



wwPDB EM Validation Summary Report ⓘ

Aug 7, 2026 – 01:35 AM JST

PDB ID : 8WMW / pdb_00008wmw
EMDB ID : EMD-37660
Title : The structure of PSI-11CAC at the stationary growth phase
Authors : Zhang, S.M.; Si, L.; Li, M.
Deposited on : 2023-10-04
Resolution : 3.30 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:

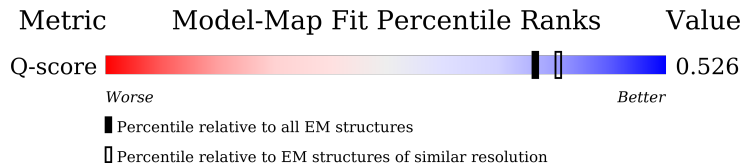
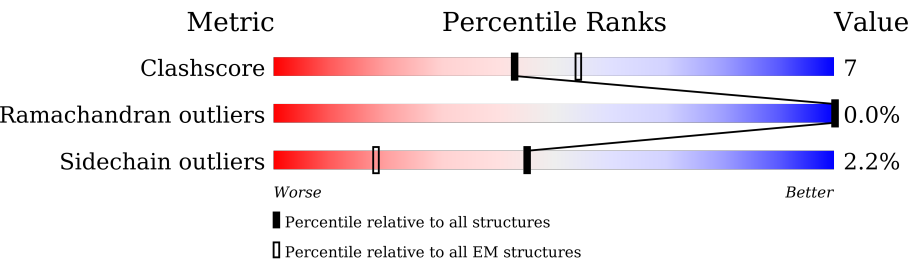
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 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.



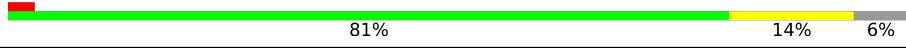
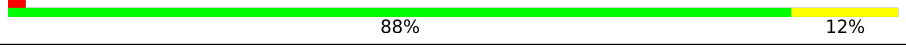
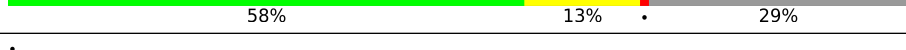
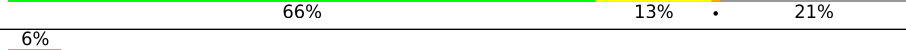
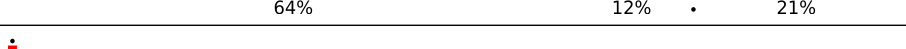
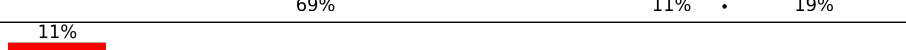
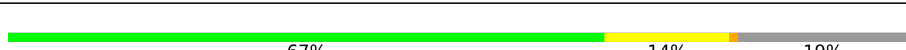
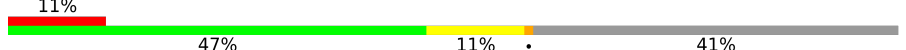
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	752	87% 11% .
2	B	734	88% 12% .
3	C	81	86% 12% .
4	D	141	85% 13% .

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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	c	216	
14	a	216	
15	b	223	
16	h	225	
17	e	203	
18	k	241	
19	f	212	
19	j	212	
20	i	218	
21	d	213	
22	g	255	
23	R	129	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	SF4	A	854	-	-	X	-
29	SF4	C	101	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 51054 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
			485	309	84	92		

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called PsaO.

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

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

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

- Molecule 13 is a protein called CAC-c.

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

- Molecule 14 is a protein called CAC-a.

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

- Molecule 15 is a protein called CAC-b.

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

- Molecule 16 is a protein called CAC-h.

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

- Molecule 17 is a protein called CAC-e.

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

- Molecule 18 is a protein called CAC-k.

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

- Molecule 19 is a protein called CAC-f.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	174	Total	C	N	O	S	0	0
			1302	842	212	240	8		
19	j	172	Total	C	N	O	S	0	0
			1293	834	212	239	8		

- Molecule 20 is a protein called CAC-i.

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

- Molecule 21 is a protein called CAC-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	126	Total	C	N	O	S	0	0
			950	609	165	167	9		

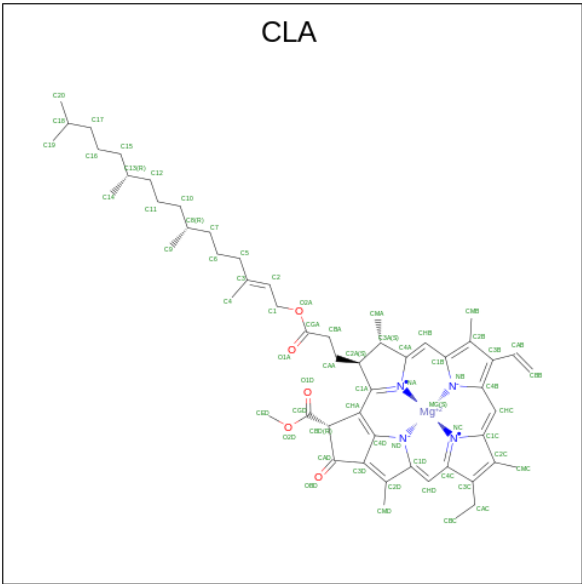
- Molecule 22 is a protein called CAC-g.

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

- Molecule 23 is a protein called PsaR.

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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
24	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	F	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	J	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	L	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	L	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	K	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	K	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	c	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	c	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	h	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	e	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	k	1	Total 51	C 41	Mg 1	N 4	O 5	0

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

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

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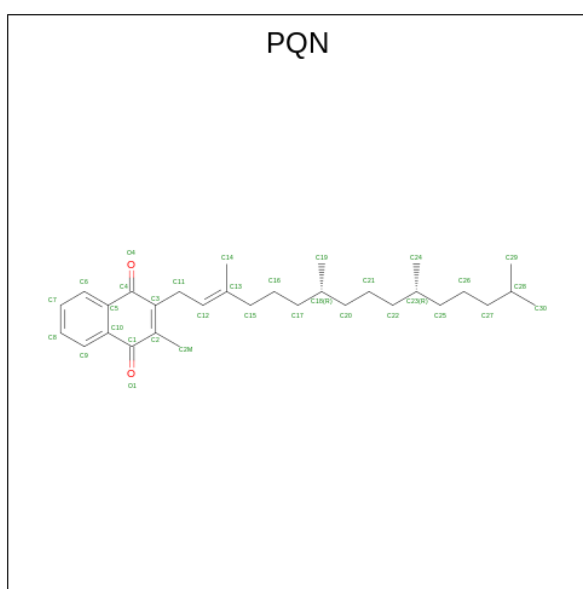
Mol	Chain	Residues	Atoms					AltConf
24	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	d	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	g	1	Total 51	C 41	Mg 1	N 4	O 5	0

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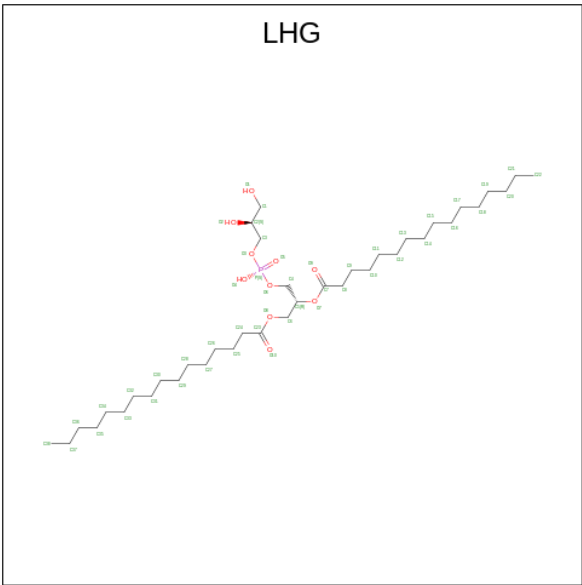
Mol	Chain	Residues	Atoms					AltConf
24	g	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	R	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



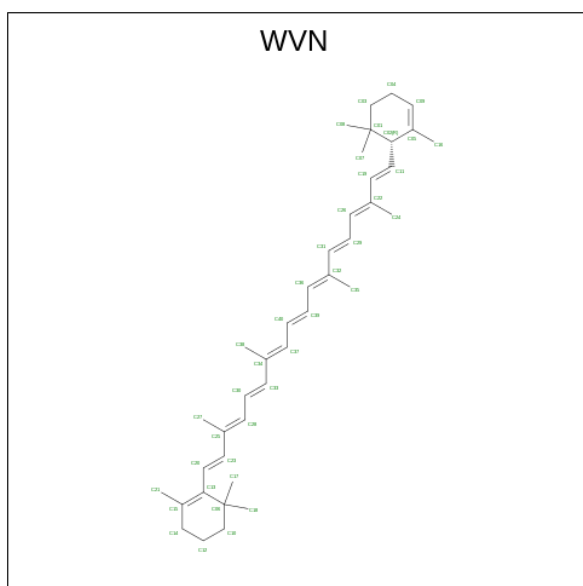
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			48	37	10	1	
26	A	1	Total	C	O	P	0
			27	16	10	1	
26	B	1	Total	C	O	P	0
			38	27	10	1	
26	J	1	Total	C	O	P	0
			49	38	10	1	
26	c	1	Total	C	O	P	0
			37	26	10	1	
26	c	1	Total	C	O	P	0
			37	26	10	1	
26	a	1	Total	C	O	P	0
			49	38	10	1	
26	b	1	Total	C	O	P	0
			49	38	10	1	
26	b	1	Total	C	O	P	0
			49	38	10	1	
26	e	1	Total	C	O	P	0
			37	26	10	1	
26	k	1	Total	C	O	P	0
			37	26	10	1	
26	f	1	Total	C	O	P	0
			37	26	10	1	
26	f	1	Total	C	O	P	0
			49	38	10	1	
26	i	1	Total	C	O	P	0
			37	26	10	1	

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Mol	Chain	Residues	Atoms				AltConf
26	j	1	Total	C	O	P	0
			30	19	10	1	
26	d	1	Total	C	O	P	0
			37	26	10	1	
26	g	1	Total	C	O	P	0
			49	38	10	1	
26	g	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 27 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).



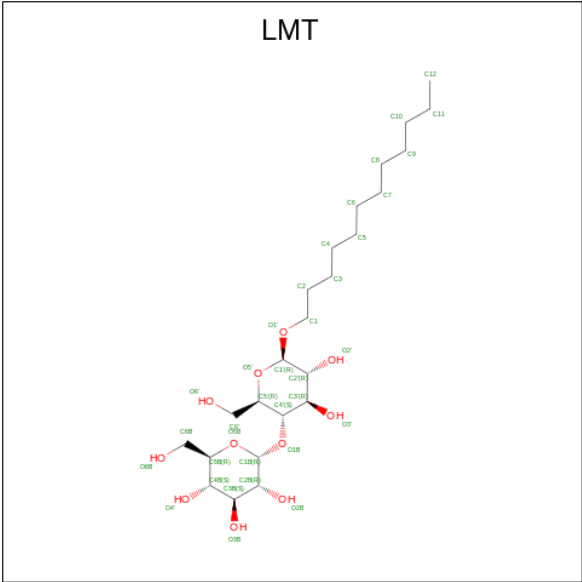
Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	B	1	Total	C	0
			40	40	

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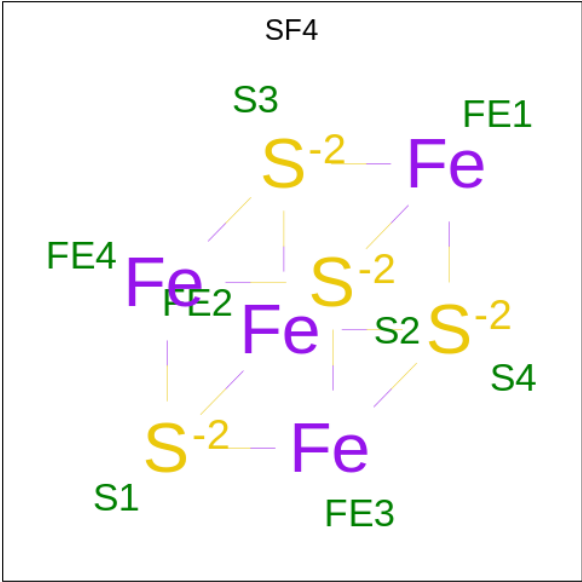
Mol	Chain	Residues	Atoms	AltConf
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	I	1	Total C 40 40	0
27	J	1	Total C 40 40	0
27	J	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	M	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	h	1	Total C 40 40	0
27	e	1	Total C 40 40	0
27	j	1	Total C 40 40	0
27	R	1	Total C 40 40	0
27	R	1	Total C 40 40	0

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



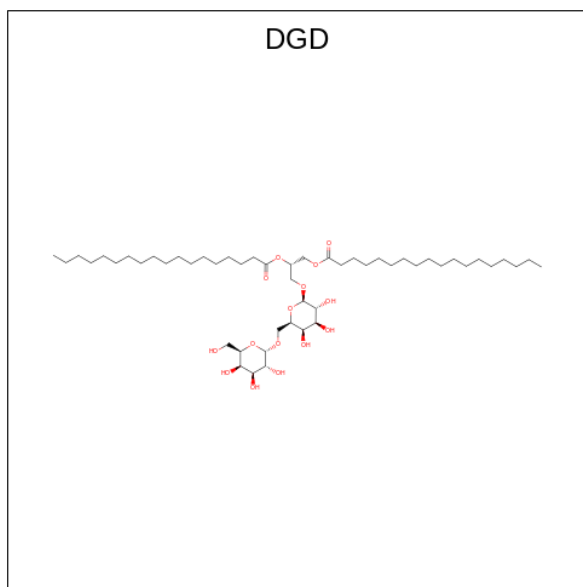
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			35	24	11	
28	F	1	Total	C	O	0
			24	18	6	
28	a	1	Total	C	O	0
			35	24	11	
28	b	1	Total	C	O	0
			24	18	6	

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



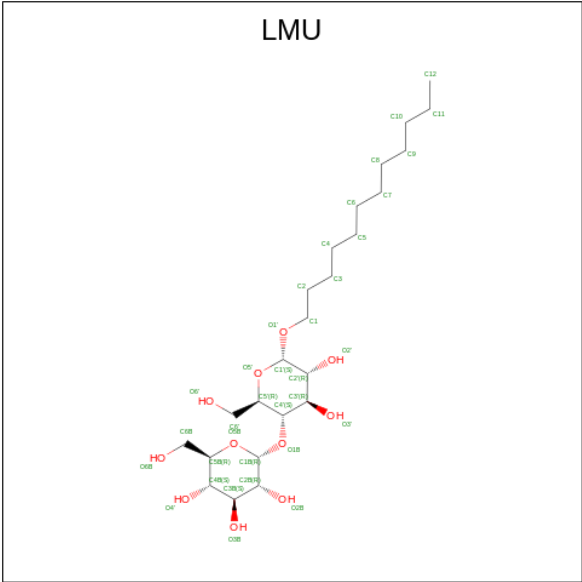
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



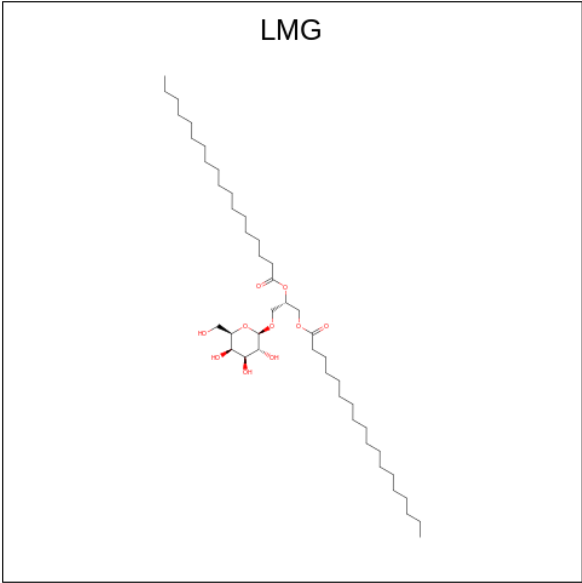
Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			60	45	15	

- Molecule 31 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			35	24	11	

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



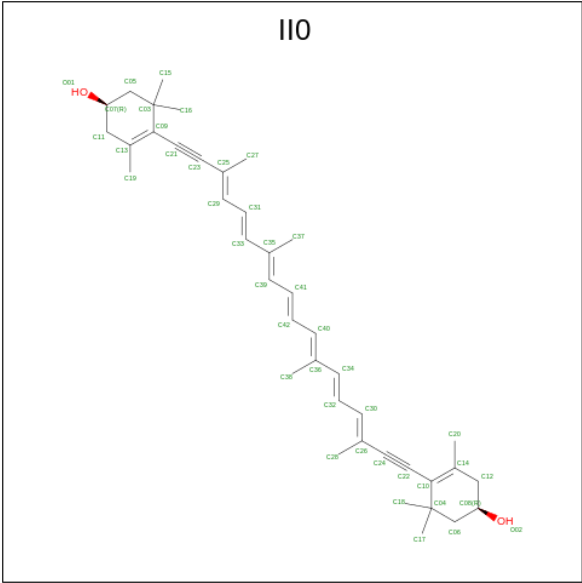
Mol	Chain	Residues	Atoms			AltConf
32	F	1	Total	C	O	0
			48	38	10	
32	J	1	Total	C	O	0
			55	45	10	

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Mol	Chain	Residues	Atoms			AltConf
32	L	1	Total	C	O	0
			55	45	10	
32	O	1	Total	C	O	0
			26	16	10	
32	b	1	Total	C	O	0
			55	45	10	

- Molecule 33 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: C₄₀H₅₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
33	J	1	Total	C	O	0
			42	40	2	
33	O	1	Total	C	O	0
			42	40	2	
33	c	1	Total	C	O	0
			42	40	2	
33	c	1	Total	C	O	0
			42	40	2	
33	c	1	Total	C	O	0
			42	40	2	
33	a	1	Total	C	O	0
			42	40	2	
33	a	1	Total	C	O	0
			42	40	2	

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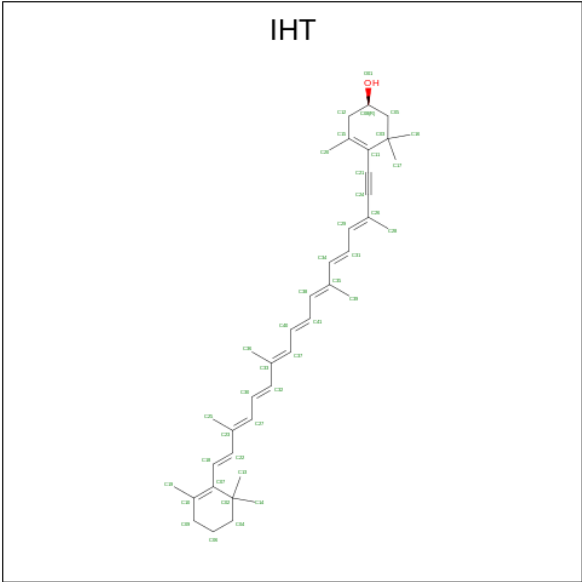
Mol	Chain	Residues	Atoms			AltConf
33	a	1	Total 42	C 40	O 2	0
33	a	1	Total 42	C 40	O 2	0
33	b	1	Total 42	C 40	O 2	0
33	b	1	Total 42	C 40	O 2	0
33	b	1	Total 42	C 40	O 2	0
33	h	1	Total 28	C 27	O 1	0
33	h	1	Total 42	C 40	O 2	0
33	h	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	f	1	Total 42	C 40	O 2	0
33	f	1	Total 42	C 40	O 2	0
33	f	1	Total 42	C 40	O 2	0
33	f	1	Total 42	C 40	O 2	0

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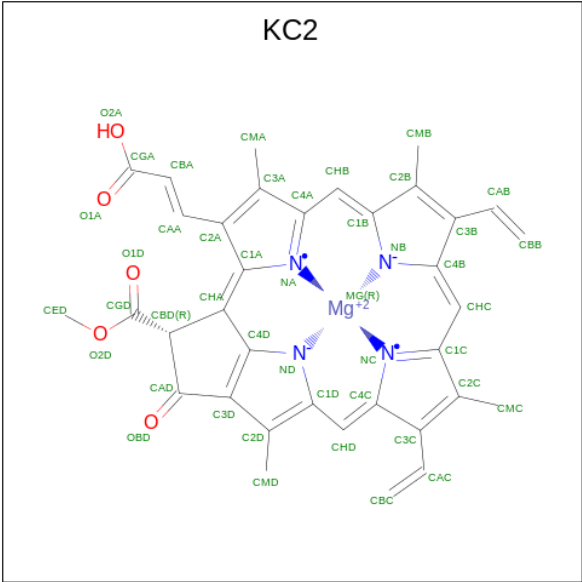
Mol	Chain	Residues	Atoms			AltConf
33	i	1	Total	C	O	0
			42	40	2	
33	i	1	Total	C	O	0
			42	40	2	
33	i	1	Total	C	O	0
			42	40	2	
33	j	1	Total	C	O	0
			42	40	2	
33	j	1	Total	C	O	0
			42	40	2	
33	j	1	Total	C	O	0
			42	40	2	
33	d	1	Total	C	O	0
			42	40	2	
33	d	1	Total	C	O	0
			42	40	2	
33	d	1	Total	C	O	0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

- Molecule 34 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
34	O	1	Total	C	O	0
			41	40	1	
34	c	1	Total	C	O	0
			41	40	1	
34	a	1	Total	C	O	0
			41	40	1	
34	b	1	Total	C	O	0
			41	40	1	
34	b	1	Total	C	O	0
			41	40	1	
34	k	1	Total	C	O	0
			41	40	1	
34	f	1	Total	C	O	0
			41	40	1	
34	j	1	Total	C	O	0
			41	40	1	
34	g	1	Total	C	O	0
			41	40	1	
34	R	1	Total	C	O	0
			41	40	1	

- Molecule 35 is Chlorophyll c2 (CCD ID: KC2) (formula: C₃₅H₂₈MgN₄O₅).



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

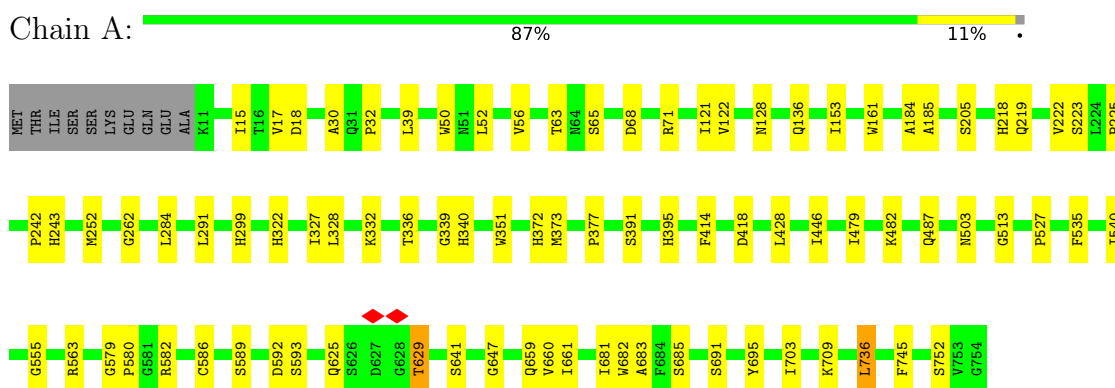
- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	A	50	Total 50	O 50	0
36	B	59	Total 59	O 59	0
36	C	7	Total 7	O 7	0
36	D	1	Total 1	O 1	0
36	F	3	Total 3	O 3	0
36	I	1	Total 1	O 1	0
36	J	1	Total 1	O 1	0
36	L	1	Total 1	O 1	0
36	O	1	Total 1	O 1	0
36	K	1	Total 1	O 1	0
36	a	1	Total 1	O 1	0
36	b	1	Total 1	O 1	0
36	h	1	Total 1	O 1	0
36	e	4	Total 4	O 4	0

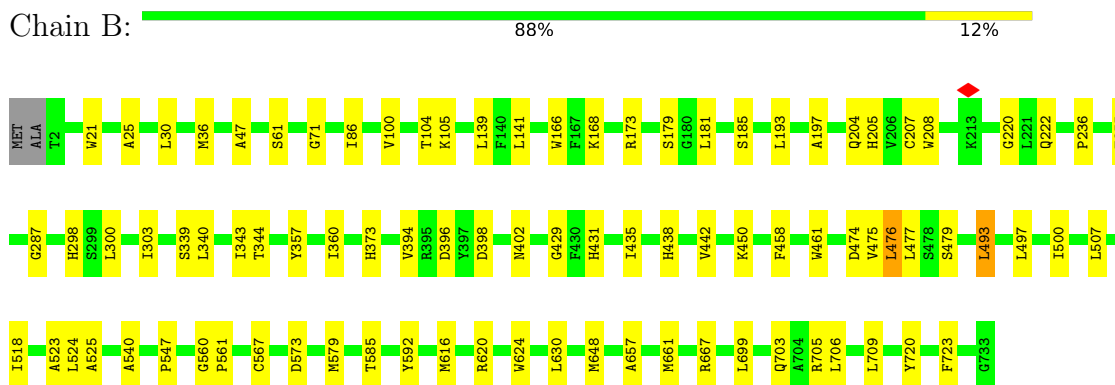
3 Residue-property plots

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.

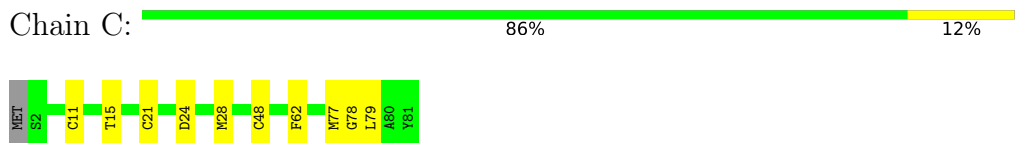
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



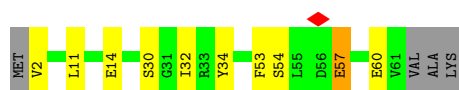
- Molecule 4: Photosystem I reaction center subunit II

Chain D:  85% 13%



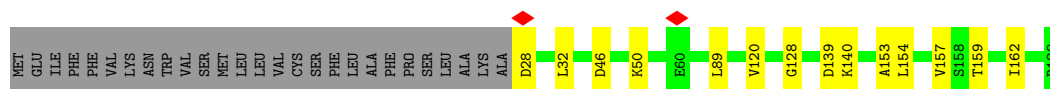
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  78% 14% 6%



- Molecule 6: Photosystem I reaction center subunit III

Chain F:  78% 7% 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:  90% 8% ..

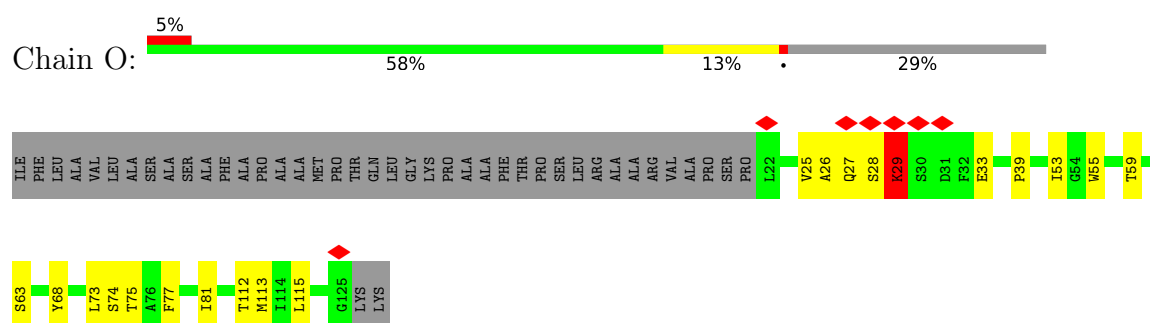


- Molecule 10: Photosystem I reaction center subunit XII

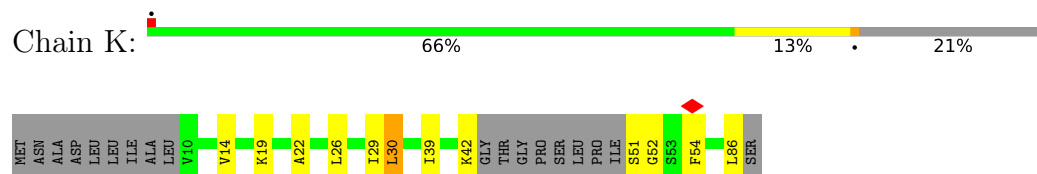
Chain M:  87% 13%



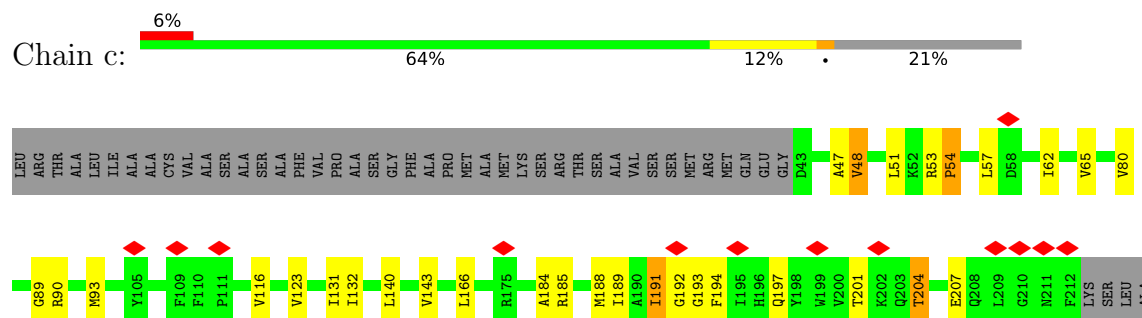
- Molecule 11: PsaO



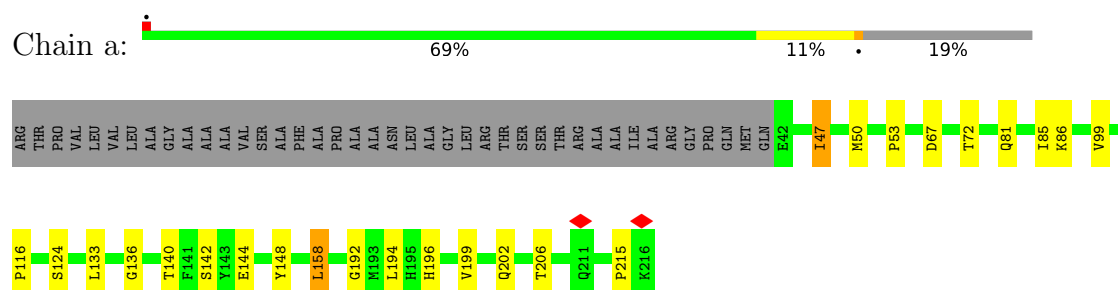
• Molecule 12: Photosystem I reaction center subunit PsaK



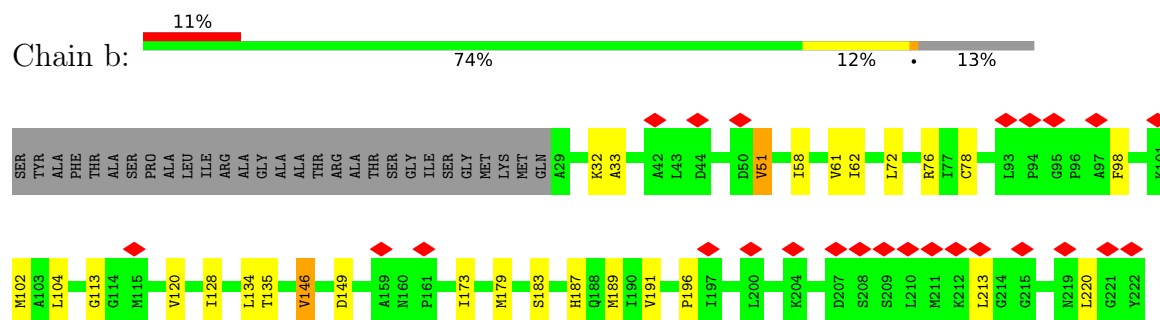
• Molecule 13: CAC-c



• Molecule 14: CAC-a

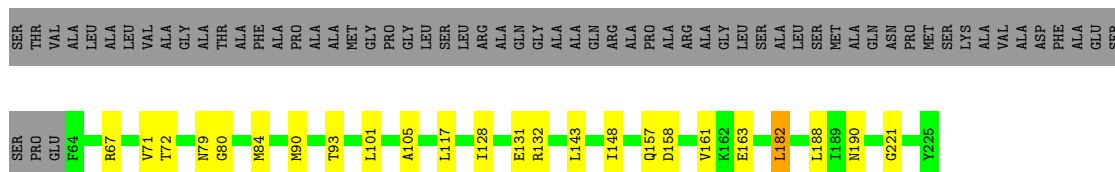


• Molecule 15: CAC-b



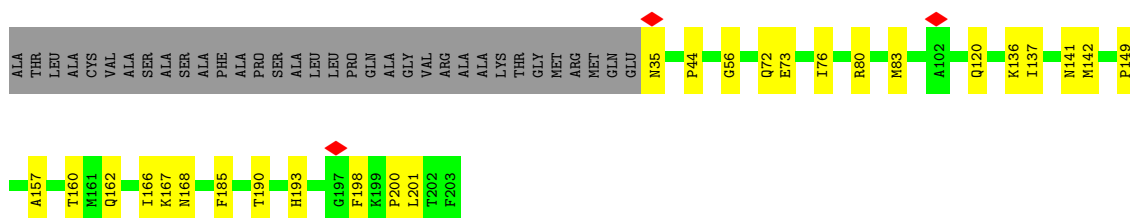
• Molecule 16: CAC-h

Chain h:  61% 10% 28%



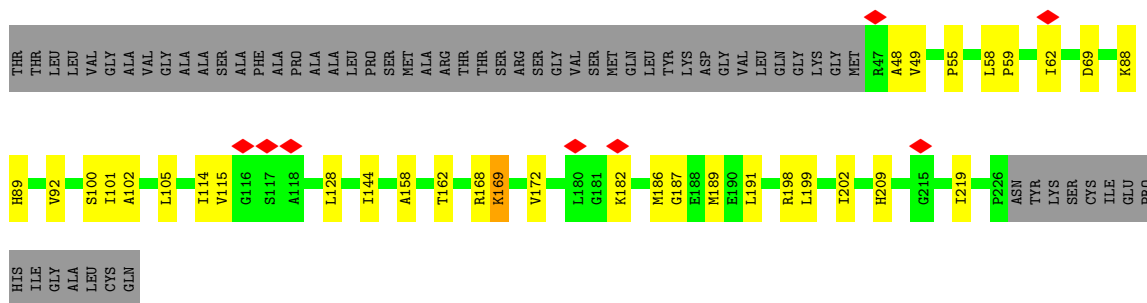
• Molecule 17: CAC-e

Chain e:  70% 13% 17%



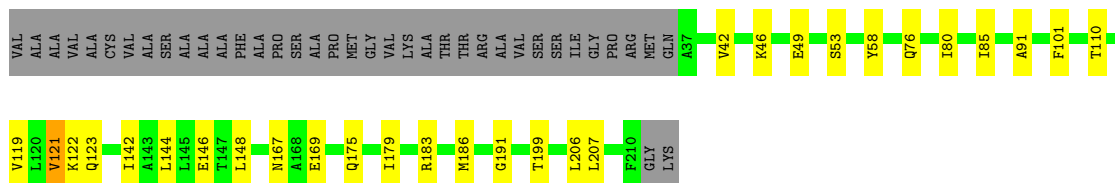
• Molecule 18: CAC-k

Chain k:  61% 13% 25%



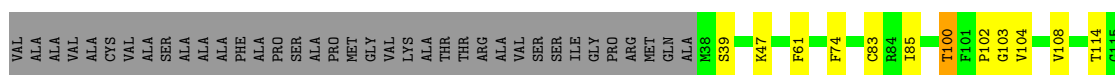
• Molecule 19: CAC-f

Chain f:  68% 13% 18%



• Molecule 19: CAC-f

Chain j:  67% 14% 19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31215	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.140	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size ($\text{\AA}$)	332.8131, 332.8131, 332.8131	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.040041, 1.040041, 1.040041	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, CLA, SF4, WVN, II0, PQN, LMG, DGD, IHT, LMU, KC2, 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	0.48	0/6019	0.57	0/8204
2	B	0.48	0/6045	0.60	1/8254 (0.0%)
3	C	0.42	0/601	0.61	0/813
4	D	0.40	0/1109	0.57	0/1500
5	E	0.45	0/493	0.60	0/667
6	F	0.44	0/1287	0.57	0/1747
7	I	0.43	0/271	0.57	0/370
8	J	0.43	0/364	0.63	0/495
9	L	0.48	0/1175	0.69	0/1599
10	M	0.35	0/233	0.60	0/315
11	O	0.66	0/799	0.88	0/1094
12	K	0.36	0/495	0.59	0/672
13	c	0.39	0/1396	0.72	3/1889 (0.2%)
14	a	0.35	0/1406	0.59	0/1903
15	b	0.38	0/1469	0.66	0/1983
16	h	0.41	0/1226	0.65	2/1667 (0.1%)
17	e	0.38	0/1324	0.66	0/1795
18	k	0.48	0/1380	0.78	0/1869
19	f	0.55	0/1328	0.81	5/1790 (0.3%)
19	j	0.41	0/1318	0.71	0/1775
20	i	0.35	0/1359	0.74	2/1835 (0.1%)
21	d	0.60	0/969	0.87	0/1304
22	g	0.41	0/1673	0.73	4/2264 (0.2%)
23	R	0.36	0/686	0.50	0/940
All	All	0.45	0/34425	0.66	17/46744 (0.0%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	c	192	GLY	N-CA-C	-6.48	107.37	115.08
20	i	194	GLY	CA-C-N	5.92	128.50	120.44
20	i	194	GLY	C-N-CA	5.92	128.50	120.44
13	c	54	PRO	CA-C-N	5.58	132.20	121.54
13	c	54	PRO	C-N-CA	5.58	132.20	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5825	0	5678	66	0
2	B	5826	0	5642	67	0
3	C	592	0	574	8	0
4	D	1084	0	1080	11	0
5	E	485	0	489	6	0
6	F	1254	0	1264	11	0
7	I	264	0	276	4	0
8	J	351	0	344	4	0
9	L	1146	0	1160	12	0
10	M	232	0	265	4	0
11	O	773	0	763	19	0
12	K	488	0	516	8	0
13	c	1357	0	1337	21	0
14	a	1361	0	1305	16	0
15	b	1439	0	1456	23	0
16	h	1200	0	1228	13	0
17	e	1286	0	1262	18	0
18	k	1346	0	1349	22	0
19	f	1302	0	1320	11	0
19	j	1293	0	1321	20	0
20	i	1324	0	1298	9	0
21	d	950	0	949	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	g	1630	0	1644	21	0
23	R	664	0	647	4	0
24	A	2758	0	2820	94	0
24	B	2403	0	2442	70	0
24	F	117	0	115	9	0
24	I	65	0	72	2	0
24	J	93	0	72	3	0
24	K	93	0	72	1	0
24	L	215	0	191	7	0
24	O	130	0	144	9	0
24	R	51	0	41	0	0
24	a	601	0	551	11	0
24	b	673	0	696	33	0
24	c	586	0	520	17	0
24	d	498	0	407	6	0
24	e	582	0	578	20	0
24	f	700	0	695	23	0
24	g	661	0	611	15	0
24	h	440	0	398	3	0
24	i	528	0	451	7	0
24	j	637	0	556	9	0
24	k	596	0	534	18	0
25	A	33	0	46	2	0
25	B	33	0	46	5	0
26	A	75	0	93	1	0
26	B	38	0	49	3	0
26	J	49	0	74	8	0
26	a	49	0	74	0	0
26	b	98	0	148	7	0
26	c	74	0	88	1	0
26	d	37	0	44	0	0
26	e	37	0	44	2	0
26	f	86	0	118	6	0
26	g	86	0	118	1	0
26	i	37	0	44	0	0
26	j	30	0	30	0	0
26	k	37	0	44	0	0
27	A	200	0	0	0	0
27	B	200	0	0	0	0
27	F	80	0	0	0	0
27	I	40	0	0	0	0
27	J	80	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	K	40	0	0	0	0
27	L	120	0	0	0	0
27	M	40	0	0	0	0
27	R	80	0	0	0	0
27	e	40	0	0	0	0
27	h	40	0	0	0	0
27	j	40	0	0	0	0
28	A	35	0	42	1	0
28	F	24	0	33	0	0
28	a	35	0	45	2	0
28	b	24	0	34	2	0
29	A	8	0	0	2	0
29	C	16	0	0	3	0
30	B	60	0	81	3	0
31	B	35	0	46	1	0
32	F	48	0	69	2	0
32	J	55	0	86	6	0
32	L	55	0	86	3	0
32	O	26	0	22	0	0
32	b	55	0	86	6	0
33	J	42	0	0	0	0
33	O	42	0	0	0	0
33	a	168	0	0	1	0
33	b	126	0	0	1	0
33	c	126	0	0	0	0
33	d	126	0	0	0	0
33	e	168	0	0	0	0
33	f	168	0	0	0	0
33	g	168	0	0	0	0
33	h	112	0	0	0	0
33	i	126	0	0	0	0
33	j	126	0	0	0	0
33	k	210	0	0	2	0
34	O	41	0	0	0	0
34	R	41	0	0	0	0
34	a	41	0	0	0	0
34	b	82	0	0	0	0
34	c	41	0	0	0	0
34	f	41	0	0	0	0
34	g	41	0	0	1	0
34	j	41	0	0	1	0
34	k	41	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	c	45	0	0	0	0
35	d	90	0	0	1	0
35	e	45	0	0	2	0
35	f	45	0	0	0	0
35	g	135	0	0	2	0
35	i	90	0	0	0	0
35	j	45	0	0	0	0
35	k	135	0	0	0	0
36	A	50	0	0	0	0
36	B	59	0	0	1	0
36	C	7	0	0	0	0
36	D	1	0	0	0	0
36	F	3	0	0	0	0
36	I	1	0	0	0	0
36	J	1	0	0	0	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	O	1	0	0	0	0
36	a	1	0	0	0	0
36	b	1	0	0	1	0
36	e	4	0	0	0	0
36	h	1	0	0	0	0
All	All	51054	0	46823	640	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 640 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)
1:A:586:CYS:HG	29:A:854:SF4:FE2	0.77	0.96
3:C:11:CYS:HG	29:C:102:SF4:FE4	0.66	0.95
3:C:48:CYS:HG	29:C:101:SF4:FE4	0.73	0.94
2:B:438:HIS:HE1	24:B:829:CLA:NA	1.62	0.92
29:A:854:SF4:FE1	2:B:567:CYS:HG	0.68	0.92

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/752 (98%)	723 (98%)	17 (2%)	0	100	100
2	B	731/734 (100%)	708 (97%)	23 (3%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
5	E	58/64 (91%)	55 (95%)	3 (5%)	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%)	92 (90%)	9 (9%)	1 (1%)	12	40
12	K	65/87 (75%)	65 (100%)	0	0	100	100
13	c	168/216 (78%)	167 (99%)	1 (1%)	0	100	100
14	a	173/216 (80%)	171 (99%)	2 (1%)	0	100	100
15	b	192/223 (86%)	191 (100%)	1 (0%)	0	100	100
16	h	160/225 (71%)	159 (99%)	1 (1%)	0	100	100
17	e	167/203 (82%)	164 (98%)	3 (2%)	0	100	100
18	k	178/241 (74%)	174 (98%)	4 (2%)	0	100	100
19	f	172/212 (81%)	167 (97%)	5 (3%)	0	100	100
19	j	170/212 (80%)	167 (98%)	3 (2%)	0	100	100
20	i	171/218 (78%)	165 (96%)	6 (4%)	0	100	100
21	d	120/213 (56%)	120 (100%)	0	0	100	100
22	g	217/255 (85%)	206 (95%)	11 (5%)	0	100	100
23	R	88/129 (68%)	87 (99%)	1 (1%)	0	100	100
All	All	4295/5017 (86%)	4194 (98%)	100 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	O	29	LYS

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	83
2	B	593/593 (100%)	589 (99%)	4 (1%)	76	80
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	116/117 (99%)	115 (99%)	1 (1%)	70	78
5	E	55/58 (95%)	53 (96%)	2 (4%)	31	58
6	F	133/157 (85%)	133 (100%)	0	100	100
7	I	28/29 (97%)	28 (100%)	0	100	100
8	J	39/39 (100%)	39 (100%)	0	100	100
9	L	124/126 (98%)	123 (99%)	1 (1%)	73	79
10	M	25/25 (100%)	25 (100%)	0	100	100
11	O	81/110 (74%)	80 (99%)	1 (1%)	63	75
12	K	52/66 (79%)	49 (94%)	3 (6%)	18	47
13	c	138/171 (81%)	132 (96%)	6 (4%)	26	54
14	a	139/165 (84%)	132 (95%)	7 (5%)	22	50
15	b	149/168 (89%)	146 (98%)	3 (2%)	48	68
16	h	123/162 (76%)	118 (96%)	5 (4%)	27	55
17	e	130/155 (84%)	128 (98%)	2 (2%)	57	72
18	k	138/186 (74%)	134 (97%)	4 (3%)	37	62
19	f	135/161 (84%)	123 (91%)	12 (9%)	9	32
19	j	136/161 (84%)	129 (95%)	7 (5%)	21	50
20	i	138/168 (82%)	133 (96%)	5 (4%)	31	58
21	d	94/157 (60%)	89 (95%)	5 (5%)	20	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	g	171/199 (86%)	166 (97%)	5 (3%)	37	62
23	R	69/98 (70%)	69 (100%)	0	100	100
All	All	3480/3955 (88%)	3404 (98%)	76 (2%)	45	66

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	i	204	LYS
22	g	45	LEU
19	j	39	SER
19	j	204	LEU
22	g	251	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
11	O	84	ASN
22	g	80	GLN
15	b	100	GLN
20	i	166	ASN
15	b	92	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

342 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$
24	CLA	B	825	2	69,73,73	1.26	12 (17%)	83,113,113	1.41	11 (13%)
24	CLA	j	308	19	55,59,73	1.39	7 (12%)	66,96,113	1.24	6 (9%)
27	WVN	R	201	-	40,41,41	1.89	14 (35%)	50,56,56	1.84	12 (24%)
26	LHG	k	620	24	36,36,48	1.14	2 (5%)	39,42,54	1.15	5 (12%)
24	CLA	f	606	19	55,59,73	1.39	7 (12%)	66,96,113	1.45	7 (10%)
24	CLA	j	303	19	54,58,73	1.41	8 (14%)	65,95,113	1.25	7 (10%)
35	KC2	k	613	35	49,53,53	2.81	21 (42%)	62,89,89	4.10	33 (53%)
24	CLA	B	808	2	69,73,73	1.26	8 (11%)	83,113,113	1.19	9 (10%)
24	CLA	a	305	36	69,73,73	1.22	10 (14%)	83,113,113	1.27	10 (12%)
34	IHT	g	319	-	40,42,42	6.12	25 (62%)	53,58,58	2.33	19 (35%)
24	CLA	B	836	2	69,73,73	1.26	11 (15%)	83,113,113	1.44	10 (12%)
24	CLA	A	813	1	49,53,73	1.48	8 (16%)	59,89,113	1.49	8 (13%)
27	WVN	j	301	-	40,41,41	1.92	14 (35%)	50,56,56	2.11	18 (36%)
24	CLA	A	801	1	69,73,73	1.23	7 (10%)	83,113,113	1.23	8 (9%)
33	II0	g	320	-	39,43,43	6.78	21 (53%)	50,60,60	2.13	19 (38%)
24	CLA	A	804	1	69,73,73	1.22	10 (14%)	83,113,113	1.39	9 (10%)
24	CLA	d	302	21	55,59,73	1.44	8 (14%)	66,96,113	1.36	12 (18%)
27	WVN	M	101	-	40,41,41	1.87	14 (35%)	50,56,56	2.11	15 (30%)
24	CLA	B	827	2	54,58,73	1.37	8 (14%)	65,95,113	1.32	9 (13%)
35	KC2	e	609	17	49,53,53	2.69	19 (38%)	62,89,89	4.10	34 (54%)
33	II0	j	315	-	39,43,43	6.61	20 (51%)	50,60,60	2.53	18 (36%)
24	CLA	i	611	20	55,59,73	1.40	6 (10%)	66,96,113	1.34	10 (15%)
24	CLA	d	308	21	45,49,73	1.50	8 (17%)	54,84,113	1.33	5 (9%)
24	CLA	h	306	16	61,65,73	1.37	7 (11%)	73,103,113	1.16	6 (8%)
24	CLA	B	806	2	69,73,73	1.26	10 (14%)	83,113,113	1.34	10 (12%)
24	CLA	A	820	36	69,73,73	1.27	10 (14%)	83,113,113	1.38	9 (10%)
24	CLA	e	611	17	69,73,73	1.25	8 (11%)	83,113,113	1.33	11 (13%)
24	CLA	b	312	15	69,73,73	1.27	8 (11%)	83,113,113	1.25	9 (10%)
24	CLA	B	805	2	69,73,73	1.21	9 (13%)	83,113,113	1.35	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	II0	b	318	-	39,43,43	6.81	23 (58%)	50,60,60	2.34	21 (42%)
33	II0	f	614	-	39,43,43	6.70	21 (53%)	50,60,60	2.36	15 (30%)
35	KC2	j	312	19	49,53,53	2.69	19 (38%)	62,89,89	4.19	35 (56%)
24	CLA	A	830	1	54,58,73	1.41	11 (20%)	65,95,113	1.45	9 (13%)
24	CLA	g	307	22	55,59,73	1.37	8 (14%)	66,96,113	1.36	10 (15%)
24	CLA	b	308	15	65,69,73	1.30	7 (10%)	78,108,113	1.54	12 (15%)
30	DGD	B	843	-	61,61,67	0.88	2 (3%)	75,75,81	1.19	8 (10%)
24	CLA	e	602	17	54,58,73	1.37	9 (16%)	65,95,113	1.37	6 (9%)
24	CLA	A	817	1	69,73,73	1.27	10 (14%)	83,113,113	1.37	11 (13%)
24	CLA	A	840	1	69,73,73	1.20	10 (14%)	83,113,113	1.25	8 (9%)
24	CLA	L	207	36	55,59,73	1.36	8 (14%)	66,96,113	1.36	8 (12%)
35	KC2	i	616	-	49,53,53	2.82	20 (40%)	62,89,89	4.07	35 (56%)
24	CLA	a	306	14	49,53,73	1.49	8 (16%)	59,89,113	1.56	5 (8%)
25	PQN	A	843	-	34,34,34	1.89	5 (14%)	42,45,45	1.23	5 (11%)
24	CLA	h	305	16	69,73,73	1.23	9 (13%)	83,113,113	1.25	8 (9%)
33	II0	c	616	-	39,43,43	6.90	22 (56%)	50,60,60	2.05	16 (32%)
24	CLA	B	830	36	69,73,73	1.26	9 (13%)	83,113,113	1.26	8 (9%)
24	CLA	c	612	13	69,73,73	1.21	5 (7%)	83,113,113	1.23	11 (13%)
24	CLA	k	610	26	55,59,73	1.37	7 (12%)	66,96,113	1.32	6 (9%)
24	CLA	j	309	19	49,53,73	1.47	9 (18%)	59,89,113	1.42	8 (13%)
33	II0	e	616	-	39,43,43	6.81	21 (53%)	50,60,60	2.02	18 (36%)
33	II0	i	612	-	39,43,43	6.65	23 (58%)	50,60,60	2.50	16 (32%)
24	CLA	j	310	19	55,59,73	1.38	9 (16%)	66,96,113	1.29	9 (13%)
24	CLA	K	102	12	46,50,73	1.48	10 (21%)	55,85,113	1.59	11 (20%)
24	CLA	f	608	19	69,73,73	1.21	7 (10%)	83,113,113	1.26	9 (10%)
24	CLA	A	809	1	60,64,73	1.35	8 (13%)	72,102,113	1.28	8 (11%)
33	II0	e	613	-	39,43,43	6.70	23 (58%)	50,60,60	2.04	16 (32%)
24	CLA	g	302	22	46,50,73	1.46	10 (21%)	55,85,113	1.65	10 (18%)
24	CLA	B	819	2	50,54,73	1.39	8 (16%)	60,90,113	1.42	9 (15%)
27	WVN	A	848	-	40,41,41	1.81	13 (32%)	50,56,56	1.74	12 (24%)
26	LHG	b	302	24	48,48,48	0.93	2 (4%)	51,54,54	1.20	5 (9%)
24	CLA	F	202	6	56,60,73	1.36	8 (14%)	67,97,113	1.52	11 (16%)
24	CLA	A	828	1	69,73,73	1.22	9 (13%)	83,113,113	1.34	7 (8%)
29	SF4	A	854	1,2	0,12,12	-	-	-	-	-
34	IHT	f	617	-	40,42,42	6.19	25 (62%)	53,58,58	3.99	25 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	II0	J	104	-	39,43,43	6.60	20 (51%)	50,60,60	2.09	16 (32%)
24	CLA	j	302	19	55,59,73	1.42	8 (14%)	66,96,113	1.28	5 (7%)
24	CLA	k	604	18	69,73,73	1.24	7 (10%)	83,113,113	1.28	8 (9%)
24	CLA	A	812	1	69,73,73	1.22	9 (13%)	83,113,113	1.46	10 (12%)
34	IHT	R	204	-	40,42,42	6.26	25 (62%)	53,58,58	2.19	19 (35%)
24	CLA	L	202	9	53,57,73	1.45	9 (16%)	62,93,113	1.42	8 (12%)
24	CLA	A	853	1	69,73,73	1.24	9 (13%)	83,113,113	1.34	11 (13%)
24	CLA	A	815	36	49,53,73	1.49	10 (20%)	59,89,113	1.59	8 (13%)
24	CLA	B	841	26	69,73,73	1.24	9 (13%)	83,113,113	1.30	10 (12%)
29	SF4	C	101	3	0,12,12	-	-	-	-	-
24	CLA	j	314	19	69,73,73	1.22	6 (8%)	83,113,113	1.26	8 (9%)
33	II0	i	613	-	39,43,43	6.81	23 (58%)	50,60,60	1.96	14 (28%)
35	KC2	d	311	21	49,53,53	2.79	20 (40%)	62,89,89	4.04	37 (59%)
24	CLA	g	306	22	55,59,73	1.40	8 (14%)	66,96,113	1.23	6 (9%)
24	CLA	i	603	20	55,59,73	1.40	9 (16%)	66,96,113	1.39	7 (10%)
24	CLA	B	835	36	69,73,73	1.24	8 (11%)	83,113,113	1.15	7 (8%)
34	IHT	k	618	-	40,42,42	6.25	25 (62%)	53,58,58	1.79	15 (28%)
24	CLA	L	204	36	54,58,73	1.38	10 (18%)	65,95,113	1.43	7 (10%)
24	CLA	b	306	15	69,73,73	1.30	11 (15%)	83,113,113	1.48	8 (9%)
24	CLA	A	855	36	69,73,73	1.30	10 (14%)	83,113,113	1.43	11 (13%)
28	LMT	F	203	-	24,24,36	1.07	1 (4%)	29,29,47	0.98	2 (6%)
33	II0	k	617	-	39,43,43	6.87	22 (56%)	50,60,60	2.61	18 (36%)
24	CLA	B	832	2	62,66,73	1.29	11 (17%)	74,104,113	1.40	10 (13%)
27	WVN	R	202	-	40,41,41	1.88	13 (32%)	50,56,56	2.49	17 (34%)
27	WVN	B	847	-	40,41,41	1.85	13 (32%)	50,56,56	2.34	17 (34%)
33	II0	g	318	-	39,43,43	6.79	21 (53%)	50,60,60	2.18	19 (38%)
24	CLA	B	803	2	69,73,73	1.22	7 (10%)	83,113,113	1.32	9 (10%)
24	CLA	e	604	36	69,73,73	1.23	8 (11%)	83,113,113	1.39	9 (10%)
24	CLA	B	822	36	69,73,73	1.27	10 (14%)	83,113,113	1.63	17 (20%)
33	II0	f	615	-	39,43,43	6.71	21 (53%)	50,60,60	1.98	17 (34%)
33	II0	i	614	-	39,43,43	6.76	22 (56%)	50,60,60	2.42	17 (34%)
24	CLA	g	305	22	69,73,73	1.19	9 (13%)	83,113,113	1.29	8 (9%)
33	II0	f	616	-	39,43,43	6.64	22 (56%)	50,60,60	2.44	19 (38%)
24	CLA	a	312	14	52,56,73	1.44	10 (19%)	62,92,113	1.41	11 (17%)
28	LMT	b	319	-	24,24,36	1.06	2 (8%)	29,29,47	1.03	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	KC2	g	314	35	49,53,53	2.79	20 (40%)	62,89,89	4.13	35 (56%)
34	IHT	c	615	-	40,42,42	6.27	25 (62%)	53,58,58	2.17	16 (30%)
24	CLA	B	824	2	69,73,73	1.21	10 (14%)	83,113,113	1.29	9 (10%)
24	CLA	A	839	1	69,73,73	1.31	9 (13%)	83,113,113	1.35	9 (10%)
33	II0	f	618	-	39,43,43	6.71	20 (51%)	50,60,60	2.38	17 (34%)
24	CLA	h	302	16	54,58,73	1.38	10 (18%)	65,95,113	1.39	10 (15%)
24	CLA	g	308	22	69,73,73	1.21	9 (13%)	83,113,113	1.24	8 (9%)
33	II0	d	314	-	39,43,43	6.70	23 (58%)	50,60,60	2.23	15 (30%)
24	CLA	j	307	19	55,59,73	1.44	10 (18%)	66,96,113	1.59	8 (12%)
27	WVN	A	849	-	40,41,41	1.90	14 (35%)	50,56,56	2.43	20 (40%)
24	CLA	A	819	1	49,53,73	1.48	10 (20%)	59,89,113	1.66	14 (23%)
24	CLA	A	837	1	69,73,73	1.23	8 (11%)	83,113,113	1.49	13 (15%)
24	CLA	B	838	2	61,65,73	1.36	10 (16%)	73,103,113	1.28	8 (10%)
24	CLA	k	607	18	55,59,73	1.43	8 (14%)	66,96,113	1.37	9 (13%)
33	II0	j	318	-	39,43,43	6.70	23 (58%)	50,60,60	2.29	18 (36%)
26	LHG	J	107	24	48,48,48	1.01	2 (4%)	51,54,54	1.08	3 (5%)
32	LMG	L	208	24	55,55,55	0.90	2 (3%)	63,63,63	1.43	10 (15%)
34	IHT	j	317	-	40,42,42	6.22	25 (62%)	53,58,58	2.34	18 (33%)
28	LMT	a	318	-	36,36,36	1.21	5 (13%)	47,47,47	1.15	3 (6%)
33	II0	O	202	-	39,43,43	6.77	22 (56%)	50,60,60	2.15	12 (24%)
24	CLA	B	809	2	69,73,73	1.26	10 (14%)	83,113,113	1.35	10 (12%)
33	II0	b	314	-	39,43,43	6.91	23 (58%)	50,60,60	2.20	13 (26%)
24	CLA	A	808	1	69,73,73	1.23	10 (14%)	83,113,113	1.43	11 (13%)
33	II0	h	309	-	26,28,43	6.13	12 (46%)	31,37,60	2.13	12 (38%)
24	CLA	A	836	1	69,73,73	1.23	8 (11%)	83,113,113	1.47	12 (14%)
24	CLA	A	821	1	53,57,73	1.37	9 (16%)	62,93,113	1.50	8 (12%)
24	CLA	A	802	-	69,73,73	1.25	9 (13%)	83,113,113	1.44	13 (15%)
24	CLA	k	605	18	49,53,73	1.44	8 (16%)	59,89,113	1.38	7 (11%)
24	CLA	i	604	20	69,73,73	1.27	6 (8%)	83,113,113	1.57	9 (10%)
24	CLA	k	602	18	54,58,73	1.44	9 (16%)	65,95,113	1.40	8 (12%)
27	WVN	e	615	-	40,41,41	1.93	14 (35%)	50,56,56	2.15	15 (30%)
24	CLA	e	608	26	50,54,73	1.43	9 (18%)	60,90,113	1.60	6 (10%)
35	KC2	k	612	35,18	49,53,53	2.80	20 (40%)	62,89,89	4.19	41 (66%)
24	CLA	e	606	17	69,73,73	1.22	6 (8%)	83,113,113	1.21	7 (8%)
24	CLA	k	609	18	69,73,73	1.27	7 (10%)	83,113,113	1.33	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	303	15	55,59,73	1.37	8 (14%)	66,96,113	1.47	8 (12%)
24	CLA	F	201	36	69,73,73	1.28	9 (13%)	83,113,113	1.21	8 (9%)
24	CLA	A	832	1	69,73,73	1.24	7 (10%)	83,113,113	1.63	15 (18%)
24	CLA	c	604	13	69,73,73	1.25	9 (13%)	83,113,113	1.18	9 (10%)
27	WVN	B	846	-	40,41,41	1.86	13 (32%)	50,56,56	2.10	16 (32%)
24	CLA	A	805	1	69,73,73	1.24	9 (13%)	83,113,113	1.41	11 (13%)
35	KC2	k	611	18	49,53,53	2.70	19 (38%)	62,89,89	4.12	36 (58%)
24	CLA	A	826	1	69,73,73	1.25	9 (13%)	83,113,113	1.45	14 (16%)
24	CLA	f	604	19	69,73,73	1.20	7 (10%)	83,113,113	1.29	8 (9%)
24	CLA	d	312	21	55,59,73	1.39	6 (10%)	66,96,113	1.53	13 (19%)
24	CLA	A	822	1	55,59,73	1.40	8 (14%)	66,96,113	1.41	10 (15%)
24	CLA	J	103	8	46,50,73	1.49	9 (19%)	55,85,113	1.49	8 (14%)
26	LHG	f	619	24	36,36,48	1.07	2 (5%)	39,42,54	1.21	3 (7%)
33	II0	k	615	-	39,43,43	6.67	21 (53%)	50,60,60	2.20	21 (42%)
24	CLA	b	310	26	69,73,73	1.29	6 (8%)	83,113,113	1.21	12 (14%)
24	CLA	d	304	21	55,59,73	1.42	5 (9%)	66,96,113	1.39	8 (12%)
33	II0	h	310	-	39,43,43	6.55	20 (51%)	50,60,60	2.22	20 (40%)
24	CLA	A	816	1	69,73,73	1.20	9 (13%)	83,113,113	1.49	12 (14%)
24	CLA	j	313	-	55,59,73	1.42	8 (14%)	66,96,113	1.32	6 (9%)
24	CLA	c	608	13	69,73,73	1.24	7 (10%)	83,113,113	1.31	12 (14%)
24	CLA	h	301	16	54,58,73	1.38	8 (14%)	65,95,113	1.32	5 (7%)
24	CLA	A	827	1	66,70,73	1.24	9 (13%)	79,109,113	1.33	10 (12%)
24	CLA	A	810	1	66,70,73	1.24	8 (12%)	79,109,113	1.18	8 (10%)
24	CLA	B	829	2	54,58,73	1.43	10 (18%)	65,95,113	1.44	5 (7%)
33	II0	c	614	-	39,43,43	6.93	21 (53%)	50,60,60	2.21	17 (34%)
24	CLA	A	806	1	69,73,73	1.27	8 (11%)	83,113,113	1.33	9 (10%)
26	LHG	j	319	24	29,29,48	1.26	2 (6%)	32,35,54	1.34	4 (12%)
33	II0	a	317	-	39,43,43	7.00	22 (56%)	50,60,60	2.40	18 (36%)
24	CLA	b	304	15	59,63,73	1.32	9 (15%)	71,101,113	1.40	6 (8%)
24	CLA	e	603	17	55,59,73	1.42	6 (10%)	66,96,113	1.44	12 (18%)
24	CLA	c	602	13	54,58,73	1.41	9 (16%)	65,95,113	1.44	10 (15%)
34	IHT	O	203	-	40,42,42	6.22	26 (65%)	53,58,58	2.34	19 (35%)
26	LHG	d	316	24	36,36,48	1.10	2 (5%)	39,42,54	1.23	5 (12%)
24	CLA	e	607	17	69,73,73	1.19	6 (8%)	83,113,113	1.24	8 (9%)
24	CLA	A	807	1	69,73,73	1.23	7 (10%)	83,113,113	1.33	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	j	305	19	69,73,73	1.22	7 (10%)	83,113,113	1.29	9 (10%)
33	II0	a	314	-	39,43,43	6.70	22 (56%)	50,60,60	2.13	20 (40%)
24	CLA	A	842	1	69,73,73	1.23	10 (14%)	83,113,113	1.41	11 (13%)
24	CLA	a	304	14	55,59,73	1.37	7 (12%)	66,96,113	1.37	4 (6%)
24	CLA	B	811	2	59,63,73	1.38	8 (13%)	71,101,113	1.29	6 (8%)
35	KC2	g	313	22,35	49,53,53	2.75	19 (38%)	62,89,89	4.09	35 (56%)
24	CLA	f	609	19	69,73,73	1.23	7 (10%)	83,113,113	1.23	7 (8%)
24	CLA	B	818	36,2	69,73,73	1.28	8 (11%)	83,113,113	1.29	8 (9%)
33	II0	g	317	-	39,43,43	6.68	23 (58%)	50,60,60	2.28	19 (38%)
33	II0	c	613	-	39,43,43	6.76	21 (53%)	50,60,60	2.15	17 (34%)
24	CLA	c	607	13	50,54,73	1.44	8 (16%)	60,90,113	1.22	5 (8%)
26	LHG	g	321	24	36,36,48	1.08	2 (5%)	39,42,54	1.54	9 (23%)
35	KC2	i	609	20	49,53,53	2.75	19 (38%)	62,89,89	4.21	37 (59%)
24	CLA	B	821	2	57,61,73	1.33	8 (14%)	68,98,113	1.29	7 (10%)
24	CLA	k	606	18	55,59,73	1.37	9 (16%)	66,96,113	1.34	7 (10%)
33	II0	g	316	-	39,43,43	6.82	21 (53%)	50,60,60	2.01	20 (40%)
33	II0	h	311	-	39,43,43	6.75	22 (56%)	50,60,60	2.14	20 (40%)
24	CLA	k	614	18	55,59,73	1.41	6 (10%)	66,96,113	1.33	8 (12%)
33	II0	e	612	-	39,43,43	6.72	21 (53%)	50,60,60	2.22	16 (32%)
24	CLA	B	823	36	68,72,73	1.26	13 (19%)	81,111,113	1.38	10 (12%)
24	CLA	c	605	13	55,59,73	1.39	7 (12%)	66,96,113	1.45	11 (16%)
24	CLA	f	603	19	55,59,73	1.38	8 (14%)	66,96,113	1.45	10 (15%)
24	CLA	f	602	19	69,73,73	1.24	8 (11%)	83,113,113	1.25	8 (9%)
24	CLA	j	311	26	65,69,73	1.29	7 (10%)	78,108,113	1.12	4 (5%)
24	CLA	c	609	26	49,53,73	1.49	8 (16%)	59,89,113	1.33	10 (16%)
24	CLA	a	303	14	54,58,73	1.38	8 (14%)	65,95,113	1.35	9 (13%)
24	CLA	B	820	2	59,63,73	1.32	8 (13%)	71,101,113	1.33	9 (12%)
27	WVN	F	204	-	40,41,41	1.86	14 (35%)	50,56,56	2.20	15 (30%)
32	LMG	J	106	-	55,55,55	0.85	3 (5%)	63,63,63	0.96	4 (6%)
24	CLA	B	831	36	49,53,73	1.49	10 (20%)	59,89,113	1.40	9 (15%)
24	CLA	A	833	1	54,58,73	1.41	10 (18%)	65,95,113	1.35	6 (9%)
24	CLA	A	824	36	69,73,73	1.25	10 (14%)	83,113,113	1.28	10 (12%)
24	CLA	f	607	19	69,73,73	1.24	9 (13%)	83,113,113	1.18	7 (8%)
24	CLA	h	312	36	69,73,73	1.22	7 (10%)	83,113,113	1.30	7 (8%)
24	CLA	f	613	19	69,73,73	1.26	8 (11%)	83,113,113	1.19	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LHG	a	301	24	48,48,48	0.93	2 (4%)	51,54,54	1.17	4 (7%)
24	CLA	j	306	19	49,53,73	1.49	8 (16%)	59,89,113	1.62	10 (16%)
24	CLA	c	611	-	49,53,73	1.46	8 (16%)	59,89,113	1.69	10 (16%)
24	CLA	d	301	21	54,58,73	1.43	7 (12%)	65,95,113	1.37	5 (7%)
24	CLA	A	835	1	69,73,73	1.26	8 (11%)	83,113,113	1.32	9 (10%)
35	KC2	c	610	13	49,53,53	2.78	20 (40%)	62,89,89	4.11	35 (56%)
24	CLA	f	605	19	49,53,73	1.47	9 (18%)	59,89,113	1.32	5 (8%)
26	LHG	e	617	24	36,36,48	1.12	2 (5%)	39,42,54	1.16	4 (10%)
27	WVN	B	849	-	40,41,41	1.90	14 (35%)	50,56,56	1.67	10 (20%)
32	LMG	F	206	-	48,48,55	0.96	2 (4%)	56,56,63	1.26	5 (8%)
27	WVN	h	308	-	40,41,41	1.89	13 (32%)	50,56,56	2.29	19 (38%)
26	LHG	g	301	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	2 (3%)
27	WVN	J	101	-	40,41,41	1.88	14 (35%)	50,56,56	2.02	15 (30%)
24	CLA	f	601	19	51,55,73	1.43	7 (13%)	61,91,113	1.34	4 (6%)
27	WVN	L	206	-	40,41,41	1.84	13 (32%)	50,56,56	2.33	20 (40%)
24	CLA	A	803	1	59,63,73	1.32	7 (11%)	71,101,113	1.52	11 (15%)
26	LHG	c	617	24	36,36,48	1.08	2 (5%)	39,42,54	1.24	5 (12%)
24	CLA	k	608	18	69,73,73	1.23	7 (10%)	83,113,113	1.13	5 (6%)
26	LHG	A	844	-	47,47,48	0.91	2 (4%)	50,53,54	1.15	5 (10%)
29	SF4	C	102	3	0,12,12	-	-	-	-	-
24	CLA	A	829	1	69,73,73	1.24	8 (11%)	83,113,113	1.26	9 (10%)
24	CLA	g	311	26	58,62,73	1.34	7 (12%)	69,99,113	1.20	4 (5%)
33	II0	d	313	-	39,43,43	6.84	23 (58%)	50,60,60	2.23	18 (36%)
26	LHG	A	845	24	26,26,48	1.25	2 (7%)	29,32,54	1.53	5 (17%)
24	CLA	A	814	1	54,58,73	1.40	6 (11%)	65,95,113	1.52	13 (20%)
24	CLA	j	304	19	55,59,73	1.37	6 (10%)	66,96,113	1.41	9 (13%)
24	CLA	i	601	20	55,59,73	1.41	7 (12%)	66,96,113	1.38	3 (4%)
24	CLA	i	608	26	50,54,73	1.45	7 (14%)	60,90,113	1.23	4 (6%)
28	LMT	A	851	-	36,36,36	1.22	6 (16%)	47,47,47	1.36	5 (10%)
24	CLA	B	814	2	63,67,73	1.26	8 (12%)	75,105,113	1.34	7 (9%)
24	CLA	d	303	21	69,73,73	1.28	9 (13%)	83,113,113	1.34	10 (12%)
24	CLA	k	603	18	55,59,73	1.41	8 (14%)	66,96,113	1.56	12 (18%)
31	LMU	B	844	-	36,36,36	1.13	2 (5%)	47,47,47	1.08	4 (8%)
27	WVN	A	850	-	40,41,41	1.89	14 (35%)	50,56,56	2.09	12 (24%)
27	WVN	A	847	-	40,41,41	1.90	14 (35%)	50,56,56	2.99	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	II0	k	621	-	39,43,43	6.93	22 (56%)	50,60,60	2.05	14 (28%)
26	LHG	c	618	24	36,36,48	1.11	2 (5%)	39,42,54	1.20	6 (15%)
24	CLA	c	606	13	56,60,73	1.45	7 (12%)	67,97,113	1.31	8 (11%)
24	CLA	O	205	-	69,73,73	1.32	11 (15%)	83,113,113	1.56	21 (25%)
33	II0	a	313	-	39,43,43	6.70	22 (56%)	50,60,60	2.15	16 (32%)
24	CLA	J	105	26	55,59,73	1.40	8 (14%)	66,96,113	1.51	8 (12%)
24	CLA	g	322	32	69,73,73	1.22	9 (13%)	83,113,113	1.26	6 (7%)
33	II0	e	614	-	39,43,43	6.91	20 (51%)	50,60,60	2.10	20 (40%)
24	CLA	L	203	9	69,73,73	1.24	9 (13%)	83,113,113	1.28	12 (14%)
33	II0	b	315	-	39,43,43	6.72	21 (53%)	50,60,60	2.77	21 (42%)
24	CLA	B	807	2	69,73,73	1.18	9 (13%)	83,113,113	1.46	7 (8%)
24	CLA	A	834	1	55,59,73	1.41	9 (16%)	66,96,113	1.61	14 (21%)
24	CLA	A	841	36	69,73,73	1.23	8 (11%)	83,113,113	1.29	8 (9%)
34	IHT	b	317	-	40,42,42	6.31	26 (65%)	53,58,58	2.85	17 (32%)
24	CLA	g	315	22	55,59,73	1.39	7 (12%)	66,96,113	1.26	8 (12%)
24	CLA	A	852	36	69,73,73	1.25	10 (14%)	83,113,113	1.38	12 (14%)
24	CLA	a	311	14	51,55,73	1.44	9 (17%)	61,91,113	1.81	12 (19%)
24	CLA	i	602	20	54,58,73	1.39	8 (14%)	65,95,113	1.37	6 (9%)
24	CLA	O	201	-	69,73,73	1.27	11 (15%)	83,113,113	1.30	8 (9%)
24	CLA	B	817	2	61,65,73	1.28	9 (14%)	73,103,113	1.44	10 (13%)
24	CLA	k	601	18	55,59,73	1.44	9 (16%)	66,96,113	1.50	6 (9%)
33	II0	a	315	-	39,43,43	6.97	23 (58%)	50,60,60	1.88	15 (30%)
24	CLA	B	801	36	69,73,73	1.25	10 (14%)	83,113,113	1.38	10 (12%)
33	II0	j	316	-	39,43,43	6.68	22 (56%)	50,60,60	2.17	21 (42%)
24	CLA	B	810	2	58,62,73	1.41	10 (17%)	73,100,113	1.24	7 (9%)
27	WVN	J	102	-	40,41,41	1.86	14 (35%)	50,56,56	2.17	16 (32%)
24	CLA	d	309	26	45,49,73	1.50	7 (15%)	54,84,113	1.29	6 (11%)
24	CLA	B	804	-	69,73,73	1.24	11 (15%)	83,113,113	1.51	12 (14%)
32	LMG	b	301	-	55,55,55	0.89	2 (3%)	63,63,63	1.13	5 (7%)
27	WVN	I	101	-	40,41,41	1.85	14 (35%)	50,56,56	1.78	15 (30%)
24	CLA	A	818	1	69,73,73	1.26	8 (11%)	83,113,113	1.40	12 (14%)
24	CLA	g	304	22	55,59,73	1.40	11 (20%)	66,96,113	1.45	13 (19%)
24	CLA	A	825	36	69,73,73	1.20	9 (13%)	83,113,113	1.27	9 (10%)
27	WVN	A	846	-	40,41,41	1.92	14 (35%)	50,56,56	2.27	14 (28%)
24	CLA	h	304	16	55,59,73	1.36	8 (14%)	66,96,113	1.28	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	d	307	21	50,54,73	1.40	6 (12%)	60,90,113	1.36	5 (8%)
24	CLA	c	603	13	55,59,73	1.39	10 (18%)	66,96,113	1.33	6 (9%)
24	CLA	e	601	17	49,53,73	1.49	9 (18%)	59,89,113	1.48	6 (10%)
24	CLA	B	833	2	69,73,73	1.20	10 (14%)	83,113,113	1.38	11 (13%)
24	CLA	b	307	36	69,73,73	1.27	6 (8%)	83,113,113	1.36	11 (13%)
24	CLA	B	839	2	69,73,73	1.28	8 (11%)	83,113,113	1.29	8 (9%)
24	CLA	i	606	20	65,69,73	1.28	7 (10%)	78,108,113	1.12	4 (5%)
24	CLA	B	828	2	53,57,73	1.35	9 (16%)	62,93,113	1.44	8 (12%)
32	LMG	O	204	-	26,26,55	1.26	2 (7%)	34,34,63	1.31	4 (11%)
24	CLA	K	101	36	55,59,73	1.38	10 (18%)	66,96,113	1.53	11 (16%)
35	KC2	g	312	22	49,53,53	2.79	18 (36%)	62,89,89	4.39	39 (62%)
26	LHG	i	615	24	36,36,48	1.12	2 (5%)	39,42,54	1.19	3 (7%)
24	CLA	A	856	26	45,49,73	1.53	10 (22%)	54,84,113	2.02	12 (22%)
24	CLA	g	309	22	69,73,73	1.25	7 (10%)	83,113,113	1.25	8 (9%)
24	CLA	g	303	22	54,58,73	1.39	9 (16%)	65,95,113	1.35	10 (15%)
33	II0	d	315	-	39,43,43	6.91	23 (58%)	50,60,60	2.30	16 (32%)
24	CLA	A	811	1	58,62,73	1.38	8 (13%)	69,99,113	1.40	10 (14%)
35	KC2	d	310	21	49,53,53	2.75	21 (42%)	62,89,89	4.15	35 (56%)
34	IHT	b	316	-	40,42,42	6.23	25 (62%)	53,58,58	2.19	17 (32%)
24	CLA	b	313	15	69,73,73	1.28	8 (11%)	83,113,113	1.14	7 (8%)
24	CLA	d	306	21	55,59,73	1.39	9 (16%)	66,96,113	1.09	3 (4%)
27	WVN	K	103	-	40,41,41	1.93	13 (32%)	50,56,56	2.08	17 (34%)
24	CLA	B	816	2	63,67,73	1.29	8 (12%)	75,105,113	1.40	12 (16%)
35	KC2	f	611	19	49,53,53	2.69	19 (38%)	62,89,89	4.30	34 (54%)
24	CLA	f	612	-	55,59,73	1.40	10 (18%)	66,96,113	1.44	13 (19%)
24	CLA	c	601	13	55,59,73	1.39	9 (16%)	66,96,113	1.36	8 (12%)
27	WVN	B	848	-	40,41,41	1.90	14 (35%)	50,56,56	2.42	15 (30%)
24	CLA	g	310	22	55,59,73	1.39	9 (16%)	66,96,113	1.33	9 (13%)
26	LHG	f	620	-	48,48,48	0.89	2 (4%)	51,54,54	1.09	3 (5%)
24	CLA	B	826	2	69,73,73	1.22	9 (13%)	83,113,113	1.24	9 (10%)
24	CLA	h	303	16	55,59,73	1.40	10 (18%)	66,96,113	1.42	11 (16%)
24	CLA	d	305	-	55,59,73	1.37	9 (16%)	66,96,113	1.27	10 (15%)
24	CLA	b	309	15	69,73,73	1.29	9 (13%)	83,113,113	1.30	11 (13%)
24	CLA	B	812	2	69,73,73	1.25	11 (15%)	83,113,113	1.33	8 (9%)
27	WVN	L	201	-	40,41,41	1.91	13 (32%)	50,56,56	2.28	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	311	15	55,59,73	1.40	9 (16%)	66,96,113	1.44	10 (15%)
24	CLA	b	305	15	69,73,73	1.24	6 (8%)	83,113,113	1.30	6 (7%)
24	CLA	e	610	36	69,73,73	1.27	10 (14%)	83,113,113	1.34	10 (12%)
27	WVN	L	205	-	40,41,41	1.92	13 (32%)	50,56,56	2.03	15 (30%)
24	CLA	B	815	2	59,63,73	1.36	7 (11%)	71,101,113	1.28	9 (12%)
24	CLA	A	831	1	69,73,73	1.25	10 (14%)	83,113,113	1.31	7 (8%)
27	WVN	B	845	-	40,41,41	1.90	13 (32%)	50,56,56	2.42	18 (36%)
26	LHG	b	320	24	48,48,48	0.94	2 (4%)	51,54,54	1.12	5 (9%)
24	CLA	B	834	2	51,55,73	1.39	9 (17%)	61,91,113	1.55	7 (11%)
27	WVN	F	205	-	40,41,41	1.92	14 (35%)	50,56,56	3.08	18 (36%)
24	CLA	i	607	20	55,59,73	1.39	8 (14%)	66,96,113	1.32	10 (15%)
24	CLA	a	307	14	69,73,73	1.25	7 (10%)	83,113,113	1.27	11 (13%)
24	CLA	e	605	17	69,73,73	1.21	8 (11%)	83,113,113	1.23	7 (8%)
24	CLA	a	302	14	56,60,73	1.37	10 (17%)	67,97,113	1.38	7 (10%)
24	CLA	i	605	20	55,59,73	1.43	9 (16%)	66,96,113	1.21	6 (9%)
33	II0	k	619	-	39,43,43	6.75	21 (53%)	50,60,60	2.28	18 (36%)
24	CLA	A	823	1	59,63,73	1.35	8 (13%)	71,101,113	1.25	6 (8%)
24	CLA	a	309	26	52,56,73	1.43	8 (15%)	62,92,113	1.25	7 (11%)
24	CLA	B	813	2	64,68,73	1.27	8 (12%)	77,107,113	1.29	9 (11%)
24	CLA	R	203	23	55,59,73	1.37	8 (14%)	66,96,113	1.47	10 (15%)
24	CLA	I	102	36	69,73,73	1.26	9 (13%)	83,113,113	1.32	9 (10%)
24	CLA	B	840	2	69,73,73	1.26	9 (13%)	83,113,113	1.37	9 (10%)
24	CLA	A	838	26	56,60,73	1.36	11 (19%)	67,97,113	1.34	9 (13%)
25	PQN	B	842	-	34,34,34	1.86	5 (14%)	42,45,45	1.29	6 (14%)
24	CLA	a	310	14	69,73,73	1.23	7 (10%)	83,113,113	1.30	6 (7%)
24	CLA	a	308	14	69,73,73	1.22	10 (14%)	83,113,113	1.39	8 (9%)
24	CLA	f	610	26	69,73,73	1.24	7 (10%)	83,113,113	1.25	6 (7%)
34	IHT	a	316	-	40,42,42	6.19	25 (62%)	53,58,58	2.12	19 (35%)
33	II0	k	616	-	39,43,43	6.84	22 (56%)	50,60,60	2.14	16 (32%)
26	LHG	B	802	-	37,37,48	1.04	2 (5%)	40,43,54	1.14	4 (10%)
24	CLA	h	307	16	55,59,73	1.41	9 (16%)	66,96,113	1.48	8 (12%)
24	CLA	i	610	-	55,59,73	1.42	9 (16%)	66,96,113	1.47	10 (15%)
24	CLA	B	837	2	69,73,73	1.22	10 (14%)	83,113,113	1.31	8 (9%)

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
24	CLA	B	825	2	-	11/39/115/115	-
24	CLA	j	308	19	-	10/23/99/115	-
27	WVN	R	201	-	-	6/29/63/63	0/2/2/2
26	LHG	k	620	24	-	14/41/41/53	-
24	CLA	f	606	19	-	4/23/99/115	-
24	CLA	j	303	19	-	2/21/97/115	-
35	KC2	k	613	35	-	7/15/71/71	-
24	CLA	B	808	2	-	13/39/115/115	-
24	CLA	a	305	36	-	9/39/115/115	-
34	IHT	g	319	-	-	11/25/65/65	0/2/2/2
24	CLA	B	836	2	-	25/39/115/115	-
24	CLA	A	813	1	-	7/15/91/115	-
27	WVN	j	301	-	-	9/29/63/63	0/2/2/2
24	CLA	A	801	1	-	10/39/115/115	-
33	II0	g	320	-	-	4/21/67/67	0/2/2/2
24	CLA	A	804	1	-	7/39/115/115	-
24	CLA	d	302	21	-	3/23/99/115	-
27	WVN	M	101	-	-	9/29/63/63	0/2/2/2
24	CLA	B	827	2	-	11/21/97/115	-
35	KC2	e	609	17	-	5/15/71/71	-
33	II0	j	315	-	-	5/21/67/67	0/2/2/2
24	CLA	i	611	20	-	13/23/99/115	-
24	CLA	d	308	21	-	3/10/86/115	-
24	CLA	h	306	16	-	9/30/106/115	-
24	CLA	B	806	2	-	14/39/115/115	-
24	CLA	A	820	36	-	5/39/115/115	-
24	CLA	e	611	17	-	16/39/115/115	-
24	CLA	b	312	15	-	22/39/115/115	-
24	CLA	B	805	2	-	17/39/115/115	-
33	II0	b	318	-	-	4/21/67/67	0/2/2/2
33	II0	f	614	-	-	4/21/67/67	0/2/2/2
35	KC2	j	312	19	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	830	1	-	5/21/97/115	-
24	CLA	g	307	22	-	9/23/99/115	-
24	CLA	b	308	15	-	14/35/111/115	-
30	DGD	B	843	-	-	5/49/89/95	0/2/2/2
24	CLA	e	602	17	-	6/21/97/115	-
24	CLA	A	817	1	-	15/39/115/115	-
24	CLA	A	840	1	-	16/39/115/115	-
24	CLA	L	207	36	-	5/23/99/115	-
35	KC2	i	616	-	-	10/15/71/71	-
24	CLA	a	306	14	-	8/15/91/115	-
25	PQN	A	843	-	-	6/23/43/43	0/2/2/2
24	CLA	h	305	16	-	11/39/115/115	-
33	II0	c	616	-	-	3/21/67/67	0/2/2/2
24	CLA	B	830	36	-	13/39/115/115	-
24	CLA	c	612	13	-	11/39/115/115	-
24	CLA	k	610	26	-	13/23/99/115	-
24	CLA	j	309	19	-	6/15/91/115	-
33	II0	e	616	-	-	5/21/67/67	0/2/2/2
33	II0	i	612	-	-	7/21/67/67	0/2/2/2
24	CLA	j	310	19	-	5/23/99/115	-
24	CLA	K	102	12	-	7/12/88/115	-
24	CLA	f	608	19	-	9/39/115/115	-
24	CLA	A	809	1	-	9/29/105/115	-
33	II0	e	613	-	-	6/21/67/67	0/2/2/2
24	CLA	g	302	22	-	0/12/88/115	-
24	CLA	B	819	2	-	3/17/93/115	-
27	WVN	A	848	-	-	9/29/63/63	0/2/2/2
26	LHG	b	302	24	-	13/53/53/53	-
24	CLA	F	202	6	-	13/24/100/115	-
24	CLA	A	828	1	-	8/39/115/115	-
29	SF4	A	854	1,2	-	-	0/6/5/5
34	IHT	f	617	-	-	4/25/65/65	0/2/2/2
33	II0	J	104	-	-	7/21/67/67	0/2/2/2
24	CLA	j	302	19	-	7/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	k	604	18	-	11/39/115/115	-
24	CLA	A	812	1	-	22/39/115/115	-
34	IHT	R	204	-	-	4/25/65/65	0/2/2/2
24	CLA	L	202	9	-	9/20/96/115	-
24	CLA	A	853	1	-	16/39/115/115	-
24	CLA	A	815	36	-	7/15/91/115	-
24	CLA	B	841	26	-	3/39/115/115	-
29	SF4	C	101	3	-	-	0/6/5/5
24	CLA	j	314	19	-	14/39/115/115	-
33	II0	i	613	-	-	4/21/67/67	0/2/2/2
35	KC2	d	311	21	-	7/15/71/71	-
24	CLA	g	306	22	-	9/23/99/115	-
24	CLA	i	603	20	-	4/23/99/115	-
24	CLA	B	835	36	-	11/39/115/115	-
34	IHT	k	618	-	-	7/25/65/65	0/2/2/2
24	CLA	L	204	36	-	7/21/97/115	-
24	CLA	b	306	15	-	19/39/115/115	-
24	CLA	A	855	36	-	16/39/115/115	-
28	LMT	F	203	-	-	4/15/35/61	0/1/1/2
33	II0	k	617	-	-	3/21/67/67	0/2/2/2
24	CLA	B	832	2	-	8/31/107/115	-
27	WVN	R	202	-	-	10/29/63/63	0/2/2/2
27	WVN	B	847	-	-	12/29/63/63	0/2/2/2
33	II0	g	318	-	-	2/21/67/67	0/2/2/2
24	CLA	B	803	2	-	21/39/115/115	-
24	CLA	e	604	36	-	11/39/115/115	-
24	CLA	B	822	36	-	10/39/115/115	-
33	II0	f	615	-	-	4/21/67/67	0/2/2/2
33	II0	i	614	-	-	4/21/67/67	0/2/2/2
24	CLA	g	305	22	-	16/39/115/115	-
33	II0	f	616	-	-	5/21/67/67	0/2/2/2
24	CLA	a	312	14	-	6/19/95/115	-
28	LMT	b	319	-	-	9/15/35/61	0/1/1/2
35	KC2	g	314	35	-	9/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	IHT	c	615	-	-	10/25/65/65	0/2/2/2
24	CLA	B	824	2	-	3/39/115/115	-
24	CLA	A	839	1	-	15/39/115/115	-
33	II0	f	618	-	-	7/21/67/67	0/2/2/2
24	CLA	h	302	16	-	11/21/97/115	-
24	CLA	g	308	22	-	18/39/115/115	-
33	II0	d	314	-	-	5/21/67/67	0/2/2/2
24	CLA	j	307	19	-	11/23/99/115	-
27	WVN	A	849	-	-	8/29/63/63	0/2/2/2
24	CLA	A	819	1	-	6/15/91/115	-
24	CLA	A	837	1	-	11/39/115/115	-
24	CLA	B	838	2	-	11/30/106/115	-
24	CLA	k	607	18	-	9/23/99/115	-
33	II0	j	318	-	-	5/21/67/67	0/2/2/2
26	LHG	J	107	24	-	19/53/53/53	-
32	LMG	L	208	24	-	19/50/70/70	0/1/1/1
34	IHT	j	317	-	-	7/25/65/65	0/2/2/2
28	LMT	a	318	-	-	3/21/61/61	0/2/2/2
33	II0	O	202	-	-	3/21/67/67	0/2/2/2
24	CLA	B	809	2	-	11/39/115/115	-
33	II0	b	314	-	-	7/21/67/67	0/2/2/2
24	CLA	A	808	1	-	11/39/115/115	-
33	II0	h	309	-	-	3/17/40/67	0/1/1/2
24	CLA	A	836	1	-	8/39/115/115	-
24	CLA	A	821	1	-	7/20/96/115	-
24	CLA	A	802	-	-	16/39/115/115	-
24	CLA	k	605	18	-	7/15/91/115	-
24	CLA	i	604	20	-	12/39/115/115	-
24	CLA	k	602	18	-	6/21/97/115	-
27	WVN	e	615	-	-	11/29/63/63	0/2/2/2
24	CLA	e	608	26	-	12/17/93/115	-
35	KC2	k	612	35,18	-	8/15/71/71	-
24	CLA	e	606	17	-	11/39/115/115	-
24	CLA	k	609	18	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	303	15	-	9/23/99/115	-
24	CLA	F	201	36	-	14/39/115/115	-
24	CLA	A	832	1	-	14/39/115/115	-
24	CLA	c	604	13	-	5/39/115/115	-
27	WVN	B	846	-	-	0/29/63/63	0/2/2/2
24	CLA	A	805	1	-	7/39/115/115	-
35	KC2	k	611	18	-	7/15/71/71	-
24	CLA	A	826	1	-	8/39/115/115	-
24	CLA	f	604	19	-	8/39/115/115	-
24	CLA	d	312	21	-	5/23/99/115	-
24	CLA	A	822	1	-	8/23/99/115	-
24	CLA	J	103	8	-	5/12/88/115	-
26	LHG	f	619	24	-	22/41/41/53	-
33	II0	k	615	-	-	5/21/67/67	0/2/2/2
24	CLA	b	310	26	-	11/39/115/115	-
24	CLA	d	304	21	-	11/23/99/115	-
33	II0	h	310	-	-	8/21/67/67	0/2/2/2
24	CLA	A	816	1	-	16/39/115/115	-
24	CLA	j	313	-	-	6/23/99/115	-
24	CLA	c	608	13	-	17/39/115/115	-
24	CLA	h	301	16	-	8/21/97/115	-
24	CLA	A	827	1	-	9/36/112/115	-
24	CLA	A	810	1	-	10/36/112/115	-
24	CLA	B	829	2	-	7/21/97/115	-
33	II0	c	614	-	-	1/21/67/67	0/2/2/2
24	CLA	A	806	1	-	10/39/115/115	-
26	LHG	j	319	24	-	5/34/34/53	-
33	II0	a	317	-	-	7/21/67/67	0/2/2/2
24	CLA	b	304	15	-	8/27/103/115	-
24	CLA	e	603	17	-	5/23/99/115	-
24	CLA	c	602	13	-	13/21/97/115	-
34	IHT	O	203	-	-	5/25/65/65	0/2/2/2
26	LHG	d	316	24	-	11/41/41/53	-
24	CLA	e	607	17	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	807	1	-	9/39/115/115	-
24	CLA	j	305	19	-	11/39/115/115	-
33	II0	a	314	-	-	7/21/67/67	0/2/2/2
24	CLA	A	842	1	-	22/39/115/115	-
24	CLA	a	304	14	-	3/23/99/115	-
24	CLA	B	811	2	-	6/27/103/115	-
35	KC2	g	313	22,35	-	2/15/71/71	-
24	CLA	f	609	19	-	5/39/115/115	-
24	CLA	B	818	36,2	-	7/39/115/115	-
33	II0	g	317	-	-	5/21/67/67	0/2/2/2
33	II0	c	613	-	-	3/21/67/67	0/2/2/2
24	CLA	c	607	13	-	3/17/93/115	-
26	LHG	g	321	24	-	12/41/41/53	-
35	KC2	i	609	20	-	9/15/71/71	-
24	CLA	B	821	2	-	9/25/101/115	-
24	CLA	k	606	18	-	8/23/99/115	-
33	II0	g	316	-	-	7/21/67/67	0/2/2/2
33	II0	h	311	-	-	7/21/67/67	0/2/2/2
24	CLA	k	614	18	-	9/23/99/115	-
33	II0	e	612	-	-	4/21/67/67	0/2/2/2
24	CLA	B	823	36	-	11/38/114/115	-
24	CLA	c	605	13	-	9/23/99/115	-
24	CLA	f	603	19	-	5/23/99/115	-
24	CLA	f	602	19	-	19/39/115/115	-
24	CLA	j	311	26	-	15/35/111/115	-
24	CLA	c	609	26	-	4/15/91/115	-
24	CLA	a	303	14	-	6/21/97/115	-
24	CLA	B	820	2	-	10/27/103/115	-
27	WVN	F	204	-	-	10/29/63/63	0/2/2/2
32	LMG	J	106	-	-	13/50/70/70	0/1/1/1
24	CLA	B	831	36	-	6/15/91/115	-
24	CLA	A	833	1	-	6/21/97/115	-
24	CLA	A	824	36	-	11/39/115/115	-
24	CLA	f	607	19	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	h	312	36	-	9/39/115/115	-
24	CLA	f	613	19	-	22/39/115/115	-
26	LHG	a	301	24	-	15/53/53/53	-
24	CLA	j	306	19	-	7/15/91/115	-
24	CLA	c	611	-	-	7/15/91/115	-
24	CLA	d	301	21	-	7/21/97/115	-
24	CLA	A	835	1	-	13/39/115/115	-
35	KC2	c	610	13	-	10/15/71/71	-
24	CLA	f	605	19	-	9/15/91/115	-
26	LHG	e	617	24	-	11/41/41/53	-
27	WVN	B	849	-	-	13/29/63/63	0/2/2/2
32	LMG	F	206	-	-	11/43/63/70	0/1/1/1
27	WVN	h	308	-	-	5/29/63/63	0/2/2/2
26	LHG	g	301	-	-	14/53/53/53	-
27	WVN	J	101	-	-	8/29/63/63	0/2/2/2
24	CLA	f	601	19	-	12/18/94/115	-
27	WVN	L	206	-	-	3/29/63/63	0/2/2/2
24	CLA	A	803	1	-	6/27/103/115	-
26	LHG	c	617	24	-	14/41/41/53	-
24	CLA	k	608	18	-	14/39/115/115	-
26	LHG	A	844	-	-	7/52/52/53	-
29	SF4	C	102	3	-	-	0/6/5/5
24	CLA	A	829	1	-	14/39/115/115	-
24	CLA	g	311	26	-	12/26/102/115	-
33	II0	d	313	-	-	6/21/67/67	0/2/2/2
26	LHG	A	845	24	-	6/31/31/53	-
24	CLA	A	814	1	-	9/21/97/115	-
24	CLA	j	304	19	-	0/23/99/115	-
24	CLA	i	601	20	-	9/23/99/115	-
24	CLA	i	608	26	-	7/17/93/115	-
28	LMT	A	851	-	-	9/21/61/61	0/2/2/2
24	CLA	B	814	2	-	13/32/108/115	-
24	CLA	d	303	21	-	17/39/115/115	-
24	CLA	k	603	18	-	3/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMU	B	844	-	-	8/21/61/61	0/2/2/2
27	WVN	A	850	-	-	14/29/63/63	0/2/2/2
27	WVN	A	847	-	-	10/29/63/63	0/2/2/2
33	II0	k	621	-	-	4/21/67/67	0/2/2/2
26	LHG	c	618	24	-	11/41/41/53	-
24	CLA	c	606	13	-	8/24/100/115	-
24	CLA	O	205	-	-	18/39/115/115	-
33	II0	a	313	-	-	1/21/67/67	0/2/2/2
24	CLA	J	105	26	-	7/23/99/115	-
24	CLA	g	322	32	-	15/39/115/115	-
33	II0	e	614	-	-	3/21/67/67	0/2/2/2
24	CLA	L	203	9	-	13/39/115/115	-
33	II0	b	315	-	-	5/21/67/67	0/2/2/2
24	CLA	B	807	2	-	10/39/115/115	-
24	CLA	A	834	1	-	4/23/99/115	-
24	CLA	A	841	36	-	22/39/115/115	-
34	IHT	b	317	-	-	7/25/65/65	0/2/2/2
24	CLA	g	315	22	-	9/23/99/115	-
24	CLA	A	852	36	-	3/39/115/115	-
24	CLA	a	311	14	-	10/18/94/115	-
24	CLA	i	602	20	-	9/21/97/115	-
24	CLA	O	201	-	-	16/39/115/115	-
24	CLA	B	817	2	-	7/30/106/115	-
24	CLA	k	601	18	-	12/23/99/115	-
33	II0	a	315	-	-	3/21/67/67	0/2/2/2
24	CLA	B	801	36	-	13/39/115/115	-
33	II0	j	316	-	-	2/21/67/67	0/2/2/2
24	CLA	B	810	2	-	5/25/101/115	-
27	WVN	J	102	-	-	8/29/63/63	0/2/2/2
24	CLA	d	309	26	-	2/10/86/115	-
24	CLA	B	804	-	-	9/39/115/115	-
32	LMG	b	301	-	-	17/50/70/70	0/1/1/1
27	WVN	I	101	-	-	9/29/63/63	0/2/2/2
24	CLA	A	818	1	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	g	304	22	-	4/23/99/115	-
24	CLA	A	825	36	-	10/39/115/115	-
27	WVN	A	846	-	-	8/29/63/63	0/2/2/2
24	CLA	h	304	16	-	6/23/99/115	-
24	CLA	d	307	21	-	6/17/93/115	-
24	CLA	c	603	13	-	3/23/99/115	-
24	CLA	e	601	17	-	9/15/91/115	-
24	CLA	B	833	2	-	9/39/115/115	-
24	CLA	b	307	36	-	10/39/115/115	-
24	CLA	B	839	2	-	10/39/115/115	-
24	CLA	i	606	20	-	11/35/111/115	-
24	CLA	B	828	2	-	4/20/96/115	-
32	LMG	O	204	-	-	7/21/41/70	0/1/1/1
24	CLA	K	101	36	-	3/23/99/115	-
35	KC2	g	312	22	-	9/15/71/71	-
26	LHG	i	615	24	-	12/41/41/53	-
24	CLA	A	856	26	-	6/10/86/115	-
24	CLA	g	309	22	-	6/39/115/115	-
24	CLA	g	303	22	-	8/21/97/115	-
33	II0	d	315	-	-	8/21/67/67	0/2/2/2
24	CLA	A	811	1	-	7/26/102/115	-
35	KC2	d	310	21	-	5/15/71/71	-
34	IHT	b	316	-	-	3/25/65/65	0/2/2/2
24	CLA	b	313	15	-	25/39/115/115	-
24	CLA	d	306	21	-	12/23/99/115	-
27	WVN	K	103	-	-	6/29/63/63	0/2/2/2
24	CLA	B	816	2	-	9/32/108/115	-
35	KC2	f	611	19	-	7/15/71/71	-
24	CLA	f	612	-	-	6/23/99/115	-
24	CLA	c	601	13	-	12/23/99/115	-
27	WVN	B	848	-	-	7/29/63/63	0/2/2/2
24	CLA	g	310	22	-	6/23/99/115	-
26	LHG	f	620	-	-	17/53/53/53	-
24	CLA	B	826	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	h	303	16	-	5/23/99/115	-
24	CLA	d	305	-	-	7/23/99/115	-
24	CLA	b	309	15	-	20/39/115/115	-
24	CLA	B	812	2	-	14/39/115/115	-
27	WVN	L	201	-	-	10/29/63/63	0/2/2/2
24	CLA	b	311	15	-	6/23/99/115	-
24	CLA	b	305	15	-	13/39/115/115	-
24	CLA	e	610	36	-	14/39/115/115	-
27	WVN	L	205	-	-	6/29/63/63	0/2/2/2
24	CLA	B	815	2	-	7/27/103/115	-
24	CLA	A	831	1	-	11/39/115/115	-
27	WVN	B	845	-	-	6/29/63/63	0/2/2/2
26	LHG	b	320	24	-	17/53/53/53	-
24	CLA	B	834	2	-	4/18/94/115	-
27	WVN	F	205	-	-	12/29/63/63	0/2/2/2
24	CLA	i	607	20	-	1/23/99/115	-
24	CLA	a	307	14	-	16/39/115/115	-
24	CLA	e	605	17	-	17/39/115/115	-
24	CLA	a	302	14	-	11/24/100/115	-
24	CLA	i	605	20	-	8/23/99/115	-
33	II0	k	619	-	-	5/21/67/67	0/2/2/2
24	CLA	A	823	1	-	8/27/103/115	-
24	CLA	a	309	26	-	8/19/95/115	-
24	CLA	B	813	2	-	14/33/109/115	-
24	CLA	R	203	23	-	9/23/99/115	-
24	CLA	I	102	36	-	17/39/115/115	-
24	CLA	B	840	2	-	11/39/115/115	-
24	CLA	A	838	26	-	5/24/100/115	-
25	PQN	B	842	-	-	13/23/43/43	0/2/2/2
24	CLA	a	310	14	-	13/39/115/115	-
24	CLA	a	308	14	-	14/39/115/115	-
24	CLA	f	610	26	-	15/39/115/115	-
34	IHT	a	316	-	-	9/25/65/65	0/2/2/2
33	II0	k	616	-	-	6/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	B	802	-	-	16/42/42/53	-
24	CLA	h	307	16	-	11/23/99/115	-
24	CLA	i	610	-	-	7/23/99/115	-
24	CLA	B	837	2	-	15/39/115/115	-

The worst 5 of 3669 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	317	IHT	C15-C11	25.48	1.63	1.34
34	R	204	IHT	C15-C11	25.36	1.63	1.34
34	c	615	IHT	C15-C11	25.20	1.63	1.34
34	k	618	IHT	C15-C11	25.15	1.63	1.34
34	j	317	IHT	C15-C11	25.06	1.62	1.34

The worst 5 of 3844 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	f	617	IHT	C40-C37-C33	-13.58	107.93	127.31
35	f	611	KC2	C1A-NA-C4A	-12.51	101.08	106.71
34	b	317	IHT	C40-C37-C33	-12.44	109.55	127.31
35	k	613	KC2	C1A-NA-C4A	-11.85	101.38	106.71
34	f	617	IHT	C30-C27-C23	-11.73	110.57	127.31

There are no chirality outliers.

5 of 3092 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	801	CLA	CBD-CGD-O2D-CED
24	A	802	CLA	C1A-C2A-CAA-CBA
24	A	802	CLA	CBA-CGA-O2A-C1
24	A	802	CLA	O1A-CGA-O2A-C1
24	A	802	CLA	C11-C10-C8-C9

There are no ring outliers.

200 monomers are involved in 400 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	825	CLA	2	0
24	j	308	CLA	1	0
24	f	606	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	808	CLA	1	0
34	g	319	IHT	1	0
24	B	836	CLA	4	0
24	A	813	CLA	2	0
24	A	801	CLA	2	0
24	A	804	CLA	3	0
24	B	827	CLA	3	0
35	e	609	KC2	2	0
24	i	611	CLA	1	0
24	B	806	CLA	2	0
24	A	820	CLA	3	0
24	e	611	CLA	3	0
24	b	312	CLA	6	0
24	B	805	CLA	1	0
24	A	830	CLA	1	0
24	g	307	CLA	1	0
24	b	308	CLA	6	0
30	B	843	DGD	3	0
24	e	602	CLA	1	0
24	A	817	CLA	4	0
24	A	840	CLA	5	0
24	L	207	CLA	1	0
25	A	843	PQN	2	0
24	h	305	CLA	1	0
24	B	830	CLA	2	0
24	c	612	CLA	2	0
24	k	610	CLA	2	0
24	j	309	CLA	2	0
24	f	608	CLA	4	0
24	A	809	CLA	2	0
24	B	819	CLA	1	0
26	b	302	LHG	2	0
24	F	202	CLA	2	0
24	A	828	CLA	2	0
29	A	854	SF4	2	0
24	j	302	CLA	1	0
24	k	604	CLA	1	0
24	A	812	CLA	1	0
24	L	202	CLA	2	0
24	A	853	CLA	4	0
24	A	815	CLA	2	0
24	B	841	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	C	101	SF4	2	0
35	d	311	KC2	1	0
24	B	835	CLA	3	0
34	k	618	IHT	2	0
24	b	306	CLA	2	0
24	A	855	CLA	6	0
24	B	832	CLA	2	0
24	B	803	CLA	2	0
24	e	604	CLA	1	0
24	B	822	CLA	4	0
28	b	319	LMT	2	0
24	B	824	CLA	1	0
24	A	839	CLA	4	0
24	h	302	CLA	1	0
24	g	308	CLA	5	0
24	A	819	CLA	1	0
24	A	837	CLA	2	0
24	k	607	CLA	2	0
26	J	107	LHG	8	0
32	L	208	LMG	3	0
34	j	317	IHT	1	0
28	a	318	LMT	2	0
24	A	836	CLA	3	0
24	A	821	CLA	1	0
24	A	802	CLA	6	0
24	k	602	CLA	3	0
24	e	608	CLA	1	0
24	e	606	CLA	4	0
24	k	609	CLA	2	0
24	b	303	CLA	1	0
24	F	201	CLA	7	0
24	A	805	CLA	1	0
24	f	604	CLA	1	0
24	A	822	CLA	2	0
26	f	619	LHG	3	0
33	k	615	II0	1	0
24	b	310	CLA	3	0
24	d	304	CLA	1	0
24	j	313	CLA	1	0
24	c	608	CLA	2	0
24	A	827	CLA	4	0
24	B	829	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	806	CLA	5	0
24	b	304	CLA	2	0
24	c	602	CLA	2	0
24	e	607	CLA	3	0
24	A	807	CLA	1	0
33	a	314	II0	1	0
24	A	842	CLA	6	0
24	B	811	CLA	1	0
35	g	313	KC2	1	0
24	f	609	CLA	2	0
24	c	607	CLA	2	0
24	B	821	CLA	1	0
24	k	614	CLA	1	0
24	B	823	CLA	5	0
24	c	605	CLA	1	0
24	f	603	CLA	1	0
24	f	602	CLA	4	0
24	j	311	CLA	2	0
24	a	303	CLA	1	0
24	B	820	CLA	4	0
32	J	106	LMG	6	0
24	B	831	CLA	1	0
24	A	824	CLA	1	0
24	f	607	CLA	3	0
24	f	613	CLA	1	0
24	j	306	CLA	2	0
24	c	611	CLA	1	0
24	d	301	CLA	1	0
24	A	835	CLA	2	0
26	e	617	LHG	2	0
32	F	206	LMG	2	0
26	g	301	LHG	1	0
24	f	601	CLA	2	0
24	A	803	CLA	3	0
24	k	608	CLA	3	0
26	A	844	LHG	1	0
29	C	102	SF4	1	0
24	A	829	CLA	3	0
24	A	814	CLA	3	0
24	i	601	CLA	1	0
28	A	851	LMT	1	0
24	B	814	CLA	1	0

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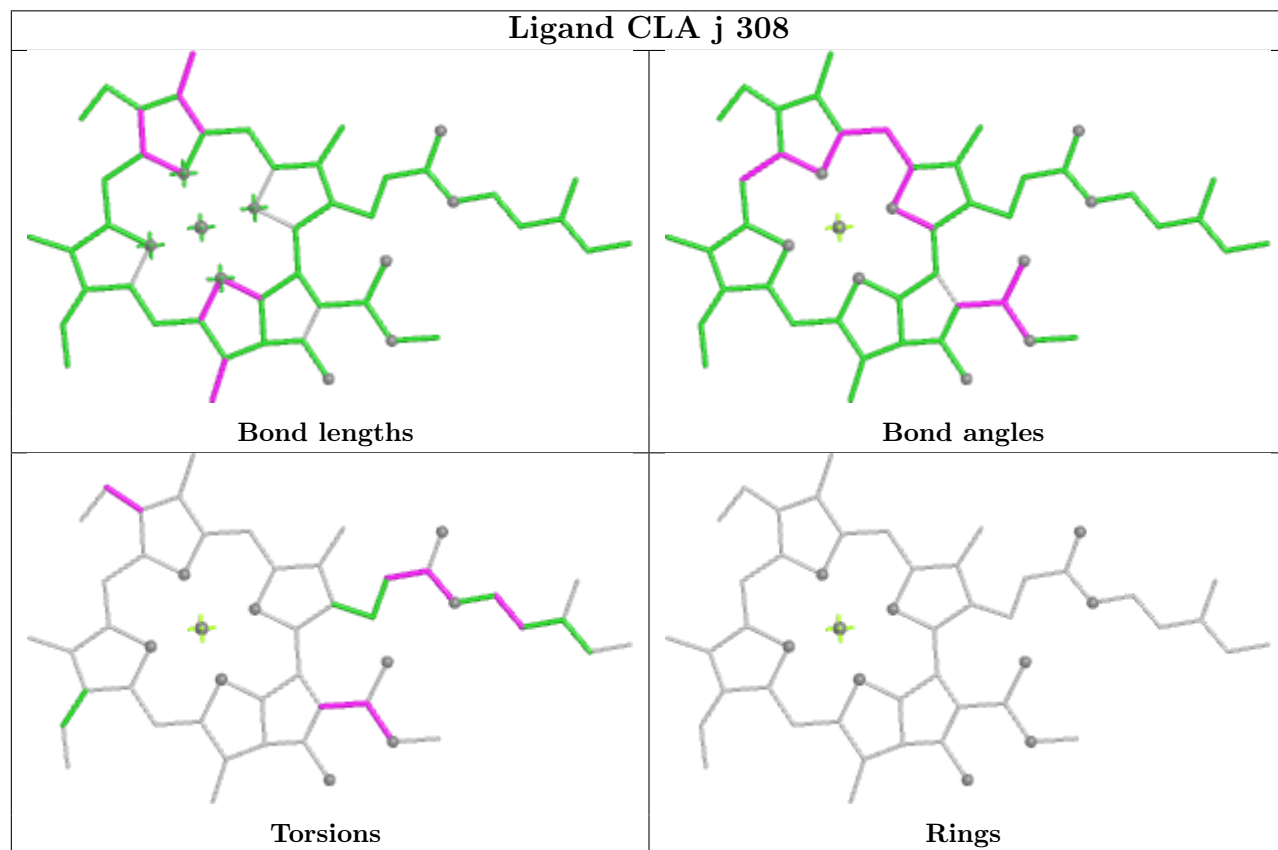
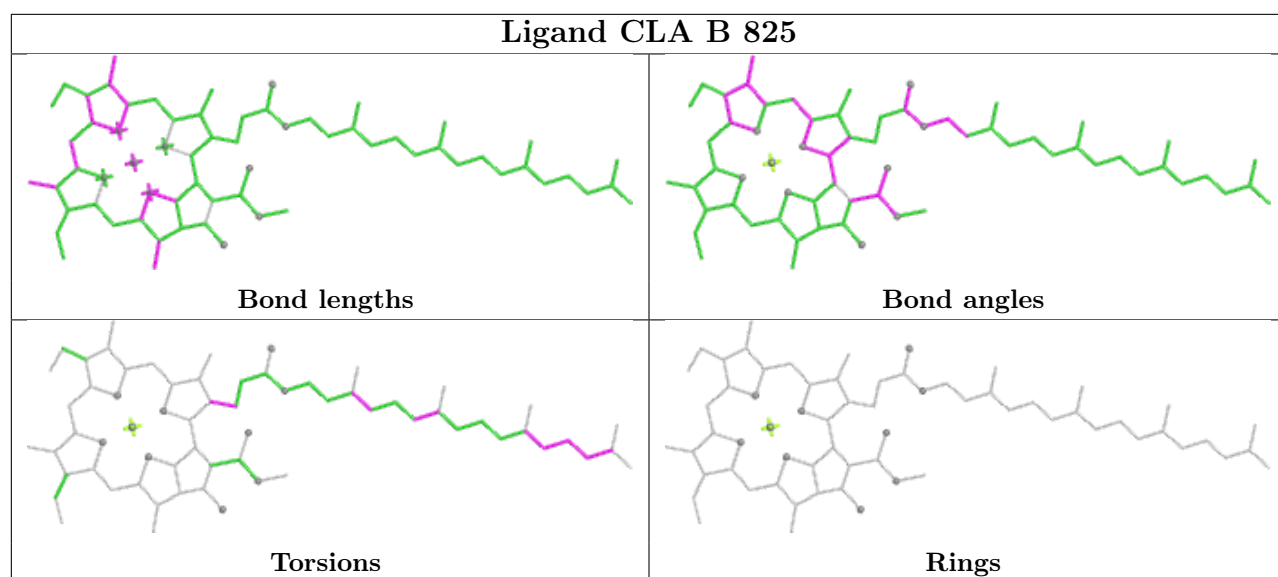
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24	k	603	CLA	3	0
31	B	844	LMU	1	0
26	c	618	LHG	1	0
24	c	606	CLA	5	0
24	O	205	CLA	6	0
24	J	105	CLA	3	0
24	g	322	CLA	2	0
24	L	203	CLA	4	0
33	b	315	II0	1	0
24	B	807	CLA	2	0
24	A	841	CLA	3	0
24	A	852	CLA	1	0
24	a	311	CLA	4	0
24	i	602	CLA	1	0
24	O	201	CLA	3	0
24	B	817	CLA	2	0
24	k	601	CLA	3	0
24	B	801	CLA	6	0
24	B	810	CLA	2	0
24	B	804	CLA	3	0
32	b	301	LMG	6	0
24	A	818	CLA	3	0
24	g	304	CLA	1	0
24	c	603	CLA	1	0
24	e	601	CLA	1	0
24	B	833	CLA	3	0
24	b	307	CLA	3	0
24	B	839	CLA	2	0
24	i	606	CLA	1	0
24	B	828	CLA	3	0
24	K	101	CLA	1	0
35	g	312	KC2	1	0
24	A	856	CLA	5	0
24	g	309	CLA	4	0
24	g	303	CLA	2	0
24	A	811	CLA	2	0
24	b	313	CLA	6	0
24	d	306	CLA	1	0
24	B	816	CLA	2	0
24	c	601	CLA	1	0
24	g	310	CLA	1	0

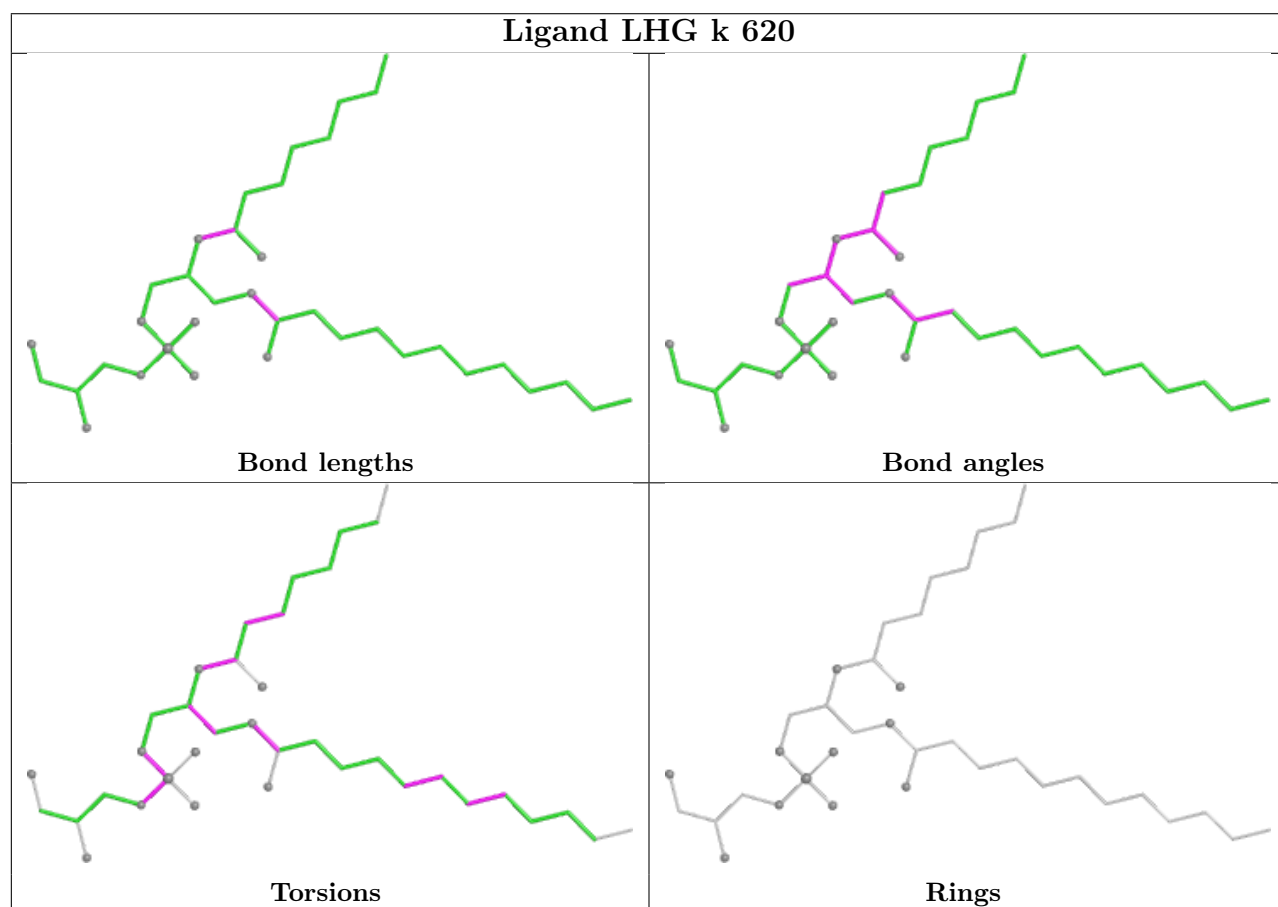
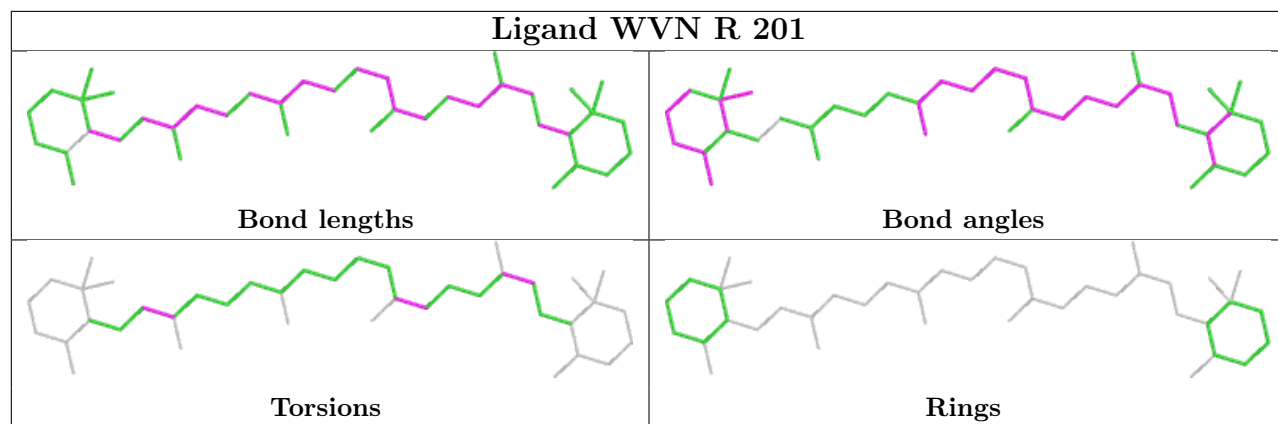
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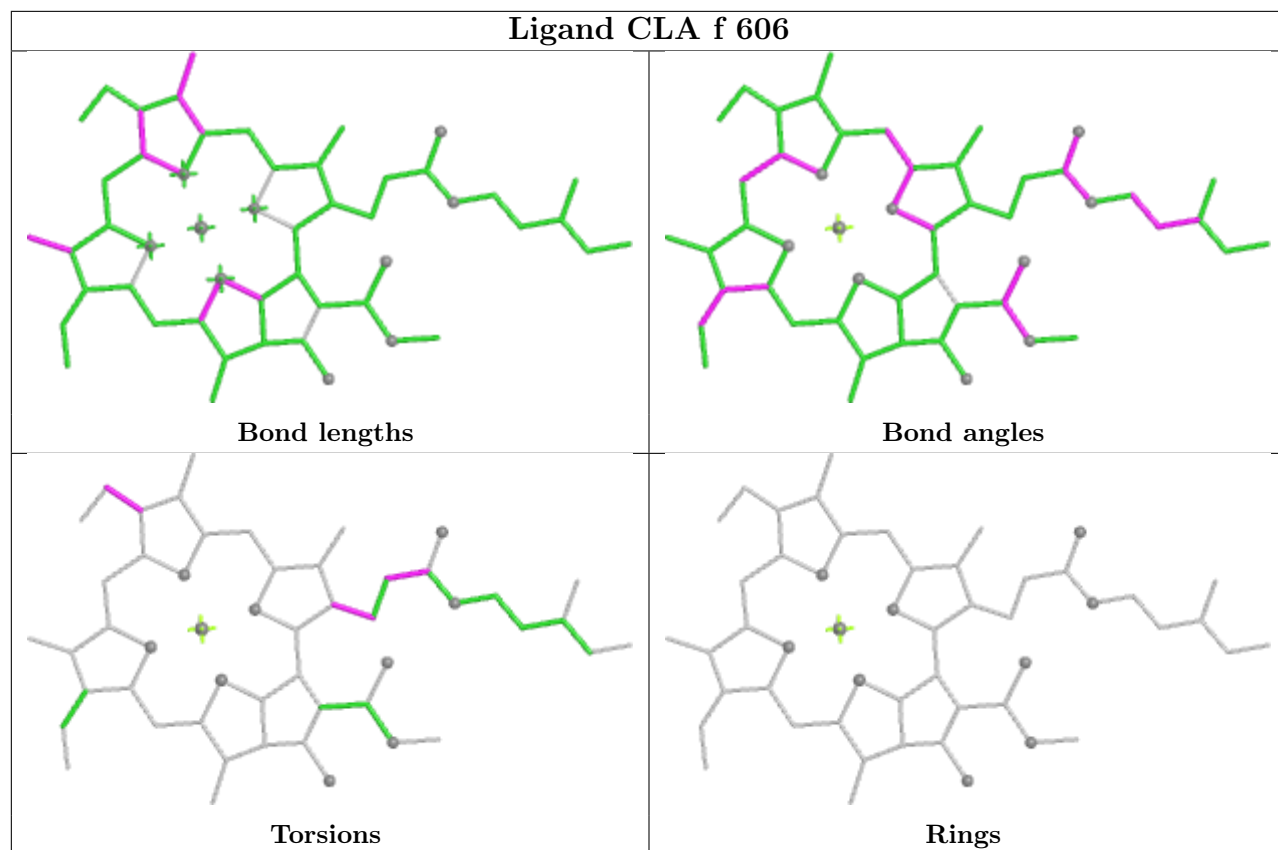
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	f	620	LHG	3	0
24	B	826	CLA	1	0
24	d	305	CLA	1	0
24	b	309	CLA	2	0
24	B	812	CLA	3	0
24	b	305	CLA	3	0
24	e	610	CLA	3	0
24	B	815	CLA	1	0
24	A	831	CLA	1	0
26	b	320	LHG	5	0
24	B	834	CLA	1	0
24	i	607	CLA	1	0
24	a	307	CLA	3	0
24	e	605	CLA	3	0
24	a	302	CLA	1	0
24	i	605	CLA	1	0
24	A	823	CLA	2	0
24	I	102	CLA	2	0
24	B	840	CLA	1	0
24	A	838	CLA	1	0
25	B	842	PQN	5	0
24	a	310	CLA	2	0
24	a	308	CLA	2	0
24	f	610	CLA	4	0
33	k	616	II0	1	0
26	B	802	LHG	3	0
24	h	307	CLA	1	0
24	i	610	CLA	1	0
24	B	837	CLA	4	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.

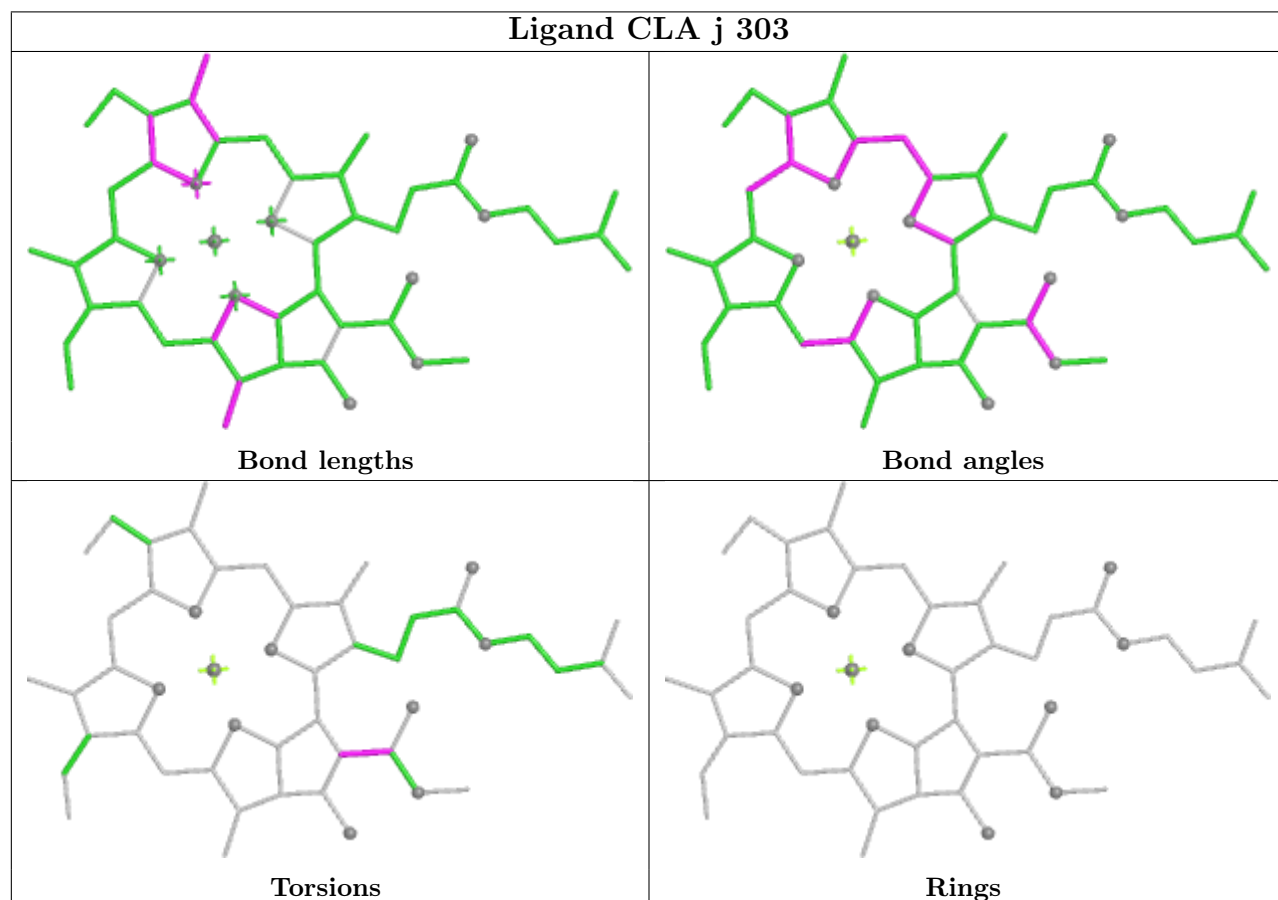




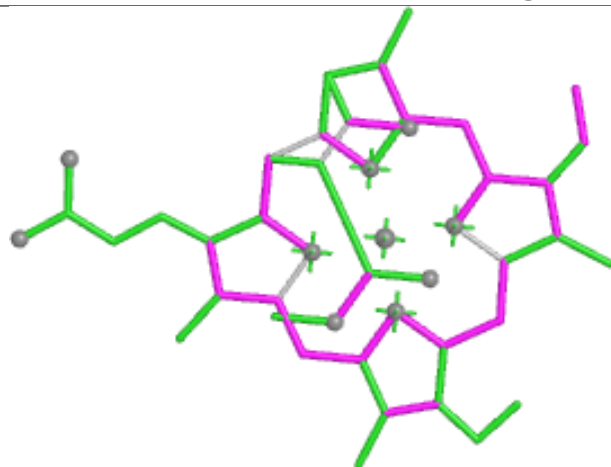
Ligand CLA f 606



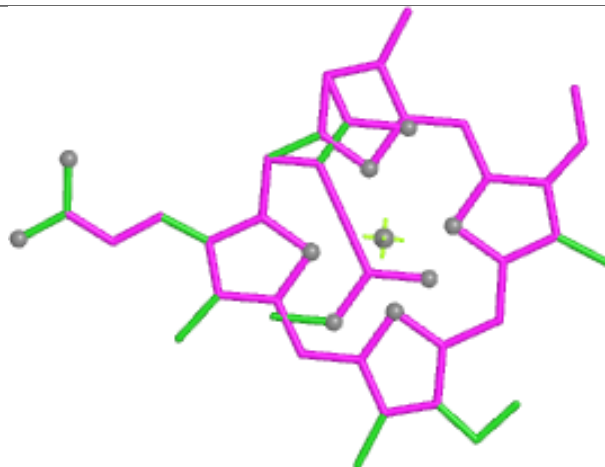
Ligand CLA j 303



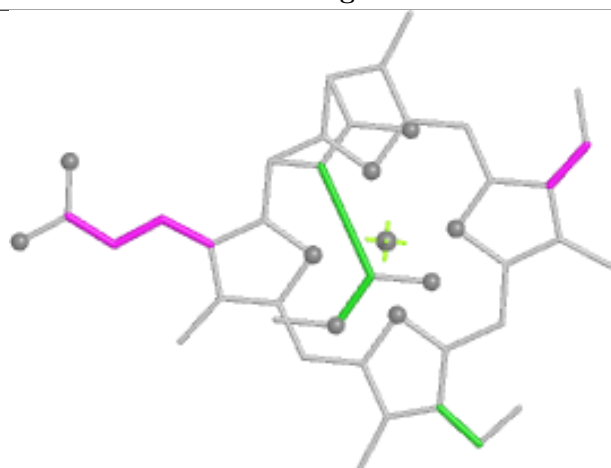
Ligand KC2 k 613



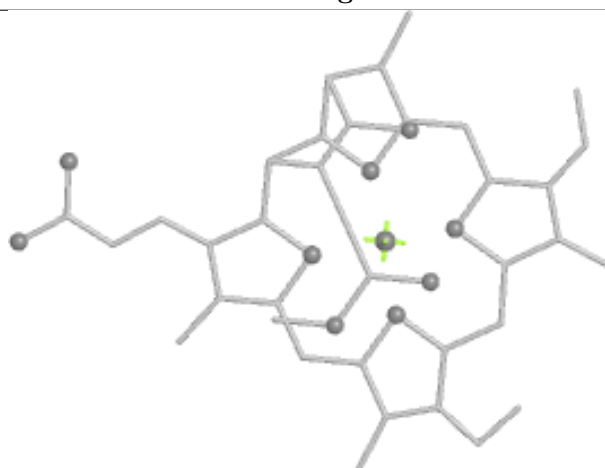
Bond lengths



Bond angles

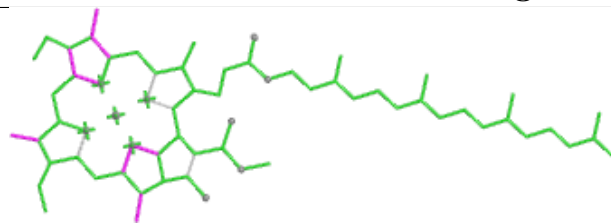


Torsions

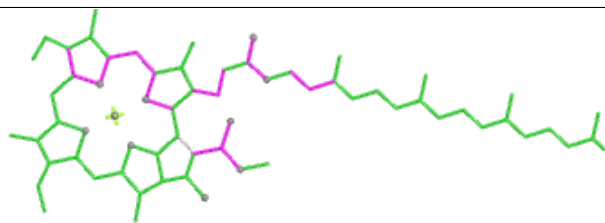


Rings

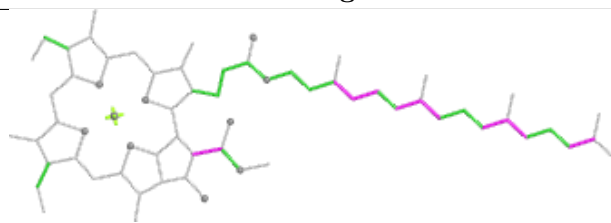
Ligand CLA B 808



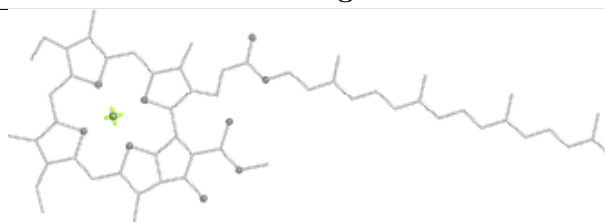
Bond lengths



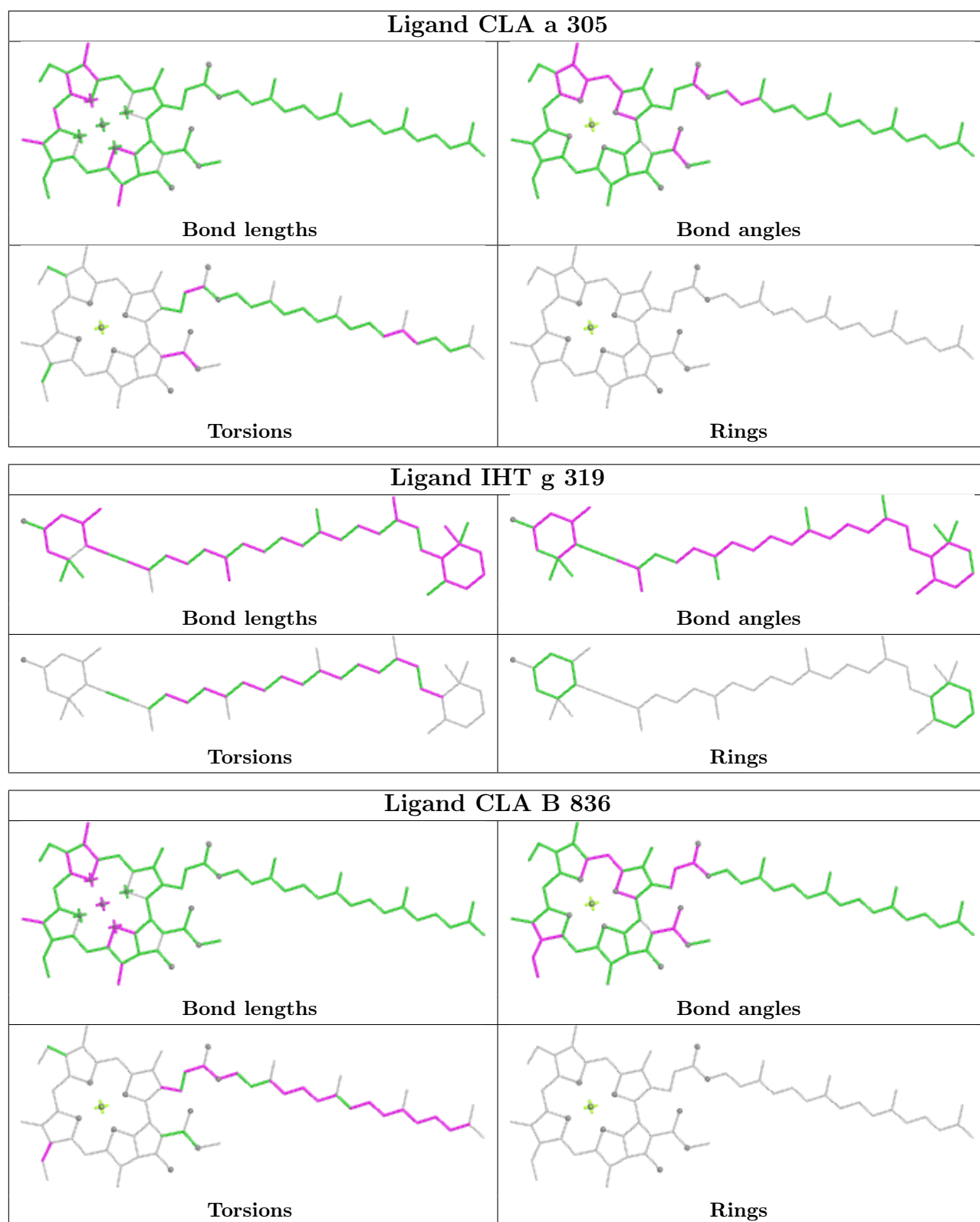
Bond angles

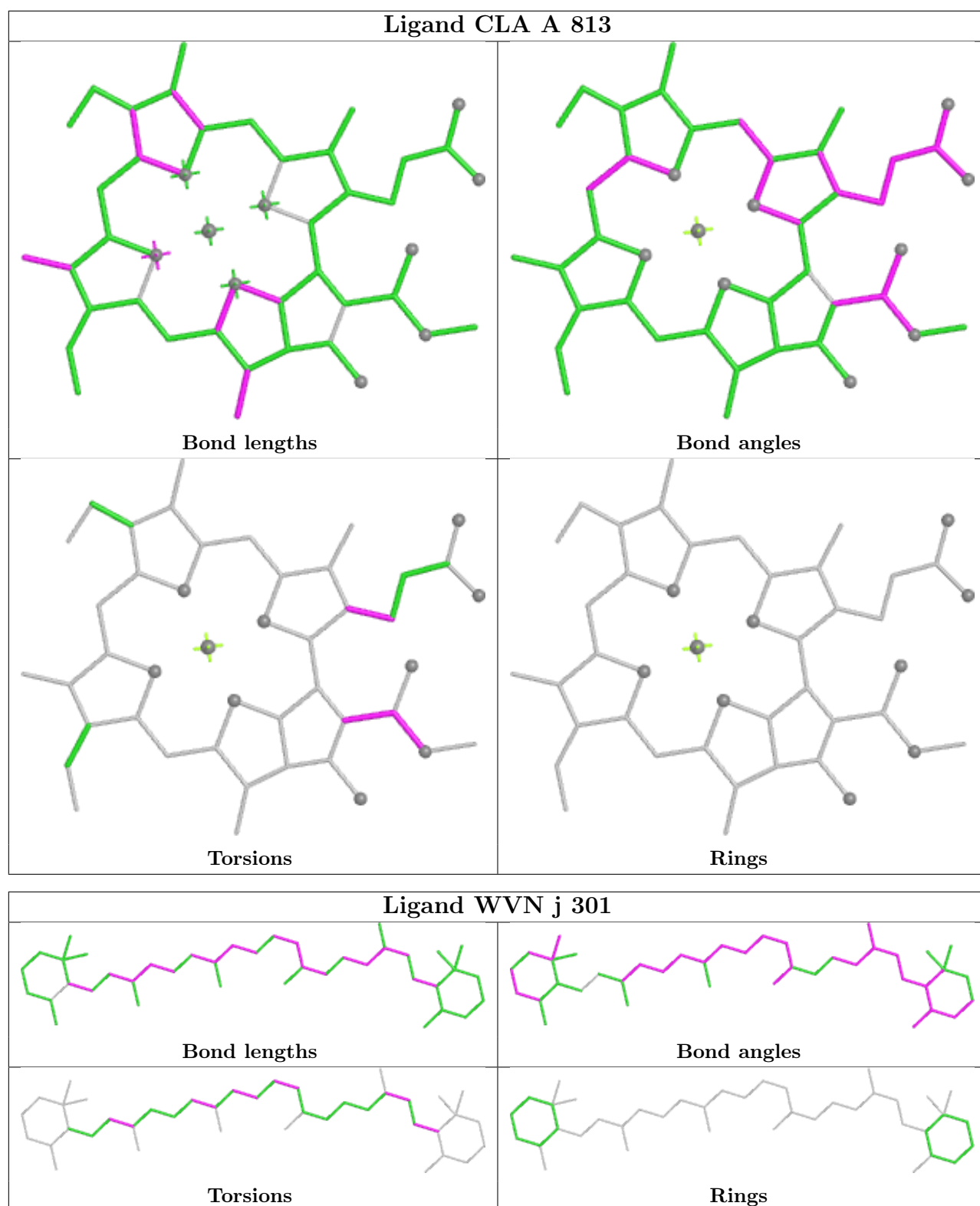


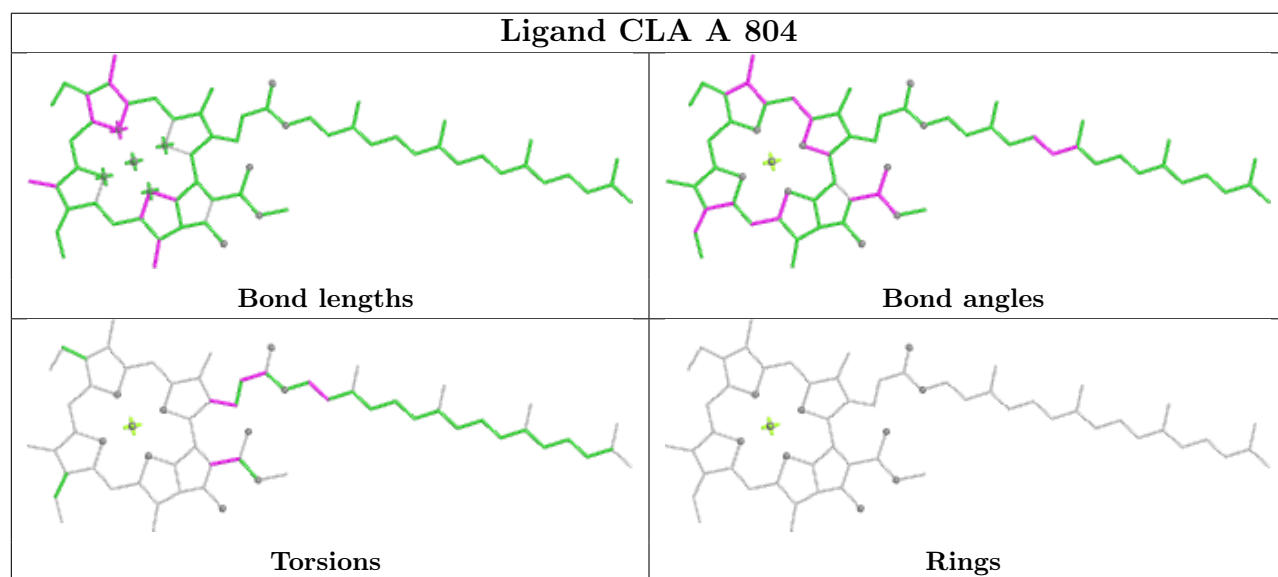
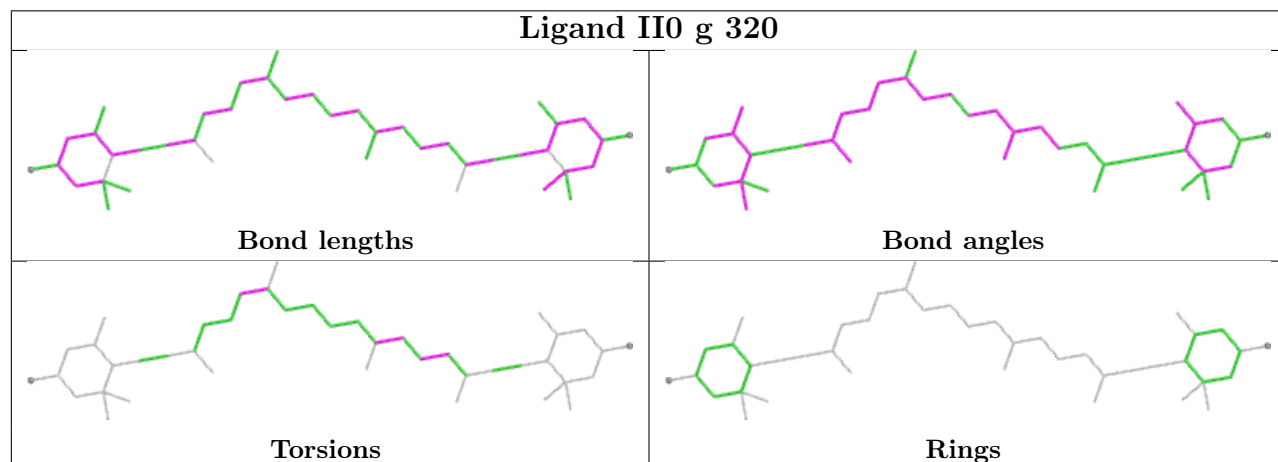
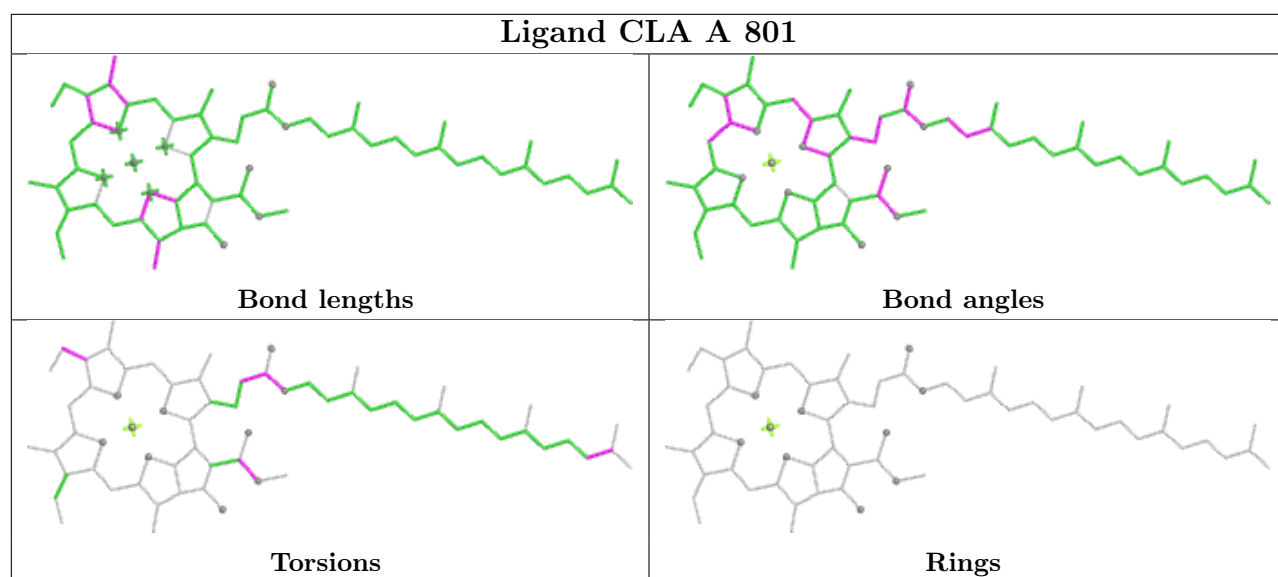
Torsions

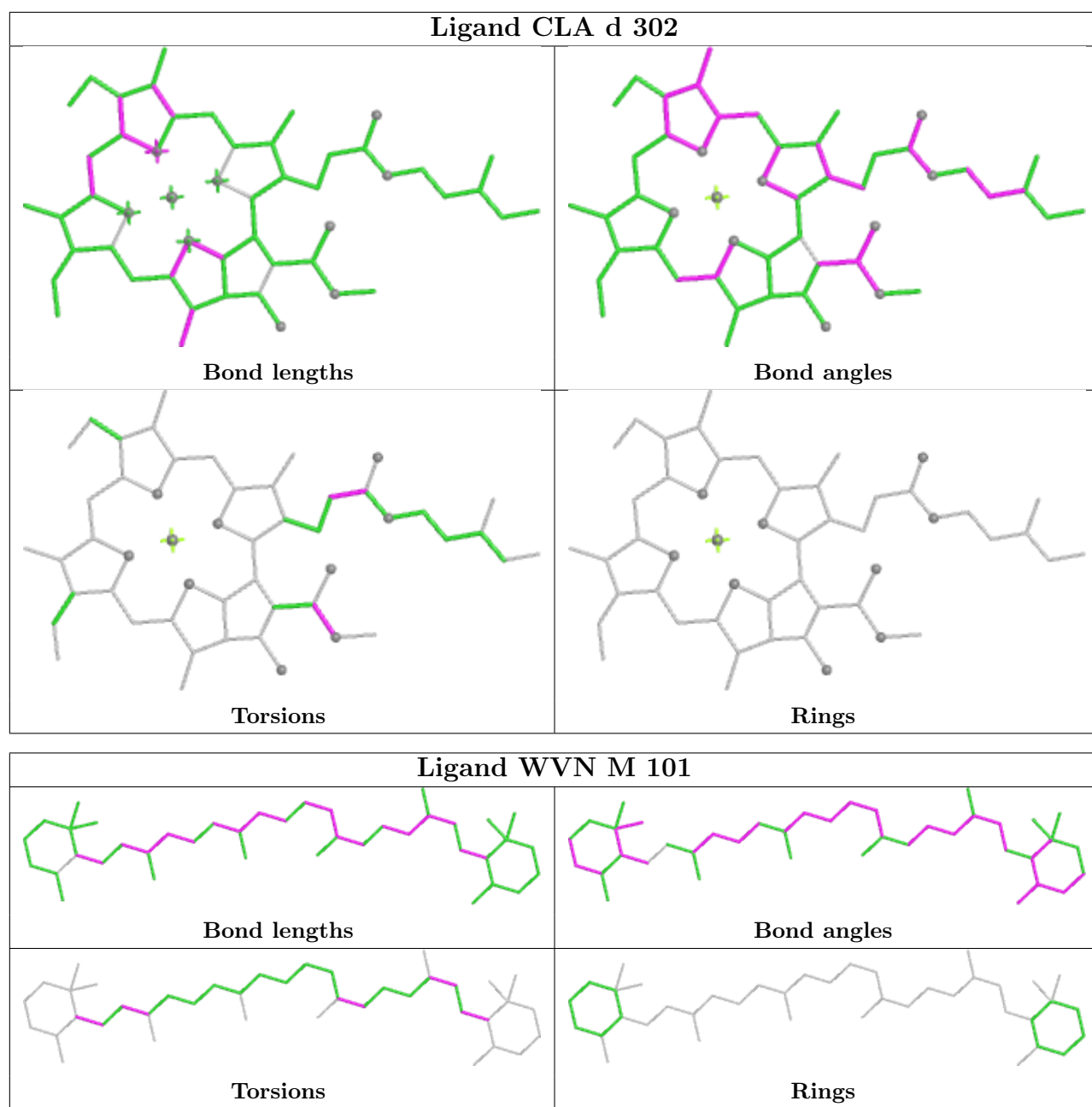


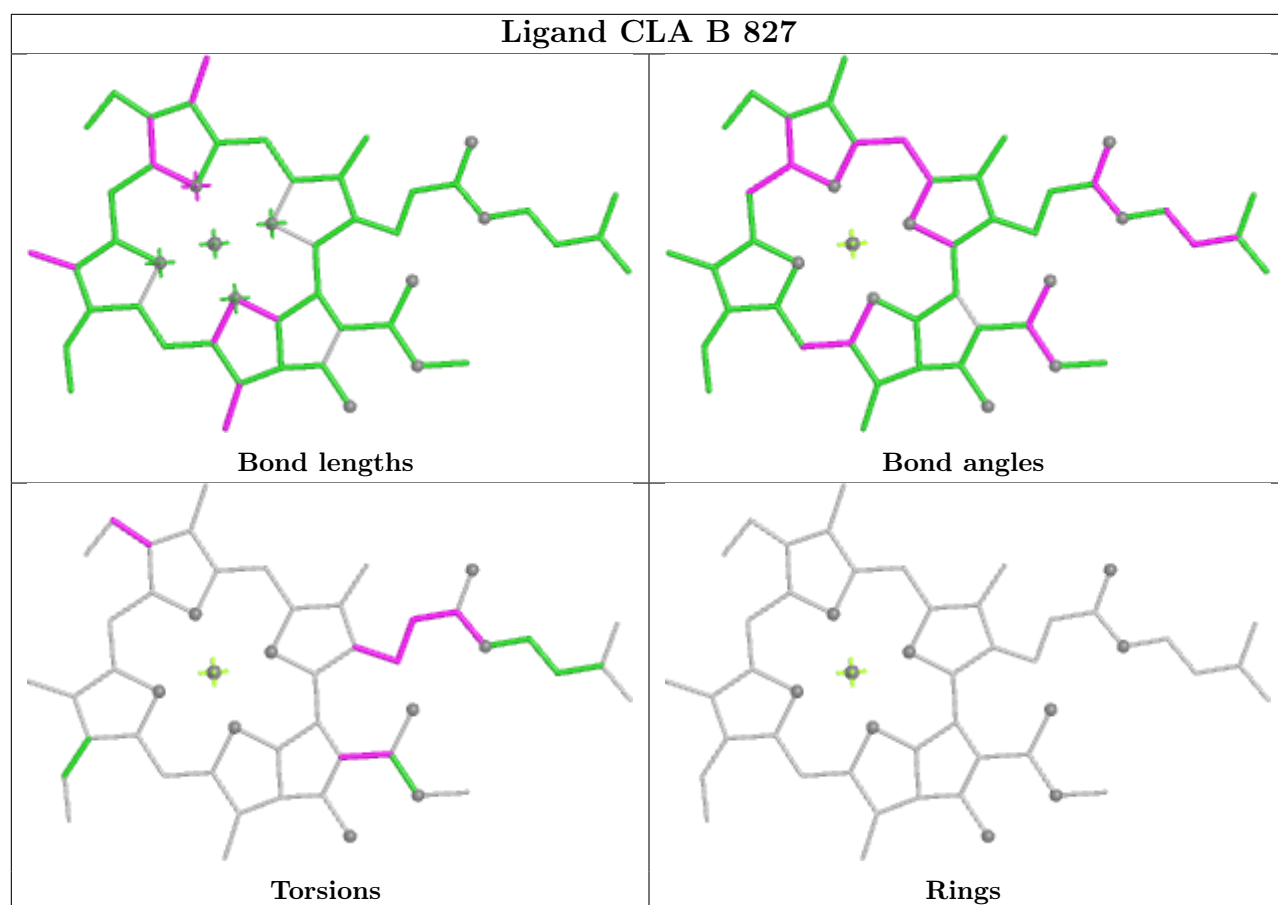
Rings



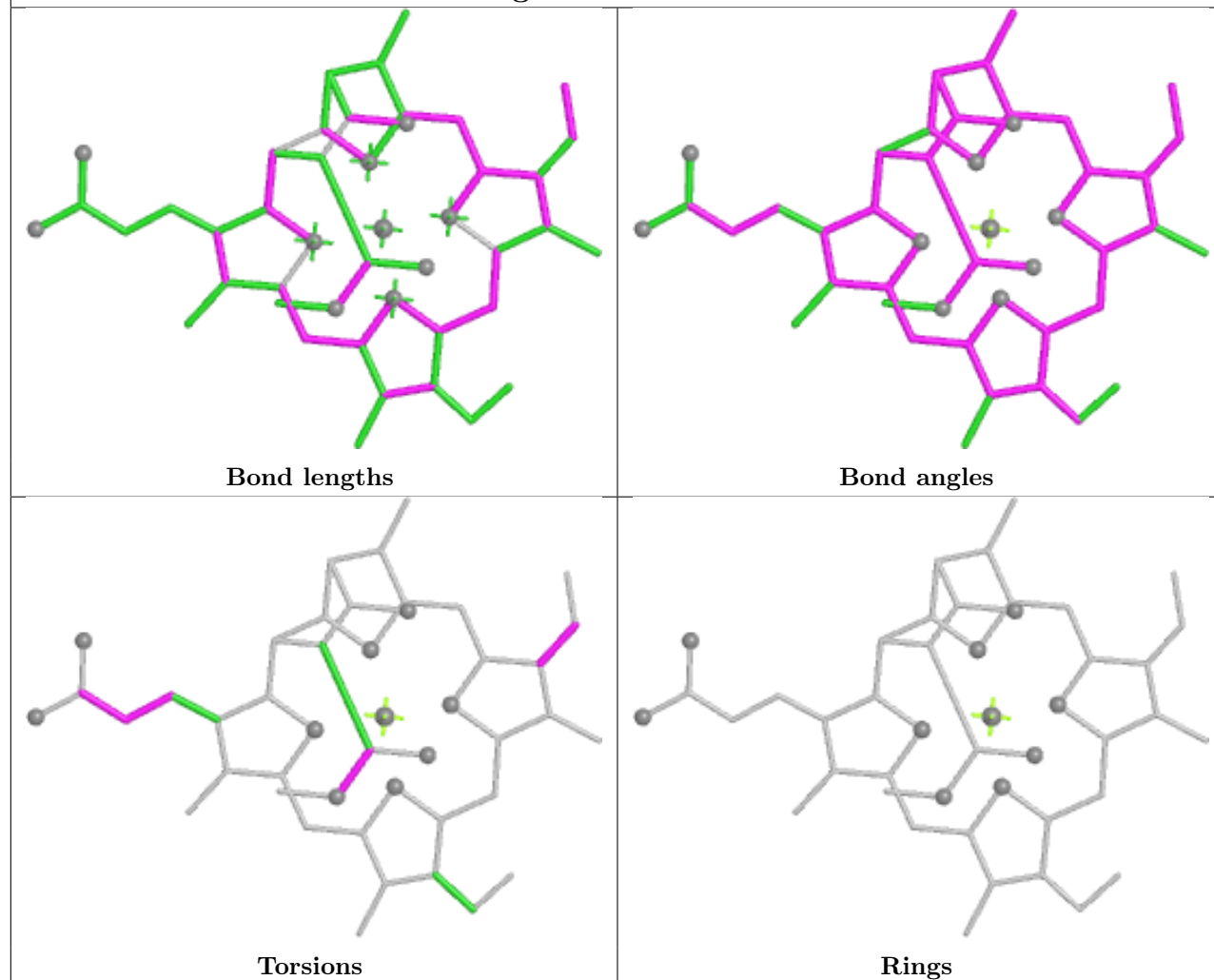




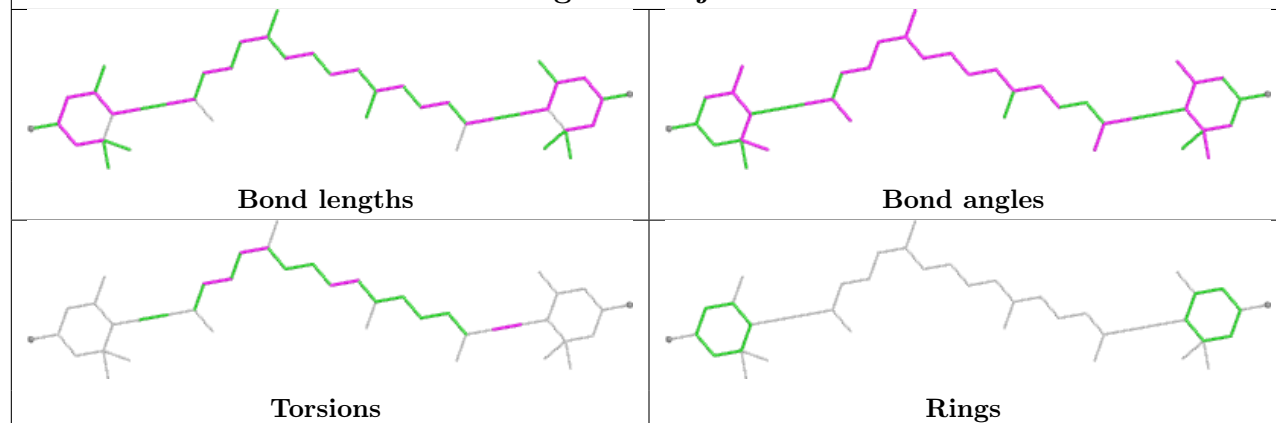


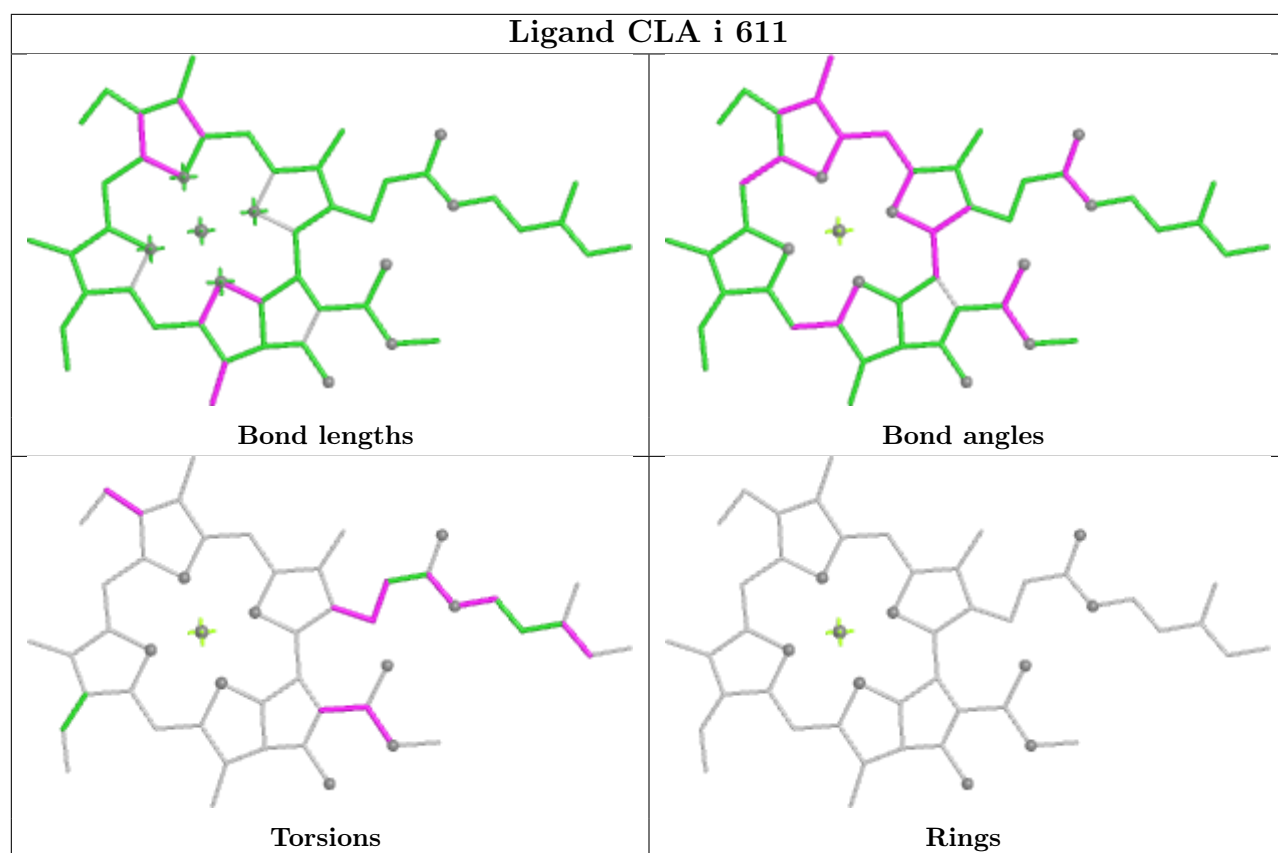


Ligand KC2 e 609

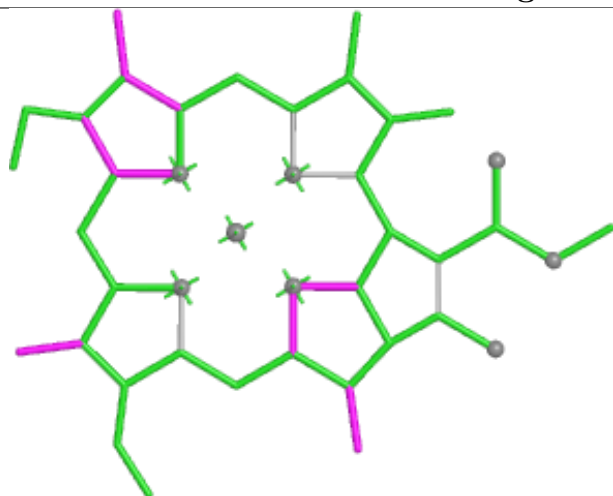


Ligand II0 j 315





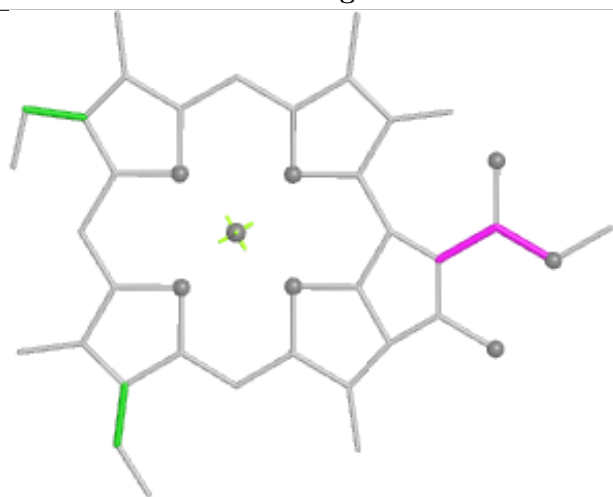
Ligand CLA d 308



Bond lengths



Bond angles

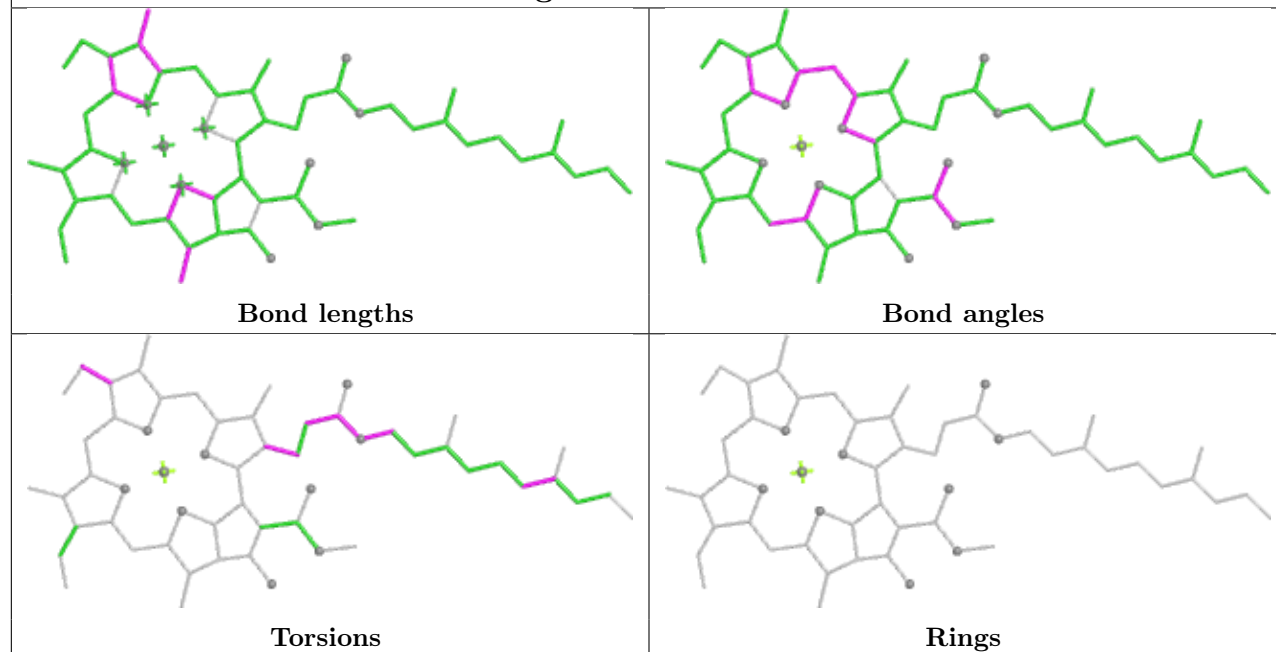


Torsions

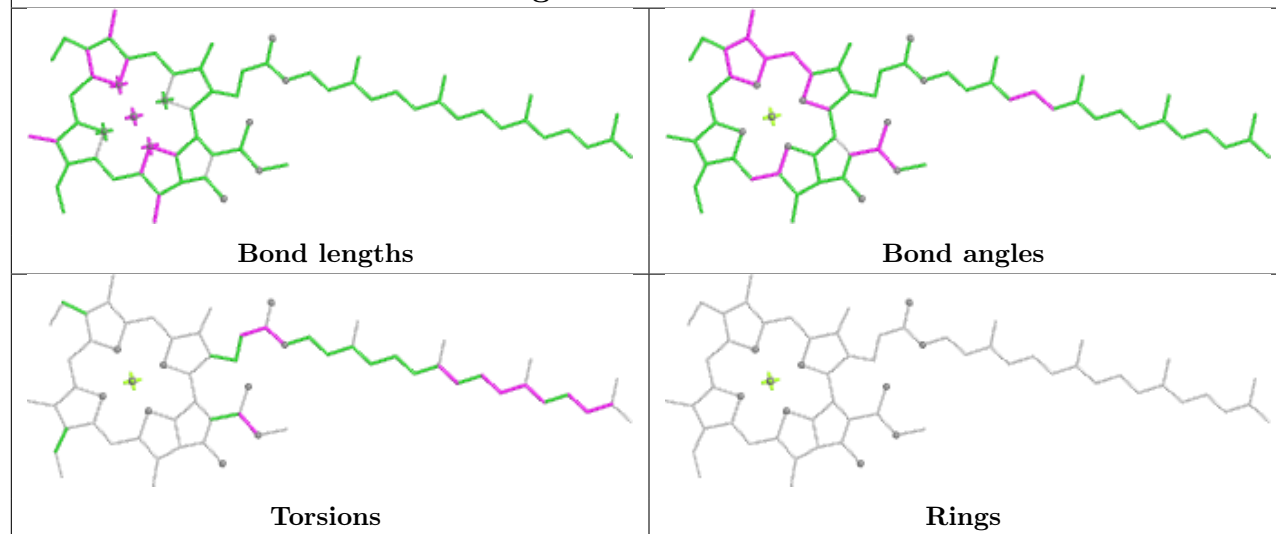


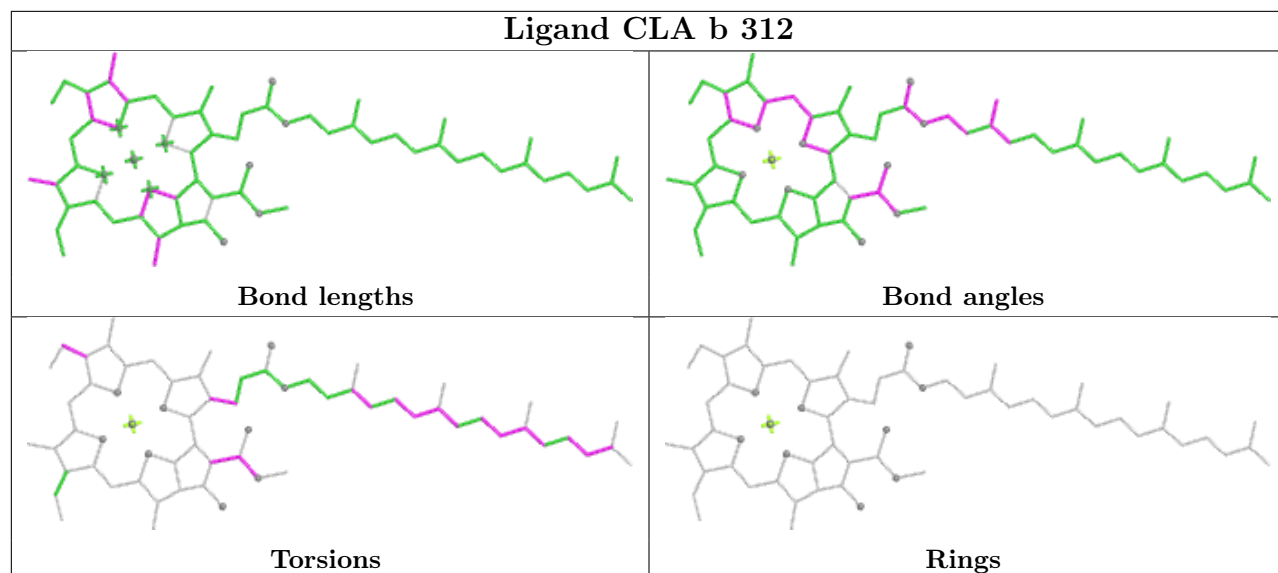
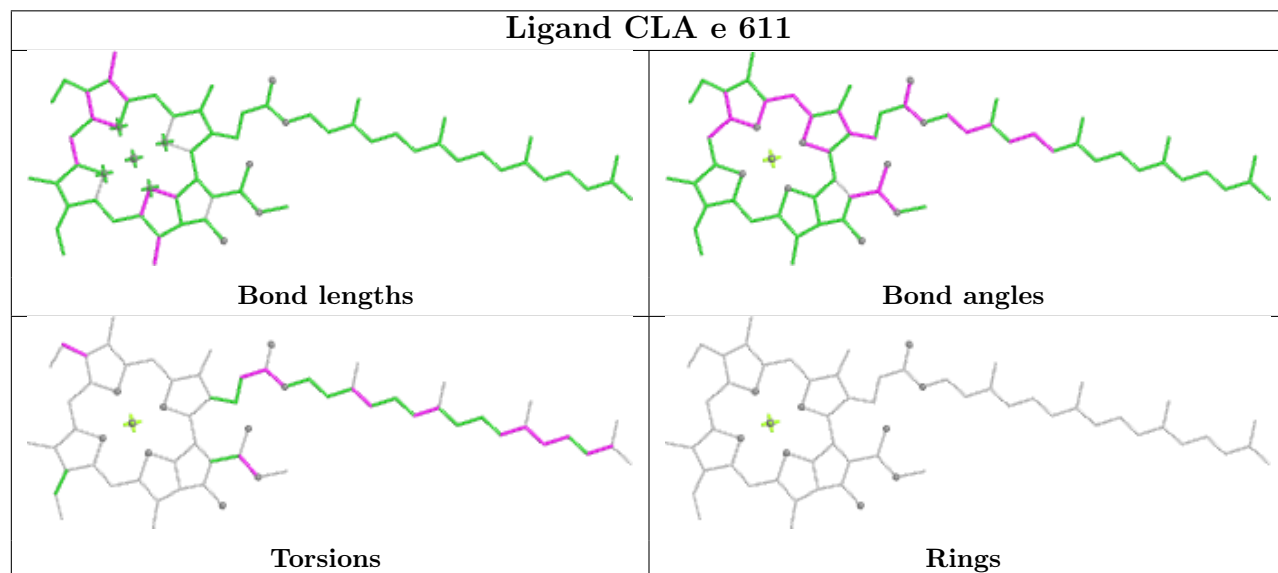
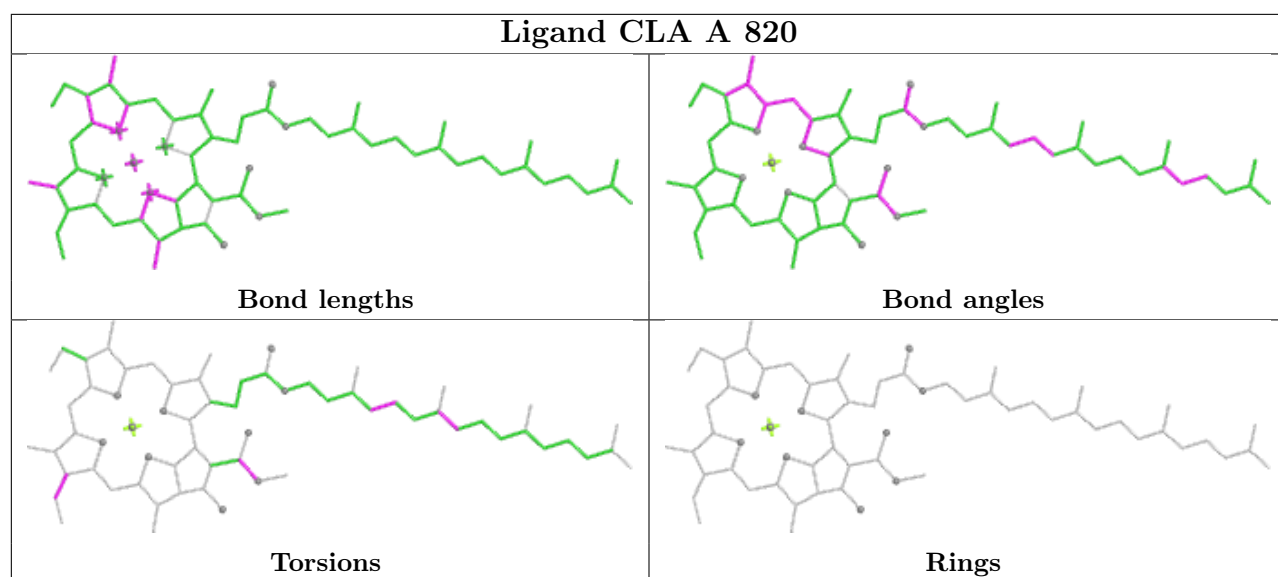
Rings

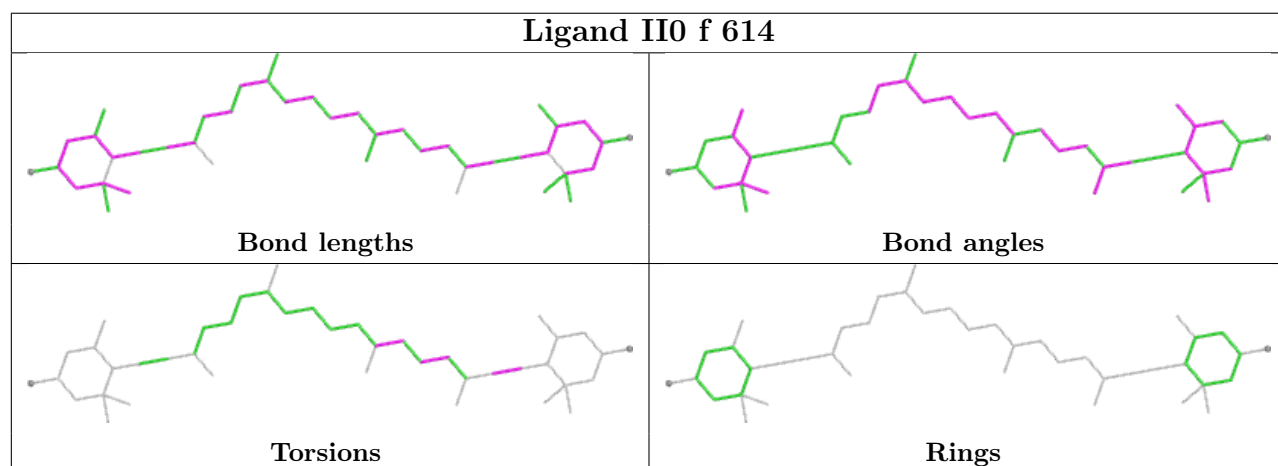
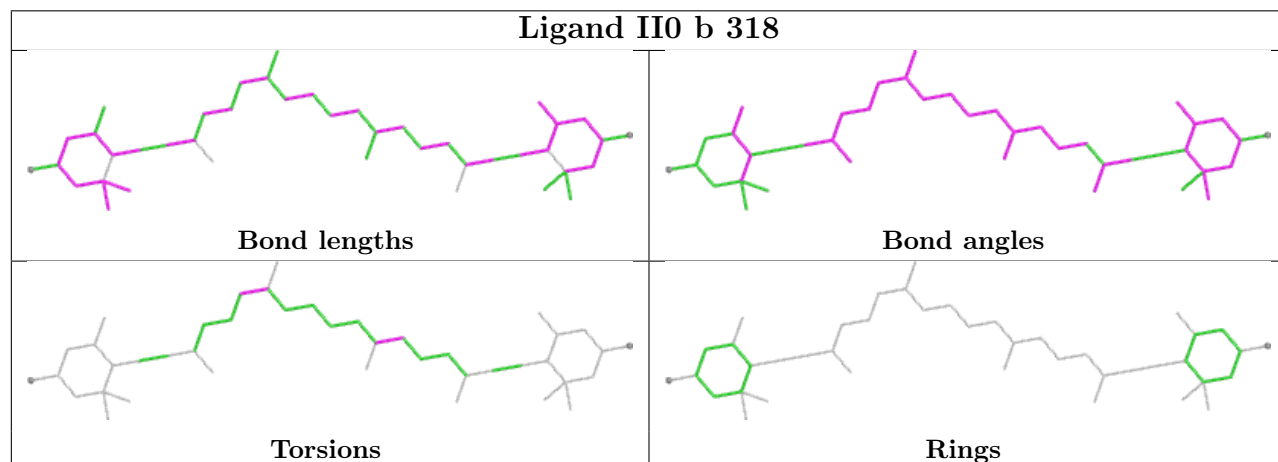
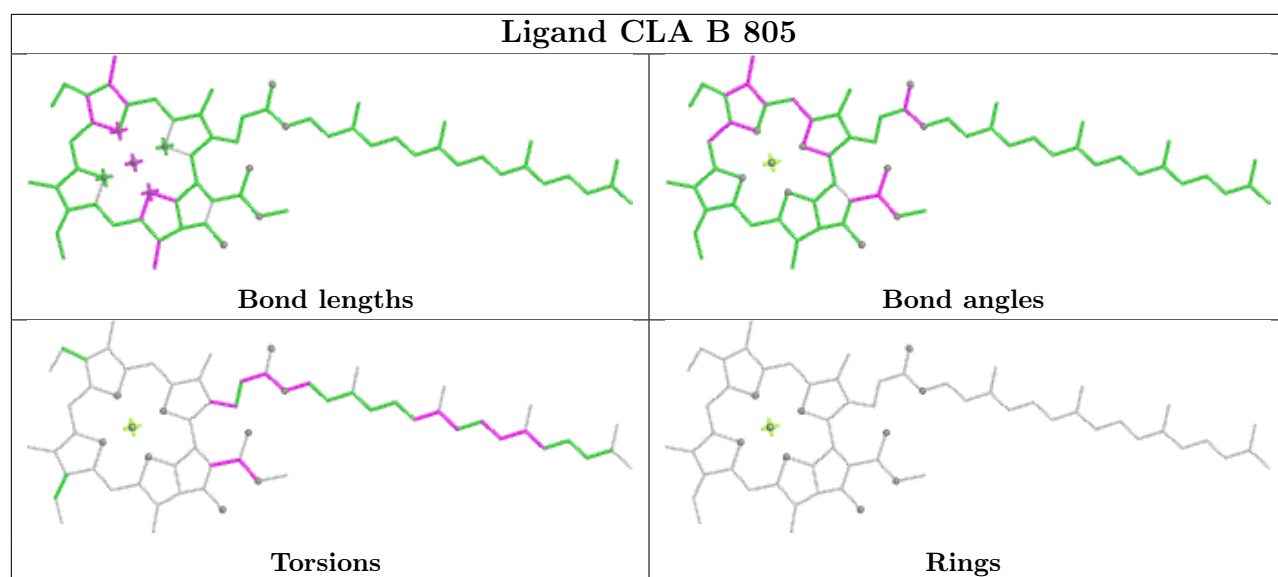
Ligand CLA h 306



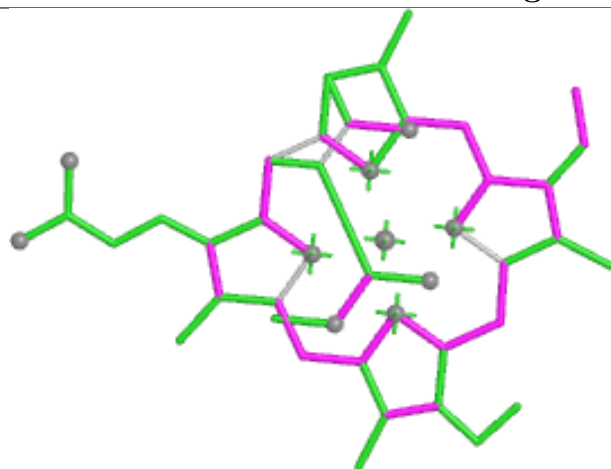
Ligand CLA B 806



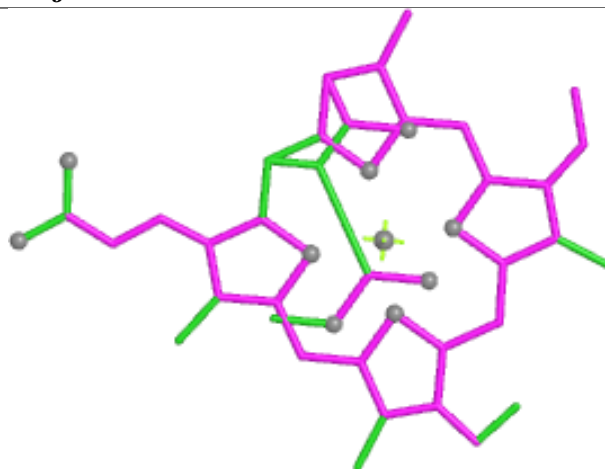




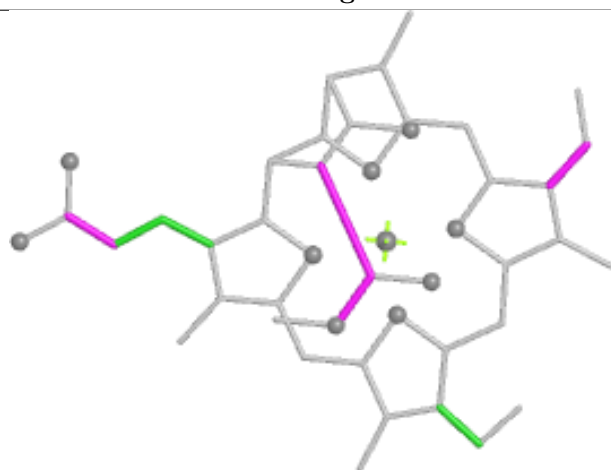
Ligand KC2 j 312



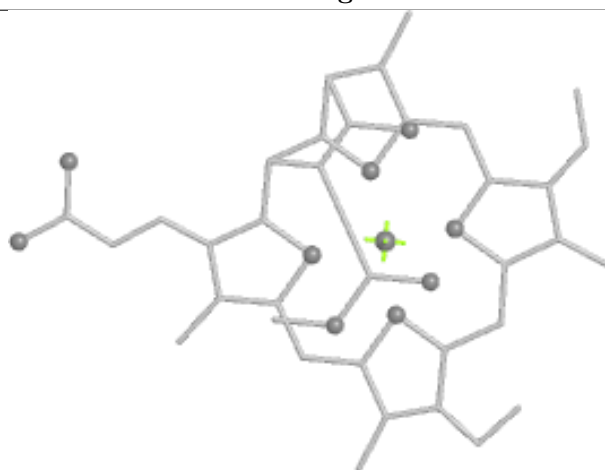
Bond lengths



Bond angles

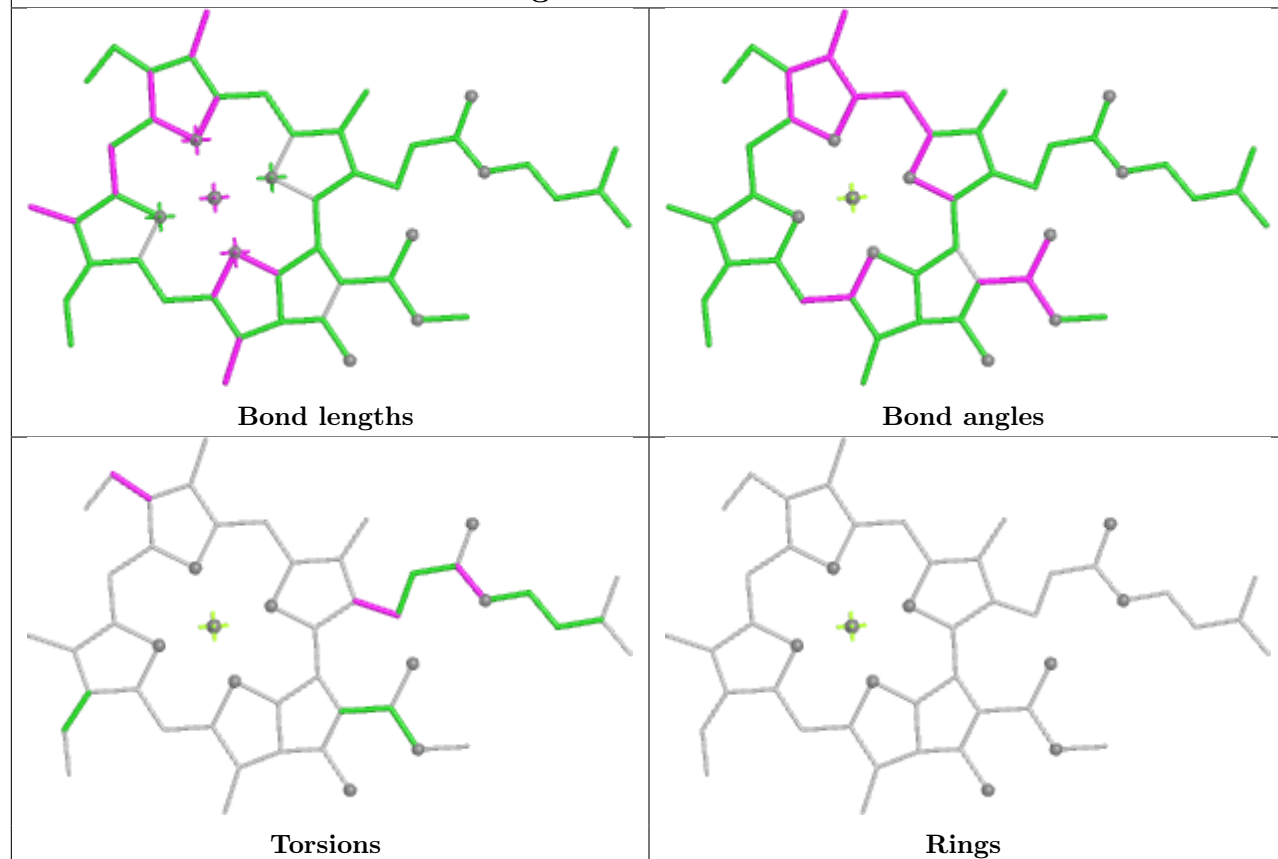


Torsions

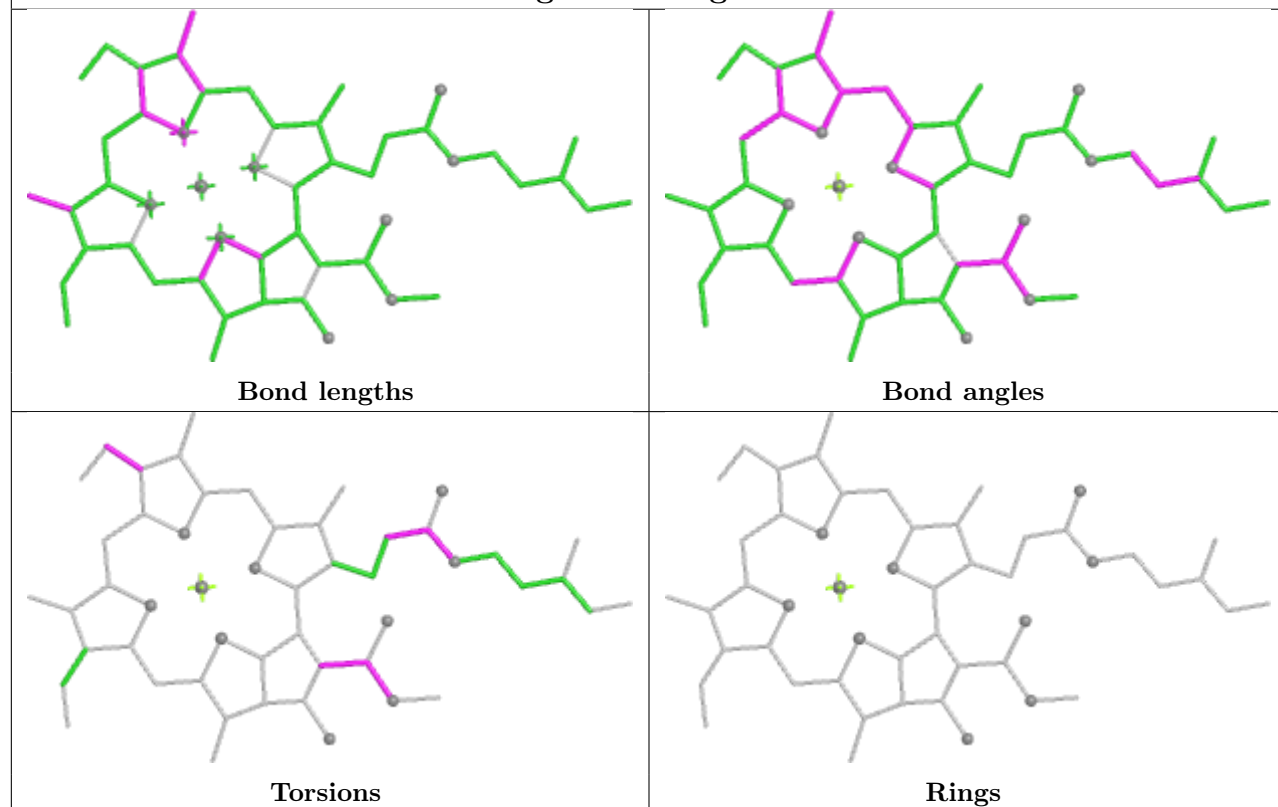


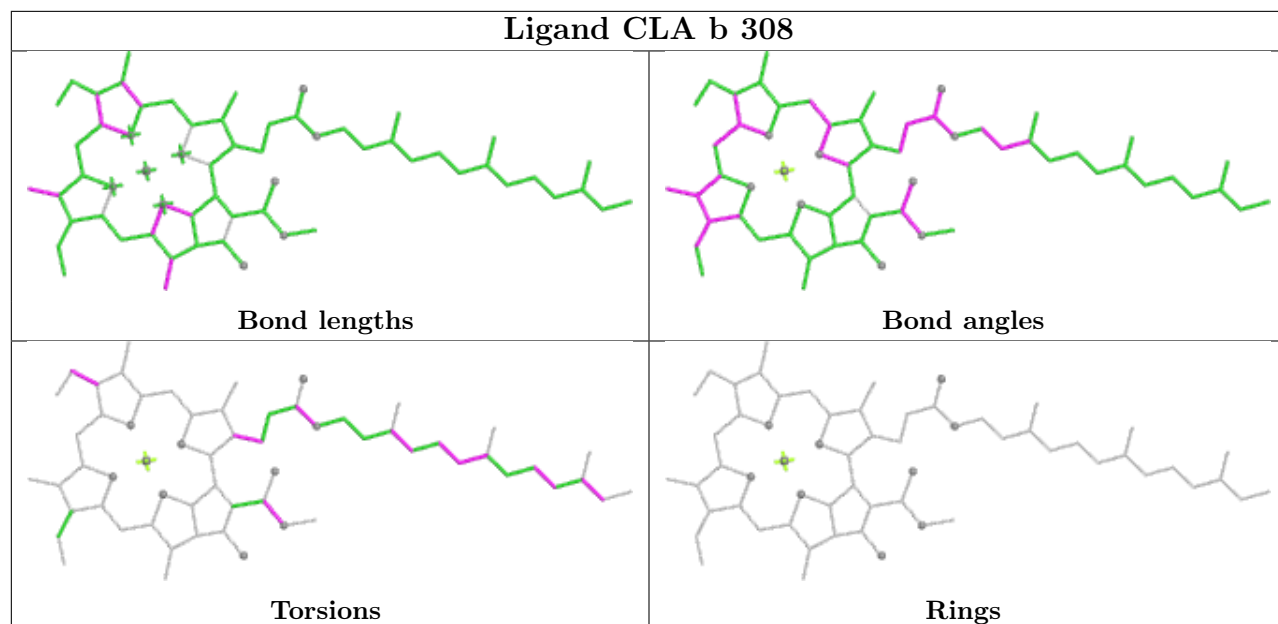
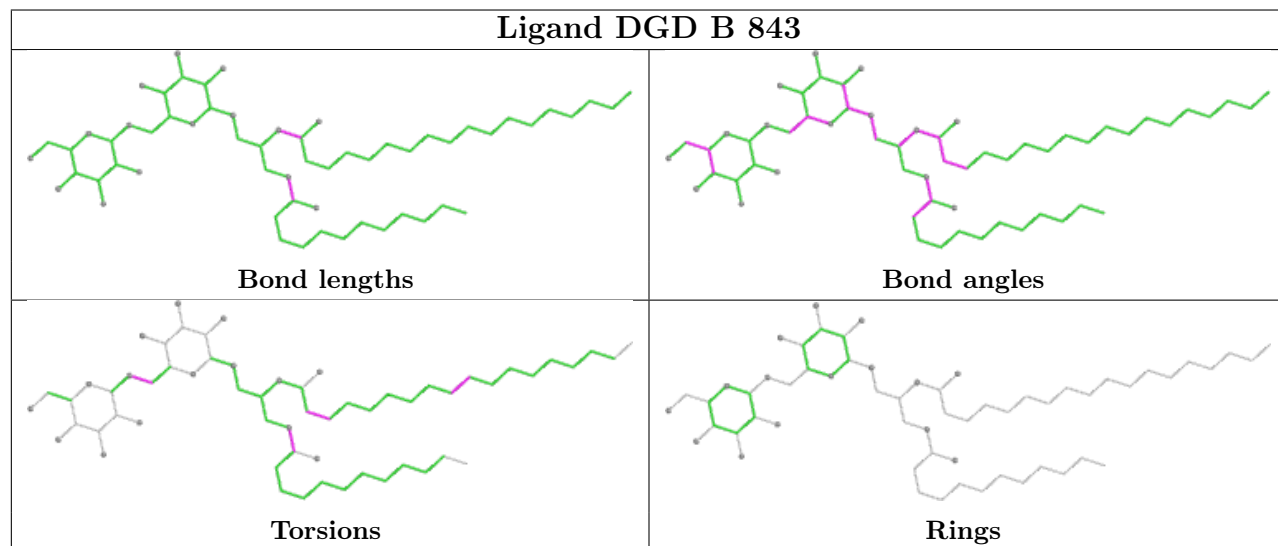
Rings

Ligand CLA A 830

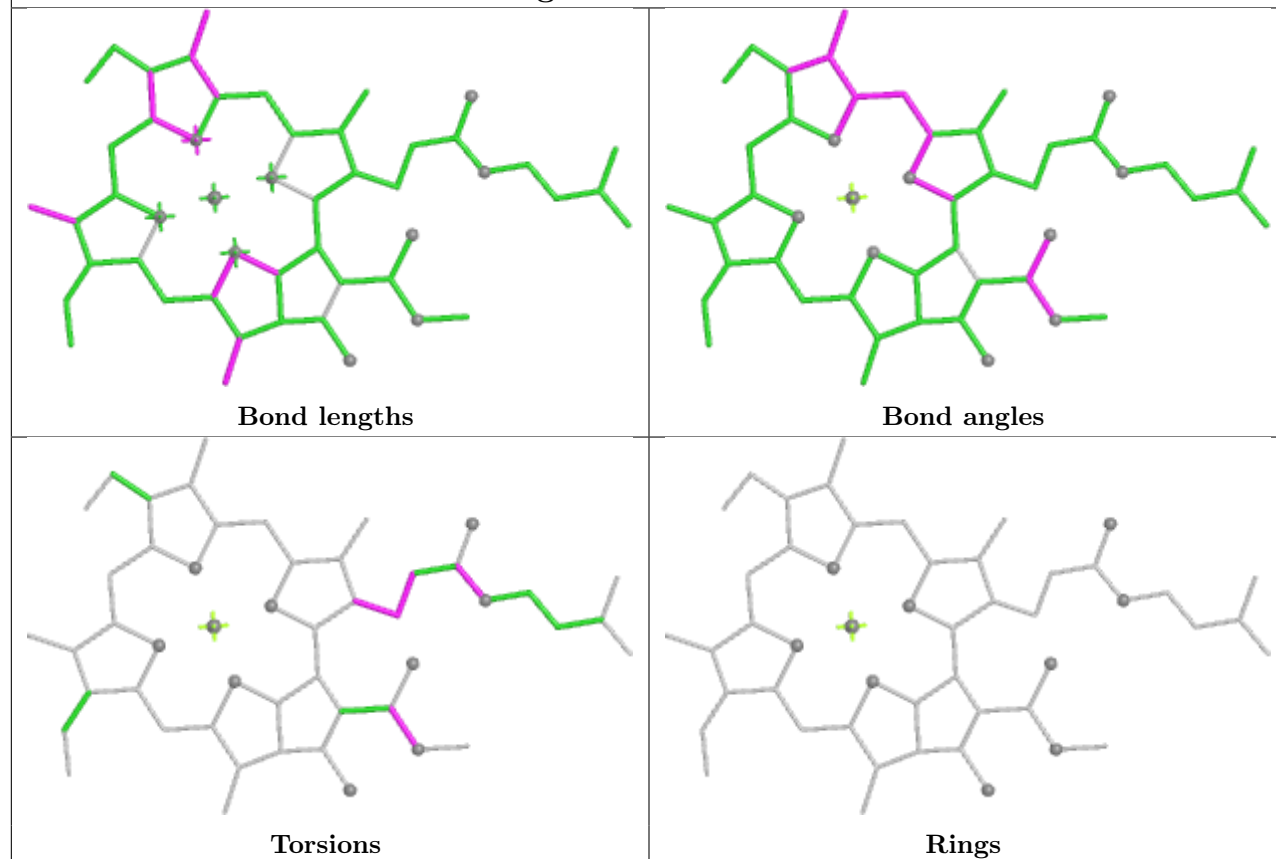


Ligand CLA g 307

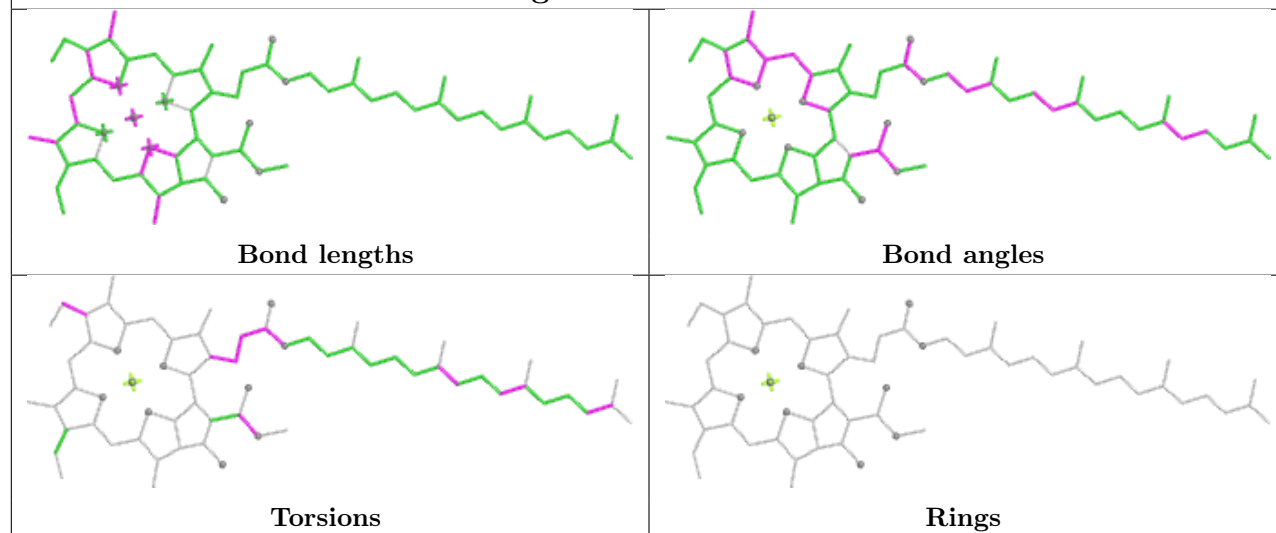


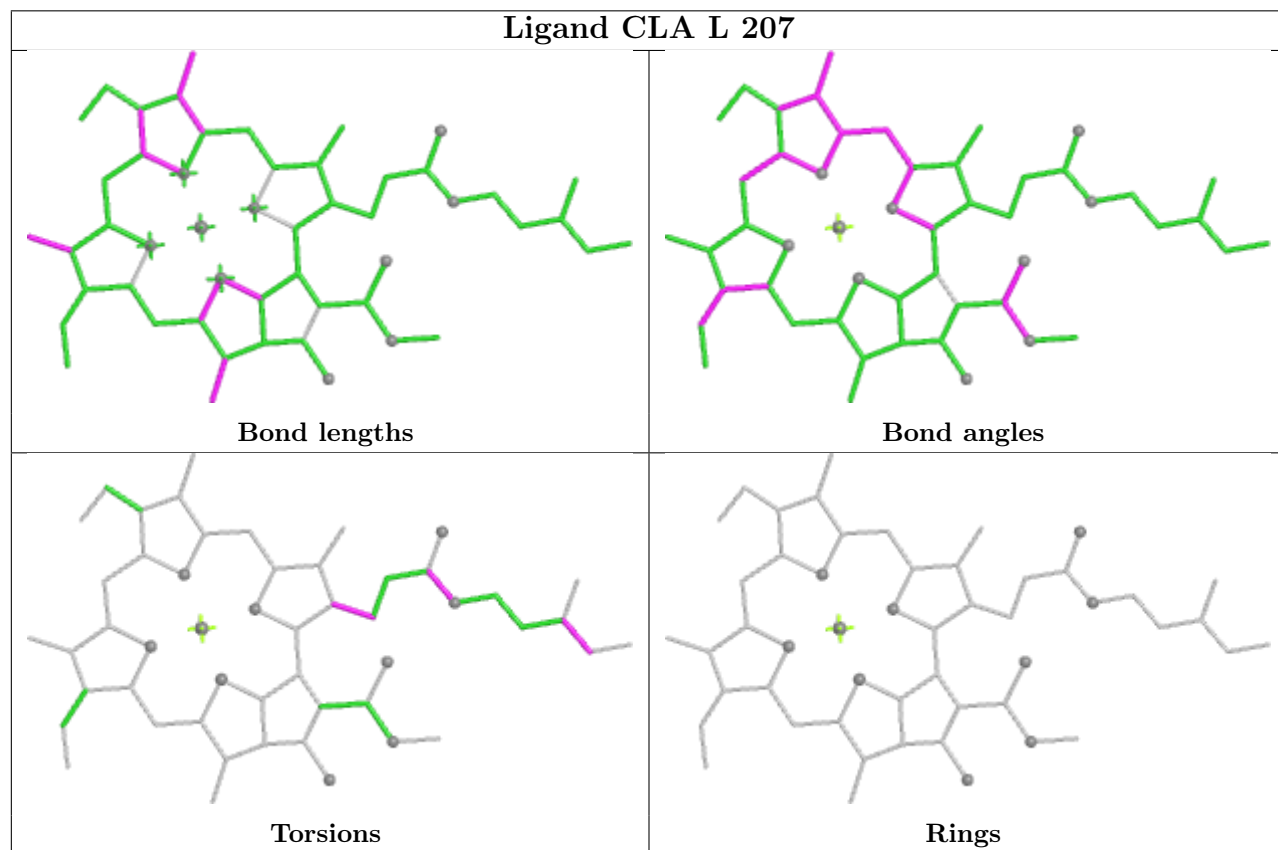
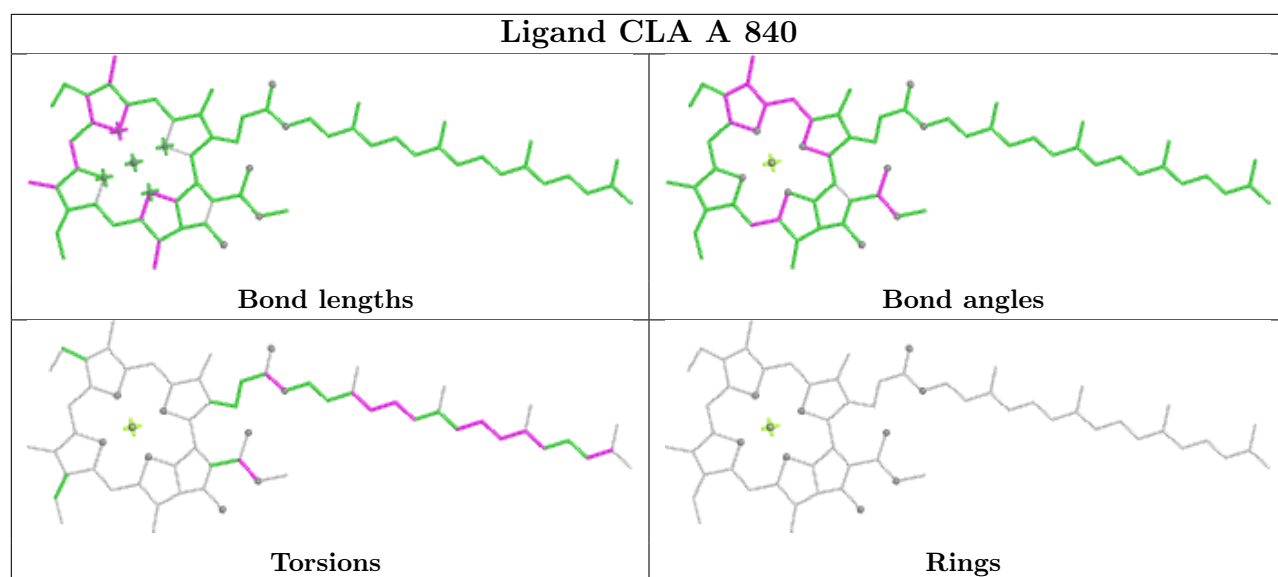
Ligand CLA b 308**Ligand DGD B 843**

Ligand CLA e 602

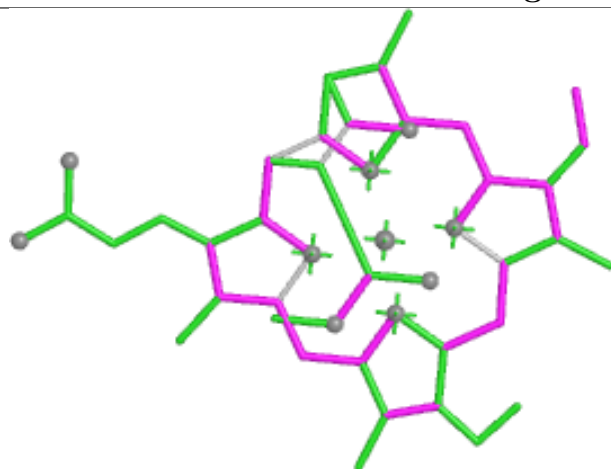


Ligand CLA A 817

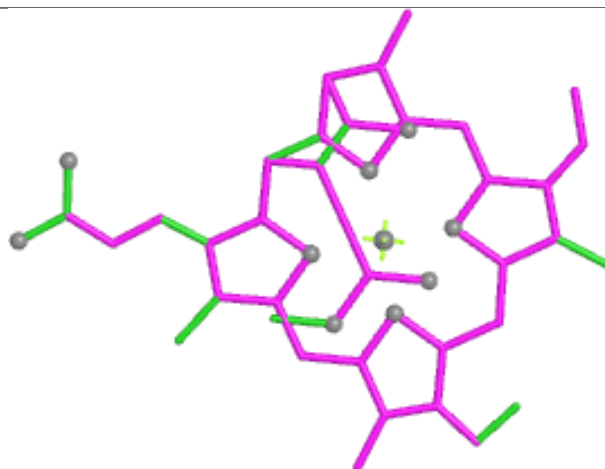




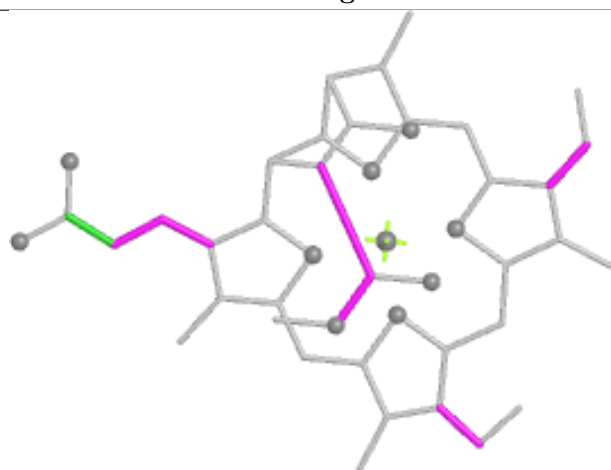
Ligand KC2 i 616



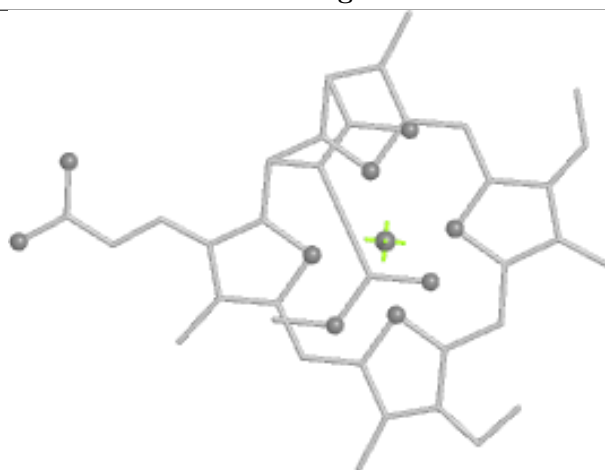
Bond lengths



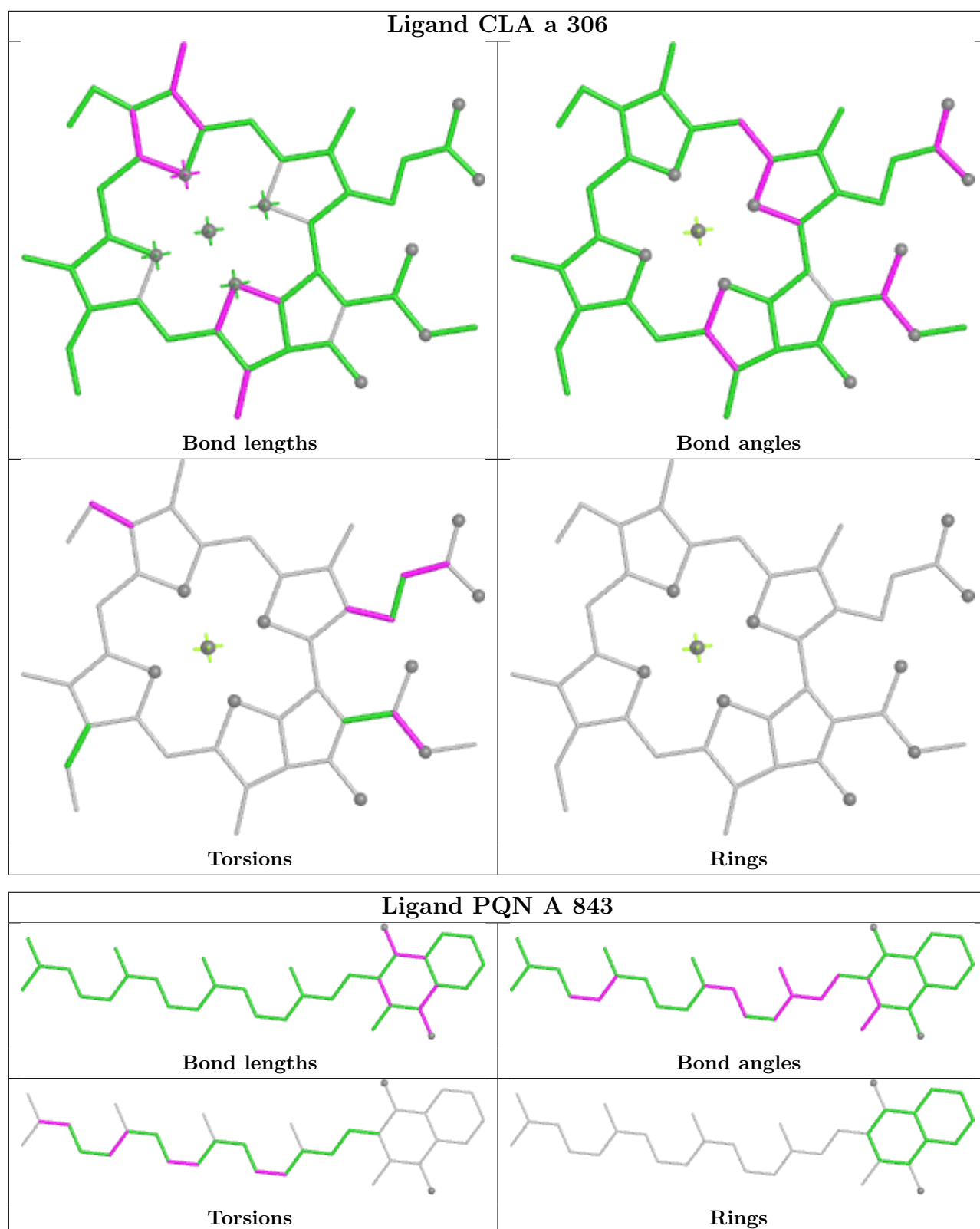
Bond angles



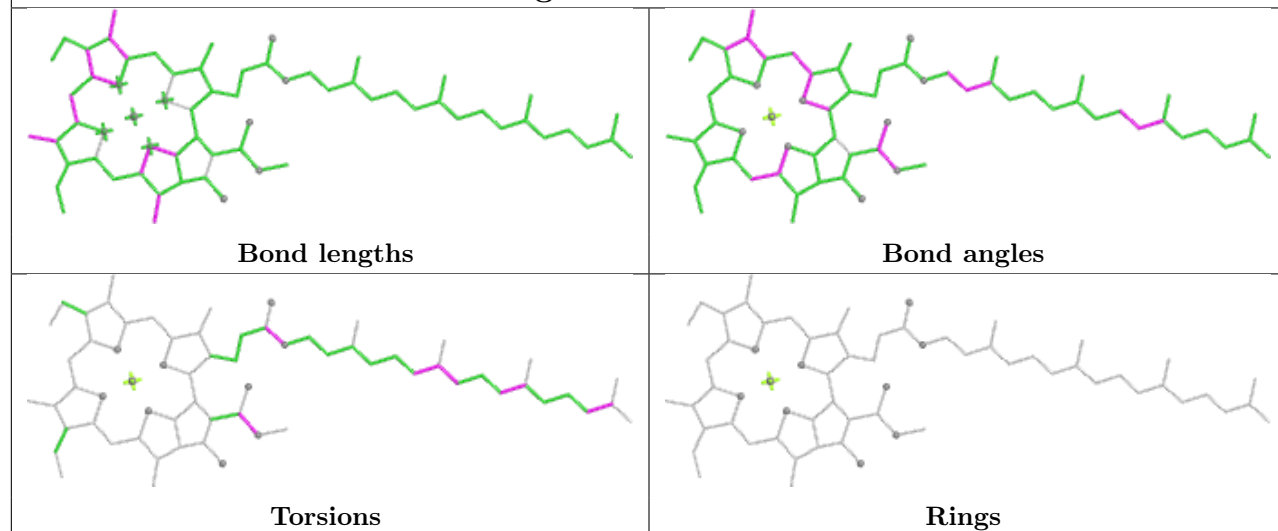
Torsions



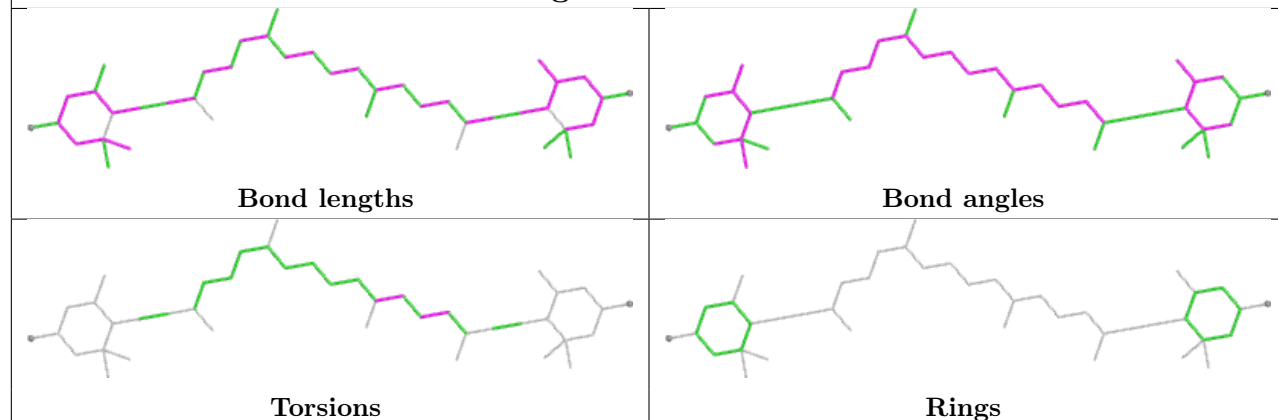
Rings



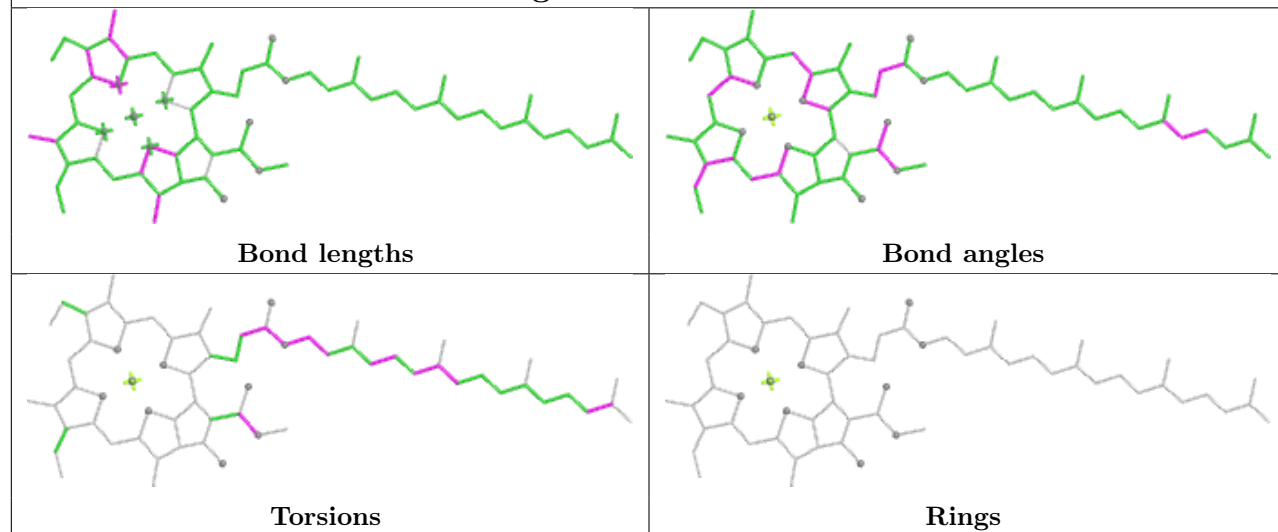
Ligand CLA h 305

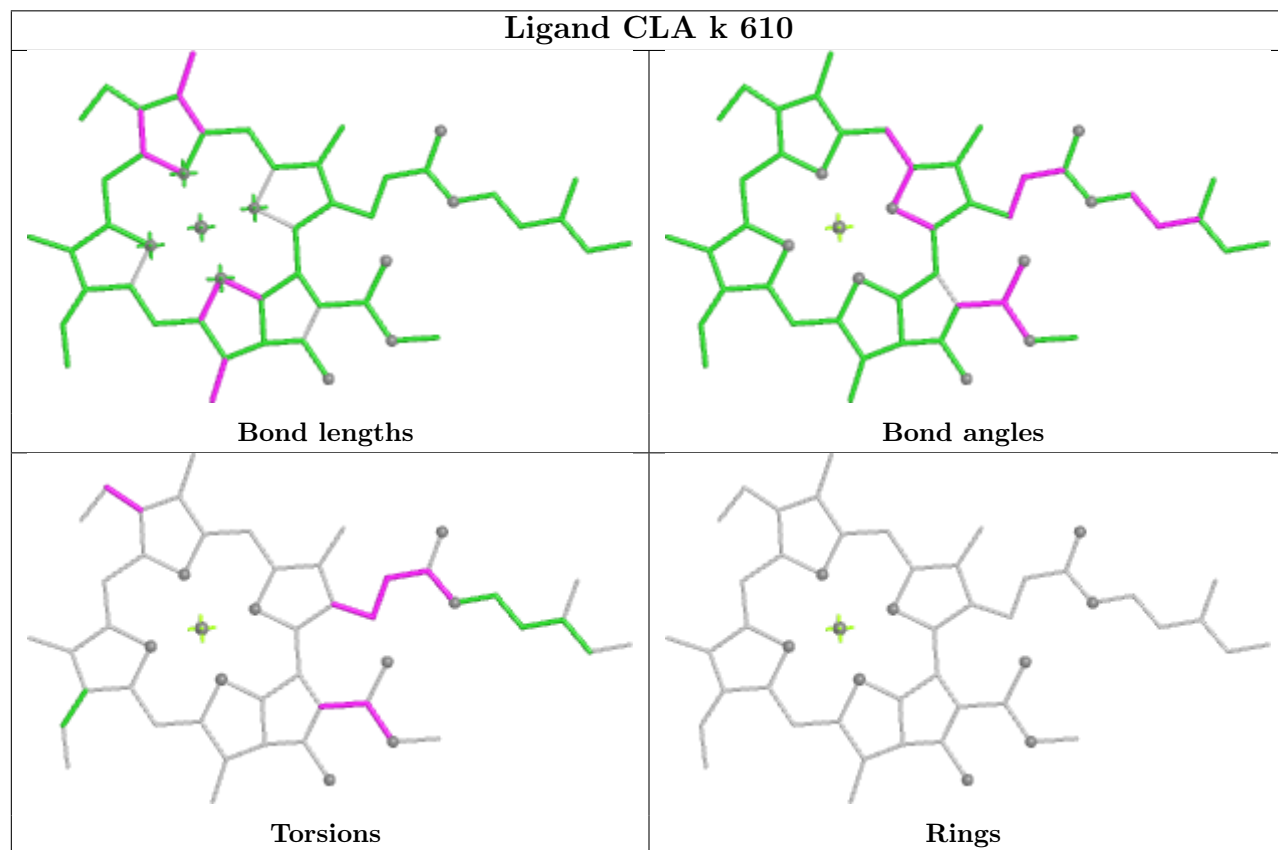
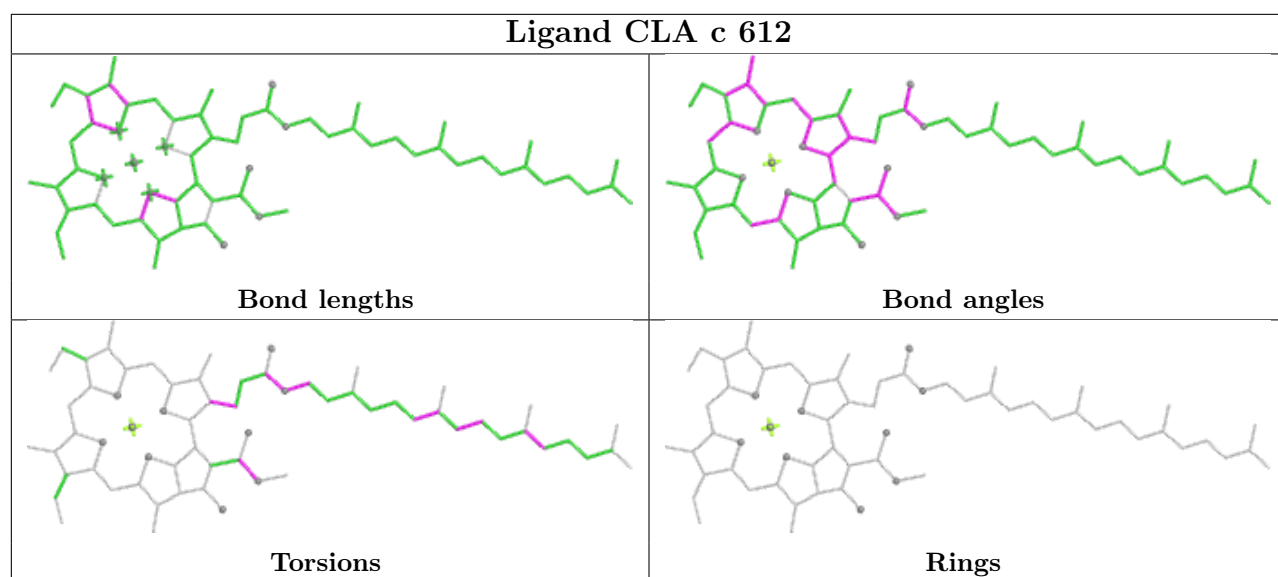


Ligand II0 c 616

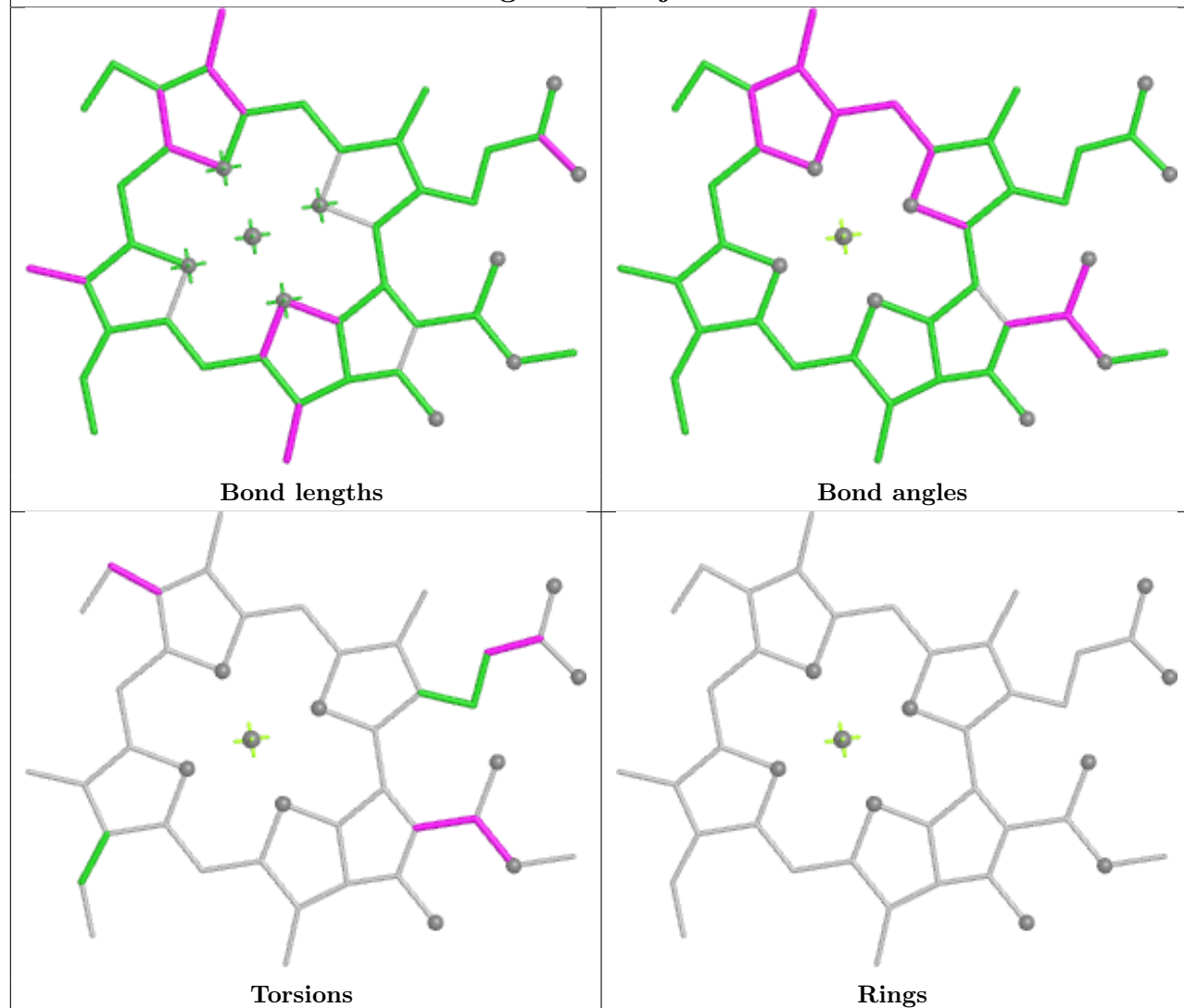


Ligand CLA B 830

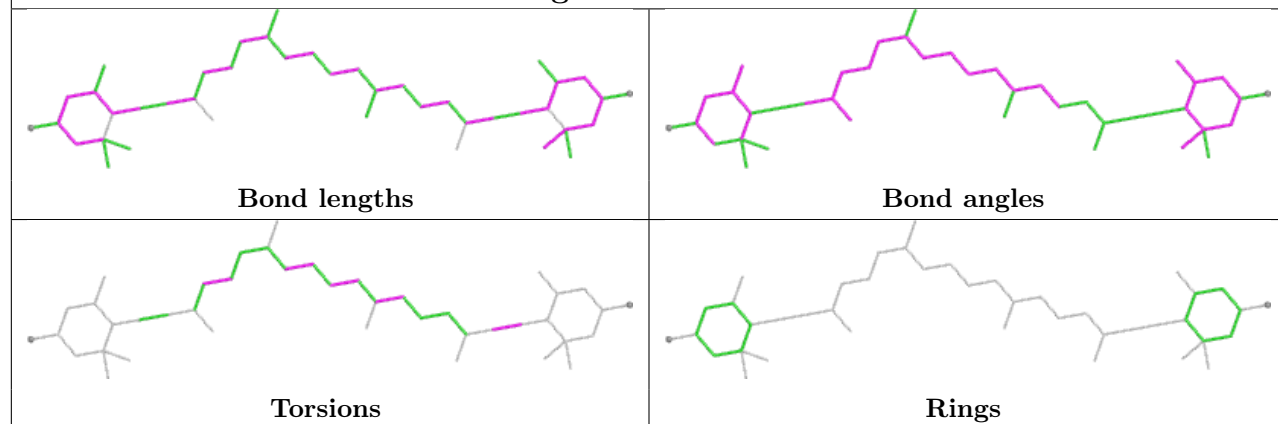


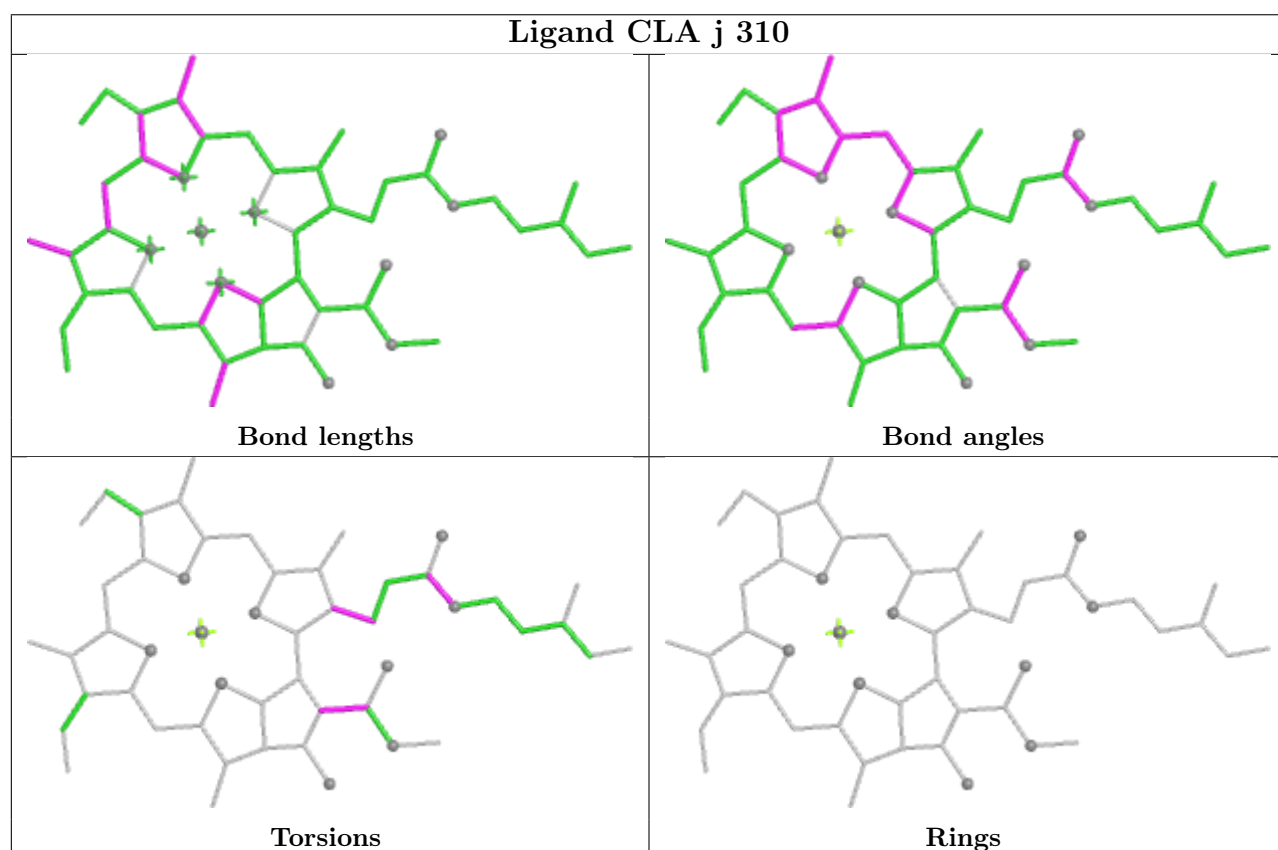
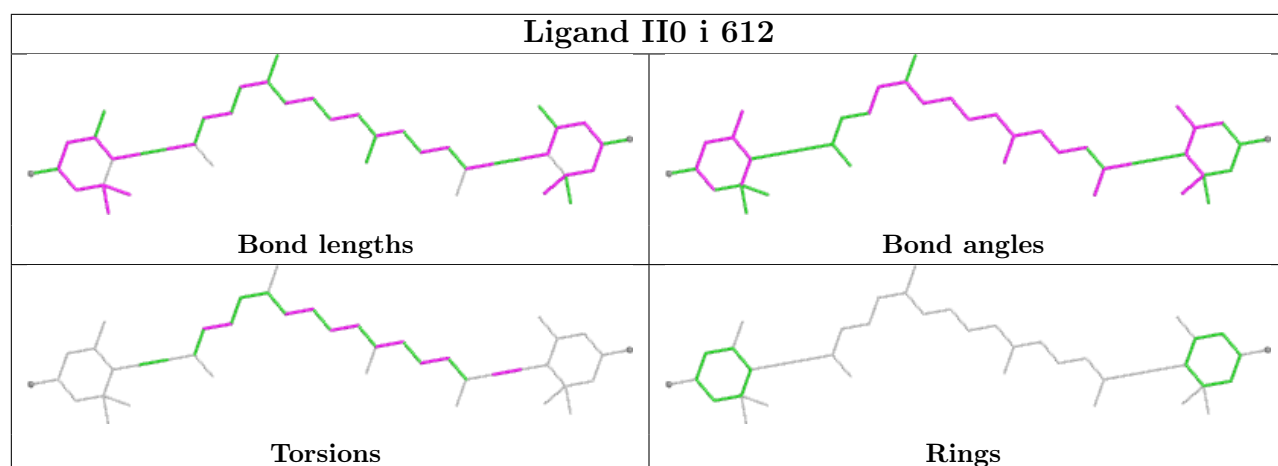


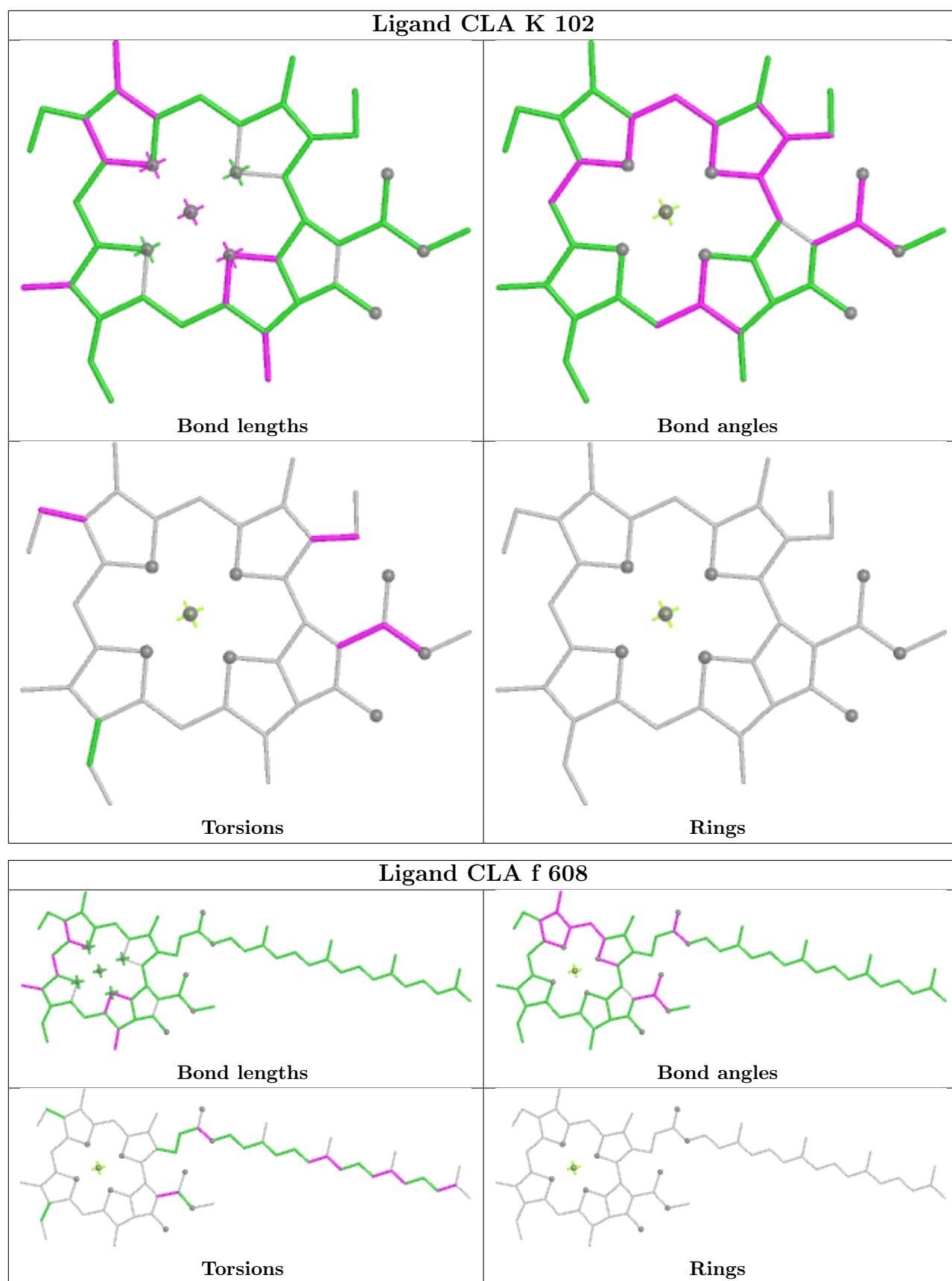
Ligand CLA j 309

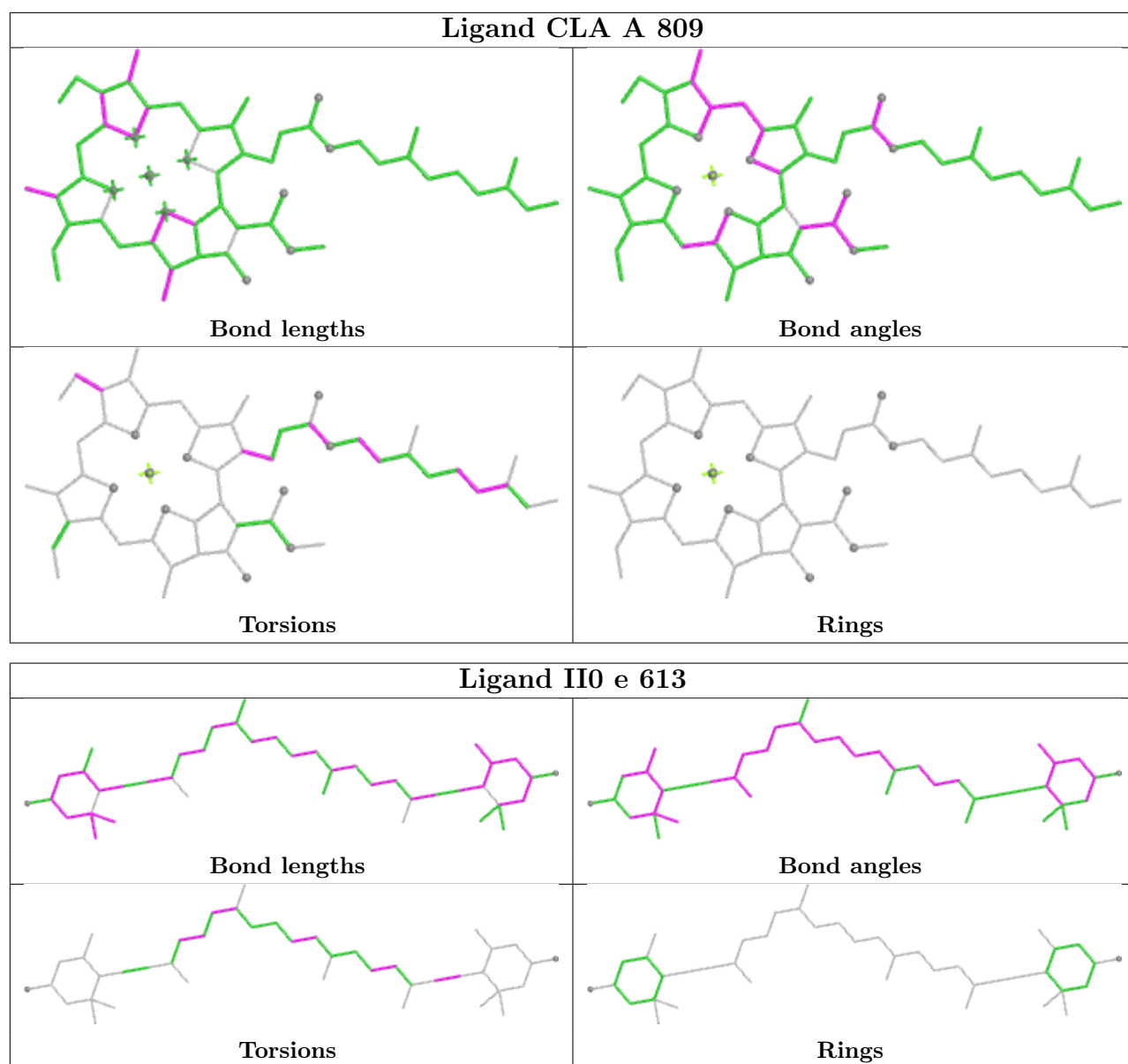


Ligand II0 e 616

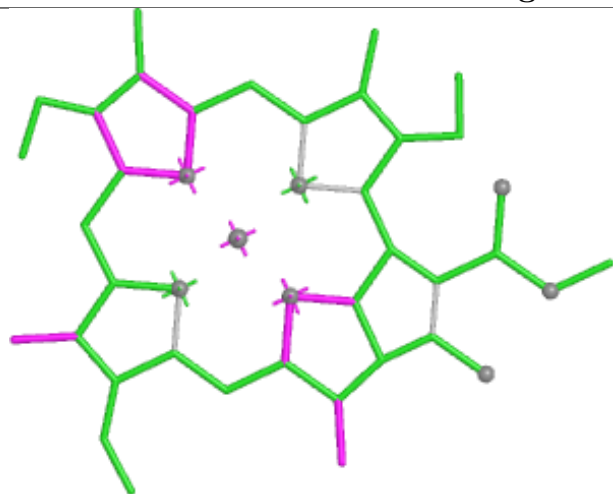




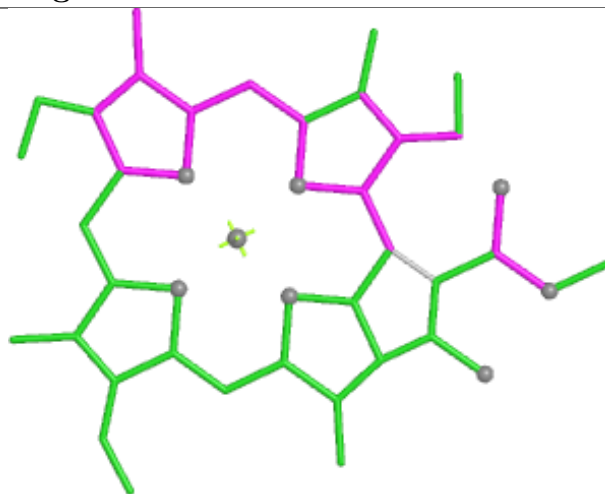




Ligand CLA g 302



Bond lengths



Bond angles

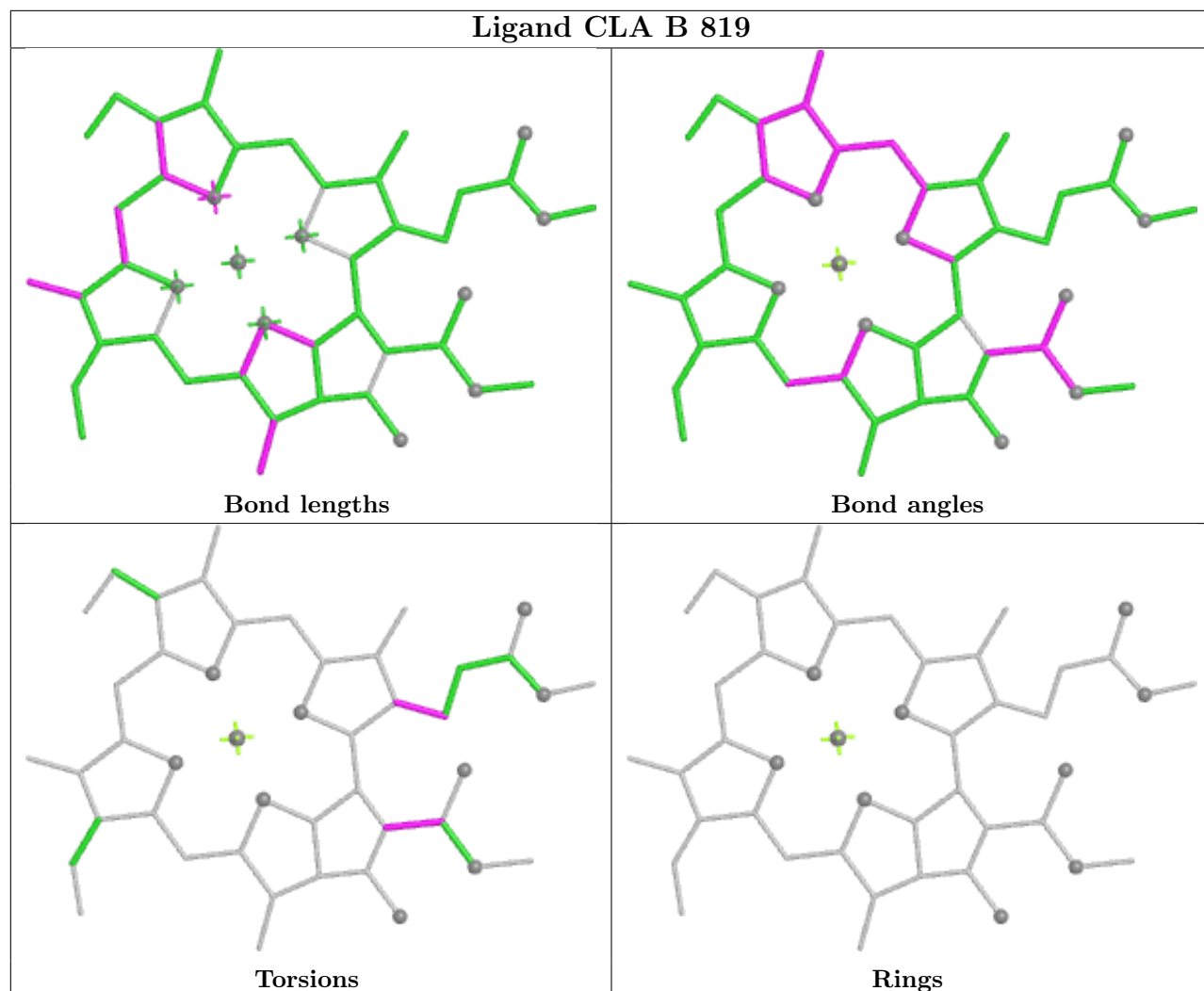


Torsions

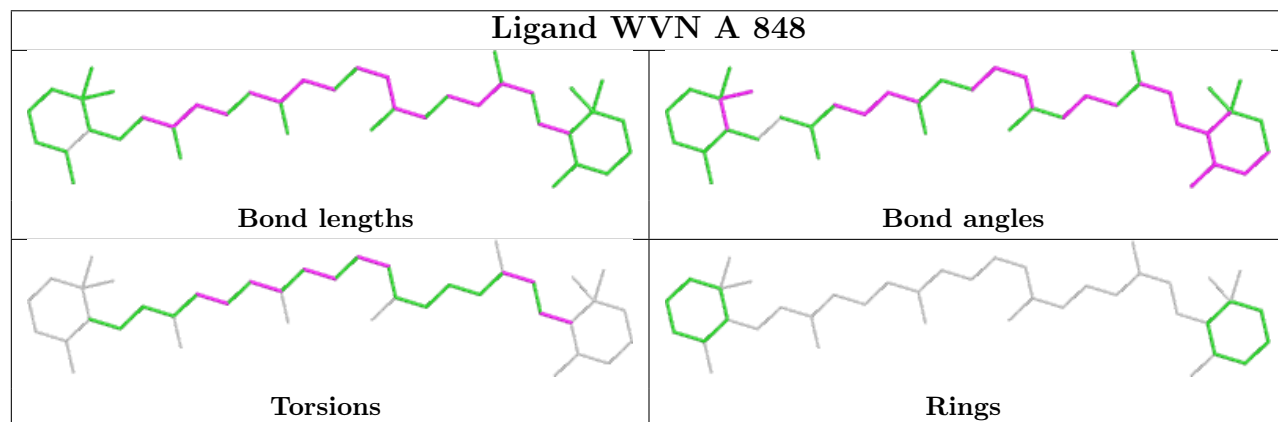


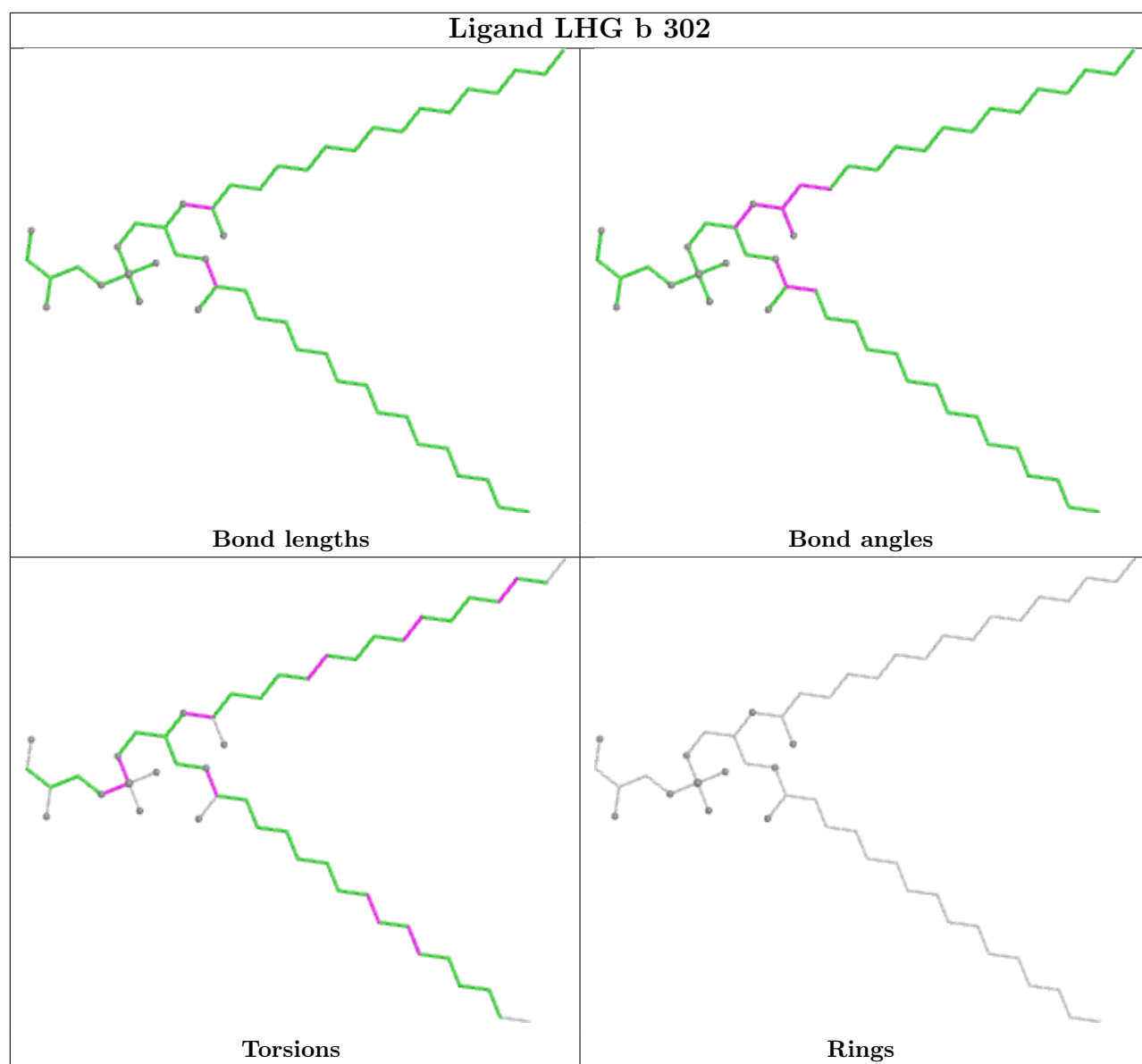
Rings

Ligand CLA B 819

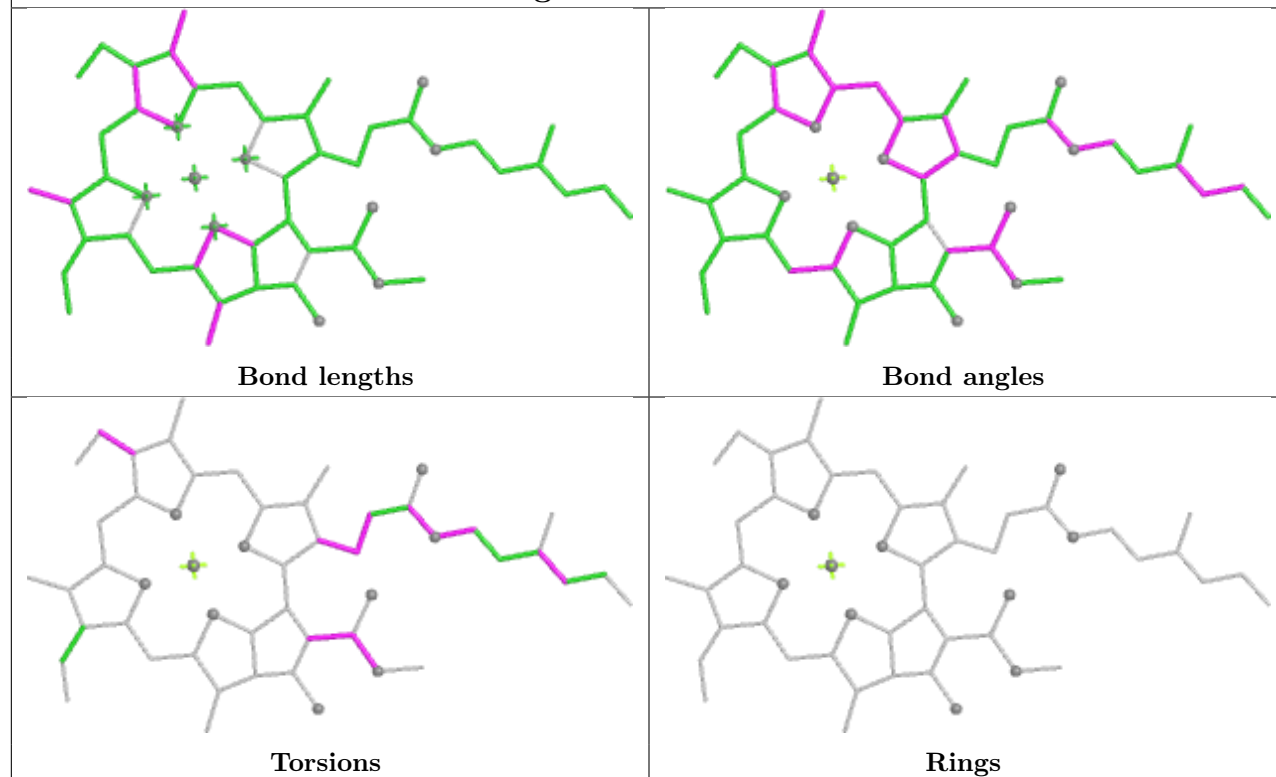


Ligand WVN A 848

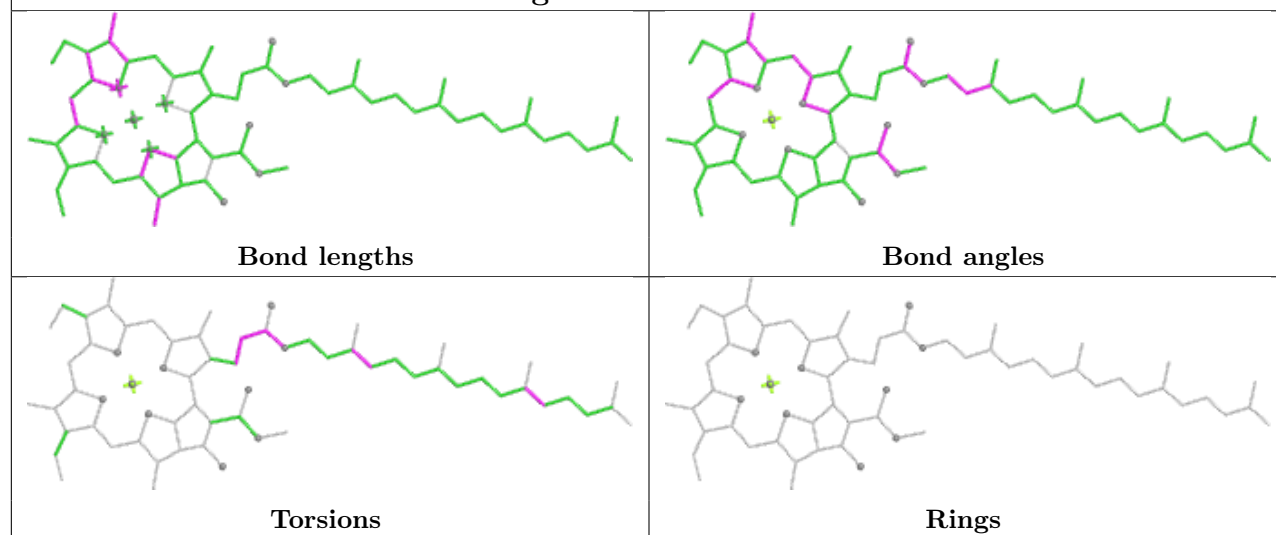


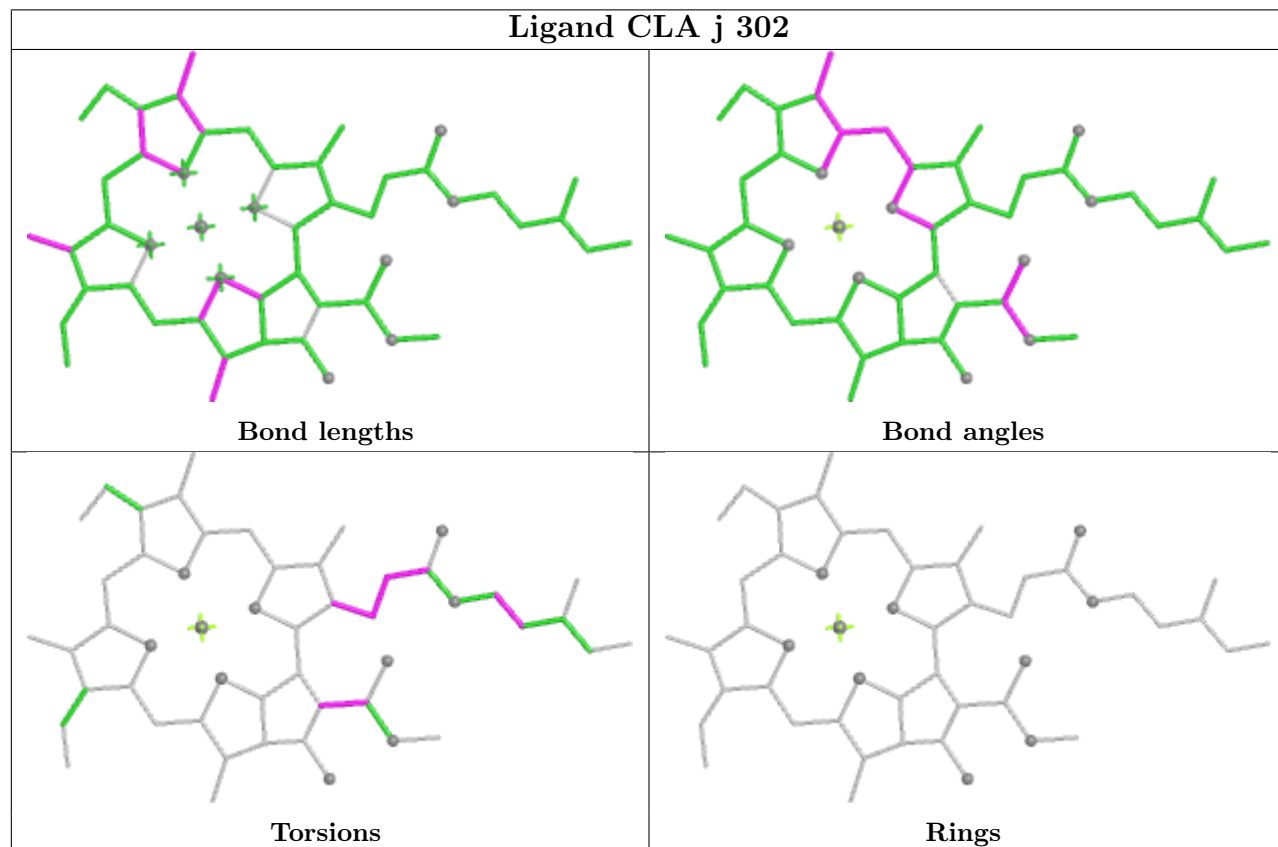
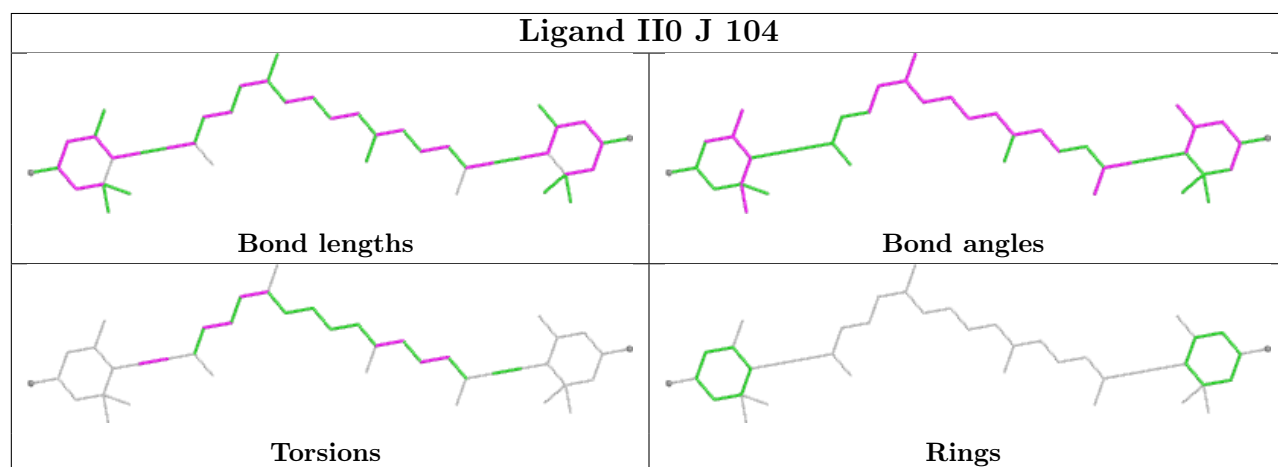
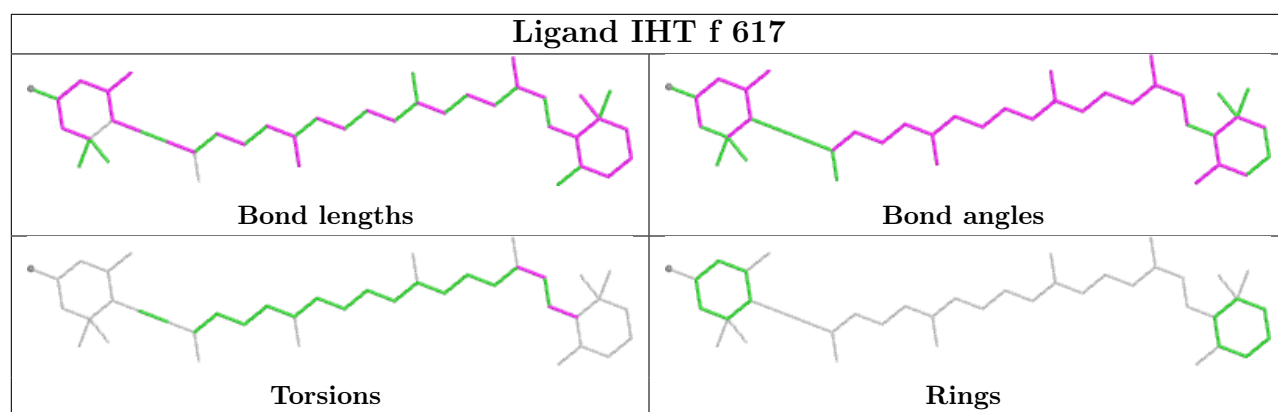


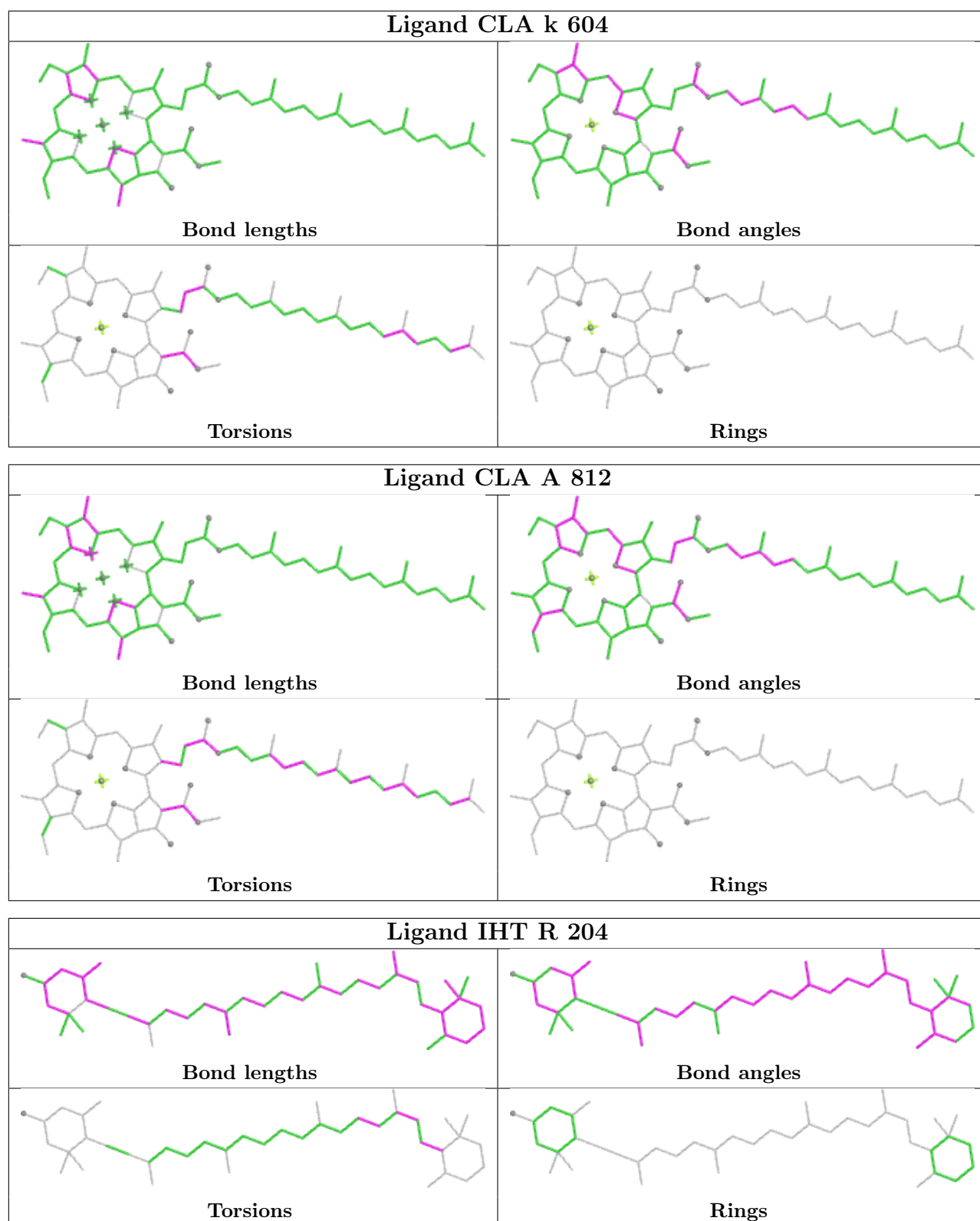
Ligand CLA F 202



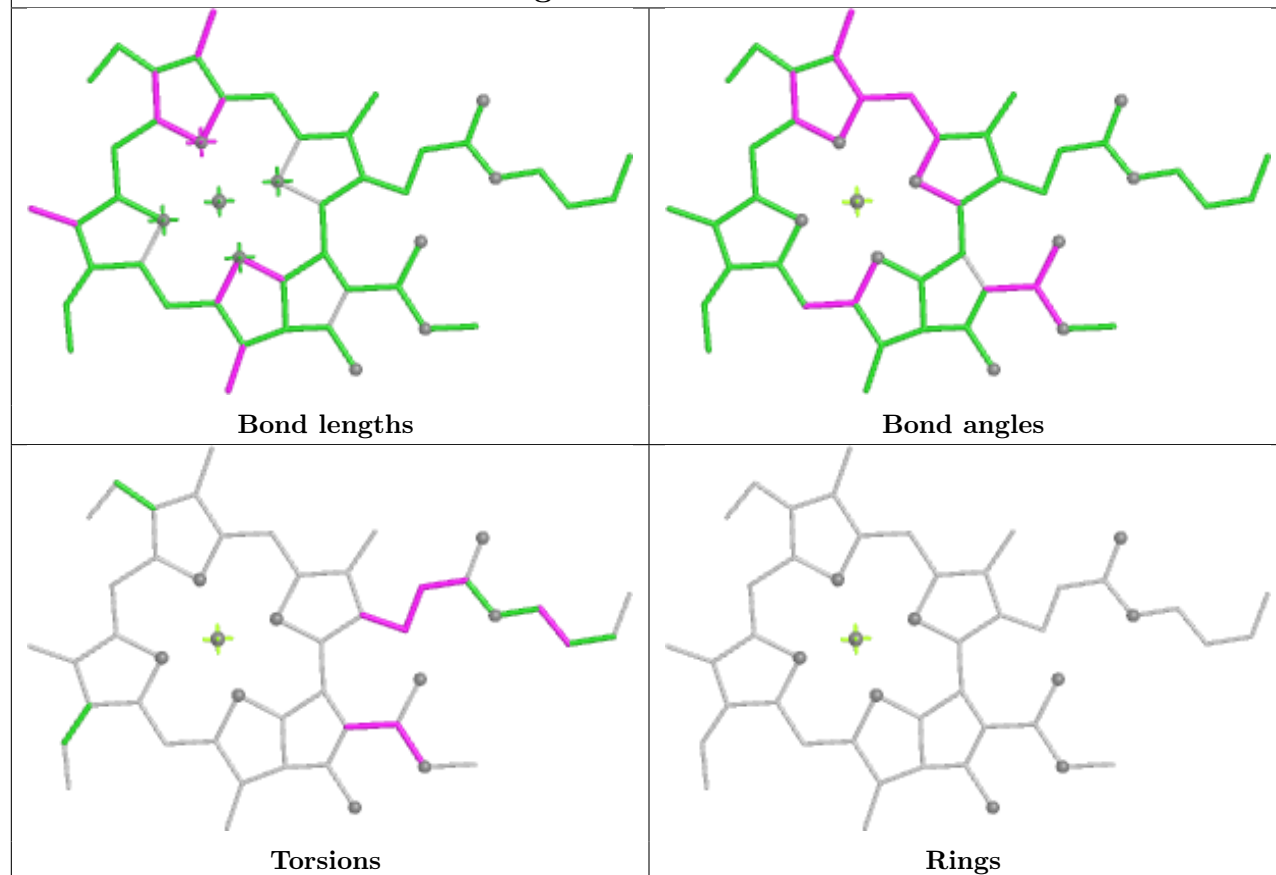
Ligand CLA A 828



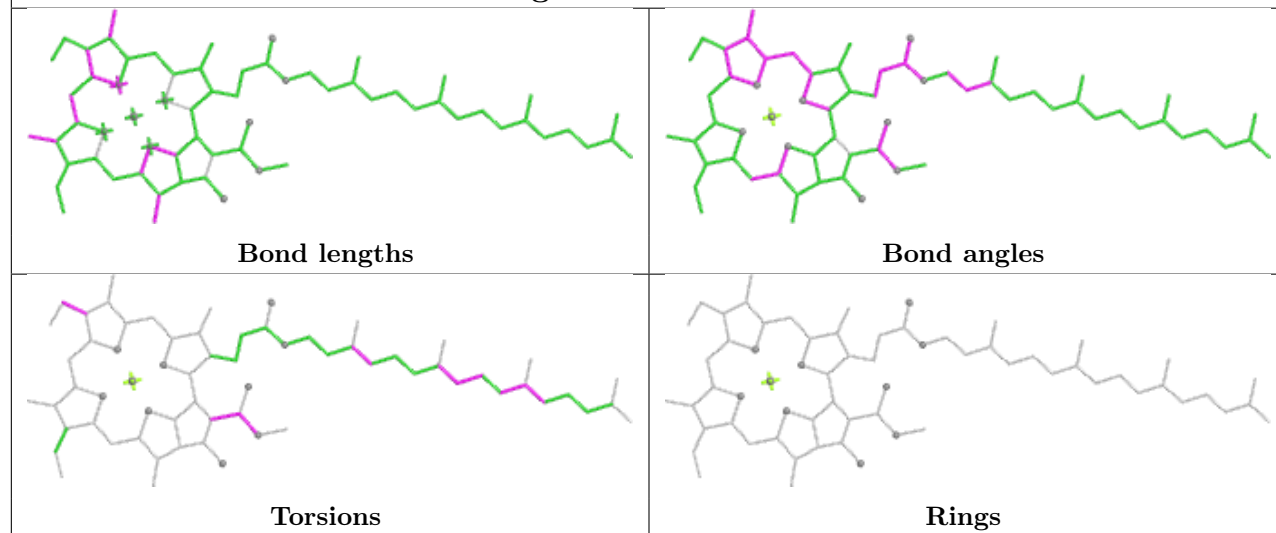


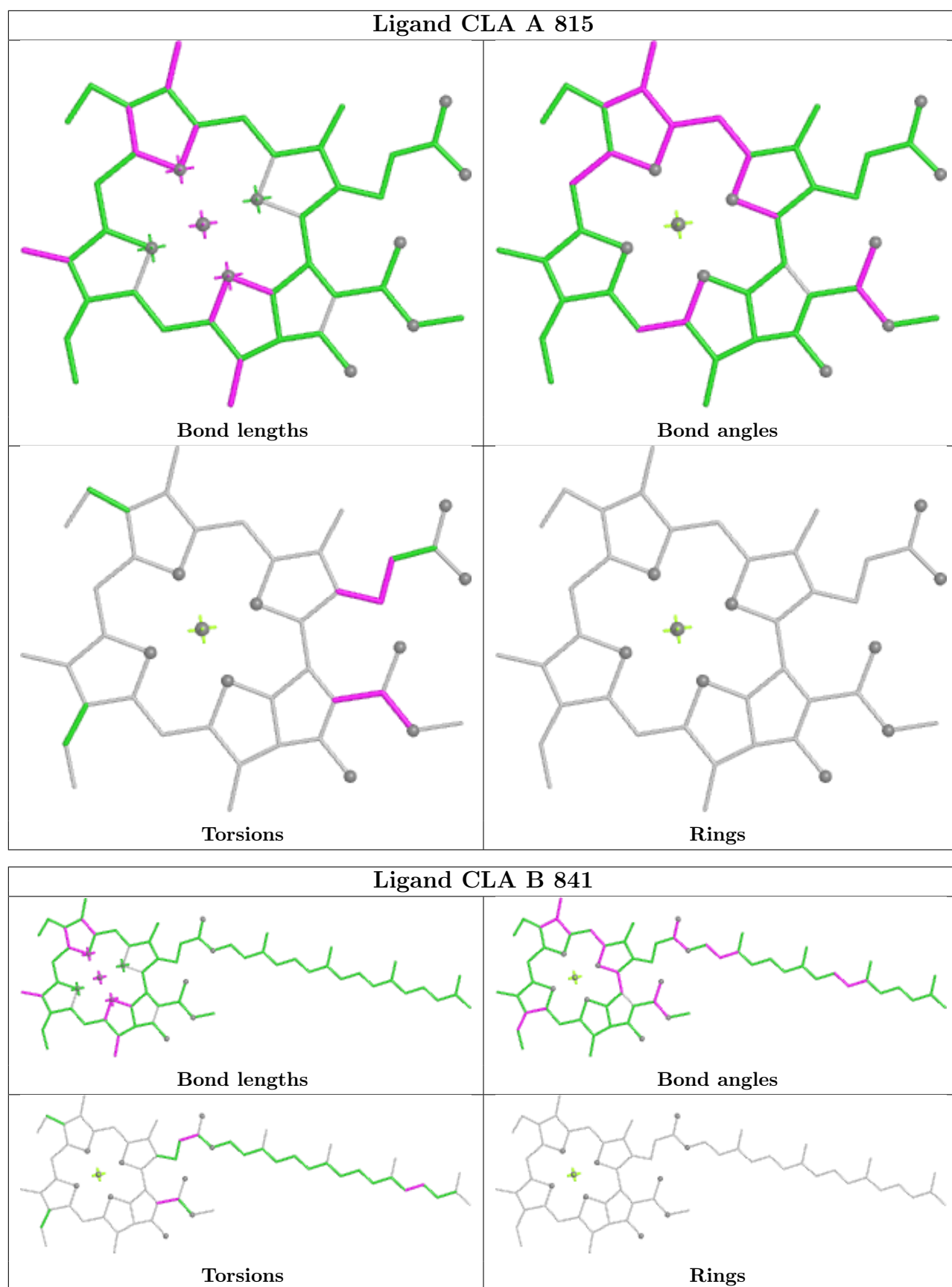


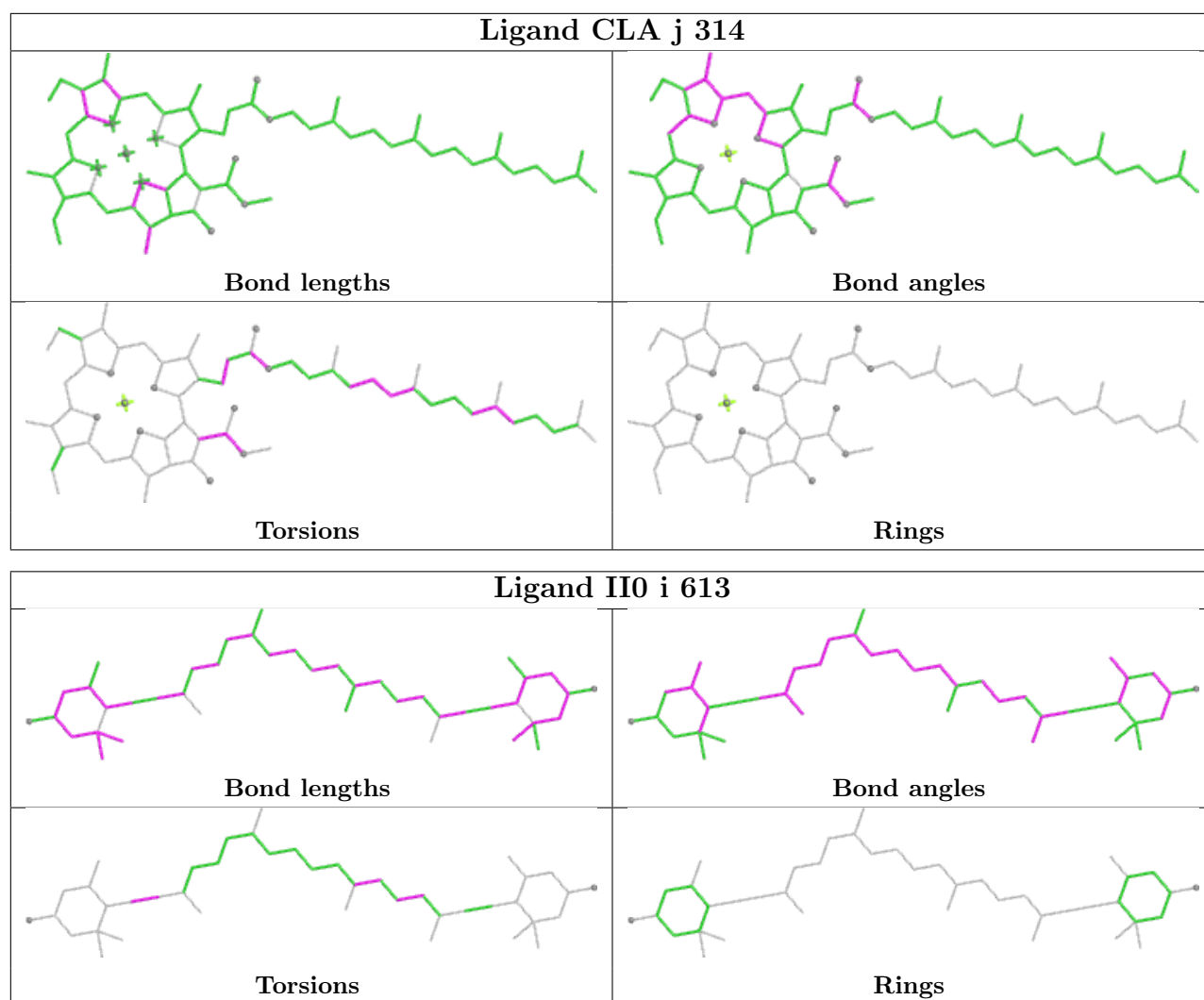
Ligand CLA L 202



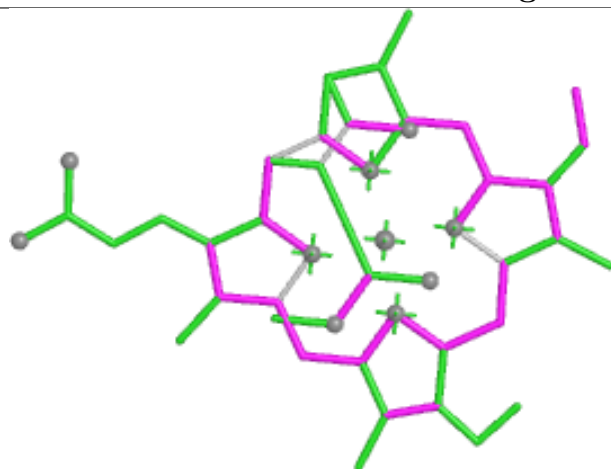
Ligand CLA A 853



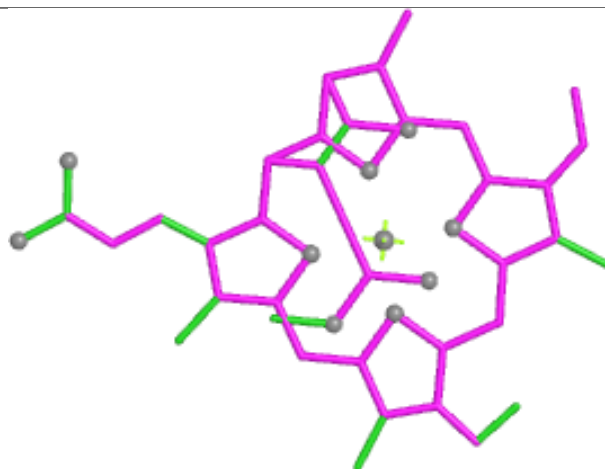




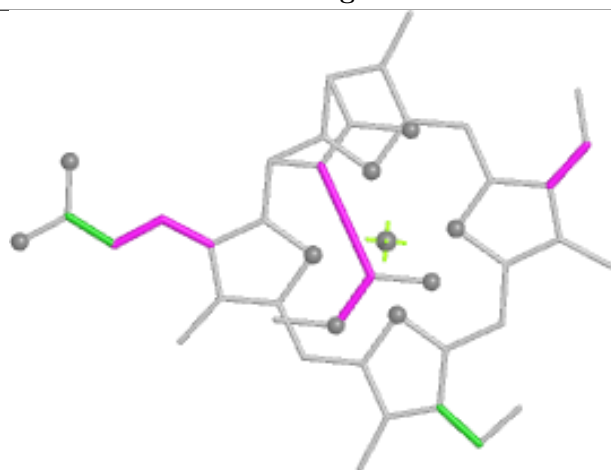
Ligand KC2 d 311



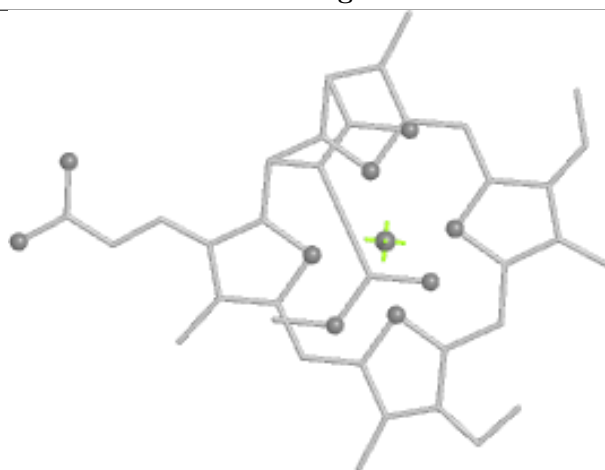
Bond lengths



Bond angles

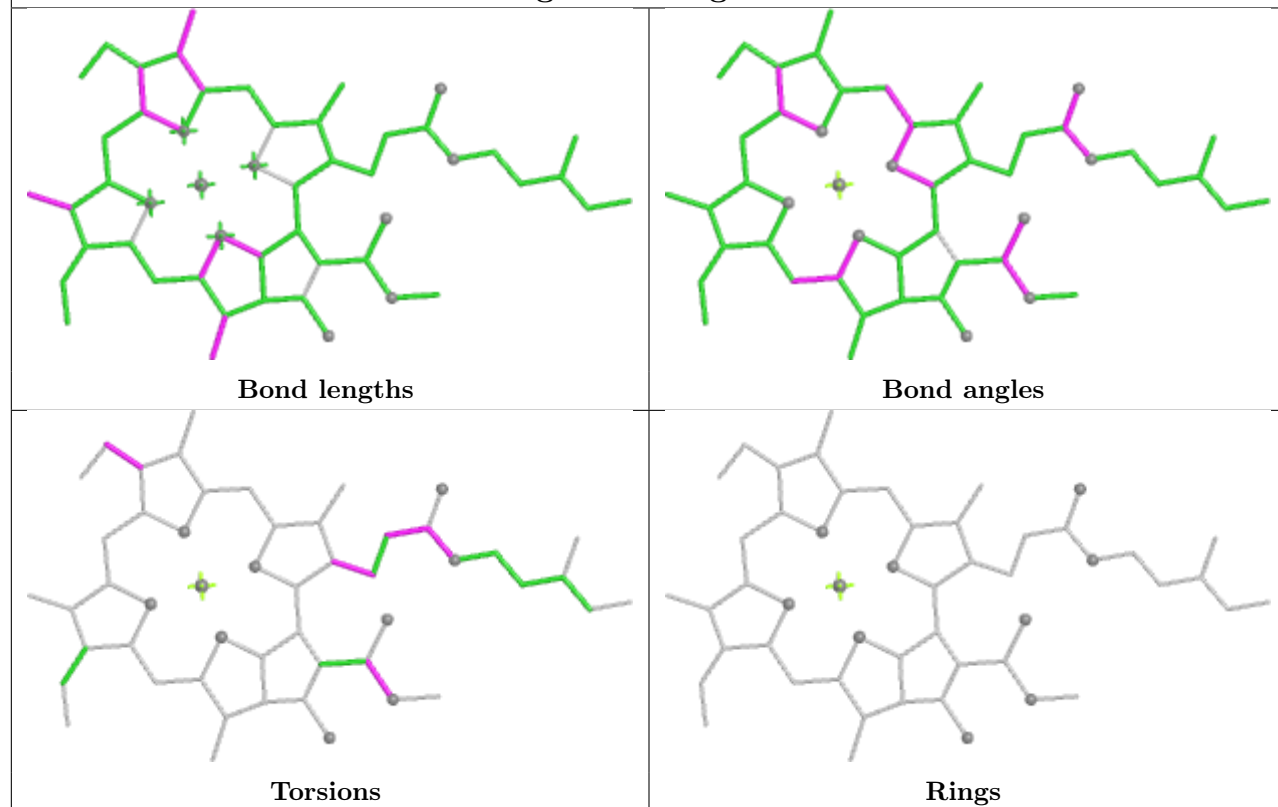


Torsions

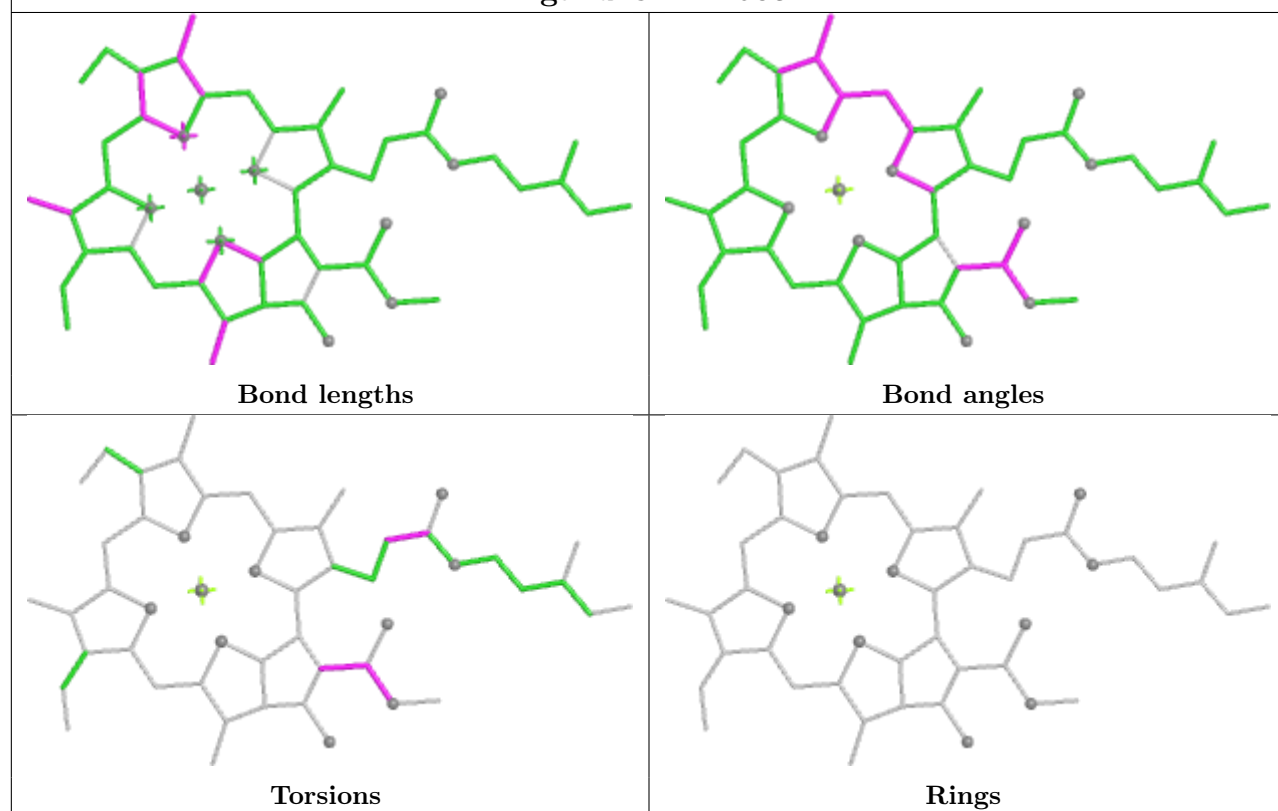


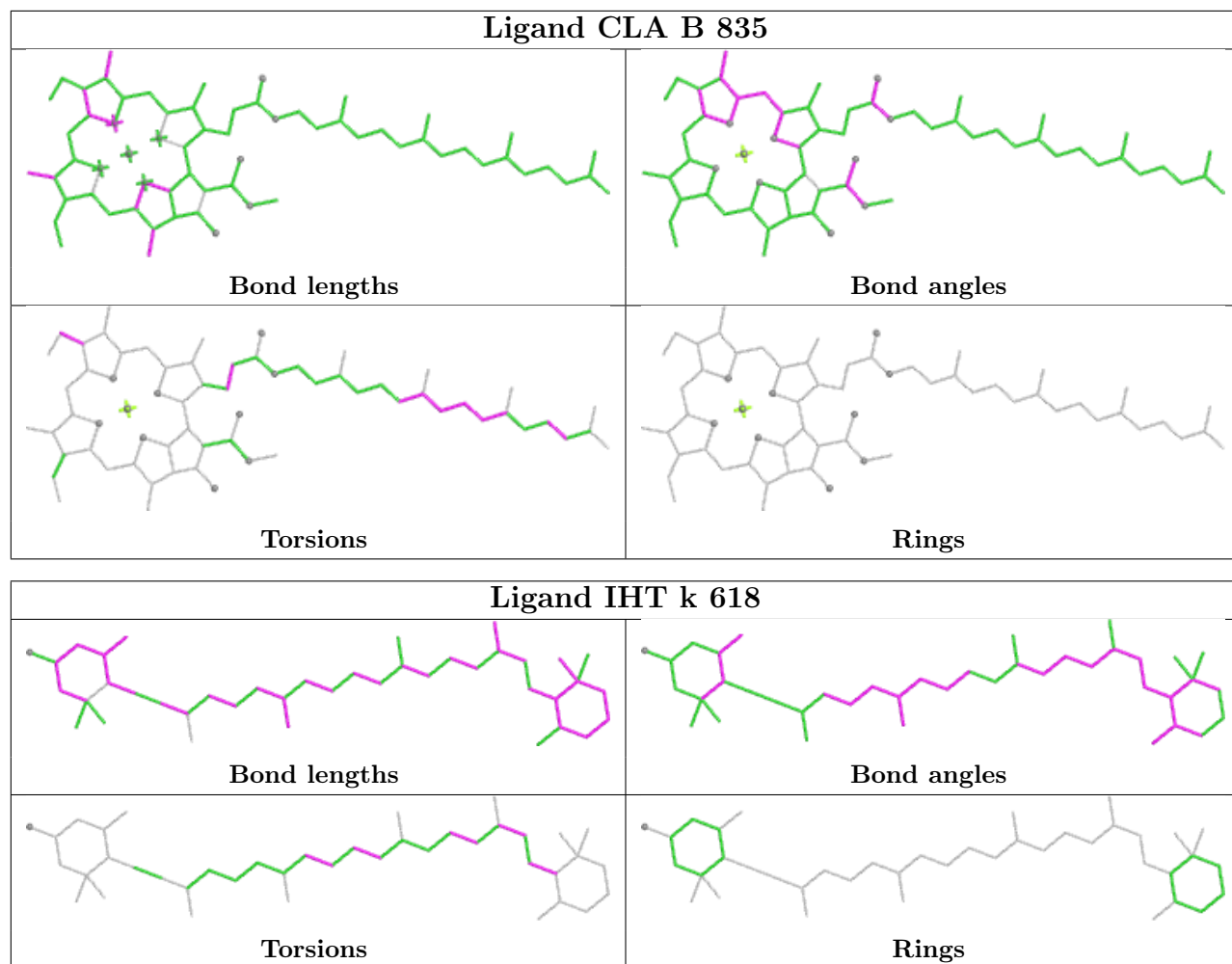
Rings

Ligand CLA g 306

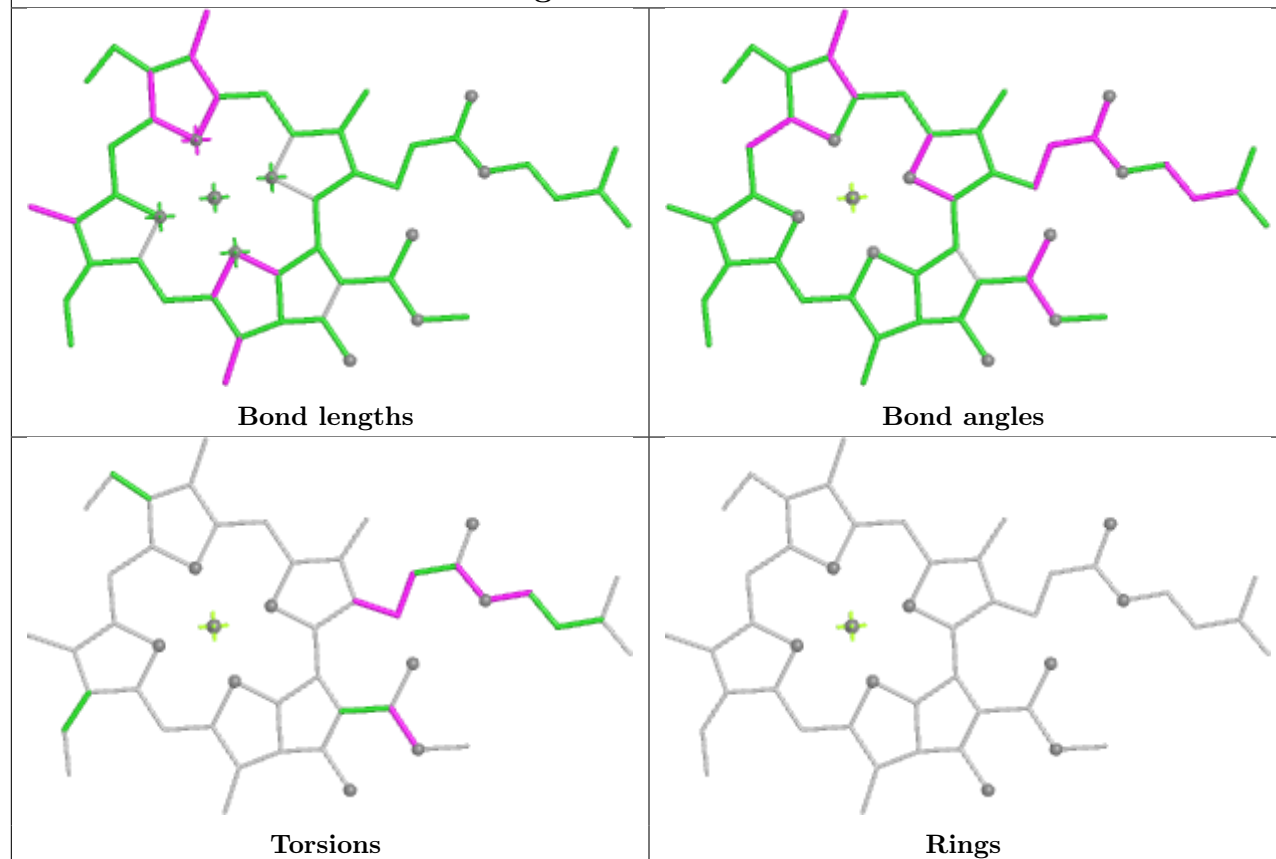


Ligand CLA i 603

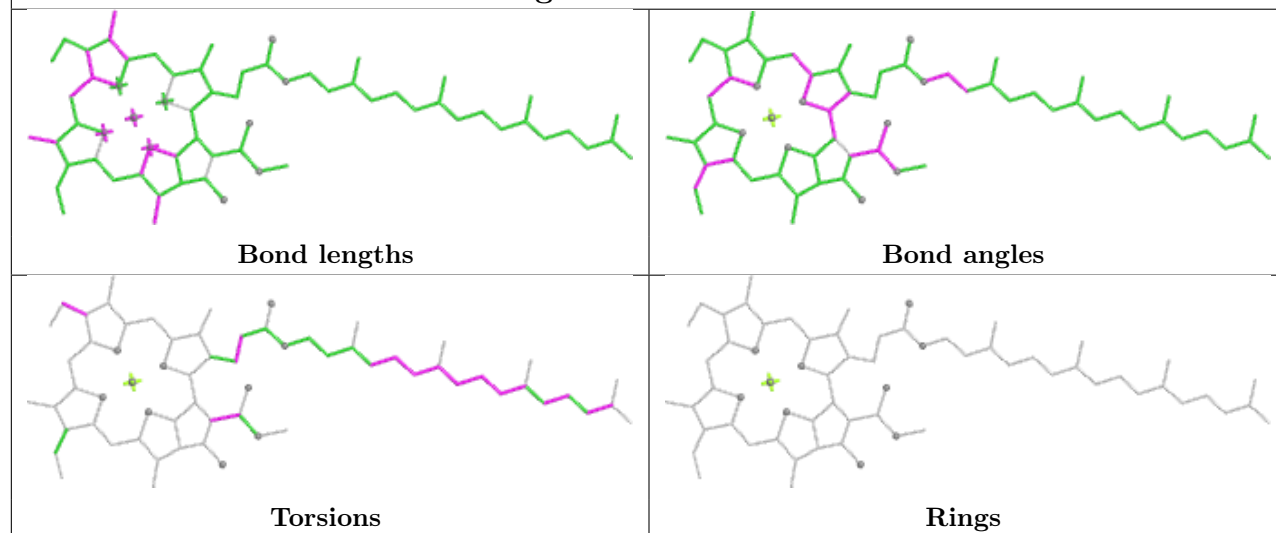


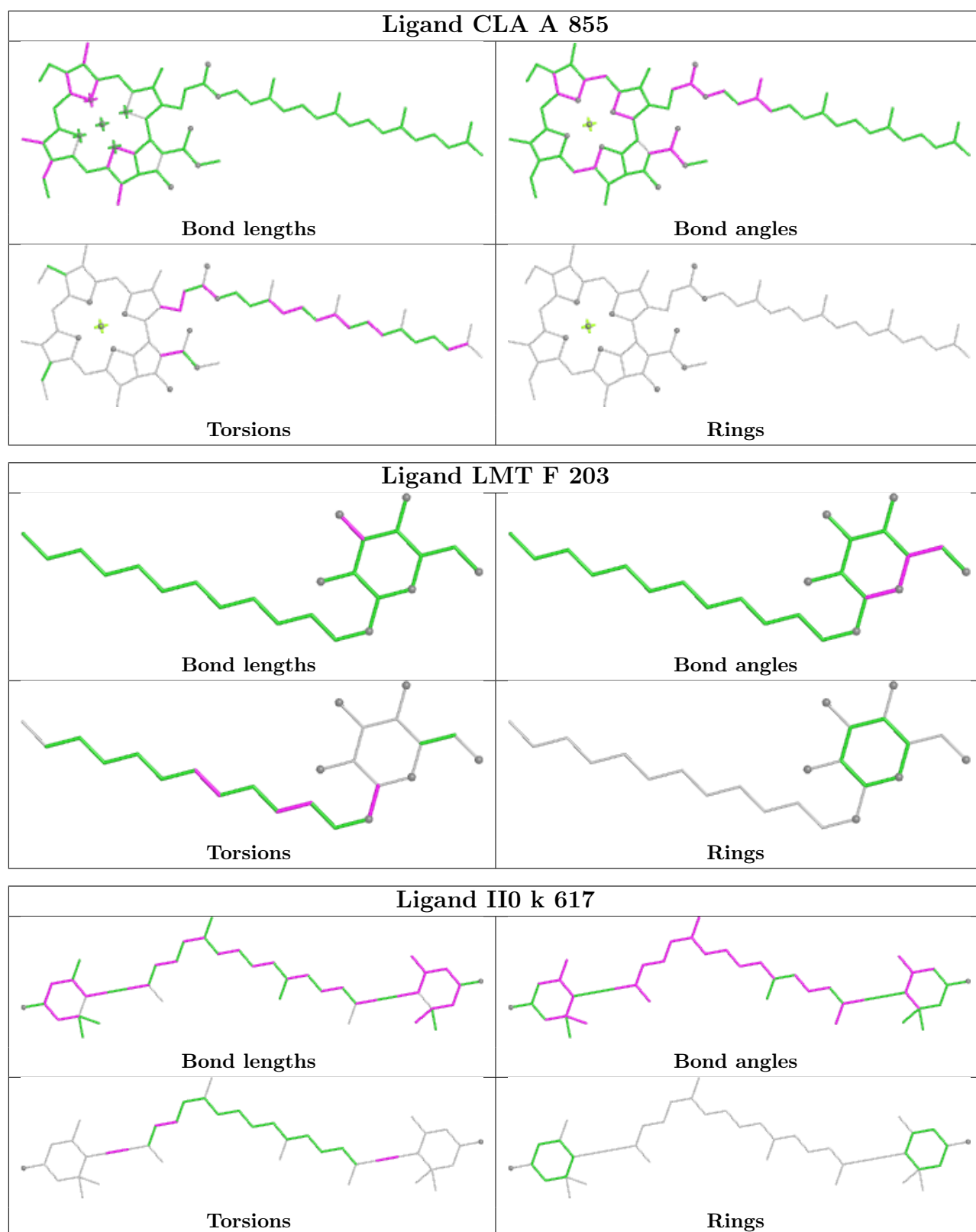


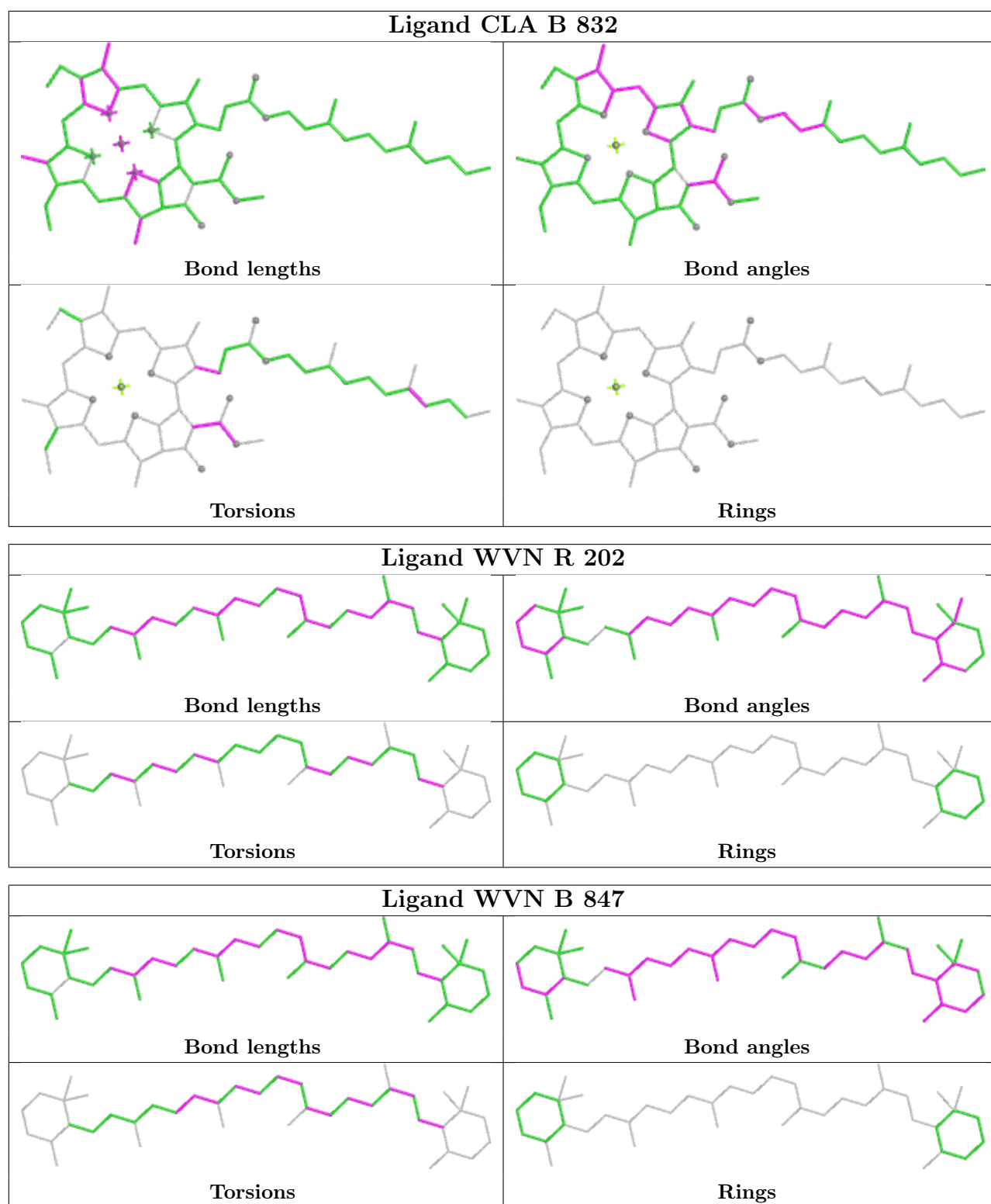
Ligand CLA L 204

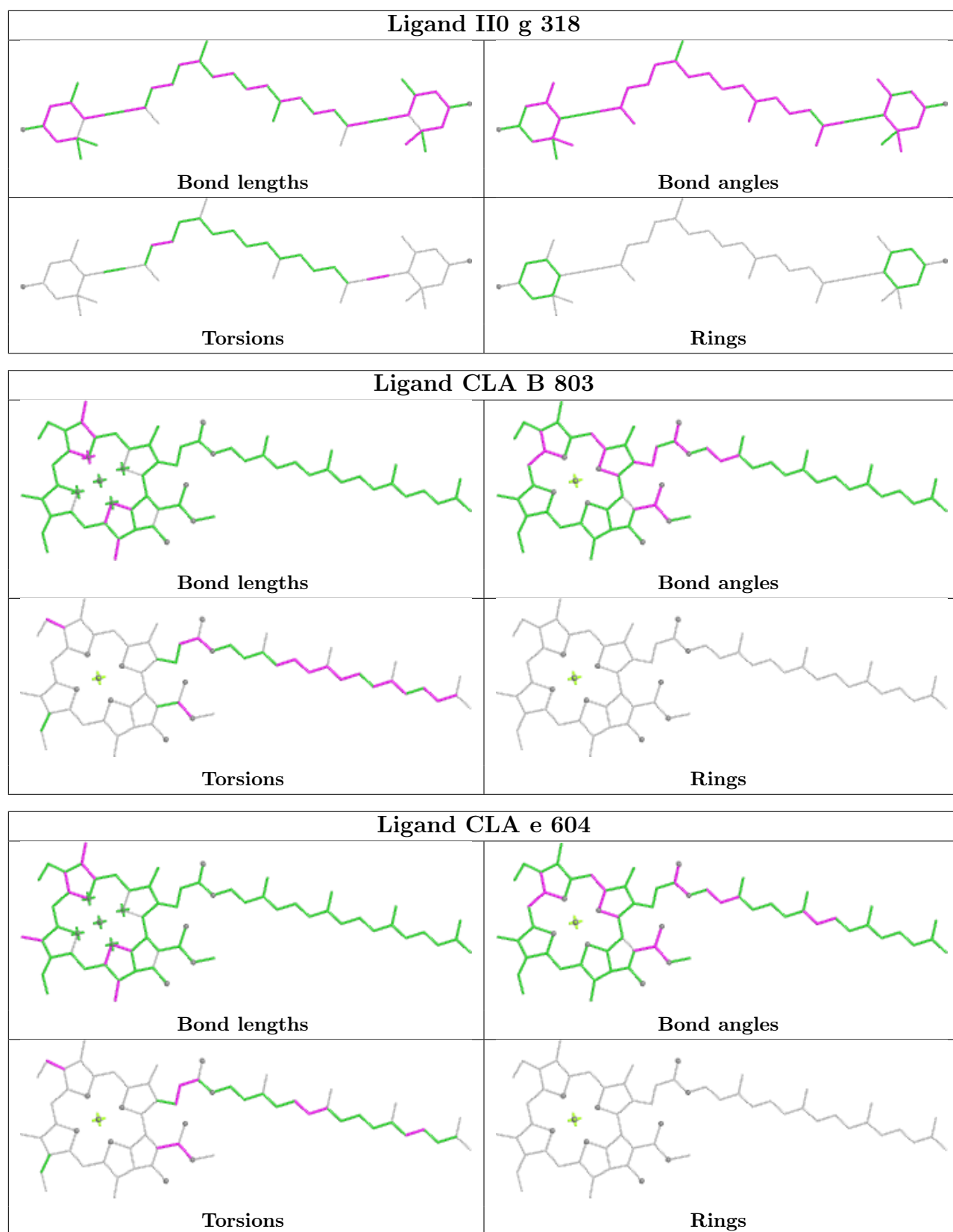


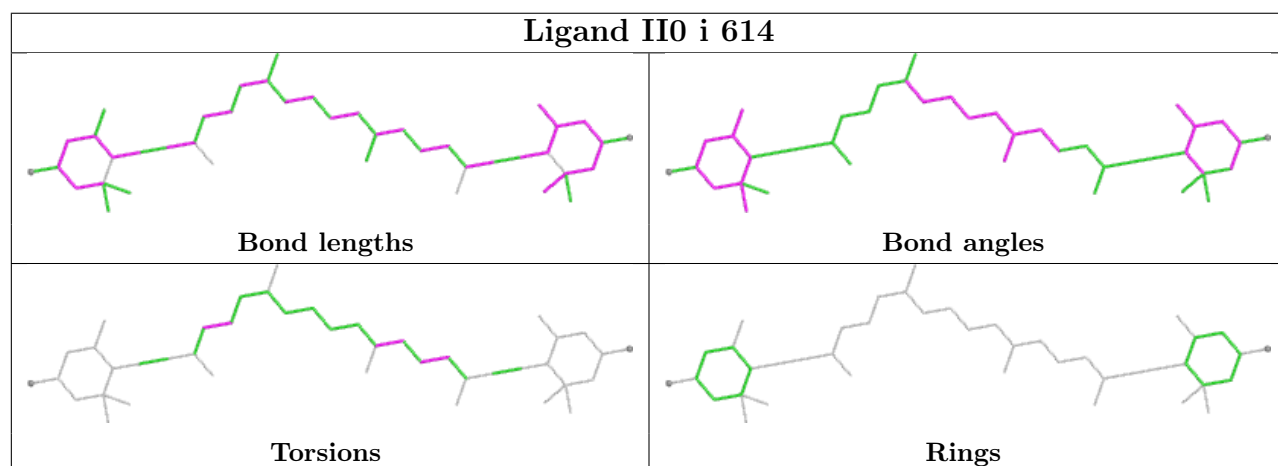
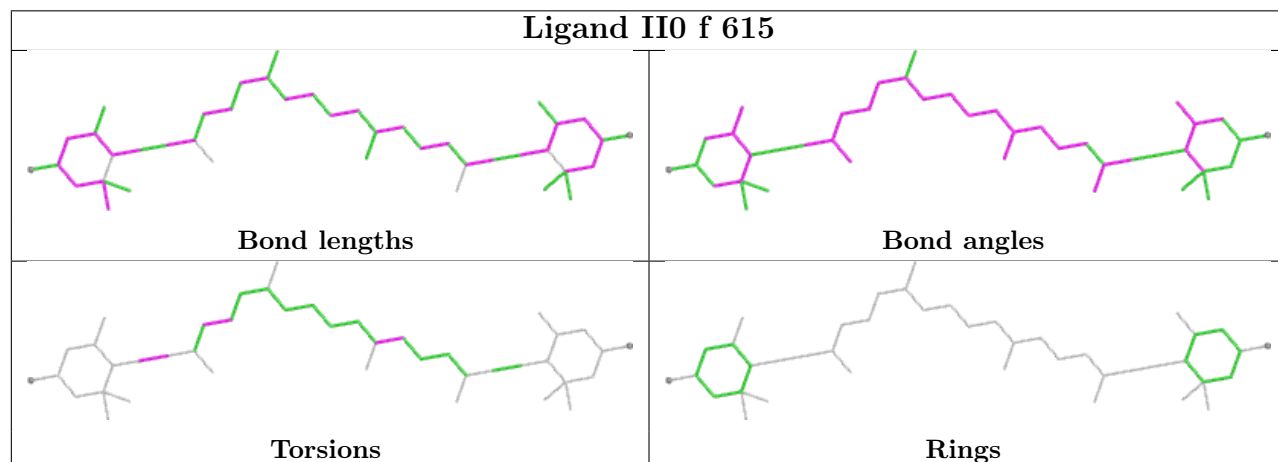
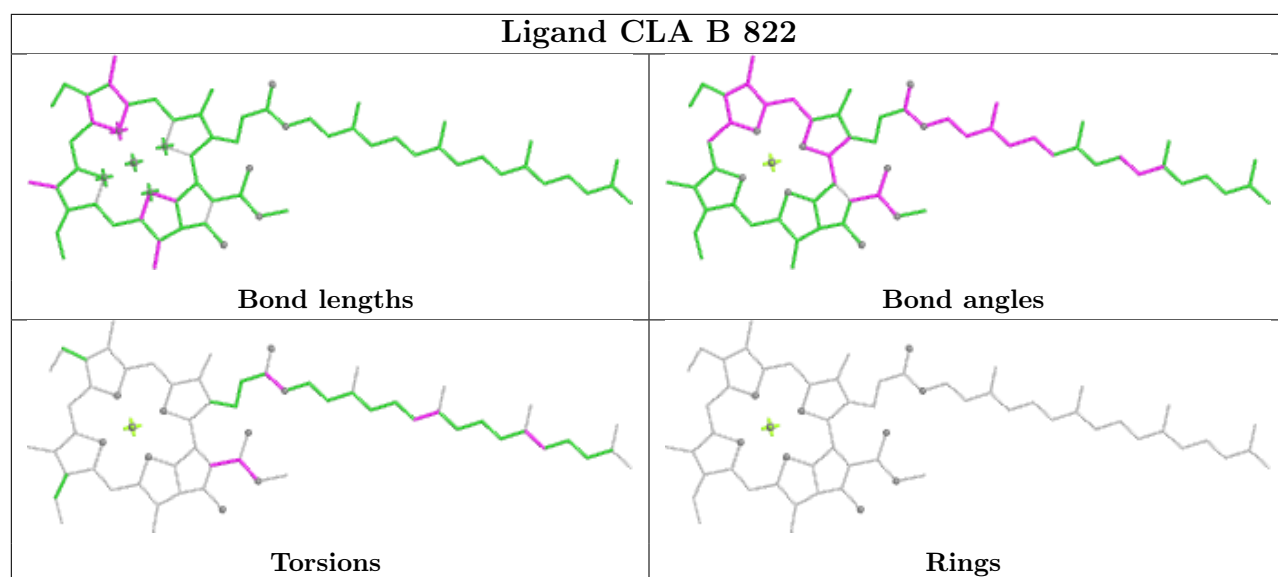
Ligand CLA b 306

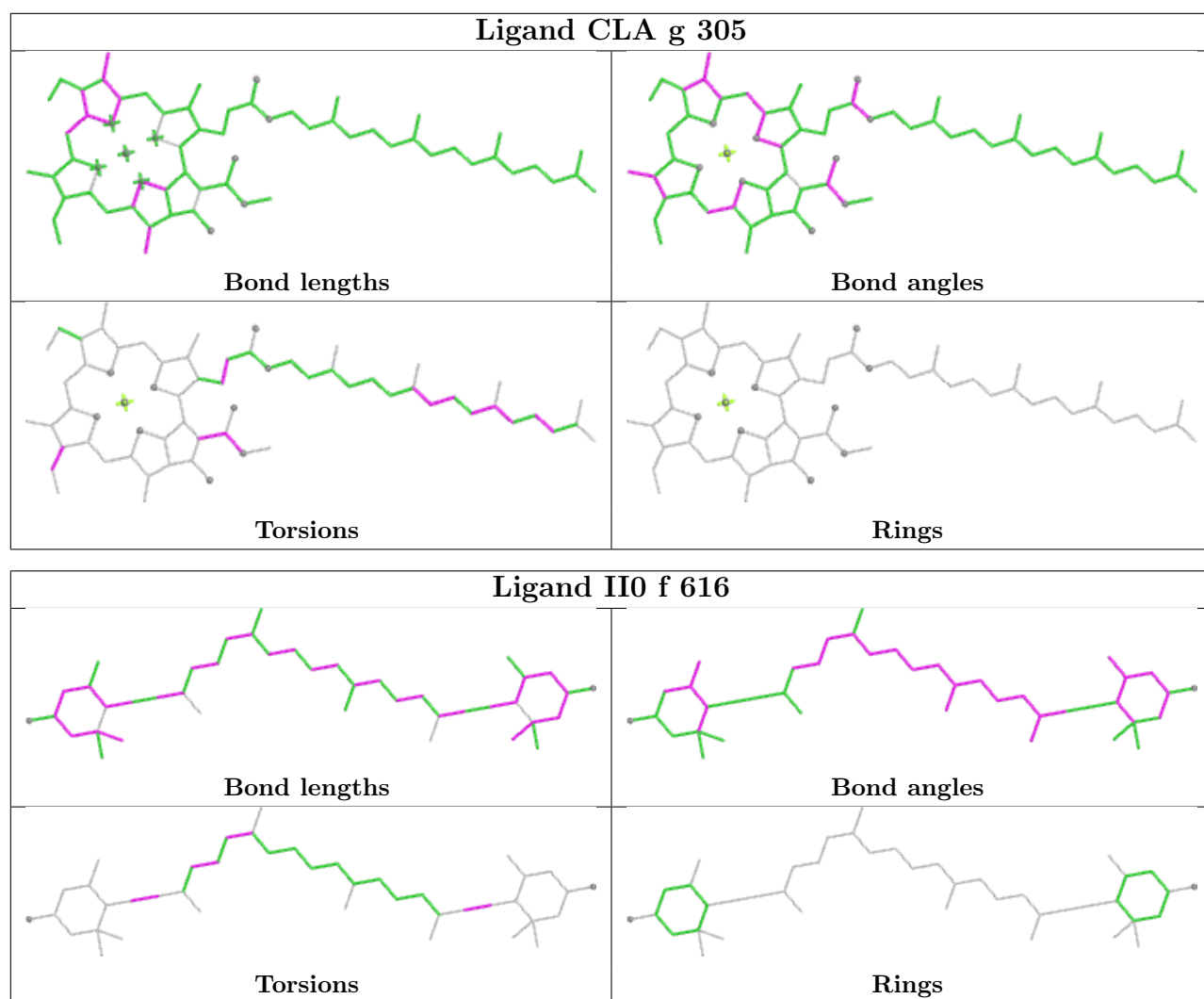




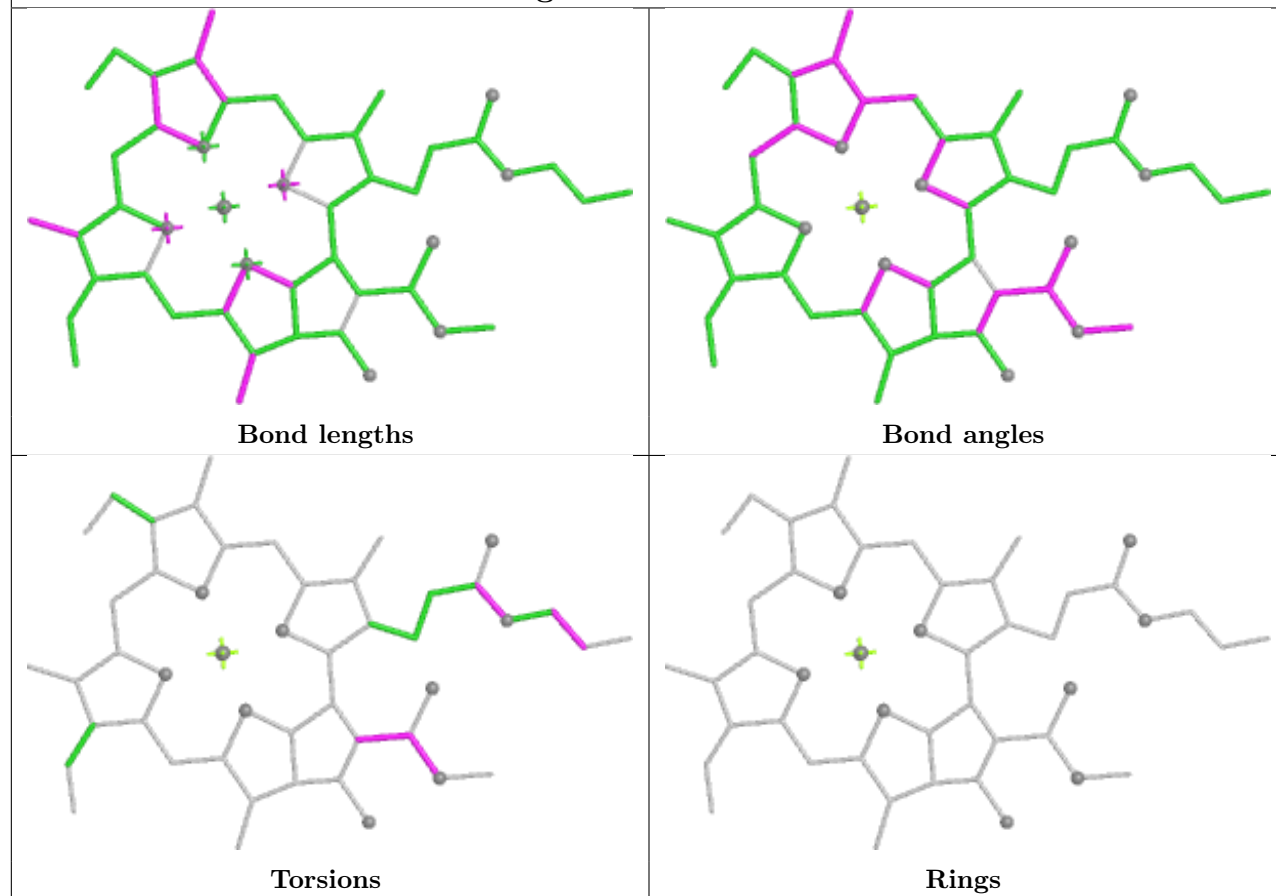




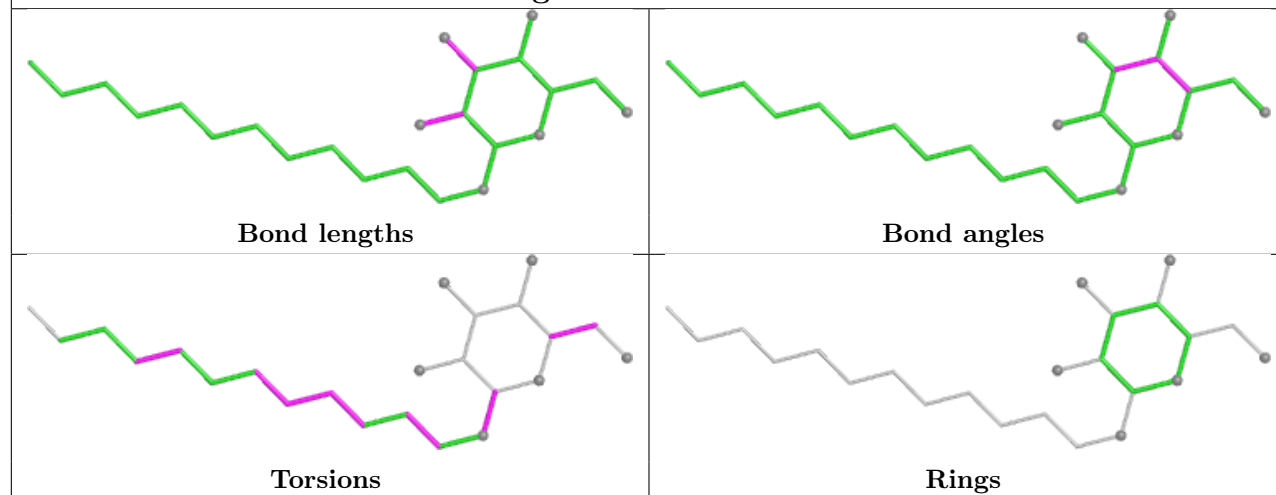




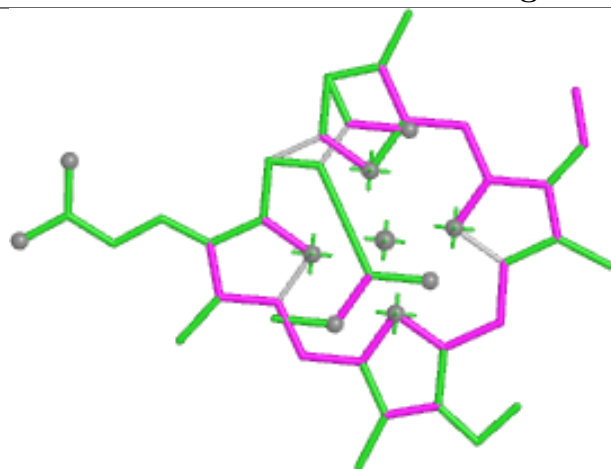
Ligand CLA a 312



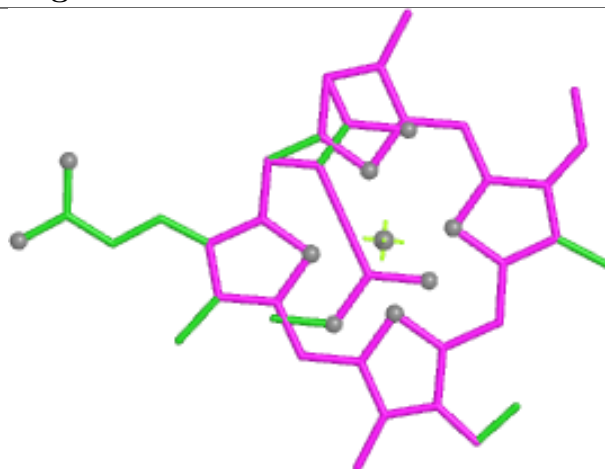
Ligand LMT b 319



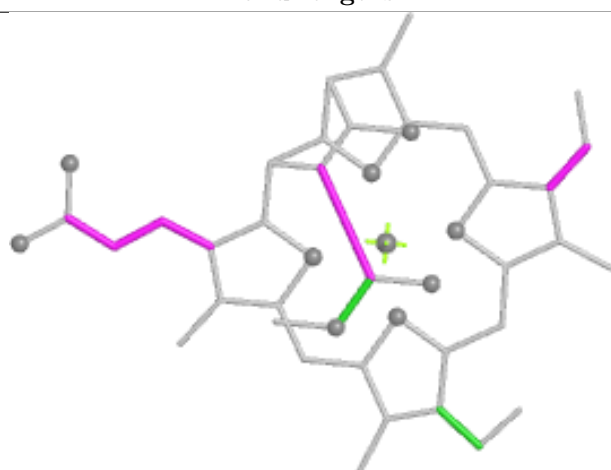
Ligand KC2 g 314



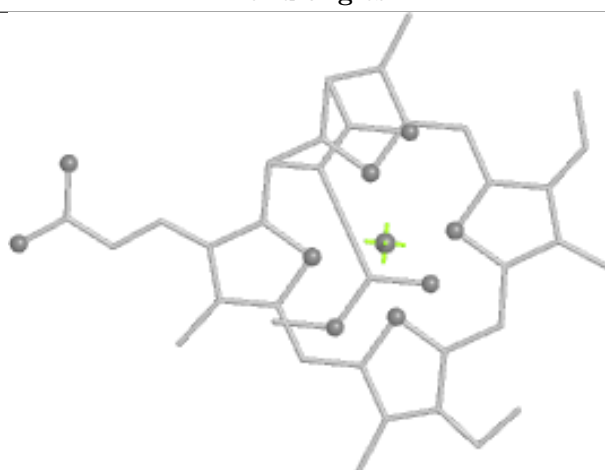
Bond lengths



Bond angles

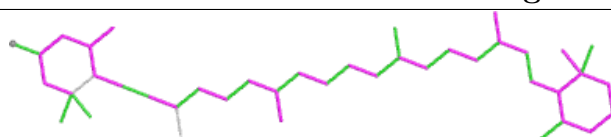


Torsions



Rings

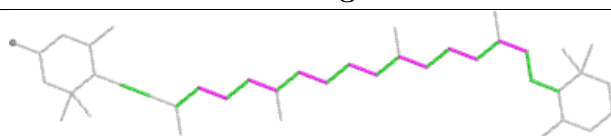
Ligand IHT c 615



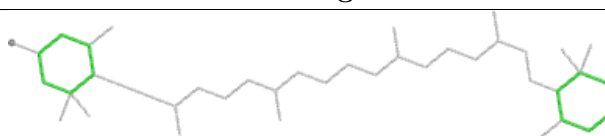
Bond lengths



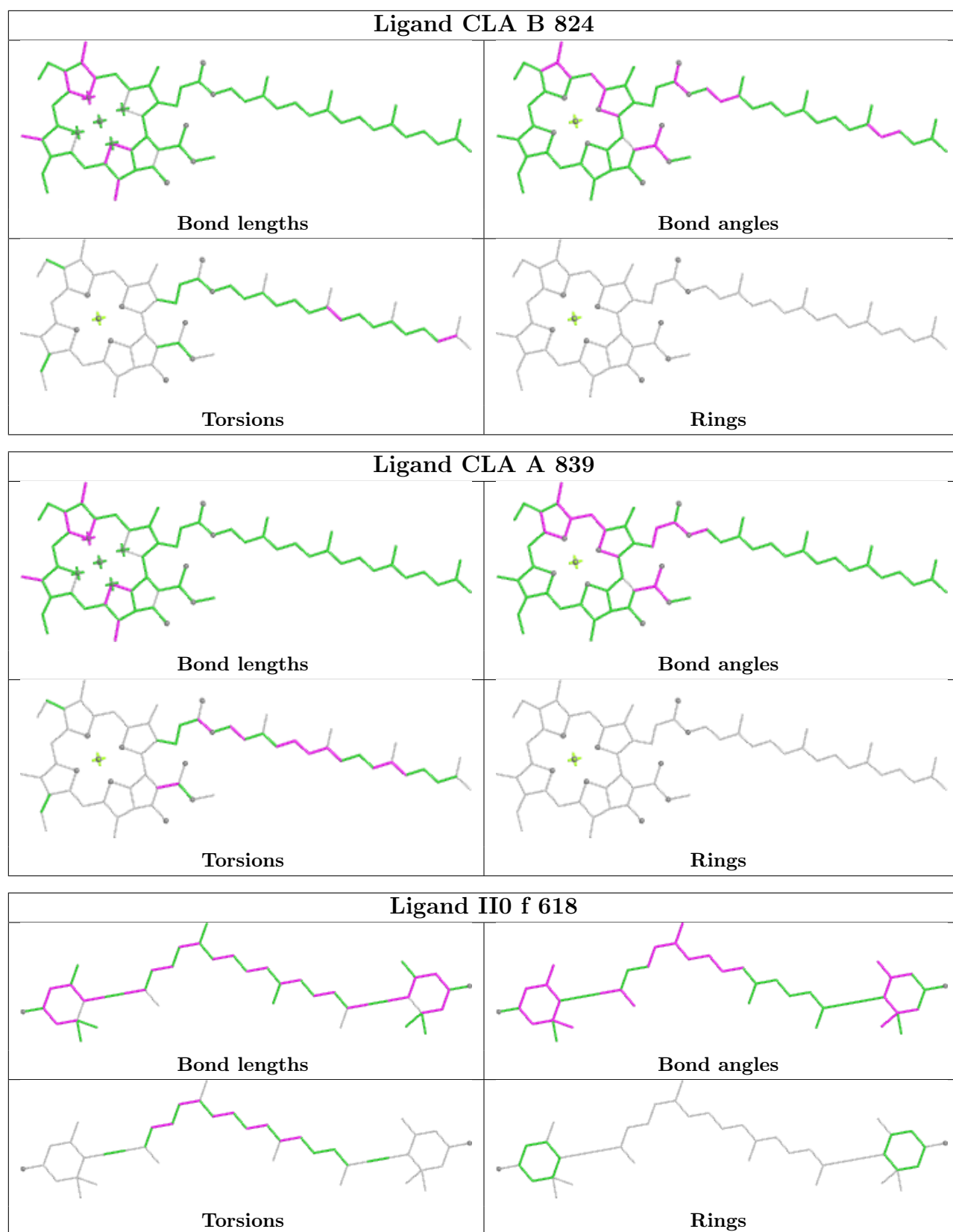
Bond angles



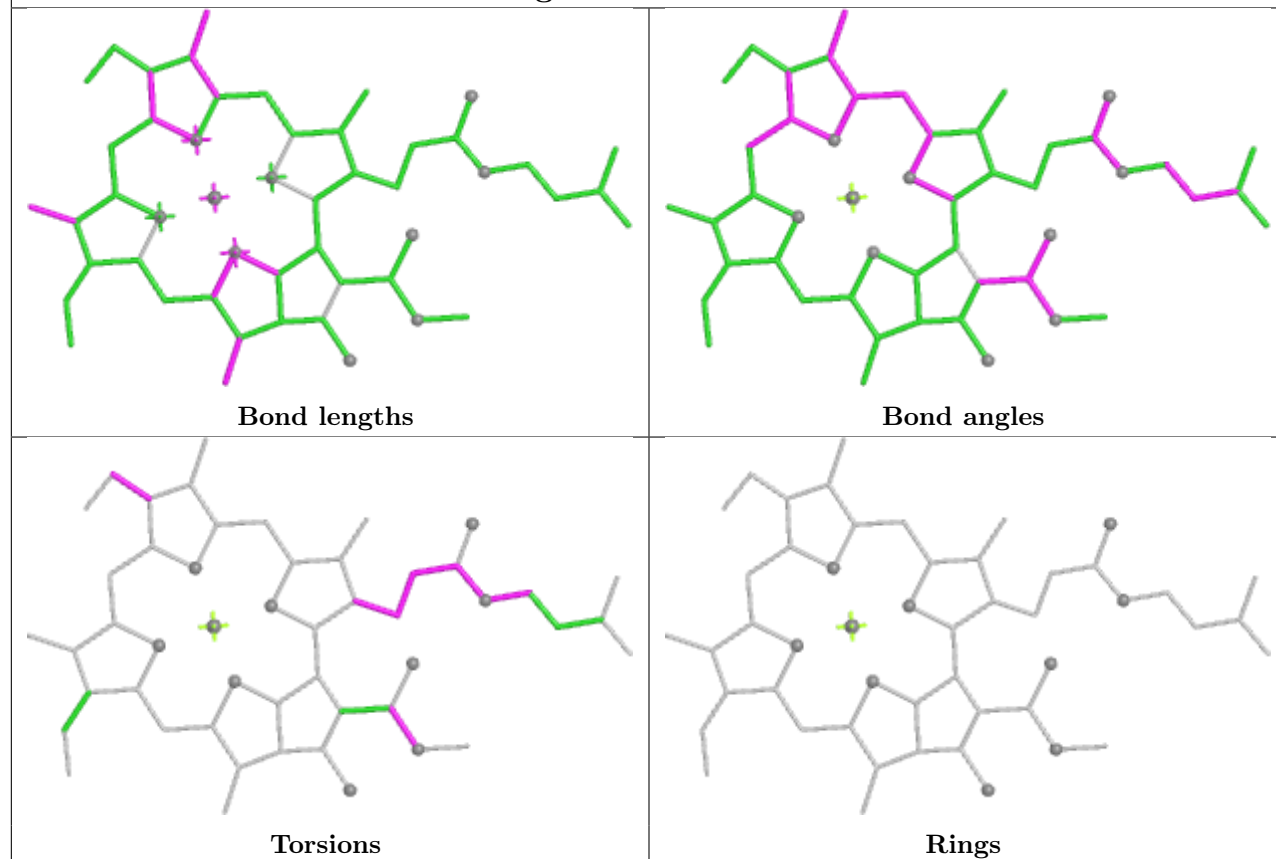
Torsions



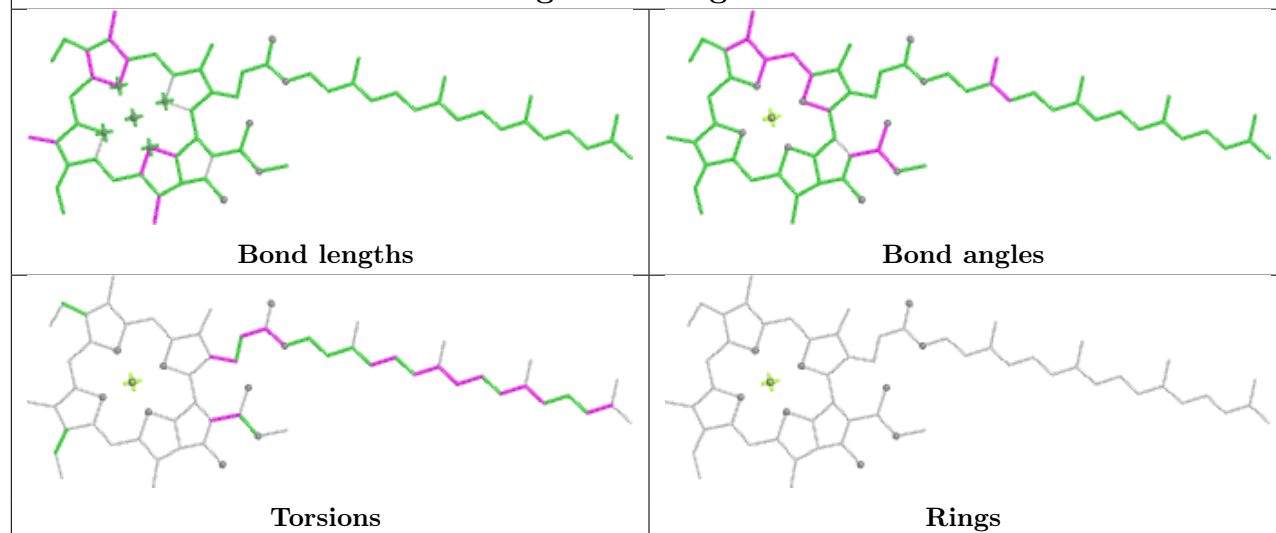
Rings



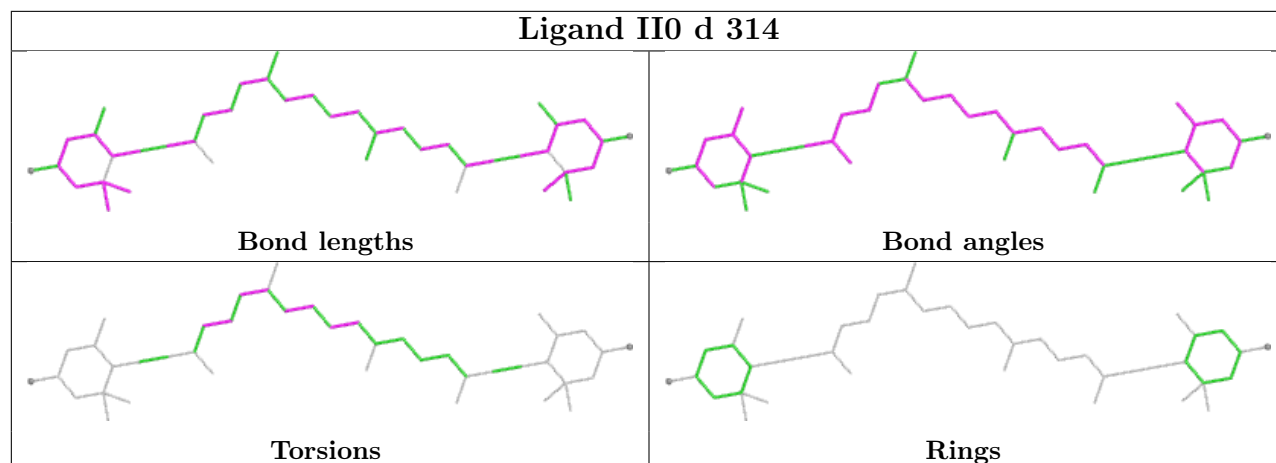
Ligand CLA h 302



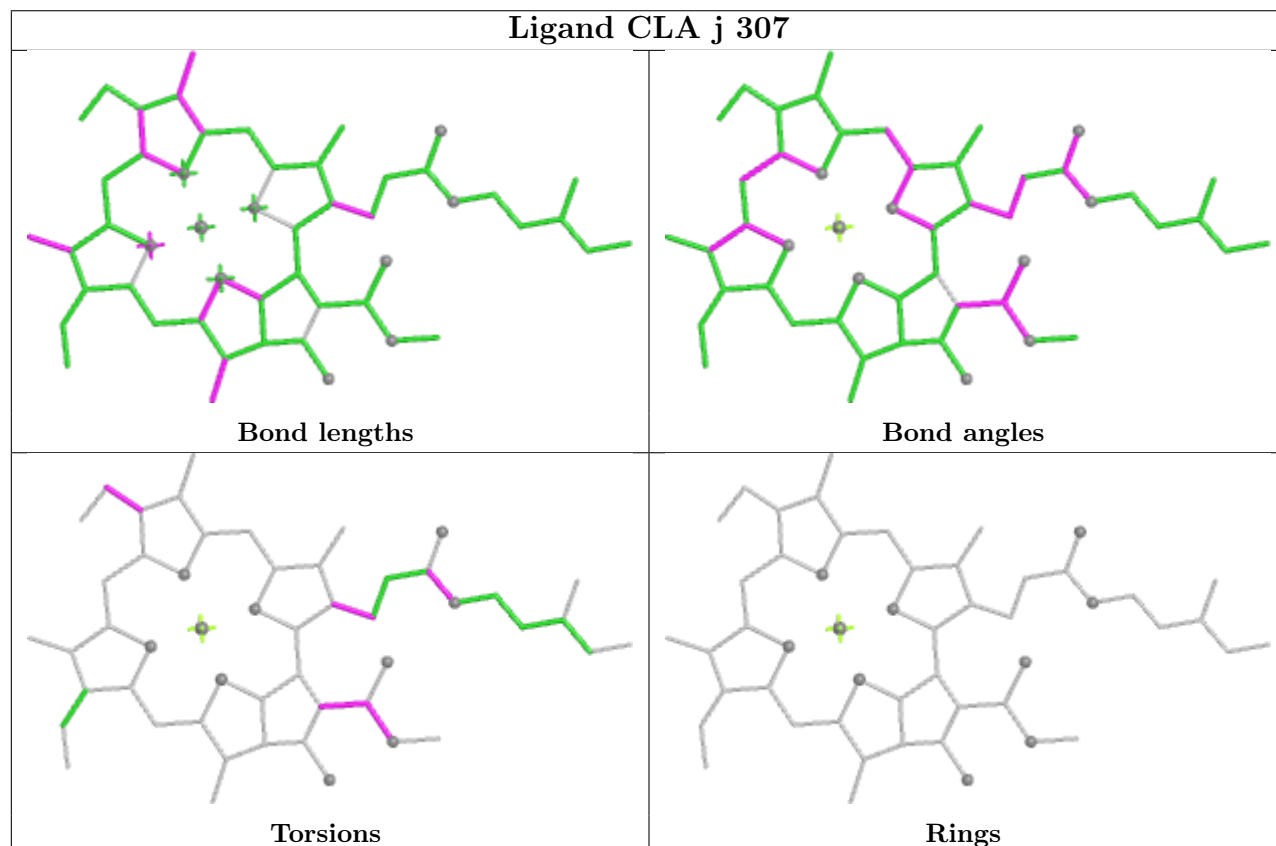
Ligand CLA g 308



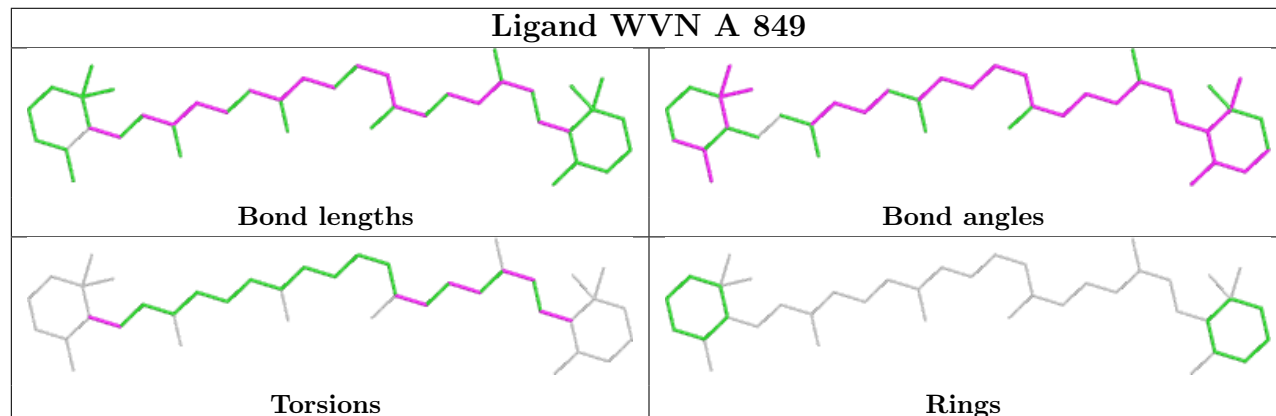
Ligand II0 d 314



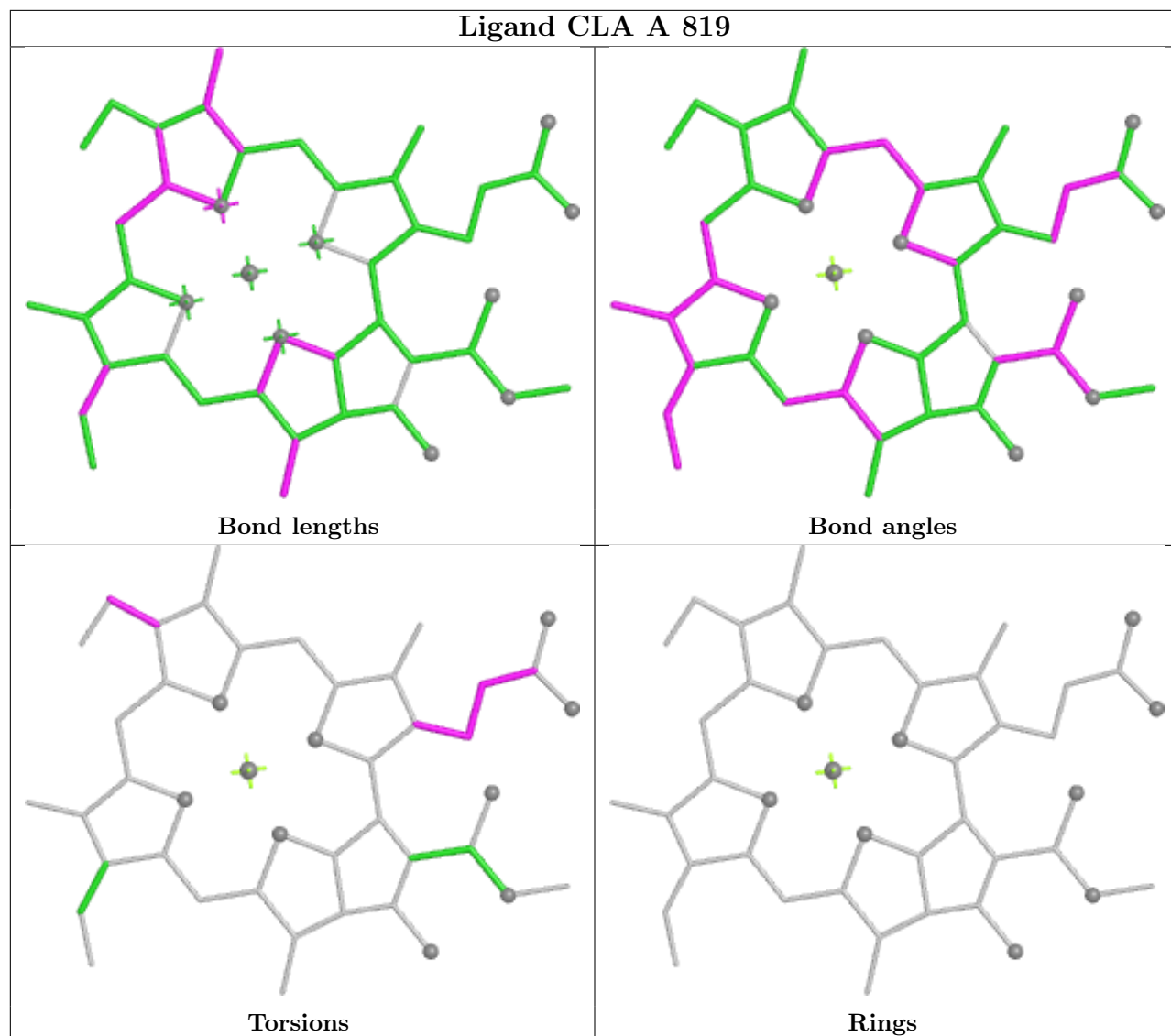
Ligand CLA j 307



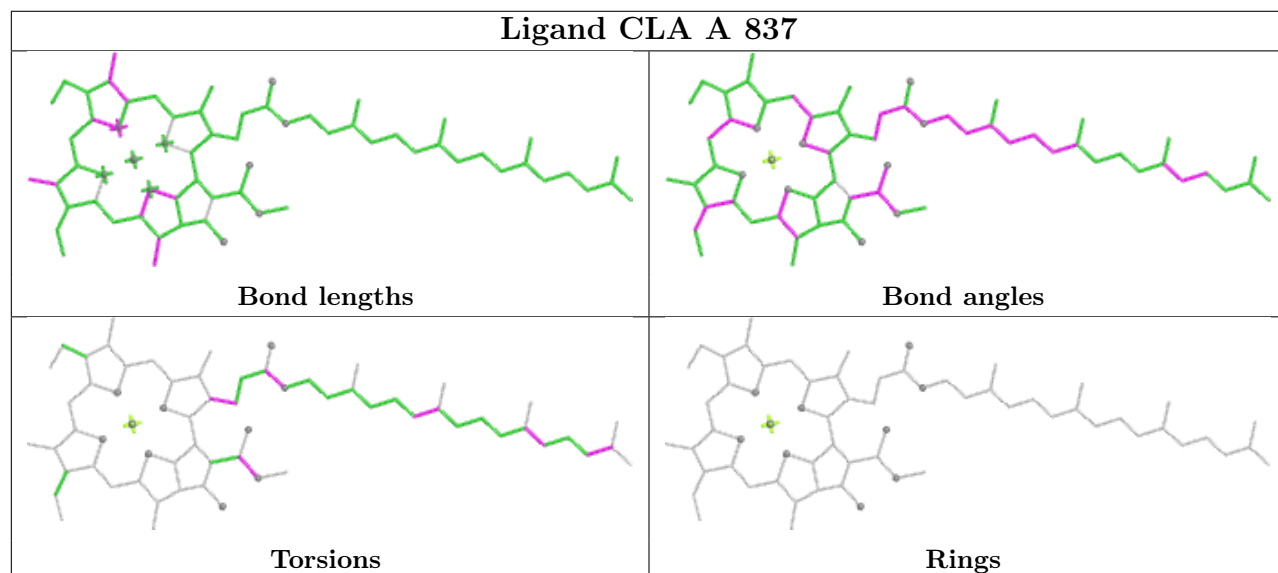
Ligand WVN A 849



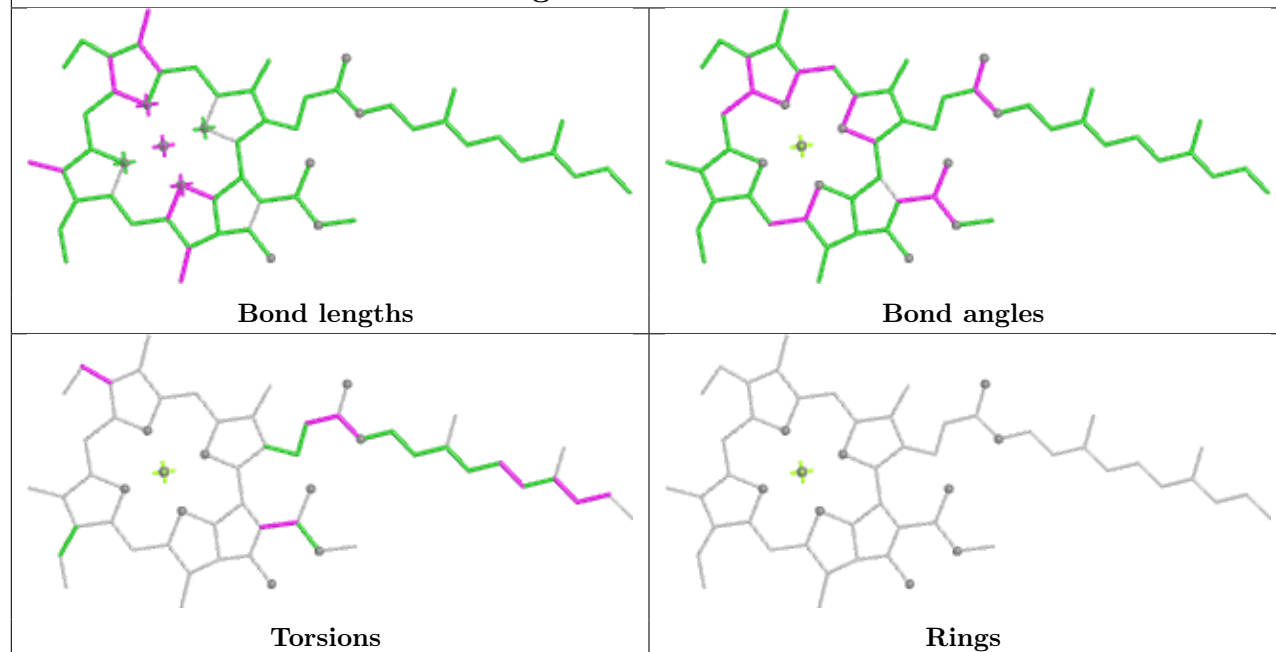
Ligand CLA A 819



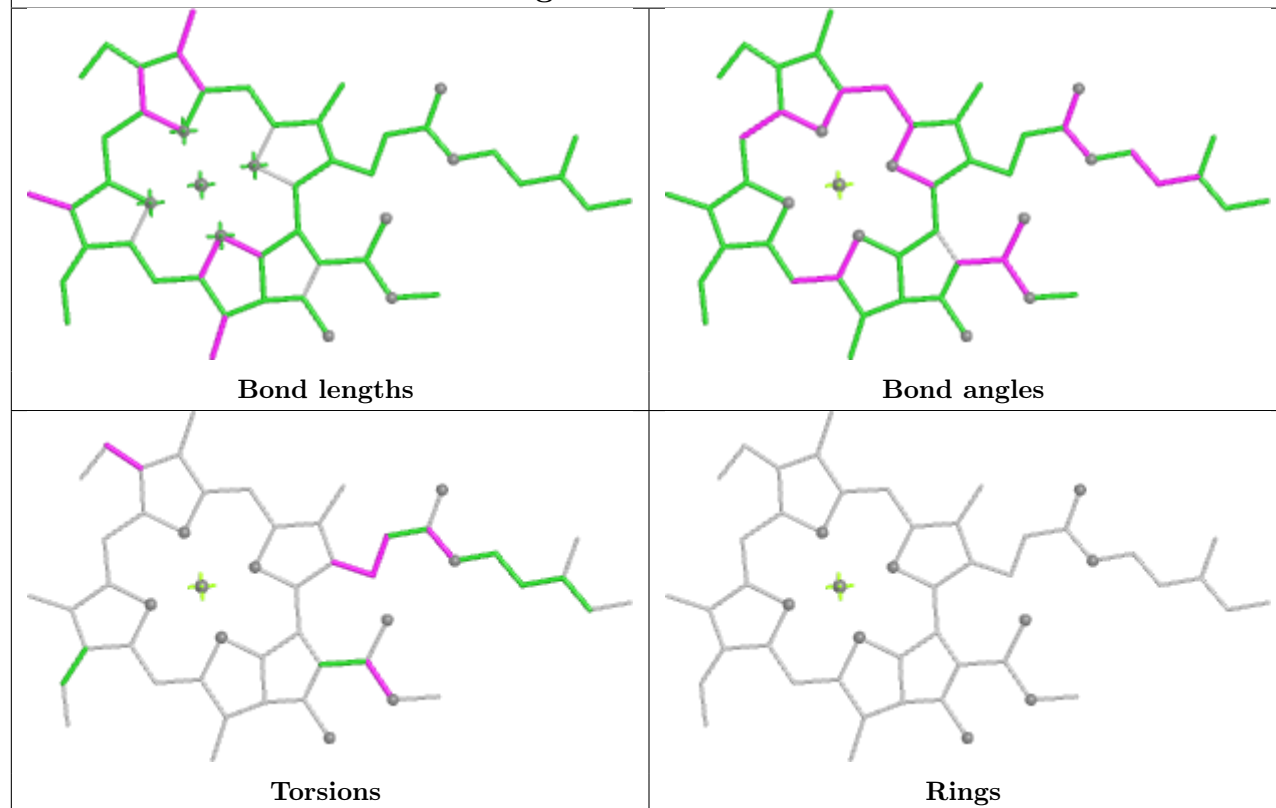
Ligand CLA A 837

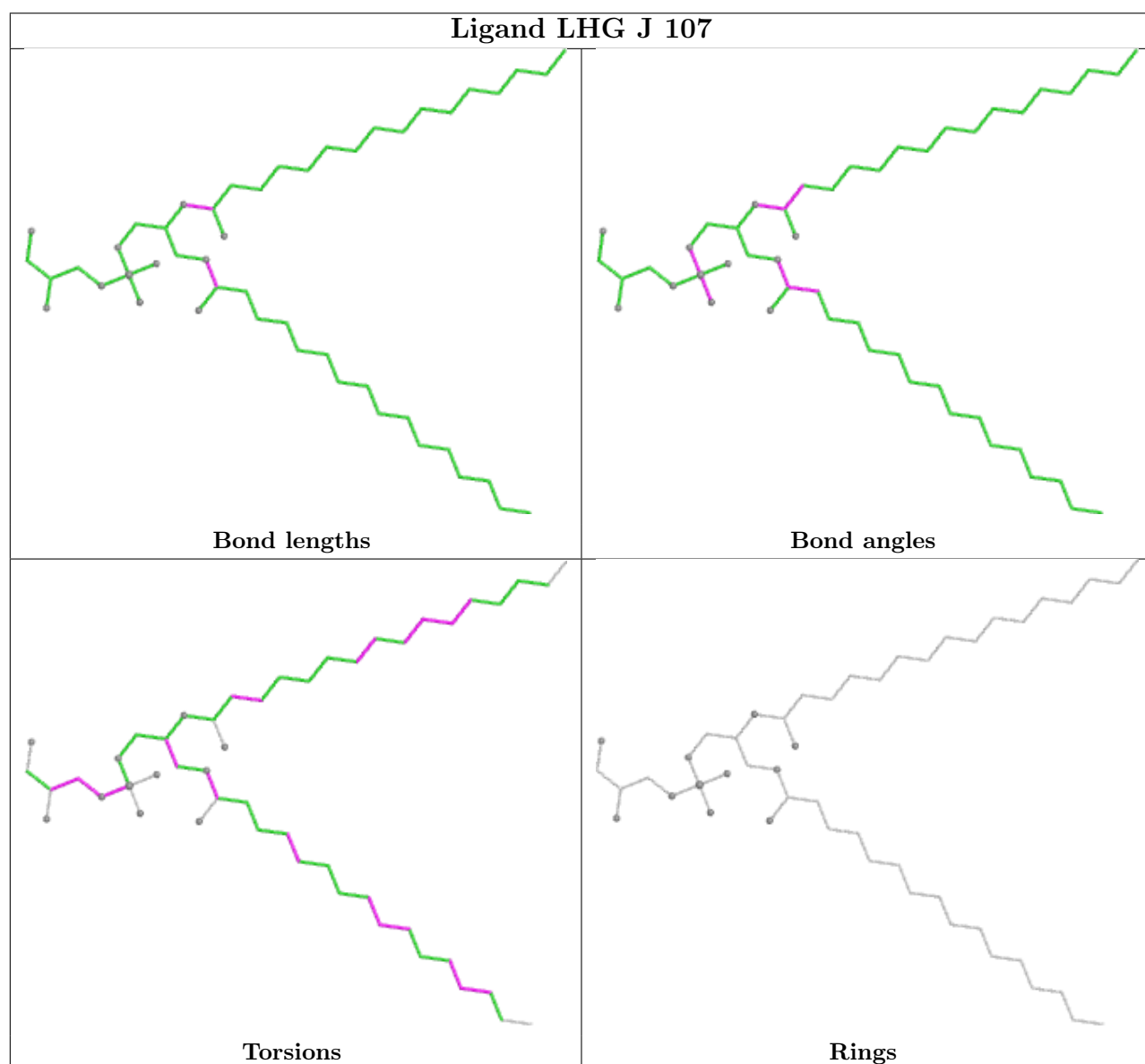
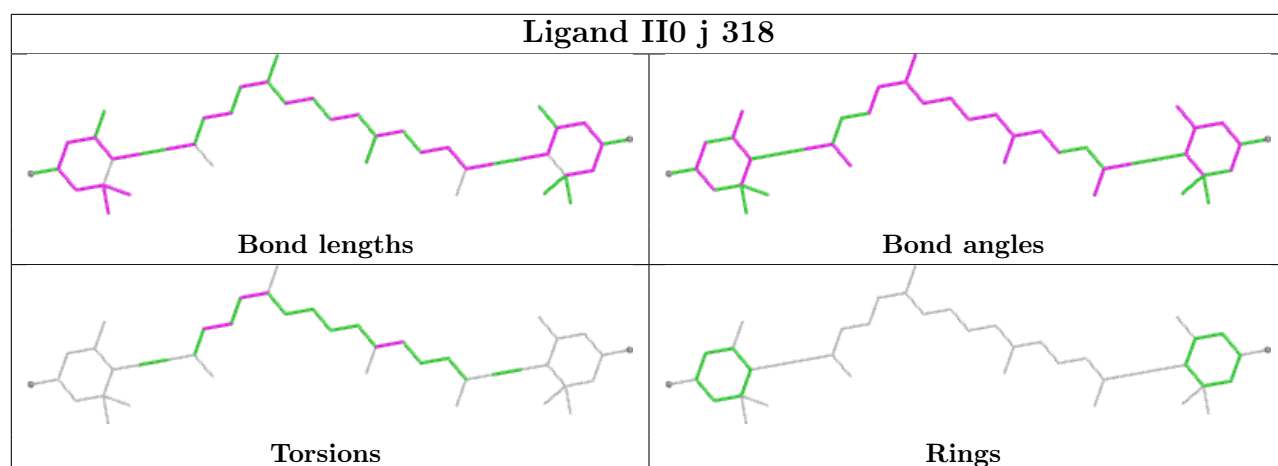


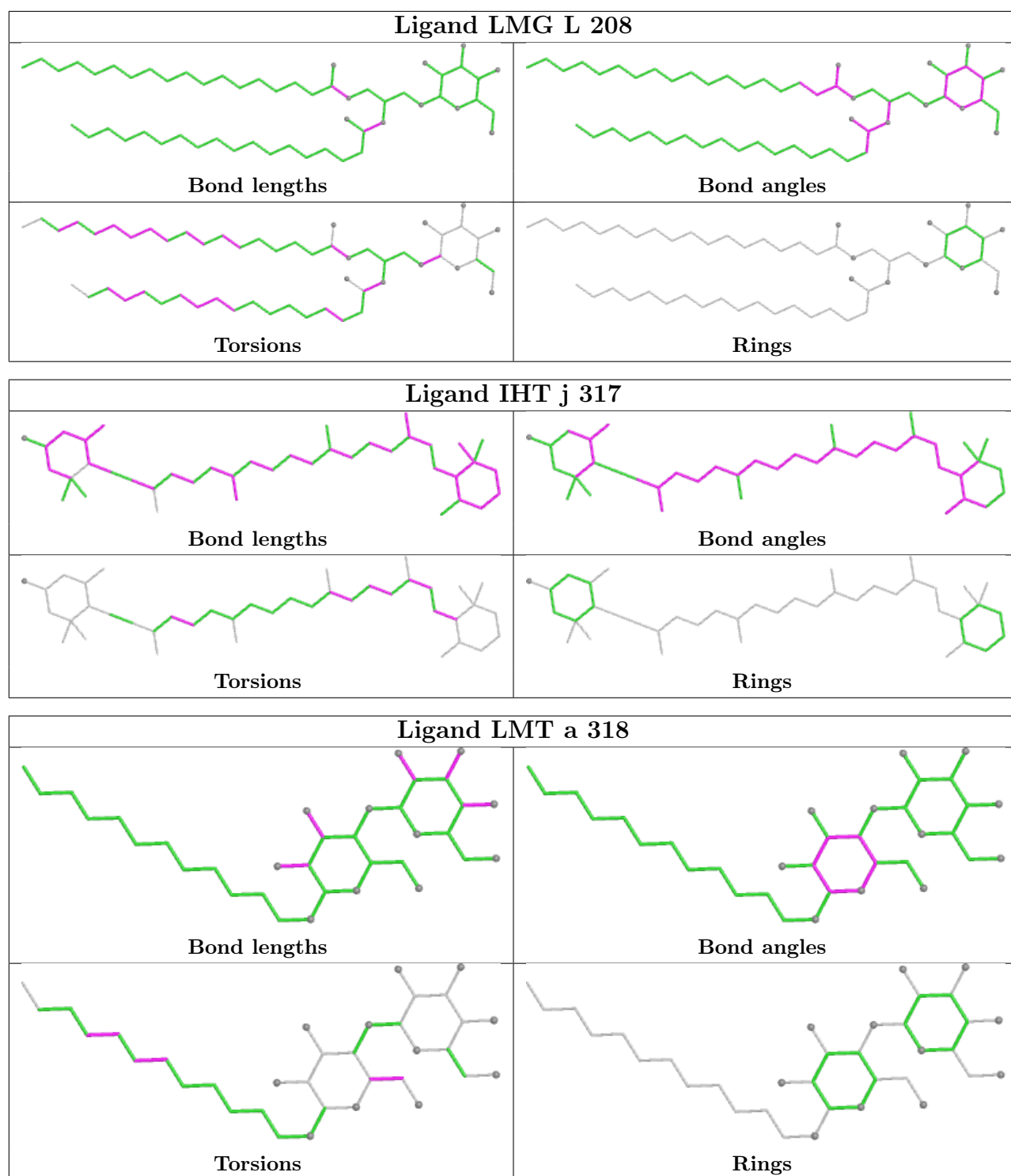
Ligand CLA B 838



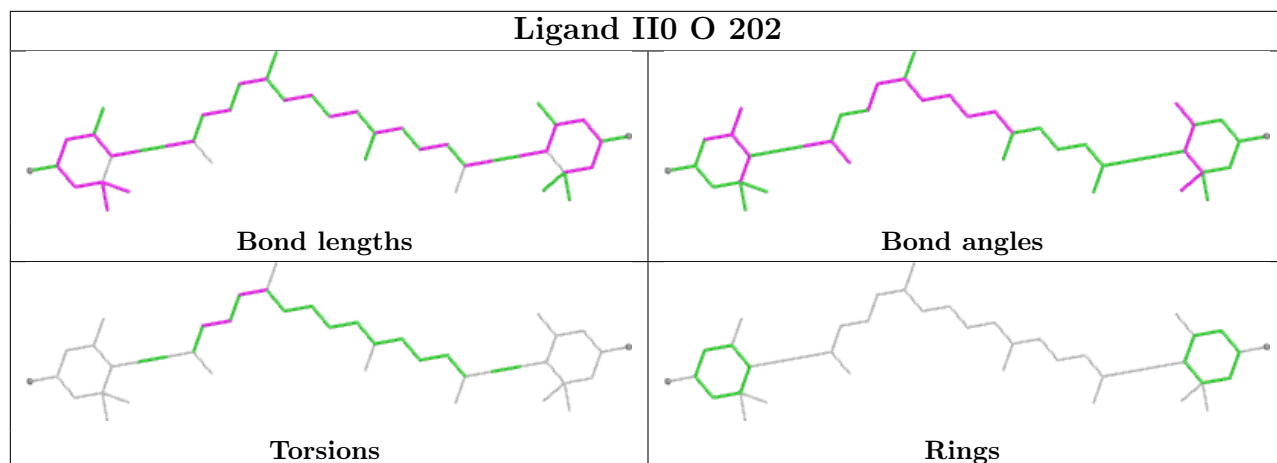
Ligand CLA k 607



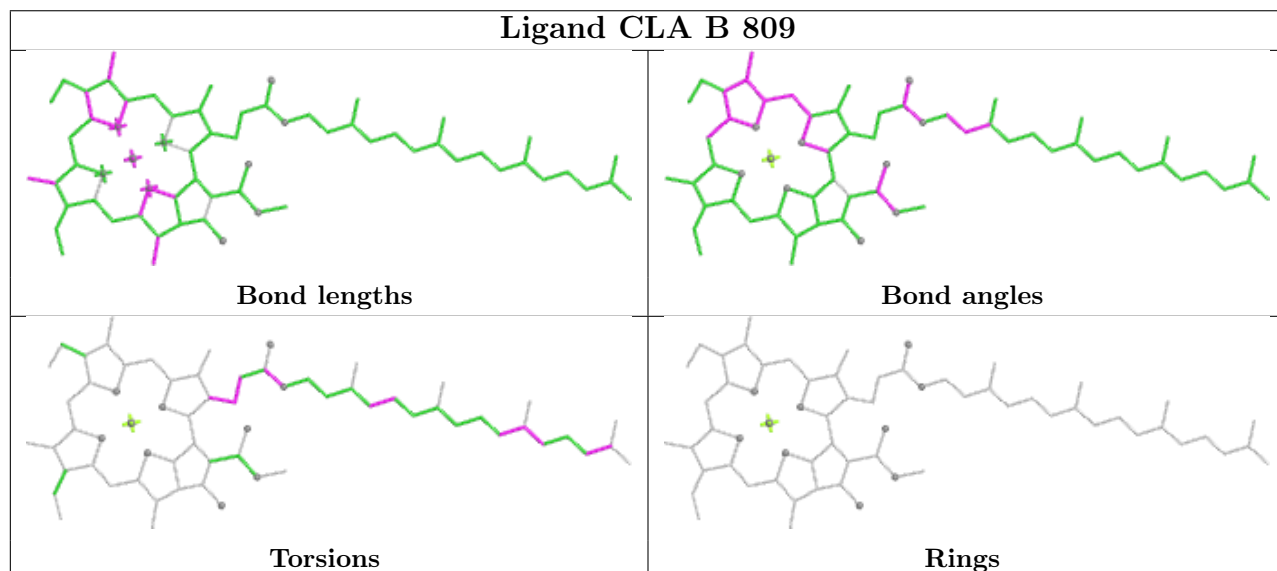




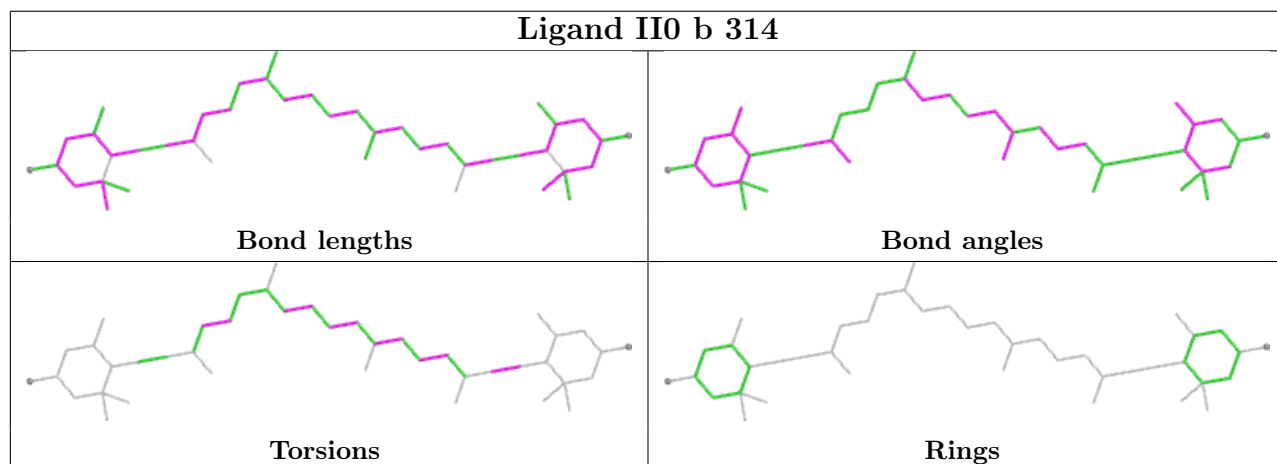
Ligand II0 O 202

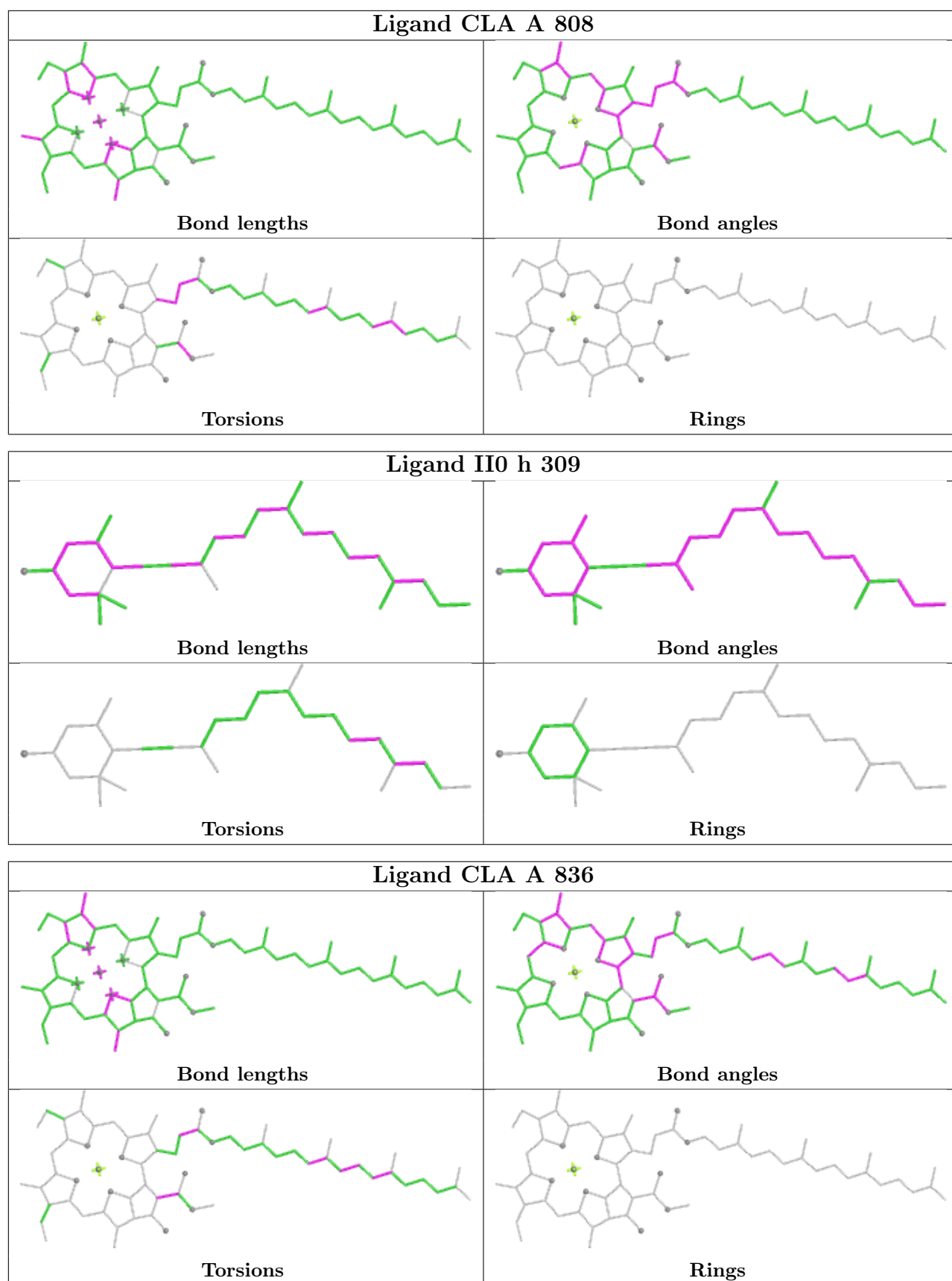


Ligand CLA B 809

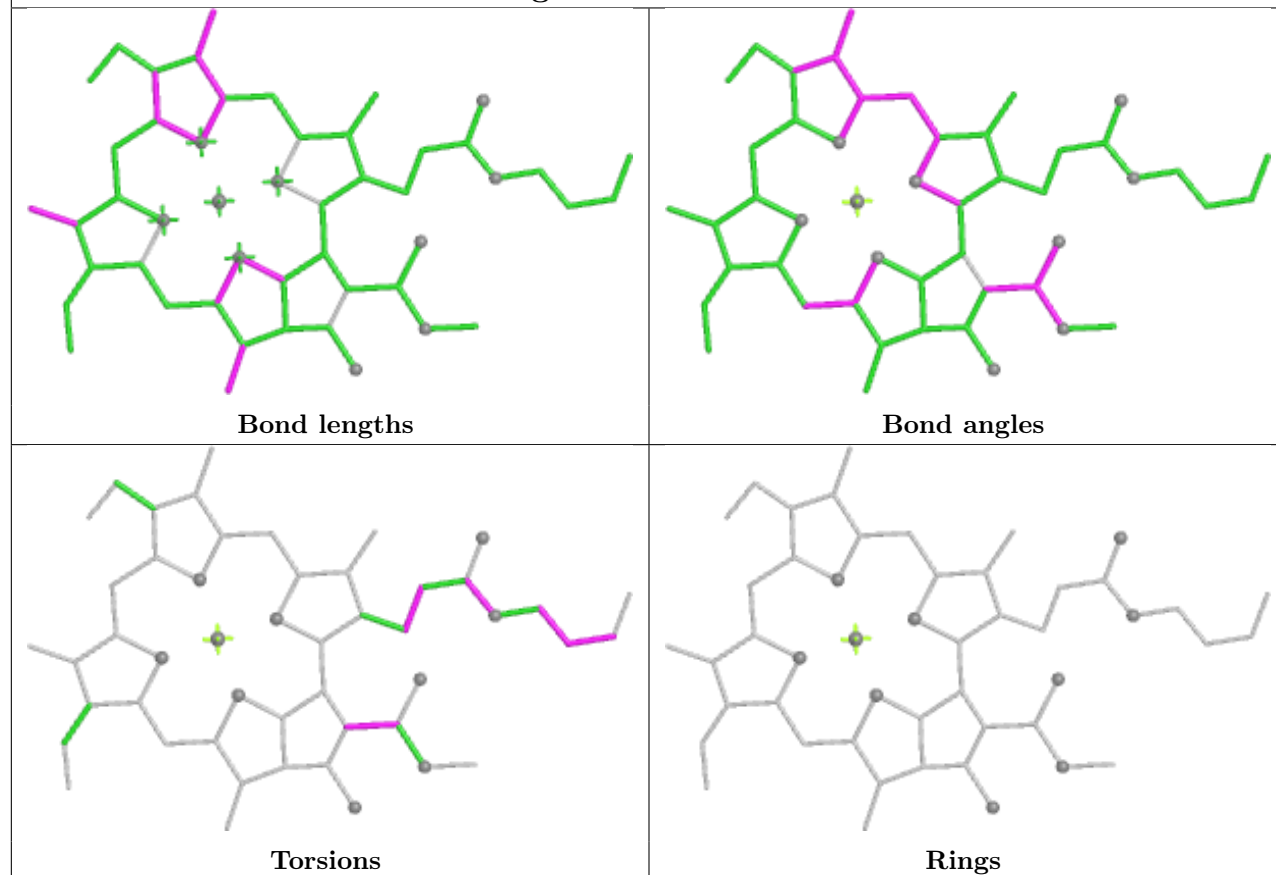


Ligand II0 b 314

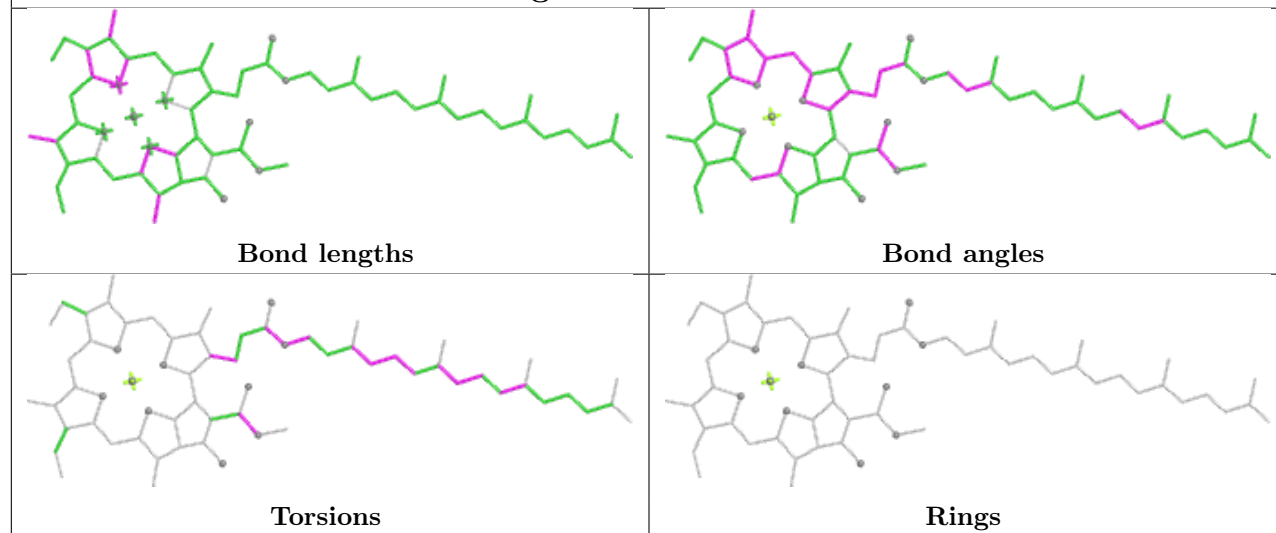




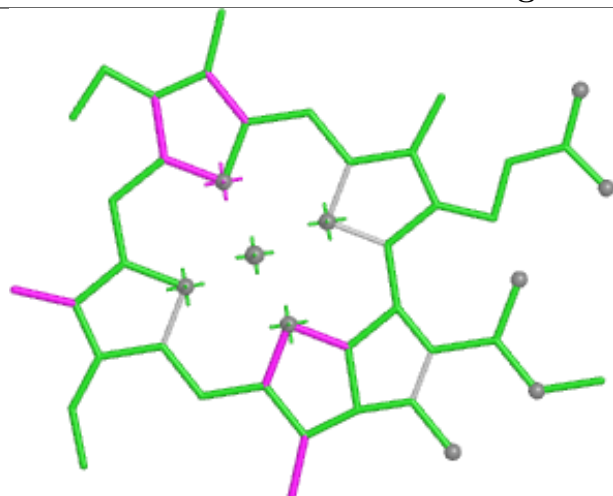
Ligand CLA A 821



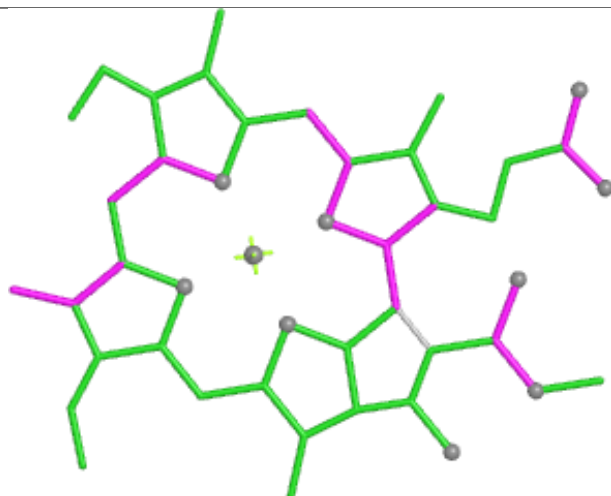
Ligand CLA A 802



Ligand CLA k 605



Bond lengths



Bond angles

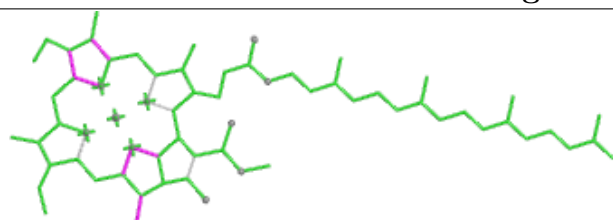


Torsions

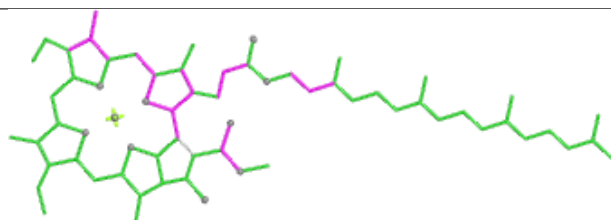


Rings

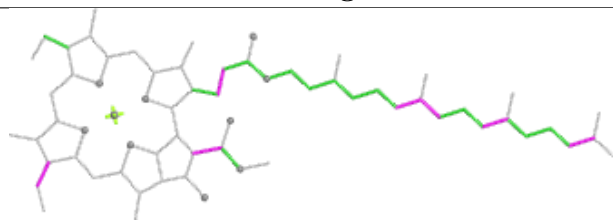
Ligand CLA i 604



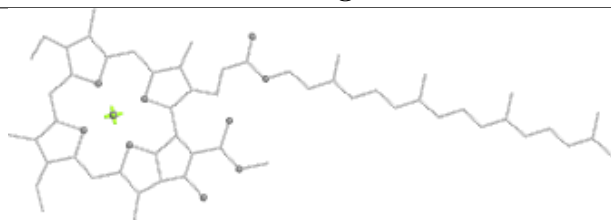
Bond lengths



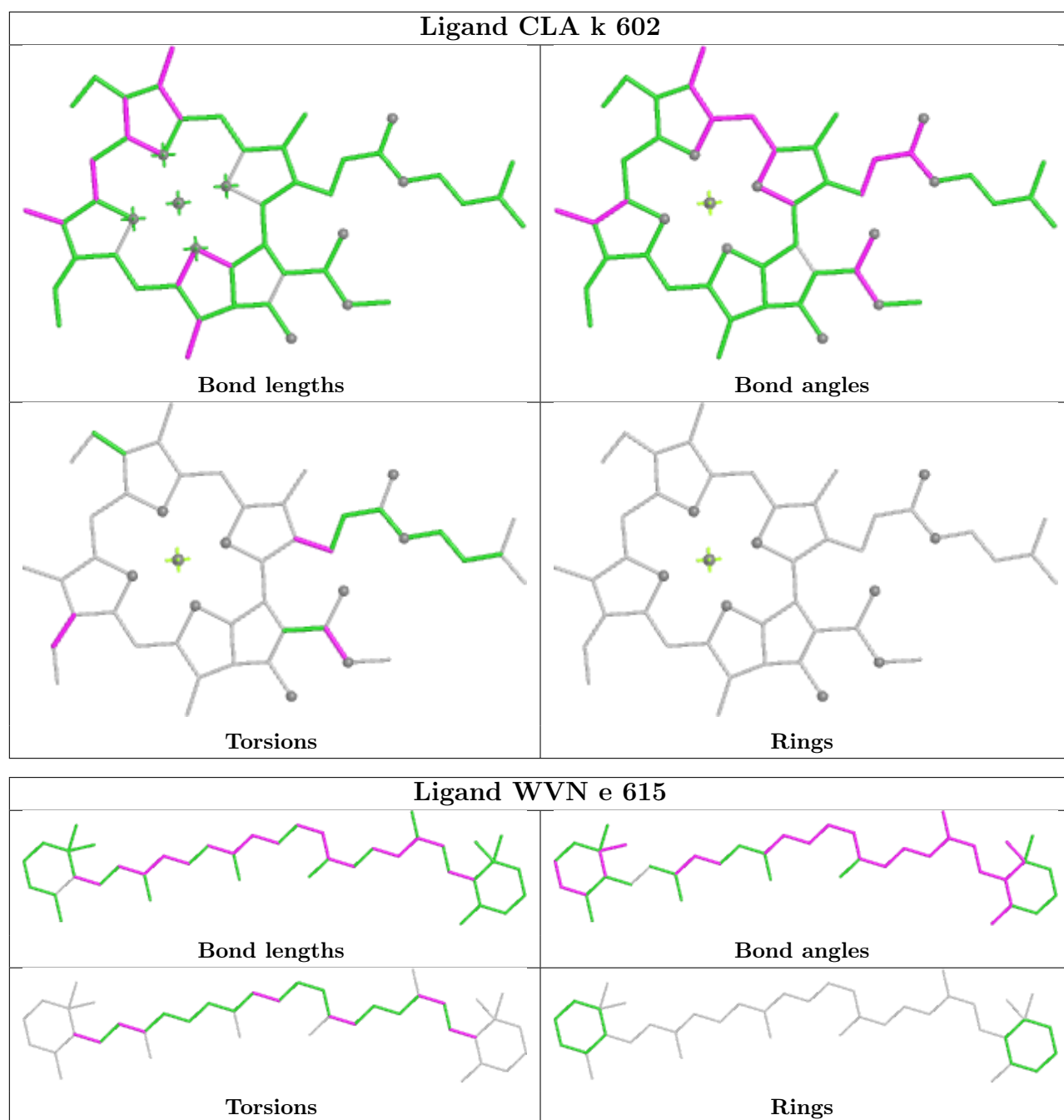
Bond angles



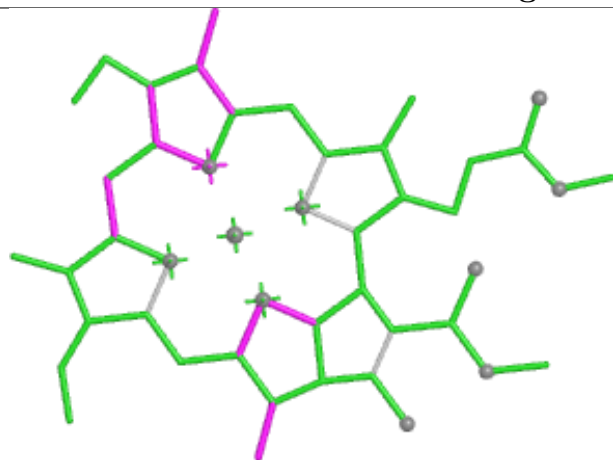
Torsions



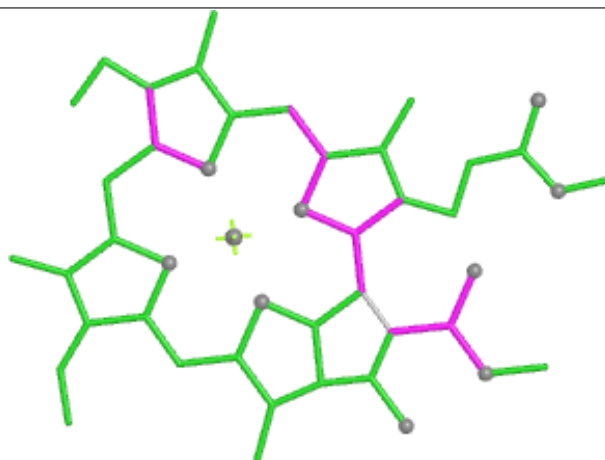
Rings



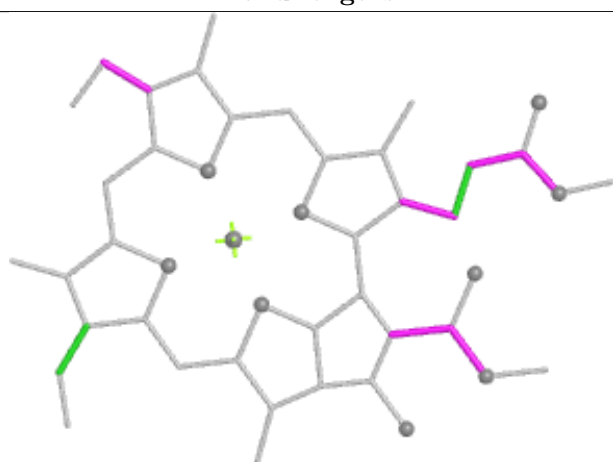
Ligand CLA e 608



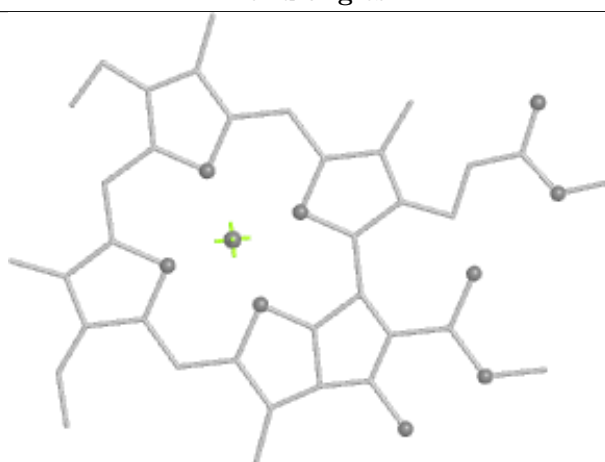
Bond lengths



Bond angles

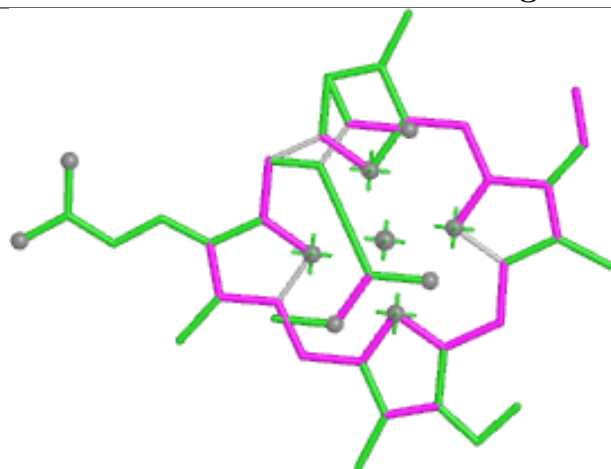


Torsions

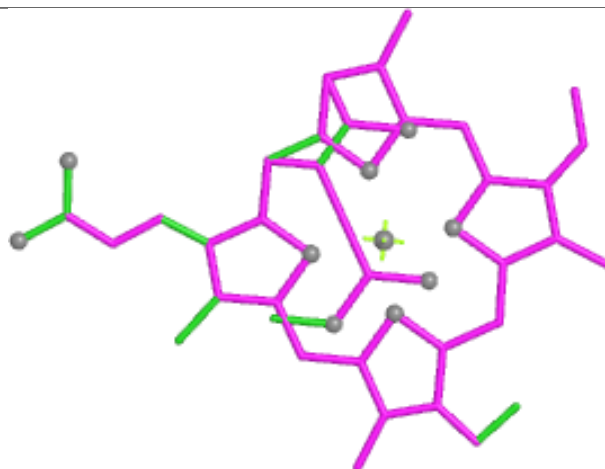


Rings

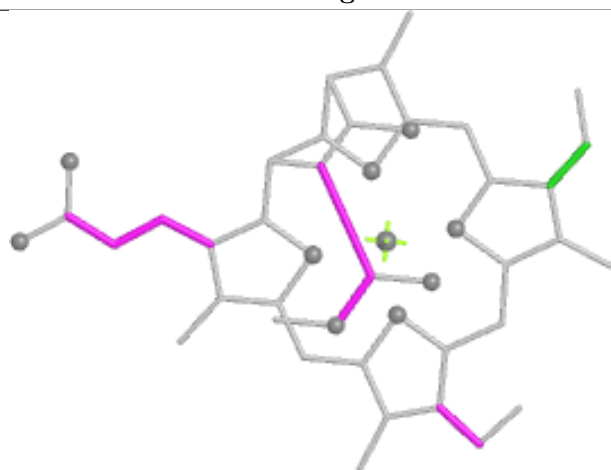
Ligand KC2 k 612



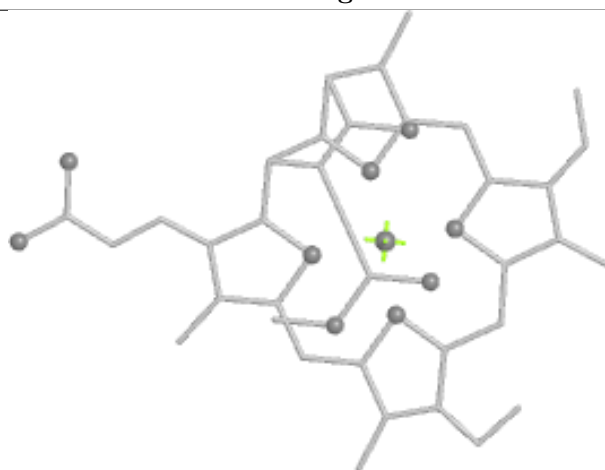
Bond lengths



Bond angles

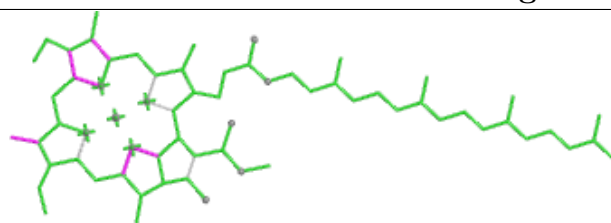


Torsions

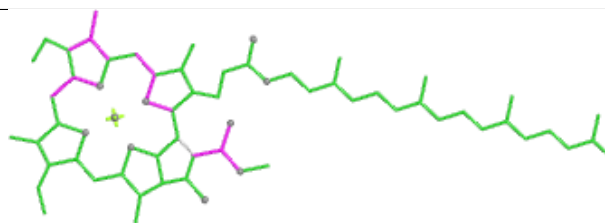


Rings

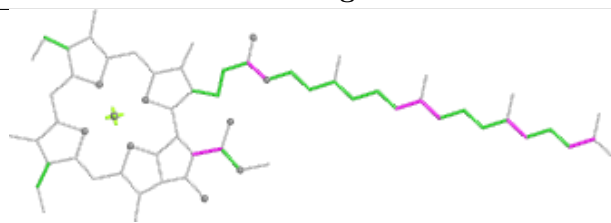
Ligand CLA e 606



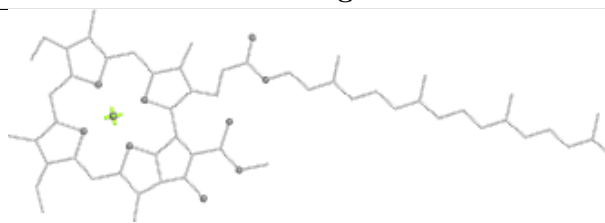
Bond lengths



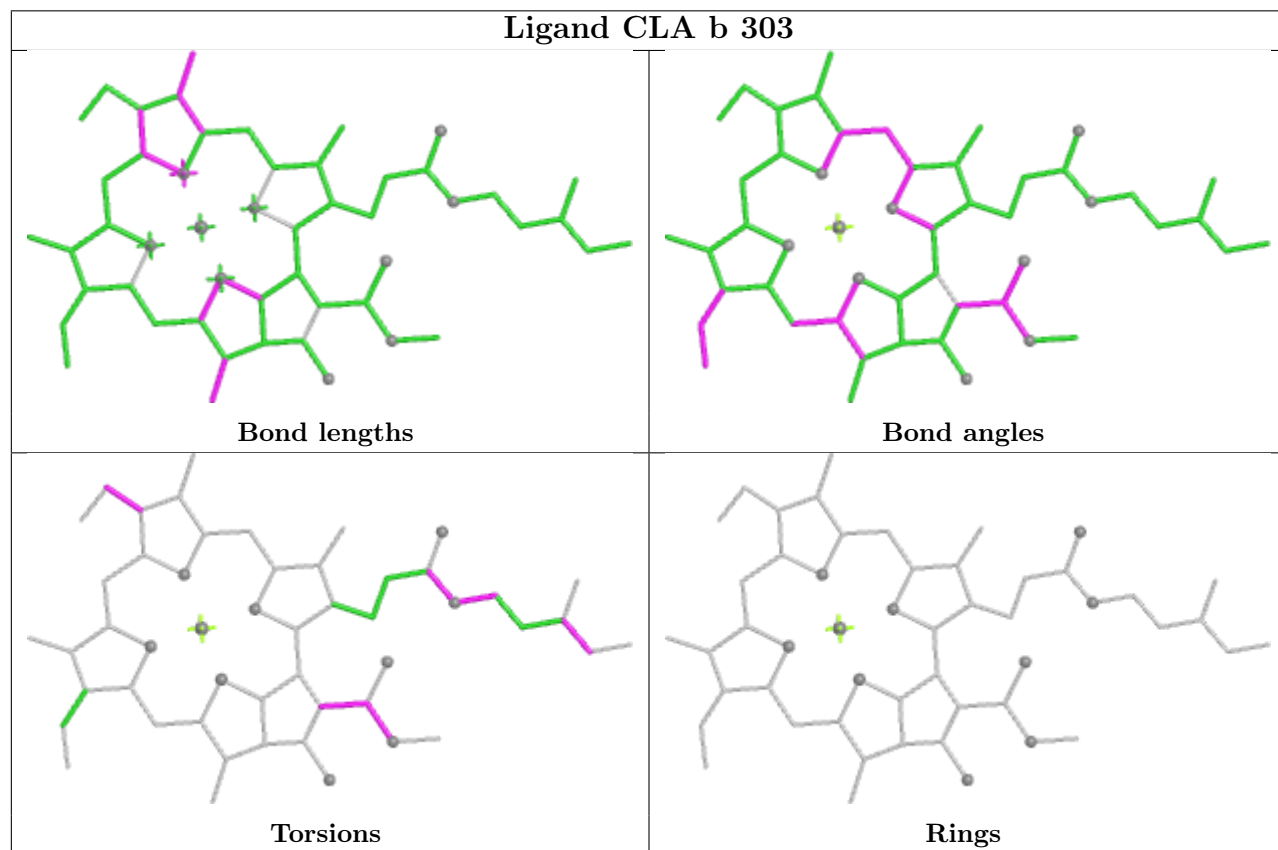
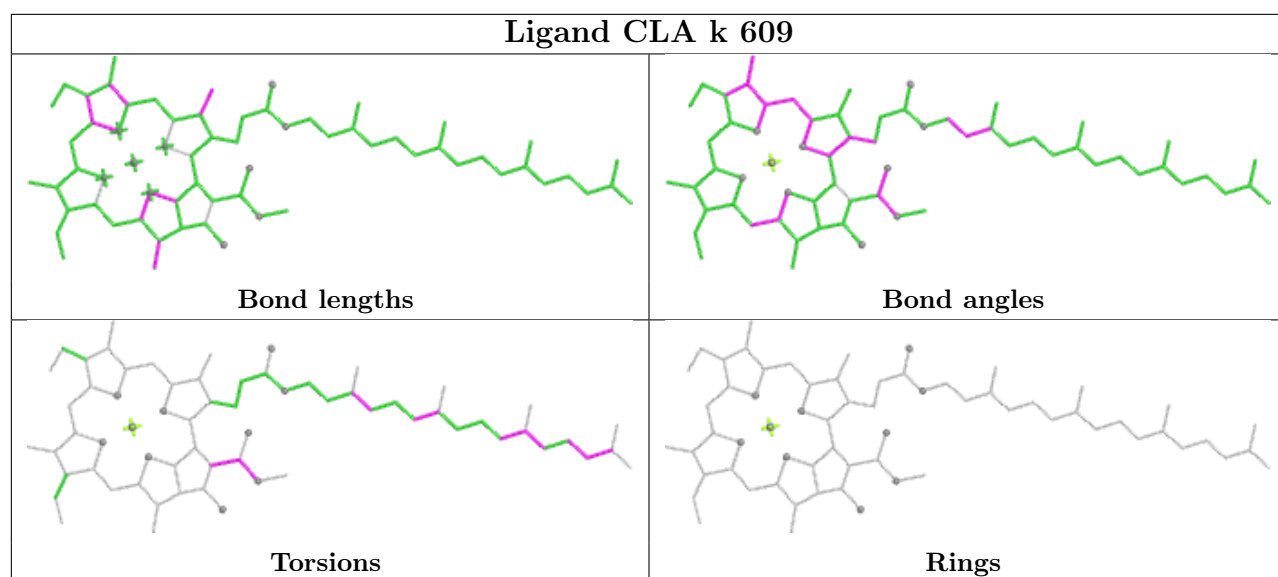
Bond angles

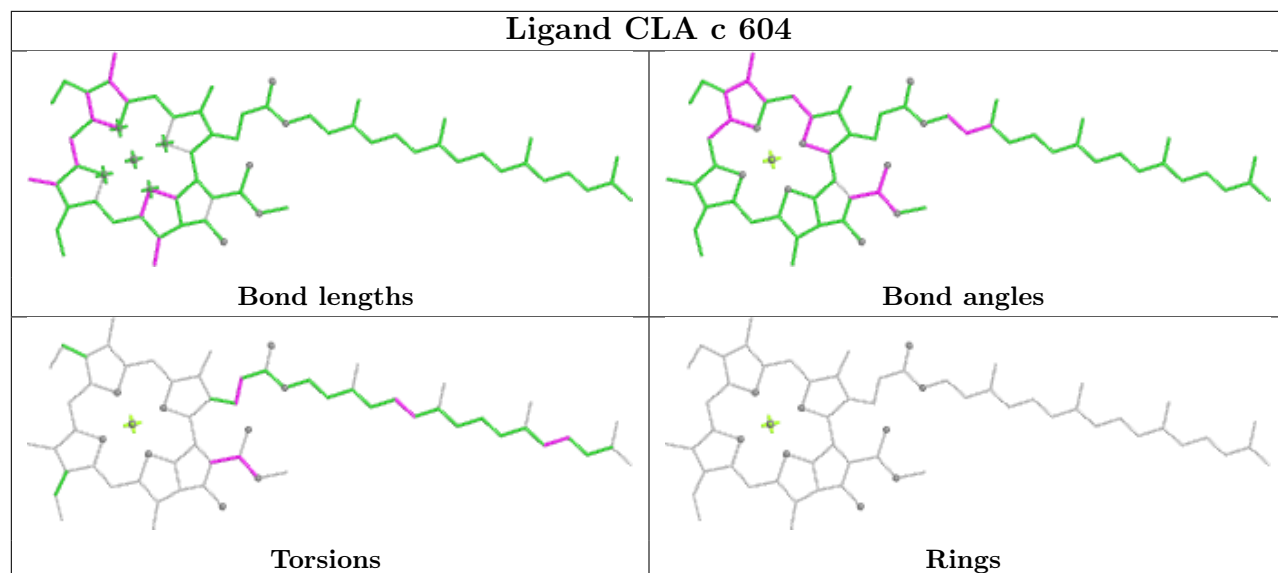
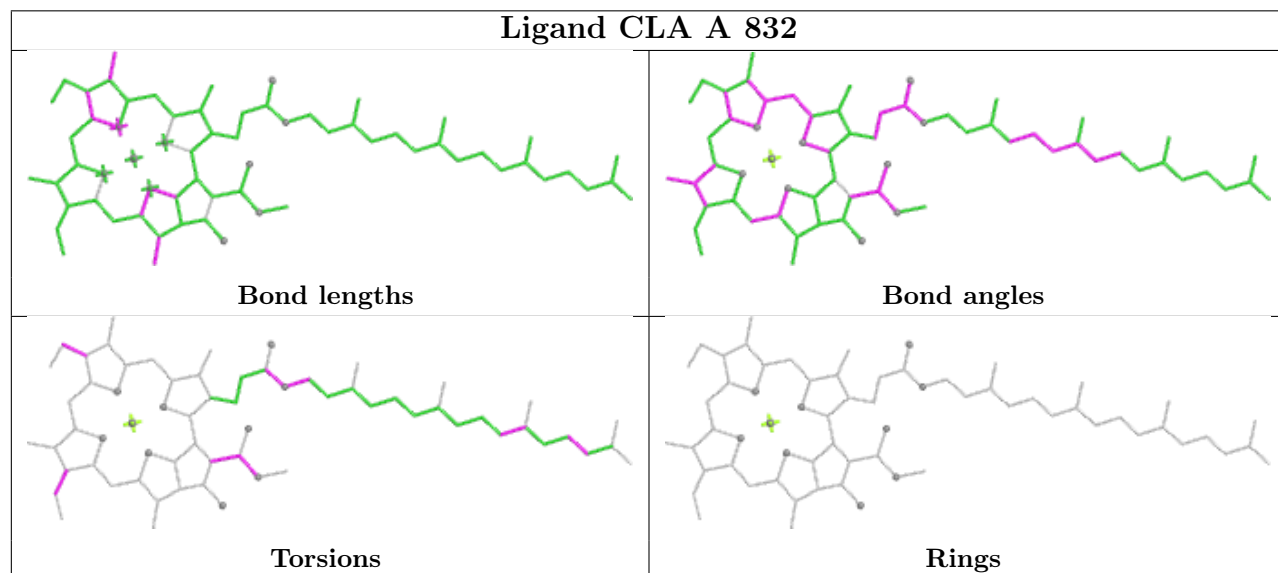
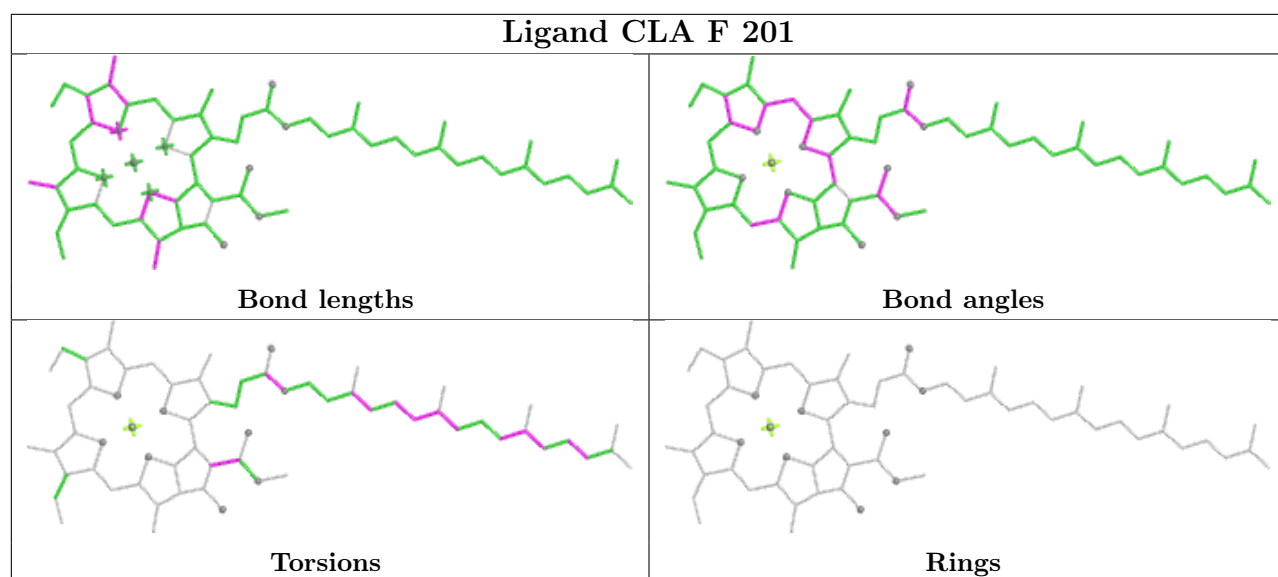


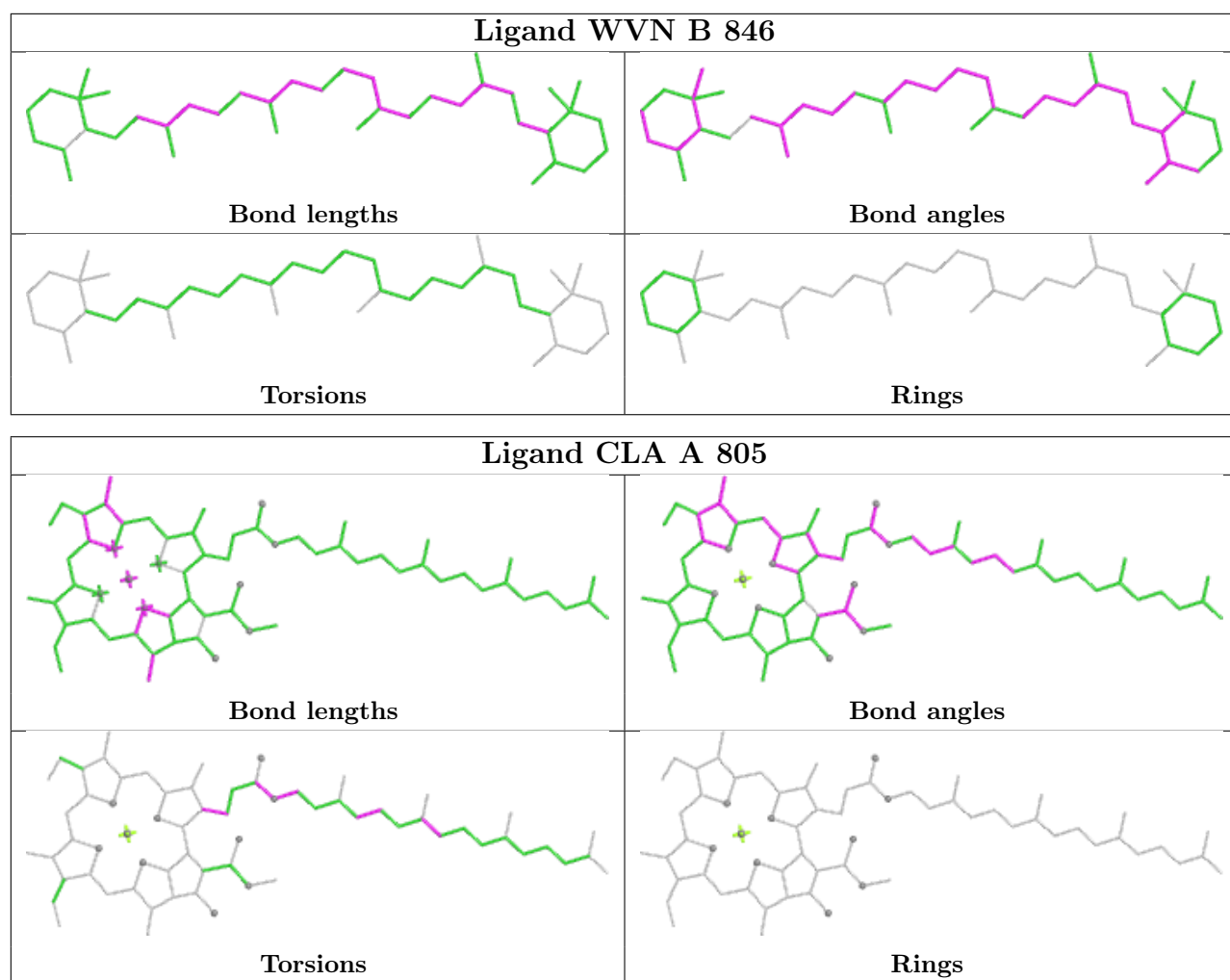
Torsions



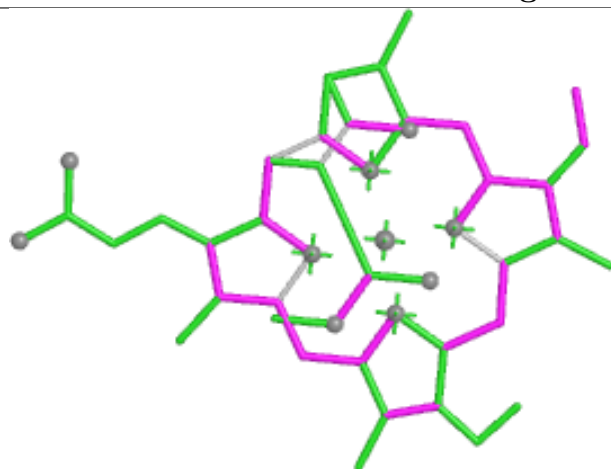
Rings



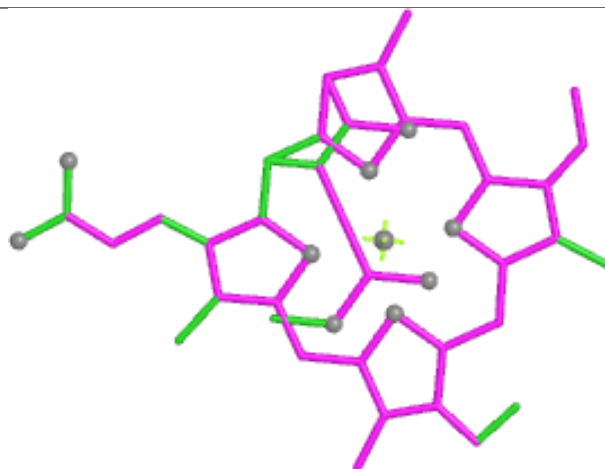




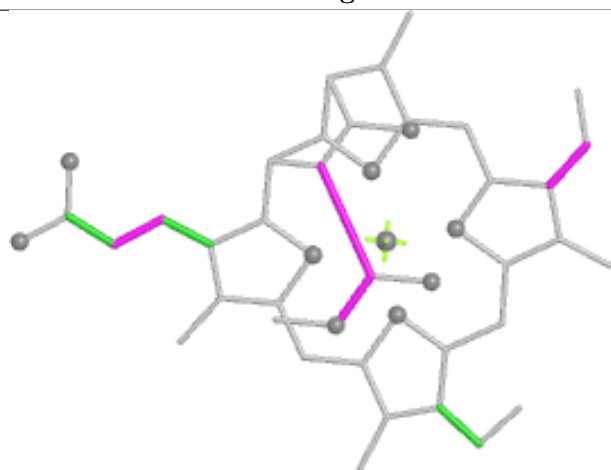
Ligand KC2 k 611



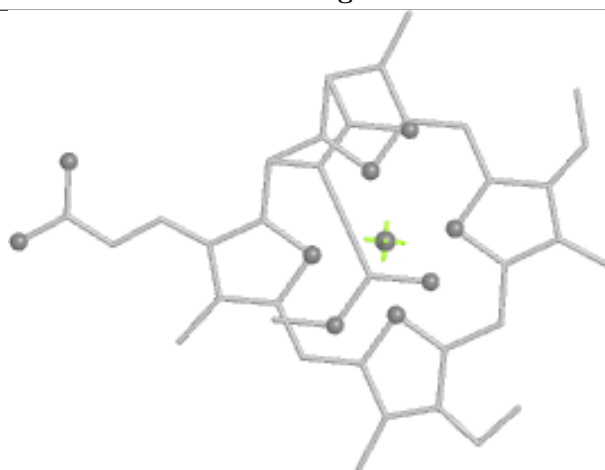
Bond lengths



Bond angles

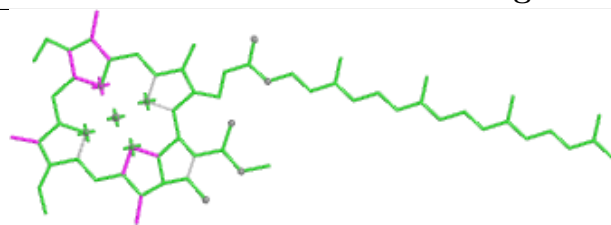


Torsions

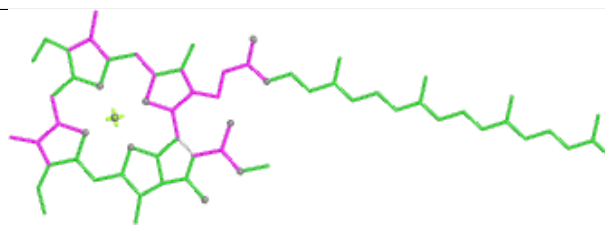


Rings

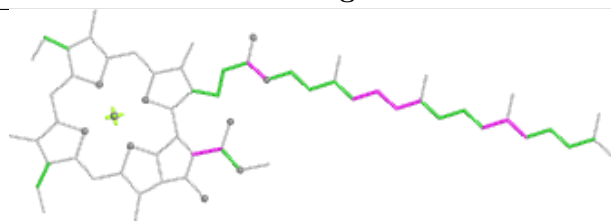
Ligand CLA A 826



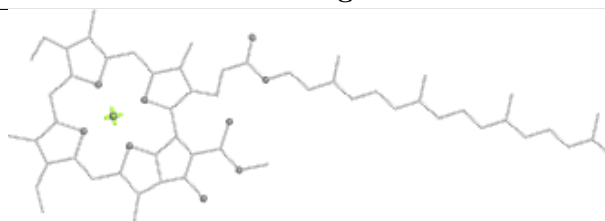
Bond lengths



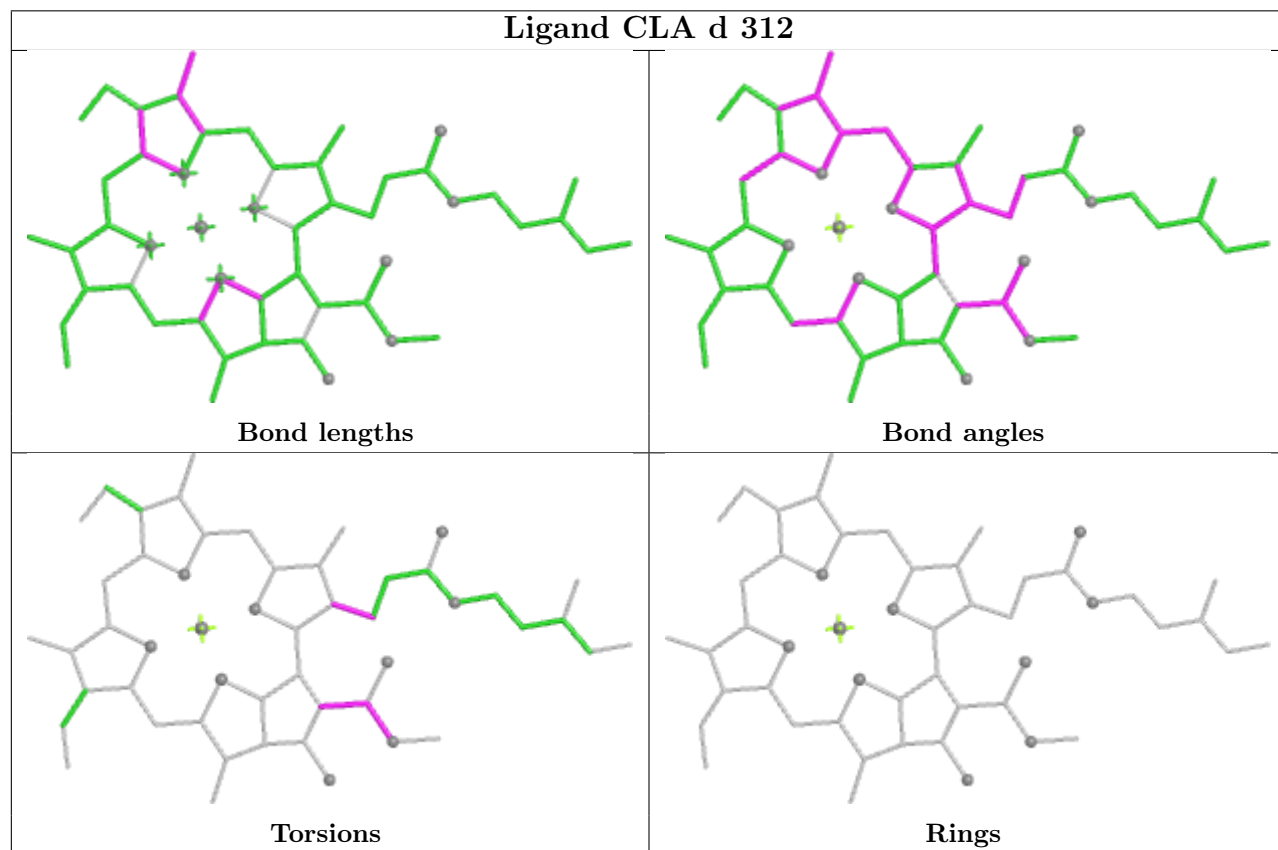
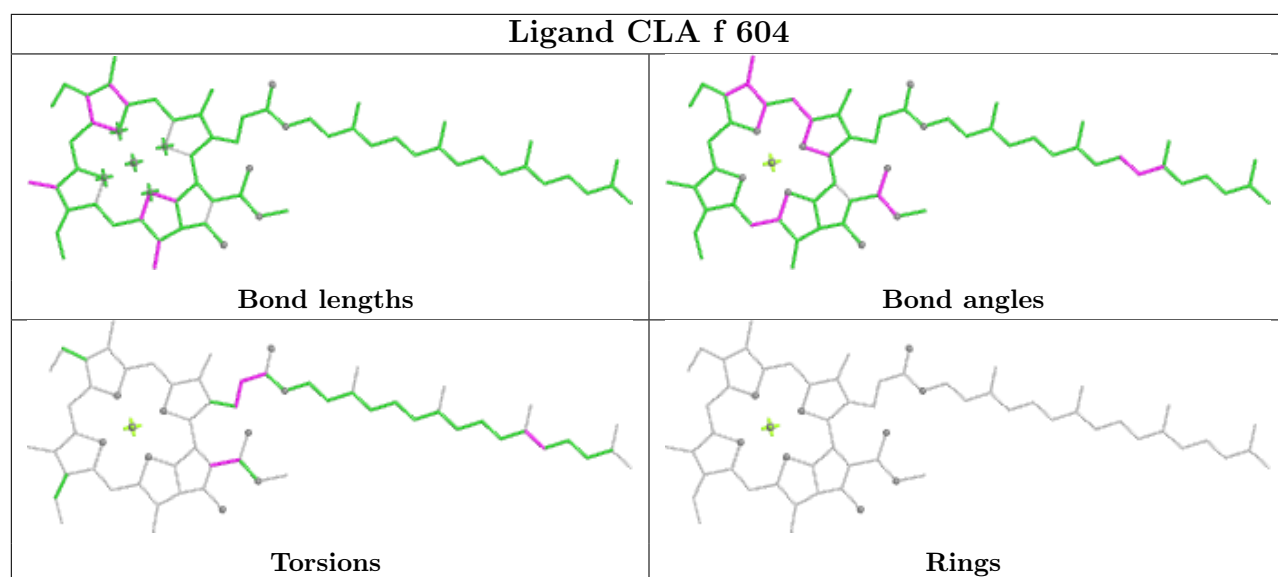
Bond angles

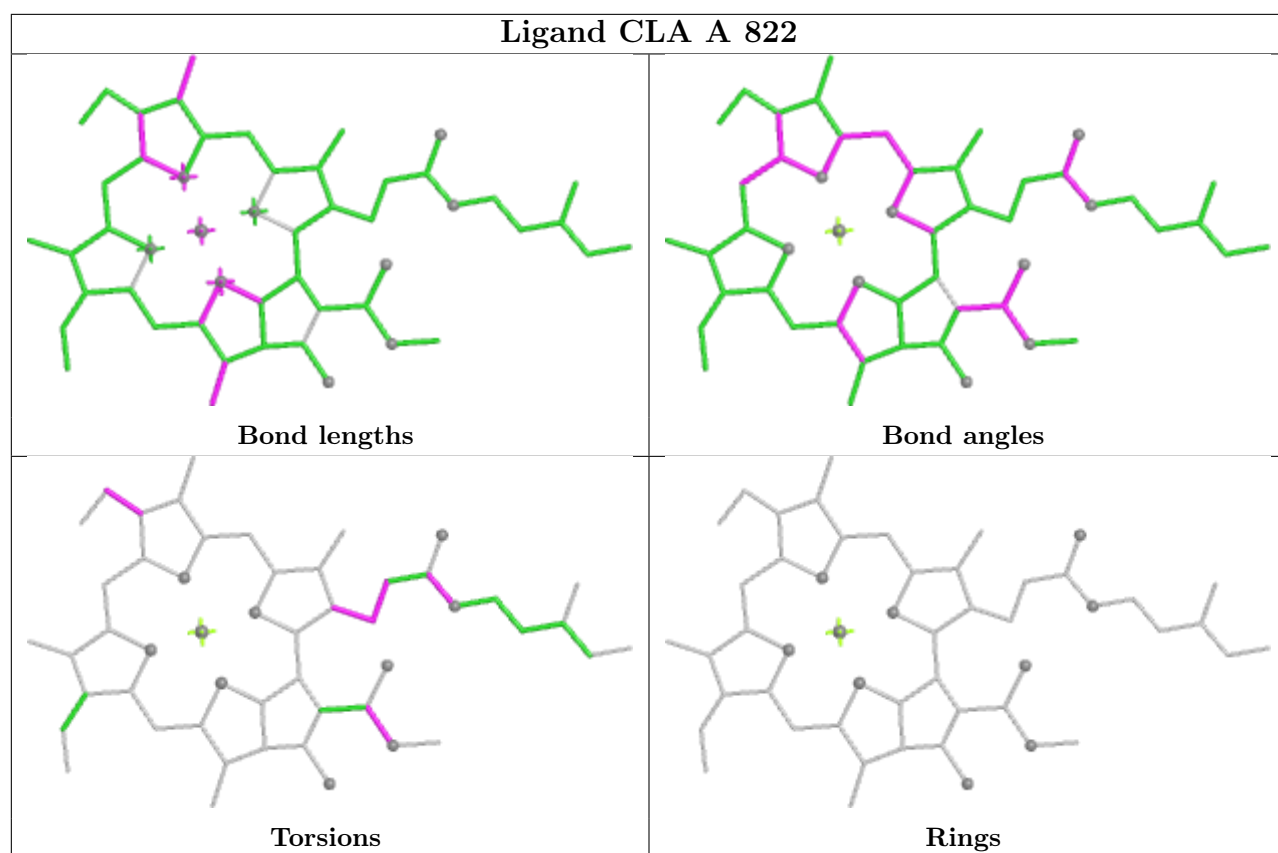


Torsions

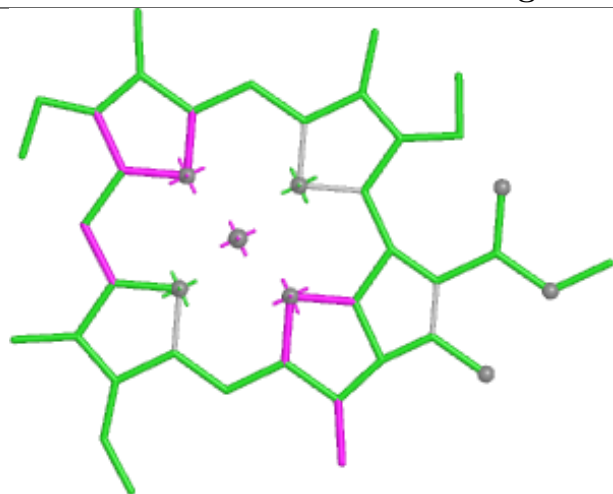


Rings

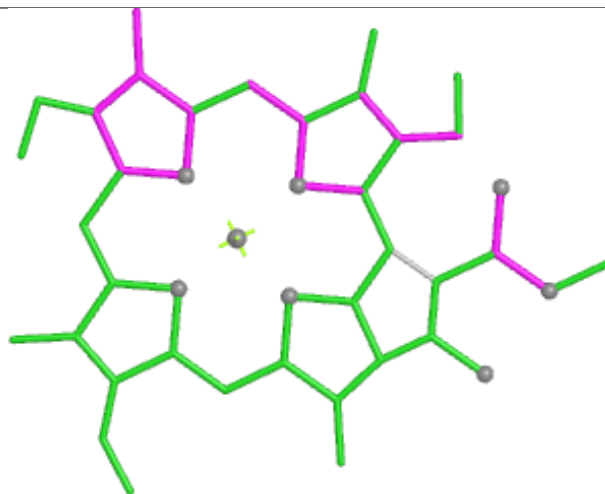




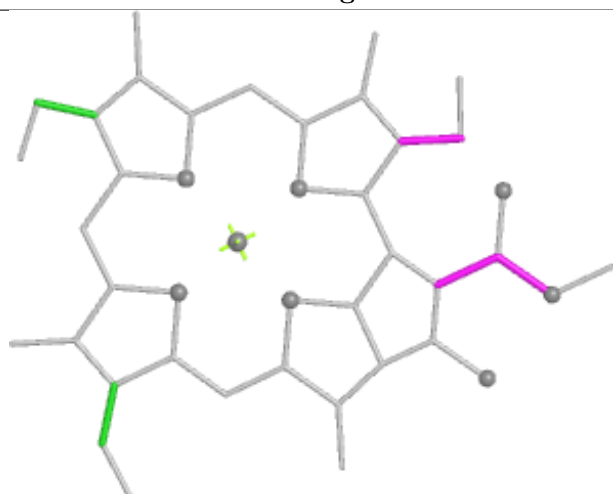
Ligand CLA J 103



Bond lengths



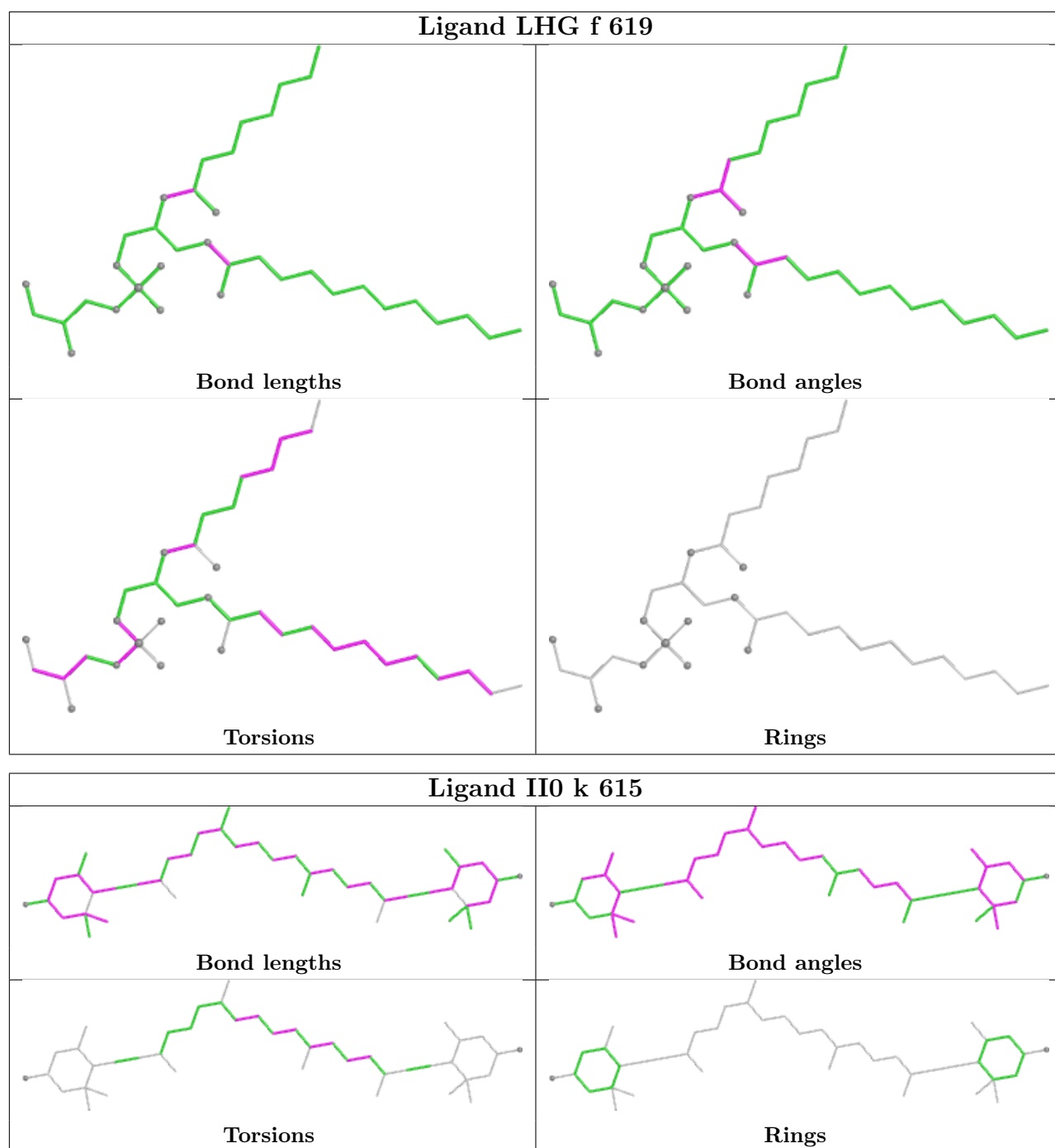
Bond angles

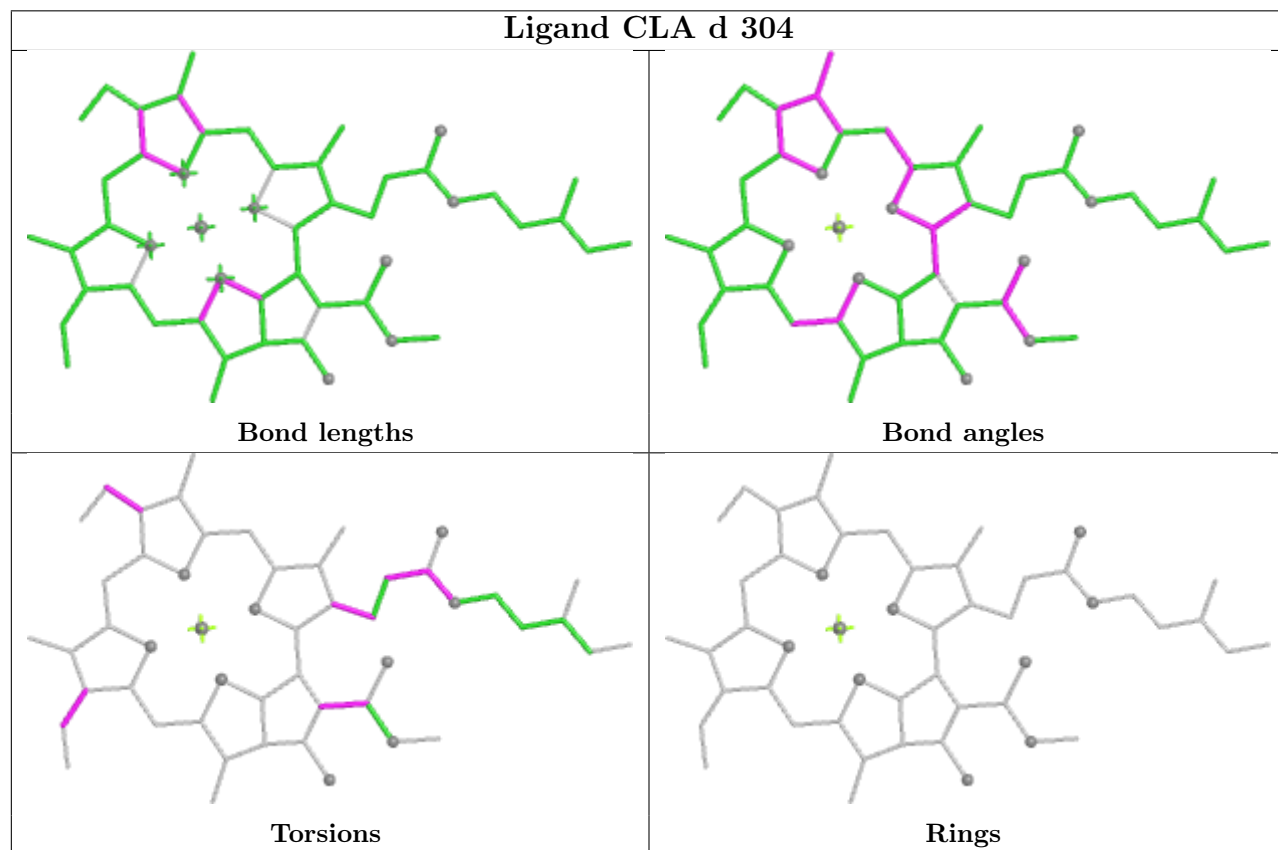
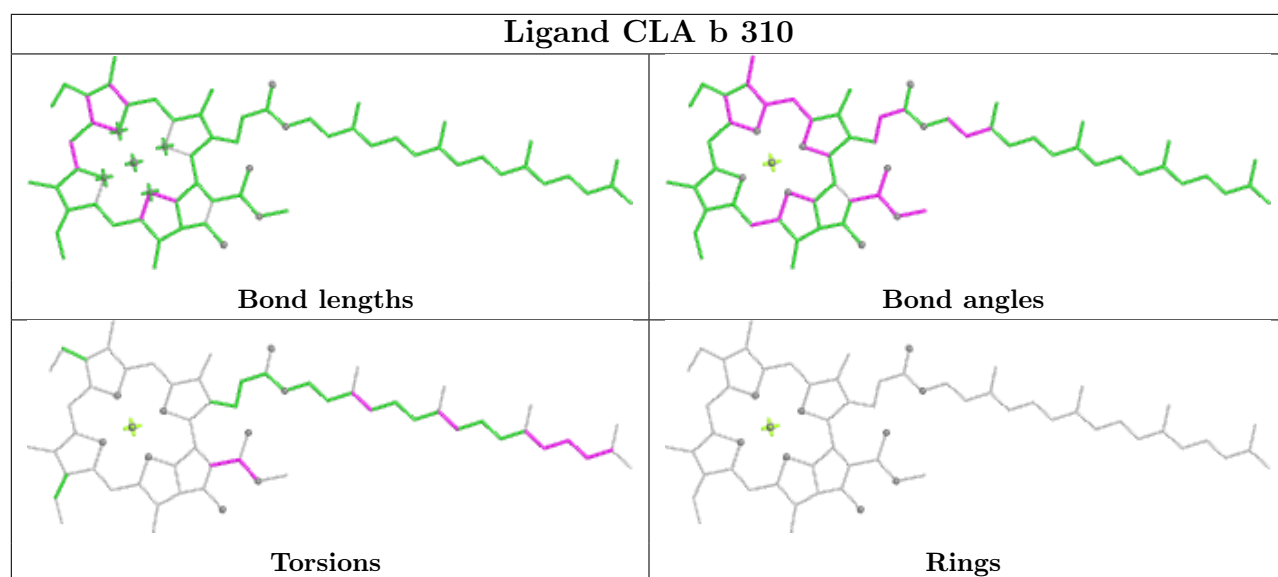


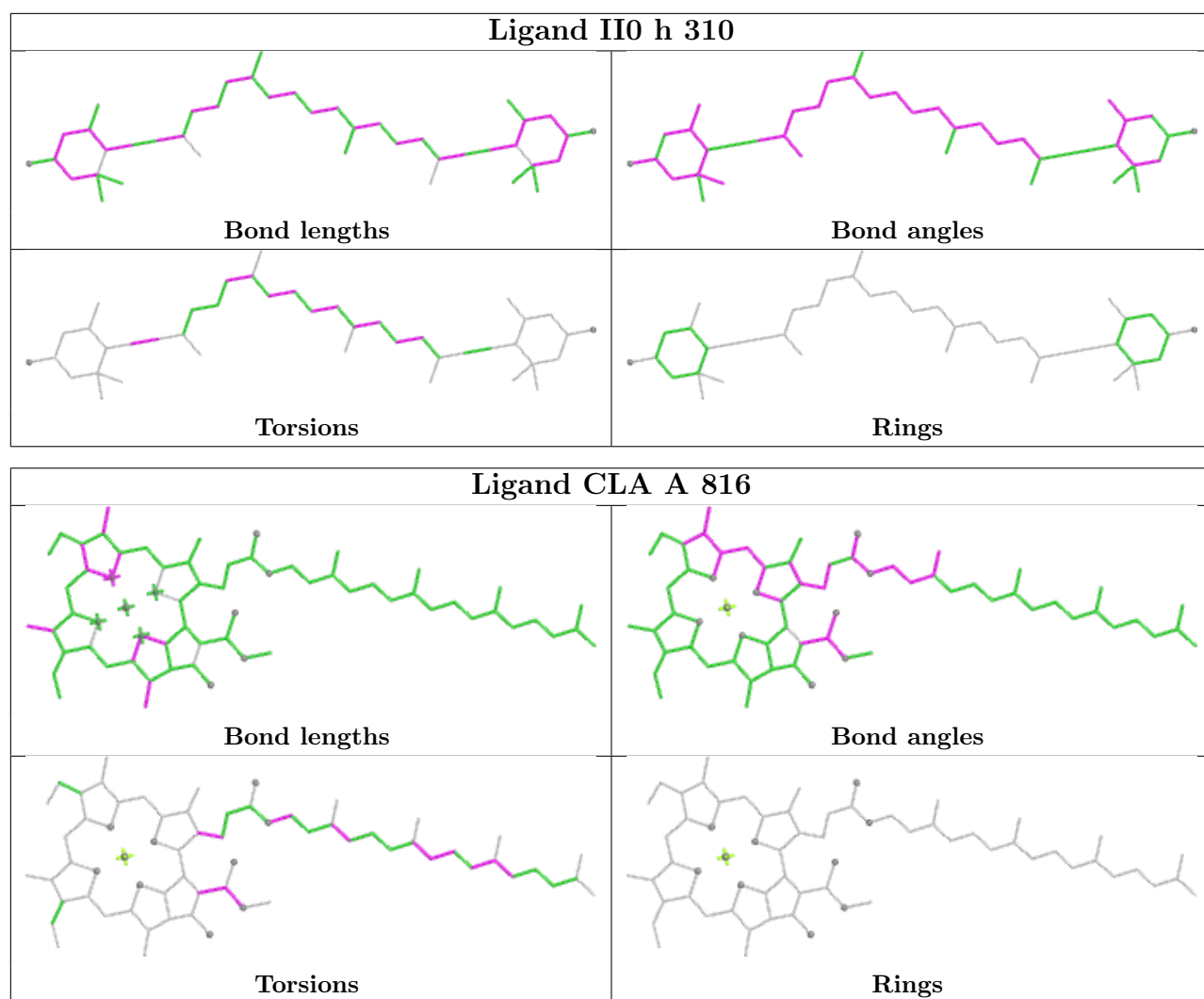
Torsions

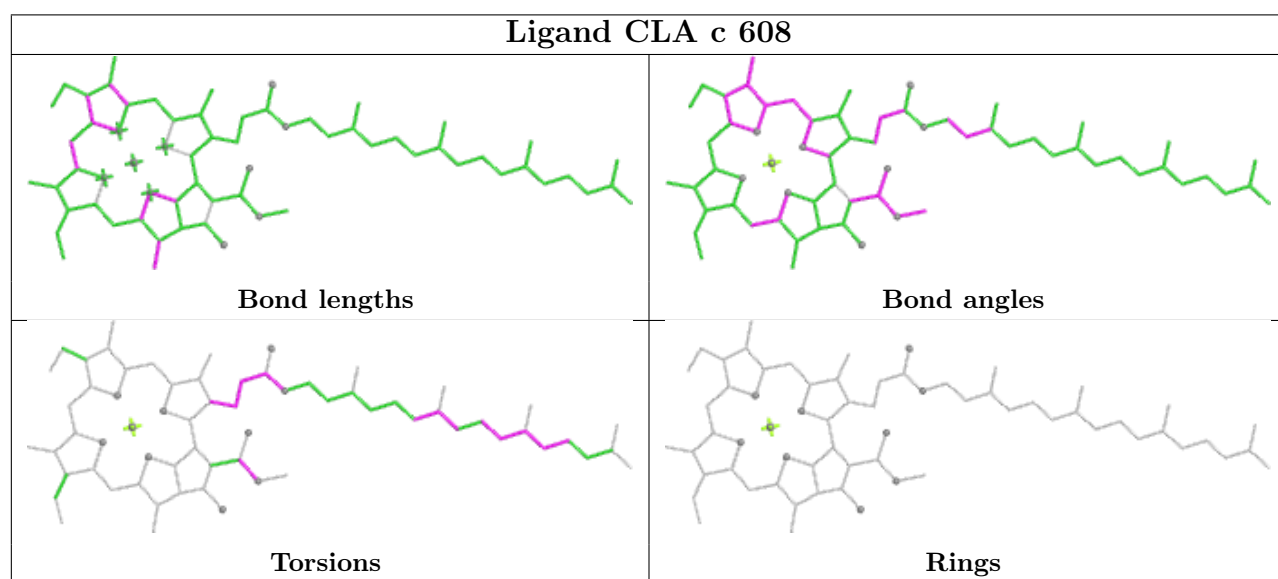
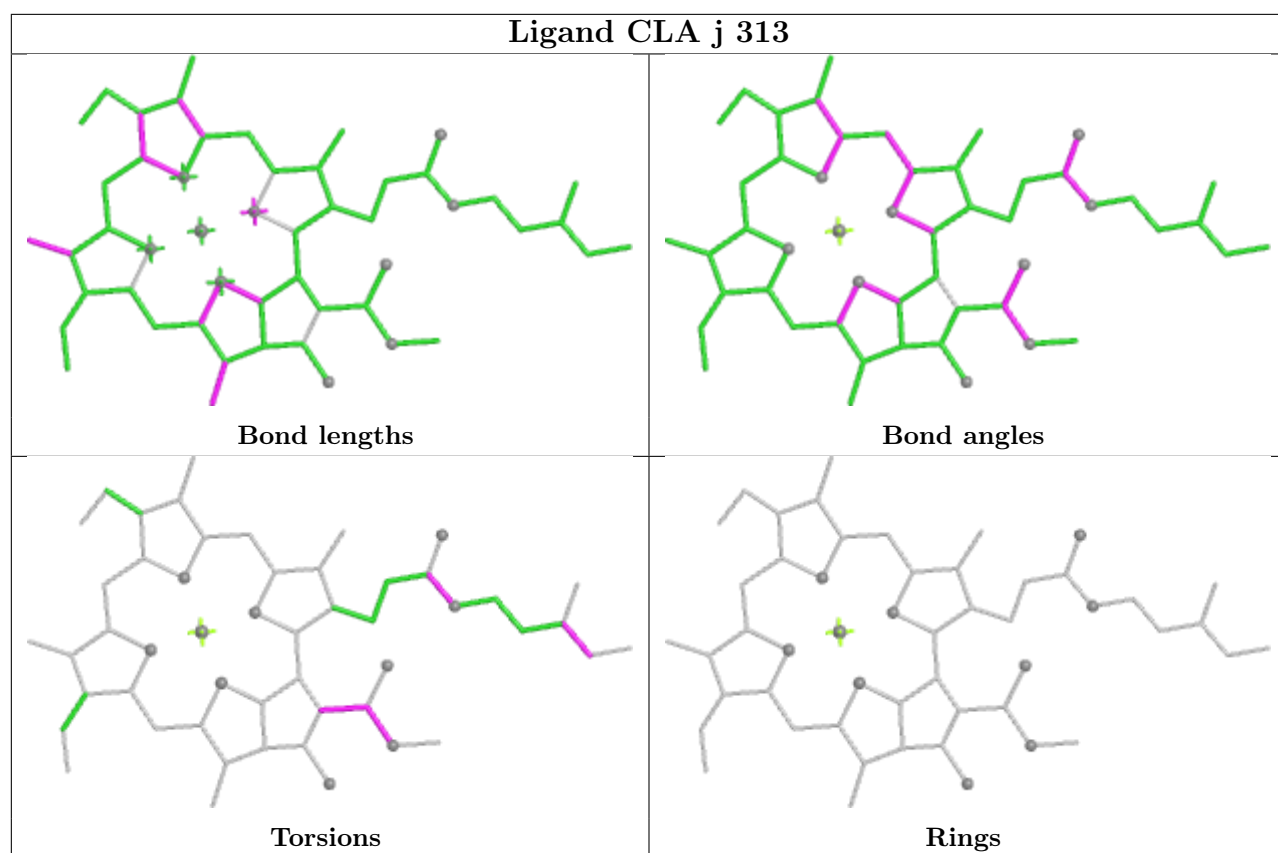


Rings

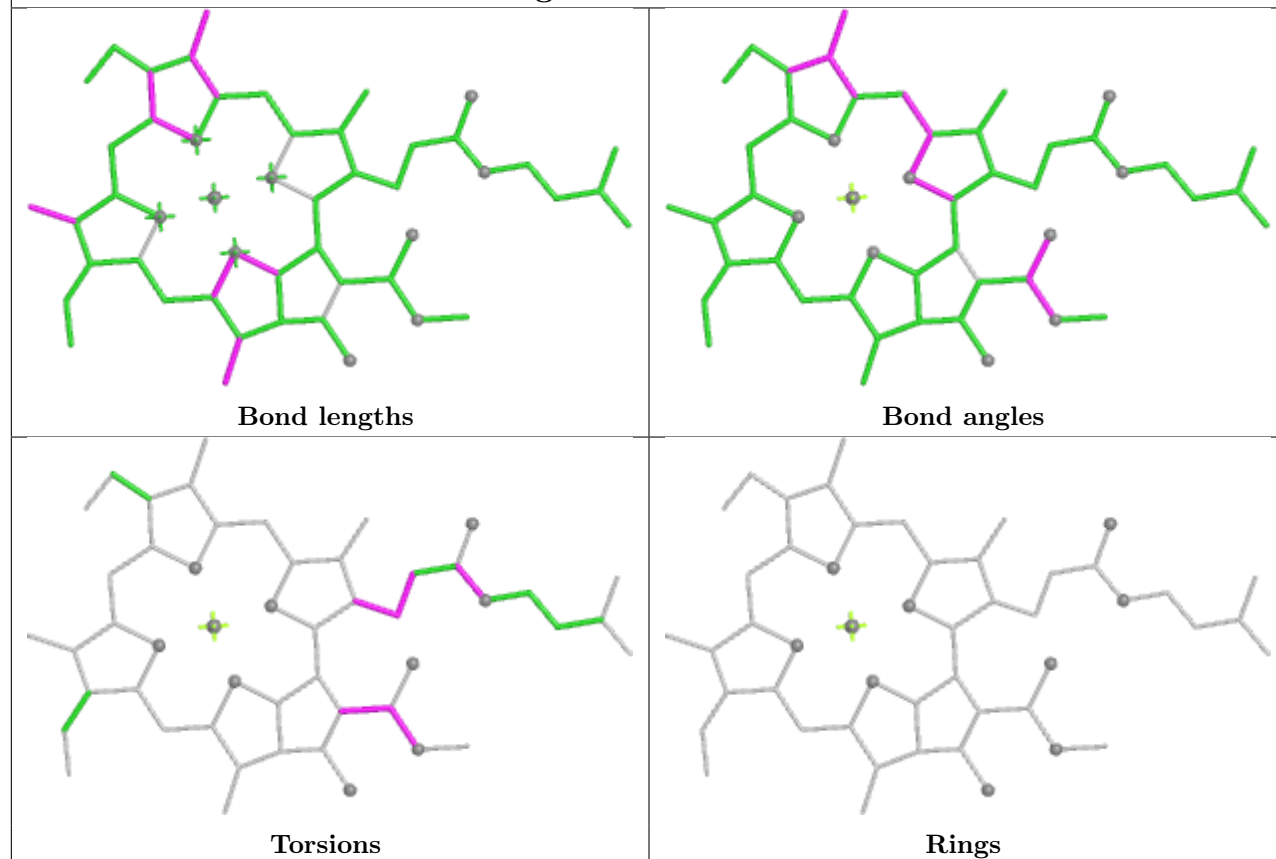




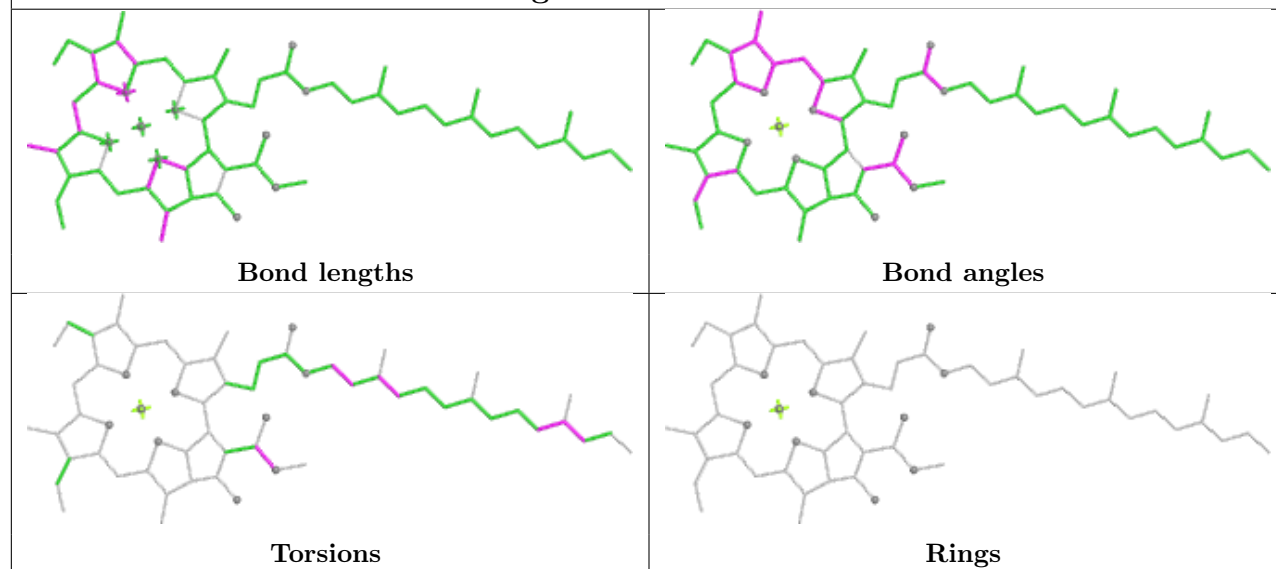




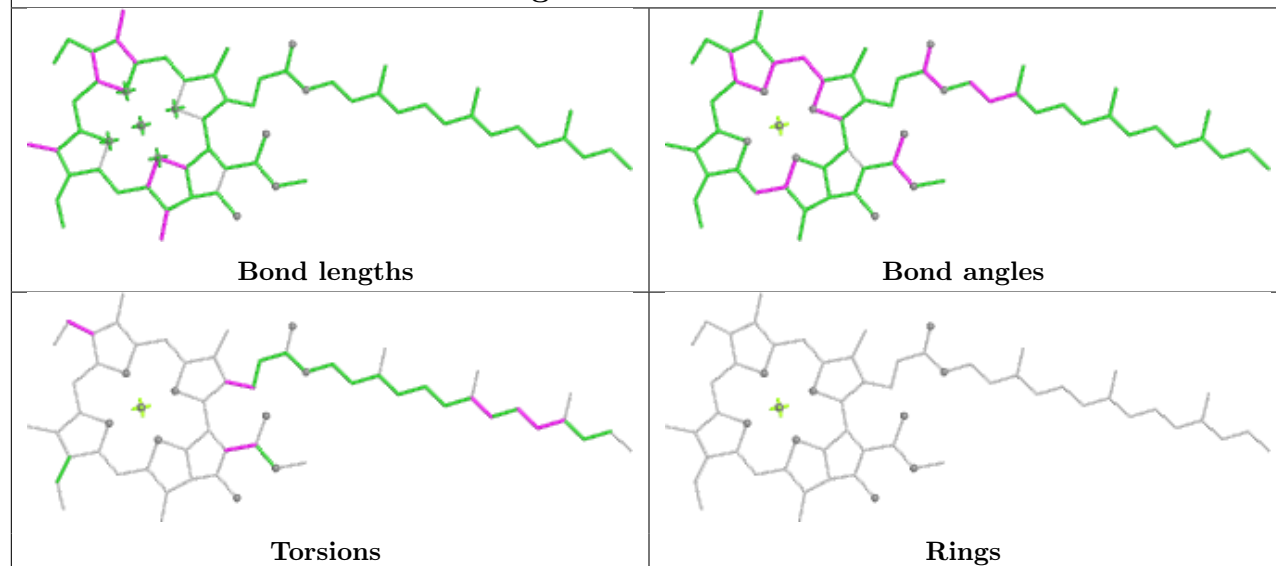
Ligand CLA h 301



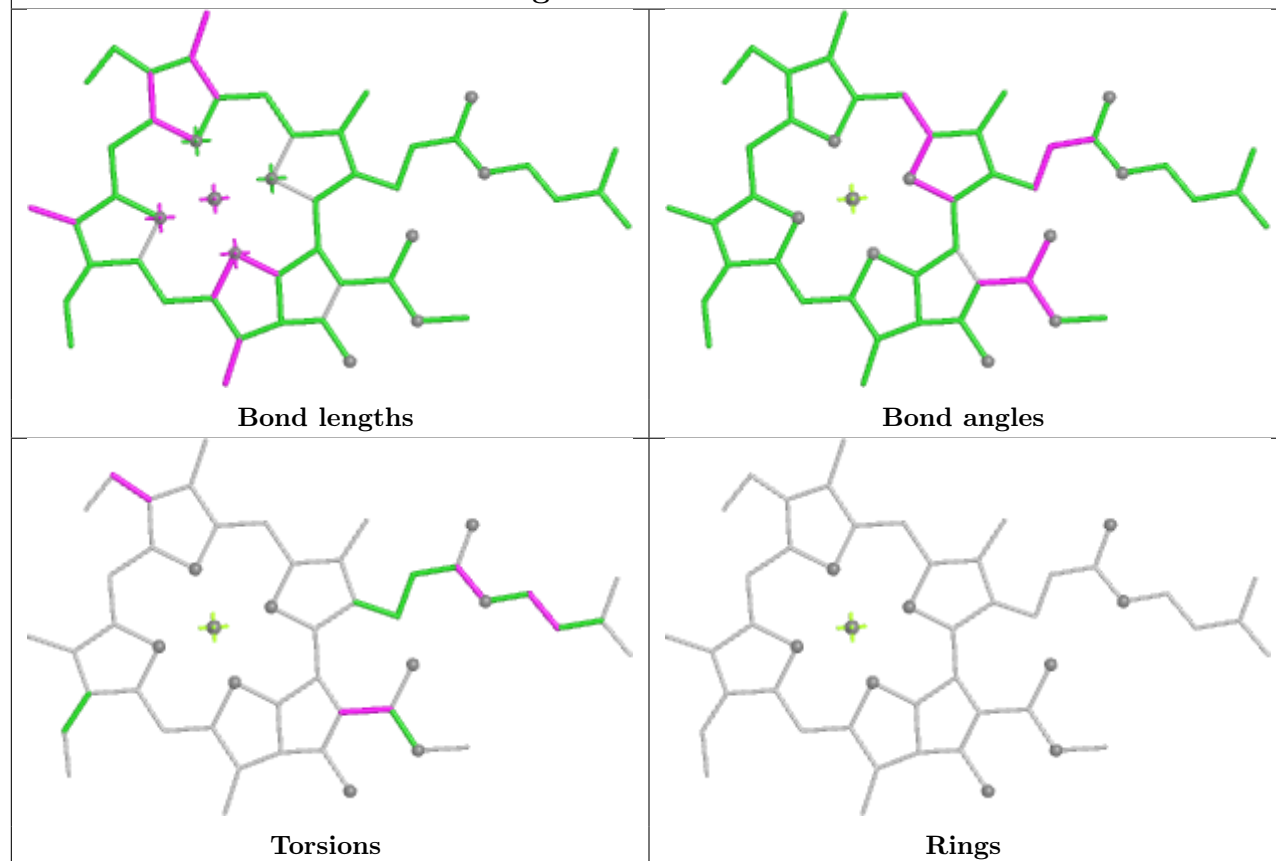
Ligand CLA A 827

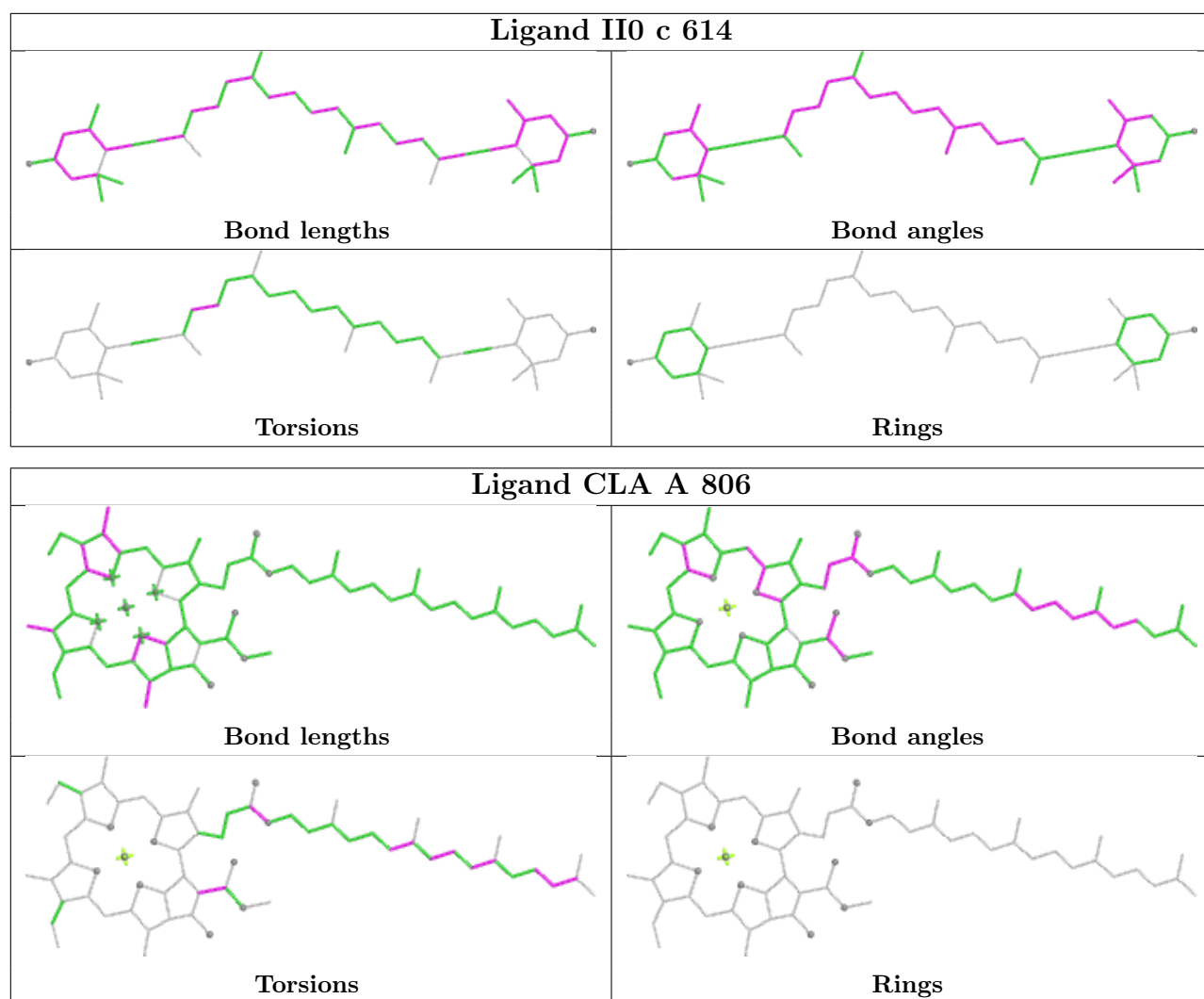


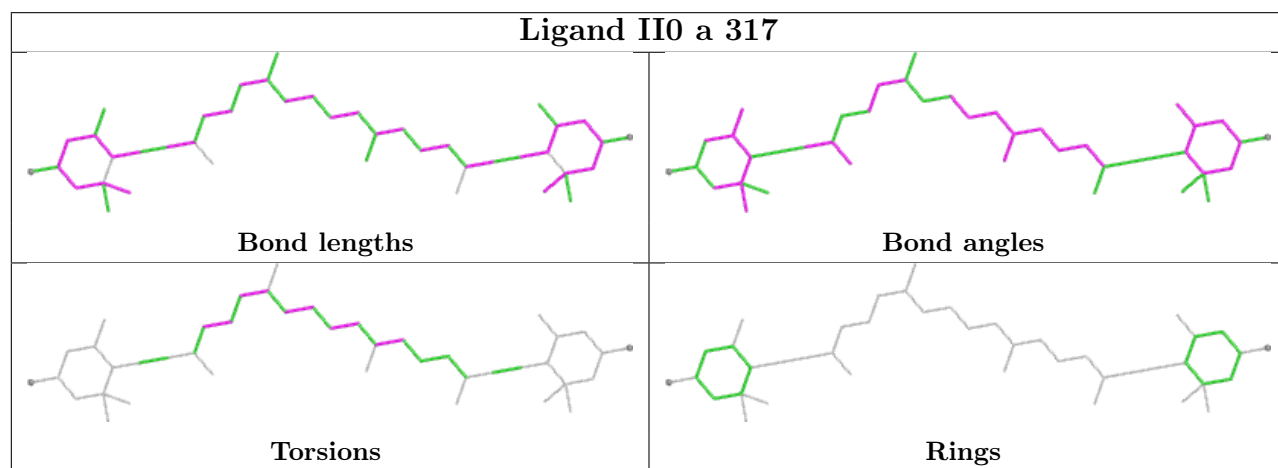
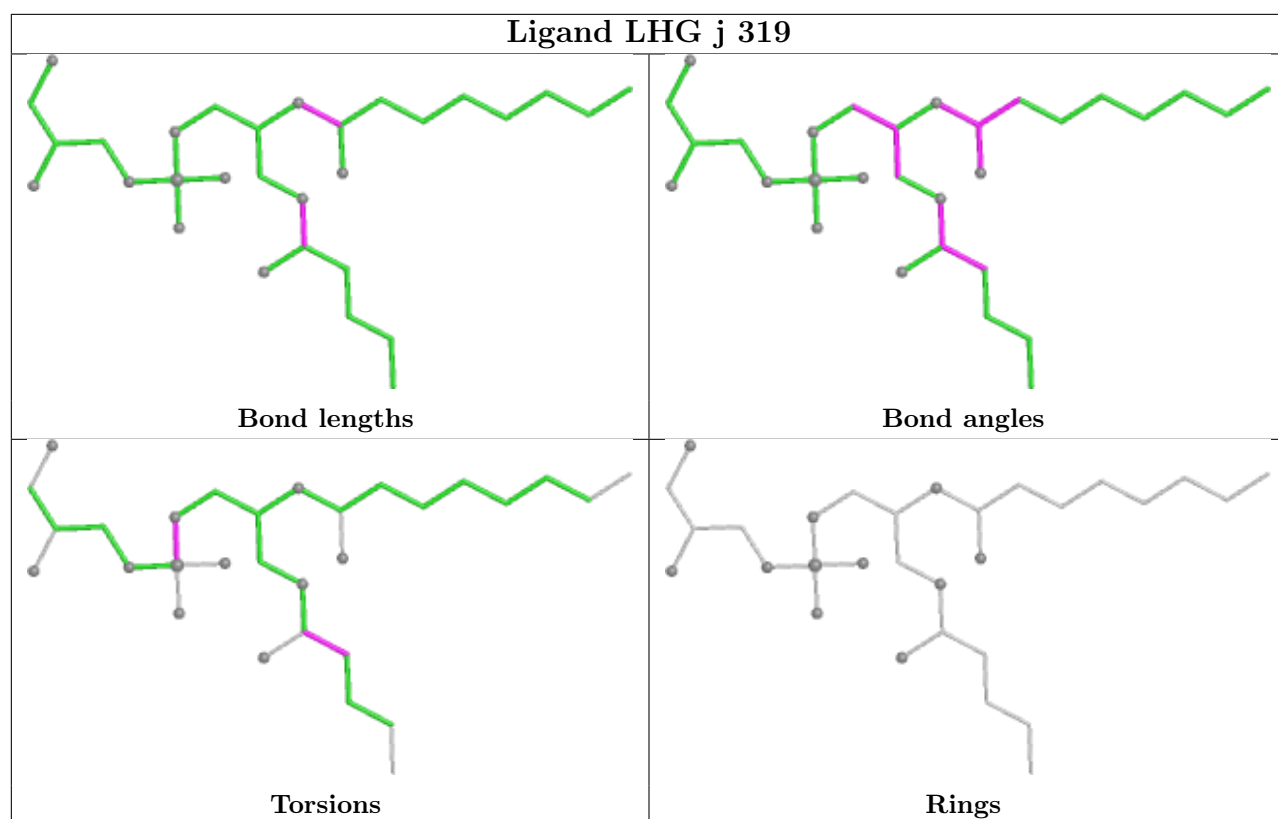
Ligand CLA A 810



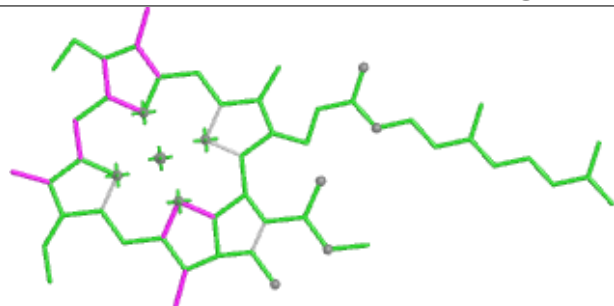
Ligand CLA B 829



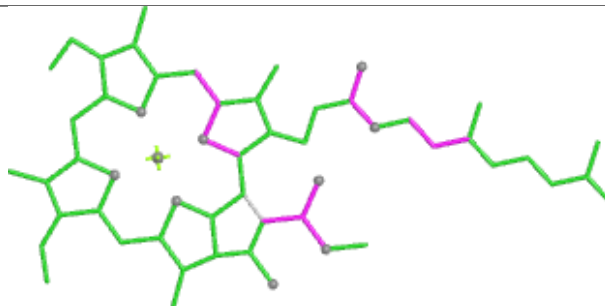




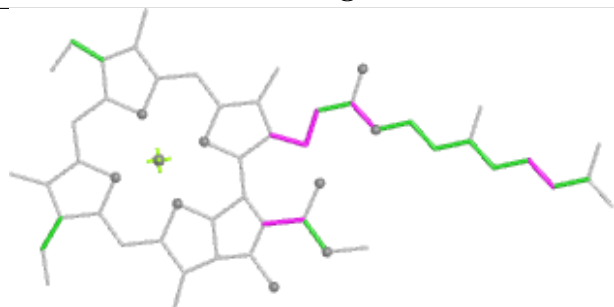
Ligand CLA b 304



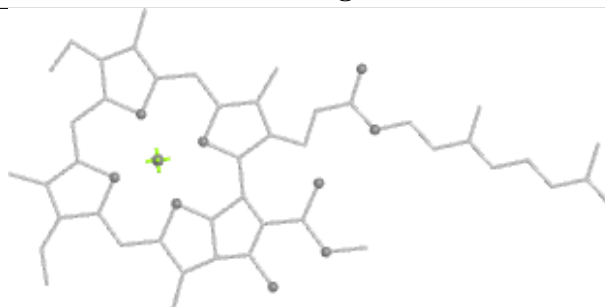
Bond lengths



Bond angles

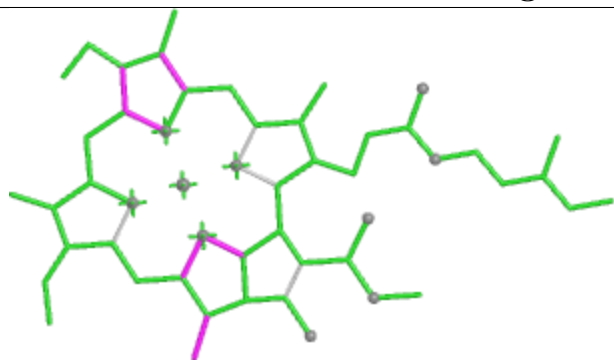


Torsions

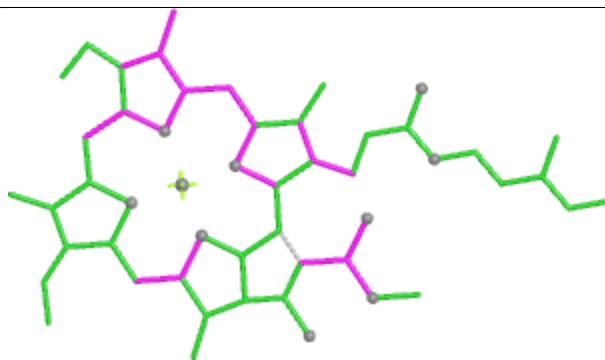


Rings

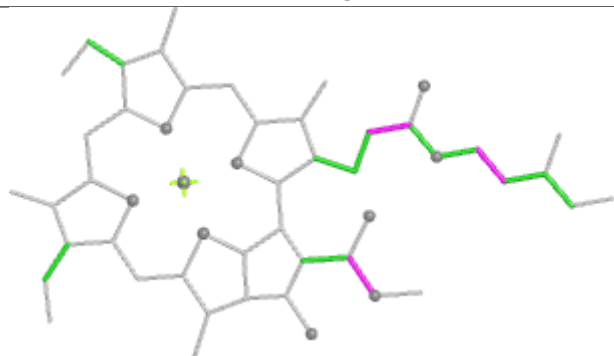
Ligand CLA e 603



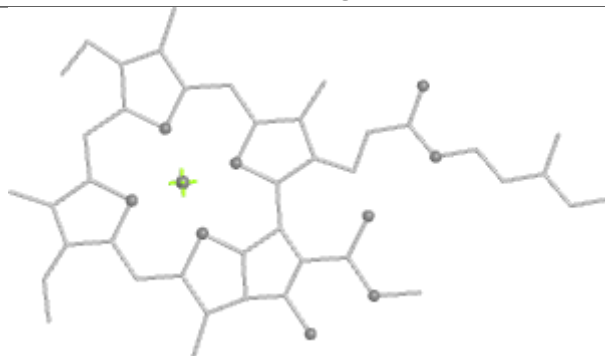
Bond lengths



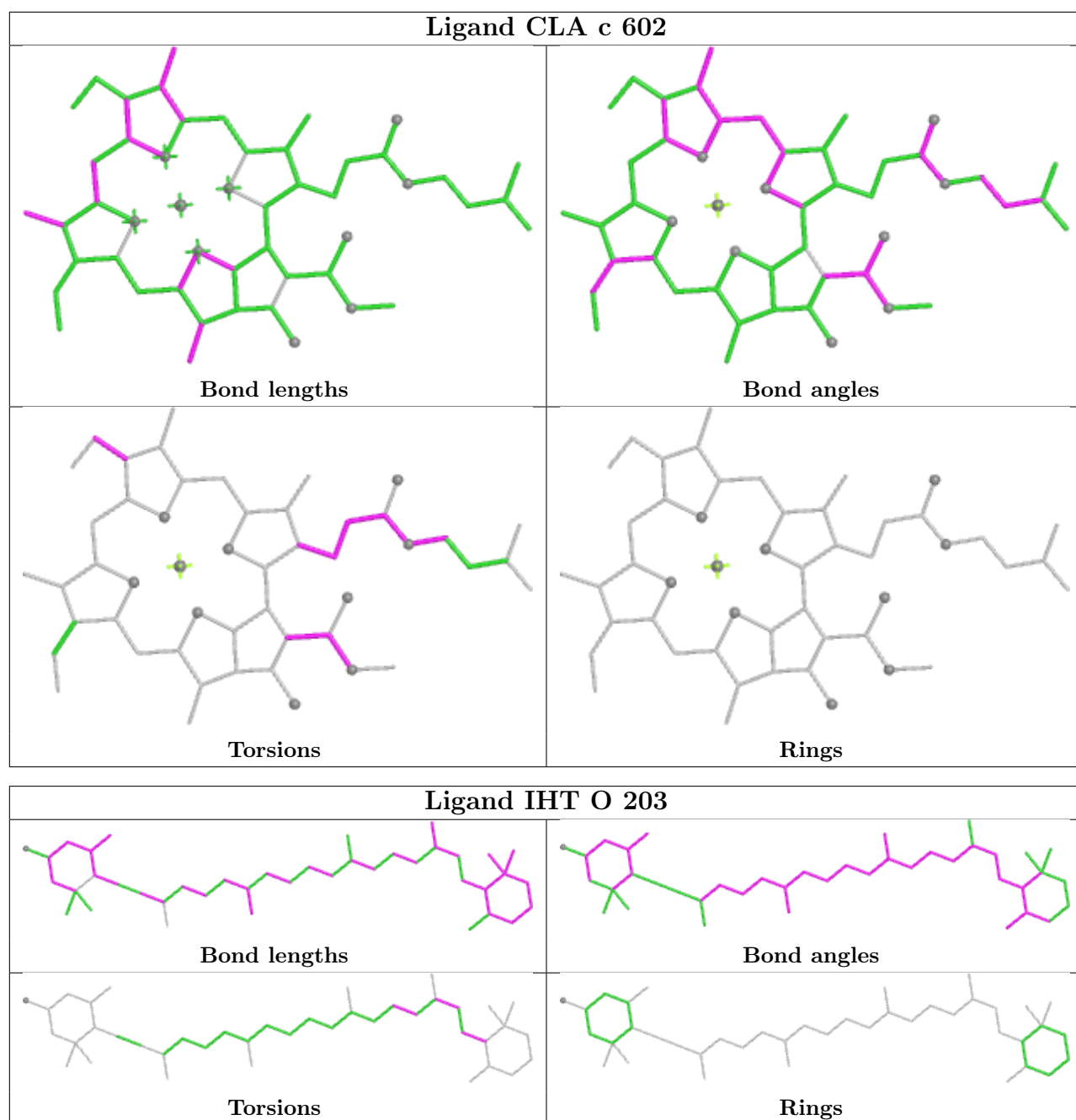
Bond angles

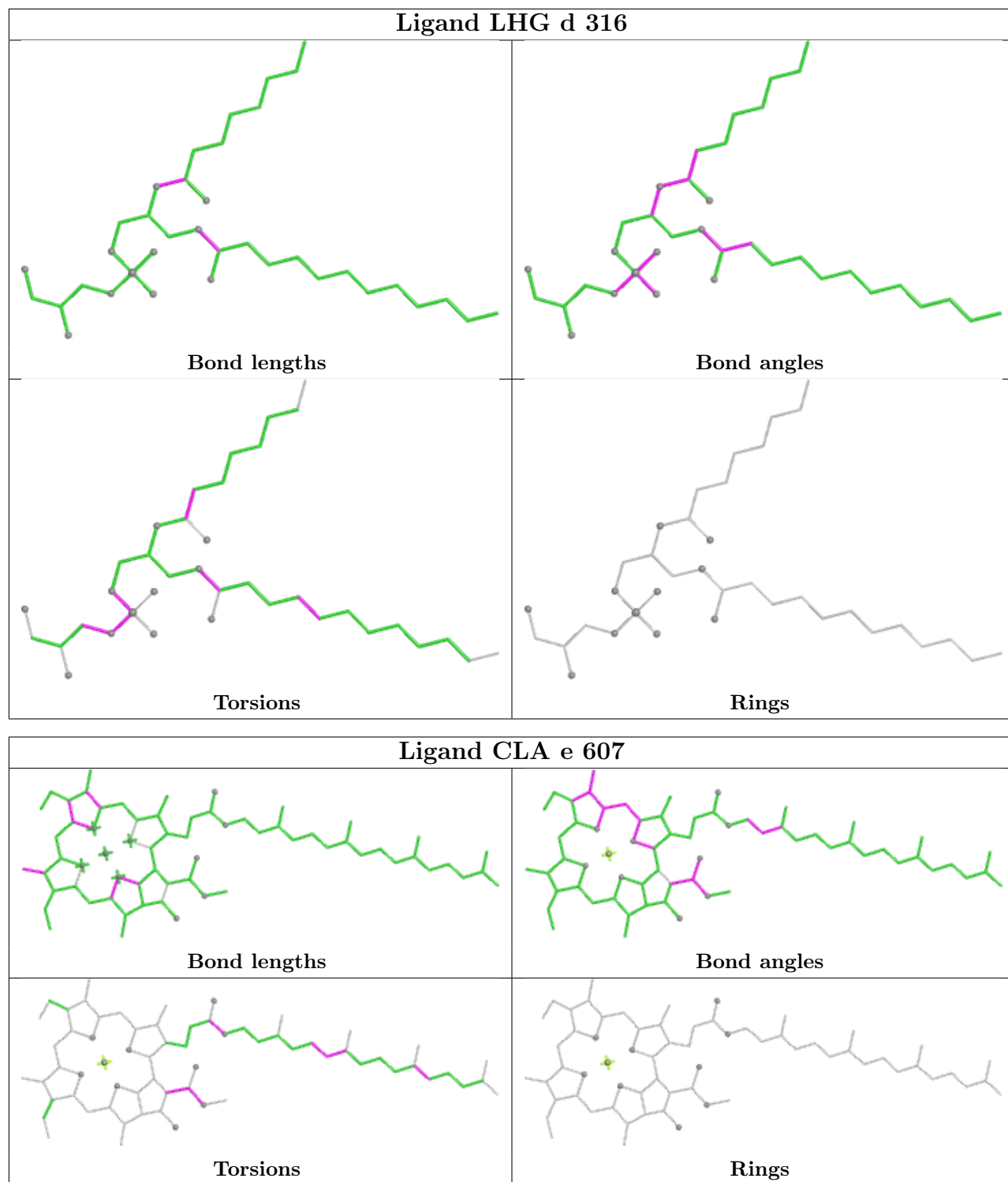


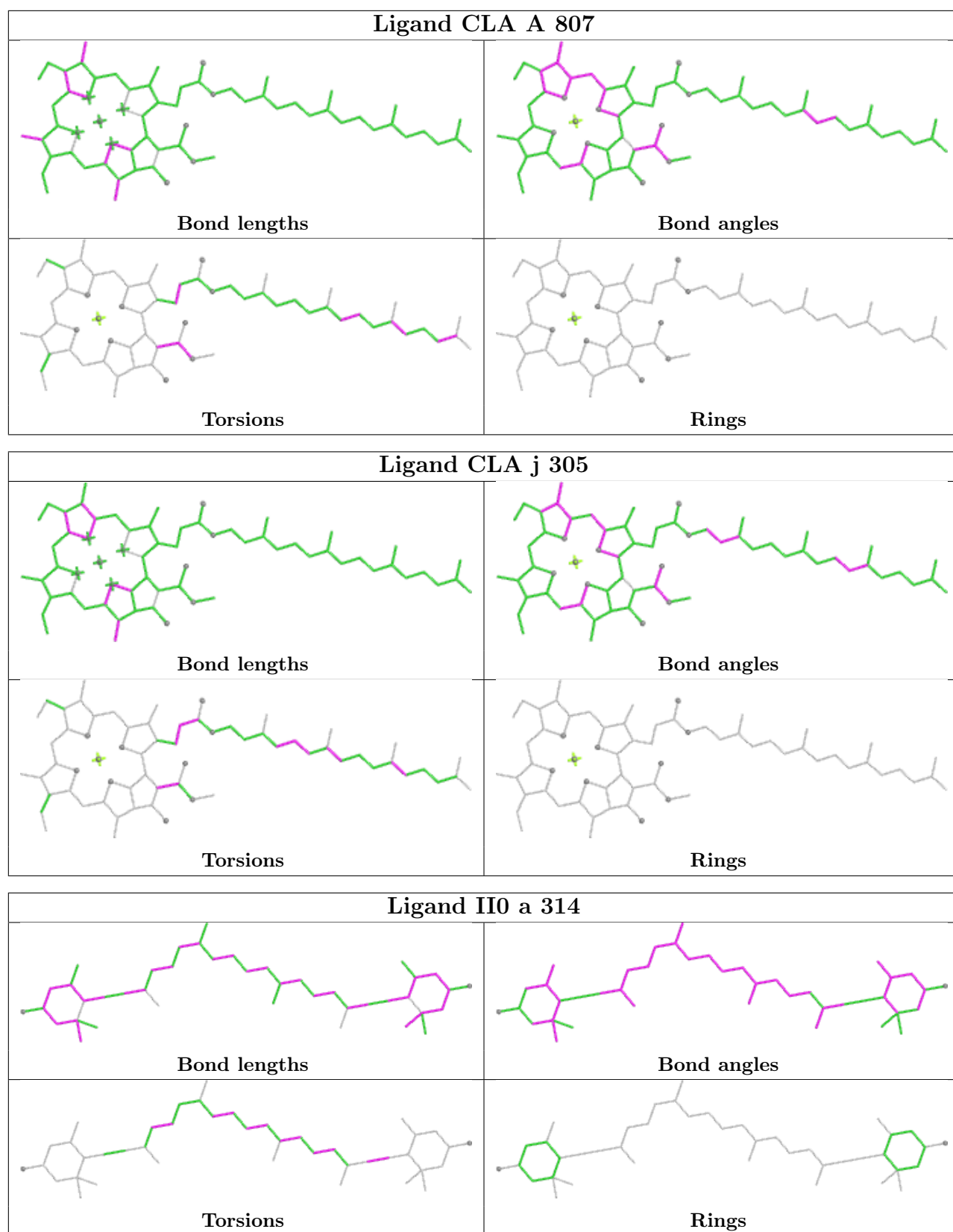
Torsions

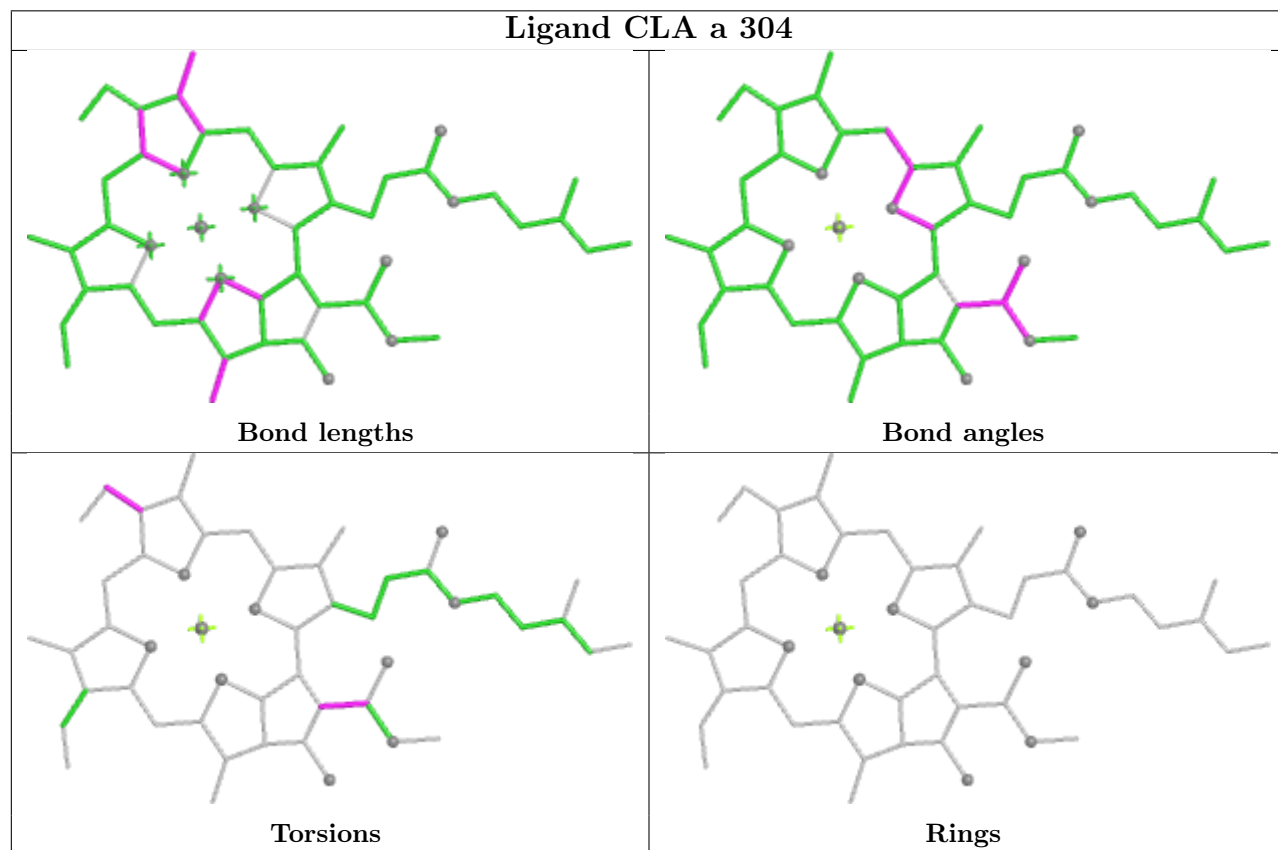
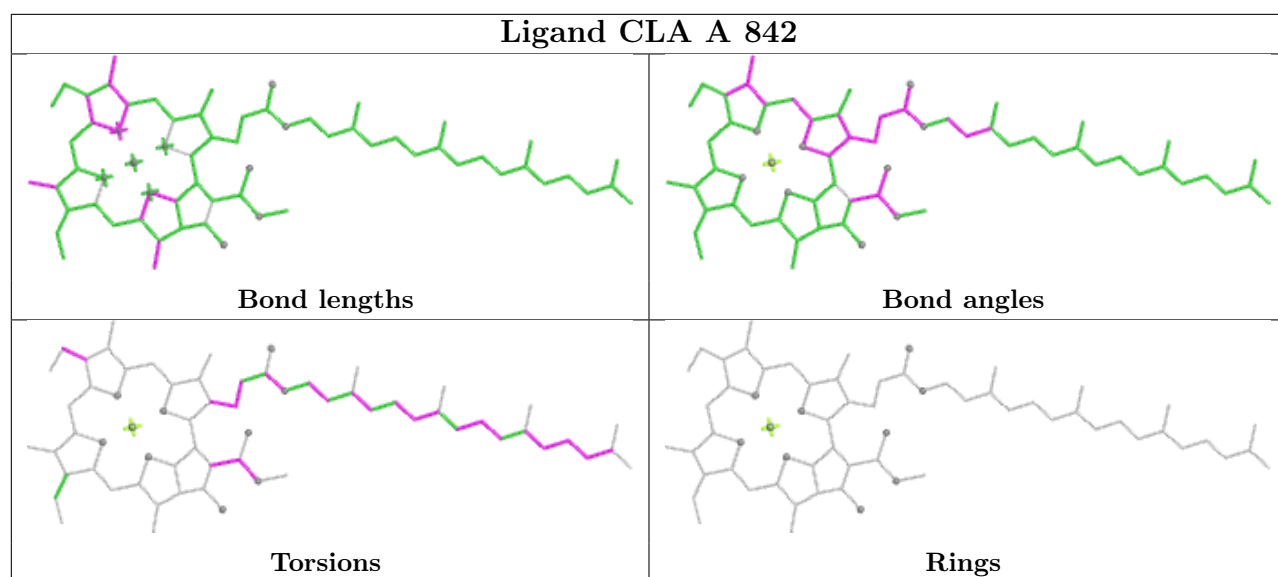


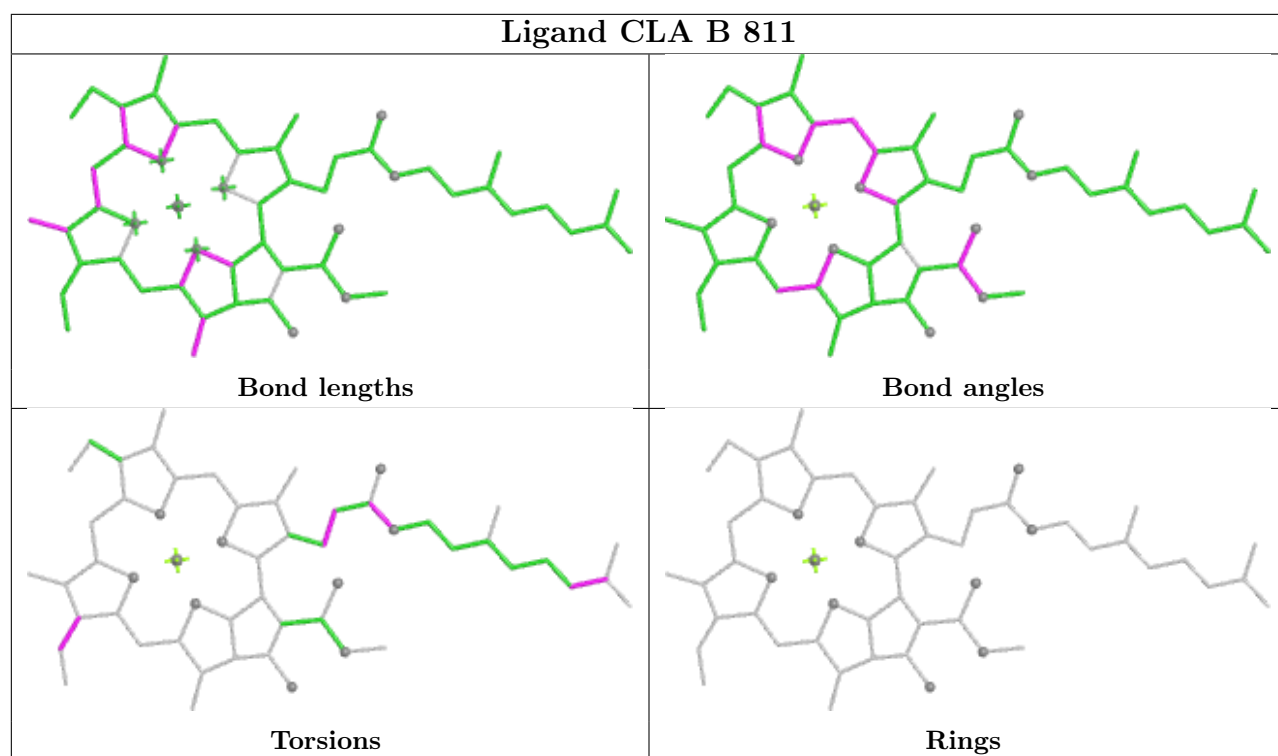
Rings



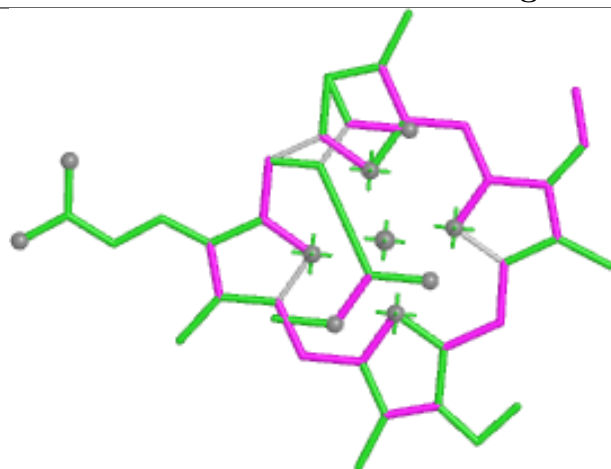




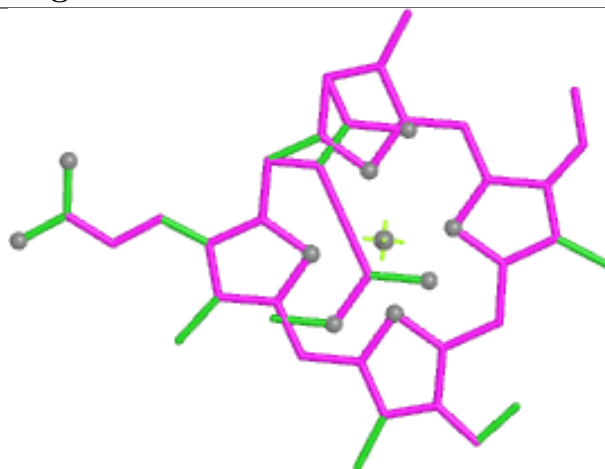




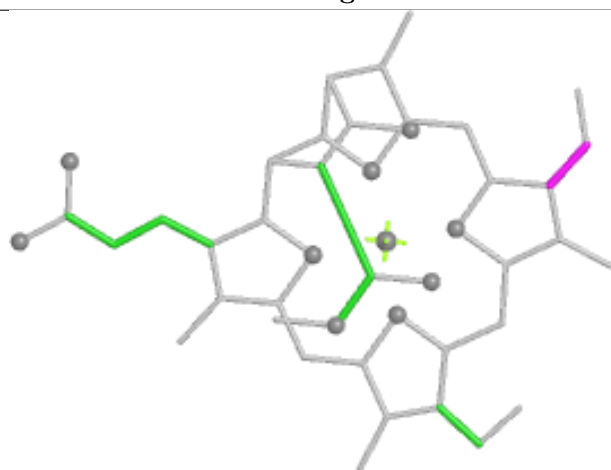
Ligand KC2 g 313



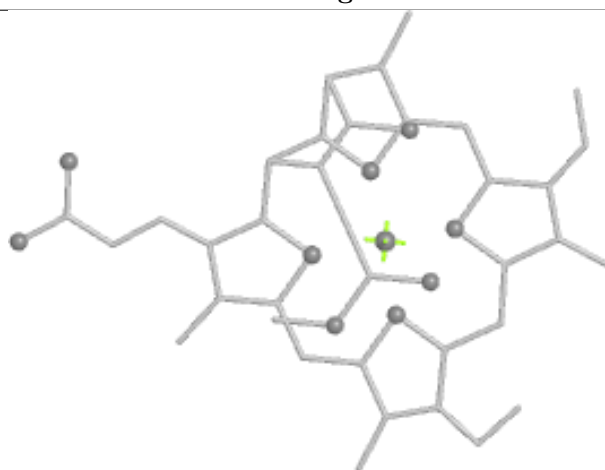
Bond lengths



Bond angles

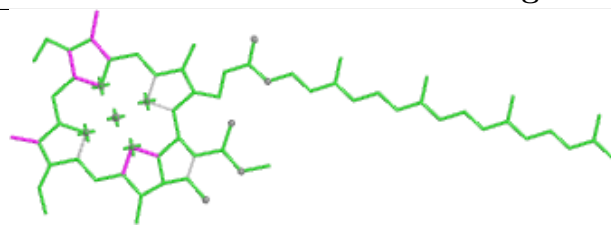


Torsions

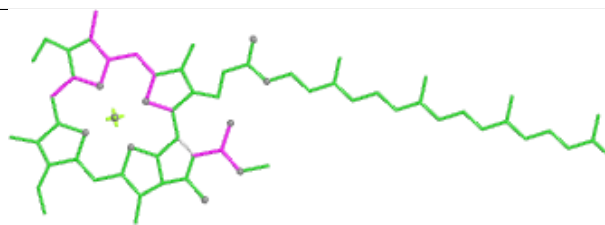


Rings

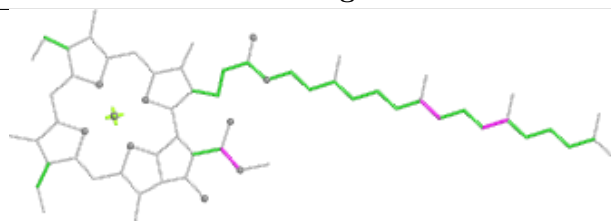
Ligand CLA f 609



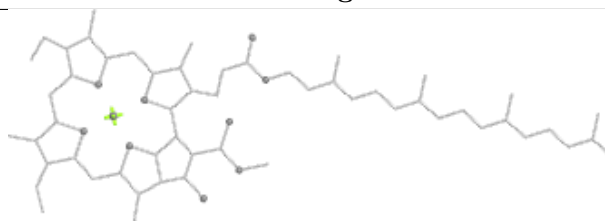
Bond lengths



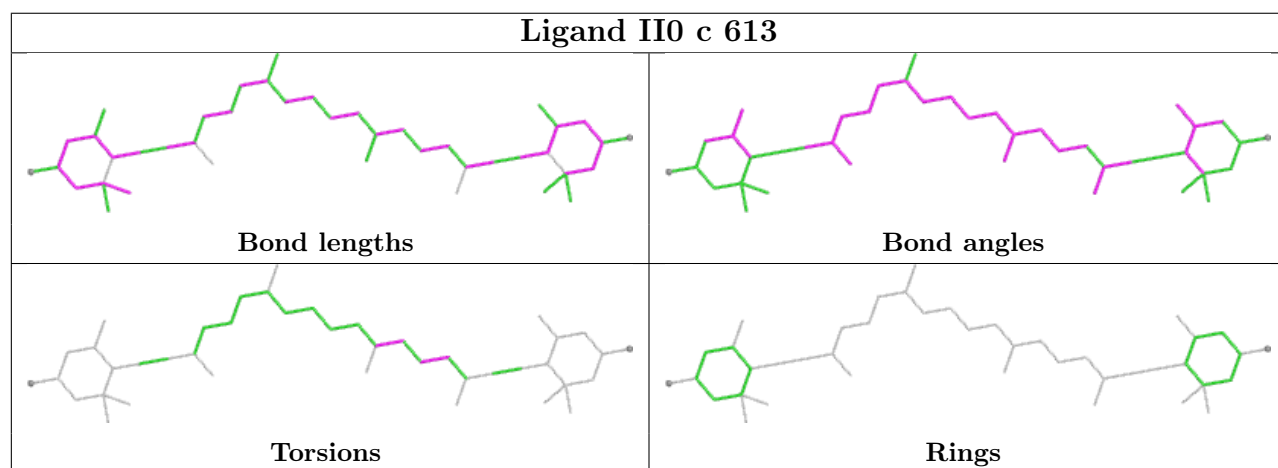
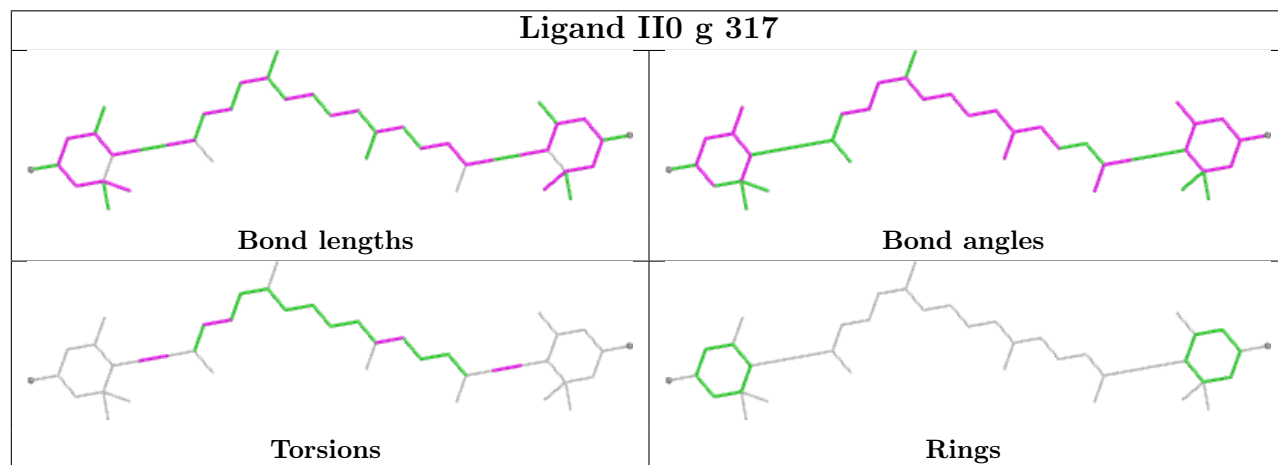
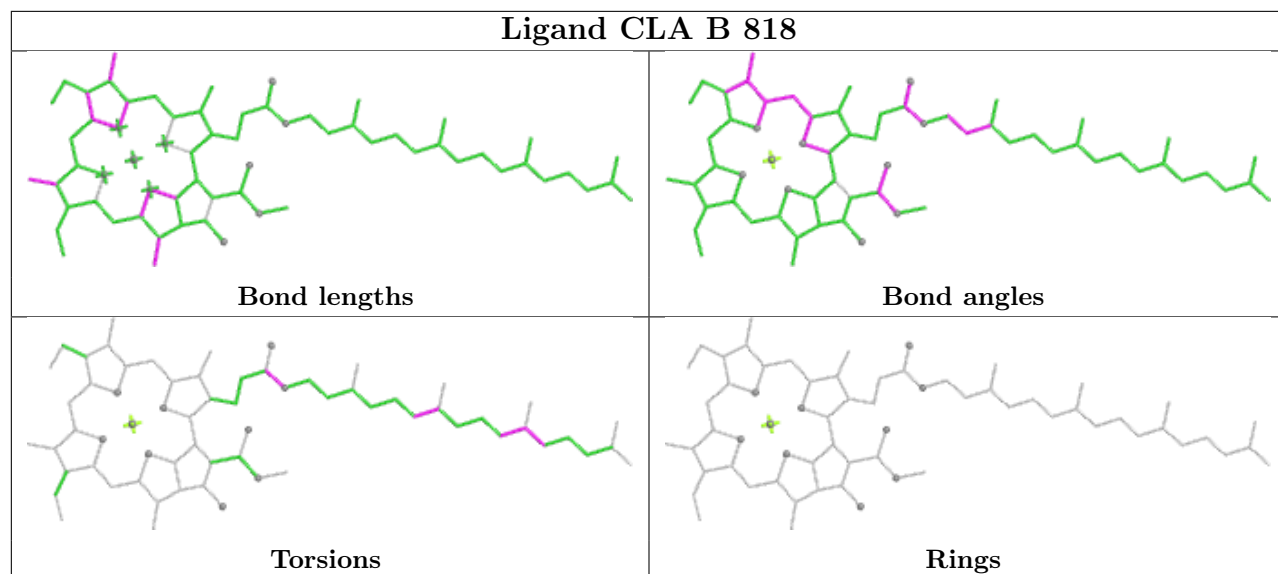
Bond angles



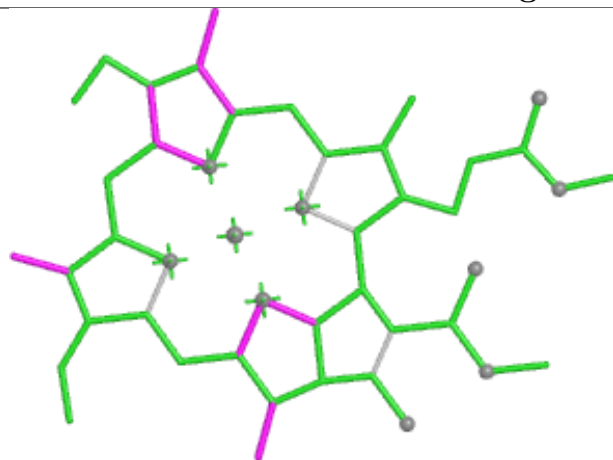
Torsions



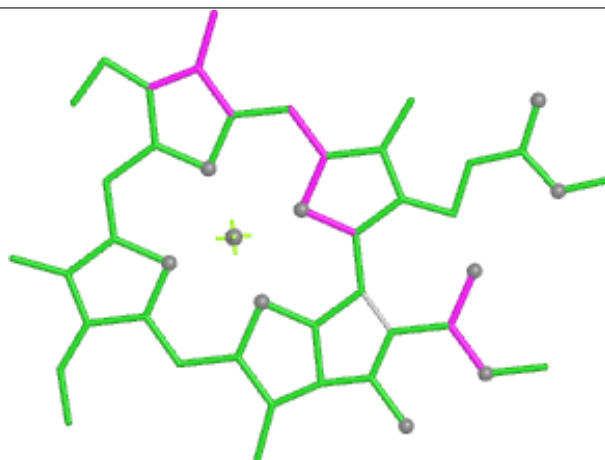
Rings



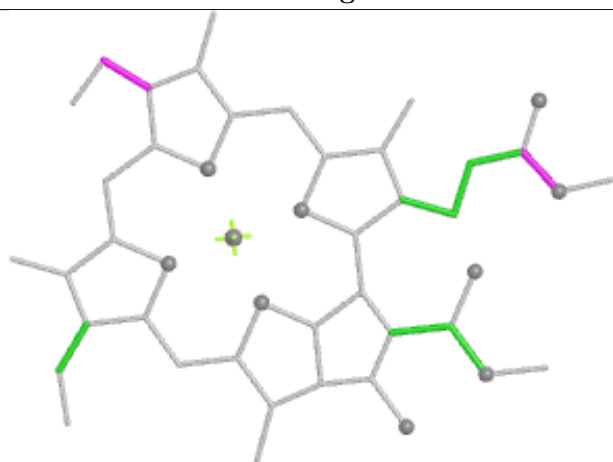
Ligand CLA c 607



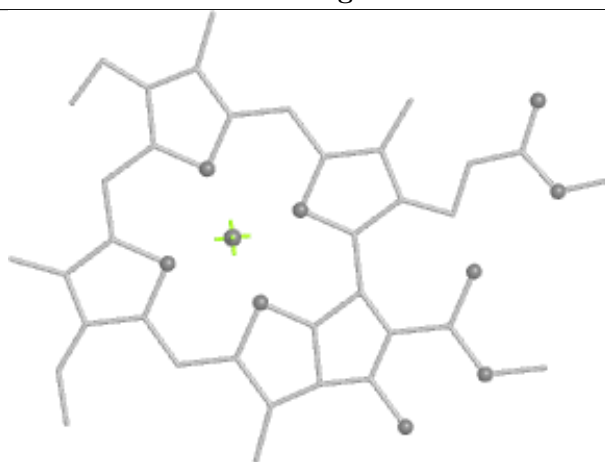
Bond lengths



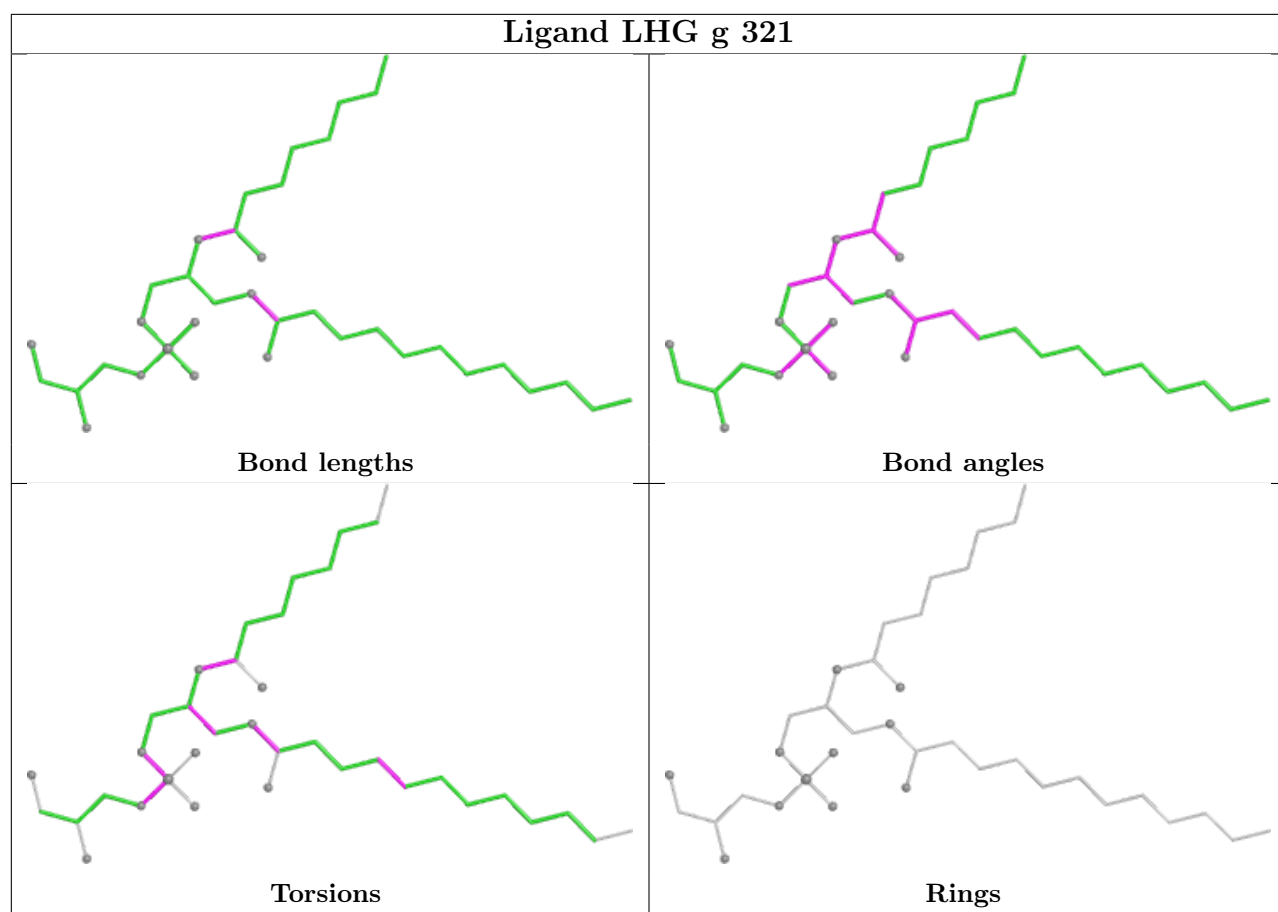
Bond angles



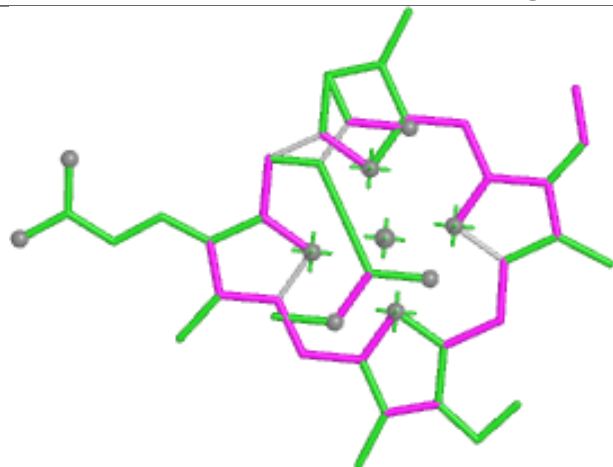
Torsions



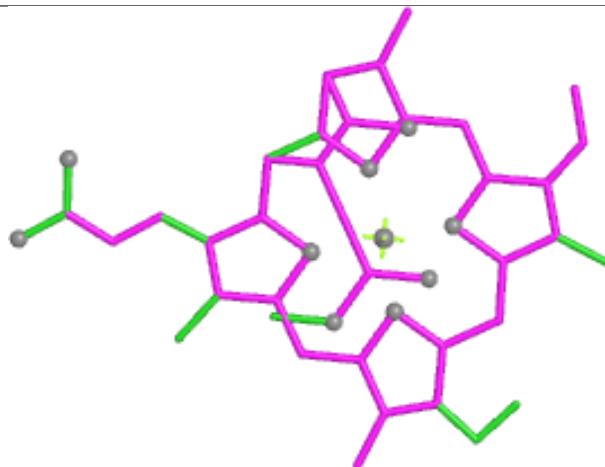
Rings



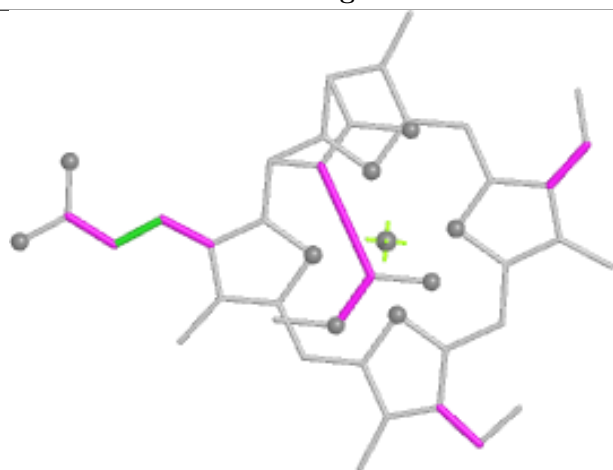
Ligand KC2 i 609



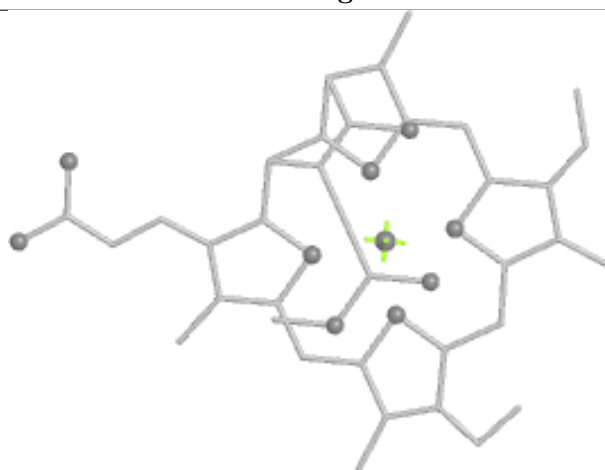
Bond lengths



Bond angles

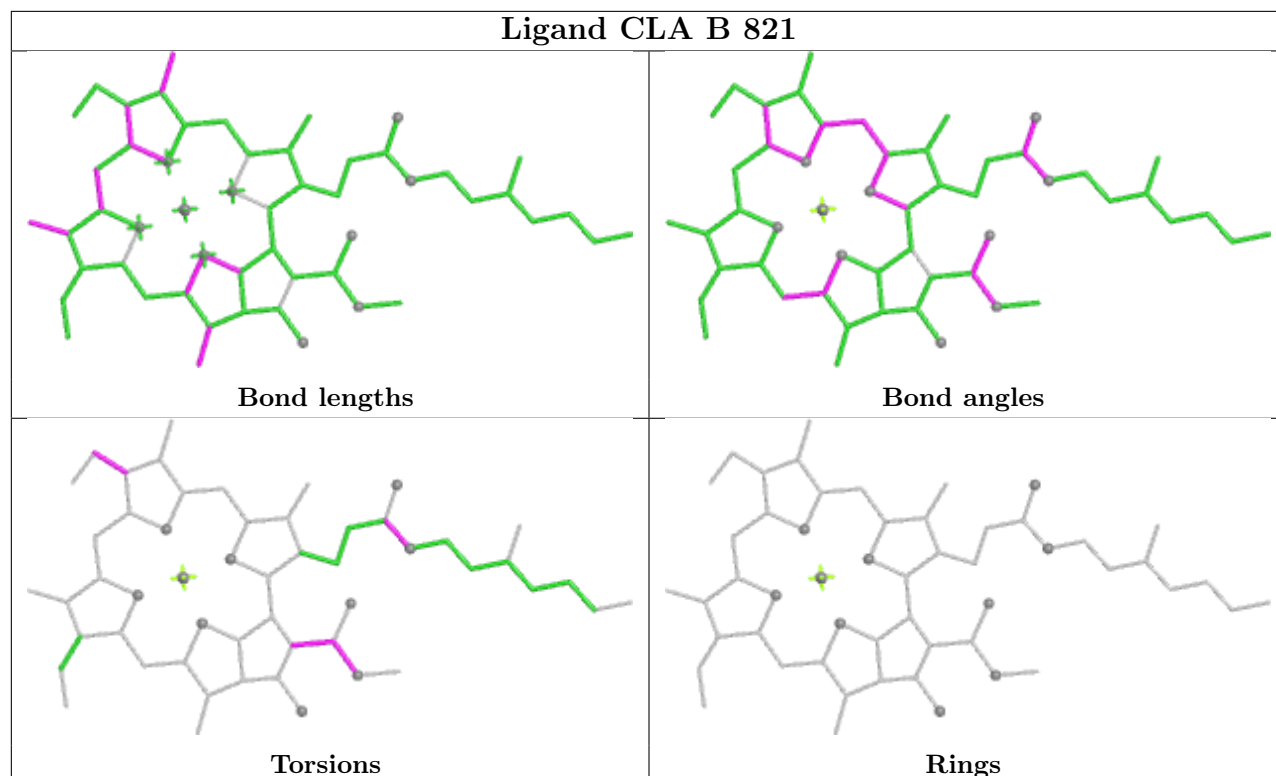


Torsions

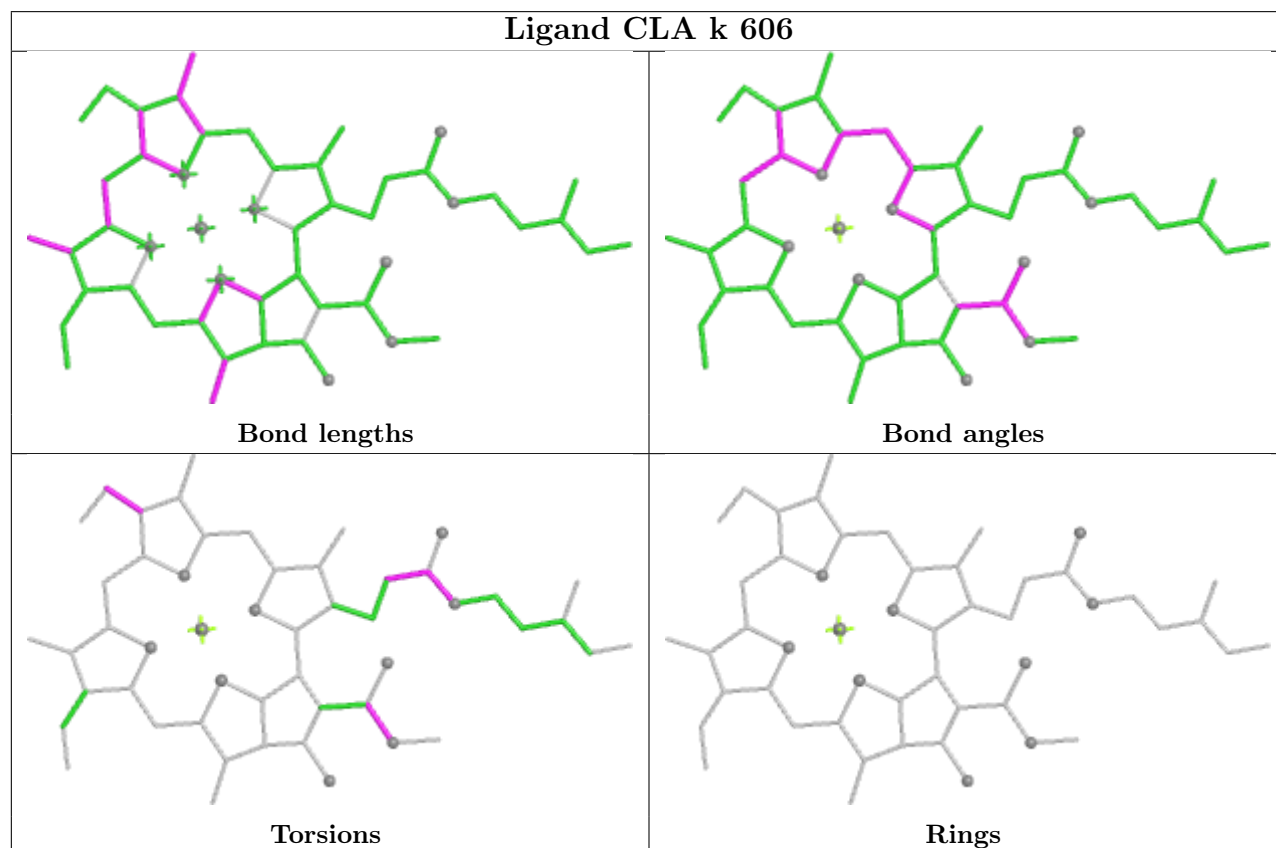


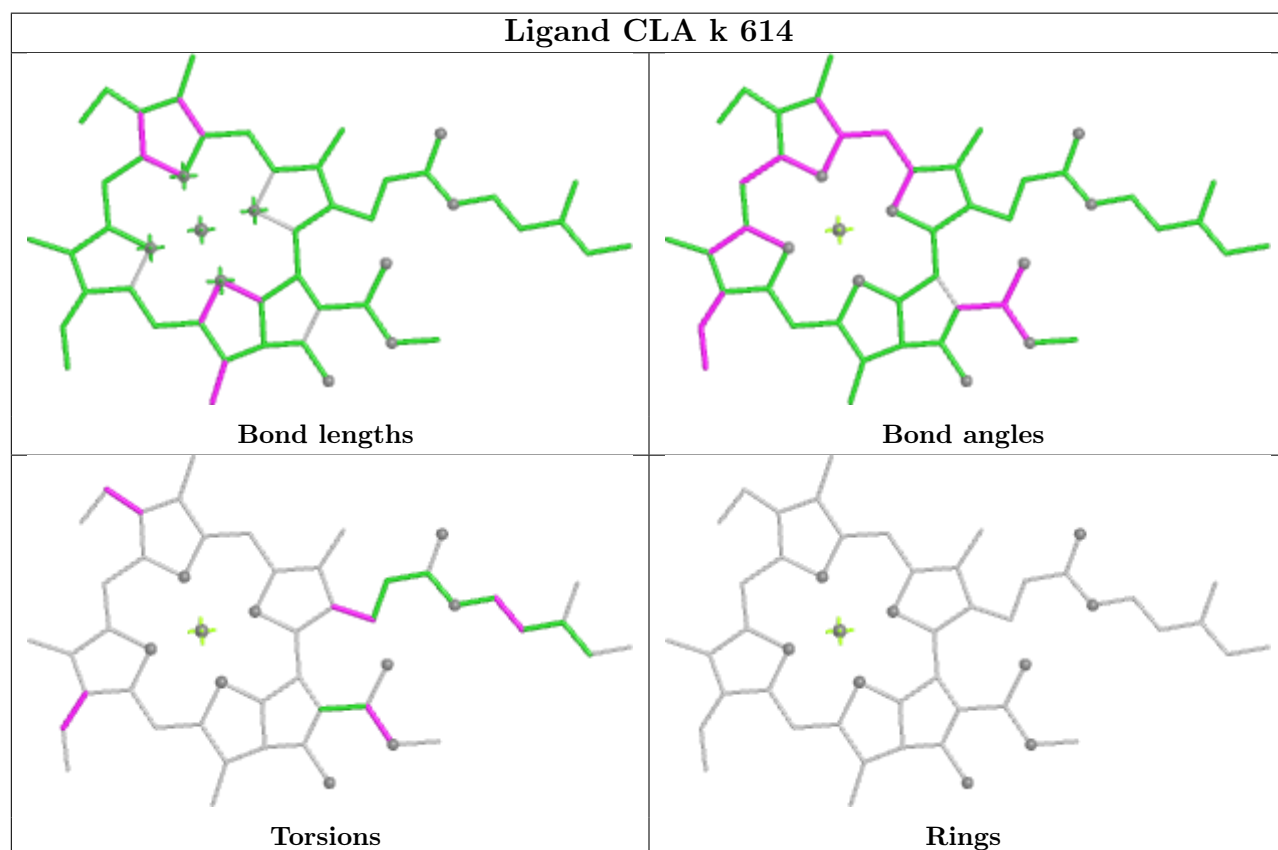
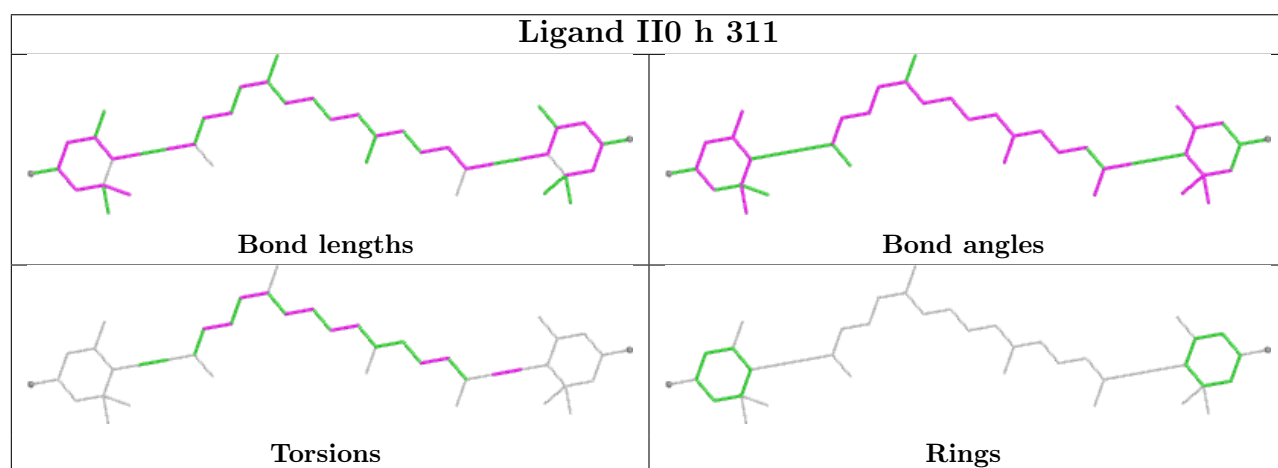
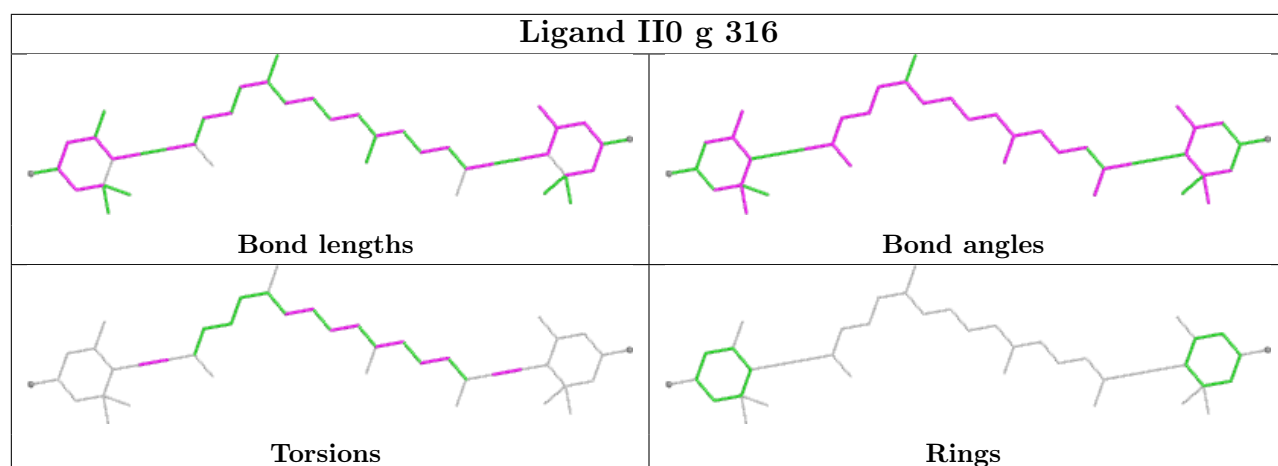
Rings

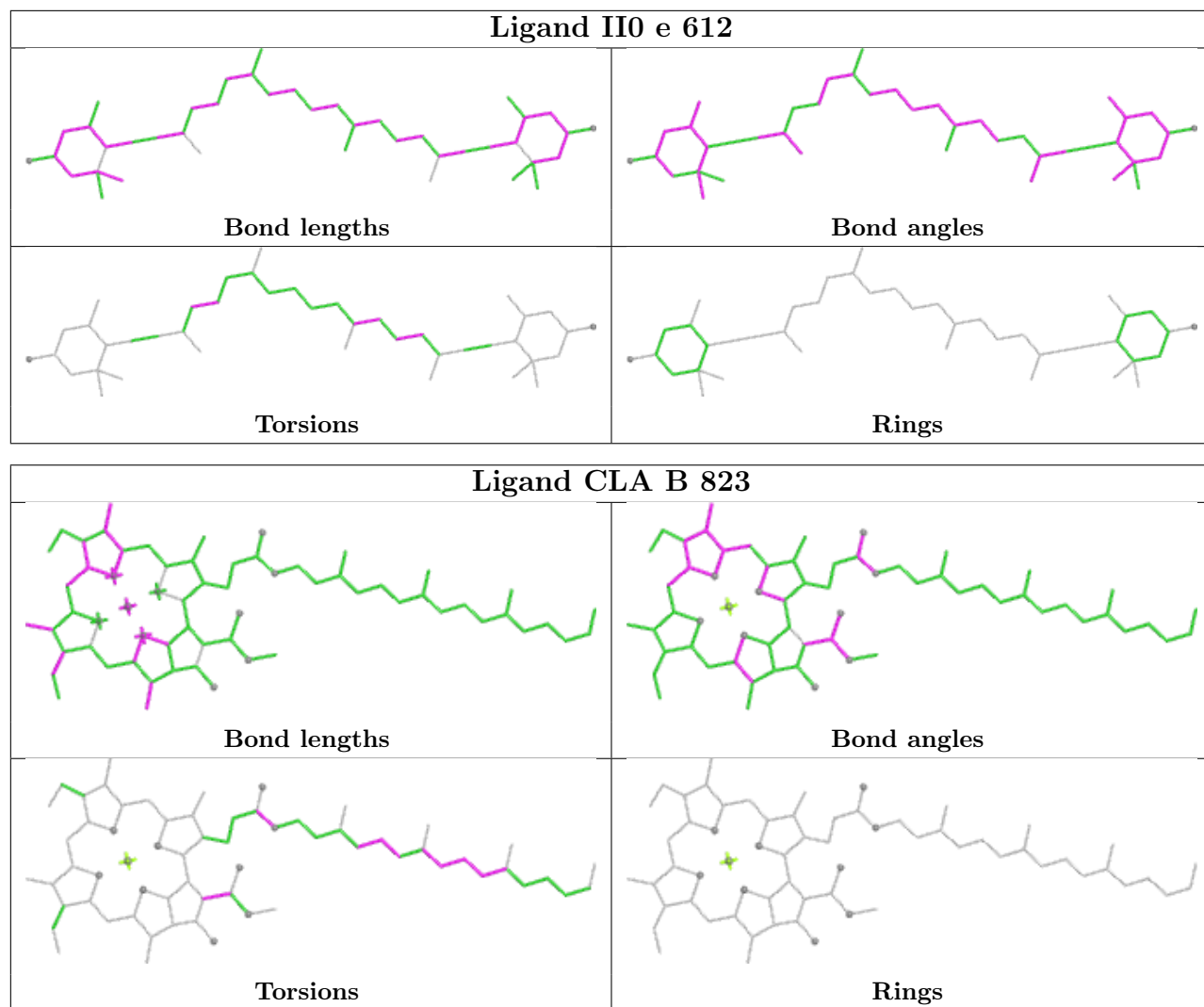
Ligand CLA B 821



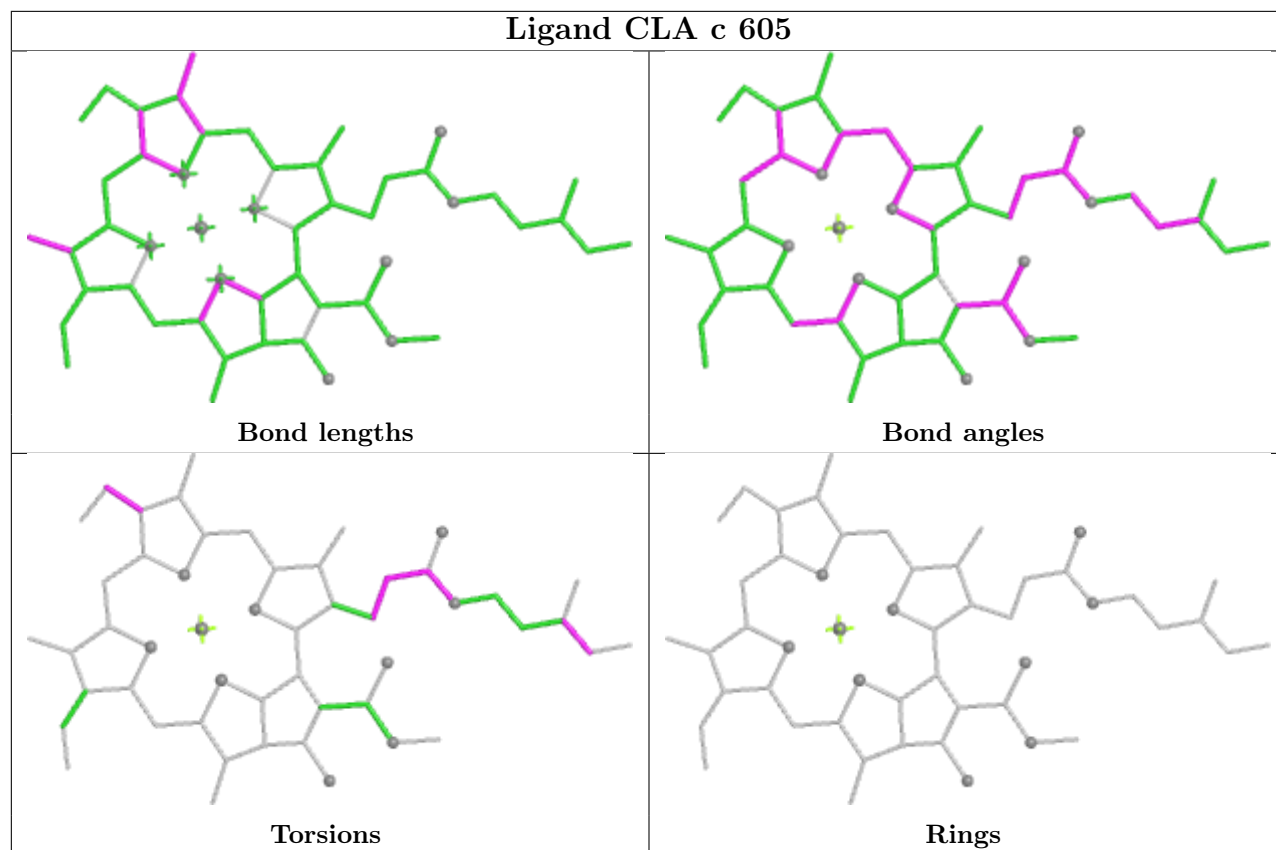
Ligand CLA k 606



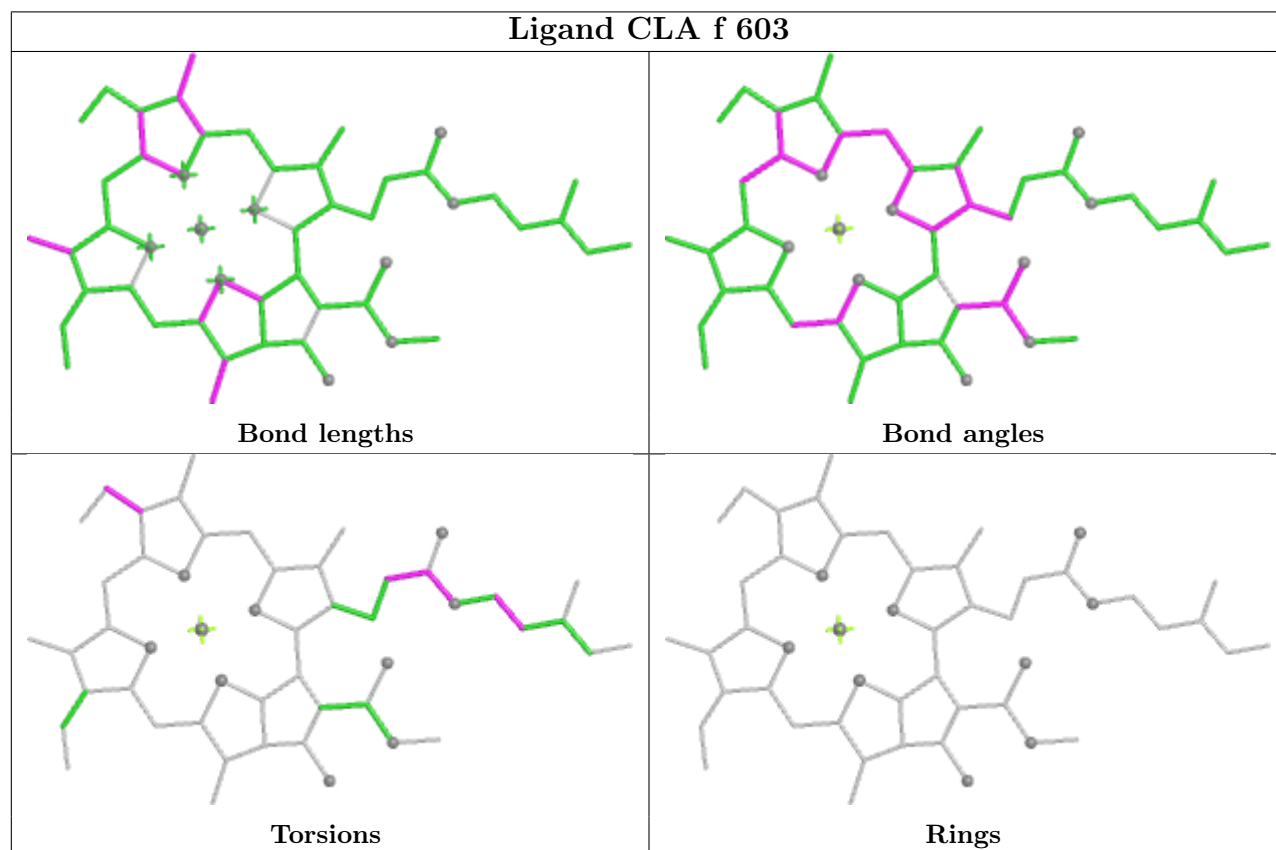


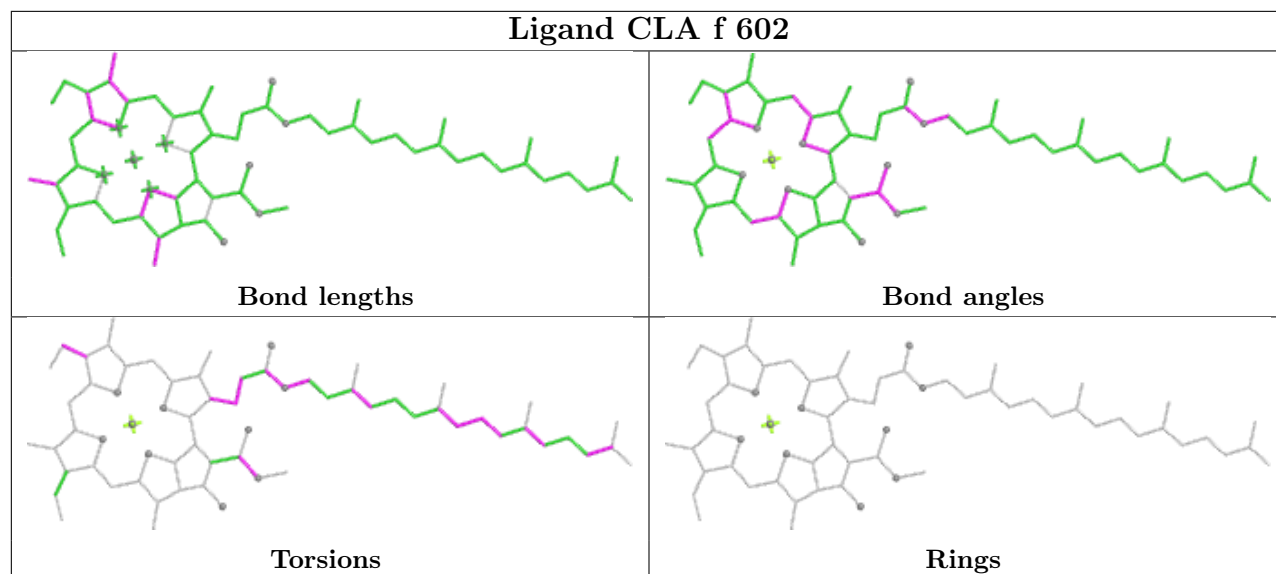
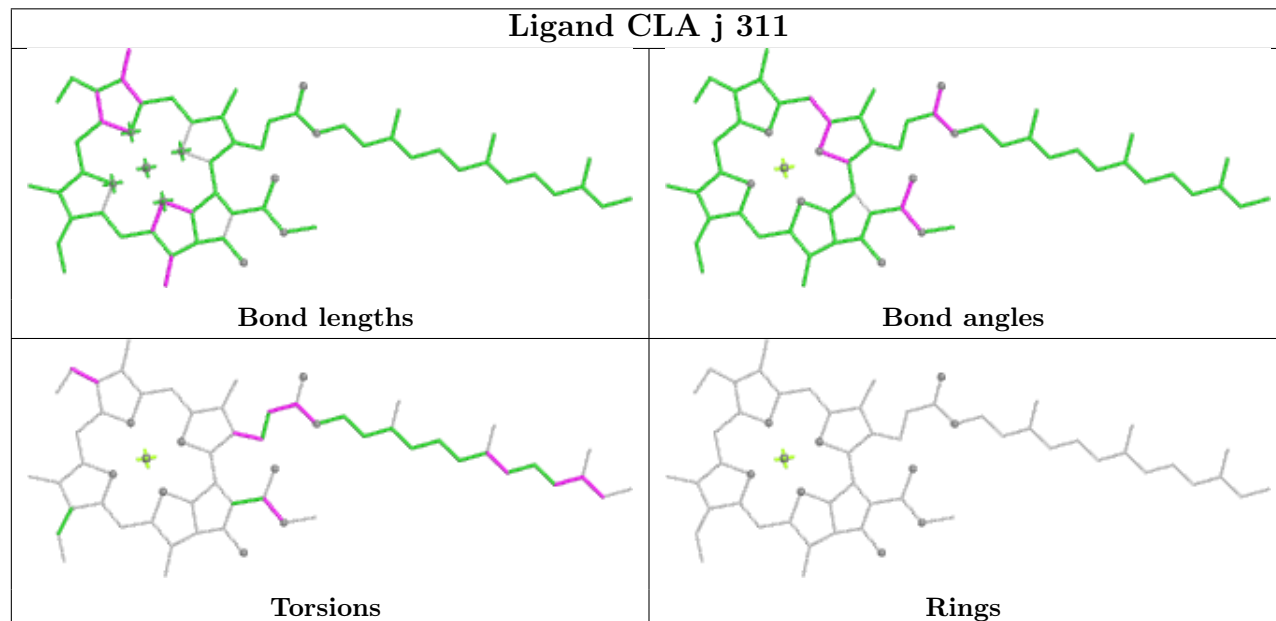


Ligand CLA c 605

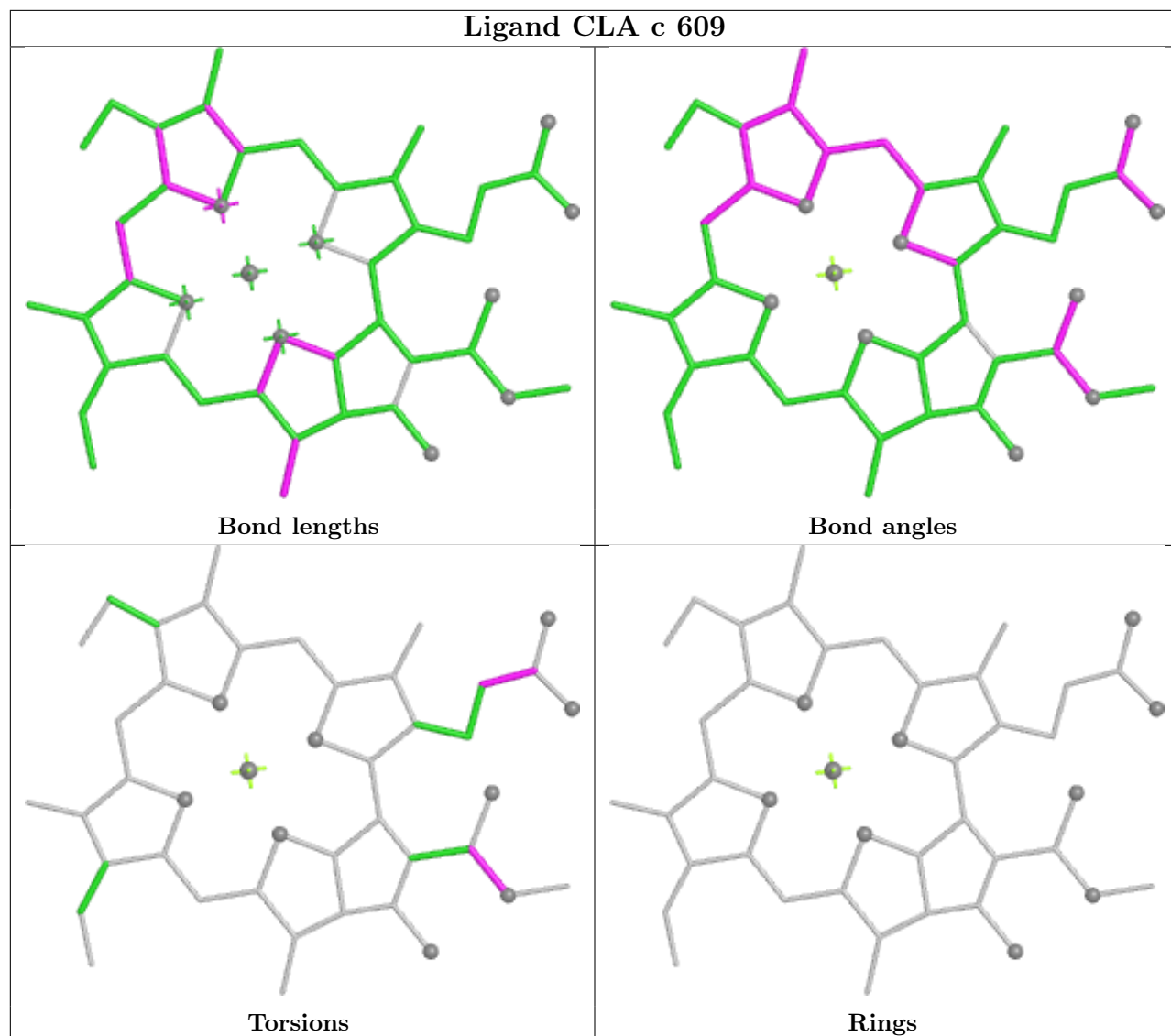


Ligand CLA f 603

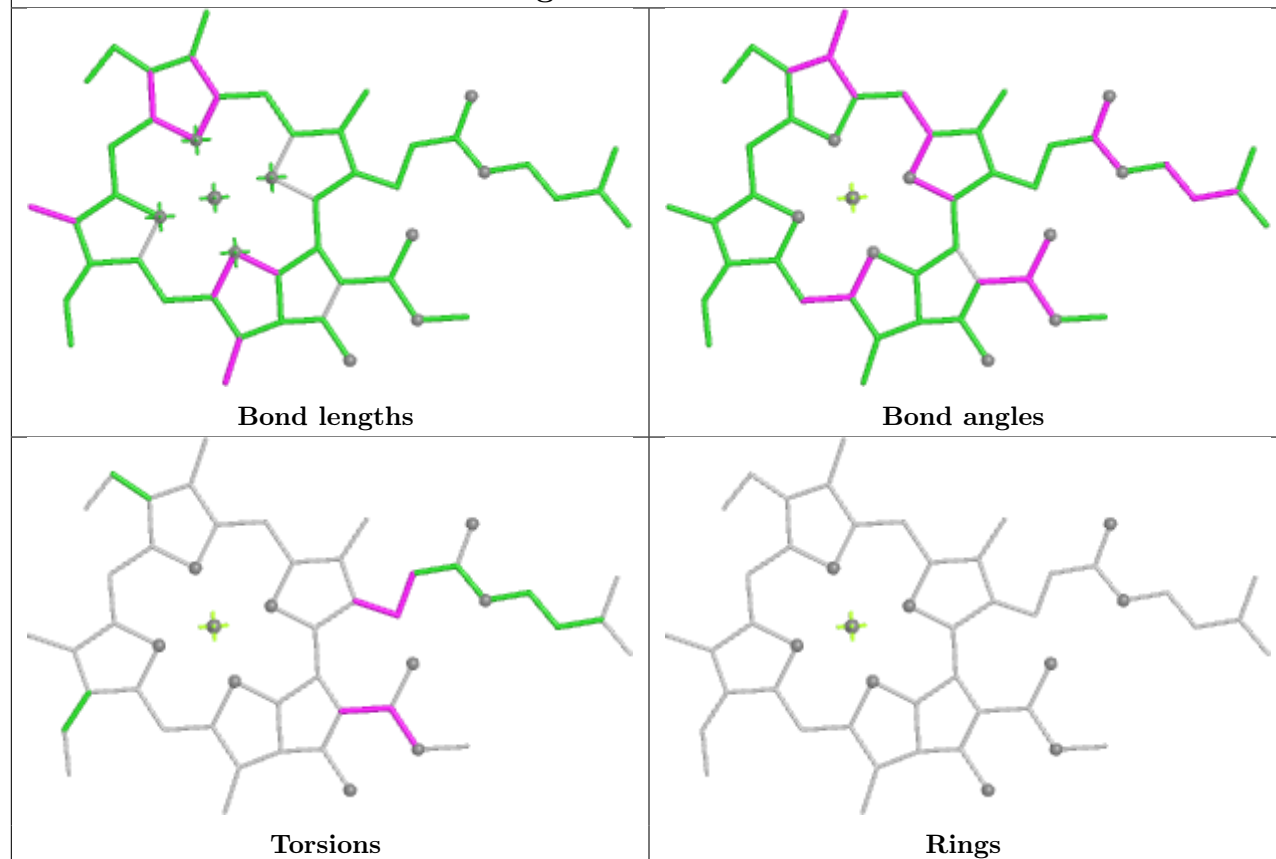


Ligand CLA f 602**Ligand CLA j 311**

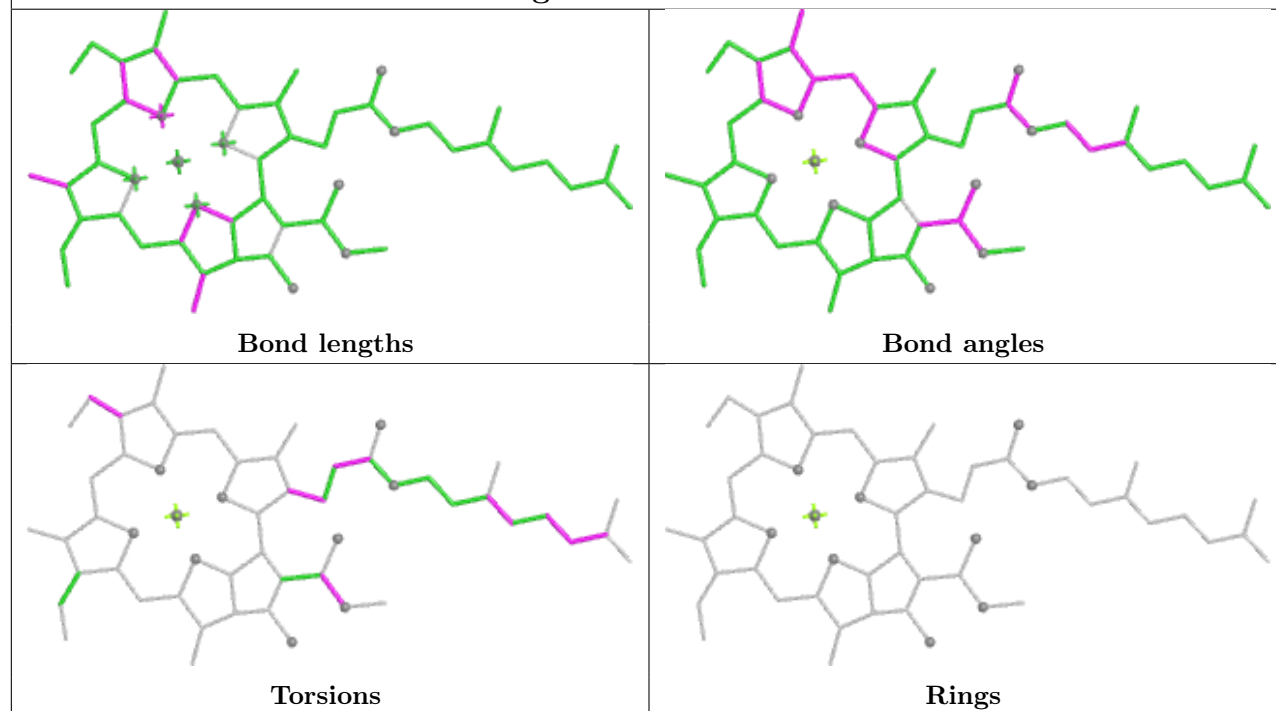
Ligand CLA c 609

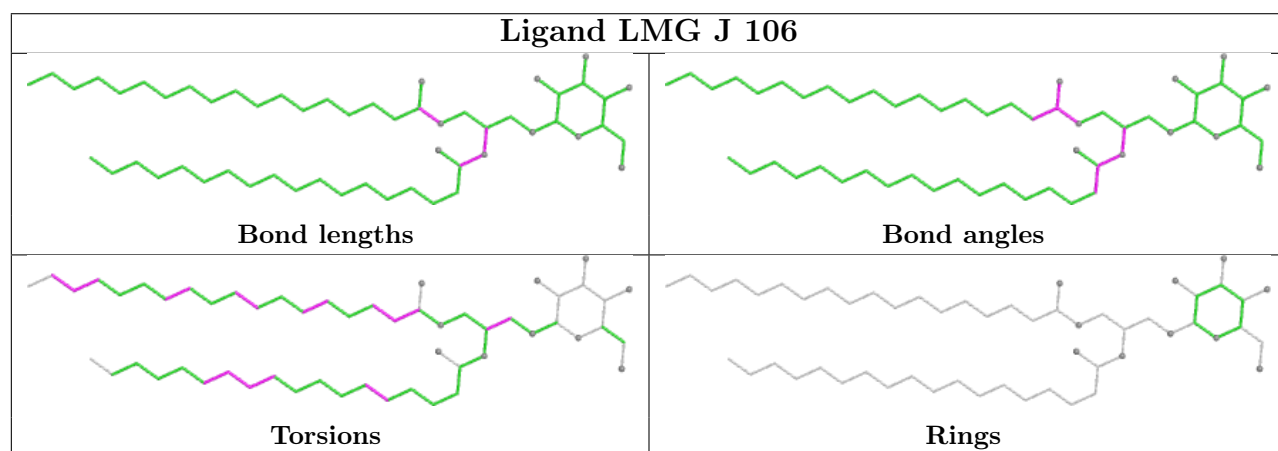
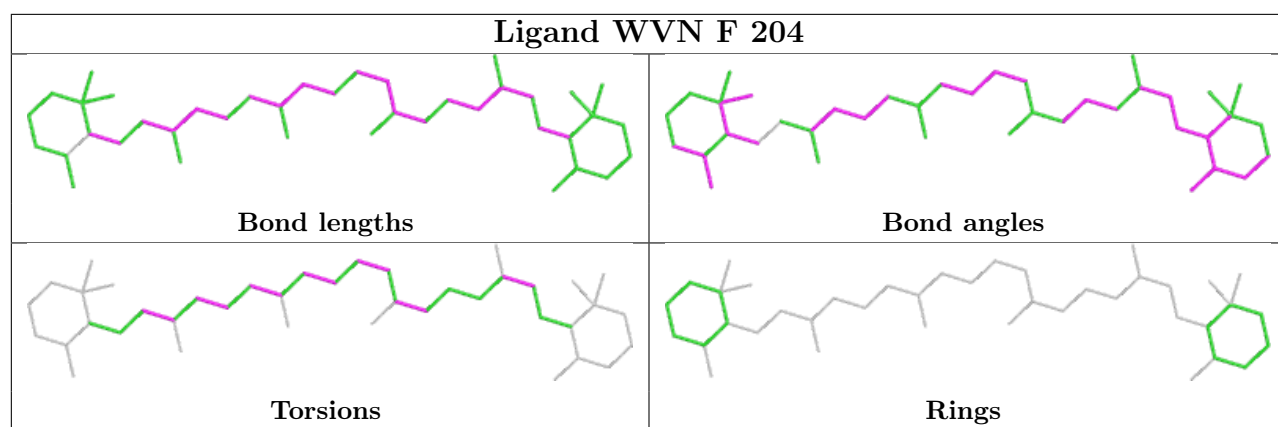


Ligand CLA a 303

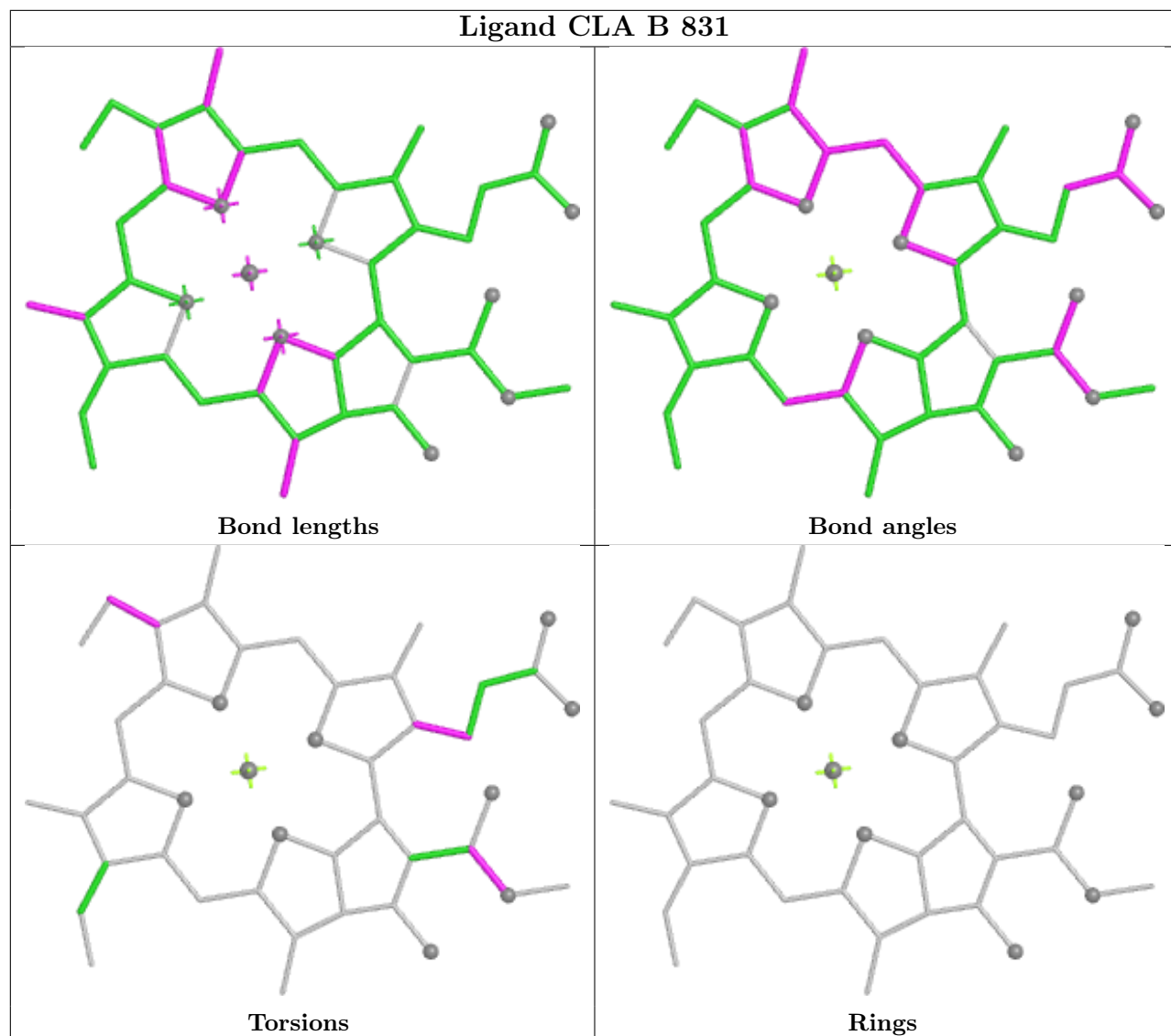


Ligand CLA B 820

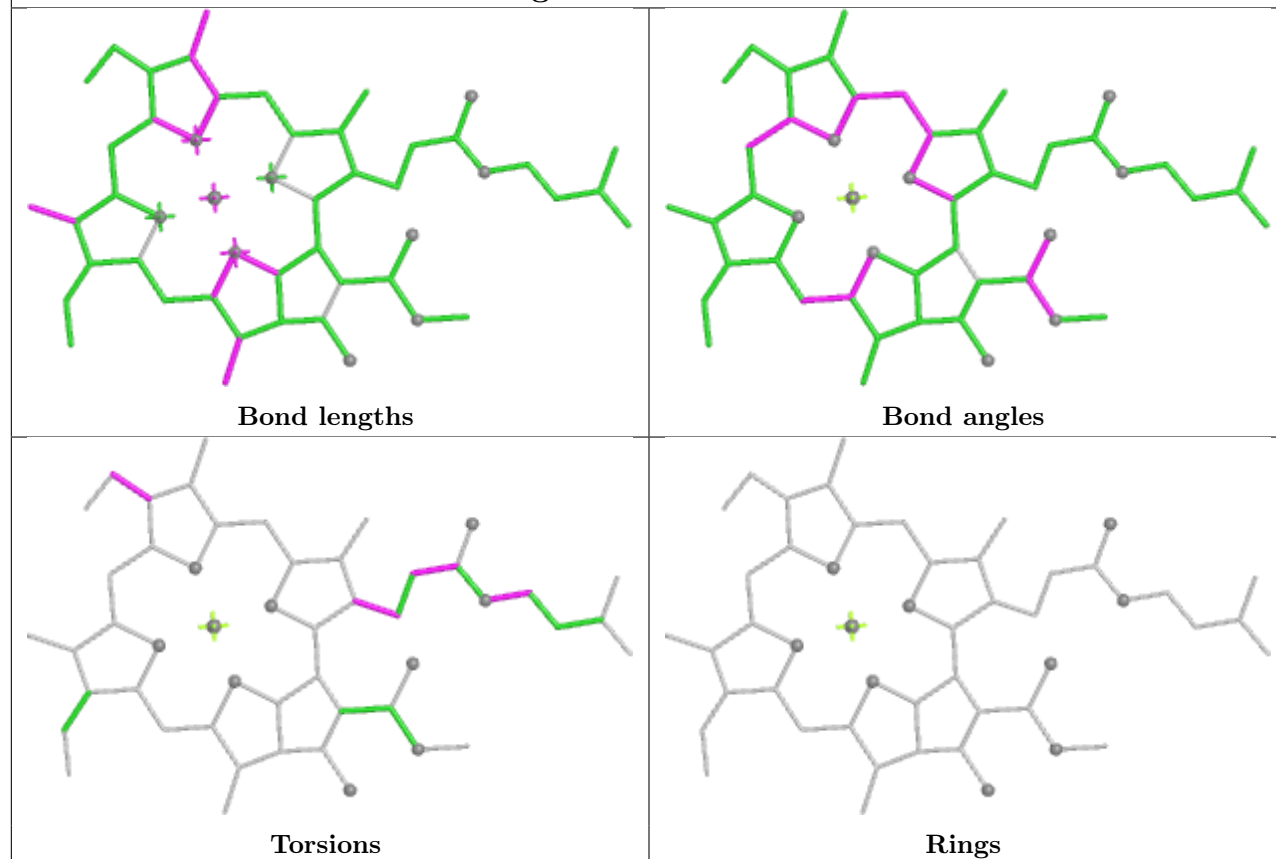




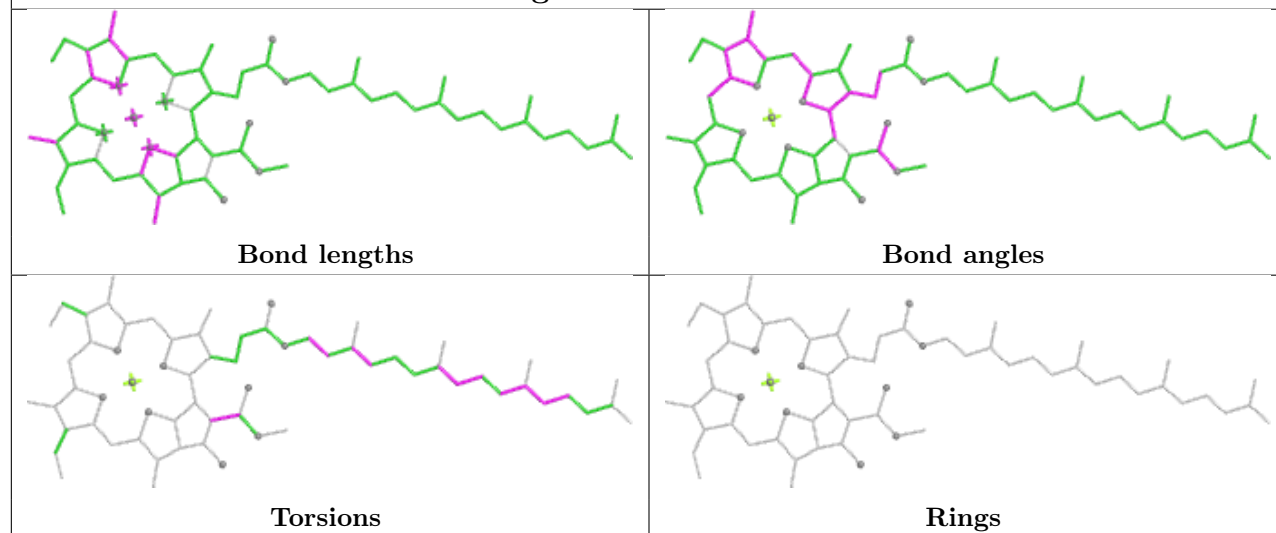
Ligand CLA B 831

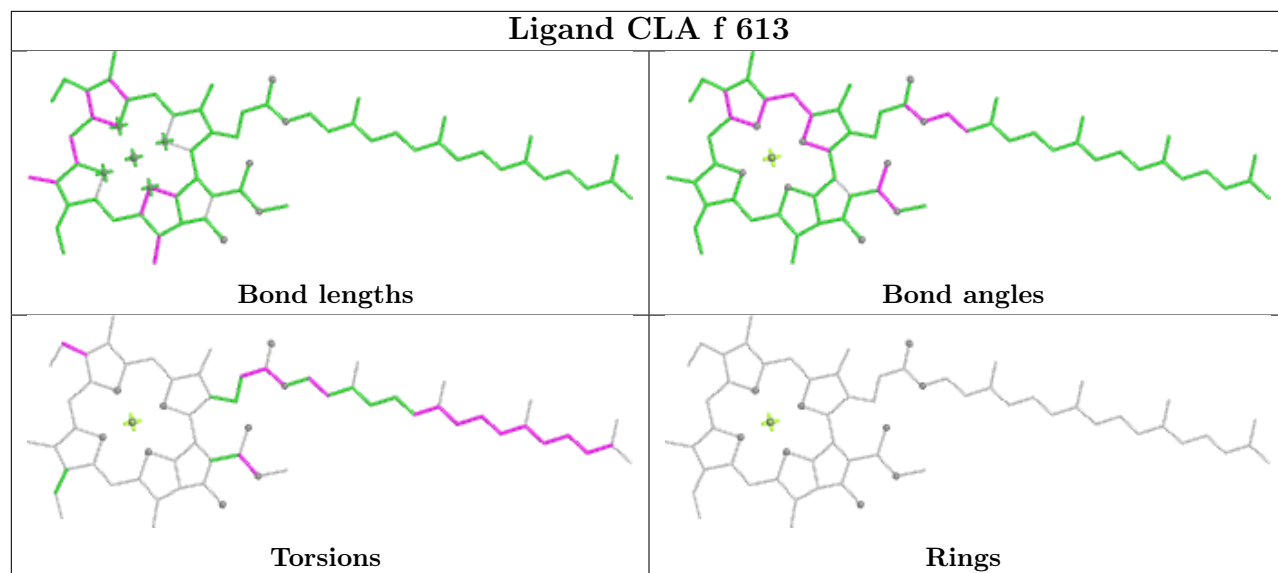
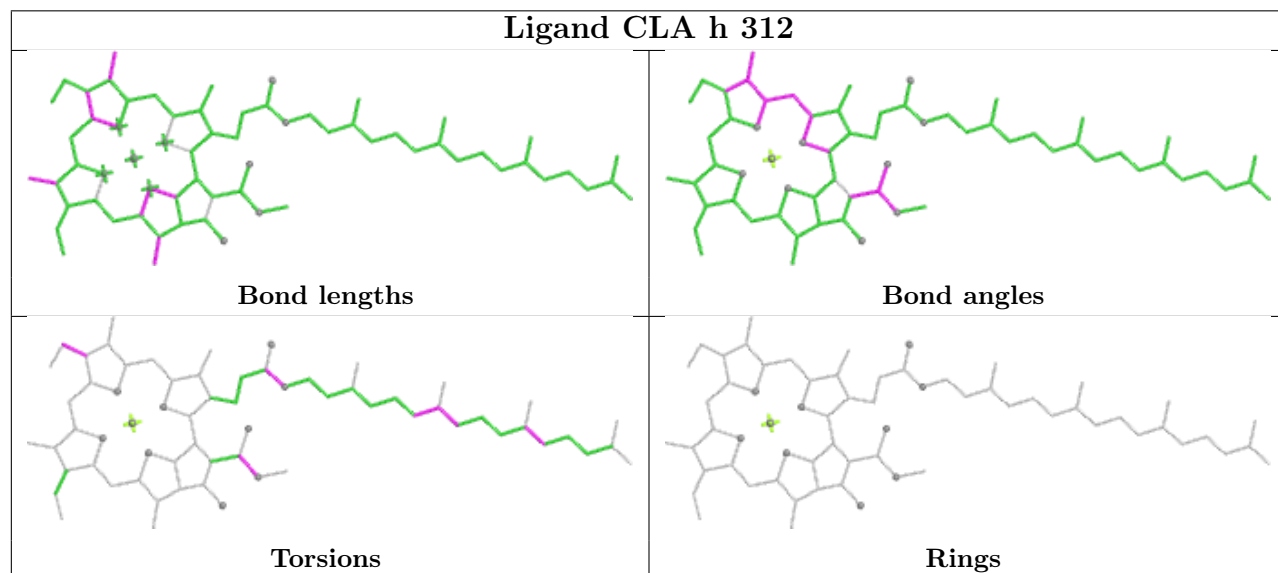
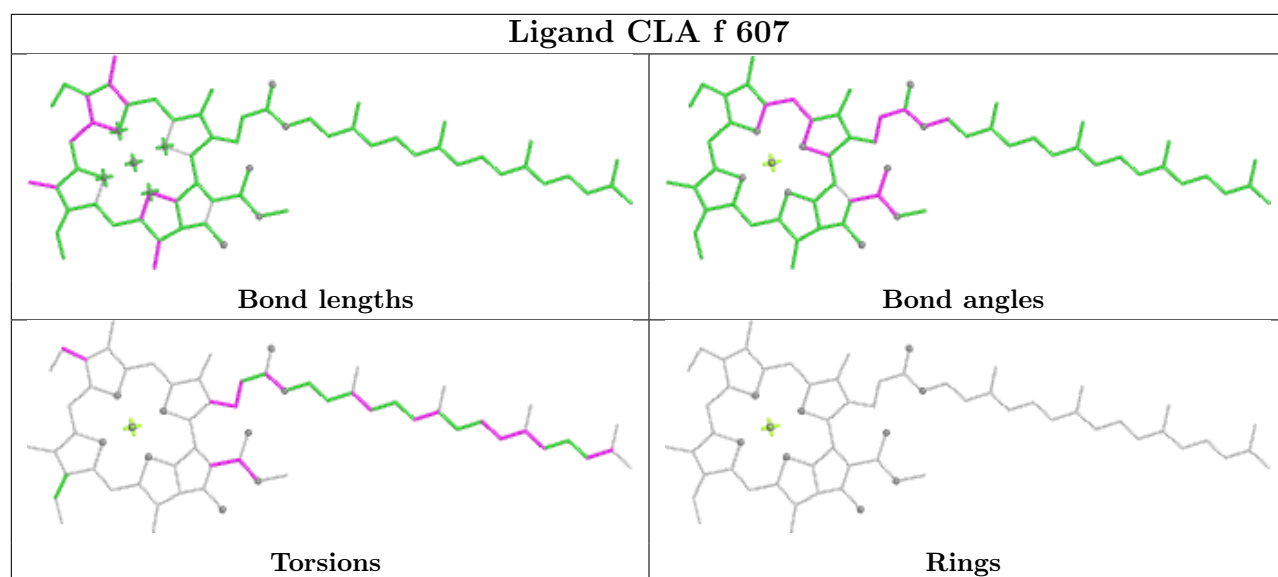


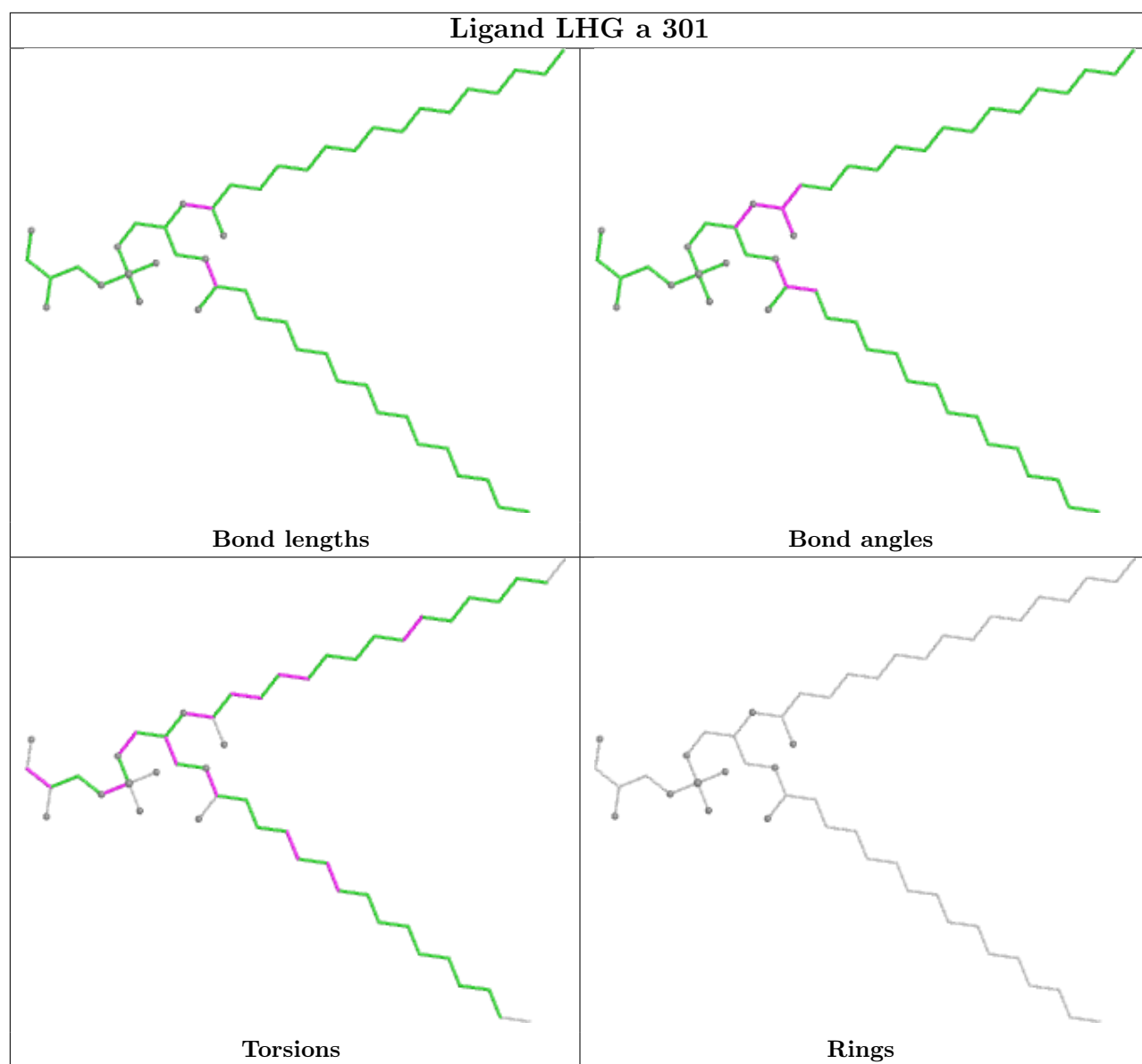
Ligand CLA A 833



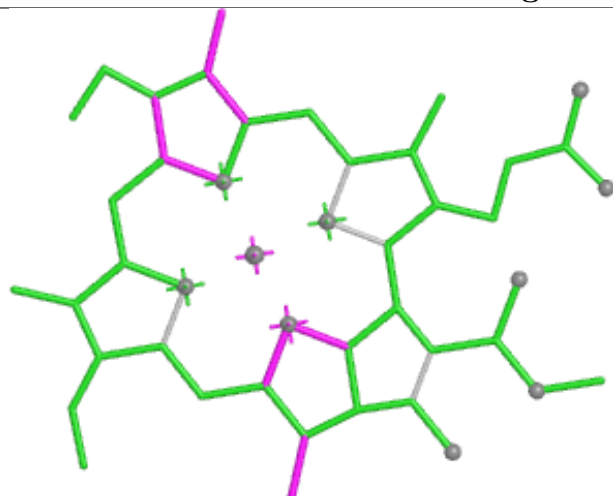
Ligand CLA A 824



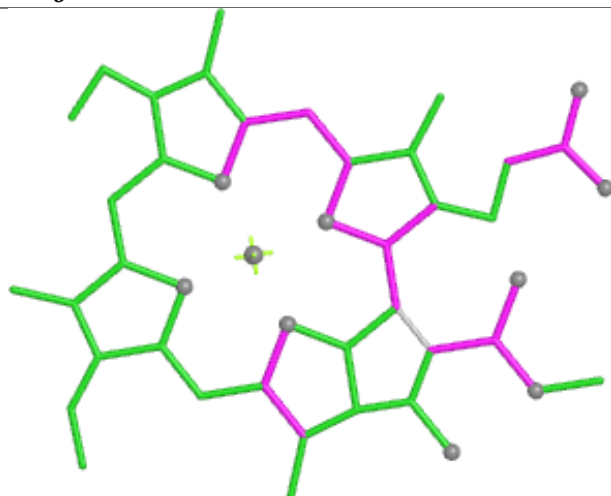




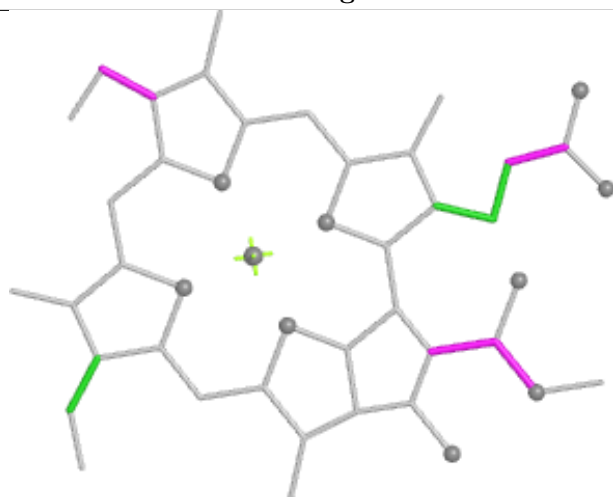
Ligand CLA j 306



Bond lengths



Bond angles

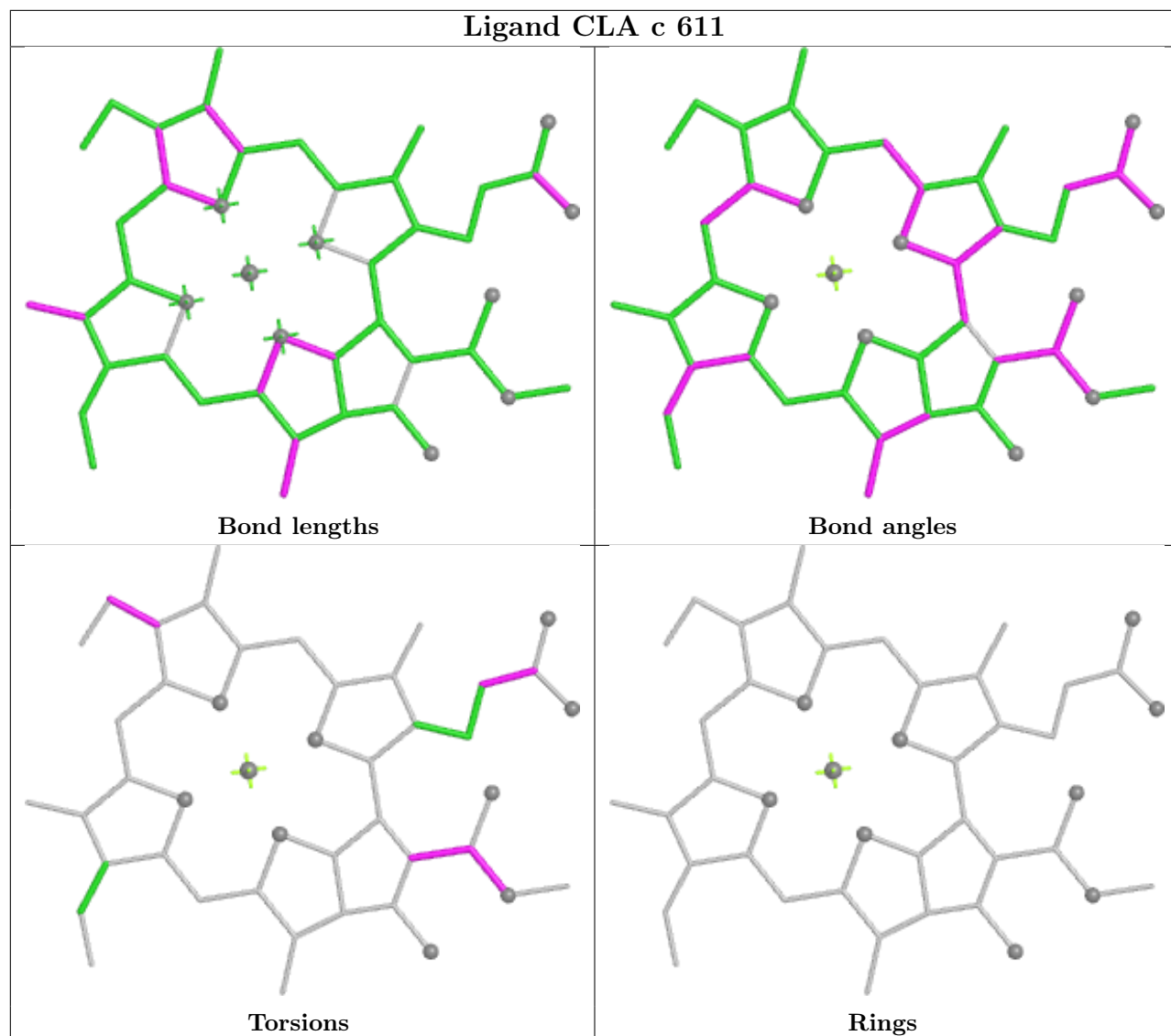


Torsions

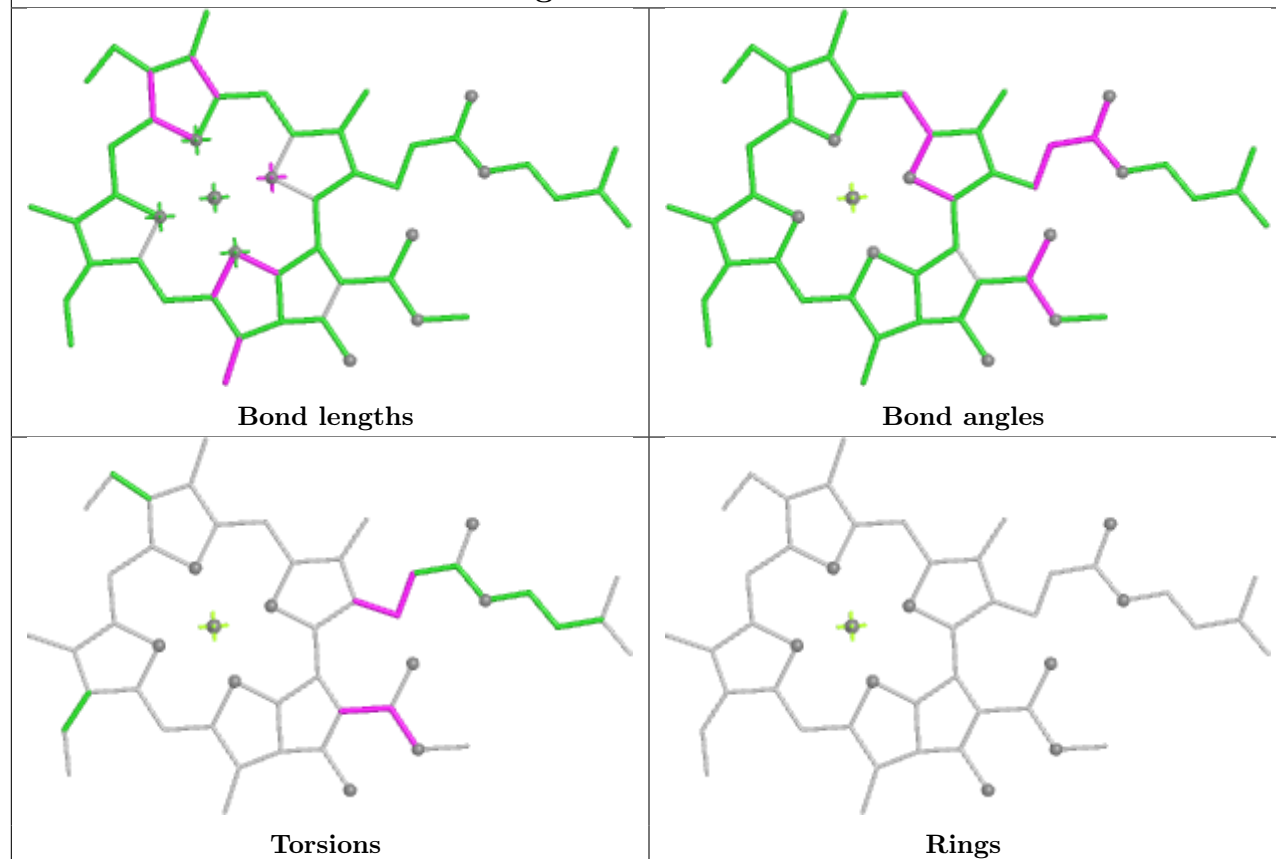


Rings

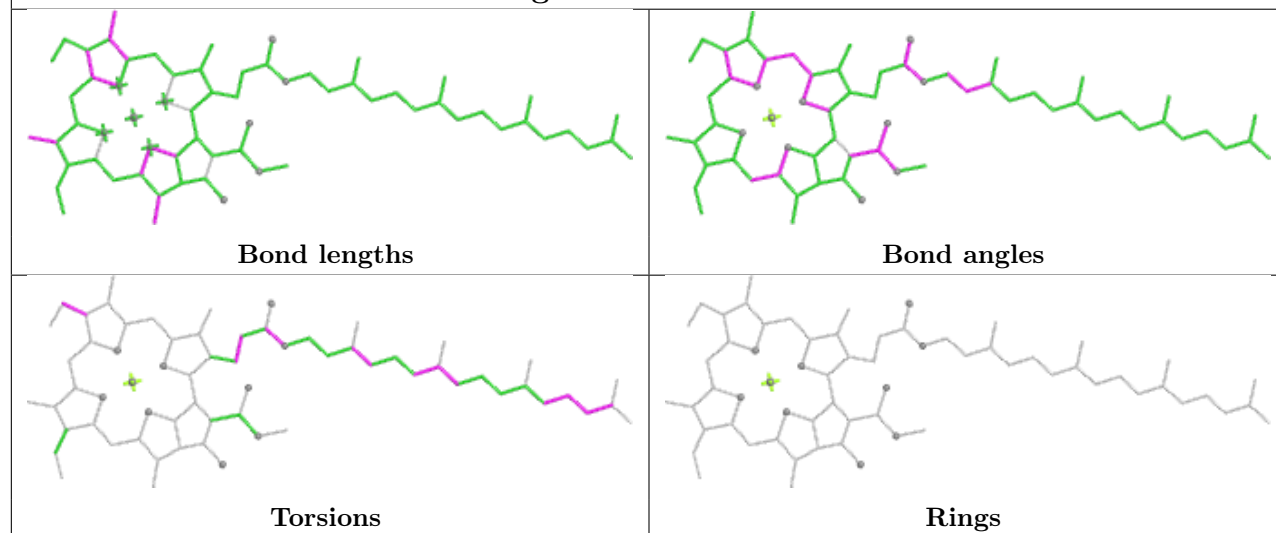
Ligand CLA c 611



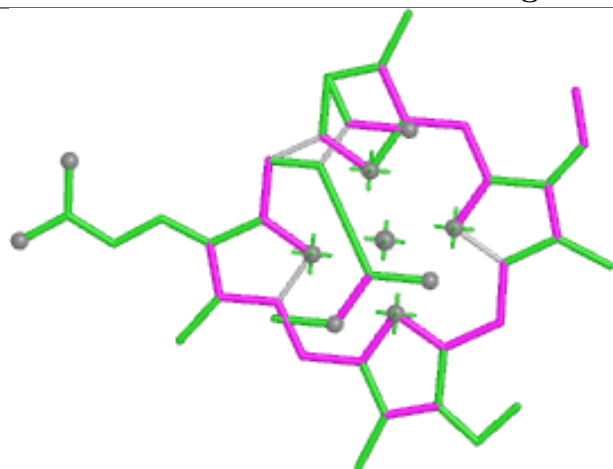
Ligand CLA d 301



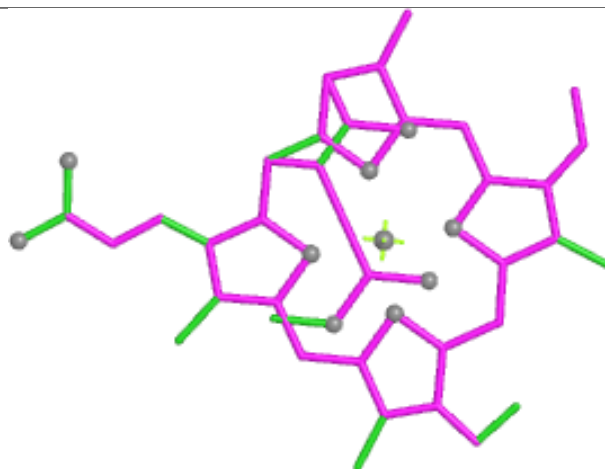
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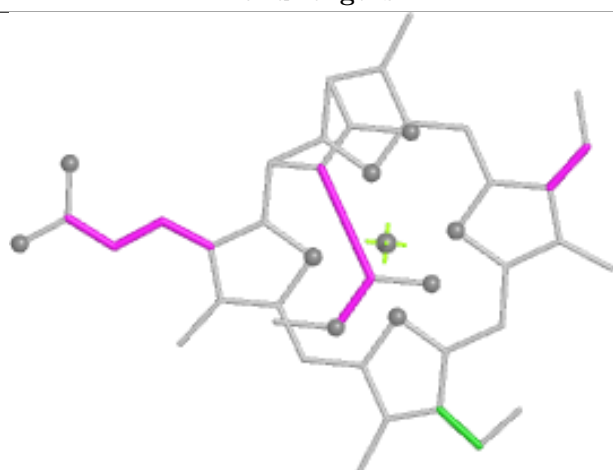
Ligand KC2 c 610



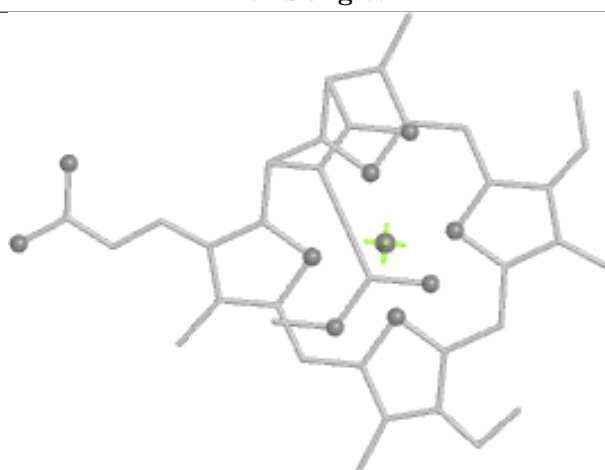
Bond lengths



Bond angles

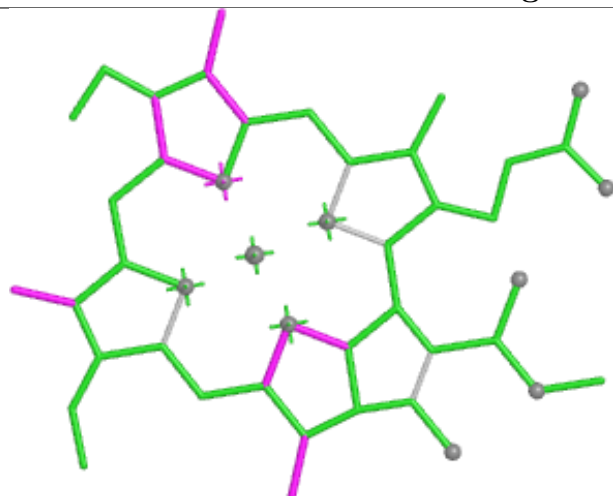


Torsions

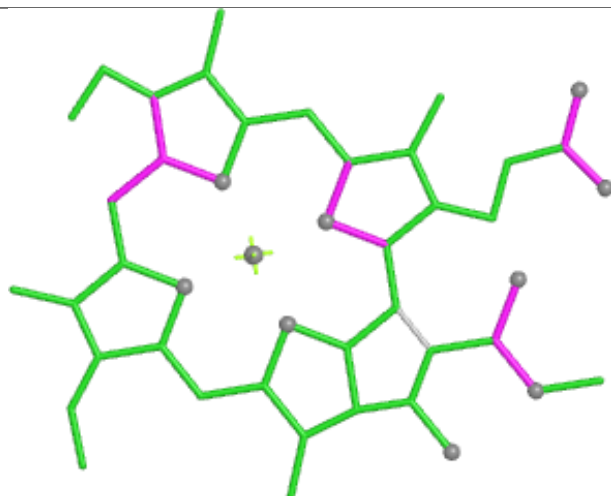


Rings

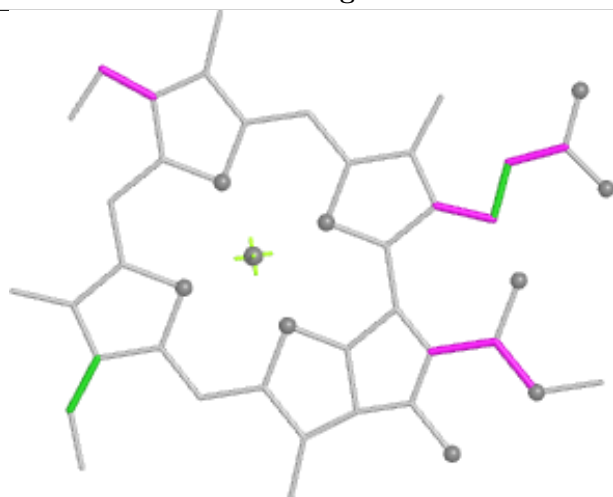
Ligand CLA f 605



Bond lengths



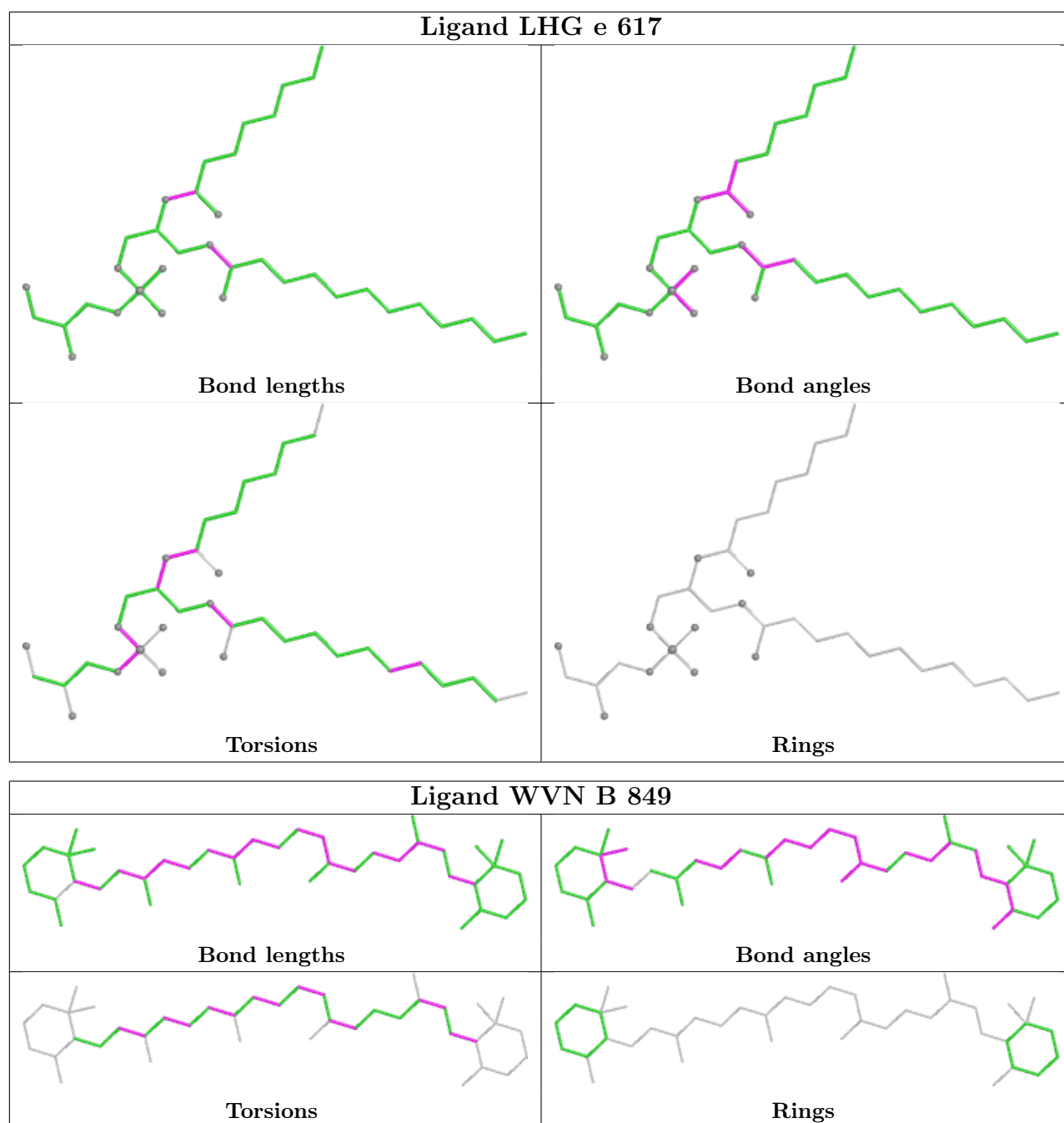
Bond angles

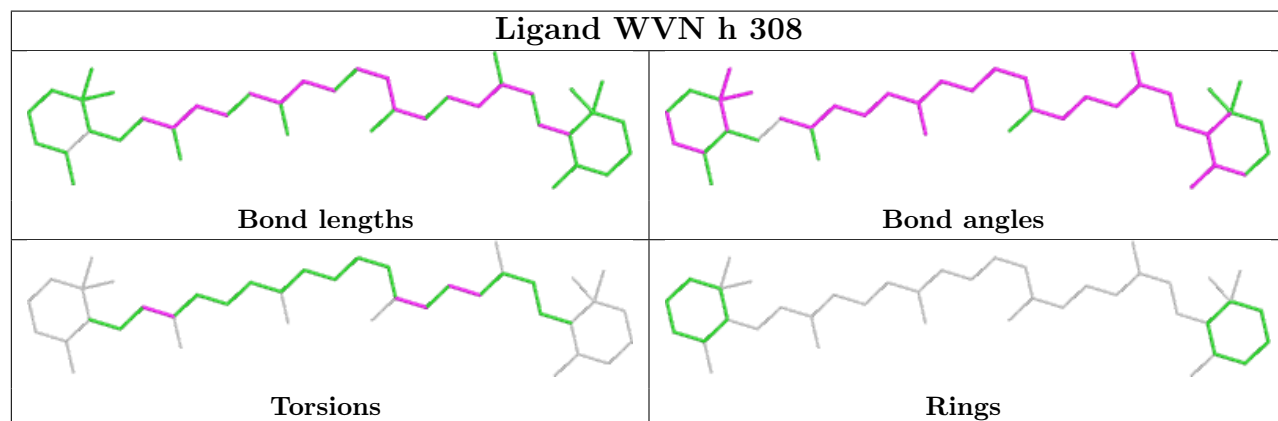
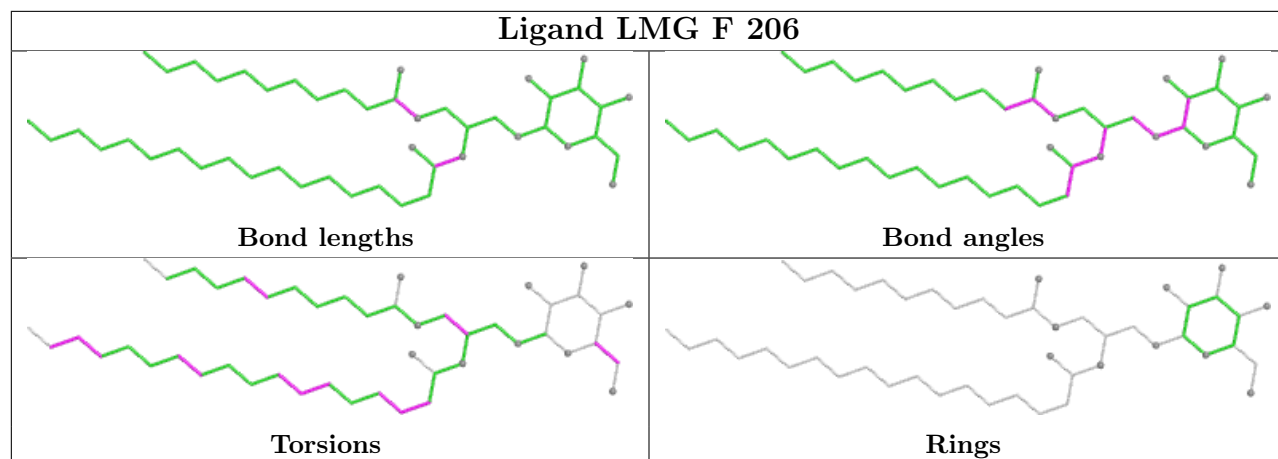


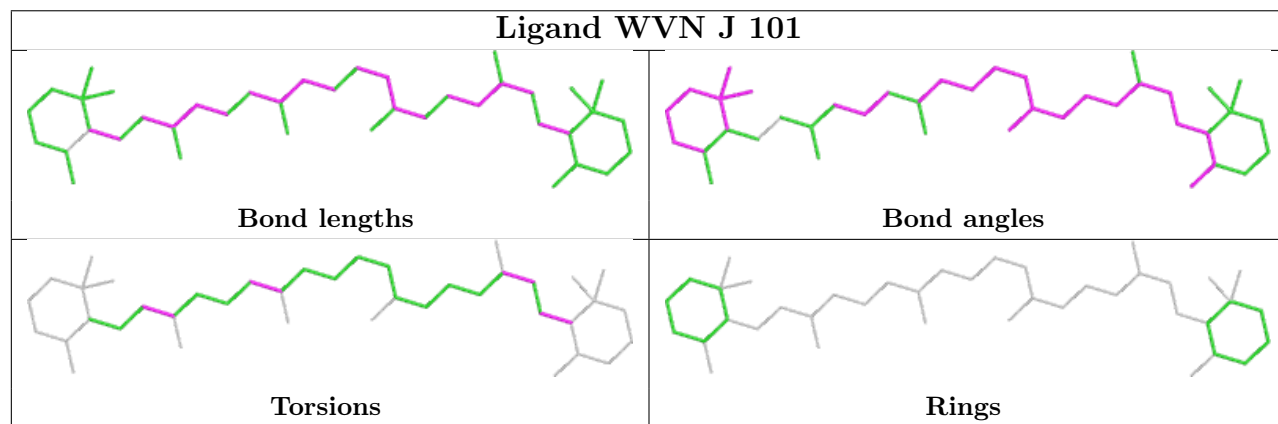
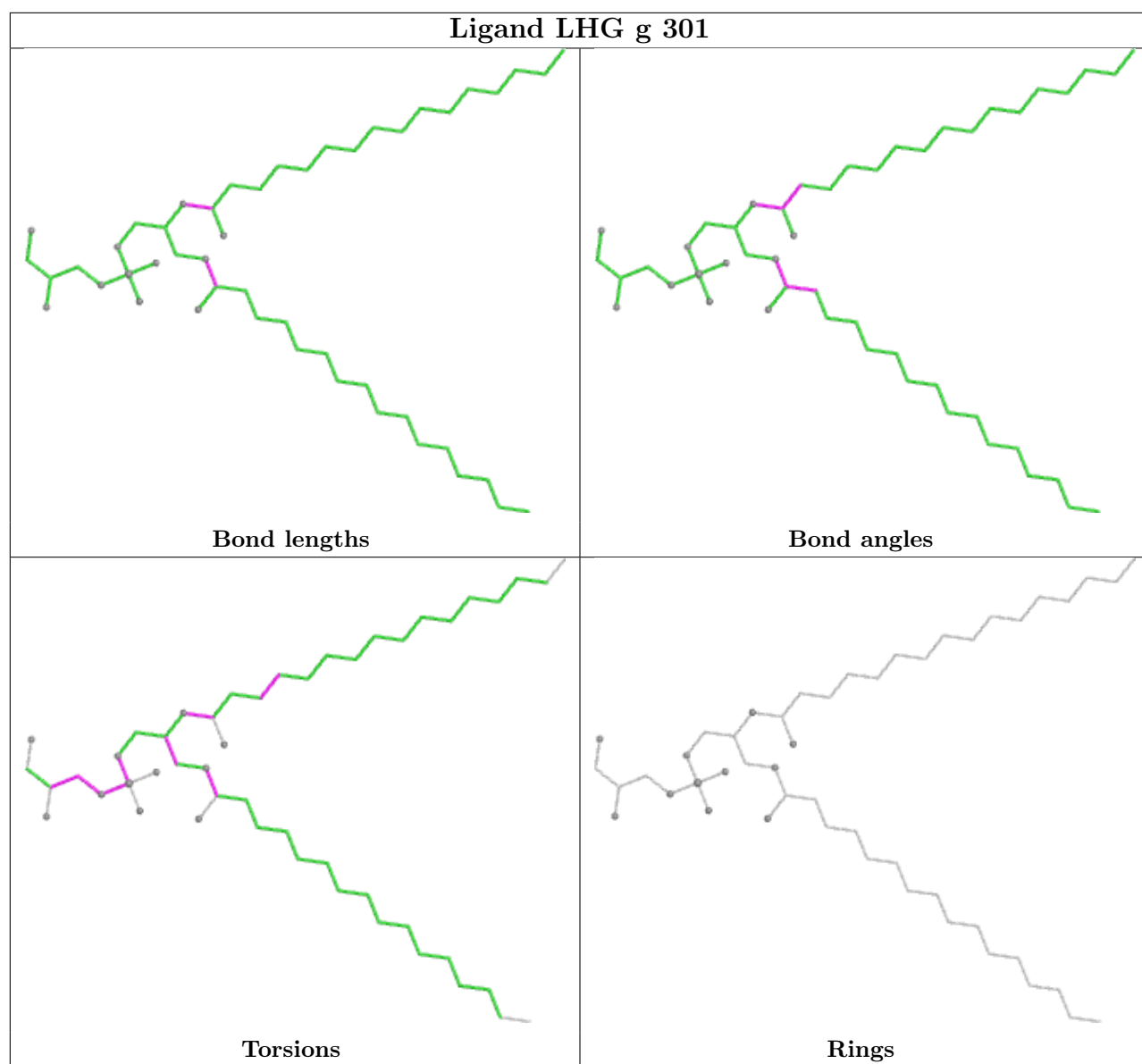
Torsions



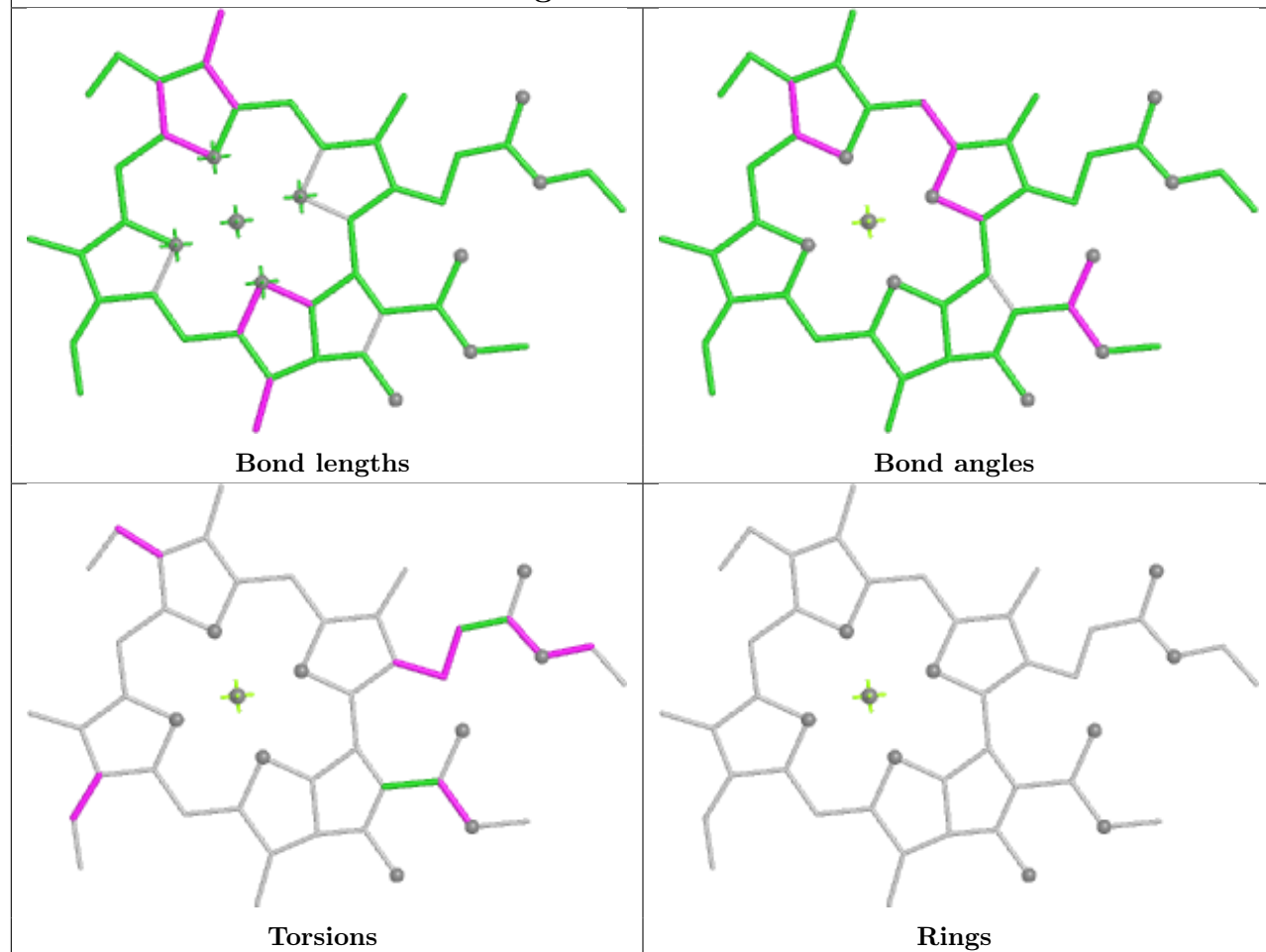
Rings



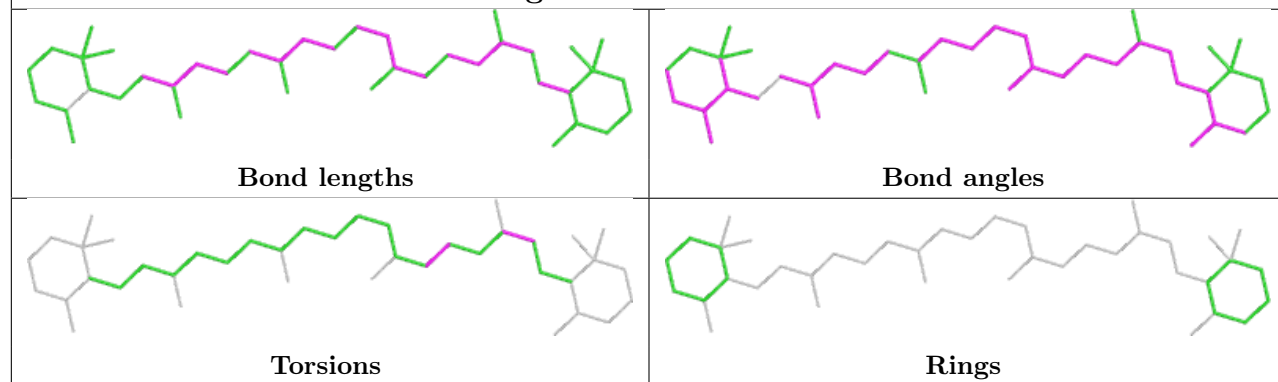


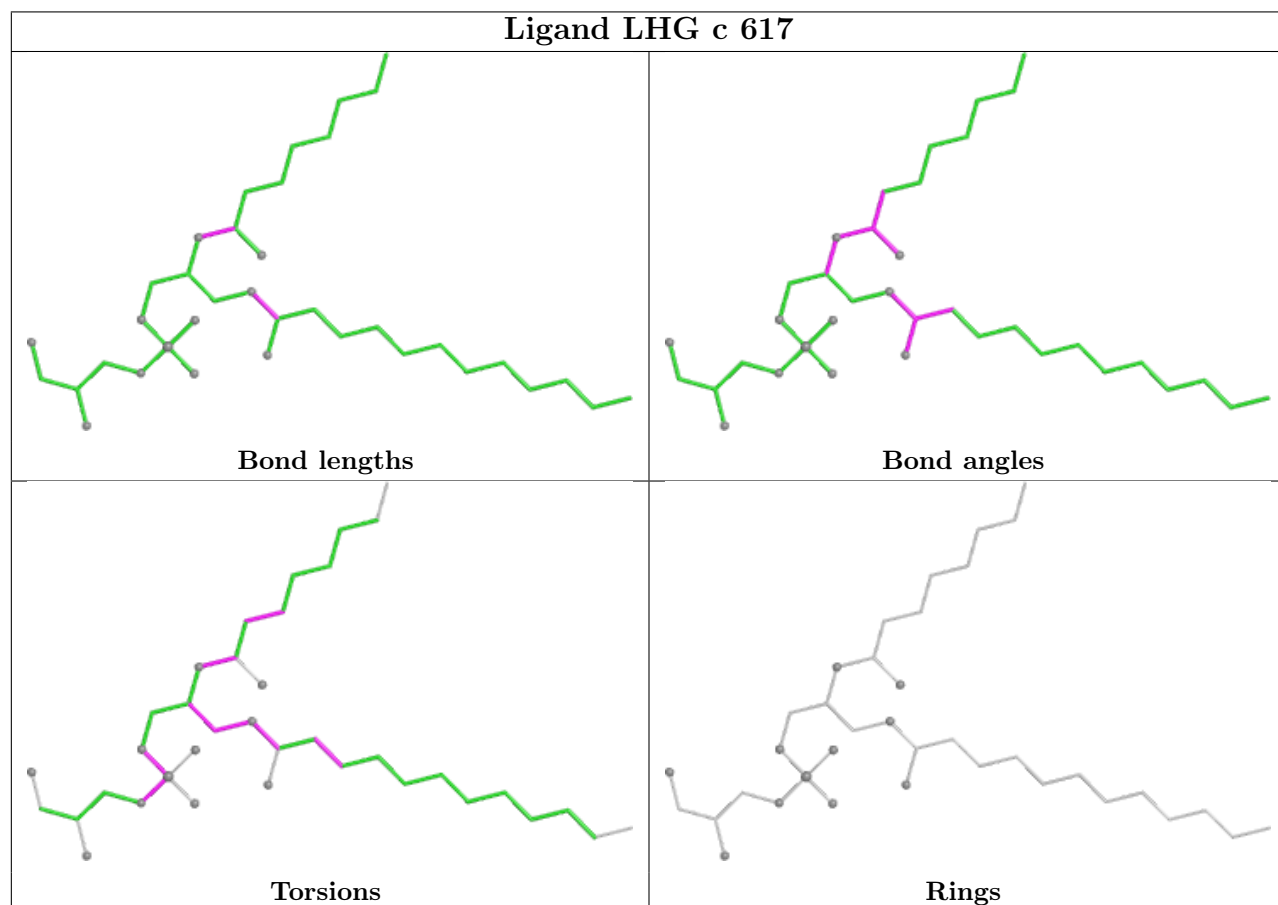
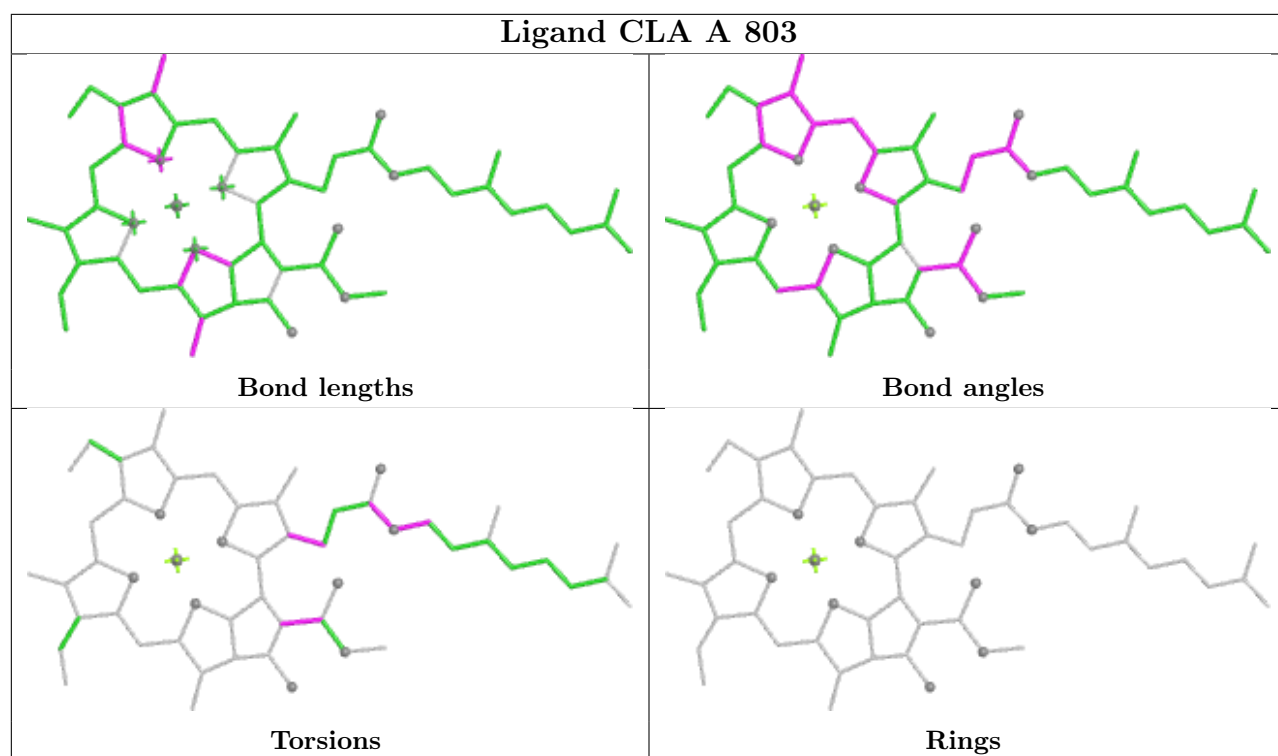


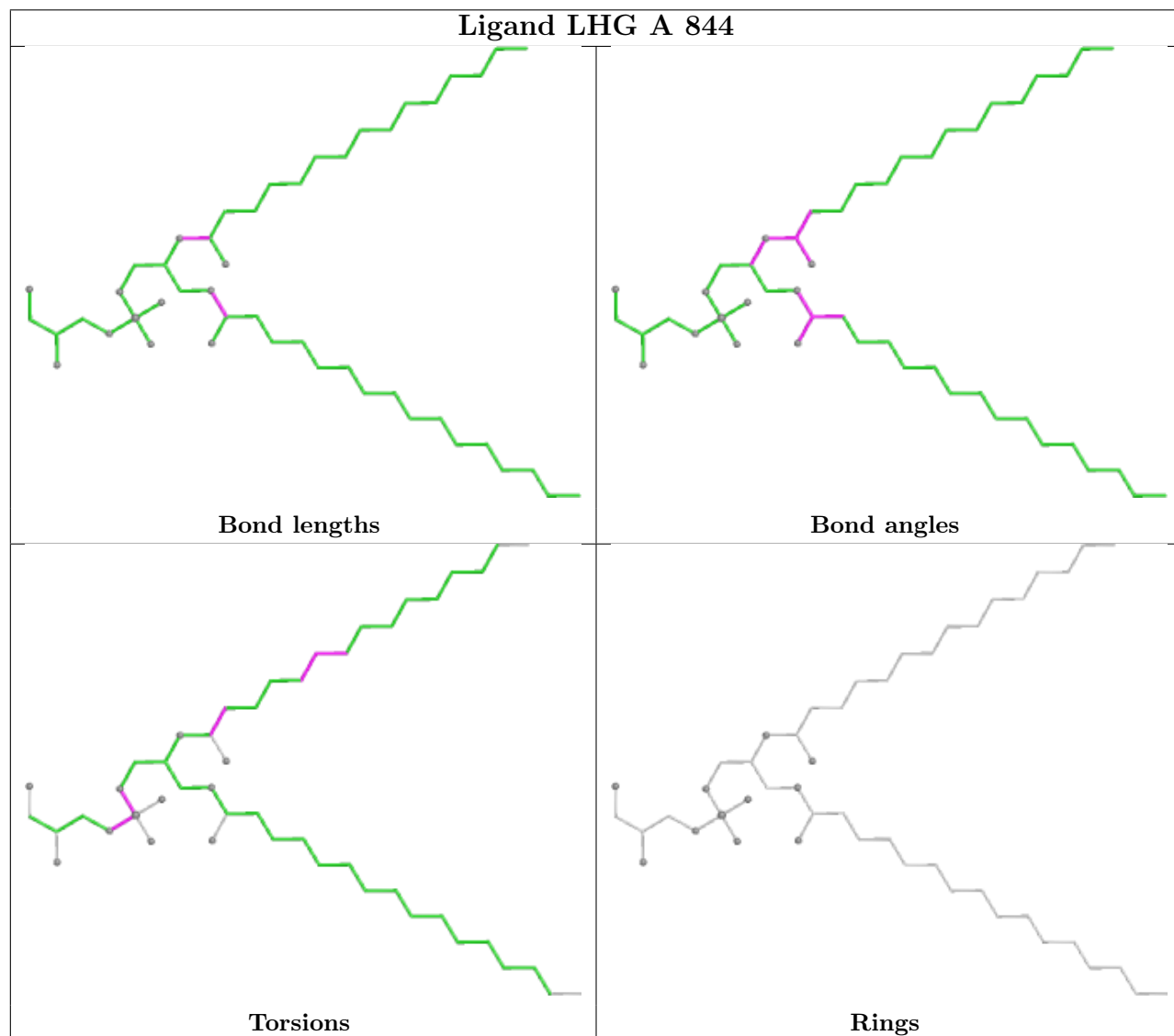
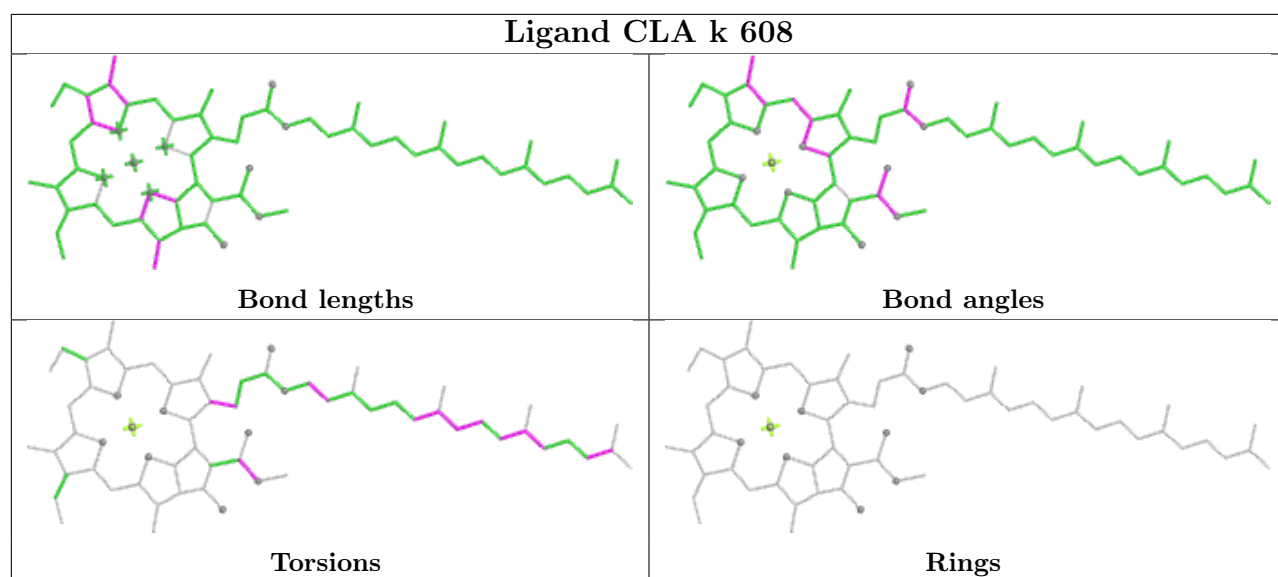
Ligand CLA f 601

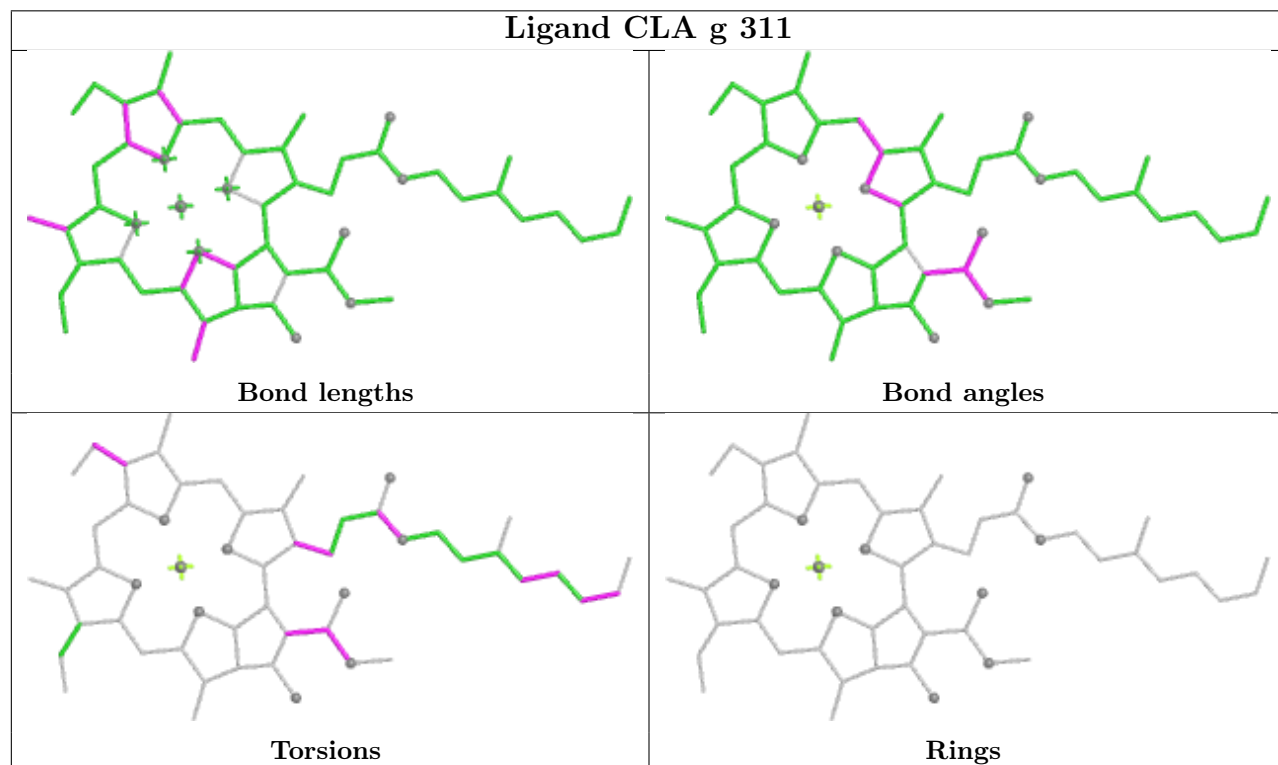
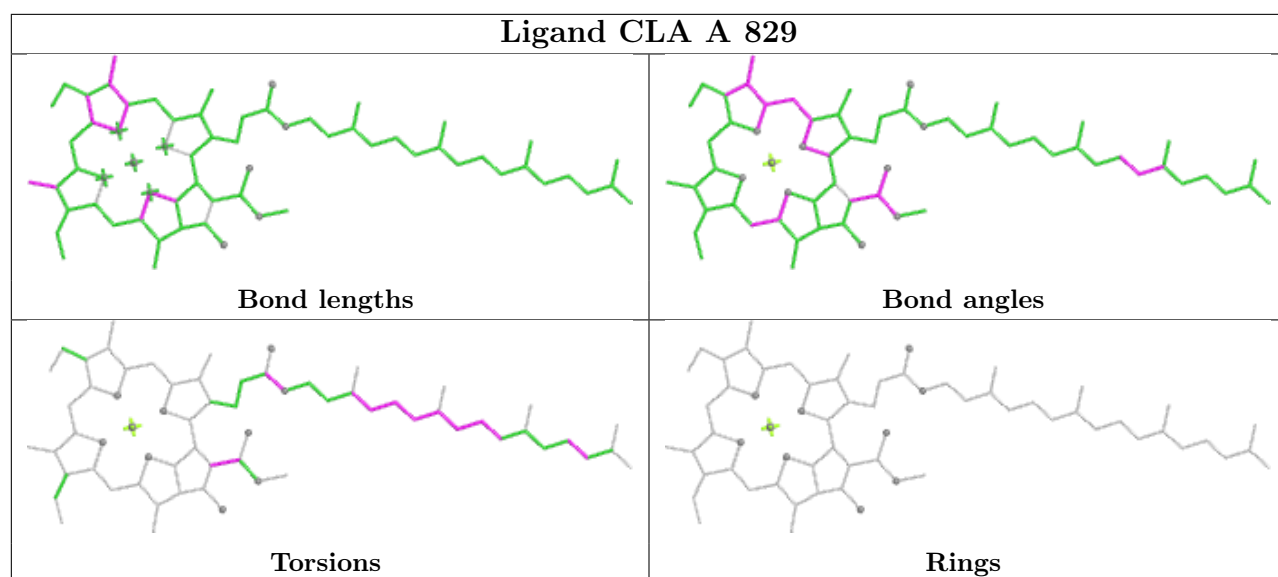


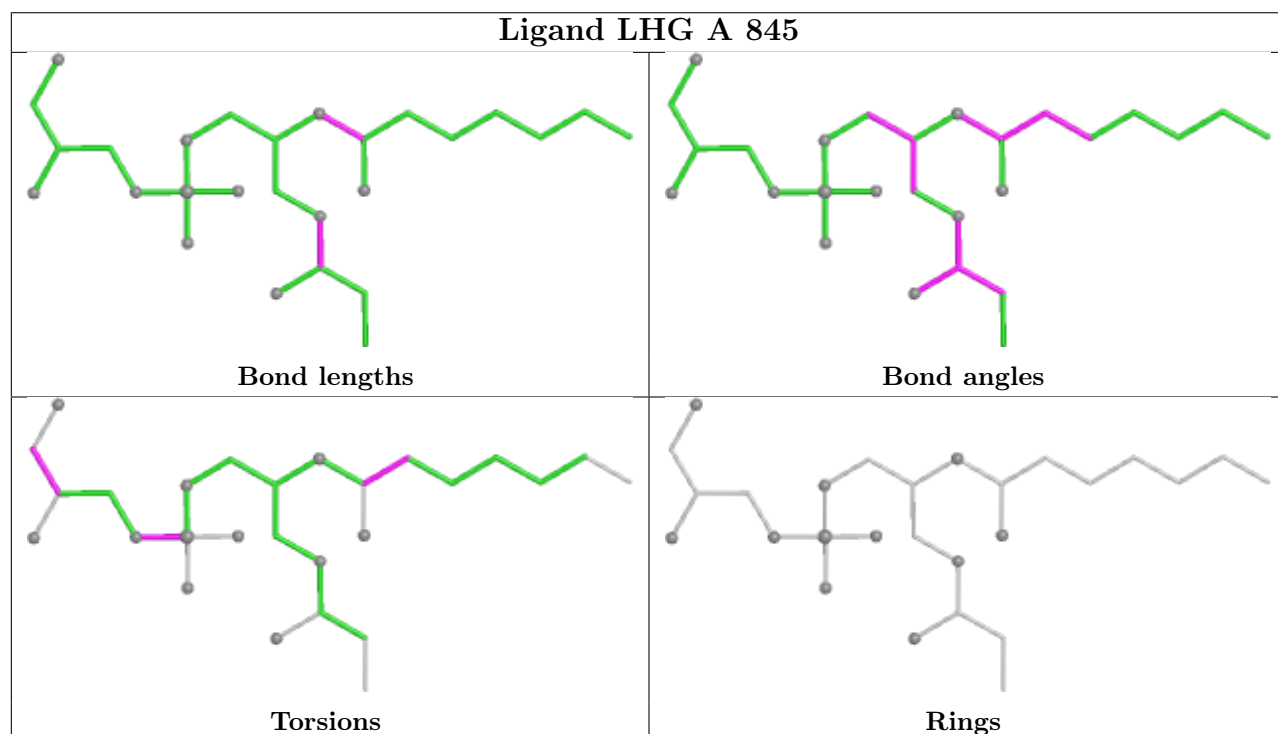
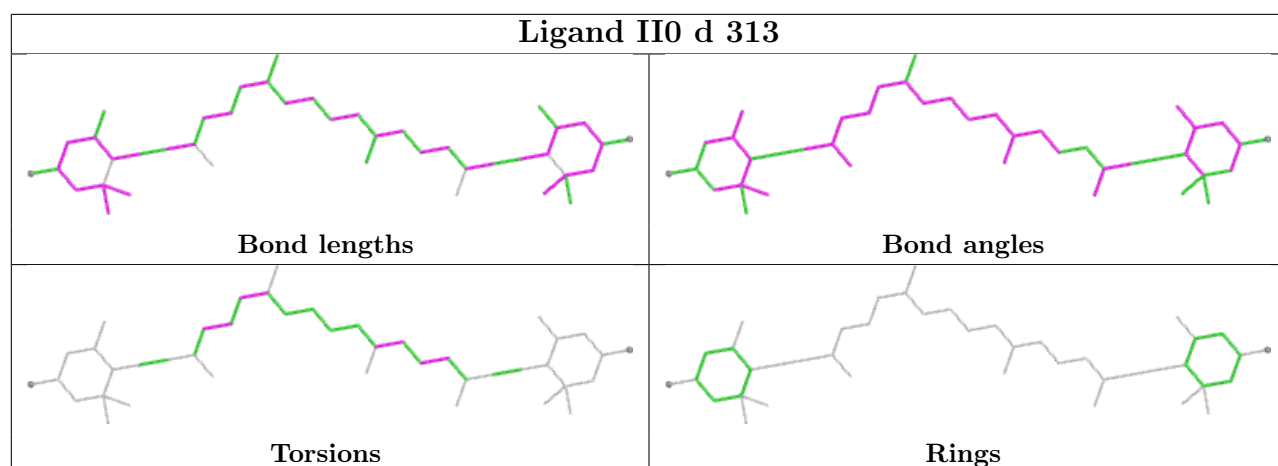
Ligand WVN L 206



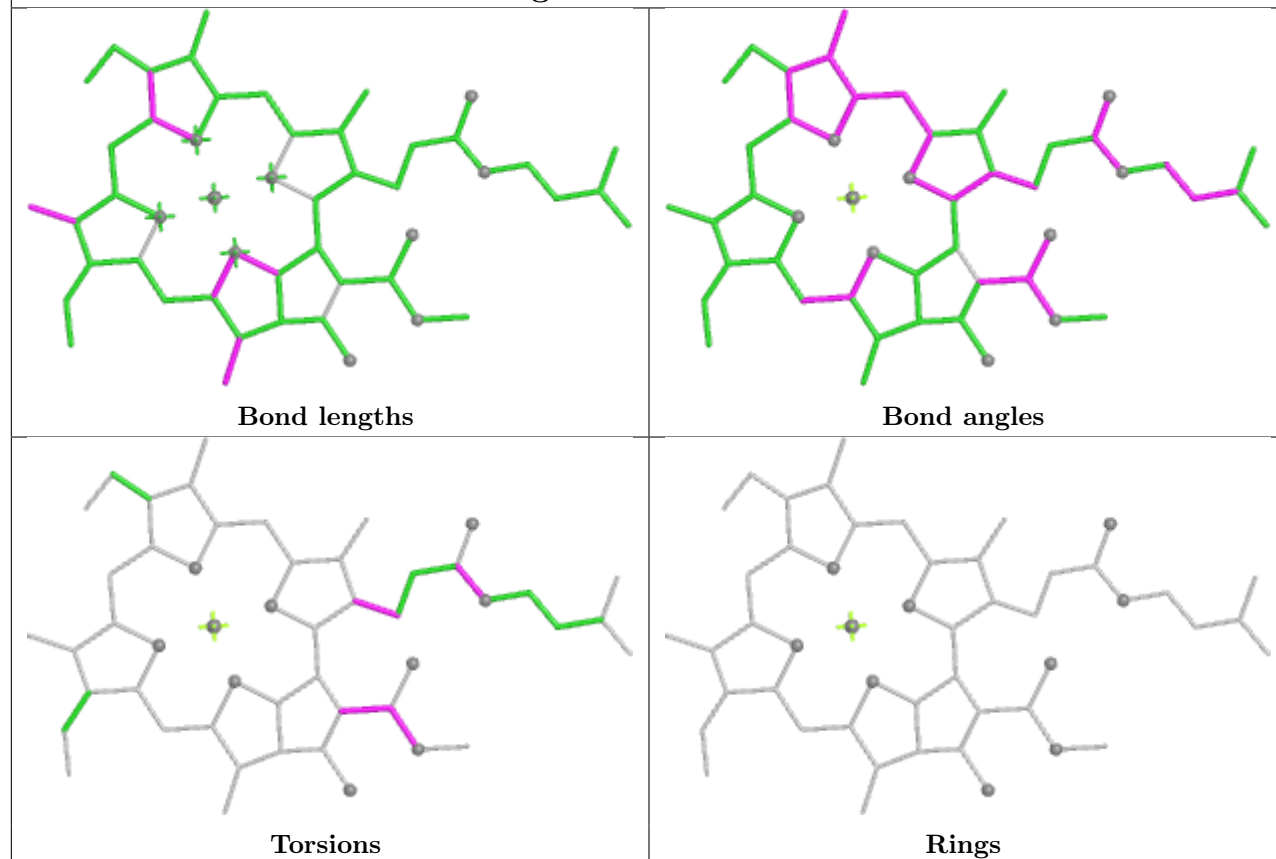




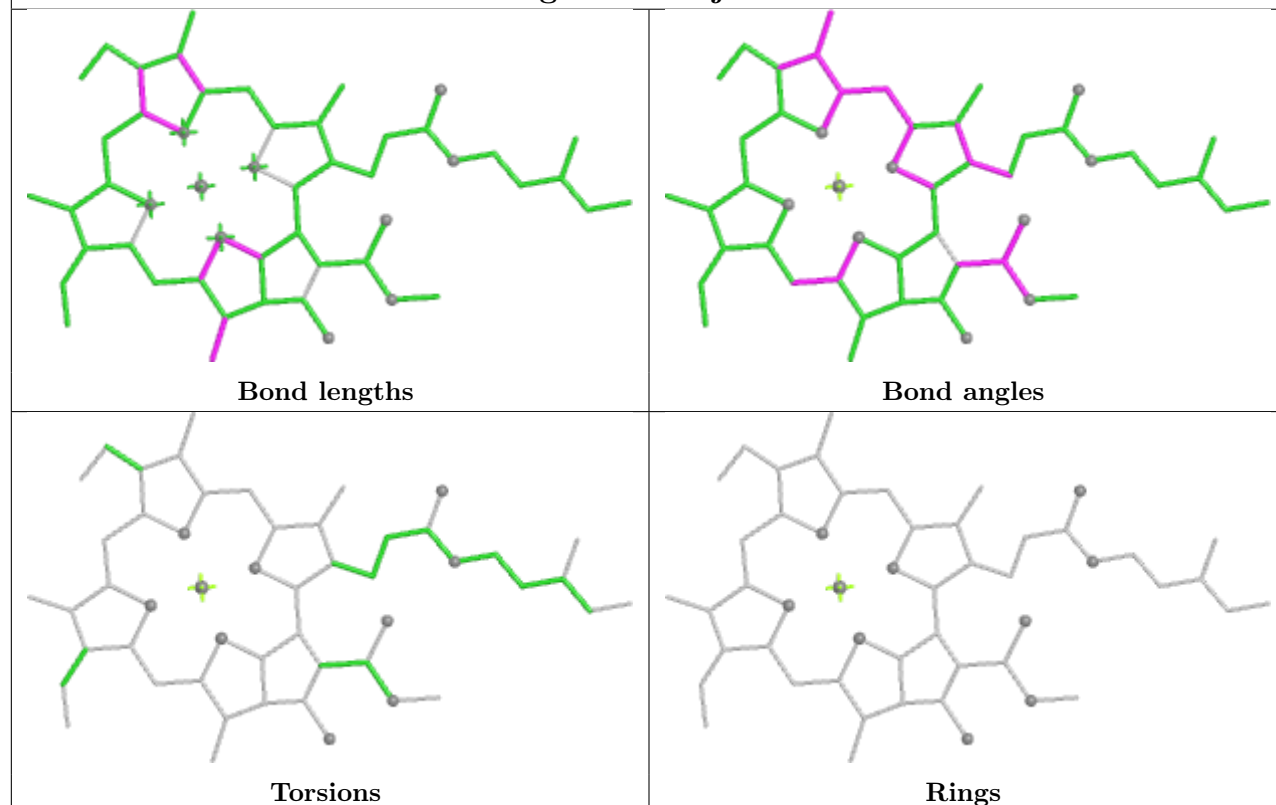


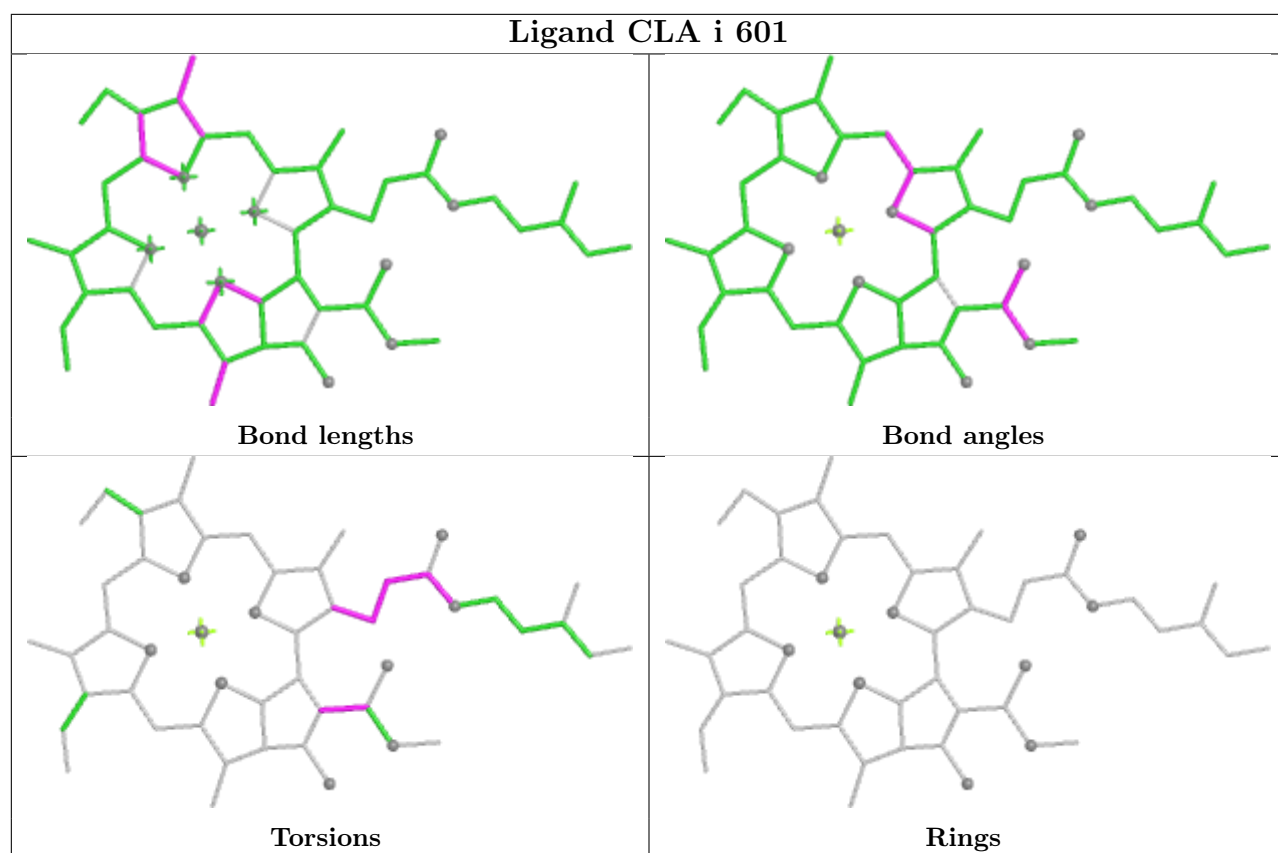


Ligand CLA A 814

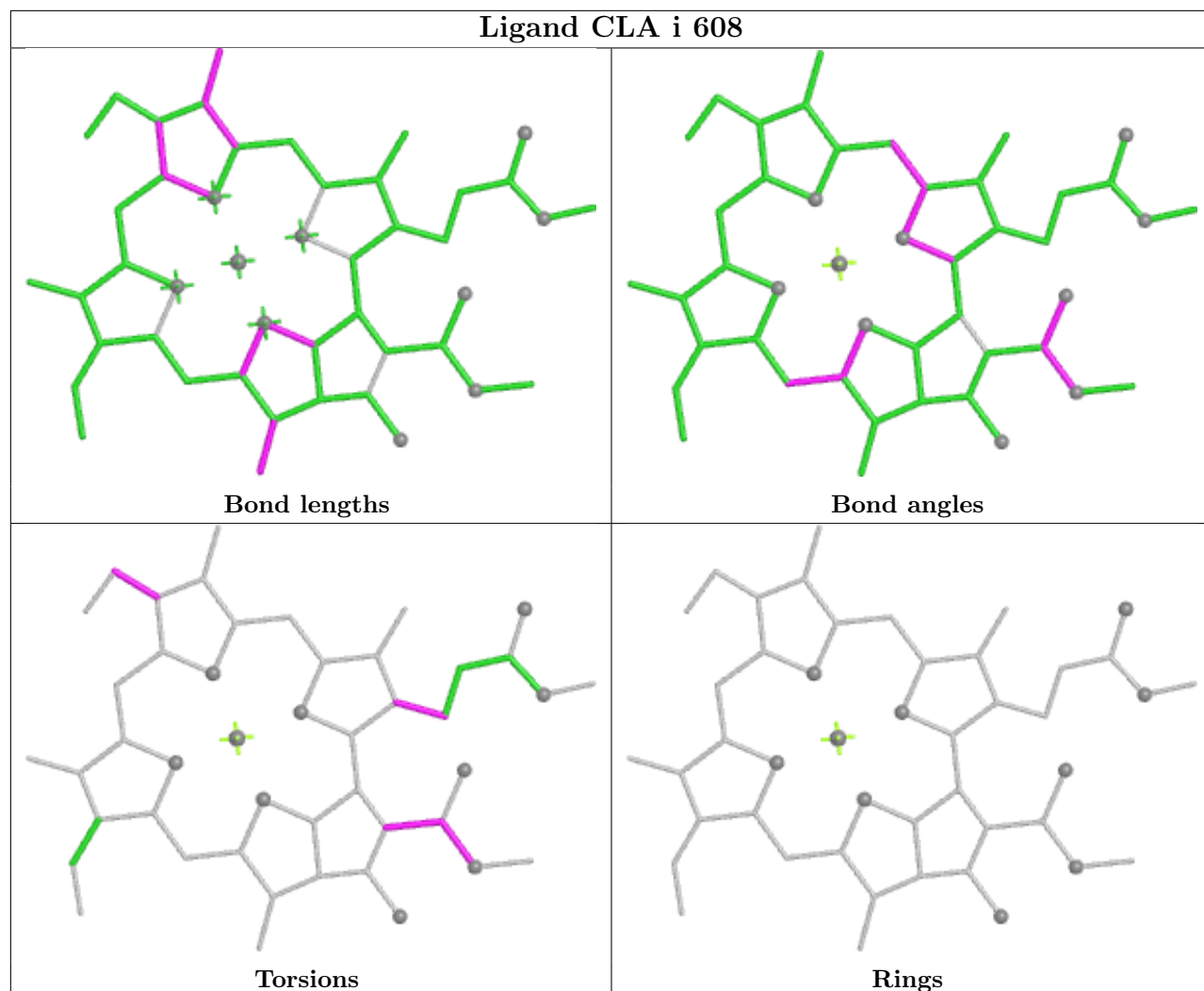


Ligand CLA j 304

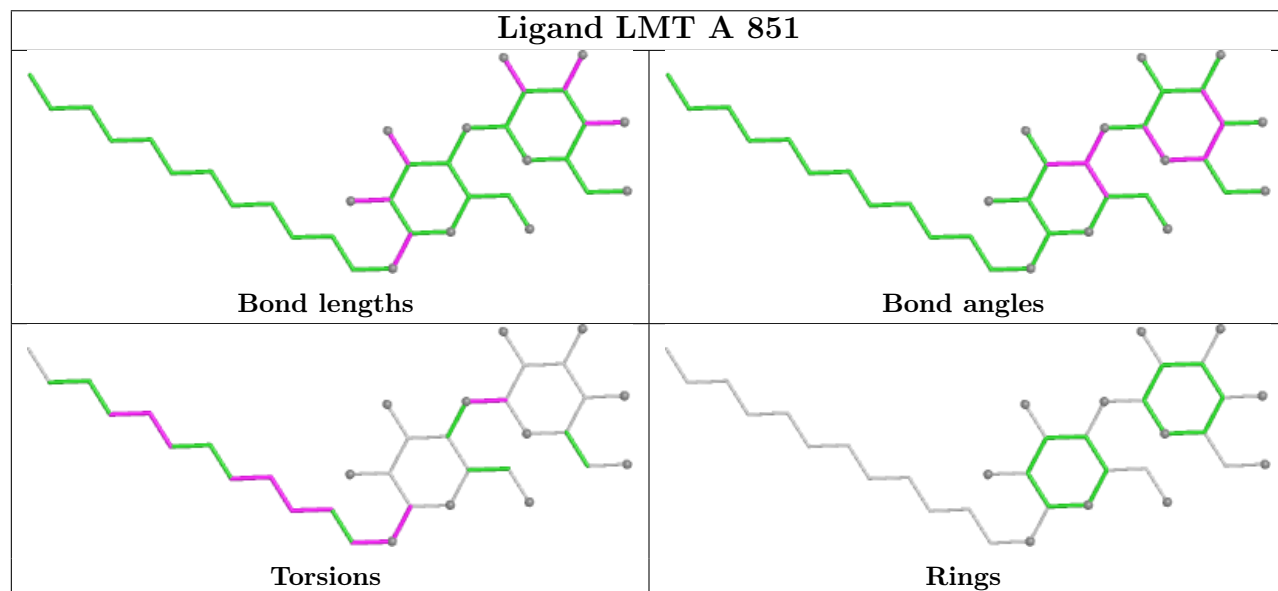


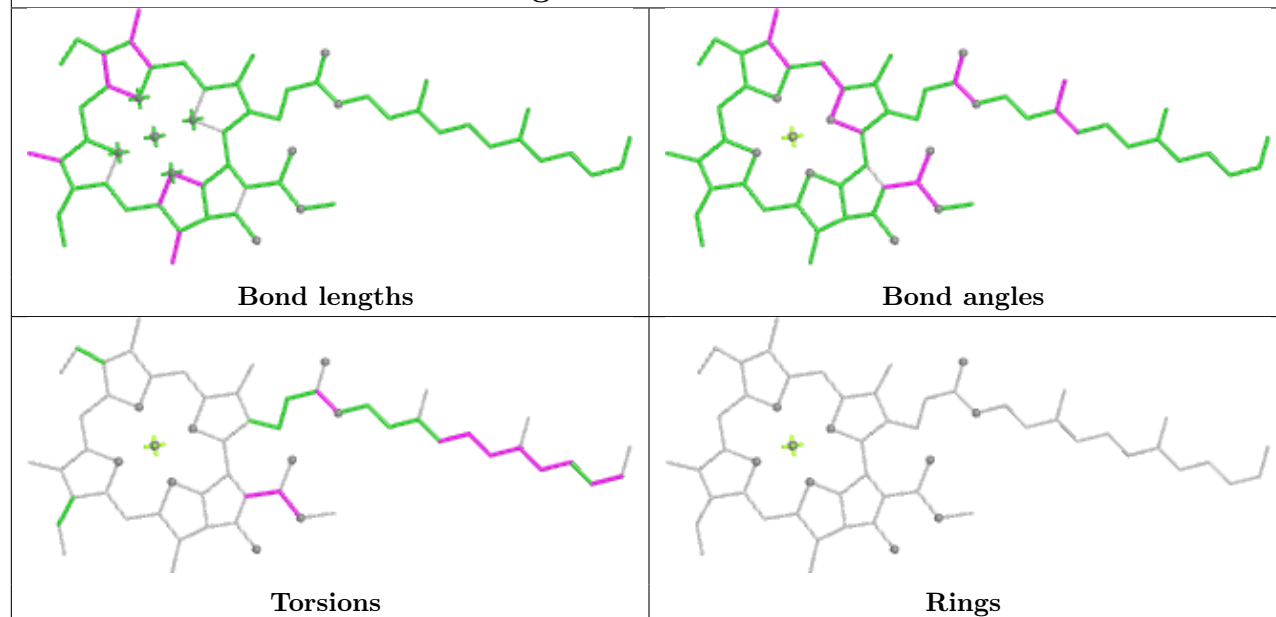
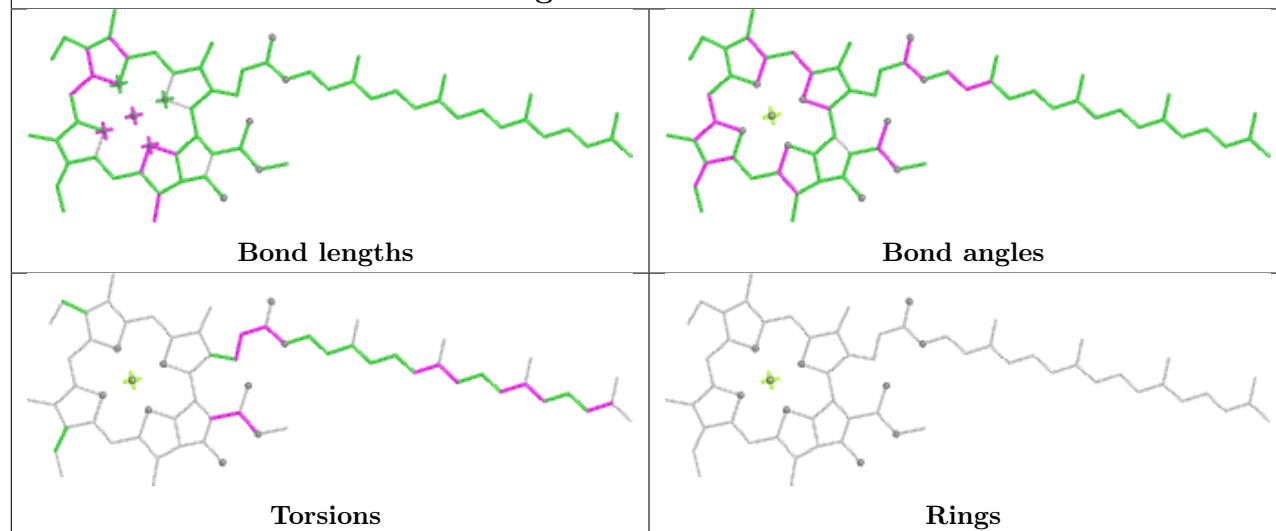


Ligand CLA i 608

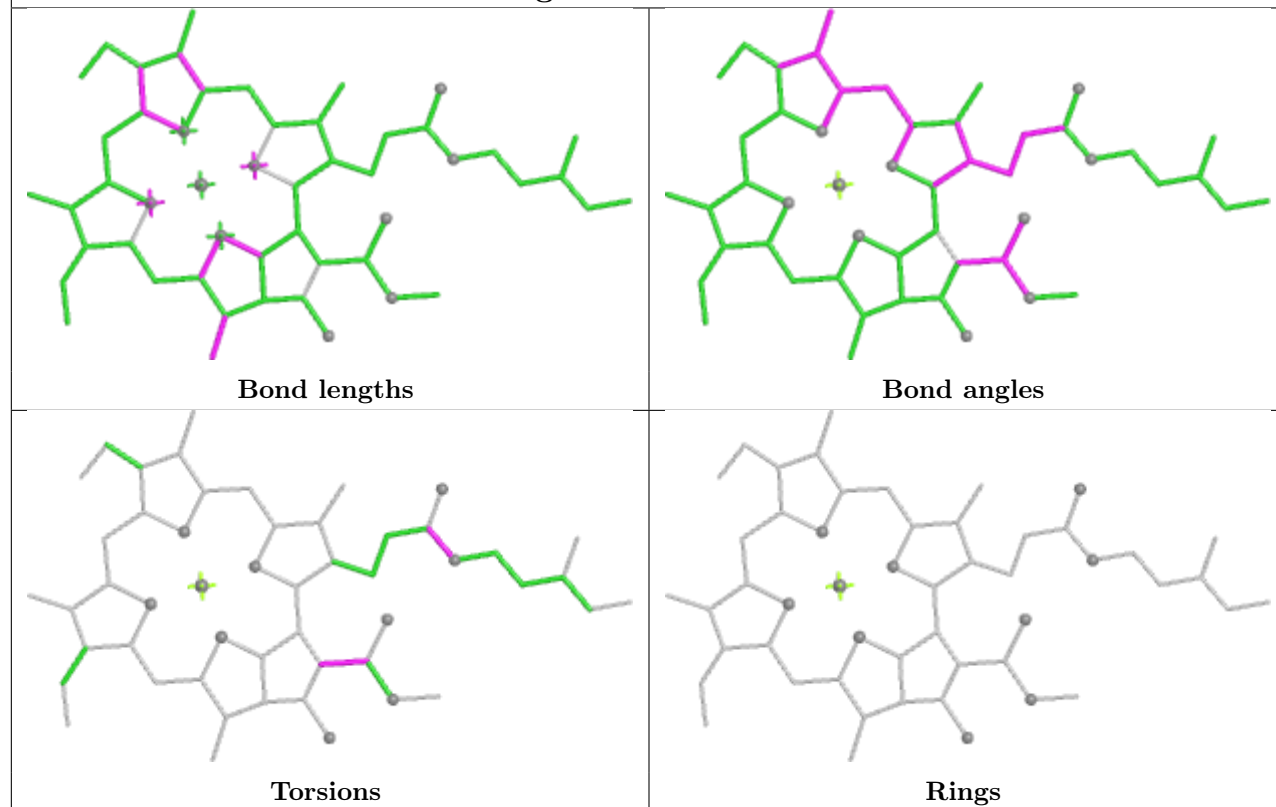


Ligand LMT A 851

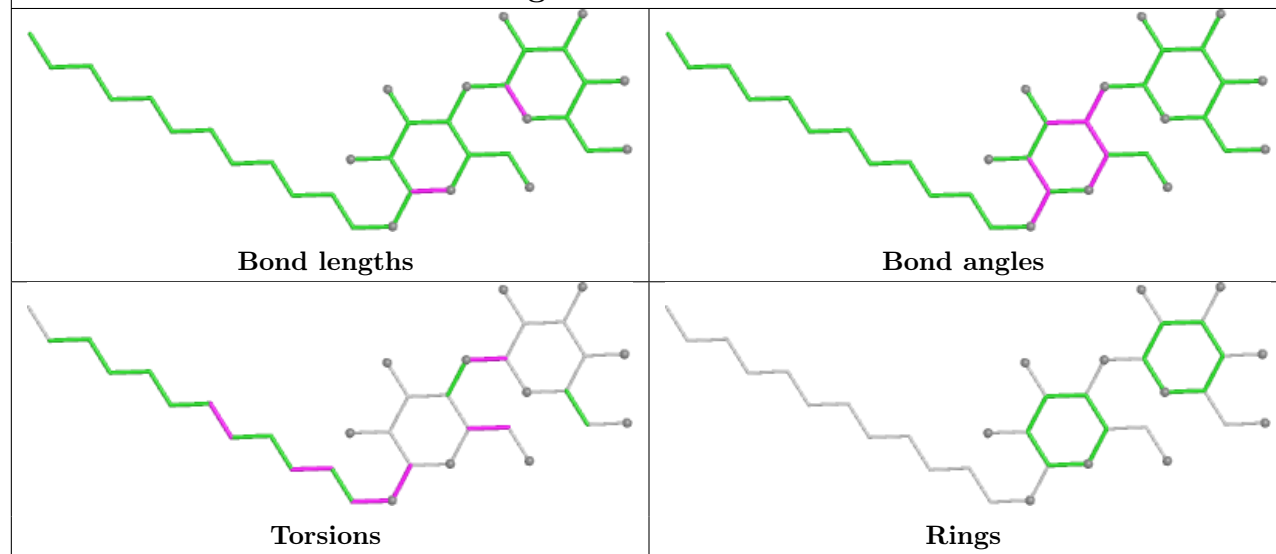


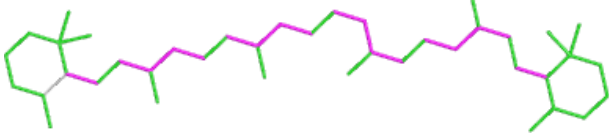
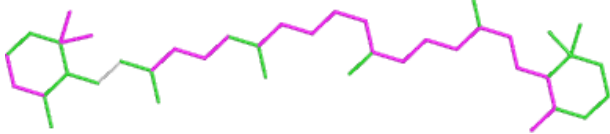
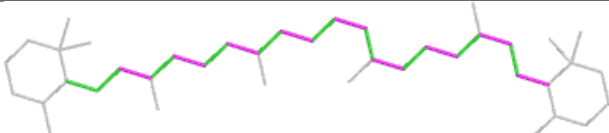
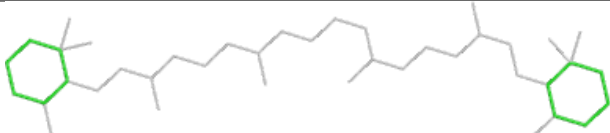
Ligand CLA B 814**Ligand CLA d 303**

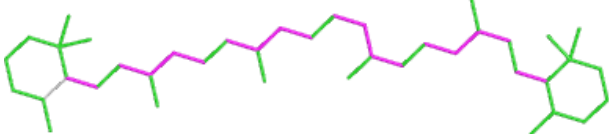
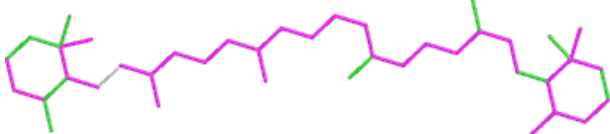
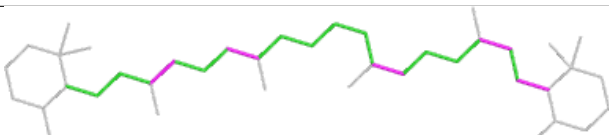
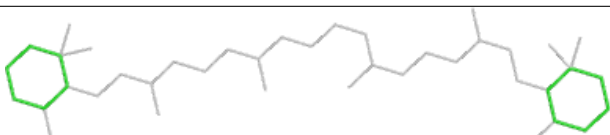
Ligand CLA k 603

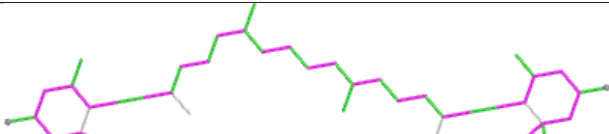
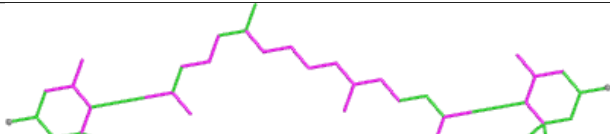
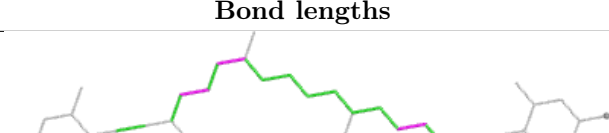
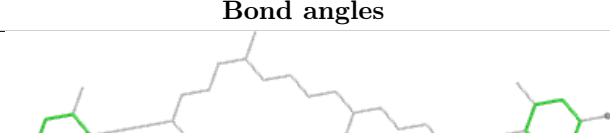


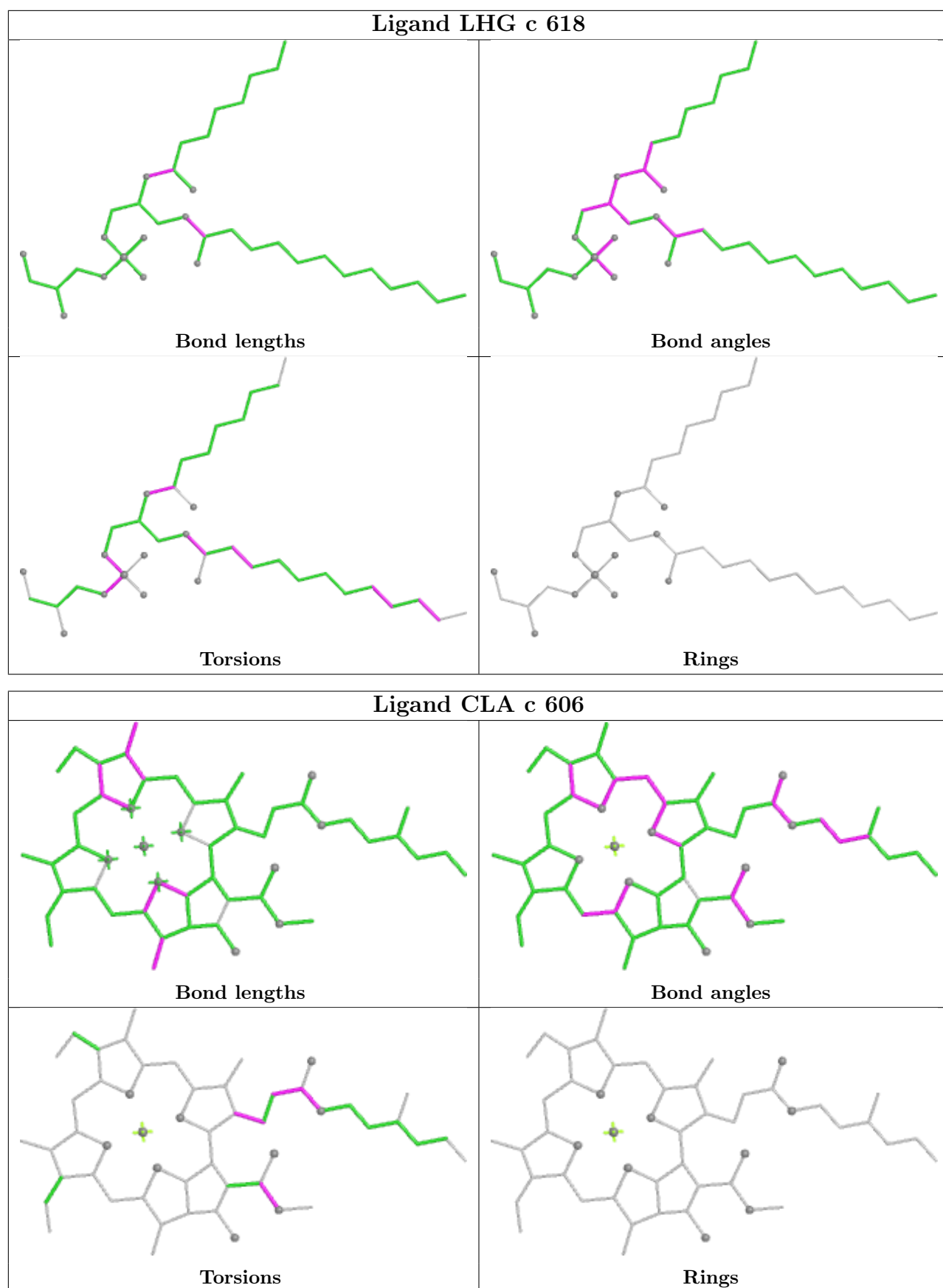
Ligand LMU B 844

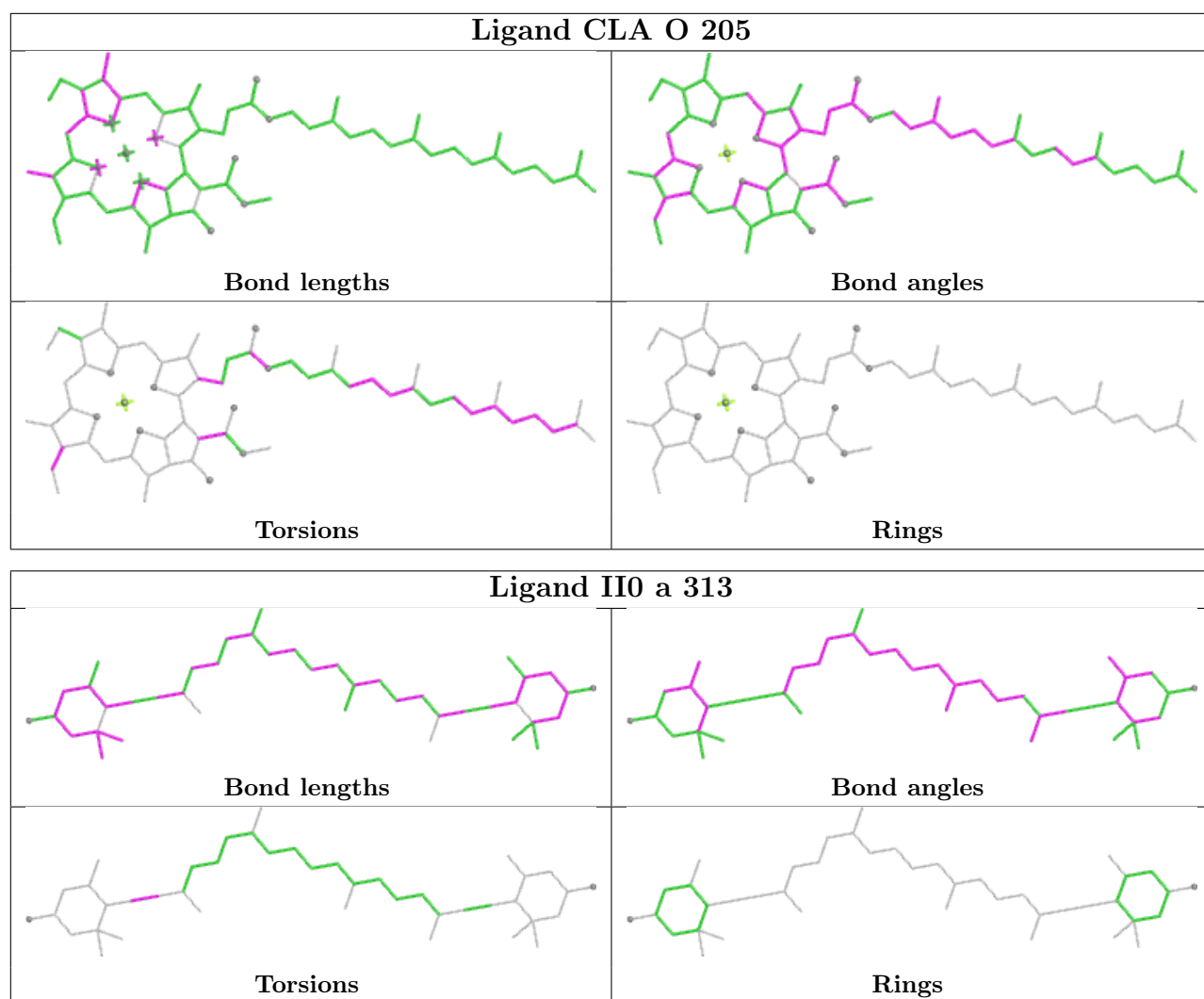


Ligand WVN A 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

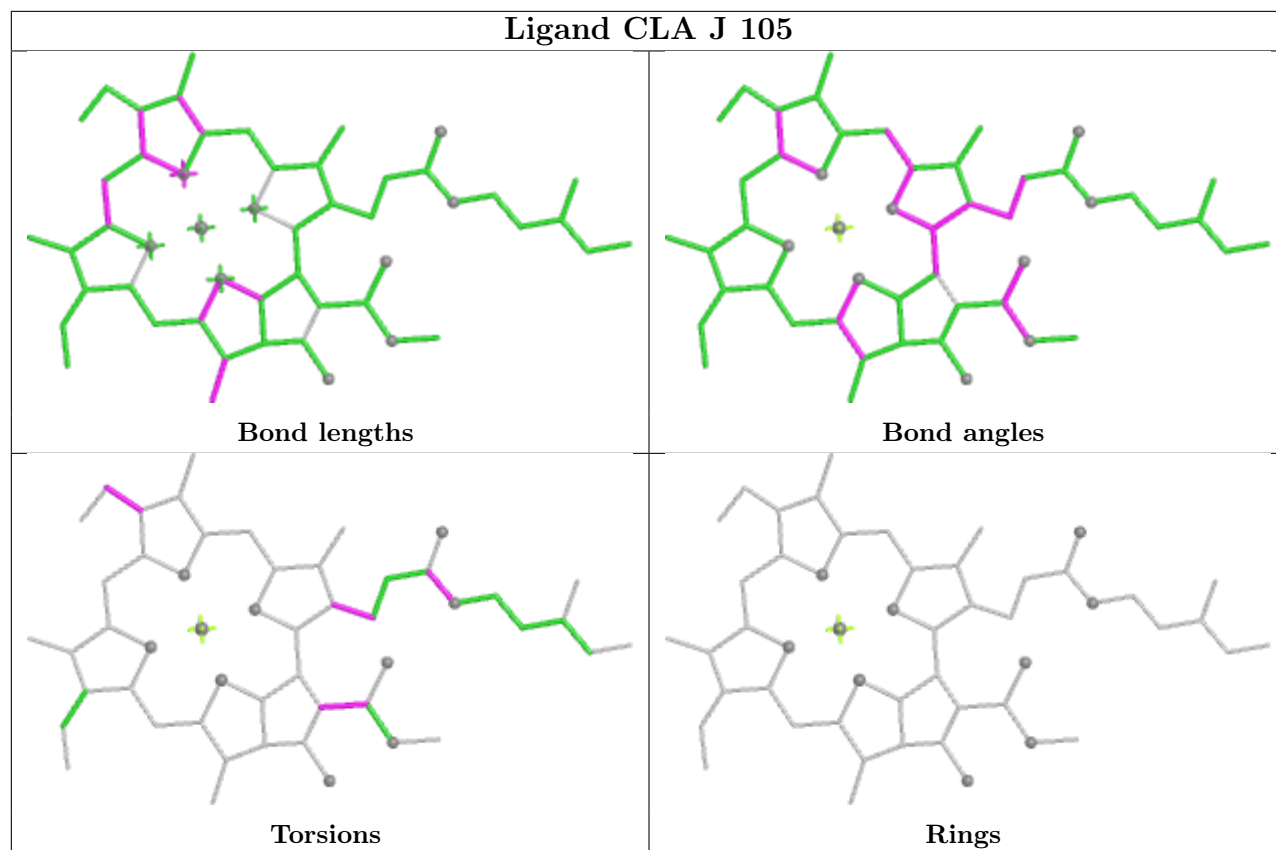
Ligand WVN A 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 k 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

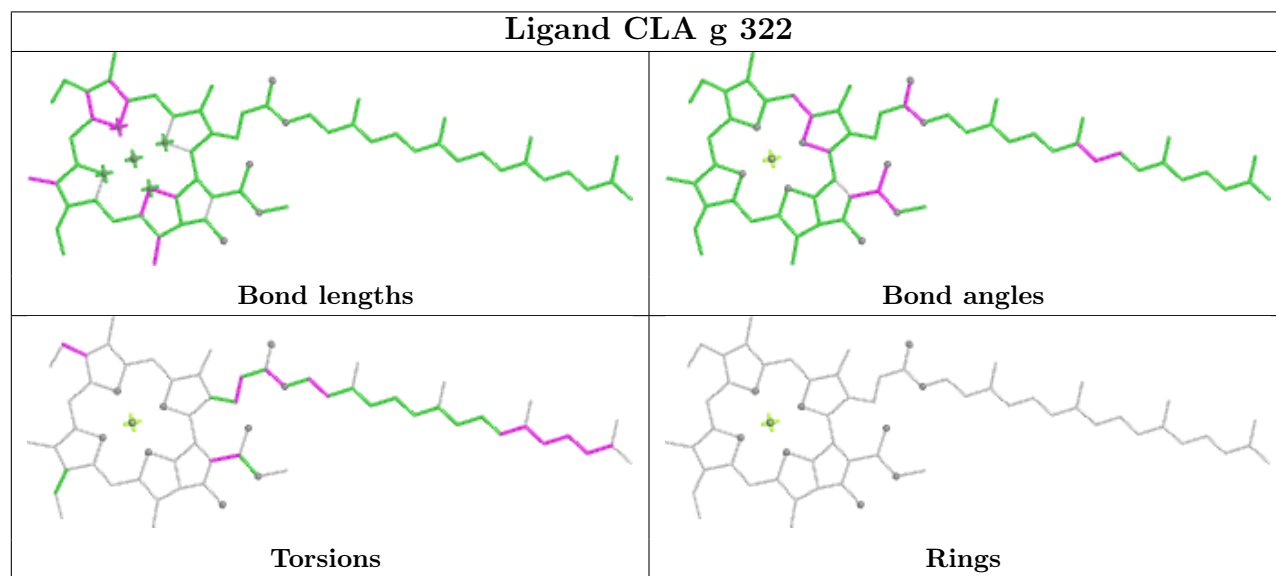


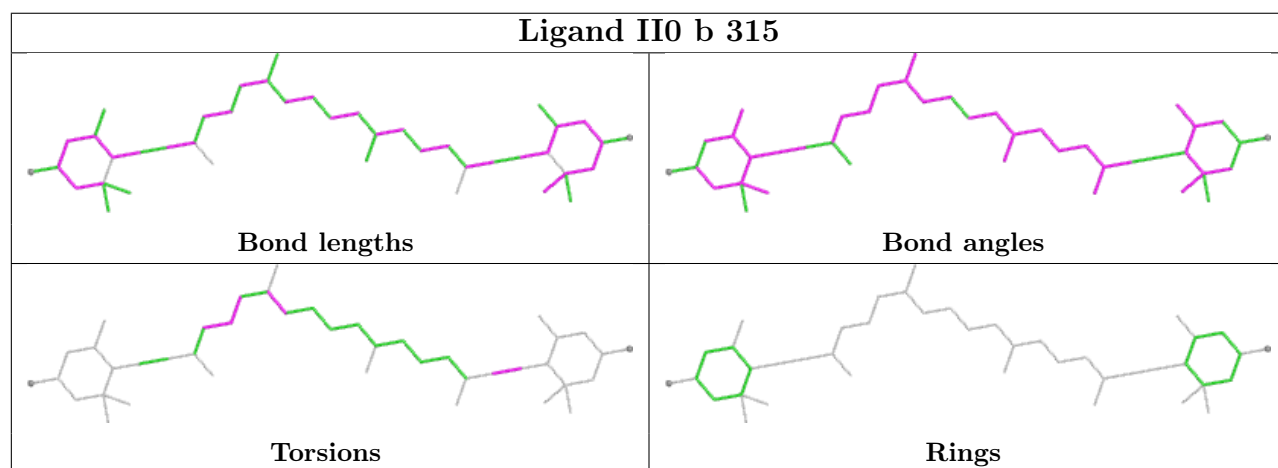
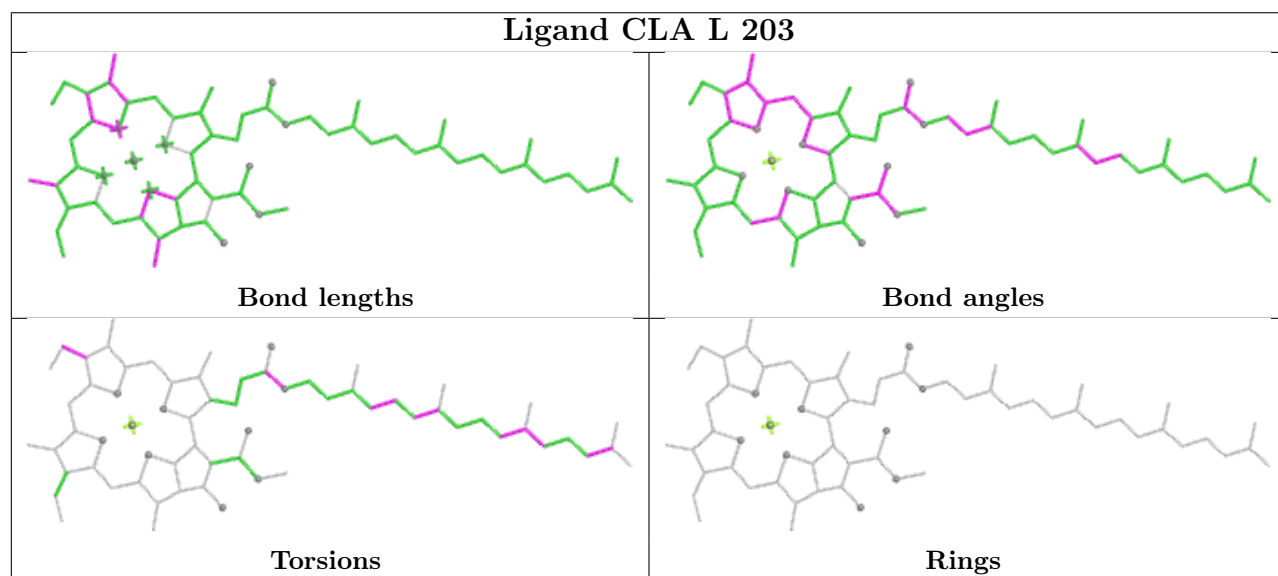
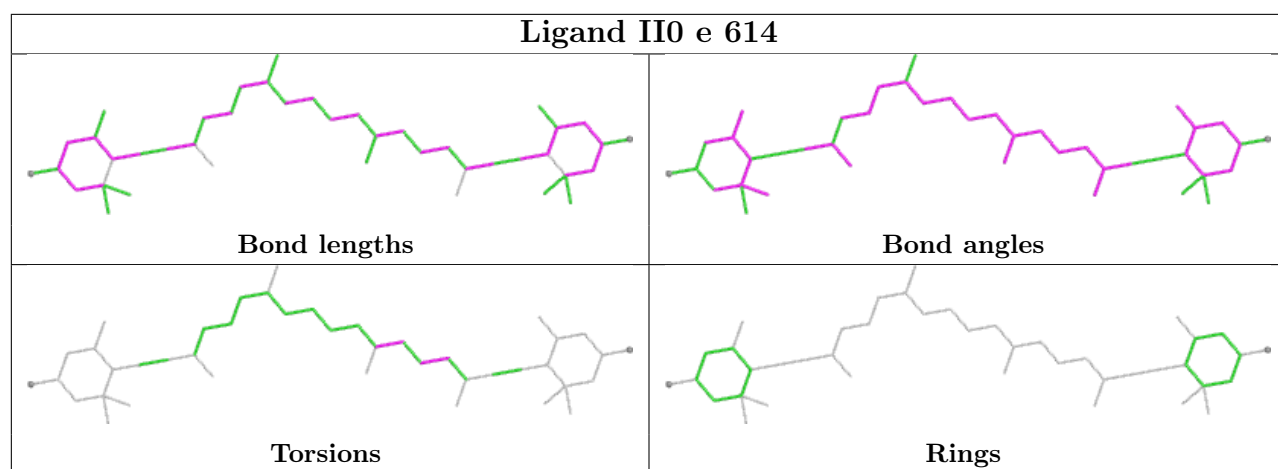


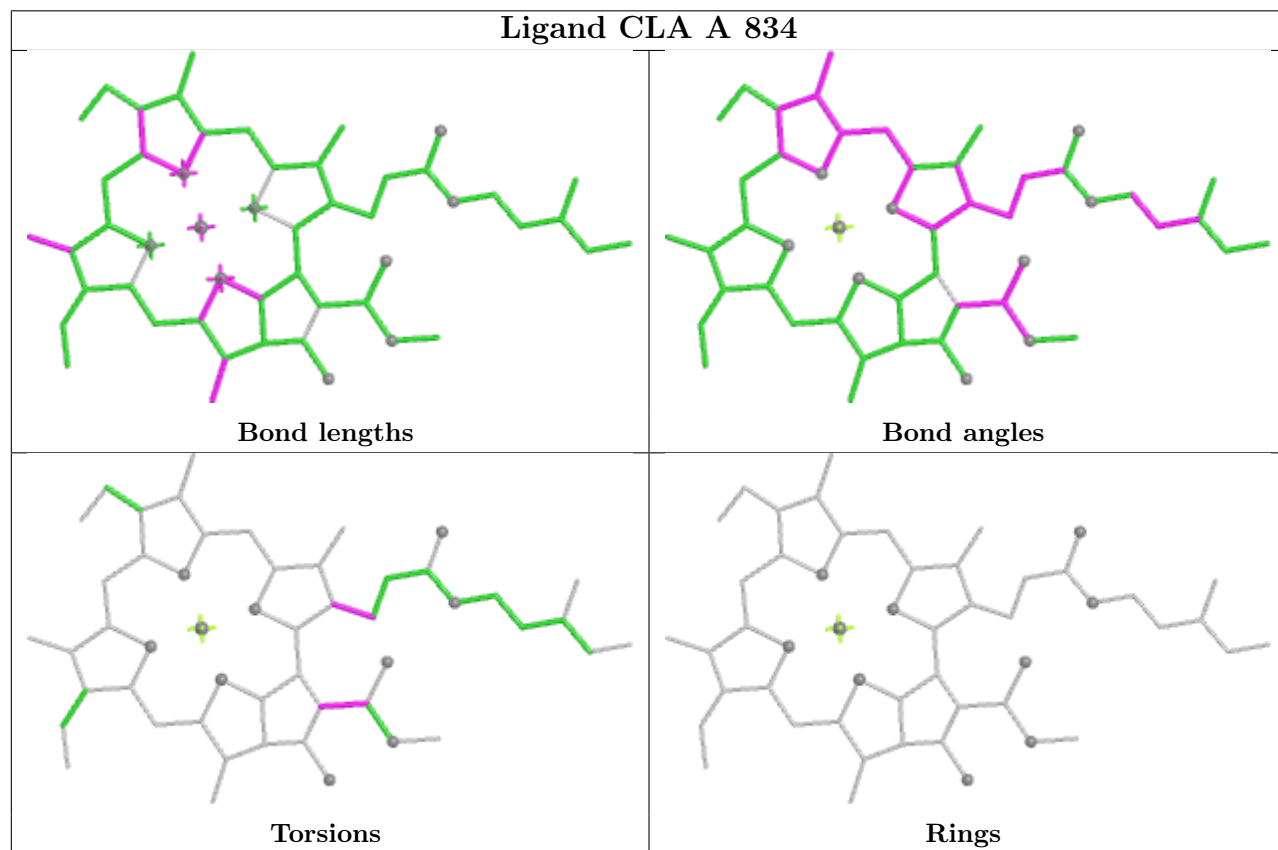
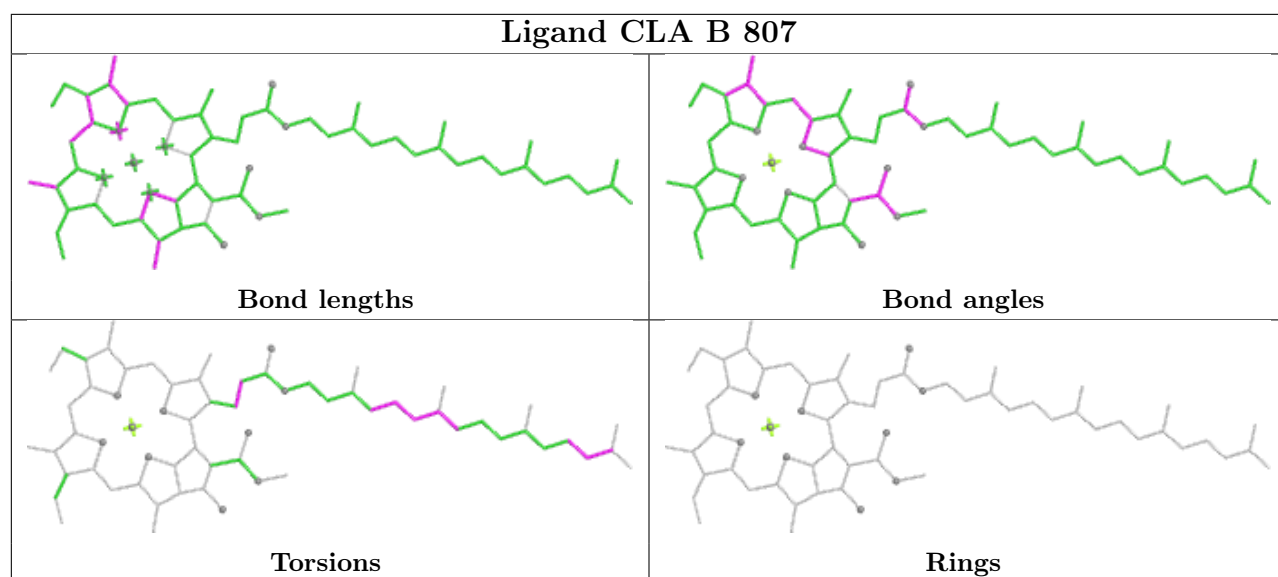
Ligand CLA J 105

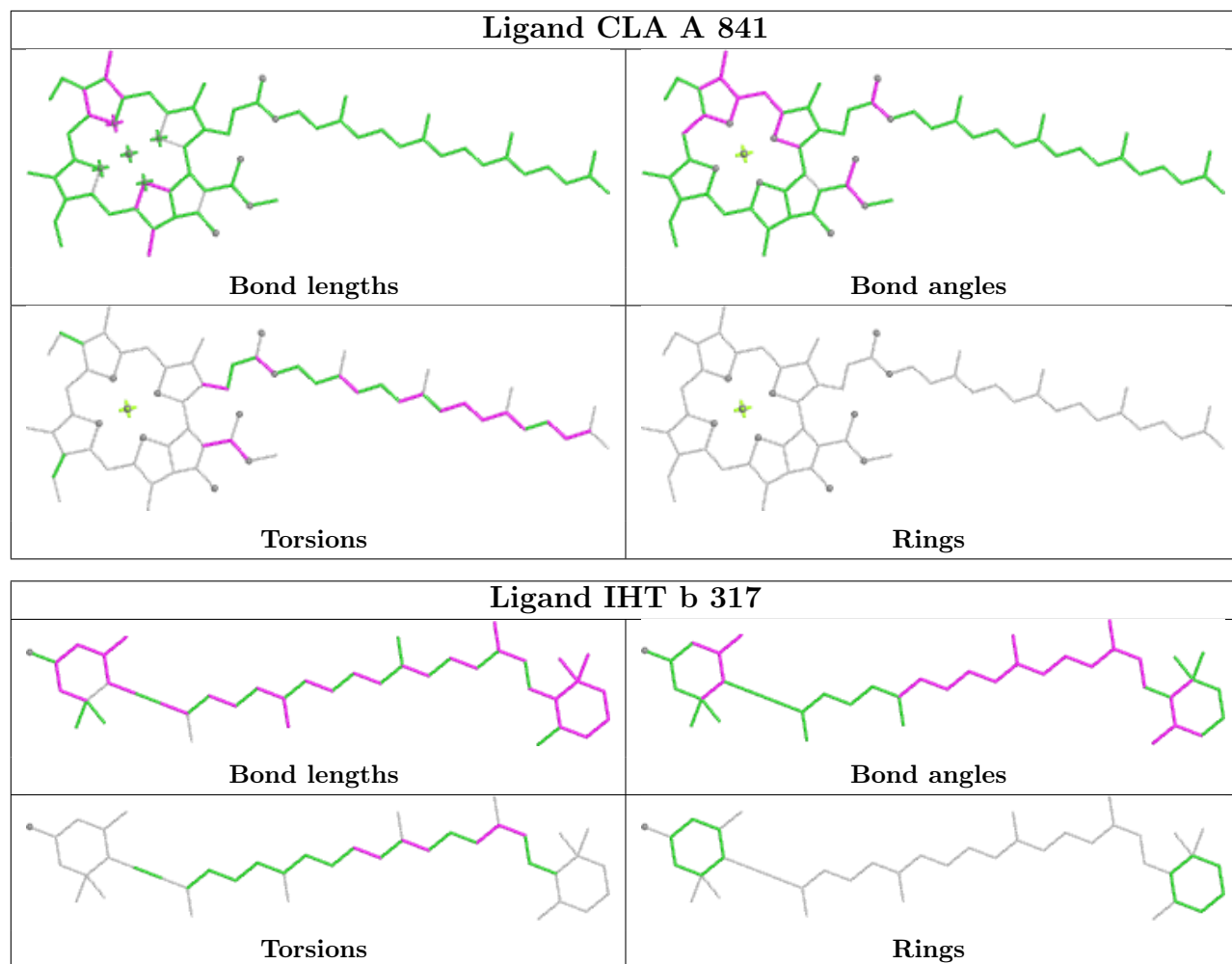


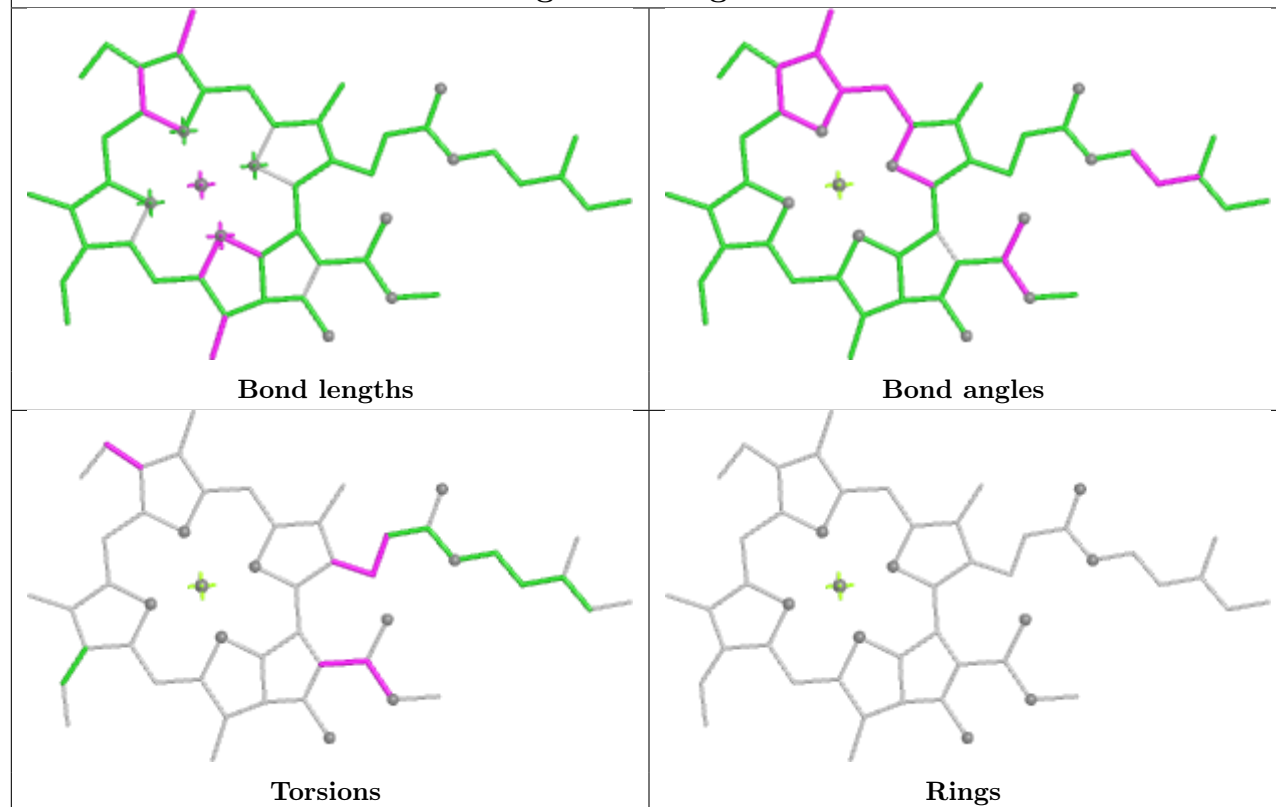
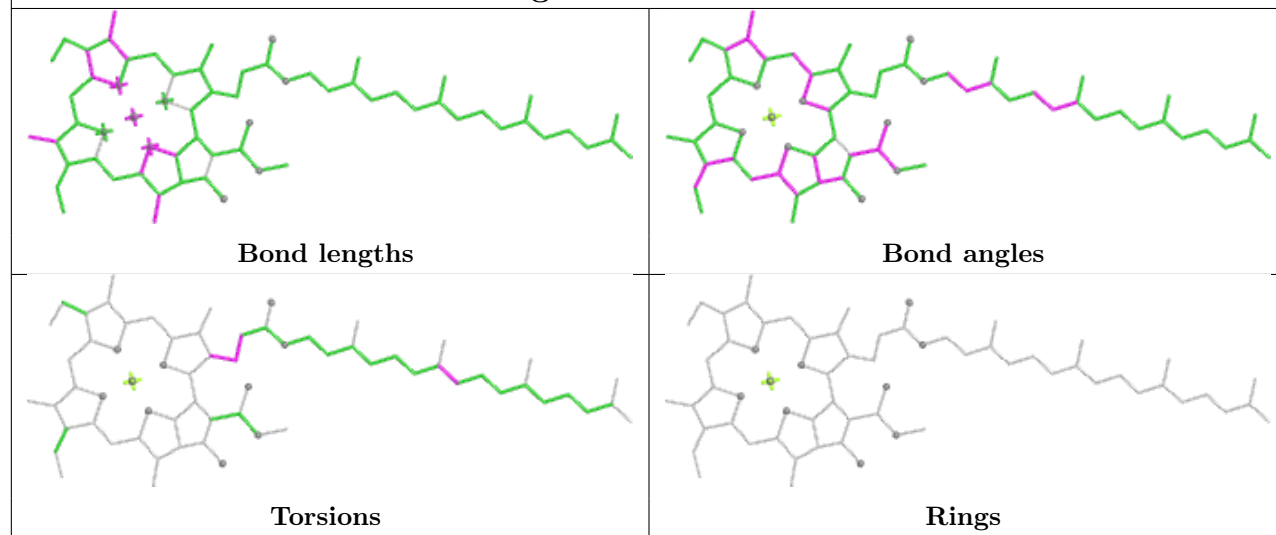
Ligand CLA g 322



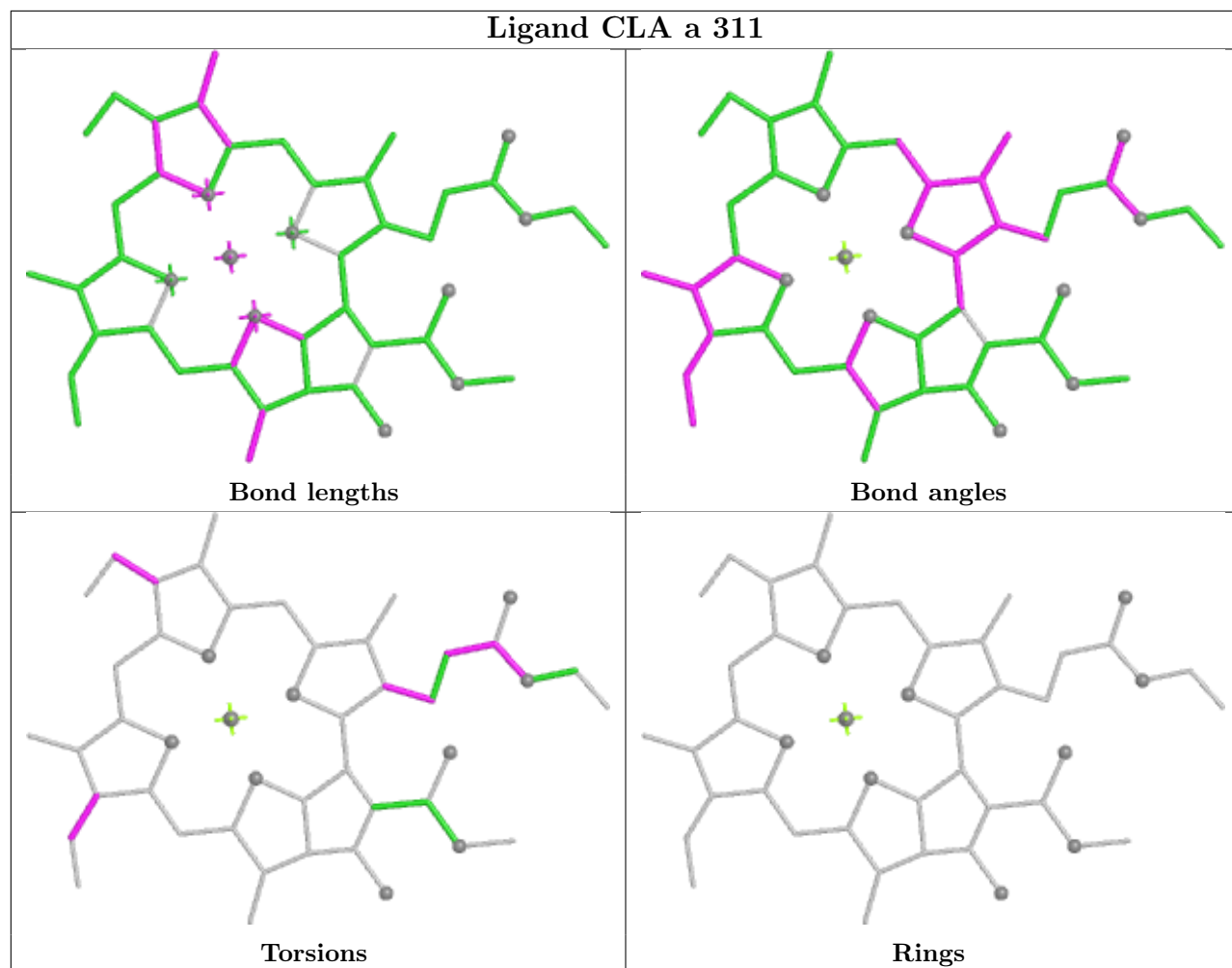




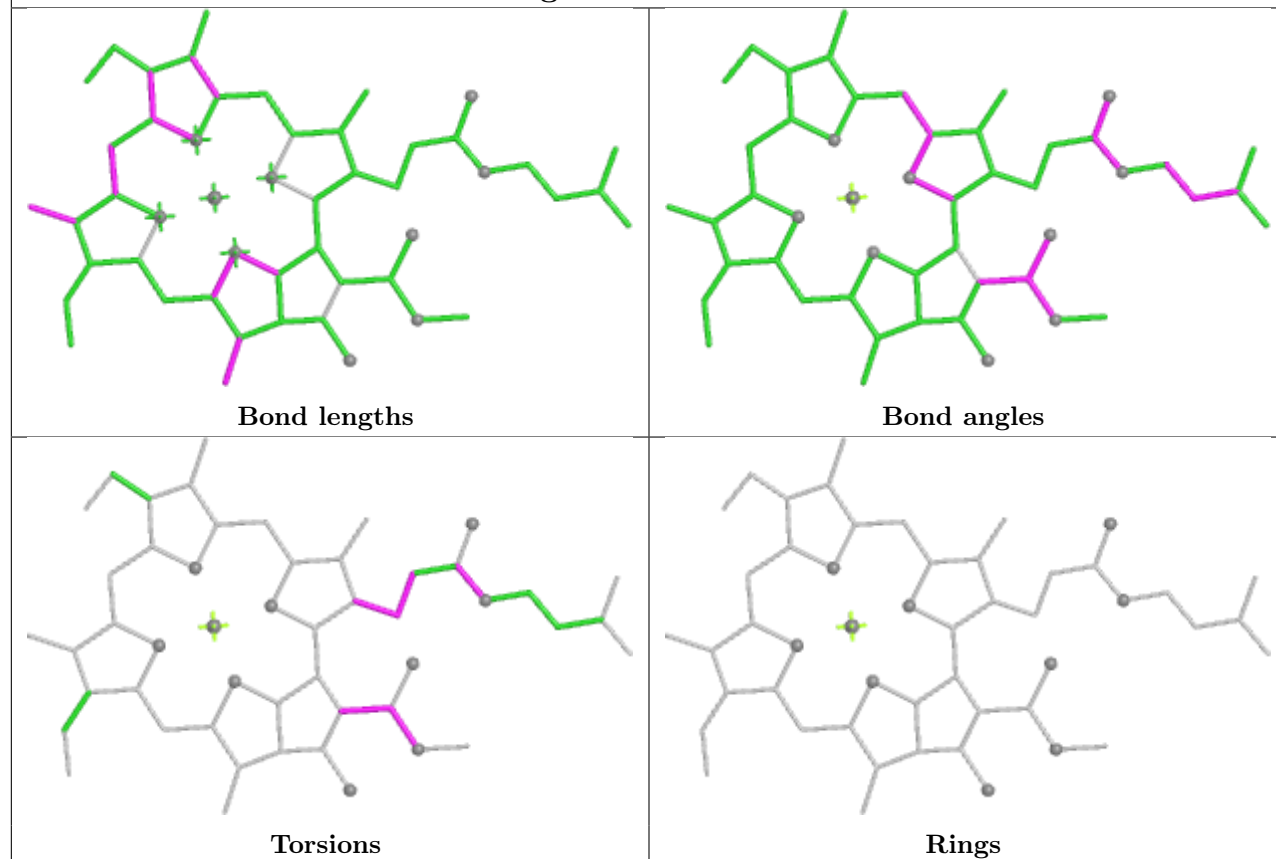


Ligand CLA g 315**Ligand CLA A 852**

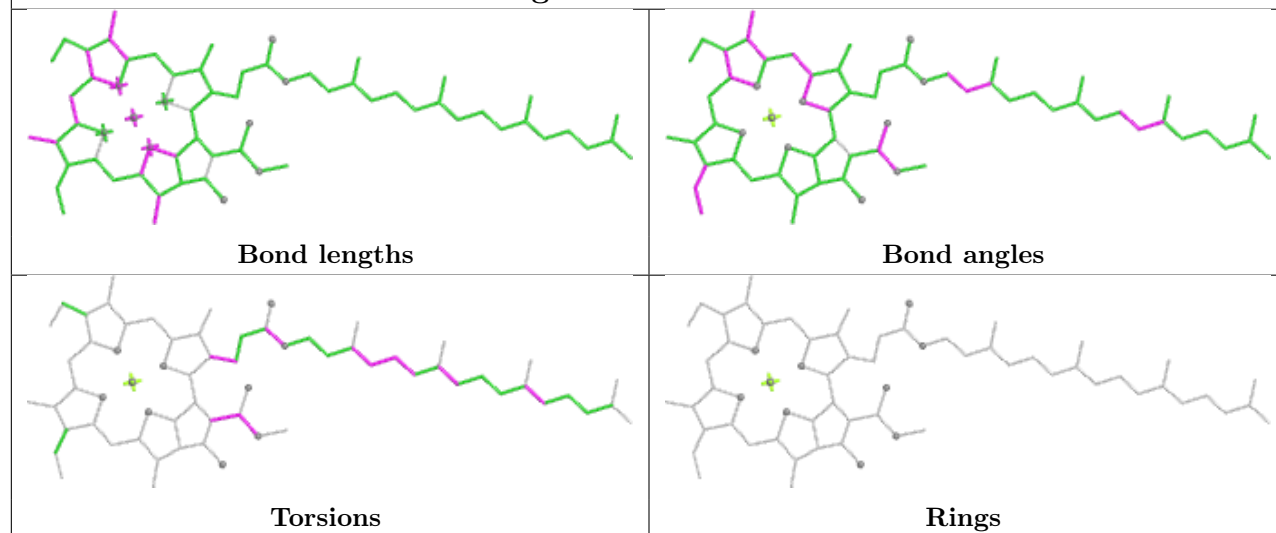
Ligand CLA a 311



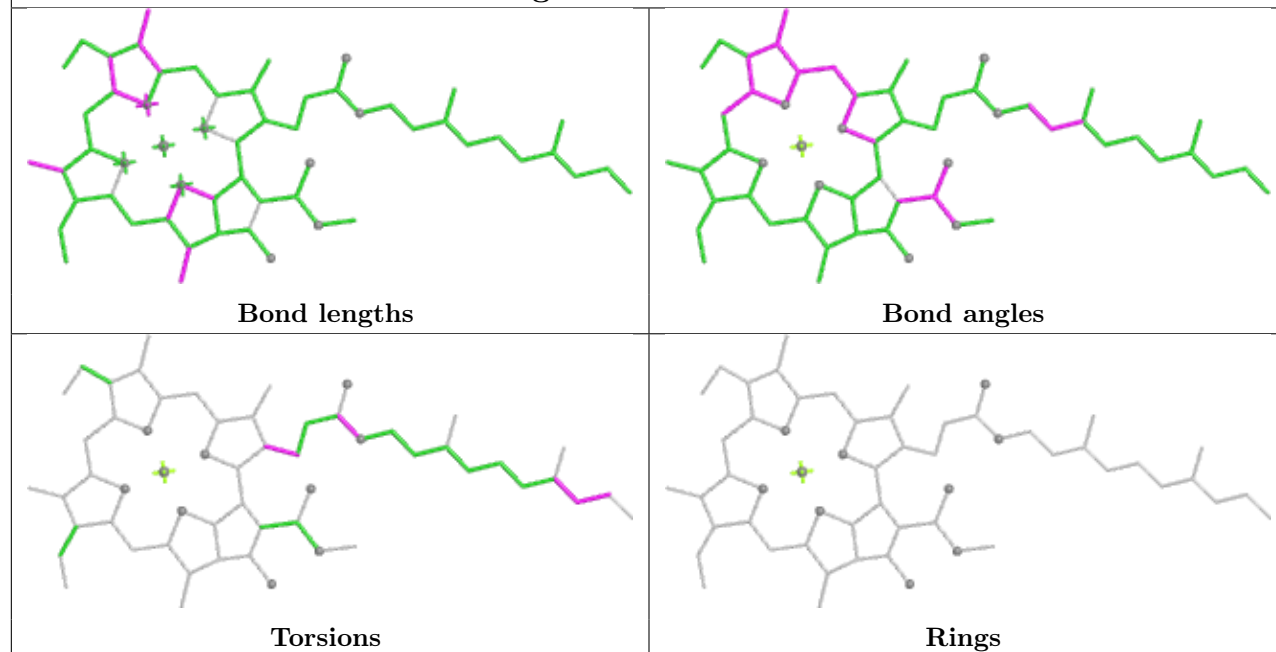
Ligand CLA i 602



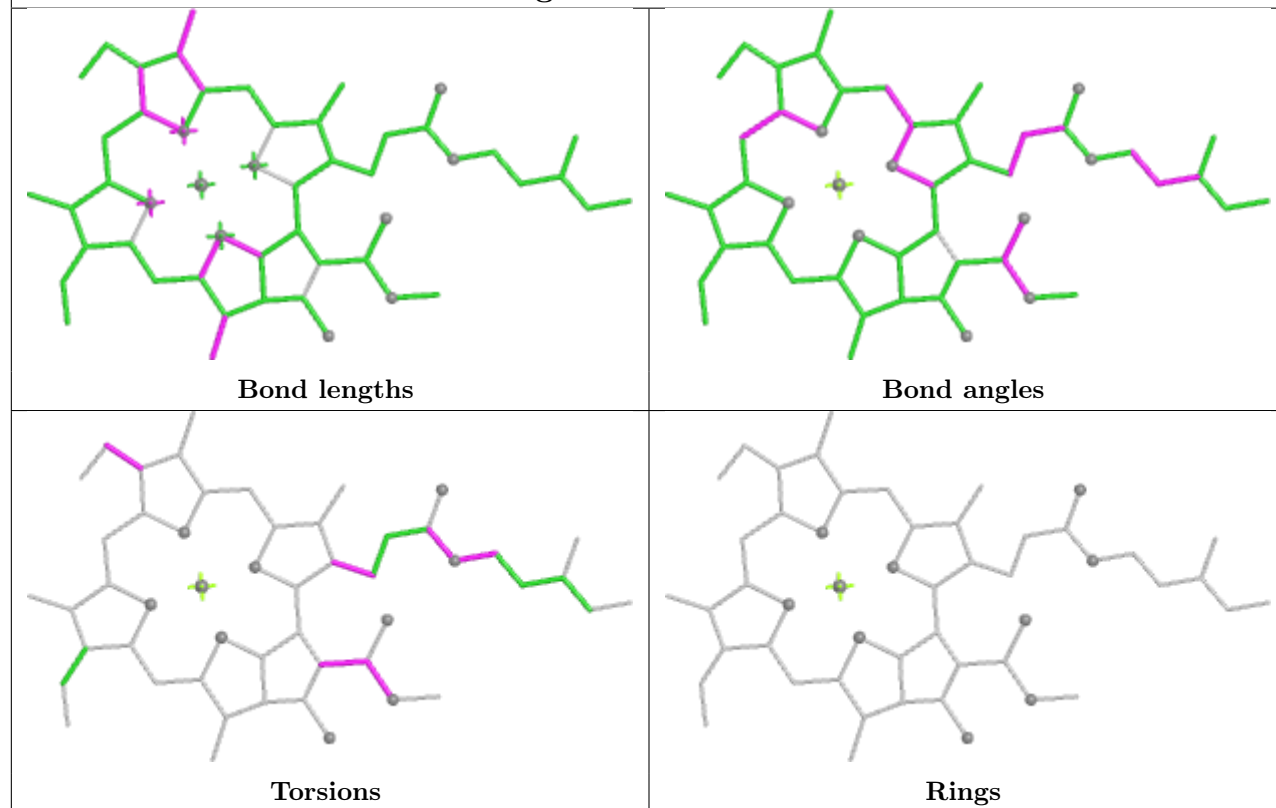
Ligand CLA O 201

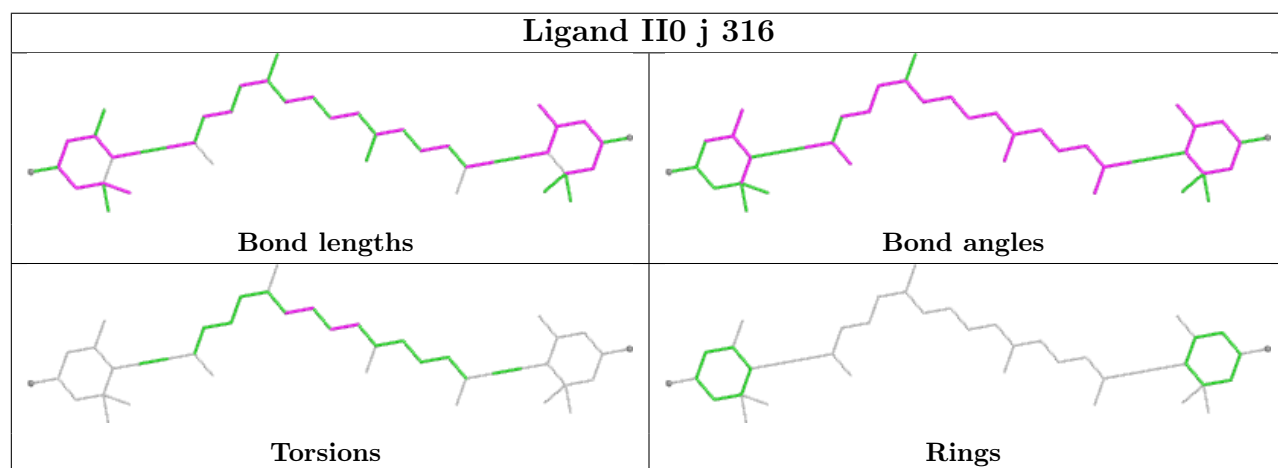
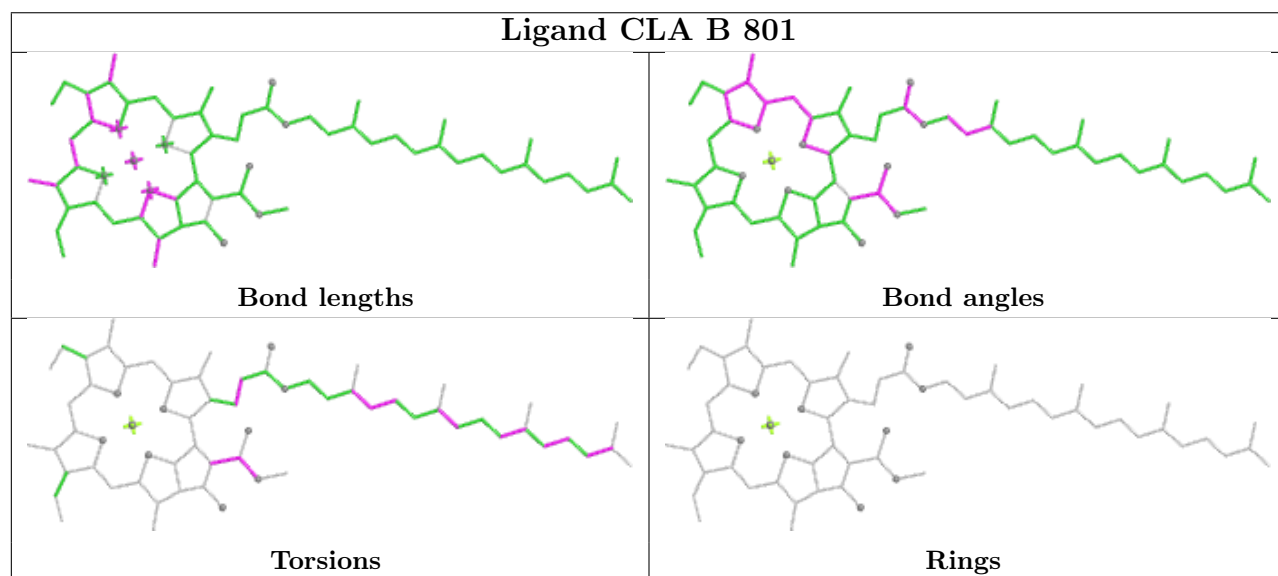
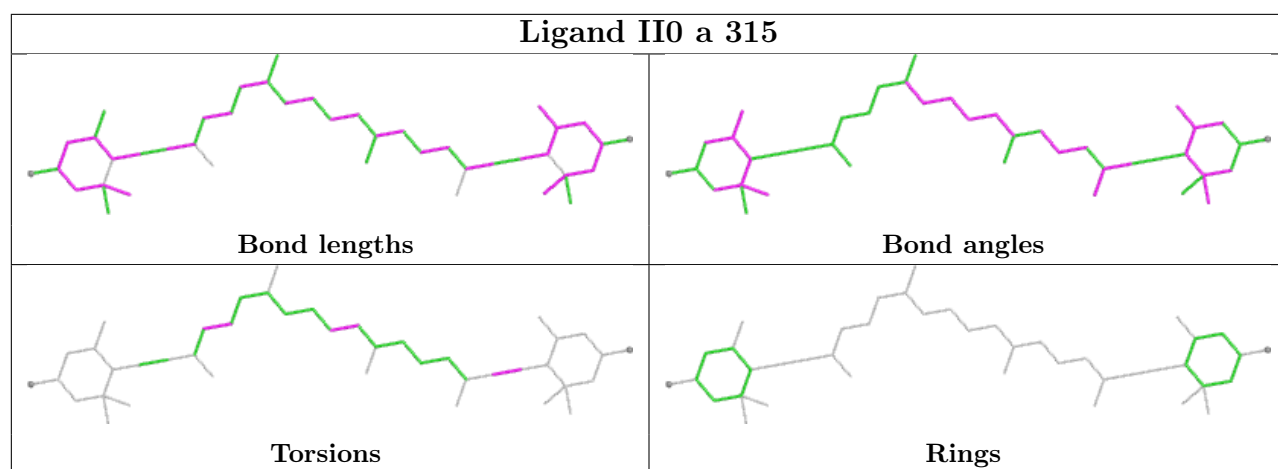


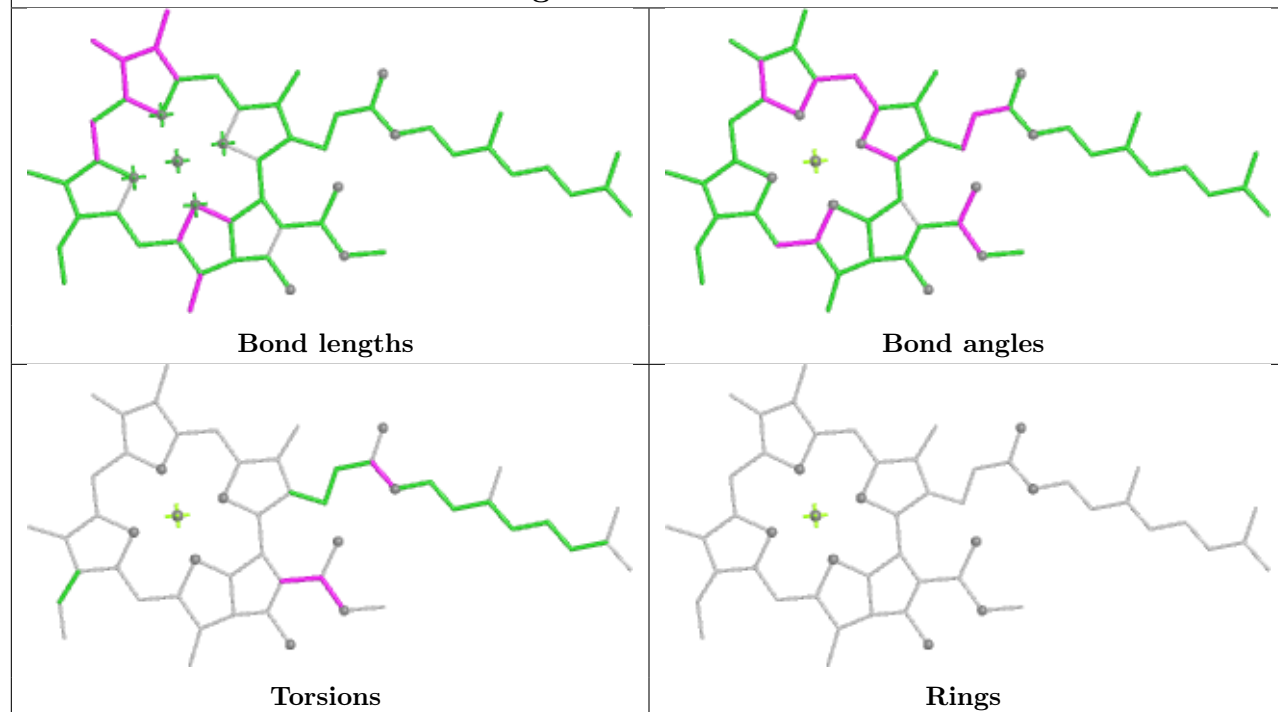
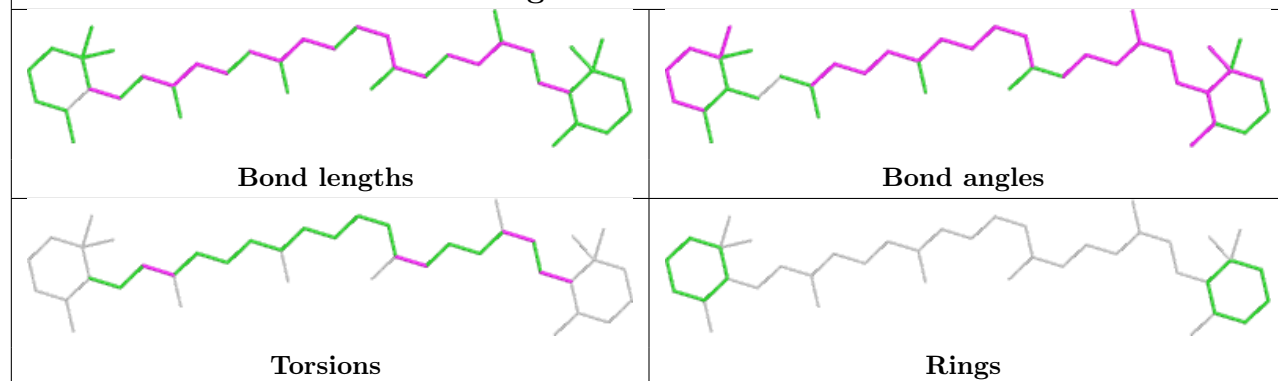
Ligand CLA B 817



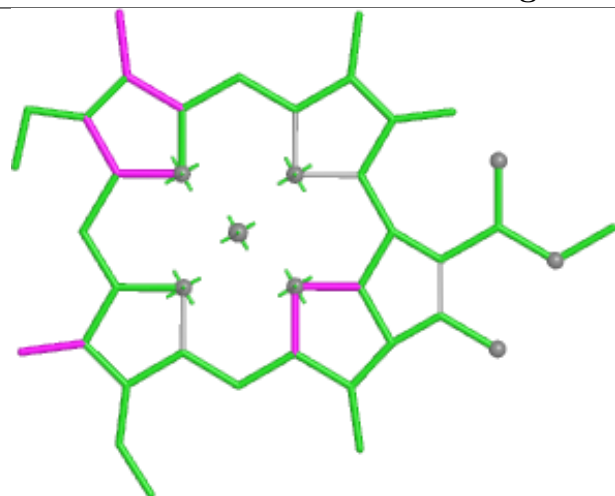
Ligand CLA k 601



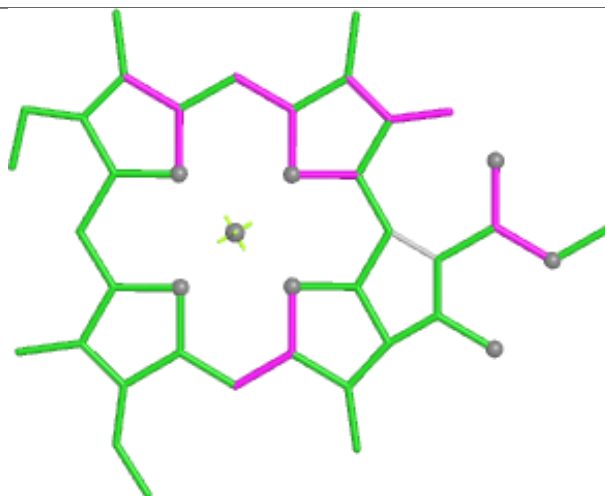


Ligand CLA B 810**Ligand WVN J 102**

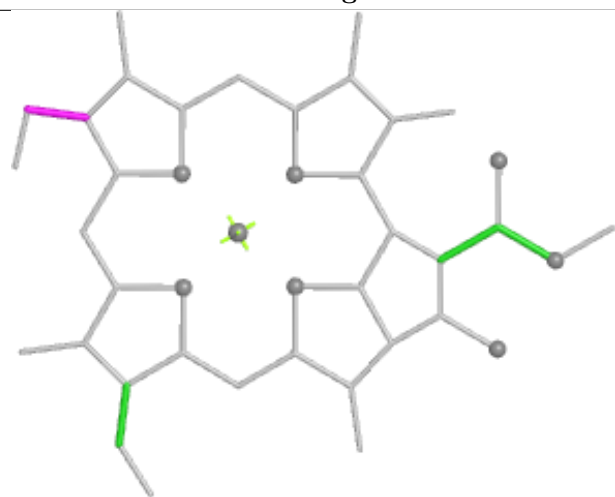
Ligand CLA d 309



Bond lengths



Bond angles

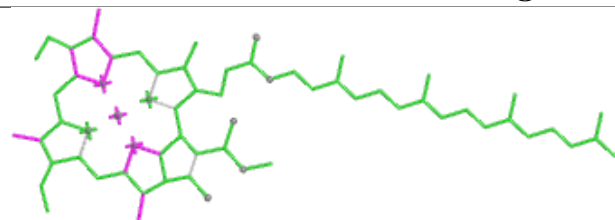


Torsions

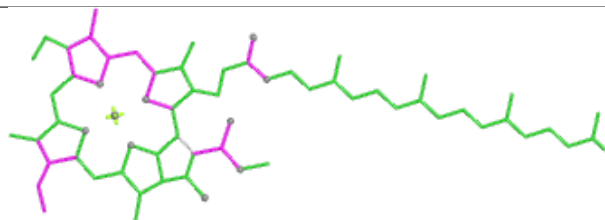


Rings

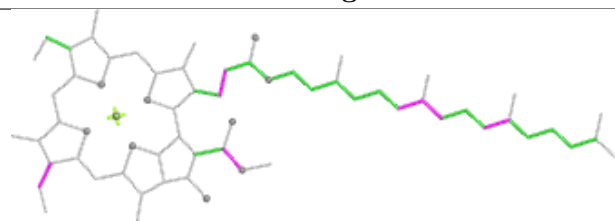
Ligand CLA B 804



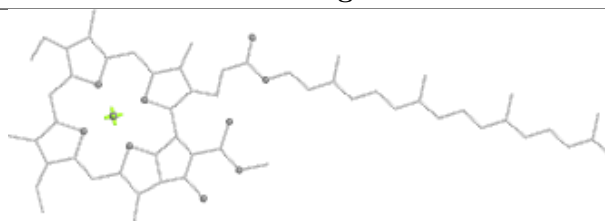
Bond lengths



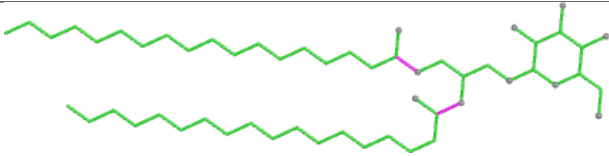
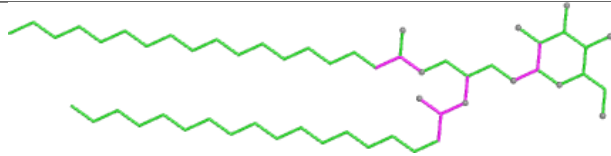
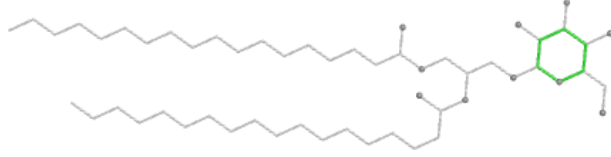
Bond angles

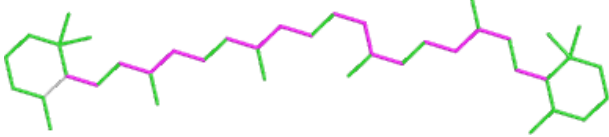
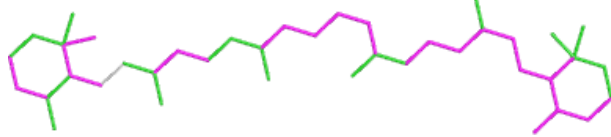
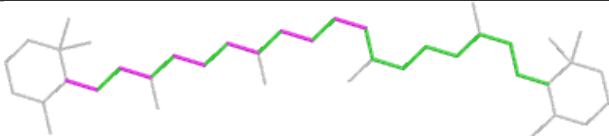
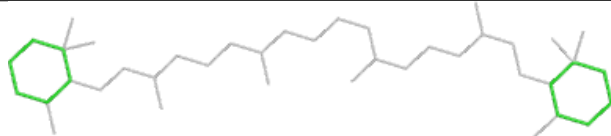


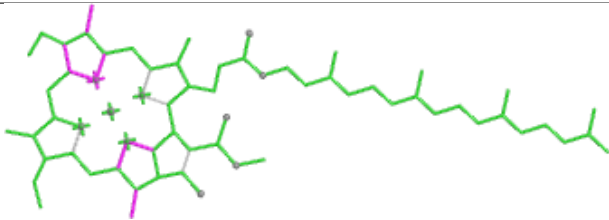
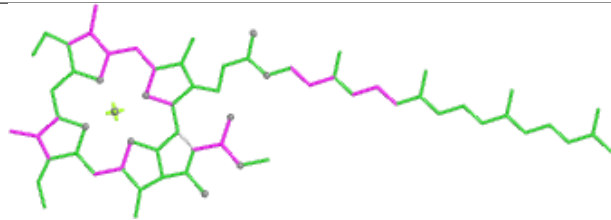
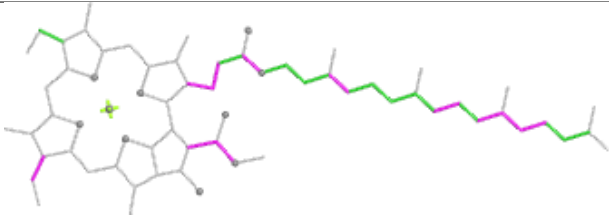
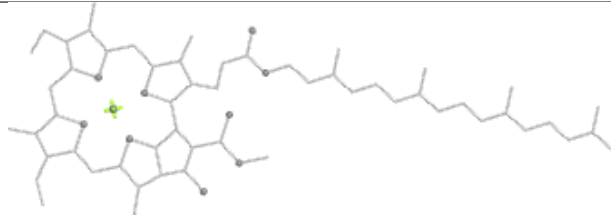
Torsions

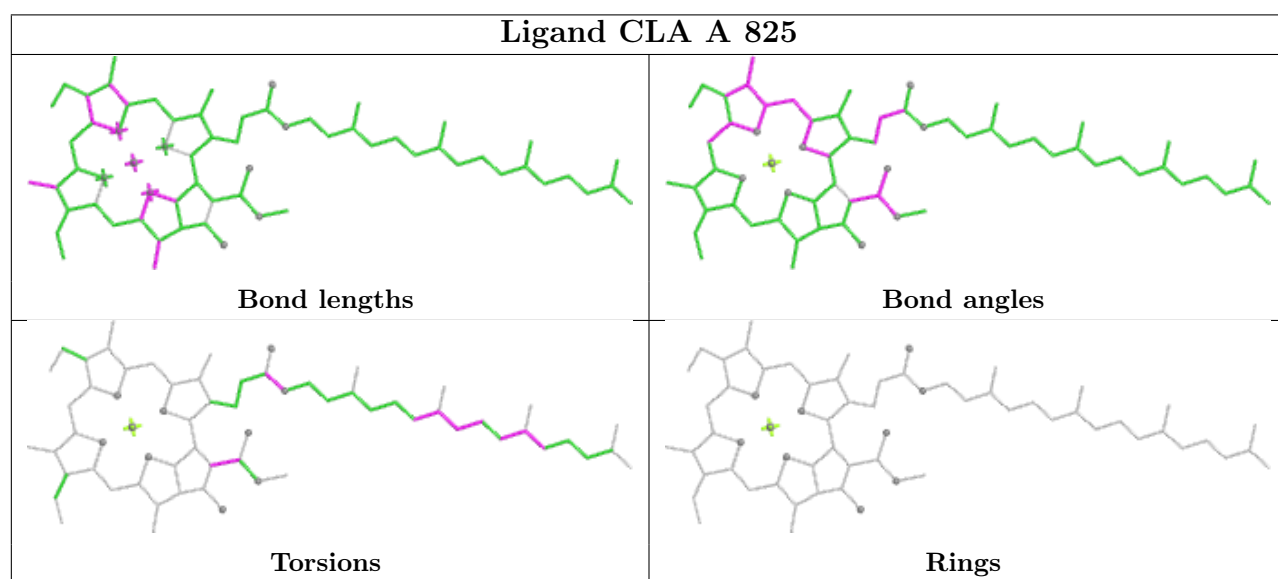
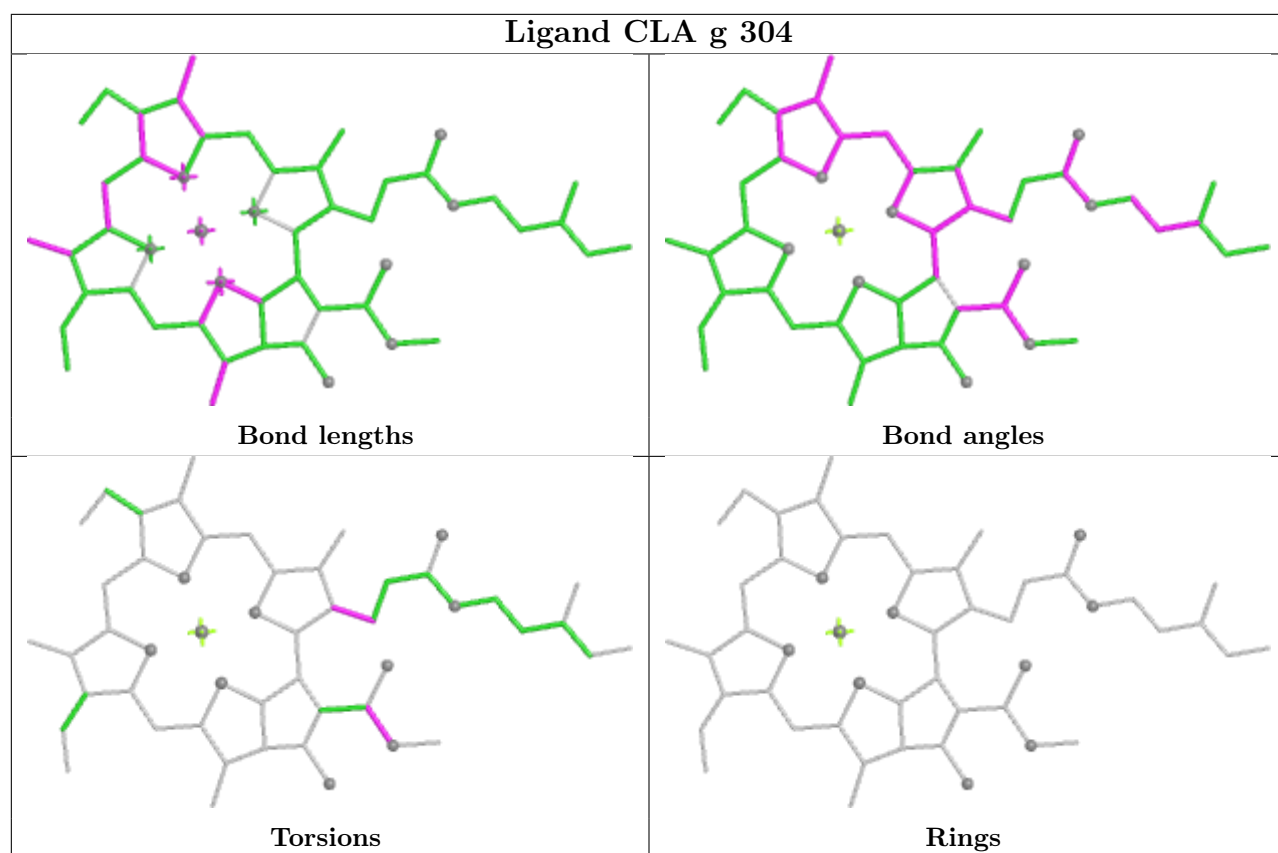


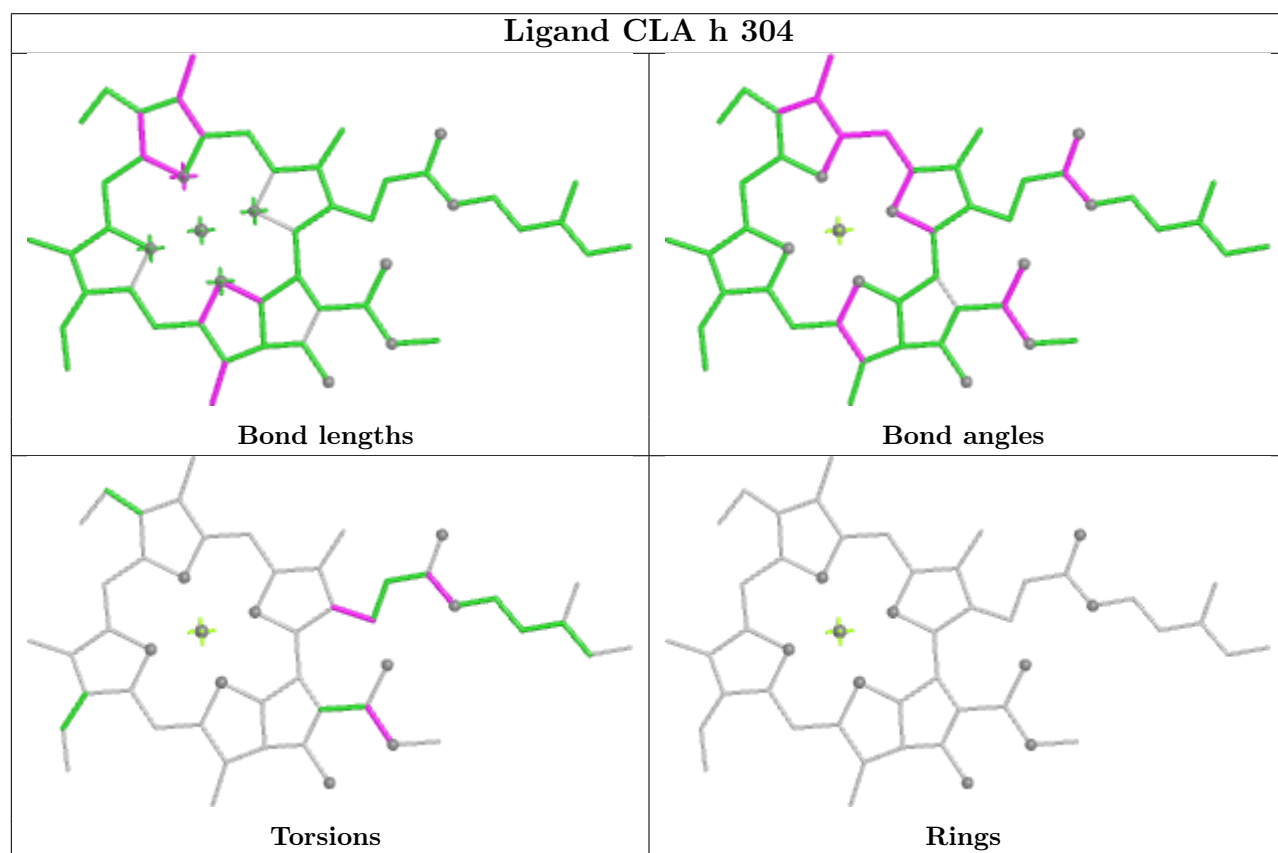
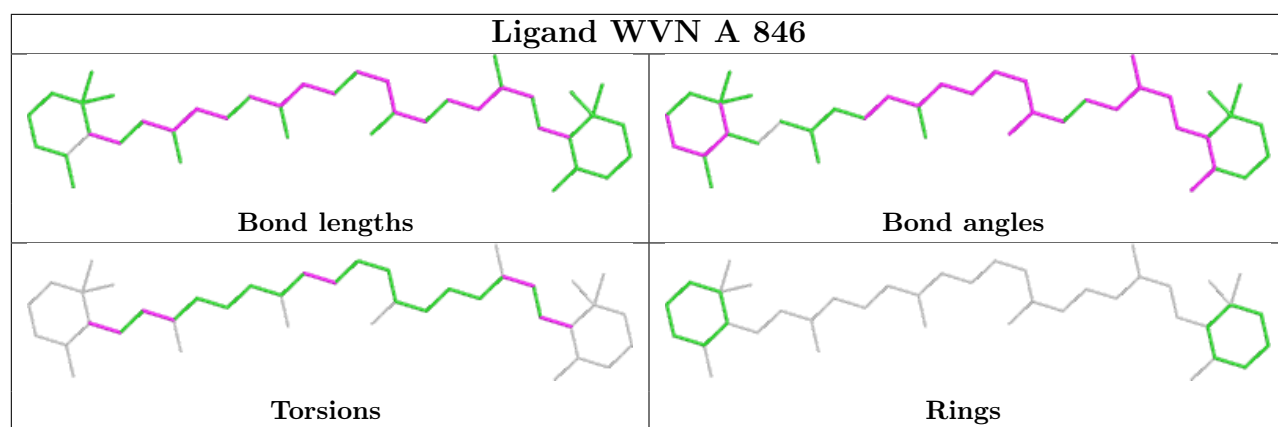
Rings

Ligand LMG b 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

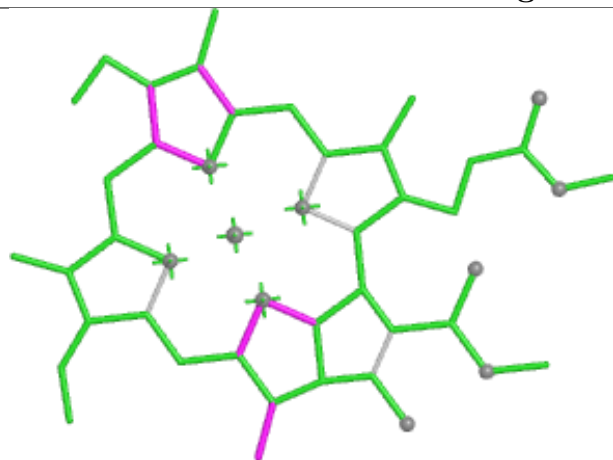
Ligand WVN I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

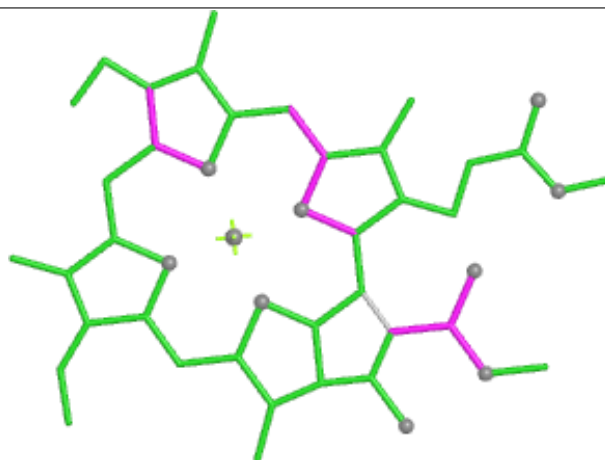




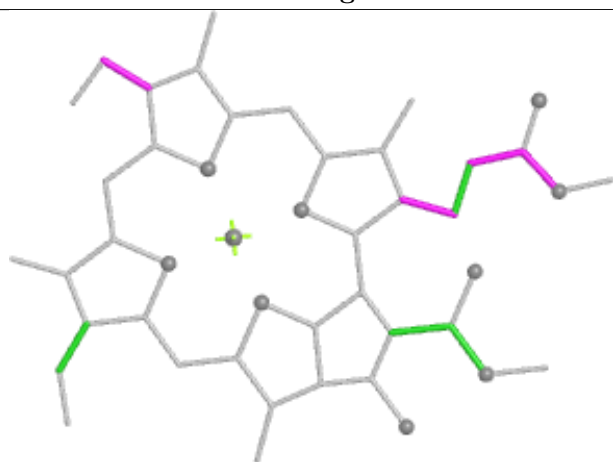
Ligand CLA d 307



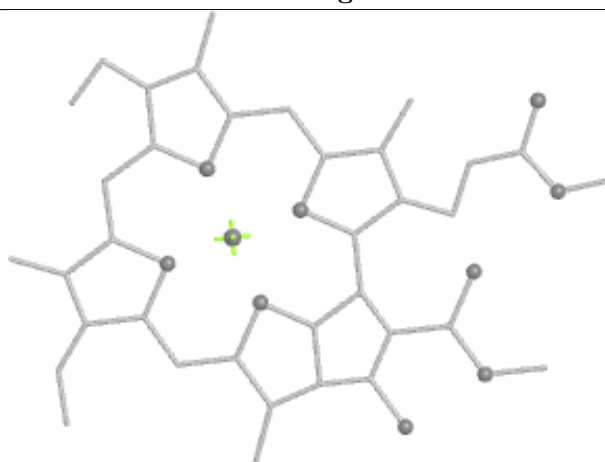
Bond lengths



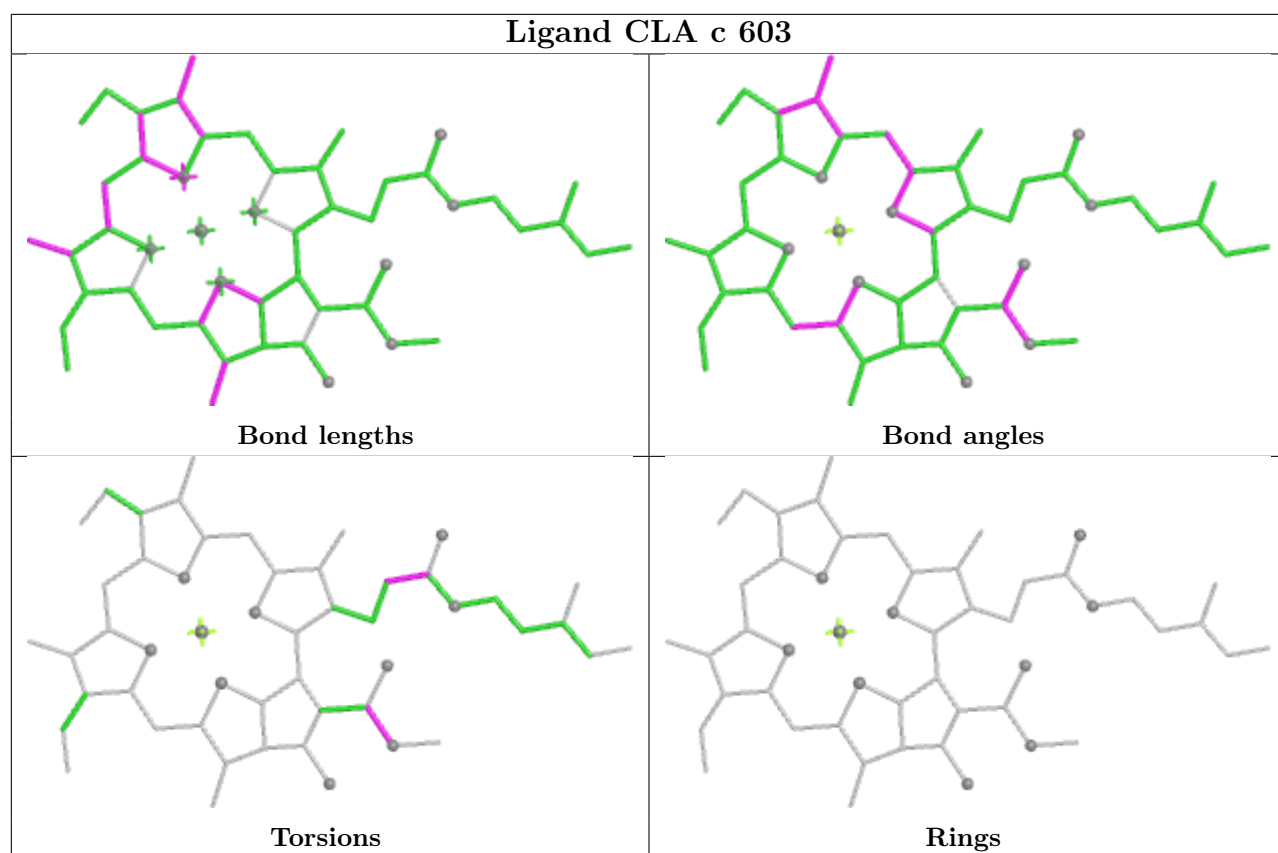
Bond angles

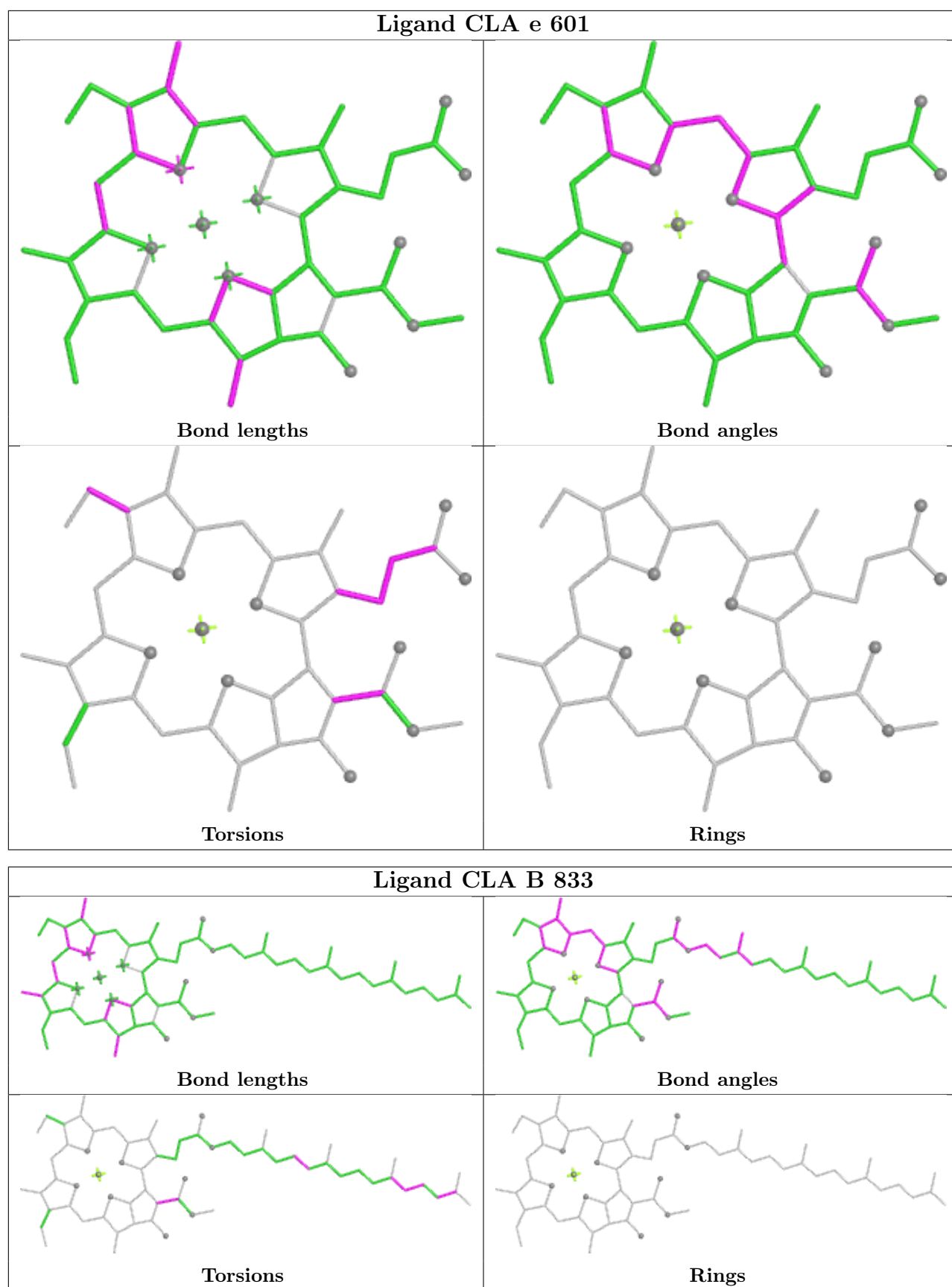


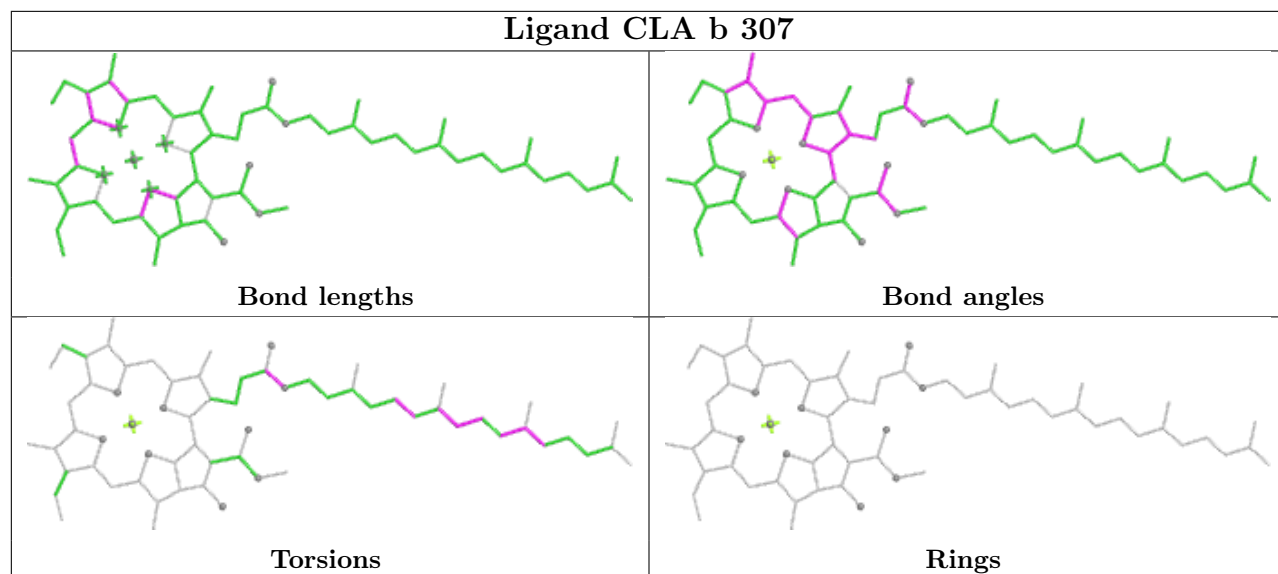
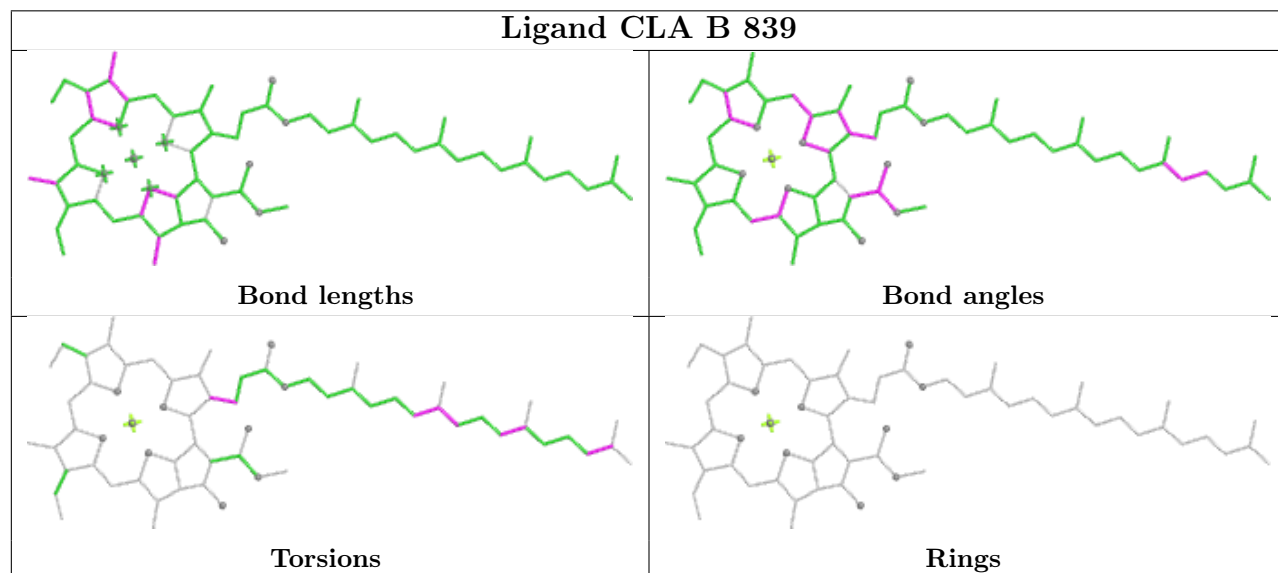
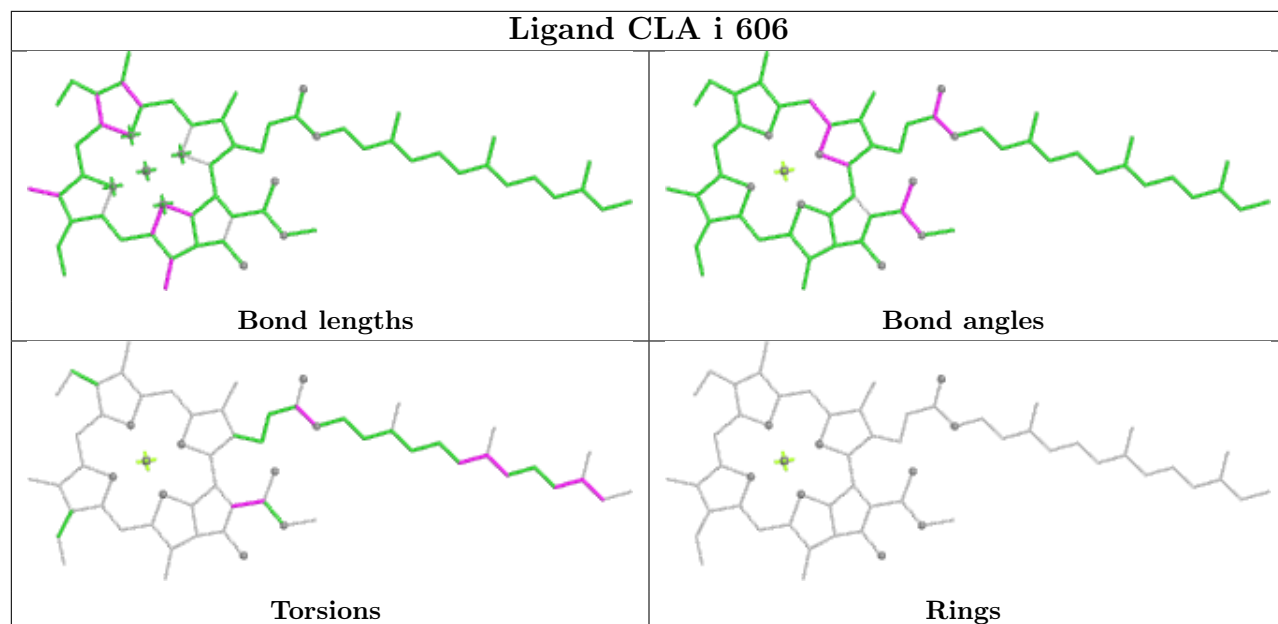
Torsions



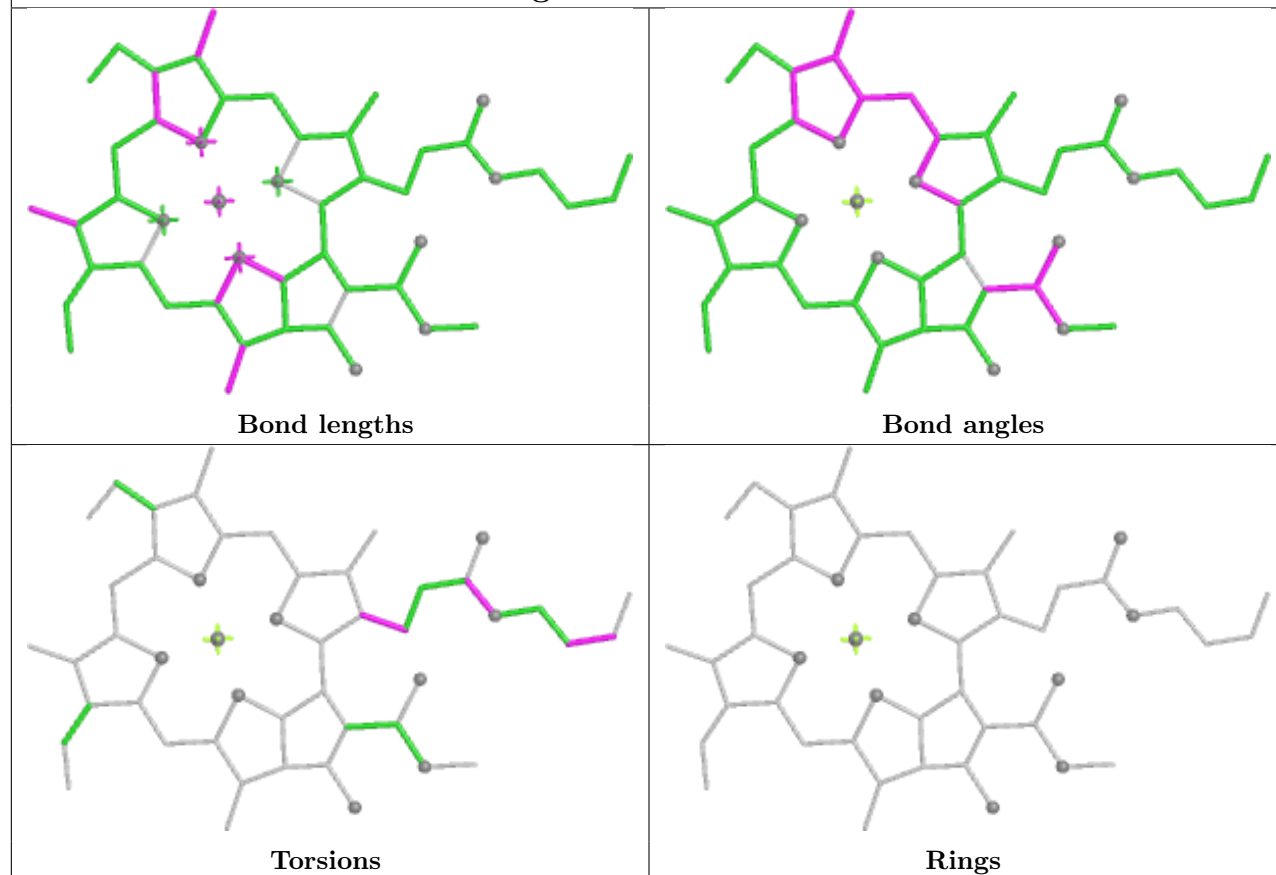
Rings



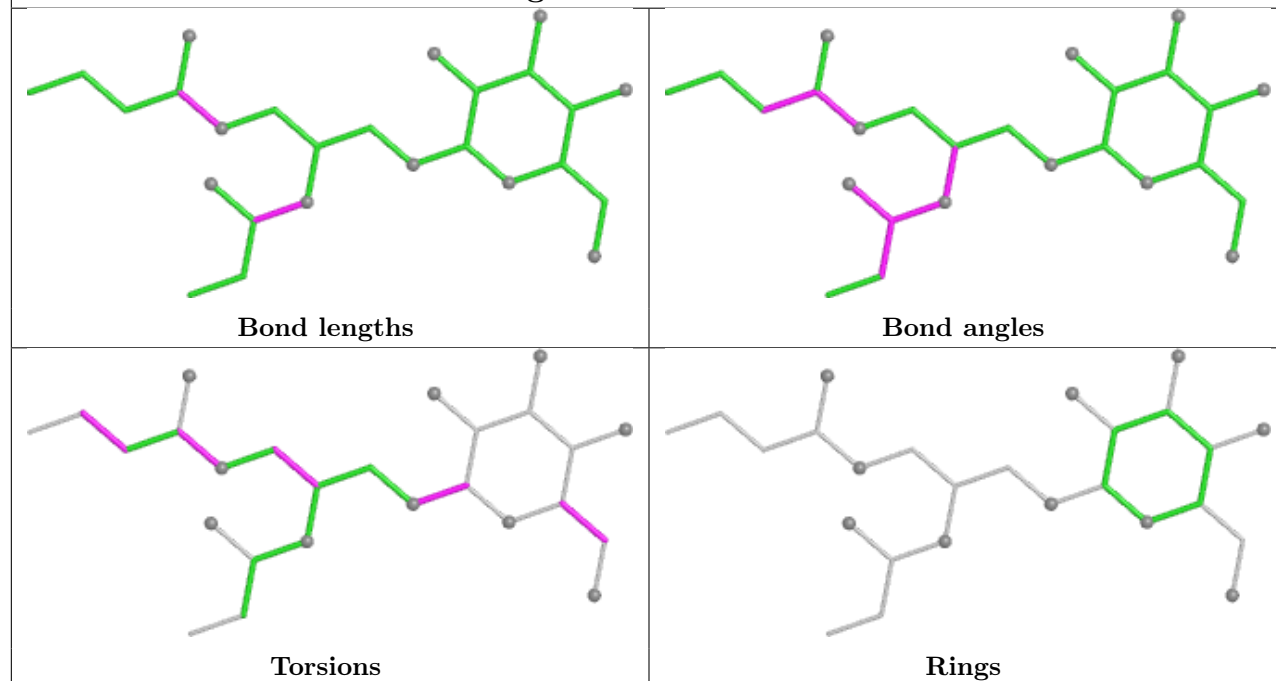


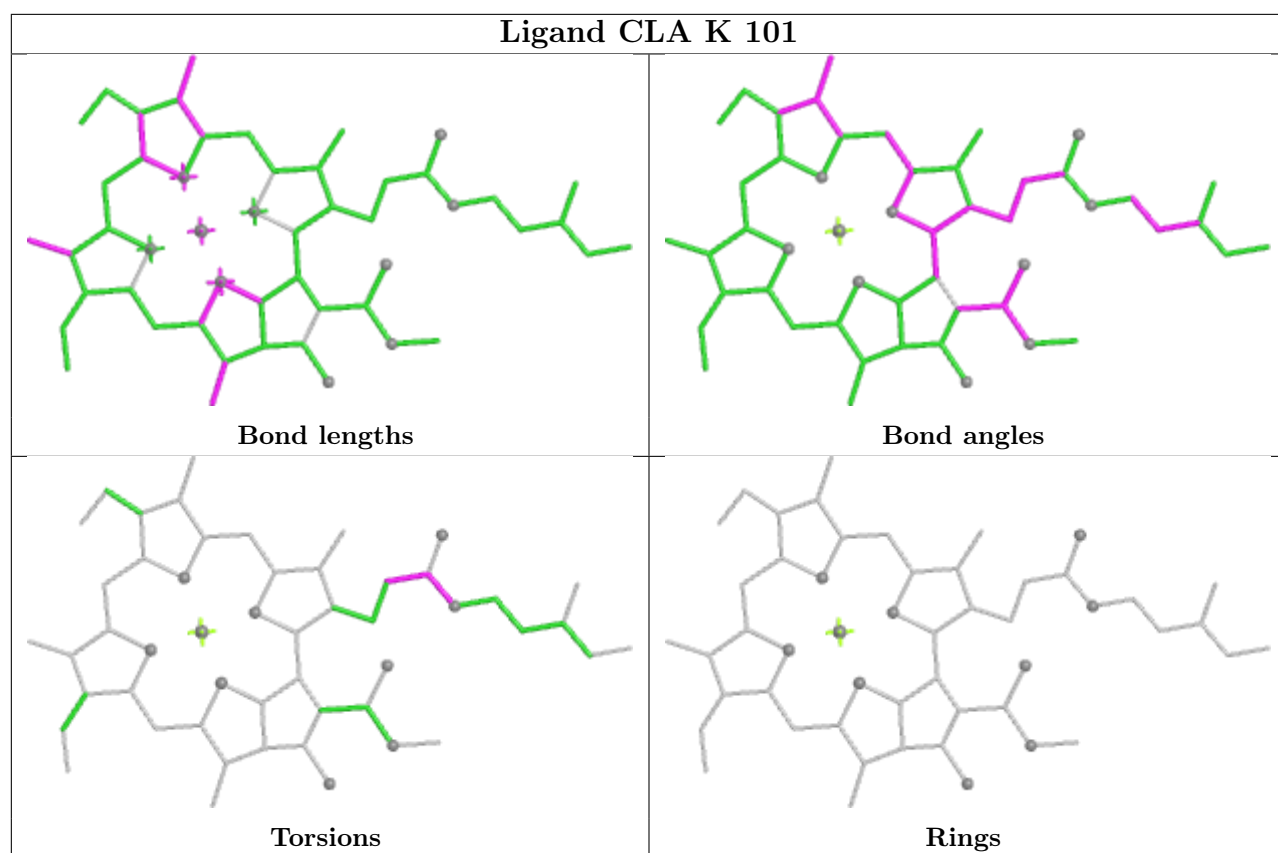
Ligand CLA b 307**Ligand CLA B 839****Ligand CLA i 606**

Ligand CLA B 828

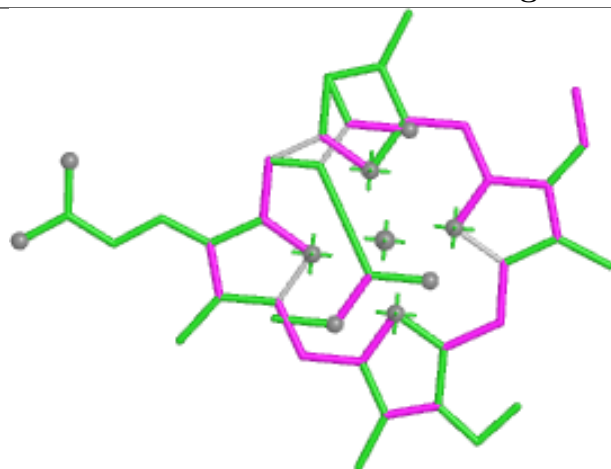


Ligand LMG O 204

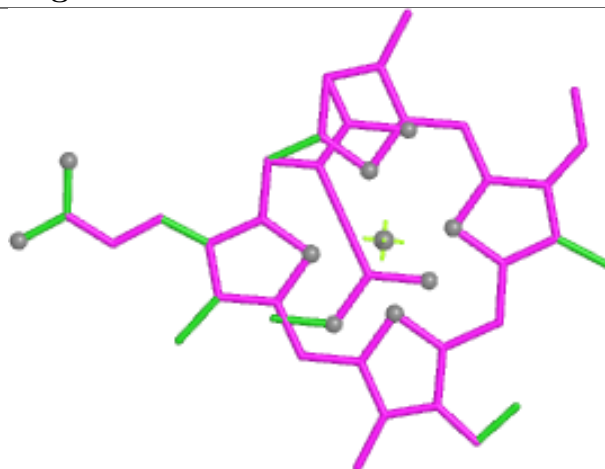




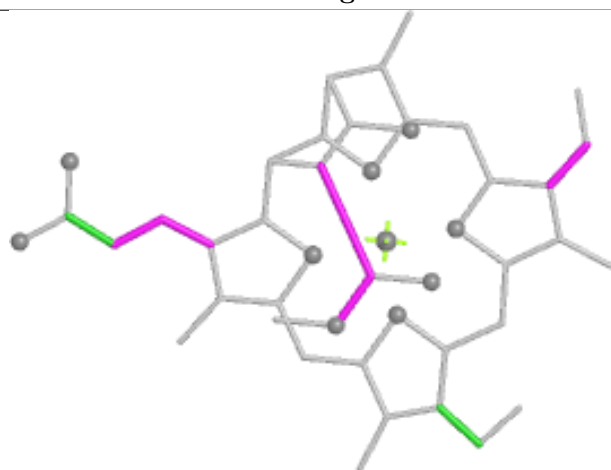
Ligand KC2 g 312



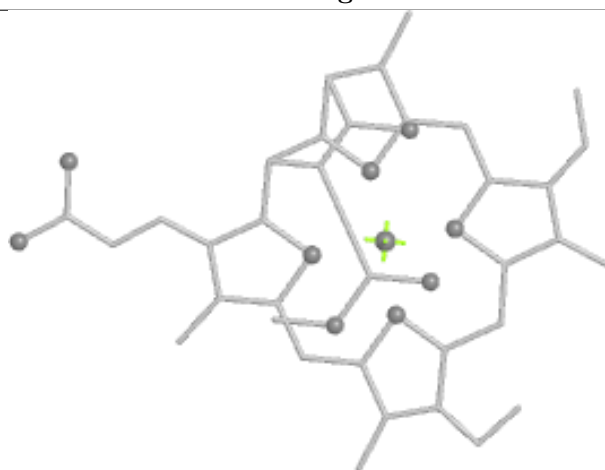
Bond lengths



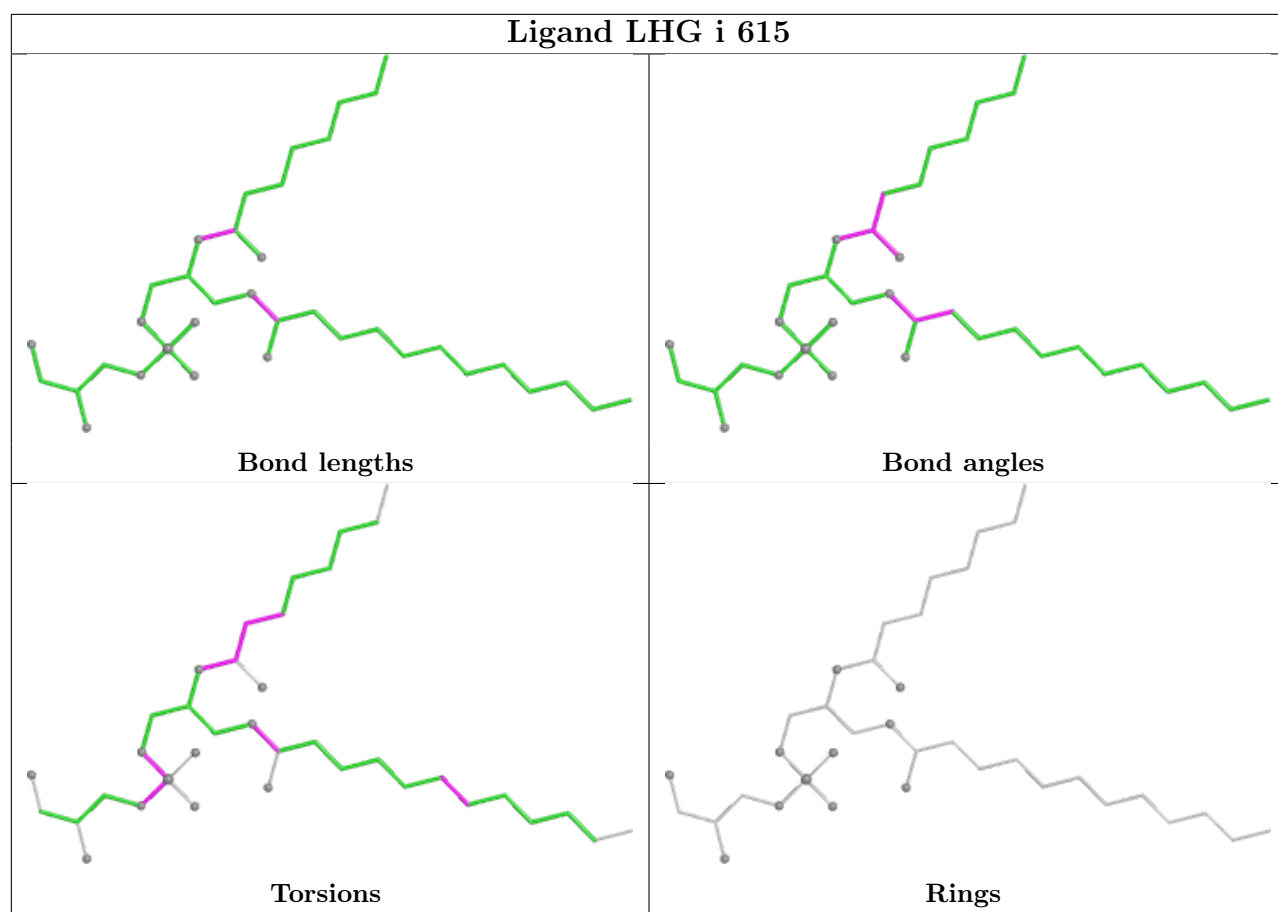
Bond angles



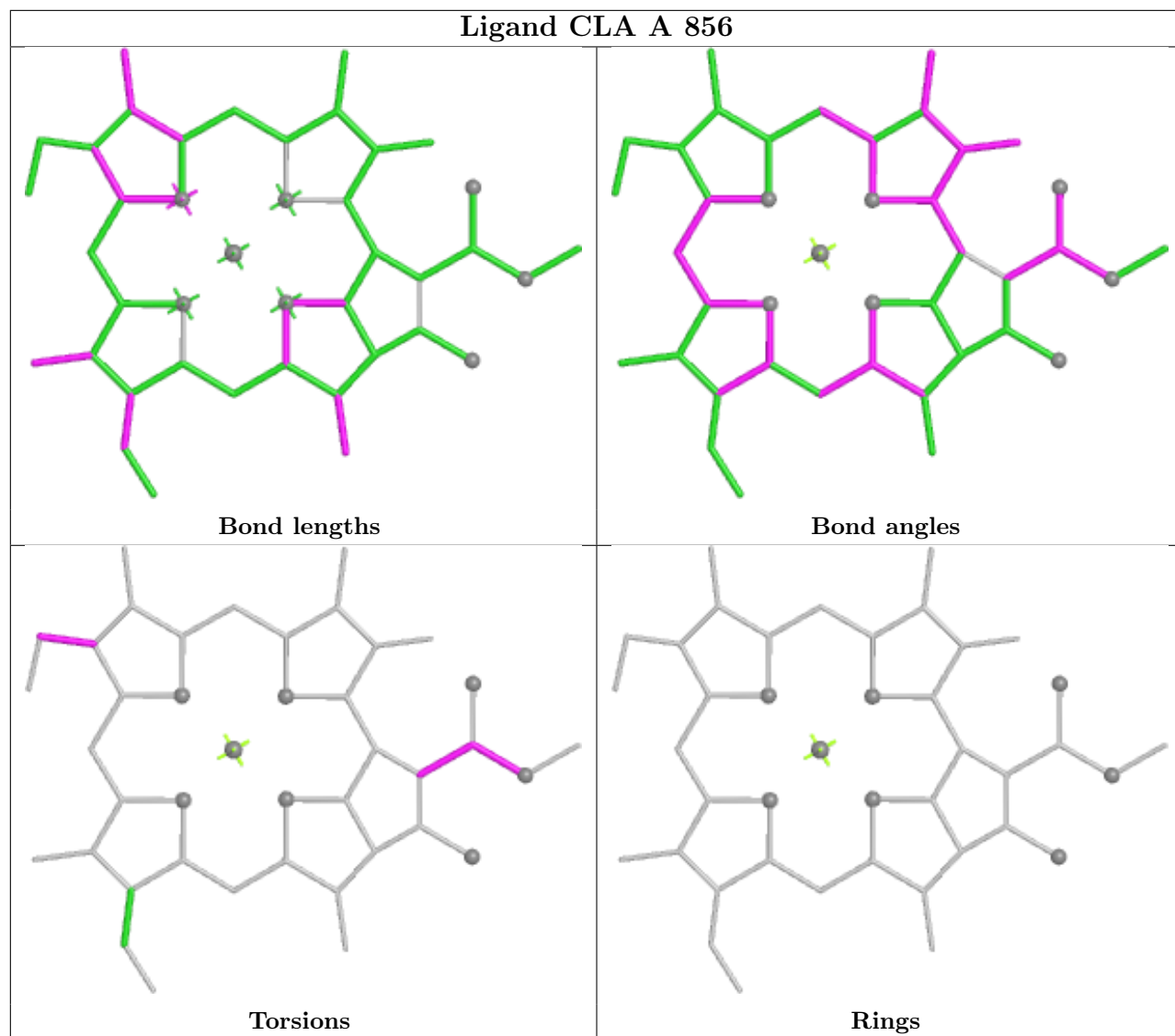
Torsions



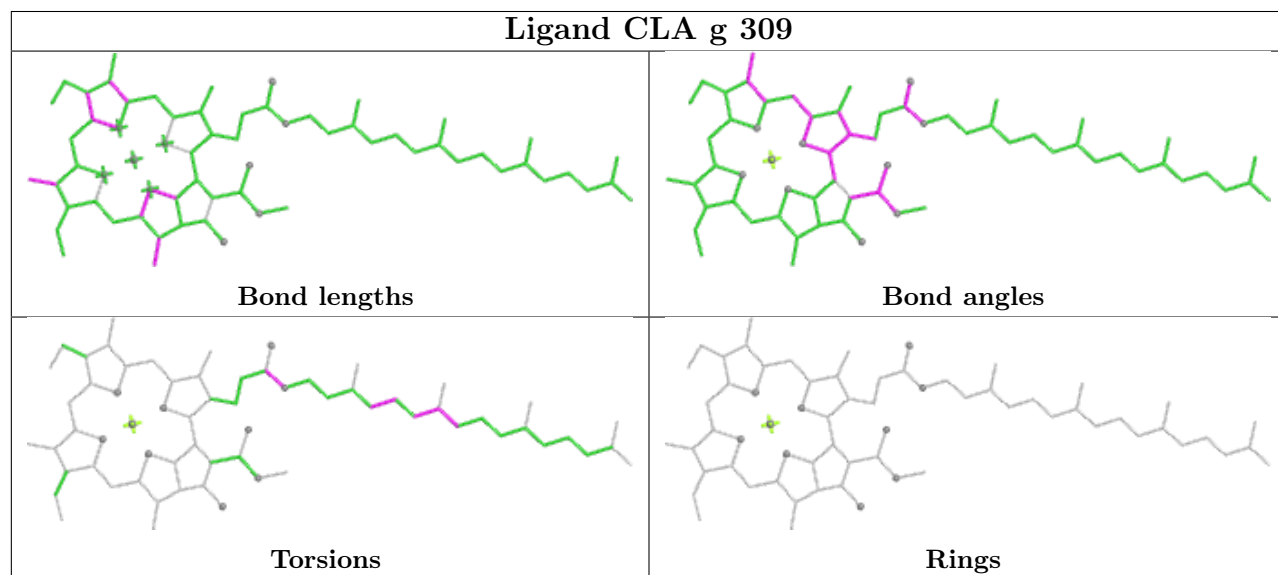
Rings



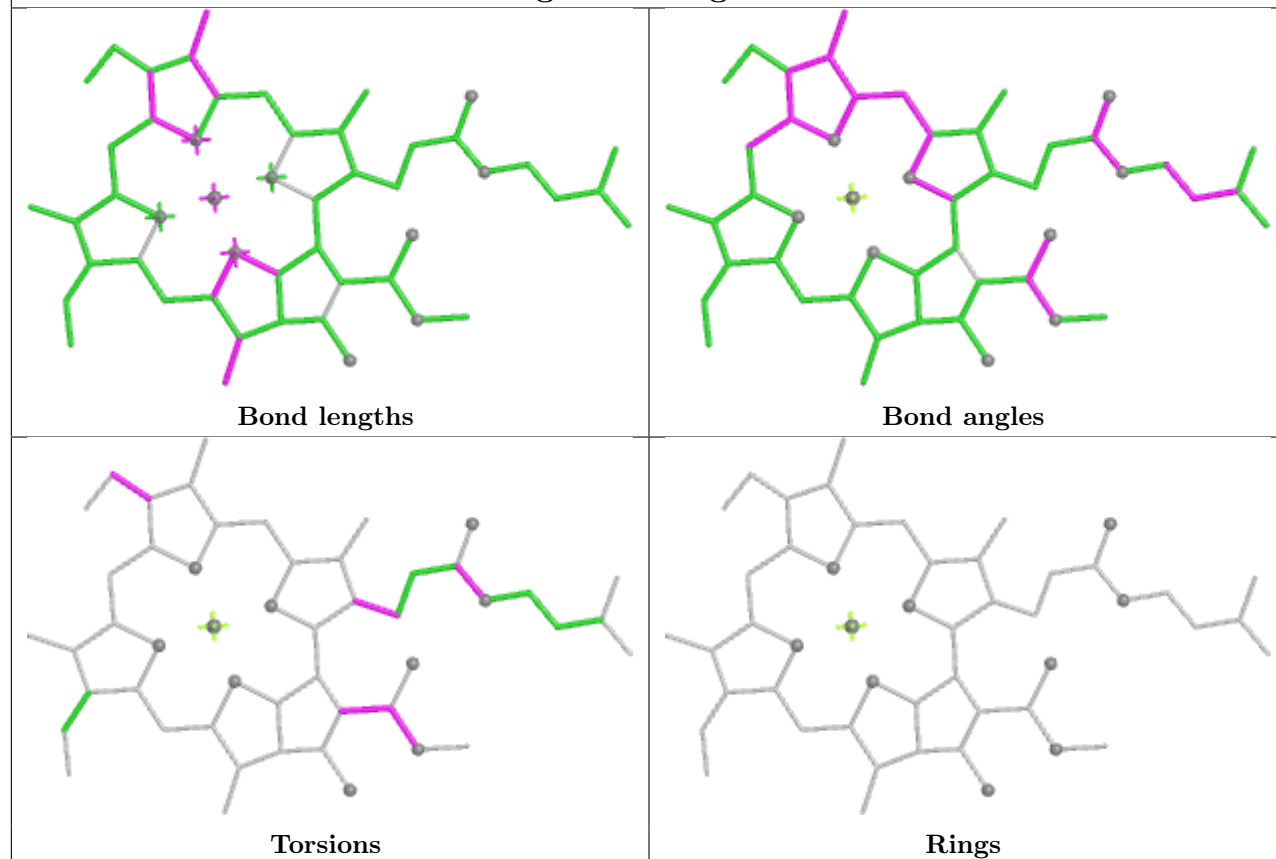
Ligand CLA A 856



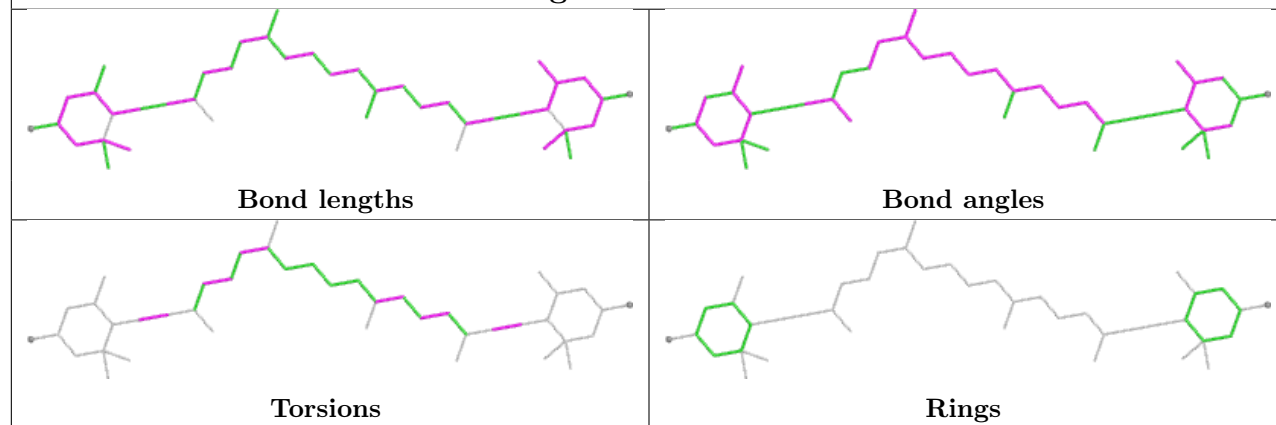
Ligand CLA g 309

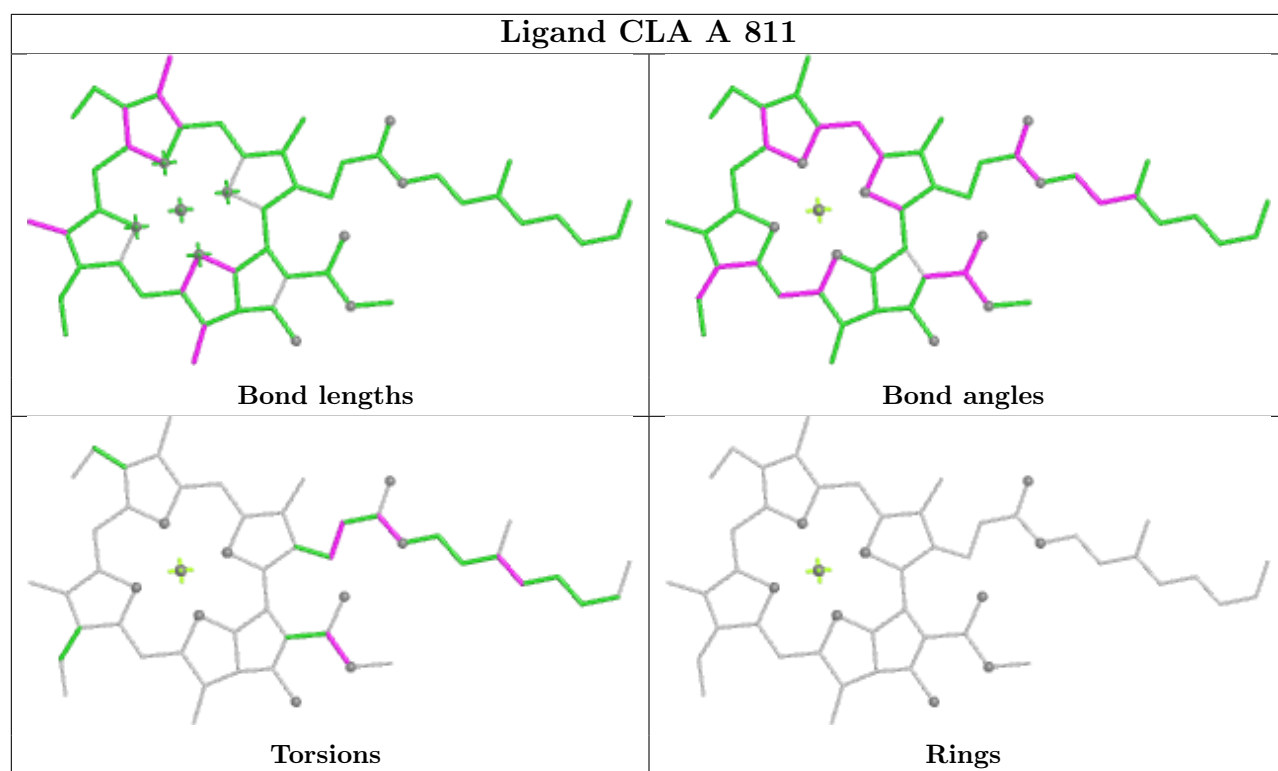


Ligand CLA g 303

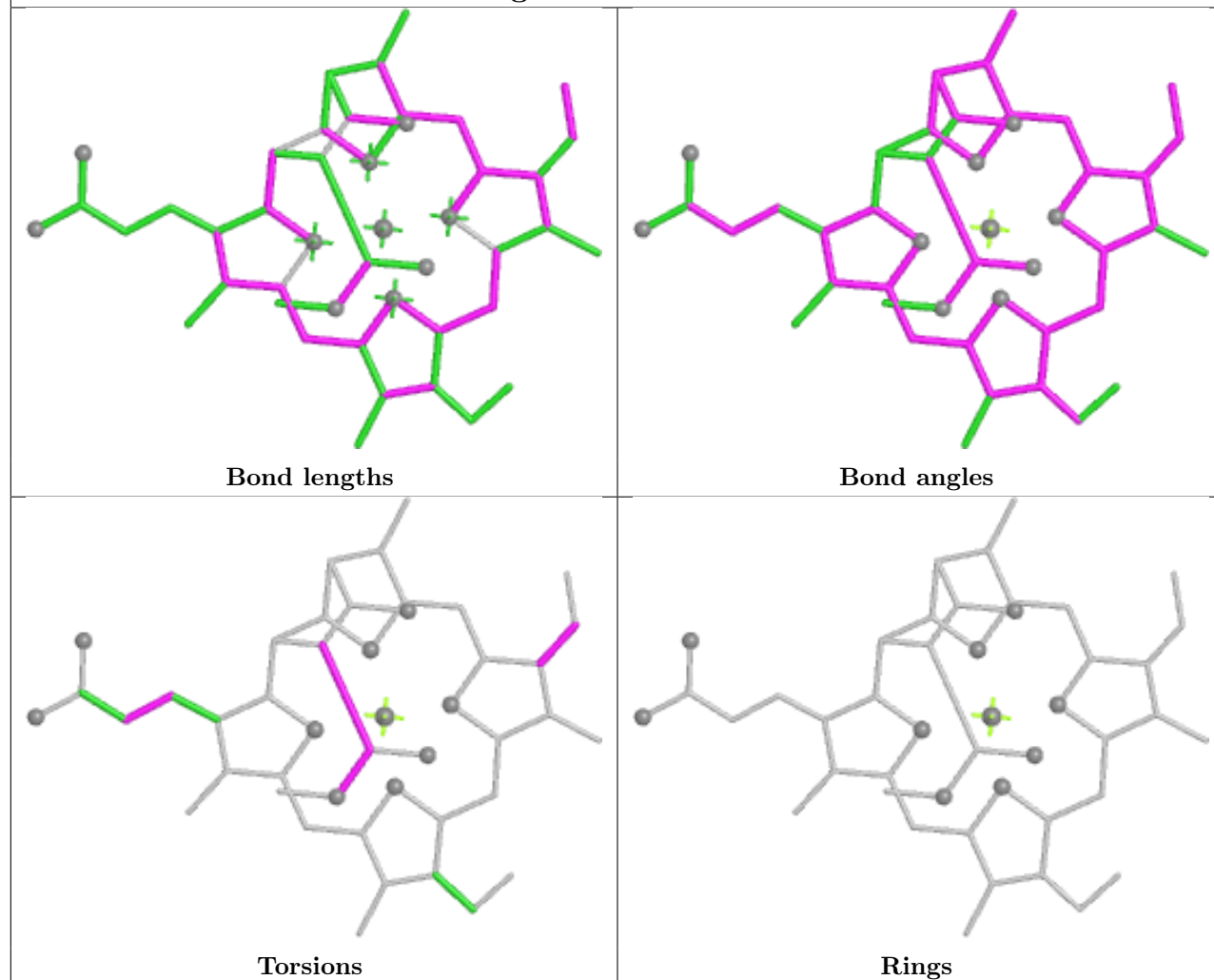


Ligand II0 d 315

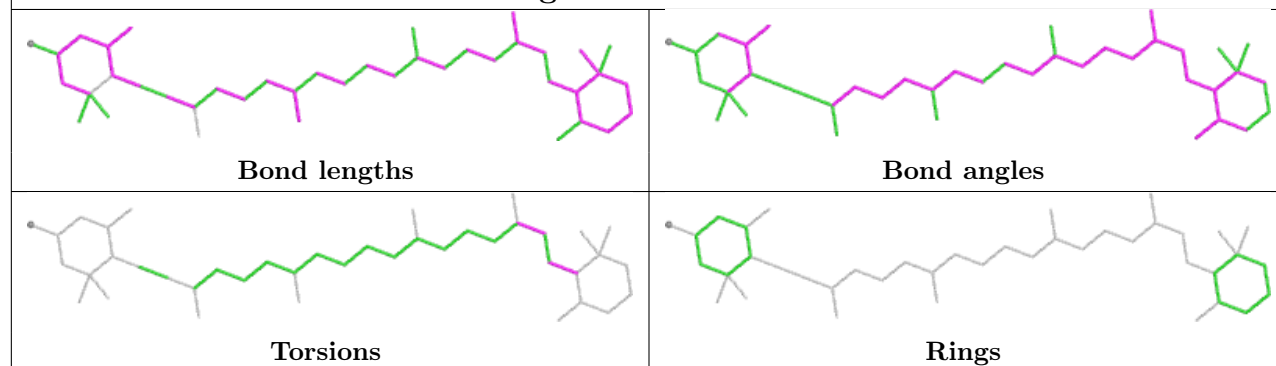




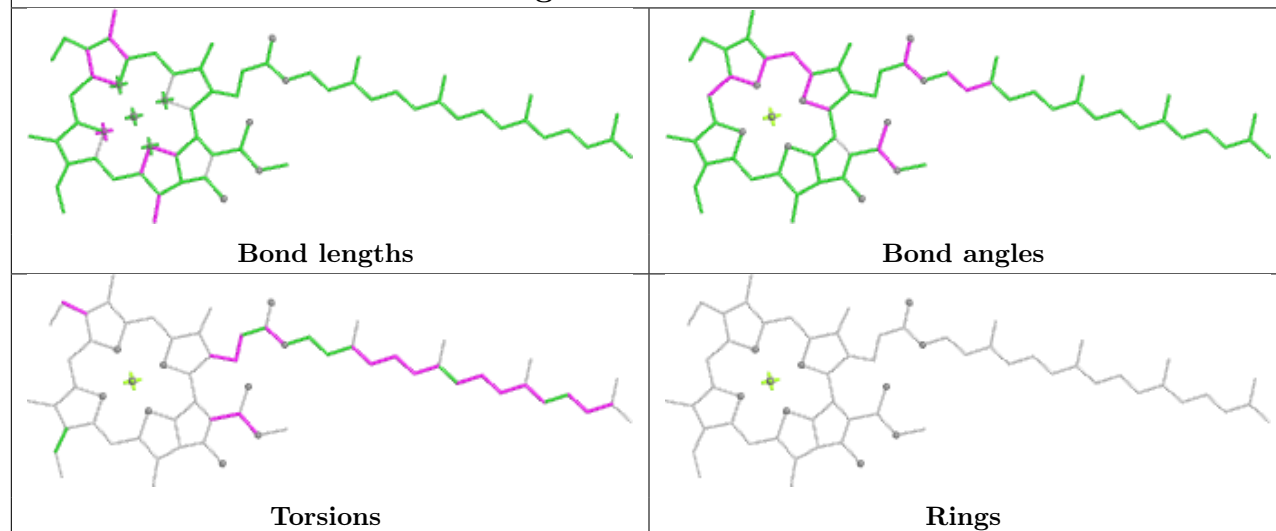
Ligand KC2 d 310



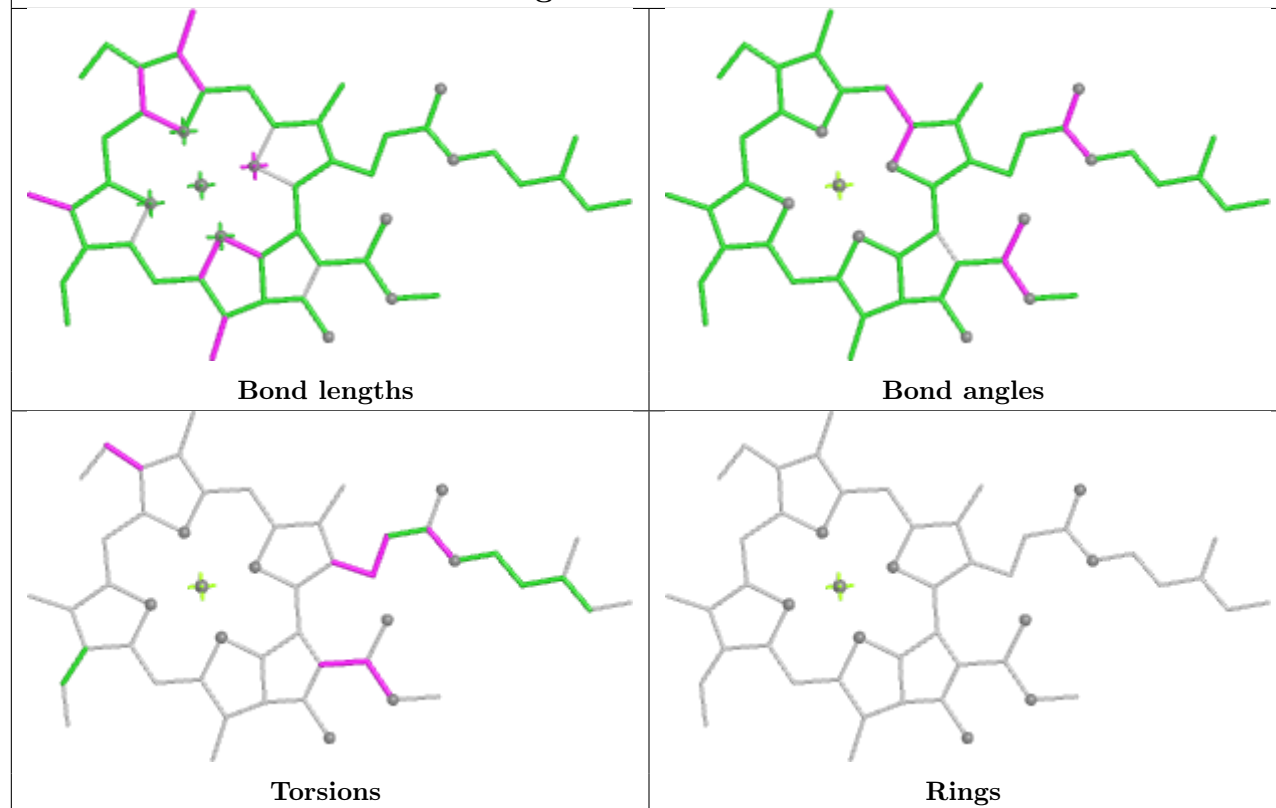
Ligand IHT b 316

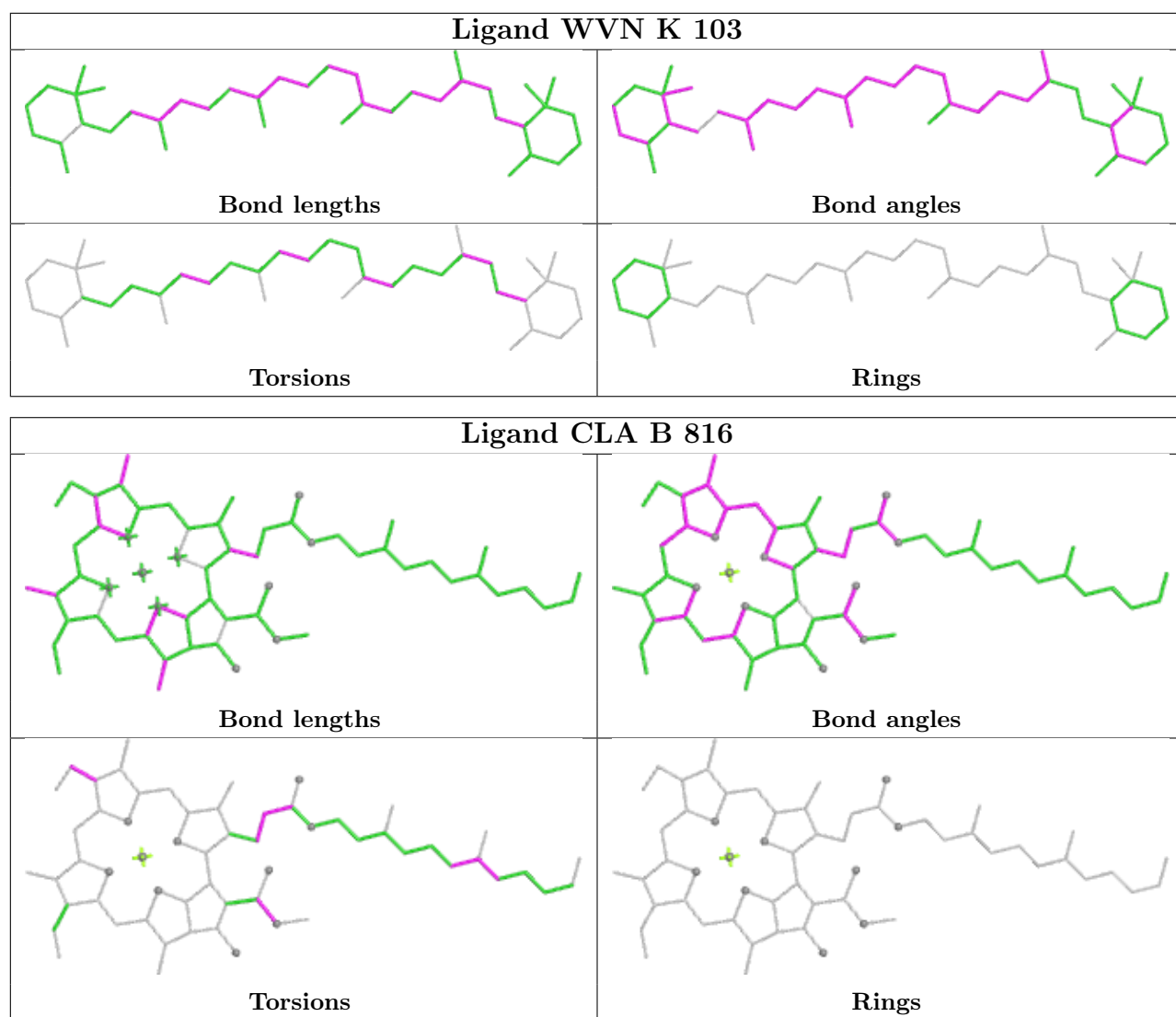


Ligand CLA b 313

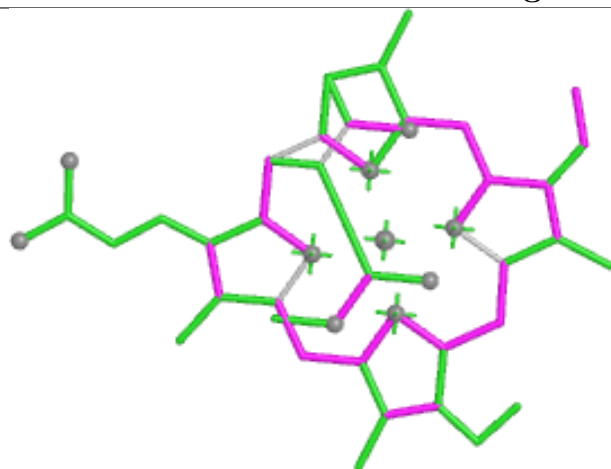


Ligand CLA d 306

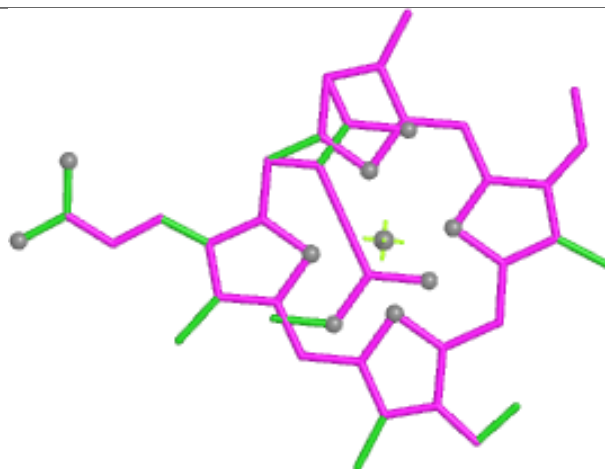




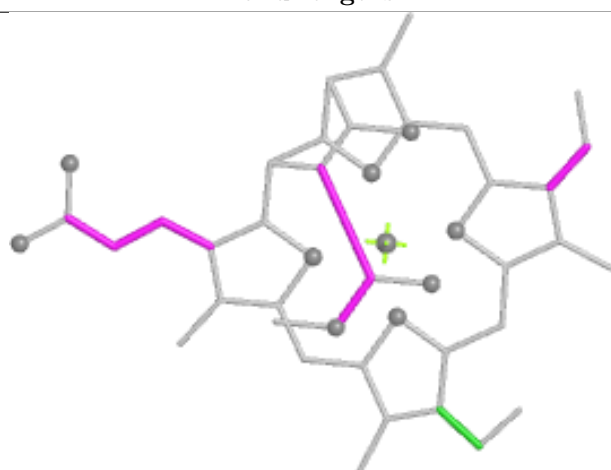
Ligand KC2 f 611



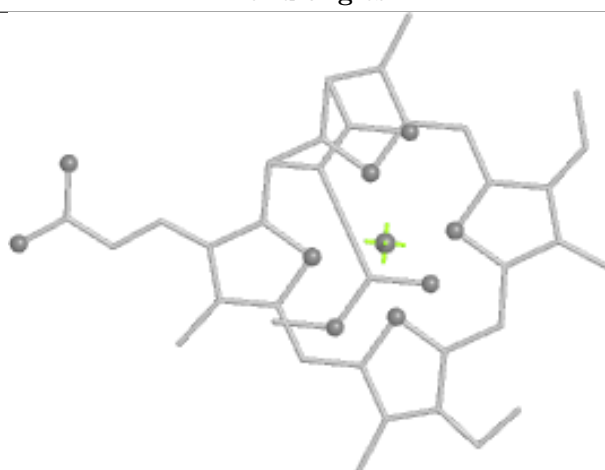
Bond lengths



Bond angles

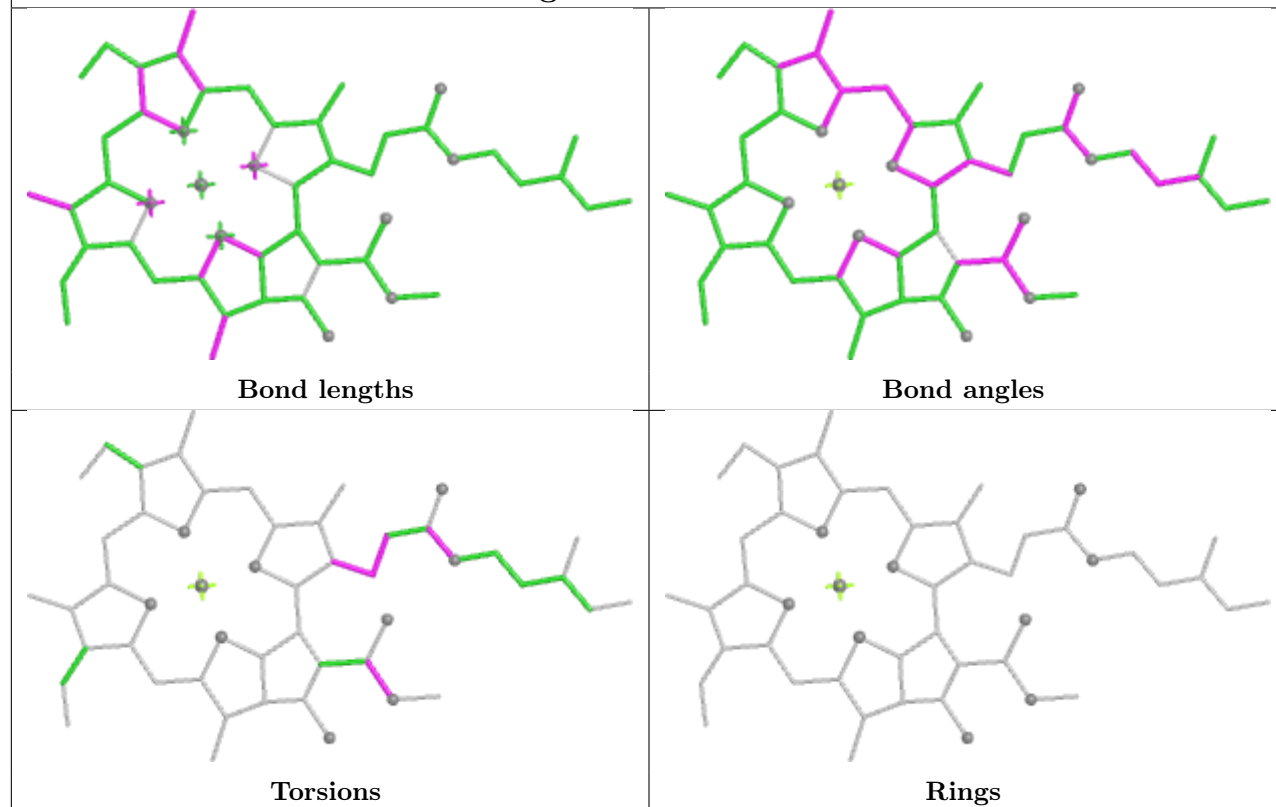


Torsions

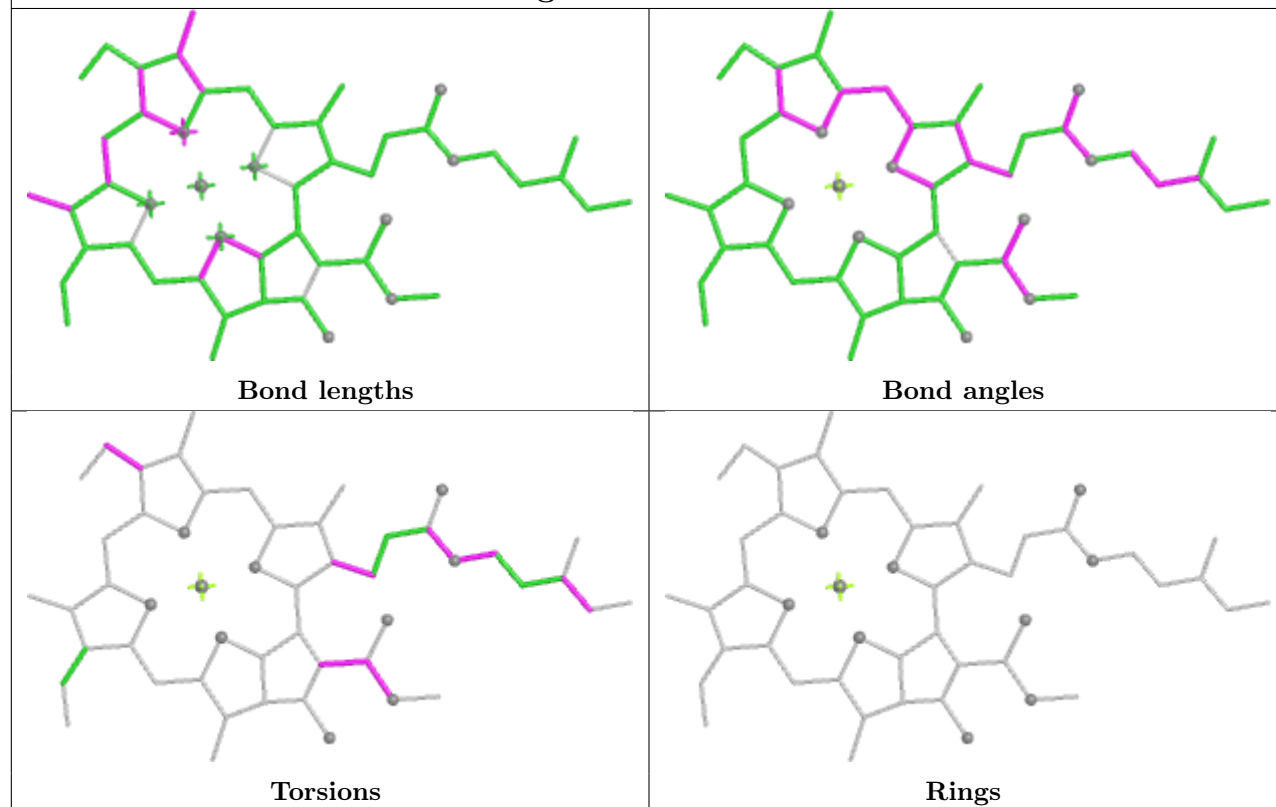


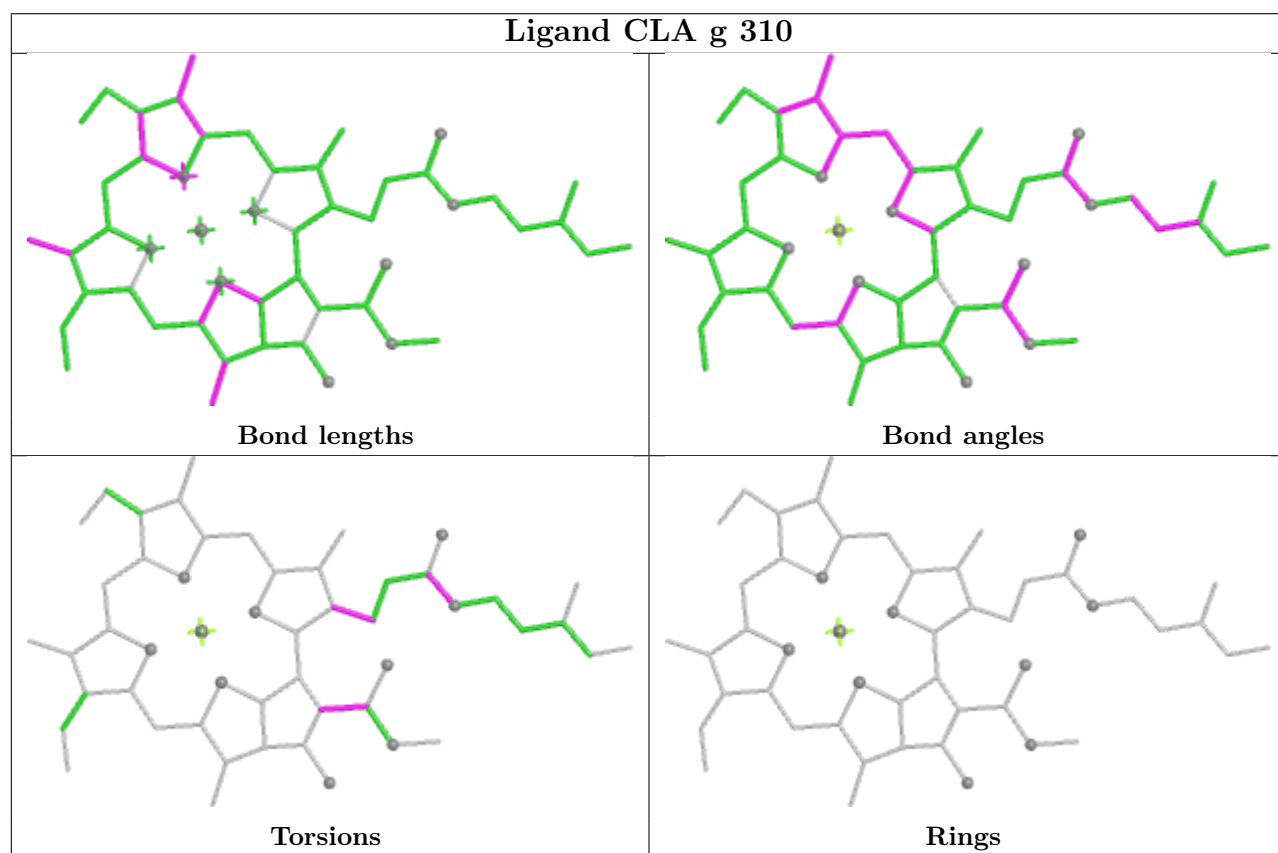
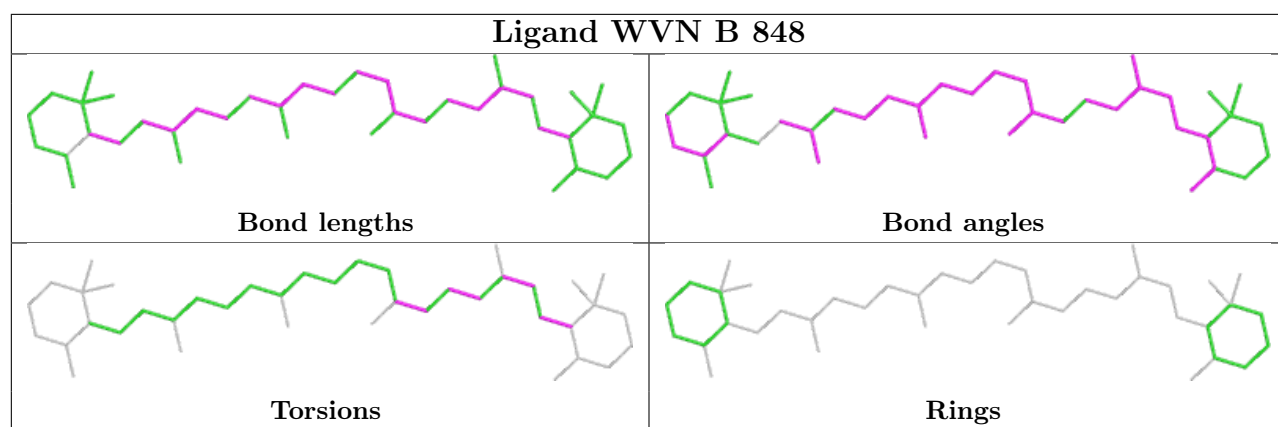
Rings

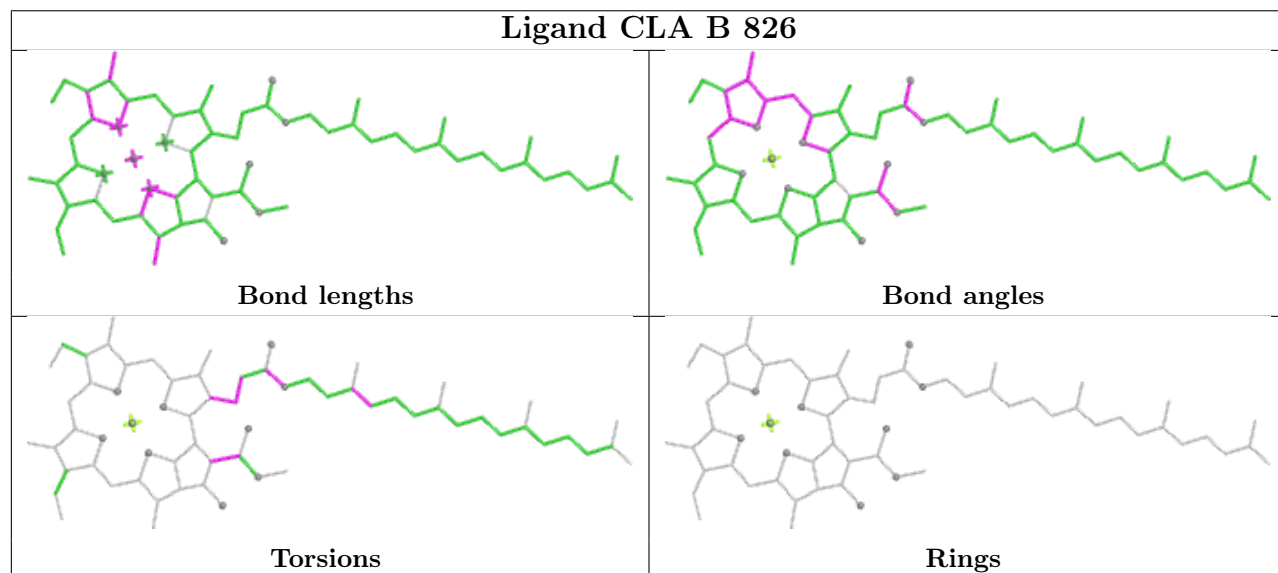
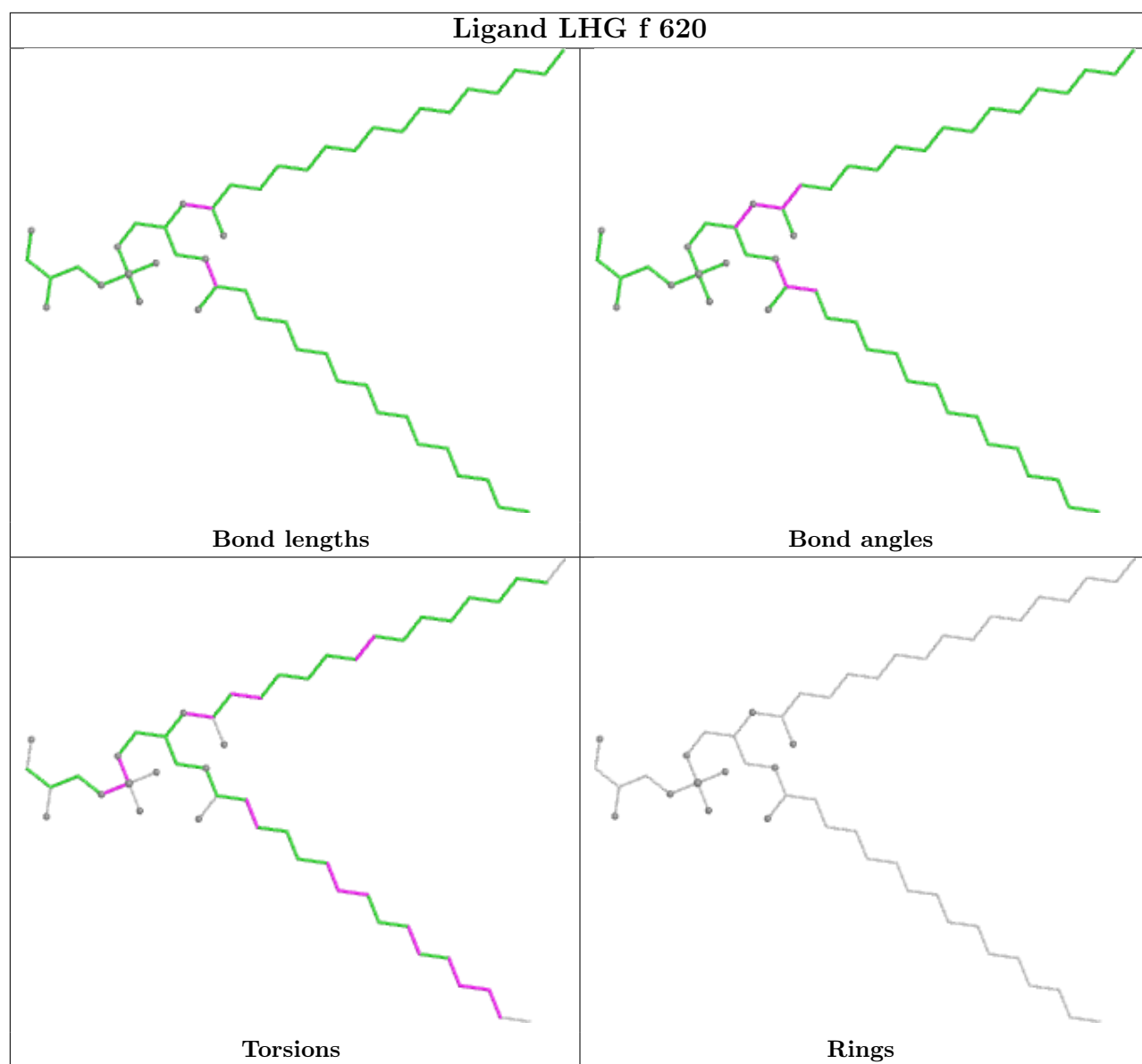
Ligand CLA f 612



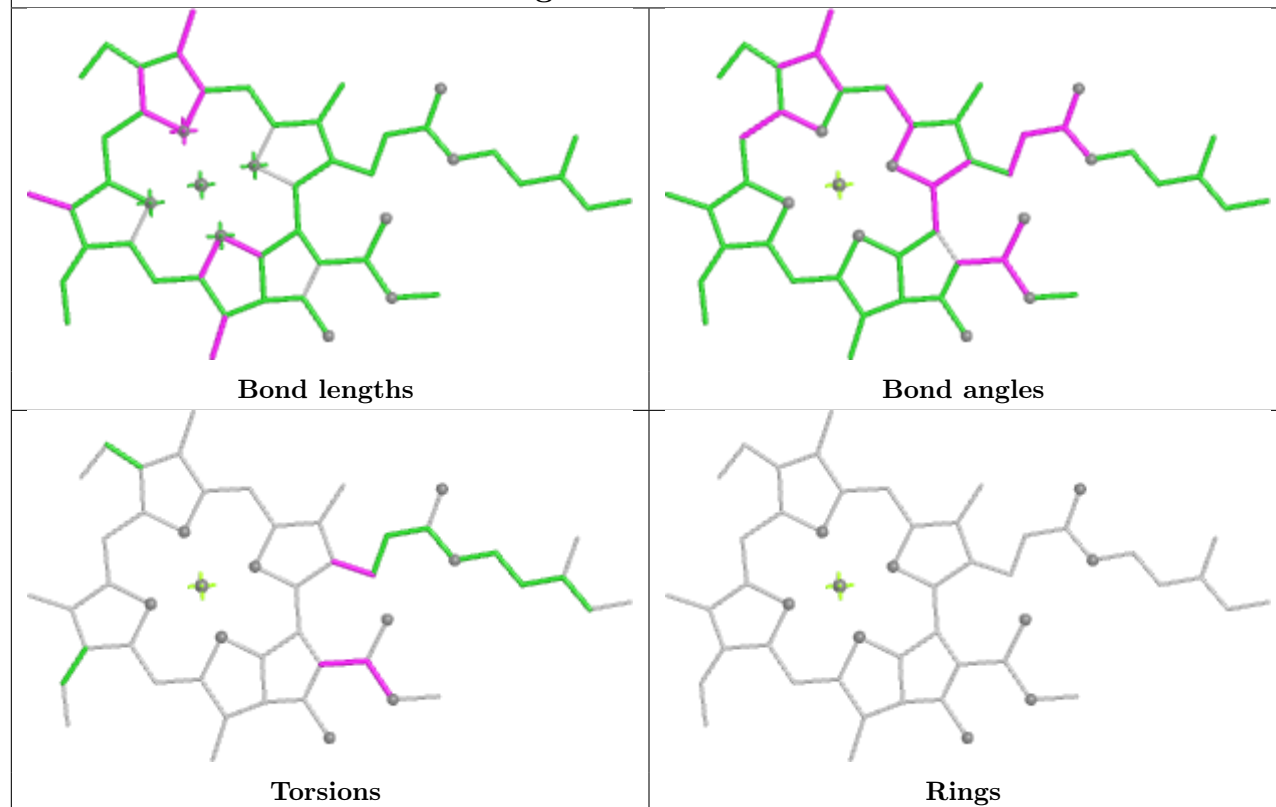
Ligand CLA c 601



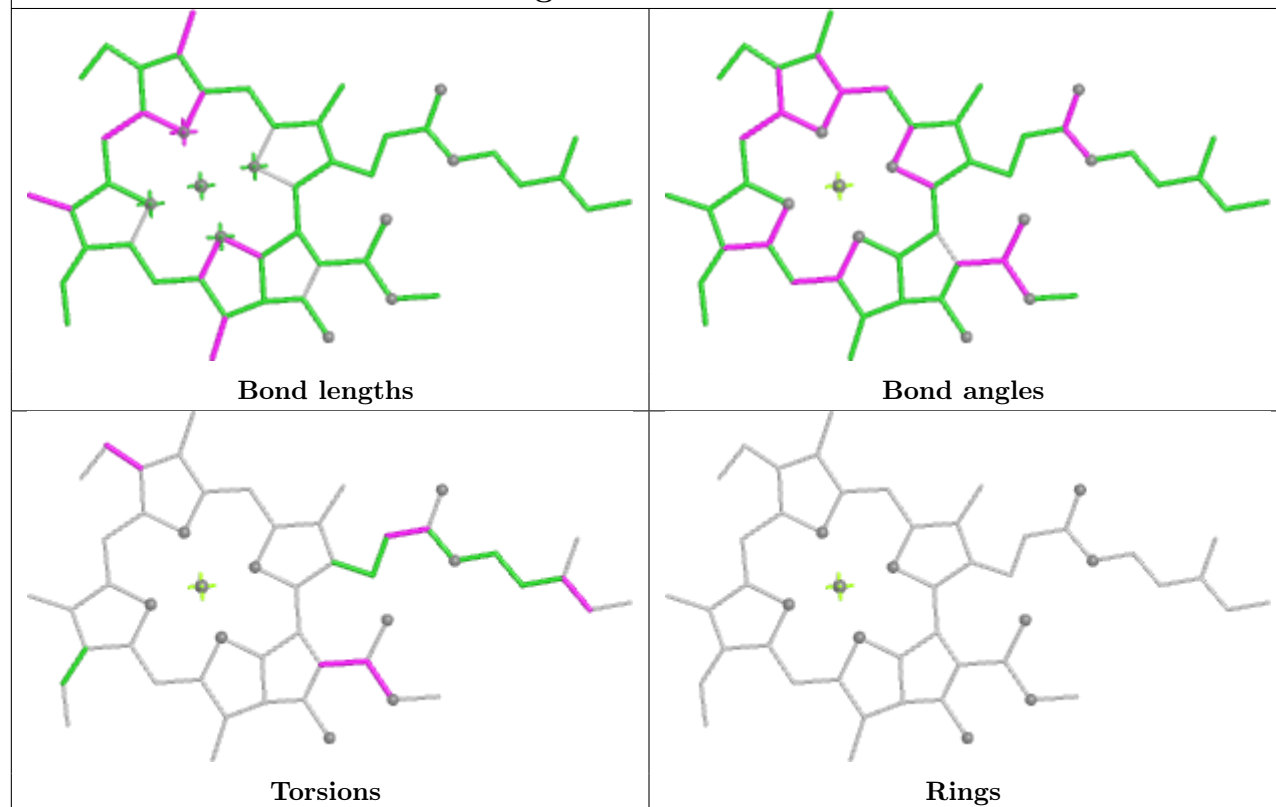


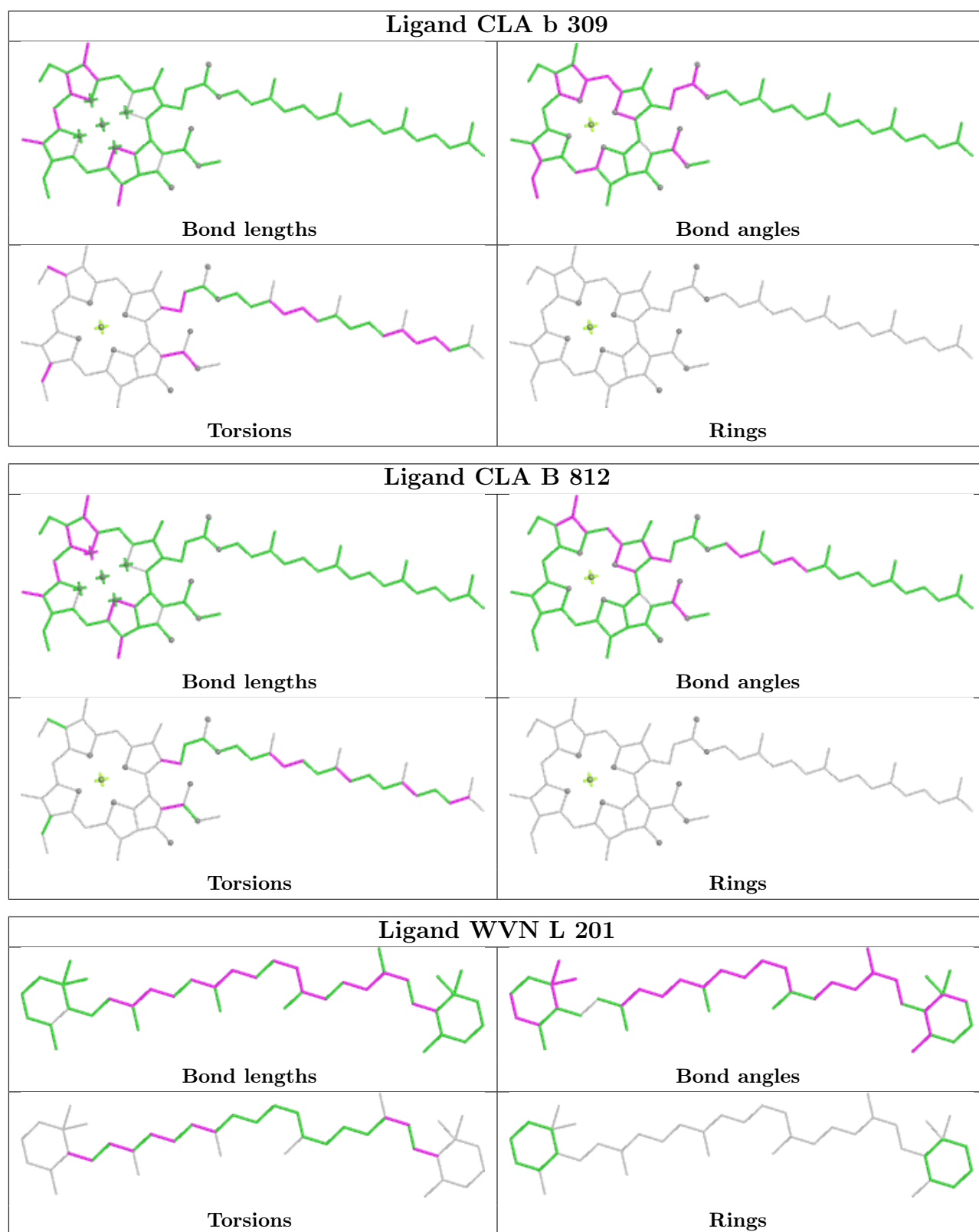


Ligand CLA h 303

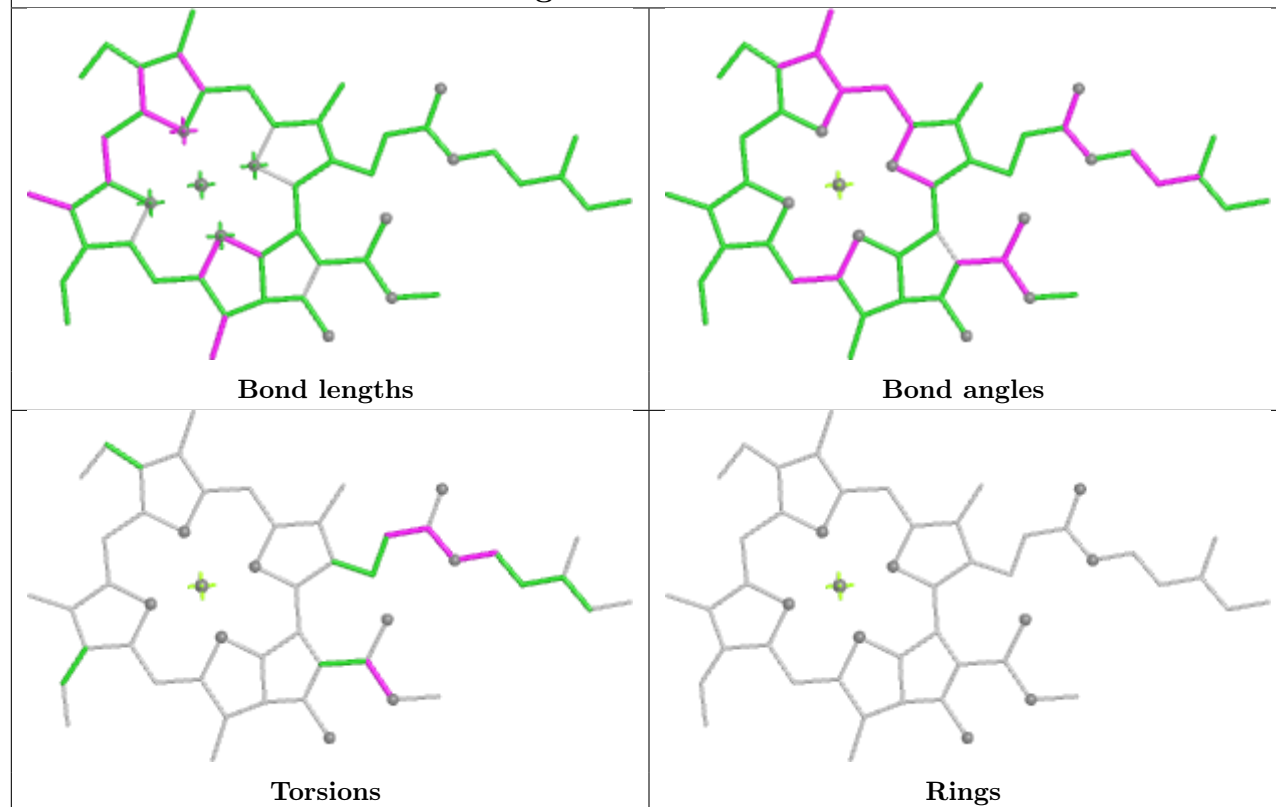


Ligand CLA d 305

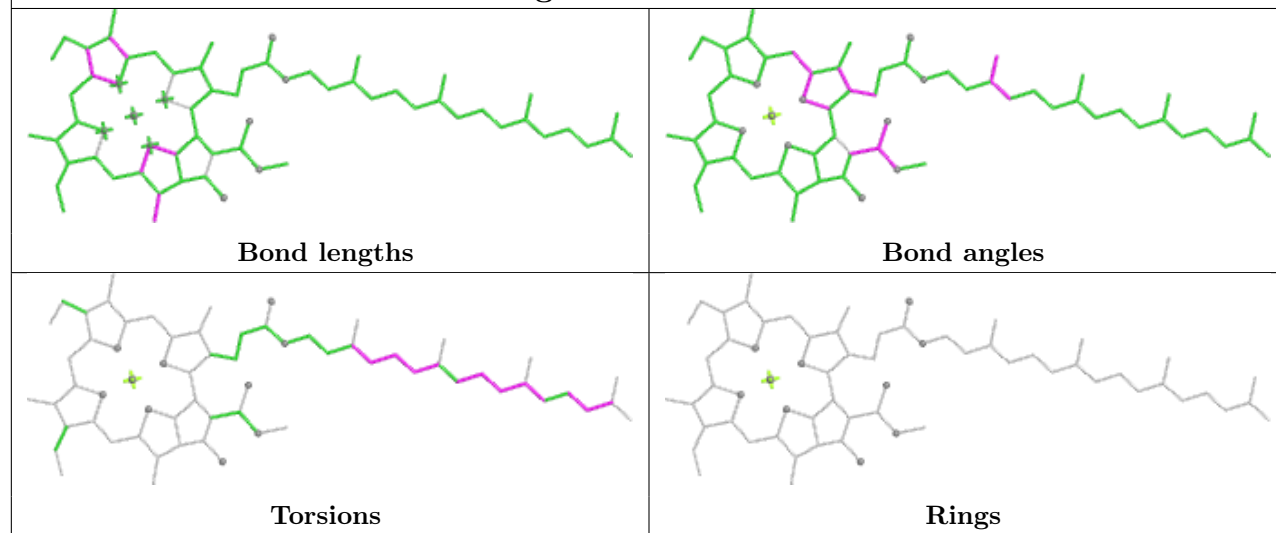


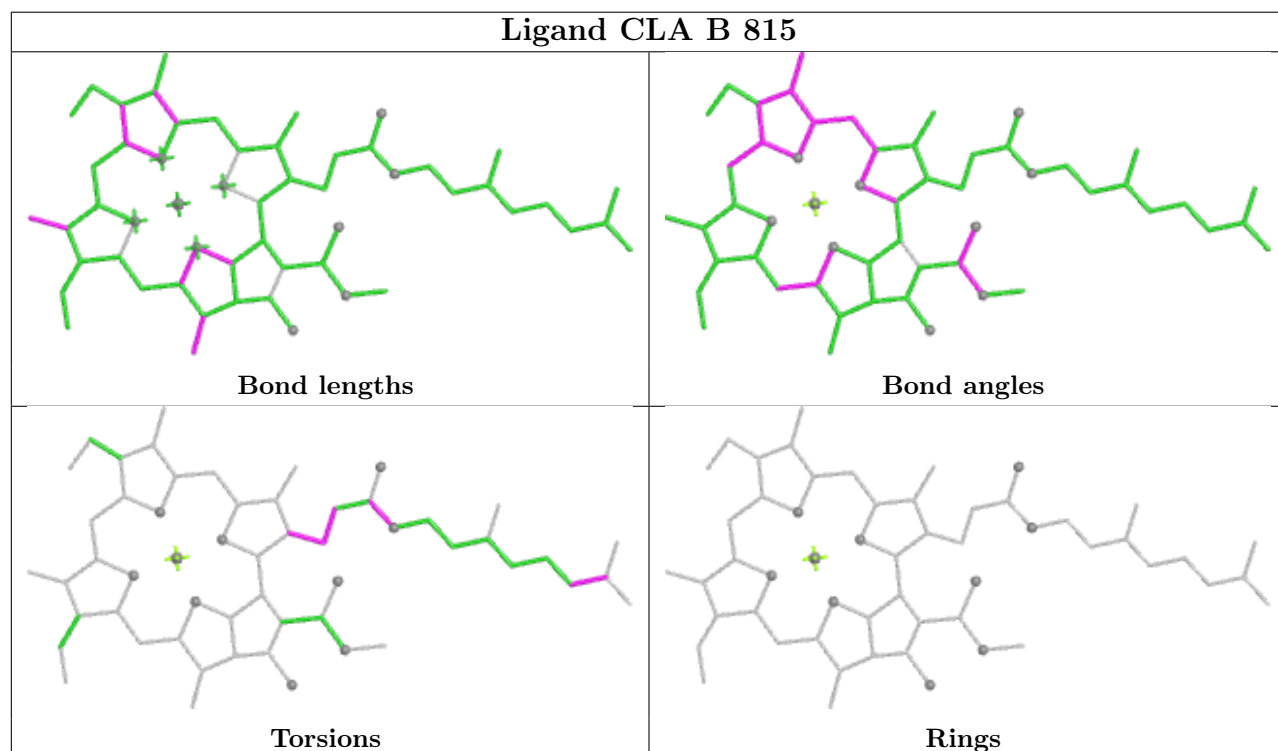
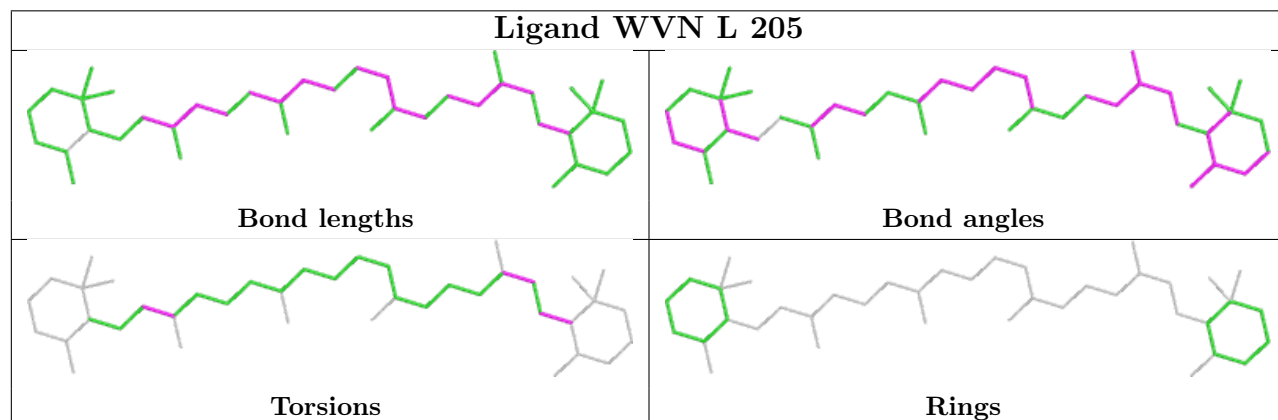
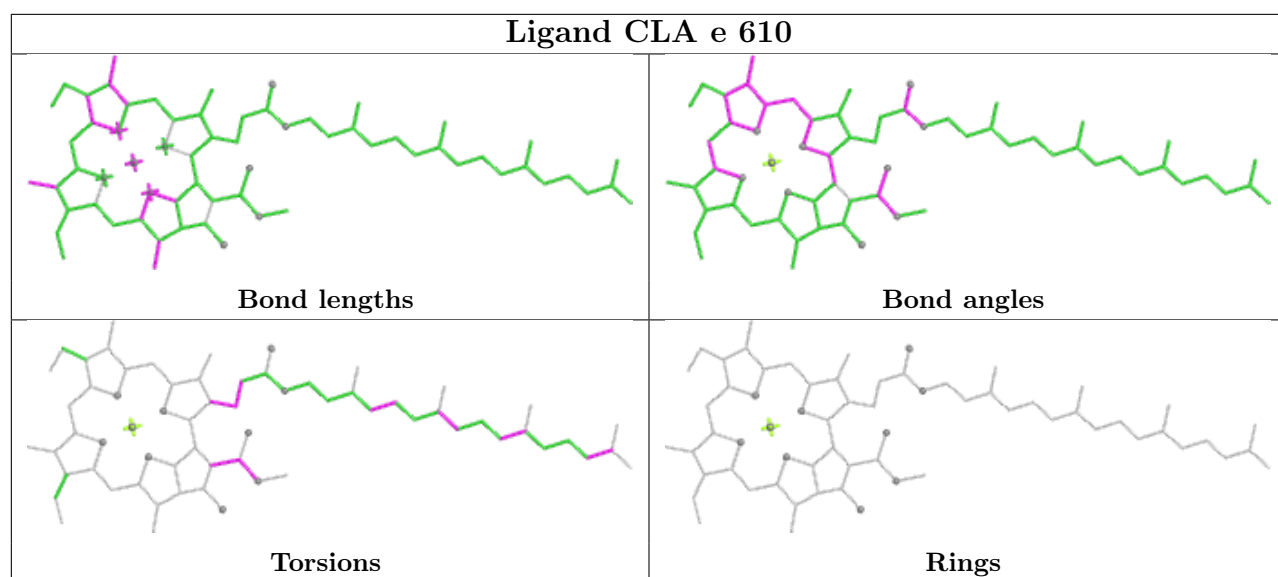


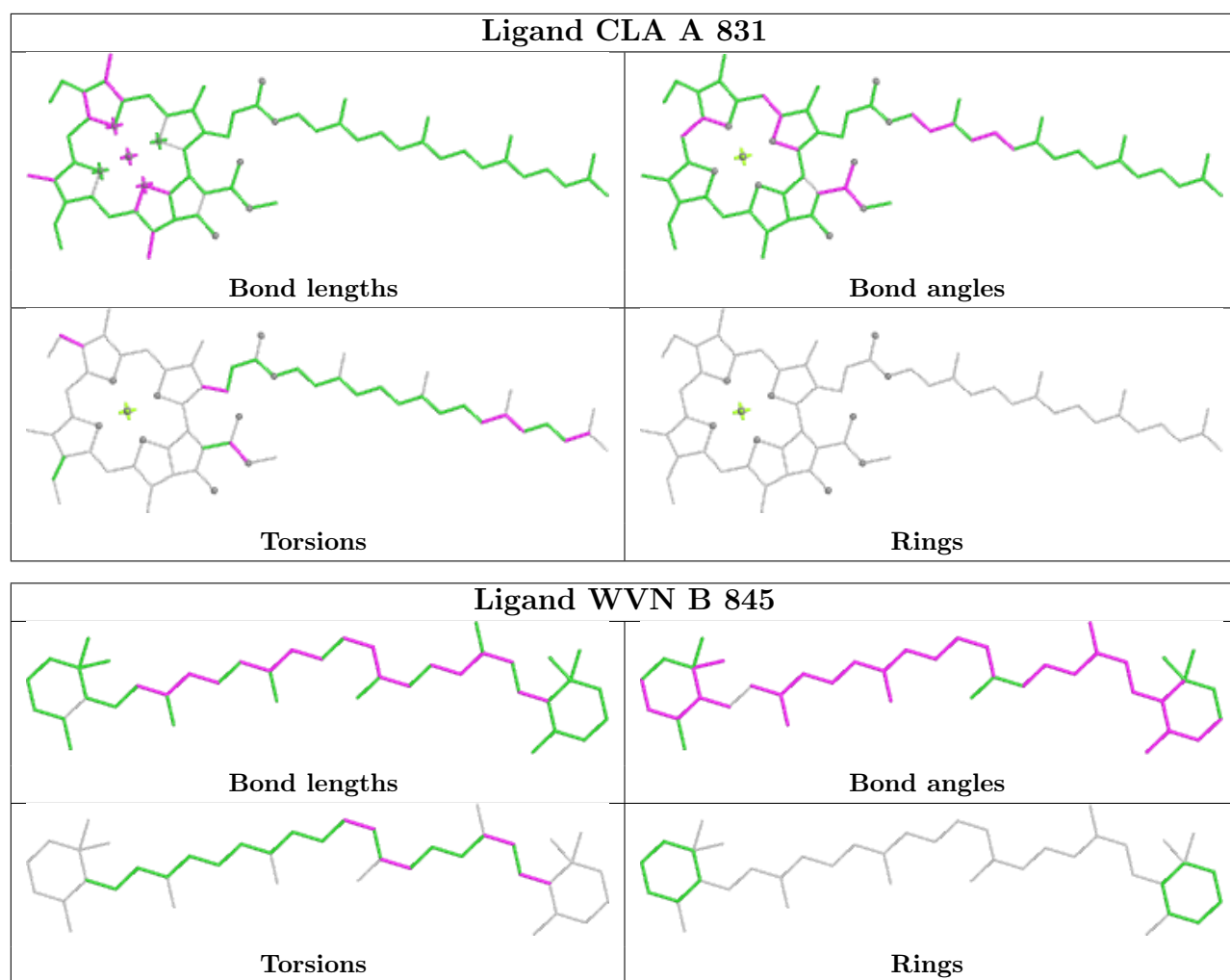
Ligand CLA b 311

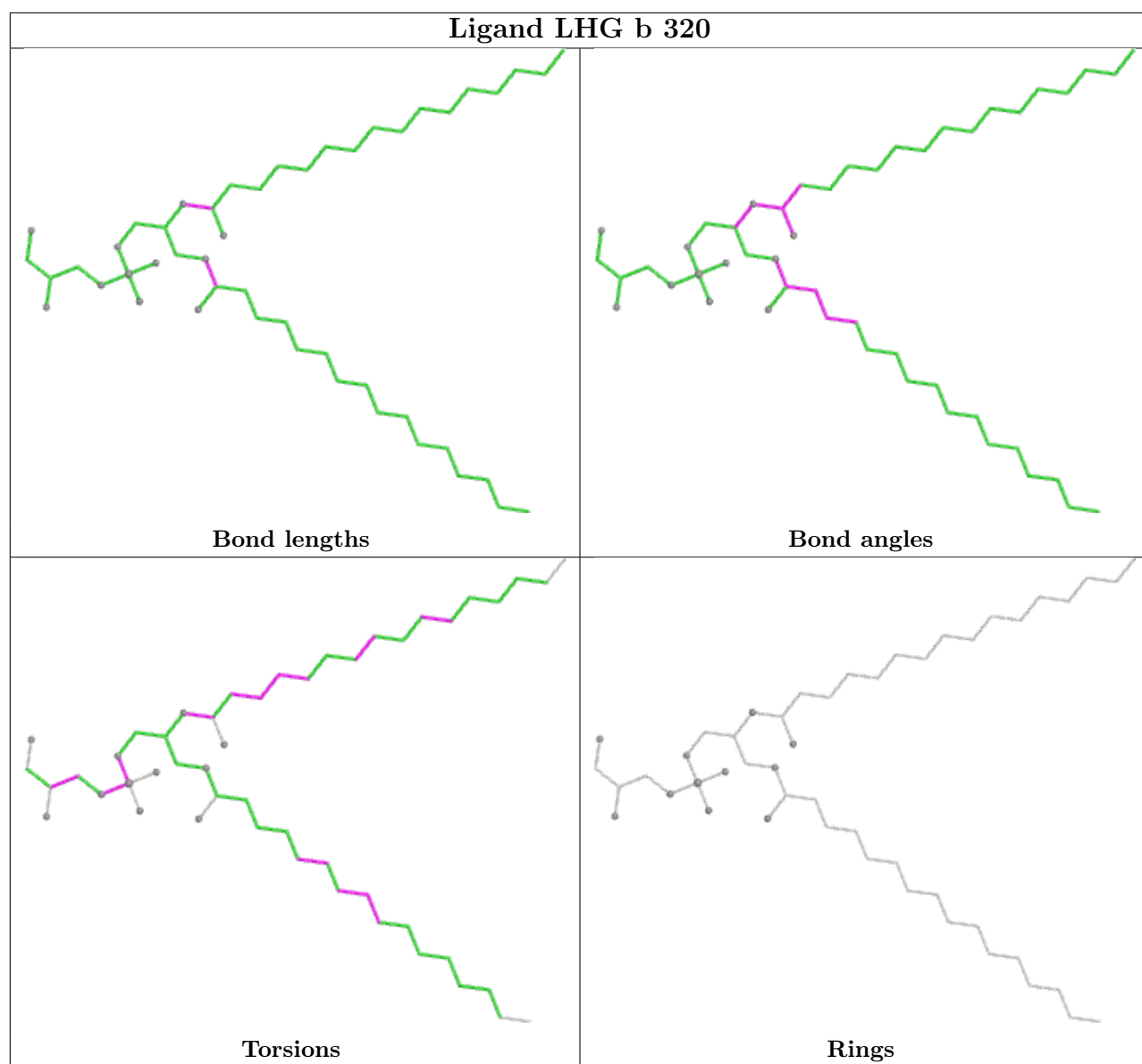


Ligand CLA b 305

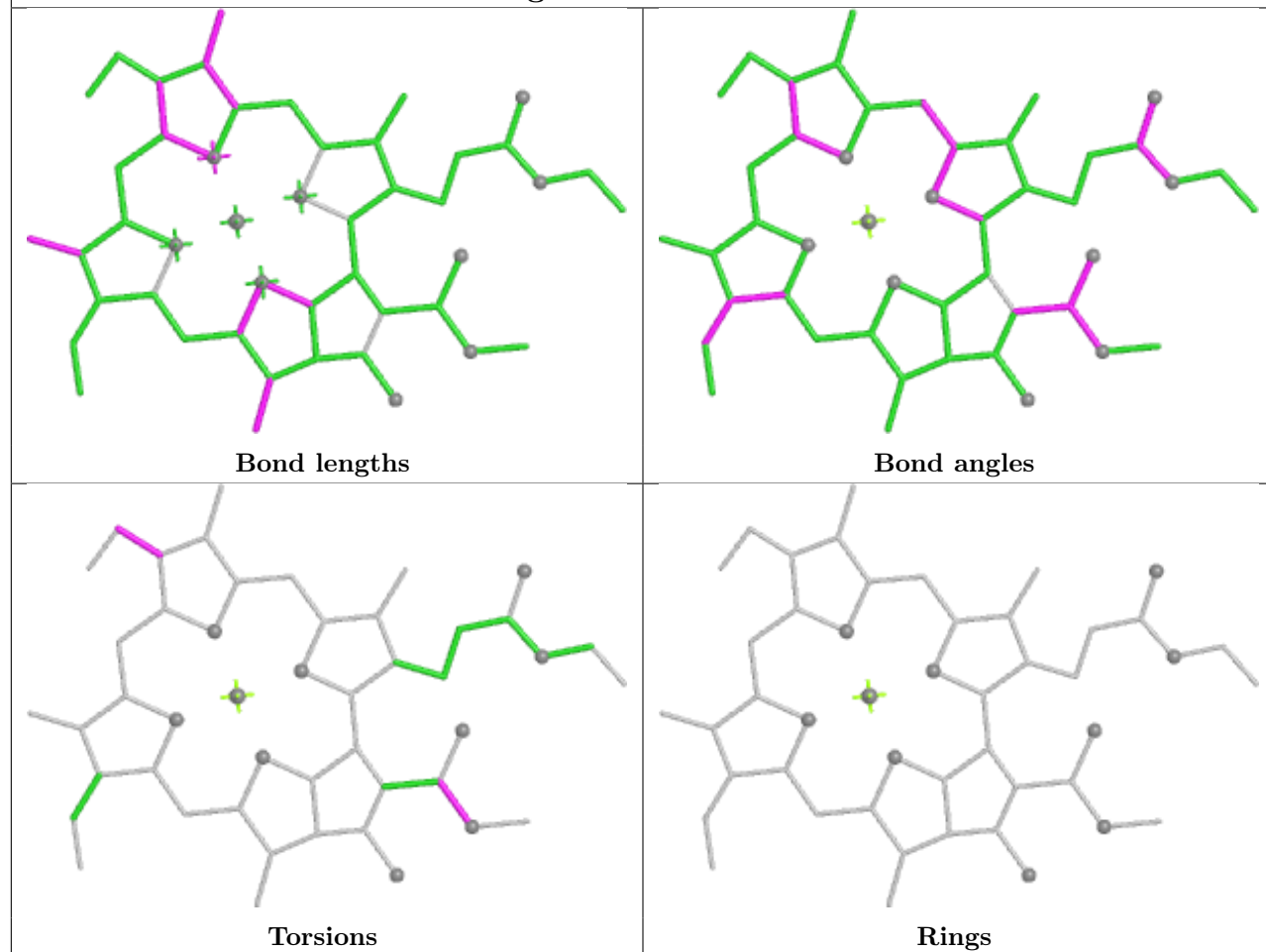




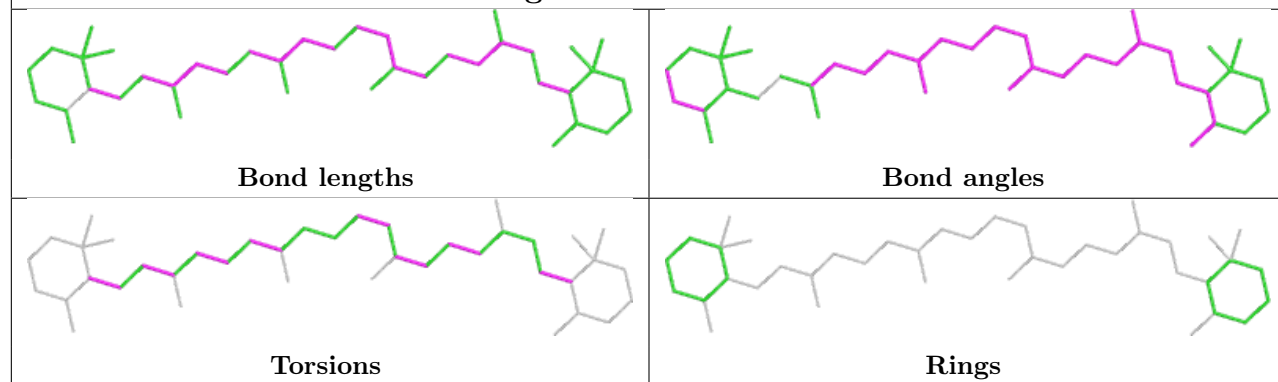


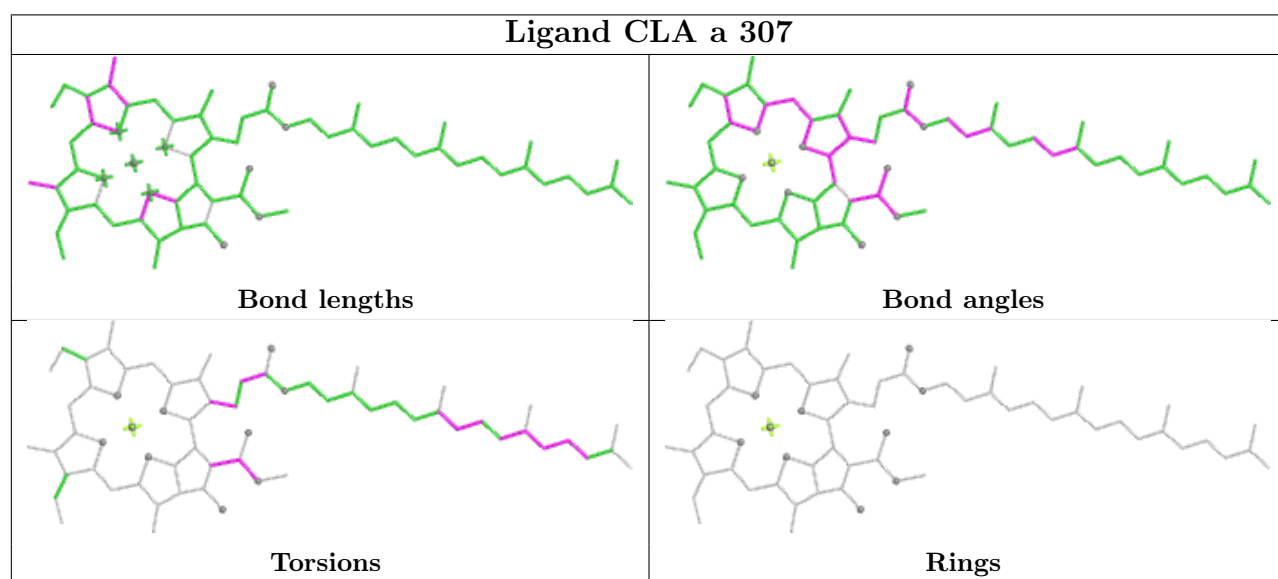
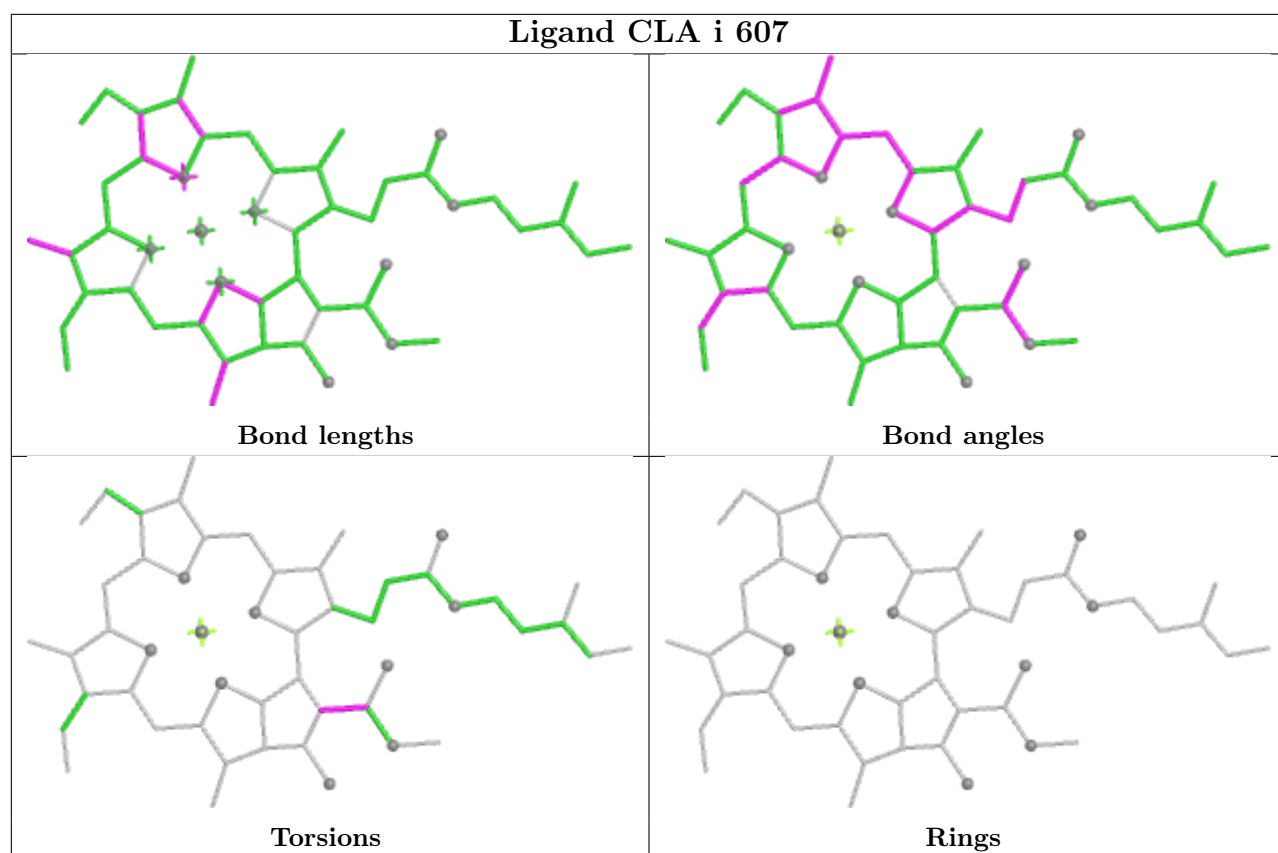


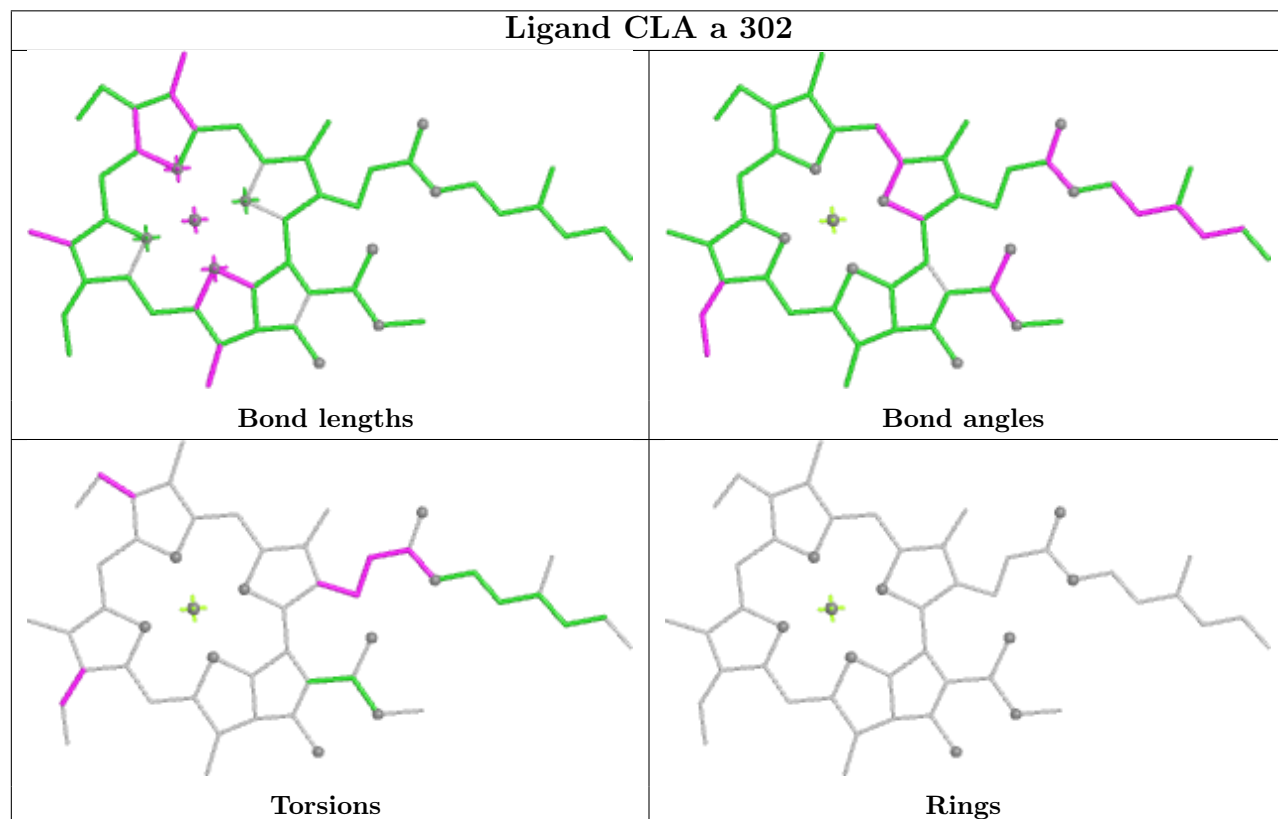
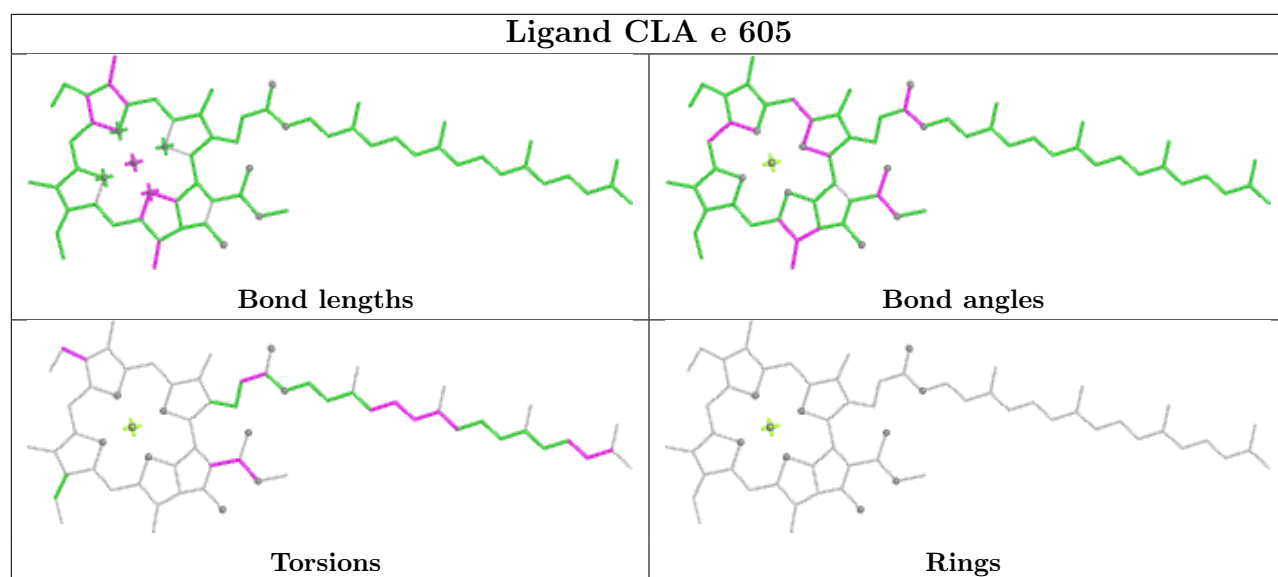
Ligand CLA B 834

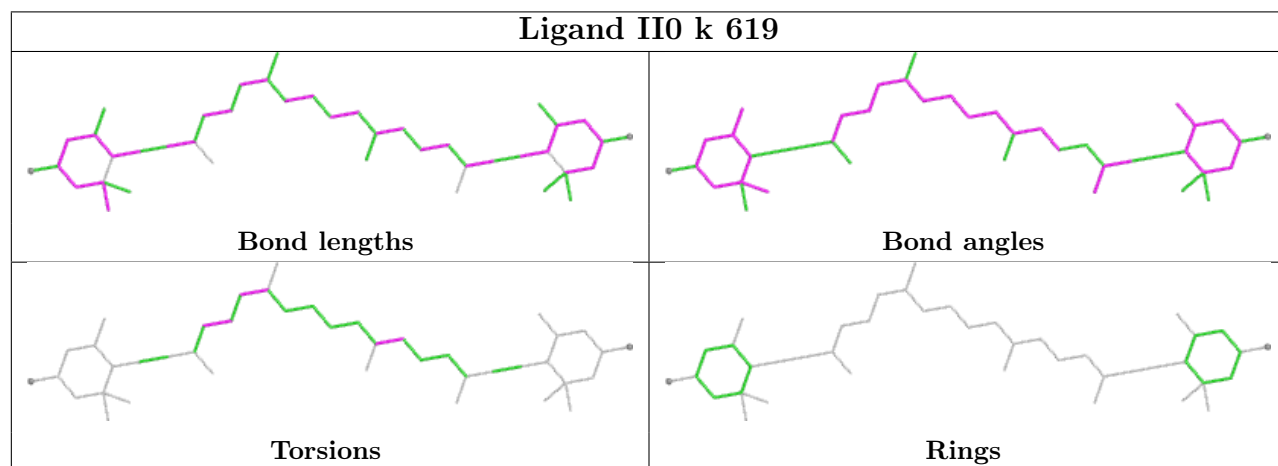
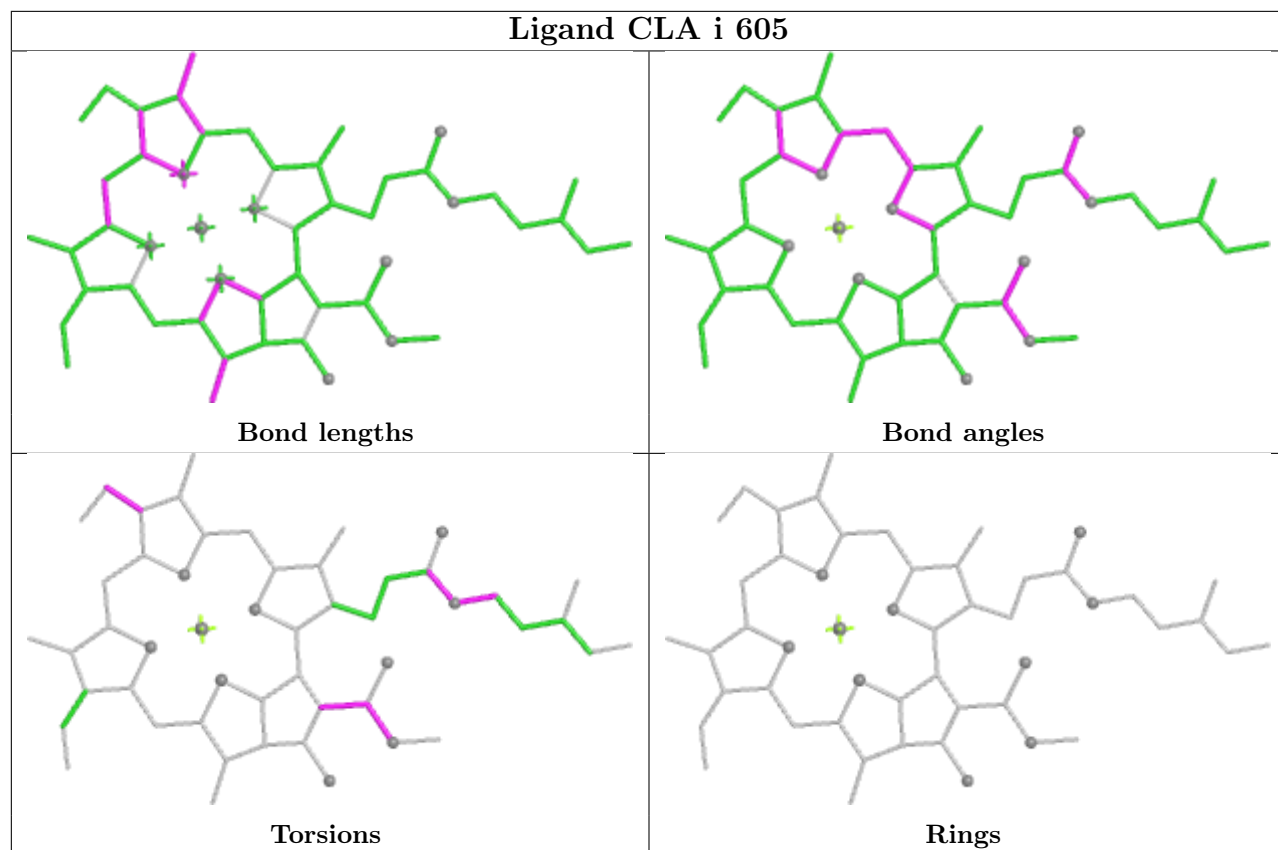


Ligand WVN F 205

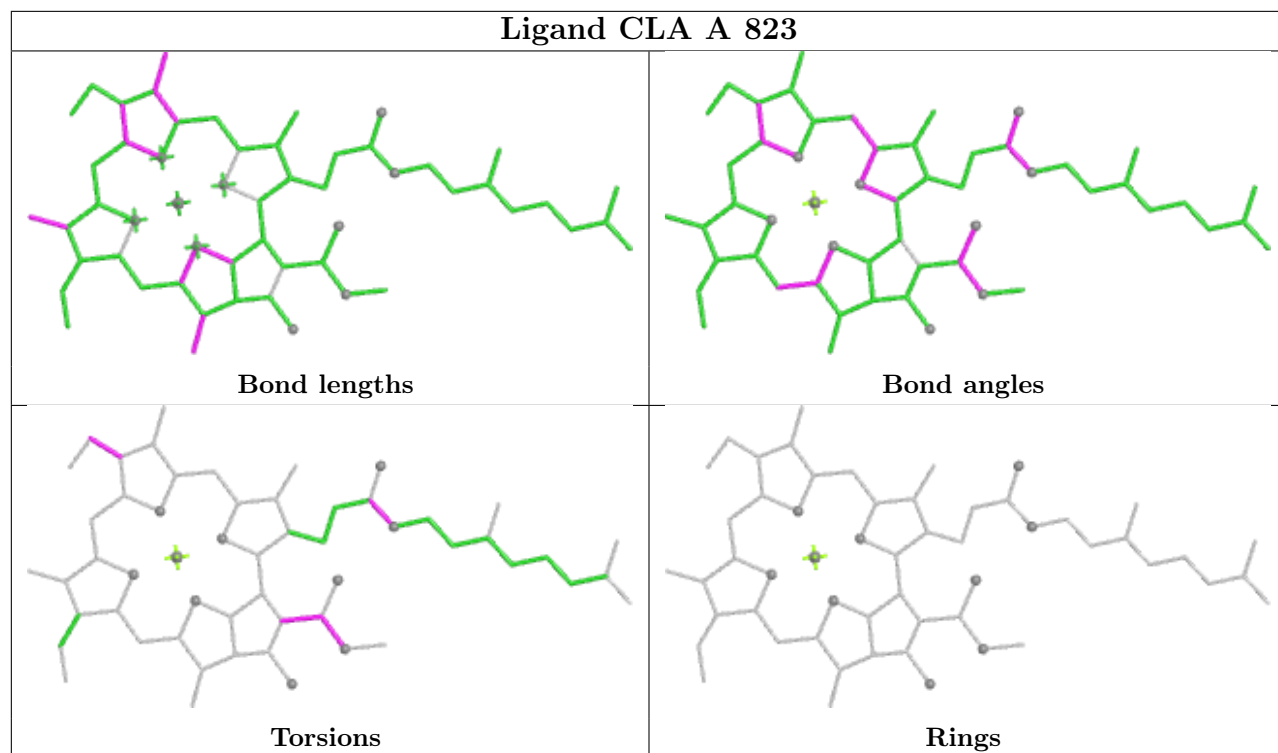




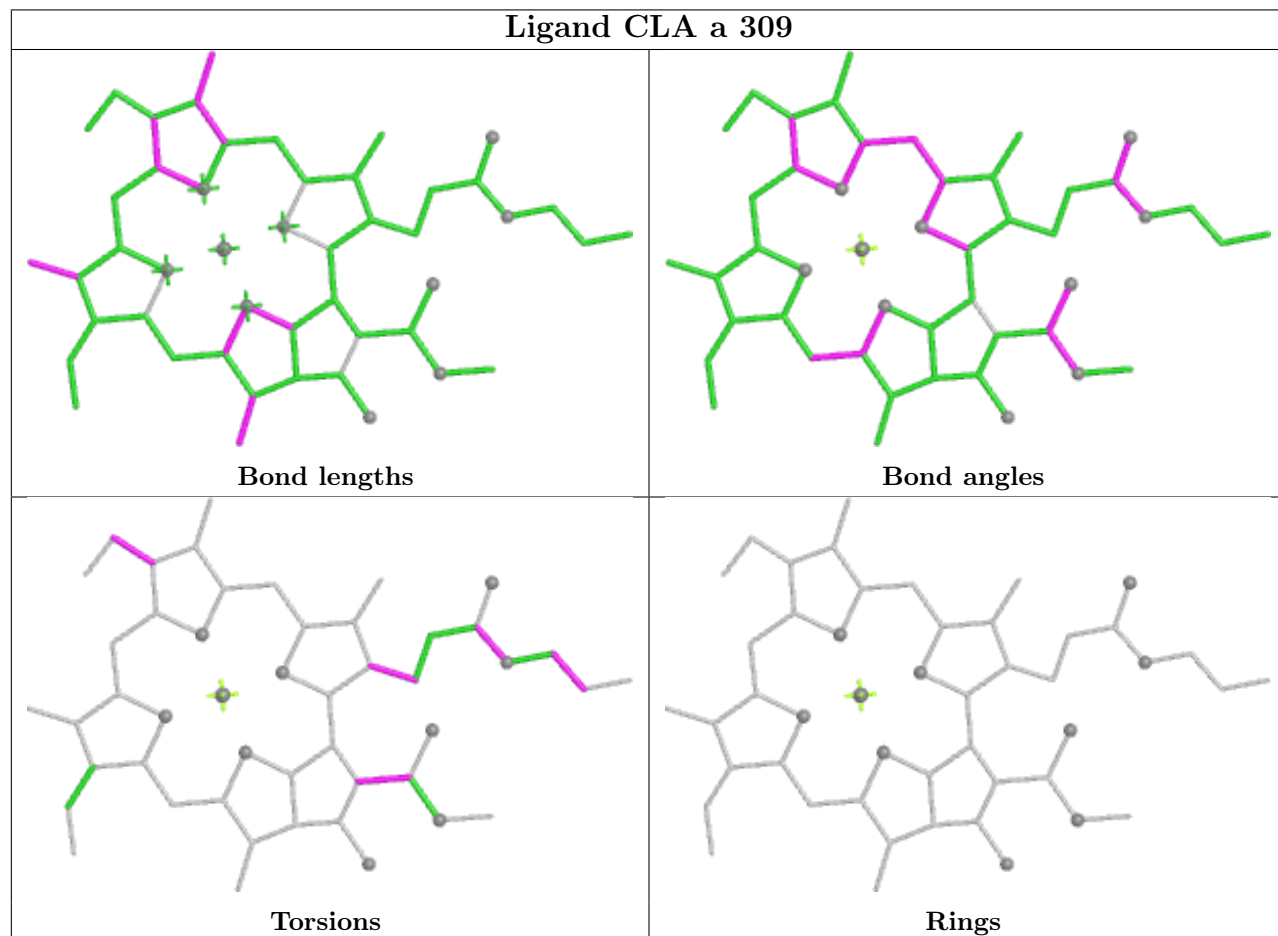




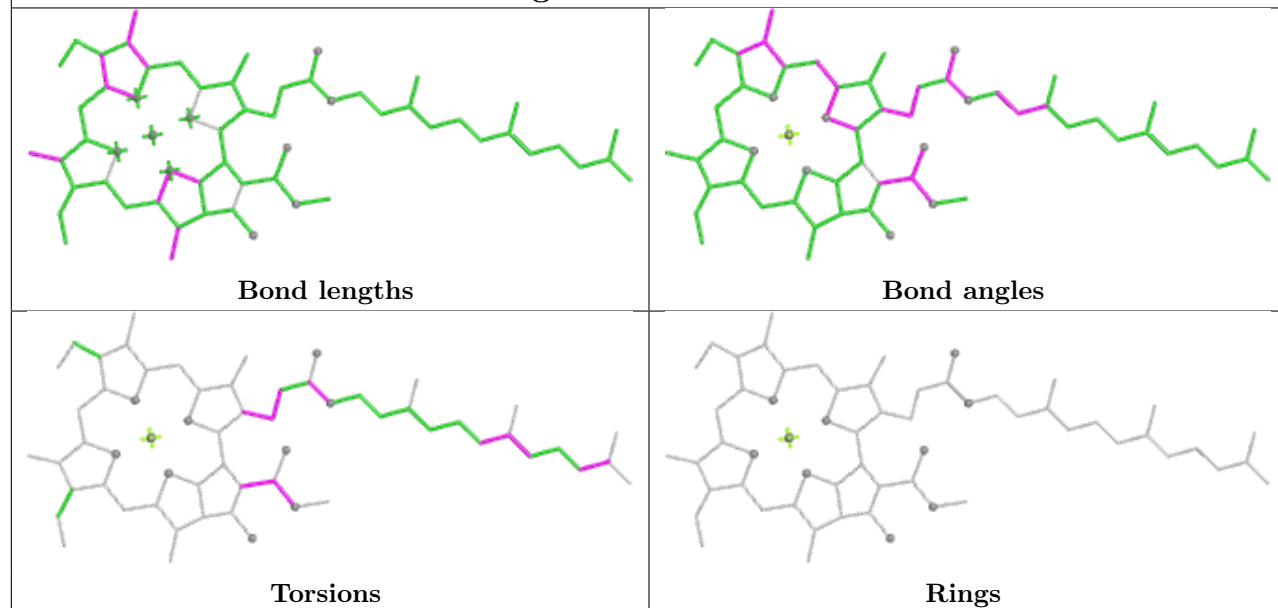
Ligand CLA A 823



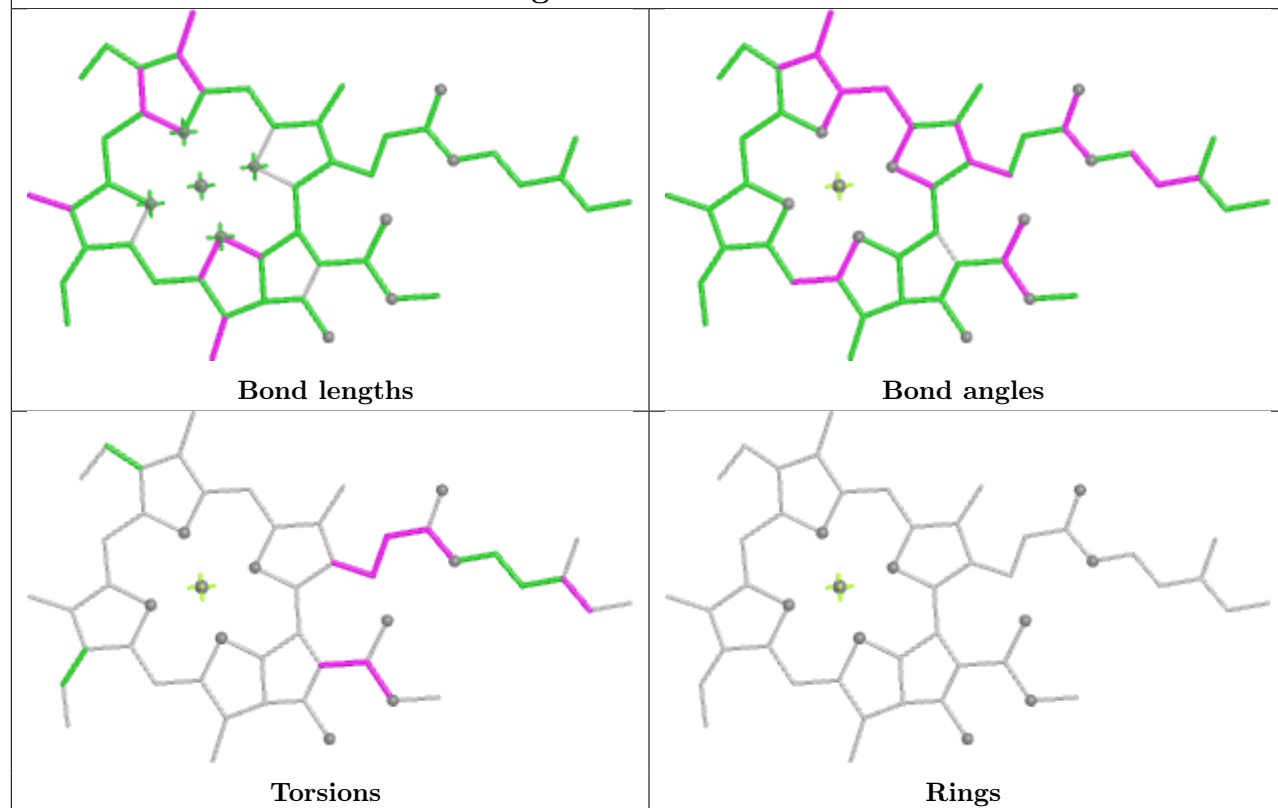
Ligand CLA a 309

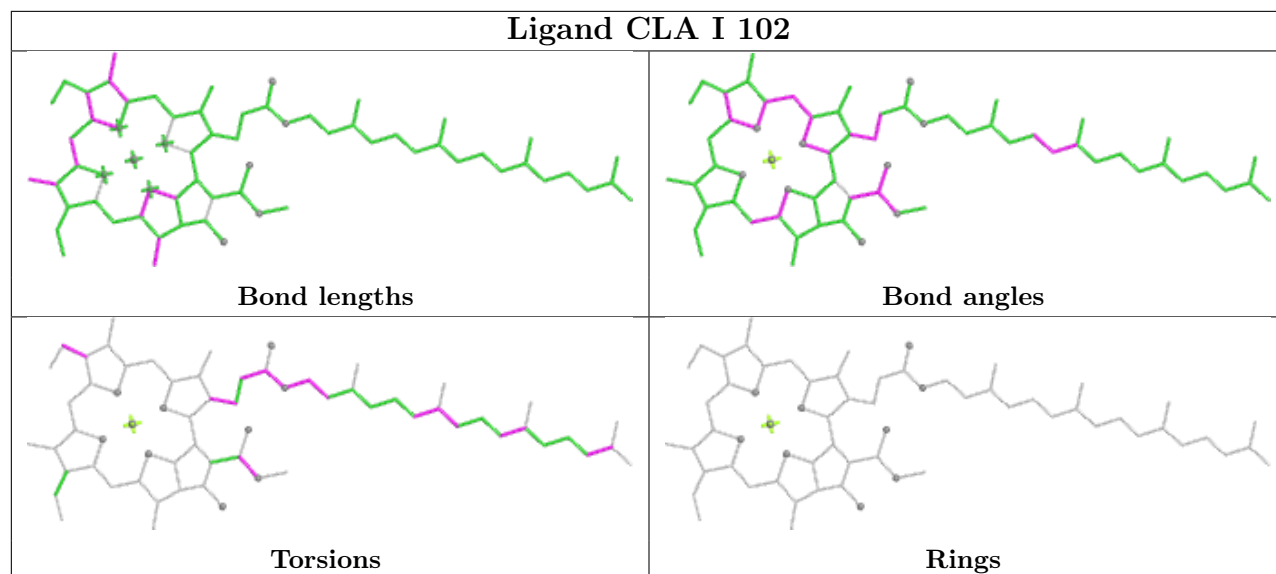
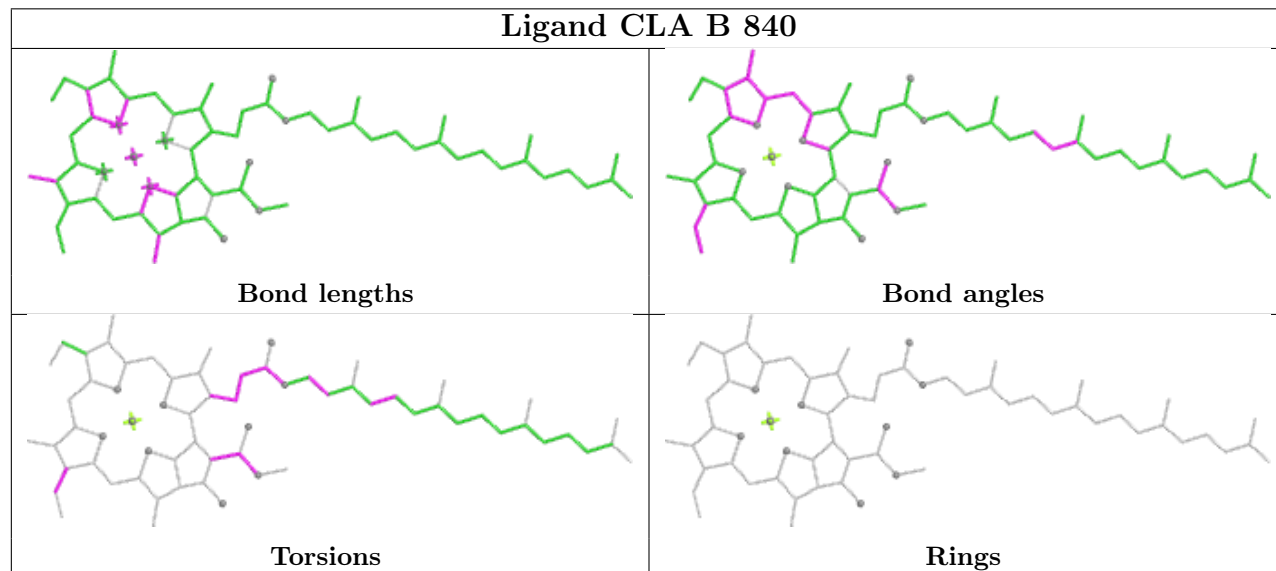


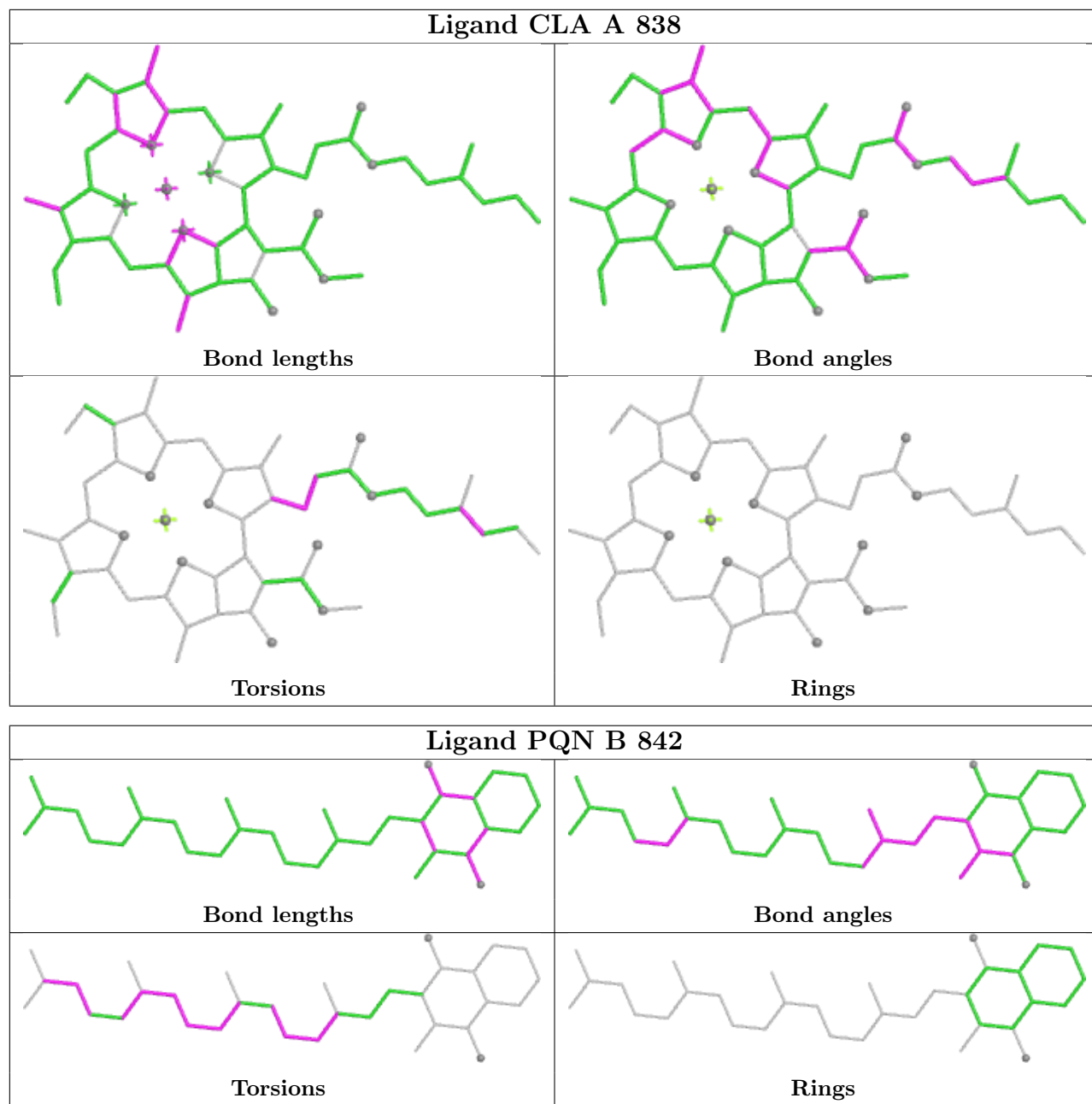
Ligand CLA B 813

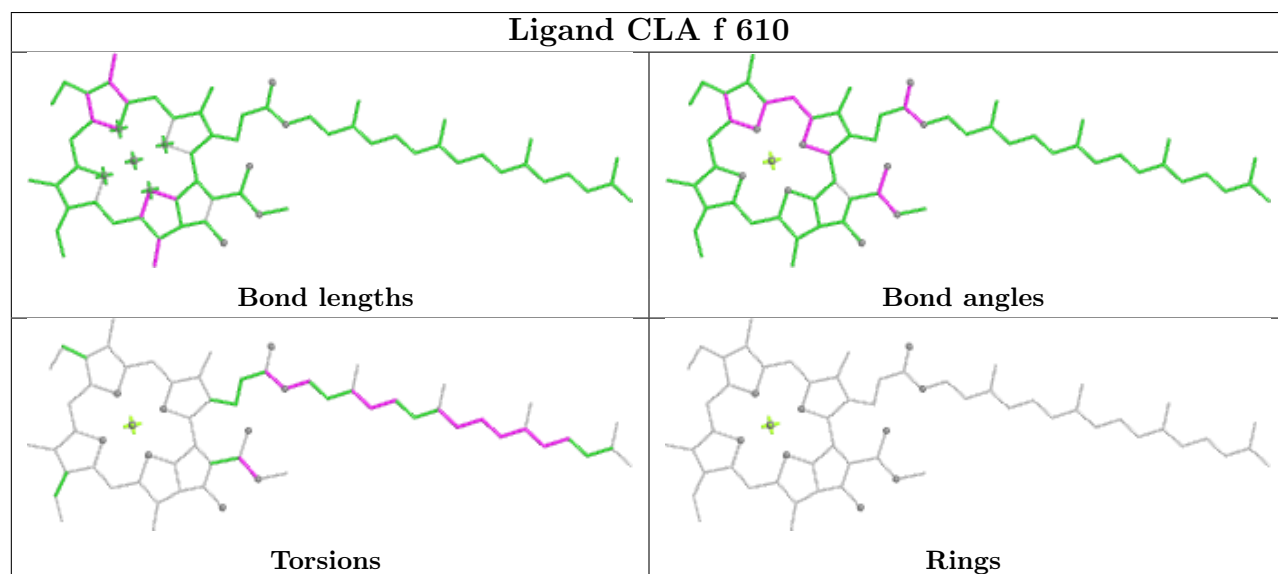
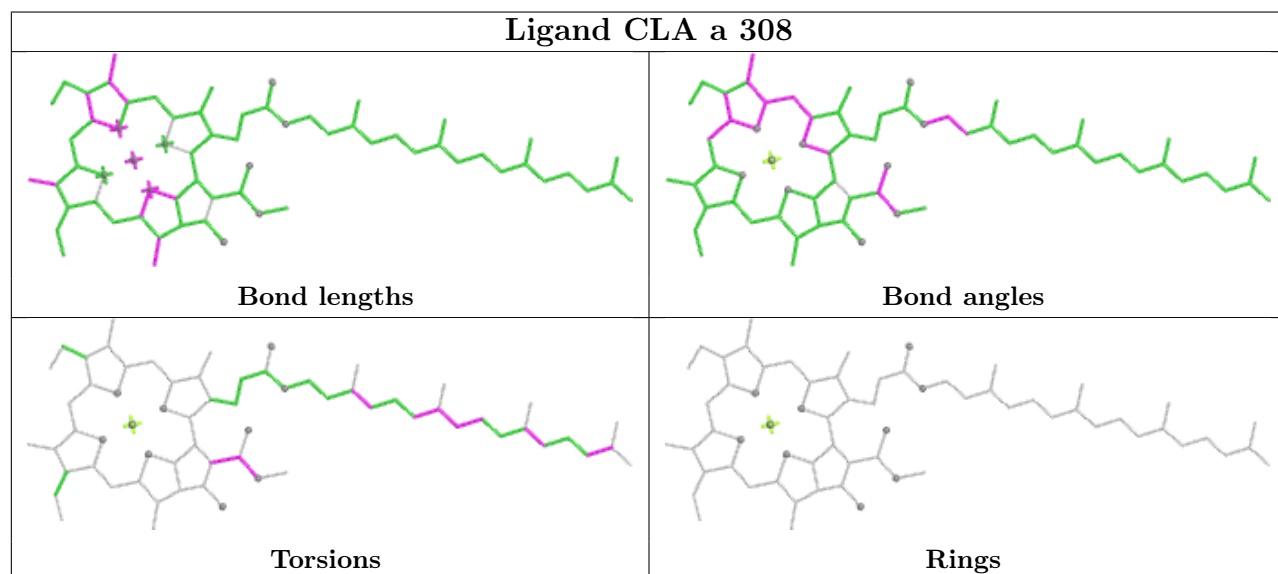
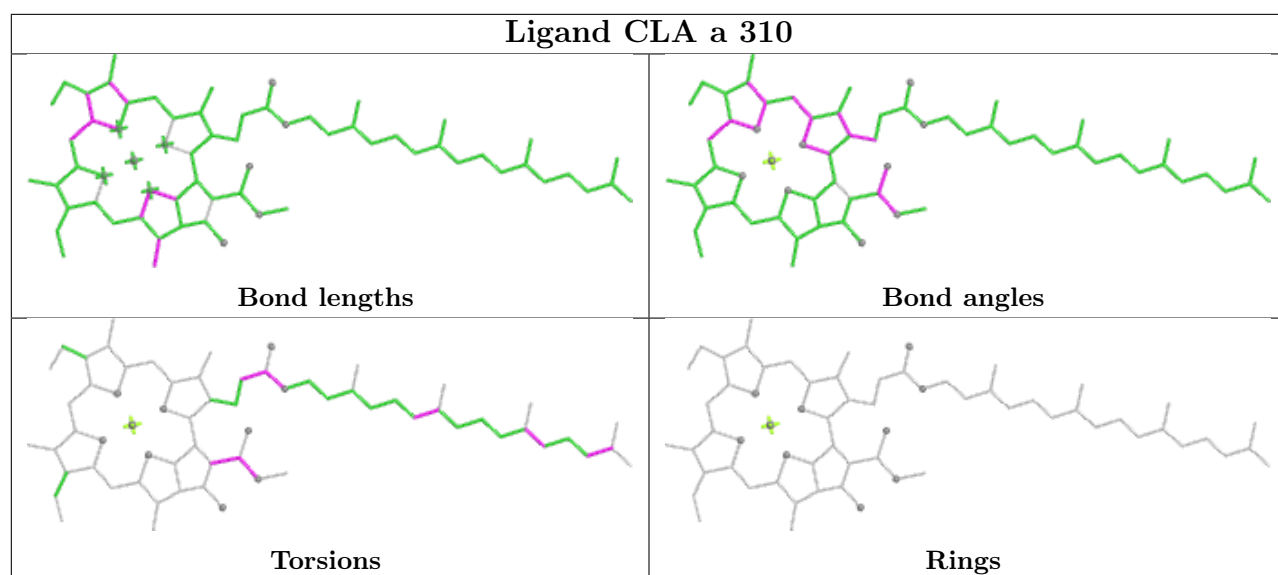


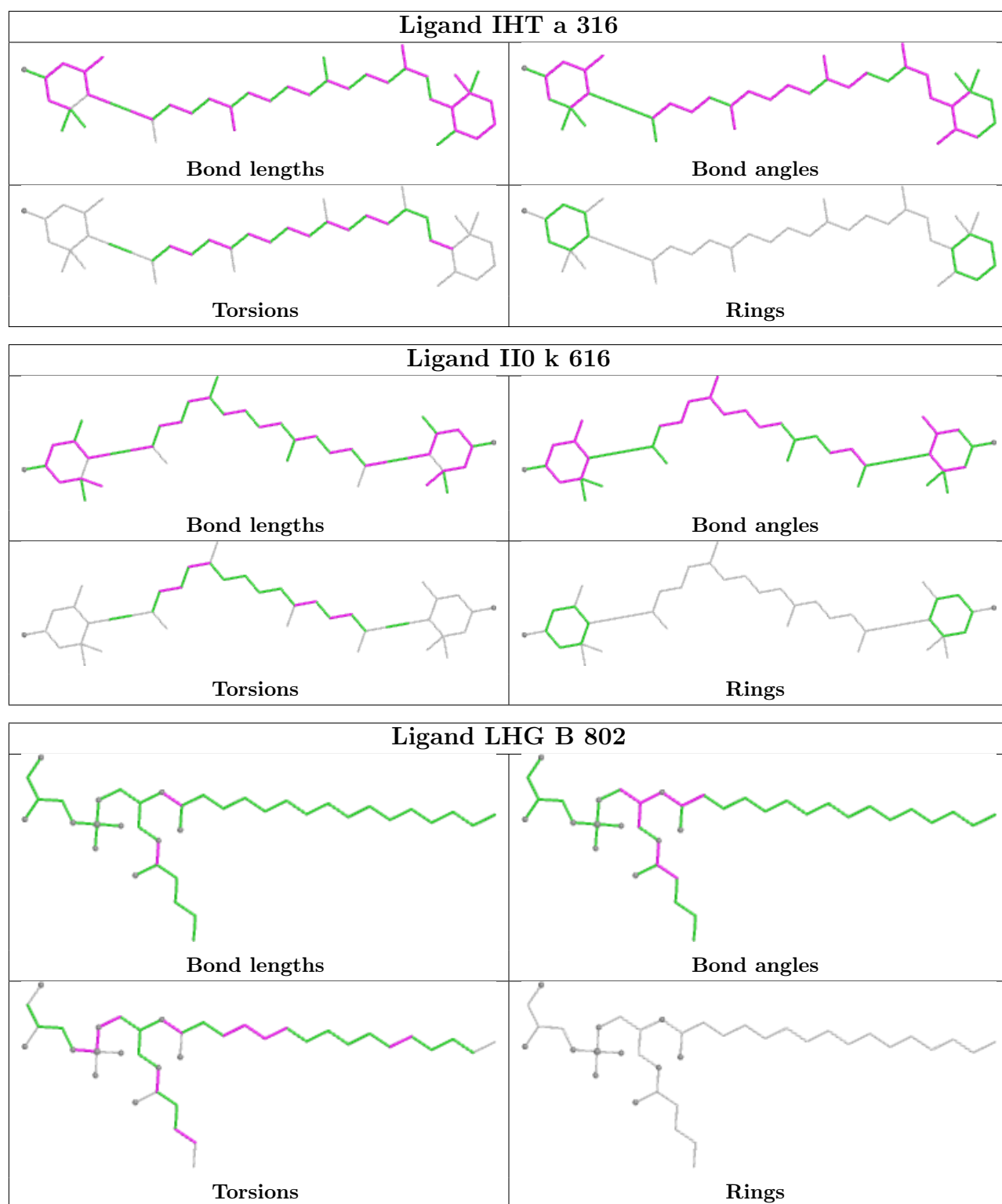
Ligand CLA R 203



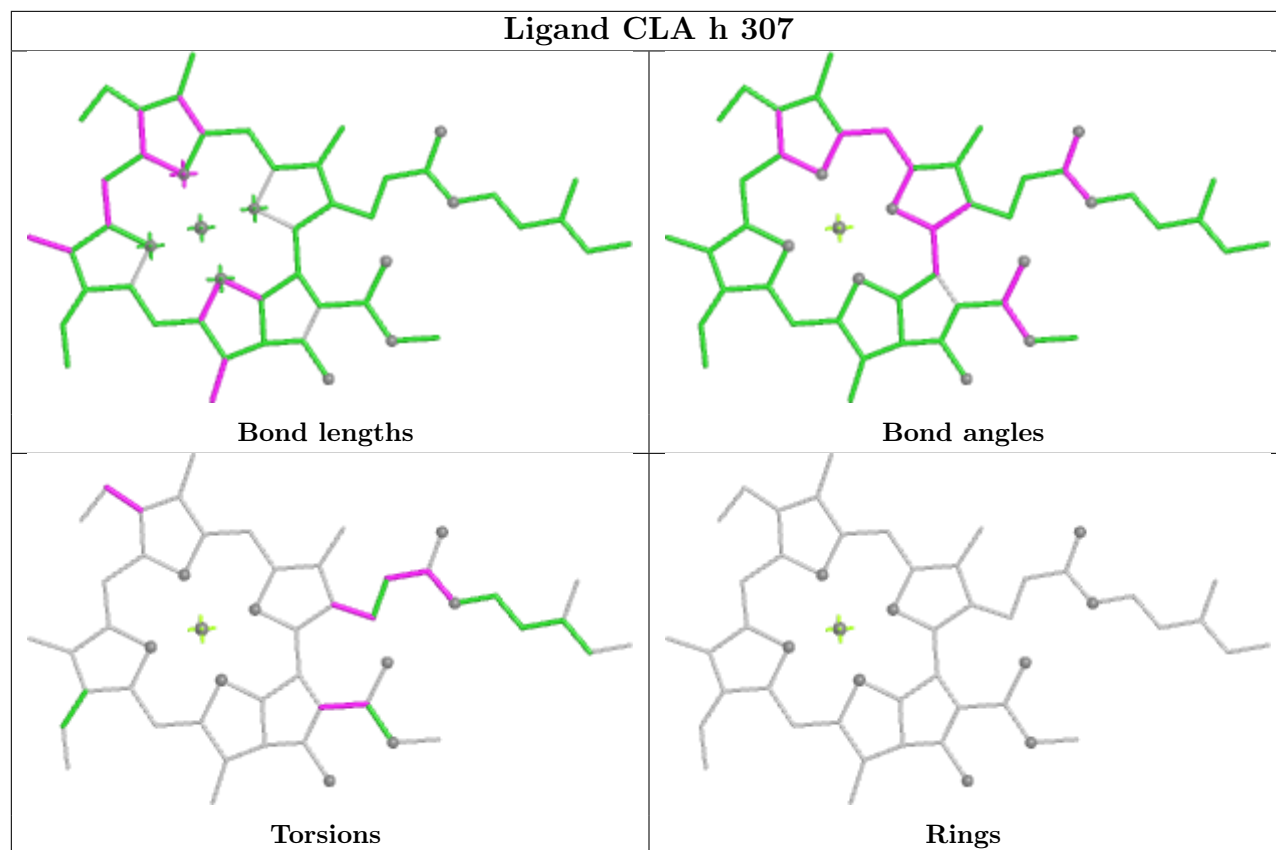
Ligand CLA I 102**Ligand CLA B 840**



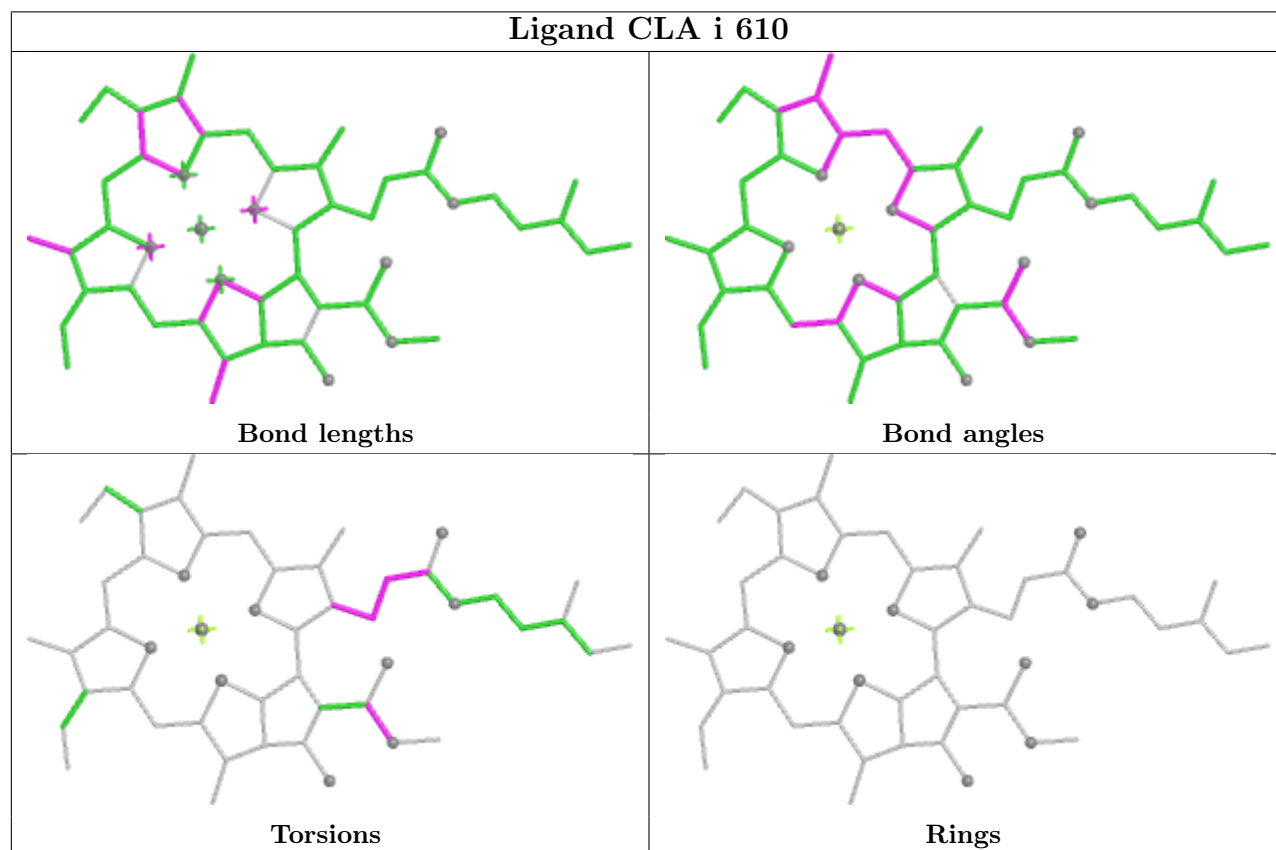


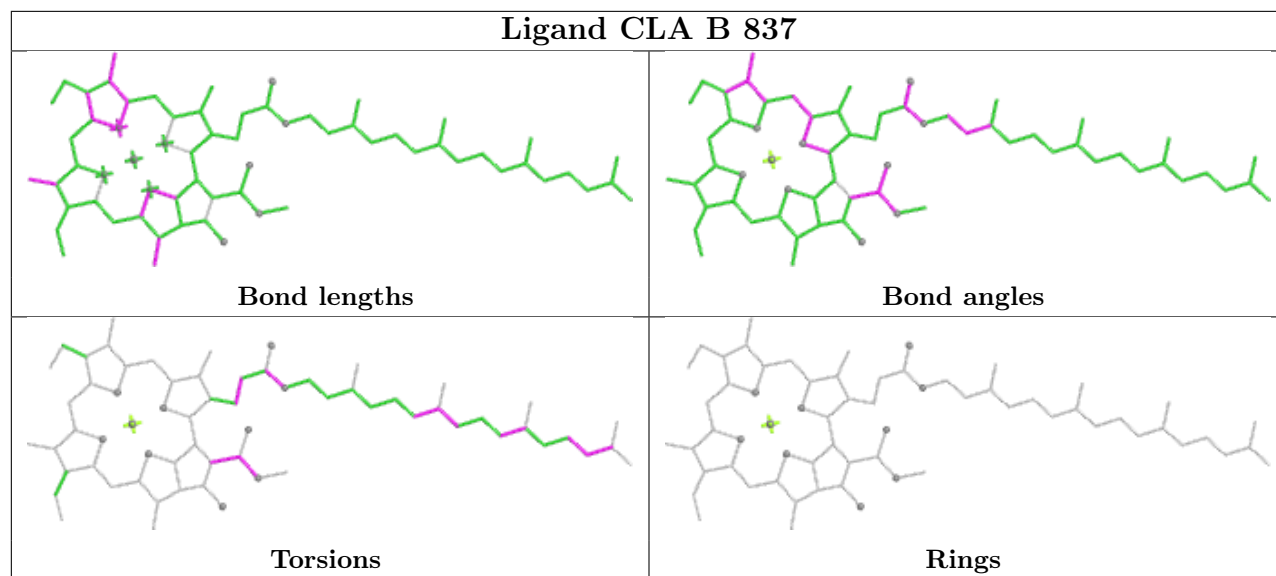


Ligand CLA h 307



Ligand CLA i 610





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.

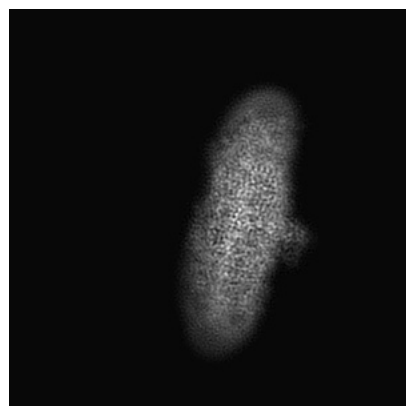
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37660. These allow visual inspection of the internal detail of the map and identification of artifacts.

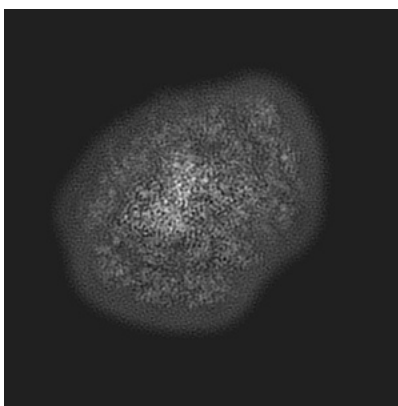
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

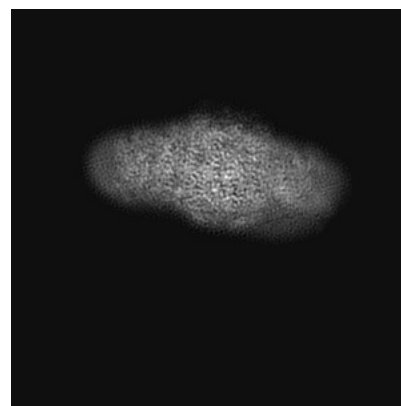
6.1.1 Primary map



X

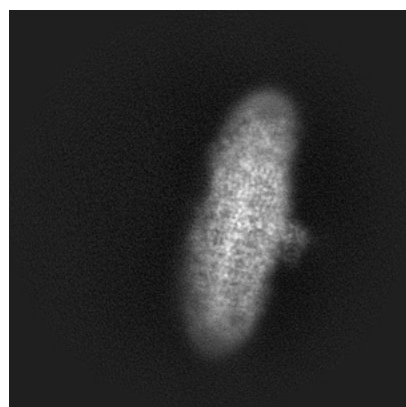


Y

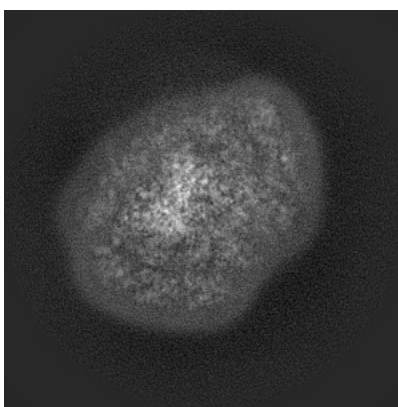


Z

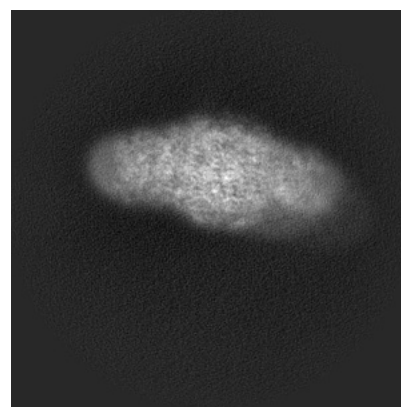
6.1.2 Raw map



X



Y

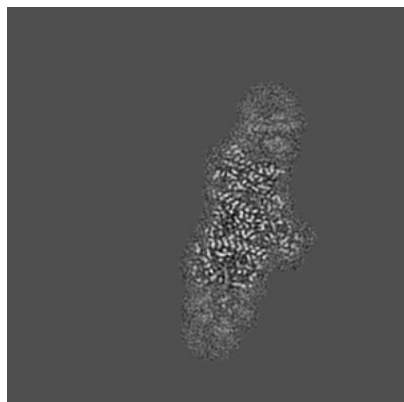


Z

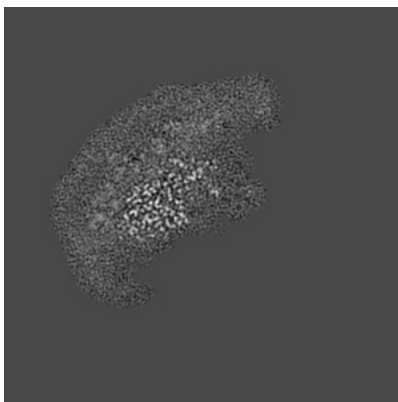
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

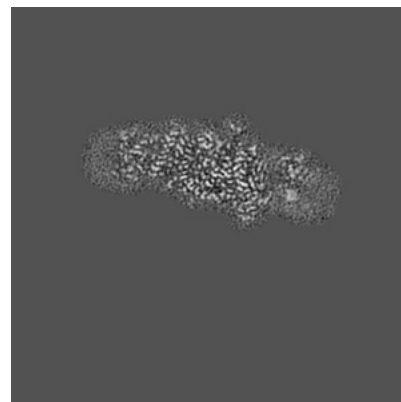
6.2.1 Primary map



X Index: 160

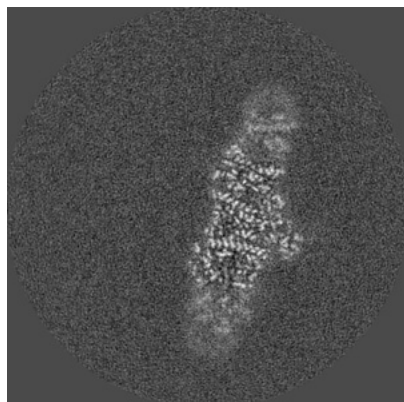


Y Index: 160

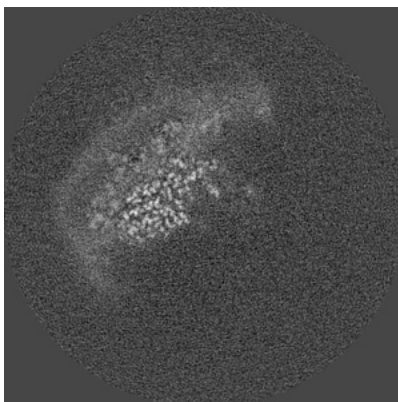


Z Index: 160

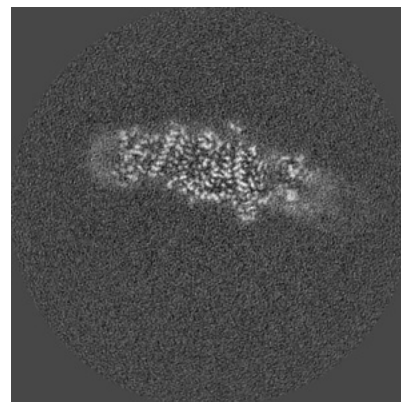
6.2.2 Raw map



X Index: 160



Y Index: 160

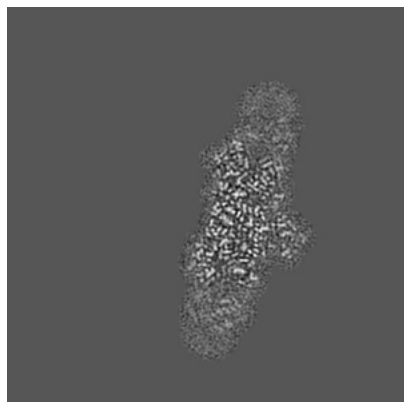


Z Index: 160

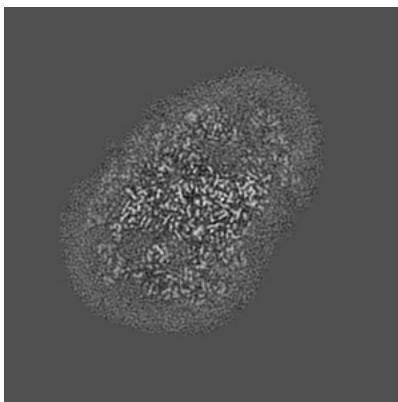
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

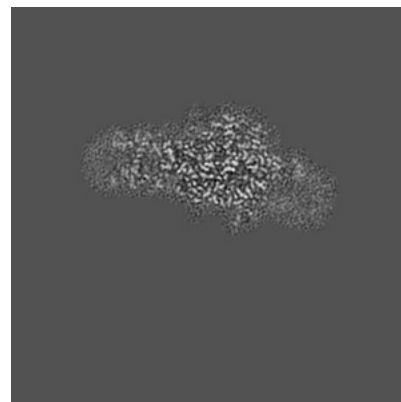
6.3.1 Primary map



X Index: 164

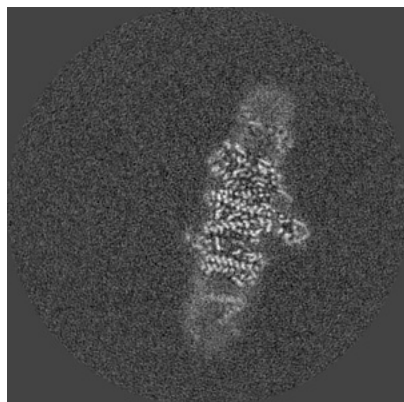


Y Index: 185

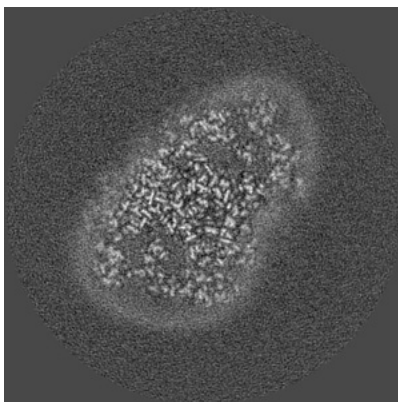


Z Index: 148

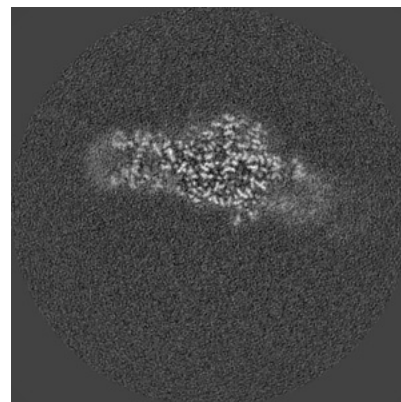
6.3.2 Raw map



X Index: 173



Y Index: 189

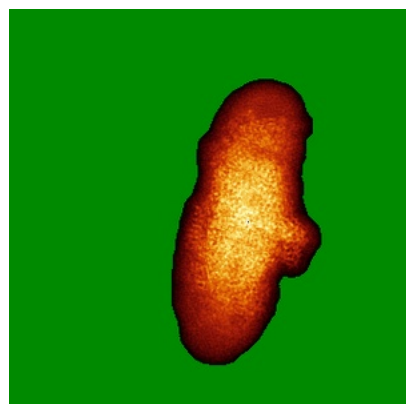


Z Index: 148

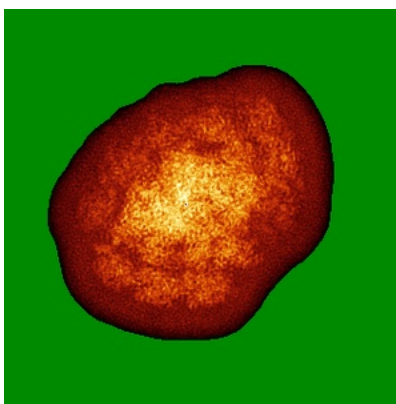
The images above show the largest variance slices of the map in three orthogonal directions.

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

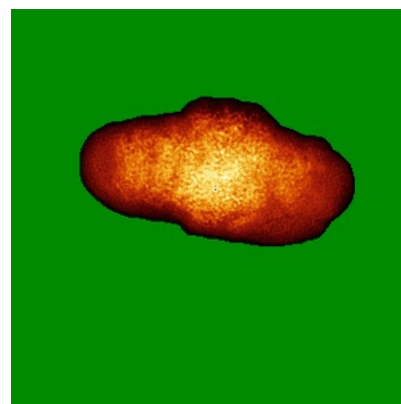
6.4.1 Primary map



X

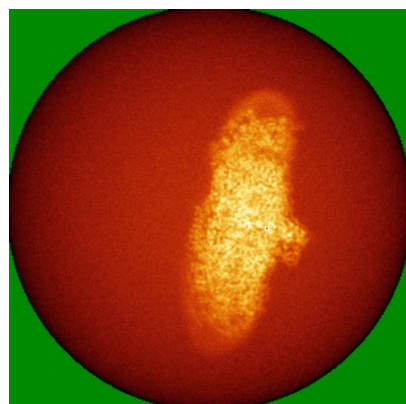


Y

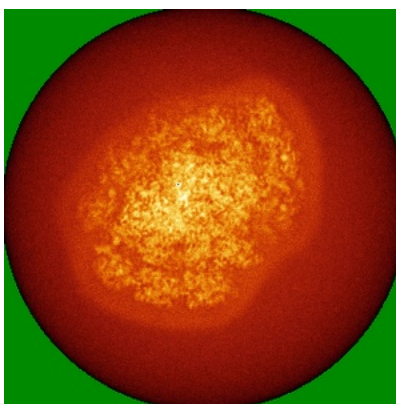


Z

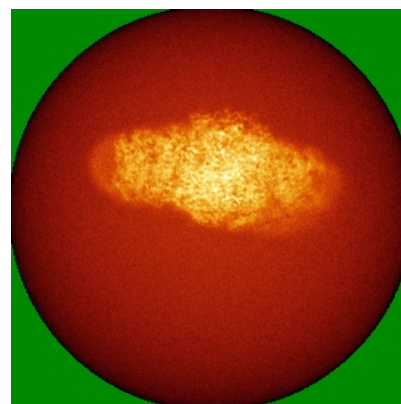
6.4.2 Raw map



X



Y

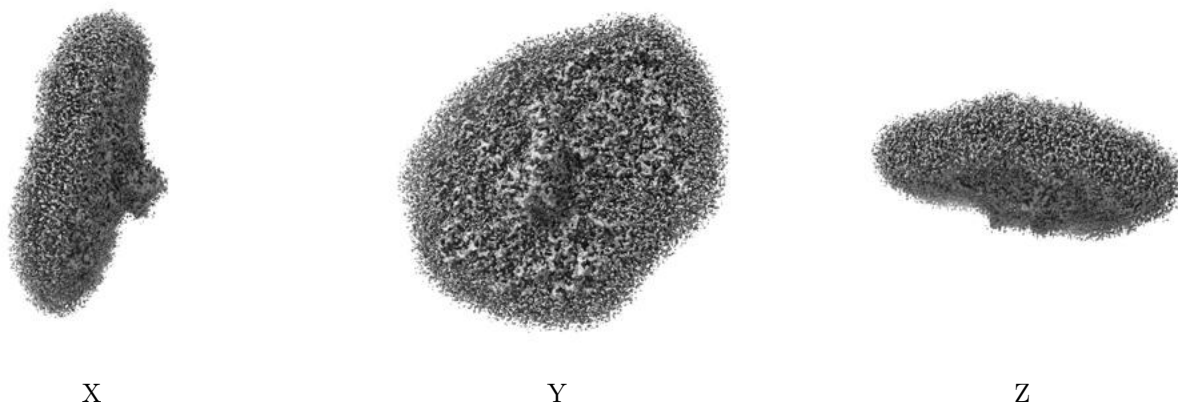


Z

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.

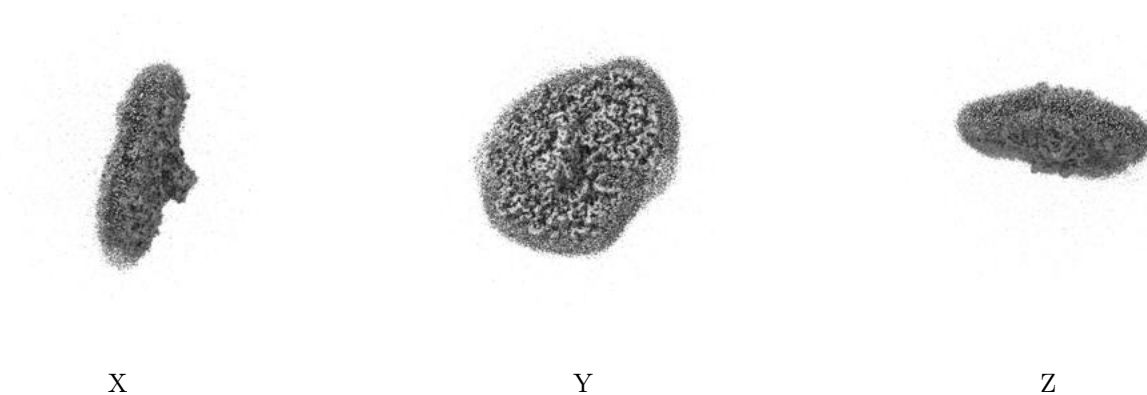
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

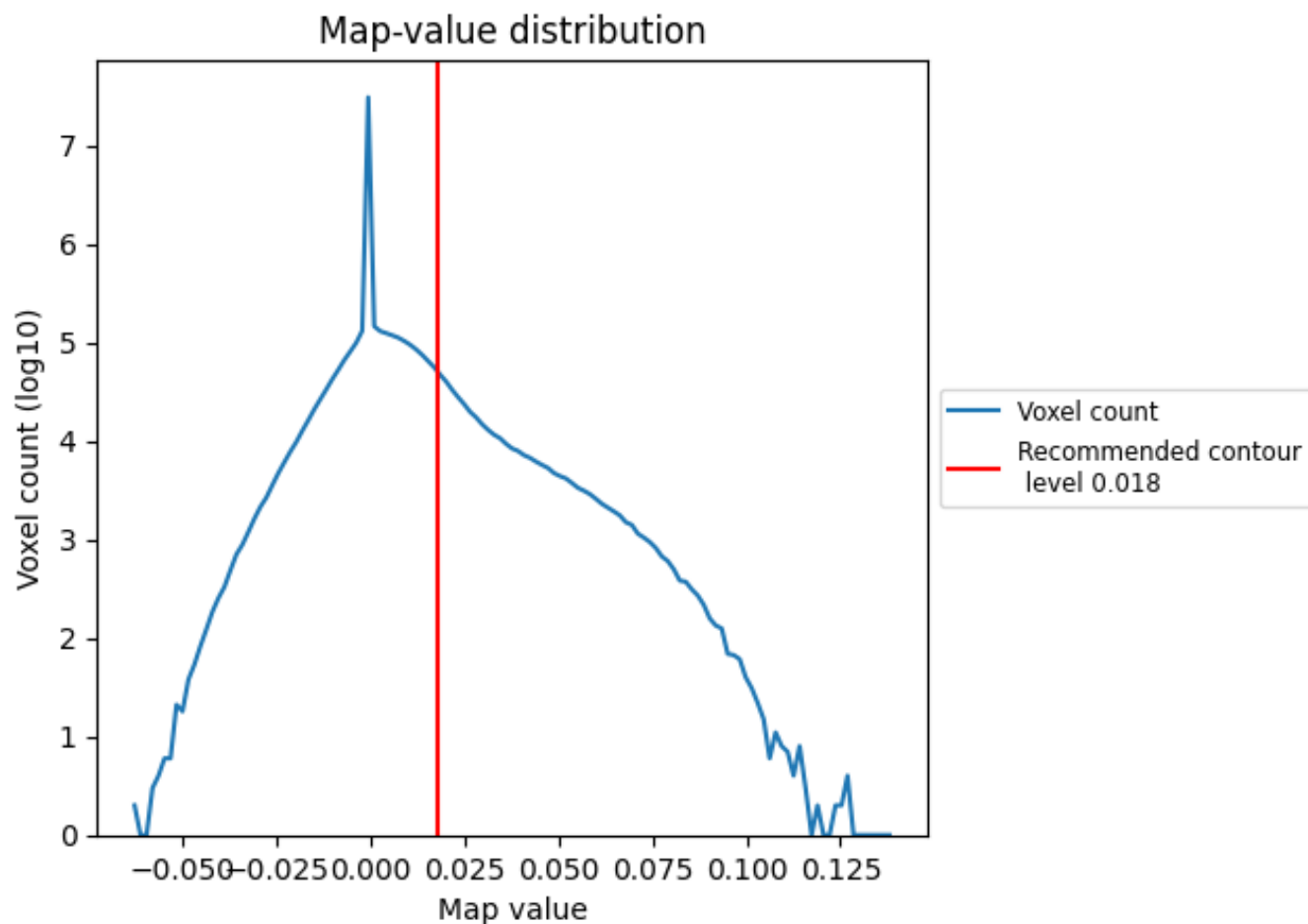
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

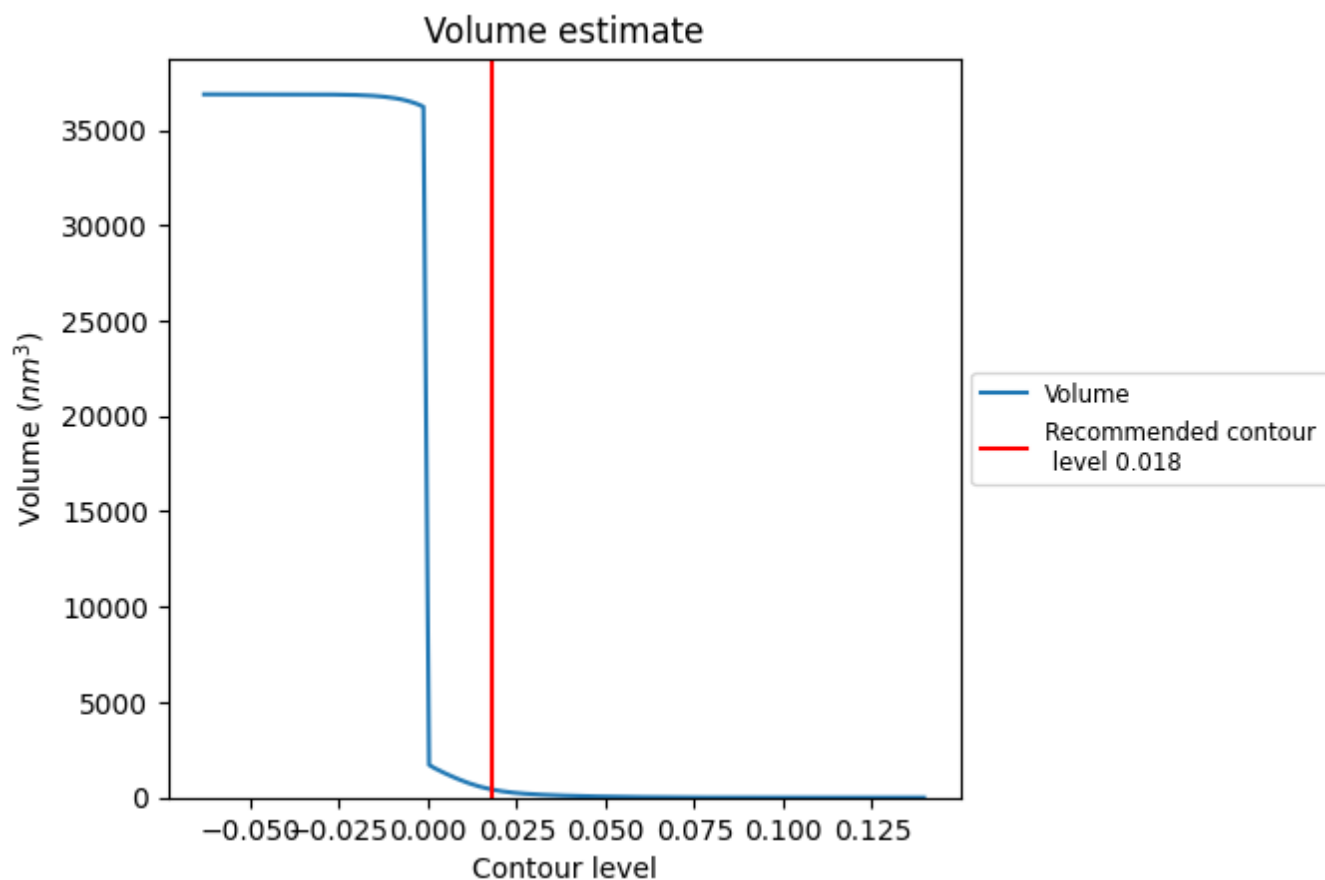
This section contains the results of statistical analysis of the map.

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.

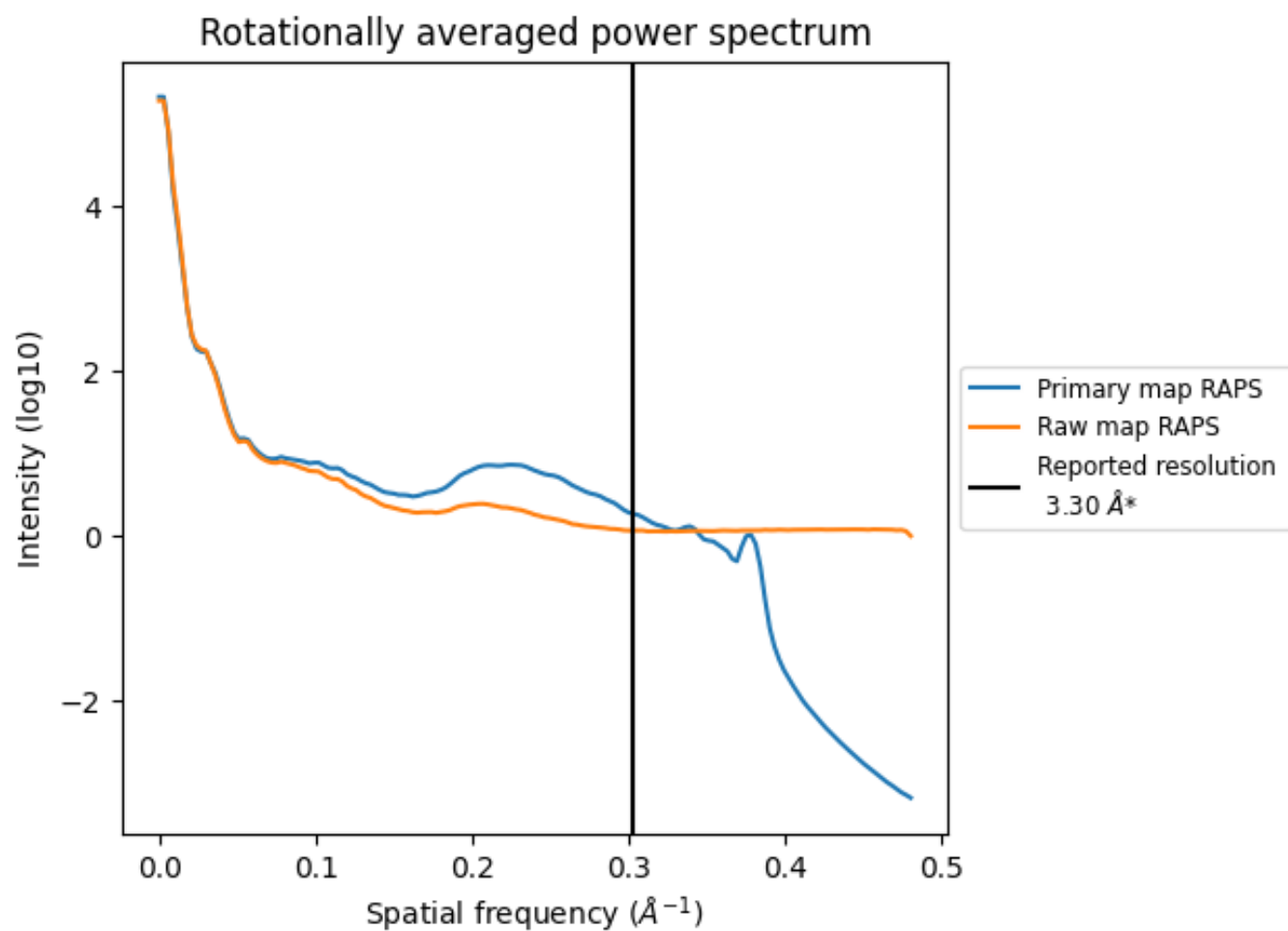
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 425 nm³; this corresponds to an approximate mass of 384 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 ⓘ

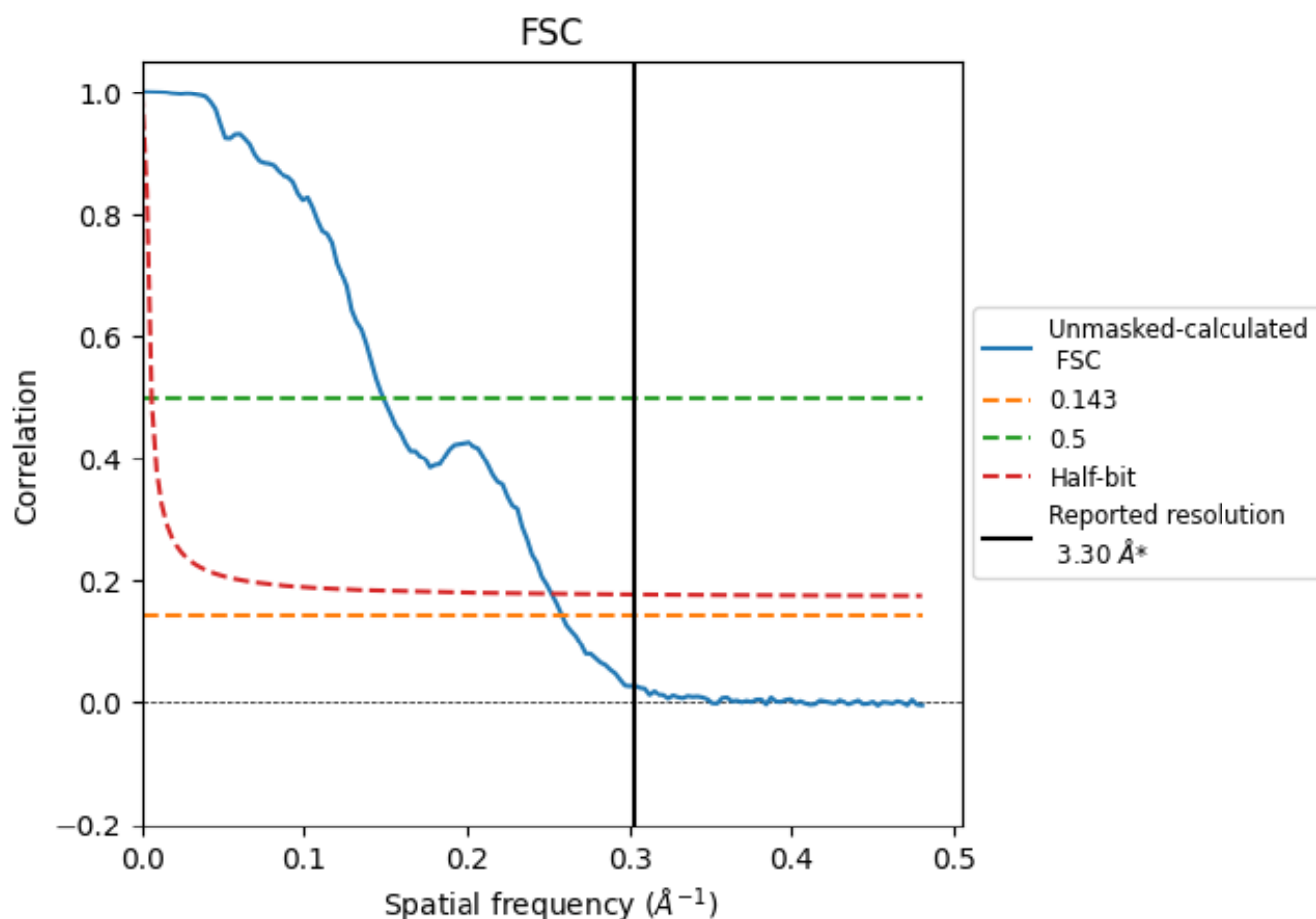


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

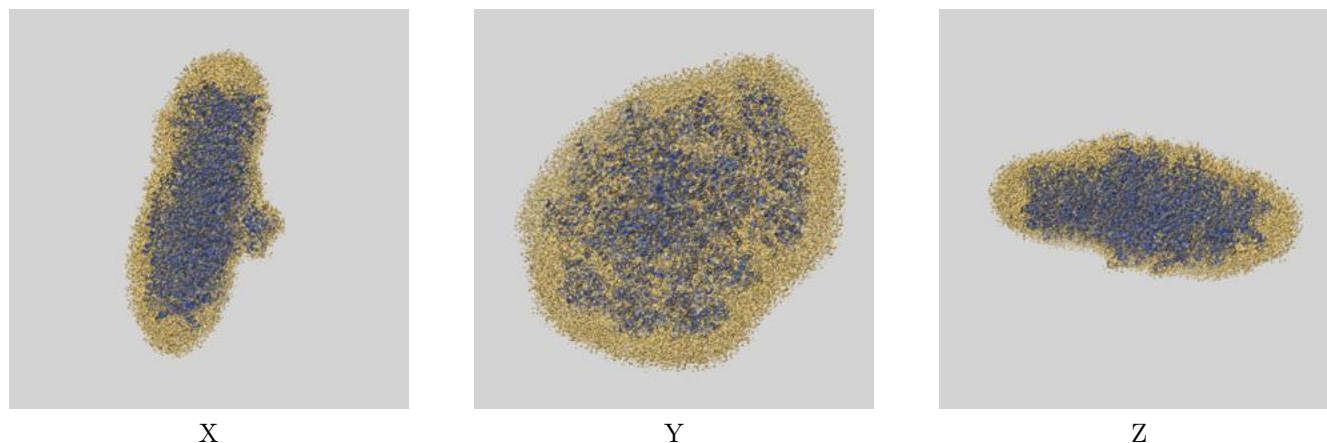
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	6.73	3.96

*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 3.86 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

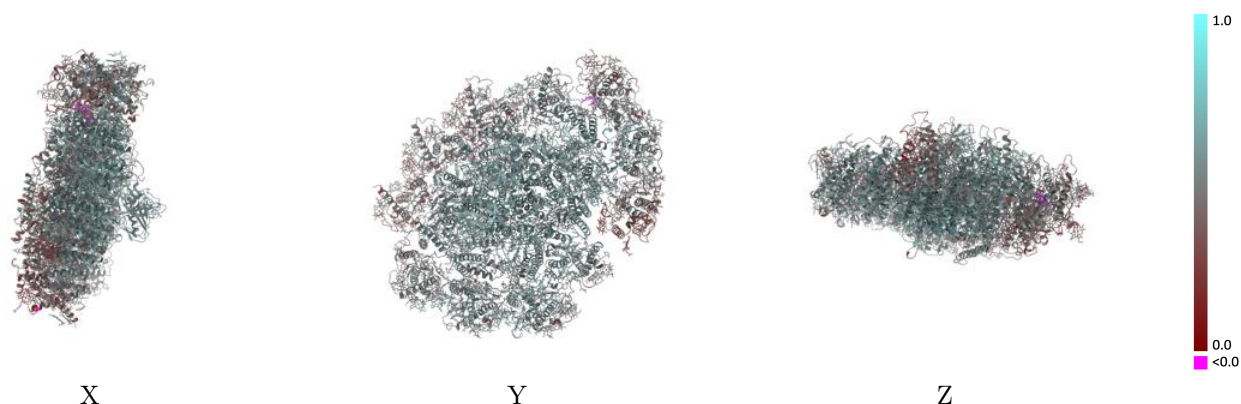
This section contains information regarding the fit between EMDB map EMD-37660 and PDB model 8WMW. Per-residue inclusion information can be found in section [3](#) on page [31](#).

9.1 Map-model overlay [i](#)



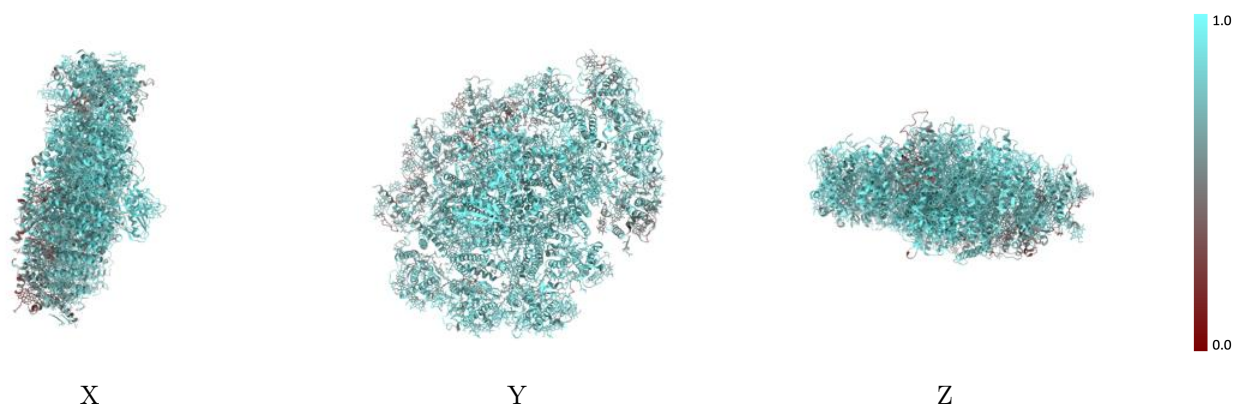
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



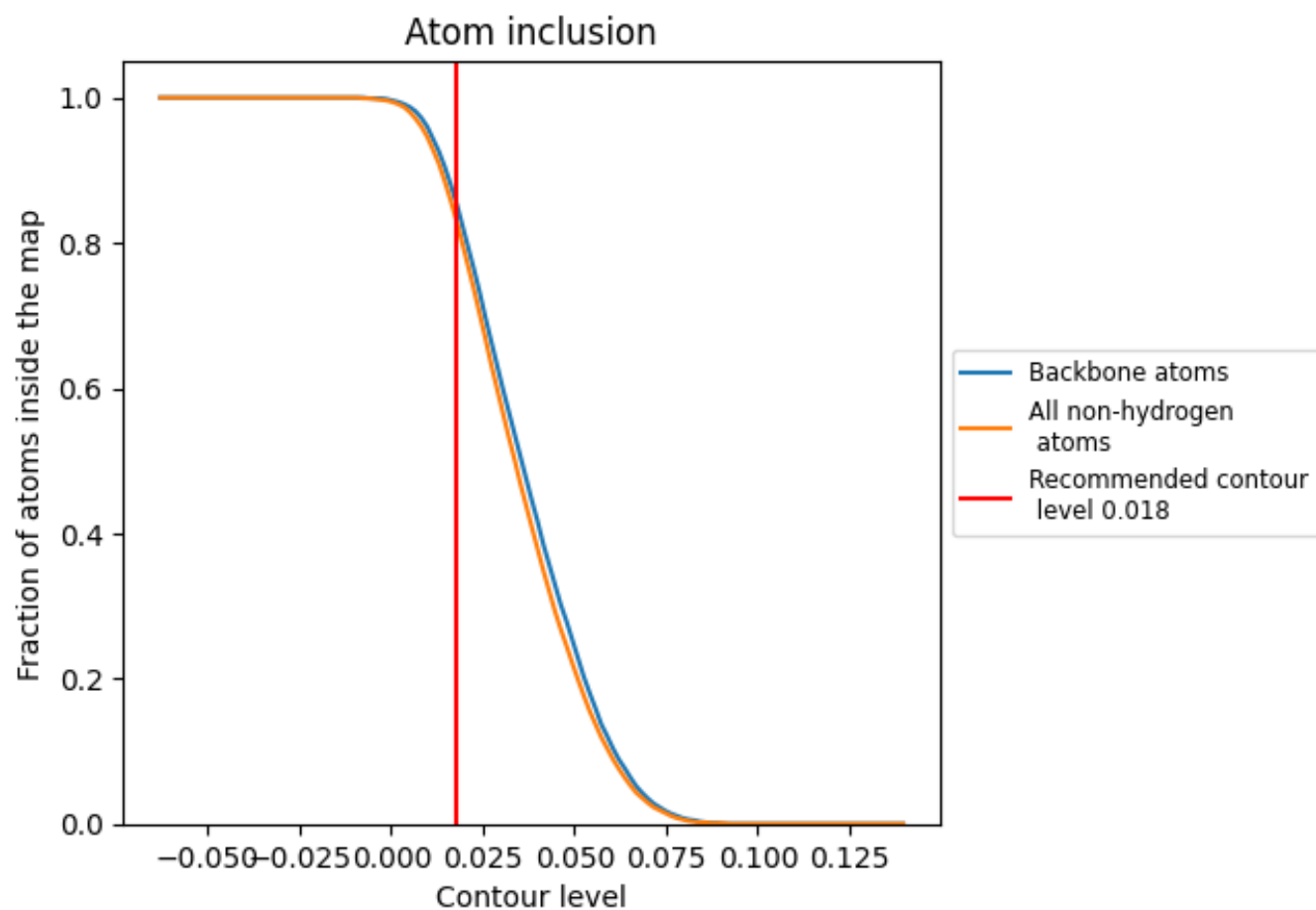
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8280	 0.5260
A	 0.9240	 0.5940
B	 0.9400	 0.6010
C	 0.9580	 0.5970
D	 0.8850	 0.5460
E	 0.8530	 0.5280
F	 0.8620	 0.5410
I	 0.9090	 0.5670
J	 0.7980	 0.5290
K	 0.8520	 0.5270
L	 0.8780	 0.5610
M	 0.8990	 0.5650
O	 0.8330	 0.5300
R	 0.8860	 0.5630
a	 0.7950	 0.4970
b	 0.6090	 0.4170
c	 0.6560	 0.4220
d	 0.6030	 0.3760
e	 0.7660	 0.4850
f	 0.8260	 0.5290
g	 0.8100	 0.5240
h	 0.8530	 0.5400
i	 0.6260	 0.3890
j	 0.8120	 0.5130
k	 0.7100	 0.4220

