



wwPDB EM Validation Summary Report ⓘ

Oct 4, 2026 – 04:45 PM JST

PDB ID : 8WM6 / pdb_00008wm6
EMDB ID : EMD-37642
Title : The structure of PSI-CAC(L-14)of R.salina at 2.7 angstroms resolution
Authors : Zhang, S.M.; Si, L.; Li, M.
Deposited on : 2023-10-03
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
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) : 2.51

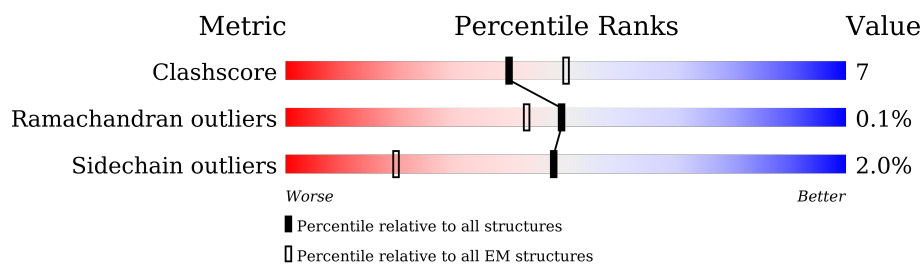
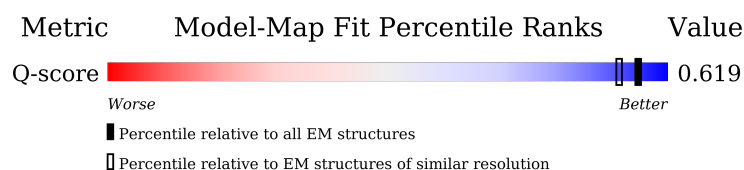
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	
27	Q	234	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 61164 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called PsaO.

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

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

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

- Molecule 13 is a protein called chain s.

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

- Molecule 14 is a protein called cac-c.

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

- Molecule 15 is a protein called cac-a.

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

- Molecule 16 is a protein called cac-b.

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

- Molecule 17 is a protein called cac-h.

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

- Molecule 18 is a protein called cac-f.

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

- Molecule 19 is a protein called cac-e.

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

- Molecule 20 is a protein called cac-l.

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

- Molecule 21 is a protein called cac-k.

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

- Molecule 22 is a protein called cac-i.

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

- Molecule 23 is a protein called cac-d.

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

- Molecule 24 is a protein called cac-g.

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

- Molecule 25 is a protein called PsaR.

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

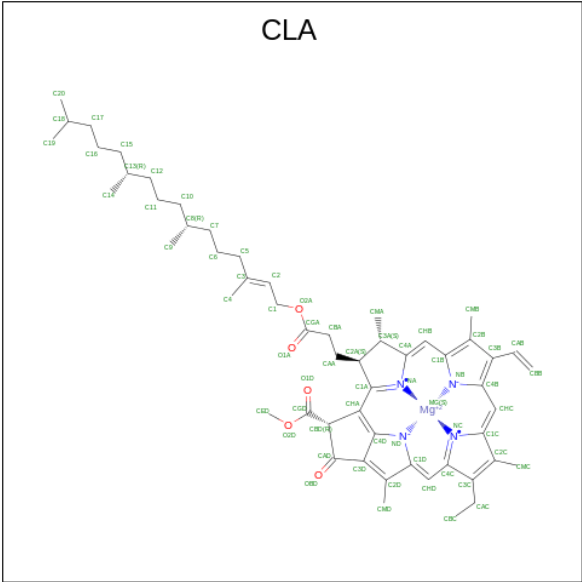
- Molecule 26 is a protein called cac-n.

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

- Molecule 27 is a protein called PsaQ.

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

- Molecule 28 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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

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

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

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

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

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

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

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

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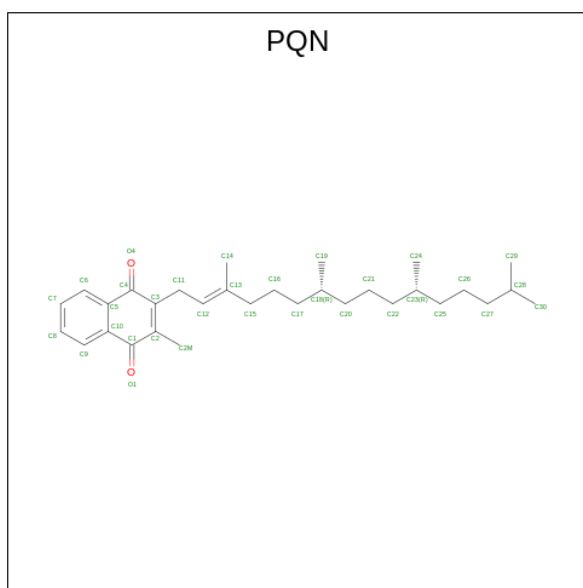
Mol	Chain	Residues	Atoms					AltConf
28	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	d	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	g	1	Total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

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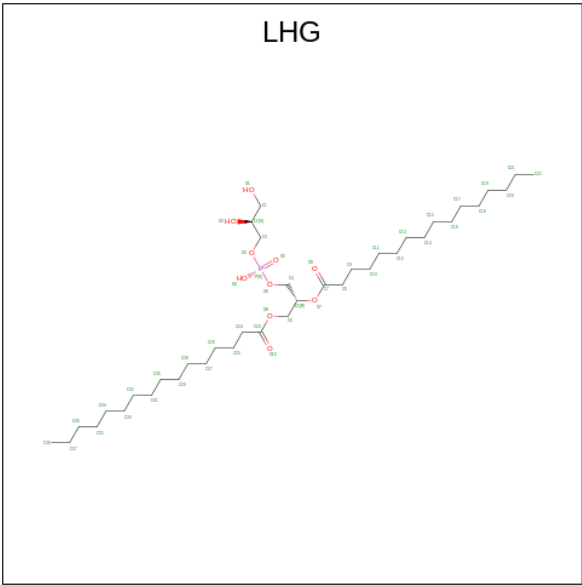
Mol	Chain	Residues	Atoms					AltConf
28	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0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

- Molecule 29 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



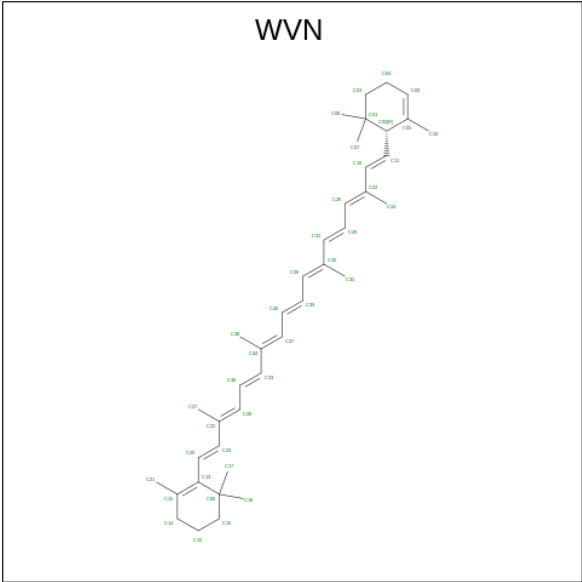
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			48	37	10	1	
30	A	1	Total	C	O	P	0
			27	16	10	1	
30	A	1	Total	C	O	P	0
			38	27	10	1	
30	J	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	c	1	Total	C	O	P	0
			37	26	10	1	
30	c	1	Total	C	O	P	0
			37	26	10	1	
30	a	1	Total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

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

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



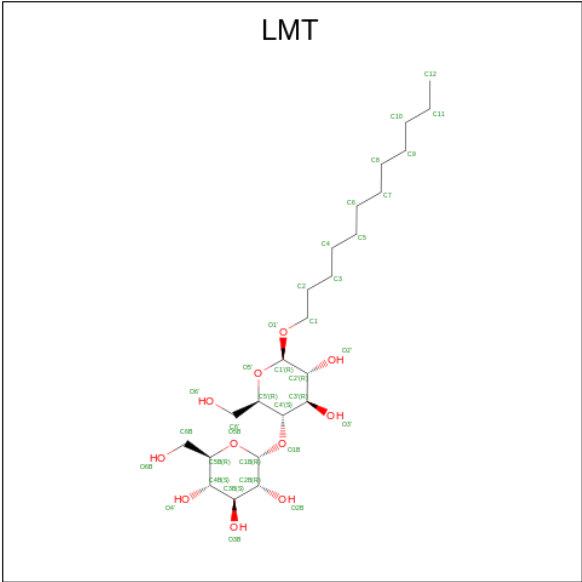
Mol	Chain	Residues	Atoms		AltConf
31	A	1	Total	C	0
			40	40	
31	A	1	Total	C	0
			40	40	
31	A	1	Total	C	0
			40	40	
31	A	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	F	1	Total	C	0
			40	40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

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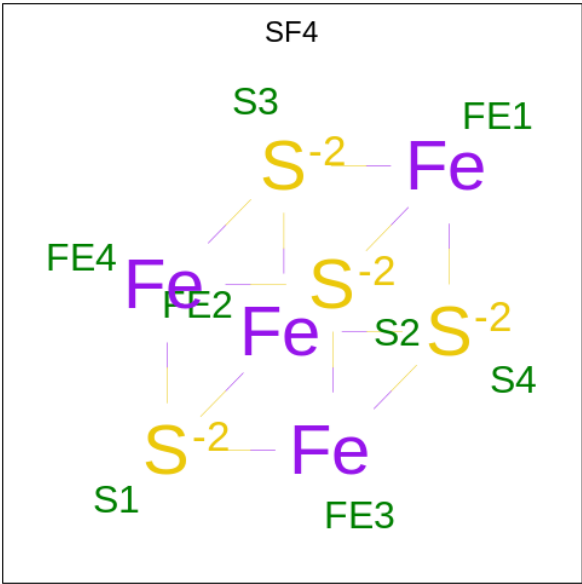
Mol	Chain	Residues	Atoms	AltConf
31	L	1	Total C 40 40	0
31	L	1	Total C 40 40	0
31	L	1	Total C 40 40	0
31	M	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	s	1	Total C 40 40	0
31	s	1	Total C 40 40	0
31	h	1	Total C 40 40	0
31	e	1	Total C 40 40	0
31	l	1	Total C 40 40	0
31	l	1	Total C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

- Molecule 32 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



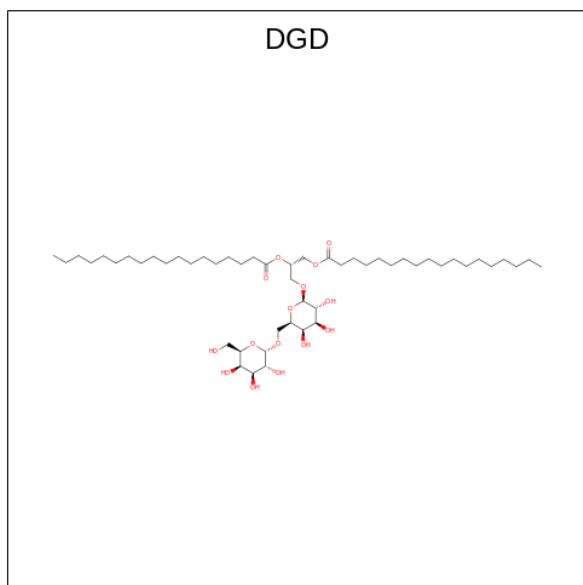
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			35	24	11	
32	a	1	Total	C	O	0
			24	18	6	
32	a	1	Total	C	O	0
			35	24	11	
32	b	1	Total	C	O	0
			24	18	6	

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



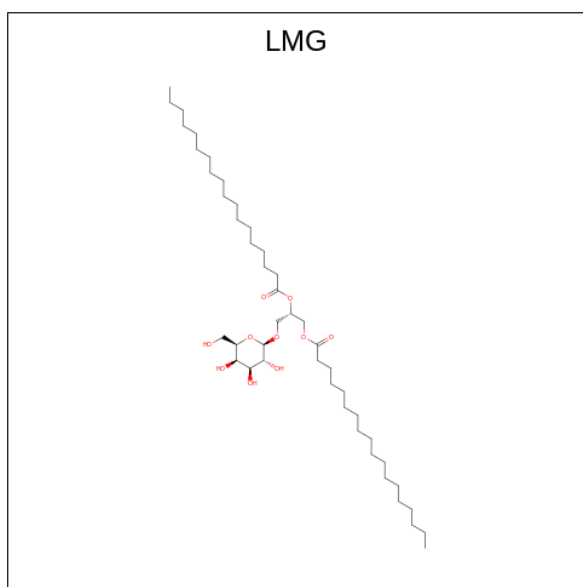
Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	Fe	S	0
			8	4	4	
33	C	1	Total	Fe	S	0
			8	4	4	
33	C	1	Total	Fe	S	0
			8	4	4	

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



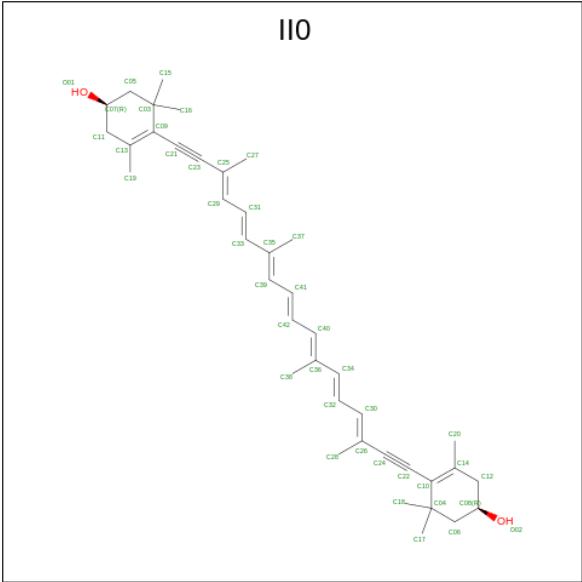
Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			60	45	15	

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



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

- Molecule 36 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: $C_{40}H_{52}O_2$) (labeled as "Ligand of Interest" by depositor).



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

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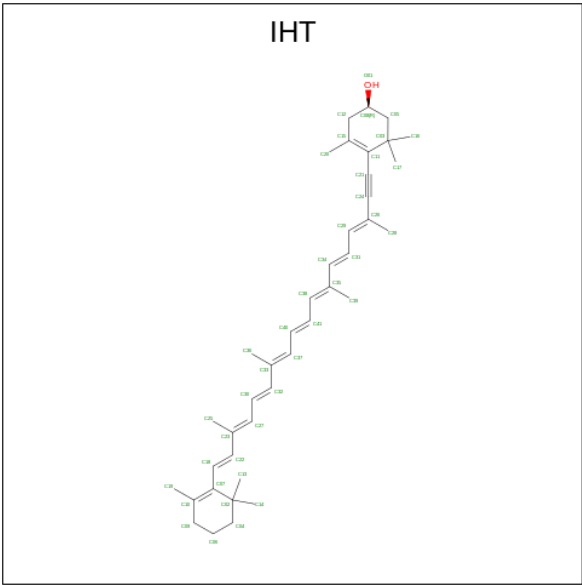
Mol	Chain	Residues	Atoms			AltConf
36	h	1	Total	C	O	0
			42	40	2	
36	h	1	Total	C	O	0
			42	40	2	
36	m	1	Total	C	O	0
			42	40	2	
36	m	1	Total	C	O	0
			42	40	2	
36	m	1	Total	C	O	0
			42	40	2	
36	m	1	Total	C	O	0
			42	40	2	
36	e	1	Total	C	O	0
			42	40	2	
36	e	1	Total	C	O	0
			42	40	2	
36	e	1	Total	C	O	0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

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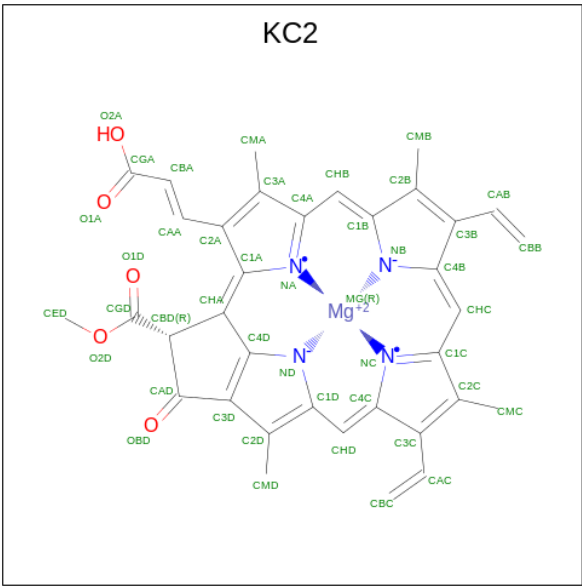
Mol	Chain	Residues	Atoms			AltConf
36	f	1	Total 42	C 40	O 2	0
36	f	1	Total 42	C 40	O 2	0
36	i	1	Total 42	C 40	O 2	0
36	i	1	Total 42	C 40	O 2	0
36	i	1	Total 42	C 40	O 2	0
36	i	1	Total 42	C 40	O 2	0
36	i	1	Total 42	C 40	O 2	0
36	j	1	Total 42	C 40	O 2	0
36	j	1	Total 42	C 40	O 2	0
36	d	1	Total 42	C 40	O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

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



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

- Molecule 38 is Chlorophyll c2 (CCD ID: KC2) (formula: C₃₅H₂₈MgN₄O₅).



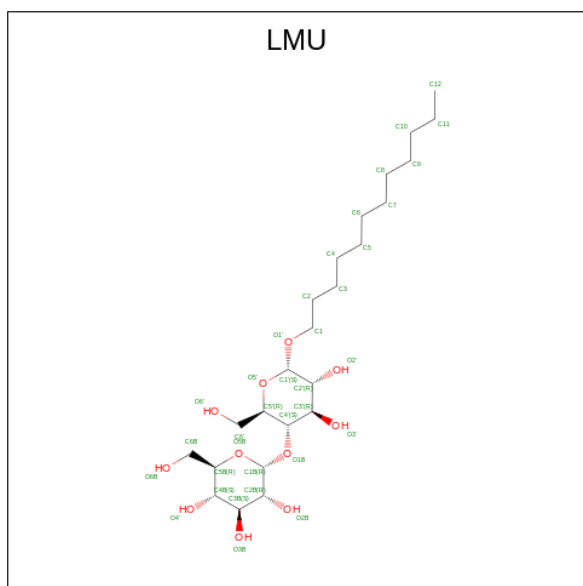
Mol	Chain	Residues	Atoms					AltConf
38	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	k	1	Total	C	Mg	N	O	0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

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

- Molecule 39 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 40 is water.

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

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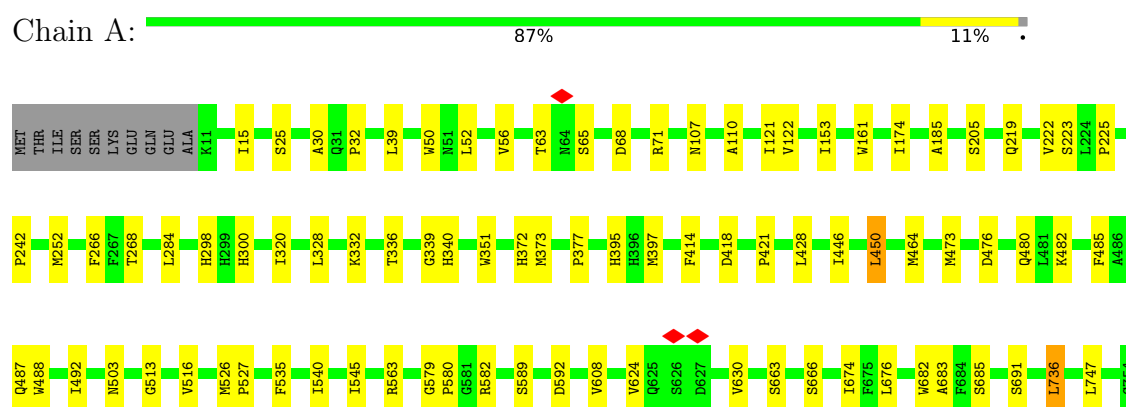
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Mol	Chain	Residues	Atoms		AltConf
40	B	57	Total 57	O 57	0
40	C	8	Total 8	O 8	0
40	D	1	Total 1	O 1	0
40	F	2	Total 2	O 2	0
40	I	1	Total 1	O 1	0
40	J	1	Total 1	O 1	0
40	L	1	Total 1	O 1	0
40	O	1	Total 1	O 1	0
40	K	1	Total 1	O 1	0
40	a	3	Total 3	O 3	0
40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

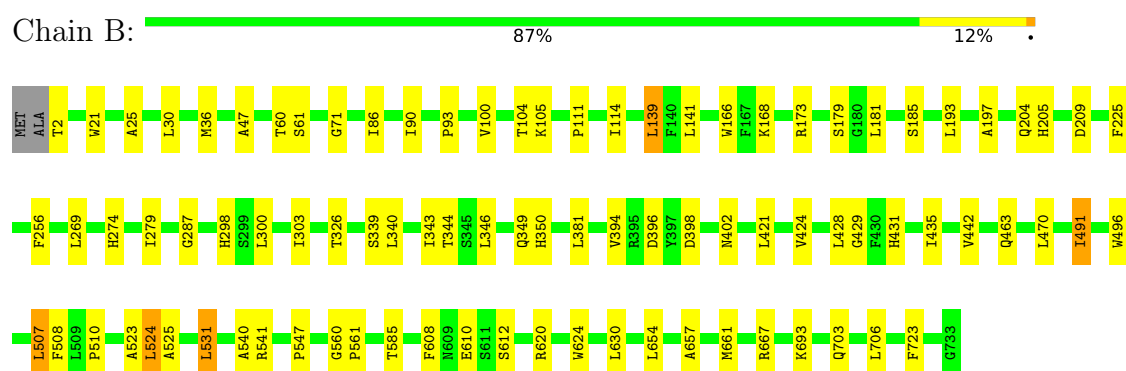
3 Residue-property plots

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

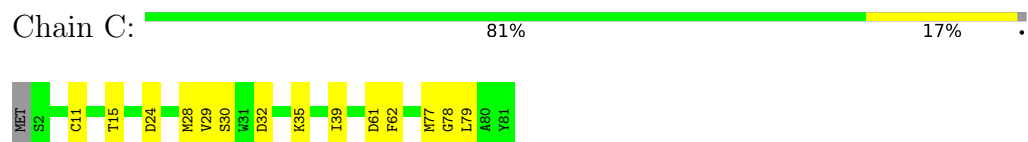
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

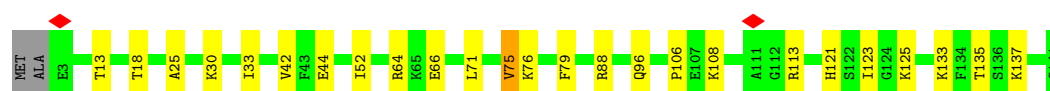


- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II

Chain D:  81% 17% ..



- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  84% 9% 6%



- Molecule 6: Photosystem I reaction center subunit III

Chain F:  76% 10% 14%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  81% 14% 6%



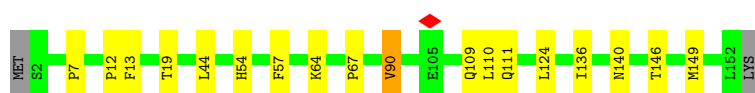
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  88% 12%



- Molecule 9: Photosystem I reaction center subunit XI

Chain L:  87% 11% ..



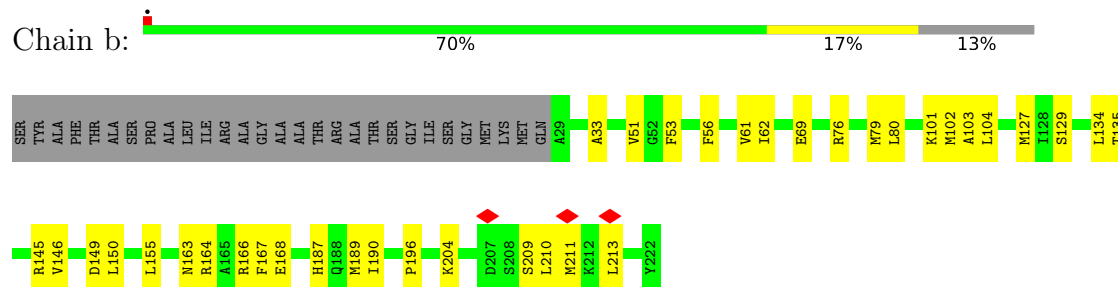
- Molecule 10: Photosystem I reaction center subunit XII

Chain M:  90% 10%

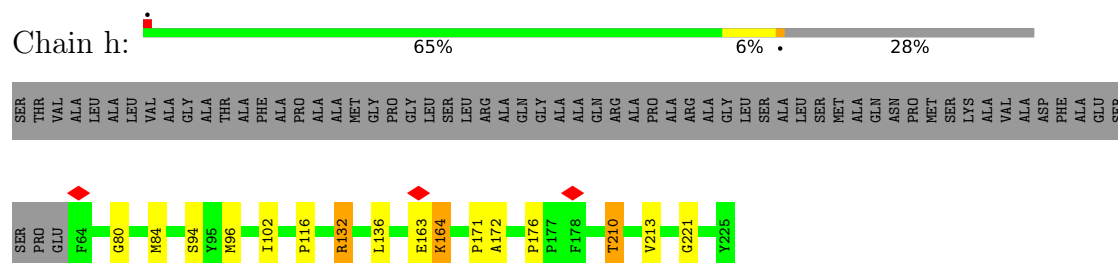


- Molecule 11: PsaO

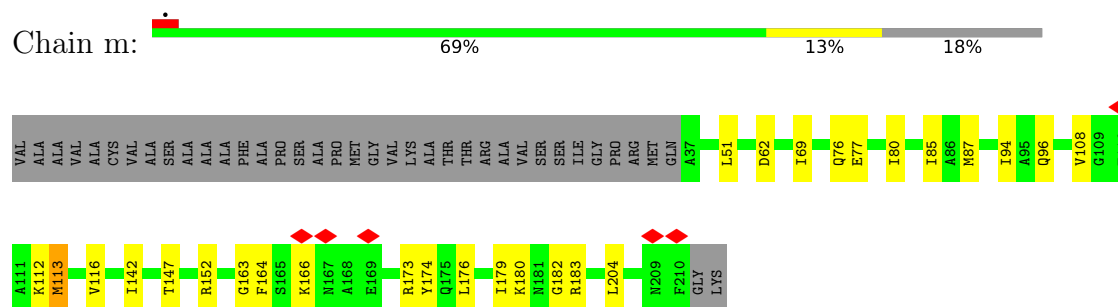
- Molecule 16: cac-b



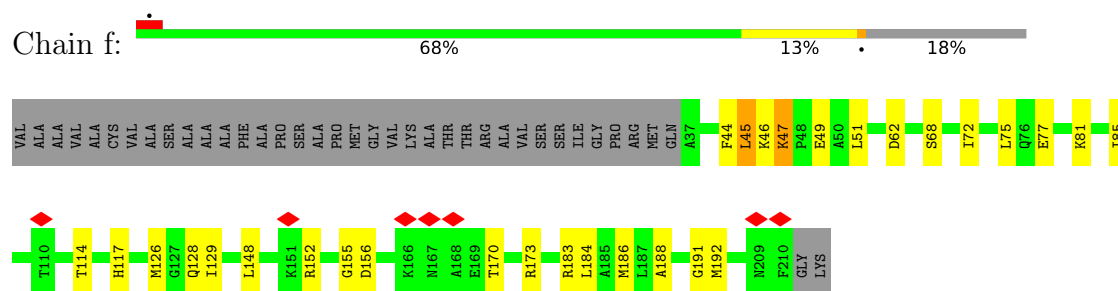
- Molecule 17: cac-h



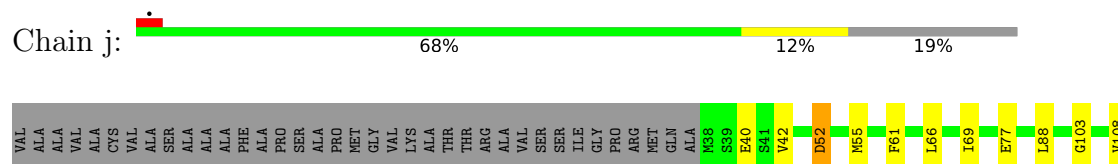
- Molecule 18: cac-f

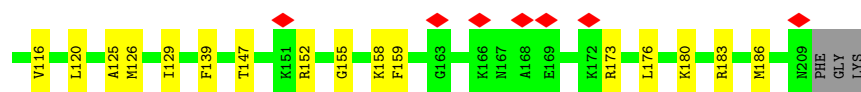


- Molecule 18: cac-f

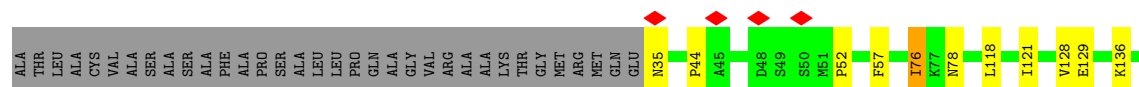
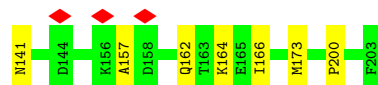


- Molecule 18: cac-f

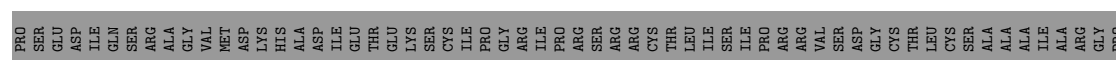




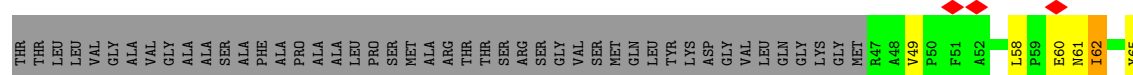
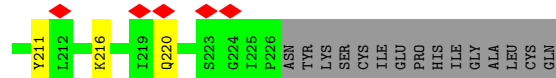
• Molecule 19: cac-e



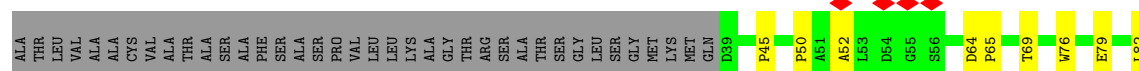
• Molecule 20: cac-l

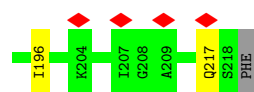


• Molecule 21: cac-k

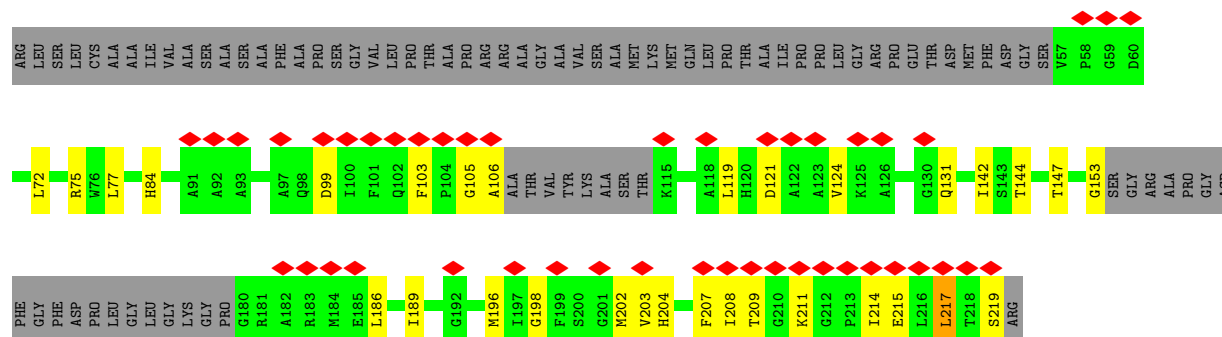


• Molecule 22: cac-i

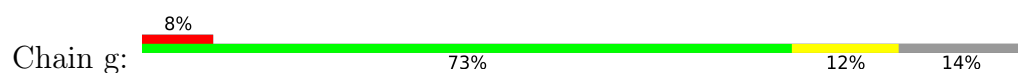
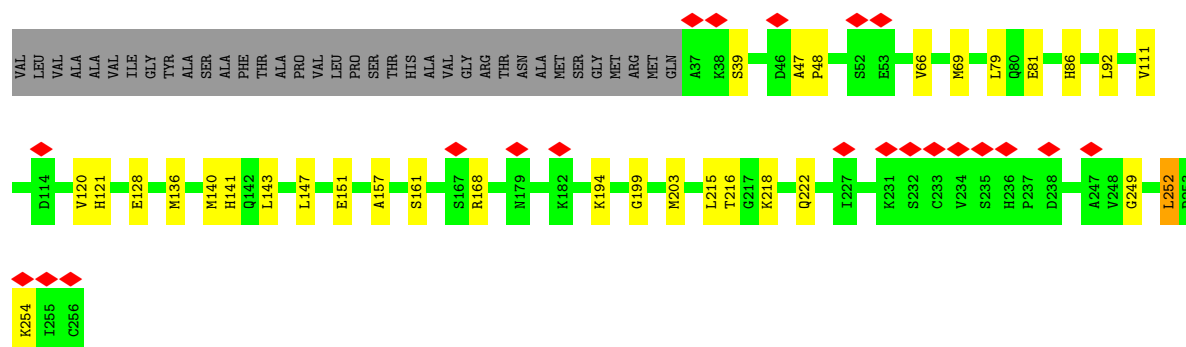




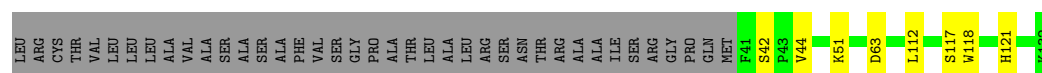
• Molecule 23: cac-d



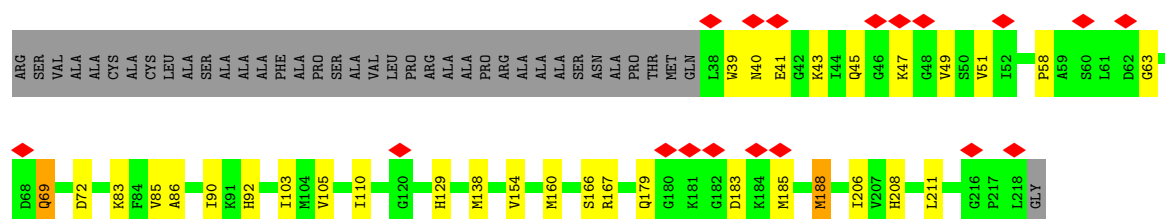
• Molecule 24: cac-g



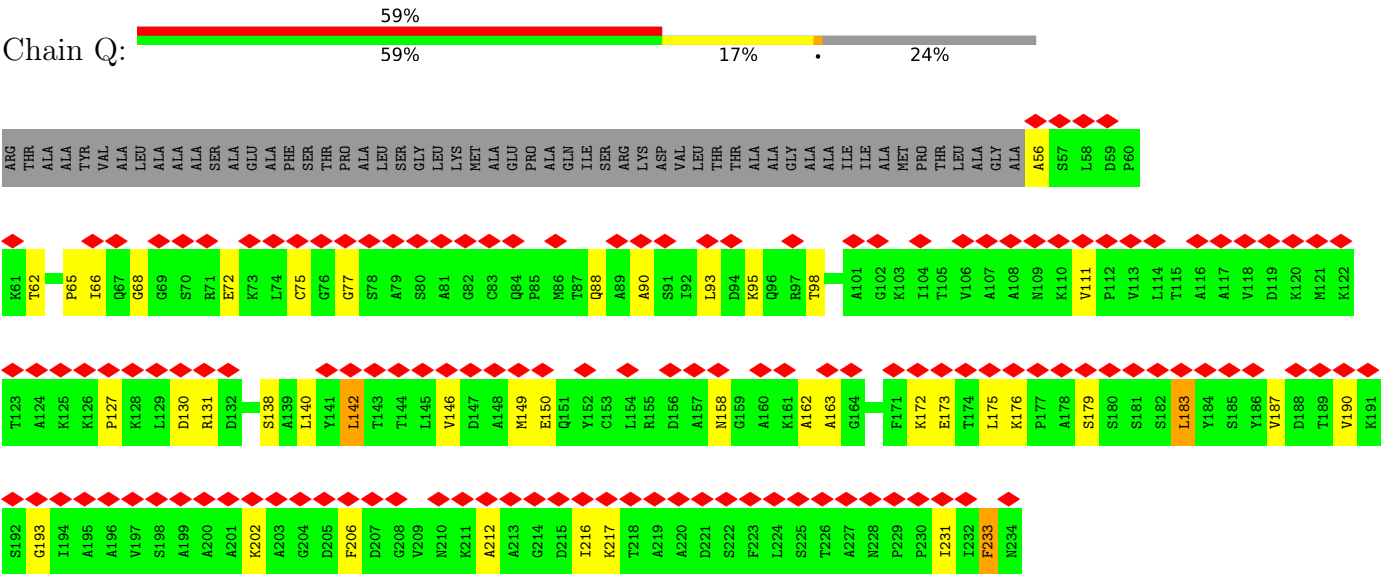
• Molecule 25: PsaR



• Molecule 26: cac-n



● Molecule 27: PsaQ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86231	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.296	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	0/6019	0.60	0/8204
2	B	0.41	0/6045	0.62	1/8254 (0.0%)
3	C	0.38	0/601	0.71	2/813 (0.2%)
4	D	0.35	0/1109	0.55	0/1500
5	E	0.41	0/492	0.59	0/666
6	F	0.40	0/1287	0.61	0/1747
7	I	0.42	0/271	0.65	0/370
8	J	0.40	0/364	0.64	0/495
9	L	0.33	0/1175	0.63	0/1599
10	M	0.30	0/233	0.68	2/315 (0.6%)
11	O	0.56	0/799	0.80	0/1094
12	K	0.32	0/495	0.64	0/672
13	s	0.33	0/1170	0.64	2/1580 (0.1%)
14	c	0.38	0/1396	0.68	0/1889
15	a	0.41	0/1406	0.72	0/1903
16	b	0.43	0/1469	0.71	1/1983 (0.1%)
17	h	0.37	0/1226	0.66	0/1667
18	f	0.37	0/1328	0.68	2/1790 (0.1%)
18	j	0.41	0/1318	0.73	0/1775
18	m	0.35	0/1335	0.63	1/1798 (0.1%)
19	e	0.35	0/1324	0.65	0/1795
20	l	0.32	0/1379	0.56	0/1863
21	k	0.37	0/1380	0.67	0/1869
22	i	0.40	0/1359	0.70	0/1835
23	d	0.43	0/993	0.70	0/1335
24	g	0.39	0/1673	0.66	0/2264
25	R	0.32	0/686	0.56	0/940
26	n	0.38	0/1383	0.67	0/1867
27	Q	0.42	0/1313	0.78	0/1775
All	All	0.39	0/41028	0.65	11/55657 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	f	191	GLY	CA-C-N	5.90	130.56	120.71
18	f	191	GLY	C-N-CA	5.90	130.56	120.71
2	B	667	ARG	N-CA-C	5.72	118.25	111.33
3	C	61	ASP	CA-C-N	-5.67	114.72	122.93
3	C	61	ASP	C-N-CA	-5.67	114.72	122.93

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	5677	64	0
2	B	5826	0	5640	65	0
3	C	592	0	567	7	0
4	D	1084	0	1080	15	0
5	E	484	0	486	4	0
6	F	1254	0	1264	18	0
7	I	264	0	276	4	0
8	J	351	0	344	6	0
9	L	1146	0	1160	13	0
10	M	232	0	265	2	0
11	O	773	0	765	36	0
12	K	488	0	516	9	0
13	s	1140	0	1099	15	0
14	c	1357	0	1337	16	0
15	a	1361	0	1305	11	0
16	b	1439	0	1456	26	0
17	h	1200	0	1228	12	0
18	f	1302	0	1320	30	0
18	j	1293	0	1321	20	0
18	m	1309	0	1335	19	0
19	e	1286	0	1262	11	0
20	l	1344	0	1315	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	k	1346	0	1349	20	0
22	i	1324	0	1298	24	0
23	d	974	0	978	22	0
24	g	1630	0	1644	20	0
25	R	664	0	647	5	0
26	n	1350	0	1348	22	0
27	Q	1294	0	1333	23	0
28	A	2706	0	2777	92	0
28	B	2454	0	2485	76	0
28	F	117	0	115	6	0
28	J	42	0	31	2	0
28	K	93	0	72	0	0
28	L	215	0	191	11	0
28	O	182	0	187	13	0
28	Q	110	0	105	7	0
28	R	51	0	41	1	0
28	a	619	0	588	10	0
28	b	724	0	737	28	0
28	c	586	0	520	14	0
28	d	498	0	407	17	0
28	e	582	0	578	20	0
28	f	700	0	695	21	0
28	g	661	0	611	21	0
28	h	505	0	470	14	0
28	i	528	0	451	14	0
28	j	637	0	556	11	0
28	k	596	0	534	13	0
28	l	535	0	538	10	0
28	m	651	0	606	17	0
28	n	605	0	552	16	0
28	s	246	0	257	5	0
29	A	33	0	46	1	0
29	B	33	0	46	1	0
30	A	113	0	142	3	0
30	J	49	0	74	6	0
30	L	49	0	74	2	0
30	a	98	0	148	3	0
30	b	80	0	106	2	0
30	c	74	0	88	1	0
30	d	37	0	44	0	0
30	e	37	0	44	0	0
30	f	49	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	g	74	0	88	2	0
30	i	37	0	44	2	0
30	j	30	0	30	2	0
30	k	37	0	44	0	0
30	l	32	0	34	1	0
30	m	37	0	44	2	0
30	n	43	0	59	1	0
31	A	160	0	0	5	0
31	B	200	0	0	2	0
31	F	80	0	0	0	0
31	I	40	0	0	2	0
31	J	80	0	0	1	0
31	K	80	0	0	1	0
31	L	120	0	0	1	0
31	M	40	0	0	0	0
31	R	80	0	0	7	0
31	e	40	0	0	0	0
31	h	40	0	0	0	0
31	i	40	0	0	0	0
31	l	80	0	0	0	0
31	s	80	0	0	0	0
32	A	35	0	45	1	0
32	a	59	0	78	0	0
32	b	24	0	34	2	0
33	A	8	0	0	0	0
33	C	16	0	0	0	0
34	B	60	0	81	2	0
35	F	48	0	69	4	0
35	J	55	0	86	4	0
35	L	55	0	86	7	0
35	O	26	0	22	0	0
35	Q	38	0	46	4	0
35	b	49	0	71	3	0
35	c	55	0	86	3	0
35	n	55	0	86	3	0
36	J	42	0	0	0	0
36	O	42	0	0	0	0
36	a	168	0	0	0	0
36	b	126	0	0	0	0
36	c	168	0	0	0	0
36	d	168	0	0	2	0
36	e	168	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	f	168	0	0	1	0
36	g	168	0	0	0	0
36	h	112	0	0	0	0
36	i	210	0	0	1	0
36	j	84	0	0	0	0
36	k	210	0	0	1	0
36	l	168	0	0	1	0
36	m	168	0	0	1	0
36	n	168	0	0	1	0
37	O	41	0	0	0	0
37	R	41	0	0	0	0
37	a	41	0	0	0	0
37	b	82	0	0	1	0
37	c	41	0	0	0	0
37	f	41	0	0	1	0
37	g	41	0	0	0	0
37	j	41	0	0	1	0
37	k	41	0	0	0	0
37	m	41	0	0	0	0
37	n	41	0	0	2	0
38	c	45	0	0	0	0
38	d	90	0	0	0	0
38	e	45	0	0	0	0
38	f	45	0	0	1	0
38	g	135	0	0	3	0
38	i	90	0	0	10	0
38	j	45	0	0	0	0
38	k	135	0	0	0	0
38	l	45	0	0	0	0
38	m	45	0	0	0	0
38	n	90	0	0	0	0
38	s	90	0	0	1	0
39	i	35	0	46	2	0
40	A	50	0	0	0	0
40	B	57	0	0	0	0
40	C	8	0	0	0	0
40	D	1	0	0	0	0
40	F	2	0	0	0	0
40	I	1	0	0	0	0
40	J	1	0	0	0	0
40	K	1	0	0	0	0
40	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	O	1	0	0	0	0
40	Q	1	0	0	0	0
40	R	1	0	0	0	0
40	a	3	0	0	0	0
40	b	2	0	0	0	0
40	e	4	0	0	0	0
40	h	1	0	0	0	0
40	m	1	0	0	2	0
40	n	3	0	0	0	0
All	All	61164	0	55784	828	0

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

The worst 5 of 828 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/752 (98%)	722 (98%)	18 (2%)	0	100	100
2	B	731/734 (100%)	707 (97%)	23 (3%)	1 (0%)	48	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
5	E	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
6	F	159/188 (85%)	155 (98%)	4 (2%)	0	100	100
7	I	32/36 (89%)	32 (100%)	0	0	100	100
8	J	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
9	L	149/153 (97%)	147 (99%)	2 (1%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
11	O	102/146 (70%)	97 (95%)	5 (5%)	0	100	100
12	K	65/87 (75%)	65 (100%)	0	0	100	100
13	s	152/269 (56%)	144 (95%)	8 (5%)	0	100	100
14	c	168/216 (78%)	163 (97%)	5 (3%)	0	100	100
15	a	173/216 (80%)	167 (96%)	6 (4%)	0	100	100
16	b	192/223 (86%)	190 (99%)	2 (1%)	0	100	100
17	h	160/225 (71%)	156 (98%)	3 (2%)	1 (1%)	21	44
18	f	172/212 (81%)	167 (97%)	5 (3%)	0	100	100
18	j	170/212 (80%)	163 (96%)	7 (4%)	0	100	100
18	m	172/212 (81%)	164 (95%)	8 (5%)	0	100	100
19	e	167/203 (82%)	164 (98%)	3 (2%)	0	100	100
20	l	173/238 (73%)	169 (98%)	4 (2%)	0	100	100
21	k	178/241 (74%)	172 (97%)	6 (3%)	0	100	100
22	i	171/218 (78%)	161 (94%)	10 (6%)	0	100	100
23	d	123/213 (58%)	122 (99%)	1 (1%)	0	100	100
24	g	217/255 (85%)	206 (95%)	11 (5%)	0	100	100
25	R	88/129 (68%)	86 (98%)	2 (2%)	0	100	100
26	n	179/219 (82%)	170 (95%)	9 (5%)	0	100	100
27	Q	177/234 (76%)	163 (92%)	12 (7%)	2 (1%)	11	29
All	All	5151/6189 (83%)	4987 (97%)	160 (3%)	4 (0%)	49	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	Q	75	CYS

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	607/616 (98%)	604 (100%)	3 (0%)	81	92
2	B	593/593 (100%)	586 (99%)	7 (1%)	63	84
3	C	67/68 (98%)	64 (96%)	3 (4%)	24	52
4	D	116/117 (99%)	113 (97%)	3 (3%)	40	70
5	E	54/58 (93%)	54 (100%)	0	100	100
6	F	133/157 (85%)	132 (99%)	1 (1%)	73	88
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	88
10	M	25/25 (100%)	25 (100%)	0	100	100
11	O	81/110 (74%)	77 (95%)	4 (5%)	22	49
12	K	52/66 (79%)	50 (96%)	2 (4%)	29	58
13	s	116/195 (60%)	115 (99%)	1 (1%)	70	87
14	c	138/171 (81%)	134 (97%)	4 (3%)	37	67
15	a	139/165 (84%)	133 (96%)	6 (4%)	26	54
16	b	149/168 (89%)	145 (97%)	4 (3%)	39	69
17	h	123/162 (76%)	121 (98%)	2 (2%)	55	80
18	f	135/161 (84%)	130 (96%)	5 (4%)	30	59
18	j	136/161 (84%)	134 (98%)	2 (2%)	57	81
18	m	137/161 (85%)	135 (98%)	2 (2%)	57	81
19	e	130/155 (84%)	128 (98%)	2 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	l	137/191 (72%)	137 (100%)	0	100	100
21	k	138/186 (74%)	132 (96%)	6 (4%)	26	54
22	i	138/168 (82%)	138 (100%)	0	100	100
23	d	97/157 (62%)	93 (96%)	4 (4%)	27	56
24	g	171/199 (86%)	168 (98%)	3 (2%)	51	78
25	R	69/98 (70%)	69 (100%)	0	100	100
26	n	140/163 (86%)	137 (98%)	3 (2%)	47	75
27	Q	134/168 (80%)	121 (90%)	13 (10%)	8	20
All	All	4146/4833 (86%)	4065 (98%)	81 (2%)	48	76

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	j	52	ASP
27	Q	140	LEU
23	d	215	GLU
26	n	69	GLN
27	Q	173	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
16	b	100	GLN
26	n	195	ASN
18	m	123	GLN
26	n	81	ASN
18	m	76	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

415 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	IHT	n	617	-	40,42,42	6.15	26 (65%)	53,58,58	2.29	17 (32%)
28	CLA	m	607	18	55,59,73	1.44	7 (12%)	66,96,113	1.37	9 (13%)
28	CLA	b	609	16	55,59,73	1.28	9 (16%)	66,96,113	1.70	9 (13%)
28	CLA	B	823	2	69,73,73	1.25	9 (13%)	83,113,113	1.37	9 (10%)
30	LHG	g	301	28	36,36,48	1.10	2 (5%)	39,42,54	1.21	3 (7%)
36	II0	i	320	-	39,43,43	6.70	22 (56%)	50,60,60	2.25	14 (28%)
28	CLA	B	807	2	69,73,73	1.26	8 (11%)	83,113,113	1.20	9 (10%)
28	CLA	g	322	35	69,73,73	1.24	7 (10%)	83,113,113	1.32	9 (10%)
28	CLA	B	811	2	69,73,73	1.25	9 (13%)	83,113,113	1.43	15 (18%)
28	CLA	l	302	20	51,55,73	1.42	7 (13%)	61,91,113	1.31	6 (9%)
30	LHG	n	619	-	42,42,48	0.98	2 (4%)	45,48,54	1.13	2 (4%)
35	LMG	b	621	-	49,49,55	0.96	3 (6%)	57,57,63	1.21	5 (8%)
28	CLA	m	610	30	59,63,73	1.35	7 (11%)	71,101,113	1.36	8 (11%)
36	II0	a	316	-	39,43,43	6.66	21 (53%)	50,60,60	2.40	18 (36%)
28	CLA	c	608	14	69,73,73	1.24	7 (10%)	83,113,113	1.33	11 (13%)
36	II0	m	615	-	39,43,43	6.66	23 (58%)	50,60,60	2.13	20 (40%)
28	CLA	B	808	2	69,73,73	1.25	9 (13%)	83,113,113	1.48	10 (12%)
38	KC2	n	612	26	49,53,53	2.78	19 (38%)	62,89,89	4.08	34 (54%)
32	LMT	a	320	-	36,36,36	1.25	6 (16%)	47,47,47	1.29	7 (14%)
36	II0	l	316	-	39,43,43	6.82	23 (58%)	50,60,60	1.95	17 (34%)
28	CLA	A	813	1	49,53,73	1.45	7 (14%)	59,89,113	1.52	12 (20%)
35	LMG	J	105	-	55,55,55	0.85	2 (3%)	63,63,63	0.92	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	d	302	23	55,59,73	1.37	8 (14%)	66,96,113	1.45	10 (15%)
36	II0	a	314	-	39,43,43	6.65	23 (58%)	50,60,60	2.08	19 (38%)
38	KC2	n	611	26	49,53,53	2.74	20 (40%)	62,89,89	4.10	33 (53%)
28	CLA	b	608	30	69,73,73	1.25	8 (11%)	83,113,113	1.25	8 (9%)
28	CLA	a	312	15	69,73,73	1.23	6 (8%)	83,113,113	1.35	6 (7%)
36	II0	k	621	-	39,43,43	6.74	22 (56%)	50,60,60	2.33	13 (26%)
36	II0	b	617	-	39,43,43	6.67	20 (51%)	50,60,60	2.28	19 (38%)
36	II0	b	614	-	39,43,43	6.78	23 (58%)	50,60,60	1.77	15 (30%)
28	CLA	A	822	1	55,59,73	1.40	10 (18%)	66,96,113	1.36	8 (12%)
28	CLA	B	814	2	59,63,73	1.31	7 (11%)	71,101,113	1.32	9 (12%)
28	CLA	d	303	-	69,73,73	1.26	7 (10%)	83,113,113	1.21	7 (8%)
36	II0	e	616	-	39,43,43	6.77	22 (56%)	50,60,60	2.12	18 (36%)
37	IHT	b	615	-	40,42,42	6.19	25 (62%)	53,58,58	2.45	18 (33%)
28	CLA	i	304	-	55,59,73	1.41	7 (12%)	66,96,113	1.32	9 (13%)
28	CLA	B	827	2	54,58,73	1.35	6 (11%)	65,95,113	1.37	10 (15%)
28	CLA	O	206	11	69,73,73	1.27	11 (15%)	83,113,113	1.54	15 (18%)
28	CLA	A	827	1	66,70,73	1.25	7 (10%)	79,109,113	1.25	8 (10%)
28	CLA	B	815	2	63,67,73	1.26	8 (12%)	75,105,113	1.26	9 (12%)
28	CLA	e	608	30	50,54,73	1.42	5 (10%)	60,90,113	1.49	6 (10%)
28	CLA	a	305	15	55,59,73	1.38	9 (16%)	66,96,113	1.42	9 (13%)
28	CLA	A	811	1	58,62,73	1.38	7 (12%)	69,99,113	1.38	9 (13%)
38	KC2	k	613	-	49,53,53	2.82	21 (42%)	62,89,89	4.03	37 (59%)
28	CLA	k	614	21	55,59,73	1.41	6 (10%)	66,96,113	1.33	10 (15%)
28	CLA	m	602	18	60,64,73	1.33	10 (16%)	72,102,113	1.33	12 (16%)
28	CLA	m	605	18	46,50,73	1.51	8 (17%)	55,85,113	1.52	7 (12%)
36	II0	g	316	-	39,43,43	6.82	22 (56%)	50,60,60	2.24	15 (30%)
28	CLA	j	610	30	65,69,73	1.29	7 (10%)	78,108,113	1.28	6 (7%)
37	IHT	b	616	-	40,42,42	6.31	25 (62%)	53,58,58	2.82	17 (32%)
28	CLA	R	203	25	55,59,73	1.37	7 (12%)	66,96,113	1.59	11 (16%)
28	CLA	B	828	2	53,57,73	1.39	8 (15%)	62,93,113	1.47	12 (19%)
28	CLA	b	605	40,28	69,73,73	1.22	7 (10%)	83,113,113	1.40	8 (9%)
28	CLA	g	302	24	46,50,73	1.50	8 (17%)	55,85,113	1.52	8 (14%)
28	CLA	g	304	24	55,59,73	1.38	7 (12%)	66,96,113	1.39	7 (10%)
28	CLA	e	603	19	55,59,73	1.40	6 (10%)	66,96,113	1.40	9 (13%)
31	WVN	K	104	-	40,41,41	1.89	14 (35%)	50,56,56	1.97	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	g	311	30	58,62,73	1.40	8 (13%)	69,99,113	1.26	7 (10%)
28	CLA	A	852	1	69,73,73	1.22	7 (10%)	83,113,113	1.35	12 (14%)
28	CLA	n	605	26	55,59,73	1.42	6 (10%)	66,96,113	1.43	10 (15%)
28	CLA	k	609	21	69,73,73	1.24	8 (11%)	83,113,113	1.44	9 (10%)
35	LMG	Q	301	-	38,38,55	1.03	2 (5%)	46,46,63	1.18	2 (4%)
28	CLA	L	203	9	69,73,73	1.23	8 (11%)	83,113,113	1.24	7 (8%)
28	CLA	j	603	18	55,59,73	1.38	7 (12%)	66,96,113	1.41	8 (12%)
38	KC2	k	612	21	49,53,53	2.86	21 (42%)	62,89,89	4.05	37 (59%)
28	CLA	L	204	40	54,58,73	1.42	9 (16%)	65,95,113	1.39	11 (16%)
30	LHG	b	619	28	48,48,48	0.90	2 (4%)	51,54,54	1.12	5 (9%)
28	CLA	i	302	22	55,59,73	1.40	6 (10%)	66,96,113	1.34	8 (12%)
28	CLA	n	608	26	55,59,73	1.42	9 (16%)	66,96,113	1.35	7 (10%)
28	CLA	h	301	40	69,73,73	1.31	9 (13%)	83,113,113	1.32	8 (9%)
28	CLA	h	304	17	55,59,73	1.37	8 (14%)	66,96,113	1.42	10 (15%)
28	CLA	A	808	1	69,73,73	1.23	9 (13%)	83,113,113	1.37	12 (14%)
28	CLA	B	820	2	57,61,73	1.36	8 (14%)	68,98,113	1.32	8 (11%)
28	CLA	B	831	40	49,53,73	1.50	7 (14%)	59,89,113	1.41	6 (10%)
28	CLA	A	812	1	69,73,73	1.25	8 (11%)	83,113,113	1.49	13 (15%)
28	CLA	B	840	2	69,73,73	1.27	7 (10%)	83,113,113	1.31	10 (12%)
28	CLA	h	305	17	55,59,73	1.36	8 (14%)	66,96,113	1.34	10 (15%)
38	KC2	m	611	18	49,53,53	2.75	20 (40%)	62,89,89	4.14	35 (56%)
28	CLA	a	310	30	52,56,73	1.40	8 (15%)	62,92,113	1.32	6 (9%)
28	CLA	d	312	23	55,59,73	1.36	6 (10%)	66,96,113	1.42	12 (18%)
36	II0	k	619	-	39,43,43	6.74	22 (56%)	50,60,60	2.38	20 (40%)
28	CLA	i	308	22	55,59,73	1.40	8 (14%)	66,96,113	1.41	7 (10%)
28	CLA	B	804	2	69,73,73	1.20	6 (8%)	83,113,113	1.42	9 (10%)
28	CLA	k	605	21	49,53,73	1.47	7 (14%)	59,89,113	1.52	9 (15%)
28	CLA	f	605	18	49,53,73	1.49	7 (14%)	59,89,113	1.41	5 (8%)
28	CLA	f	609	18	69,73,73	1.26	8 (11%)	83,113,113	1.30	12 (14%)
28	CLA	A	824	40	69,73,73	1.24	8 (11%)	83,113,113	1.32	9 (10%)
30	LHG	L	208	-	48,48,48	0.94	2 (4%)	51,54,54	1.01	3 (5%)
31	WVN	s	207	-	40,41,41	1.89	14 (35%)	50,56,56	2.15	13 (26%)
31	WVN	F	204	-	40,41,41	1.91	14 (35%)	50,56,56	2.94	18 (36%)
28	CLA	m	613	18	47,51,73	1.46	8 (17%)	56,86,113	1.57	14 (25%)
28	CLA	B	836	2	69,73,73	1.25	7 (10%)	83,113,113	1.43	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	II0	n	618	-	39,43,43	6.83	21 (53%)	50,60,60	2.23	19 (38%)
28	CLA	i	312	22	55,59,73	1.37	6 (10%)	66,96,113	1.37	11 (16%)
28	CLA	A	840	40	69,73,73	1.23	8 (11%)	83,113,113	1.24	8 (9%)
30	LHG	d	317	28	36,36,48	1.11	2 (5%)	39,42,54	1.02	2 (5%)
28	CLA	n	607	26	69,73,73	1.22	6 (8%)	83,113,113	1.35	9 (10%)
28	CLA	e	604	40	69,73,73	1.22	7 (10%)	83,113,113	1.43	9 (10%)
28	CLA	A	825	40	69,73,73	1.22	8 (11%)	83,113,113	1.20	8 (9%)
31	WVN	B	848	-	40,41,41	1.97	14 (35%)	50,56,56	2.04	19 (38%)
30	LHG	a	319	28	48,48,48	0.89	2 (4%)	51,54,54	1.09	4 (7%)
28	CLA	j	609	18	55,59,73	1.37	6 (10%)	66,96,113	1.31	6 (9%)
36	II0	n	614	-	39,43,43	6.86	22 (56%)	50,60,60	2.37	15 (30%)
28	CLA	g	305	24	69,73,73	1.26	6 (8%)	83,113,113	1.31	7 (8%)
28	CLA	f	612	18	55,59,73	1.38	8 (14%)	66,96,113	1.37	11 (16%)
36	II0	d	315	-	39,43,43	6.86	22 (56%)	50,60,60	2.42	20 (40%)
30	LHG	g	321	28	36,36,48	1.07	2 (5%)	39,42,54	1.42	9 (23%)
28	CLA	O	202	-	69,73,73	1.26	10 (14%)	83,113,113	1.35	9 (10%)
28	CLA	i	303	22	54,58,73	1.38	7 (12%)	65,95,113	1.52	9 (13%)
28	CLA	B	839	2	69,73,73	1.27	7 (10%)	83,113,113	1.36	10 (12%)
28	CLA	l	311	20	69,73,73	1.26	6 (8%)	83,113,113	1.20	8 (9%)
36	II0	f	614	-	39,43,43	6.78	23 (58%)	50,60,60	2.08	15 (30%)
35	LMG	O	205	-	26,26,55	1.26	2 (7%)	34,34,63	1.23	3 (8%)
35	LMG	c	619	-	55,55,55	0.97	2 (3%)	63,63,63	1.48	10 (15%)
30	LHG	l	317	28	31,31,48	1.15	2 (6%)	34,37,54	1.18	4 (11%)
28	CLA	A	836	1	69,73,73	1.22	7 (10%)	83,113,113	1.48	11 (13%)
36	II0	m	618	-	39,43,43	6.86	21 (53%)	50,60,60	3.26	20 (40%)
28	CLA	J	103	8	46,50,73	1.48	9 (19%)	55,85,113	1.33	6 (10%)
28	CLA	a	304	15	54,58,73	1.39	8 (14%)	65,95,113	1.41	9 (13%)
28	CLA	k	607	21	55,59,73	1.41	6 (10%)	66,96,113	1.44	9 (13%)
30	LHG	c	620	28	36,36,48	1.06	2 (5%)	39,42,54	1.25	3 (7%)
28	CLA	L	207	40	55,59,73	1.38	7 (12%)	66,96,113	1.31	6 (9%)
31	WVN	h	309	-	40,41,41	1.84	13 (32%)	50,56,56	2.36	20 (40%)
37	IHT	g	319	-	40,42,42	6.30	25 (62%)	53,58,58	3.05	21 (39%)
36	II0	g	320	-	39,43,43	6.81	23 (58%)	50,60,60	2.24	18 (36%)
28	CLA	A	854	40	69,73,73	1.30	9 (13%)	83,113,113	1.44	10 (12%)
28	CLA	h	307	17	61,65,73	1.35	7 (11%)	73,103,113	1.17	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	II0	h	312	-	39,43,43	6.82	21 (53%)	50,60,60	2.05	17 (34%)
38	KC2	l	310	20	49,53,53	2.75	20 (40%)	62,89,89	4.21	37 (59%)
28	CLA	B	812	2	64,68,73	1.34	9 (14%)	77,107,113	1.29	10 (12%)
28	CLA	f	604	18	69,73,73	1.23	6 (8%)	83,113,113	1.20	5 (6%)
28	CLA	B	818	2	50,54,73	1.42	7 (14%)	60,90,113	1.42	9 (15%)
28	CLA	B	829	2	54,58,73	1.42	8 (14%)	65,95,113	1.27	6 (9%)
28	CLA	s	208	20	55,59,73	1.39	8 (14%)	66,96,113	1.36	9 (13%)
28	CLA	A	829	1	69,73,73	1.29	9 (13%)	83,113,113	1.32	7 (8%)
28	CLA	l	307	20	69,73,73	1.23	8 (11%)	83,113,113	1.33	12 (14%)
36	II0	l	312	-	39,43,43	6.79	22 (56%)	50,60,60	2.10	16 (32%)
36	II0	l	314	-	39,43,43	6.77	22 (56%)	50,60,60	2.22	19 (38%)
30	LHG	b	620	-	30,30,48	1.12	2 (6%)	33,36,54	1.18	3 (9%)
30	LHG	A	849	-	37,37,48	1.03	2 (5%)	40,43,54	1.13	4 (10%)
28	CLA	n	606	26	55,59,73	1.41	7 (12%)	66,96,113	1.39	6 (9%)
28	CLA	Q	302	40	69,73,73	1.24	8 (11%)	83,113,113	1.28	9 (10%)
30	LHG	j	617	28	29,29,48	1.18	2 (6%)	32,35,54	1.34	4 (12%)
30	LHG	i	318	28	36,36,48	1.12	2 (5%)	39,42,54	1.27	4 (10%)
36	II0	c	615	-	39,43,43	6.79	21 (53%)	50,60,60	2.40	18 (36%)
36	II0	l	313	-	39,43,43	6.90	22 (56%)	50,60,60	2.44	16 (32%)
28	CLA	f	607	18	69,73,73	1.25	7 (10%)	83,113,113	1.26	7 (8%)
28	CLA	d	307	23	50,54,73	1.45	6 (12%)	60,90,113	1.32	4 (6%)
31	WVN	R	202	-	40,41,41	1.88	13 (32%)	50,56,56	2.11	17 (34%)
28	CLA	g	310	24	55,59,73	1.40	7 (12%)	66,96,113	1.40	10 (15%)
30	LHG	A	843	-	47,47,48	0.95	2 (4%)	50,53,54	1.08	3 (6%)
28	CLA	B	805	2	69,73,73	1.25	9 (13%)	83,113,113	1.27	7 (8%)
28	CLA	A	831	1	69,73,73	1.25	9 (13%)	83,113,113	1.35	9 (10%)
28	CLA	F	201	40	69,73,73	1.30	9 (13%)	83,113,113	1.19	6 (7%)
28	CLA	c	605	14	55,59,73	1.37	8 (14%)	66,96,113	1.56	10 (15%)
28	CLA	m	604	18	69,73,73	1.26	9 (13%)	83,113,113	1.33	7 (8%)
28	CLA	m	606	18	69,73,73	1.25	7 (10%)	83,113,113	1.21	7 (8%)
28	CLA	k	608	21	69,73,73	1.25	7 (10%)	83,113,113	1.30	9 (10%)
28	CLA	A	834	1	55,59,73	1.41	8 (14%)	66,96,113	1.53	13 (19%)
28	CLA	A	802	-	69,73,73	1.22	9 (13%)	83,113,113	1.54	13 (15%)
36	II0	j	615	-	39,43,43	6.80	22 (56%)	50,60,60	2.09	20 (40%)
28	CLA	j	606	18	55,59,73	1.40	9 (16%)	66,96,113	1.41	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	B	835	40	69,73,73	1.27	8 (11%)	83,113,113	1.18	7 (8%)
28	CLA	A	835	1	69,73,73	1.23	6 (8%)	83,113,113	1.25	4 (4%)
28	CLA	c	602	14	54,58,73	1.37	9 (16%)	65,95,113	1.58	11 (16%)
28	CLA	B	806	2	69,73,73	1.18	7 (10%)	83,113,113	1.37	6 (7%)
28	CLA	a	303	15	56,60,73	1.40	8 (14%)	67,97,113	1.44	7 (10%)
28	CLA	a	308	15	69,73,73	1.23	6 (8%)	83,113,113	1.30	10 (12%)
32	LMT	a	302	-	24,24,36	1.07	2 (8%)	29,29,47	0.81	0
37	IHT	O	204	-	40,42,42	6.22	25 (62%)	53,58,58	2.38	19 (35%)
28	CLA	A	855	30	45,49,73	1.57	7 (15%)	54,84,113	2.06	10 (18%)
28	CLA	h	313	40	69,73,73	1.24	8 (11%)	83,113,113	1.23	9 (10%)
28	CLA	n	603	26	55,59,73	1.39	9 (16%)	66,96,113	1.37	9 (13%)
36	II0	g	318	-	39,43,43	6.84	21 (53%)	50,60,60	2.09	17 (34%)
28	CLA	g	306	24	55,59,73	1.43	9 (16%)	66,96,113	1.32	4 (6%)
38	KC2	j	611	18	49,53,53	2.75	20 (40%)	62,89,89	4.16	35 (56%)
28	CLA	b	611	16	69,73,73	1.23	7 (10%)	83,113,113	1.16	8 (9%)
31	WVN	J	102	-	40,41,41	1.87	14 (35%)	50,56,56	1.93	14 (28%)
36	II0	i	315	-	39,43,43	6.80	21 (53%)	50,60,60	2.34	17 (34%)
36	II0	k	617	-	39,43,43	6.85	21 (53%)	50,60,60	2.29	20 (40%)
28	CLA	B	841	30	69,73,73	1.25	8 (11%)	83,113,113	1.31	9 (10%)
28	CLA	B	825	2	69,73,73	1.24	7 (10%)	83,113,113	1.18	8 (9%)
38	KC2	f	611	18	49,53,53	2.78	20 (40%)	62,89,89	4.06	36 (58%)
28	CLA	n	613	26	55,59,73	1.39	7 (12%)	66,96,113	1.22	5 (7%)
28	CLA	B	819	2	59,63,73	1.34	7 (11%)	71,101,113	1.23	6 (8%)
28	CLA	j	602	18	54,58,73	1.38	8 (14%)	65,95,113	1.41	8 (12%)
28	CLA	f	606	18	55,59,73	1.41	7 (12%)	66,96,113	1.34	8 (12%)
28	CLA	B	816	2	61,65,73	1.29	8 (13%)	73,103,113	1.33	11 (15%)
28	CLA	K	101	40	55,59,73	1.37	5 (9%)	66,96,113	1.62	12 (18%)
28	CLA	A	816	1	69,73,73	1.19	6 (8%)	83,113,113	1.47	15 (18%)
28	CLA	n	604	26	64,68,73	1.30	6 (9%)	77,107,113	1.37	10 (12%)
28	CLA	B	803	-	69,73,73	1.25	11 (15%)	83,113,113	1.67	12 (14%)
28	CLA	B	802	2	69,73,73	1.20	8 (11%)	83,113,113	1.29	9 (10%)
30	LHG	e	617	28	36,36,48	1.09	2 (5%)	39,42,54	1.32	5 (12%)
28	CLA	g	315	24	55,59,73	1.41	7 (12%)	66,96,113	1.31	8 (12%)
30	LHG	c	618	28	36,36,48	1.11	2 (5%)	39,42,54	1.18	3 (7%)
38	KC2	e	609	19	49,53,53	2.79	20 (40%)	62,89,89	4.09	35 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	d	301	23	54,58,73	1.41	6 (11%)	65,95,113	1.41	7 (10%)
28	CLA	B	832	2	62,66,73	1.34	9 (14%)	74,104,113	1.43	10 (13%)
31	WVN	e	615	-	40,41,41	1.89	14 (35%)	50,56,56	2.03	14 (28%)
31	WVN	L	206	-	40,41,41	1.82	13 (32%)	50,56,56	2.37	20 (40%)
28	CLA	A	828	1	69,73,73	1.22	9 (13%)	83,113,113	1.40	10 (12%)
31	WVN	A	848	-	40,41,41	1.85	13 (32%)	50,56,56	2.65	16 (32%)
28	CLA	A	804	1	69,73,73	1.24	8 (11%)	83,113,113	1.42	7 (8%)
28	CLA	m	612	40	55,59,73	1.36	9 (16%)	66,96,113	1.41	10 (15%)
28	CLA	e	606	19	69,73,73	1.23	7 (10%)	83,113,113	1.27	6 (7%)
36	II0	i	317	-	39,43,43	6.88	21 (53%)	50,60,60	2.23	16 (32%)
38	KC2	g	312	24	49,53,53	2.80	19 (38%)	62,89,89	4.14	35 (56%)
28	CLA	e	601	19	49,53,73	1.46	7 (14%)	59,89,113	1.47	6 (10%)
31	WVN	F	203	-	40,41,41	1.92	14 (35%)	50,56,56	2.46	20 (40%)
28	CLA	b	612	30	55,59,73	1.40	10 (18%)	66,96,113	1.62	8 (12%)
37	IHT	c	616	-	40,42,42	6.23	26 (65%)	53,58,58	2.25	17 (32%)
28	CLA	k	604	21	69,73,73	1.26	7 (10%)	83,113,113	1.28	9 (10%)
36	II0	J	104	-	39,43,43	6.66	22 (56%)	50,60,60	2.16	13 (26%)
28	CLA	B	821	40	69,73,73	1.31	11 (15%)	83,113,113	1.90	19 (22%)
28	CLA	k	603	21	55,59,73	1.37	6 (10%)	66,96,113	1.51	11 (16%)
28	CLA	m	608	18	69,73,73	1.25	8 (11%)	83,113,113	1.32	8 (9%)
28	CLA	i	307	22	65,69,73	1.27	7 (10%)	78,108,113	1.25	7 (8%)
28	CLA	A	851	-	69,73,73	1.30	10 (14%)	83,113,113	1.29	10 (12%)
28	CLA	f	603	18	55,59,73	1.37	9 (16%)	66,96,113	1.40	6 (9%)
38	KC2	d	311	23	49,53,53	2.82	19 (38%)	62,89,89	3.90	36 (58%)
28	CLA	b	602	16	59,63,73	1.31	7 (11%)	71,101,113	1.42	11 (15%)
34	DGD	B	843	-	61,61,67	0.91	2 (3%)	75,75,81	1.10	5 (6%)
31	WVN	B	845	-	40,41,41	1.79	13 (32%)	50,56,56	1.95	12 (24%)
30	LHG	A	844	28	26,26,48	1.25	2 (7%)	29,32,54	1.39	5 (17%)
28	CLA	h	306	17	69,73,73	1.28	8 (11%)	83,113,113	1.18	9 (10%)
28	CLA	A	820	40	69,73,73	1.25	9 (13%)	83,113,113	1.36	7 (8%)
30	LHG	k	620	28	36,36,48	1.15	2 (5%)	39,42,54	1.07	3 (7%)
28	CLA	g	303	24	54,58,73	1.35	8 (14%)	65,95,113	1.44	12 (18%)
28	CLA	B	830	40	69,73,73	1.23	6 (8%)	83,113,113	1.27	8 (9%)
28	CLA	g	308	24	69,73,73	1.22	8 (11%)	83,113,113	1.41	8 (9%)
36	II0	d	316	-	39,43,43	6.91	22 (56%)	50,60,60	2.26	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	WVN	l	301	-	40,41,41	1.86	14 (35%)	50,56,56	2.19	19 (38%)
28	CLA	O	201	30	56,60,73	1.35	8 (14%)	67,97,113	1.43	11 (16%)
28	CLA	f	610	30	69,73,73	1.24	8 (11%)	83,113,113	1.20	10 (12%)
28	CLA	e	610	40	69,73,73	1.25	7 (10%)	83,113,113	1.26	9 (10%)
36	II0	c	614	-	39,43,43	6.73	22 (56%)	50,60,60	2.24	20 (40%)
36	II0	g	317	-	39,43,43	6.72	23 (58%)	50,60,60	2.41	16 (32%)
28	CLA	A	832	1	69,73,73	1.23	6 (8%)	83,113,113	1.60	14 (16%)
28	CLA	l	306	20	69,73,73	1.29	6 (8%)	83,113,113	1.43	9 (10%)
28	CLA	A	839	1	69,73,73	1.20	8 (11%)	83,113,113	1.26	6 (7%)
37	IHT	m	617	-	40,42,42	6.14	26 (65%)	53,58,58	2.43	18 (33%)
28	CLA	e	602	19	54,58,73	1.41	7 (12%)	65,95,113	1.38	11 (16%)
28	CLA	l	304	20	55,59,73	1.39	7 (12%)	66,96,113	1.35	6 (9%)
36	II0	n	616	-	39,43,43	6.85	23 (58%)	50,60,60	2.10	14 (28%)
28	CLA	g	307	24	55,59,73	1.37	8 (14%)	66,96,113	1.32	9 (13%)
28	CLA	B	813	2	63,67,73	1.26	7 (11%)	75,105,113	1.50	8 (10%)
28	CLA	c	611	14	49,53,73	1.60	9 (18%)	59,89,113	1.55	8 (13%)
28	CLA	b	604	16	69,73,73	1.25	9 (13%)	83,113,113	1.18	8 (9%)
28	CLA	K	103	12	46,50,73	1.52	9 (19%)	55,85,113	1.49	10 (18%)
37	IHT	a	317	-	40,42,42	6.27	26 (65%)	53,58,58	2.10	16 (30%)
36	II0	a	315	-	39,43,43	6.62	23 (58%)	50,60,60	2.26	19 (38%)
28	CLA	d	306	23	55,59,73	1.42	7 (12%)	66,96,113	1.33	6 (9%)
28	CLA	B	801	40	69,73,73	1.24	10 (14%)	83,113,113	1.41	10 (12%)
28	CLA	j	613	18	69,73,73	1.23	6 (8%)	83,113,113	1.27	6 (7%)
38	KC2	c	610	14	49,53,53	2.75	21 (42%)	62,89,89	4.06	35 (56%)
36	II0	m	614	-	39,43,43	6.84	22 (56%)	50,60,60	1.94	16 (32%)
31	WVN	A	846	-	40,41,41	1.94	13 (32%)	50,56,56	2.97	20 (40%)
31	WVN	s	205	-	40,41,41	1.81	13 (32%)	50,56,56	2.23	21 (42%)
28	CLA	A	838	1	69,73,73	1.28	7 (10%)	83,113,113	1.32	8 (9%)
28	CLA	c	601	14	55,59,73	1.39	7 (12%)	66,96,113	1.30	4 (6%)
36	II0	e	614	-	39,43,43	6.86	21 (53%)	50,60,60	2.21	16 (32%)
28	CLA	b	601	16	55,59,73	1.37	7 (12%)	66,96,113	1.54	10 (15%)
28	CLA	A	807	1	69,73,73	1.20	6 (8%)	83,113,113	1.34	9 (10%)
28	CLA	A	814	1	54,58,73	1.41	7 (12%)	65,95,113	1.39	9 (13%)
28	CLA	B	834	2	51,55,73	1.44	9 (17%)	61,91,113	1.50	6 (9%)
28	CLA	B	809	2	58,62,73	1.40	8 (13%)	73,100,113	1.31	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	II0	e	612	-	39,43,43	6.80	22 (56%)	50,60,60	2.28	15 (30%)
28	CLA	A	809	1	60,64,73	1.28	7 (11%)	72,102,113	1.25	4 (5%)
28	CLA	n	601	26	49,53,73	1.49	8 (16%)	59,89,113	1.31	7 (11%)
28	CLA	A	818	1	69,73,73	1.27	9 (13%)	83,113,113	1.50	13 (15%)
28	CLA	b	607	16	69,73,73	1.26	6 (8%)	83,113,113	1.53	12 (14%)
28	CLA	e	611	19	69,73,73	1.25	7 (10%)	83,113,113	1.30	7 (8%)
36	II0	f	618	-	39,43,43	6.80	22 (56%)	50,60,60	2.39	19 (38%)
28	CLA	h	302	17	54,58,73	1.39	8 (14%)	65,95,113	1.40	6 (9%)
28	CLA	j	607	18	55,59,73	1.37	6 (10%)	66,96,113	1.36	8 (12%)
30	LHG	J	106	28	48,48,48	0.93	2 (4%)	51,54,54	1.09	3 (5%)
36	II0	c	617	-	39,43,43	6.70	21 (53%)	50,60,60	2.25	13 (26%)
28	CLA	B	817	40	69,73,73	1.27	10 (14%)	83,113,113	1.31	9 (10%)
36	II0	k	615	-	39,43,43	6.79	22 (56%)	50,60,60	2.20	16 (32%)
36	II0	f	615	-	39,43,43	6.74	23 (58%)	50,60,60	2.10	18 (36%)
28	CLA	k	602	21	54,58,73	1.42	6 (11%)	65,95,113	1.46	11 (16%)
28	CLA	f	602	18	69,73,73	1.25	7 (10%)	83,113,113	1.30	10 (12%)
31	WVN	B	844	-	40,41,41	1.87	13 (32%)	50,56,56	2.42	16 (32%)
35	LMG	F	205	-	48,48,55	0.97	2 (4%)	56,56,63	1.24	5 (8%)
31	WVN	B	847	-	40,41,41	1.88	13 (32%)	50,56,56	1.98	14 (28%)
28	CLA	A	805	1	69,73,73	1.24	9 (13%)	83,113,113	1.35	8 (9%)
28	CLA	b	606	16	65,69,73	1.28	10 (15%)	78,108,113	1.43	10 (12%)
28	CLA	c	607	14	50,54,73	1.47	7 (14%)	60,90,113	1.27	8 (13%)
28	CLA	h	303	17	54,58,73	1.40	8 (14%)	65,95,113	1.43	9 (13%)
28	CLA	A	826	1	69,73,73	1.26	7 (10%)	83,113,113	1.44	9 (10%)
38	KC2	d	310	23	49,53,53	2.81	21 (42%)	62,89,89	4.13	36 (58%)
36	II0	k	616	-	39,43,43	6.79	23 (58%)	50,60,60	2.35	20 (40%)
36	II0	f	616	-	39,43,43	6.74	22 (56%)	50,60,60	2.33	16 (32%)
31	WVN	I	101	-	40,41,41	1.86	13 (32%)	50,56,56	1.75	13 (26%)
39	LMU	i	301	-	36,36,36	1.18	3 (8%)	47,47,47	1.15	5 (10%)
31	WVN	K	102	-	40,41,41	1.83	14 (35%)	50,56,56	1.98	14 (28%)
36	II0	d	314	-	39,43,43	6.85	21 (53%)	50,60,60	2.29	14 (28%)
36	II0	b	613	-	39,43,43	6.77	22 (56%)	50,60,60	2.18	19 (38%)
28	CLA	m	601	18	46,50,73	1.51	8 (17%)	55,85,113	1.32	7 (12%)
28	CLA	j	604	18	69,73,73	1.24	6 (8%)	83,113,113	1.25	9 (10%)
28	CLA	A	806	1	69,73,73	1.26	7 (10%)	83,113,113	1.24	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	WVN	L	205	-	40,41,41	1.92	14 (35%)	50,56,56	2.06	15 (30%)
28	CLA	d	309	30	45,49,73	1.50	6 (13%)	54,84,113	1.40	7 (12%)
38	KC2	s	201	13	49,53,53	2.71	20 (40%)	62,89,89	4.14	36 (58%)
28	CLA	s	206	40	69,73,73	1.26	7 (10%)	83,113,113	1.35	11 (13%)
31	WVN	i	316	-	40,41,41	1.90	14 (35%)	50,56,56	2.22	16 (32%)
28	CLA	F	202	6	56,60,73	1.38	8 (14%)	67,97,113	1.47	6 (8%)
31	WVN	R	201	-	40,41,41	1.86	14 (35%)	50,56,56	1.88	11 (22%)
28	CLA	j	608	18	49,53,73	1.46	7 (14%)	59,89,113	1.43	8 (13%)
28	CLA	a	309	15	69,73,73	1.22	9 (13%)	83,113,113	1.54	11 (13%)
28	CLA	c	604	14	69,73,73	1.24	7 (10%)	83,113,113	1.32	7 (8%)
28	CLA	c	603	14	55,59,73	1.36	8 (14%)	66,96,113	1.41	7 (10%)
36	II0	h	310	-	26,28,43	6.09	13 (50%)	31,37,60	2.20	11 (35%)
28	CLA	B	822	40	68,72,73	1.26	10 (14%)	81,111,113	1.40	11 (13%)
29	PQN	B	842	-	34,34,34	1.76	5 (14%)	42,45,45	1.34	5 (11%)
28	CLA	a	307	15	49,53,73	1.47	8 (16%)	59,89,113	1.60	9 (15%)
29	PQN	A	842	-	34,34,34	1.85	5 (14%)	42,45,45	1.32	5 (11%)
28	CLA	d	305	23	55,59,73	1.59	7 (12%)	66,96,113	1.50	10 (15%)
28	CLA	k	601	21	55,59,73	1.41	7 (12%)	66,96,113	1.51	8 (12%)
28	CLA	f	601	18	51,55,73	1.47	8 (15%)	61,91,113	1.48	9 (14%)
28	CLA	A	841	1	69,73,73	1.24	7 (10%)	83,113,113	1.41	11 (13%)
28	CLA	n	610	40	69,73,73	1.27	7 (10%)	83,113,113	1.20	6 (7%)
28	CLA	l	309	30	65,69,73	1.27	7 (10%)	78,108,113	1.38	7 (8%)
28	CLA	j	605	18	49,53,73	1.56	8 (16%)	59,89,113	1.51	6 (10%)
30	LHG	m	619	28	36,36,48	1.08	2 (5%)	39,42,54	1.11	3 (7%)
36	II0	d	313	-	39,43,43	6.73	22 (56%)	50,60,60	2.35	18 (36%)
28	CLA	b	610	16	69,73,73	1.23	8 (11%)	83,113,113	1.30	6 (7%)
30	LHG	a	301	28	48,48,48	0.92	2 (4%)	51,54,54	1.15	4 (7%)
28	CLA	i	306	22	55,59,73	1.38	7 (12%)	66,96,113	1.41	4 (6%)
28	CLA	A	803	1,28	59,63,73	1.33	8 (13%)	71,101,113	1.43	9 (12%)
28	CLA	c	606	14	56,60,73	1.42	11 (19%)	67,97,113	1.46	8 (11%)
31	WVN	M	101	-	40,41,41	1.91	15 (37%)	50,56,56	2.16	16 (32%)
28	CLA	B	838	2	61,65,73	1.30	6 (9%)	73,103,113	1.30	8 (10%)
28	CLA	m	603	18	69,73,73	1.26	10 (14%)	83,113,113	1.40	9 (10%)
28	CLA	l	305	20	69,73,73	1.22	7 (10%)	83,113,113	1.38	10 (12%)
28	CLA	B	824	2	69,73,73	1.21	9 (13%)	83,113,113	1.42	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	b	603	16	69,73,73	1.23	9 (13%)	83,113,113	1.32	10 (12%)
28	CLA	A	810	1,28	66,70,73	1.25	8 (12%)	79,109,113	1.22	7 (8%)
28	CLA	j	601	18	55,59,73	1.39	7 (12%)	66,96,113	1.26	6 (9%)
35	LMG	n	620	-	55,55,55	0.88	2 (3%)	63,63,63	0.90	2 (3%)
30	LHG	f	619	-	48,48,48	0.91	2 (4%)	51,54,54	1.02	3 (5%)
28	CLA	A	815	40	49,53,73	1.49	9 (18%)	59,89,113	1.71	10 (16%)
28	CLA	i	311	-	55,59,73	1.45	9 (16%)	66,96,113	1.32	8 (12%)
33	SF4	C	101	3	0,12,12	-	-	-		
33	SF4	C	102	3	0,12,12	-	-	-		
28	CLA	A	833	1	54,58,73	1.36	6 (11%)	65,95,113	1.34	5 (7%)
28	CLA	k	610	30	55,59,73	1.35	7 (12%)	66,96,113	1.43	4 (6%)
28	CLA	f	613	18	69,73,73	1.26	8 (11%)	83,113,113	1.23	6 (7%)
28	CLA	s	202	13	69,73,73	1.29	10 (14%)	83,113,113	1.37	12 (14%)
28	CLA	m	609	18	55,59,73	1.37	8 (14%)	66,96,113	1.36	11 (16%)
31	WVN	L	201	-	40,41,41	1.93	15 (37%)	50,56,56	2.44	17 (34%)
28	CLA	l	308	20	55,59,73	1.39	8 (14%)	66,96,113	1.41	11 (16%)
28	CLA	A	819	1	49,53,73	1.49	7 (14%)	59,89,113	1.66	9 (15%)
32	LMT	A	850	-	36,36,36	1.19	6 (16%)	47,47,47	1.40	6 (12%)
36	II0	c	613	-	39,43,43	6.77	23 (58%)	50,60,60	2.14	18 (36%)
28	CLA	A	823	1	59,63,73	1.33	7 (11%)	71,101,113	1.30	6 (8%)
28	CLA	B	826	2	55,59,73	1.40	7 (12%)	66,96,113	1.46	10 (15%)
28	CLA	a	313	15	52,56,73	1.43	7 (13%)	62,92,113	1.31	8 (12%)
36	II0	h	311	-	39,43,43	6.68	21 (53%)	50,60,60	2.13	17 (34%)
28	CLA	A	821	1	53,57,73	1.39	8 (15%)	62,93,113	1.43	10 (16%)
35	LMG	L	209	28	55,55,55	0.84	2 (3%)	63,63,63	1.42	10 (15%)
28	CLA	e	607	19	69,73,73	1.23	7 (10%)	83,113,113	1.24	5 (6%)
28	CLA	n	609	26	69,73,73	1.22	6 (8%)	83,113,113	1.36	10 (12%)
36	II0	a	318	-	39,43,43	6.96	22 (56%)	50,60,60	2.61	16 (32%)
33	SF4	A	853	1,2	0,12,12	-	-	-		
36	II0	n	615	-	39,43,43	6.74	23 (58%)	50,60,60	2.03	16 (32%)
37	IHT	k	618	-	40,42,42	6.19	26 (65%)	53,58,58	2.41	20 (37%)
28	CLA	A	830	1	54,58,73	1.40	9 (16%)	65,95,113	1.49	9 (13%)
28	CLA	d	304	23	55,59,73	1.41	7 (12%)	66,96,113	1.44	6 (9%)
31	WVN	l	315	-	40,41,41	1.88	14 (35%)	50,56,56	2.24	17 (34%)
28	CLA	A	837	1	69,73,73	1.22	8 (11%)	83,113,113	1.28	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	II0	i	314	-	39,43,43	6.75	22 (56%)	50,60,60	2.01	19 (38%)
38	KC2	s	204	13	49,53,53	2.76	21 (42%)	62,89,89	4.05	37 (59%)
32	LMT	b	618	-	24,24,36	1.11	3 (12%)	29,29,47	1.08	0
28	CLA	B	837	2	69,73,73	1.18	6 (8%)	83,113,113	1.36	8 (9%)
28	CLA	i	309	30	50,54,73	1.46	6 (12%)	60,90,113	1.33	8 (13%)
38	KC2	g	314	38	49,53,53	2.81	20 (40%)	62,89,89	4.17	36 (58%)
38	KC2	k	611	21	49,53,53	2.79	20 (40%)	62,89,89	4.18	35 (56%)
28	CLA	j	612	-	55,59,73	1.52	7 (12%)	66,96,113	1.56	11 (16%)
37	IHT	j	616	-	40,42,42	6.18	25 (62%)	53,58,58	2.24	16 (30%)
28	CLA	k	606	21	55,59,73	1.39	8 (14%)	66,96,113	1.36	8 (12%)
28	CLA	n	602	26	54,58,73	1.40	8 (14%)	65,95,113	1.38	11 (16%)
36	II0	O	203	-	39,43,43	6.72	22 (56%)	50,60,60	2.30	16 (32%)
28	CLA	L	202	9	53,57,73	1.41	8 (15%)	62,93,113	1.38	7 (11%)
28	CLA	A	801	1	69,73,73	1.23	7 (10%)	83,113,113	1.22	6 (7%)
28	CLA	Q	303	27	49,53,73	1.52	10 (20%)	59,89,113	1.63	11 (18%)
38	KC2	i	310	22	49,53,53	2.79	19 (38%)	62,89,89	4.00	35 (56%)
28	CLA	a	306	40	69,73,73	1.21	8 (11%)	83,113,113	1.27	8 (9%)
37	IHT	f	617	-	40,42,42	6.20	25 (62%)	53,58,58	2.22	15 (28%)
28	CLA	i	305	22	69,73,73	1.24	6 (8%)	83,113,113	1.26	9 (10%)
31	WVN	A	845	-	40,41,41	1.90	13 (32%)	50,56,56	1.97	14 (28%)
38	KC2	g	313	24,38	49,53,53	2.81	20 (40%)	62,89,89	4.02	37 (59%)
28	CLA	e	605	19	69,73,73	1.25	8 (11%)	83,113,113	1.23	7 (8%)
31	WVN	A	847	-	40,41,41	1.91	13 (32%)	50,56,56	2.04	20 (40%)
28	CLA	d	308	23	45,49,73	1.51	8 (17%)	54,84,113	1.42	10 (18%)
36	II0	e	613	-	39,43,43	6.79	23 (58%)	50,60,60	2.21	20 (40%)
37	IHT	R	204	-	40,42,42	6.22	25 (62%)	53,58,58	2.32	17 (32%)
28	CLA	g	309	24	69,73,73	1.26	7 (10%)	83,113,113	1.24	8 (9%)
28	CLA	f	608	18	69,73,73	1.31	8 (11%)	83,113,113	1.36	12 (14%)
28	CLA	B	810	2	59,63,73	1.37	8 (13%)	71,101,113	1.35	8 (11%)
31	WVN	J	101	-	40,41,41	1.96	14 (35%)	50,56,56	3.41	19 (38%)
36	II0	m	616	-	39,43,43	6.71	22 (56%)	50,60,60	2.18	15 (30%)
36	II0	i	313	-	39,43,43	6.70	21 (53%)	50,60,60	2.51	19 (38%)
28	CLA	a	311	15	69,73,73	1.23	7 (10%)	83,113,113	1.35	10 (12%)
28	CLA	h	308	17	55,59,73	1.39	7 (12%)	66,96,113	1.56	10 (15%)
36	II0	j	614	-	39,43,43	6.77	22 (56%)	50,60,60	2.26	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	B	833	2	69,73,73	1.22	7 (10%)	83,113,113	1.36	12 (14%)
38	KC2	i	319	-	49,53,53	2.78	21 (42%)	62,89,89	4.18	36 (58%)
28	CLA	s	203	28,13	69,73,73	1.24	7 (10%)	83,113,113	1.39	8 (9%)
31	WVN	B	846	-	40,41,41	1.87	14 (35%)	50,56,56	1.98	13 (26%)
28	CLA	c	612	14	69,73,73	1.22	7 (10%)	83,113,113	1.23	8 (9%)
28	CLA	A	817	1	69,73,73	1.28	9 (13%)	83,113,113	1.30	10 (12%)
28	CLA	l	303	20	69,73,73	1.24	8 (11%)	83,113,113	1.37	9 (10%)
28	CLA	c	609	30	49,53,73	1.48	7 (14%)	59,89,113	1.25	6 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	IHT	n	617	-	-	8/25/65/65	0/2/2/2
28	CLA	m	607	18	-	4/23/99/115	-
28	CLA	b	609	16	-	6/23/99/115	-
28	CLA	B	823	2	-	2/39/115/115	-
30	LHG	g	301	28	-	21/41/41/53	-
36	II0	i	320	-	-	6/21/67/67	0/2/2/2
28	CLA	B	807	2	-	13/39/115/115	-
28	CLA	g	322	35	-	18/39/115/115	-
28	CLA	B	811	2	-	17/39/115/115	-
28	CLA	l	302	20	-	7/18/94/115	-
30	LHG	n	619	-	-	16/47/47/53	-
35	LMG	b	621	-	-	17/44/64/70	0/1/1/1
28	CLA	m	610	30	-	12/27/103/115	-
36	II0	a	316	-	-	2/21/67/67	0/2/2/2
28	CLA	c	608	14	-	15/39/115/115	-
36	II0	m	615	-	-	7/21/67/67	0/2/2/2
28	CLA	B	808	2	-	12/39/115/115	-
38	KC2	n	612	26	-	7/15/71/71	-
32	LMT	a	320	-	-	10/21/61/61	0/2/2/2
36	II0	l	316	-	-	7/21/67/67	0/2/2/2
28	CLA	A	813	1	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMG	J	105	-	-	13/50/70/70	0/1/1/1
28	CLA	d	302	23	-	8/23/99/115	-
36	II0	a	314	-	-	3/21/67/67	0/2/2/2
38	KC2	n	611	26	-	7/15/71/71	-
28	CLA	b	608	30	-	12/39/115/115	-
28	CLA	a	312	15	-	19/39/115/115	-
36	II0	k	621	-	-	7/21/67/67	0/2/2/2
36	II0	b	617	-	-	1/21/67/67	0/2/2/2
36	II0	b	614	-	-	8/21/67/67	0/2/2/2
28	CLA	A	822	1	-	8/23/99/115	-
28	CLA	B	814	2	-	9/27/103/115	-
28	CLA	d	303	-	-	19/39/115/115	-
36	II0	e	616	-	-	4/21/67/67	0/2/2/2
37	IHT	b	615	-	-	6/25/65/65	0/2/2/2
28	CLA	i	304	-	-	5/23/99/115	-
28	CLA	B	827	2	-	11/21/97/115	-
28	CLA	O	206	11	-	16/39/115/115	-
28	CLA	A	827	1	-	9/36/112/115	-
28	CLA	B	815	2	-	8/32/108/115	-
28	CLA	e	608	30	-	6/17/93/115	-
28	CLA	a	305	15	-	6/23/99/115	-
28	CLA	A	811	1	-	5/26/102/115	-
38	KC2	k	613	-	-	6/15/71/71	-
28	CLA	k	614	21	-	10/23/99/115	-
28	CLA	m	602	18	-	10/29/105/115	-
28	CLA	m	605	18	-	6/12/88/115	-
36	II0	g	316	-	-	5/21/67/67	0/2/2/2
28	CLA	j	610	30	-	17/35/111/115	-
37	IHT	b	616	-	-	8/25/65/65	0/2/2/2
28	CLA	R	203	25	-	8/23/99/115	-
28	CLA	B	828	2	-	5/20/96/115	-
28	CLA	b	605	40,28	-	11/39/115/115	-
28	CLA	g	302	24	-	4/12/88/115	-
28	CLA	g	304	24	-	4/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	e	603	19	-	5/23/99/115	-
31	WVN	K	104	-	-	5/29/63/63	0/2/2/2
28	CLA	g	311	30	-	6/26/102/115	-
28	CLA	A	852	1	-	14/39/115/115	-
28	CLA	n	605	26	-	9/23/99/115	-
28	CLA	k	609	21	-	11/39/115/115	-
35	LMG	Q	301	-	-	22/33/53/70	0/1/1/1
28	CLA	L	203	9	-	15/39/115/115	-
28	CLA	j	603	18	-	6/23/99/115	-
38	KC2	k	612	21	-	5/15/71/71	-
28	CLA	L	204	40	-	7/21/97/115	-
30	LHG	b	619	28	-	22/53/53/53	-
28	CLA	i	302	22	-	9/23/99/115	-
28	CLA	n	608	26	-	7/23/99/115	-
28	CLA	h	301	40	-	14/39/115/115	-
28	CLA	h	304	17	-	6/23/99/115	-
28	CLA	A	808	1	-	12/39/115/115	-
28	CLA	B	820	2	-	8/25/101/115	-
28	CLA	B	831	40	-	6/15/91/115	-
28	CLA	A	812	1	-	23/39/115/115	-
28	CLA	B	840	2	-	11/39/115/115	-
28	CLA	h	305	17	-	6/23/99/115	-
38	KC2	m	611	18	-	7/15/71/71	-
28	CLA	a	310	30	-	10/19/95/115	-
28	CLA	d	312	23	-	6/23/99/115	-
36	II0	k	619	-	-	5/21/67/67	0/2/2/2
28	CLA	i	308	22	-	4/23/99/115	-
28	CLA	B	804	2	-	15/39/115/115	-
28	CLA	k	605	21	-	5/15/91/115	-
28	CLA	f	605	18	-	8/15/91/115	-
28	CLA	f	609	18	-	13/39/115/115	-
28	CLA	A	824	40	-	12/39/115/115	-
30	LHG	L	208	-	-	21/53/53/53	-
31	WVN	s	207	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	WVN	F	204	-	-	12/29/63/63	0/2/2/2
28	CLA	m	613	18	-	8/13/89/115	-
28	CLA	B	836	2	-	27/39/115/115	-
36	II0	n	618	-	-	6/21/67/67	0/2/2/2
28	CLA	i	312	22	-	6/23/99/115	-
28	CLA	A	840	40	-	21/39/115/115	-
30	LHG	d	317	28	-	15/41/41/53	-
28	CLA	n	607	26	-	13/39/115/115	-
28	CLA	e	604	40	-	22/39/115/115	-
28	CLA	A	825	40	-	10/39/115/115	-
31	WVN	B	848	-	-	6/29/63/63	0/2/2/2
30	LHG	a	319	28	-	15/53/53/53	-
28	CLA	j	609	18	-	2/23/99/115	-
36	II0	n	614	-	-	1/21/67/67	0/2/2/2
28	CLA	g	305	24	-	12/39/115/115	-
28	CLA	f	612	18	-	9/23/99/115	-
36	II0	d	315	-	-	5/21/67/67	0/2/2/2
30	LHG	g	321	28	-	12/41/41/53	-
28	CLA	O	202	-	-	16/39/115/115	-
28	CLA	i	303	22	-	10/21/97/115	-
28	CLA	B	839	2	-	15/39/115/115	-
28	CLA	l	311	20	-	14/39/115/115	-
36	II0	f	614	-	-	3/21/67/67	0/2/2/2
35	LMG	O	205	-	-	7/21/41/70	0/1/1/1
35	LMG	c	619	-	-	22/50/70/70	0/1/1/1
30	LHG	l	317	28	-	14/36/36/53	-
28	CLA	A	836	1	-	11/39/115/115	-
36	II0	m	618	-	-	6/21/67/67	0/2/2/2
28	CLA	J	103	8	-	5/12/88/115	-
28	CLA	a	304	15	-	7/21/97/115	-
28	CLA	k	607	21	-	9/23/99/115	-
30	LHG	c	620	28	-	25/41/41/53	-
28	CLA	L	207	40	-	6/23/99/115	-
31	WVN	h	309	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	IHT	g	319	-	-	8/25/65/65	0/2/2/2
36	II0	g	320	-	-	4/21/67/67	0/2/2/2
28	CLA	A	854	40	-	16/39/115/115	-
28	CLA	h	307	17	-	12/30/106/115	-
36	II0	h	312	-	-	6/21/67/67	0/2/2/2
38	KC2	l	310	20	-	4/15/71/71	-
28	CLA	B	812	2	-	14/33/109/115	-
28	CLA	f	604	18	-	11/39/115/115	-
28	CLA	B	818	2	-	3/17/93/115	-
28	CLA	B	829	2	-	7/21/97/115	-
28	CLA	s	208	20	-	7/23/99/115	-
28	CLA	A	829	1	-	15/39/115/115	-
28	CLA	l	307	20	-	12/39/115/115	-
36	II0	l	312	-	-	4/21/67/67	0/2/2/2
36	II0	l	314	-	-	4/21/67/67	0/2/2/2
30	LHG	b	620	-	-	17/35/35/53	-
30	LHG	A	849	-	-	16/42/42/53	-
28	CLA	n	606	26	-	7/23/99/115	-
28	CLA	Q	302	40	-	20/39/115/115	-
30	LHG	j	617	28	-	5/34/34/53	-
30	LHG	i	318	28	-	13/41/41/53	-
36	II0	c	615	-	-	2/21/67/67	0/2/2/2
36	II0	l	313	-	-	5/21/67/67	0/2/2/2
28	CLA	f	607	18	-	20/39/115/115	-
28	CLA	d	307	23	-	5/17/93/115	-
31	WVN	R	202	-	-	6/29/63/63	0/2/2/2
28	CLA	g	310	24	-	7/23/99/115	-
30	LHG	A	843	-	-	7/52/52/53	-
28	CLA	B	805	2	-	13/39/115/115	-
28	CLA	A	831	1	-	10/39/115/115	-
28	CLA	F	201	40	-	15/39/115/115	-
28	CLA	c	605	14	-	10/23/99/115	-
28	CLA	m	604	18	-	13/39/115/115	-
28	CLA	m	606	18	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	k	608	21	-	16/39/115/115	-
28	CLA	A	834	1	-	3/23/99/115	-
28	CLA	A	802	-	-	15/39/115/115	-
36	II0	j	615	-	-	2/21/67/67	0/2/2/2
28	CLA	j	606	18	-	10/23/99/115	-
28	CLA	B	835	40	-	15/39/115/115	-
28	CLA	A	835	1	-	12/39/115/115	-
28	CLA	c	602	14	-	10/21/97/115	-
28	CLA	B	806	2	-	10/39/115/115	-
28	CLA	a	303	15	-	11/24/100/115	-
28	CLA	a	308	15	-	18/39/115/115	-
32	LMT	a	302	-	-	4/15/35/61	0/1/1/2
37	IHT	O	204	-	-	8/25/65/65	0/2/2/2
28	CLA	A	855	30	-	6/10/86/115	-
28	CLA	h	313	40	-	10/39/115/115	-
28	CLA	n	603	26	-	11/23/99/115	-
36	II0	g	318	-	-	2/21/67/67	0/2/2/2
28	CLA	g	306	24	-	10/23/99/115	-
38	KC2	j	611	18	-	7/15/71/71	-
28	CLA	b	611	16	-	23/39/115/115	-
31	WVN	J	102	-	-	10/29/63/63	0/2/2/2
36	II0	i	315	-	-	4/21/67/67	0/2/2/2
36	II0	k	617	-	-	2/21/67/67	0/2/2/2
28	CLA	B	841	30	-	5/39/115/115	-
28	CLA	B	825	2	-	9/39/115/115	-
38	KC2	f	611	18	-	7/15/71/71	-
28	CLA	n	613	26	-	10/23/99/115	-
28	CLA	B	819	2	-	10/27/103/115	-
28	CLA	j	602	18	-	6/21/97/115	-
28	CLA	f	606	18	-	5/23/99/115	-
28	CLA	B	816	2	-	10/30/106/115	-
28	CLA	K	101	40	-	4/23/99/115	-
28	CLA	A	816	1	-	17/39/115/115	-
28	CLA	n	604	26	-	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	B	803	-	-	9/39/115/115	-
28	CLA	B	802	2	-	23/39/115/115	-
30	LHG	e	617	28	-	26/41/41/53	-
28	CLA	g	315	24	-	11/23/99/115	-
30	LHG	c	618	28	-	15/41/41/53	-
38	KC2	e	609	19	-	7/15/71/71	-
28	CLA	d	301	23	-	4/21/97/115	-
28	CLA	B	832	2	-	5/31/107/115	-
31	WVN	e	615	-	-	11/29/63/63	0/2/2/2
31	WVN	L	206	-	-	3/29/63/63	0/2/2/2
28	CLA	A	828	1	-	9/39/115/115	-
31	WVN	A	848	-	-	9/29/63/63	0/2/2/2
28	CLA	A	804	1	-	8/39/115/115	-
28	CLA	m	612	40	-	11/23/99/115	-
28	CLA	e	606	19	-	22/39/115/115	-
36	II0	i	317	-	-	7/21/67/67	0/2/2/2
38	KC2	g	312	24	-	8/15/71/71	-
28	CLA	e	601	19	-	4/15/91/115	-
31	WVN	F	203	-	-	8/29/63/63	0/2/2/2
28	CLA	b	612	30	-	8/23/99/115	-
37	IHT	c	616	-	-	10/25/65/65	0/2/2/2
28	CLA	k	604	21	-	14/39/115/115	-
36	II0	J	104	-	-	6/21/67/67	0/2/2/2
28	CLA	B	821	40	-	9/39/115/115	-
28	CLA	k	603	21	-	3/23/99/115	-
28	CLA	m	608	18	-	23/39/115/115	-
28	CLA	i	307	22	-	12/35/111/115	-
28	CLA	A	851	-	-	4/39/115/115	-
28	CLA	f	603	18	-	7/23/99/115	-
38	KC2	d	311	23	-	5/15/71/71	-
28	CLA	b	602	16	-	10/27/103/115	-
34	DGD	B	843	-	-	5/49/89/95	0/2/2/2
31	WVN	B	845	-	-	0/29/63/63	0/2/2/2
30	LHG	A	844	28	-	6/31/31/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	h	306	17	-	21/39/115/115	-
28	CLA	A	820	40	-	3/39/115/115	-
30	LHG	k	620	28	-	19/41/41/53	-
28	CLA	g	303	24	-	2/21/97/115	-
28	CLA	B	830	40	-	15/39/115/115	-
28	CLA	g	308	24	-	17/39/115/115	-
36	II0	d	316	-	-	8/21/67/67	0/2/2/2
31	WVN	l	301	-	-	4/29/63/63	0/2/2/2
28	CLA	O	201	30	-	5/24/100/115	-
28	CLA	f	610	30	-	15/39/115/115	-
28	CLA	e	610	40	-	15/39/115/115	-
36	II0	c	614	-	-	1/21/67/67	0/2/2/2
36	II0	g	317	-	-	5/21/67/67	0/2/2/2
28	CLA	A	832	1	-	14/39/115/115	-
28	CLA	l	306	20	-	21/39/115/115	-
28	CLA	A	839	1	-	16/39/115/115	-
37	IHT	m	617	-	-	9/25/65/65	0/2/2/2
28	CLA	e	602	19	-	10/21/97/115	-
28	CLA	l	304	20	-	6/23/99/115	-
36	II0	n	616	-	-	4/21/67/67	0/2/2/2
28	CLA	g	307	24	-	8/23/99/115	-
28	CLA	B	813	2	-	14/32/108/115	-
28	CLA	c	611	14	-	7/15/91/115	-
28	CLA	b	604	16	-	18/39/115/115	-
28	CLA	K	103	12	-	7/12/88/115	-
37	IHT	a	317	-	-	8/25/65/65	0/2/2/2
36	II0	a	315	-	-	2/21/67/67	0/2/2/2
28	CLA	d	306	23	-	11/23/99/115	-
28	CLA	B	801	40	-	12/39/115/115	-
28	CLA	j	613	18	-	17/39/115/115	-
38	KC2	c	610	14	-	6/15/71/71	-
36	II0	m	614	-	-	3/21/67/67	0/2/2/2
31	WVN	A	846	-	-	10/29/63/63	0/2/2/2
31	WVN	s	205	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	A	838	1	-	15/39/115/115	-
28	CLA	c	601	14	-	8/23/99/115	-
36	II0	e	614	-	-	3/21/67/67	0/2/2/2
28	CLA	b	601	16	-	10/23/99/115	-
28	CLA	A	807	1	-	10/39/115/115	-
28	CLA	A	814	1	-	9/21/97/115	-
28	CLA	B	834	2	-	4/18/94/115	-
28	CLA	B	809	2	-	4/25/101/115	-
36	II0	e	612	-	-	5/21/67/67	0/2/2/2
28	CLA	A	809	1	-	10/29/105/115	-
28	CLA	n	601	26	-	6/15/91/115	-
28	CLA	A	818	1	-	19/39/115/115	-
28	CLA	b	607	16	-	19/39/115/115	-
28	CLA	e	611	19	-	23/39/115/115	-
36	II0	f	618	-	-	7/21/67/67	0/2/2/2
28	CLA	h	302	17	-	7/21/97/115	-
28	CLA	j	607	18	-	8/23/99/115	-
30	LHG	J	106	28	-	27/53/53/53	-
36	II0	c	617	-	-	4/21/67/67	0/2/2/2
28	CLA	B	817	40	-	11/39/115/115	-
36	II0	k	615	-	-	6/21/67/67	0/2/2/2
36	II0	f	615	-	-	5/21/67/67	0/2/2/2
28	CLA	k	602	21	-	8/21/97/115	-
28	CLA	f	602	18	-	16/39/115/115	-
31	WVN	B	844	-	-	5/29/63/63	0/2/2/2
35	LMG	F	205	-	-	11/43/63/70	0/1/1/1
31	WVN	B	847	-	-	2/29/63/63	0/2/2/2
28	CLA	A	805	1	-	7/39/115/115	-
28	CLA	b	606	16	-	15/35/111/115	-
28	CLA	c	607	14	-	3/17/93/115	-
28	CLA	h	303	17	-	8/21/97/115	-
28	CLA	A	826	1	-	10/39/115/115	-
38	KC2	d	310	23	-	6/15/71/71	-
36	II0	k	616	-	-	8/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	II0	f	616	-	-	3/21/67/67	0/2/2/2
31	WVN	I	101	-	-	9/29/63/63	0/2/2/2
39	LMU	i	301	-	-	8/21/61/61	0/2/2/2
31	WVN	K	102	-	-	5/29/63/63	0/2/2/2
36	II0	d	314	-	-	3/21/67/67	0/2/2/2
36	II0	b	613	-	-	2/21/67/67	0/2/2/2
28	CLA	m	601	18	-	4/12/88/115	-
28	CLA	j	604	18	-	13/39/115/115	-
28	CLA	A	806	1	-	10/39/115/115	-
31	WVN	L	205	-	-	6/29/63/63	0/2/2/2
28	CLA	d	309	30	-	3/10/86/115	-
38	KC2	s	201	13	-	8/15/71/71	-
28	CLA	s	206	40	-	14/39/115/115	-
31	WVN	i	316	-	-	9/29/63/63	0/2/2/2
28	CLA	F	202	6	-	13/24/100/115	-
31	WVN	R	201	-	-	6/29/63/63	0/2/2/2
28	CLA	j	608	18	-	6/15/91/115	-
28	CLA	a	309	15	-	11/39/115/115	-
28	CLA	c	604	14	-	4/39/115/115	-
28	CLA	c	603	14	-	3/23/99/115	-
36	II0	h	310	-	-	3/17/40/67	0/1/1/2
28	CLA	B	822	40	-	11/38/114/115	-
29	PQN	B	842	-	-	5/23/43/43	0/2/2/2
28	CLA	a	307	15	-	4/15/91/115	-
29	PQN	A	842	-	-	8/23/43/43	0/2/2/2
28	CLA	d	305	23	-	9/23/99/115	-
28	CLA	k	601	21	-	12/23/99/115	-
28	CLA	f	601	18	-	10/18/94/115	-
28	CLA	A	841	1	-	21/39/115/115	-
28	CLA	n	610	40	-	16/39/115/115	-
28	CLA	l	309	30	-	14/35/111/115	-
28	CLA	j	605	18	-	8/15/91/115	-
30	LHG	m	619	28	-	19/41/41/53	-
36	II0	d	313	-	-	5/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	b	610	16	-	22/39/115/115	-
30	LHG	a	301	28	-	12/53/53/53	-
28	CLA	i	306	22	-	12/23/99/115	-
28	CLA	A	803	1,28	-	7/27/103/115	-
28	CLA	c	606	14	-	11/24/100/115	-
31	WVN	M	101	-	-	7/29/63/63	0/2/2/2
28	CLA	B	838	2	-	10/30/106/115	-
28	CLA	m	603	18	-	11/39/115/115	-
28	CLA	l	305	20	-	16/39/115/115	-
28	CLA	B	824	2	-	9/39/115/115	-
28	CLA	b	603	16	-	18/39/115/115	-
28	CLA	A	810	1,28	-	10/36/112/115	-
28	CLA	j	601	18	-	6/23/99/115	-
35	LMG	n	620	-	-	12/50/70/70	0/1/1/1
30	LHG	f	619	-	-	38/53/53/53	-
28	CLA	A	815	40	-	6/15/91/115	-
28	CLA	i	311	-	-	7/23/99/115	-
33	SF4	C	101	3	-	-	0/6/5/5
33	SF4	C	102	3	-	-	0/6/5/5
28	CLA	A	833	1	-	6/21/97/115	-
28	CLA	k	610	30	-	13/23/99/115	-
28	CLA	f	613	18	-	23/39/115/115	-
28	CLA	s	202	13	-	21/39/115/115	-
28	CLA	m	609	18	-	6/23/99/115	-
31	WVN	L	201	-	-	9/29/63/63	0/2/2/2
28	CLA	l	308	20	-	9/23/99/115	-
28	CLA	A	819	1	-	5/15/91/115	-
32	LMT	A	850	-	-	11/21/61/61	0/2/2/2
36	II0	c	613	-	-	4/21/67/67	0/2/2/2
28	CLA	A	823	1	-	8/27/103/115	-
28	CLA	B	826	2	-	5/23/99/115	-
28	CLA	a	313	15	-	10/19/95/115	-
36	II0	h	311	-	-	7/21/67/67	0/2/2/2
28	CLA	A	821	1	-	6/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMG	L	209	28	-	19/50/70/70	0/1/1/1
28	CLA	e	607	19	-	22/39/115/115	-
28	CLA	n	609	26	-	11/39/115/115	-
36	II0	a	318	-	-	7/21/67/67	0/2/2/2
33	SF4	A	853	1,2	-	-	0/6/5/5
36	II0	n	615	-	-	4/21/67/67	0/2/2/2
37	IHT	k	618	-	-	11/25/65/65	0/2/2/2
28	CLA	A	830	1	-	7/21/97/115	-
28	CLA	d	304	23	-	9/23/99/115	-
31	WVN	l	315	-	-	9/29/63/63	0/2/2/2
28	CLA	A	837	1	-	9/39/115/115	-
36	II0	i	314	-	-	5/21/67/67	0/2/2/2
38	KC2	s	204	13	-	5/15/71/71	-
32	LMT	b	618	-	-	9/15/35/61	0/1/1/2
28	CLA	B	837	2	-	14/39/115/115	-
28	CLA	i	309	30	-	5/17/93/115	-
38	KC2	g	314	38	-	5/15/71/71	-
38	KC2	k	611	21	-	5/15/71/71	-
28	CLA	j	612	-	-	10/23/99/115	-
37	IHT	j	616	-	-	5/25/65/65	0/2/2/2
28	CLA	k	606	21	-	12/23/99/115	-
28	CLA	n	602	26	-	4/21/97/115	-
36	II0	O	203	-	-	3/21/67/67	0/2/2/2
28	CLA	L	202	9	-	10/20/96/115	-
28	CLA	A	801	1	-	13/39/115/115	-
28	CLA	Q	303	27	-	8/15/91/115	-
38	KC2	i	310	22	-	7/15/71/71	-
28	CLA	a	306	40	-	15/39/115/115	-
37	IHT	f	617	-	-	7/25/65/65	0/2/2/2
28	CLA	i	305	22	-	9/39/115/115	-
31	WVN	A	845	-	-	7/29/63/63	0/2/2/2
38	KC2	g	313	24,38	-	2/15/71/71	-
28	CLA	e	605	19	-	19/39/115/115	-
31	WVN	A	847	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	d	308	23	-	3/10/86/115	-
36	II0	e	613	-	-	4/21/67/67	0/2/2/2
37	IHT	R	204	-	-	3/25/65/65	0/2/2/2
28	CLA	g	309	24	-	12/39/115/115	-
28	CLA	f	608	18	-	17/39/115/115	-
28	CLA	B	810	2	-	6/27/103/115	-
31	WVN	J	101	-	-	11/29/63/63	0/2/2/2
36	II0	m	616	-	-	3/21/67/67	0/2/2/2
36	II0	i	313	-	-	7/21/67/67	0/2/2/2
28	CLA	a	311	15	-	12/39/115/115	-
28	CLA	h	308	17	-	9/23/99/115	-
36	II0	j	614	-	-	6/21/67/67	0/2/2/2
28	CLA	B	833	2	-	11/39/115/115	-
38	KC2	i	319	-	-	6/15/71/71	-
28	CLA	s	203	28,13	-	18/39/115/115	-
31	WVN	B	846	-	-	6/29/63/63	0/2/2/2
28	CLA	c	612	14	-	15/39/115/115	-
28	CLA	A	817	1	-	15/39/115/115	-
28	CLA	l	303	20	-	24/39/115/115	-
28	CLA	c	609	30	-	4/15/91/115	-

The worst 5 of 4378 bond length outliers are listed below:

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

The worst 5 of 4747 bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 3969 torsion outliers are listed below:

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

There are no ring outliers.

247 monomers are involved in 487 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	n	617	IHT	2	0
28	m	607	CLA	1	0
28	B	823	CLA	2	0
30	g	301	LHG	2	0
36	i	320	II0	1	0
28	B	807	CLA	2	0
28	g	322	CLA	5	0
28	B	811	CLA	2	0
30	n	619	LHG	1	0
35	b	621	LMG	3	0
28	m	610	CLA	2	0
28	c	608	CLA	2	0
36	m	615	II0	1	0
28	B	808	CLA	1	0
28	A	813	CLA	1	0
35	J	105	LMG	4	0
28	d	302	CLA	3	0
28	b	608	CLA	3	0
28	a	312	CLA	1	0
36	k	621	II0	1	0
28	A	822	CLA	2	0
28	B	814	CLA	1	0
28	d	303	CLA	10	0
37	b	615	IHT	1	0
28	B	827	CLA	2	0
28	O	206	CLA	8	0
28	A	827	CLA	1	0
28	B	815	CLA	6	0
28	a	305	CLA	1	0
28	A	811	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	m	602	CLA	3	0
28	j	610	CLA	3	0
28	R	203	CLA	1	0
28	B	828	CLA	1	0
28	b	605	CLA	1	0
28	A	852	CLA	3	0
28	n	605	CLA	1	0
28	k	609	CLA	2	0
35	Q	301	LMG	4	0
28	L	203	CLA	4	0
28	L	204	CLA	3	0
30	b	619	LHG	1	0
28	i	302	CLA	3	0
28	n	608	CLA	1	0
28	h	301	CLA	4	0
28	h	304	CLA	2	0
28	B	820	CLA	1	0
28	B	831	CLA	1	0
28	B	840	CLA	2	0
28	i	308	CLA	1	0
28	B	804	CLA	1	0
28	A	824	CLA	3	0
30	L	208	LHG	2	0
28	B	836	CLA	3	0
36	n	618	II0	1	0
28	i	312	CLA	1	0
28	A	840	CLA	2	0
28	n	607	CLA	1	0
28	e	604	CLA	3	0
30	a	319	LHG	2	0
28	g	305	CLA	1	0
36	d	315	II0	1	0
28	O	202	CLA	4	0
28	i	303	CLA	2	0
28	B	839	CLA	4	0
28	l	311	CLA	2	0
35	c	619	LMG	3	0
30	l	317	LHG	1	0
28	A	836	CLA	5	0
28	J	103	CLA	2	0
28	a	304	CLA	2	0
28	k	607	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	c	620	LHG	1	0
28	L	207	CLA	2	0
28	A	854	CLA	5	0
28	h	307	CLA	1	0
28	s	208	CLA	1	0
28	A	829	CLA	2	0
28	l	307	CLA	1	0
36	l	312	II0	1	0
30	b	620	LHG	1	0
30	A	849	LHG	3	0
28	Q	302	CLA	7	0
30	j	617	LHG	2	0
30	i	318	LHG	2	0
28	f	607	CLA	4	0
28	d	307	CLA	1	0
31	R	202	WVN	7	0
28	g	310	CLA	2	0
28	B	805	CLA	3	0
28	A	831	CLA	2	0
28	F	201	CLA	5	0
28	c	605	CLA	1	0
28	m	604	CLA	1	0
28	m	606	CLA	1	0
28	k	608	CLA	3	0
28	A	834	CLA	2	0
28	A	802	CLA	7	0
28	B	835	CLA	5	0
28	A	835	CLA	4	0
28	c	602	CLA	2	0
28	B	806	CLA	1	0
28	a	303	CLA	2	0
28	a	308	CLA	2	0
28	A	855	CLA	1	0
28	n	603	CLA	4	0
28	b	611	CLA	2	0
28	B	841	CLA	1	0
28	B	825	CLA	2	0
38	f	611	KC2	1	0
28	n	613	CLA	1	0
28	B	819	CLA	1	0
28	f	606	CLA	1	0
28	A	816	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	n	604	CLA	2	0
28	B	803	CLA	4	0
28	B	802	CLA	1	0
28	g	315	CLA	1	0
28	d	301	CLA	2	0
28	B	832	CLA	3	0
31	L	206	WVN	1	0
28	A	828	CLA	4	0
31	A	848	WVN	1	0
28	A	804	CLA	2	0
28	m	612	CLA	2	0
28	e	606	CLA	6	0
38	g	312	KC2	3	0
28	e	601	CLA	2	0
28	b	612	CLA	2	0
28	B	821	CLA	5	0
28	m	608	CLA	2	0
28	i	307	CLA	3	0
28	A	851	CLA	2	0
28	b	602	CLA	1	0
34	B	843	DGD	2	0
28	h	306	CLA	4	0
28	A	820	CLA	3	0
28	g	303	CLA	2	0
28	B	830	CLA	3	0
28	g	308	CLA	5	0
36	d	316	II0	1	0
28	O	201	CLA	1	0
28	f	610	CLA	4	0
28	e	610	CLA	2	0
28	l	306	CLA	3	0
28	A	839	CLA	5	0
28	B	813	CLA	8	0
28	b	604	CLA	3	0
28	d	306	CLA	1	0
28	B	801	CLA	5	0
31	A	846	WVN	1	0
28	A	838	CLA	3	0
28	c	601	CLA	2	0
28	b	601	CLA	2	0
28	A	807	CLA	2	0
28	A	814	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B	834	CLA	2	0
28	B	809	CLA	1	0
28	A	809	CLA	2	0
28	A	818	CLA	4	0
28	b	607	CLA	4	0
28	e	611	CLA	3	0
28	h	302	CLA	1	0
28	j	607	CLA	3	0
30	J	106	LHG	6	0
28	B	817	CLA	4	0
36	f	615	II0	1	0
28	k	602	CLA	3	0
28	f	602	CLA	3	0
35	F	205	LMG	4	0
28	b	606	CLA	5	0
28	h	303	CLA	1	0
28	A	826	CLA	3	0
31	I	101	WVN	2	0
39	i	301	LMU	2	0
31	K	102	WVN	1	0
28	j	604	CLA	1	0
28	A	806	CLA	2	0
38	s	201	KC2	1	0
28	F	202	CLA	1	0
28	a	309	CLA	1	0
28	c	604	CLA	2	0
28	c	603	CLA	1	0
28	B	822	CLA	4	0
29	B	842	PQN	1	0
28	a	307	CLA	1	0
29	A	842	PQN	1	0
28	k	601	CLA	1	0
28	f	601	CLA	1	0
28	A	841	CLA	4	0
28	n	610	CLA	2	0
28	j	605	CLA	1	0
30	m	619	LHG	2	0
28	b	610	CLA	3	0
30	a	301	LHG	1	0
28	i	306	CLA	2	0
28	A	803	CLA	2	0
28	c	606	CLA	2	0

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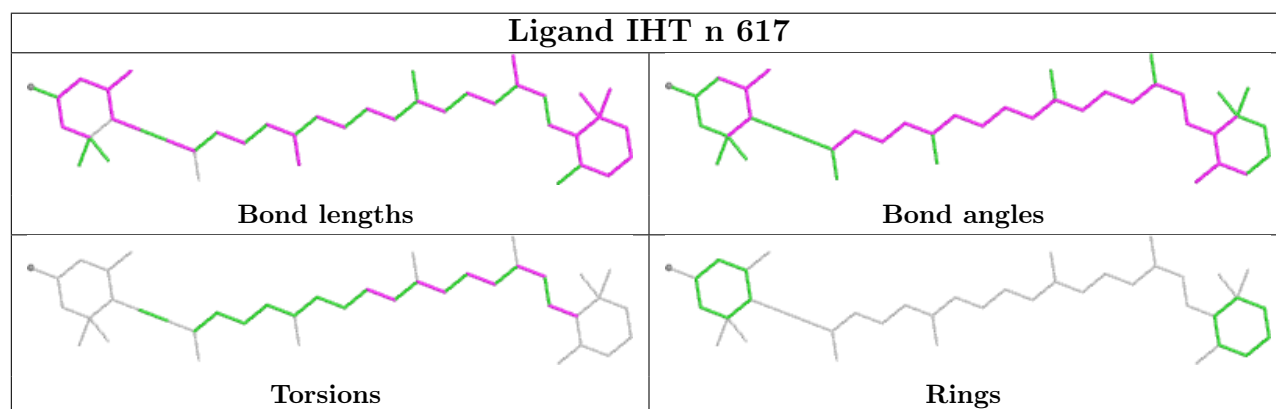
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28	l	305	CLA	2	0
28	B	824	CLA	2	0
28	b	603	CLA	2	0
28	A	810	CLA	1	0
28	j	601	CLA	3	0
35	n	620	LMG	3	0
30	f	619	LHG	2	0
28	A	815	CLA	1	0
28	i	311	CLA	1	0
28	k	610	CLA	2	0
28	f	613	CLA	2	0
28	s	202	CLA	5	0
28	m	609	CLA	1	0
28	l	308	CLA	1	0
28	A	819	CLA	1	0
32	A	850	LMT	1	0
28	A	823	CLA	2	0
28	A	821	CLA	3	0
35	L	209	LMG	7	0
28	e	607	CLA	3	0
28	n	609	CLA	3	0
28	A	830	CLA	1	0
28	d	304	CLA	2	0
28	A	837	CLA	3	0
32	b	618	LMT	2	0
28	B	837	CLA	3	0
37	j	616	IHT	1	0
28	k	606	CLA	1	0
28	n	602	CLA	2	0
28	L	202	CLA	3	0
28	A	801	CLA	3	0
37	f	617	IHT	1	0
28	i	305	CLA	1	0
28	e	605	CLA	2	0
31	A	847	WVN	3	0
28	d	308	CLA	1	0
28	g	309	CLA	6	0
28	f	608	CLA	6	0
28	B	810	CLA	1	0
31	J	101	WVN	1	0
28	a	311	CLA	2	0

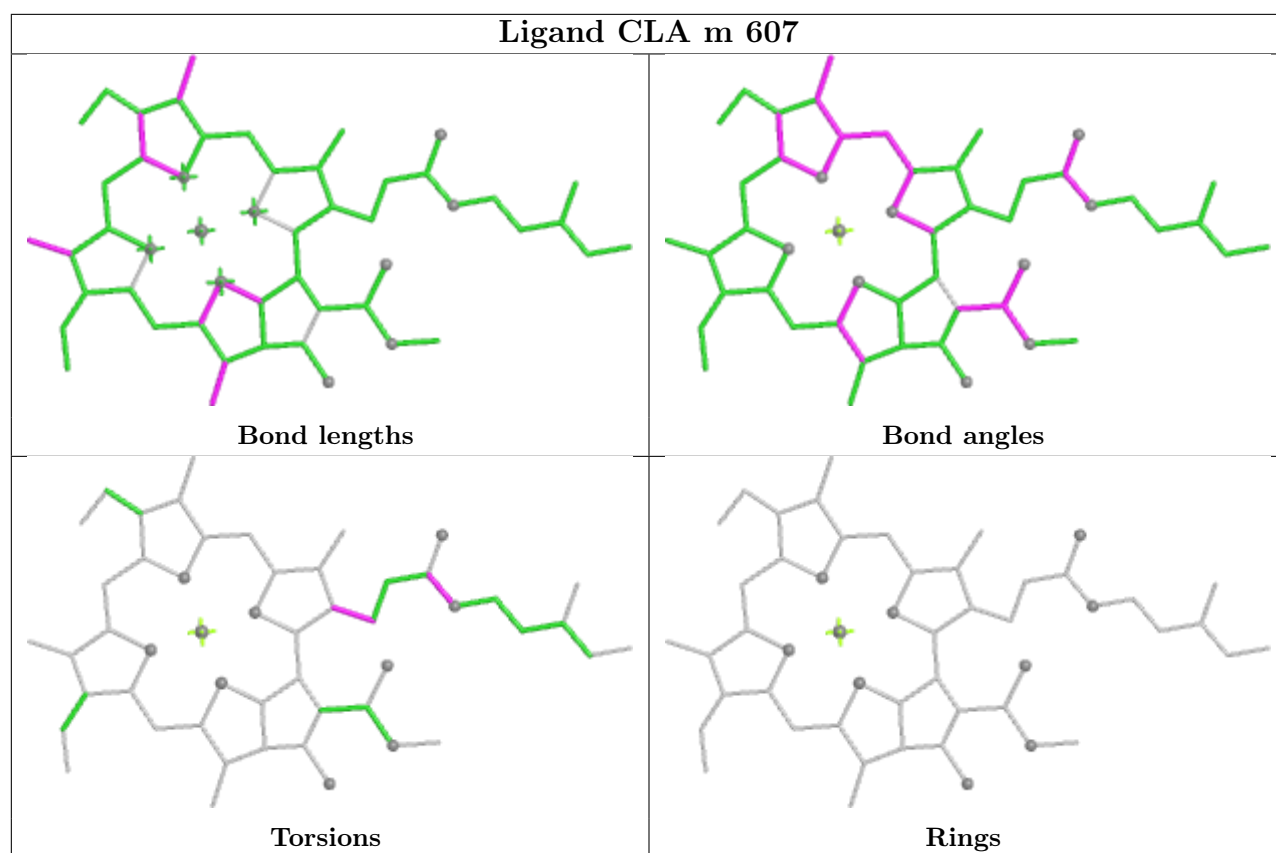
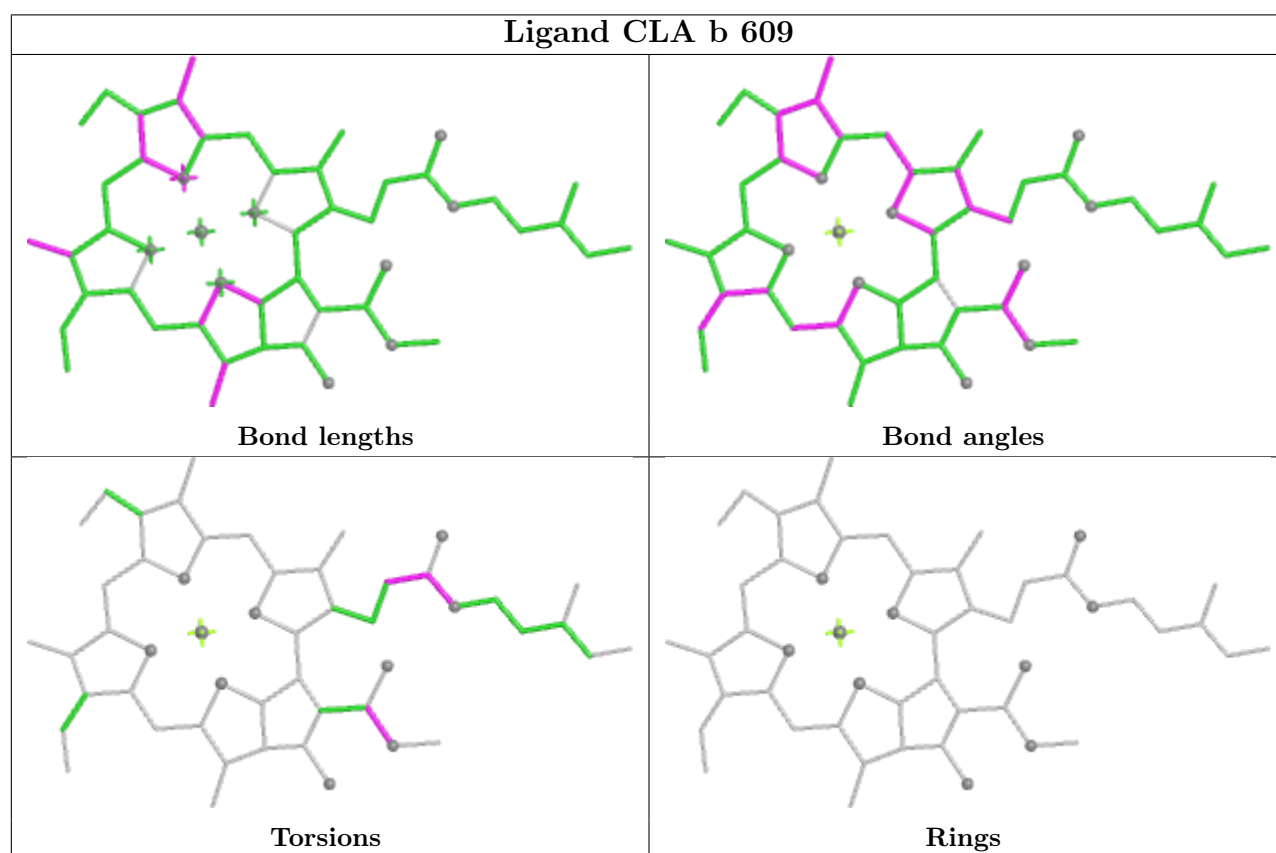
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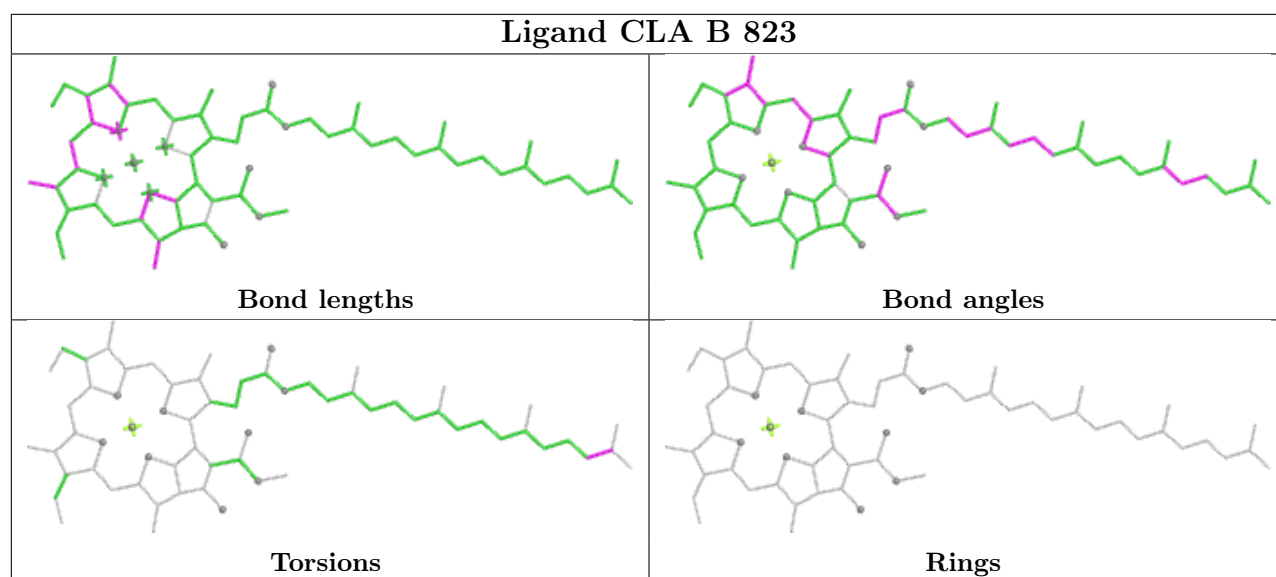
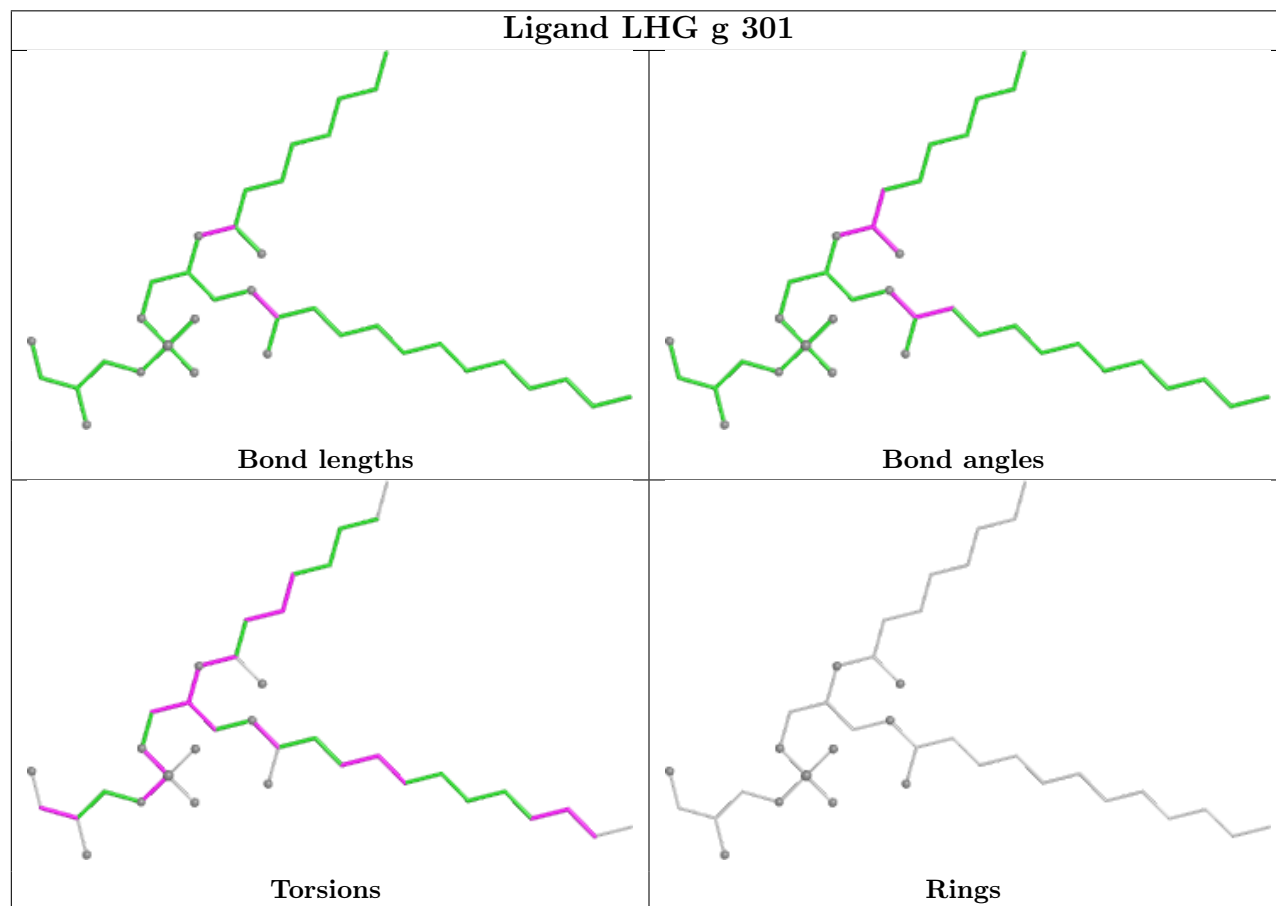
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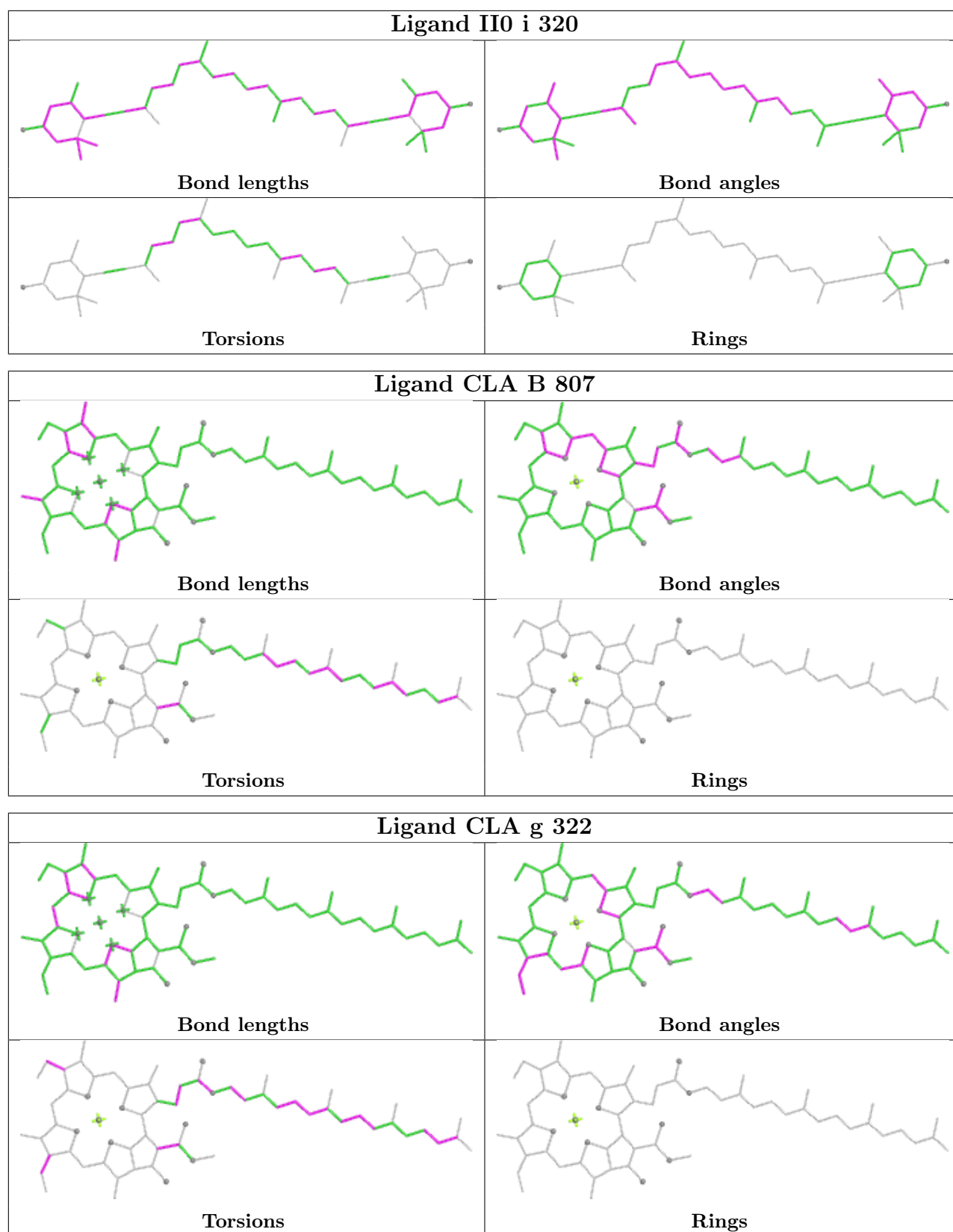
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	h	308	CLA	2	0
28	B	833	CLA	4	0
38	i	319	KC2	10	0
31	B	846	WVN	2	0
28	c	612	CLA	2	0
28	A	817	CLA	4	0
28	l	303	CLA	1	0

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

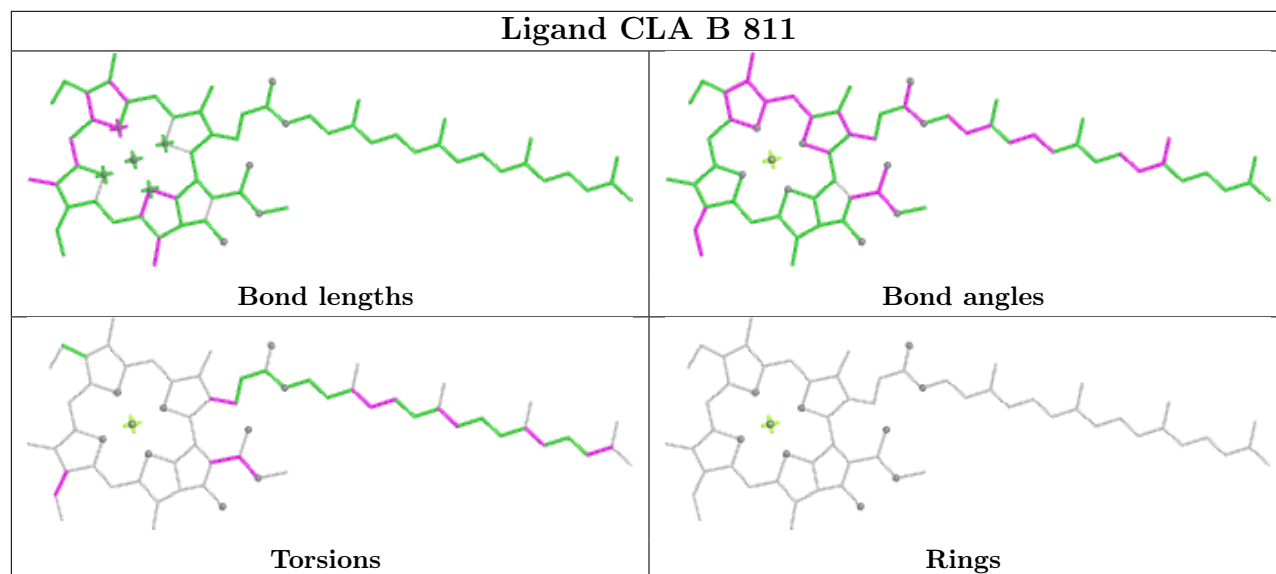




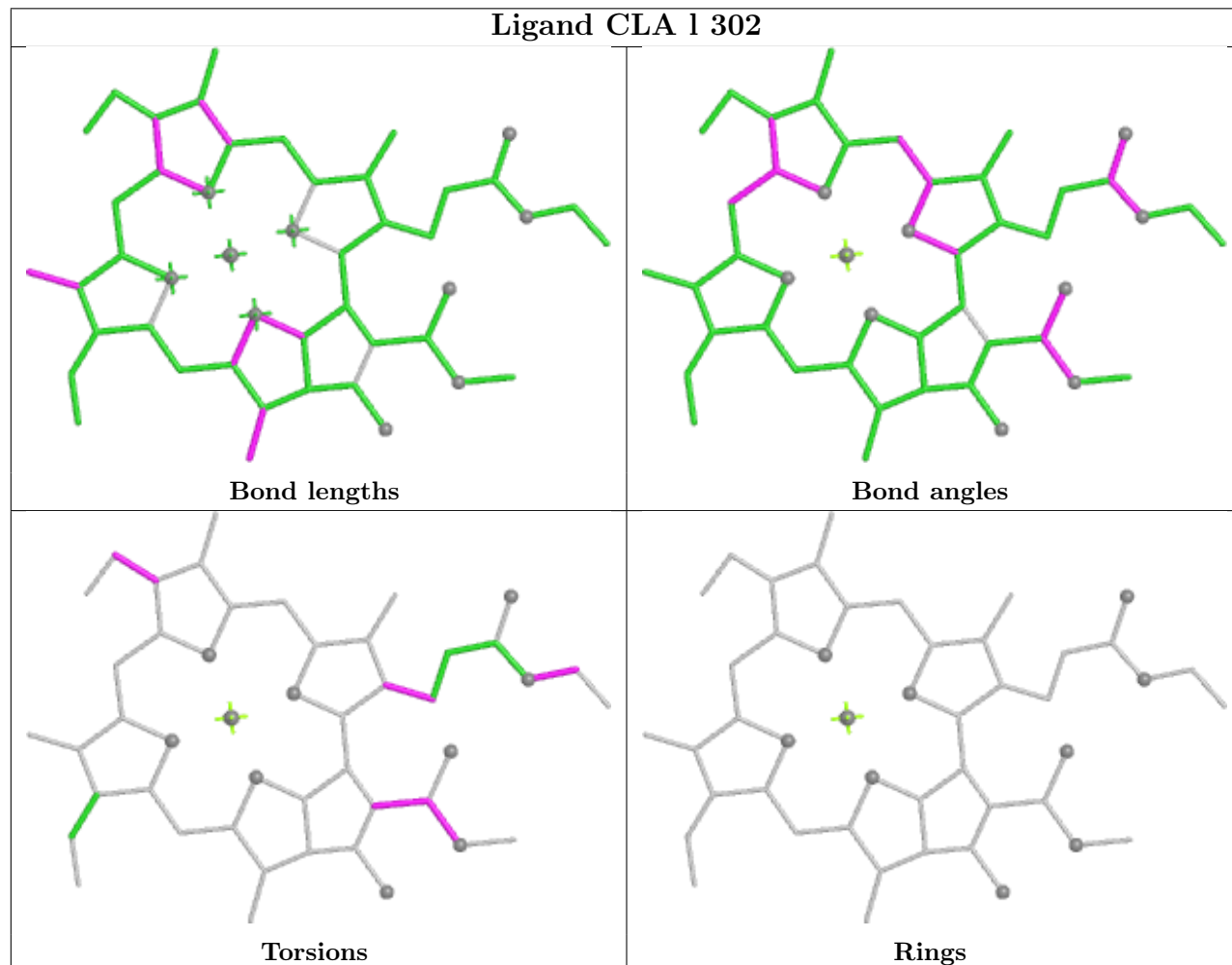


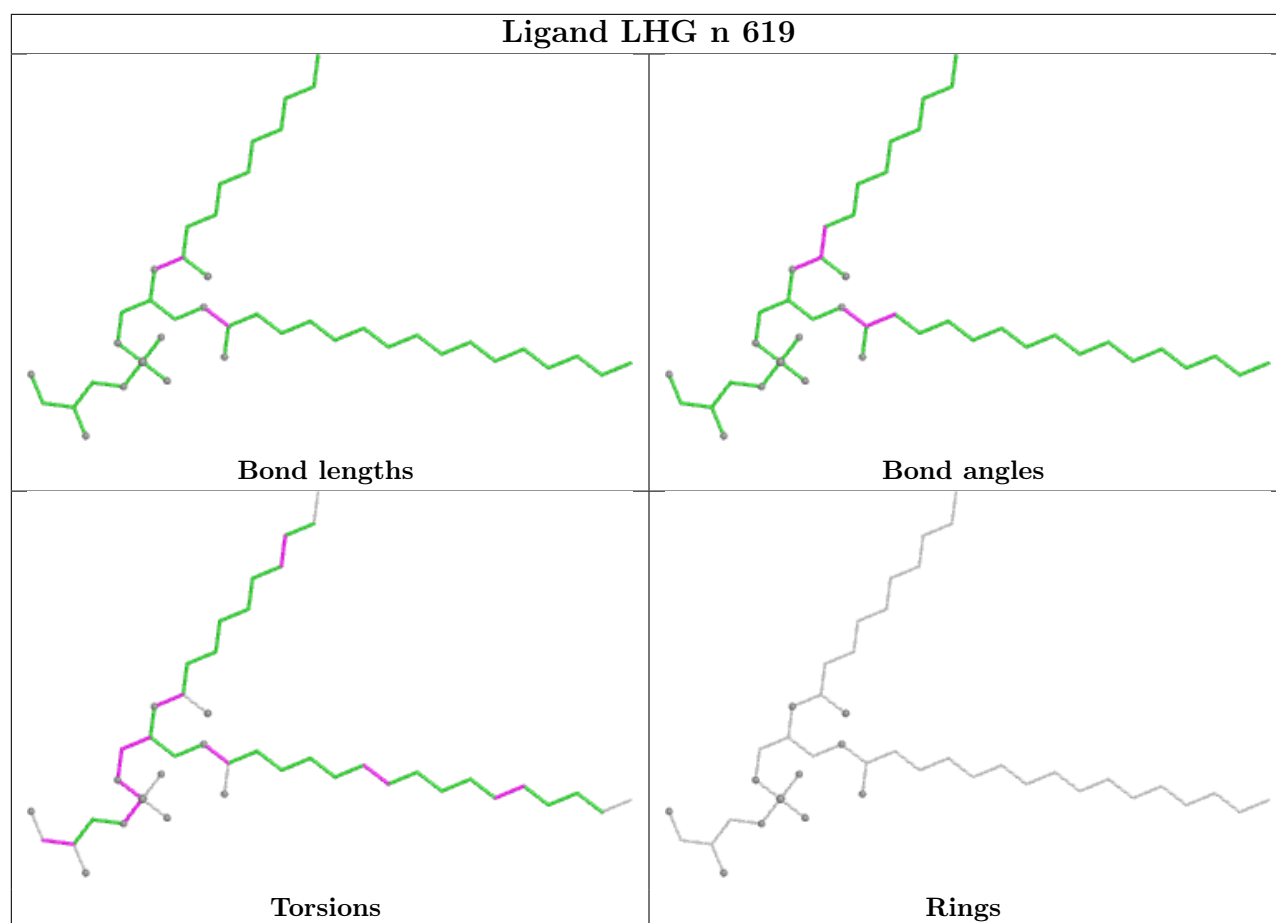
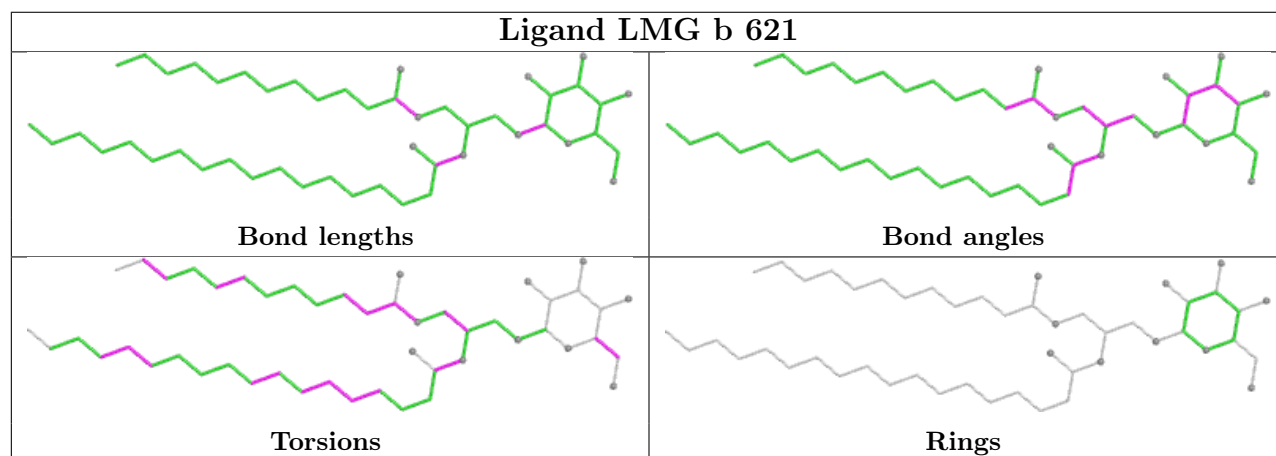


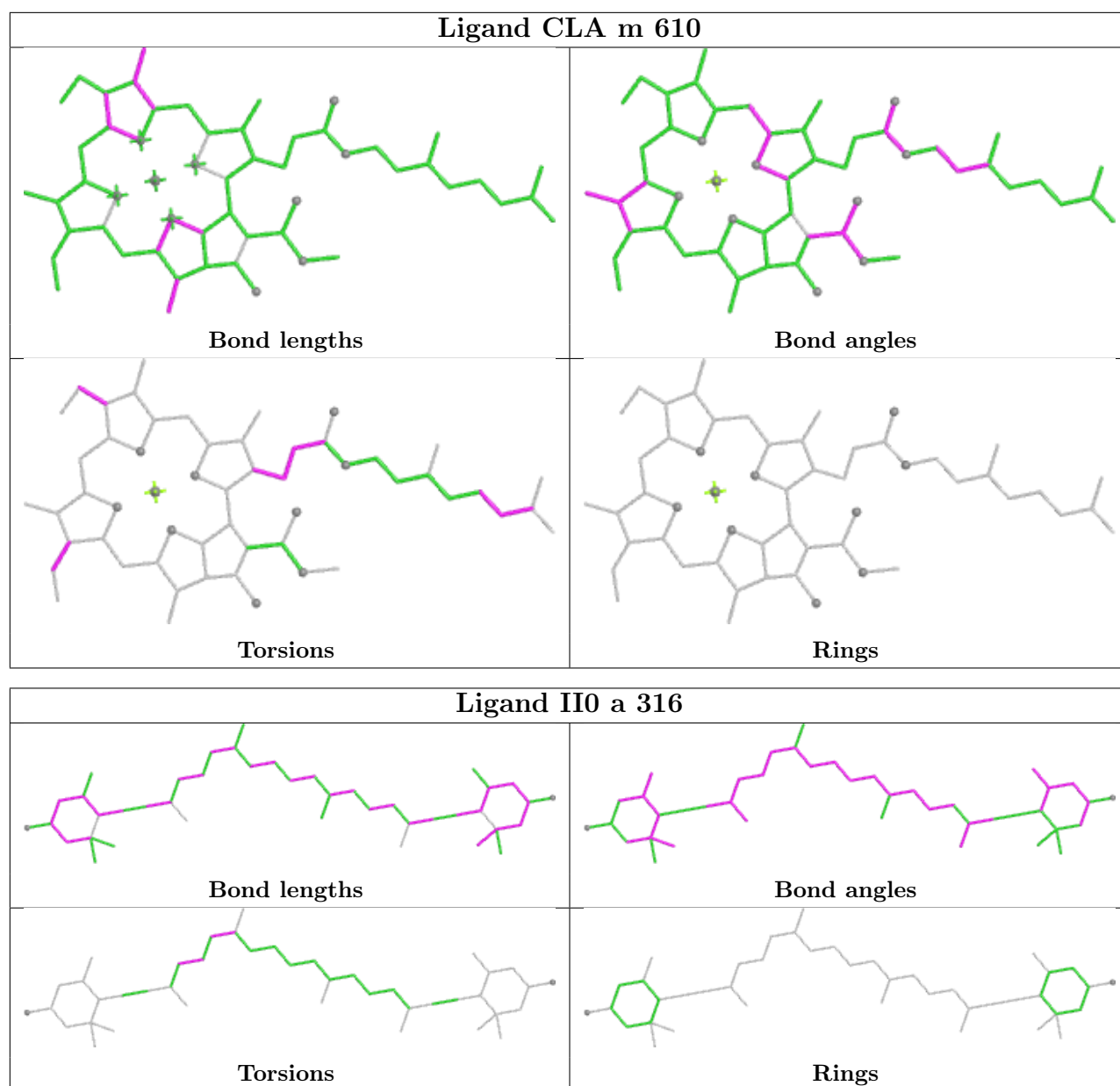
Ligand CLA B 811



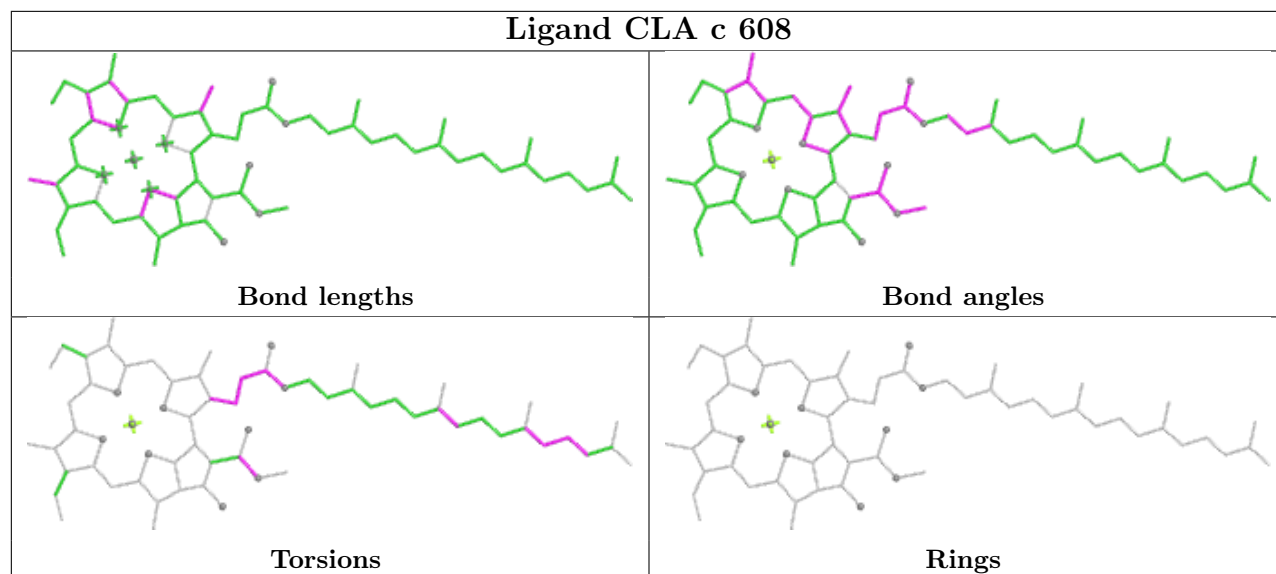
Ligand CLA I 302



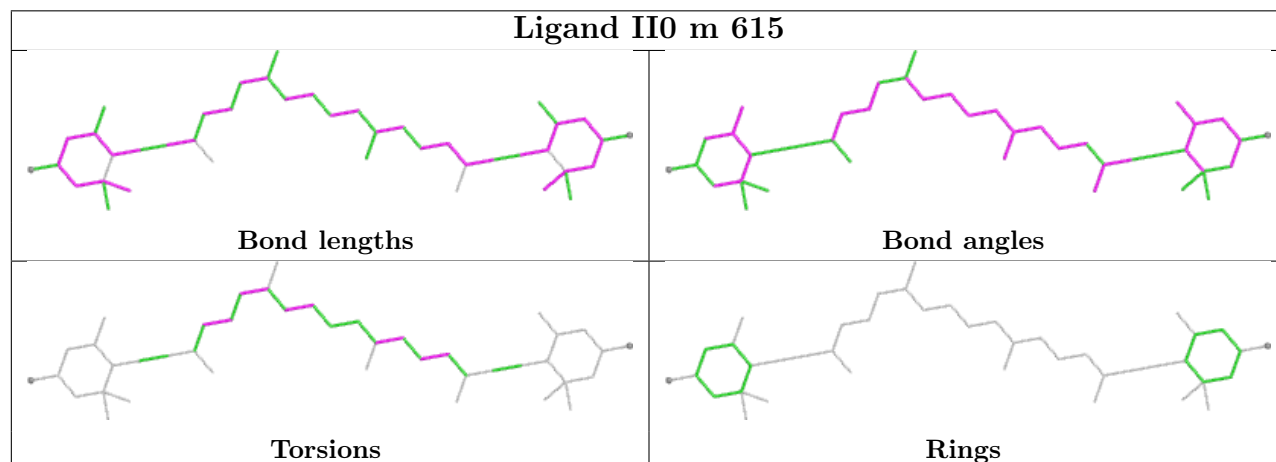




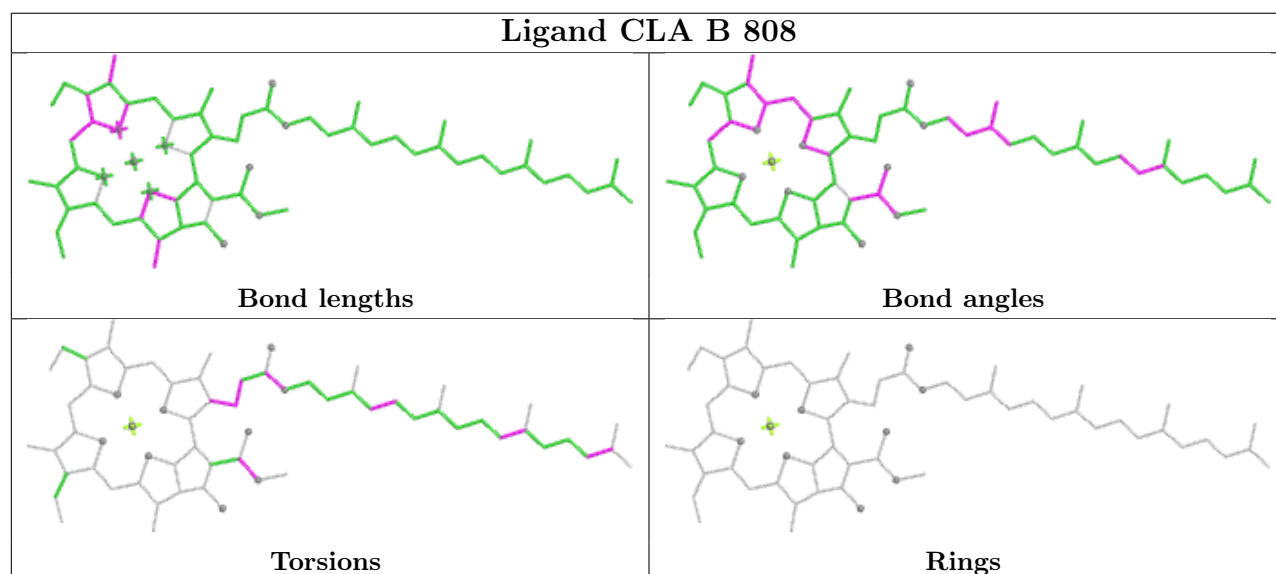
Ligand CLA c 608

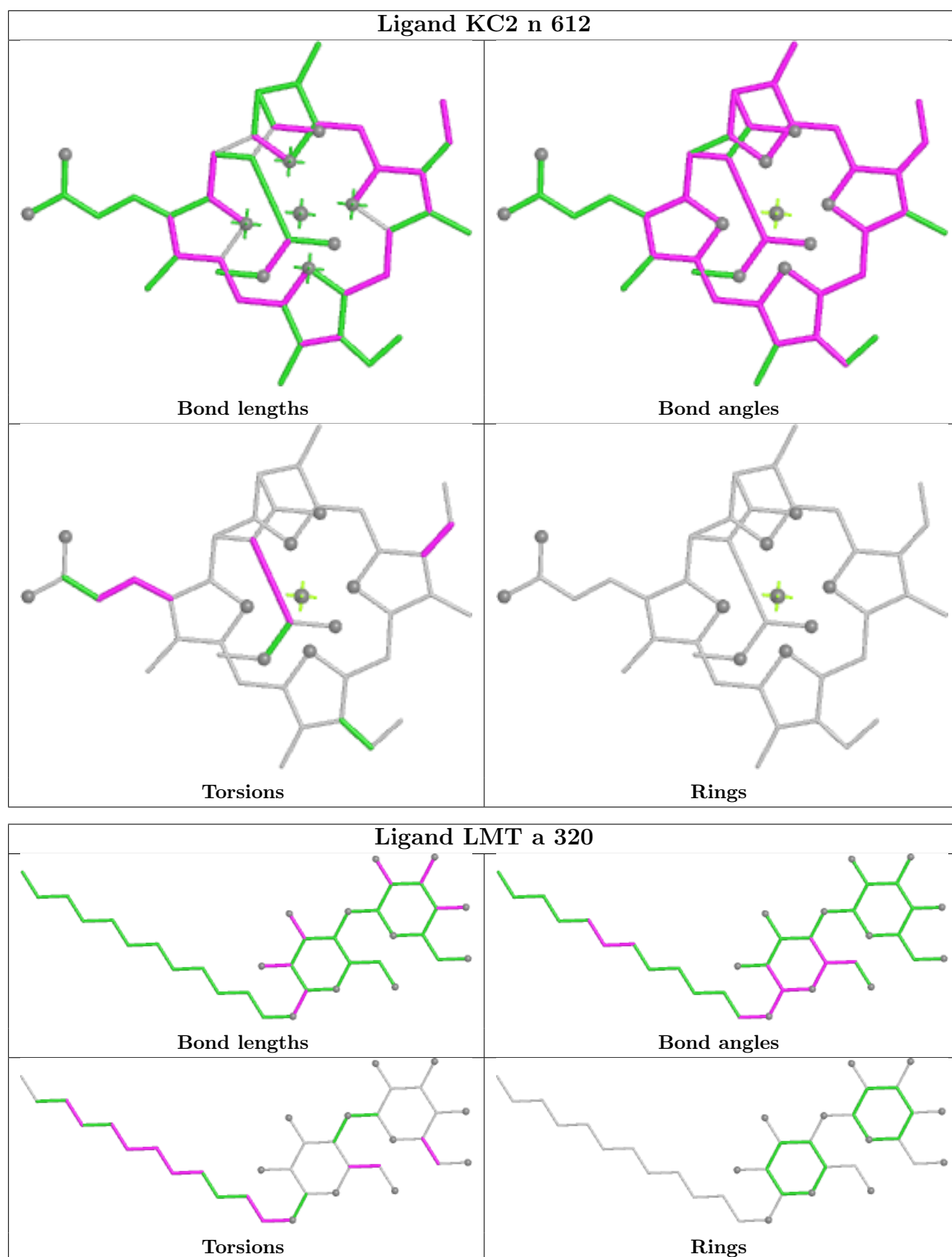


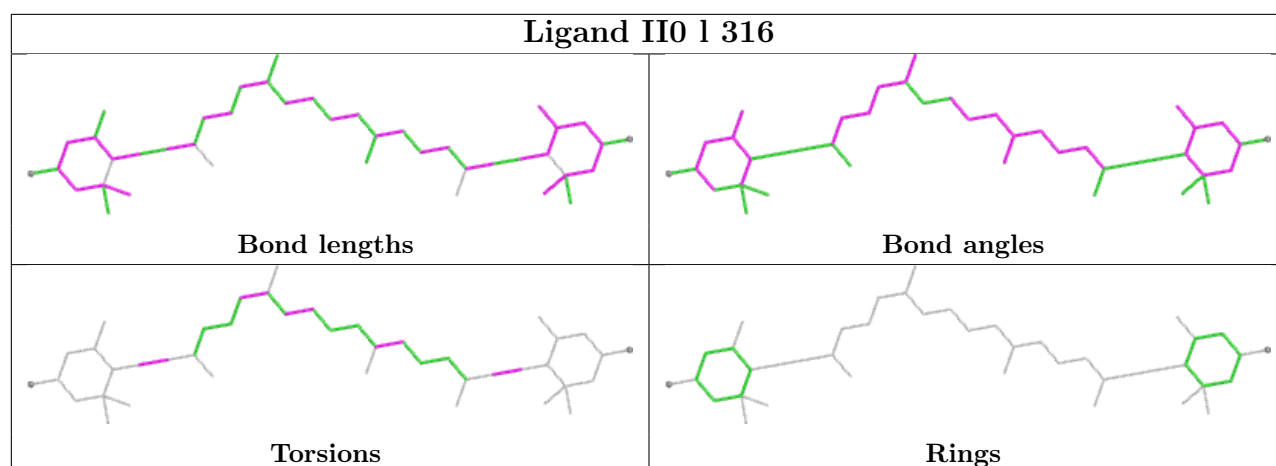
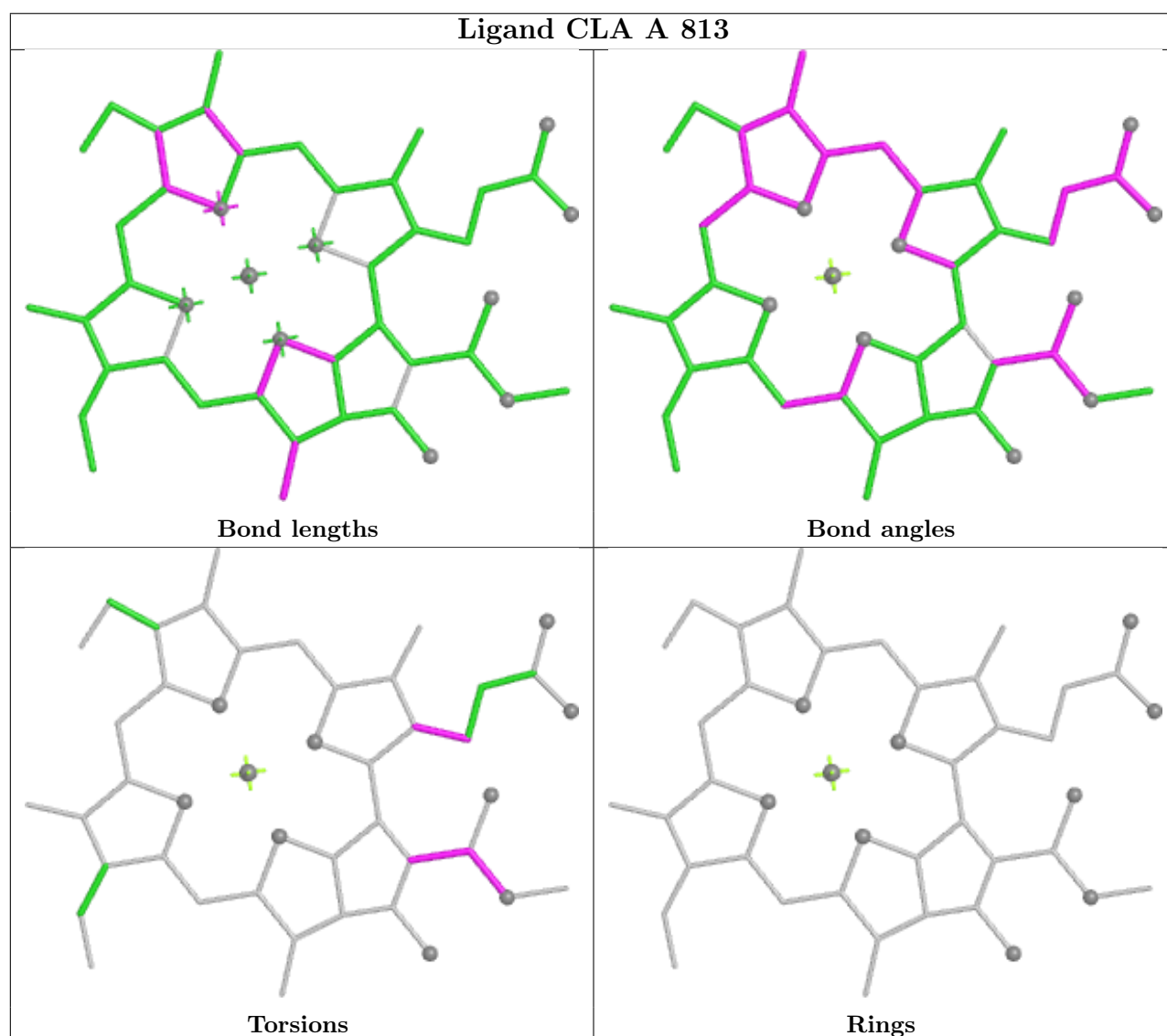
Ligand II0 m 615

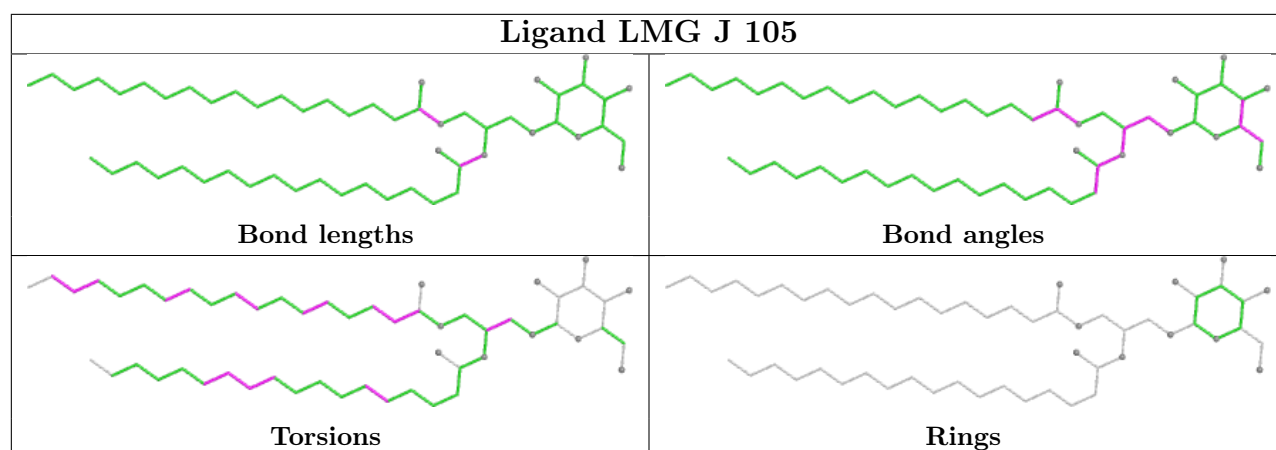
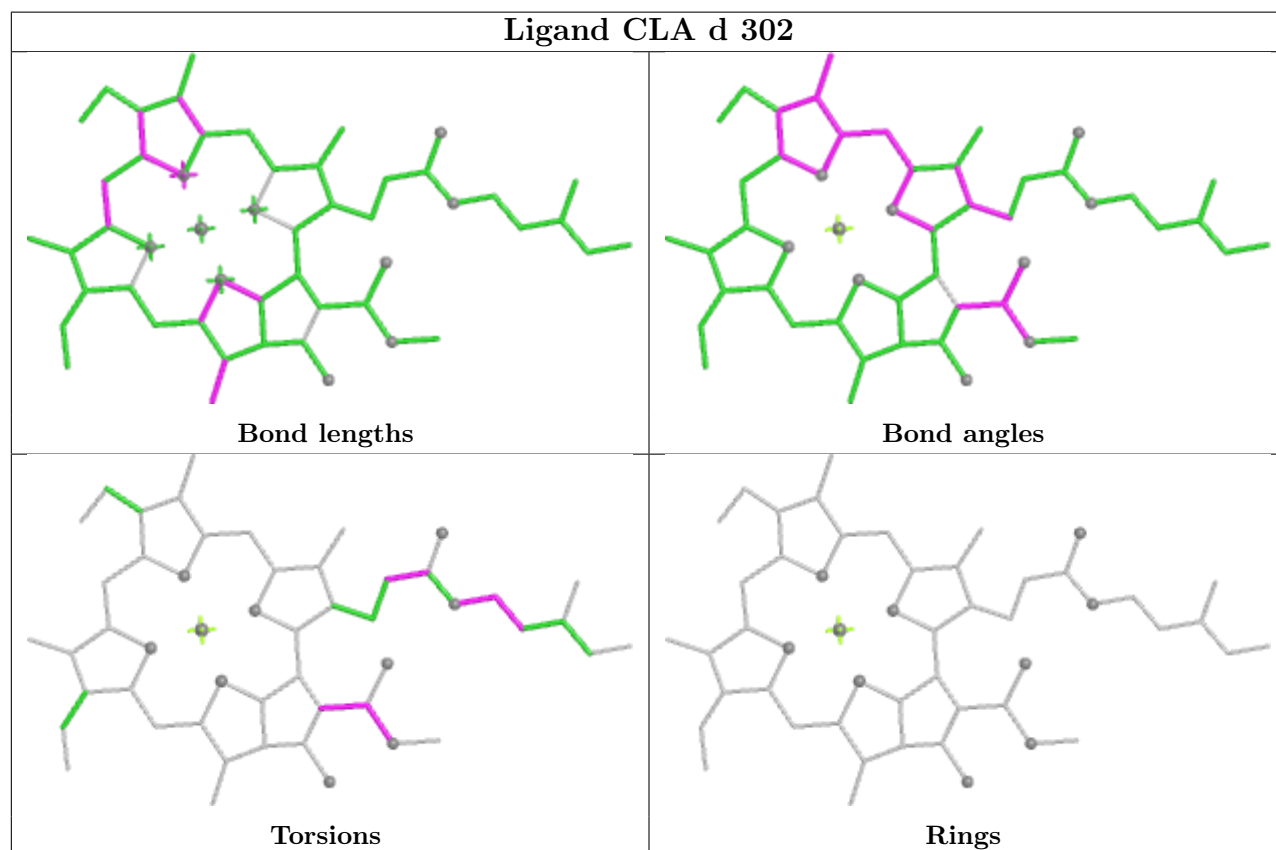
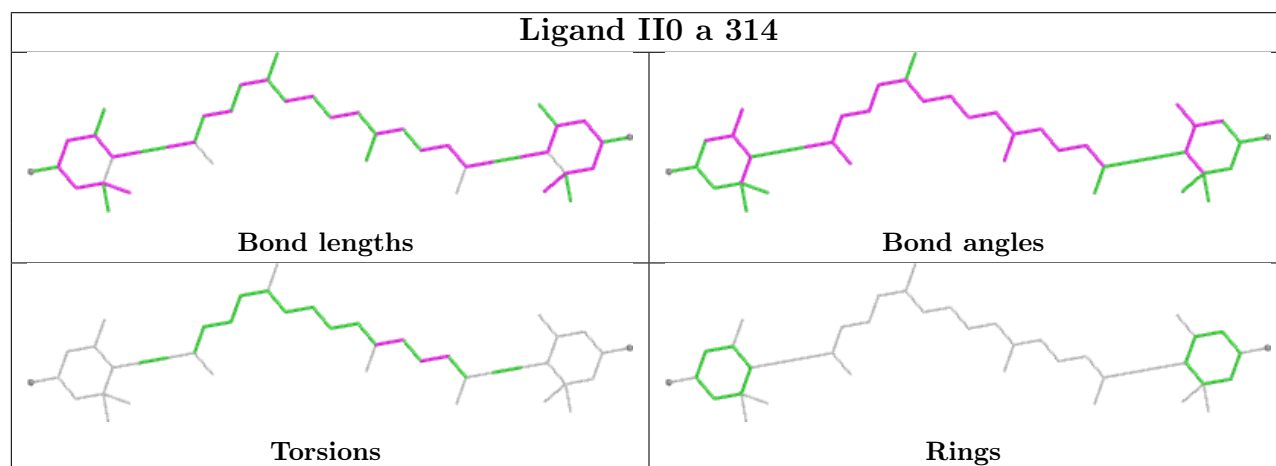


Ligand CLA B 808

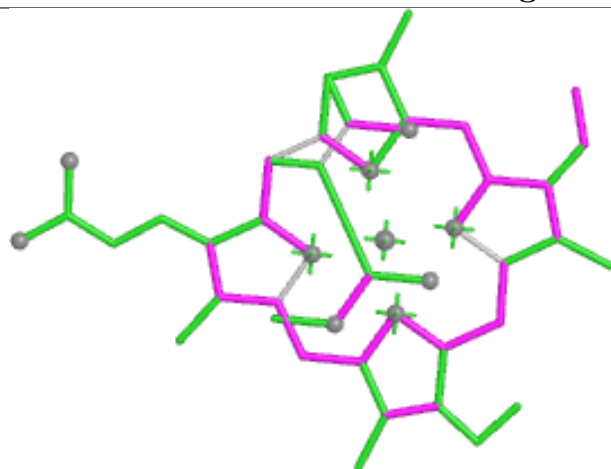




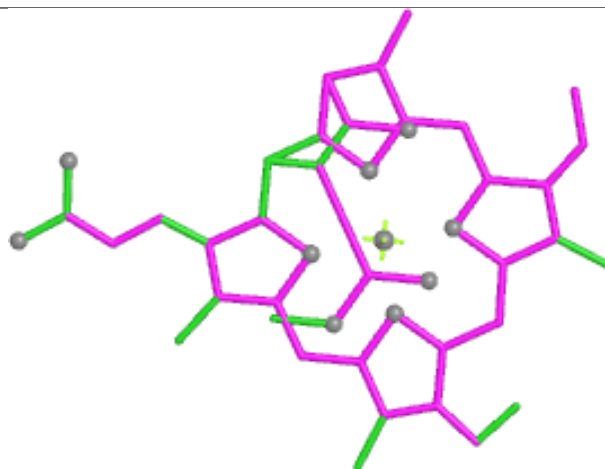




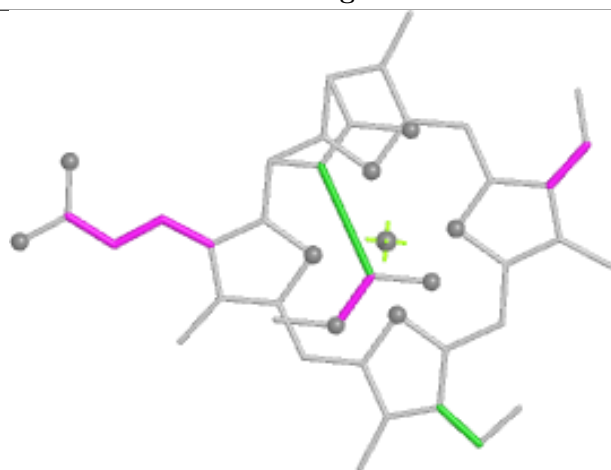
Ligand KC2 n 611



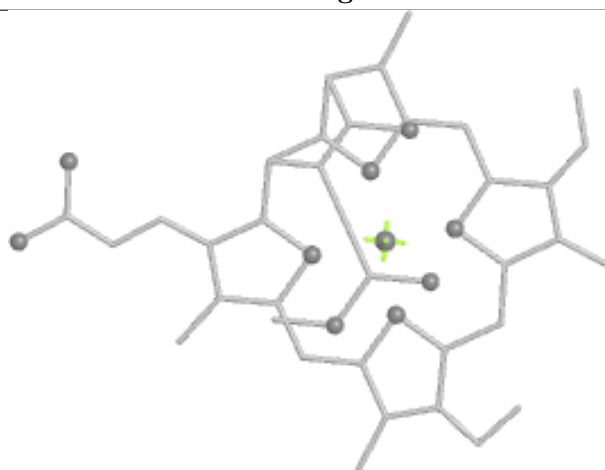
Bond lengths



Bond angles

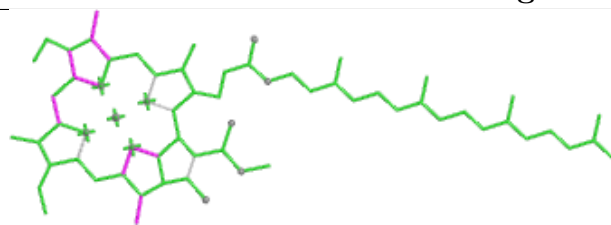


Torsions

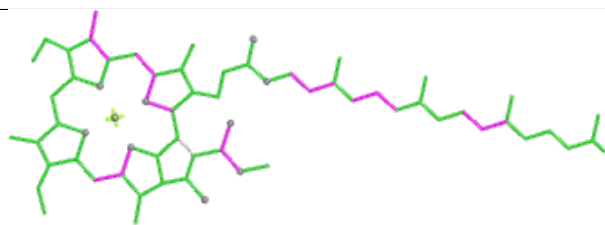


Rings

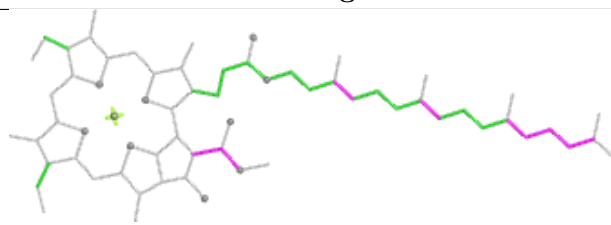
Ligand CLA b 608



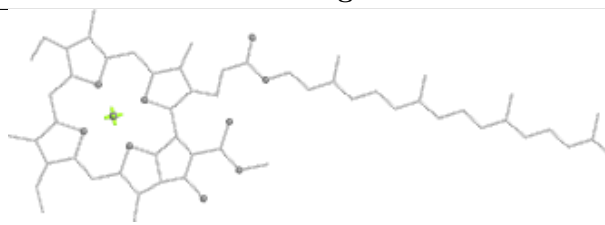
Bond lengths



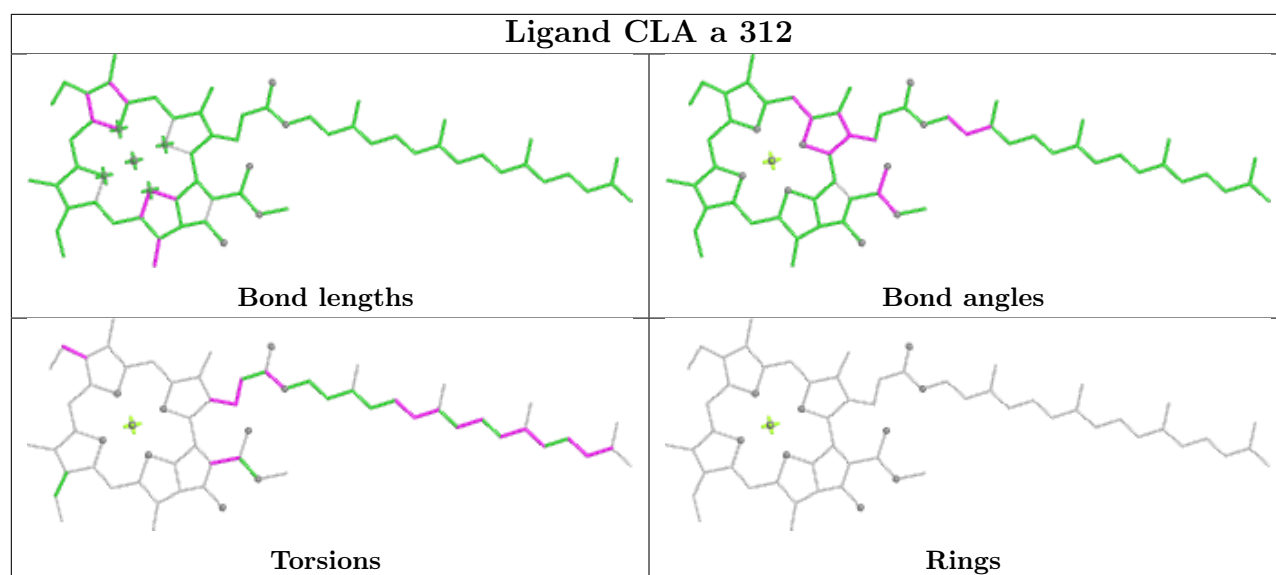
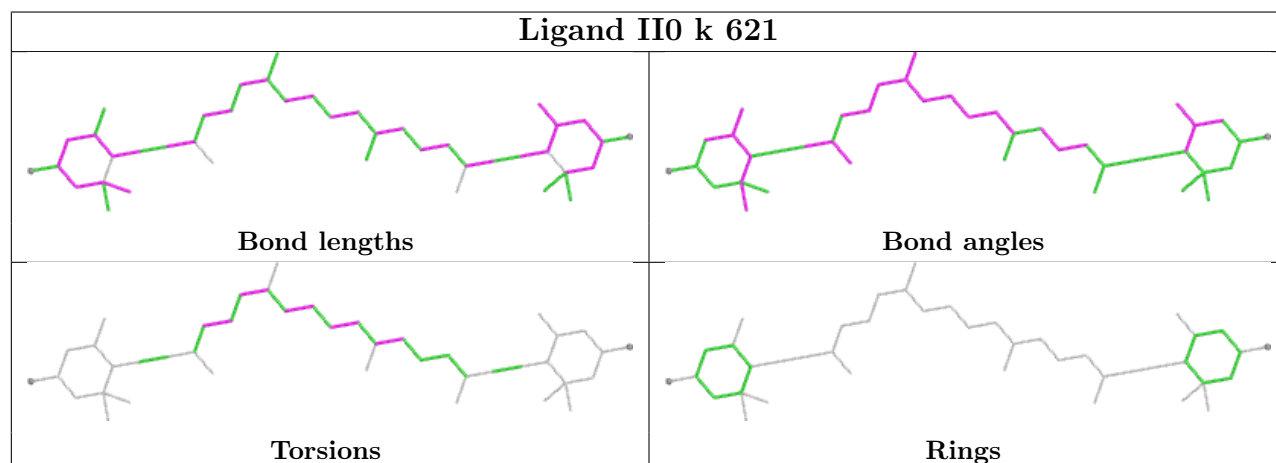
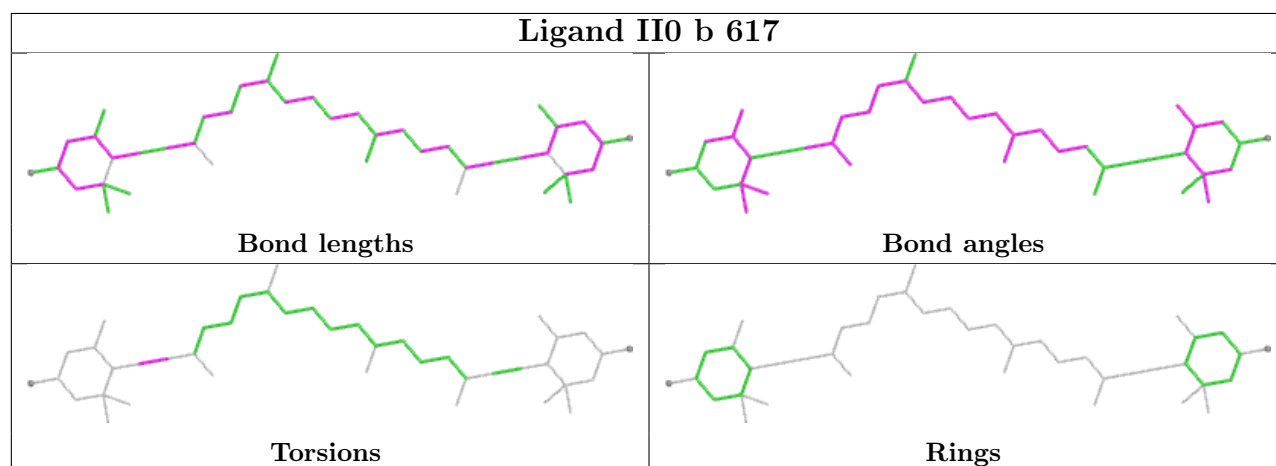
Bond angles

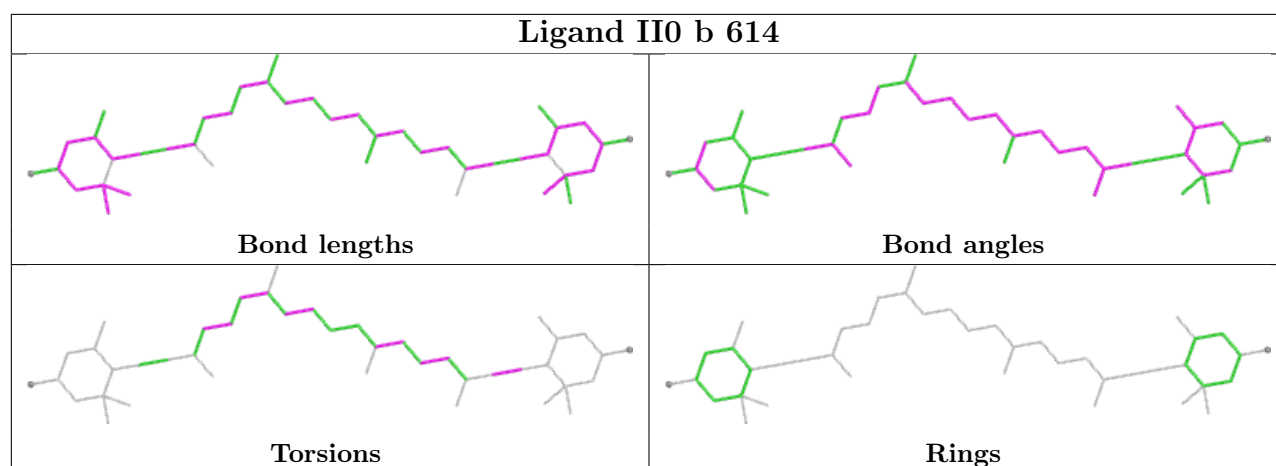
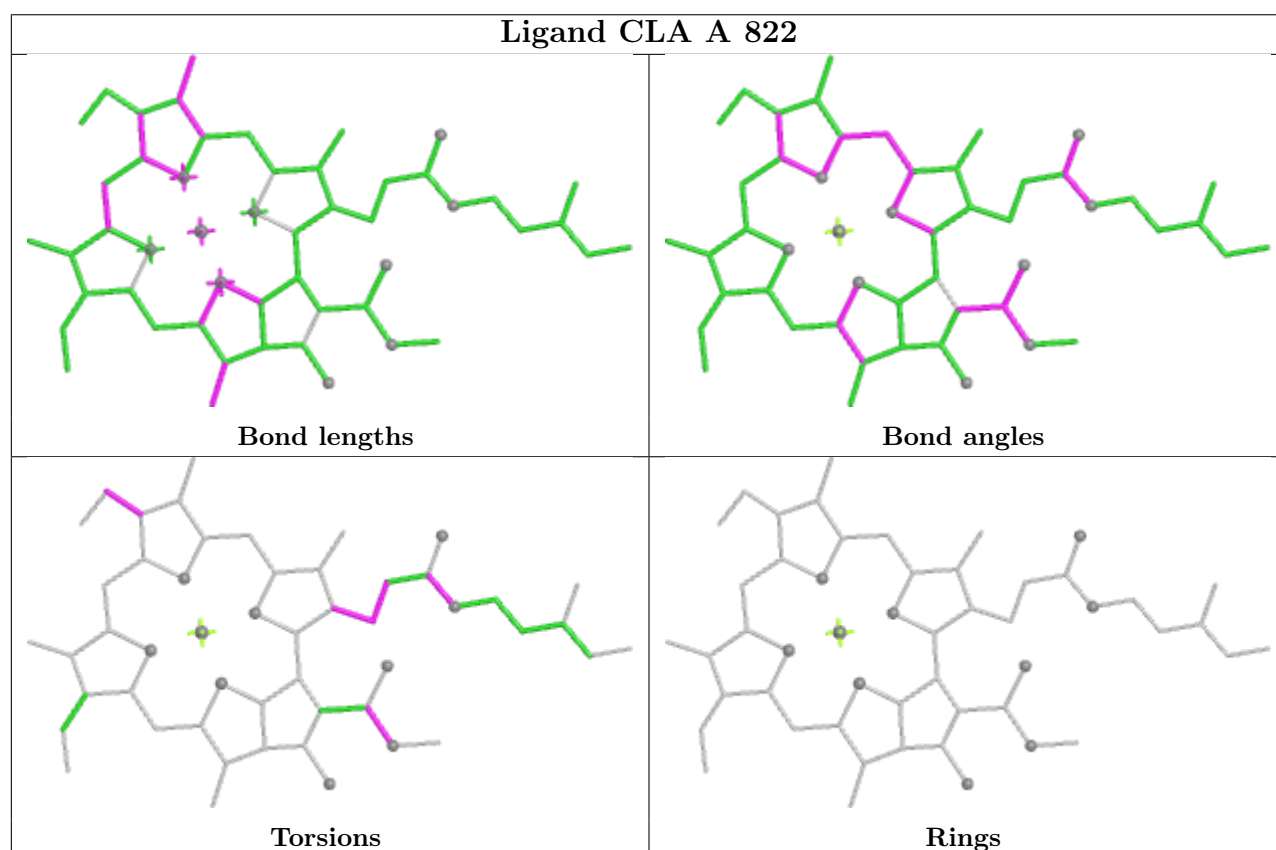


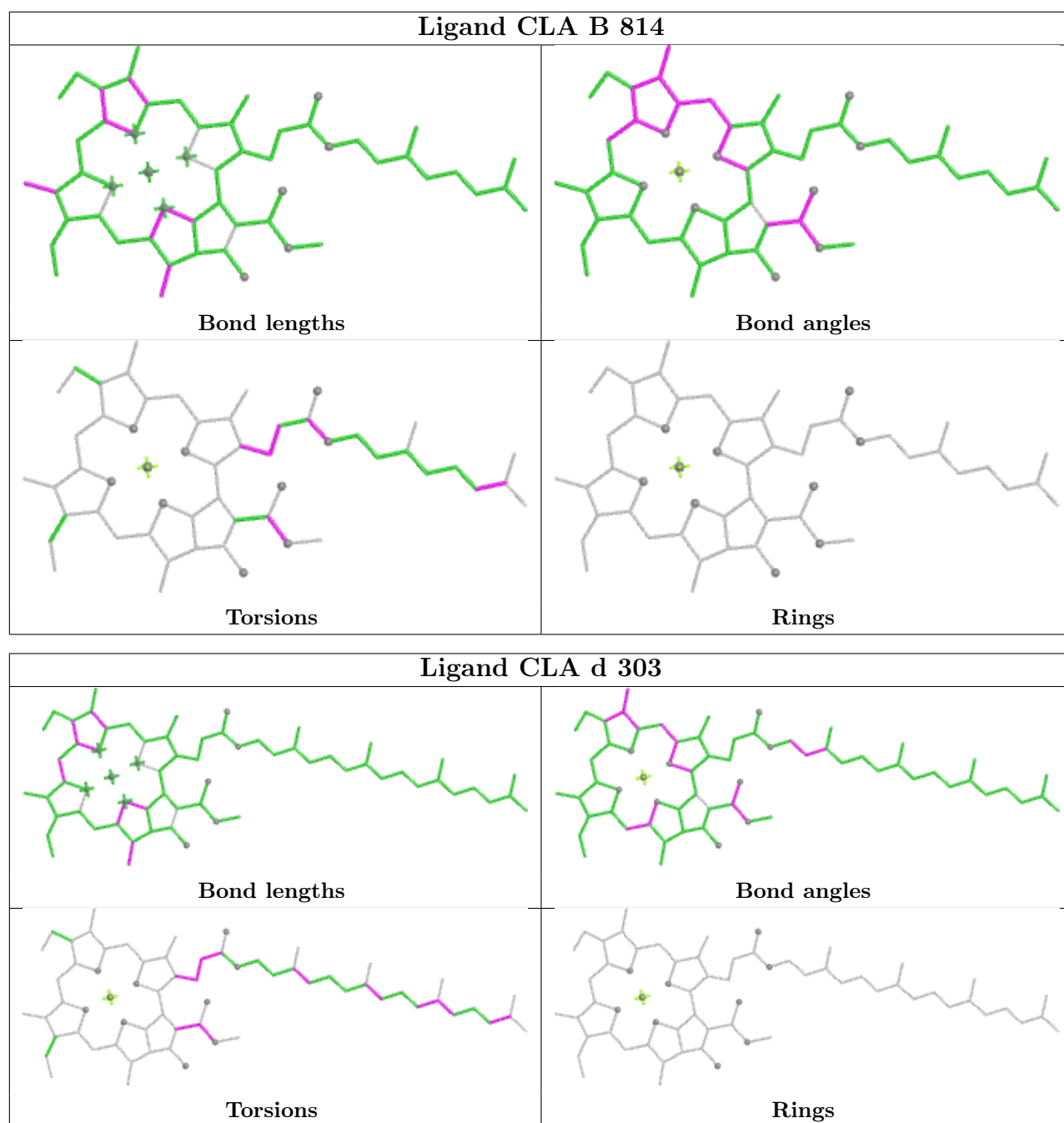
Torsions

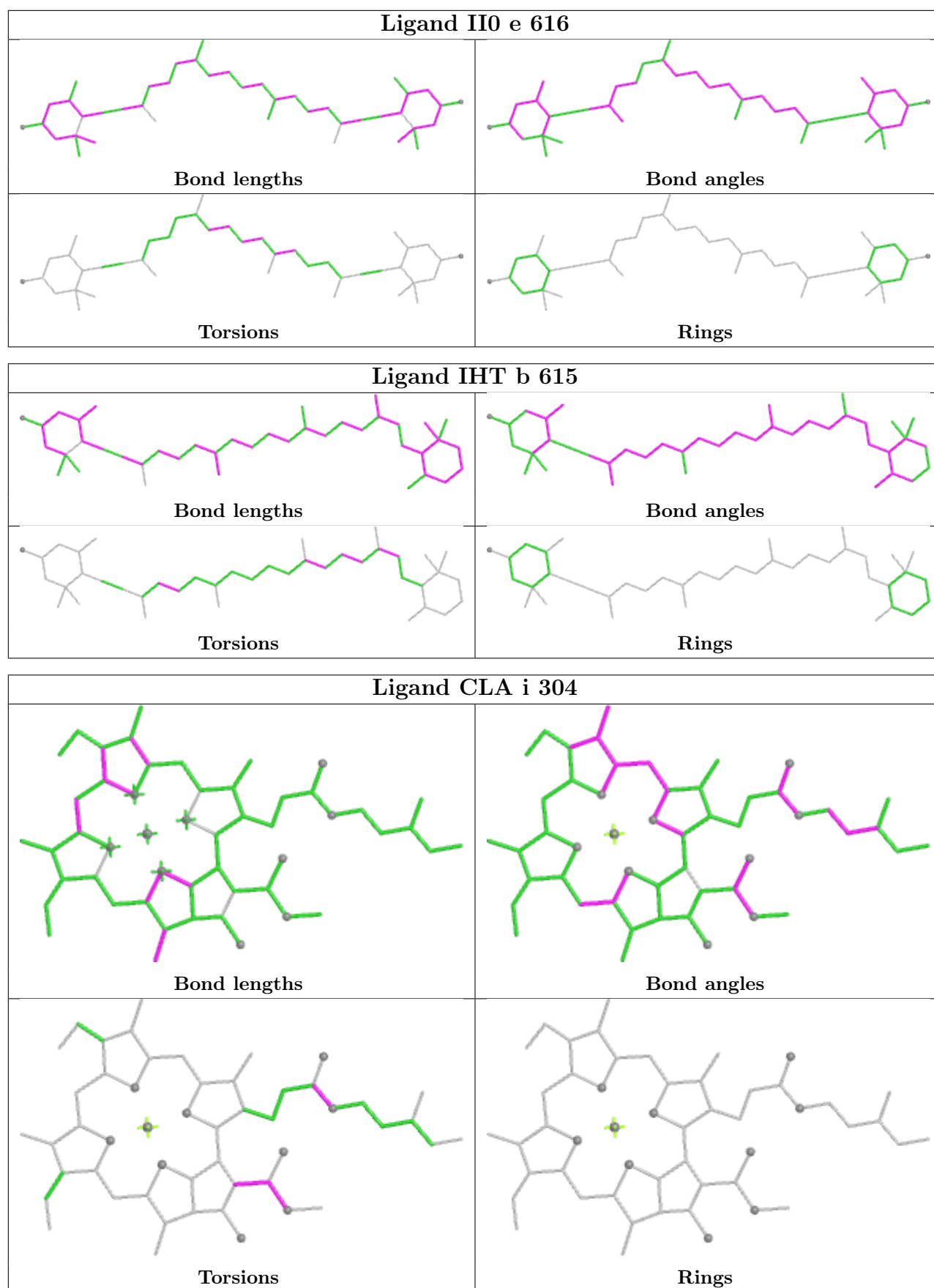


Rings

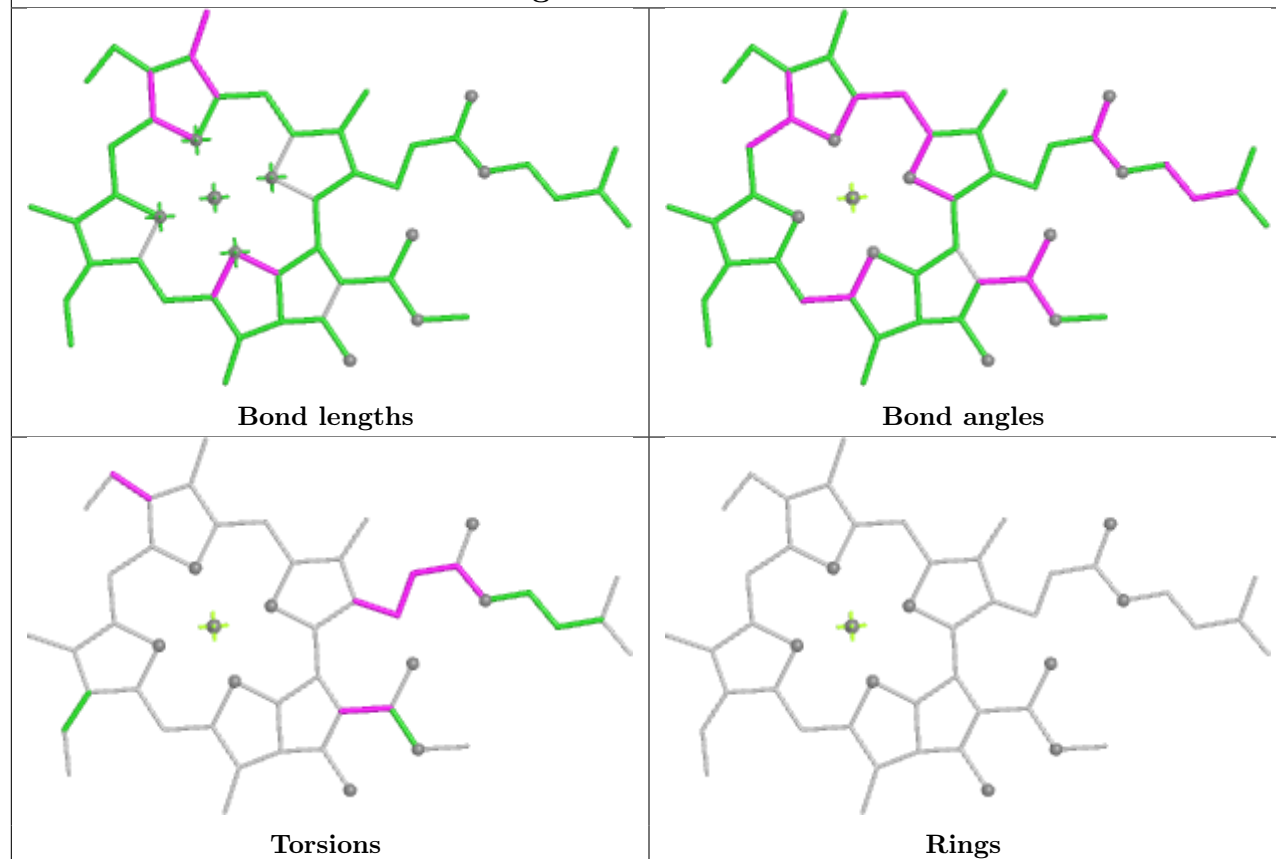




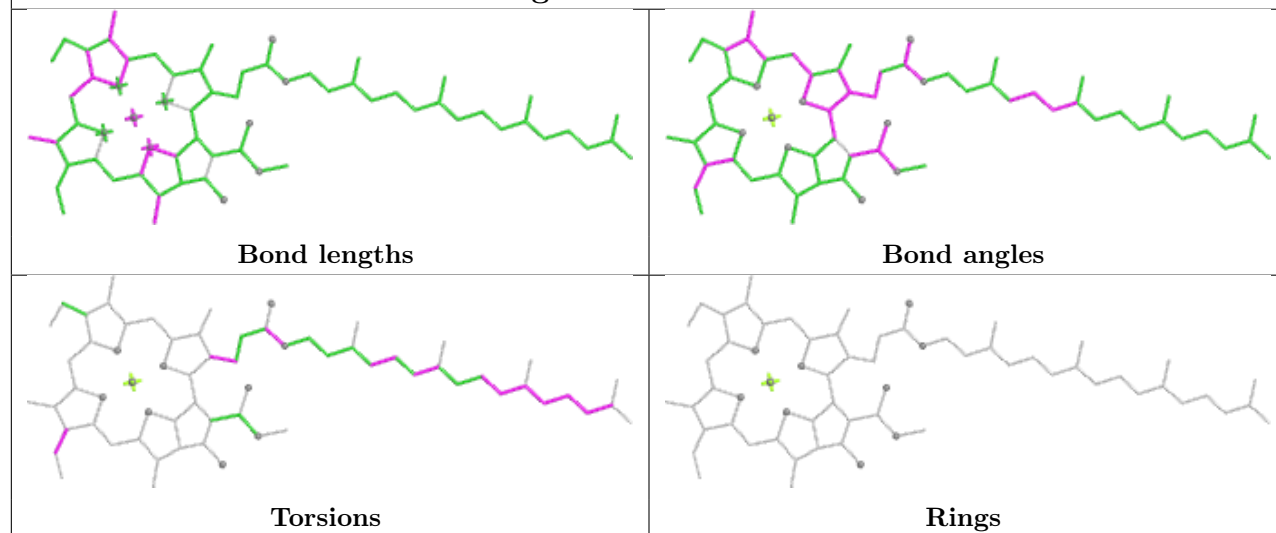


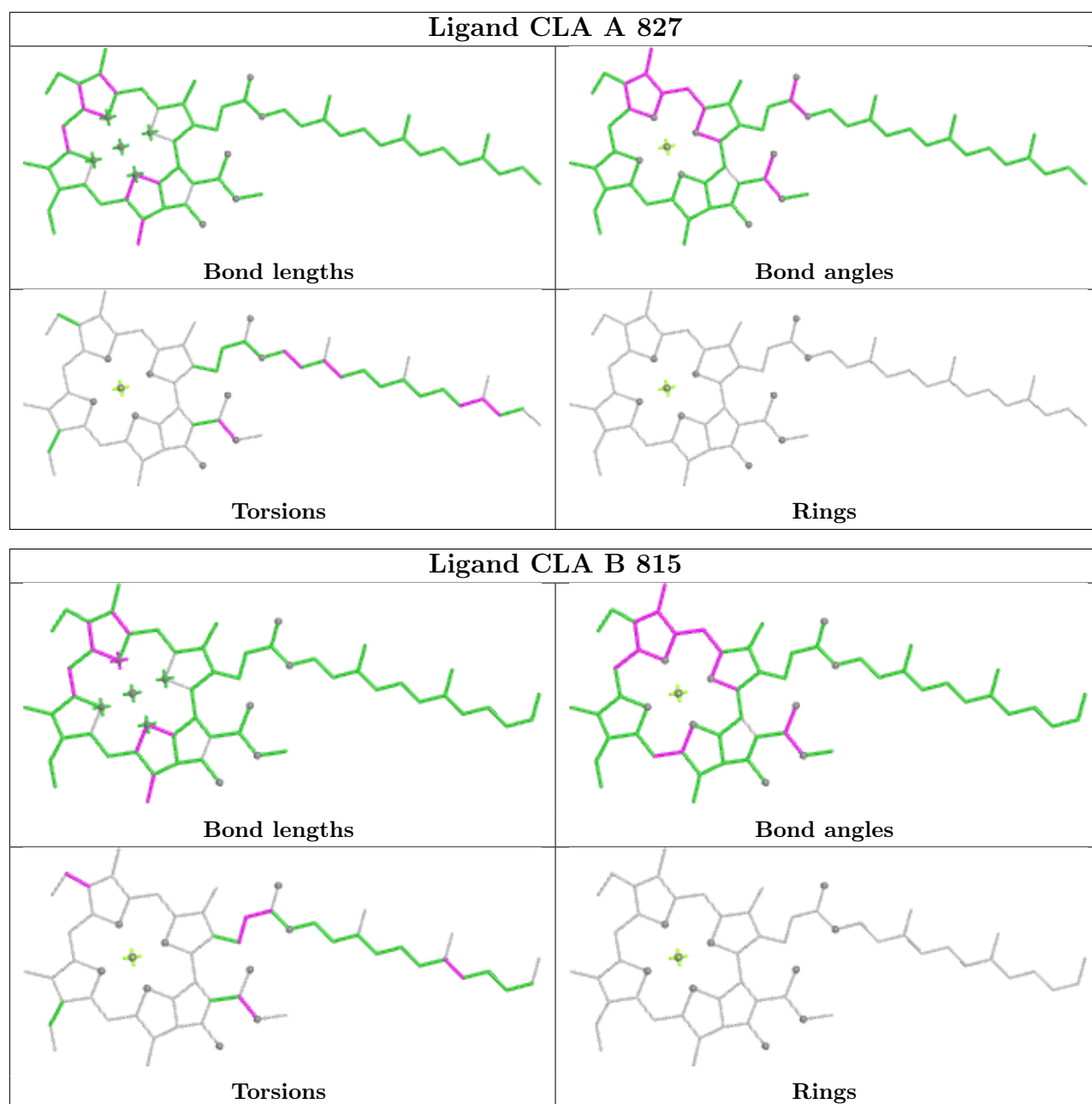


Ligand CLA B 827

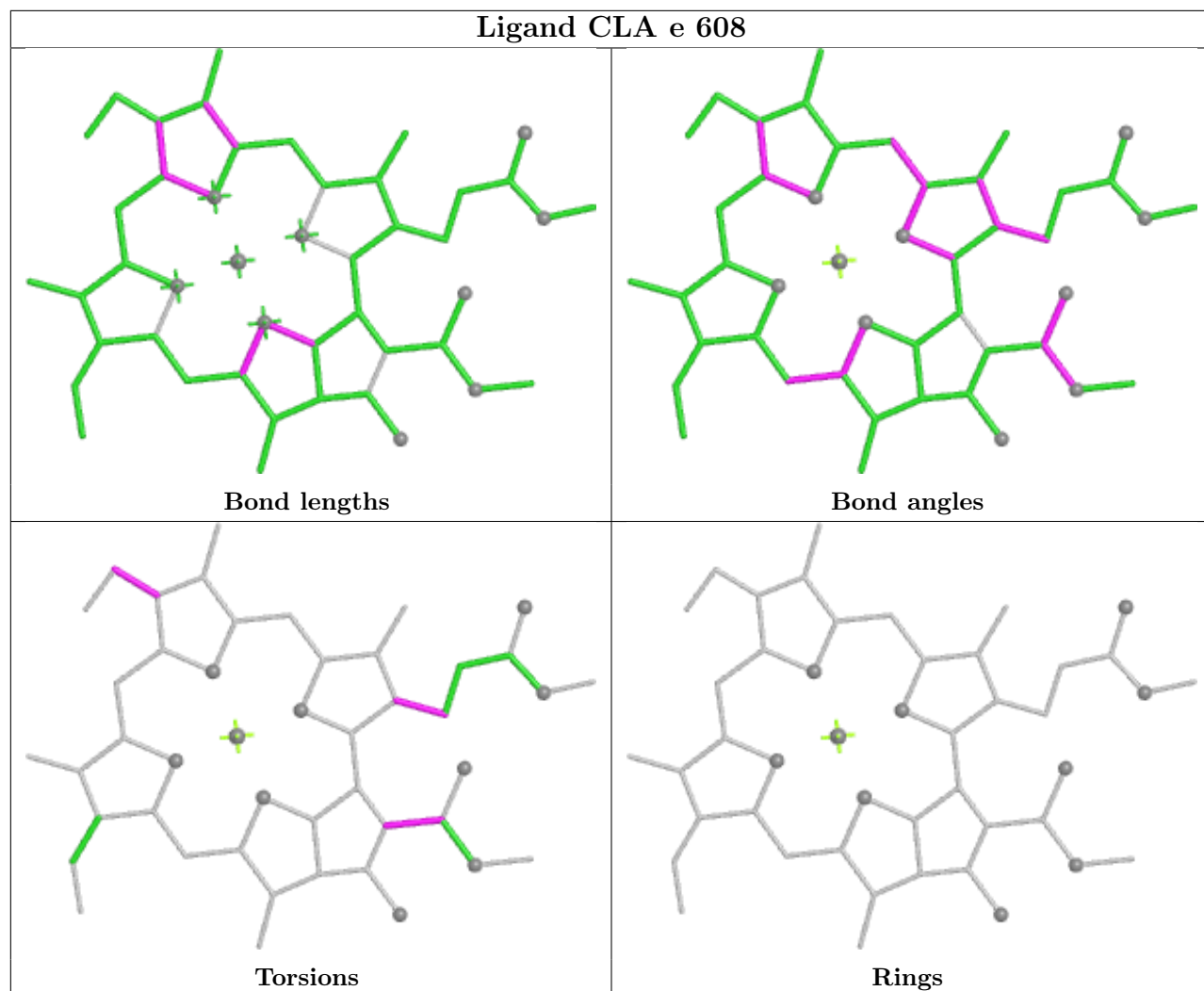


Ligand CLA O 206

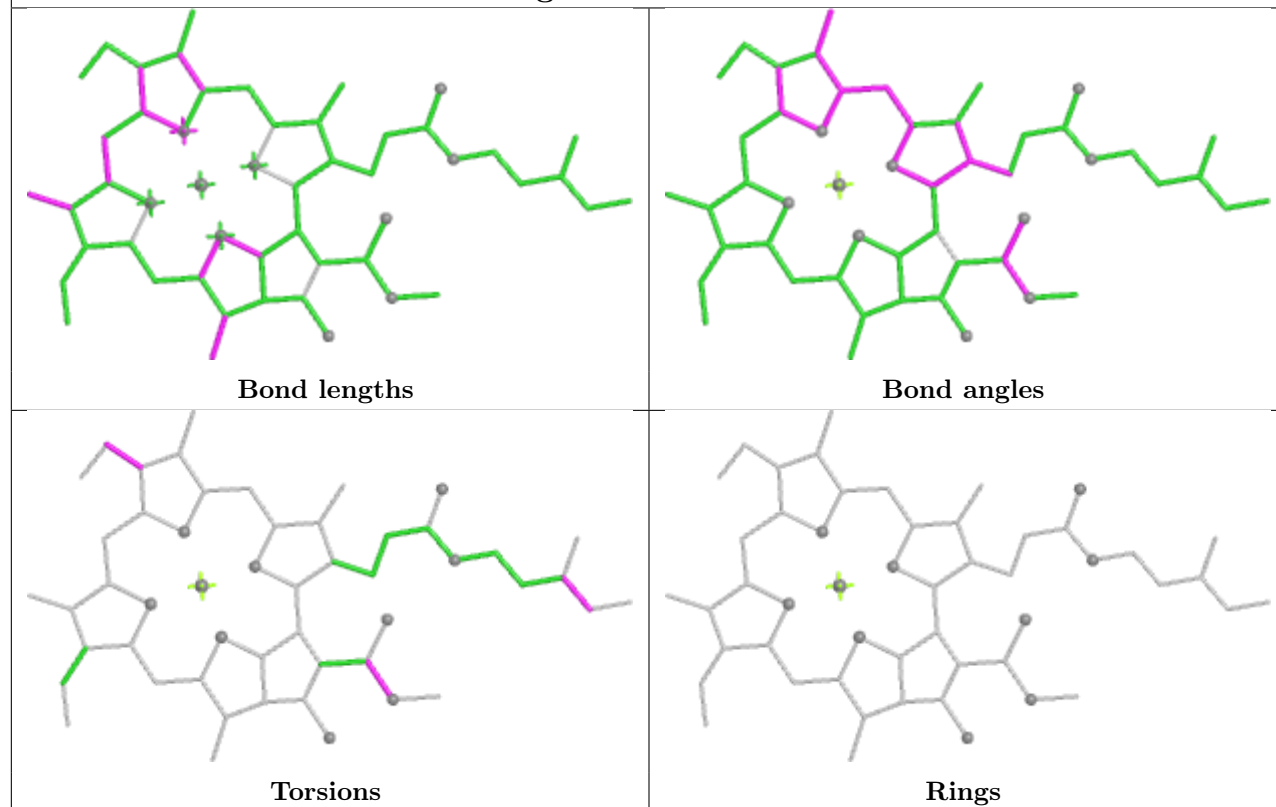




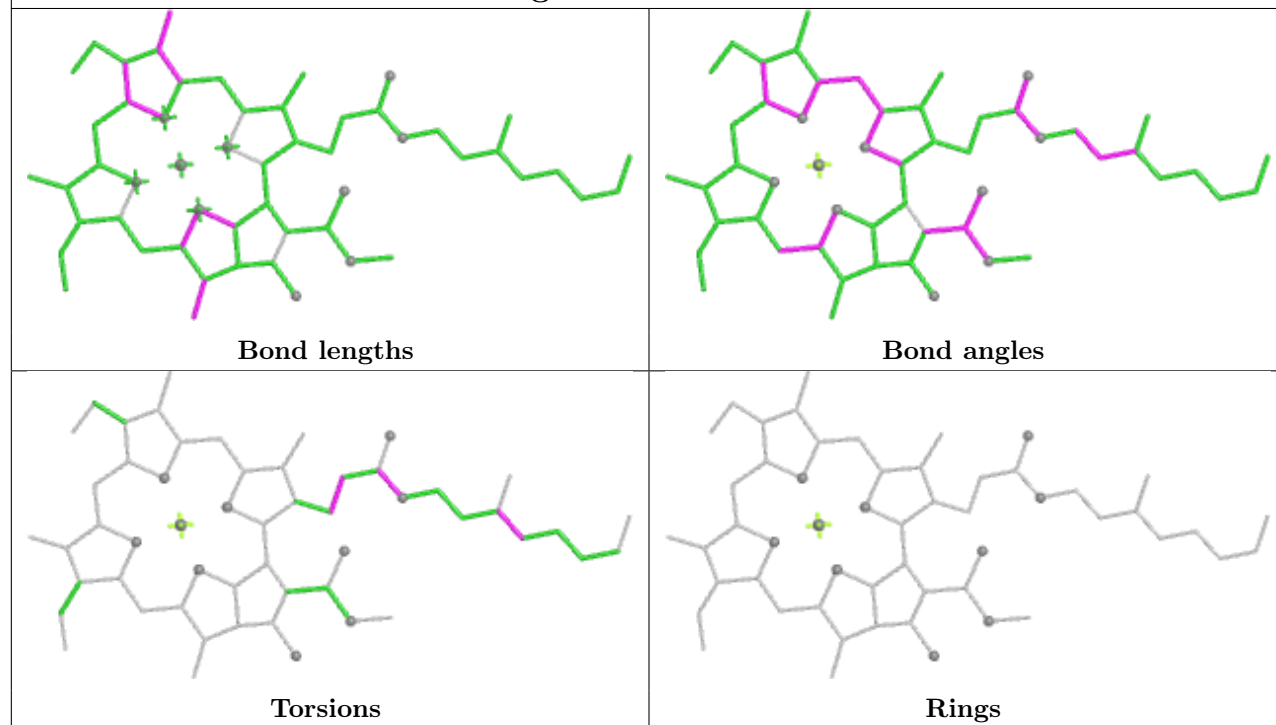
Ligand CLA e 608



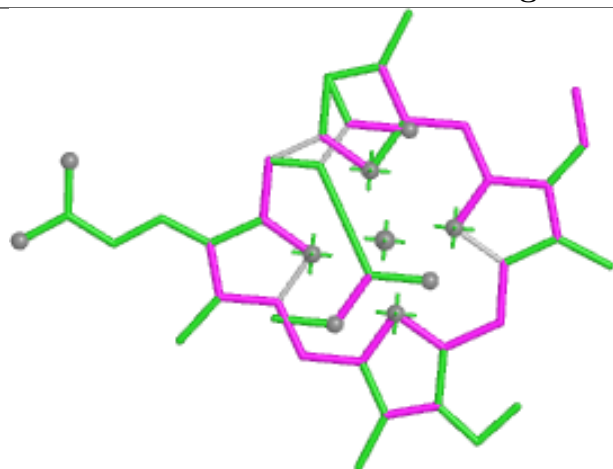
Ligand CLA a 305



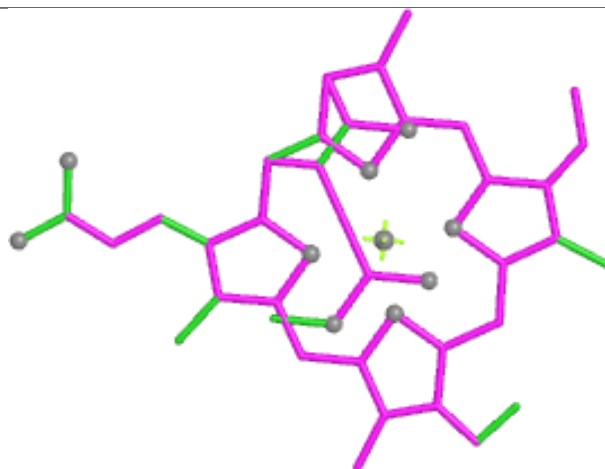
Ligand CLA A 811



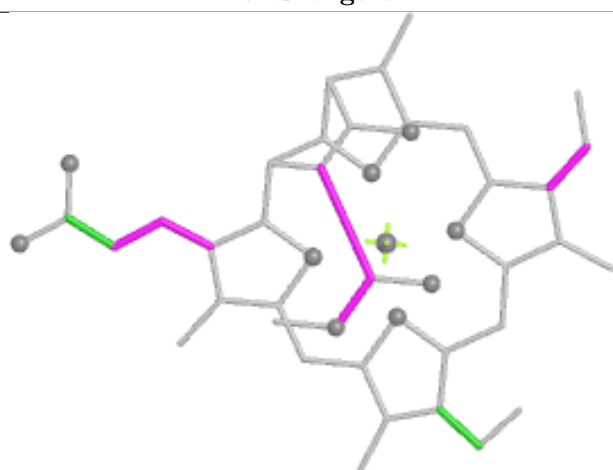
Ligand KC2 k 613



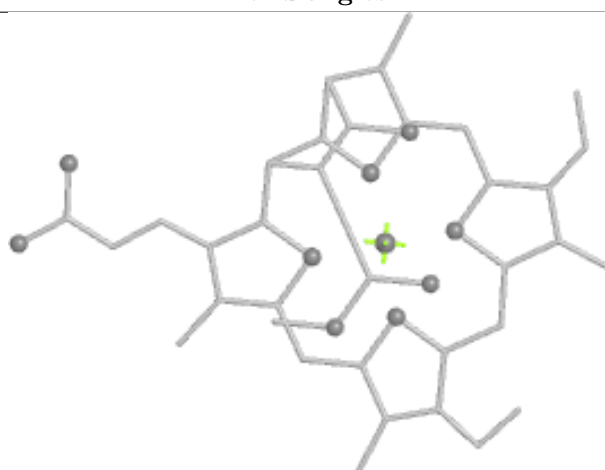
Bond lengths



Bond angles

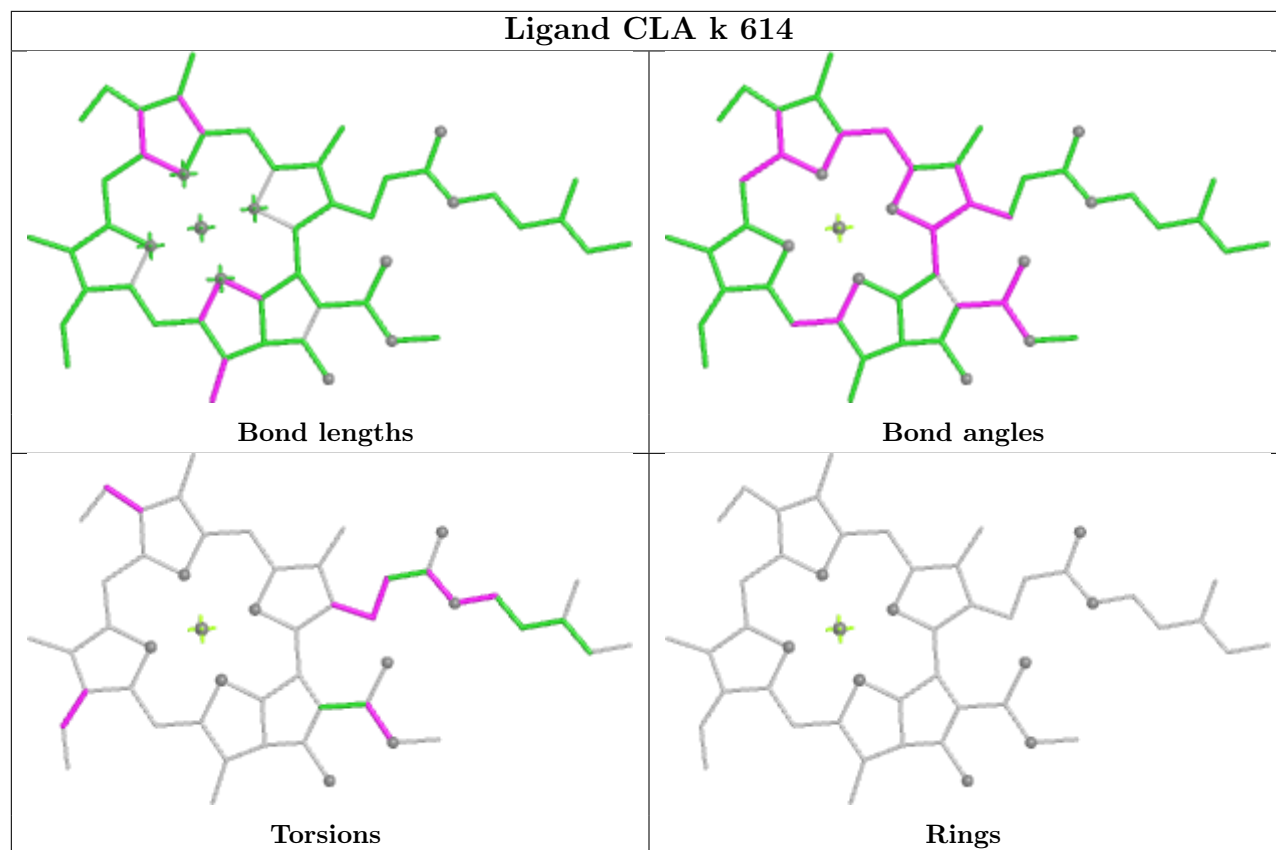


Torsions

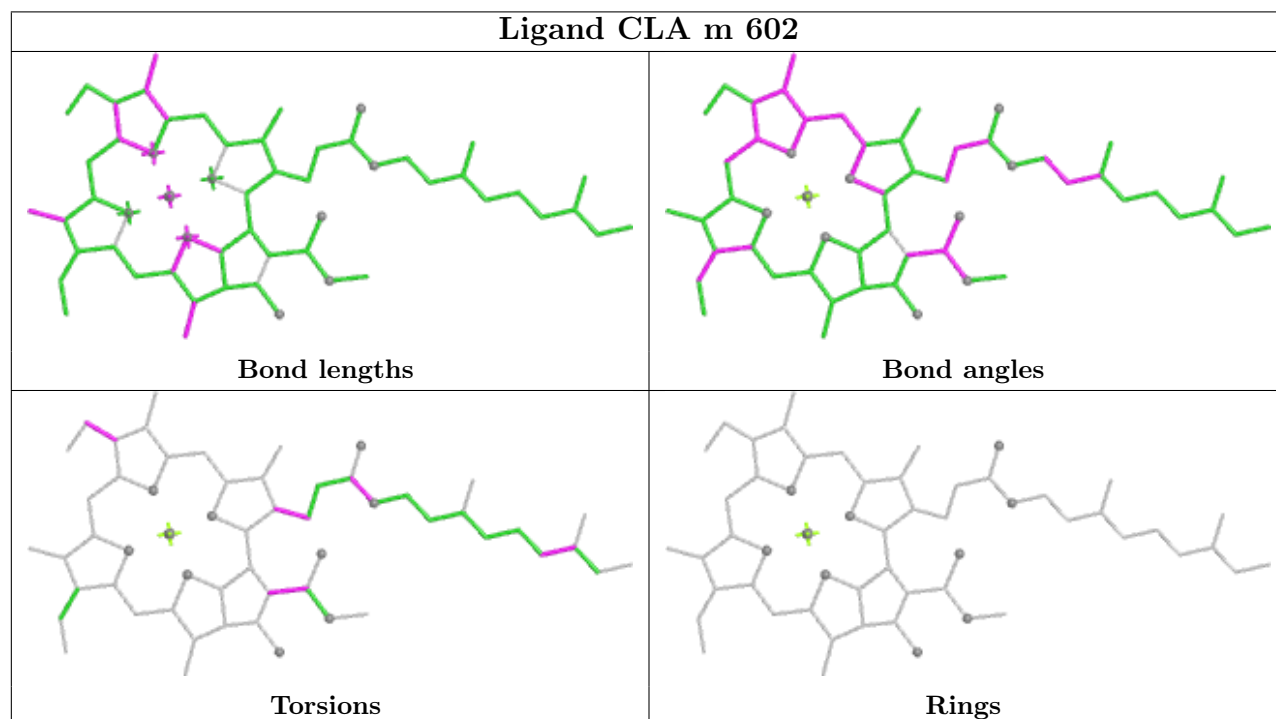


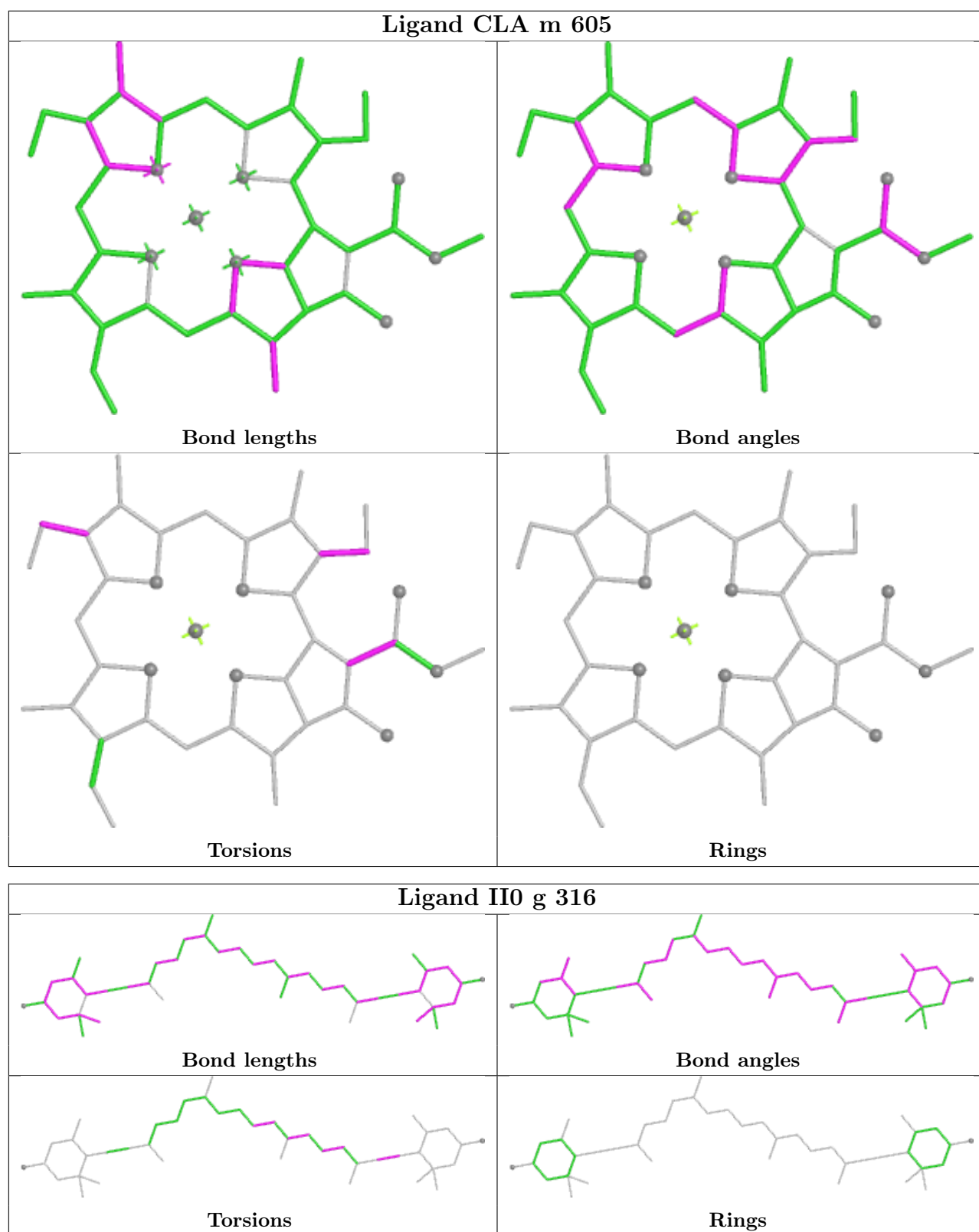
Rings

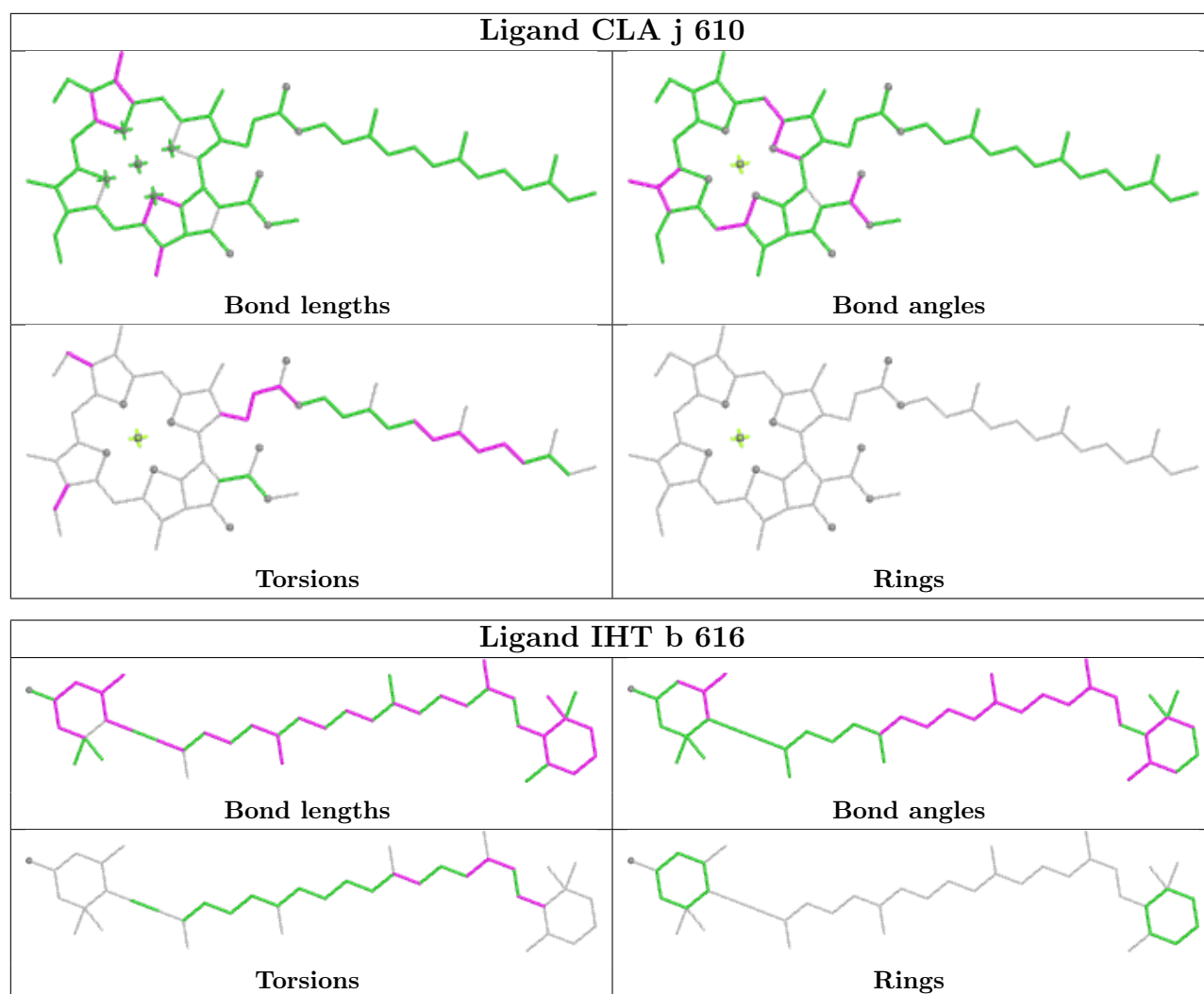
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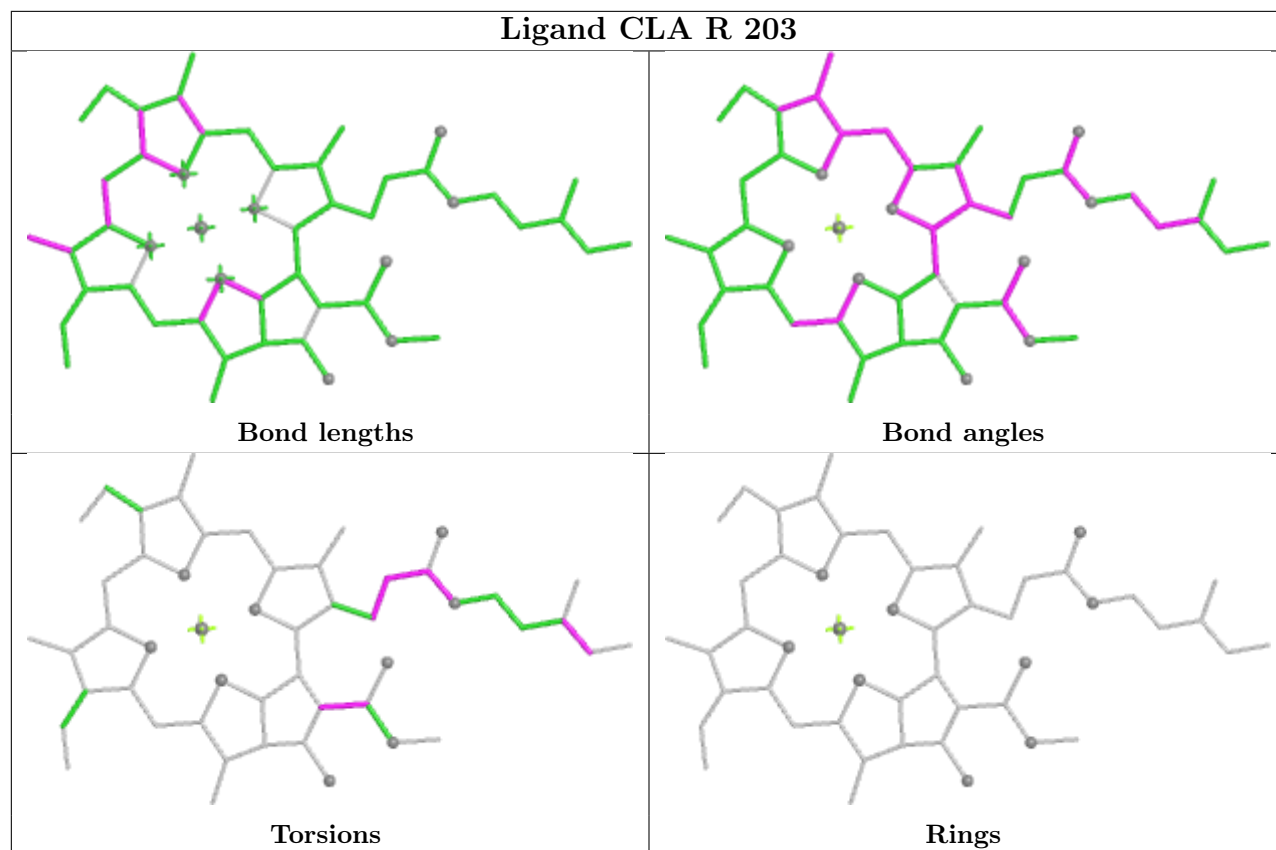
Ligand CLA m 602



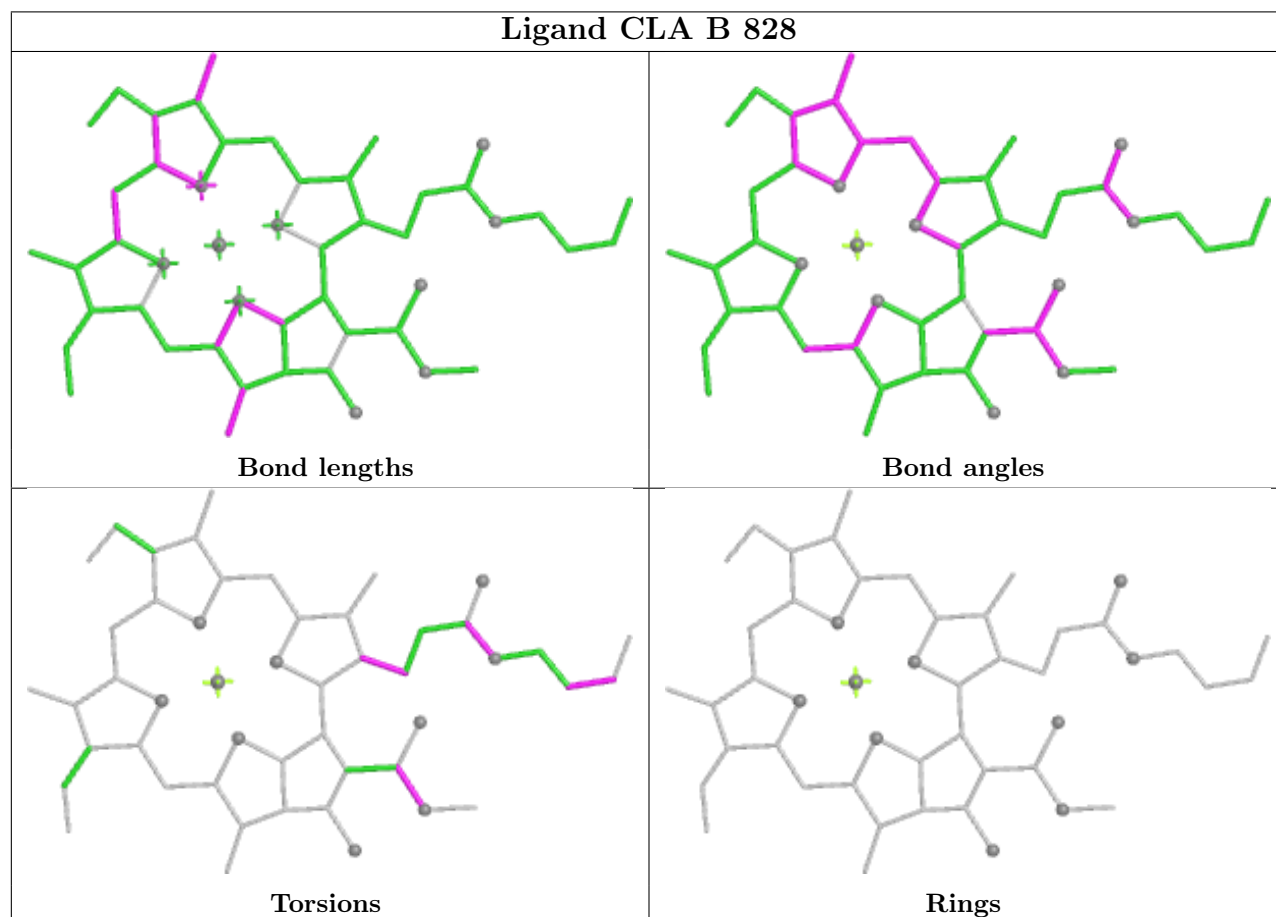




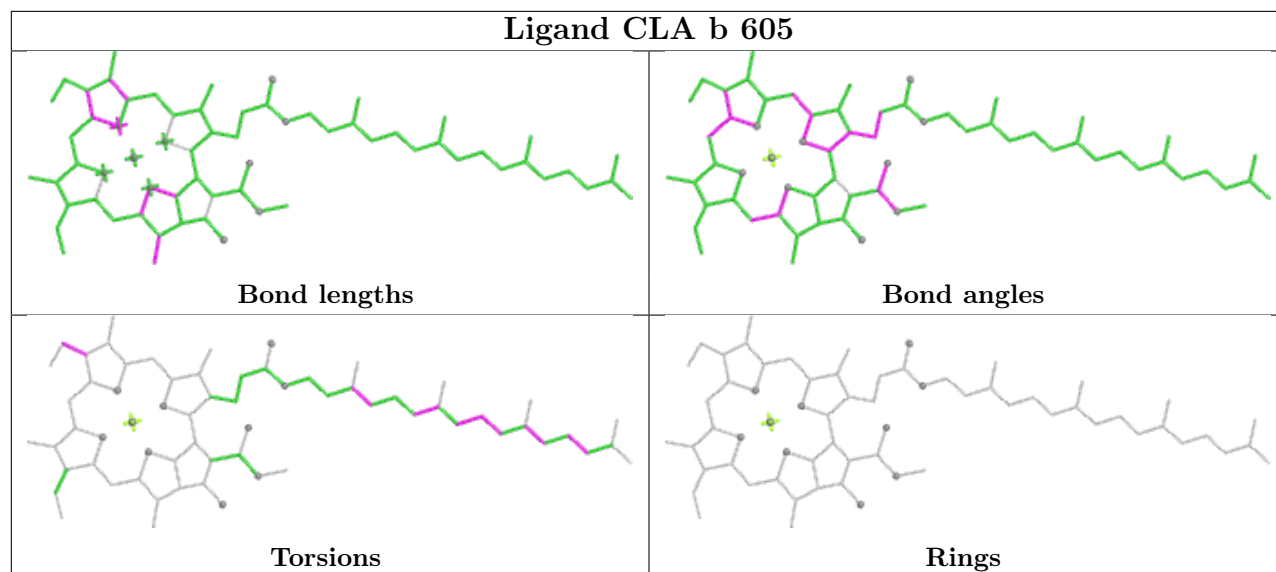
Ligand CLA R 203



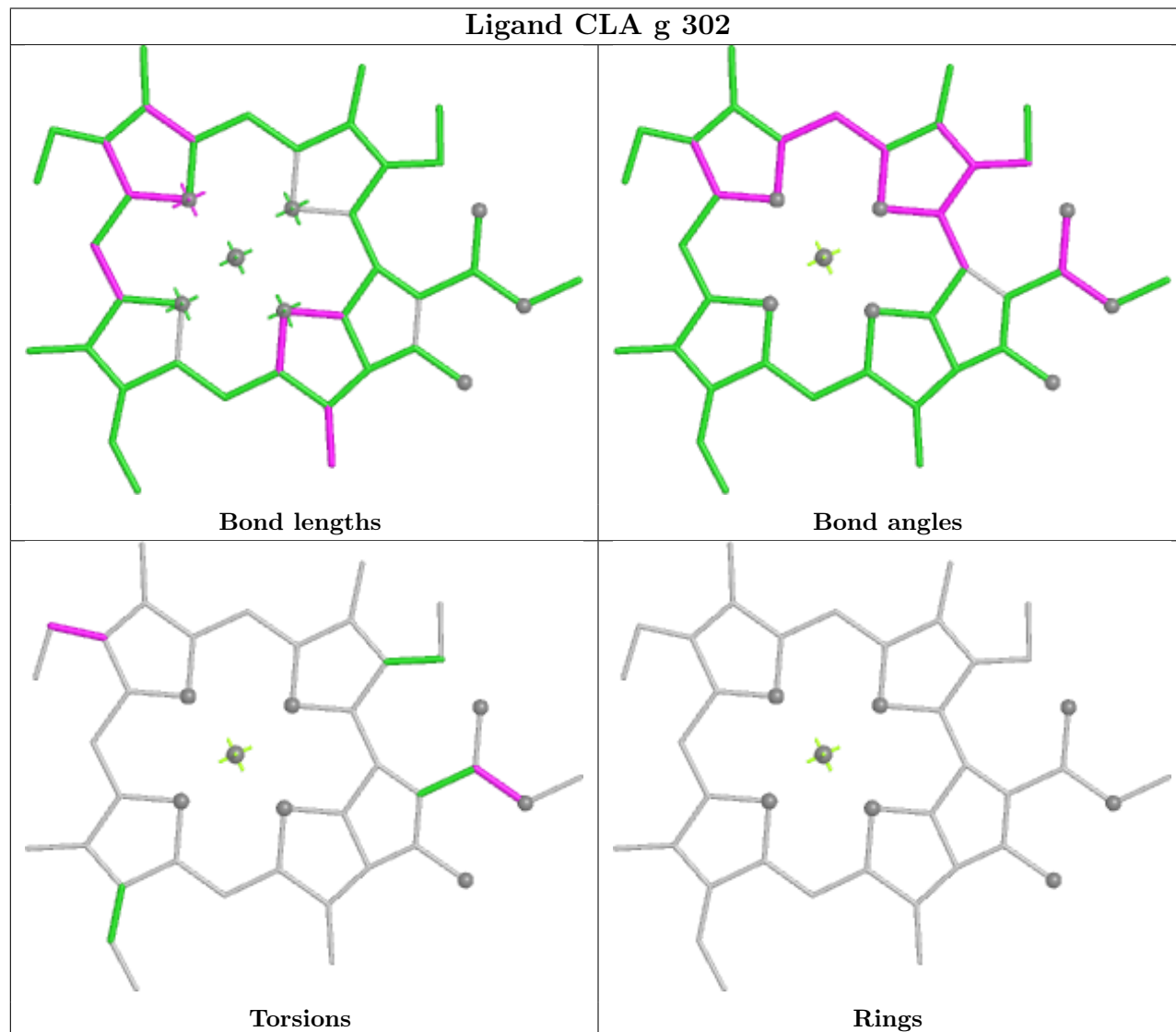
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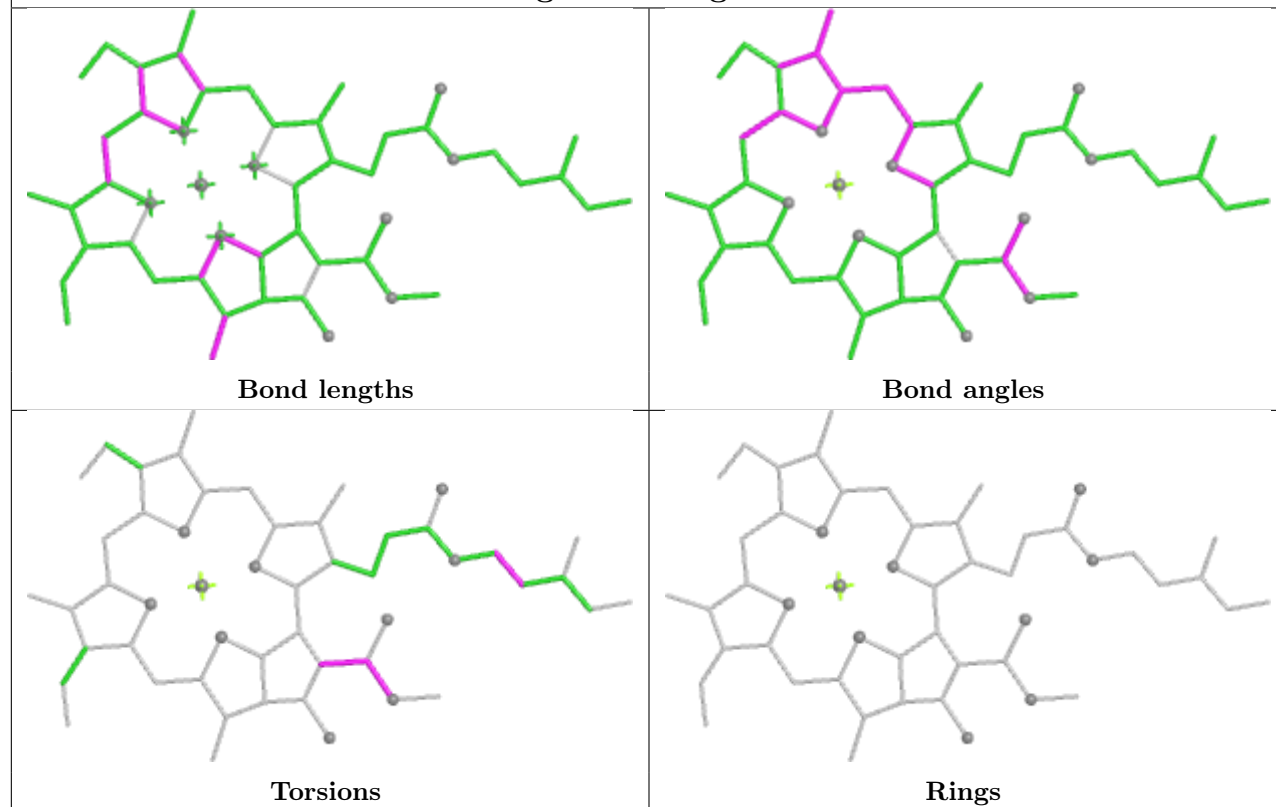
Ligand CLA b 605



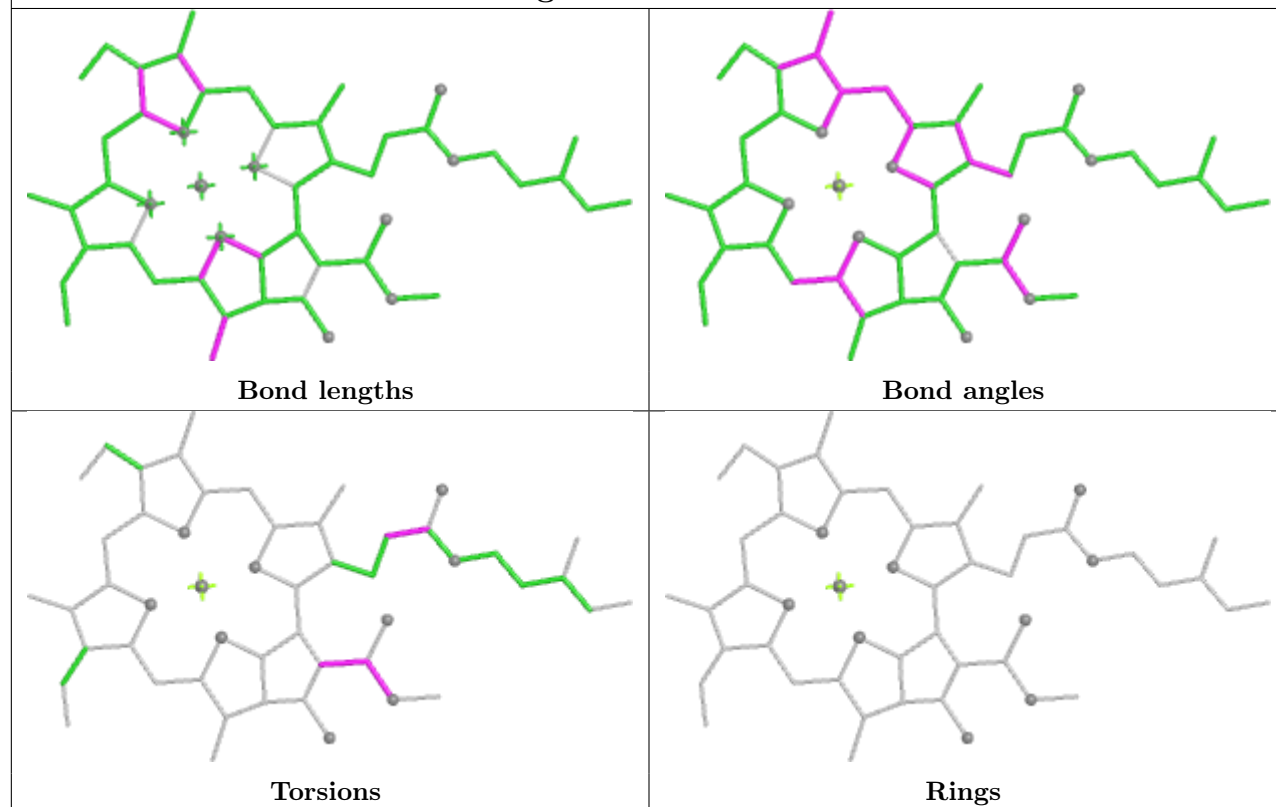
Ligand CLA g 302

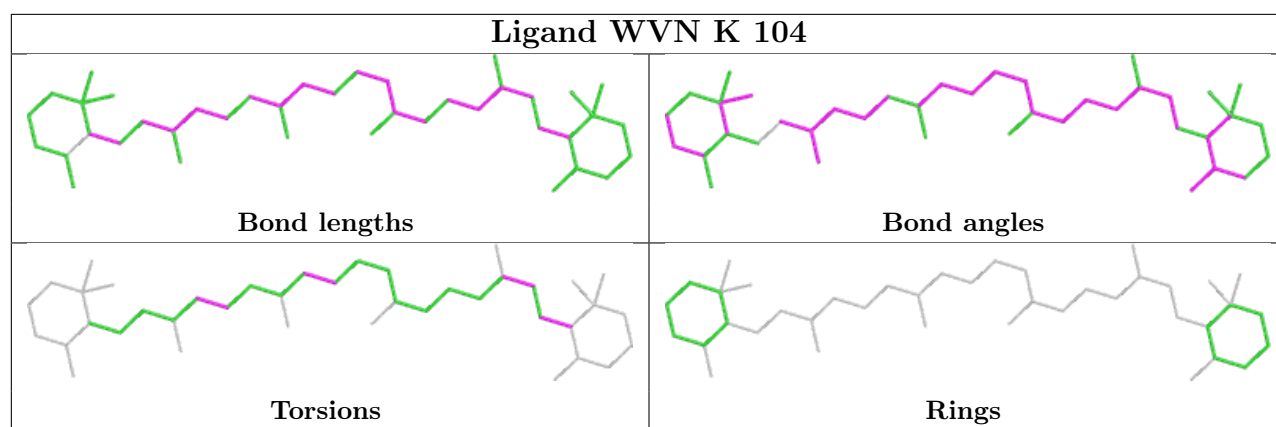
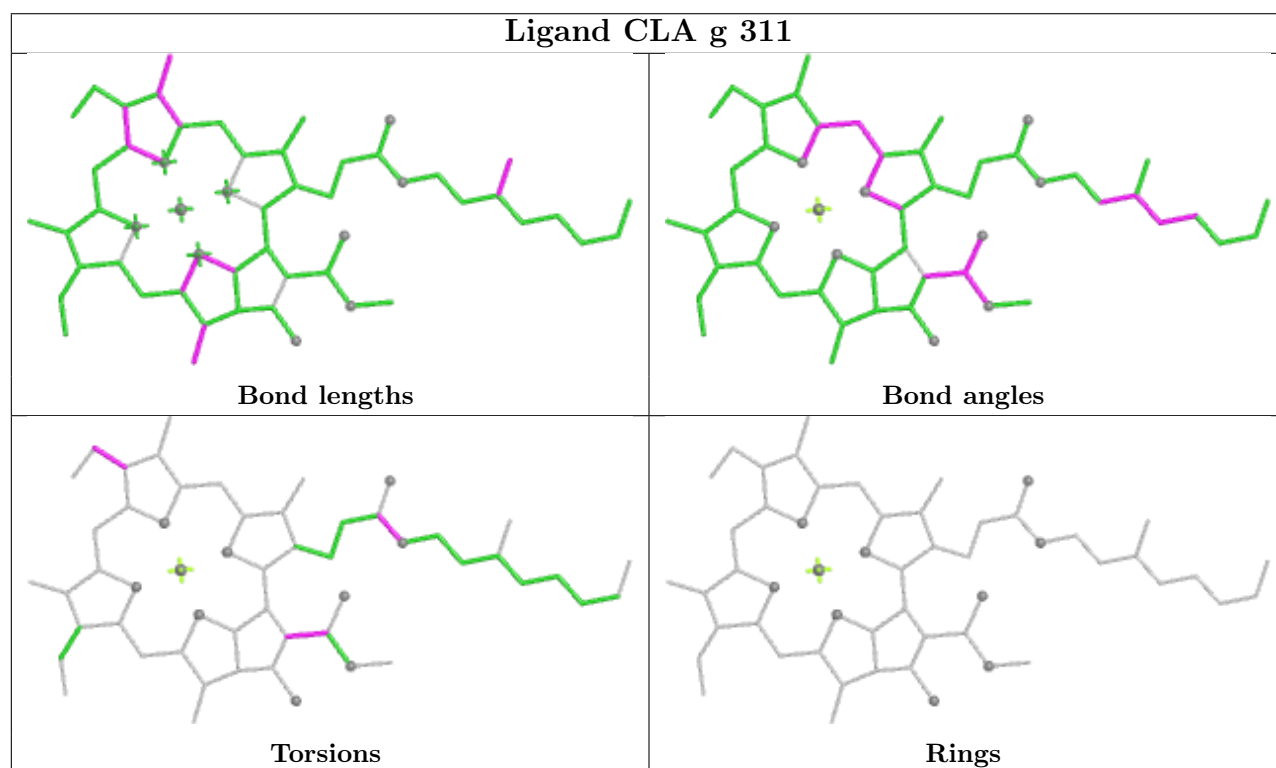
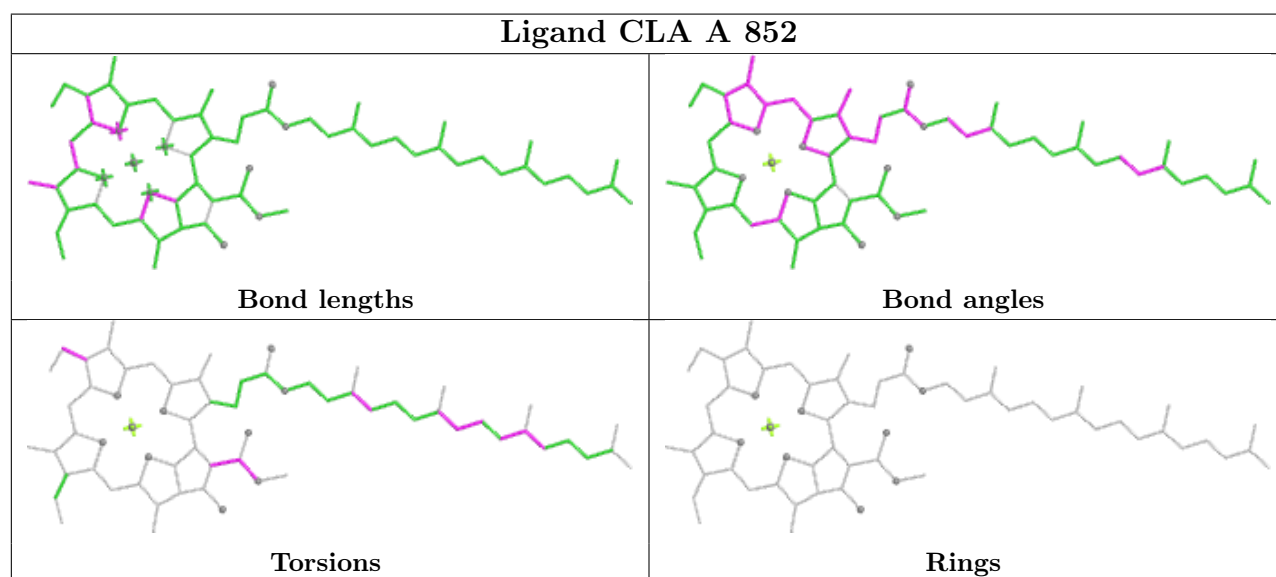


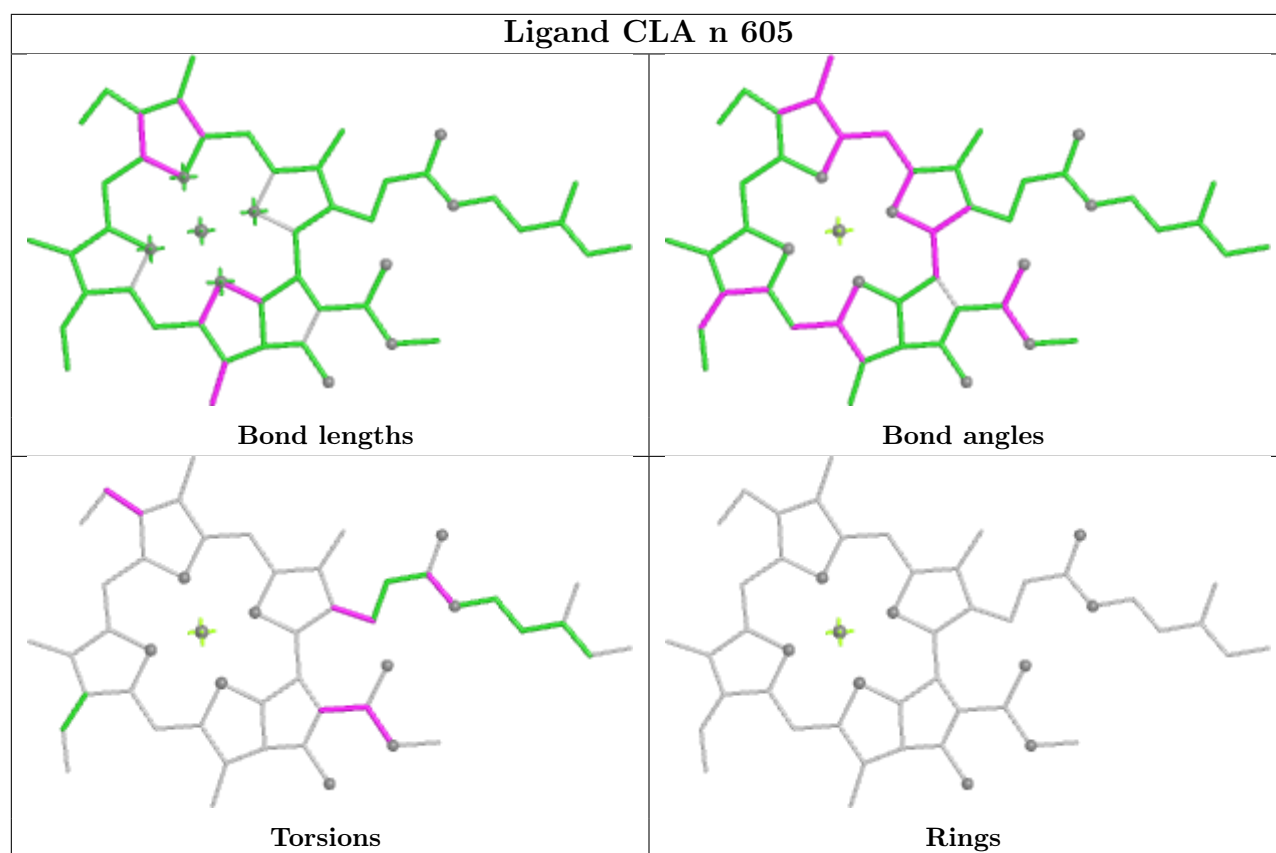
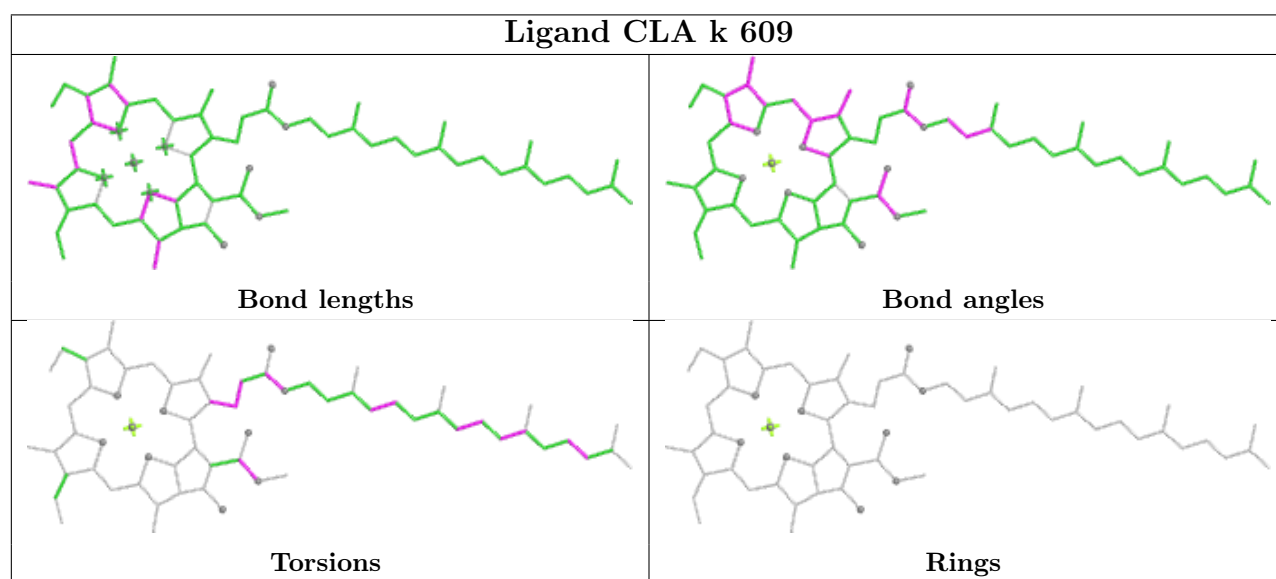
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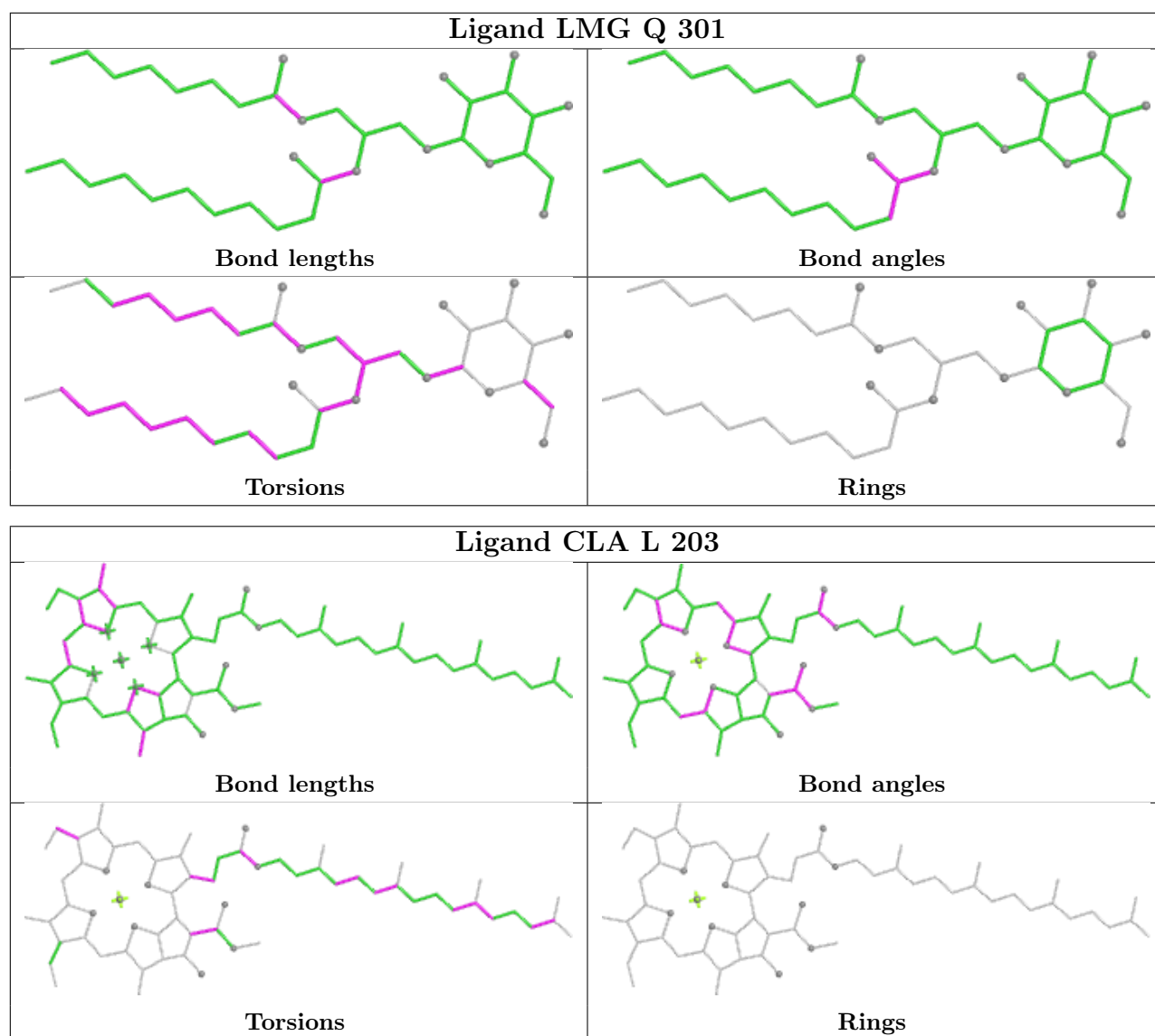


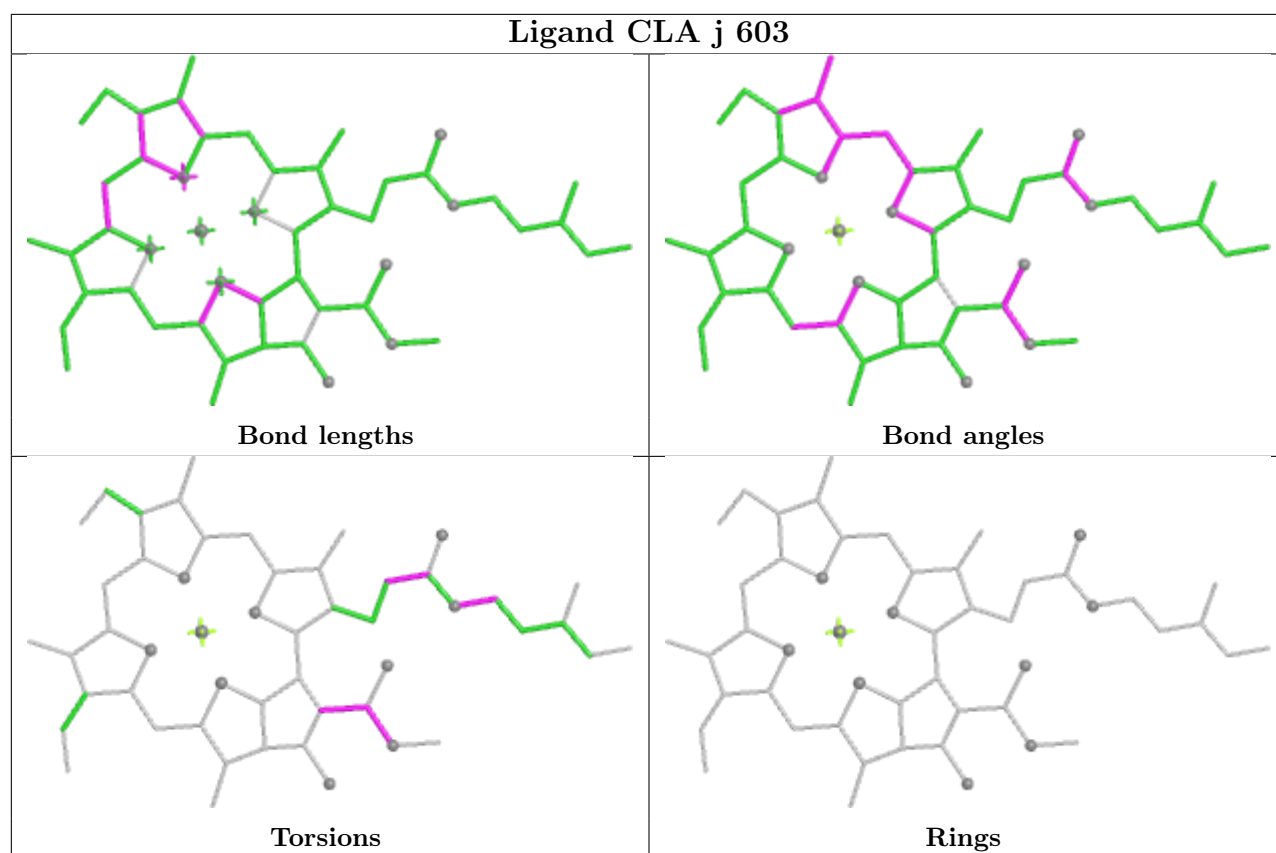
Ligand CLA e 603



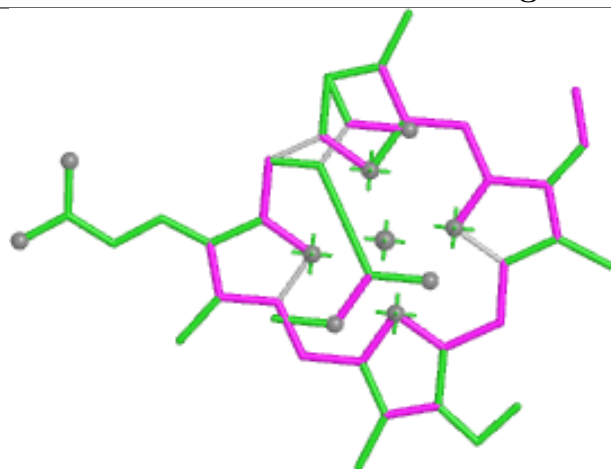




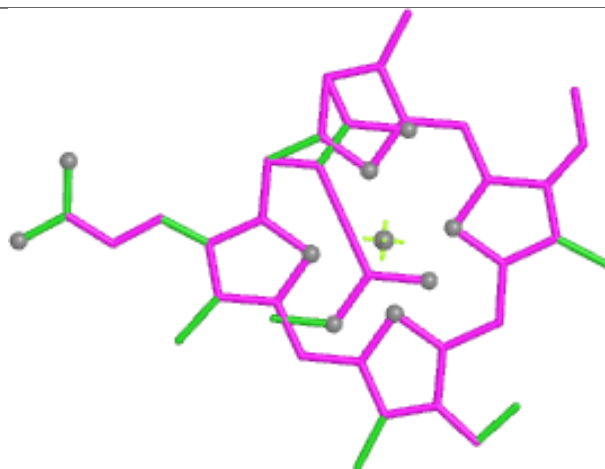




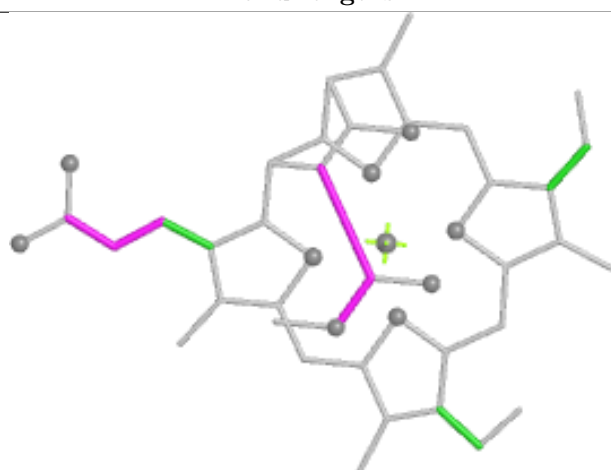
Ligand KC2 k 612



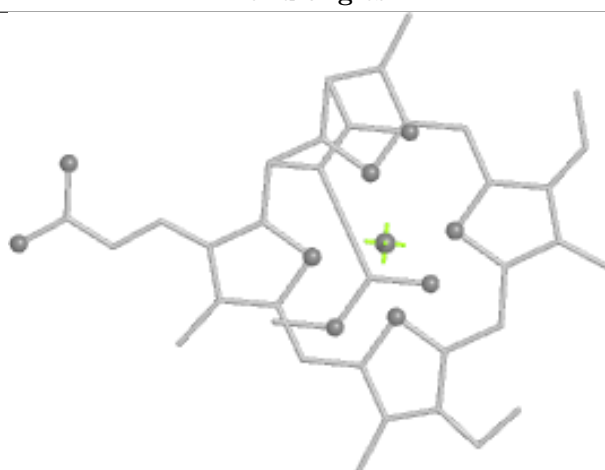
Bond lengths



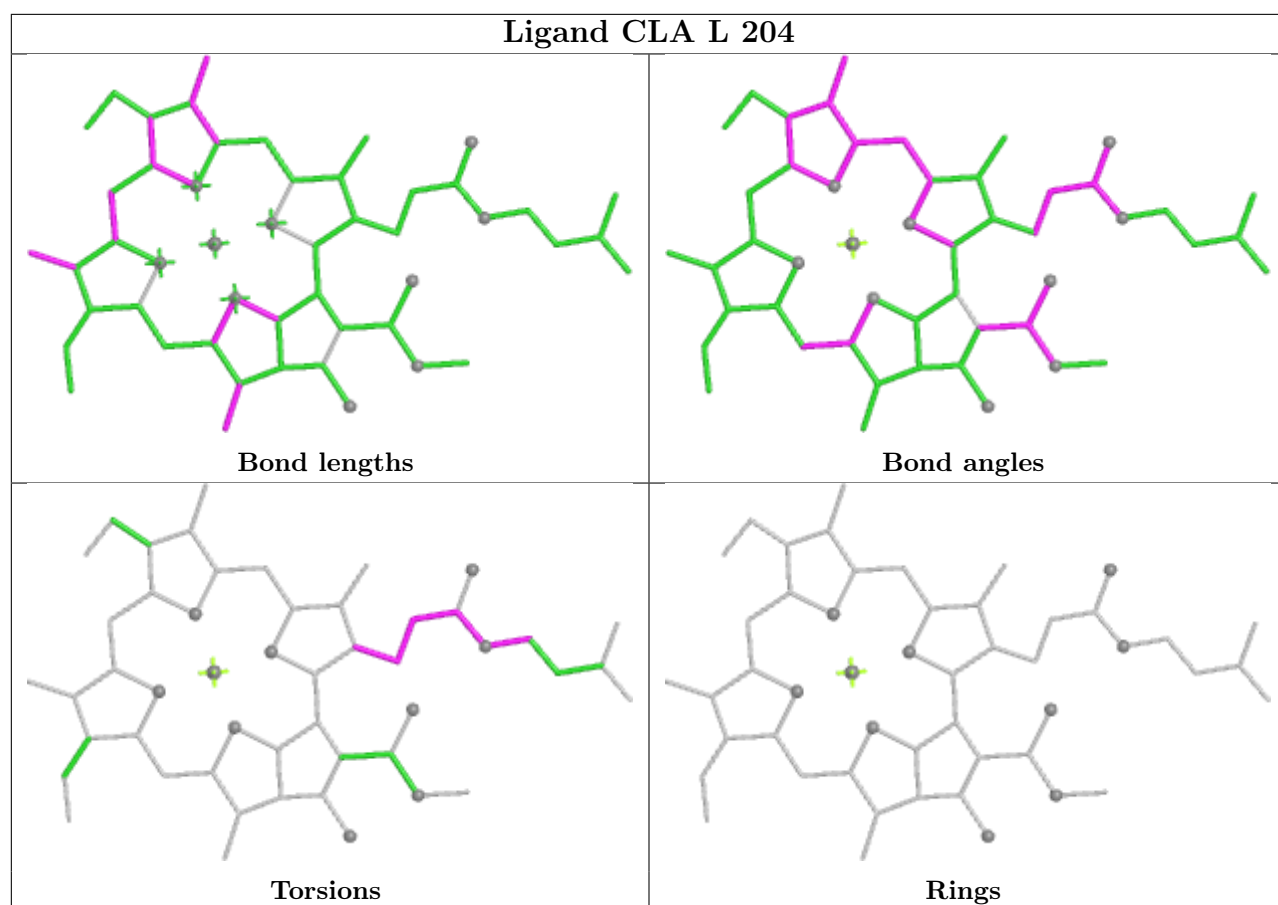
Bond angles

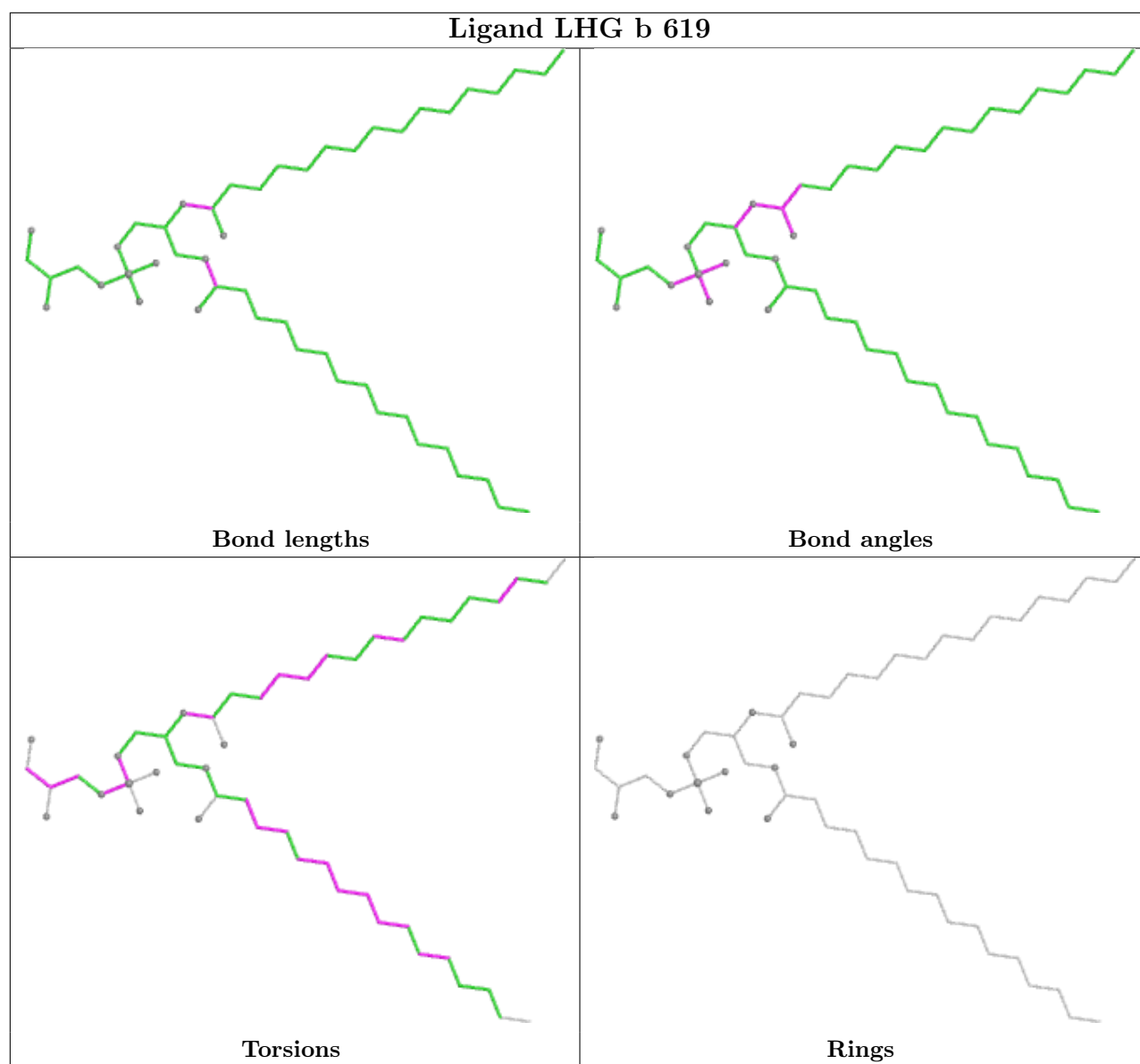


Torsions

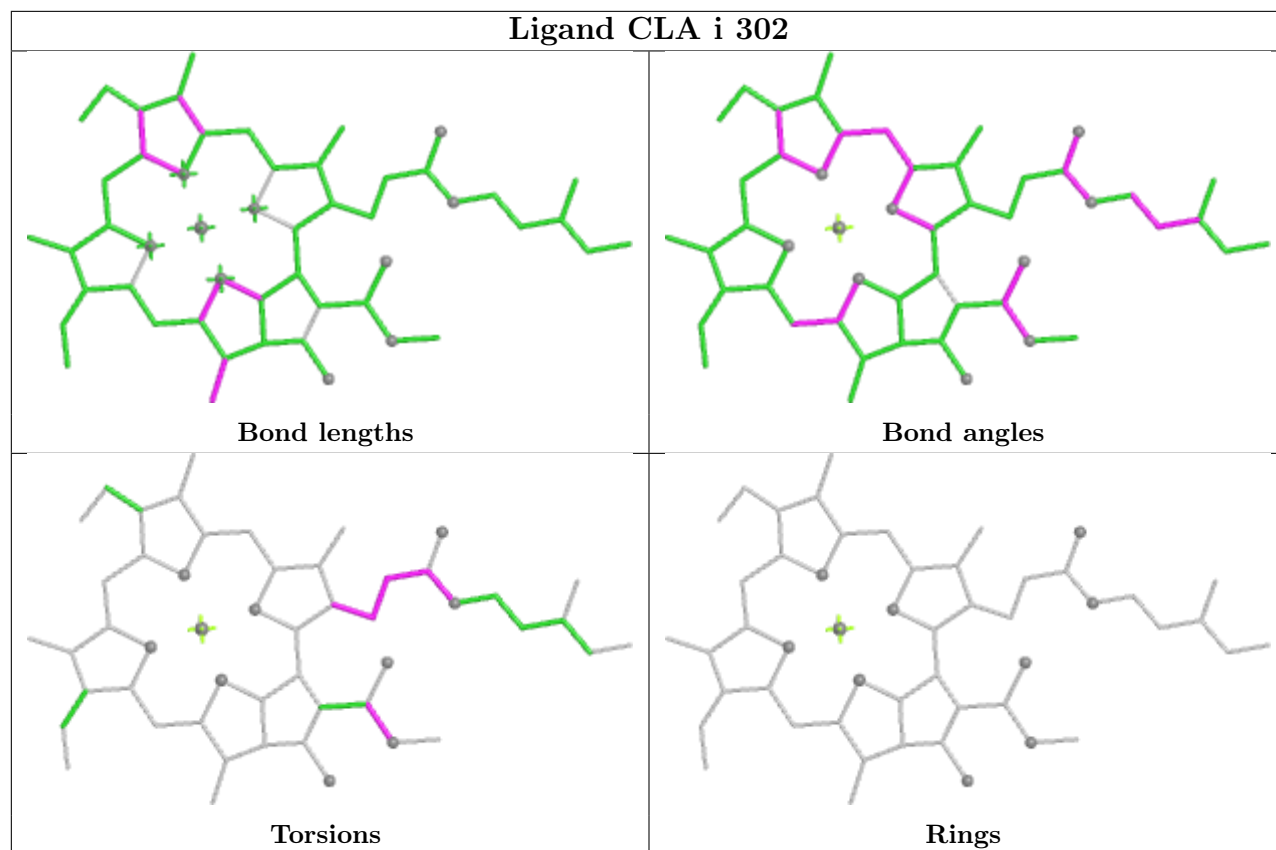


Rings

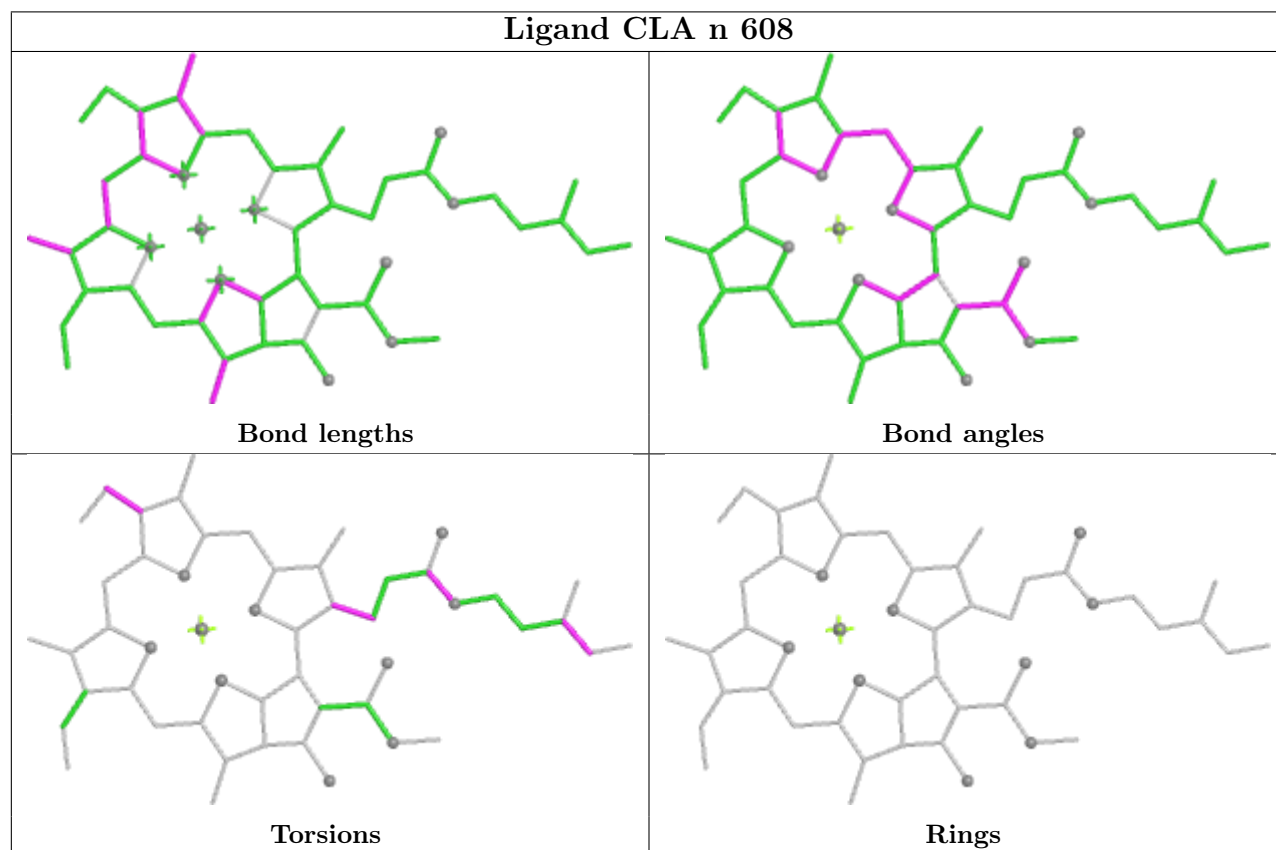




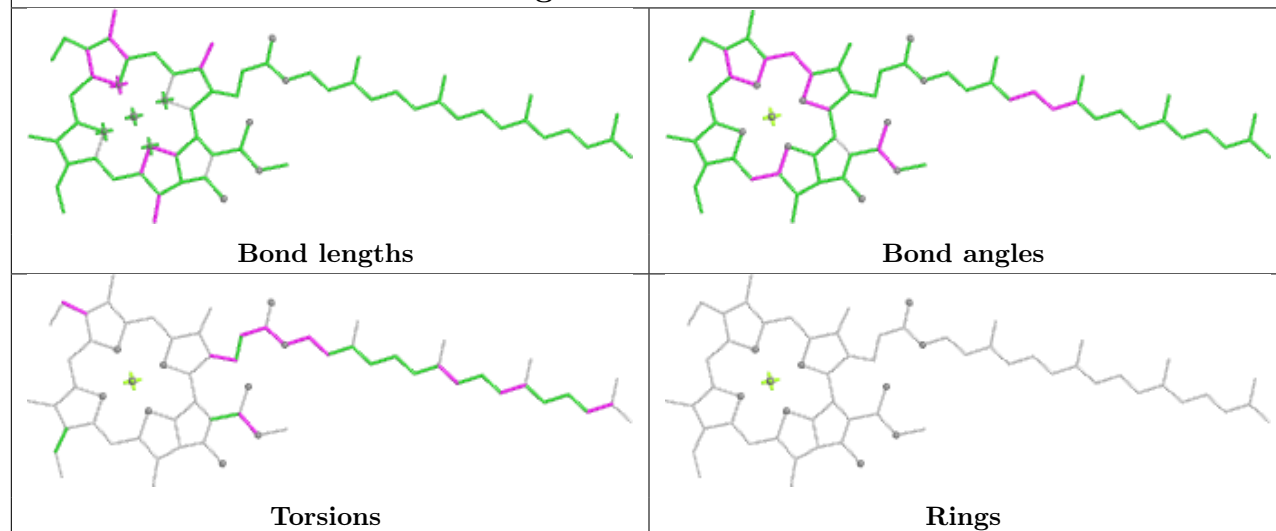
Ligand CLA i 302



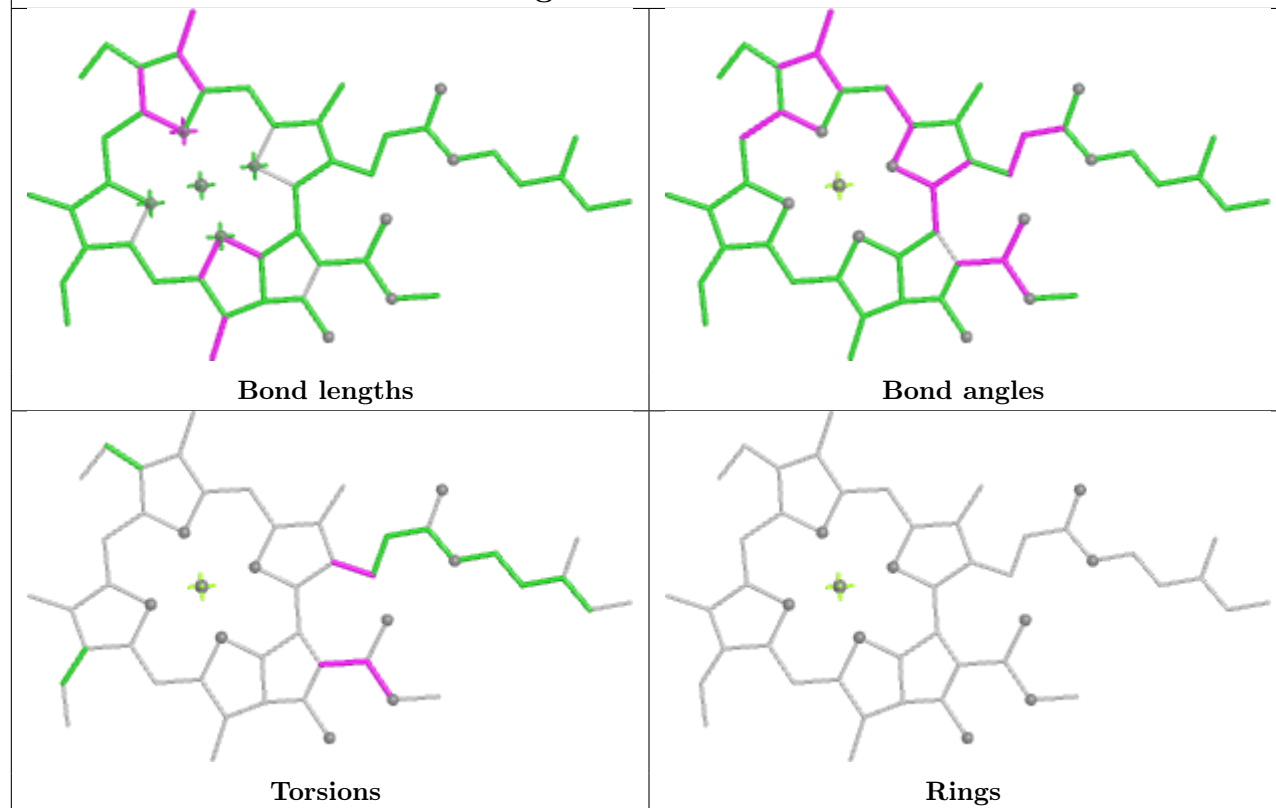
Ligand CLA n 608

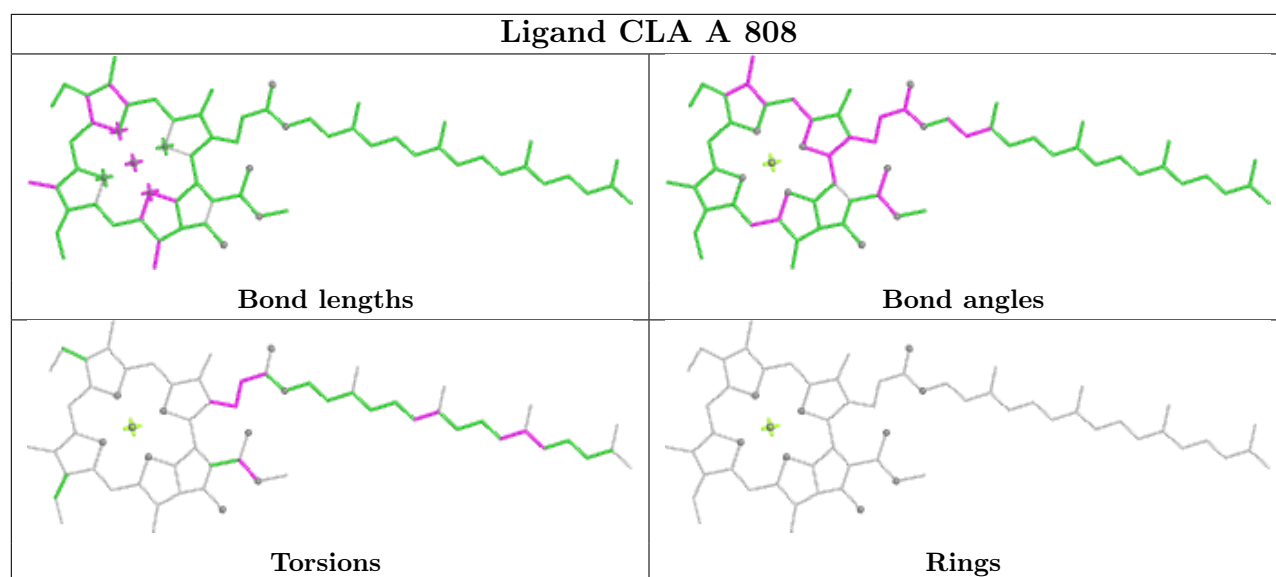
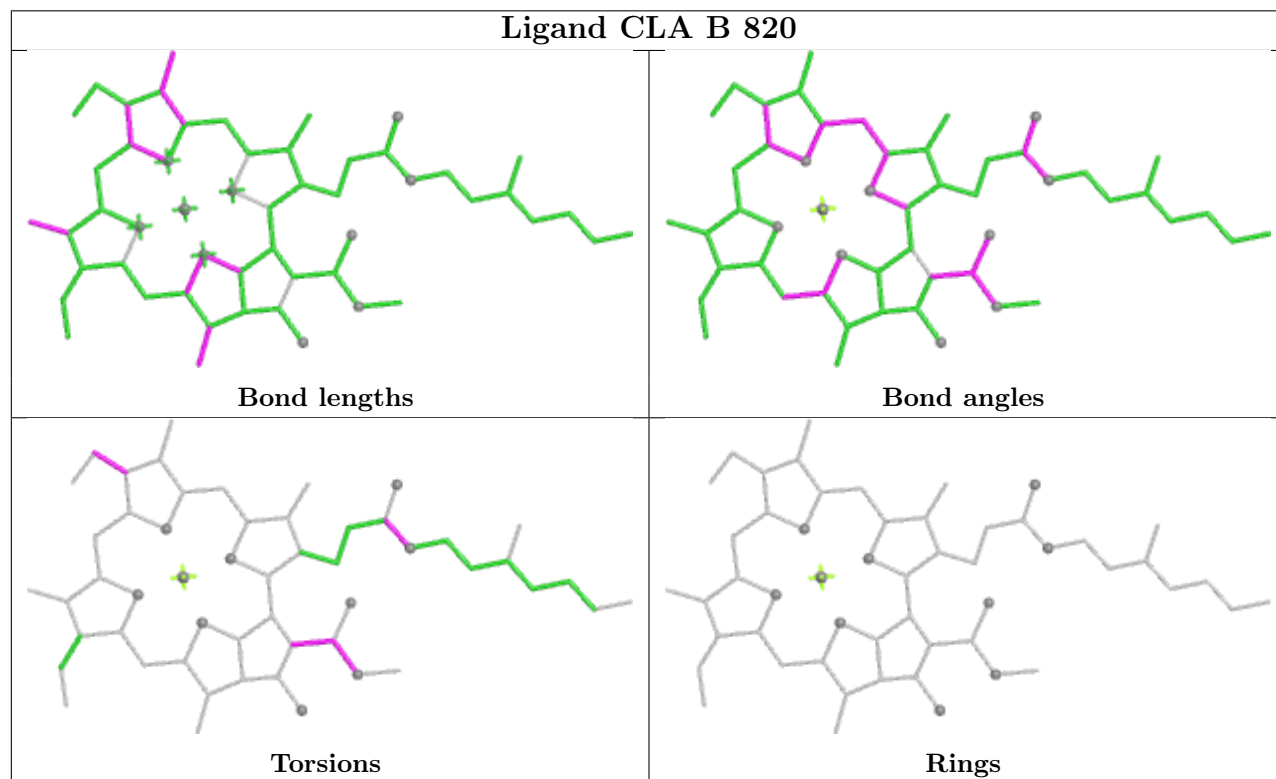


Ligand CLA h 301

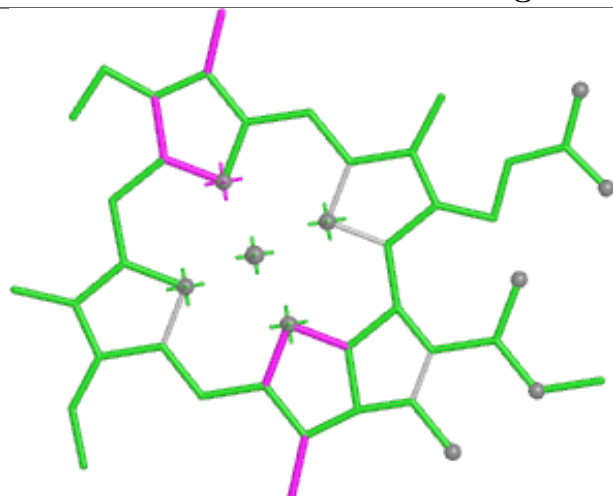


Ligand CLA h 304

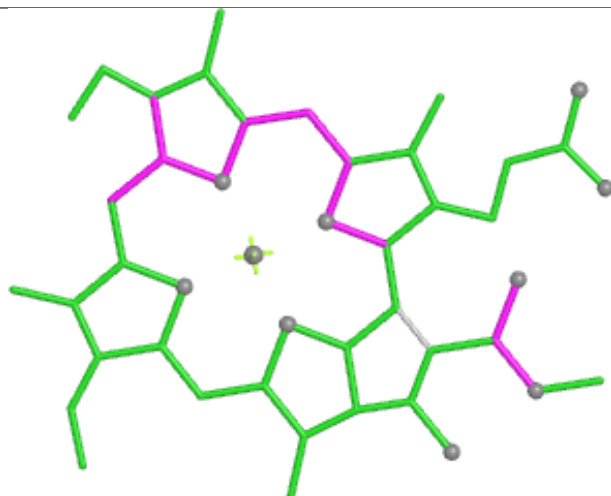




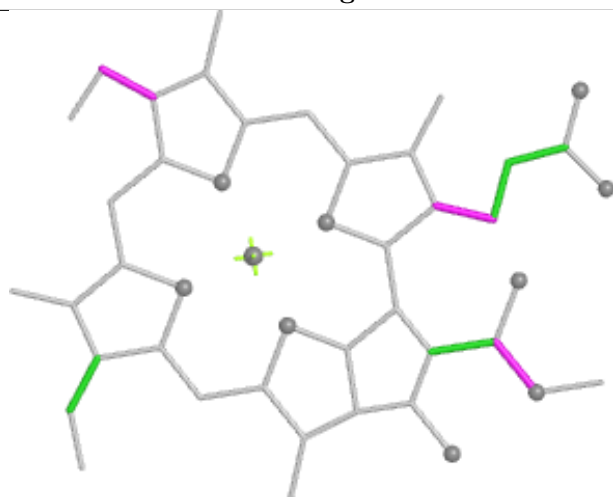
Ligand CLA B 831



Bond lengths



Bond angles

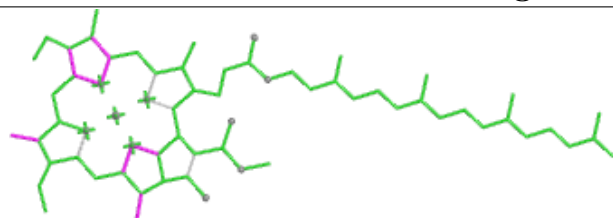


Torsions

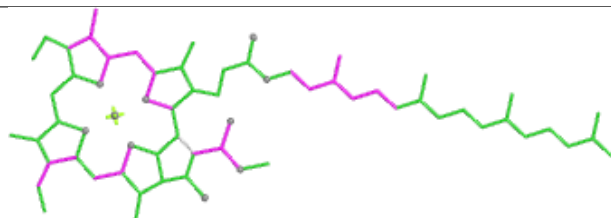


Rings

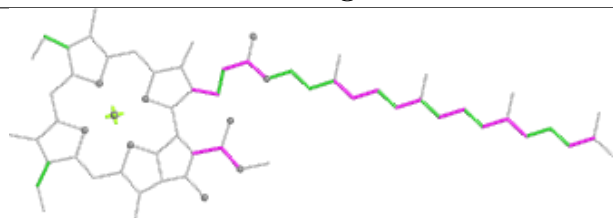
Ligand CLA A 812



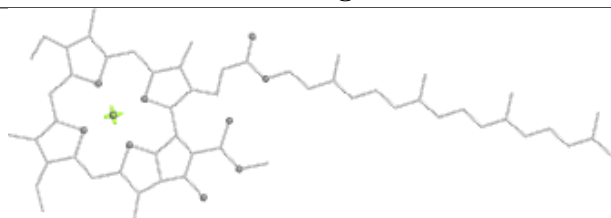
Bond lengths



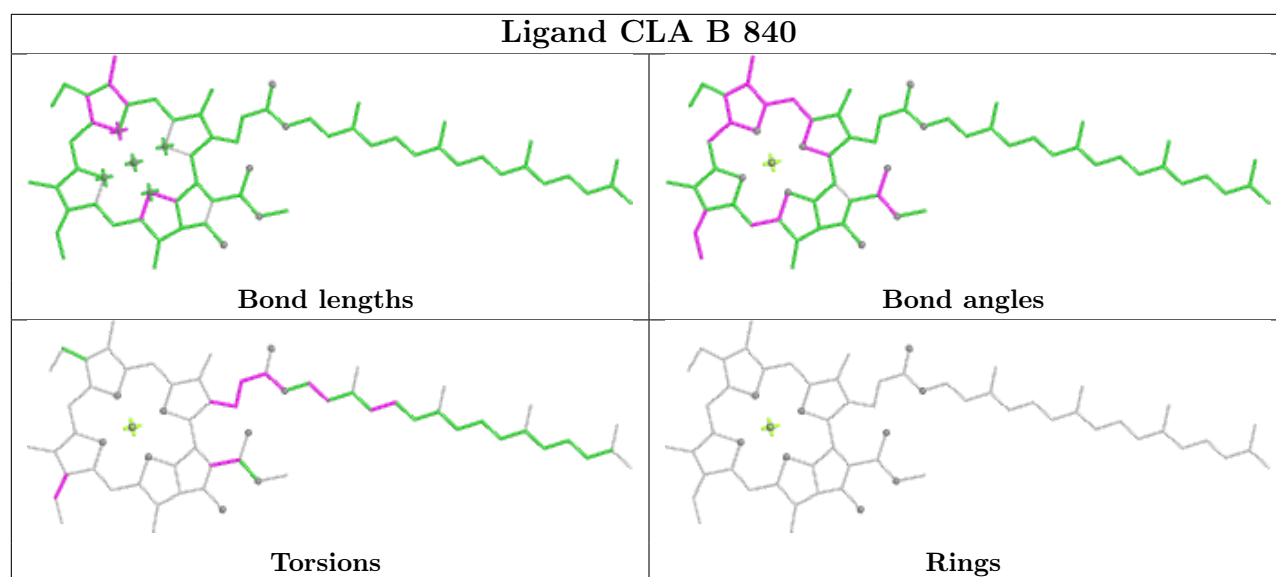
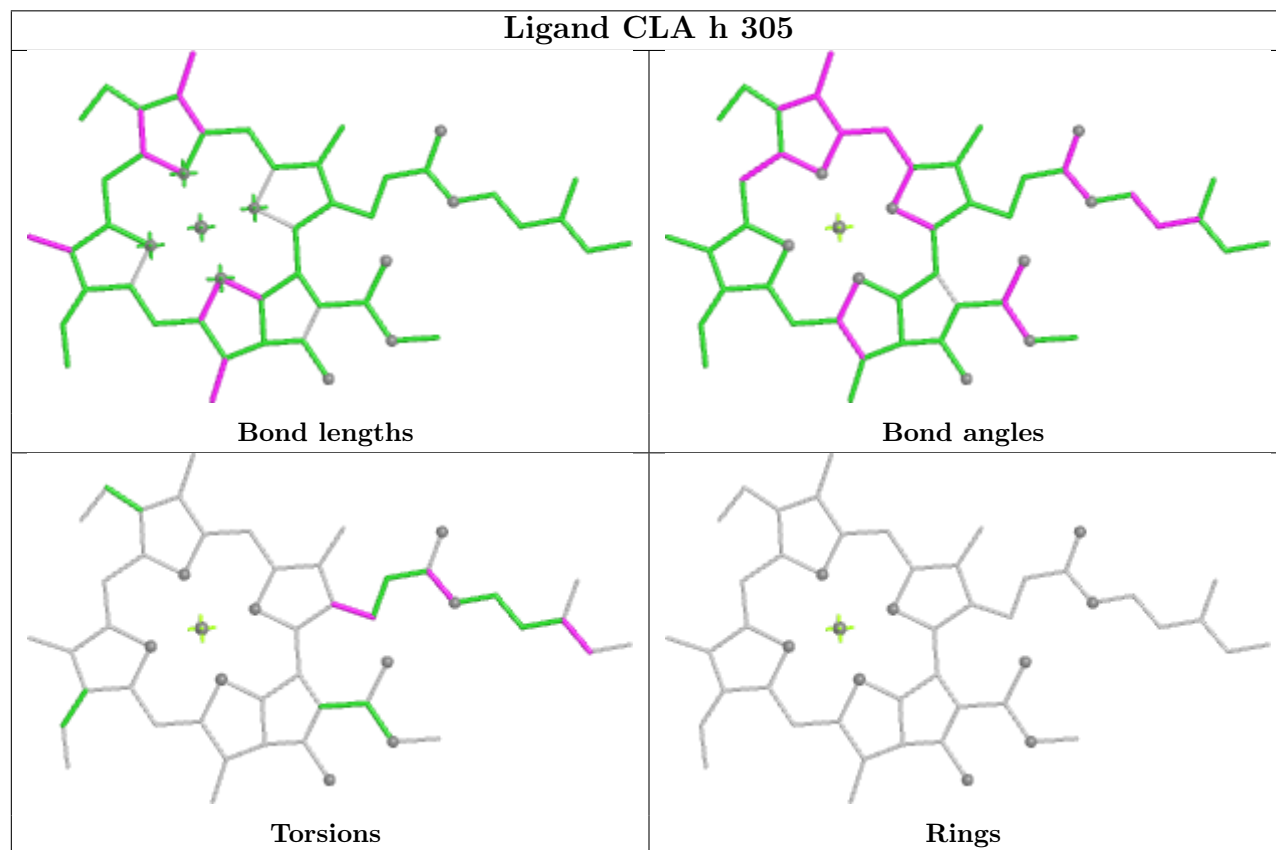
Bond angles



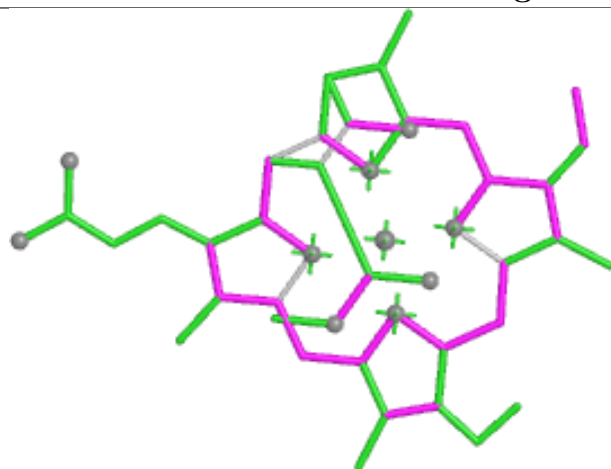
Torsions



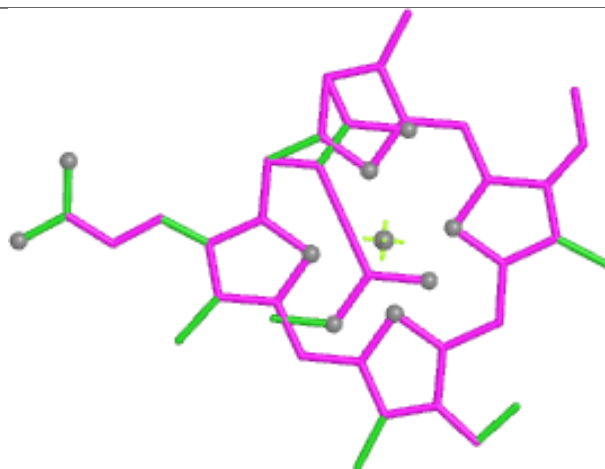
Rings



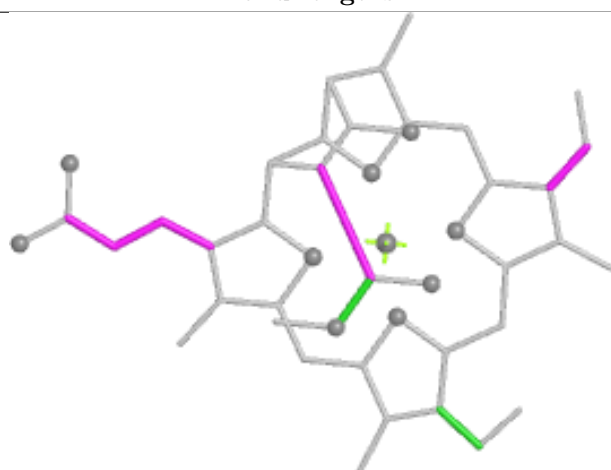
Ligand KC2 m 611



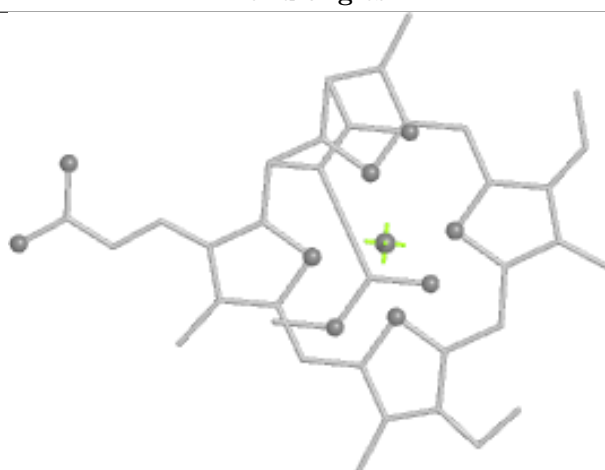
Bond lengths



Bond angles

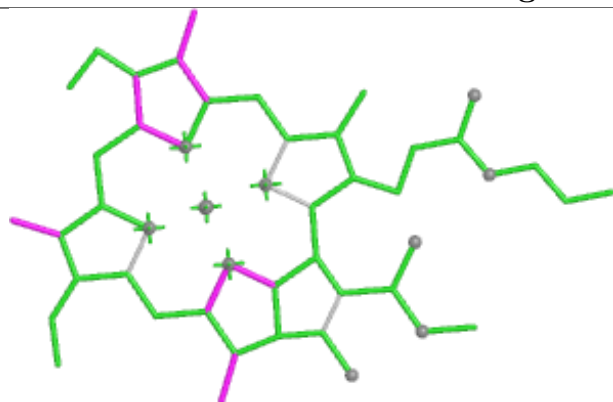


Torsions

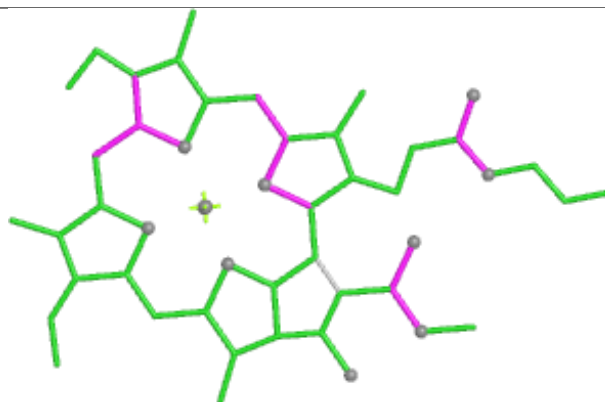


Rings

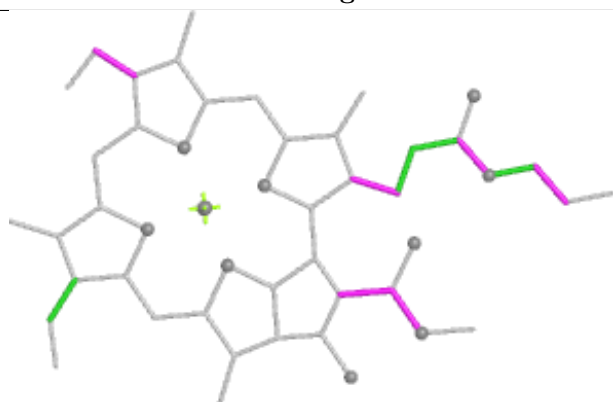
Ligand CLA a 310



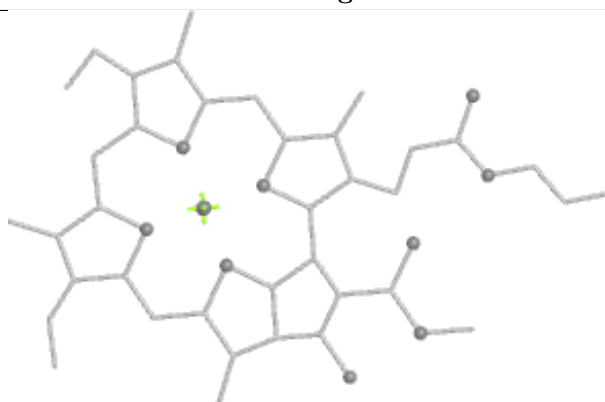
Bond lengths



Bond angles

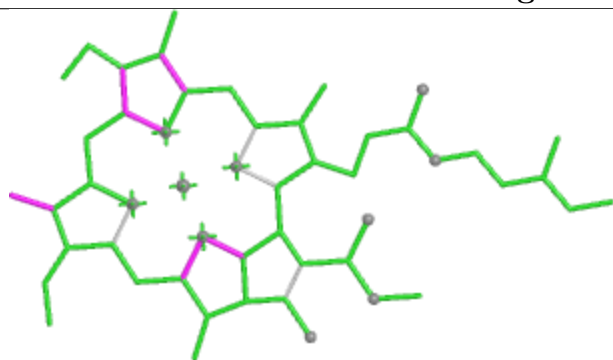


Torsions

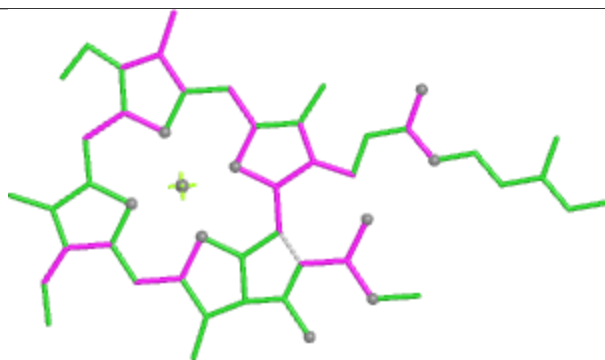


Rings

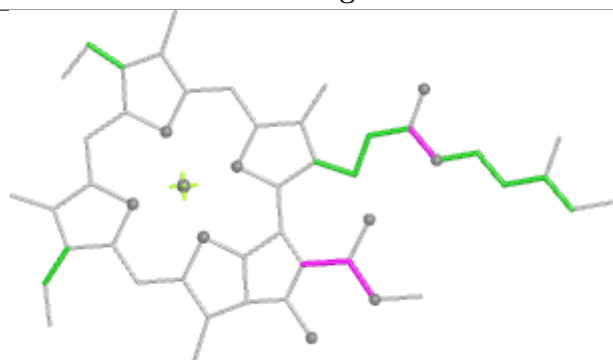
Ligand CLA d 312



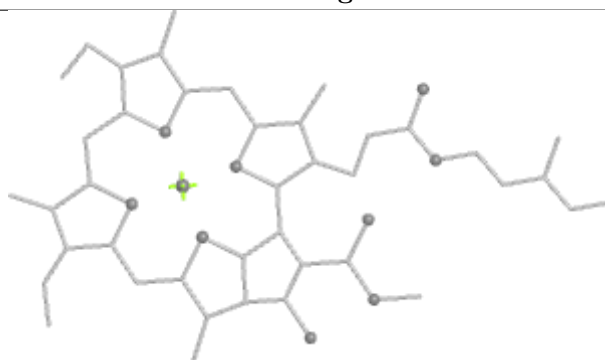
Bond lengths



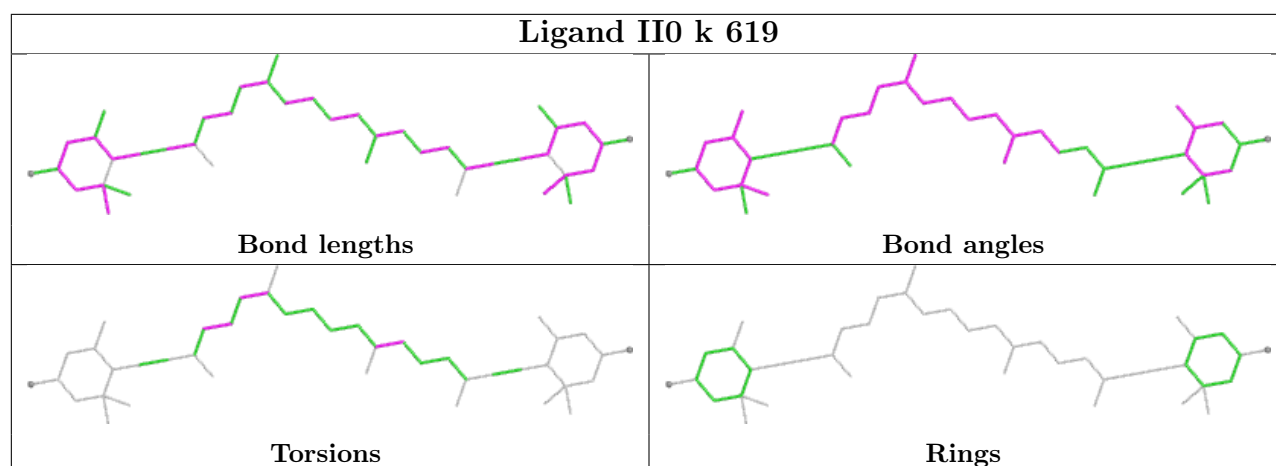
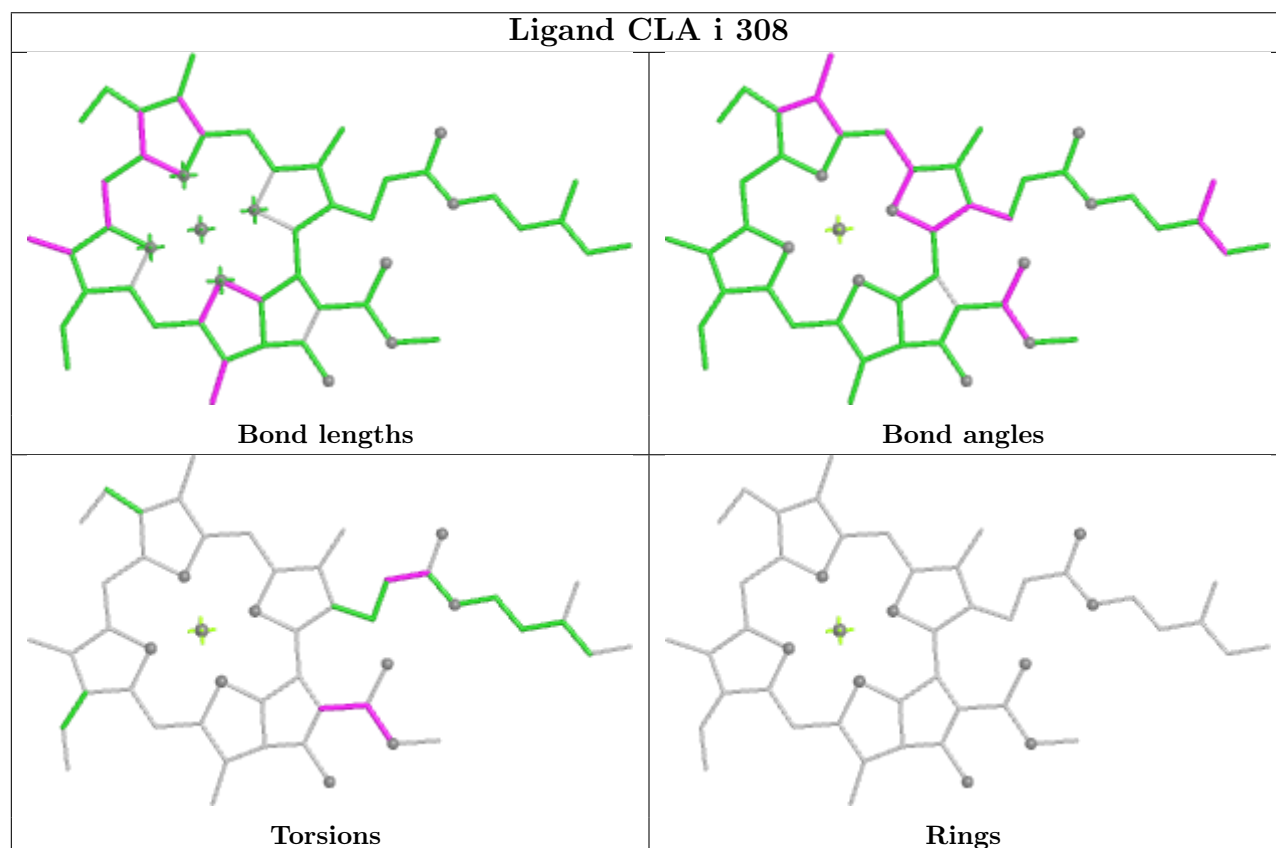
Bond angles

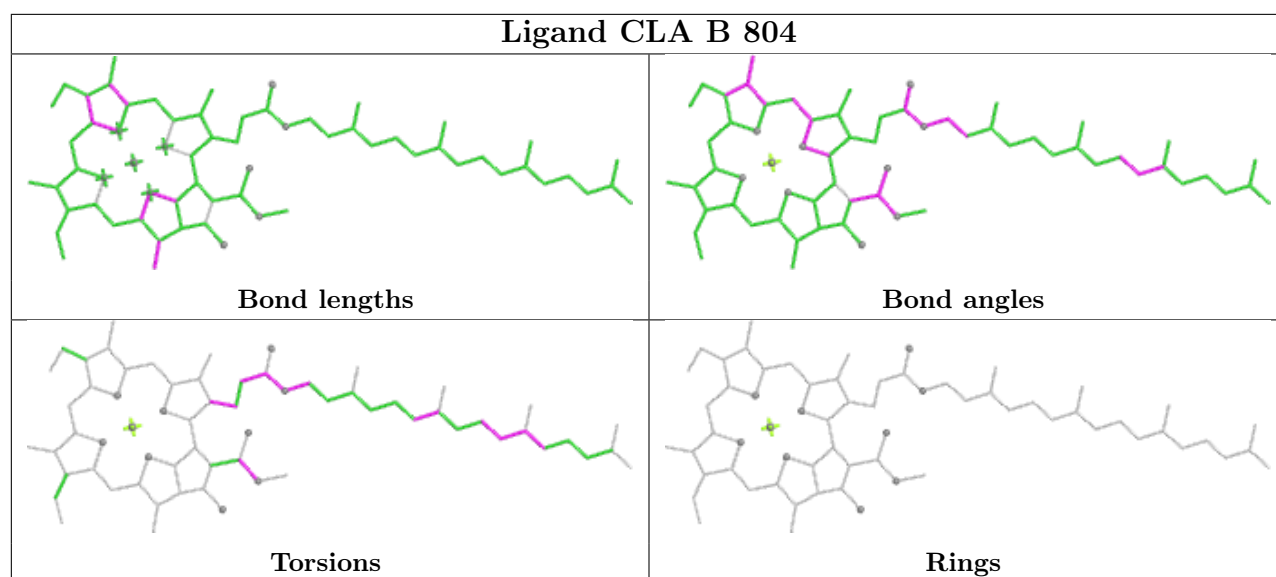
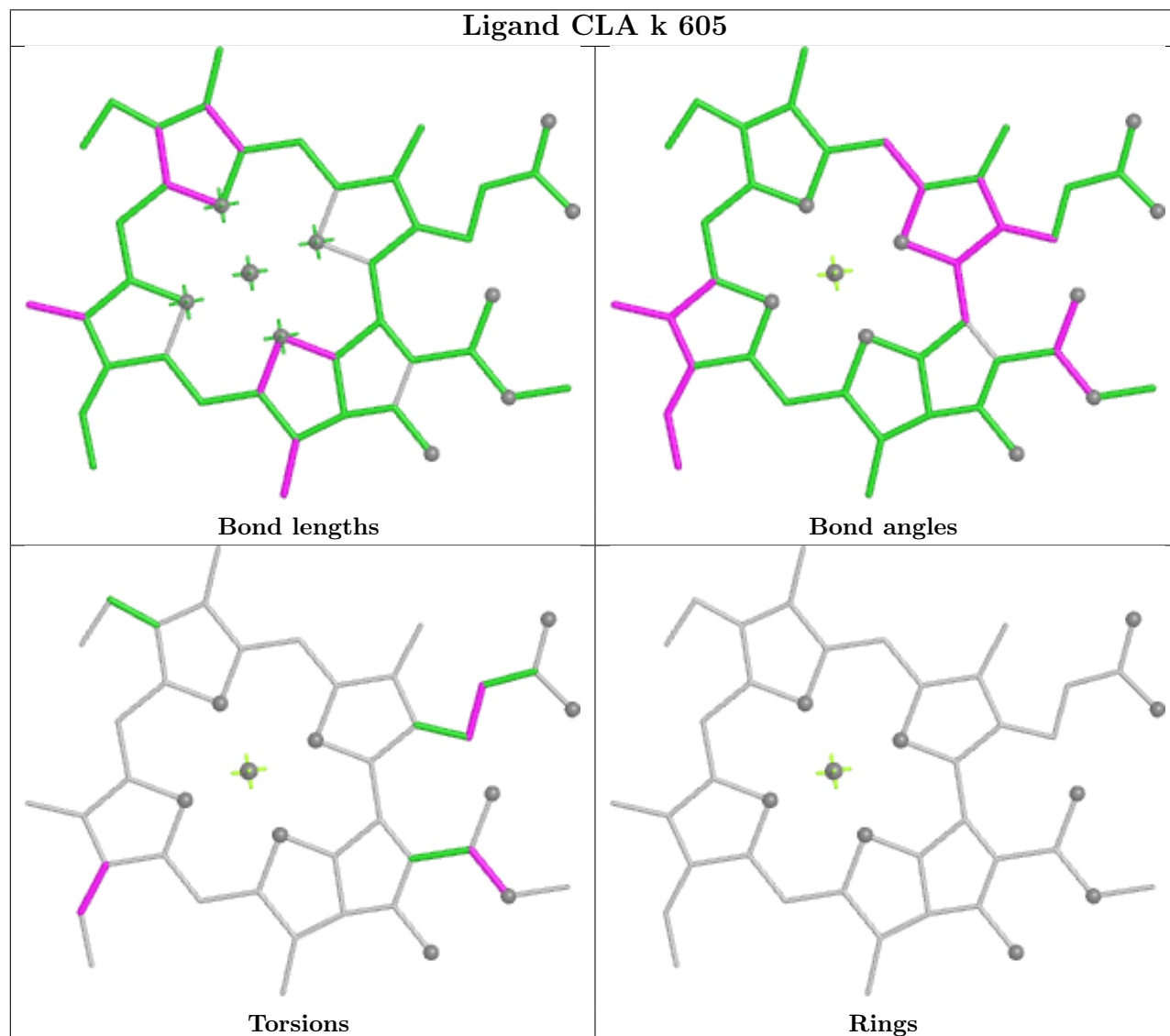


Torsions

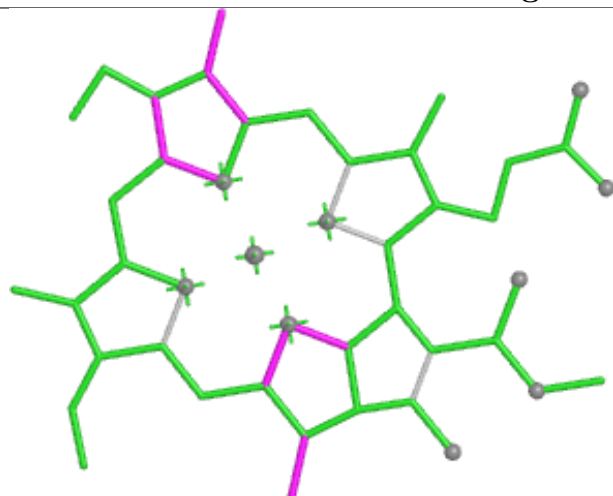


Rings

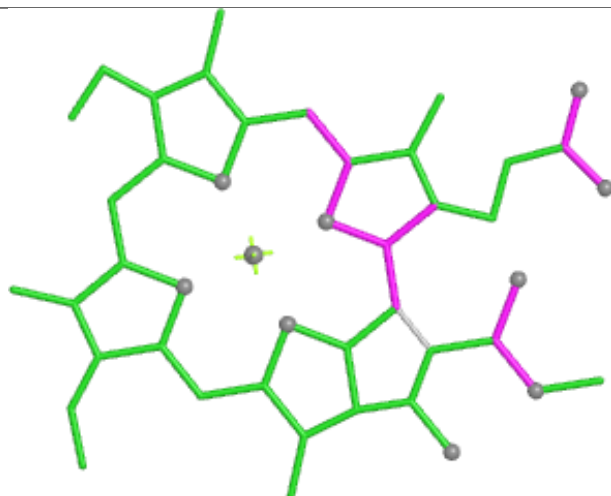




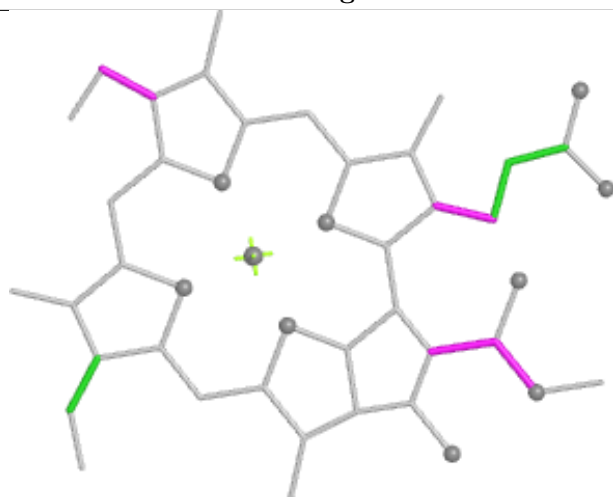
Ligand CLA f 605



Bond lengths



Bond angles

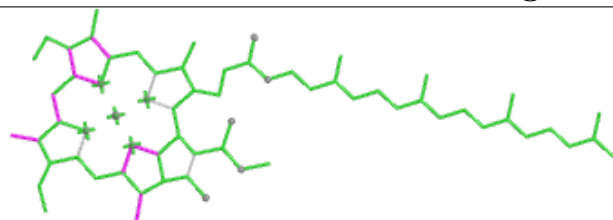


Torsions

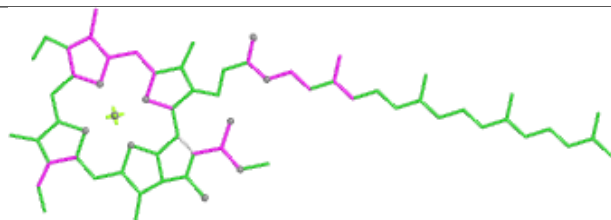


Rings

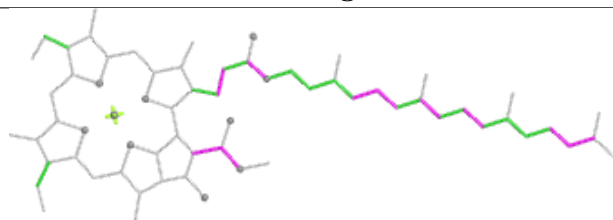
Ligand CLA f 609



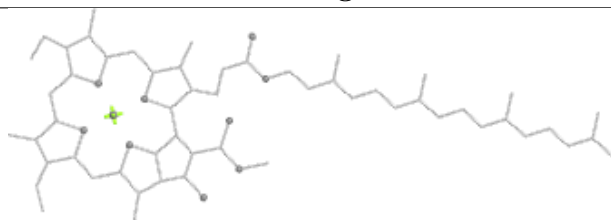
Bond lengths



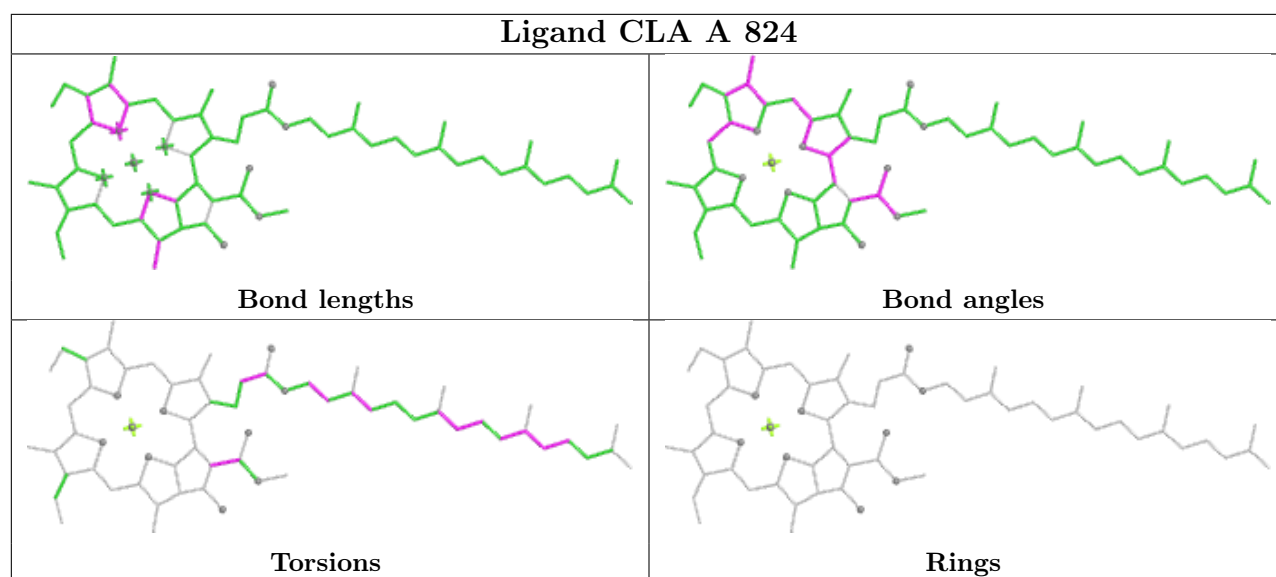
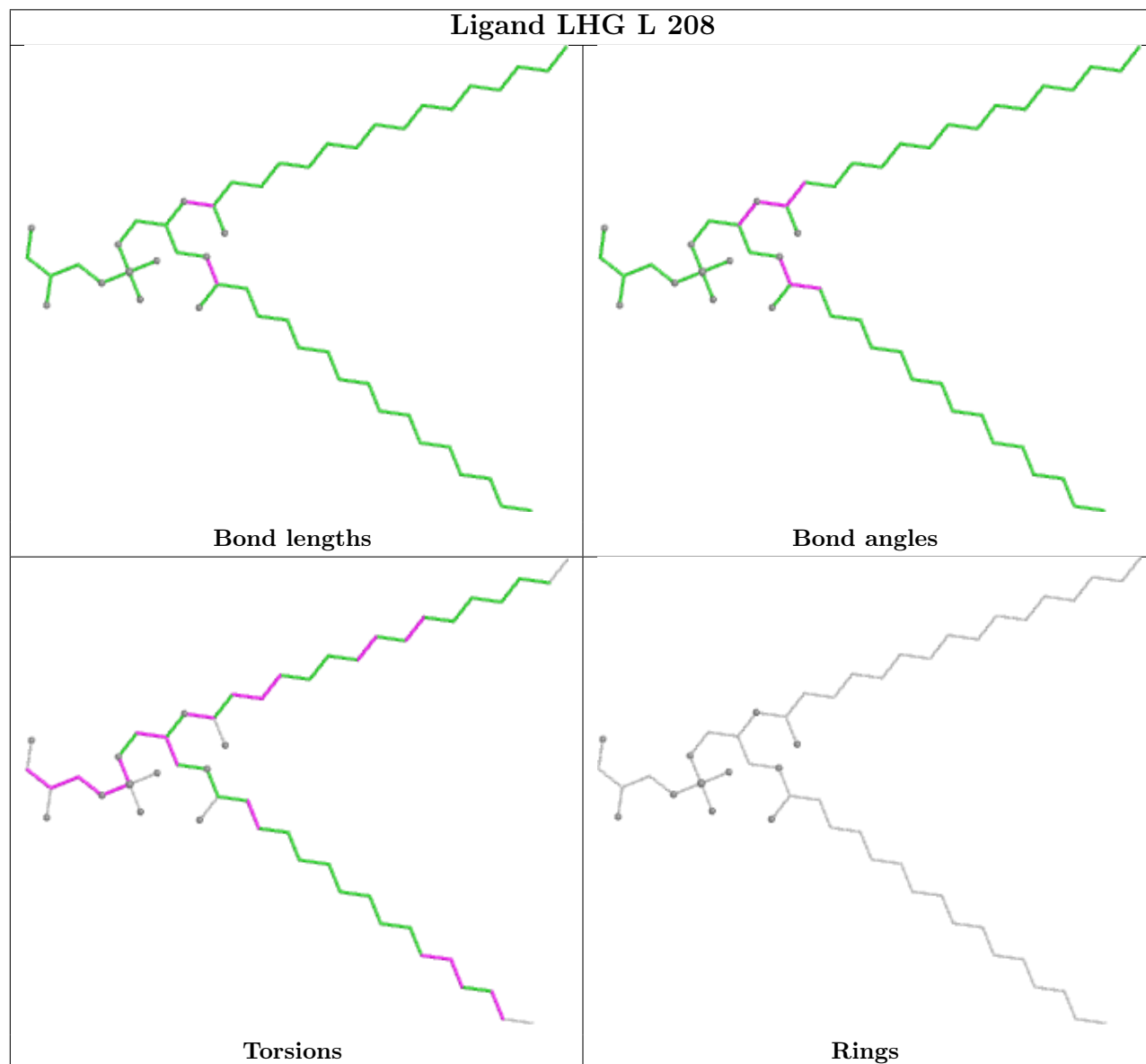
Bond angles

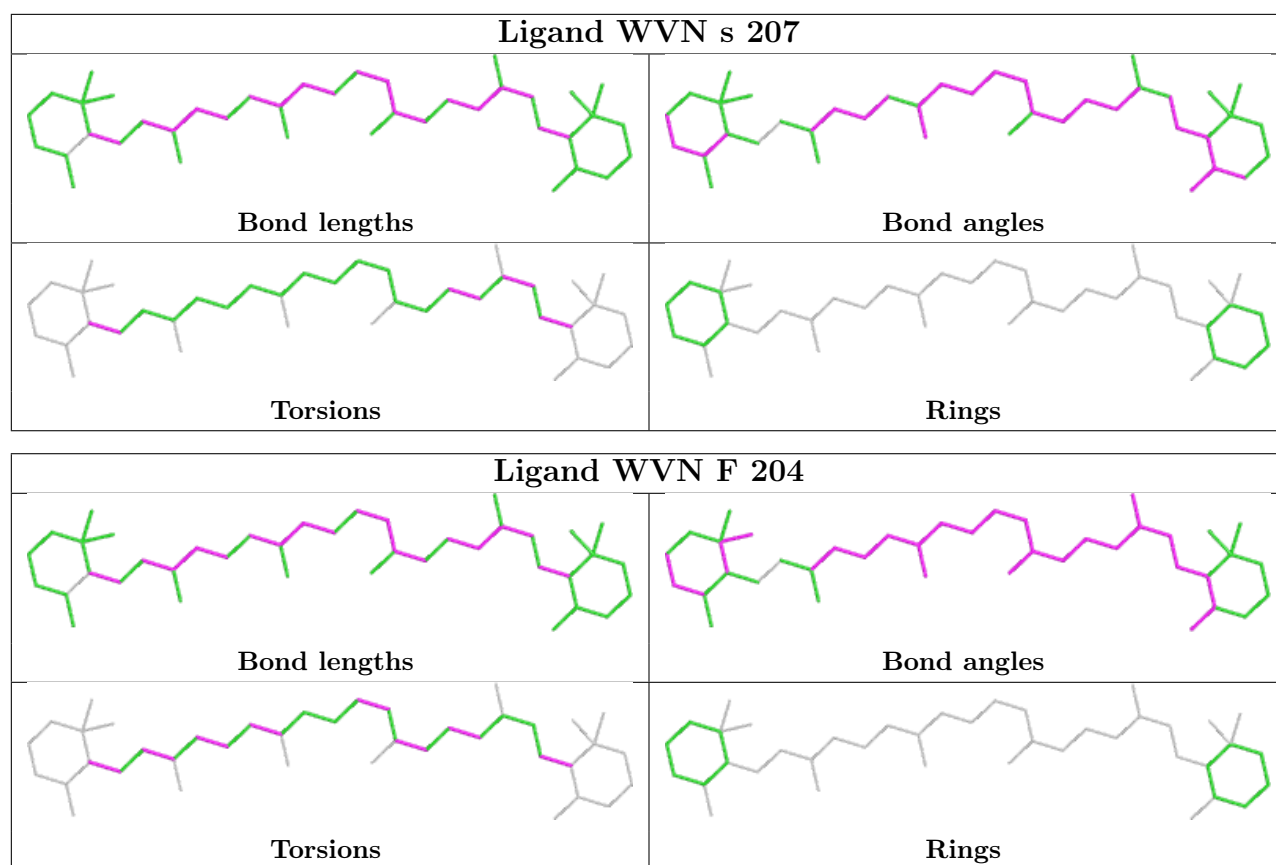


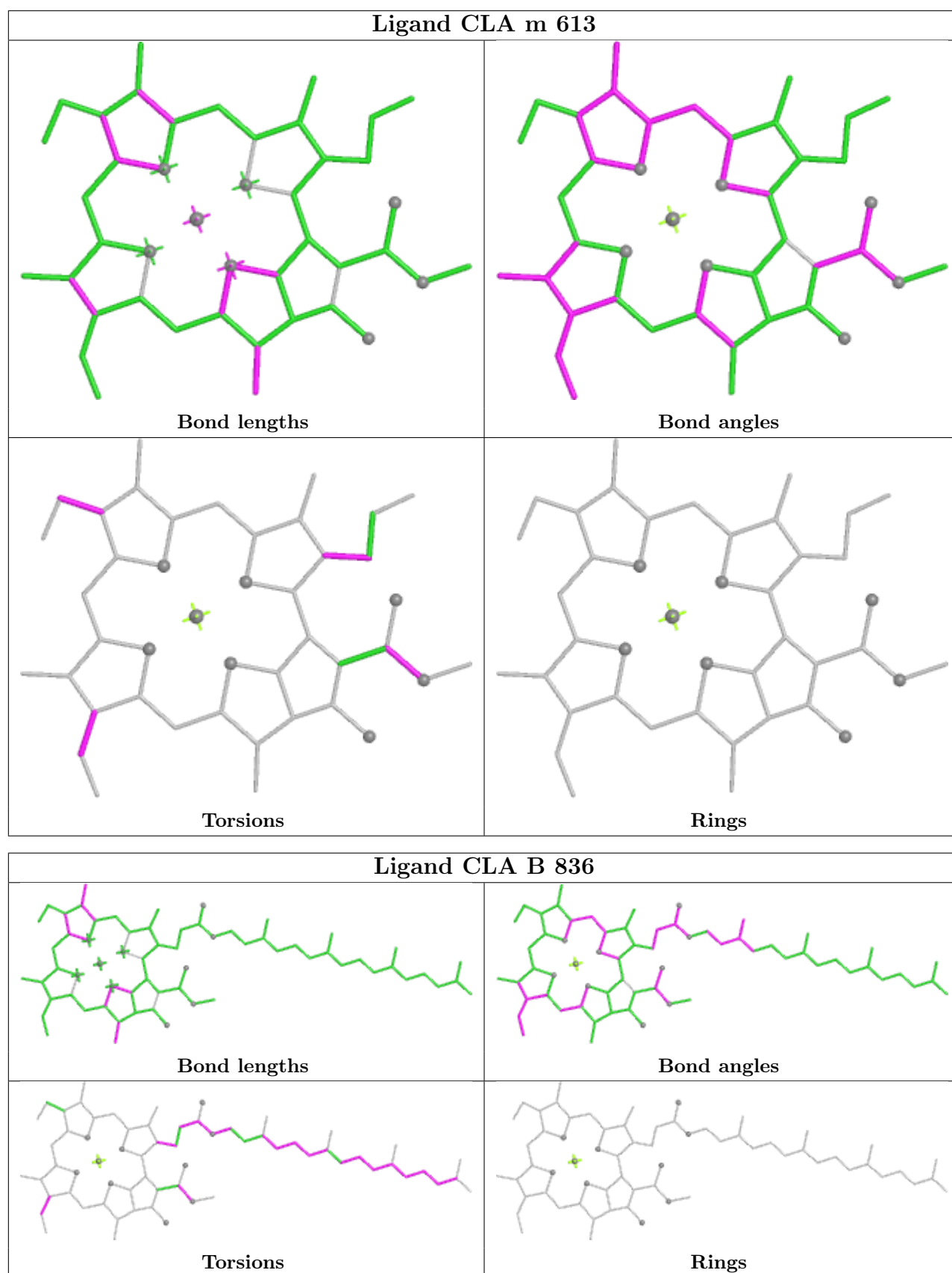
Torsions

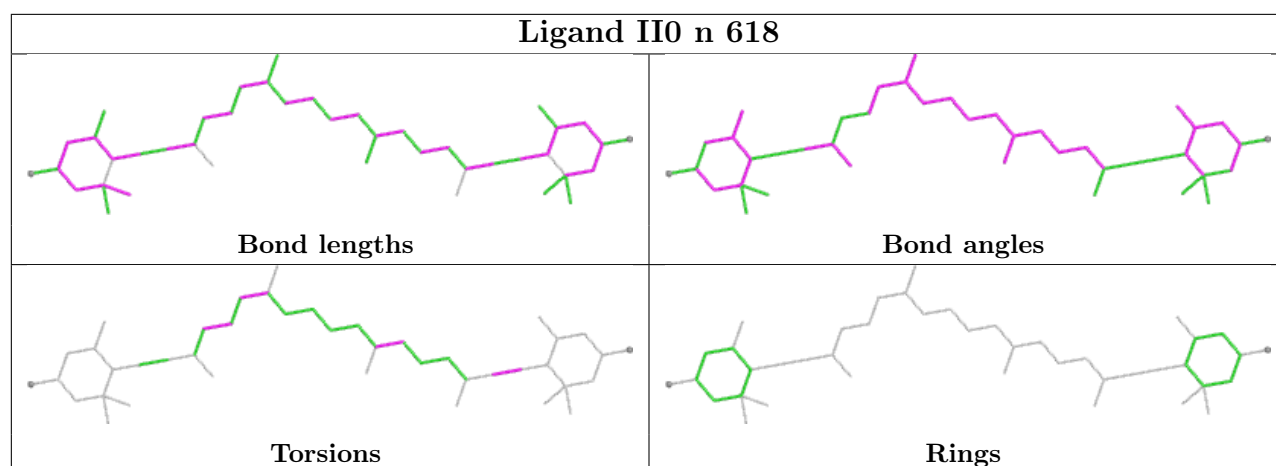
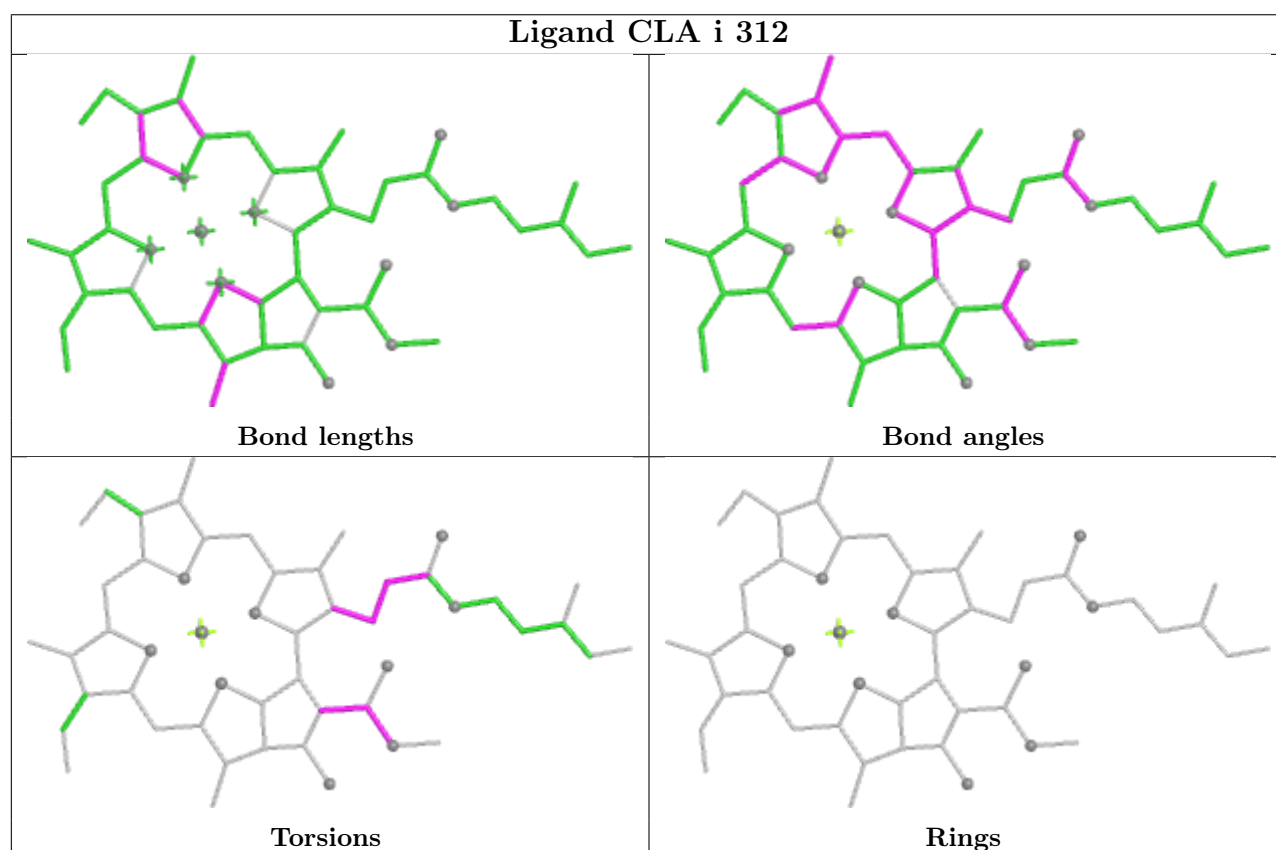


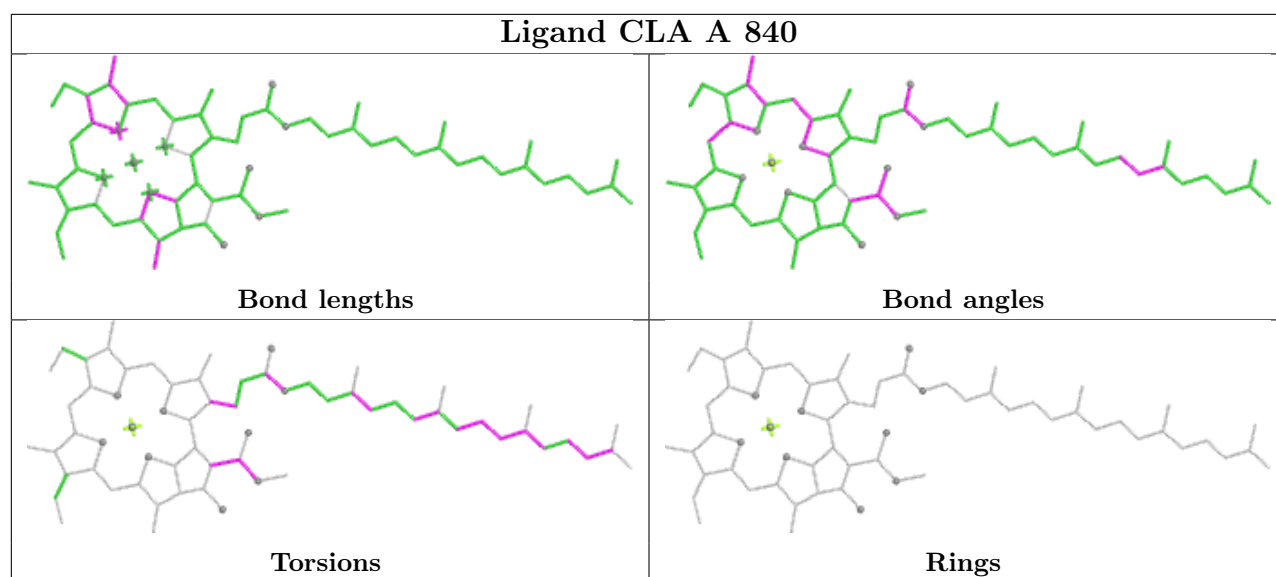
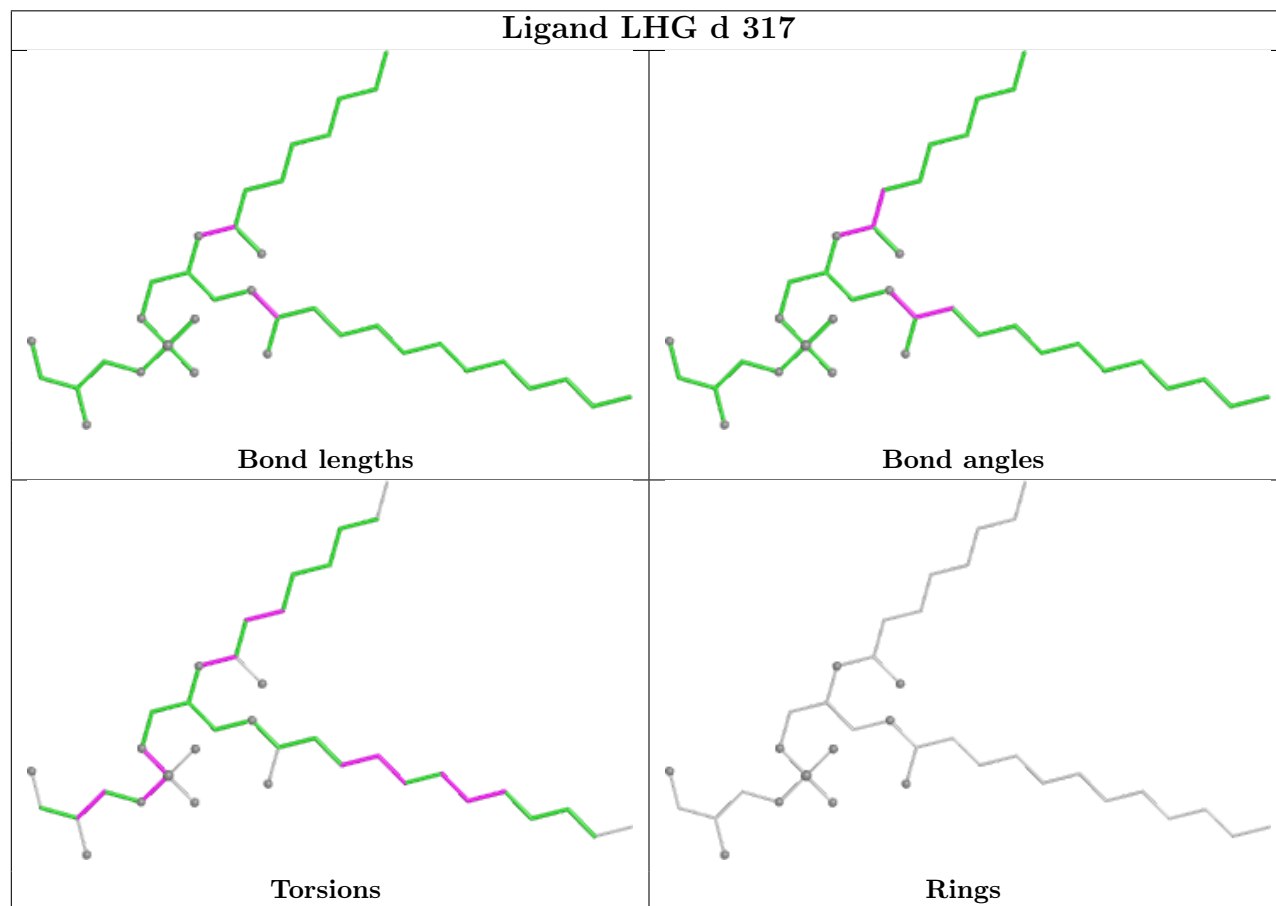
Rings

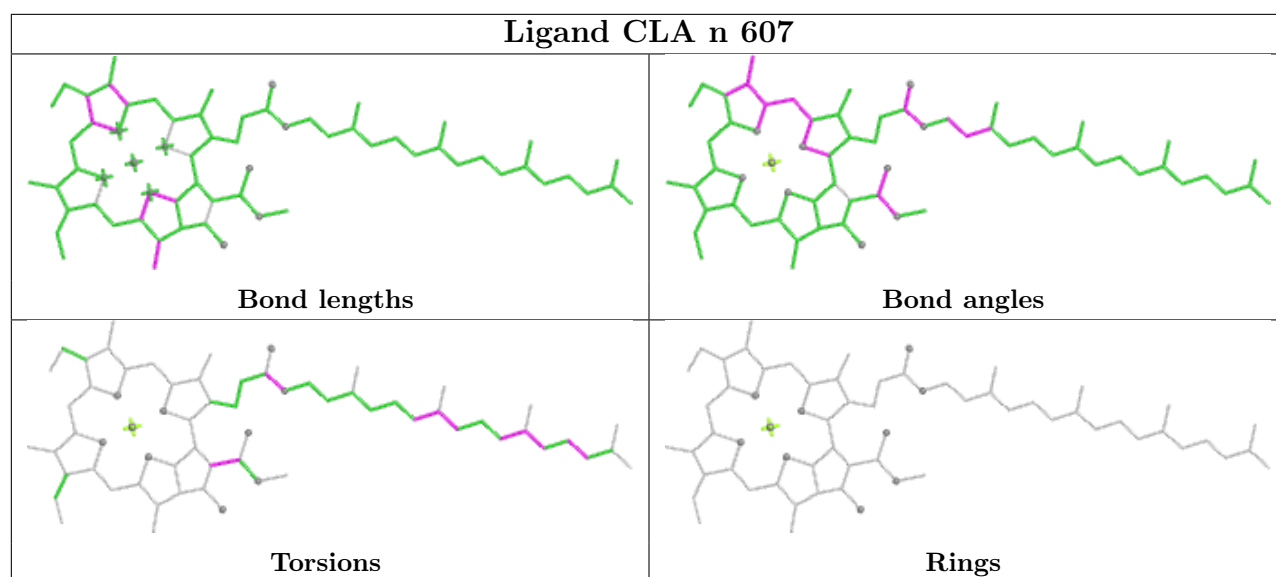
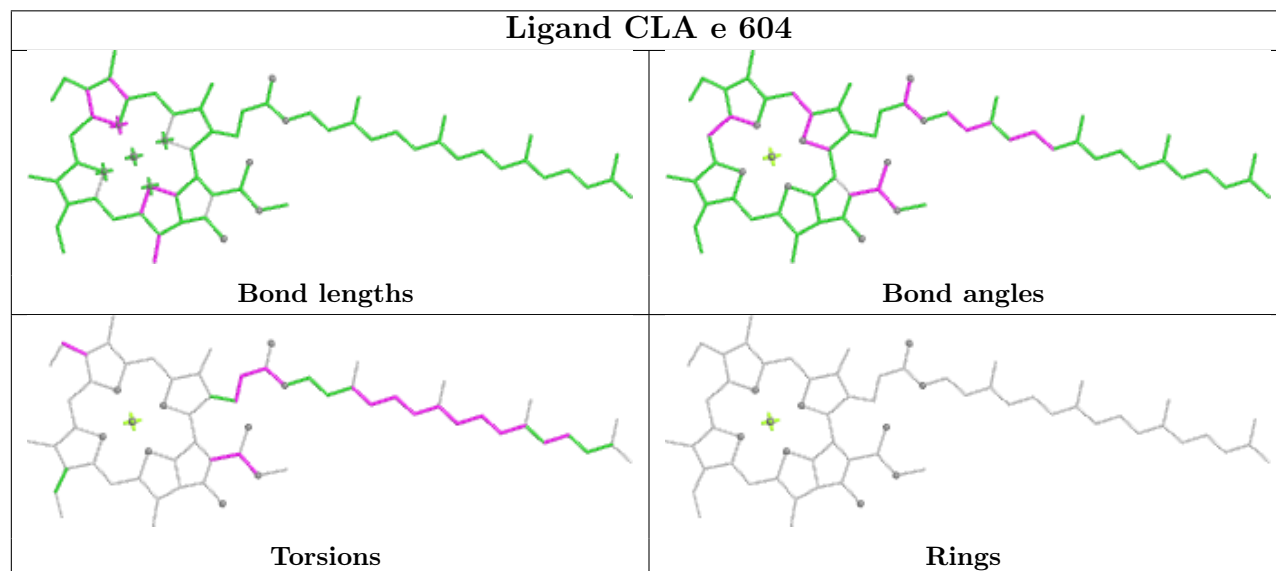
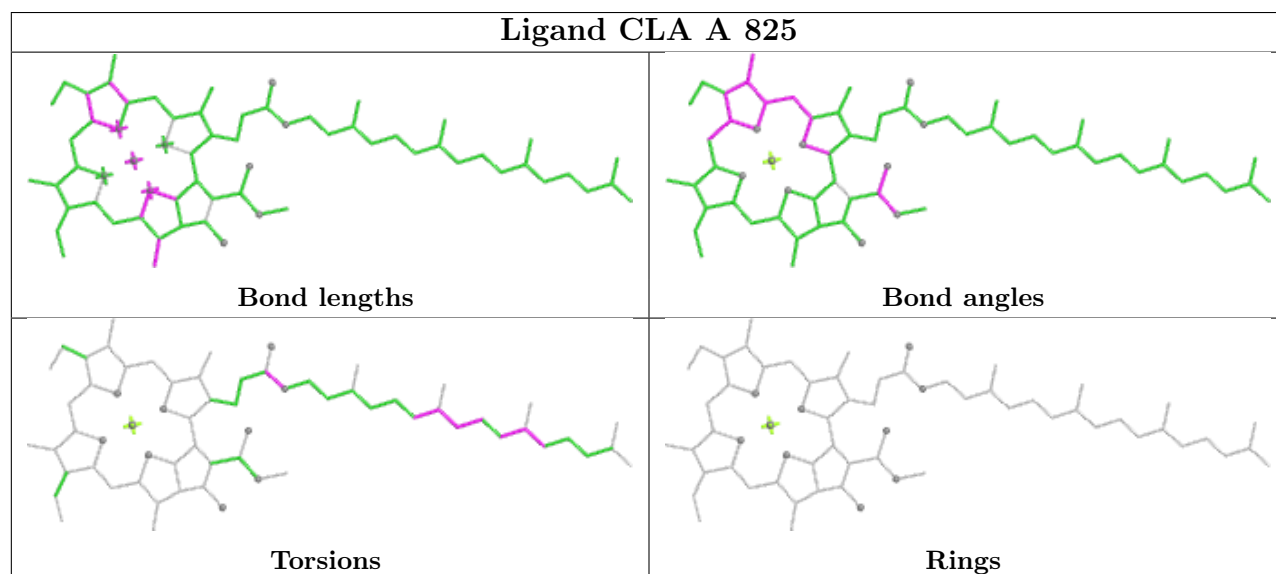


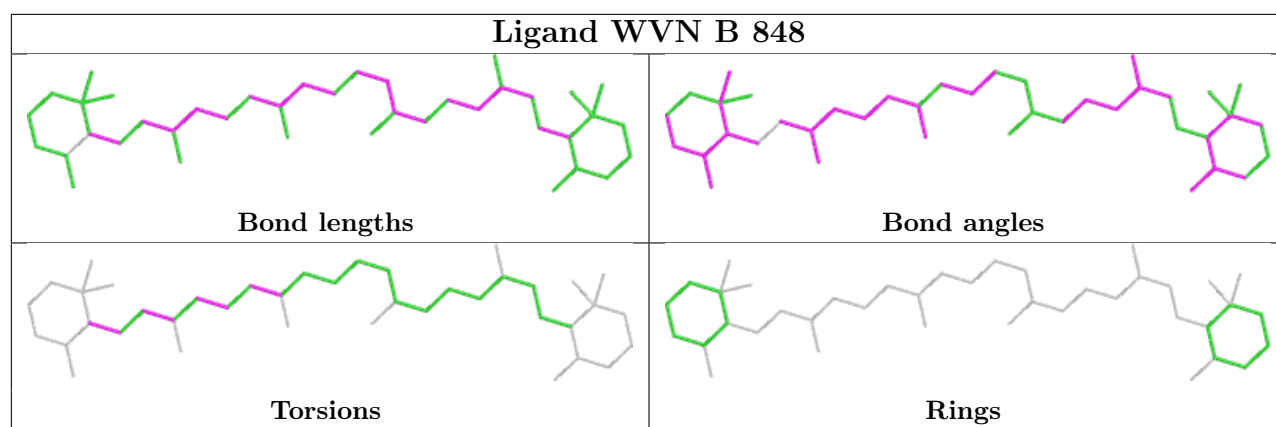
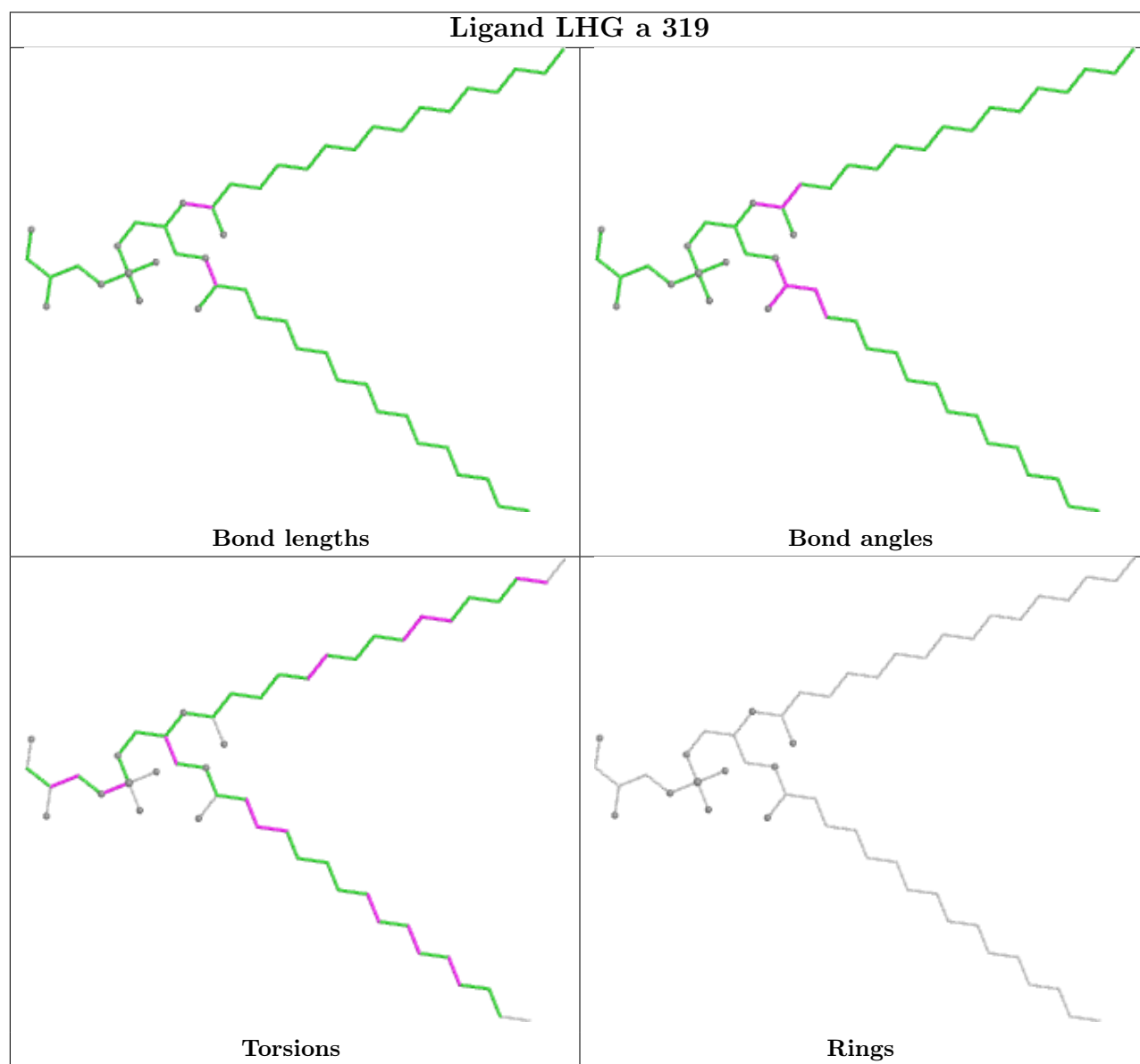


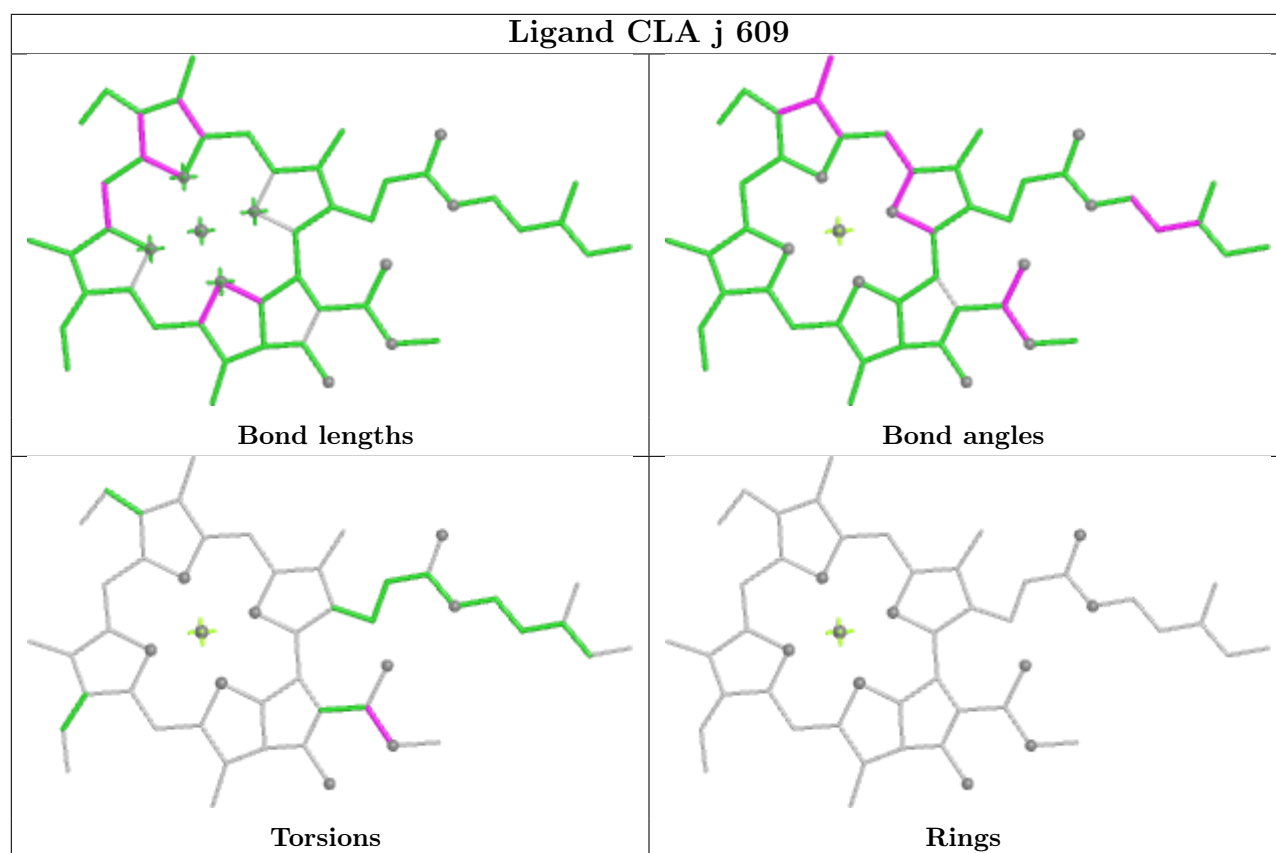
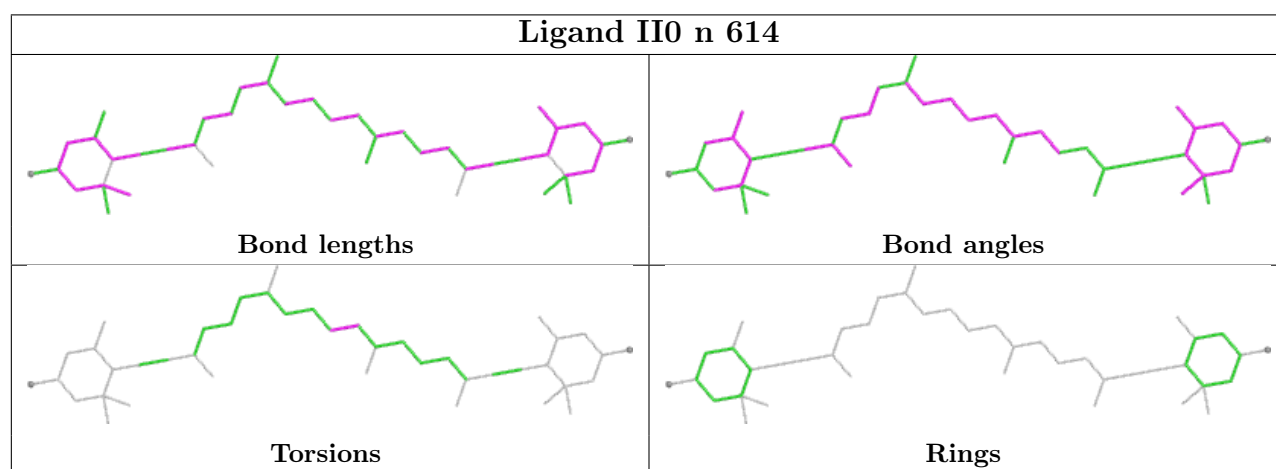


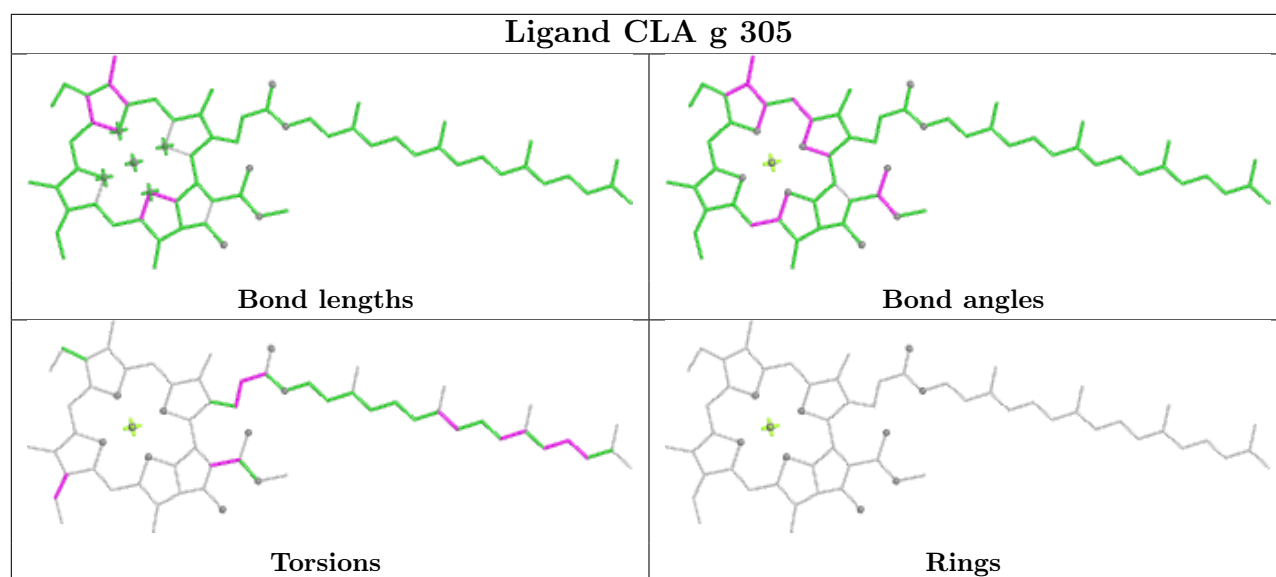
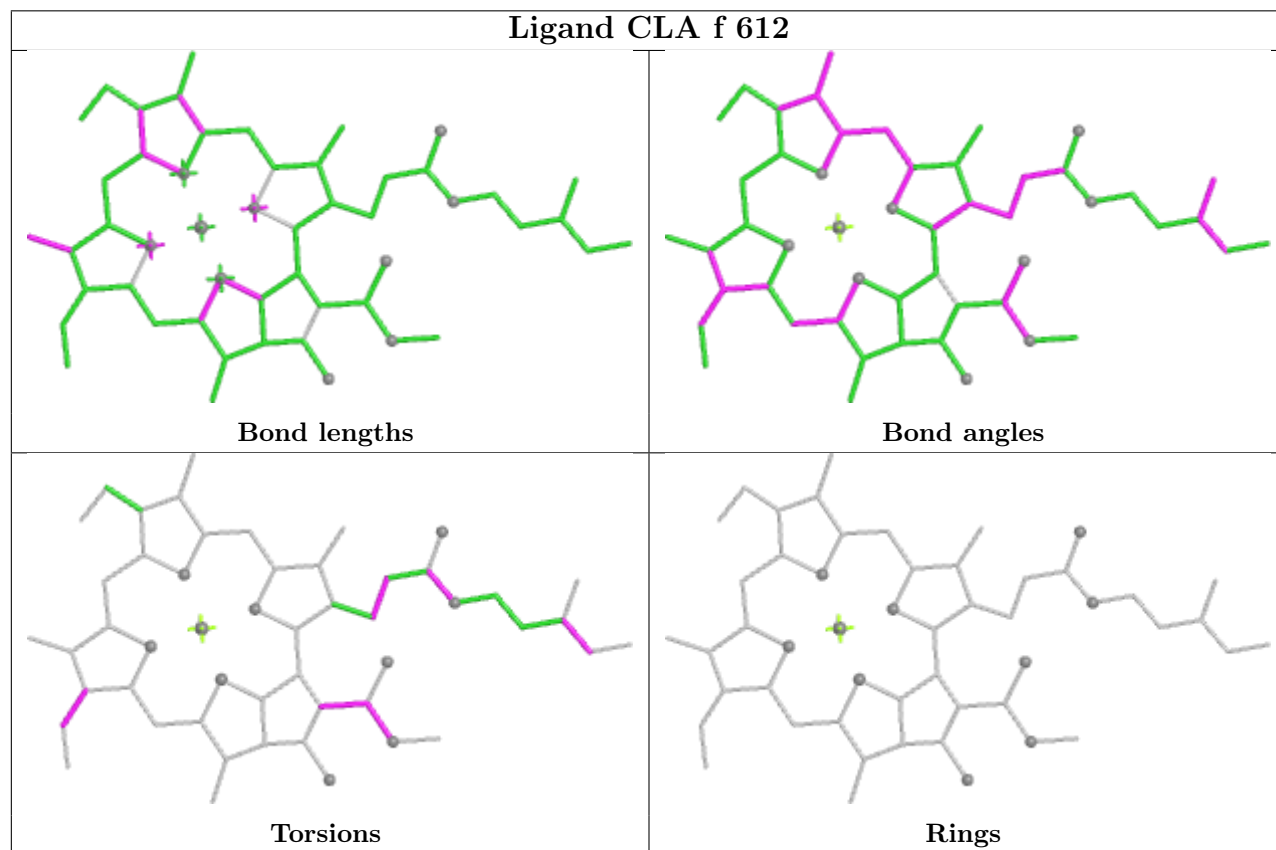


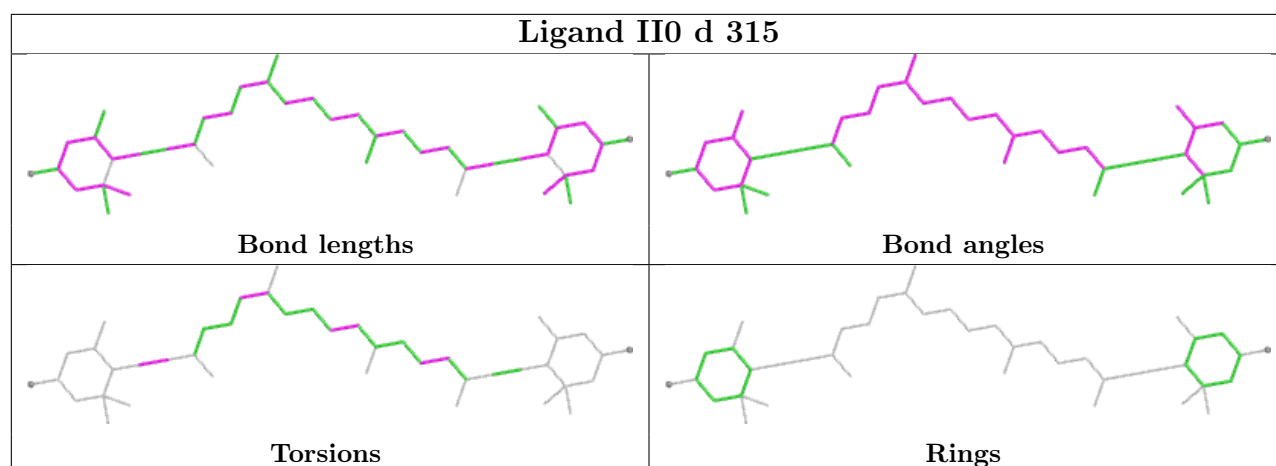
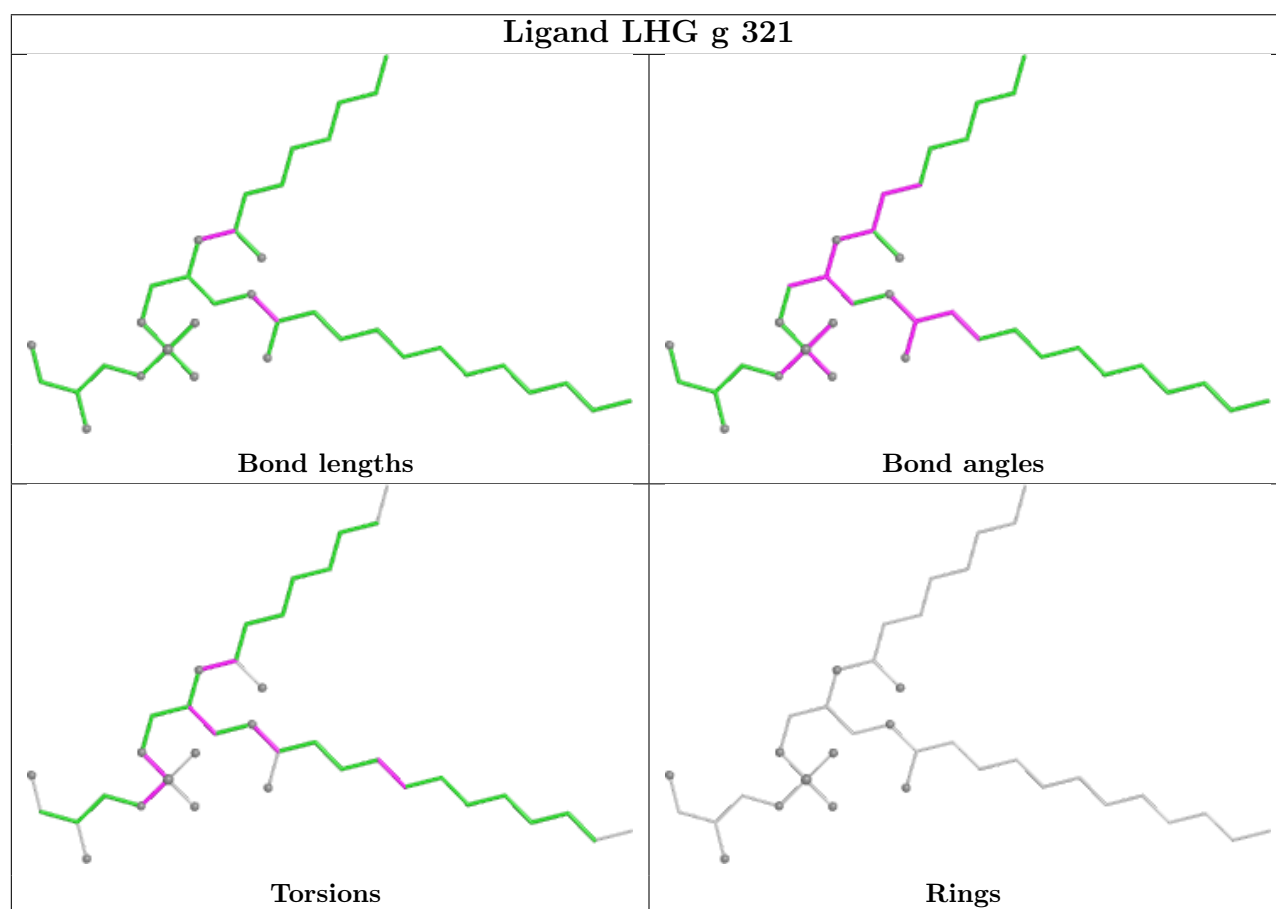




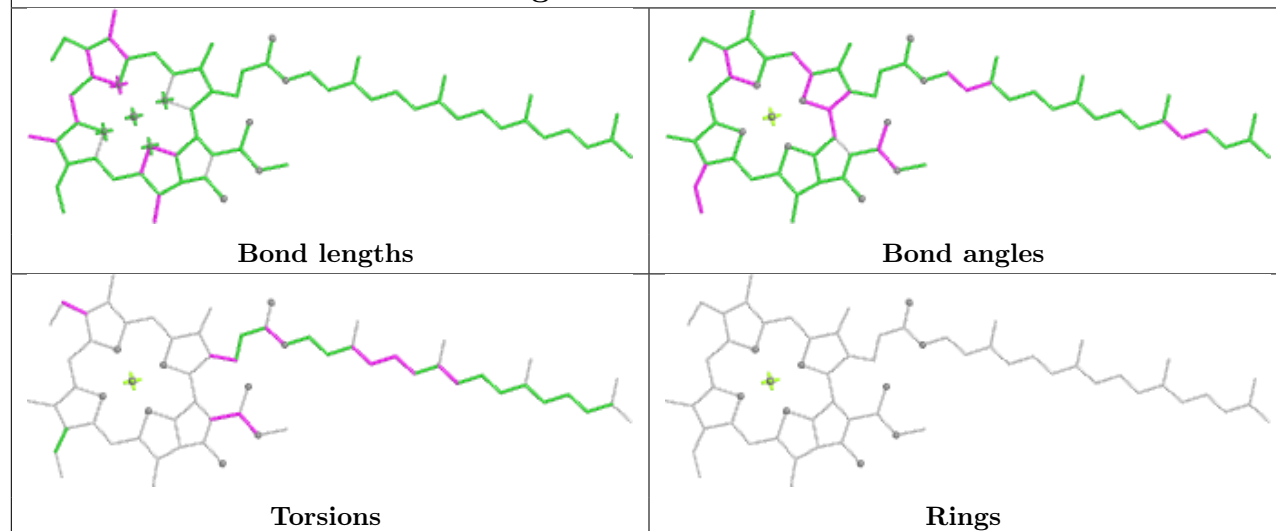




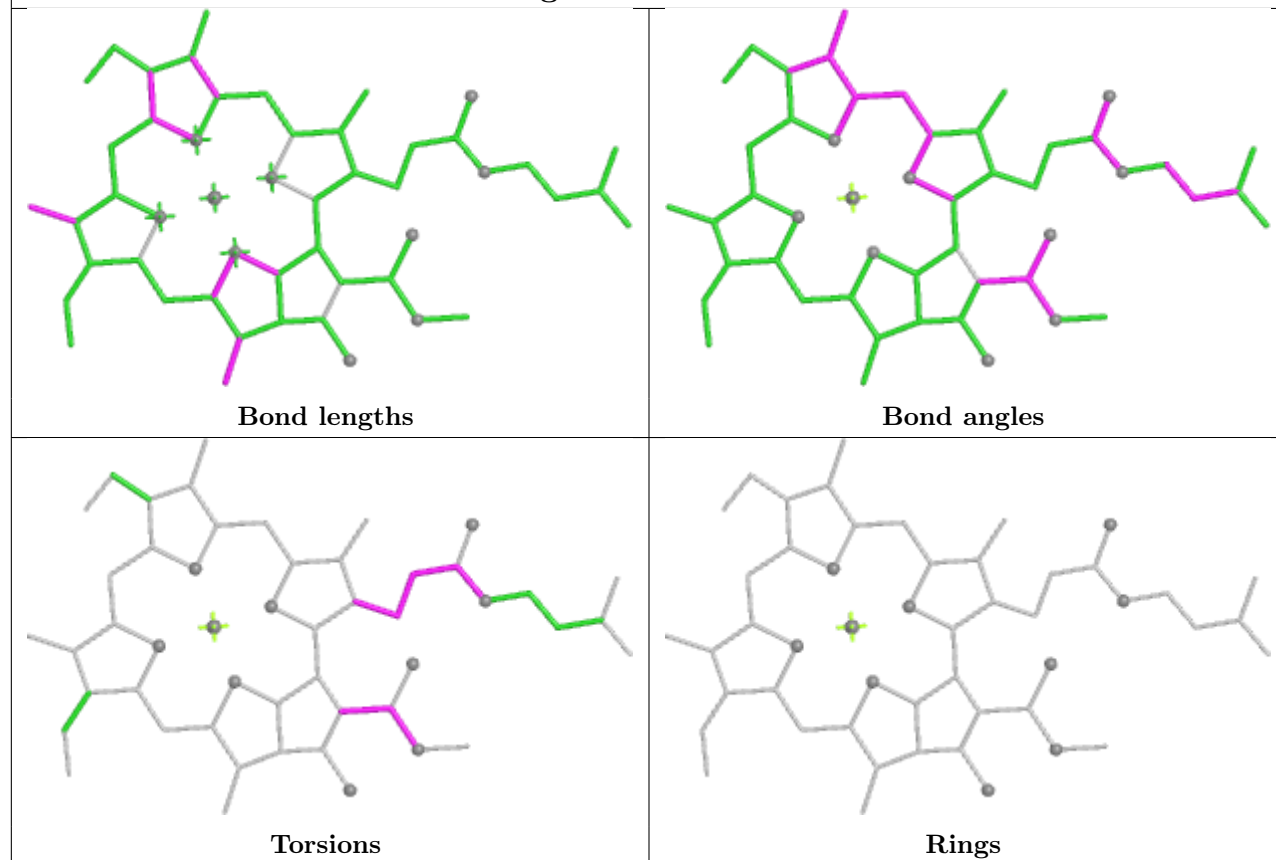


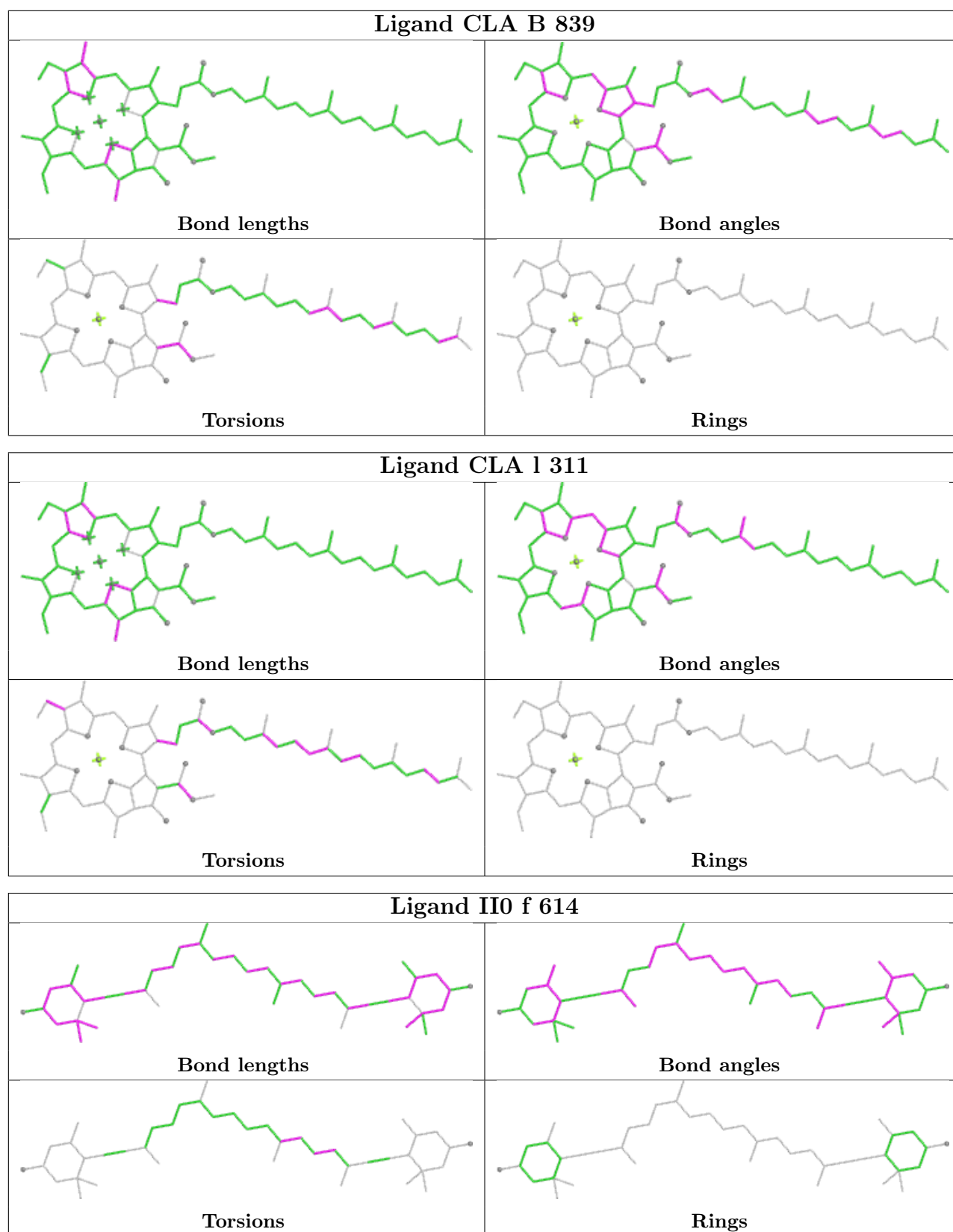


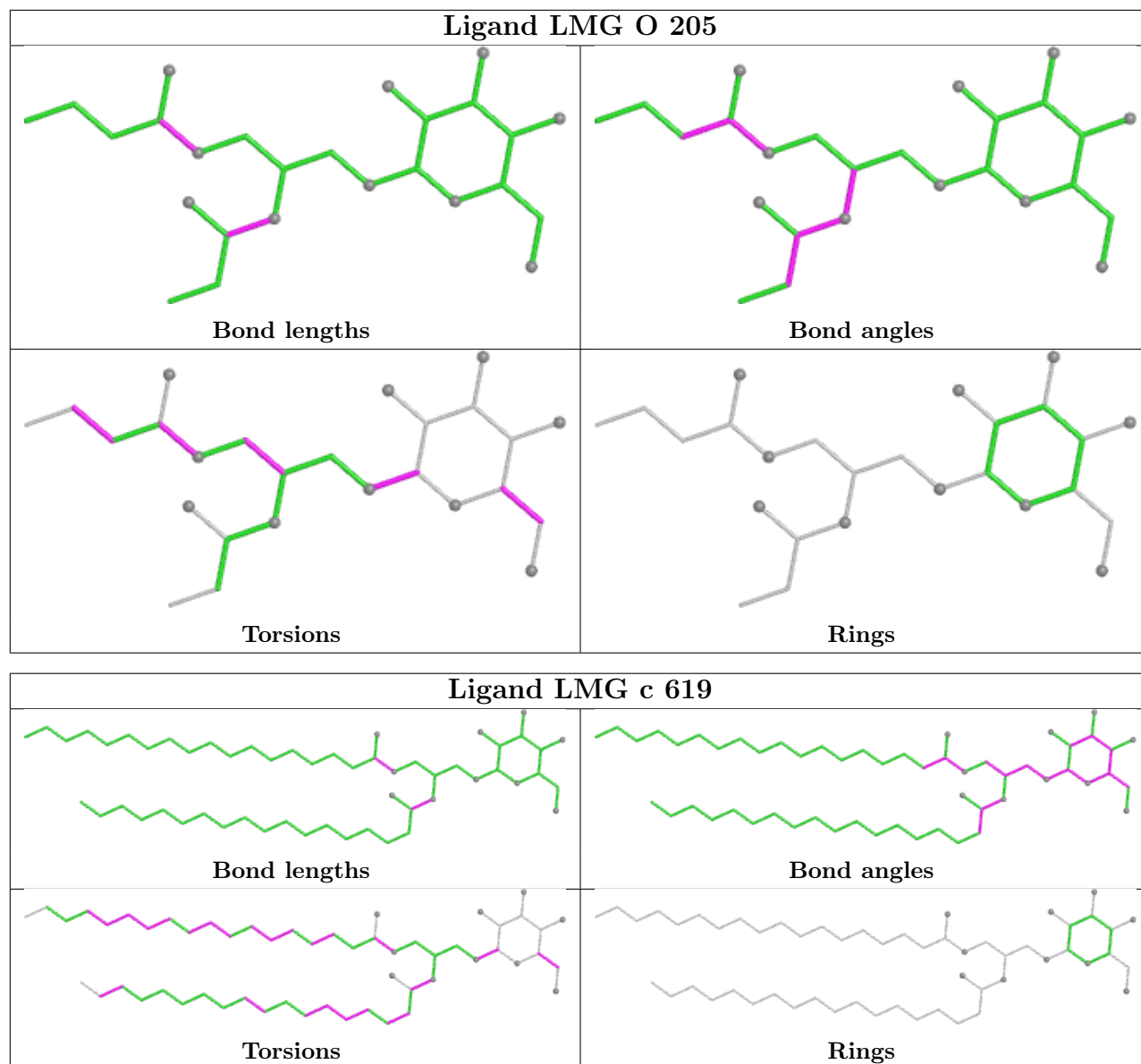
Ligand CLA O 202



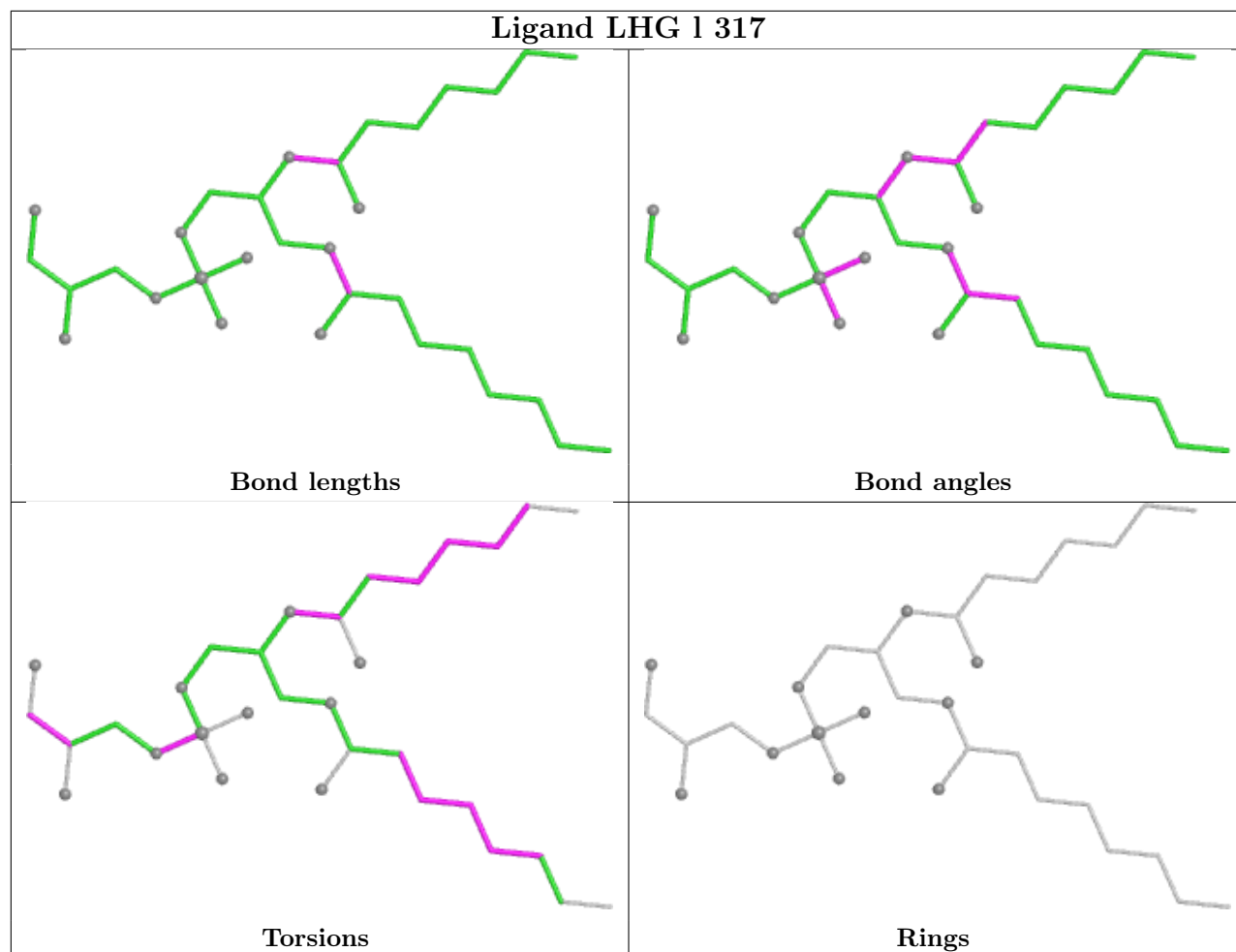
Ligand CLA i 303



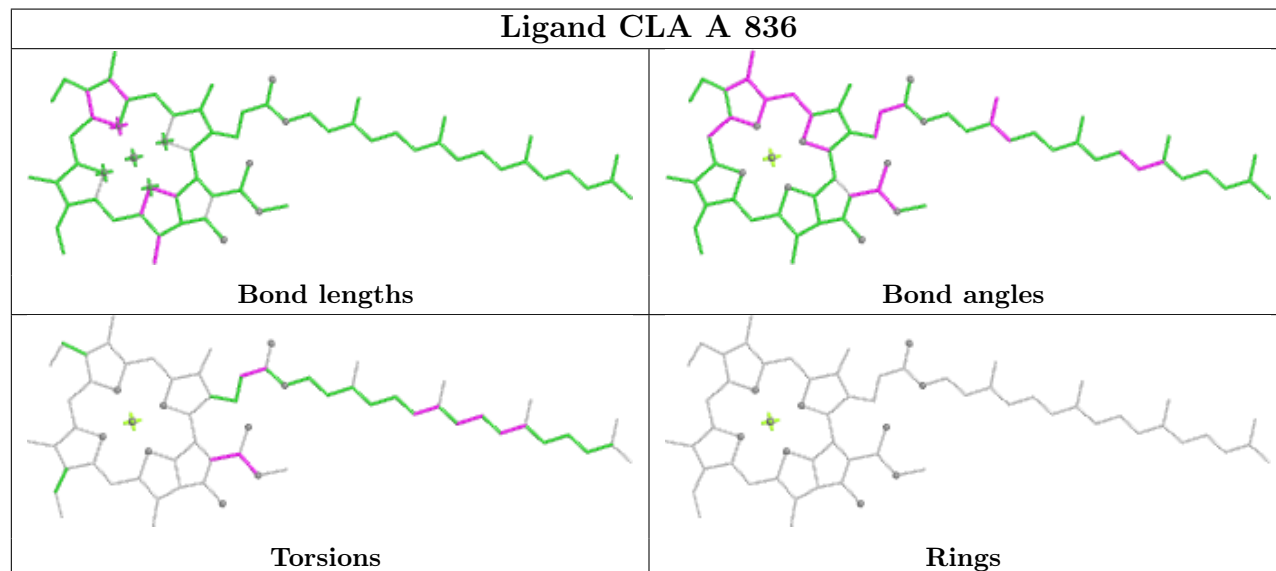




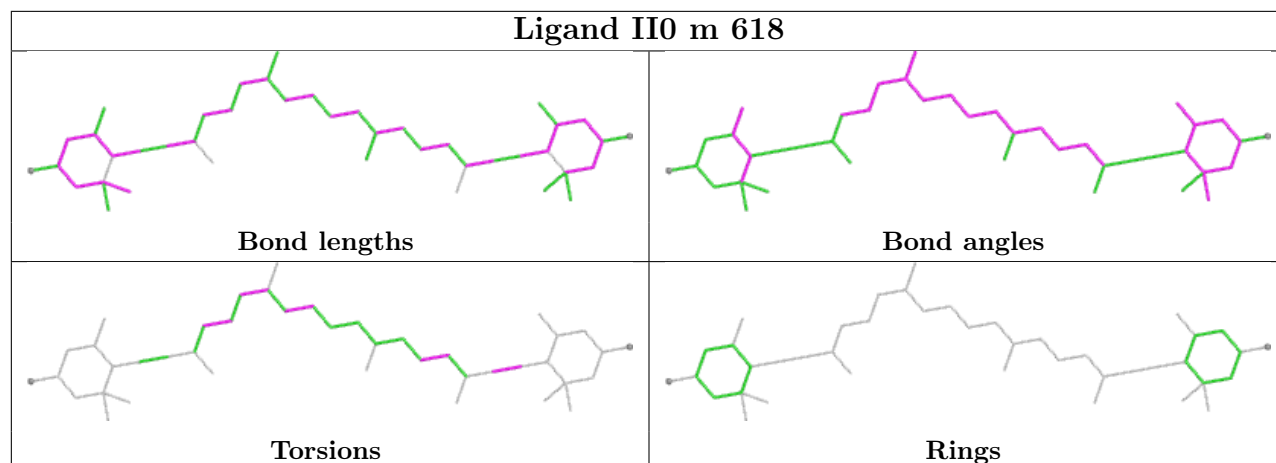
Ligand LHG 1 317



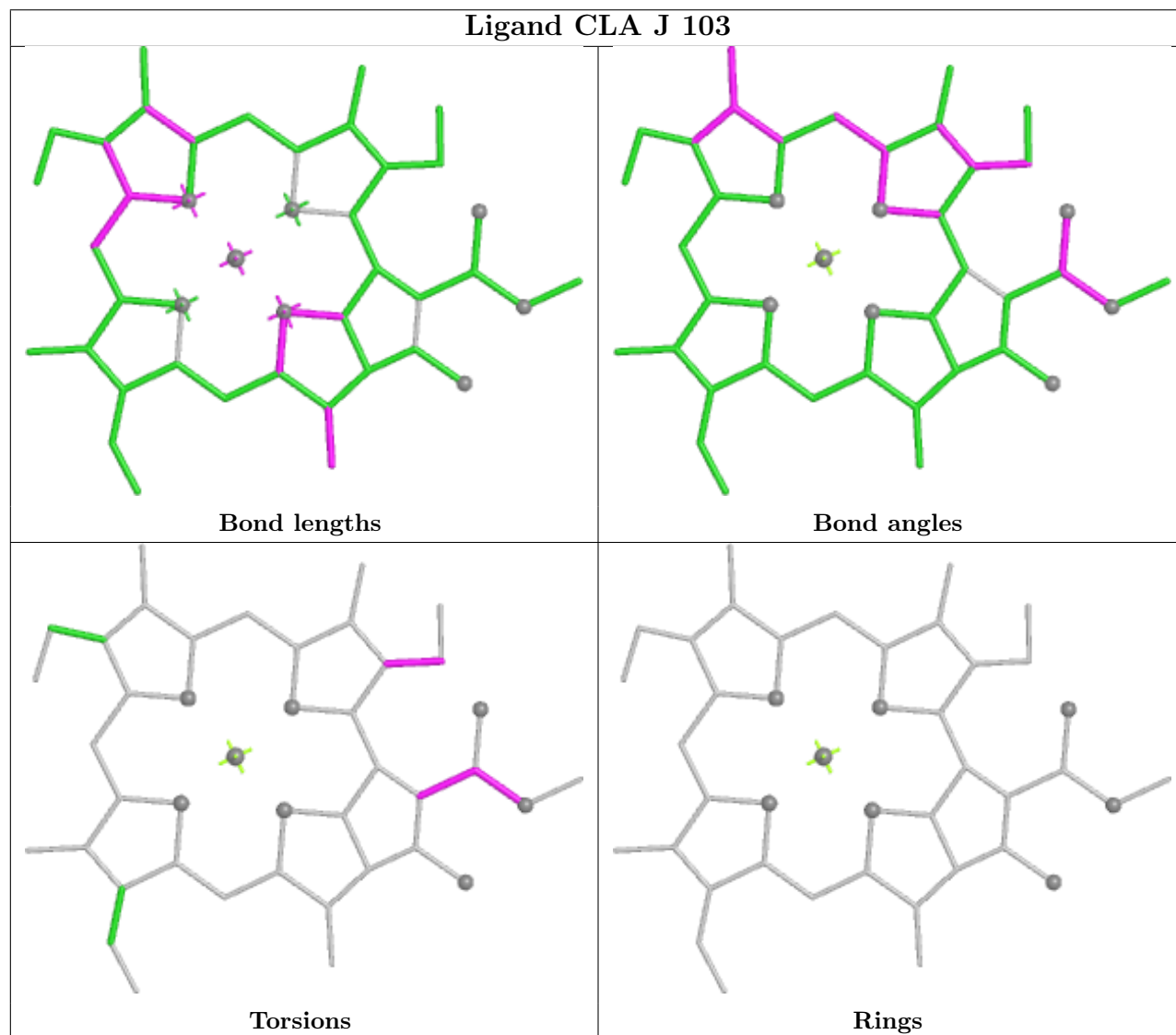
Ligand CLA A 836



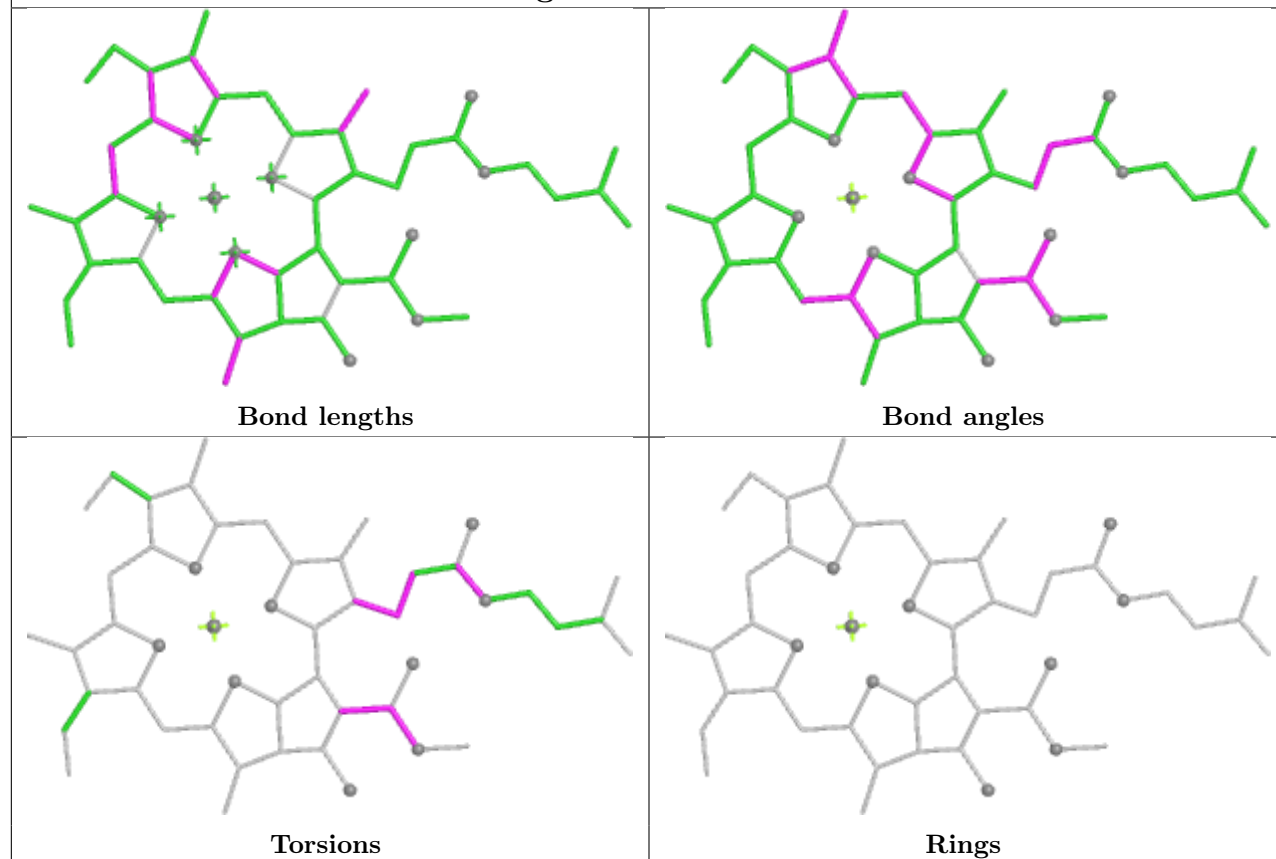
Ligand II0 m 618



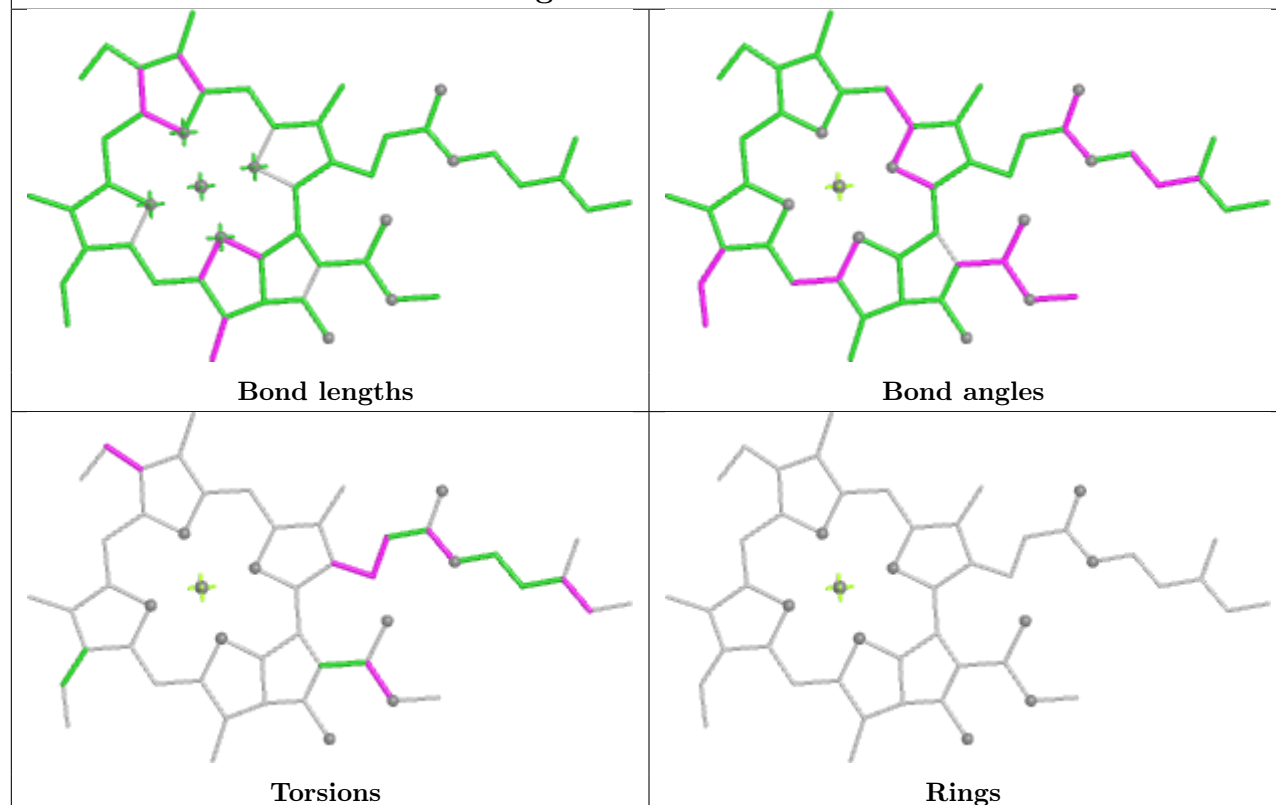
Ligand CLA J 103

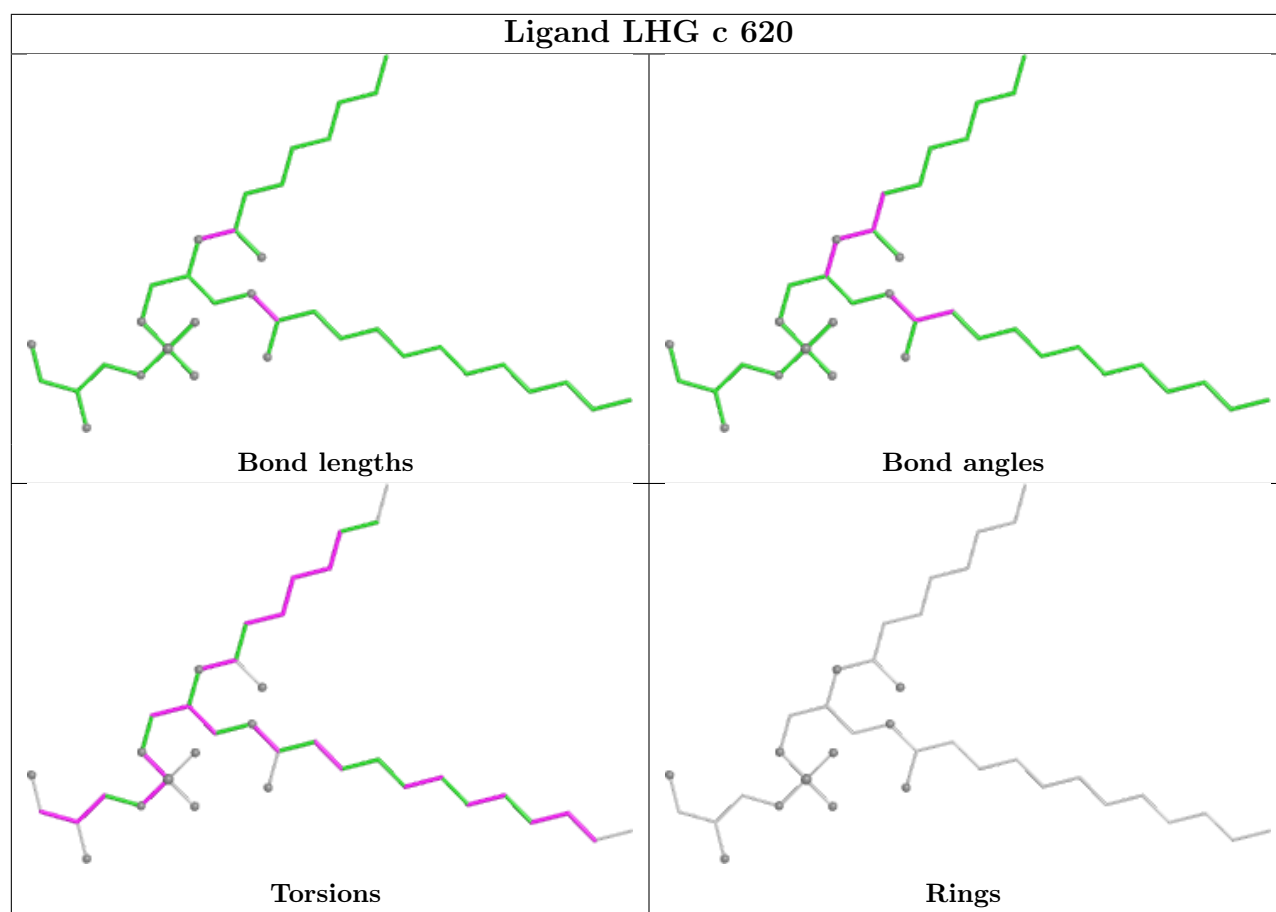
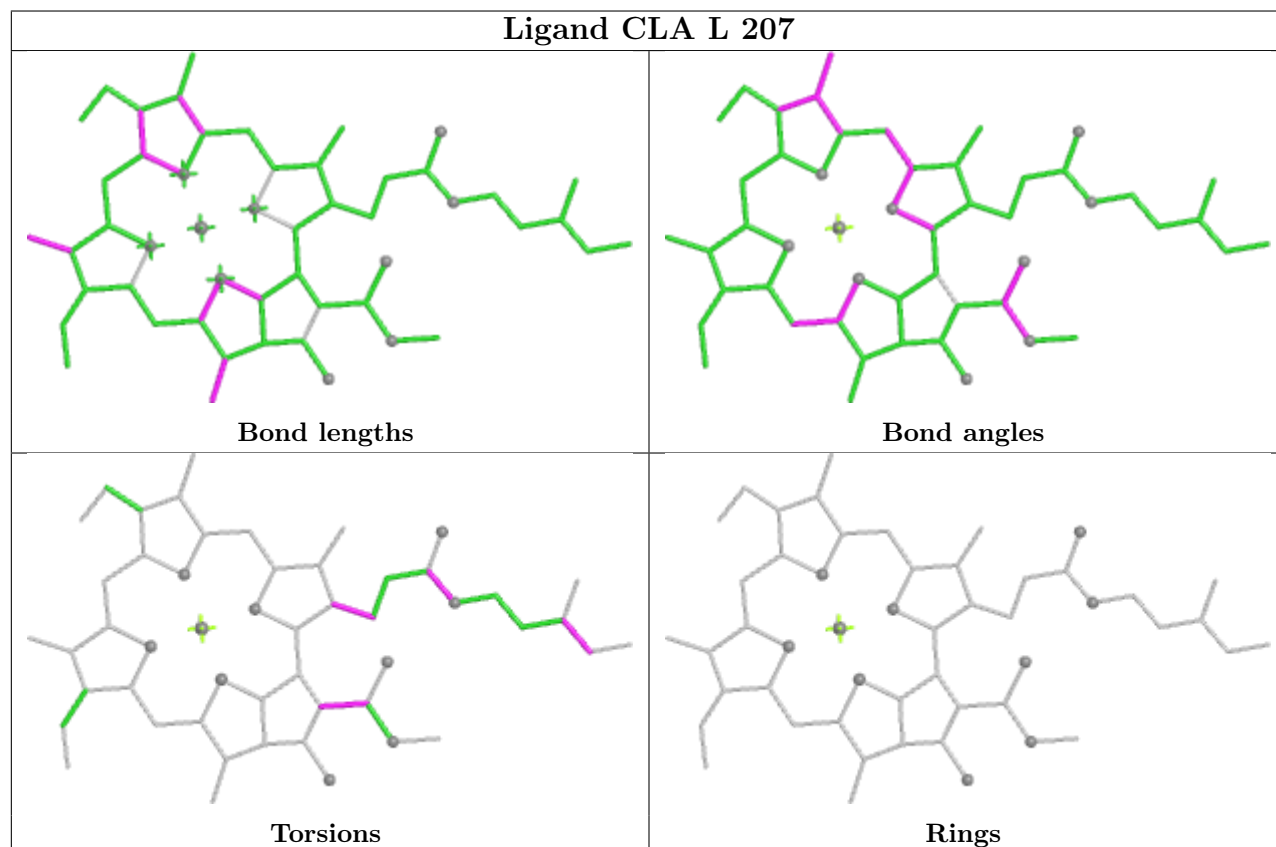


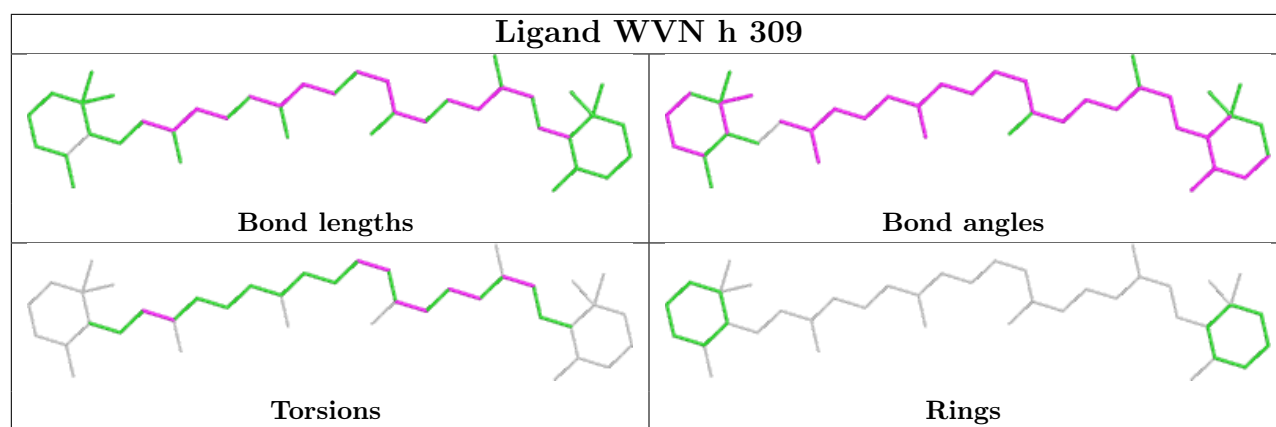
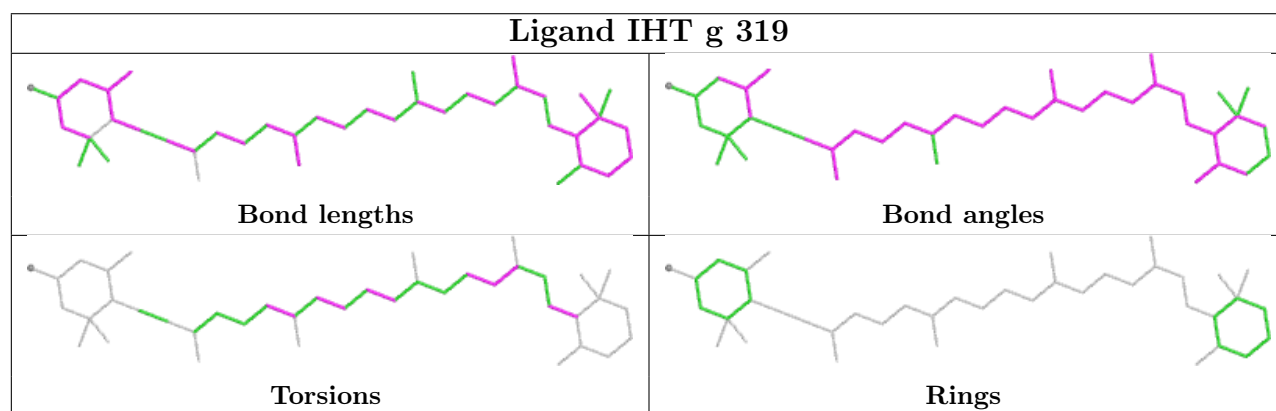
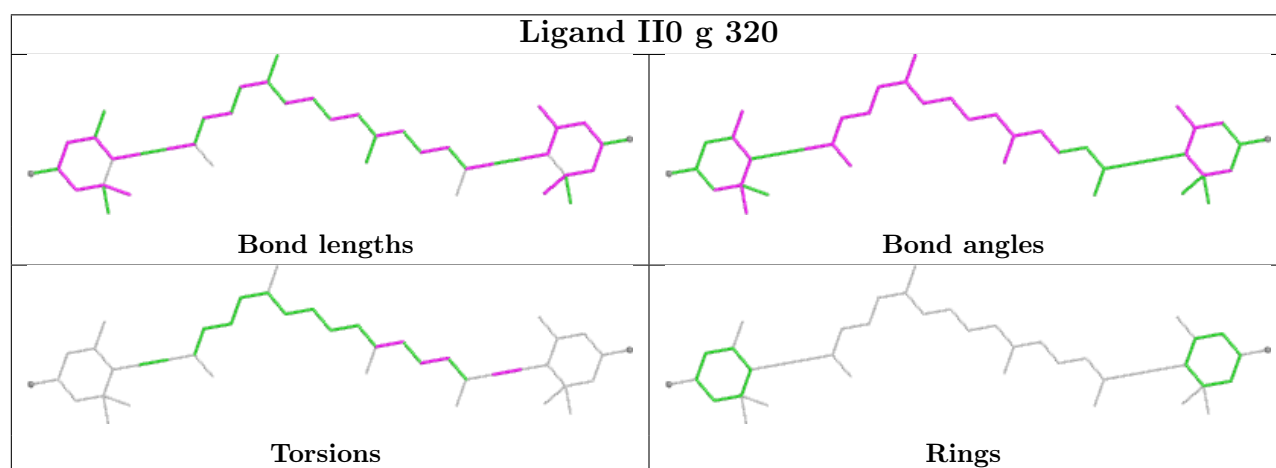
Ligand CLA a 304

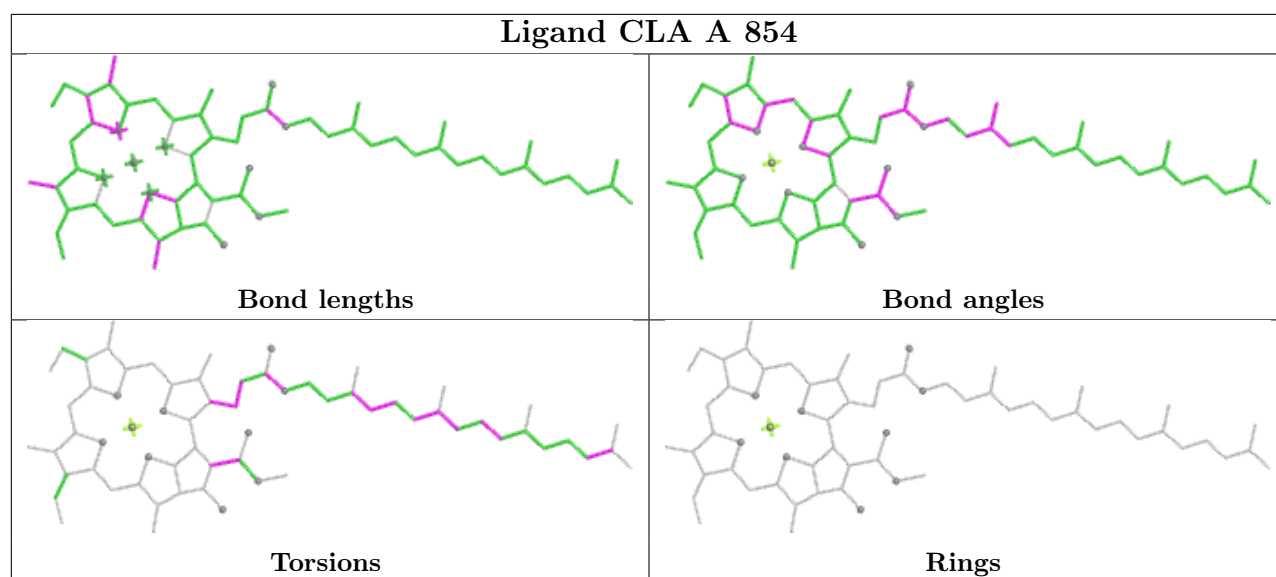
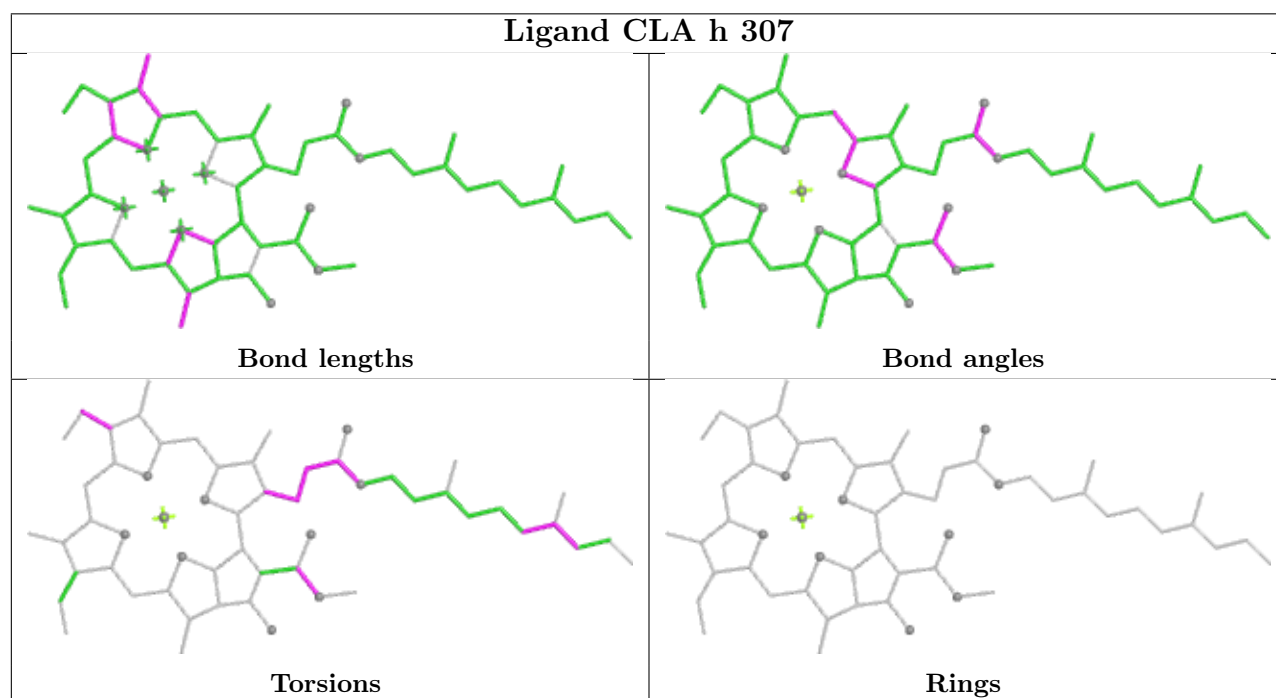
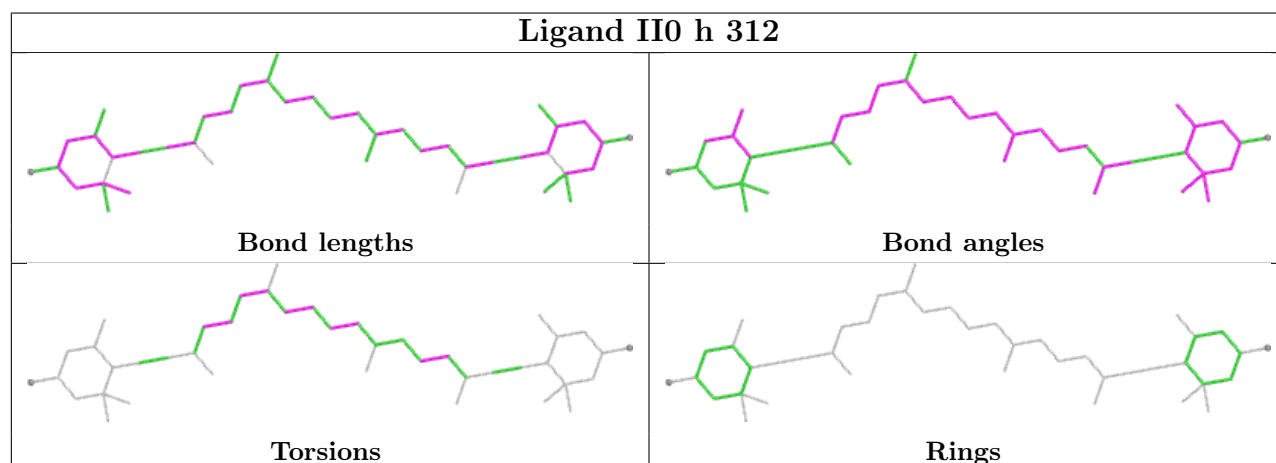


Ligand CLA k 607

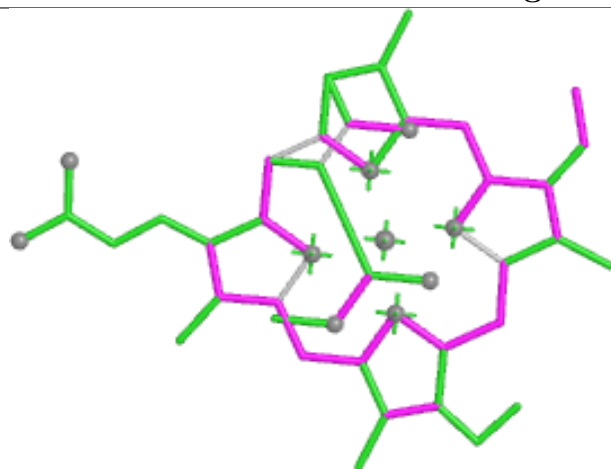




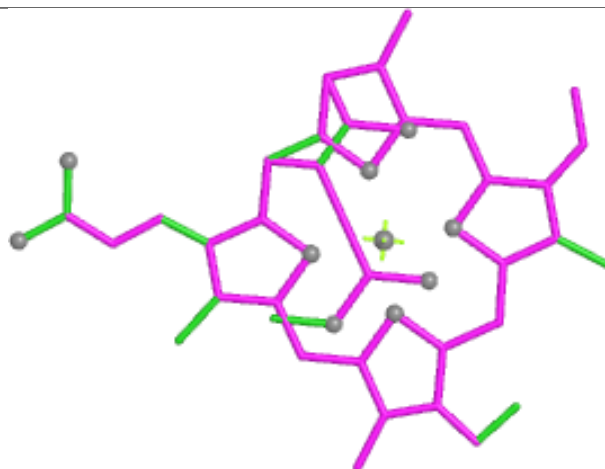




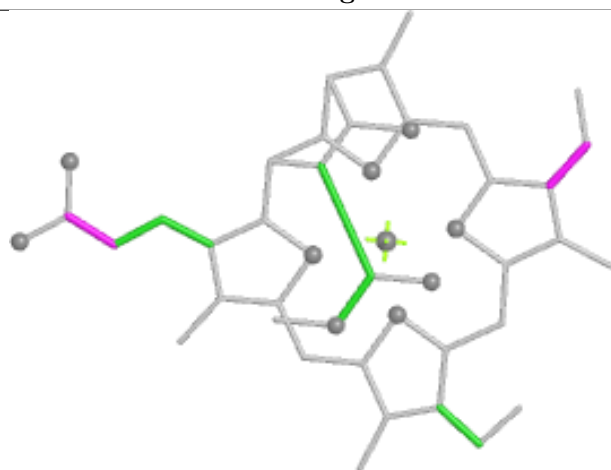
Ligand KC2 I 310



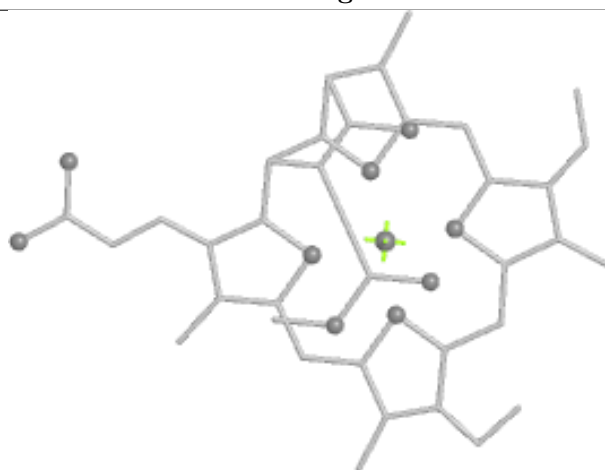
Bond lengths



Bond angles

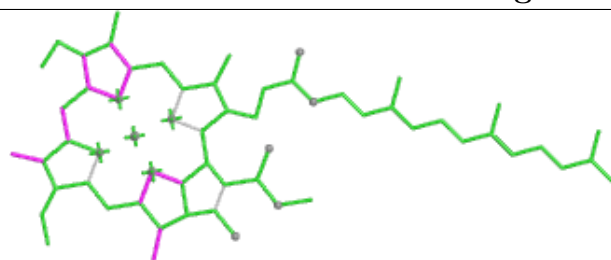


Torsions

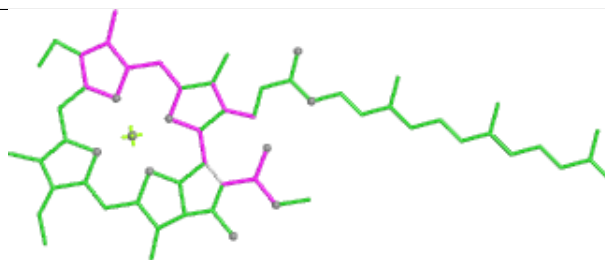


Rings

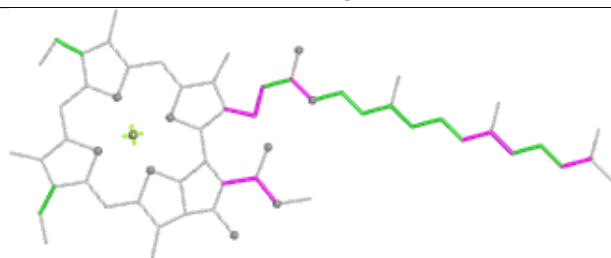
Ligand CLA B 812



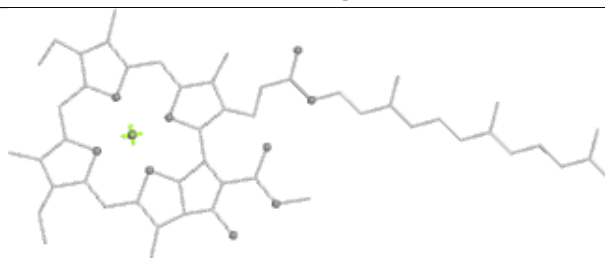
Bond lengths



Bond angles

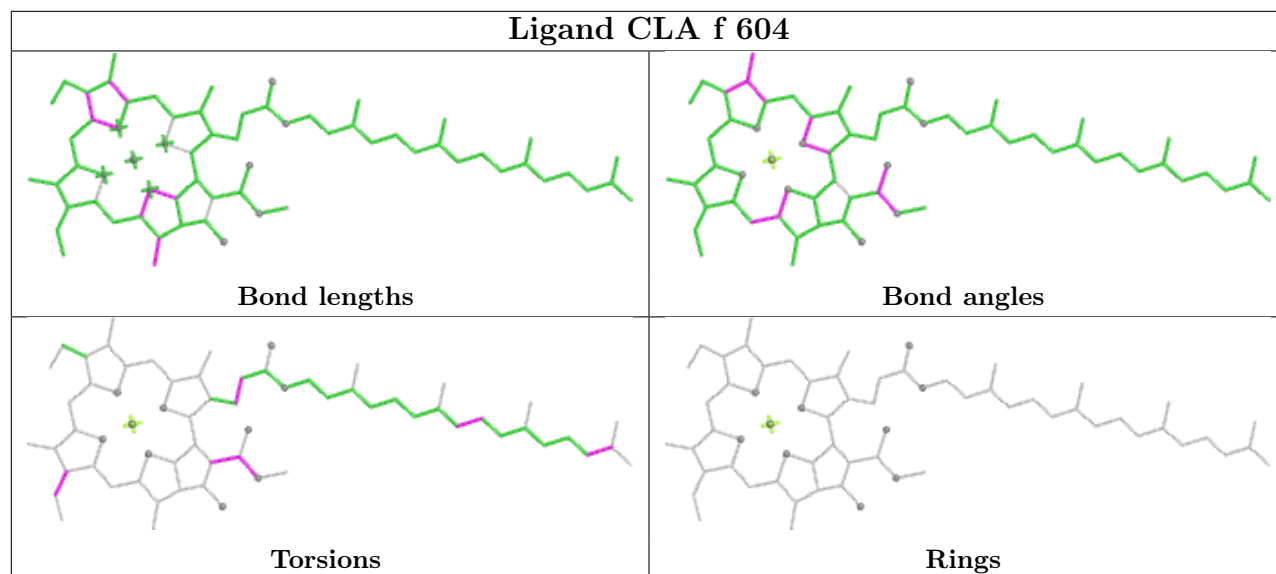


Torsions

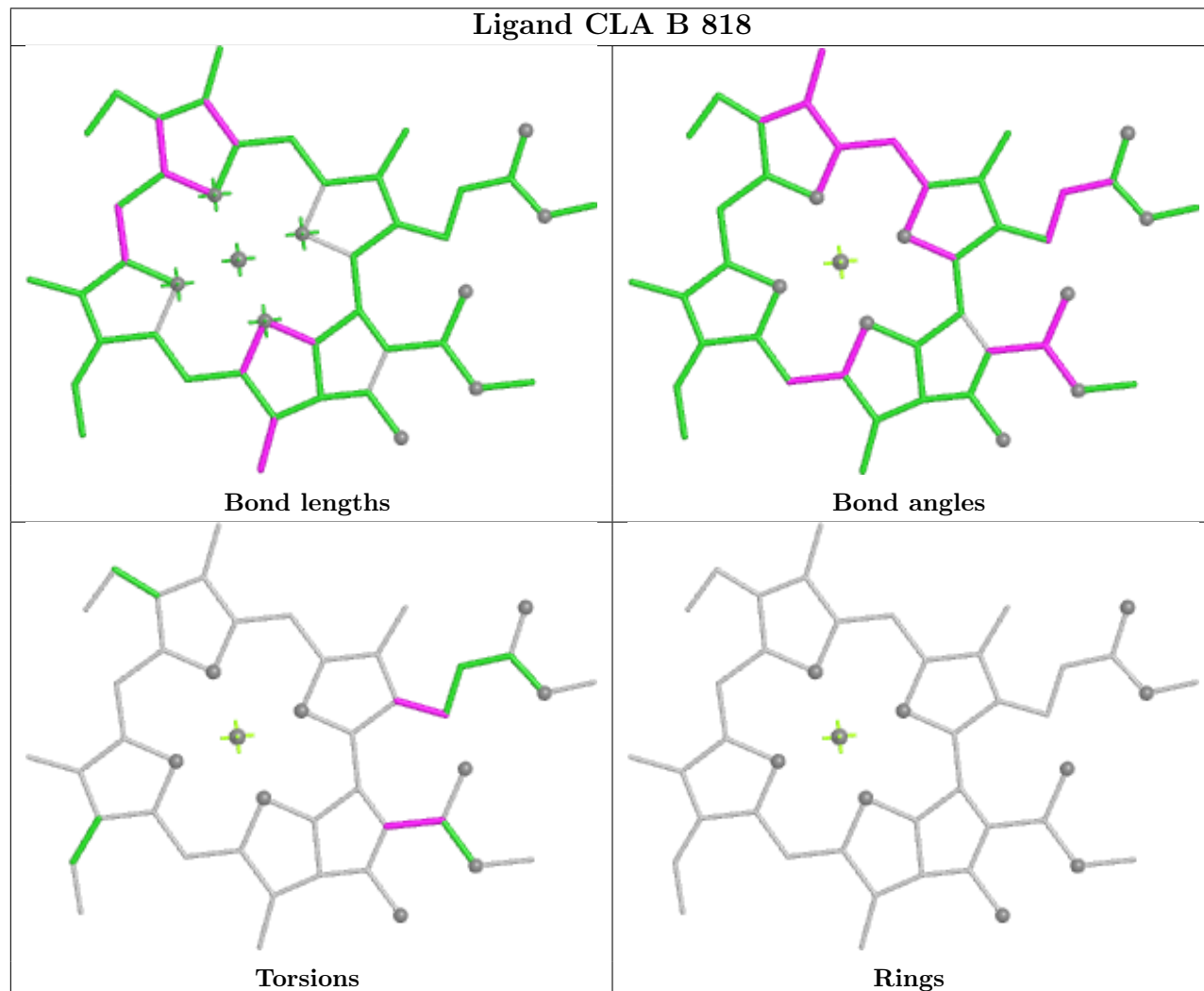


Rings

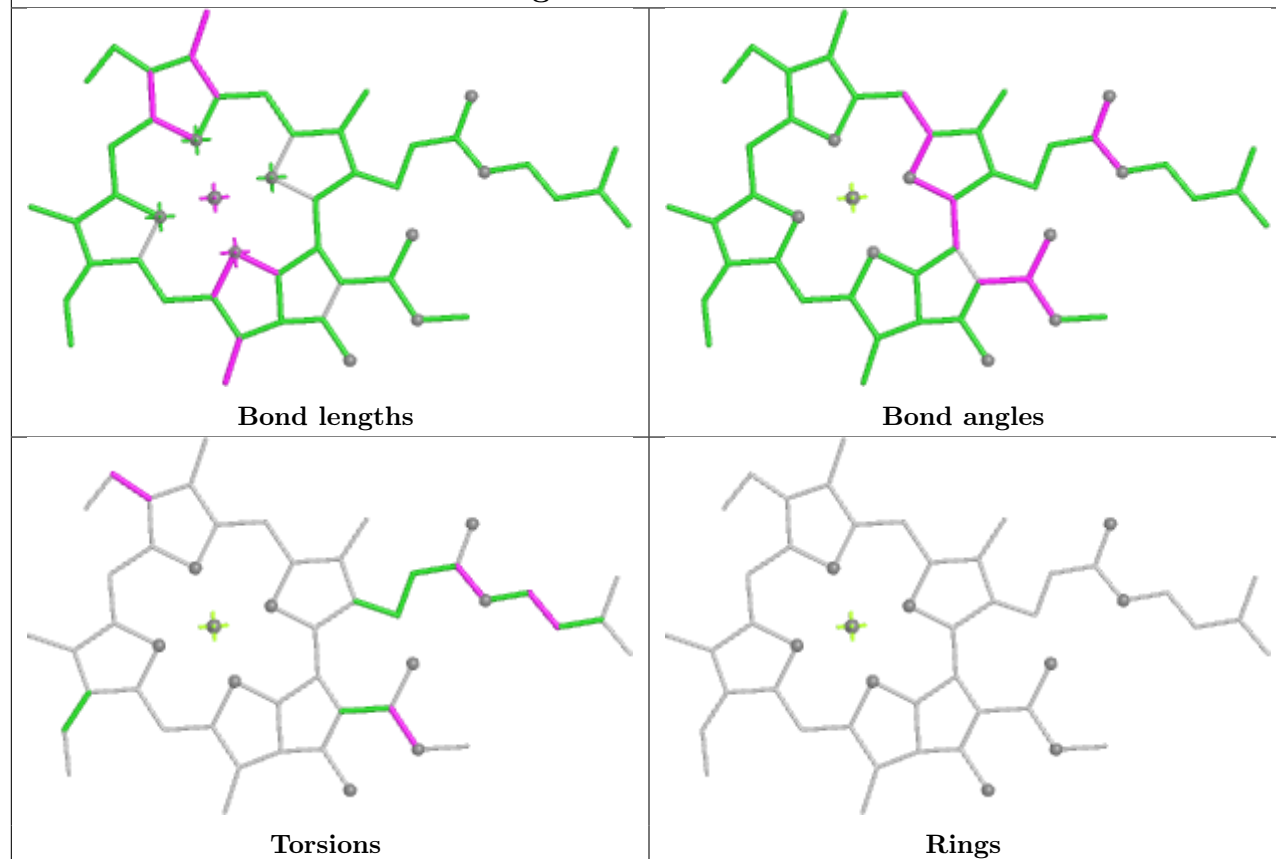
Ligand CLA f 604



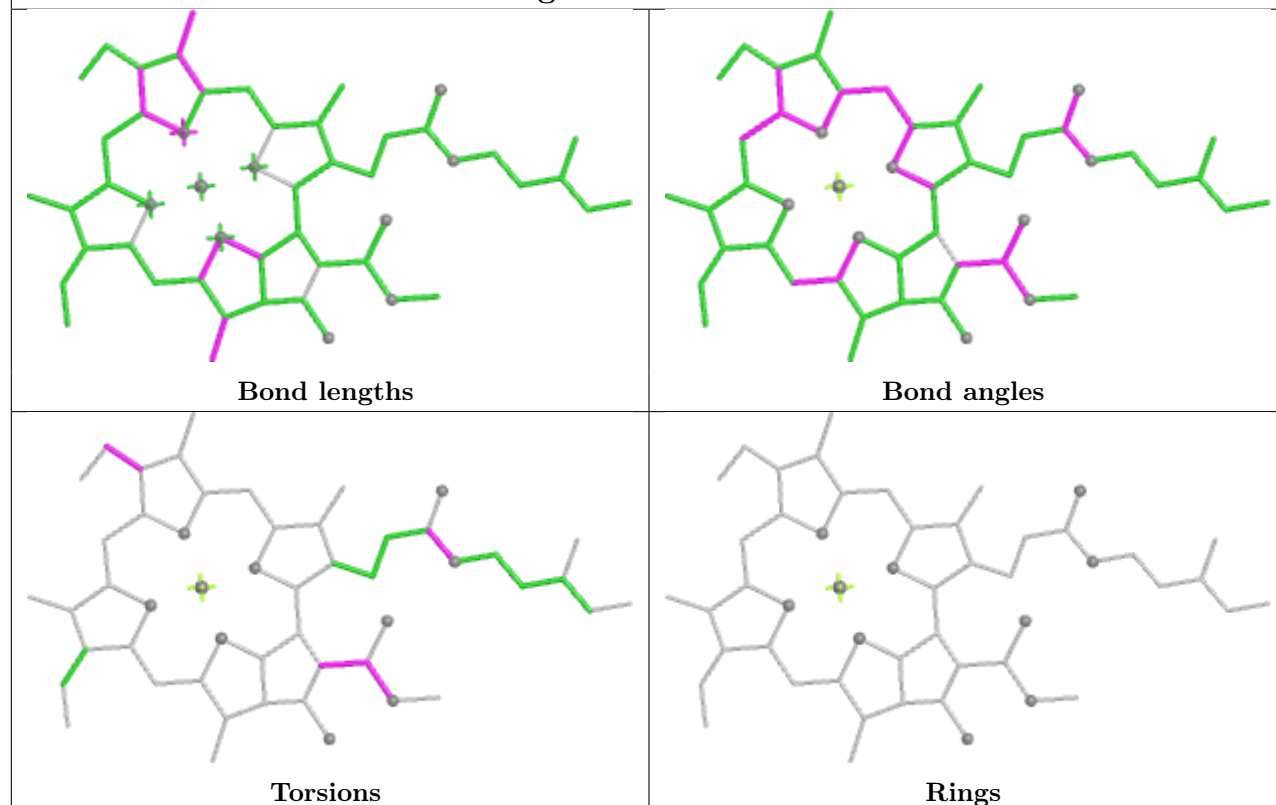
Ligand CLA B 818

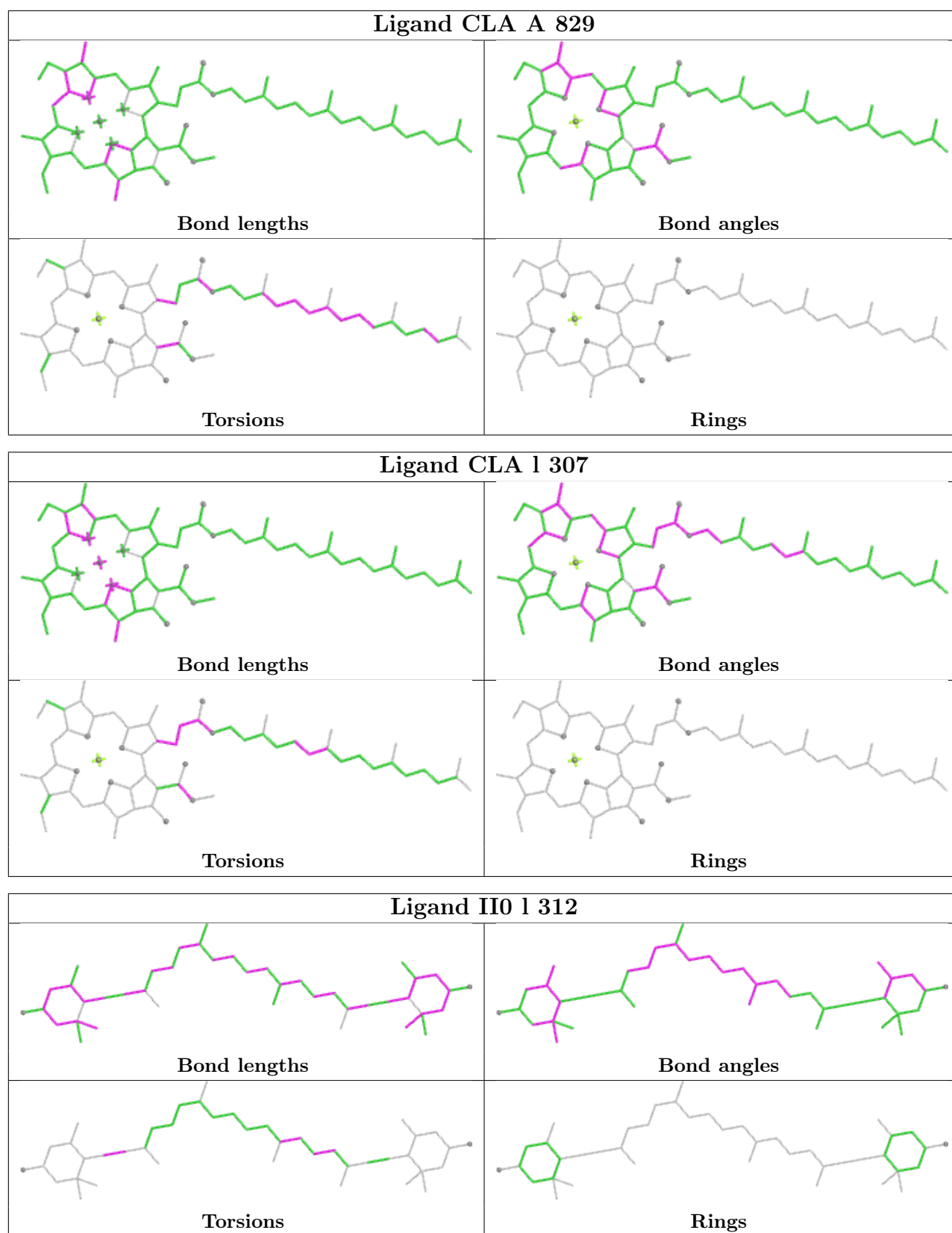


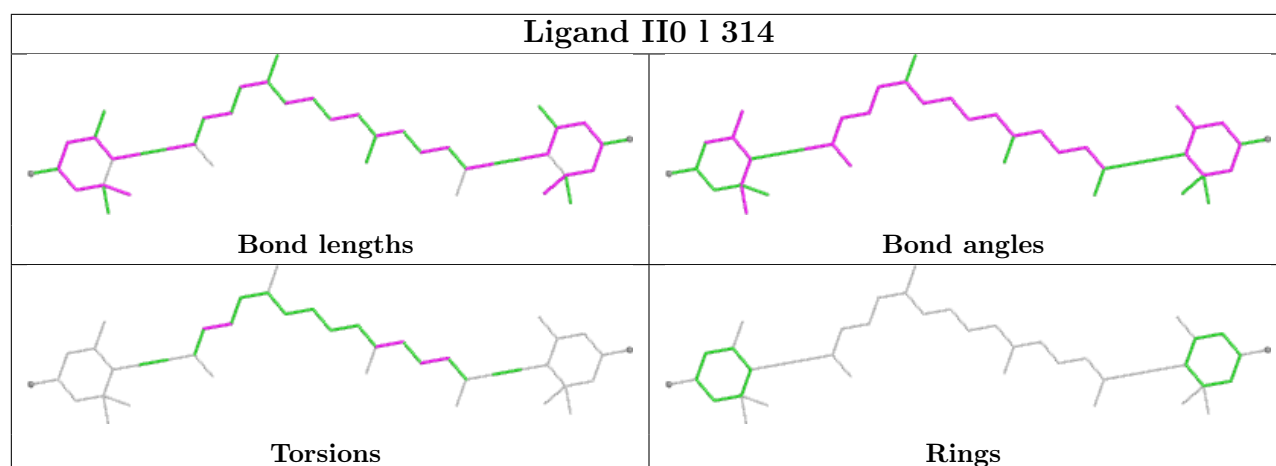
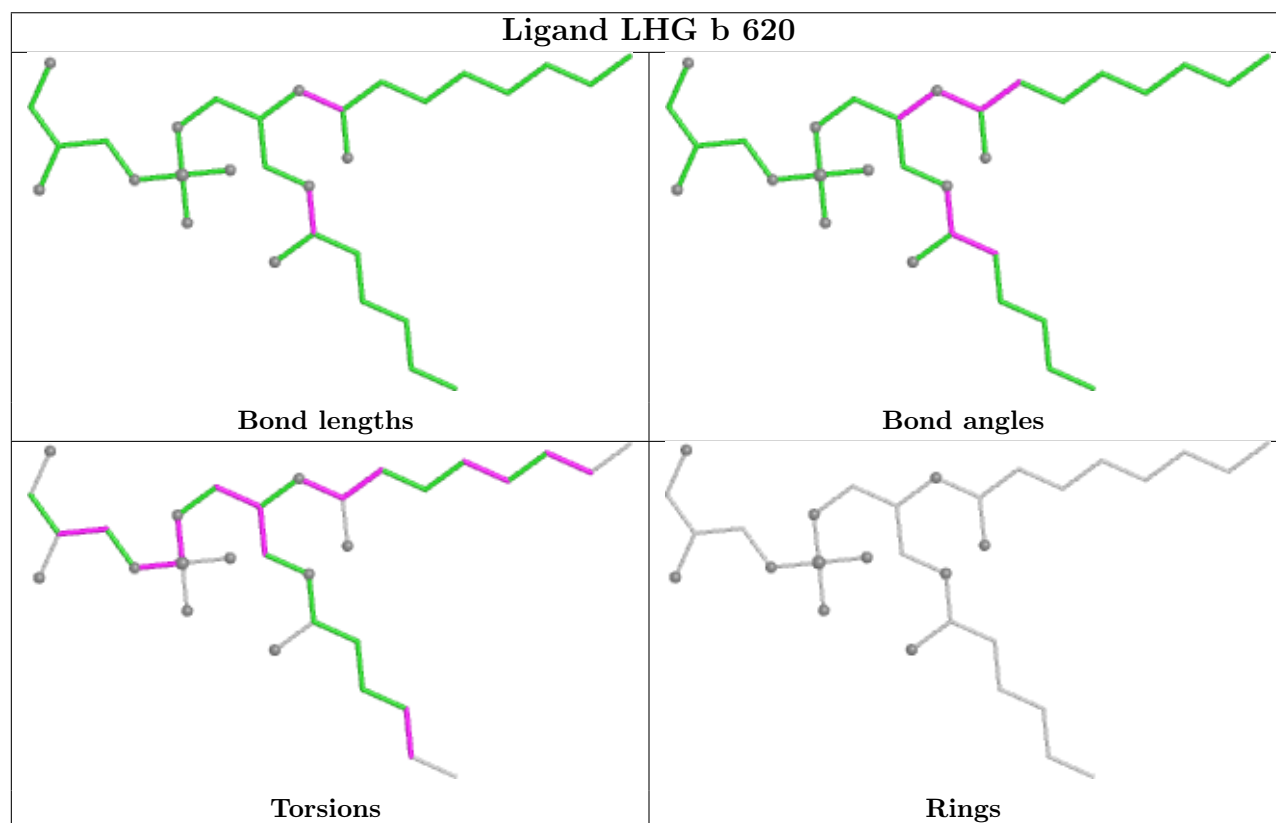
Ligand CLA B 829

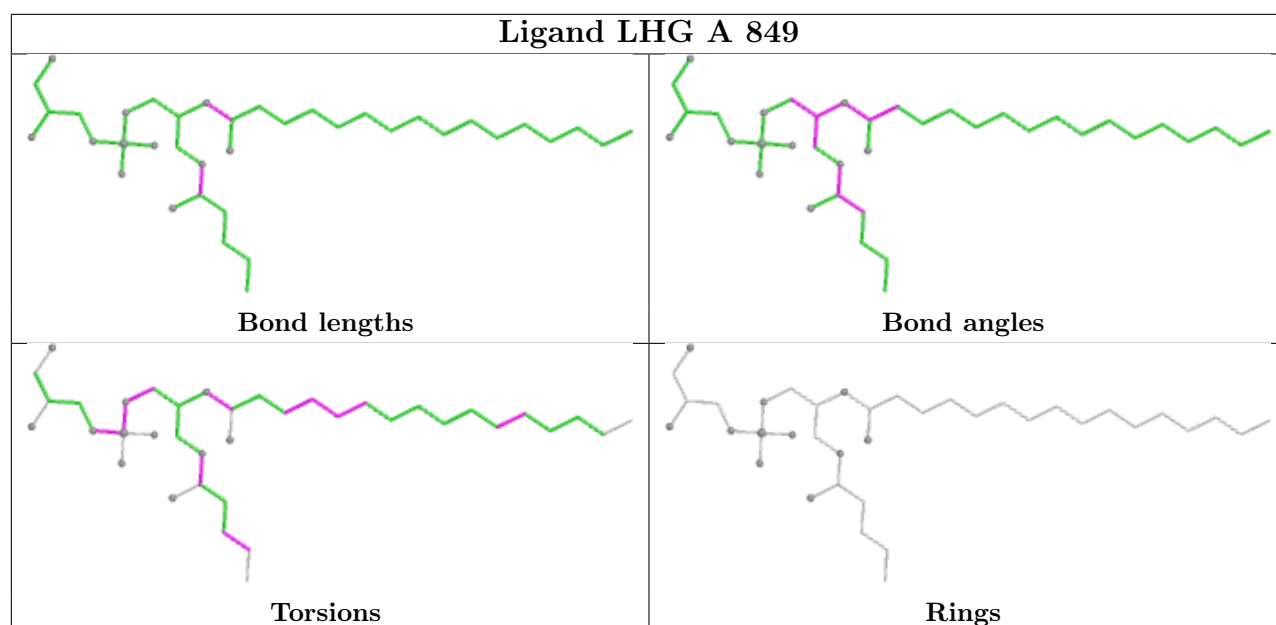
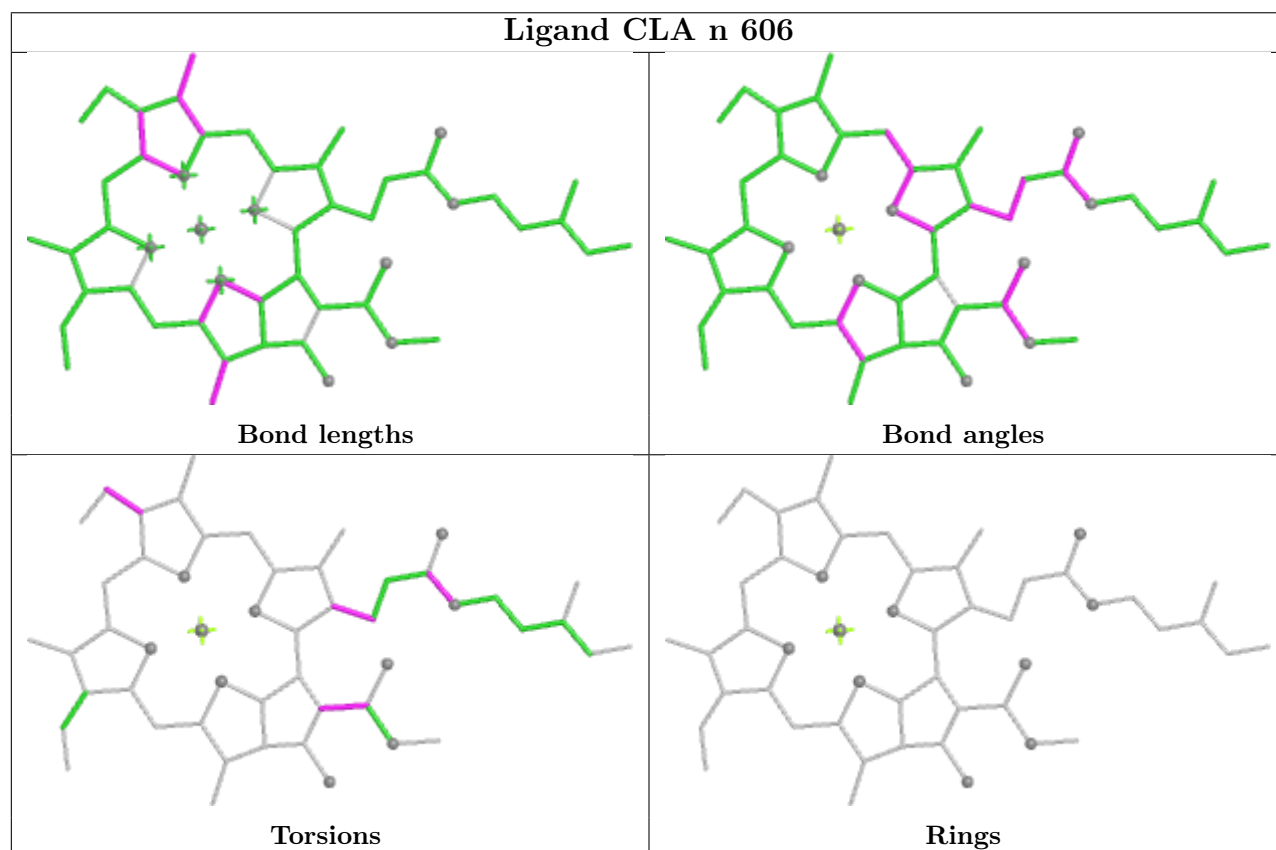


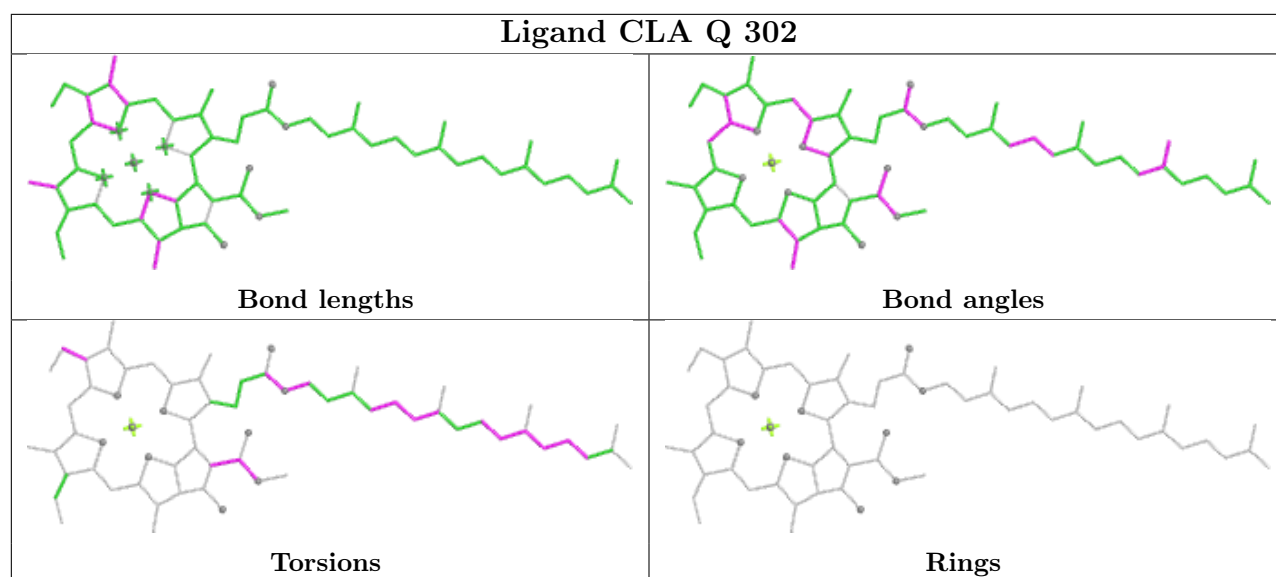
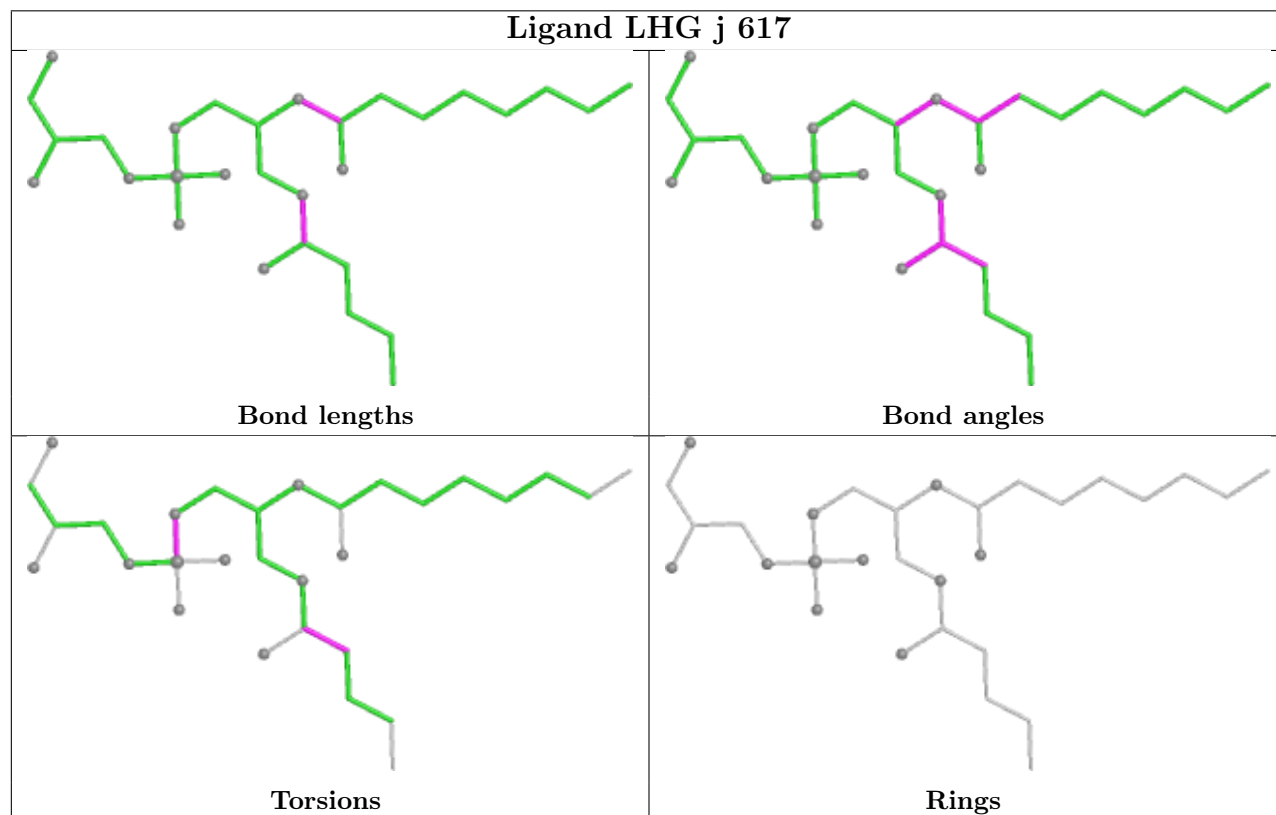
Ligand CLA s 208

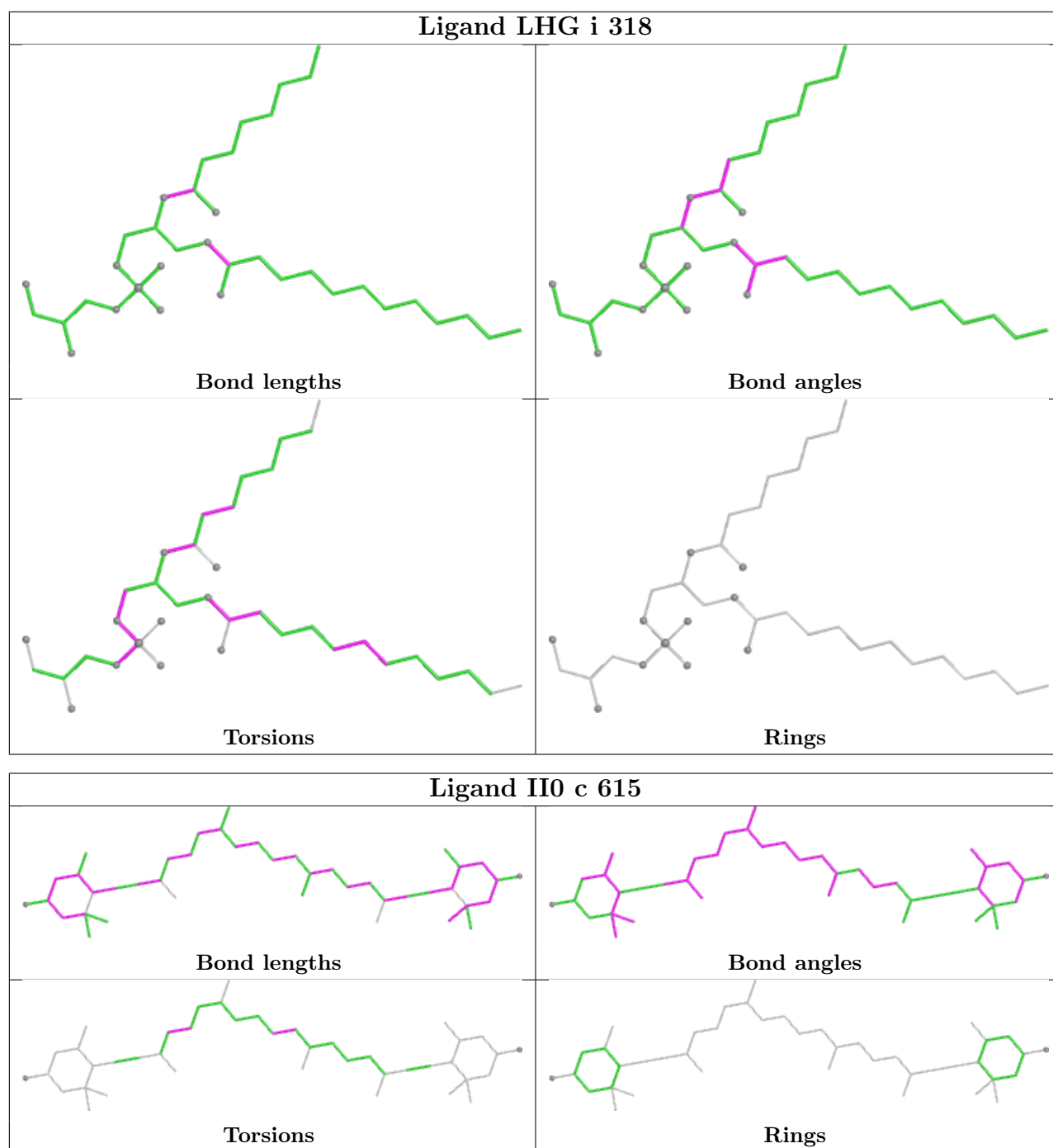


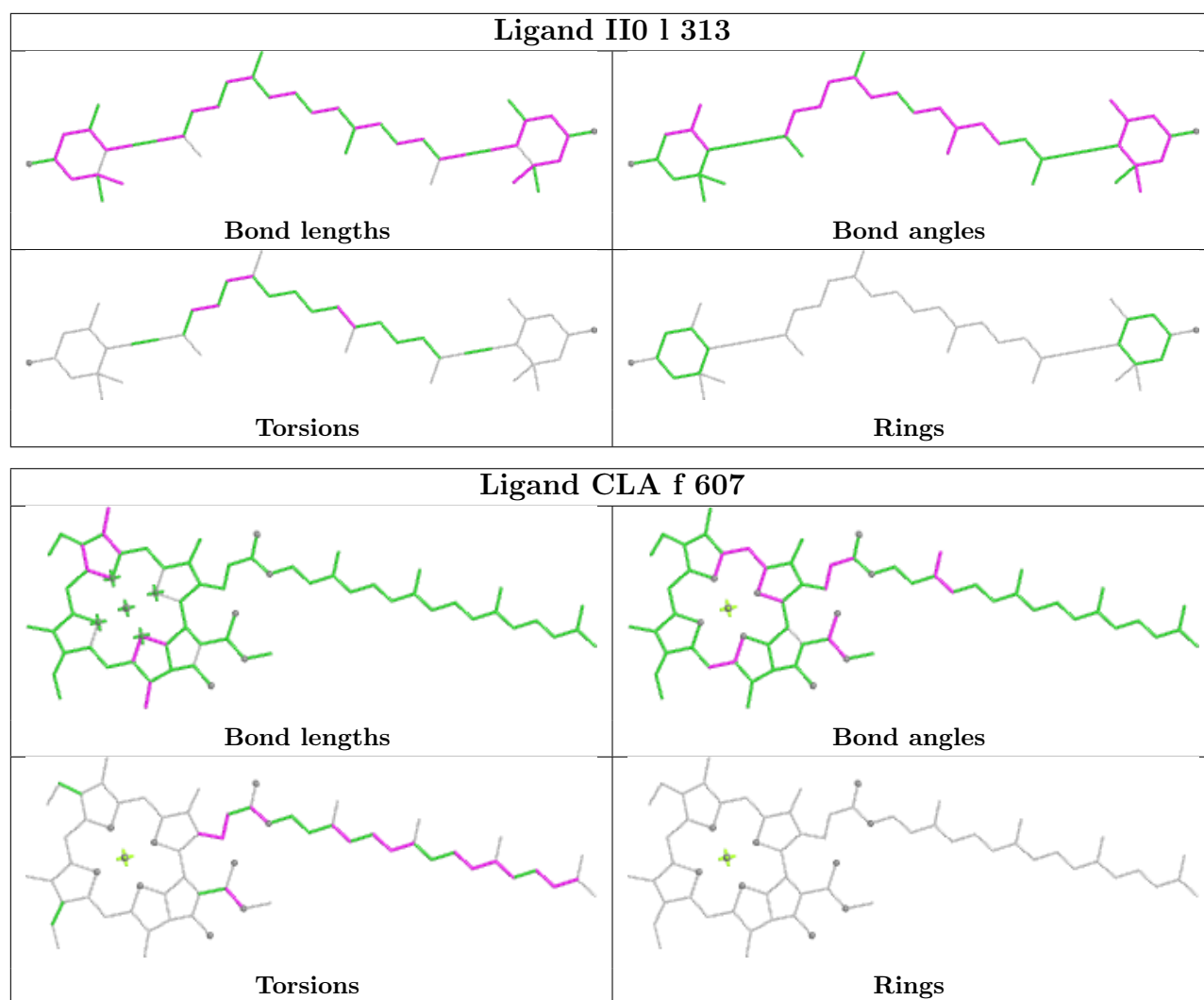




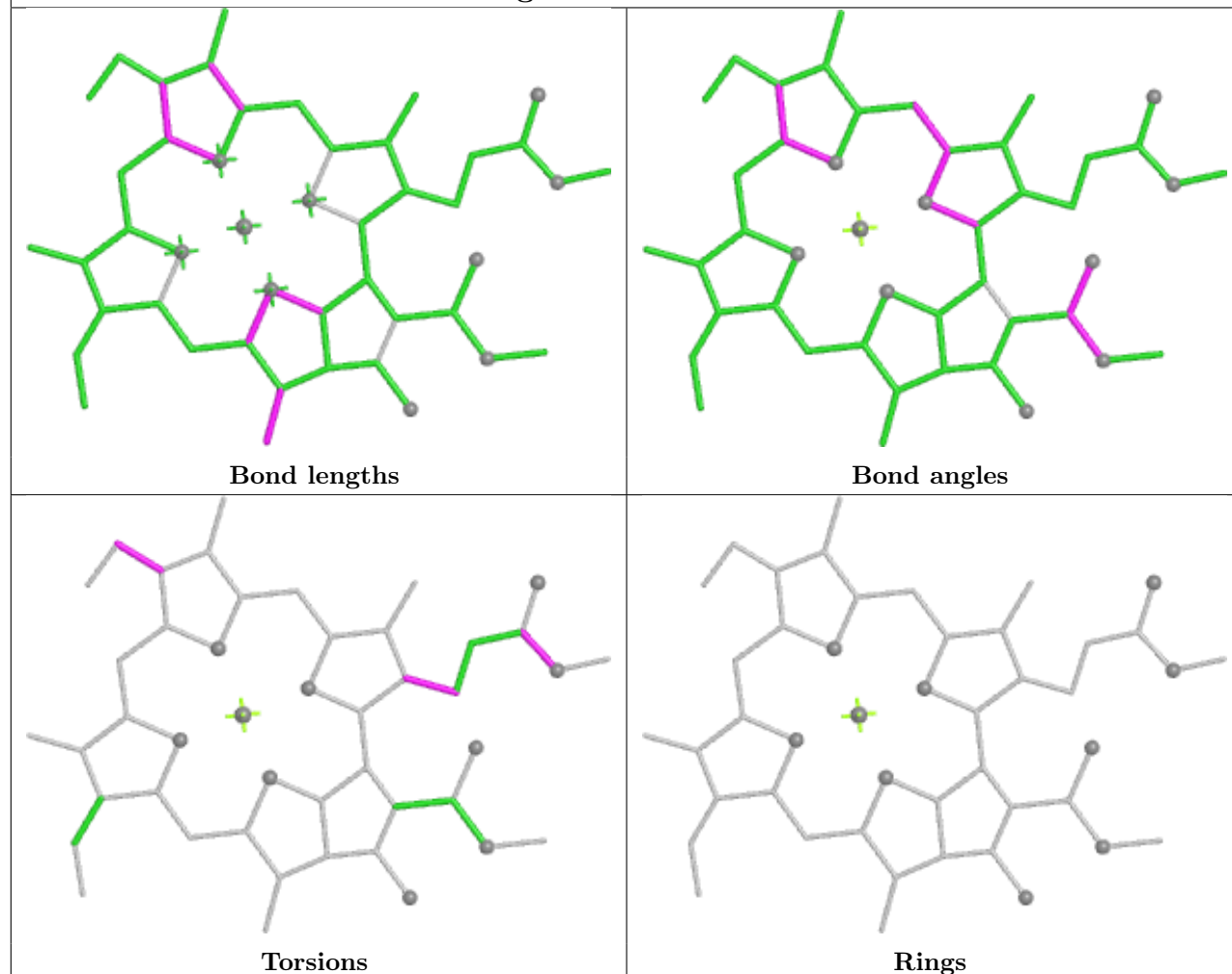




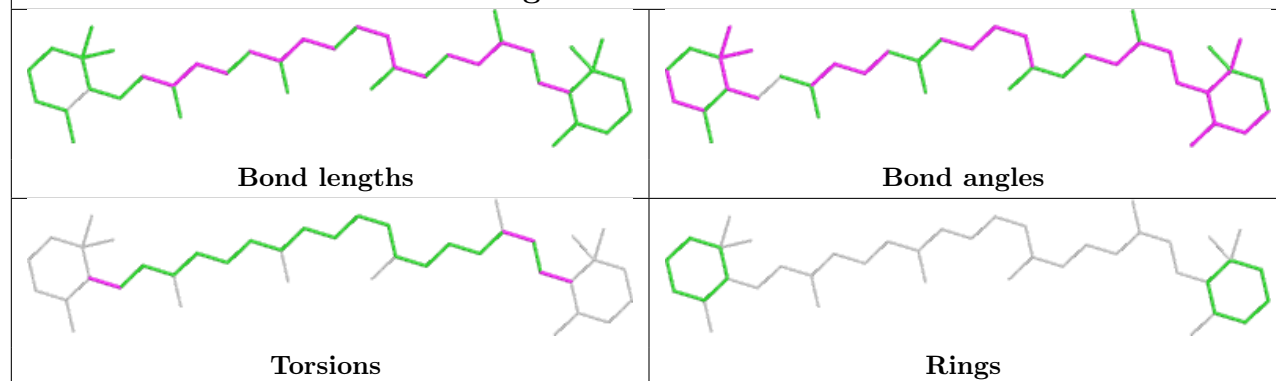


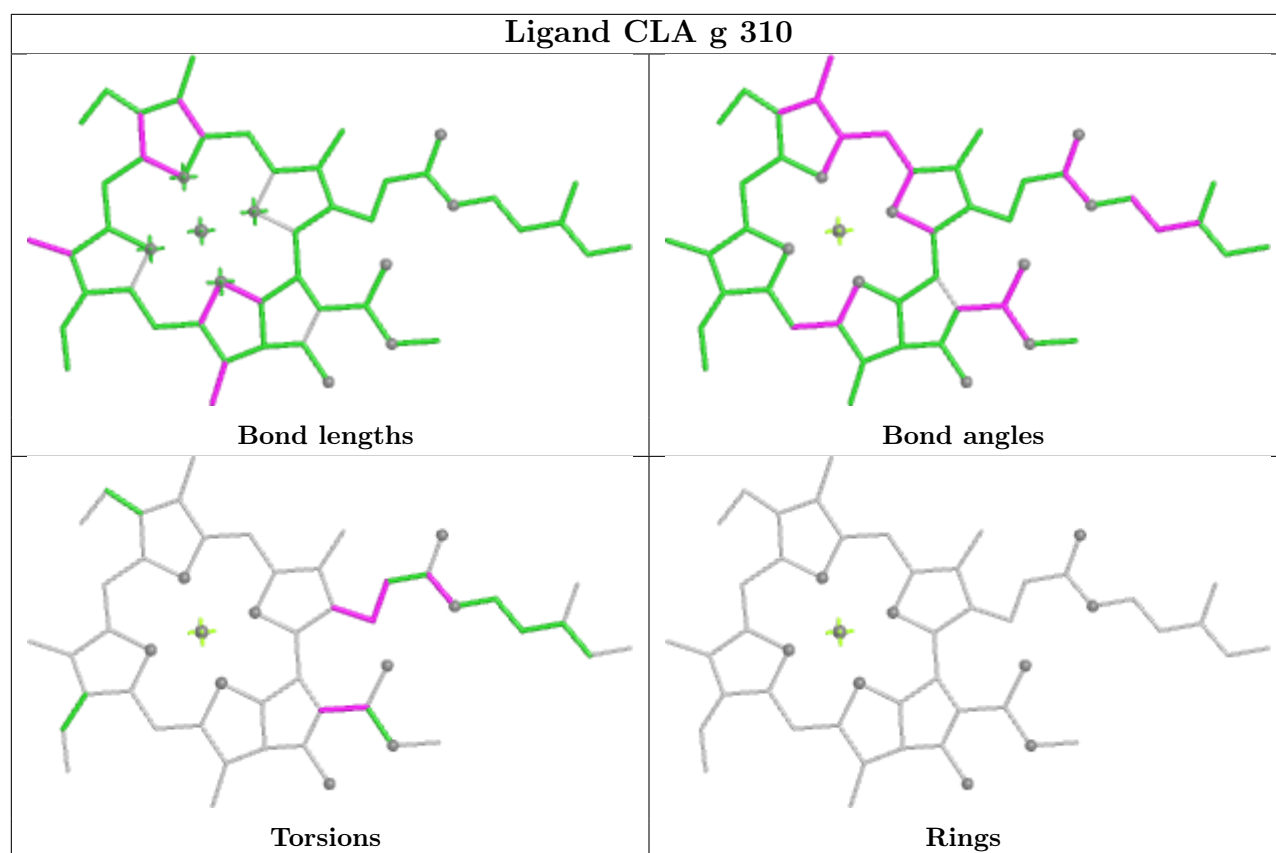


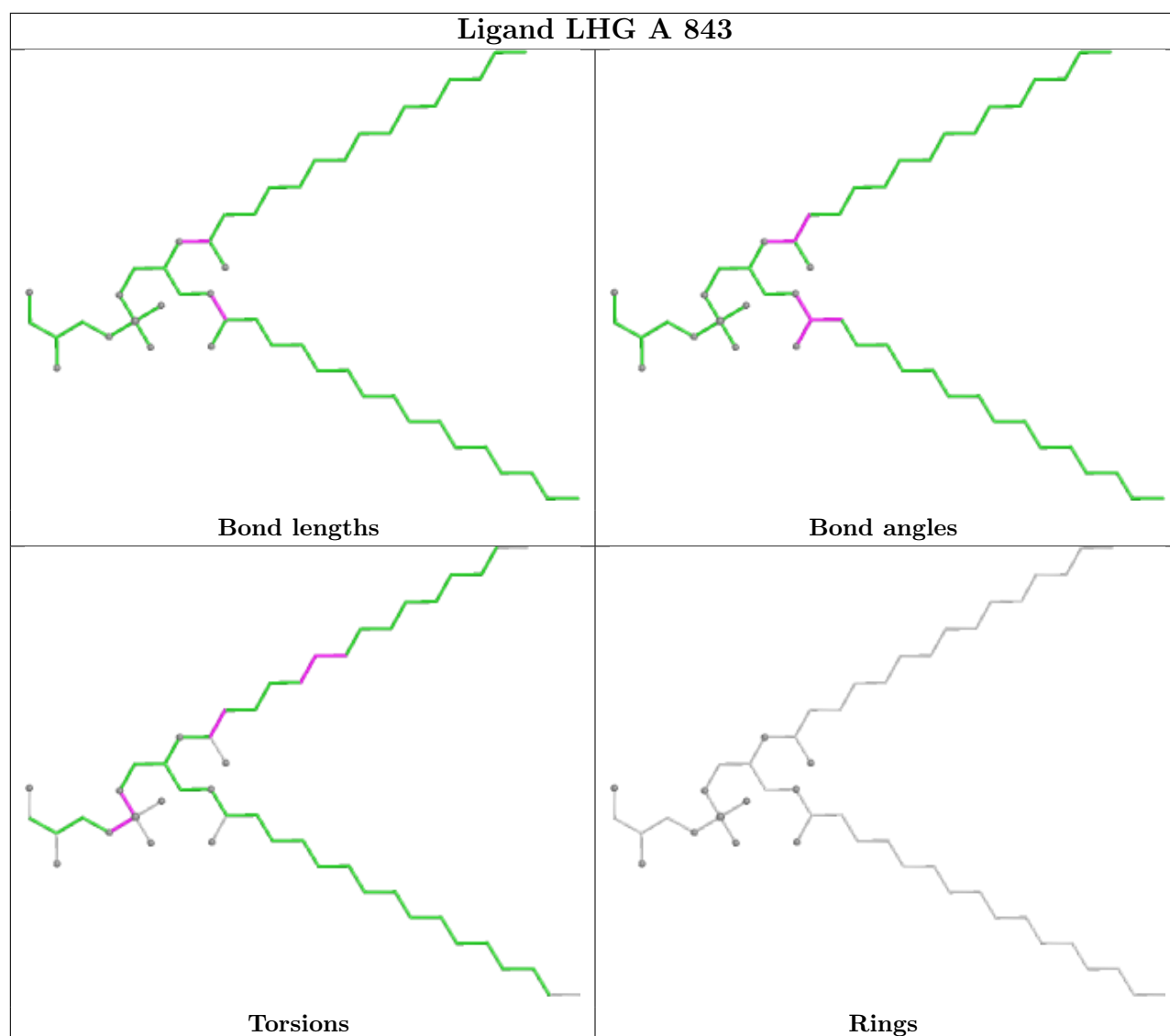
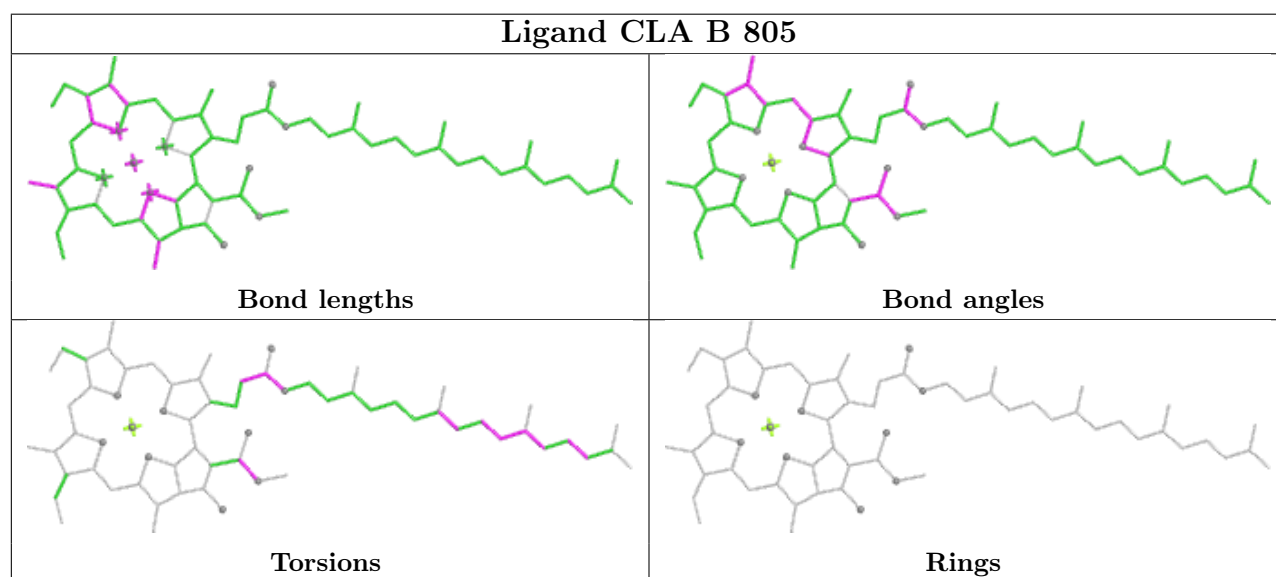
Ligand CLA d 307

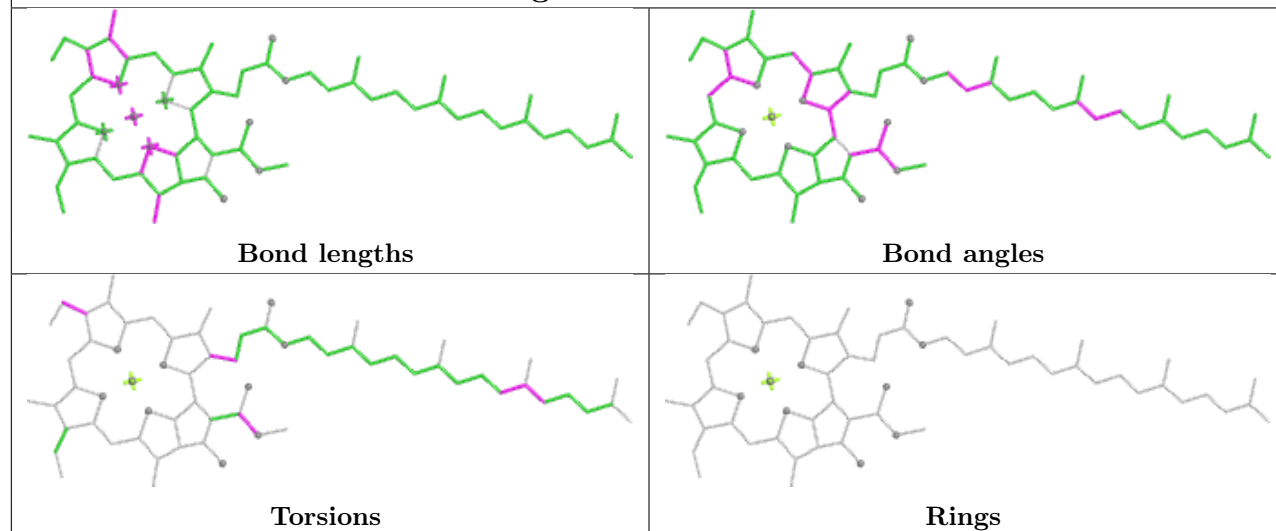
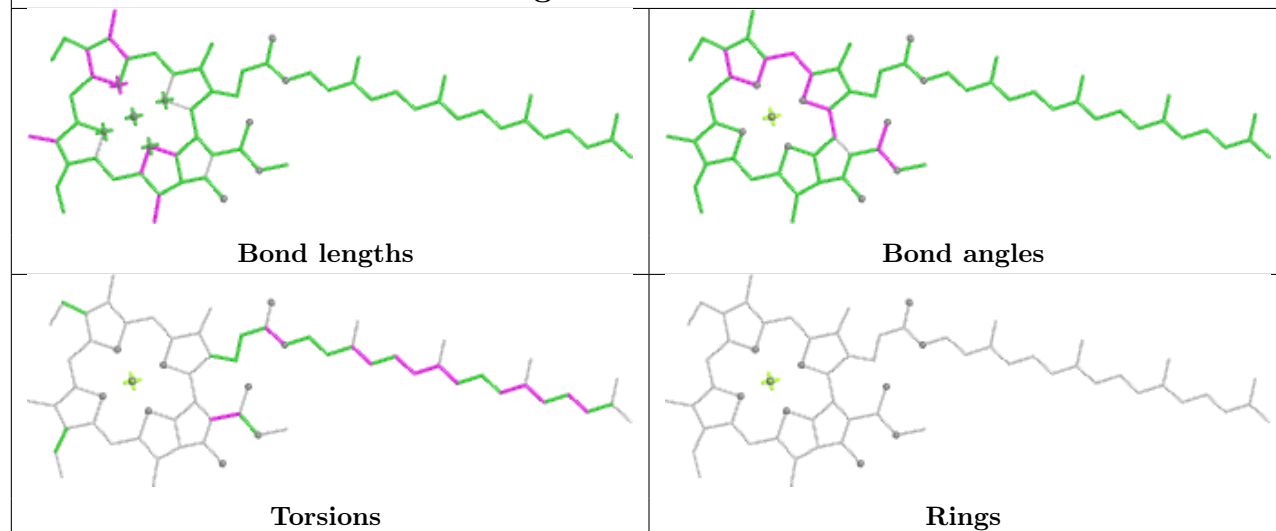


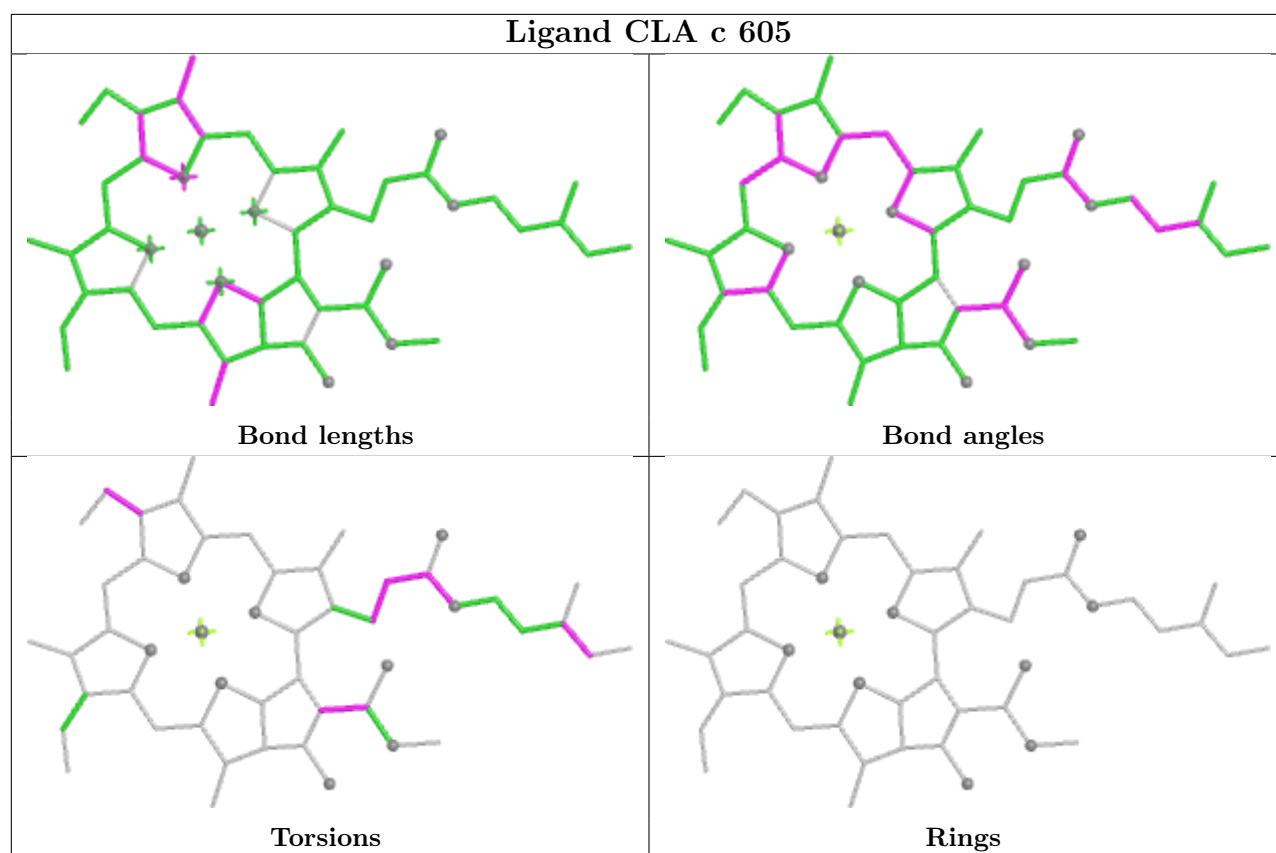
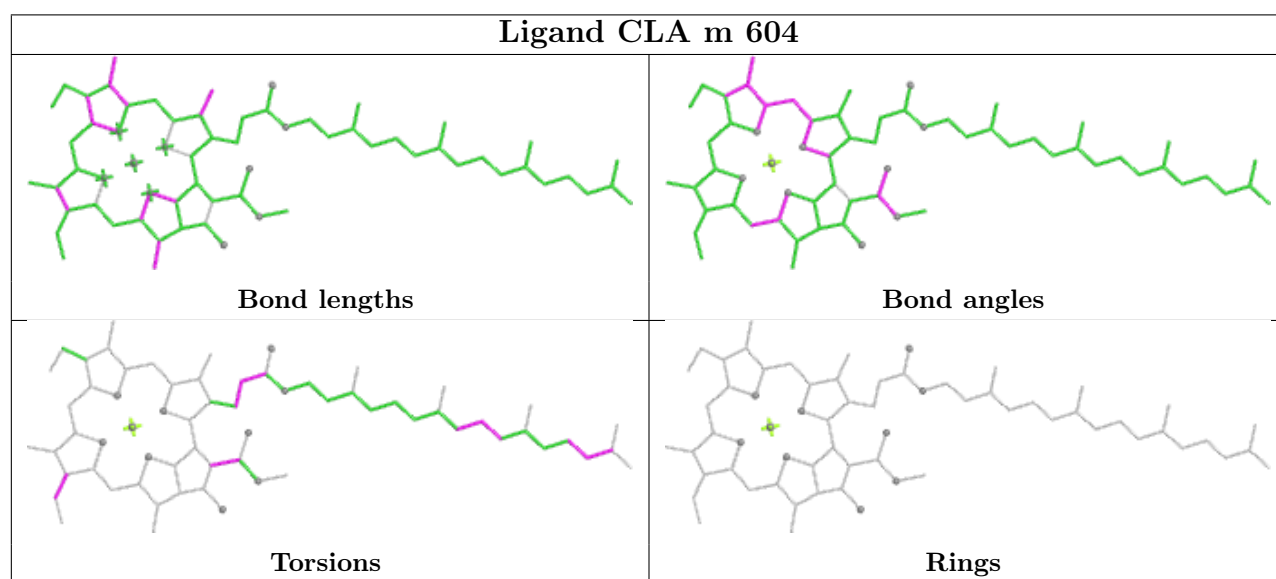
Ligand WVN R 202

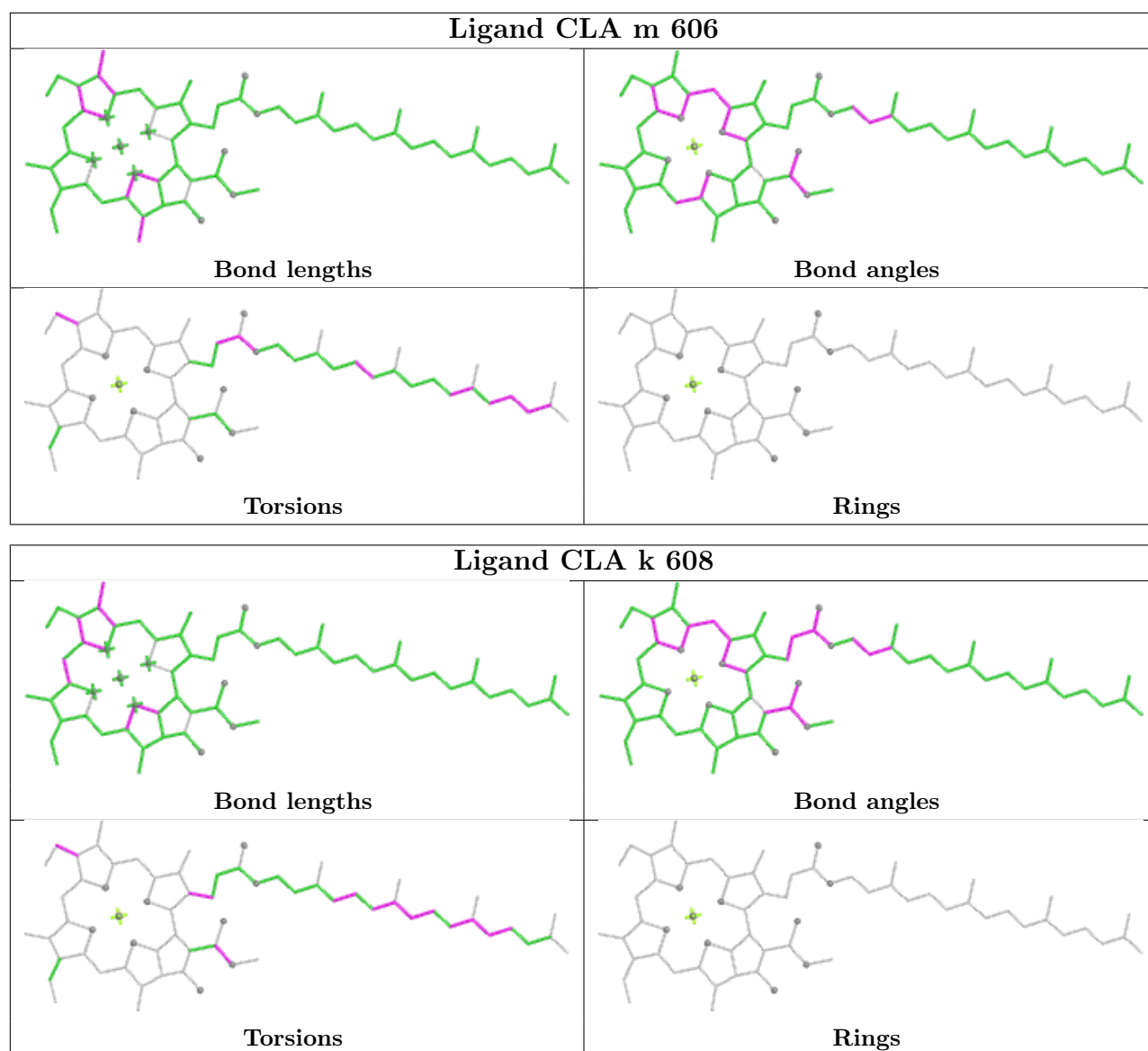


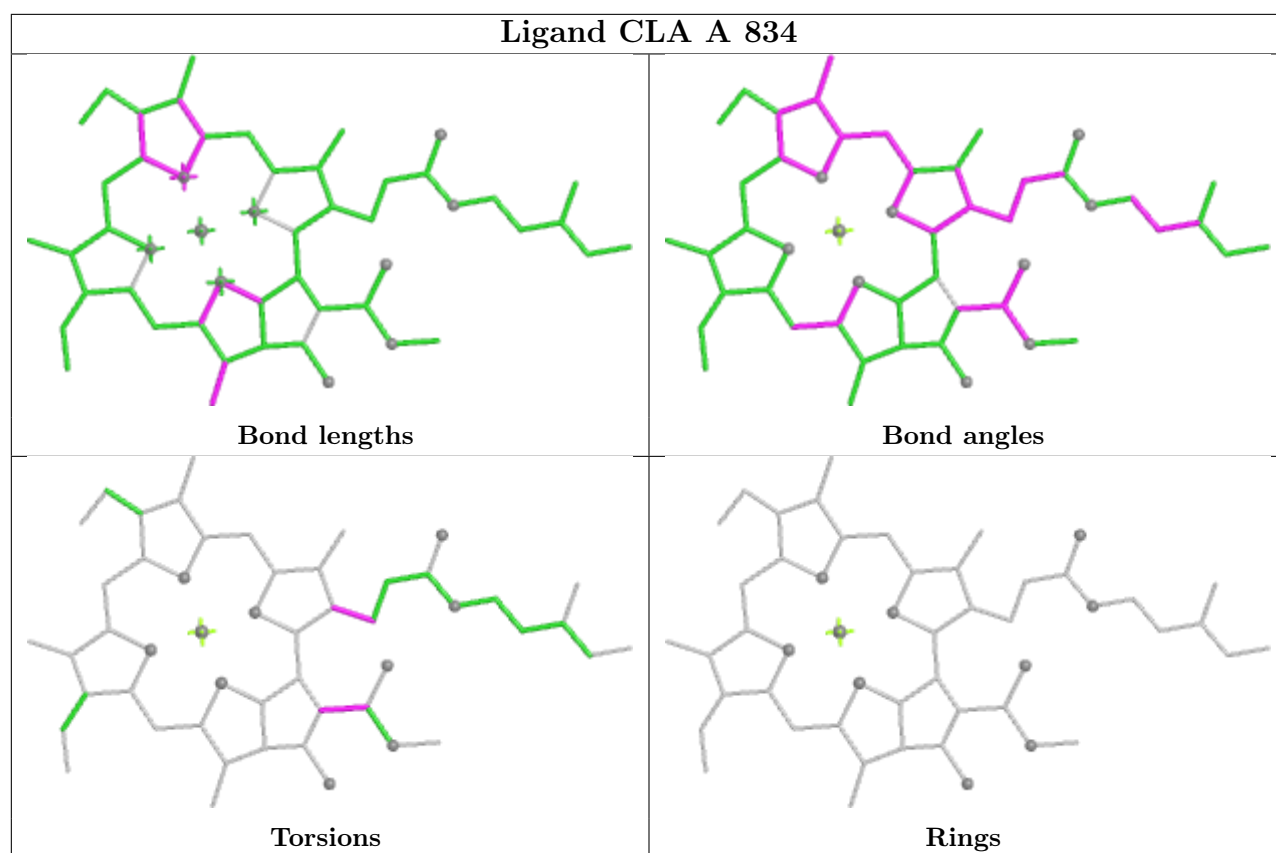
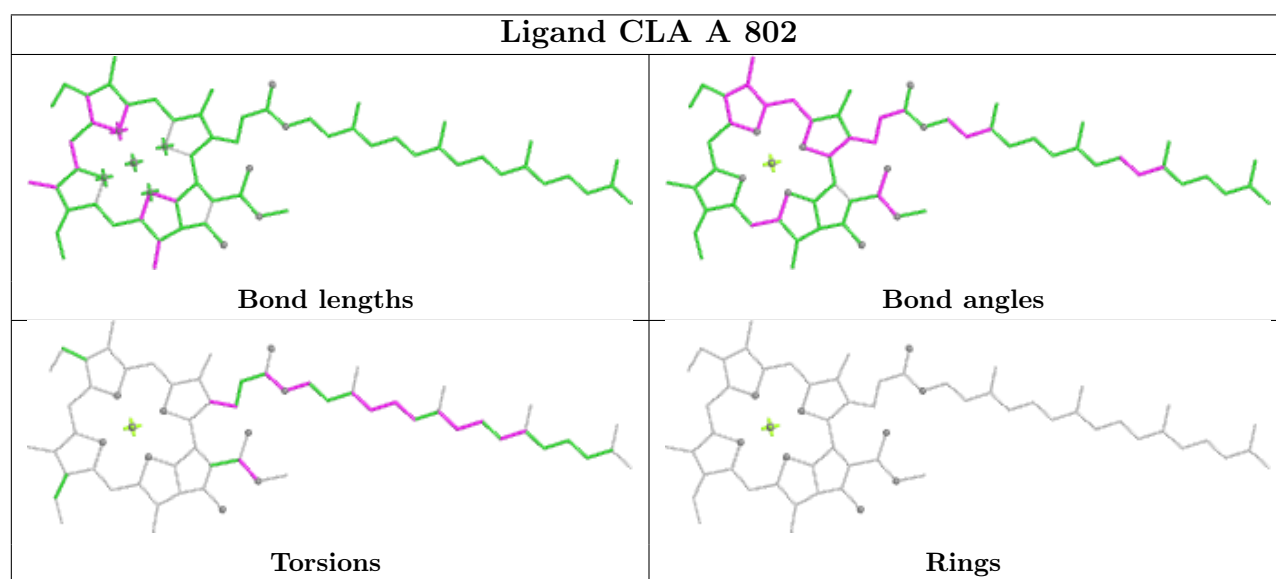


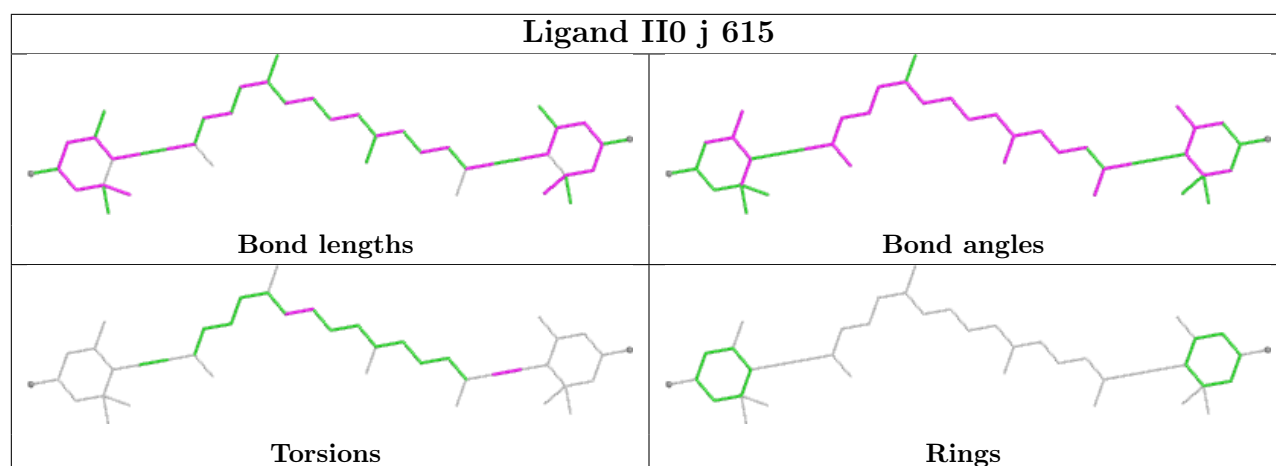
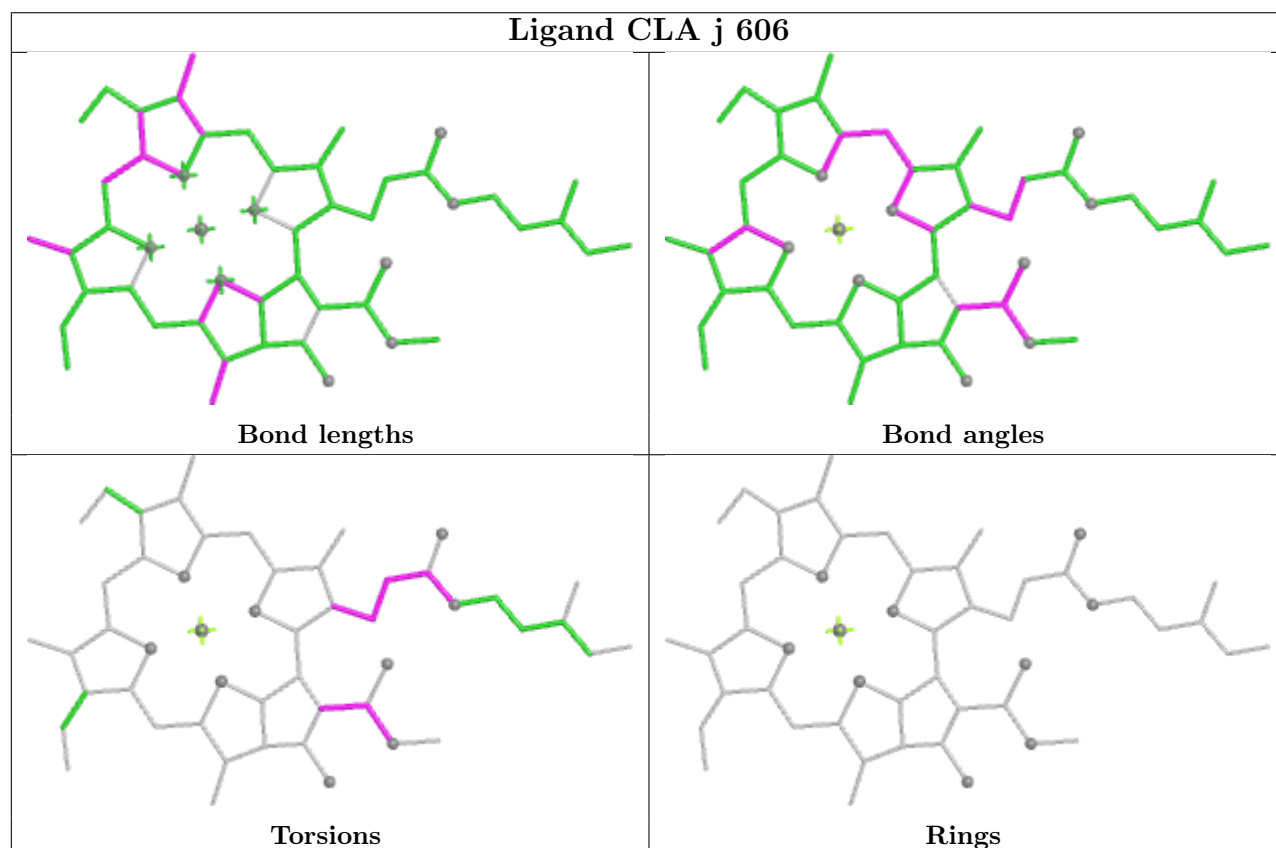


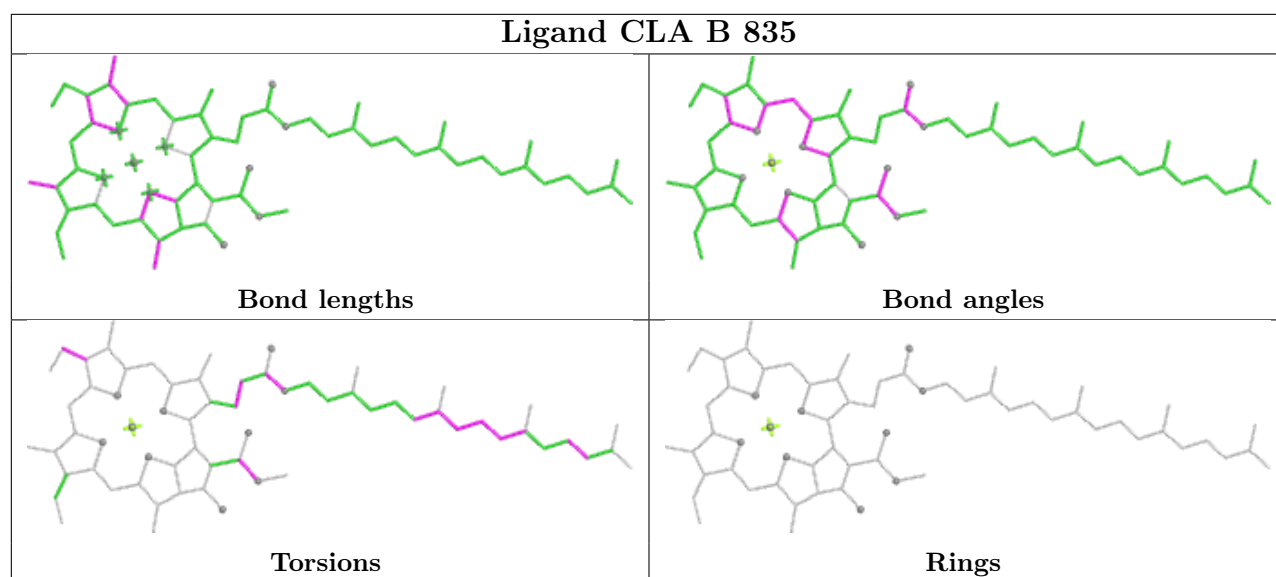
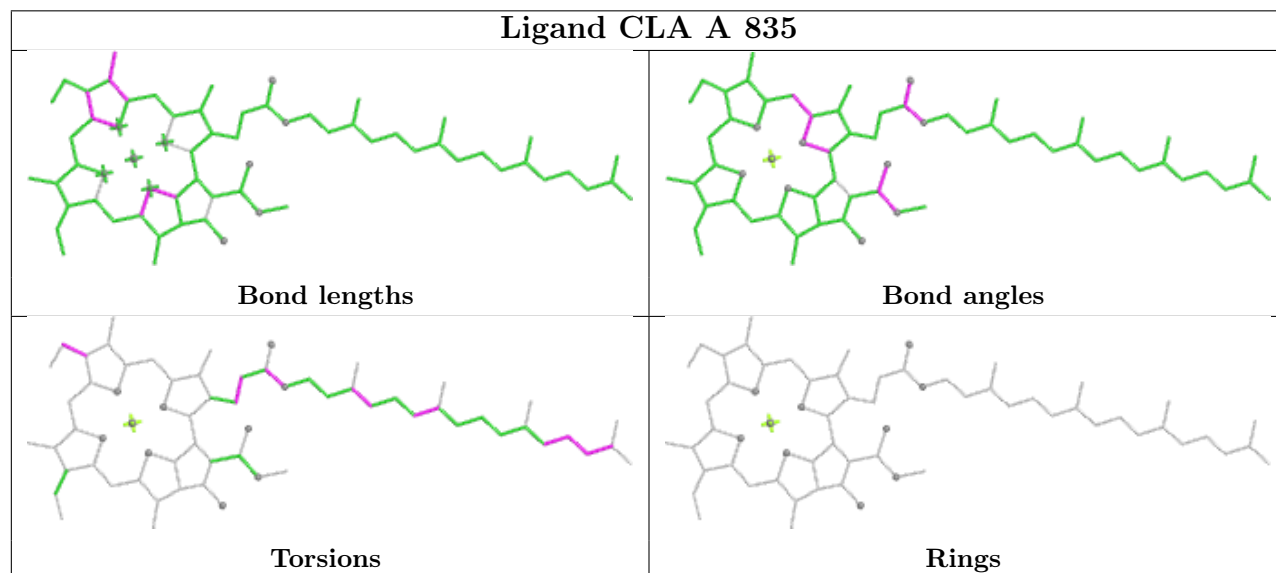
Ligand CLA A 831**Ligand CLA F 201**



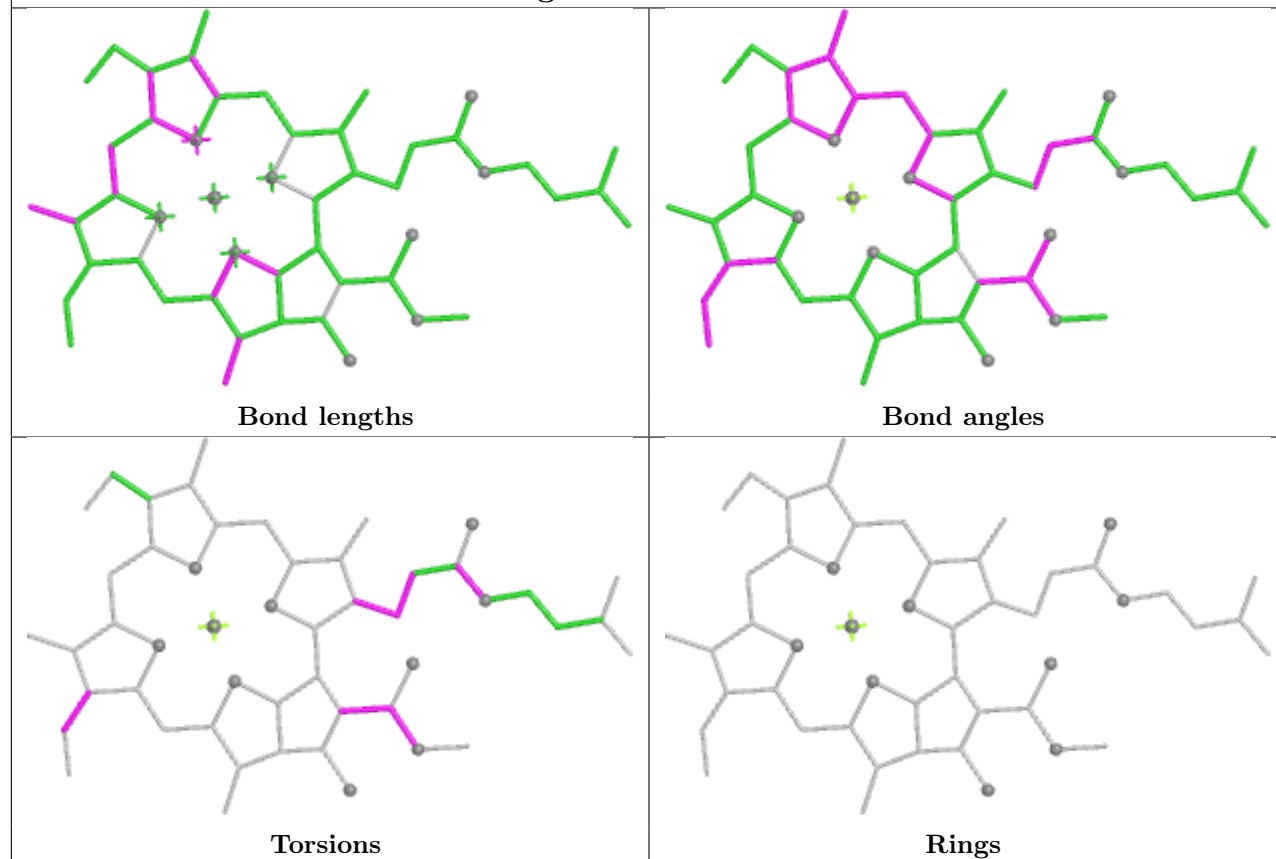




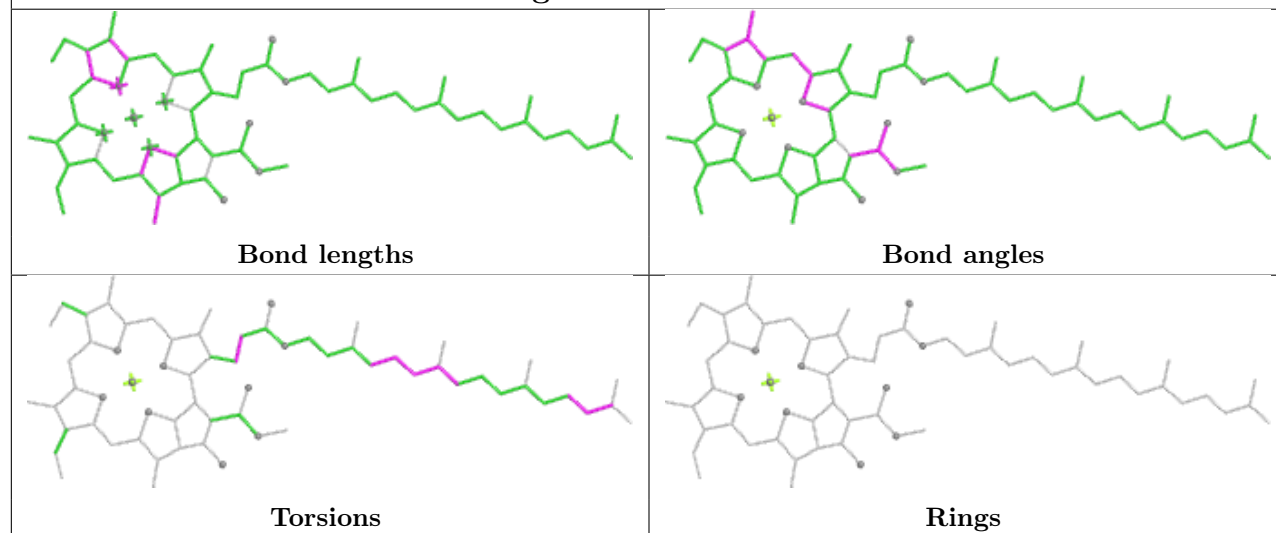




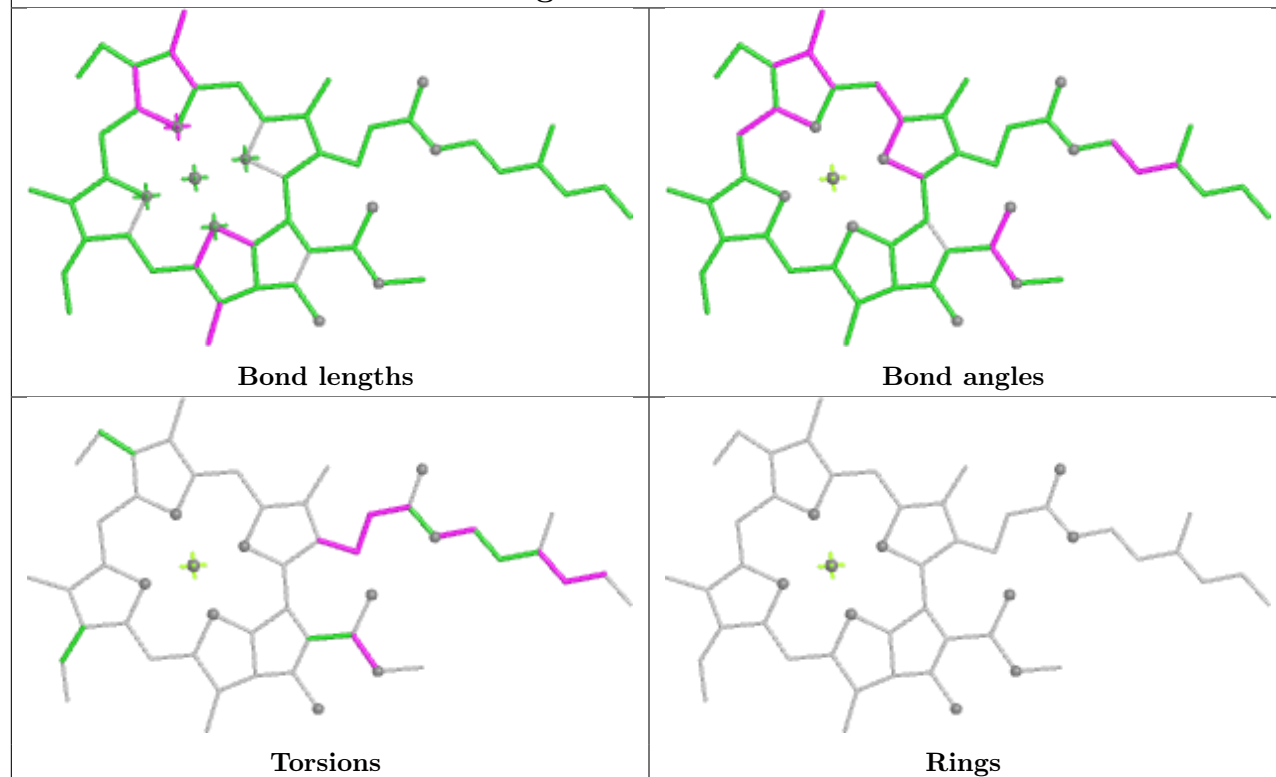
Ligand CLA c 602



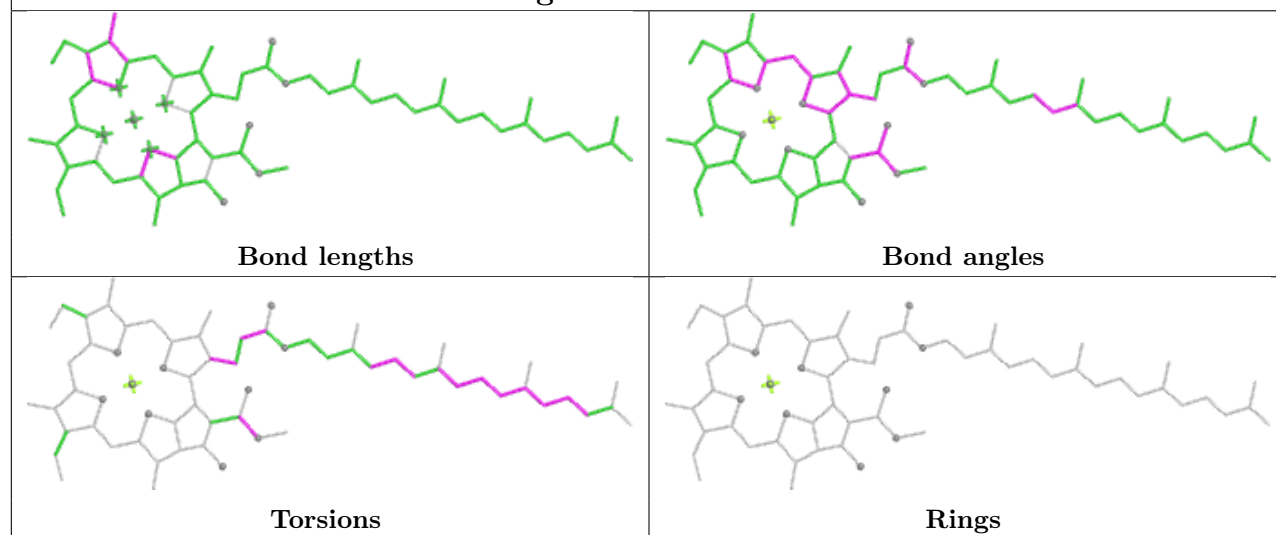
Ligand CLA B 806

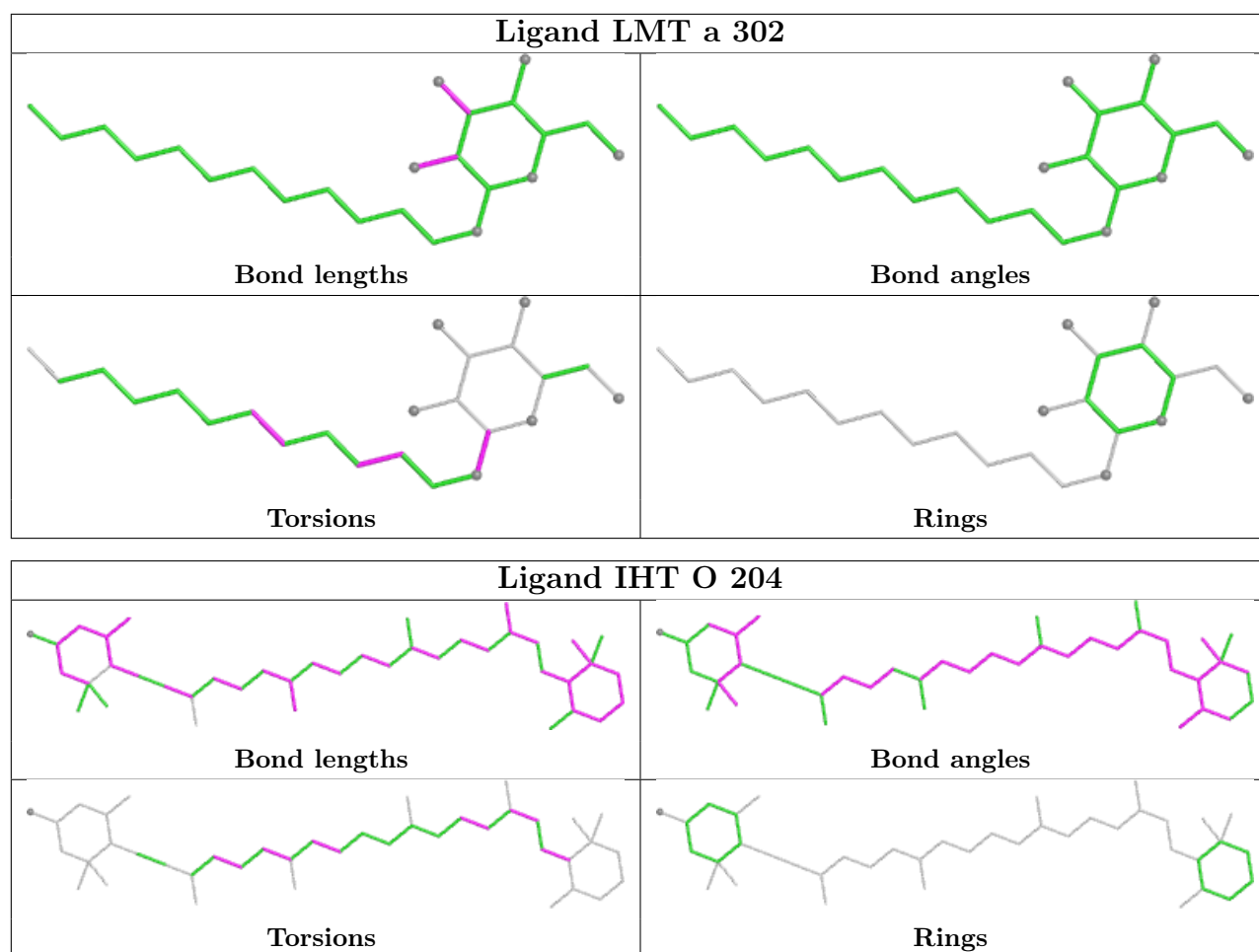


Ligand CLA a 303

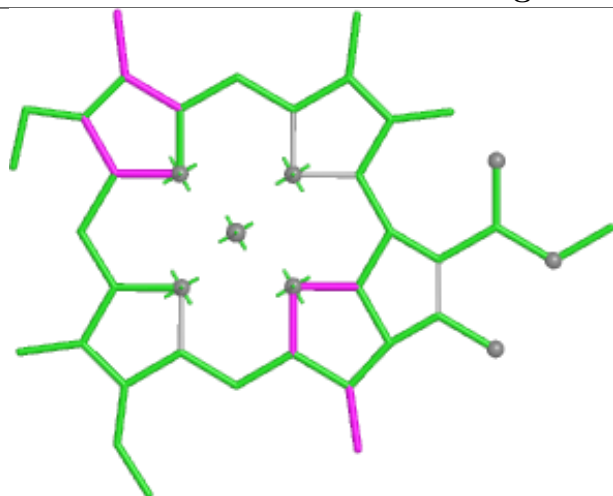


Ligand CLA a 308





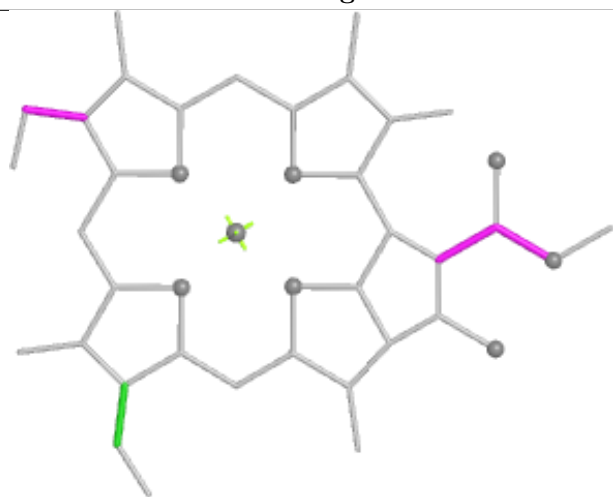
Ligand CLA A 855



Bond lengths



Bond angles

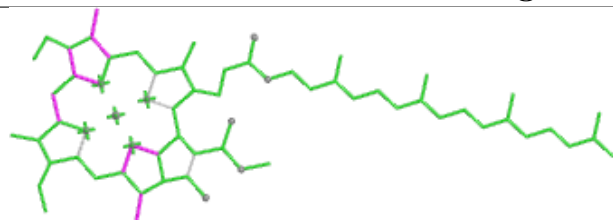


Torsions

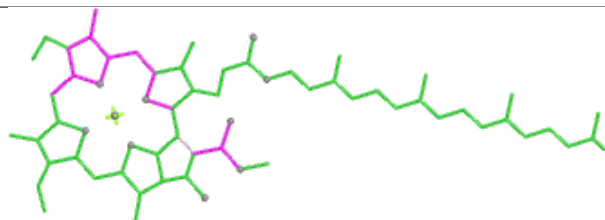


Rings

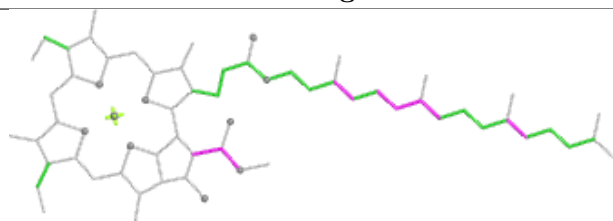
Ligand CLA h 313



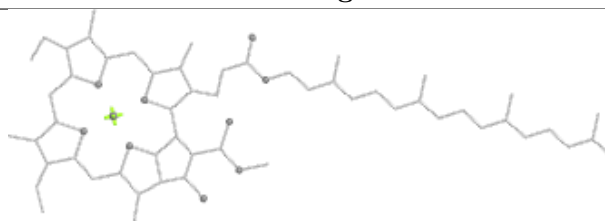
Bond lengths



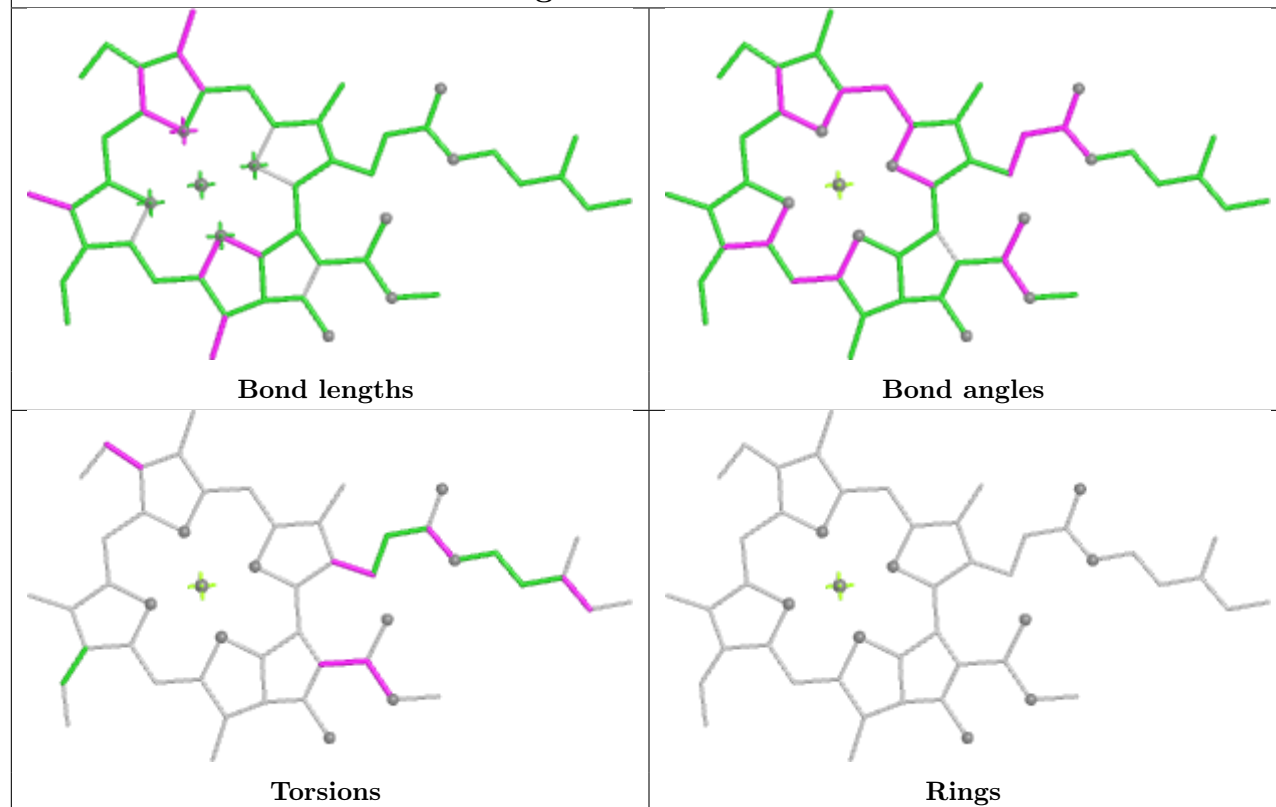
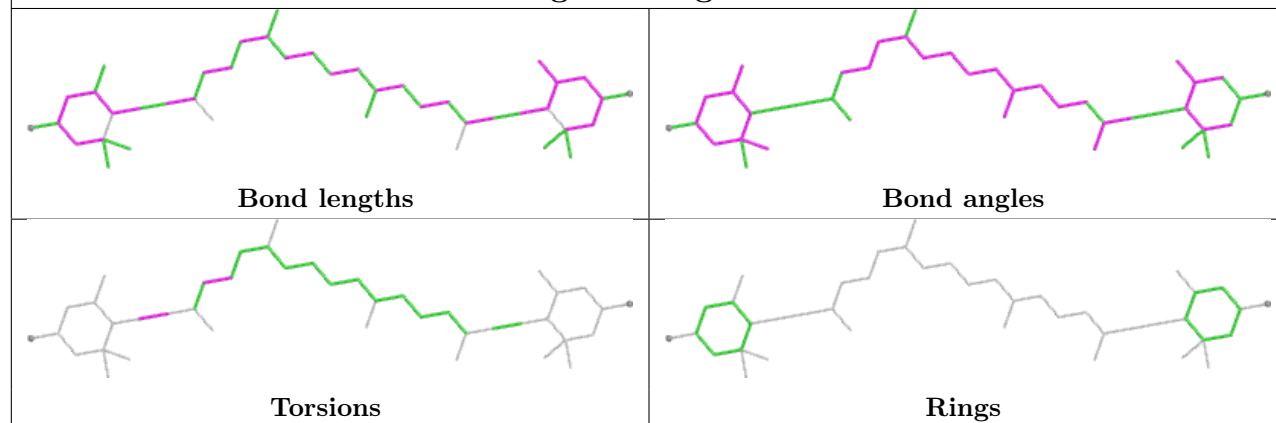
Bond angles

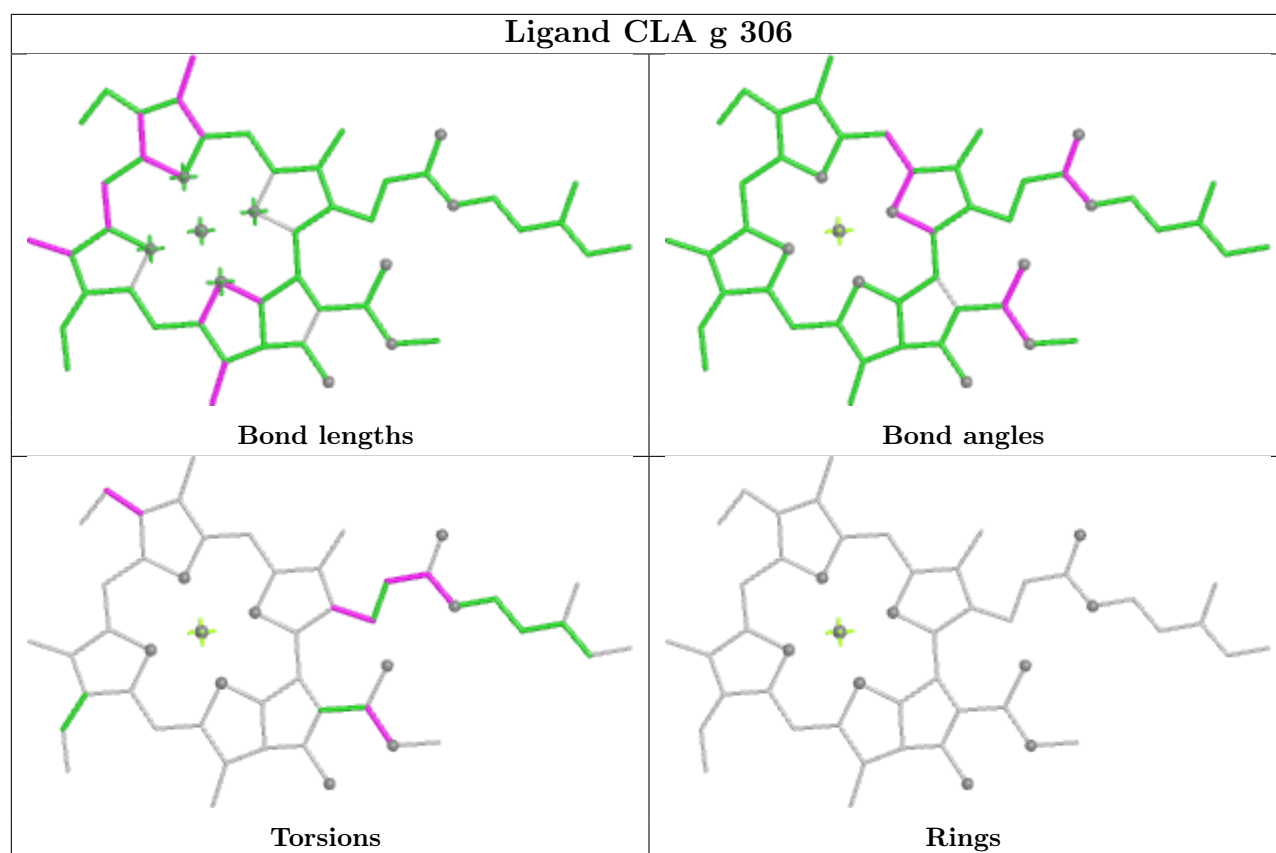


Torsions

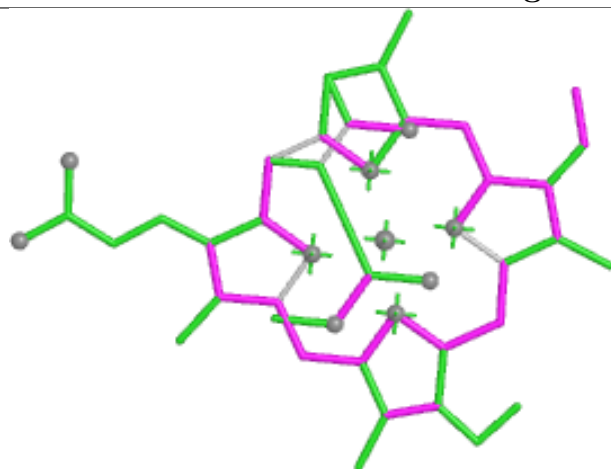


Rings

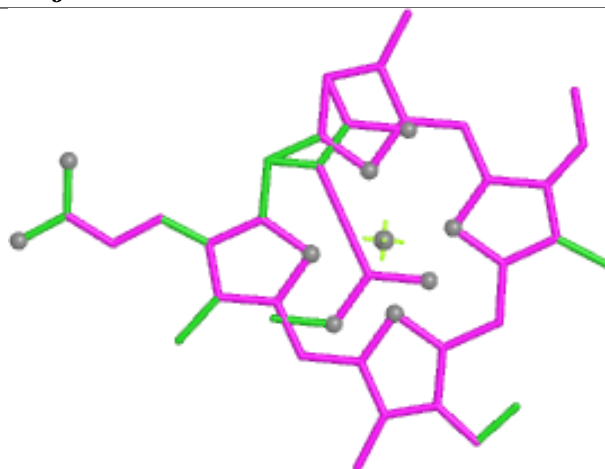
Ligand CLA n 603**Ligand II0 g 318**



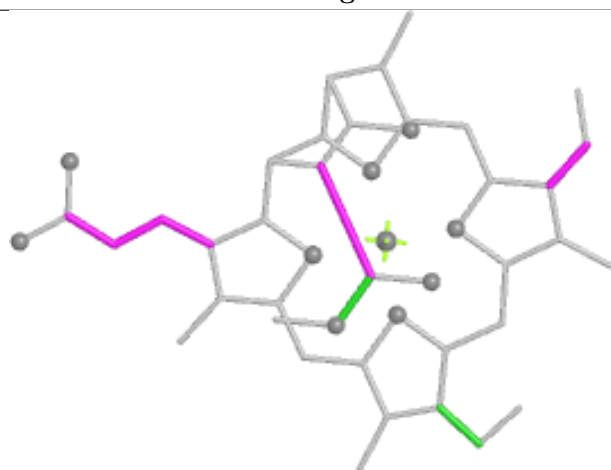
Ligand KC2 j 611



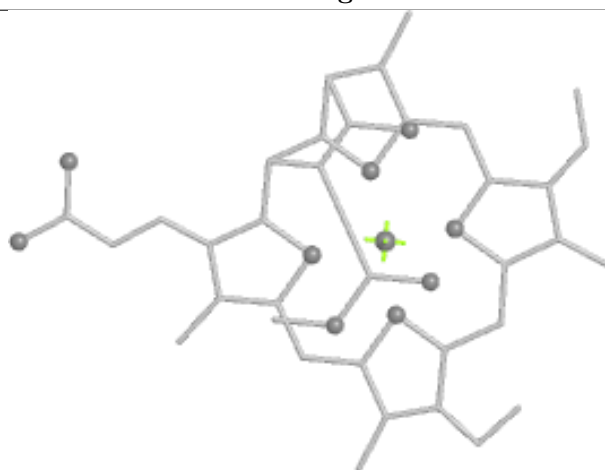
Bond lengths



Bond angles

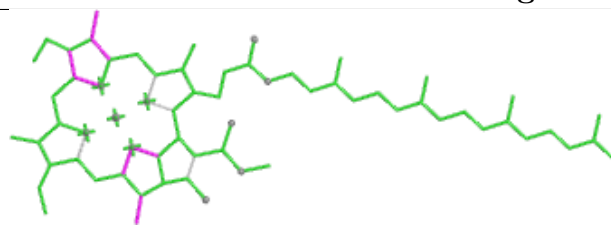


Torsions

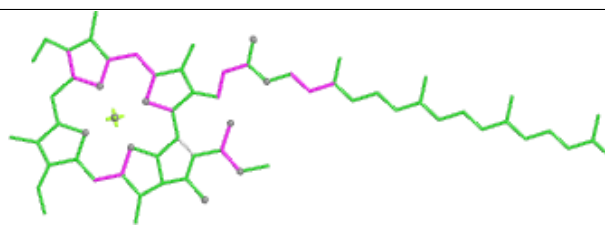


Rings

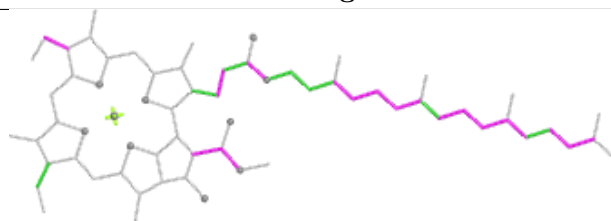
Ligand CLA b 611



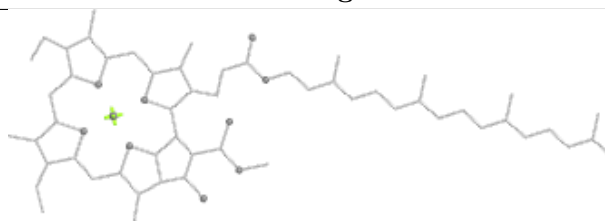
Bond lengths



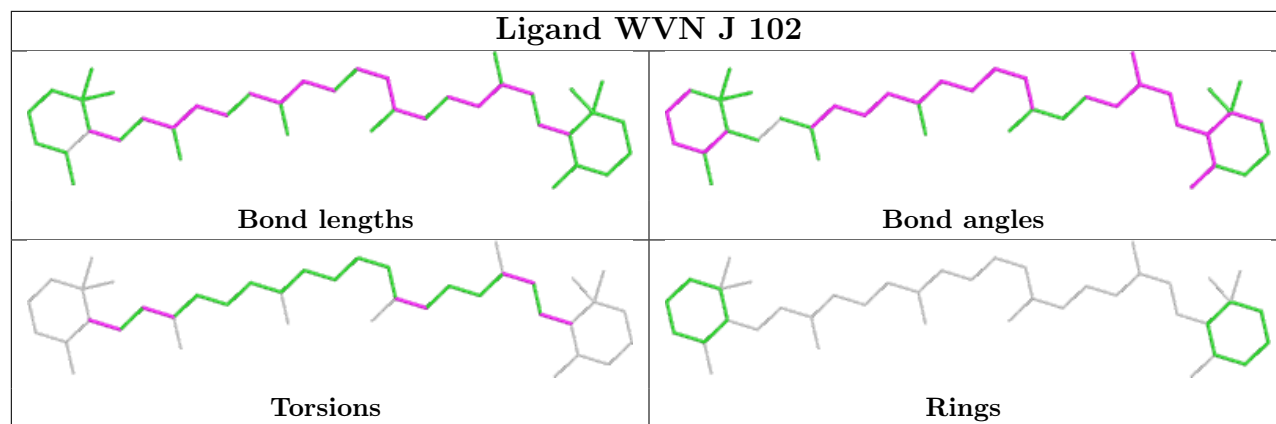
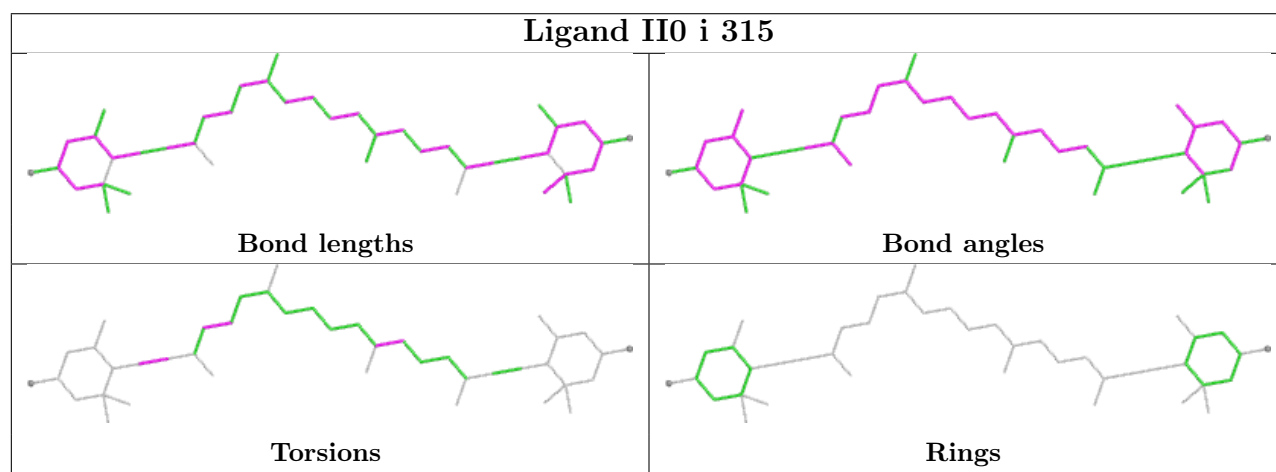
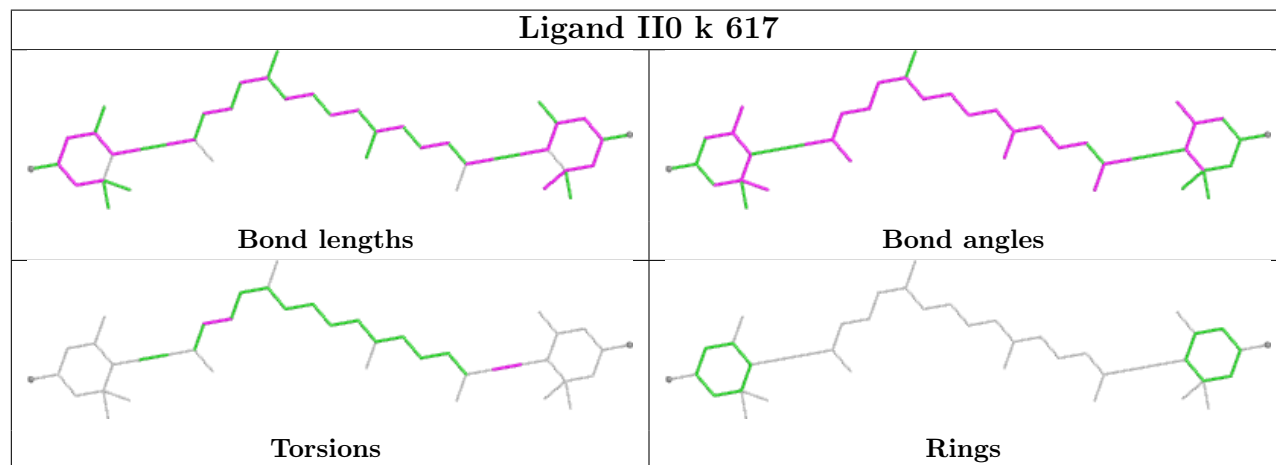
Bond angles

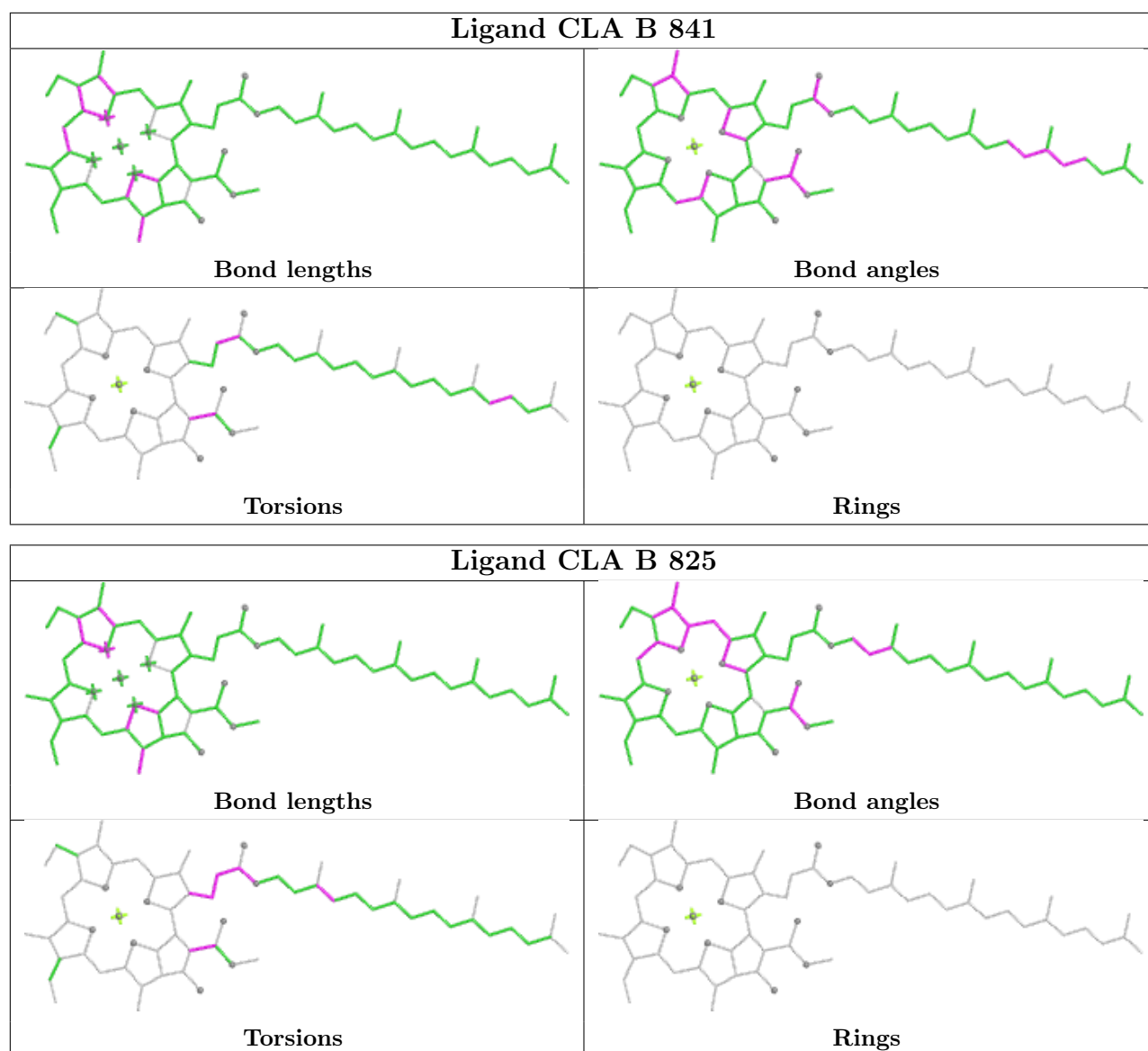


Torsions

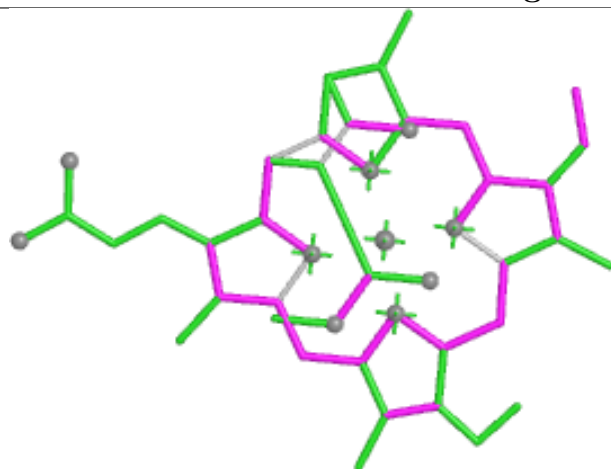


Rings

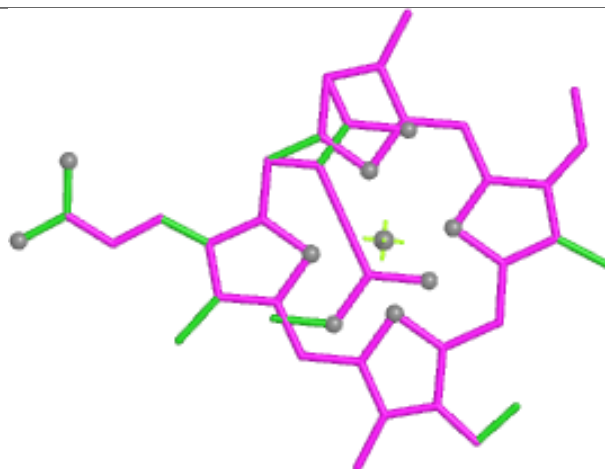




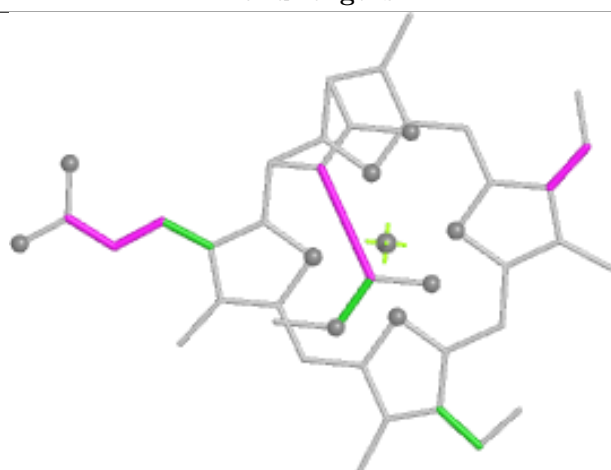
Ligand KC2 f 611



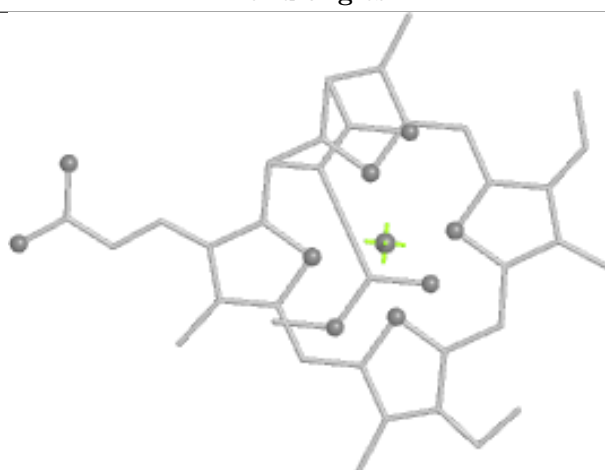
Bond lengths



Bond angles

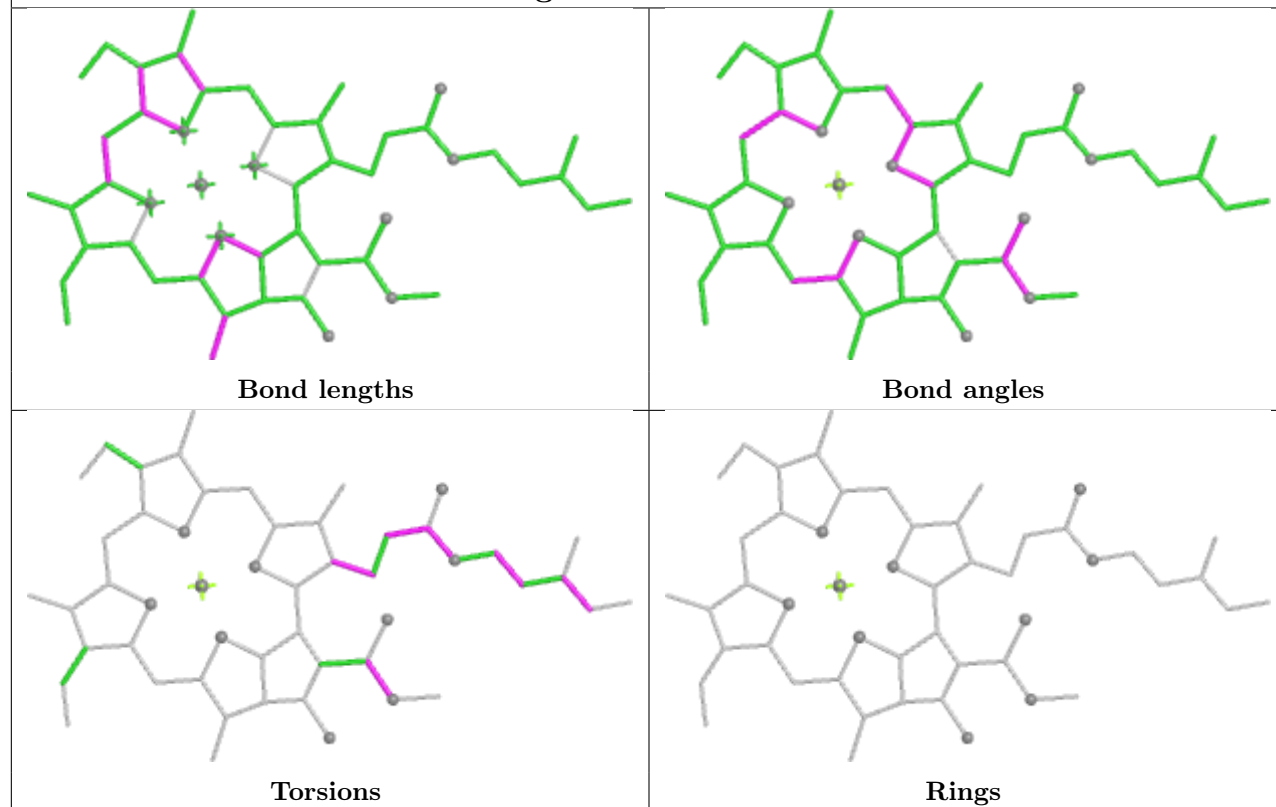


Torsions

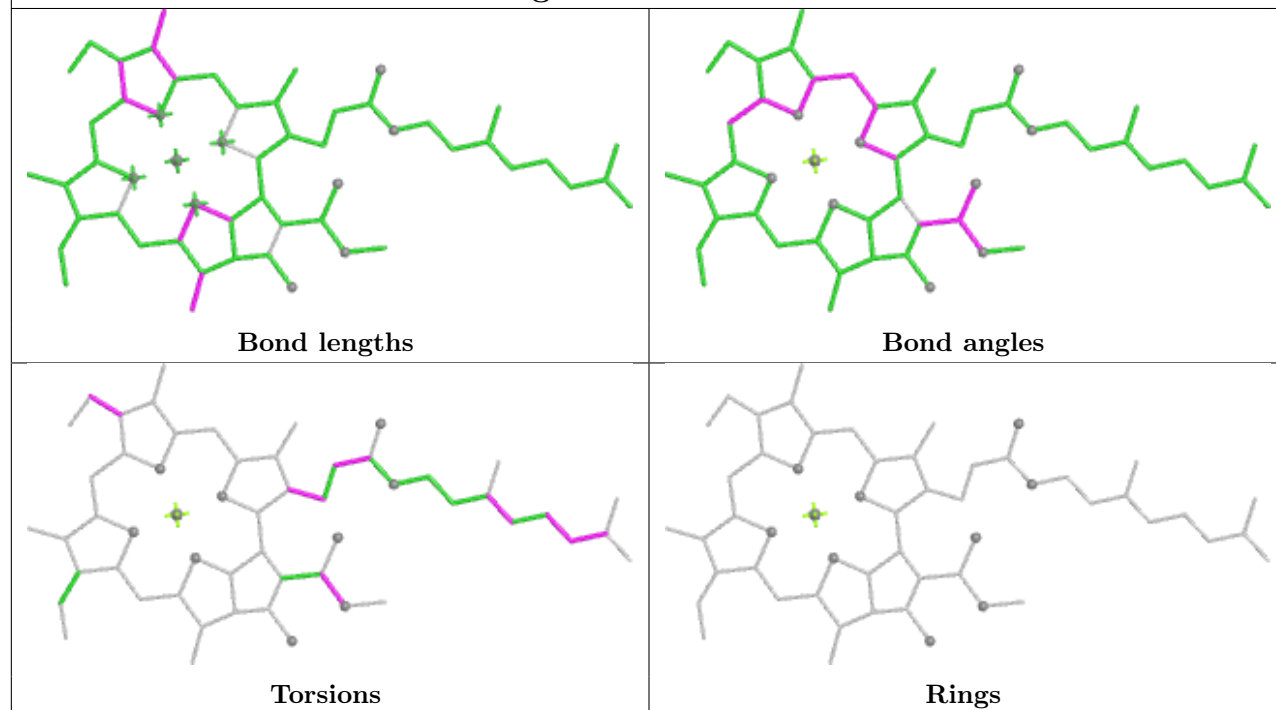


Rings

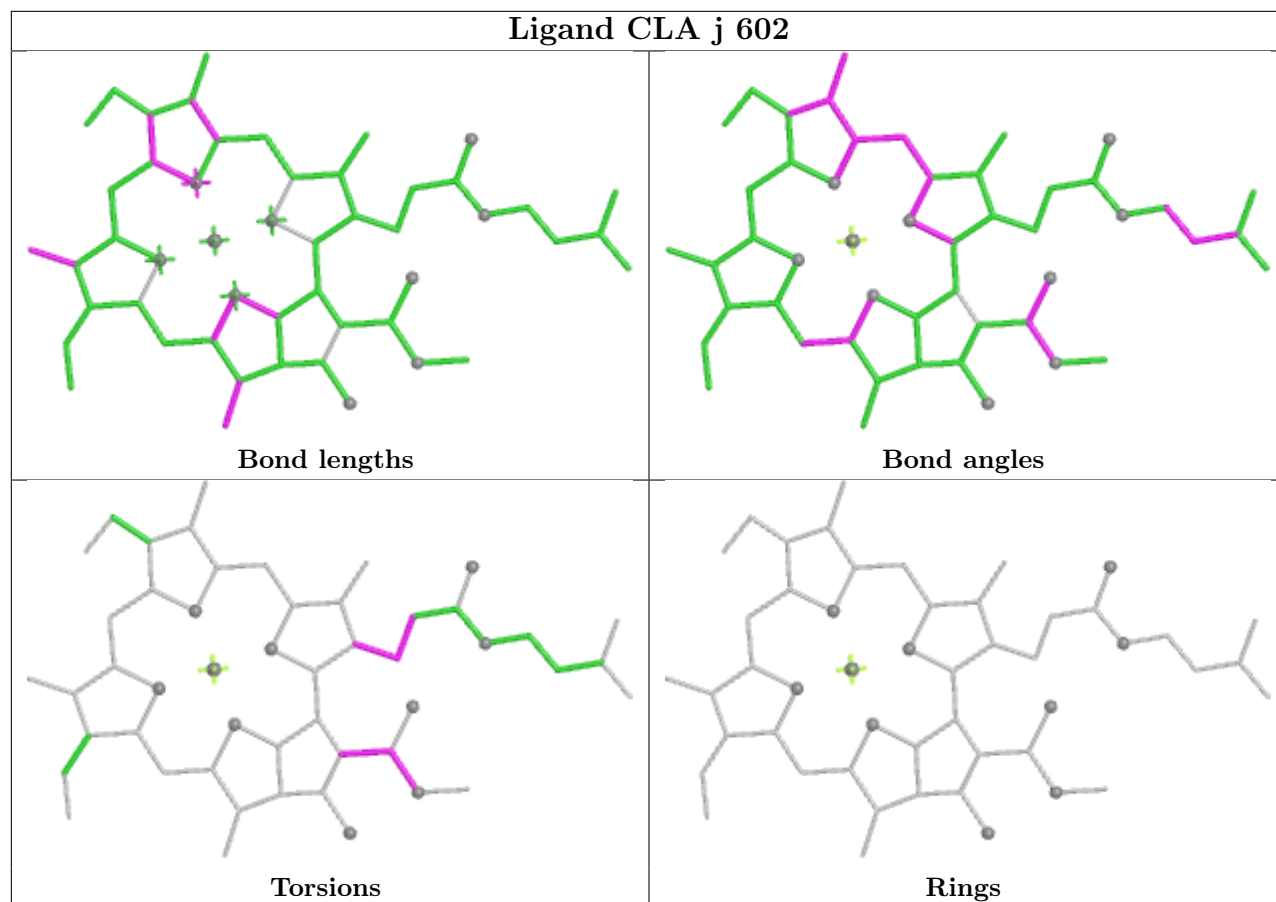
Ligand CLA n 613



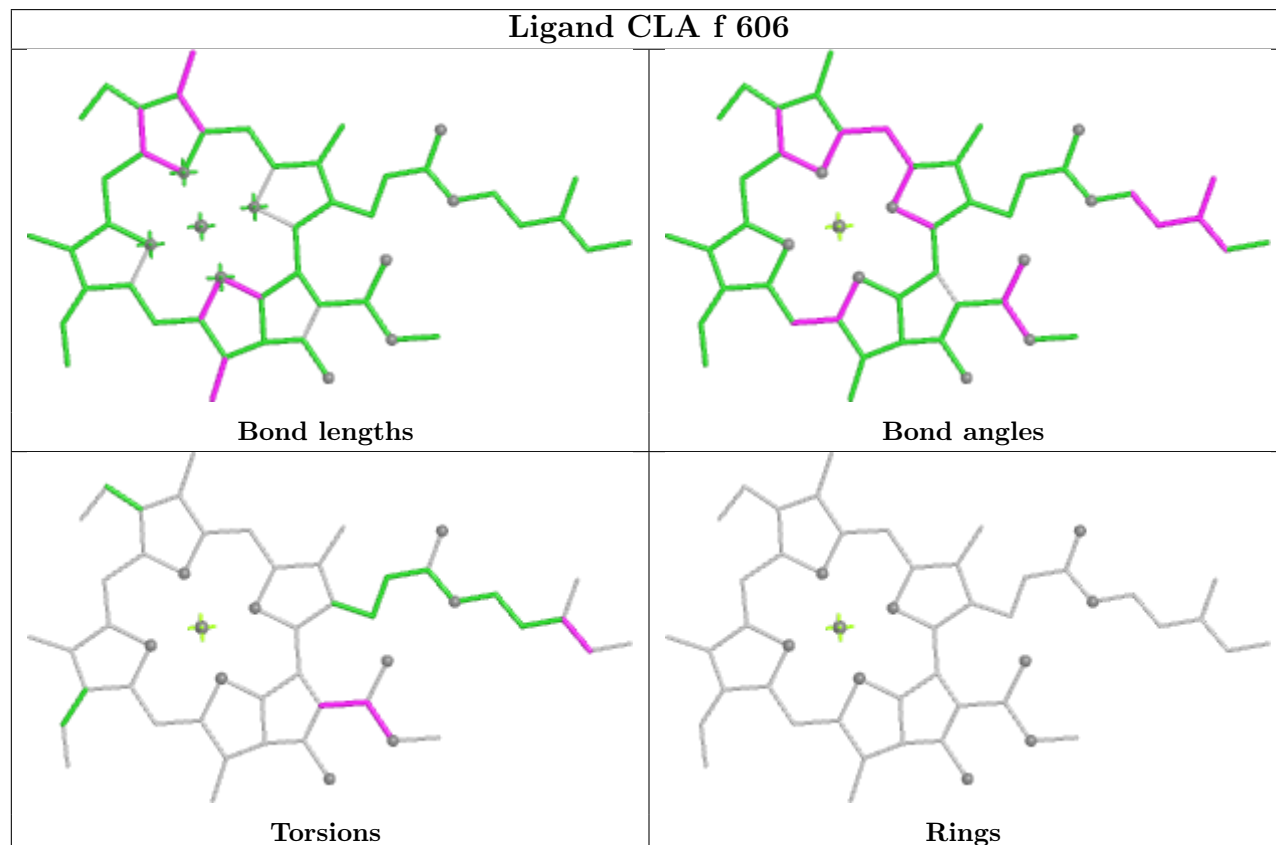
Ligand CLA B 819



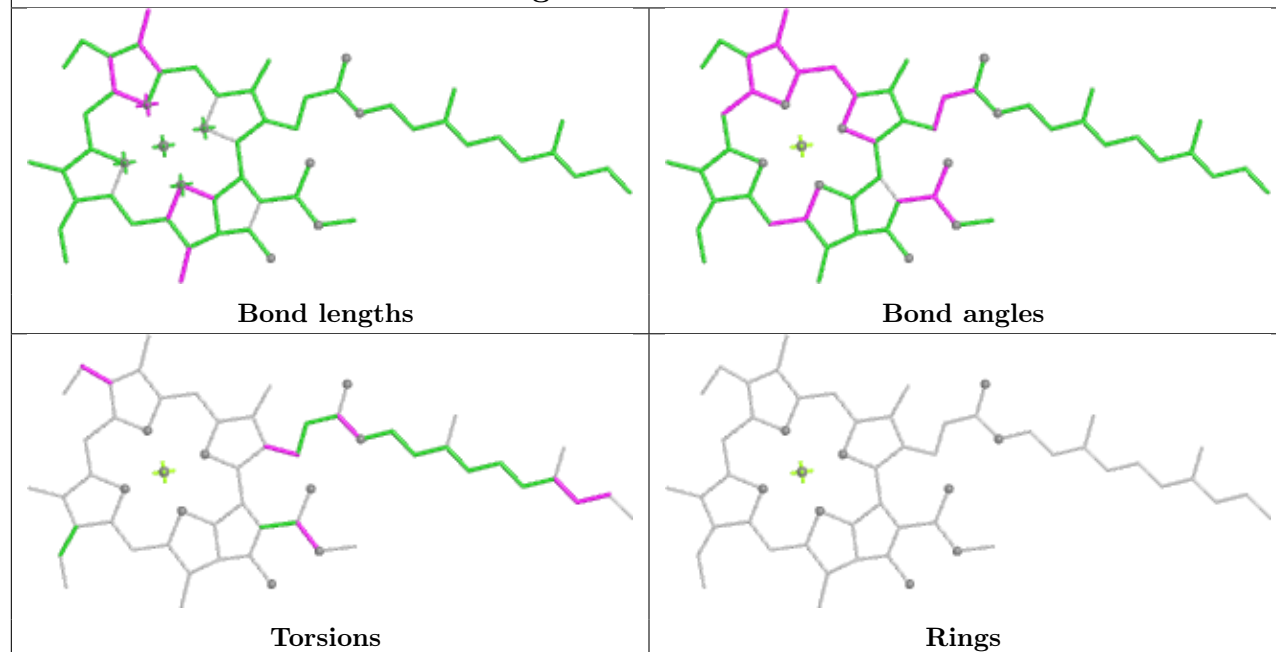
Ligand CLA j 602



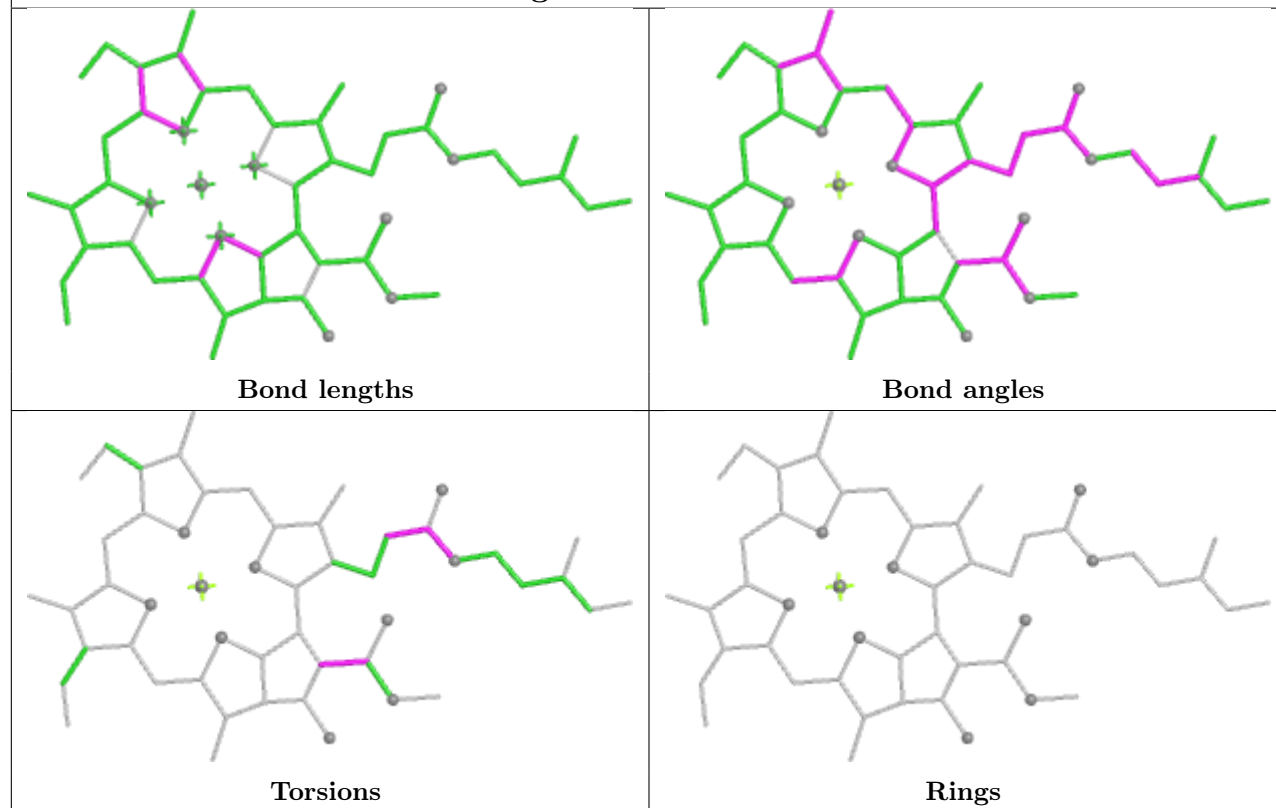
Ligand CLA f 606

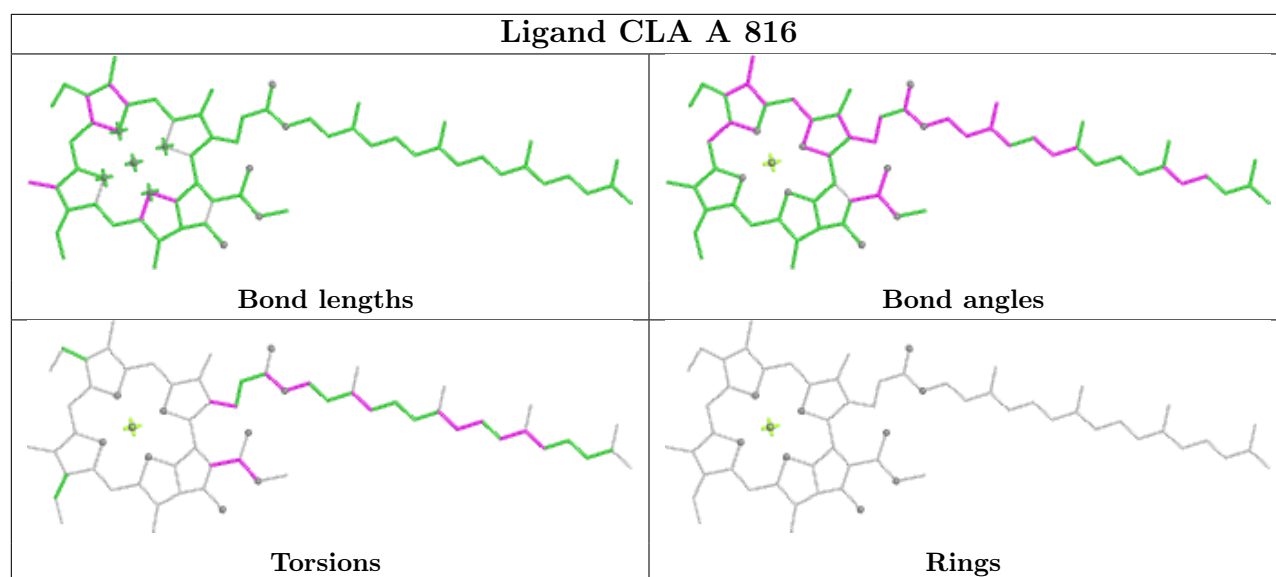
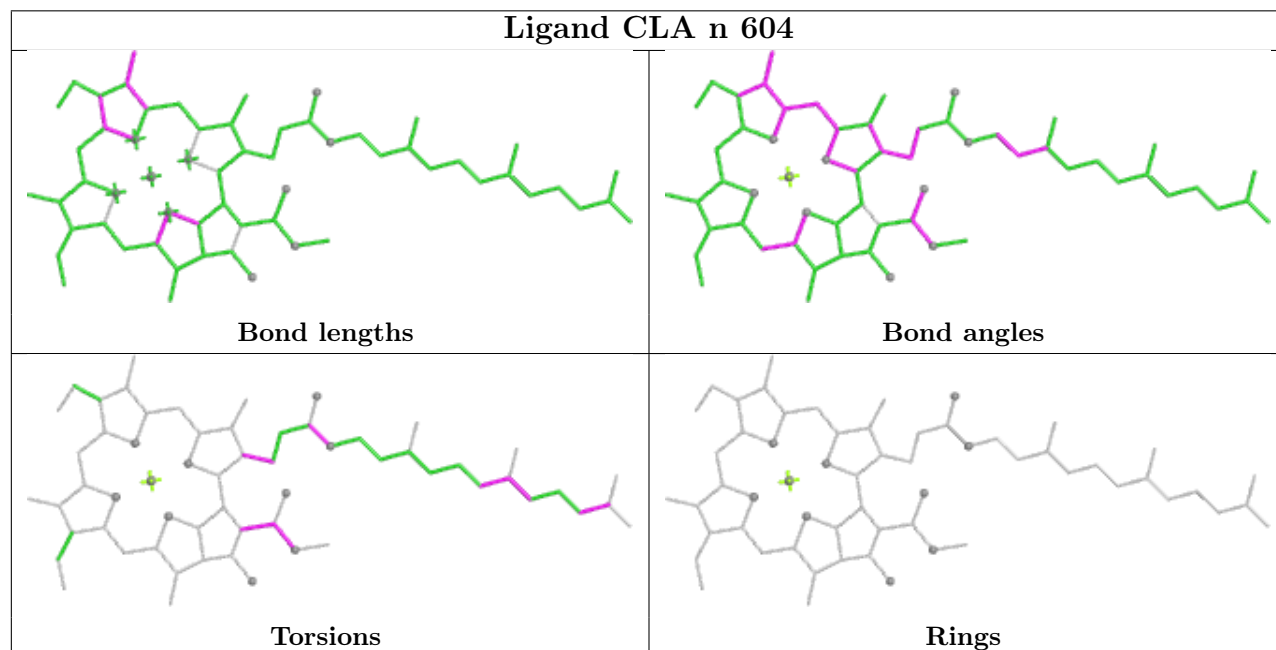


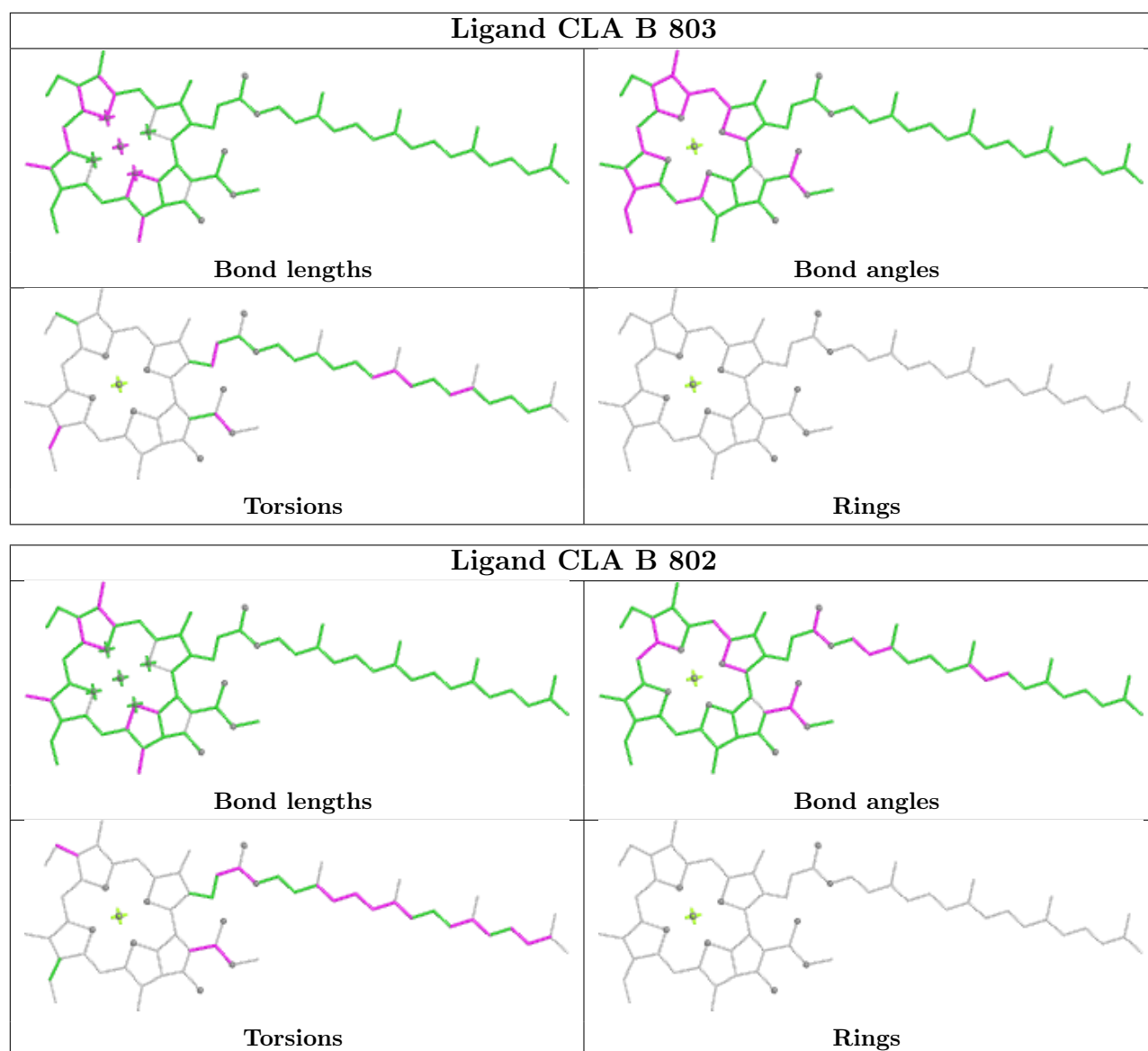
Ligand CLA B 816



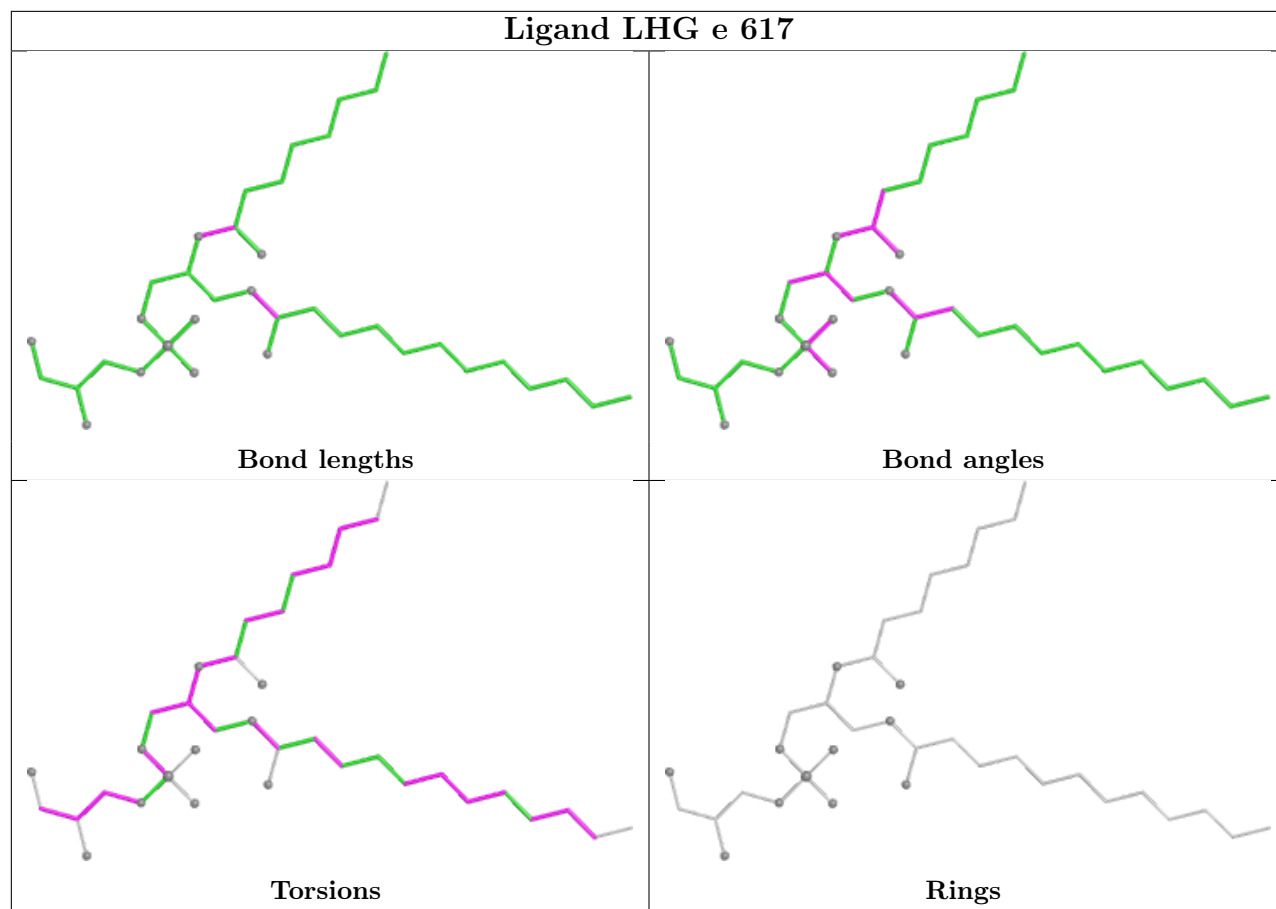
Ligand CLA K 101



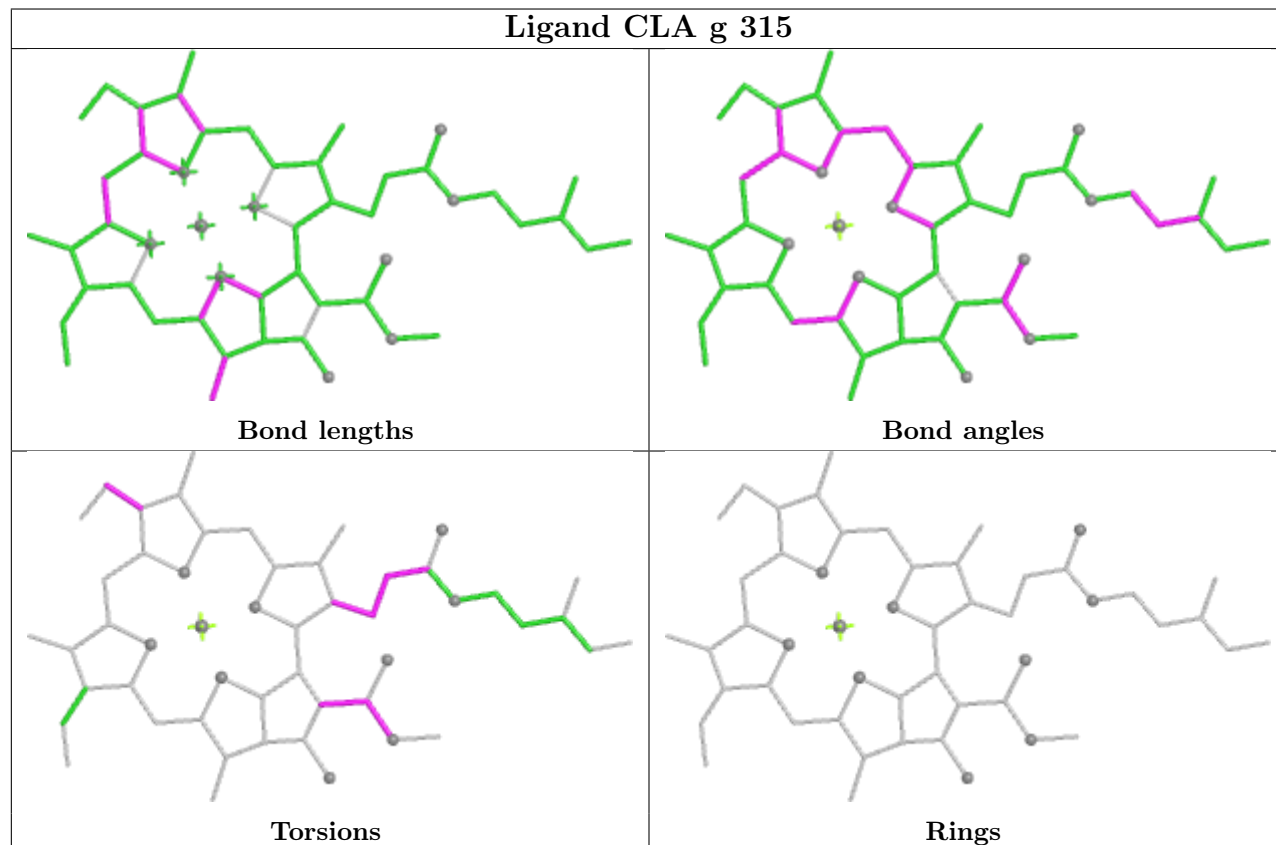


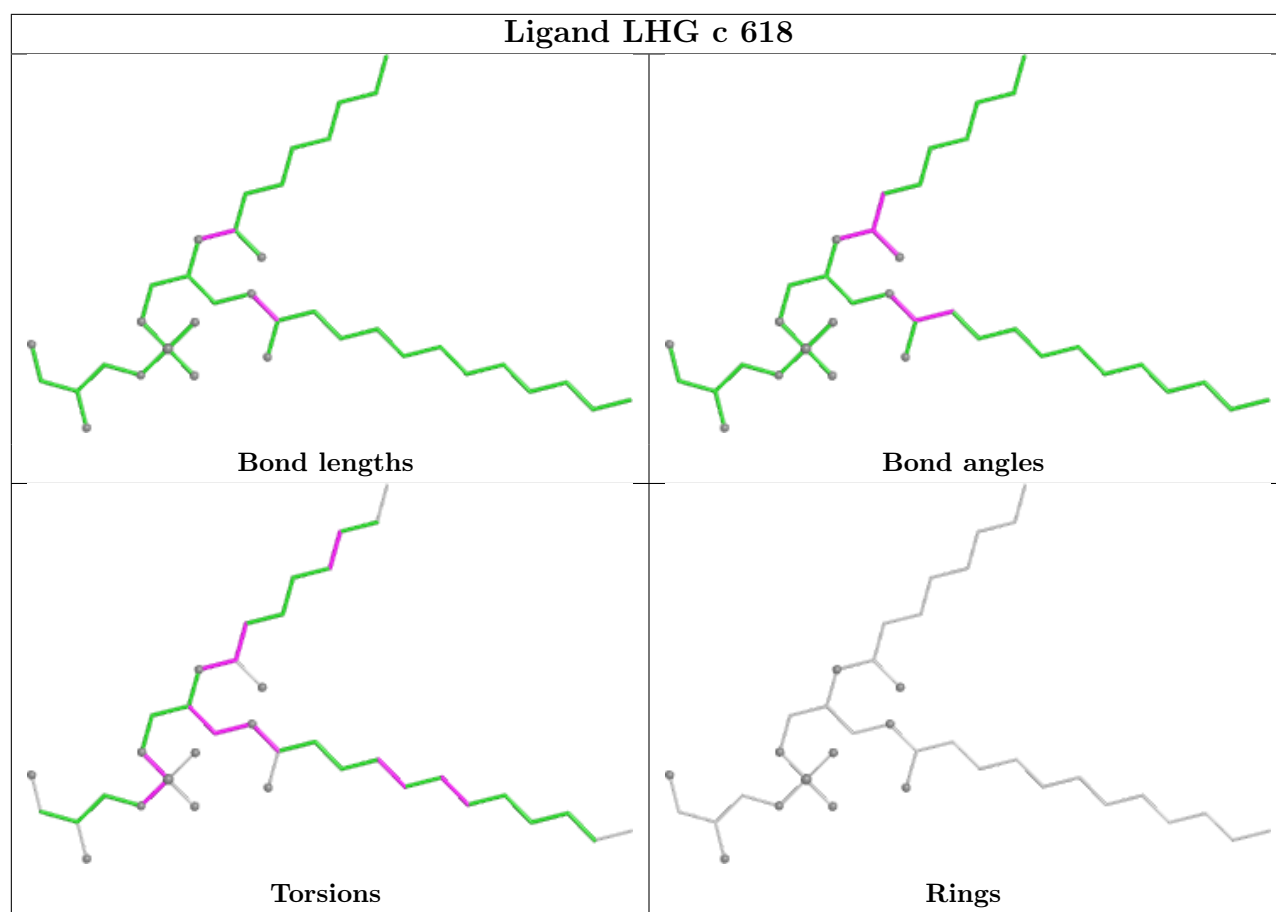


Ligand LHG e 617

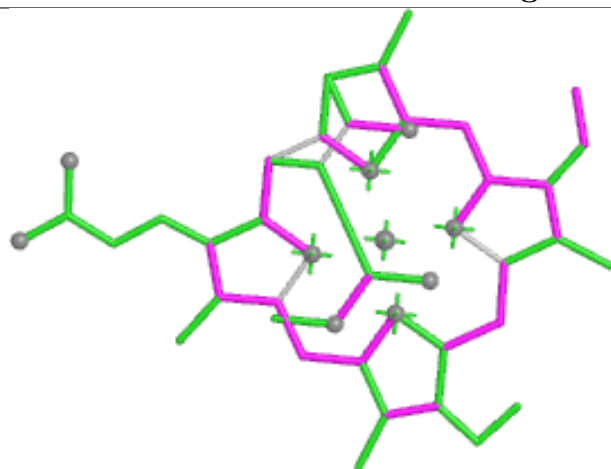


Ligand CLA g 315

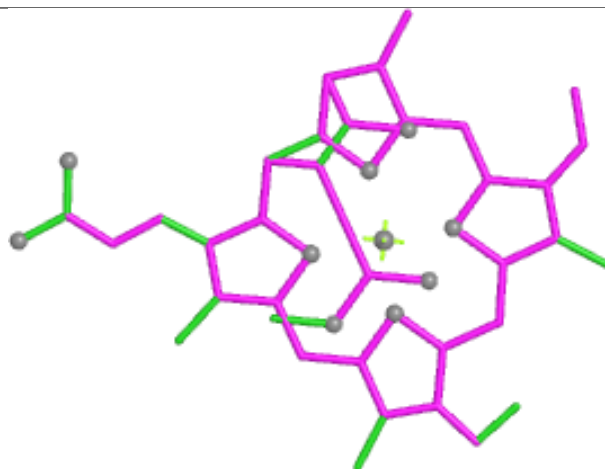




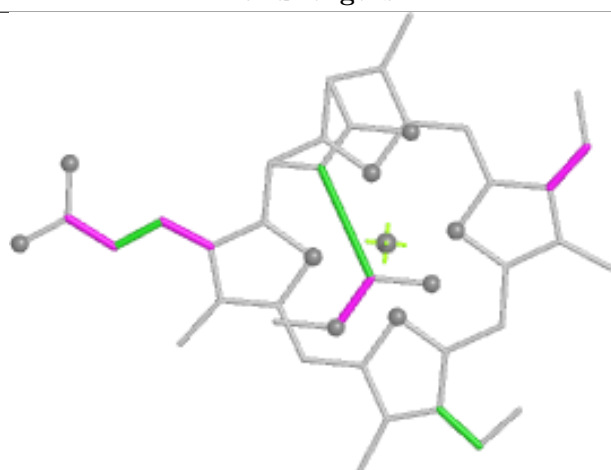
Ligand KC2 e 609



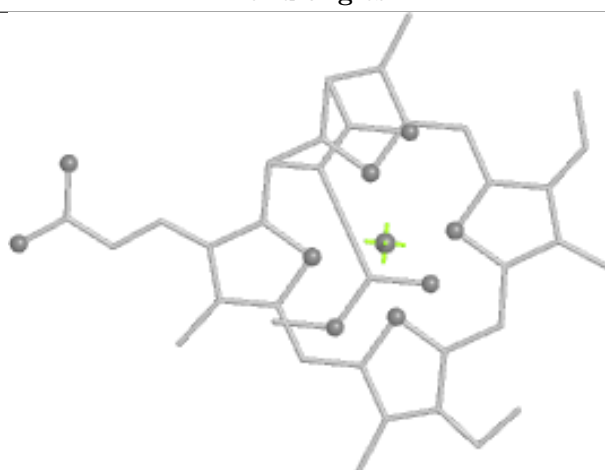
Bond lengths



Bond angles

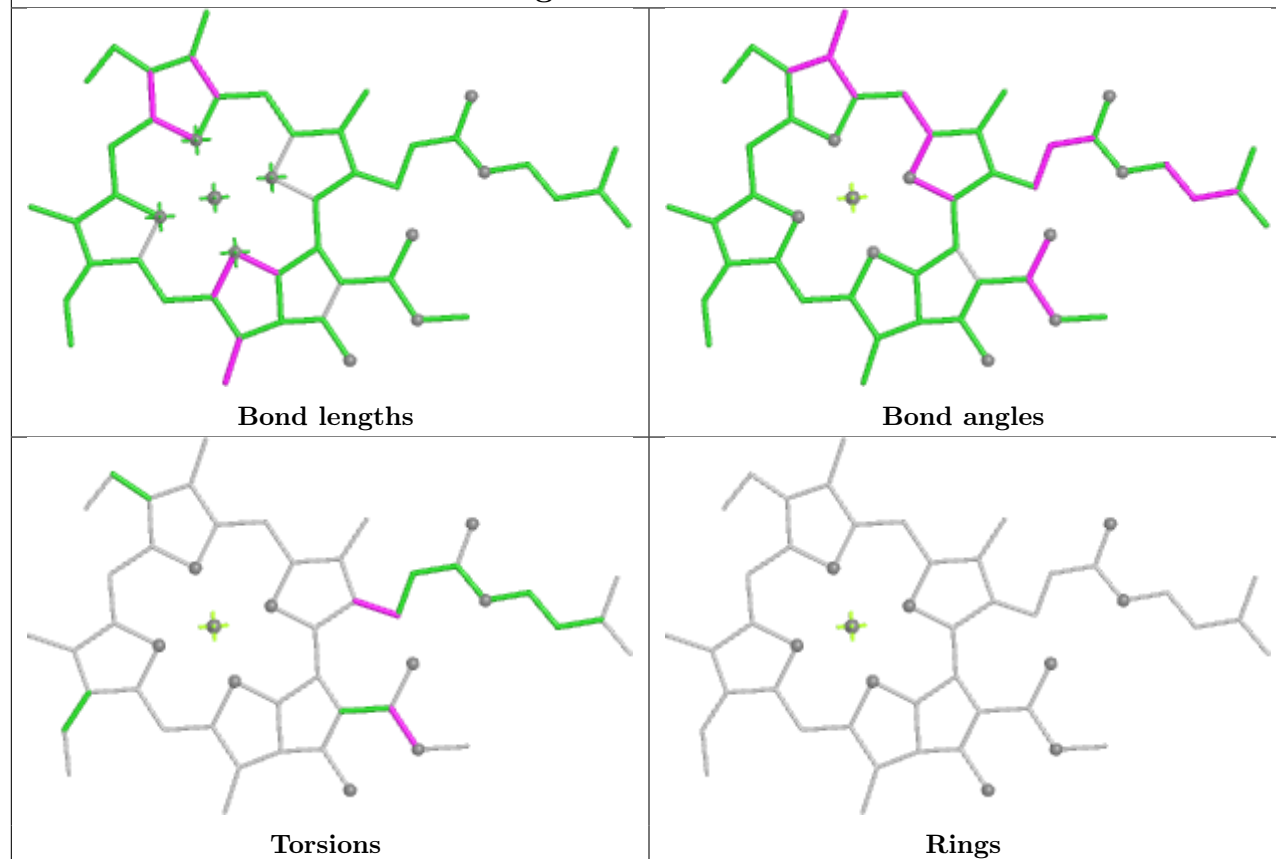


Torsions

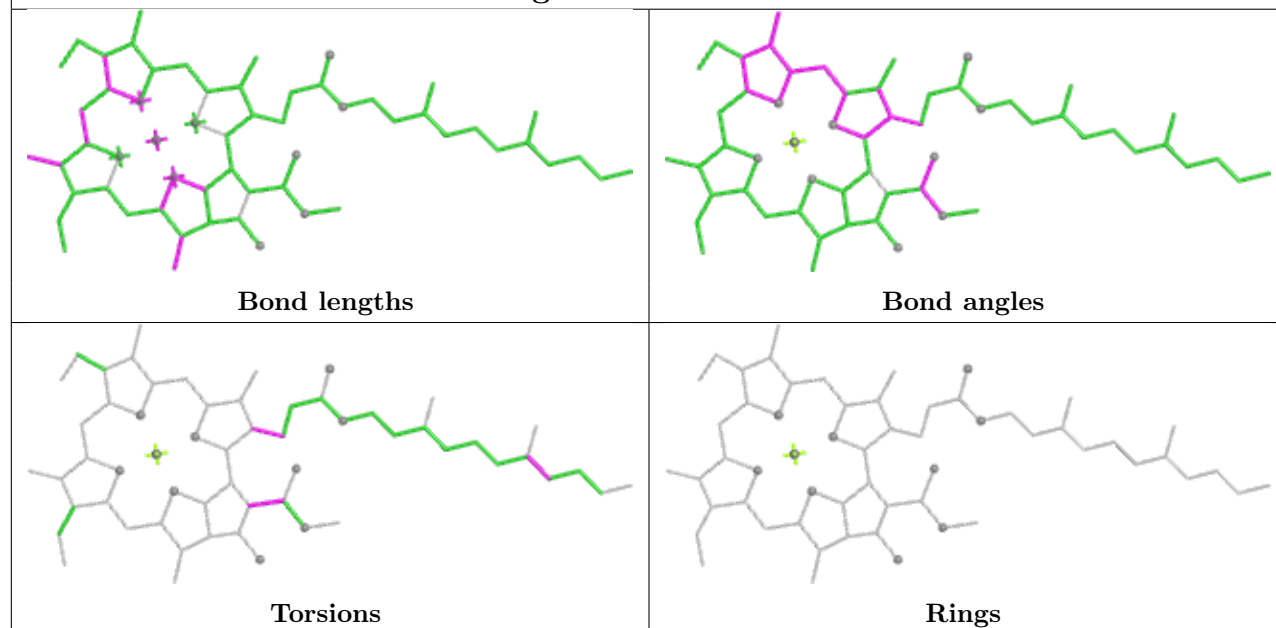


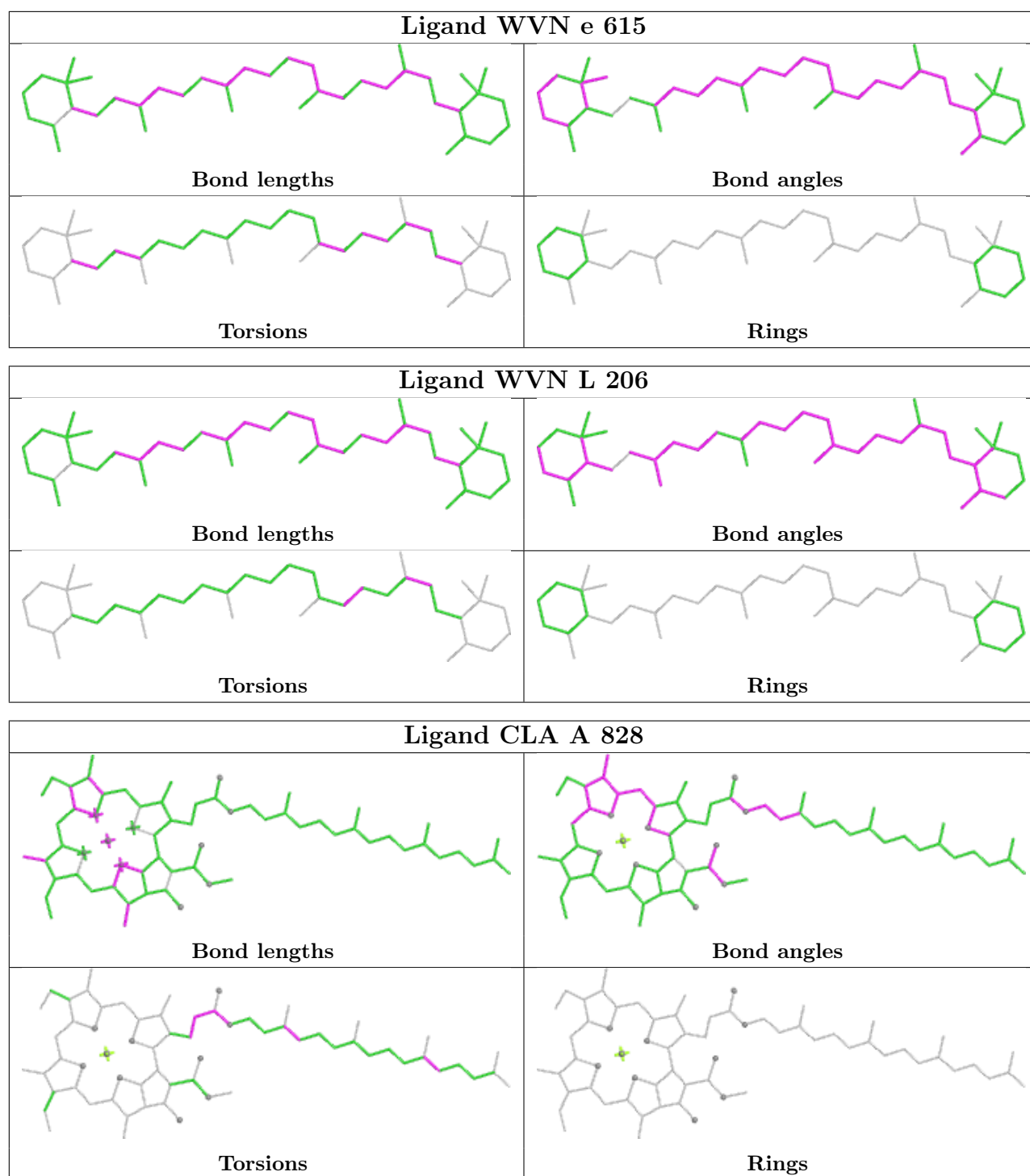
Rings

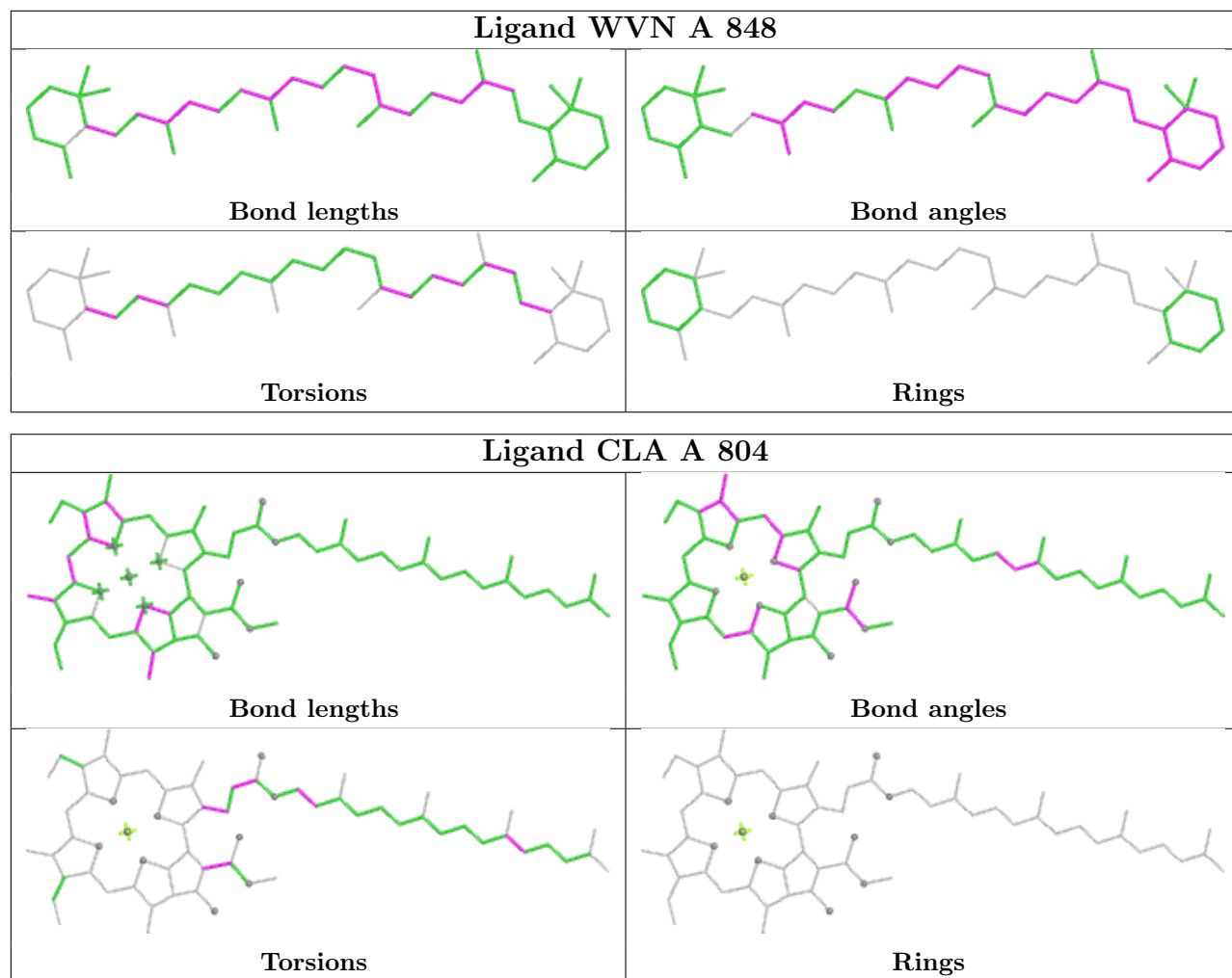
Ligand CLA d 301

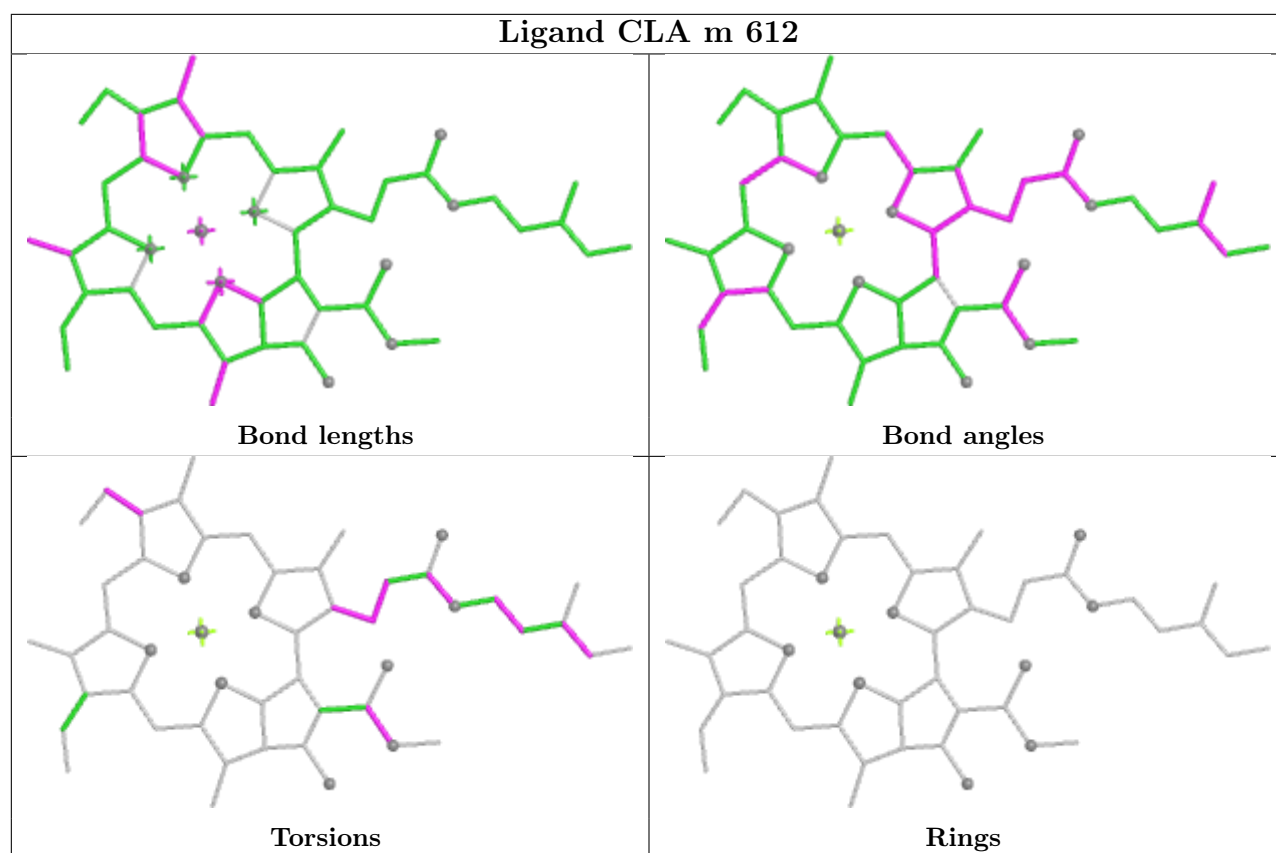
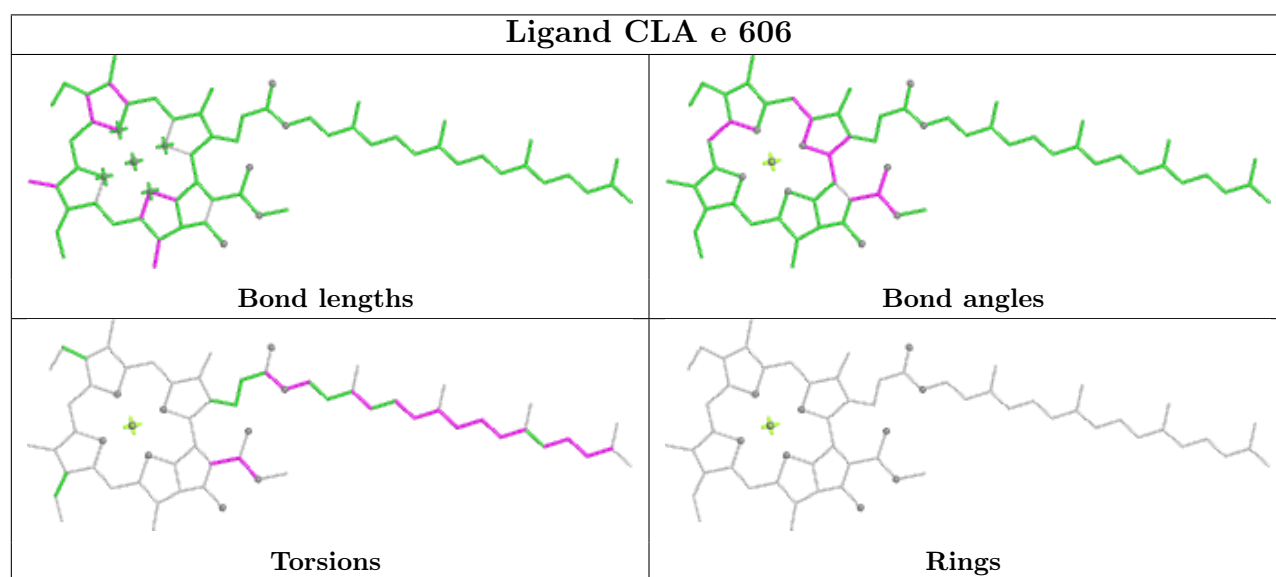


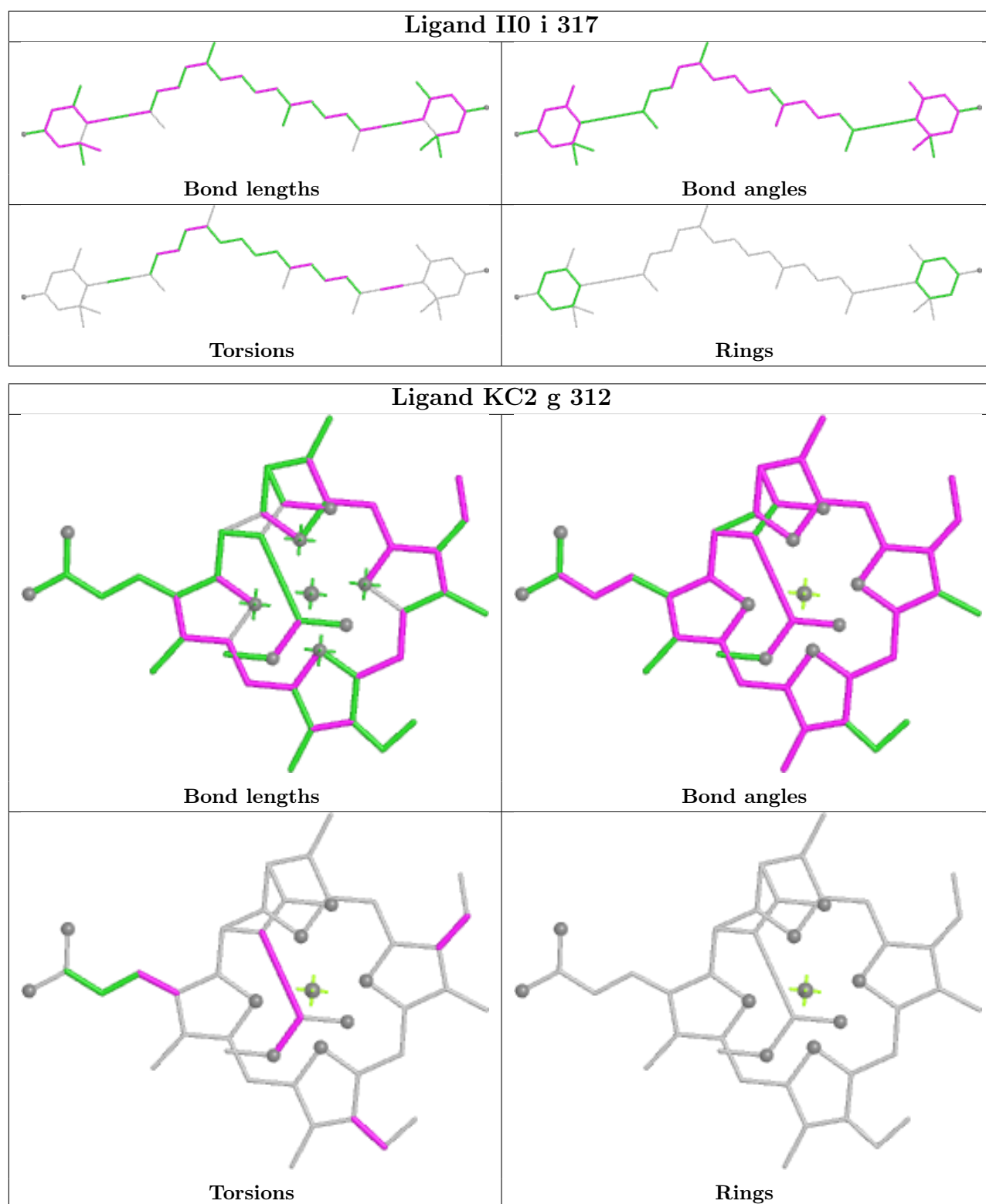
Ligand CLA B 832



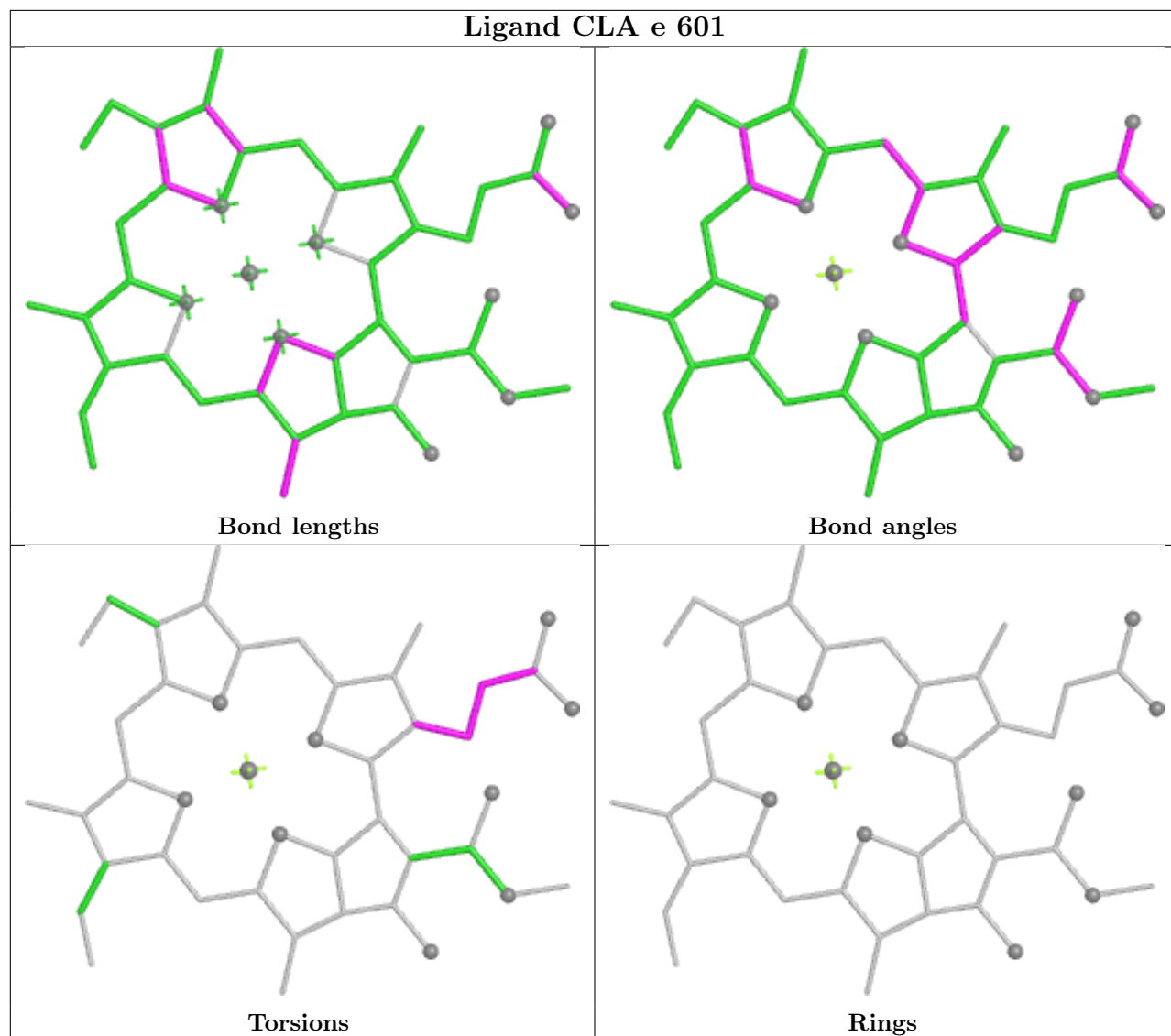




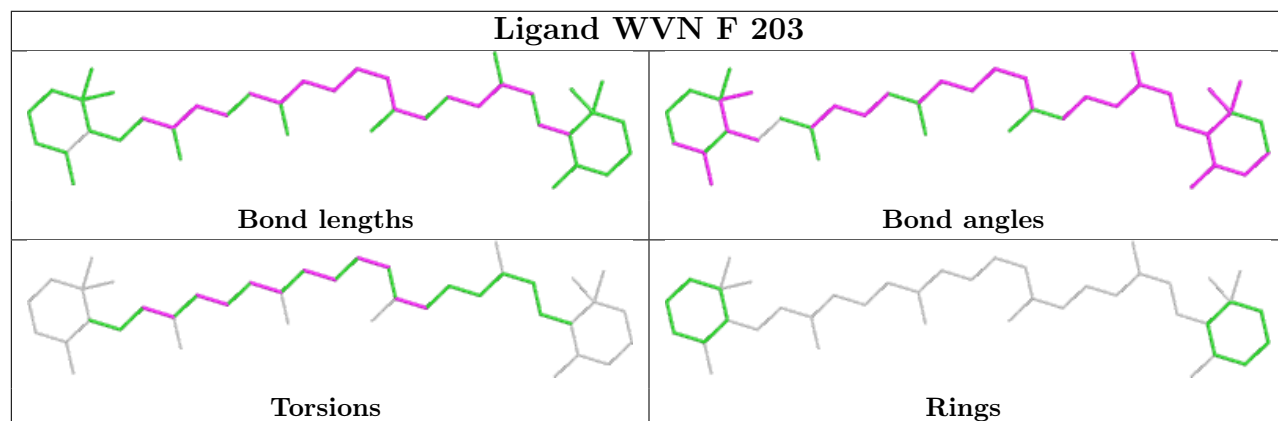


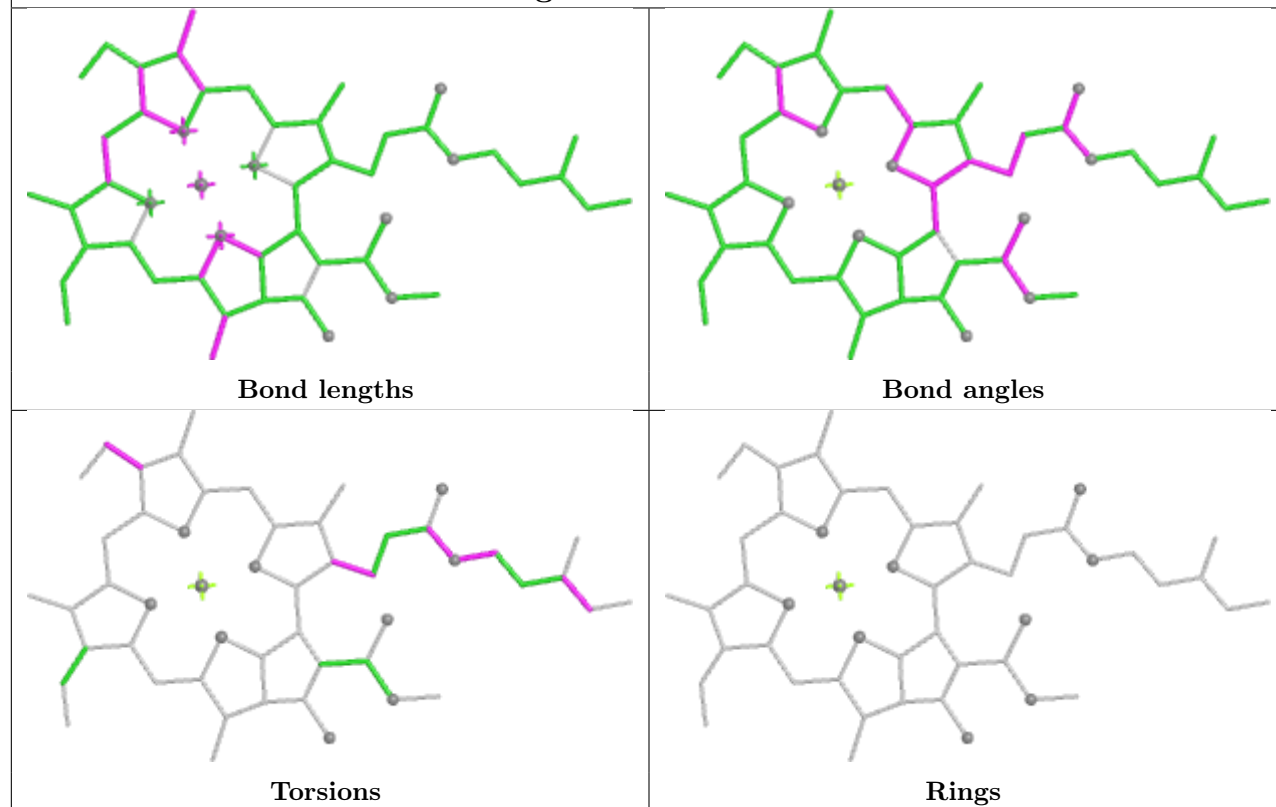
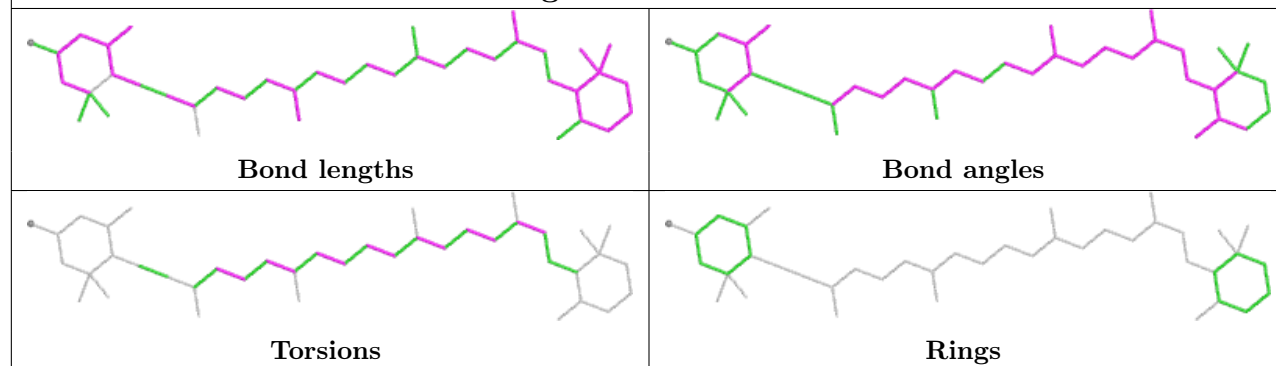


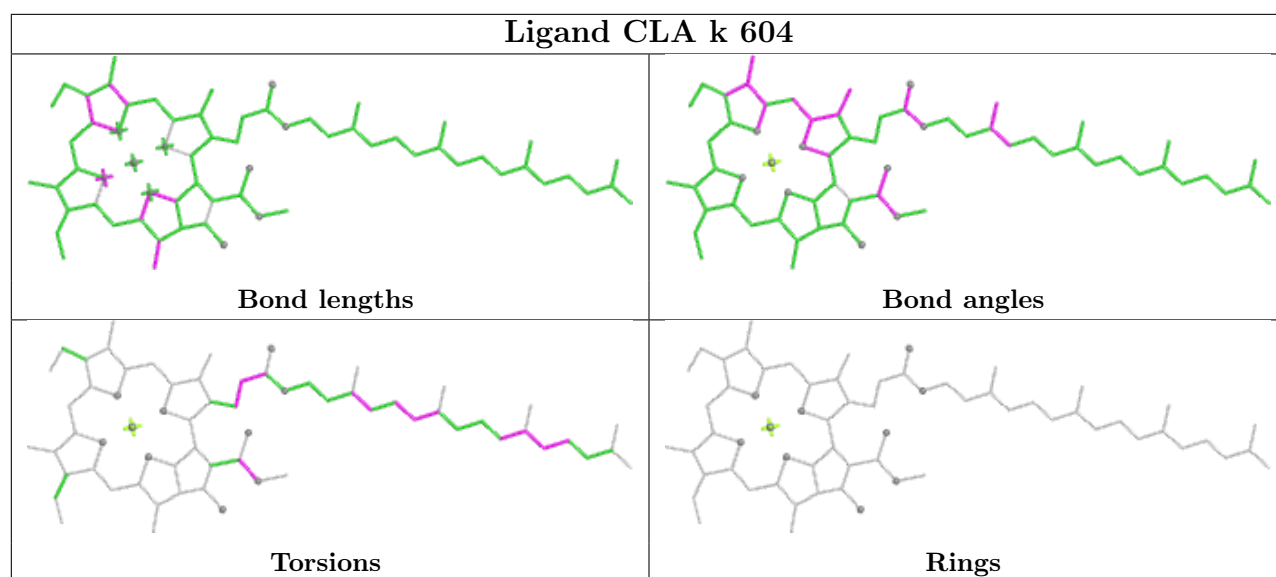
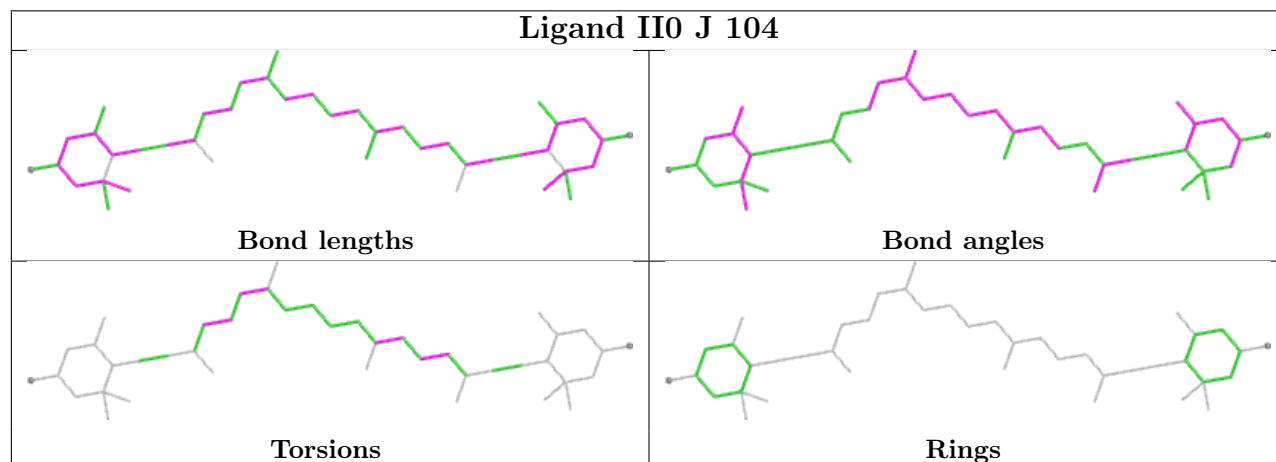
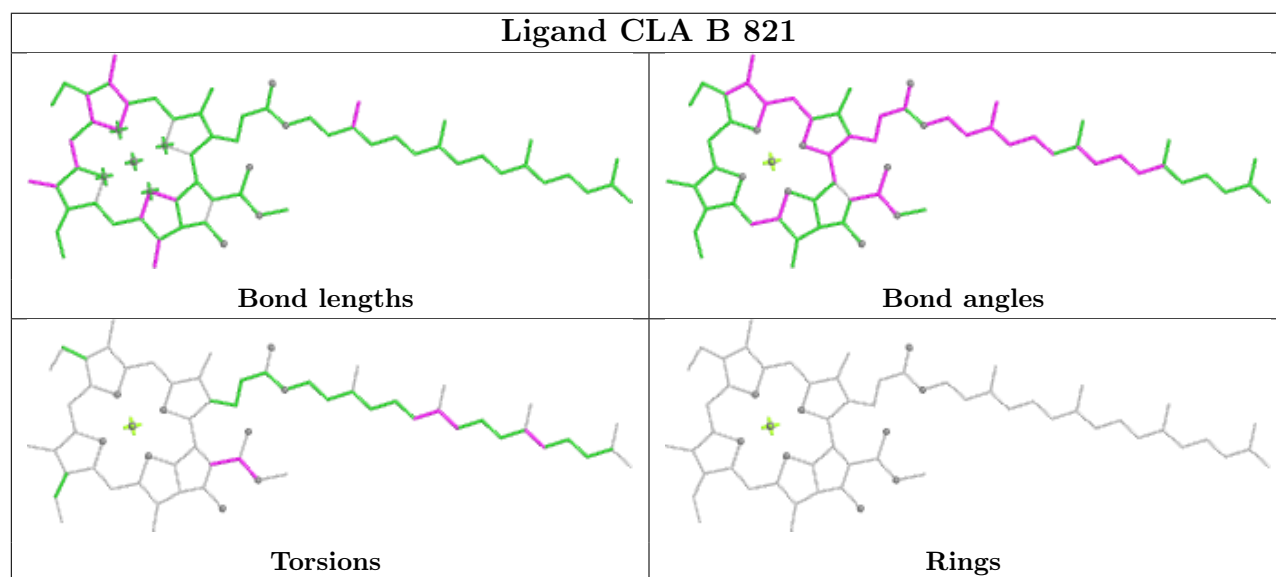
Ligand CLA e 601



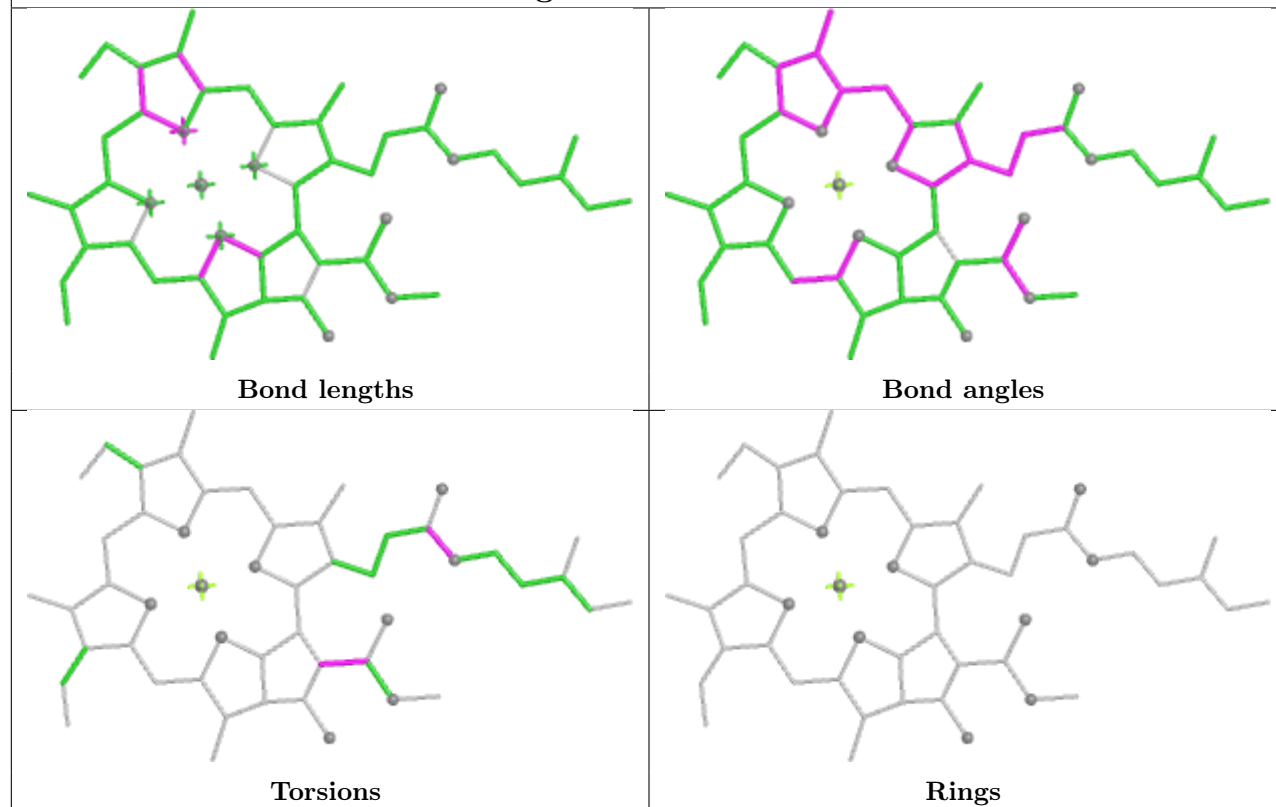
Ligand WVN F 203



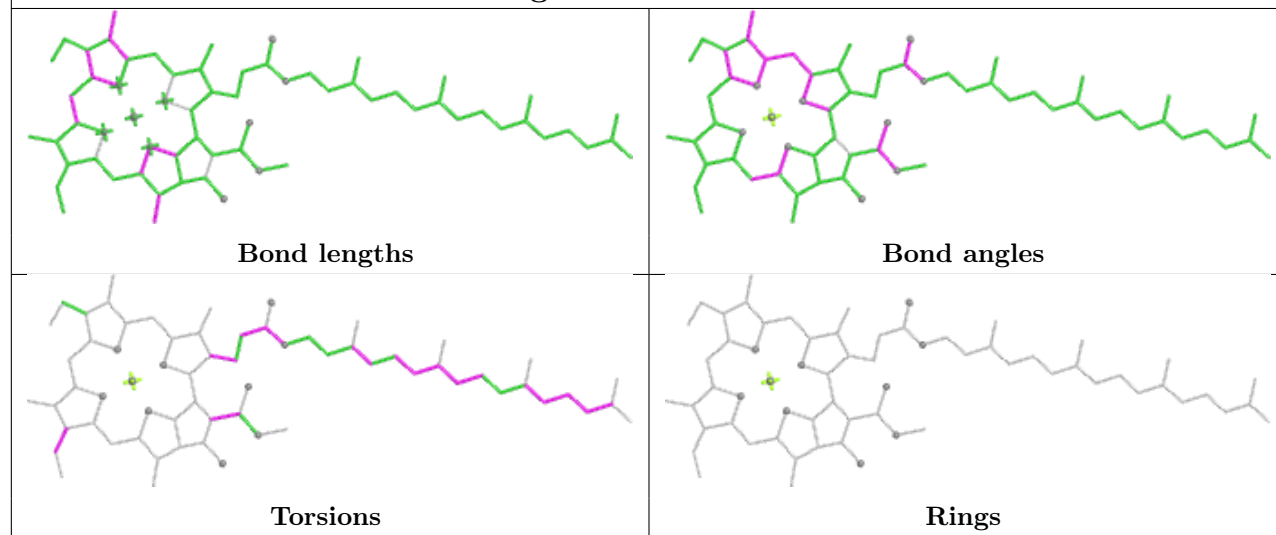
Ligand CLA b 612**Ligand IHT c 616**

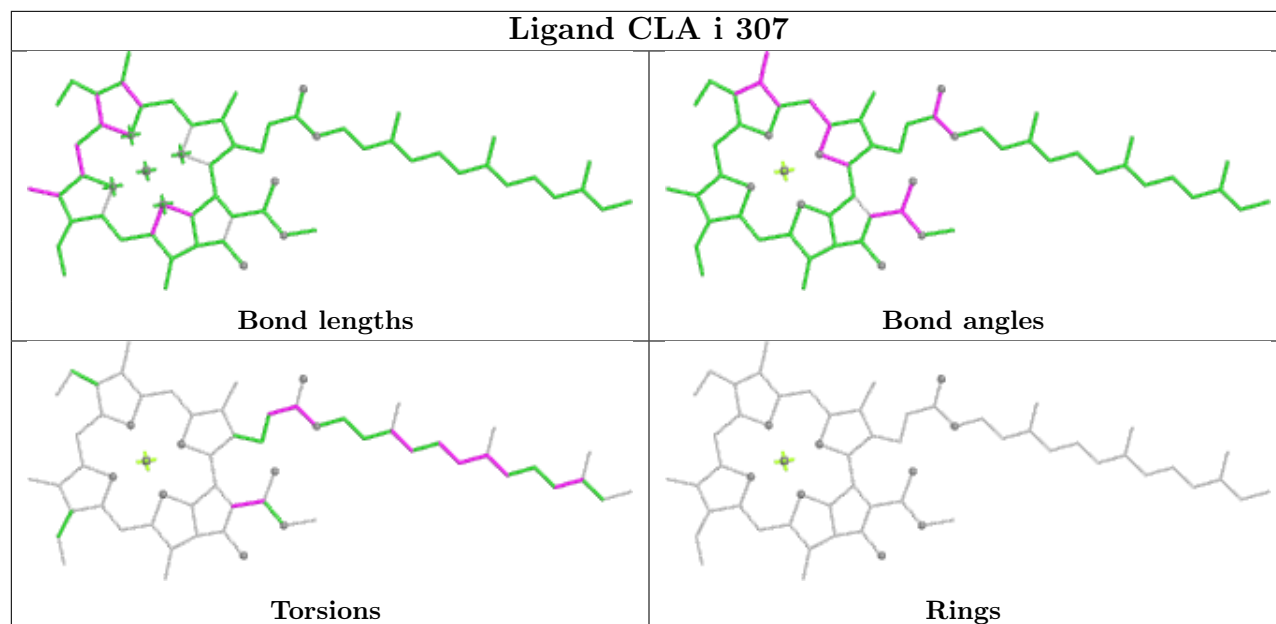
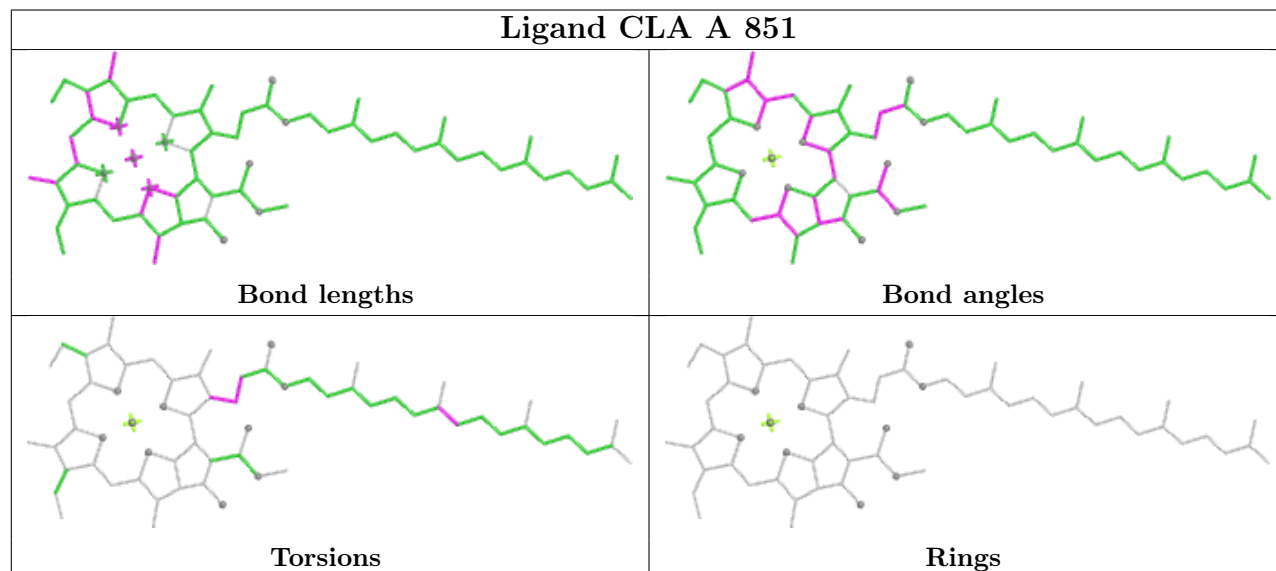


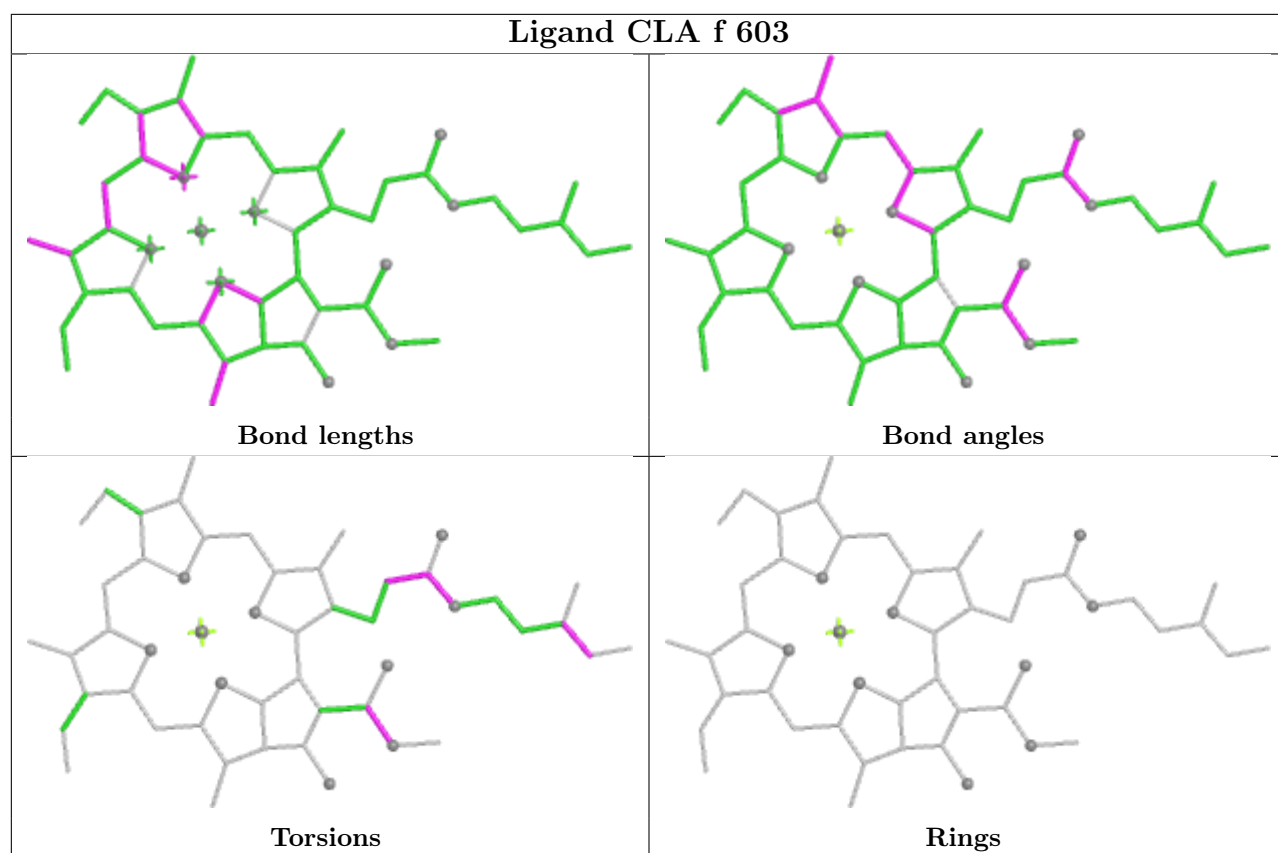
Ligand CLA k 603



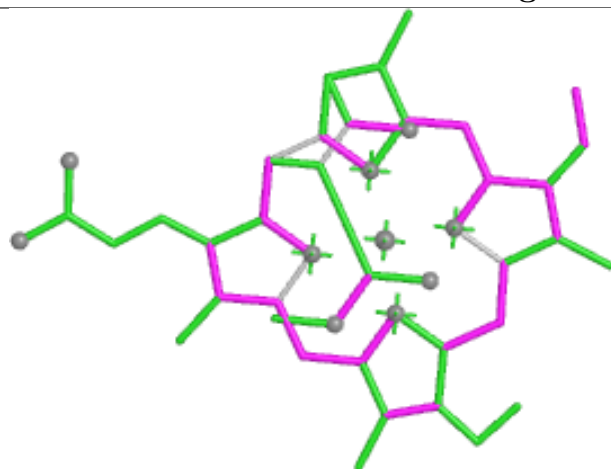
Ligand CLA m 608



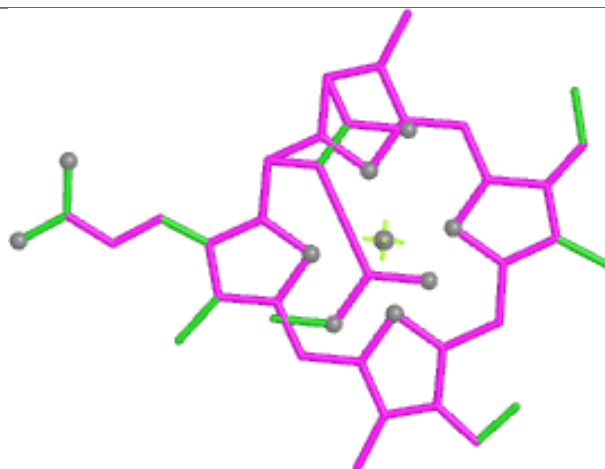
Ligand CLA i 307**Ligand CLA A 851**



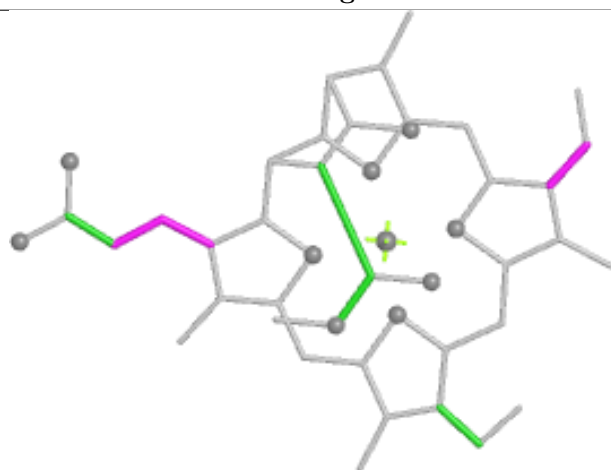
Ligand KC2 d 311



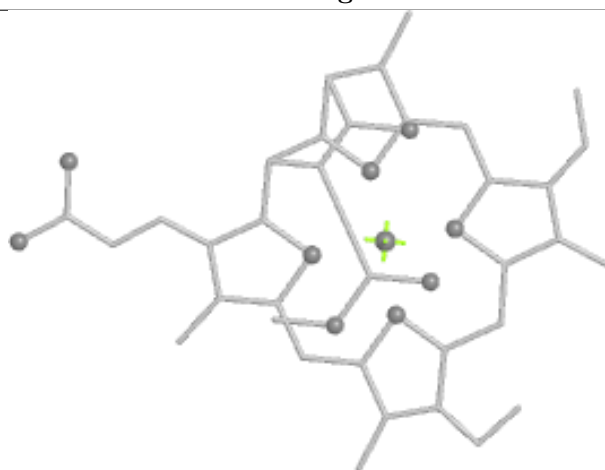
Bond lengths



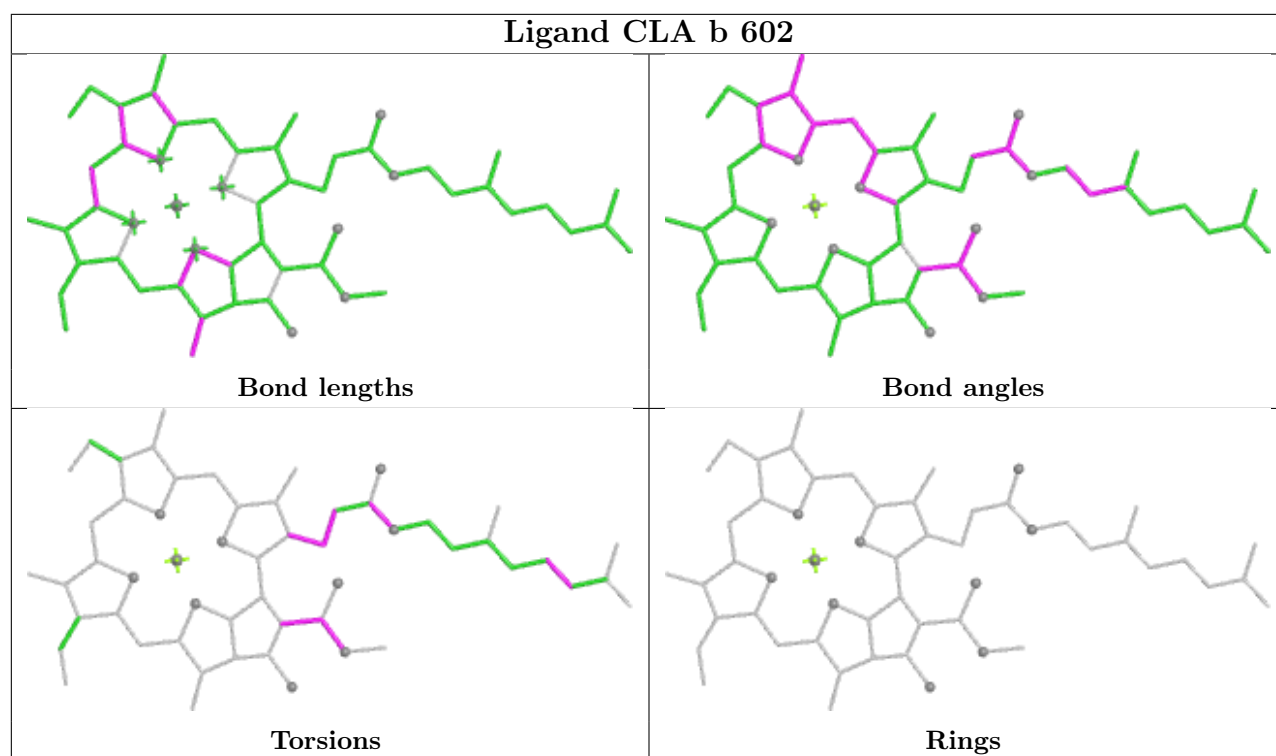
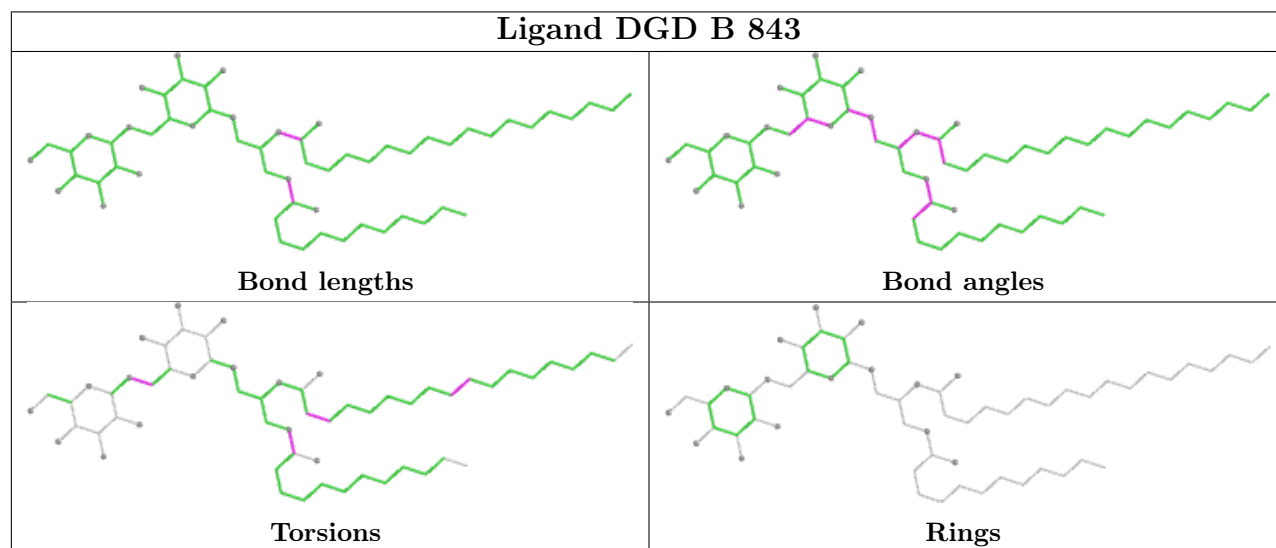
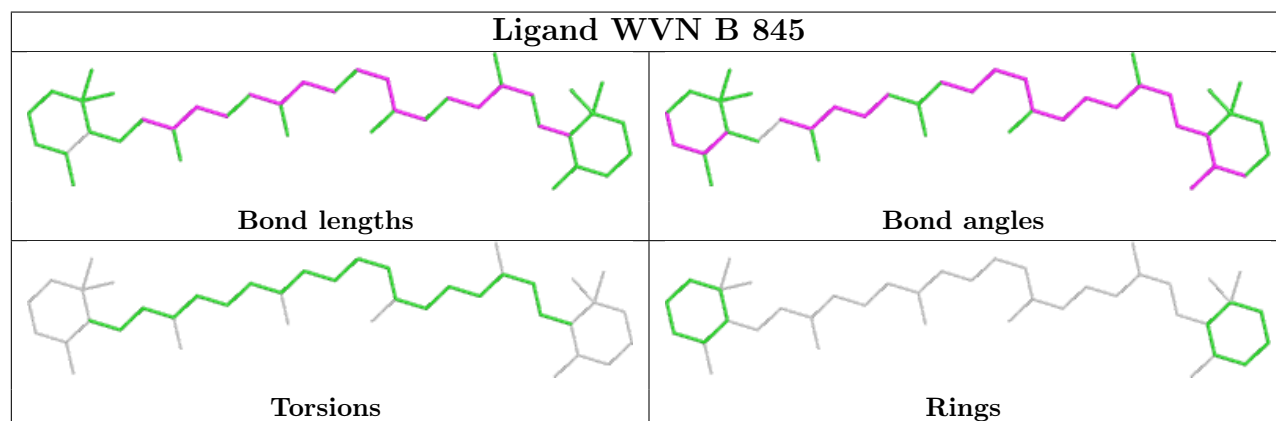
Bond angles

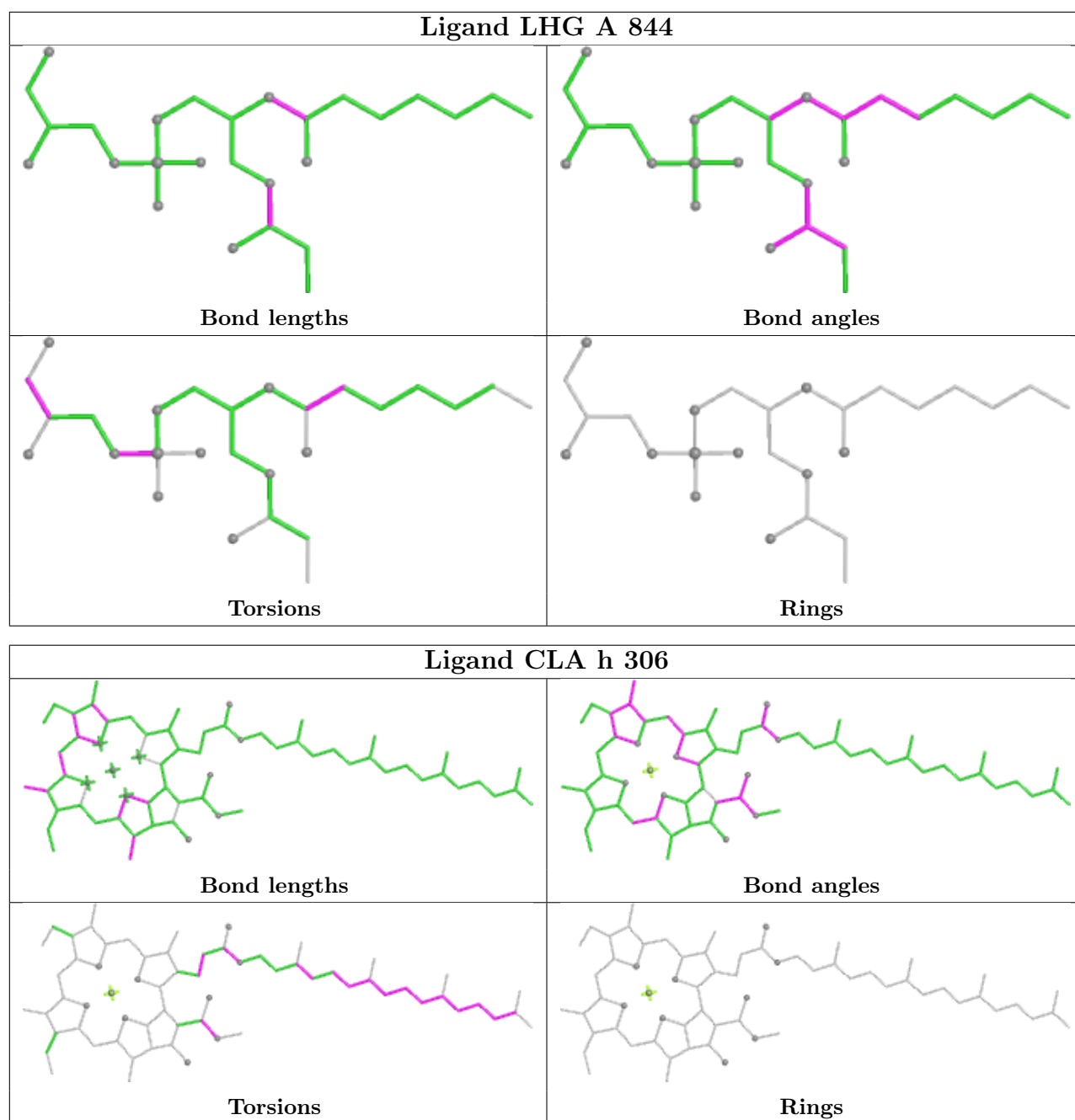


Torsions

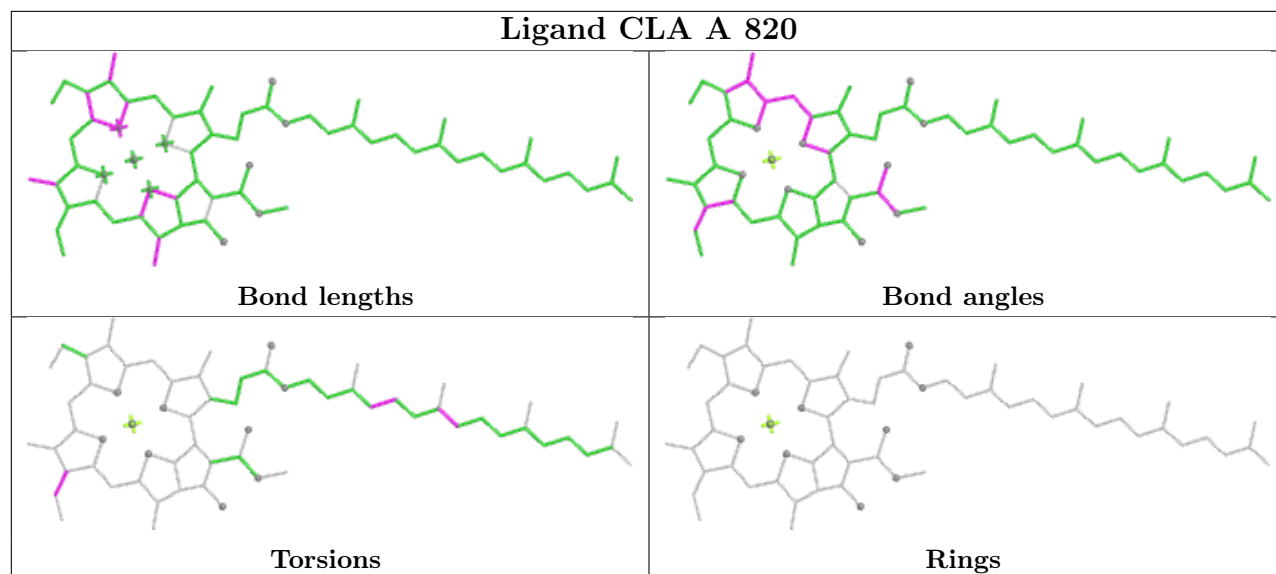


Rings

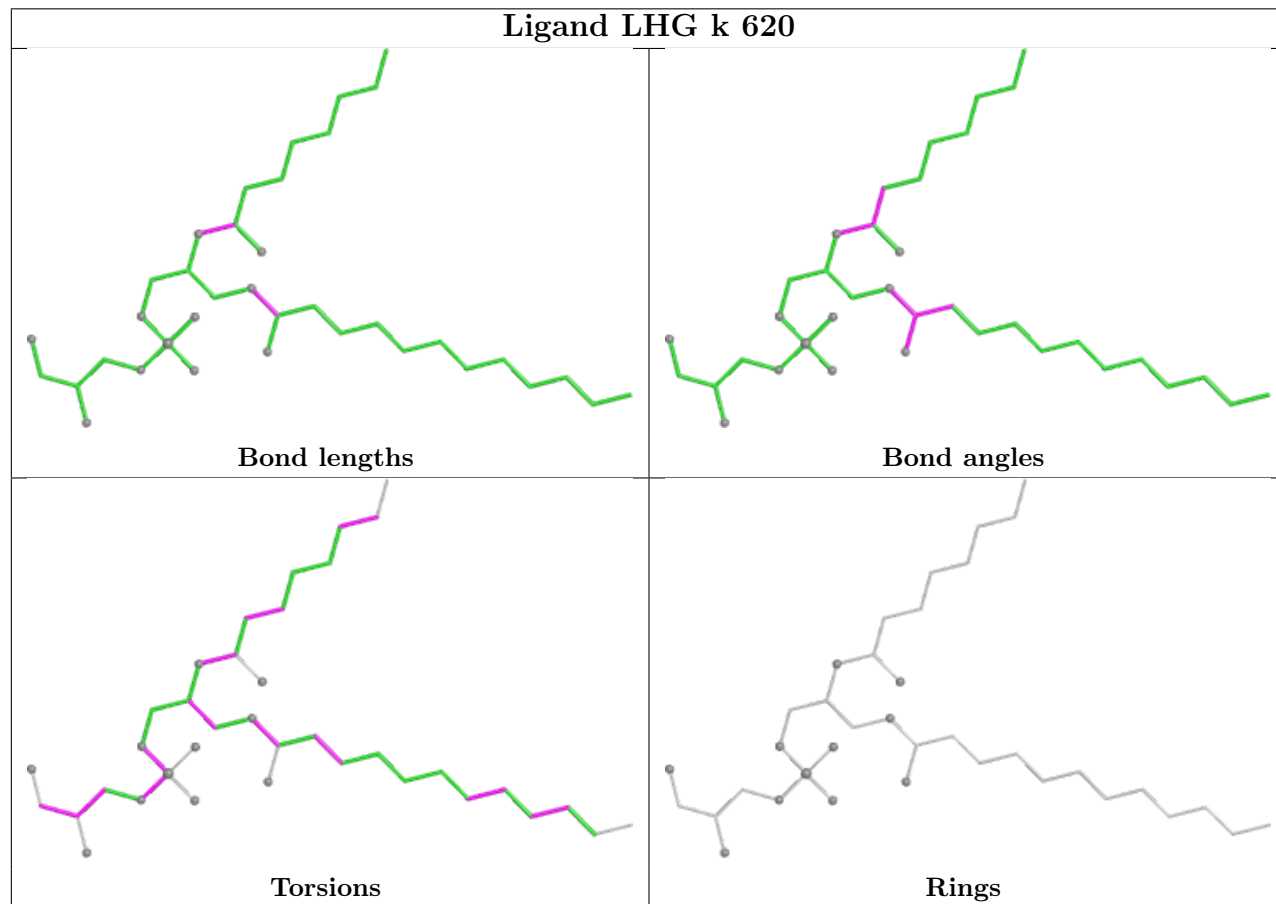




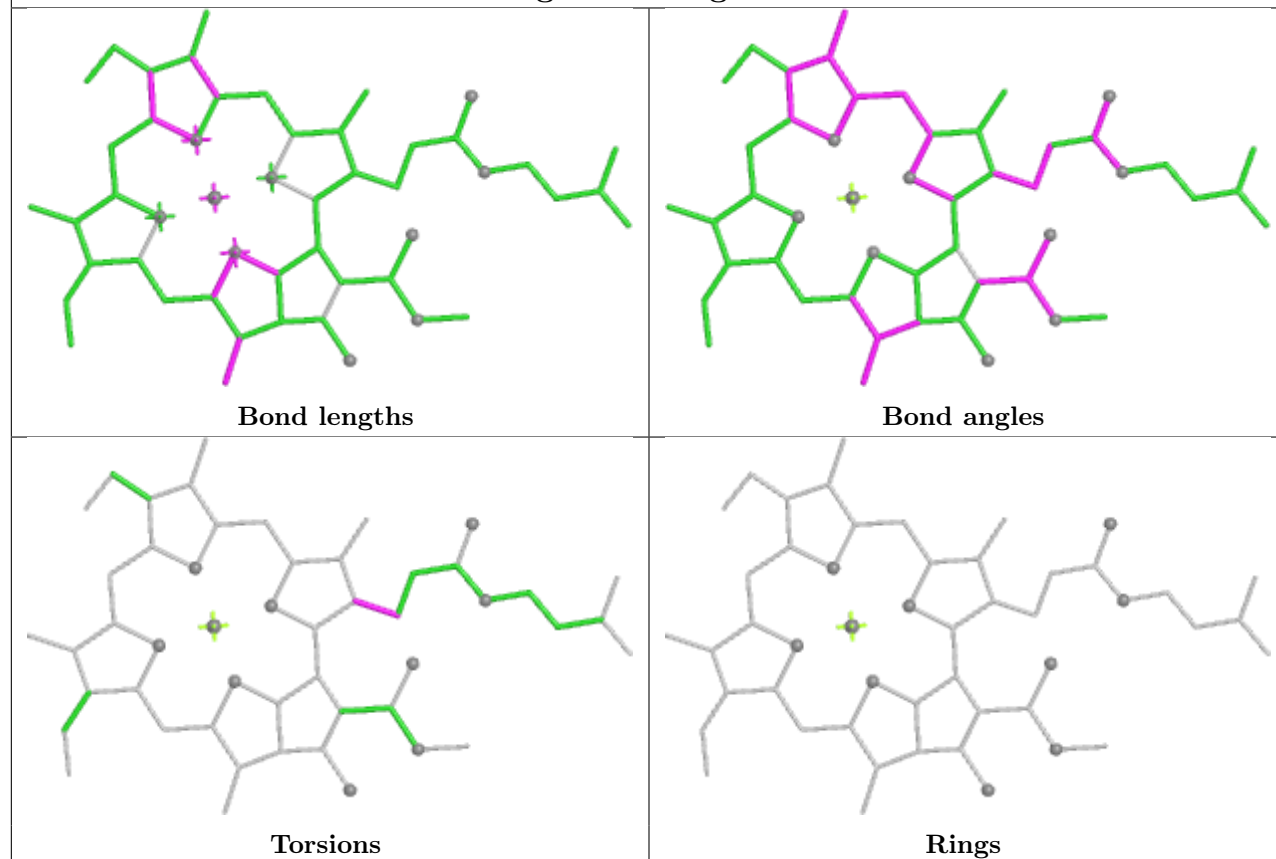
Ligand CLA A 820



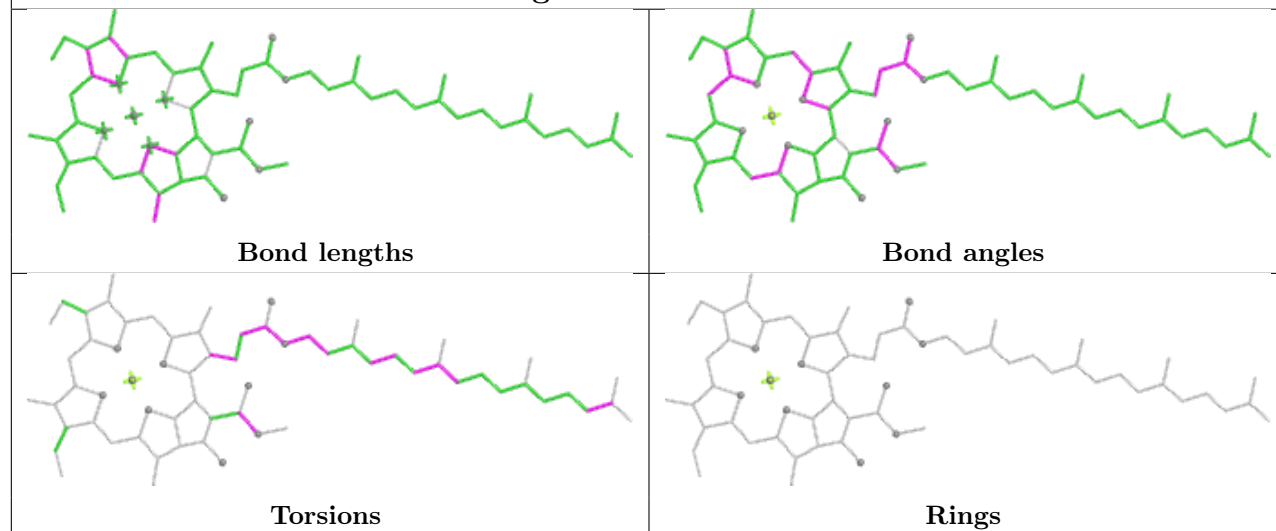
Ligand LHG k 620

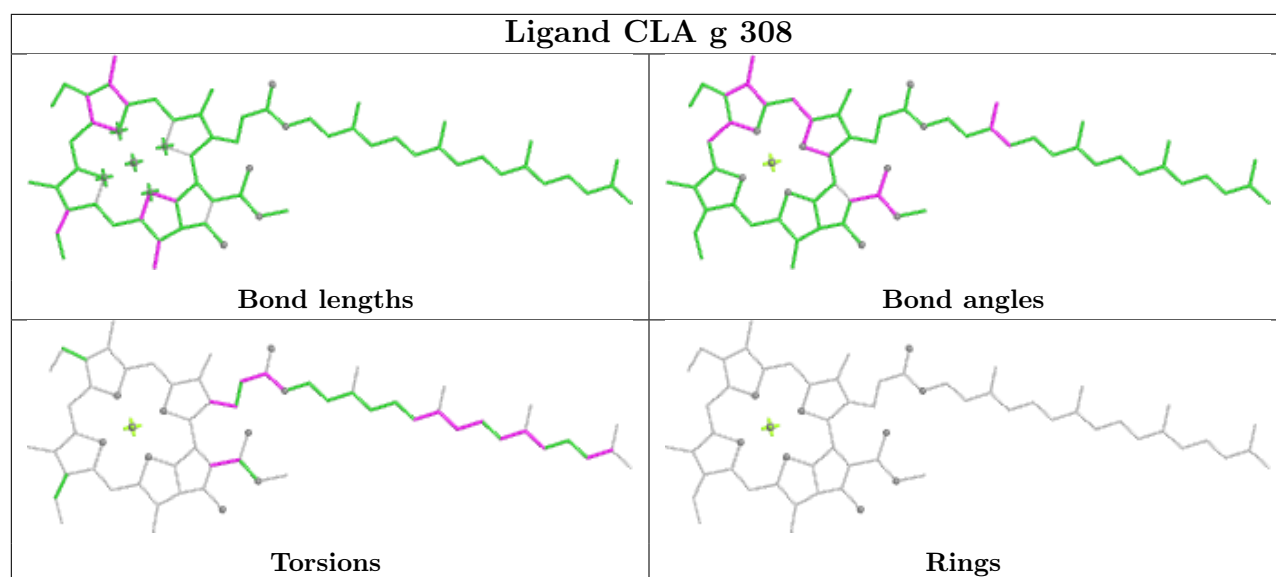
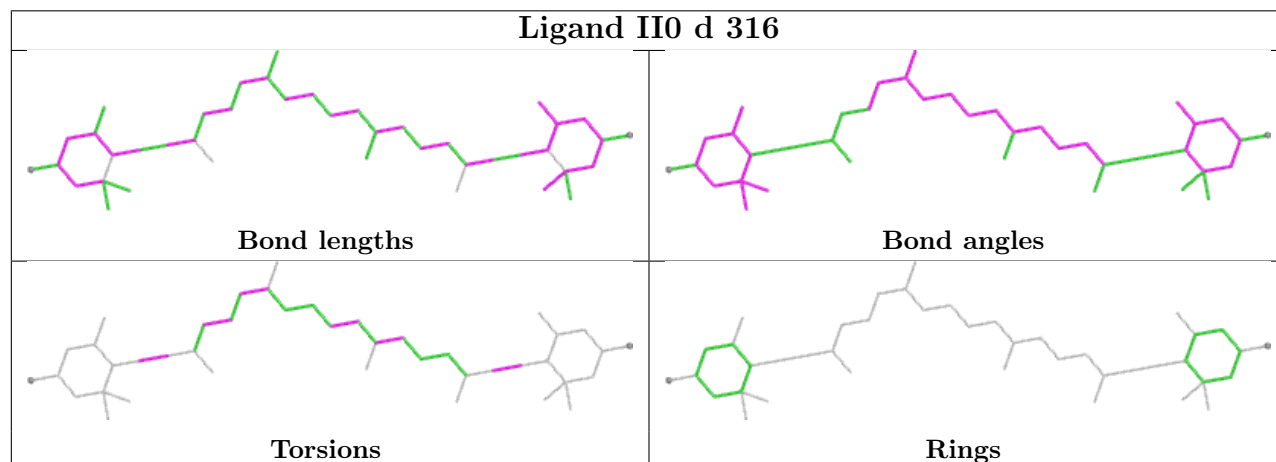
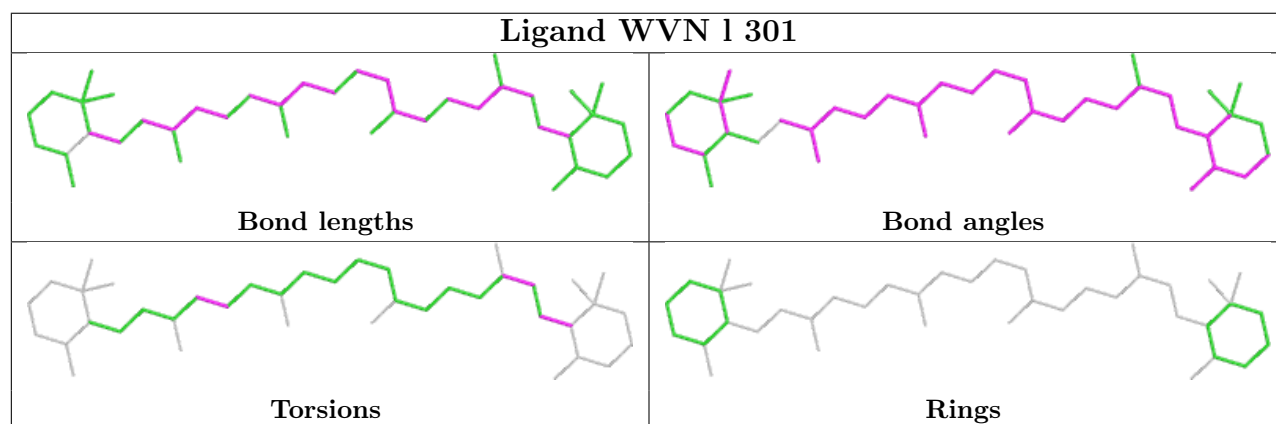


Ligand CLA g 303

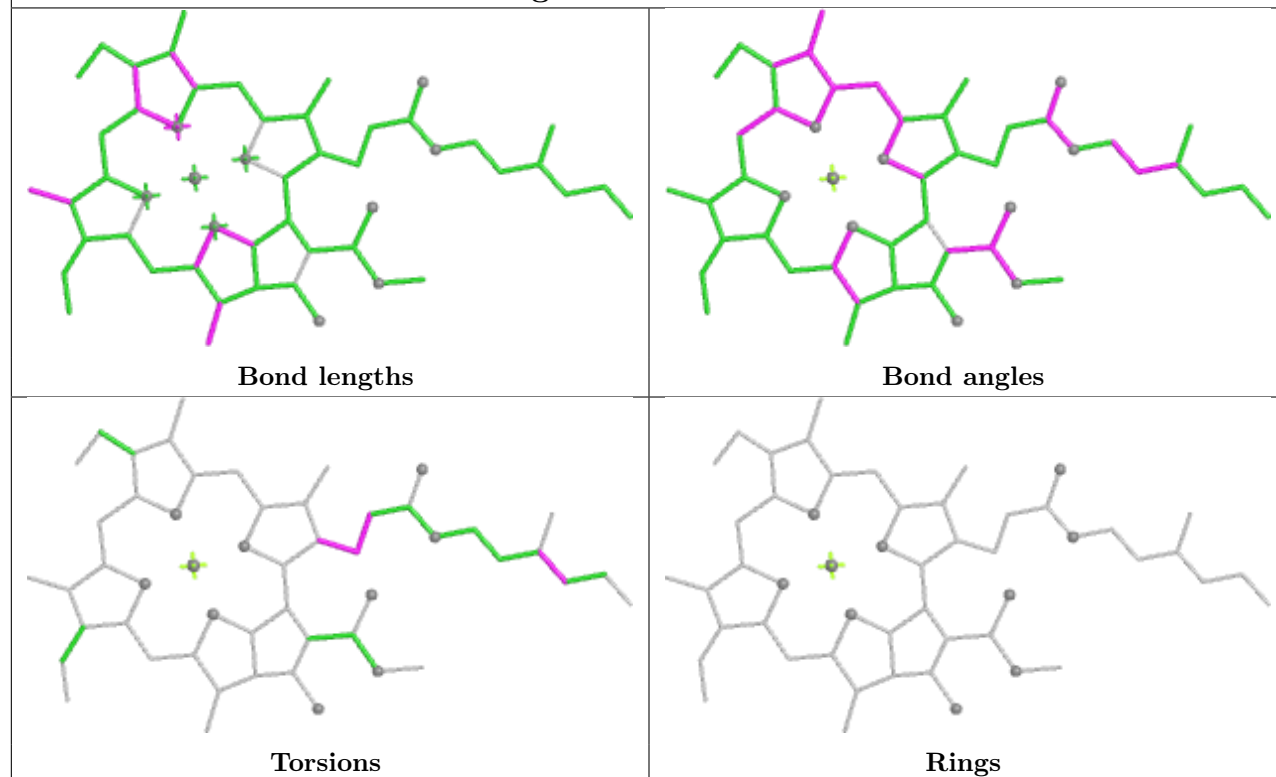


Ligand CLA B 830

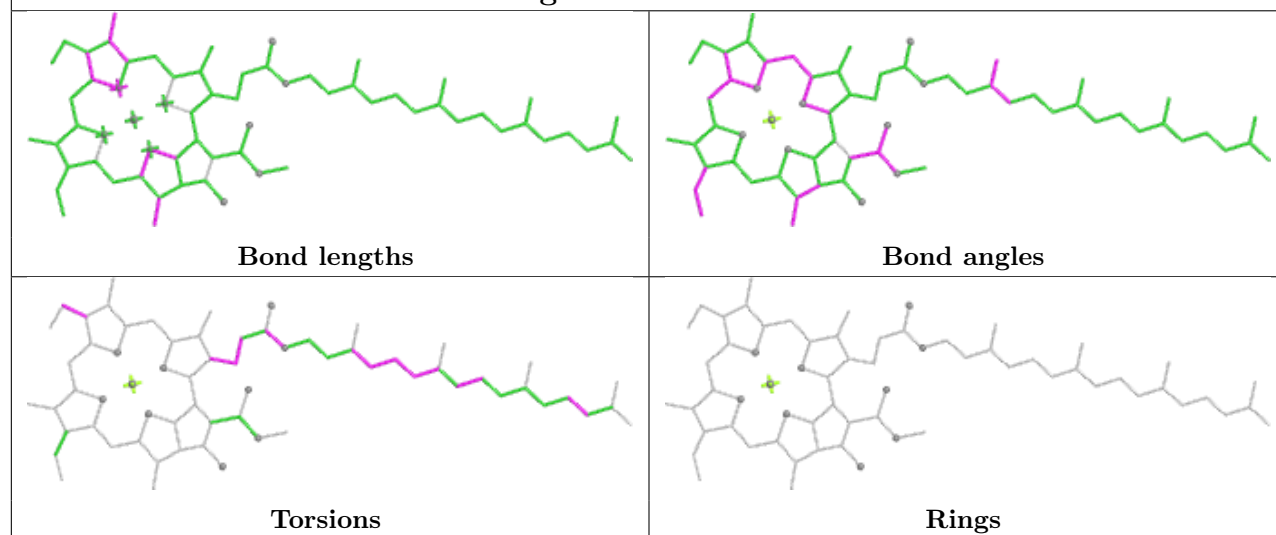


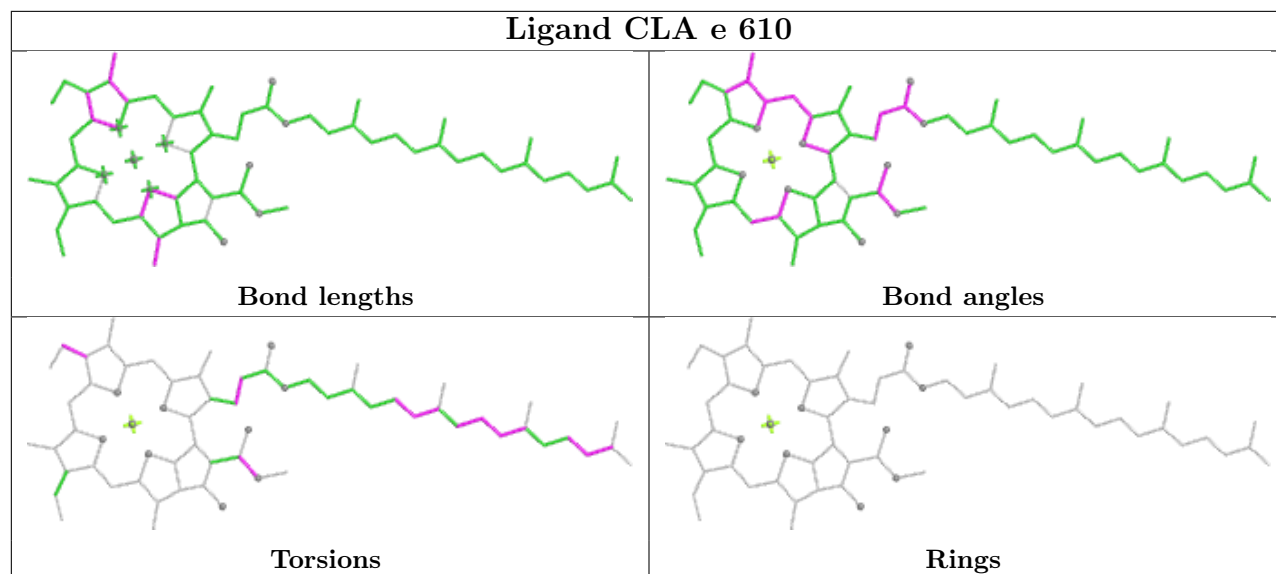
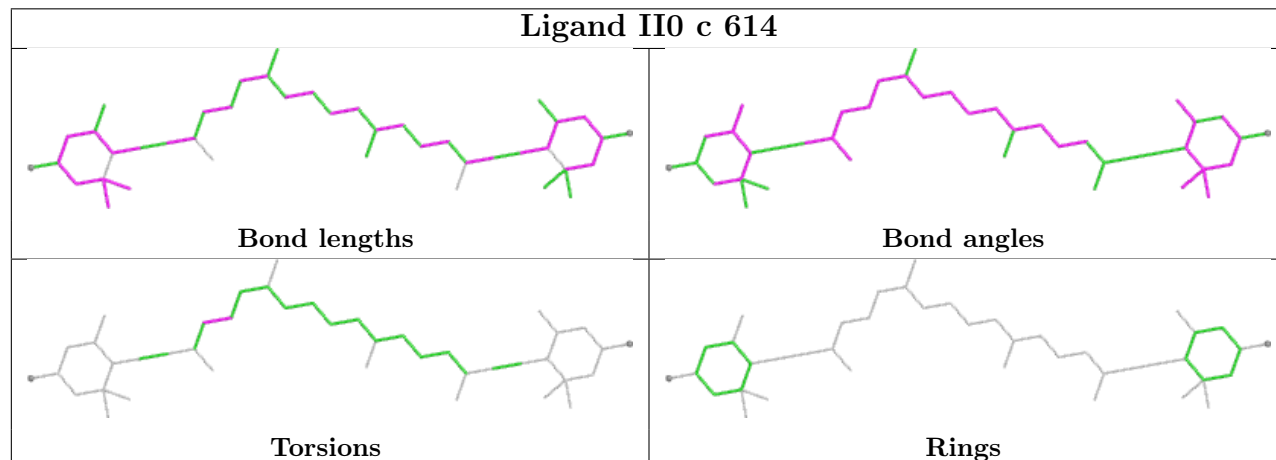
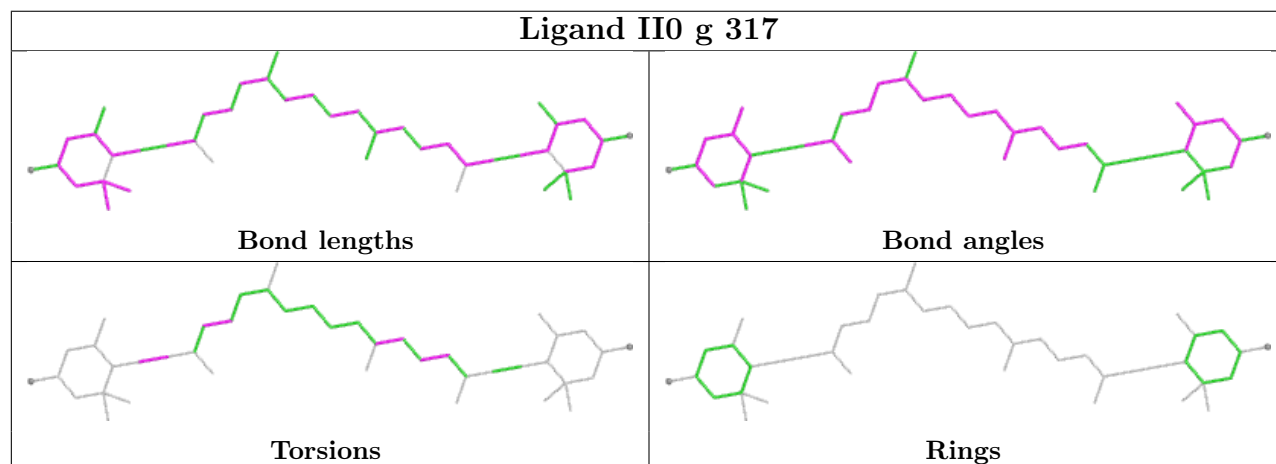


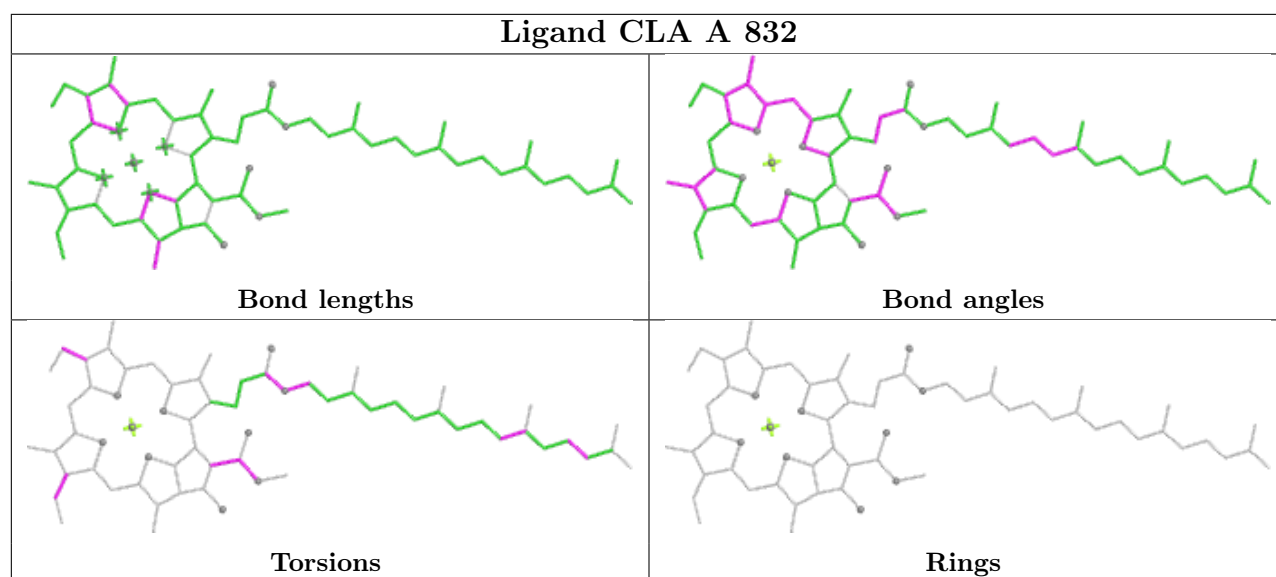
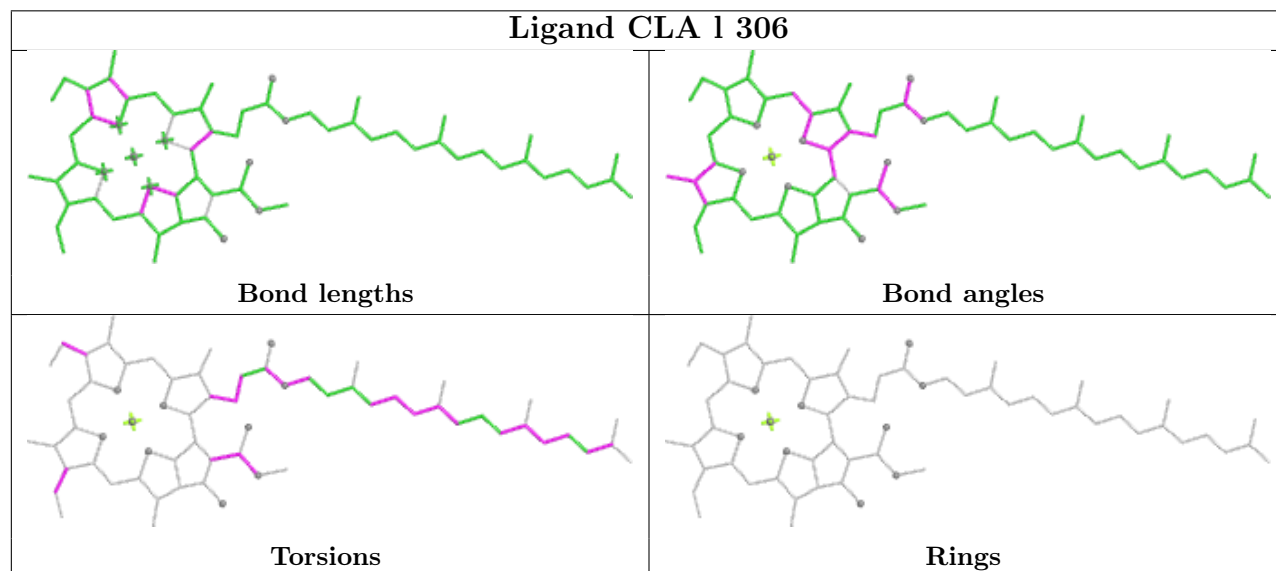
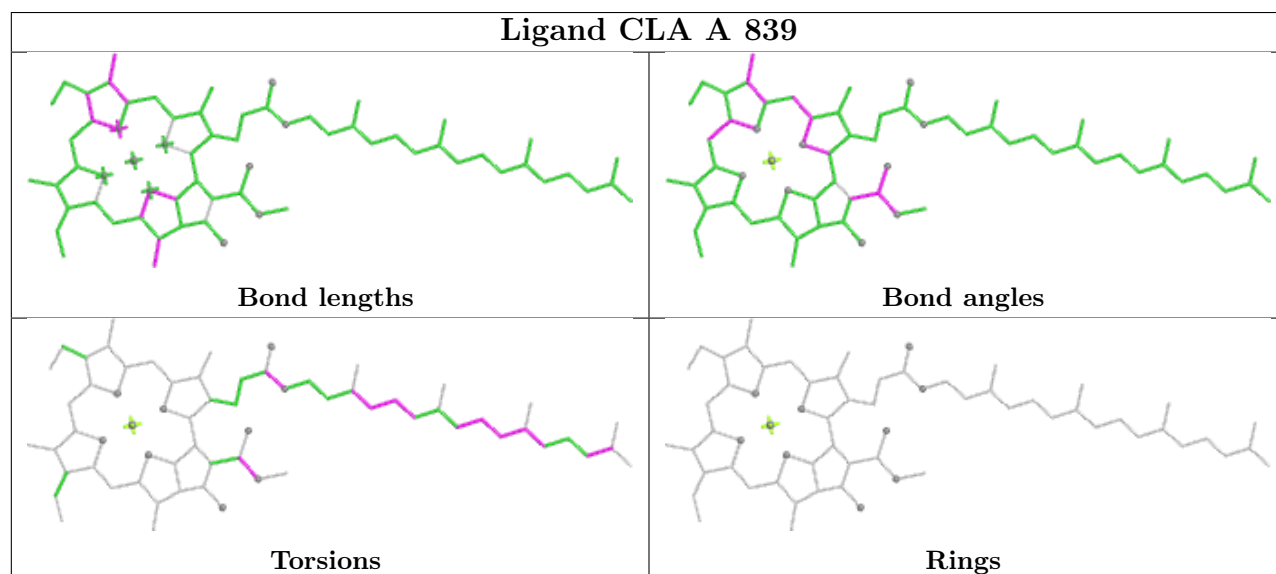
Ligand CLA O 201

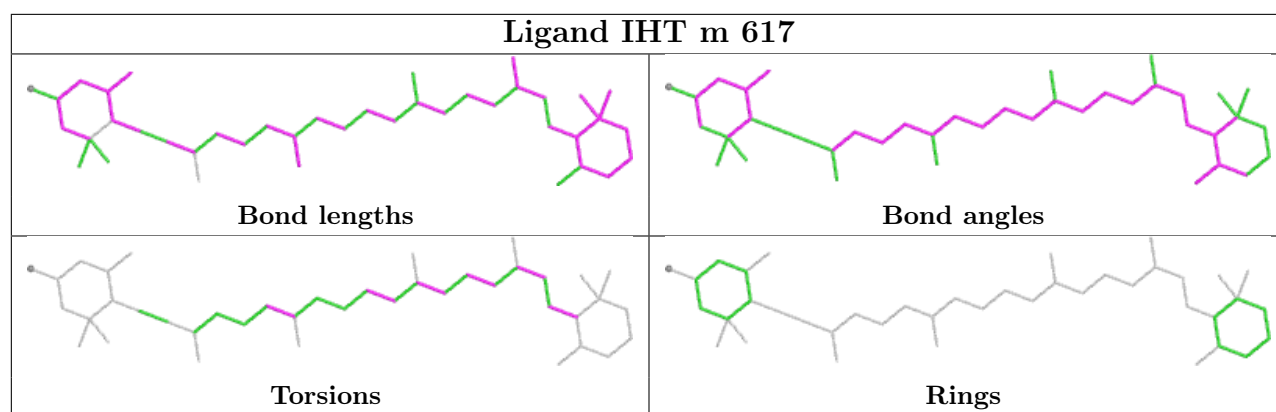
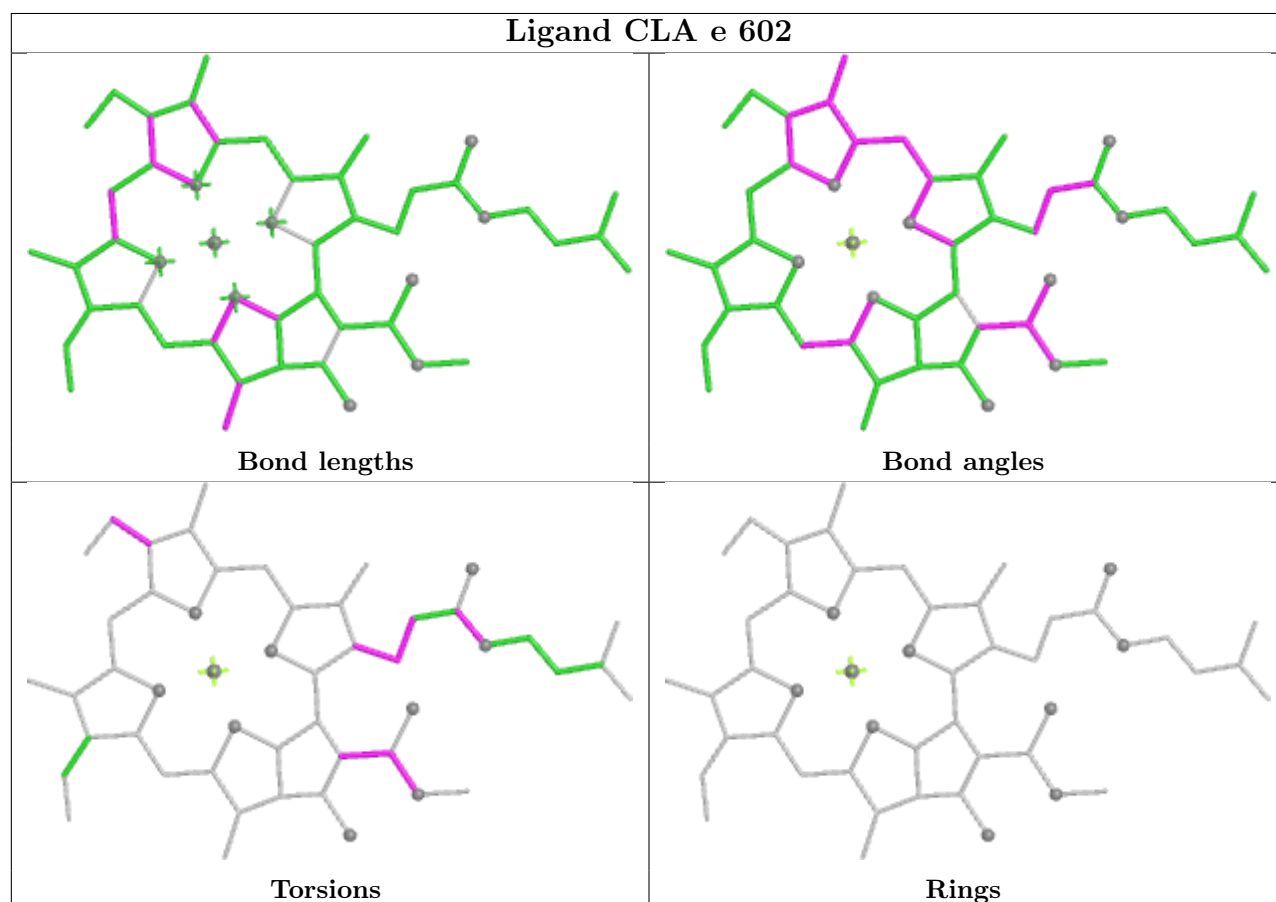


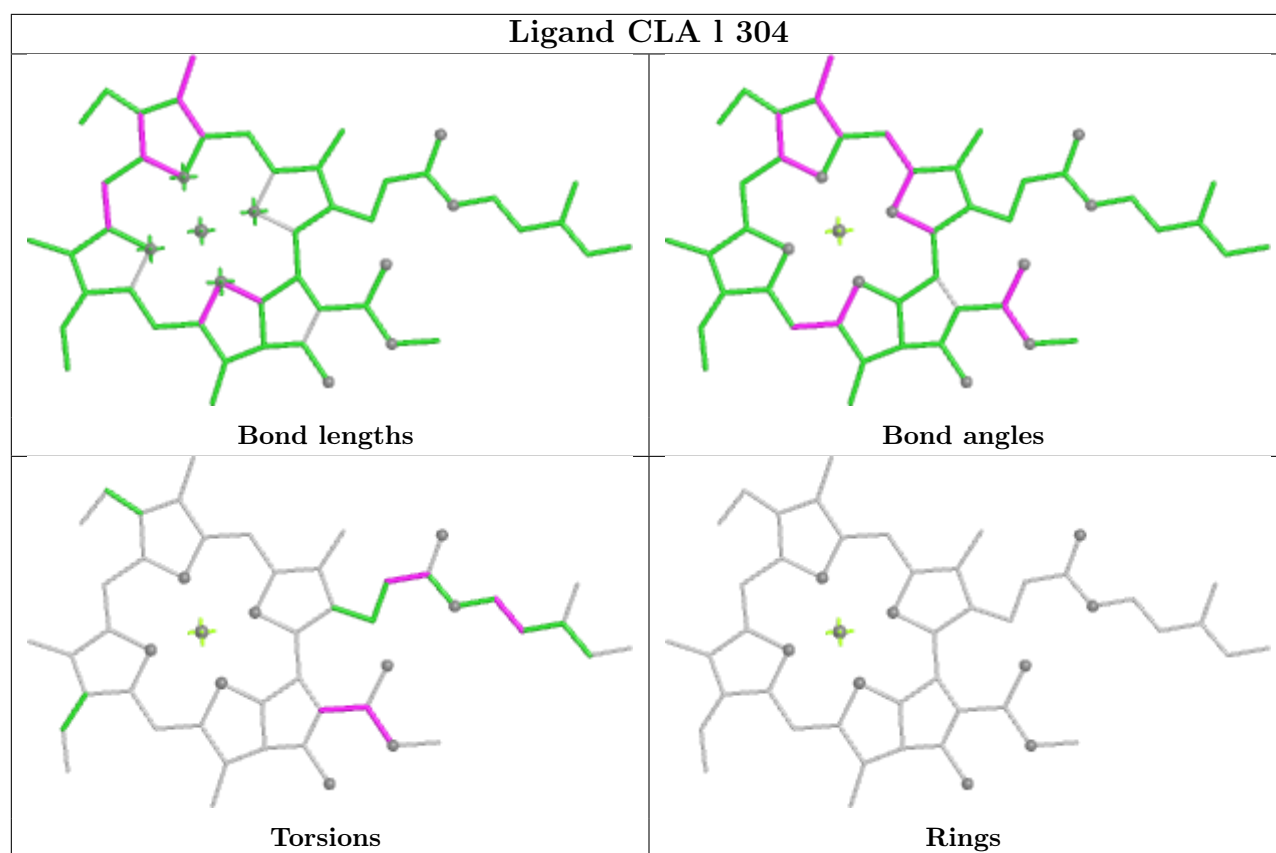
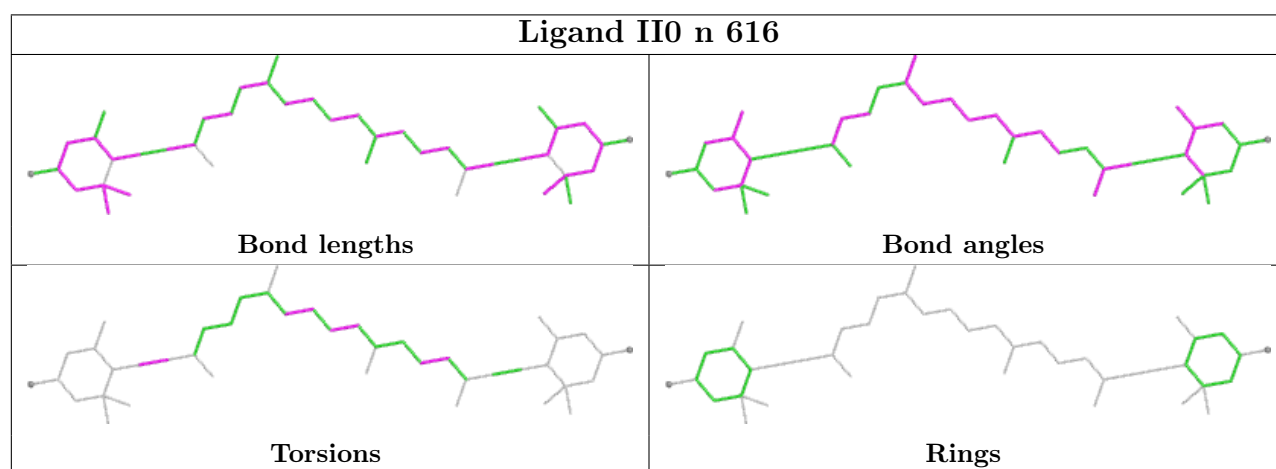
Ligand CLA f 610



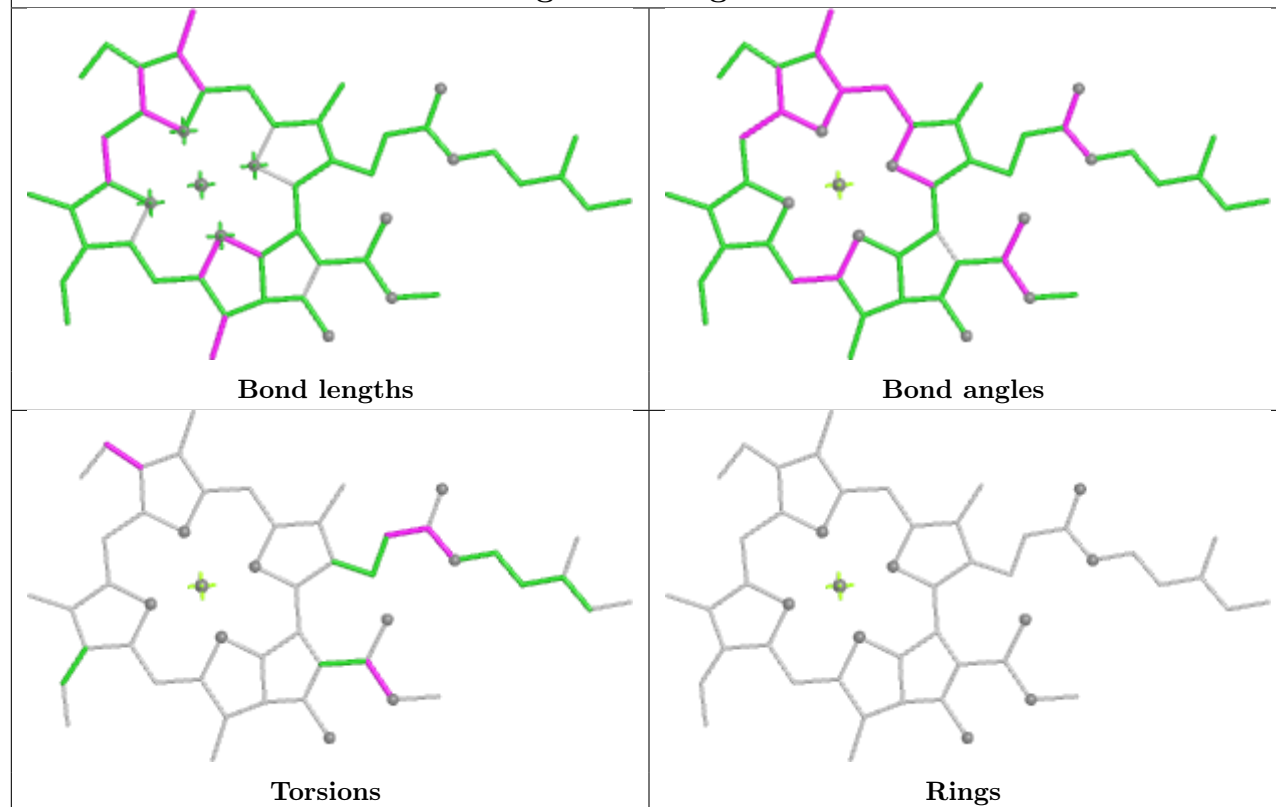
Ligand CLA e 610**Ligand II0 c 614****Ligand II0 g 317**



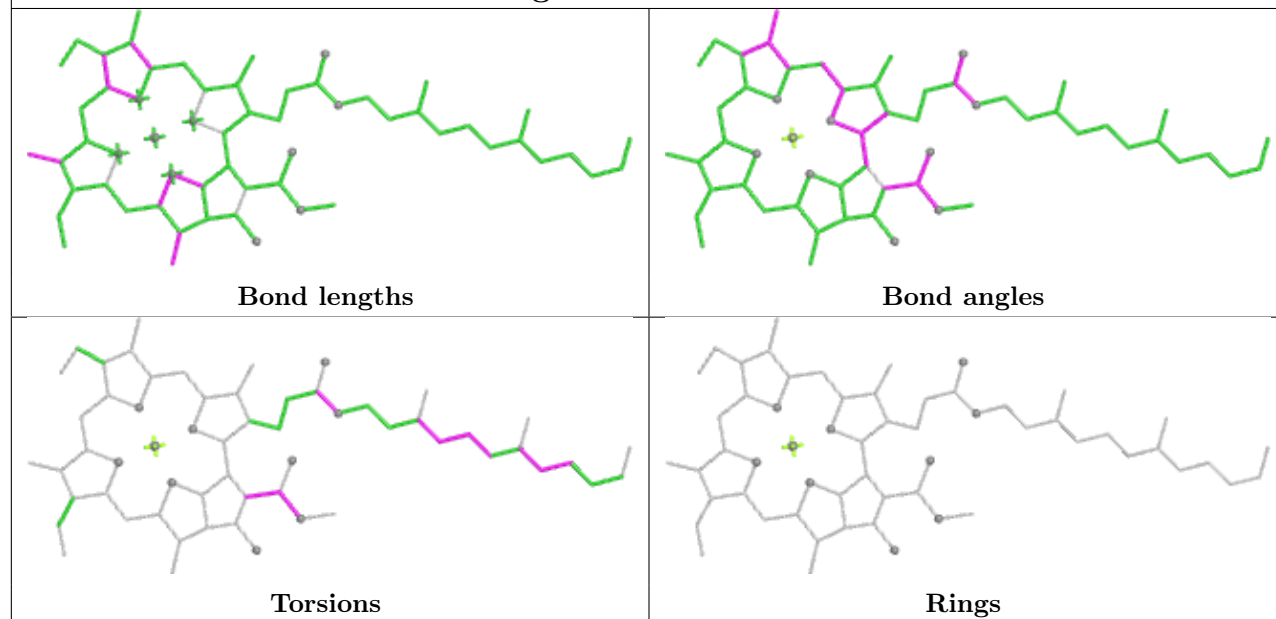




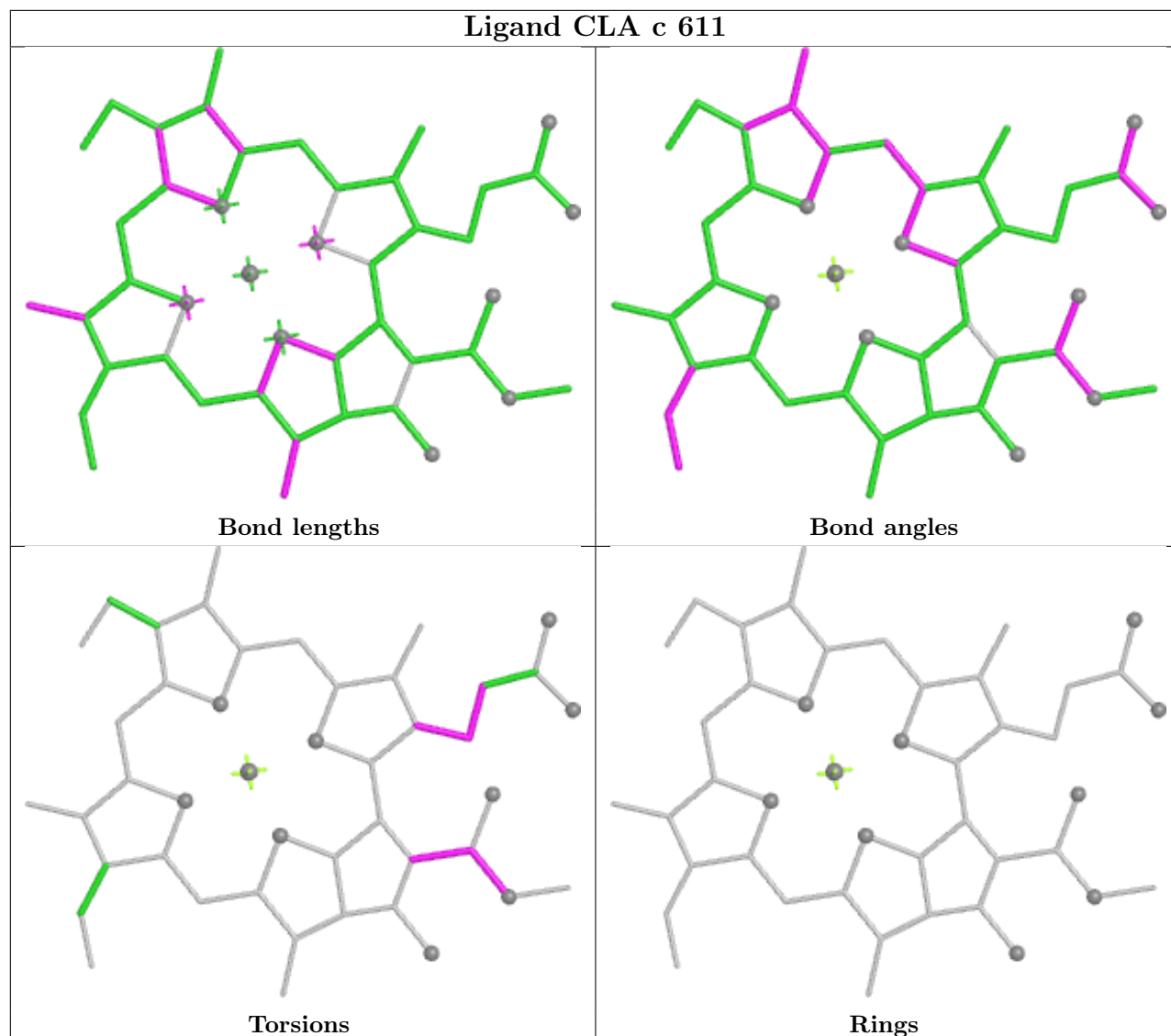
Ligand CLA g 307



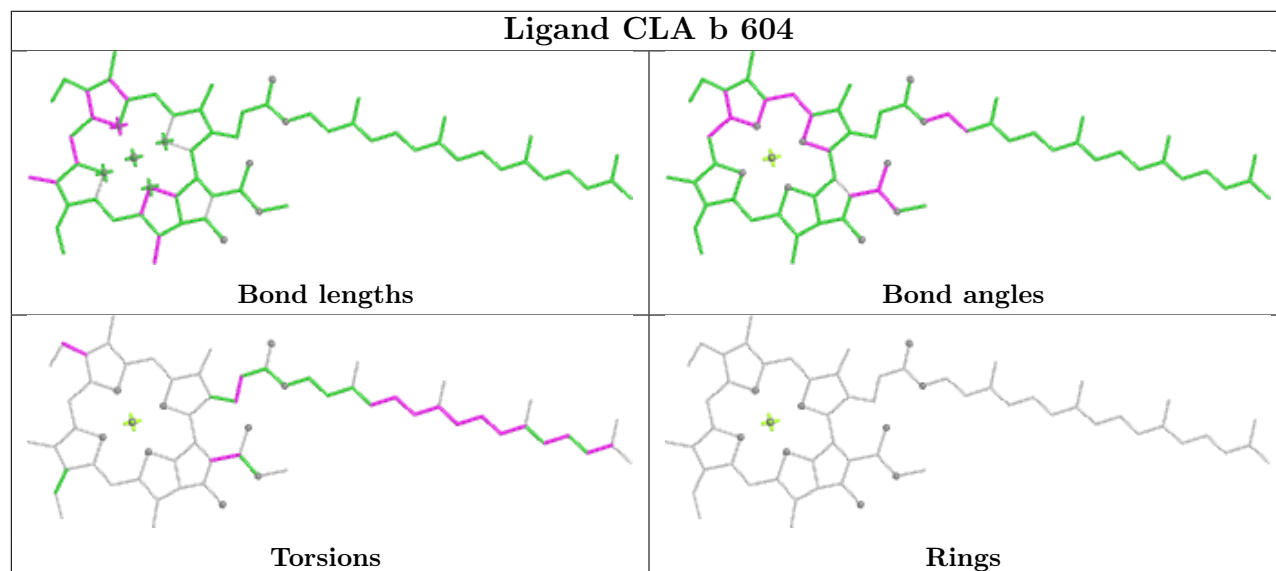
Ligand CLA B 813



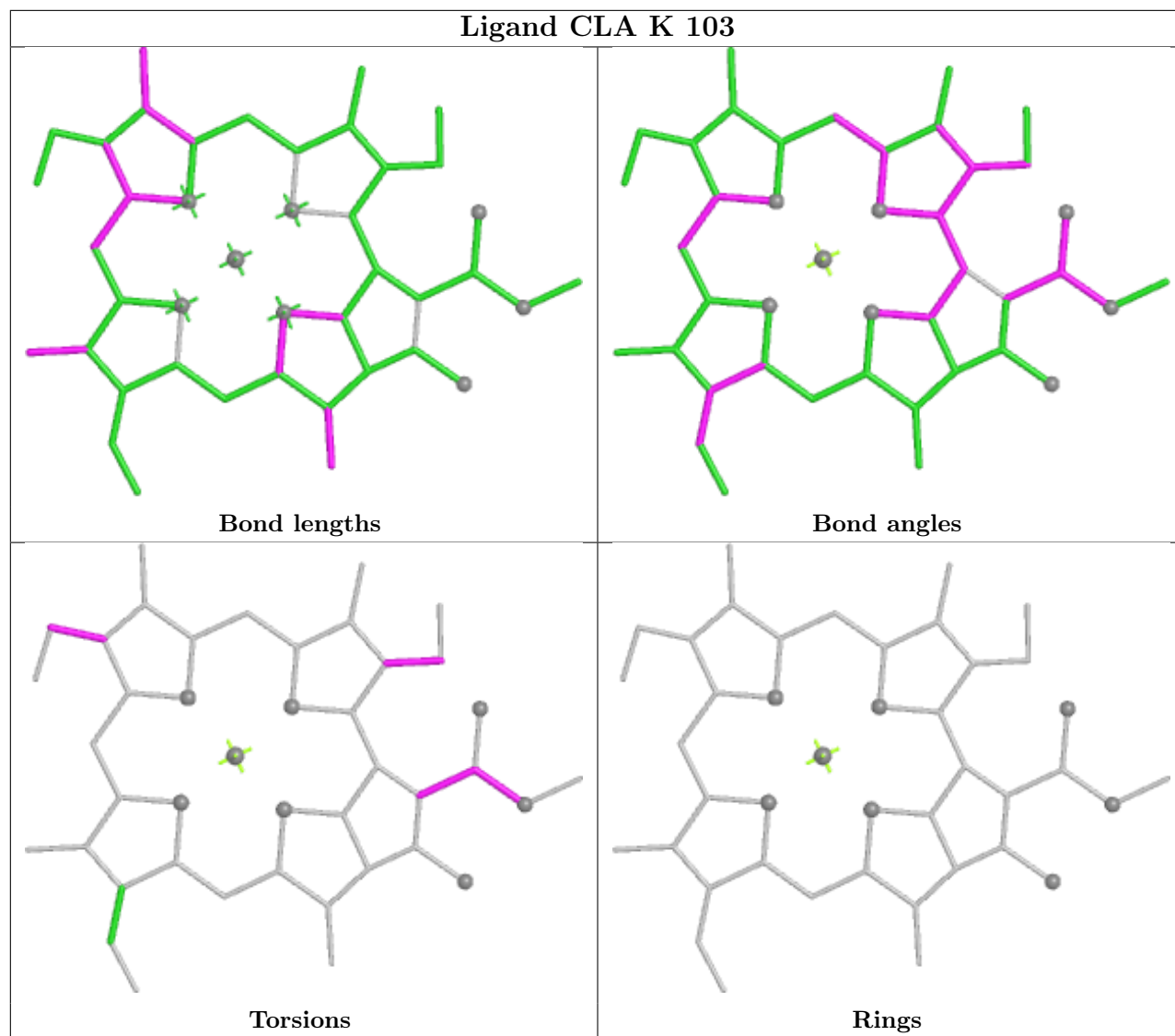
Ligand CLA c 611



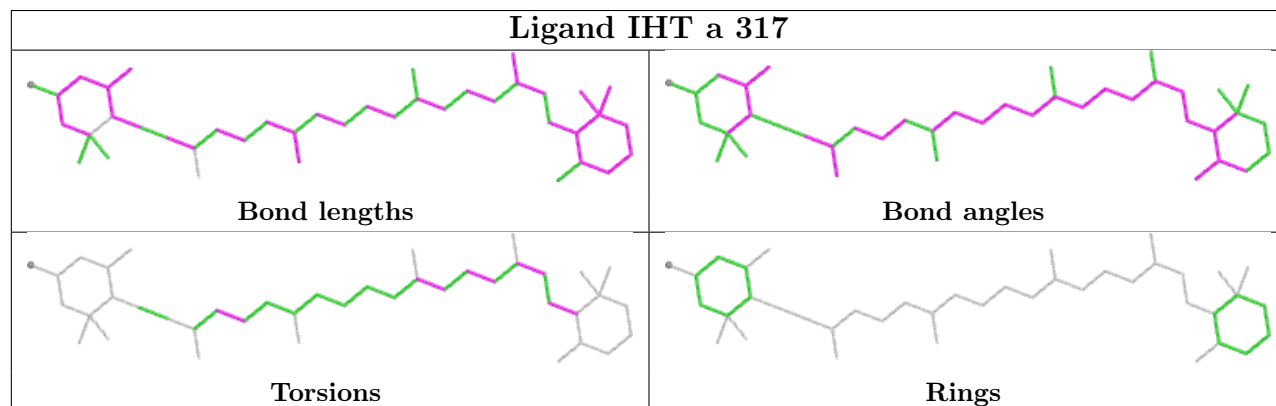
Ligand CLA b 604

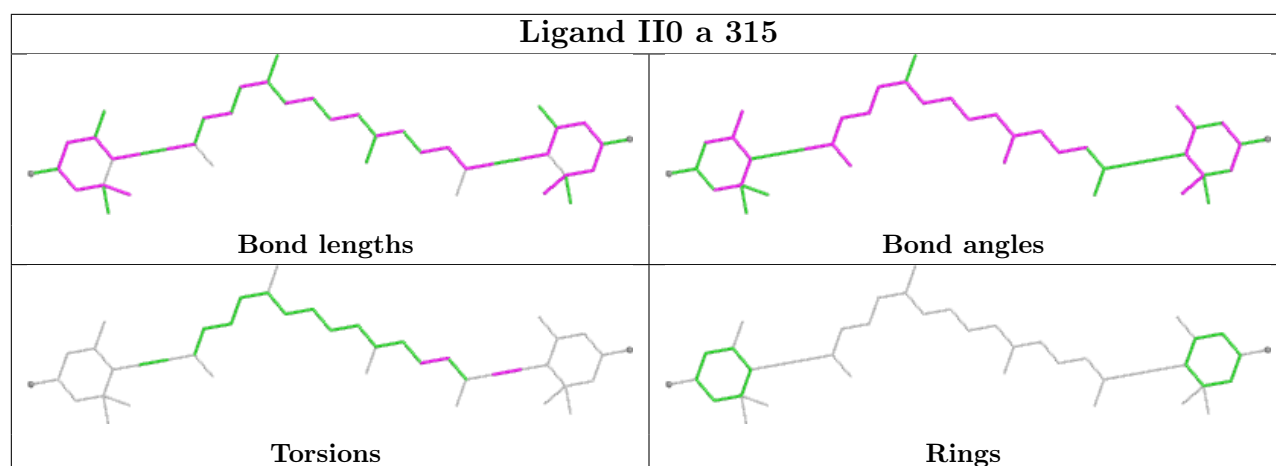
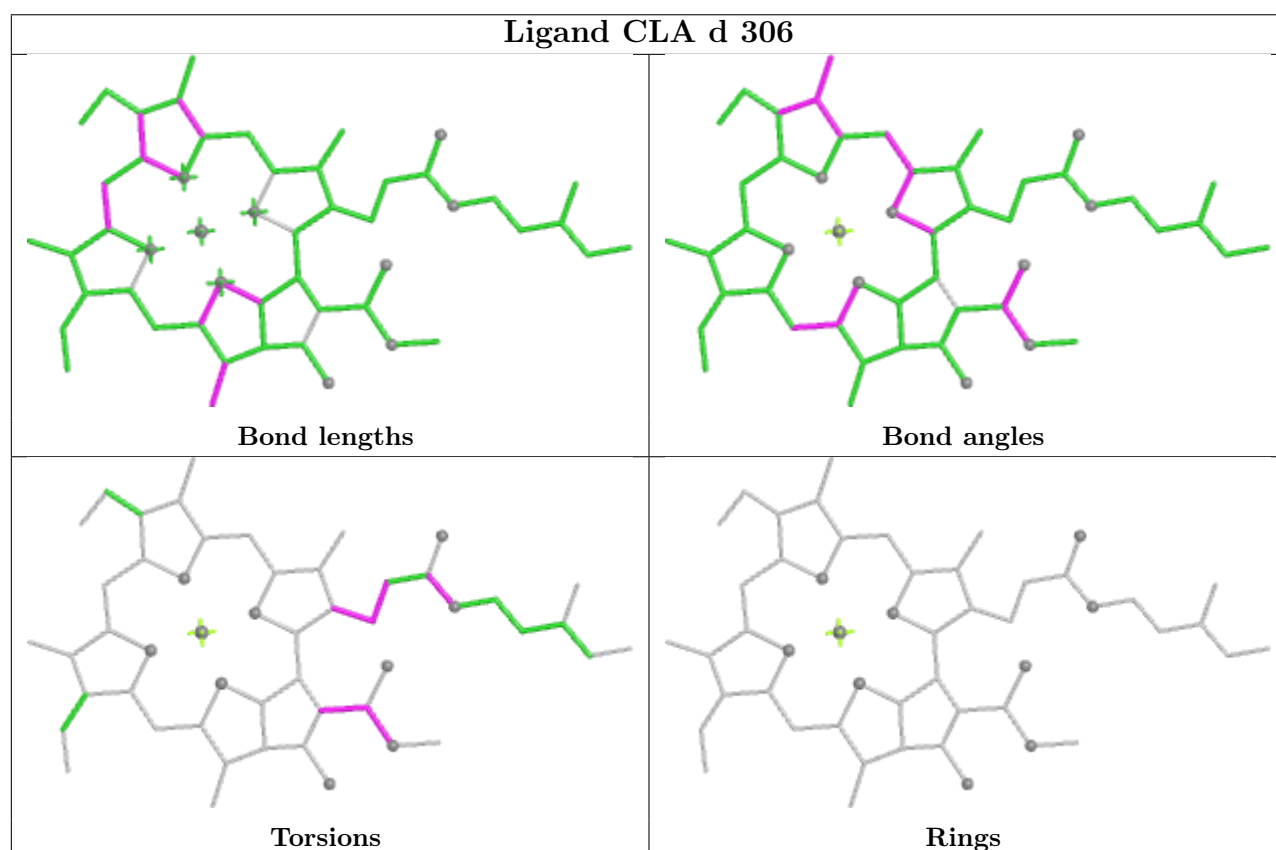


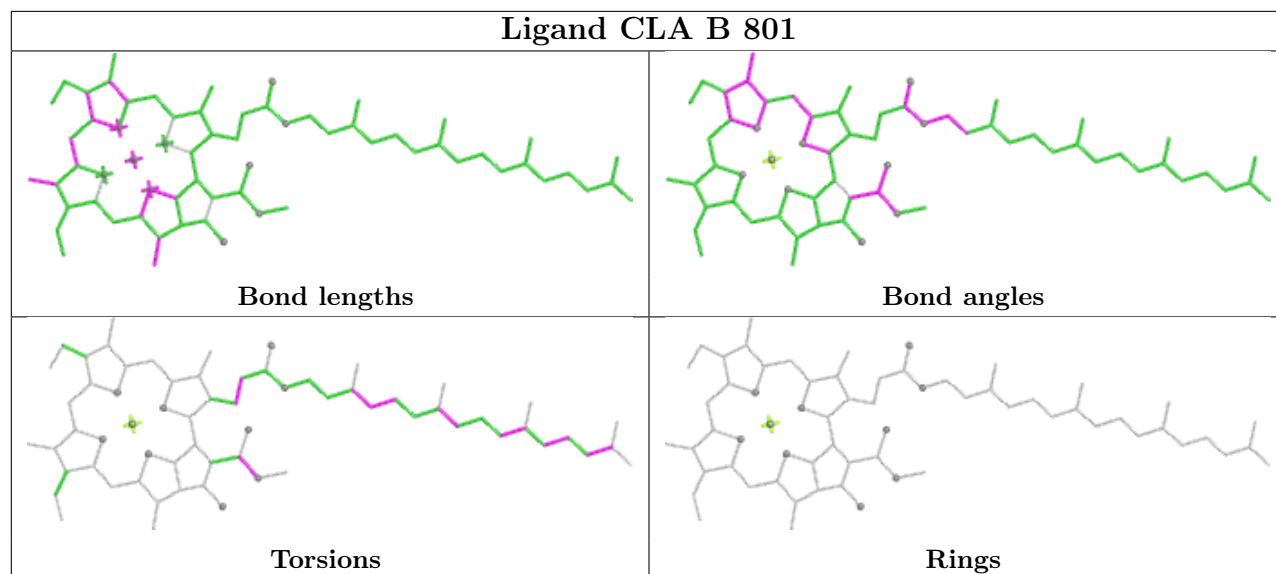
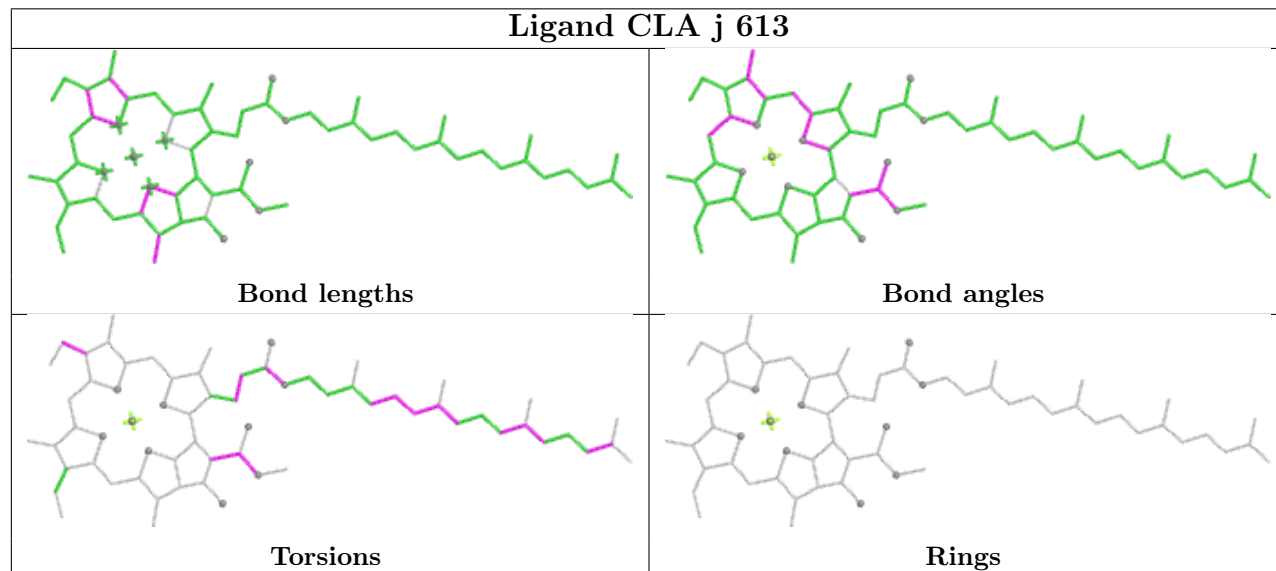
Ligand CLA K 103



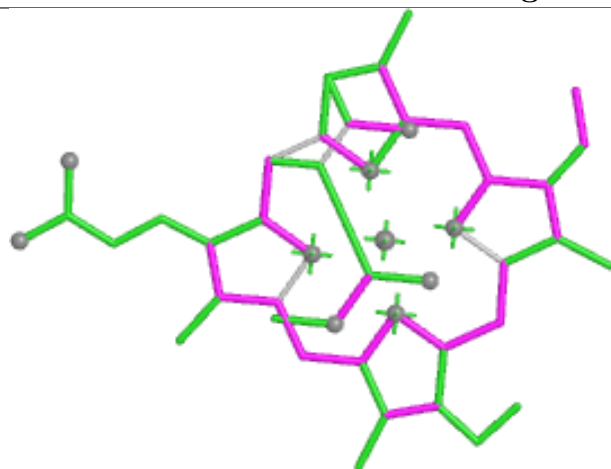
Ligand IHT a 317



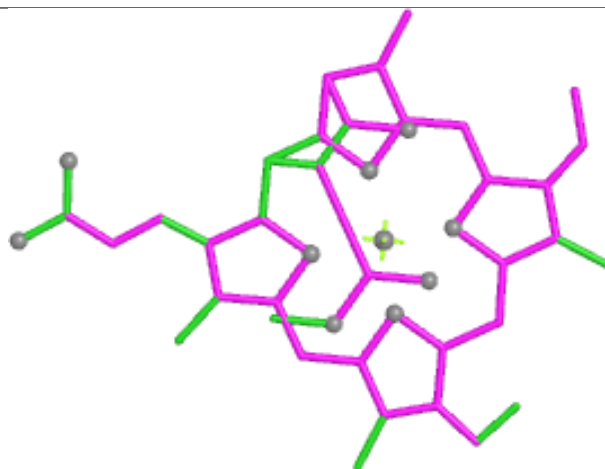


Ligand CLA B 801**Ligand CLA j 613**

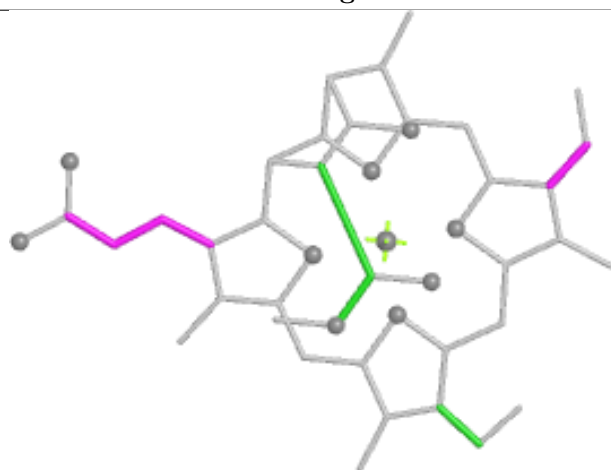
Ligand KC2 c 610



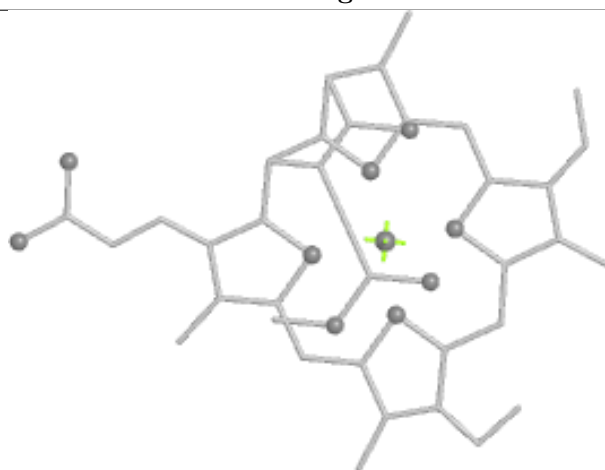
Bond lengths



Bond angles

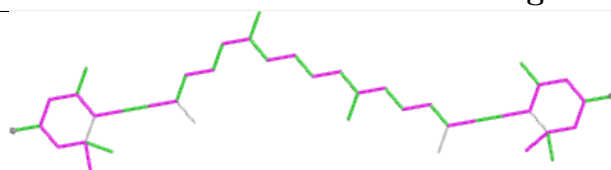


Torsions

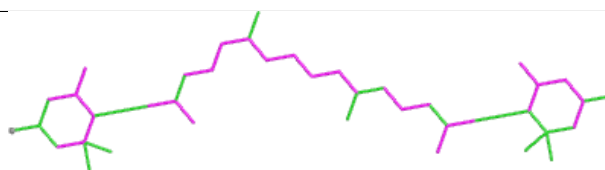


Rings

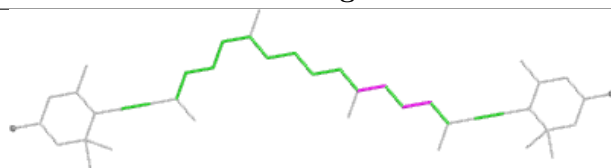
Ligand II0 m 614



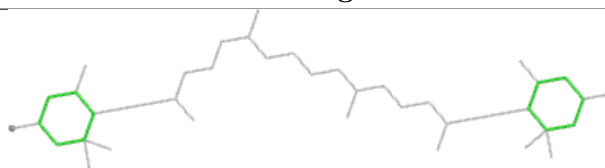
Bond lengths



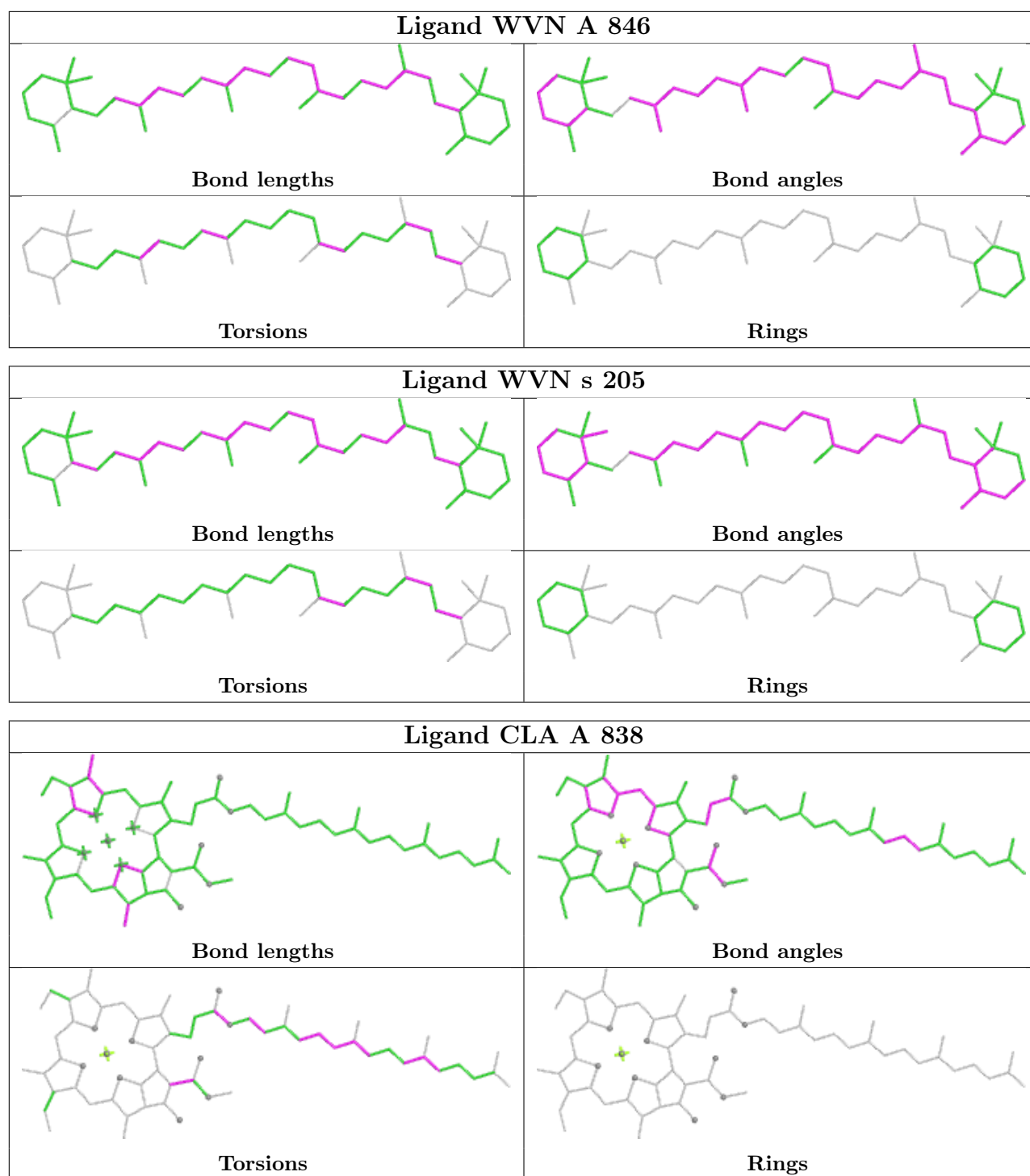
Bond angles

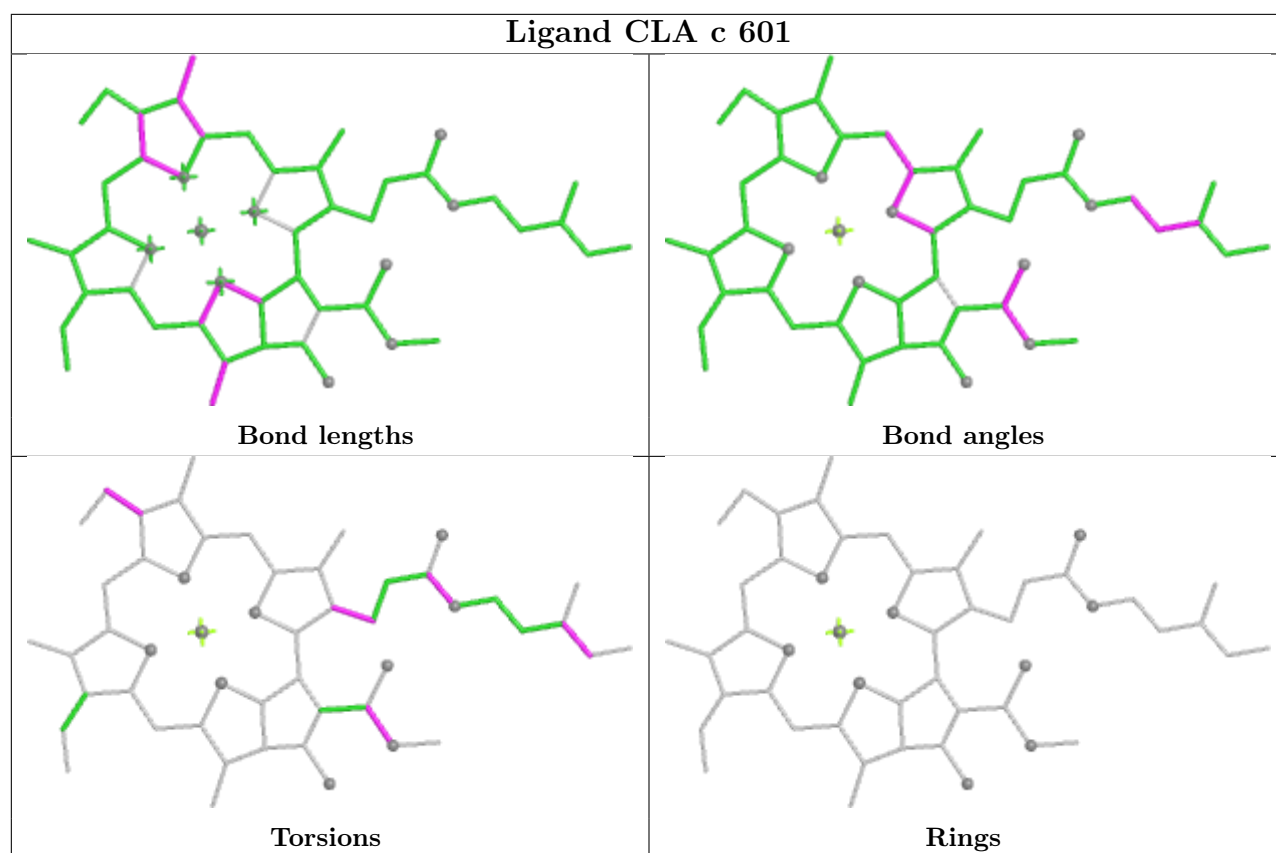
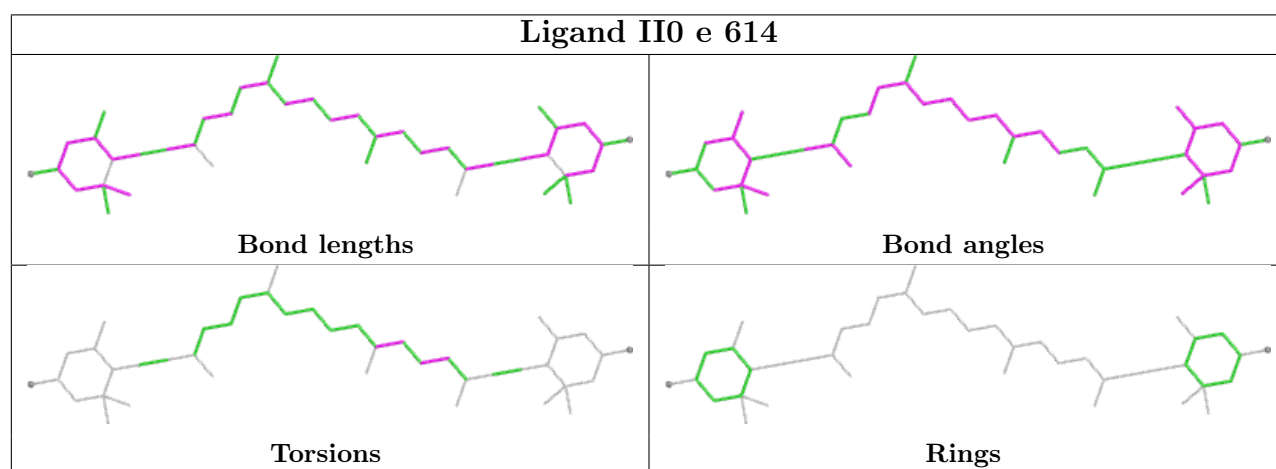


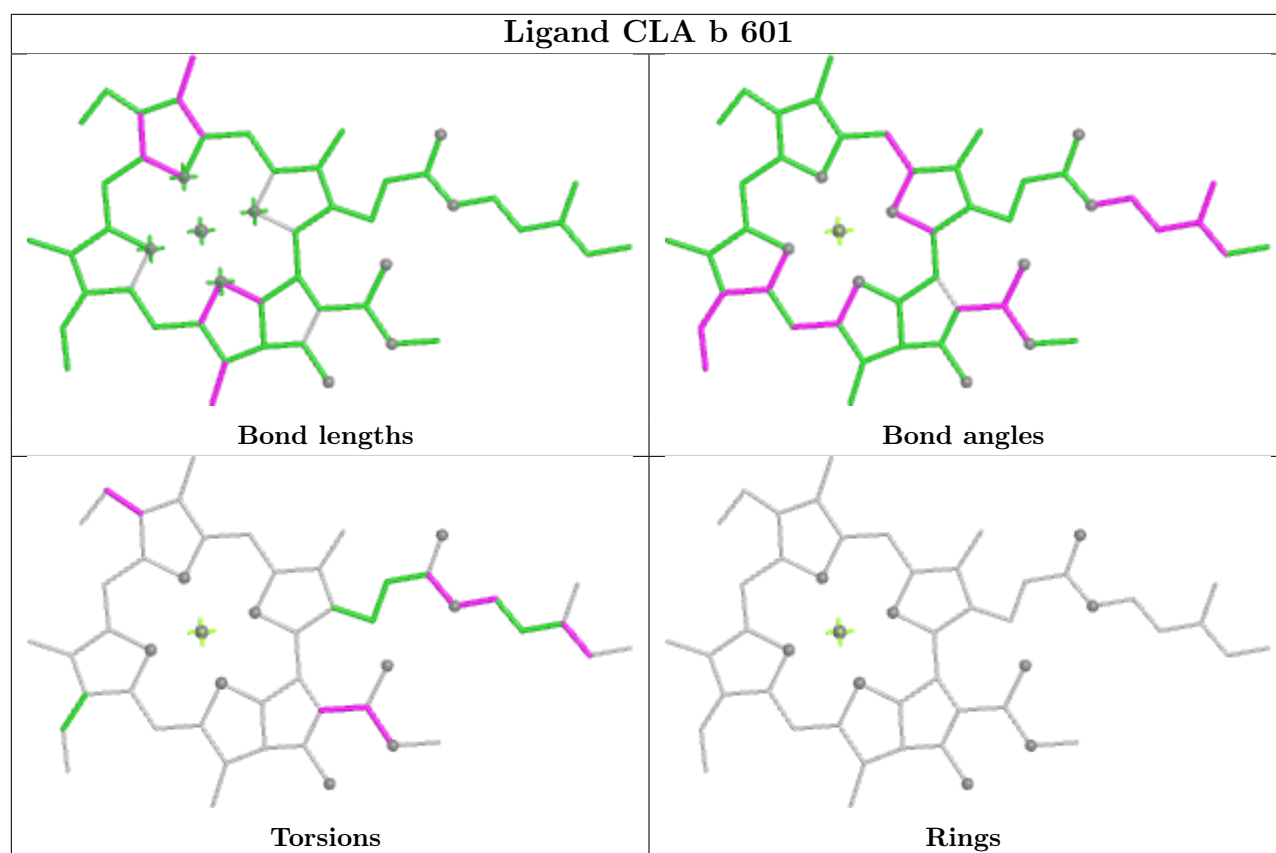
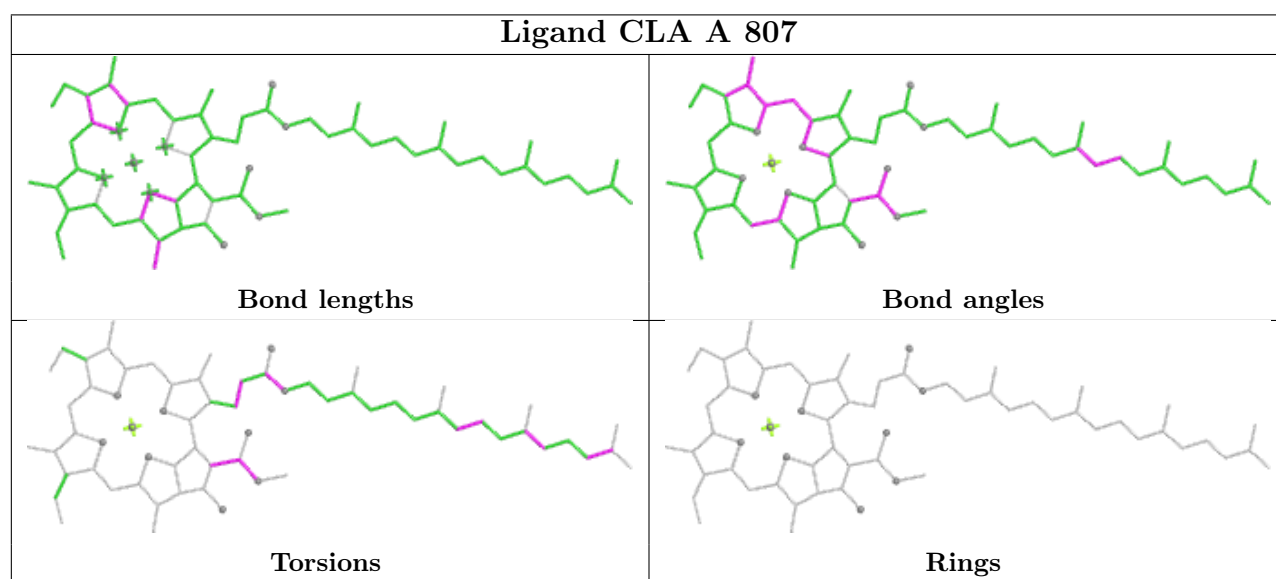
Torsions

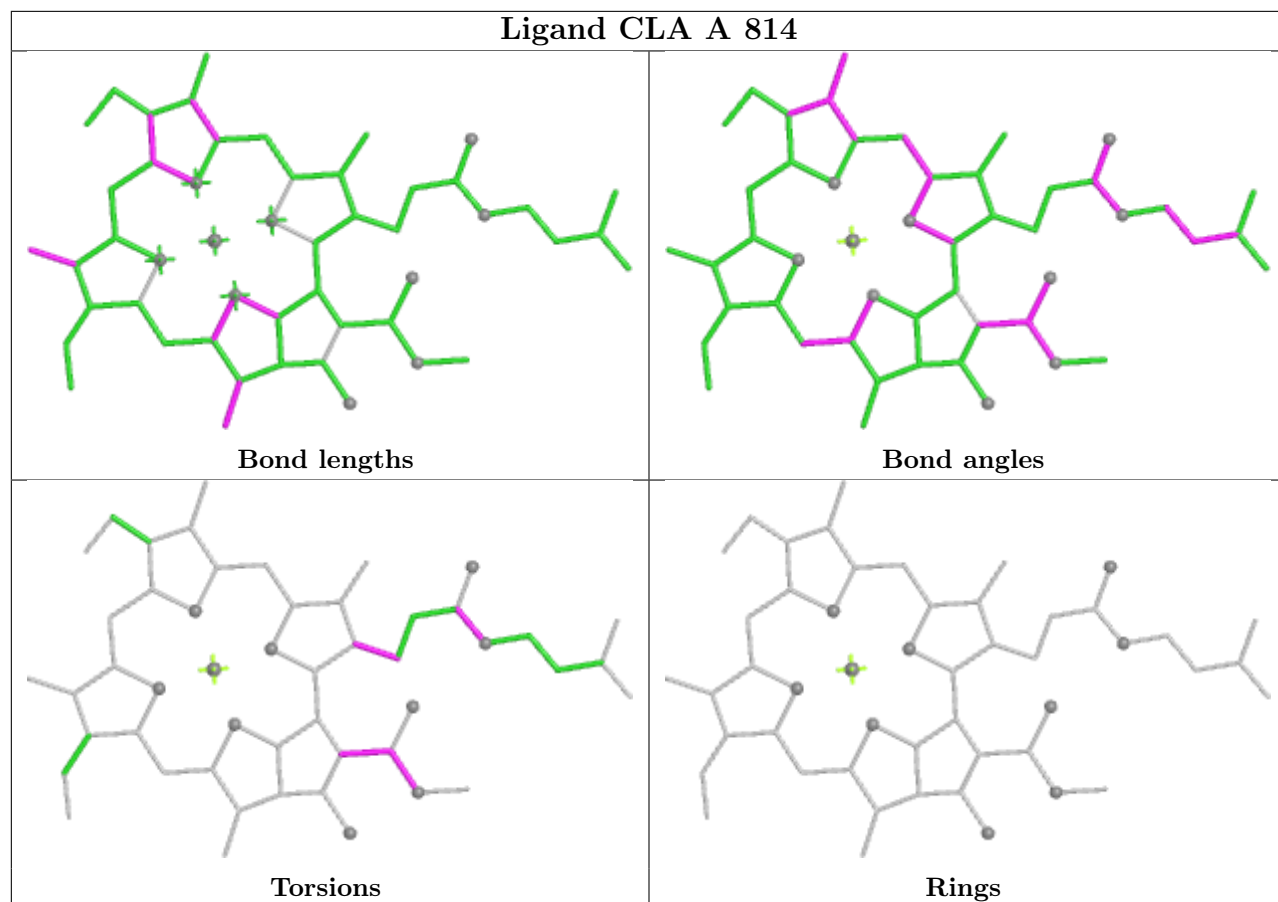


Rings

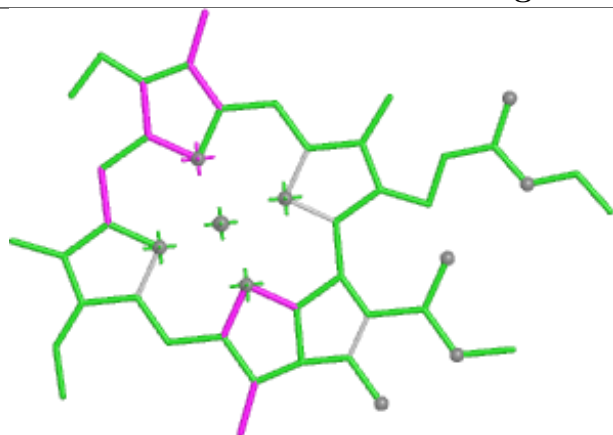




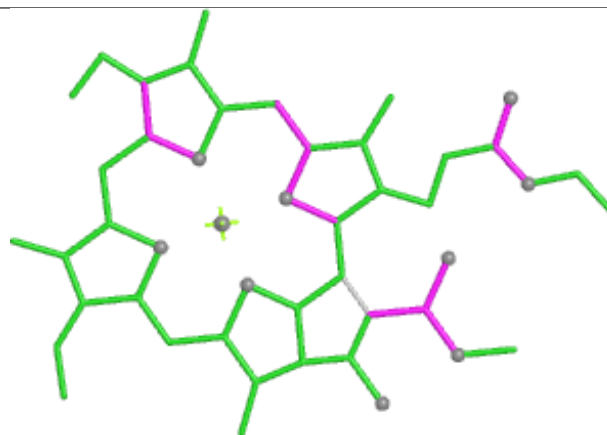




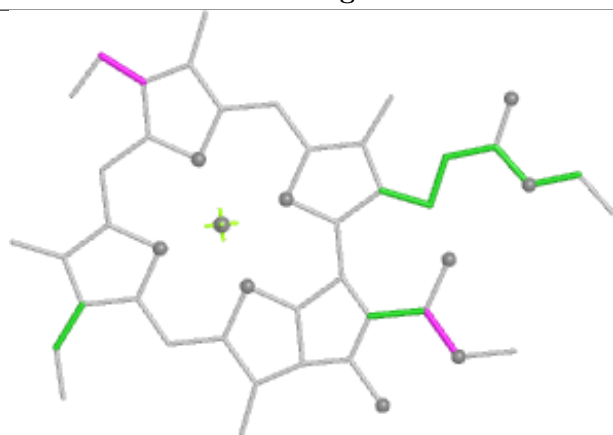
Ligand CLA B 834



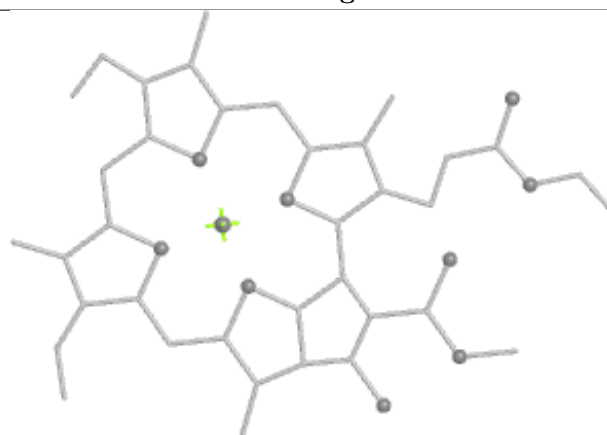
Bond lengths



Bond angles

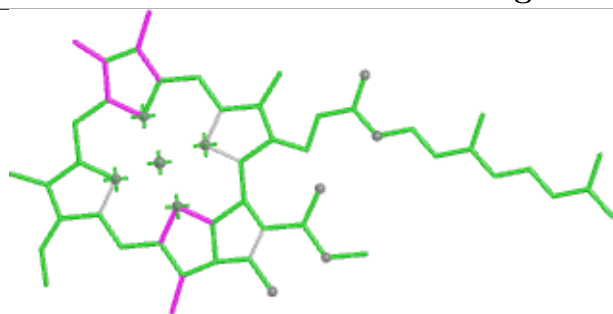


Torsions

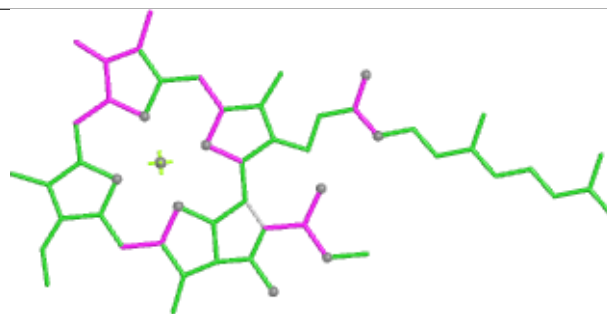


Rings

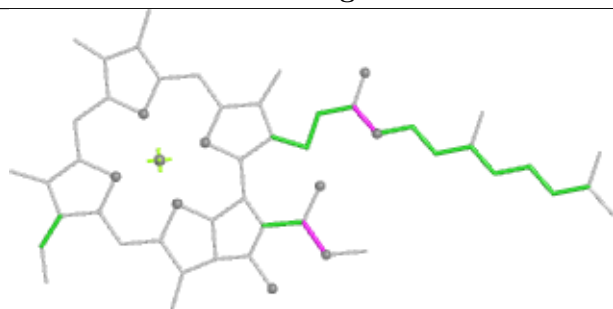
Ligand CLA B 809



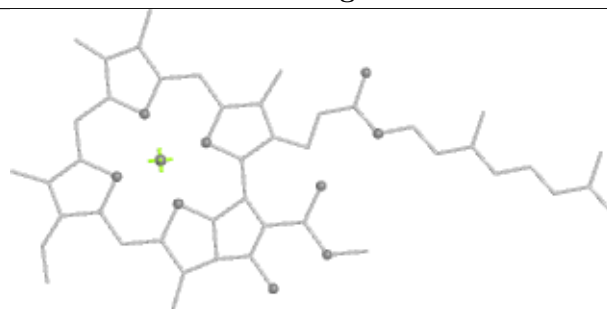
Bond lengths



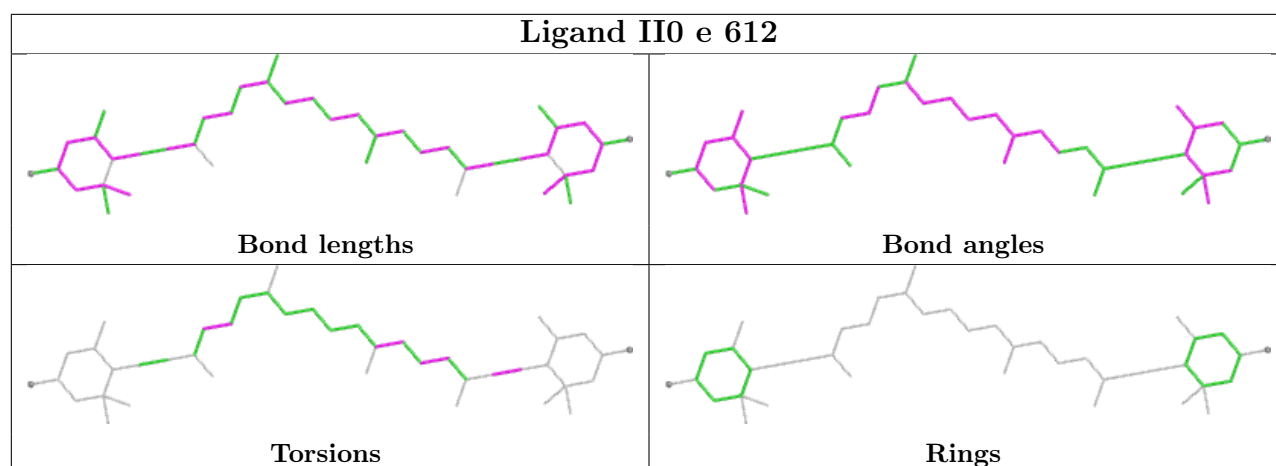
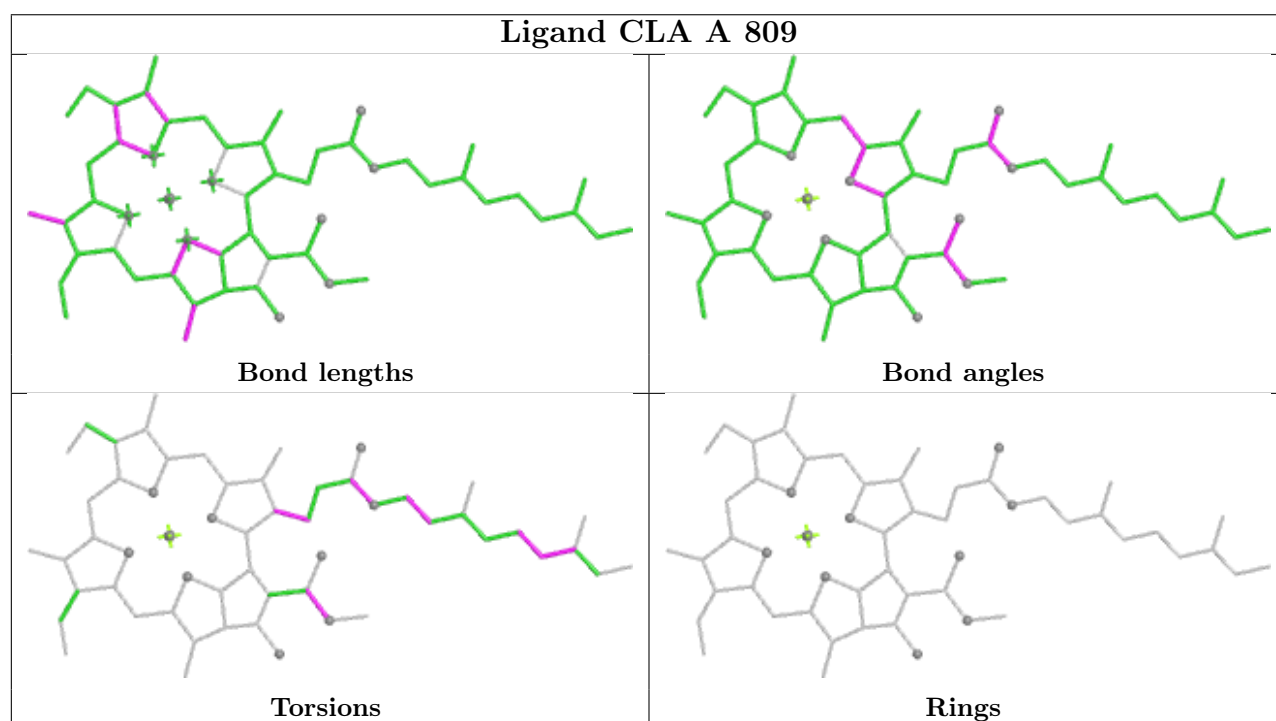
Bond angles



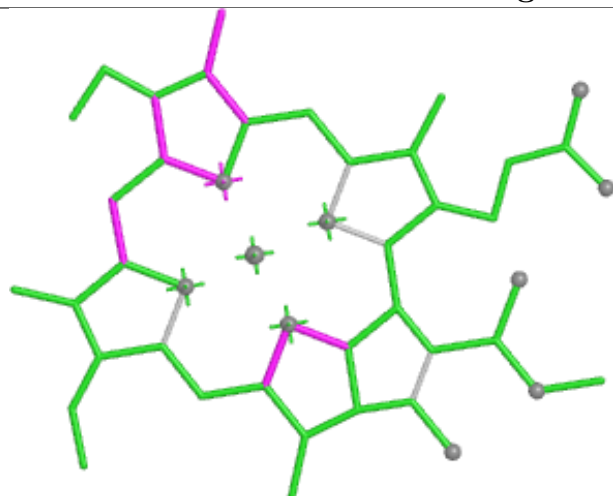
Torsions



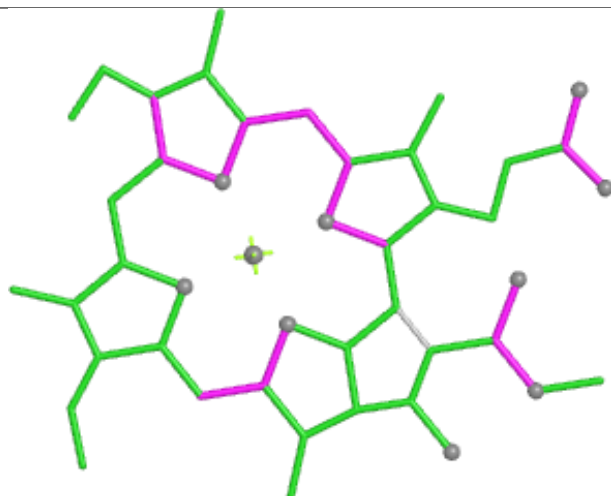
Rings



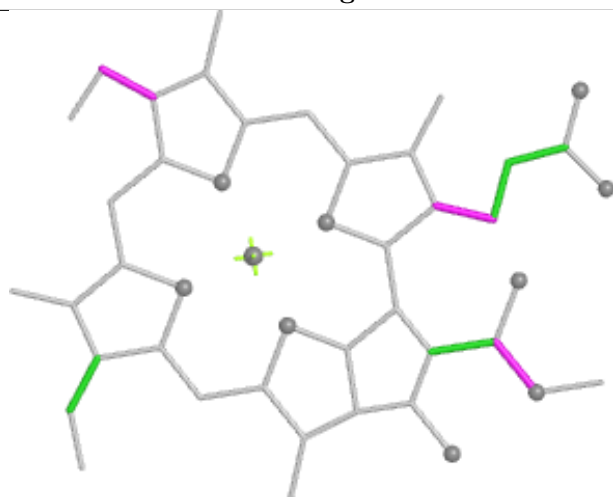
Ligand CLA n 601



Bond lengths



Bond angles

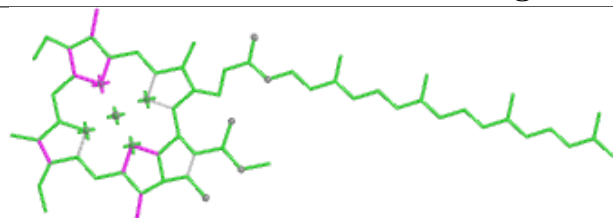


Torsions

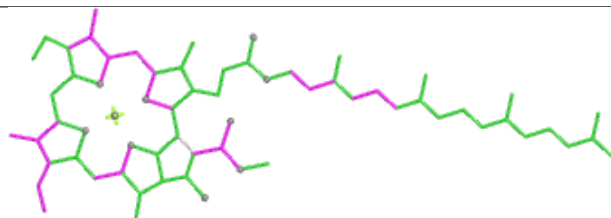


Rings

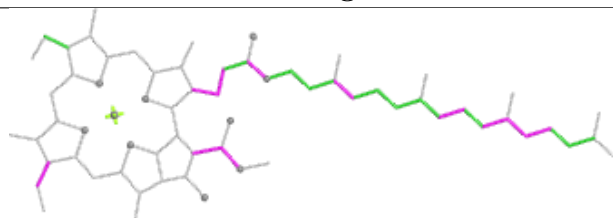
Ligand CLA A 818



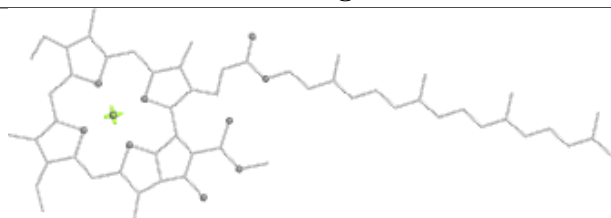
Bond lengths



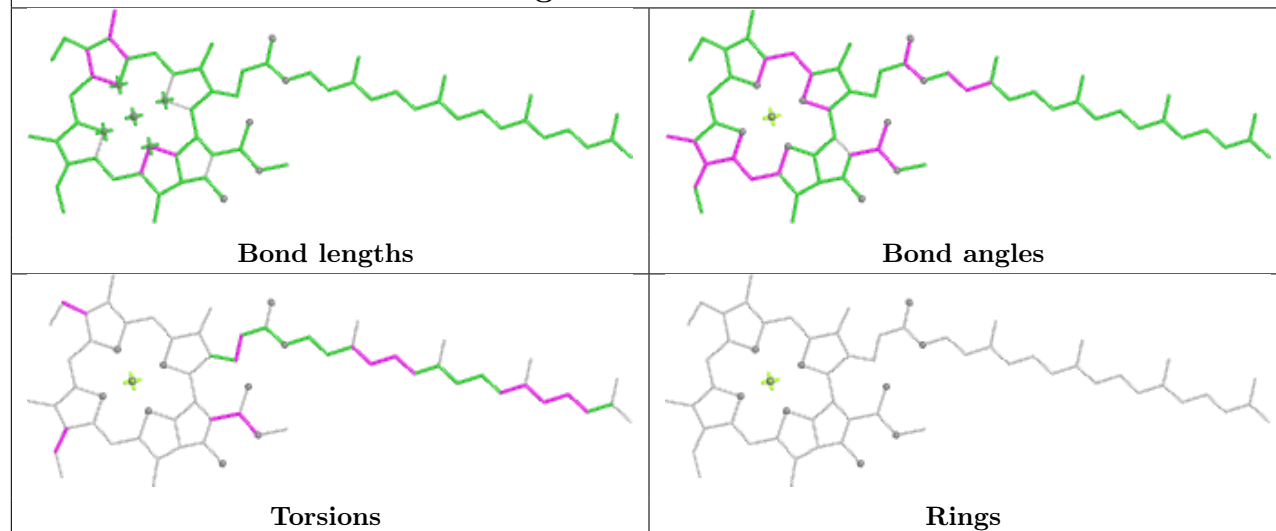
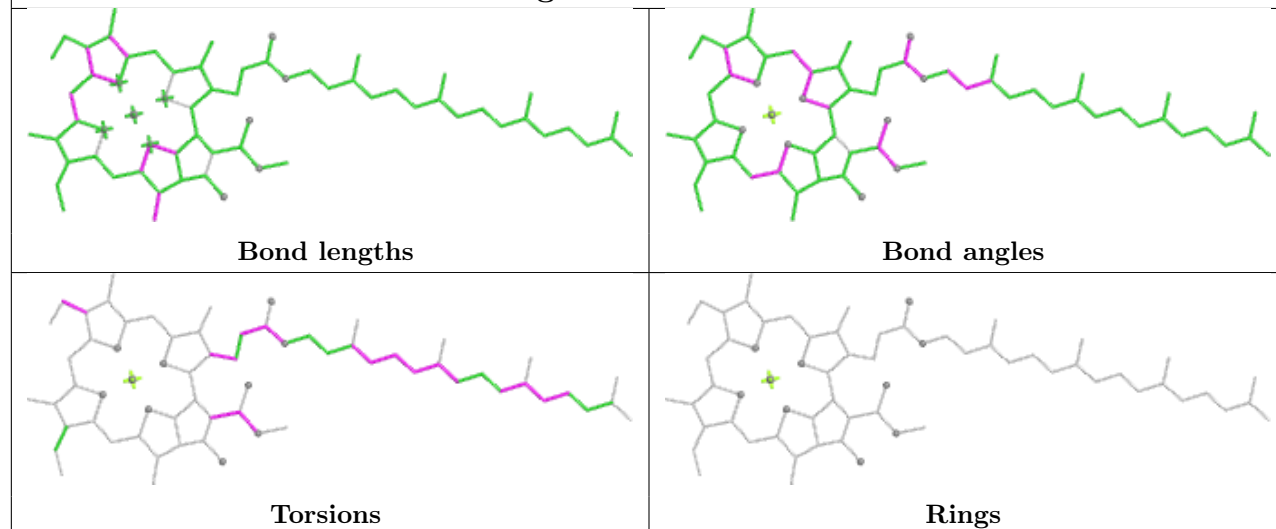
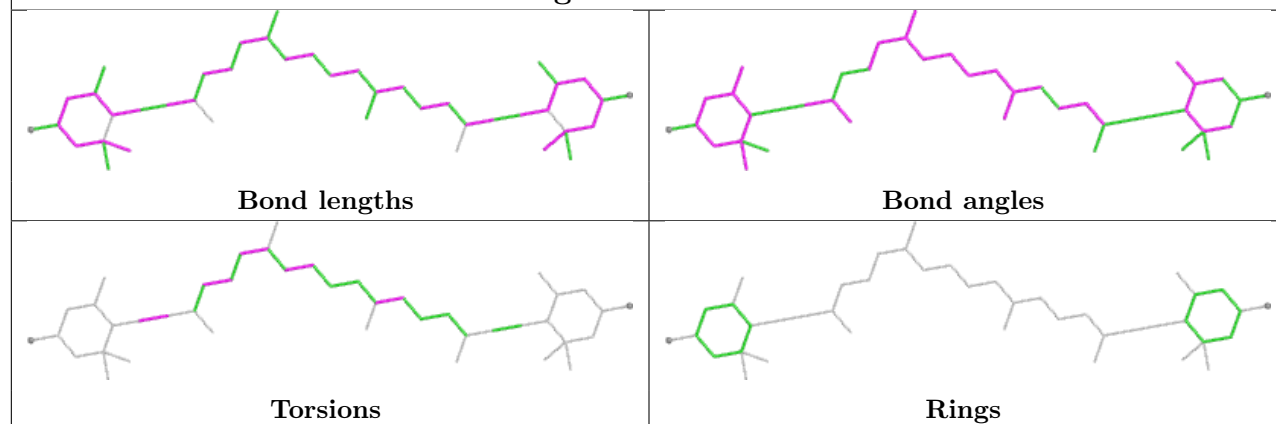
Bond angles



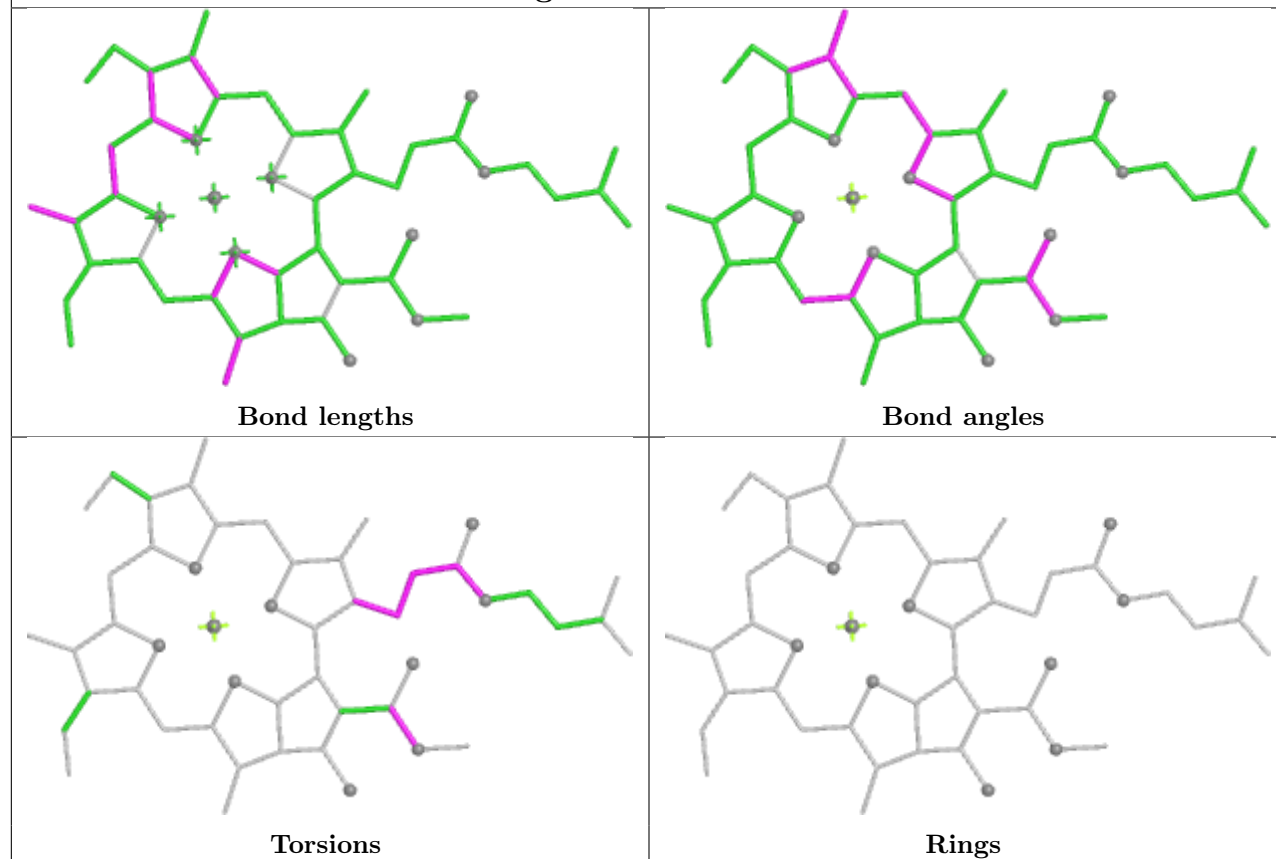
Torsions



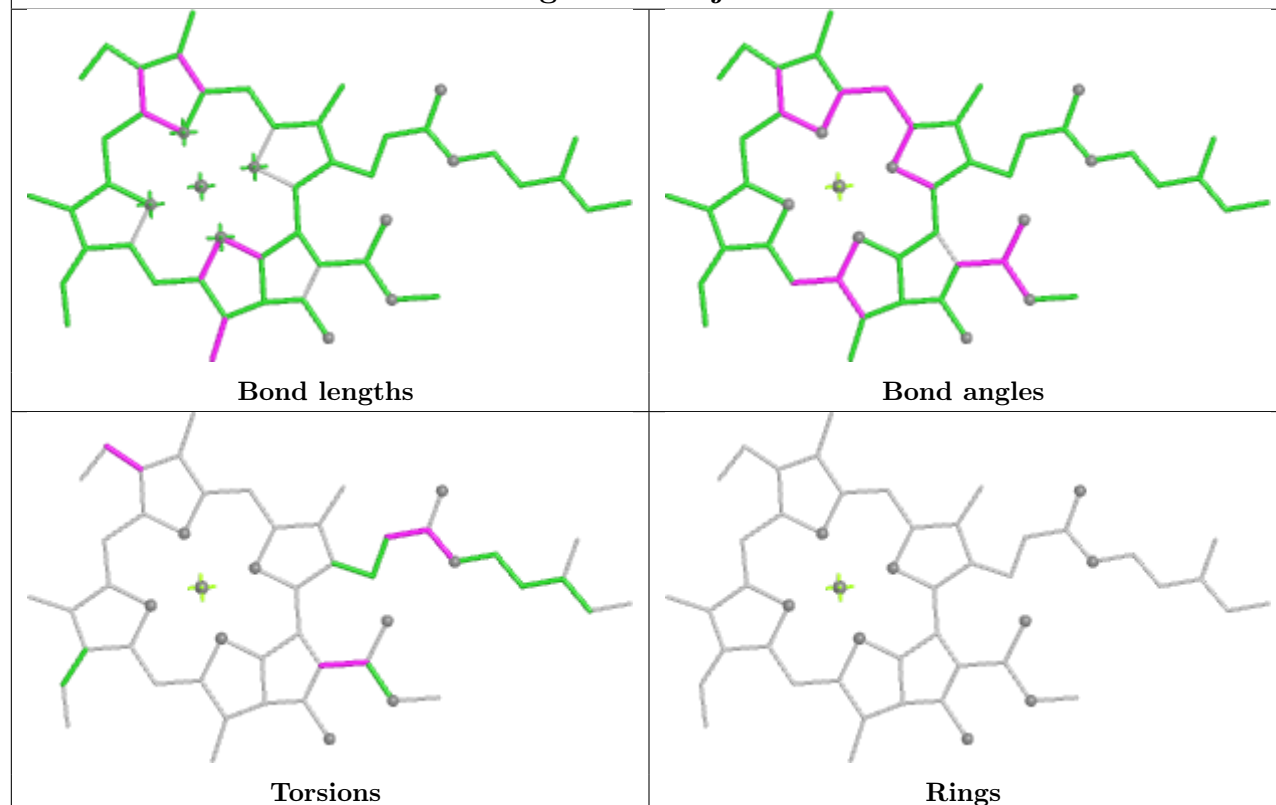
Rings

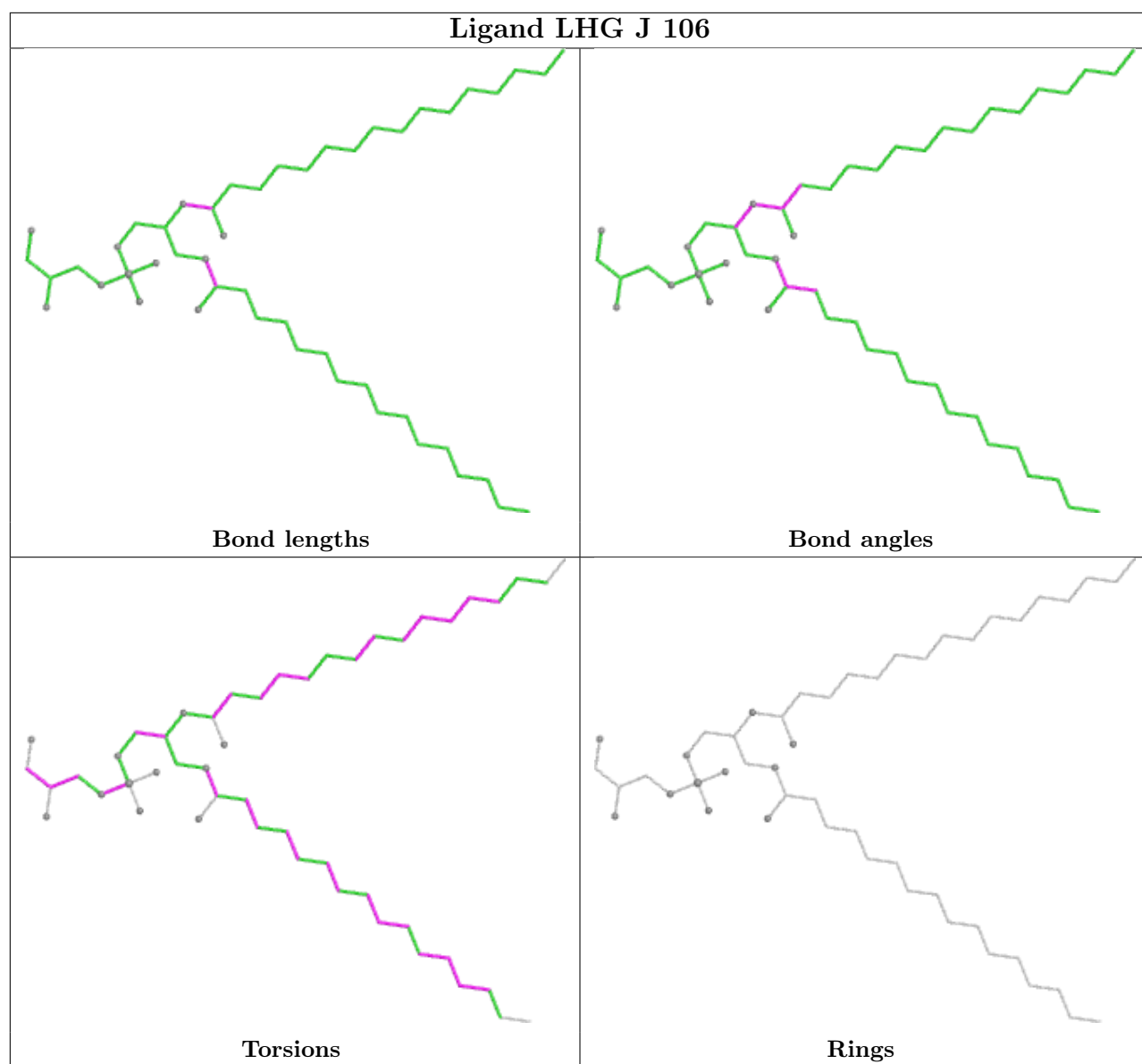
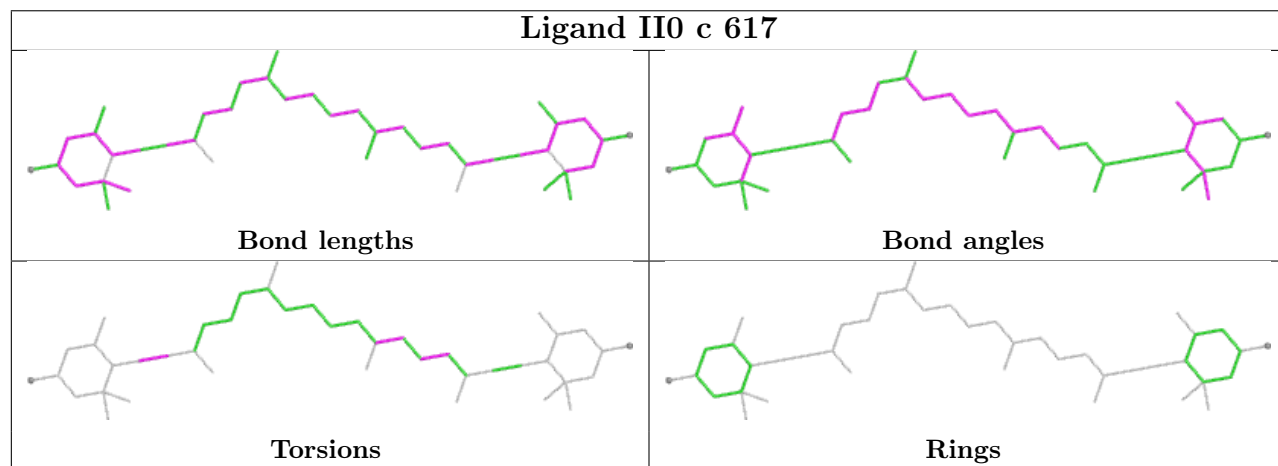
Ligand CLA b 607**Ligand CLA e 611****Ligand II0 f 618**

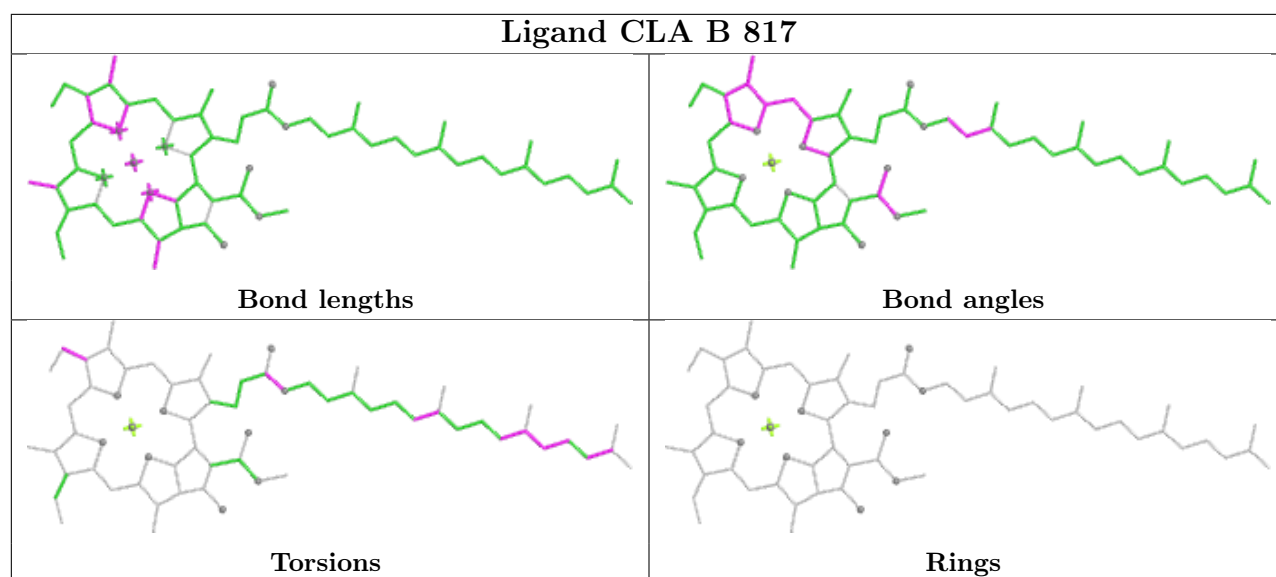
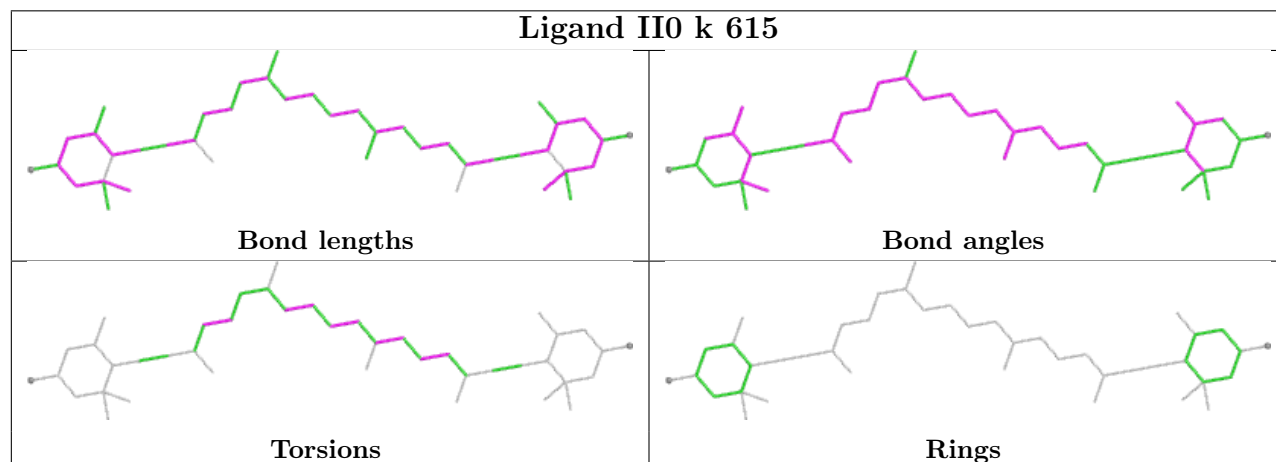
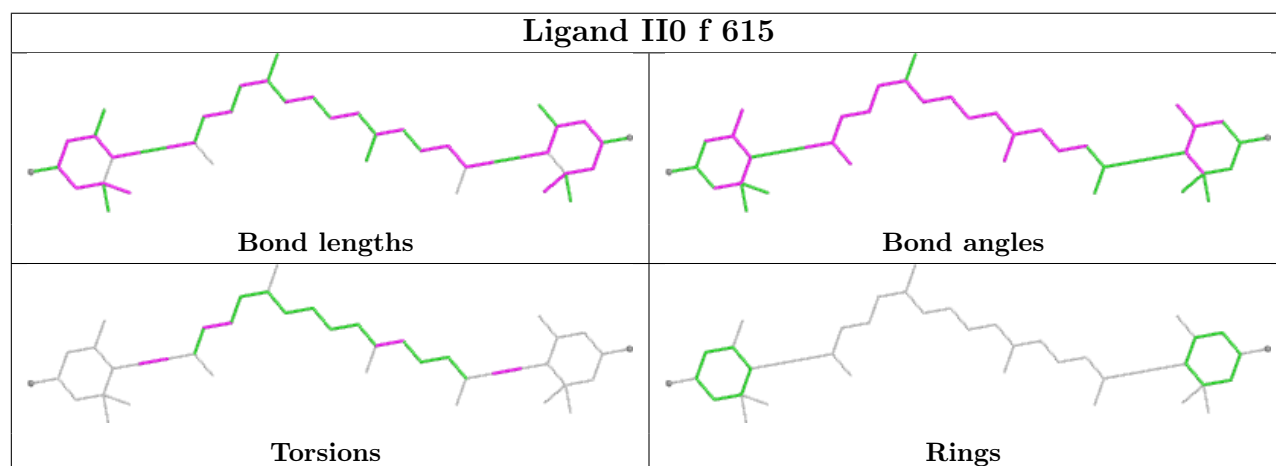
Ligand CLA h 302



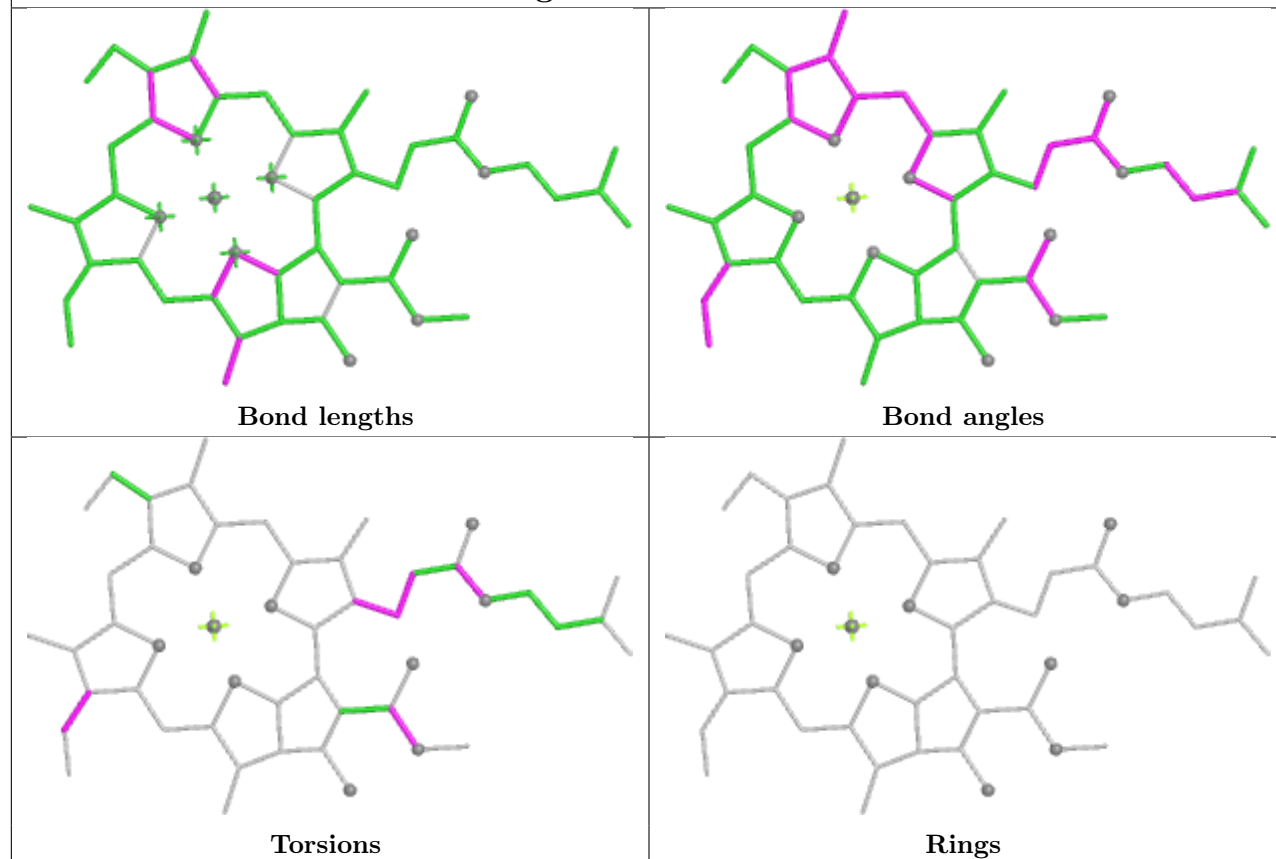
Ligand CLA j 607



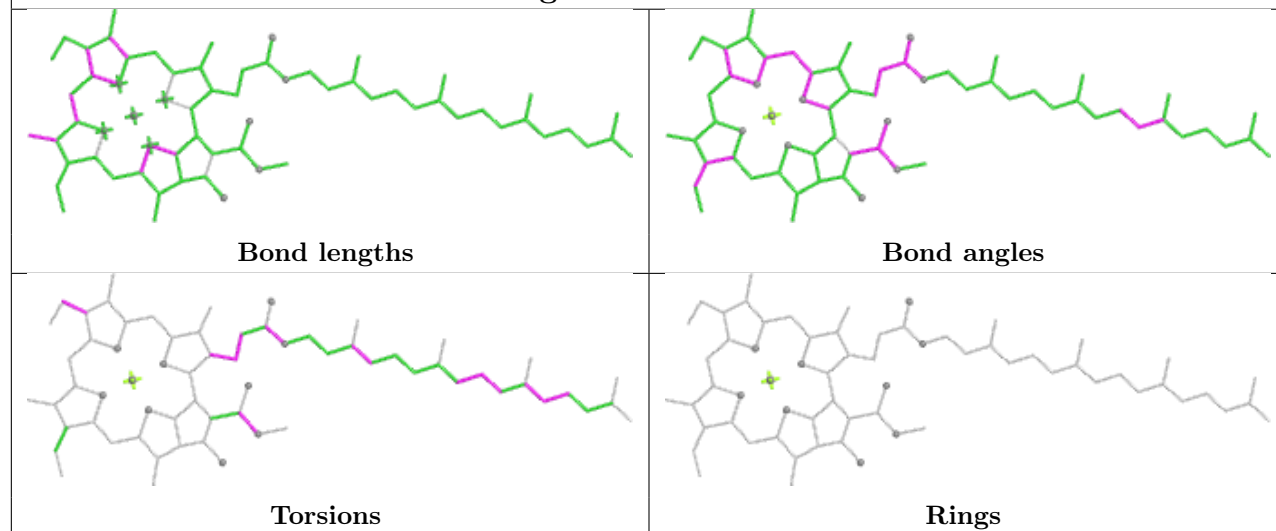


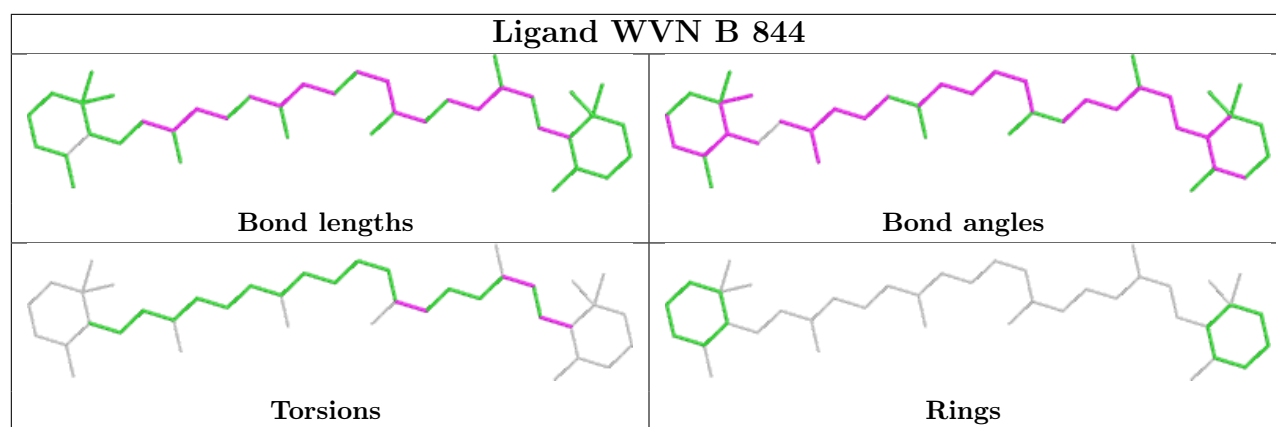
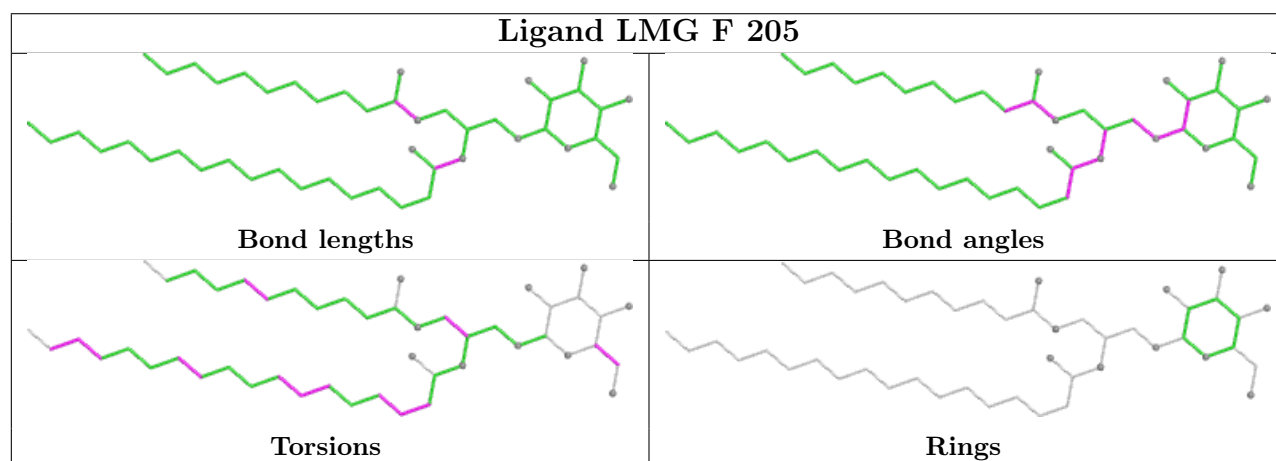
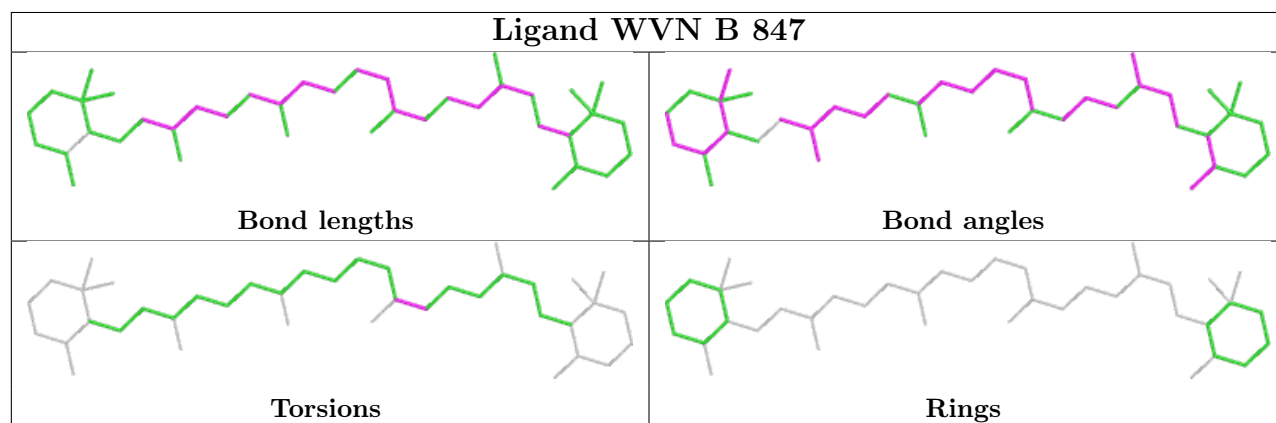


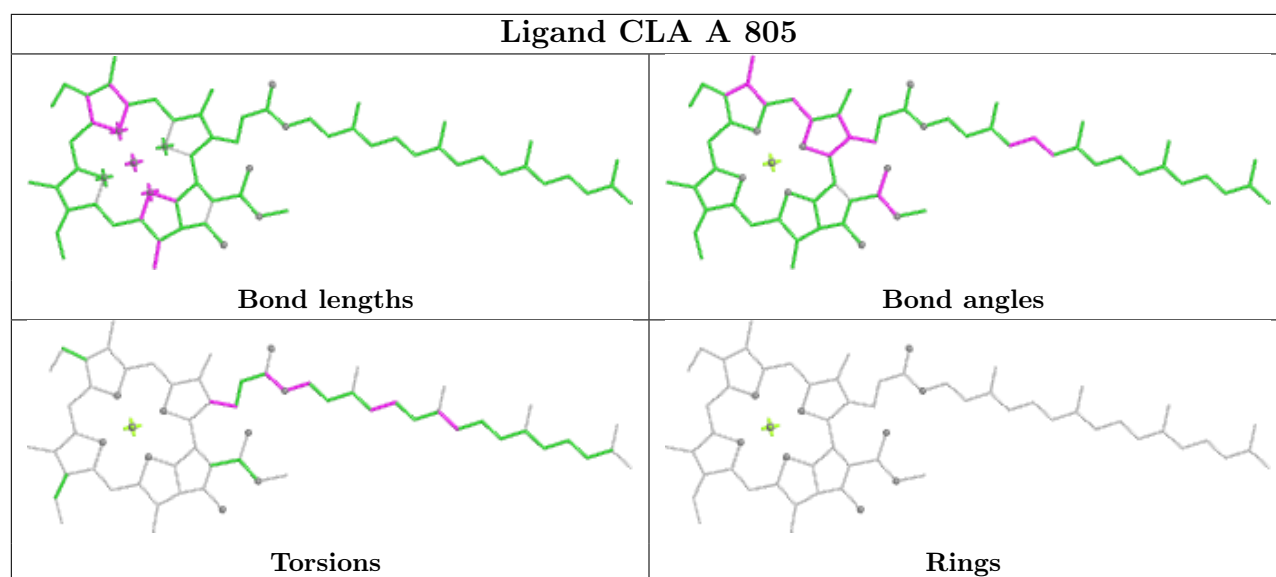
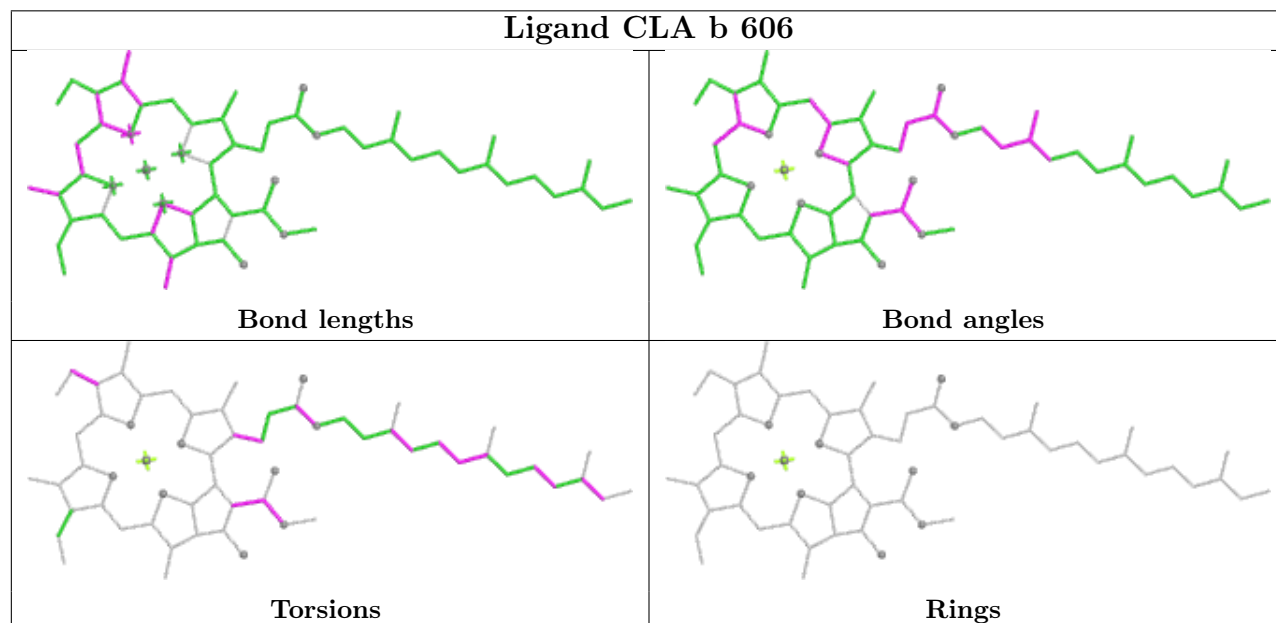
Ligand CLA k 602



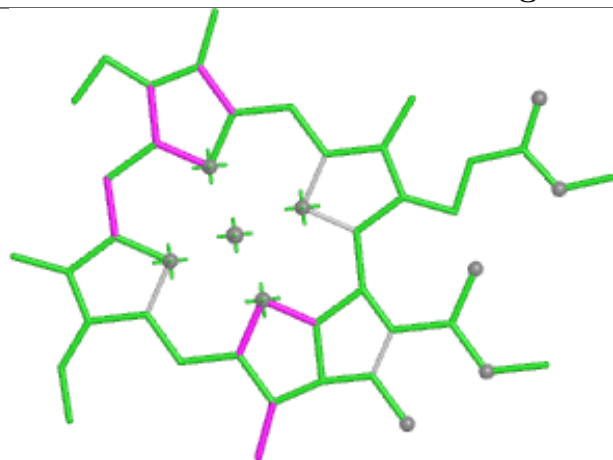
Ligand CLA f 602



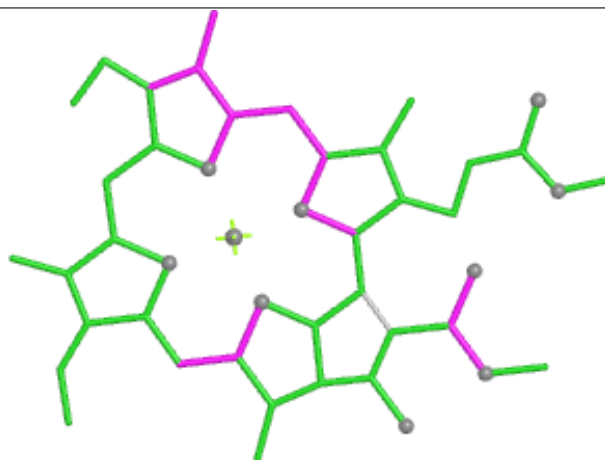




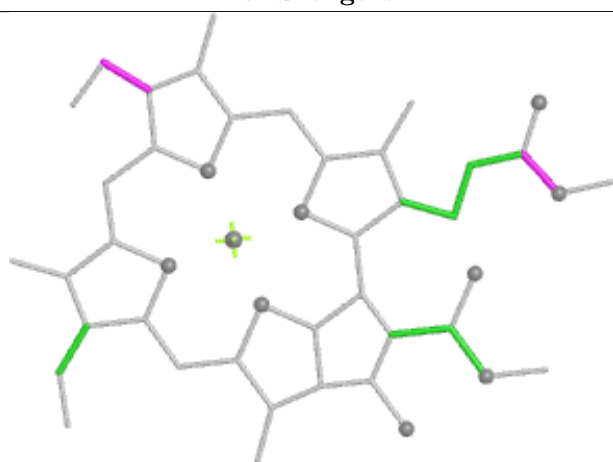
Ligand CLA c 607



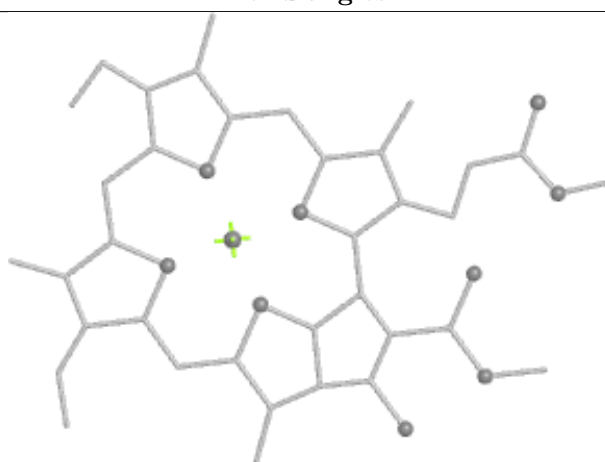
Bond lengths



Bond angles

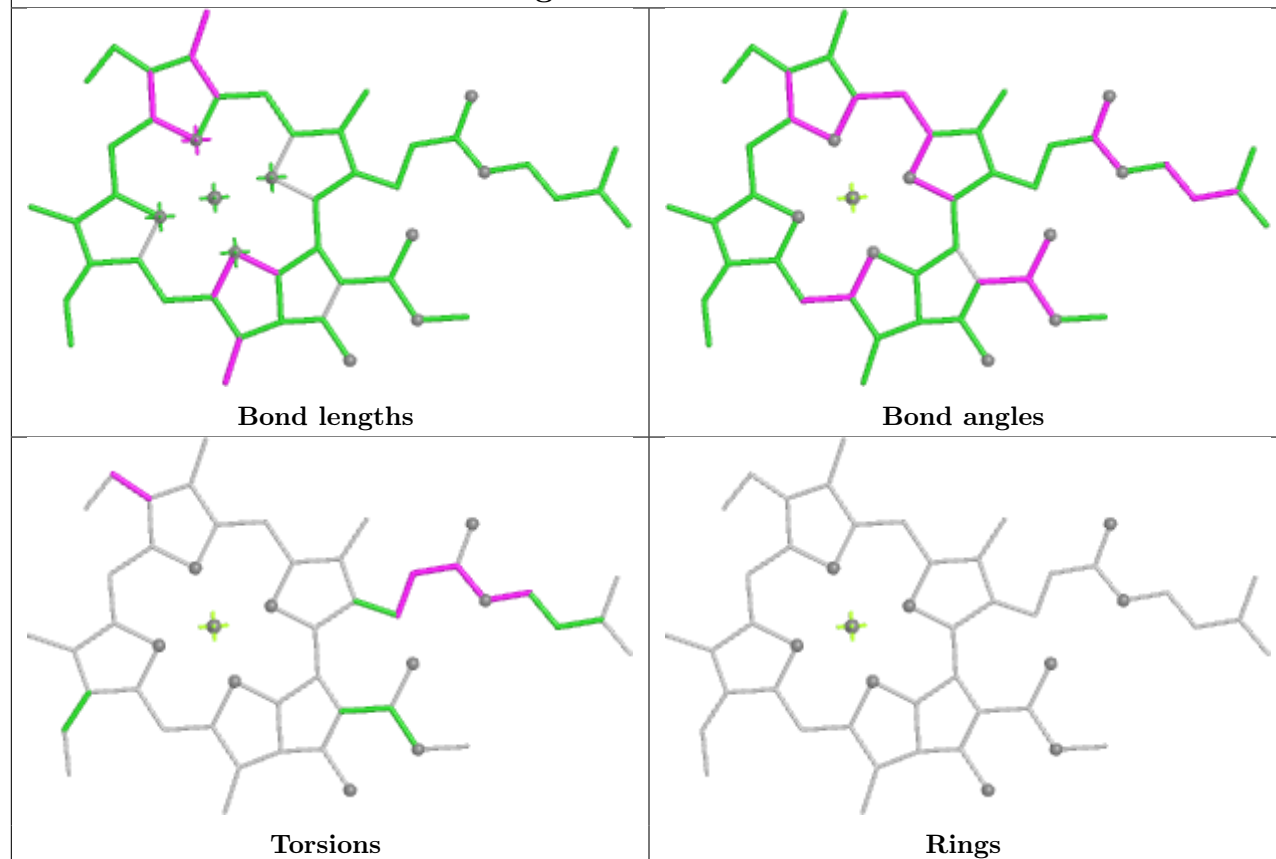


Torsions

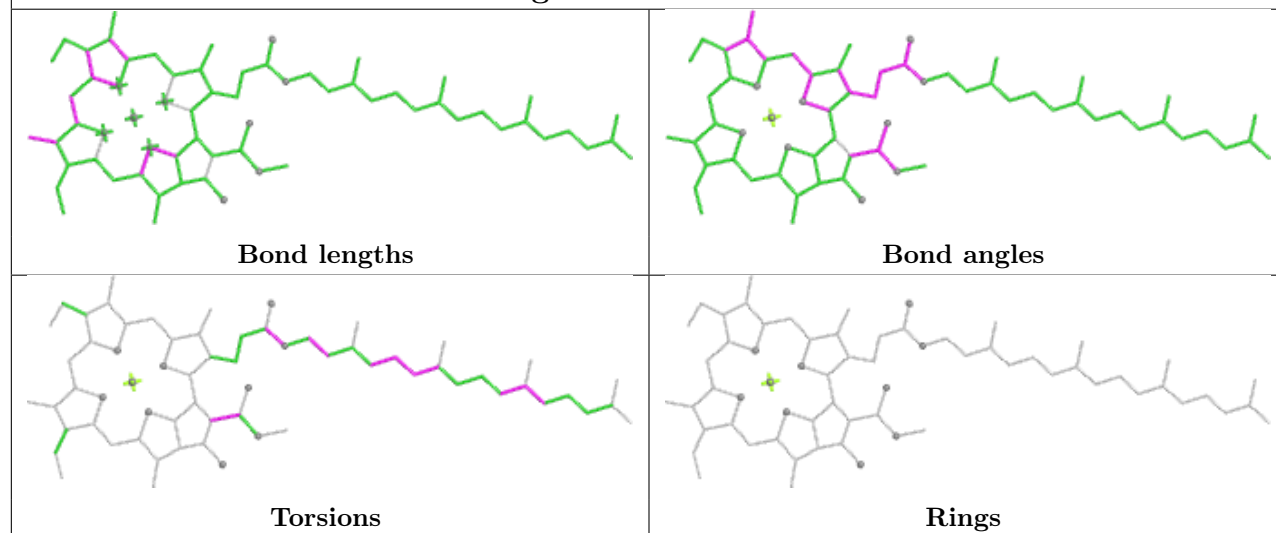


Rings

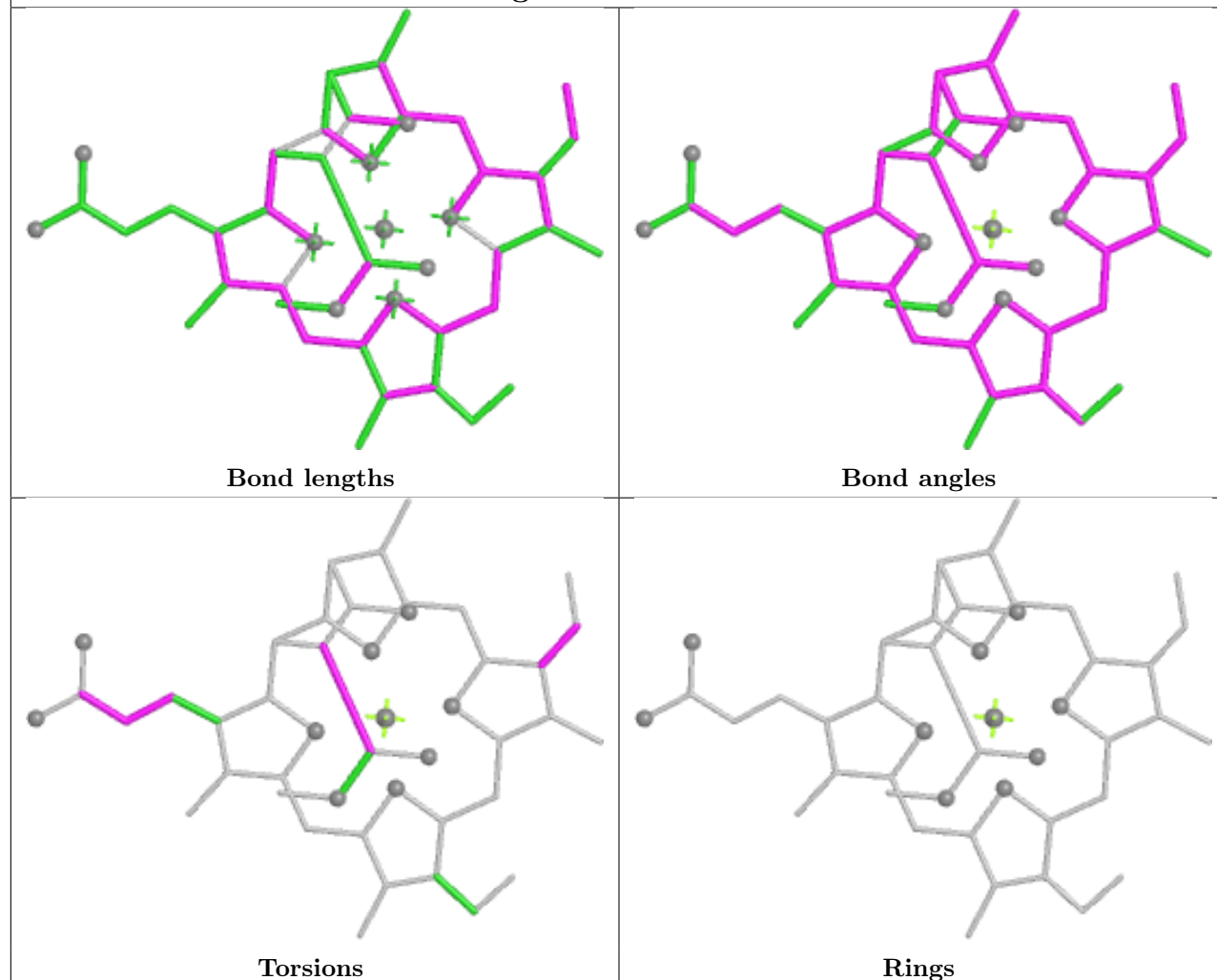
Ligand CLA h 303



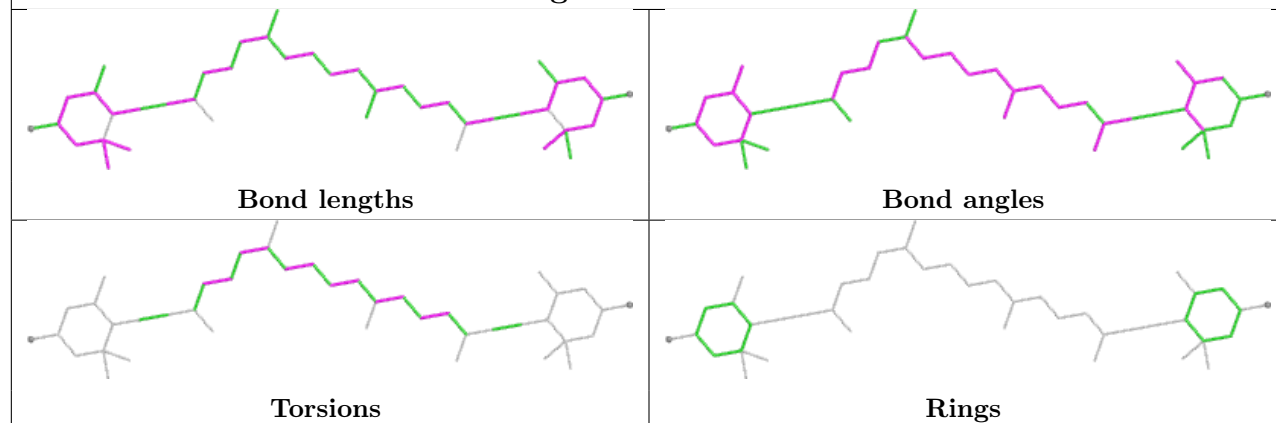
Ligand CLA A 826

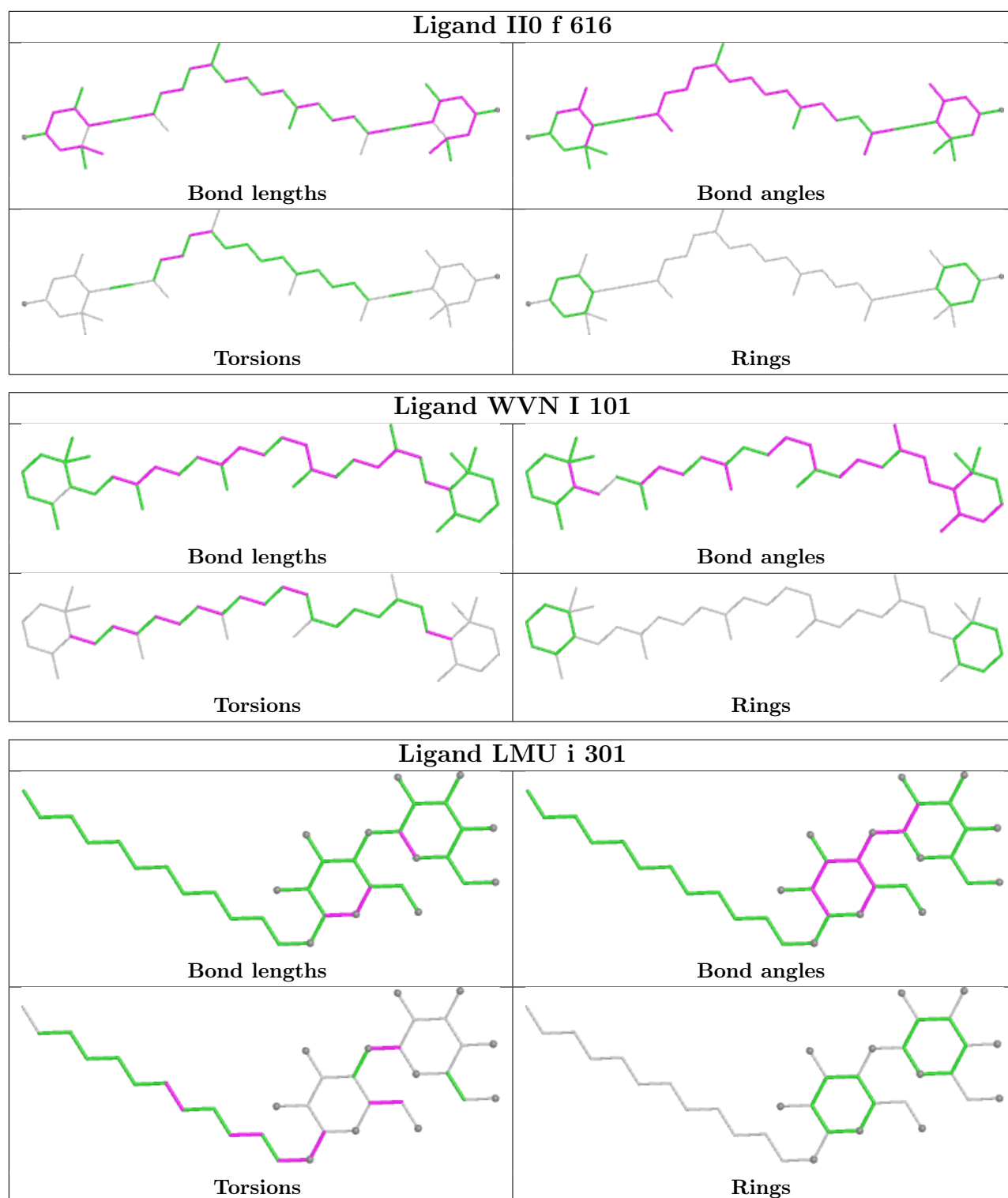


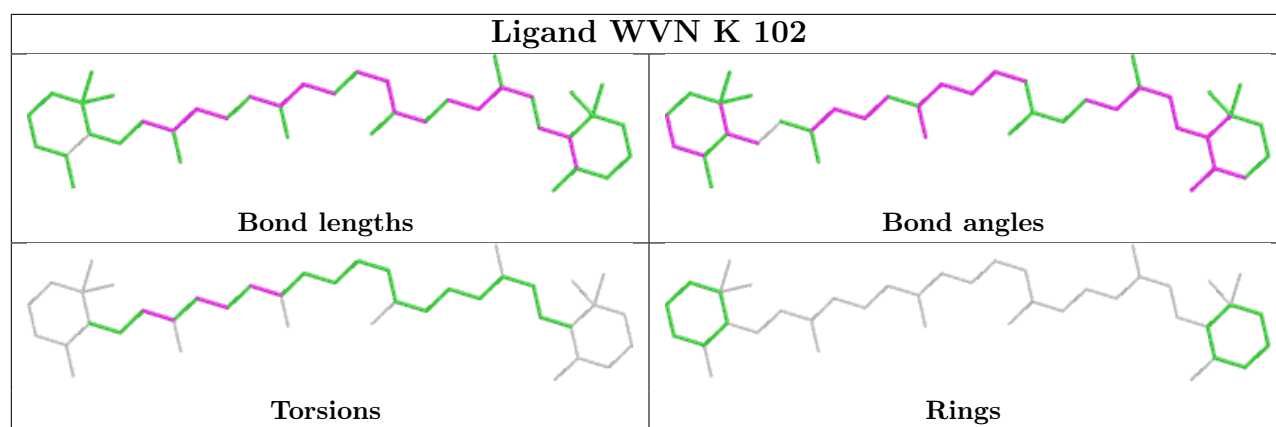
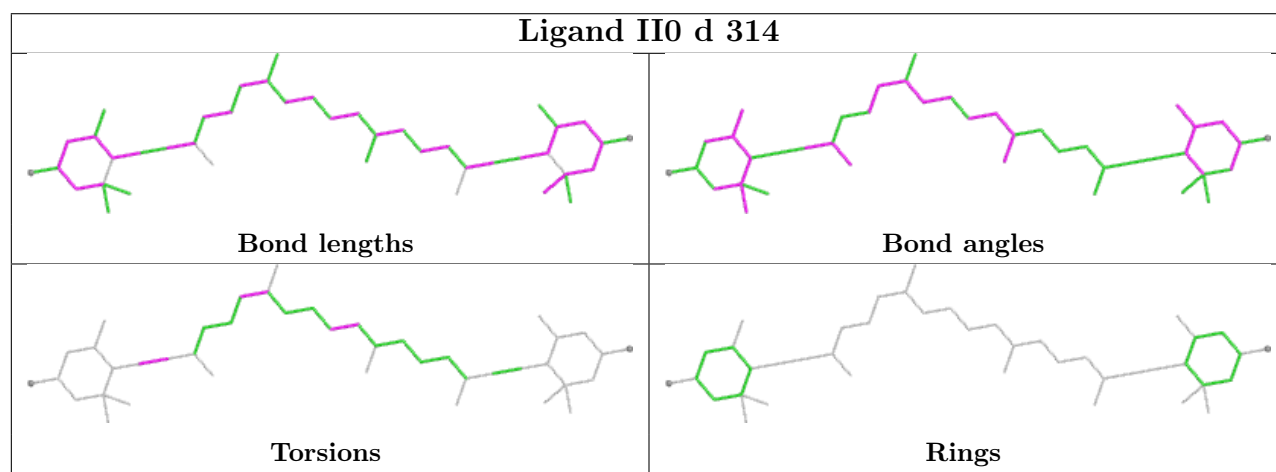
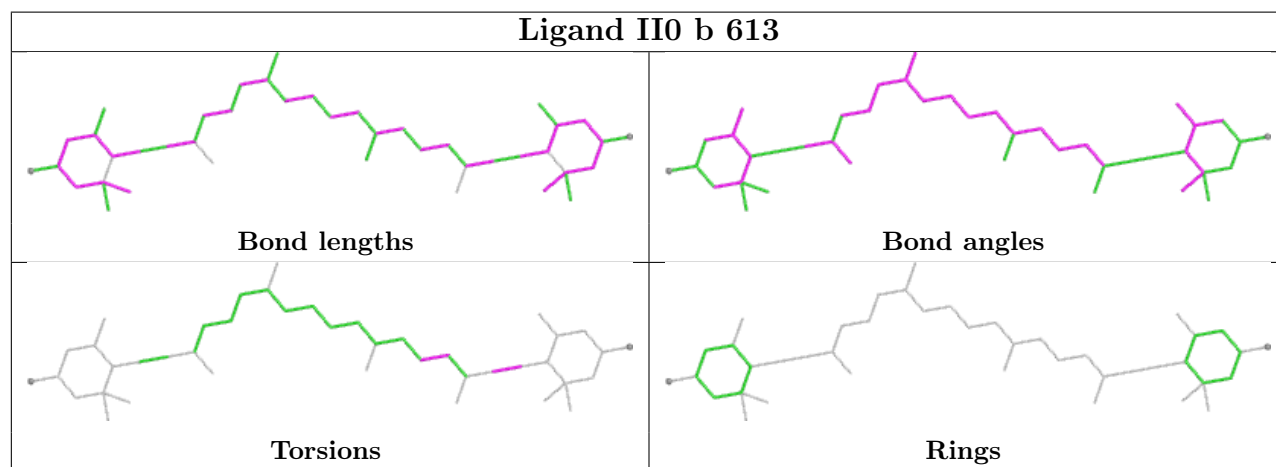
Ligand KC2 d 310

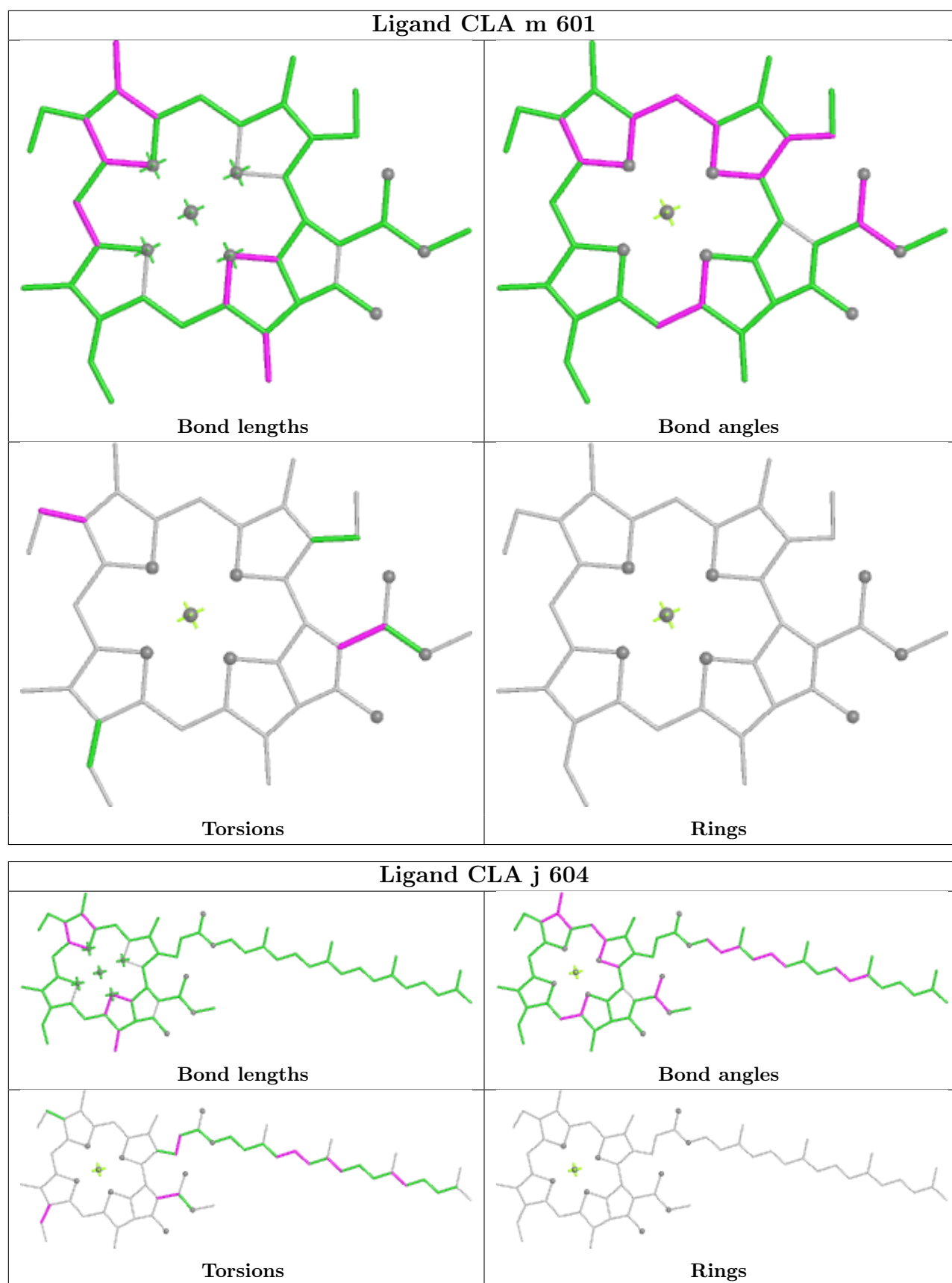


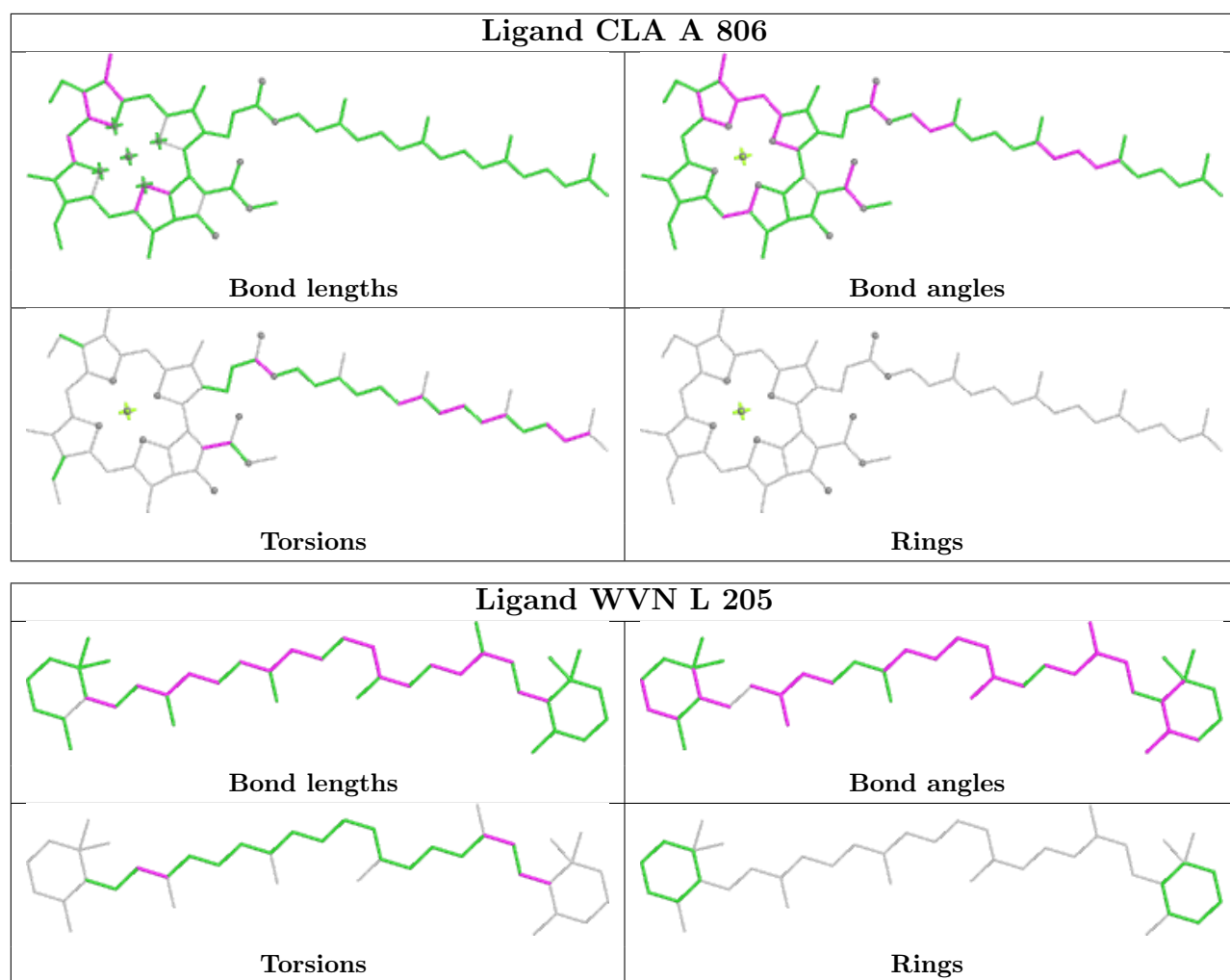
Ligand II0 k 616



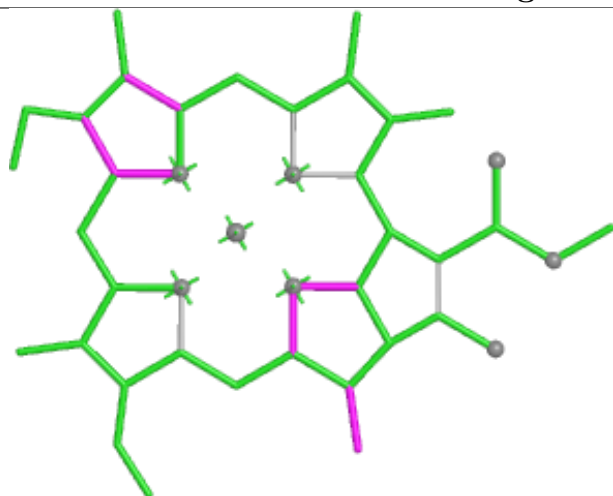




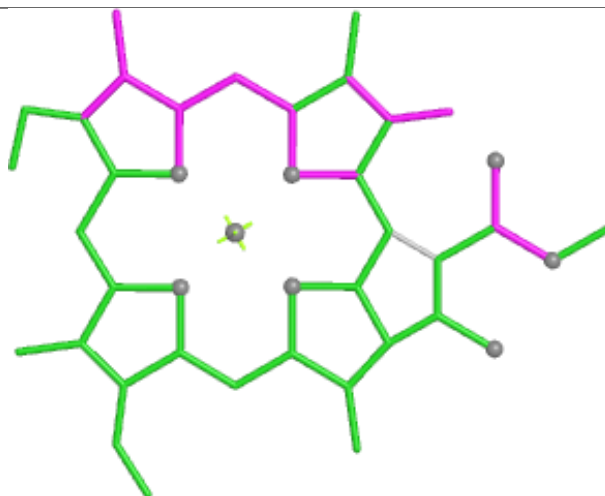




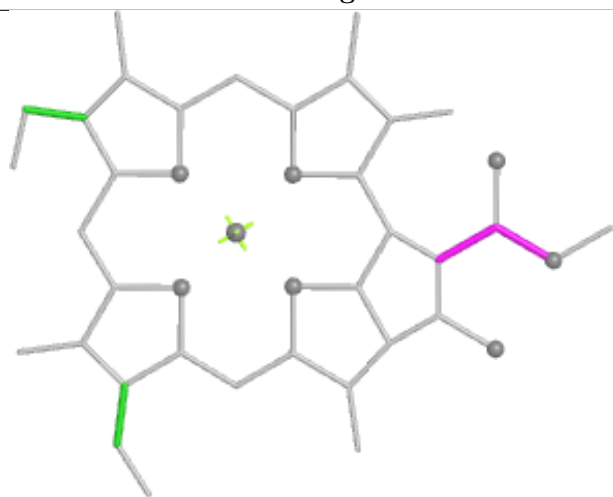
Ligand CLA d 309



Bond lengths



Bond angles

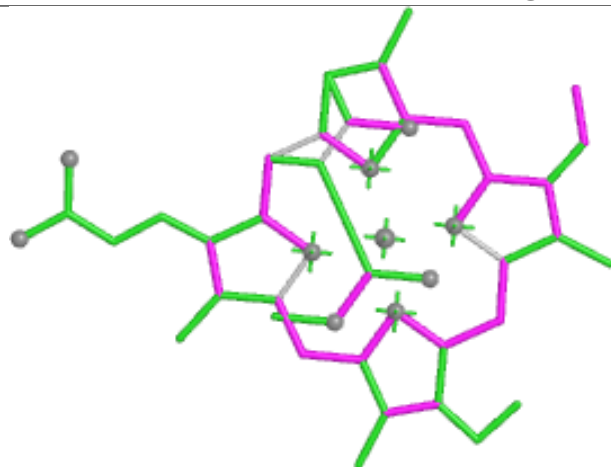


Torsions

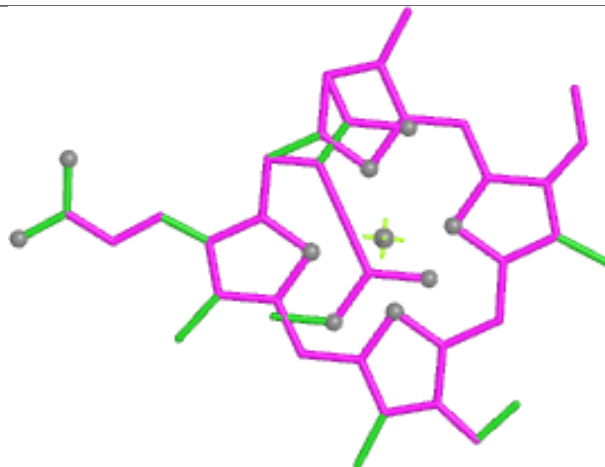


Rings

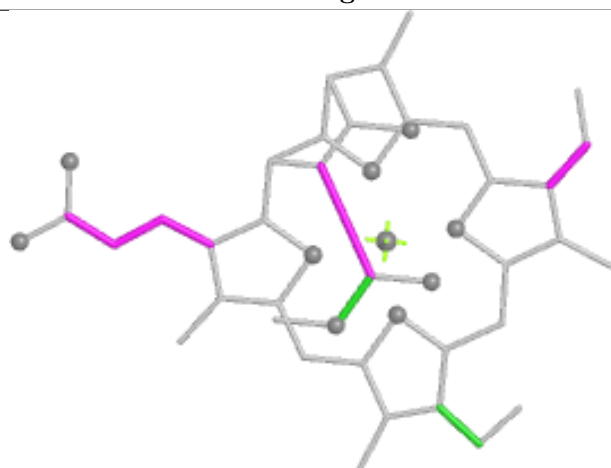
Ligand KC2 s 201



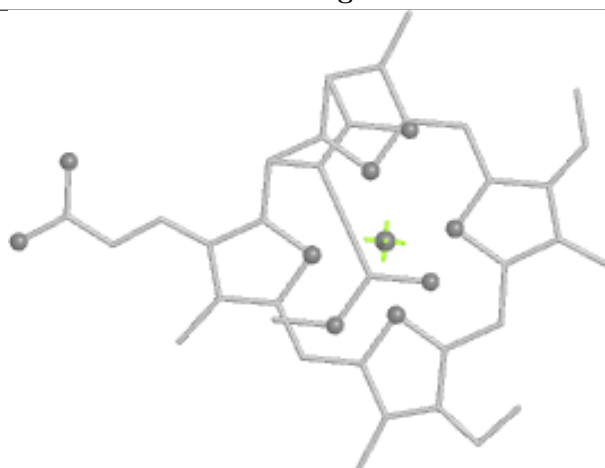
Bond lengths



Bond angles

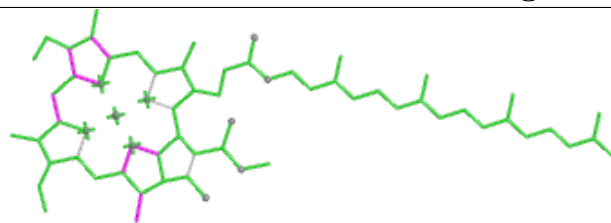


Torsions

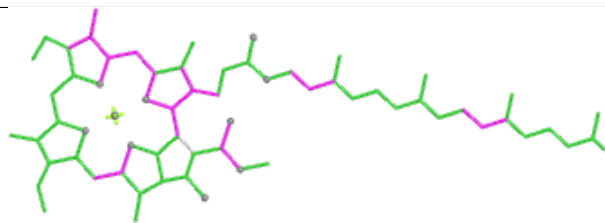


Rings

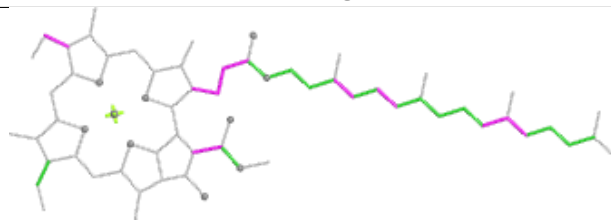
Ligand CLA s 206



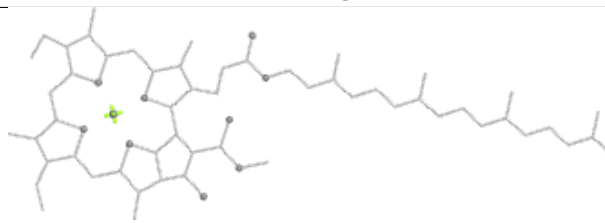
Bond lengths



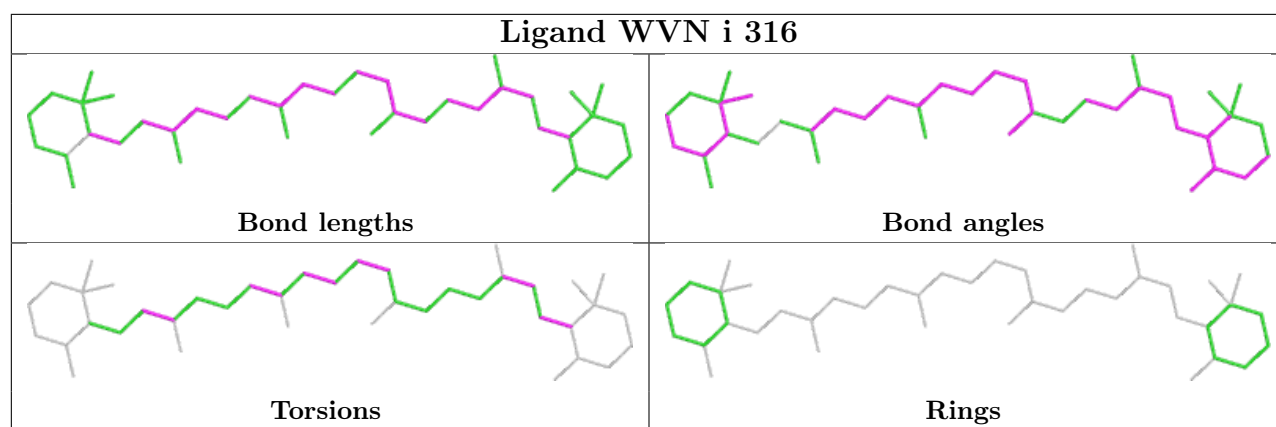
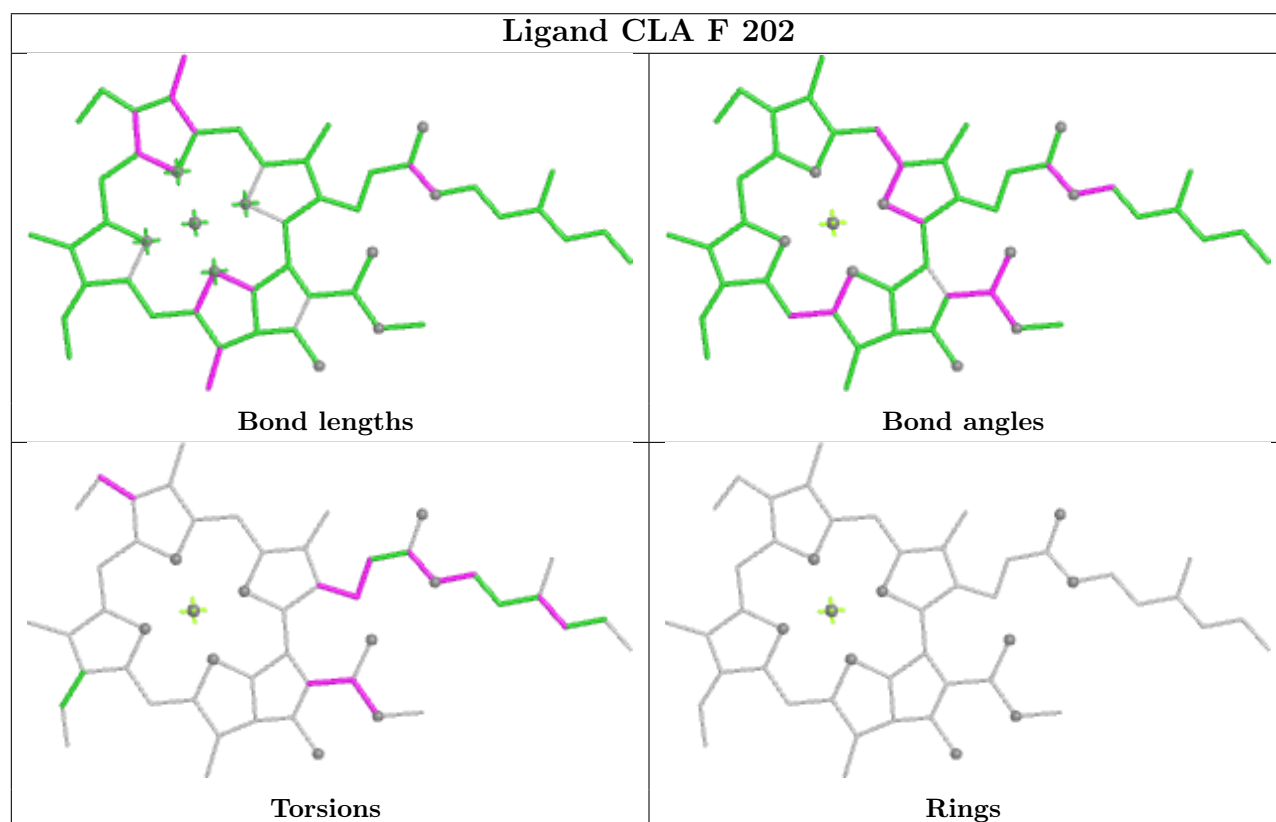
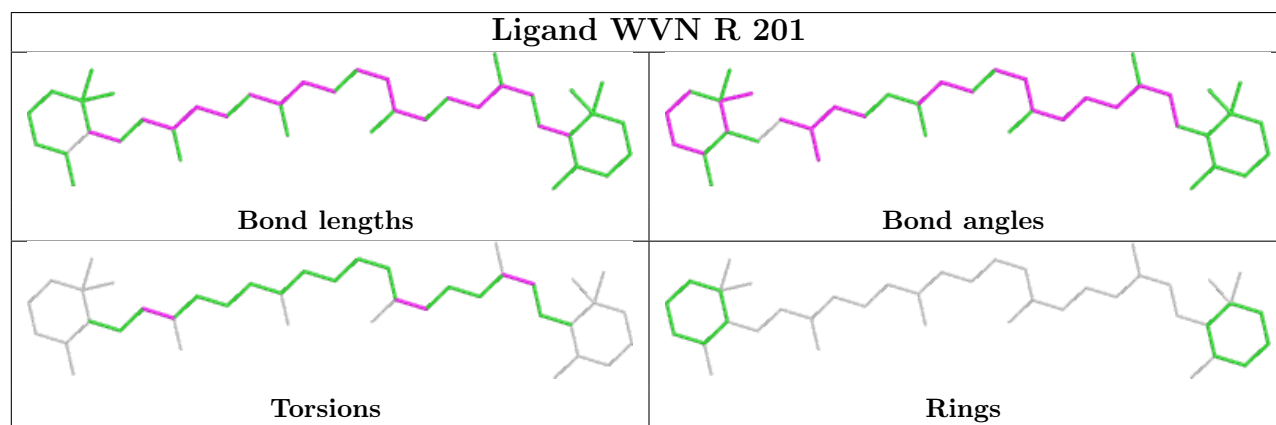
Bond angles

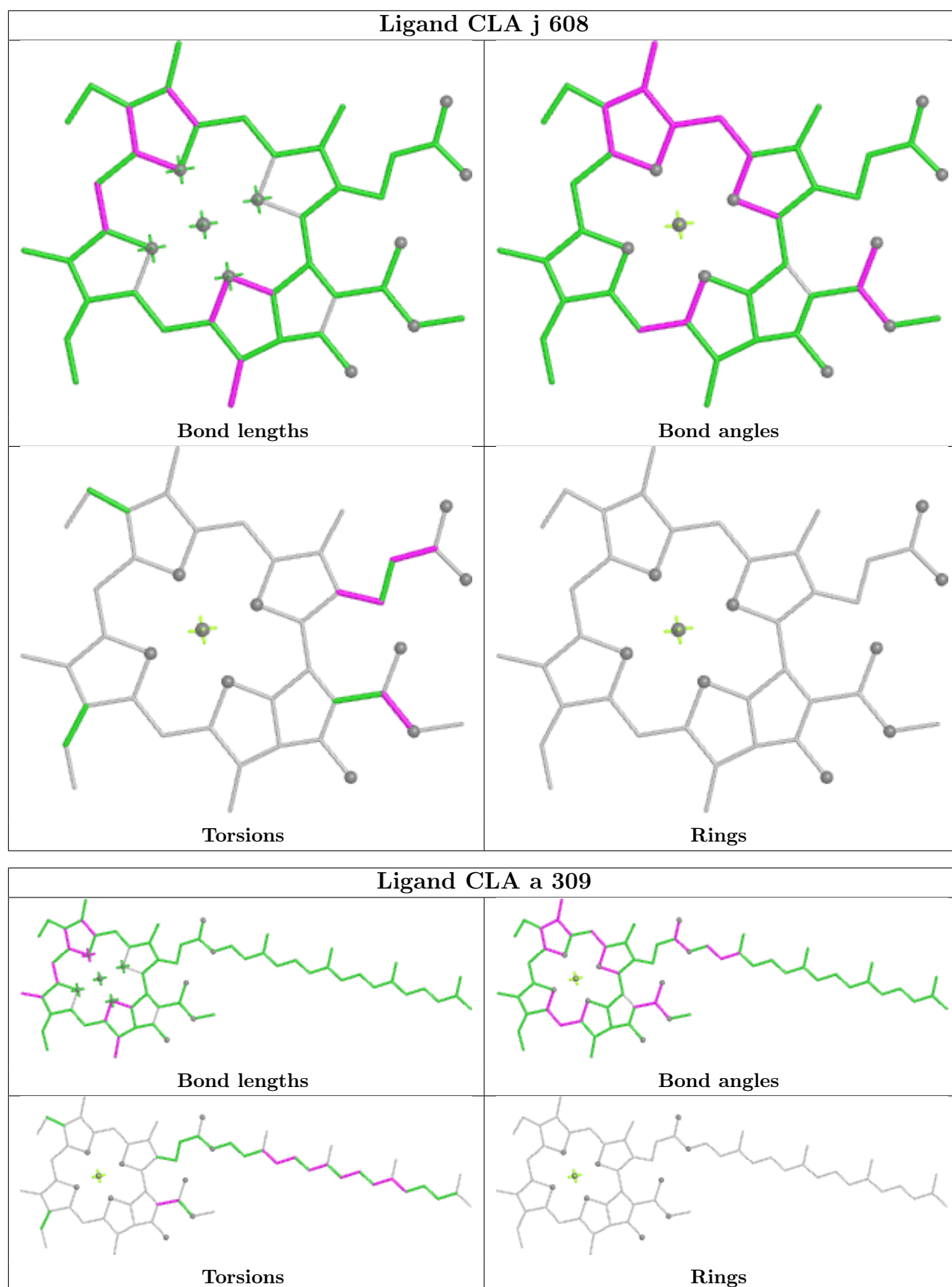


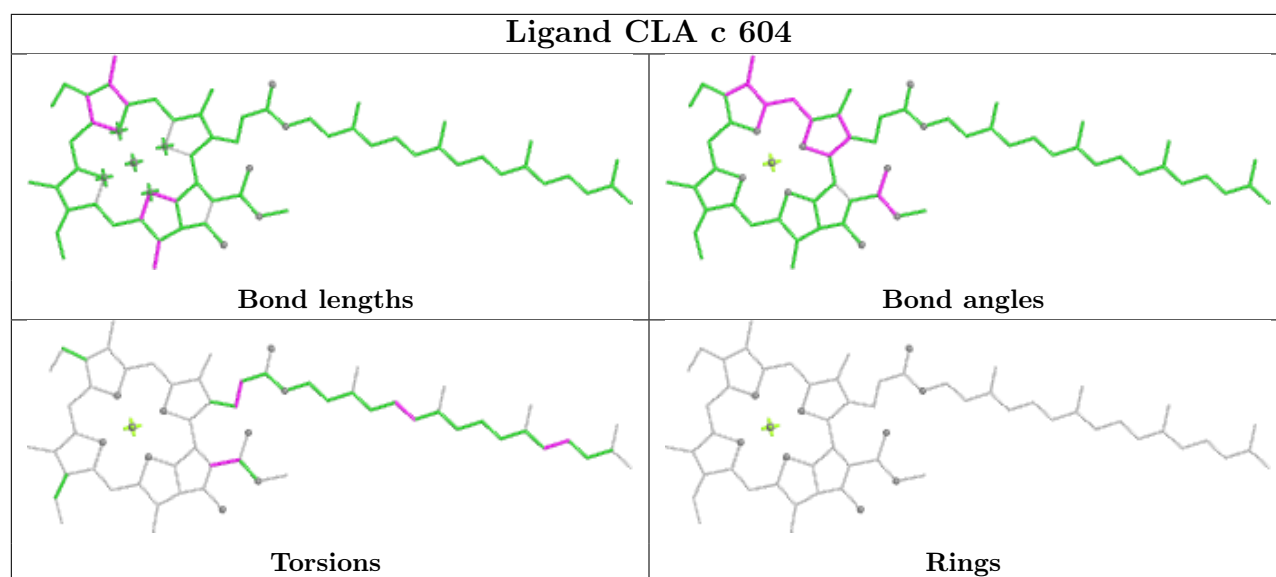
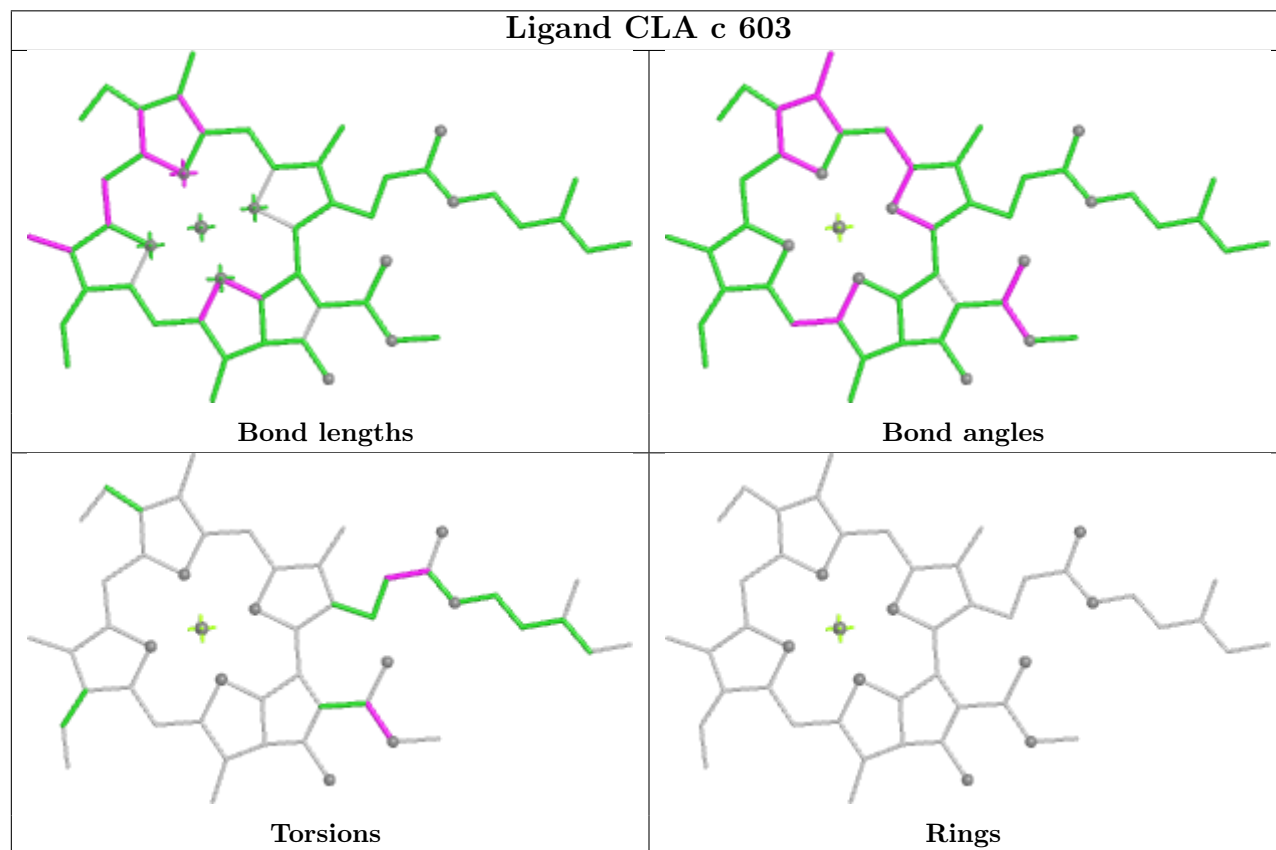
Torsions

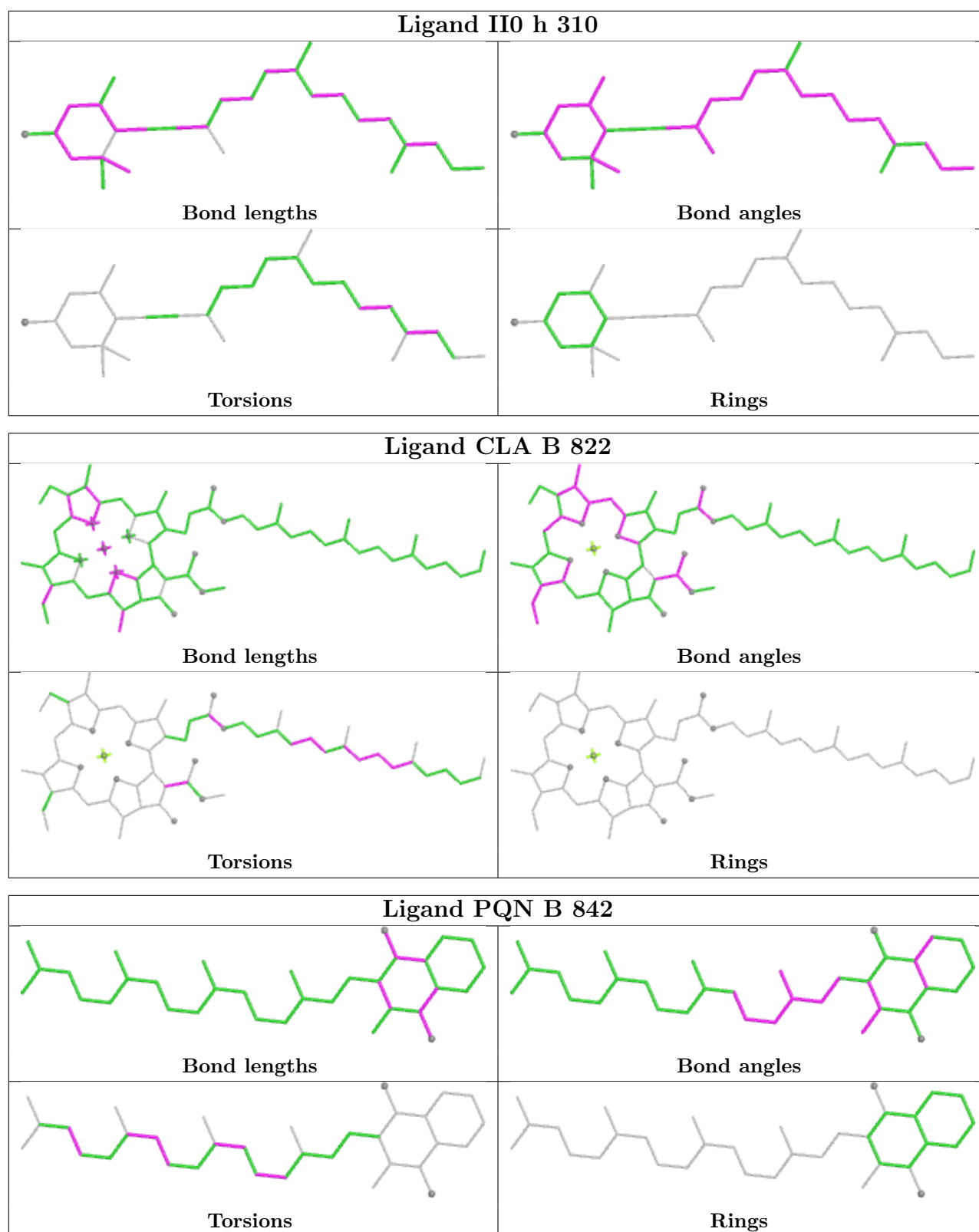


Rings

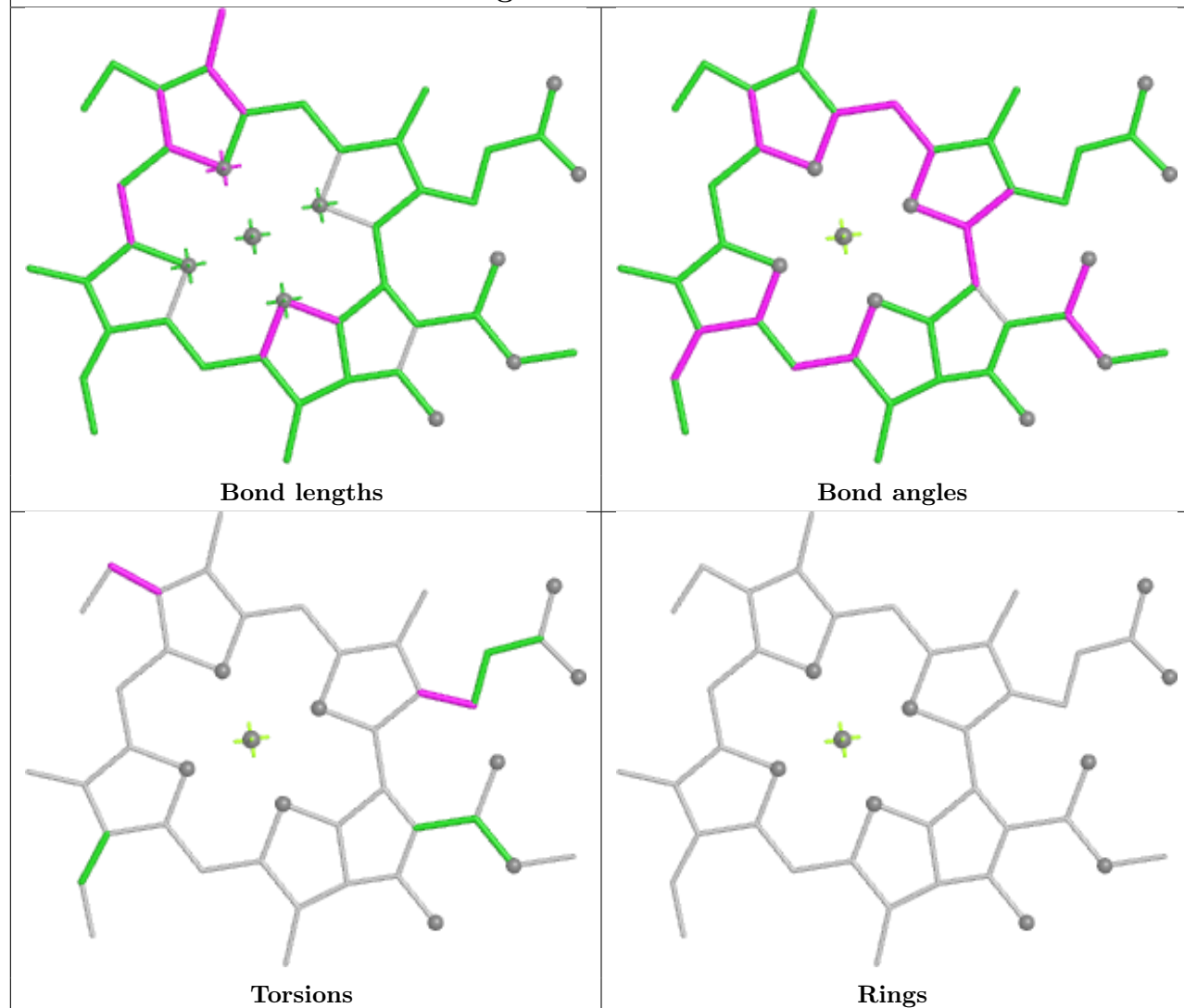




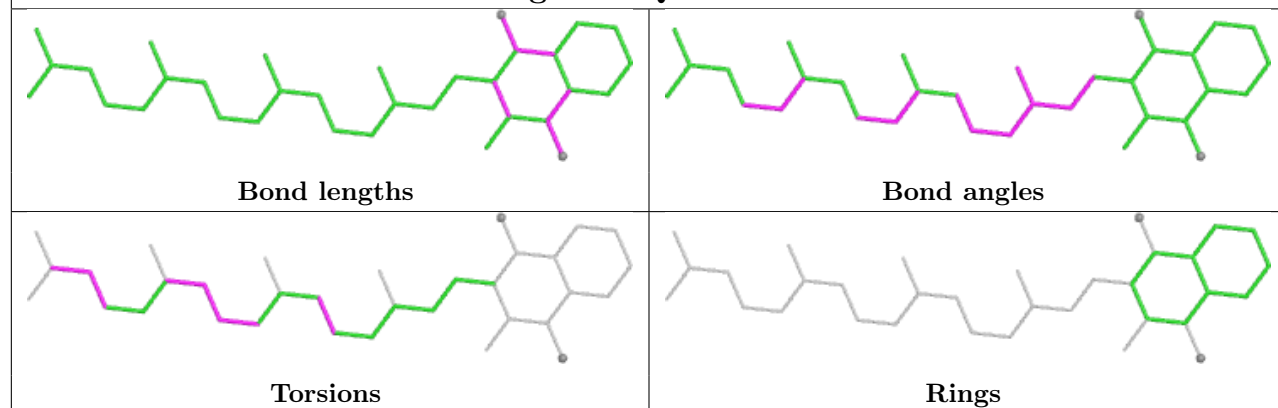




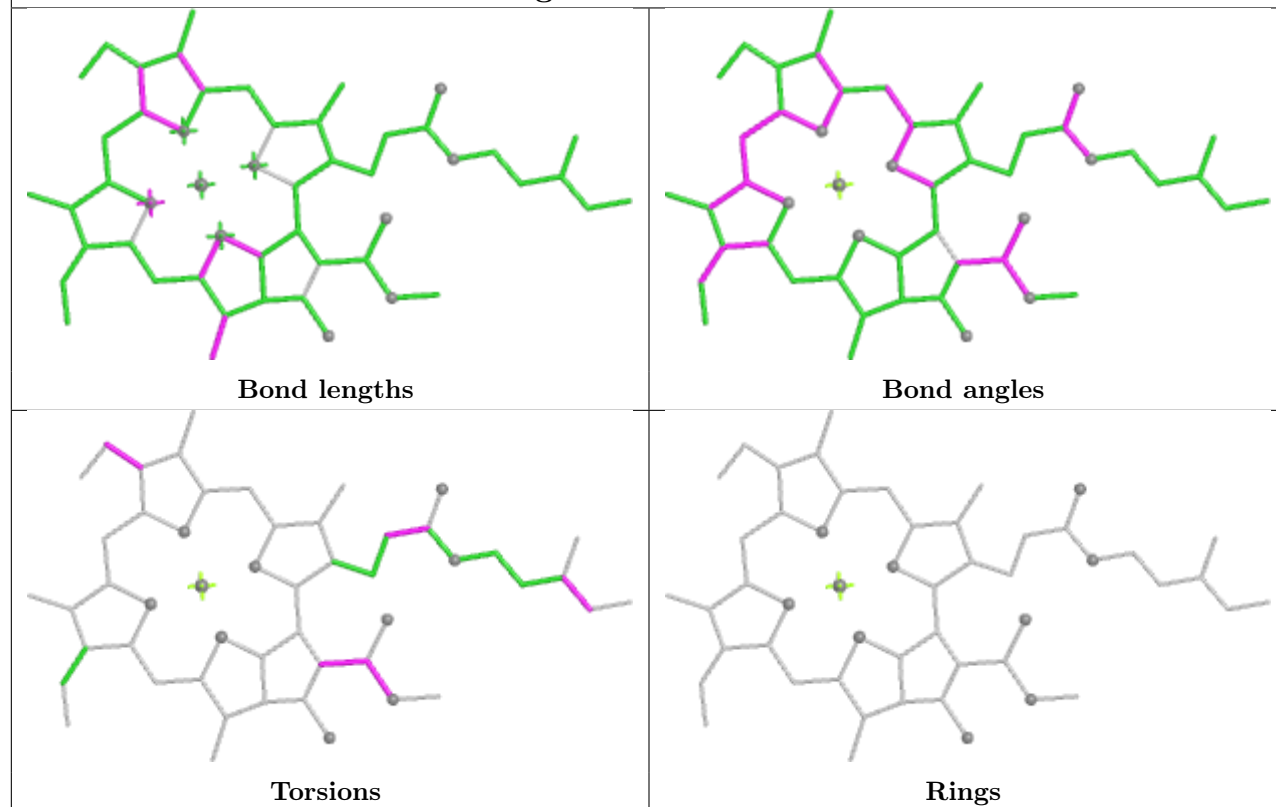
Ligand CLA a 307



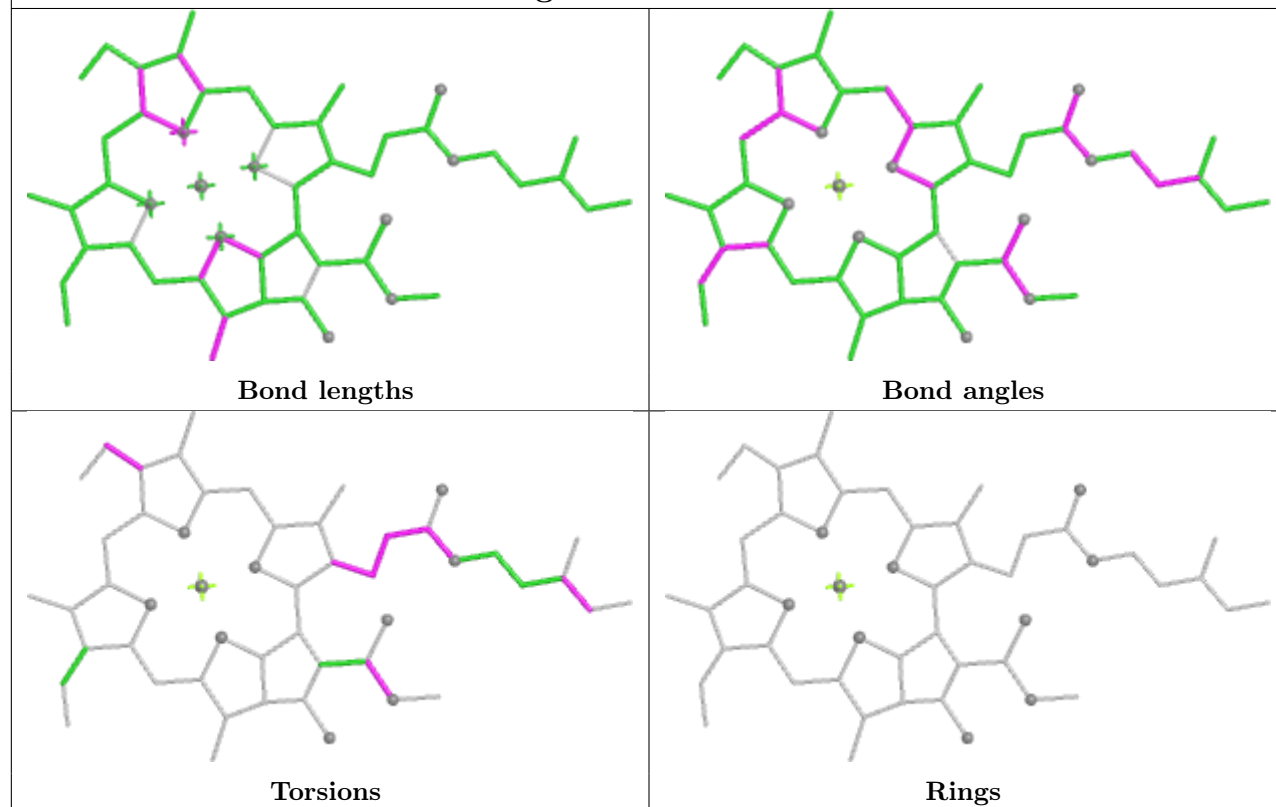
Ligand PQN A 842



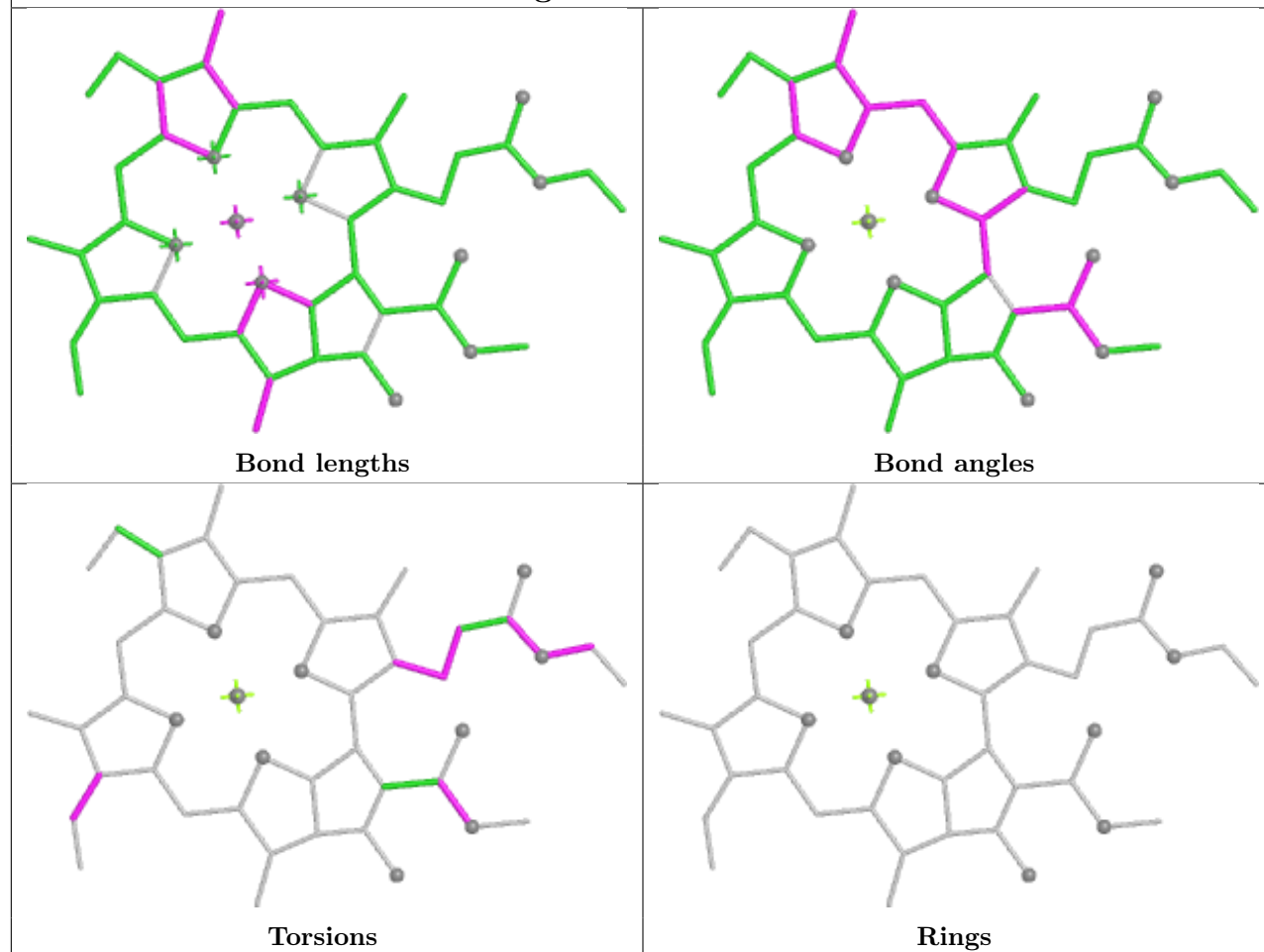
Ligand CLA d 305



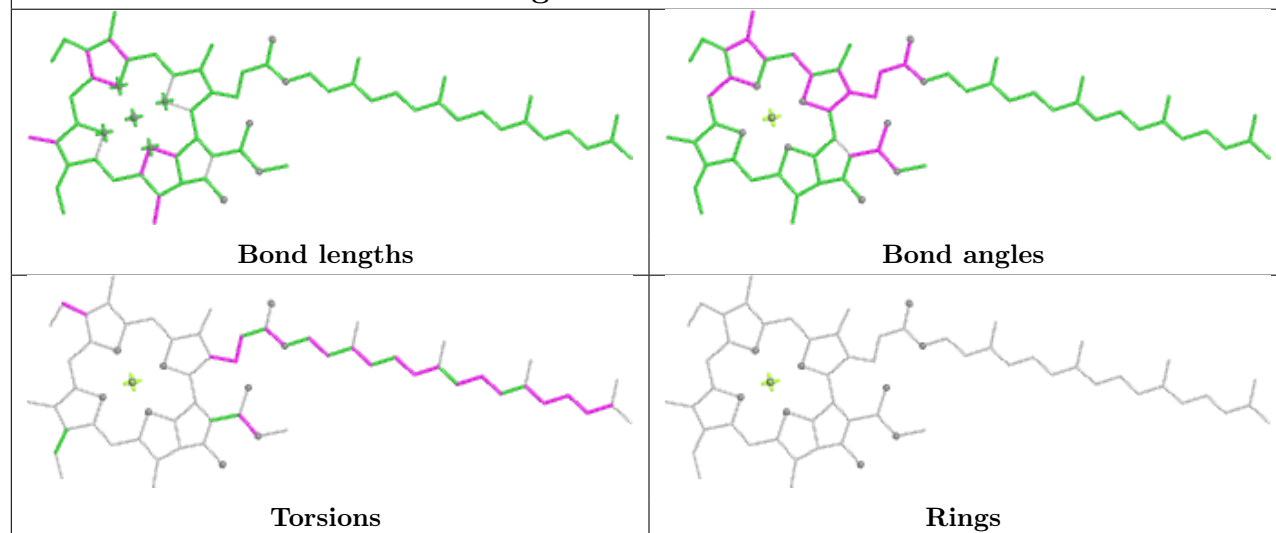
Ligand CLA k 601

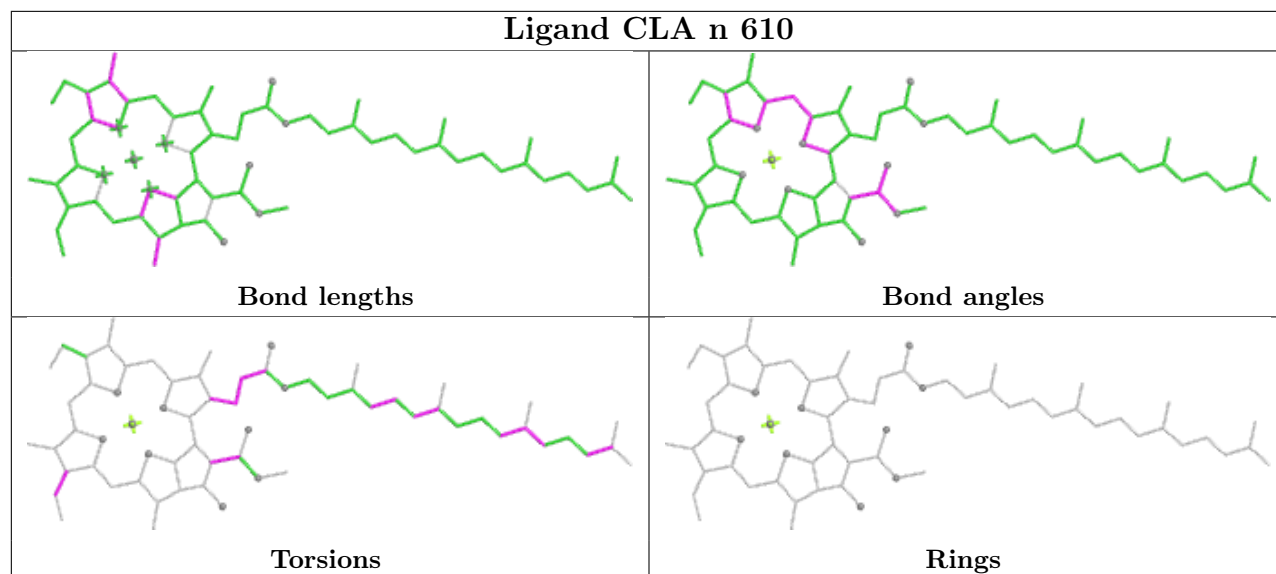
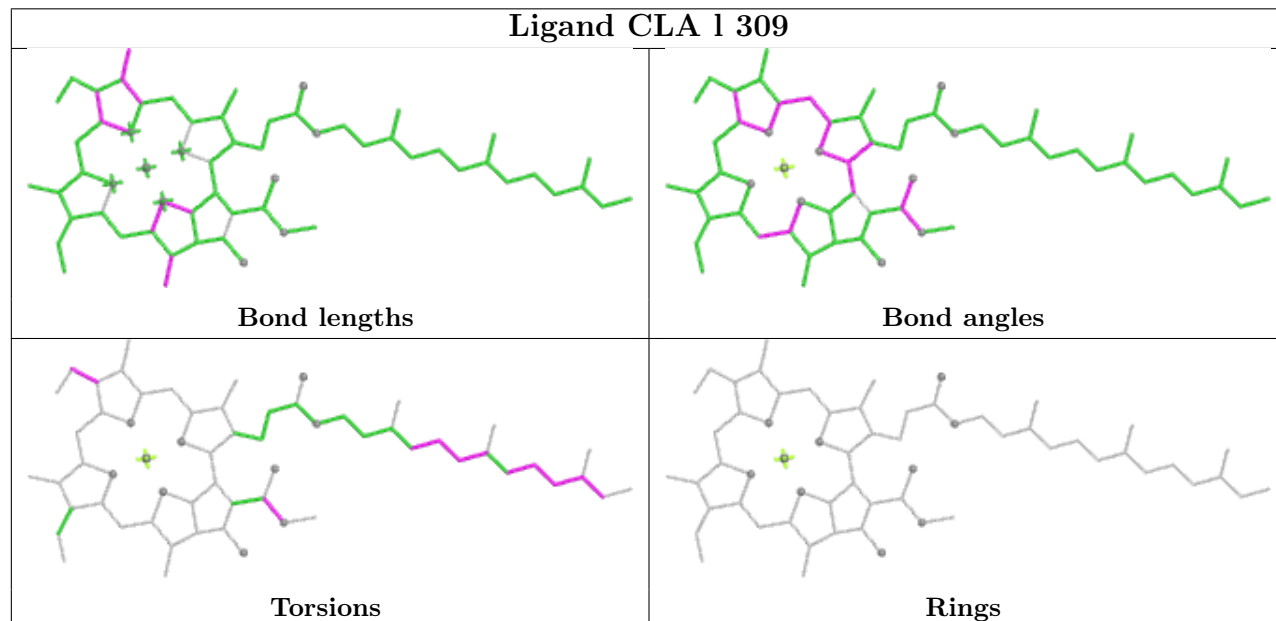


Ligand CLA f 601

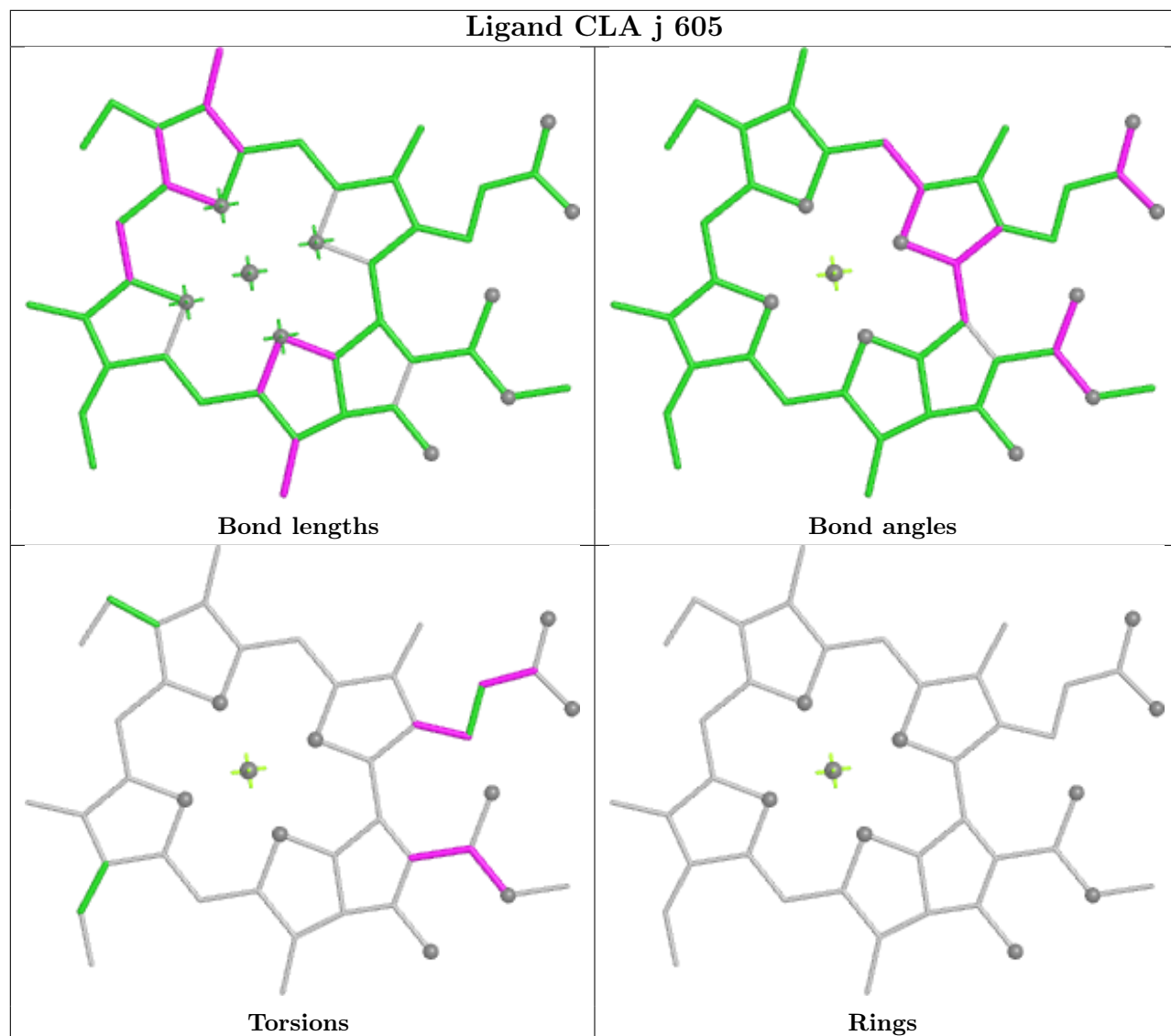


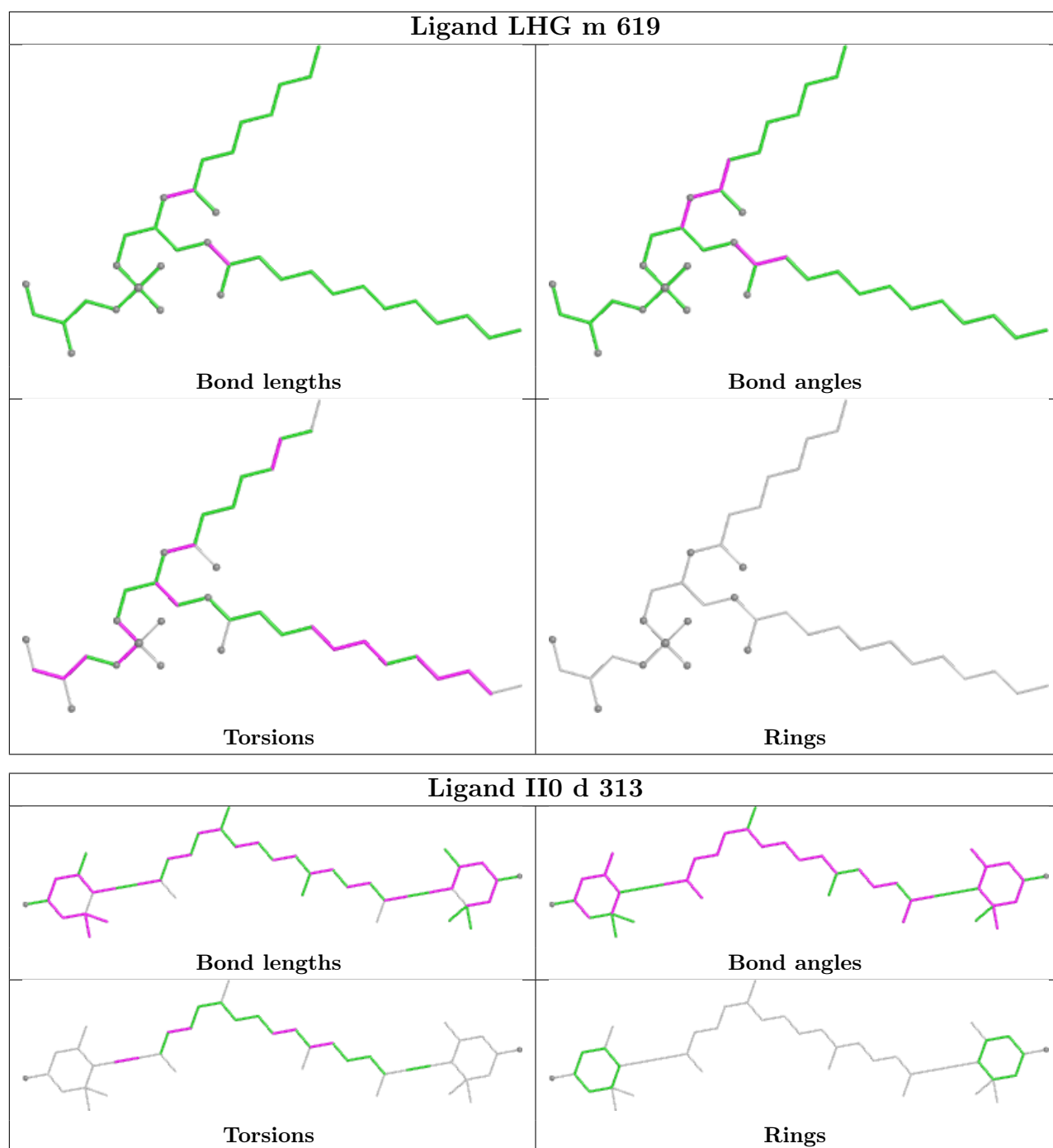
Ligand CLA A 841

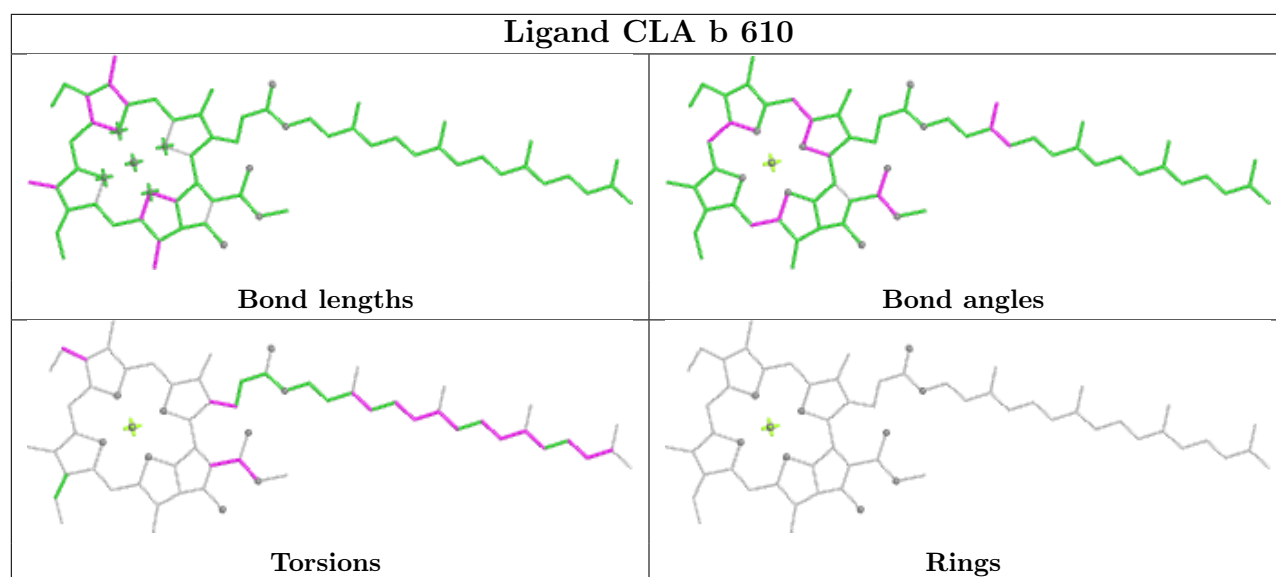
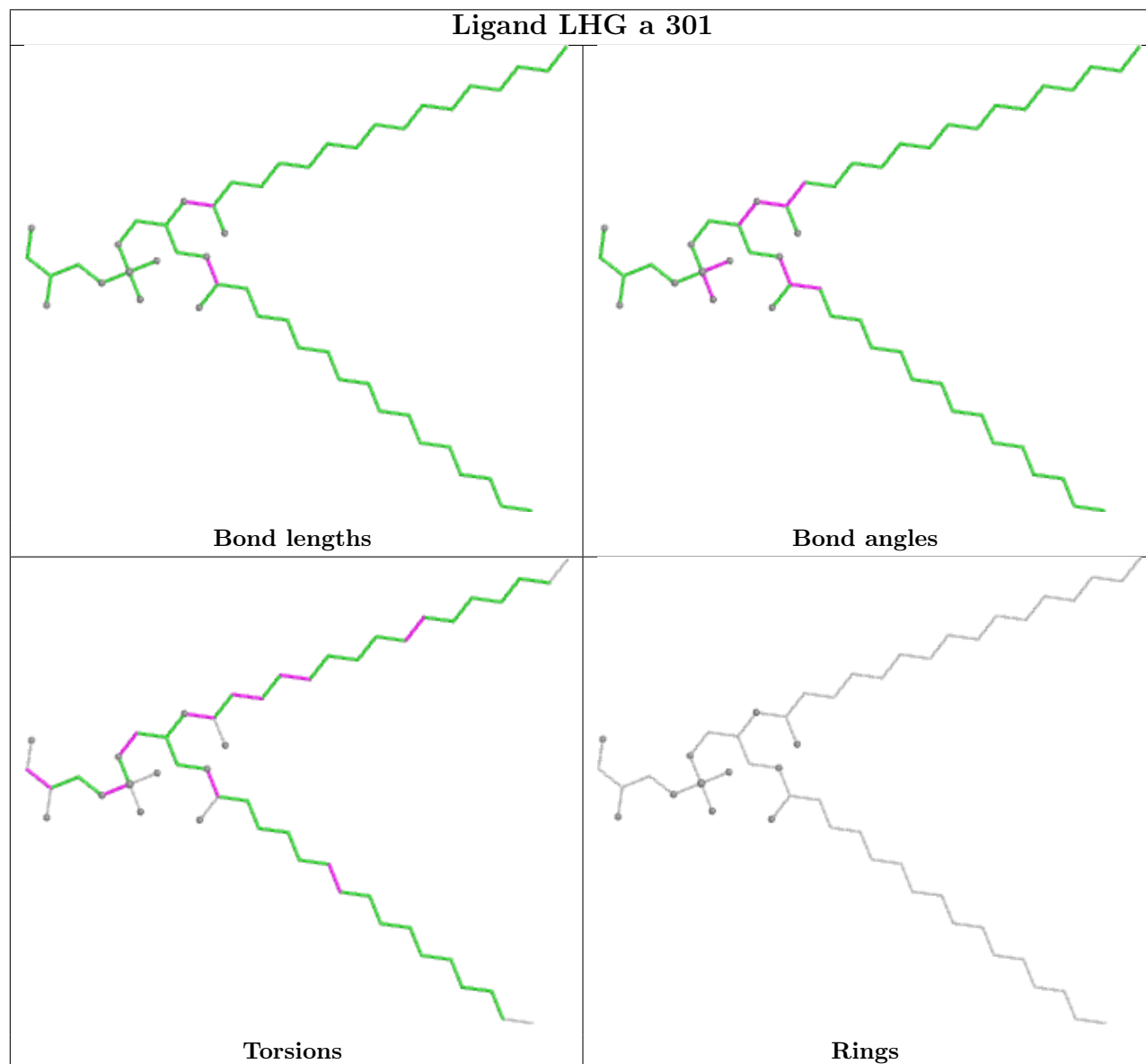


Ligand CLA n 610**Ligand CLA l 309**

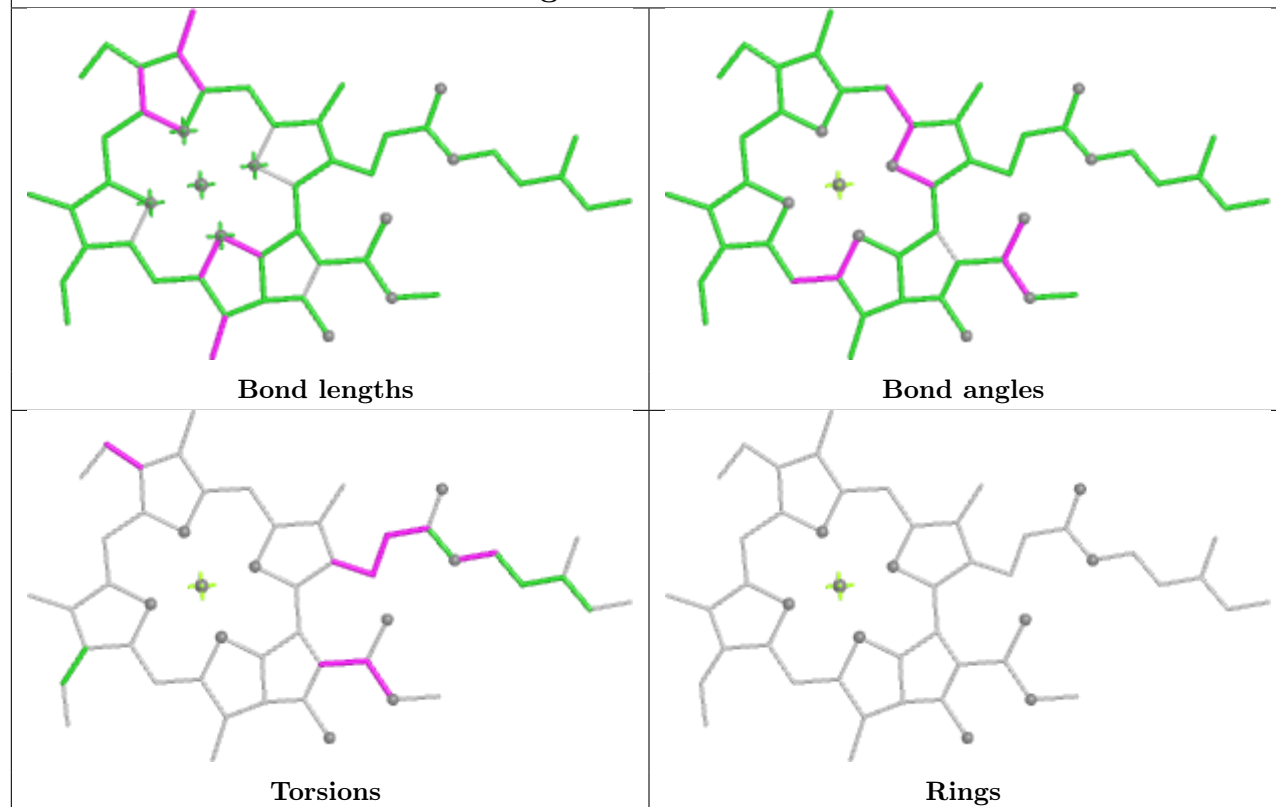
Ligand CLA j 605



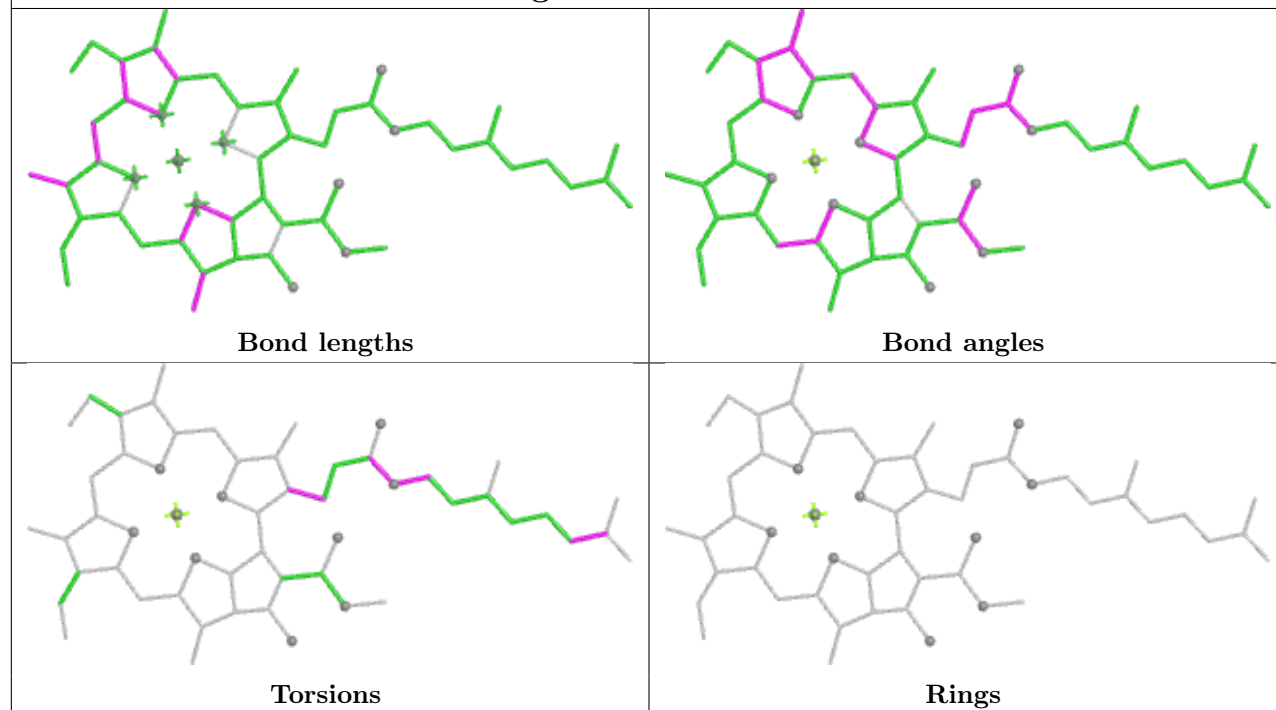


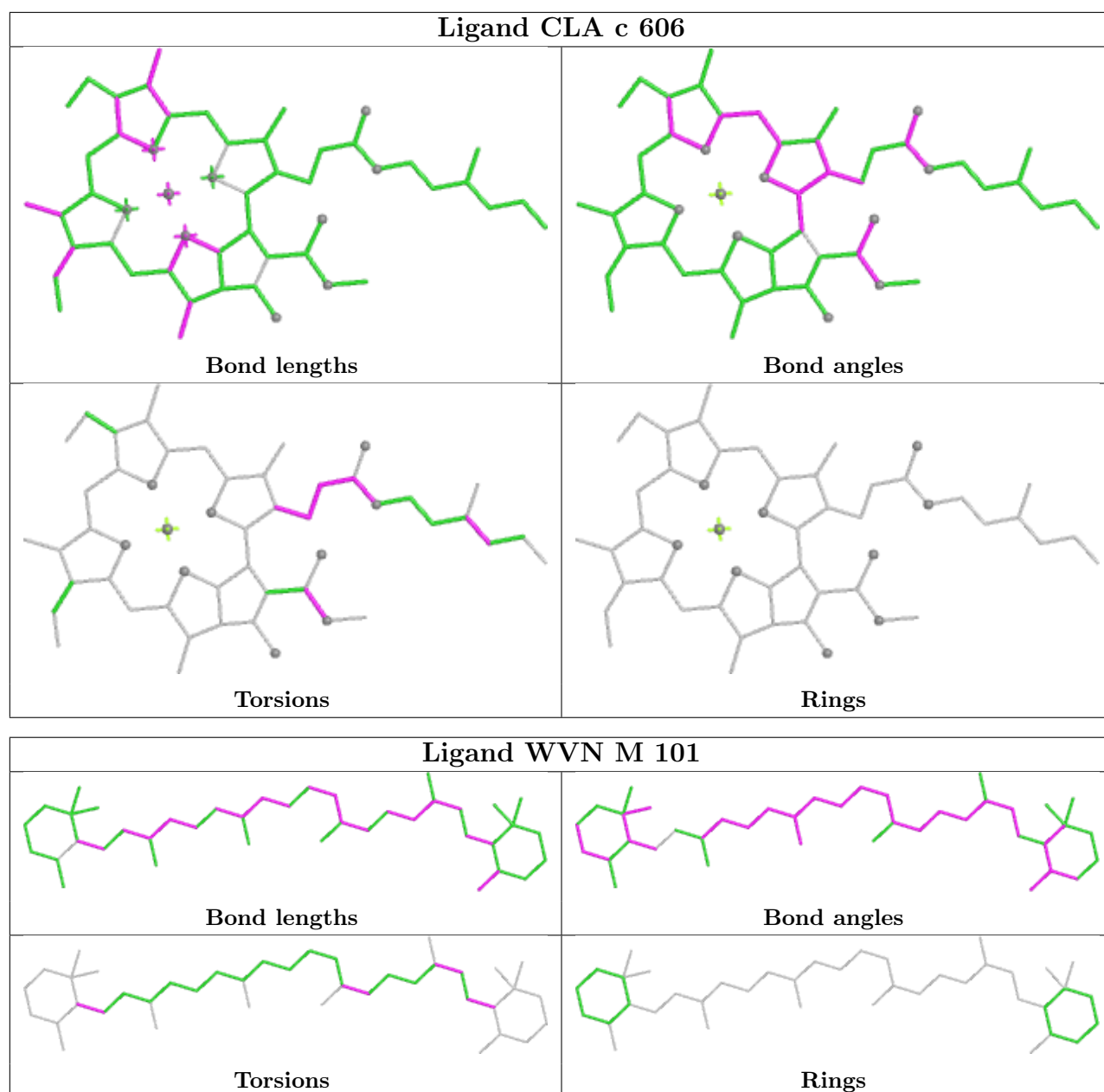


Ligand CLA i 306

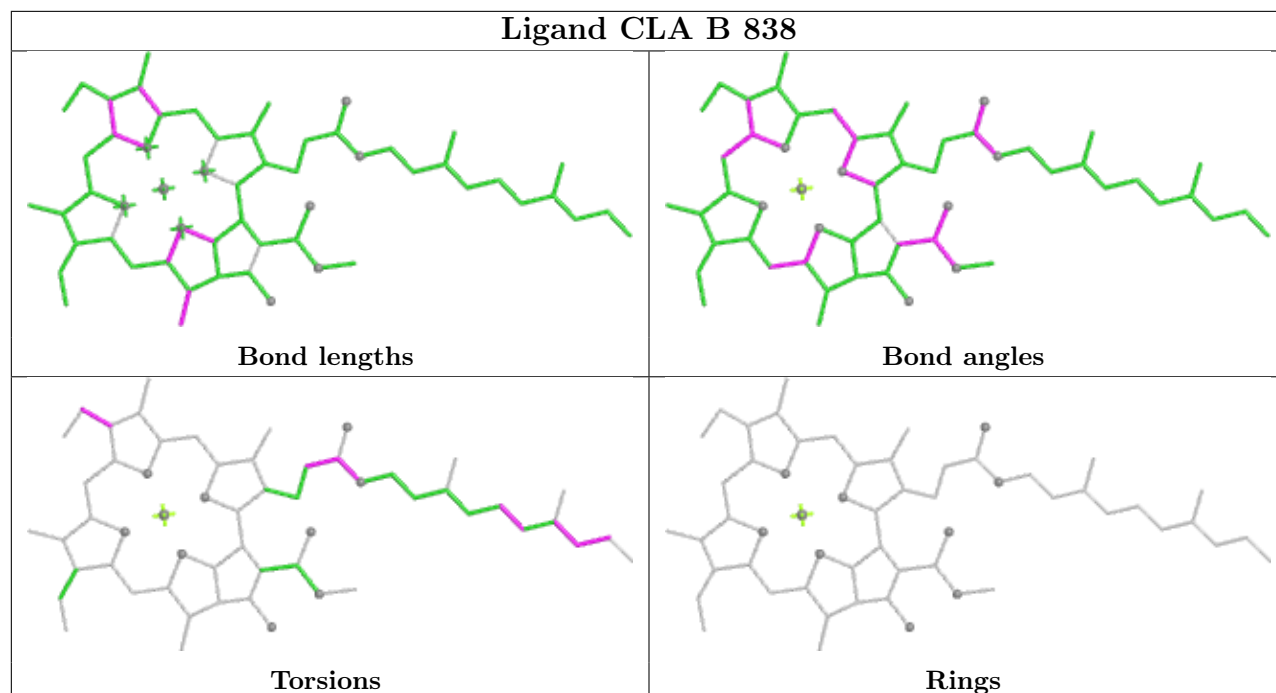


Ligand CLA A 803

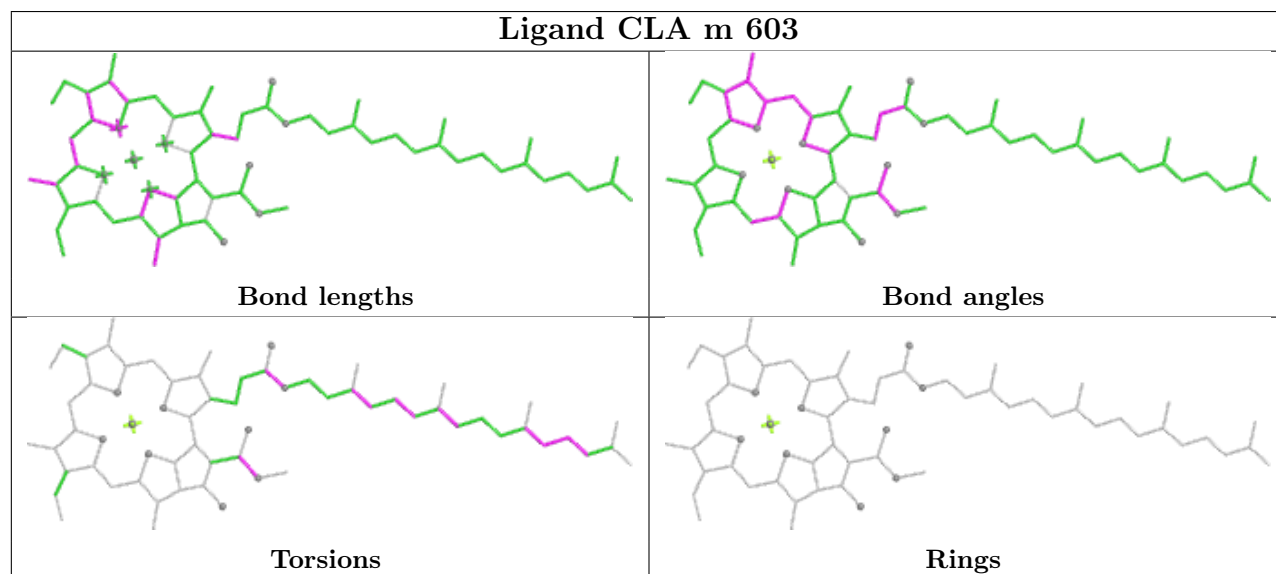


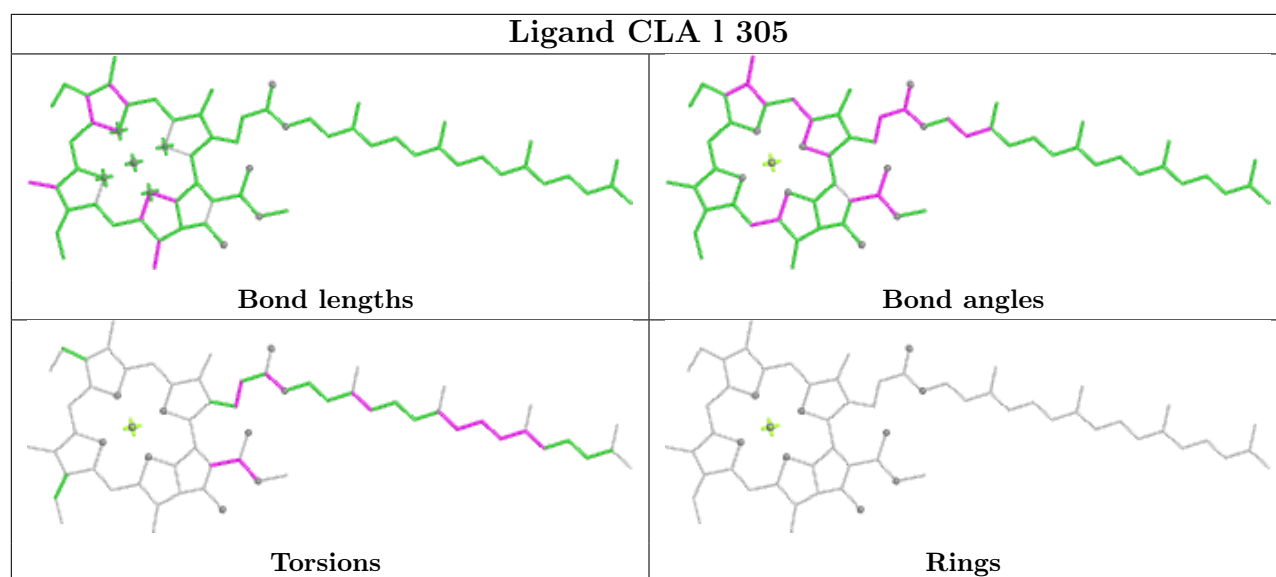
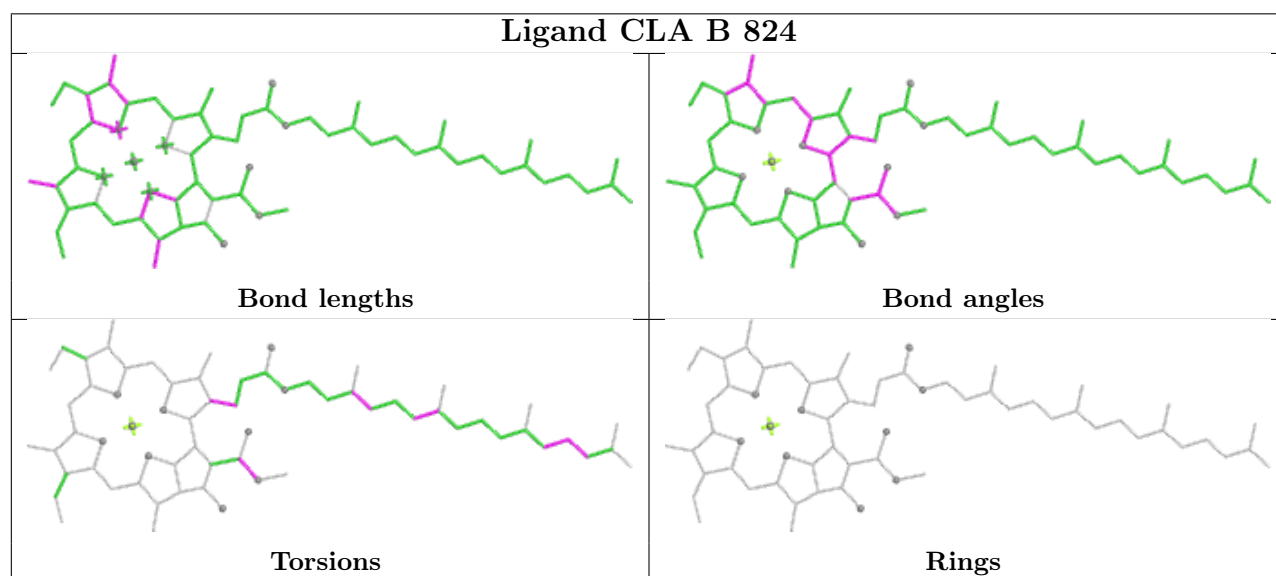
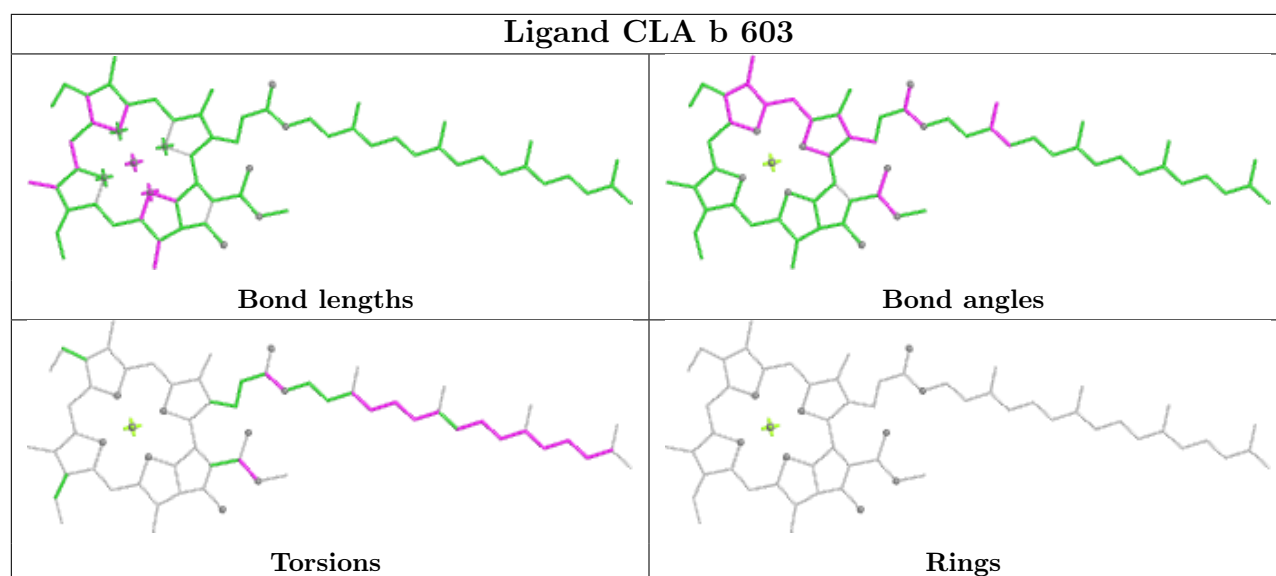


Ligand CLA B 838

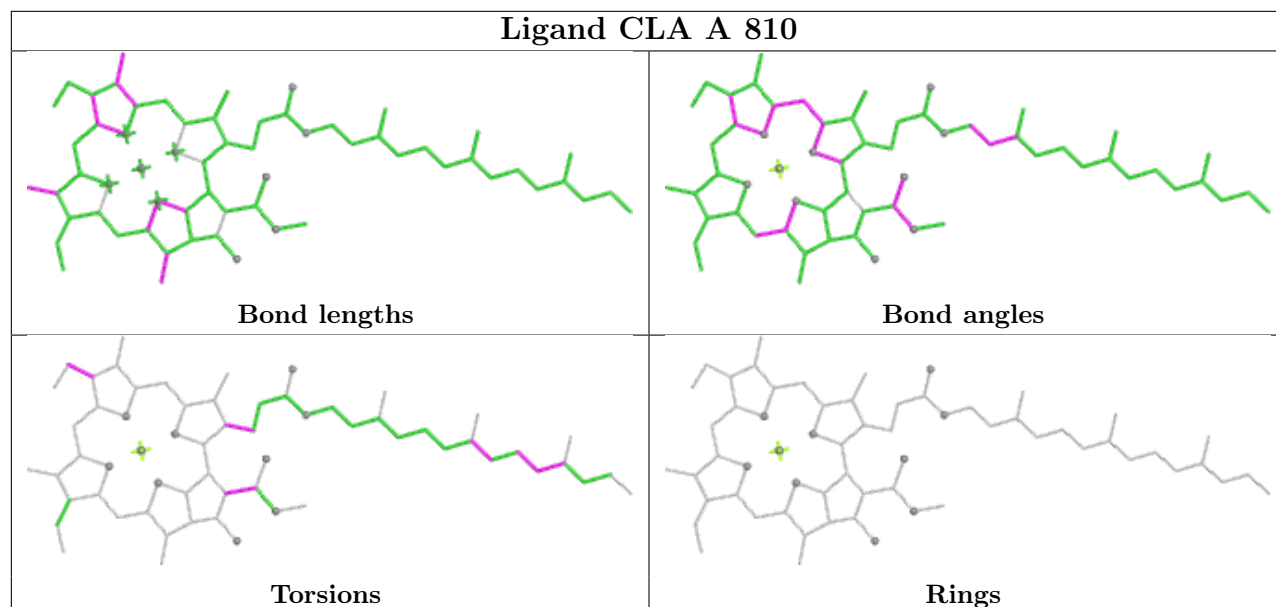


Ligand CLA m 603

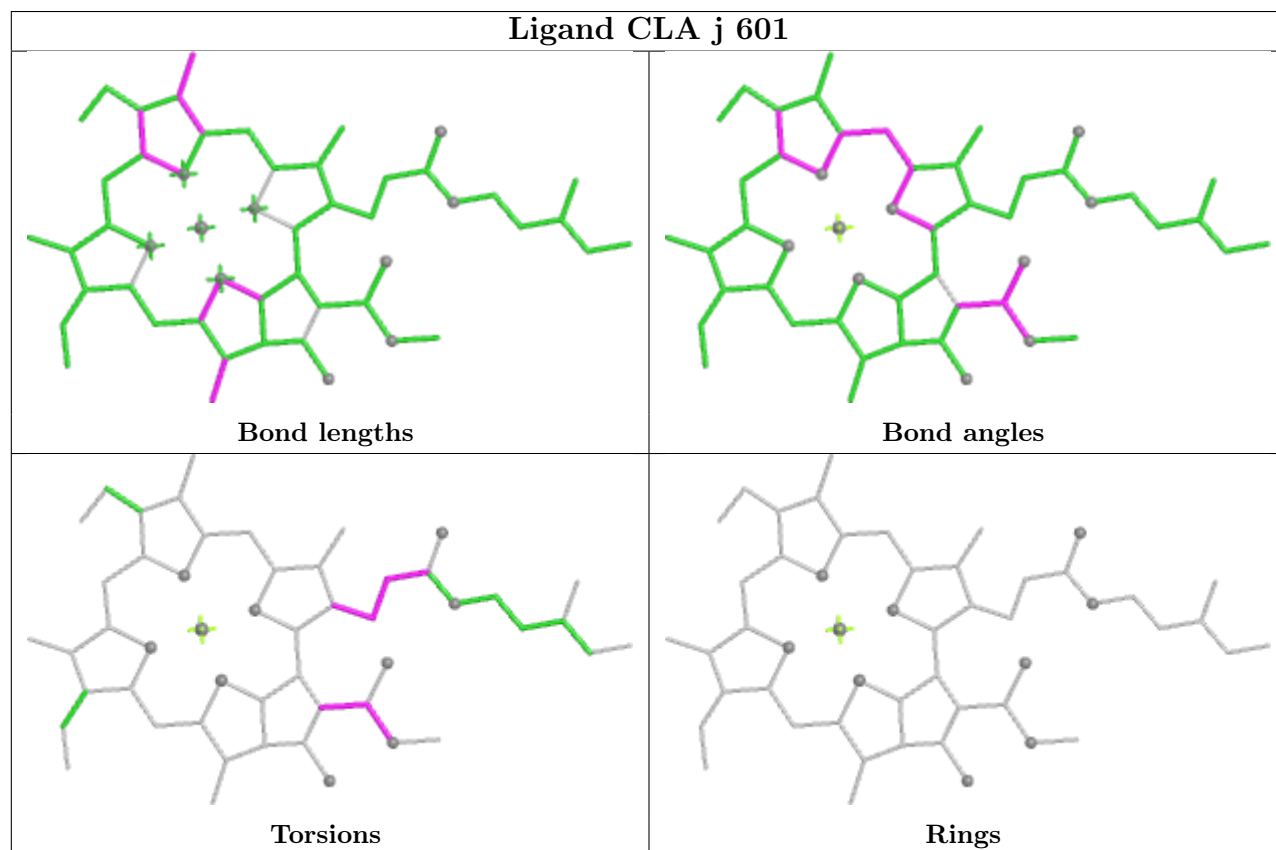


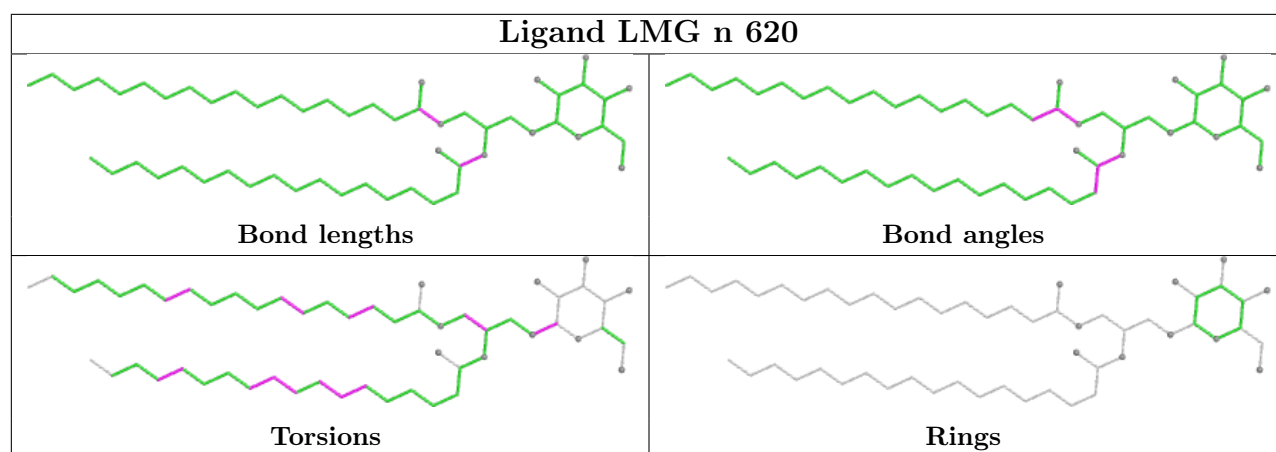
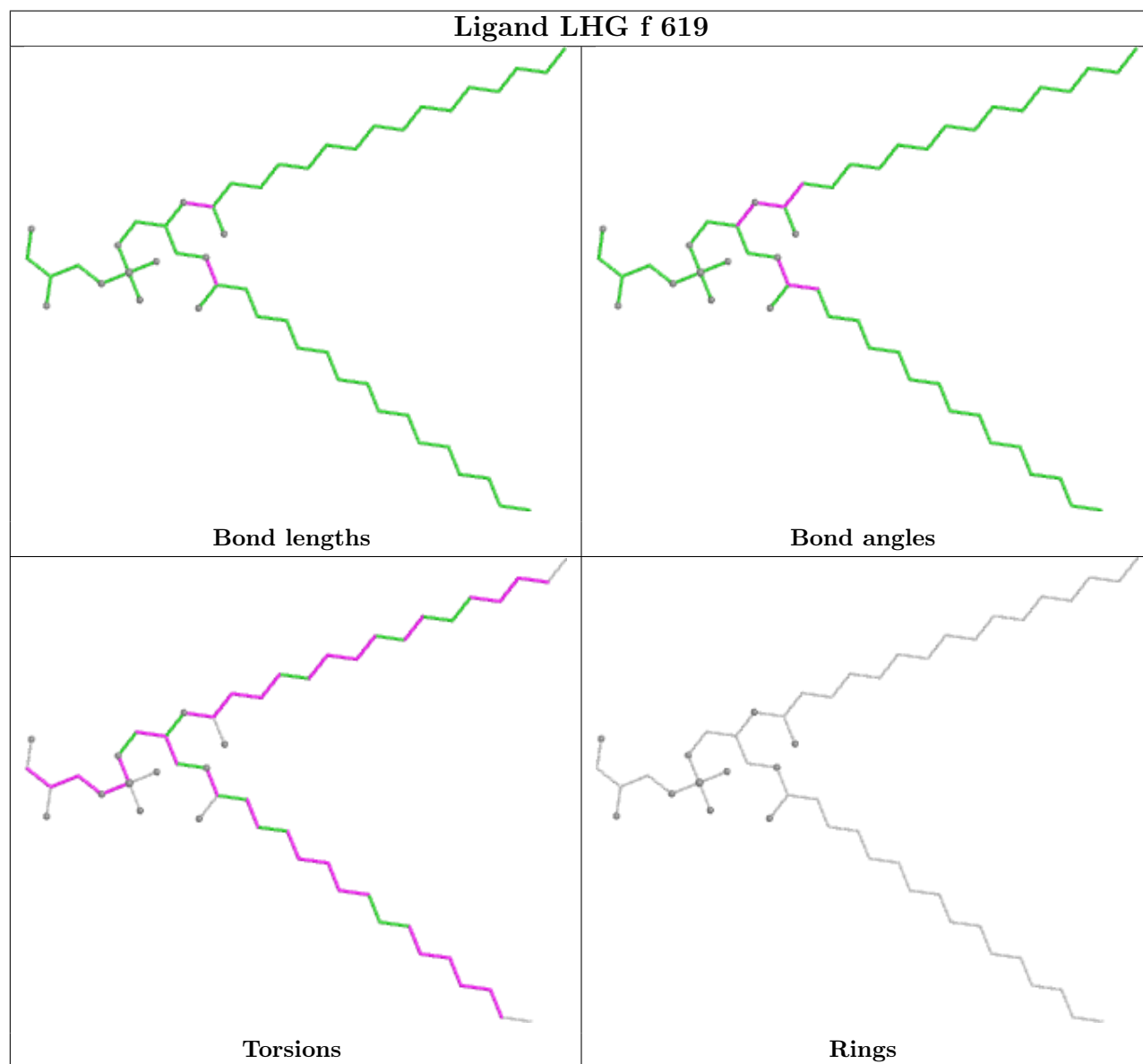


Ligand CLA A 810

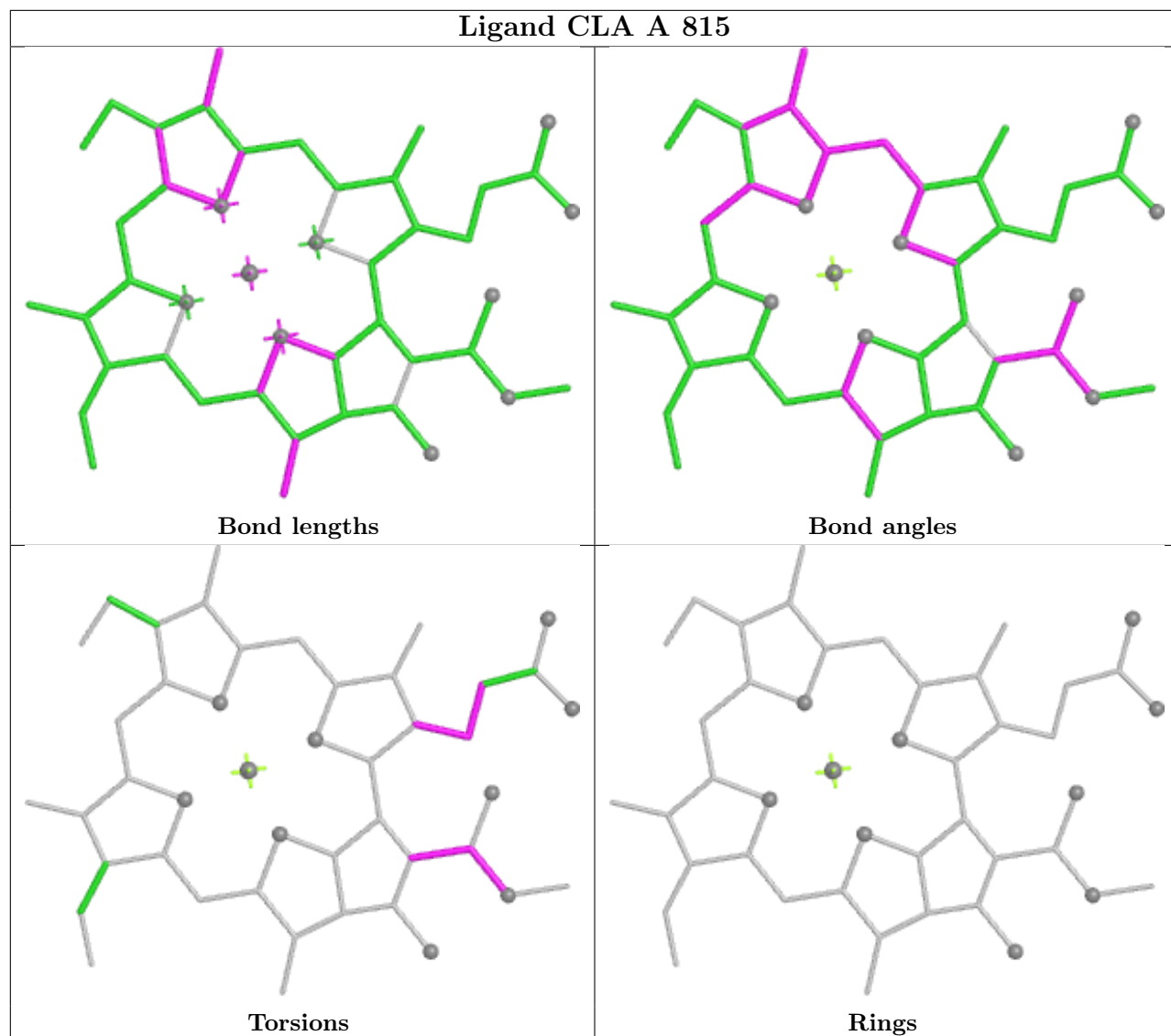


Ligand CLA j 601

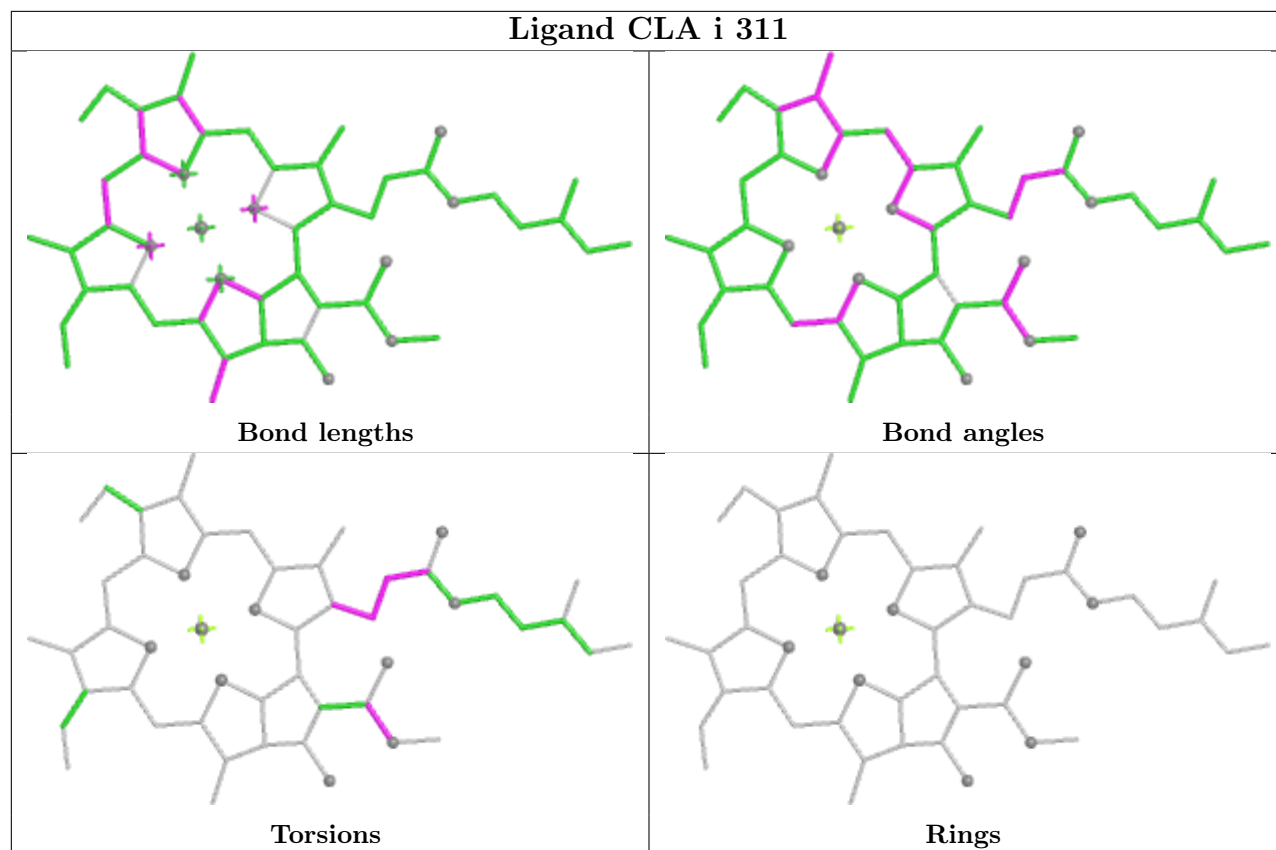




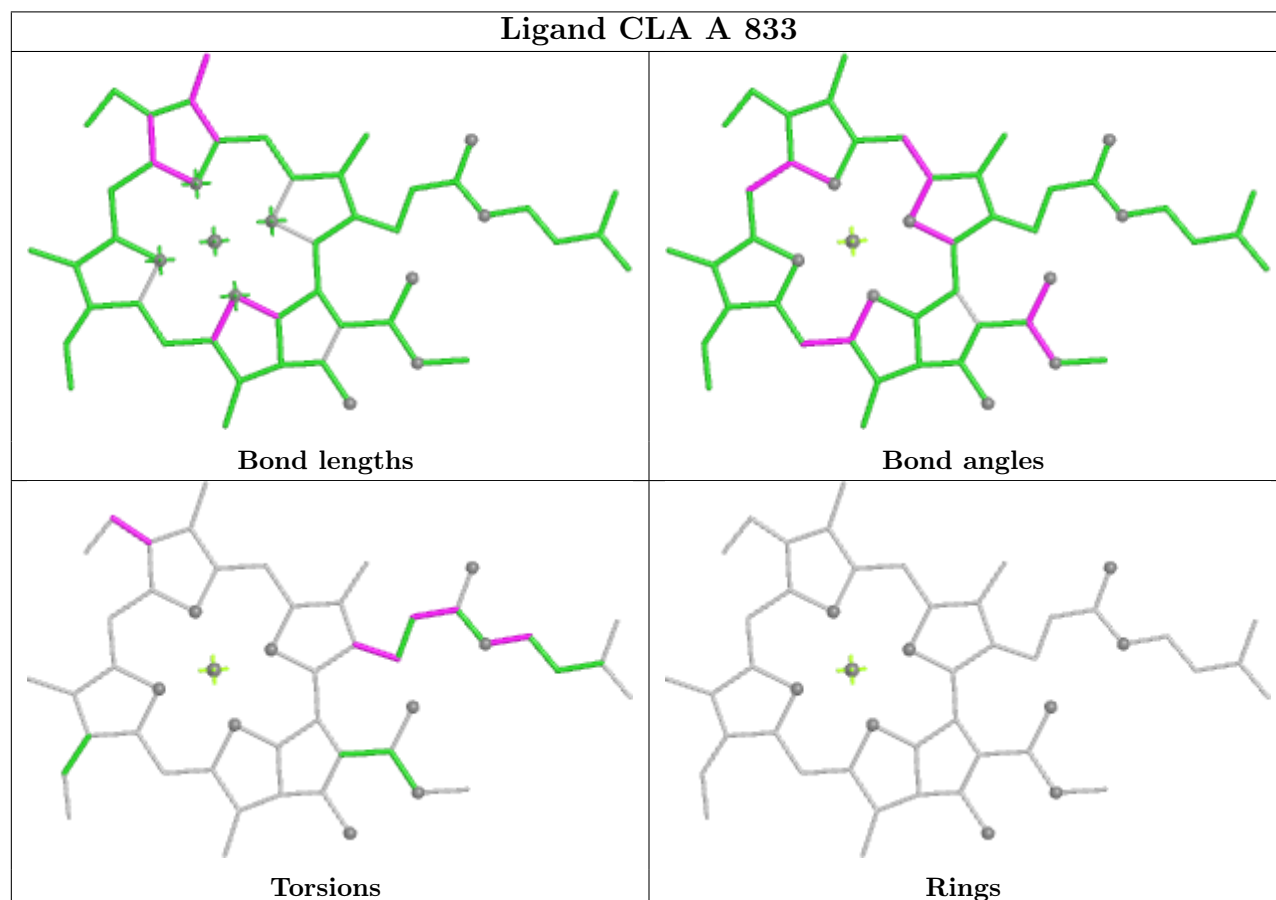
Ligand CLA A 815



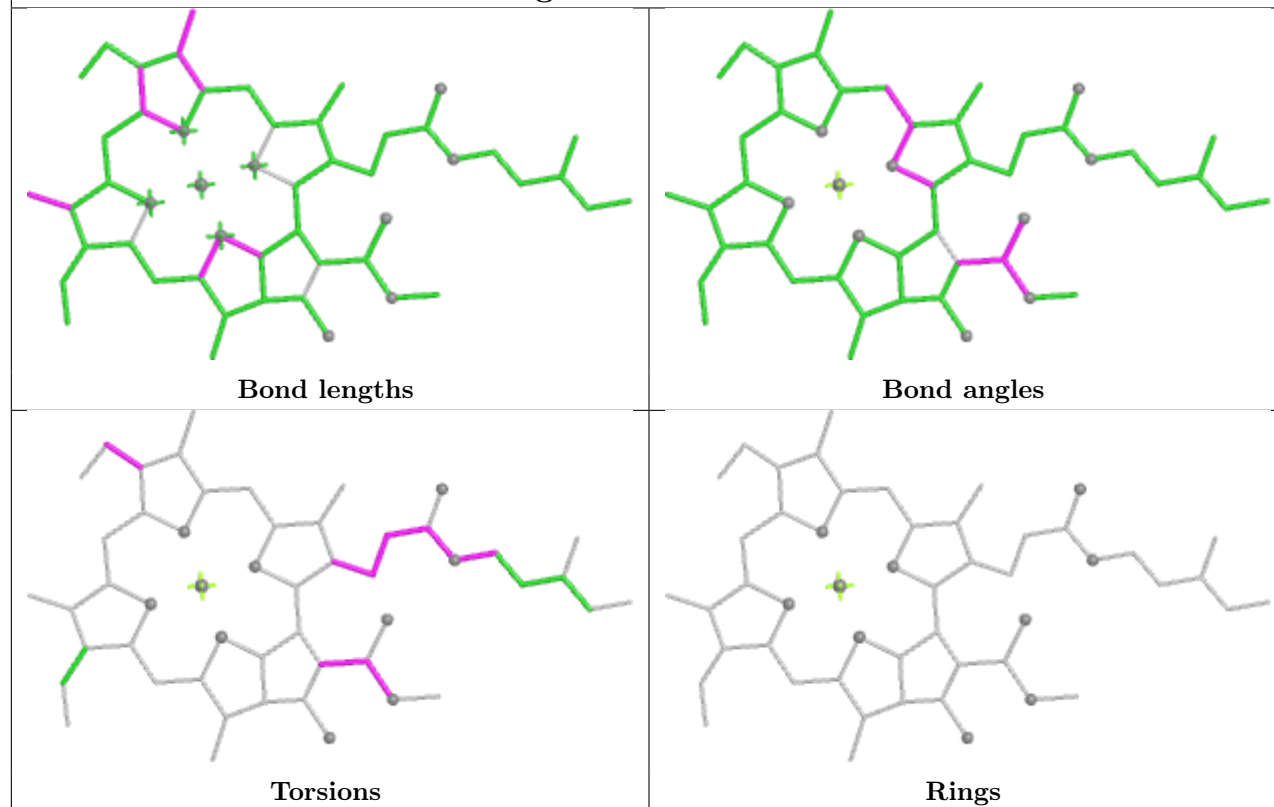
Ligand CLA i 311



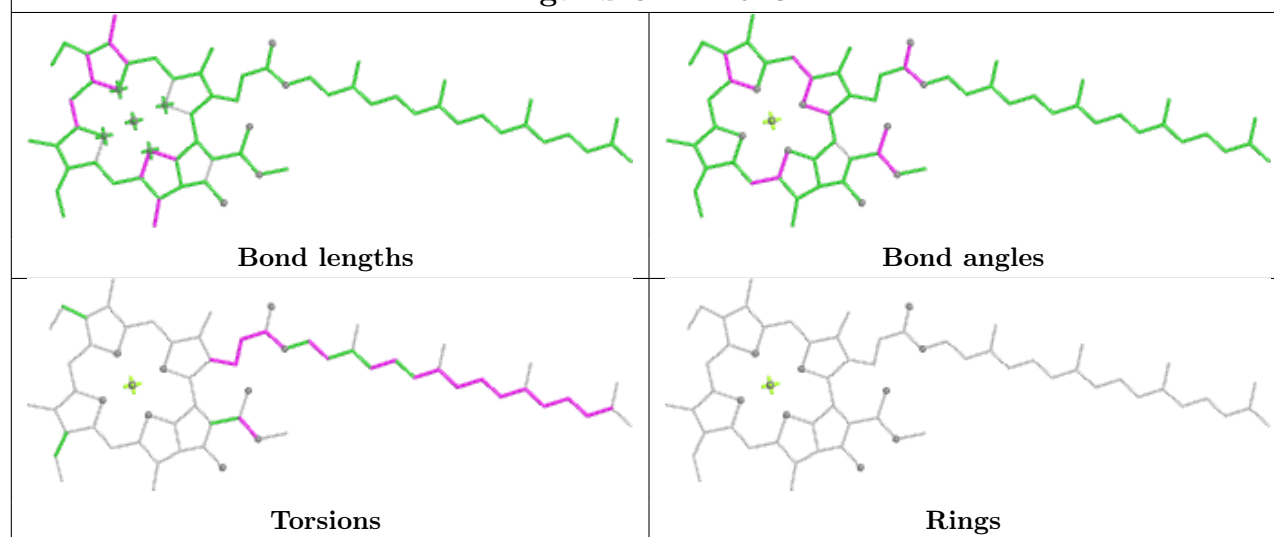
Ligand CLA A 833

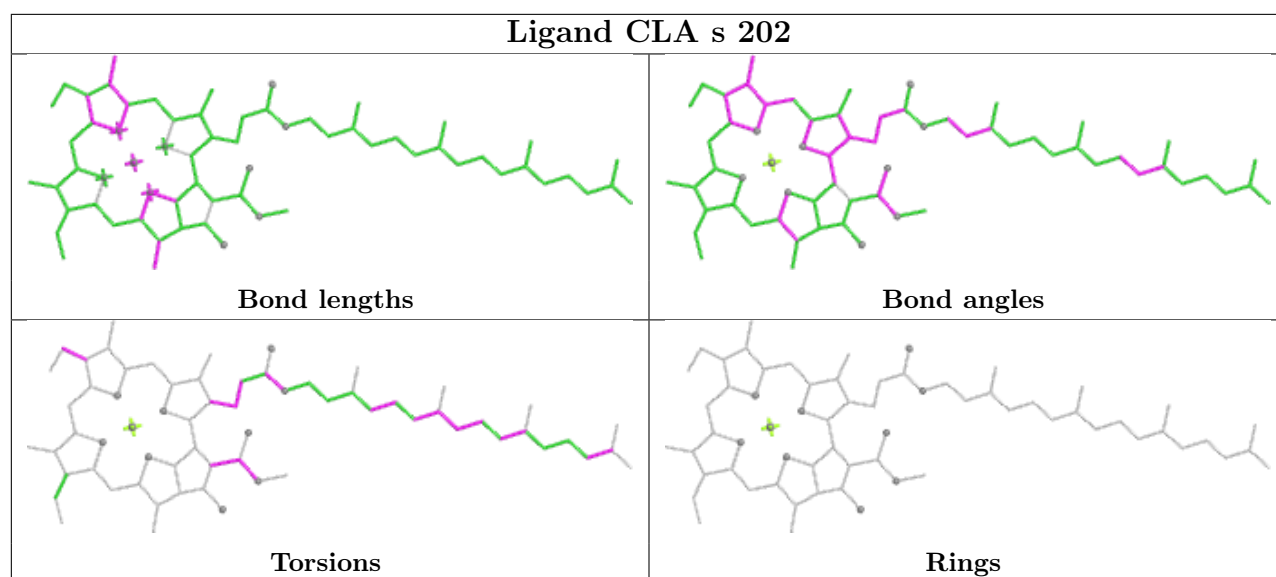
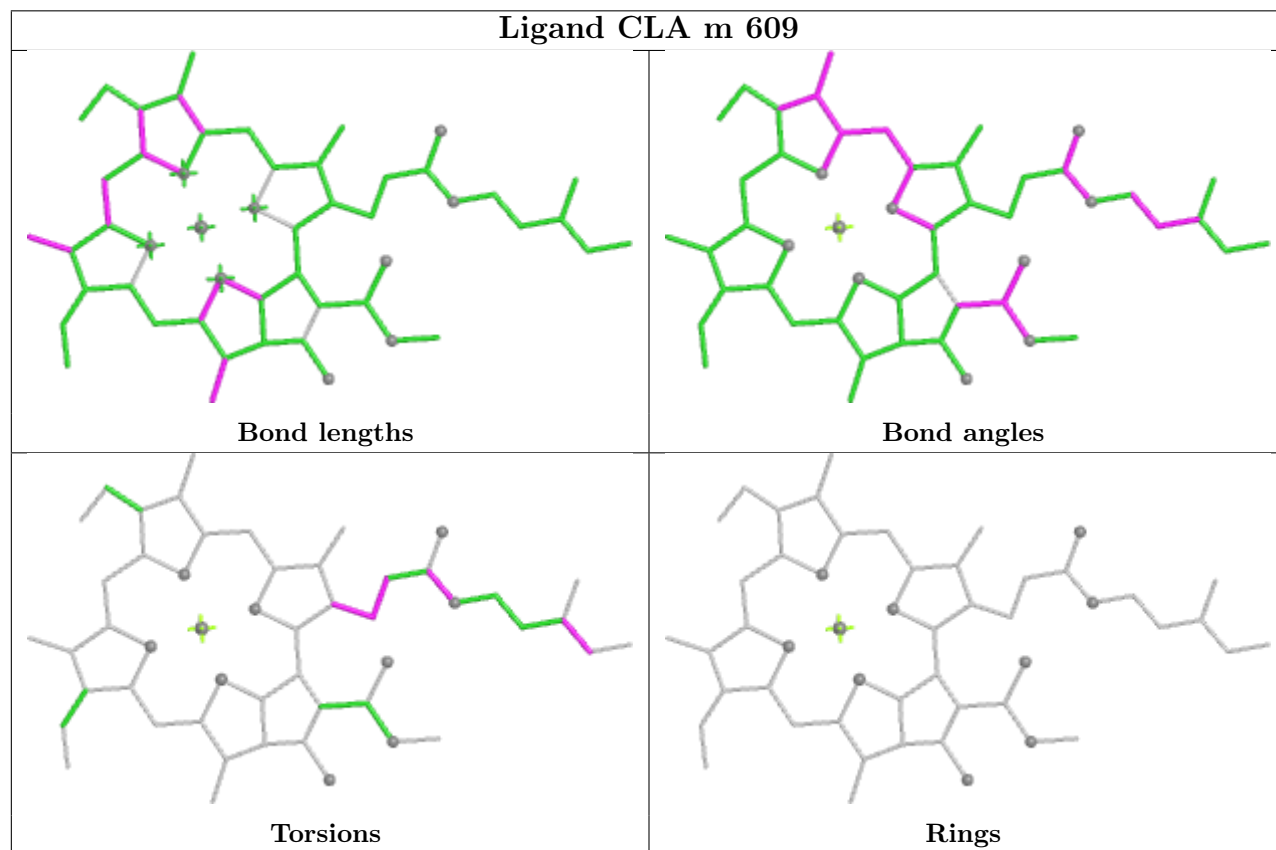


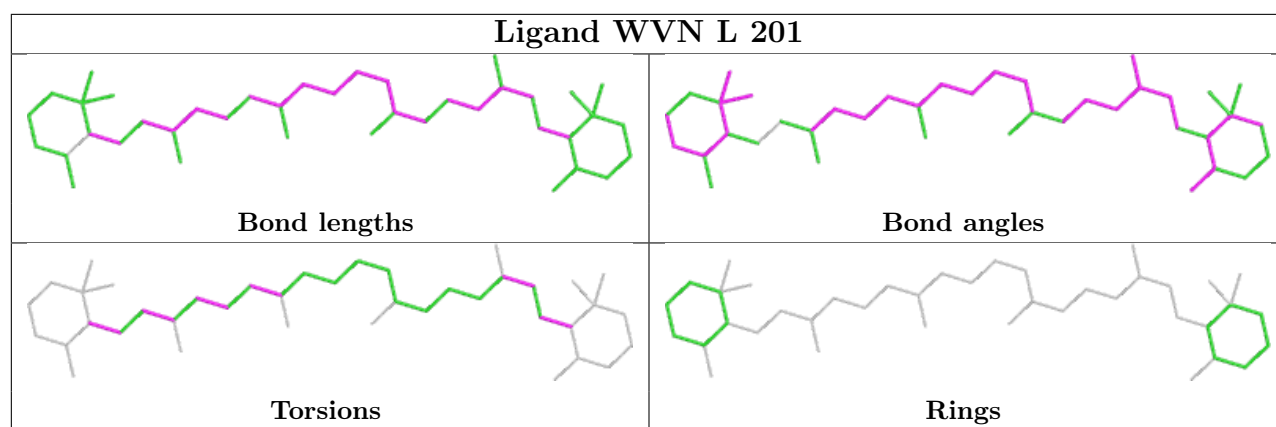
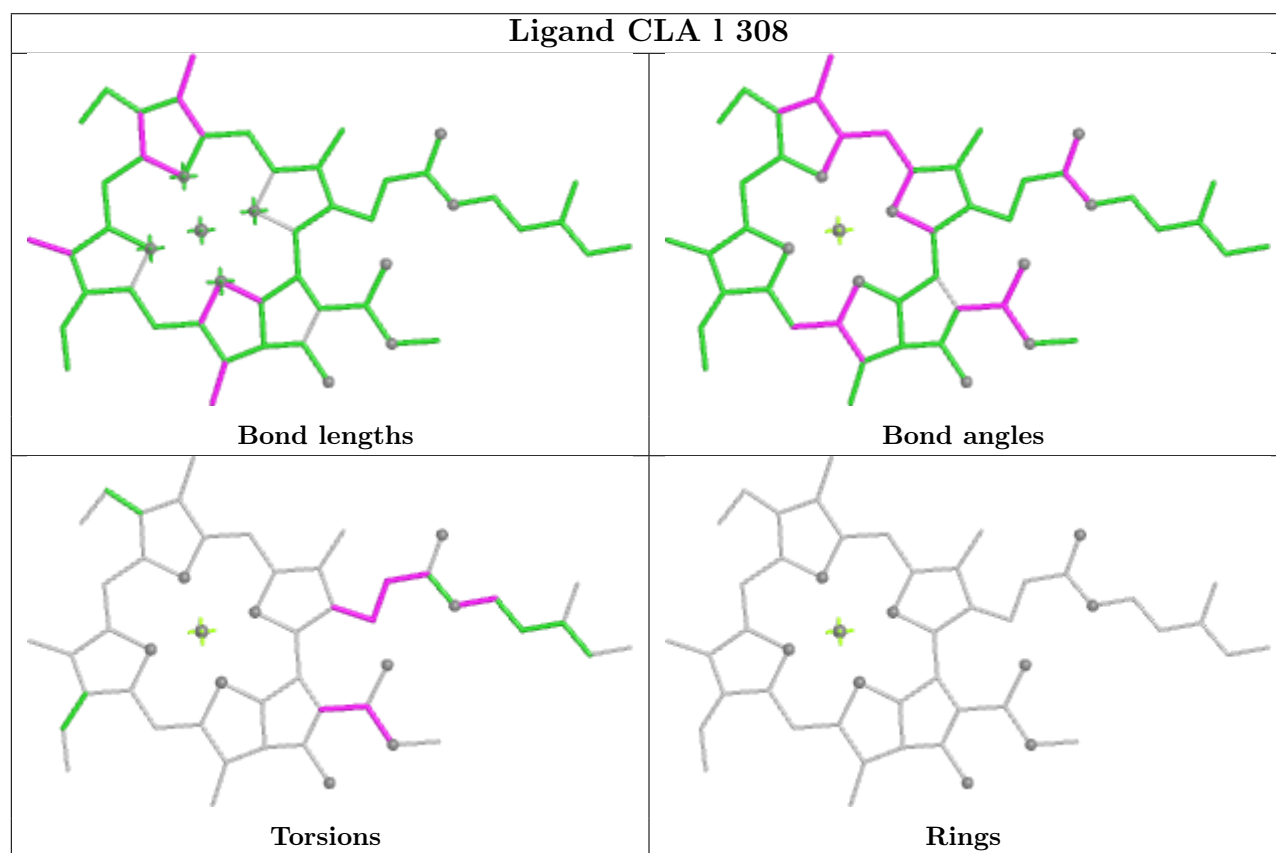
Ligand CLA k 610

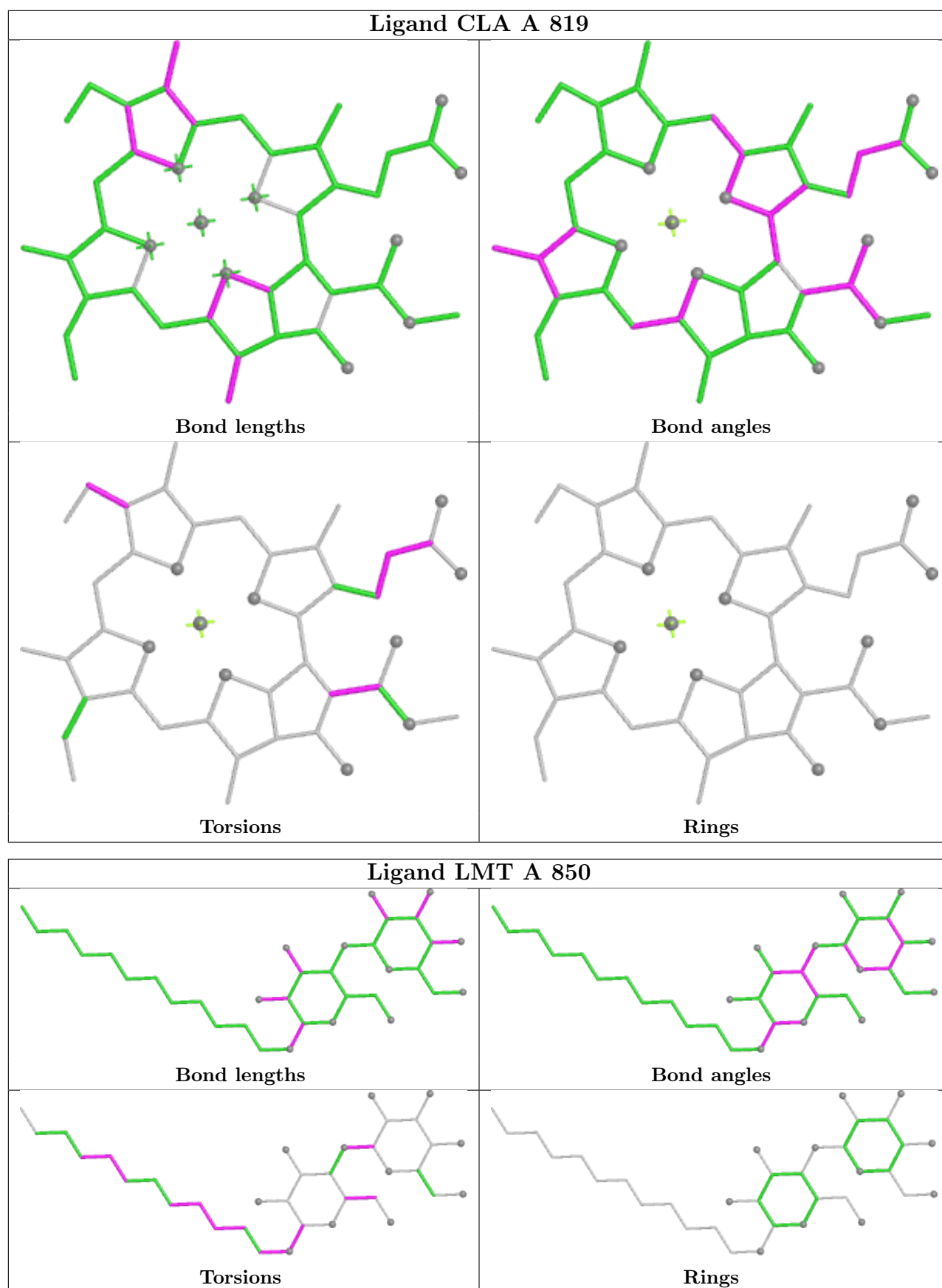


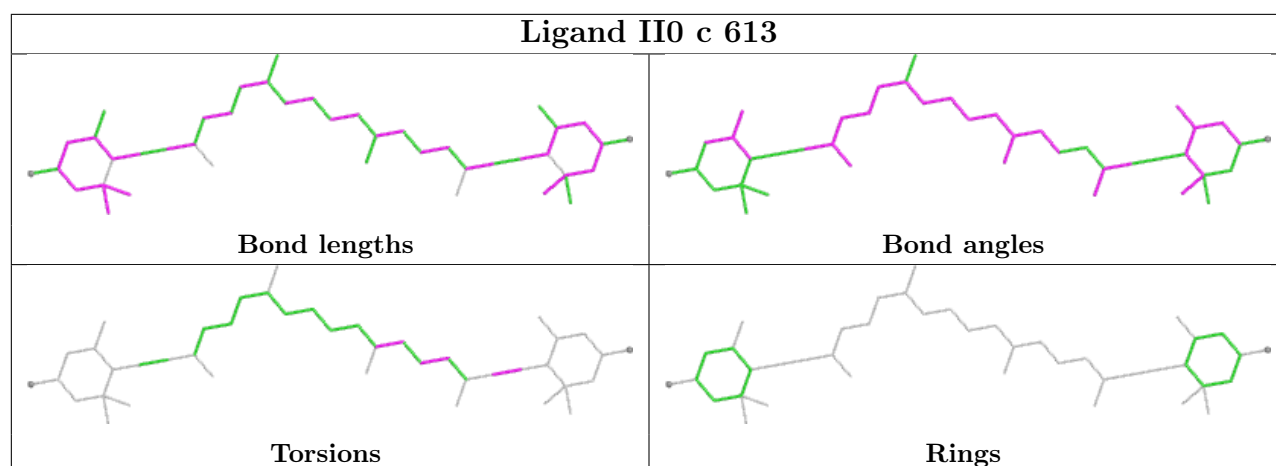
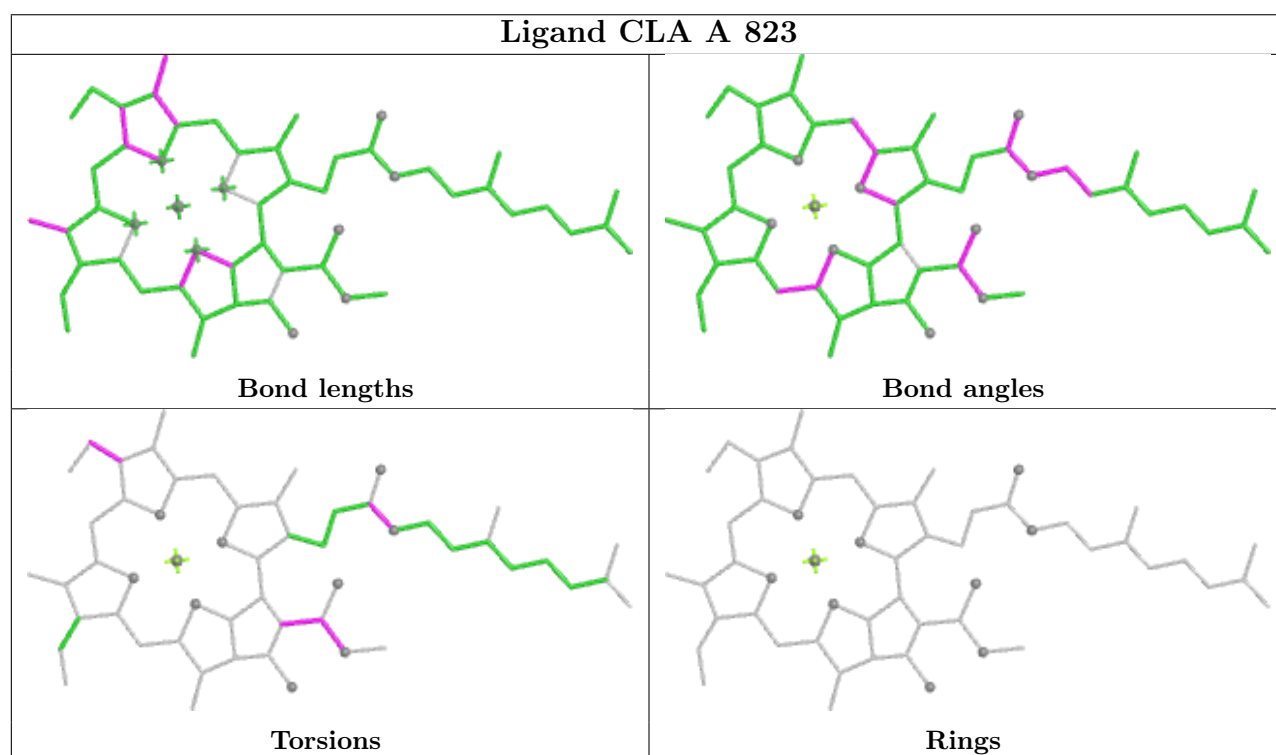
Ligand CLA f 613



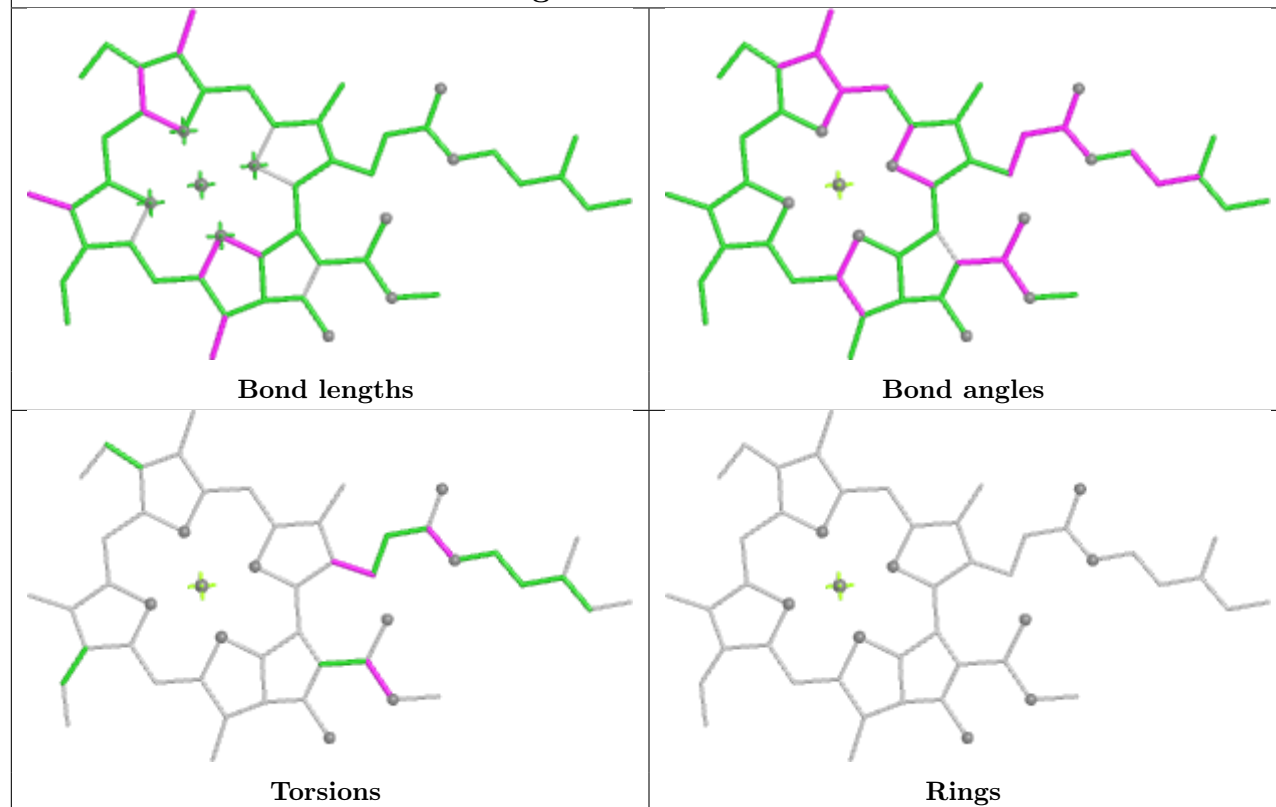




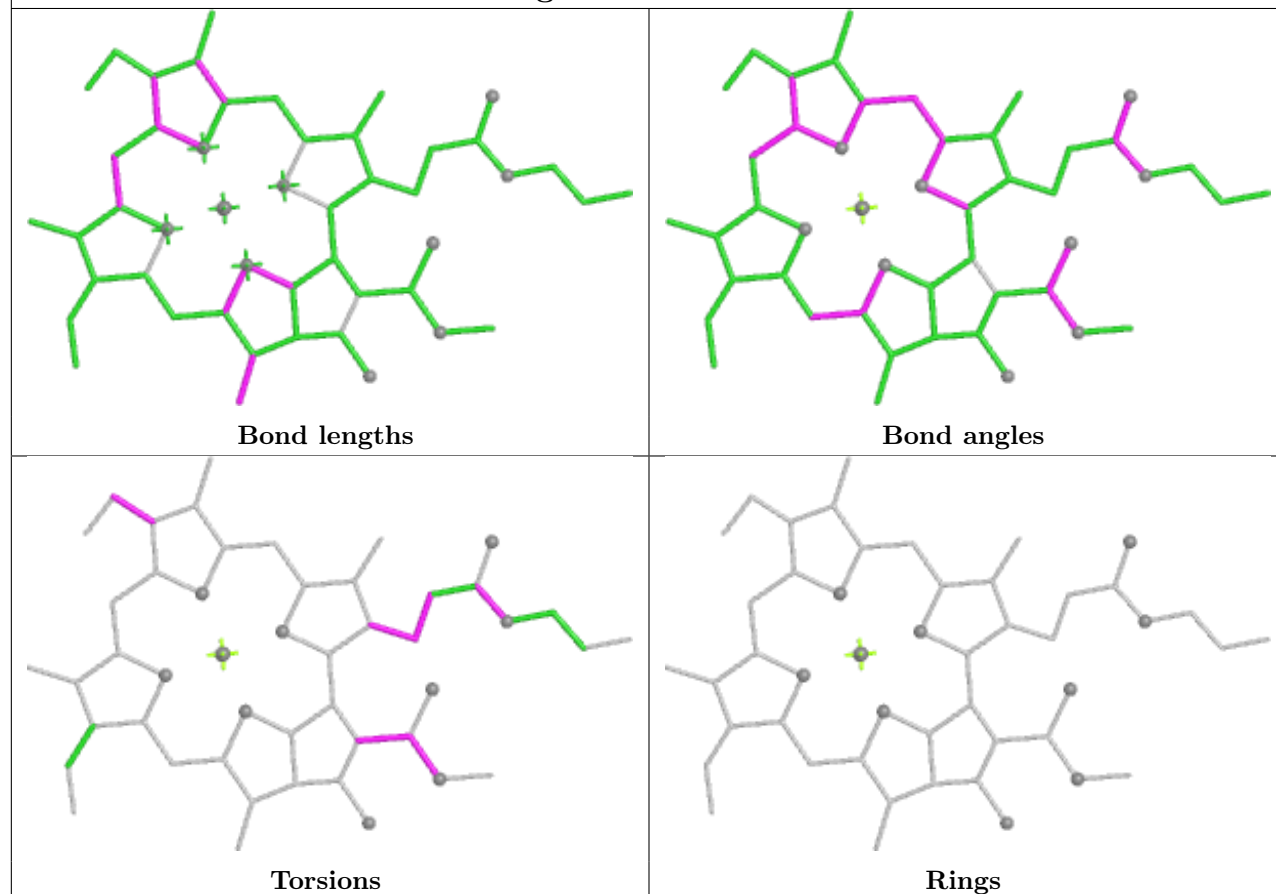


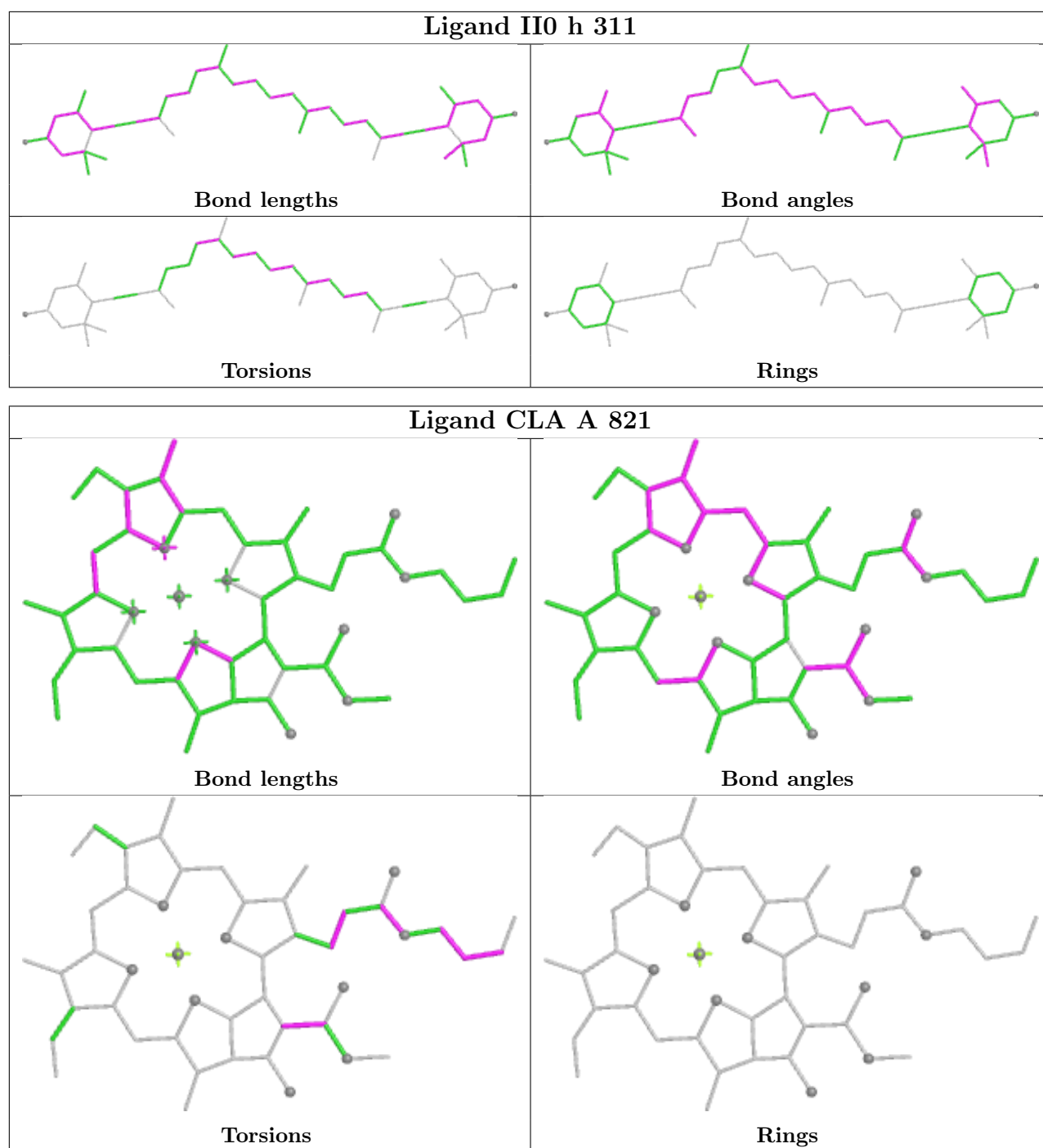


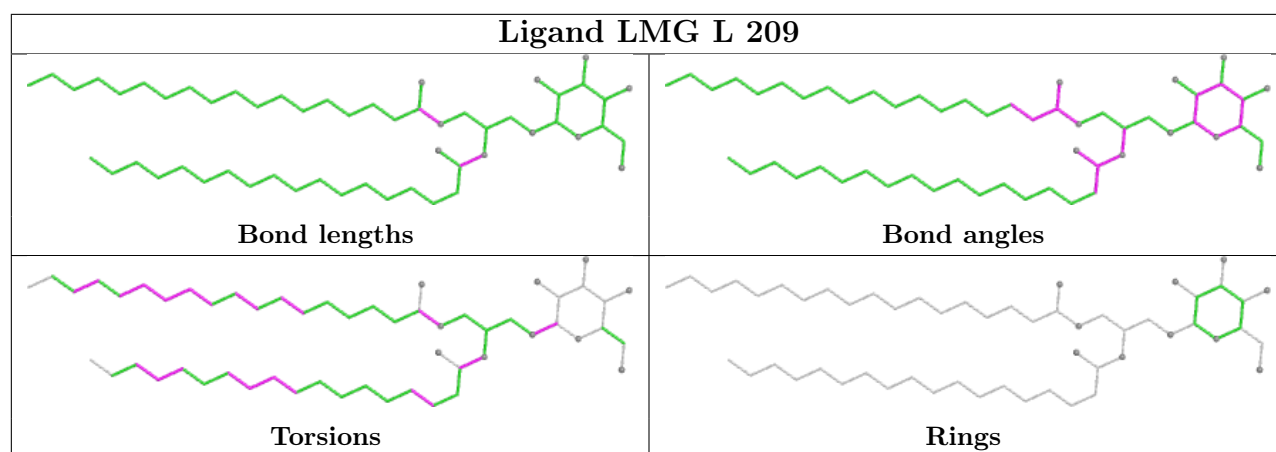
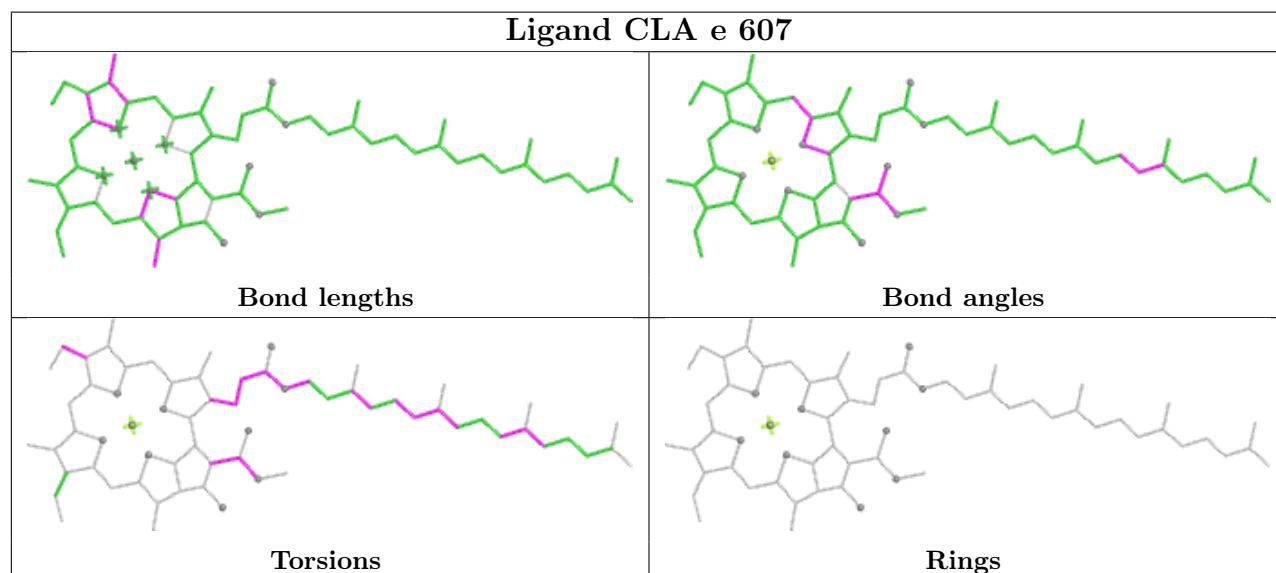
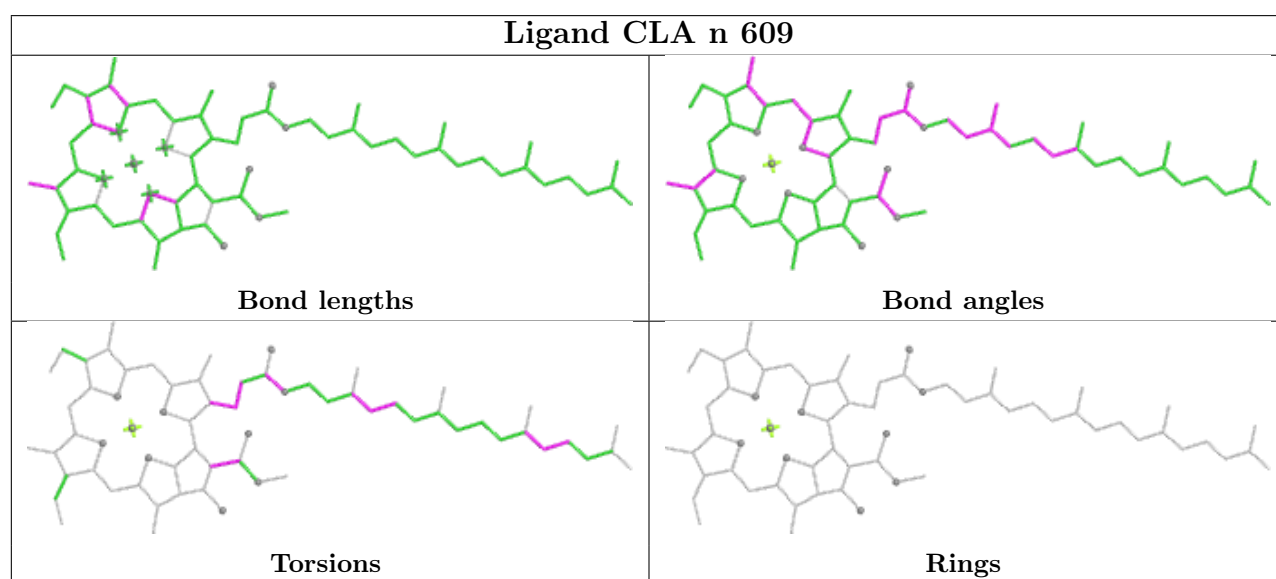
Ligand CLA B 826

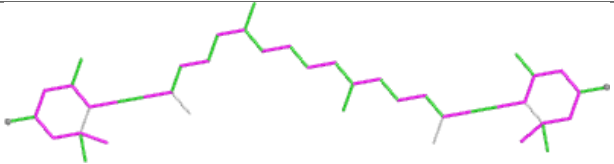
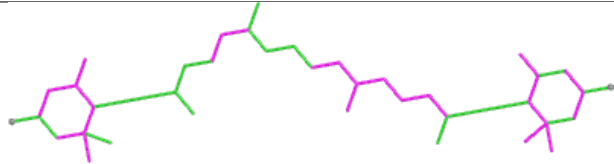
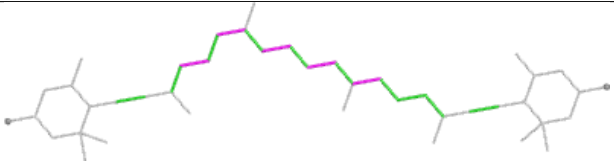
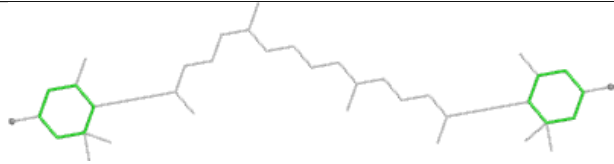


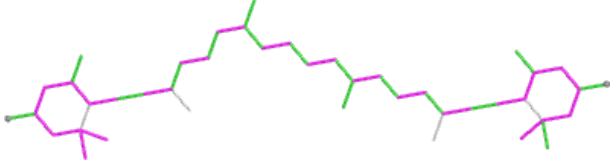
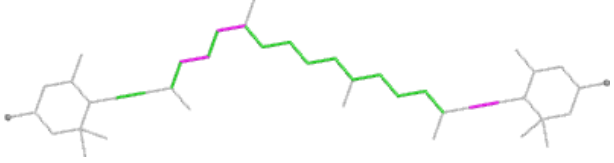
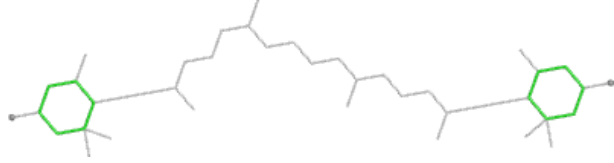
Ligand CLA a 313

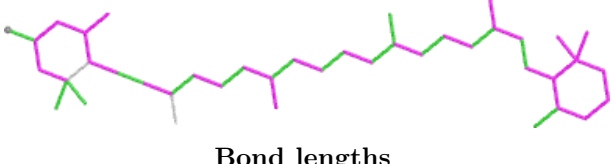
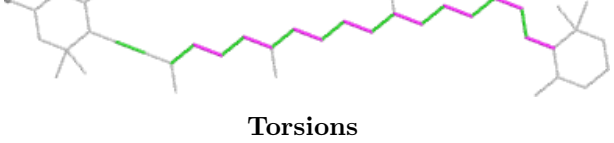
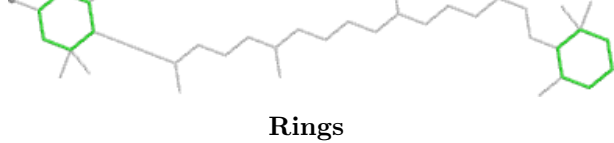




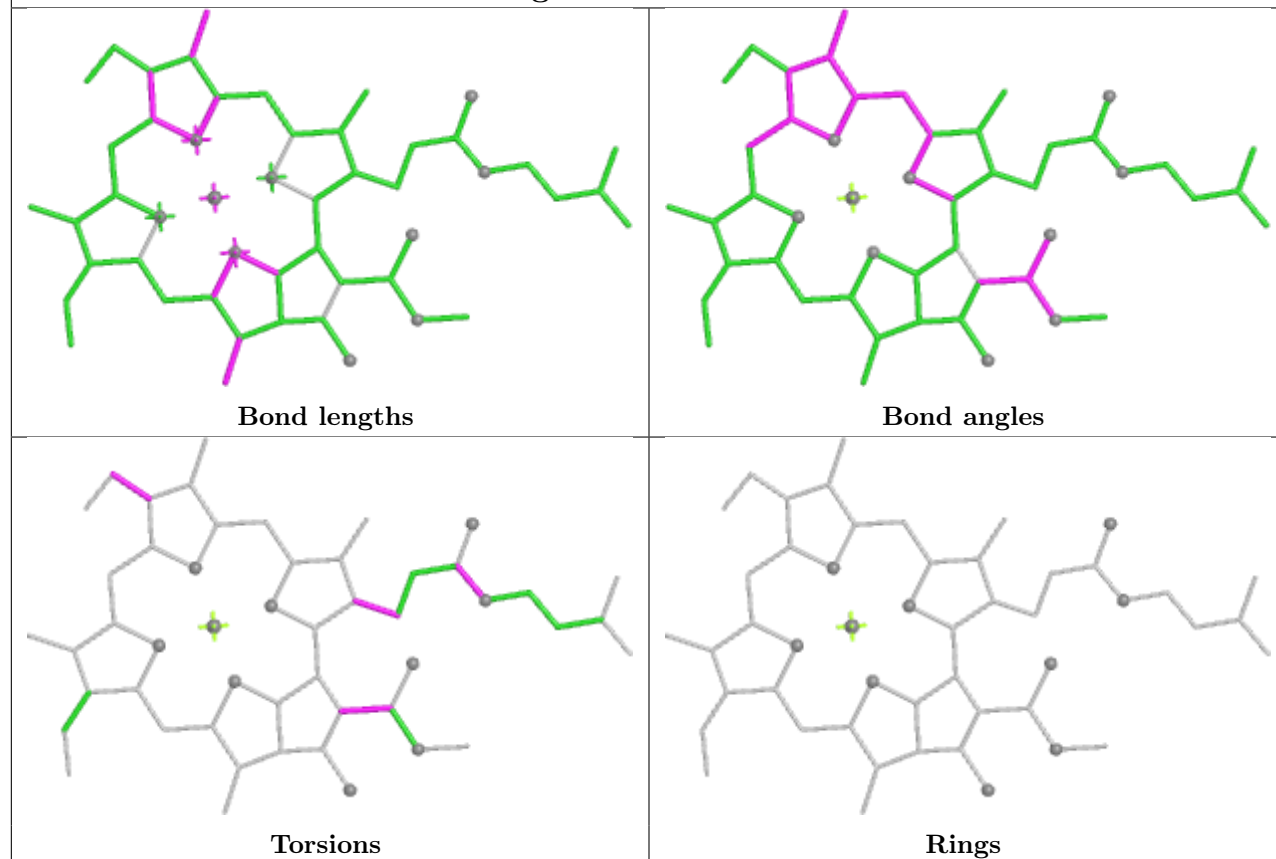


Ligand II0 a 318	
	Bond lengths
	Bond angles
	Torsions
	Rings

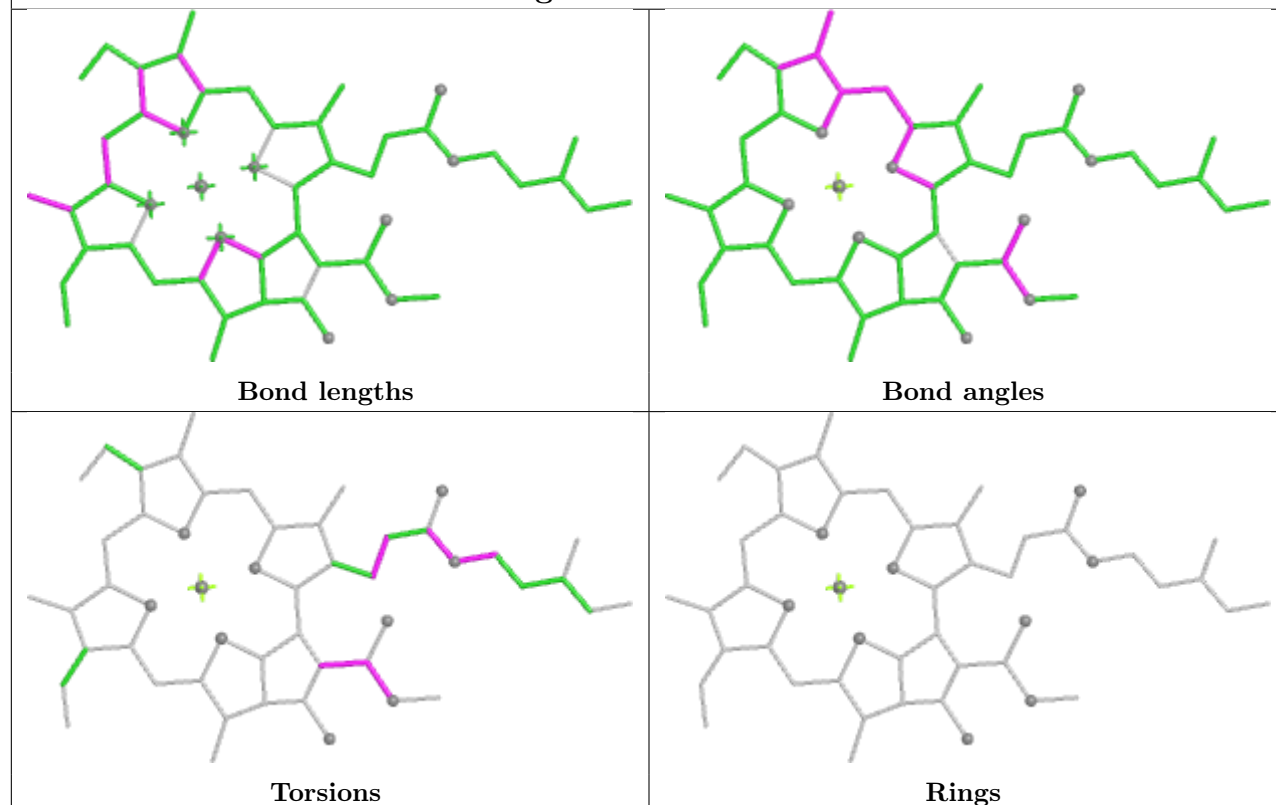
Ligand II0 n 615	
	Bond lengths
	Bond angles
	Torsions
	Rings

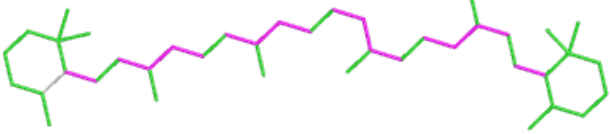
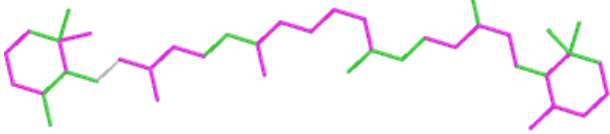
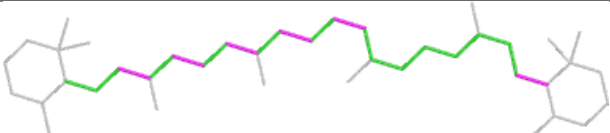
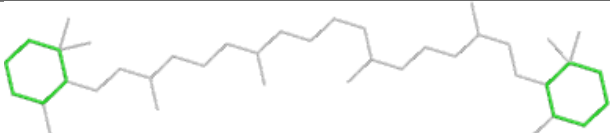
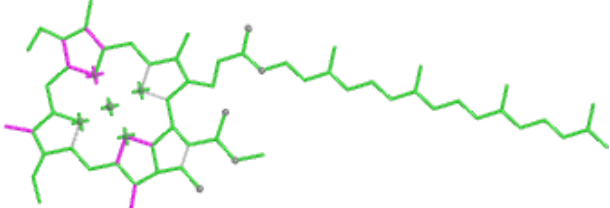
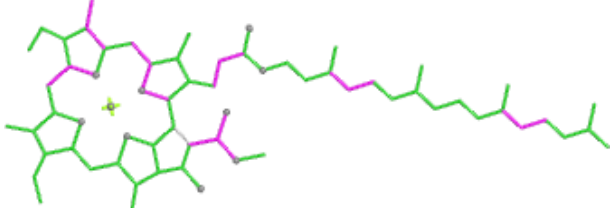
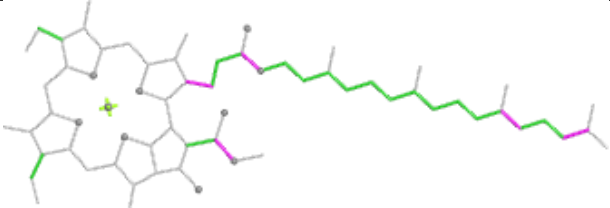
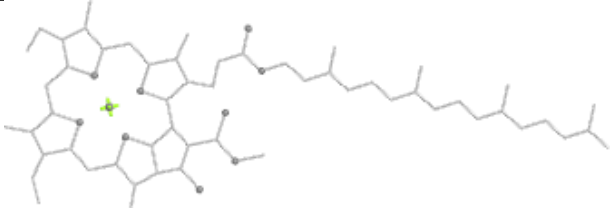
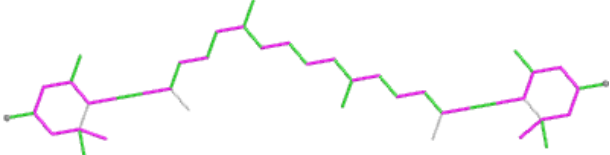
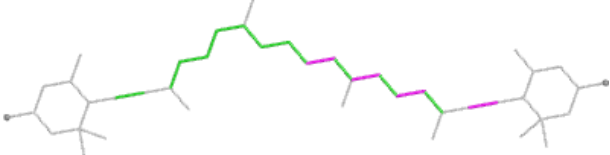
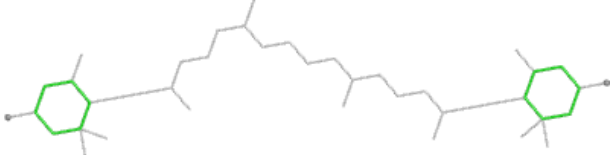
Ligand IHT k 618	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand CLA A 830

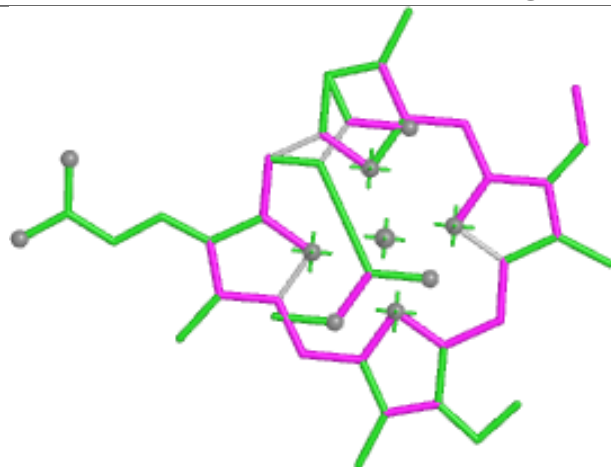


Ligand CLA d 304

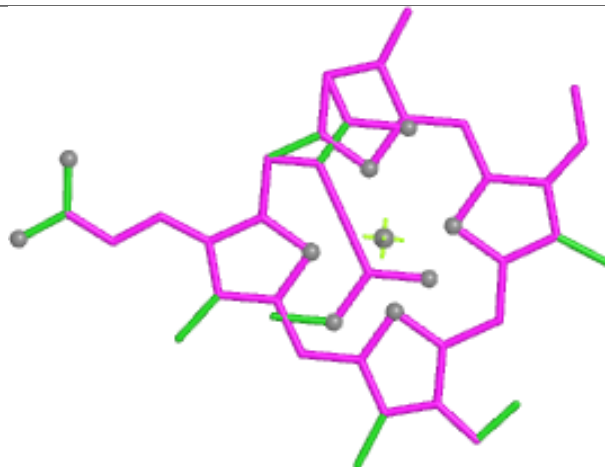


Ligand WVN 1 315	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA A 837	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand II0 i 314	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

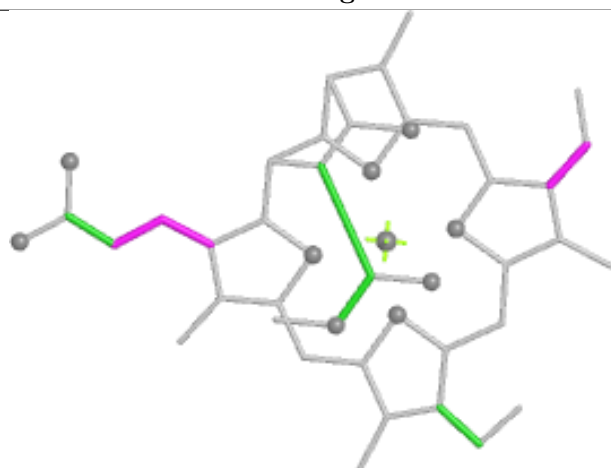
Ligand KC2 s 204



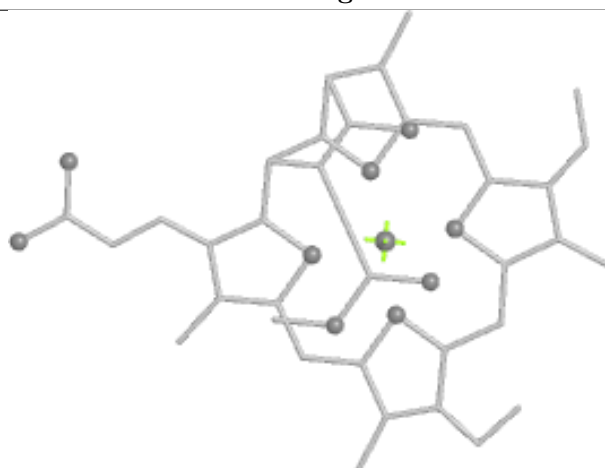
Bond lengths



Bond angles



Torsions



Rings

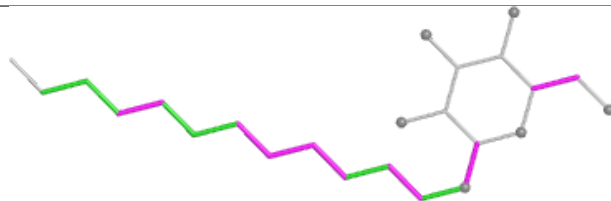
Ligand LMT b 618



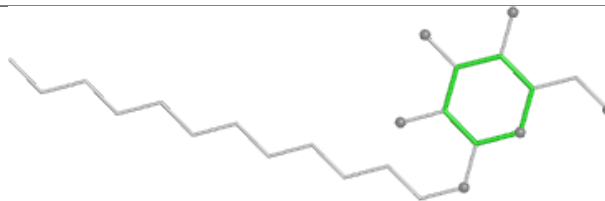
Bond lengths



Bond angles

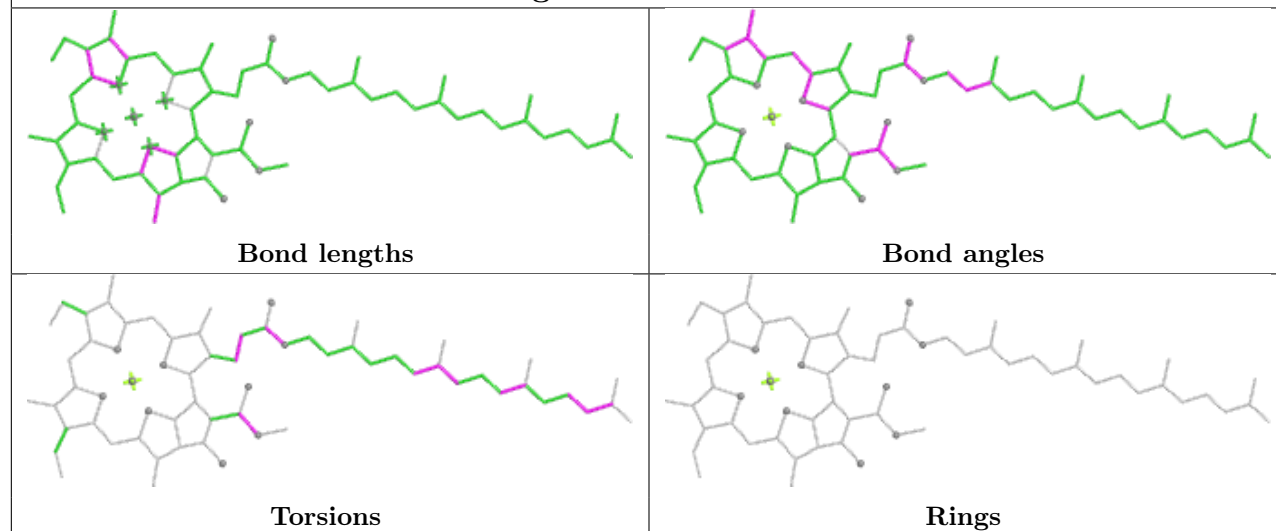


Torsions

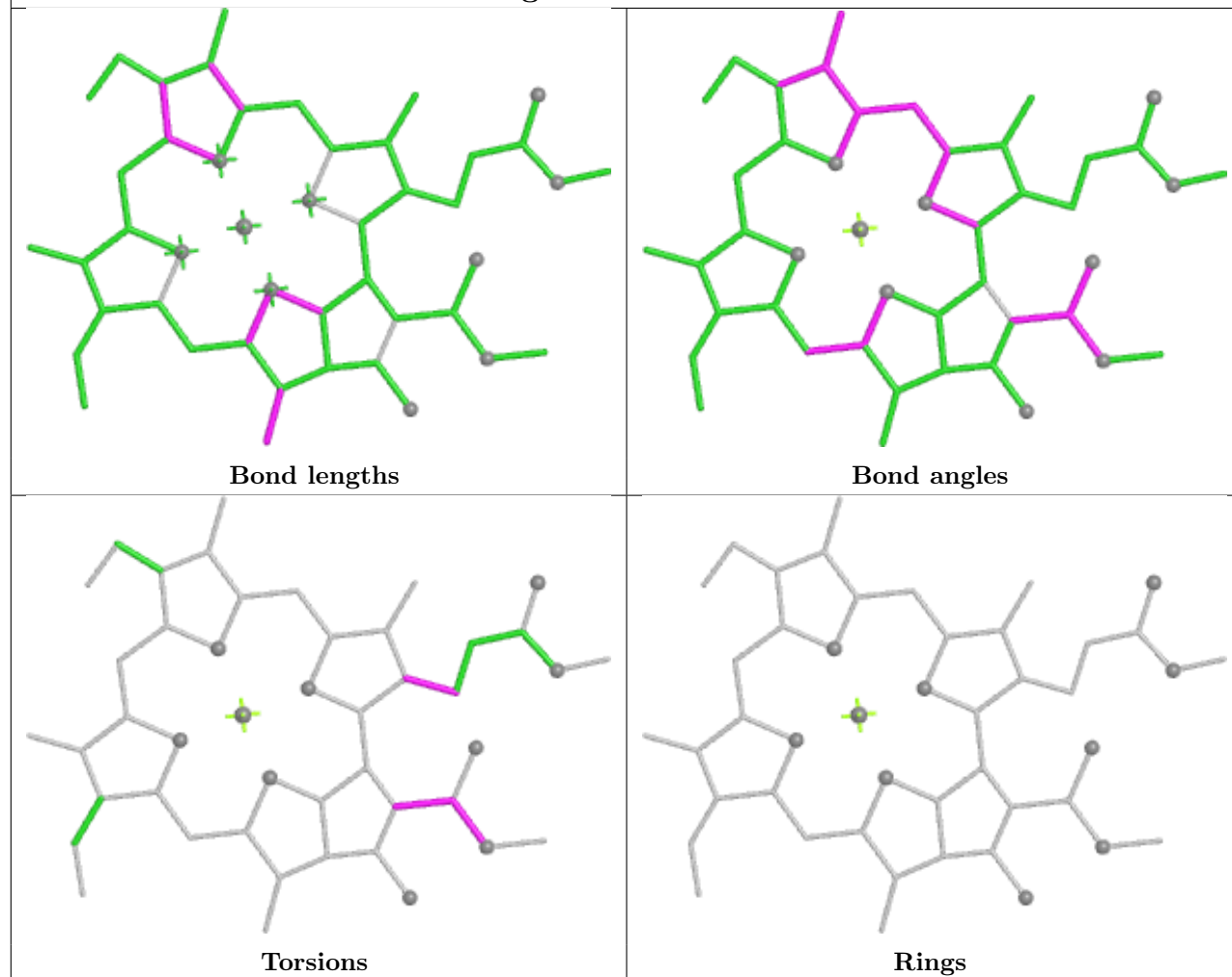


Rings

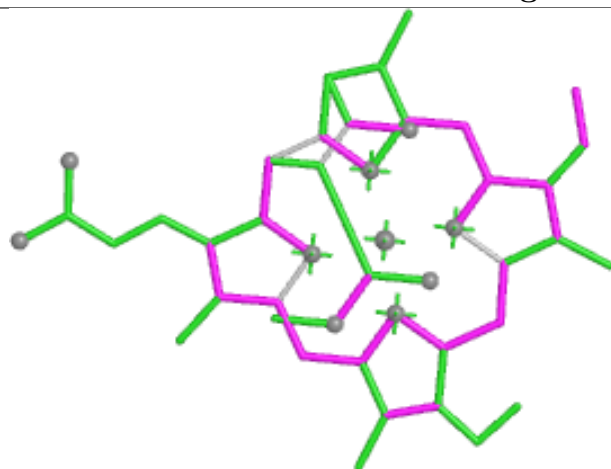
Ligand CLA B 837



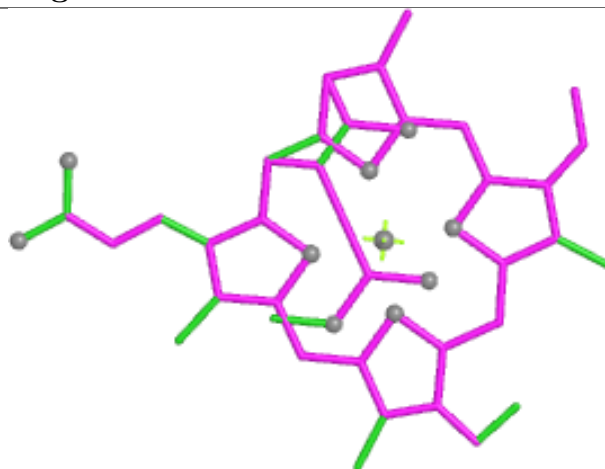
Ligand CLA i 309



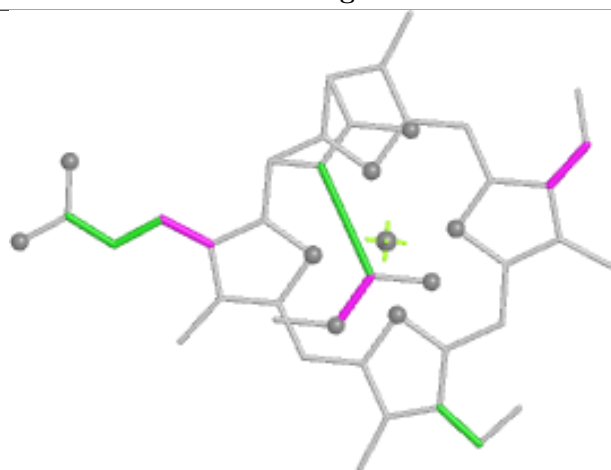
Ligand KC2 g 314



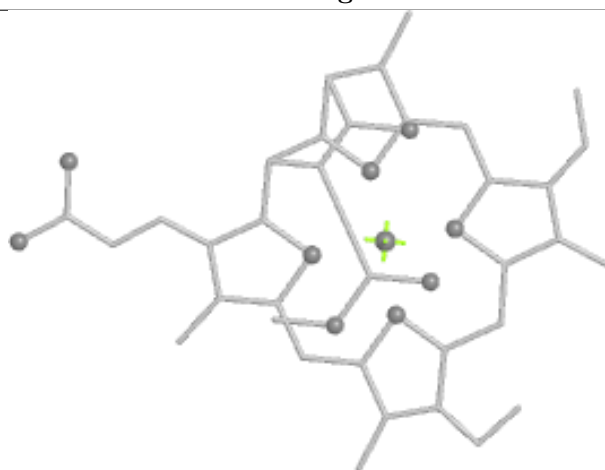
Bond lengths



Bond angles

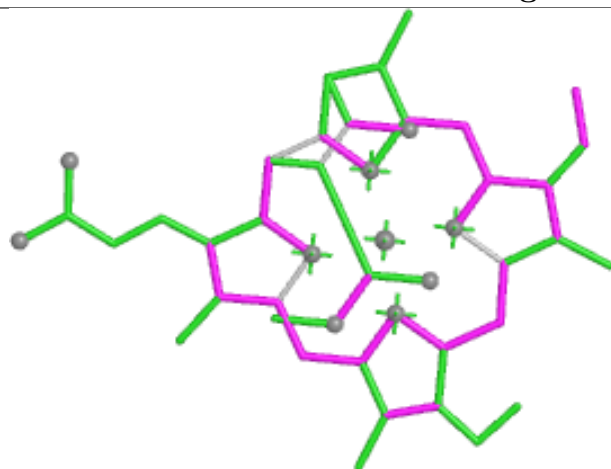


Torsions

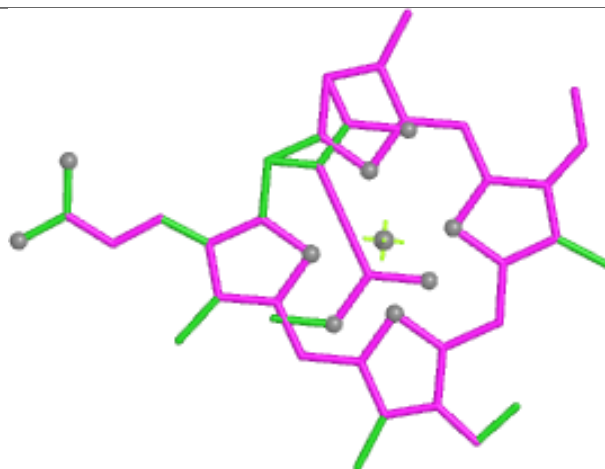


Rings

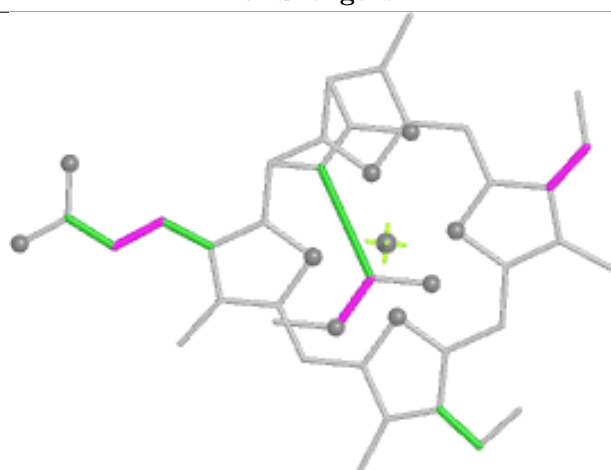
Ligand KC2 k 611



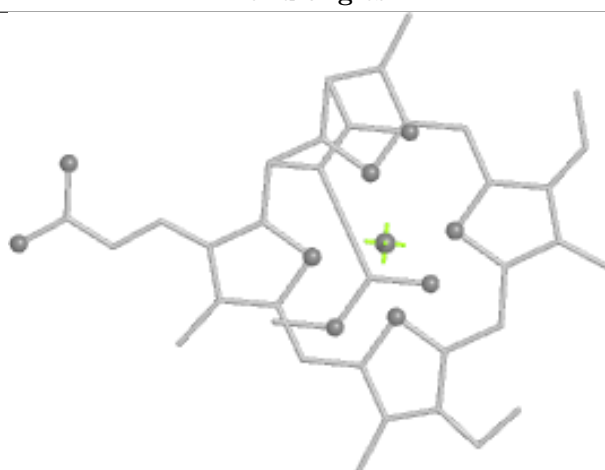
Bond lengths



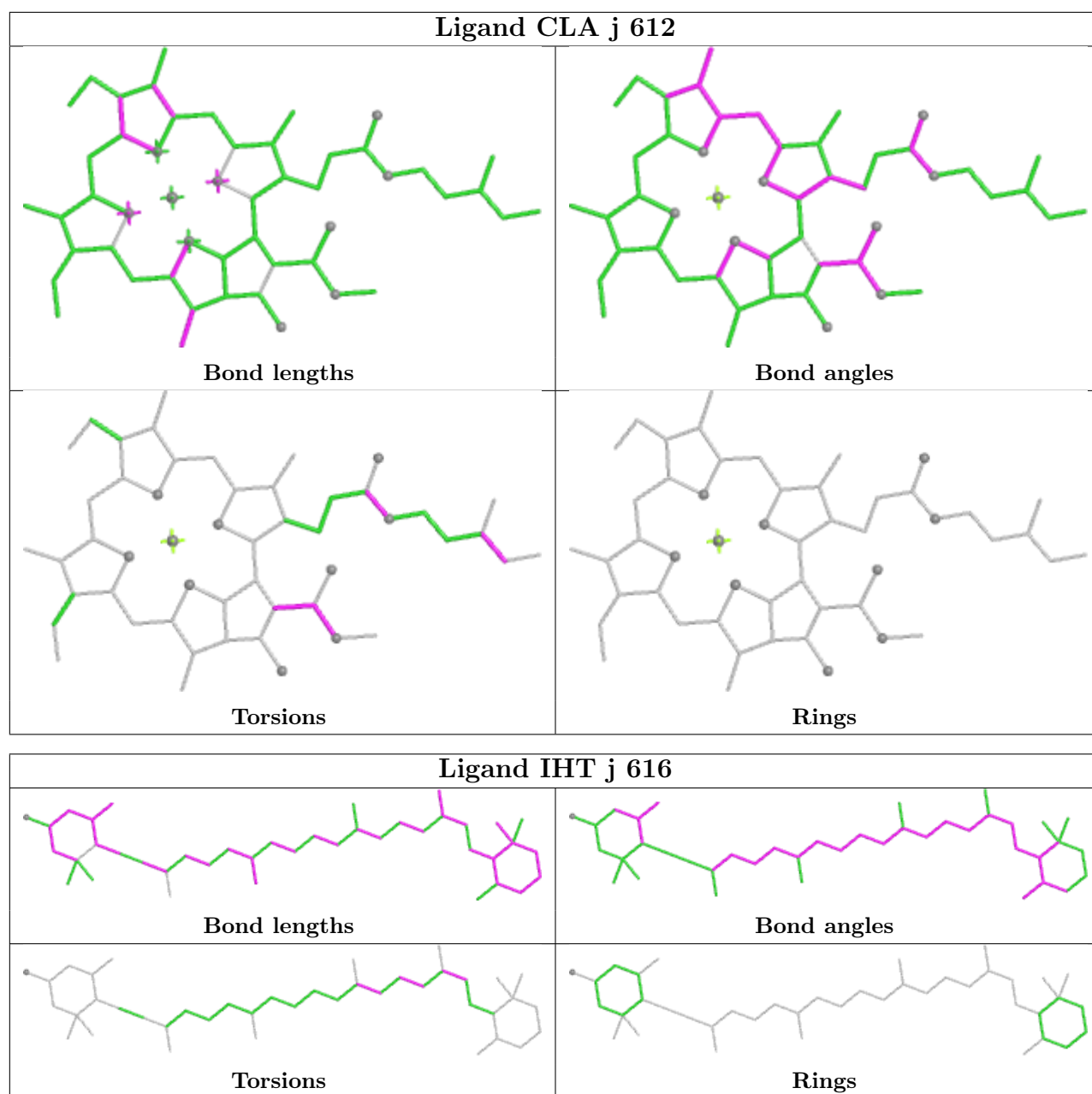
Bond angles



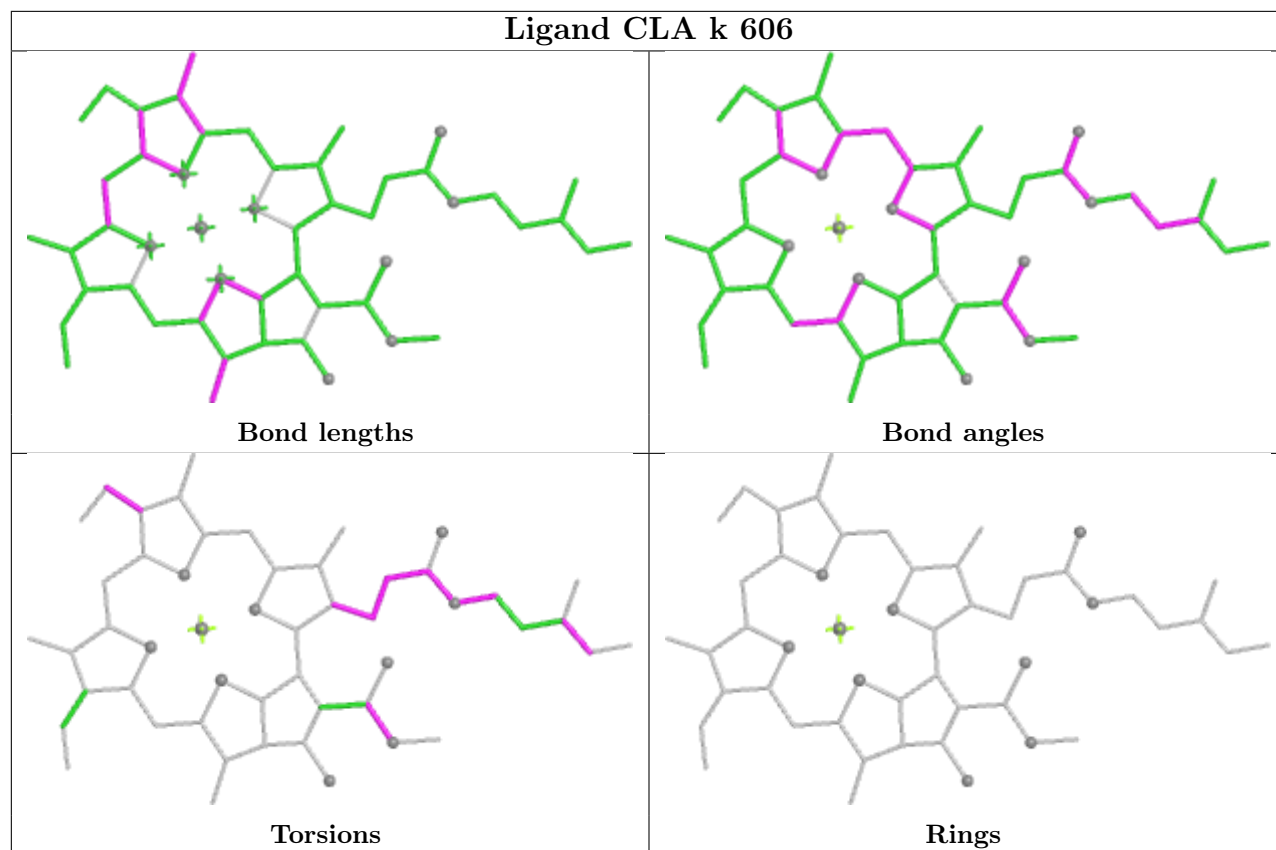
Torsions



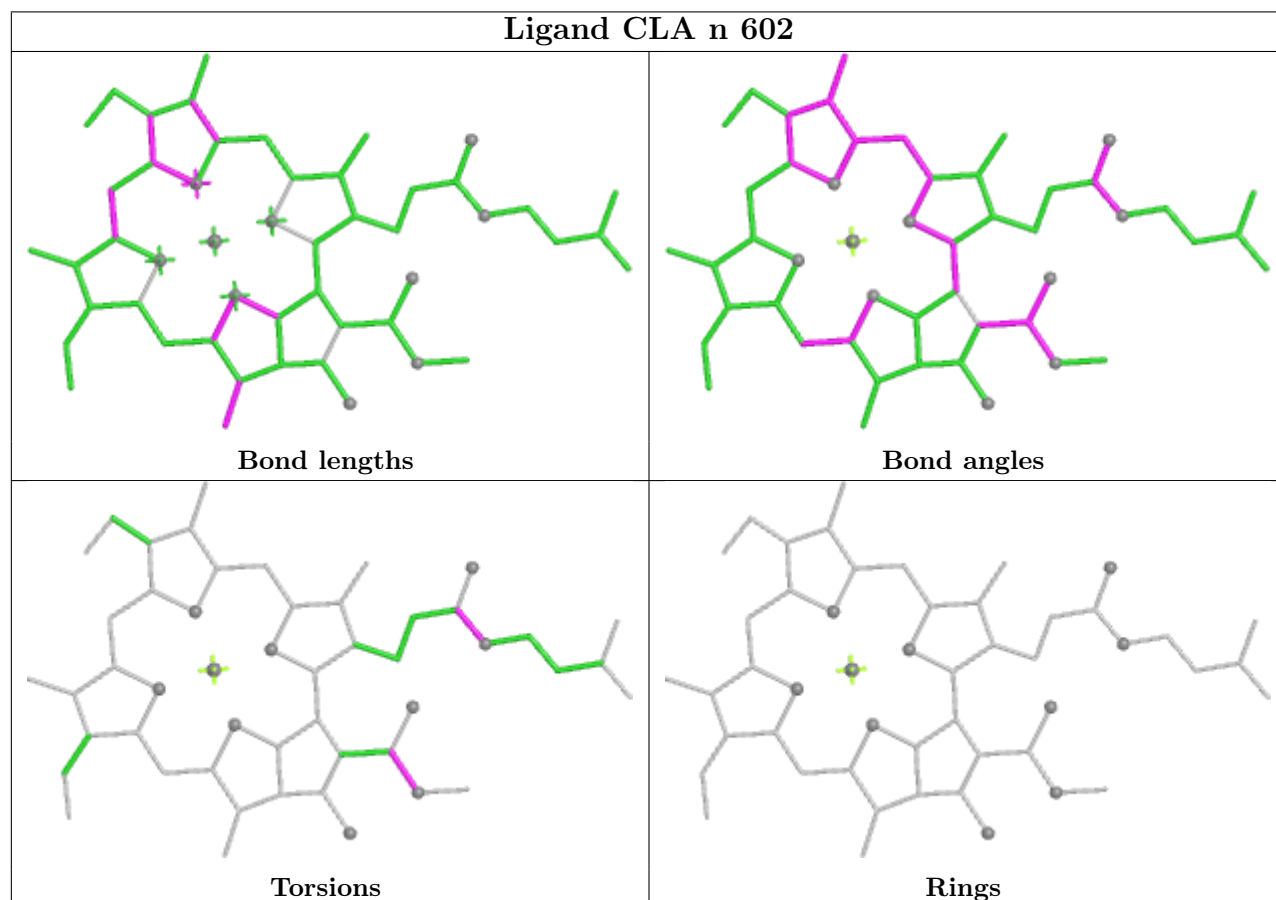
Rings



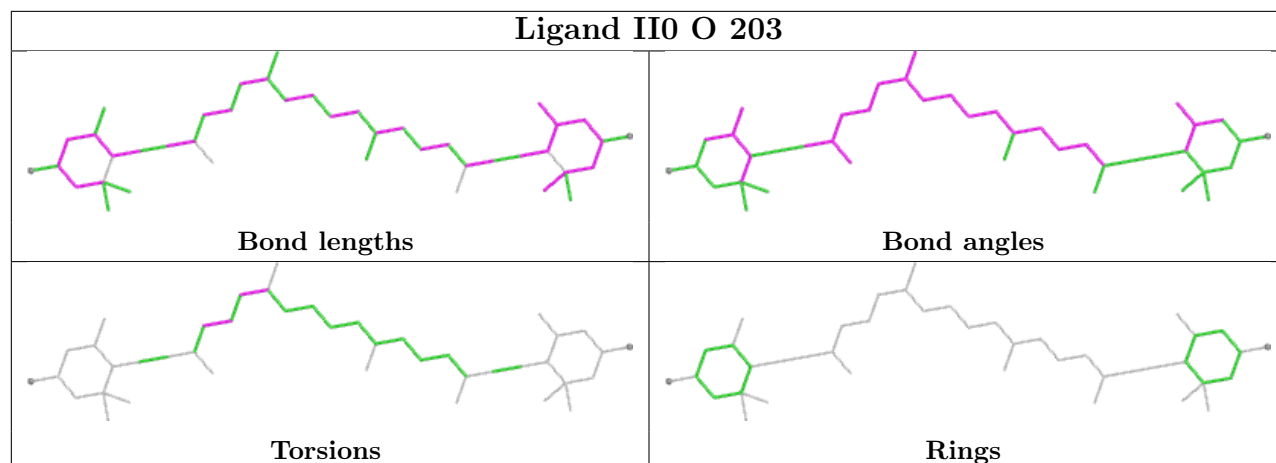
Ligand CLA k 606



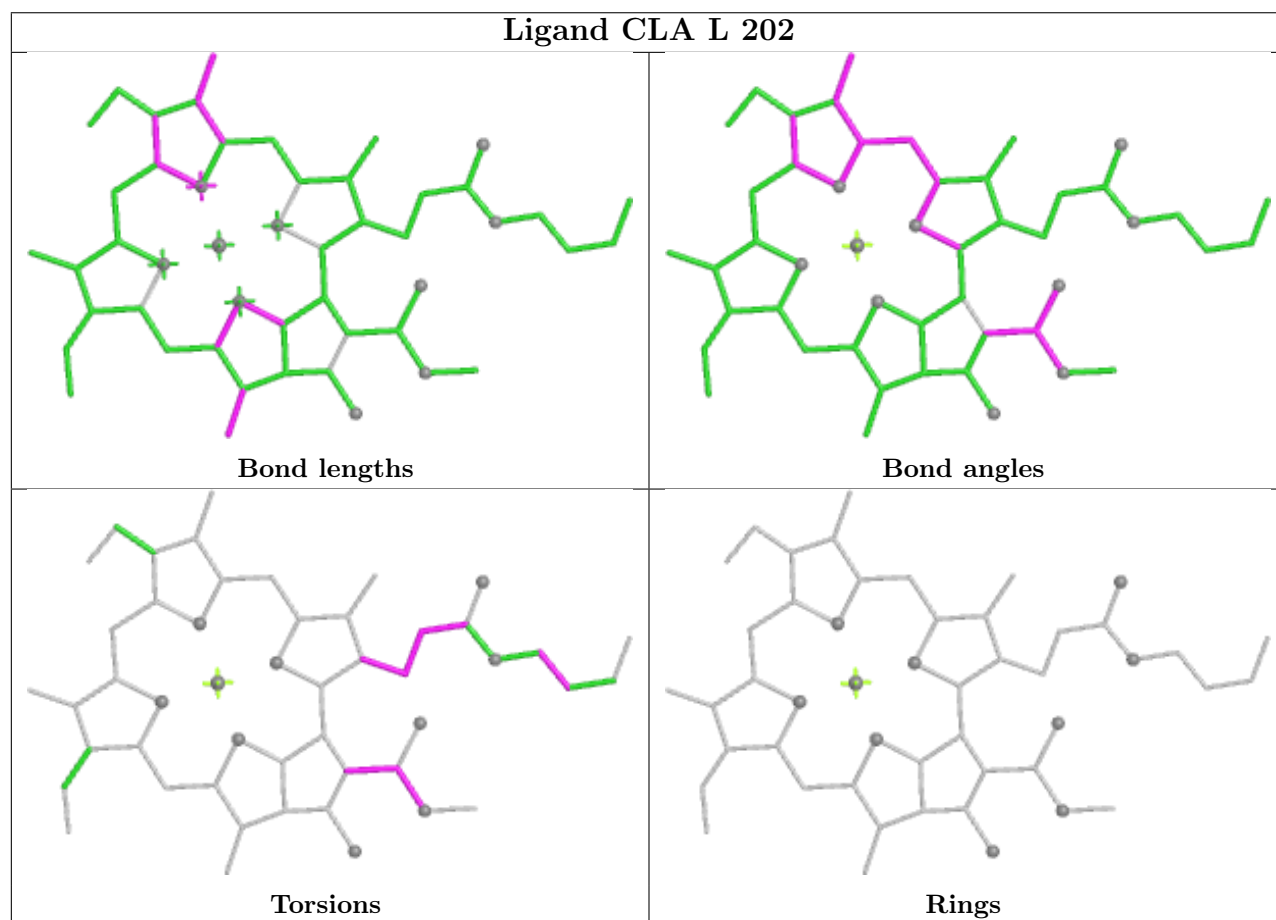
Ligand CLA n 602



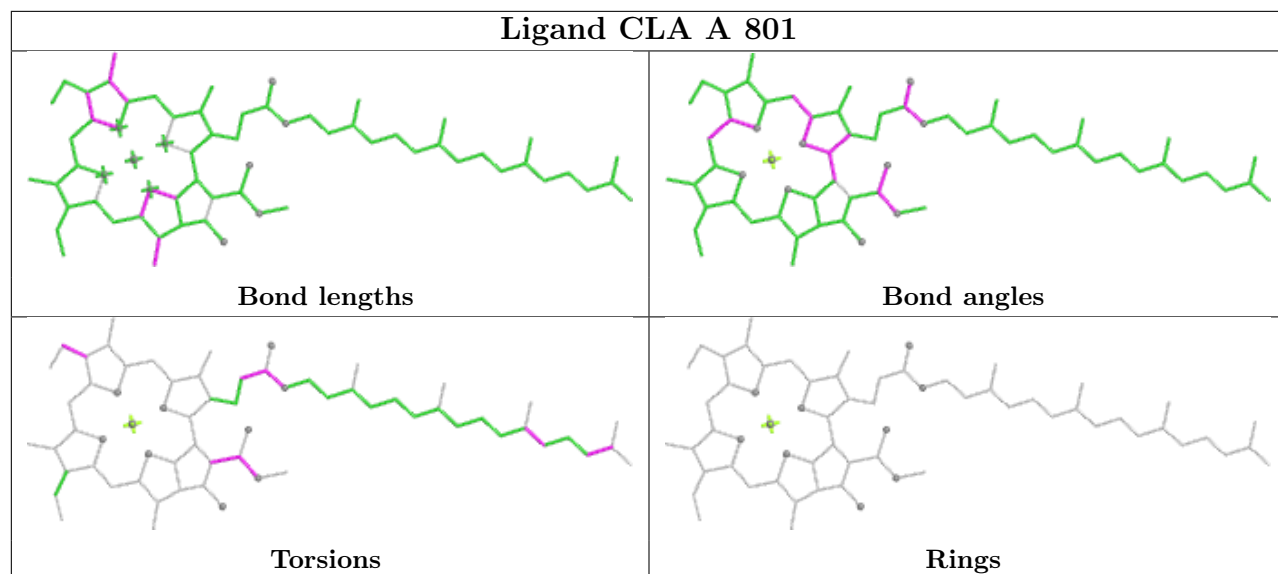
Ligand II0 O 203



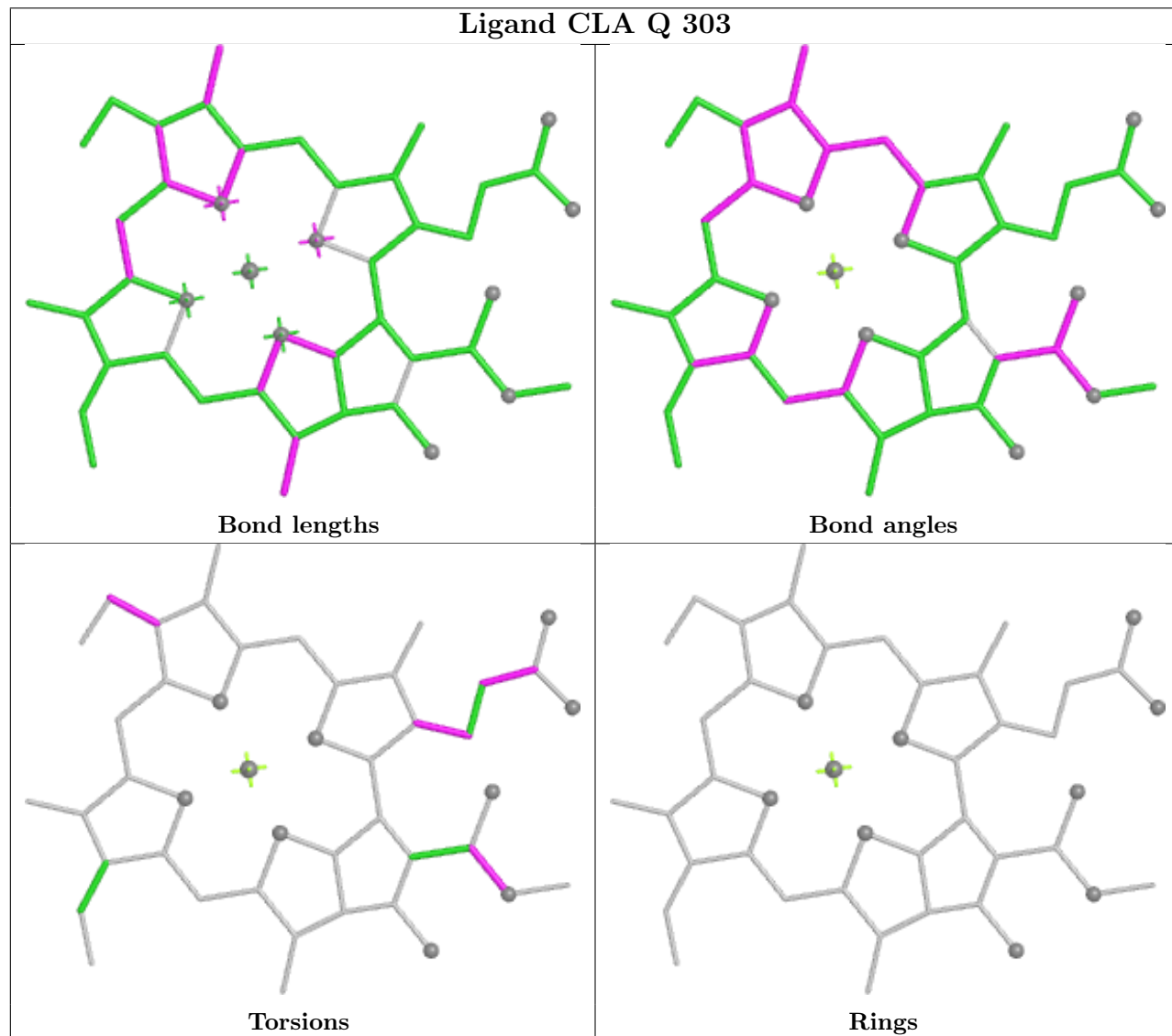
Ligand CLA L 202



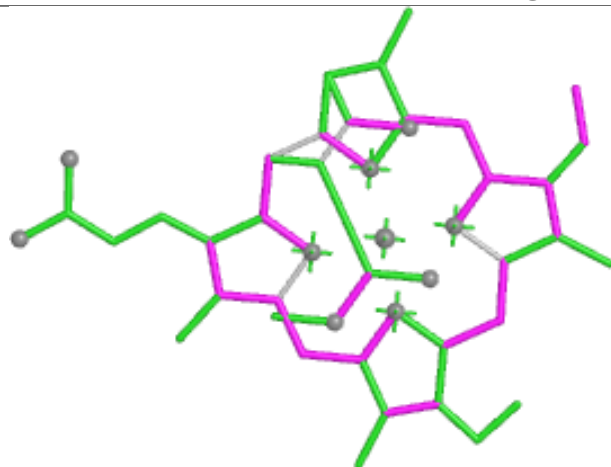
Ligand CLA A 801



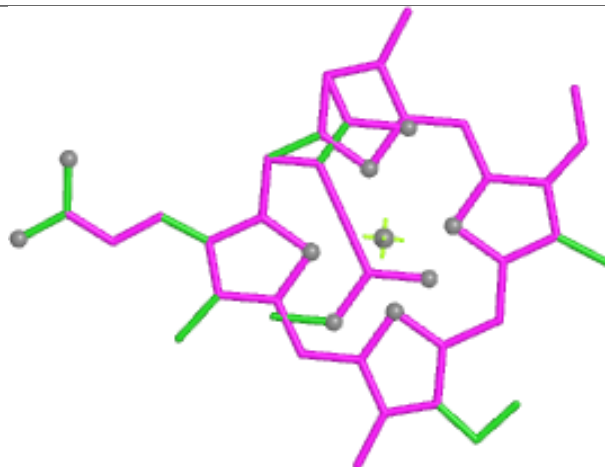
Ligand CLA Q 303



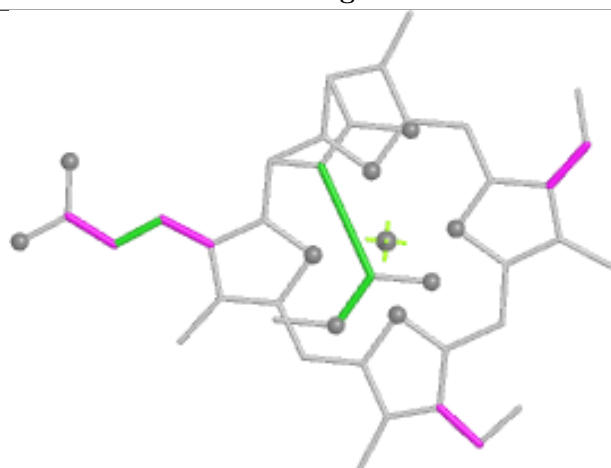
Ligand KC2 i 310



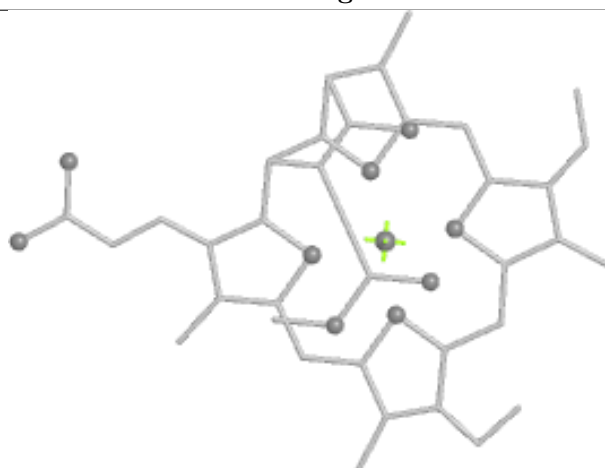
Bond lengths



Bond angles

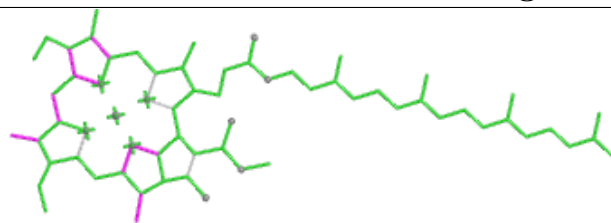


Torsions

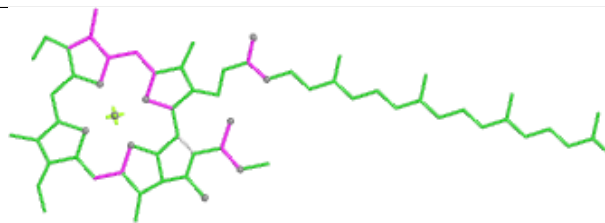


Rings

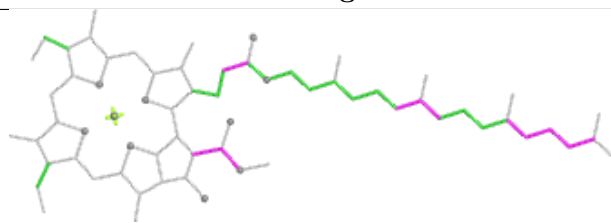
Ligand CLA a 306



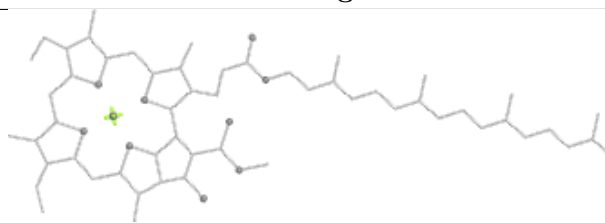
Bond lengths



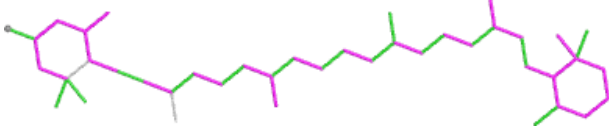
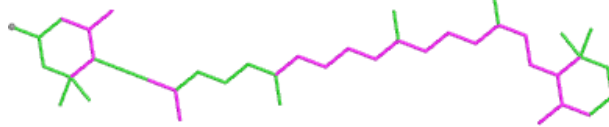
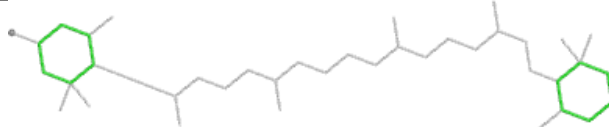
Bond angles

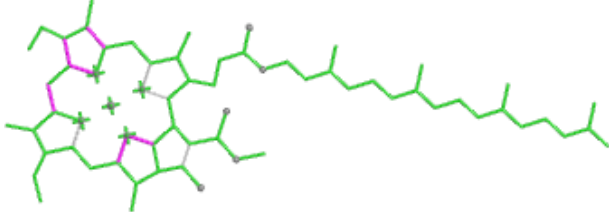
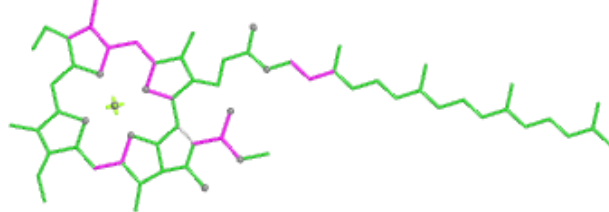
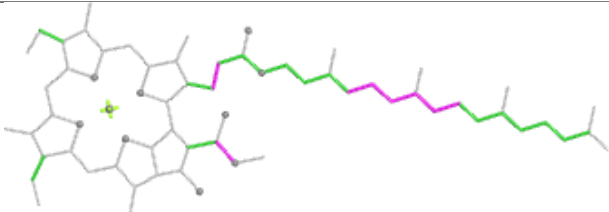
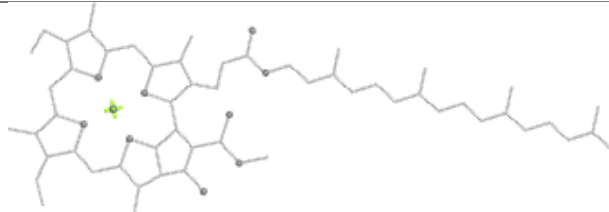


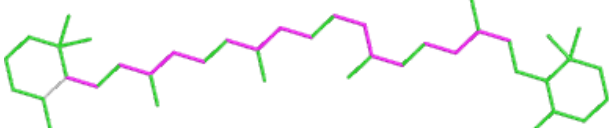
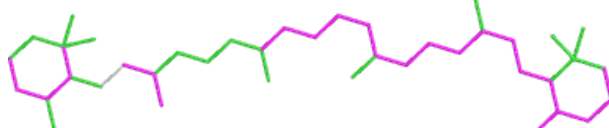
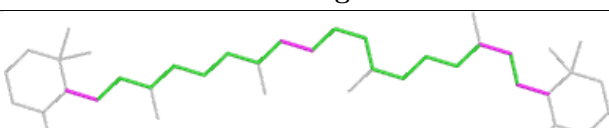
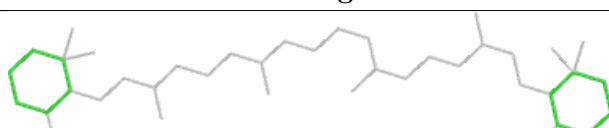
Torsions



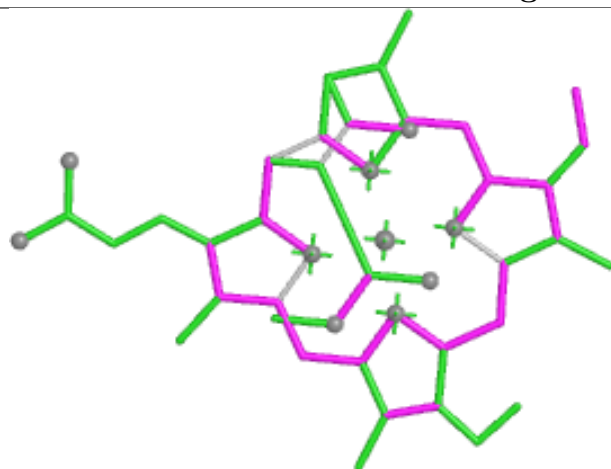
Rings

Ligand IHT f 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

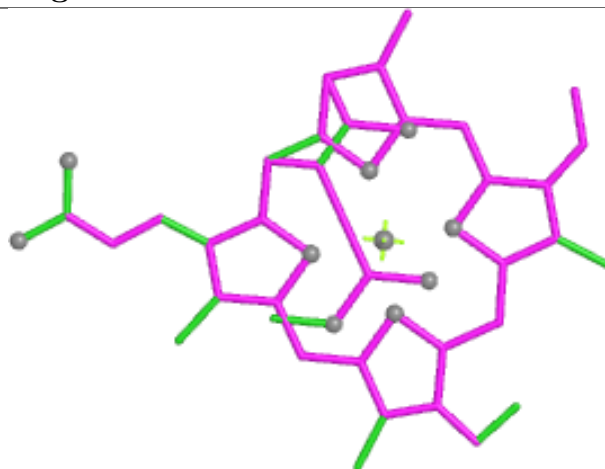
Ligand CLA i 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand WVN A 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

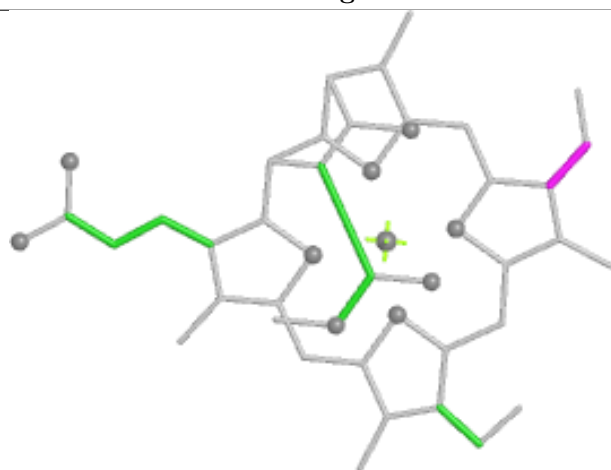
Ligand KC2 g 313



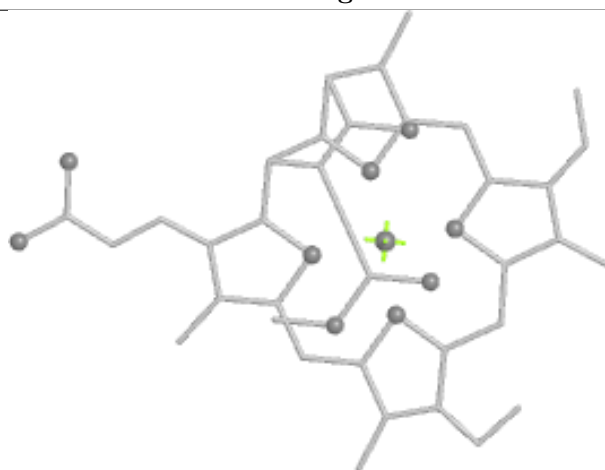
Bond lengths



Bond angles

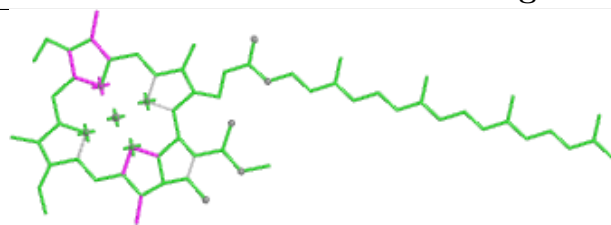


Torsions

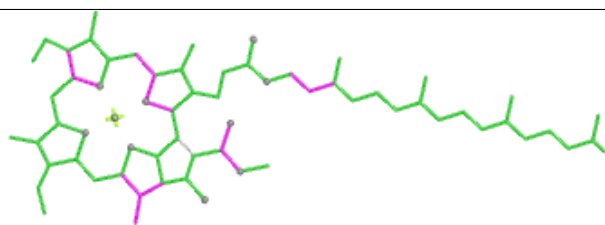


Rings

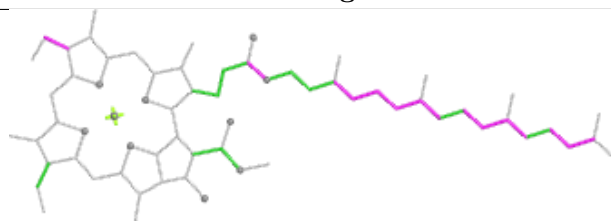
Ligand CLA e 605



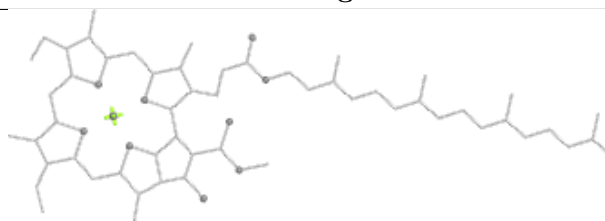
Bond lengths



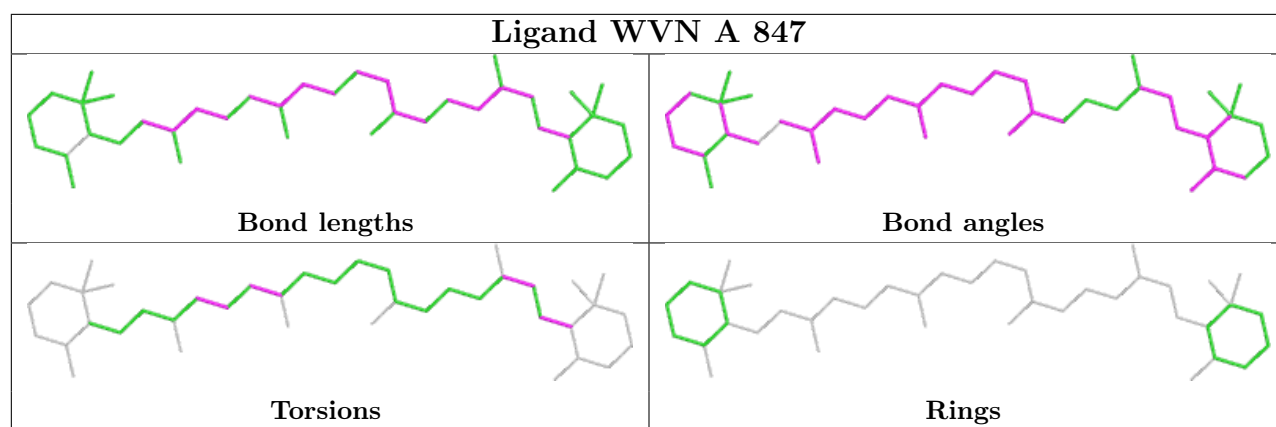
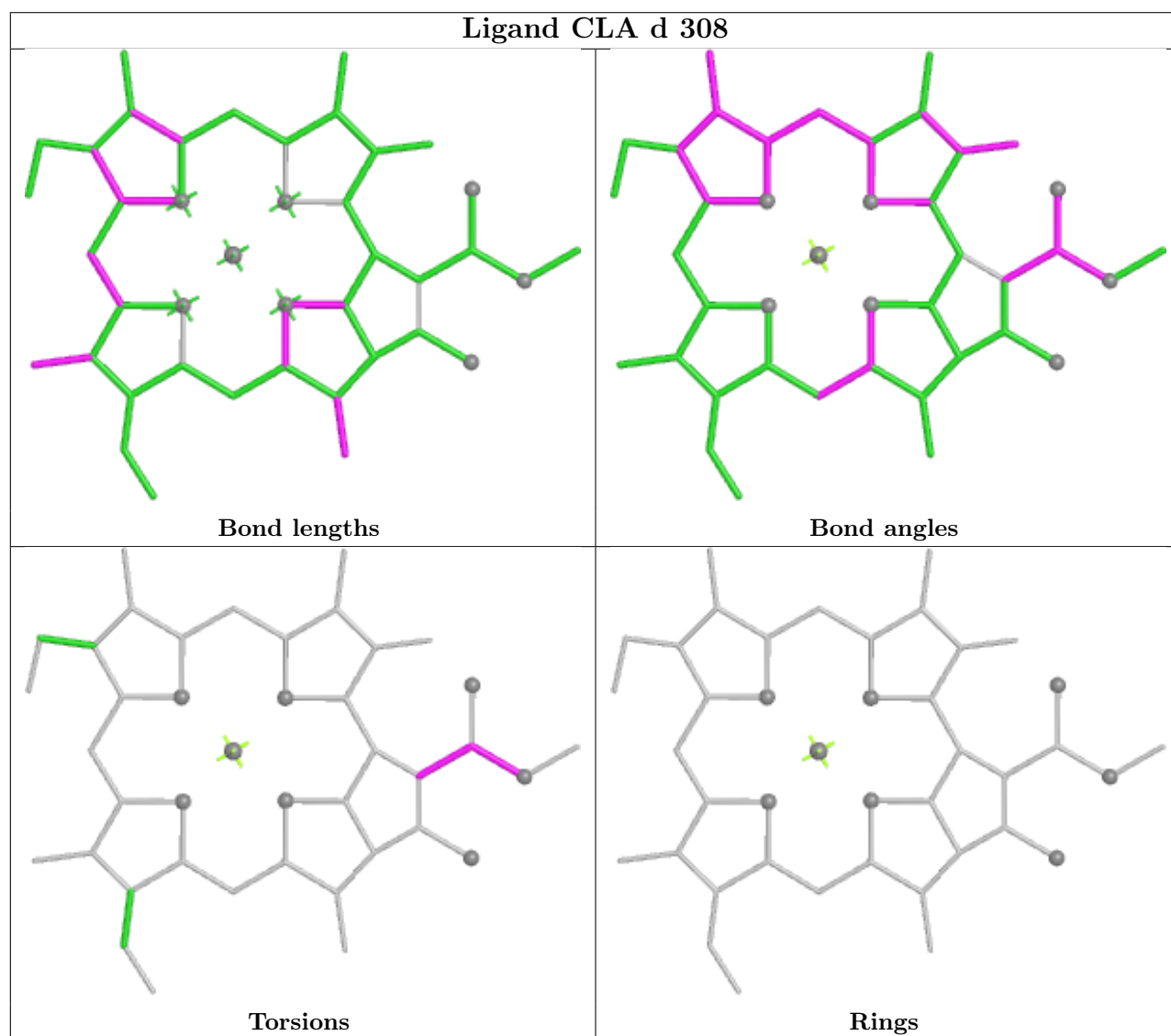
Bond angles

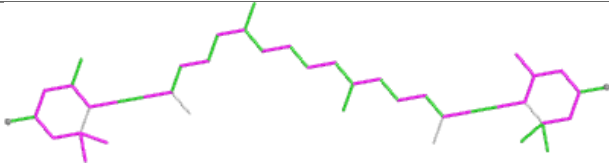
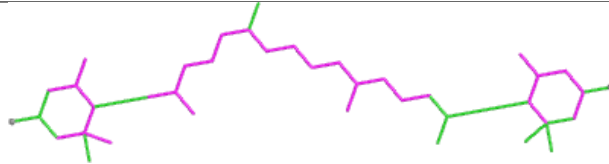
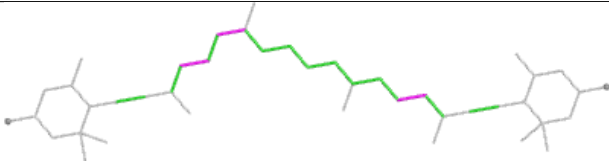
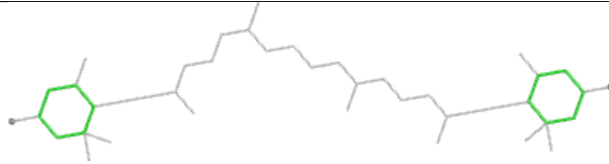


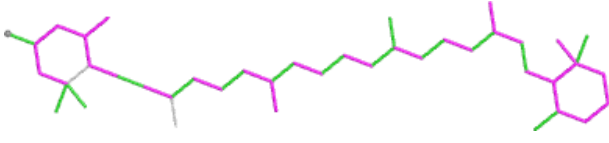
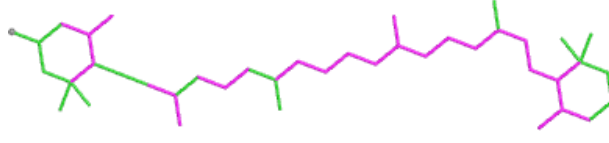
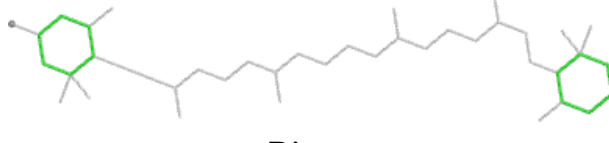
Torsions

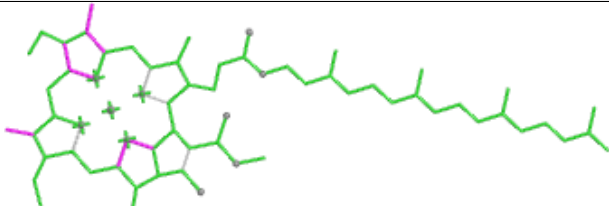
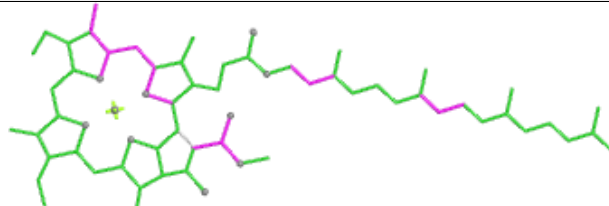
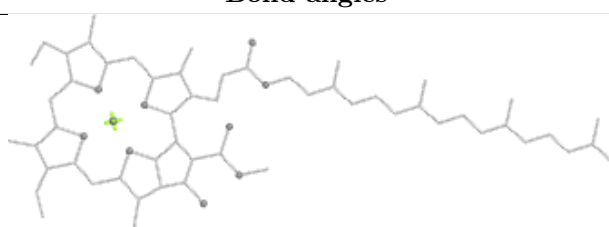


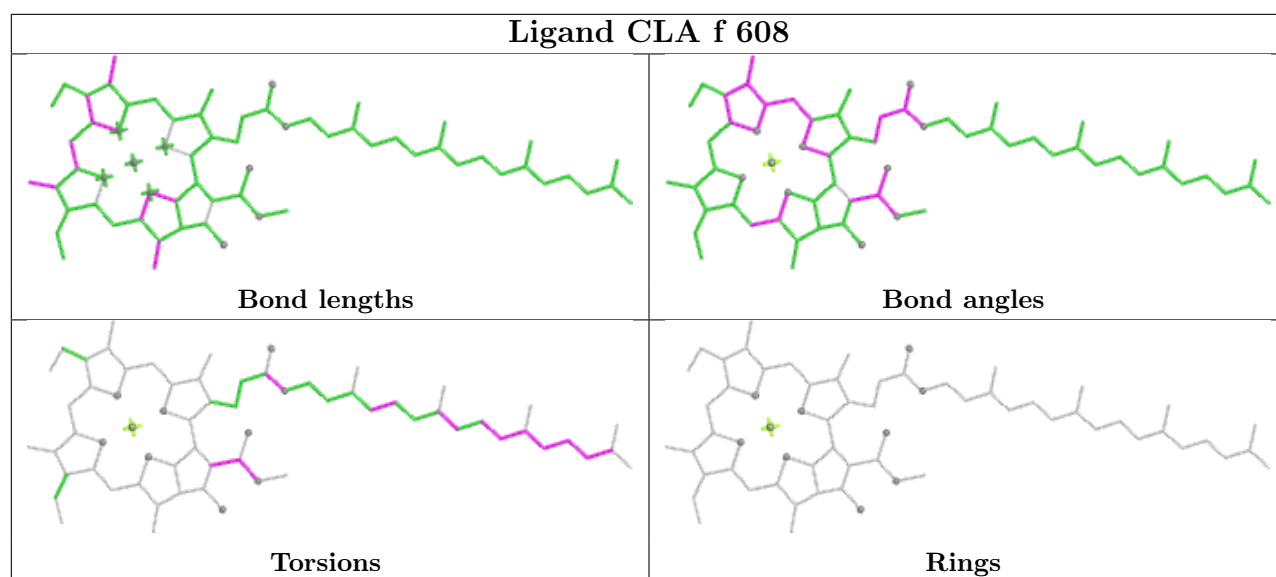
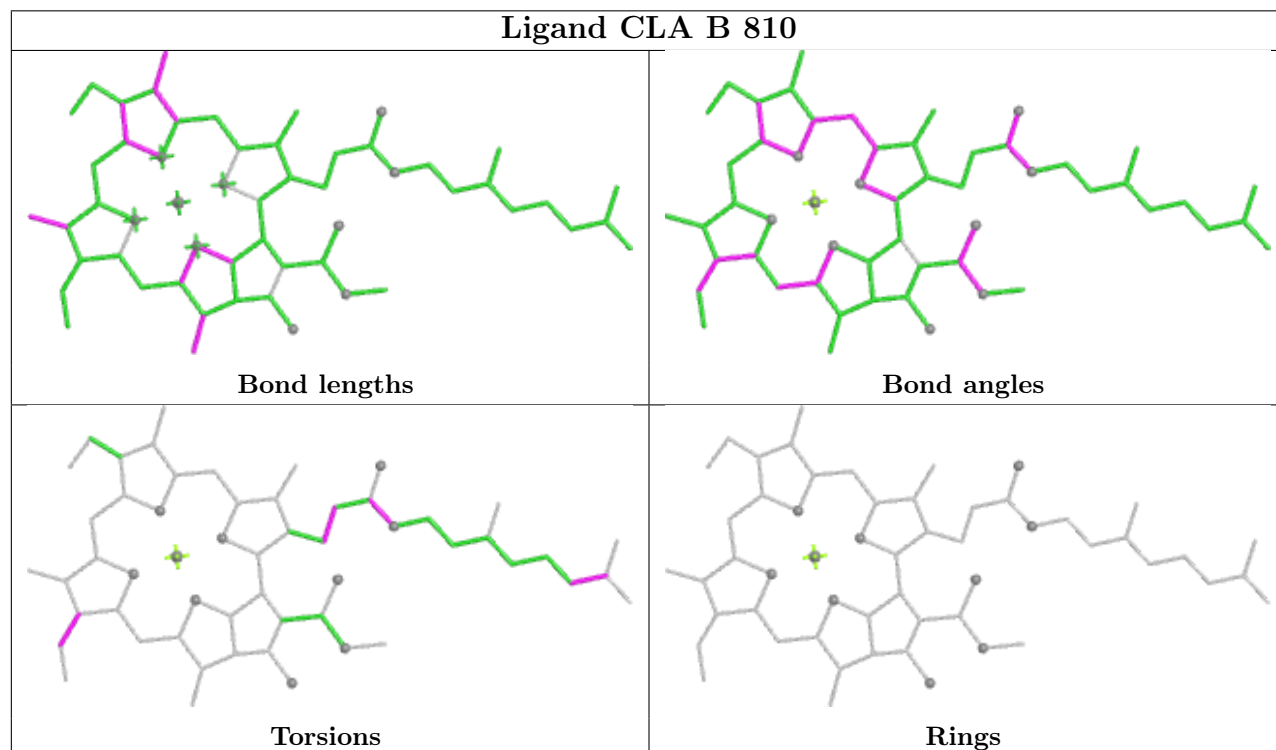
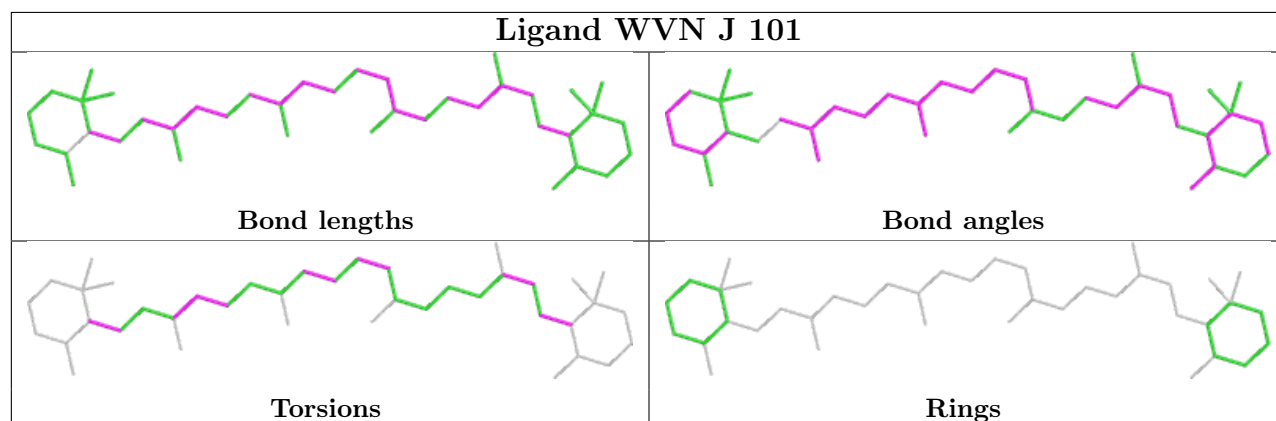
Rings

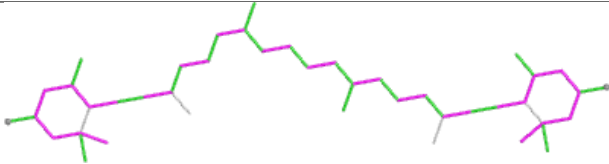
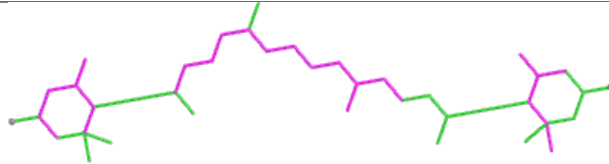
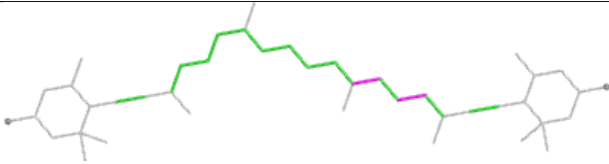
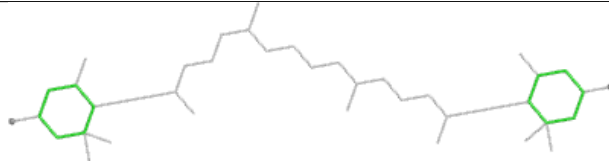


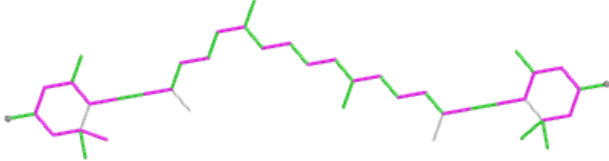
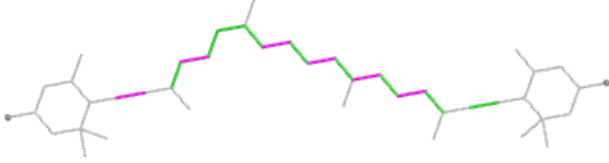
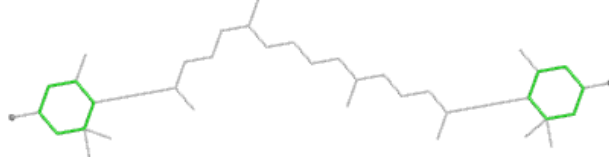
Ligand II0 e 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

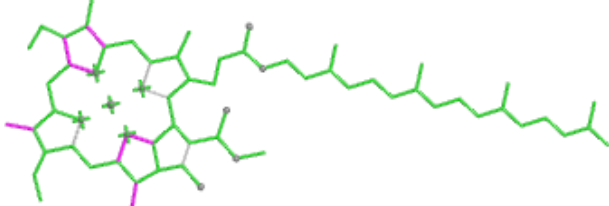
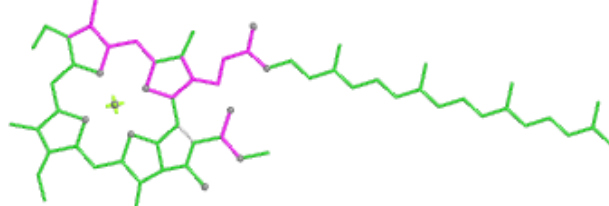
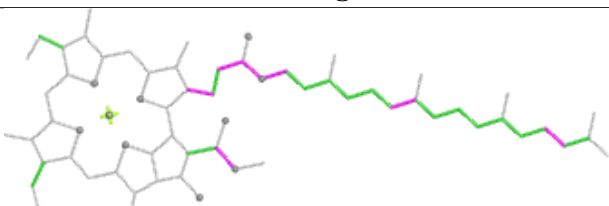
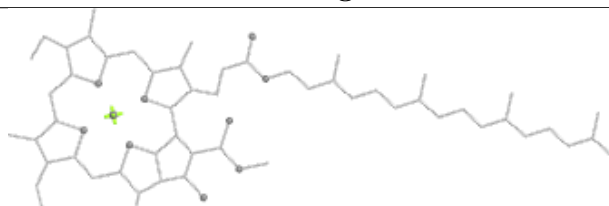
Ligand IHT R 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA g 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

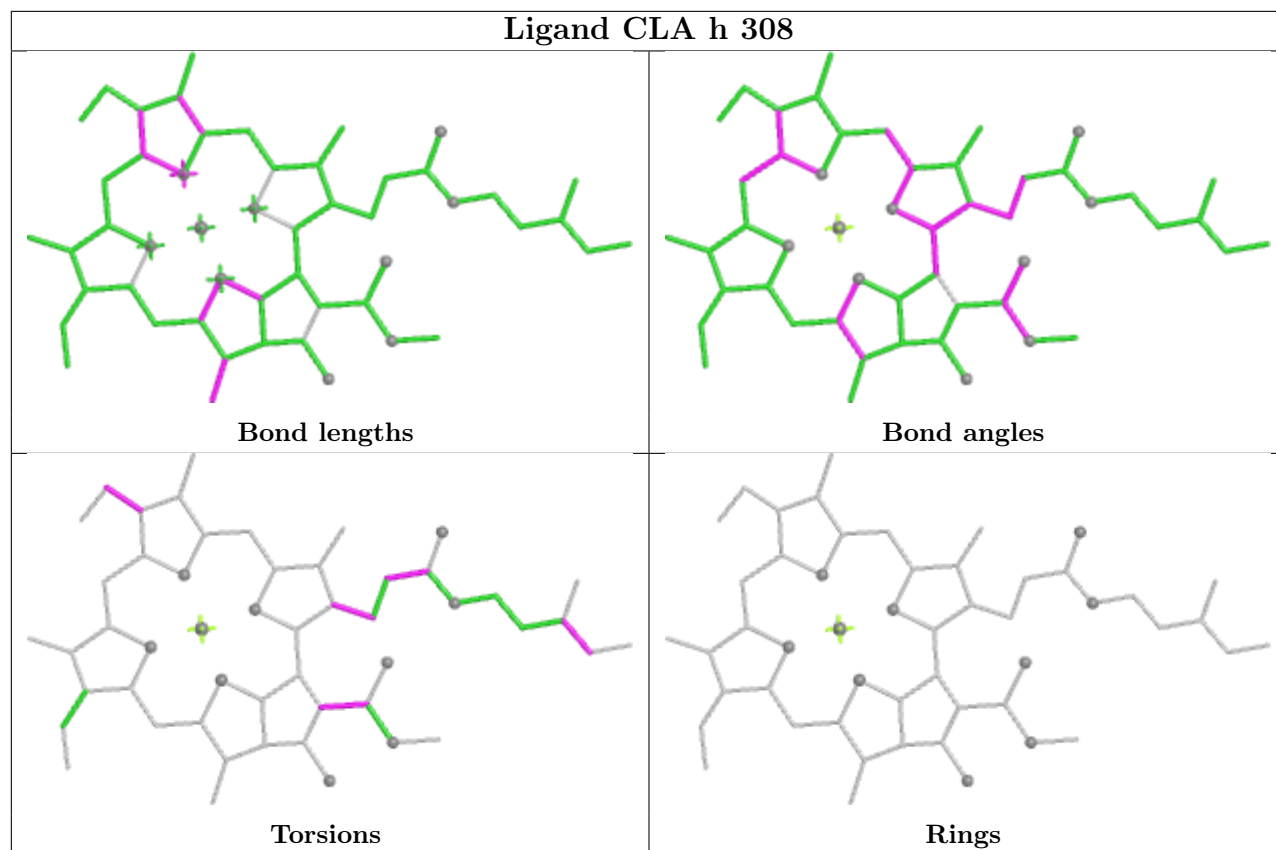


Ligand II0 m 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

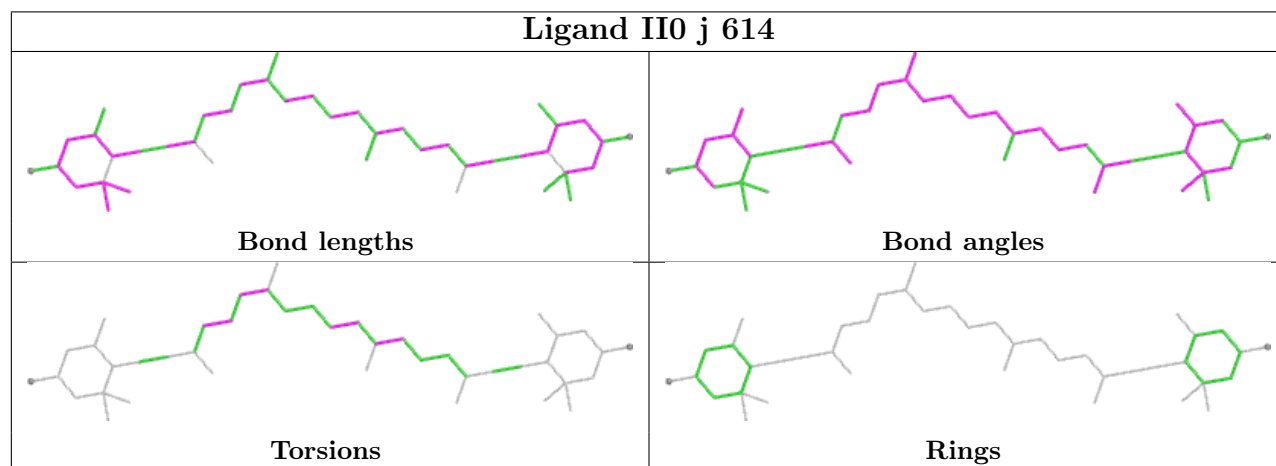
Ligand II0 i 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

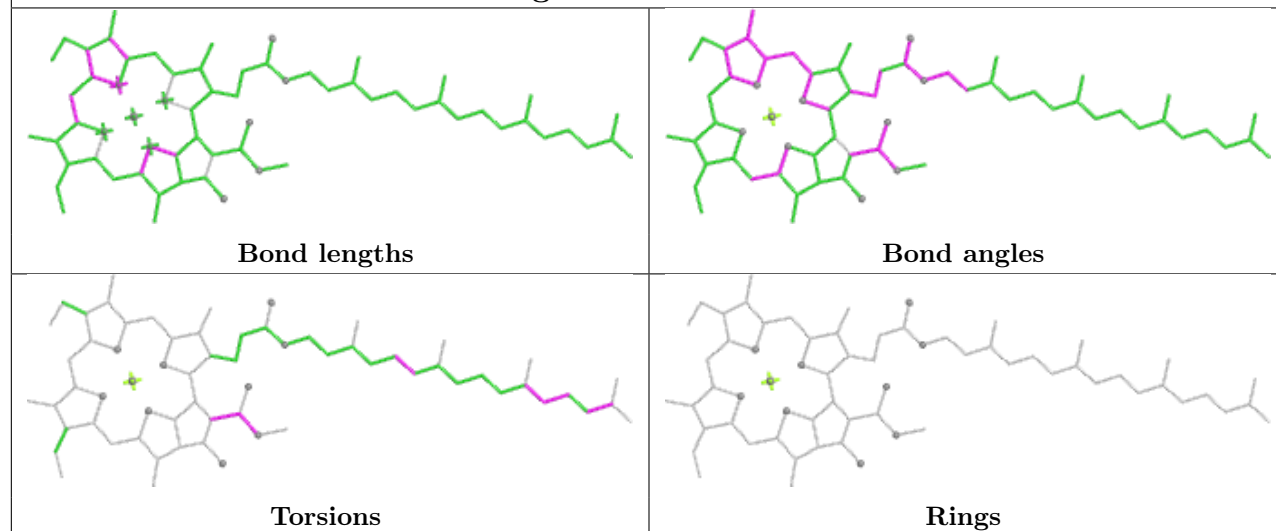
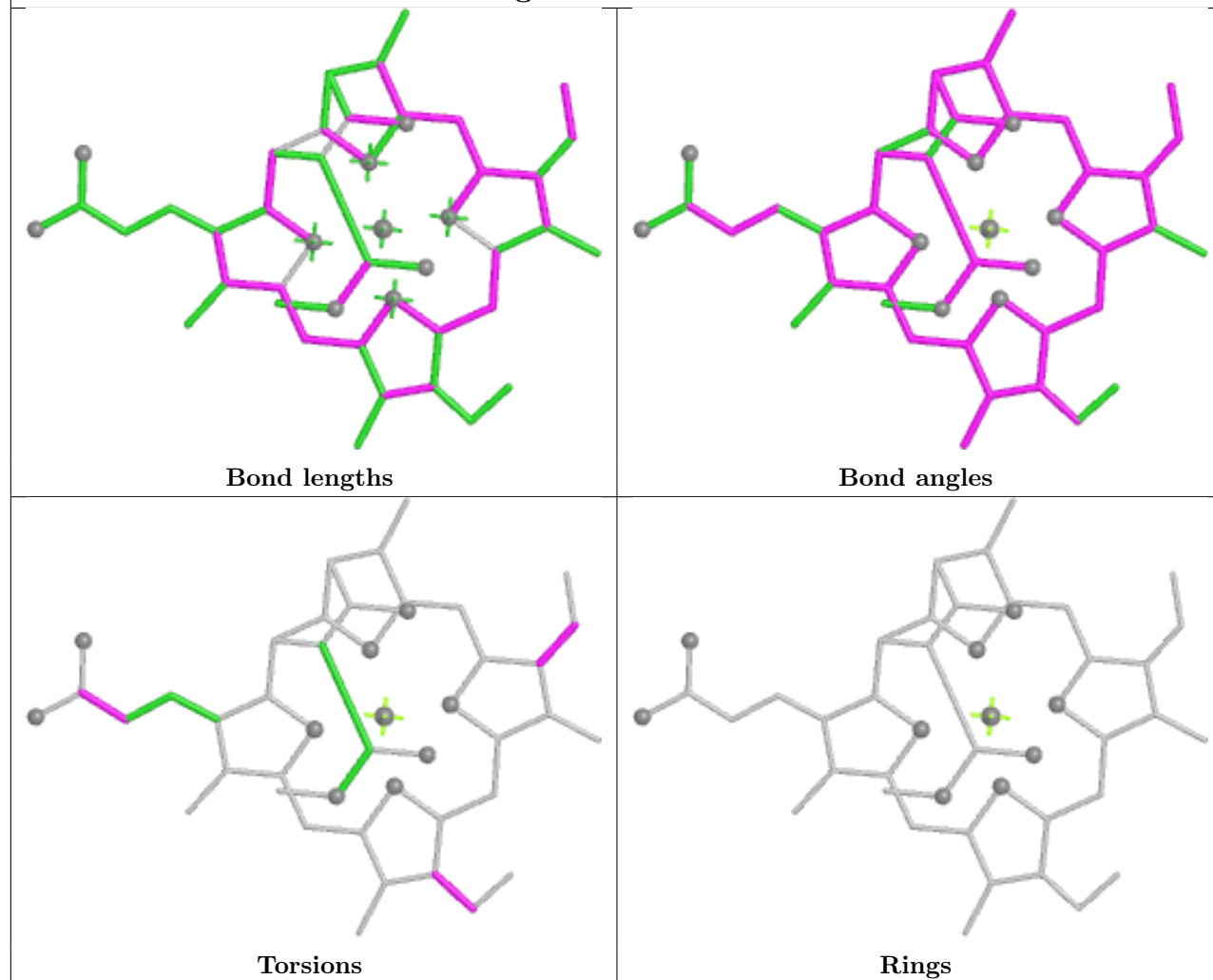
Ligand CLA a 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

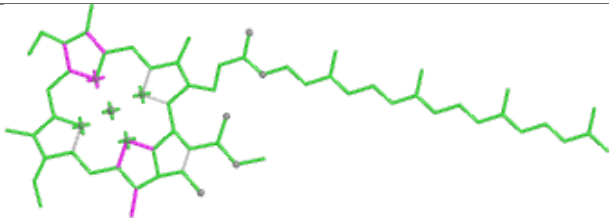
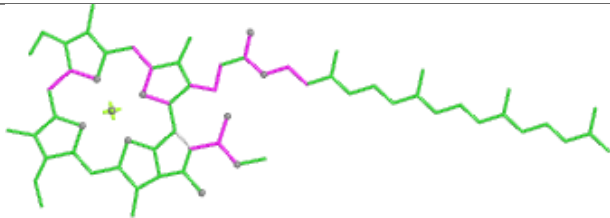
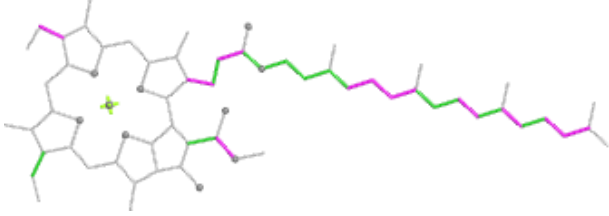
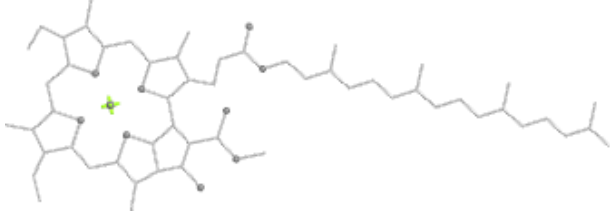
Ligand CLA h 308

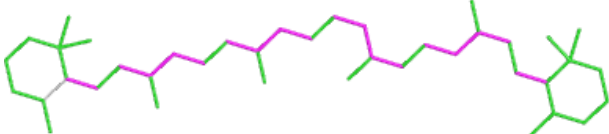
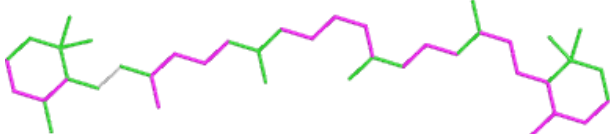
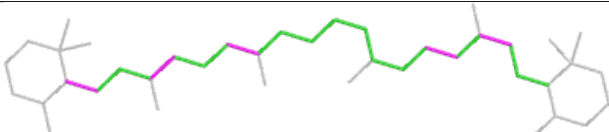
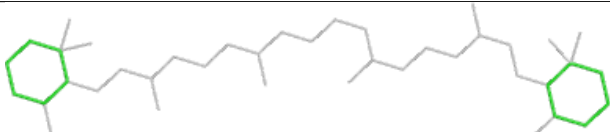


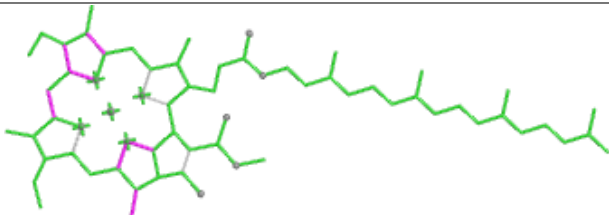
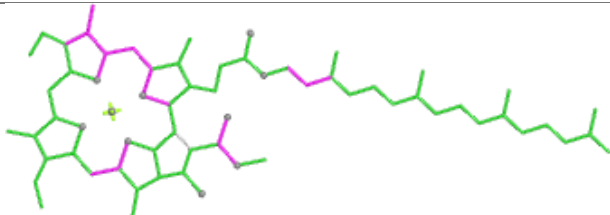
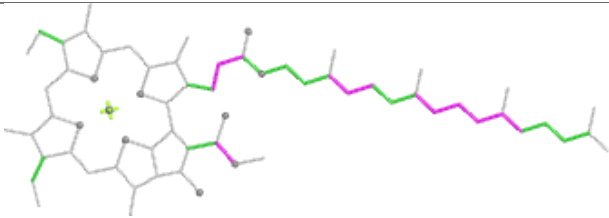
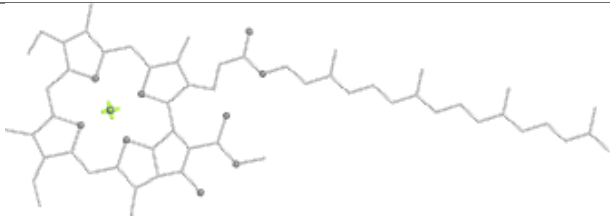
Ligand II0 j 614

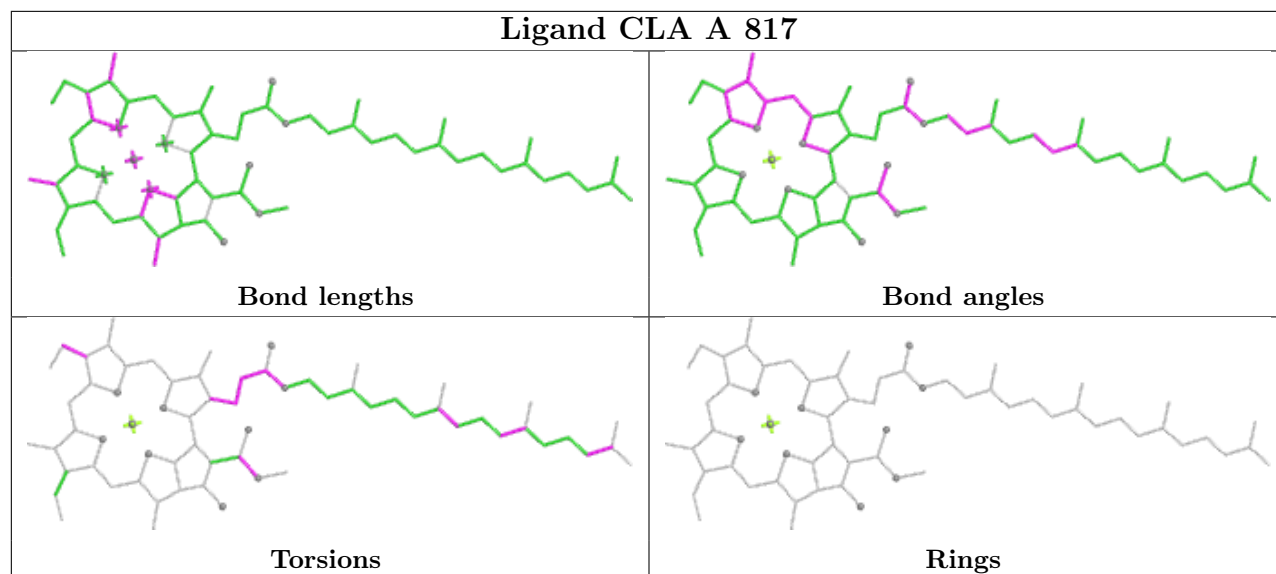
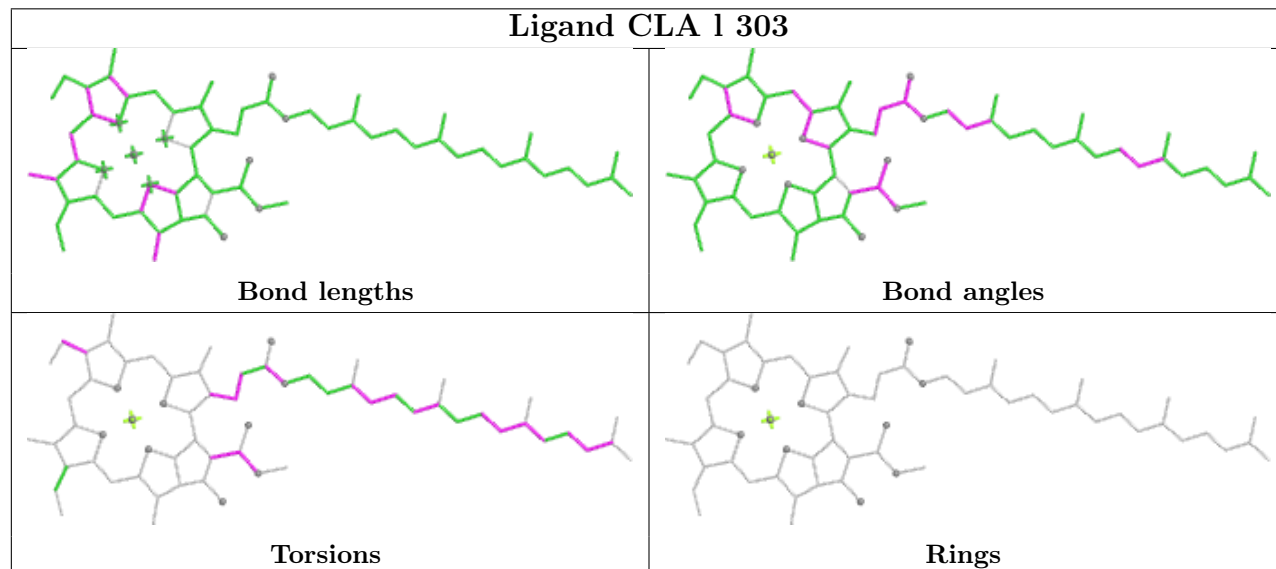


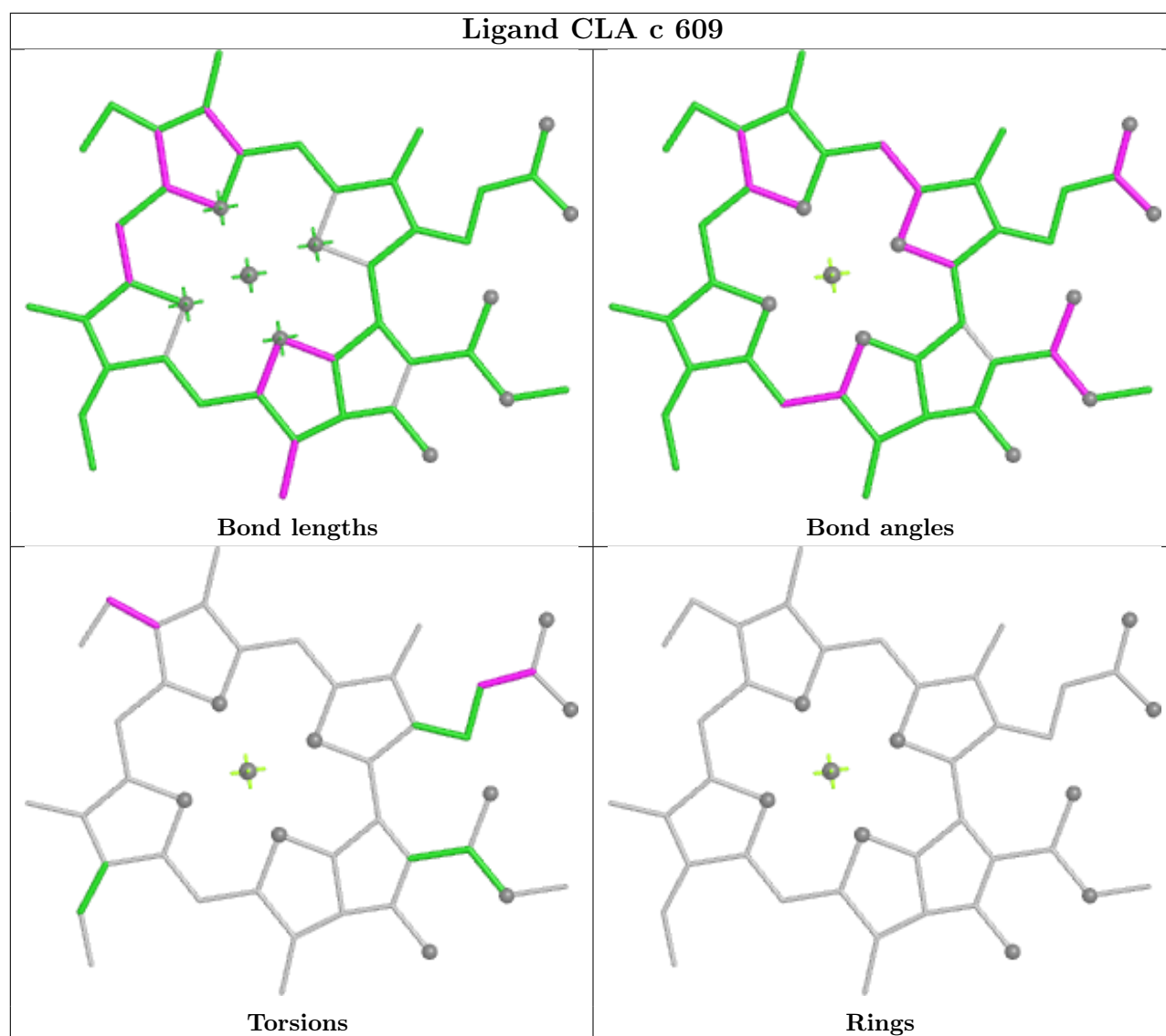
Ligand CLA B 833**Ligand KC2 i 319**

Ligand CLA s 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand WVN B 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 817**Ligand CLA I 303**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

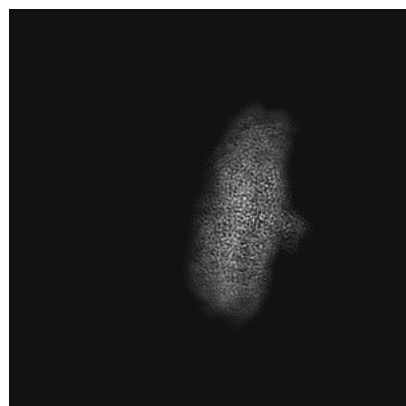
6 Map visualisation [i](#)

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

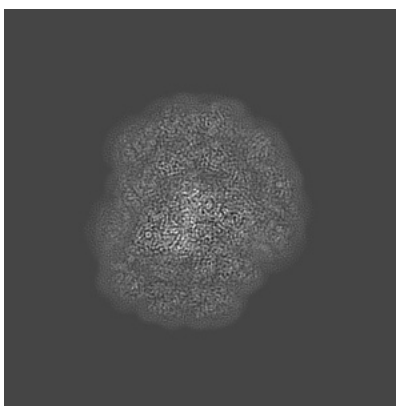
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

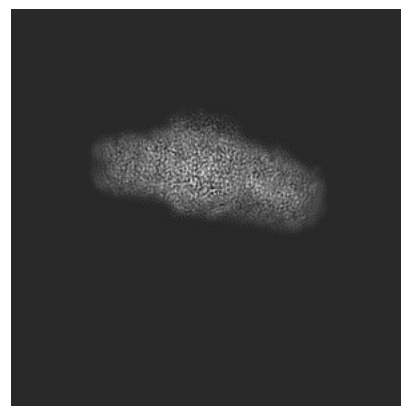
6.1.1 Primary map



X

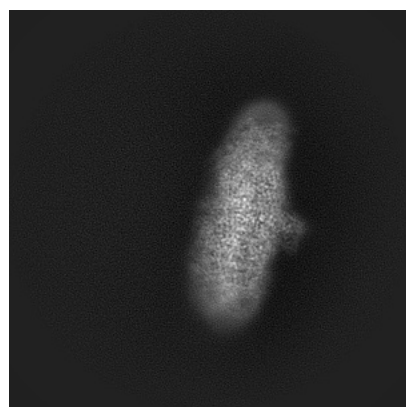


Y

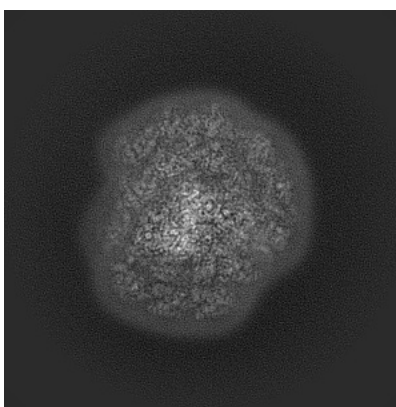


Z

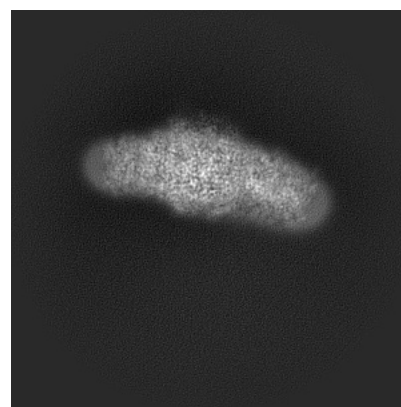
6.1.2 Raw map



X



Y

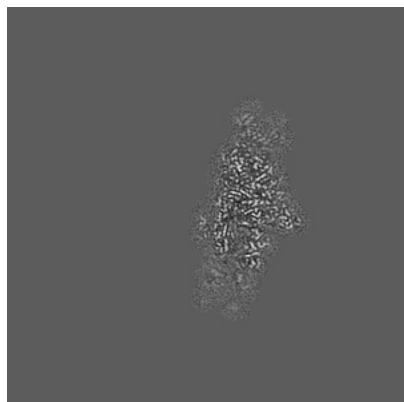


Z

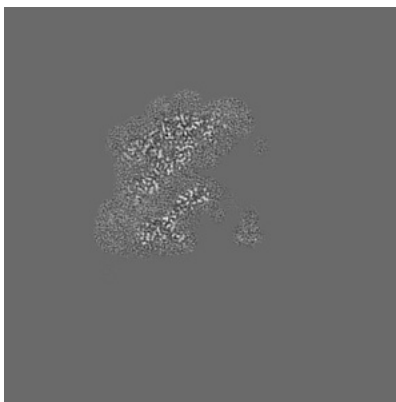
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

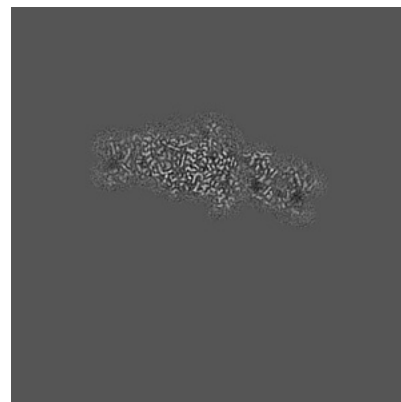
6.2.1 Primary map



X Index: 180

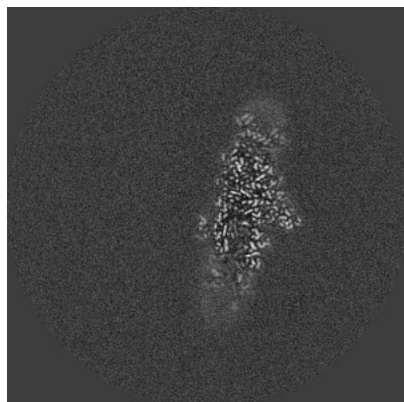


Y Index: 180

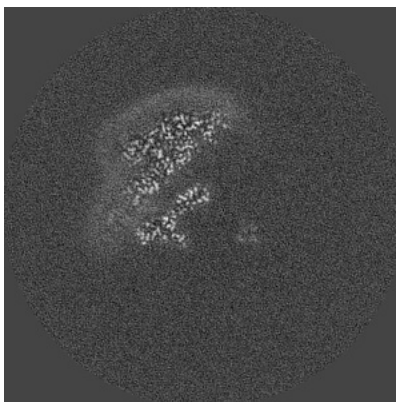


Z Index: 180

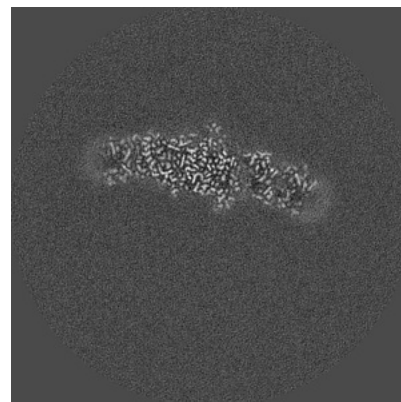
6.2.2 Raw map



X Index: 180



Y Index: 180

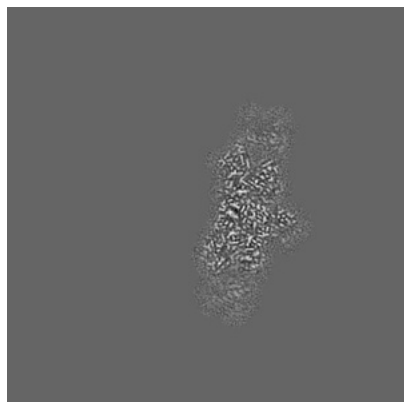


Z Index: 180

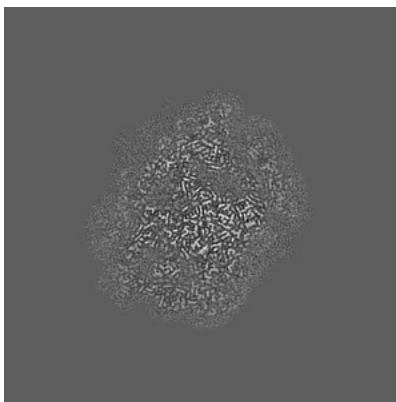
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

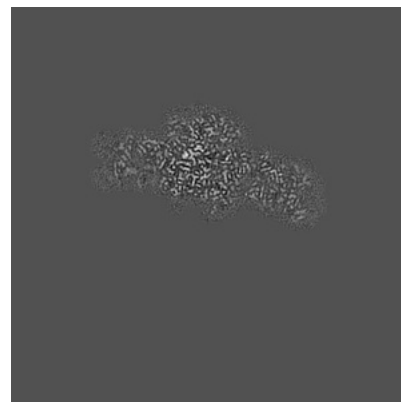
6.3.1 Primary map



X Index: 165

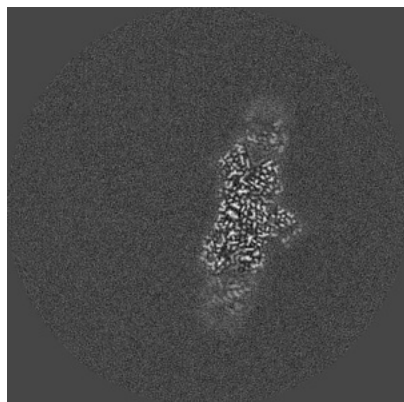


Y Index: 211

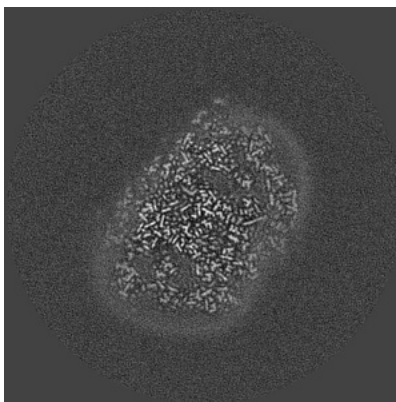


Z Index: 170

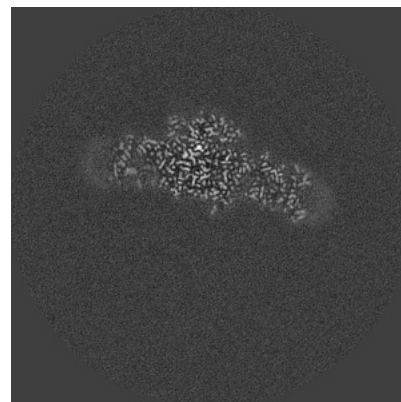
6.3.2 Raw map



X Index: 165



Y Index: 216

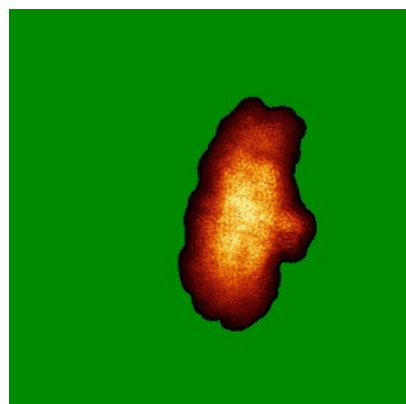


Z Index: 170

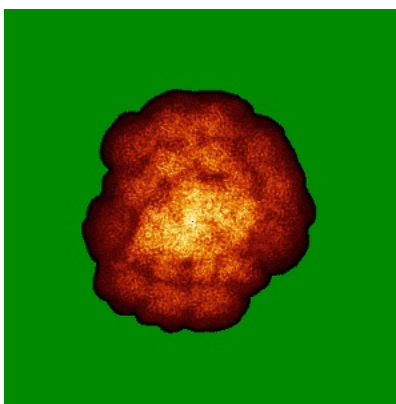
The images above show the largest variance slices of the map in three orthogonal directions.

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

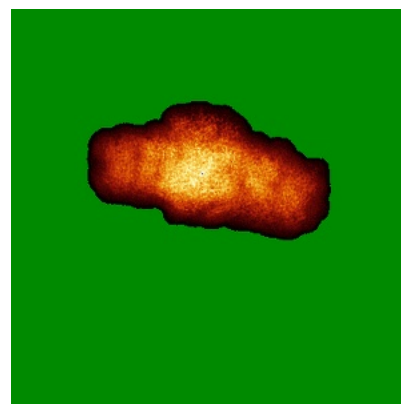
6.4.1 Primary map



X

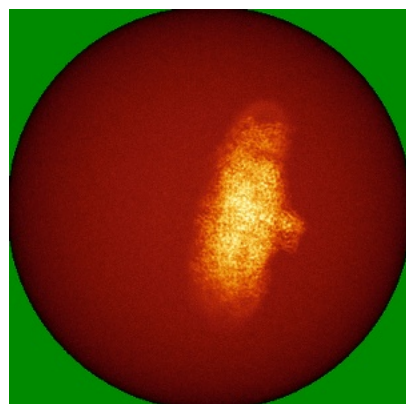


Y

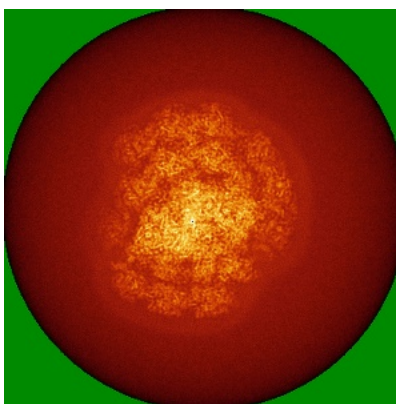


Z

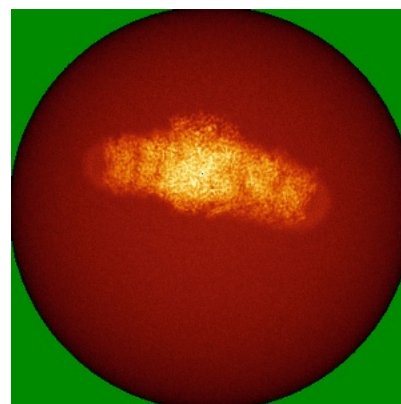
6.4.2 Raw map



X



Y

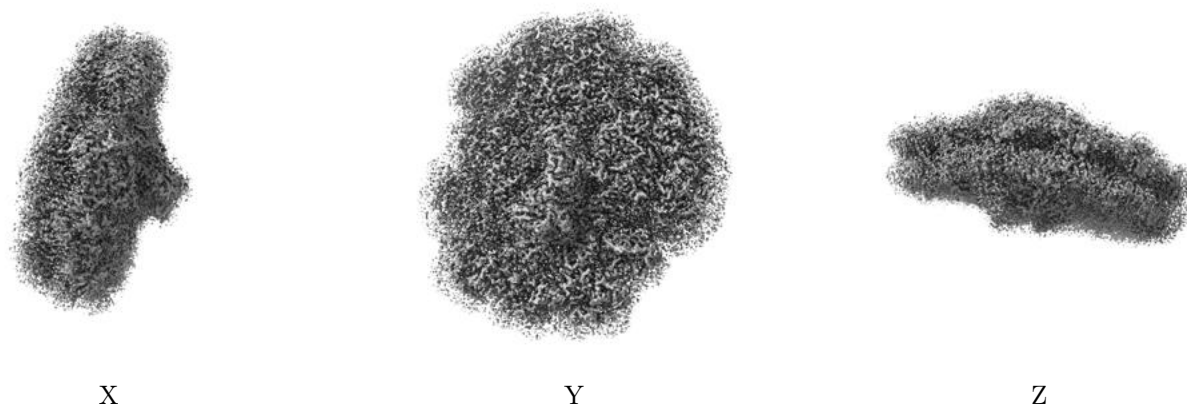


Z

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

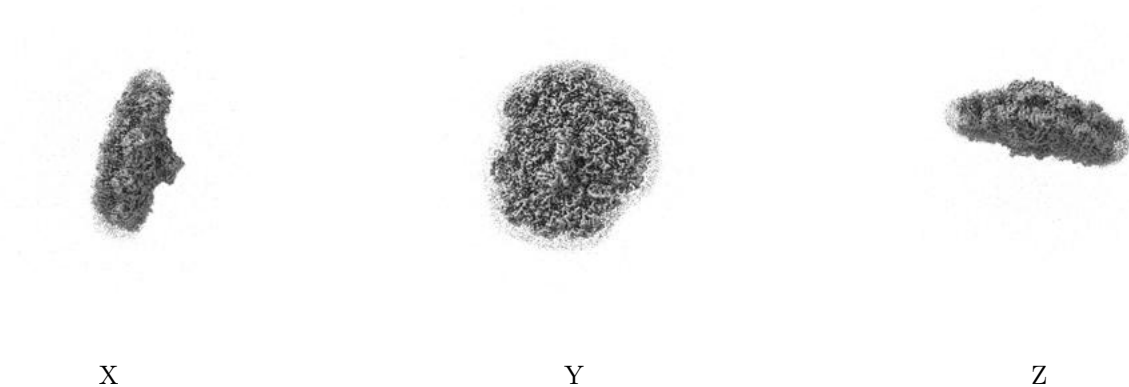
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

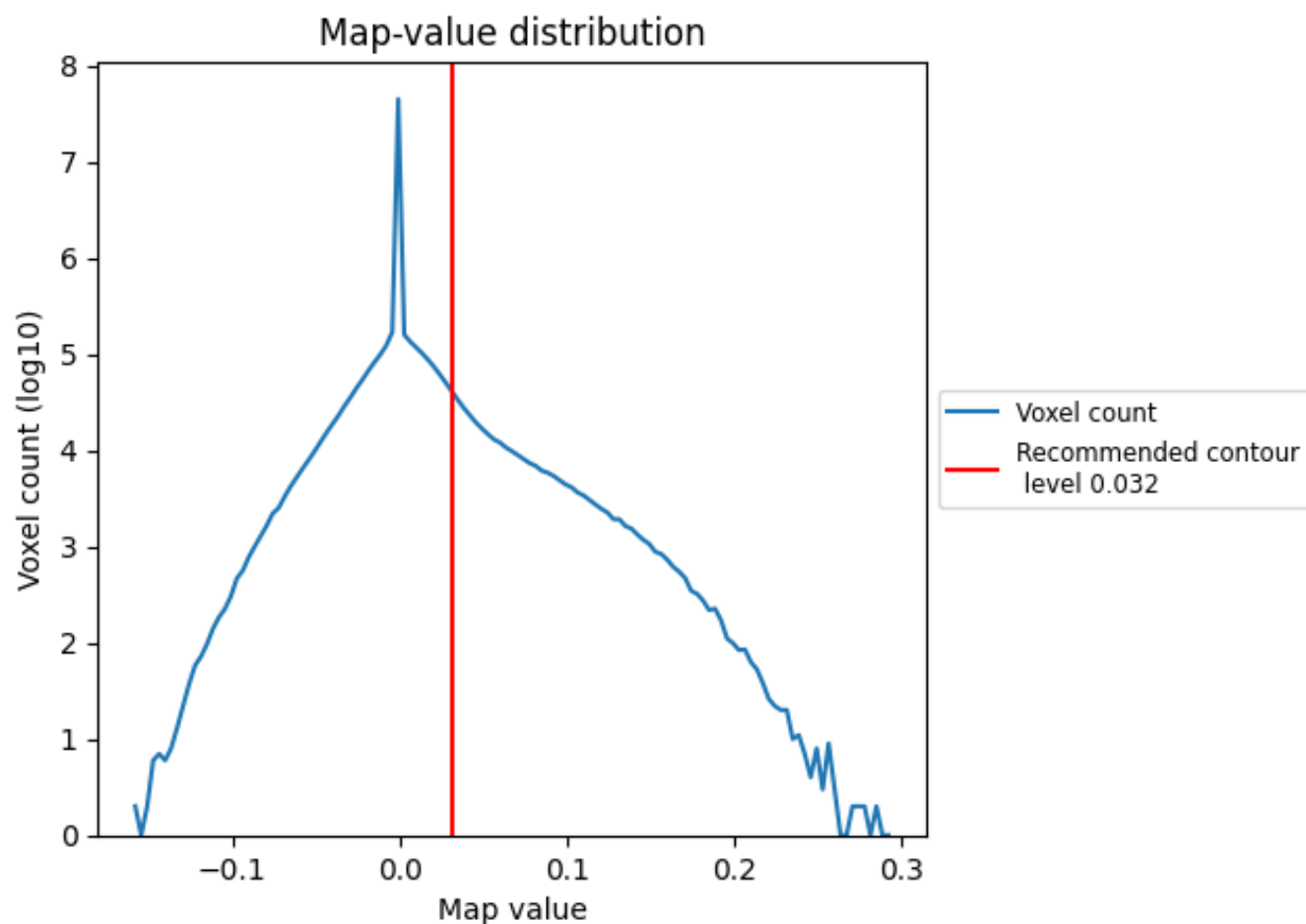
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

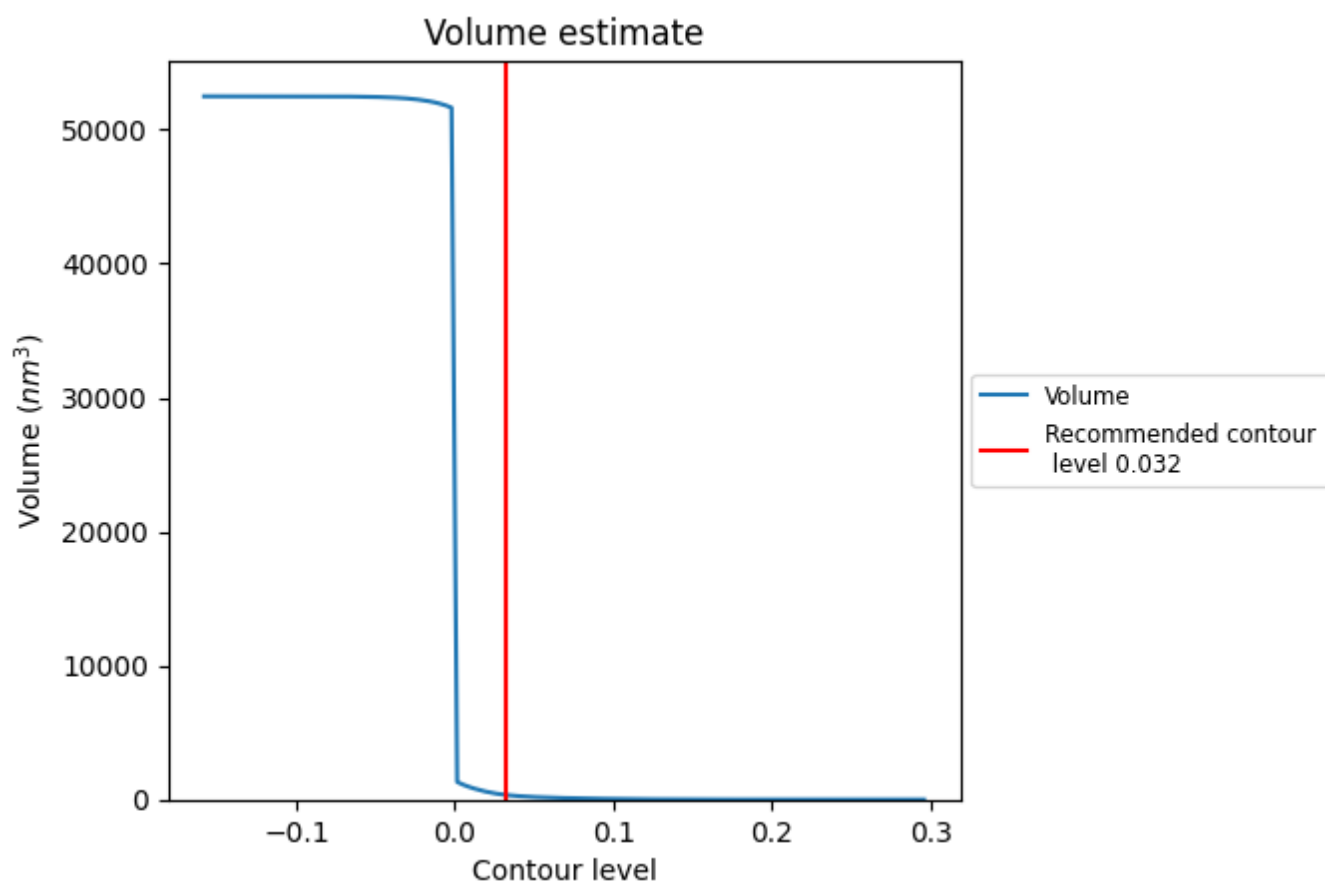
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

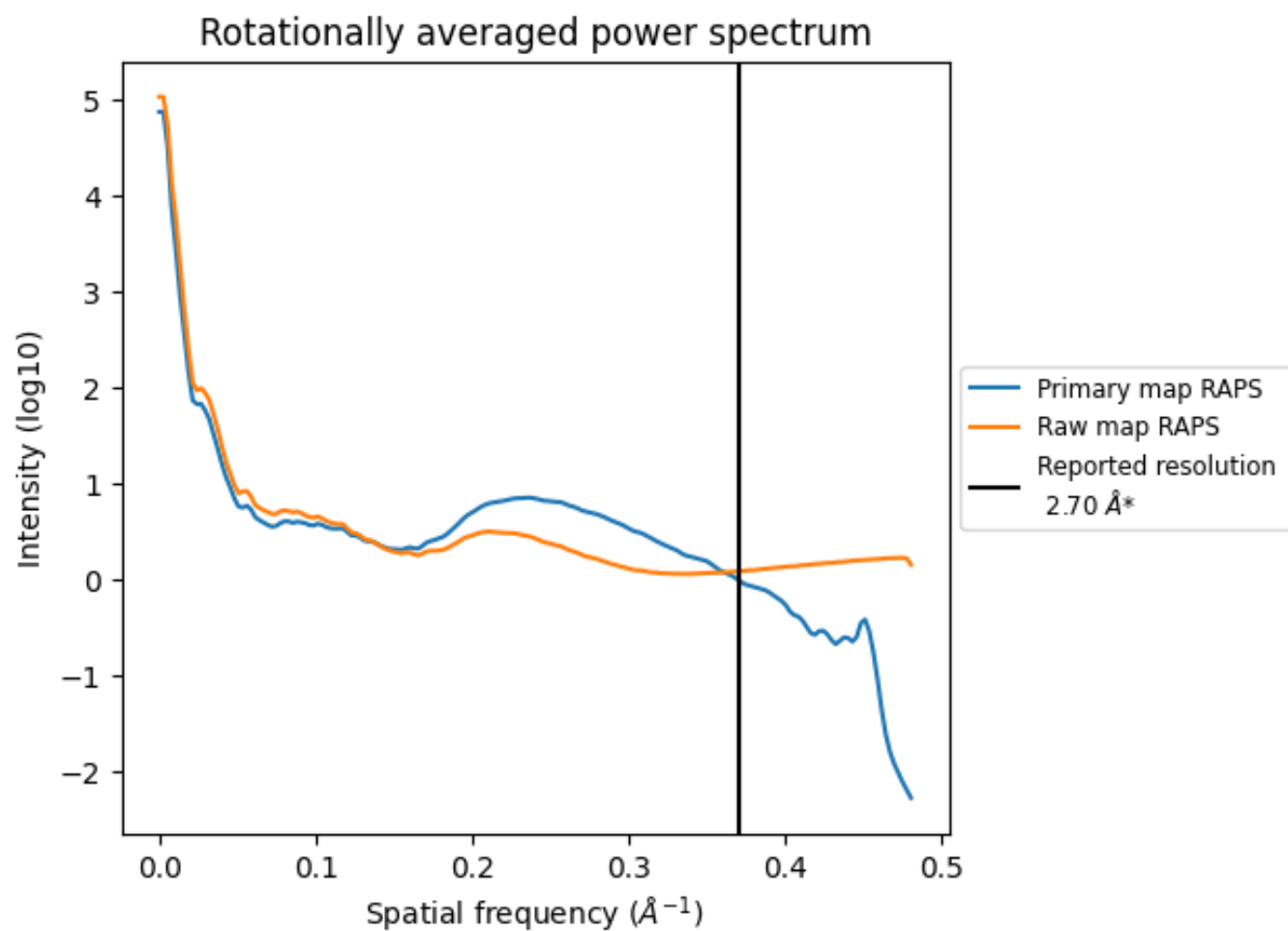
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

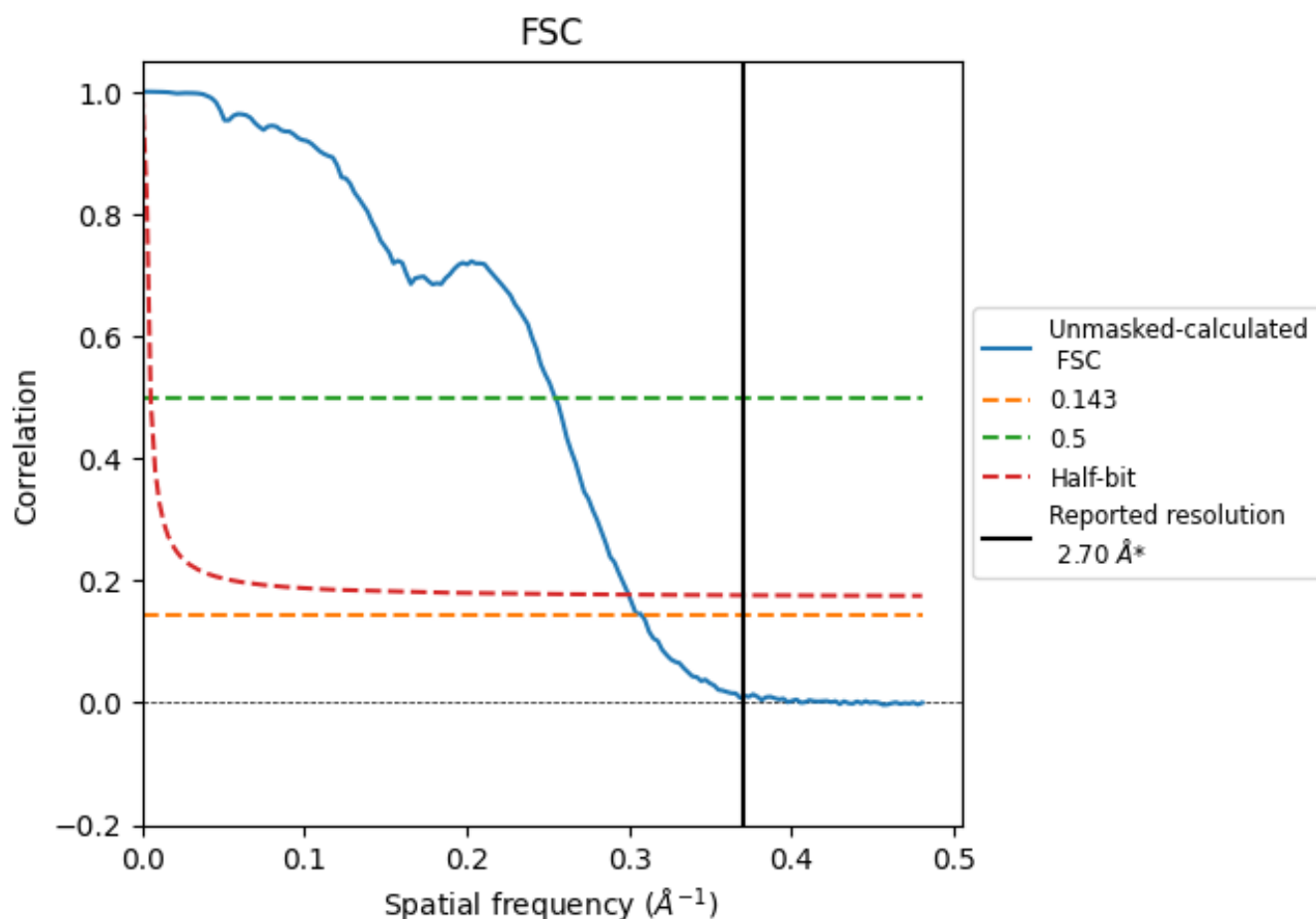


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

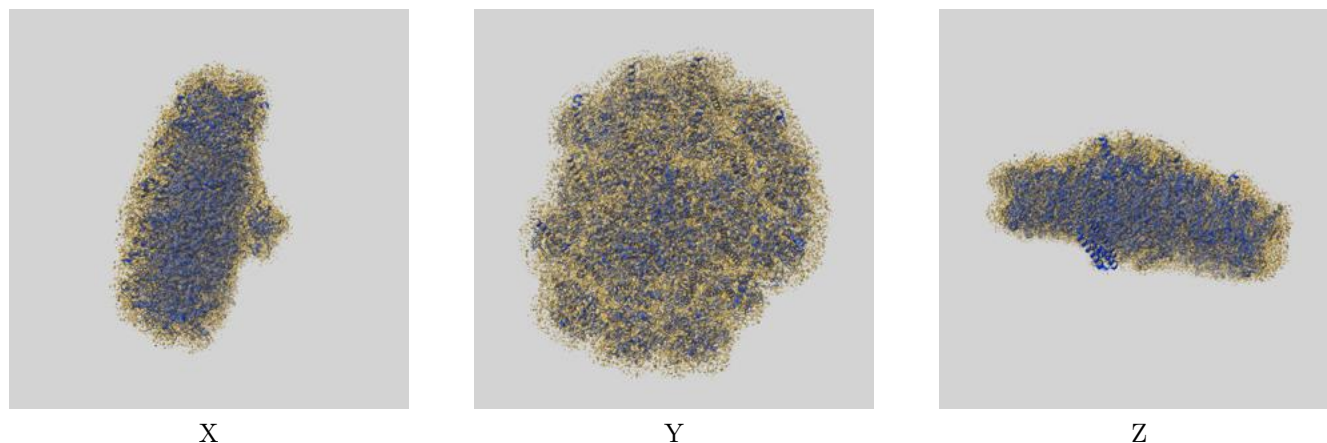
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.25	3.93	3.34

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

9 Map-model fit [i](#)

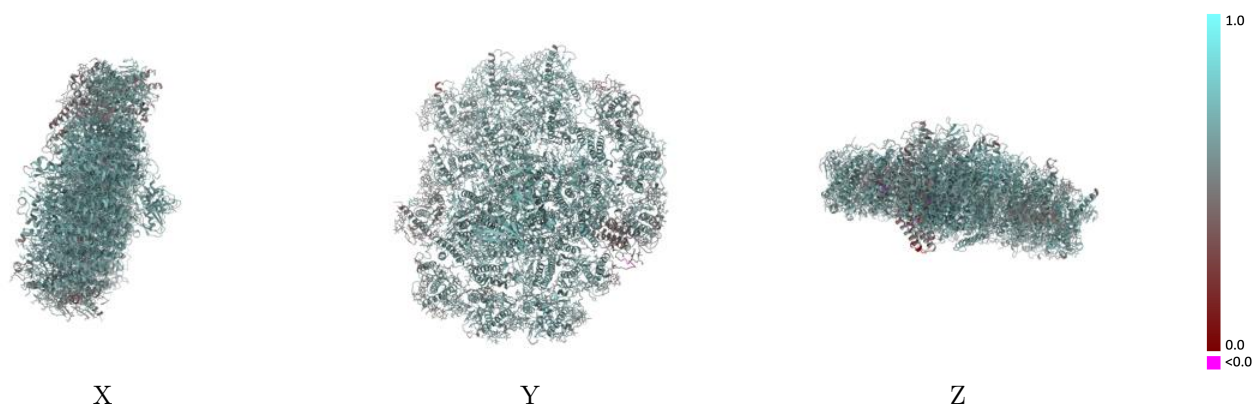
This section contains information regarding the fit between EMDB map EMD-37642 and PDB model 8WM6. Per-residue inclusion information can be found in section [3](#) on page [35](#).

9.1 Map-model overlay [i](#)



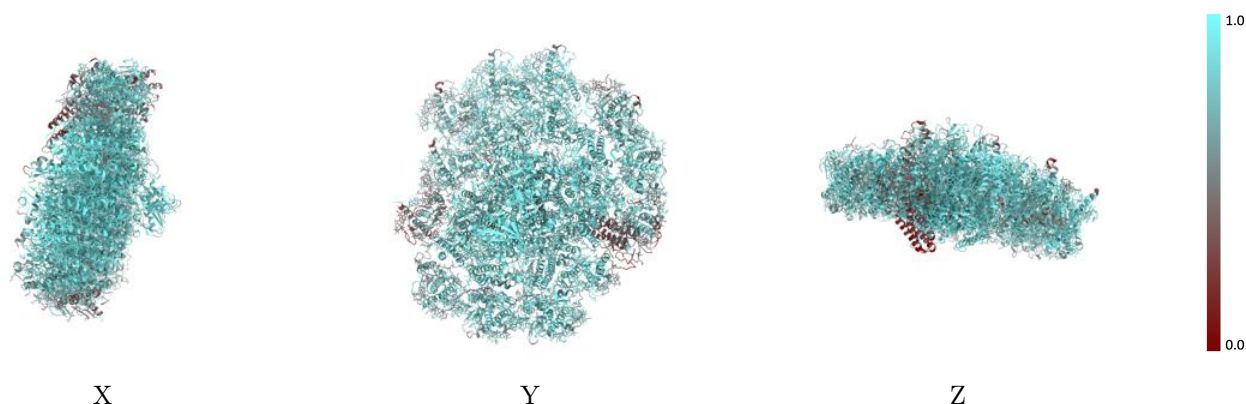
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



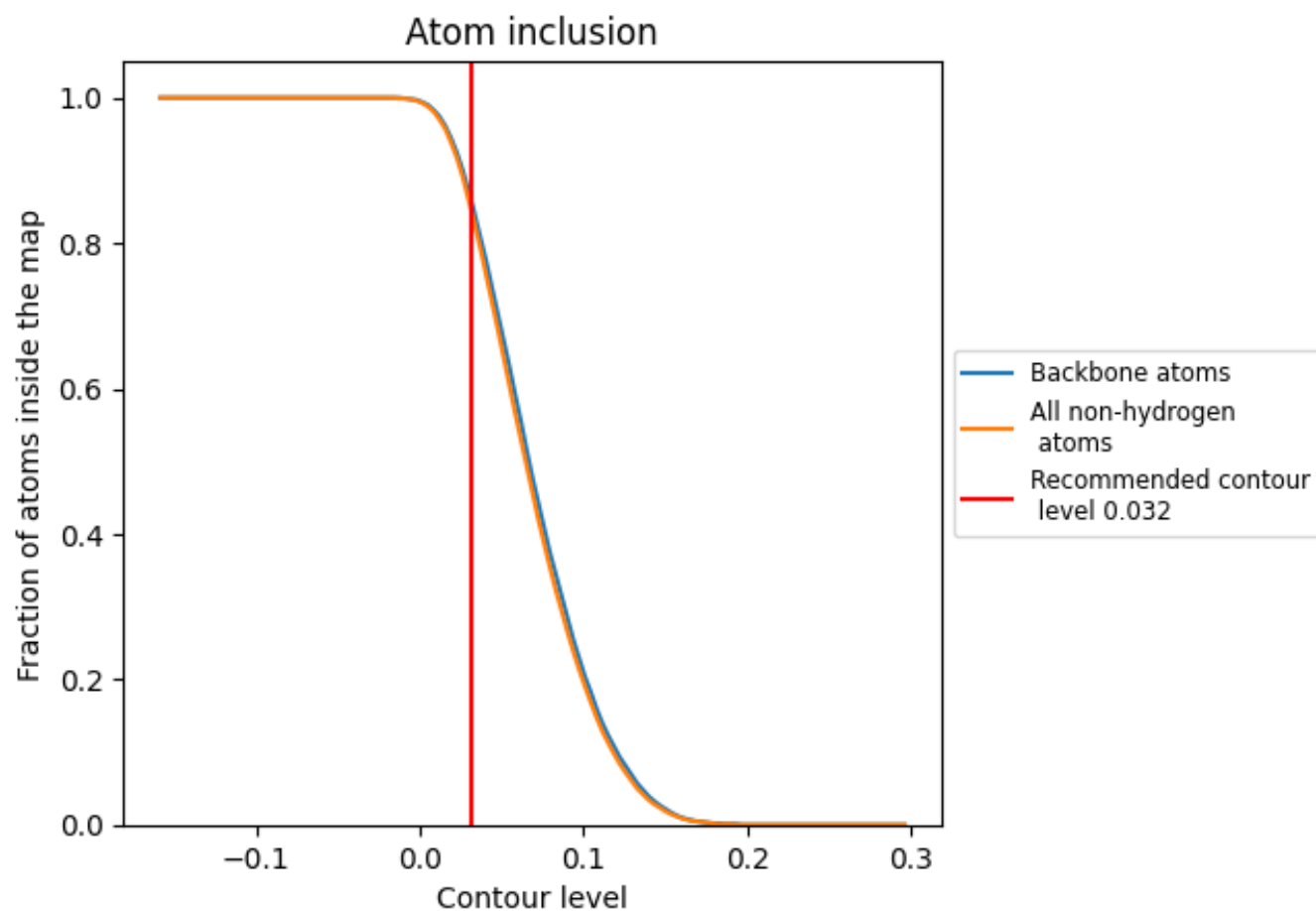
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary

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

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

