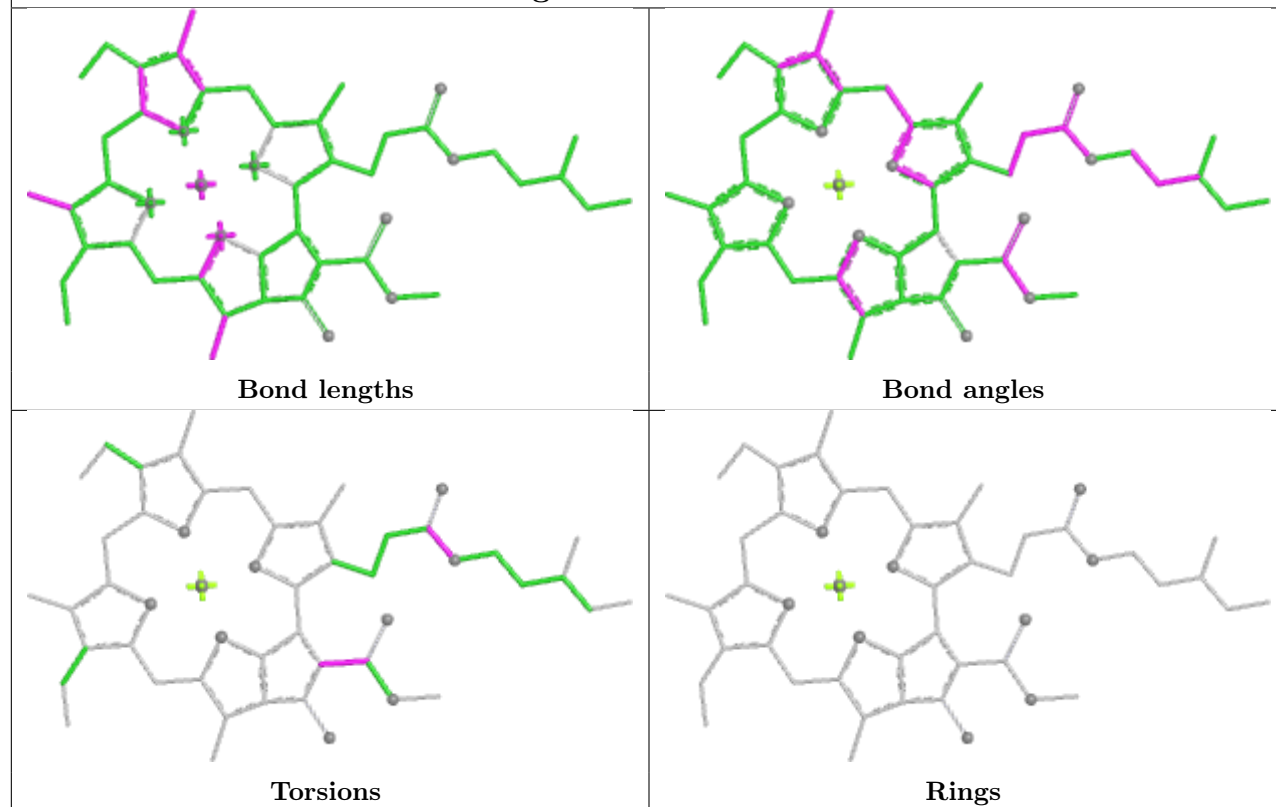
Torsions



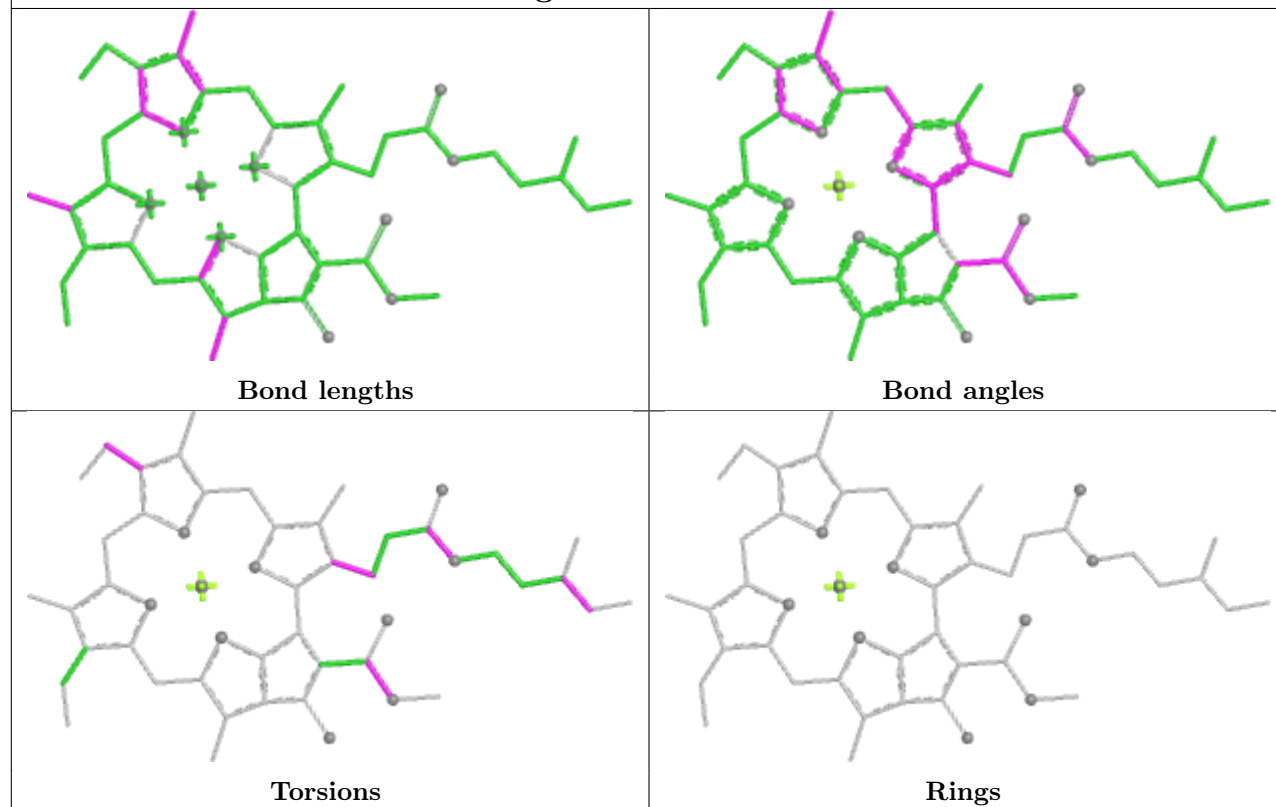
Rings



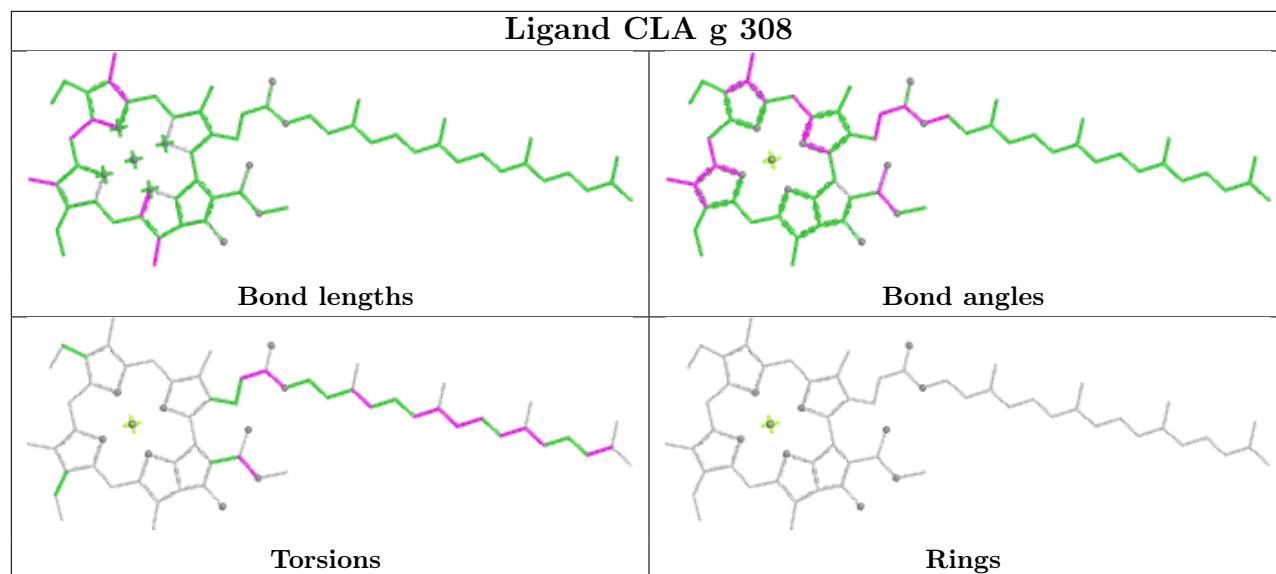
Ligand CLA B 825



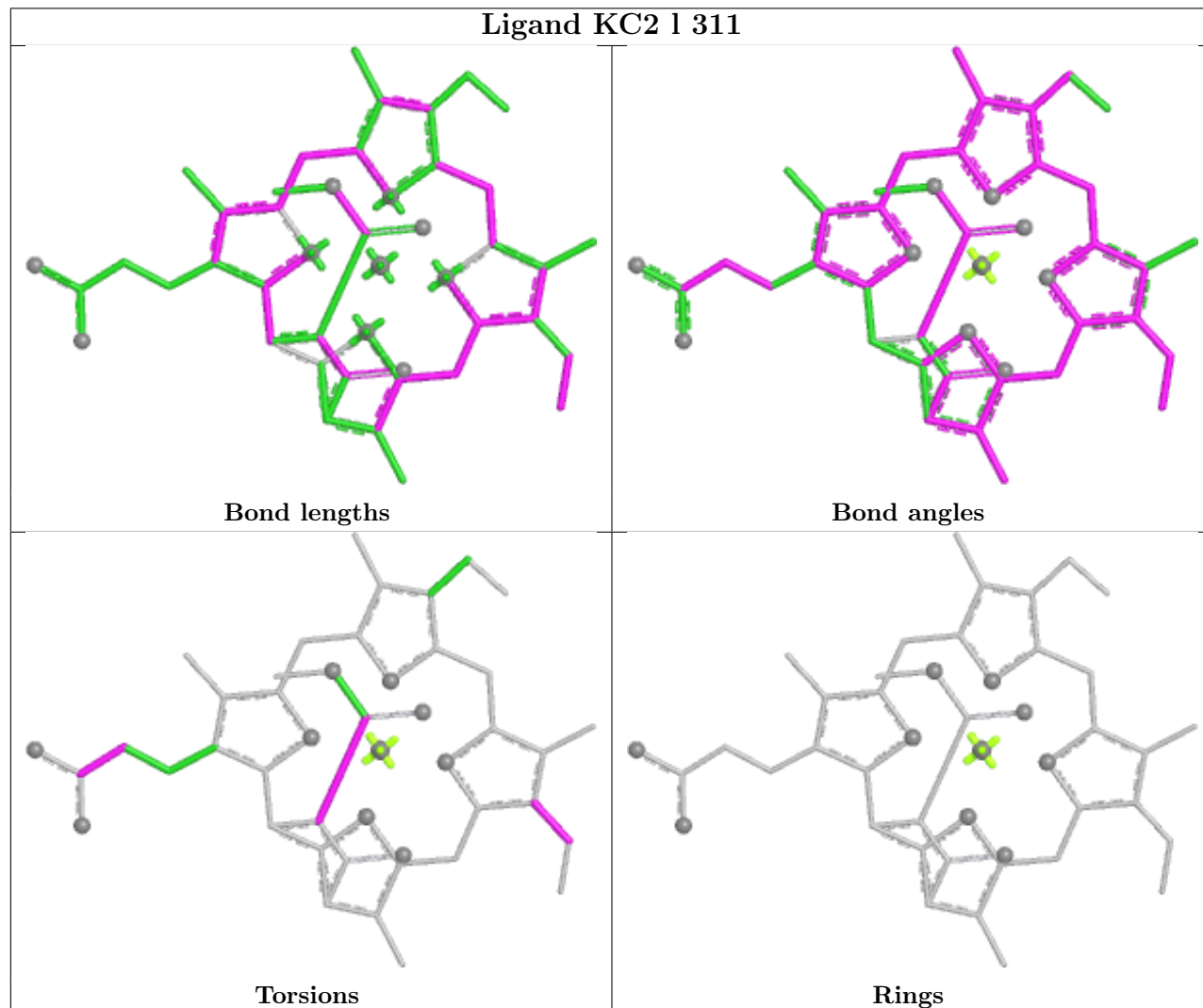
Ligand CLA n 603

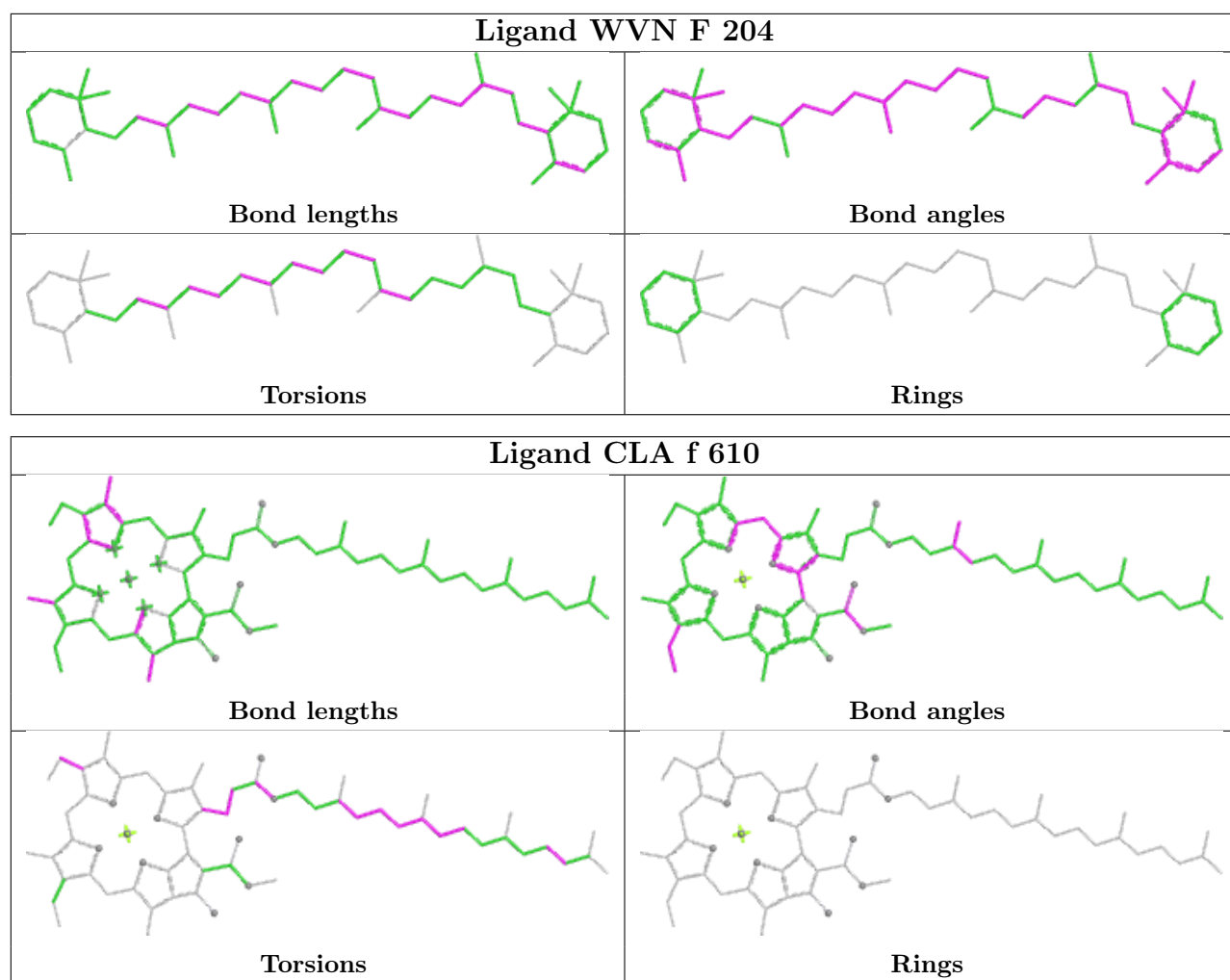


Ligand CLA g 308

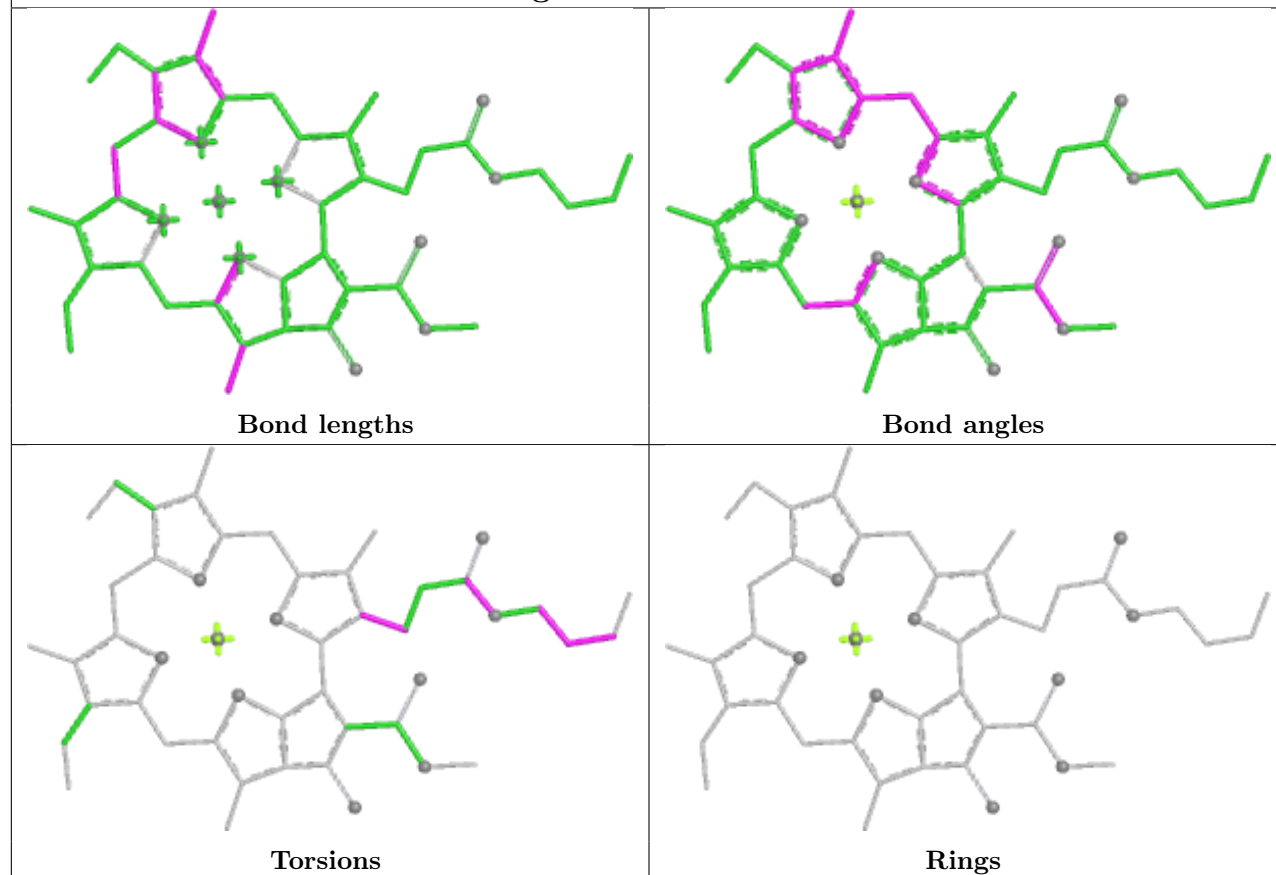


Ligand KC2 l 311

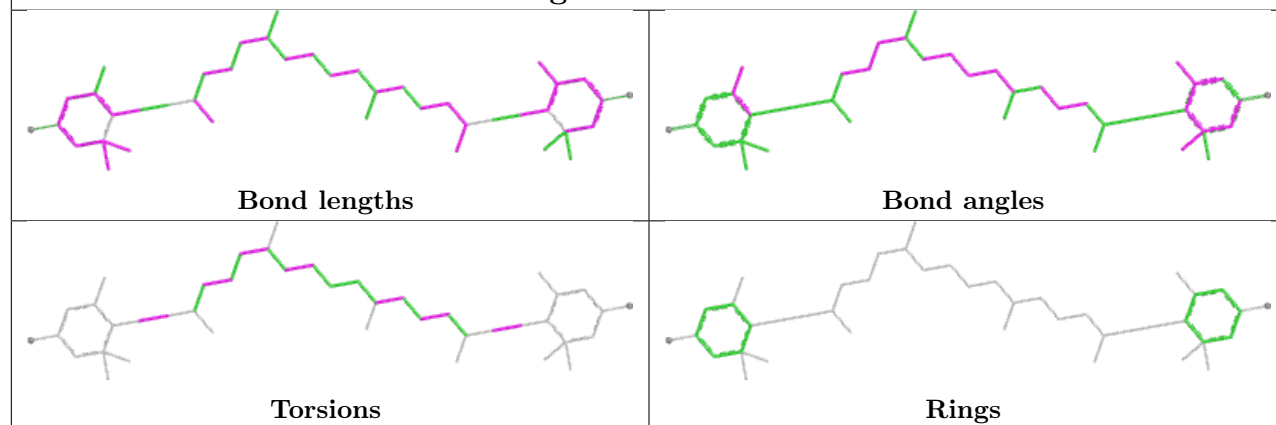


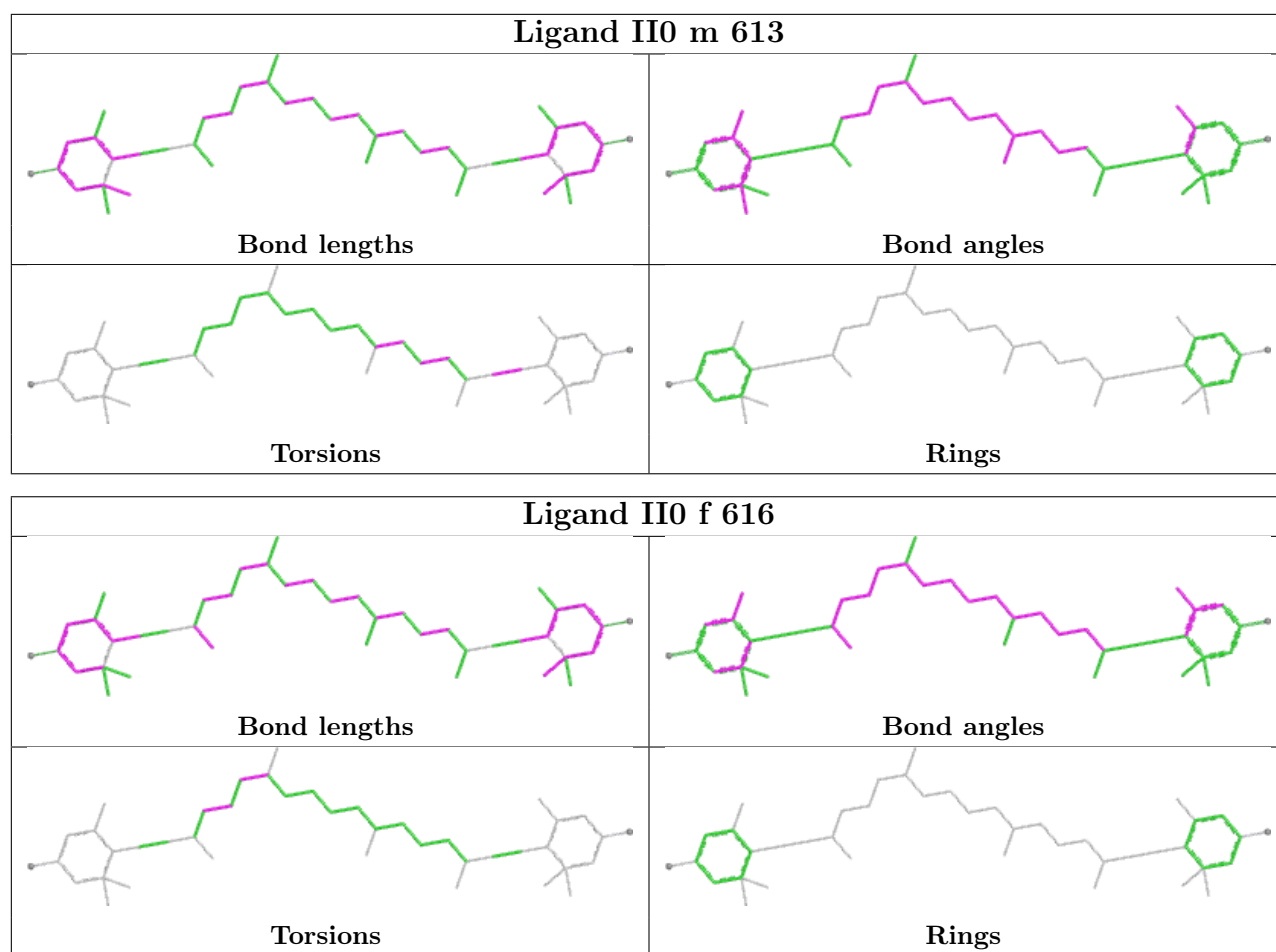


Ligand CLA B 827

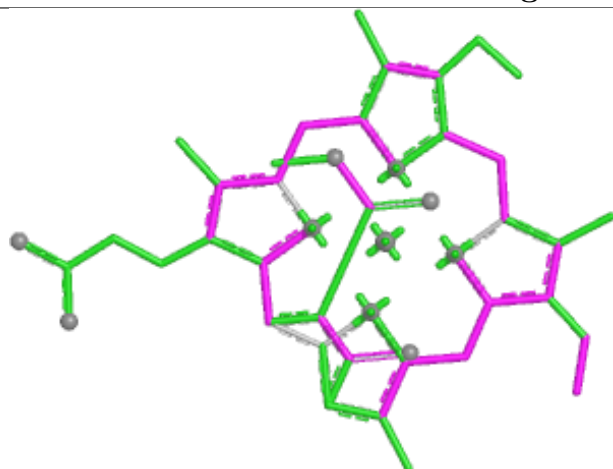


Ligand II0 b 613

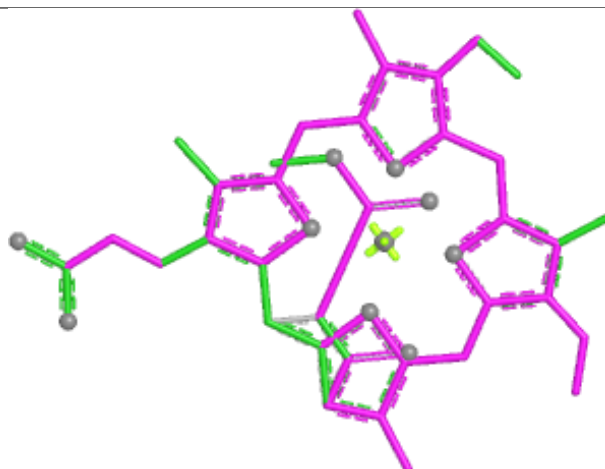




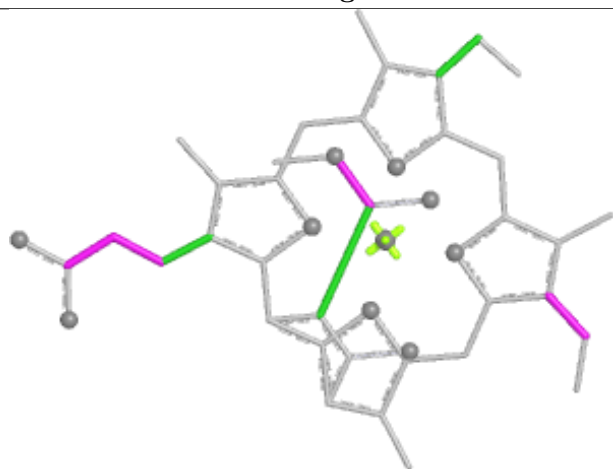
Ligand KC2 e 609



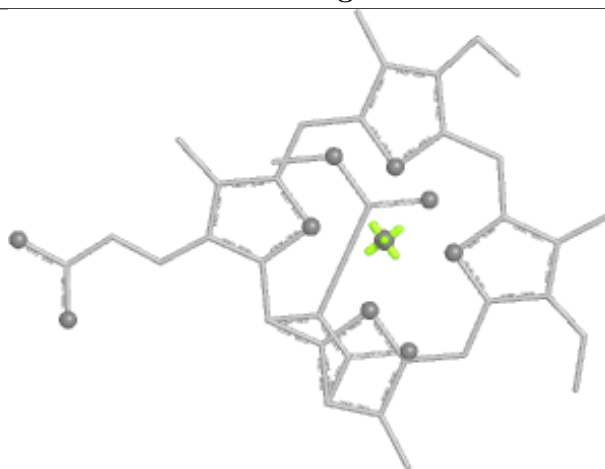
Bond lengths



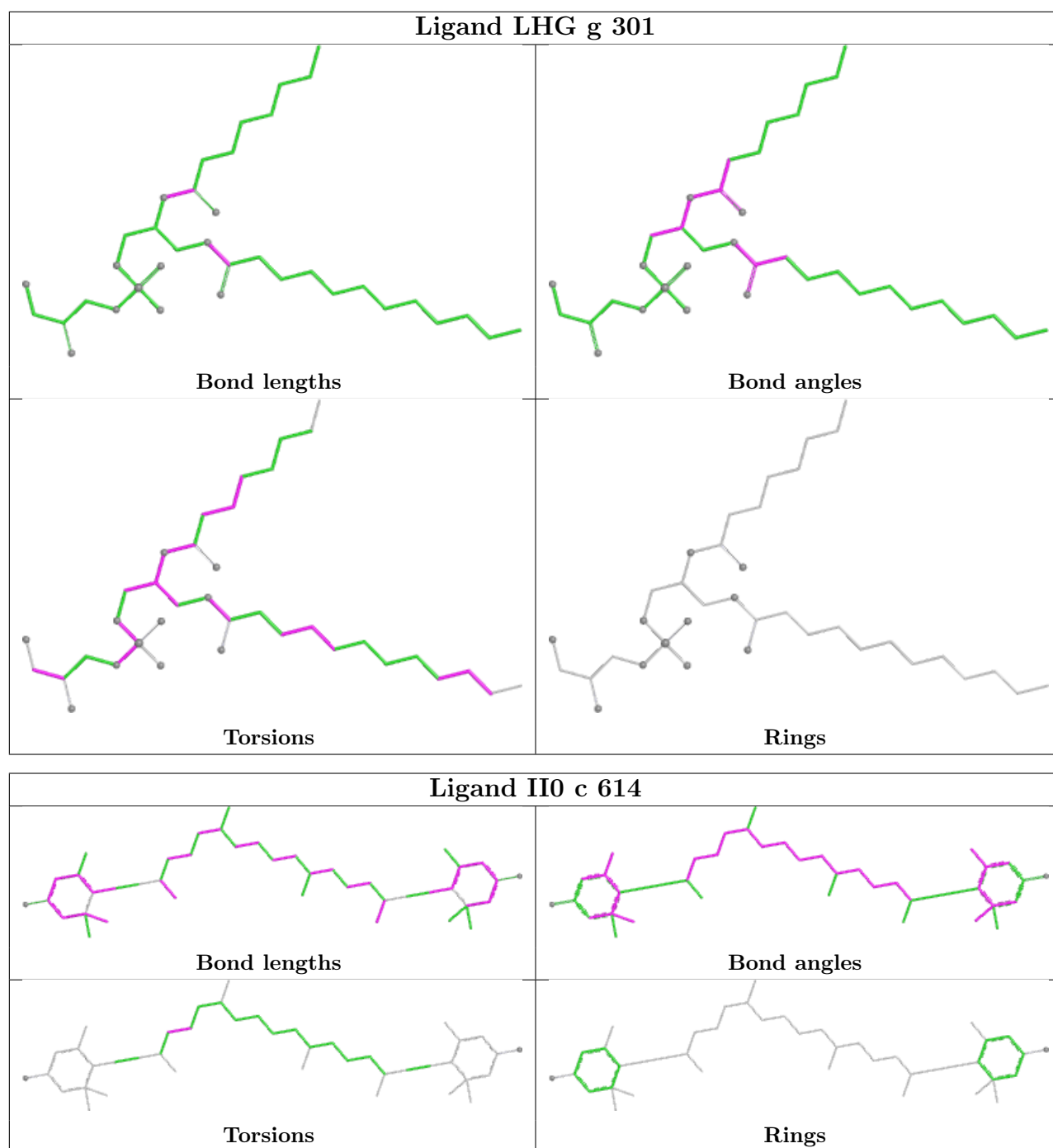
Bond angles

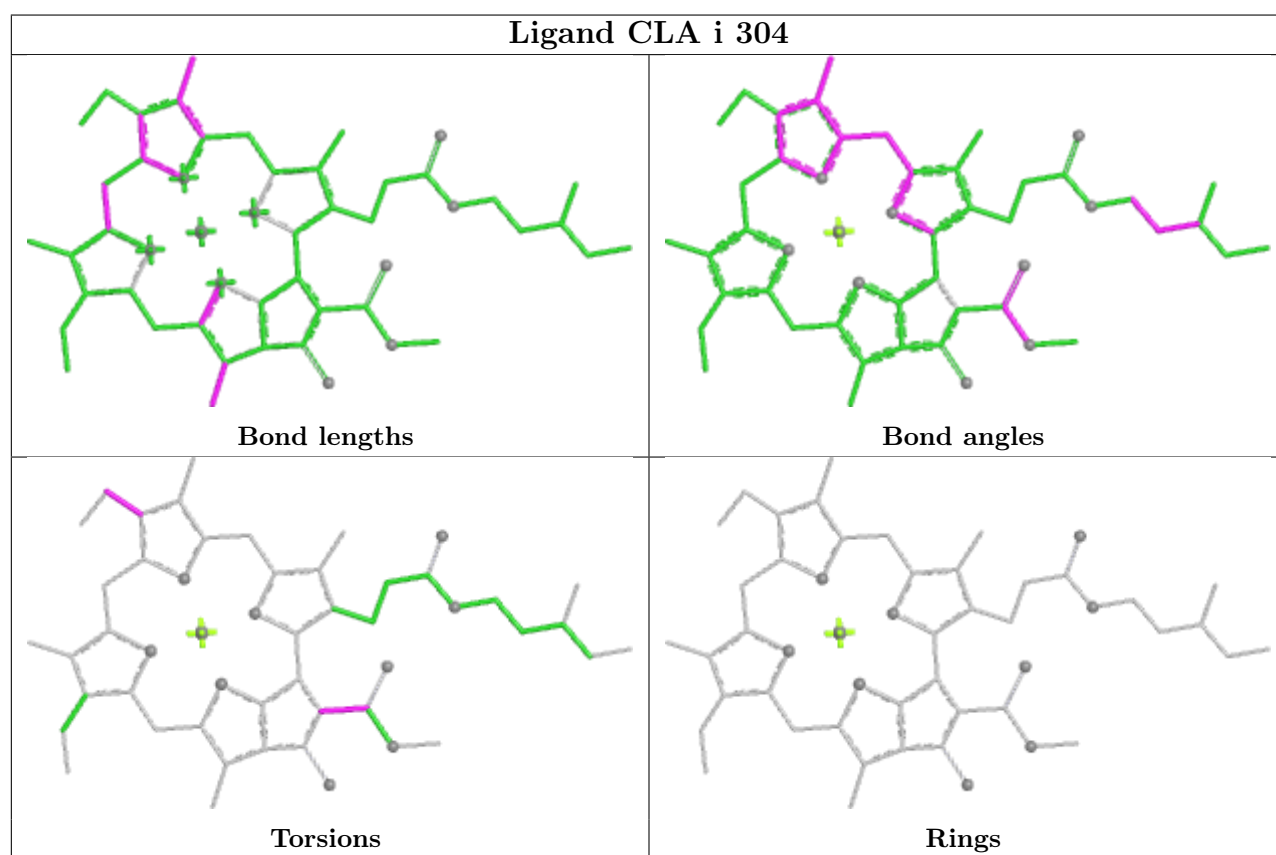
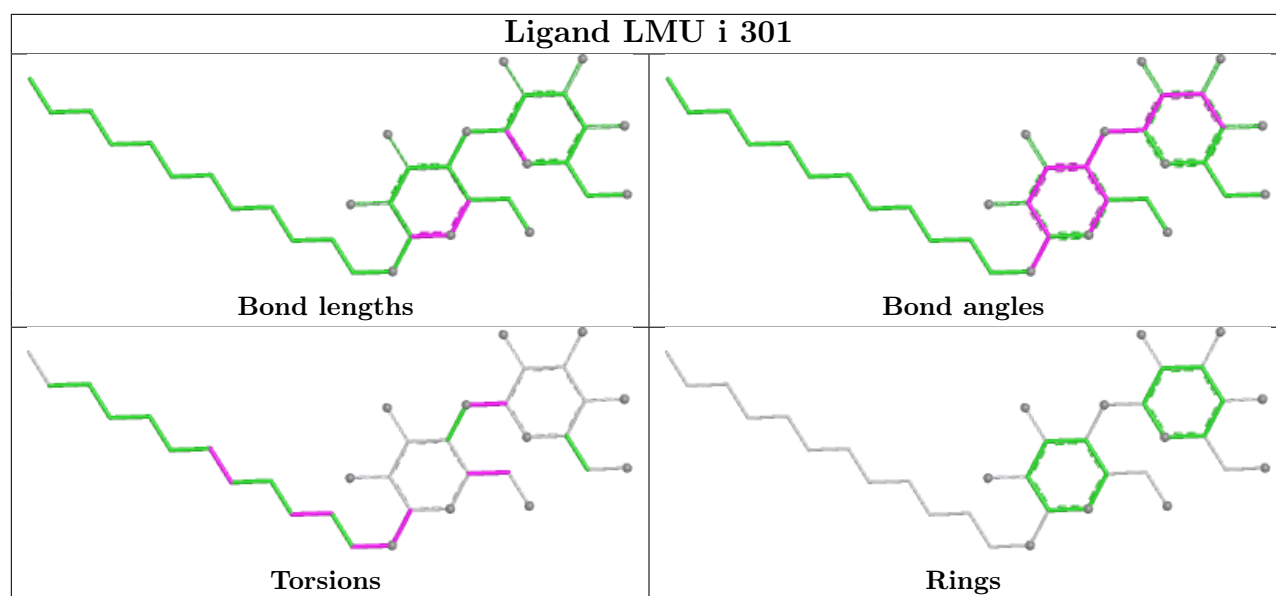


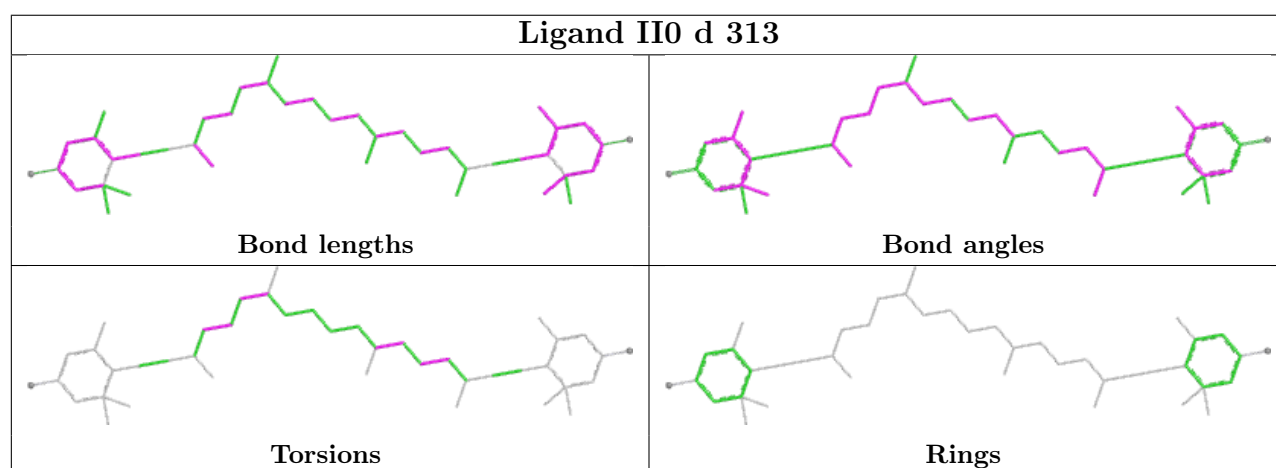
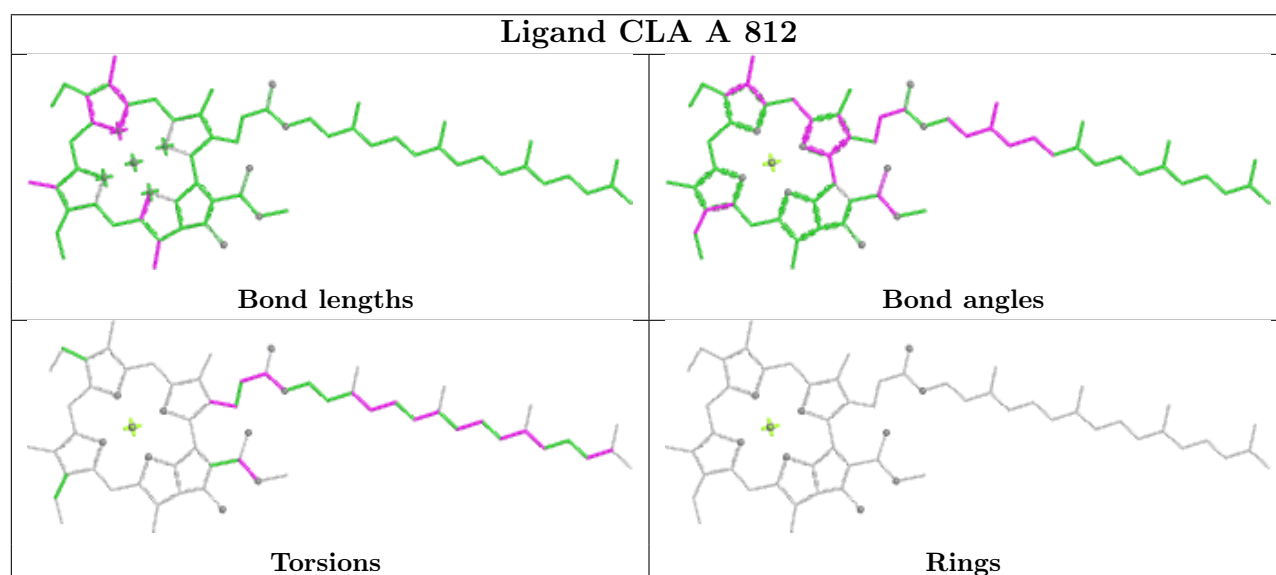
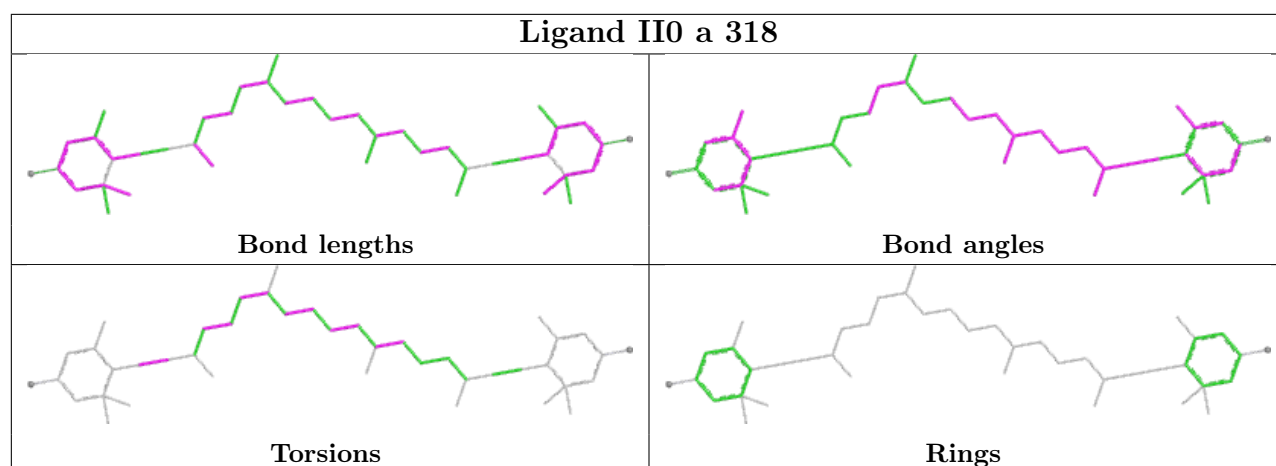
Torsions

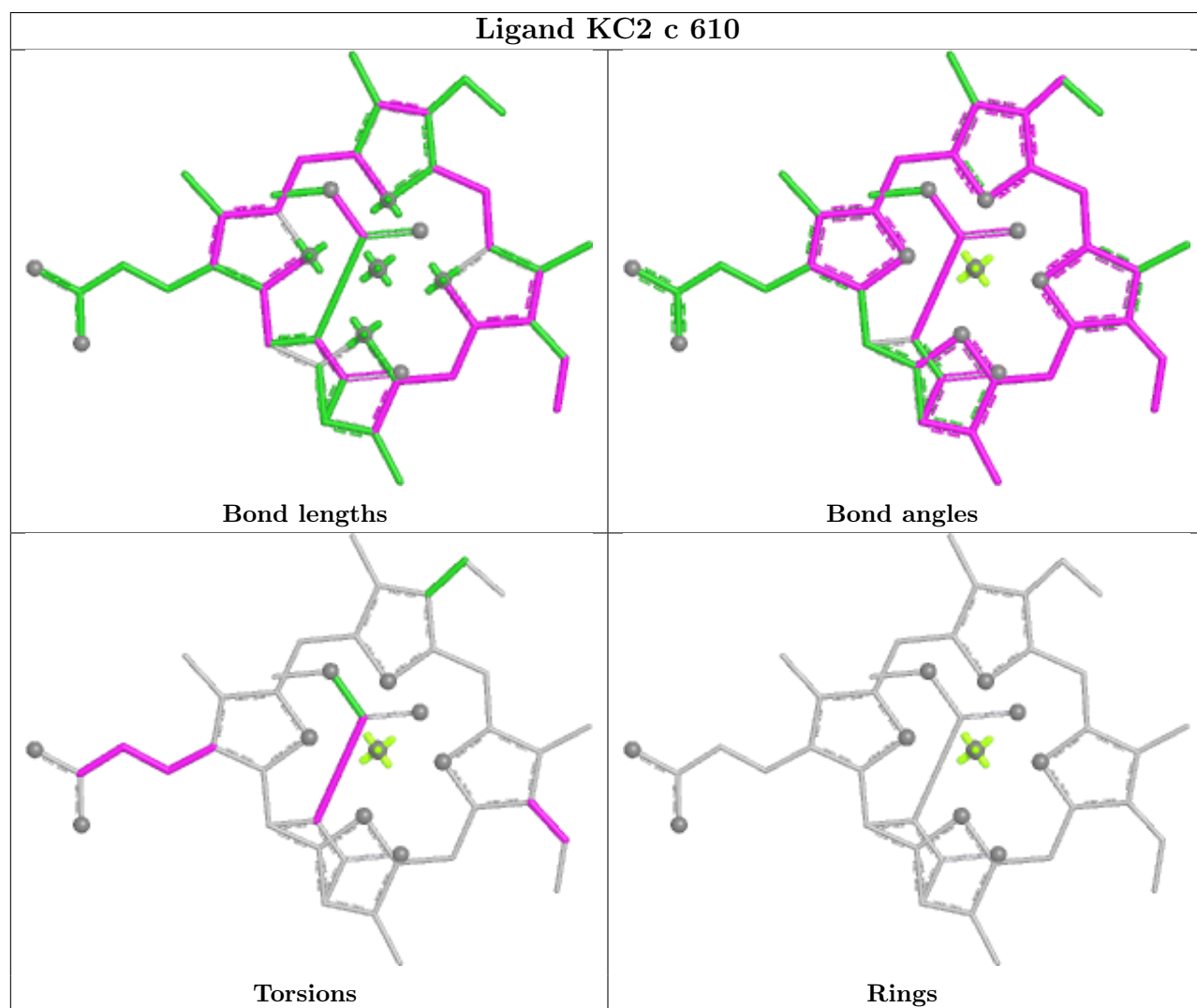
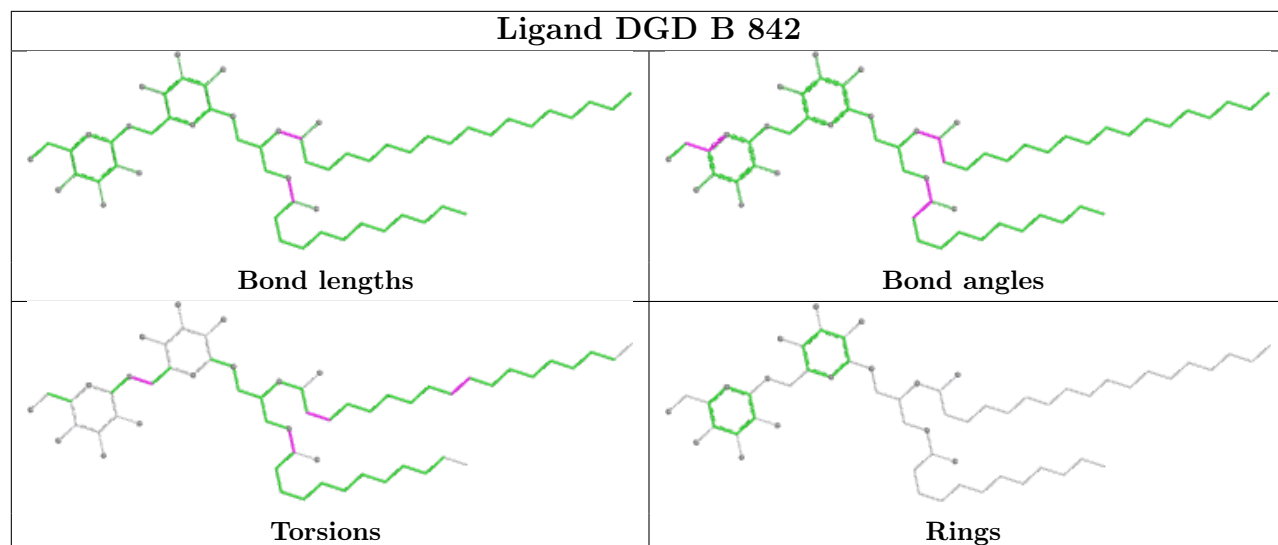


Rings

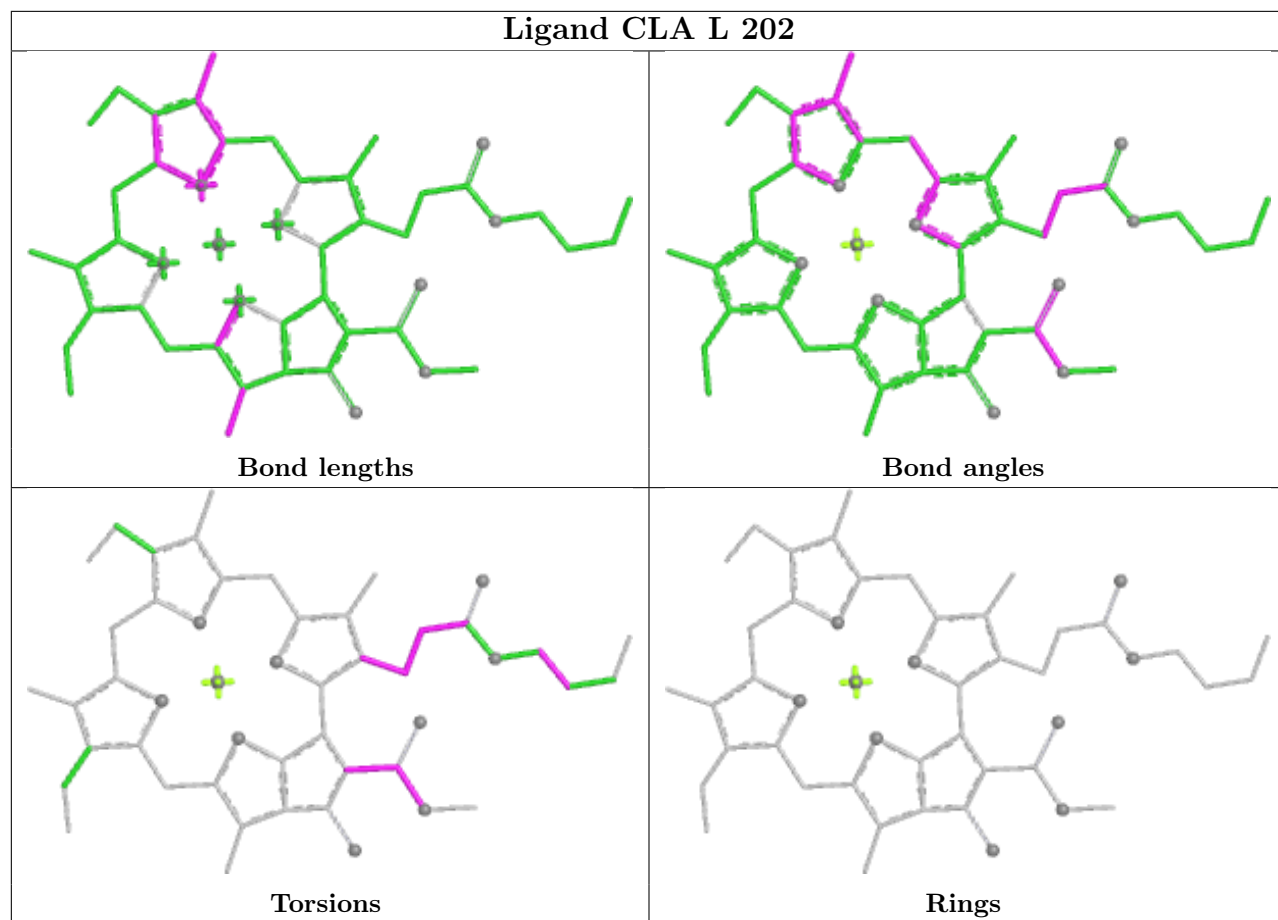


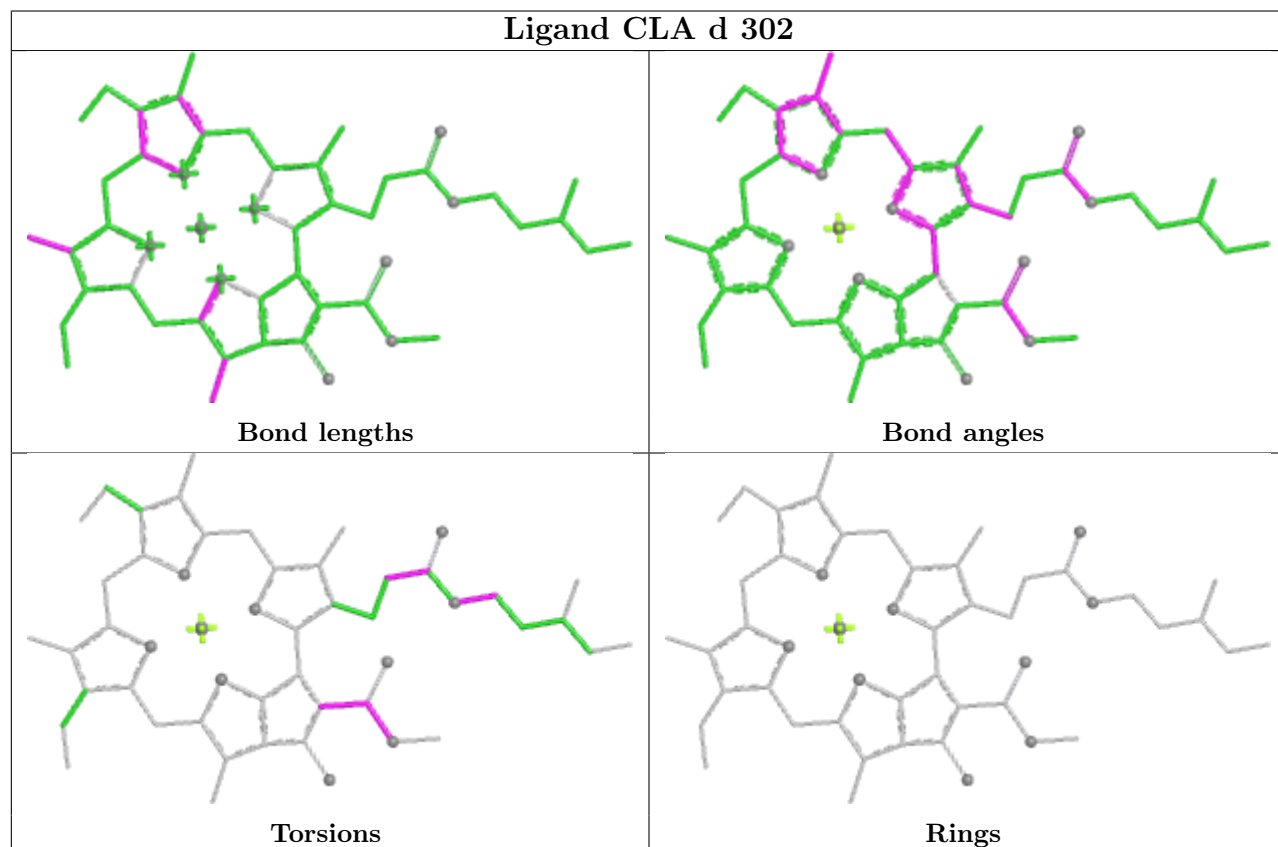
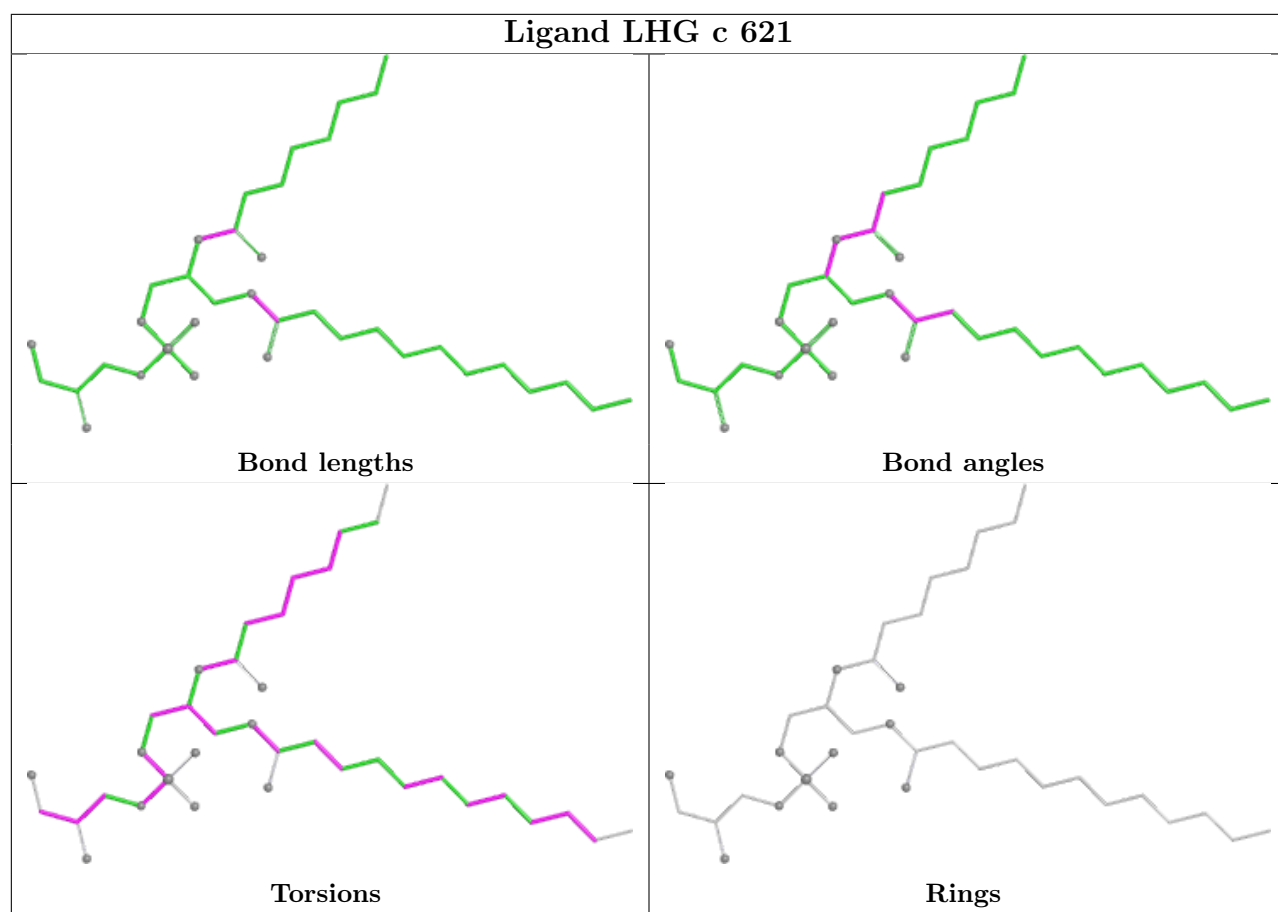




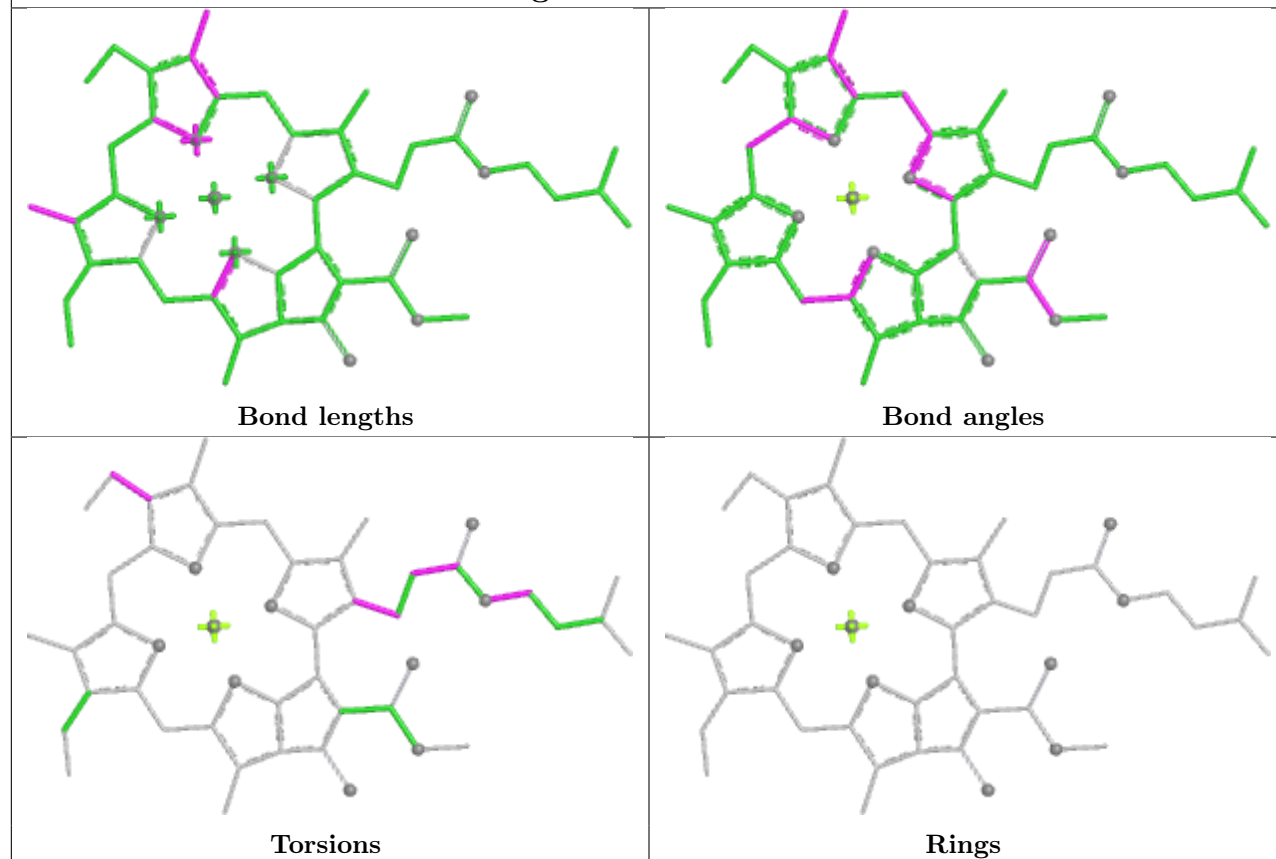


Ligand CLA L 202

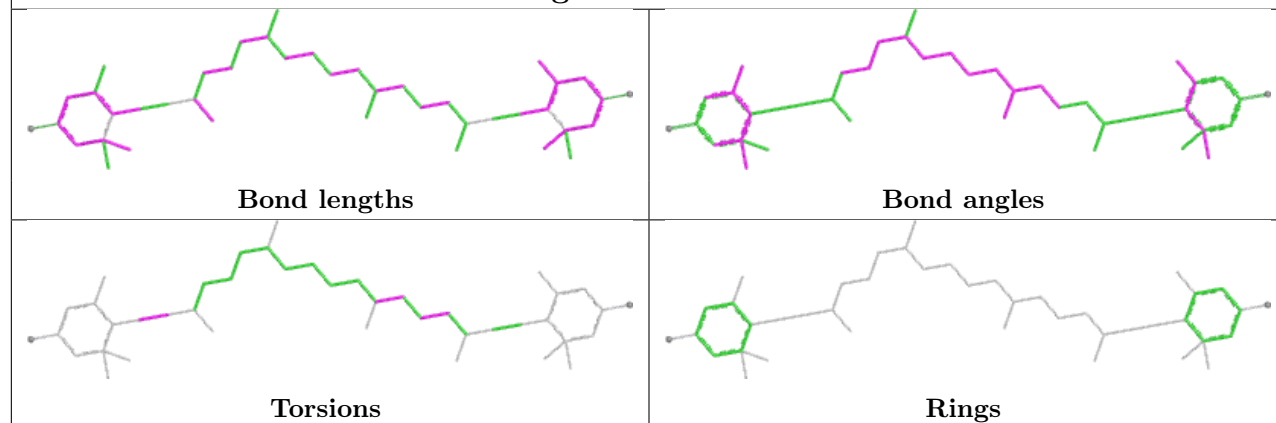


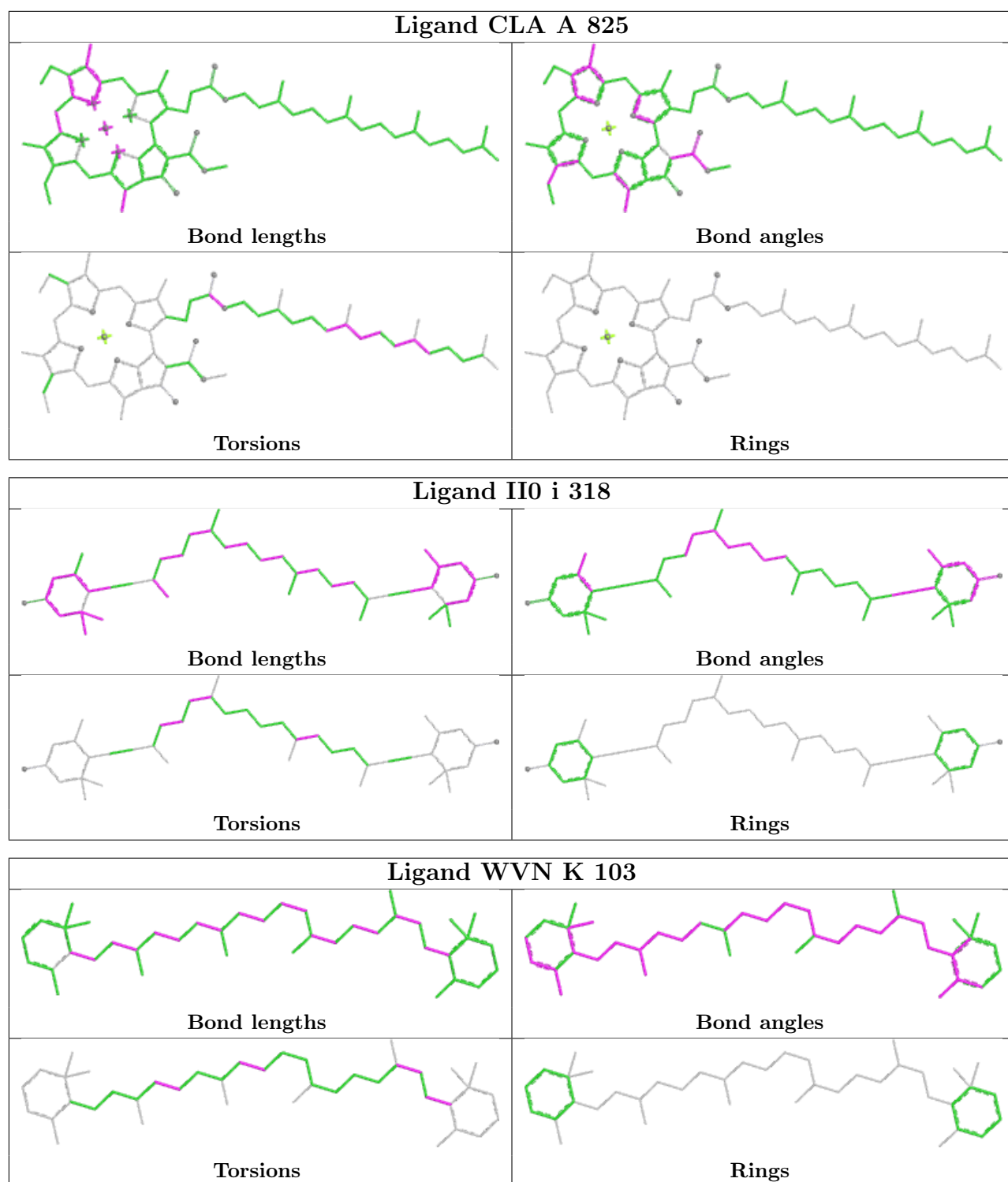


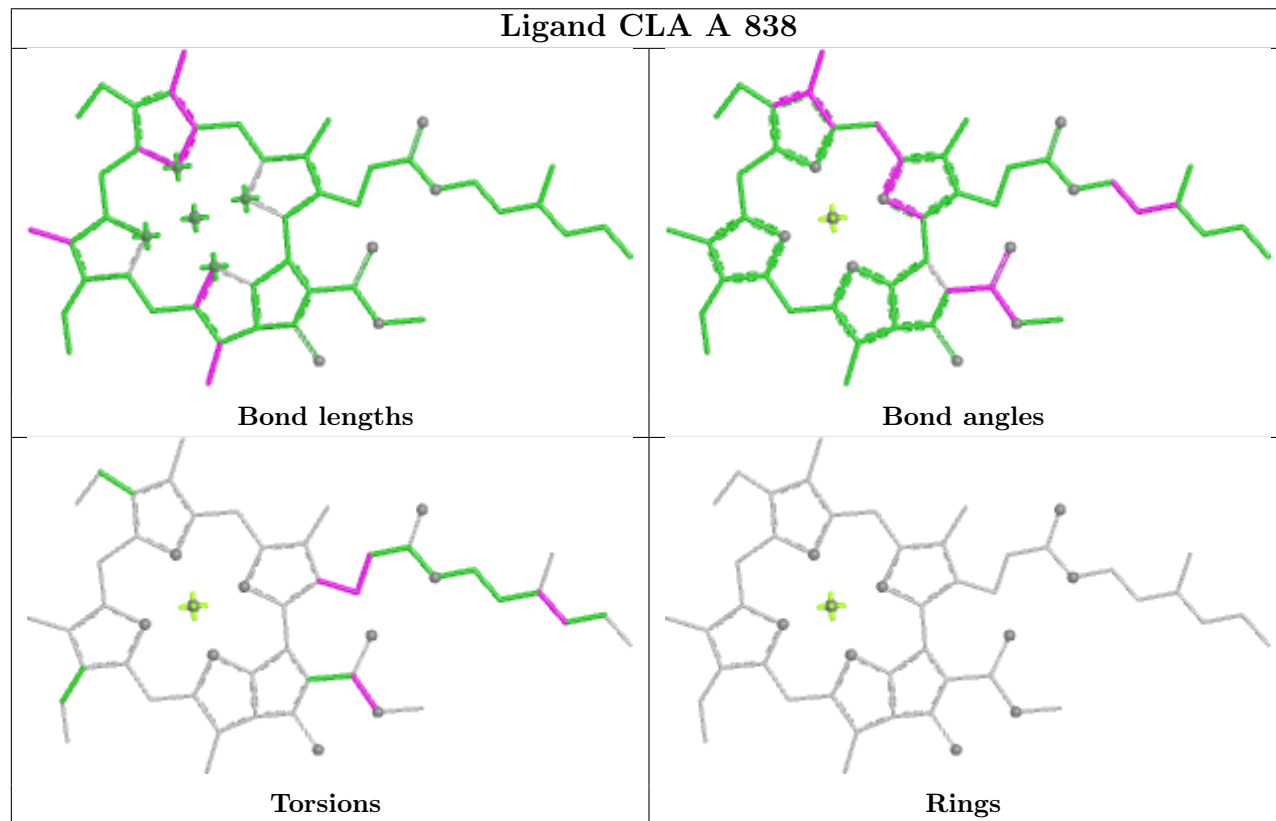
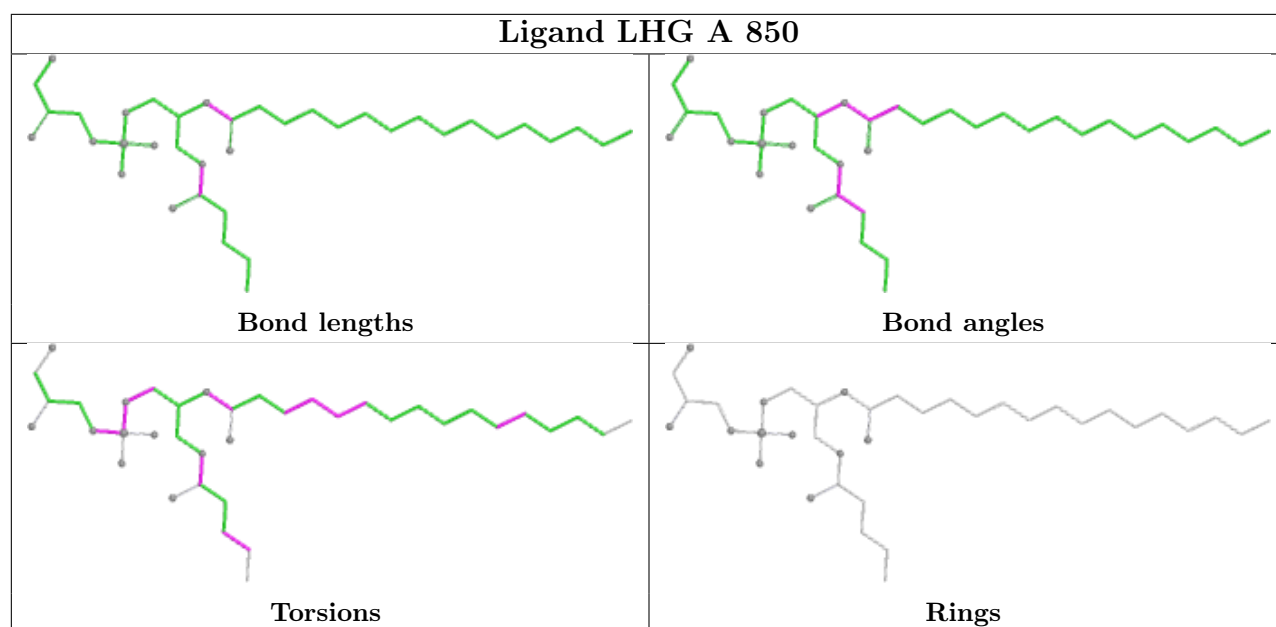
Ligand CLA A 833

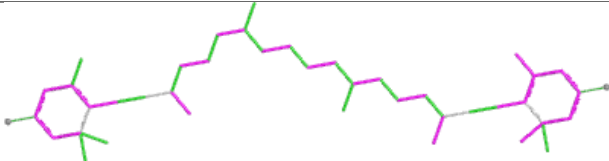
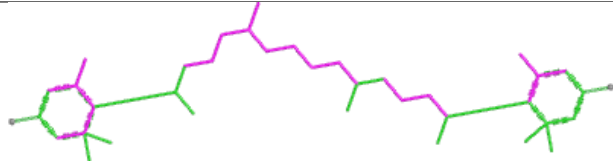
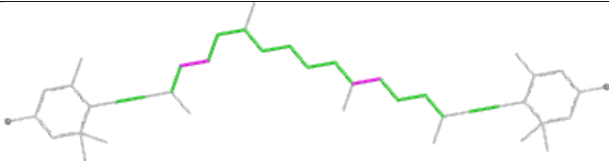
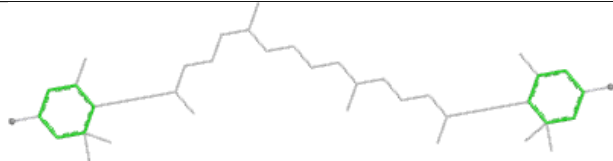


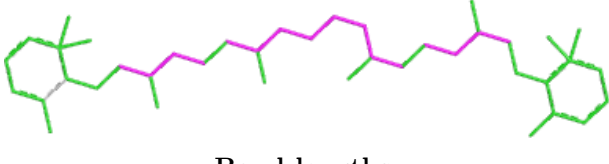
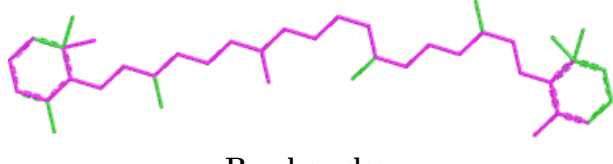
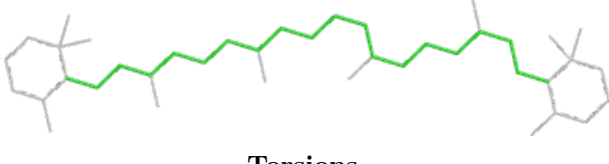
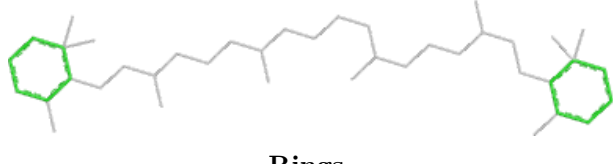
Ligand II0 c 613

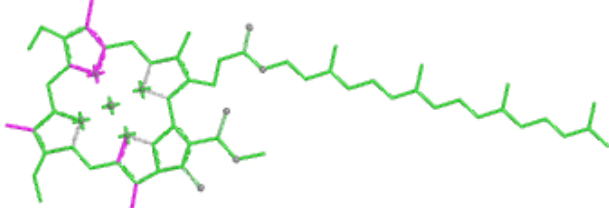
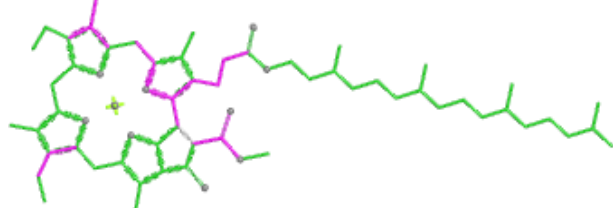
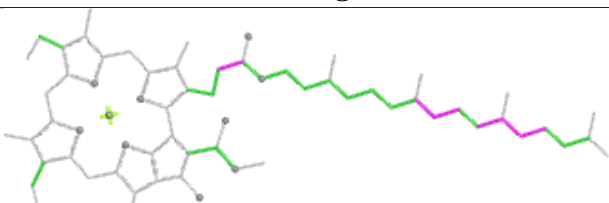
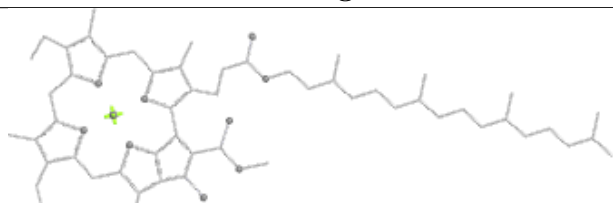




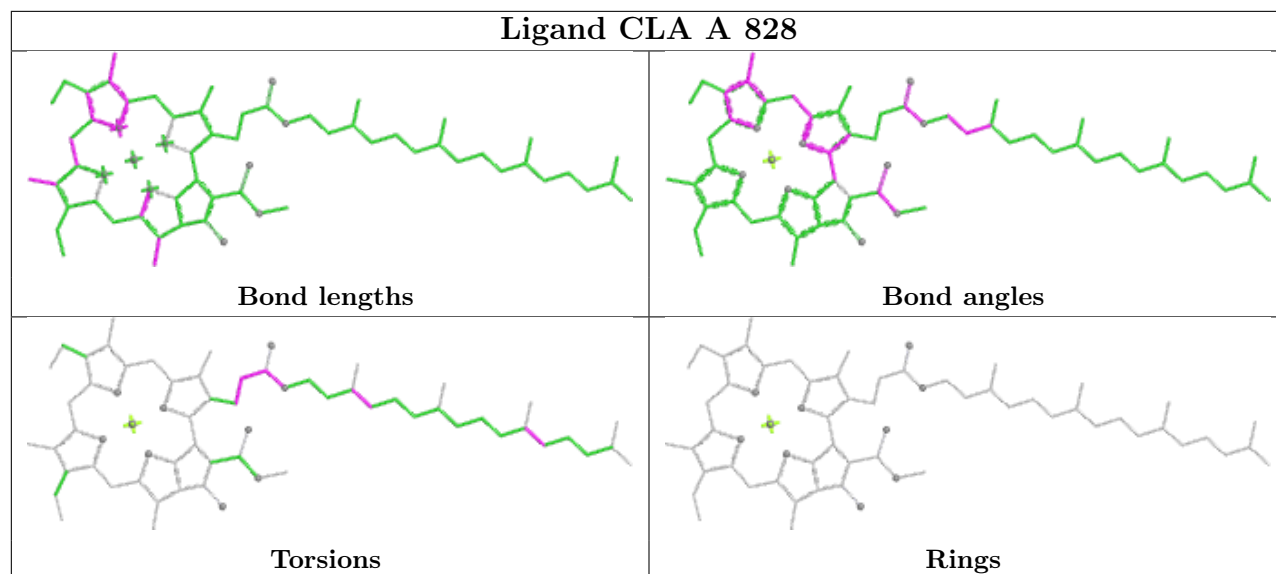


Ligand II0 i 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

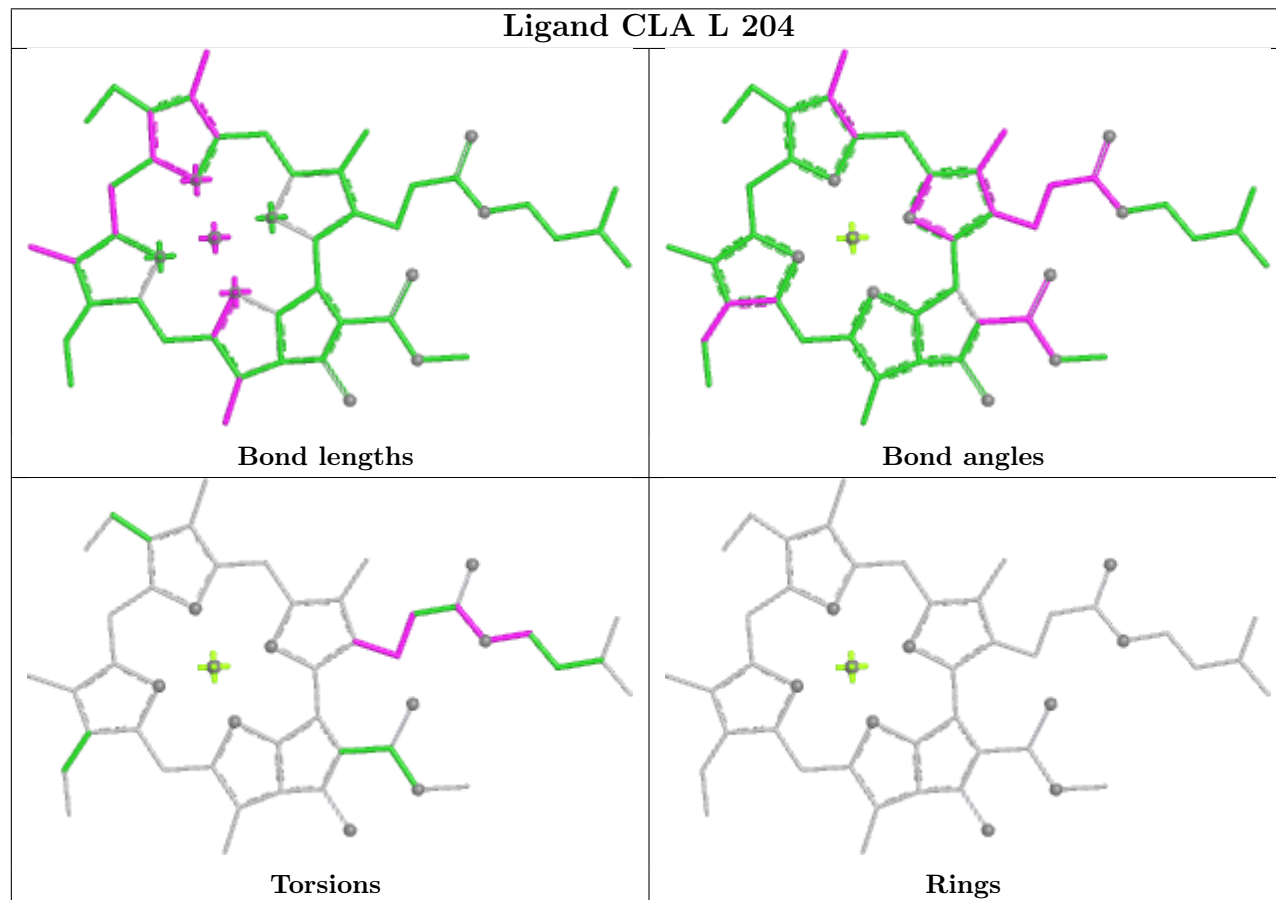
Ligand WVN B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

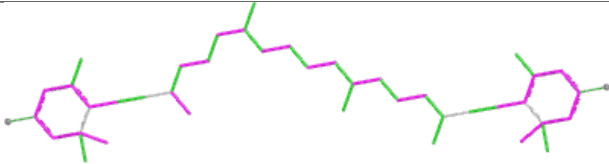
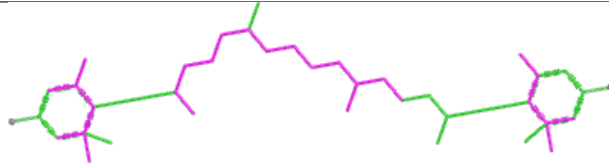
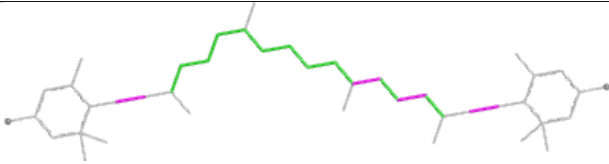
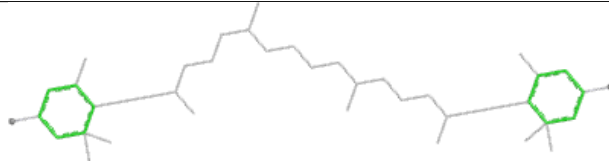
Ligand CLA A 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

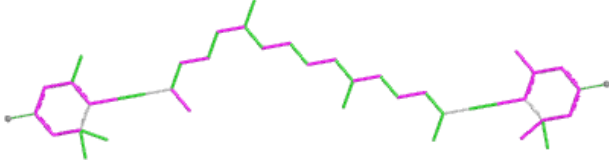
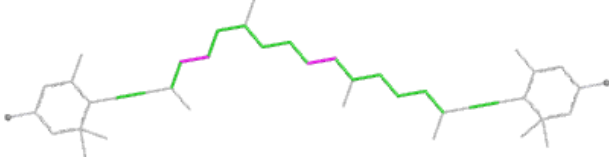
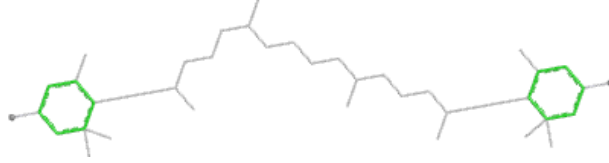
Ligand CLA A 828

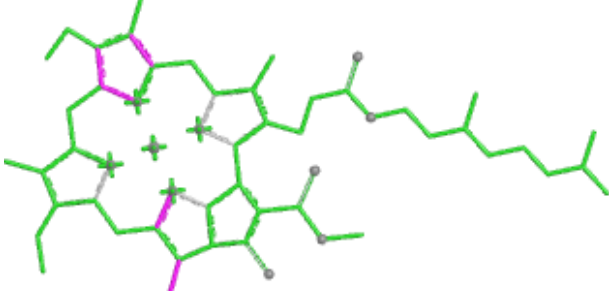
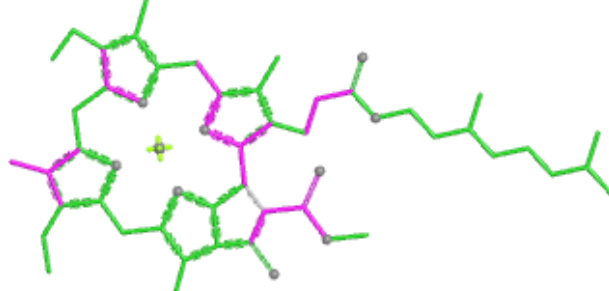
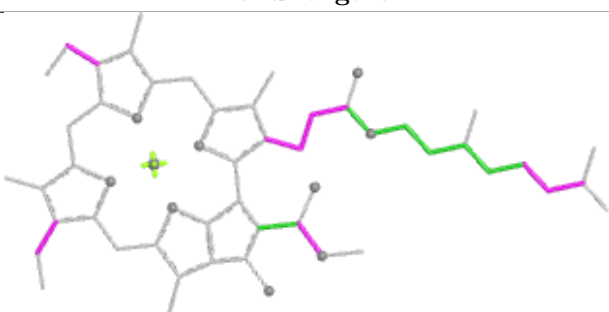
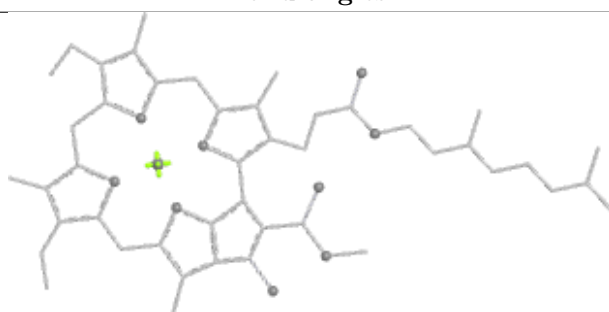


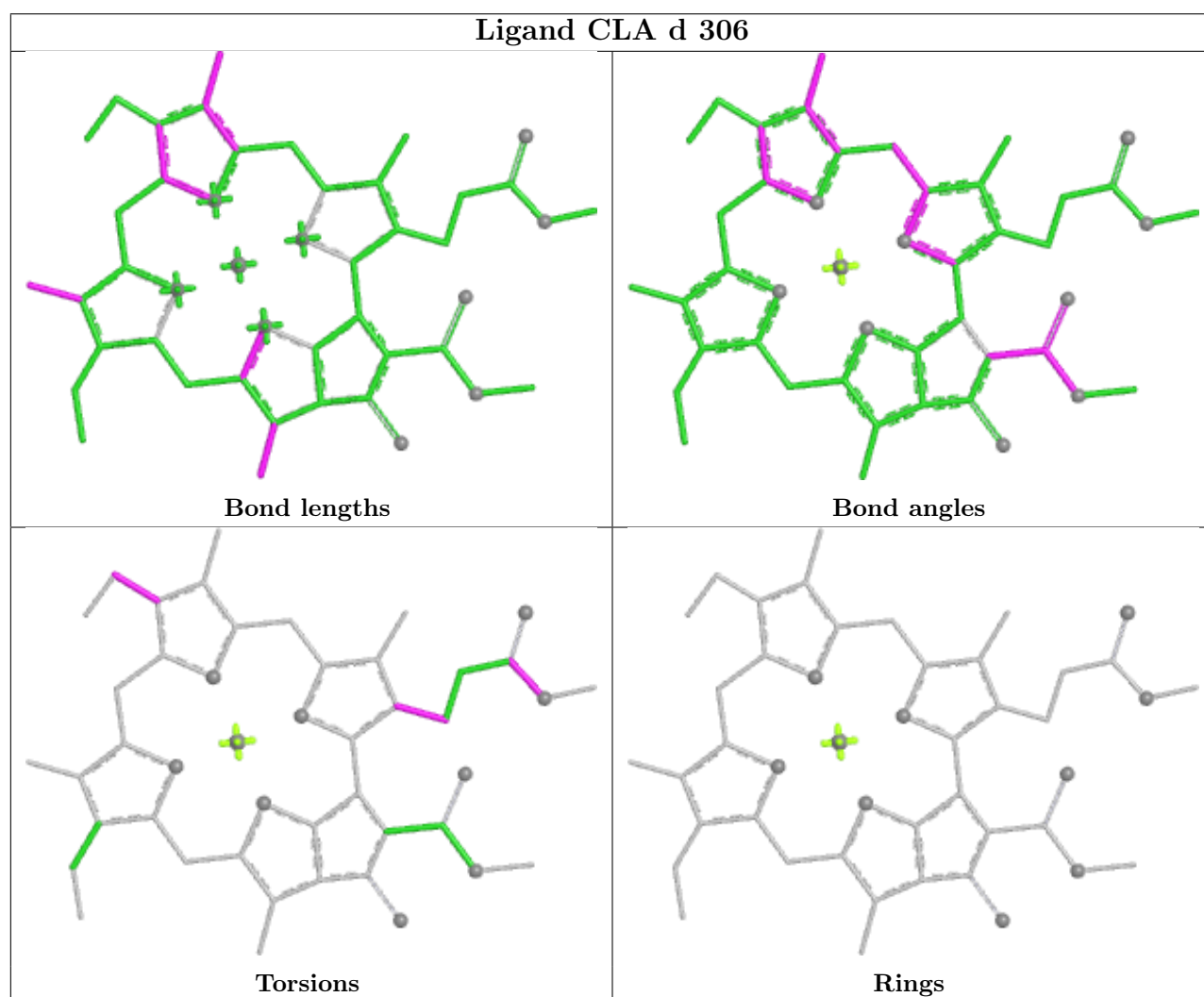
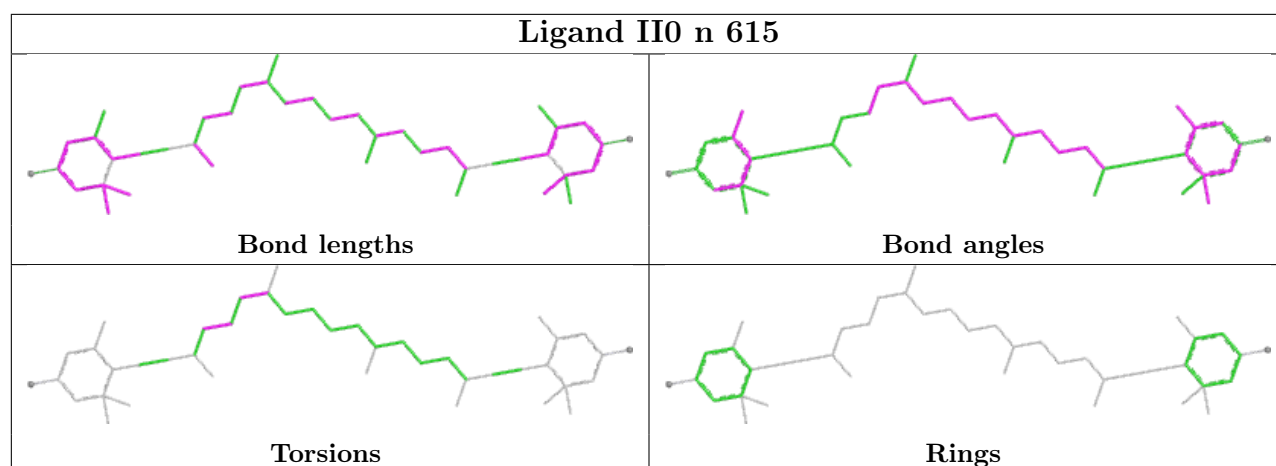
Ligand CLA L 204

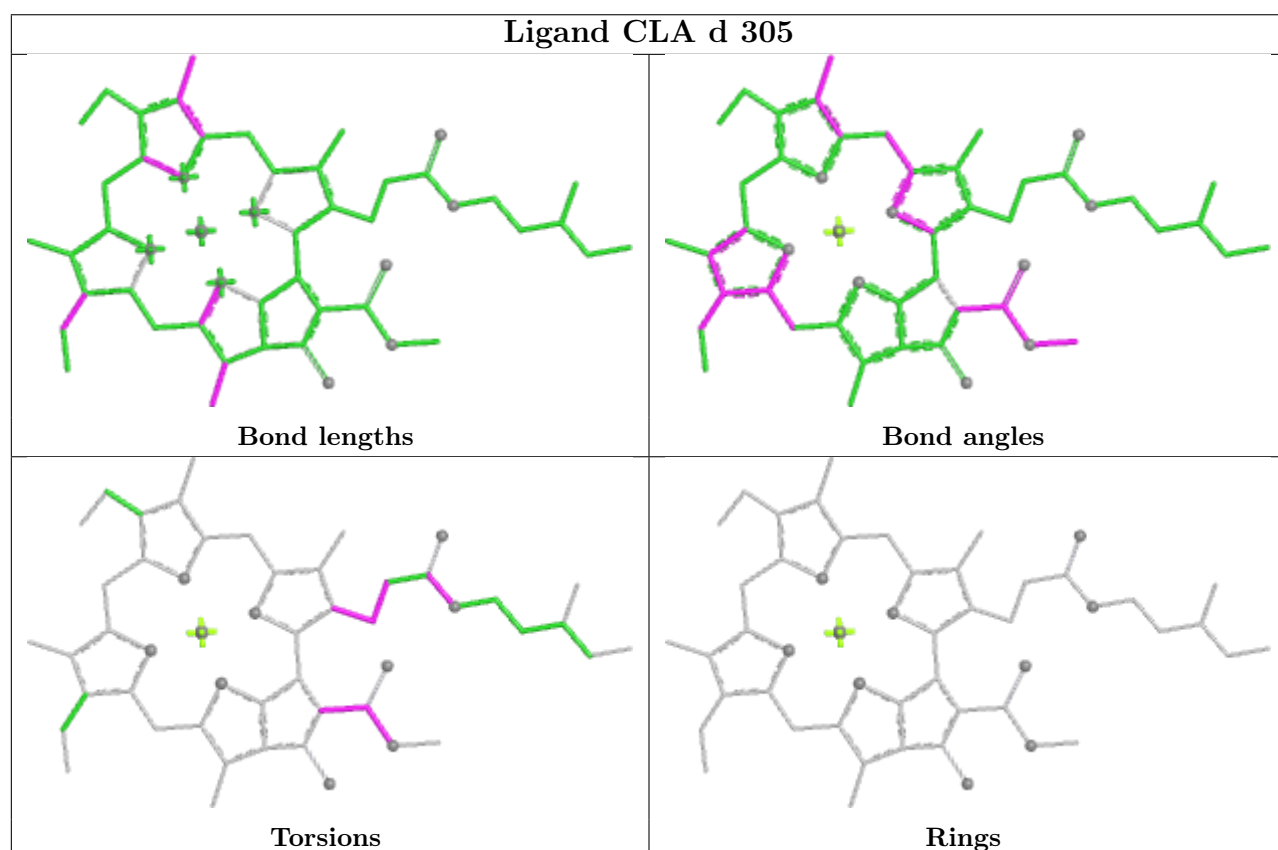
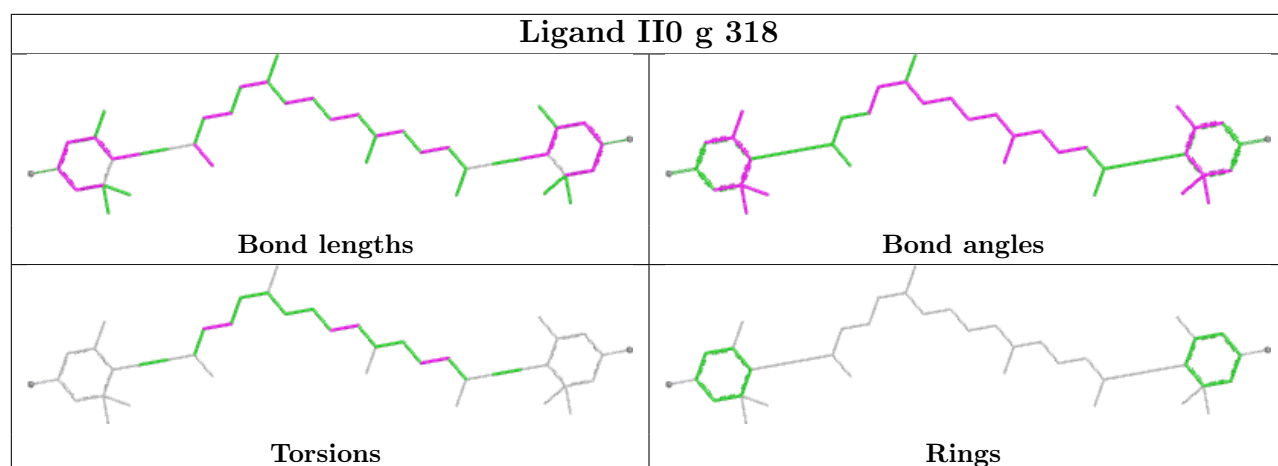


Ligand II0 c 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

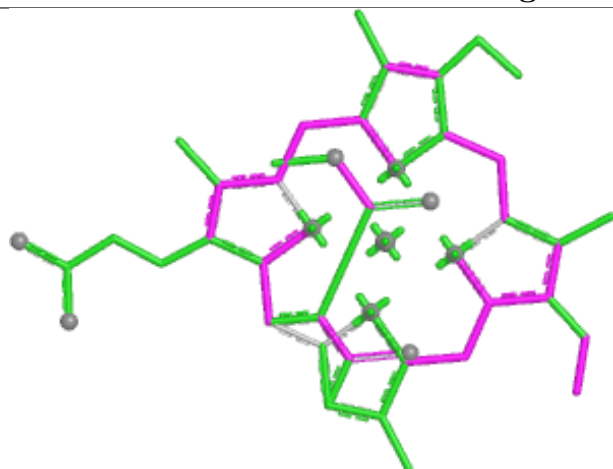
Ligand II0 a 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA m 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

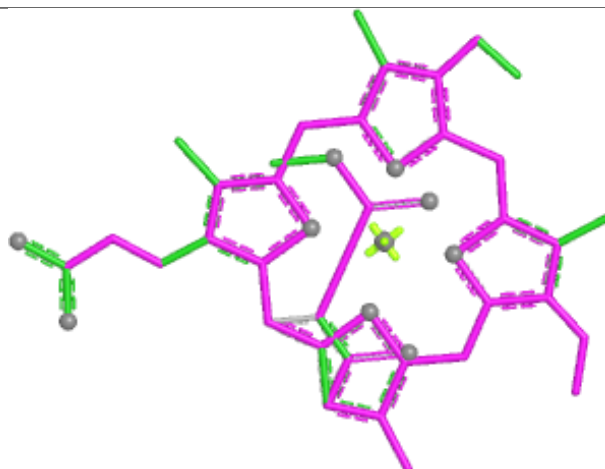




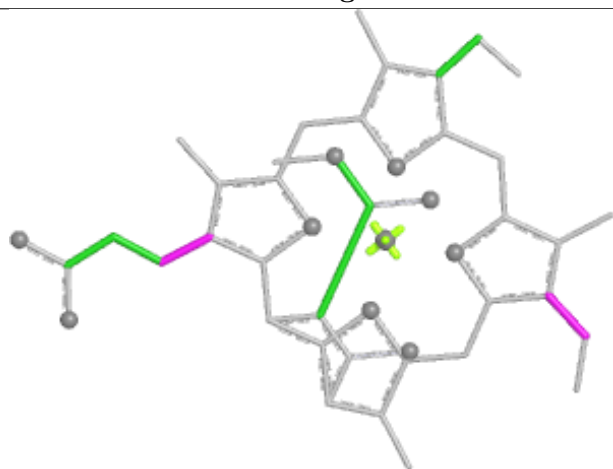
Ligand KC2 n 611



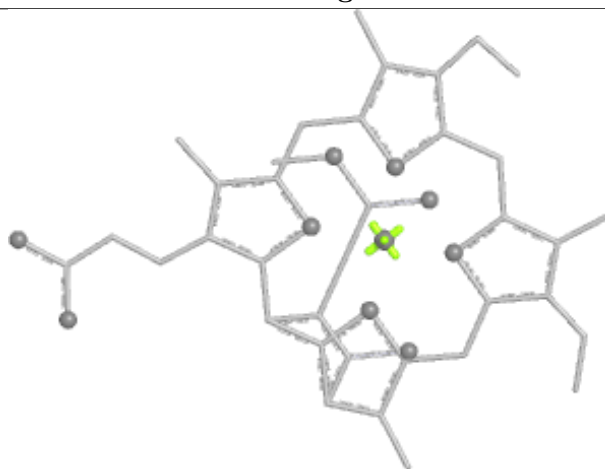
Bond lengths



Bond angles

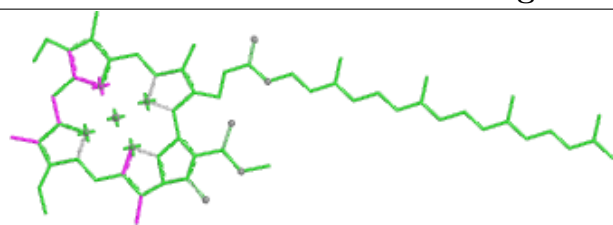


Torsions

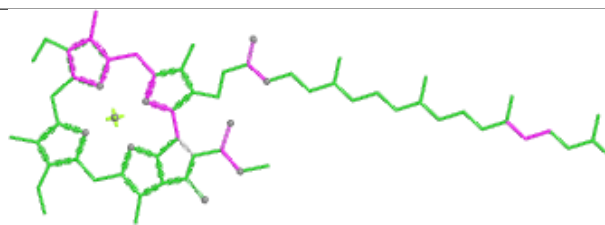


Rings

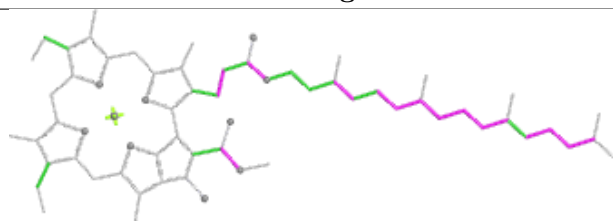
Ligand CLA h 306



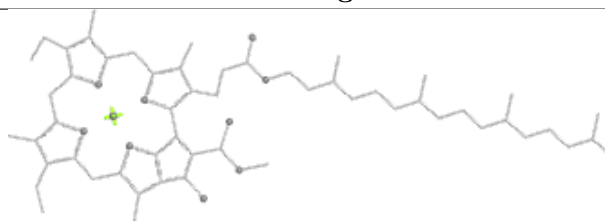
Bond lengths



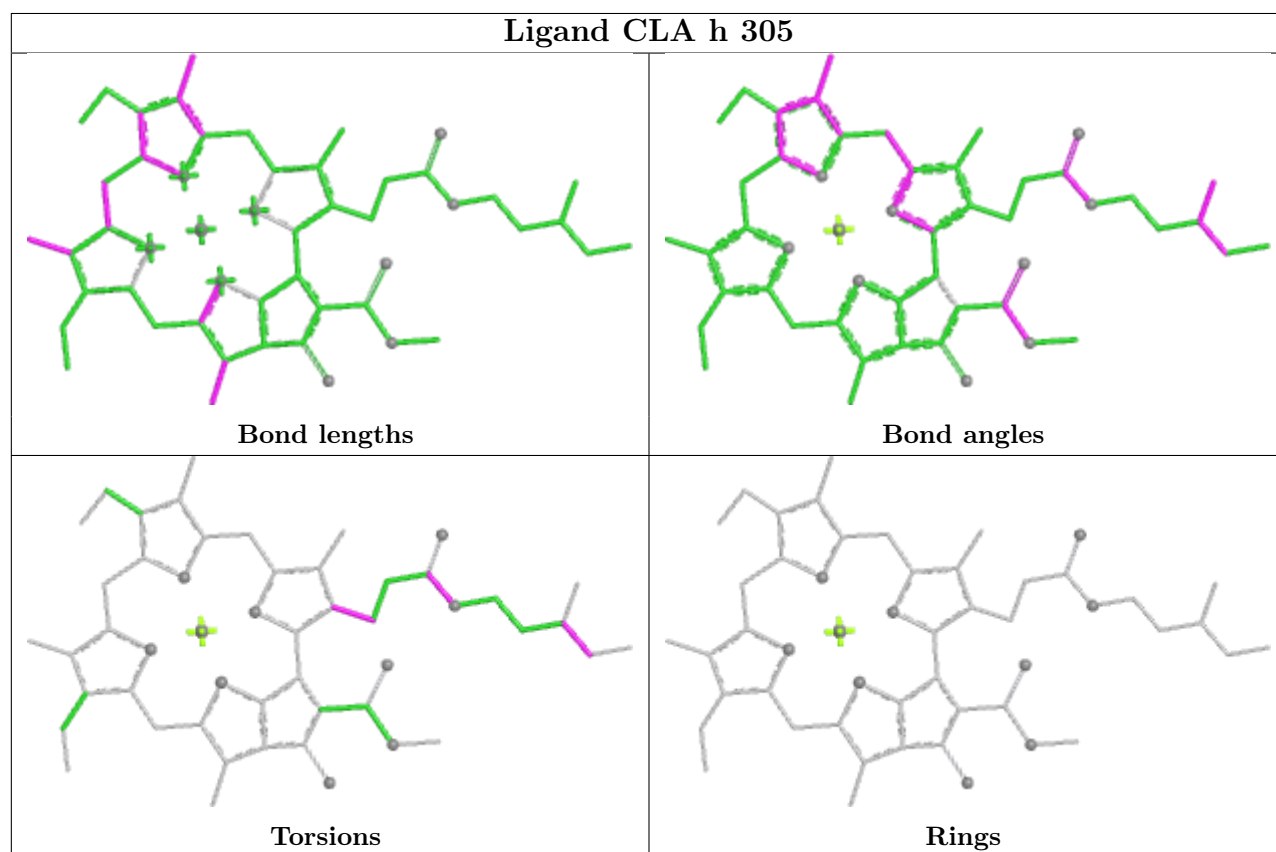
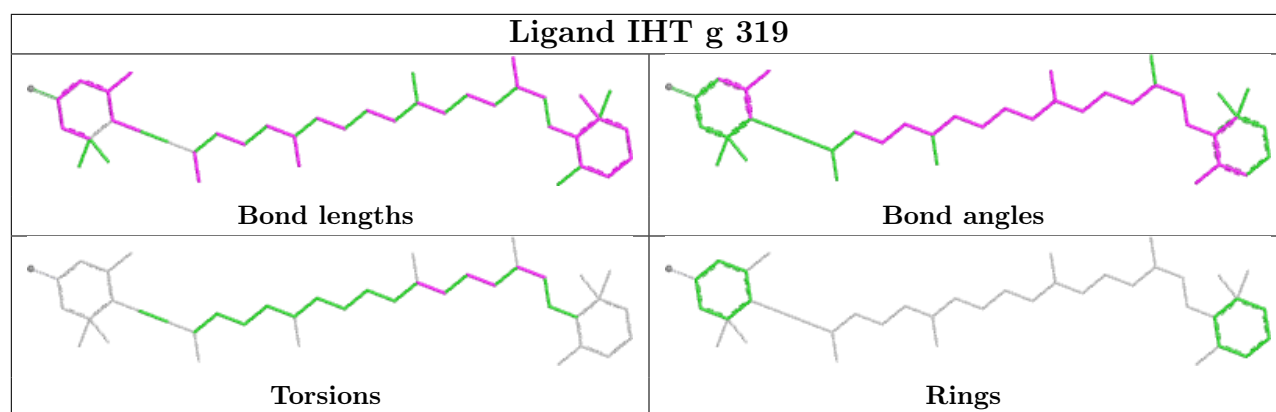
Bond angles

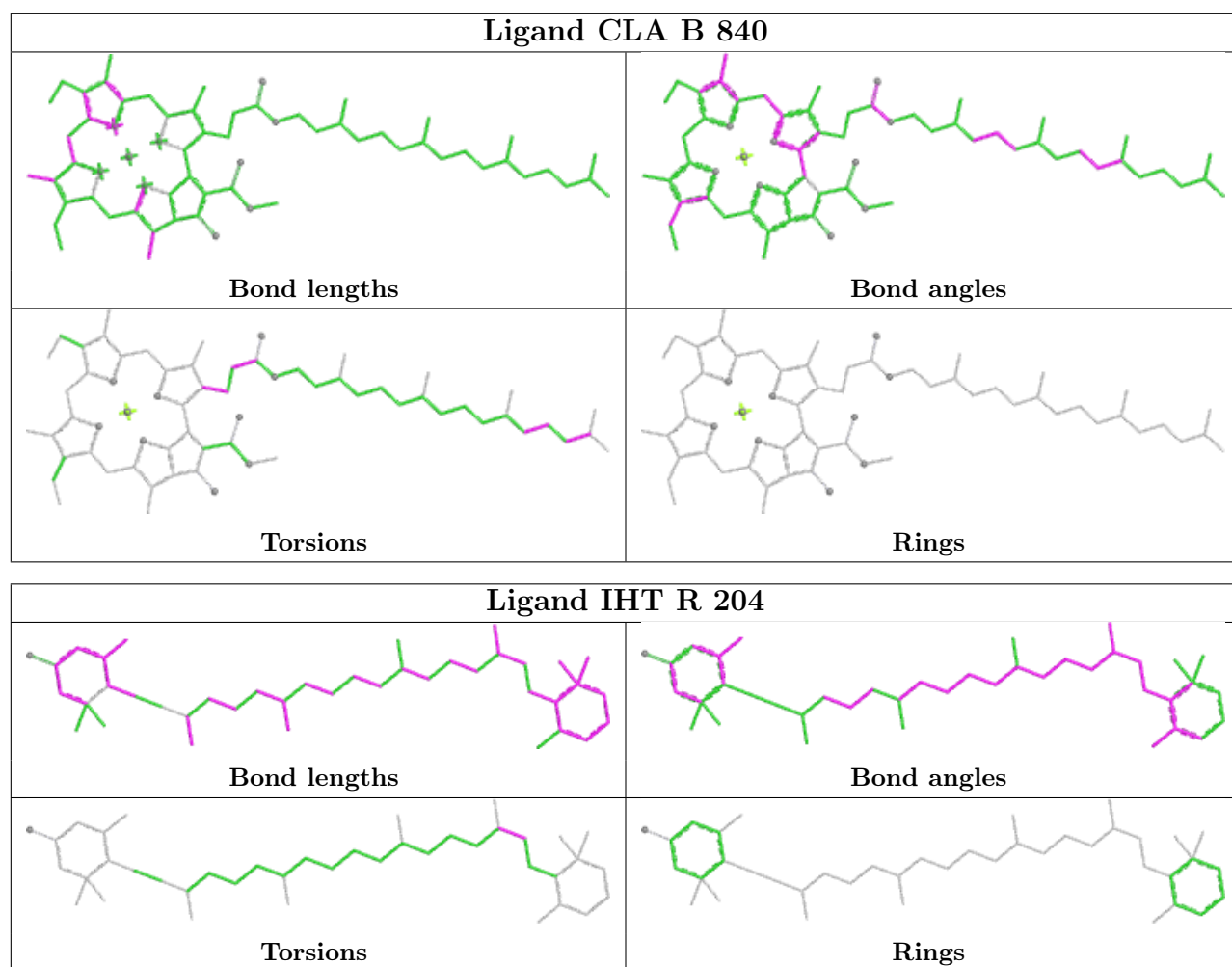


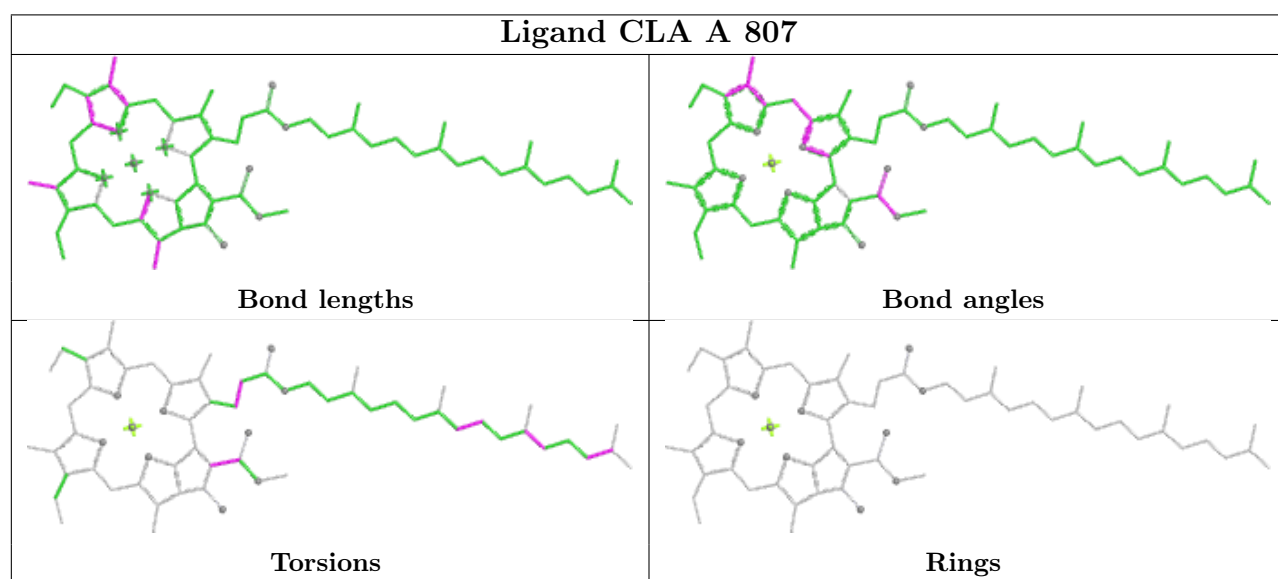
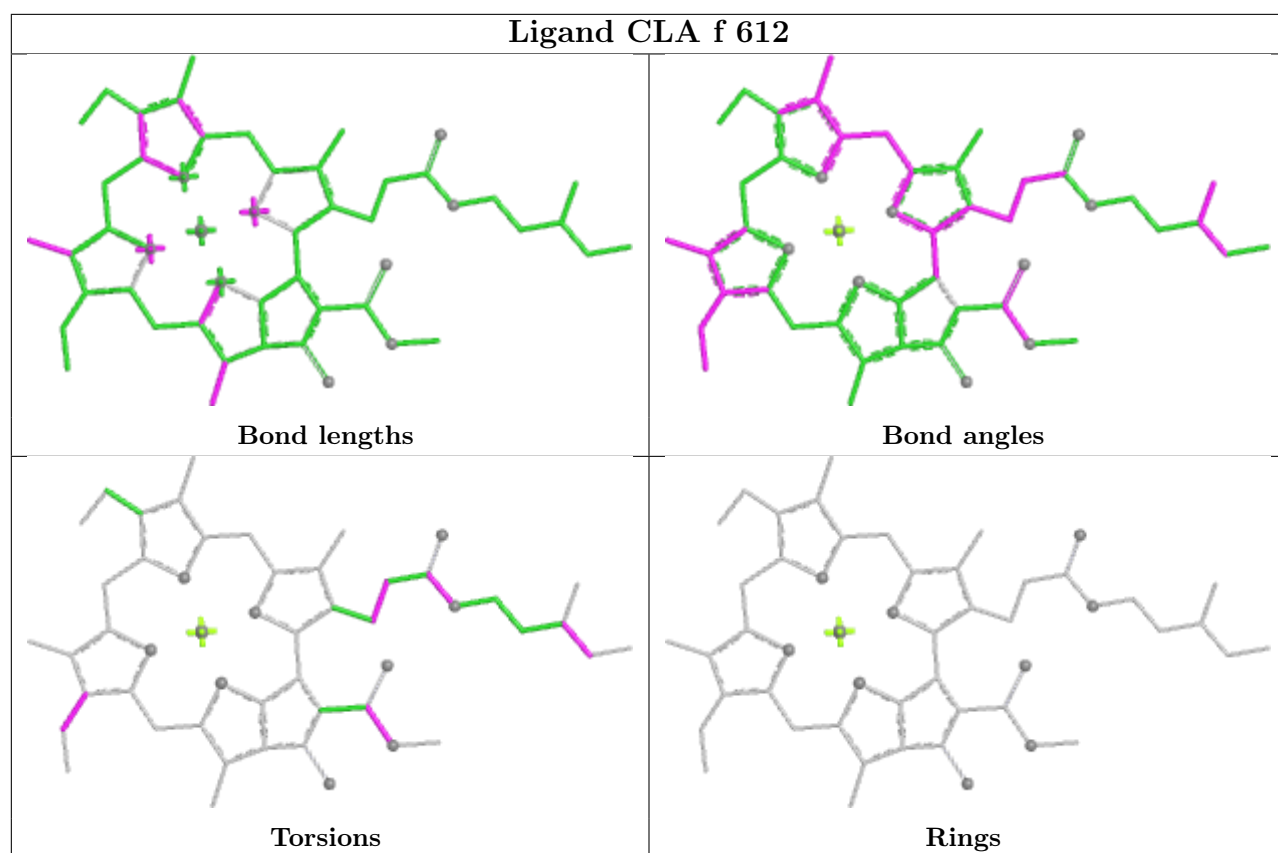
Torsions



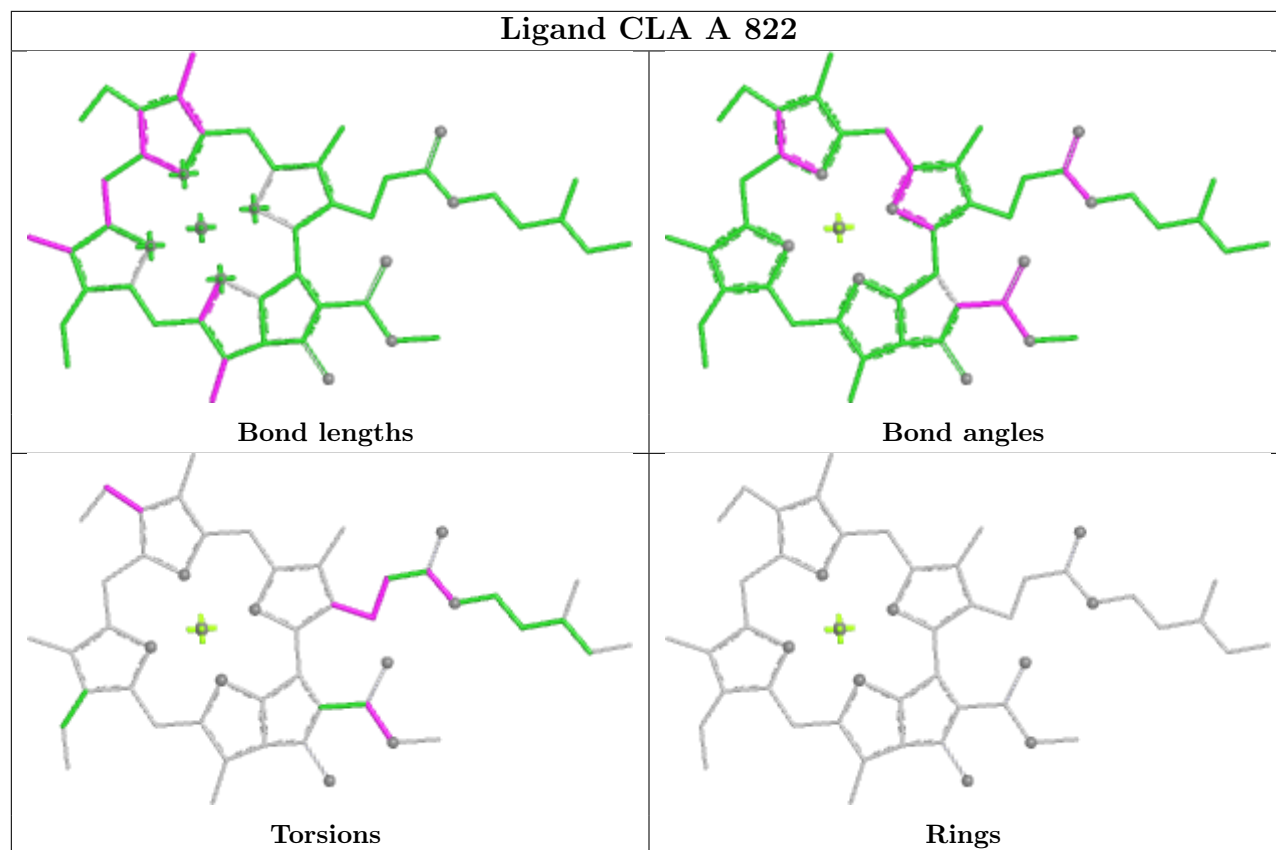
Rings



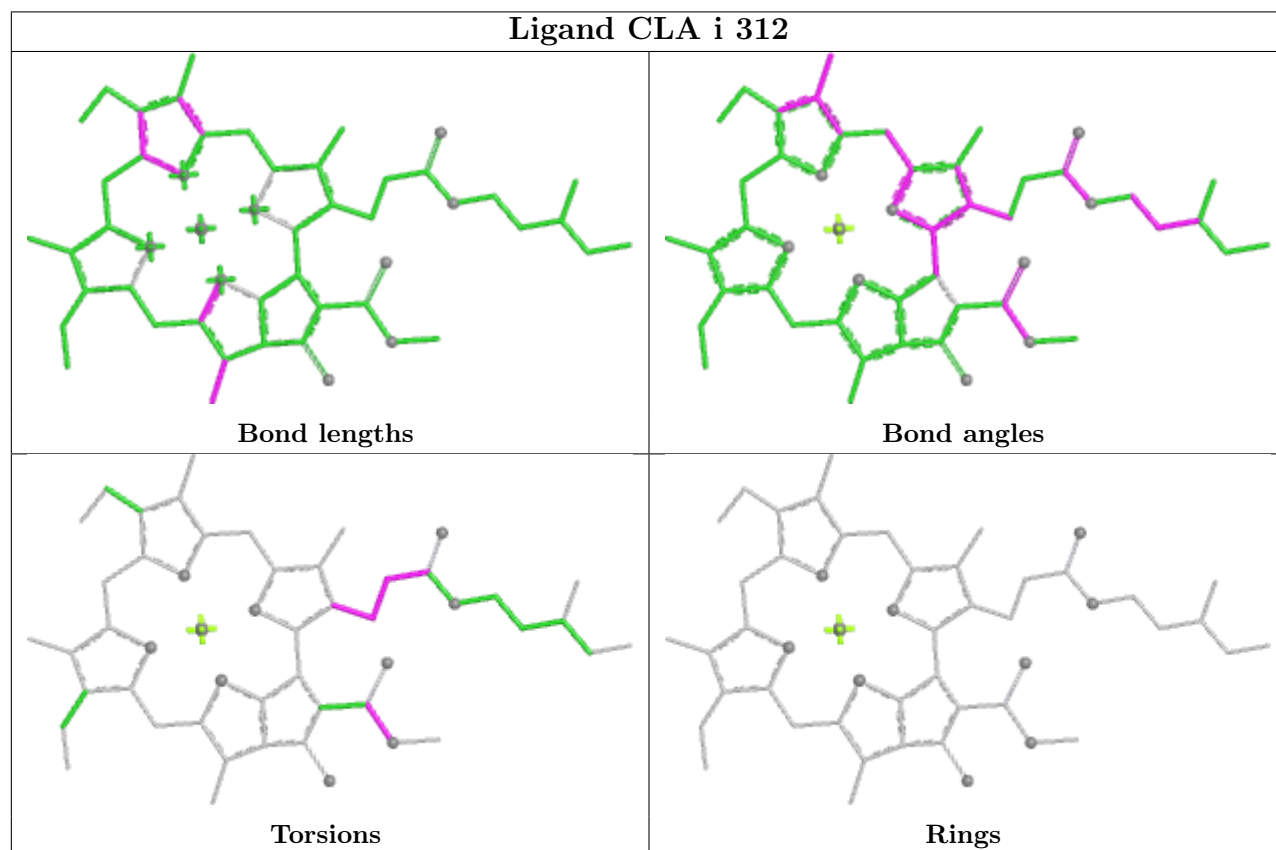




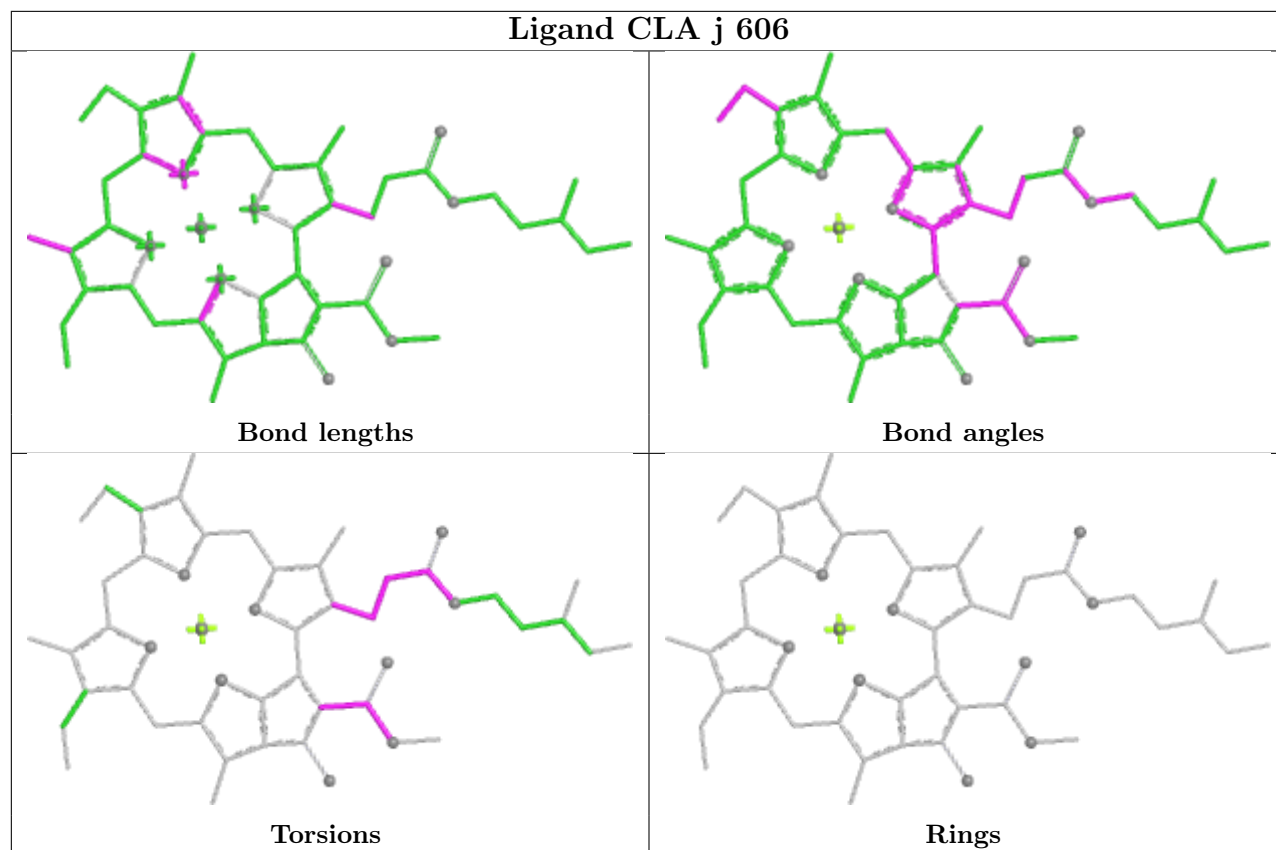
Ligand CLA A 822



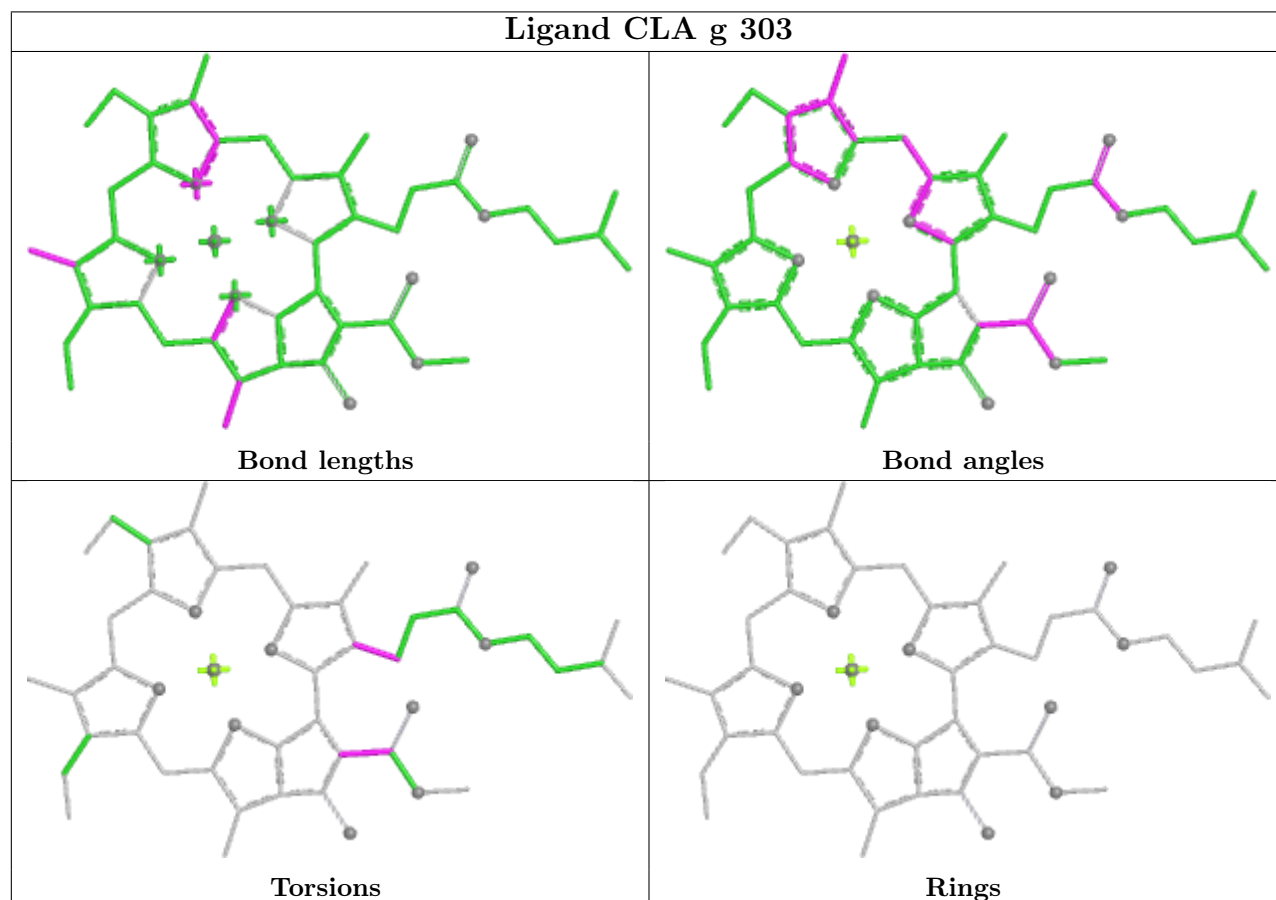
Ligand CLA i 312

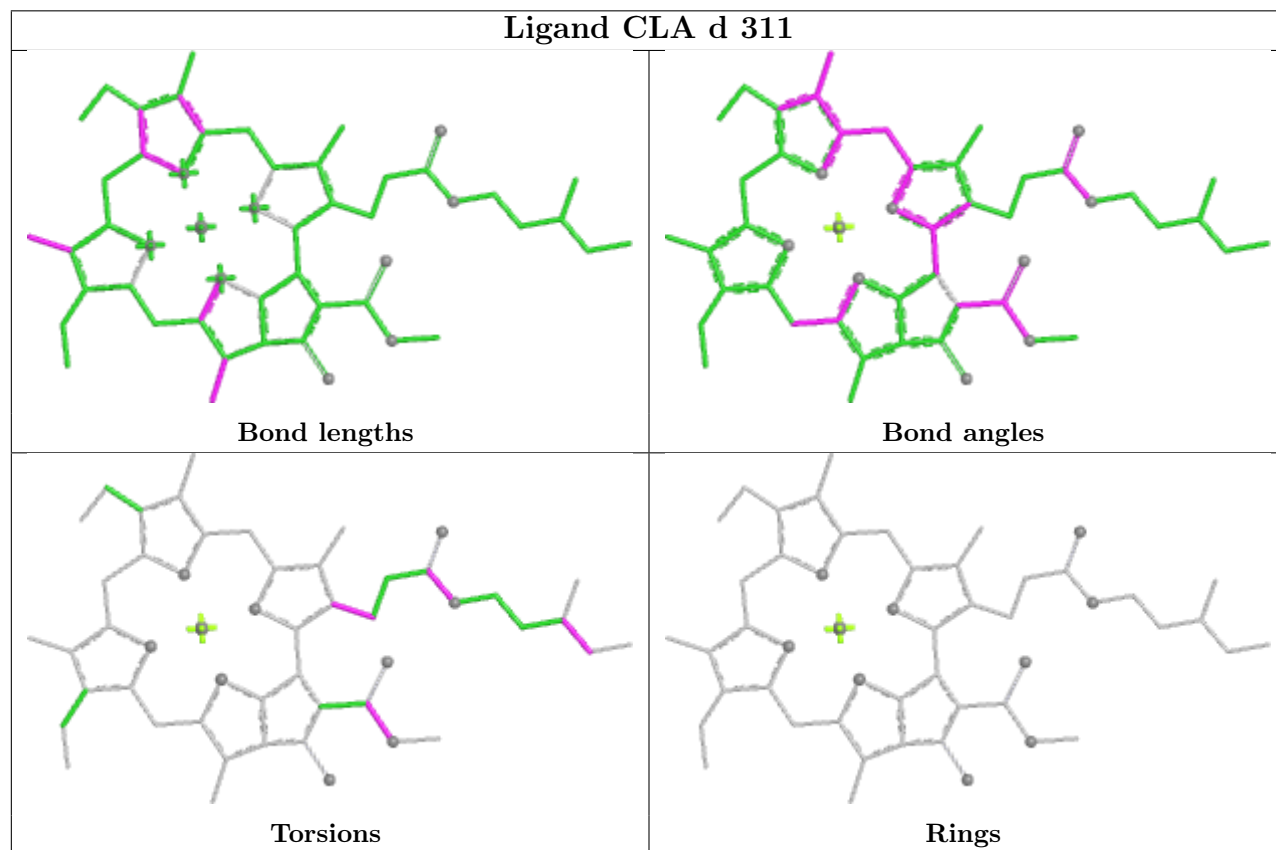
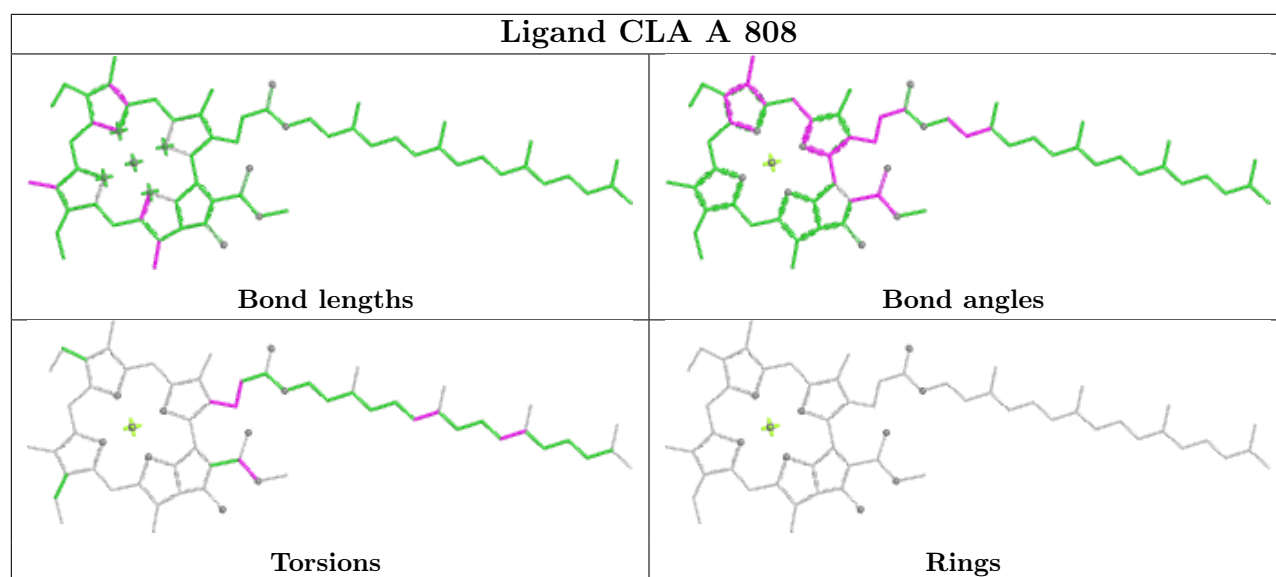


Ligand CLA j 606

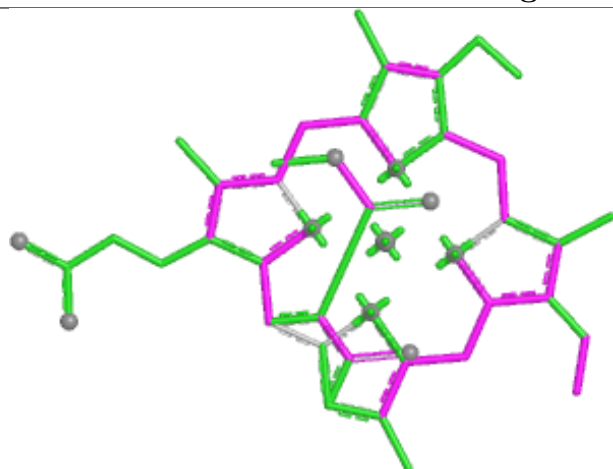


Ligand CLA g 303

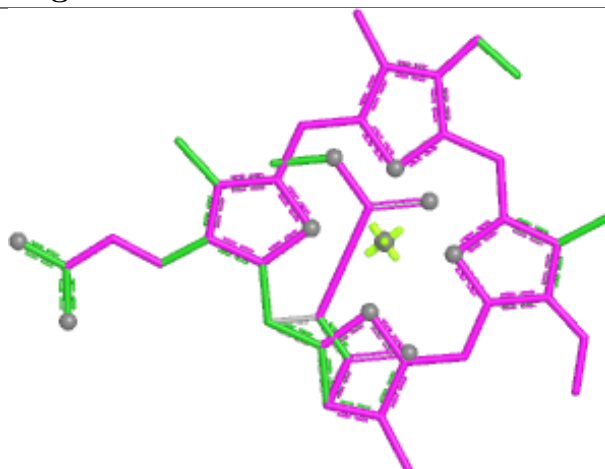




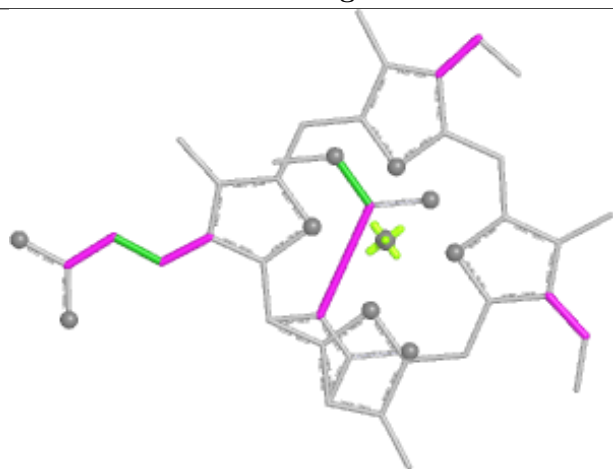
Ligand KC2 g 312



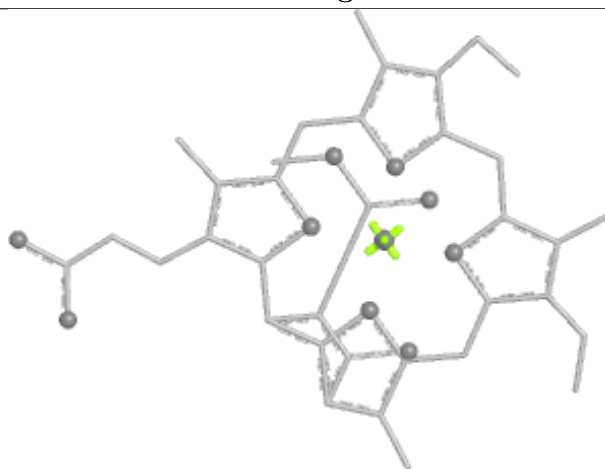
Bond lengths



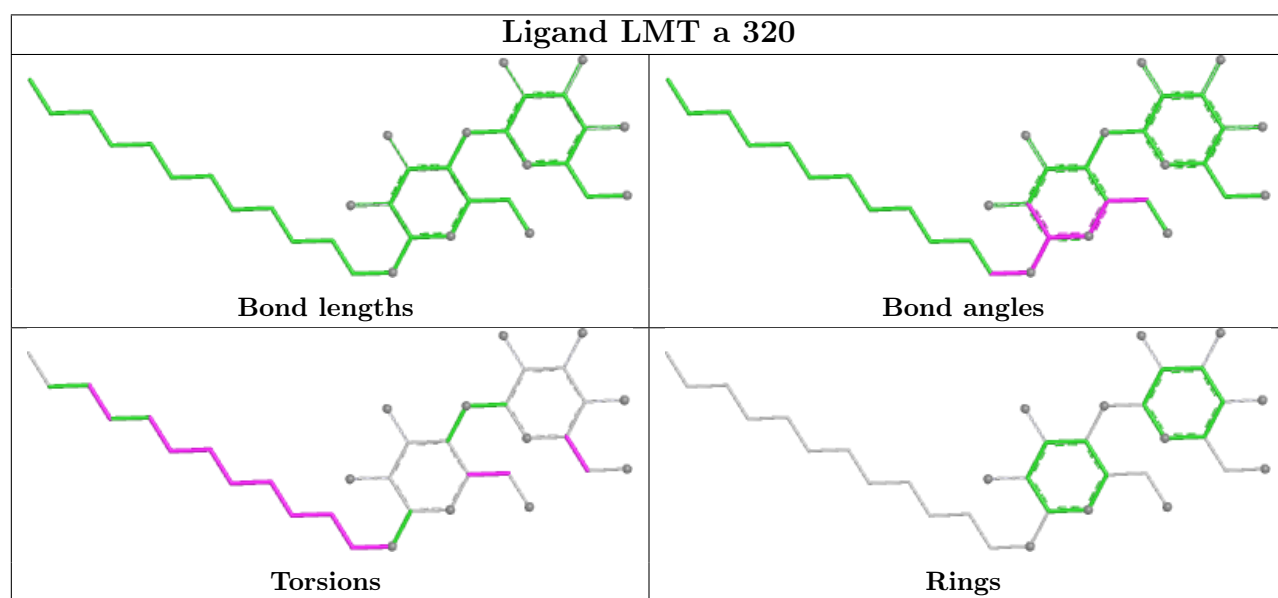
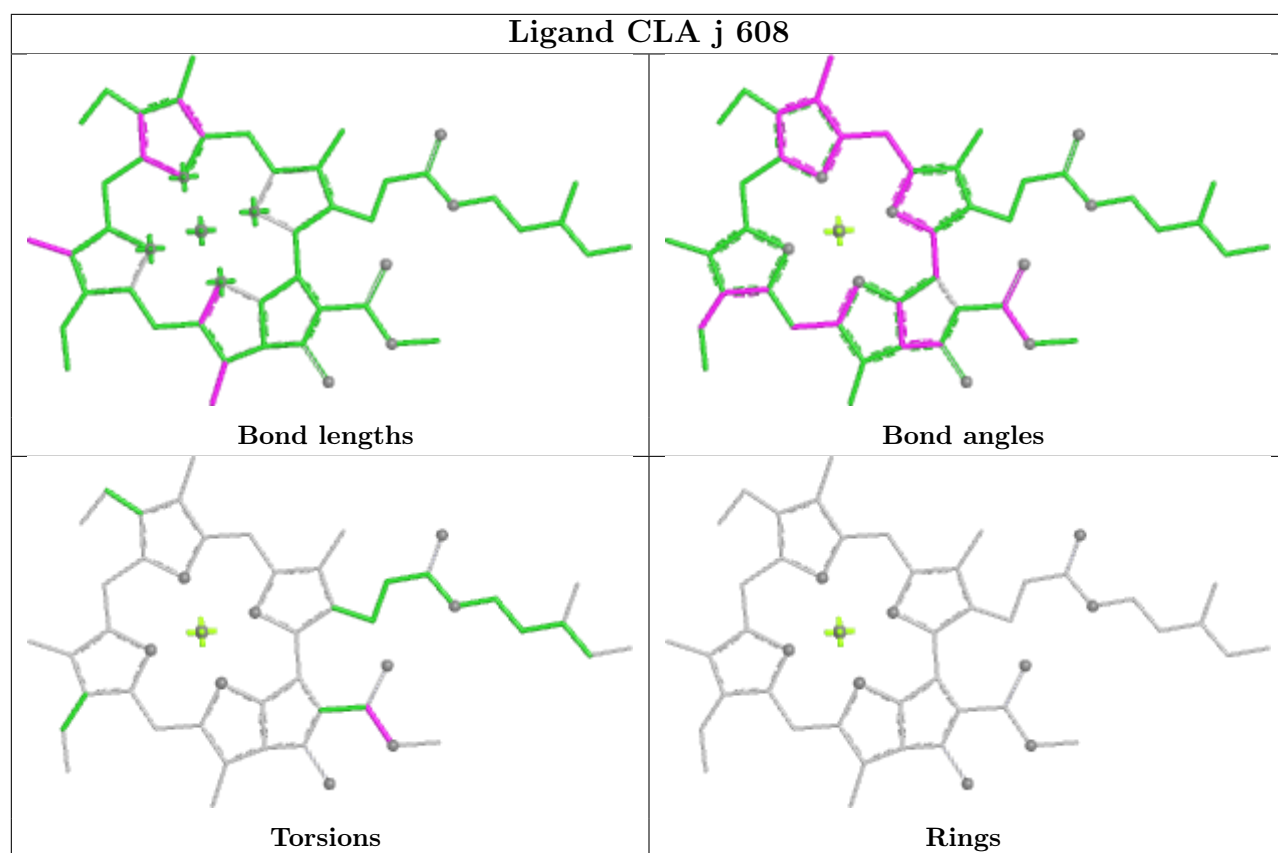
Bond angles

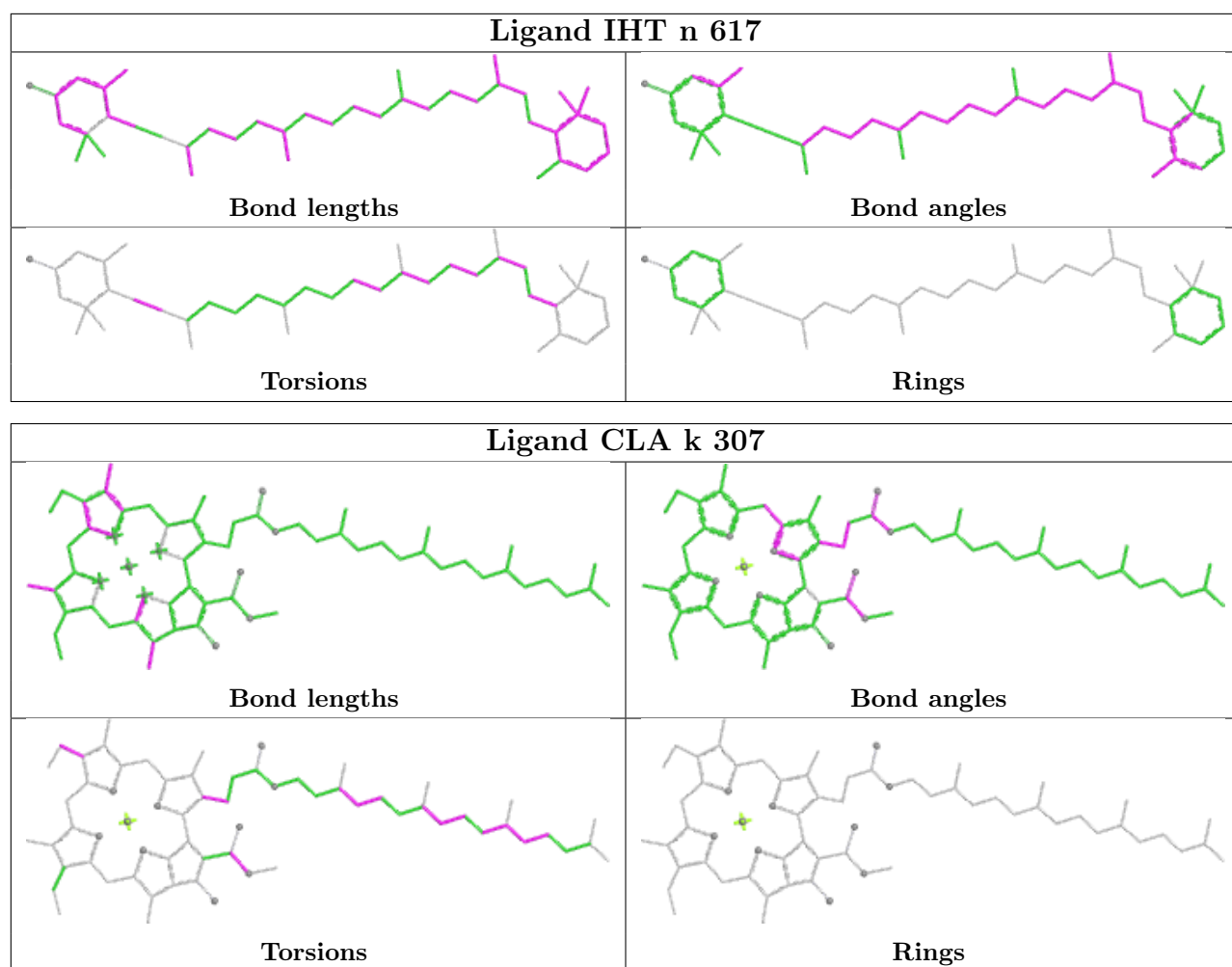


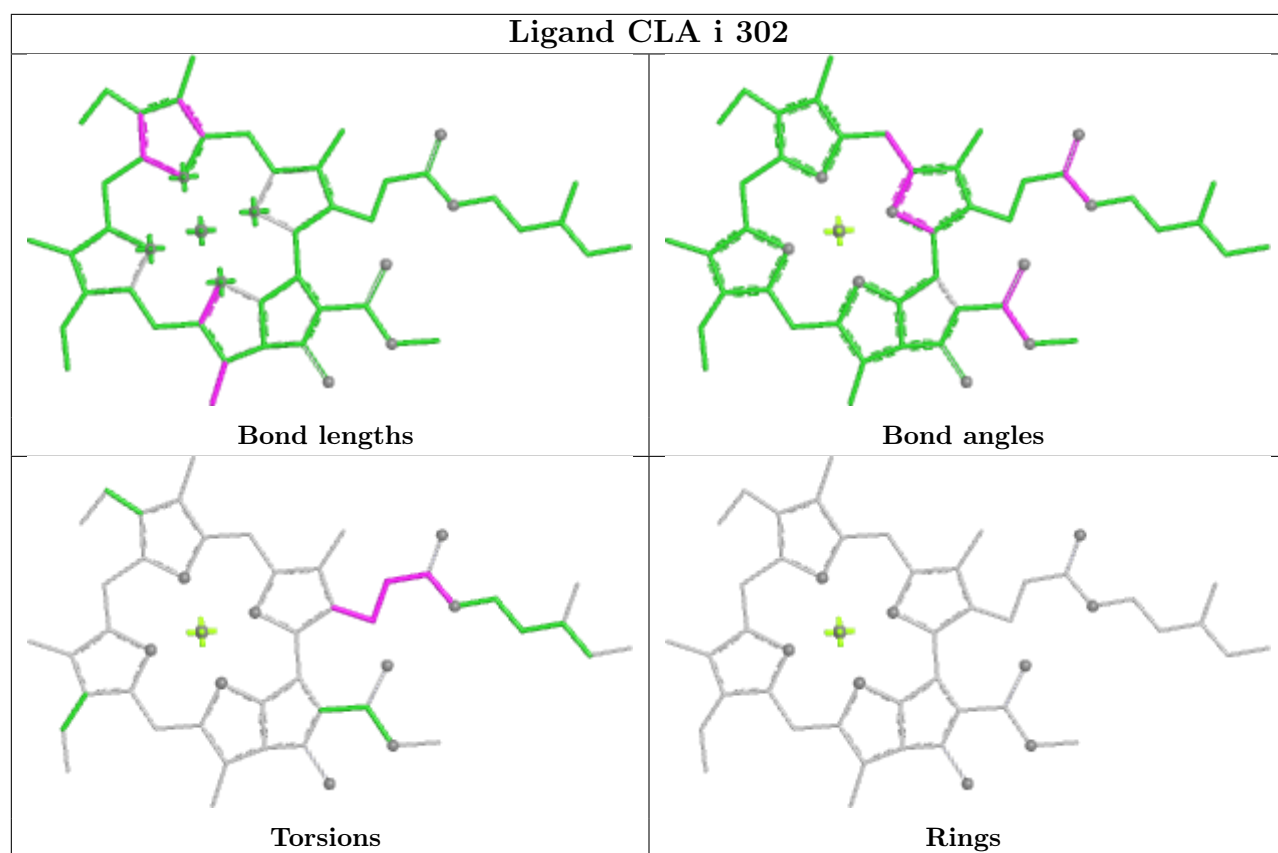
Torsions



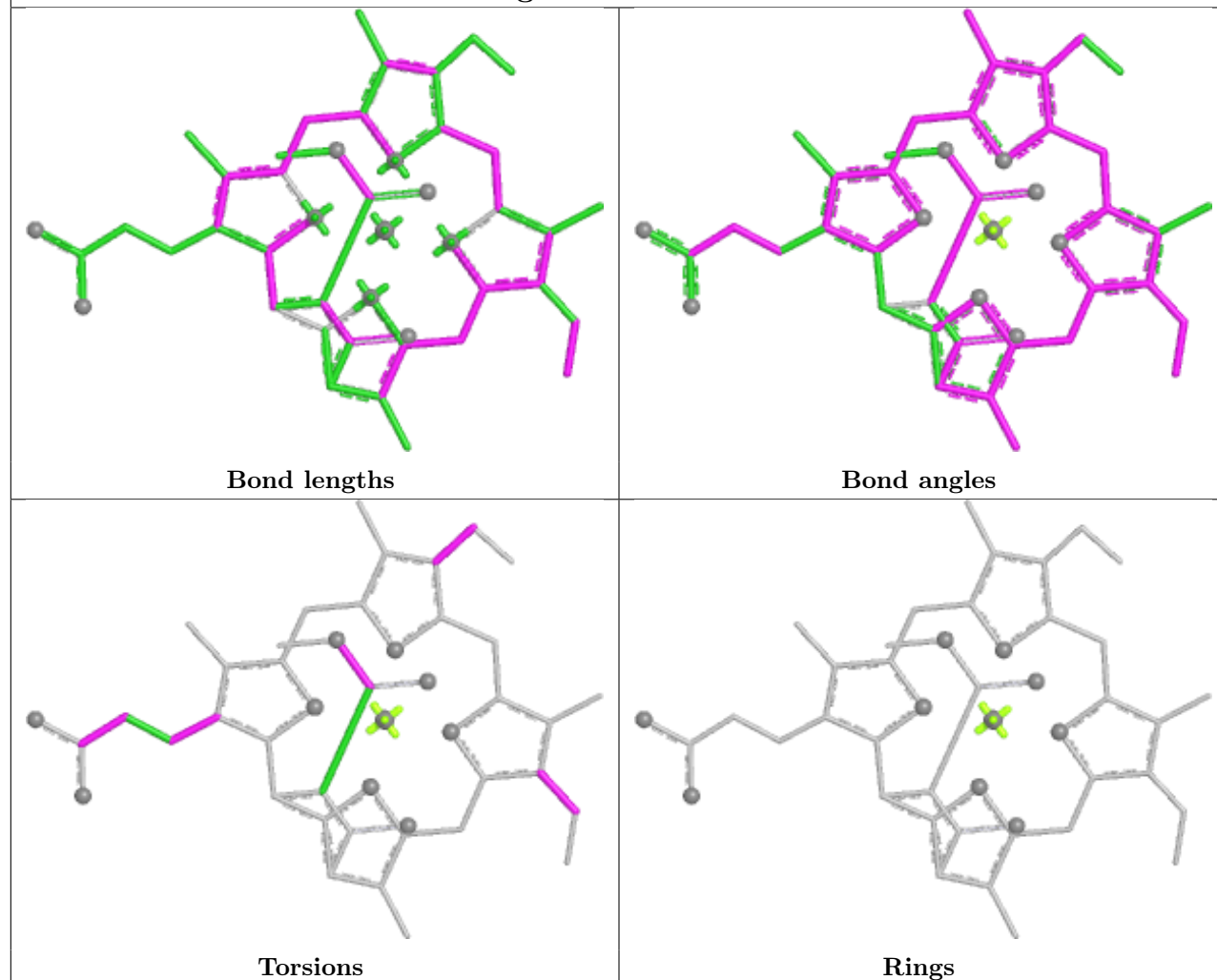
Rings



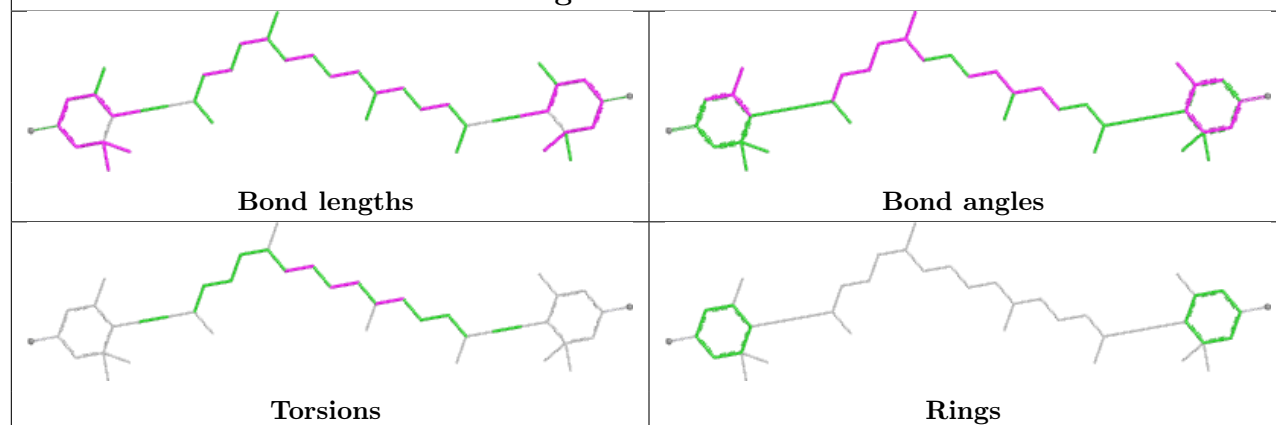




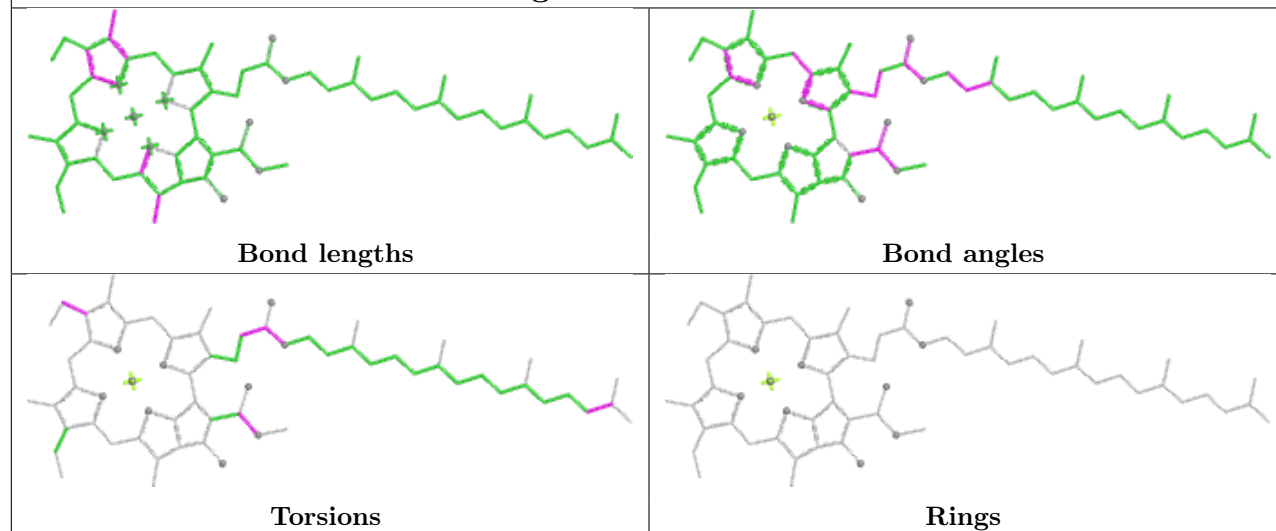
Ligand KC2 i 310



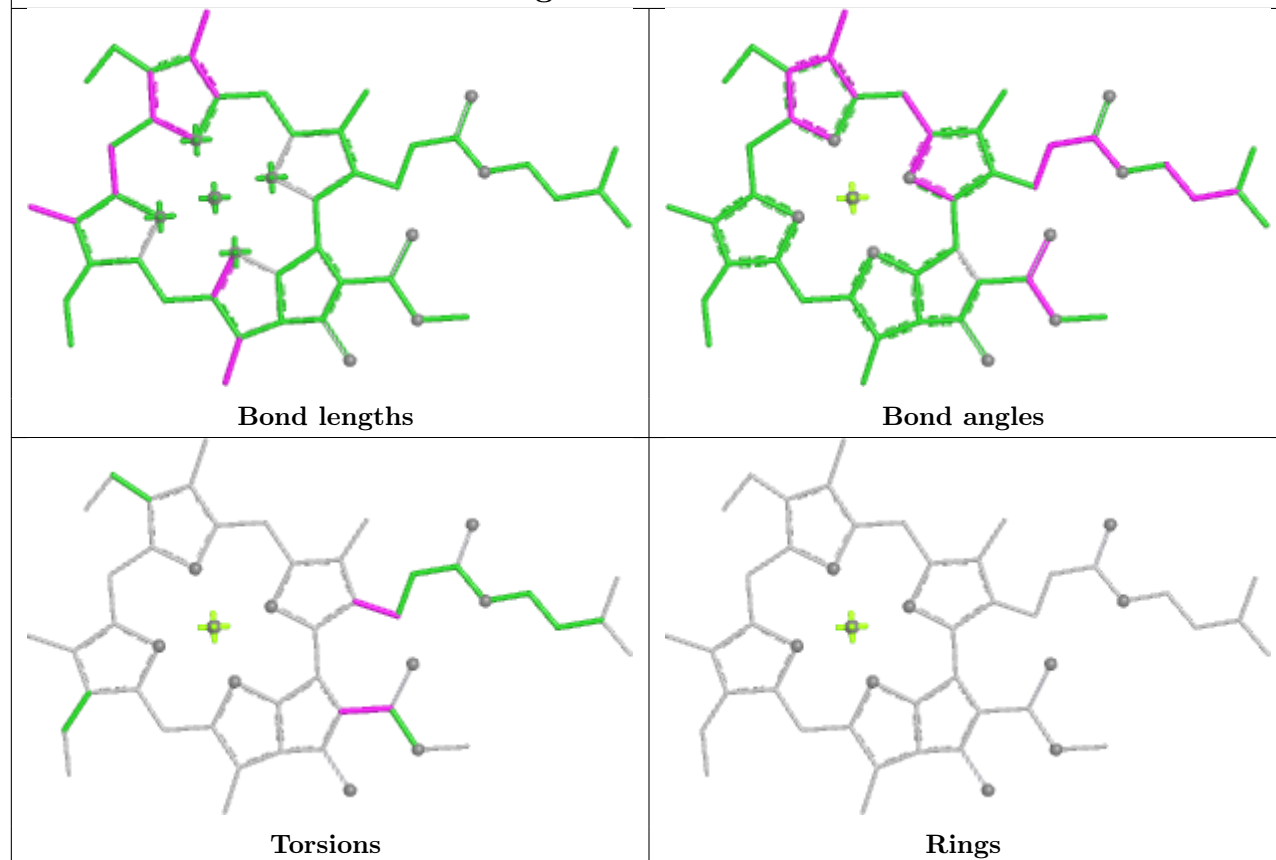
Ligand II0 l 317

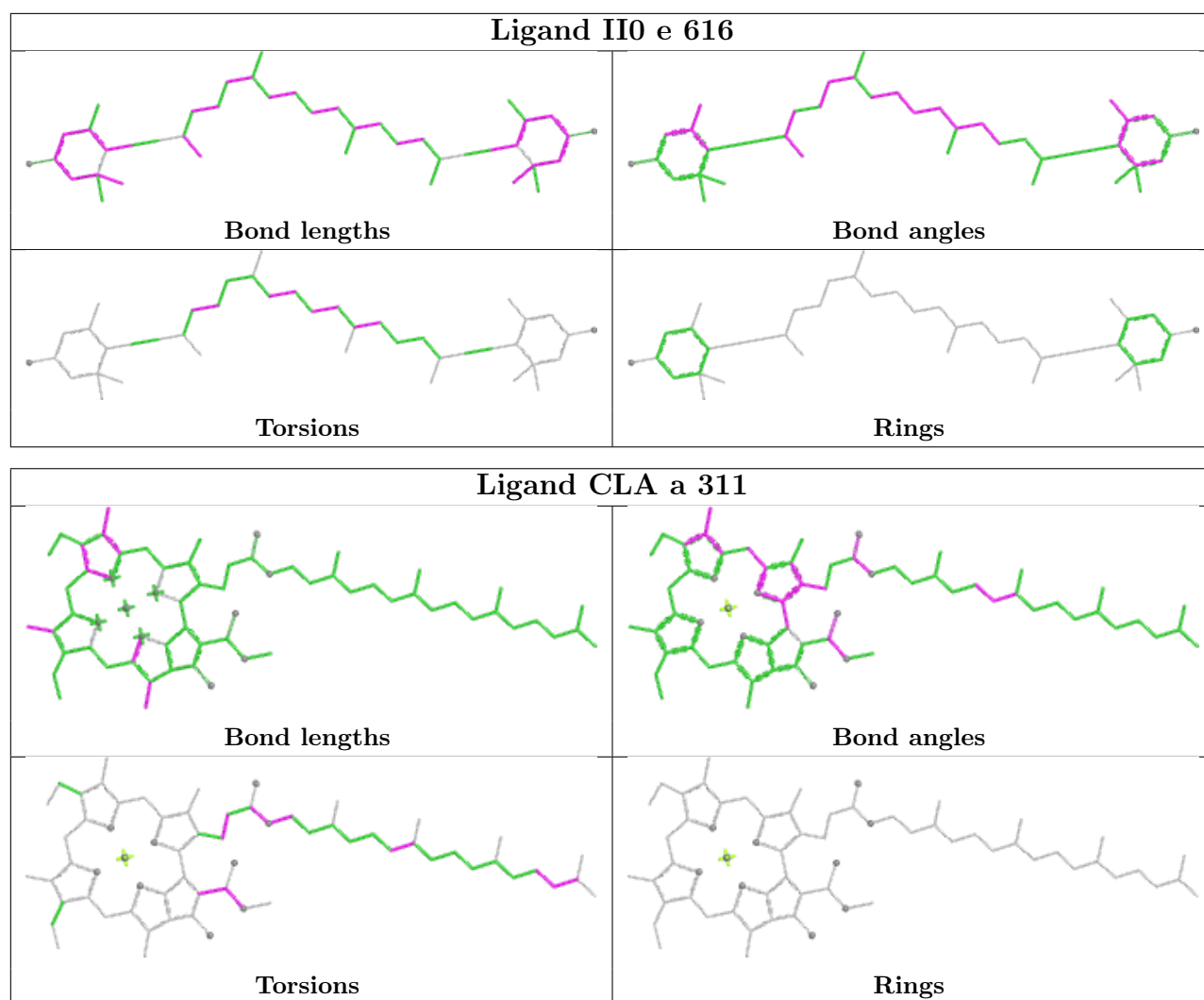


Ligand CLA A 801

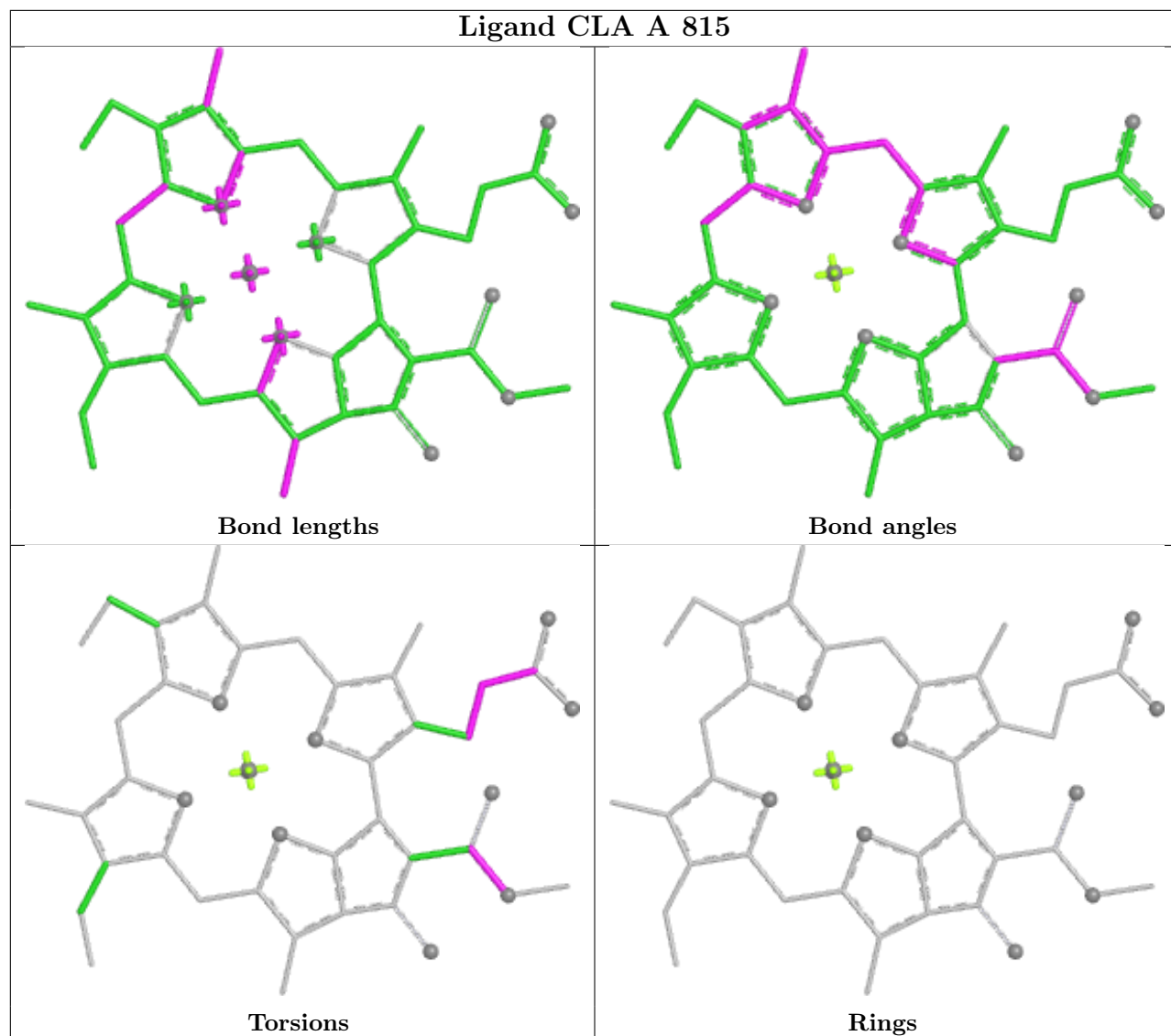


Ligand CLA d 301

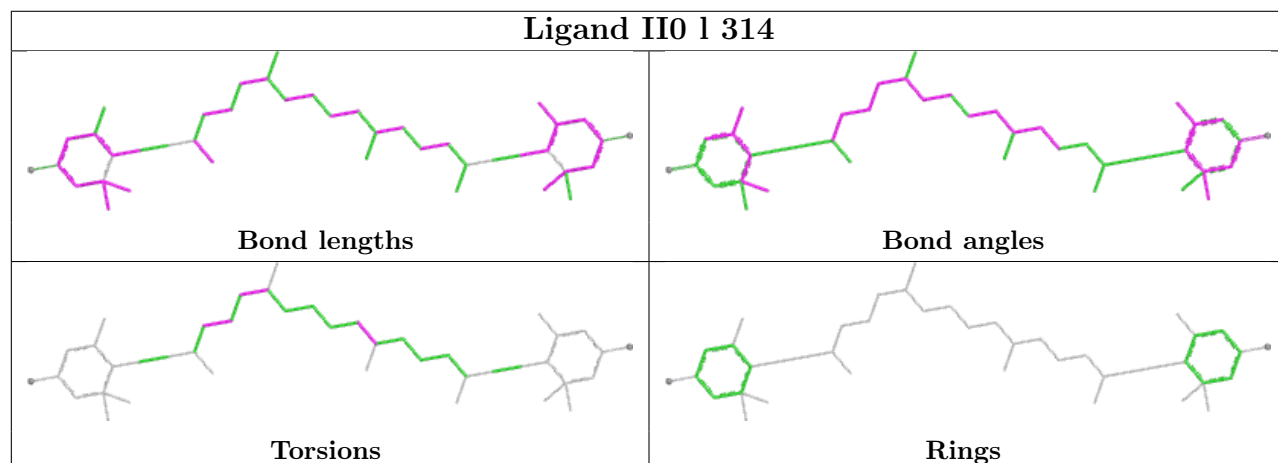


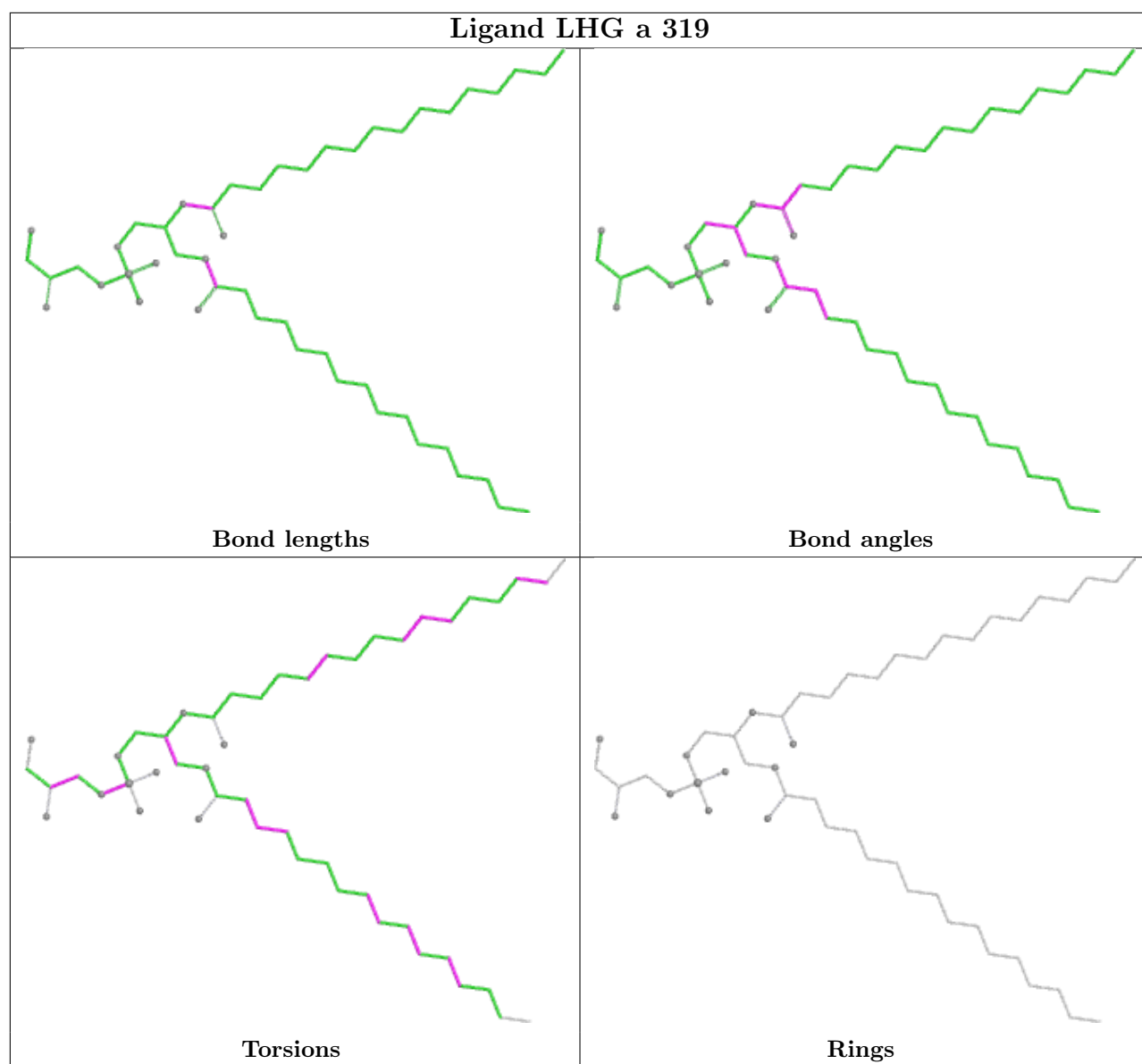


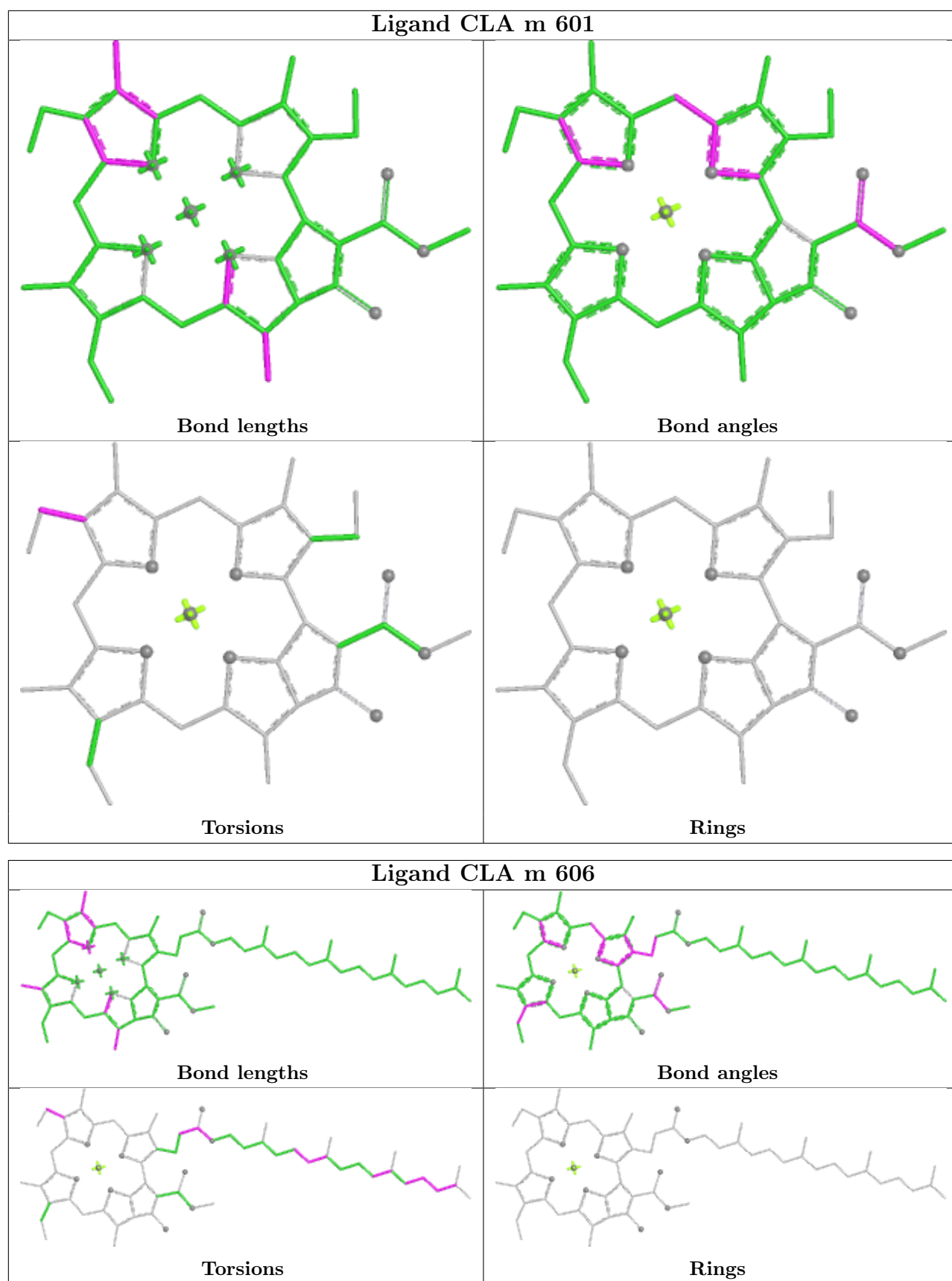
Ligand CLA A 815

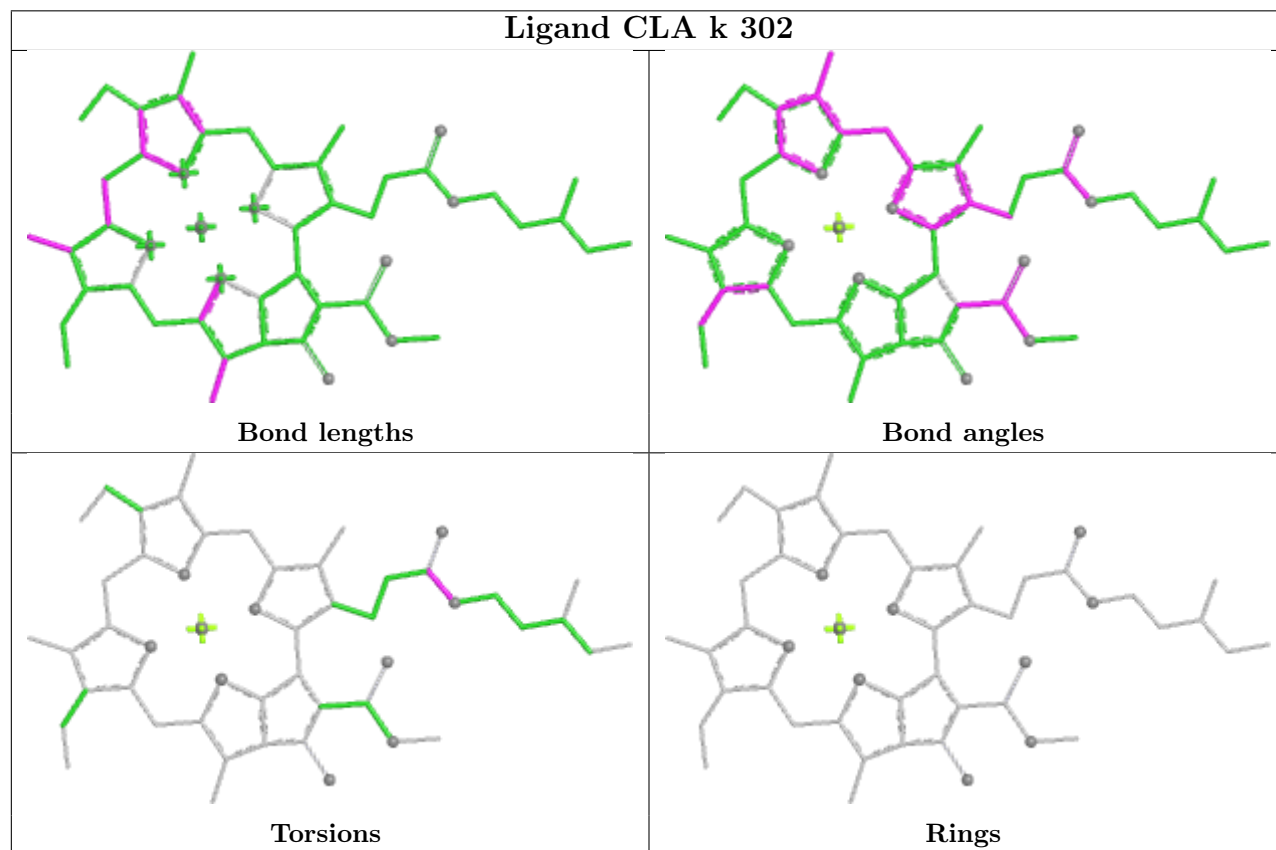
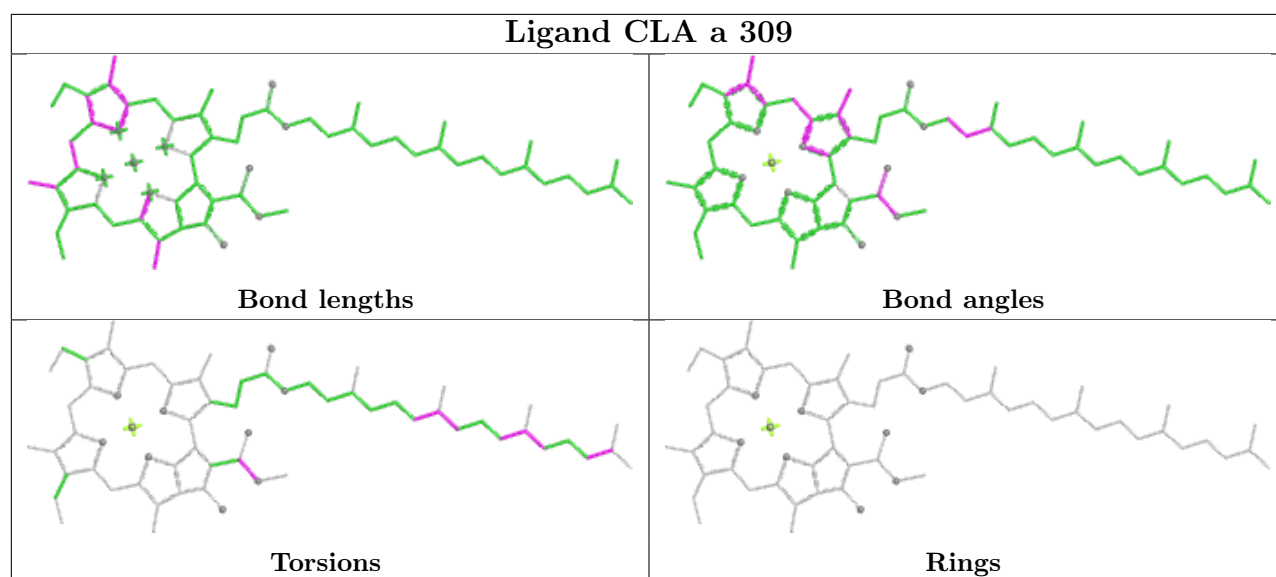


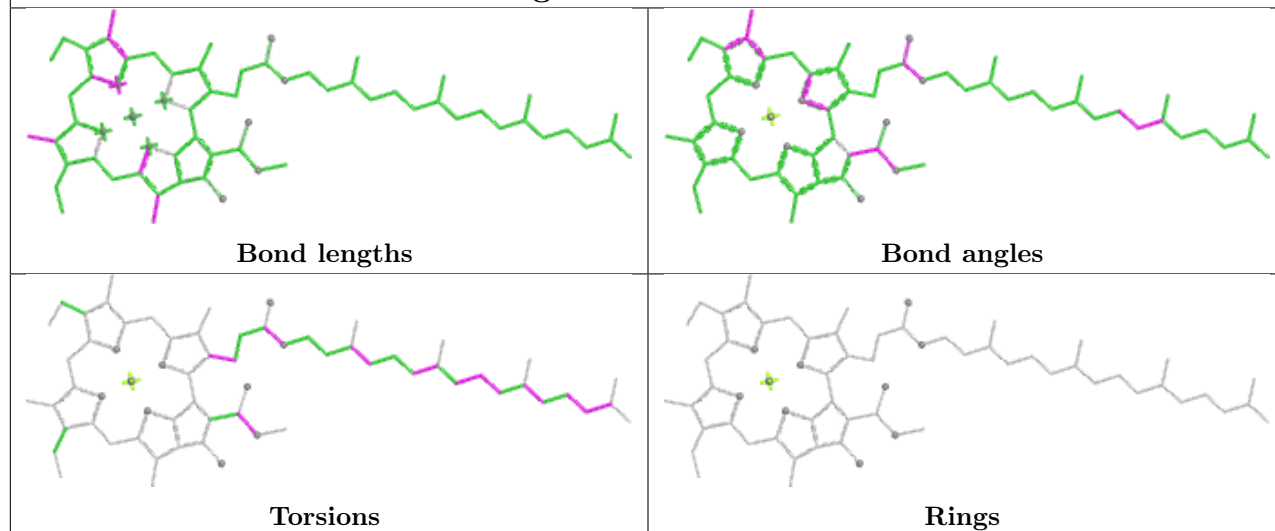
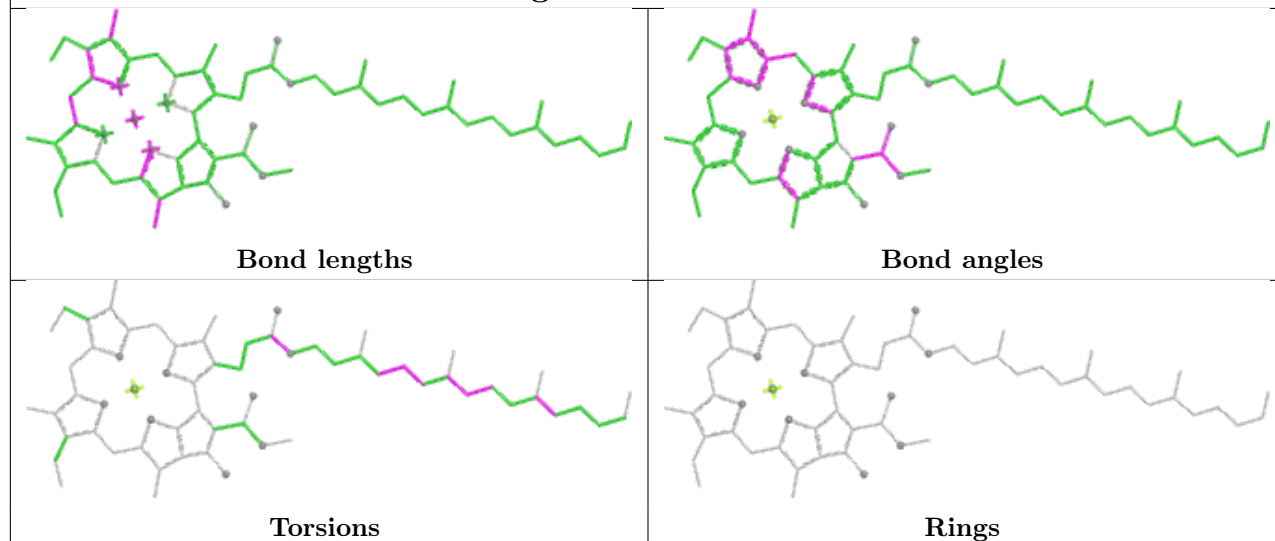
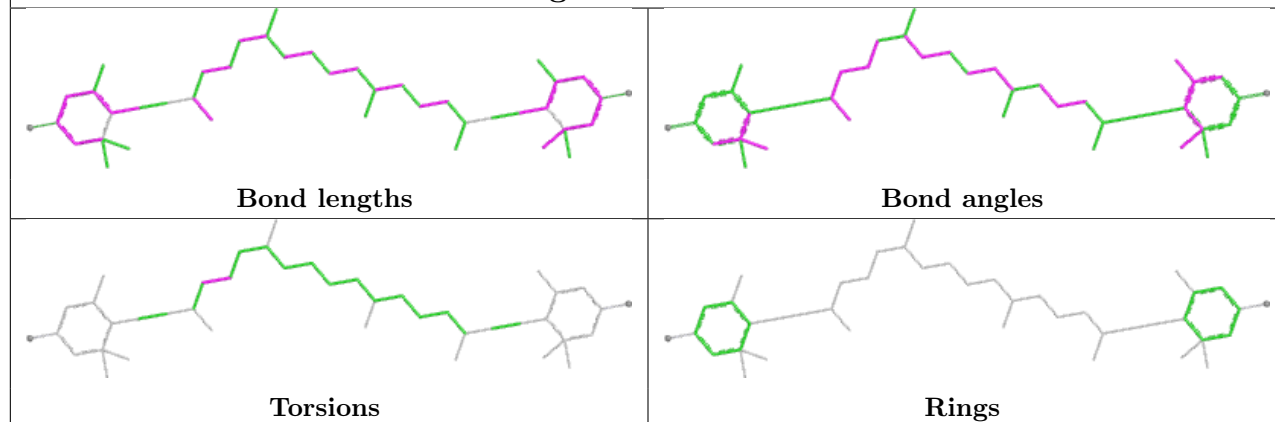
Ligand II0 1 314

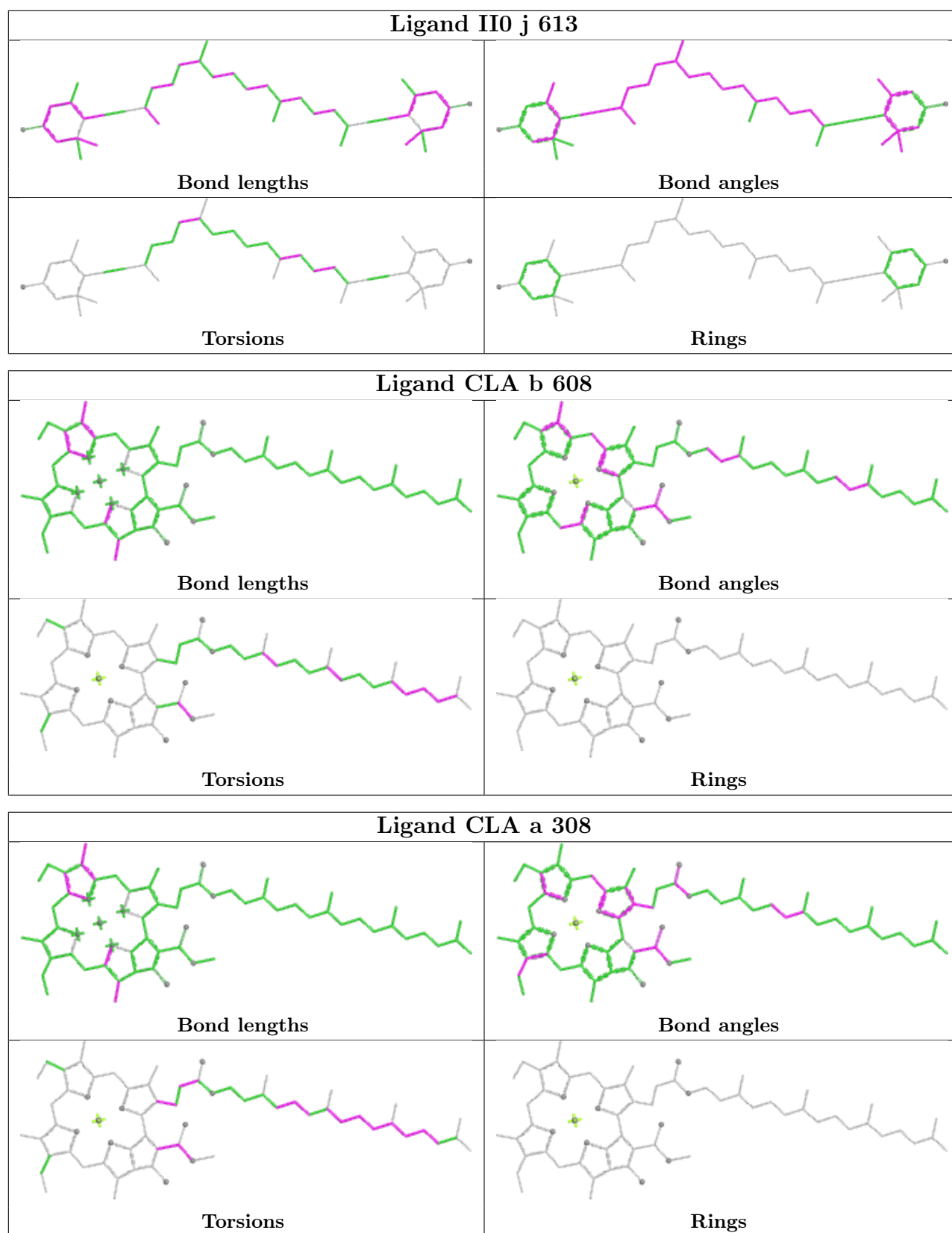




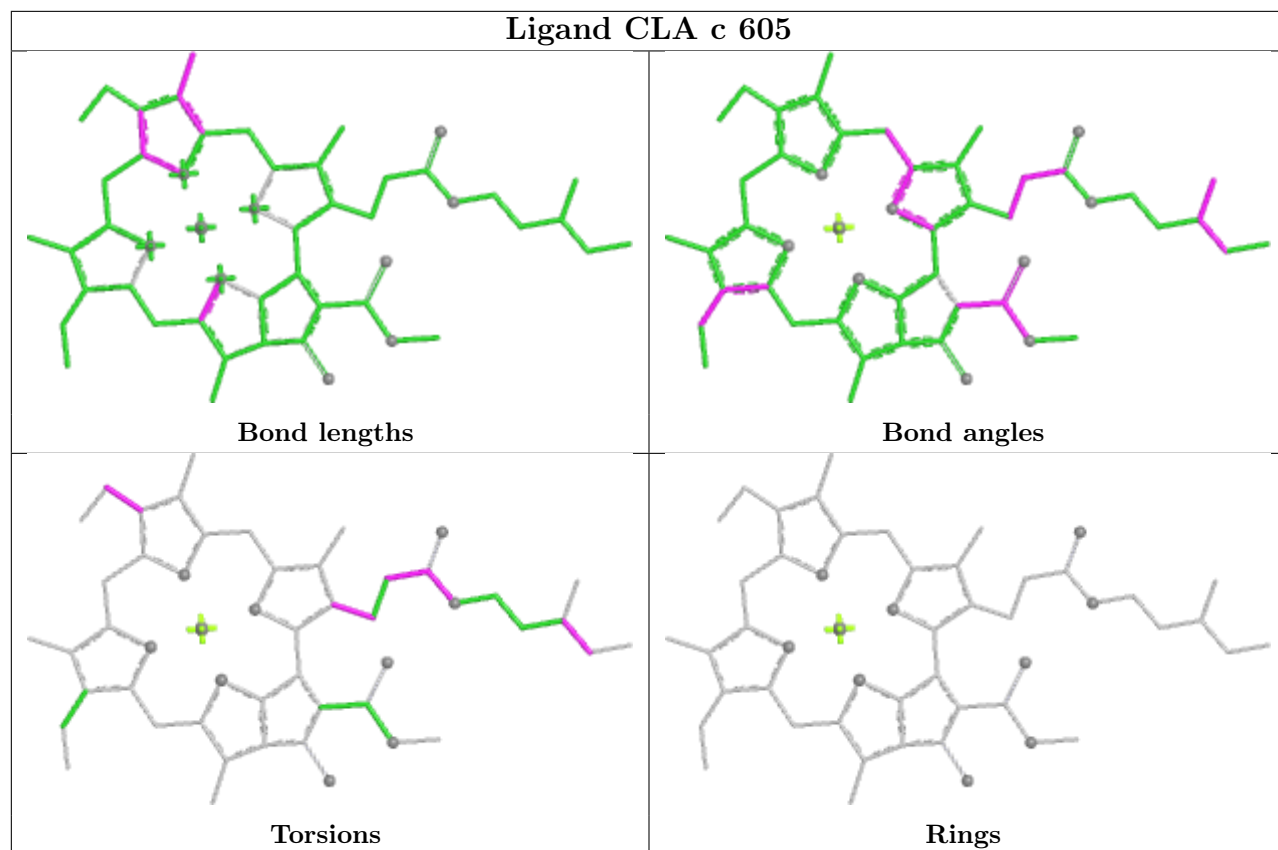




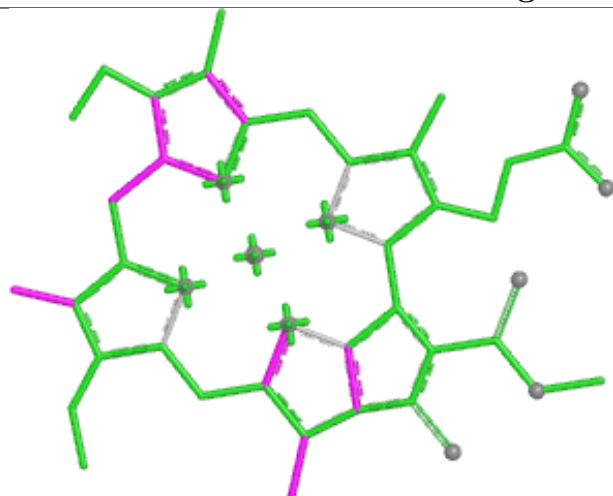
Ligand CLA F 201**Ligand CLA B 821****Ligand II0 k 316**



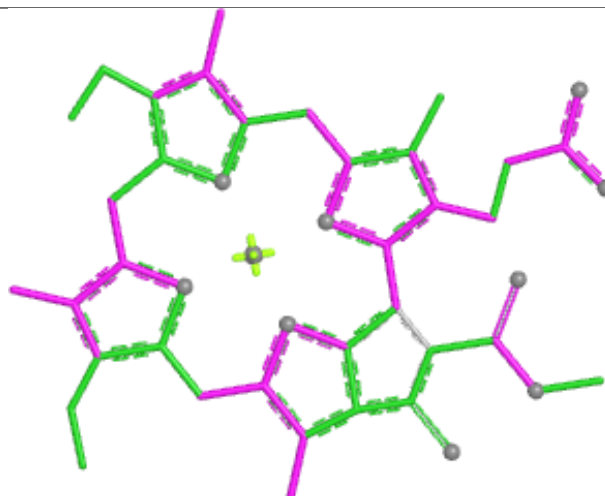
Ligand CLA c 605



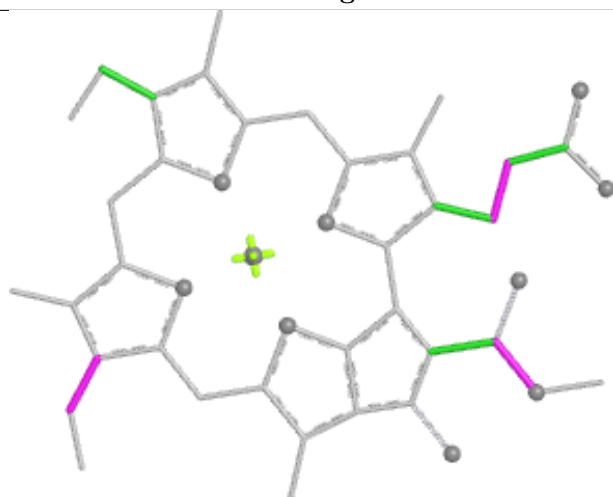
Ligand CLA k 304



Bond lengths



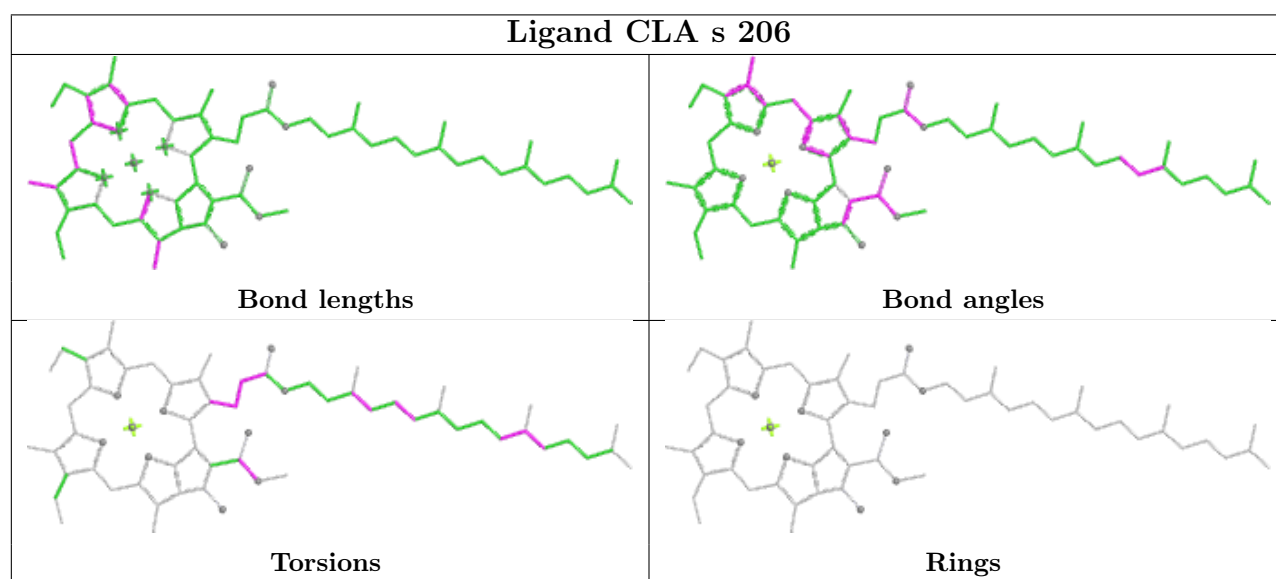
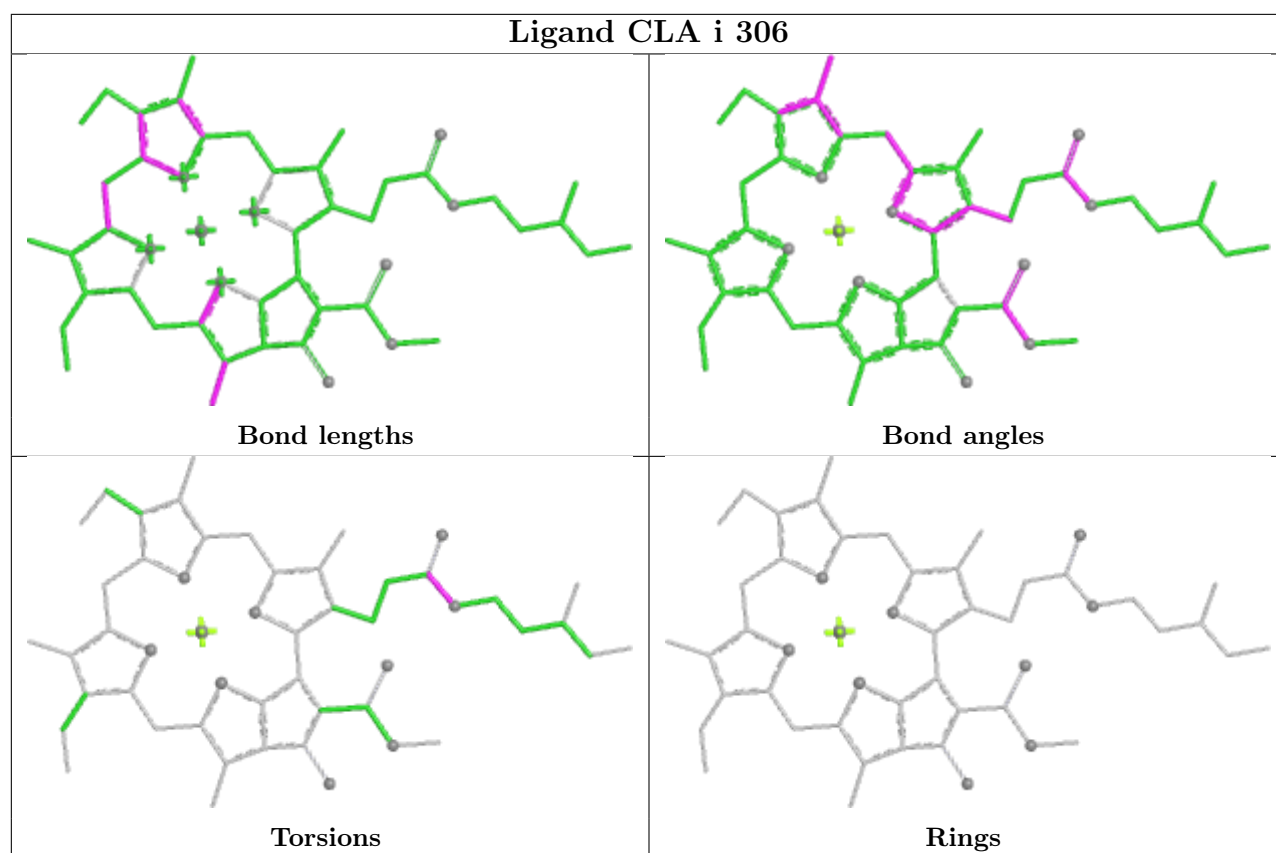
Bond angles

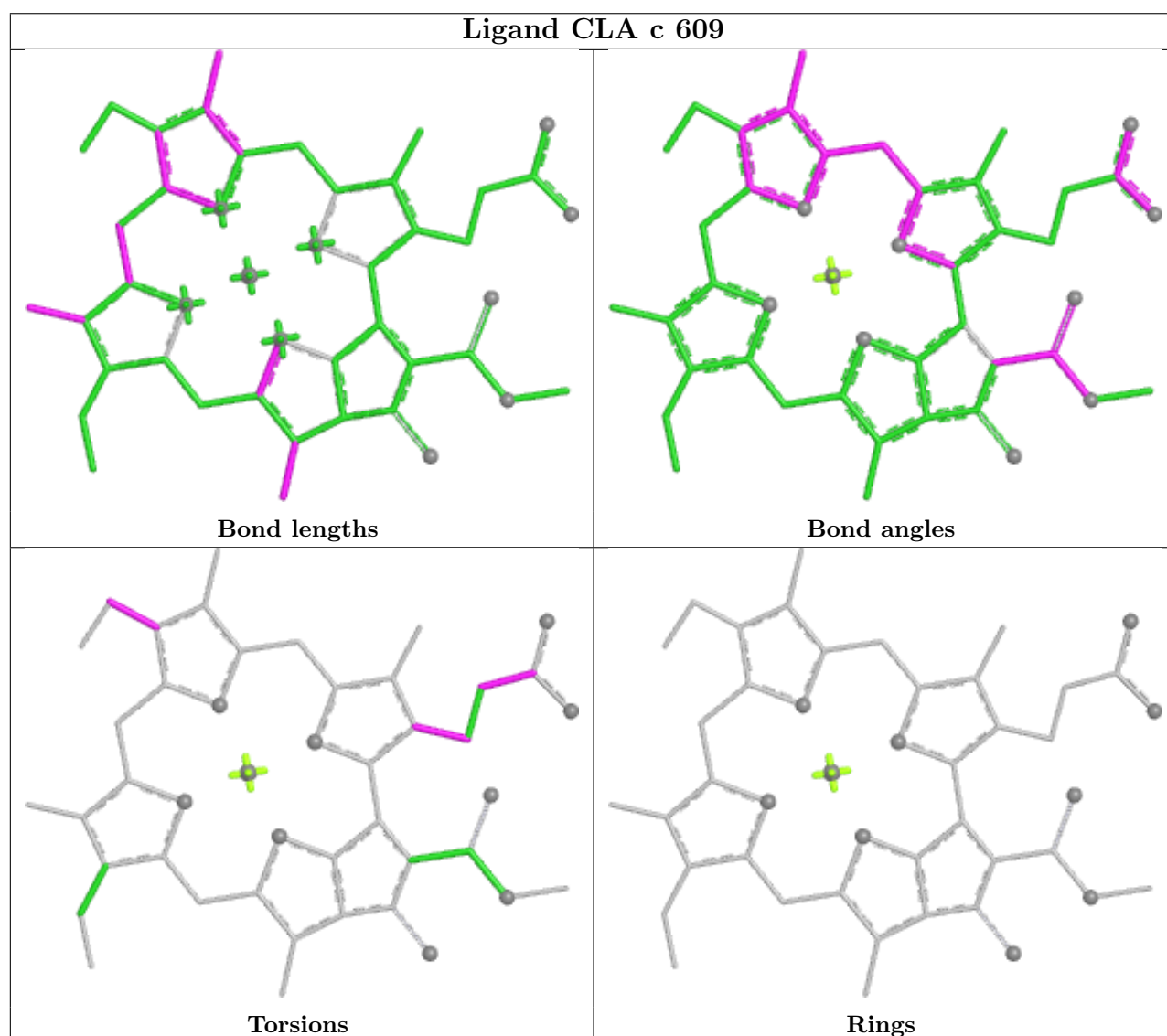
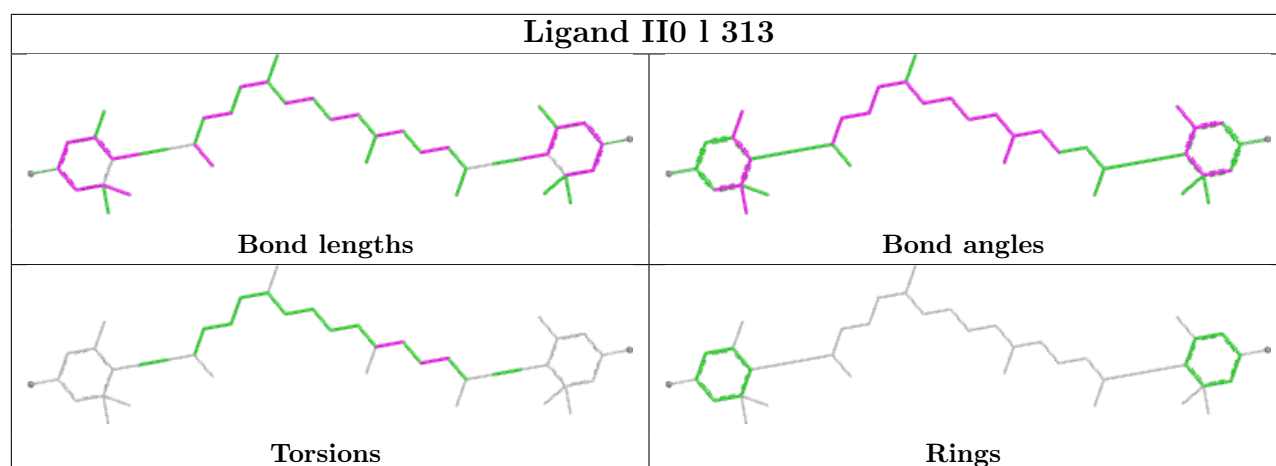


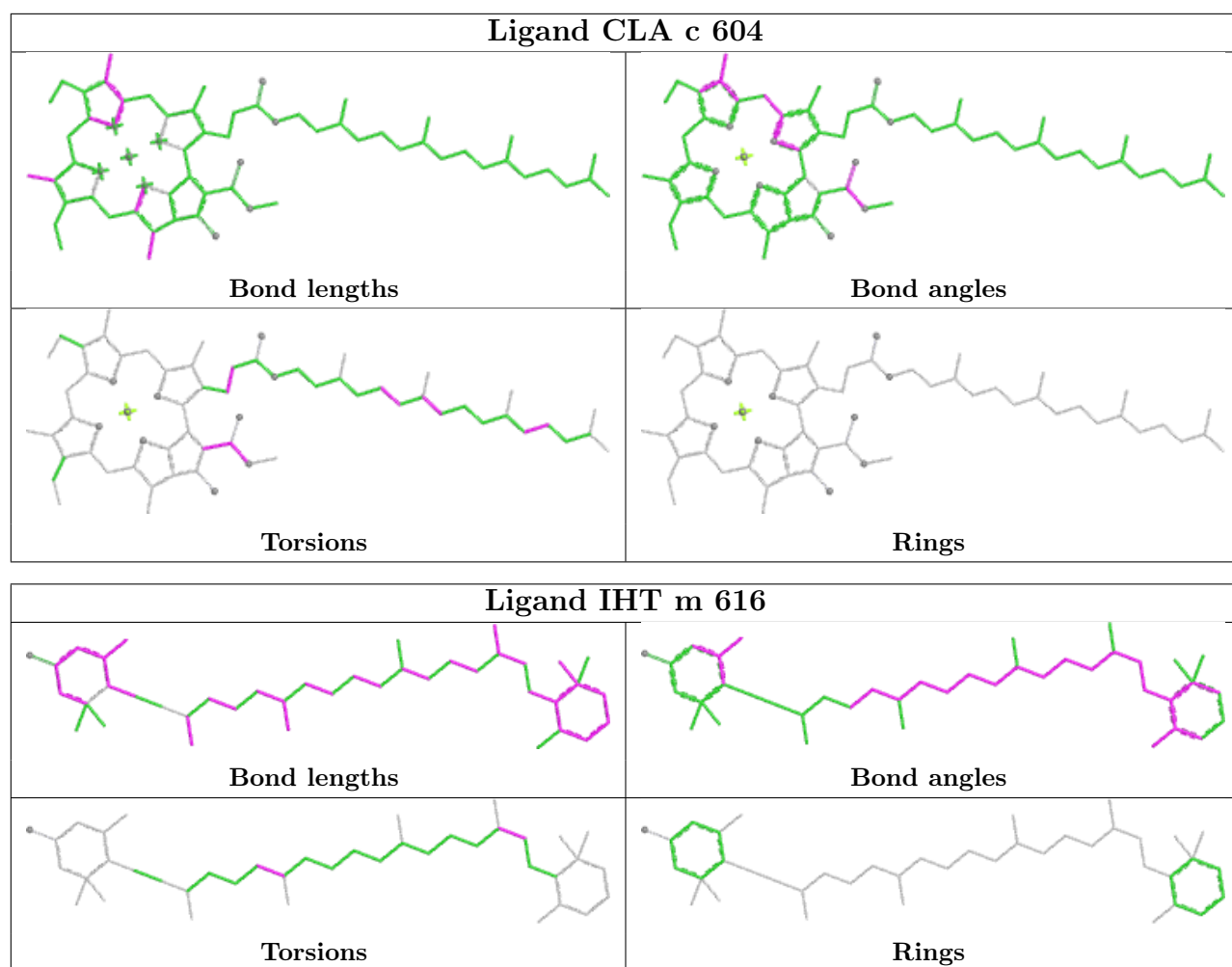
Torsions



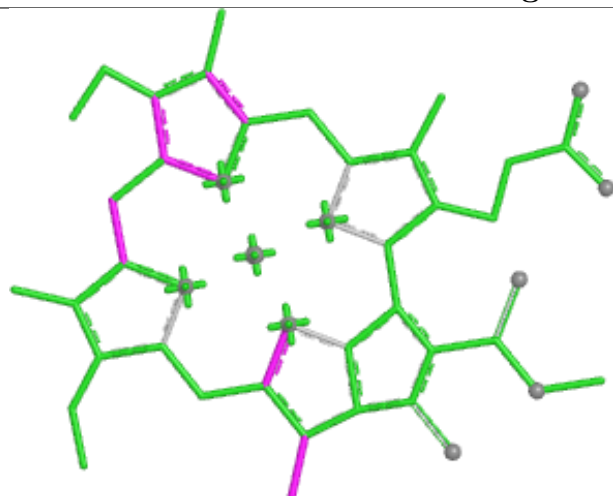
Rings



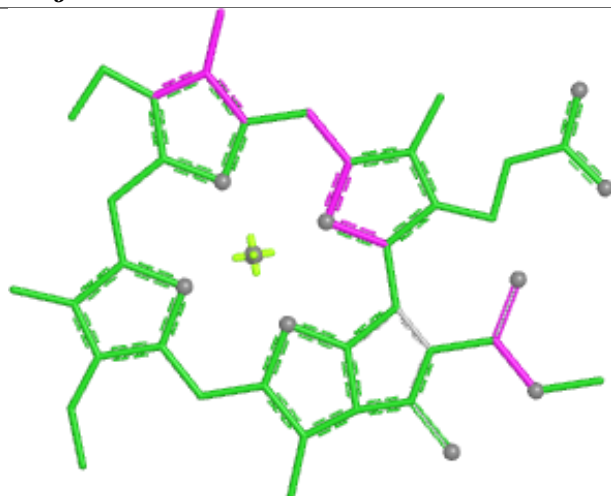




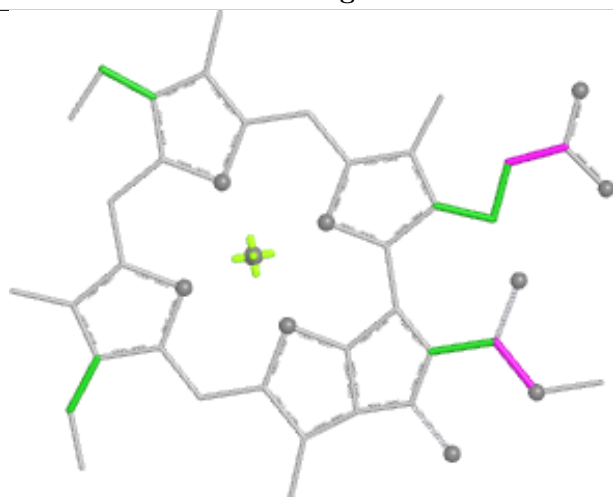
Ligand CLA j 607



Bond lengths



Bond angles

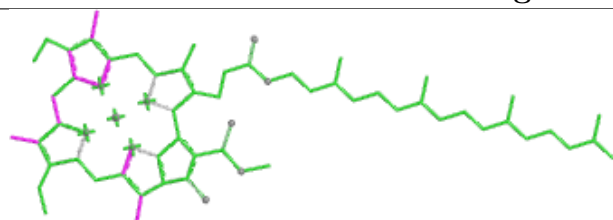


Torsions

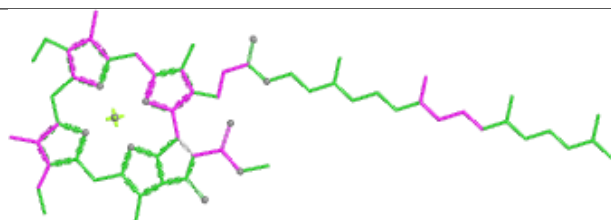


Rings

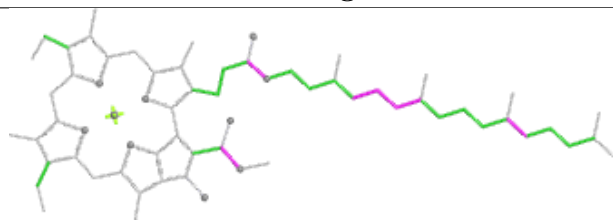
Ligand CLA A 826



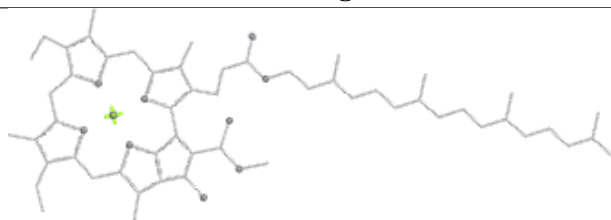
Bond lengths



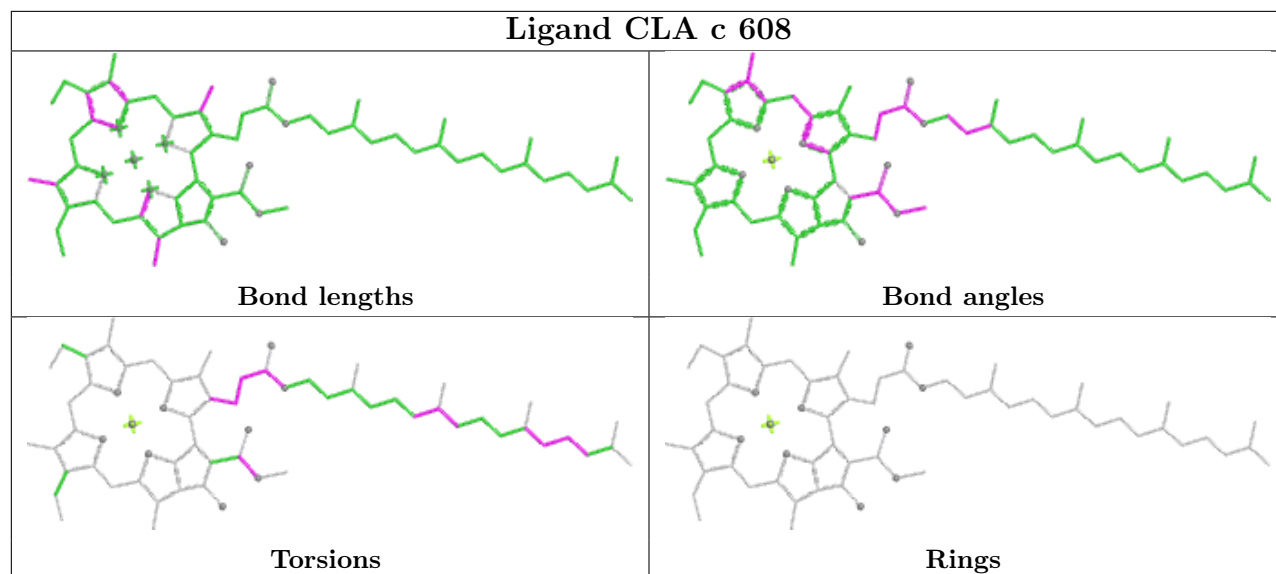
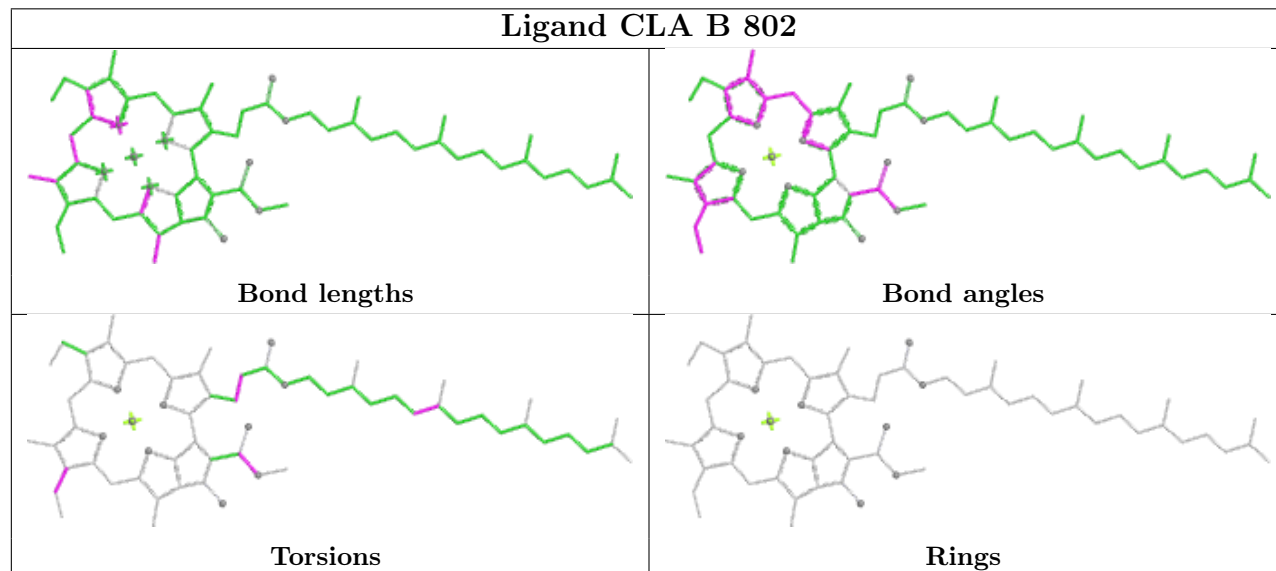
Bond angles

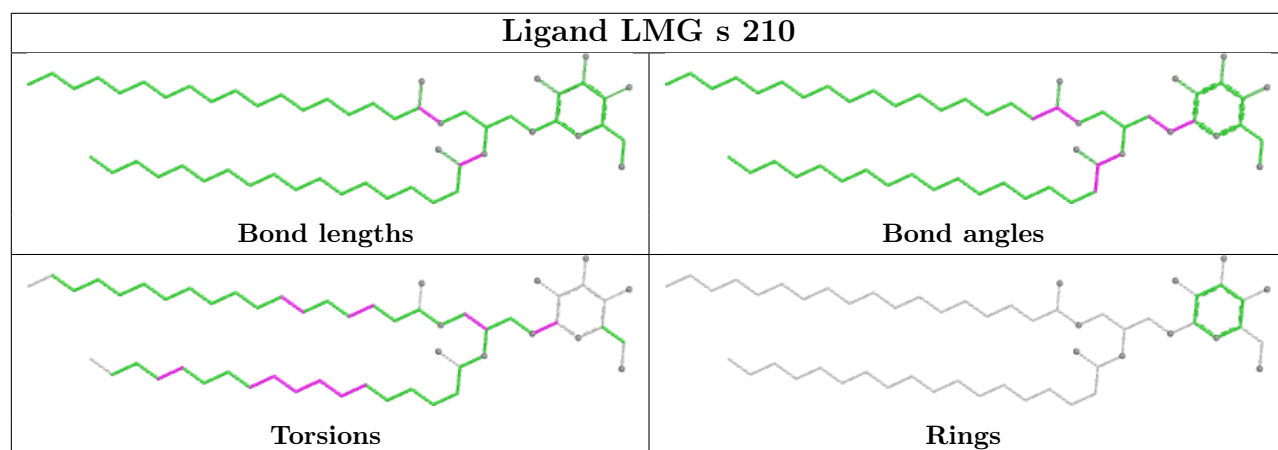
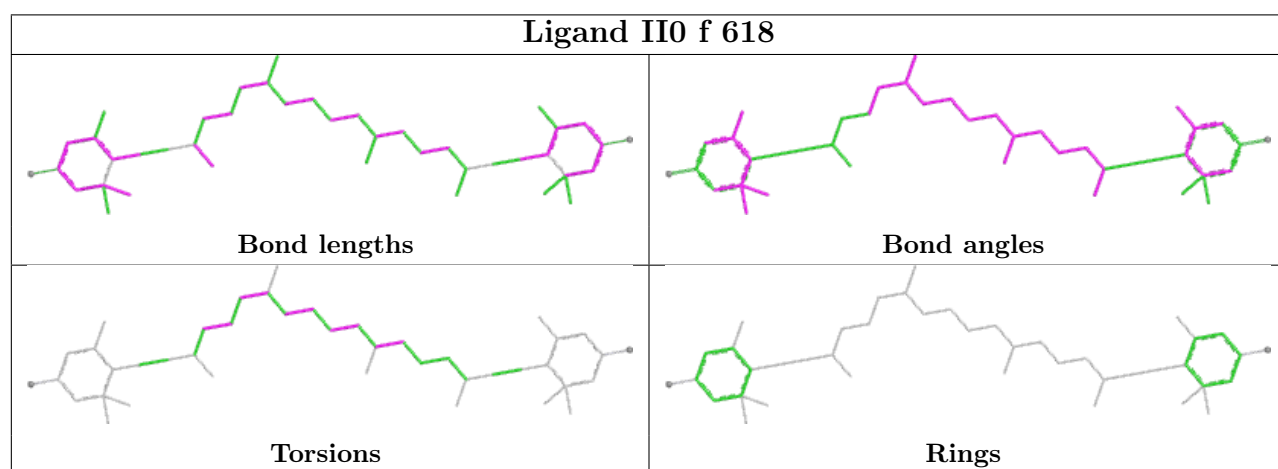
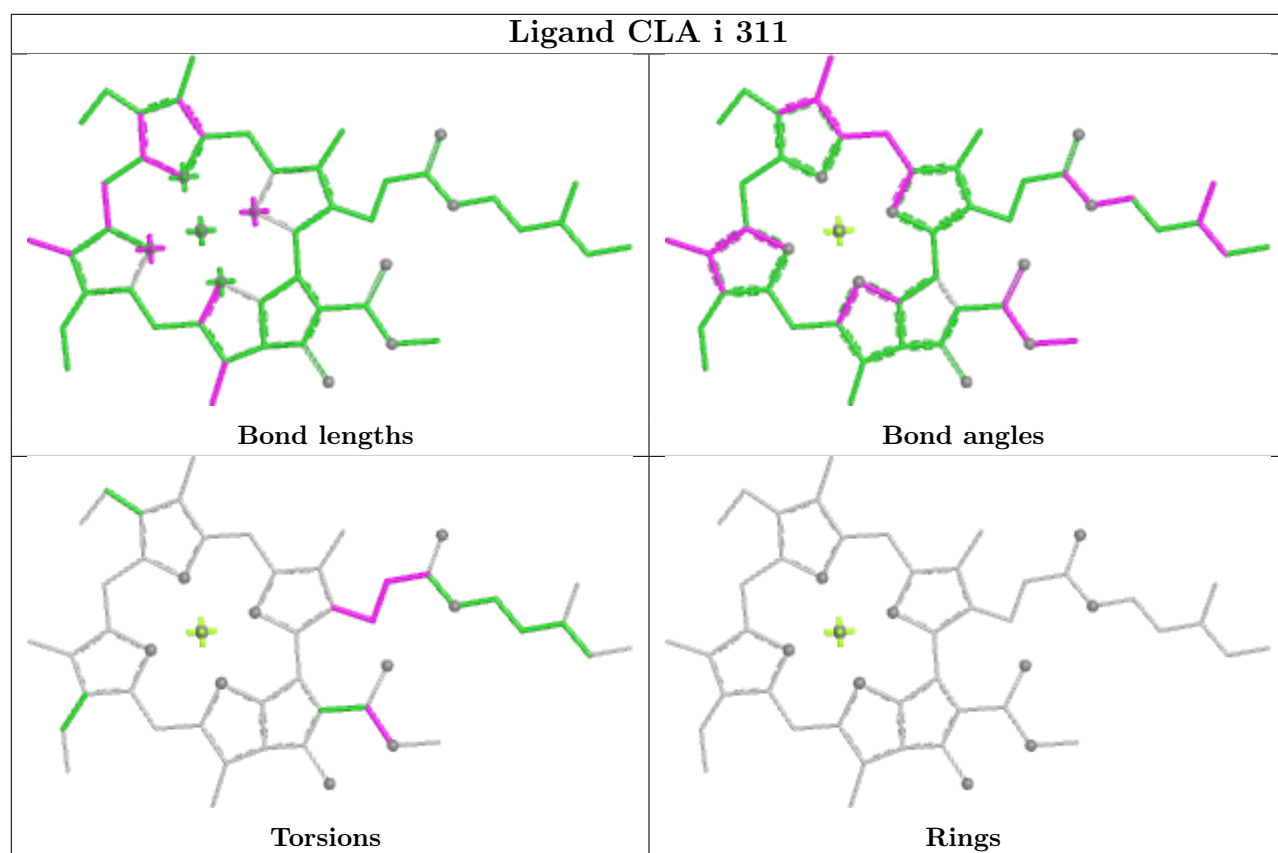


Torsions

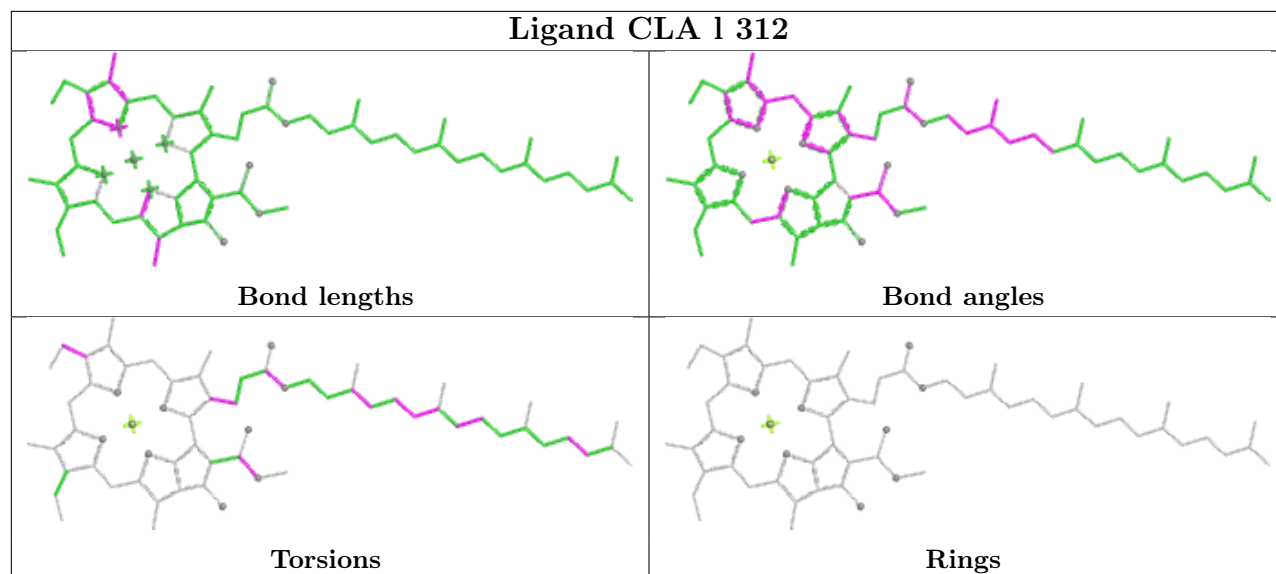


Rings

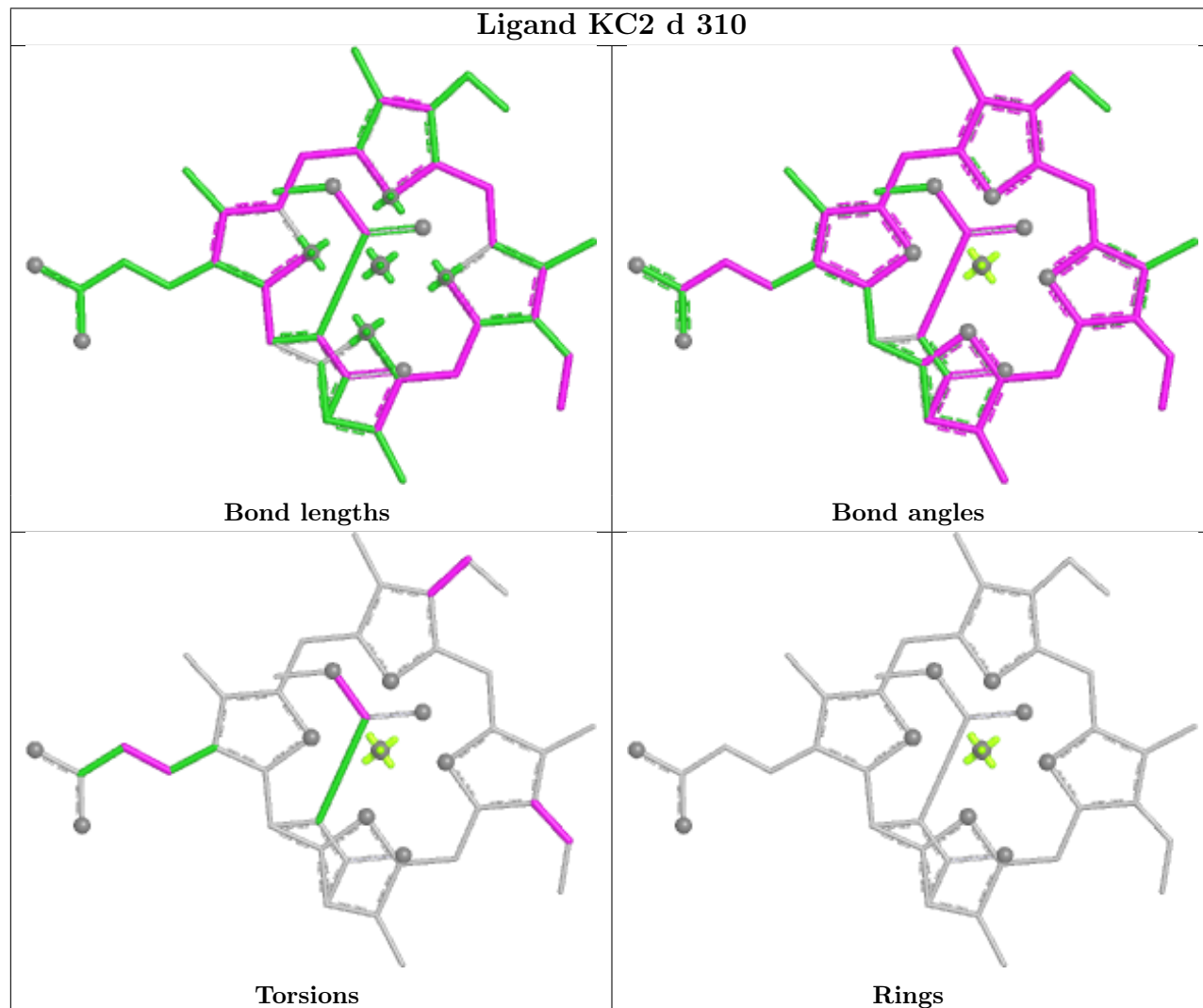
Ligand CLA c 608**Ligand CLA B 802**

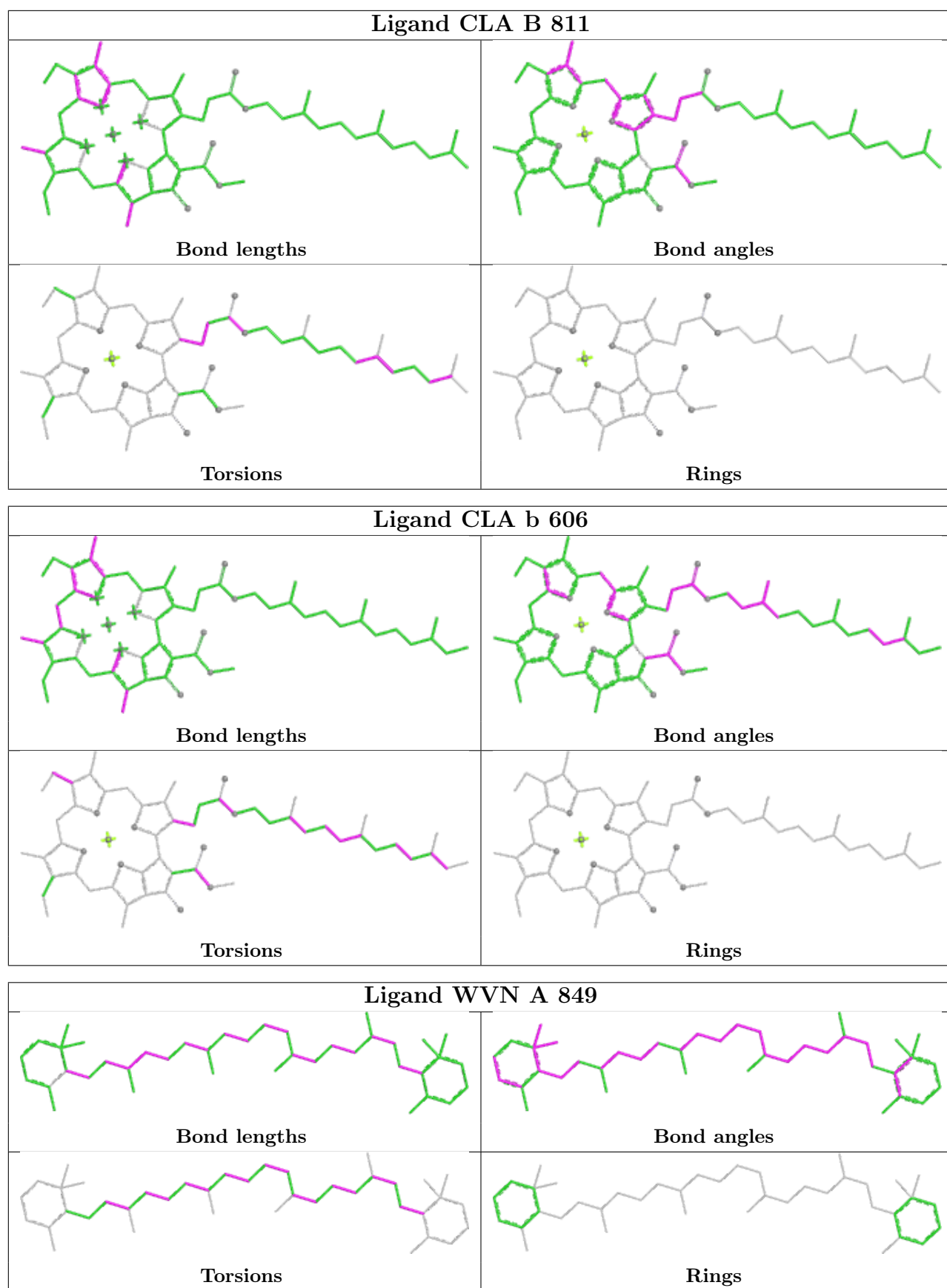


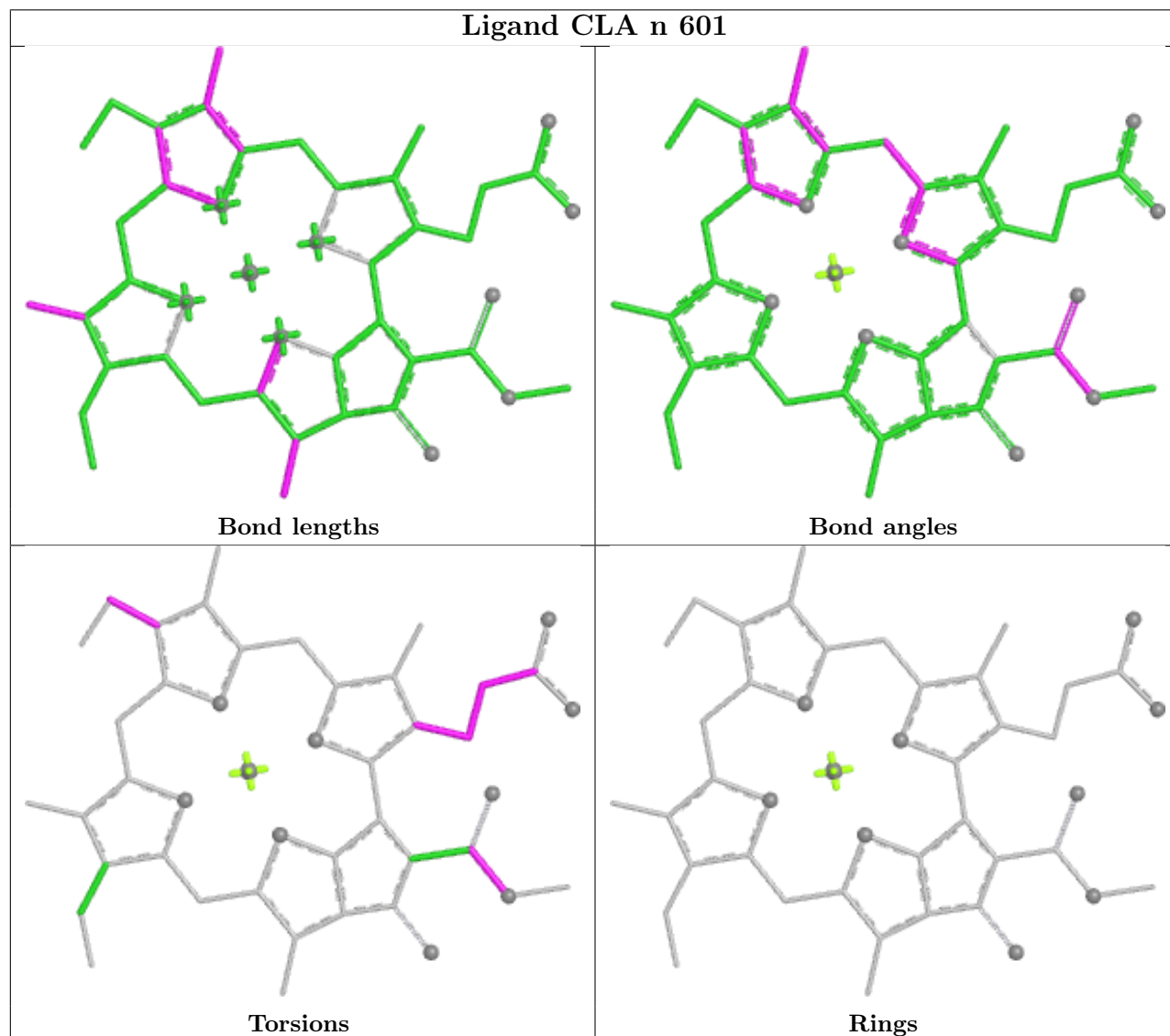
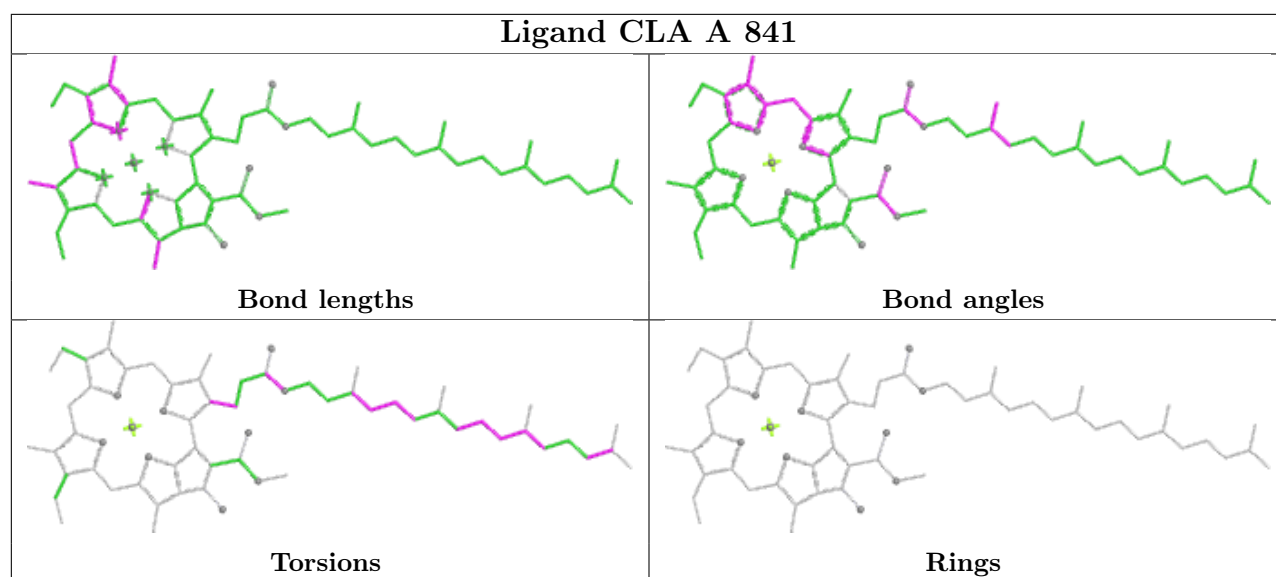
Ligand CLA l 312



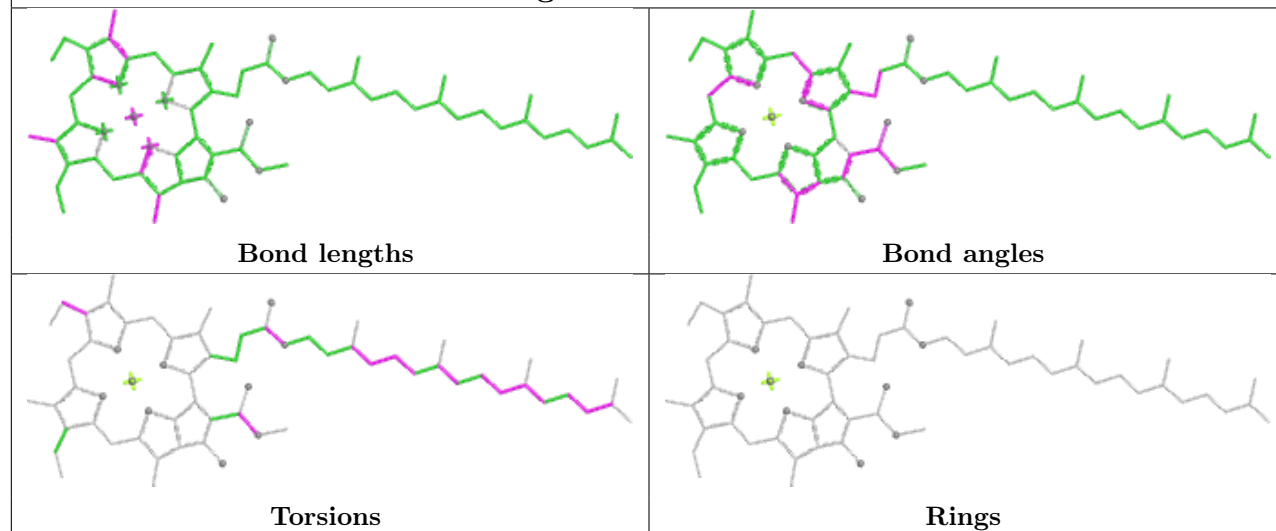
Ligand KC2 d 310



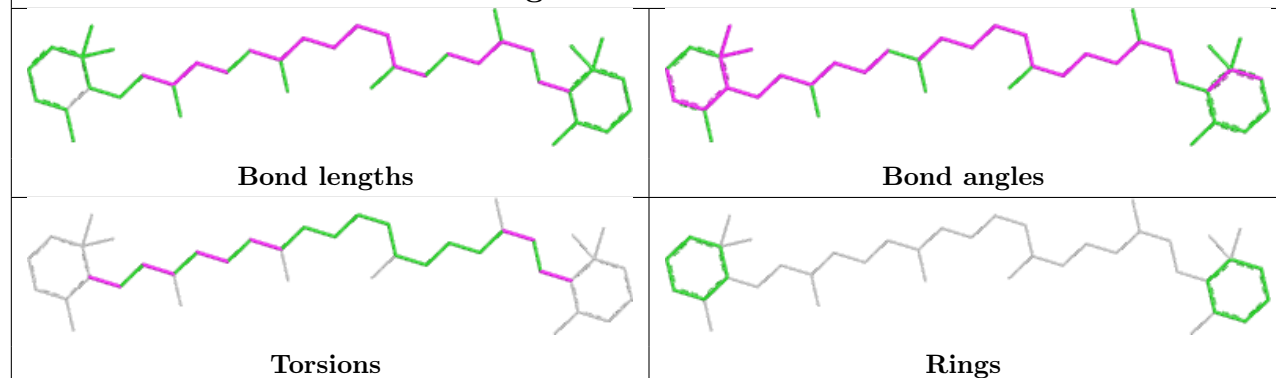




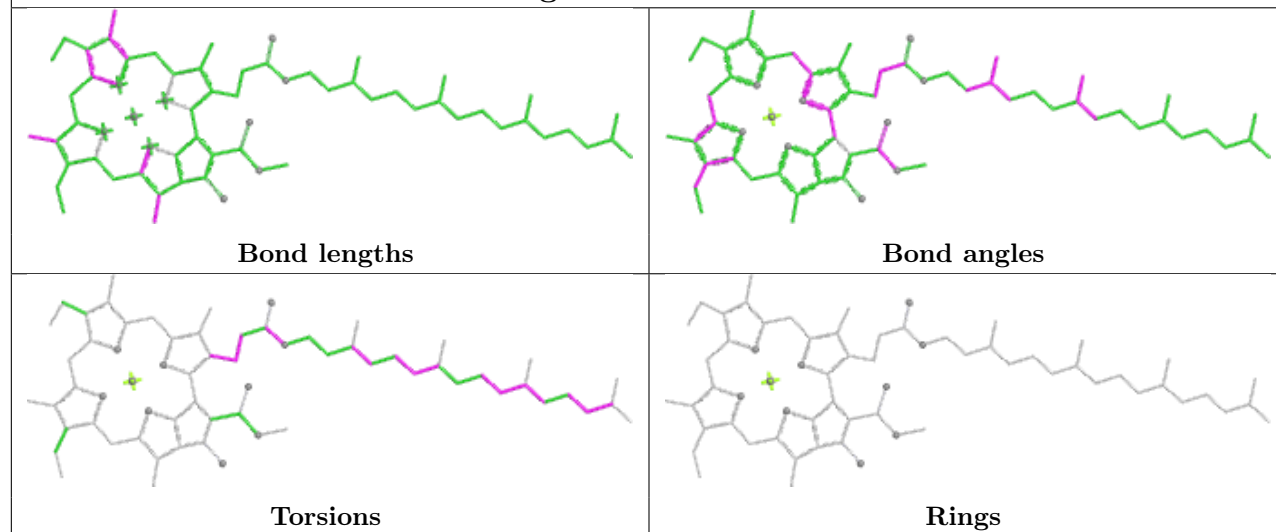
Ligand CLA e 605

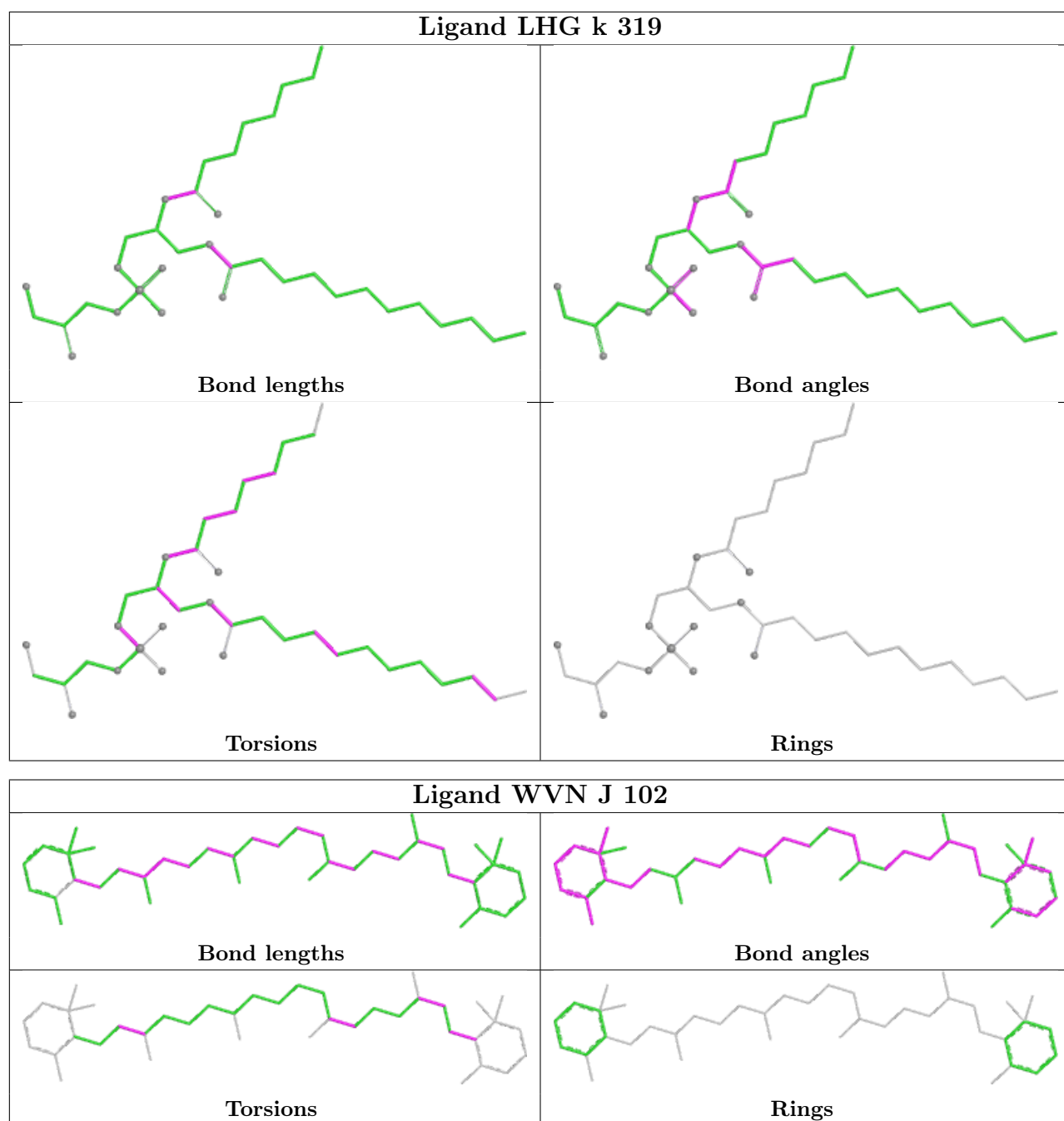


Ligand WVN L 201

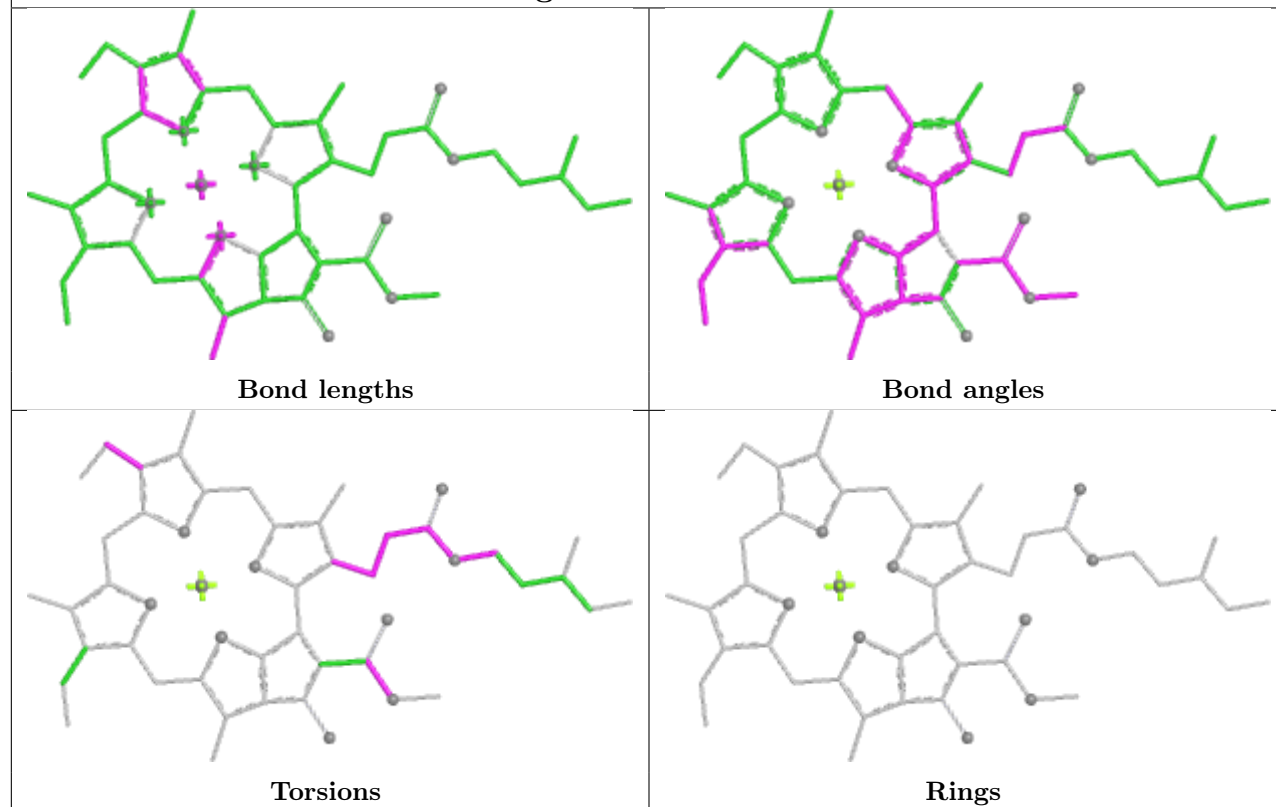


Ligand CLA f 607

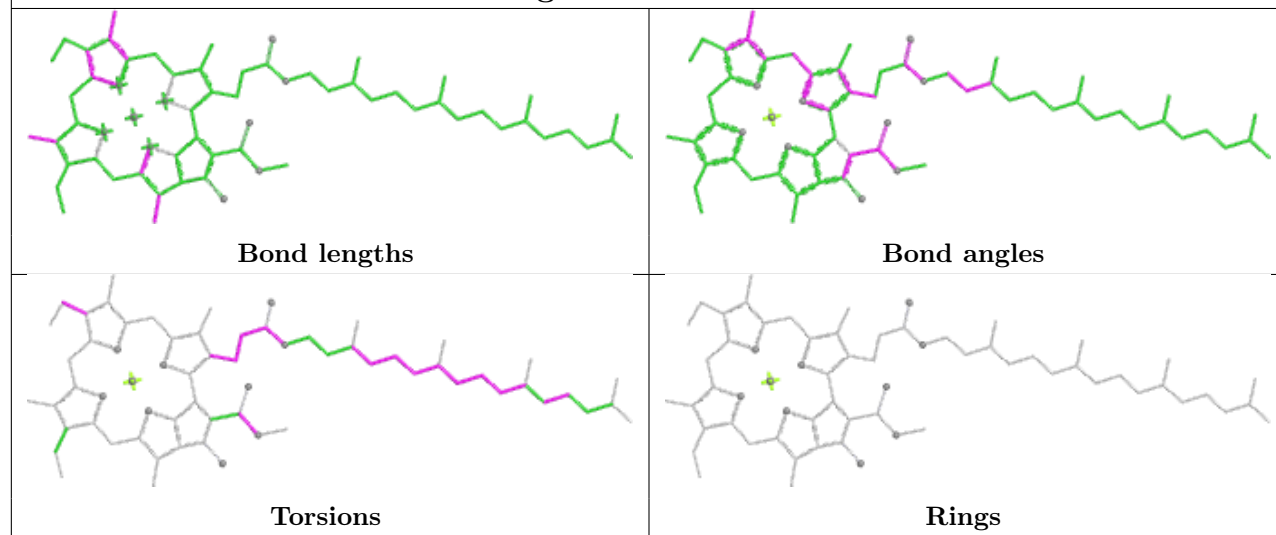


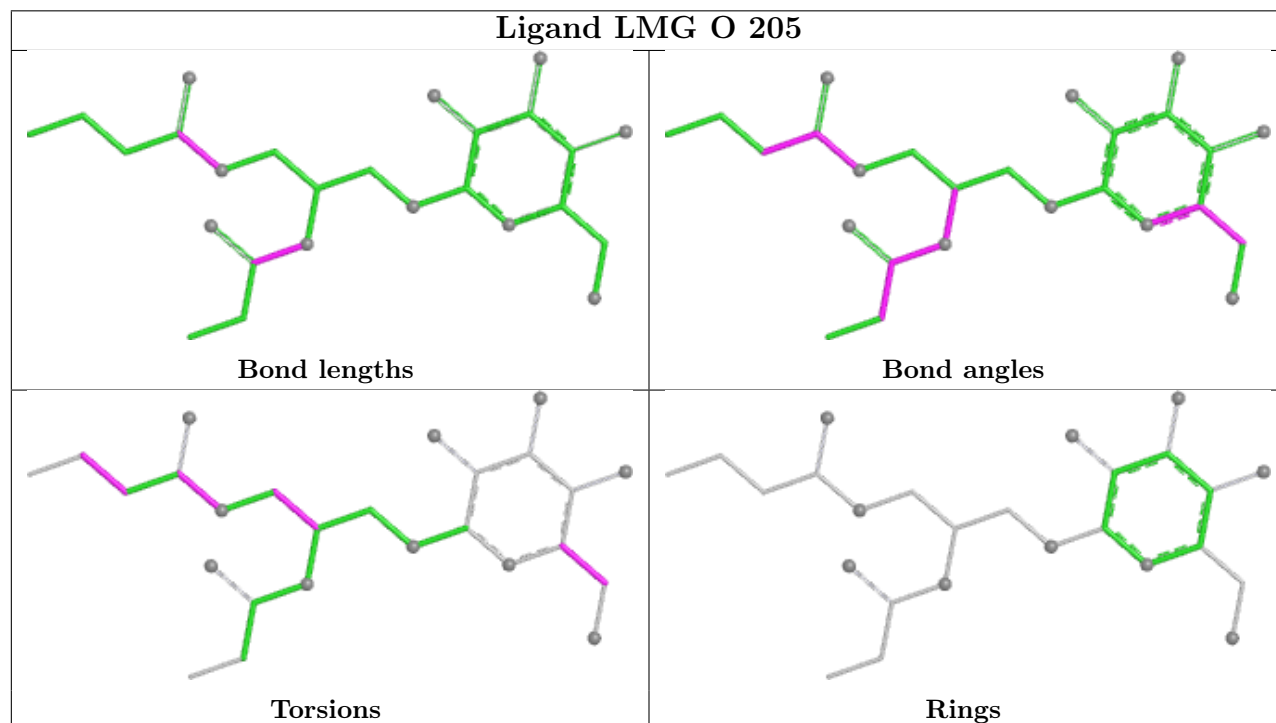
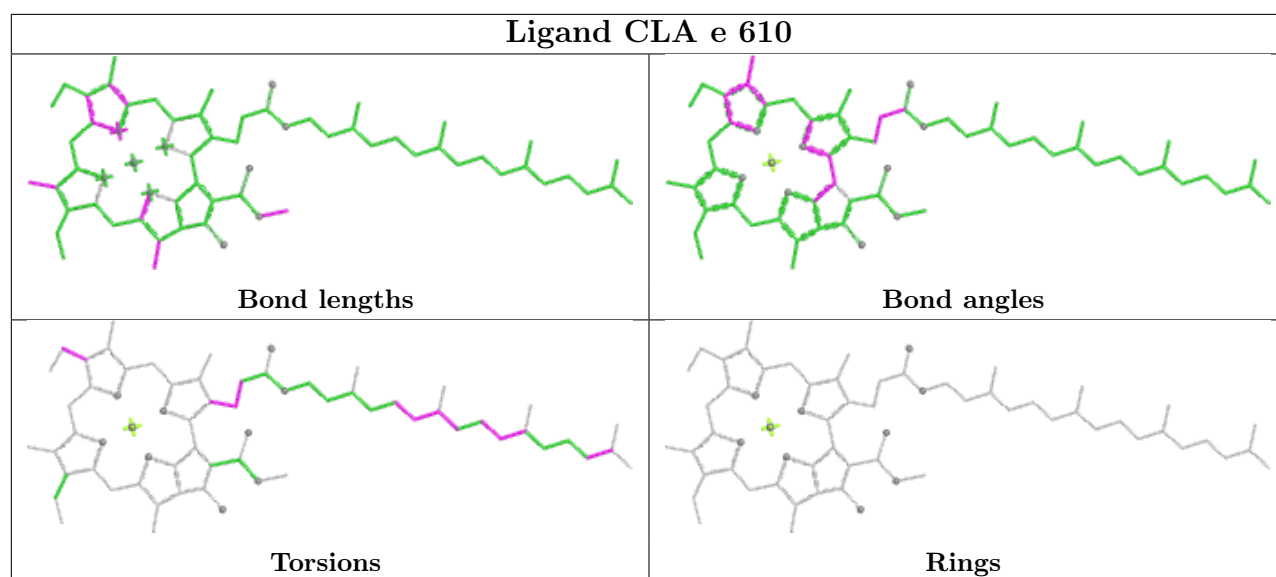


Ligand CLA k 309

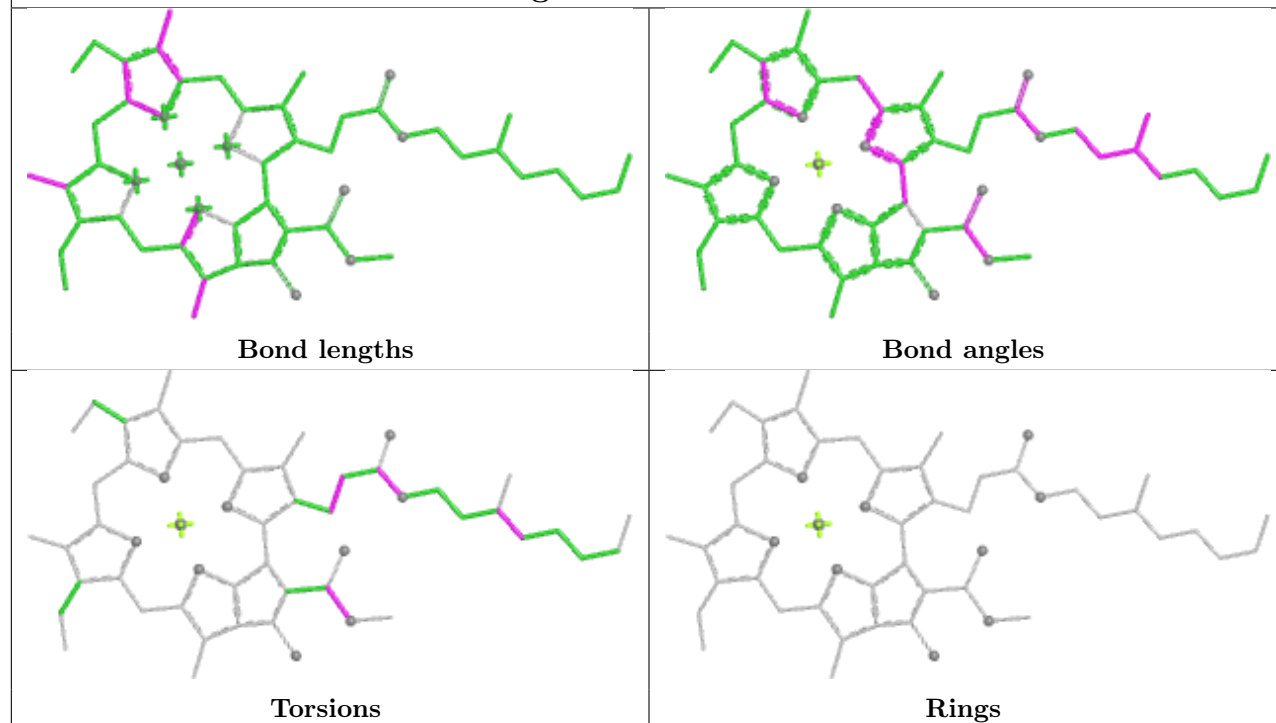


Ligand CLA e 604

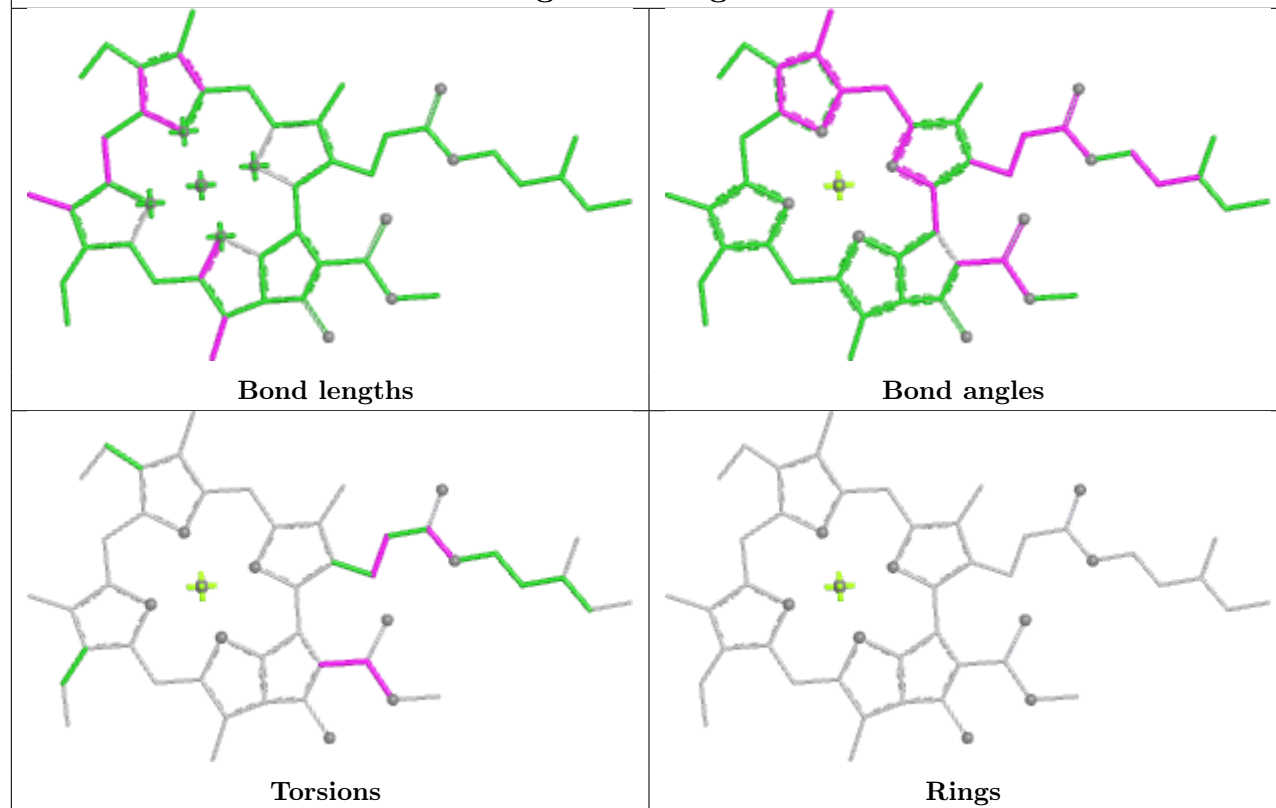




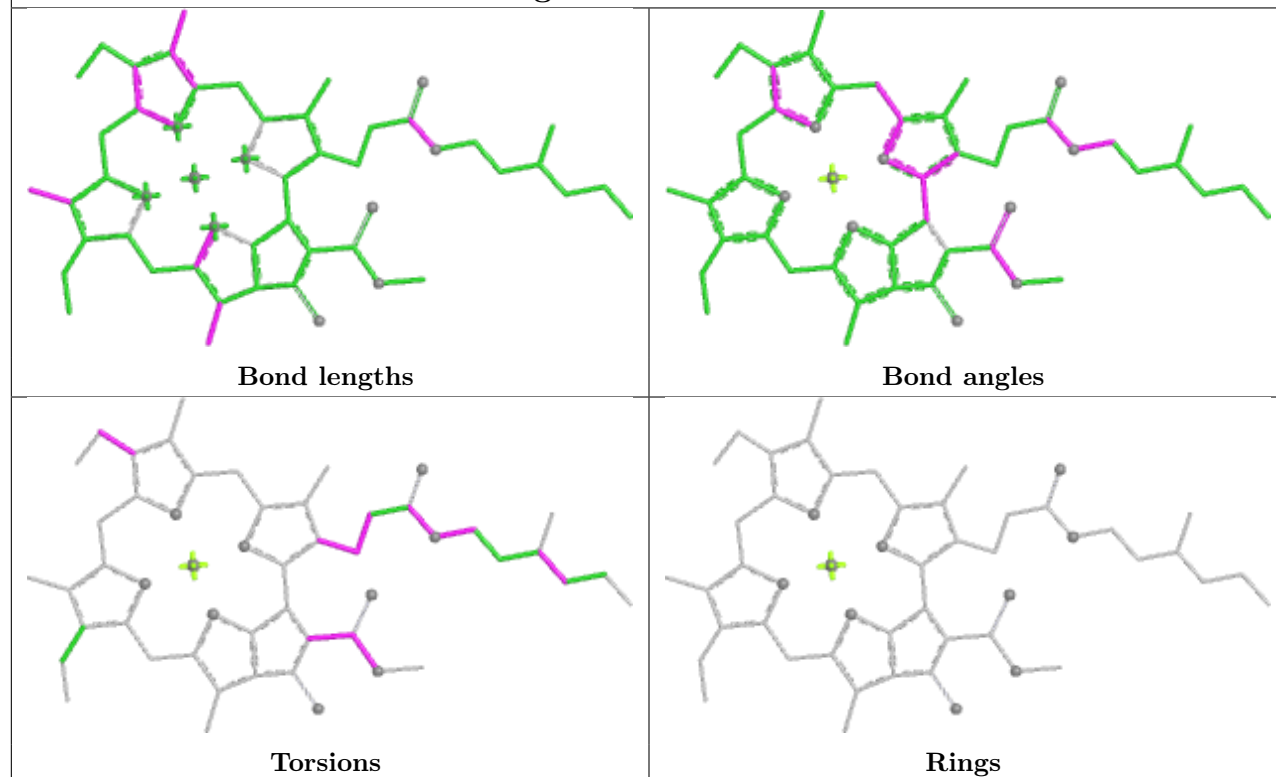
Ligand CLA A 811



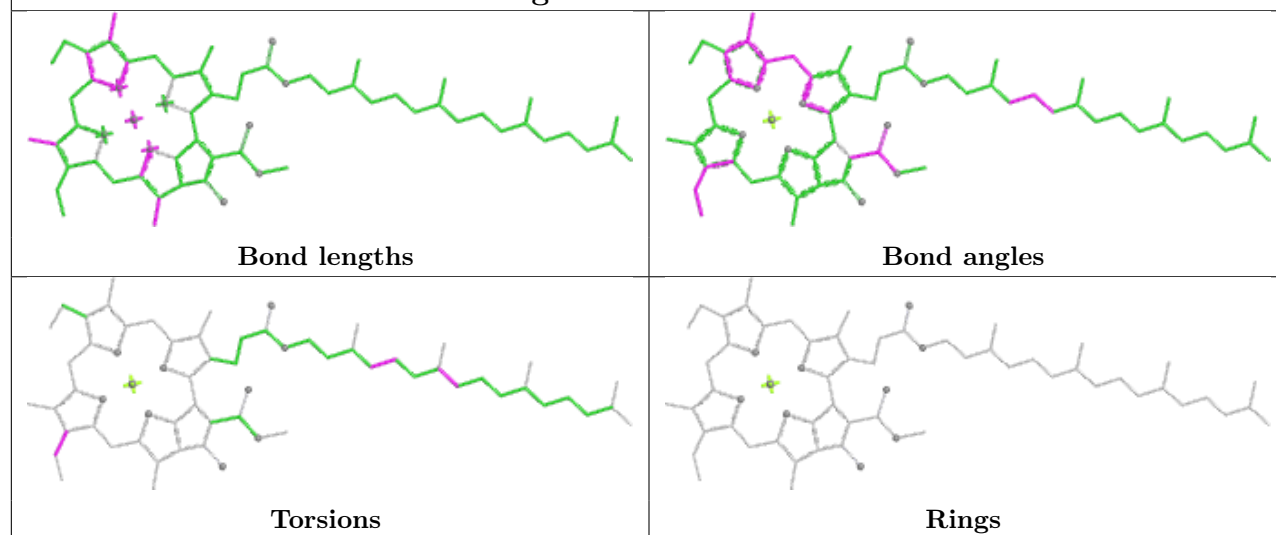
Ligand CLA g 310

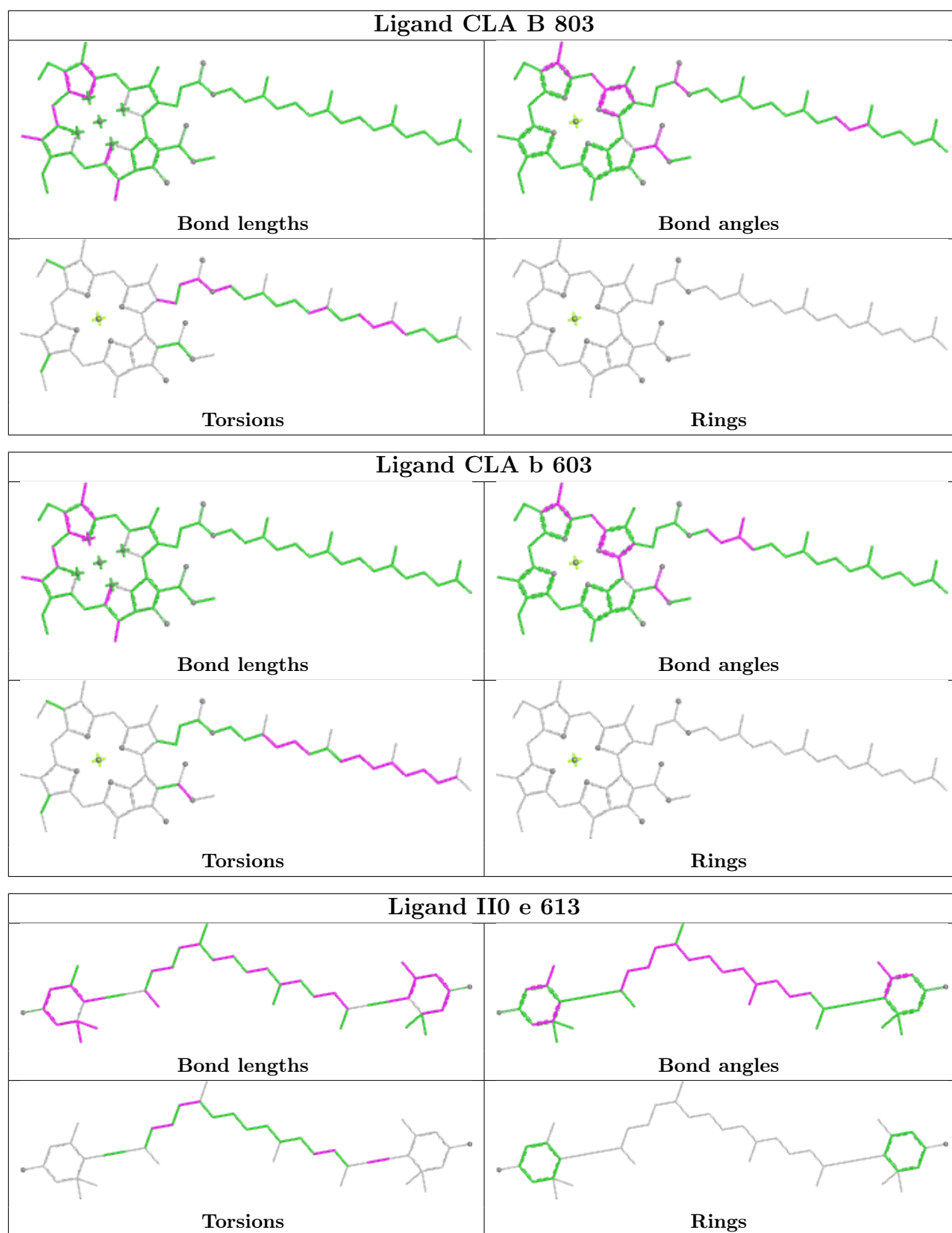


Ligand CLA F 203

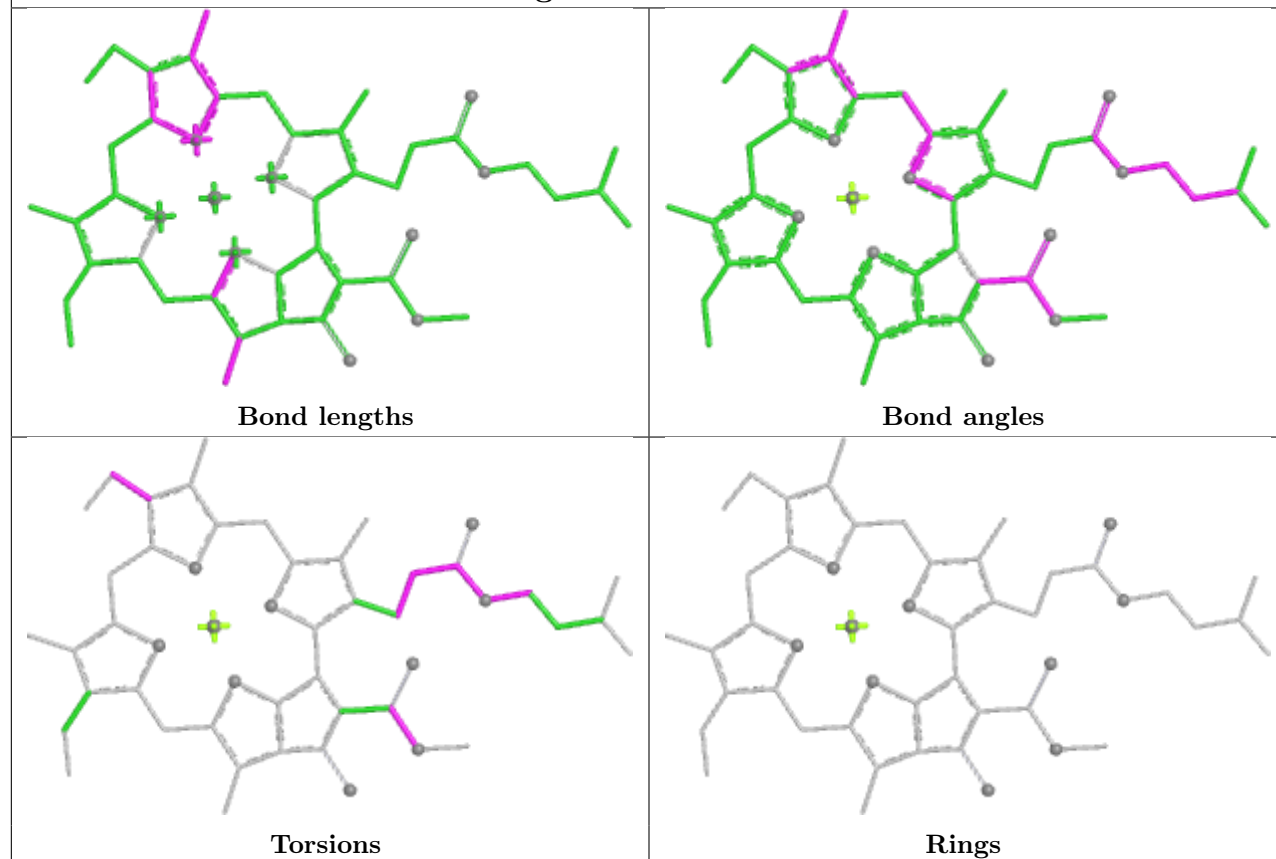


Ligand CLA A 820

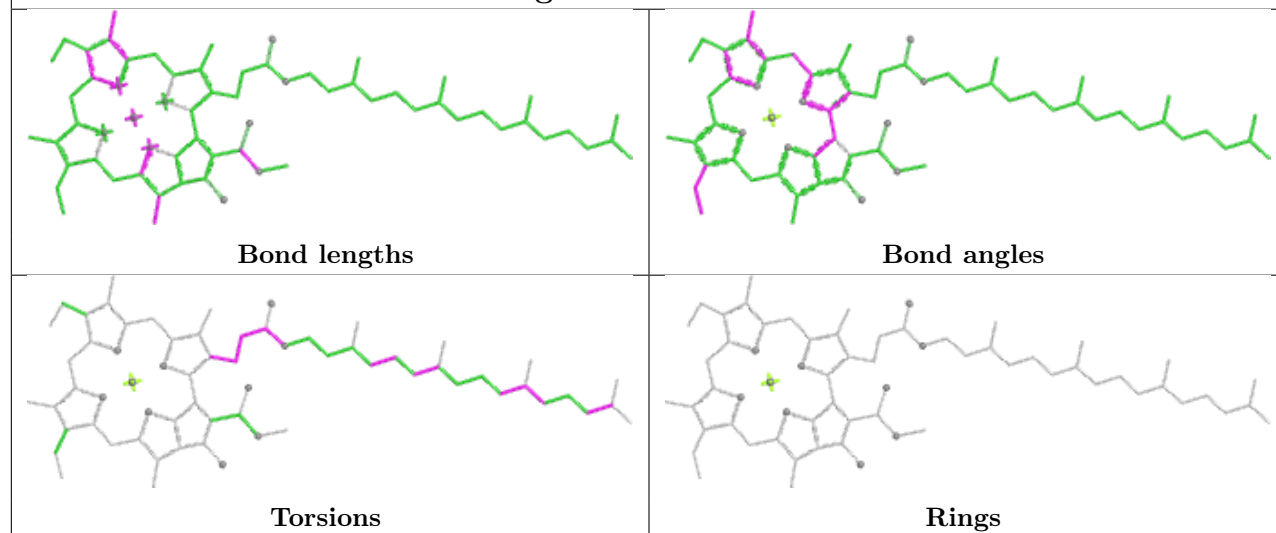




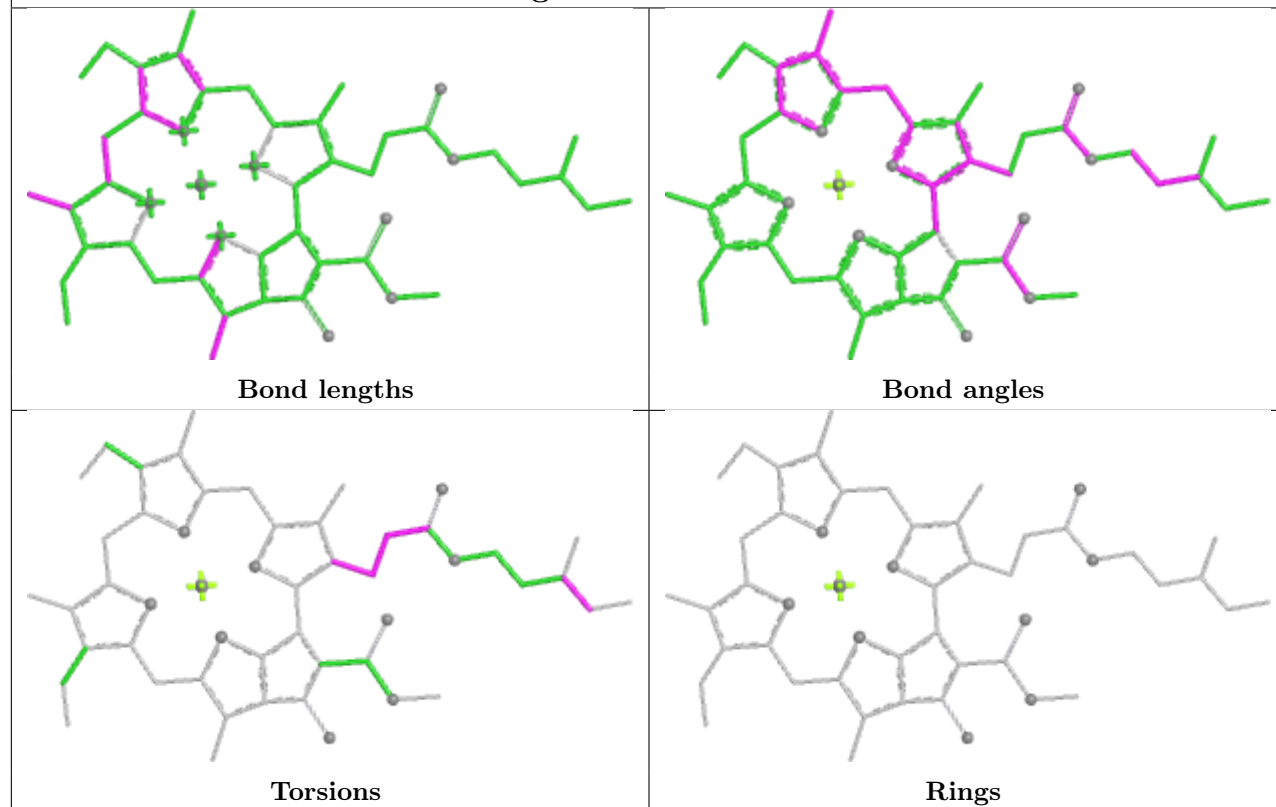
Ligand CLA h 303



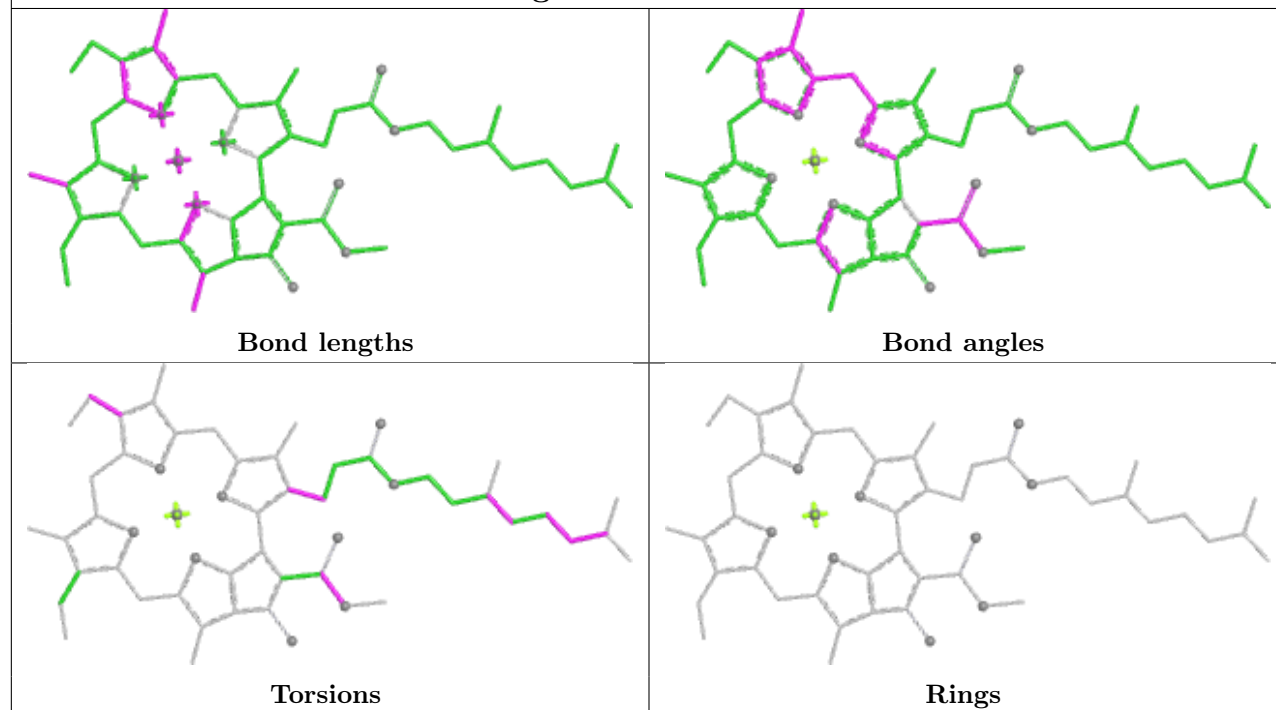
Ligand CLA n 610

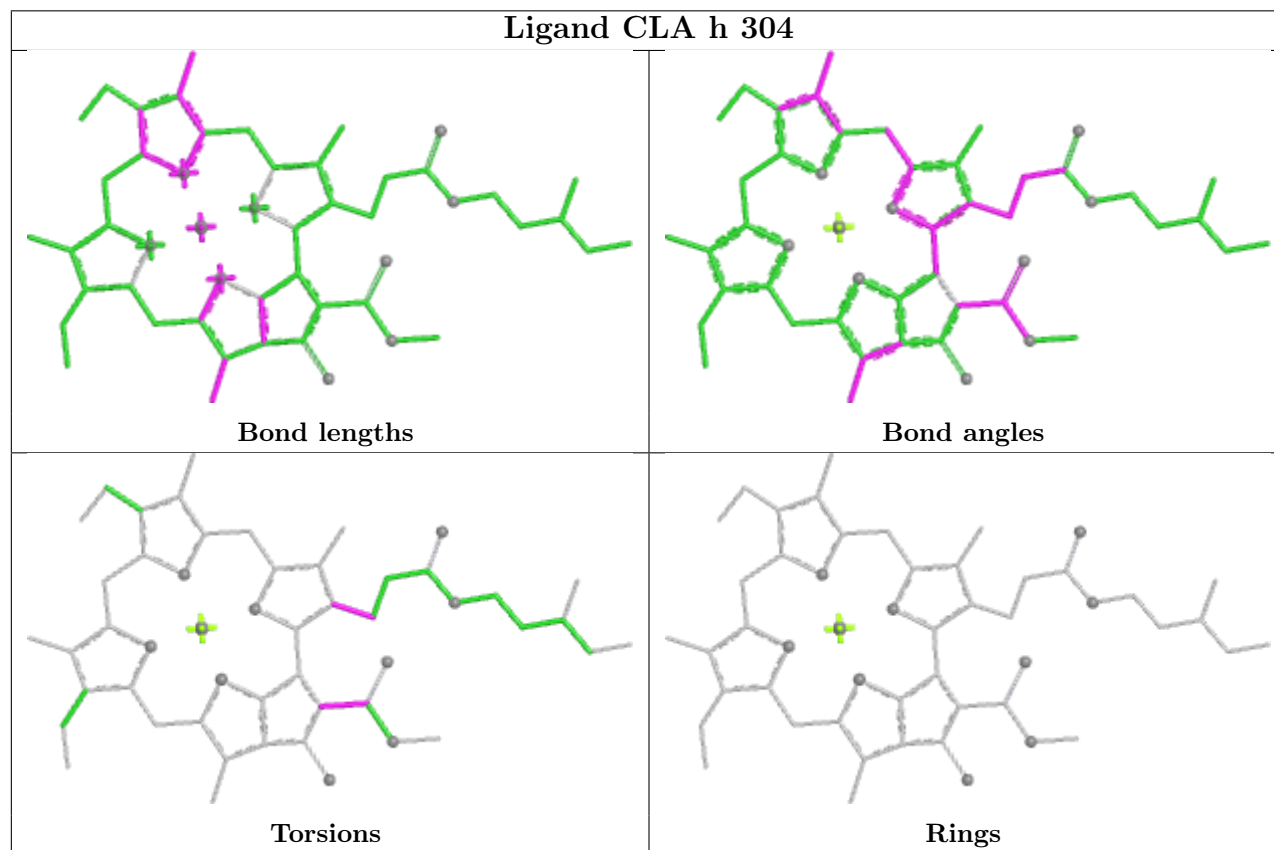
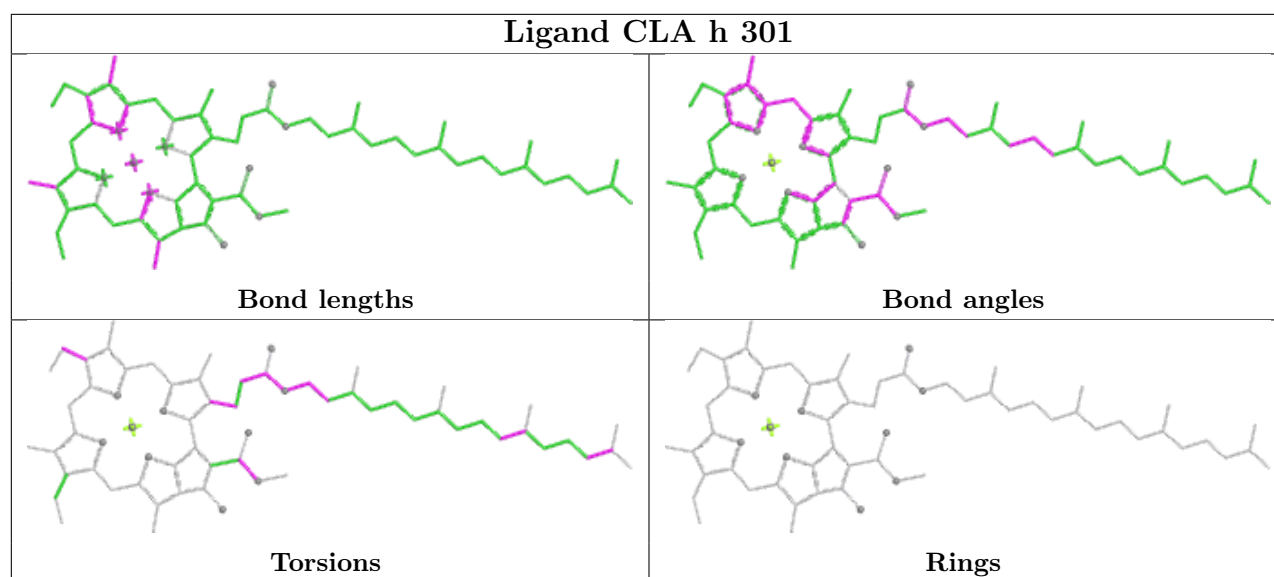


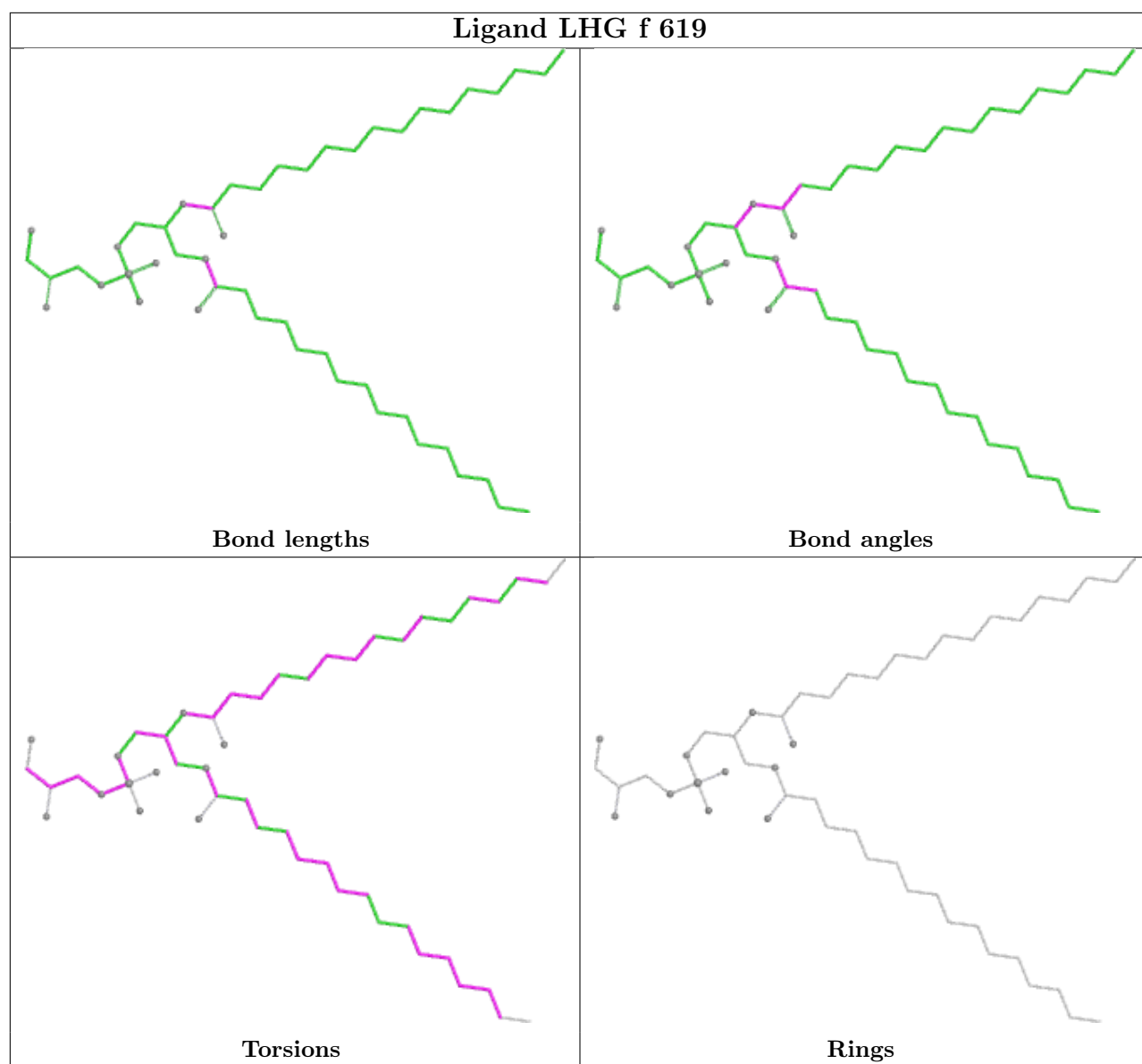
Ligand CLA R 203

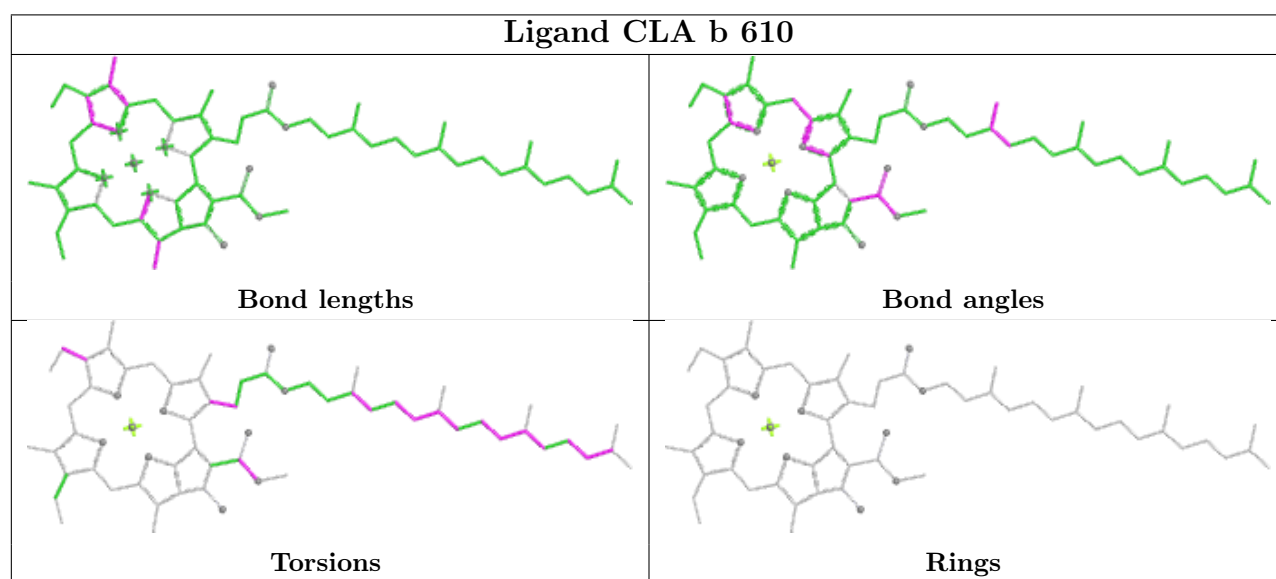
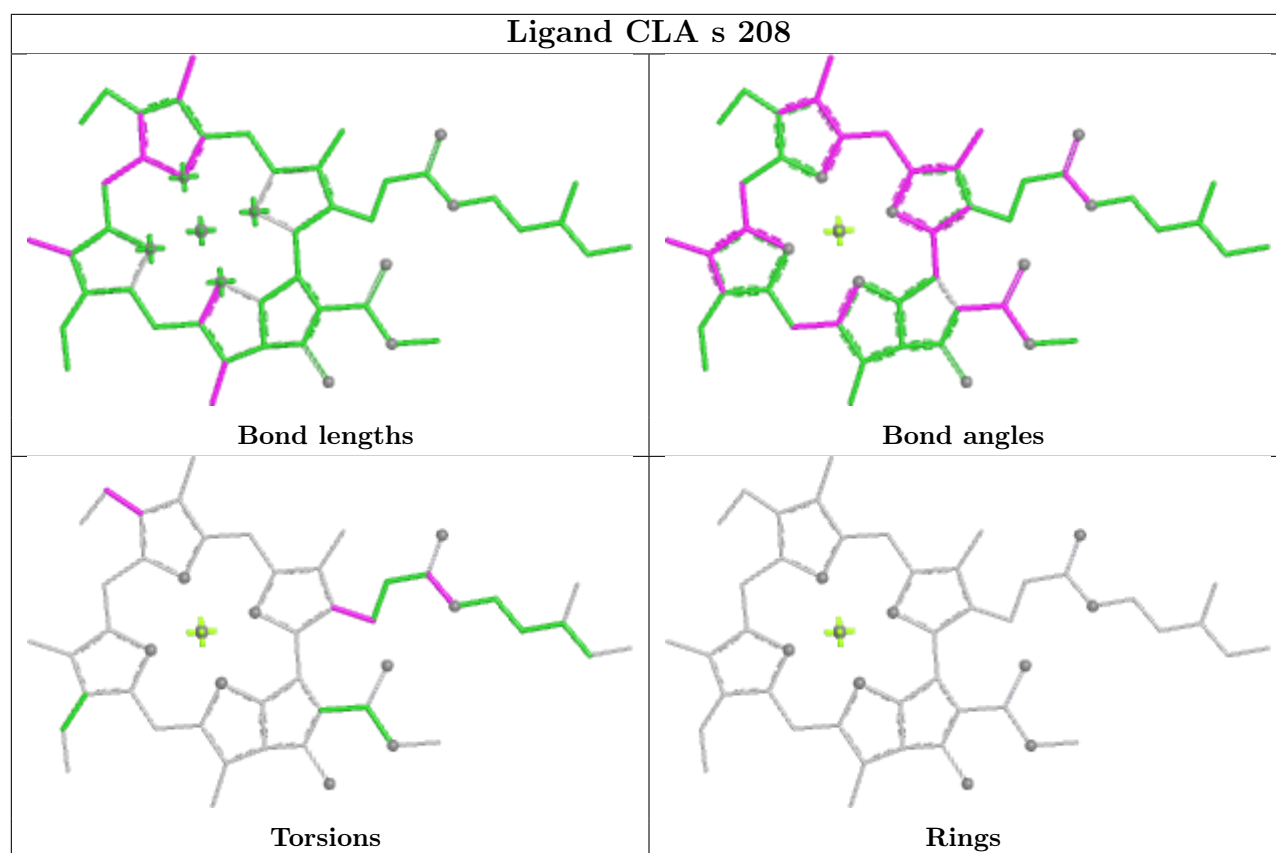


Ligand CLA B 818

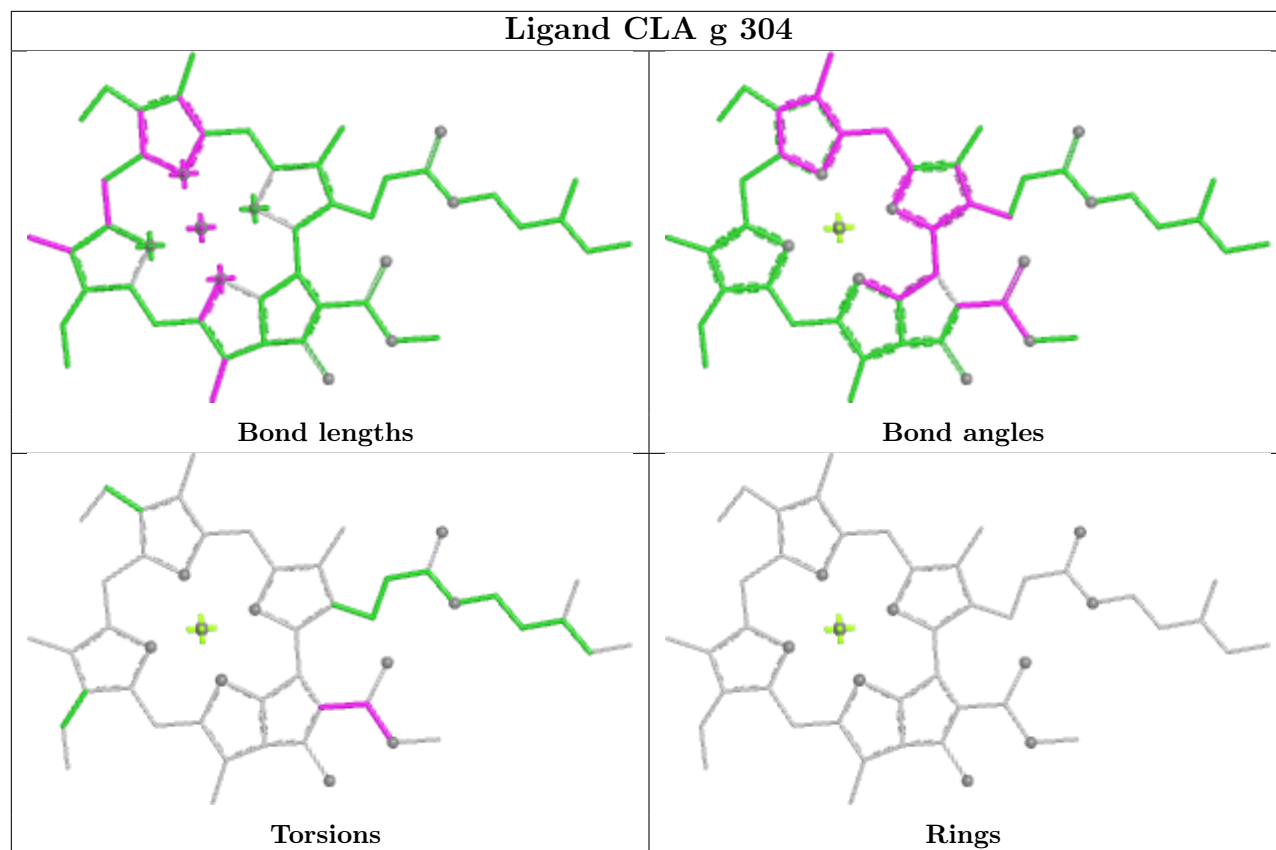




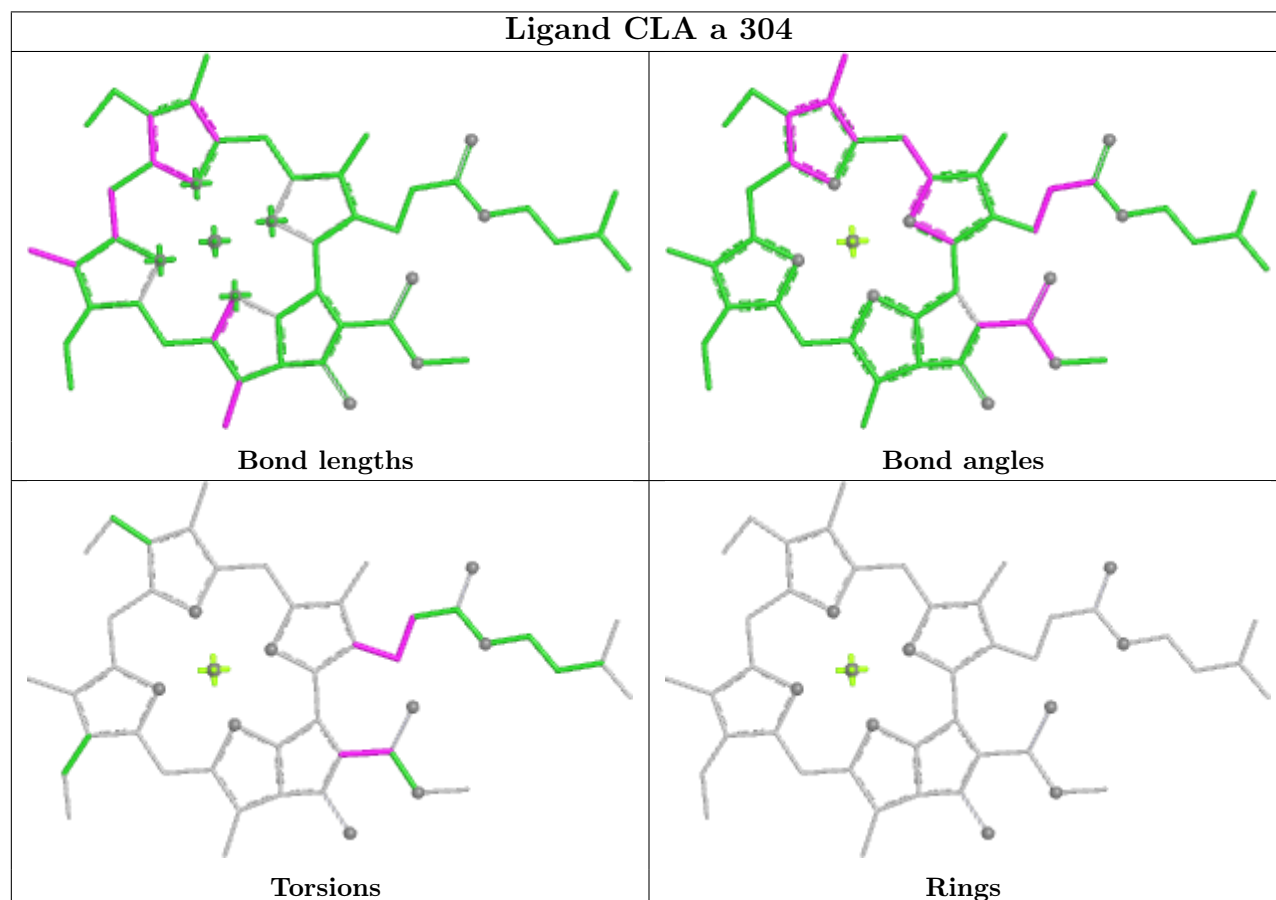


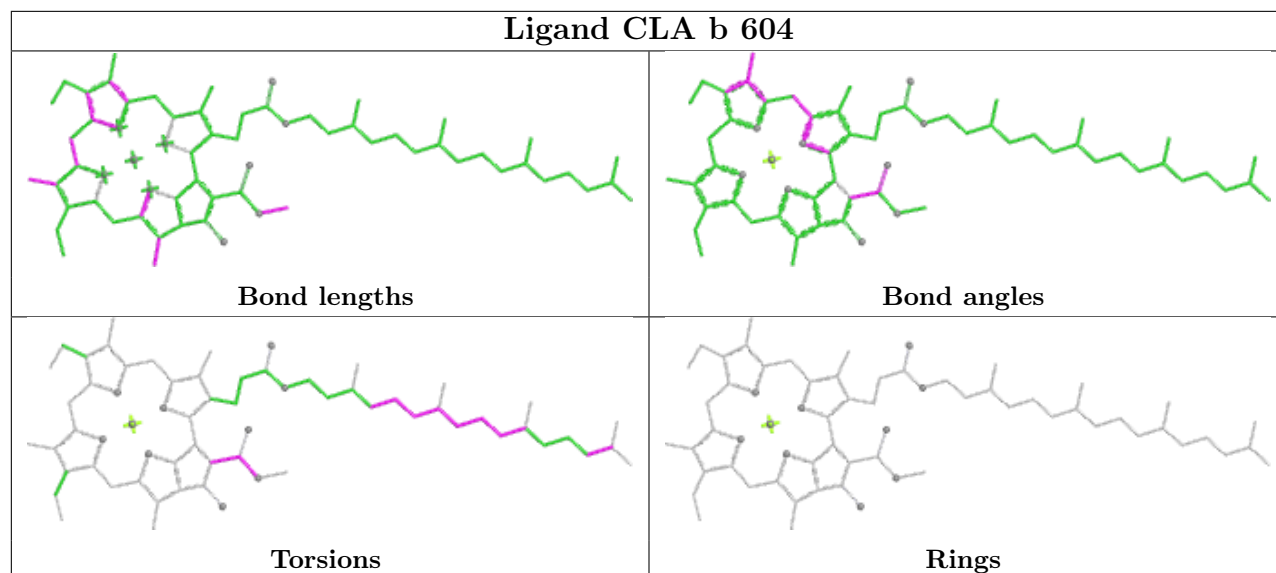
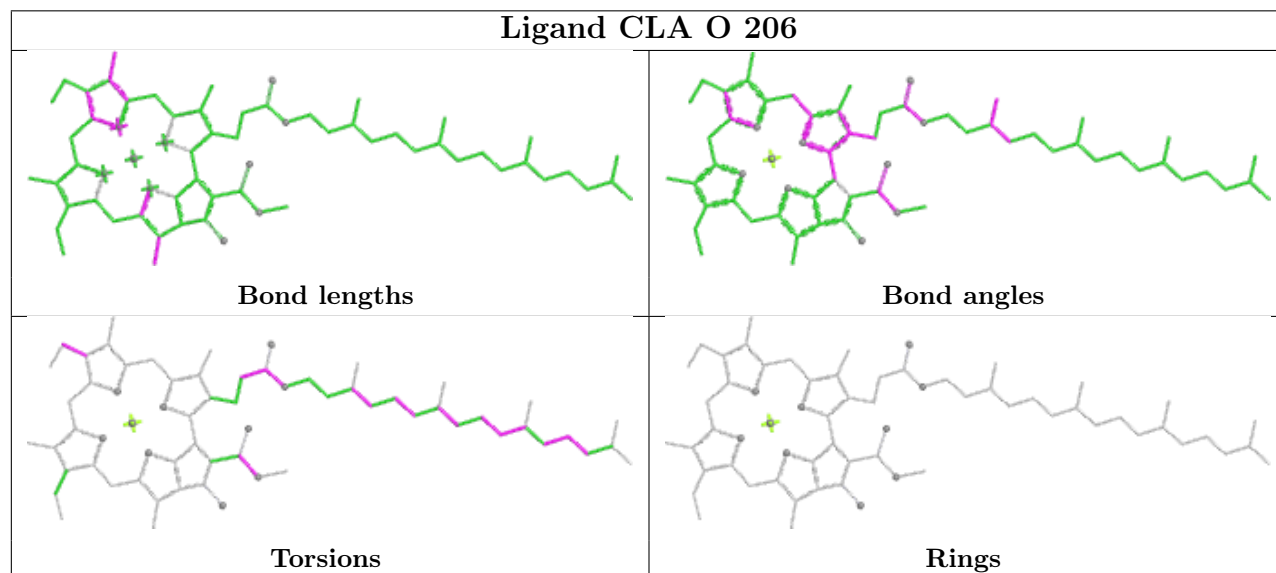
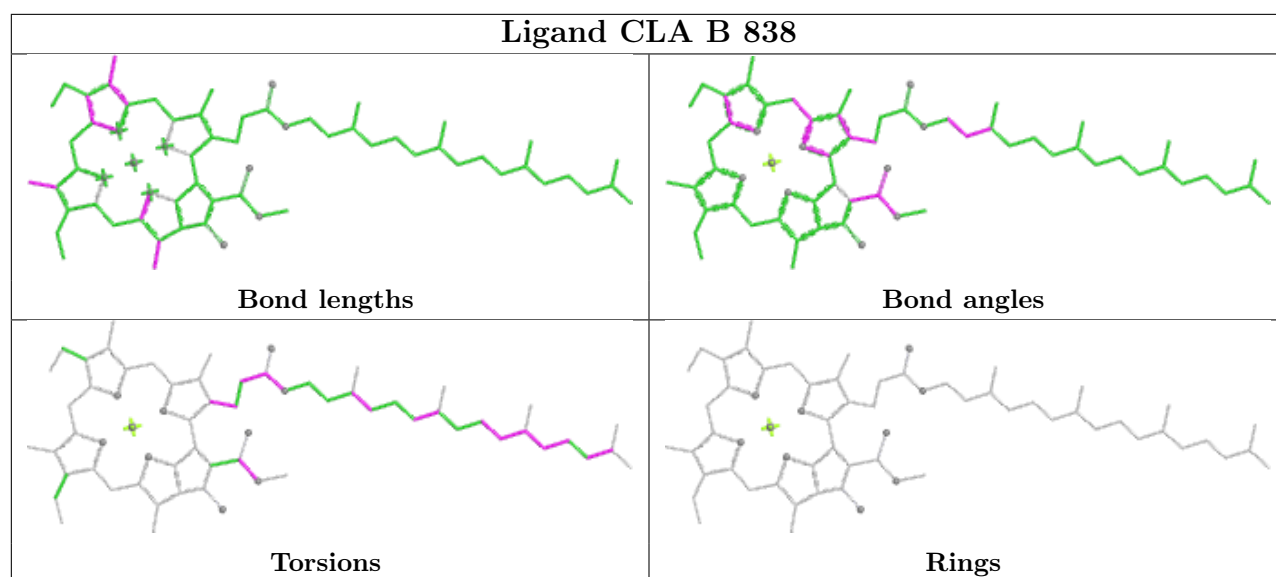


Ligand CLA g 304

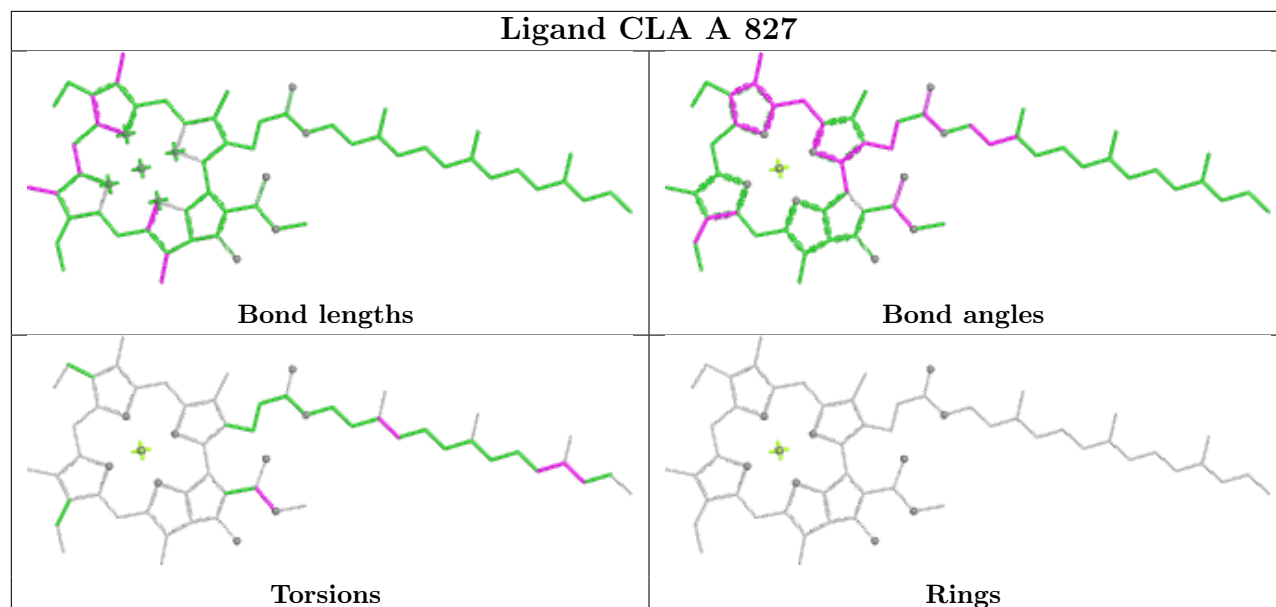


Ligand CLA a 304

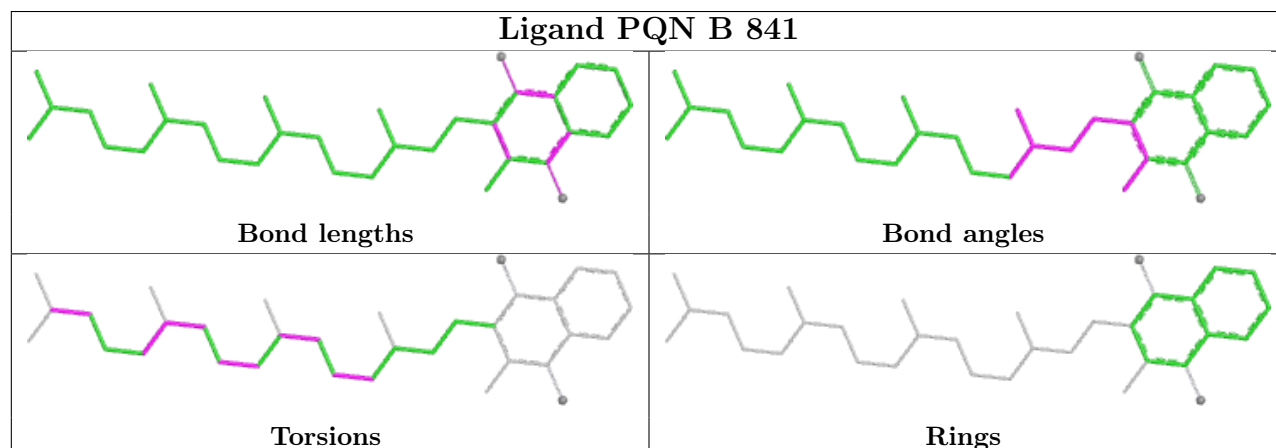




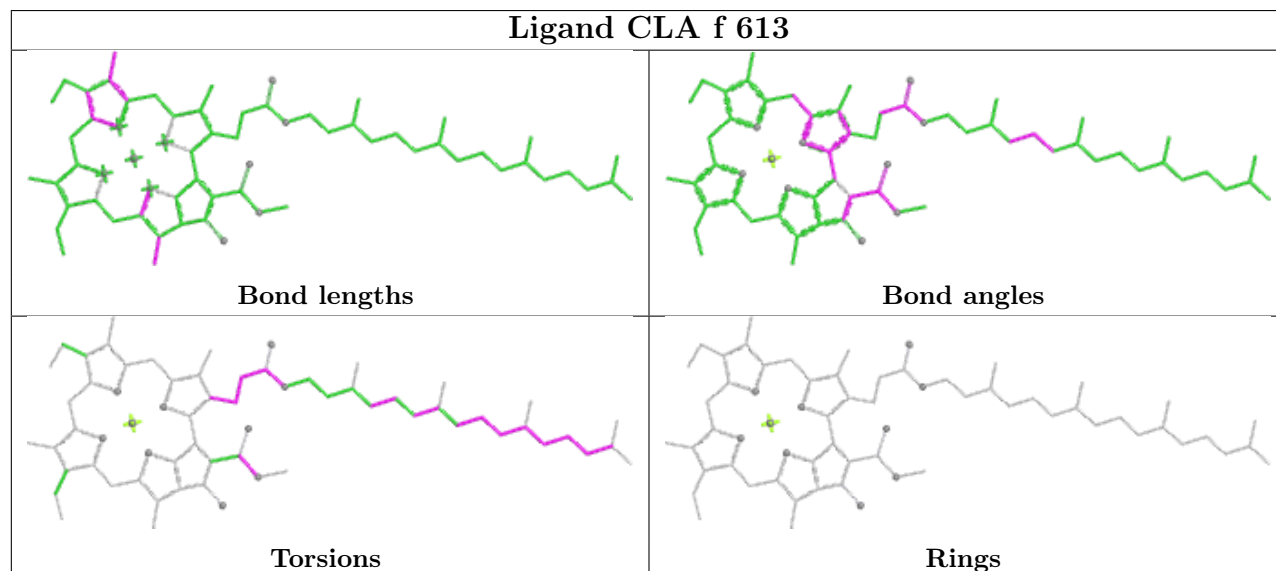
Ligand CLA A 827

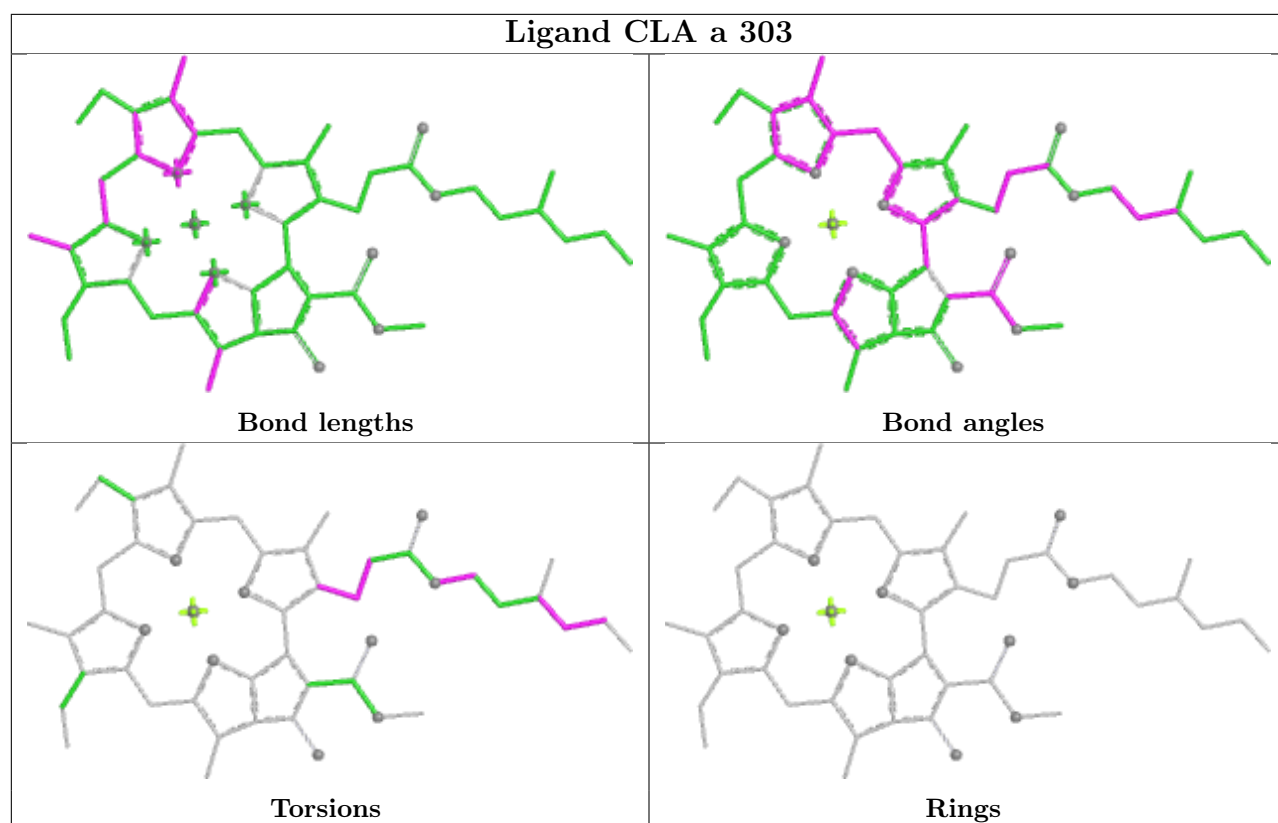


Ligand PQN B 841

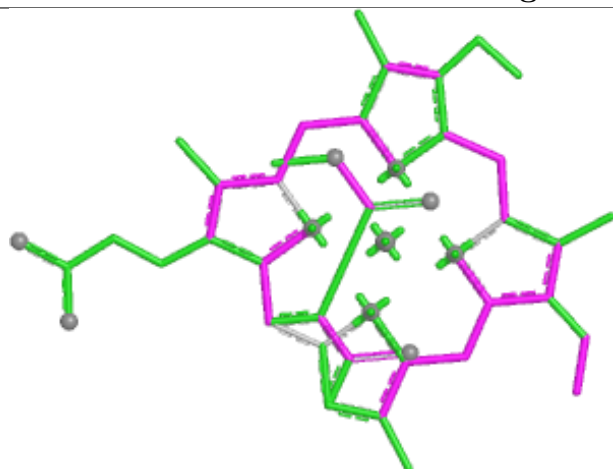


Ligand CLA f 613

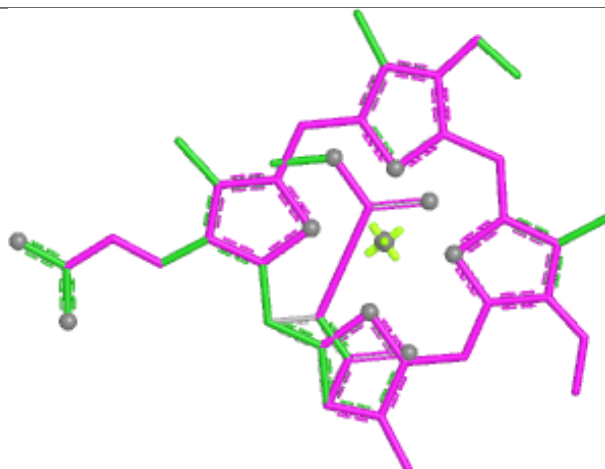




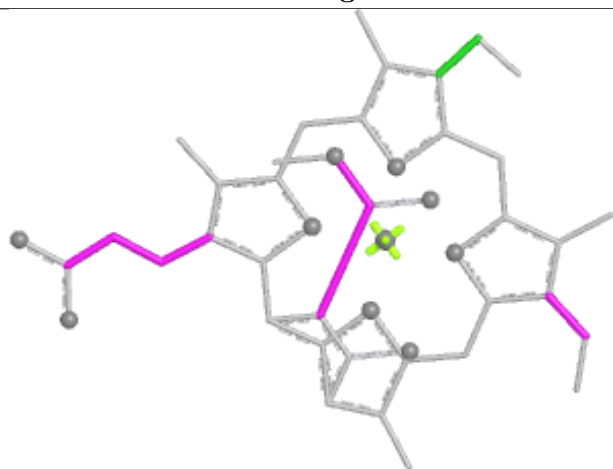
Ligand KC2 k 312



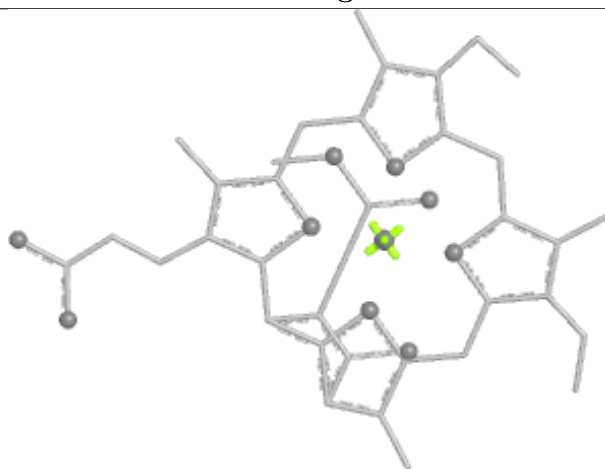
Bond lengths



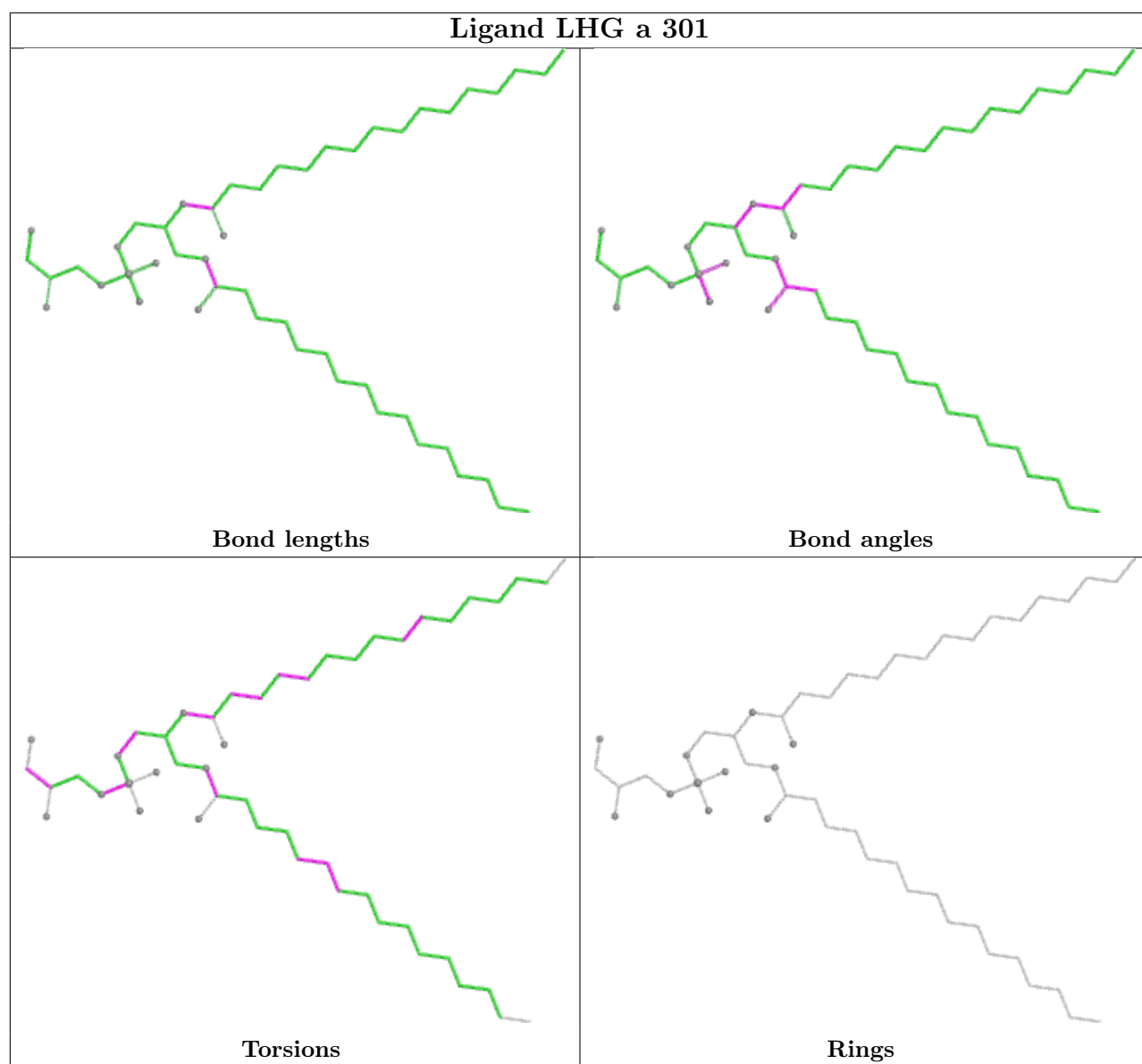
Bond angles

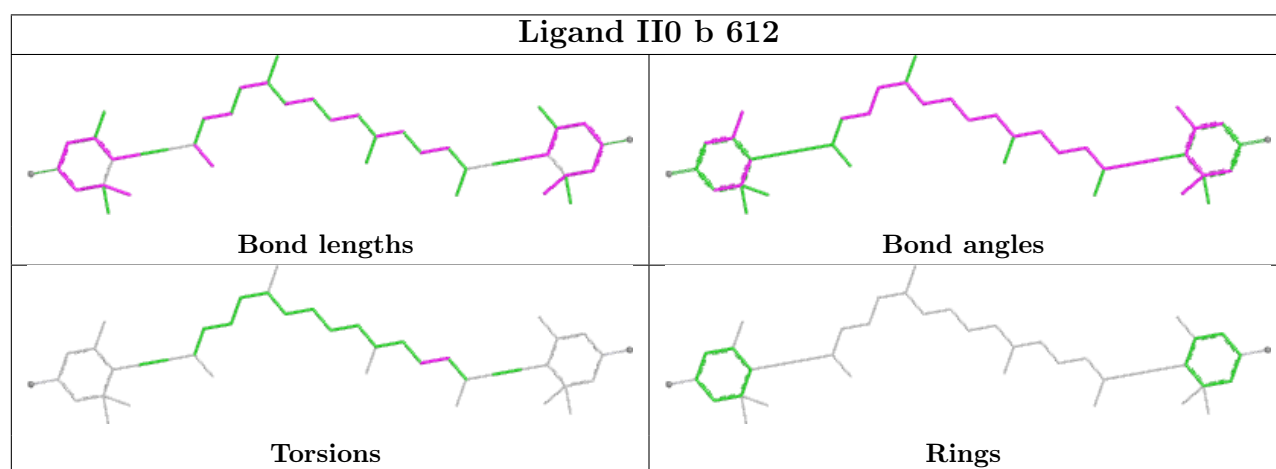
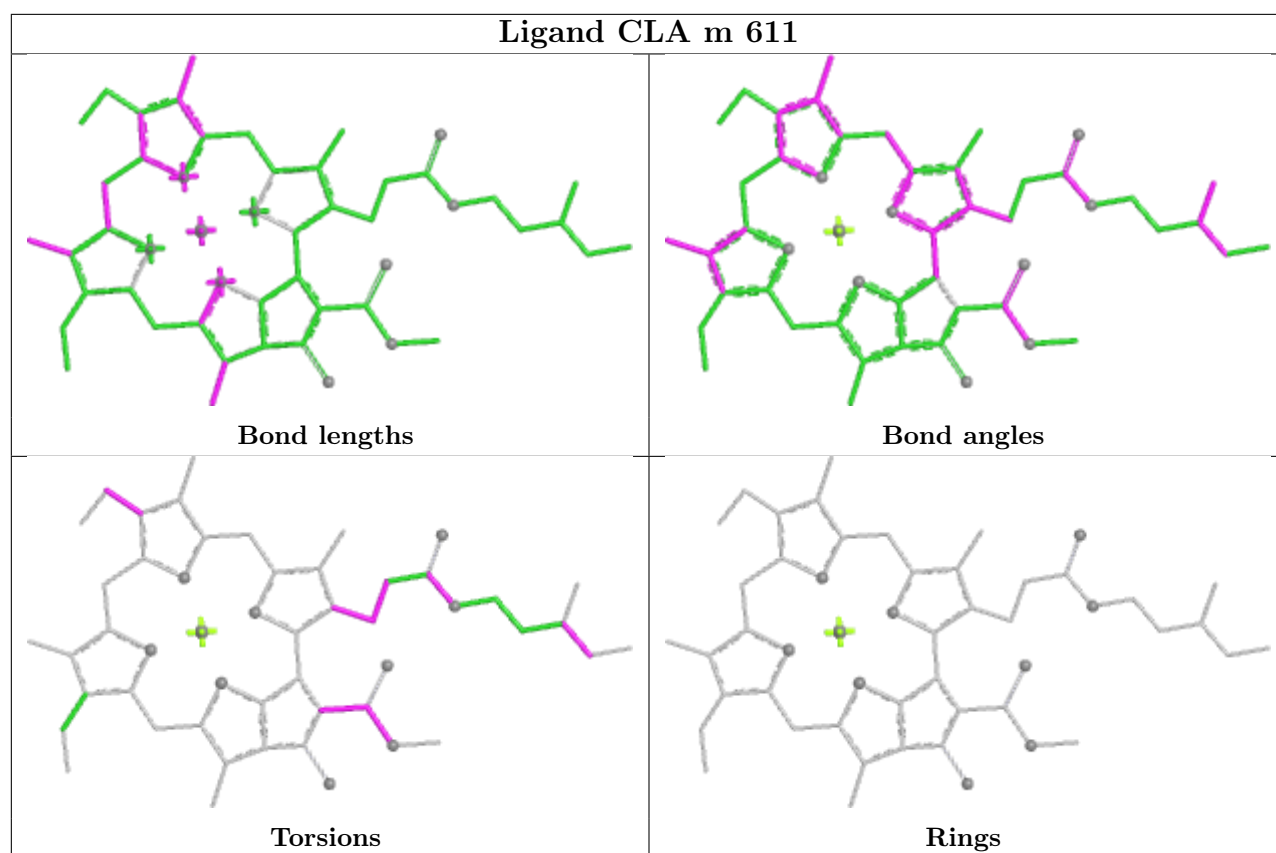


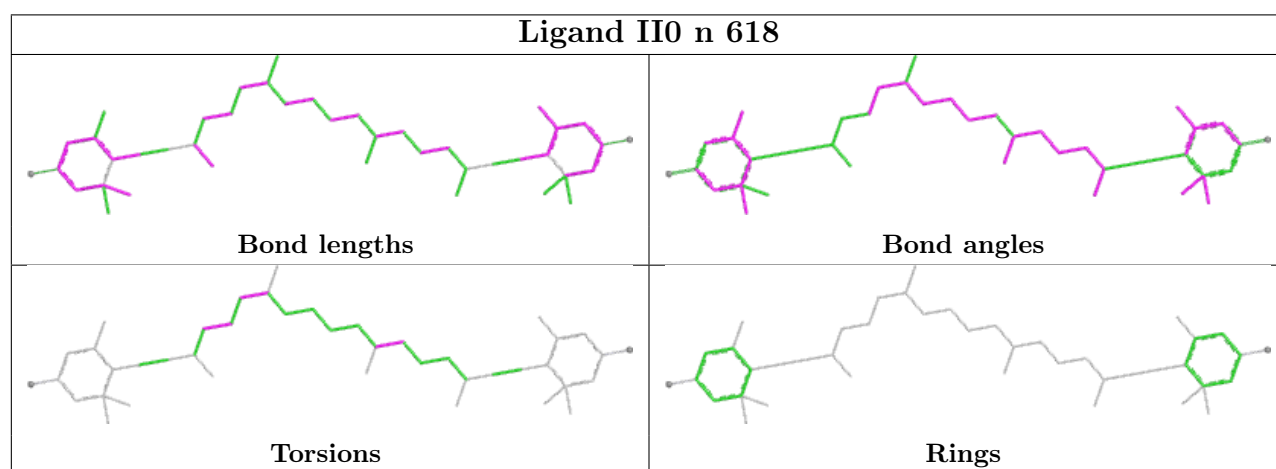
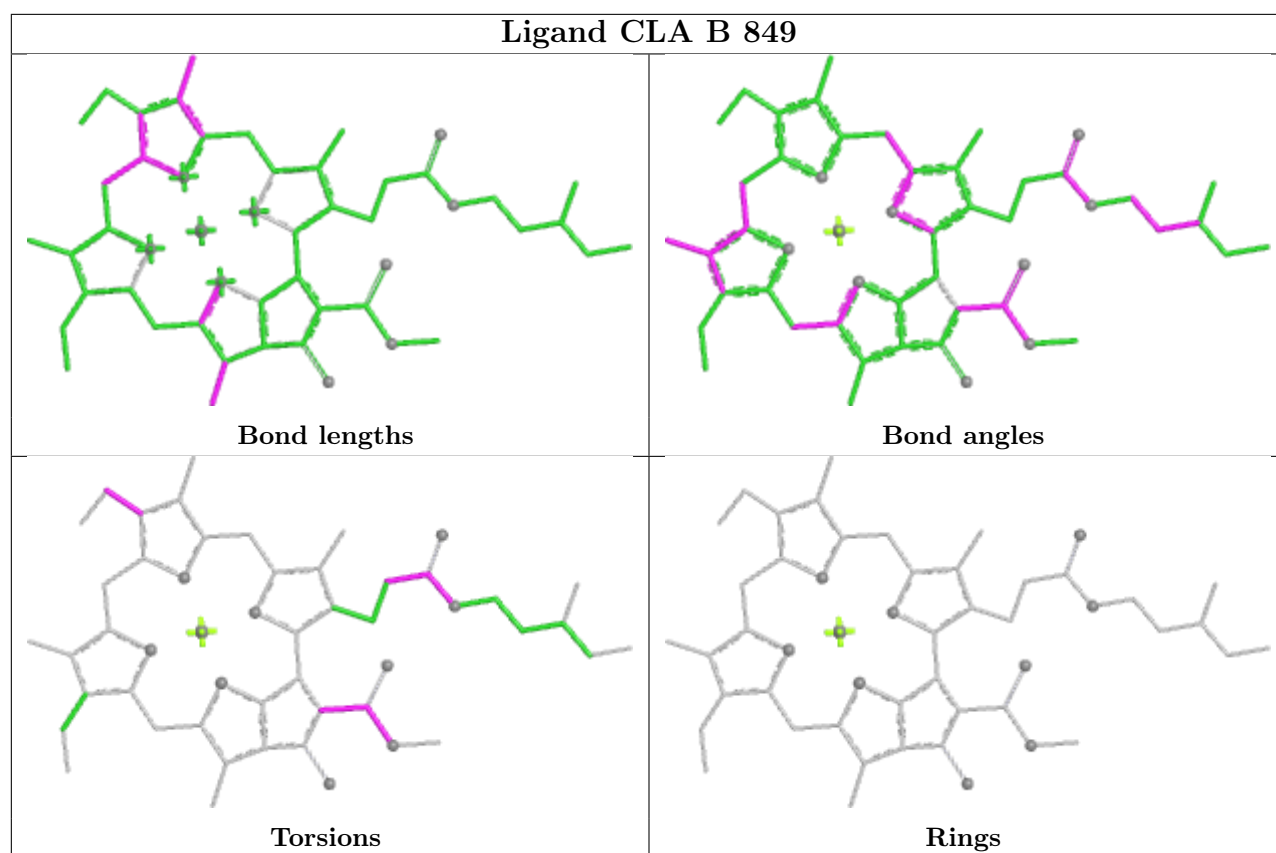
Torsions

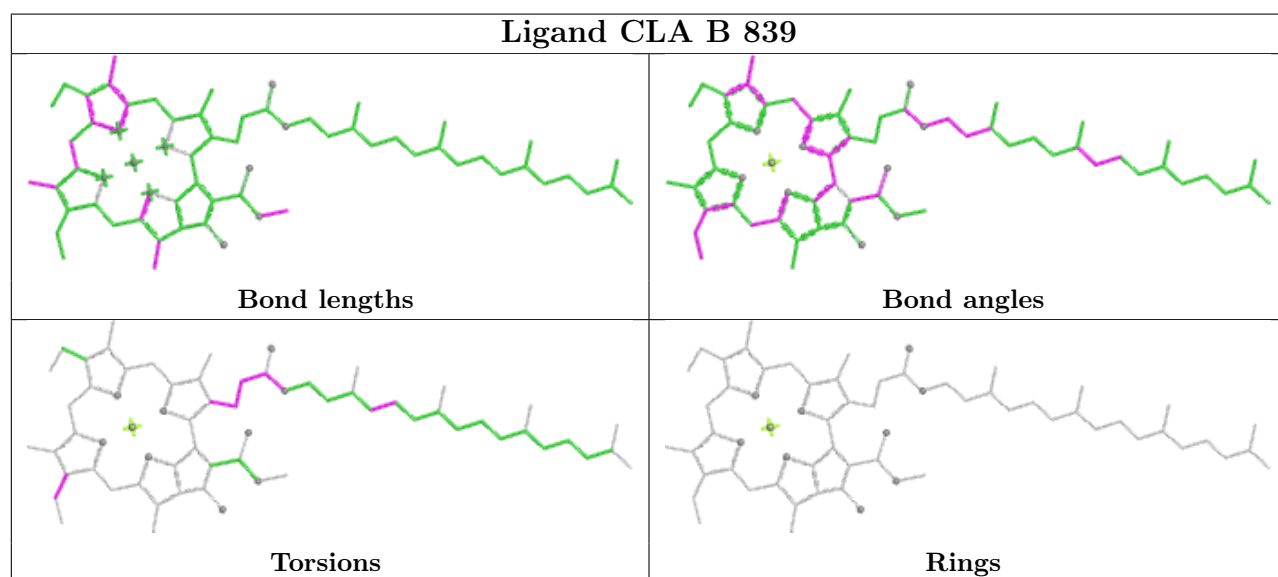
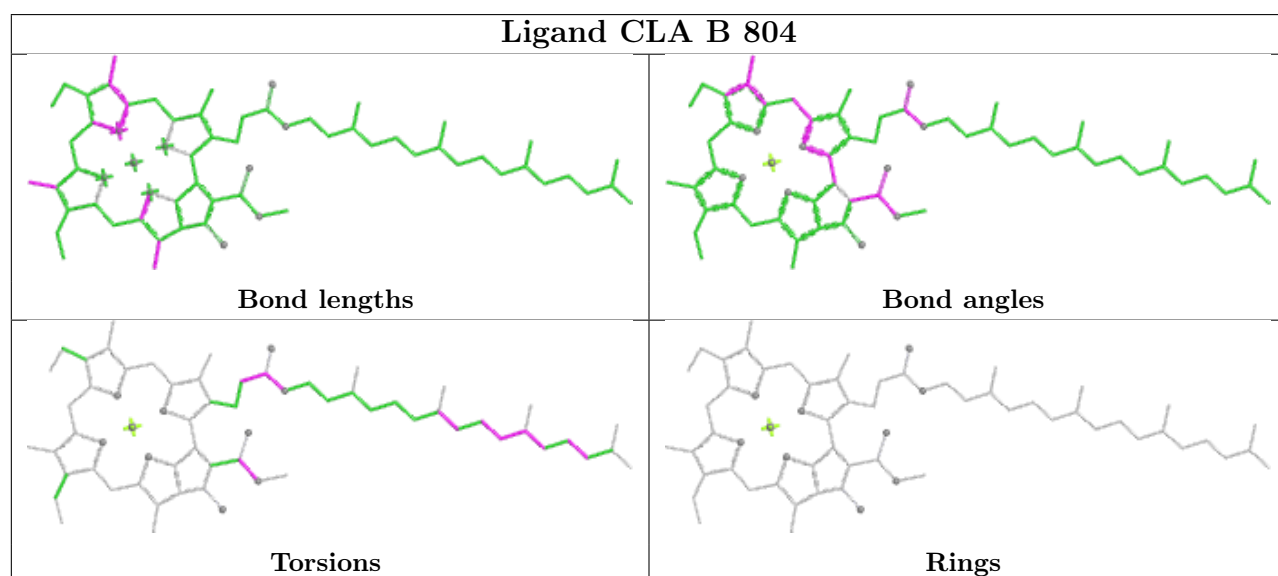
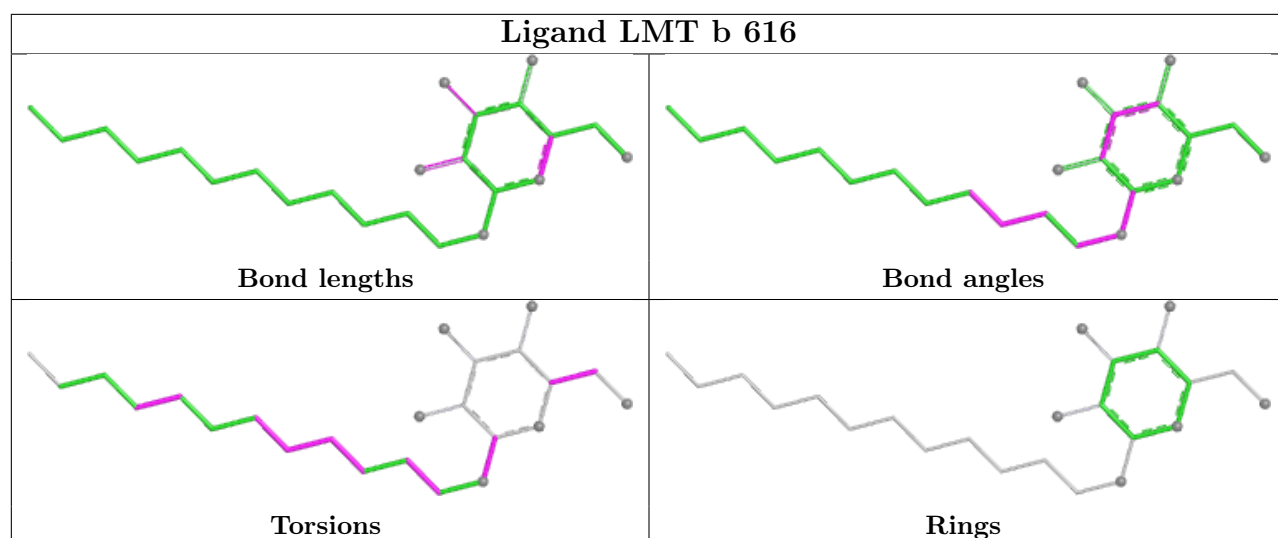


Rings

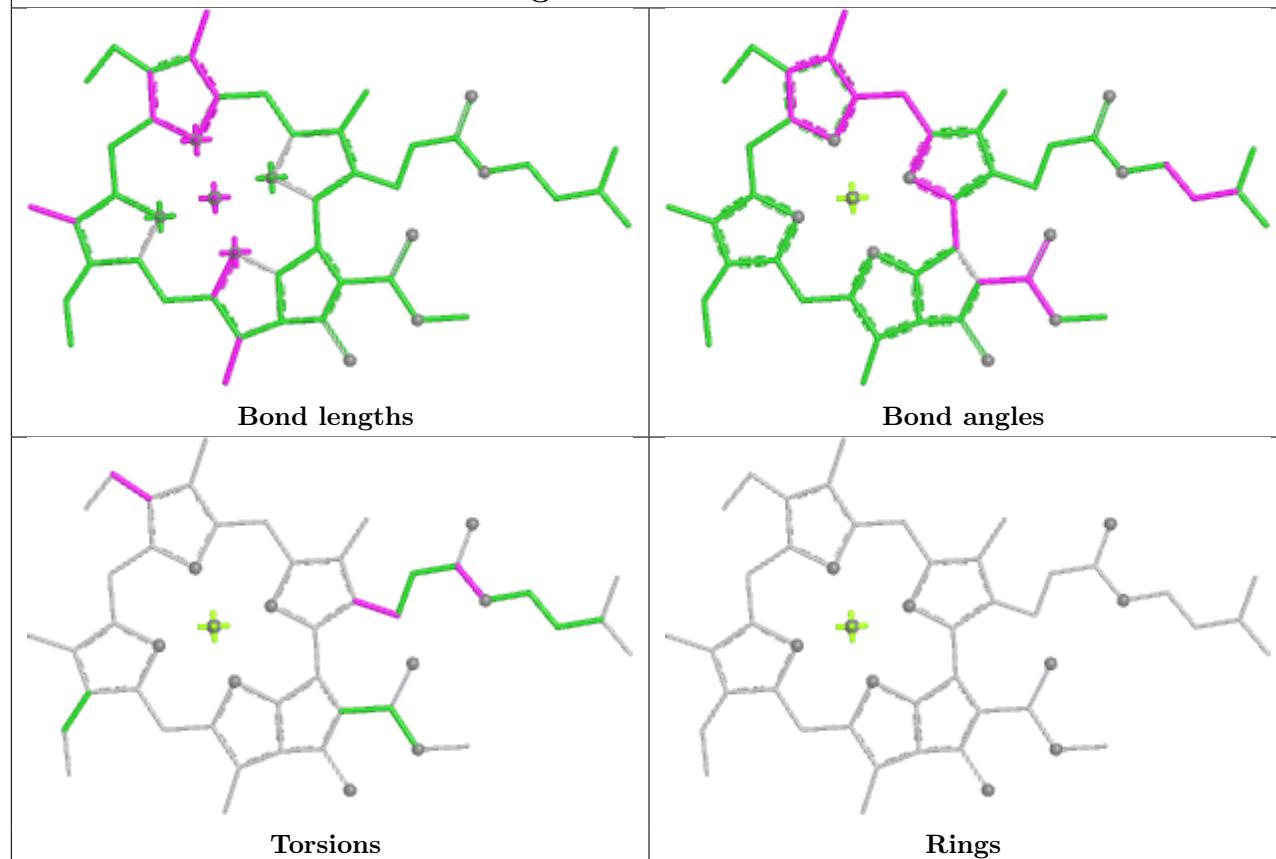




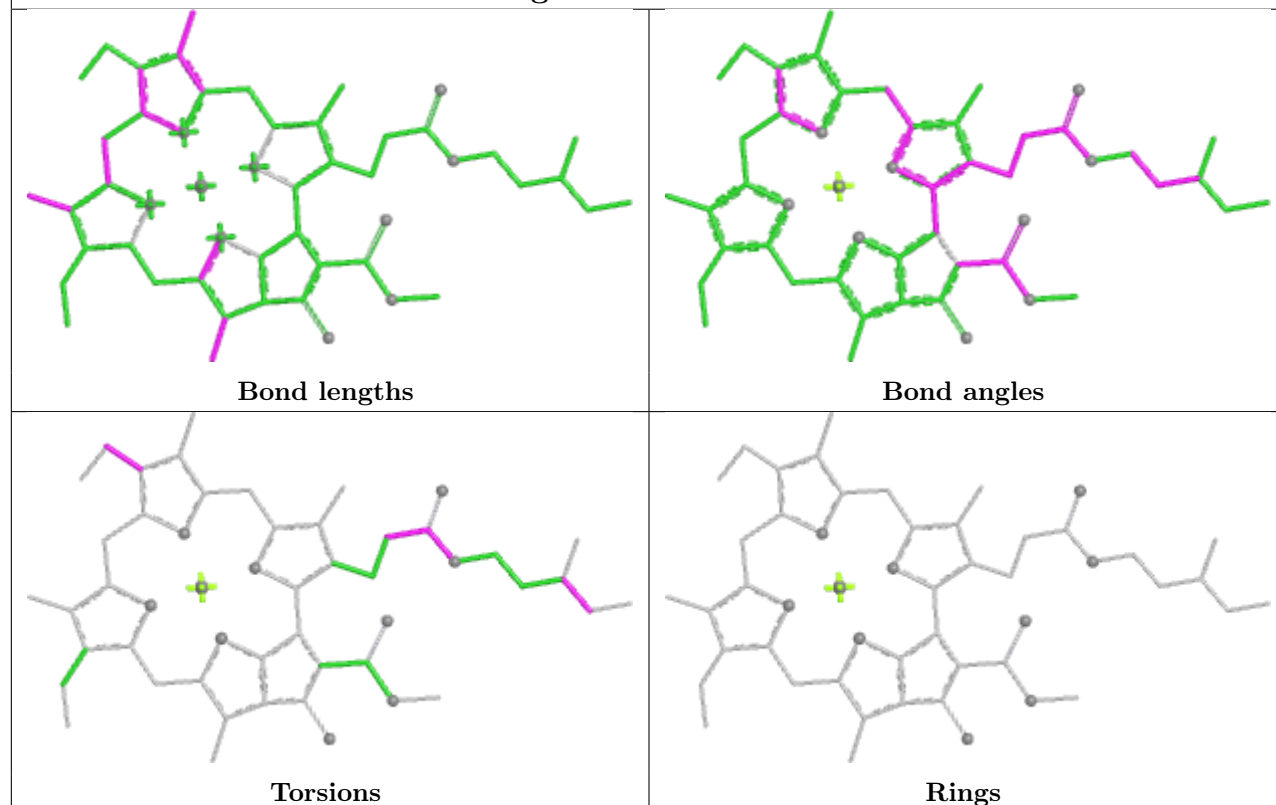


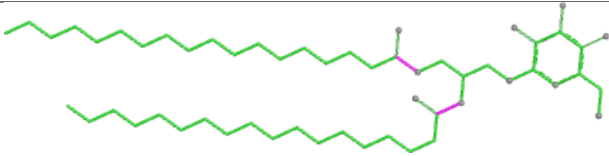
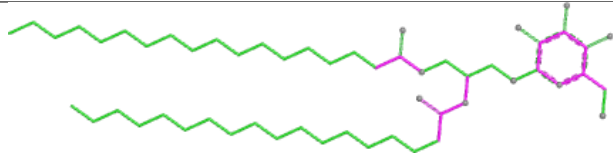
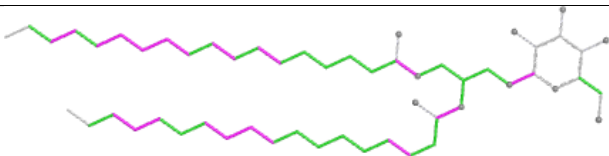
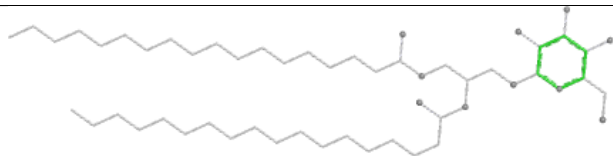


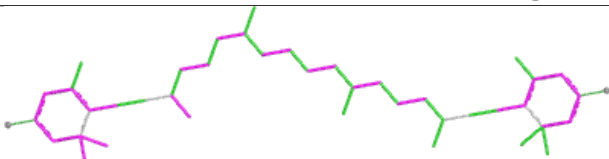
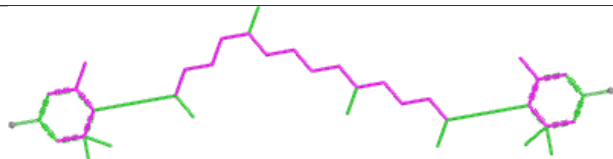
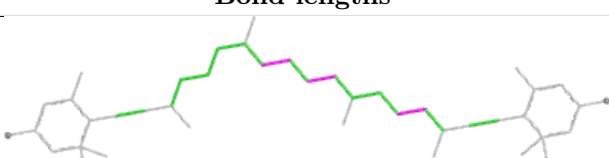
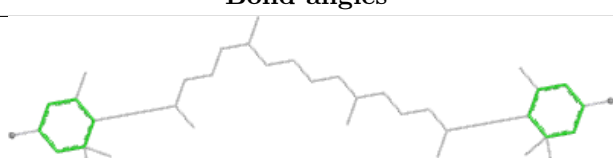
Ligand CLA A 830

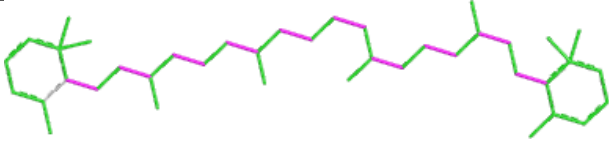
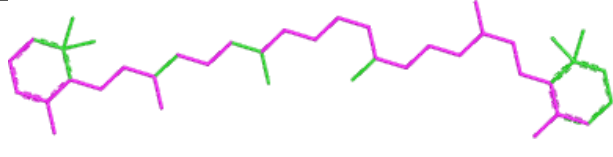
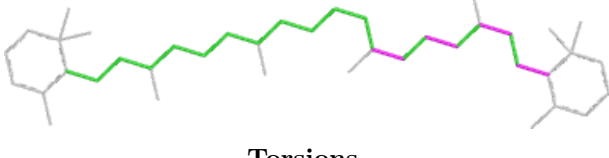
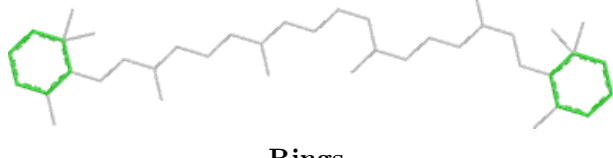


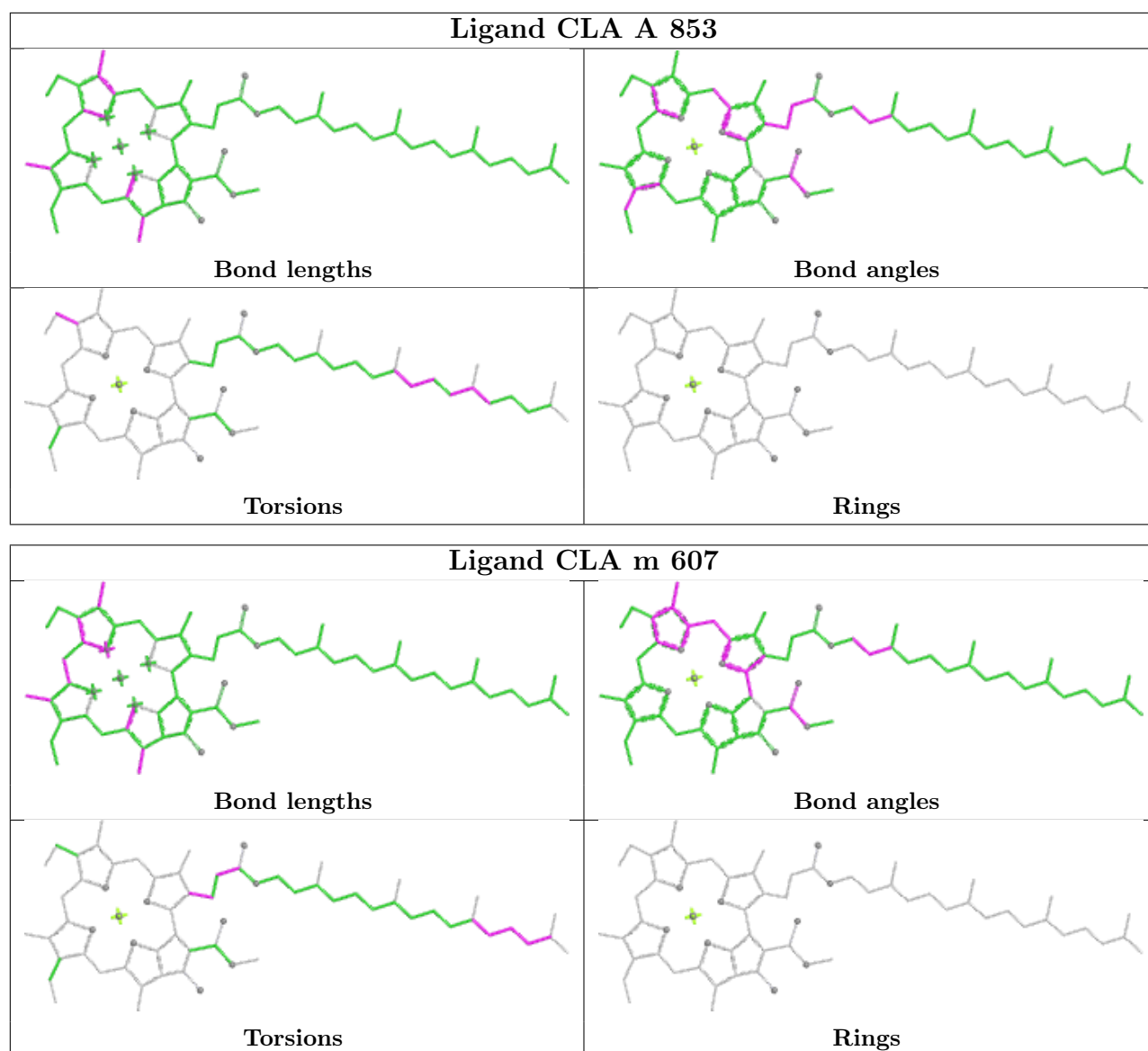
Ligand CLA K 101



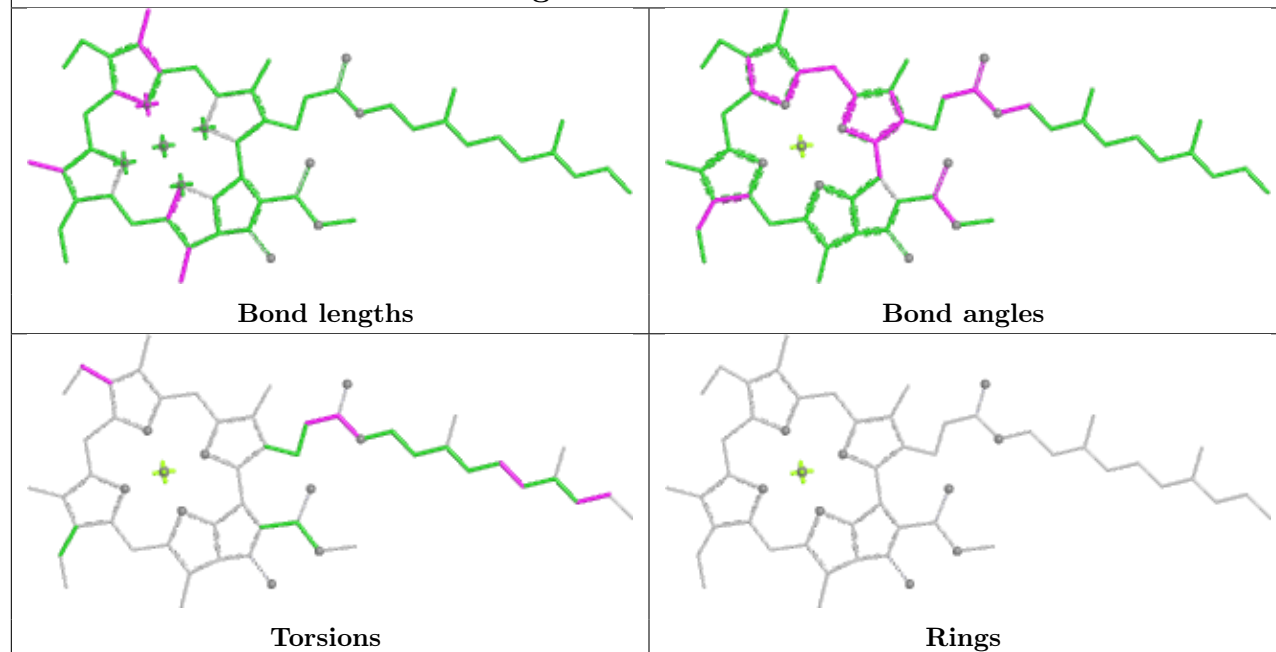
Ligand LMG L 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 n 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

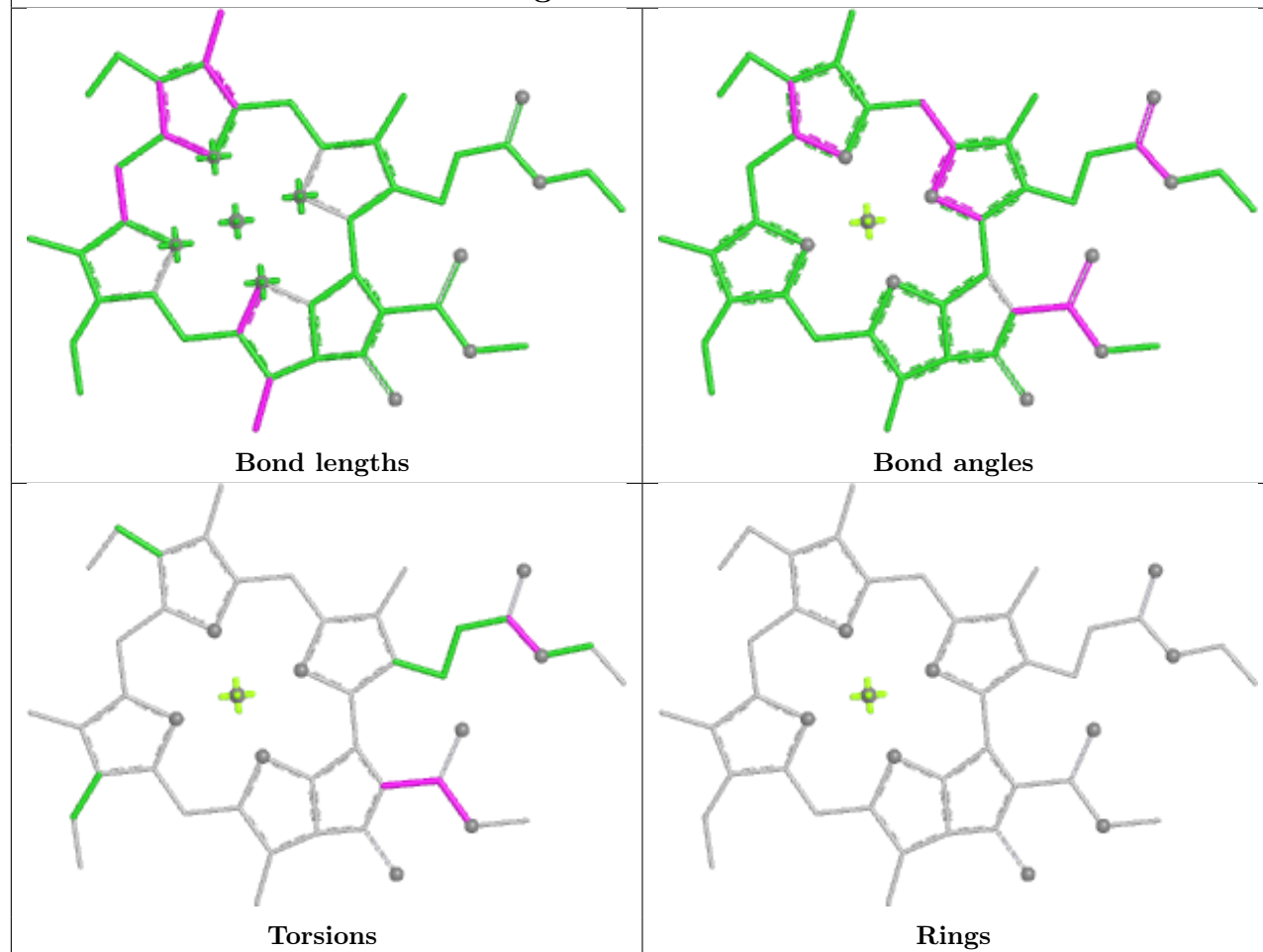
Ligand WVN B 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

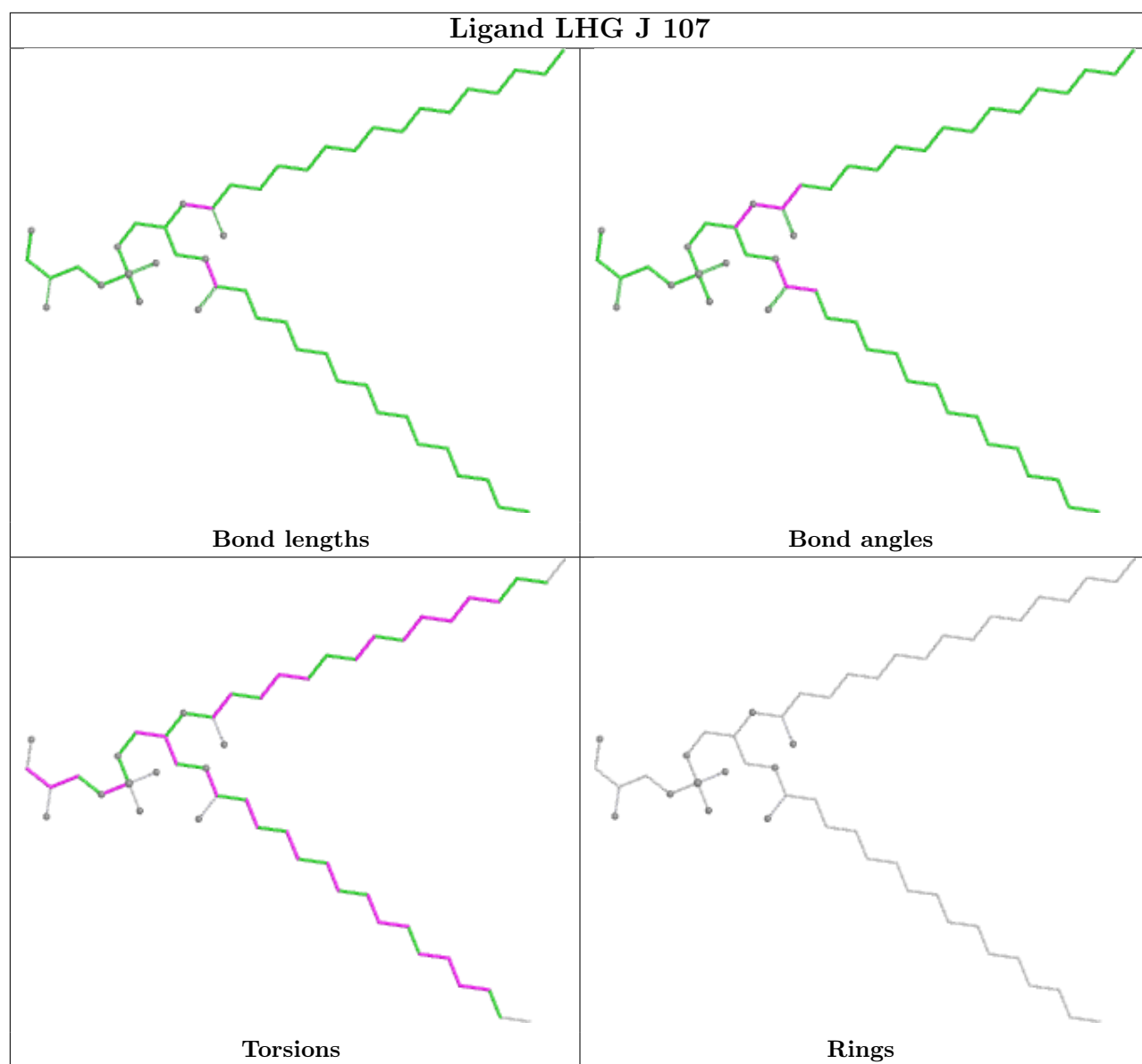


Ligand CLA B 837

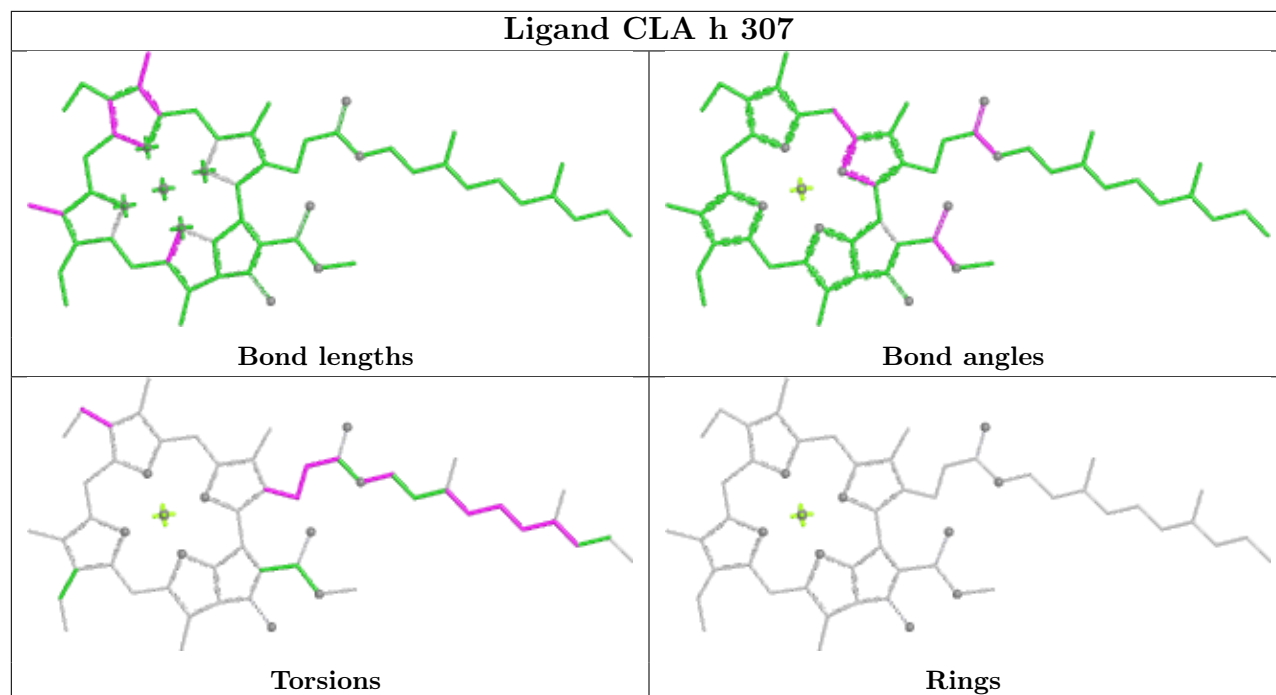


Ligand CLA f 601

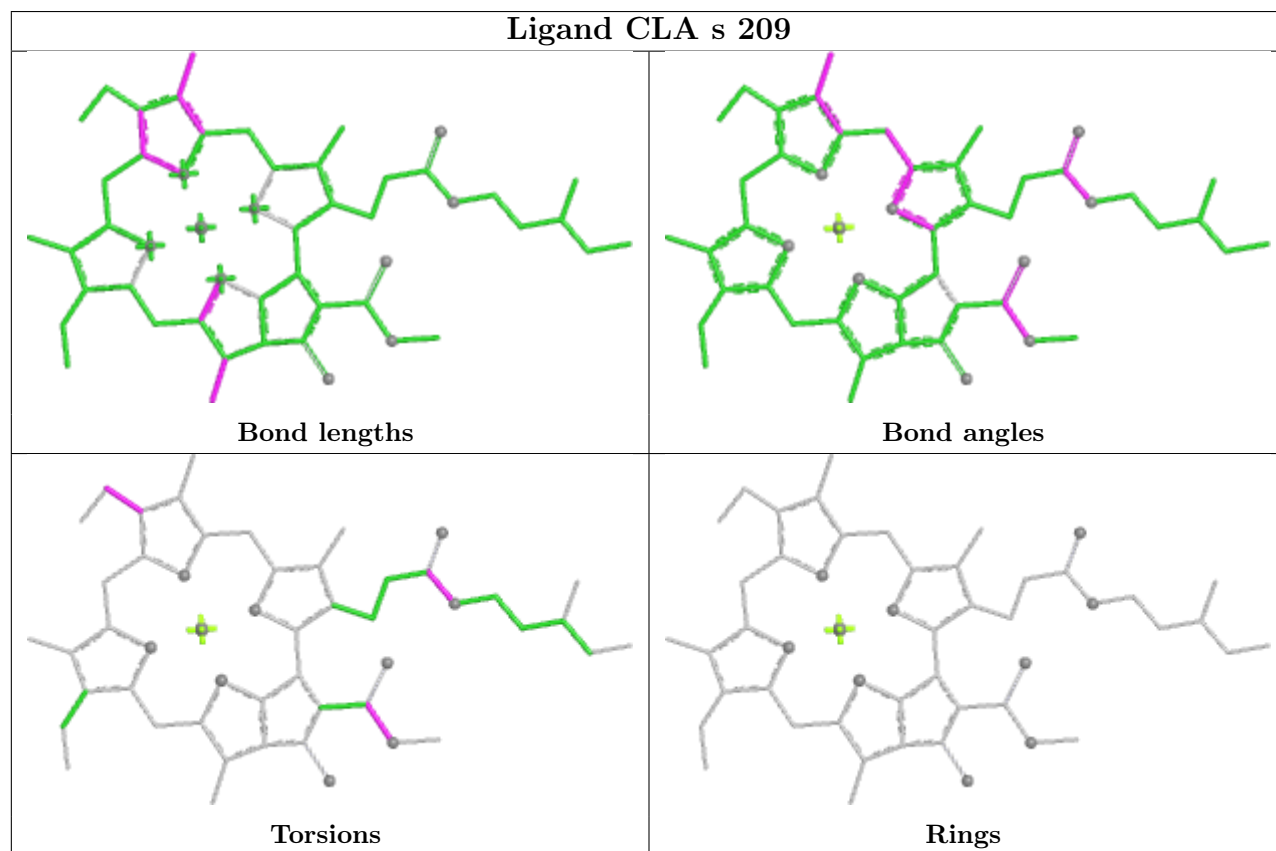


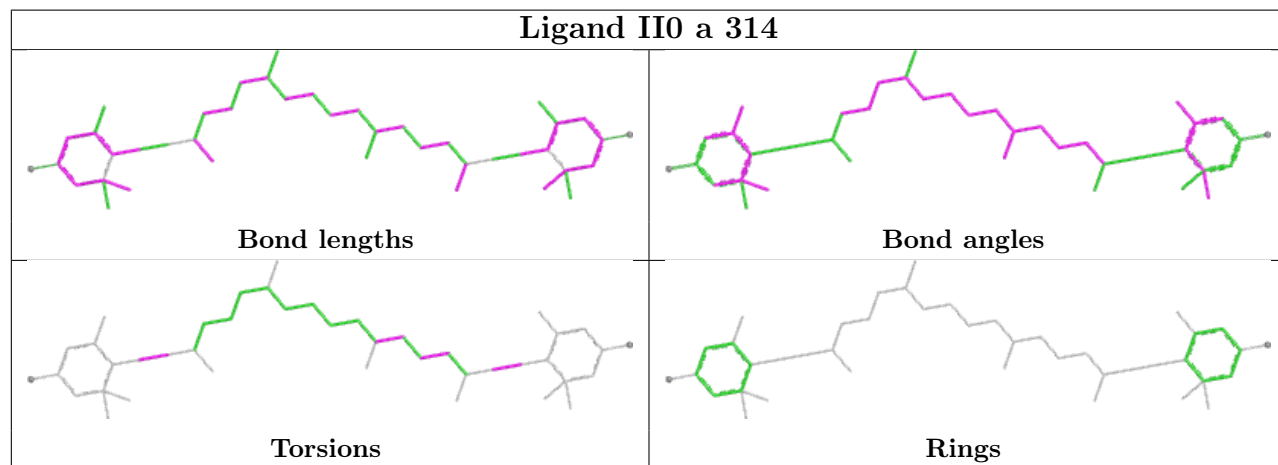
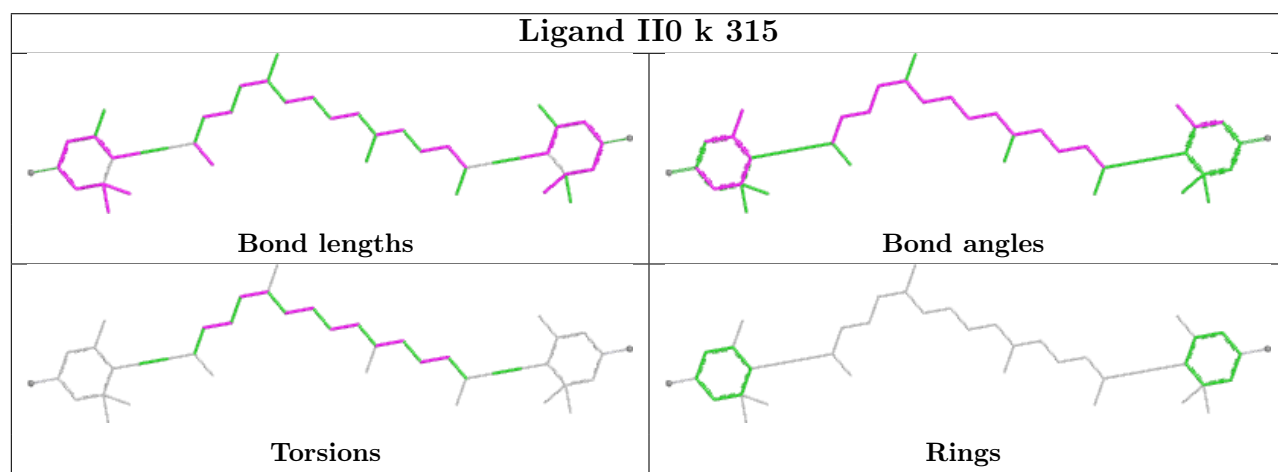
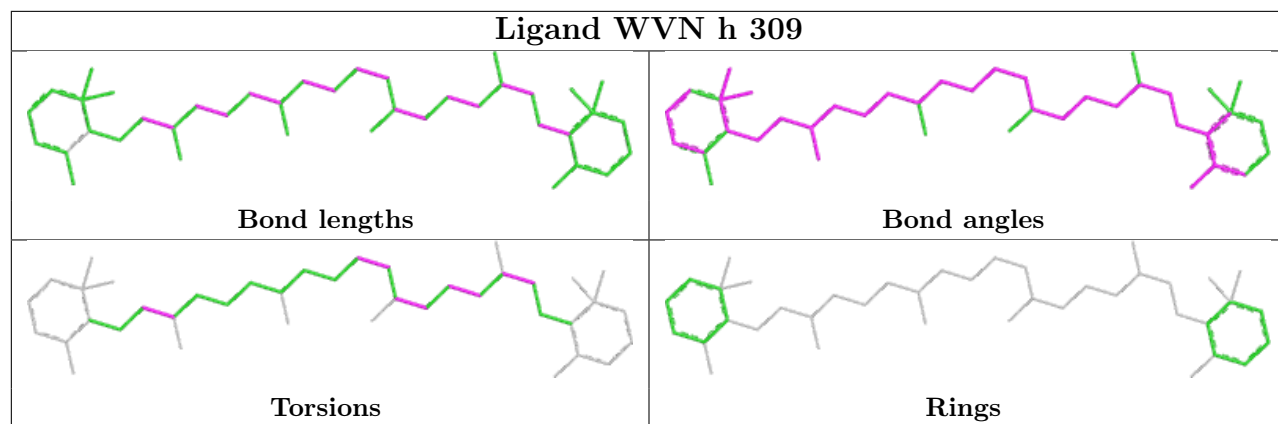


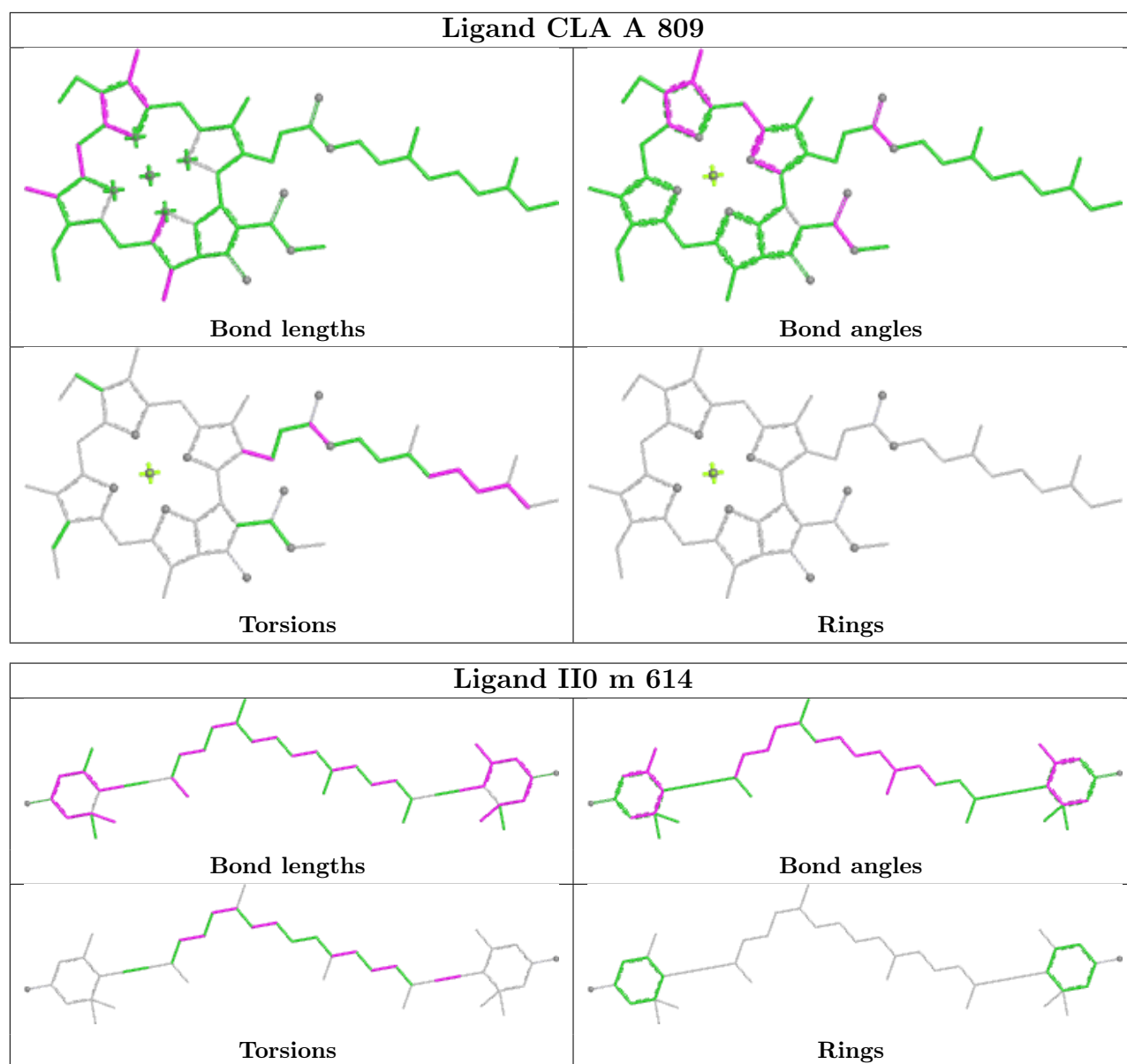
Ligand CLA h 307



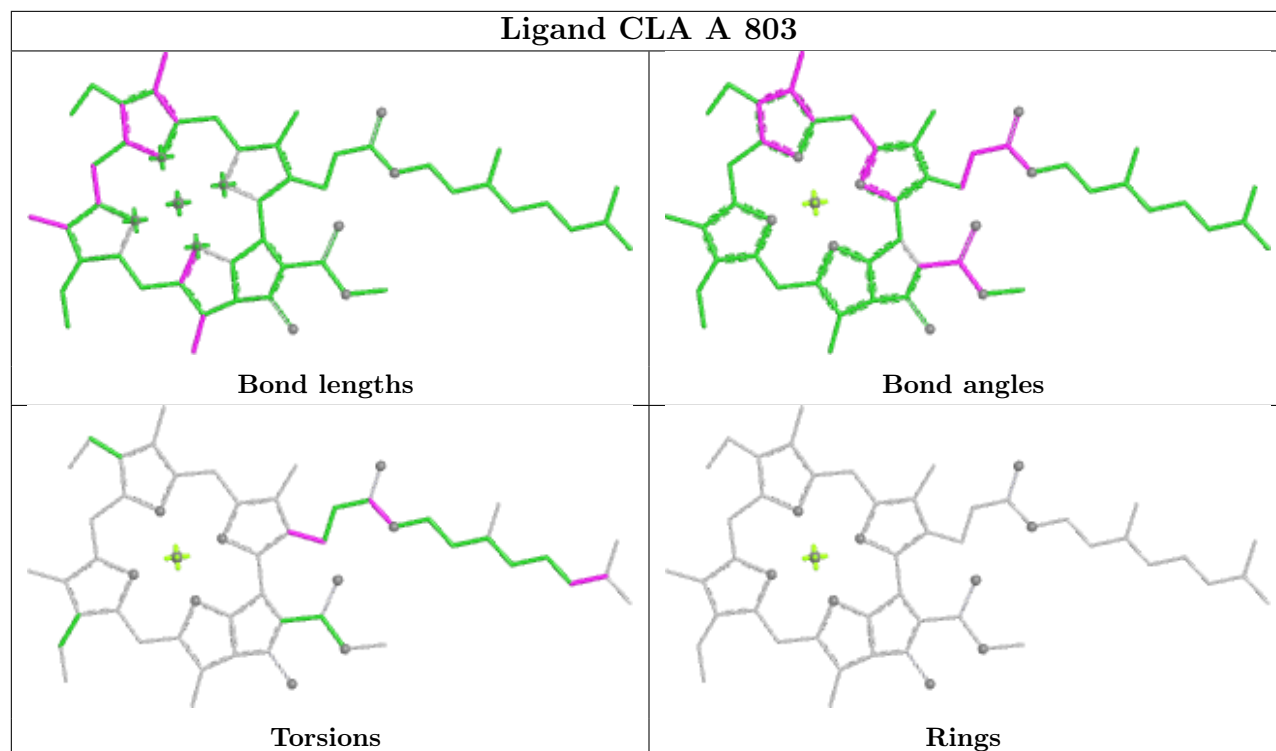
Ligand CLA s 209



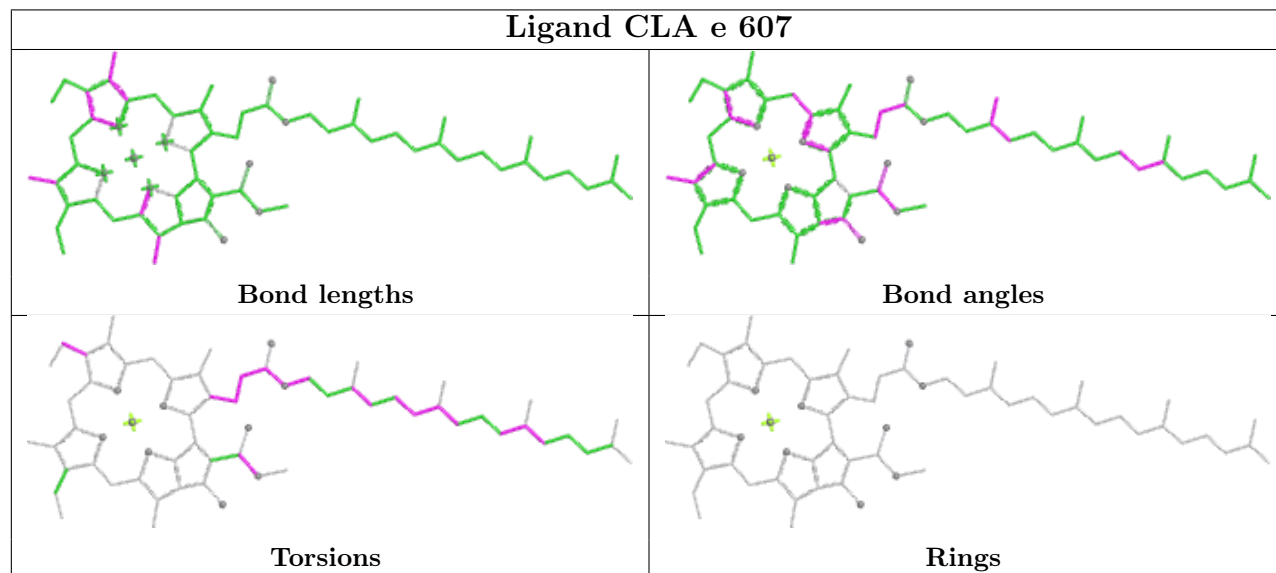




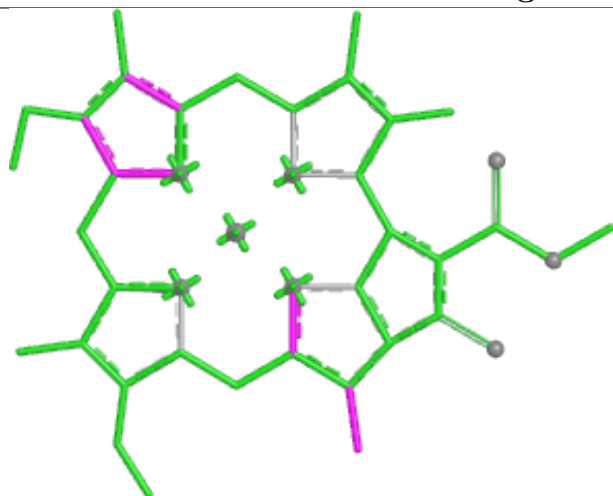
Ligand CLA A 803



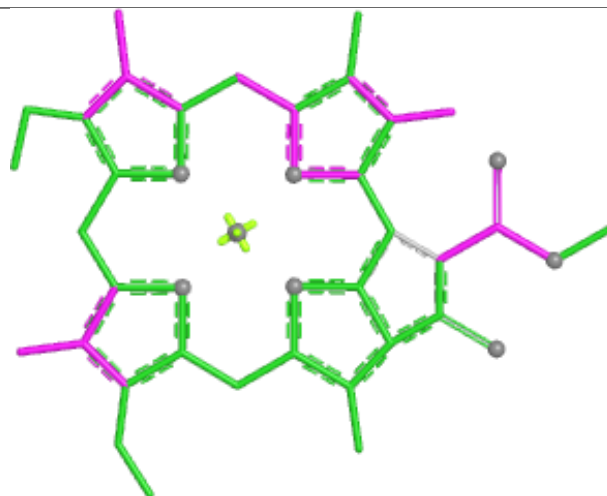
Ligand CLA e 607



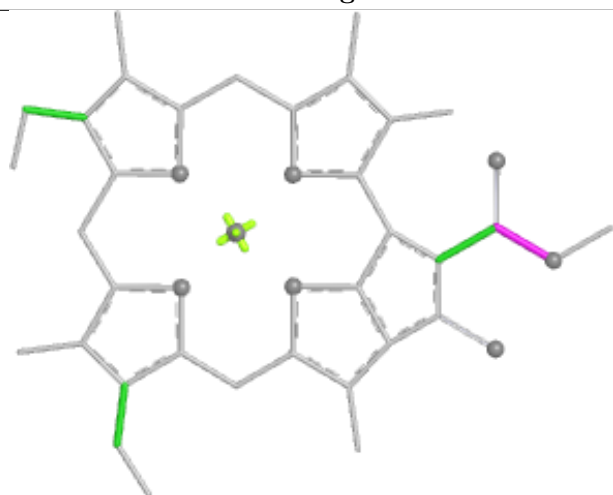
Ligand CLA d 308



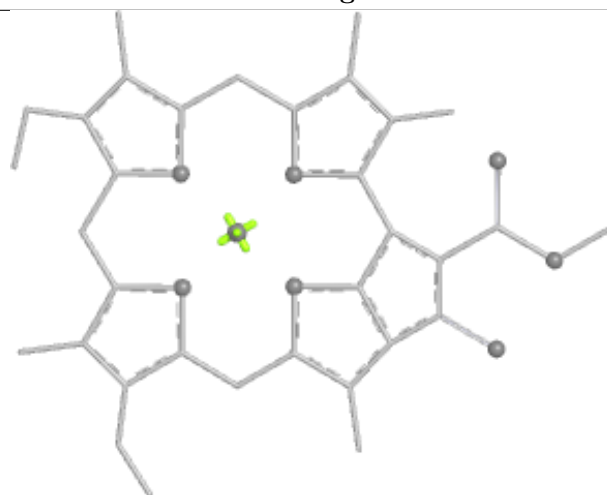
Bond lengths



Bond angles

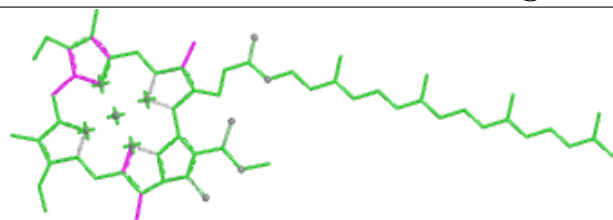


Torsions

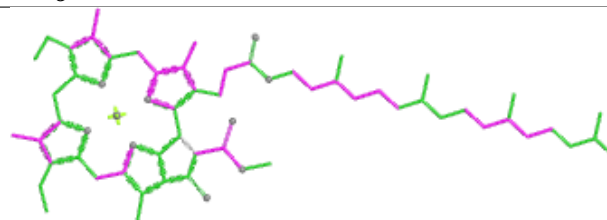


Rings

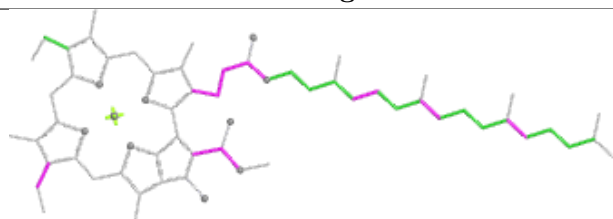
Ligand CLA j 604



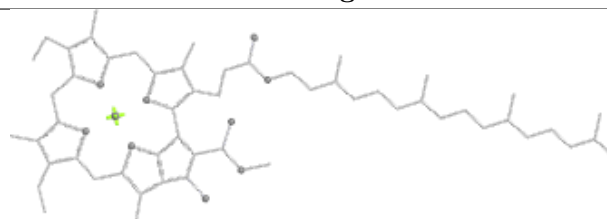
Bond lengths



Bond angles

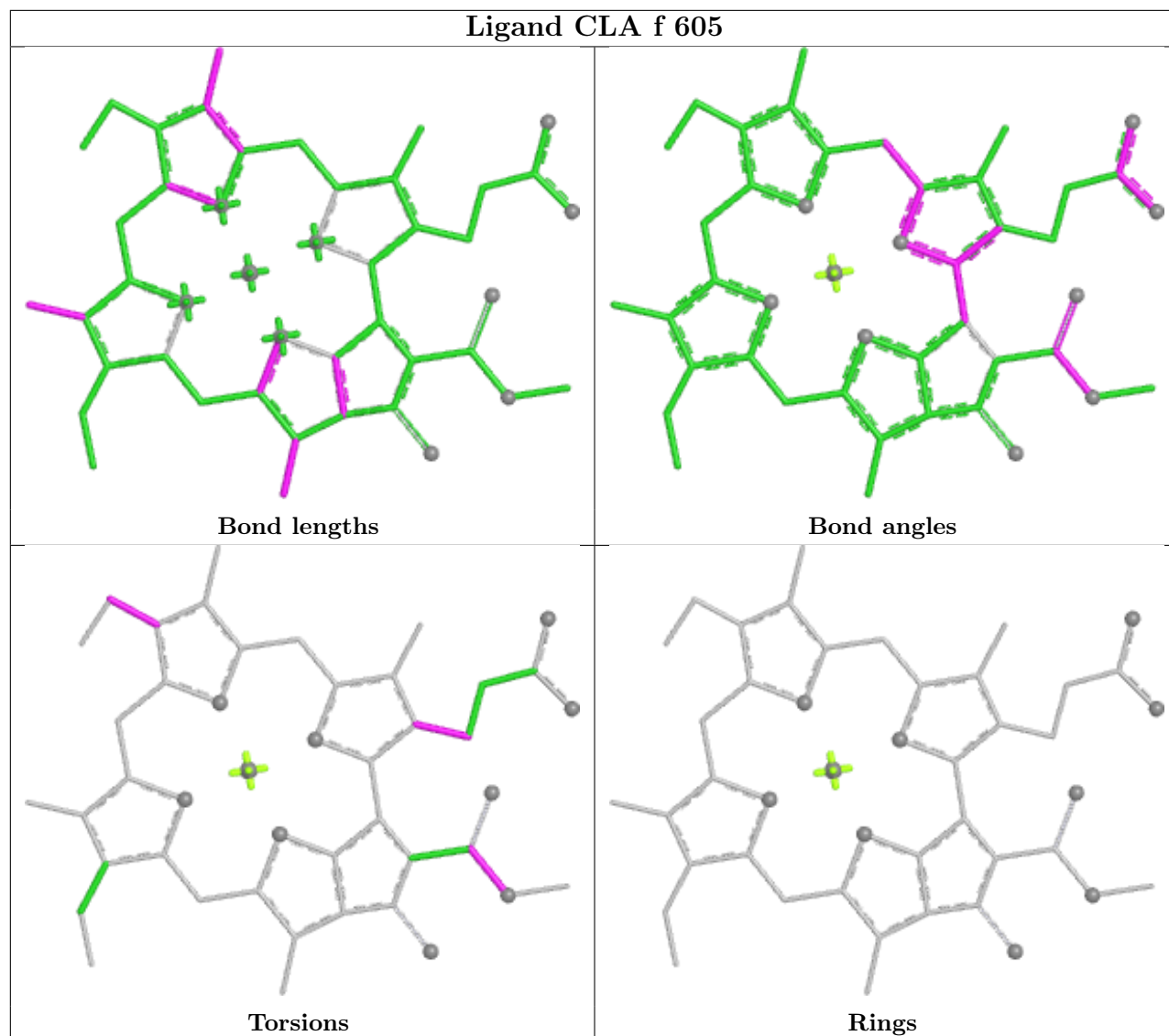


Torsions

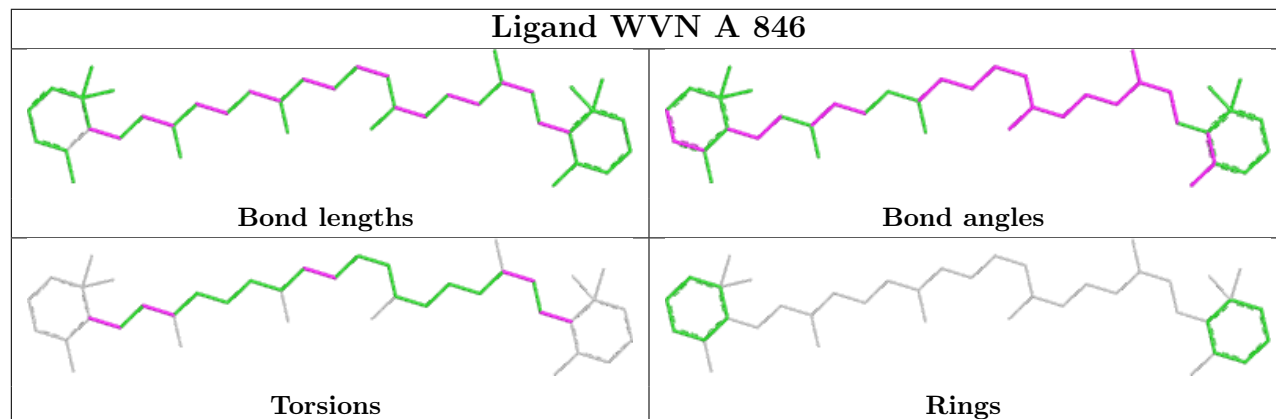


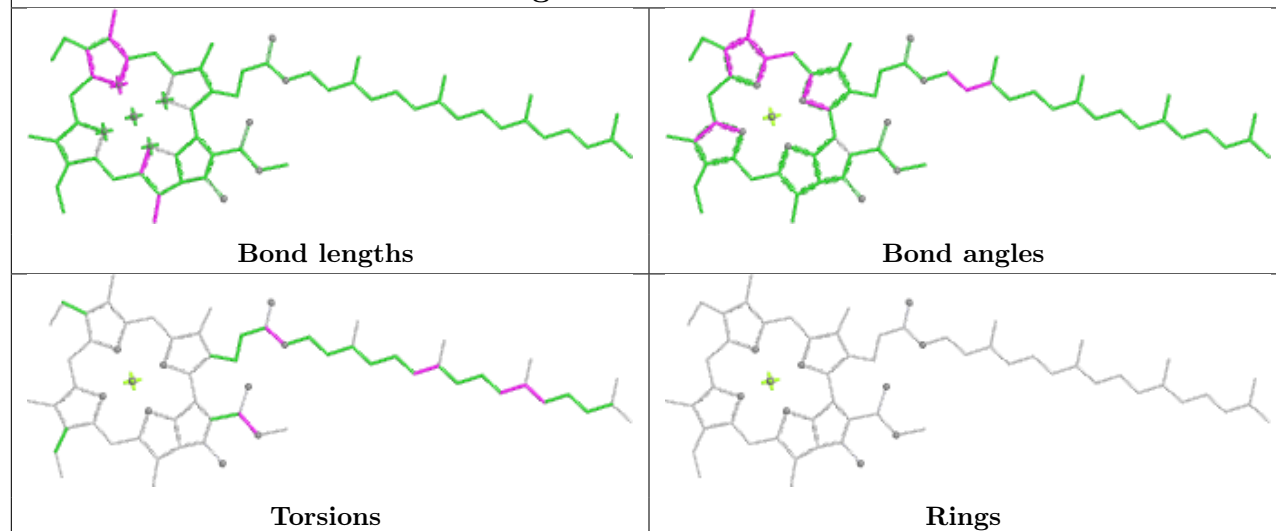
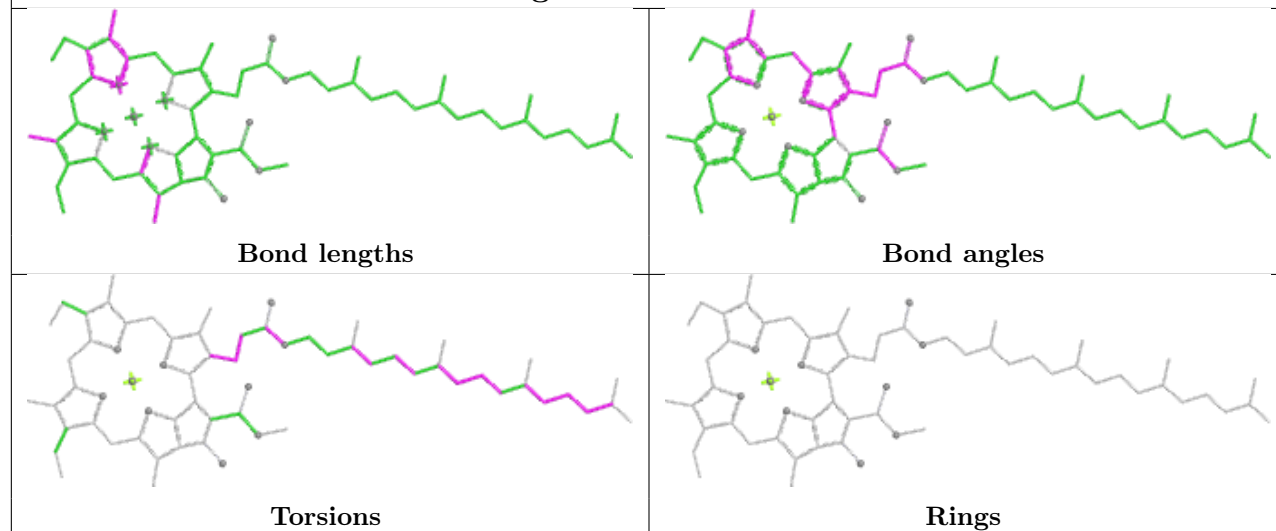
Rings

Ligand CLA f 605

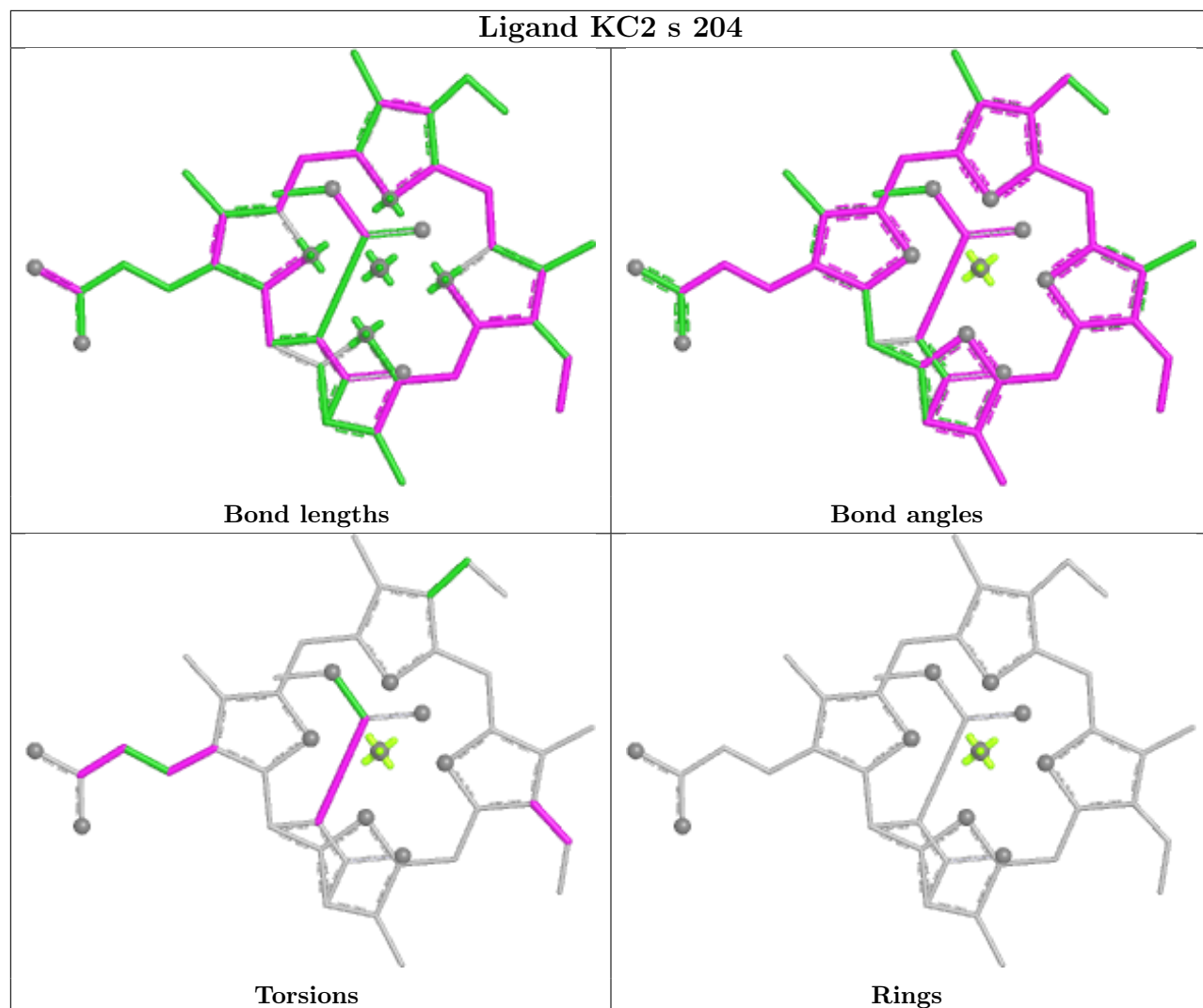


Ligand WVN A 846

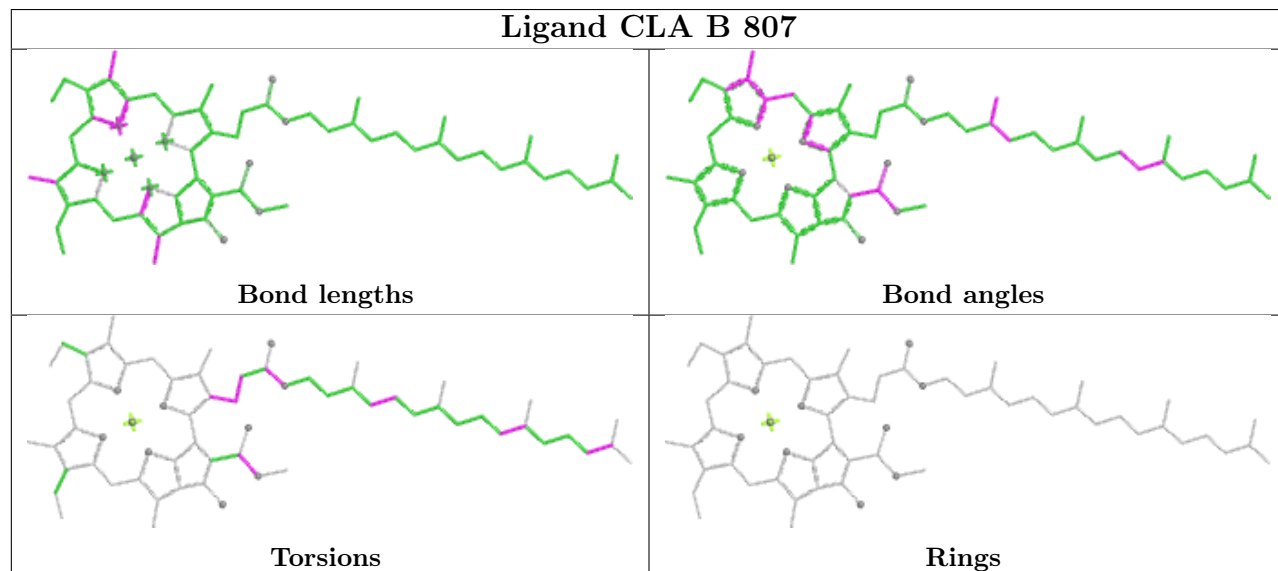


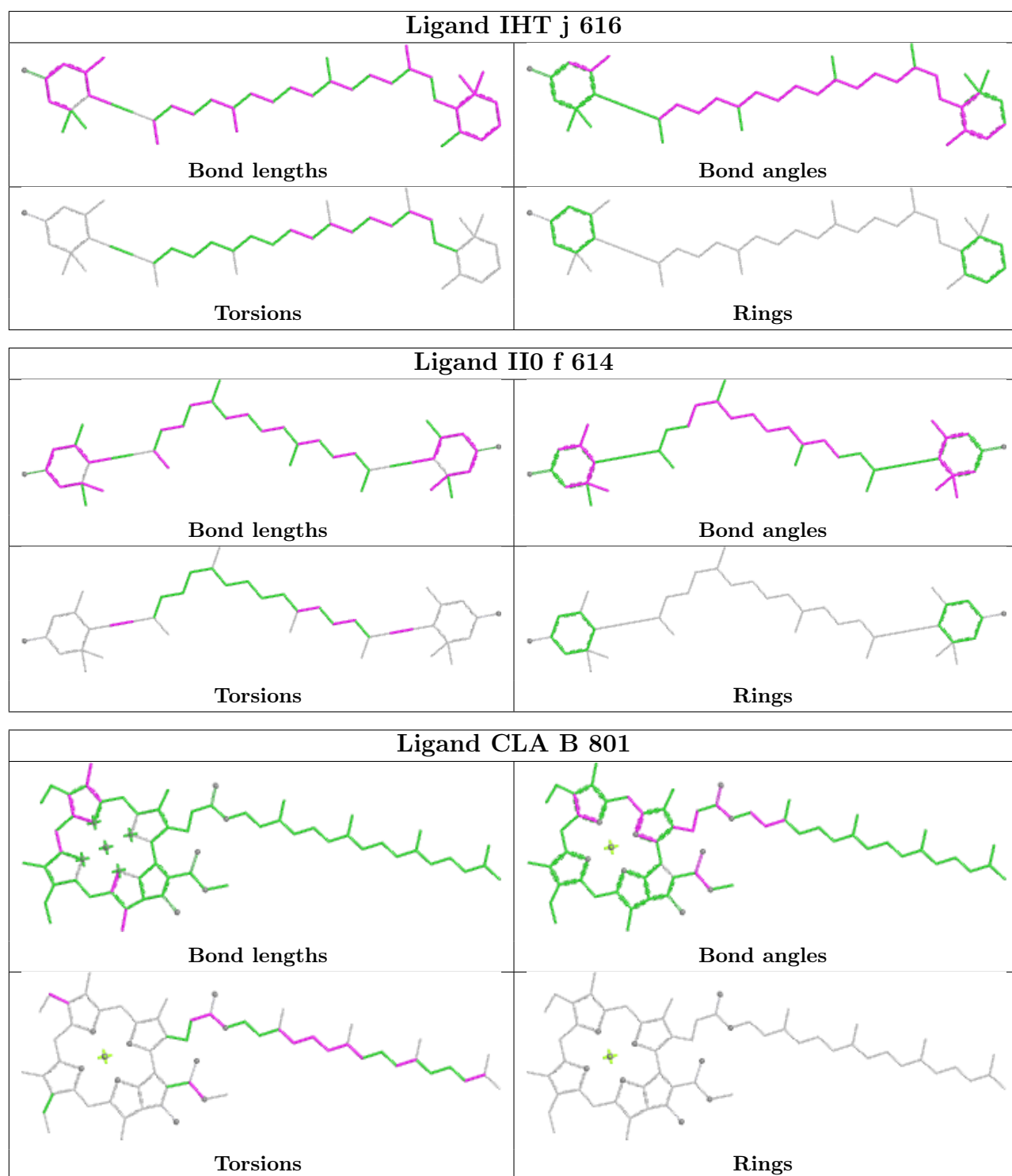
Ligand CLA B 816**Ligand CLA A 842**

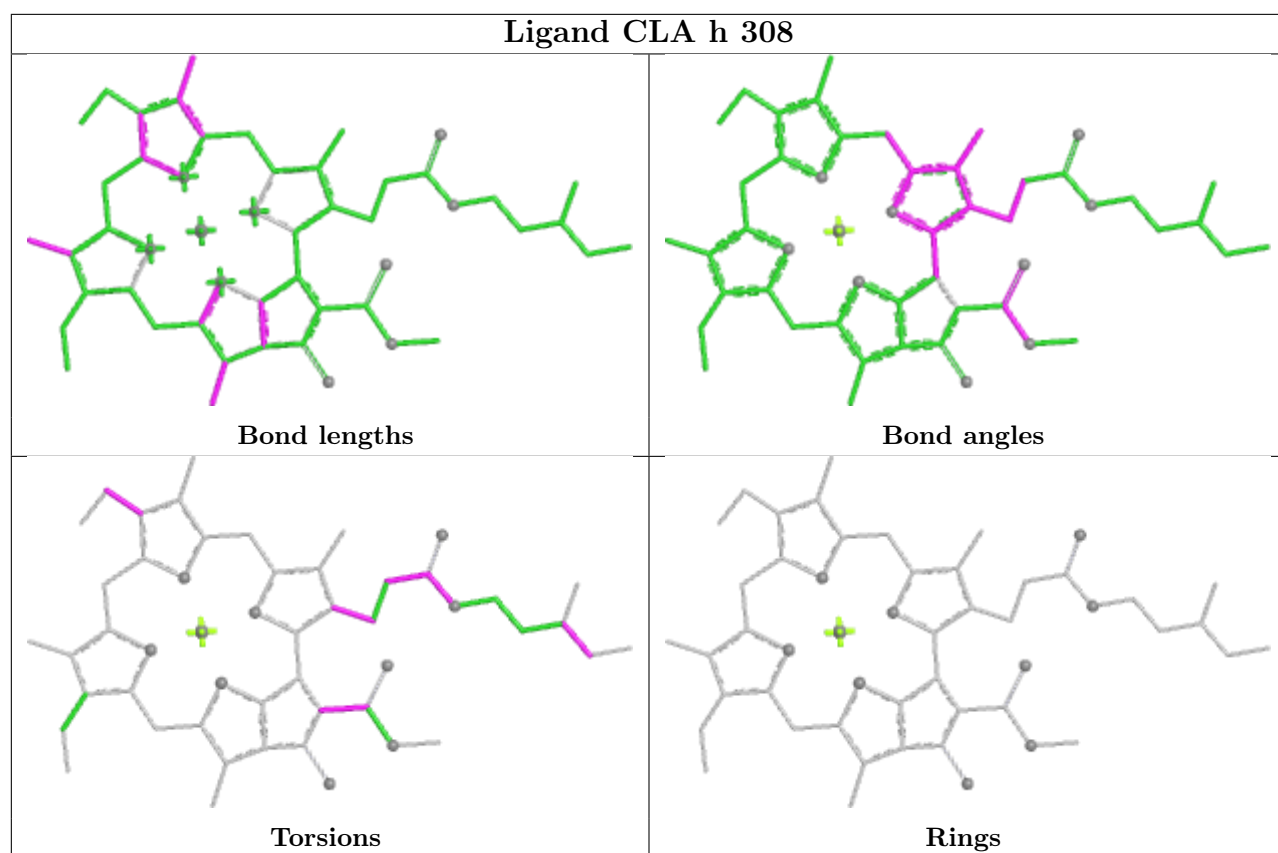
Ligand KC2 s 204

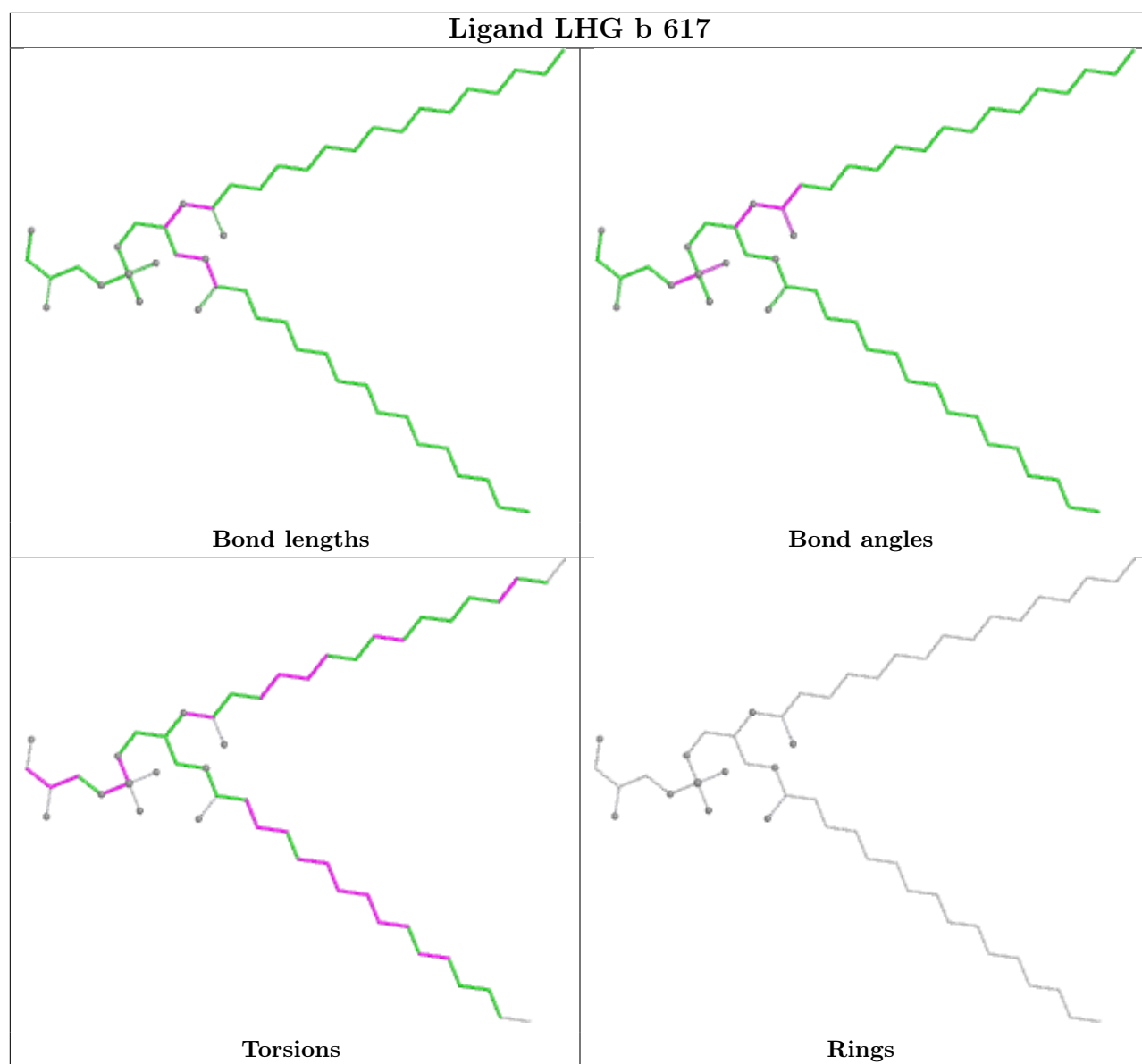


Ligand CLA B 807

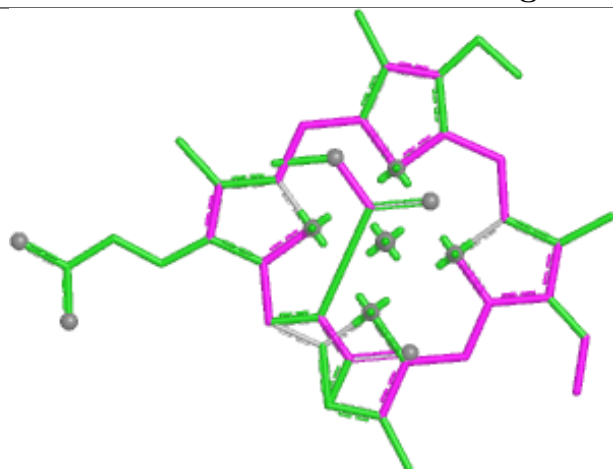




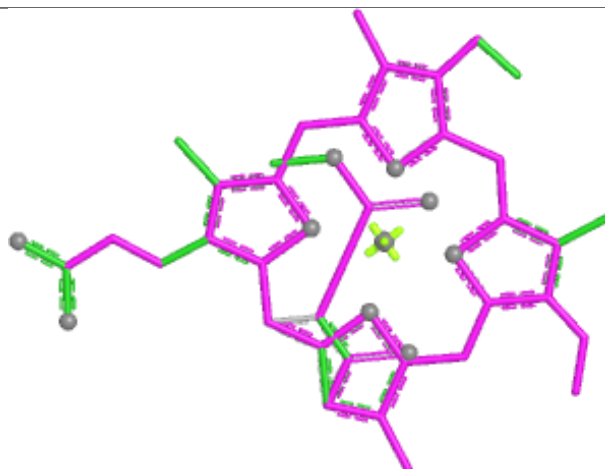




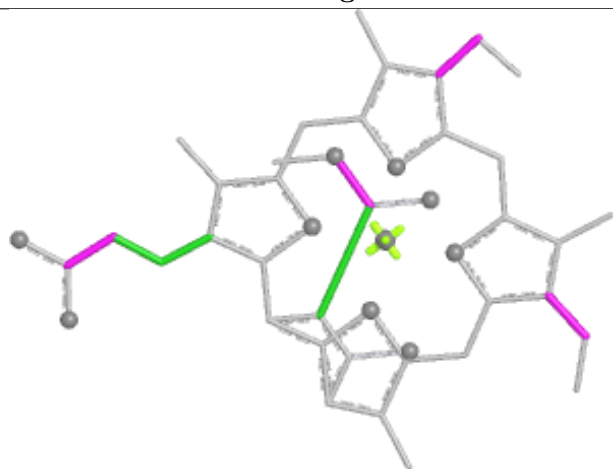
Ligand KC2 k 311



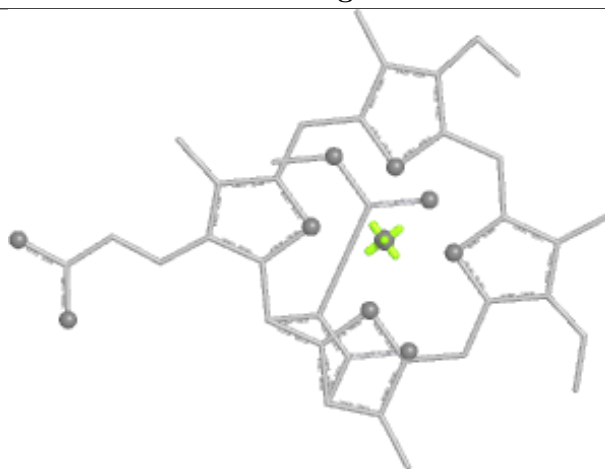
Bond lengths



Bond angles

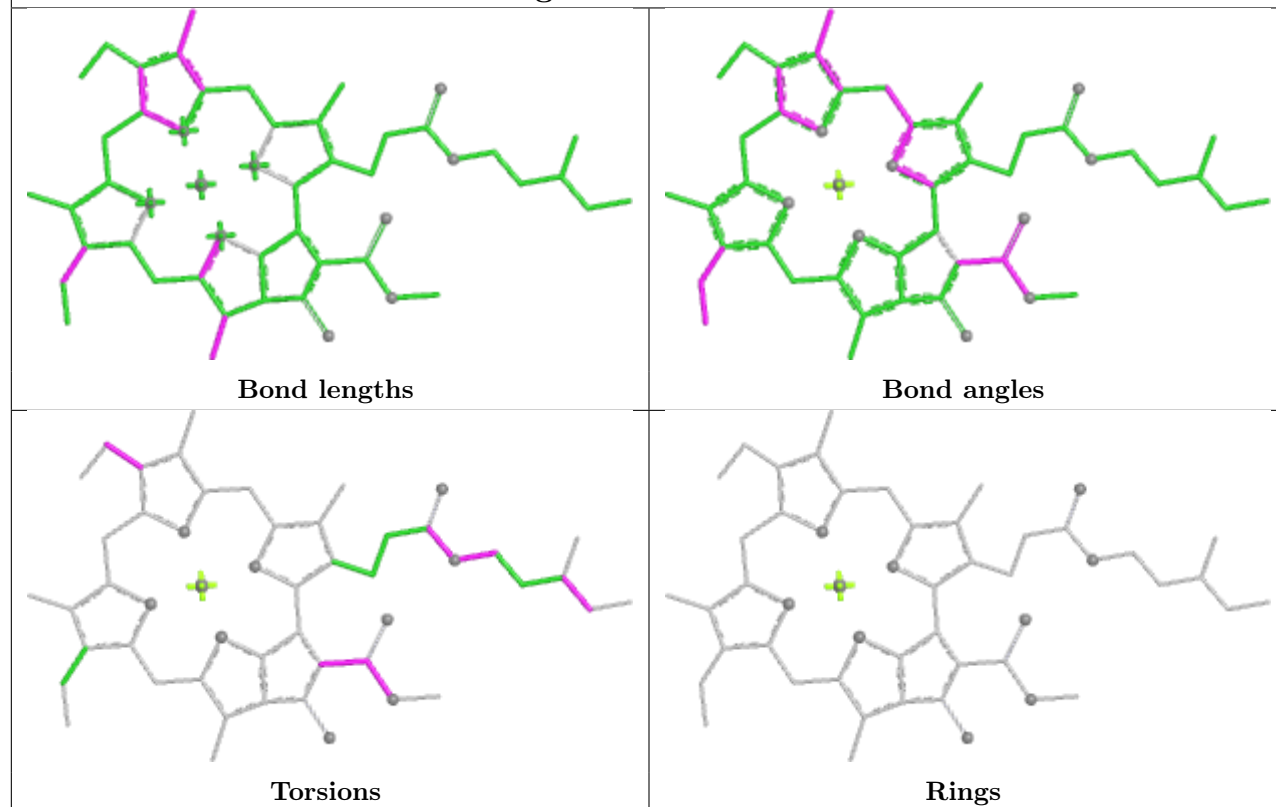


Torsions

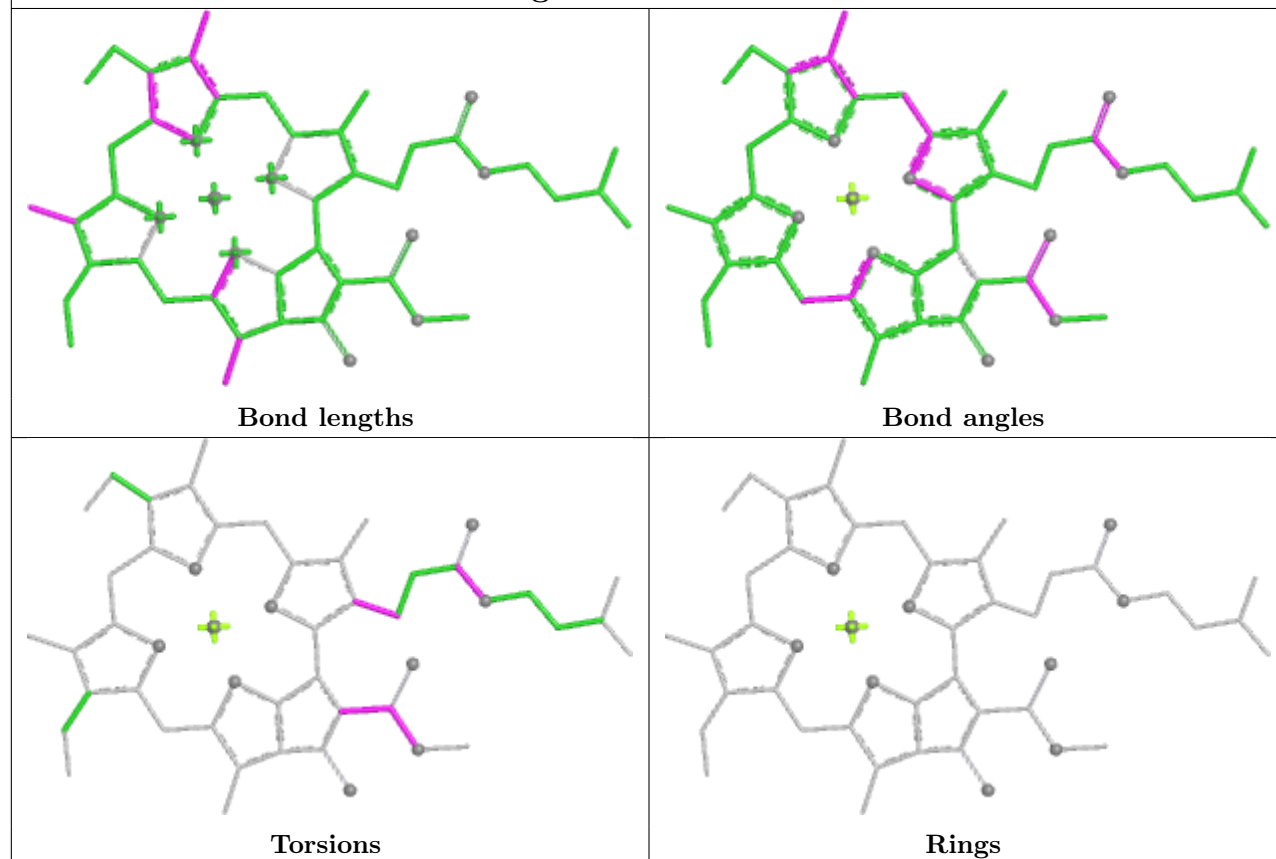


Rings

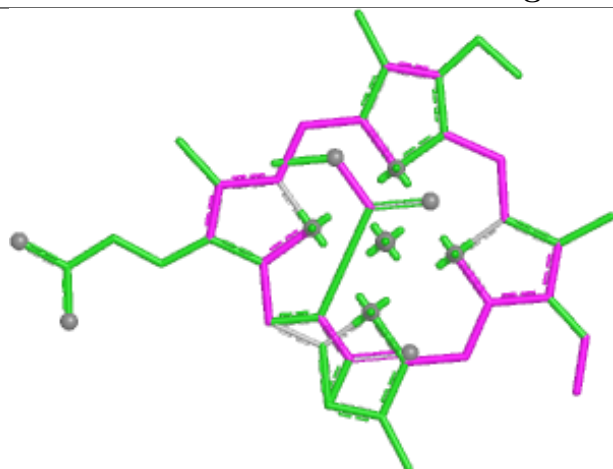
Ligand CLA b 601



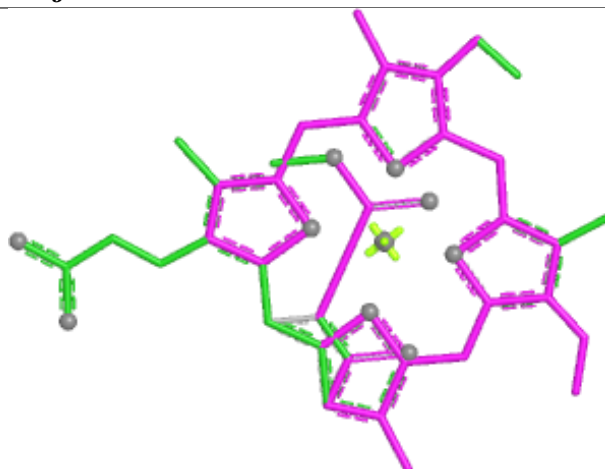
Ligand CLA A 814



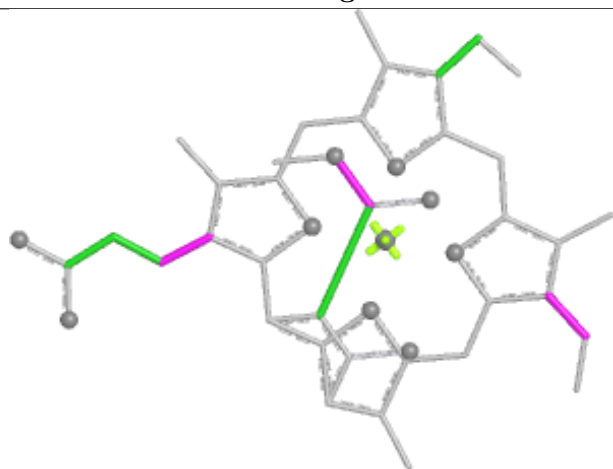
Ligand KC2 j 610



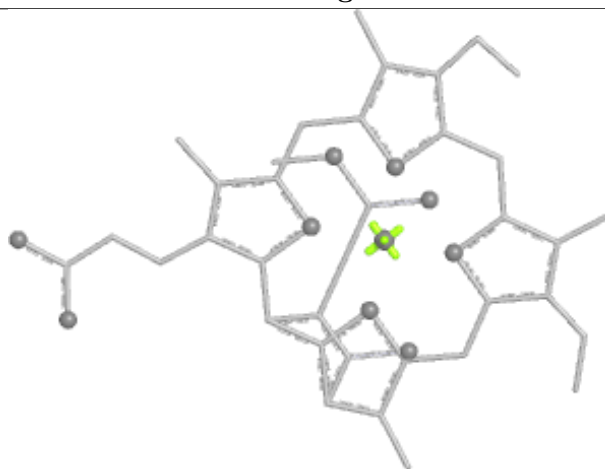
Bond lengths



Bond angles

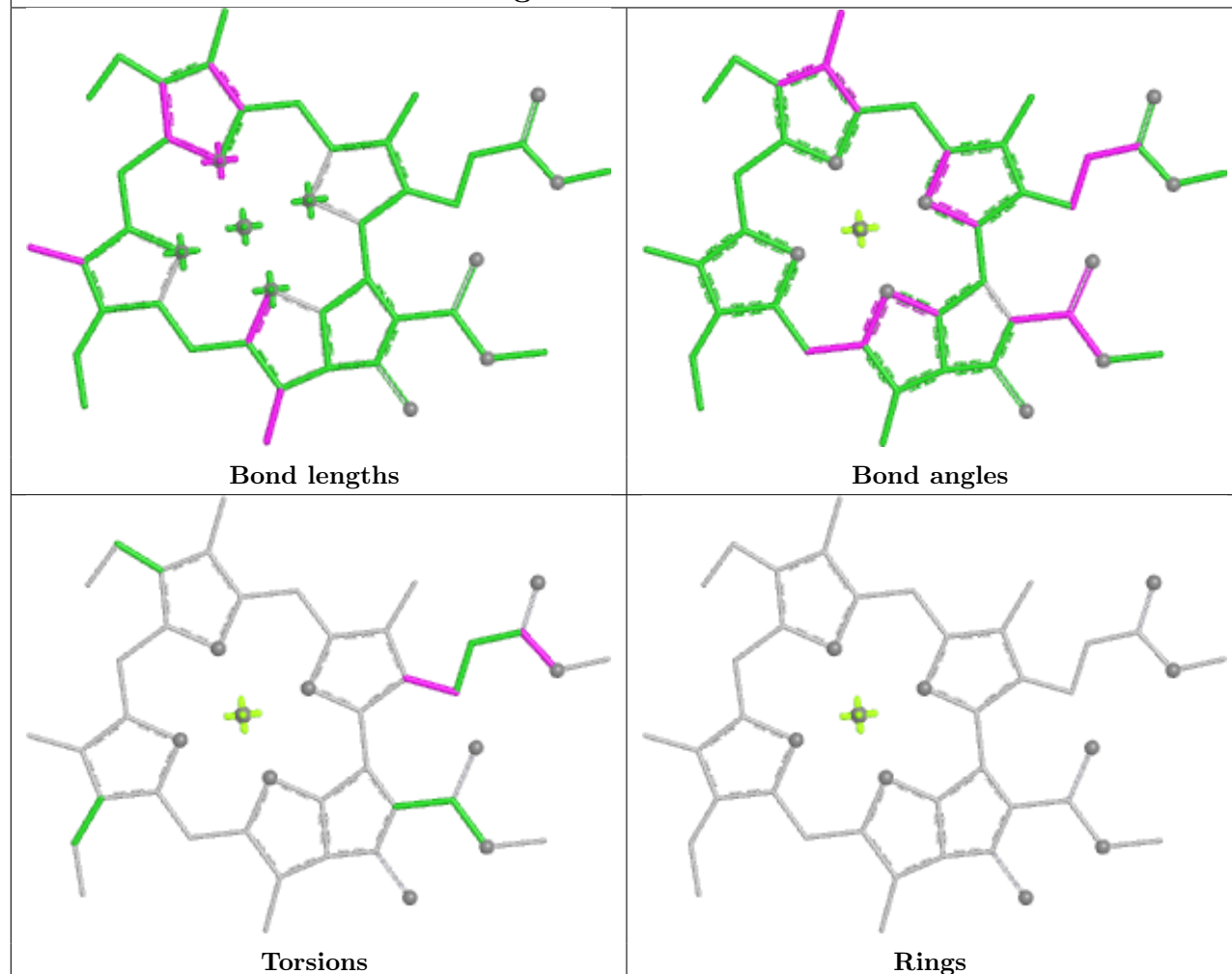


Torsions

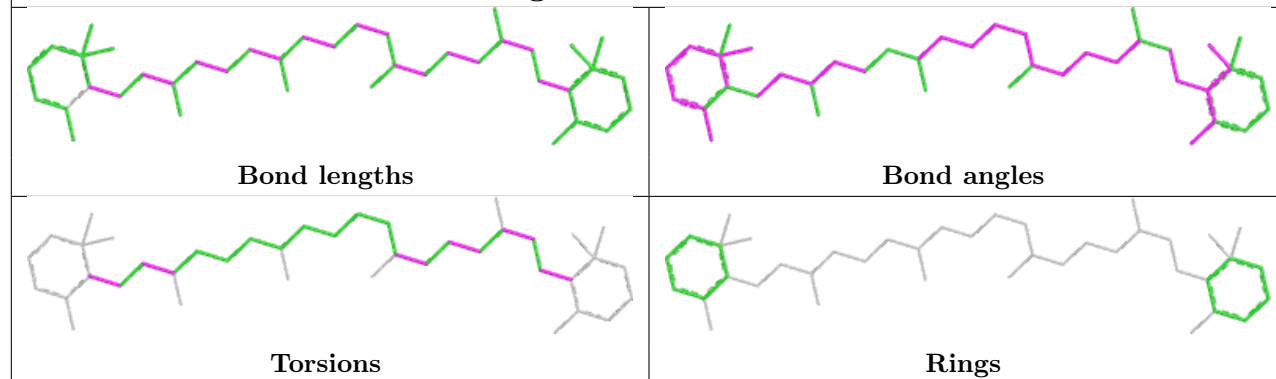


Rings

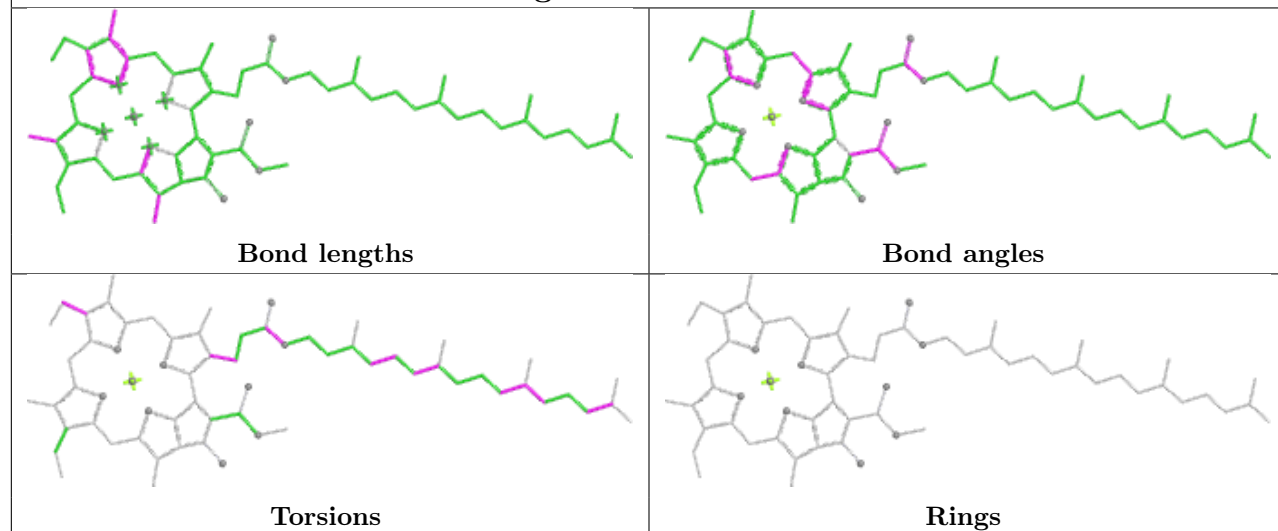
Ligand CLA B 817



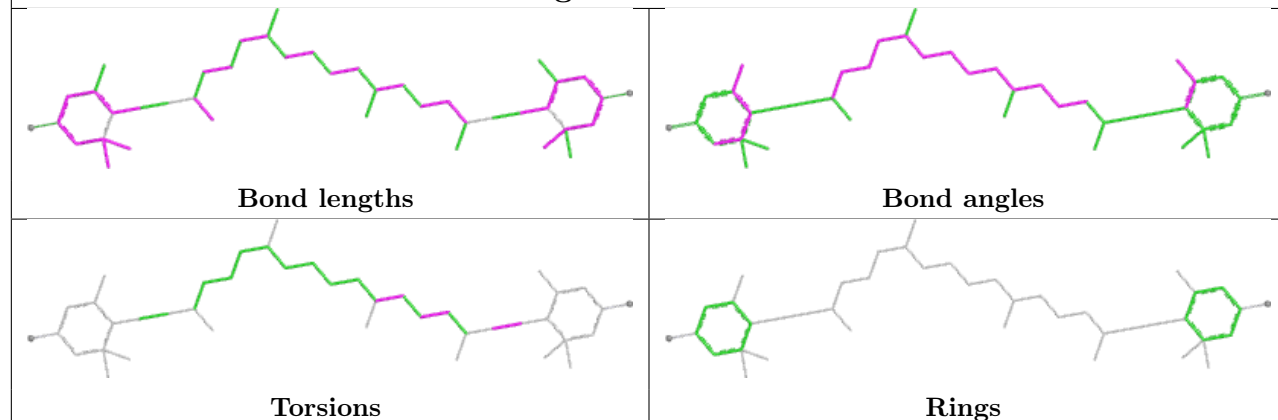
Ligand WVN e 615



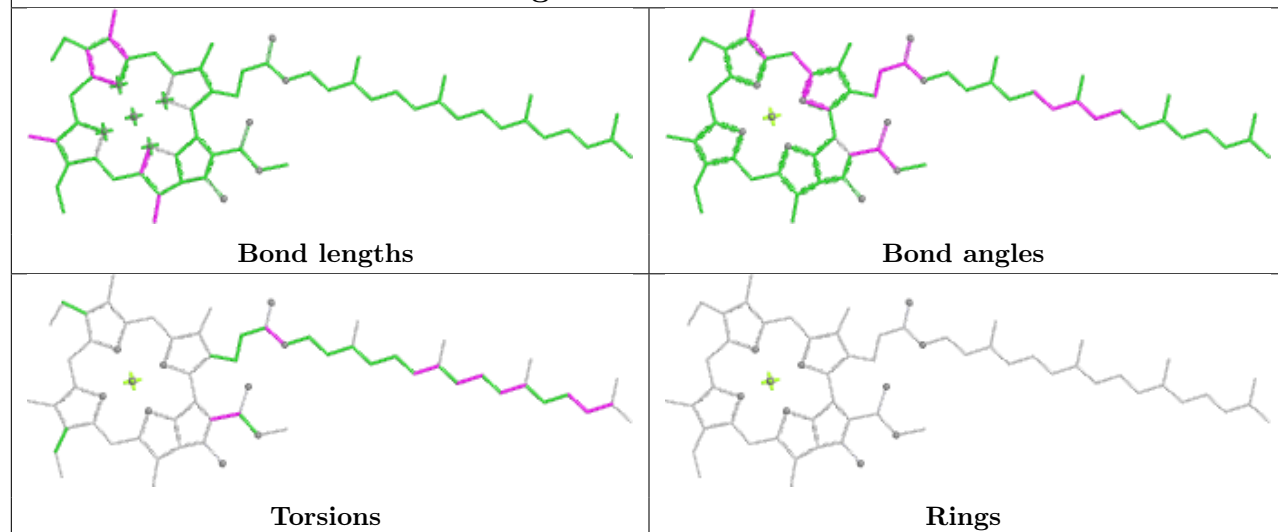
Ligand CLA L 203



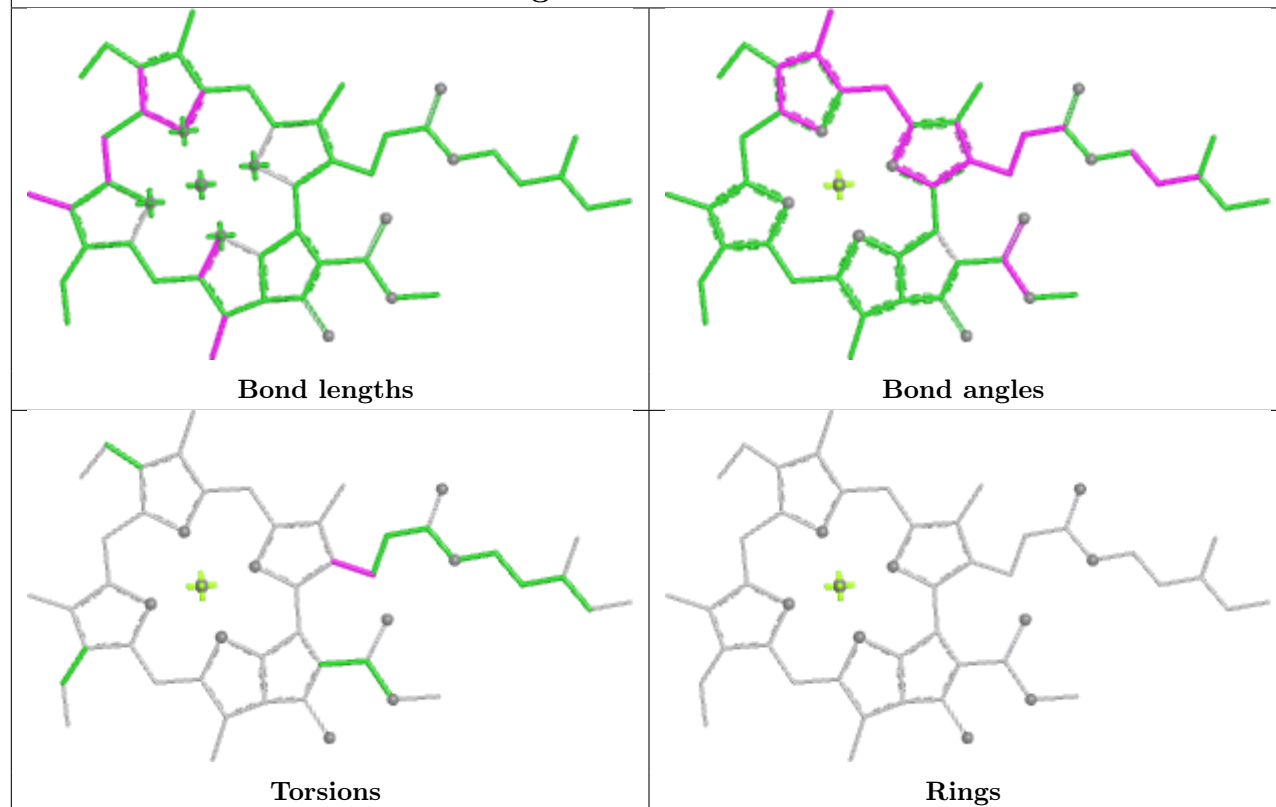
Ligand II0 i 313



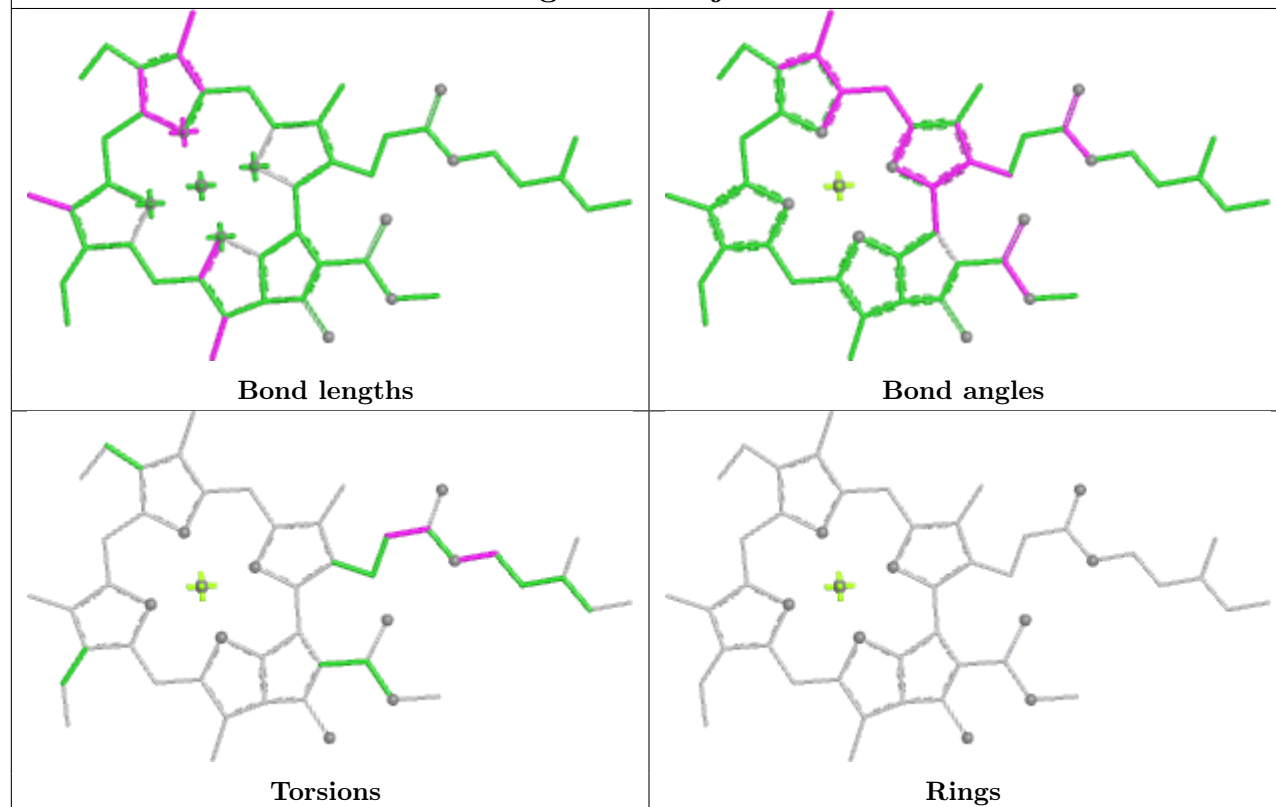
Ligand CLA A 806



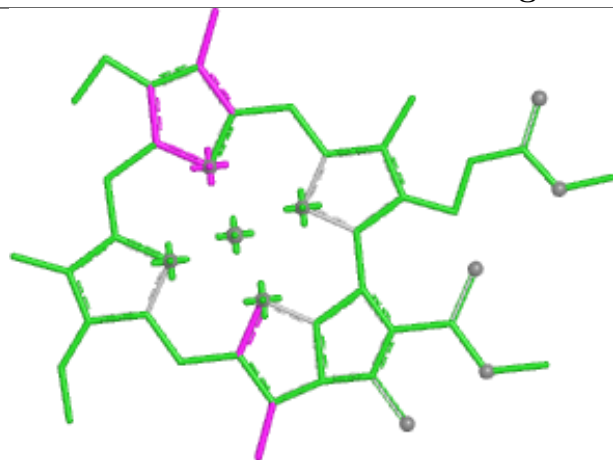
Ligand CLA A 834



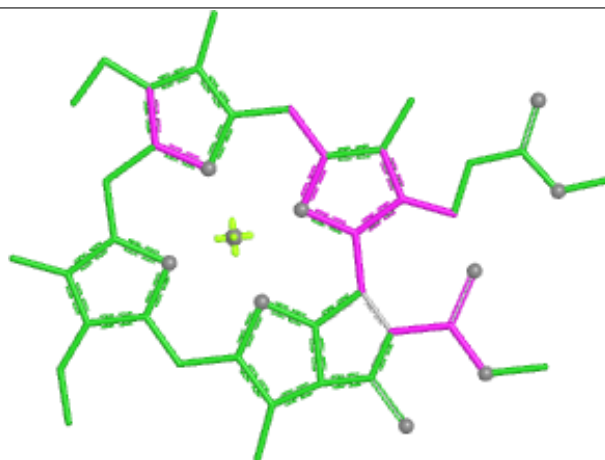
Ligand CLA j 603



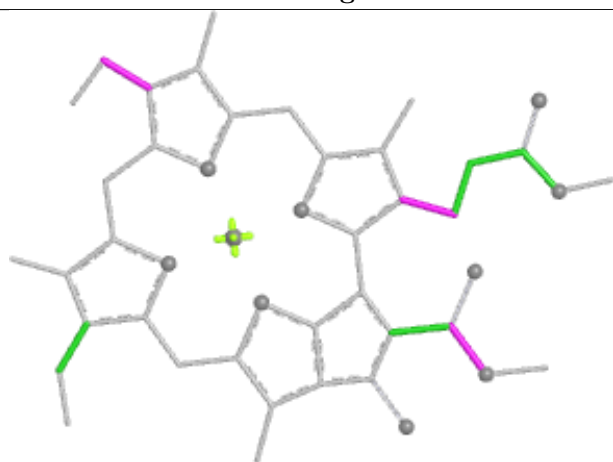
Ligand CLA e 608



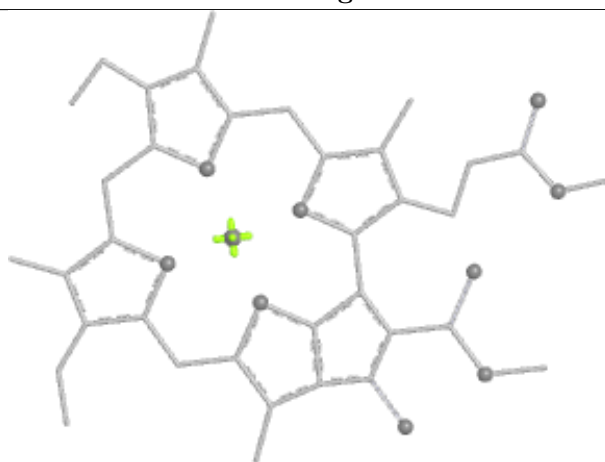
Bond lengths



Bond angles

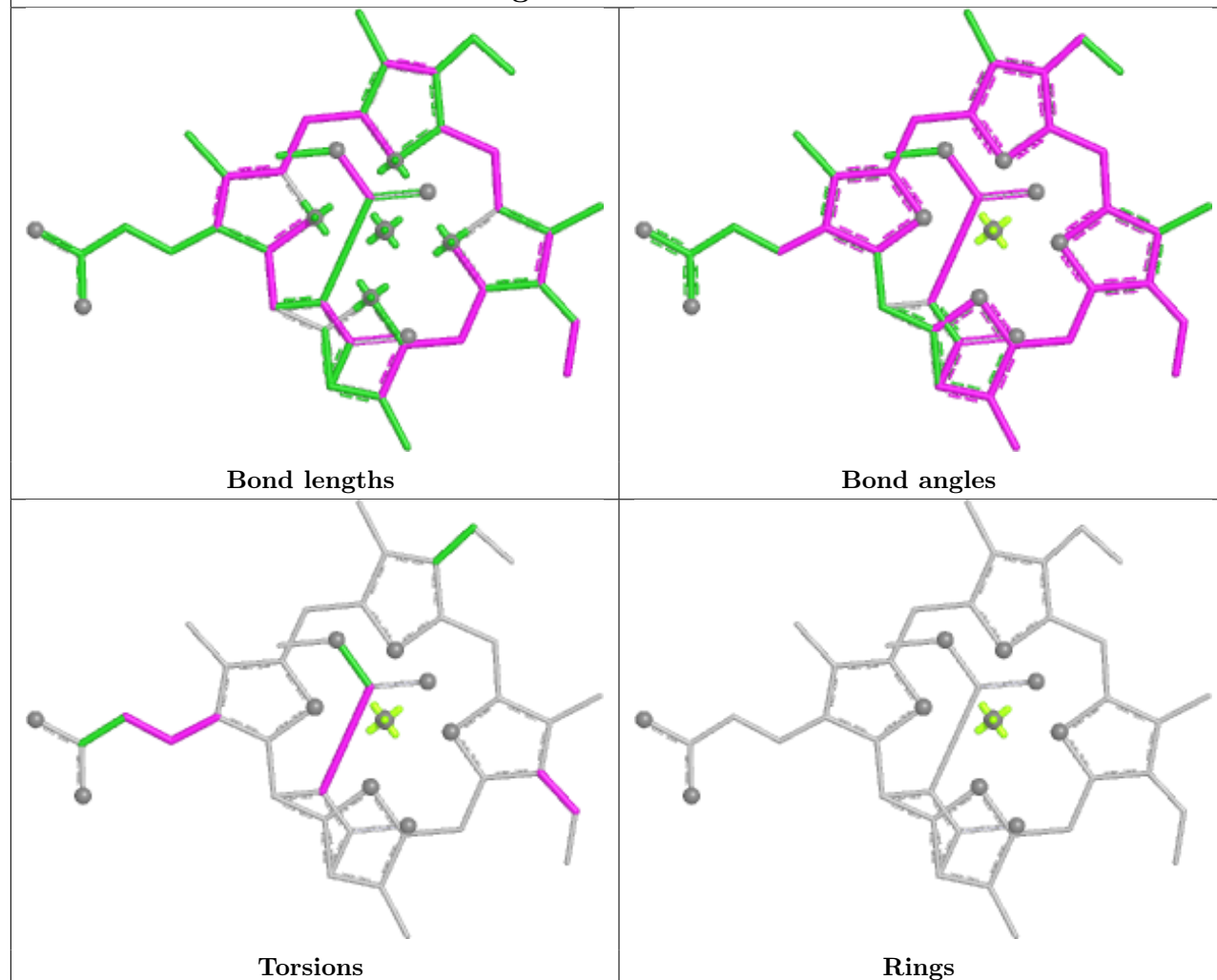


Torsions

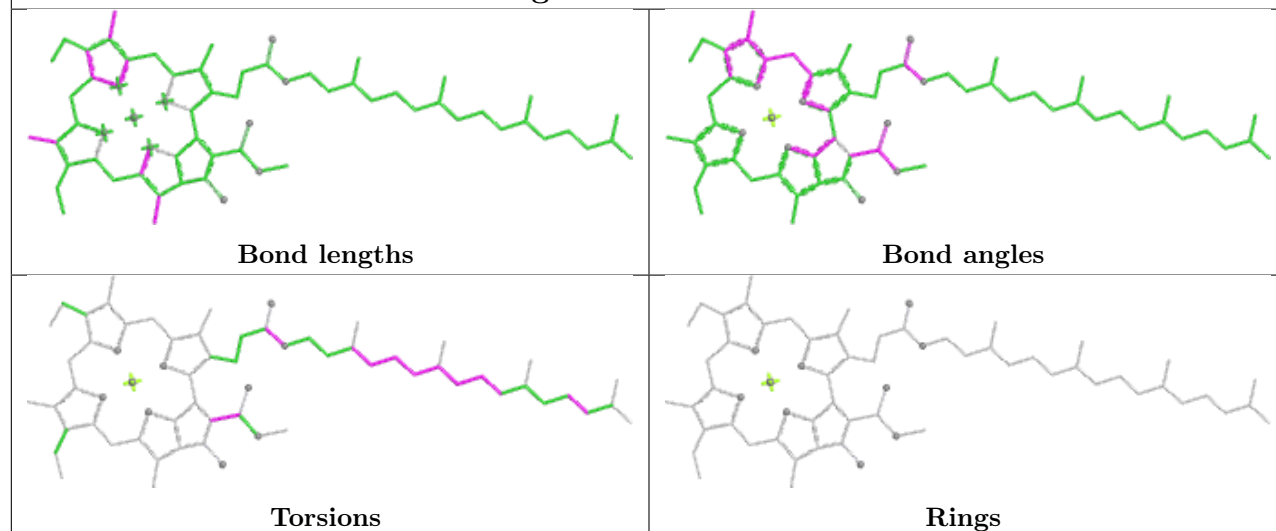


Rings

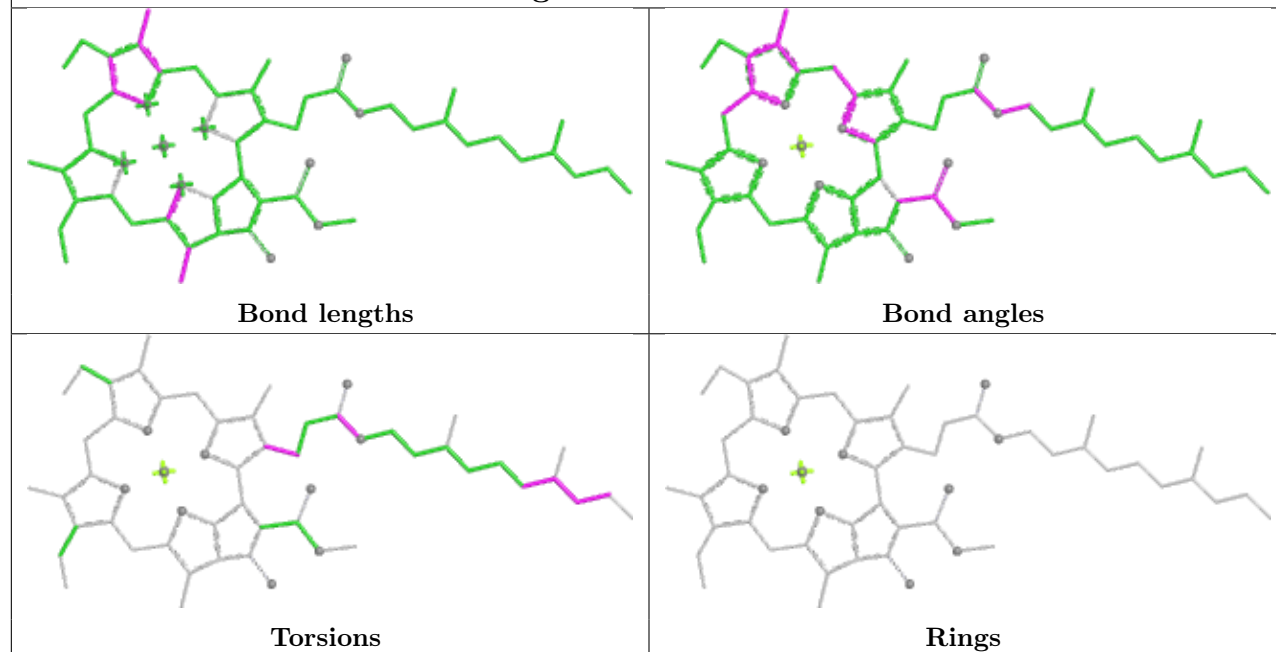
Ligand KC2 n 612



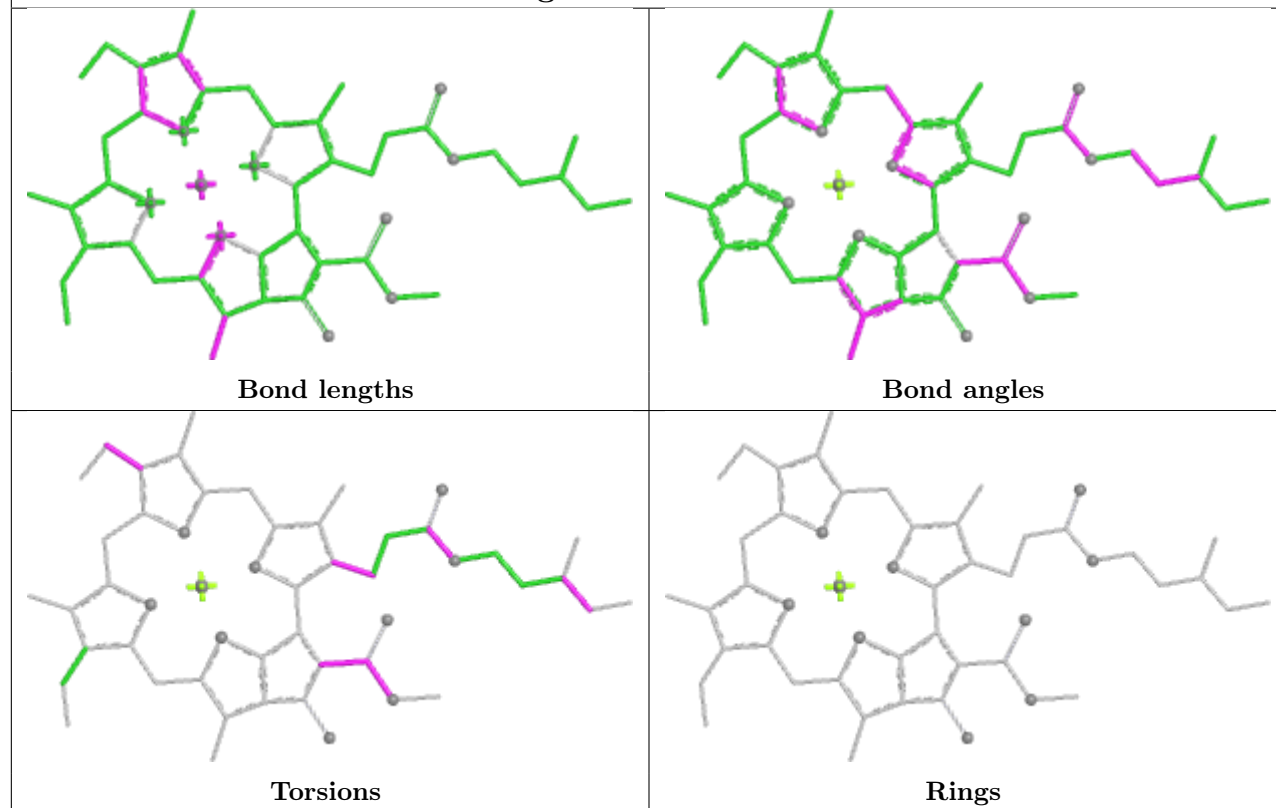
Ligand CLA A 829

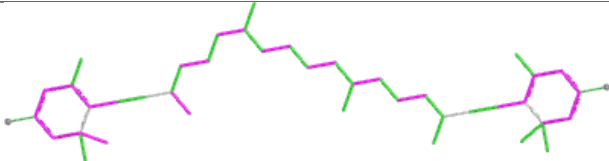
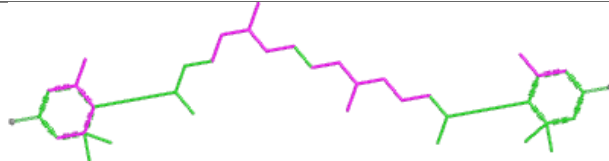
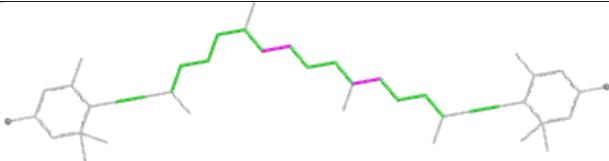
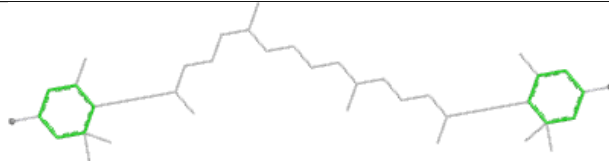


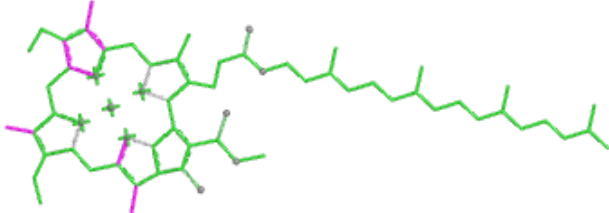
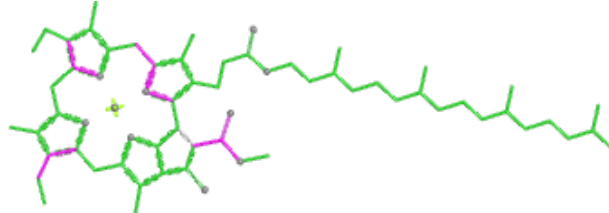
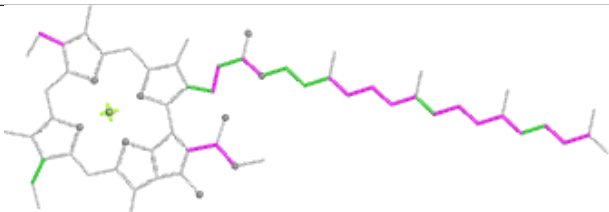
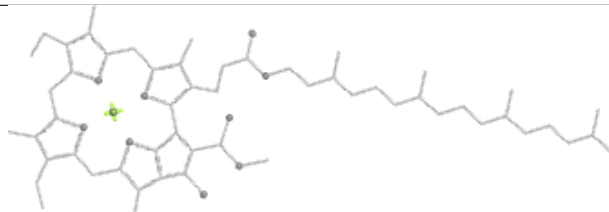
Ligand CLA B 815

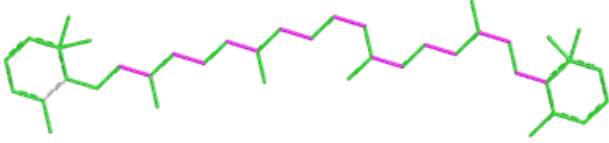
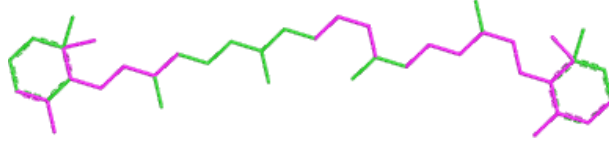
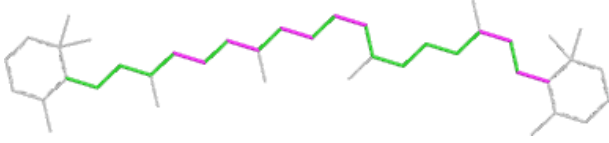
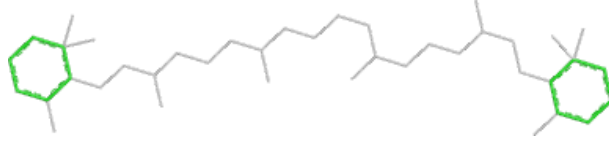


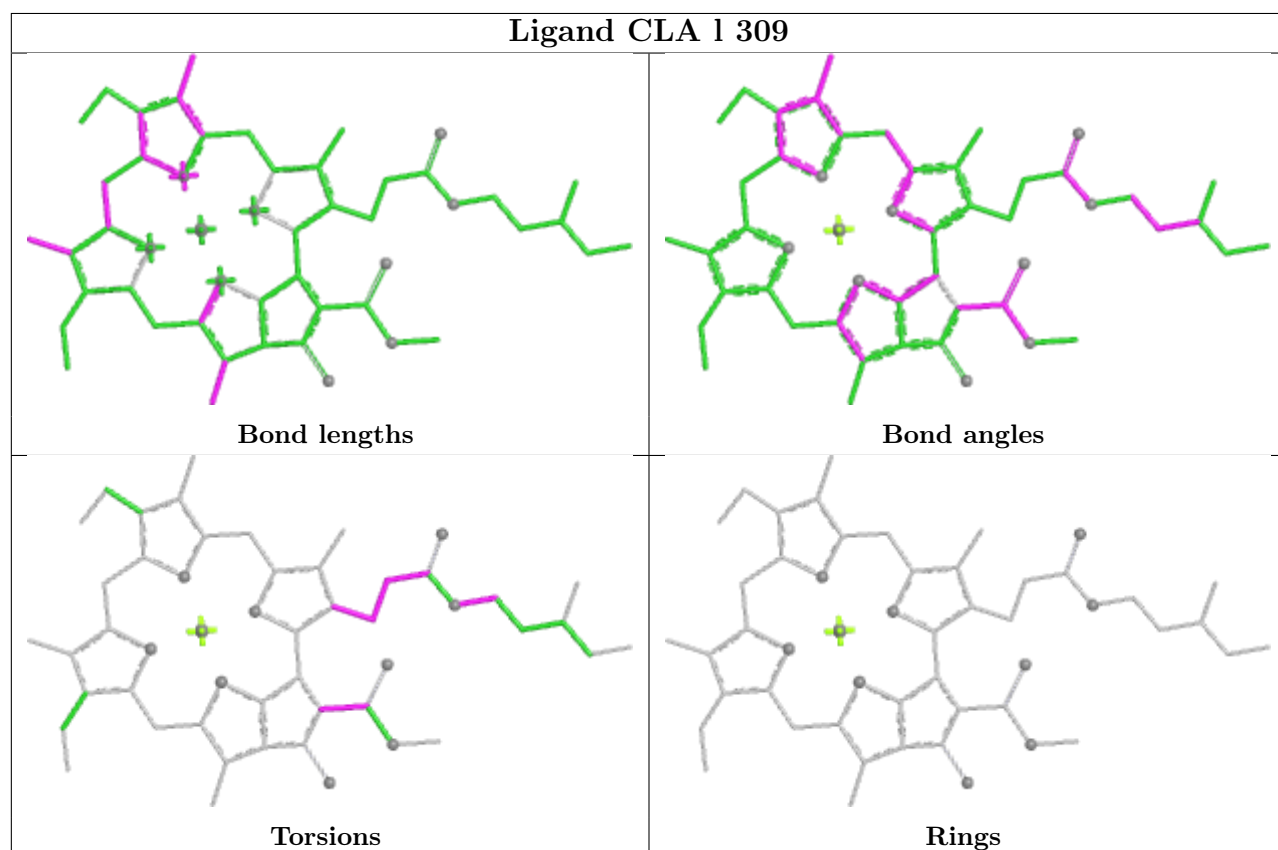
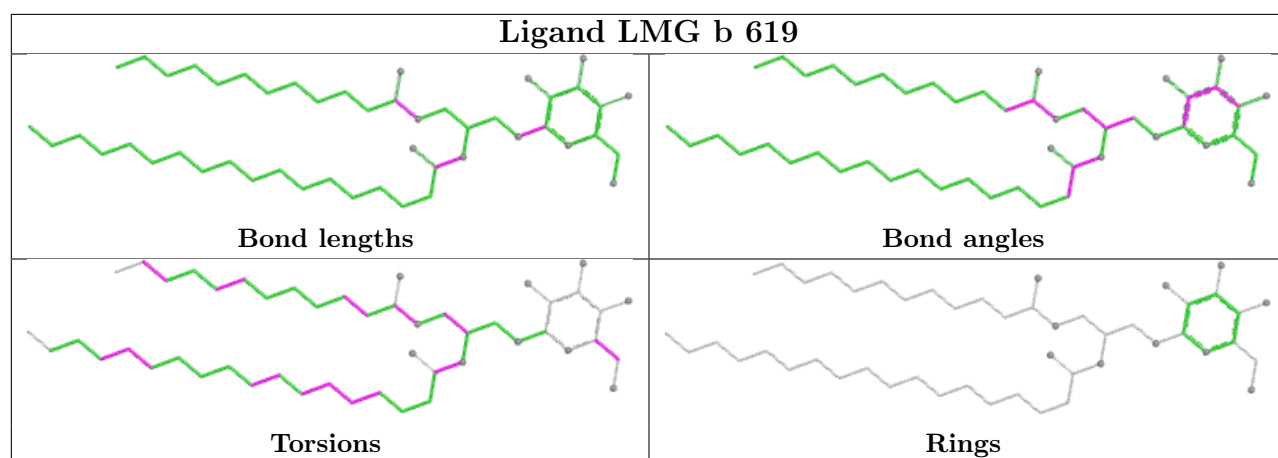
Ligand CLA c 601



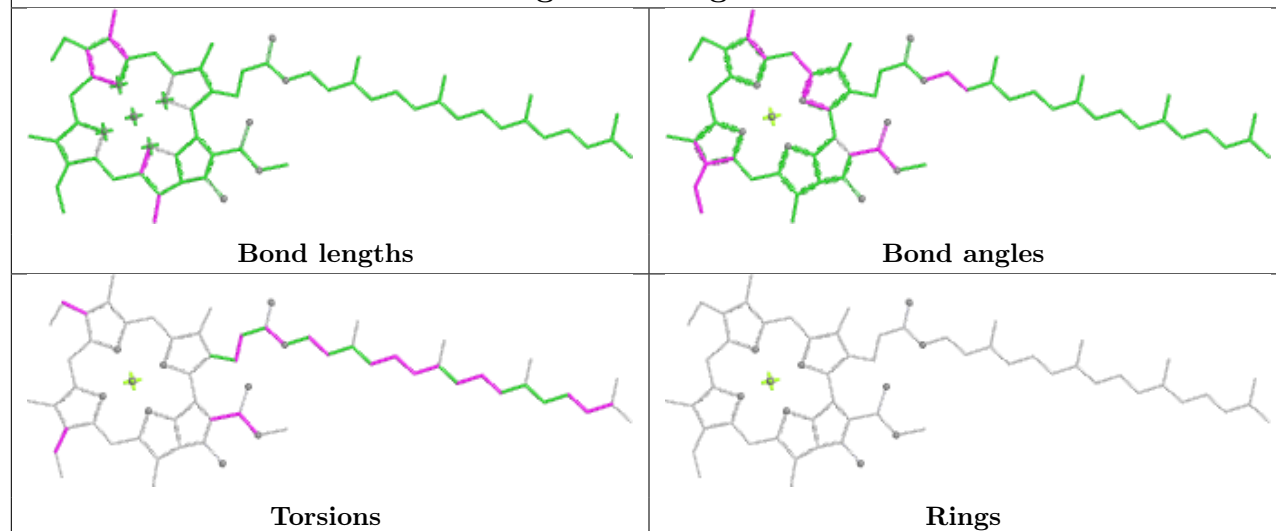
Ligand II0 k 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

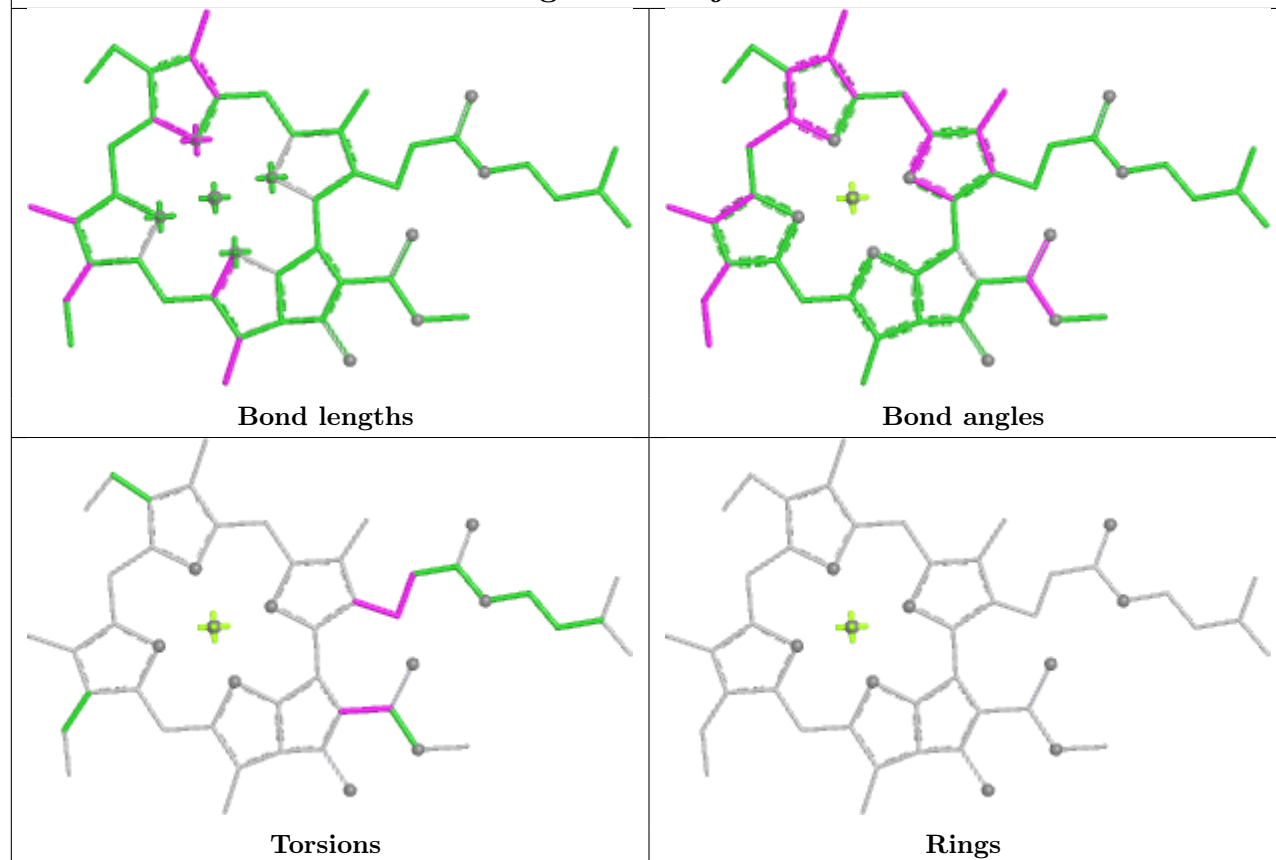
Ligand WVN O 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

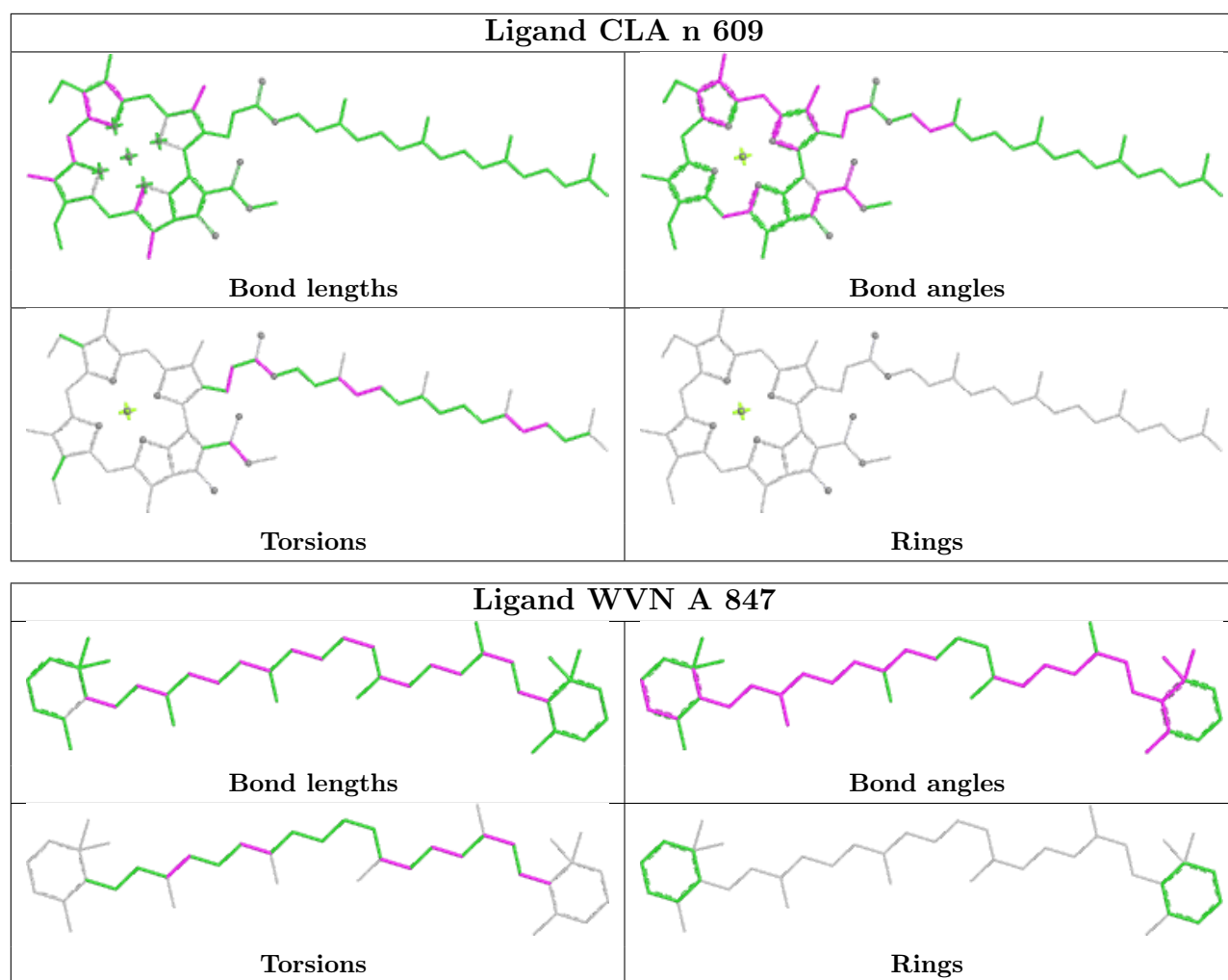


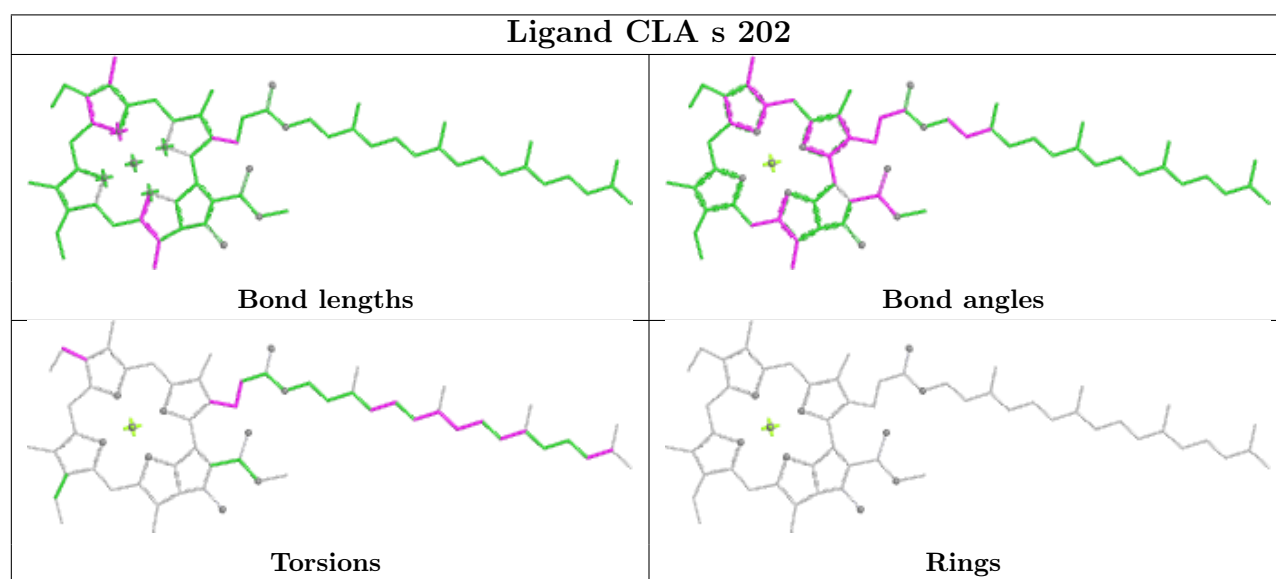
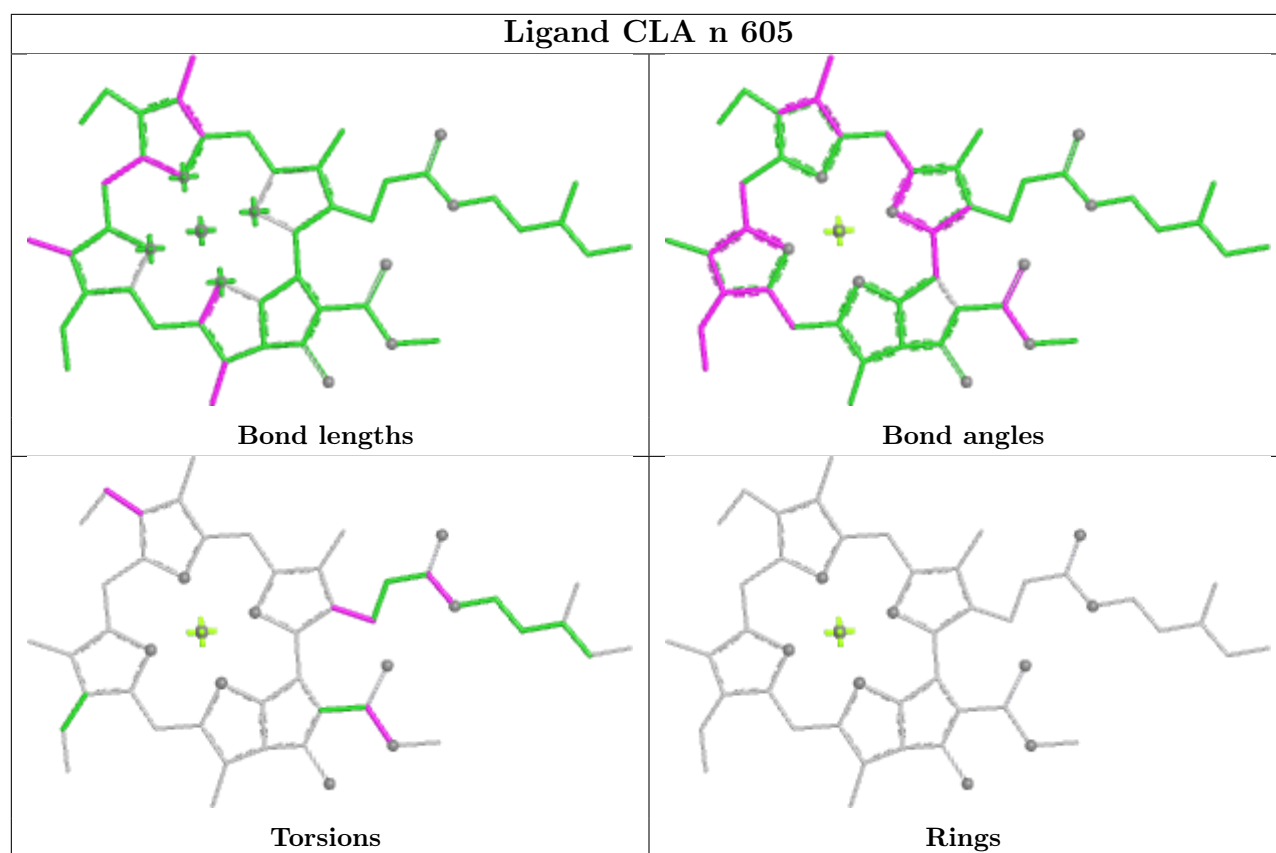
Ligand CLA g 322

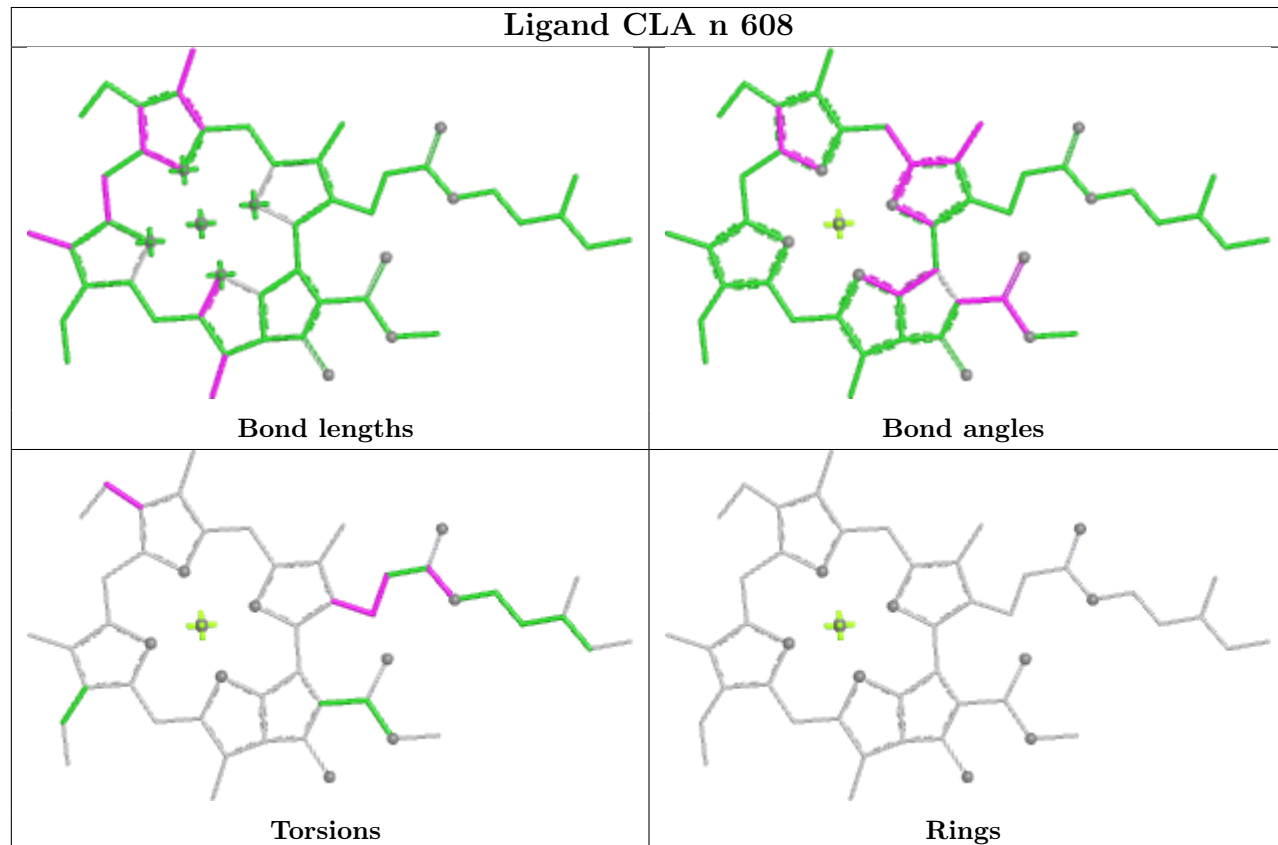
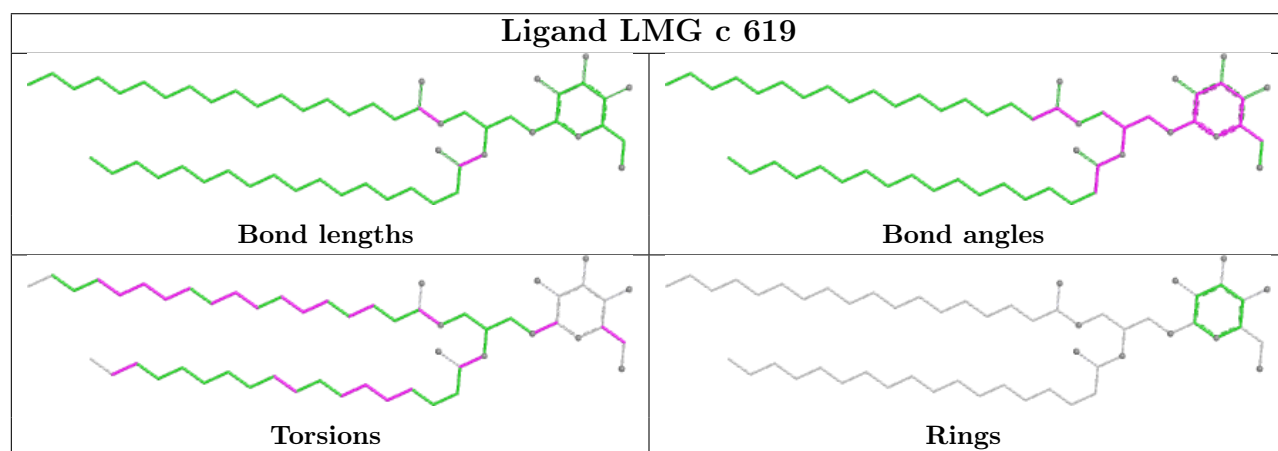
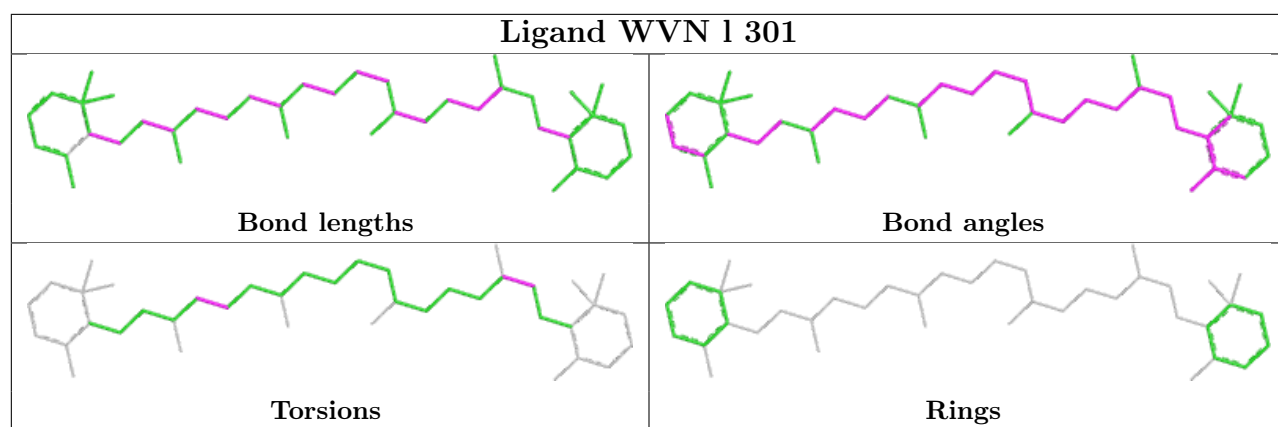


Ligand CLA j 602

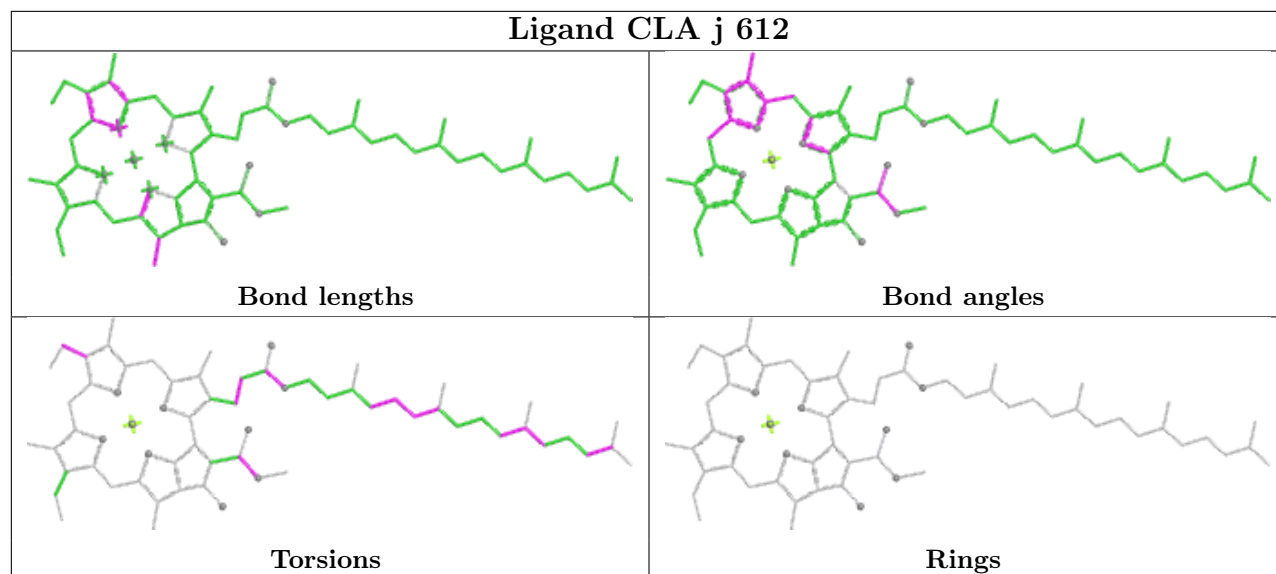




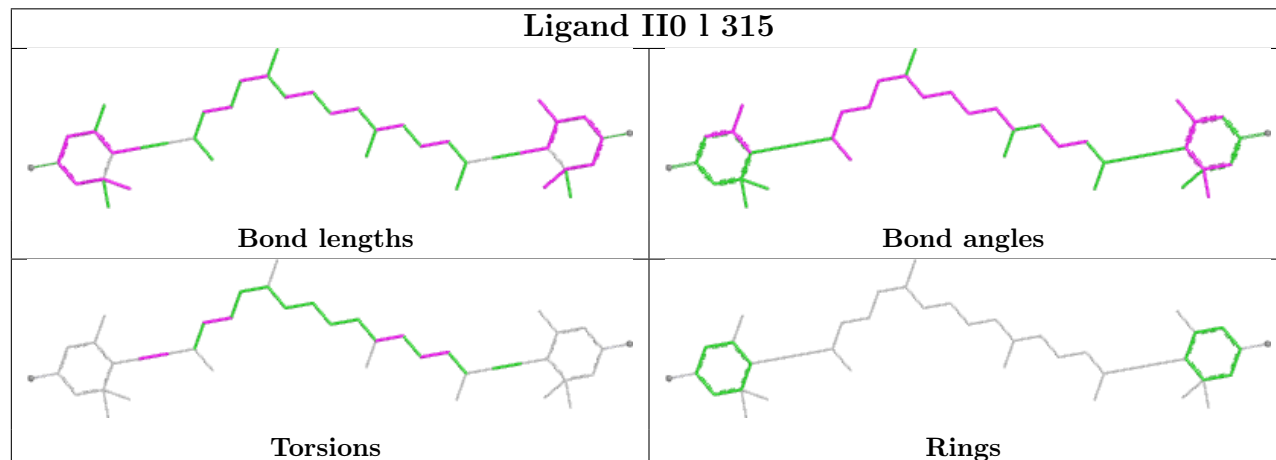




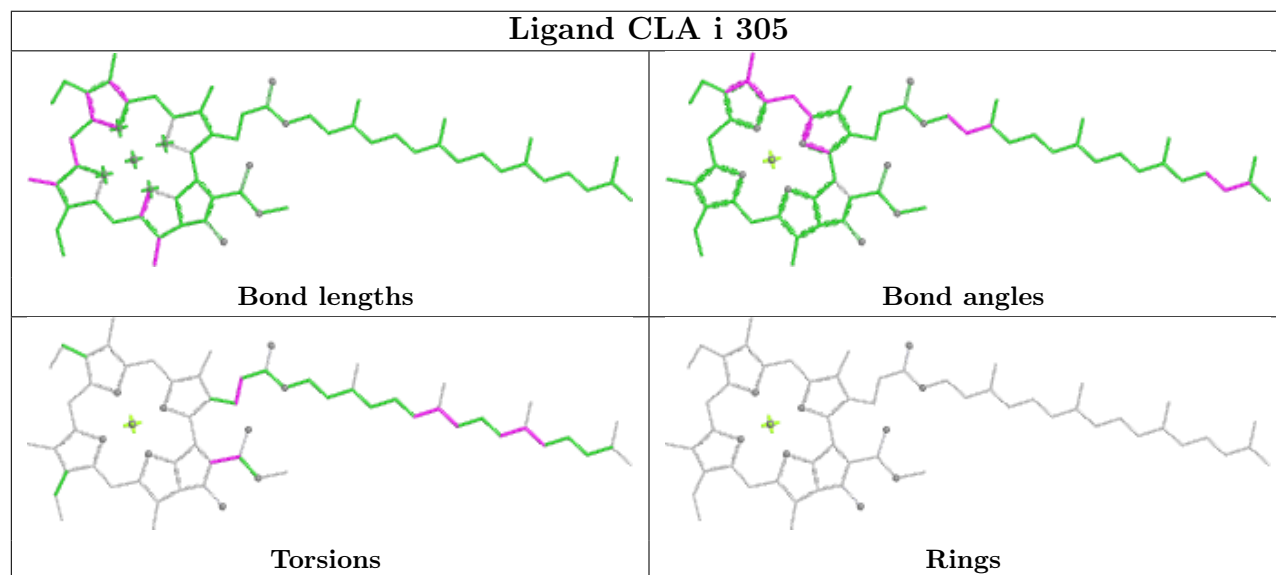
Ligand CLA j 612

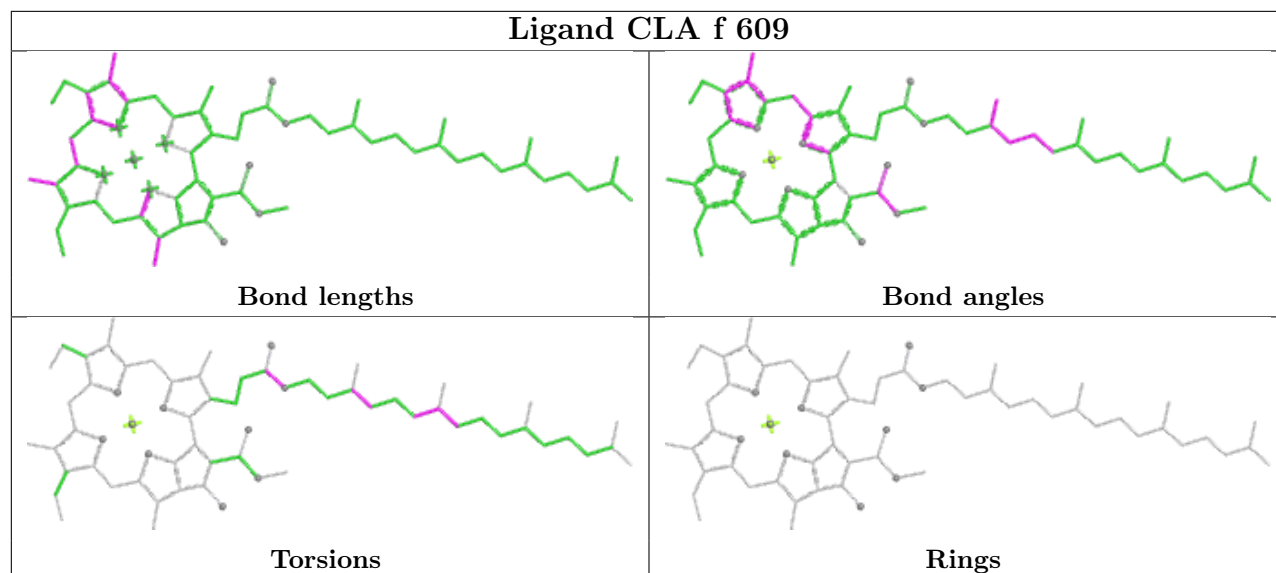
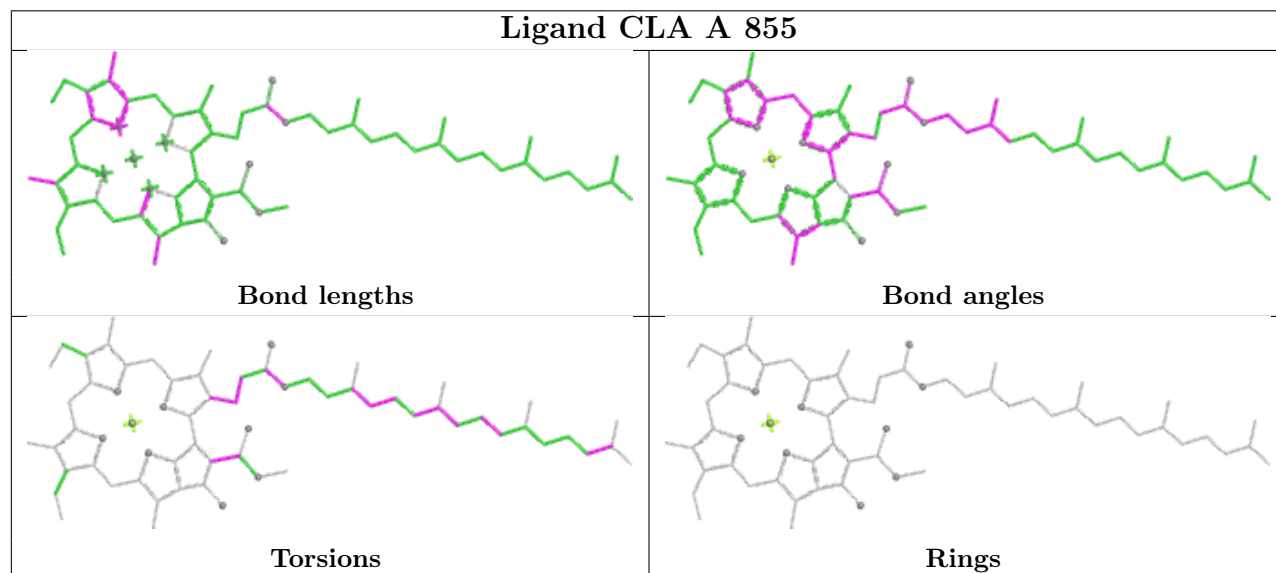
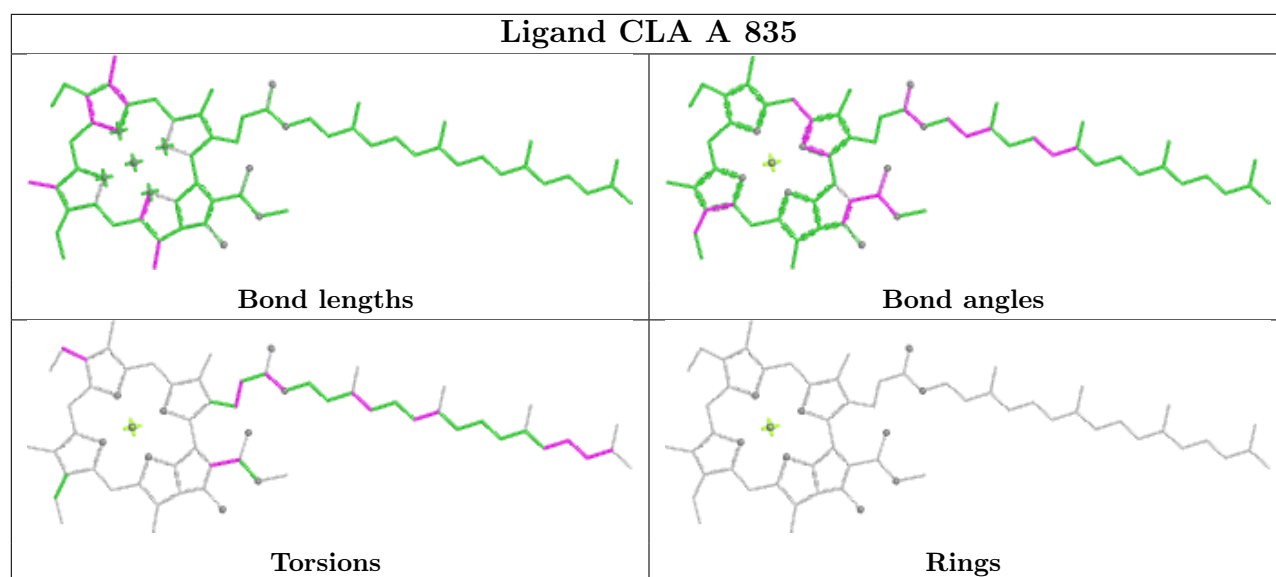


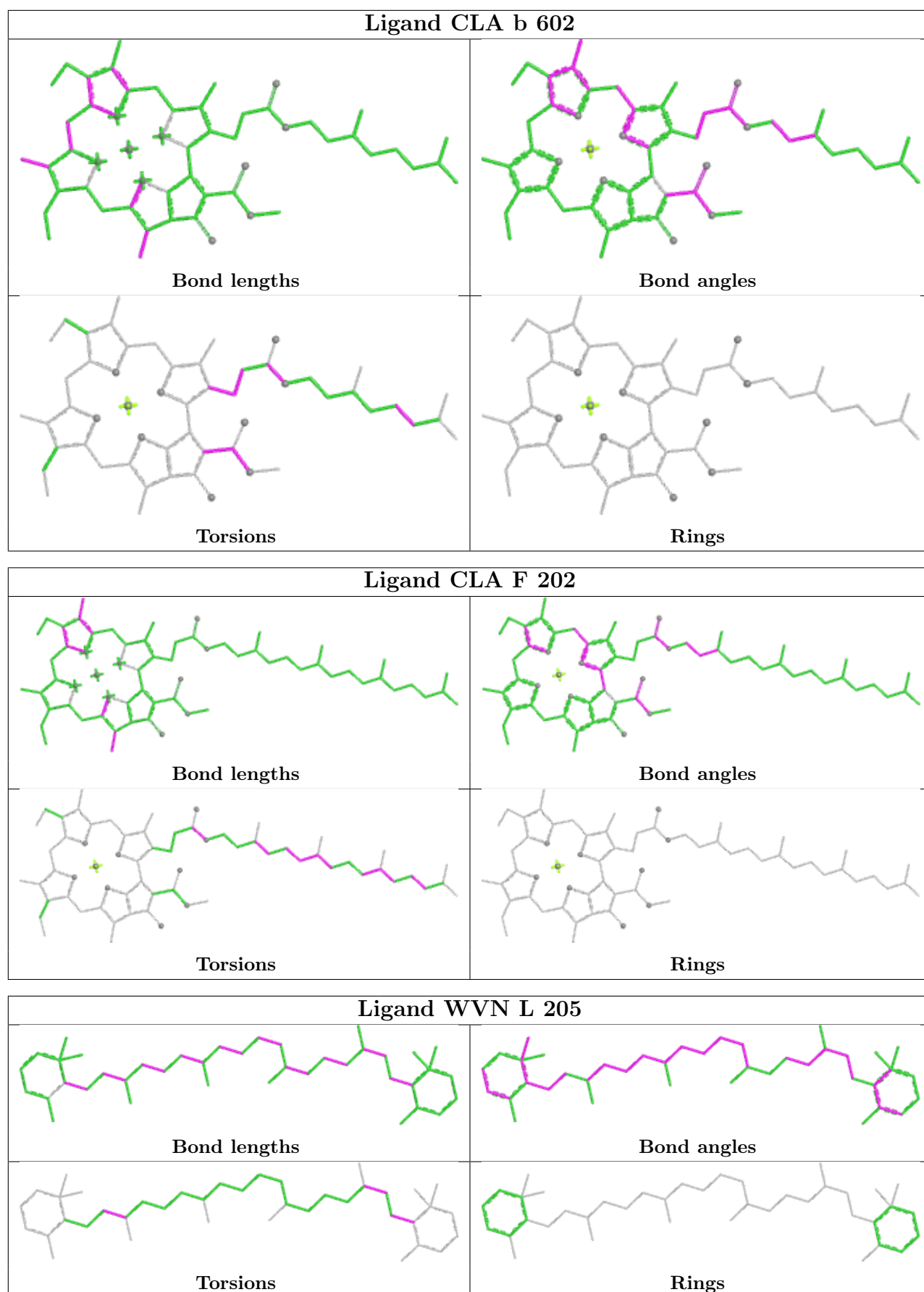
Ligand II0 l 315



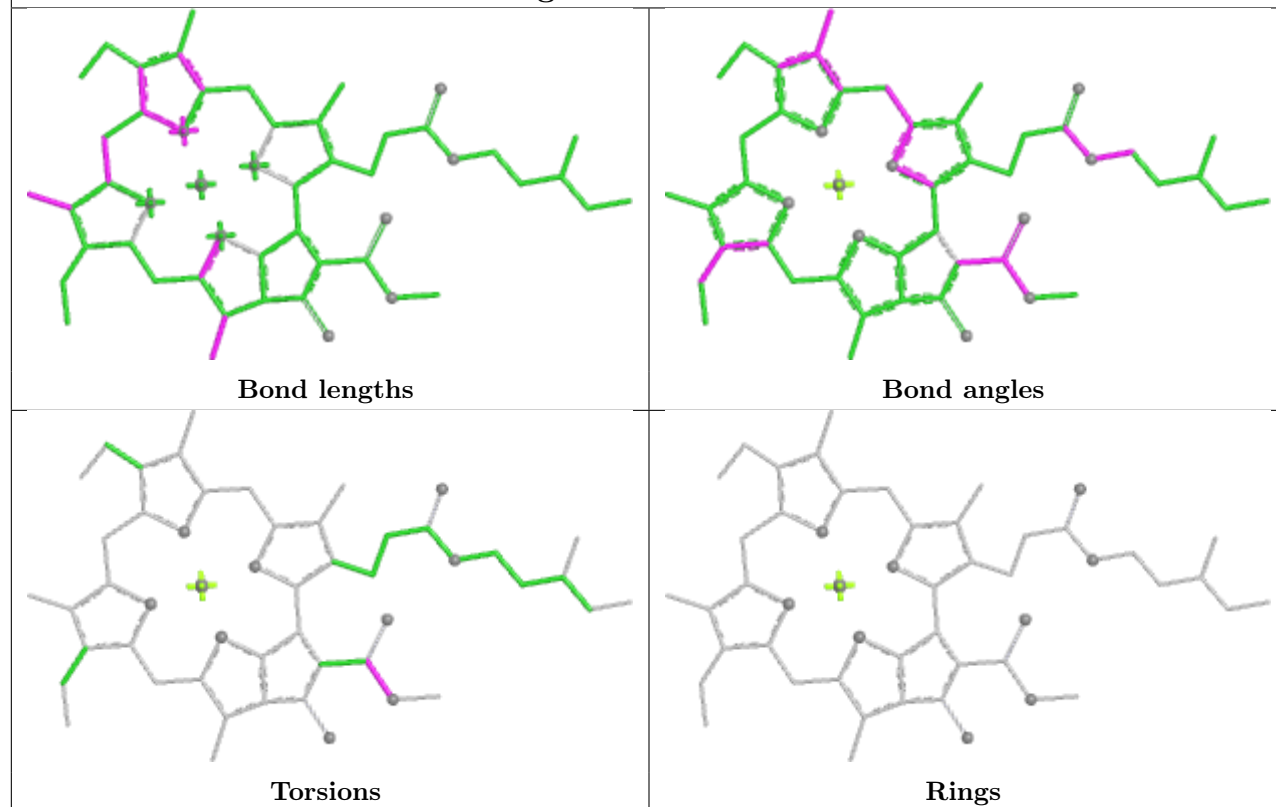
Ligand CLA i 305



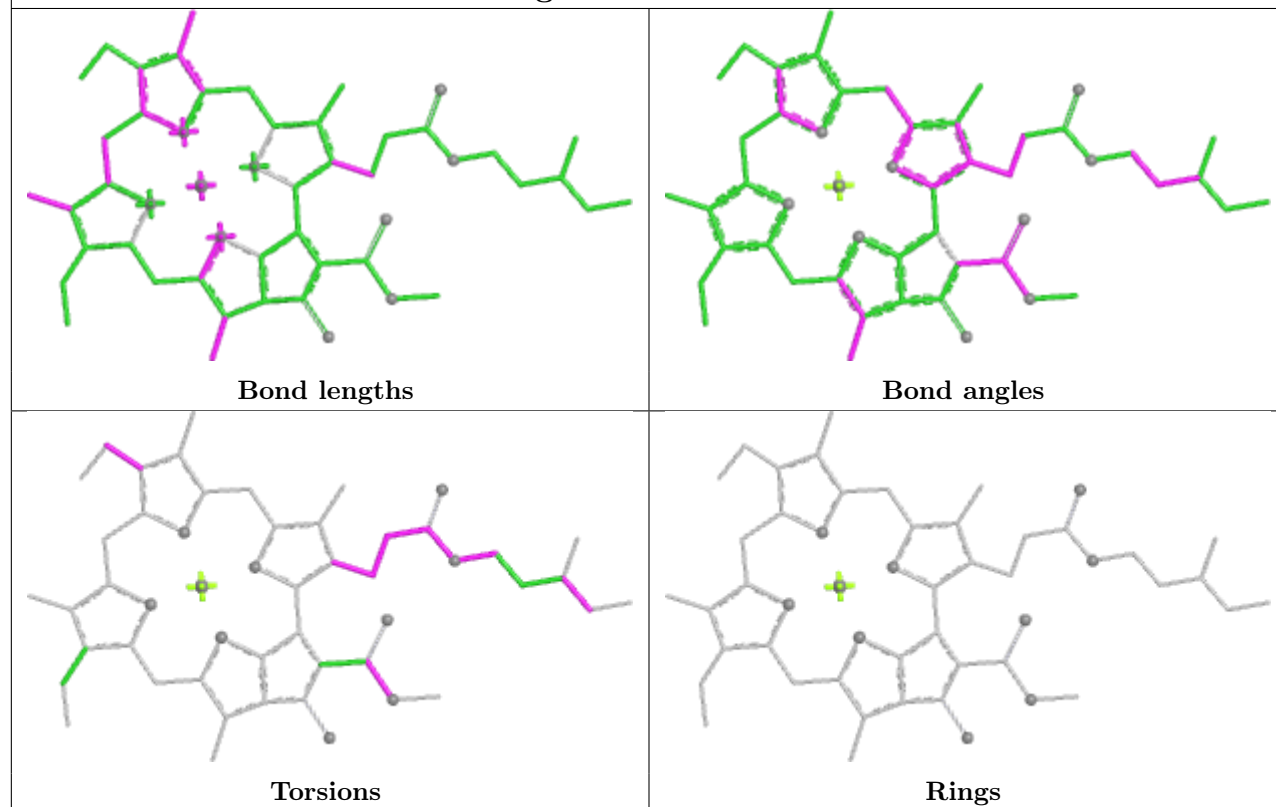


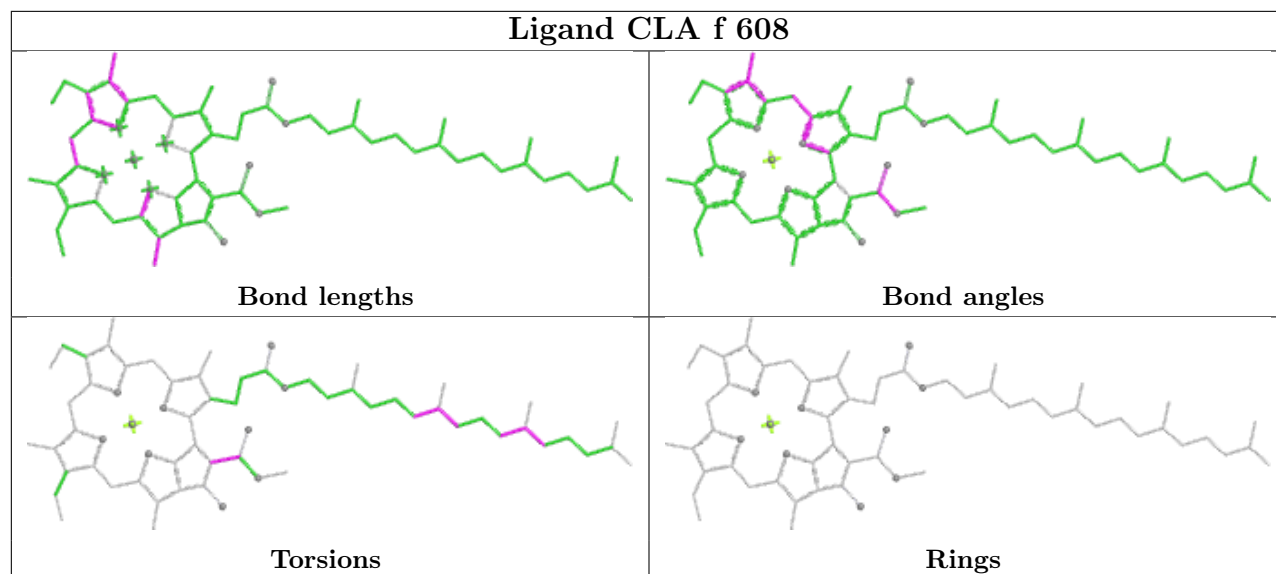
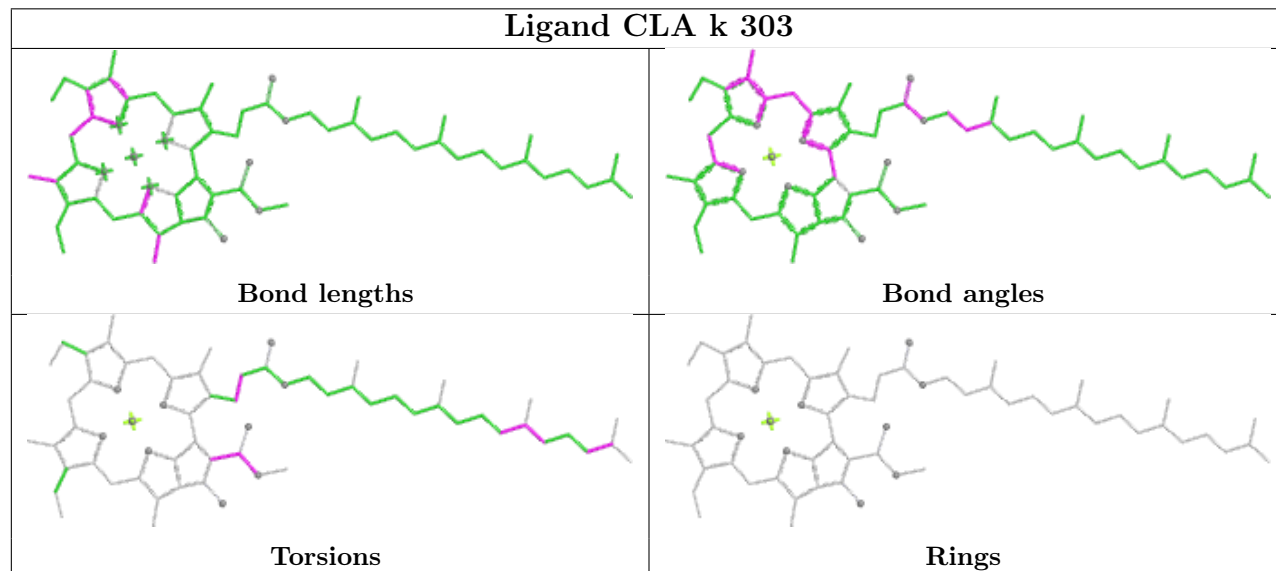


Ligand CLA c 603

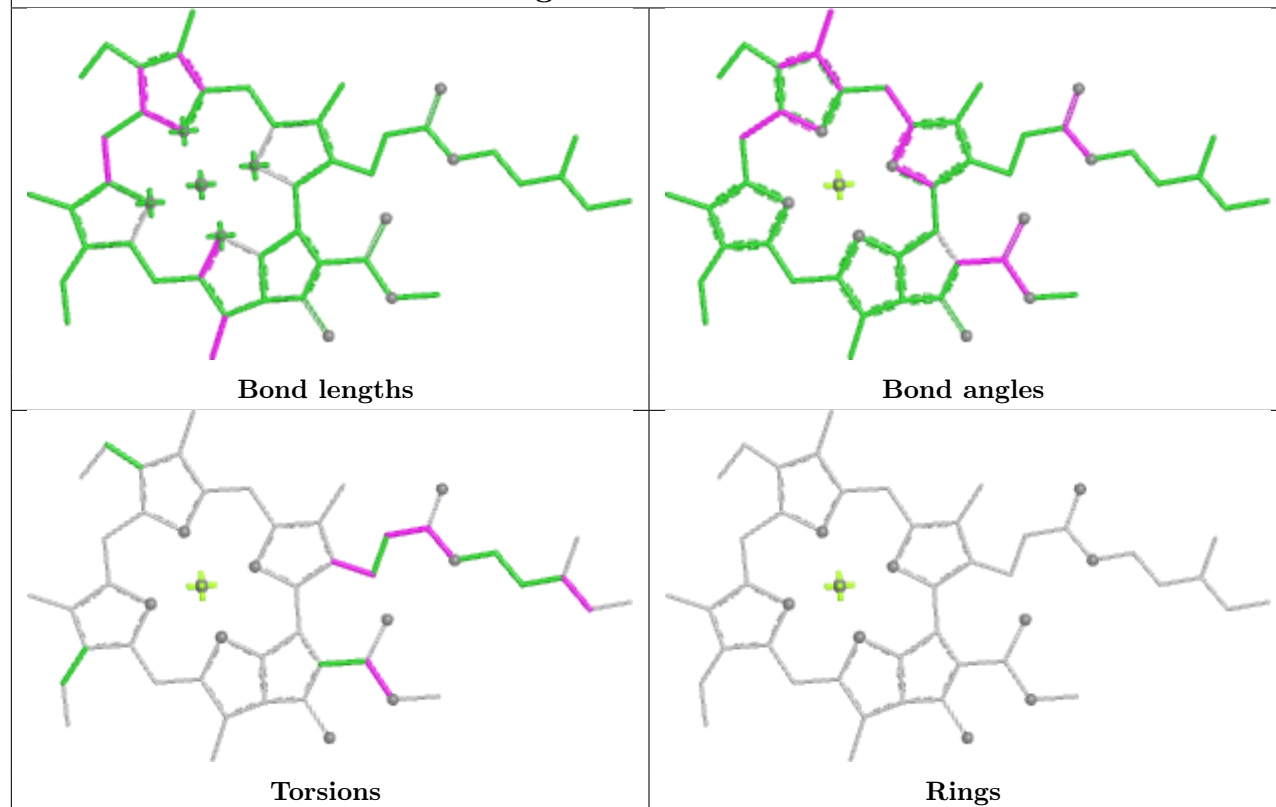


Ligand CLA k 305

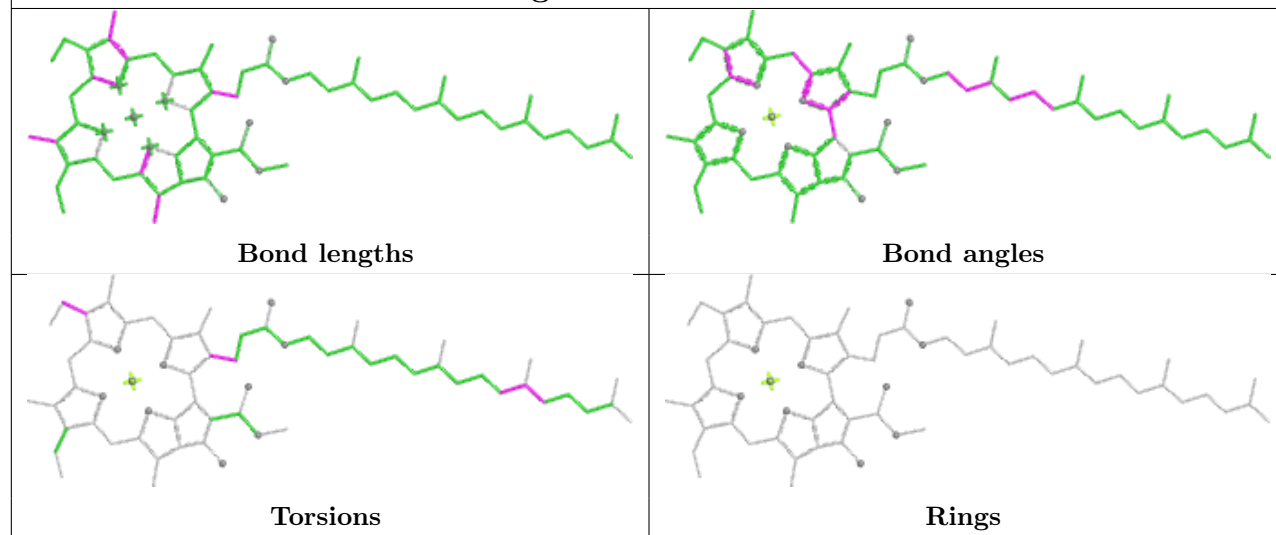


Ligand CLA f 608**Ligand CLA k 303**

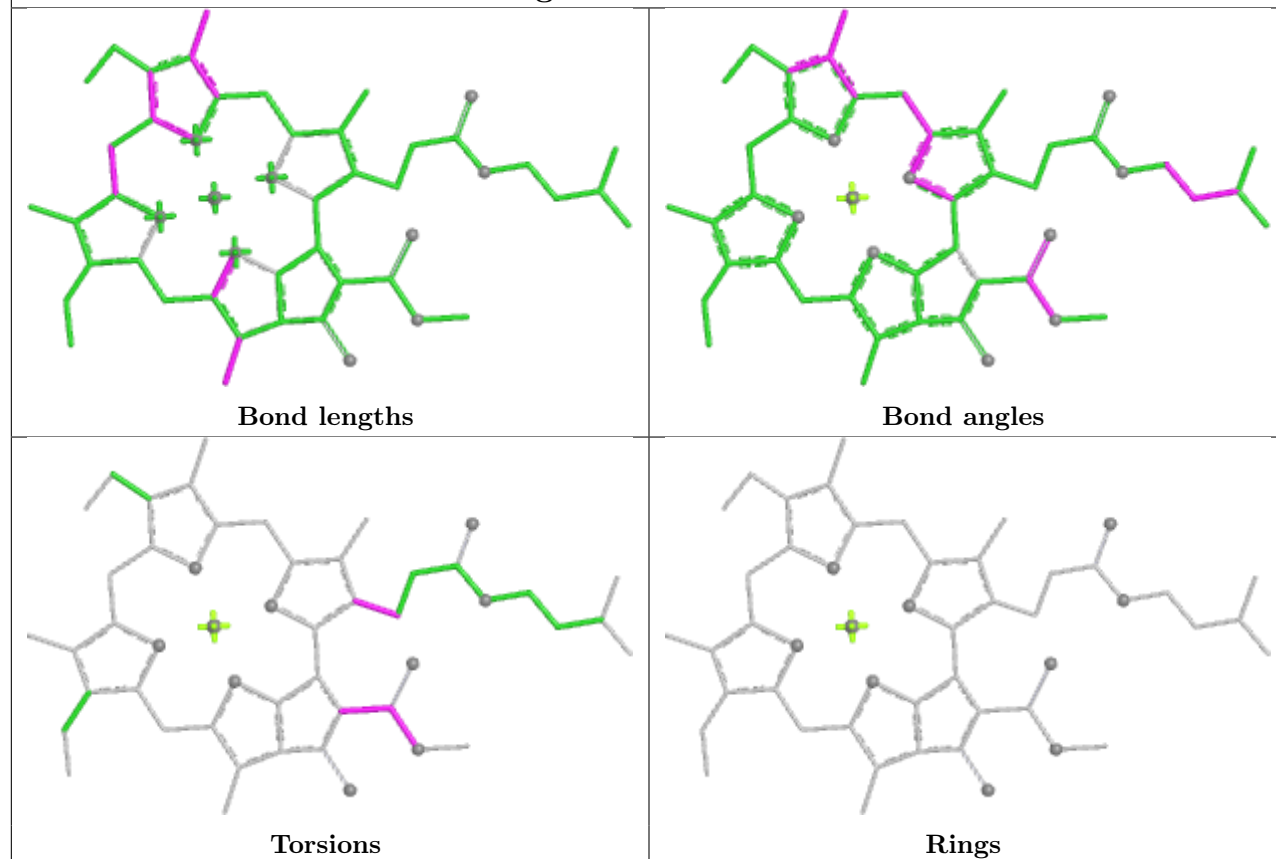
Ligand CLA n 613



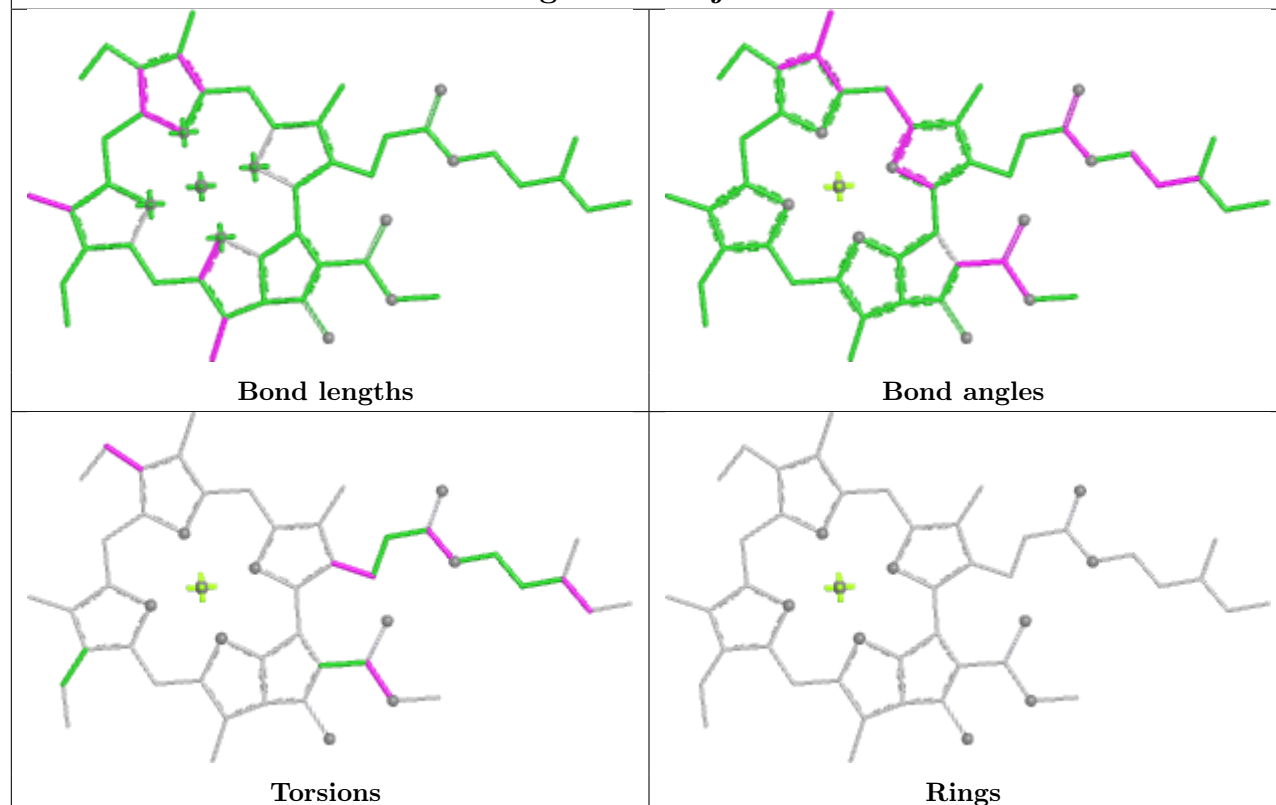
Ligand CLA A 831

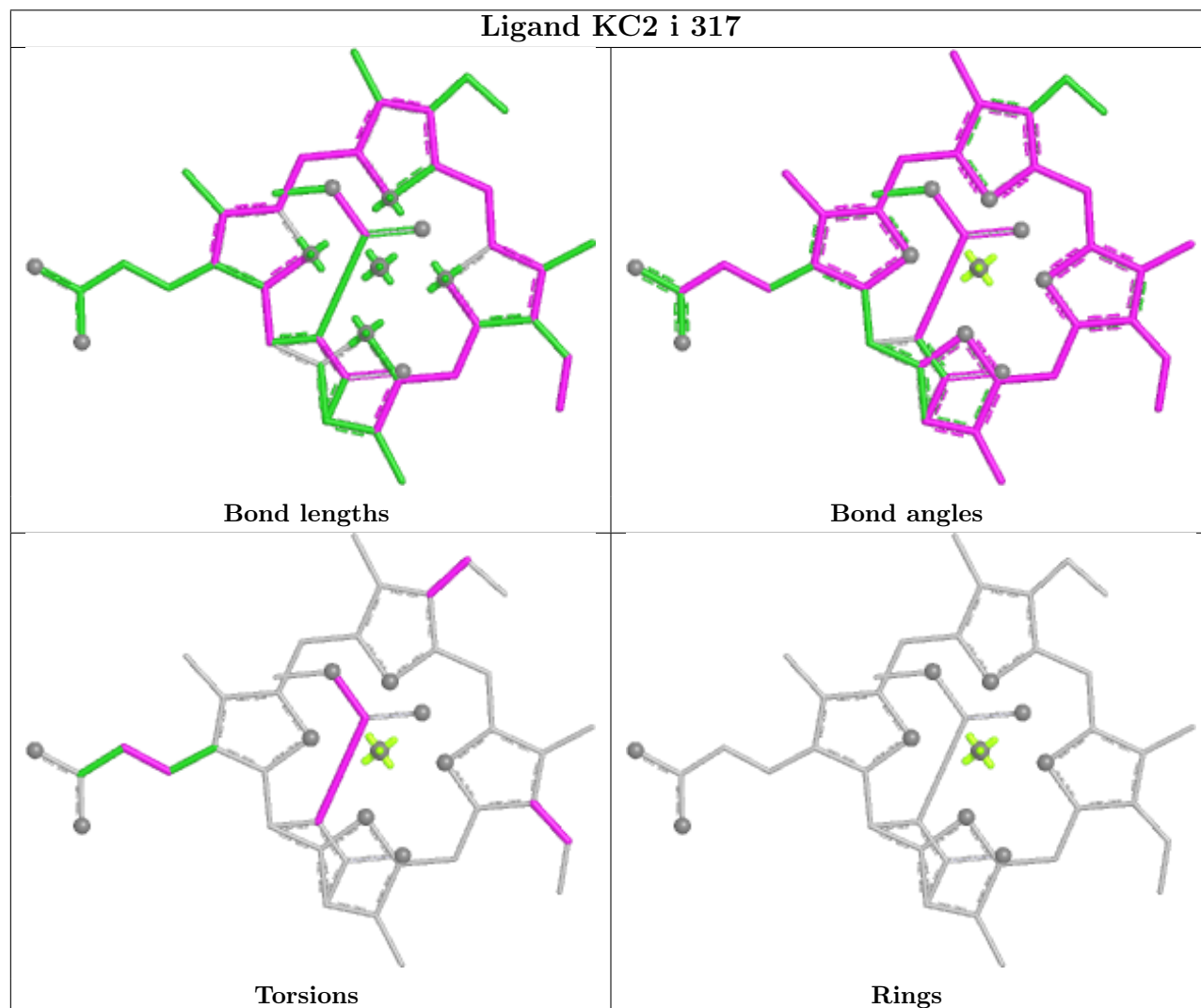
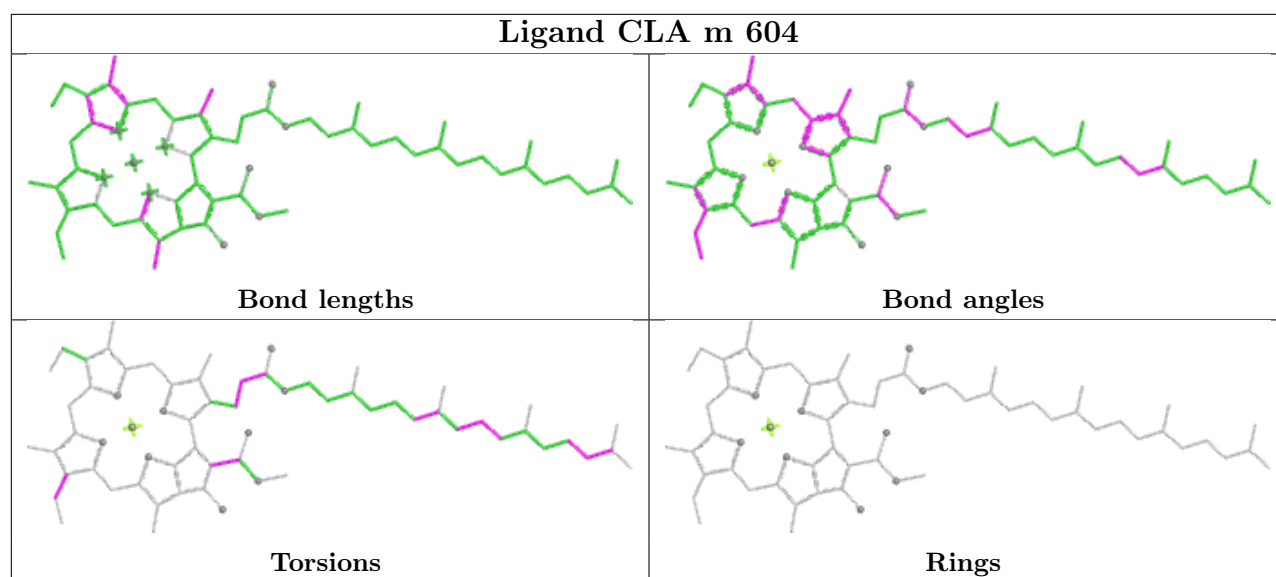


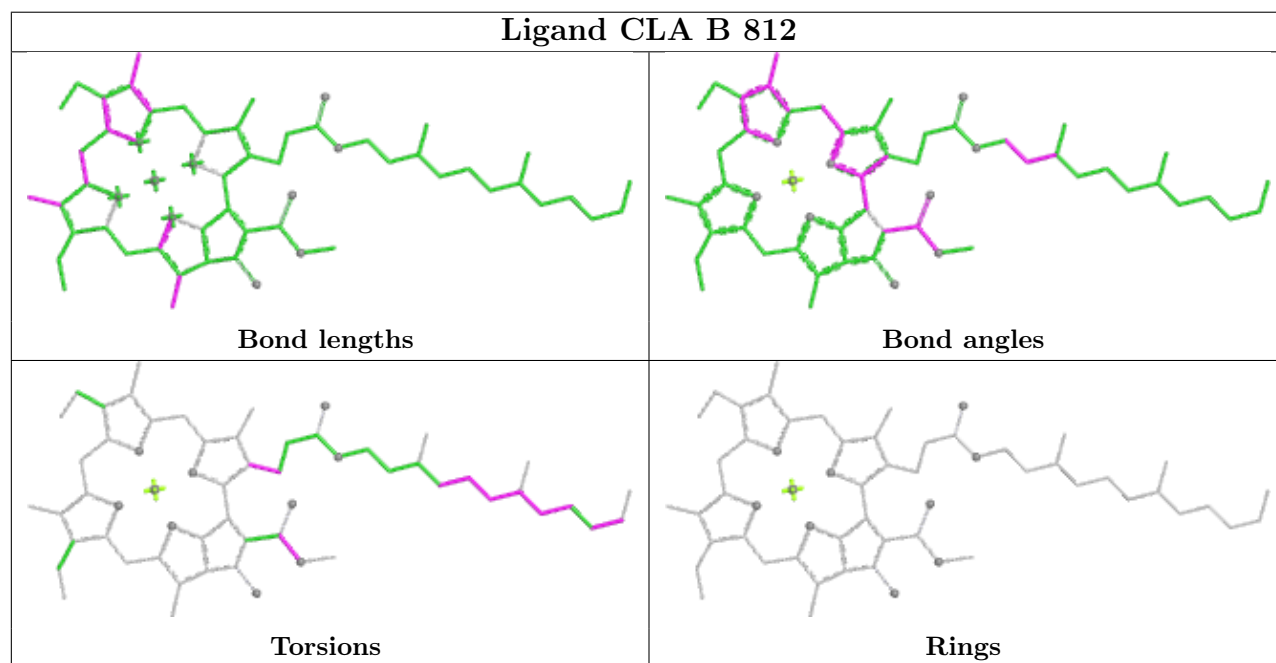
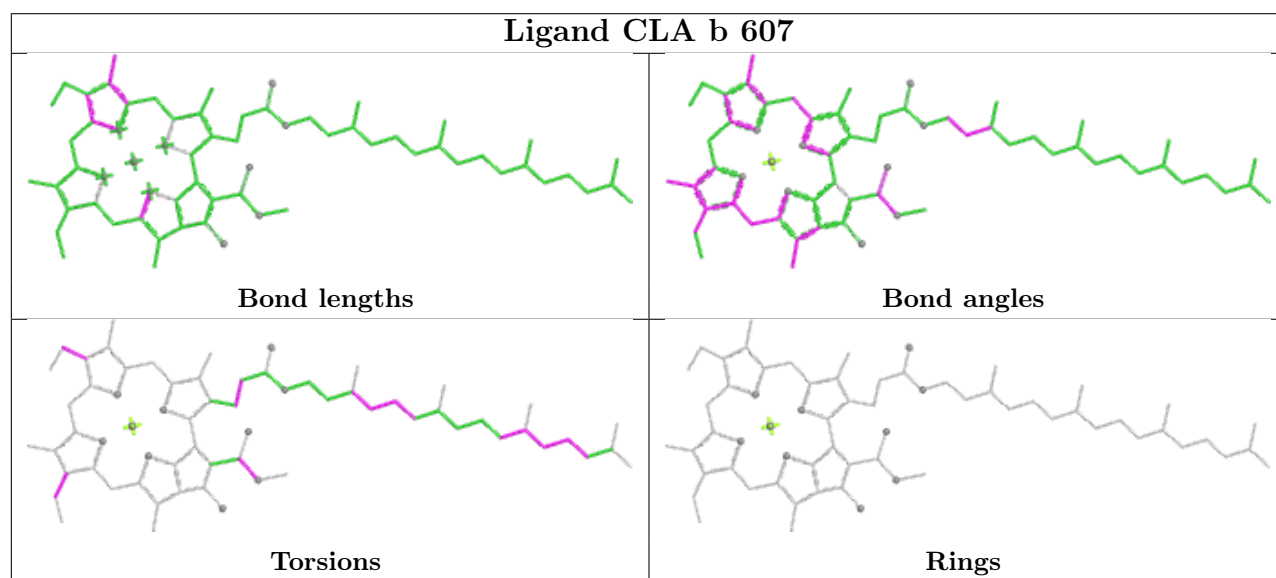
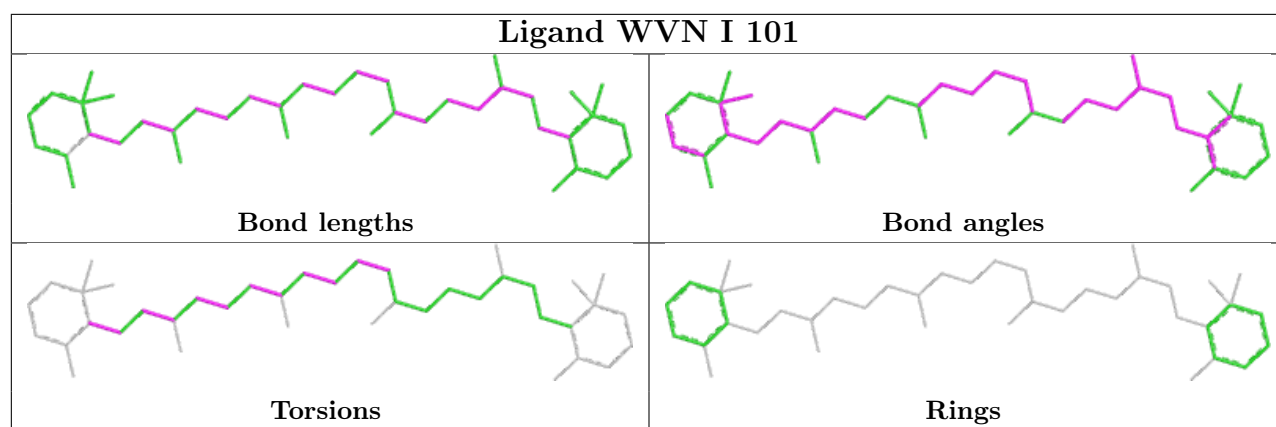
Ligand CLA k 301



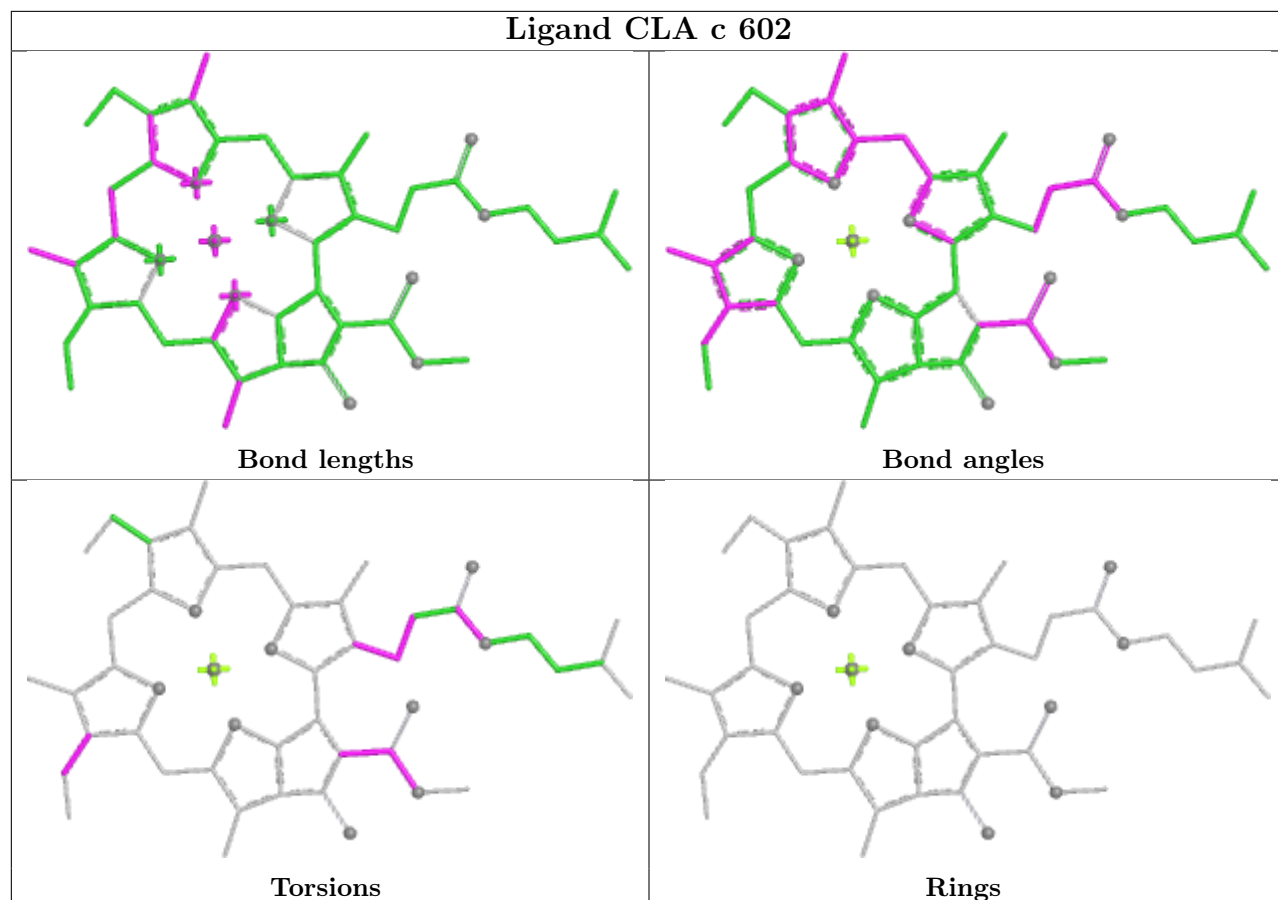
Ligand CLA j 611



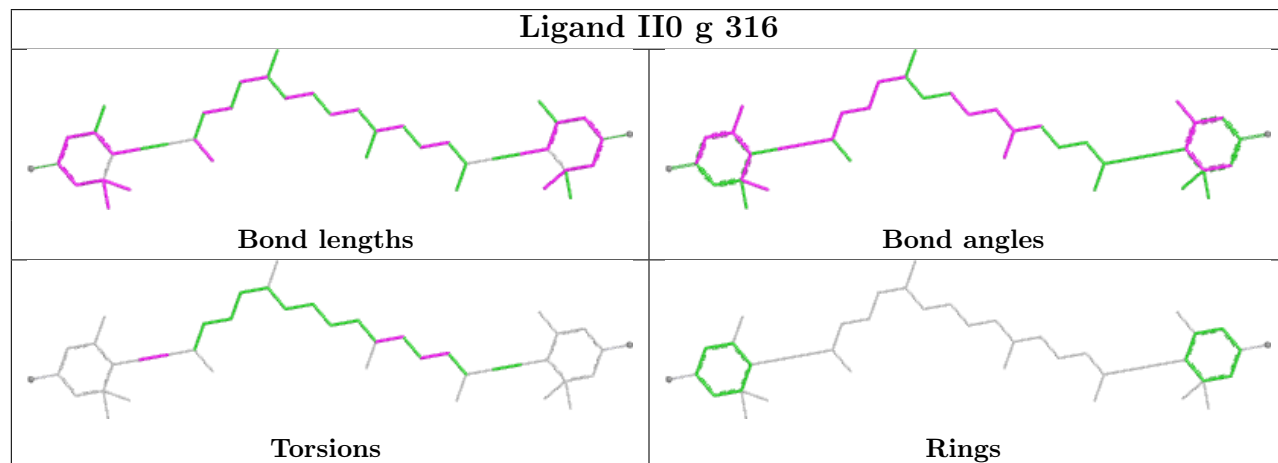


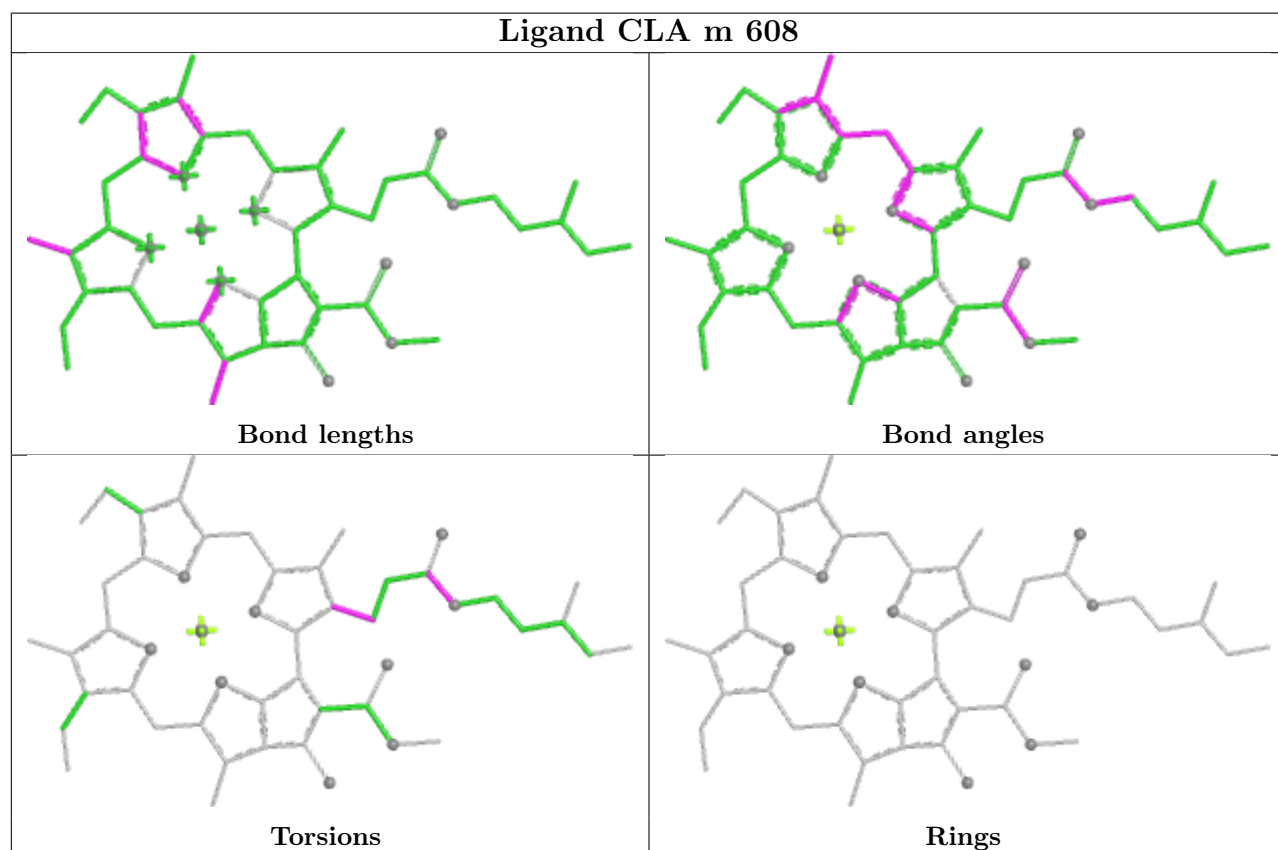
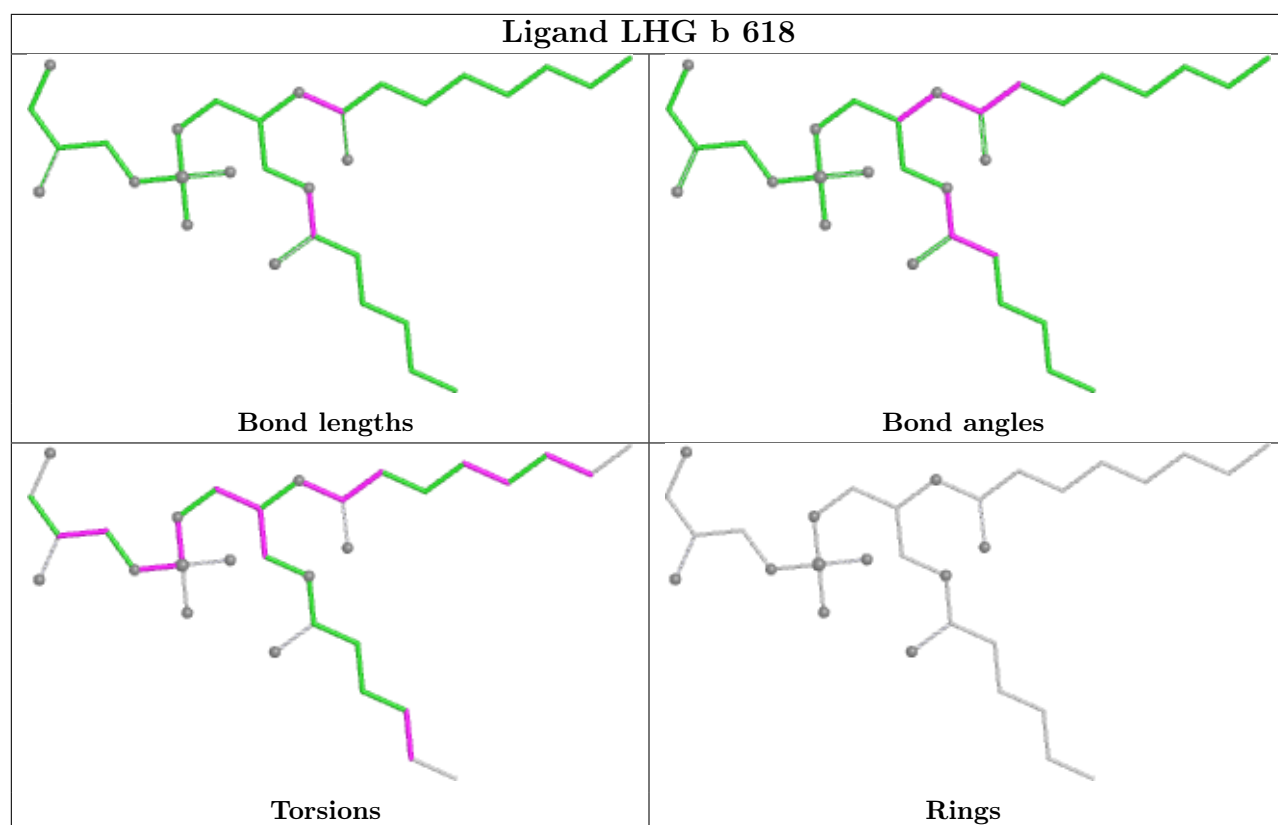


Ligand CLA c 602

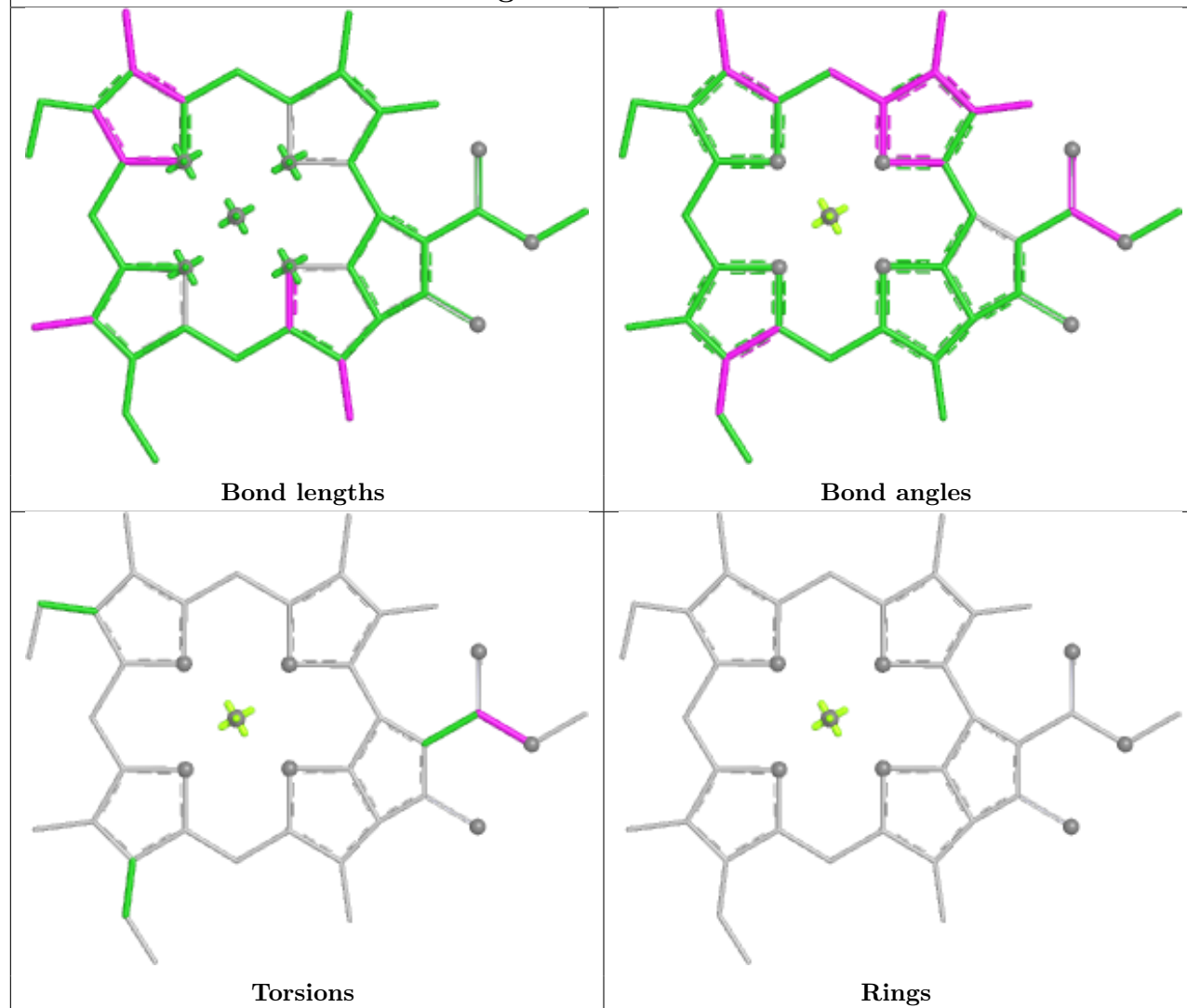


Ligand II0 g 316

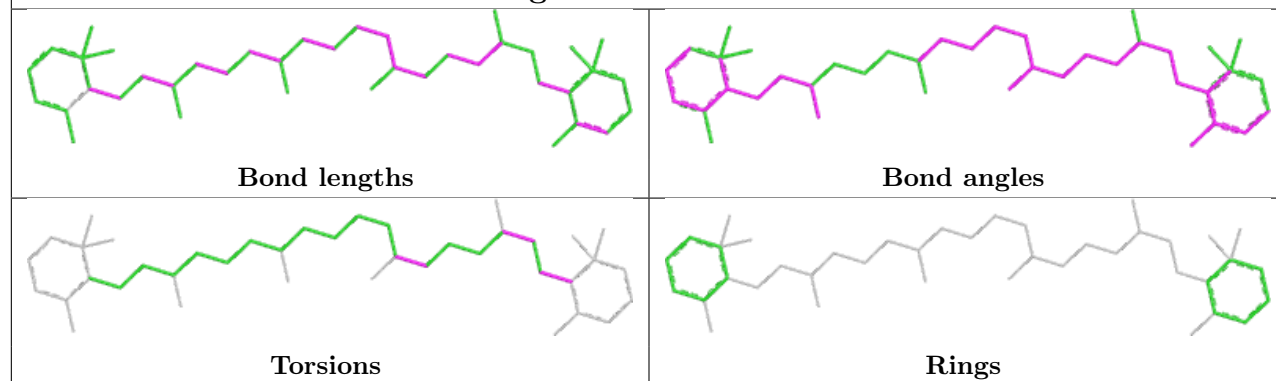




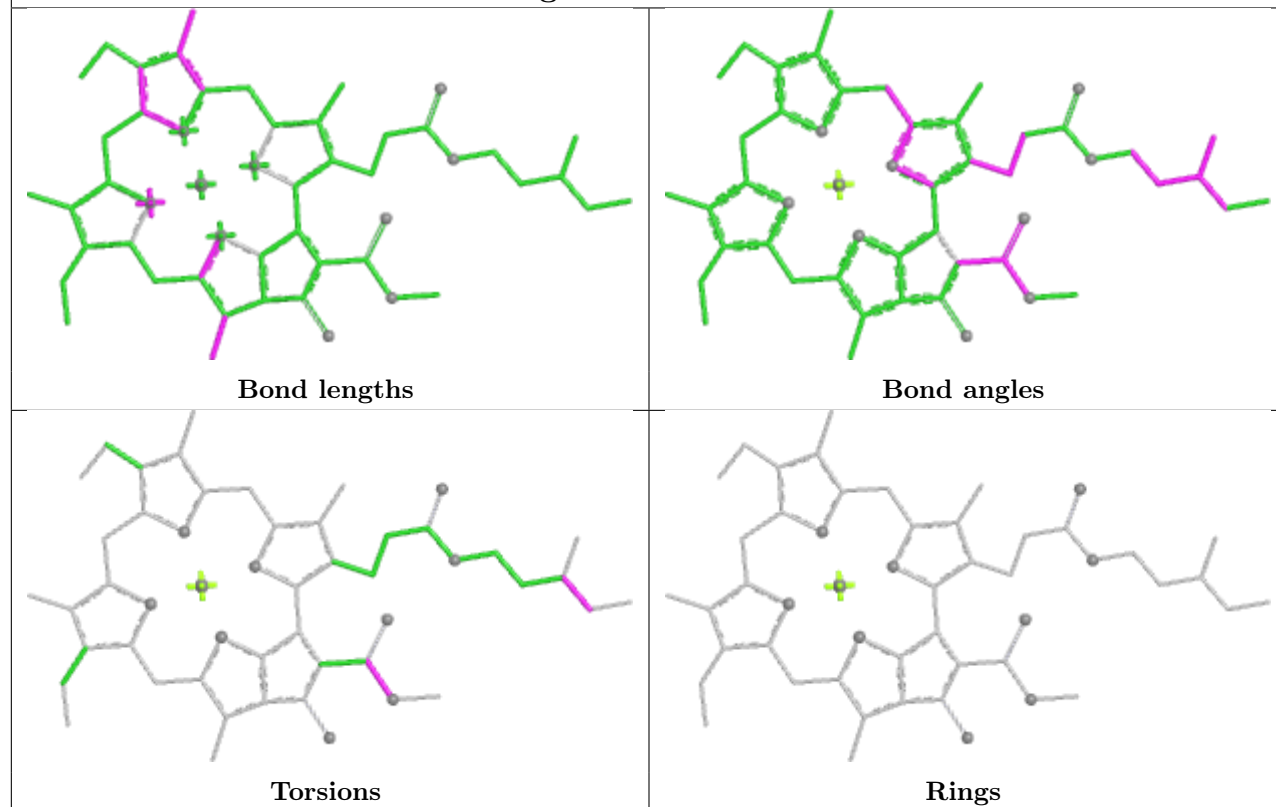
Ligand CLA d 307



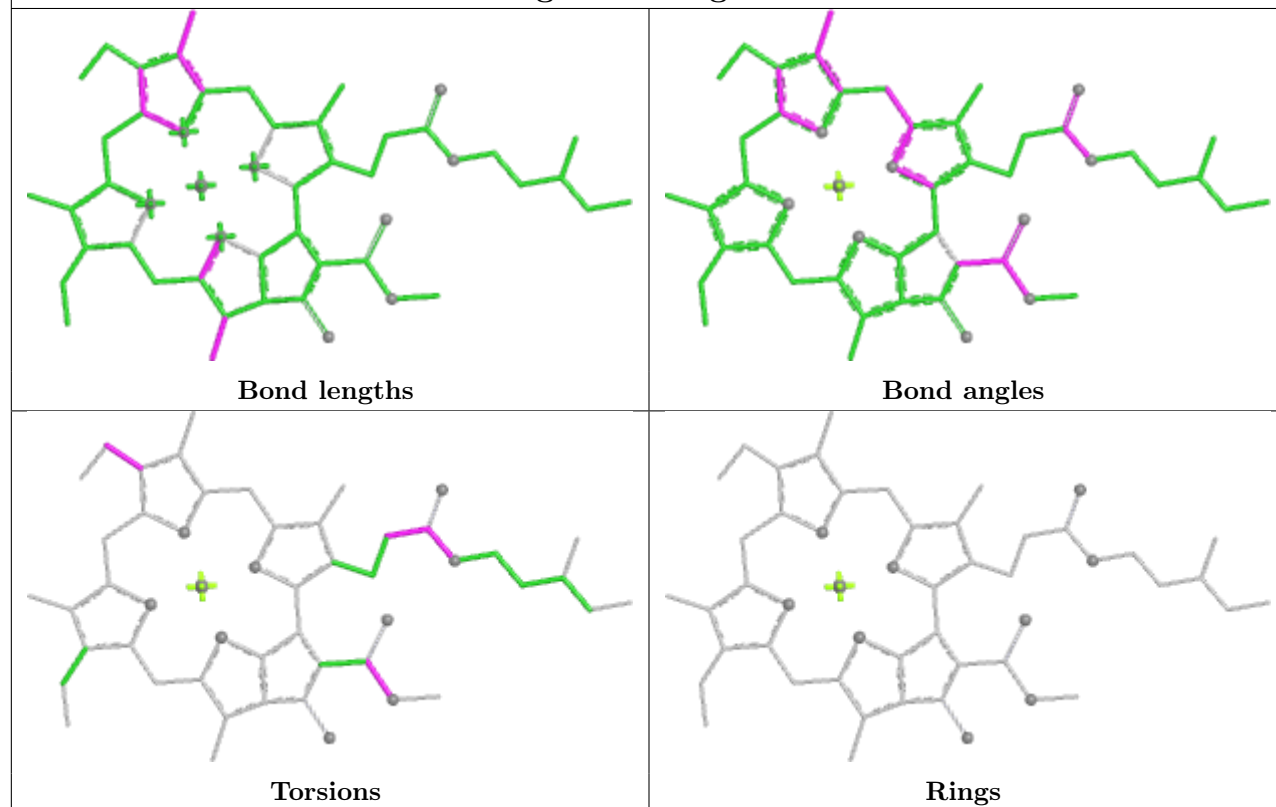
Ligand WVN s 205



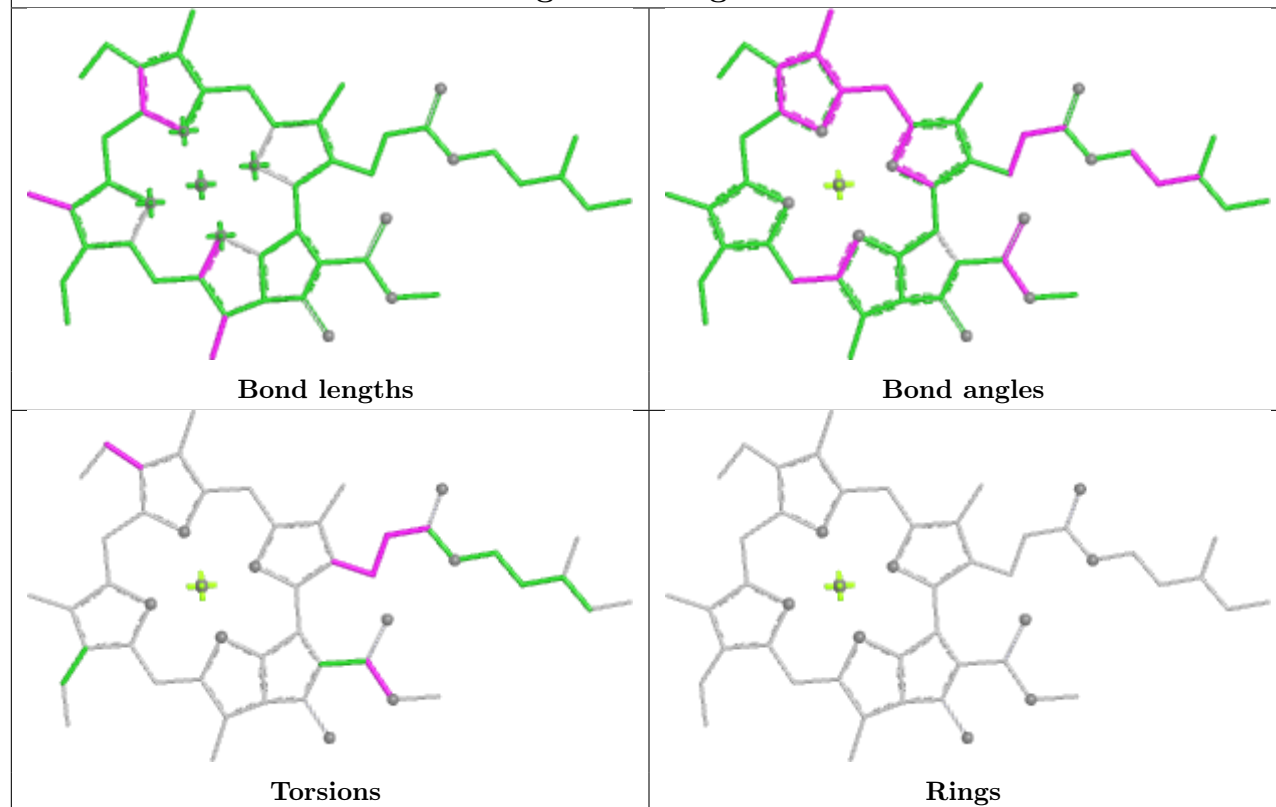
Ligand CLA f 606



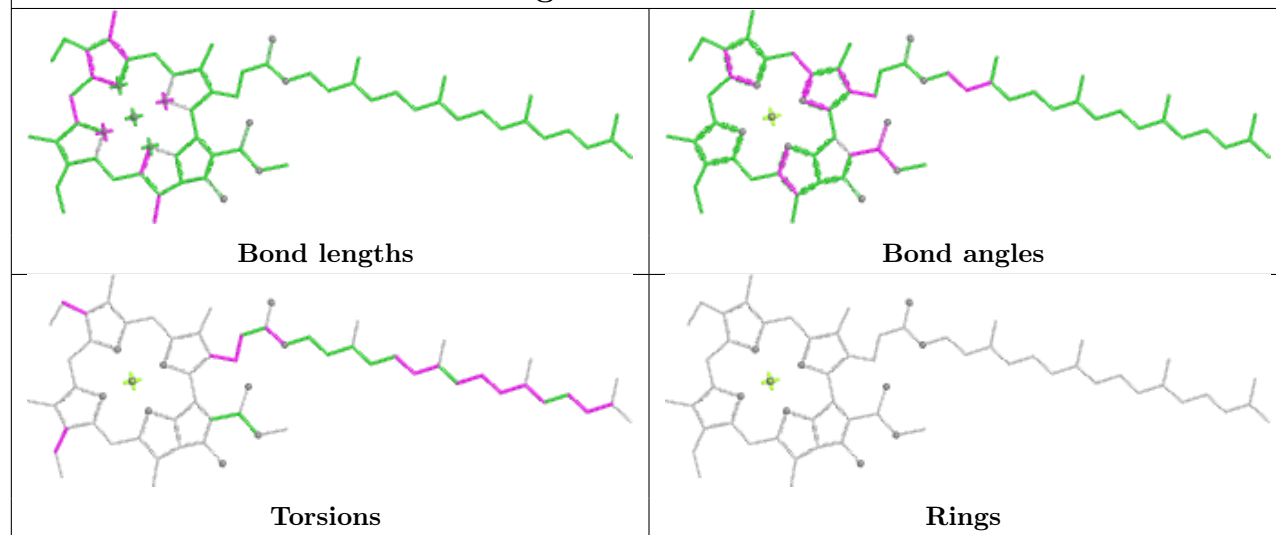
Ligand CLA g 307

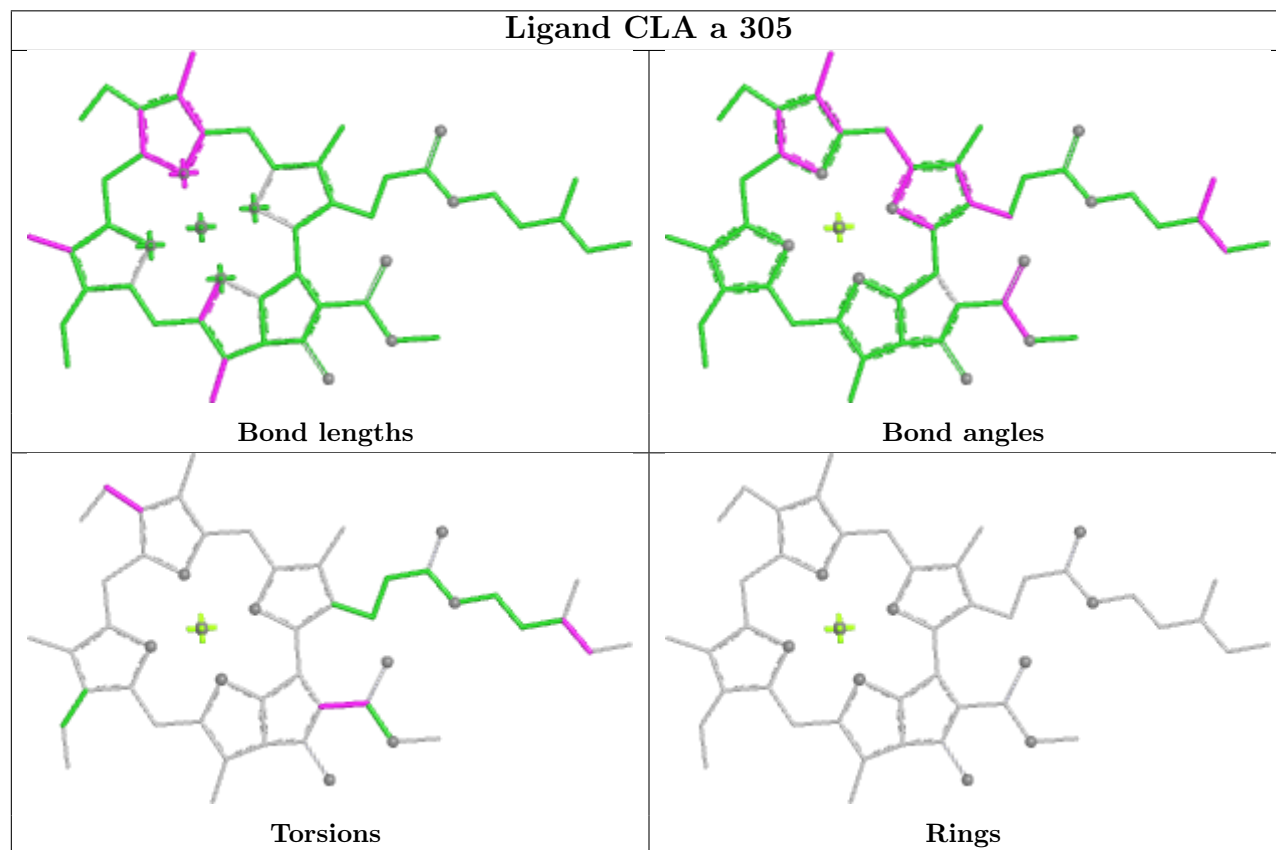
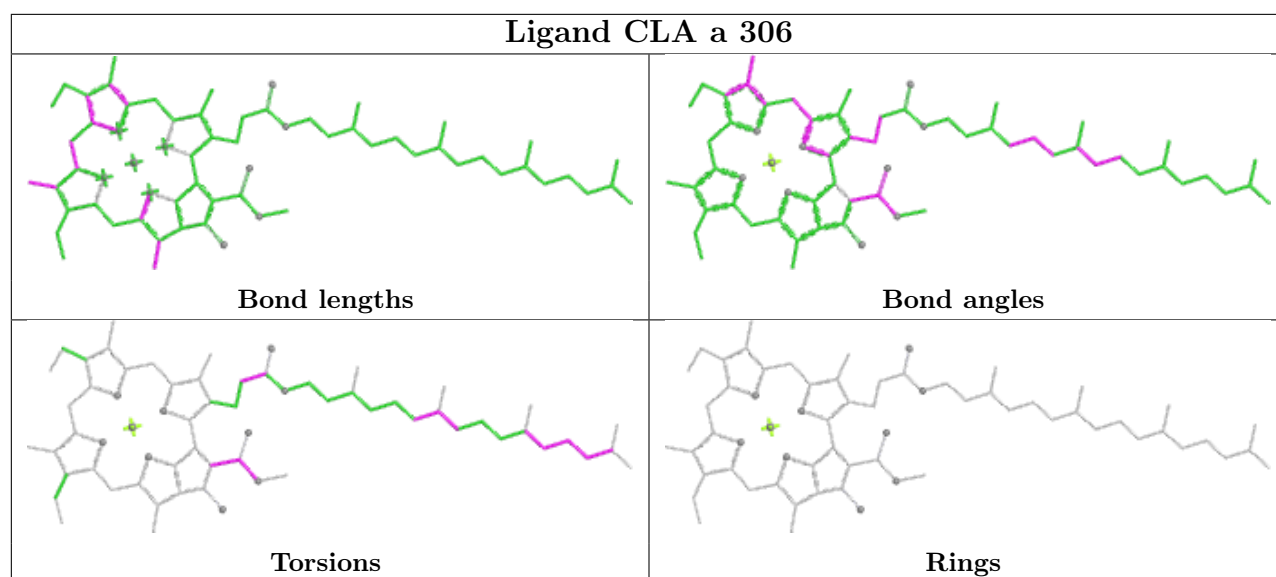


Ligand CLA g 315

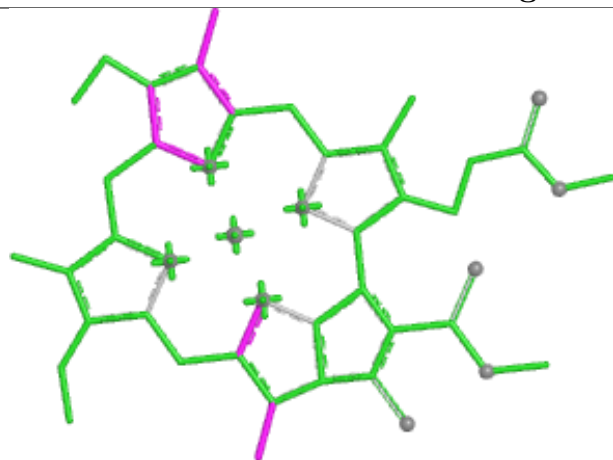


Ligand CLA a 312

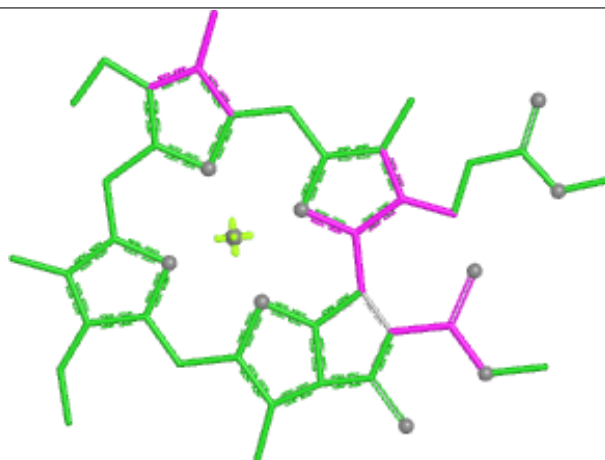




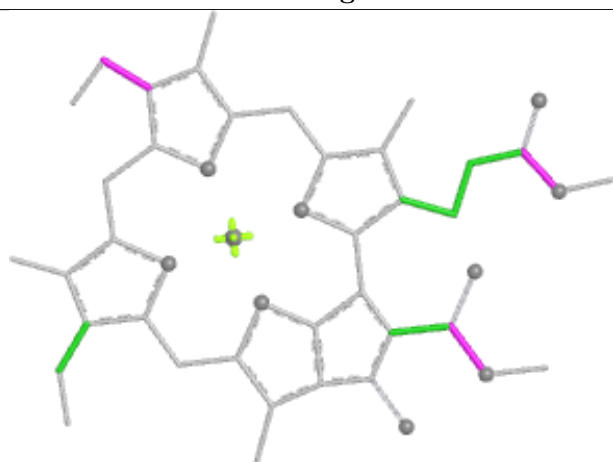
Ligand CLA c 607



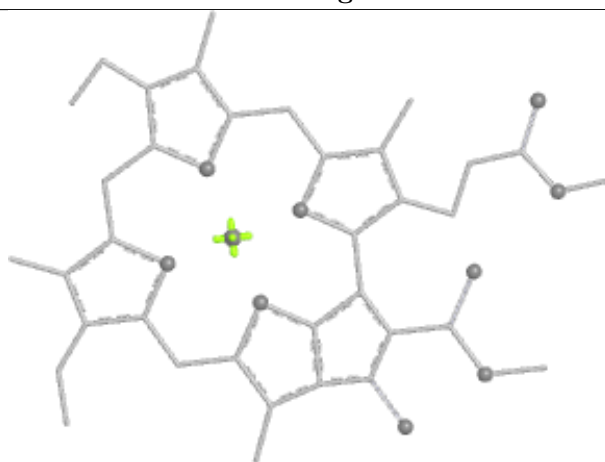
Bond lengths



Bond angles

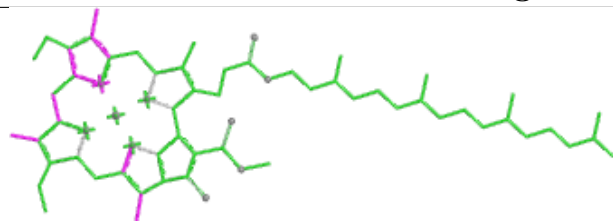


Torsions

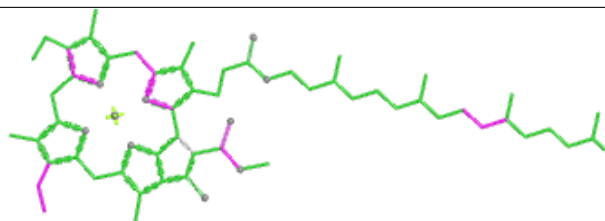


Rings

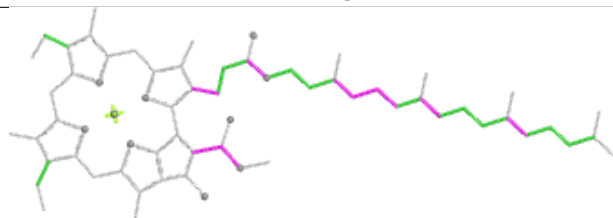
Ligand CLA O 202



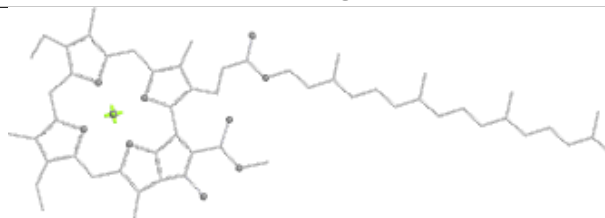
Bond lengths



Bond angles

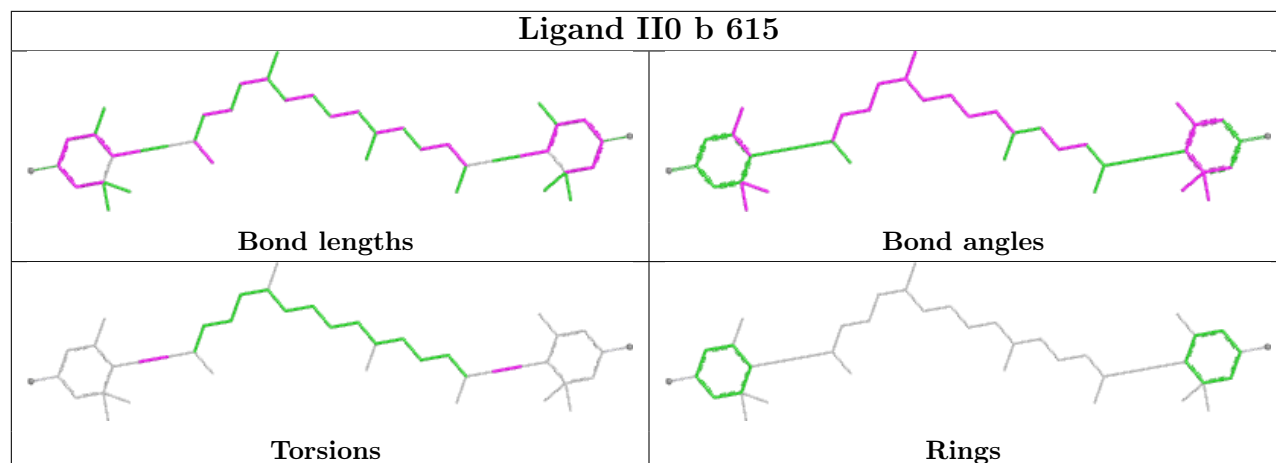


Torsions

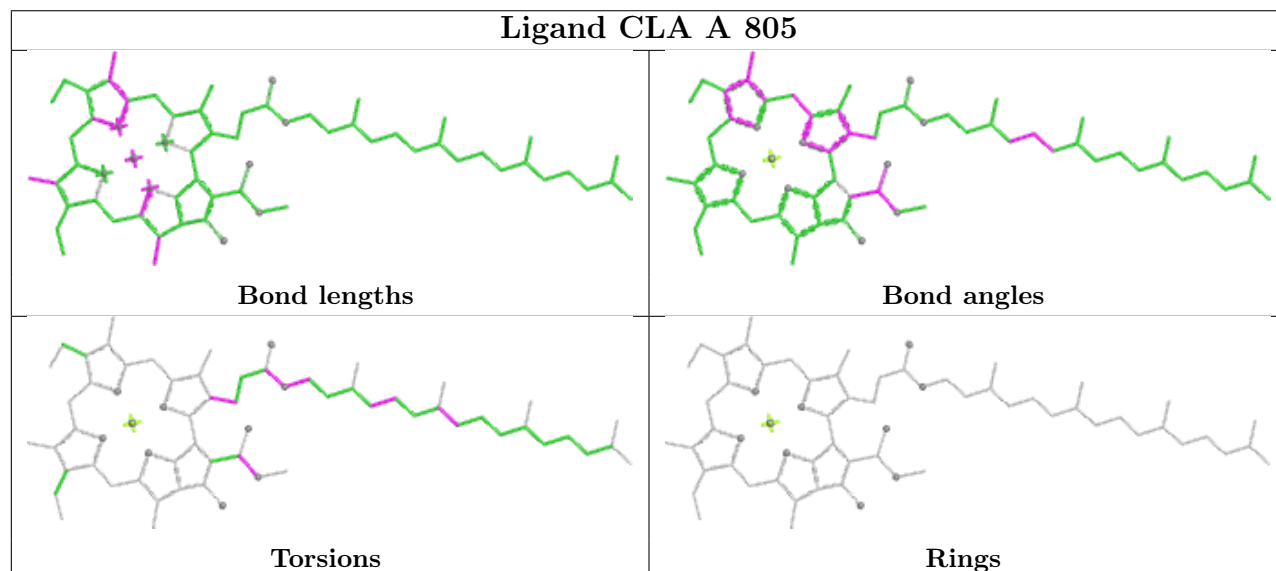


Rings

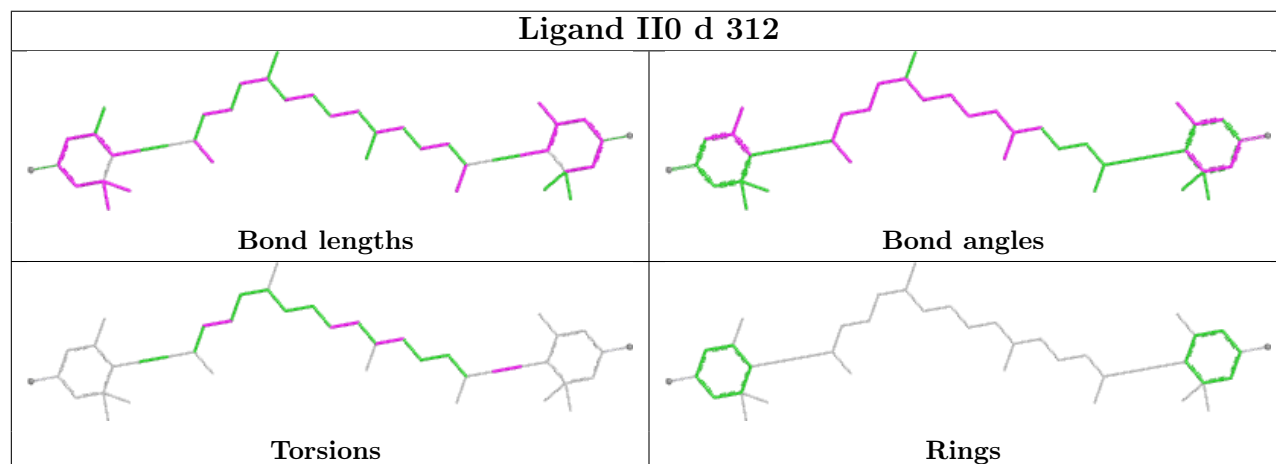
Ligand II0 b 615

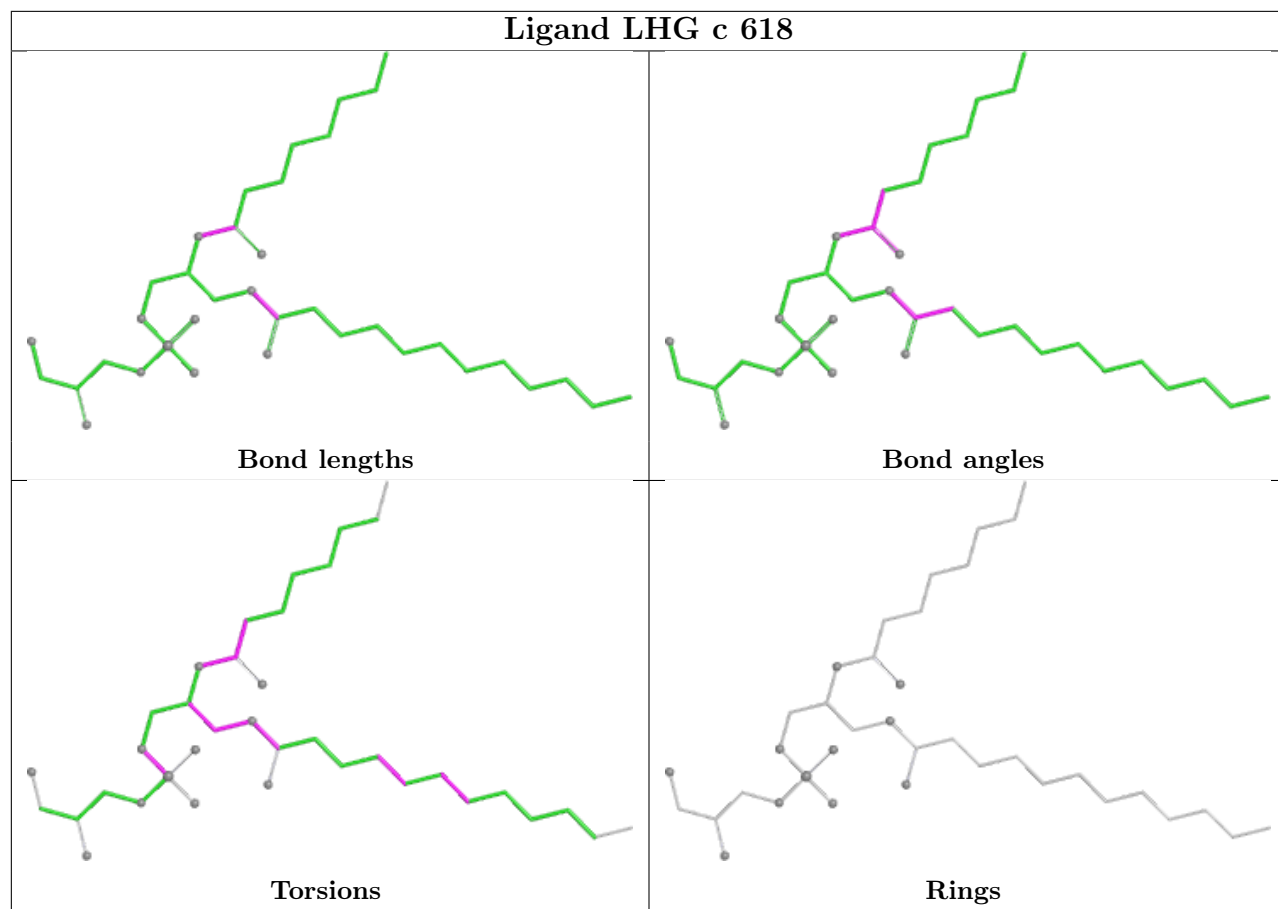


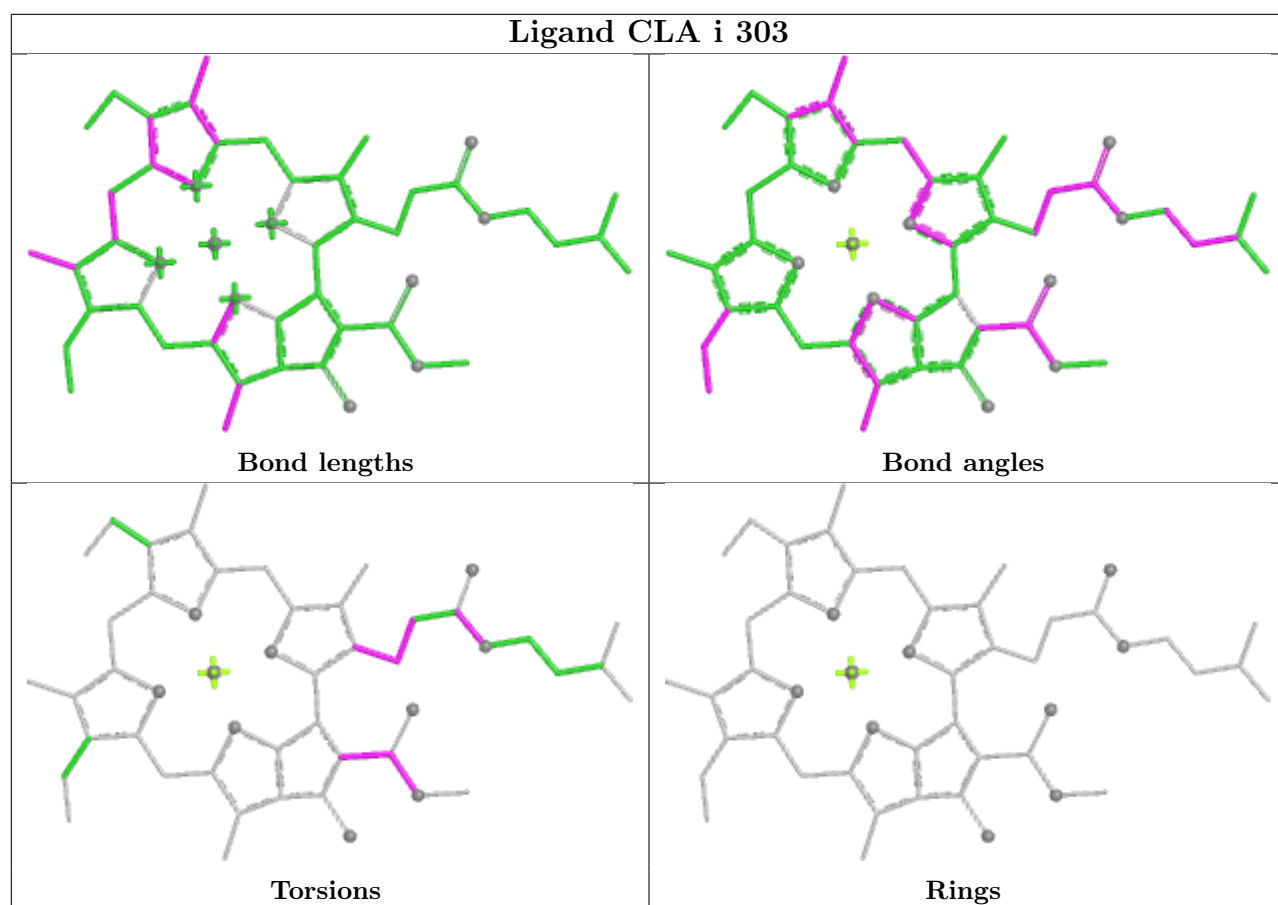
Ligand CLA A 805



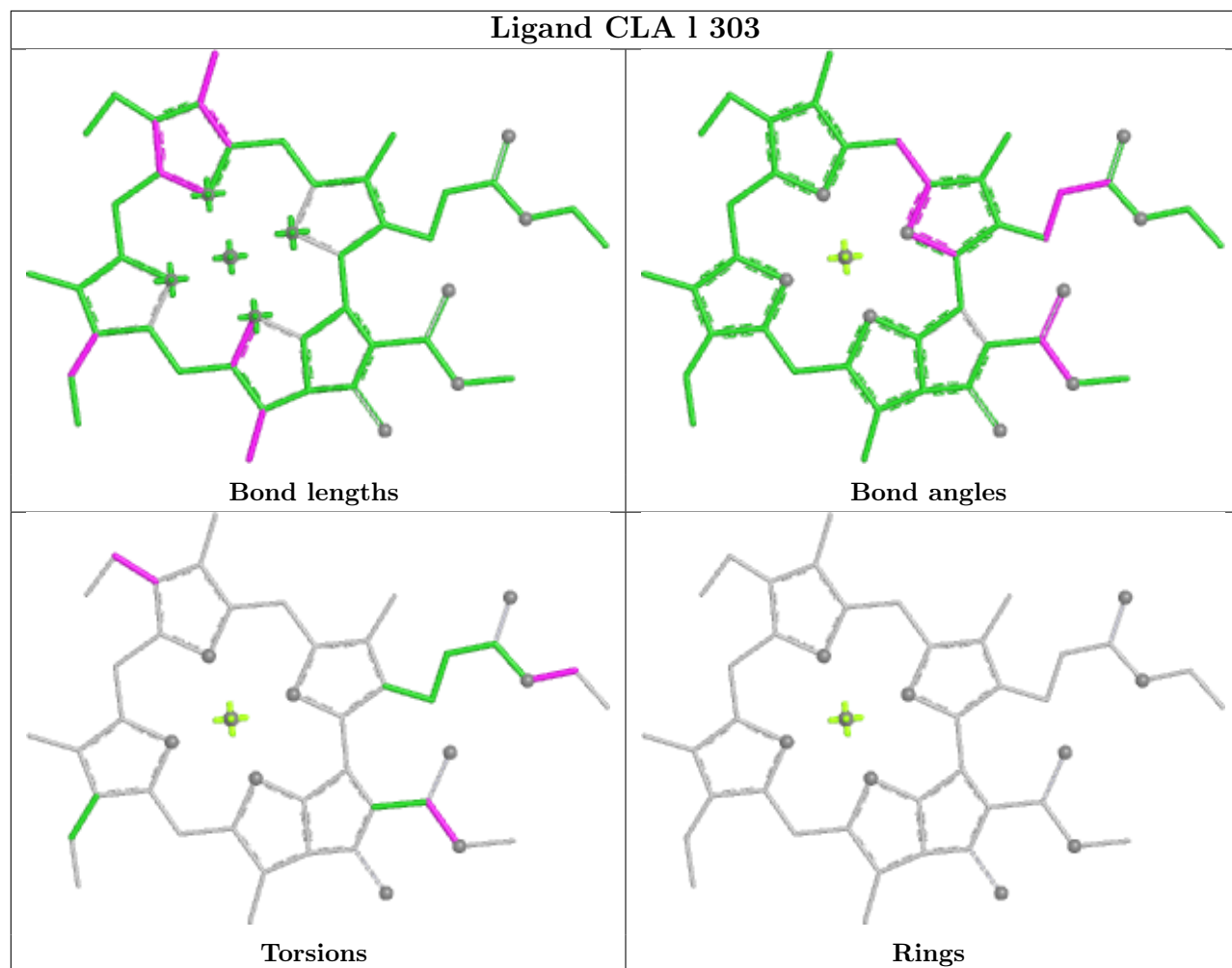
Ligand II0 d 312



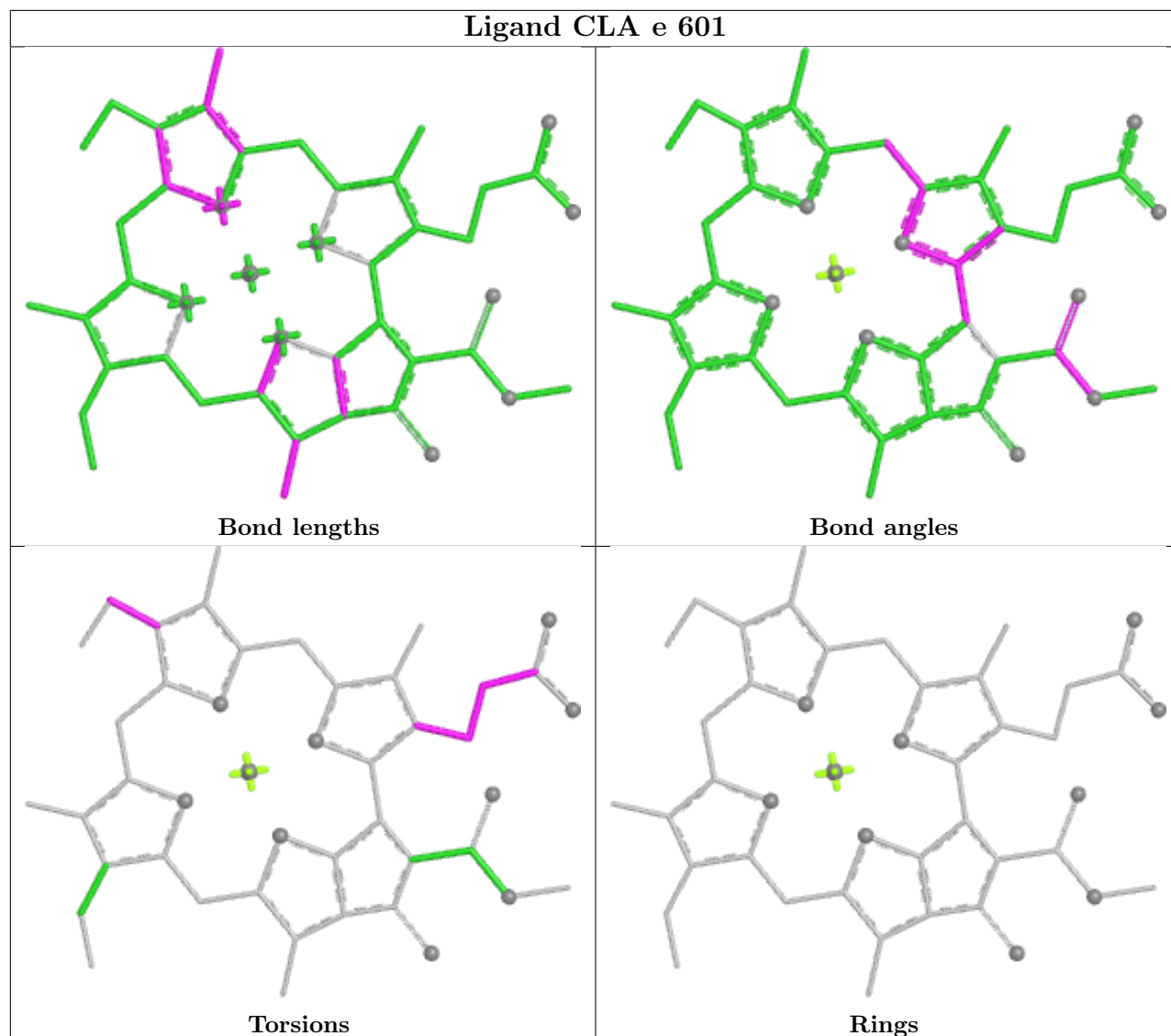




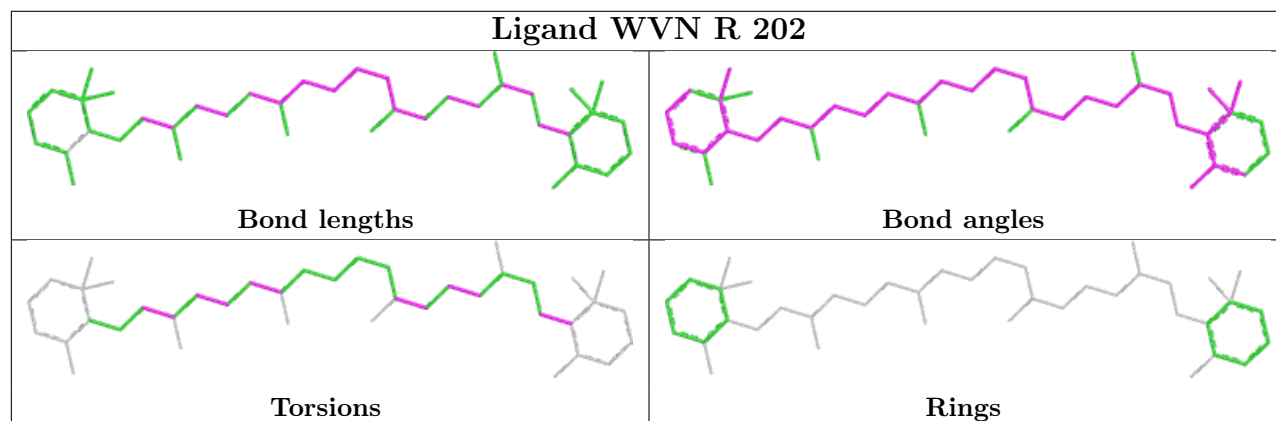
Ligand CLA 1 303

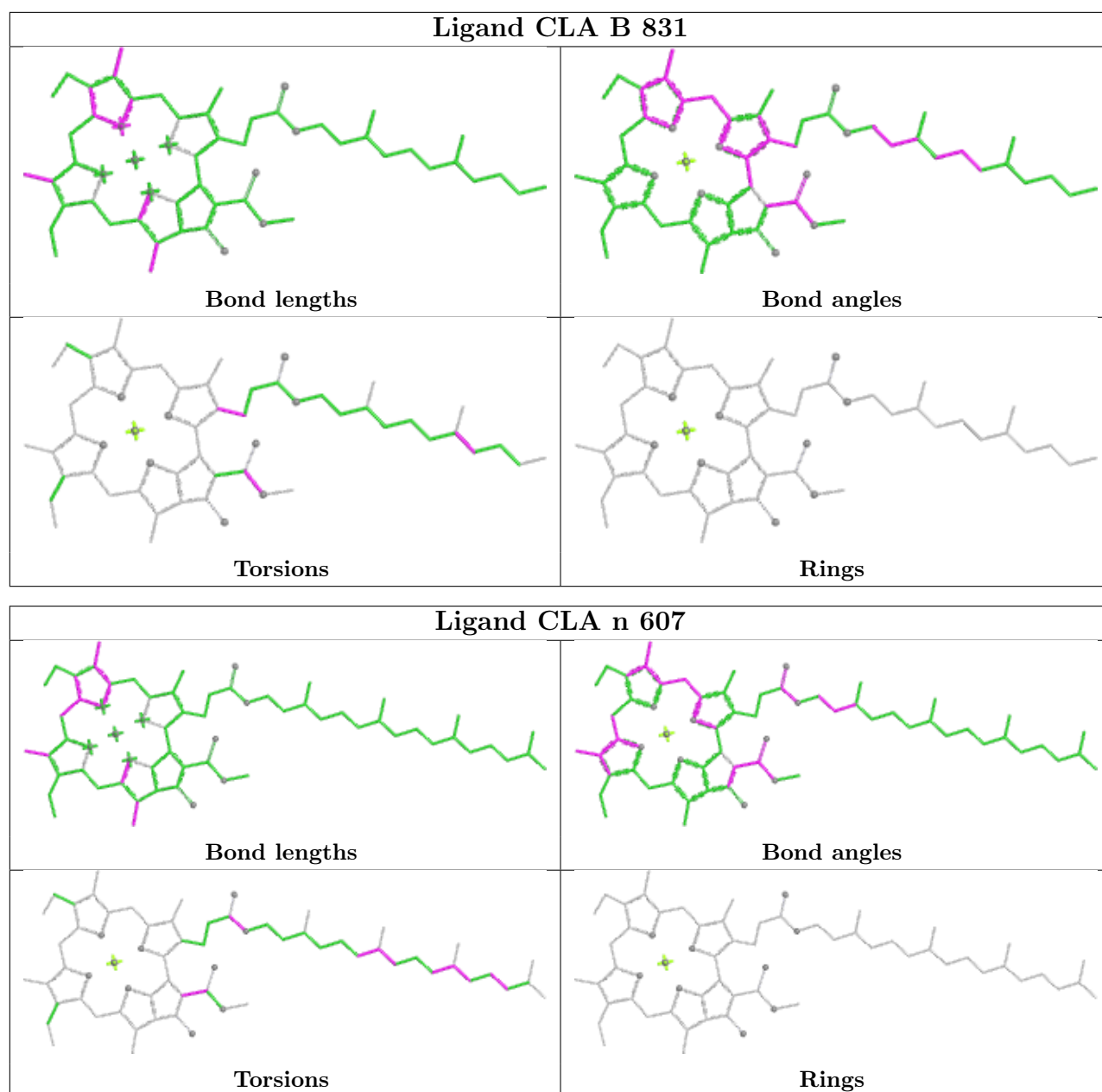


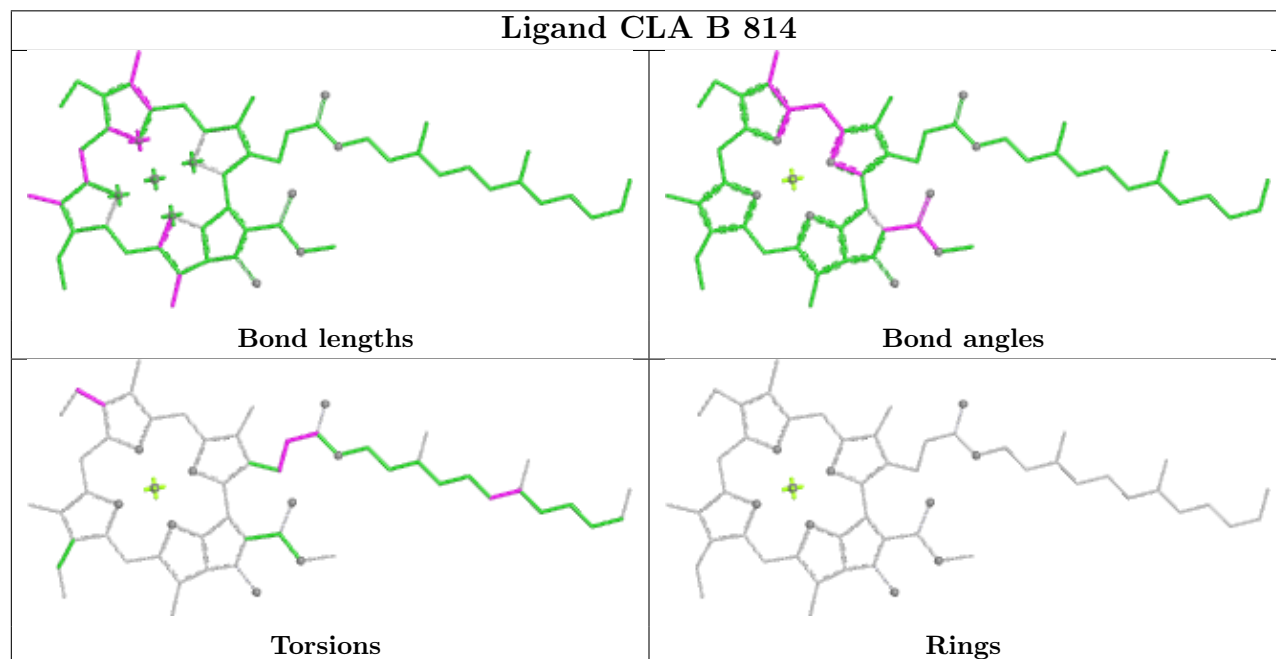
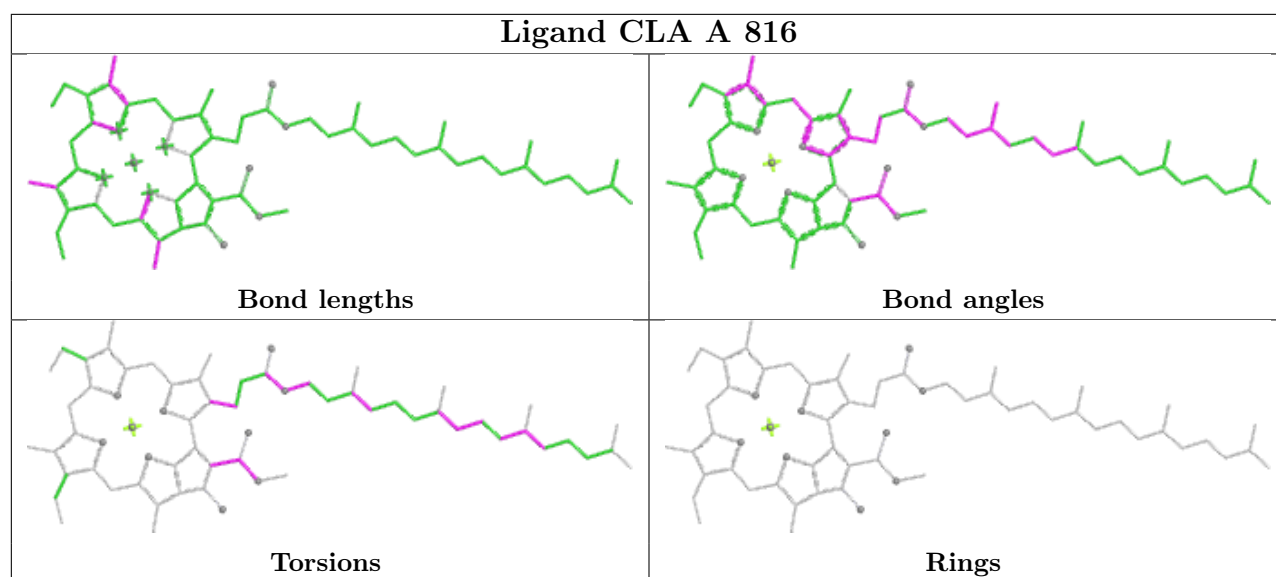
Ligand CLA e 601



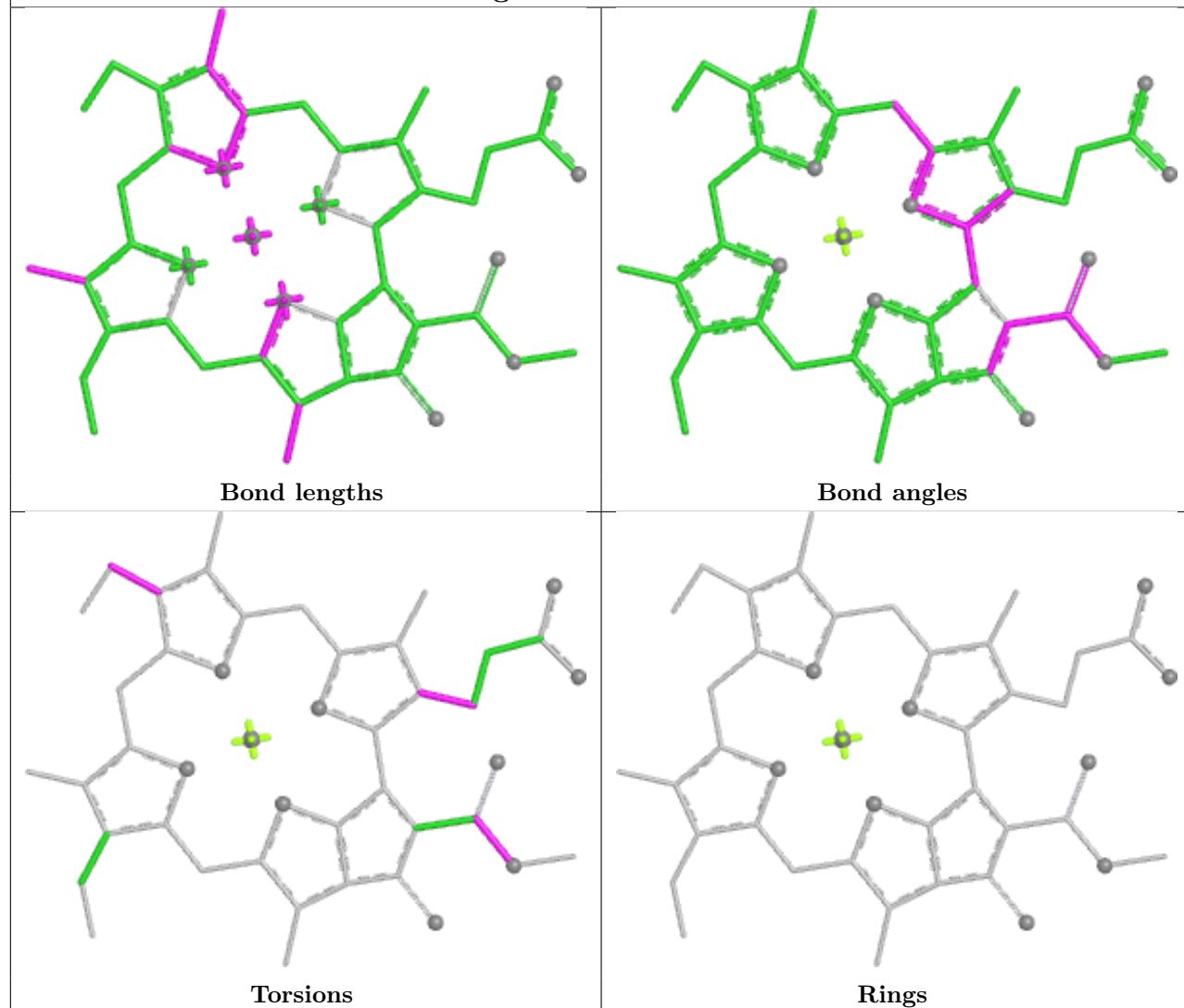
Ligand WVN R 202



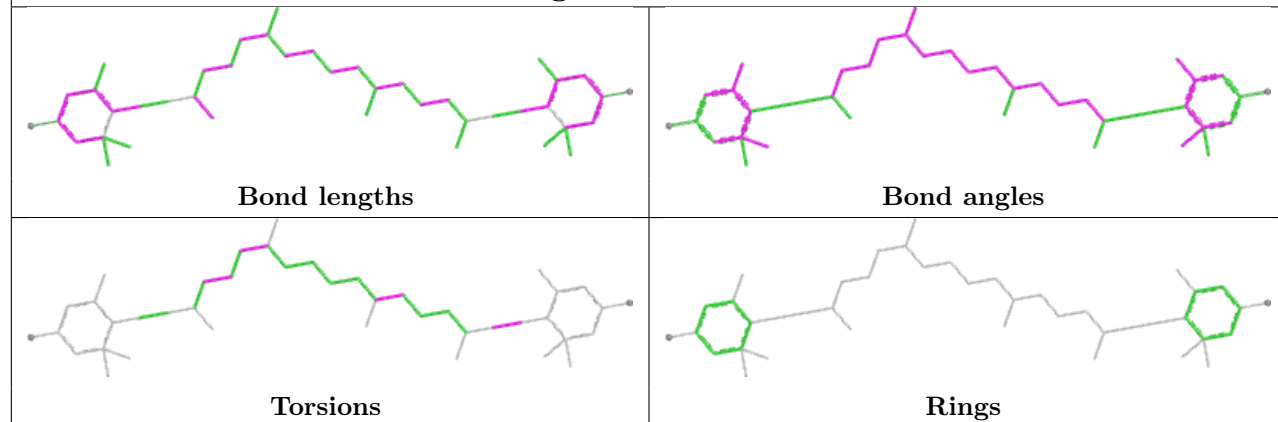




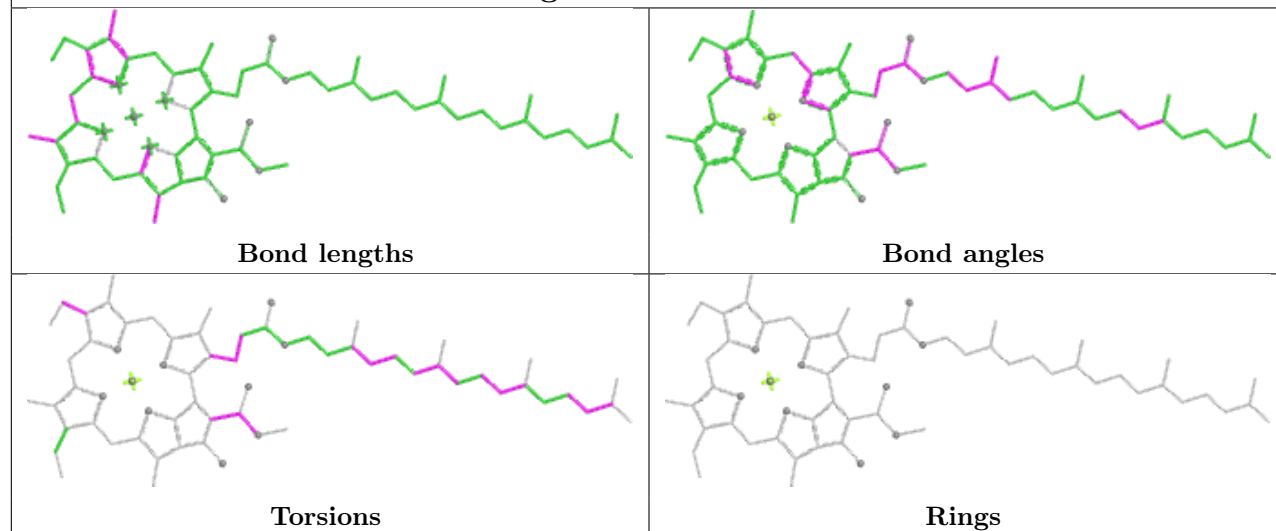
Ligand CLA B 830



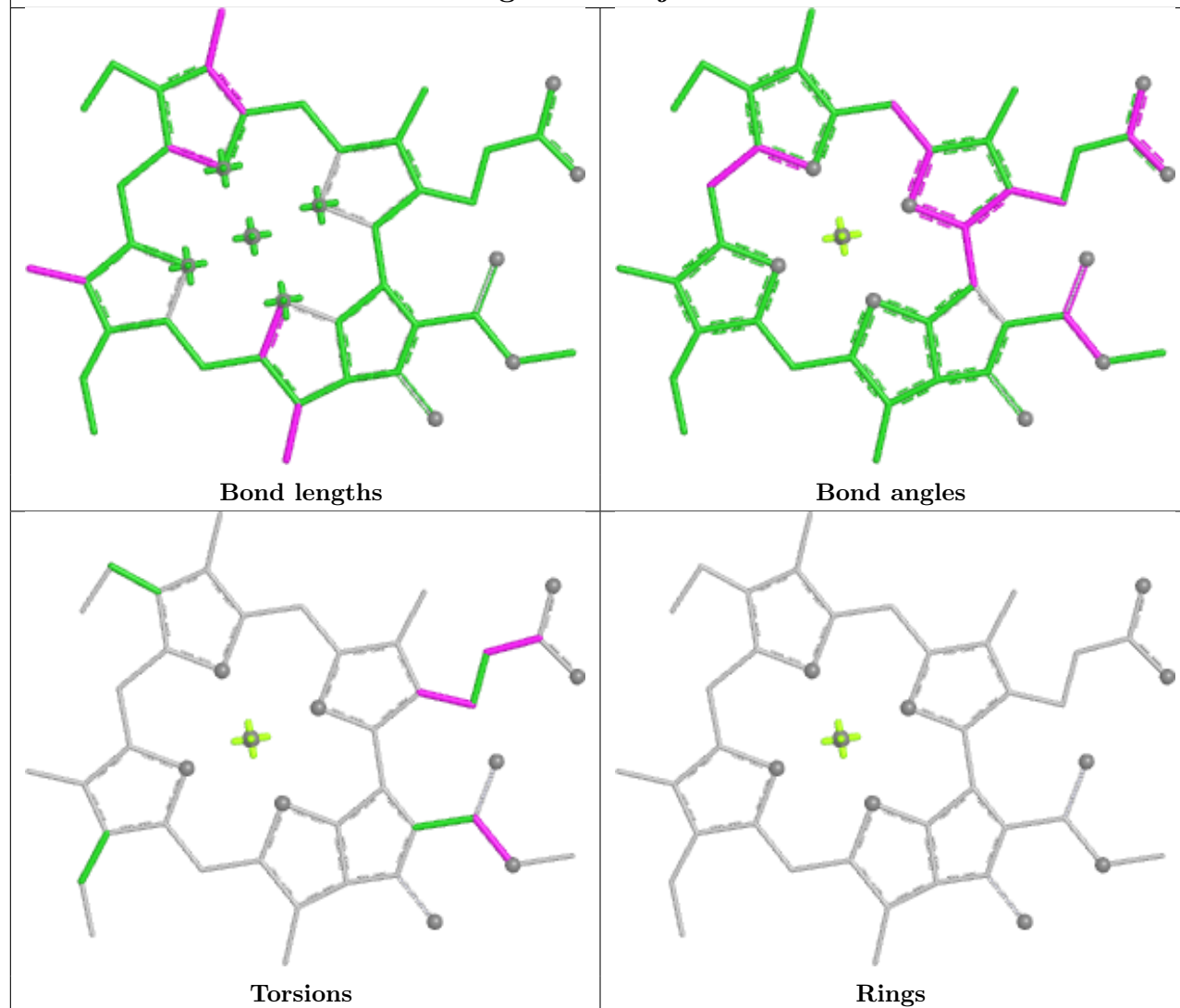
Ligand II0 k 318

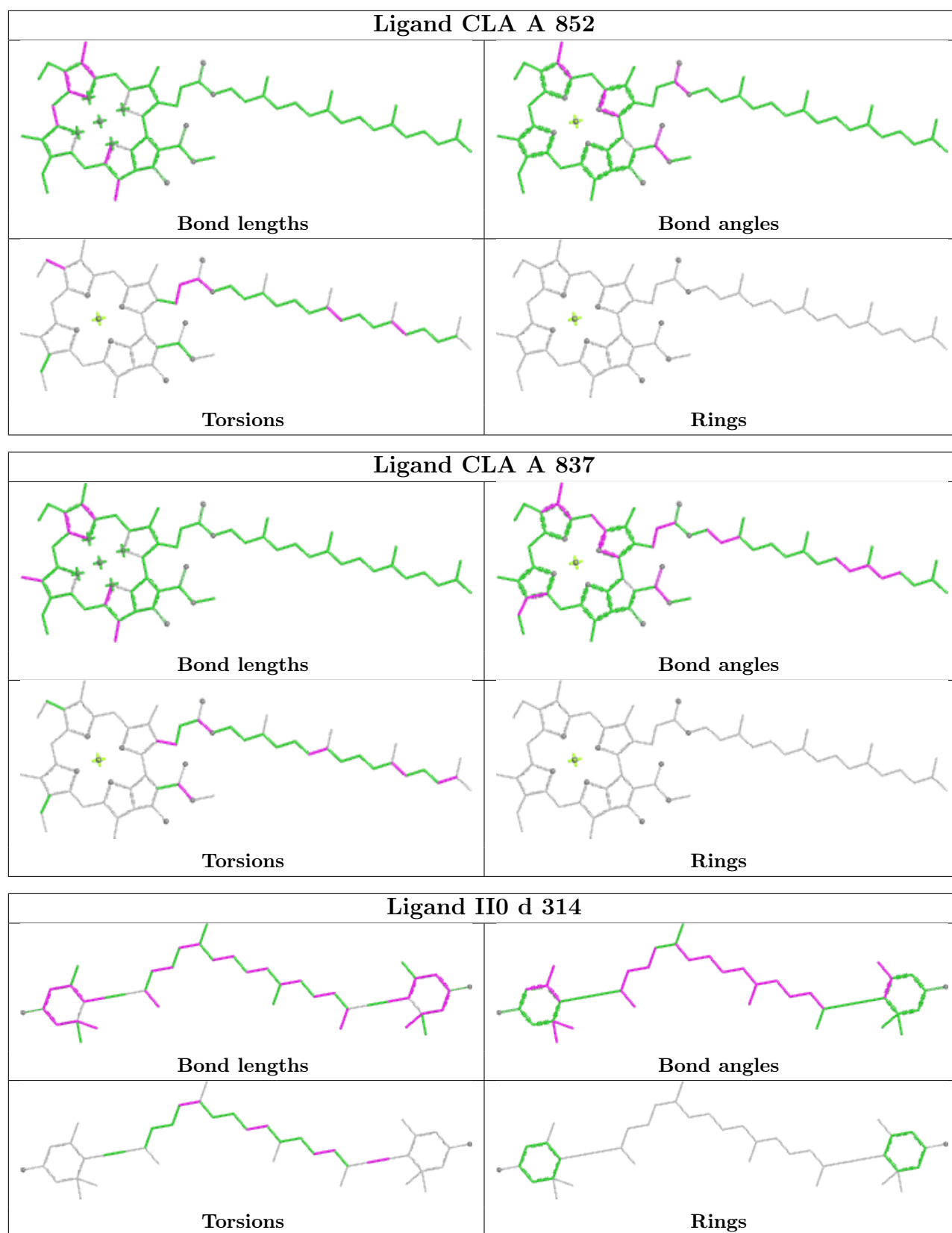


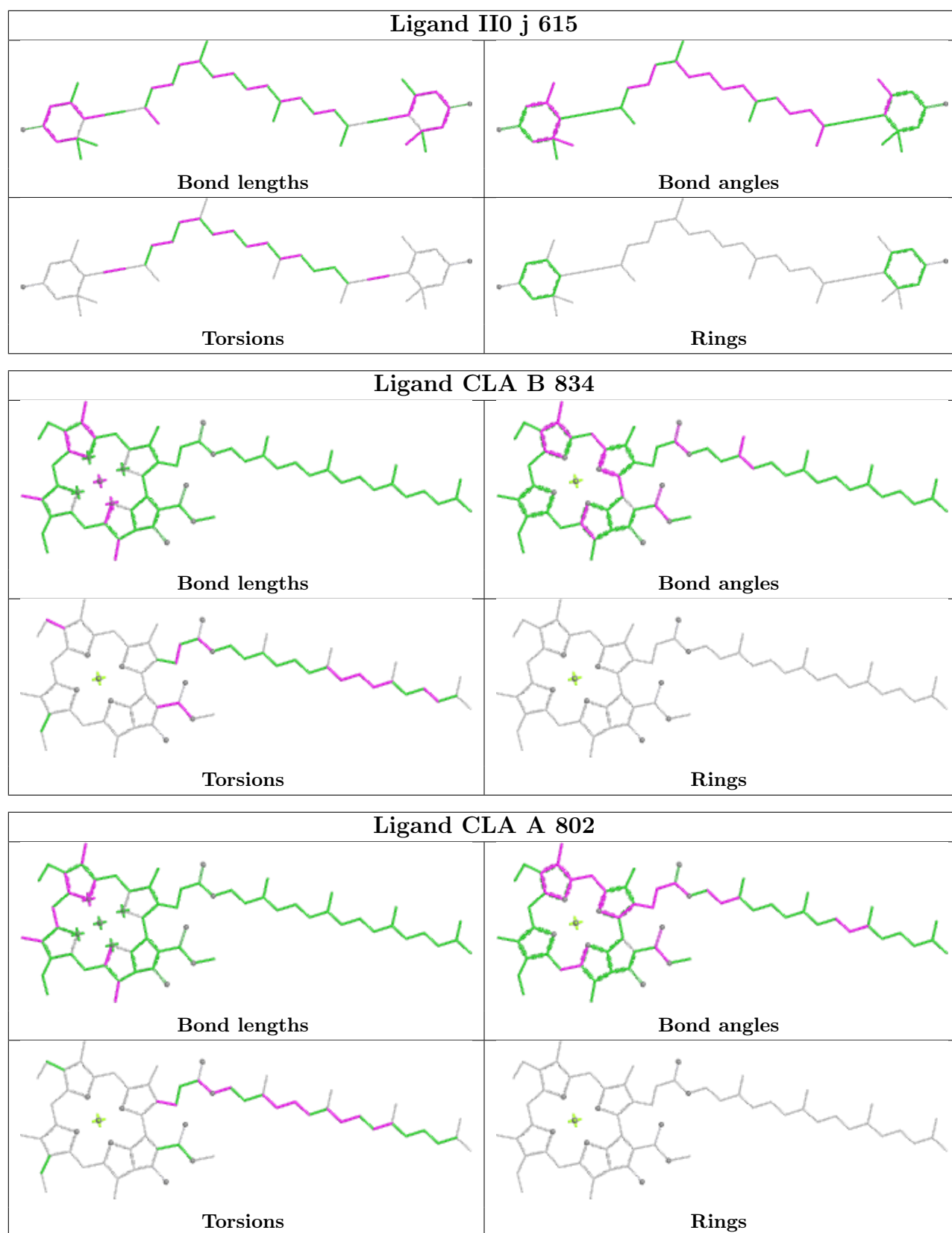
Ligand CLA l 304

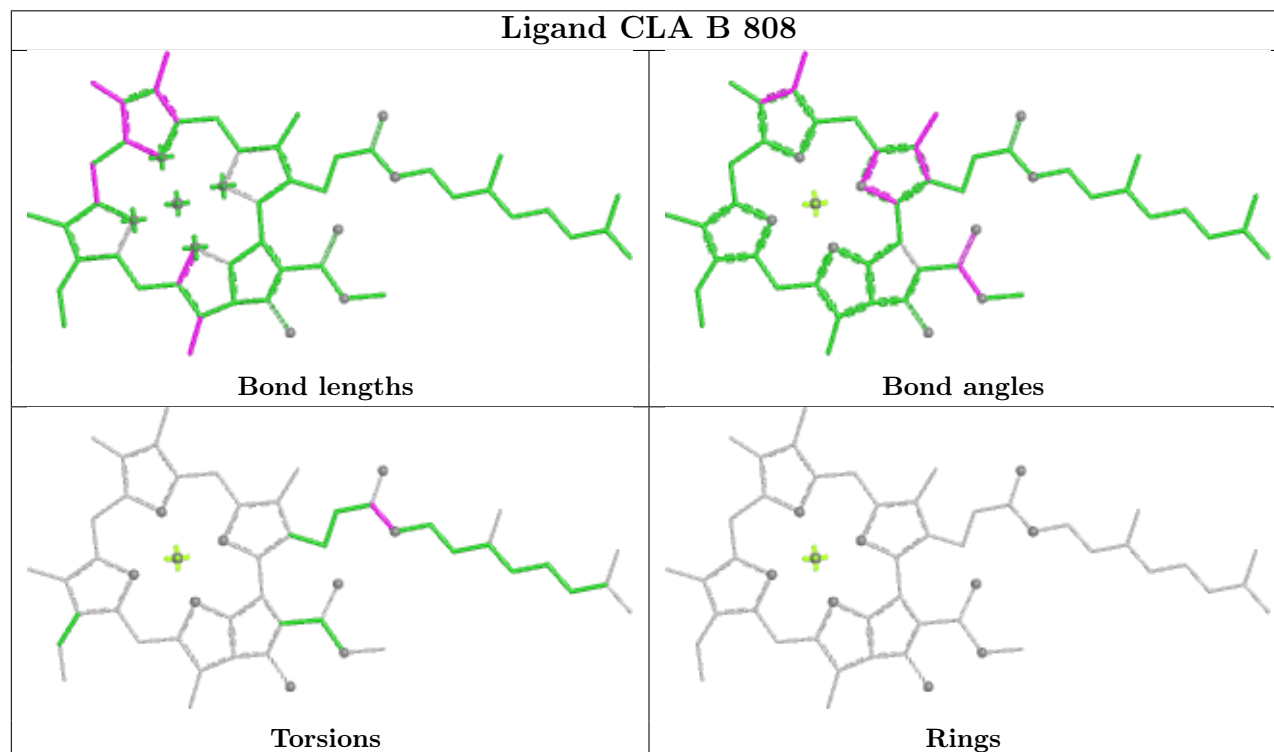
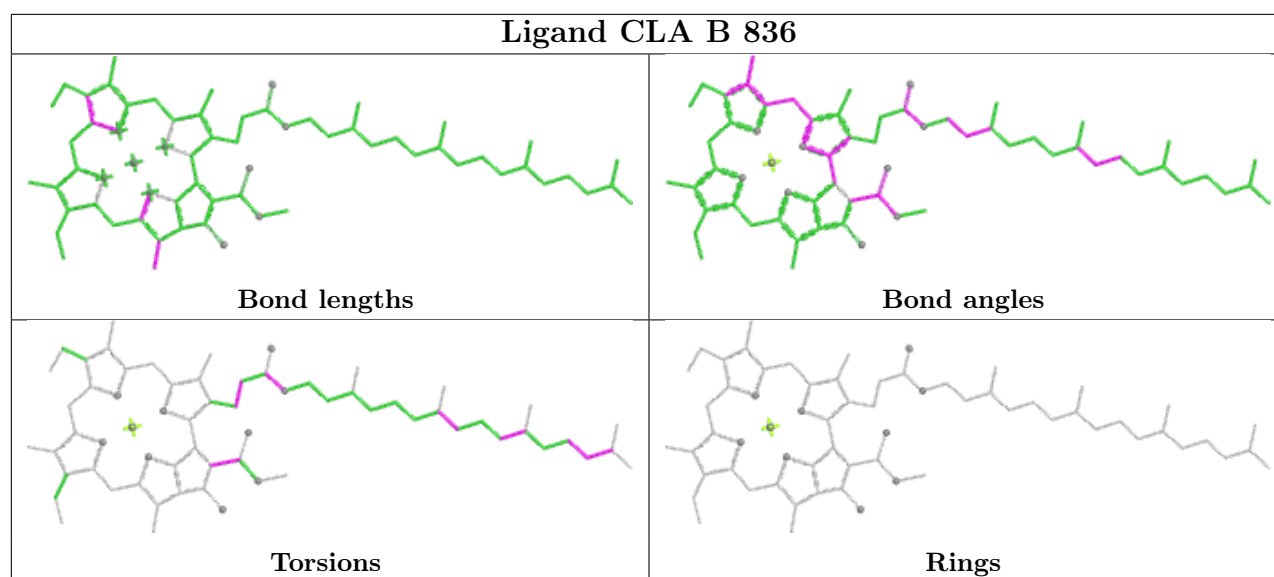


Ligand CLA j 605

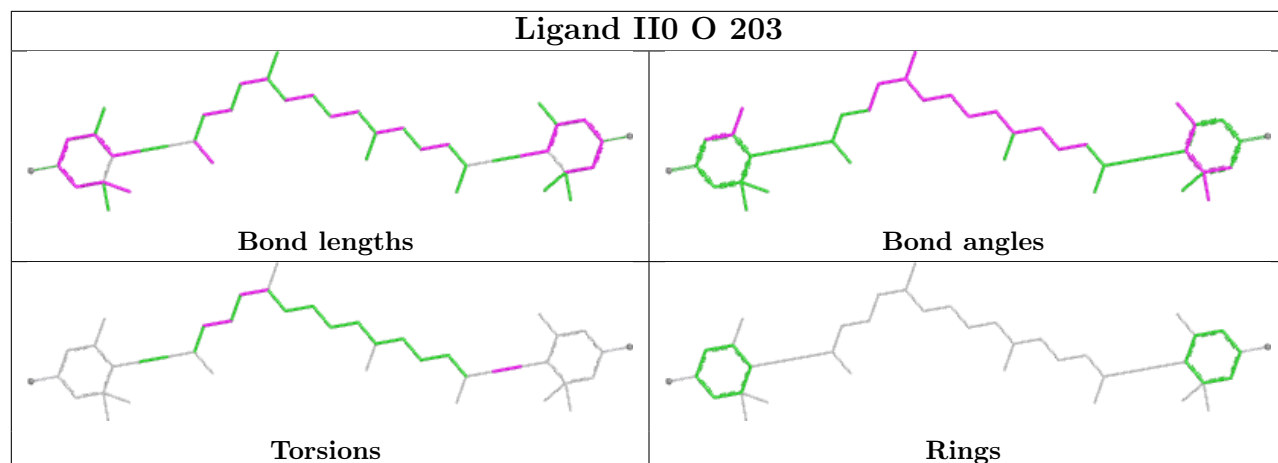




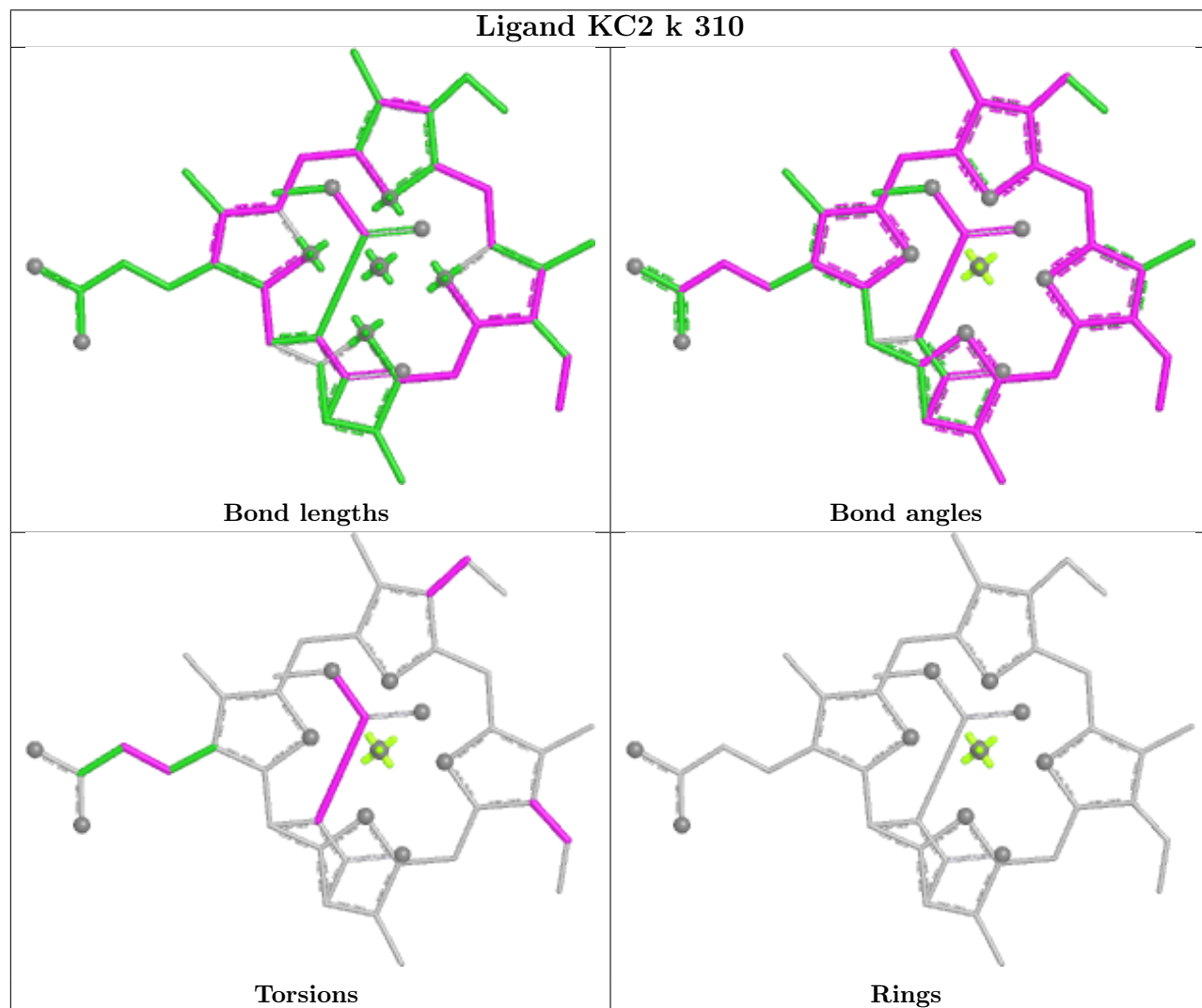


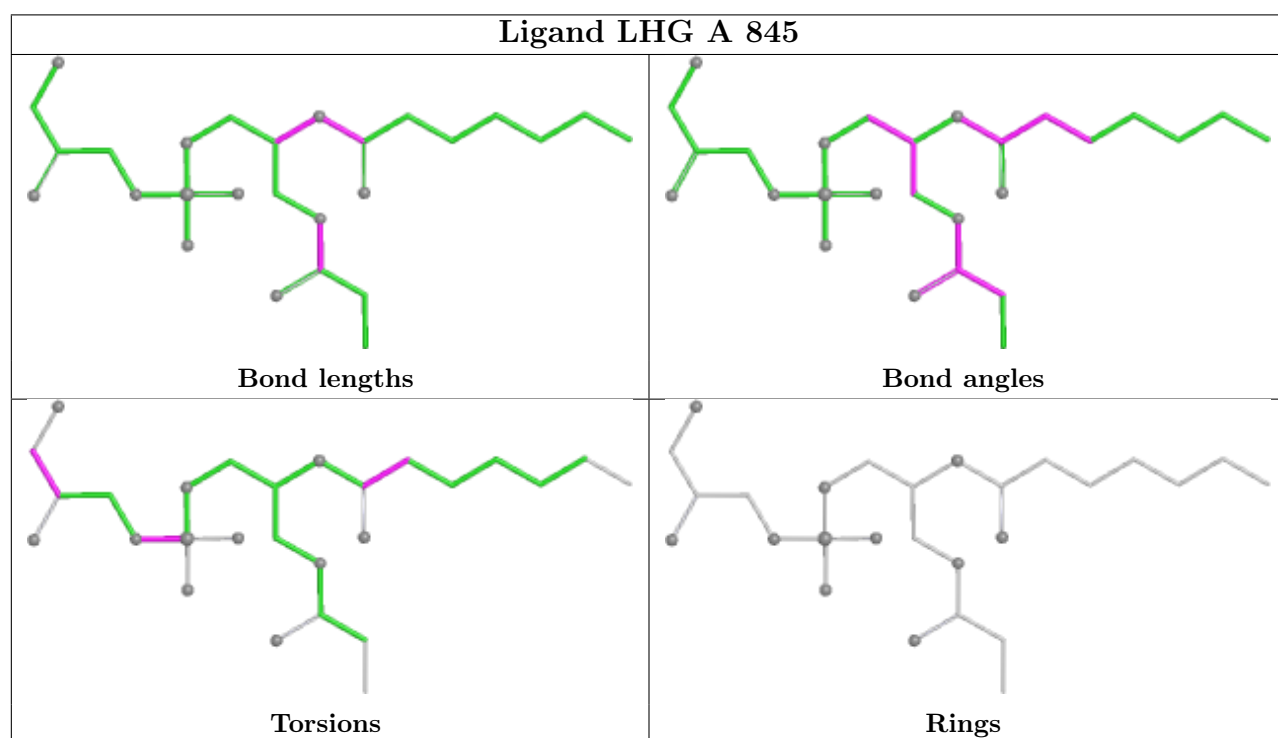
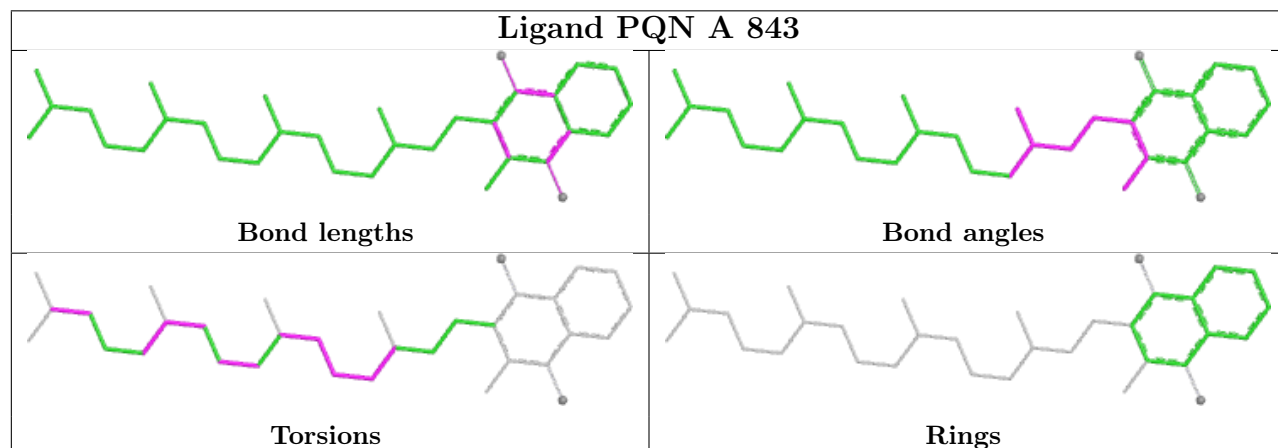
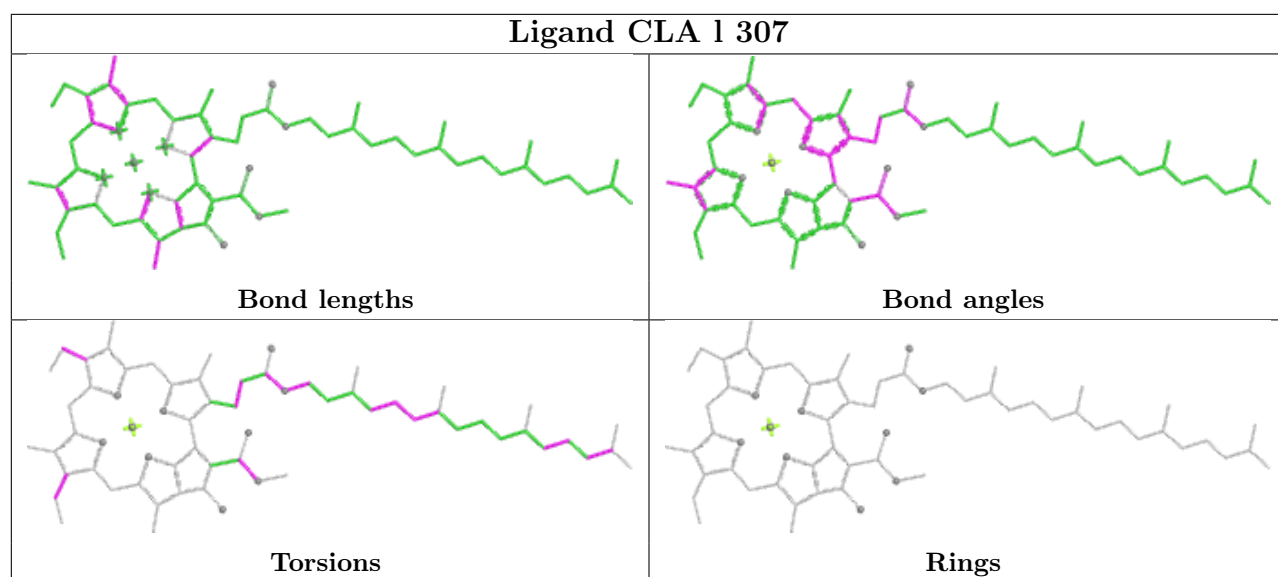


Ligand II0 O 203

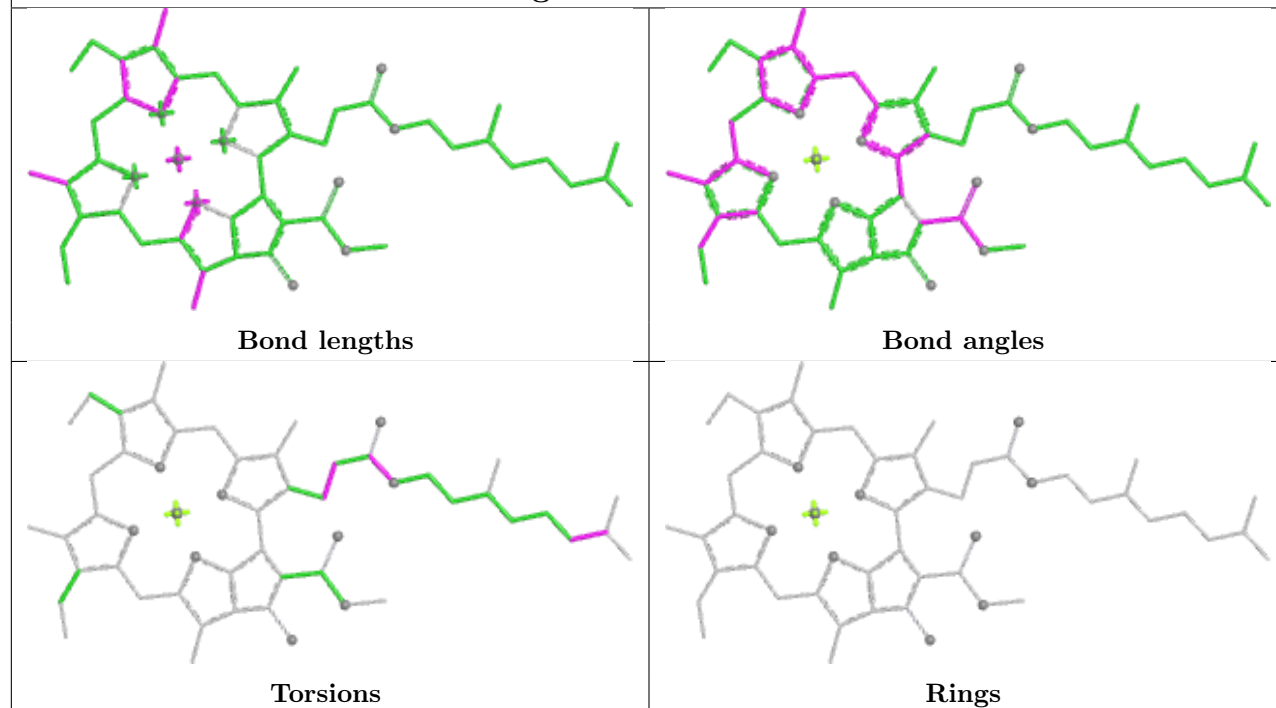


Ligand KC2 k 310

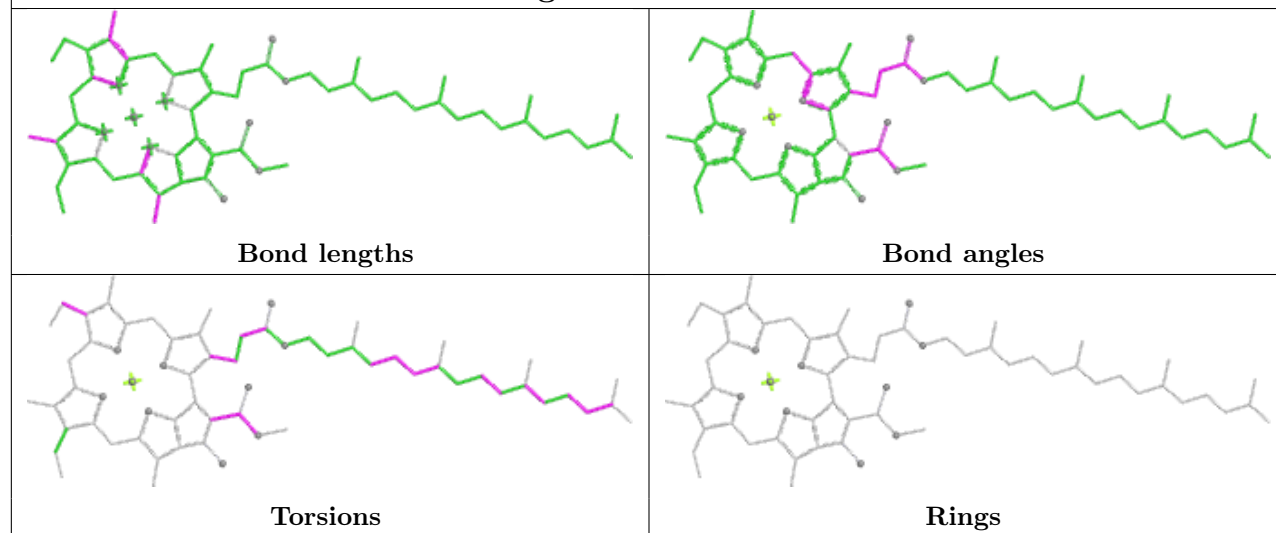


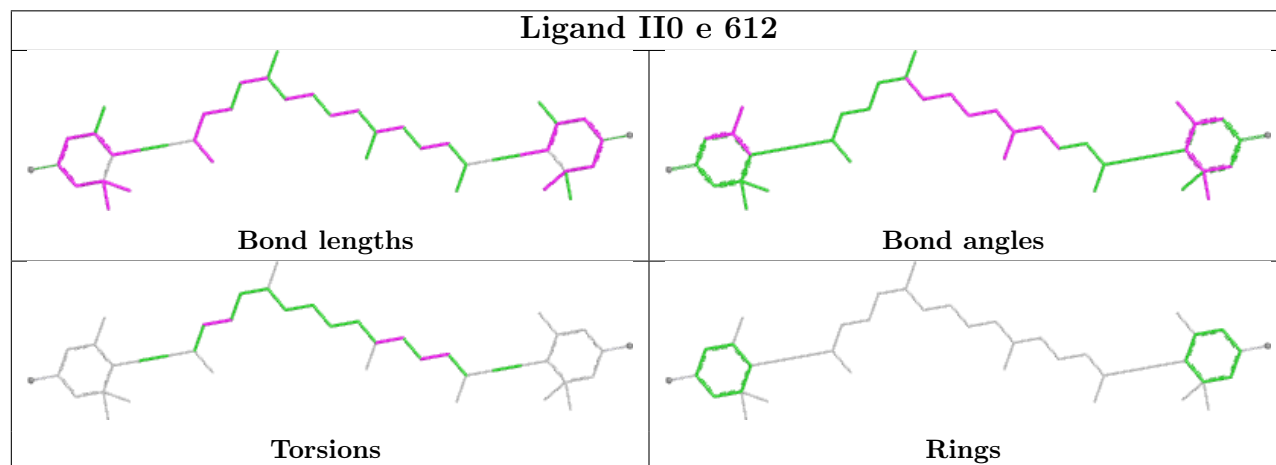
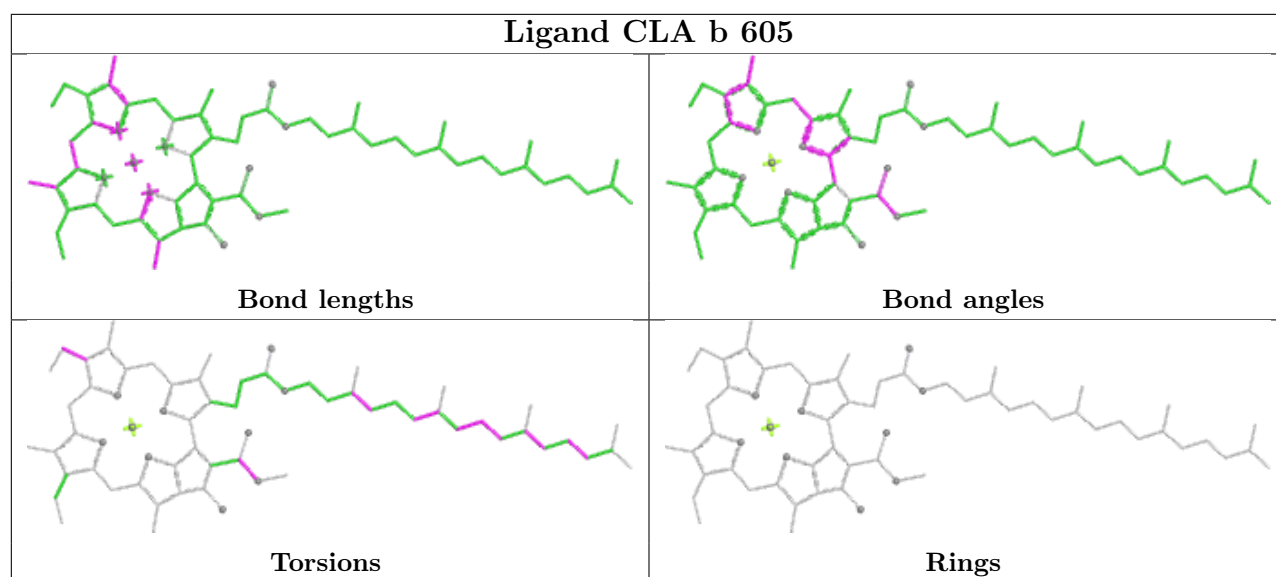


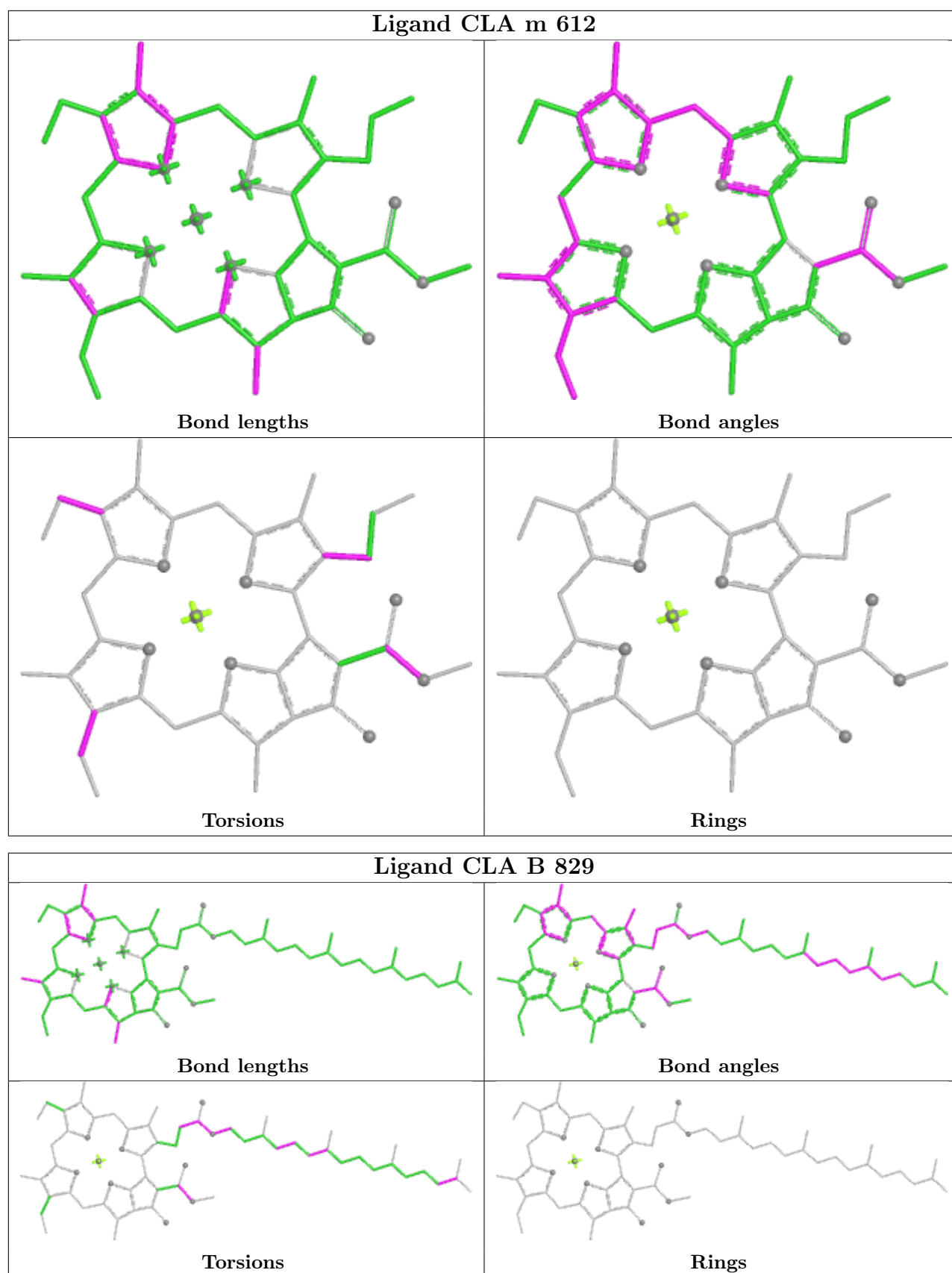
Ligand CLA B 809

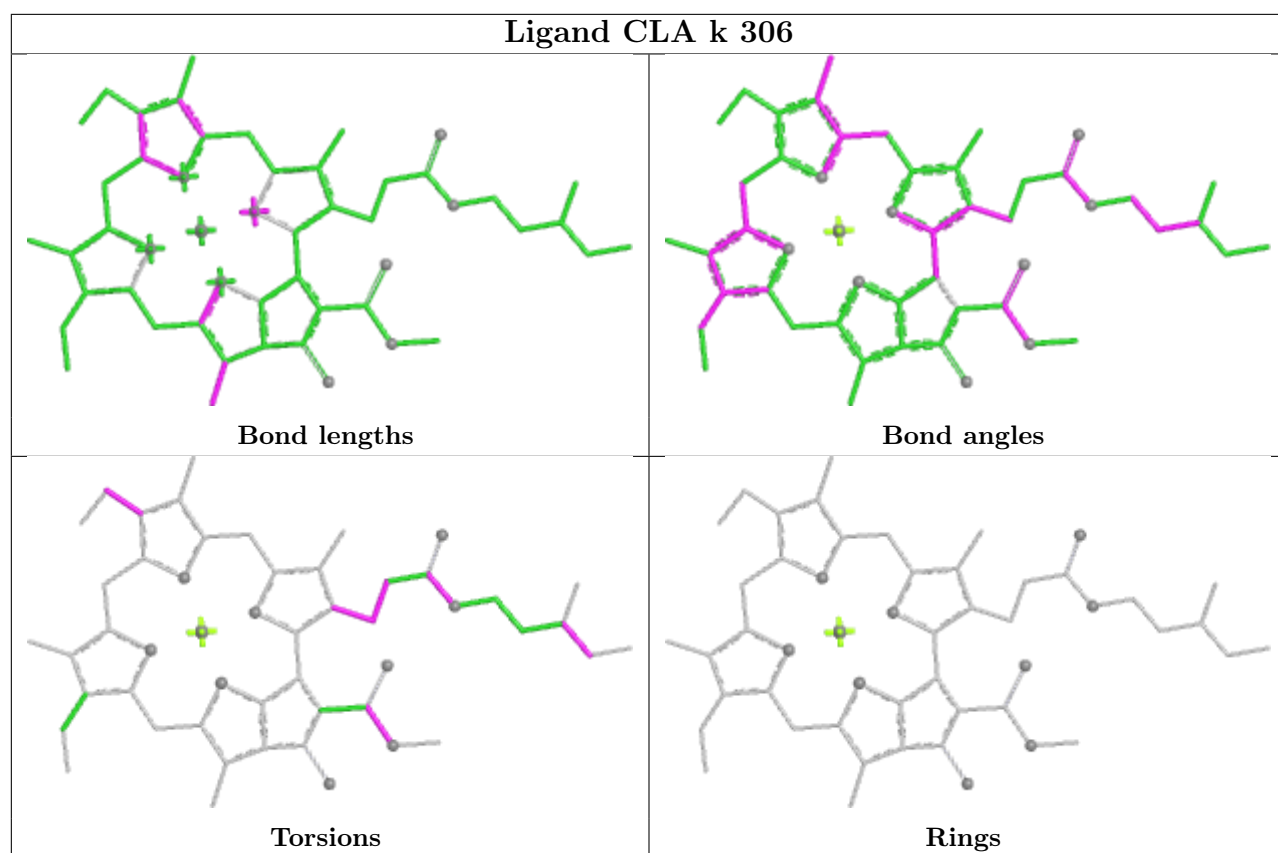


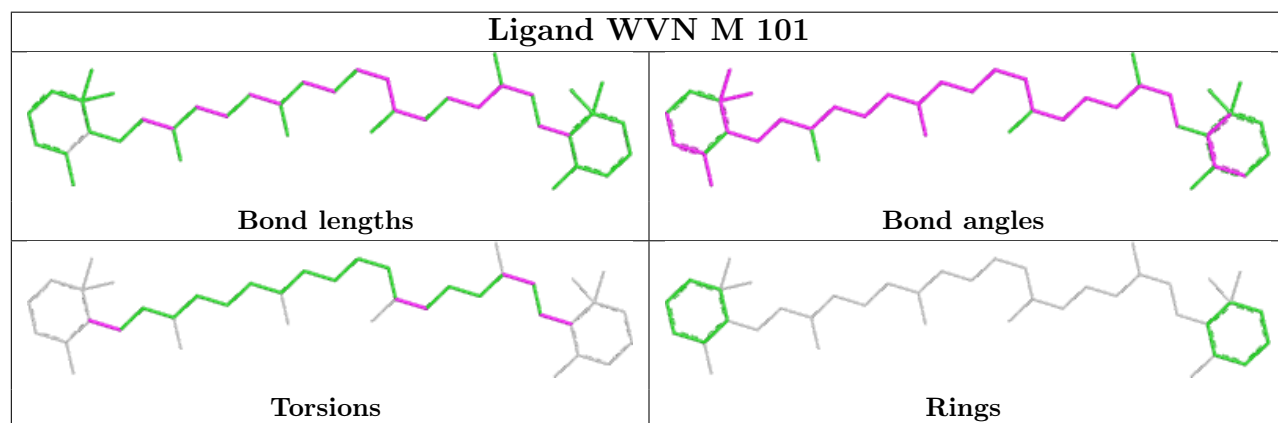
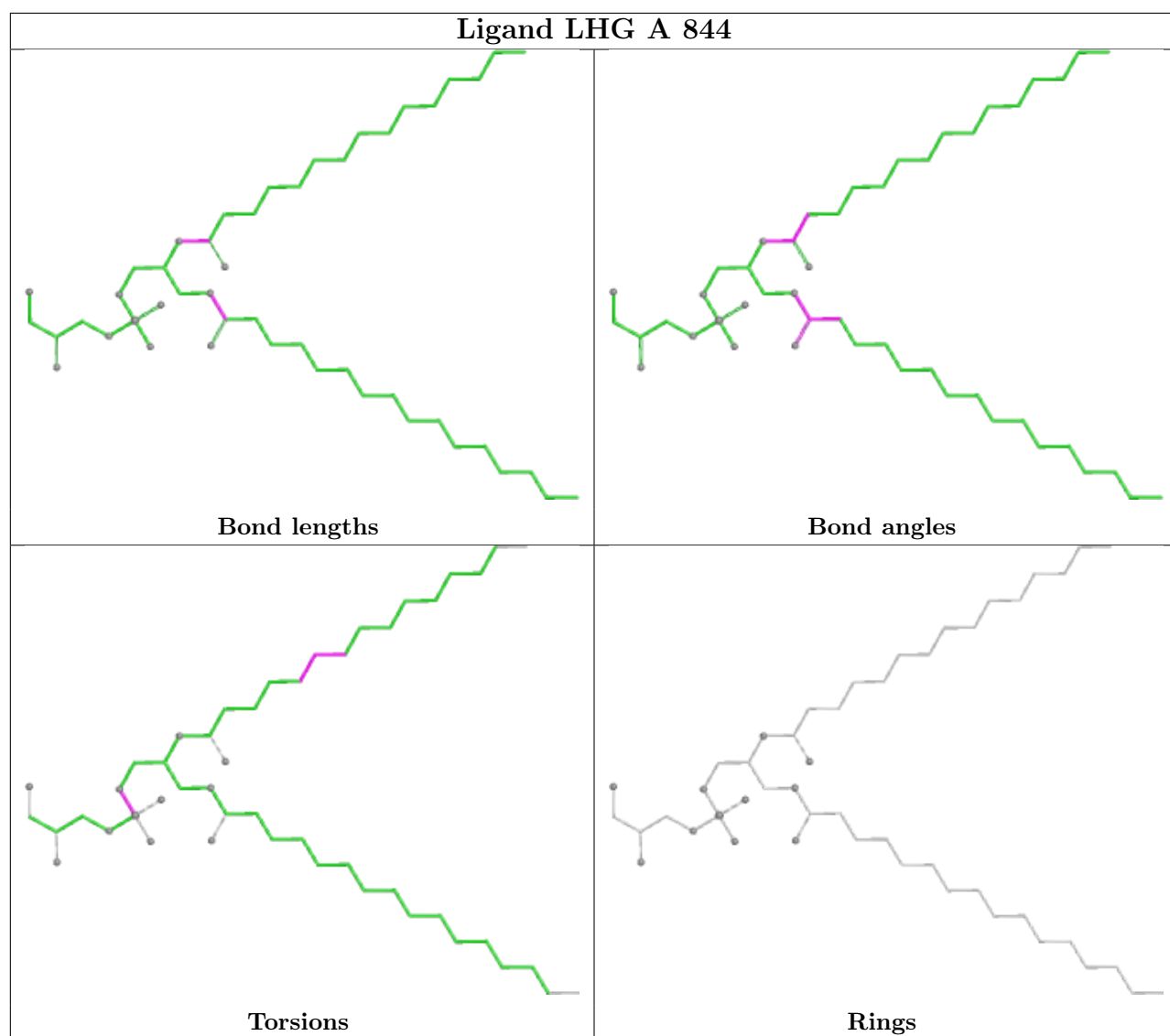
Ligand CLA s 203

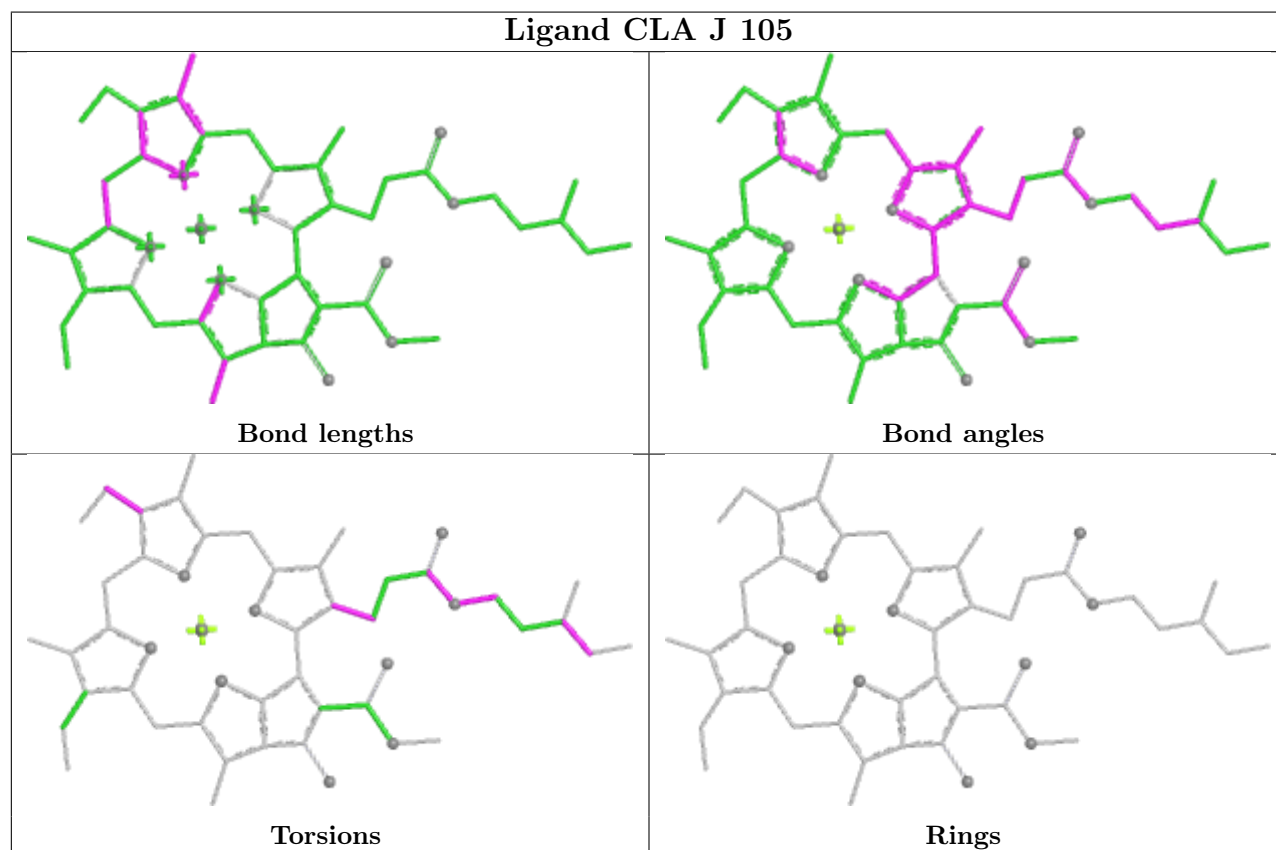
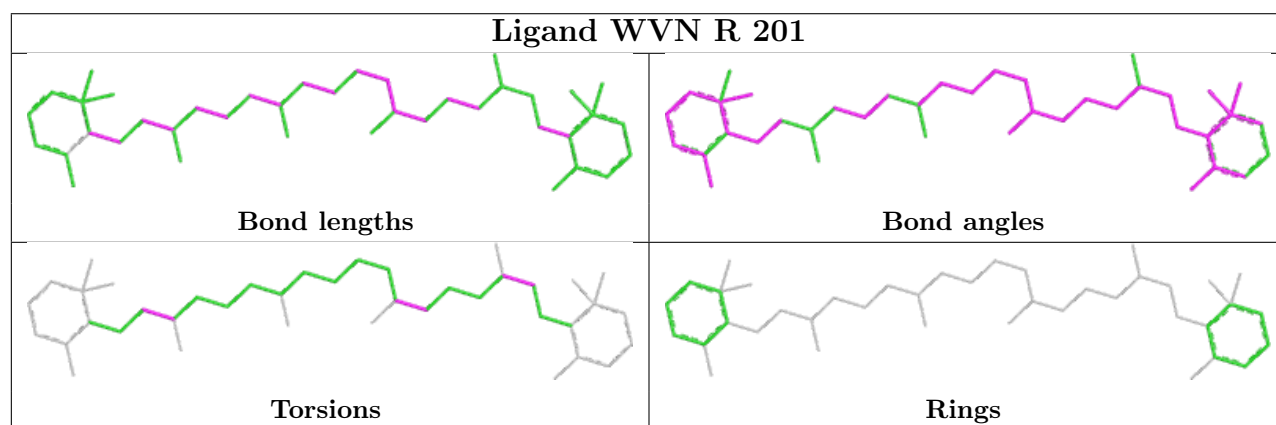
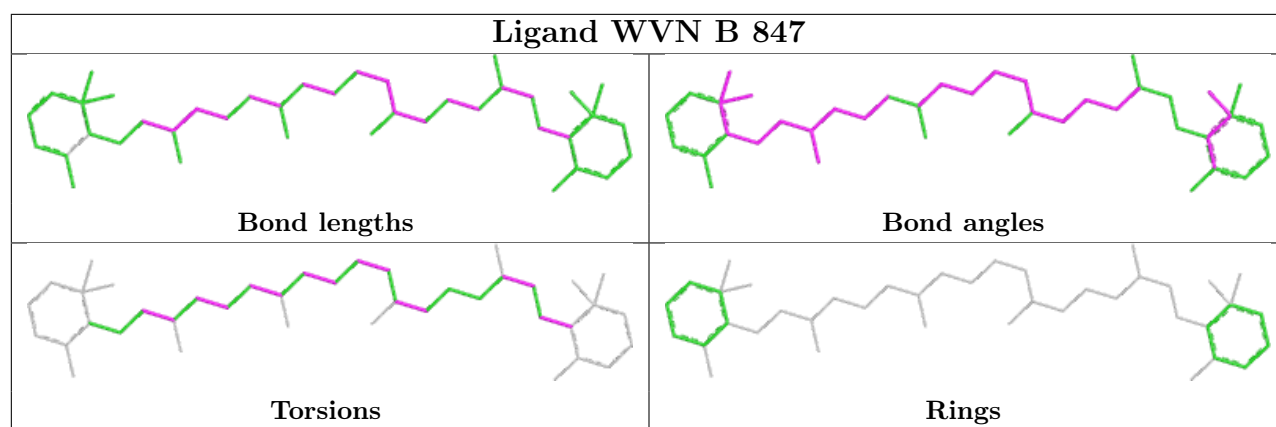


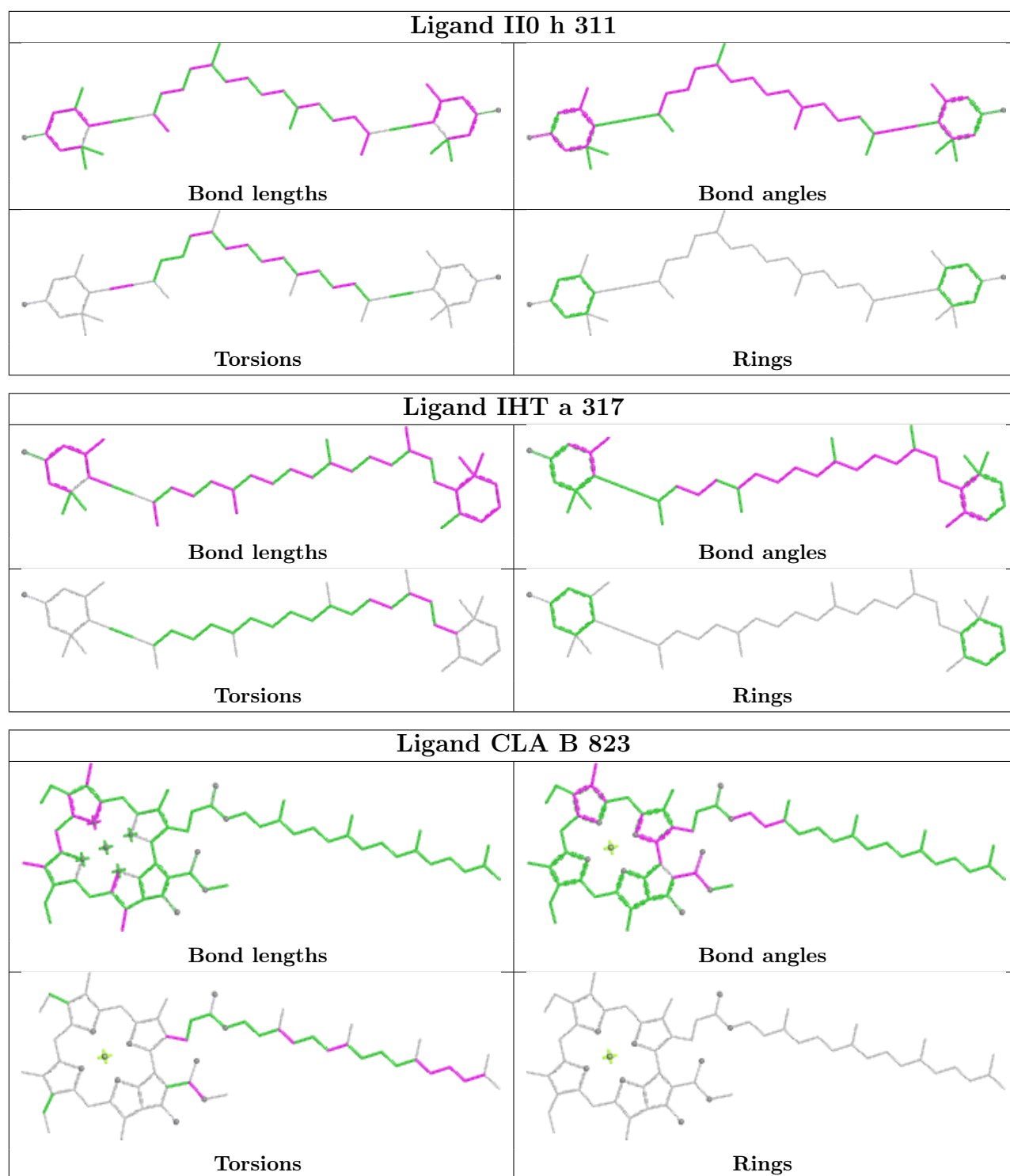


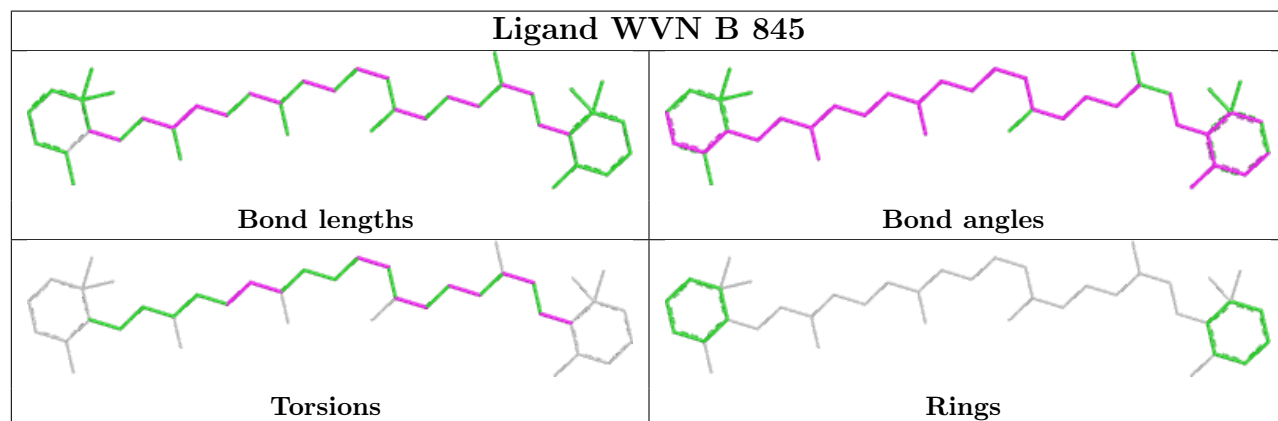
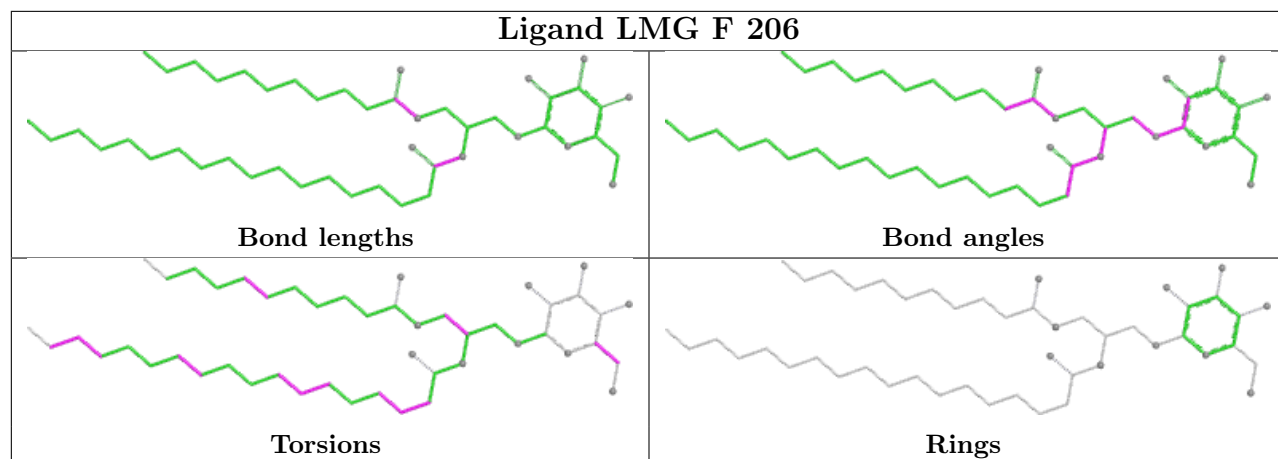


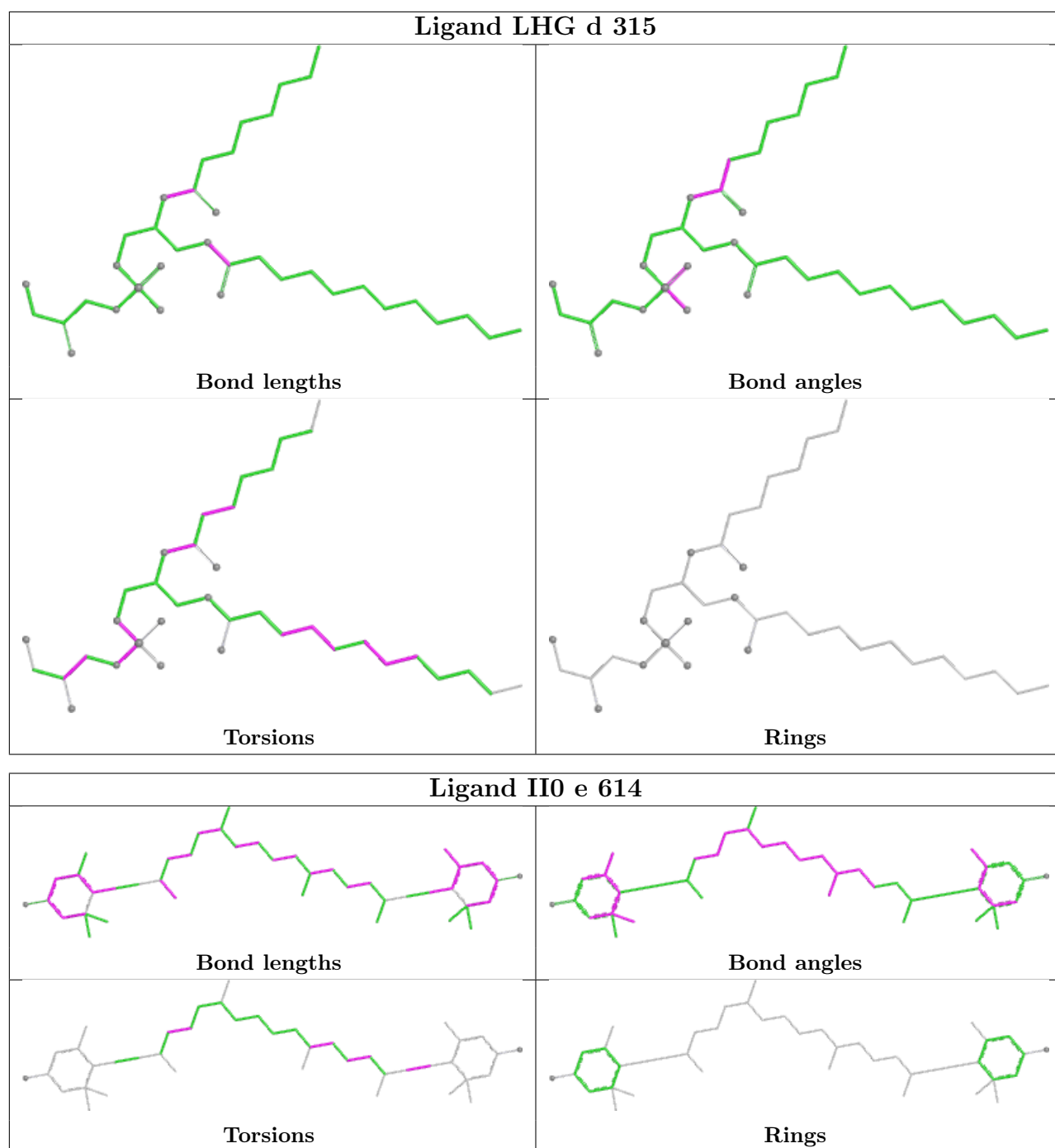




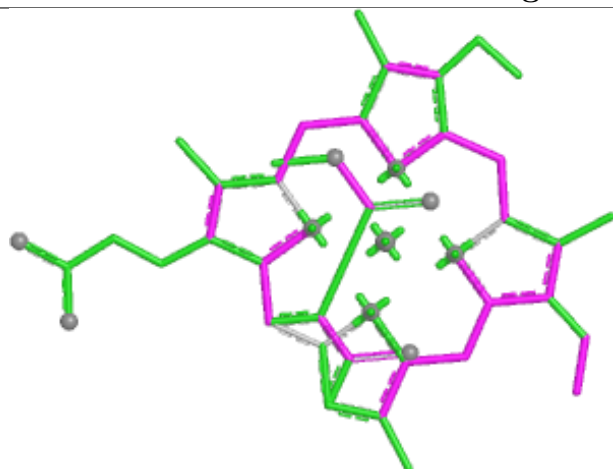




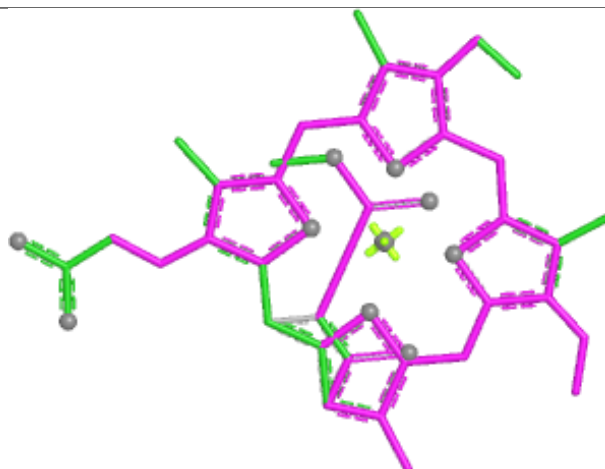




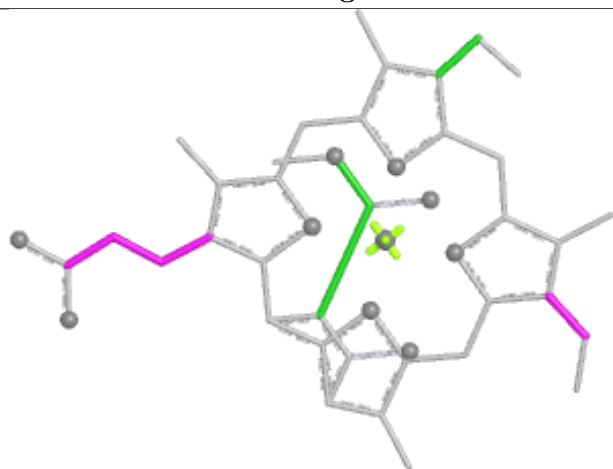
Ligand KC2 s 201



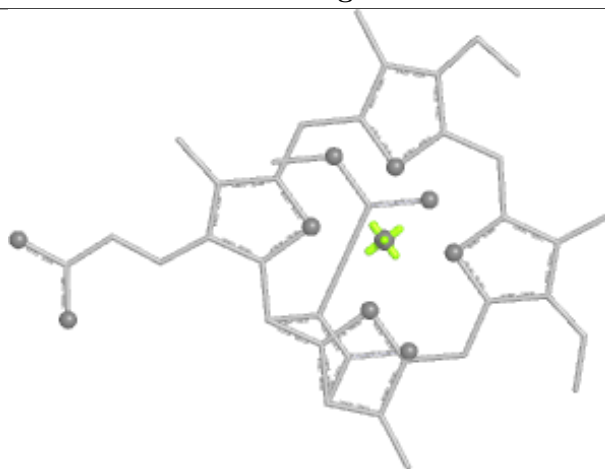
Bond lengths



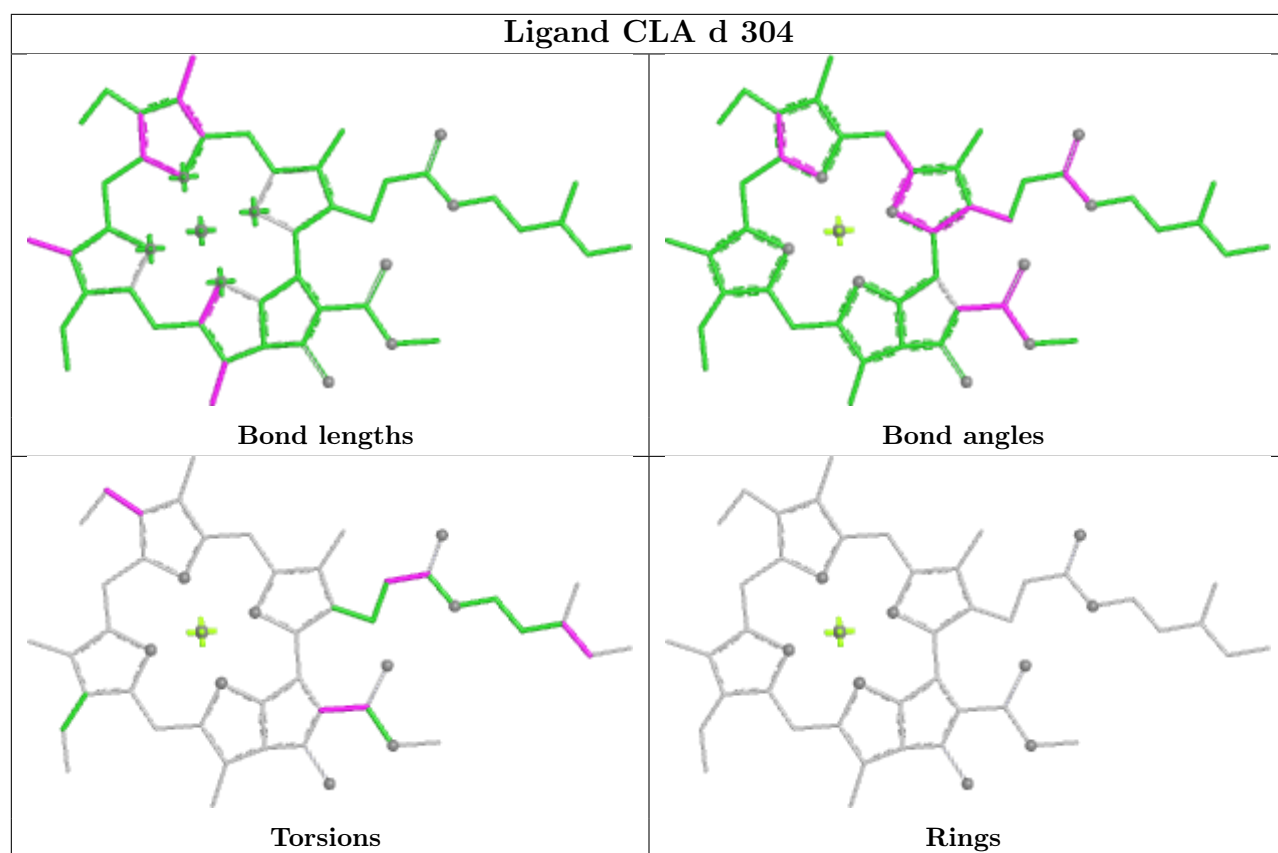
Bond angles



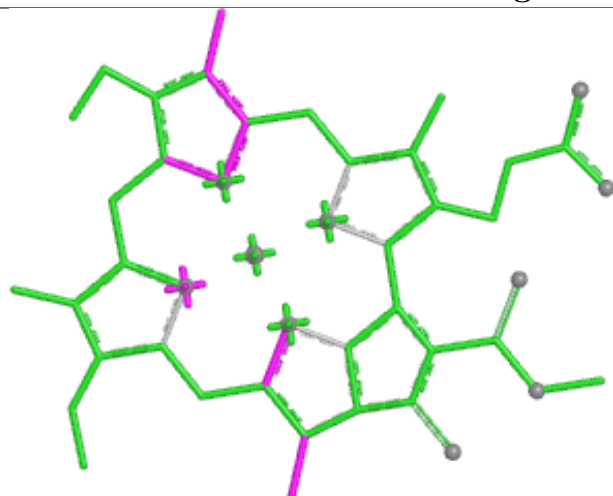
Torsions



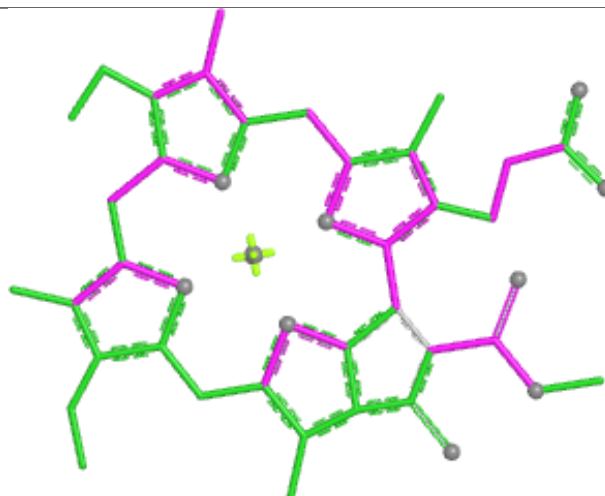
Rings



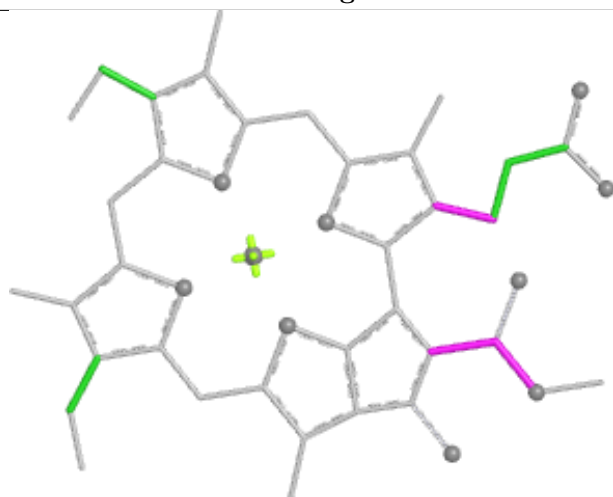
Ligand CLA A 813



Bond lengths



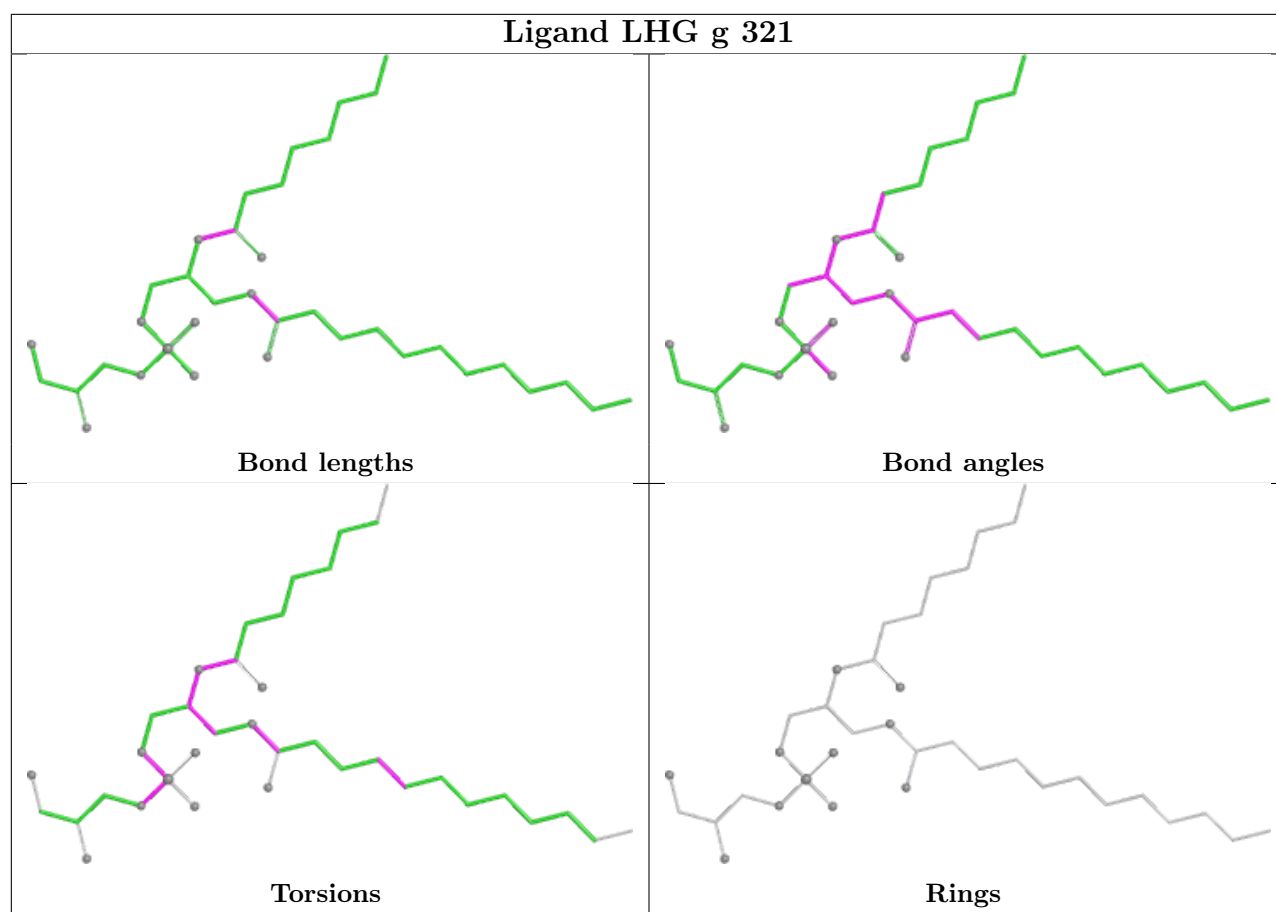
Bond angles



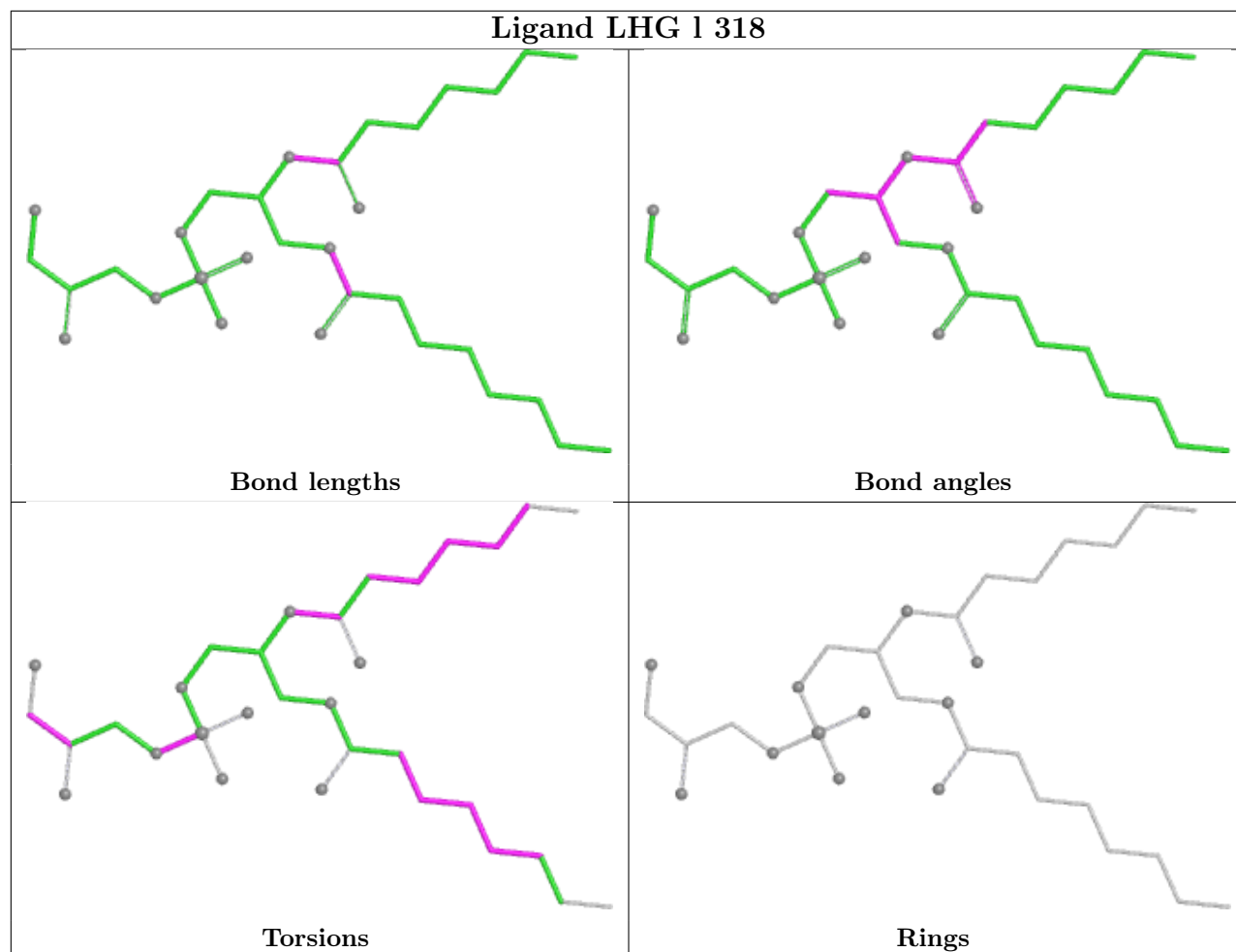
Torsions



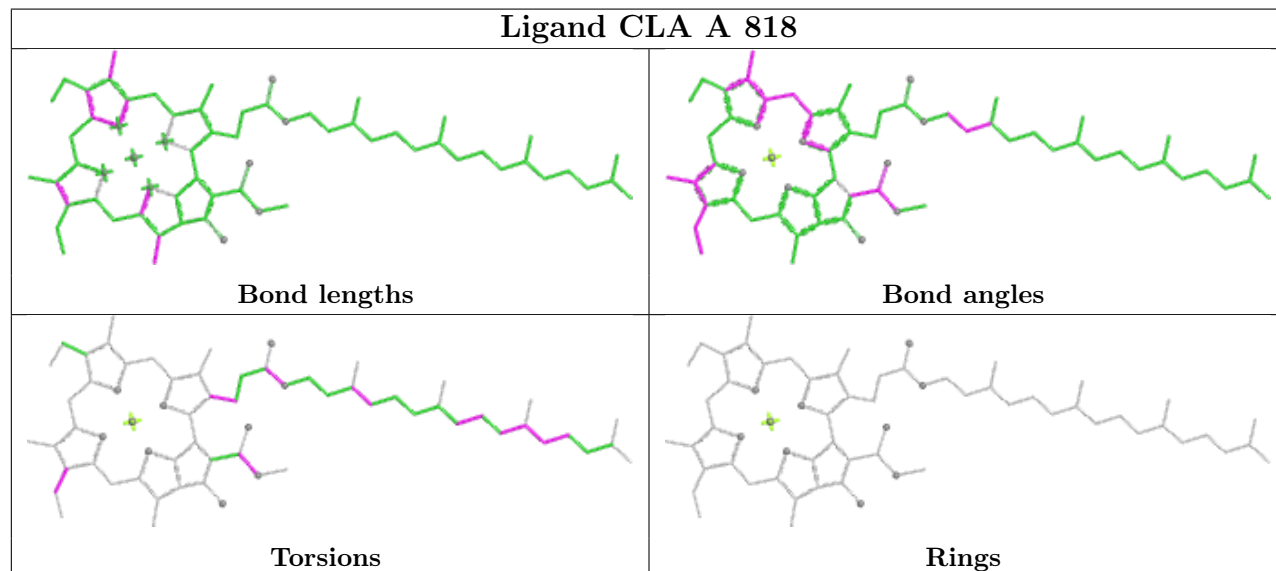
Rings



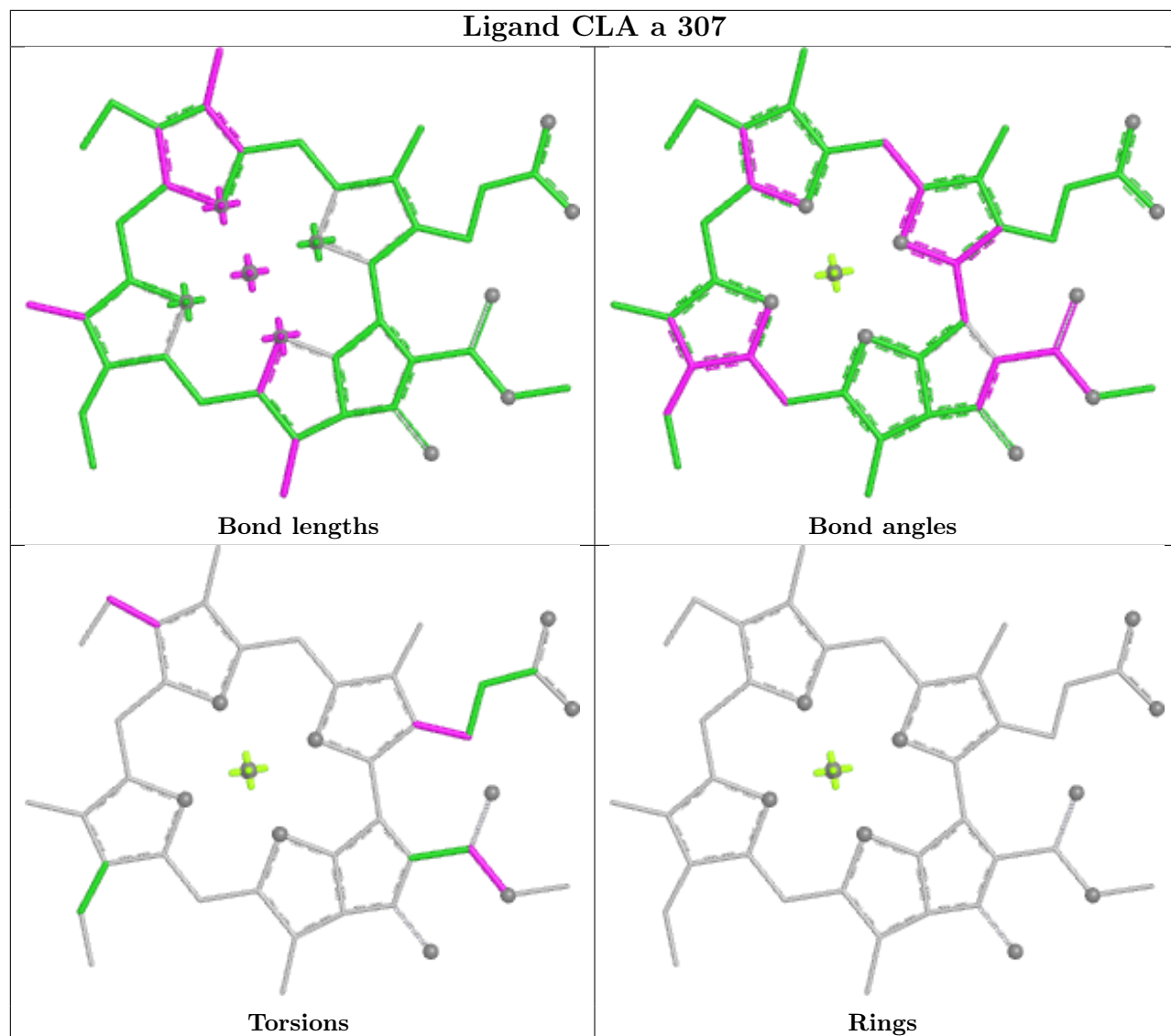
Ligand LHG 1 318



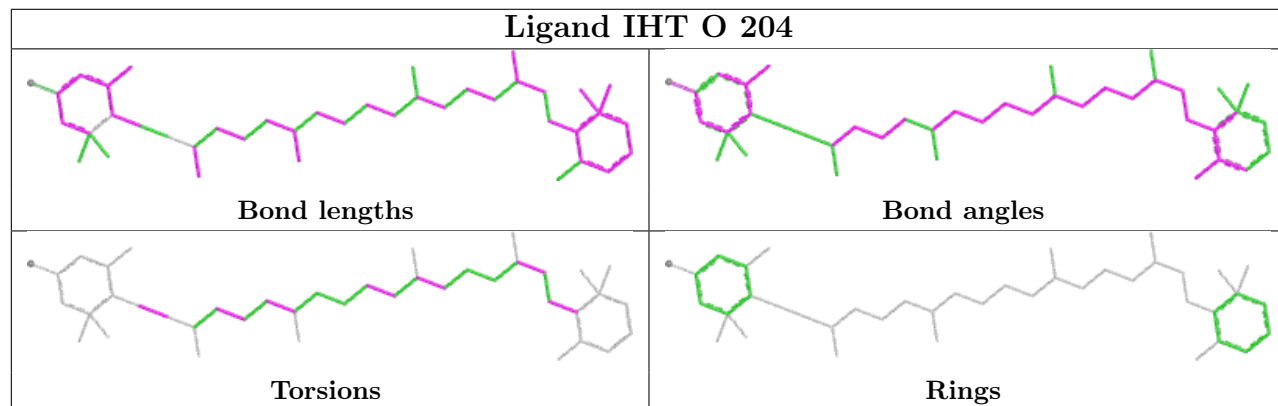
Ligand CLA A 818

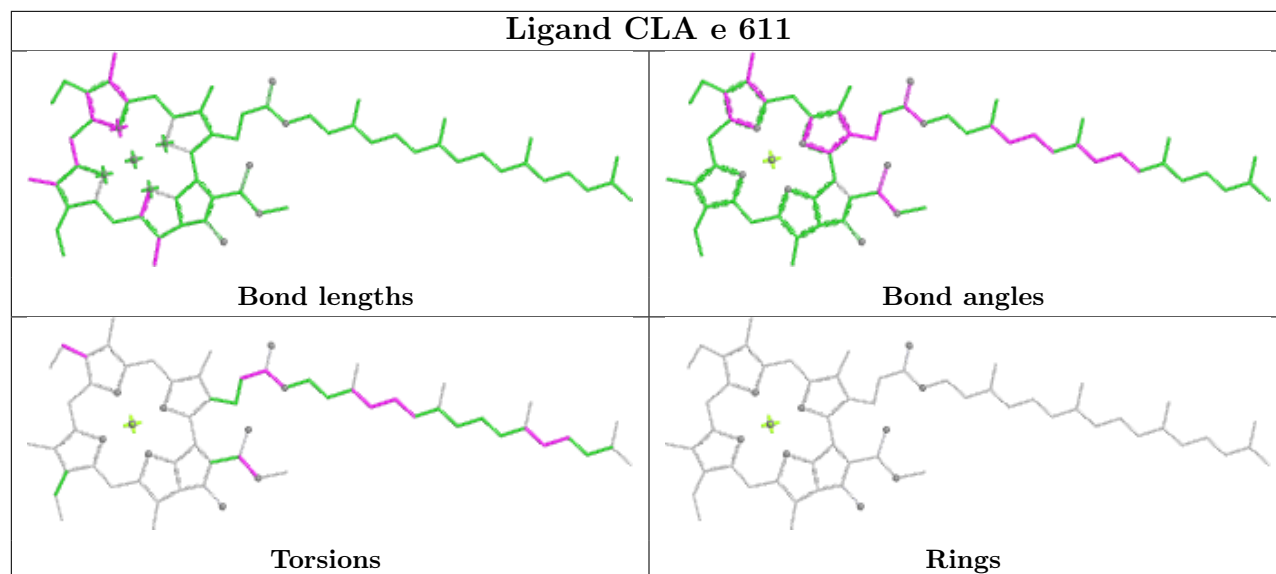
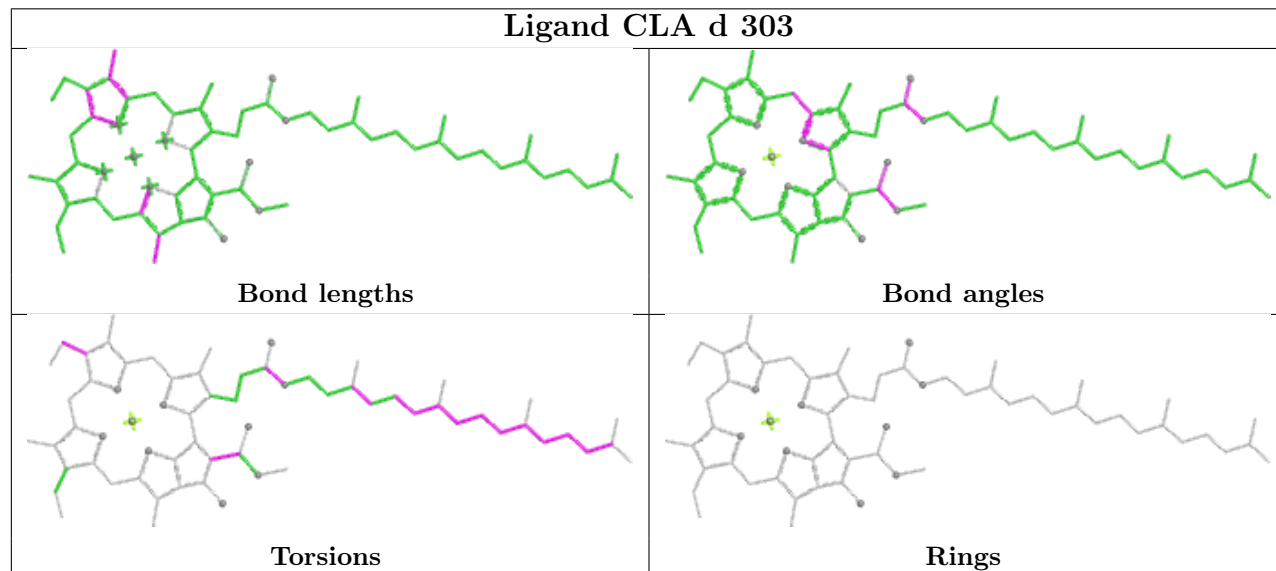


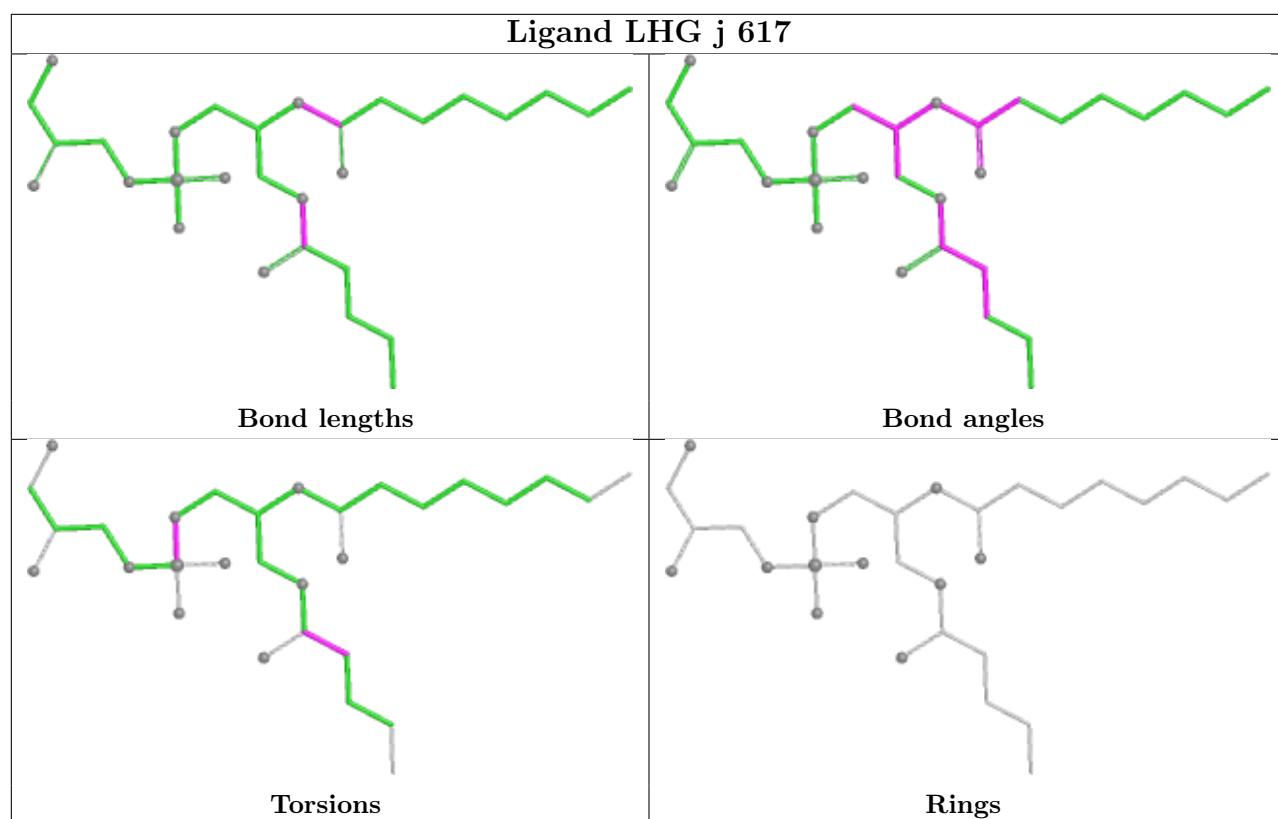
Ligand CLA a 307



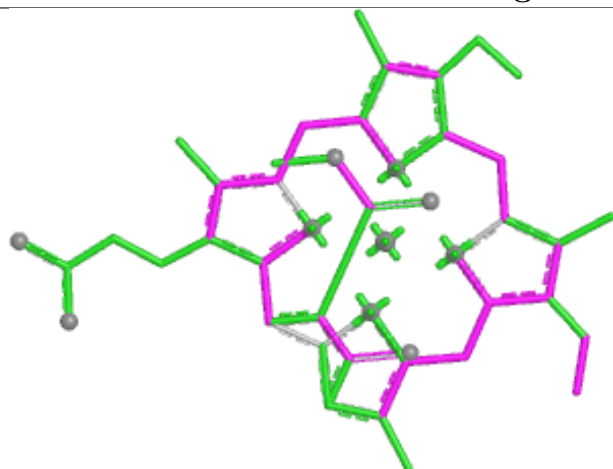
Ligand IHT O 204



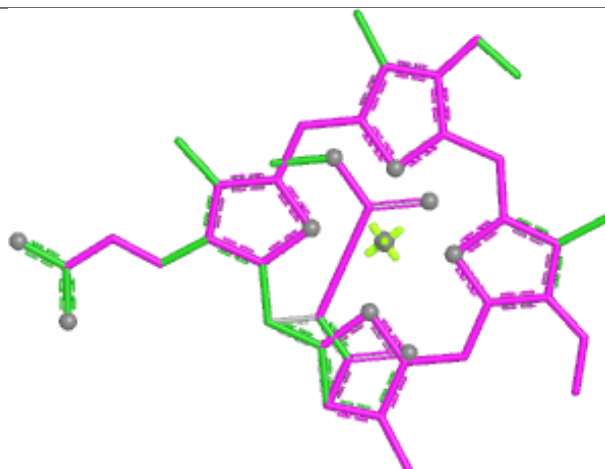
Ligand CLA e 611**Ligand CLA d 303**



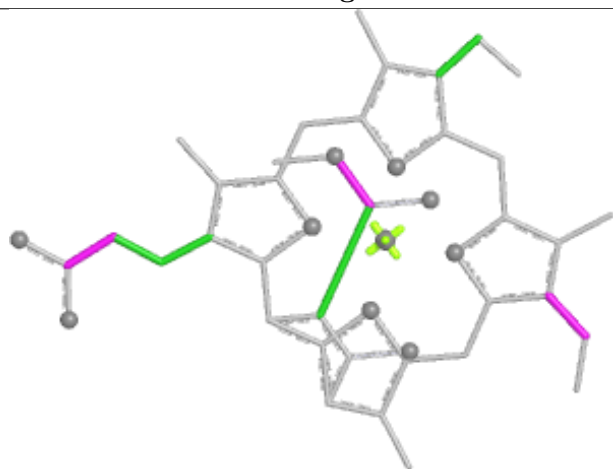
Ligand KC2 m 610



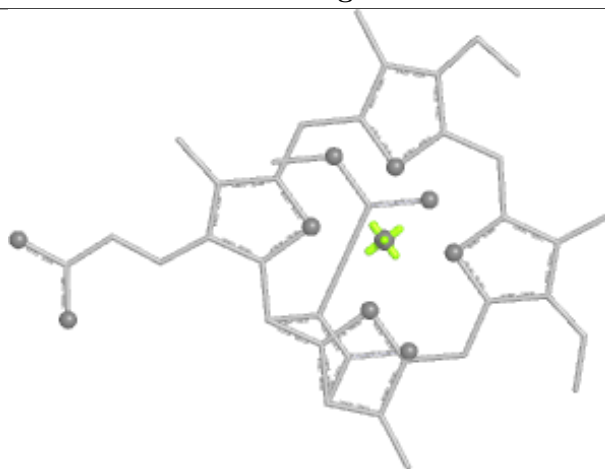
Bond lengths



Bond angles

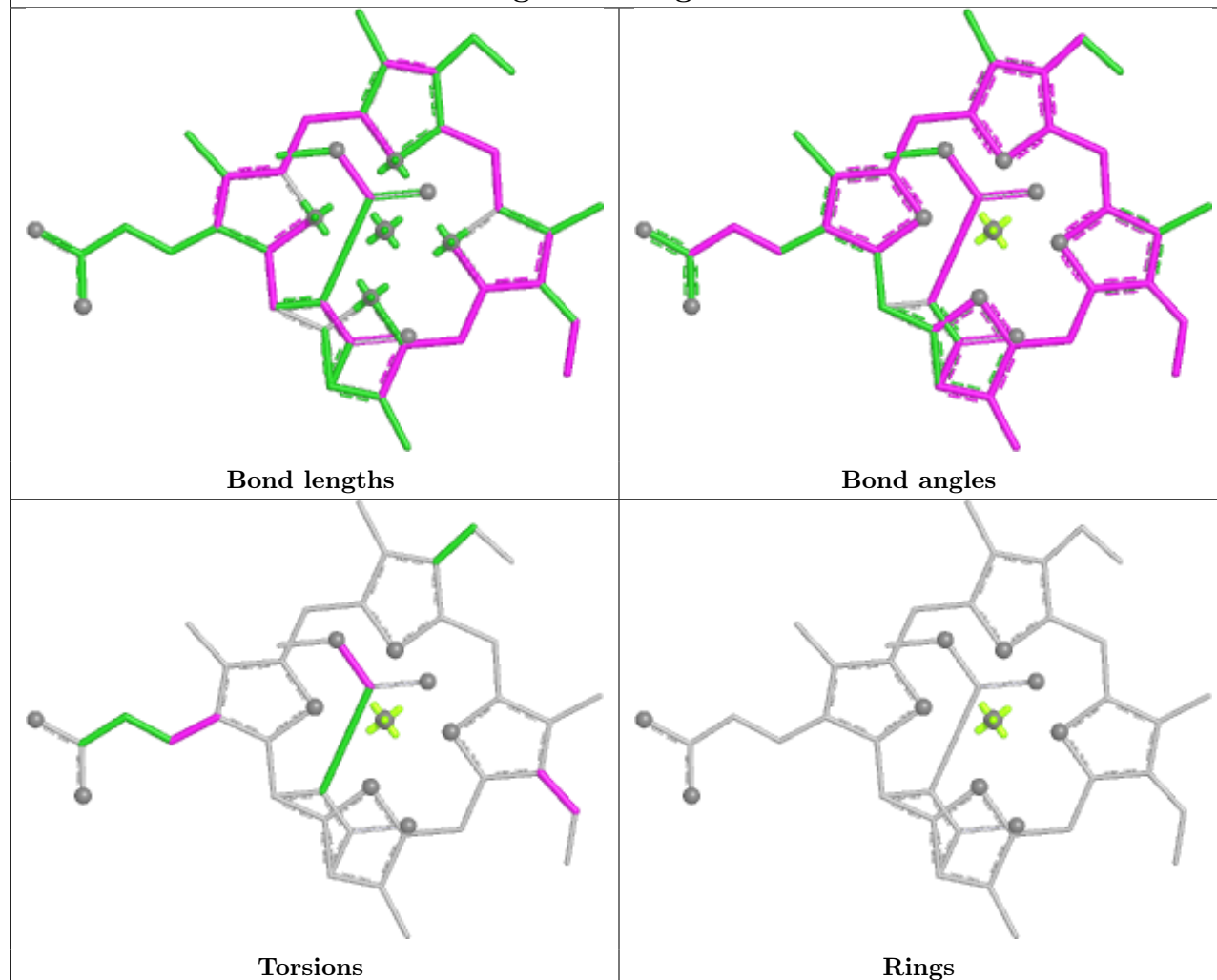


Torsions

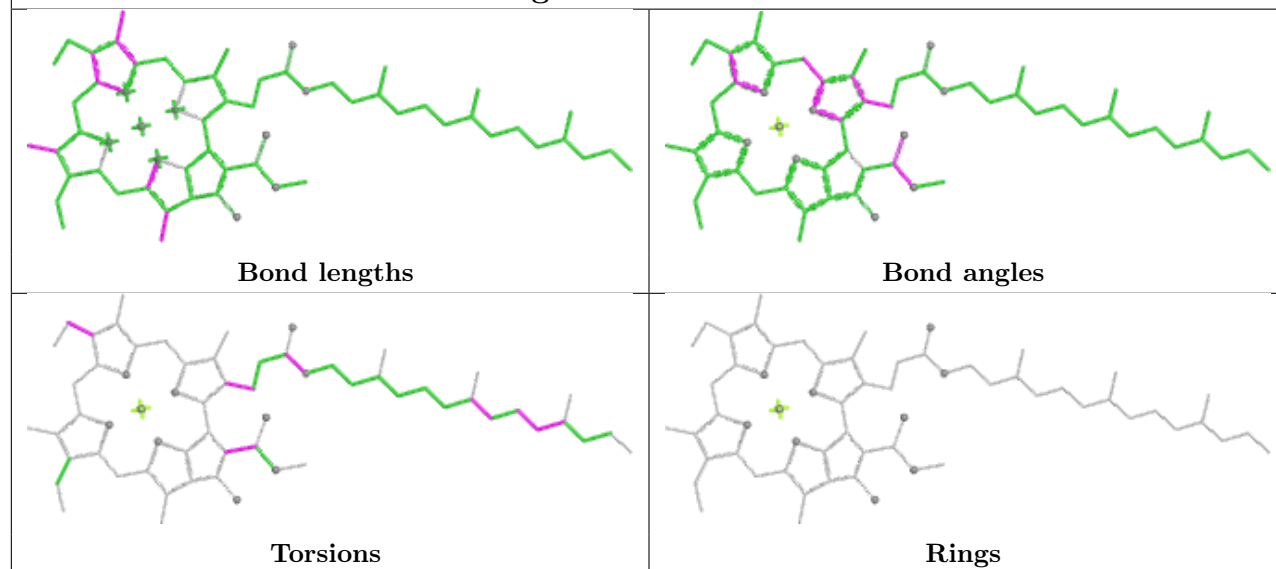


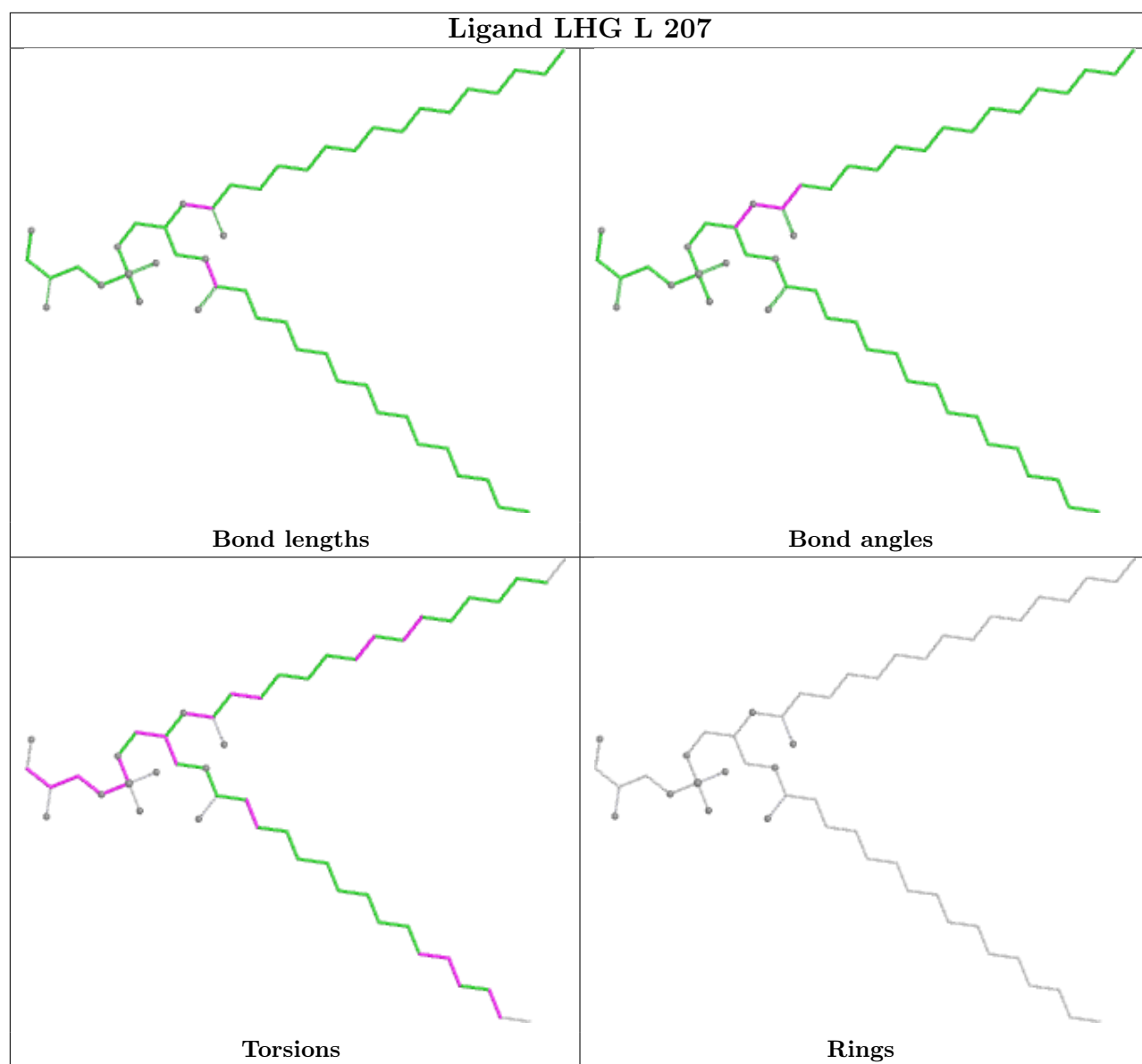
Rings

Ligand KC2 g 314

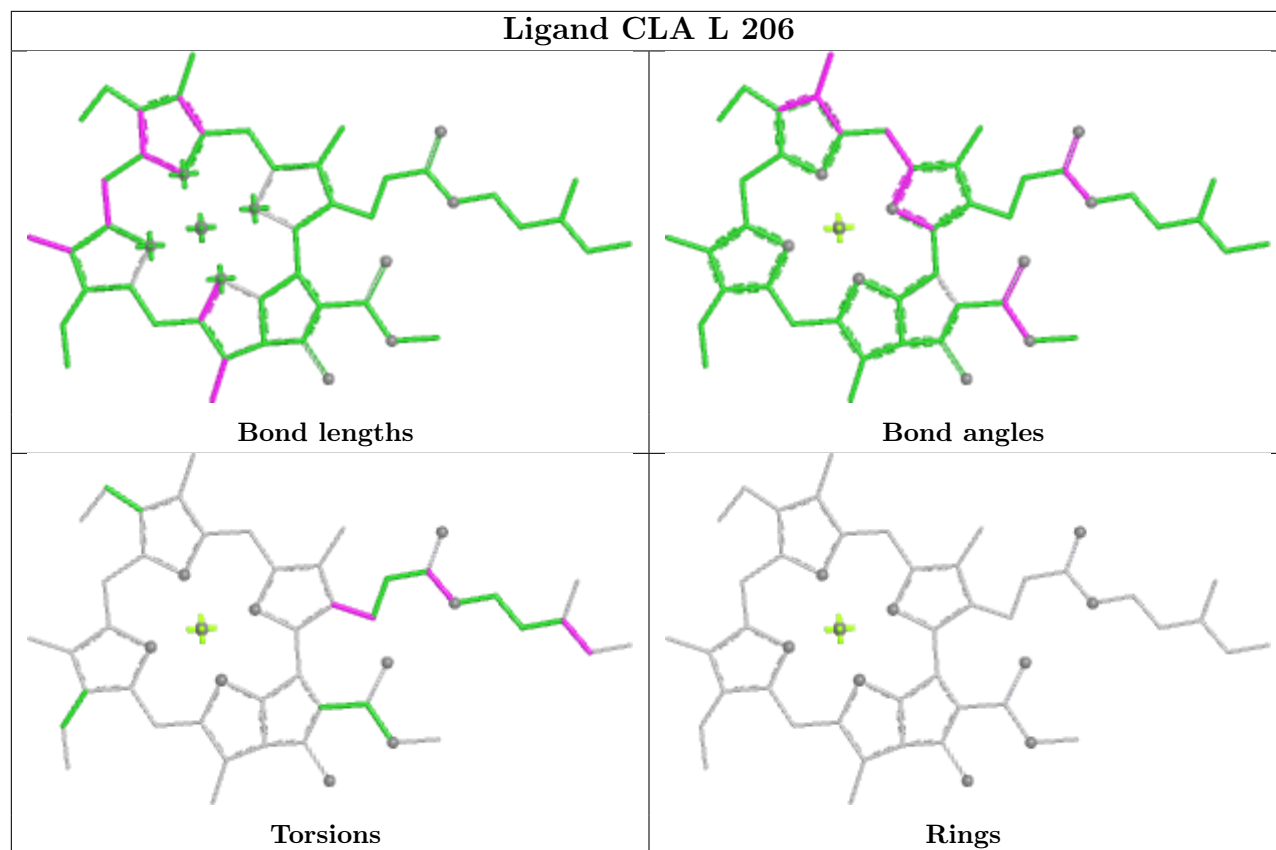


Ligand CLA A 810

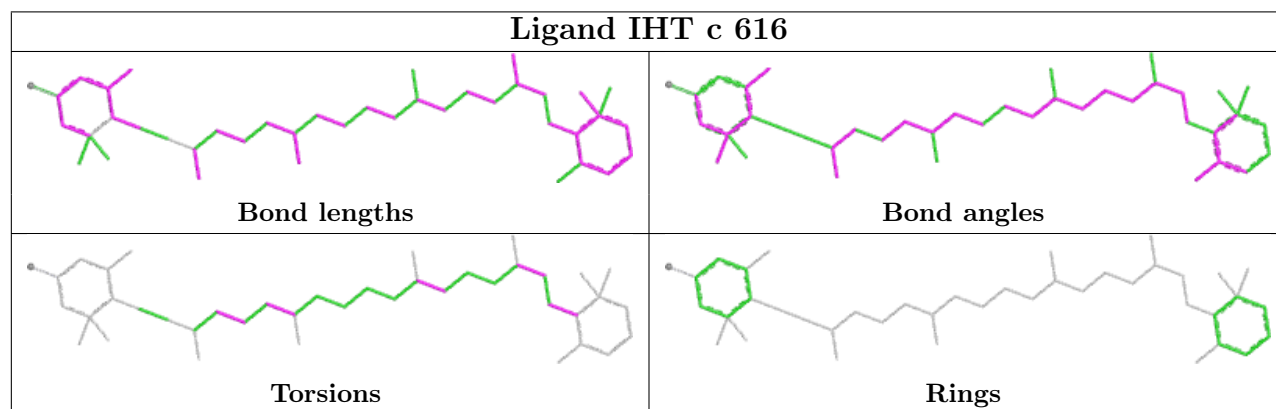


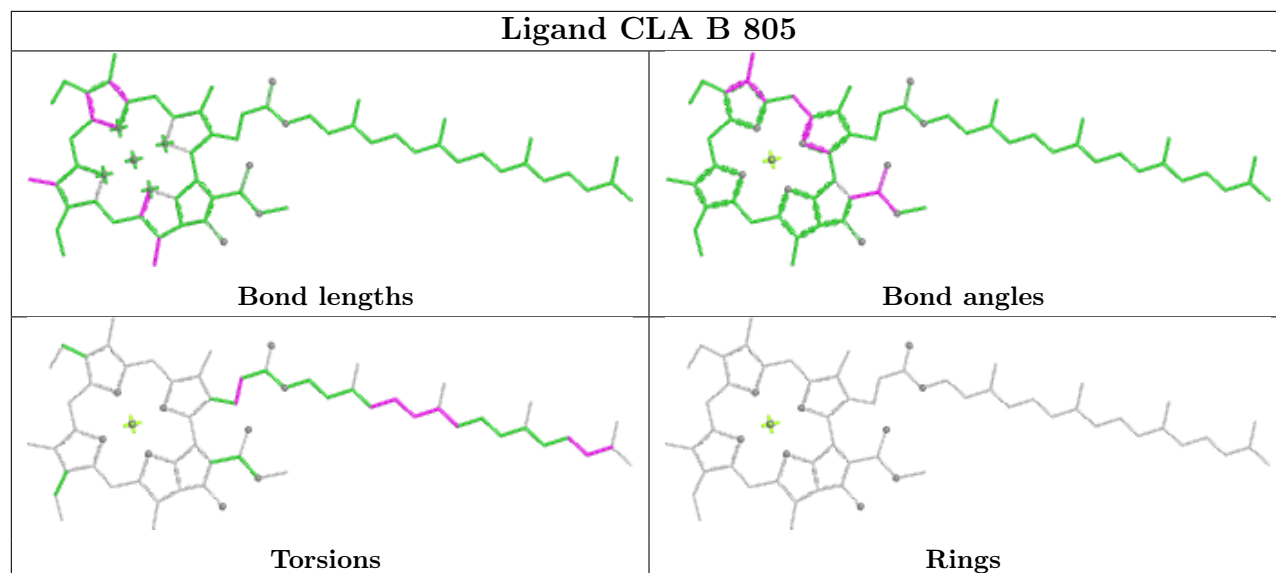
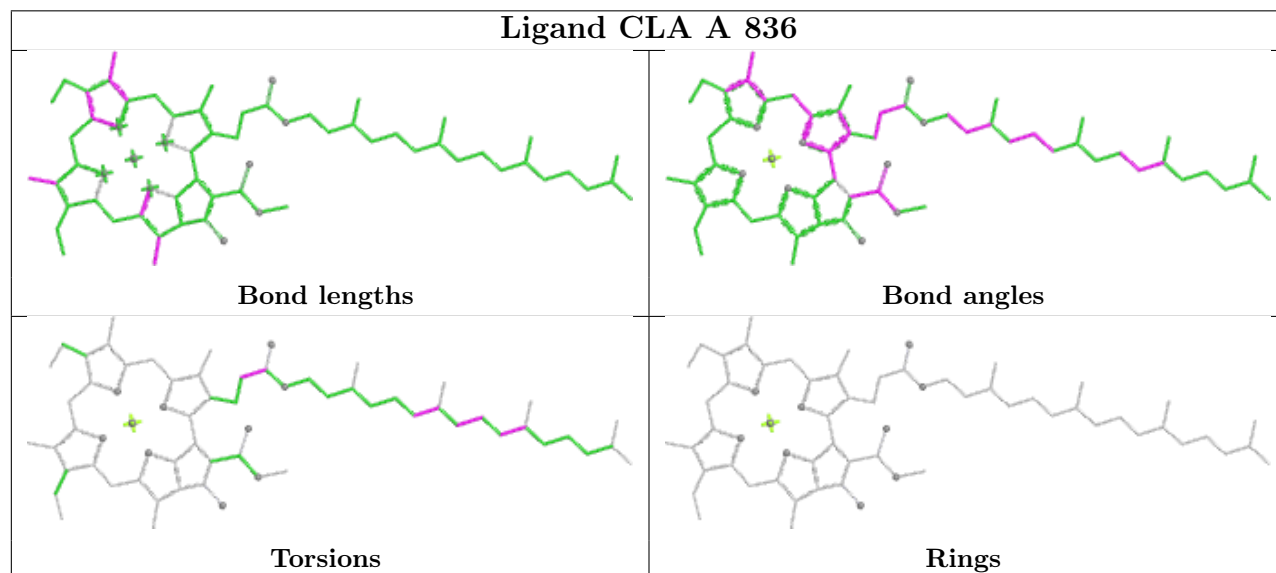
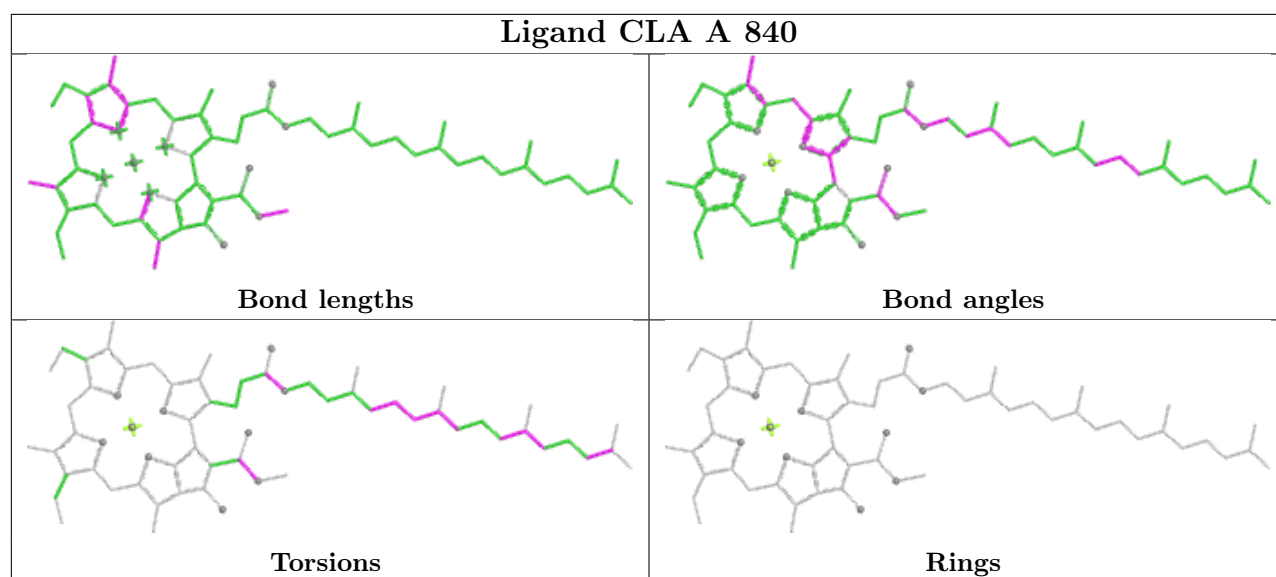


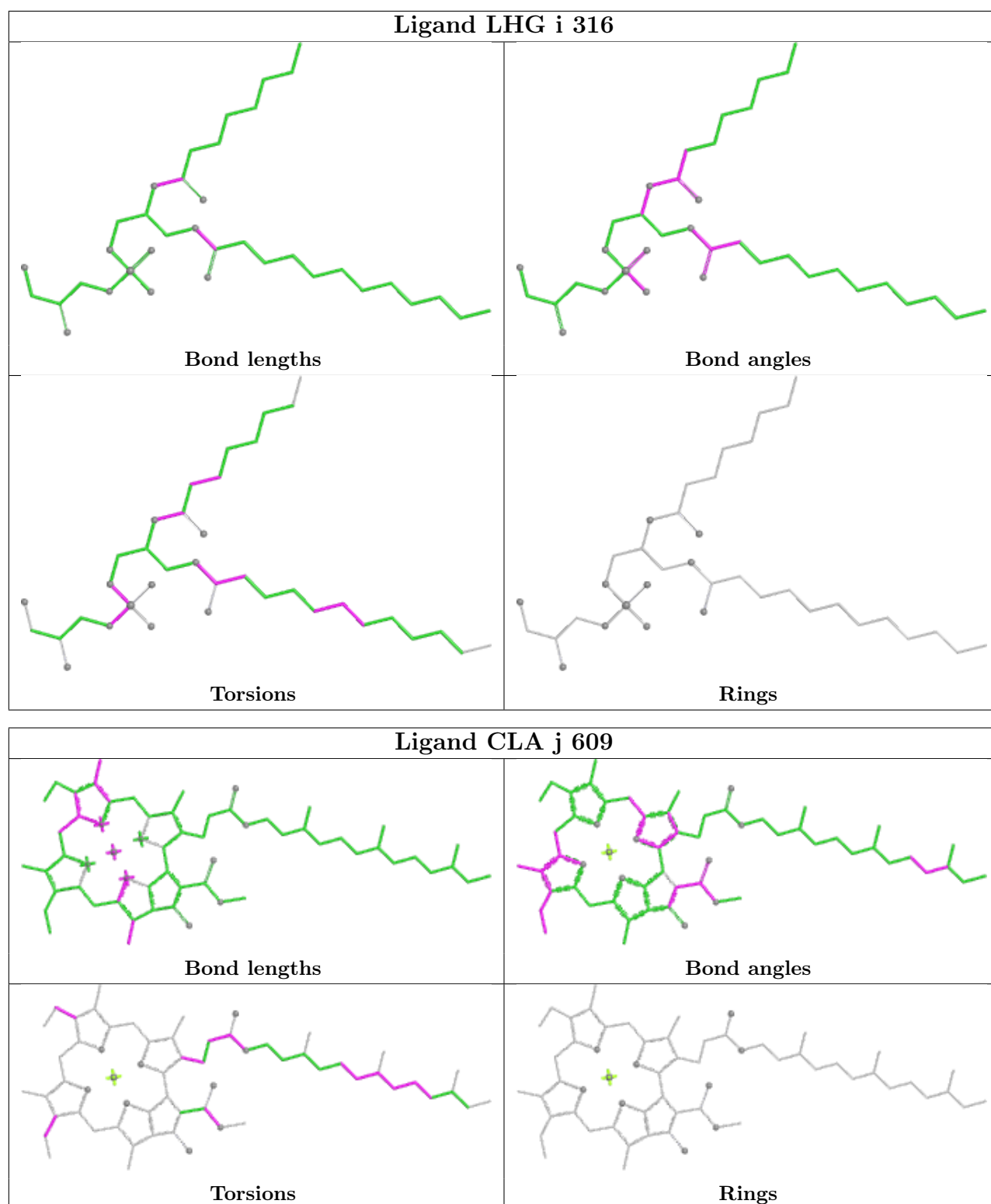
Ligand CLA L 206

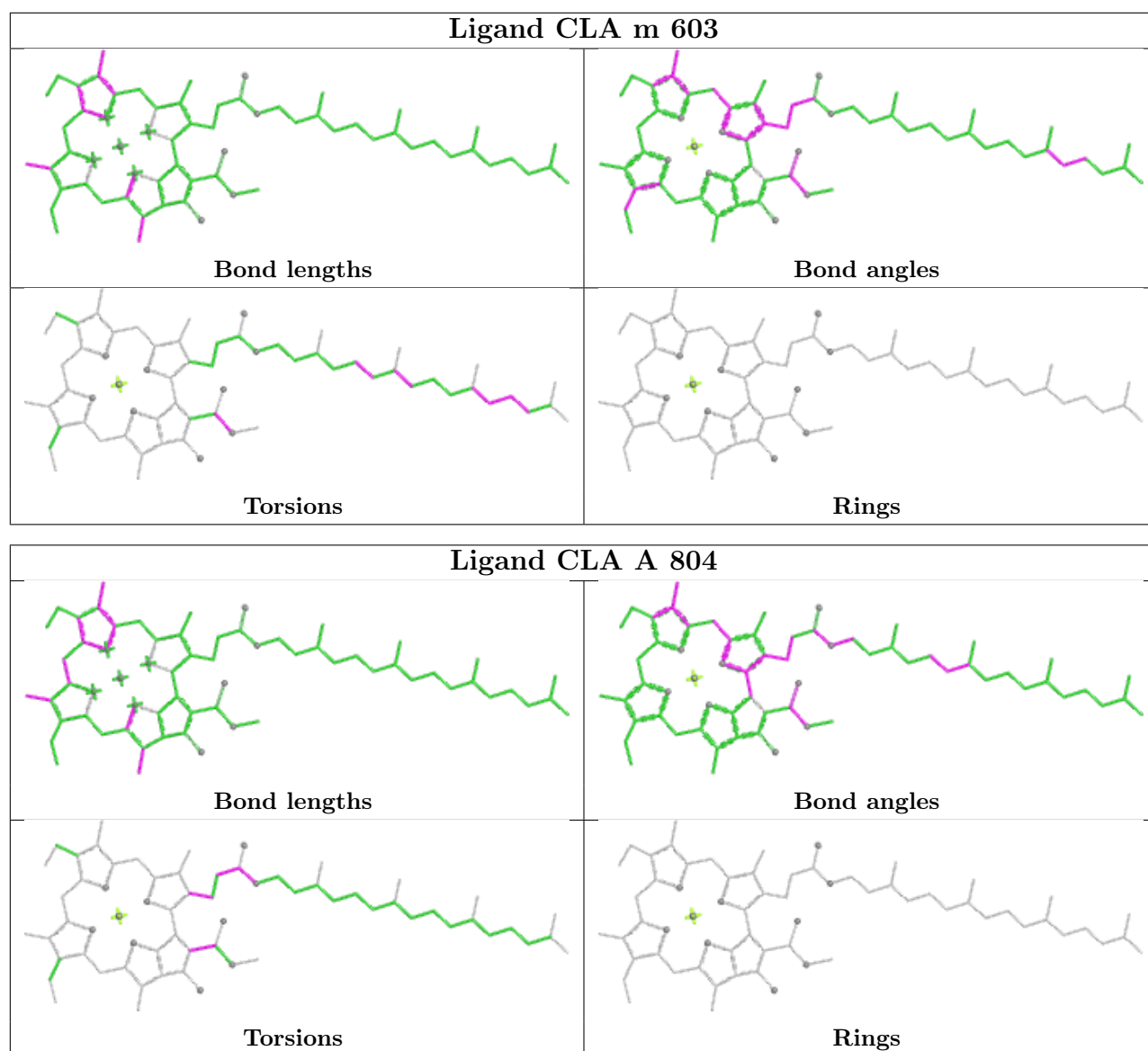


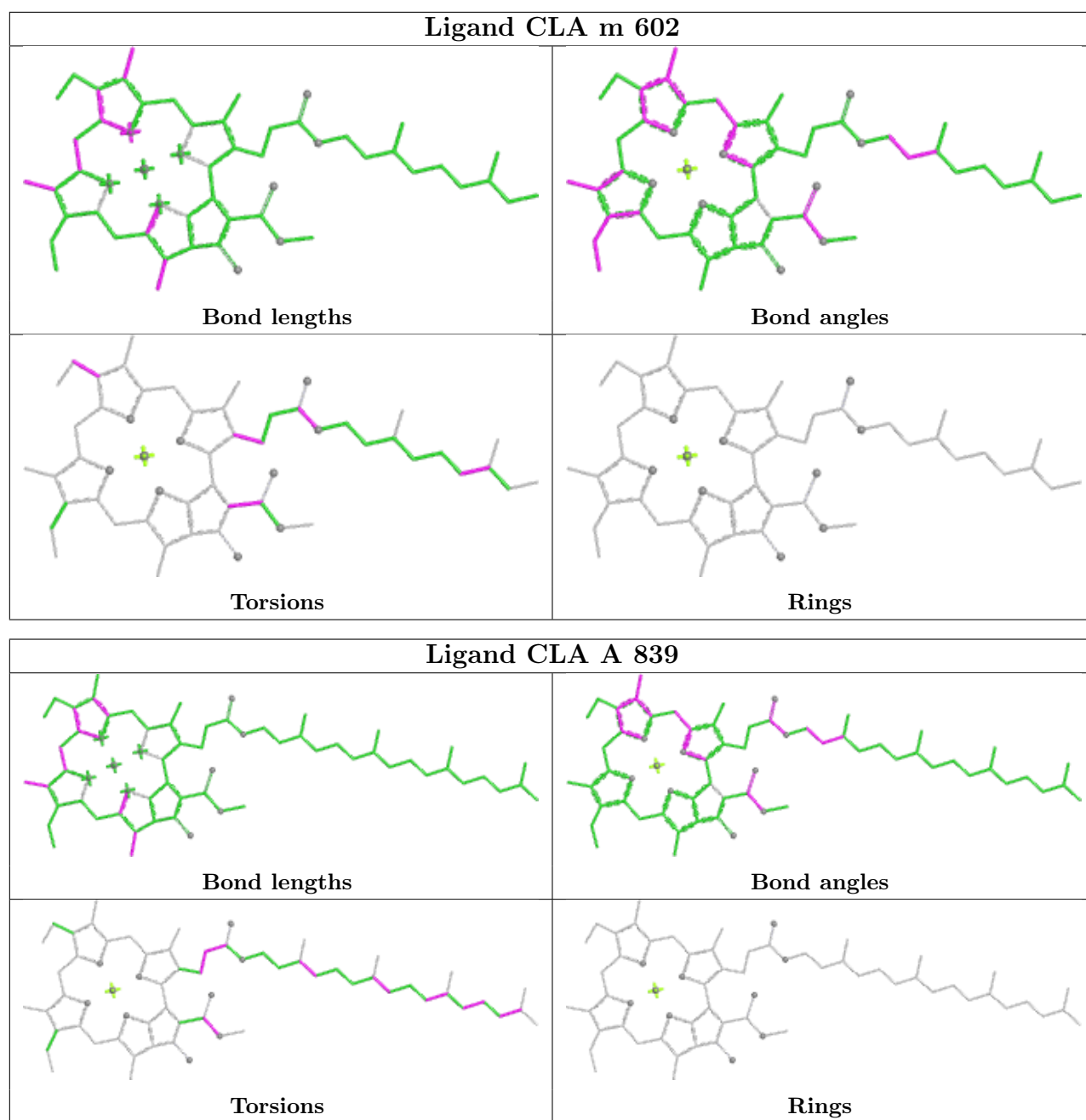
Ligand IHT c 616



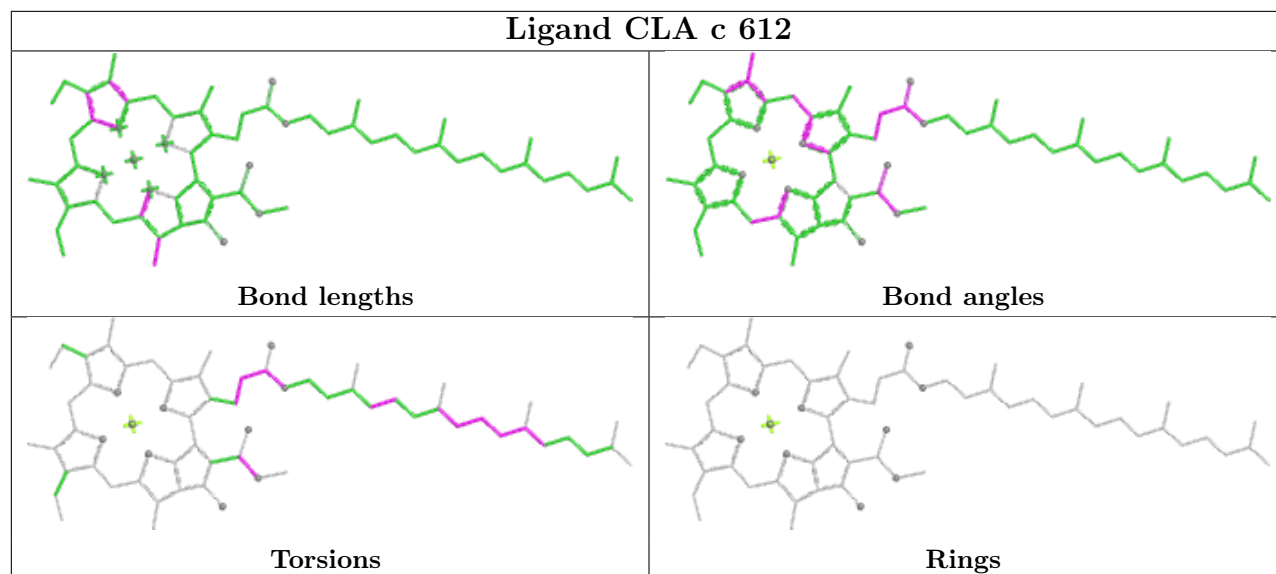




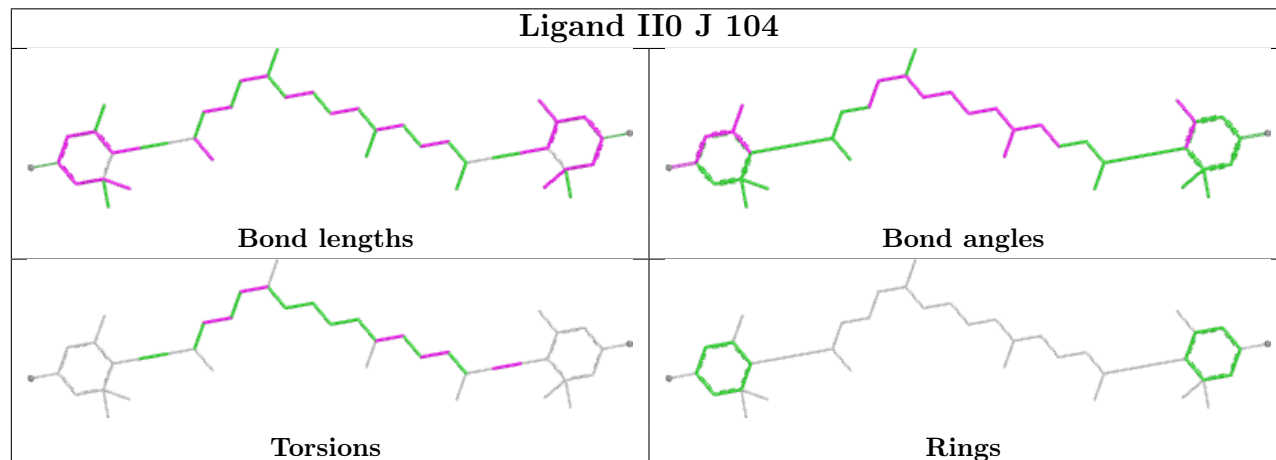




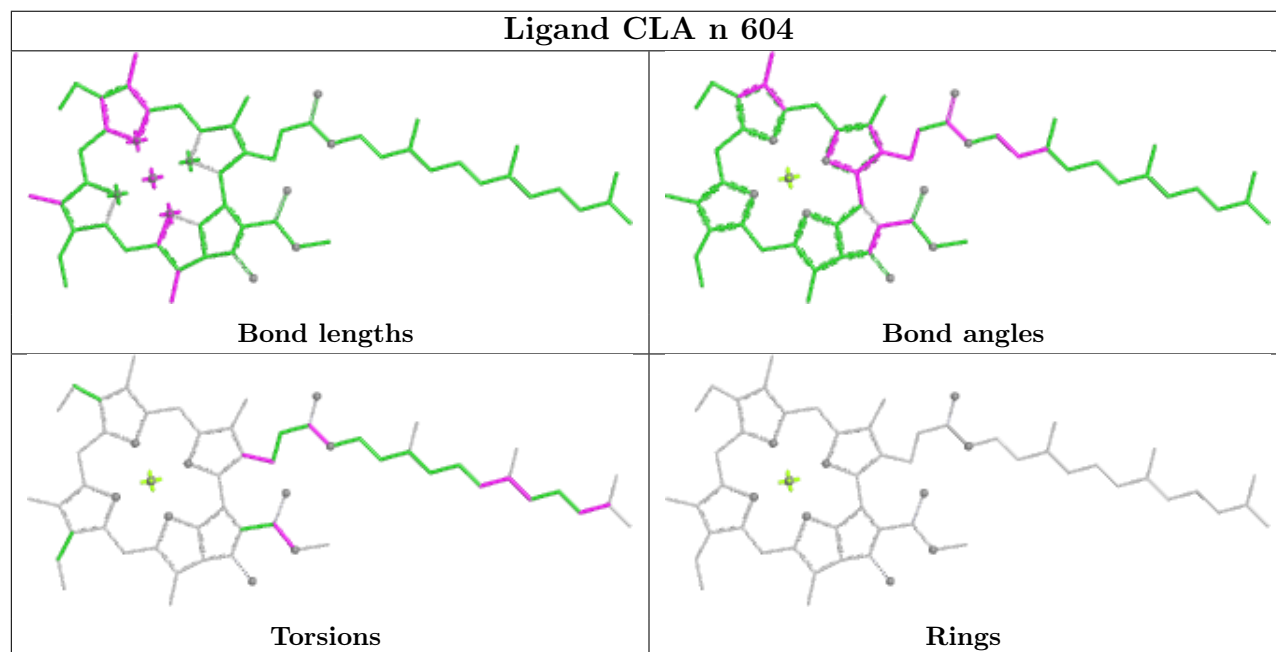
Ligand CLA c 612



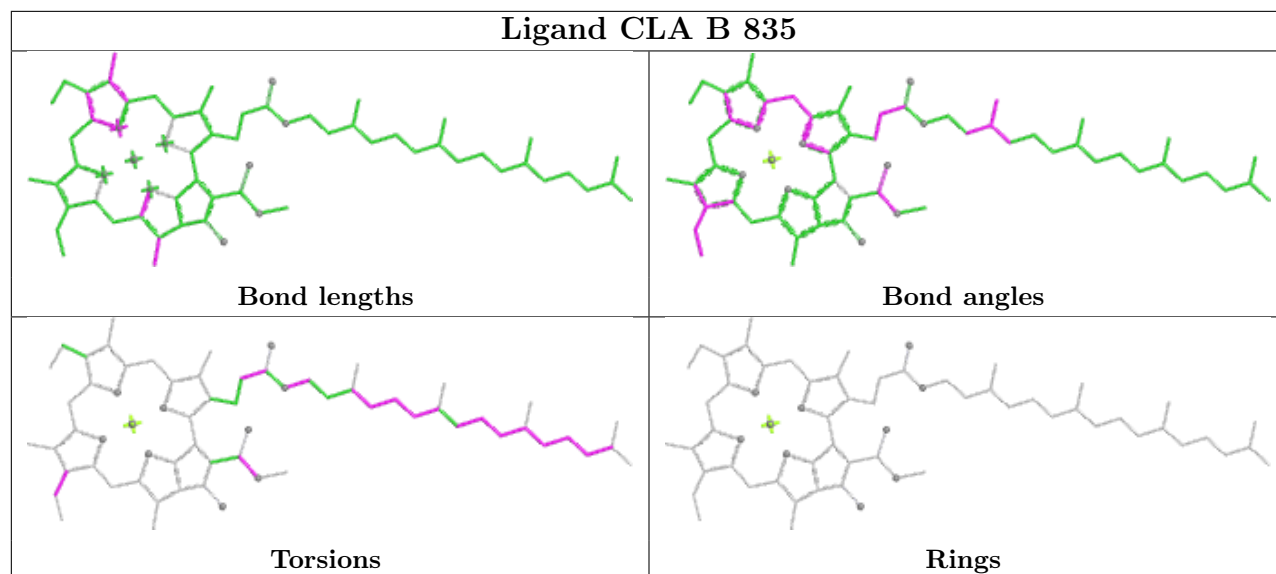
Ligand II0 J 104



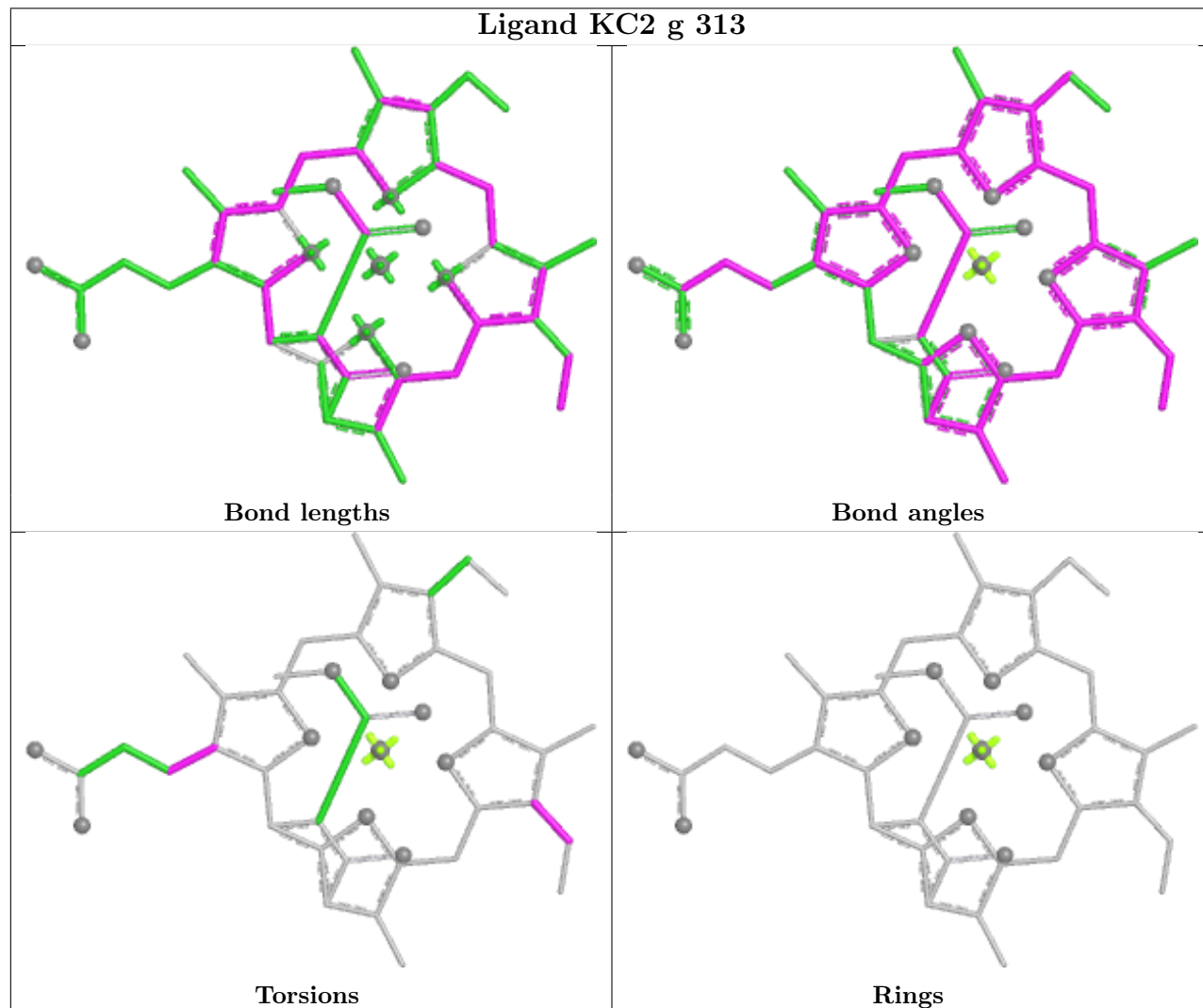
Ligand CLA n 604

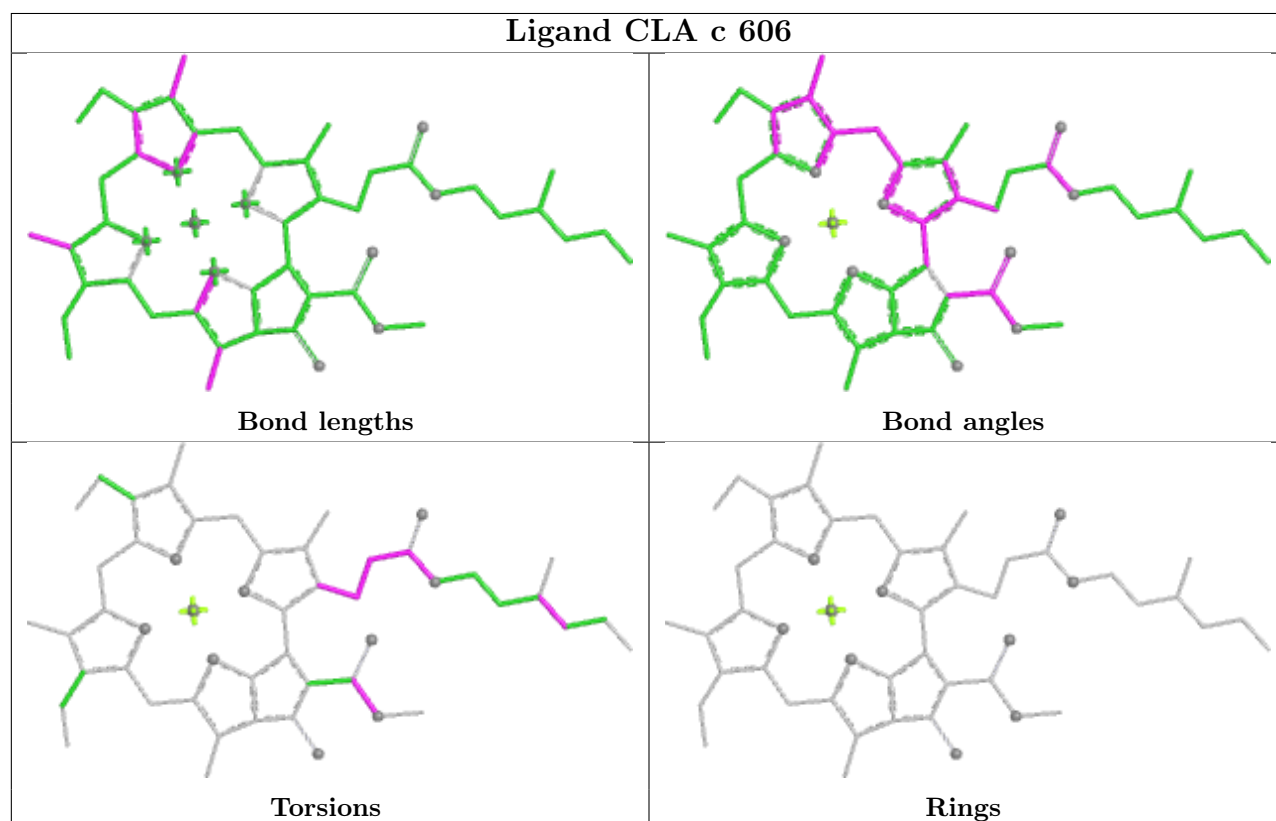
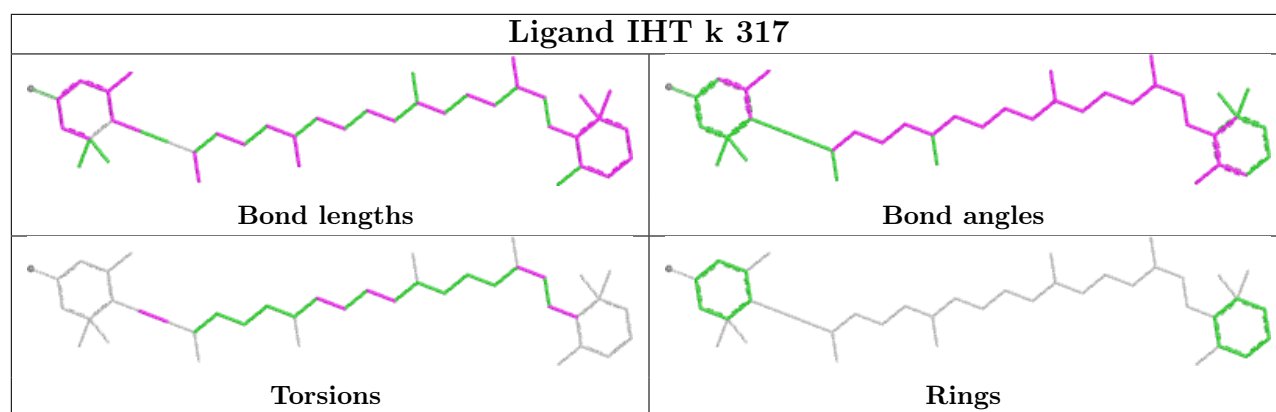


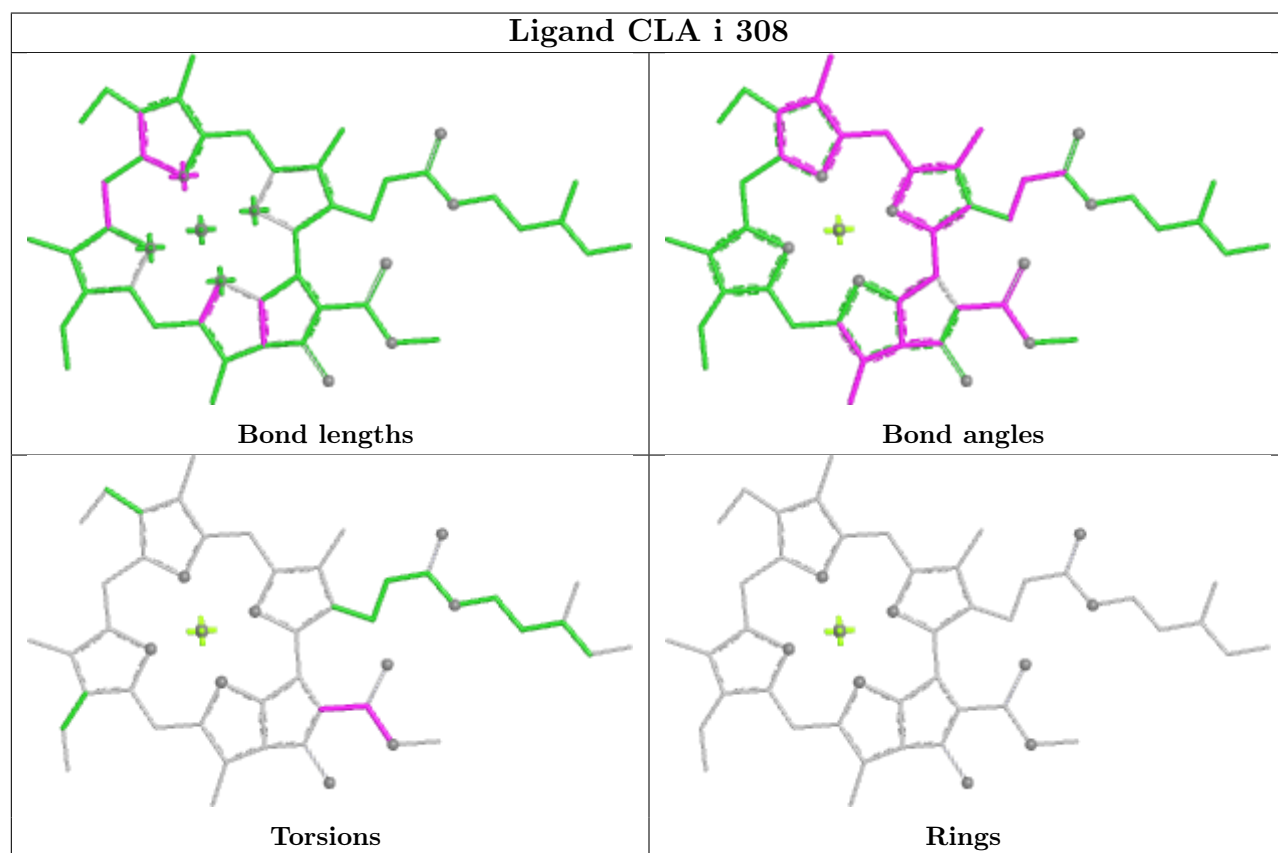
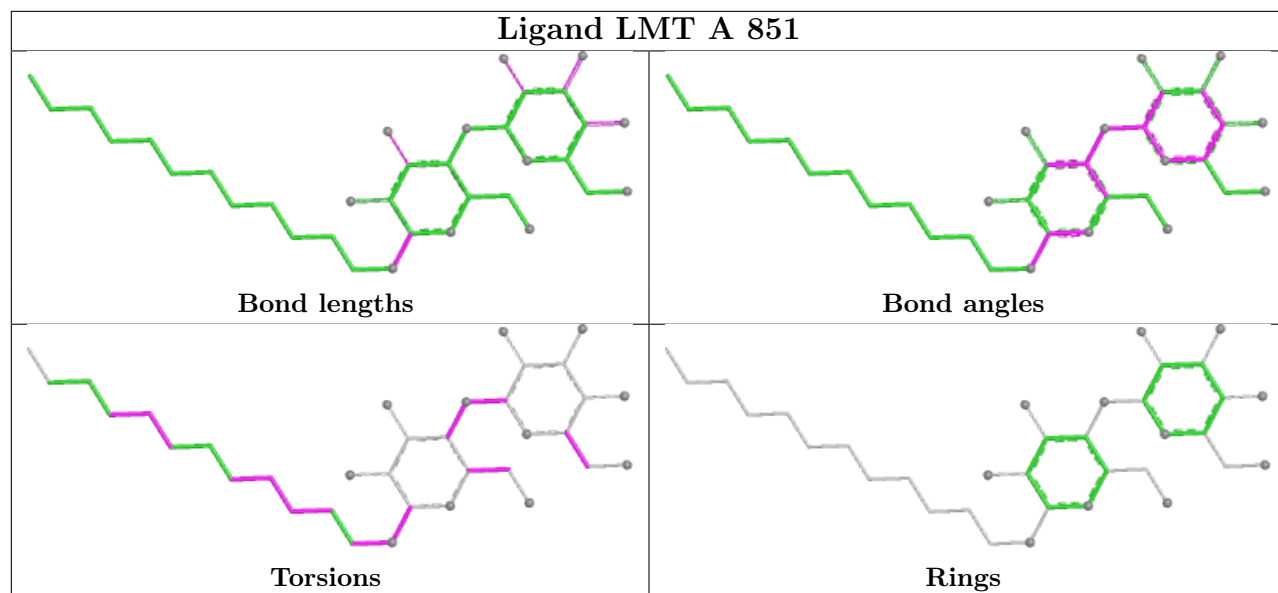
Ligand CLA B 835

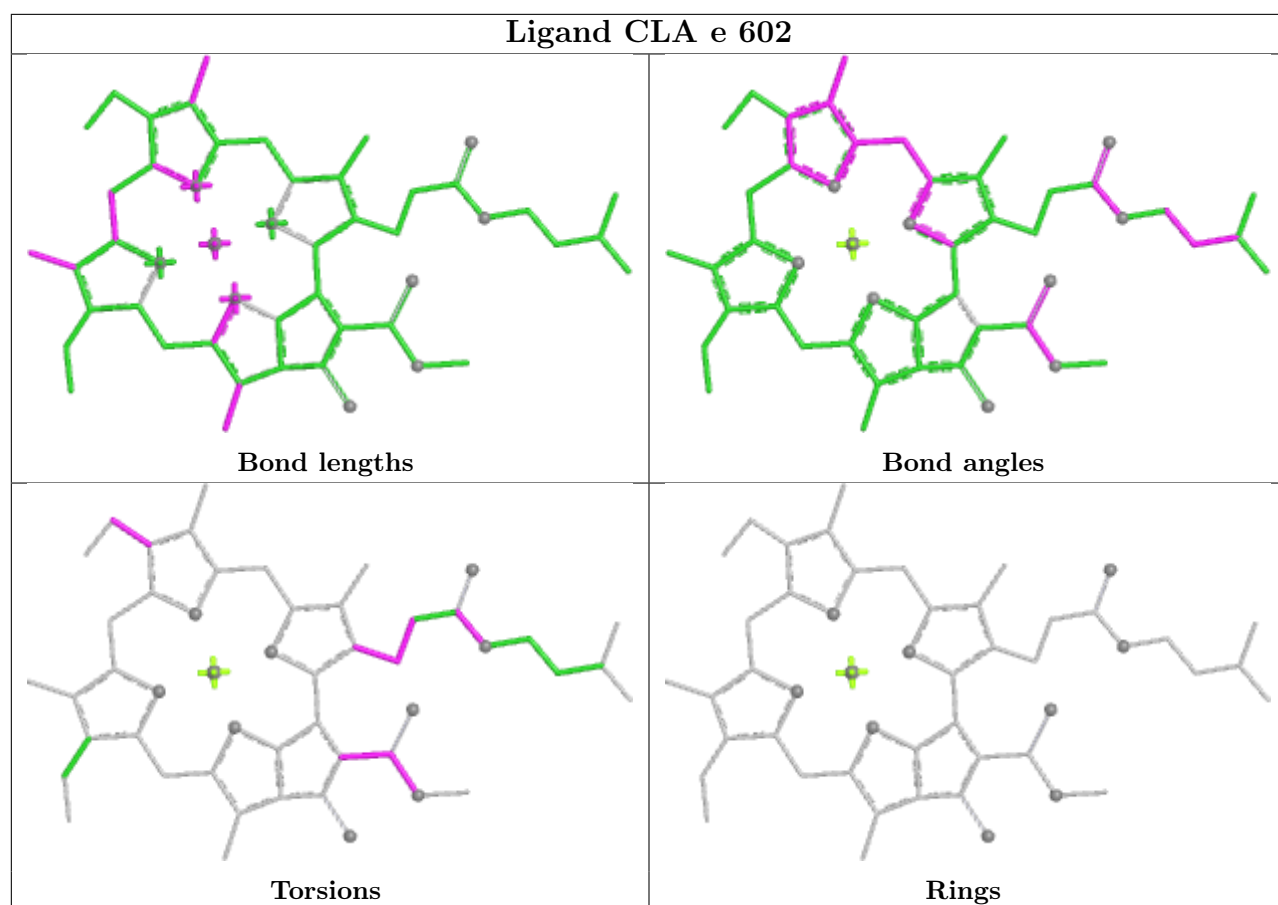


Ligand KC2 g 313

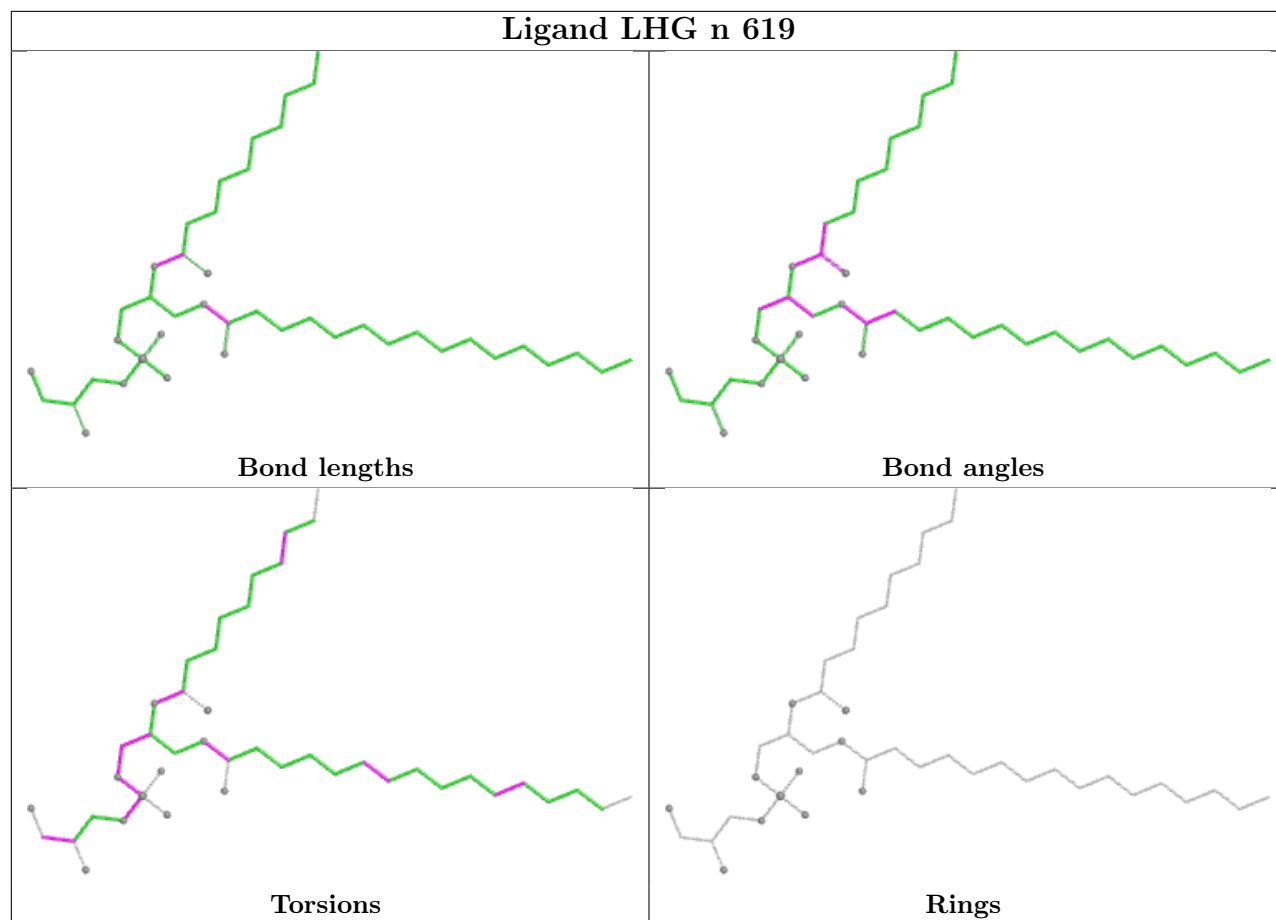




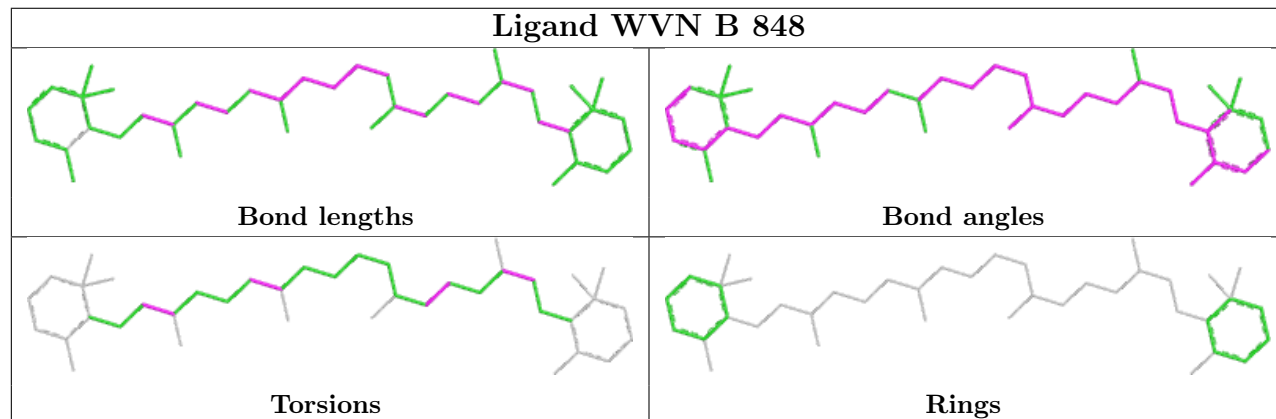




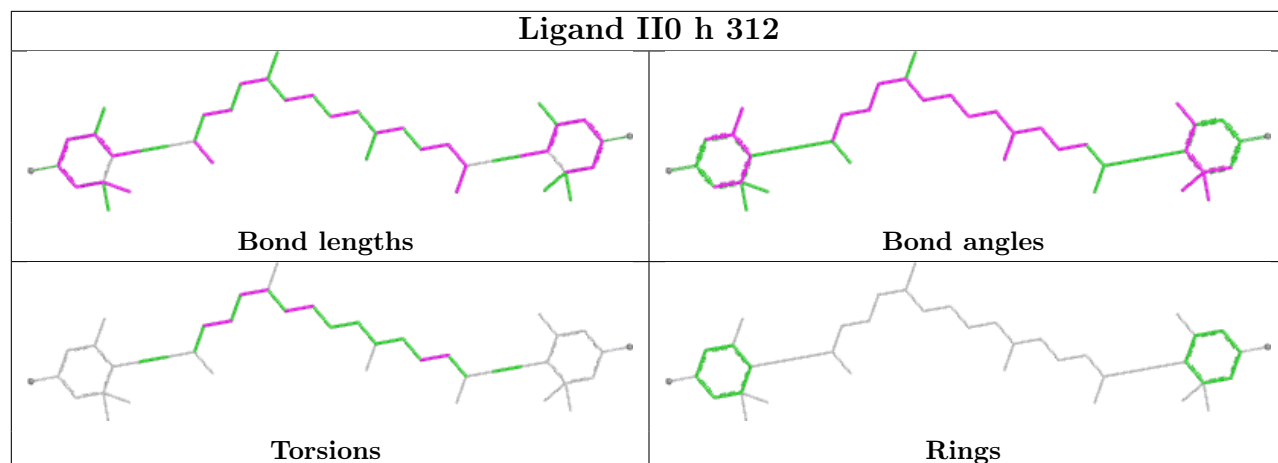
Ligand LHG n 619



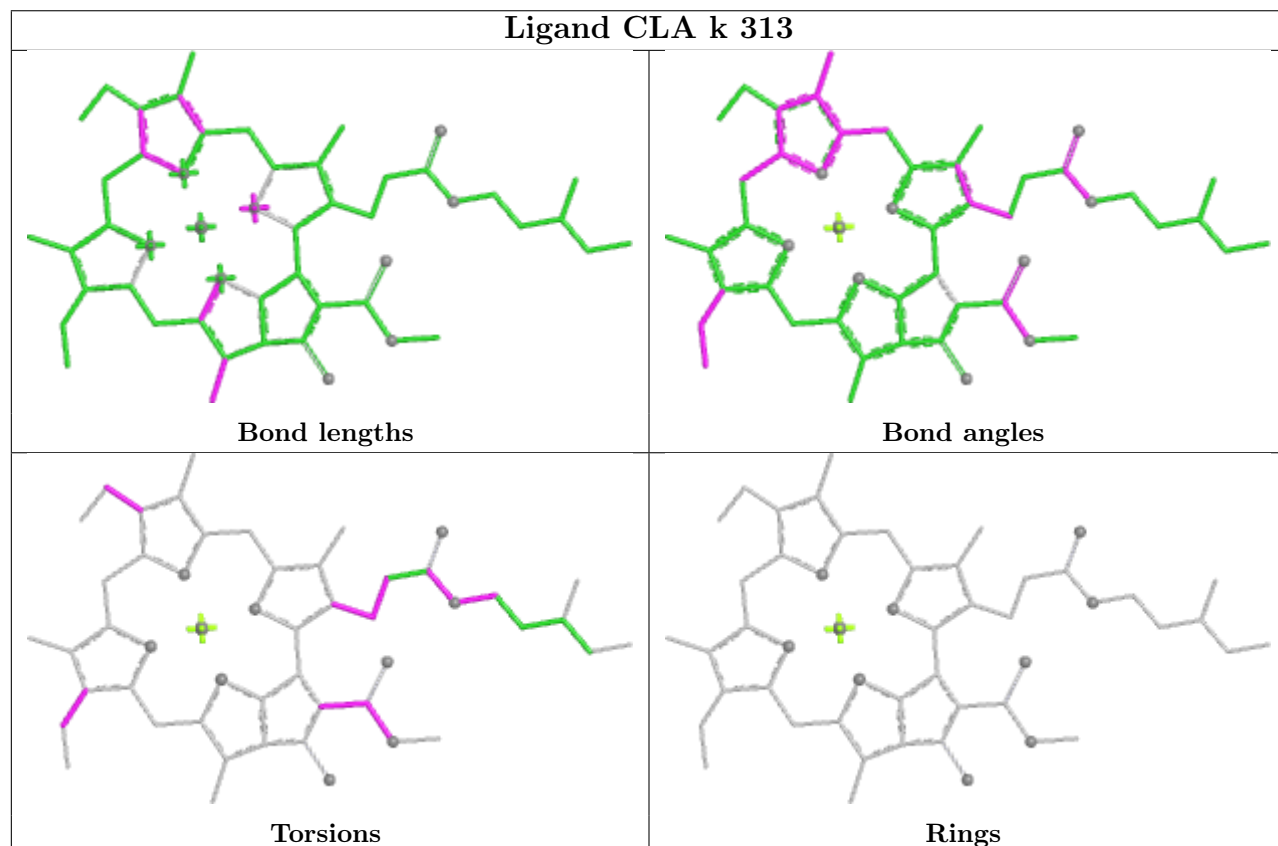
Ligand WVN B 848



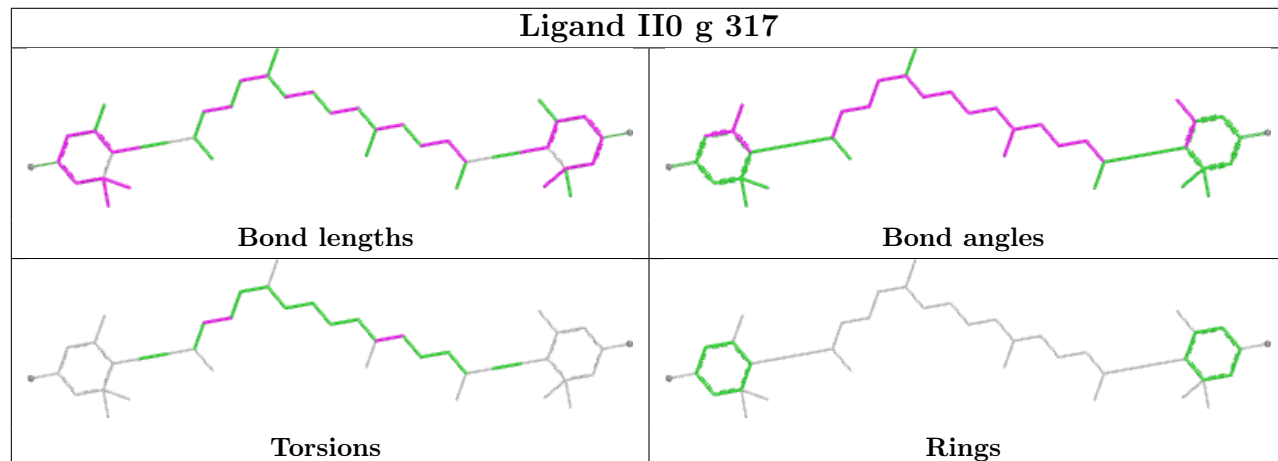
Ligand II0 h 312



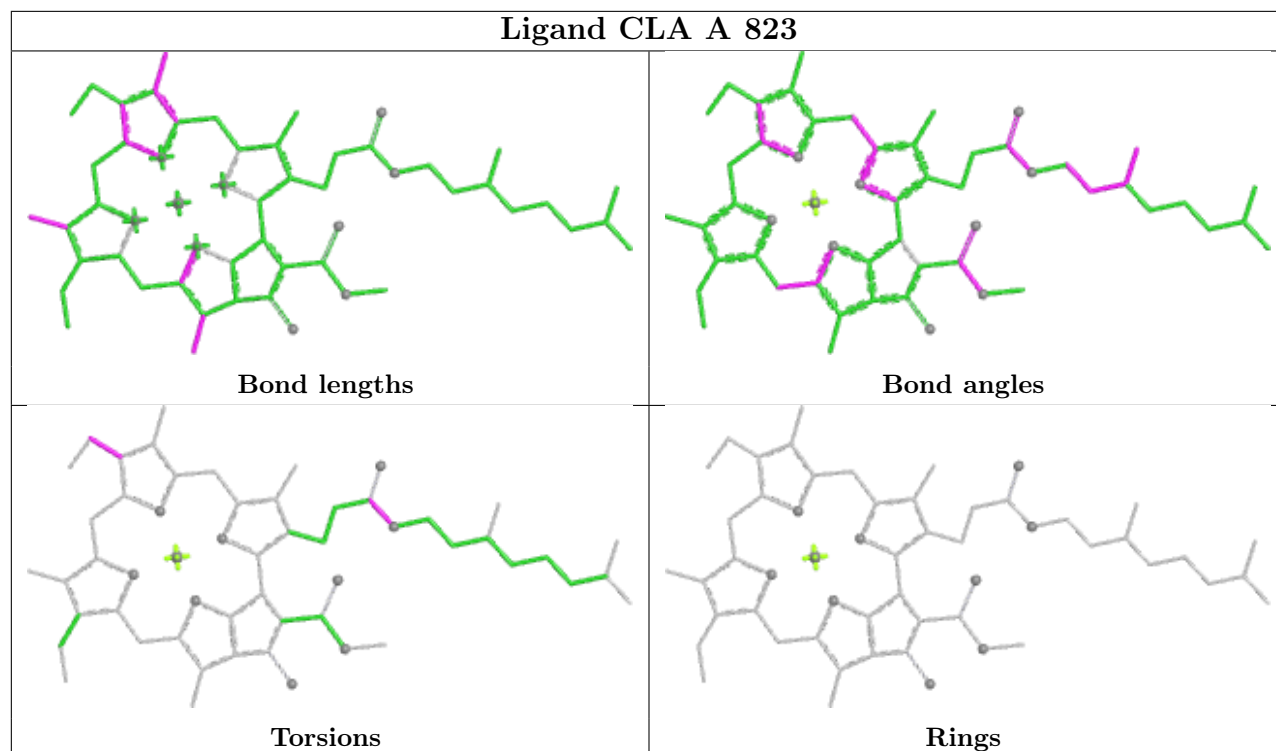
Ligand CLA k 313



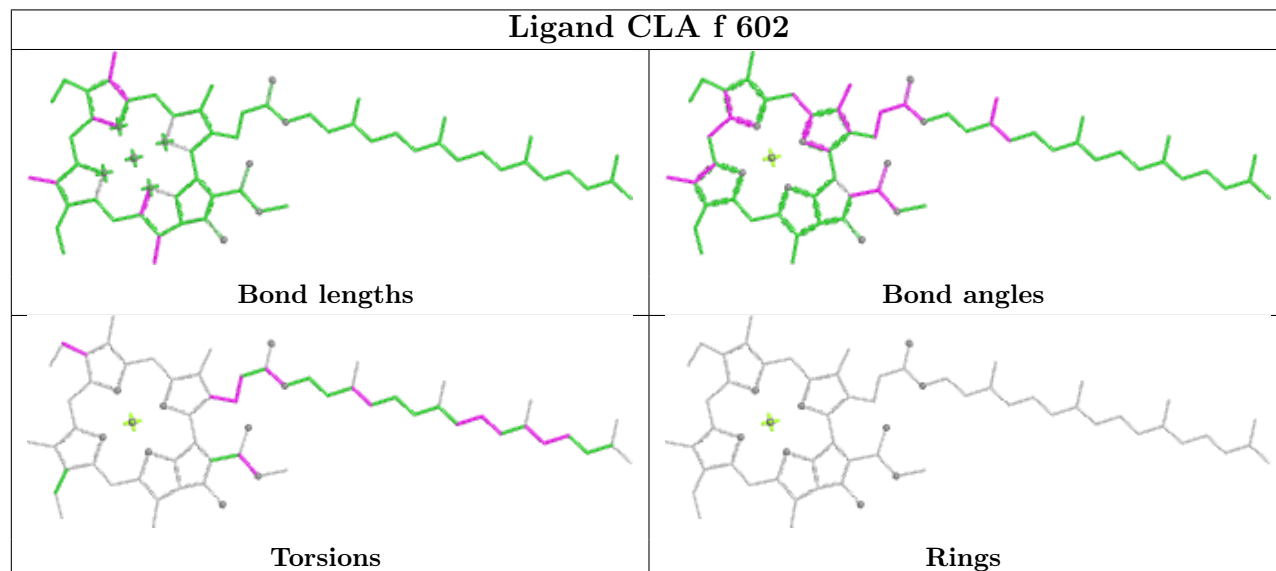
Ligand II0 g 317

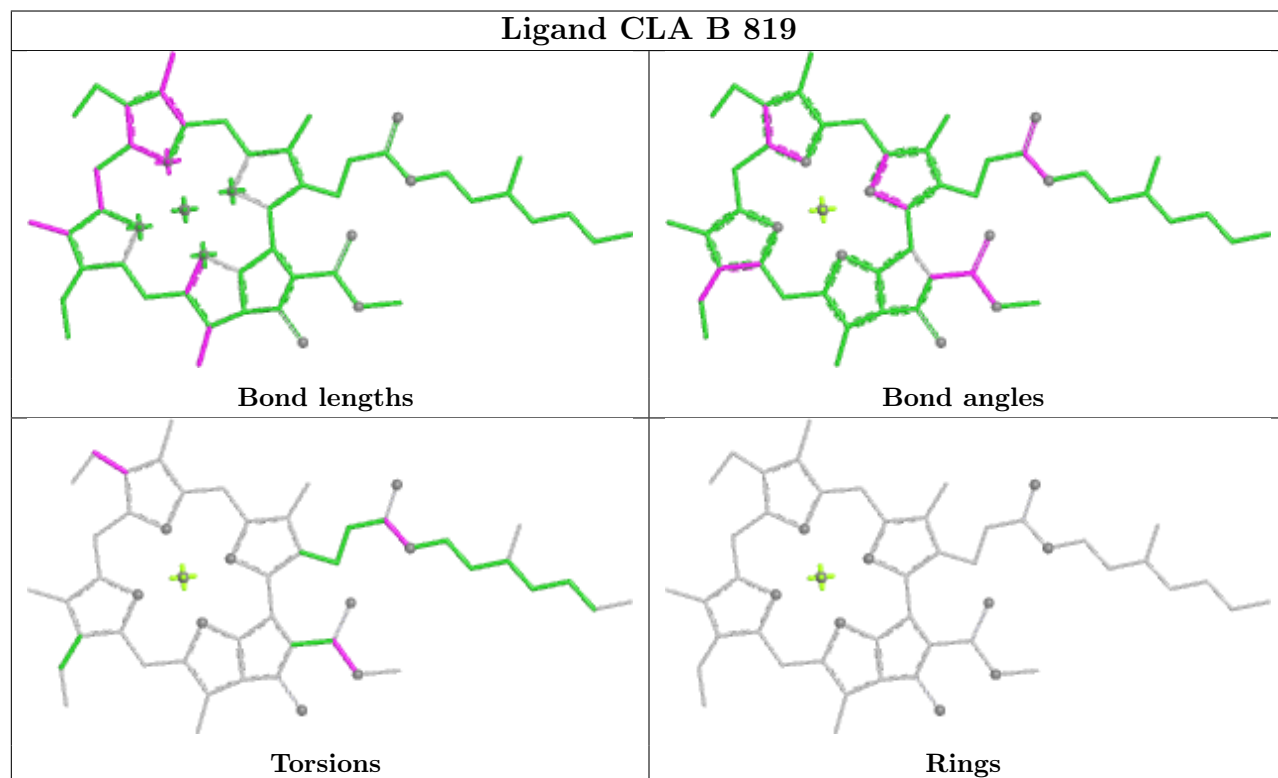
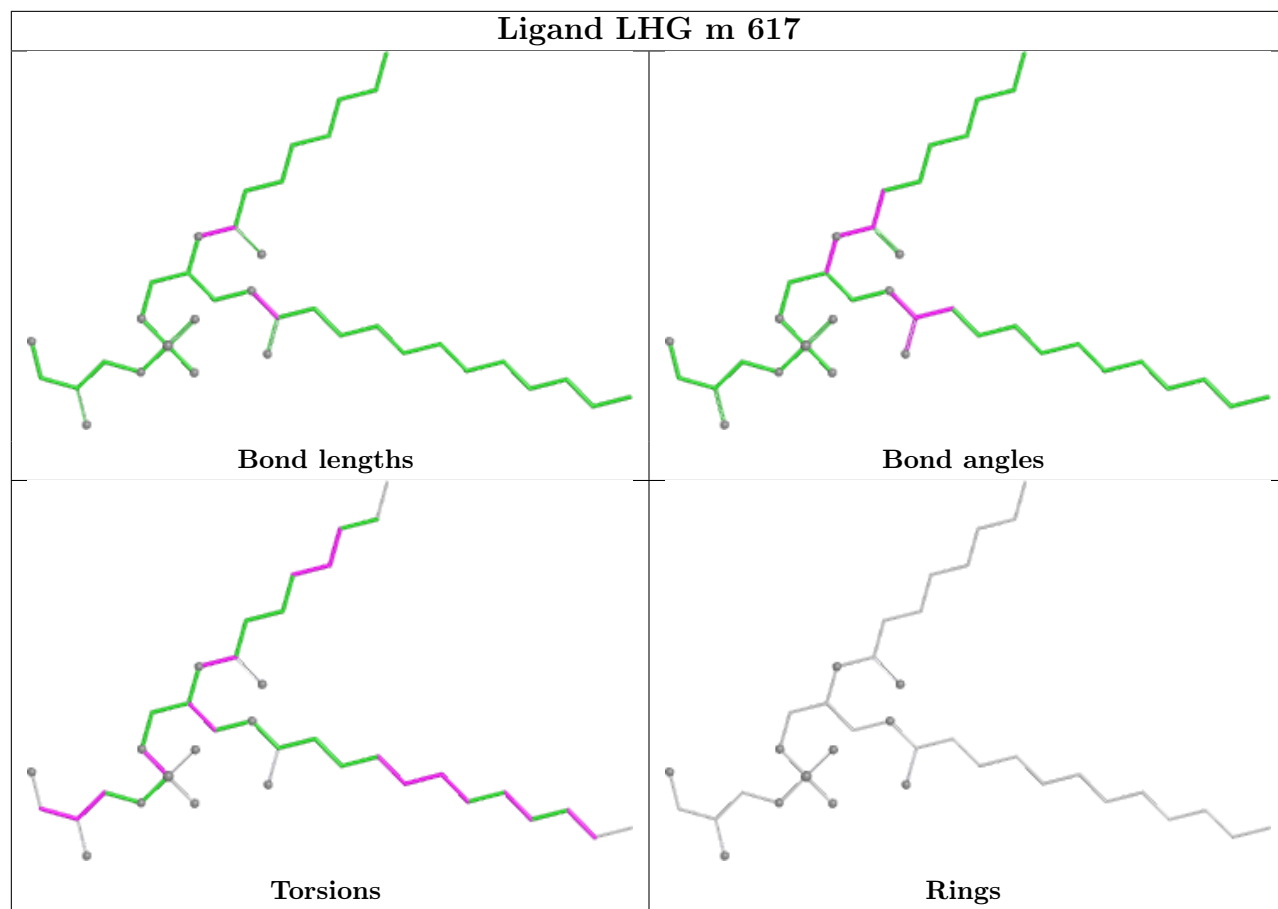


Ligand CLA A 823

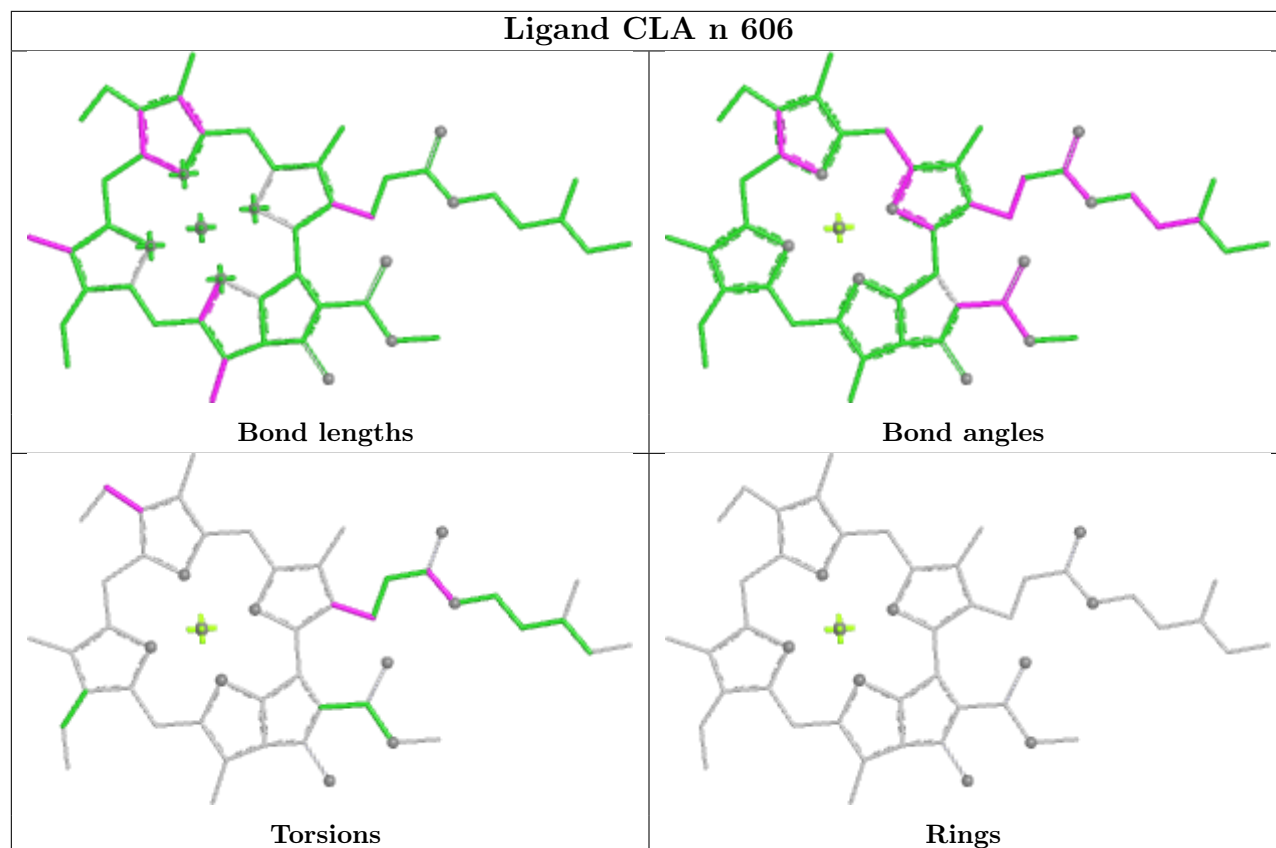


Ligand CLA f 602

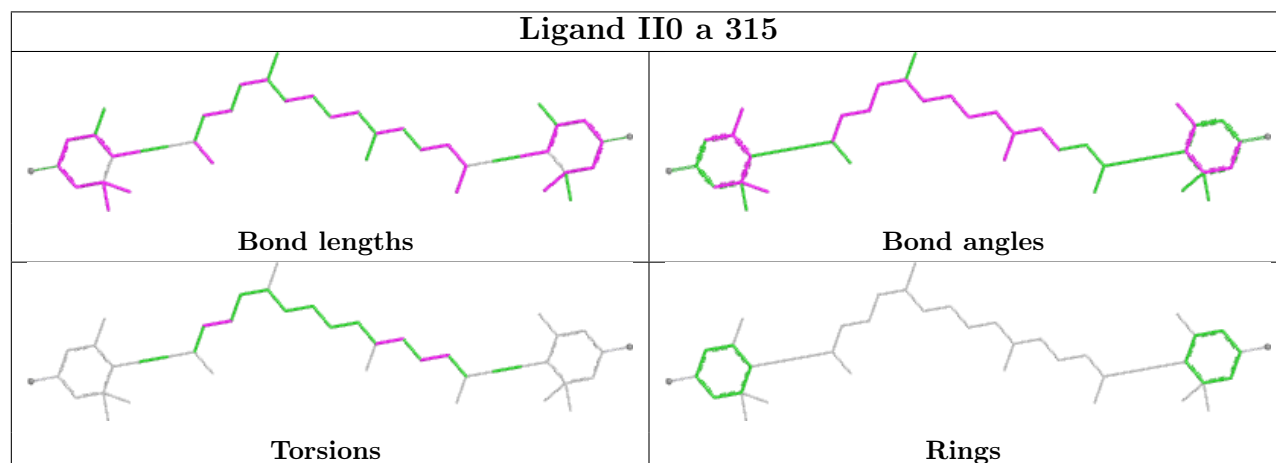




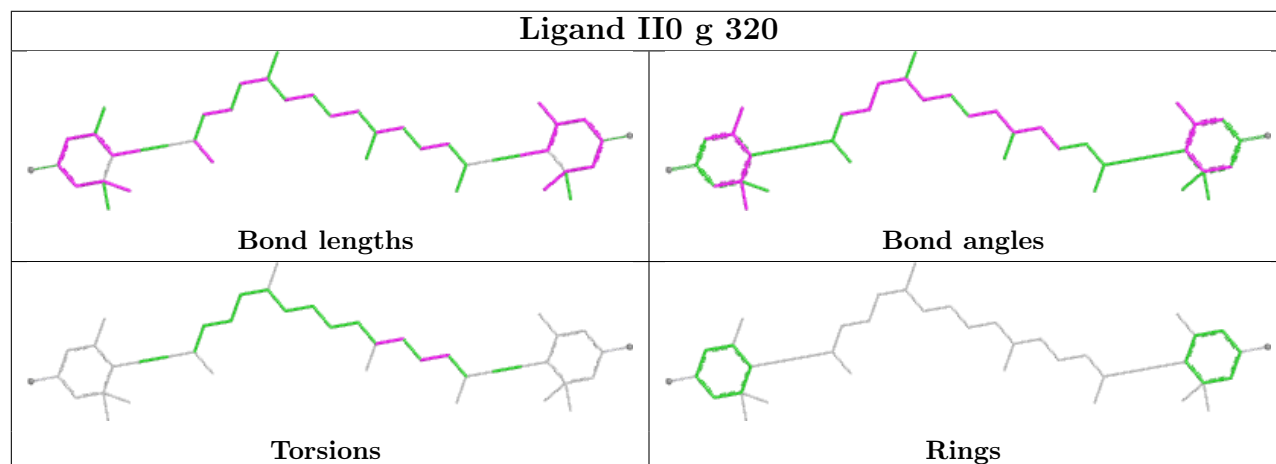
Ligand CLA n 606



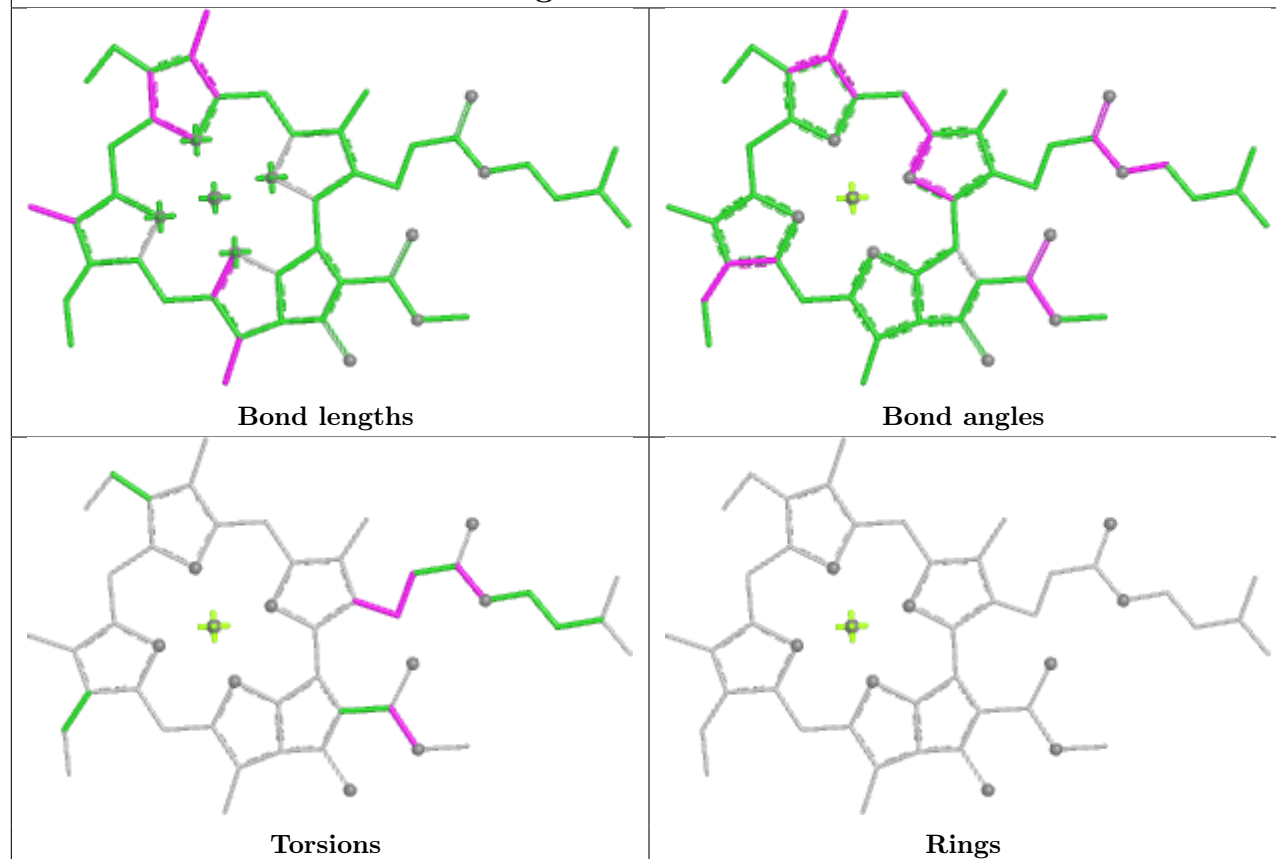
Ligand II0 a 315



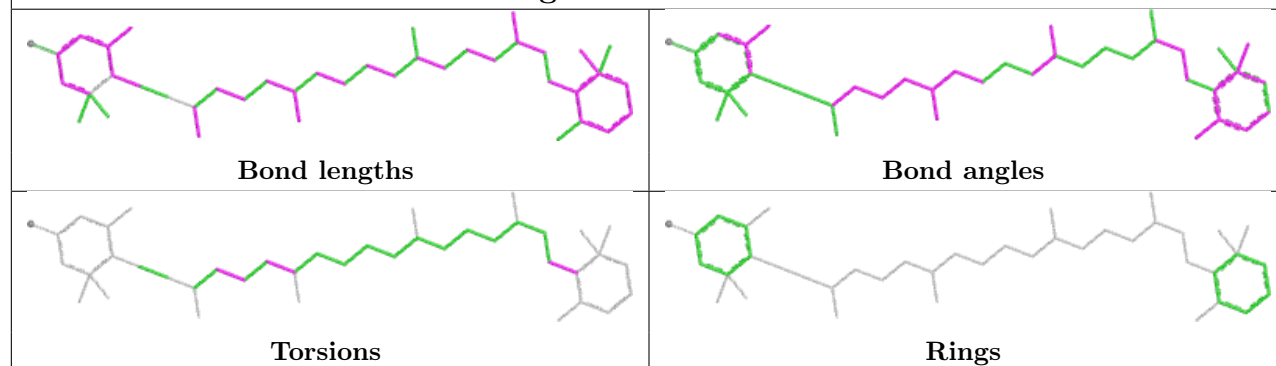
Ligand II0 g 320

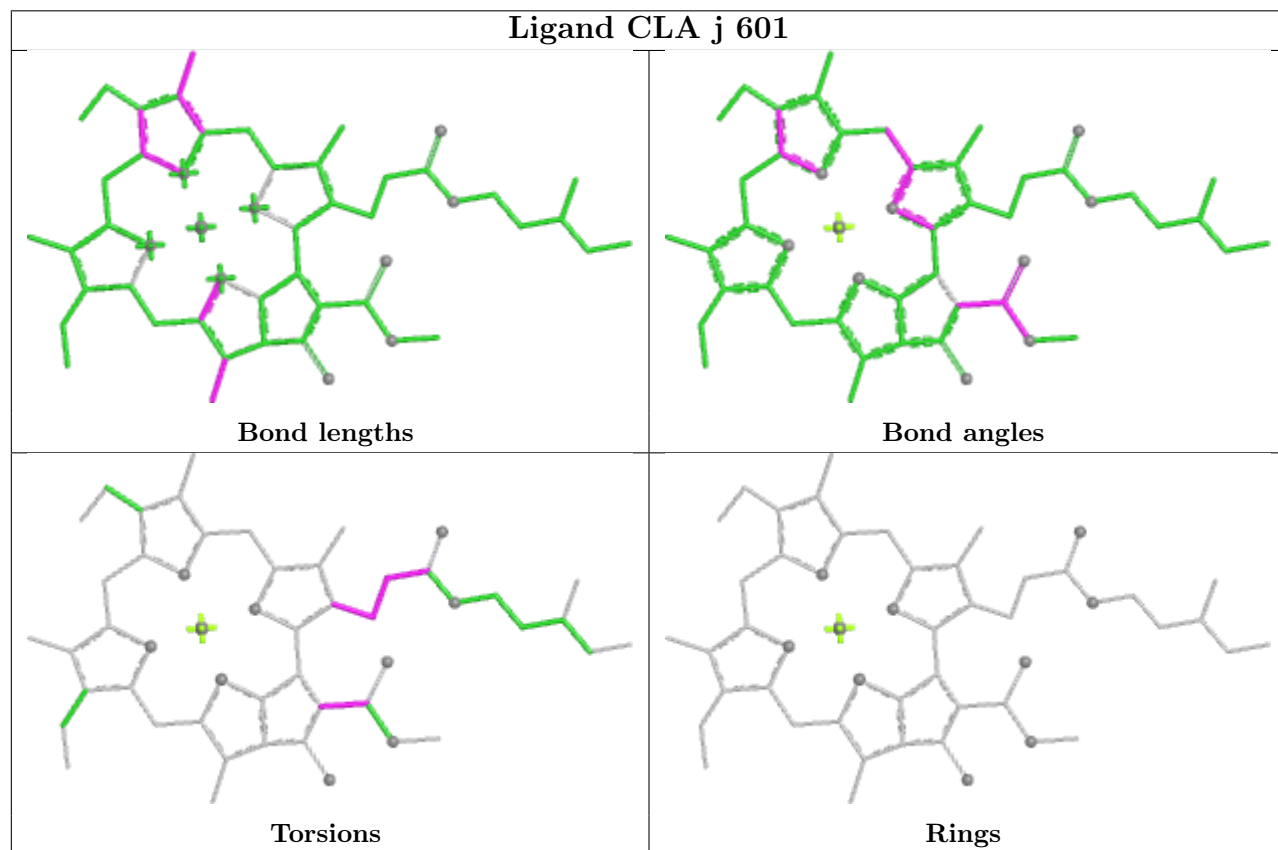
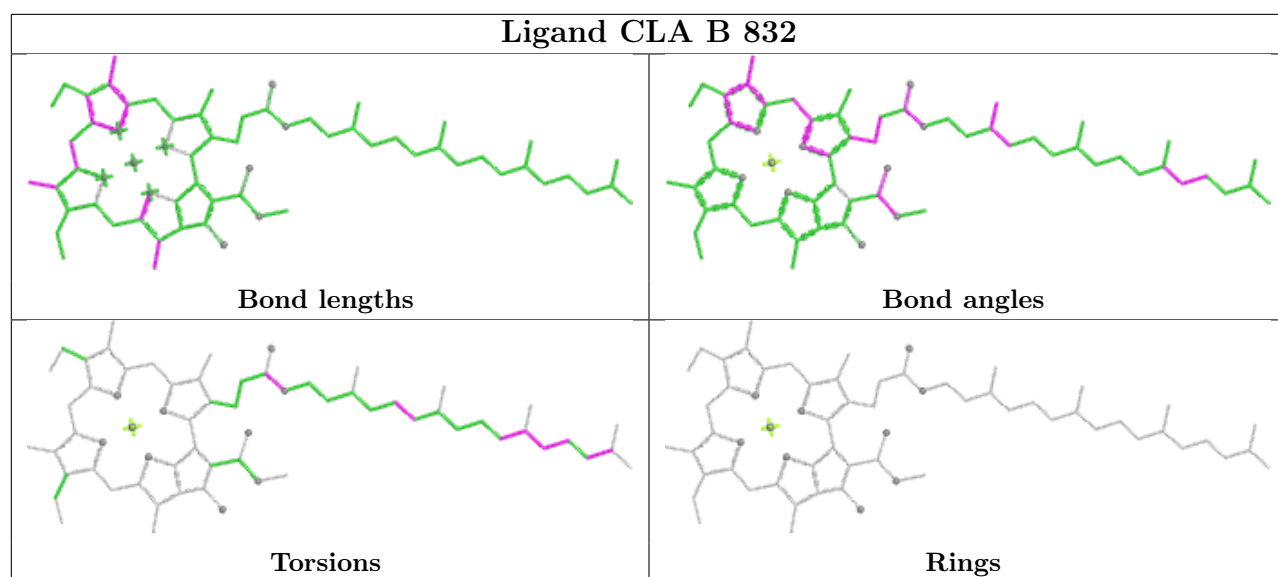


Ligand CLA h 302

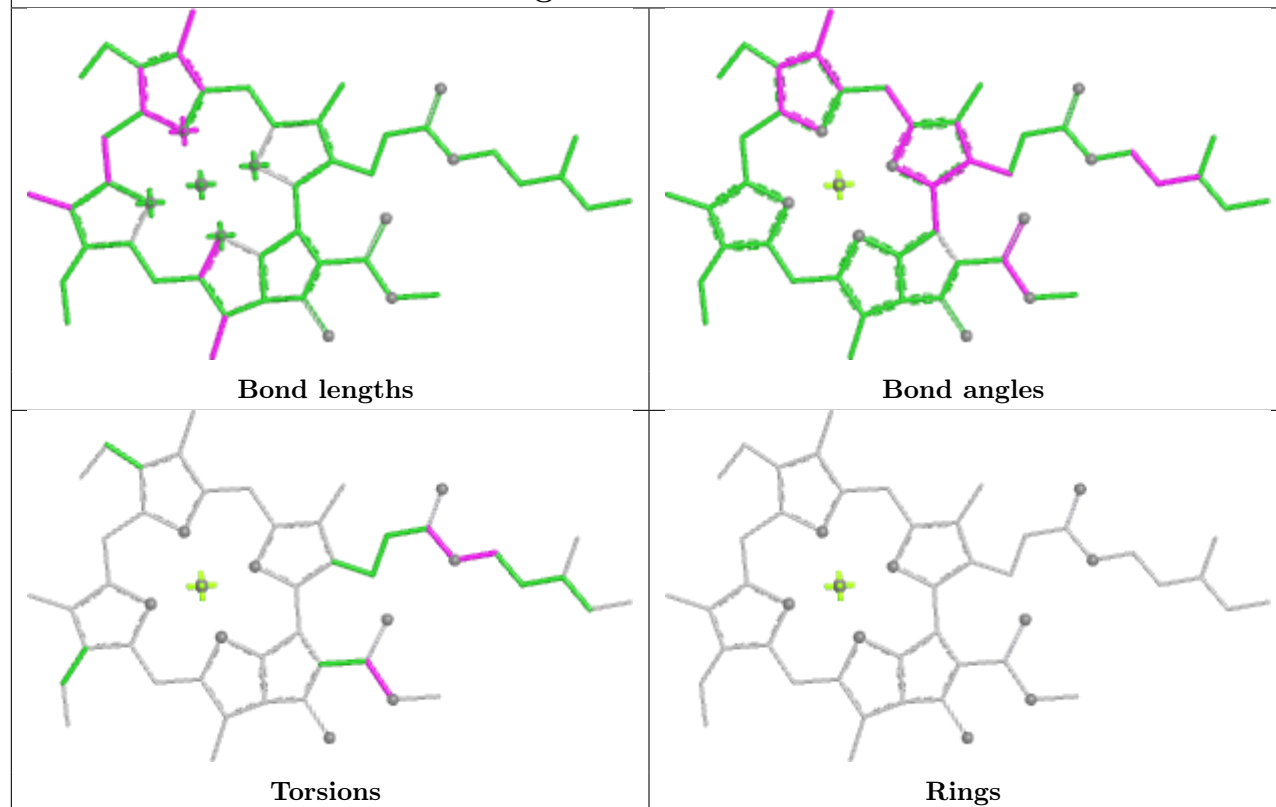


Ligand IHT b 614

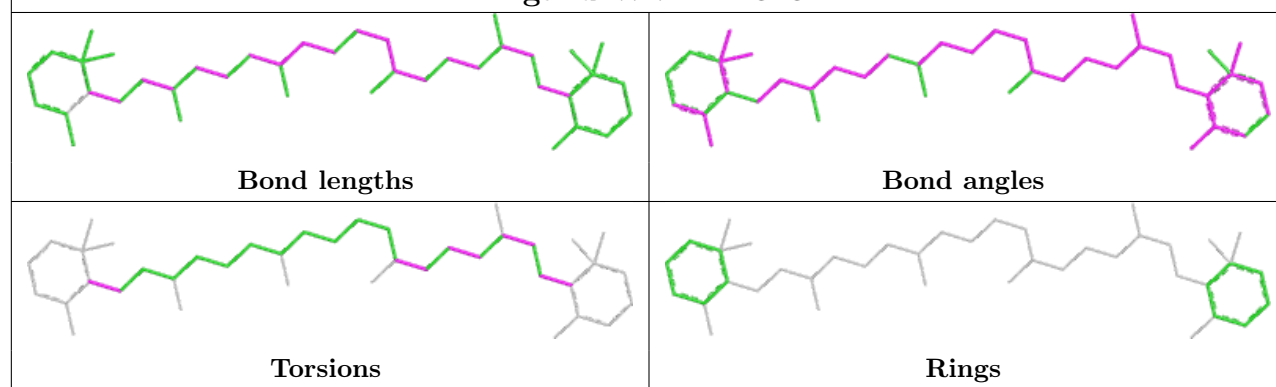


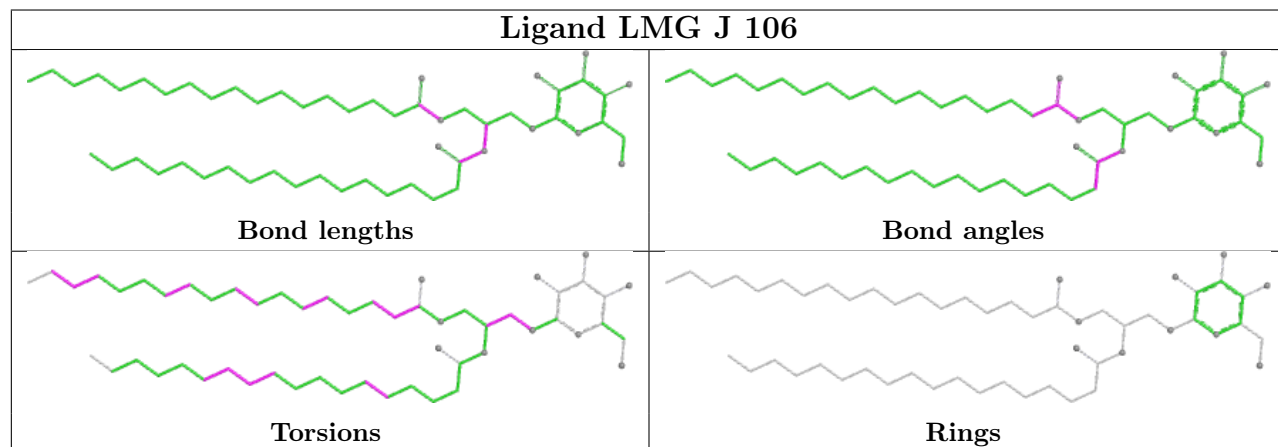
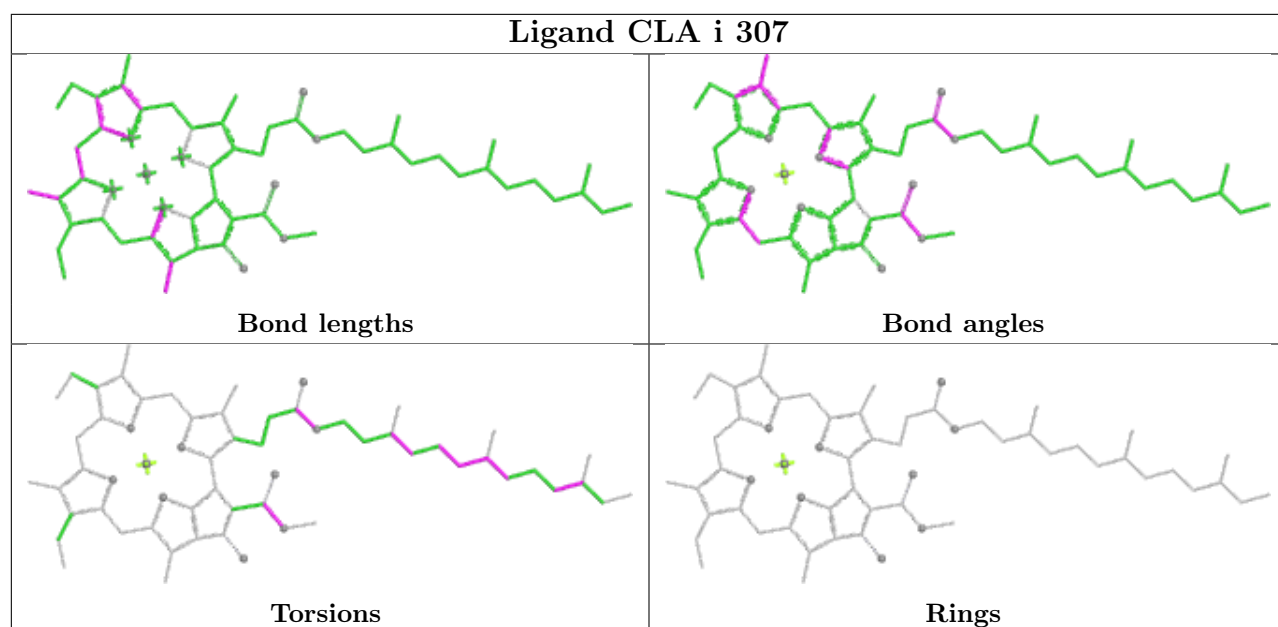


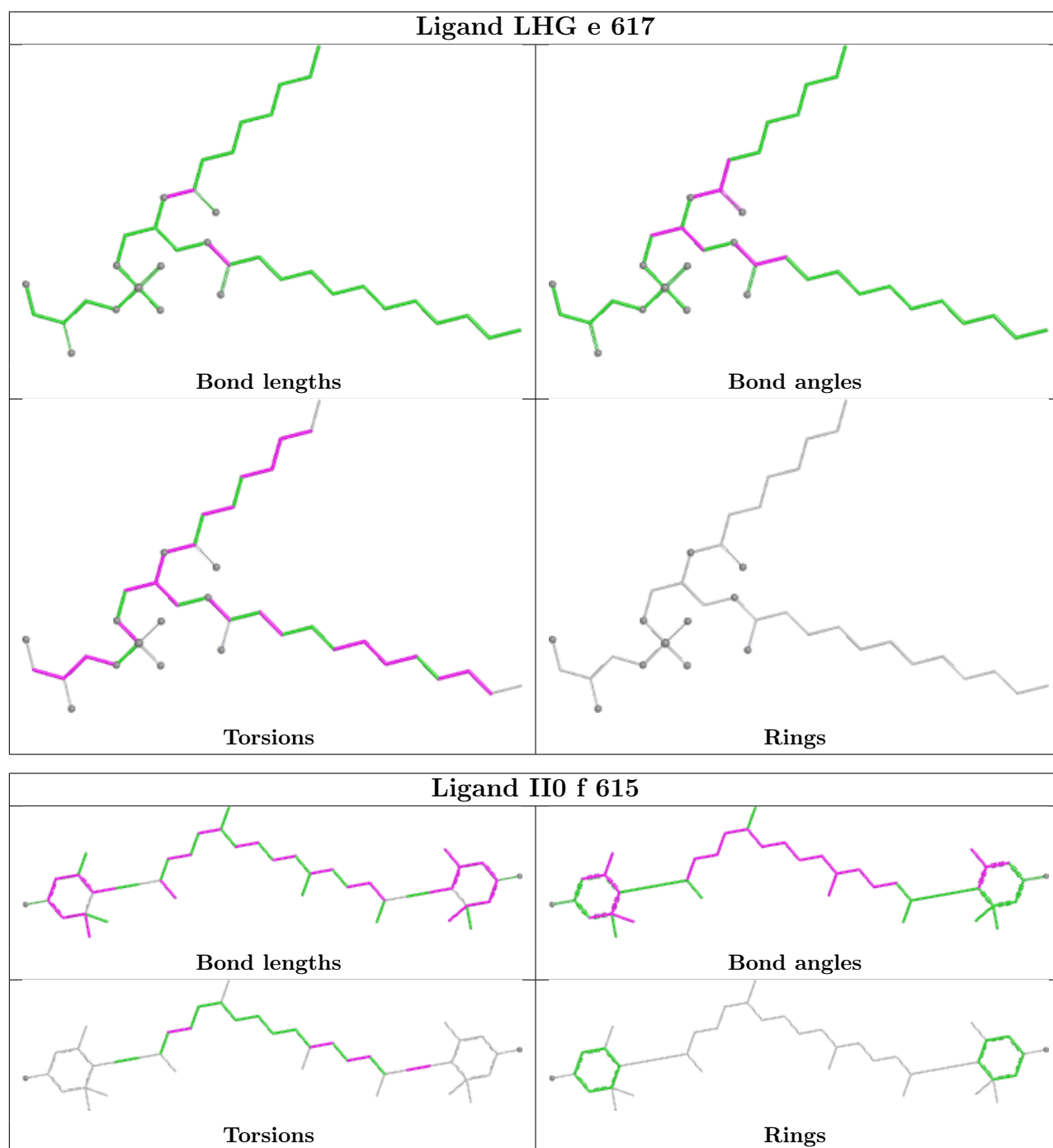
Ligand CLA b 609



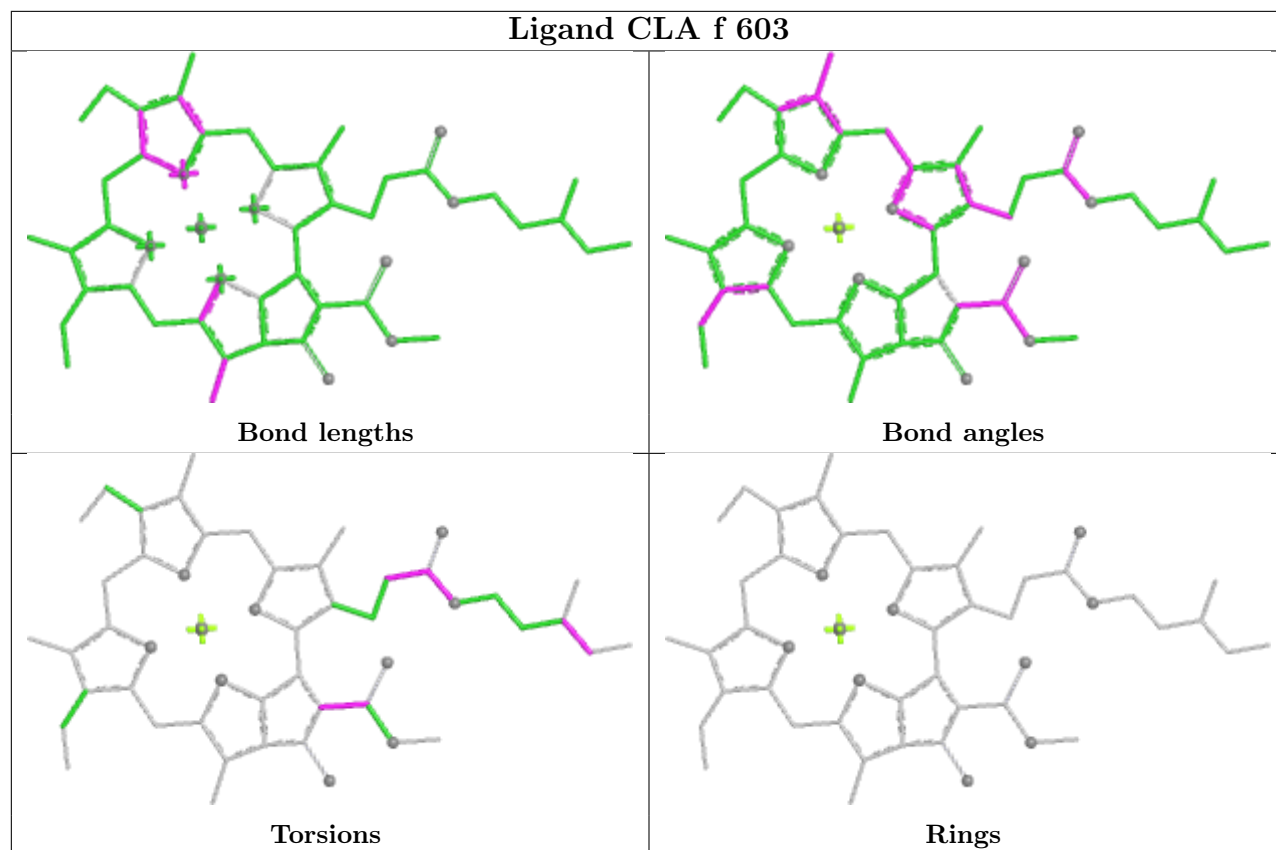
Ligand WVN A 848



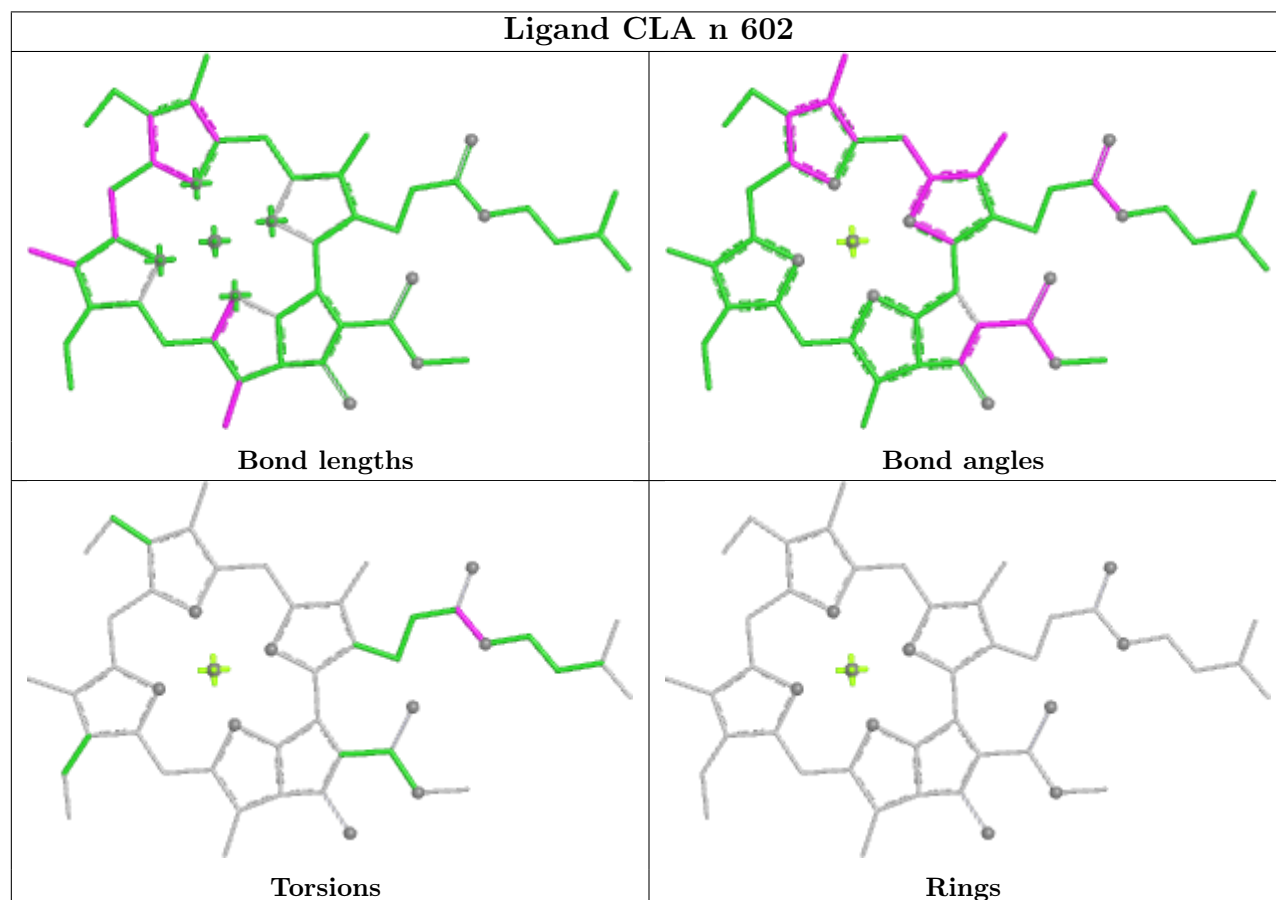




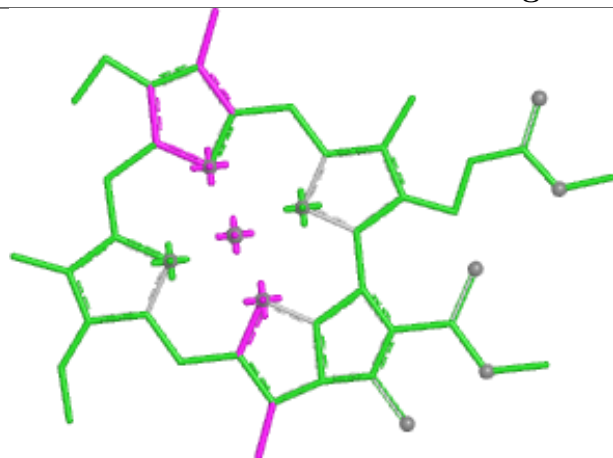
Ligand CLA f 603



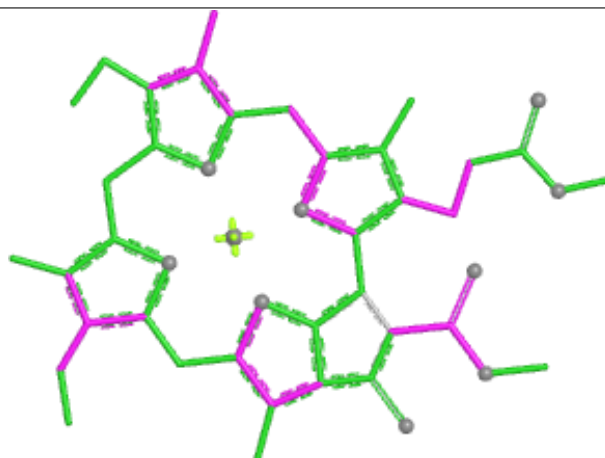
Ligand CLA n 602



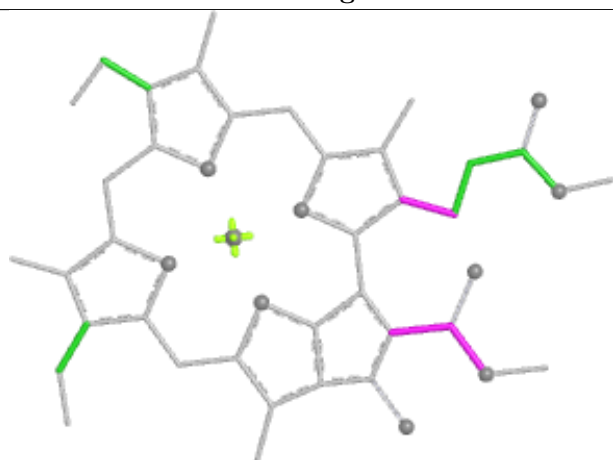
Ligand CLA i 309



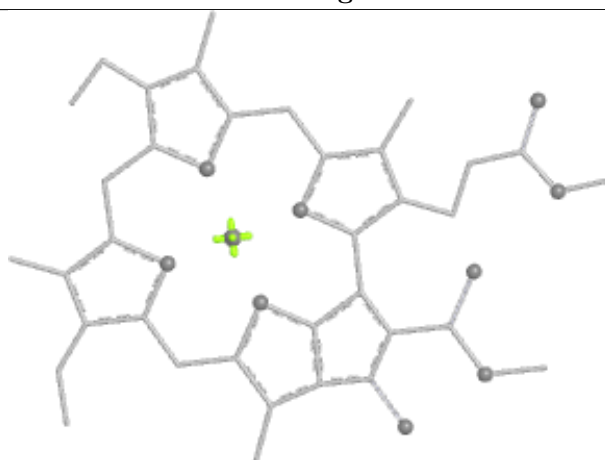
Bond lengths



Bond angles

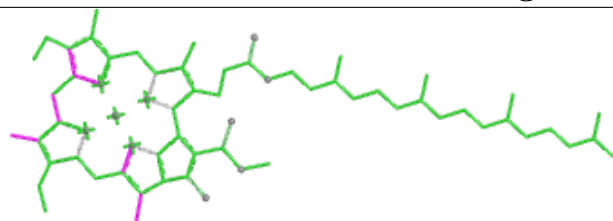


Torsions

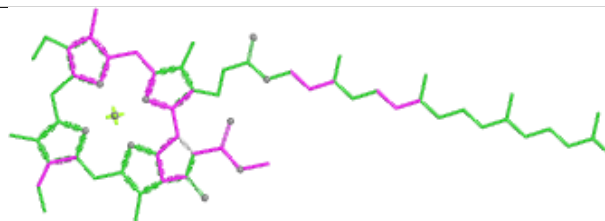


Rings

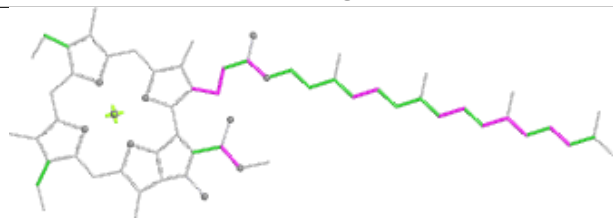
Ligand CLA k 308



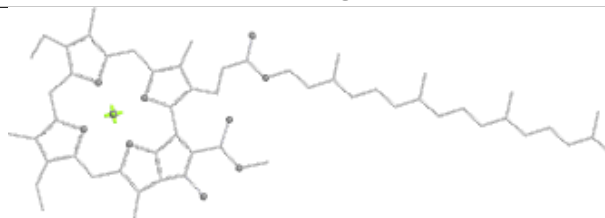
Bond lengths



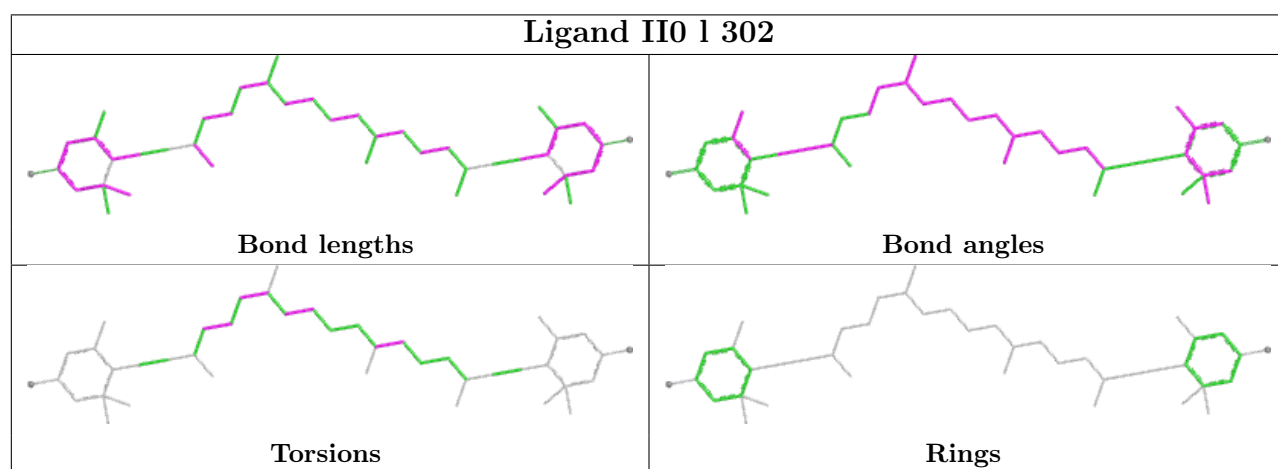
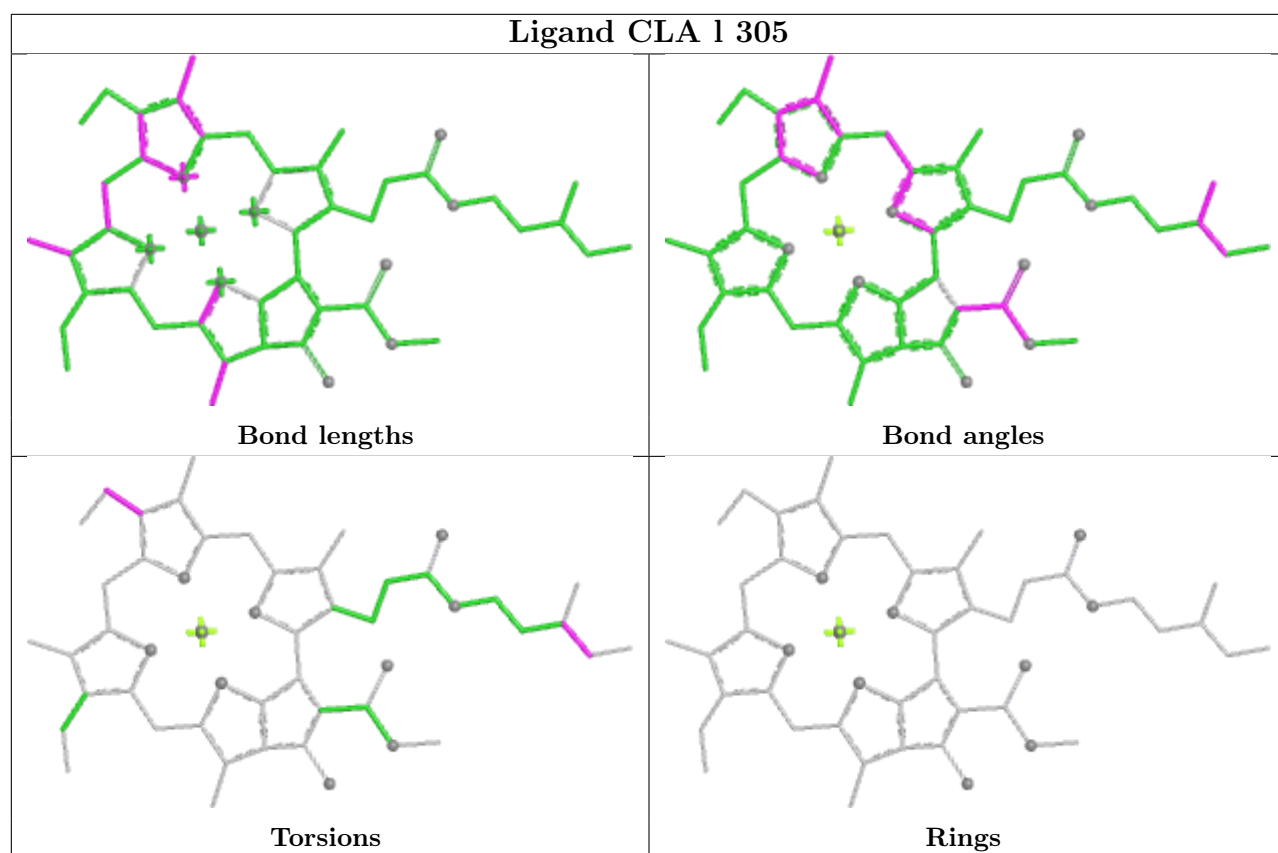
Bond angles

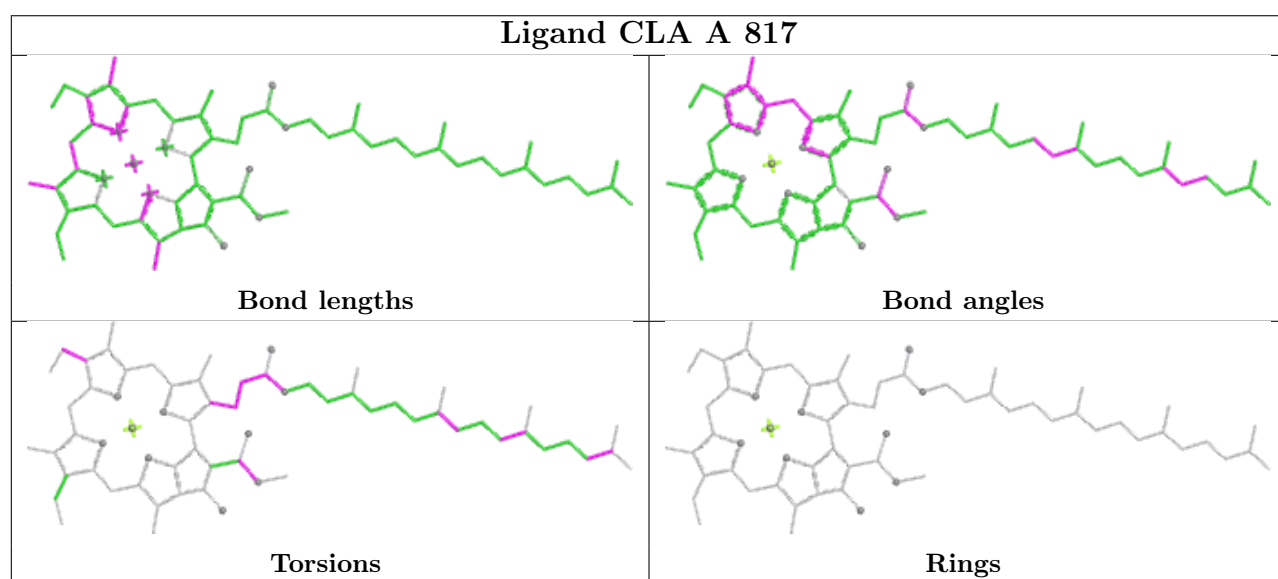
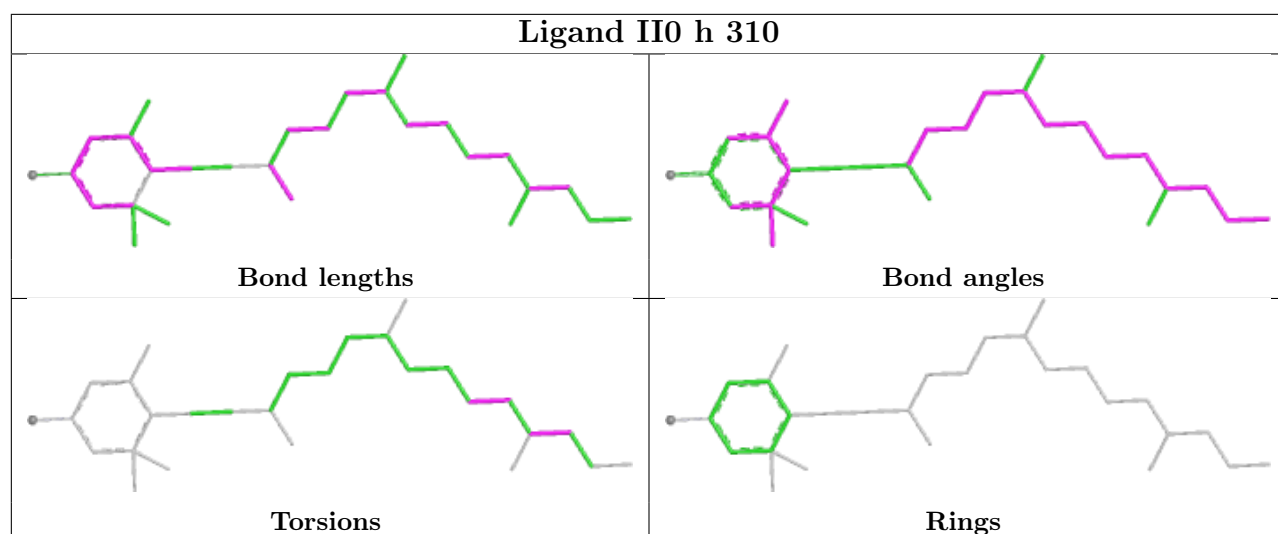


Torsions

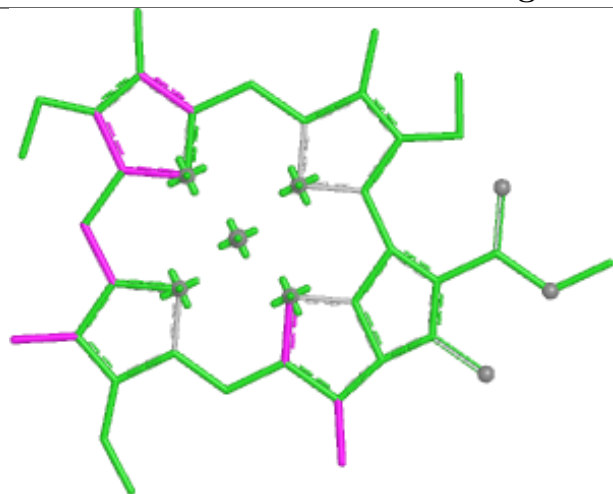


Rings





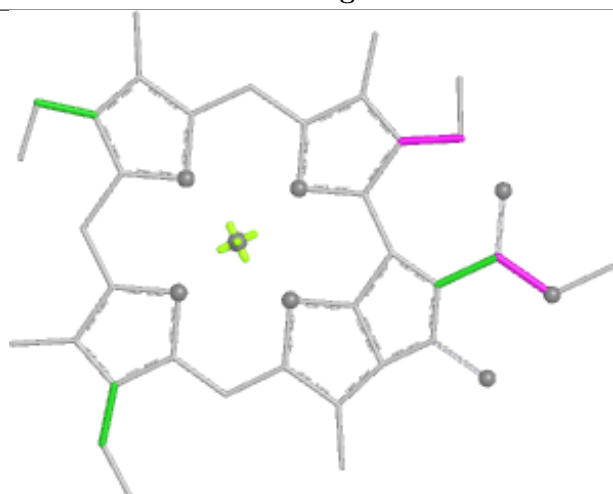
Ligand CLA J 103



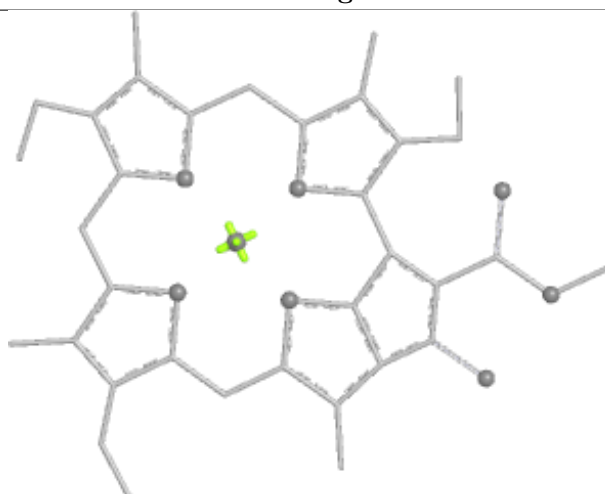
Bond lengths



Bond angles

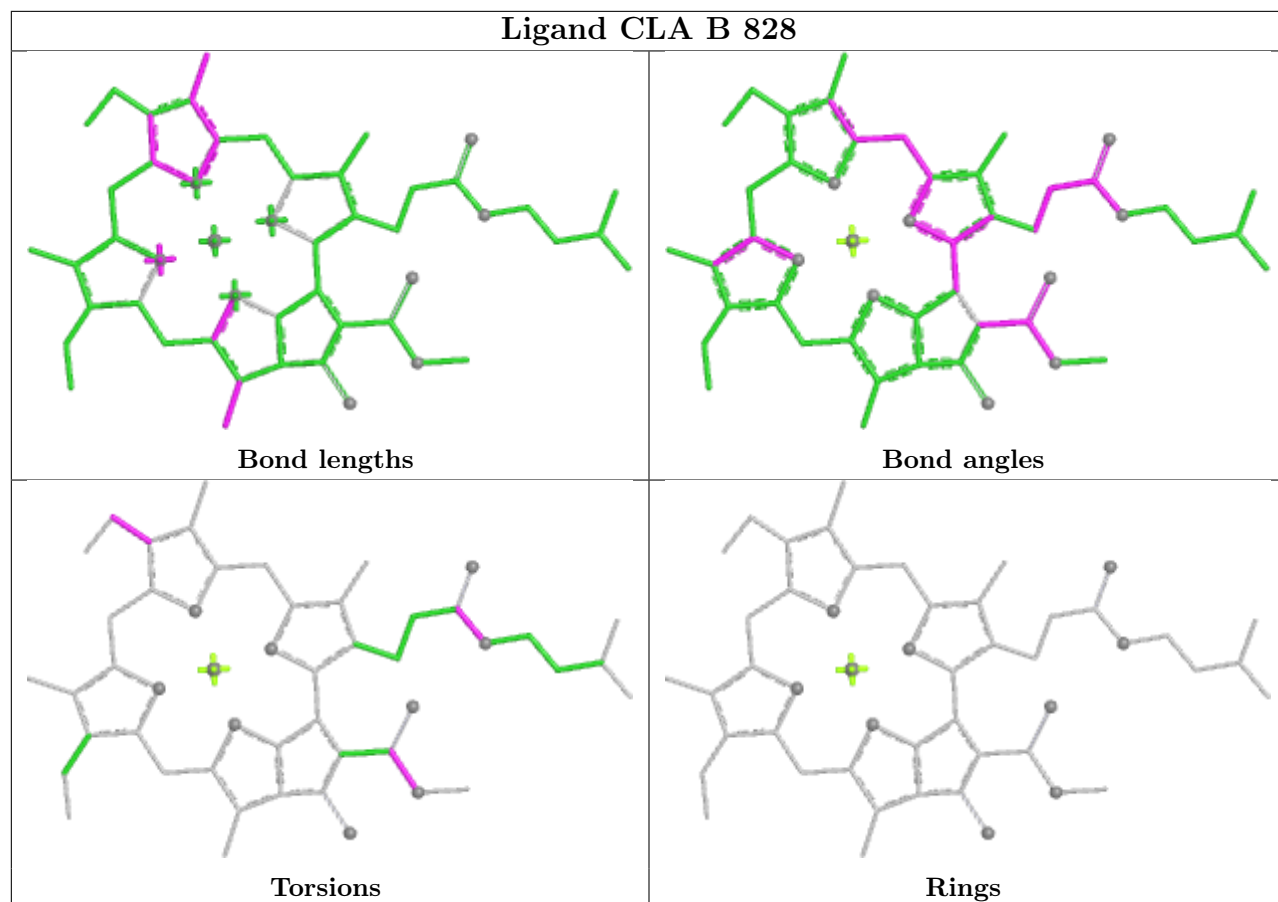


Torsions

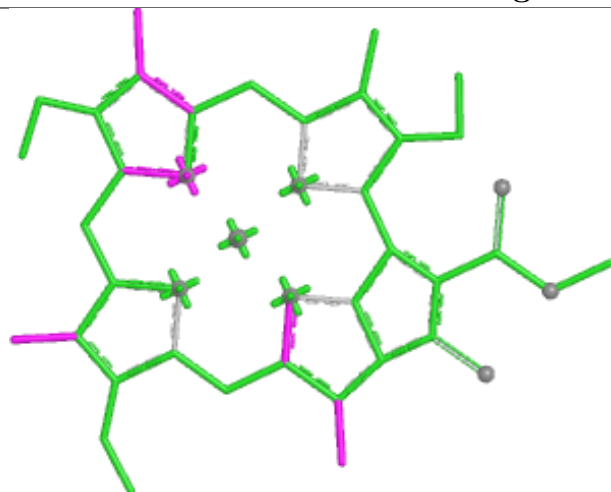


Rings

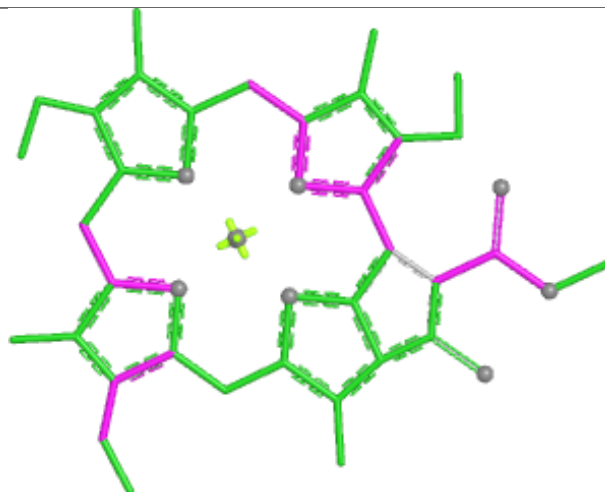
Ligand CLA B 828



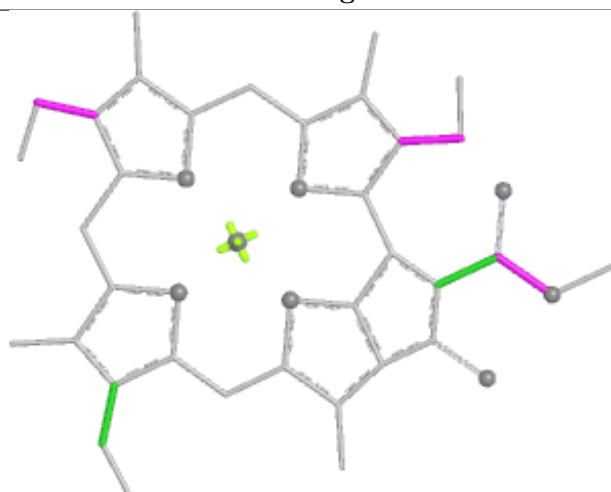
Ligand CLA K 102



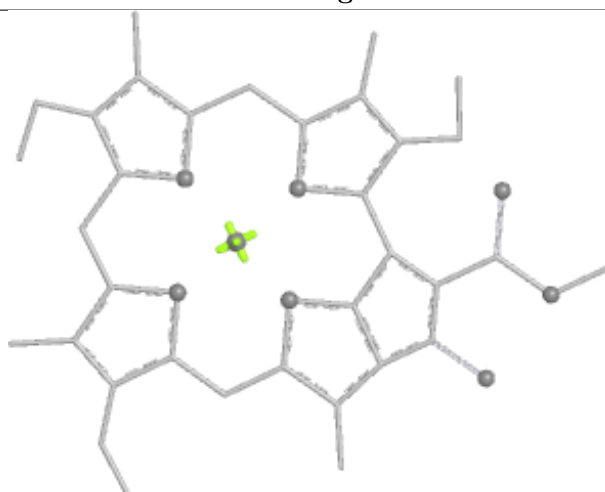
Bond lengths



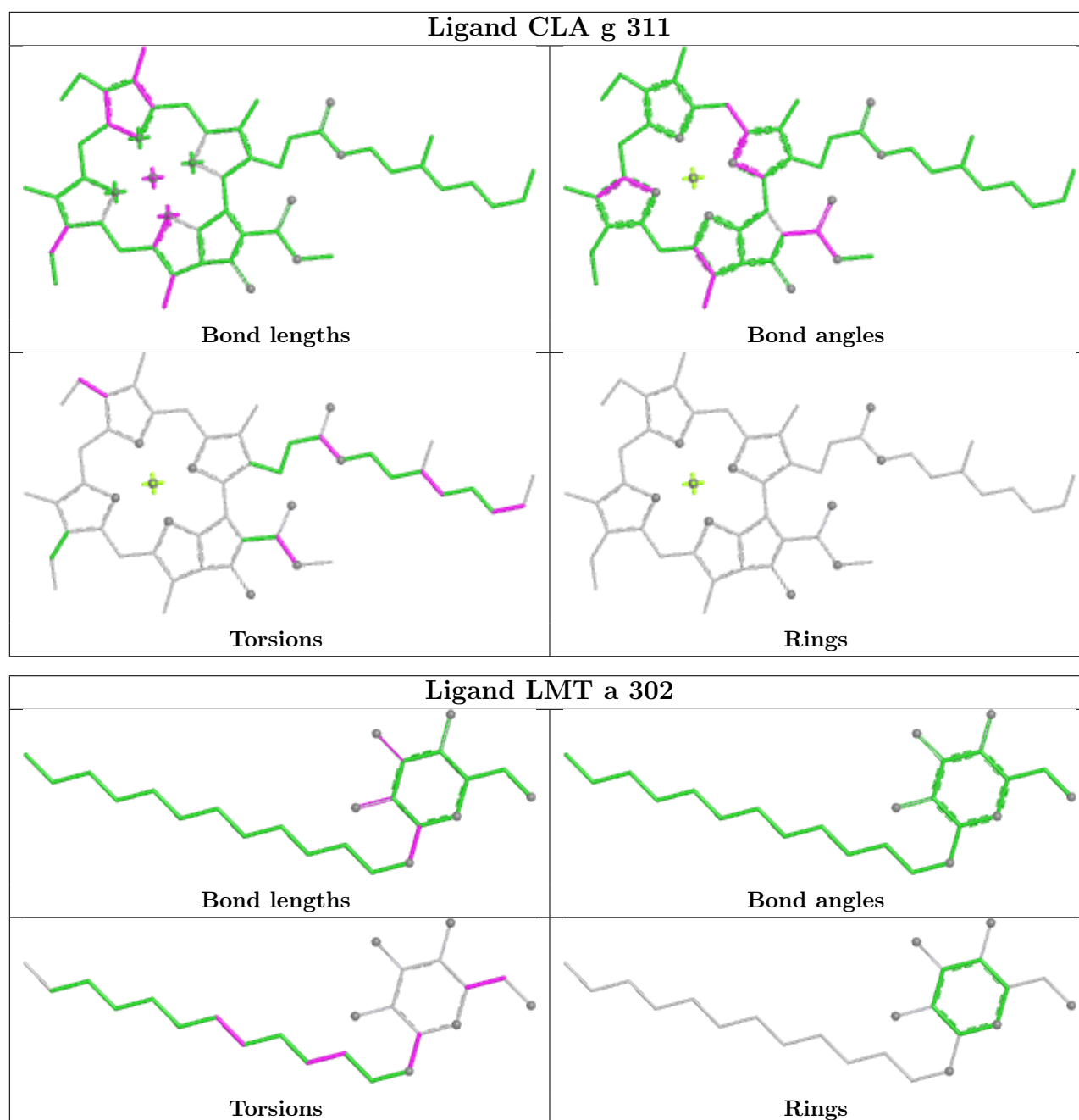
Bond angles

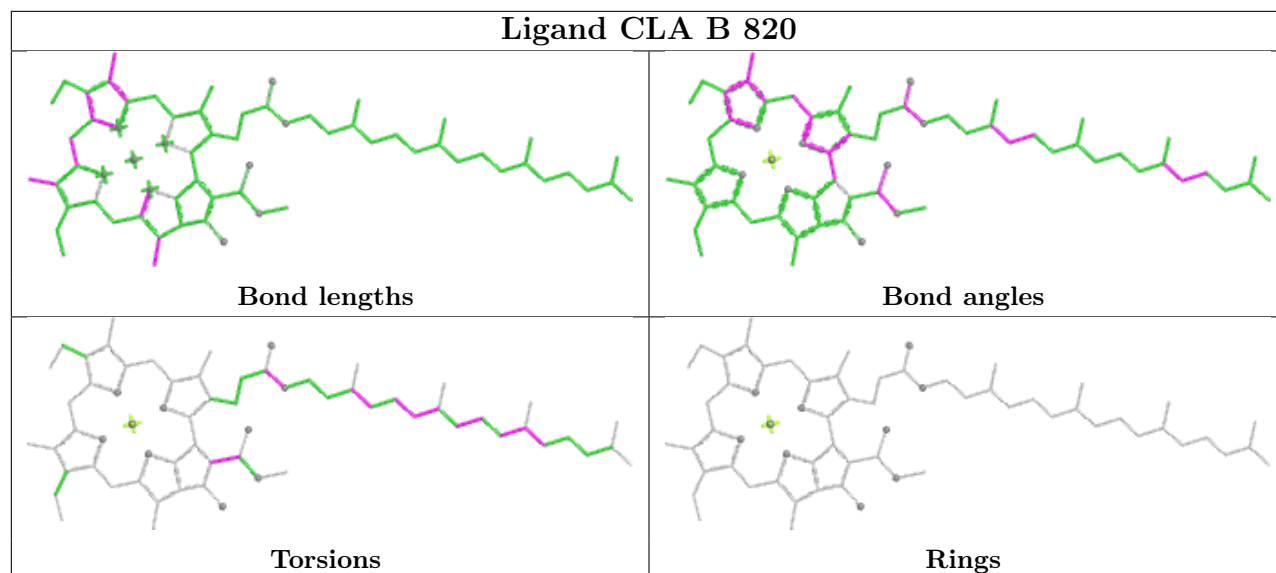
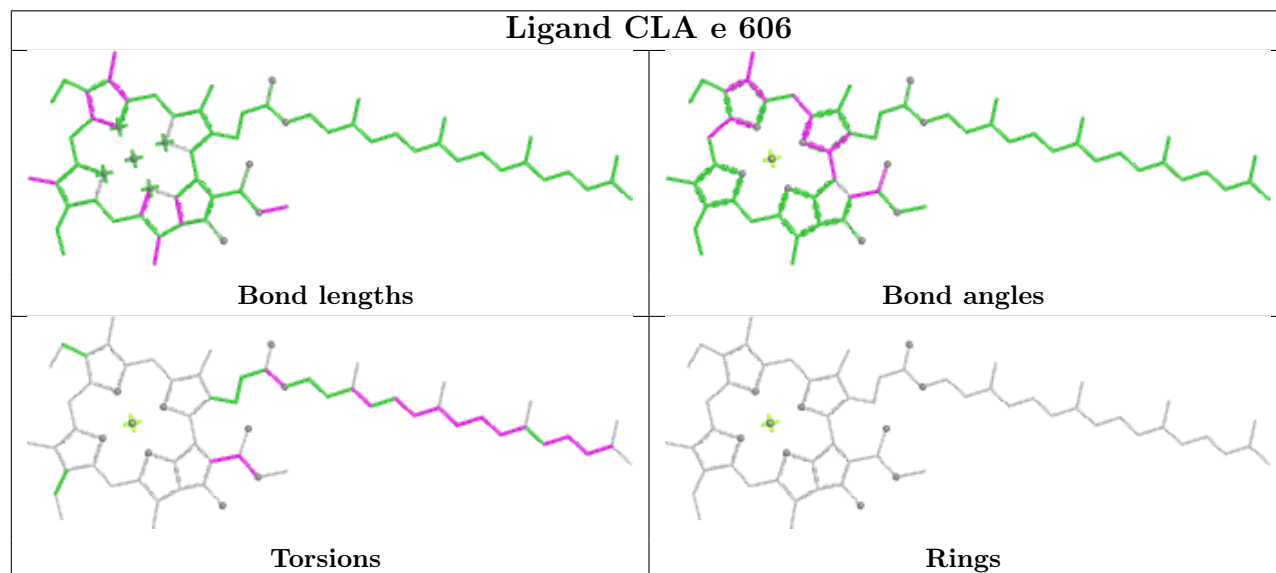
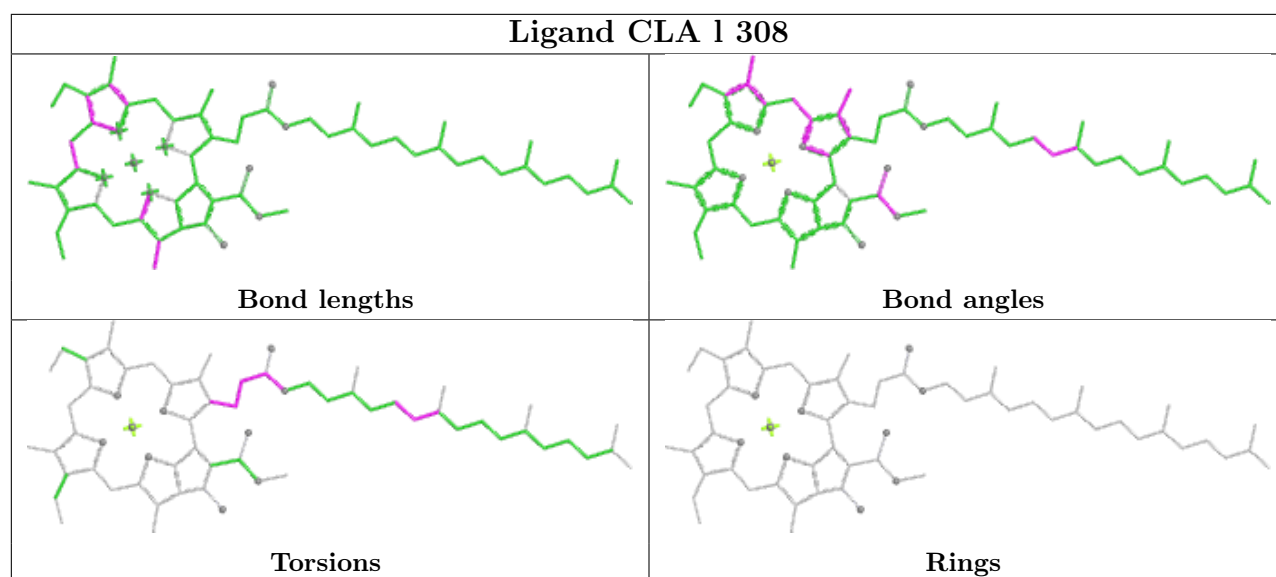


Torsions

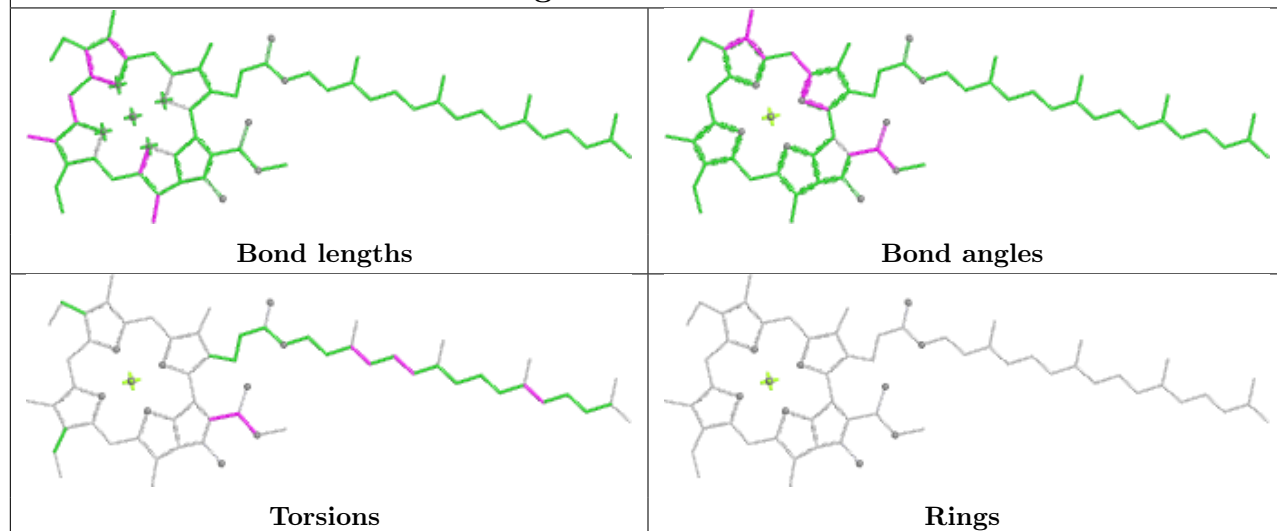


Rings

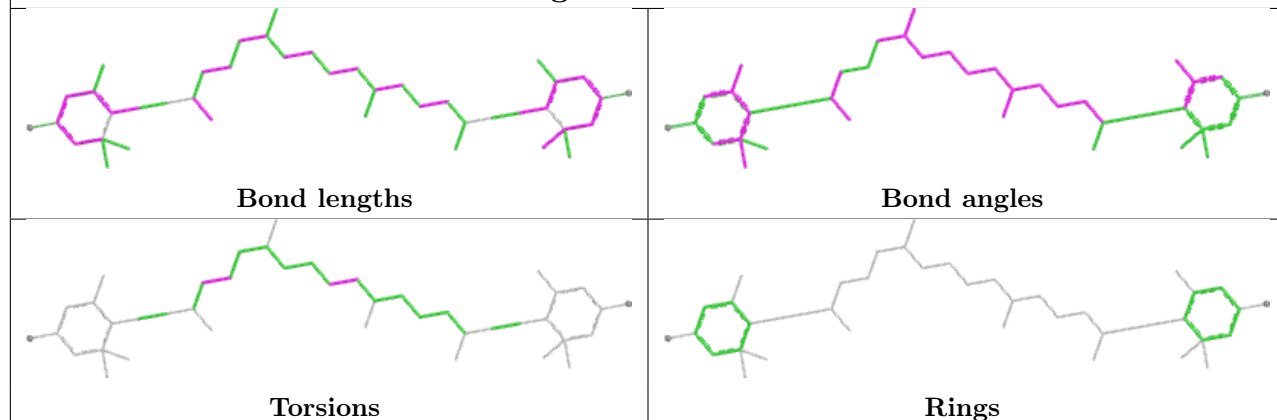




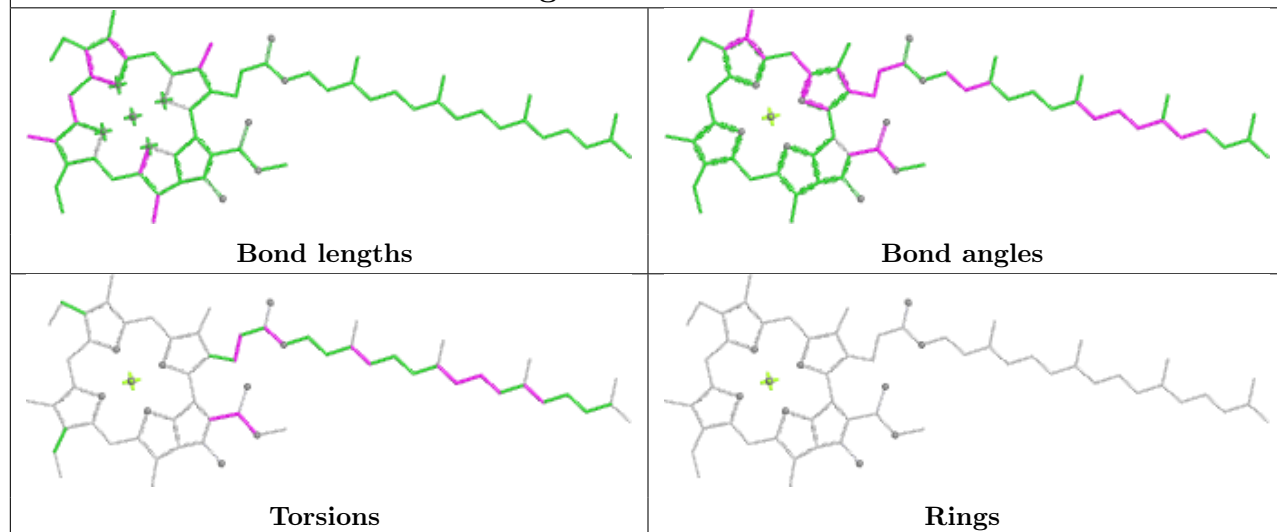
Ligand CLA h 313



Ligand II0 c 615



Ligand CLA l 306



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.

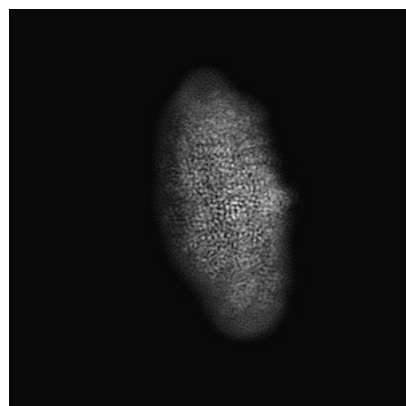
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37659. These allow visual inspection of the internal detail of the map and identification of artifacts.

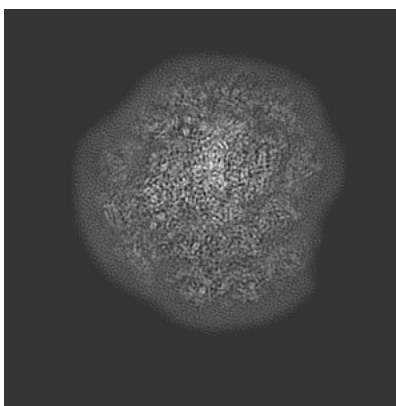
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

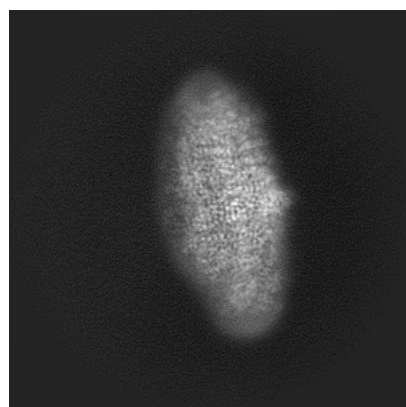


Y

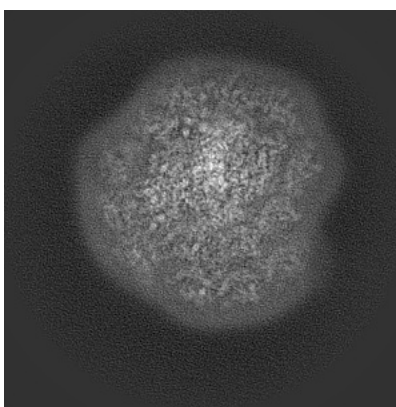


Z

6.1.2 Raw map



X



Y

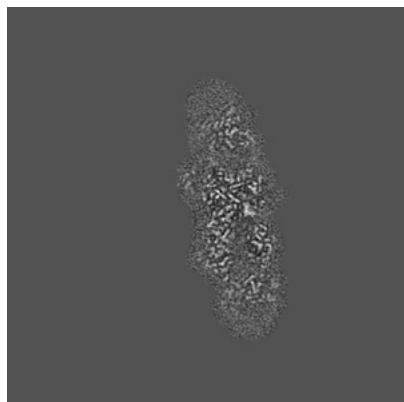


Z

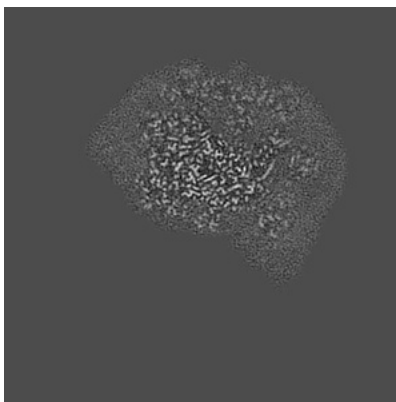
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

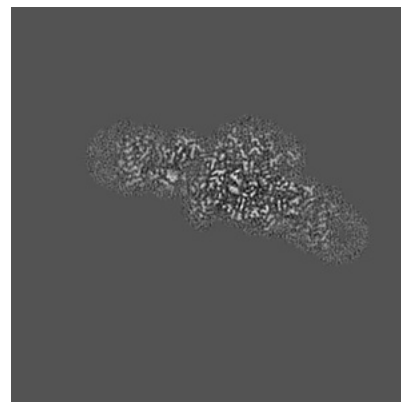
6.2.1 Primary map



X Index: 160

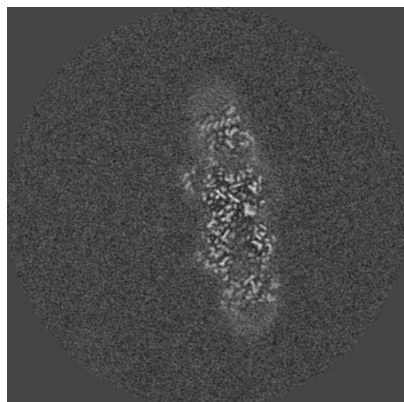


Y Index: 160

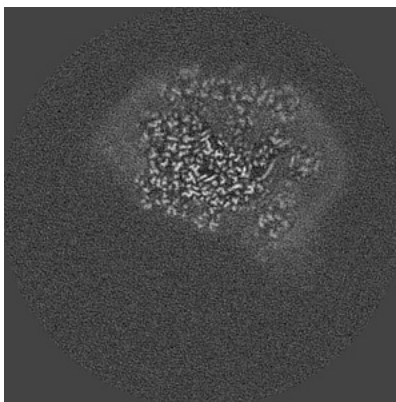


Z Index: 160

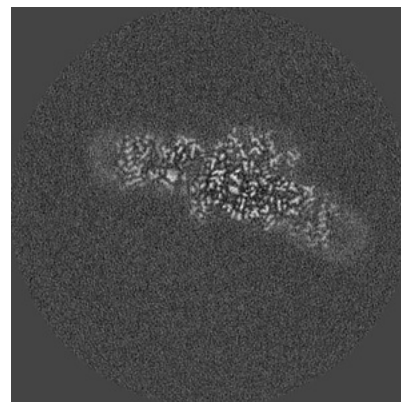
6.2.2 Raw map



X Index: 160



Y Index: 160

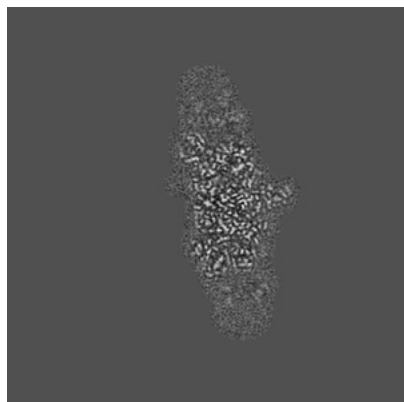


Z Index: 160

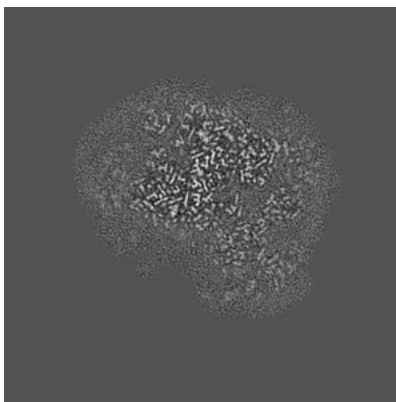
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

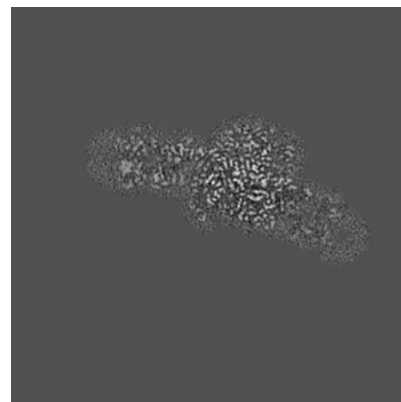
6.3.1 Primary map



X Index: 181

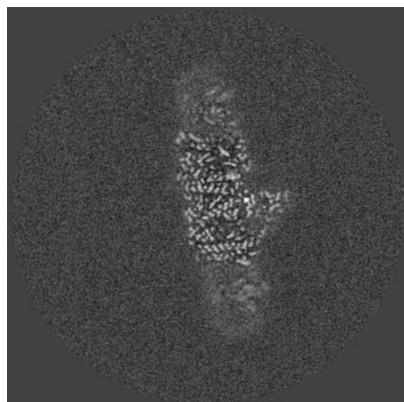


Y Index: 174

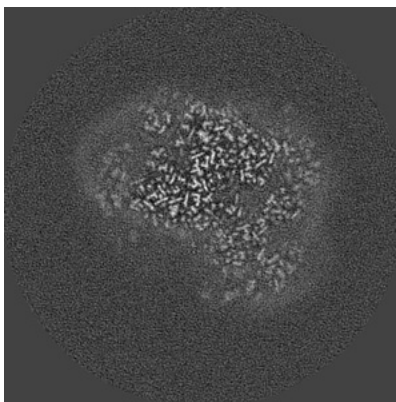


Z Index: 164

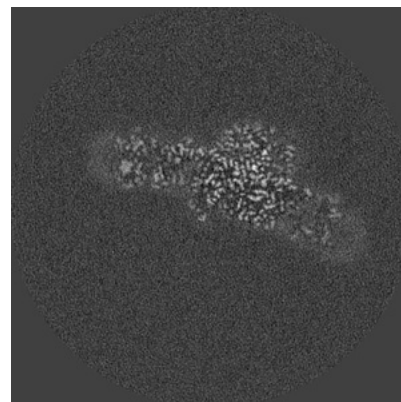
6.3.2 Raw map



X Index: 193



Y Index: 174

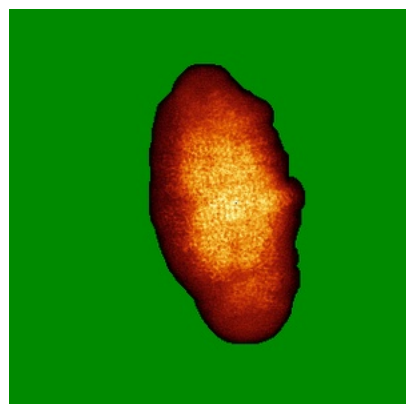


Z Index: 164

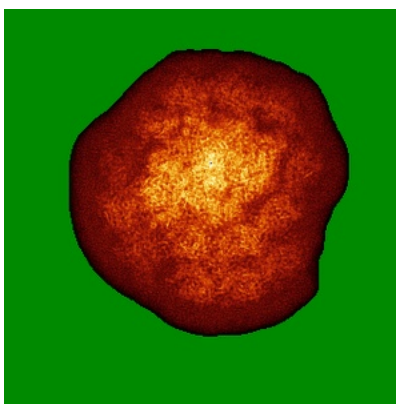
The images above show the largest variance slices of the map in three orthogonal directions.

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

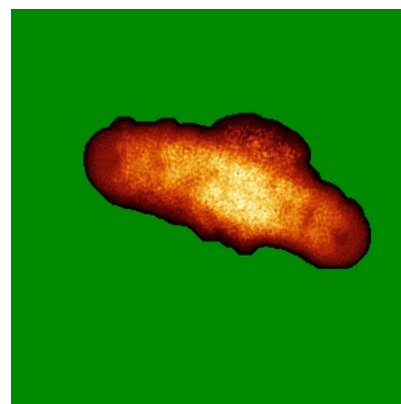
6.4.1 Primary map



X

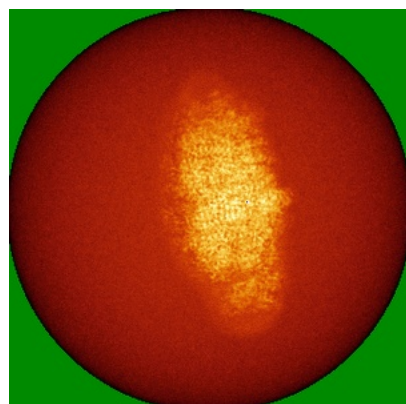


Y

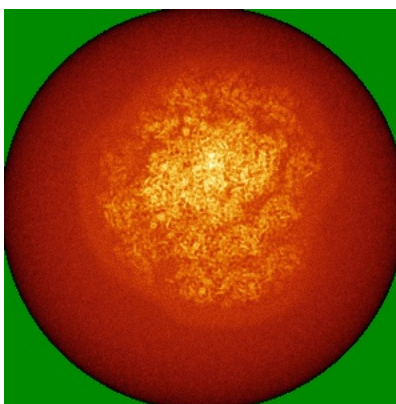


Z

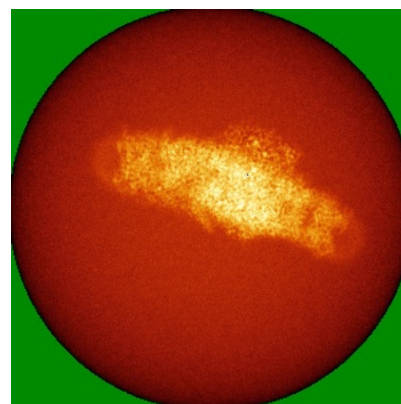
6.4.2 Raw map



X



Y

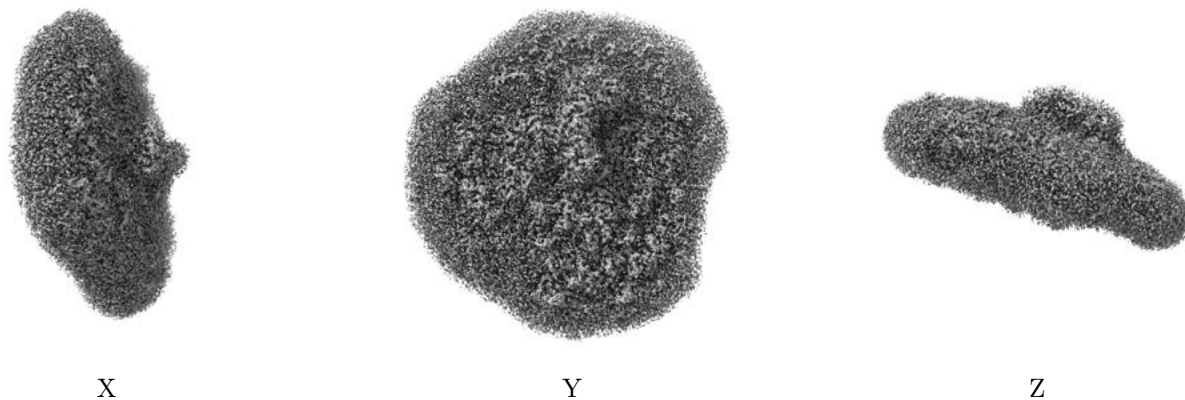


Z

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.

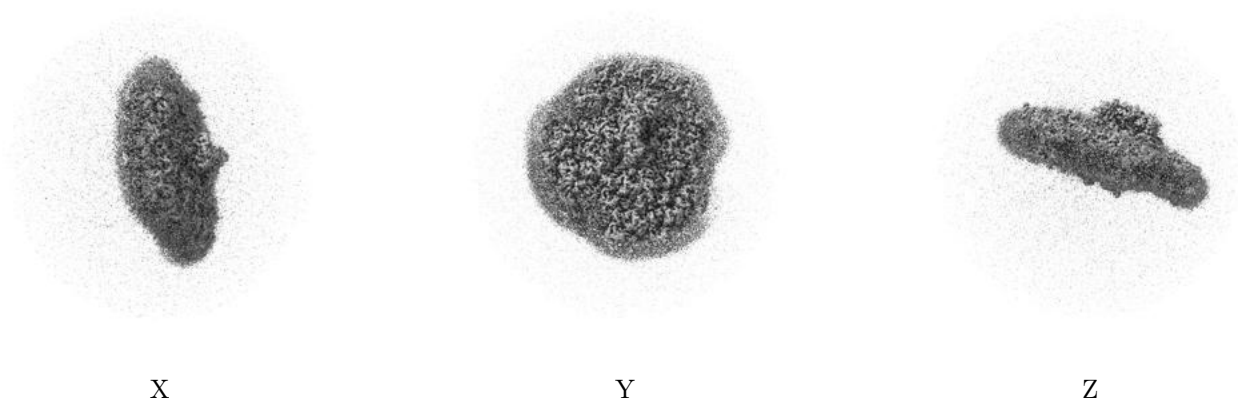
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.023. 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.

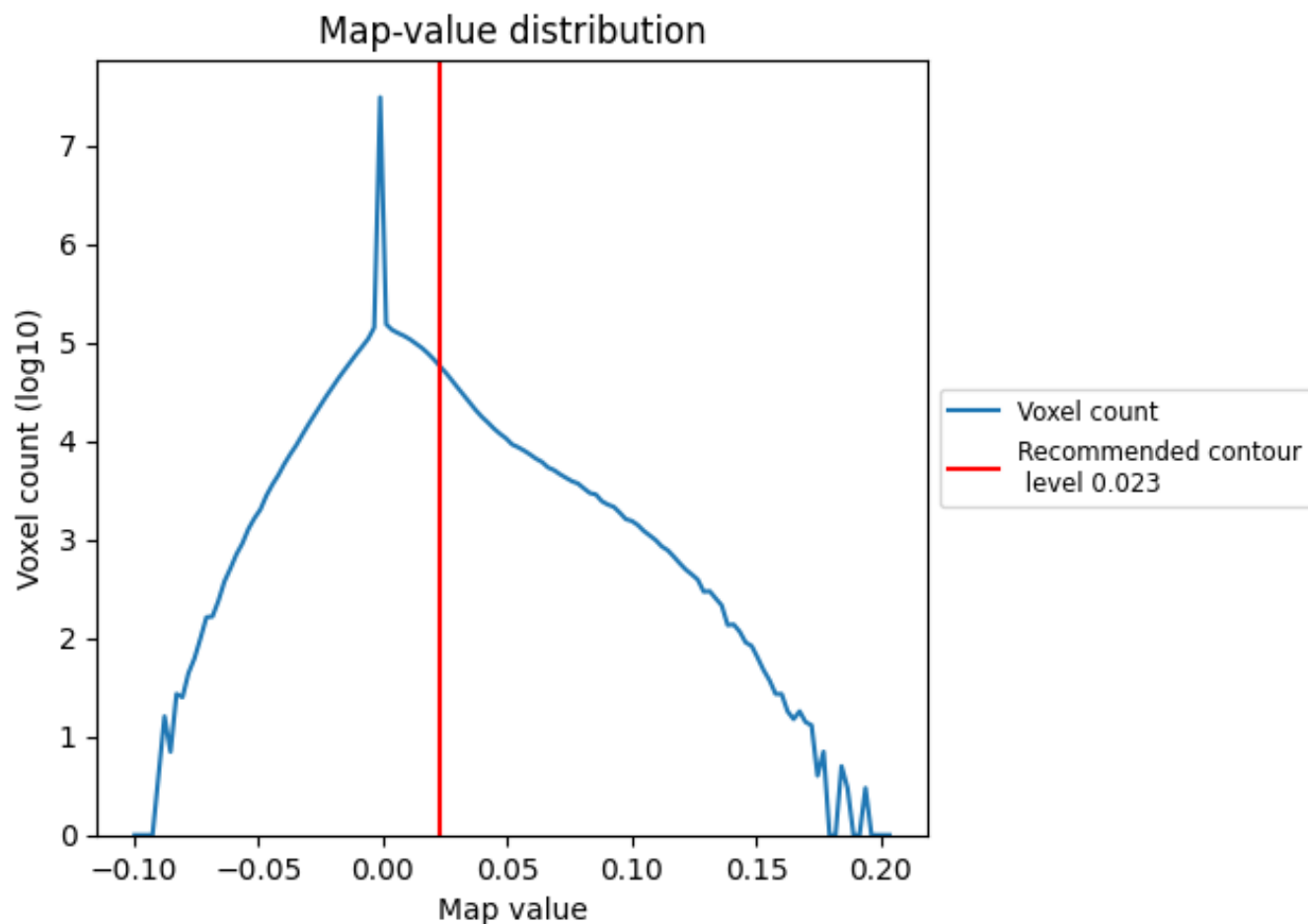
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

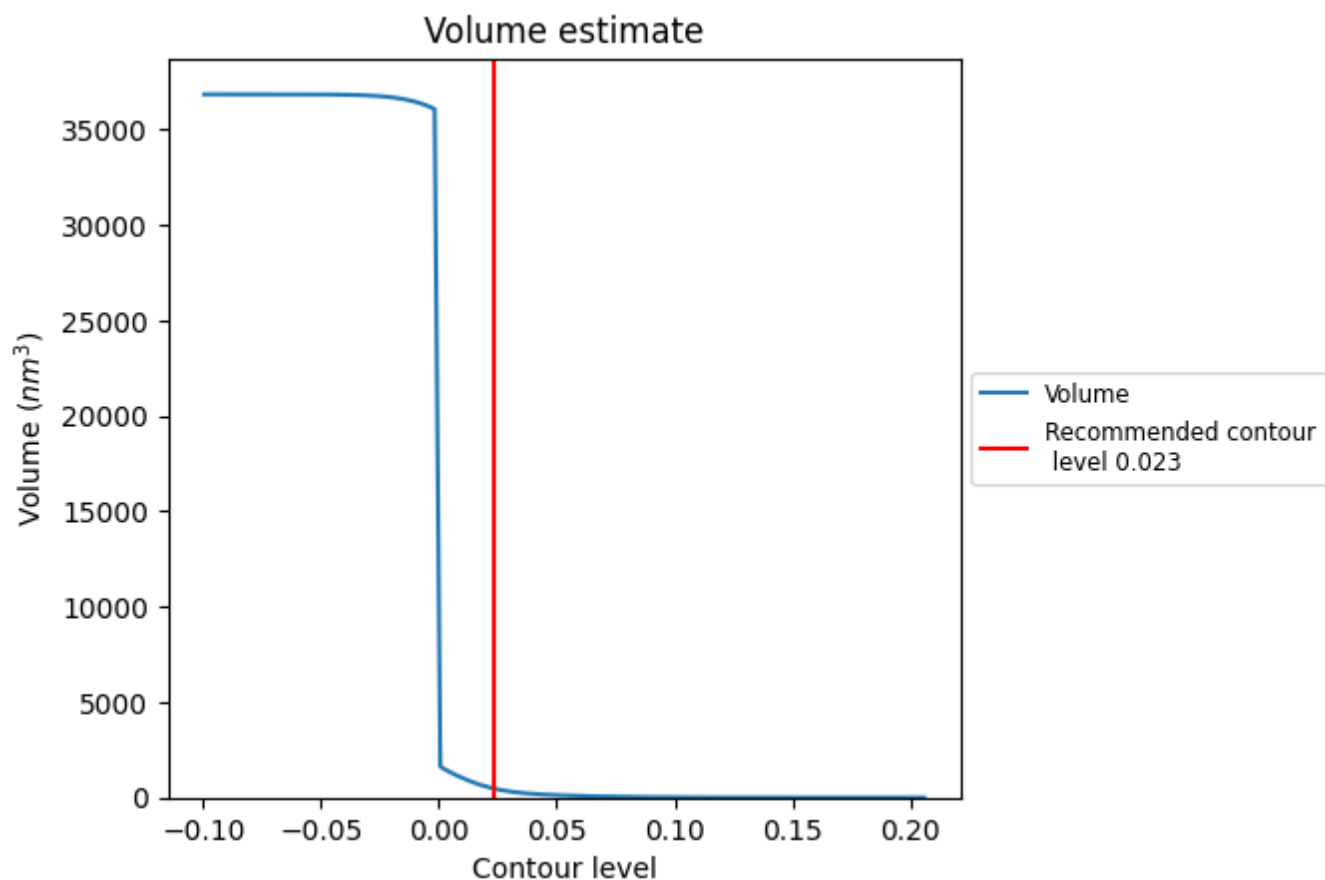
This section contains the results of statistical analysis of the map.

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.

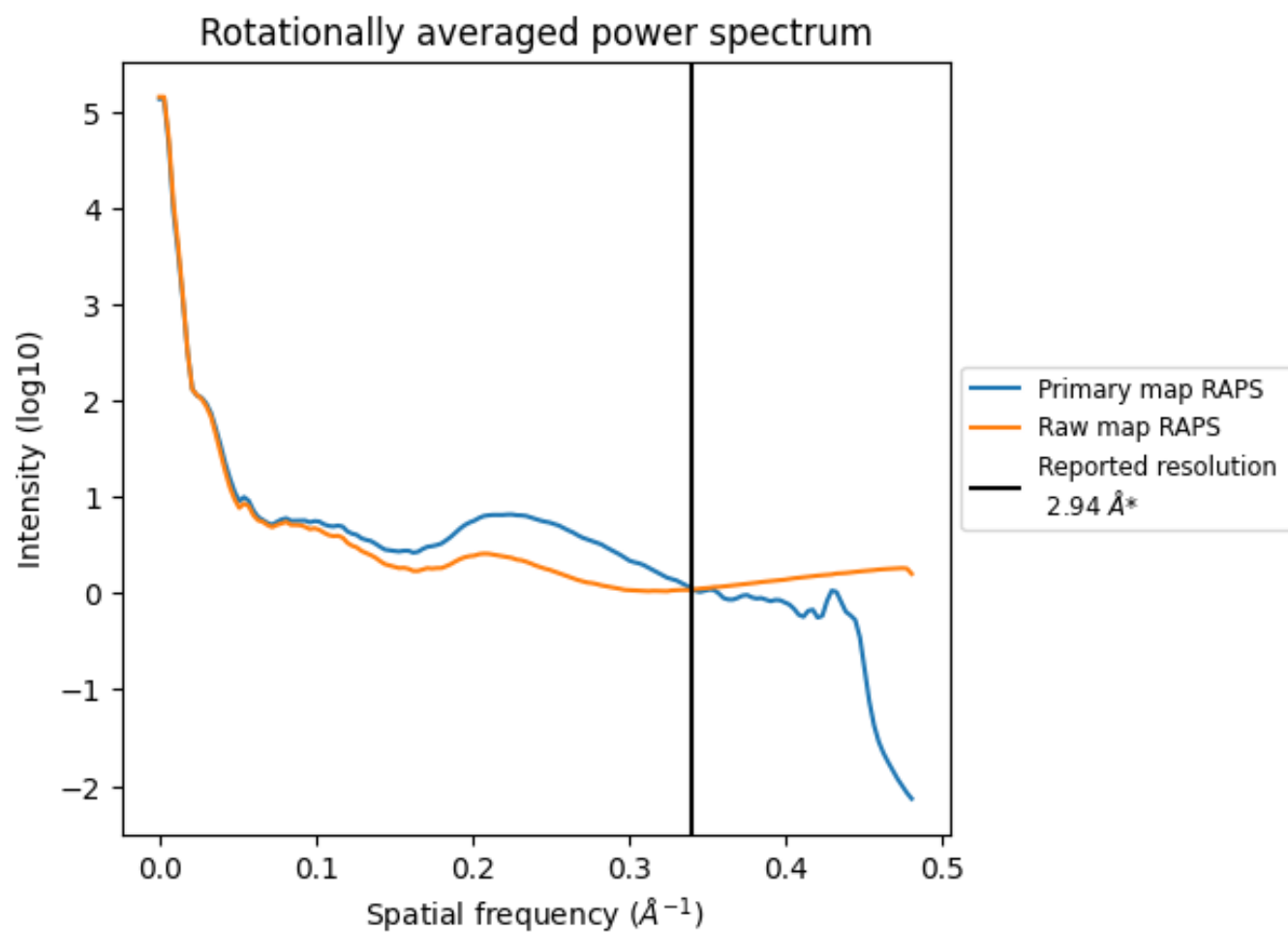
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 484 nm^3 ; this corresponds to an approximate mass of 437 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

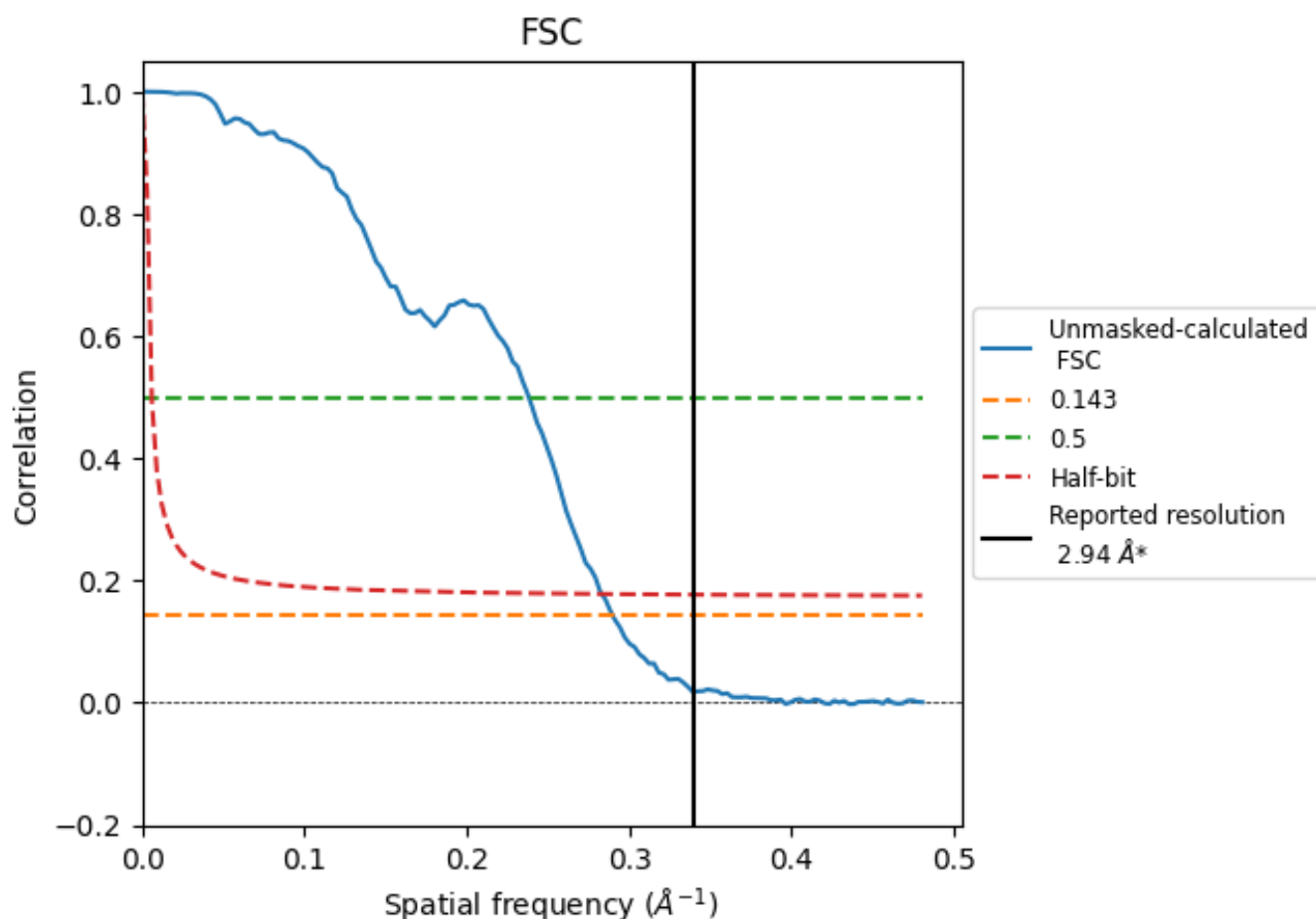


*Reported resolution corresponds to spatial frequency of 0.340 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.340 Å⁻¹

8.2 Resolution estimates [i](#)

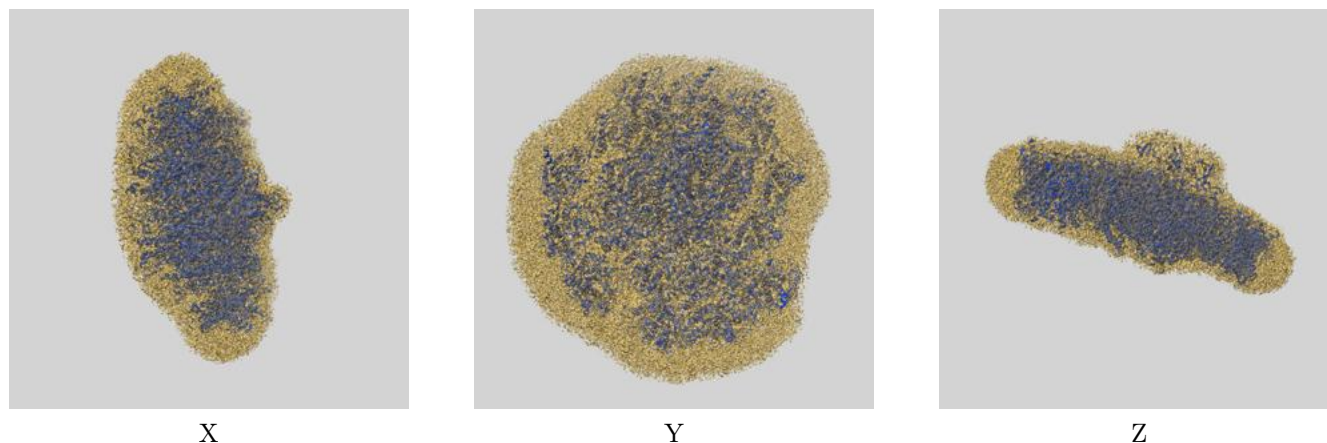
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.45	4.20	3.53

*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 3.45 differs from the reported value 2.94 by more than 10 %

9 Map-model fit [i](#)

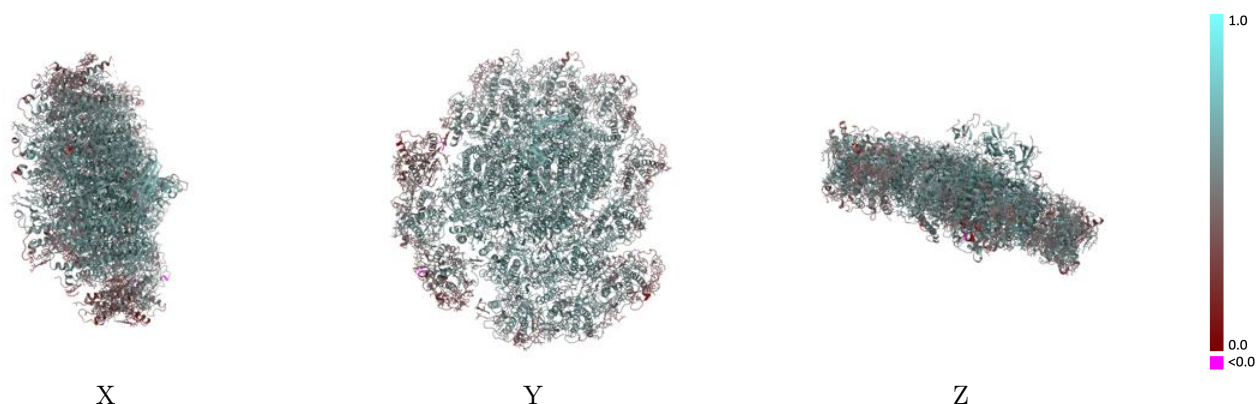
This section contains information regarding the fit between EMDB map EMD-37659 and PDB model 8WMV. Per-residue inclusion information can be found in section 3 on page 40.

9.1 Map-model overlay [i](#)



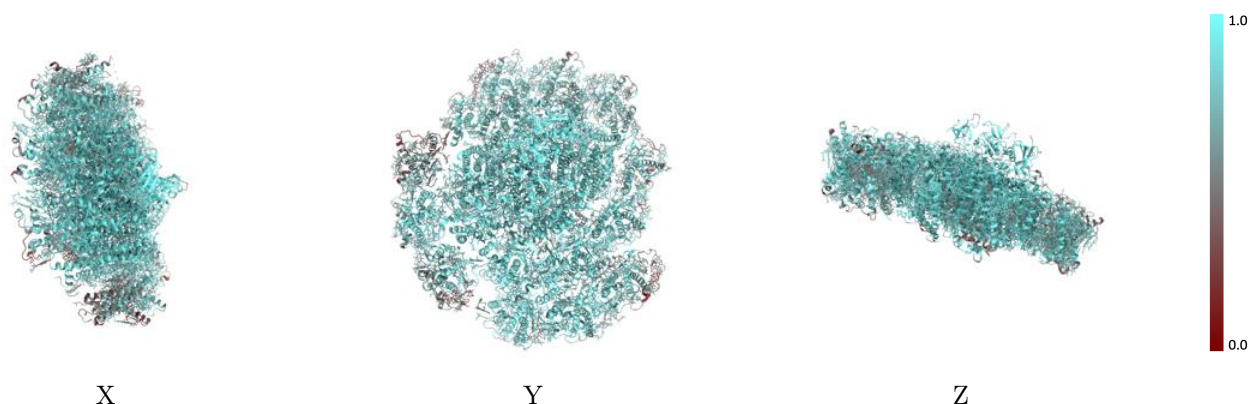
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



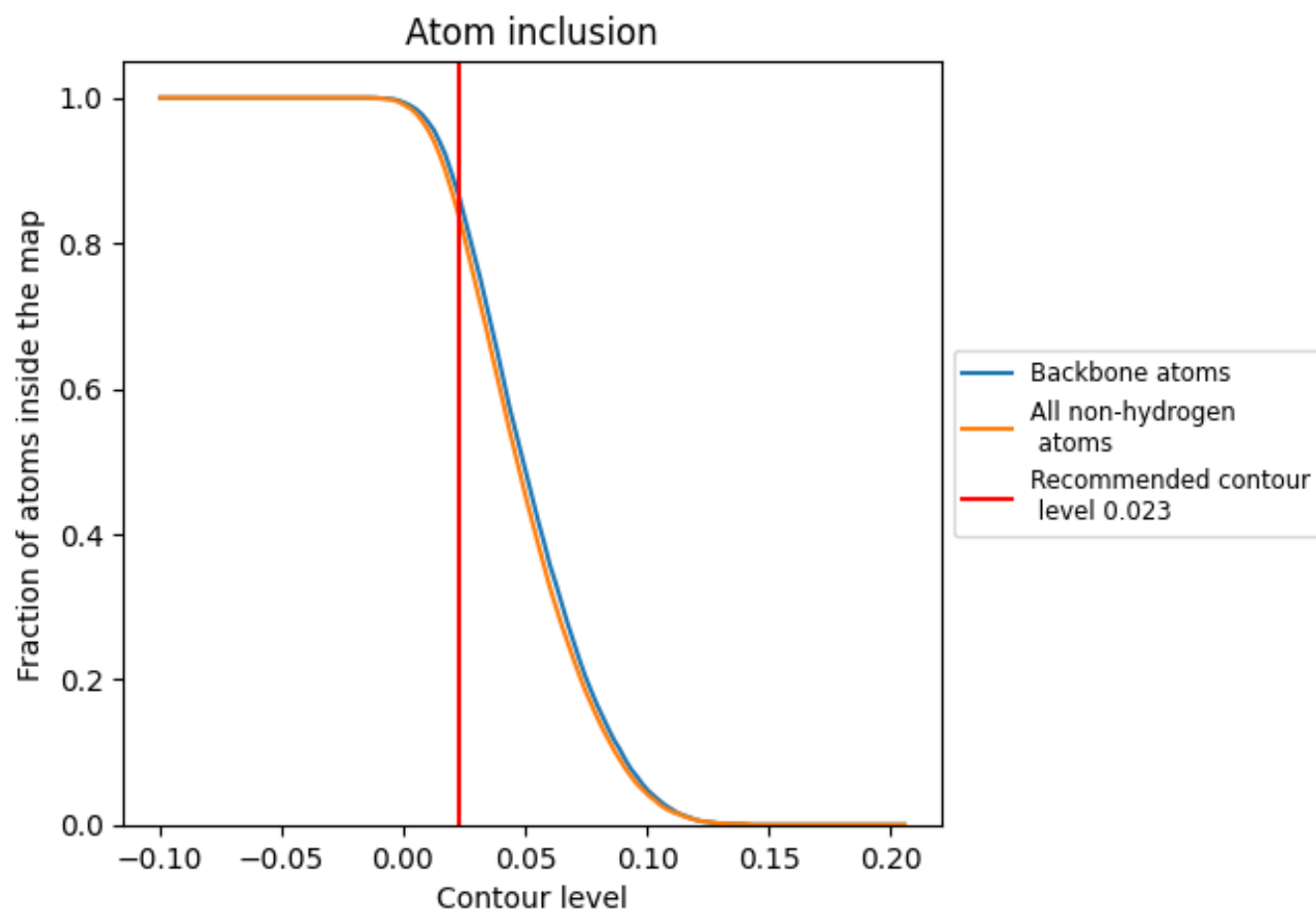
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8360	 0.5550
A	 0.9490	 0.6430
B	 0.9550	 0.6440
C	 0.9700	 0.6420
D	 0.8900	 0.5820
E	 0.8700	 0.5730
F	 0.9040	 0.6050
I	 0.9170	 0.5980
J	 0.9030	 0.6120
K	 0.8540	 0.5580
L	 0.8580	 0.5780
M	 0.8990	 0.5790
O	 0.8390	 0.5640
R	 0.9040	 0.5990
a	 0.9020	 0.5930
b	 0.8810	 0.5900
c	 0.8250	 0.5370
d	 0.6560	 0.4160
e	 0.6940	 0.4670
f	 0.7600	 0.5150
g	 0.6950	 0.4750
h	 0.8320	 0.5430
i	 0.5180	 0.3390
j	 0.7880	 0.5030
k	 0.6630	 0.4110
l	 0.8050	 0.5130
m	 0.8210	 0.5450
n	 0.6470	 0.4390
s	 0.8520	 0.5650

