



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 06:49 PM UTC

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

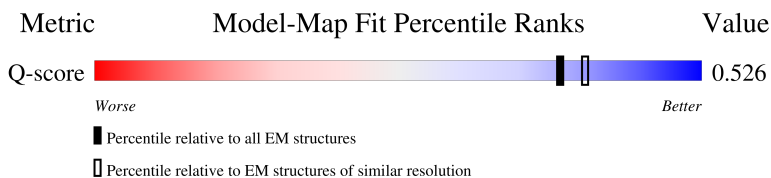
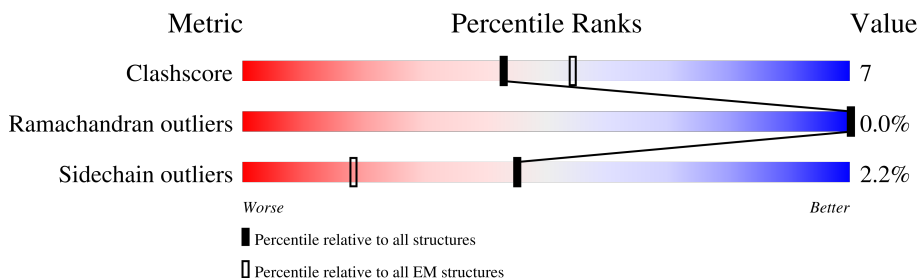
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	 85% 14% .
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
24	CLA	A	801	X	-	-	-
24	CLA	A	802	X	-	-	-
24	CLA	A	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	804	X	-	-	-
24	CLA	A	805	X	-	-	-
24	CLA	A	807	X	-	-	-
24	CLA	A	808	X	-	-	-
24	CLA	A	809	X	-	-	-
24	CLA	A	810	X	-	-	-
24	CLA	A	811	X	-	-	-
24	CLA	A	812	X	-	-	-
24	CLA	A	813	X	-	-	-
24	CLA	A	815	X	-	-	-
24	CLA	A	816	X	-	-	-
24	CLA	A	817	X	-	-	-
24	CLA	A	819	X	-	-	-
24	CLA	A	820	X	-	-	-
24	CLA	A	821	X	-	-	-
24	CLA	A	822	X	-	-	-
24	CLA	A	823	X	-	-	-
24	CLA	A	824	X	-	-	-
24	CLA	A	825	X	-	-	-
24	CLA	A	826	X	-	-	-
24	CLA	A	827	X	-	-	-
24	CLA	A	828	X	-	-	-
24	CLA	A	829	X	-	-	-
24	CLA	A	830	X	-	-	-
24	CLA	A	831	X	-	-	-
24	CLA	A	833	X	-	-	-
24	CLA	A	834	X	-	-	-
24	CLA	A	835	X	-	-	-
24	CLA	A	836	X	-	-	-
24	CLA	A	837	X	-	-	-
24	CLA	A	838	X	-	-	-
24	CLA	A	839	X	-	-	-
24	CLA	A	840	X	-	-	-
24	CLA	A	841	X	-	-	-
24	CLA	A	842	X	-	-	-
24	CLA	A	852	X	-	-	-
24	CLA	A	853	X	-	-	-
24	CLA	A	855	X	-	-	-
24	CLA	A	856	X	-	-	-
24	CLA	B	801	X	-	-	-
24	CLA	B	803	X	-	-	-
24	CLA	B	804	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	805	X	-	-	-
24	CLA	B	806	X	-	-	-
24	CLA	B	807	X	-	-	-
24	CLA	B	808	X	-	-	-
24	CLA	B	809	X	-	-	-
24	CLA	B	810	X	-	-	-
24	CLA	B	811	X	-	-	-
24	CLA	B	812	X	-	-	-
24	CLA	B	813	X	-	-	-
24	CLA	B	814	X	-	-	-
24	CLA	B	815	X	-	-	-
24	CLA	B	816	X	-	-	-
24	CLA	B	818	X	-	-	-
24	CLA	B	821	X	-	-	-
24	CLA	B	822	X	-	-	-
24	CLA	B	823	X	-	-	-
24	CLA	B	824	X	-	-	-
24	CLA	B	825	X	-	-	-
24	CLA	B	826	X	-	-	-
24	CLA	B	827	X	-	-	-
24	CLA	B	829	X	-	-	-
24	CLA	B	830	X	-	-	-
24	CLA	B	831	X	-	-	-
24	CLA	B	832	X	-	-	-
24	CLA	B	833	X	-	-	-
24	CLA	B	834	X	-	-	-
24	CLA	B	835	X	-	-	-
24	CLA	B	836	X	-	-	-
24	CLA	B	837	X	-	-	-
24	CLA	B	838	X	-	-	-
24	CLA	B	839	X	-	-	-
24	CLA	F	201	X	-	-	-
24	CLA	F	202	X	-	-	-
24	CLA	I	102	X	-	-	-
24	CLA	J	103	X	-	-	-
24	CLA	J	105	X	-	-	-
24	CLA	K	101	X	-	-	-
24	CLA	K	102	X	-	-	-
24	CLA	L	202	X	-	-	-
24	CLA	L	203	X	-	-	-
24	CLA	L	204	X	-	-	-
24	CLA	L	207	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	O	201	X	-	-	-
24	CLA	O	205	X	-	-	-
24	CLA	R	203	X	-	-	-
24	CLA	a	302	X	-	-	-
24	CLA	a	303	X	-	-	-
24	CLA	a	304	X	-	-	-
24	CLA	a	305	X	-	-	-
24	CLA	a	306	X	-	-	-
24	CLA	a	307	X	-	-	-
24	CLA	a	308	X	-	-	-
24	CLA	a	309	X	-	-	-
24	CLA	a	310	X	-	-	-
24	CLA	a	311	X	-	-	-
24	CLA	a	312	X	-	-	-
24	CLA	b	303	X	-	-	-
24	CLA	b	304	X	-	-	-
24	CLA	b	305	X	-	-	-
24	CLA	b	307	X	-	-	-
24	CLA	b	308	X	-	-	-
24	CLA	b	309	X	-	-	-
24	CLA	b	310	X	-	-	-
24	CLA	b	311	X	-	-	-
24	CLA	b	312	X	-	-	-
24	CLA	b	313	X	-	-	-
24	CLA	c	601	X	-	-	-
24	CLA	c	602	X	-	-	-
24	CLA	c	603	X	-	-	-
24	CLA	c	604	X	-	-	-
24	CLA	c	605	X	-	-	-
24	CLA	c	607	X	-	-	-
24	CLA	c	608	X	-	-	-
24	CLA	c	609	X	-	-	-
24	CLA	c	611	X	-	-	-
24	CLA	c	612	X	-	-	-
24	CLA	d	301	X	-	-	-
24	CLA	d	302	X	-	-	-
24	CLA	d	303	X	-	-	-
24	CLA	d	304	X	-	-	-
24	CLA	d	306	X	-	-	-
24	CLA	d	307	X	-	-	-
24	CLA	d	308	X	-	-	-
24	CLA	d	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	e	601	X	-	-	-
24	CLA	e	602	X	-	-	-
24	CLA	e	603	X	-	-	-
24	CLA	e	604	X	-	-	-
24	CLA	e	605	X	-	-	-
24	CLA	e	606	X	-	-	-
24	CLA	e	607	X	-	-	-
24	CLA	e	608	X	-	-	-
24	CLA	e	611	X	-	-	-
24	CLA	f	601	X	-	-	-
24	CLA	f	602	X	-	-	-
24	CLA	f	603	X	-	-	-
24	CLA	f	607	X	-	-	-
24	CLA	f	608	X	-	-	-
24	CLA	f	609	X	-	-	-
24	CLA	f	610	X	-	-	-
24	CLA	f	612	X	-	-	-
24	CLA	f	613	X	-	-	-
24	CLA	g	302	X	-	-	-
24	CLA	g	303	X	-	-	-
24	CLA	g	304	X	-	-	-
24	CLA	g	305	X	-	-	-
24	CLA	g	306	X	-	-	-
24	CLA	g	307	X	-	-	-
24	CLA	g	308	X	-	-	-
24	CLA	g	309	X	-	-	-
24	CLA	g	310	X	-	-	-
24	CLA	g	311	X	-	-	-
24	CLA	g	315	X	-	-	-
24	CLA	g	322	X	-	-	-
24	CLA	h	301	X	-	-	-
24	CLA	h	302	X	-	-	-
24	CLA	h	303	X	-	-	-
24	CLA	h	304	X	-	-	-
24	CLA	h	305	X	-	-	-
24	CLA	h	306	X	-	-	-
24	CLA	h	307	X	-	-	-
24	CLA	h	312	X	-	-	-
24	CLA	i	601	X	-	-	-
24	CLA	i	602	X	-	-	-
24	CLA	i	603	X	-	-	-
24	CLA	i	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	i	605	X	-	-	-
24	CLA	i	606	X	-	-	-
24	CLA	i	607	X	-	-	-
24	CLA	i	608	X	-	-	-
24	CLA	i	610	X	-	-	-
24	CLA	i	611	X	-	-	-
24	CLA	j	302	X	-	-	-
24	CLA	j	303	X	-	-	-
24	CLA	j	304	X	-	-	-
24	CLA	j	306	X	-	-	-
24	CLA	j	307	X	-	-	-
24	CLA	j	308	X	-	-	-
24	CLA	j	309	X	-	-	-
24	CLA	j	310	X	-	-	-
24	CLA	j	311	X	-	-	-
24	CLA	j	313	X	-	-	-
24	CLA	j	314	X	-	-	-
24	CLA	k	601	X	-	-	-
24	CLA	k	602	X	-	-	-
24	CLA	k	603	X	-	-	-
24	CLA	k	604	X	-	-	-
24	CLA	k	605	X	-	-	-
24	CLA	k	607	X	-	-	-
24	CLA	k	608	X	-	-	-
24	CLA	k	609	X	-	-	-
24	CLA	k	610	X	-	-	-
29	SF4	A	854	-	-	X	-
29	SF4	C	101	-	-	X	-
29	SF4	C	102	-	-	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		

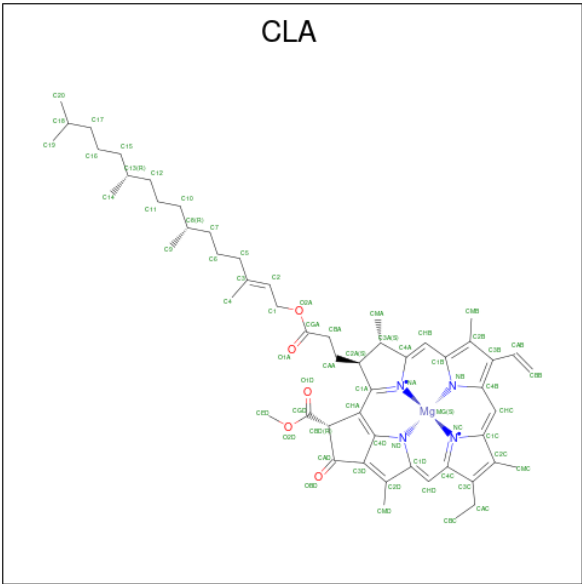
- Molecule 22 is a protein called CAC-g.

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 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 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 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 54	C 44	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 60	C 50	Mg 1	N 4	O 5	0
24	B	1	Total 59	C 49	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 59	C 49	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 46	C 36	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 53	C 43	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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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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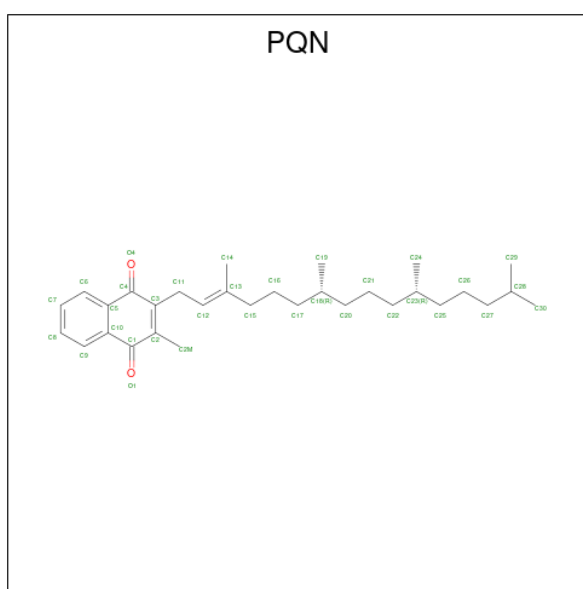
Mol	Chain	Residues	Atoms					AltConf
24	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	d	1	Total 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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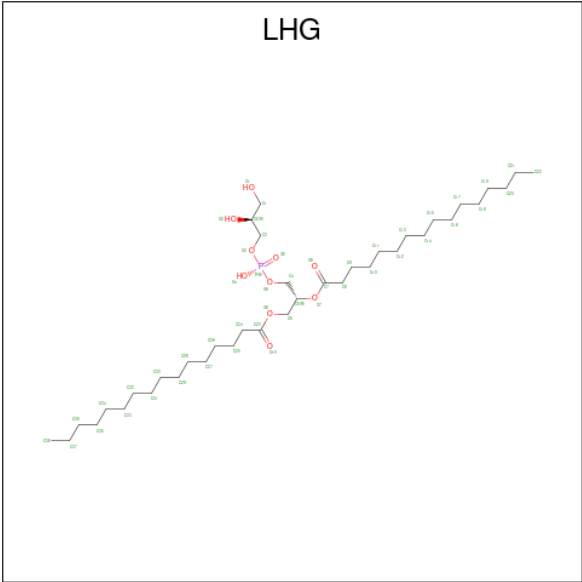
Mol	Chain	Residues	Atoms					AltConf
24	g	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	R	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

- 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: $C_{38}H_{75}O_{10}P$).



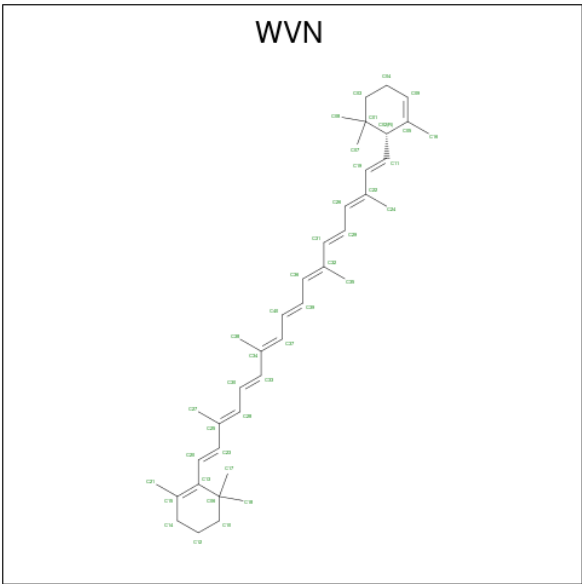
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			48	37	10	1	
26	A	1	Total	C	O	P	0
			27	16	10	1	
26	B	1	Total	C	O	P	0
			38	27	10	1	
26	J	1	Total	C	O	P	0
			49	38	10	1	
26	c	1	Total	C	O	P	0
			37	26	10	1	
26	c	1	Total	C	O	P	0
			37	26	10	1	
26	a	1	Total	C	O	P	0
			49	38	10	1	
26	b	1	Total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



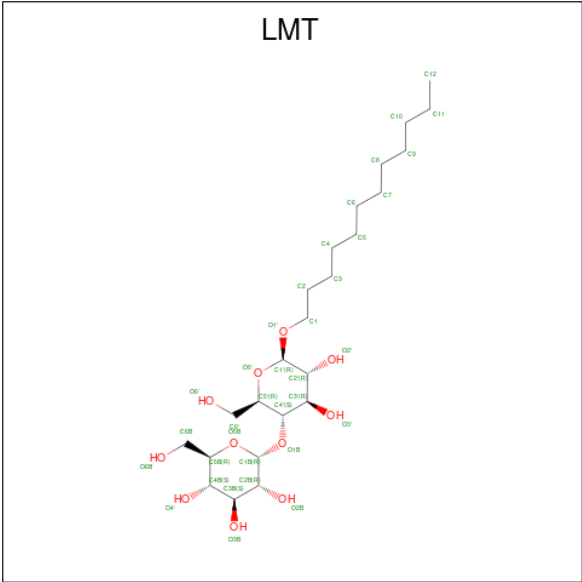
Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	B	1	Total	C	0
			40	40	

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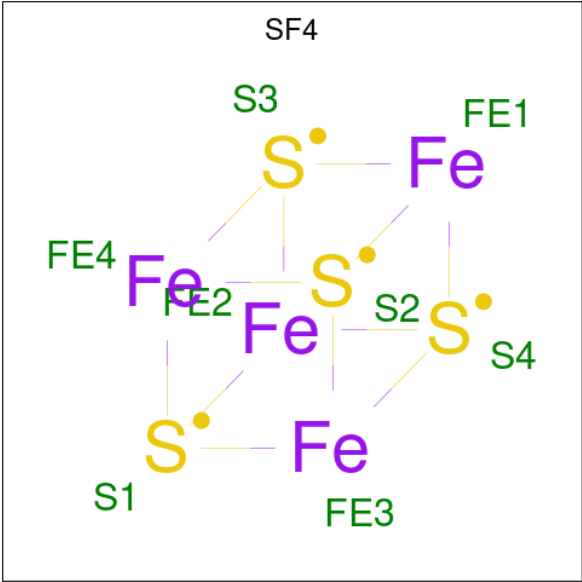
Mol	Chain	Residues	Atoms	AltConf
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	I	1	Total C 40 40	0
27	J	1	Total C 40 40	0
27	J	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 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).



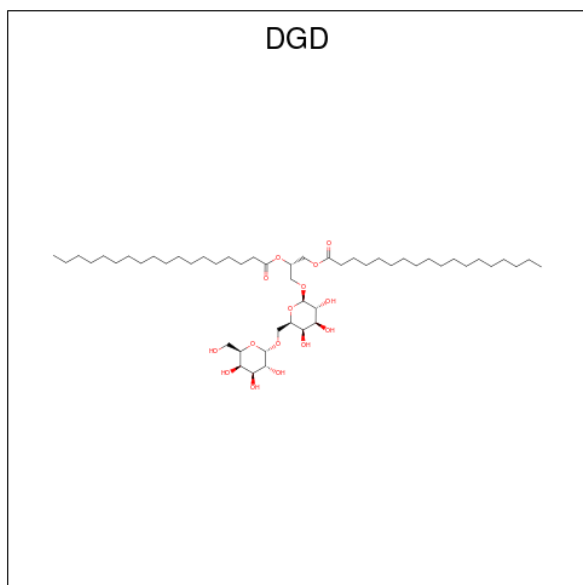
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			35	24	11	
28	F	1	Total	C	O	0
			24	18	6	
28	a	1	Total	C	O	0
			35	24	11	
28	b	1	Total	C	O	0
			24	18	6	

- 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-MALTOSIDE (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: $C_{45}H_{86}O_{10}$).



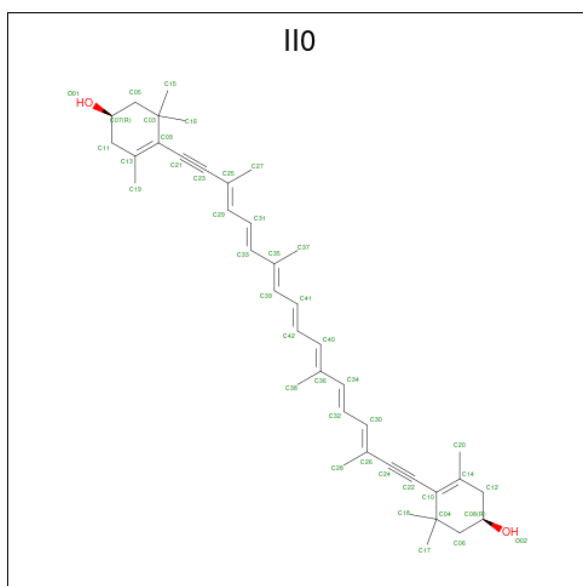
Mol	Chain	Residues	Atoms			AltConf
32	F	1	Total 48	C 38	O 10	0
32	J	1	Total 55	C 45	O 10	0

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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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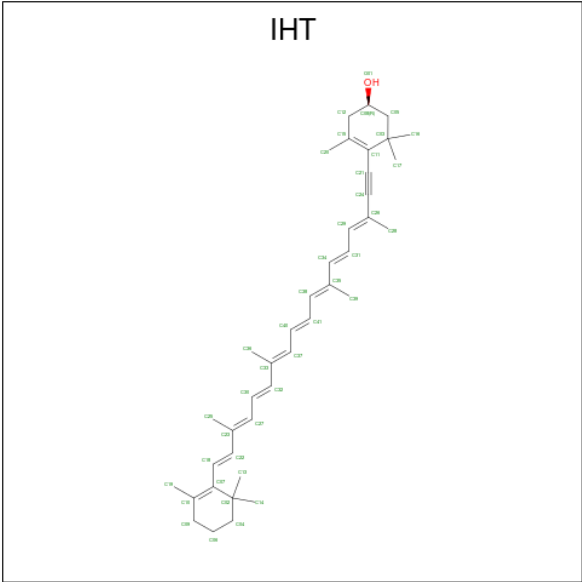
Mol	Chain	Residues	Atoms			AltConf
33	a	1	Total 42	C 40	O 2	0
33	a	1	Total 42	C 40	O 2	0
33	b	1	Total 42	C 40	O 2	0
33	b	1	Total 42	C 40	O 2	0
33	b	1	Total 42	C 40	O 2	0
33	h	1	Total 28	C 27	O 1	0
33	h	1	Total 42	C 40	O 2	0
33	h	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	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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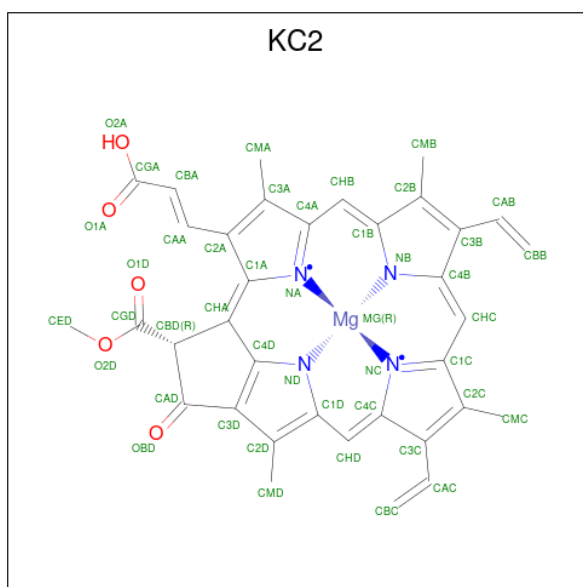
Mol	Chain	Residues	Atoms			AltConf
33	i	1	Total	C	O	0
			42	40	2	
33	i	1	Total	C	O	0
			42	40	2	
33	i	1	Total	C	O	0
			42	40	2	
33	j	1	Total	C	O	0
			42	40	2	
33	j	1	Total	C	O	0
			42	40	2	
33	j	1	Total	C	O	0
			42	40	2	
33	d	1	Total	C	O	0
			42	40	2	
33	d	1	Total	C	O	0
			42	40	2	
33	d	1	Total	C	O	0
			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 45	C 35	Mg 1	N 4	O 5	0
35	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	g	1	Total 45	C 35	Mg 1	N 4	O 5	0

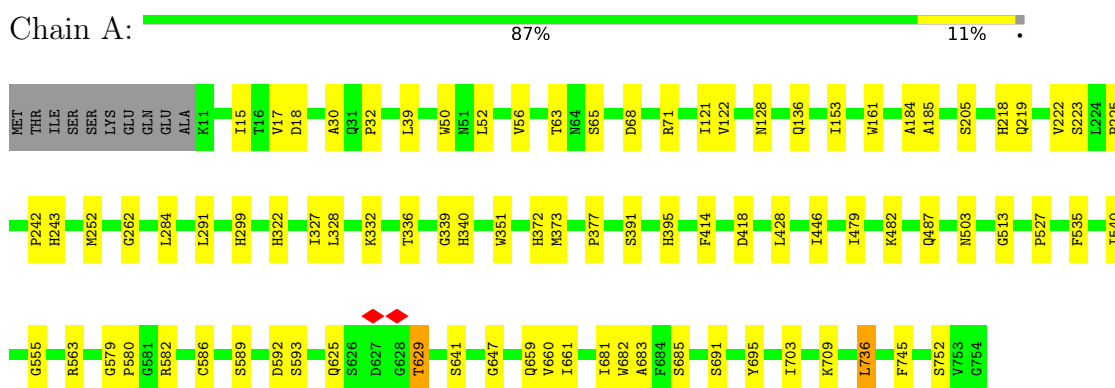
- Molecule 36 is water.

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

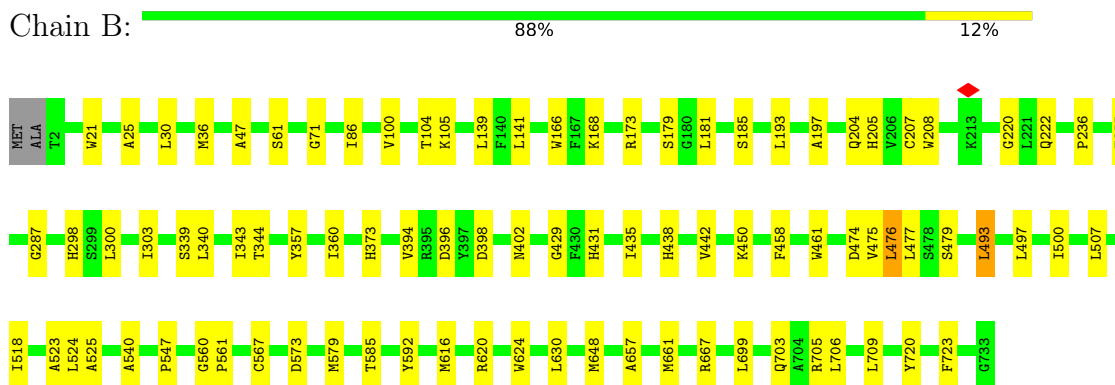
3 Residue-property plots

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.

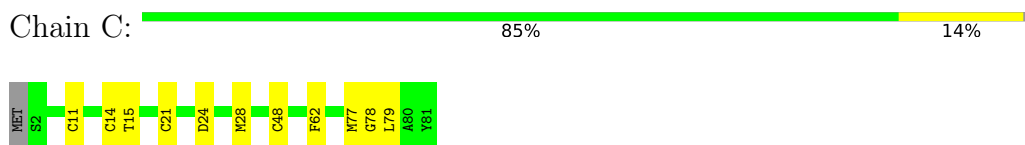
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



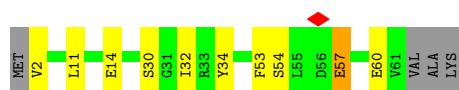
- Molecule 4: Photosystem I reaction center subunit II

Chain D:  85% 13%



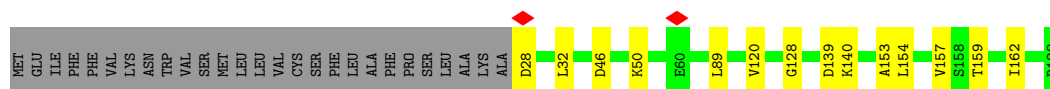
- Molecule 5: Photosystem I reaction center subunit IV

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% ..

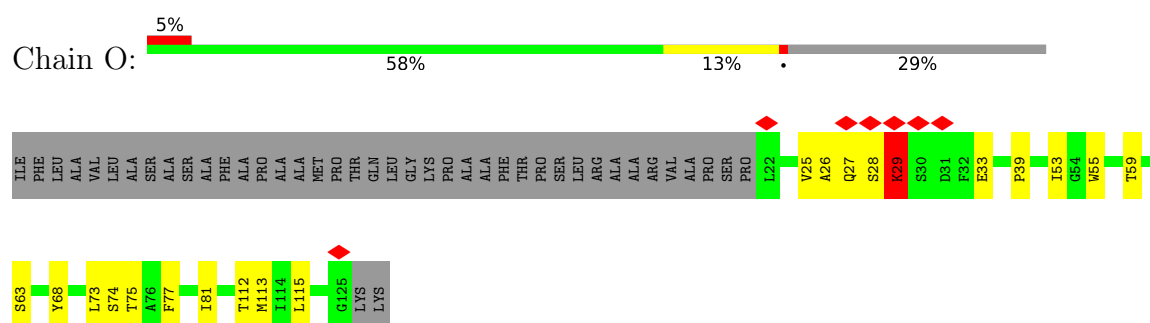


- Molecule 10: Photosystem I reaction center subunit XII

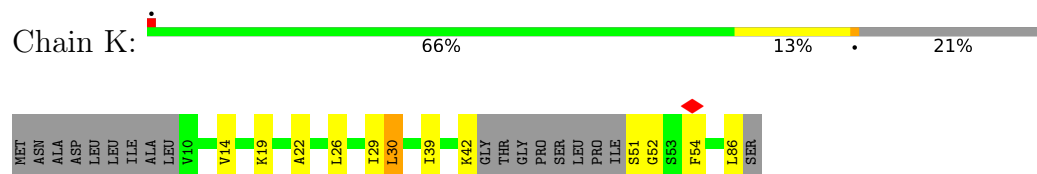
Chain M:  87% 13%



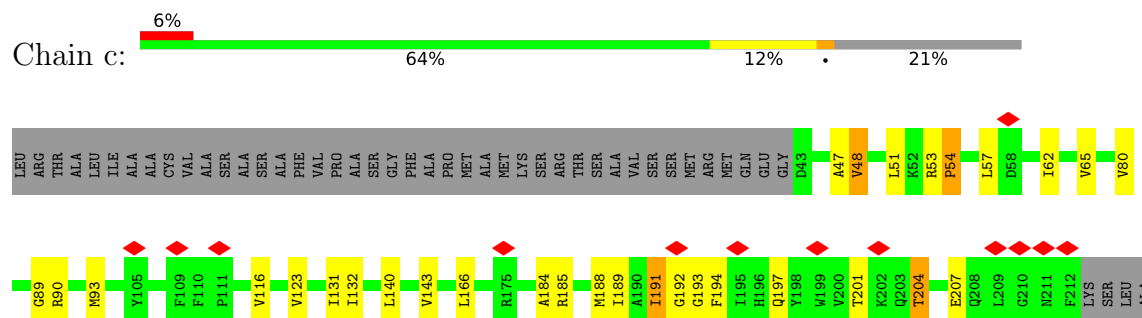
- Molecule 11: PsaO



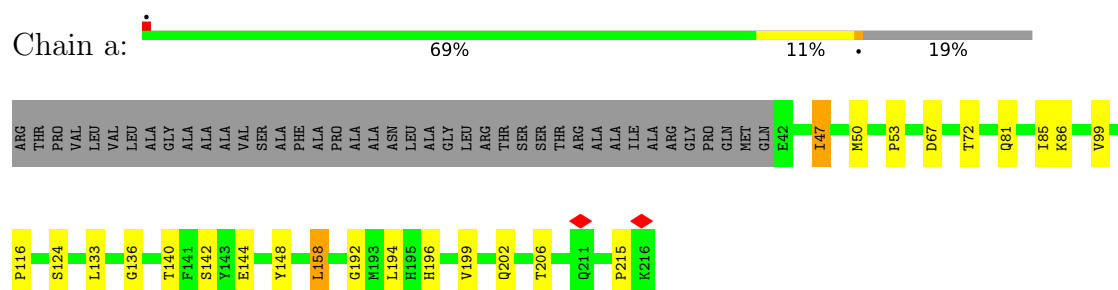
• Molecule 12: Photosystem I reaction center subunit PsaK



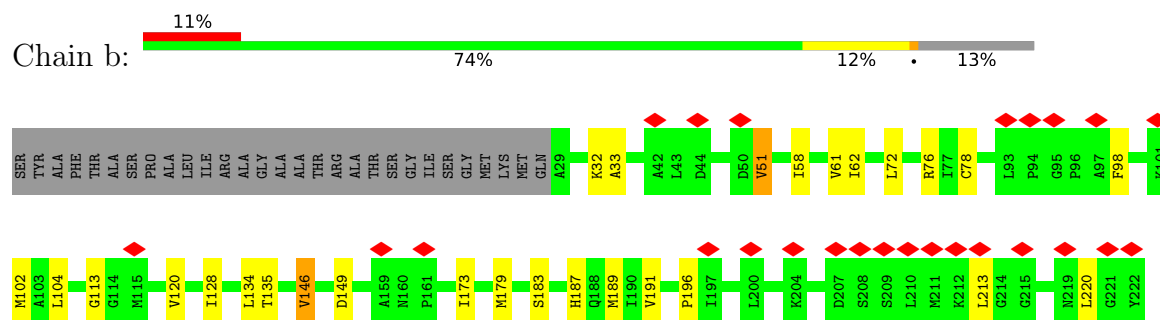
• Molecule 13: CAC-c



• Molecule 14: CAC-a

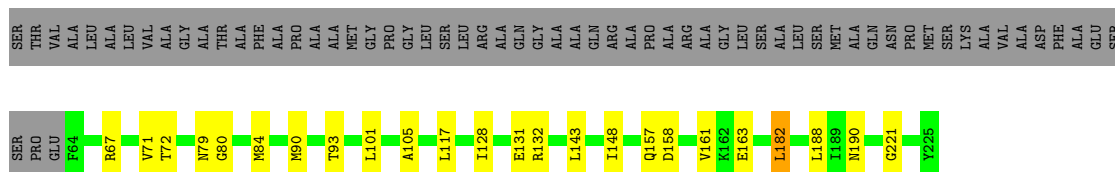


• Molecule 15: CAC-b



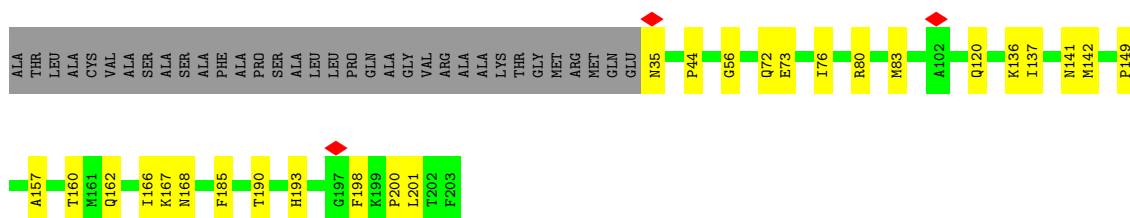
• Molecule 16: CAC-h

Chain h:  61% 10% 28%



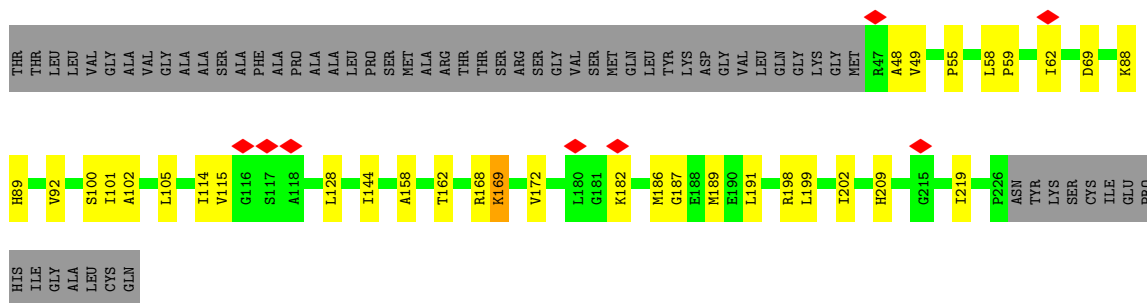
• Molecule 17: CAC-e

Chain e:  70% 13% 17%



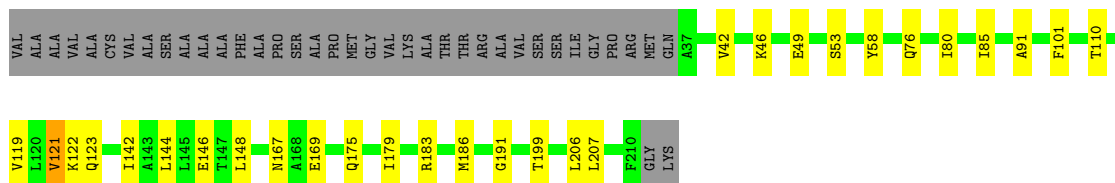
• Molecule 18: CAC-k

Chain k:  61% 13% 25%



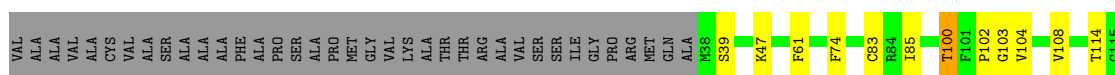
• Molecule 19: CAC-f

Chain f:  68% 13% 18%



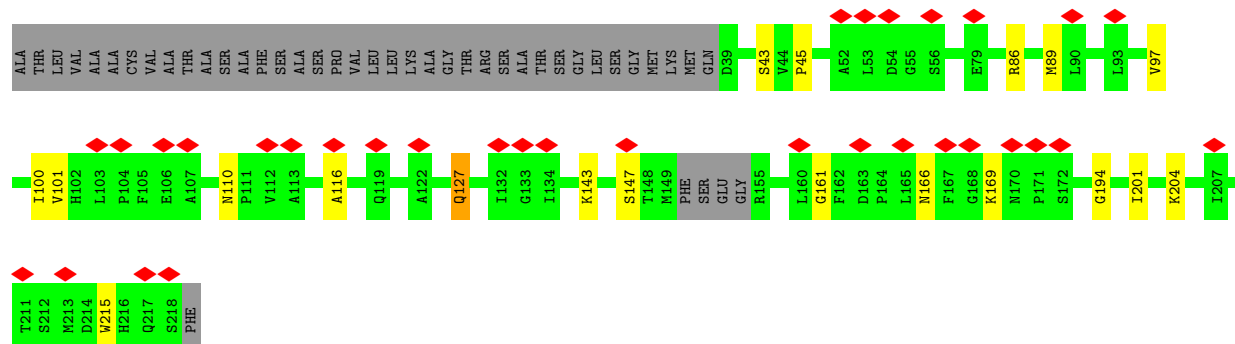
• Molecule 19: CAC-f

Chain j:  67% 14% 19%

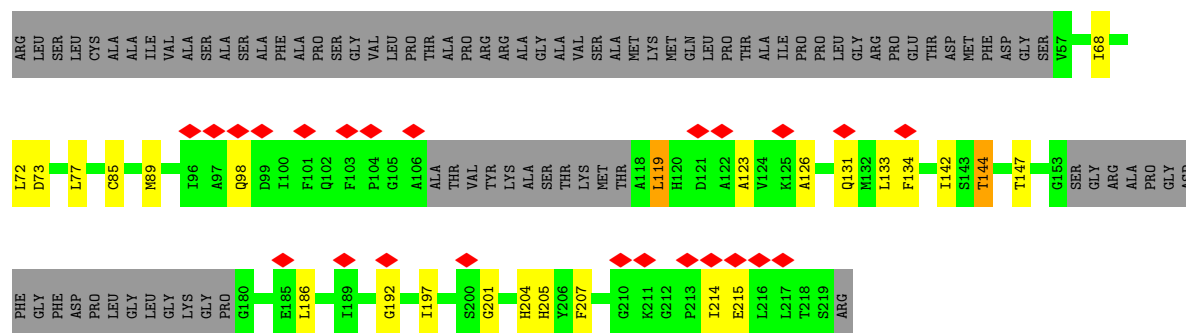




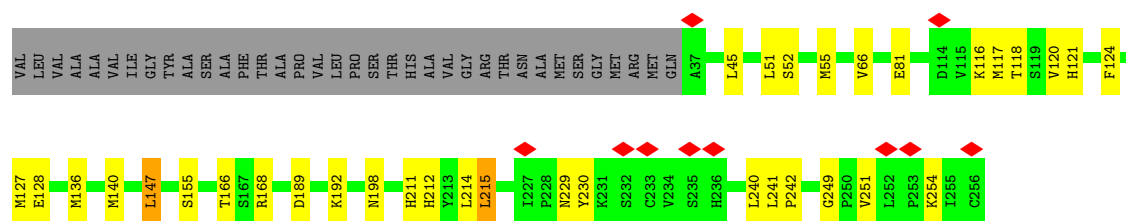
• Molecule 20: CAC-i



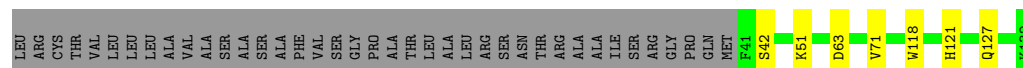
• Molecule 21: CAC-d



• Molecule 22: CAC-g



• Molecule 23: Psar



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: LMG, DGD, PQN, CLA, SF4, II0, IHT, LMU, LHG, KC2, WVN, LMT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	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	67	0
2	B	5826	0	5642	68	0
3	C	592	0	574	10	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	4	0
29	C	16	0	0	5	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	644	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 644 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	a	303	14	54,58,73	1.27	7 (12%)	64,95,113	1.33	8 (12%)
24	CLA	c	607	13	50,54,73	1.32	7 (14%)	59,90,113	1.20	5 (8%)
33	II0	f	614	-	39,43,43	6.63	21 (53%)	48,60,60	2.11	14 (29%)
24	CLA	B	837	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	8 (9%)
33	II0	i	613	-	39,43,43	6.76	22 (56%)	48,60,60	1.69	10 (20%)
24	CLA	d	307	21	50,54,73	1.30	6 (12%)	59,90,113	1.35	5 (8%)
24	CLA	b	303	15	55,59,73	1.28	6 (10%)	64,96,113	1.45	6 (9%)
24	CLA	f	605	19	49,53,73	1.36	7 (14%)	58,89,113	1.29	4 (6%)
24	CLA	a	304	-	55,59,73	1.26	5 (9%)	64,96,113	1.36	4 (6%)
24	CLA	B	817	-	61,65,73	1.19	7 (11%)	72,103,113	1.42	10 (13%)
27	WVN	j	301	-	40,41,41	1.80	10 (25%)	51,56,56	2.25	16 (31%)
24	CLA	g	303	22	54,58,73	1.27	9 (16%)	64,95,113	1.33	8 (12%)
24	CLA	B	807	-	69,73,73	1.10	7 (10%)	82,113,113	1.45	7 (8%)
24	CLA	b	304	15	59,63,73	1.22	8 (13%)	70,101,113	1.41	7 (10%)
24	CLA	h	305	16	69,73,73	1.14	8 (11%)	82,113,113	1.22	8 (9%)
24	CLA	g	304	-	55,59,73	1.29	10 (18%)	64,96,113	1.45	13 (20%)
24	CLA	a	309	26	52,56,73	1.32	7 (13%)	61,92,113	1.22	5 (8%)
24	CLA	h	307	16	55,59,73	1.32	8 (14%)	64,96,113	1.47	9 (14%)
24	CLA	B	811	-	59,63,73	1.26	8 (13%)	70,101,113	1.26	5 (7%)
33	II0	g	320	-	39,43,43	6.71	21 (53%)	48,60,60	1.96	17 (35%)
32	LMG	J	106	-	55,55,55	0.86	3 (5%)	63,63,63	0.97	4 (6%)
33	II0	k	619	-	39,43,43	6.68	20 (51%)	48,60,60	1.94	14 (29%)
24	CLA	i	608	26	50,54,73	1.34	6 (12%)	59,90,113	1.21	3 (5%)
24	CLA	j	311	26	65,69,73	1.21	6 (9%)	77,108,113	1.10	4 (5%)
24	CLA	c	601	13	55,59,73	1.29	9 (16%)	64,96,113	1.36	7 (10%)
24	CLA	B	830	36	69,73,73	1.16	7 (10%)	82,113,113	1.23	6 (7%)
24	CLA	R	203	-	55,59,73	1.26	7 (12%)	64,96,113	1.46	9 (14%)
33	II0	d	315	-	39,43,43	6.83	23 (58%)	48,60,60	2.00	14 (29%)
29	SF4	A	854	1,2	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMT	a	318	-	36,36,36	1.19	4 (11%)	47,47,47	1.16	3 (6%)
35	KC2	i	616	-	49,53,53	2.77	20 (40%)	60,89,89	3.73	32 (53%)
35	KC2	k	611	18	49,53,53	2.65	19 (38%)	60,89,89	3.84	33 (55%)
24	CLA	e	610	36	69,73,73	1.17	9 (13%)	82,113,113	1.33	10 (12%)
24	CLA	f	613	-	69,73,73	1.17	8 (11%)	82,113,113	1.16	5 (6%)
26	LHG	A	844	-	47,47,48	0.91	2 (4%)	50,53,54	1.17	5 (10%)
24	CLA	B	809	2	69,73,73	1.16	9 (13%)	82,113,113	1.31	12 (14%)
27	WVN	I	101	-	40,41,41	1.71	10 (25%)	51,56,56	1.86	19 (37%)
24	CLA	j	308	-	55,59,73	1.28	6 (10%)	64,96,113	1.20	5 (7%)
24	CLA	k	603	-	55,59,73	1.33	7 (12%)	64,96,113	1.54	10 (15%)
33	II0	O	202	-	39,43,43	6.70	21 (53%)	48,60,60	1.84	10 (20%)
33	II0	k	621	-	39,43,43	6.86	22 (56%)	48,60,60	1.80	10 (20%)
24	CLA	A	853	-	69,73,73	1.13	8 (11%)	82,113,113	1.33	10 (12%)
24	CLA	c	606	-	56,60,73	1.33	7 (12%)	65,97,113	1.30	7 (10%)
33	II0	J	104	-	39,43,43	6.53	18 (46%)	48,60,60	1.94	13 (27%)
24	CLA	d	309	26	45,49,73	1.39	8 (17%)	54,84,113	1.25	4 (7%)
24	CLA	J	105	26	55,59,73	1.34	8 (14%)	64,96,113	1.51	7 (10%)
24	CLA	k	601	18	55,59,73	1.35	8 (14%)	64,96,113	1.48	6 (9%)
26	LHG	J	107	24	48,48,48	1.01	2 (4%)	51,54,54	1.09	3 (5%)
24	CLA	g	322	32	69,73,73	1.12	8 (11%)	82,113,113	1.25	6 (7%)
33	II0	j	316	-	39,43,43	6.62	21 (53%)	48,60,60	2.04	18 (37%)
24	CLA	B	827	-	54,58,73	1.25	7 (12%)	64,95,113	1.28	8 (12%)
26	LHG	e	617	24	36,36,48	1.12	2 (5%)	39,42,54	1.18	4 (10%)
24	CLA	B	804	-	69,73,73	1.12	11 (15%)	82,113,113	1.51	11 (13%)
24	CLA	A	814	-	54,58,73	1.28	5 (9%)	64,95,113	1.48	13 (20%)
24	CLA	h	302	16	54,58,73	1.27	8 (14%)	64,95,113	1.36	9 (14%)
34	IHT	c	615	-	40,42,42	6.30	26 (65%)	52,58,58	2.17	13 (25%)
24	CLA	A	856	26	45,49,73	1.44	9 (20%)	54,84,113	1.99	8 (14%)
24	CLA	A	813	-	49,53,73	1.37	6 (12%)	58,89,113	1.47	6 (10%)
24	CLA	b	306	-	69,73,73	1.20	9 (13%)	82,113,113	1.45	7 (8%)
24	CLA	A	833	-	54,58,73	1.31	8 (14%)	64,95,113	1.30	5 (7%)
24	CLA	j	303	19	54,58,73	1.30	8 (14%)	64,95,113	1.22	5 (7%)
33	II0	i	614	-	39,43,43	6.67	21 (53%)	48,60,60	1.97	15 (31%)
24	CLA	g	306	22	55,59,73	1.30	8 (14%)	64,96,113	1.22	5 (7%)
24	CLA	c	604	13	69,73,73	1.16	8 (11%)	82,113,113	1.16	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	WVN	J	101	-	40,41,41	1.74	10 (25%)	51,56,56	2.09	17 (33%)
24	CLA	e	604	36	69,73,73	1.15	7 (10%)	82,113,113	1.39	8 (9%)
24	CLA	B	803	-	69,73,73	1.14	7 (10%)	82,113,113	1.29	9 (10%)
24	CLA	A	810	-	66,70,73	1.15	7 (10%)	78,109,113	1.17	6 (7%)
24	CLA	c	602	13	54,58,73	1.29	8 (14%)	64,95,113	1.42	11 (17%)
24	CLA	A	825	36	69,73,73	1.11	7 (10%)	82,113,113	1.26	7 (8%)
24	CLA	d	308	21	45,49,73	1.38	7 (15%)	54,84,113	1.29	4 (7%)
24	CLA	B	829	-	54,58,73	1.30	8 (14%)	64,95,113	1.43	5 (7%)
33	II0	a	314	-	39,43,43	6.71	22 (56%)	48,60,60	1.98	16 (33%)
24	CLA	e	601	17	49,53,73	1.39	8 (16%)	58,89,113	1.48	5 (8%)
24	CLA	A	812	-	69,73,73	1.13	9 (13%)	82,113,113	1.46	10 (12%)
24	CLA	B	816	-	63,67,73	1.19	7 (11%)	74,105,113	1.35	9 (12%)
24	CLA	c	612	-	69,73,73	1.12	6 (8%)	82,113,113	1.20	9 (10%)
24	CLA	O	205	-	69,73,73	1.25	10 (14%)	82,113,113	1.58	21 (25%)
33	II0	i	612	-	39,43,43	6.59	22 (56%)	48,60,60	2.09	12 (25%)
24	CLA	A	819	-	49,53,73	1.38	9 (18%)	58,89,113	1.63	10 (17%)
24	CLA	f	609	19	69,73,73	1.13	7 (10%)	82,113,113	1.19	7 (8%)
34	IHT	f	617	-	40,42,42	6.23	26 (65%)	52,58,58	4.02	21 (40%)
24	CLA	A	855	36	69,73,73	1.21	8 (11%)	82,113,113	1.41	10 (12%)
25	PQN	B	842	-	34,34,34	1.87	5 (14%)	43,45,45	1.30	6 (13%)
24	CLA	d	304	21	55,59,73	1.33	4 (7%)	64,96,113	1.38	7 (10%)
24	CLA	A	820	36	69,73,73	1.17	8 (11%)	82,113,113	1.37	10 (12%)
26	LHG	a	301	24	48,48,48	0.94	2 (4%)	51,54,54	1.19	5 (9%)
24	CLA	i	610	-	55,59,73	1.34	9 (16%)	64,96,113	1.41	8 (12%)
24	CLA	L	207	36	55,59,73	1.26	7 (12%)	64,96,113	1.34	7 (10%)
24	CLA	A	828	-	69,73,73	1.14	9 (13%)	82,113,113	1.34	7 (8%)
24	CLA	B	813	-	64,68,73	1.18	7 (10%)	76,107,113	1.29	10 (13%)
24	CLA	j	313	-	55,59,73	1.34	7 (12%)	64,96,113	1.27	7 (10%)
33	II0	f	615	-	39,43,43	6.65	23 (58%)	48,60,60	1.86	13 (27%)
24	CLA	B	808	-	69,73,73	1.17	7 (10%)	82,113,113	1.19	8 (9%)
24	CLA	B	801	36	69,73,73	1.14	9 (13%)	82,113,113	1.37	9 (10%)
24	CLA	A	822	-	55,59,73	1.30	8 (14%)	64,96,113	1.38	6 (9%)
24	CLA	k	604	18	69,73,73	1.15	6 (8%)	82,113,113	1.28	8 (9%)
24	CLA	e	606	17	69,73,73	1.13	7 (10%)	82,113,113	1.20	6 (7%)
24	CLA	A	806	-	69,73,73	1.16	7 (10%)	82,113,113	1.32	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	KC2	e	609	17	49,53,53	2.64	19 (38%)	60,89,89	3.78	33 (55%)
24	CLA	L	204	36	54,58,73	1.27	7 (12%)	64,95,113	1.42	6 (9%)
24	CLA	f	610	26	69,73,73	1.15	7 (10%)	82,113,113	1.23	5 (6%)
28	LMT	A	851	-	36,36,36	1.19	6 (16%)	47,47,47	1.38	5 (10%)
27	WVN	A	846	-	40,41,41	1.75	12 (30%)	51,56,56	2.28	17 (33%)
24	CLA	e	607	17	69,73,73	1.10	6 (8%)	82,113,113	1.23	7 (8%)
24	CLA	A	832	-	69,73,73	1.14	6 (8%)	82,113,113	1.59	18 (21%)
27	WVN	M	101	-	40,41,41	1.70	10 (25%)	51,56,56	2.21	16 (31%)
24	CLA	B	823	36	68,72,73	1.17	11 (16%)	80,111,113	1.34	8 (10%)
24	CLA	g	307	22	55,59,73	1.27	8 (14%)	64,96,113	1.33	7 (10%)
33	II0	f	616	-	39,43,43	6.56	22 (56%)	48,60,60	1.95	14 (29%)
34	IHT	k	618	-	40,42,42	6.28	26 (65%)	52,58,58	1.78	15 (28%)
24	CLA	c	611	-	49,53,73	1.36	6 (12%)	58,89,113	1.68	9 (15%)
24	CLA	g	305	22	69,73,73	1.10	7 (10%)	82,113,113	1.27	7 (8%)
24	CLA	i	606	20	65,69,73	1.19	5 (7%)	77,108,113	1.12	6 (7%)
35	KC2	i	609	20	49,53,53	2.70	19 (38%)	60,89,89	3.87	35 (58%)
24	CLA	A	852	36	69,73,73	1.16	8 (11%)	82,113,113	1.37	11 (13%)
24	CLA	c	603	-	55,59,73	1.26	9 (16%)	64,96,113	1.33	6 (9%)
24	CLA	A	811	-	58,62,73	1.28	7 (12%)	68,99,113	1.39	8 (11%)
24	CLA	f	602	19	69,73,73	1.15	7 (10%)	82,113,113	1.23	6 (7%)
24	CLA	f	601	19	51,55,73	1.34	6 (11%)	60,91,113	1.32	4 (6%)
24	CLA	A	826	-	69,73,73	1.16	8 (11%)	82,113,113	1.45	13 (15%)
24	CLA	B	838	-	61,65,73	1.26	8 (13%)	72,103,113	1.24	6 (8%)
24	CLA	d	306	-	55,59,73	1.31	7 (12%)	64,96,113	1.07	3 (4%)
24	CLA	g	308	-	69,73,73	1.13	7 (10%)	82,113,113	1.23	7 (8%)
33	II0	g	317	-	39,43,43	6.63	24 (61%)	48,60,60	1.97	16 (33%)
24	CLA	k	605	18	49,53,73	1.35	7 (14%)	58,89,113	1.37	5 (8%)
24	CLA	k	608	18	69,73,73	1.14	6 (8%)	82,113,113	1.12	6 (7%)
27	WVN	R	202	-	40,41,41	1.68	10 (25%)	51,56,56	2.65	19 (37%)
24	CLA	a	305	36	69,73,73	1.11	9 (13%)	82,113,113	1.25	10 (12%)
24	CLA	A	815	36	49,53,73	1.38	8 (16%)	58,89,113	1.55	6 (10%)
24	CLA	g	302	22	46,50,73	1.35	10 (21%)	53,85,113	1.61	8 (15%)
35	KC2	k	612	35	49,53,53	2.77	18 (36%)	60,89,89	3.86	37 (61%)
32	LMG	L	208	24	55,55,55	0.91	2 (3%)	63,63,63	1.44	10 (15%)
24	CLA	A	809	-	60,64,73	1.24	7 (11%)	71,102,113	1.27	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	WVN	B	847	-	40,41,41	1.69	9 (22%)	51,56,56	2.63	18 (35%)
27	WVN	J	102	-	40,41,41	1.71	11 (27%)	51,56,56	2.25	17 (33%)
33	II0	c	616	-	39,43,43	6.82	22 (56%)	48,60,60	1.92	18 (37%)
35	KC2	k	613	35	49,53,53	2.76	21 (42%)	60,89,89	3.76	31 (51%)
33	II0	e	612	-	39,43,43	6.67	20 (51%)	48,60,60	1.69	9 (18%)
24	CLA	a	308	14	69,73,73	1.14	9 (13%)	82,113,113	1.36	6 (7%)
24	CLA	K	102	-	46,50,73	1.38	9 (19%)	53,85,113	1.51	7 (13%)
34	IHT	j	317	-	40,42,42	6.25	26 (65%)	52,58,58	2.34	16 (30%)
24	CLA	j	307	19	55,59,73	1.34	9 (16%)	64,96,113	1.58	8 (12%)
24	CLA	i	611	-	55,59,73	1.30	5 (9%)	64,96,113	1.31	9 (14%)
24	CLA	b	311	-	55,59,73	1.30	8 (14%)	64,96,113	1.45	9 (14%)
33	II0	j	315	-	39,43,43	6.55	22 (56%)	48,60,60	2.27	15 (31%)
24	CLA	j	305	19	69,73,73	1.14	7 (10%)	82,113,113	1.27	7 (8%)
24	CLA	d	312	-	55,59,73	1.30	6 (10%)	64,96,113	1.51	10 (15%)
24	CLA	a	307	14	69,73,73	1.16	7 (10%)	82,113,113	1.27	10 (12%)
29	SF4	C	101	3	0,12,12	-	-	-	-	-
24	CLA	g	315	-	55,59,73	1.26	7 (12%)	64,96,113	1.25	10 (15%)
24	CLA	c	605	13	55,59,73	1.30	7 (12%)	64,96,113	1.44	9 (14%)
24	CLA	e	602	17	54,58,73	1.27	8 (14%)	64,95,113	1.35	5 (7%)
33	II0	b	318	-	39,43,43	6.75	23 (58%)	48,60,60	2.05	15 (31%)
29	SF4	C	102	3	0,12,12	-	-	-	-	-
33	II0	k	615	-	39,43,43	6.62	21 (53%)	48,60,60	1.89	17 (35%)
24	CLA	K	101	36	55,59,73	1.27	9 (16%)	64,96,113	1.54	11 (17%)
24	CLA	j	306	19	49,53,73	1.40	7 (14%)	58,89,113	1.60	8 (13%)
33	II0	k	617	-	39,43,43	6.80	21 (53%)	48,60,60	2.25	14 (29%)
24	CLA	A	841	36	69,73,73	1.15	6 (8%)	82,113,113	1.27	6 (7%)
27	WVN	A	849	-	40,41,41	1.73	11 (27%)	51,56,56	2.45	21 (41%)
33	II0	a	317	-	39,43,43	6.93	21 (53%)	48,60,60	2.38	15 (31%)
24	CLA	j	314	-	69,73,73	1.13	6 (8%)	82,113,113	1.23	6 (7%)
24	CLA	L	202	9	53,57,73	1.35	7 (13%)	61,93,113	1.39	8 (13%)
27	WVN	K	103	-	40,41,41	1.70	11 (27%)	51,56,56	2.24	19 (37%)
27	WVN	A	848	-	40,41,41	1.66	9 (22%)	51,56,56	1.93	13 (25%)
24	CLA	a	302	14	56,60,73	1.28	9 (16%)	65,97,113	1.35	7 (10%)
35	KC2	j	312	19	49,53,53	2.64	19 (38%)	60,89,89	3.86	33 (55%)
24	CLA	f	612	-	55,59,73	1.29	9 (16%)	64,96,113	1.38	12 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	e	608	26	50,54,73	1.34	9 (18%)	59,90,113	1.61	6 (10%)
26	LHG	j	319	24	29,29,48	1.26	2 (6%)	32,35,54	1.36	4 (12%)
24	CLA	f	603	-	55,59,73	1.28	6 (10%)	64,96,113	1.43	8 (12%)
24	CLA	A	816	-	69,73,73	1.11	8 (11%)	82,113,113	1.45	10 (12%)
24	CLA	A	824	36	69,73,73	1.15	8 (11%)	82,113,113	1.26	10 (12%)
35	KC2	g	313	35	49,53,53	2.72	19 (38%)	60,89,89	3.73	33 (55%)
24	CLA	d	301	21	54,58,73	1.33	6 (11%)	64,95,113	1.36	5 (7%)
24	CLA	A	804	-	69,73,73	1.15	7 (10%)	82,113,113	1.36	8 (9%)
33	II0	g	316	-	39,43,43	6.82	21 (53%)	48,60,60	1.83	16 (33%)
24	CLA	B	831	36	49,53,73	1.39	8 (16%)	58,89,113	1.37	7 (12%)
24	CLA	A	817	-	69,73,73	1.17	9 (13%)	82,113,113	1.36	12 (14%)
24	CLA	j	302	19	55,59,73	1.32	7 (12%)	64,96,113	1.26	5 (7%)
33	II0	h	311	-	39,43,43	6.69	21 (53%)	48,60,60	2.03	18 (37%)
33	II0	d	313	-	39,43,43	6.78	22 (56%)	48,60,60	2.04	13 (27%)
24	CLA	B	834	-	51,55,73	1.27	8 (15%)	60,91,113	1.55	7 (11%)
26	LHG	b	320	24	48,48,48	0.94	2 (4%)	51,54,54	1.12	5 (9%)
33	II0	e	616	-	39,43,43	6.73	20 (51%)	48,60,60	1.73	13 (27%)
24	CLA	A	842	-	69,73,73	1.15	9 (13%)	82,113,113	1.41	11 (13%)
33	II0	b	315	-	39,43,43	6.64	20 (51%)	48,60,60	2.73	19 (39%)
27	WVN	B	845	-	40,41,41	1.69	11 (27%)	51,56,56	2.60	20 (39%)
33	II0	a	313	-	39,43,43	6.60	22 (56%)	48,60,60	1.88	14 (29%)
24	CLA	I	102	36	69,73,73	1.18	8 (11%)	82,113,113	1.29	8 (9%)
26	LHG	f	620	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	4 (7%)
24	CLA	h	306	16	61,65,73	1.26	7 (11%)	72,103,113	1.12	5 (6%)
24	CLA	B	819	-	50,54,73	1.27	7 (14%)	59,90,113	1.40	7 (11%)
24	CLA	f	608	19	69,73,73	1.11	8 (11%)	82,113,113	1.25	8 (9%)
24	CLA	b	310	26	69,73,73	1.20	6 (8%)	82,113,113	1.19	10 (12%)
26	LHG	c	618	24	36,36,48	1.11	2 (5%)	39,42,54	1.22	6 (15%)
26	LHG	c	617	24	36,36,48	1.08	2 (5%)	39,42,54	1.26	5 (12%)
24	CLA	c	608	13	69,73,73	1.15	7 (10%)	82,113,113	1.30	10 (12%)
24	CLA	g	310	22	55,59,73	1.28	8 (14%)	64,96,113	1.32	8 (12%)
26	LHG	g	321	24	36,36,48	1.08	2 (5%)	39,42,54	1.56	9 (23%)
34	IHT	b	316	-	40,42,42	6.27	26 (65%)	52,58,58	2.17	15 (28%)
24	CLA	b	309	15	69,73,73	1.18	8 (11%)	82,113,113	1.27	10 (12%)
24	CLA	B	839	-	69,73,73	1.18	7 (10%)	82,113,113	1.29	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	KC2	d	310	21	49,53,53	2.70	21 (42%)	60,89,89	3.83	35 (58%)
24	CLA	i	601	20	55,59,73	1.29	6 (10%)	64,96,113	1.38	3 (4%)
24	CLA	f	606	19	55,59,73	1.28	6 (10%)	64,96,113	1.45	6 (9%)
27	WVN	F	204	-	40,41,41	1.69	11 (27%)	51,56,56	2.39	17 (33%)
24	CLA	B	805	-	69,73,73	1.12	7 (10%)	82,113,113	1.34	7 (8%)
24	CLA	B	812	-	69,73,73	1.16	10 (14%)	82,113,113	1.33	10 (12%)
24	CLA	B	832	-	62,66,73	1.20	9 (14%)	73,104,113	1.40	9 (12%)
24	CLA	k	602	18	54,58,73	1.32	8 (14%)	64,95,113	1.40	7 (10%)
28	LMT	F	203	-	24,24,36	1.05	2 (8%)	29,29,47	0.99	2 (6%)
24	CLA	A	838	26	56,60,73	1.27	8 (14%)	65,97,113	1.34	8 (12%)
24	CLA	B	840	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	10 (12%)
26	LHG	d	316	24	36,36,48	1.10	2 (5%)	39,42,54	1.25	5 (12%)
24	CLA	i	603	-	55,59,73	1.30	8 (14%)	64,96,113	1.39	6 (9%)
24	CLA	J	103	8	46,50,73	1.37	7 (15%)	53,85,113	1.43	6 (11%)
26	LHG	g	301	-	48,48,48	0.94	2 (4%)	51,54,54	1.05	2 (3%)
33	II0	f	618	-	39,43,43	6.64	20 (51%)	48,60,60	2.11	11 (22%)
24	CLA	k	610	26	55,59,73	1.29	6 (10%)	64,96,113	1.32	6 (9%)
24	CLA	a	310	14	69,73,73	1.14	6 (8%)	82,113,113	1.27	4 (4%)
24	CLA	a	311	-	51,55,73	1.33	7 (13%)	60,91,113	1.77	12 (20%)
24	CLA	f	607	-	69,73,73	1.14	8 (11%)	82,113,113	1.16	6 (7%)
24	CLA	j	304	-	55,59,73	1.27	5 (9%)	64,96,113	1.39	7 (10%)
25	PQN	A	843	-	34,34,34	1.90	5 (14%)	43,45,45	1.24	6 (13%)
24	CLA	d	302	-	55,59,73	1.34	8 (14%)	64,96,113	1.34	11 (17%)
24	CLA	B	836	-	69,73,73	1.17	10 (14%)	82,113,113	1.43	11 (13%)
33	II0	k	616	-	39,43,43	6.78	22 (56%)	48,60,60	1.98	15 (31%)
24	CLA	B	828	-	53,57,73	1.25	9 (16%)	61,93,113	1.41	9 (14%)
27	WVN	e	615	-	40,41,41	1.79	10 (25%)	51,56,56	2.22	17 (33%)
24	CLA	F	202	6	56,60,73	1.26	7 (12%)	65,97,113	1.49	8 (12%)
27	WVN	L	206	-	40,41,41	1.67	10 (25%)	51,56,56	2.56	22 (43%)
24	CLA	h	312	36	69,73,73	1.15	6 (8%)	82,113,113	1.27	7 (8%)
35	KC2	g	312	22	49,53,53	2.72	18 (36%)	60,89,89	4.07	37 (61%)
24	CLA	B	818	36	69,73,73	1.17	7 (10%)	82,113,113	1.31	8 (9%)
24	CLA	B	835	36	69,73,73	1.14	7 (10%)	82,113,113	1.12	6 (7%)
35	KC2	d	311	-	49,53,53	2.73	20 (40%)	60,89,89	3.69	34 (56%)
24	CLA	F	201	36	69,73,73	1.18	8 (11%)	82,113,113	1.20	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	WVN	F	205	-	40,41,41	1.79	10 (25%)	51,56,56	3.10	20 (39%)
24	CLA	j	310	19	55,59,73	1.27	8 (14%)	64,96,113	1.27	7 (10%)
33	II0	h	310	-	39,43,43	6.50	19 (48%)	48,60,60	2.08	17 (35%)
26	LHG	i	615	24	36,36,48	1.12	2 (5%)	39,42,54	1.21	3 (7%)
27	WVN	h	308	-	40,41,41	1.74	9 (22%)	51,56,56	2.43	19 (37%)
24	CLA	B	815	-	59,63,73	1.24	7 (11%)	70,101,113	1.26	6 (8%)
33	II0	d	314	-	39,43,43	6.65	23 (58%)	48,60,60	1.88	10 (20%)
24	CLA	A	830	-	54,58,73	1.31	10 (18%)	64,95,113	1.42	9 (14%)
24	CLA	e	605	17	69,73,73	1.12	7 (10%)	82,113,113	1.21	7 (8%)
24	CLA	e	603	17	55,59,73	1.33	6 (10%)	64,96,113	1.36	10 (15%)
24	CLA	B	810	-	58,62,73	1.34	9 (15%)	71,100,113	1.17	5 (7%)
24	CLA	A	821	-	53,57,73	1.27	9 (16%)	61,93,113	1.47	7 (11%)
24	CLA	i	602	20	54,58,73	1.29	7 (12%)	64,95,113	1.37	6 (9%)
24	CLA	h	301	16	54,58,73	1.29	7 (12%)	64,95,113	1.31	5 (7%)
27	WVN	L	205	-	40,41,41	1.76	9 (22%)	51,56,56	2.16	16 (31%)
24	CLA	A	808	1	69,73,73	1.15	7 (10%)	82,113,113	1.42	10 (12%)
33	II0	j	318	-	39,43,43	6.63	24 (61%)	48,60,60	1.88	12 (25%)
24	CLA	L	203	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	11 (13%)
26	LHG	B	802	-	37,37,48	1.04	3 (8%)	40,43,54	1.16	4 (10%)
24	CLA	A	801	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	9 (10%)
32	LMG	F	206	-	48,48,55	0.97	2 (4%)	56,56,63	1.26	5 (8%)
24	CLA	d	303	21	69,73,73	1.16	7 (10%)	82,113,113	1.29	12 (14%)
24	CLA	g	311	26	58,62,73	1.23	8 (13%)	68,99,113	1.18	5 (7%)
35	KC2	f	611	19	49,53,53	2.64	19 (38%)	60,89,89	3.97	34 (56%)
27	WVN	B	849	-	40,41,41	1.75	10 (25%)	51,56,56	1.87	11 (21%)
24	CLA	a	306	14	49,53,73	1.40	7 (14%)	58,89,113	1.53	4 (6%)
24	CLA	B	821	-	57,61,73	1.22	8 (14%)	67,98,113	1.26	7 (10%)
24	CLA	h	304	-	55,59,73	1.26	7 (12%)	64,96,113	1.25	7 (10%)
24	CLA	A	831	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	7 (8%)
26	LHG	f	619	24	36,36,48	1.07	2 (5%)	39,42,54	1.23	3 (7%)
24	CLA	A	818	-	69,73,73	1.16	8 (11%)	82,113,113	1.38	11 (13%)
24	CLA	i	604	20	69,73,73	1.20	6 (8%)	82,113,113	1.57	9 (10%)
24	CLA	B	841	26	69,73,73	1.16	8 (11%)	82,113,113	1.30	9 (10%)
33	II0	g	318	-	39,43,43	6.73	23 (58%)	48,60,60	1.92	14 (29%)
24	CLA	A	834	-	55,59,73	1.32	7 (12%)	64,96,113	1.61	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	308	15	65,69,73	1.19	7 (10%)	77,108,113	1.52	12 (15%)
24	CLA	b	313	-	69,73,73	1.18	7 (10%)	82,113,113	1.12	6 (7%)
35	KC2	g	314	35	49,53,53	2.73	20 (40%)	60,89,89	3.77	31 (51%)
24	CLA	i	605	20	55,59,73	1.33	8 (14%)	64,96,113	1.21	5 (7%)
24	CLA	B	825	-	69,73,73	1.17	11 (15%)	82,113,113	1.40	10 (12%)
26	LHG	A	845	24	26,26,48	1.26	2 (7%)	29,32,54	1.51	5 (17%)
24	CLA	B	824	-	69,73,73	1.12	8 (11%)	82,113,113	1.29	9 (10%)
26	LHG	k	620	24	36,36,48	1.15	2 (5%)	39,42,54	1.17	5 (12%)
35	KC2	c	610	-	49,53,53	2.73	21 (42%)	60,89,89	3.78	32 (53%)
24	CLA	e	611	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	9 (10%)
24	CLA	A	827	-	66,70,73	1.14	8 (12%)	78,109,113	1.32	11 (14%)
24	CLA	h	303	-	55,59,73	1.29	8 (14%)	64,96,113	1.42	10 (15%)
24	CLA	A	829	-	69,73,73	1.14	7 (10%)	82,113,113	1.24	7 (8%)
24	CLA	f	604	19	69,73,73	1.11	7 (10%)	82,113,113	1.25	7 (8%)
24	CLA	B	833	-	69,73,73	1.11	8 (11%)	82,113,113	1.35	9 (10%)
33	II0	c	613	-	39,43,43	6.71	22 (56%)	48,60,60	1.99	14 (29%)
27	WVN	B	848	-	40,41,41	1.75	11 (27%)	51,56,56	2.59	16 (31%)
24	CLA	O	201	-	69,73,73	1.18	10 (14%)	82,113,113	1.29	8 (9%)
30	DGD	B	843	-	61,61,67	0.88	2 (3%)	75,75,81	1.19	8 (10%)
31	LMU	B	844	-	36,36,36	1.13	2 (5%)	47,47,47	1.11	4 (8%)
24	CLA	A	839	1	69,73,73	1.20	8 (11%)	82,113,113	1.35	9 (10%)
33	II0	e	613	-	39,43,43	6.63	23 (58%)	48,60,60	1.80	14 (29%)
24	CLA	A	807	1	69,73,73	1.13	7 (10%)	82,113,113	1.31	8 (9%)
34	IHT	O	203	-	40,42,42	6.25	26 (65%)	52,58,58	2.25	16 (30%)
27	WVN	A	850	-	40,41,41	1.69	12 (30%)	51,56,56	2.19	14 (27%)
33	II0	c	614	-	39,43,43	6.84	20 (51%)	48,60,60	2.14	17 (35%)
24	CLA	A	840	-	69,73,73	1.12	9 (13%)	82,113,113	1.22	7 (8%)
24	CLA	c	609	26	49,53,73	1.39	7 (14%)	58,89,113	1.28	8 (13%)
28	LMT	b	319	-	24,24,36	1.05	2 (8%)	29,29,47	1.03	1 (3%)
24	CLA	A	836	-	69,73,73	1.15	6 (8%)	82,113,113	1.46	11 (13%)
24	CLA	j	309	19	49,53,73	1.36	8 (16%)	58,89,113	1.40	7 (12%)
33	II0	h	309	-	26,28,43	6.09	12 (46%)	30,37,60	2.03	10 (33%)
32	LMG	O	204	-	26,26,55	1.27	2 (7%)	34,34,63	1.26	4 (11%)
24	CLA	A	823	-	59,63,73	1.25	7 (11%)	70,101,113	1.22	6 (8%)
34	IHT	g	319	-	40,42,42	6.16	26 (65%)	52,58,58	2.25	16 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	WVN	R	201	-	40,41,41	1.72	10 (25%)	51,56,56	2.07	13 (25%)
32	LMG	b	301	-	55,55,55	0.90	2 (3%)	63,63,63	1.13	5 (7%)
24	CLA	k	606	18	55,59,73	1.29	8 (14%)	64,96,113	1.33	5 (7%)
24	CLA	k	614	-	55,59,73	1.31	5 (9%)	64,96,113	1.27	7 (10%)
33	II0	a	315	-	39,43,43	6.89	22 (56%)	48,60,60	1.68	12 (25%)
24	CLA	g	309	22	69,73,73	1.16	7 (10%)	82,113,113	1.25	9 (10%)
33	II0	e	614	-	39,43,43	6.85	19 (48%)	48,60,60	1.91	15 (31%)
24	CLA	A	805	1	69,73,73	1.15	7 (10%)	82,113,113	1.40	11 (13%)
27	WVN	B	846	-	40,41,41	1.65	11 (27%)	51,56,56	2.29	19 (37%)
24	CLA	A	802	-	69,73,73	1.16	9 (13%)	82,113,113	1.42	13 (15%)
24	CLA	k	607	-	55,59,73	1.34	7 (12%)	64,96,113	1.36	6 (9%)
24	CLA	A	837	-	69,73,73	1.15	7 (10%)	82,113,113	1.46	12 (14%)
24	CLA	b	307	36	69,73,73	1.19	6 (8%)	82,113,113	1.33	10 (12%)
34	IHT	b	317	-	40,42,42	6.34	26 (65%)	52,58,58	2.85	15 (28%)
24	CLA	b	312	15	69,73,73	1.17	7 (10%)	82,113,113	1.23	7 (8%)
24	CLA	A	803	-	59,63,73	1.23	7 (11%)	70,101,113	1.49	10 (14%)
24	CLA	b	305	-	69,73,73	1.14	7 (10%)	82,113,113	1.28	7 (8%)
27	WVN	L	201	-	40,41,41	1.70	11 (27%)	51,56,56	2.40	16 (31%)
33	II0	b	314	-	39,43,43	6.84	23 (58%)	48,60,60	2.02	11 (22%)
24	CLA	d	305	-	55,59,73	1.29	7 (12%)	64,96,113	1.19	8 (12%)
26	LHG	b	302	24	48,48,48	0.93	2 (4%)	51,54,54	1.21	5 (9%)
24	CLA	B	820	-	59,63,73	1.23	7 (11%)	70,101,113	1.31	9 (12%)
34	IHT	R	204	-	40,42,42	6.30	25 (62%)	52,58,58	2.18	17 (32%)
24	CLA	k	609	18	69,73,73	1.19	7 (10%)	82,113,113	1.30	10 (12%)
34	IHT	a	316	-	40,42,42	6.23	26 (65%)	52,58,58	2.07	16 (30%)
24	CLA	B	826	-	69,73,73	1.13	8 (11%)	82,113,113	1.22	7 (8%)
24	CLA	i	607	20	55,59,73	1.30	7 (12%)	64,96,113	1.30	9 (14%)
24	CLA	B	814	-	63,67,73	1.18	7 (11%)	74,105,113	1.34	8 (10%)
24	CLA	A	835	-	69,73,73	1.15	7 (10%)	82,113,113	1.31	7 (8%)
24	CLA	B	822	36	69,73,73	1.19	7 (10%)	82,113,113	1.57	15 (18%)
24	CLA	B	806	-	69,73,73	1.16	10 (14%)	82,113,113	1.31	8 (9%)
27	WVN	A	847	-	40,41,41	1.72	11 (27%)	51,56,56	3.12	23 (45%)
24	CLA	a	312	-	52,56,73	1.36	9 (17%)	61,92,113	1.36	10 (16%)

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	a	303	14	1/1/12/20	7/21/97/115	-
24	CLA	c	607	13	1/1/11/20	3/17/93/115	-
33	II0	f	614	-	-	3/21/67/67	0/2/2/2
24	CLA	B	837	-	1/1/15/20	13/39/115/115	-
33	II0	i	613	-	-	3/21/67/67	0/2/2/2
24	CLA	d	307	21	1/1/11/20	6/17/93/115	-
24	CLA	b	303	15	1/1/12/20	10/23/99/115	-
24	CLA	f	605	19	-	8/15/91/115	-
24	CLA	a	304	-	1/1/12/20	3/23/99/115	-
24	CLA	B	817	-	-	7/30/106/115	-
27	WVN	j	301	-	-	9/29/63/63	0/2/2/2
24	CLA	g	303	22	1/1/12/20	7/21/97/115	-
24	CLA	B	807	-	1/1/15/20	10/39/115/115	-
24	CLA	b	304	15	1/1/13/20	8/27/103/115	-
24	CLA	h	305	16	1/1/15/20	10/39/115/115	-
24	CLA	g	304	-	1/1/12/20	4/23/99/115	-
24	CLA	a	309	26	1/1/11/20	6/19/95/115	-
24	CLA	h	307	16	1/1/12/20	9/23/99/115	-
24	CLA	B	811	-	1/1/13/20	6/27/103/115	-
33	II0	g	320	-	-	4/21/67/67	0/2/2/2
32	LMG	J	106	-	-	13/50/70/70	0/1/1/1
33	II0	k	619	-	-	5/21/67/67	0/2/2/2
24	CLA	i	608	26	1/1/11/20	6/17/93/115	-
24	CLA	j	311	26	1/1/14/20	15/35/111/115	-
24	CLA	c	601	13	1/1/12/20	13/23/99/115	-
24	CLA	B	830	36	1/1/15/20	11/39/115/115	-
24	CLA	R	203	-	1/1/12/20	8/23/99/115	-
33	II0	d	315	-	-	8/21/67/67	0/2/2/2
29	SF4	A	854	1,2	-	-	0/6/5/5
28	LMT	a	318	-	-	3/21/61/61	0/2/2/2
35	KC2	i	616	-	-	10/15/71/71	-
35	KC2	k	611	18	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	e	610	36	-	9/39/115/115	-
24	CLA	f	613	-	1/1/15/20	21/39/115/115	-
26	LHG	A	844	-	-	4/52/52/53	-
24	CLA	B	809	2	1/1/15/20	11/39/115/115	-
27	WVN	I	101	-	-	9/29/63/63	0/2/2/2
24	CLA	j	308	-	1/1/12/20	9/23/99/115	-
24	CLA	k	603	-	1/1/12/20	2/23/99/115	-
33	II0	O	202	-	-	3/21/67/67	0/2/2/2
33	II0	k	621	-	-	4/21/67/67	0/2/2/2
24	CLA	A	853	-	1/1/15/20	11/39/115/115	-
24	CLA	c	606	-	-	7/24/100/115	-
33	II0	J	104	-	-	7/21/67/67	0/2/2/2
24	CLA	d	309	26	1/1/10/20	2/10/86/115	-
24	CLA	J	105	26	1/1/12/20	6/23/99/115	-
24	CLA	k	601	18	1/1/12/20	9/23/99/115	-
26	LHG	J	107	24	-	19/53/53/53	-
24	CLA	g	322	32	1/1/15/20	14/39/115/115	-
33	II0	j	316	-	-	3/21/67/67	0/2/2/2
24	CLA	B	827	-	1/1/12/20	11/21/97/115	-
26	LHG	e	617	24	-	11/41/41/53	-
24	CLA	B	804	-	1/1/15/20	9/39/115/115	-
24	CLA	A	814	-	-	8/21/97/115	-
24	CLA	h	302	16	1/1/12/20	10/21/97/115	-
34	IHT	c	615	-	-	10/25/65/65	0/2/2/2
24	CLA	A	856	26	1/1/10/20	4/10/86/115	-
24	CLA	A	813	-	1/1/11/20	6/15/91/115	-
24	CLA	b	306	-	-	17/39/115/115	-
24	CLA	A	833	-	1/1/12/20	5/21/97/115	-
24	CLA	j	303	19	1/1/12/20	2/21/97/115	-
33	II0	i	614	-	-	4/21/67/67	0/2/2/2
24	CLA	g	306	22	1/1/12/20	9/23/99/115	-
24	CLA	c	604	13	1/1/15/20	4/39/115/115	-
27	WVN	J	101	-	-	8/29/63/63	0/2/2/2
24	CLA	e	604	36	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	803	-	1/1/15/20	19/39/115/115	-
24	CLA	A	810	-	1/1/14/20	9/36/112/115	-
24	CLA	c	602	13	1/1/12/20	12/21/97/115	-
24	CLA	A	825	36	1/1/15/20	8/39/115/115	-
24	CLA	d	308	21	1/1/10/20	2/10/86/115	-
24	CLA	B	829	-	1/1/12/20	4/21/97/115	-
33	II0	a	314	-	-	7/21/67/67	0/2/2/2
24	CLA	e	601	17	1/1/11/20	9/15/91/115	-
24	CLA	A	812	-	1/1/15/20	20/39/115/115	-
24	CLA	B	816	-	1/1/13/20	9/32/108/115	-
24	CLA	c	612	-	1/1/15/20	12/39/115/115	-
24	CLA	O	205	-	1/1/15/20	17/39/115/115	-
33	II0	i	612	-	-	7/21/67/67	0/2/2/2
24	CLA	A	819	-	1/1/11/20	6/15/91/115	-
24	CLA	f	609	19	1/1/15/20	4/39/115/115	-
34	IHT	f	617	-	-	4/25/65/65	0/2/2/2
24	CLA	A	855	36	1/1/15/20	15/39/115/115	-
25	PQN	B	842	-	-	13/23/43/43	0/2/2/2
24	CLA	d	304	21	1/1/12/20	8/23/99/115	-
24	CLA	A	820	36	1/1/15/20	5/39/115/115	-
26	LHG	a	301	24	-	15/53/53/53	-
24	CLA	i	610	-	1/1/12/20	7/23/99/115	-
24	CLA	L	207	36	1/1/12/20	5/23/99/115	-
24	CLA	A	828	-	1/1/15/20	8/39/115/115	-
24	CLA	B	813	-	1/1/14/20	13/33/109/115	-
24	CLA	j	313	-	1/1/12/20	5/23/99/115	-
33	II0	f	615	-	-	4/21/67/67	0/2/2/2
24	CLA	B	808	-	1/1/15/20	13/39/115/115	-
24	CLA	B	801	36	1/1/15/20	12/39/115/115	-
24	CLA	A	822	-	1/1/12/20	8/23/99/115	-
24	CLA	k	604	18	1/1/15/20	8/39/115/115	-
24	CLA	e	606	17	1/1/15/20	11/39/115/115	-
24	CLA	A	806	-	-	9/39/115/115	-
35	KC2	e	609	17	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	L	204	36	1/1/12/20	7/21/97/115	-
24	CLA	f	610	26	1/1/15/20	15/39/115/115	-
28	LMT	A	851	-	-	10/21/61/61	0/2/2/2
27	WVN	A	846	-	-	8/29/63/63	0/2/2/2
24	CLA	e	607	17	1/1/15/20	10/39/115/115	-
24	CLA	A	832	-	-	14/39/115/115	-
27	WVN	M	101	-	-	9/29/63/63	0/2/2/2
24	CLA	B	823	36	1/1/14/20	9/38/114/115	-
24	CLA	g	307	22	1/1/12/20	8/23/99/115	-
33	II0	f	616	-	-	3/21/67/67	0/2/2/2
34	IHT	k	618	-	-	7/25/65/65	0/2/2/2
24	CLA	c	611	-	1/1/11/20	8/15/91/115	-
24	CLA	g	305	22	1/1/15/20	14/39/115/115	-
24	CLA	i	606	20	1/1/14/20	9/35/111/115	-
35	KC2	i	609	20	-	8/15/71/71	-
24	CLA	A	852	36	1/1/15/20	2/39/115/115	-
24	CLA	c	603	-	1/1/12/20	2/23/99/115	-
24	CLA	A	811	-	1/1/12/20	7/26/102/115	-
24	CLA	f	602	19	1/1/15/20	19/39/115/115	-
24	CLA	f	601	19	1/1/11/20	12/18/94/115	-
24	CLA	A	826	-	1/1/15/20	7/39/115/115	-
24	CLA	B	838	-	1/1/13/20	9/30/106/115	-
24	CLA	d	306	-	1/1/12/20	11/23/99/115	-
24	CLA	g	308	-	1/1/15/20	19/39/115/115	-
33	II0	g	317	-	-	5/21/67/67	0/2/2/2
24	CLA	k	605	18	1/1/11/20	5/15/91/115	-
24	CLA	k	608	18	1/1/15/20	11/39/115/115	-
27	WVN	R	202	-	-	10/29/63/63	0/2/2/2
24	CLA	a	305	36	1/1/15/20	6/39/115/115	-
24	CLA	A	815	36	1/1/11/20	5/15/91/115	-
24	CLA	g	302	22	1/1/10/20	0/12/88/115	-
35	KC2	k	612	35	-	8/15/71/71	-
32	LMG	L	208	24	-	19/50/70/70	0/1/1/1
24	CLA	A	809	-	1/1/13/20	7/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	WVN	B	847	-	-	12/29/63/63	0/2/2/2
27	WVN	J	102	-	-	8/29/63/63	0/2/2/2
33	II0	c	616	-	-	3/21/67/67	0/2/2/2
35	KC2	k	613	35	-	7/15/71/71	-
33	II0	e	612	-	-	4/21/67/67	0/2/2/2
24	CLA	a	308	14	1/1/15/20	13/39/115/115	-
24	CLA	K	102	-	1/1/10/20	5/12/88/115	-
34	IHT	j	317	-	-	7/25/65/65	0/2/2/2
24	CLA	j	307	19	1/1/12/20	10/23/99/115	-
24	CLA	i	611	-	1/1/12/20	13/23/99/115	-
24	CLA	b	311	-	1/1/12/20	5/23/99/115	-
33	II0	j	315	-	-	4/21/67/67	0/2/2/2
24	CLA	j	305	19	-	9/39/115/115	-
24	CLA	d	312	-	-	6/23/99/115	-
24	CLA	a	307	14	1/1/15/20	16/39/115/115	-
29	SF4	C	101	3	-	-	0/6/5/5
24	CLA	g	315	-	1/1/12/20	7/23/99/115	-
24	CLA	c	605	13	1/1/12/20	9/23/99/115	-
24	CLA	e	602	17	1/1/12/20	7/21/97/115	-
33	II0	b	318	-	-	5/21/67/67	0/2/2/2
29	SF4	C	102	3	-	-	0/6/5/5
33	II0	k	615	-	-	6/21/67/67	0/2/2/2
24	CLA	K	101	36	1/1/12/20	2/23/99/115	-
24	CLA	j	306	19	1/1/11/20	7/15/91/115	-
33	II0	k	617	-	-	2/21/67/67	0/2/2/2
24	CLA	A	841	36	1/1/15/20	18/39/115/115	-
27	WVN	A	849	-	-	8/29/63/63	0/2/2/2
33	II0	a	317	-	-	7/21/67/67	0/2/2/2
24	CLA	j	314	-	1/1/15/20	14/39/115/115	-
24	CLA	L	202	9	1/1/11/20	8/20/96/115	-
27	WVN	K	103	-	-	5/29/63/63	0/2/2/2
27	WVN	A	848	-	-	9/29/63/63	0/2/2/2
24	CLA	a	302	14	1/1/12/20	11/24/100/115	-
35	KC2	j	312	19	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	f	612	-	1/1/12/20	6/23/99/115	-
24	CLA	e	608	26	1/1/11/20	9/17/93/115	-
26	LHG	j	319	24	-	5/34/34/53	-
24	CLA	f	603	-	1/1/12/20	6/23/99/115	-
24	CLA	A	816	-	1/1/15/20	14/39/115/115	-
24	CLA	A	824	36	1/1/15/20	9/39/115/115	-
35	KC2	g	313	35	-	2/15/71/71	-
24	CLA	d	301	21	1/1/12/20	7/21/97/115	-
24	CLA	A	804	-	1/1/15/20	5/39/115/115	-
33	II0	g	316	-	-	7/21/67/67	0/2/2/2
24	CLA	B	831	36	1/1/11/20	6/15/91/115	-
24	CLA	A	817	-	1/1/15/20	15/39/115/115	-
24	CLA	j	302	19	1/1/12/20	2/23/99/115	-
33	II0	h	311	-	-	6/21/67/67	0/2/2/2
33	II0	d	313	-	-	6/21/67/67	0/2/2/2
24	CLA	B	834	-	1/1/11/20	4/18/94/115	-
26	LHG	b	320	24	-	16/53/53/53	-
33	II0	e	616	-	-	5/21/67/67	0/2/2/2
24	CLA	A	842	-	1/1/15/20	21/39/115/115	-
33	II0	b	315	-	-	5/21/67/67	0/2/2/2
27	WVN	B	845	-	-	7/29/63/63	0/2/2/2
33	II0	a	313	-	-	1/21/67/67	0/2/2/2
24	CLA	I	102	36	1/1/15/20	17/39/115/115	-
26	LHG	f	620	-	-	17/53/53/53	-
24	CLA	h	306	16	1/1/13/20	9/30/106/115	-
24	CLA	f	608	19	1/1/15/20	8/39/115/115	-
24	CLA	B	819	-	-	2/17/93/115	-
24	CLA	b	310	26	1/1/15/20	10/39/115/115	-
26	LHG	c	618	24	-	11/41/41/53	-
26	LHG	c	617	24	-	13/41/41/53	-
24	CLA	c	608	13	1/1/15/20	16/39/115/115	-
24	CLA	g	310	22	1/1/12/20	6/23/99/115	-
26	LHG	g	321	24	-	12/41/41/53	-
34	IHT	b	316	-	-	3/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	309	15	1/1/15/20	18/39/115/115	-
24	CLA	B	839	-	1/1/15/20	10/39/115/115	-
35	KC2	d	310	21	-	6/15/71/71	-
24	CLA	i	601	20	1/1/12/20	7/23/99/115	-
24	CLA	f	606	19	-	6/23/99/115	-
27	WVN	F	204	-	-	8/29/63/63	0/2/2/2
24	CLA	B	805	-	1/1/15/20	14/39/115/115	-
24	CLA	B	812	-	1/1/15/20	12/39/115/115	-
24	CLA	B	832	-	1/1/13/20	6/31/107/115	-
24	CLA	k	602	18	1/1/12/20	6/21/97/115	-
28	LMT	F	203	-	-	4/15/35/61	0/1/1/2
24	CLA	A	838	26	1/1/12/20	5/24/100/115	-
24	CLA	B	840	-	-	10/39/115/115	-
26	LHG	d	316	24	-	10/41/41/53	-
24	CLA	i	603	-	1/1/12/20	3/23/99/115	-
24	CLA	J	103	8	1/1/10/20	3/12/88/115	-
26	LHG	g	301	-	-	14/53/53/53	-
33	II0	f	618	-	-	7/21/67/67	0/2/2/2
24	CLA	k	610	26	1/1/12/20	11/23/99/115	-
24	CLA	a	310	14	1/1/15/20	12/39/115/115	-
24	CLA	a	311	-	1/1/11/20	10/18/94/115	-
24	CLA	f	607	-	1/1/15/20	17/39/115/115	-
24	CLA	j	304	-	1/1/12/20	0/23/99/115	-
25	PQN	A	843	-	-	5/23/43/43	0/2/2/2
24	CLA	d	302	-	1/1/12/20	4/23/99/115	-
24	CLA	B	836	-	1/1/15/20	25/39/115/115	-
33	II0	k	616	-	-	6/21/67/67	0/2/2/2
24	CLA	B	828	-	-	5/20/96/115	-
27	WVN	e	615	-	-	11/29/63/63	0/2/2/2
24	CLA	F	202	6	1/1/12/20	10/24/100/115	-
27	WVN	L	206	-	-	3/29/63/63	0/2/2/2
24	CLA	h	312	36	1/1/15/20	9/39/115/115	-
35	KC2	g	312	22	-	8/15/71/71	-
24	CLA	B	818	36	1/1/15/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	835	36	1/1/15/20	11/39/115/115	-
35	KC2	d	311	-	-	6/15/71/71	-
24	CLA	F	201	36	1/1/15/20	15/39/115/115	-
27	WVN	F	205	-	-	12/29/63/63	0/2/2/2
24	CLA	j	310	19	1/1/12/20	3/23/99/115	-
33	II0	h	310	-	-	7/21/67/67	0/2/2/2
26	LHG	i	615	24	-	11/41/41/53	-
27	WVN	h	308	-	-	5/29/63/63	0/2/2/2
24	CLA	B	815	-	1/1/13/20	7/27/103/115	-
33	II0	d	314	-	-	5/21/67/67	0/2/2/2
24	CLA	A	830	-	1/1/12/20	4/21/97/115	-
24	CLA	e	605	17	1/1/15/20	13/39/115/115	-
24	CLA	e	603	17	1/1/12/20	4/23/99/115	-
24	CLA	B	810	-	1/1/13/20	4/25/101/115	-
24	CLA	A	821	-	1/1/11/20	7/20/96/115	-
24	CLA	i	602	20	1/1/12/20	9/21/97/115	-
24	CLA	h	301	16	1/1/12/20	6/21/97/115	-
27	WVN	L	205	-	-	6/29/63/63	0/2/2/2
24	CLA	A	808	1	1/1/15/20	10/39/115/115	-
33	II0	j	318	-	-	5/21/67/67	0/2/2/2
24	CLA	L	203	-	1/1/15/20	12/39/115/115	-
26	LHG	B	802	-	-	16/42/42/53	-
24	CLA	A	801	-	1/1/15/20	10/39/115/115	-
32	LMG	F	206	-	-	11/43/63/70	0/1/1/1
24	CLA	d	303	21	1/1/15/20	13/39/115/115	-
24	CLA	g	311	26	1/1/12/20	10/26/102/115	-
35	KC2	f	611	19	-	7/15/71/71	-
27	WVN	B	849	-	-	12/29/63/63	0/2/2/2
24	CLA	a	306	14	1/1/11/20	8/15/91/115	-
24	CLA	B	821	-	1/1/12/20	6/25/101/115	-
24	CLA	h	304	-	1/1/12/20	6/23/99/115	-
24	CLA	A	831	-	1/1/15/20	11/39/115/115	-
26	LHG	f	619	24	-	22/41/41/53	-
24	CLA	A	818	-	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	i	604	20	1/1/15/20	12/39/115/115	-
24	CLA	B	841	26	-	3/39/115/115	-
33	II0	g	318	-	-	2/21/67/67	0/2/2/2
24	CLA	A	834	-	1/1/12/20	2/23/99/115	-
24	CLA	b	308	15	1/1/14/20	14/35/111/115	-
24	CLA	b	313	-	1/1/15/20	23/39/115/115	-
35	KC2	g	314	35	-	9/15/71/71	-
24	CLA	i	605	20	1/1/12/20	8/23/99/115	-
24	CLA	B	825	-	1/1/15/20	9/39/115/115	-
26	LHG	A	845	24	-	5/31/31/53	-
24	CLA	B	824	-	1/1/15/20	3/39/115/115	-
26	LHG	k	620	24	-	12/41/41/53	-
35	KC2	c	610	-	-	10/15/71/71	-
24	CLA	e	611	-	1/1/15/20	14/39/115/115	-
24	CLA	A	827	-	1/1/14/20	8/36/112/115	-
24	CLA	h	303	-	1/1/12/20	6/23/99/115	-
24	CLA	A	829	-	1/1/15/20	14/39/115/115	-
24	CLA	f	604	19	-	5/39/115/115	-
24	CLA	B	833	-	1/1/15/20	8/39/115/115	-
33	II0	c	613	-	-	3/21/67/67	0/2/2/2
27	WVN	B	848	-	-	7/29/63/63	0/2/2/2
24	CLA	O	201	-	1/1/15/20	14/39/115/115	-
30	DGD	B	843	-	-	5/49/89/95	0/2/2/2
31	LMU	B	844	-	-	8/21/61/61	0/2/2/2
24	CLA	A	839	1	1/1/15/20	12/39/115/115	-
33	II0	e	613	-	-	5/21/67/67	0/2/2/2
24	CLA	A	807	1	1/1/15/20	9/39/115/115	-
34	IHT	O	203	-	-	5/25/65/65	0/2/2/2
27	WVN	A	850	-	-	13/29/63/63	0/2/2/2
33	II0	c	614	-	-	1/21/67/67	0/2/2/2
24	CLA	A	840	-	1/1/15/20	16/39/115/115	-
24	CLA	c	609	26	1/1/11/20	4/15/91/115	-
28	LMT	b	319	-	-	9/15/35/61	0/1/1/2
24	CLA	A	836	-	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	j	309	19	1/1/11/20	5/15/91/115	-
33	II0	h	309	-	-	3/17/40/67	0/1/1/2
32	LMG	O	204	-	-	7/21/41/70	0/1/1/1
24	CLA	A	823	-	1/1/13/20	6/27/103/115	-
34	IHT	g	319	-	-	11/25/65/65	0/2/2/2
27	WVN	R	201	-	-	6/29/63/63	0/2/2/2
32	LMG	b	301	-	-	18/50/70/70	0/1/1/1
24	CLA	k	606	18	-	8/23/99/115	-
24	CLA	k	614	-	-	8/23/99/115	-
33	II0	a	315	-	-	3/21/67/67	0/2/2/2
24	CLA	g	309	22	1/1/15/20	6/39/115/115	-
33	II0	e	614	-	-	3/21/67/67	0/2/2/2
24	CLA	A	805	1	1/1/15/20	7/39/115/115	-
27	WVN	B	846	-	-	0/29/63/63	0/2/2/2
24	CLA	A	802	-	1/1/15/20	16/39/115/115	-
24	CLA	k	607	-	1/1/12/20	9/23/99/115	-
24	CLA	A	837	-	1/1/15/20	9/39/115/115	-
24	CLA	b	307	36	1/1/15/20	10/39/115/115	-
34	IHT	b	317	-	-	7/25/65/65	0/2/2/2
24	CLA	b	312	15	1/1/15/20	21/39/115/115	-
24	CLA	A	803	-	1/1/13/20	6/27/103/115	-
24	CLA	b	305	-	1/1/15/20	13/39/115/115	-
27	WVN	L	201	-	-	10/29/63/63	0/2/2/2
33	II0	b	314	-	-	7/21/67/67	0/2/2/2
24	CLA	d	305	-	-	6/23/99/115	-
26	LHG	b	302	24	-	12/53/53/53	-
24	CLA	B	820	-	-	9/27/103/115	-
34	IHT	R	204	-	-	3/25/65/65	0/2/2/2
24	CLA	k	609	18	1/1/15/20	12/39/115/115	-
34	IHT	a	316	-	-	9/25/65/65	0/2/2/2
24	CLA	B	826	-	1/1/15/20	7/39/115/115	-
24	CLA	i	607	20	1/1/12/20	1/23/99/115	-
24	CLA	B	814	-	1/1/13/20	12/32/108/115	-
24	CLA	A	835	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	822	36	1/1/15/20	10/39/115/115	-
24	CLA	B	806	-	1/1/15/20	14/39/115/115	-
27	WVN	A	847	-	-	11/29/63/63	0/2/2/2
24	CLA	a	312	-	1/1/11/20	5/19/95/115	-

The worst 5 of 3377 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	317	IHT	C15-C11	25.56	1.63	1.35
34	R	204	IHT	C15-C11	25.44	1.63	1.35
34	c	615	IHT	C15-C11	25.28	1.63	1.35
34	k	618	IHT	C15-C11	25.23	1.63	1.35
34	j	317	IHT	C15-C11	25.14	1.62	1.35

The worst 5 of 3510 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	f	617	IHT	C40-C37-C33	-13.79	107.93	127.28
34	b	317	IHT	C40-C37-C33	-12.64	109.55	127.28
35	f	611	KC2	C1A-NA-C4A	-12.27	101.08	106.68
34	f	617	IHT	C30-C27-C23	-11.91	110.57	127.28
35	k	613	KC2	C1A-NA-C4A	-11.62	101.38	106.68

5 of 197 chirality outliers are listed below:

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

5 of 2874 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 404 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	a	303	CLA	1	0
24	c	607	CLA	2	0
24	B	837	CLA	4	0
24	b	303	CLA	1	0
24	B	817	CLA	2	0
24	g	303	CLA	2	0
24	B	807	CLA	2	0
24	b	304	CLA	2	0
24	h	305	CLA	1	0
24	g	304	CLA	1	0
24	h	307	CLA	1	0
24	B	811	CLA	1	0
32	J	106	LMG	6	0
24	j	311	CLA	2	0
24	c	601	CLA	1	0
24	B	830	CLA	2	0
29	A	854	SF4	4	0
28	a	318	LMT	2	0
24	e	610	CLA	3	0
24	f	613	CLA	1	0
26	A	844	LHG	1	0
24	j	308	CLA	1	0
24	k	603	CLA	3	0
24	A	853	CLA	4	0
24	c	606	CLA	5	0
24	J	105	CLA	3	0
24	k	601	CLA	3	0
26	J	107	LHG	8	0
24	g	322	CLA	2	0
24	B	827	CLA	3	0
26	e	617	LHG	2	0
24	B	804	CLA	3	0
24	A	814	CLA	3	0
24	h	302	CLA	1	0
24	A	856	CLA	5	0
24	A	813	CLA	2	0
24	b	306	CLA	2	0
24	e	604	CLA	1	0
24	B	803	CLA	2	0
24	c	602	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	829	CLA	2	0
33	a	314	II0	1	0
24	e	601	CLA	1	0
24	A	812	CLA	1	0
24	B	816	CLA	2	0
24	c	612	CLA	2	0
24	O	205	CLA	6	0
24	A	819	CLA	1	0
24	f	609	CLA	2	0
24	A	855	CLA	6	0
25	B	842	PQN	5	0
24	d	304	CLA	1	0
24	A	820	CLA	3	0
24	i	610	CLA	1	0
24	L	207	CLA	1	0
24	A	828	CLA	2	0
24	j	313	CLA	1	0
24	B	808	CLA	1	0
24	B	801	CLA	6	0
24	A	822	CLA	2	0
24	k	604	CLA	1	0
24	e	606	CLA	4	0
24	A	806	CLA	5	0
35	e	609	KC2	2	0
24	f	610	CLA	4	0
28	A	851	LMT	1	0
24	e	607	CLA	3	0
24	B	823	CLA	5	0
24	g	307	CLA	1	0
34	k	618	IHT	2	0
24	c	611	CLA	1	0
24	i	606	CLA	1	0
24	A	852	CLA	1	0
24	c	603	CLA	1	0
24	A	811	CLA	2	0
24	f	602	CLA	4	0
24	f	601	CLA	2	0
24	d	306	CLA	1	0
24	g	308	CLA	5	0
24	k	608	CLA	3	0
24	A	815	CLA	2	0
32	L	208	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	809	CLA	2	0
24	a	308	CLA	2	0
34	j	317	IHT	1	0
24	i	611	CLA	1	0
24	a	307	CLA	3	0
29	C	101	SF4	3	0
24	c	605	CLA	1	0
24	e	602	CLA	1	0
29	C	102	SF4	2	0
33	k	615	II0	1	0
24	K	101	CLA	1	0
24	j	306	CLA	2	0
24	A	841	CLA	3	0
24	L	202	CLA	2	0
24	a	302	CLA	1	0
24	e	608	CLA	1	0
24	f	603	CLA	1	0
24	A	824	CLA	1	0
35	g	313	KC2	1	0
24	d	301	CLA	1	0
24	A	804	CLA	3	0
24	B	831	CLA	1	0
24	A	817	CLA	4	0
24	j	302	CLA	1	0
24	B	834	CLA	1	0
26	b	320	LHG	5	0
24	A	842	CLA	6	0
33	b	315	II0	1	0
24	I	102	CLA	2	0
26	f	620	LHG	3	0
24	B	819	CLA	1	0
24	f	608	CLA	4	0
24	b	310	CLA	3	0
26	c	618	LHG	1	0
24	c	608	CLA	2	0
24	g	310	CLA	1	0
24	b	309	CLA	2	0
24	B	839	CLA	2	0
24	i	601	CLA	1	0
24	f	606	CLA	2	0
24	B	805	CLA	1	0
24	B	812	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	832	CLA	2	0
24	k	602	CLA	3	0
24	A	838	CLA	1	0
24	B	840	CLA	1	0
26	g	301	LHG	1	0
24	k	610	CLA	2	0
24	a	310	CLA	2	0
24	a	311	CLA	4	0
24	f	607	CLA	3	0
25	A	843	PQN	2	0
24	B	836	CLA	4	0
33	k	616	II0	1	0
24	B	828	CLA	3	0
24	F	202	CLA	2	0
35	g	312	KC2	1	0
24	B	835	CLA	3	0
35	d	311	KC2	1	0
24	F	201	CLA	7	0
24	B	815	CLA	1	0
24	A	830	CLA	1	0
24	e	605	CLA	3	0
24	B	810	CLA	2	0
24	A	821	CLA	1	0
24	i	602	CLA	1	0
24	L	203	CLA	4	0
26	B	802	LHG	3	0
24	A	801	CLA	2	0
32	F	206	LMG	2	0
24	d	303	CLA	2	0
24	B	821	CLA	1	0
24	A	831	CLA	1	0
26	f	619	LHG	3	0
24	A	818	CLA	3	0
24	B	841	CLA	4	0
24	b	308	CLA	6	0
24	b	313	CLA	6	0
24	i	605	CLA	1	0
24	B	825	CLA	2	0
24	B	824	CLA	1	0
24	e	611	CLA	3	0
24	A	827	CLA	4	0
24	A	829	CLA	3	0

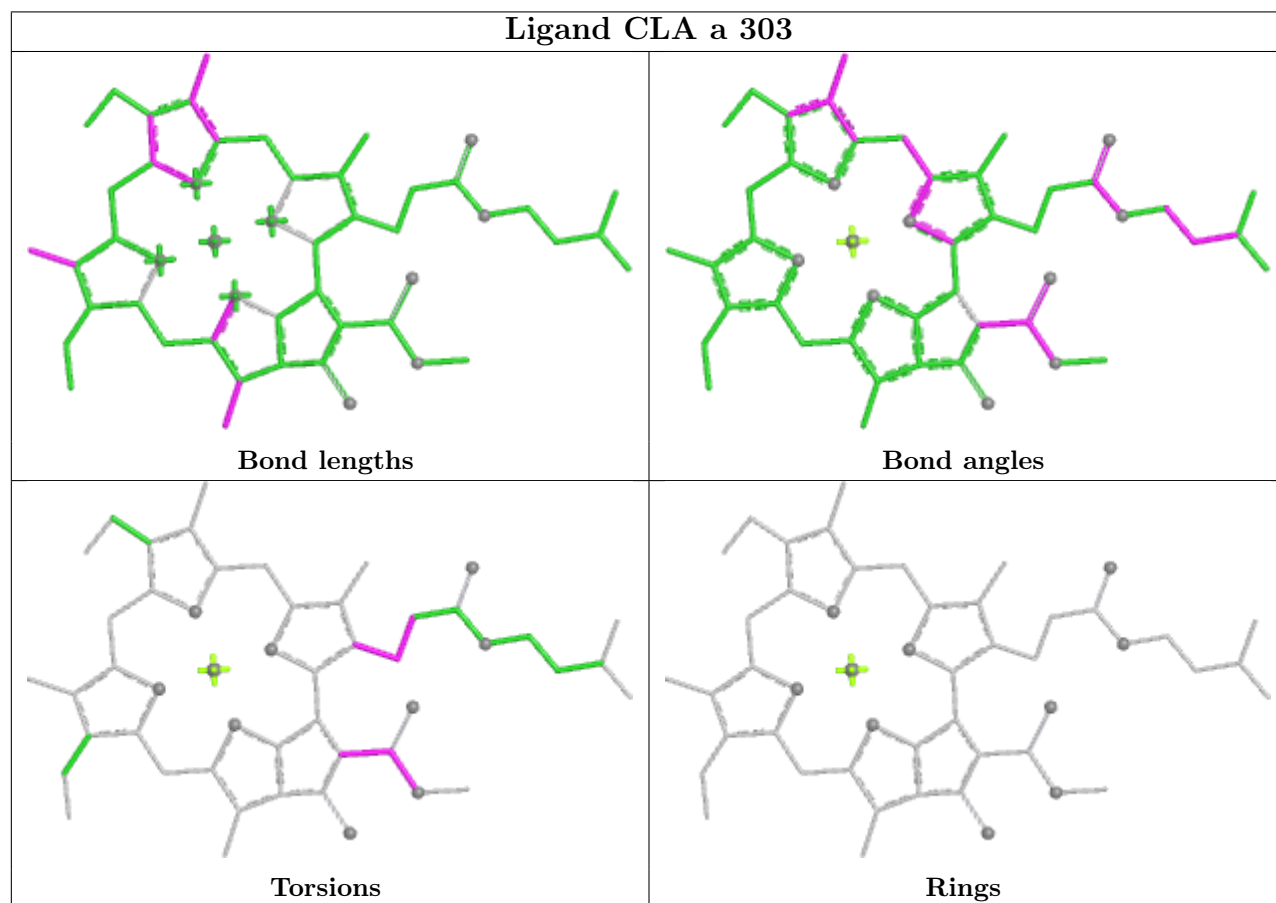
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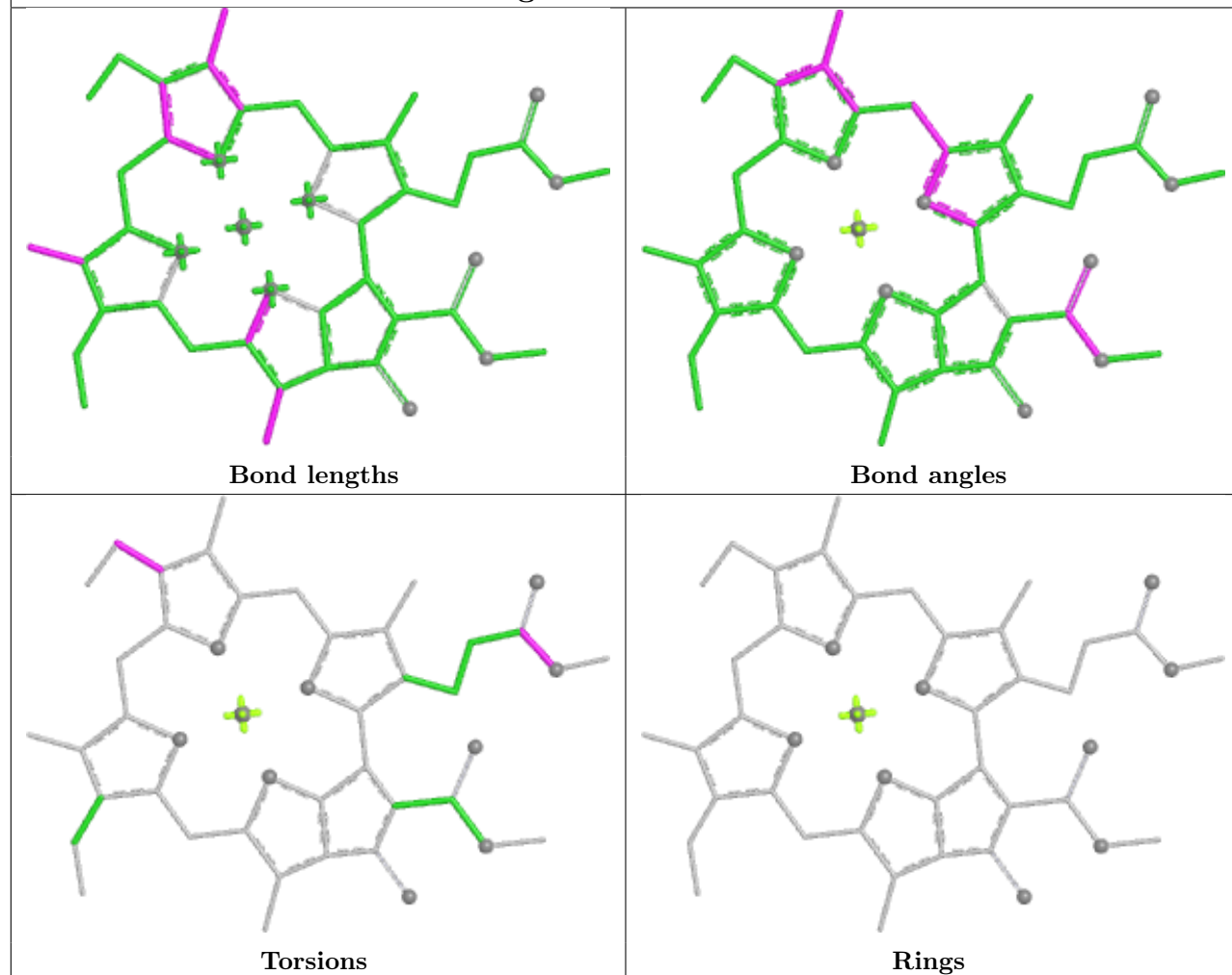
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	f	604	CLA	1	0
24	B	833	CLA	3	0
24	O	201	CLA	3	0
30	B	843	DGD	3	0
31	B	844	LMU	1	0
24	A	839	CLA	4	0
24	A	807	CLA	1	0
24	A	840	CLA	5	0
28	b	319	LMT	2	0
24	A	836	CLA	3	0
24	j	309	CLA	2	0
24	A	823	CLA	2	0
34	g	319	IHT	1	0
32	b	301	LMG	6	0
24	k	614	CLA	1	0
24	g	309	CLA	4	0
24	A	805	CLA	1	0
24	A	802	CLA	6	0
24	k	607	CLA	2	0
24	A	837	CLA	2	0
24	b	307	CLA	3	0
24	b	312	CLA	6	0
24	A	803	CLA	3	0
24	b	305	CLA	3	0
24	d	305	CLA	1	0
26	b	302	LHG	2	0
24	B	820	CLA	4	0
24	k	609	CLA	2	0
24	B	826	CLA	1	0
24	i	607	CLA	1	0
24	B	814	CLA	1	0
24	A	835	CLA	2	0
24	B	822	CLA	4	0
24	B	806	CLA	2	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

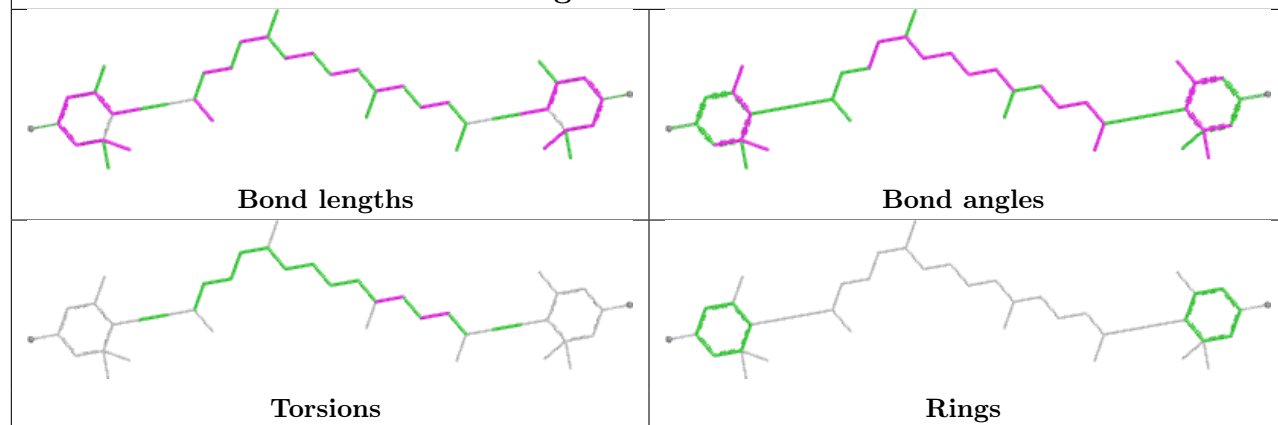
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

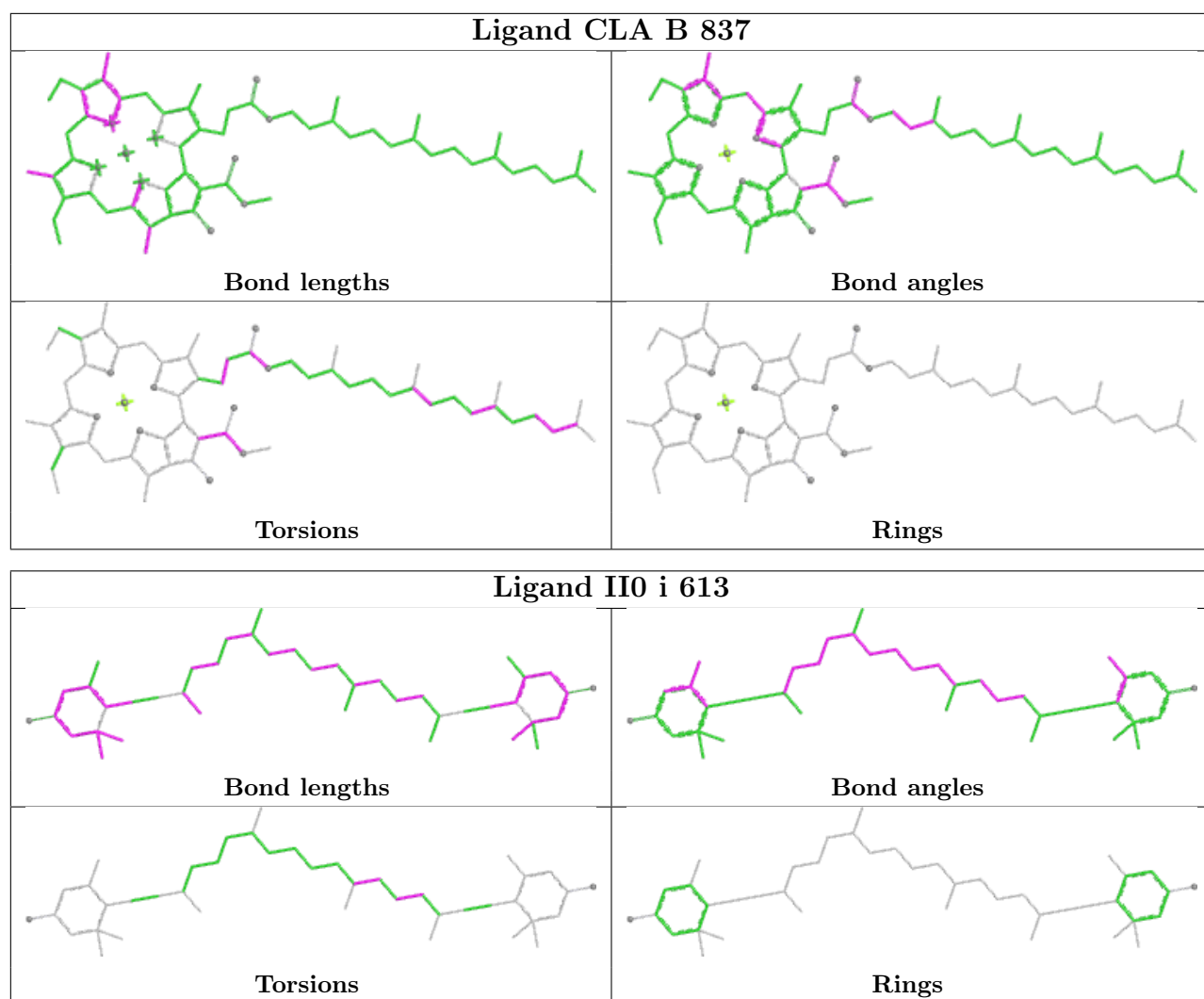


Ligand CLA c 607

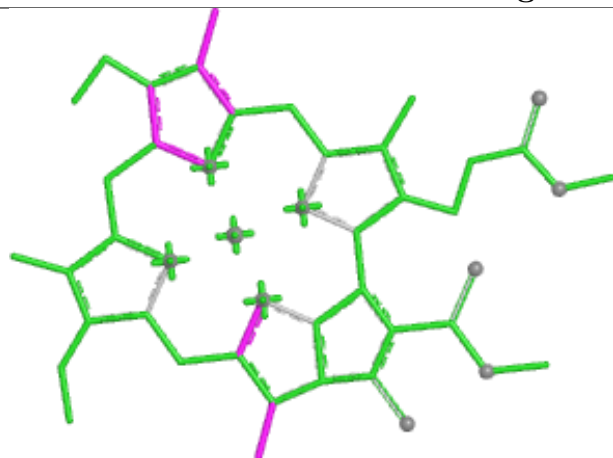


Ligand II0 f 614

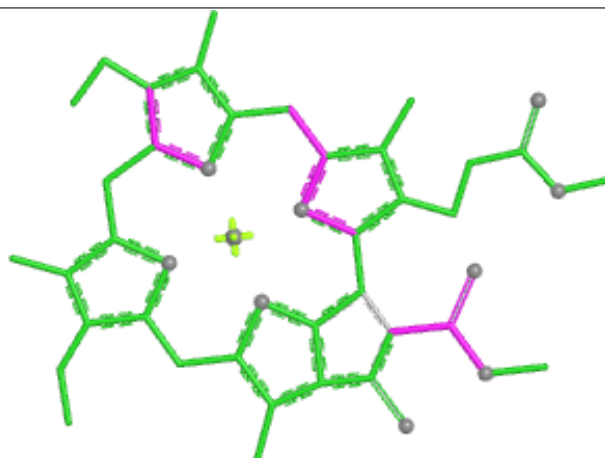




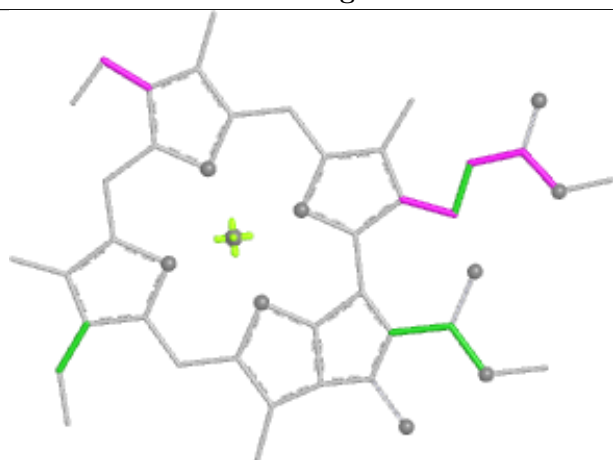
Ligand CLA d 307



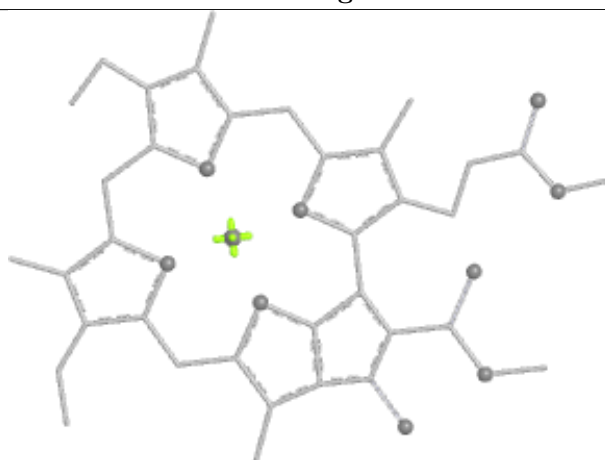
Bond lengths



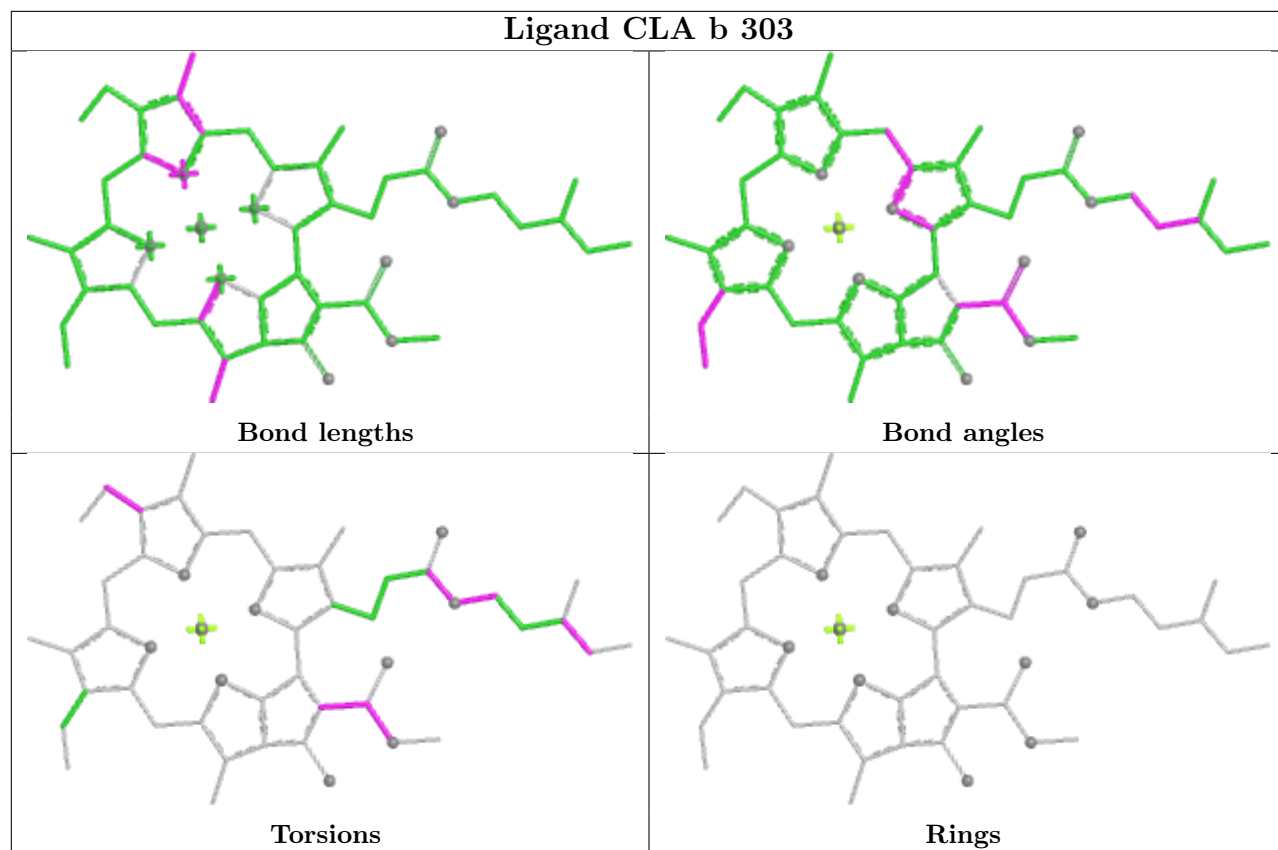
Bond angles



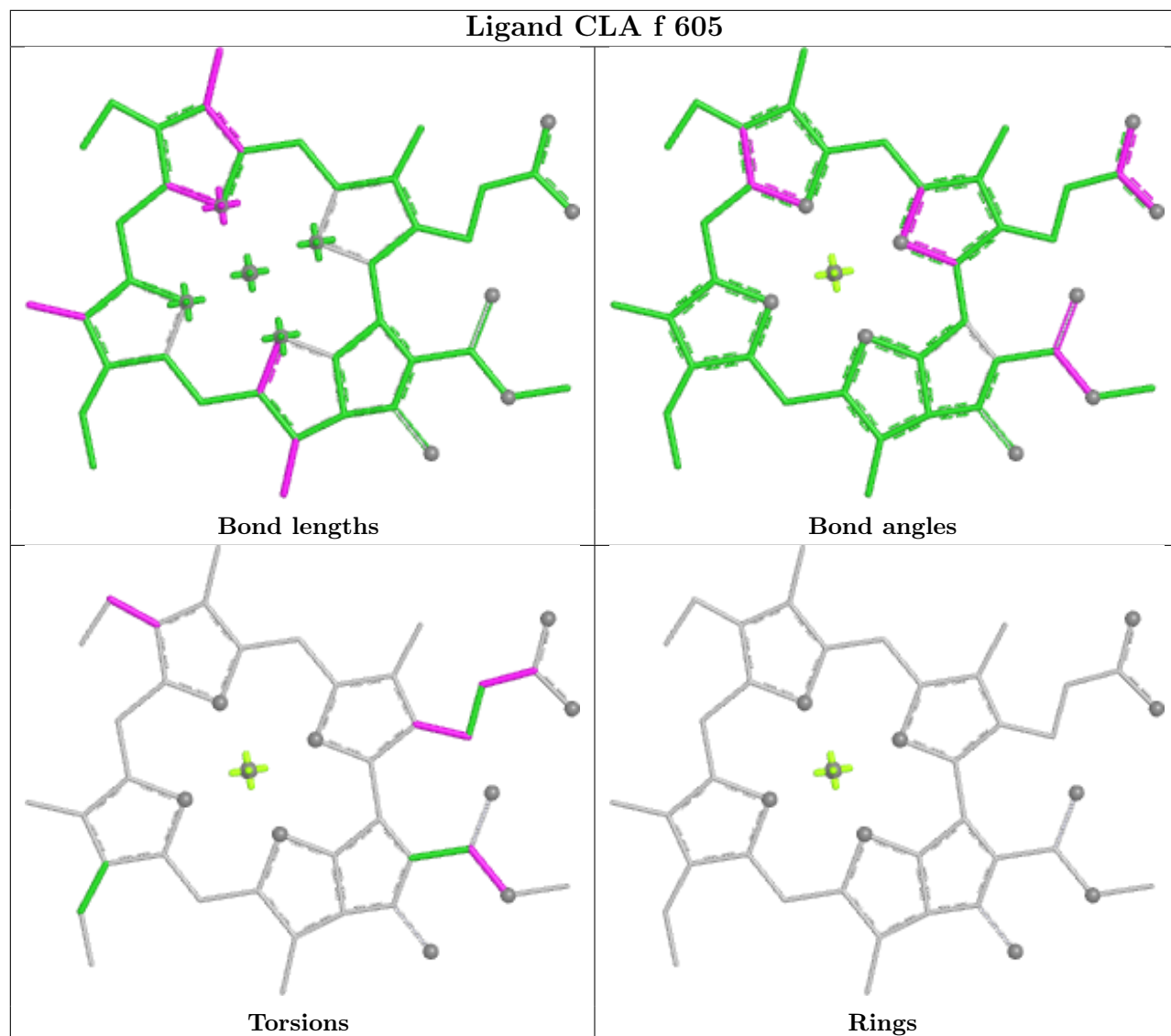
Torsions



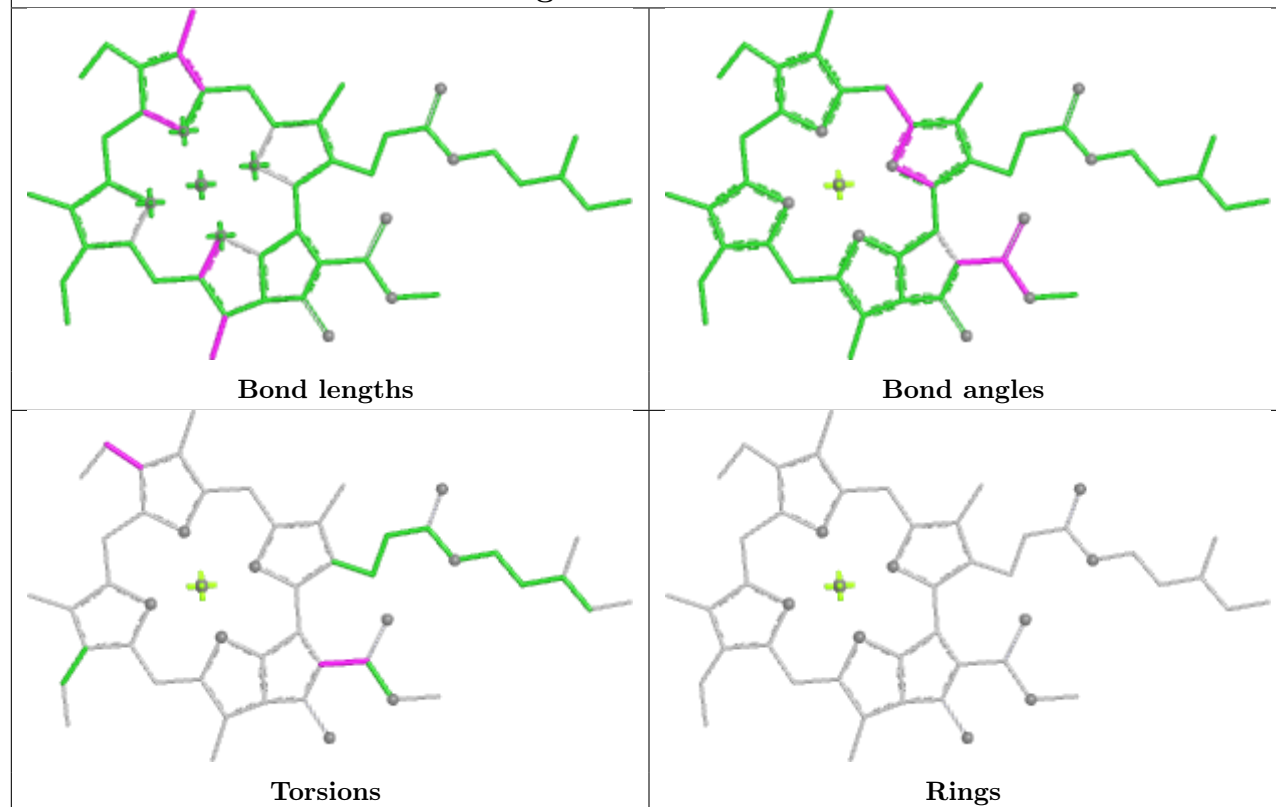
Rings



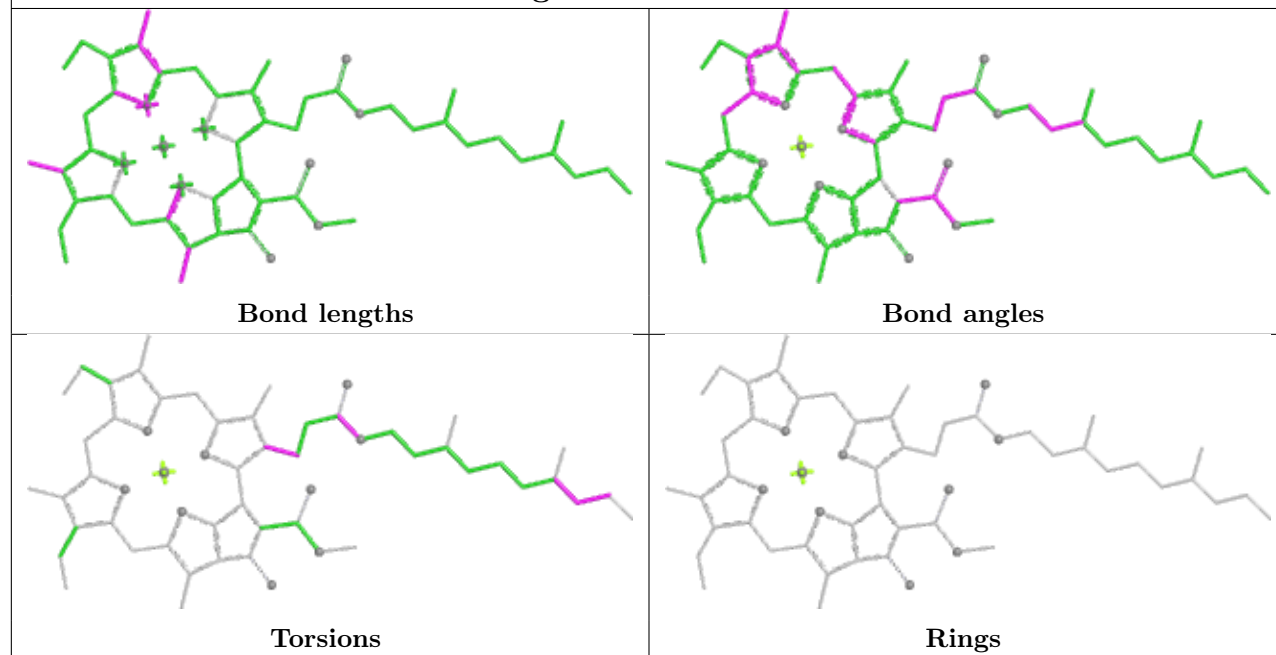
Ligand CLA f 605

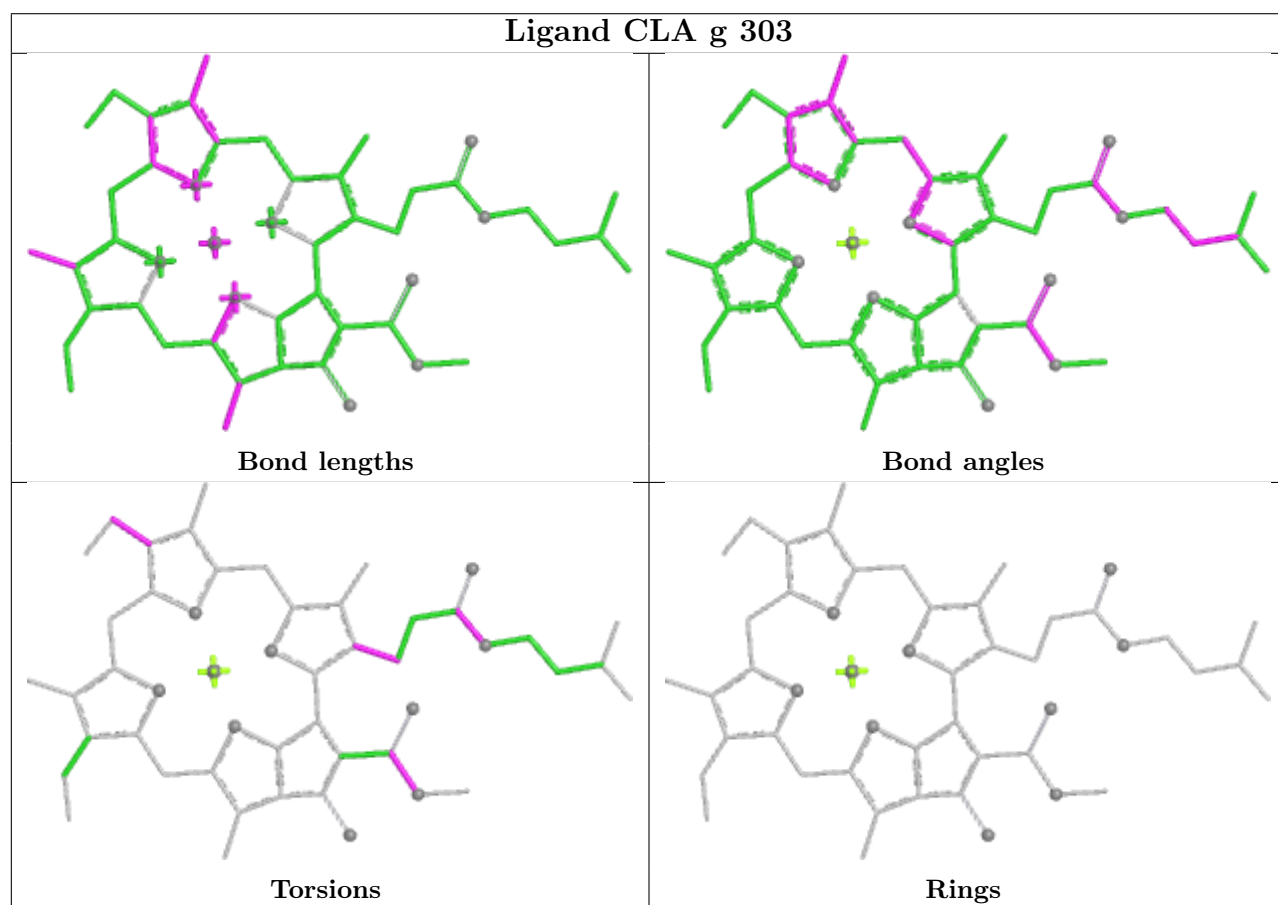
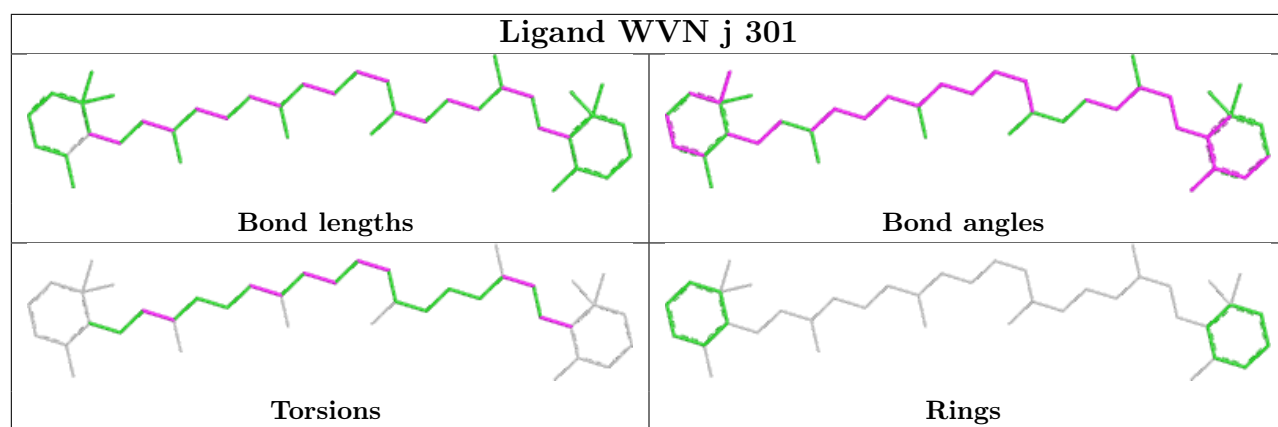


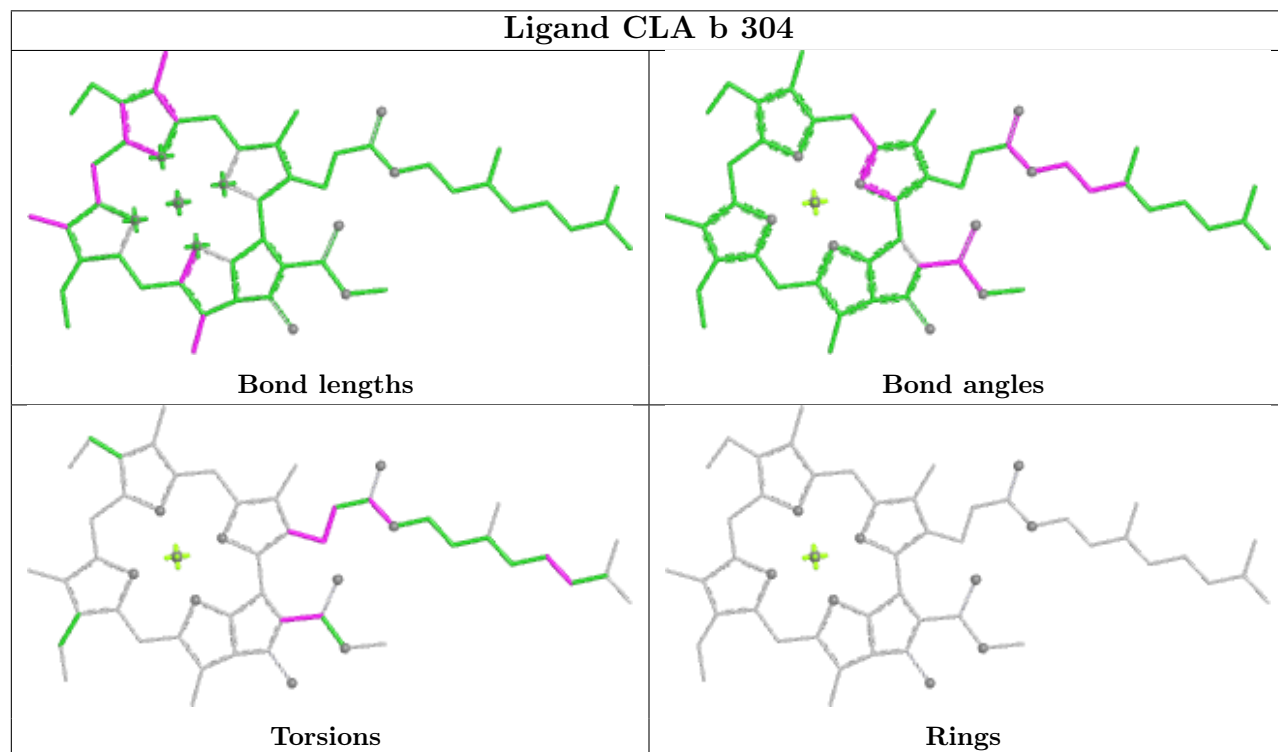
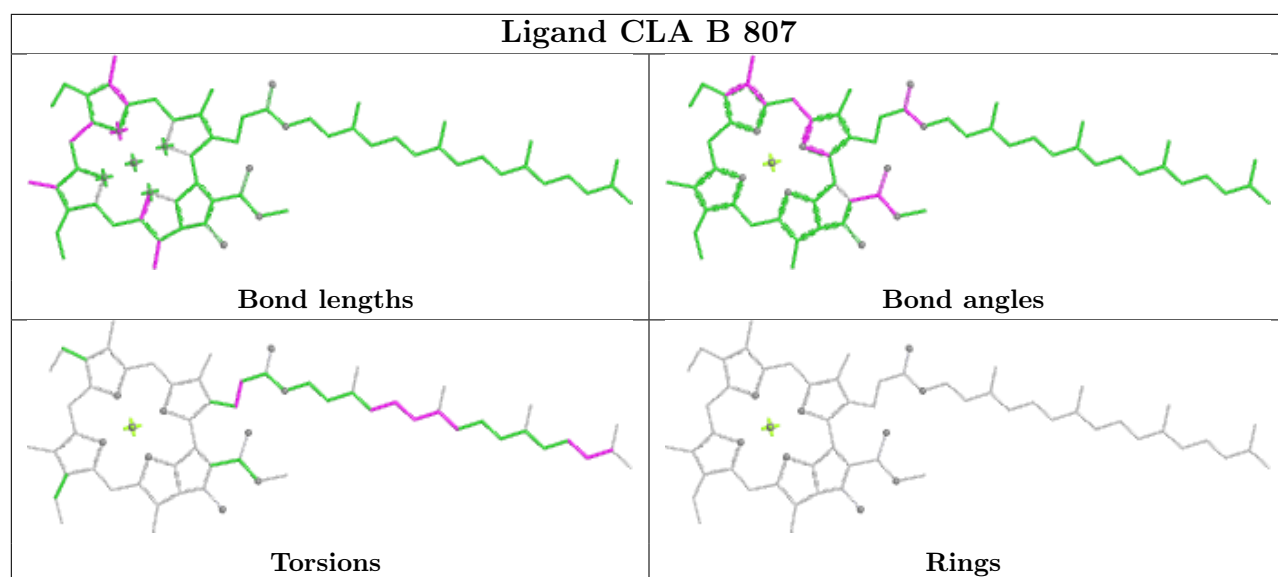
Ligand CLA a 304

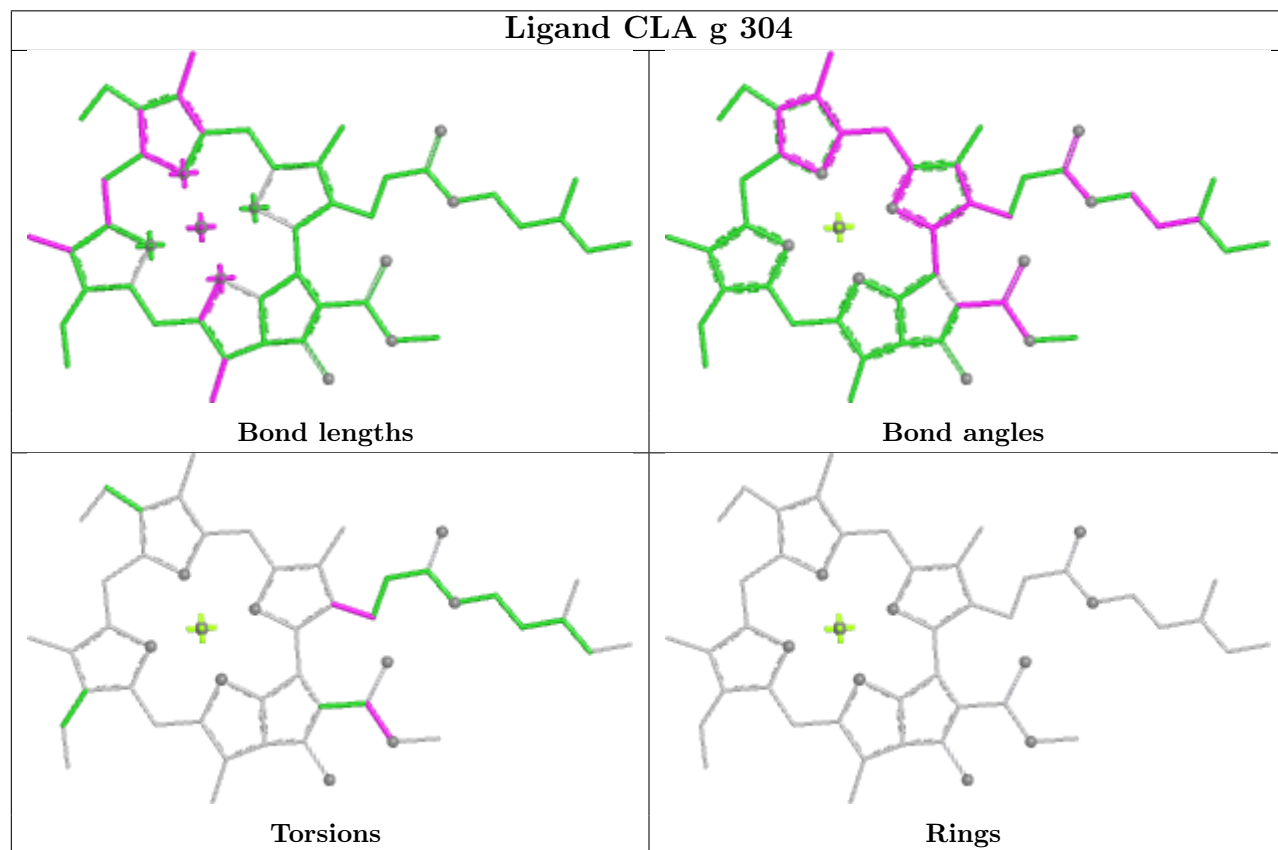
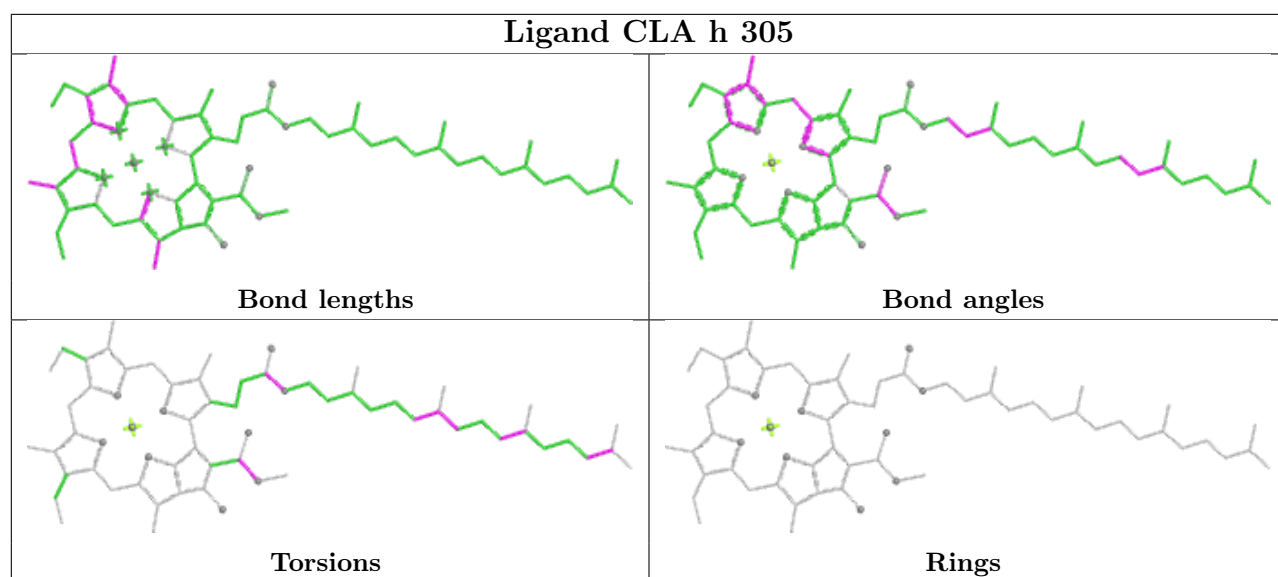


Ligand CLA B 817

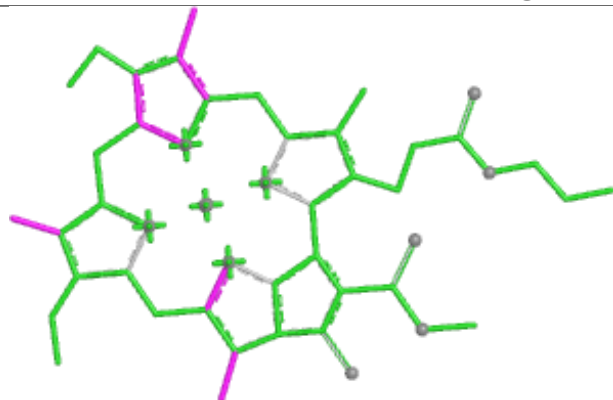




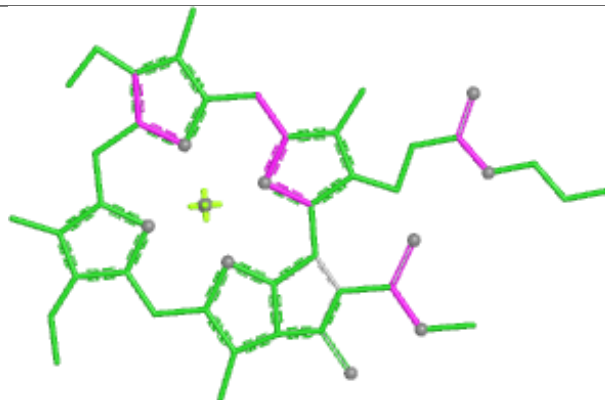




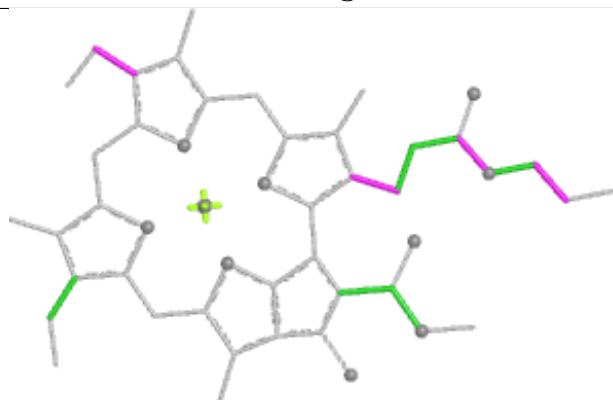
Ligand CLA a 309



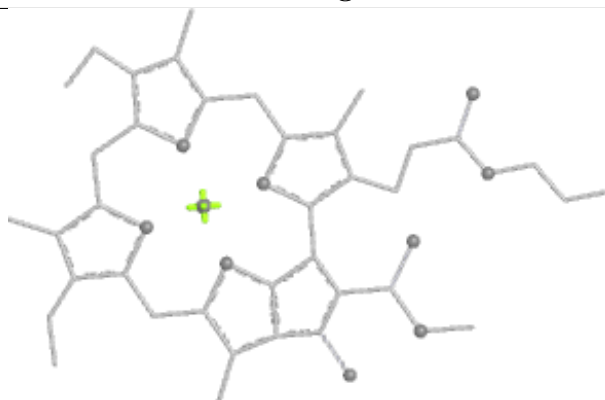
Bond lengths



Bond angles

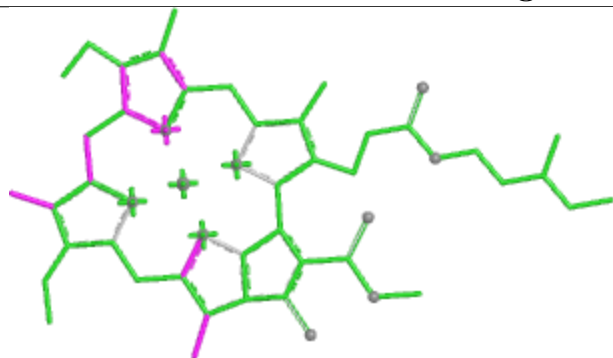


Torsions

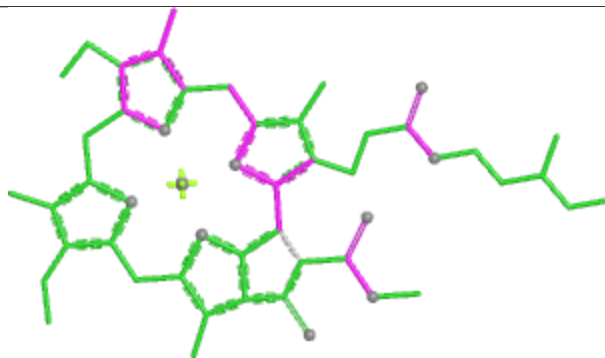


Rings

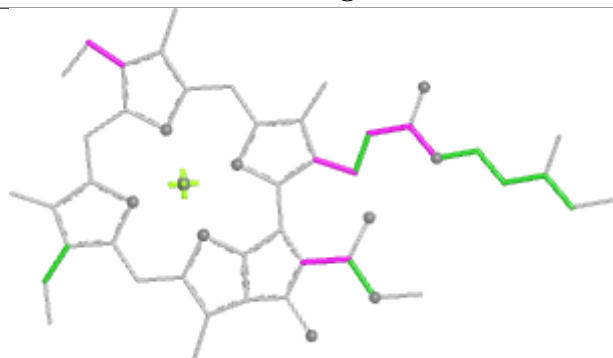
Ligand CLA h 307



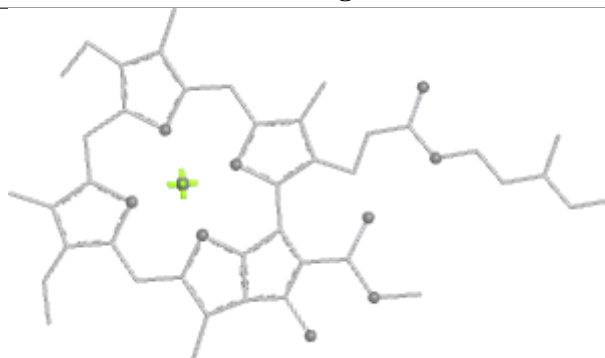
Bond lengths



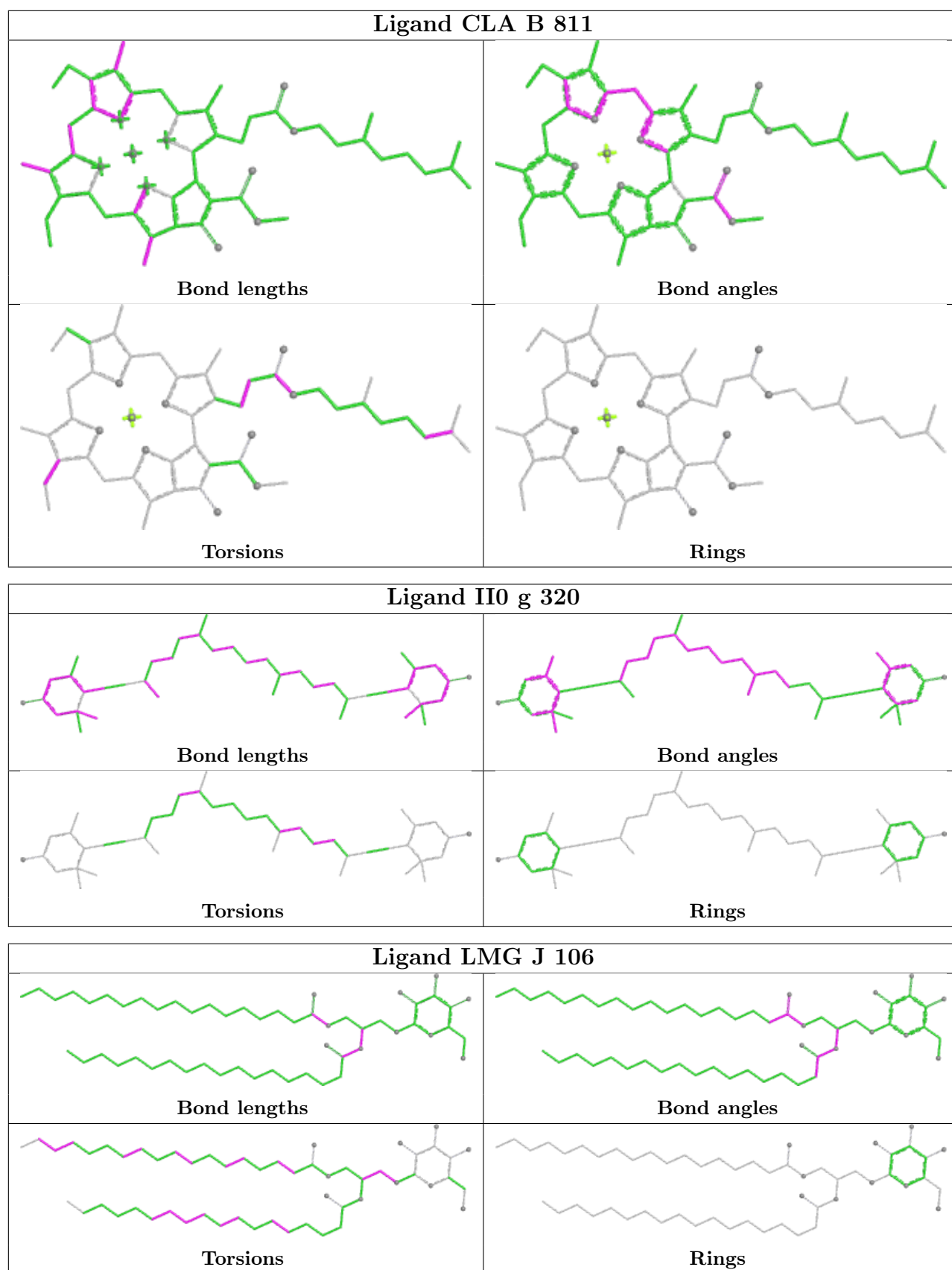
Bond angles

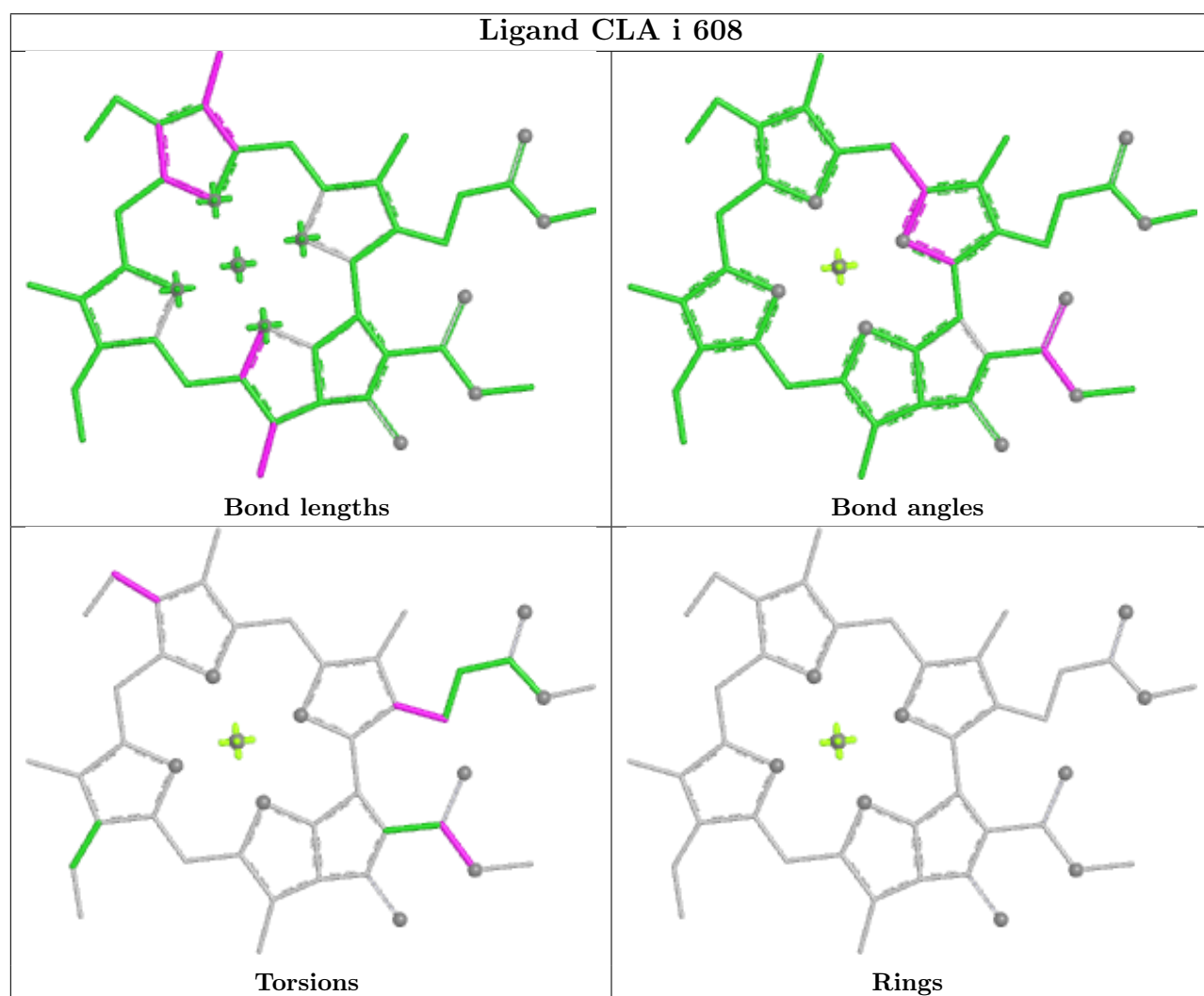
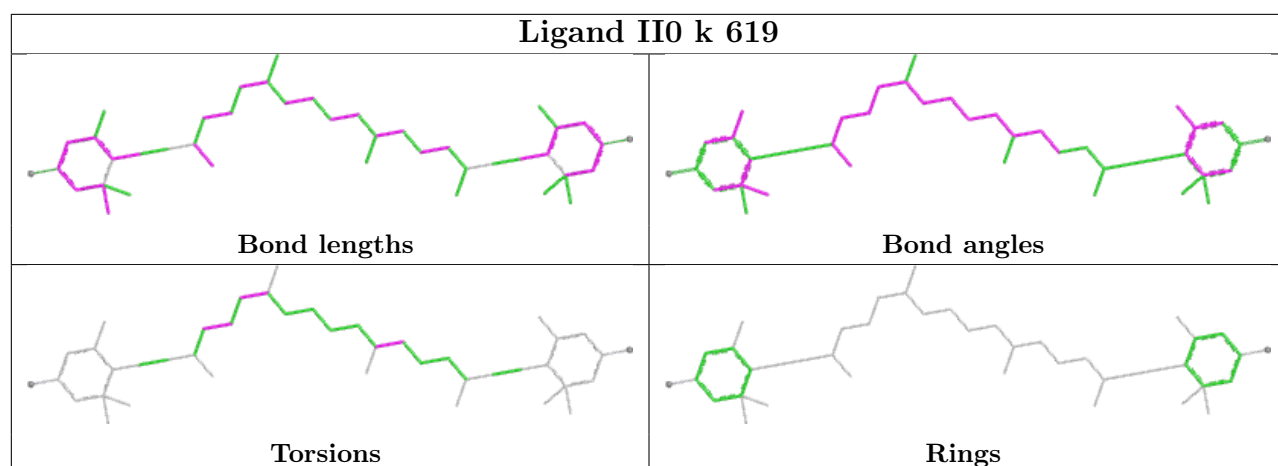


Torsions

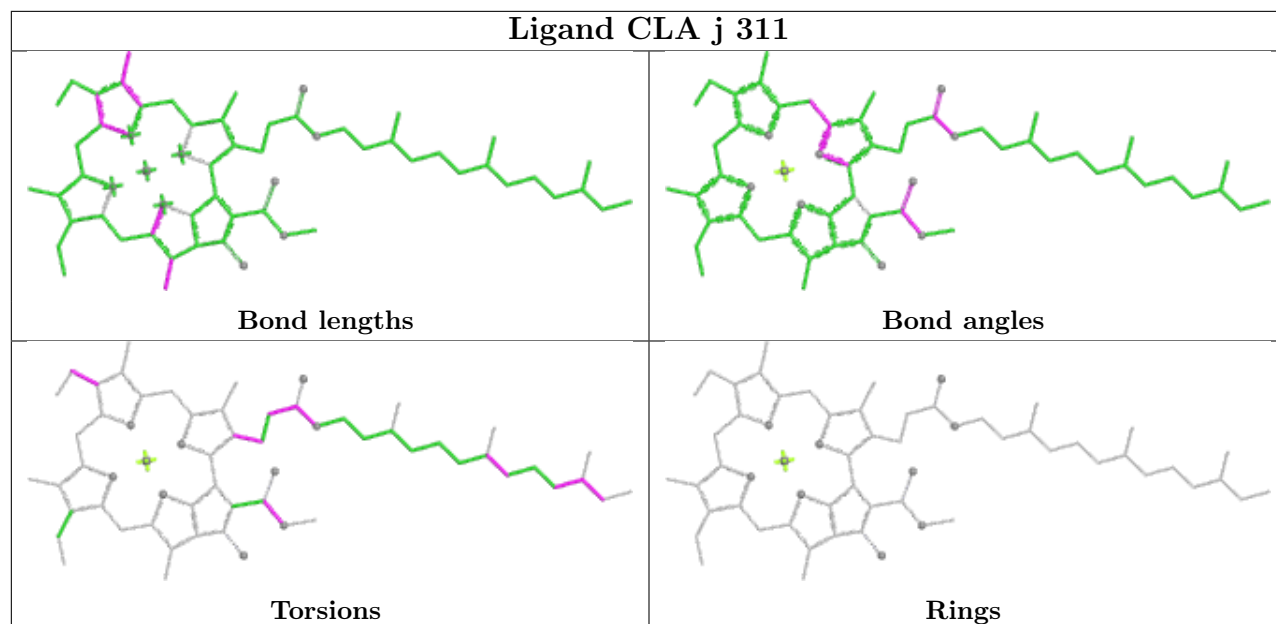


Rings

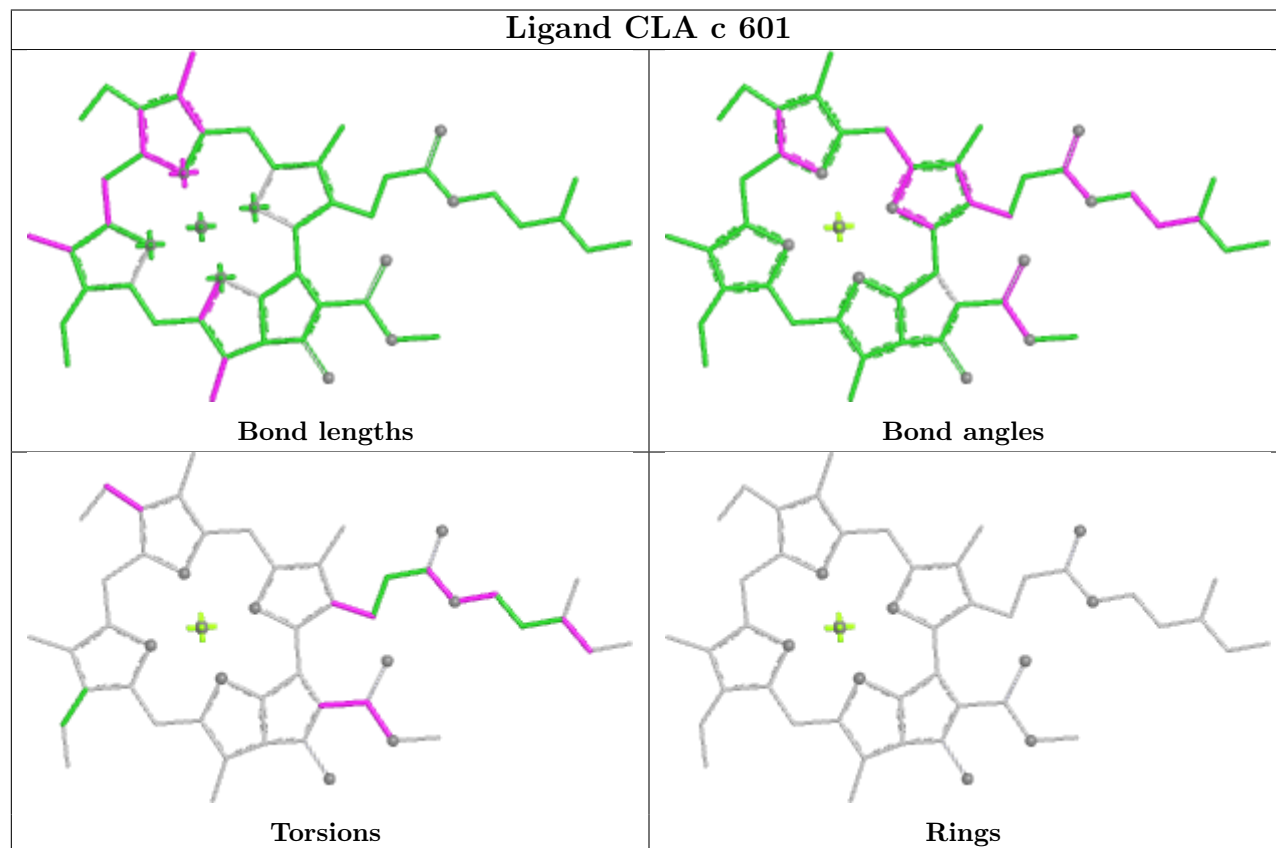


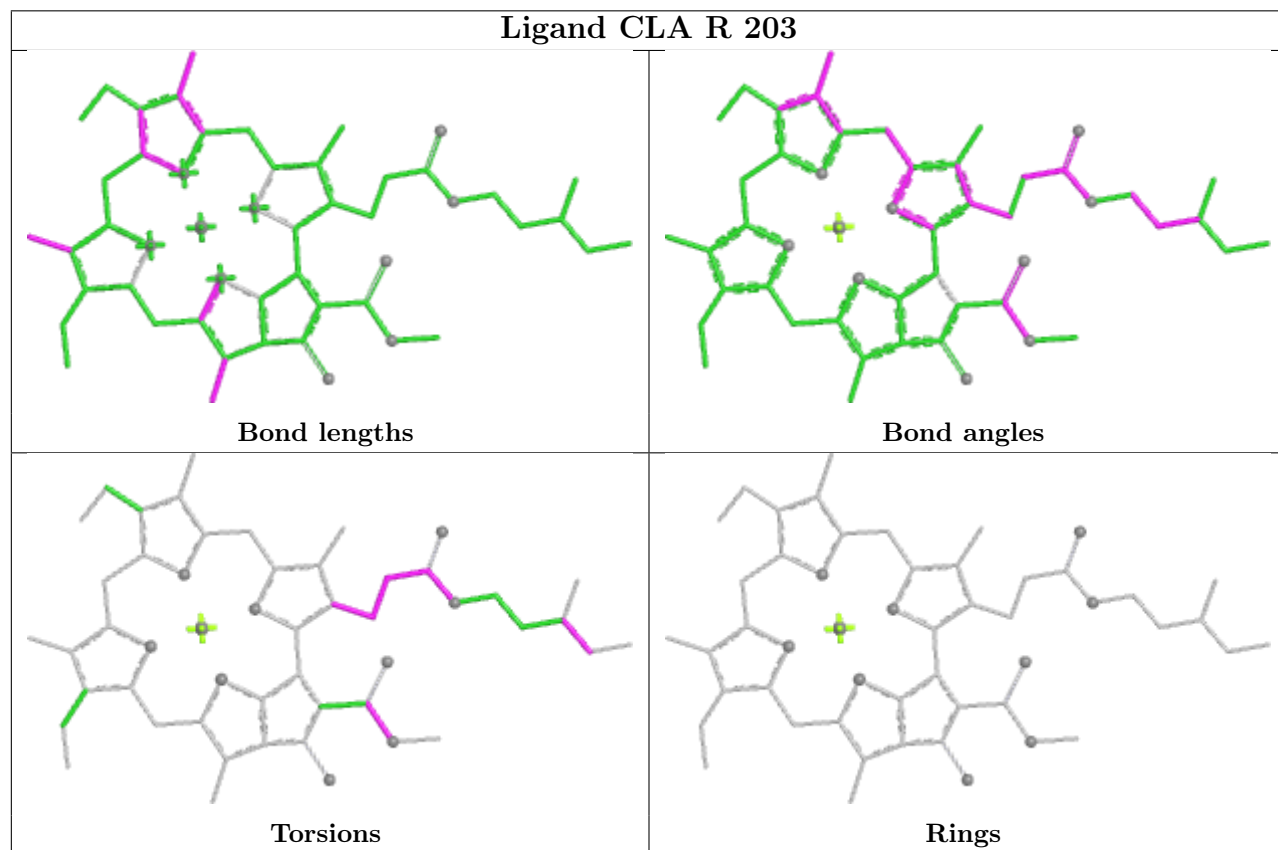
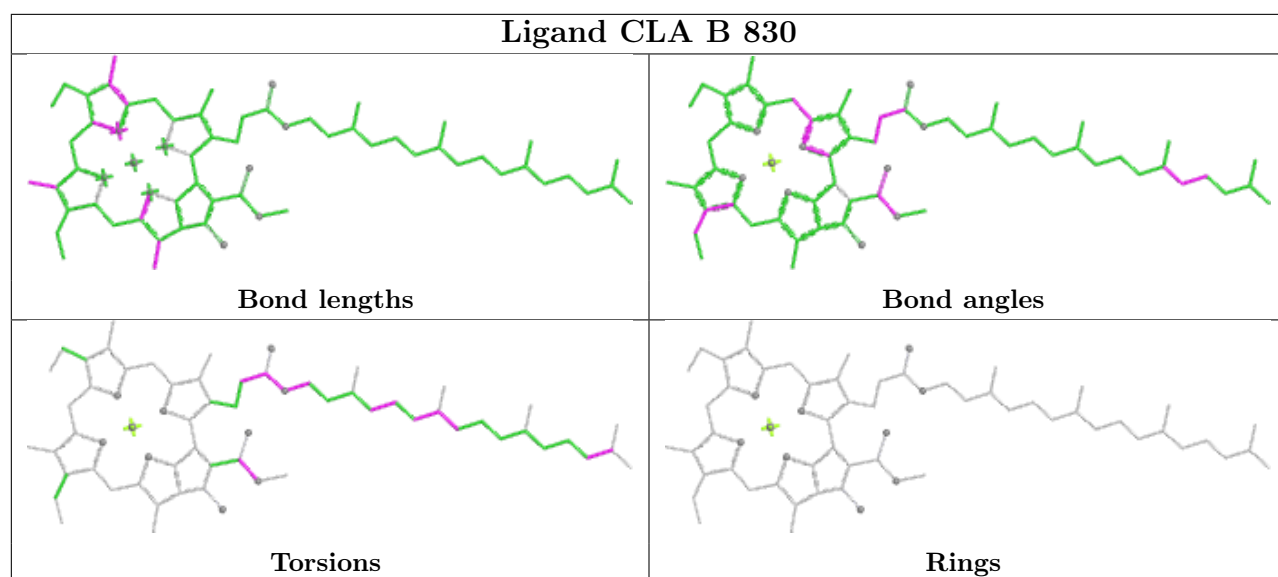


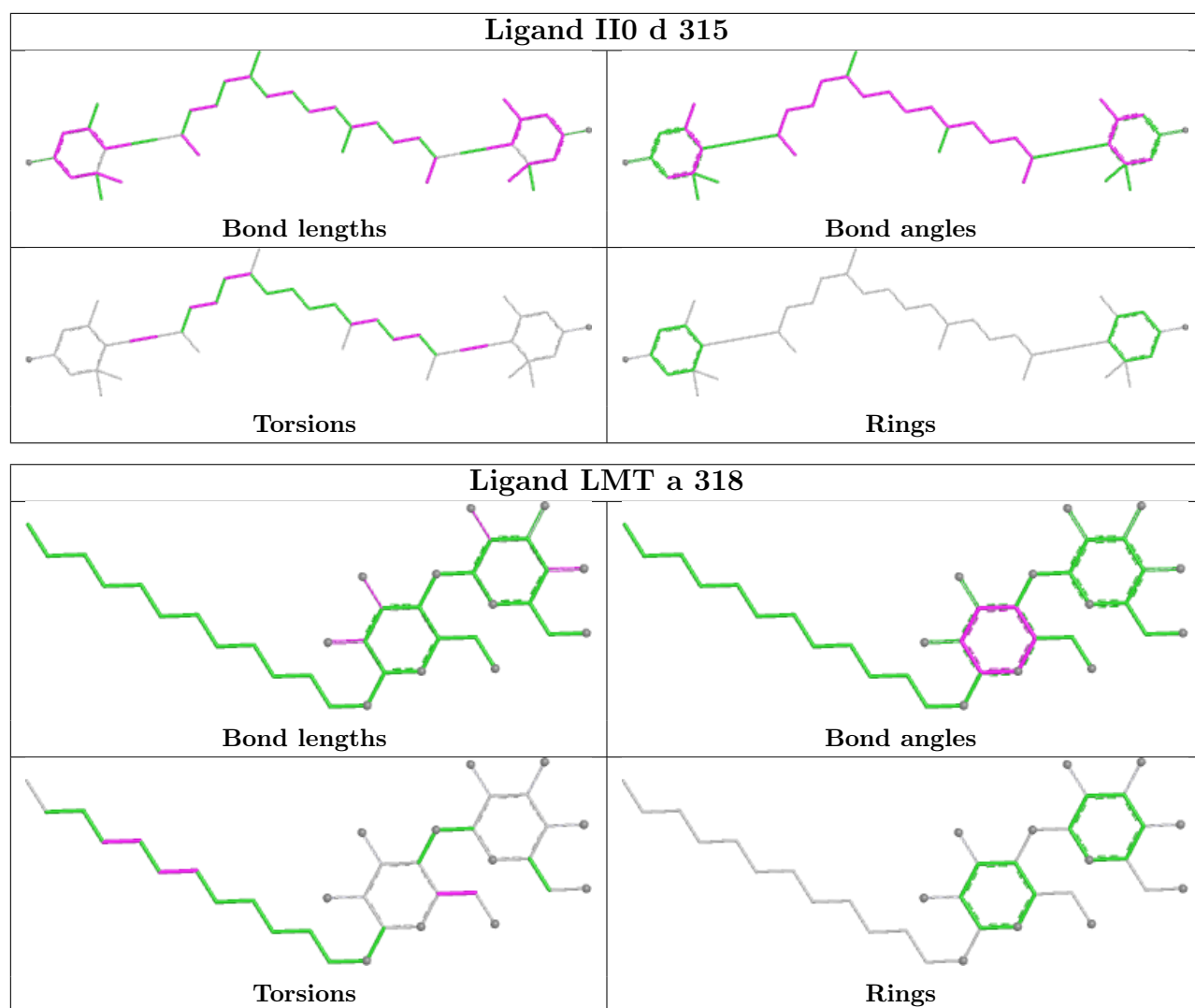
Ligand CLA j 311



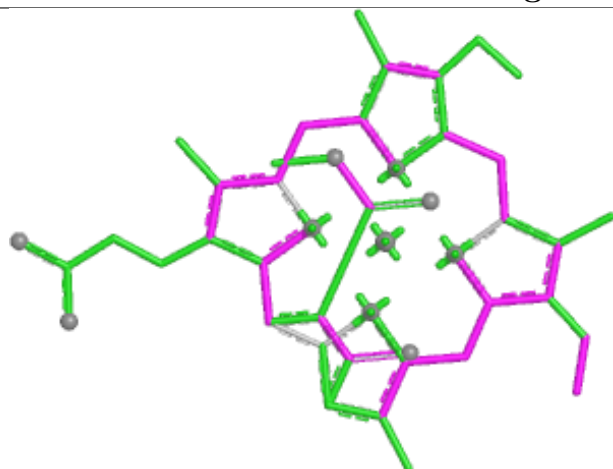
Ligand CLA c 601



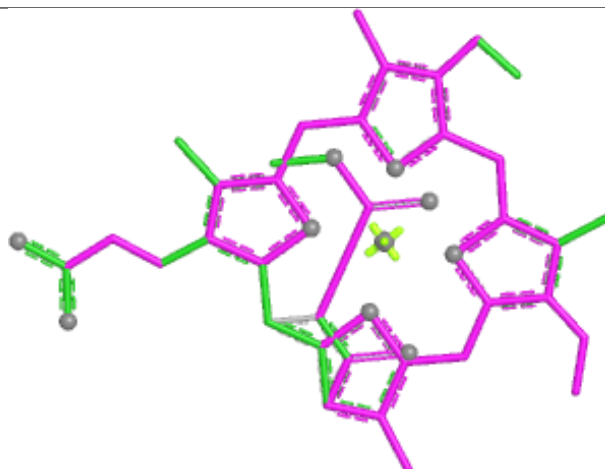




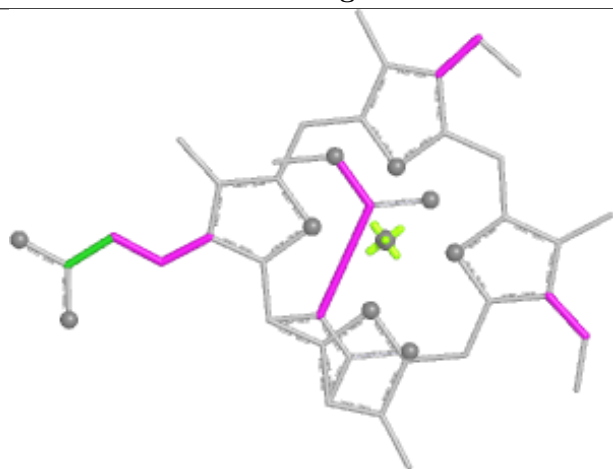
Ligand KC2 i 616



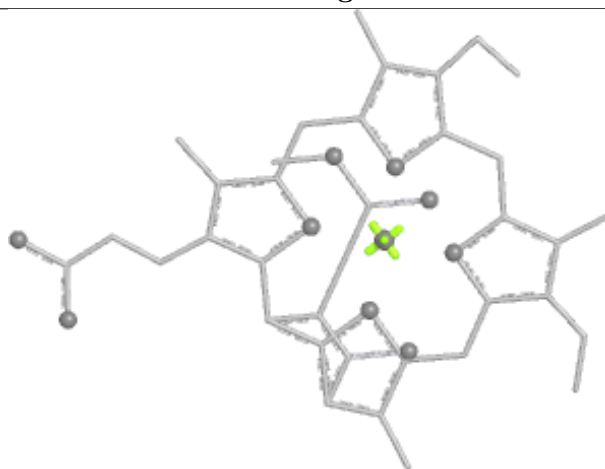
Bond lengths



Bond angles

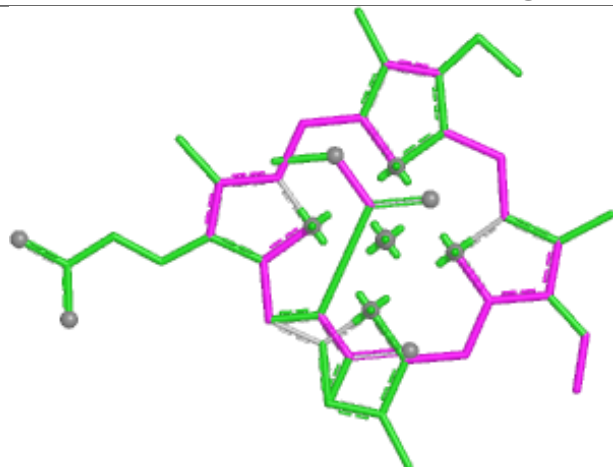


Torsions

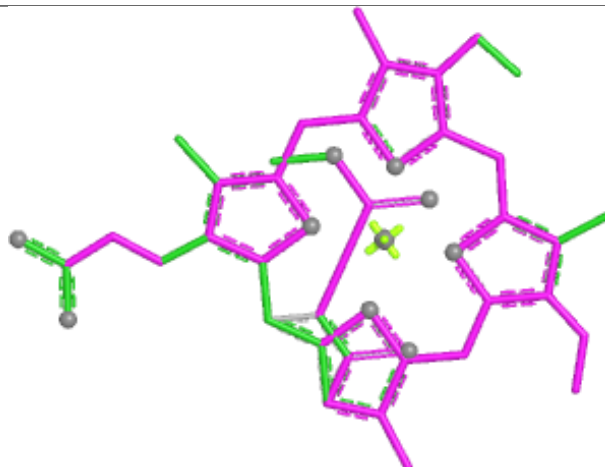


Rings

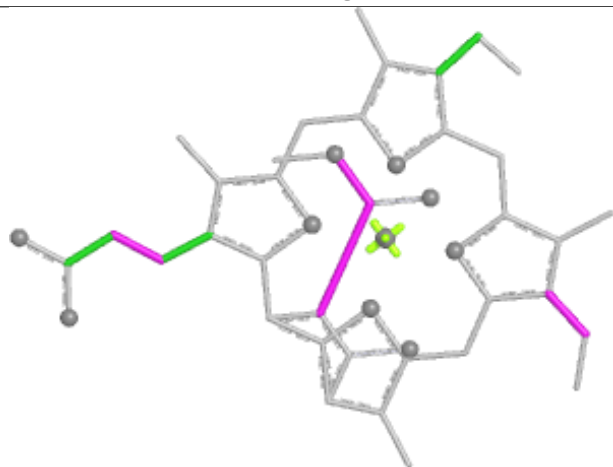
Ligand KC2 k 611



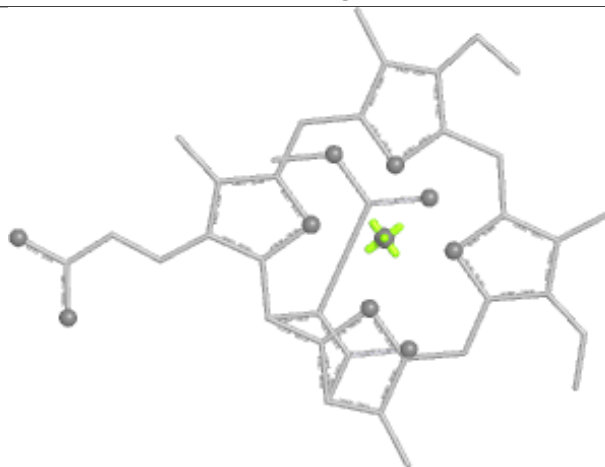
Bond lengths



Bond angles

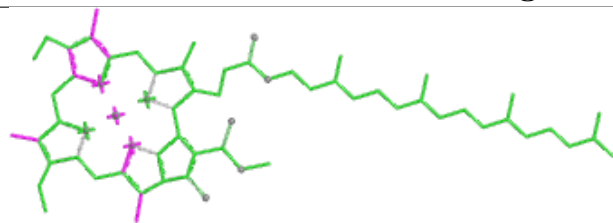


Torsions

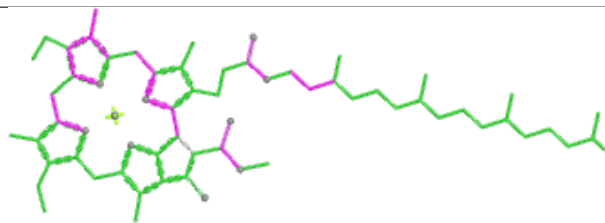


Rings

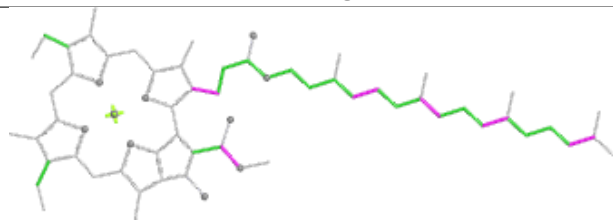
Ligand CLA e 610



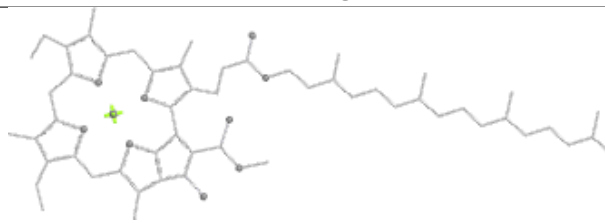
Bond lengths



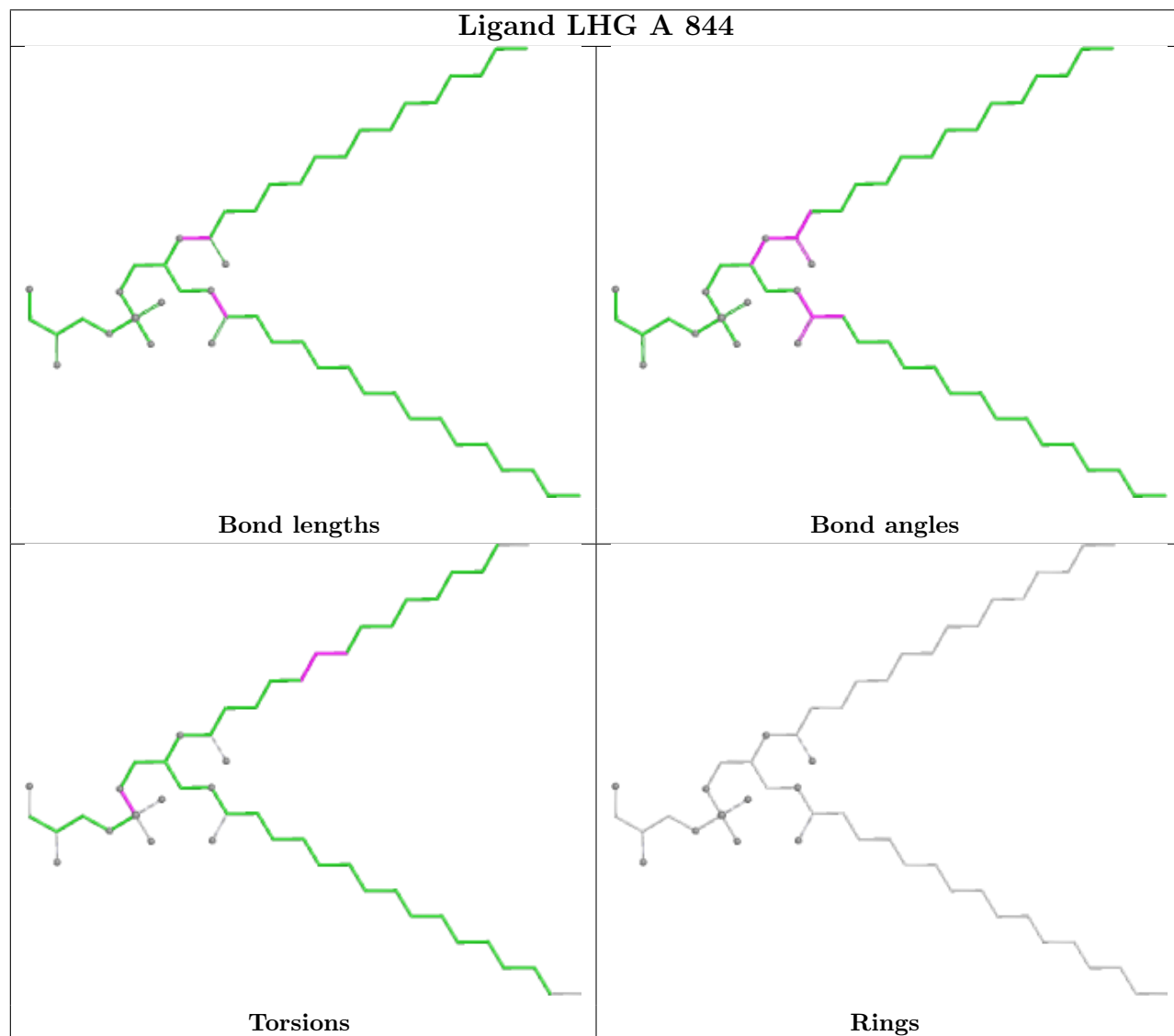
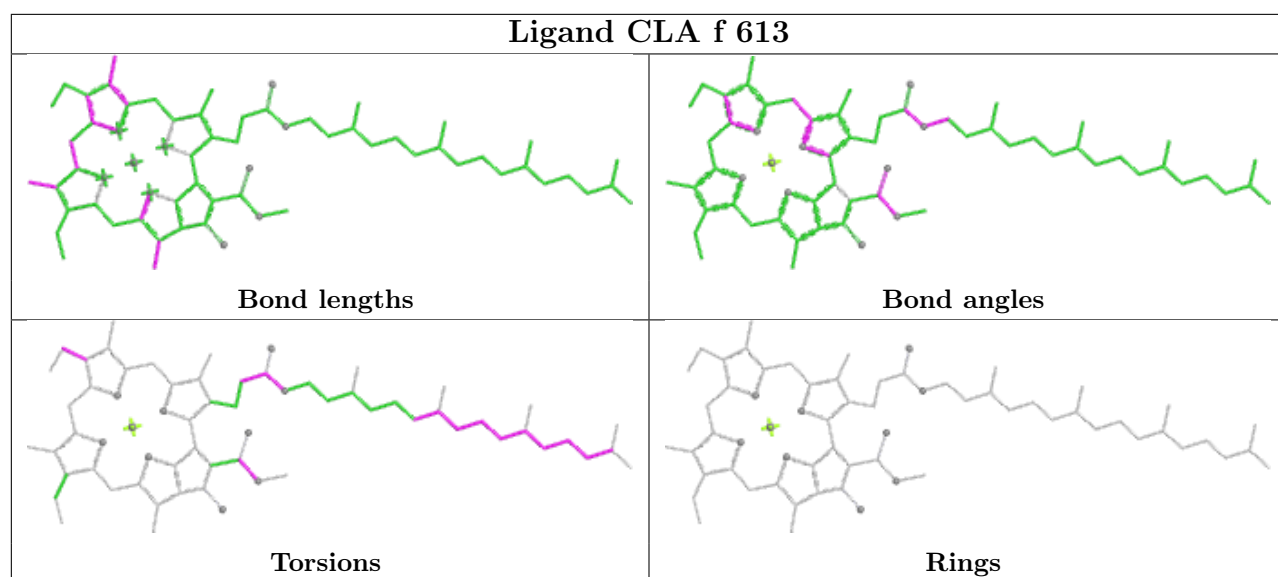
Bond angles

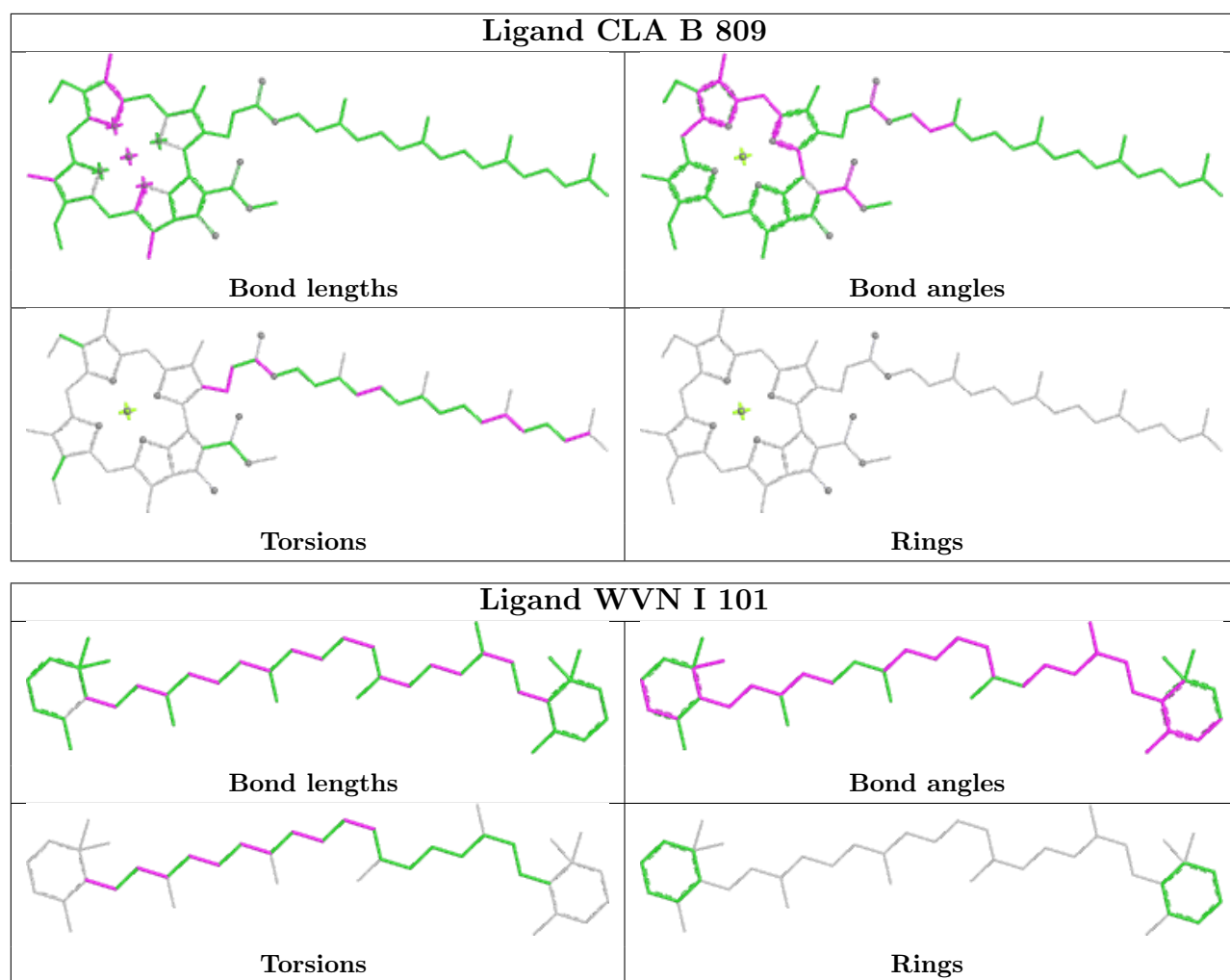


Torsions

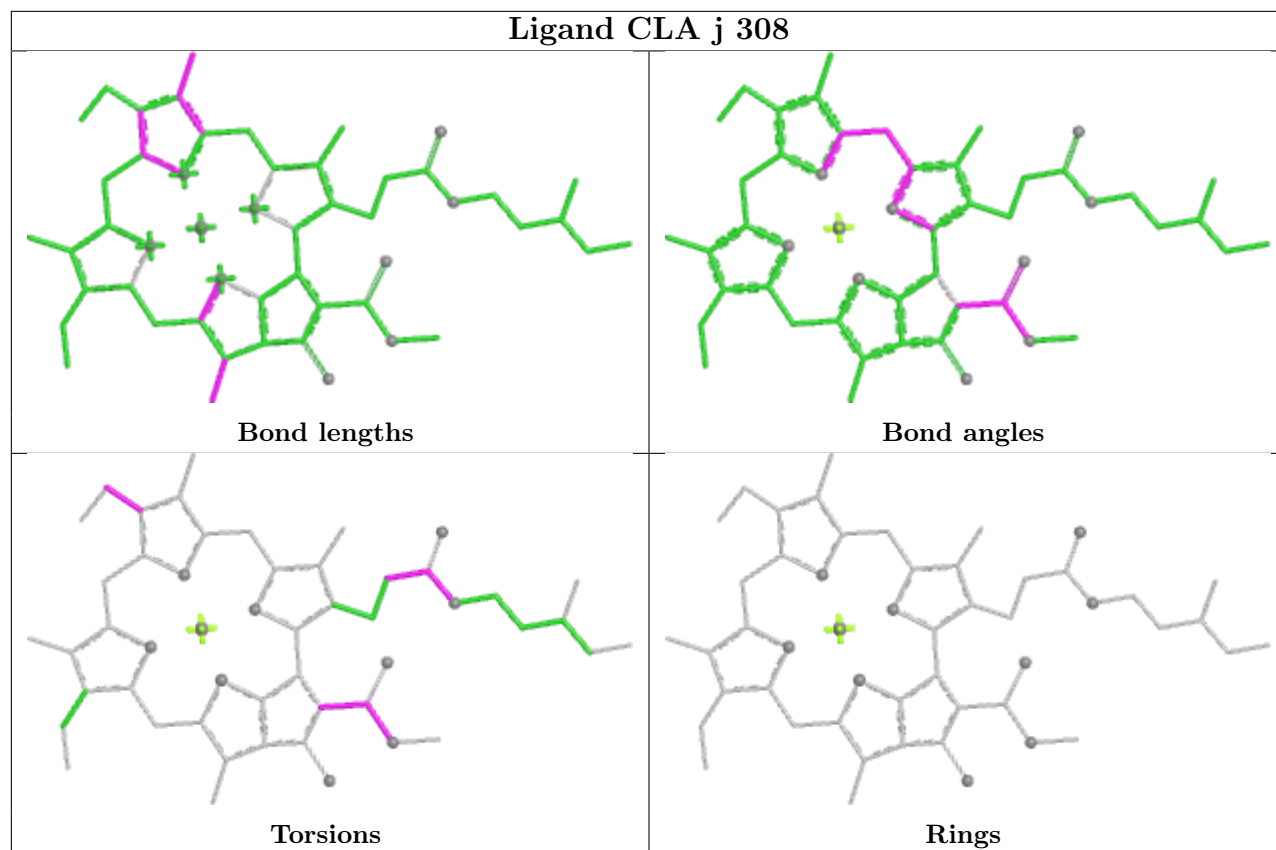


Rings

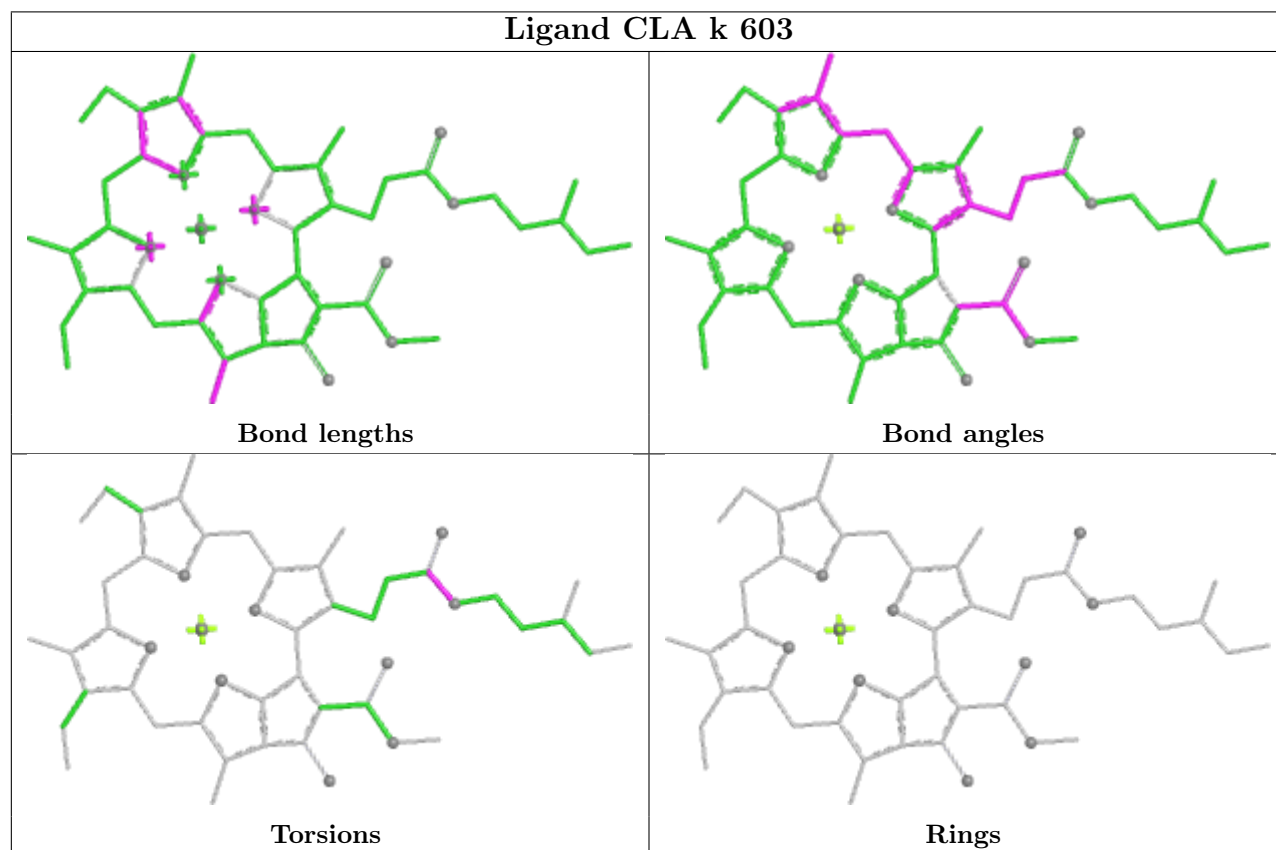


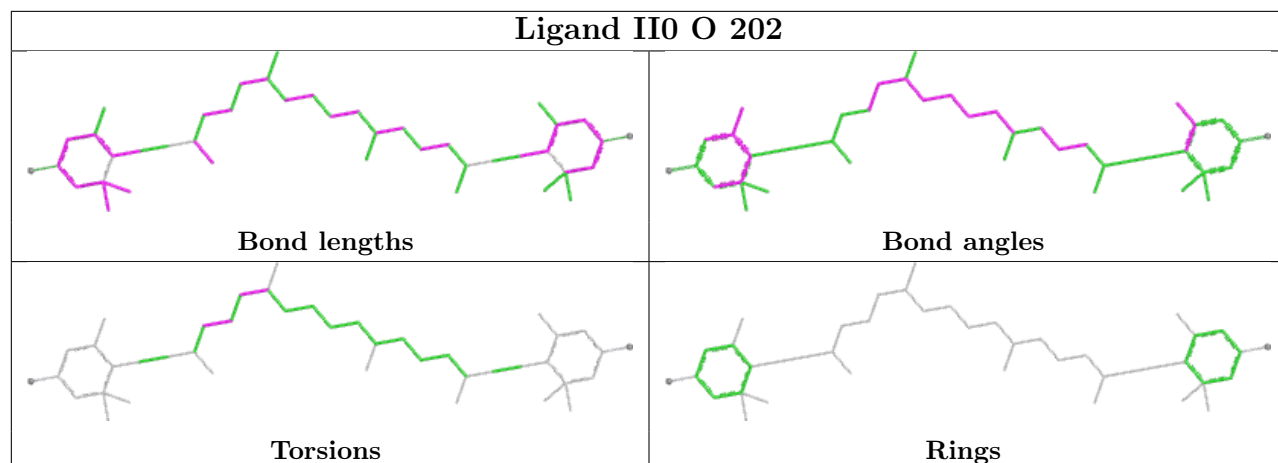
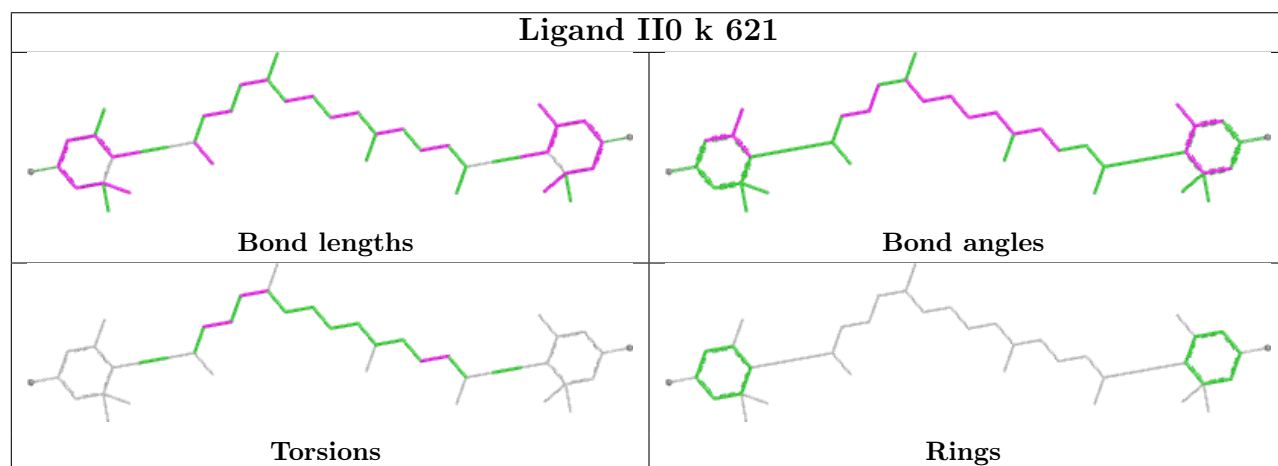
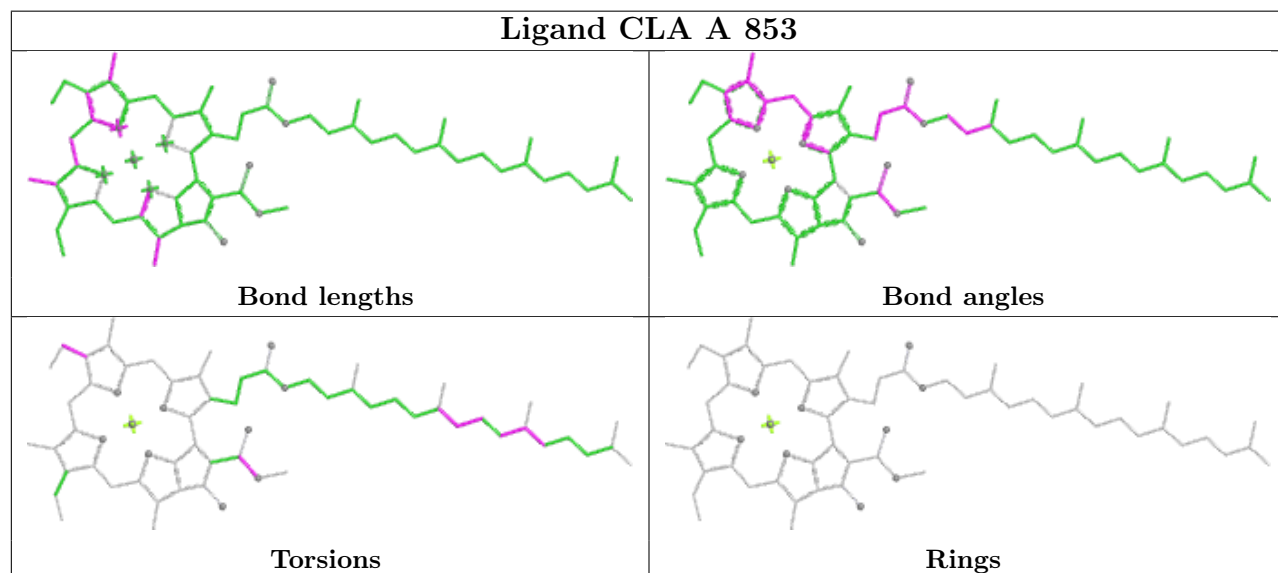


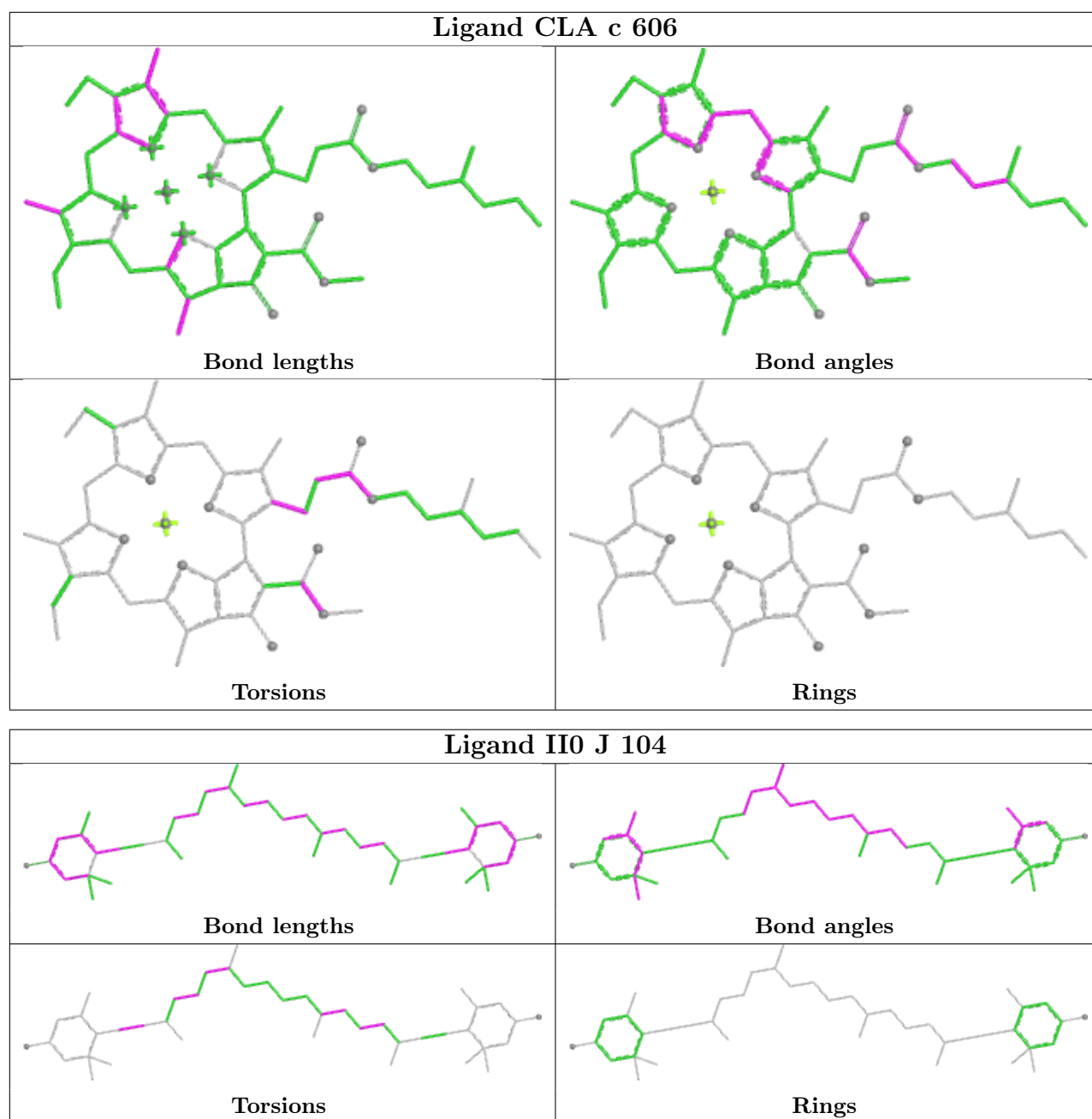
Ligand CLA j 308



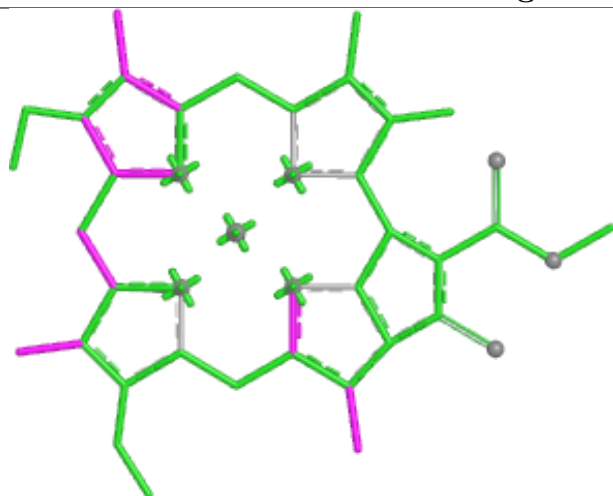
Ligand CLA k 603



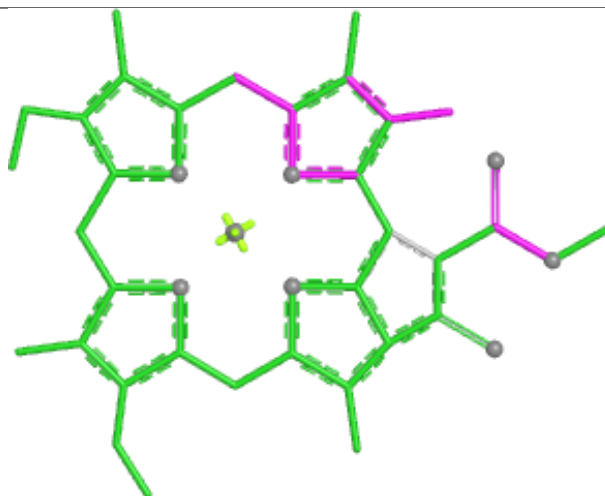
Ligand II0 O 202**Ligand II0 k 621****Ligand CLA A 853**



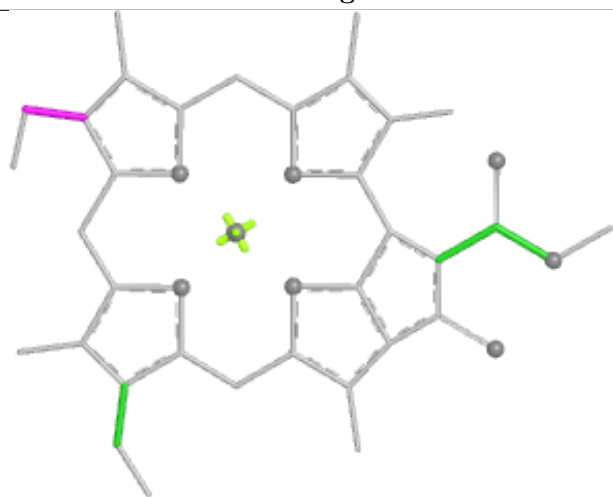
Ligand CLA d 309



Bond lengths



Bond angles

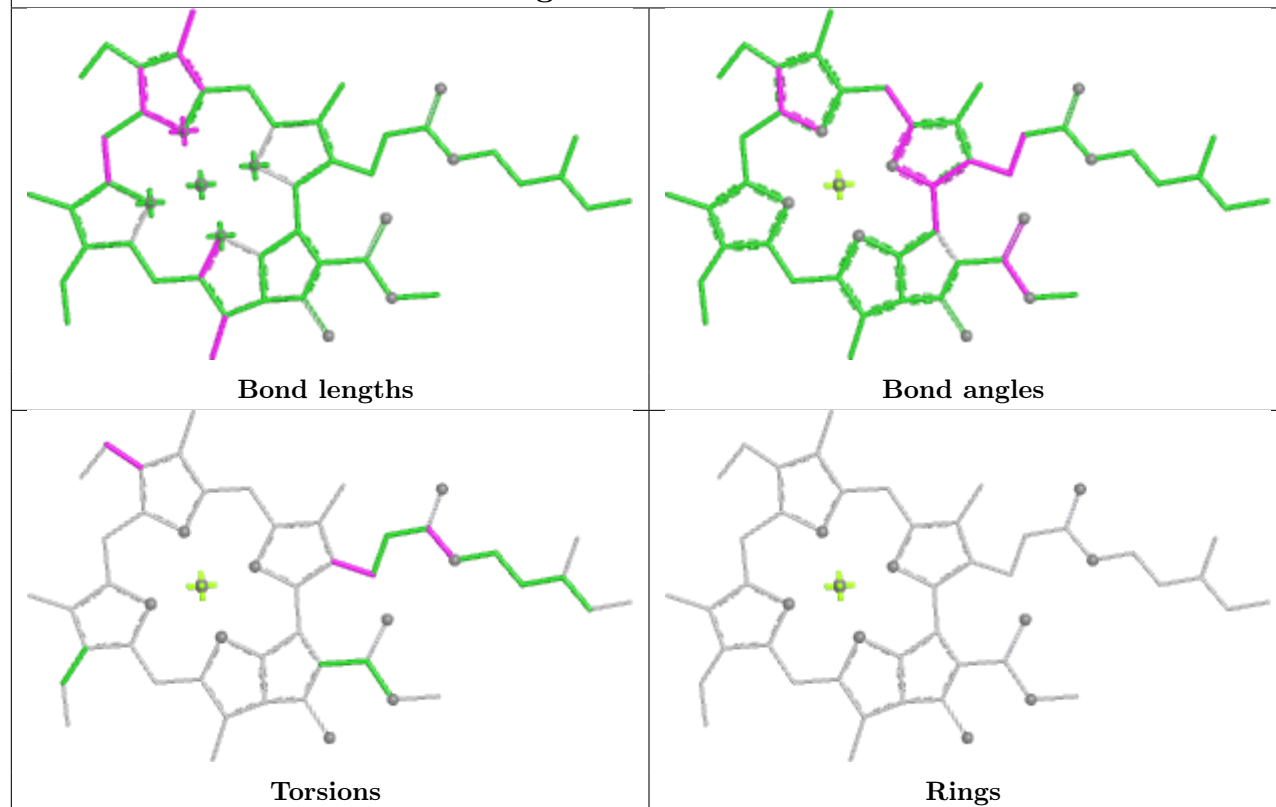


Torsions

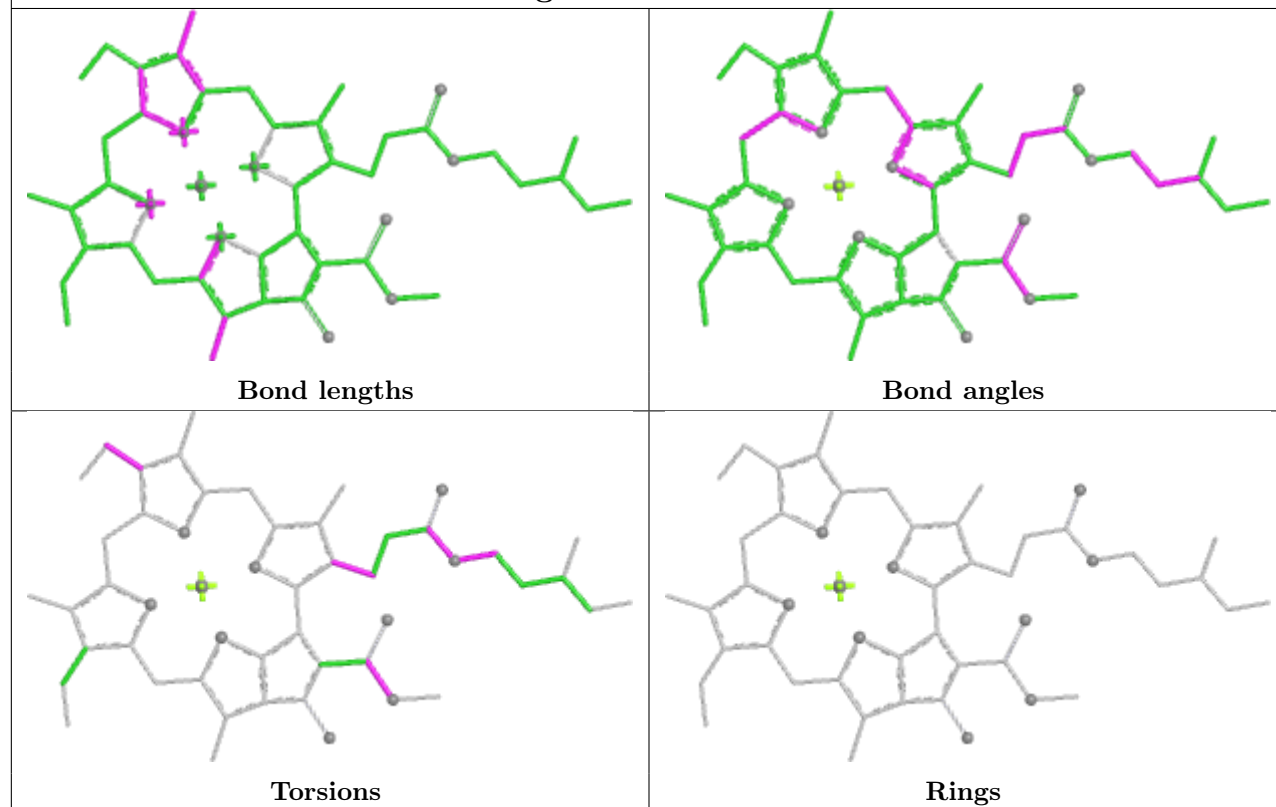


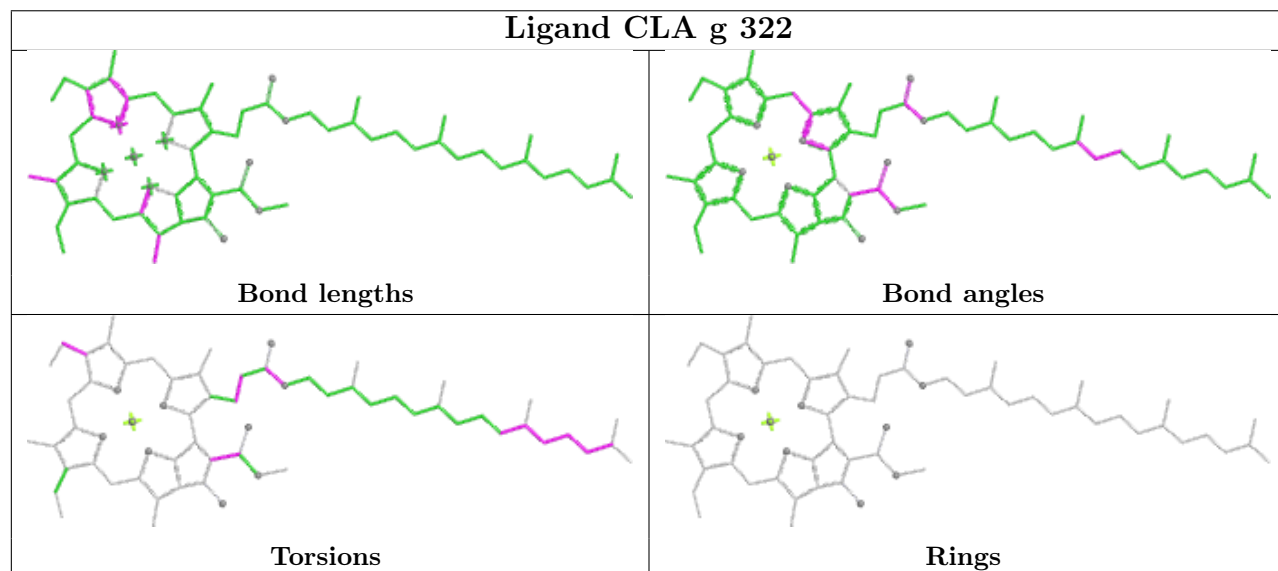
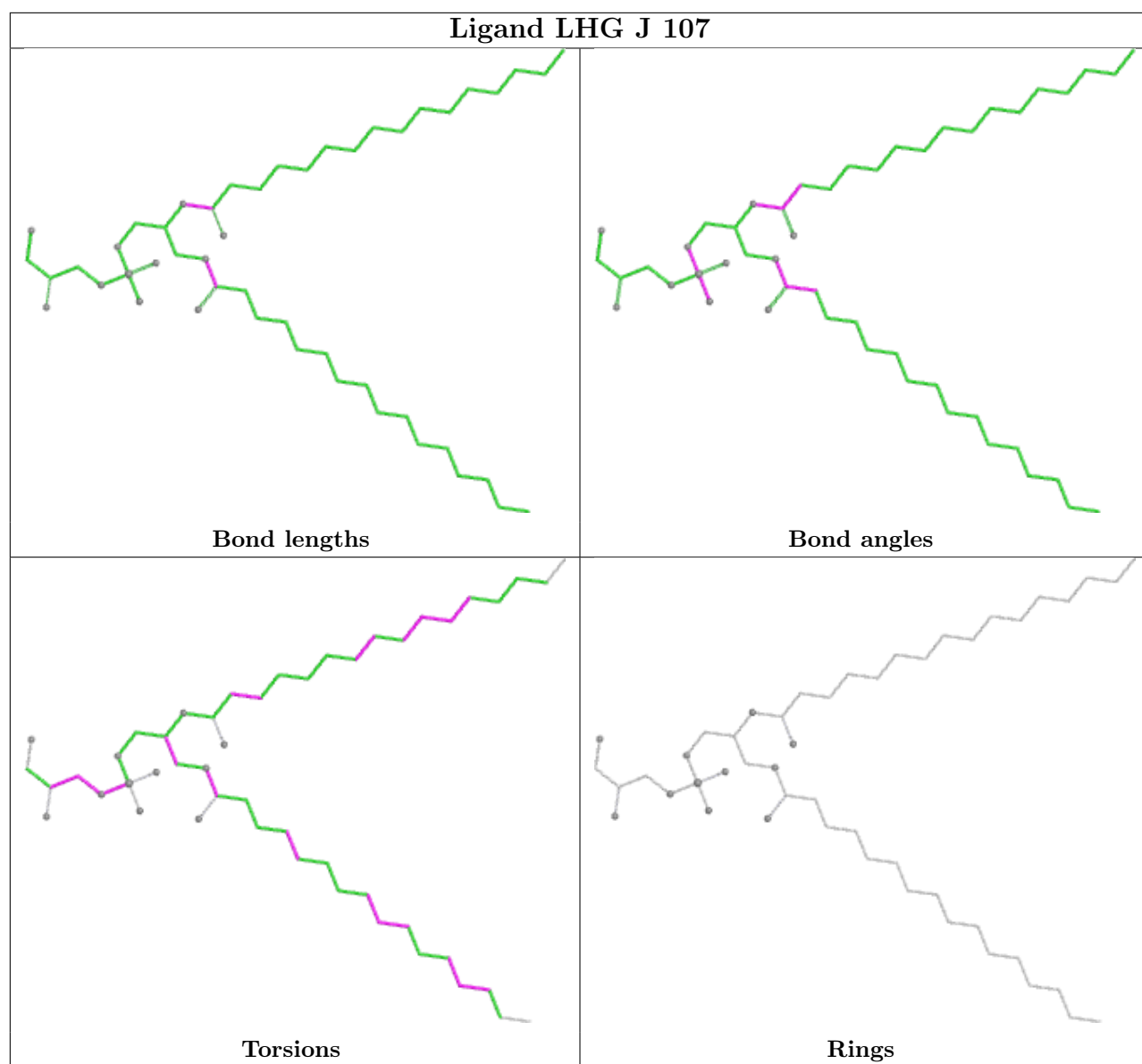
Rings

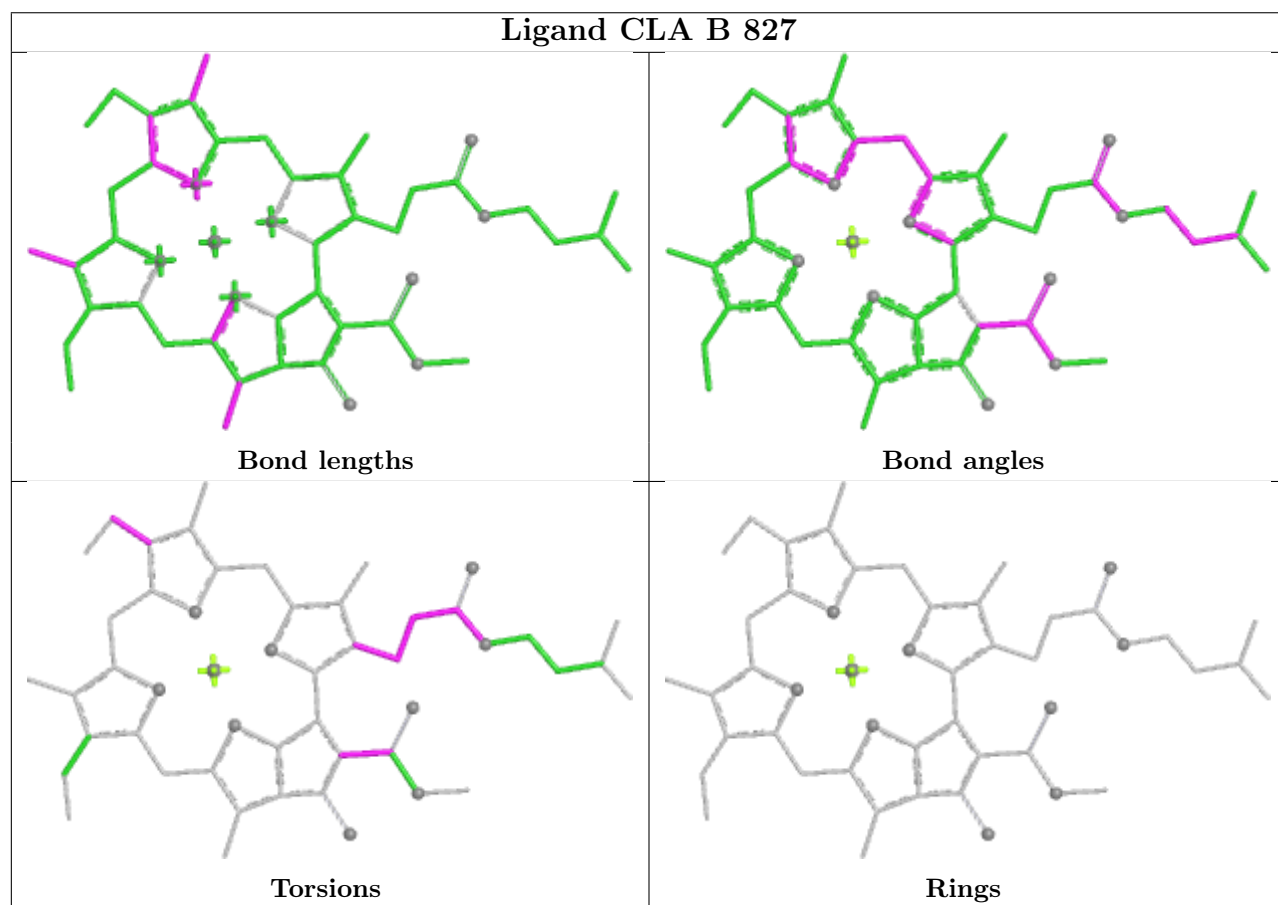
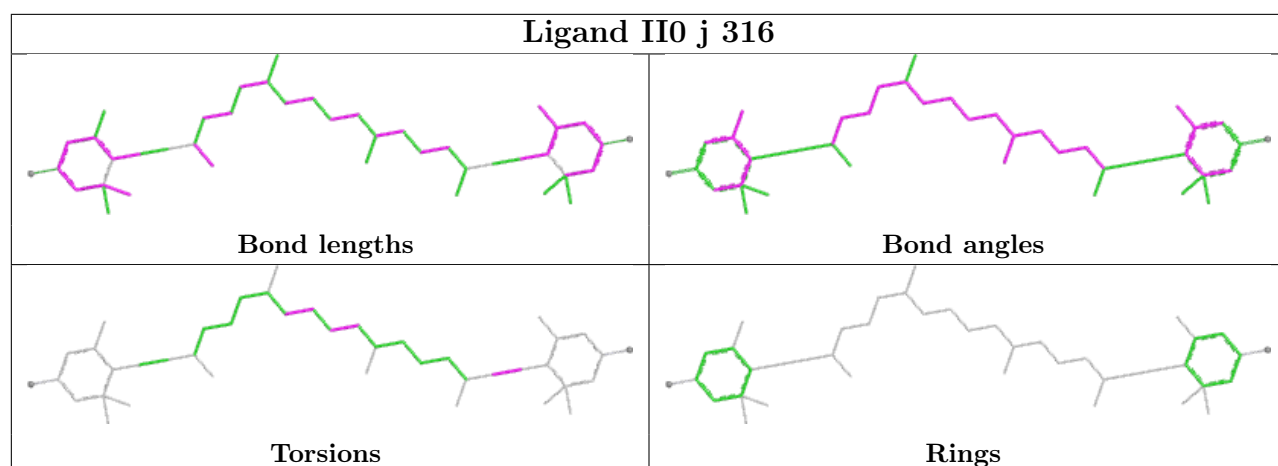
Ligand CLA J 105

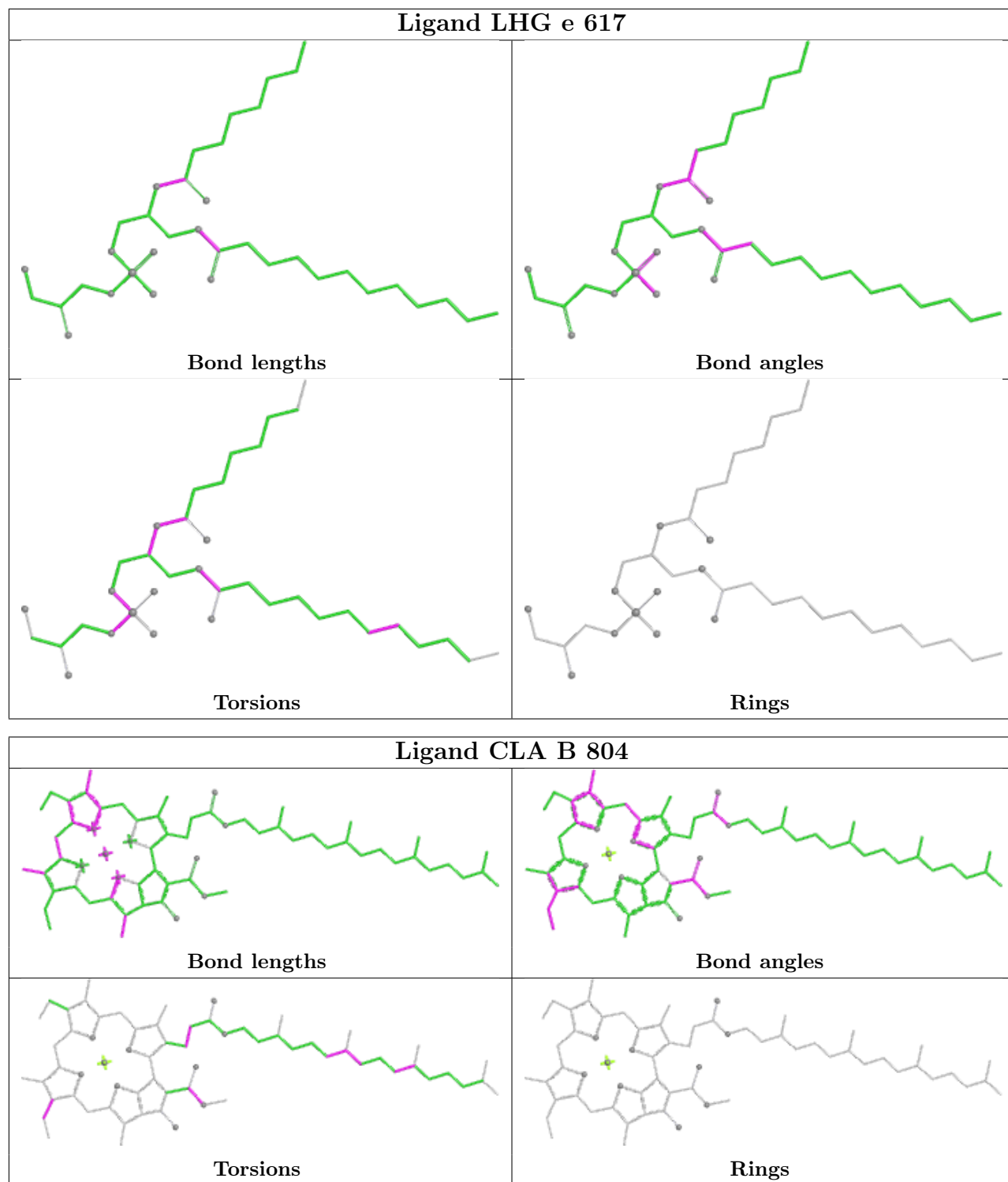


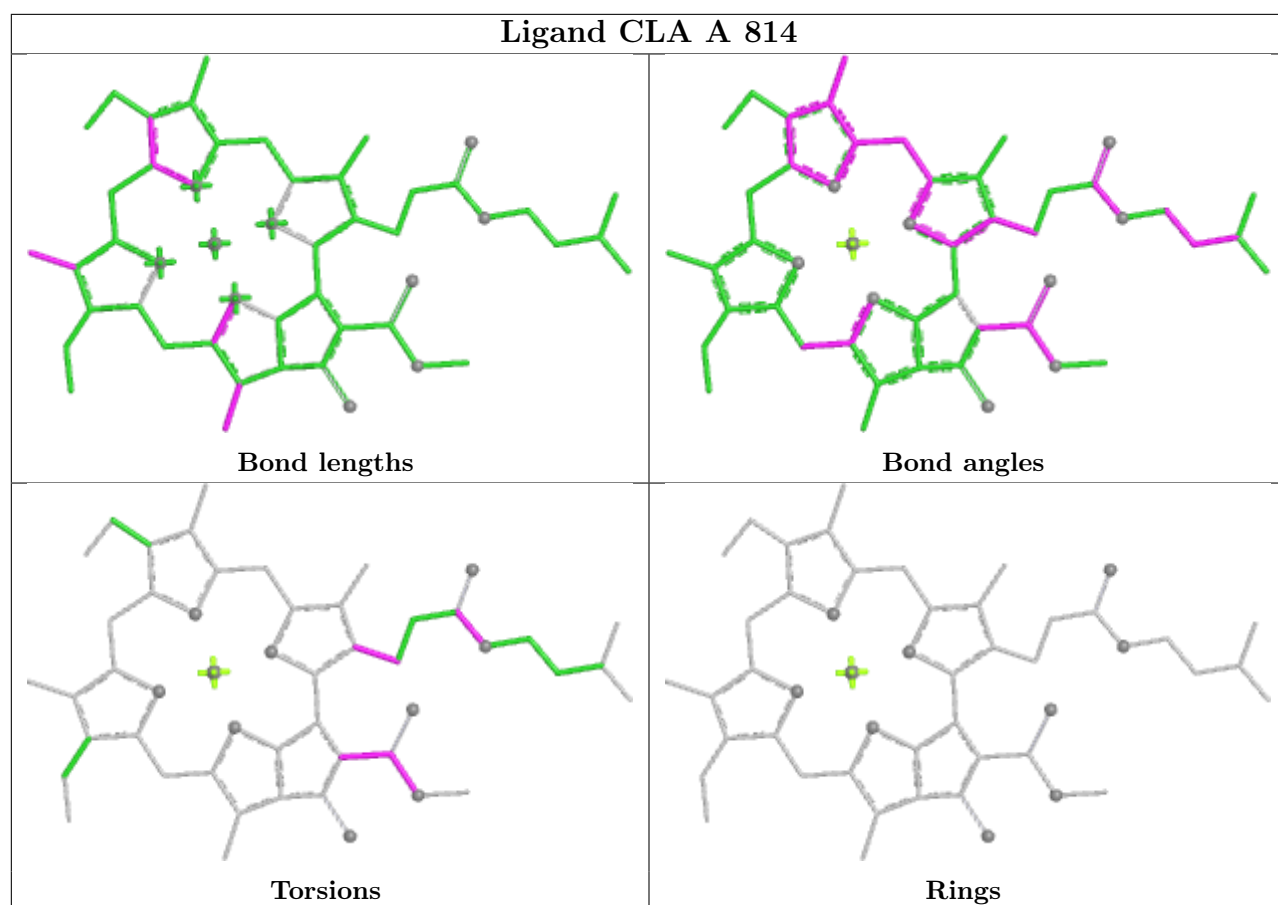
Ligand CLA k 601

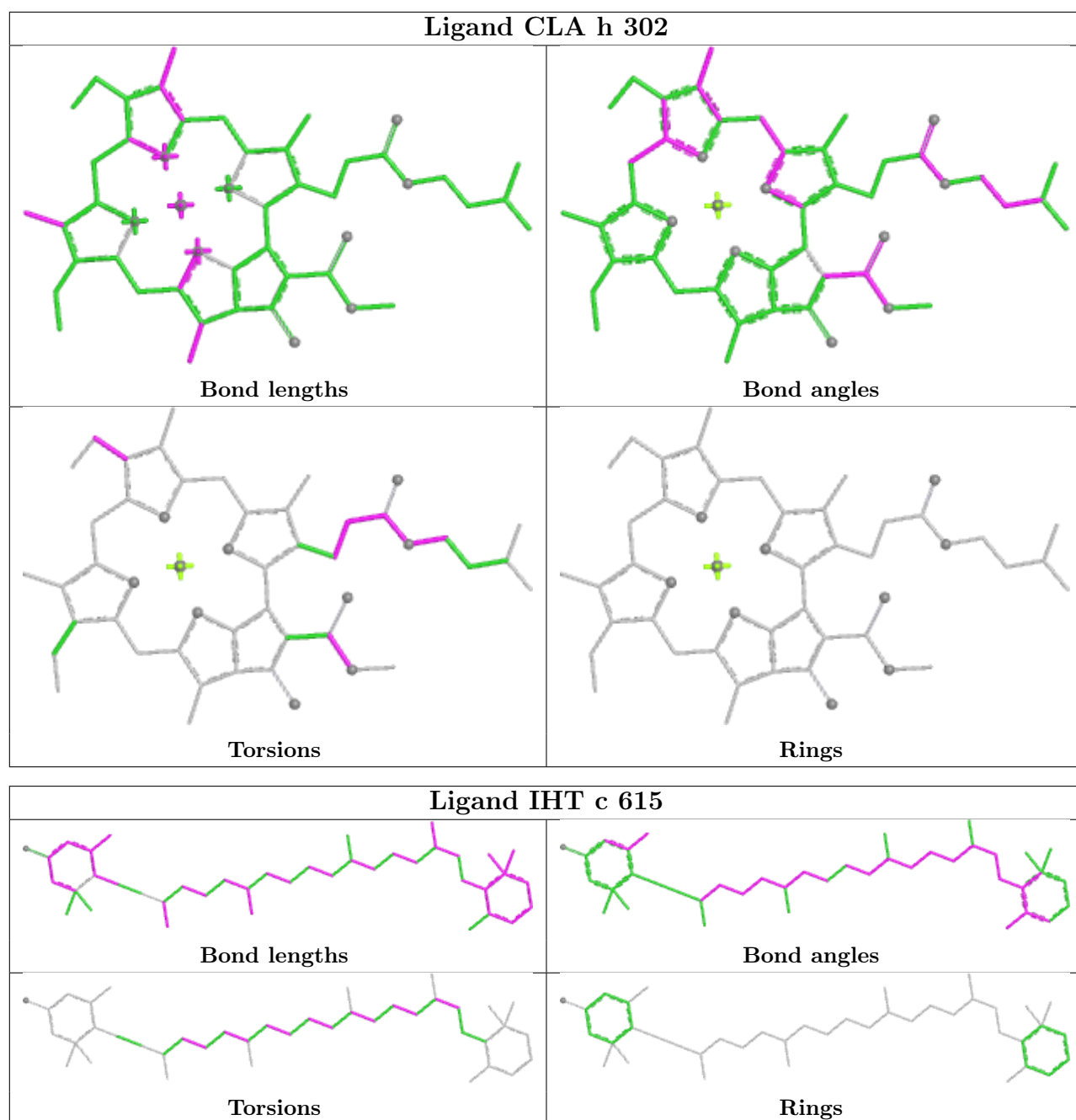




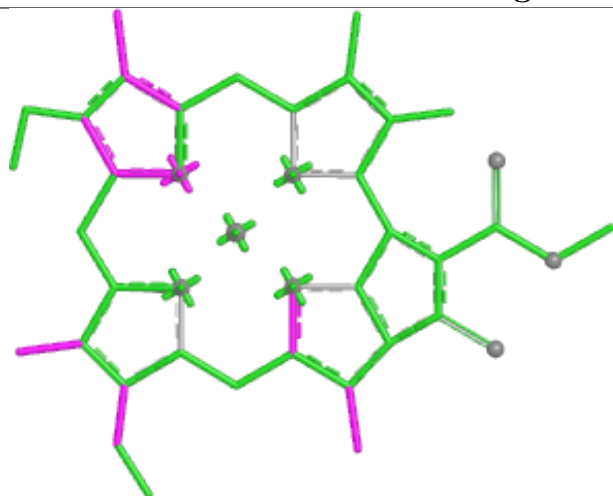




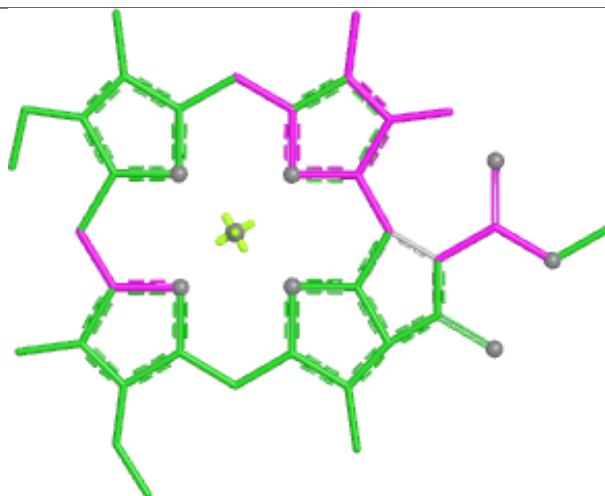




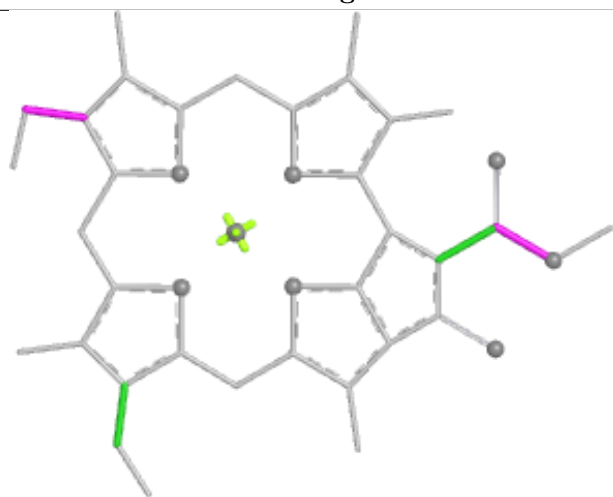
Ligand CLA A 856



Bond lengths



Bond angles

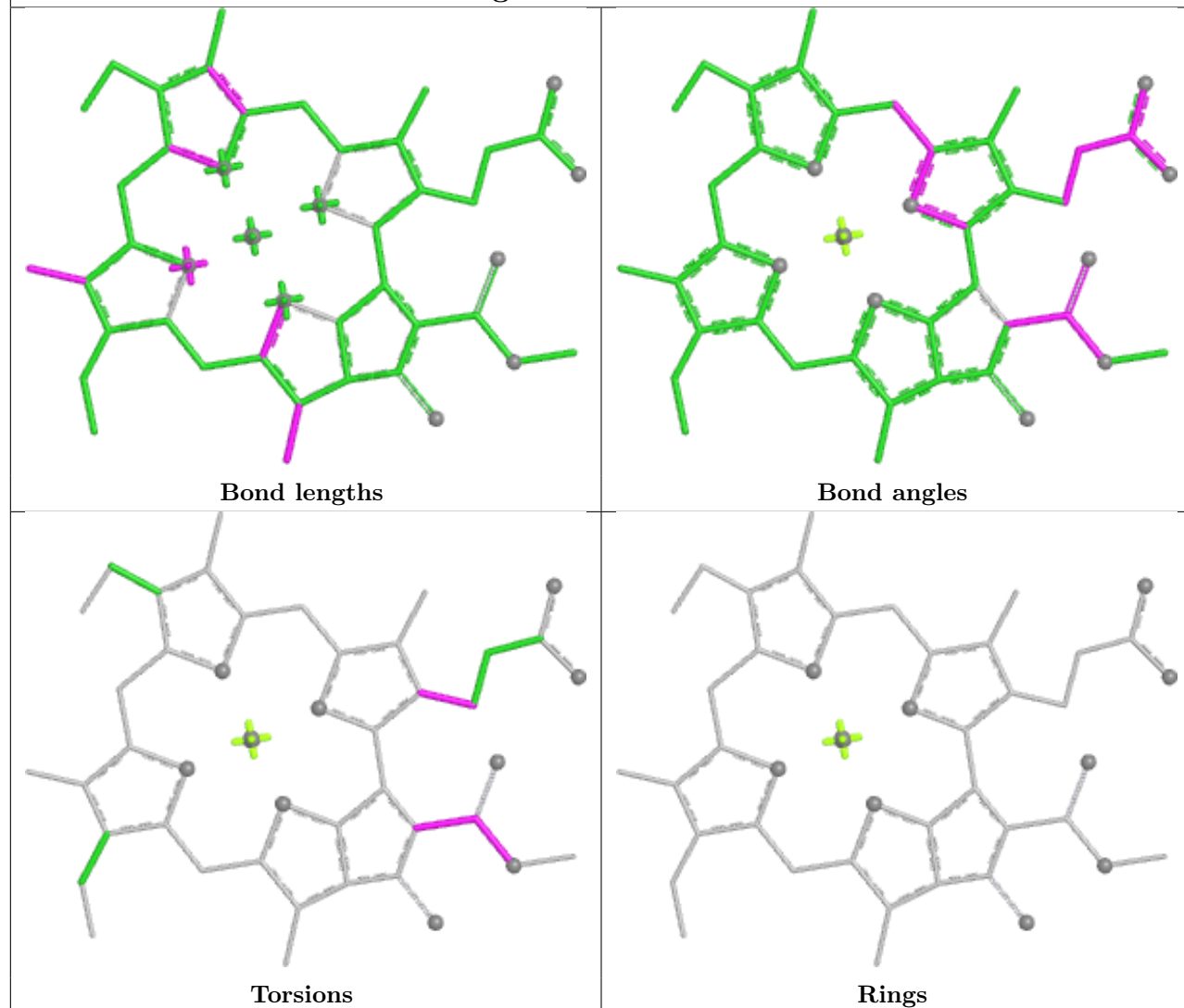


Torsions

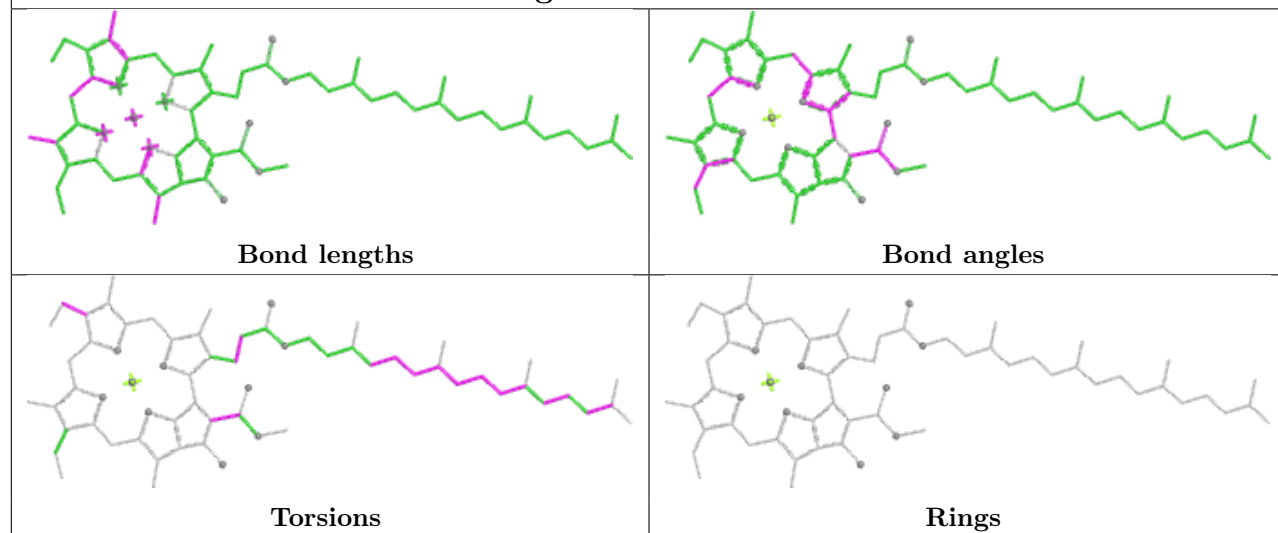


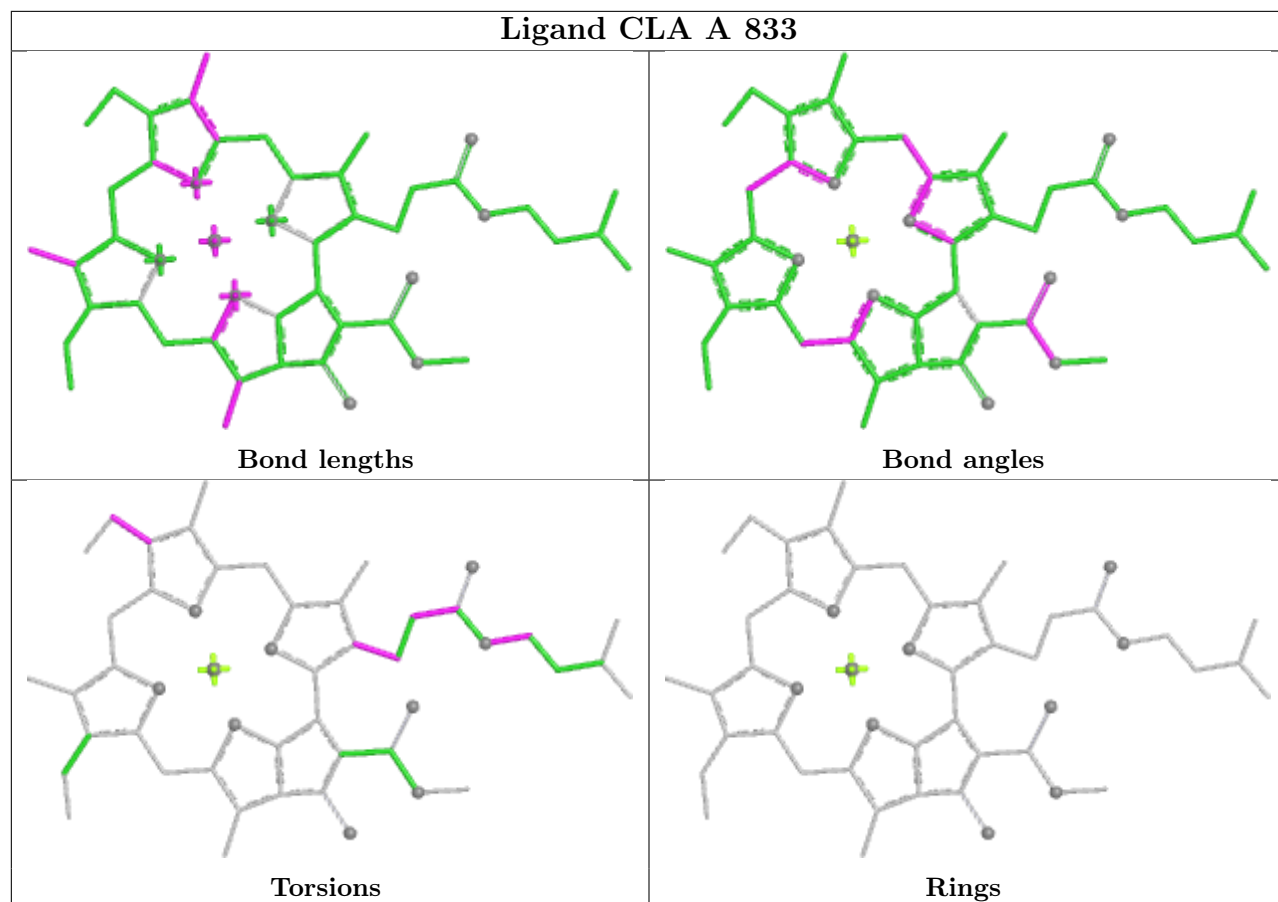
Rings

Ligand CLA A 813

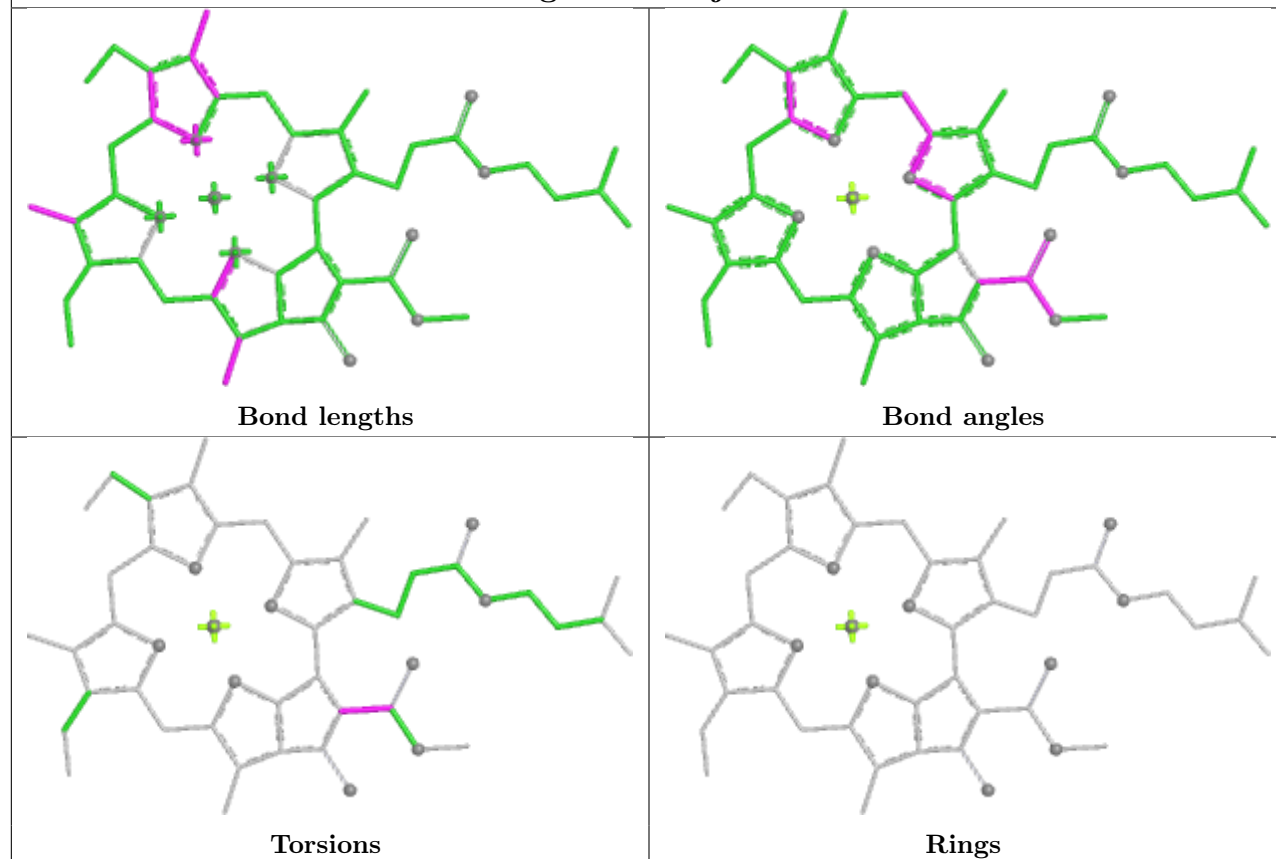


Ligand CLA b 306

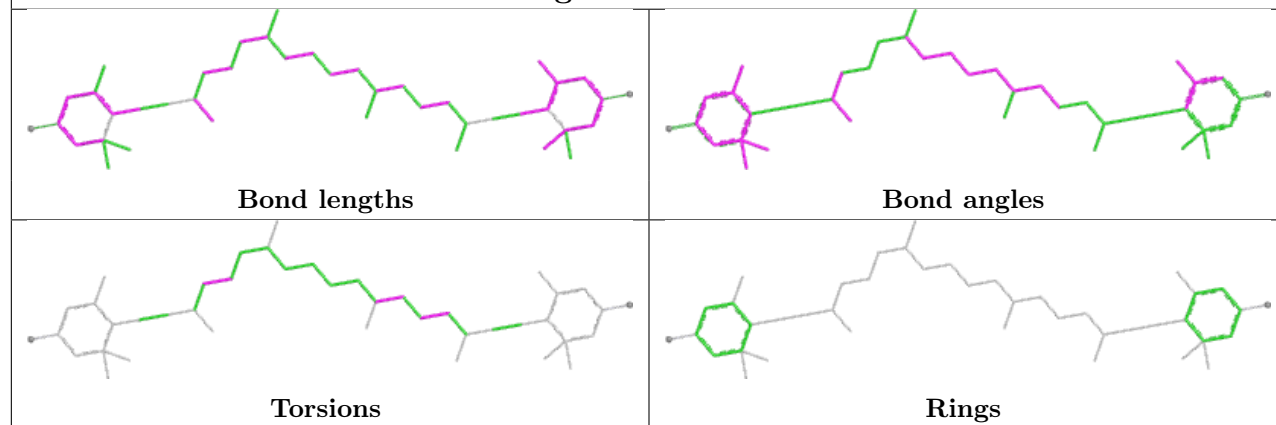




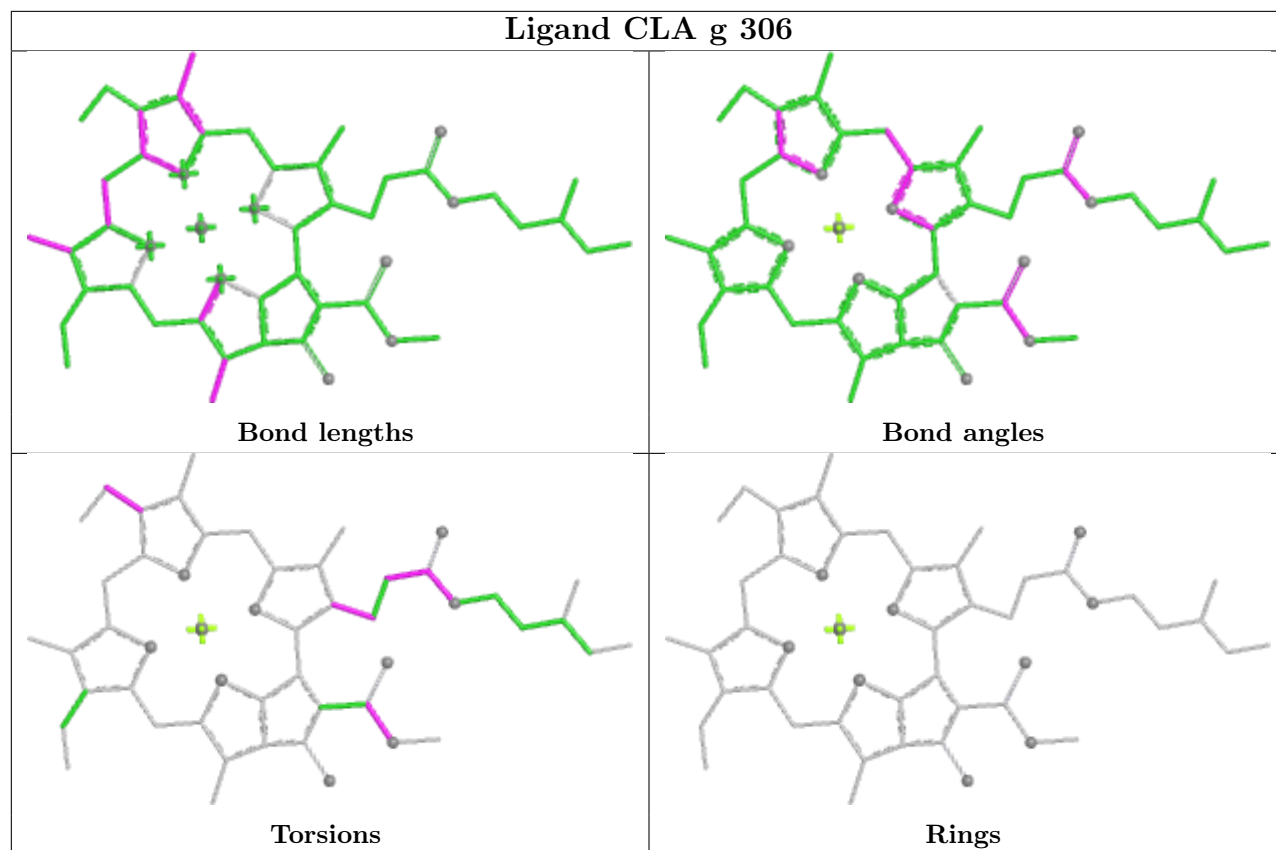
Ligand CLA j 303



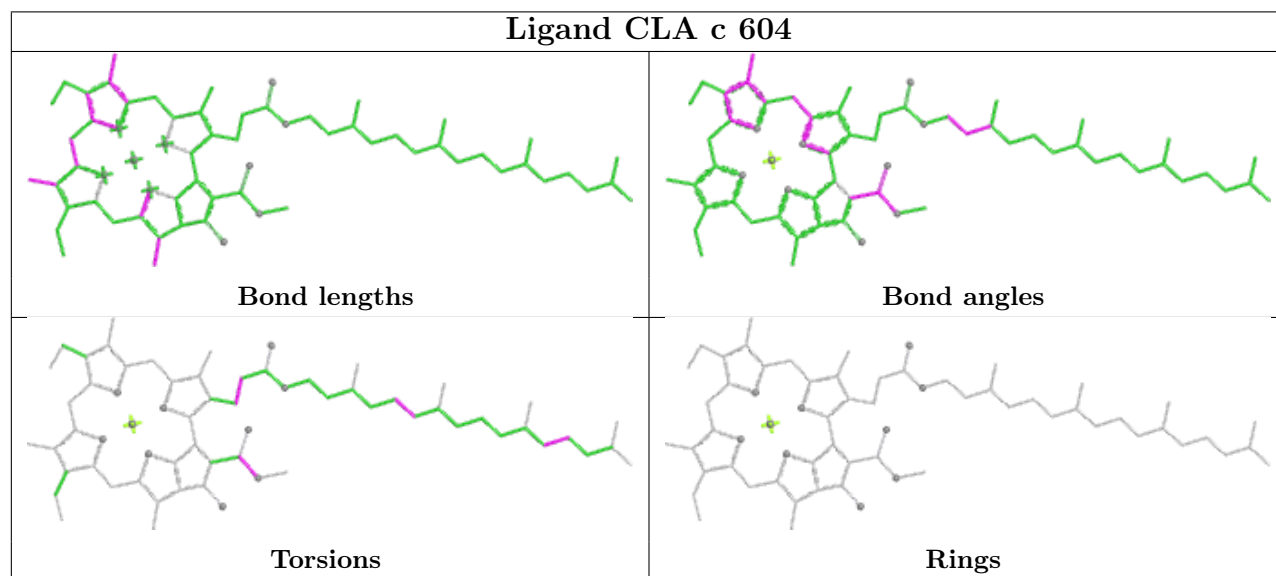
Ligand II0 i 614

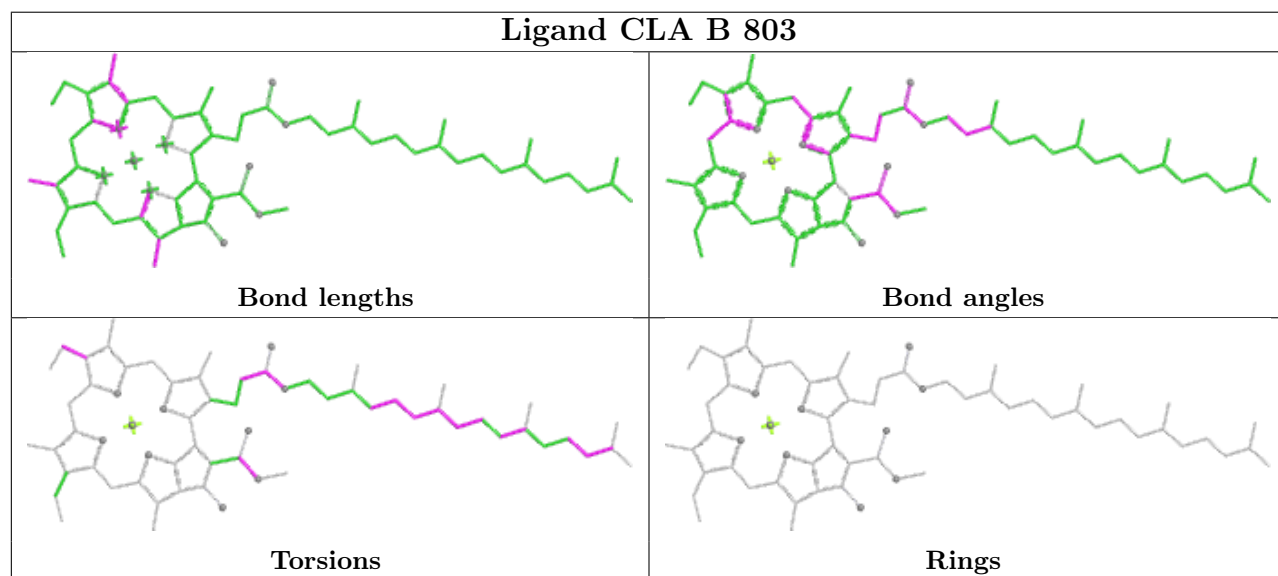
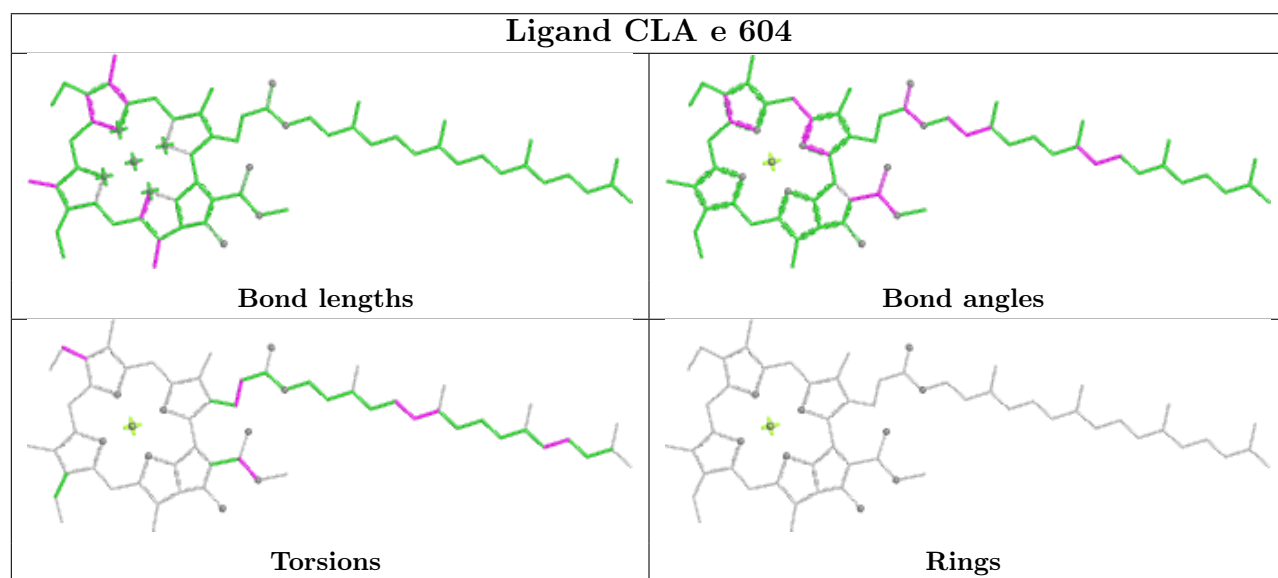
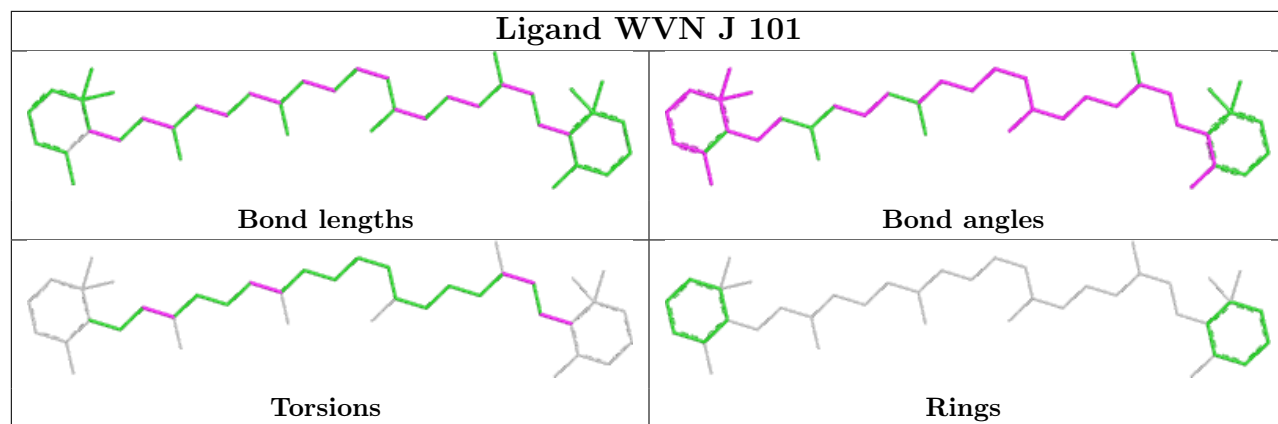


Ligand CLA g 306

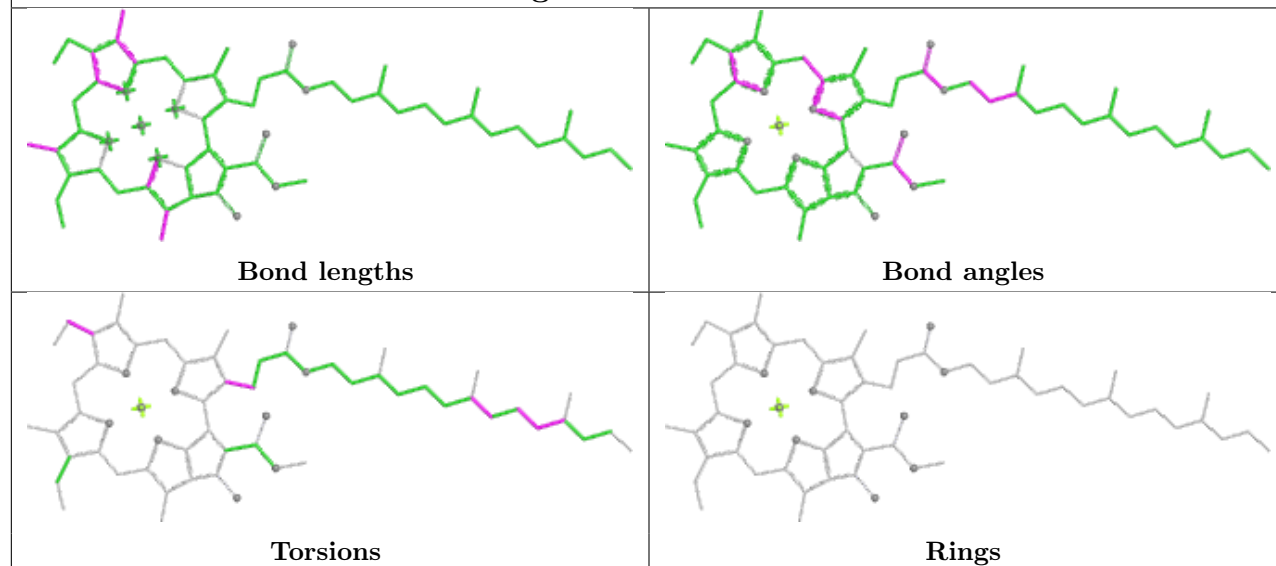


Ligand CLA c 604

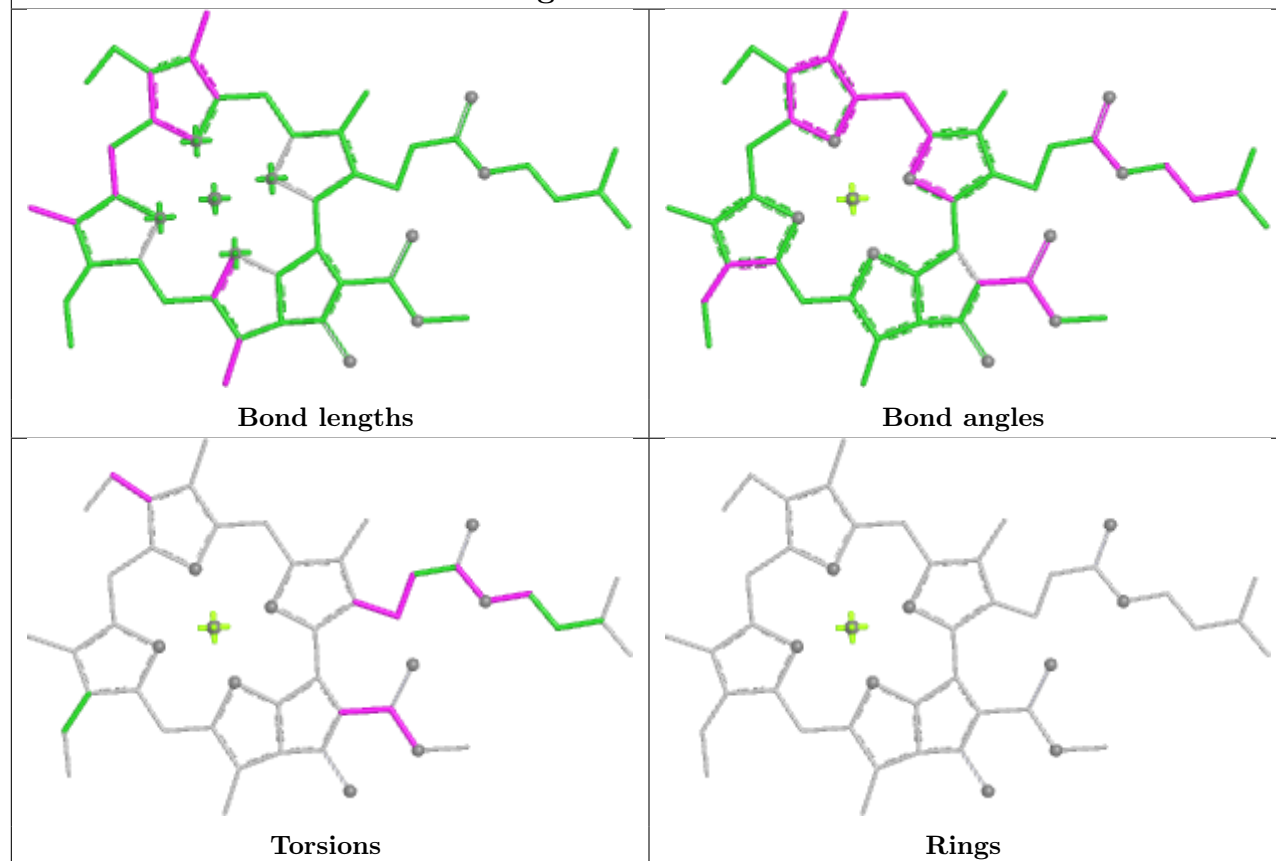




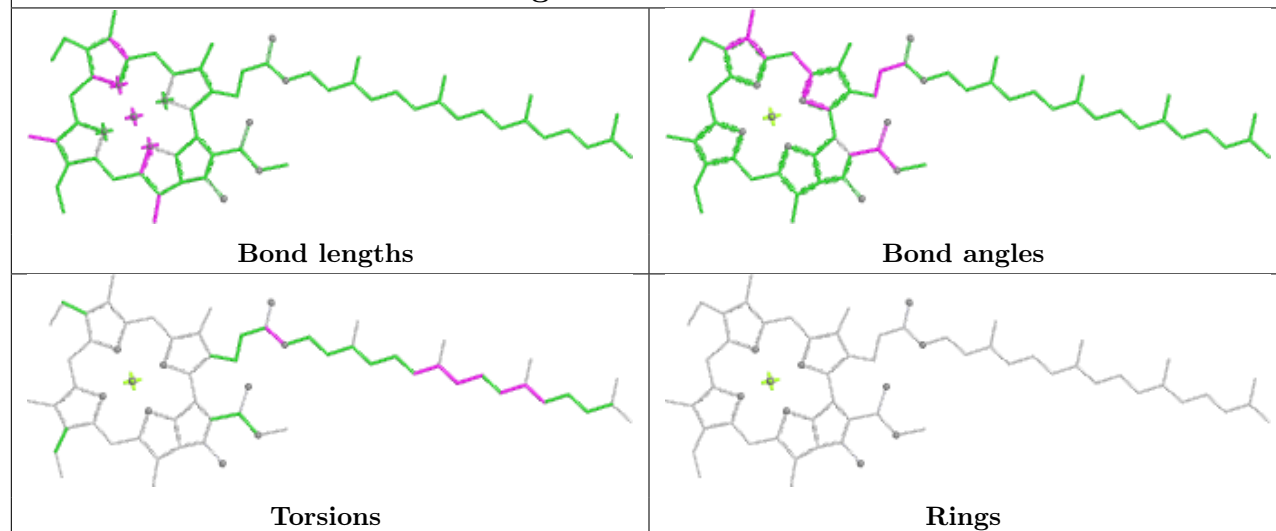
Ligand CLA A 810



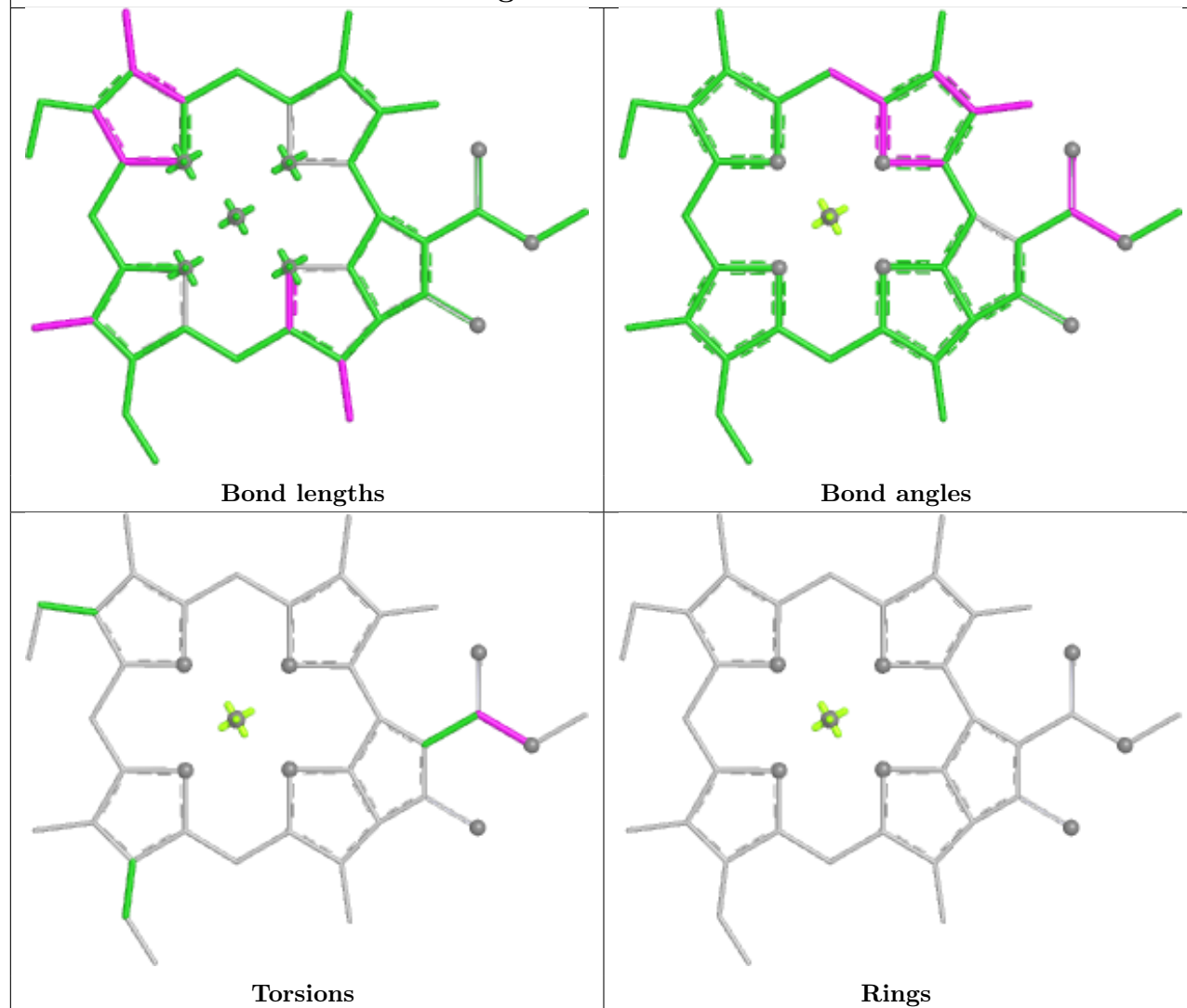
Ligand CLA c 602



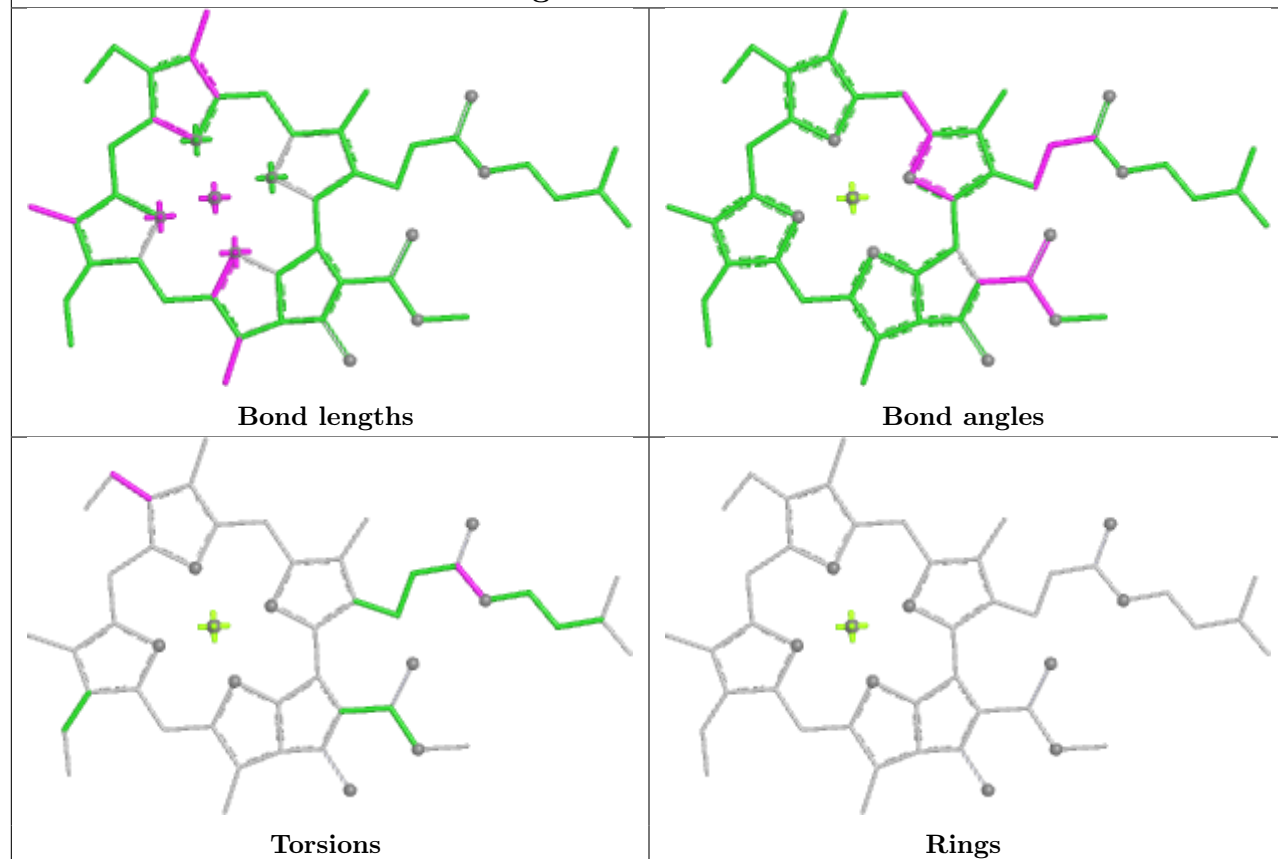
Ligand CLA A 825



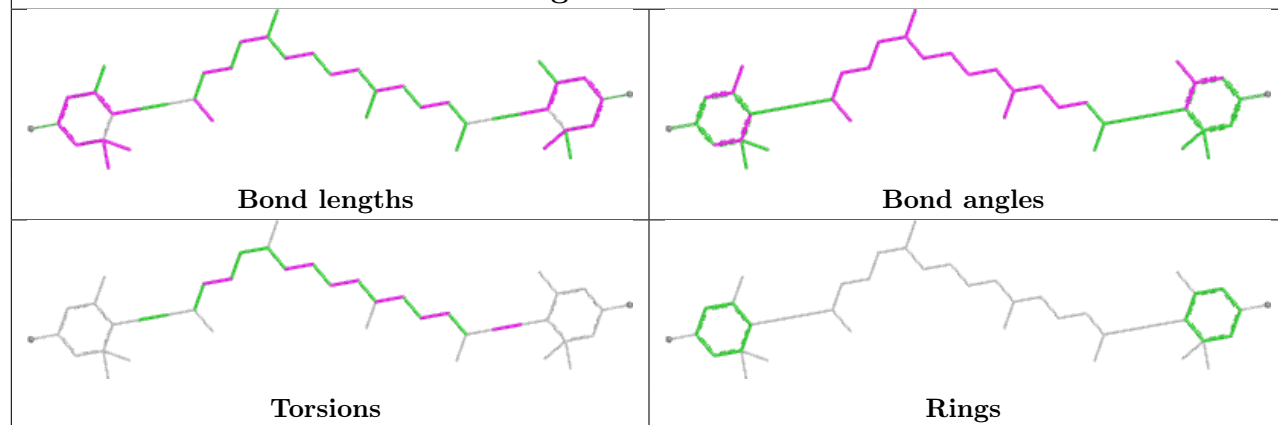
Ligand CLA d 308



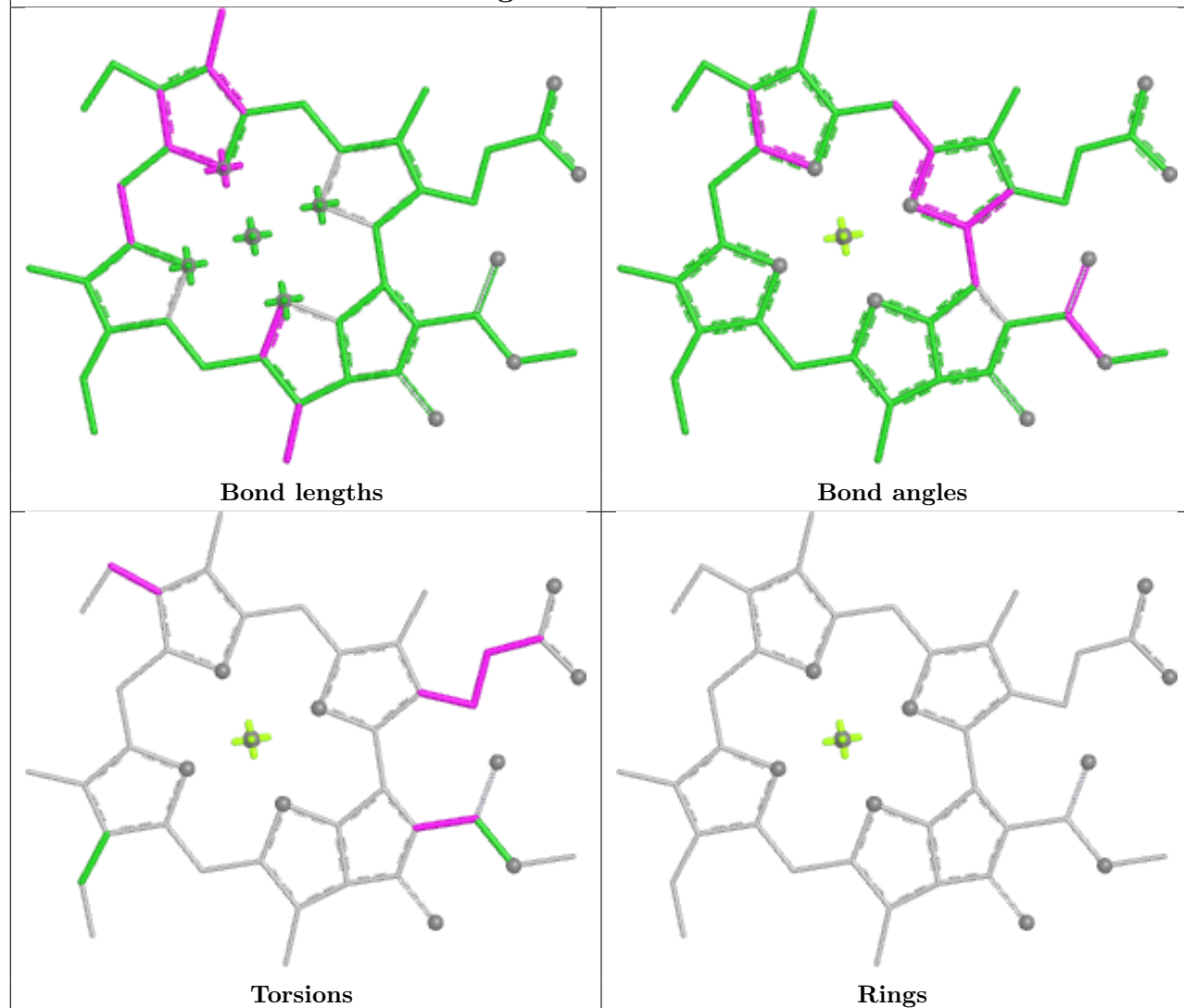
Ligand CLA B 829



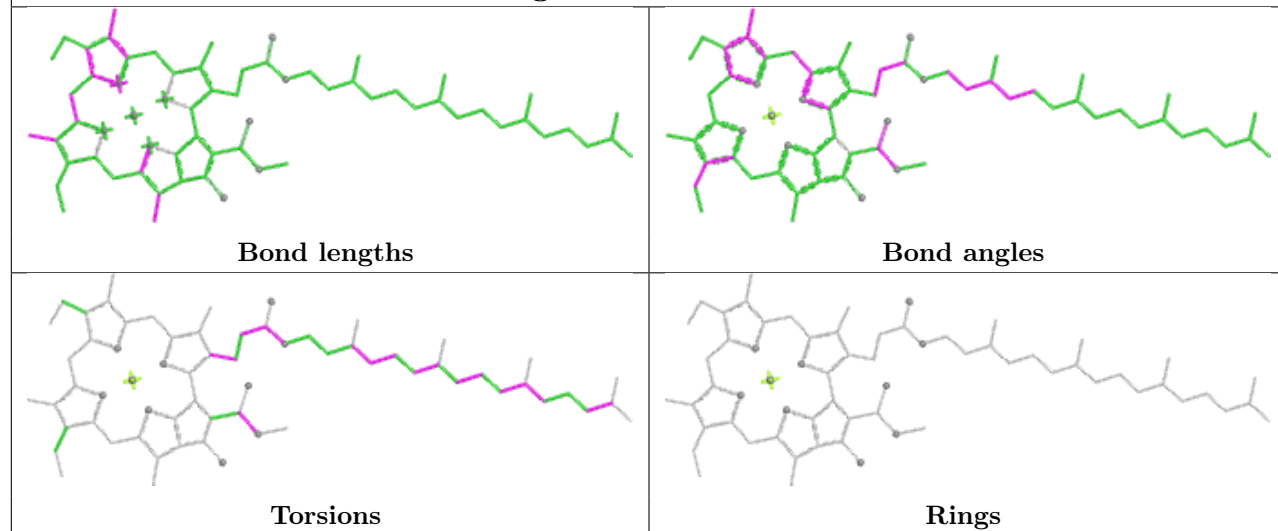
Ligand II0 a 314

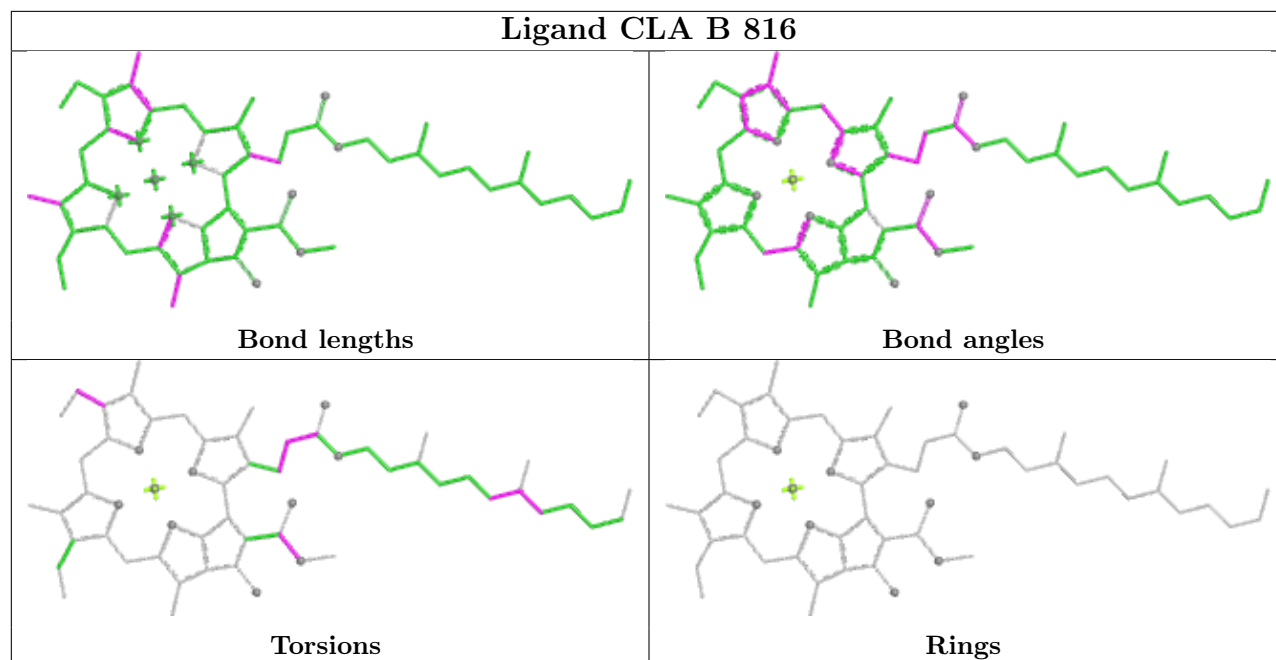
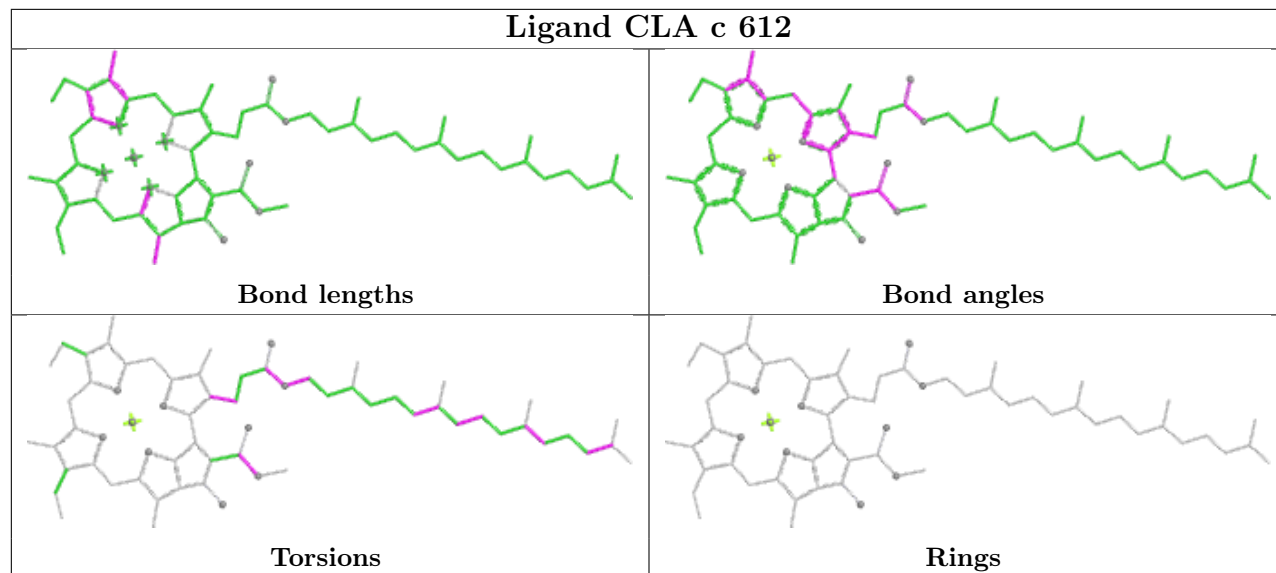


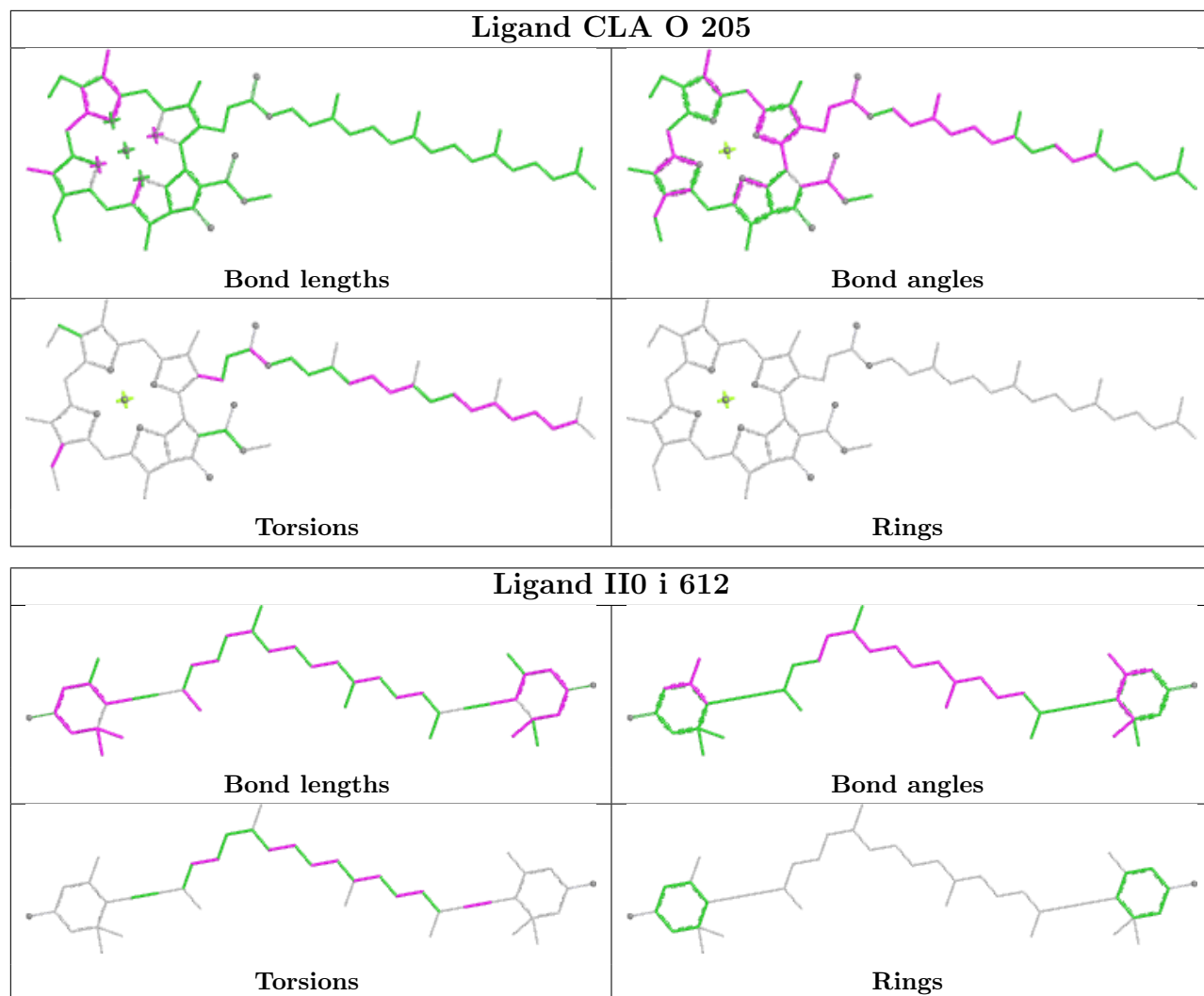
Ligand CLA e 601



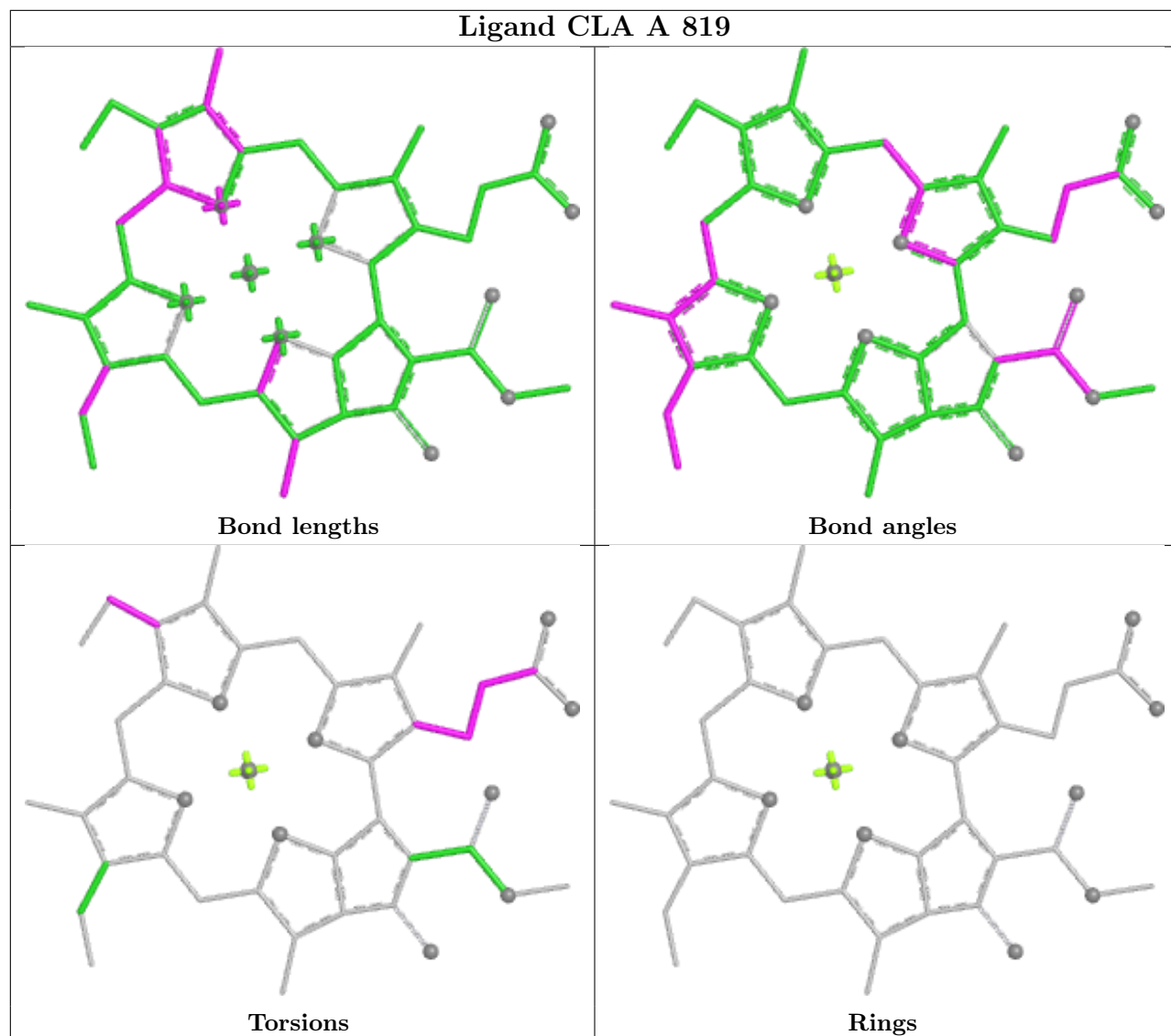
Ligand CLA A 812



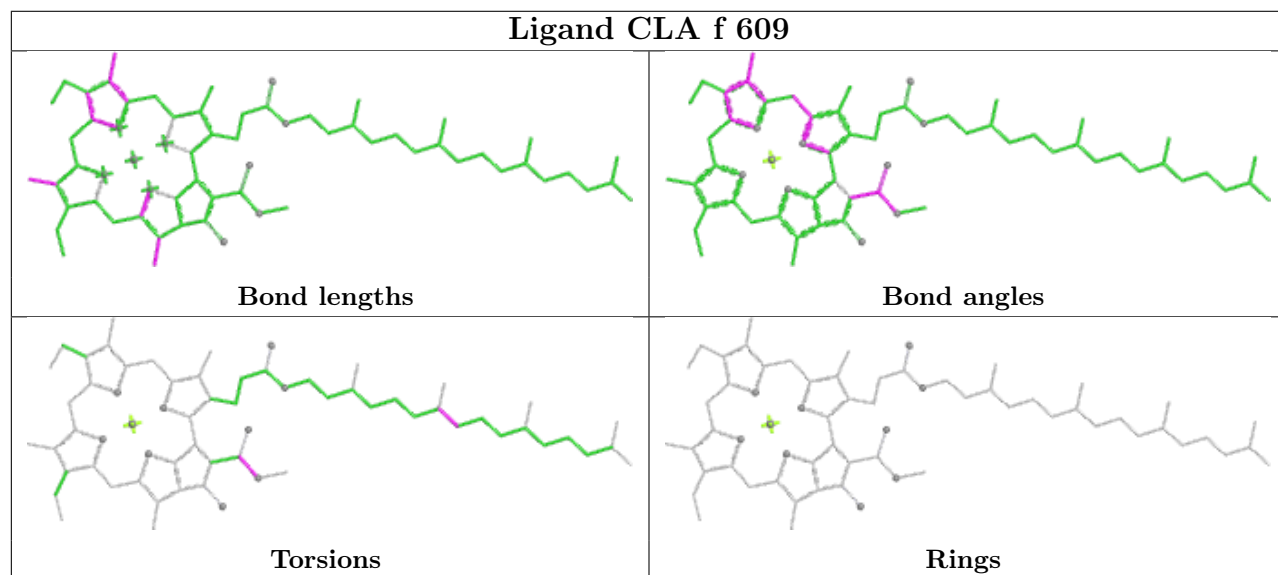
Ligand CLA B 816**Ligand CLA c 612**

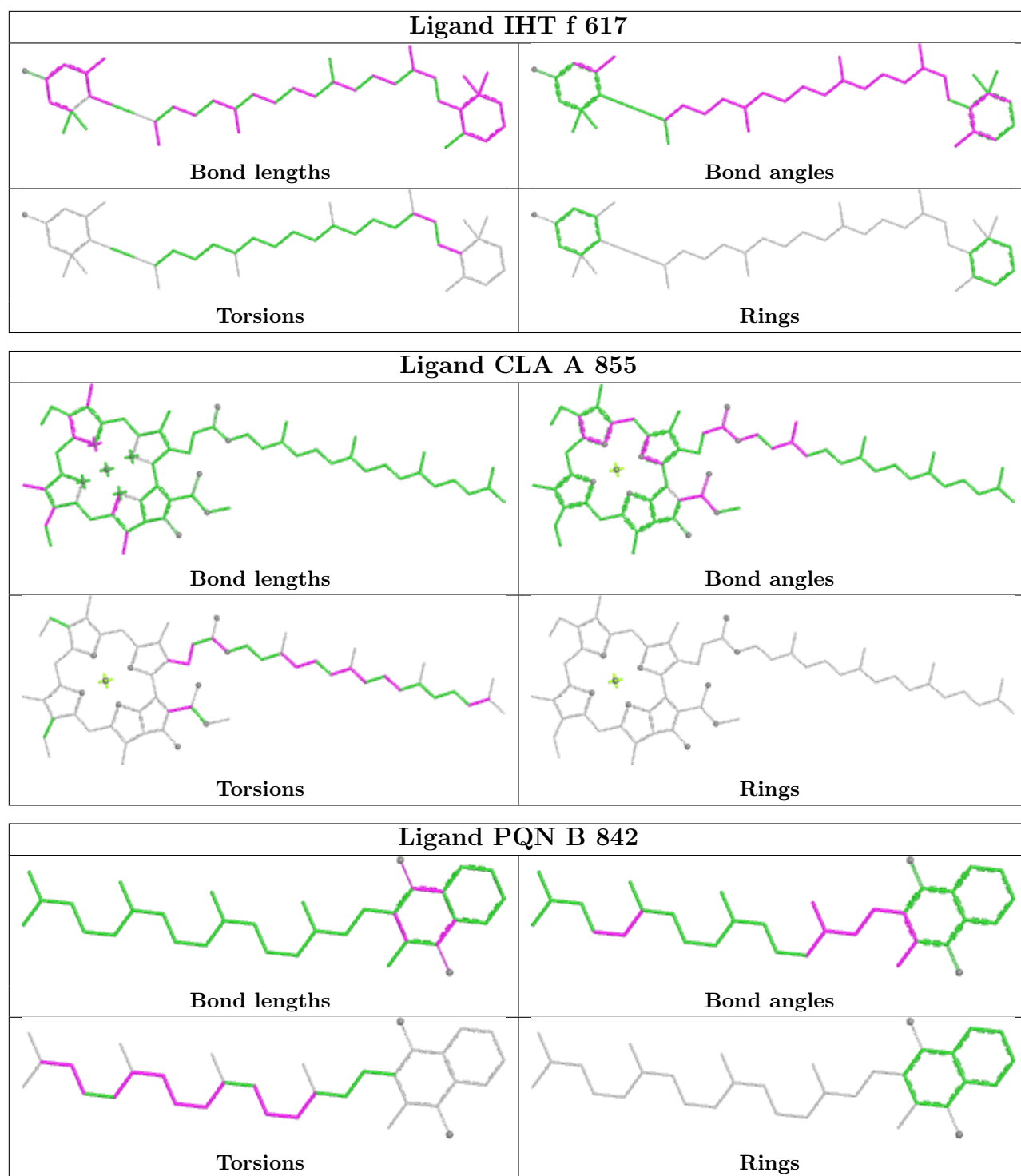


Ligand CLA A 819

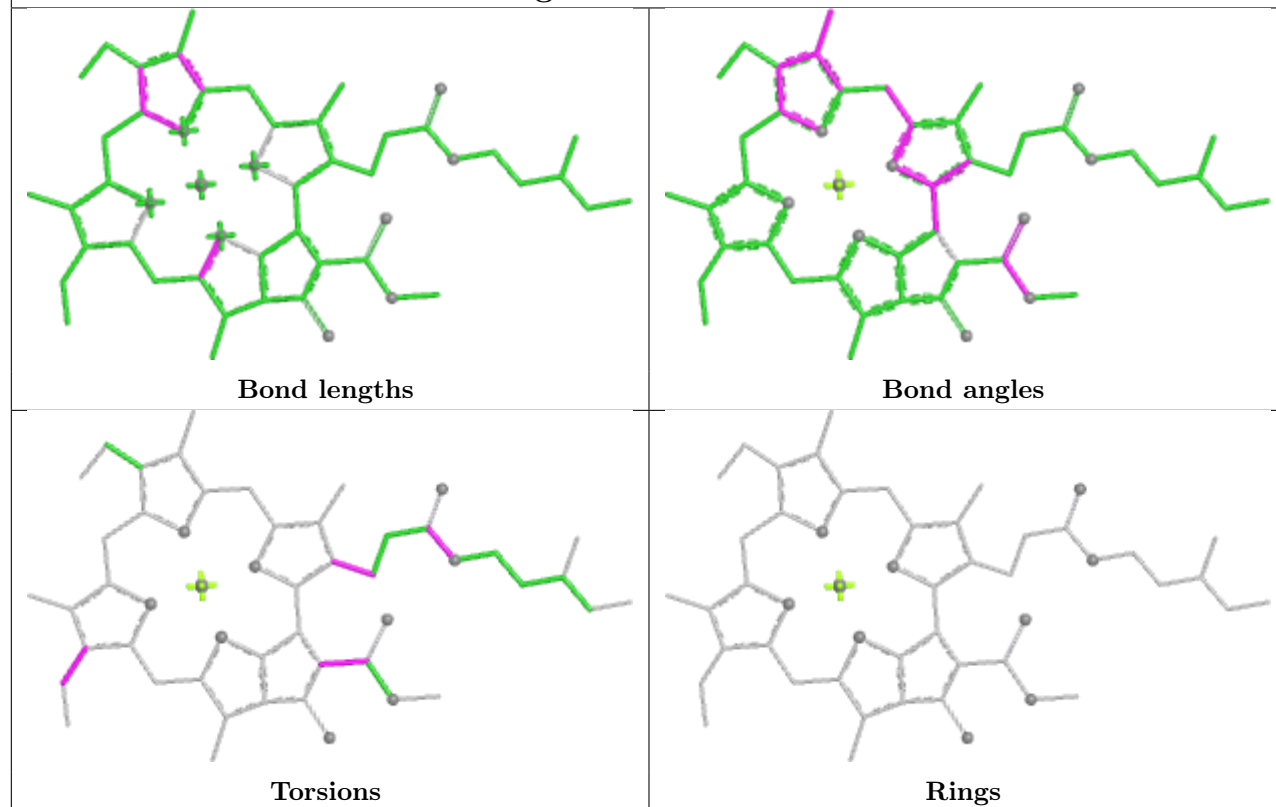


Ligand CLA f 609

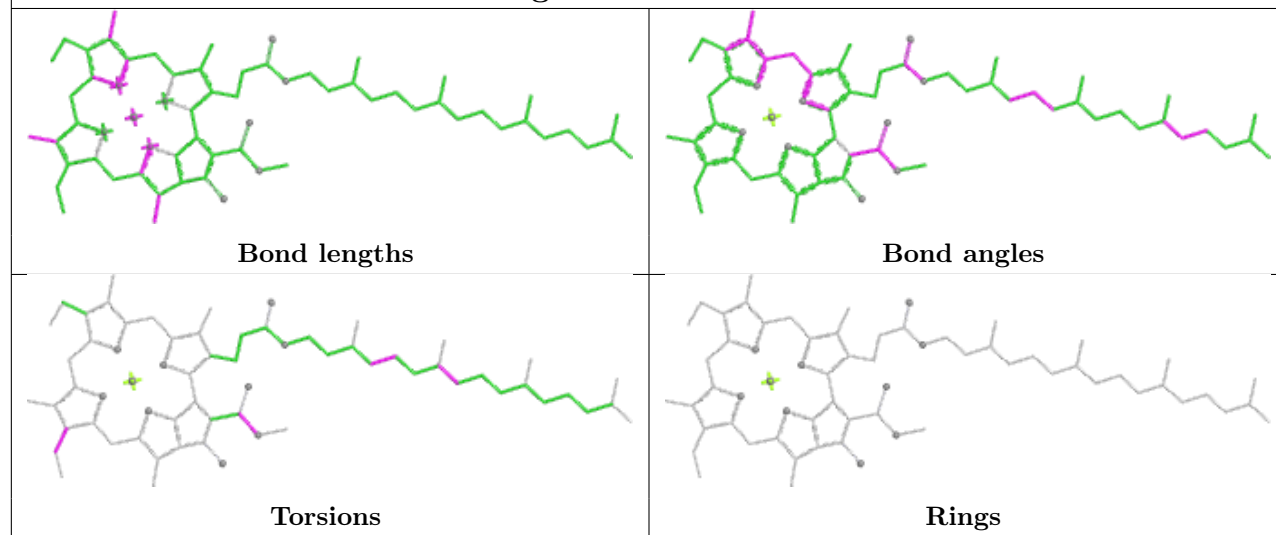


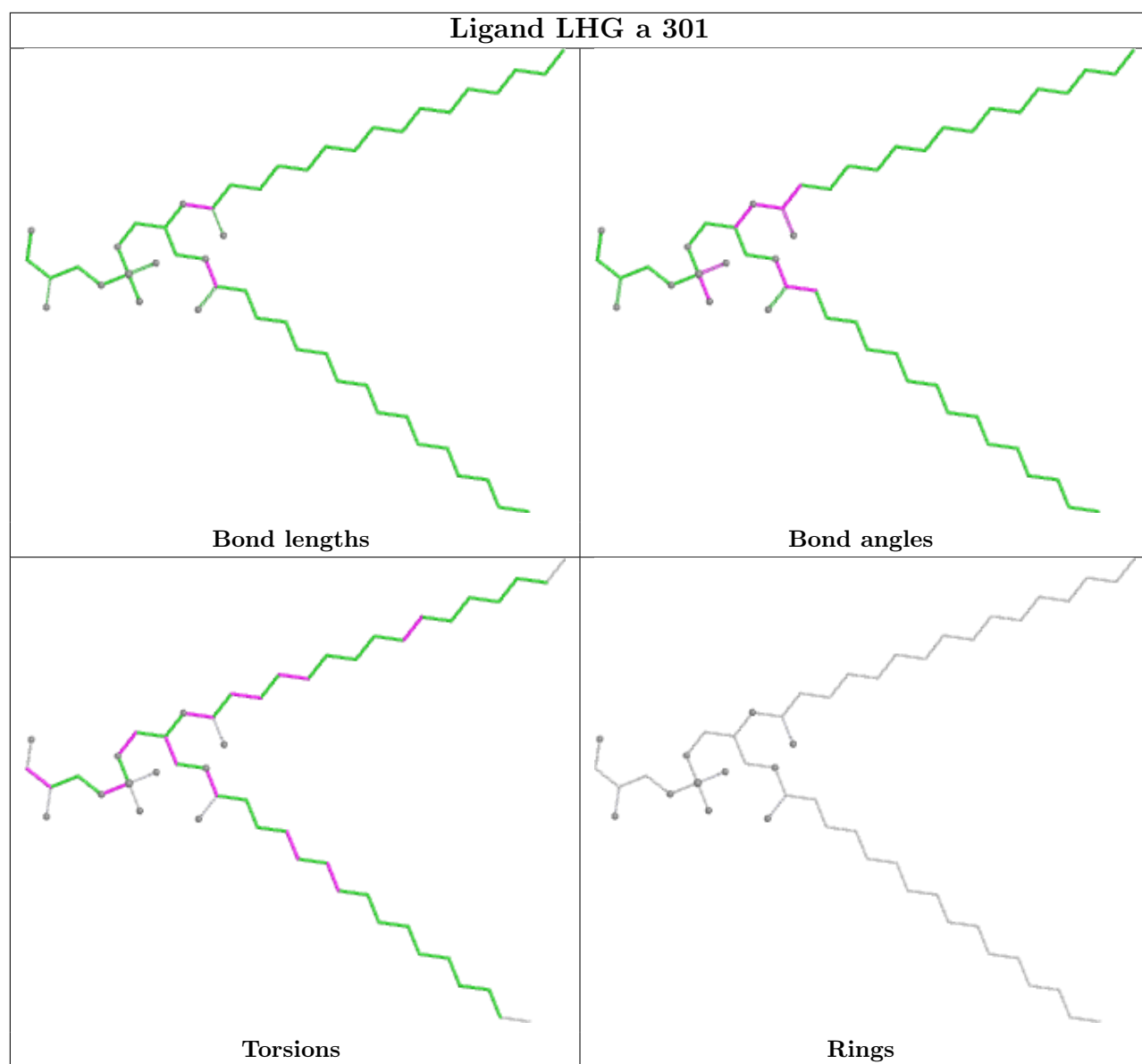


Ligand CLA d 304

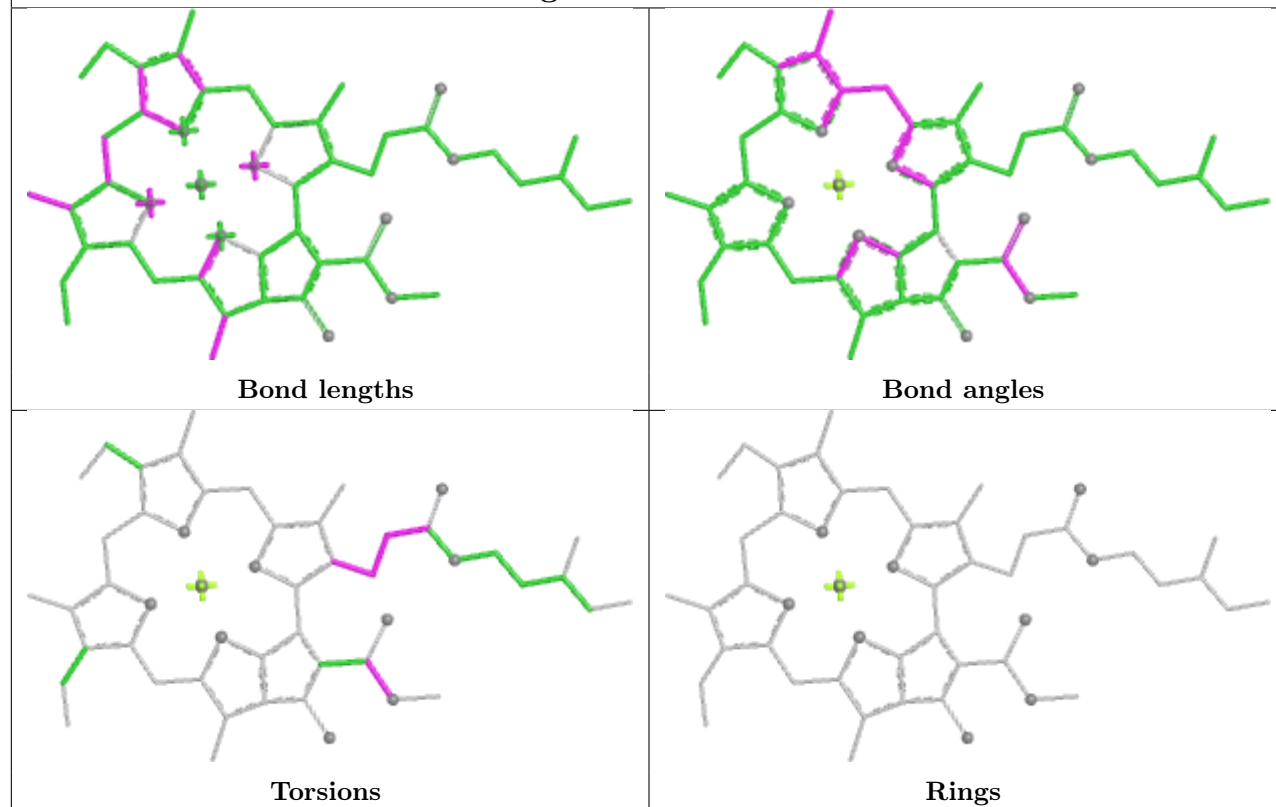


Ligand CLA A 820

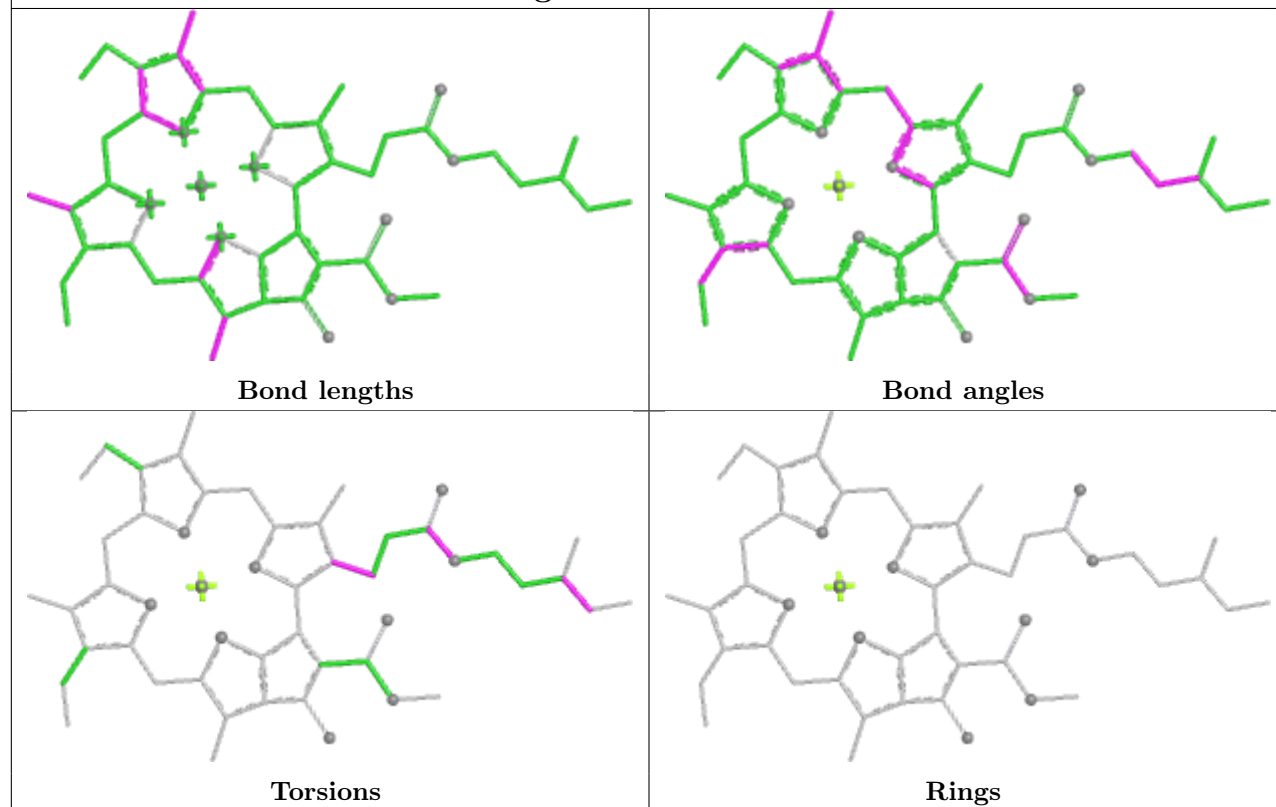


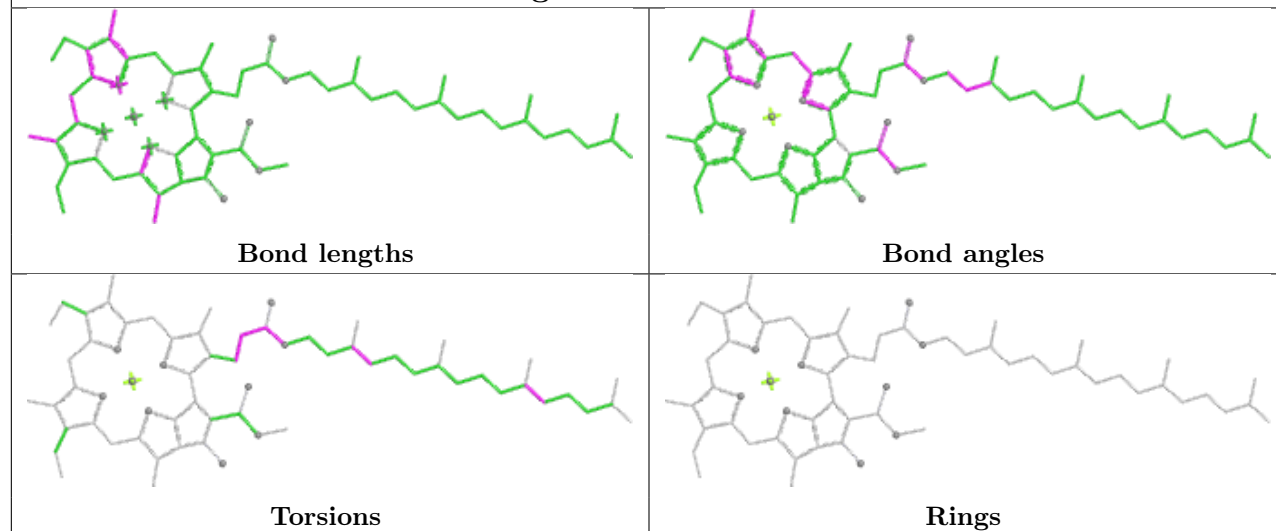
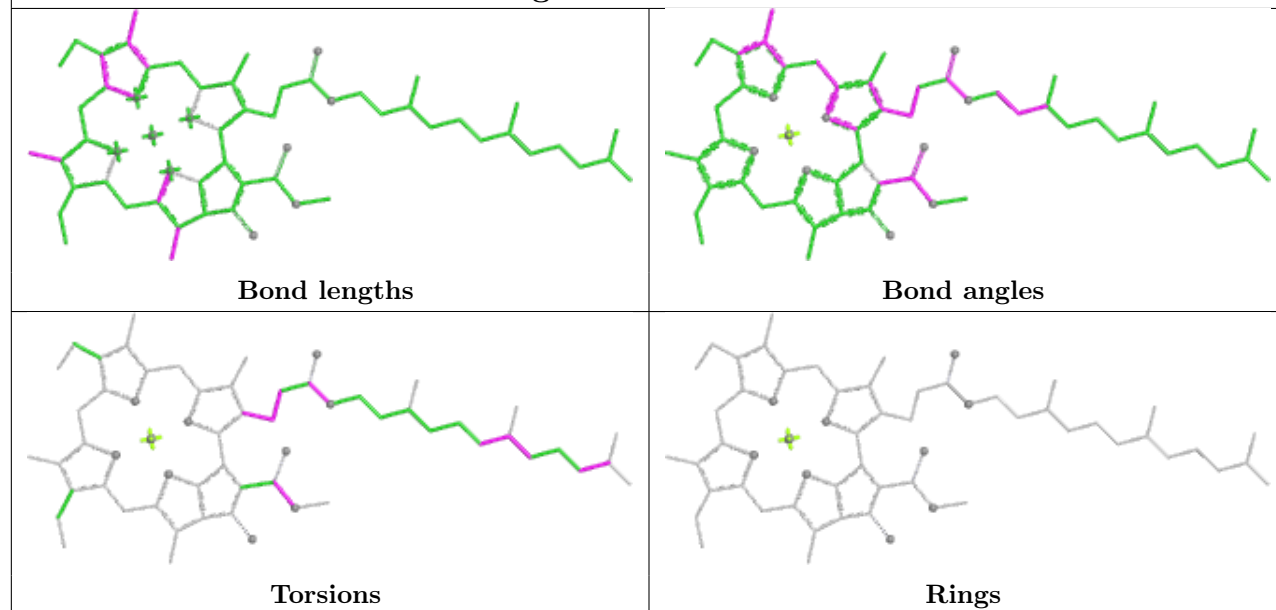


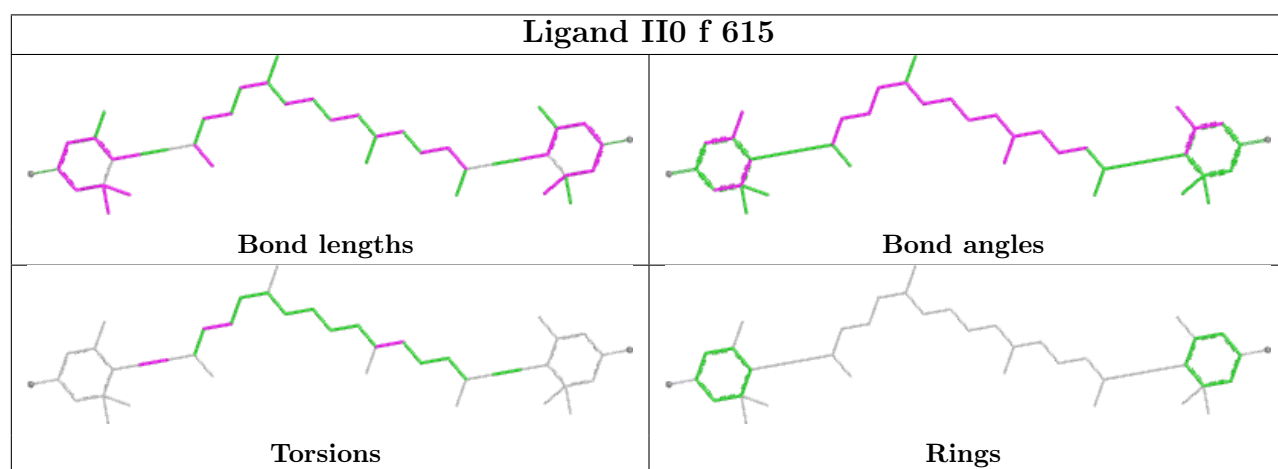
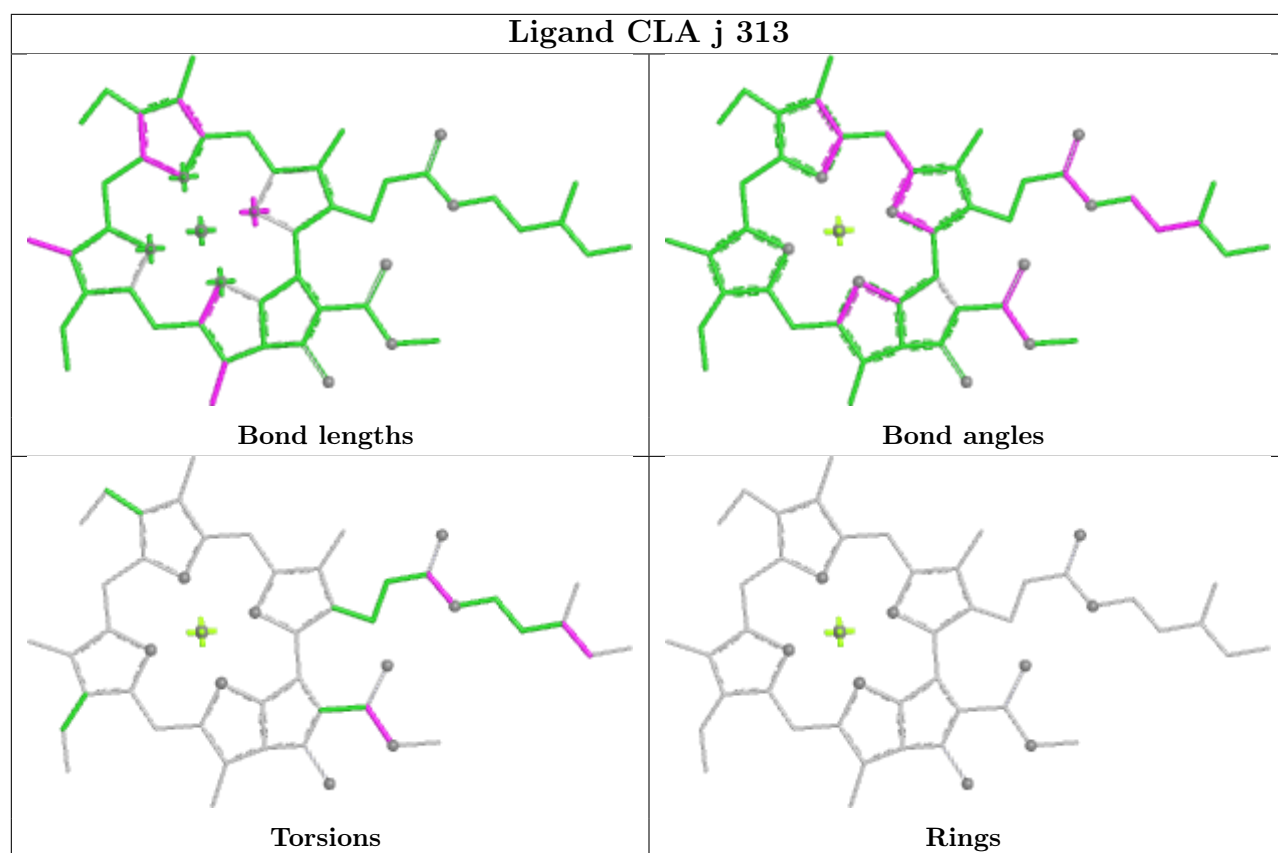
Ligand CLA i 610

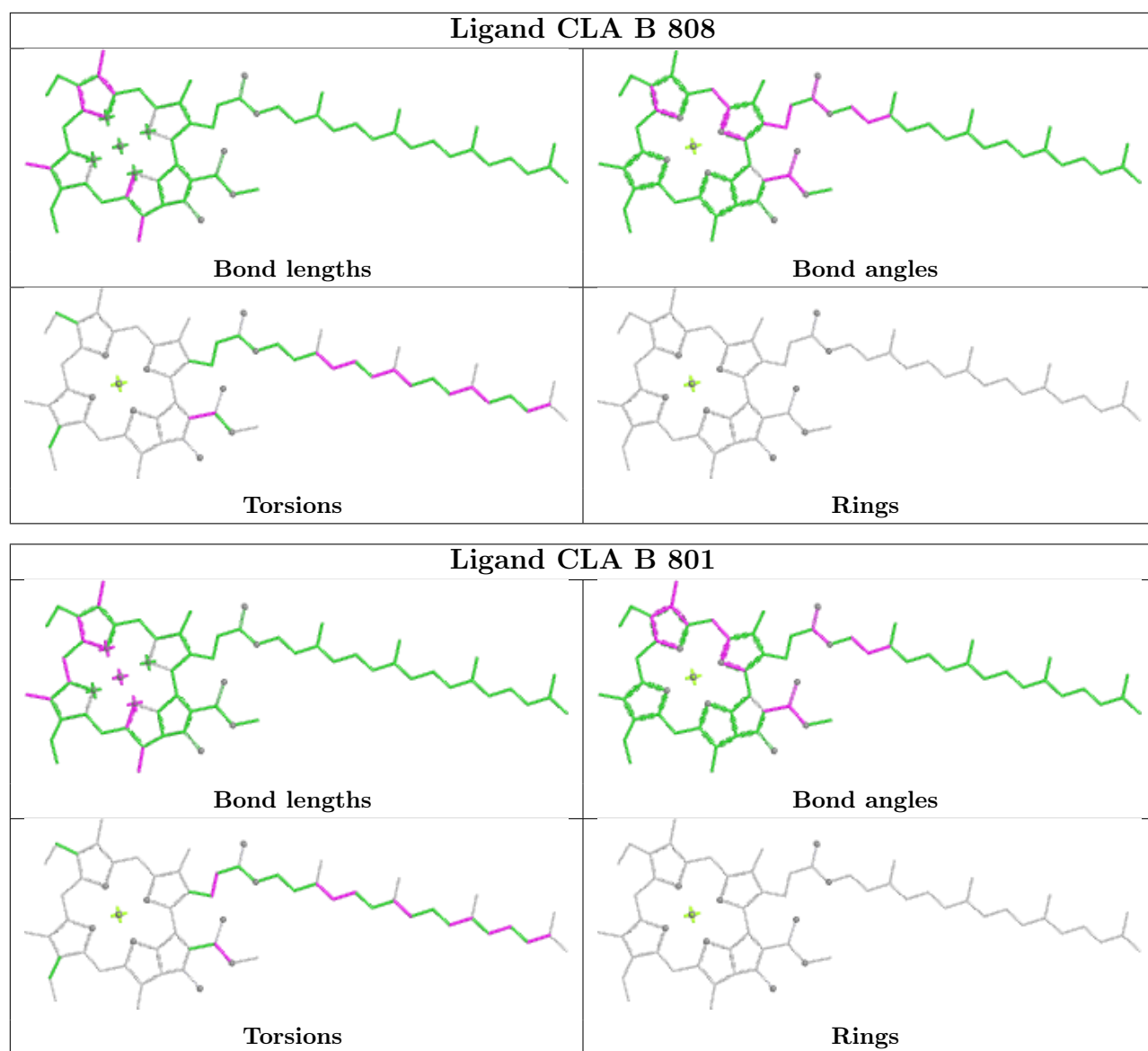


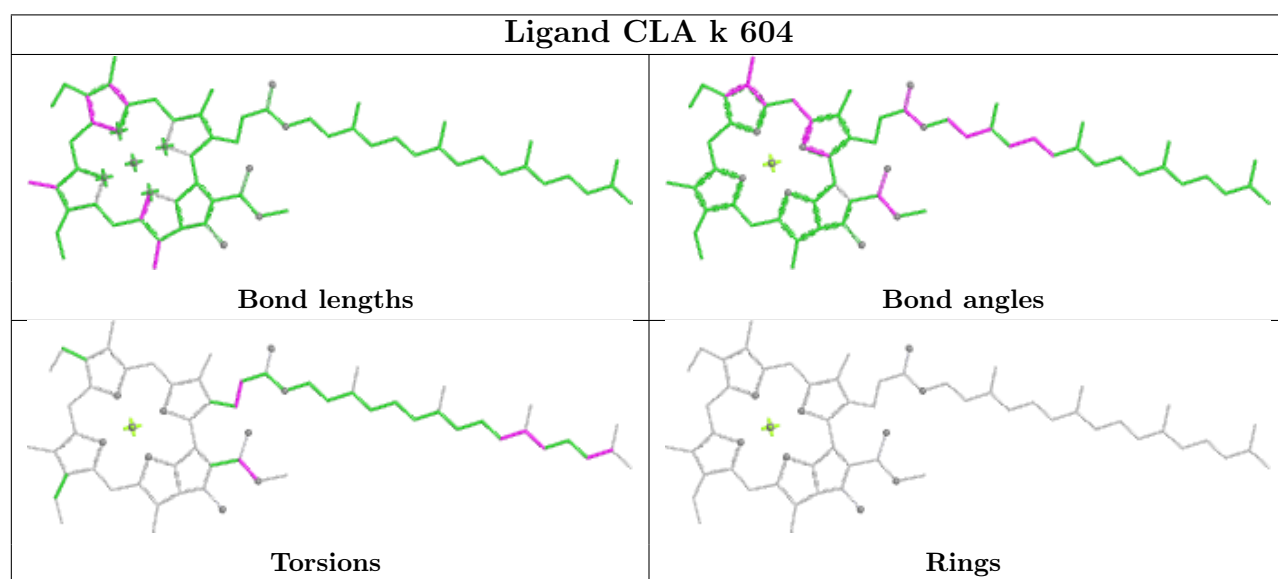
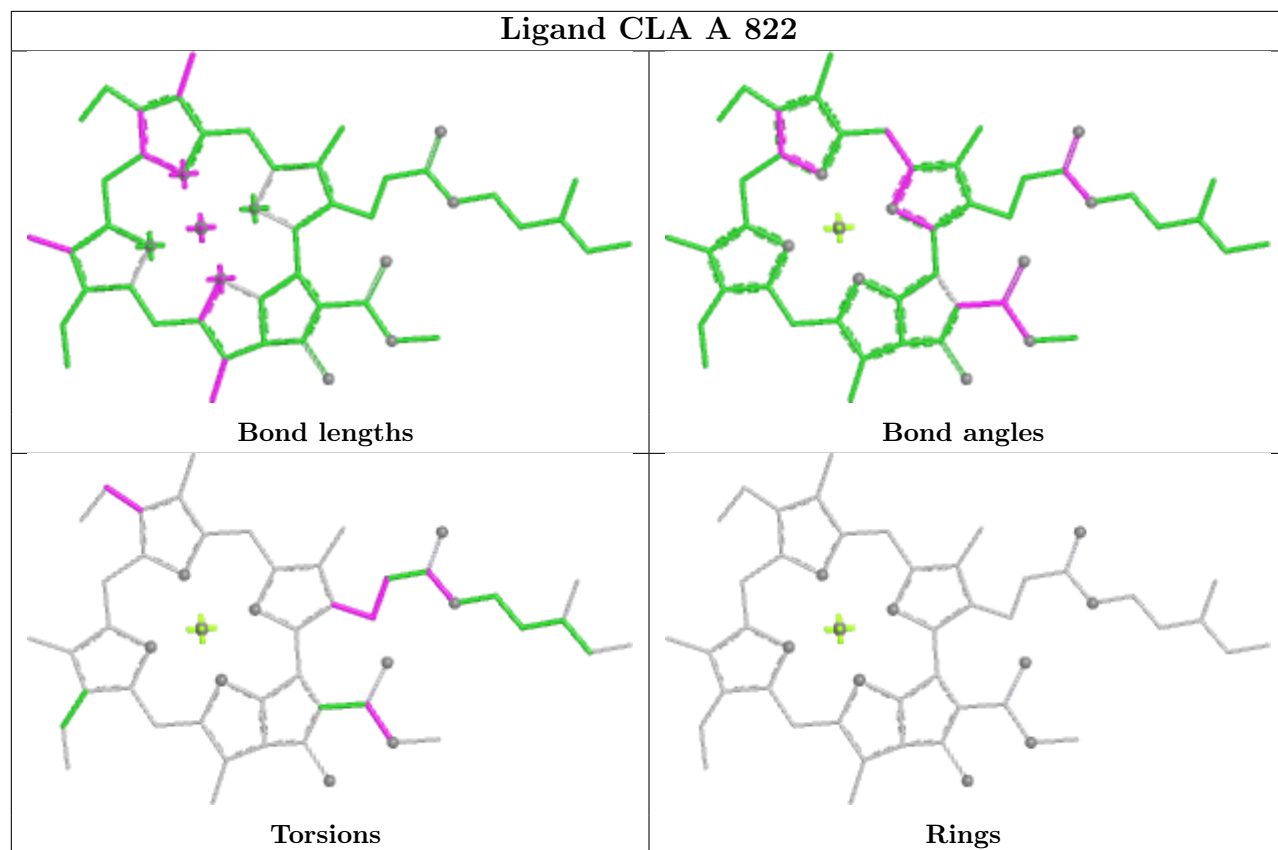
Ligand CLA L 207

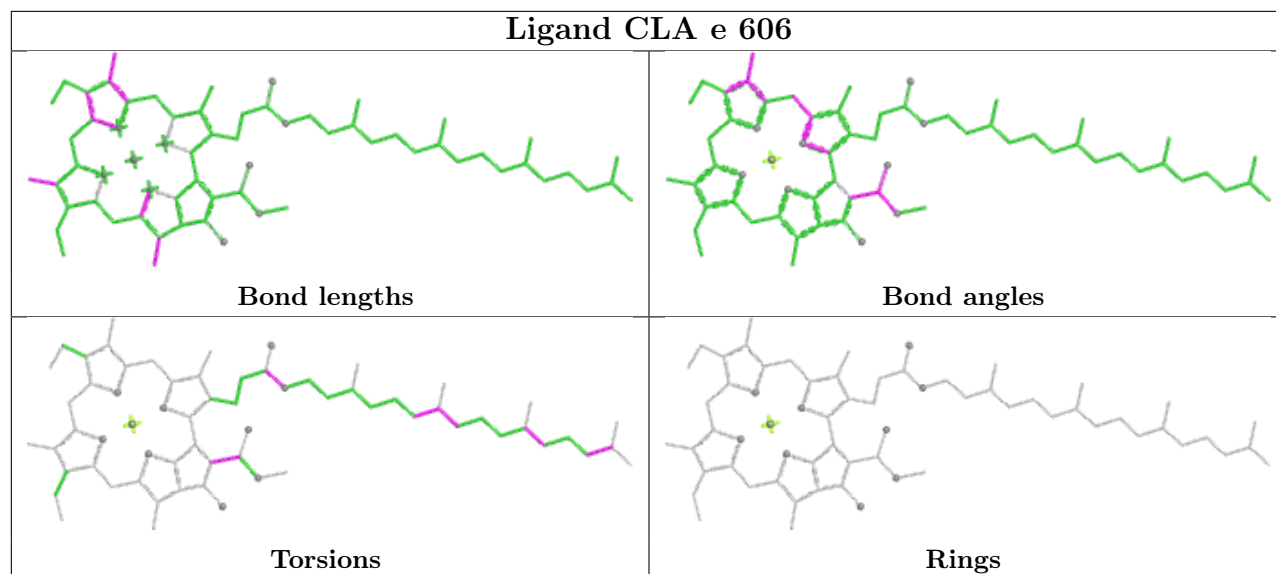
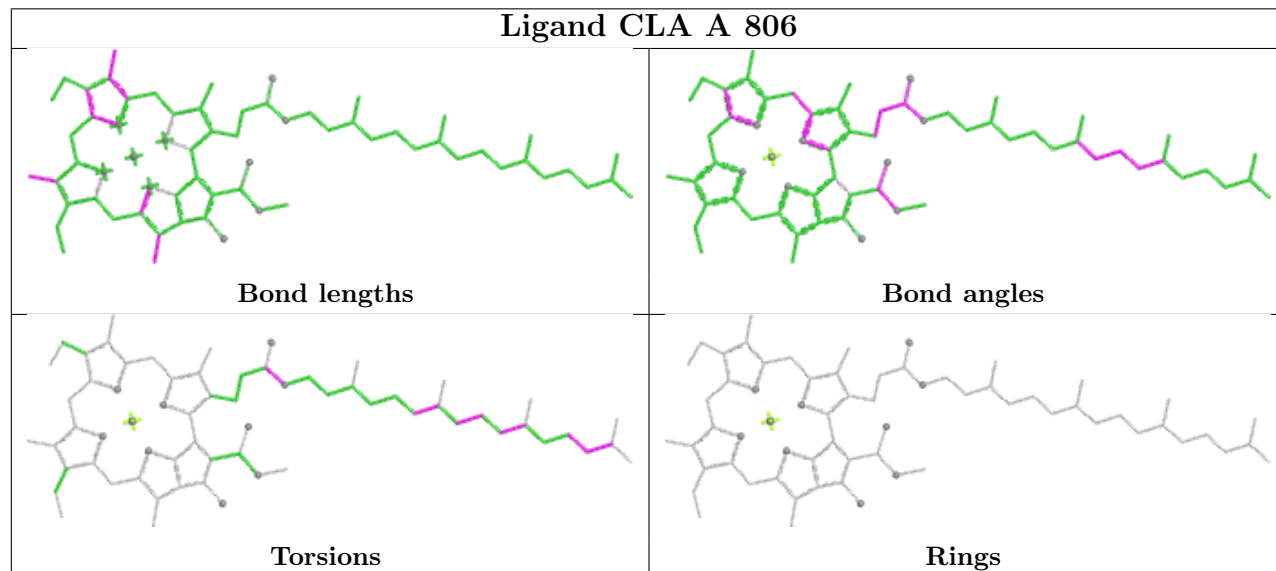


Ligand CLA A 828**Ligand CLA B 813**

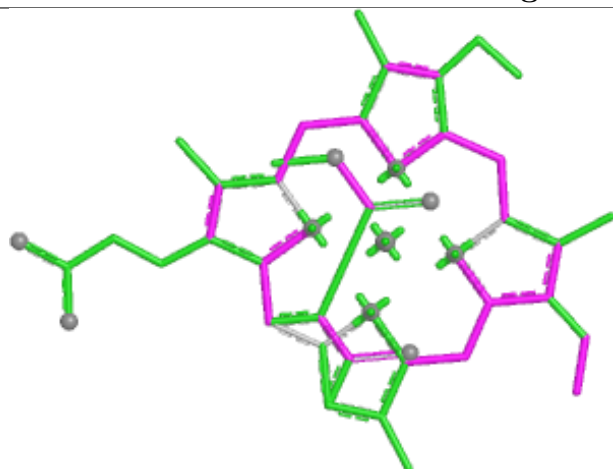




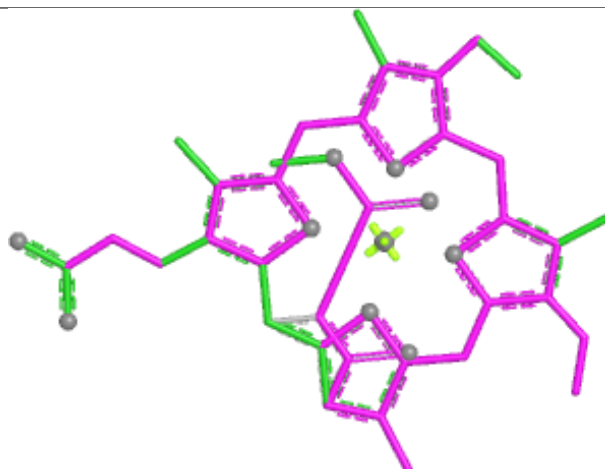


Ligand CLA e 606**Ligand CLA A 806**

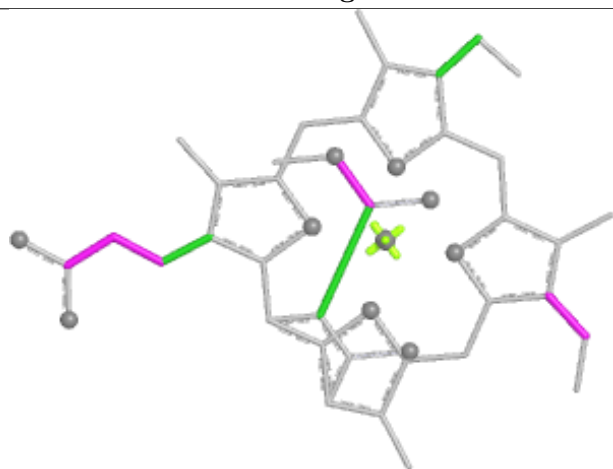
Ligand KC2 e 609



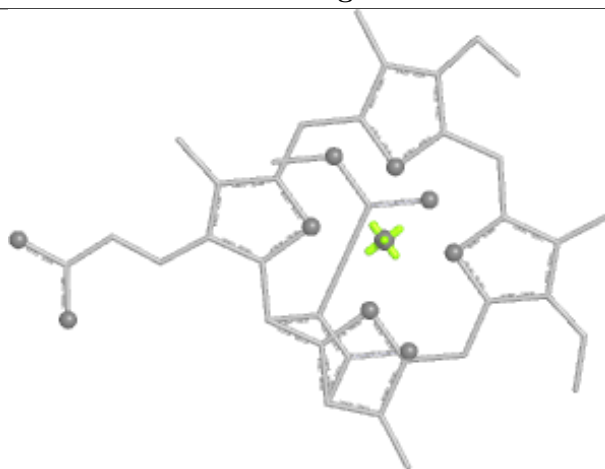
Bond lengths



Bond angles

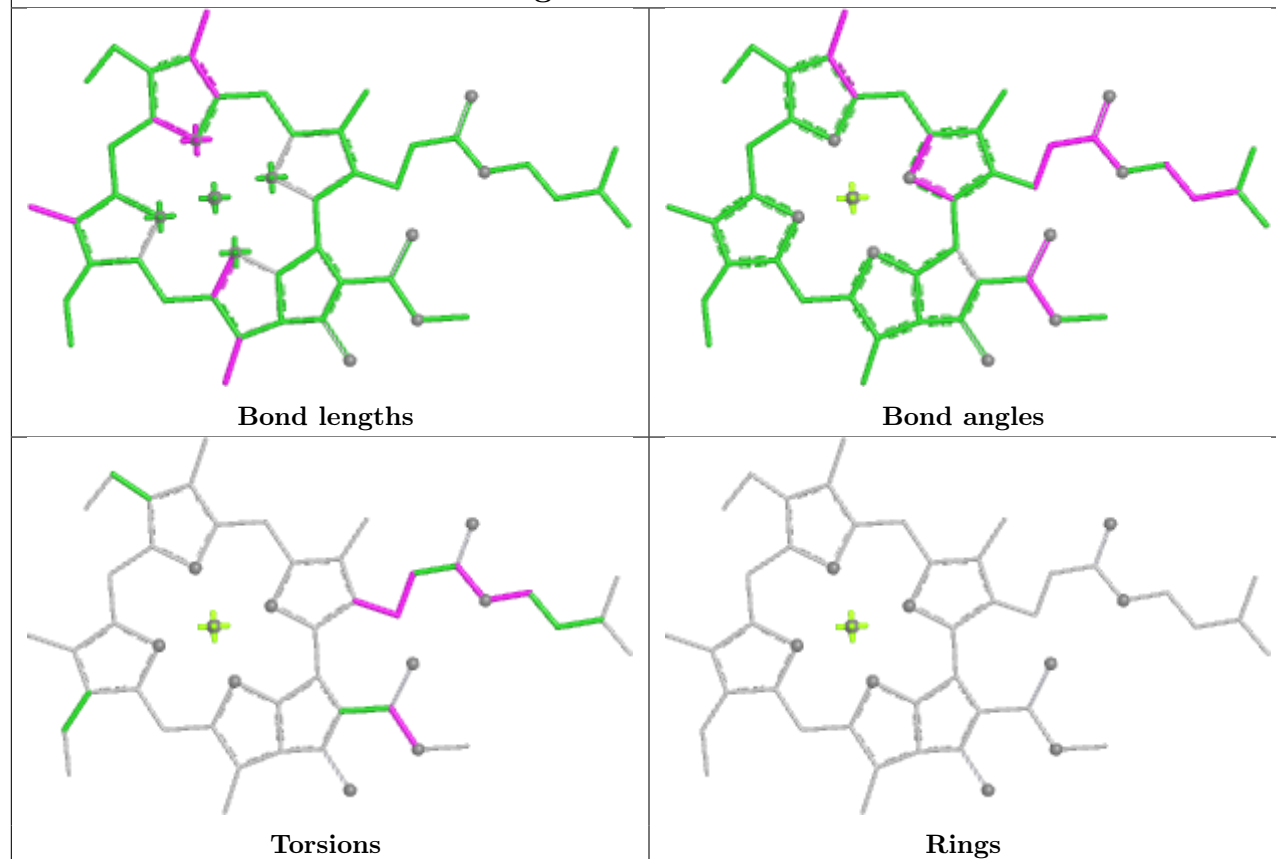


Torsions

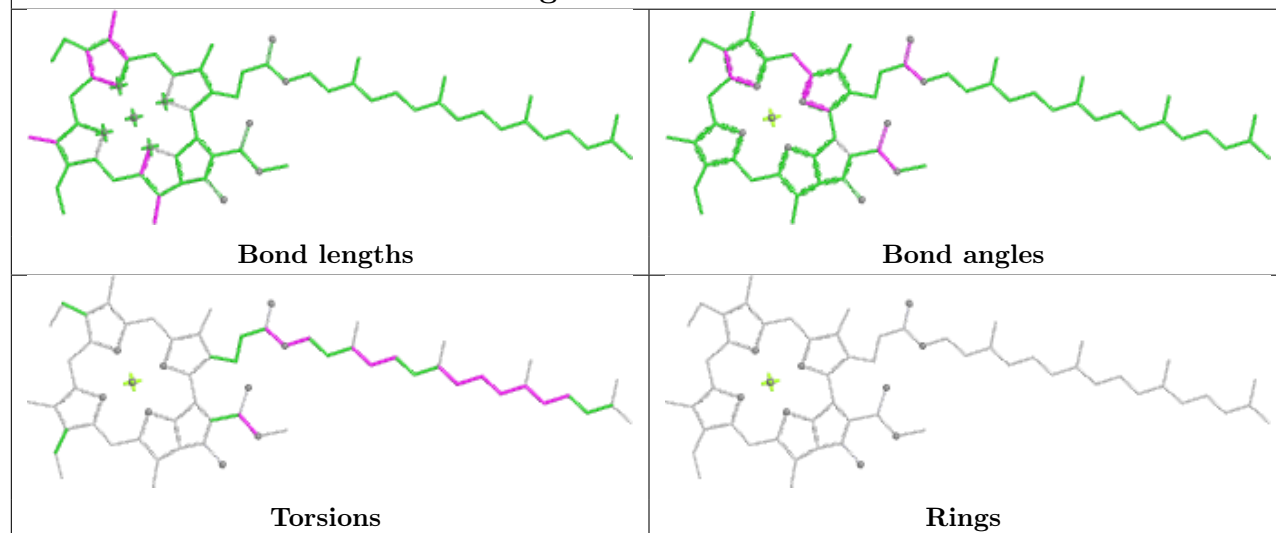


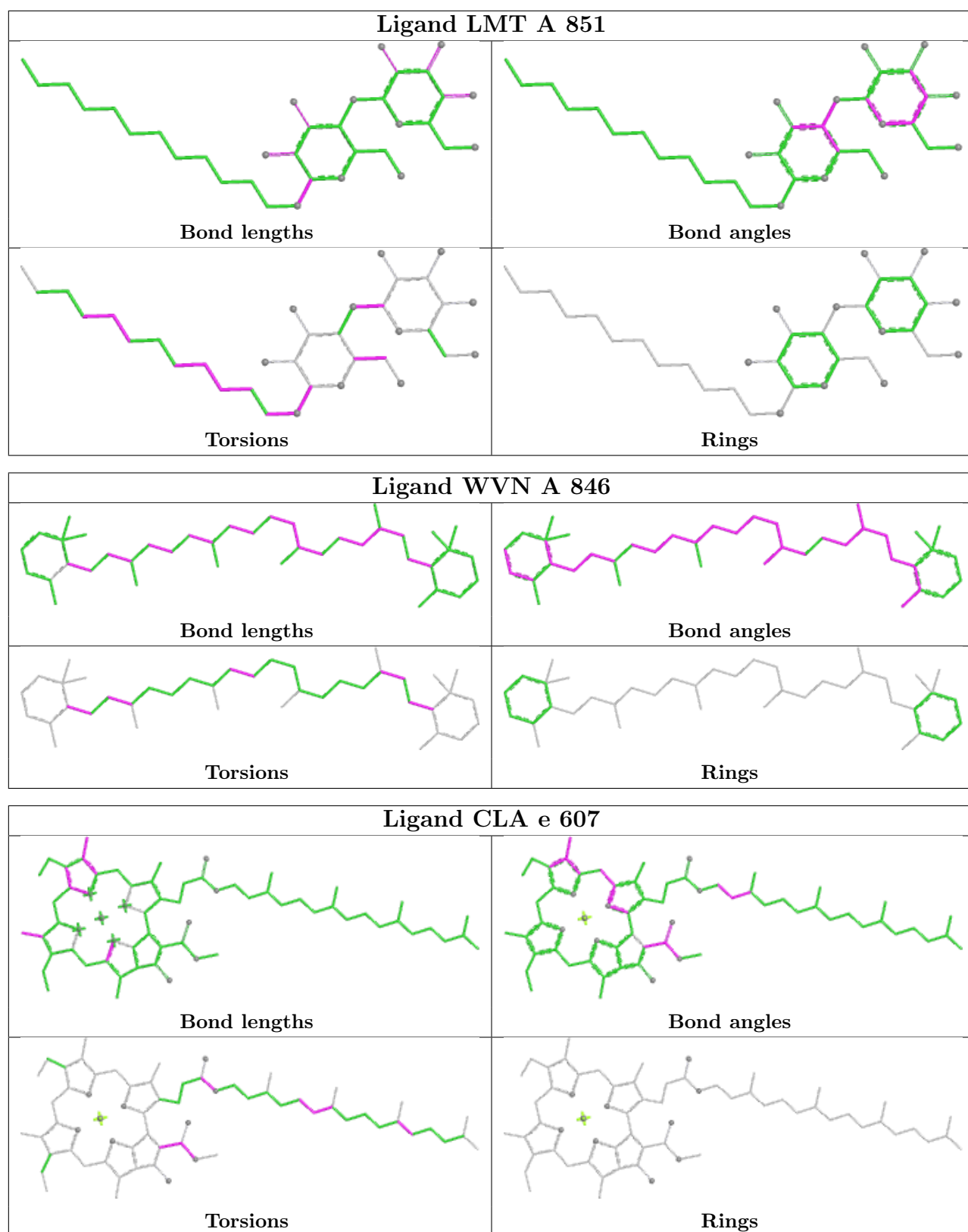
Rings

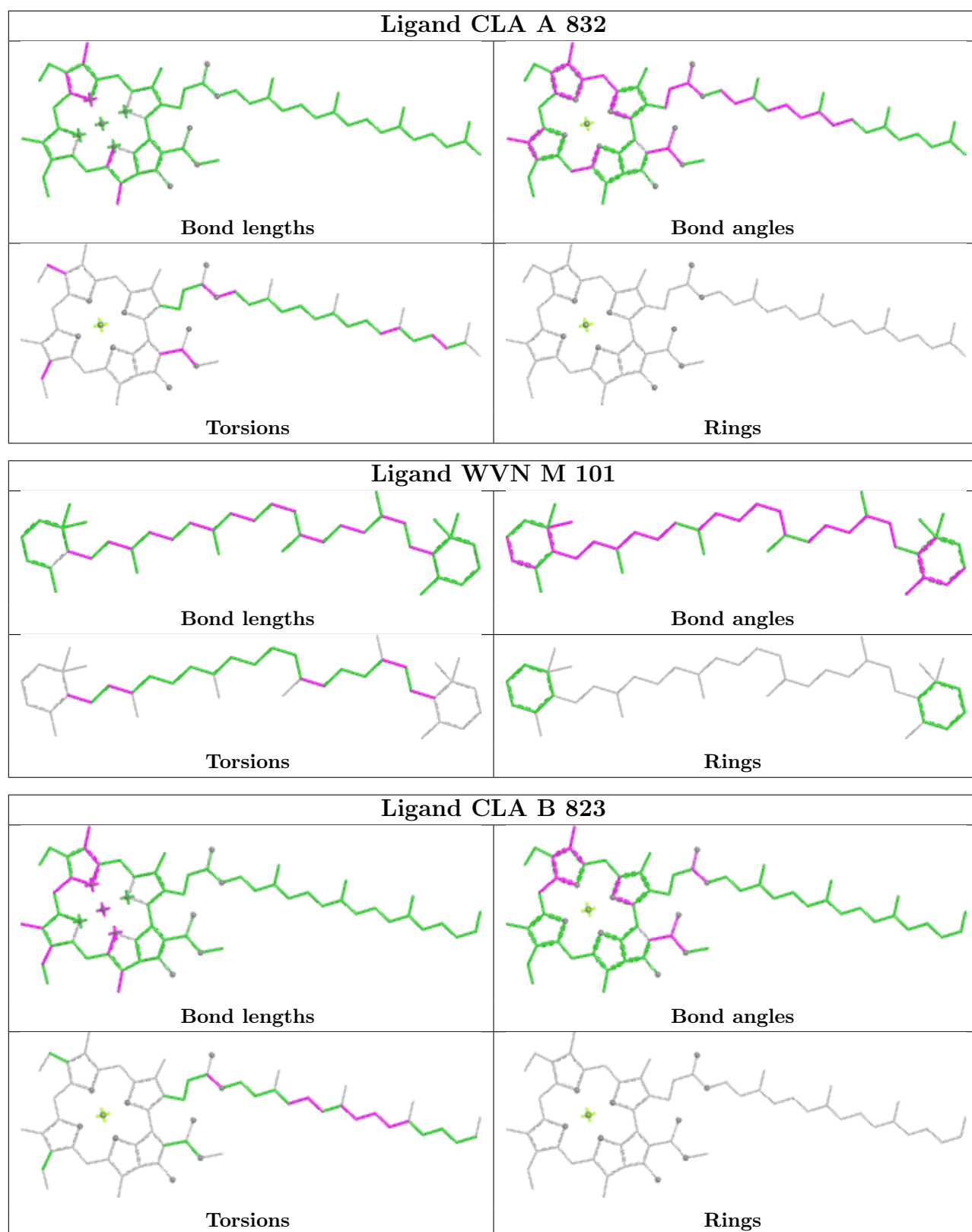
Ligand CLA L 204

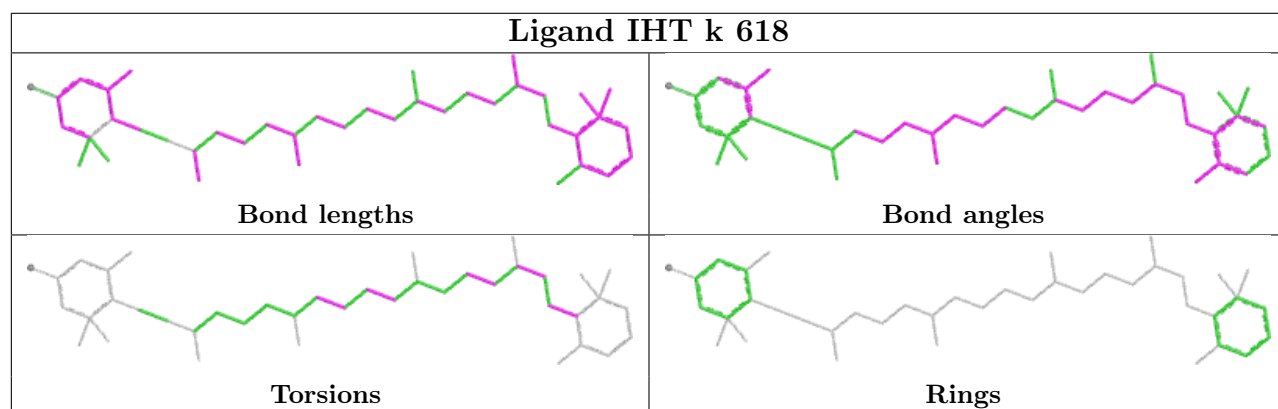
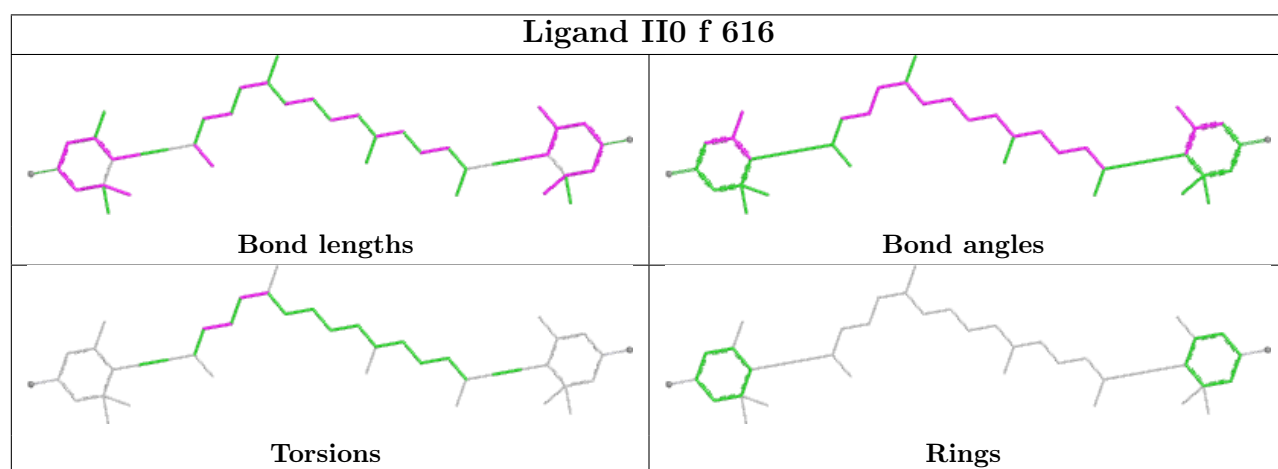
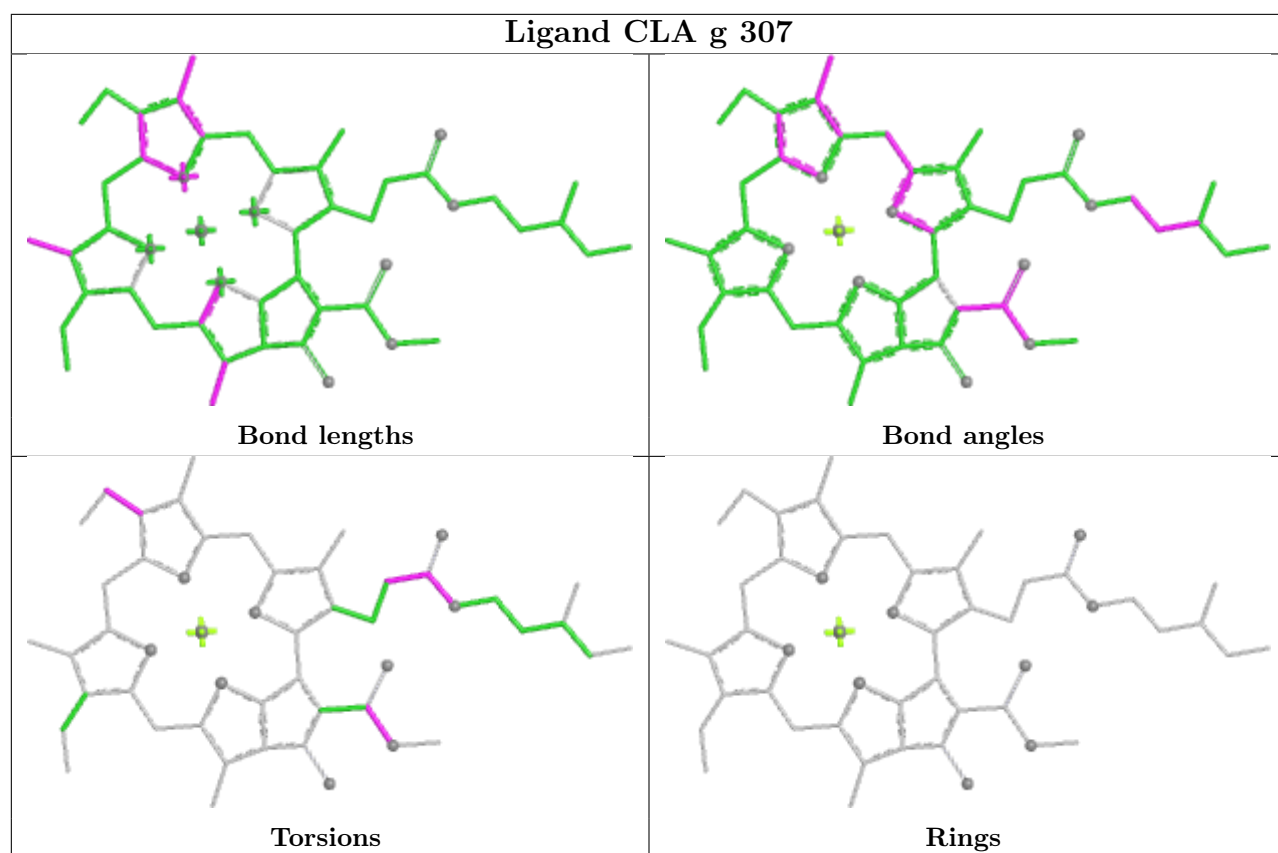


Ligand CLA f 610

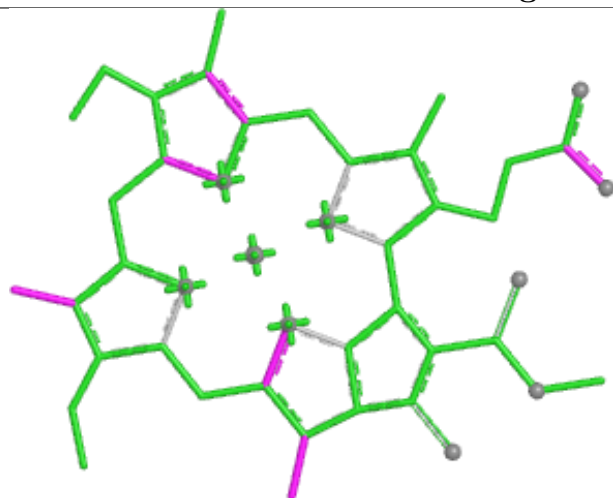




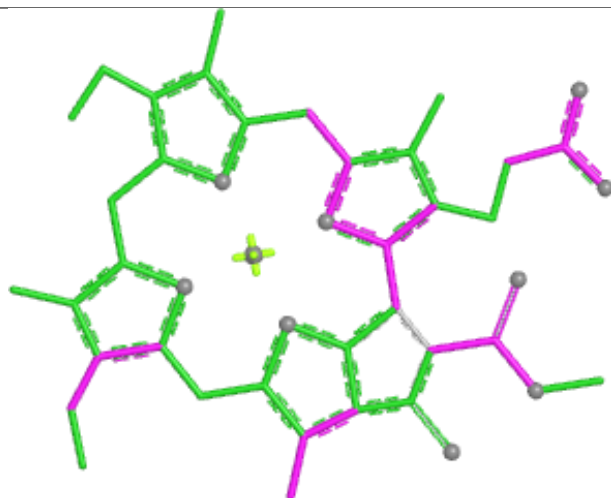




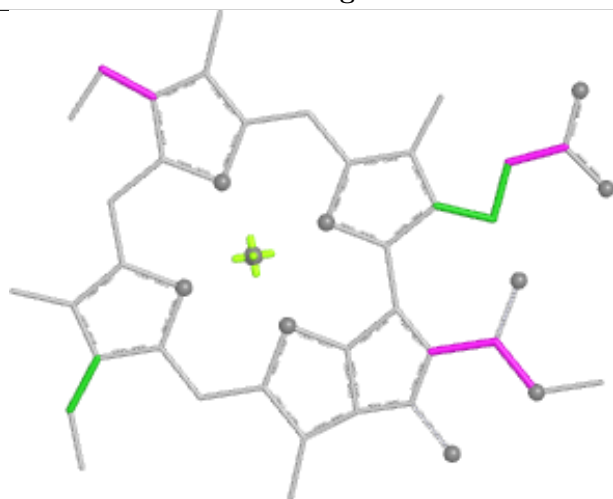
Ligand CLA c 611



Bond lengths



Bond angles

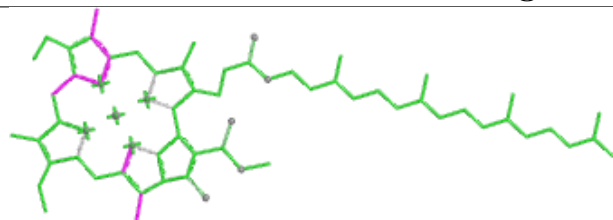


Torsions

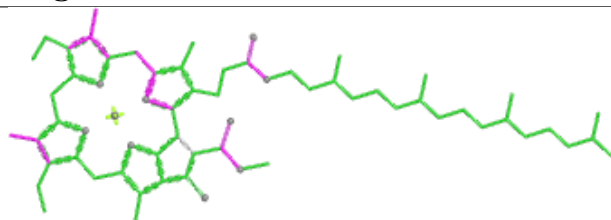


Rings

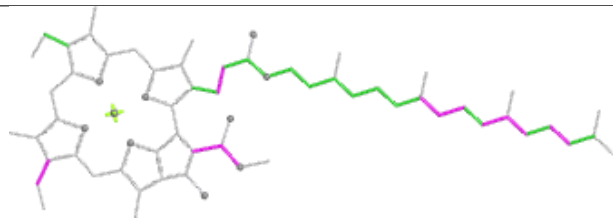
Ligand CLA g 305



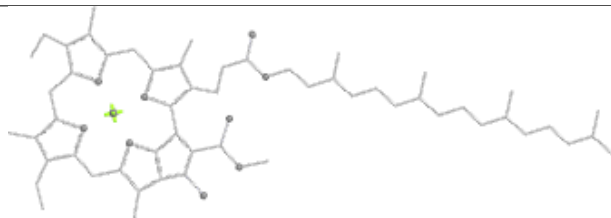
Bond lengths



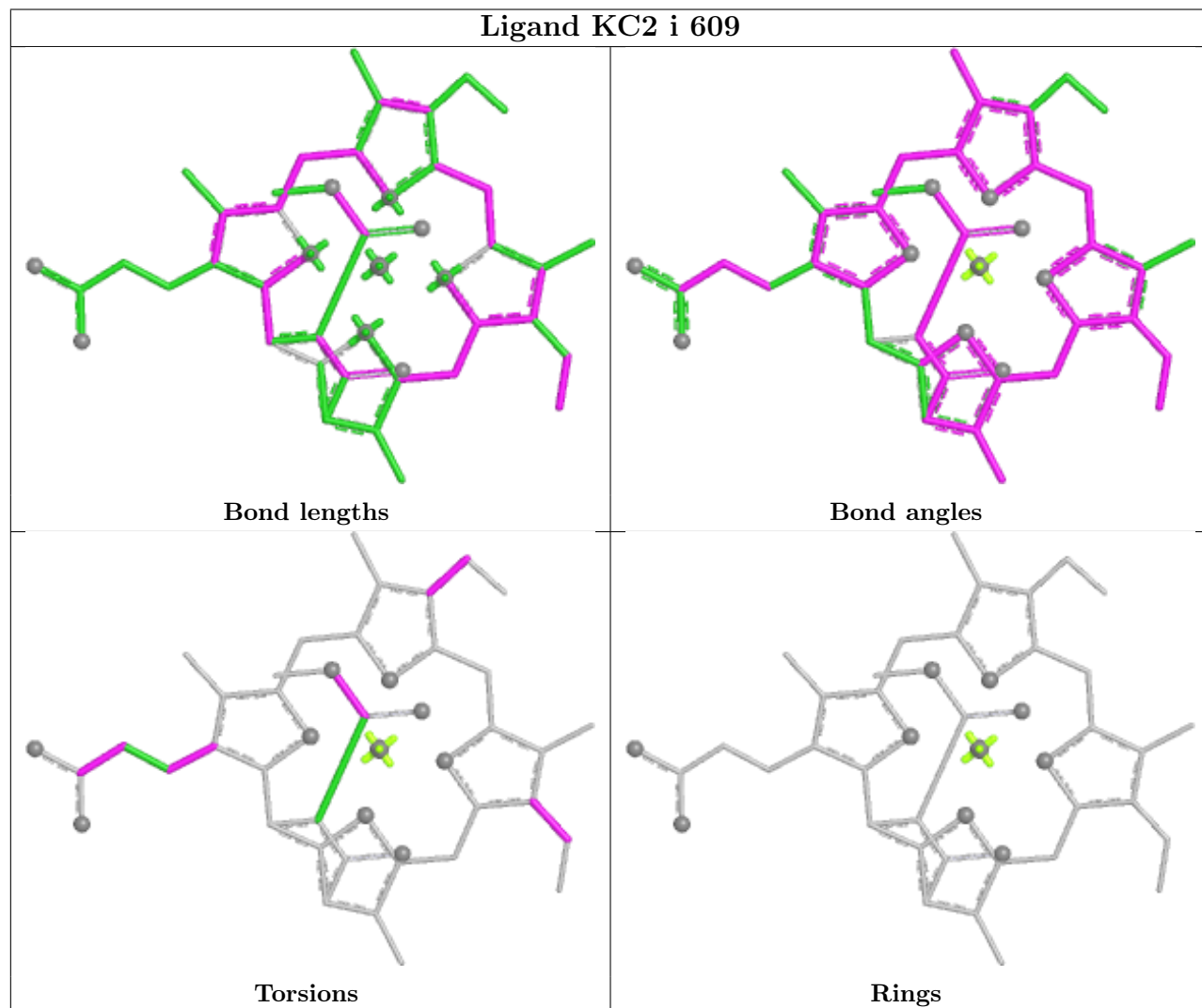
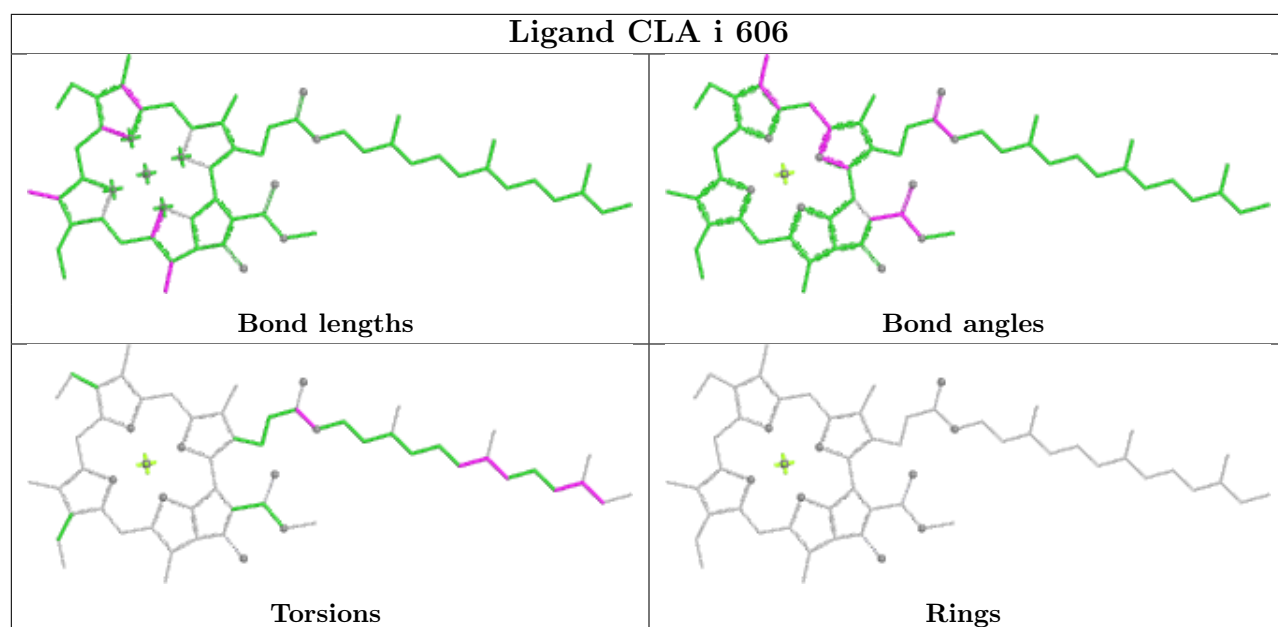
Bond angles

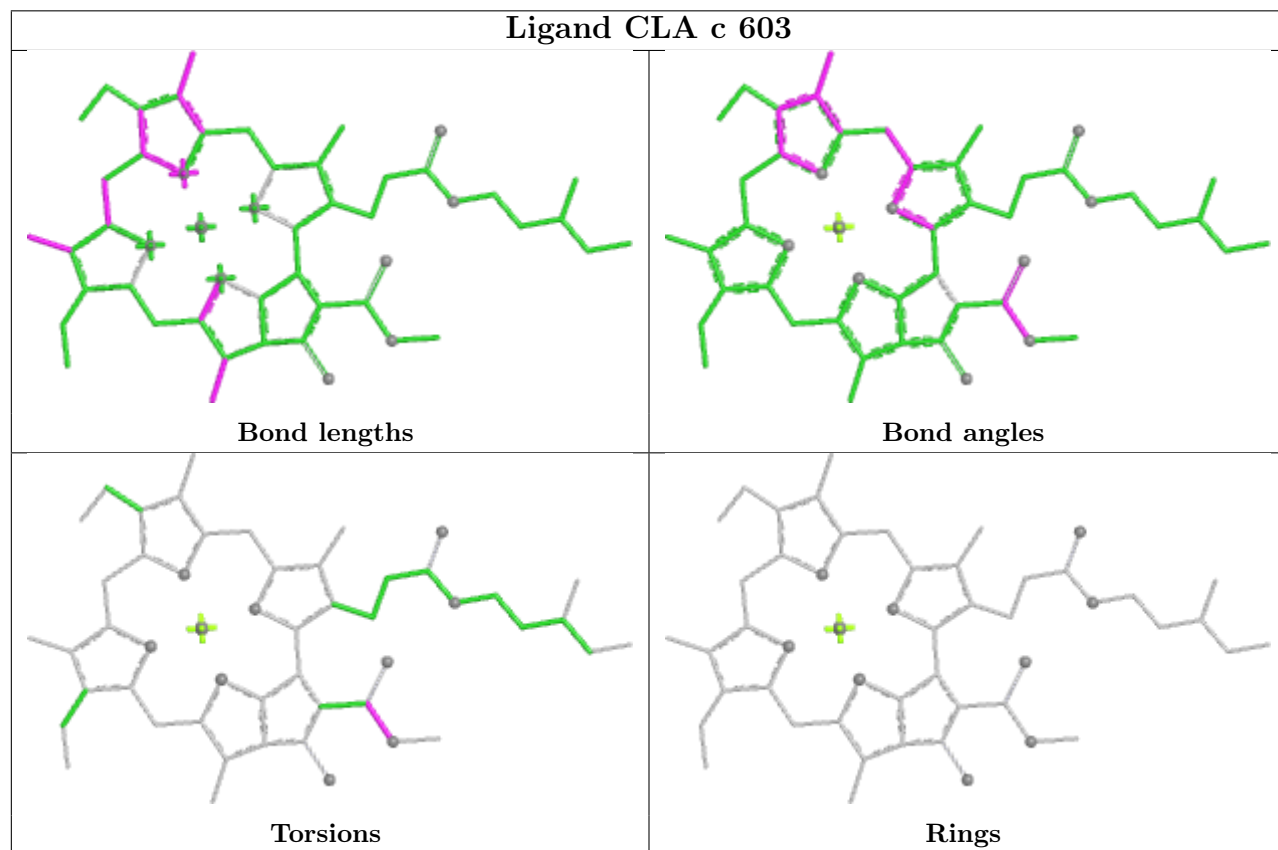
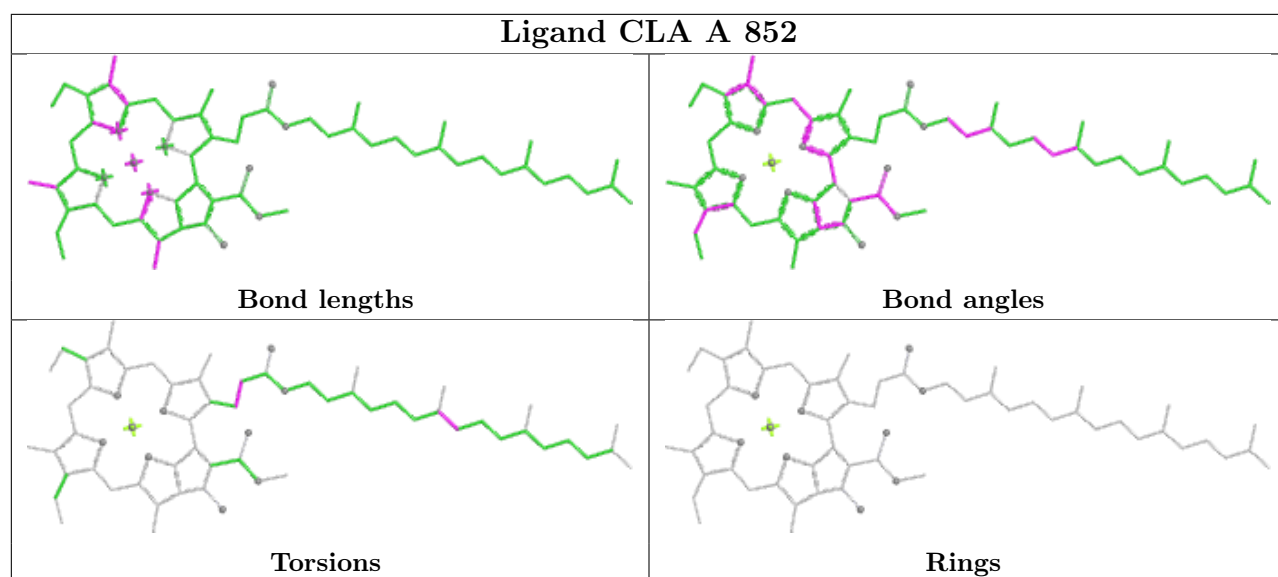


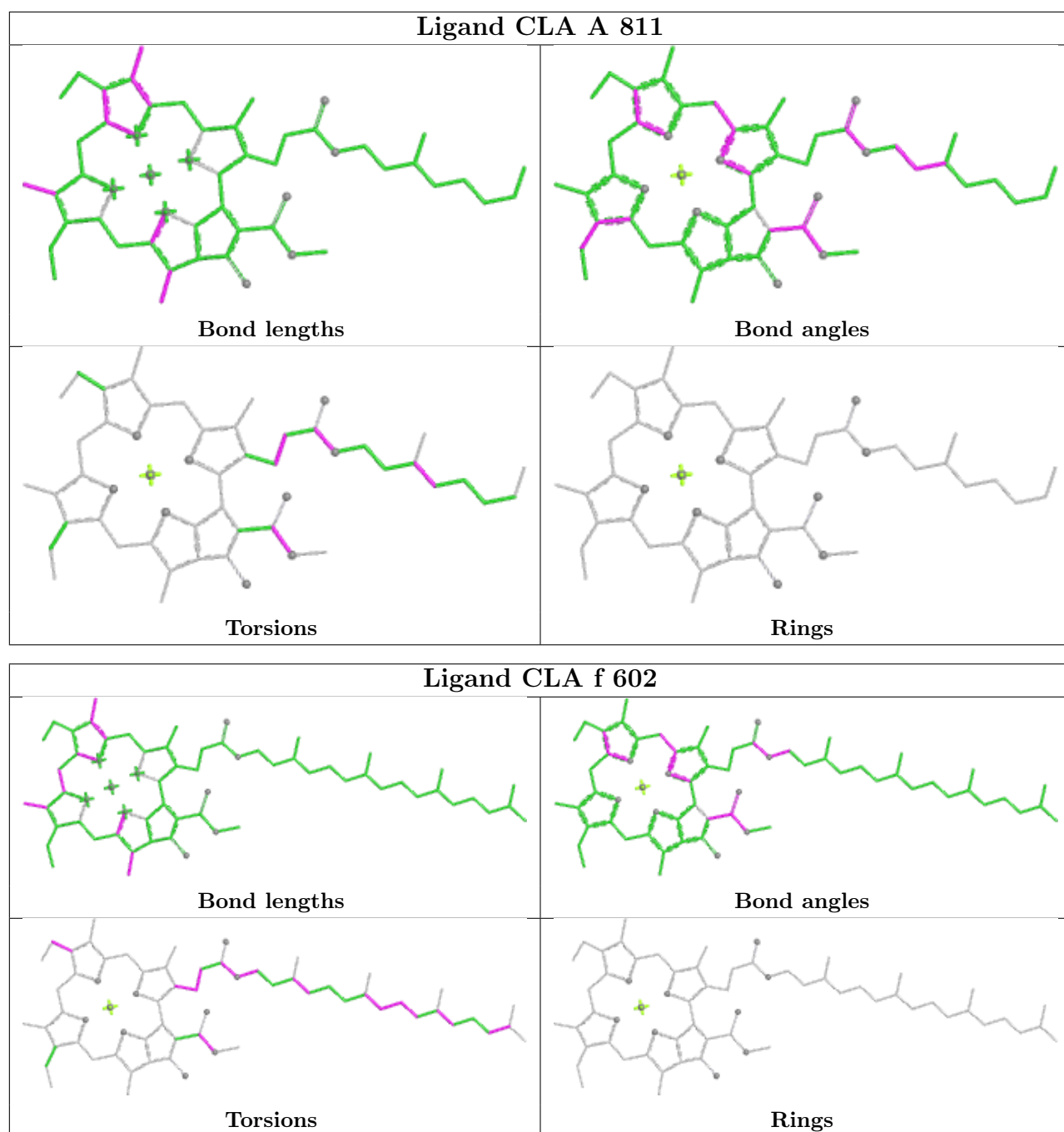
Torsions



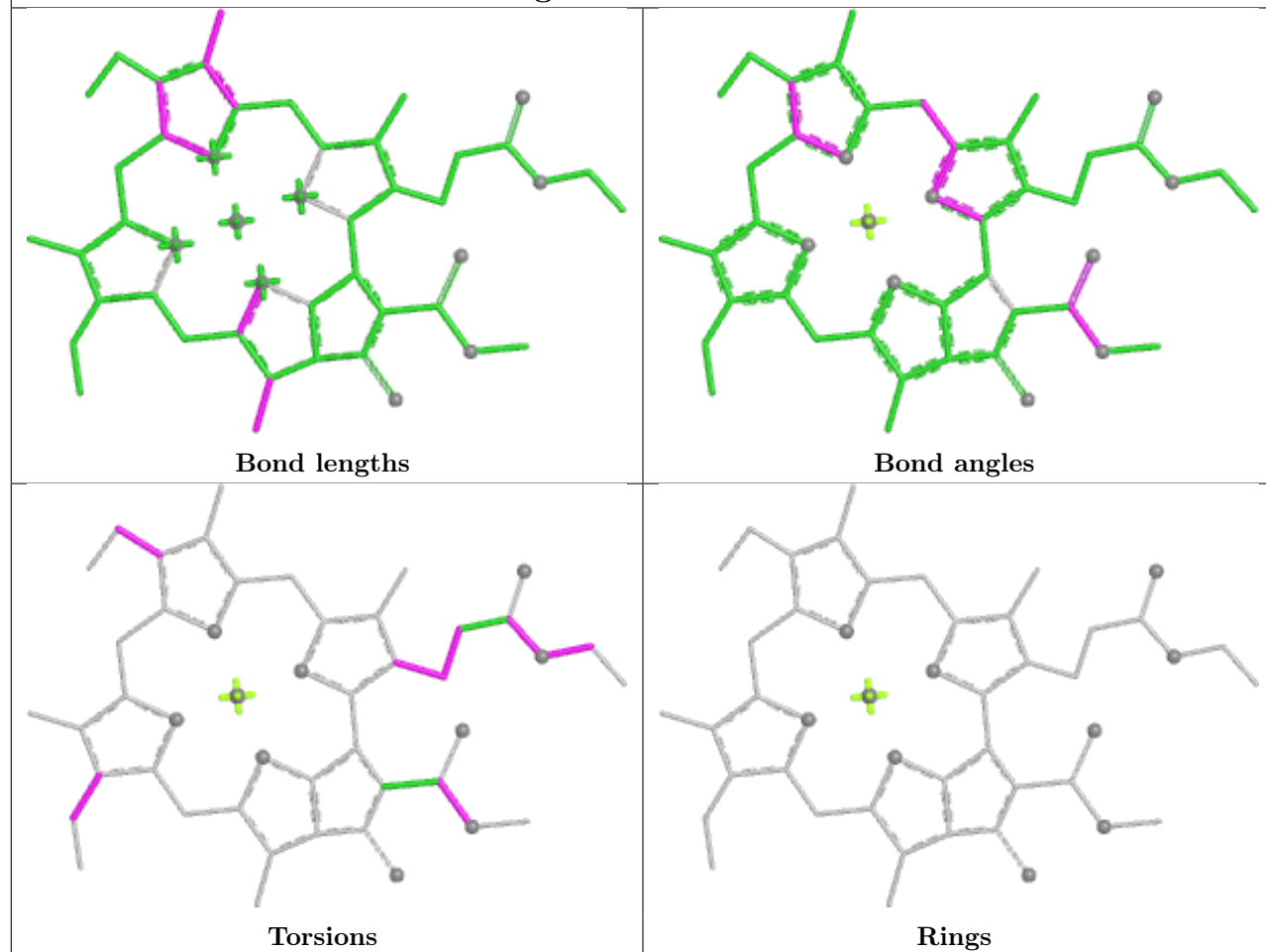
Rings



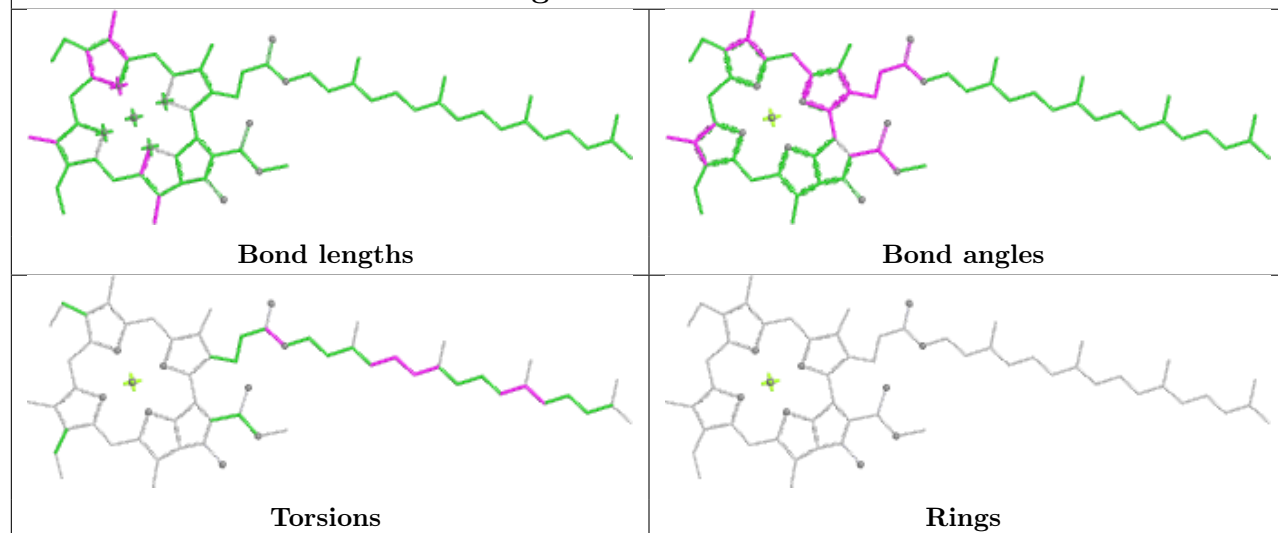




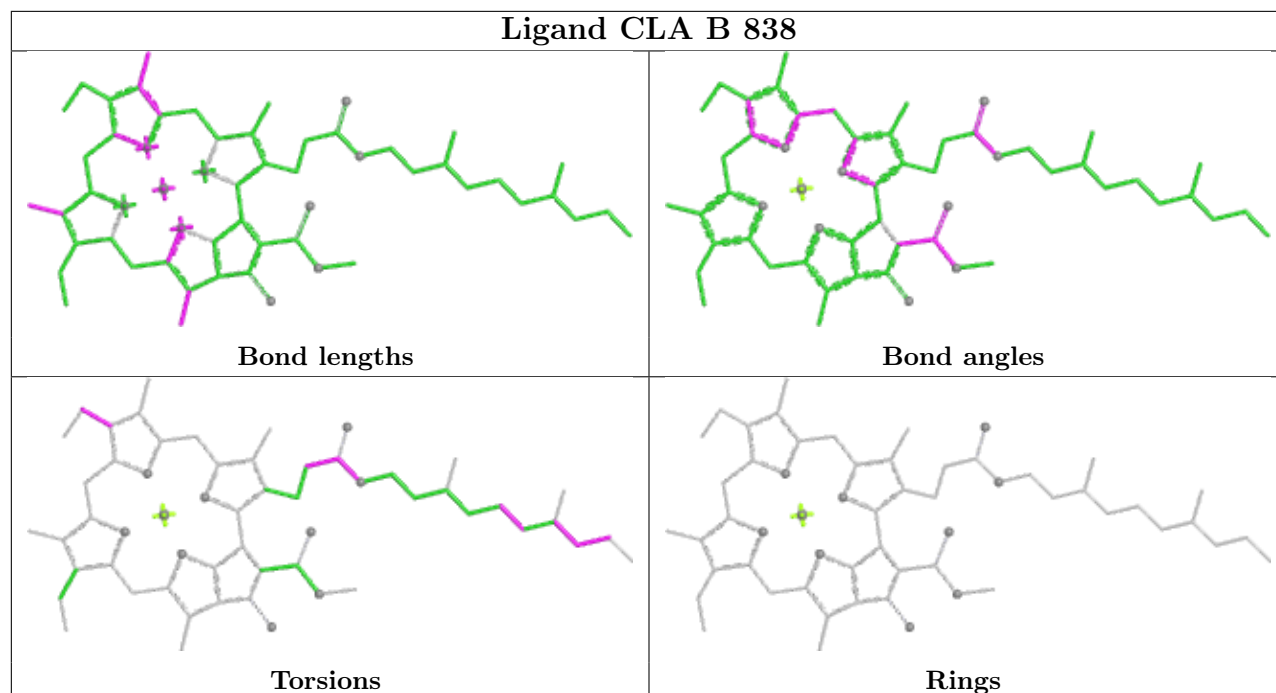
Ligand CLA f 601



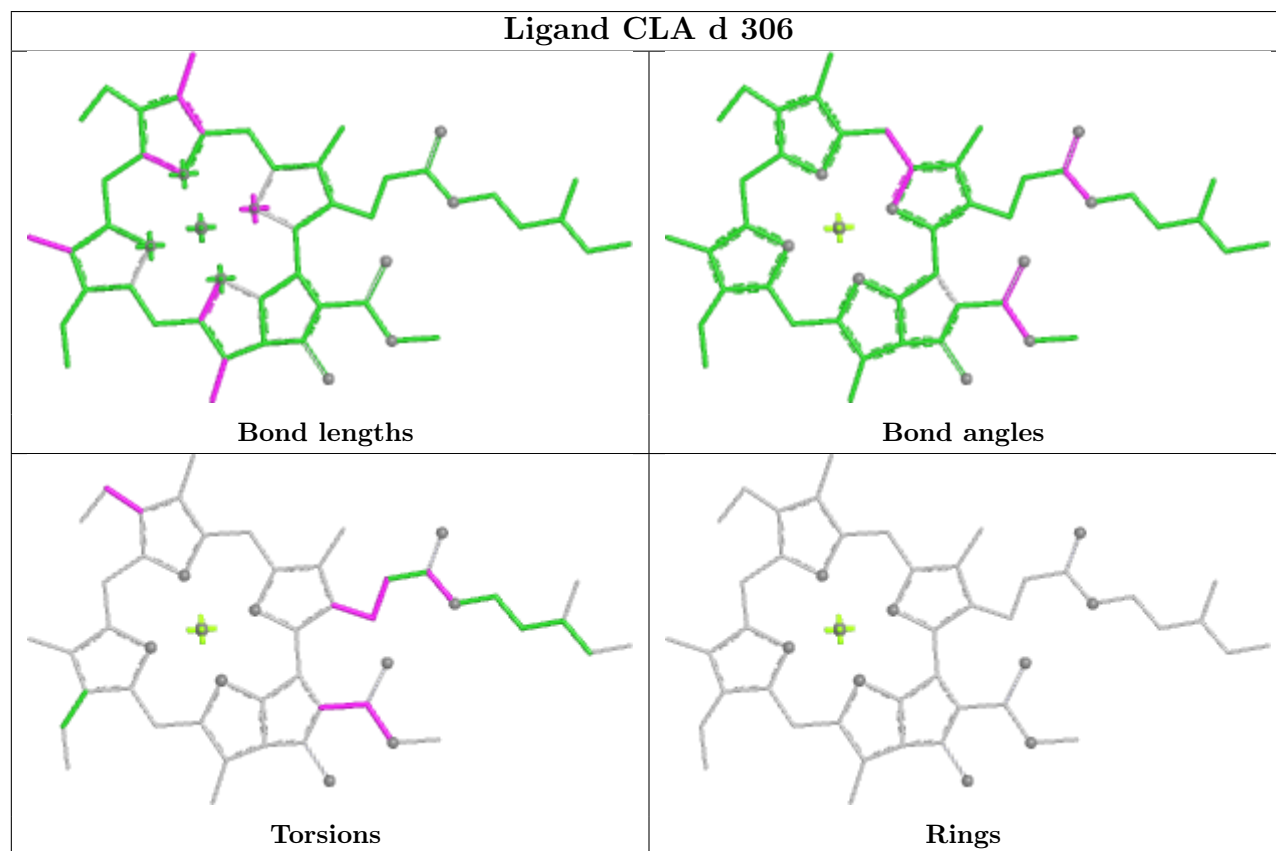
Ligand CLA A 826

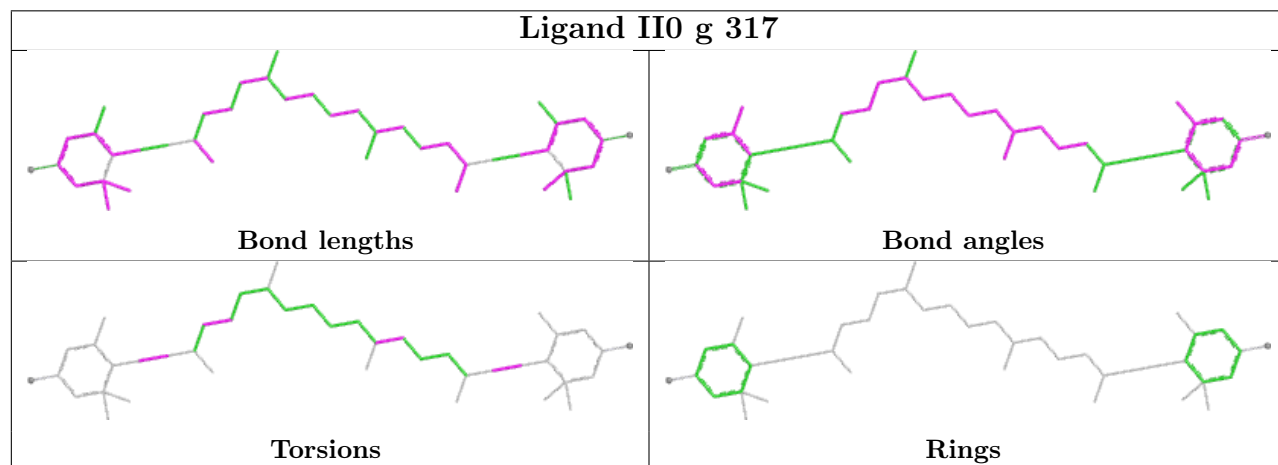
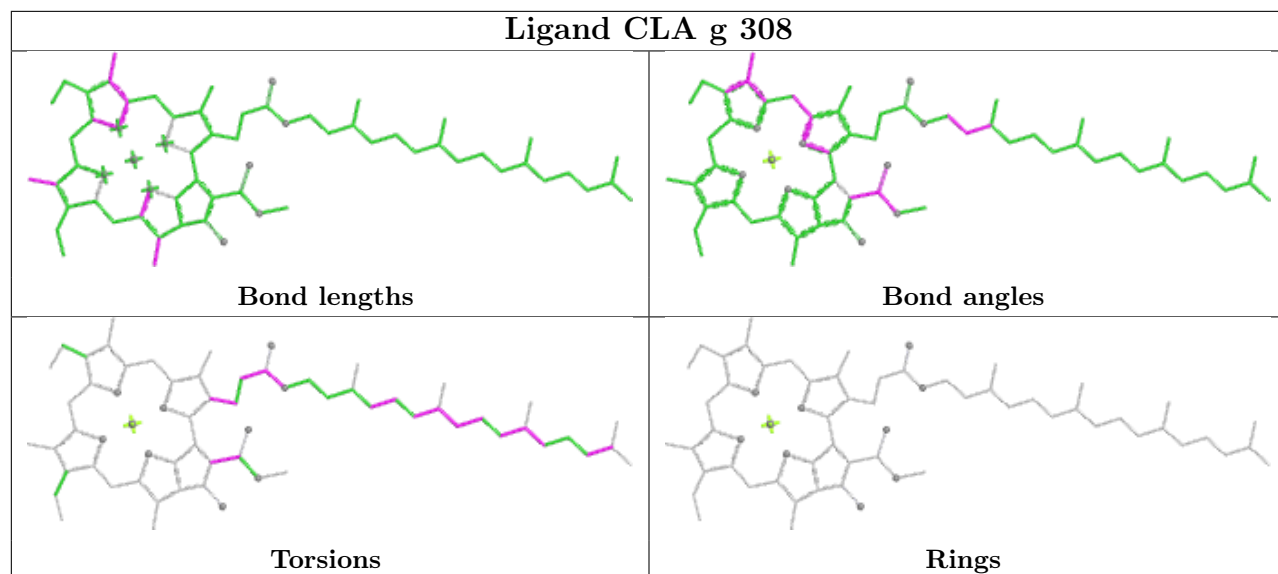


Ligand CLA B 838

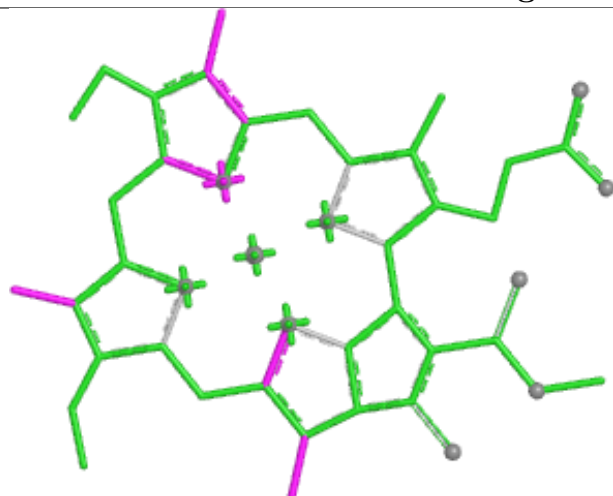


Ligand CLA d 306

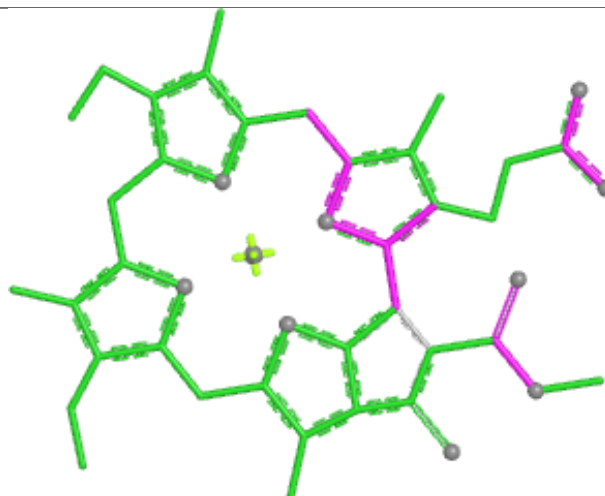




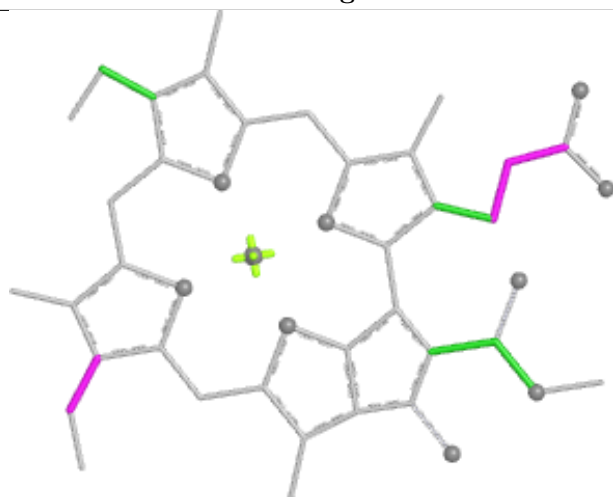
Ligand CLA k 605



Bond lengths



Bond angles

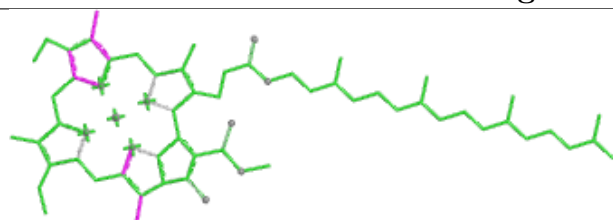


Torsions

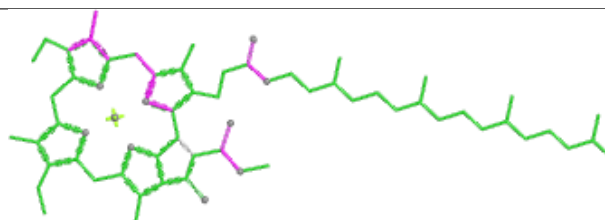


Rings

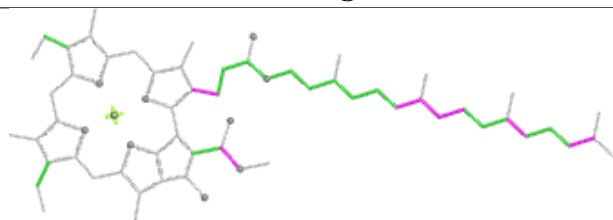
Ligand CLA k 608



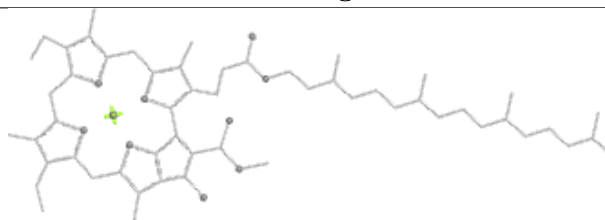
Bond lengths



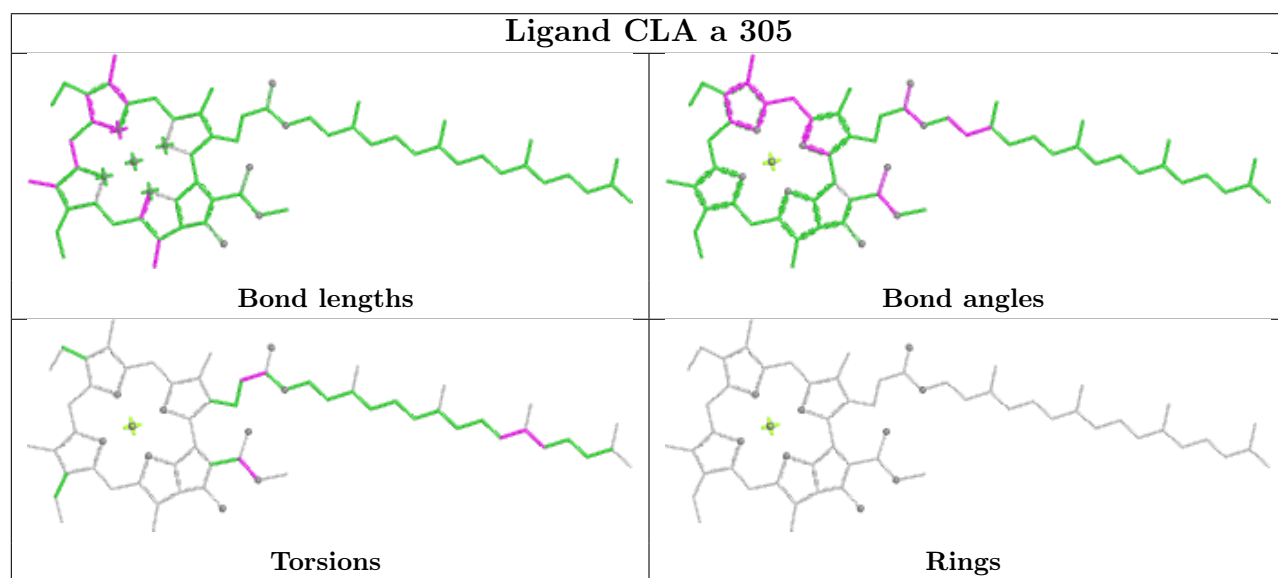
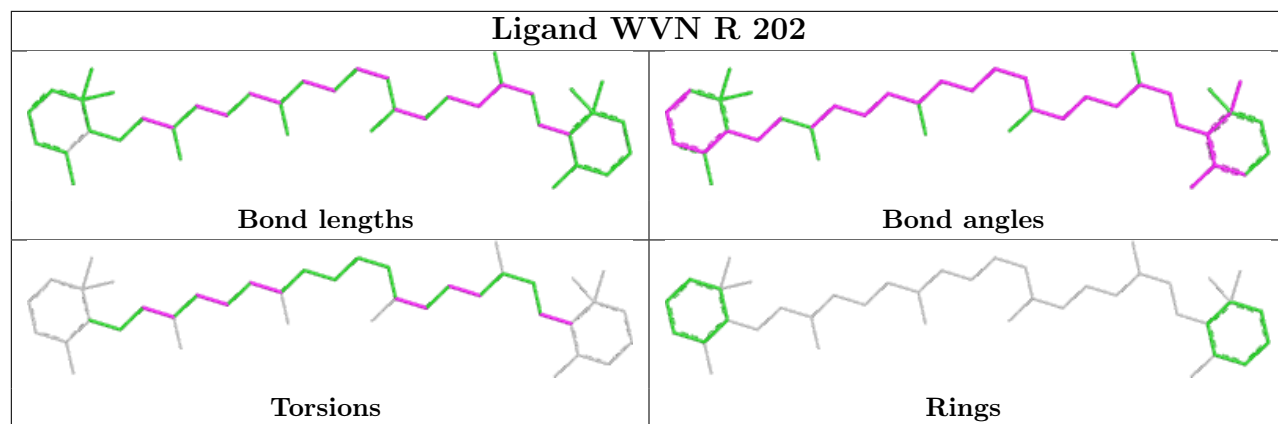
Bond angles



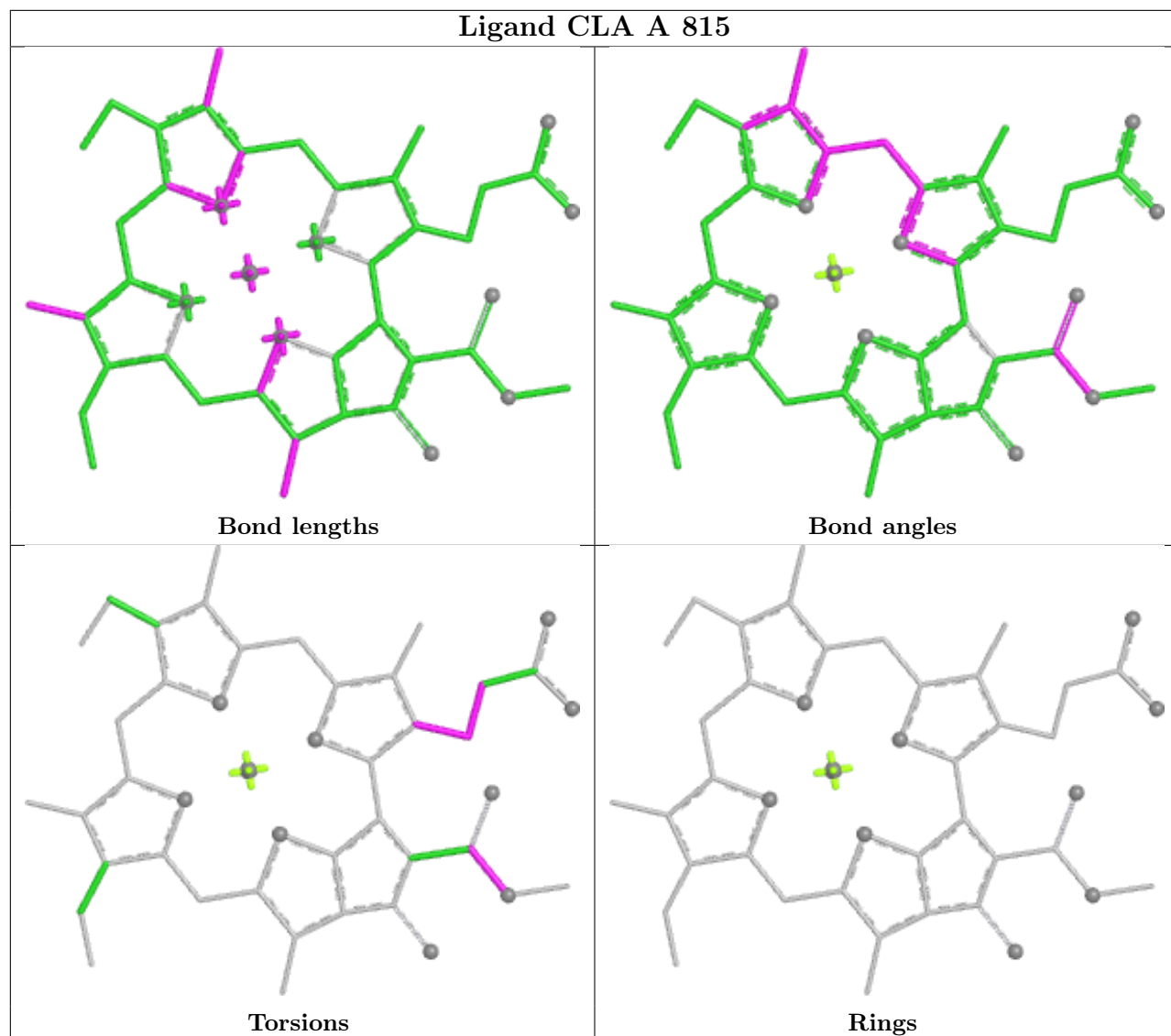
Torsions



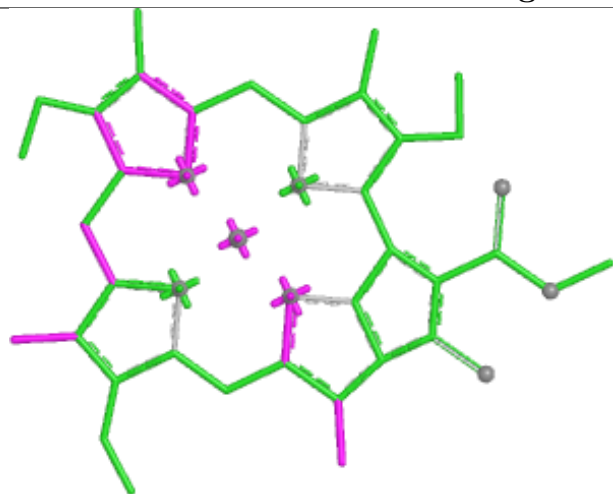
Rings



Ligand CLA A 815



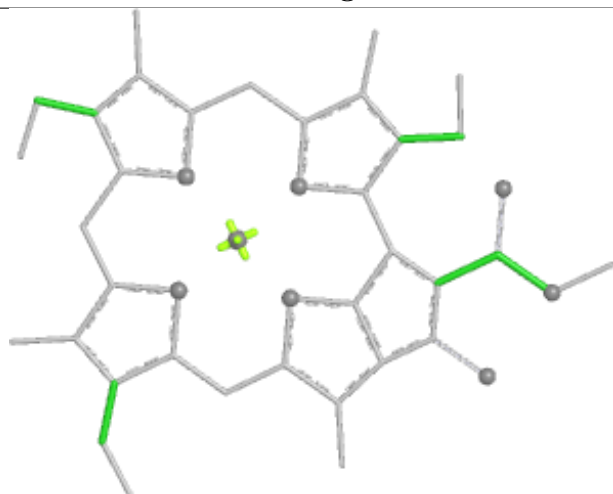
Ligand CLA g 302



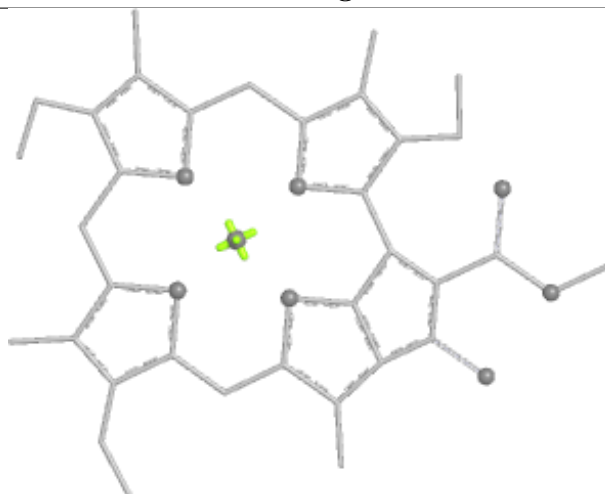
Bond lengths



Bond angles

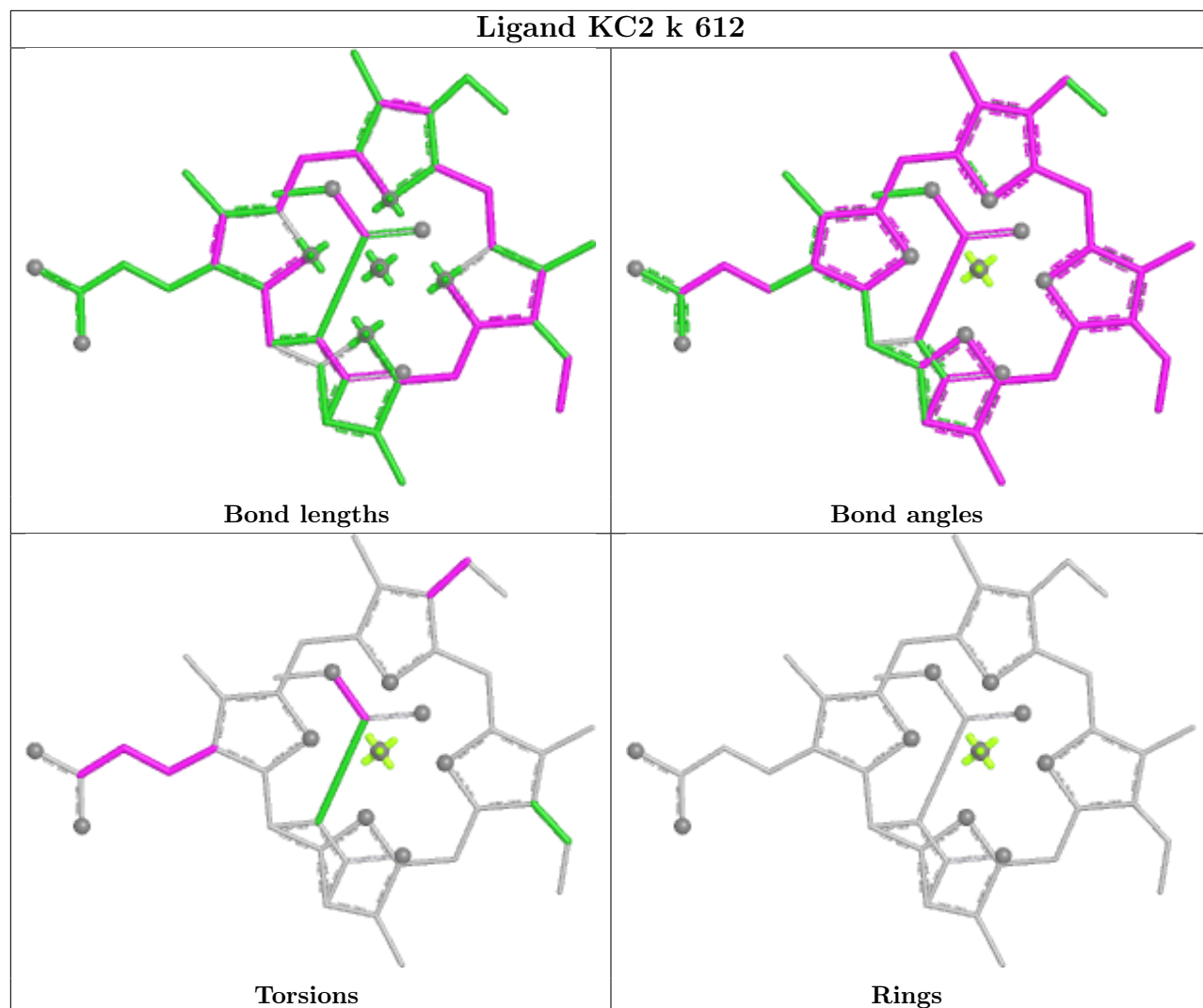


Torsions

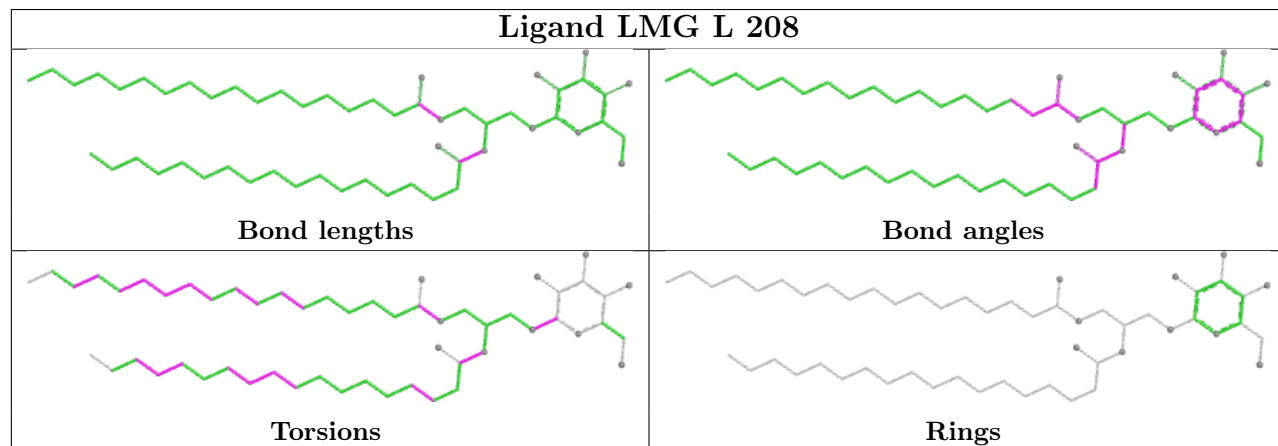


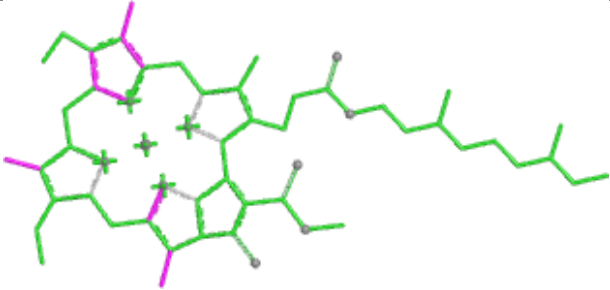
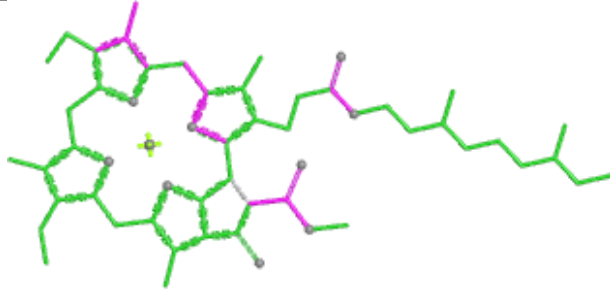
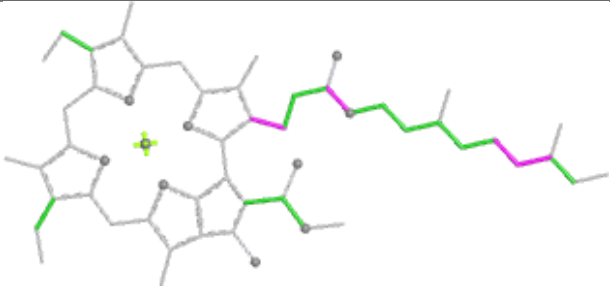
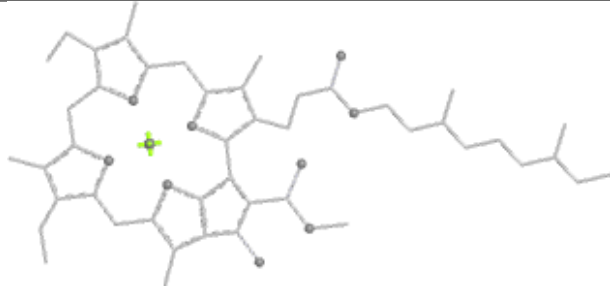
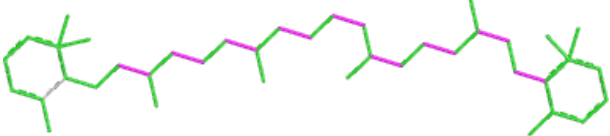
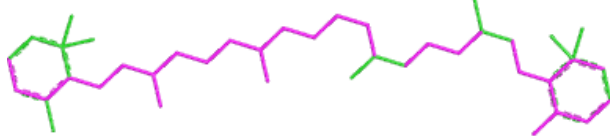
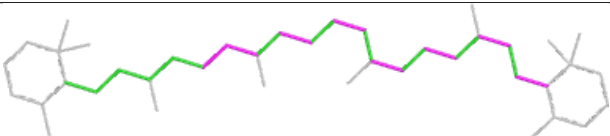
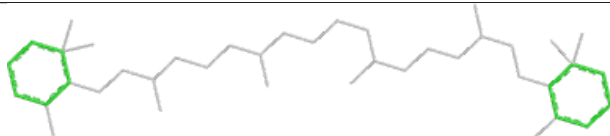
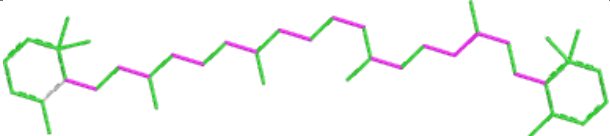
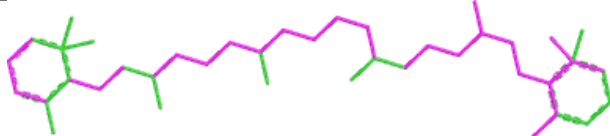
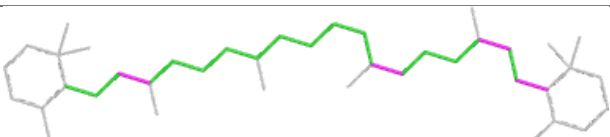
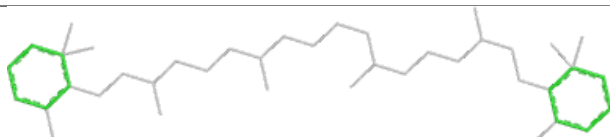
Rings

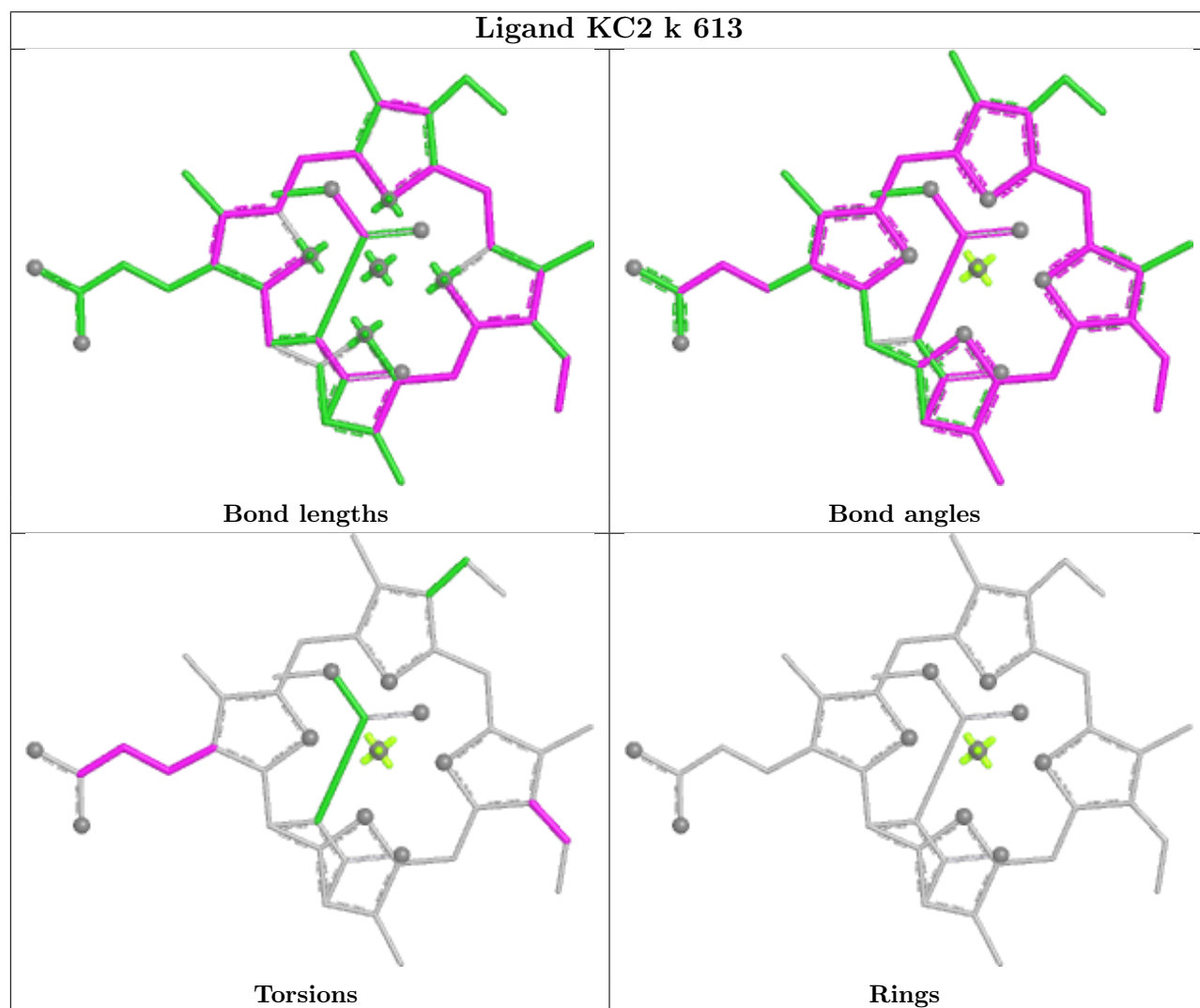
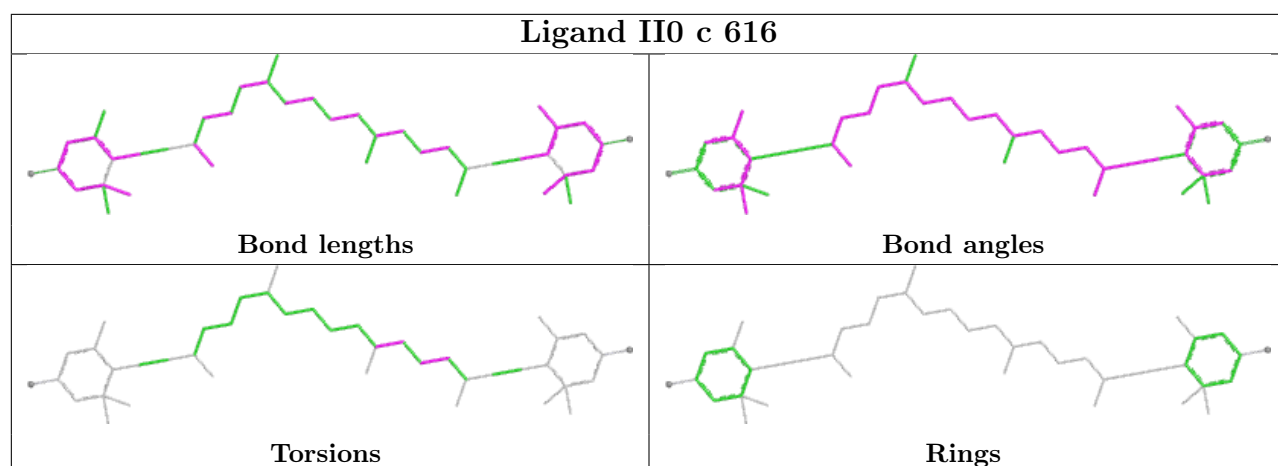
Ligand KC2 k 612

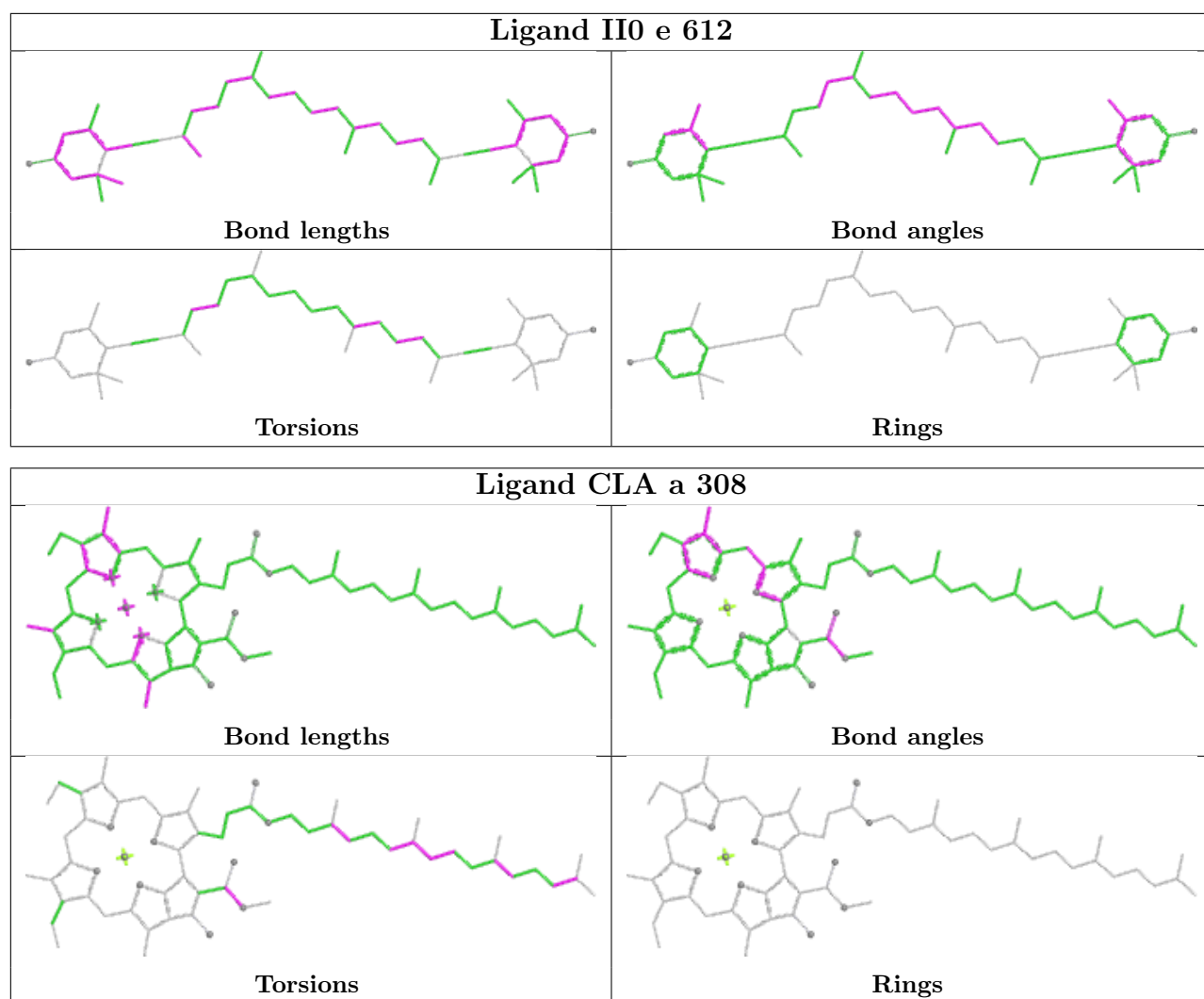


Ligand LMG L 208

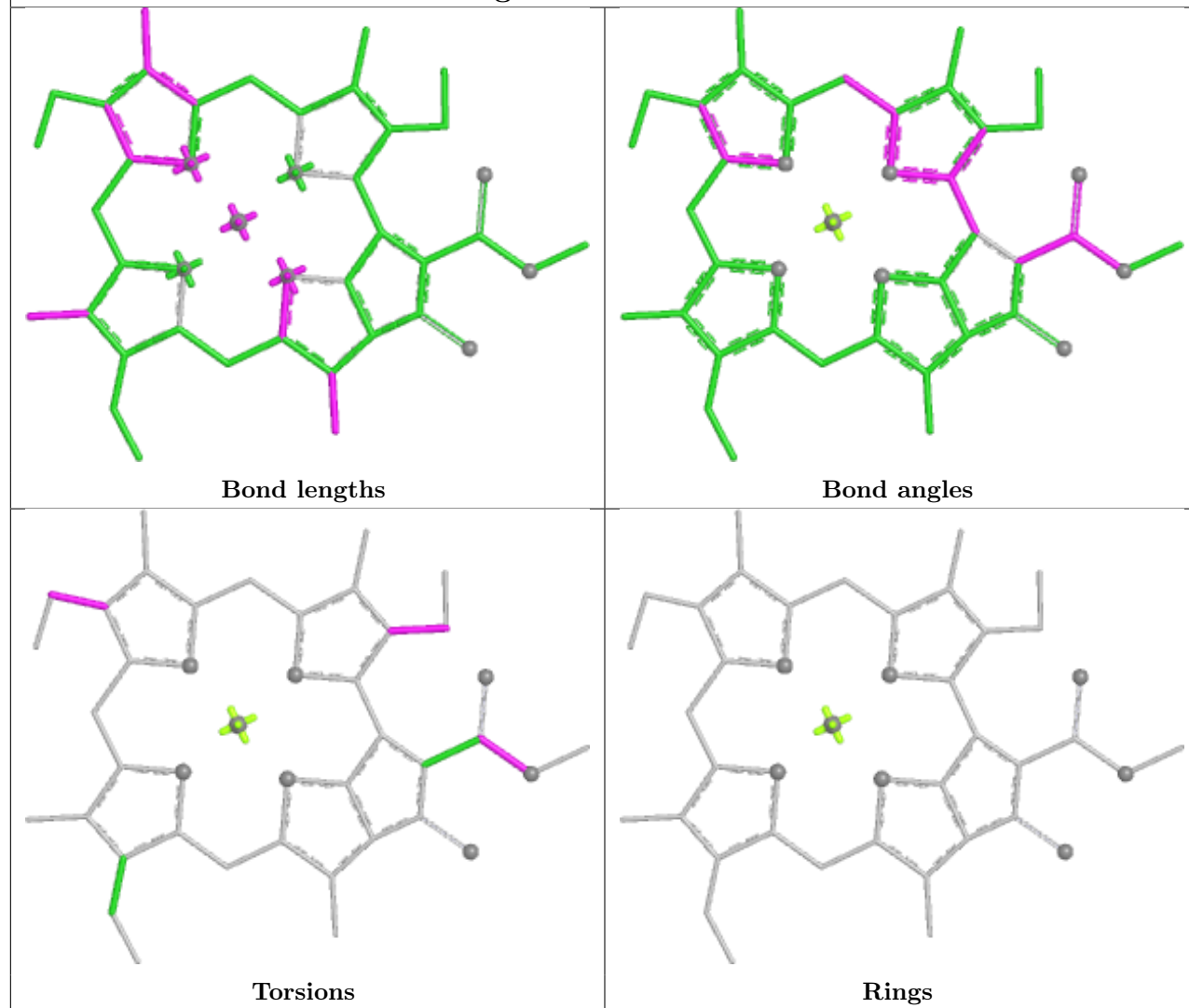


Ligand CLA A 809	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand WVN B 847	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand WVN J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

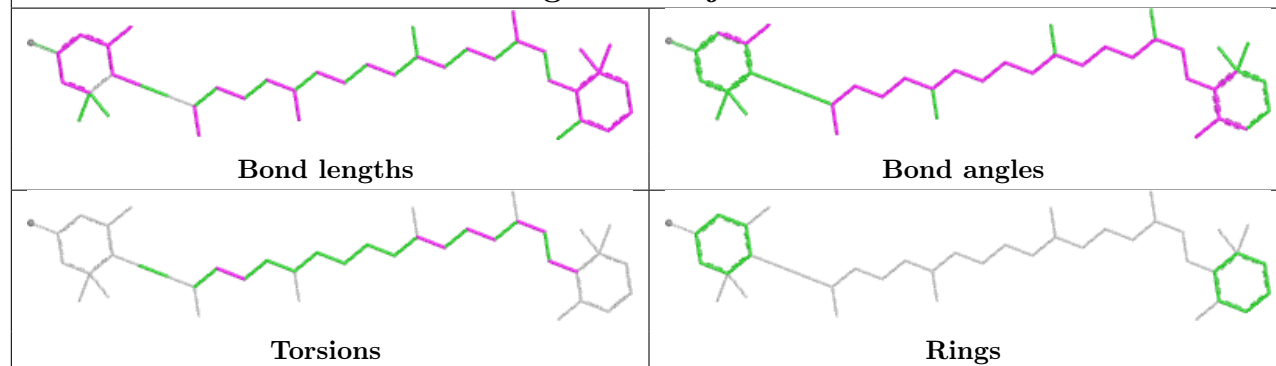




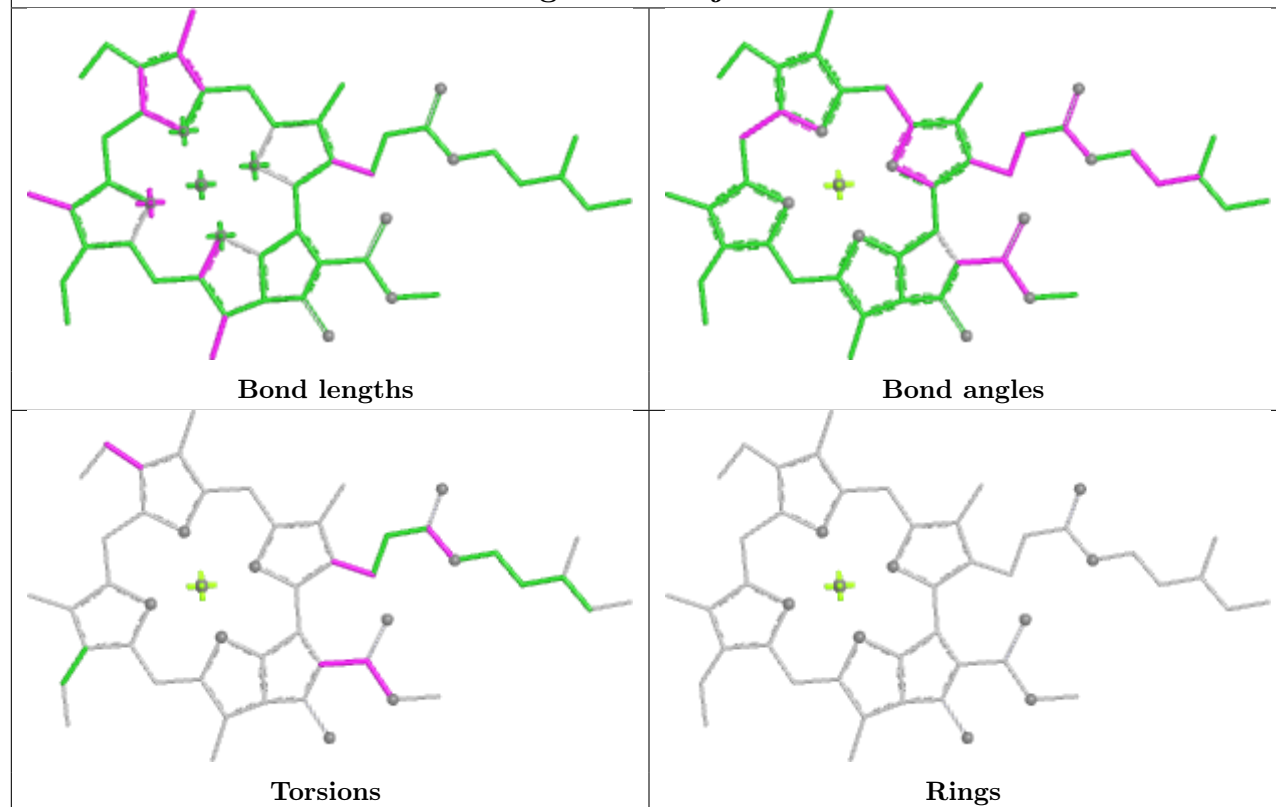
Ligand CLA K 102



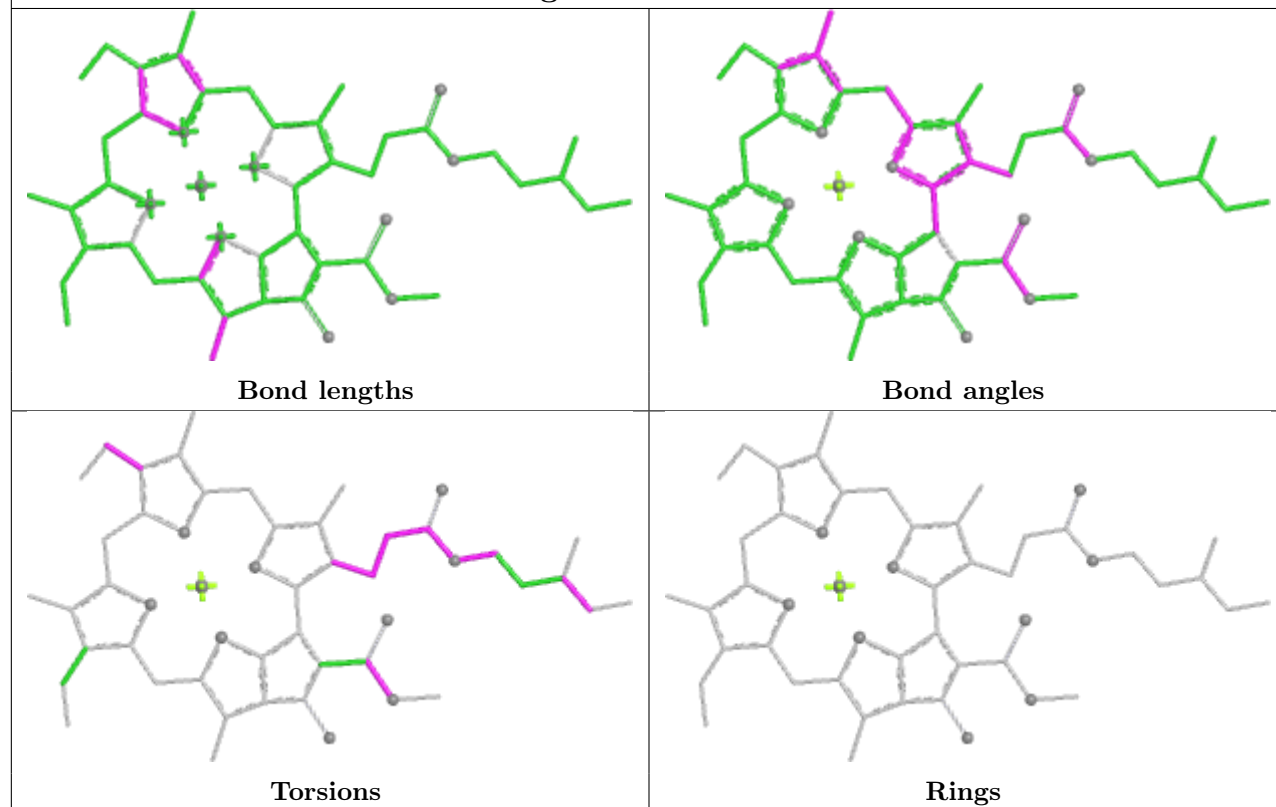
Ligand IHT j 317



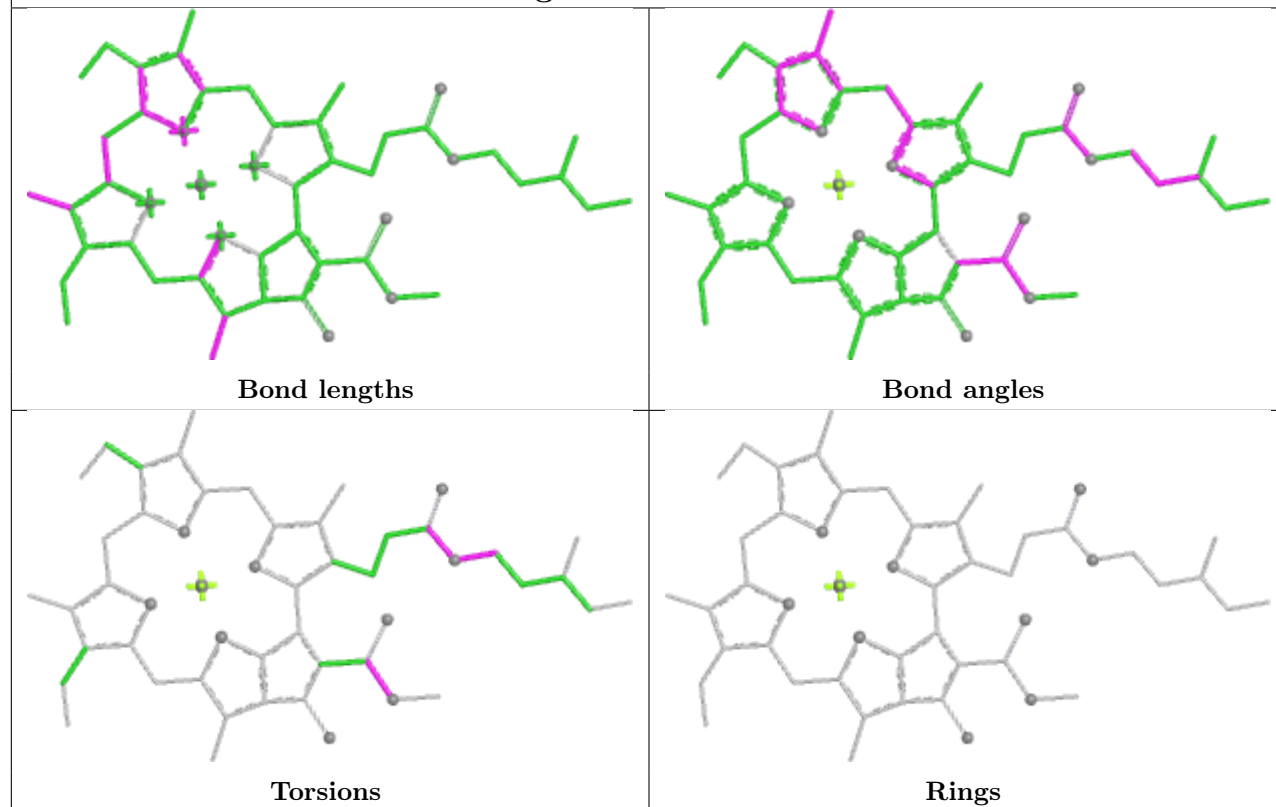
Ligand CLA j 307



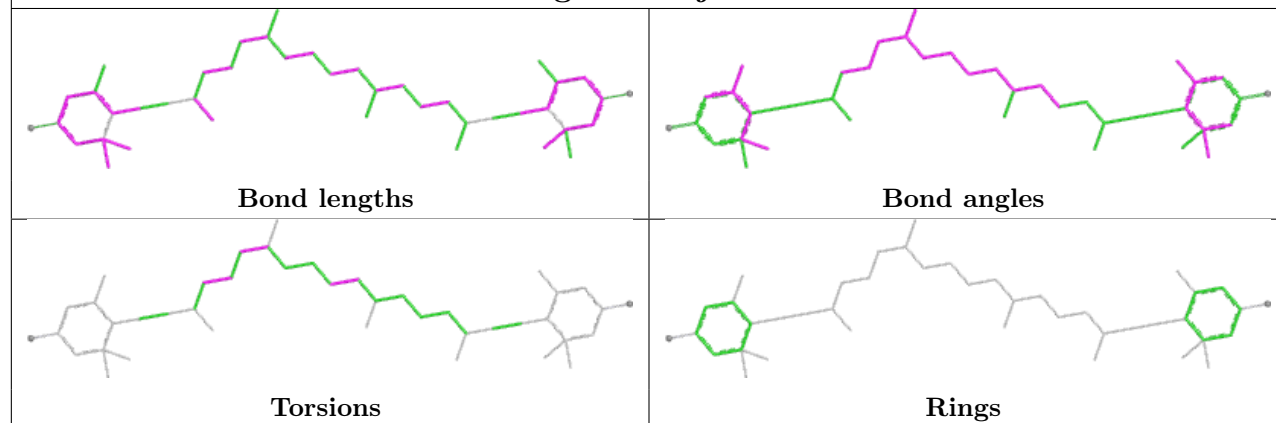
Ligand CLA i 611

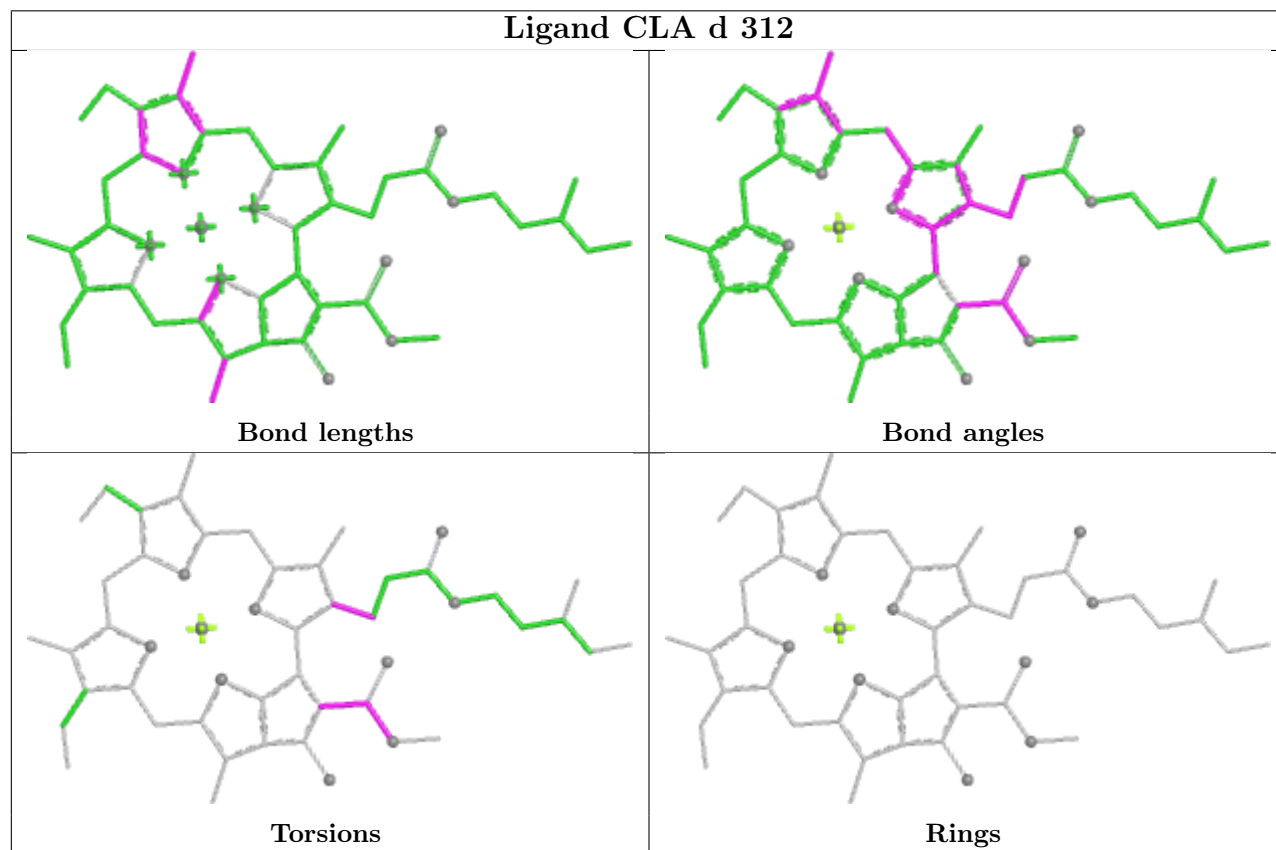
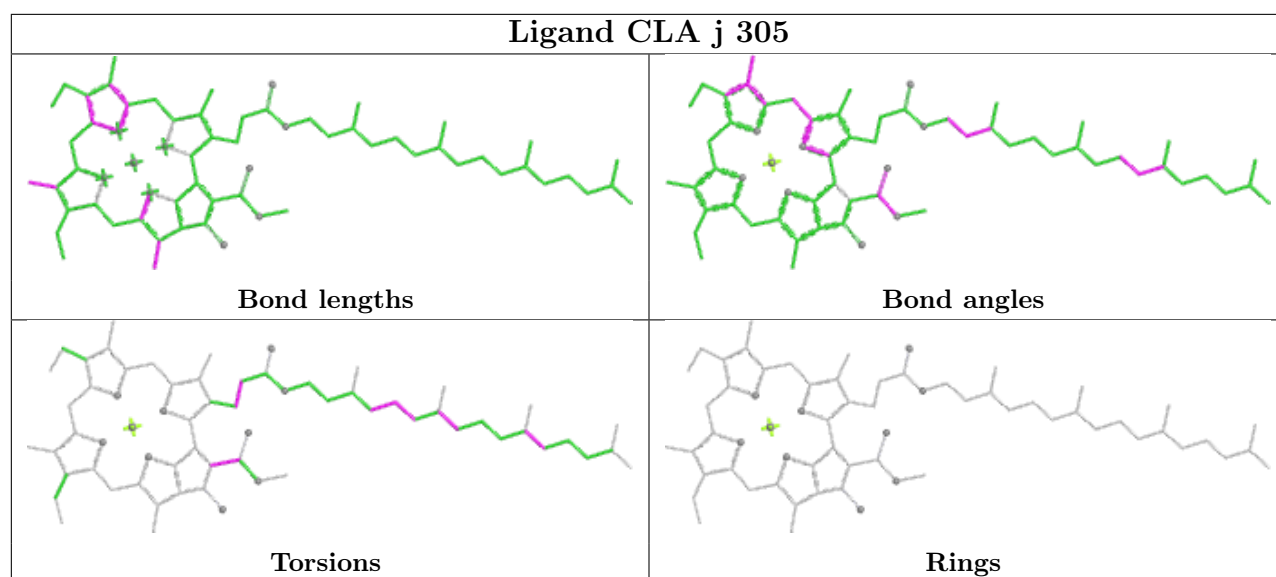


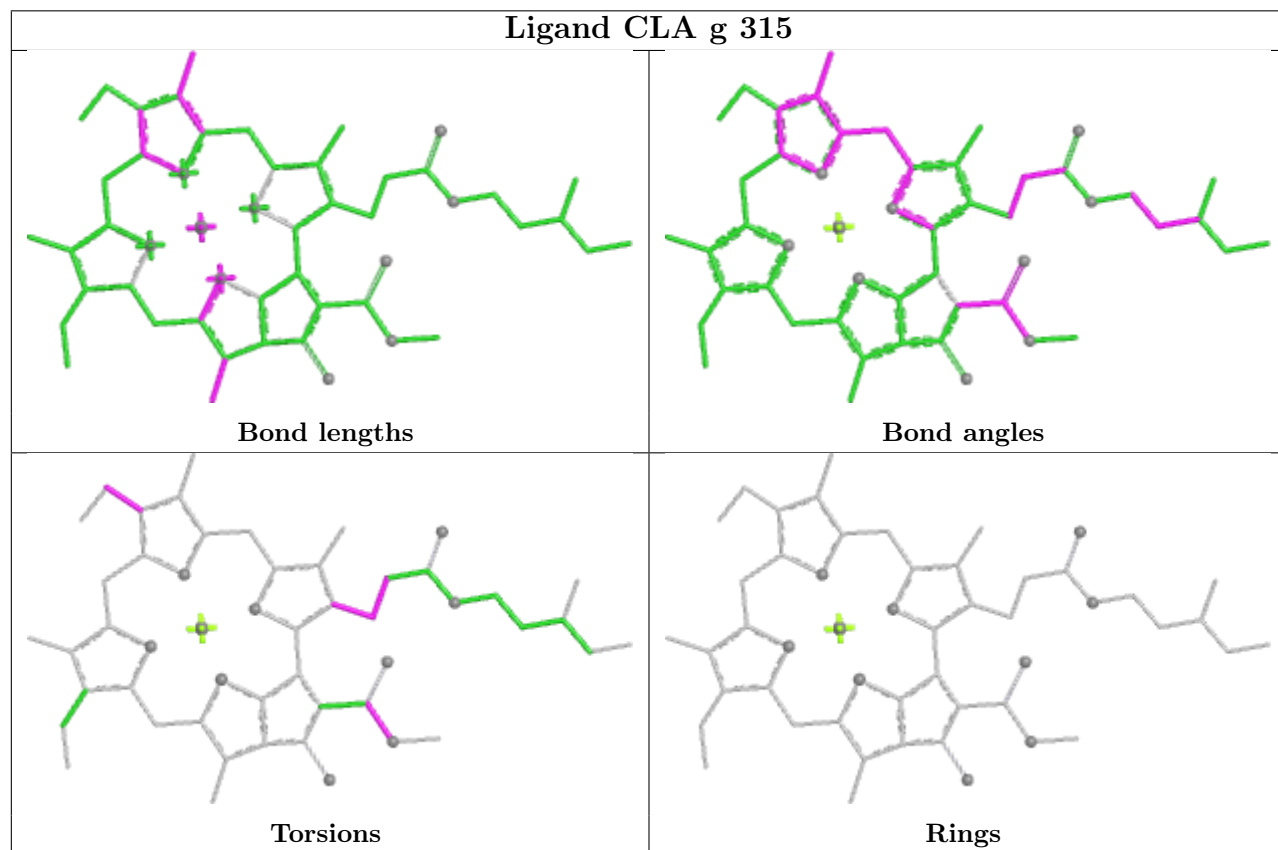
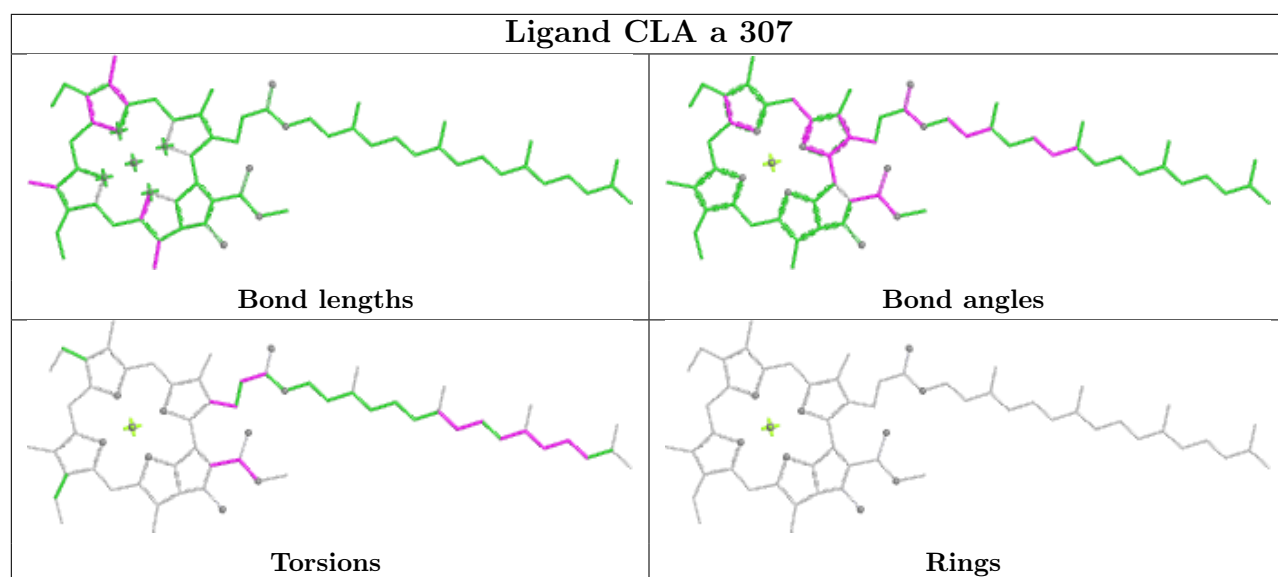
Ligand CLA b 311



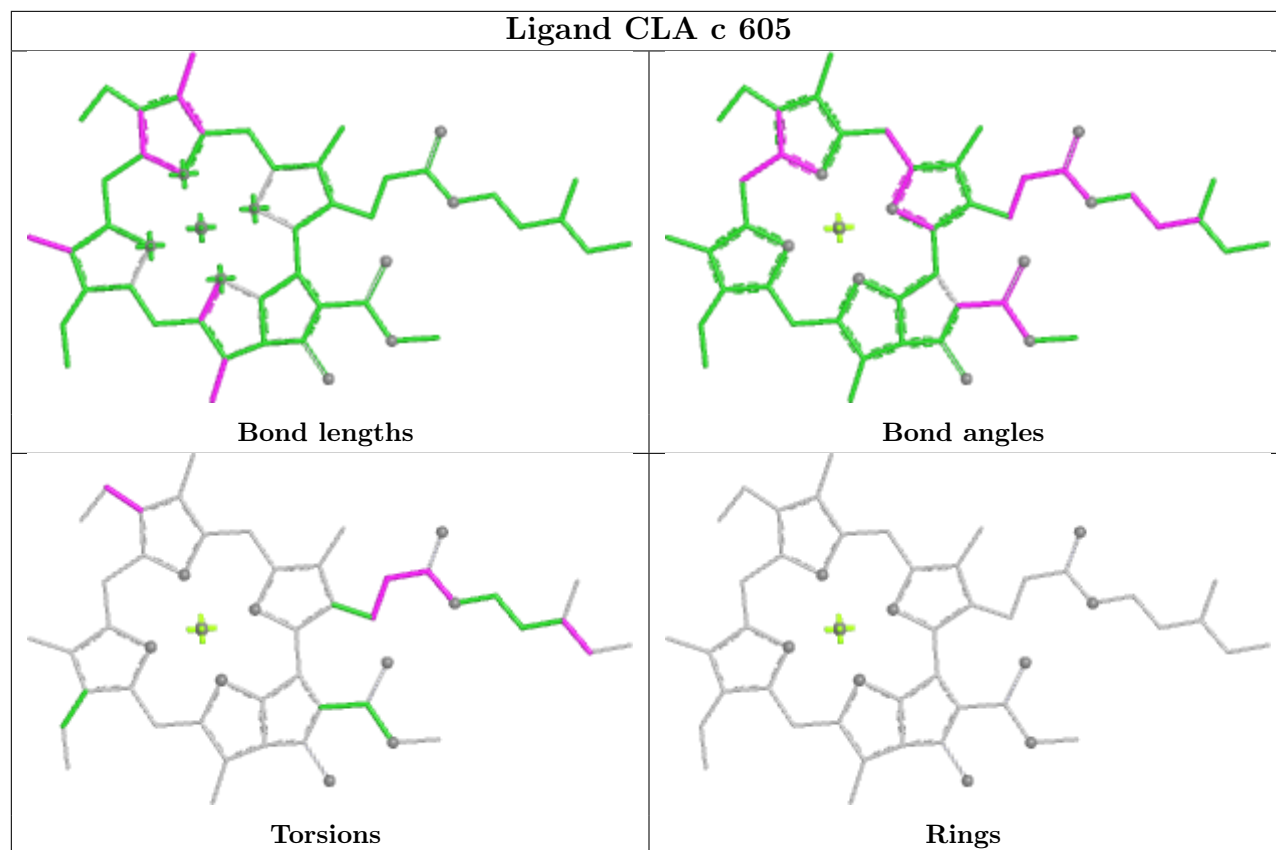
Ligand II0 j 315



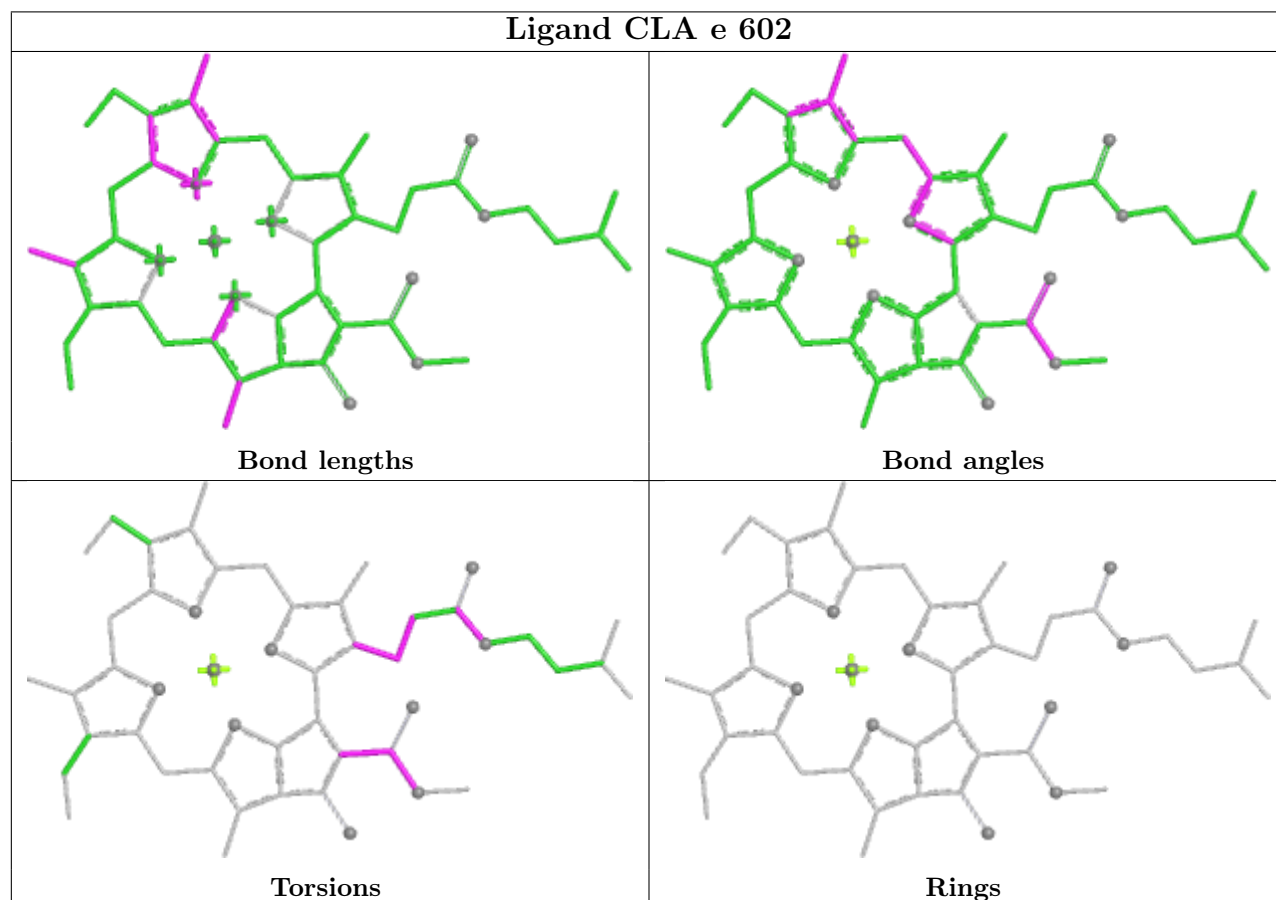


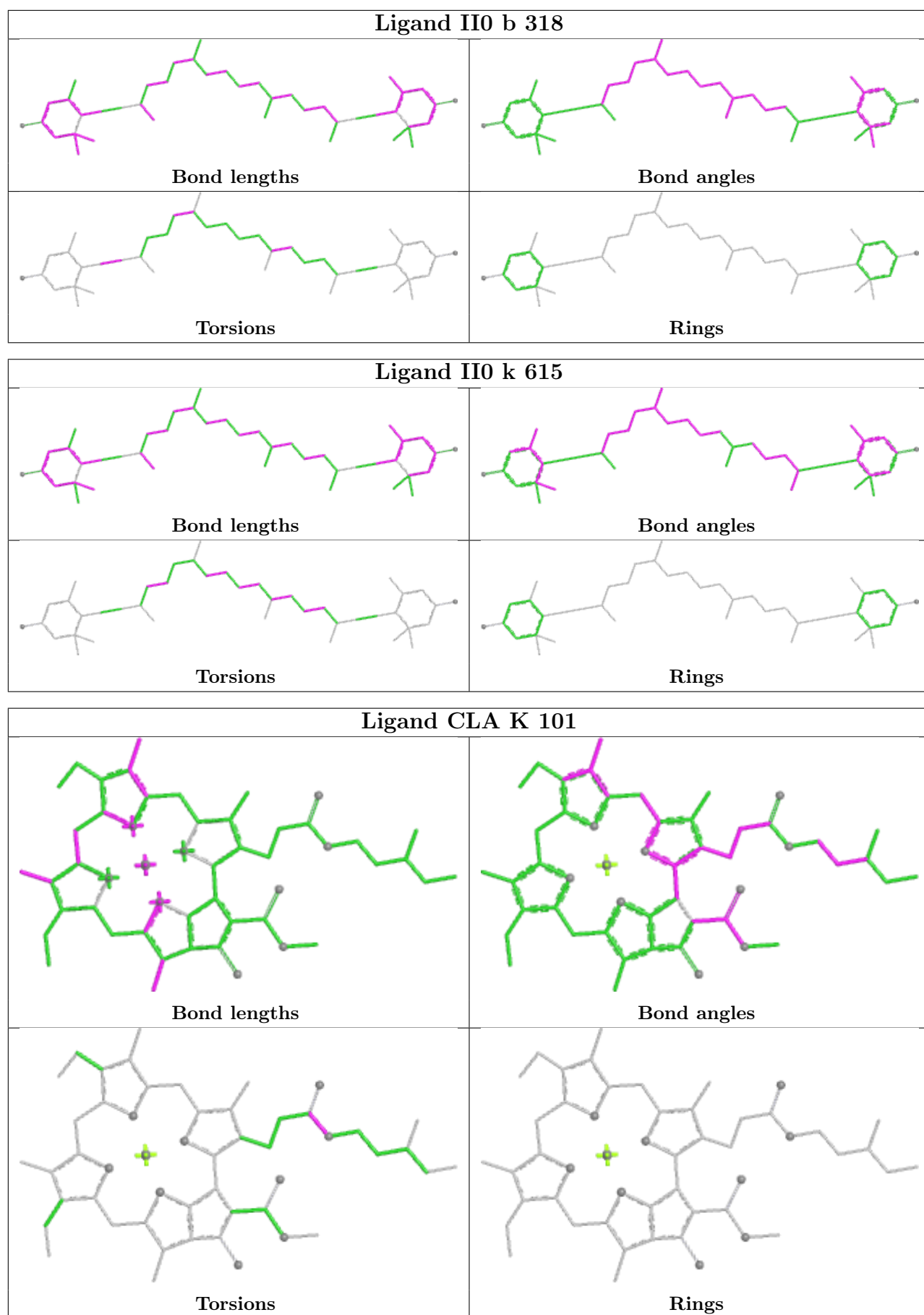


Ligand CLA c 605

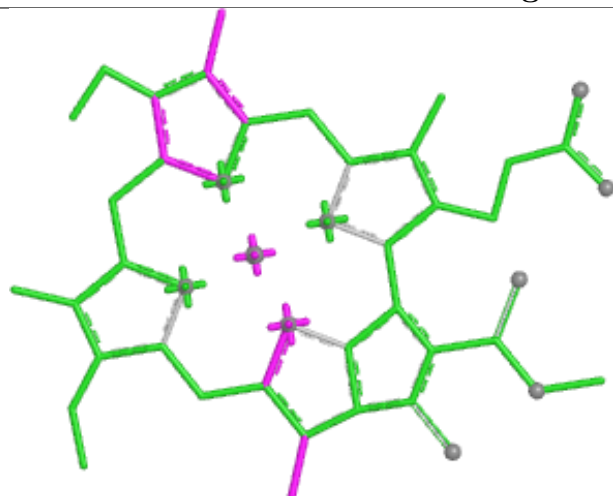


Ligand CLA e 602

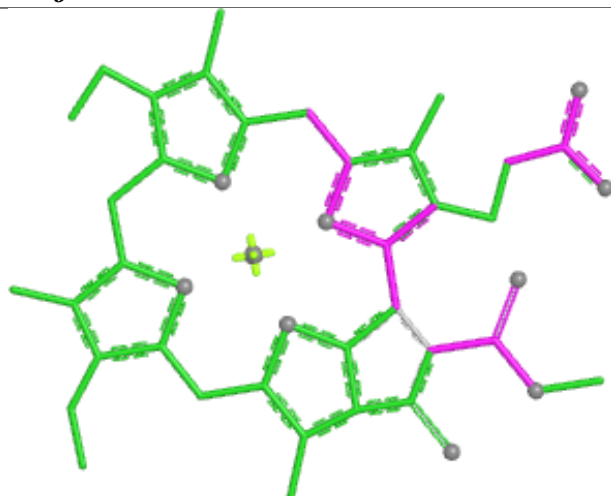




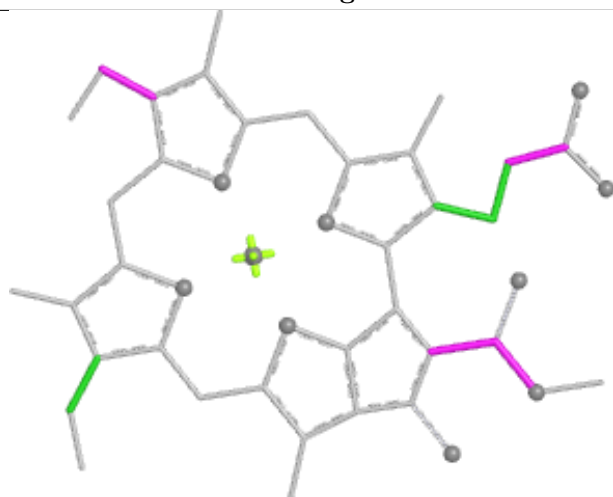
Ligand CLA j 306



Bond lengths



Bond angles

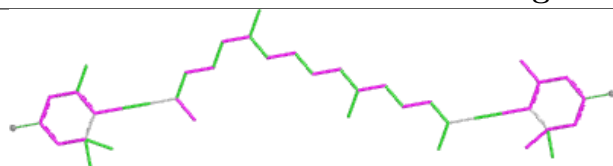


Torsions

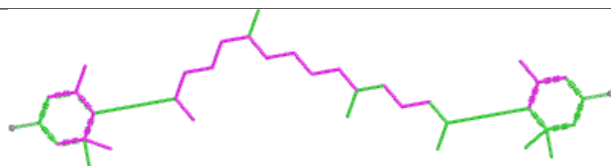


Rings

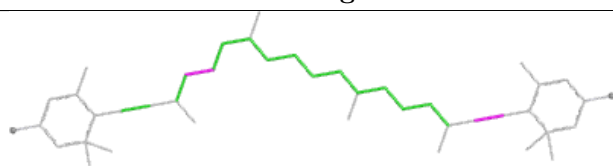
Ligand II0 k 617



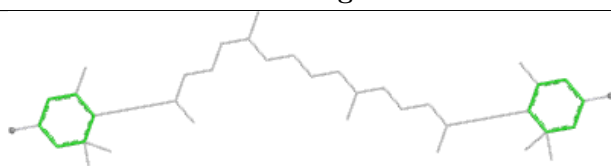
Bond lengths



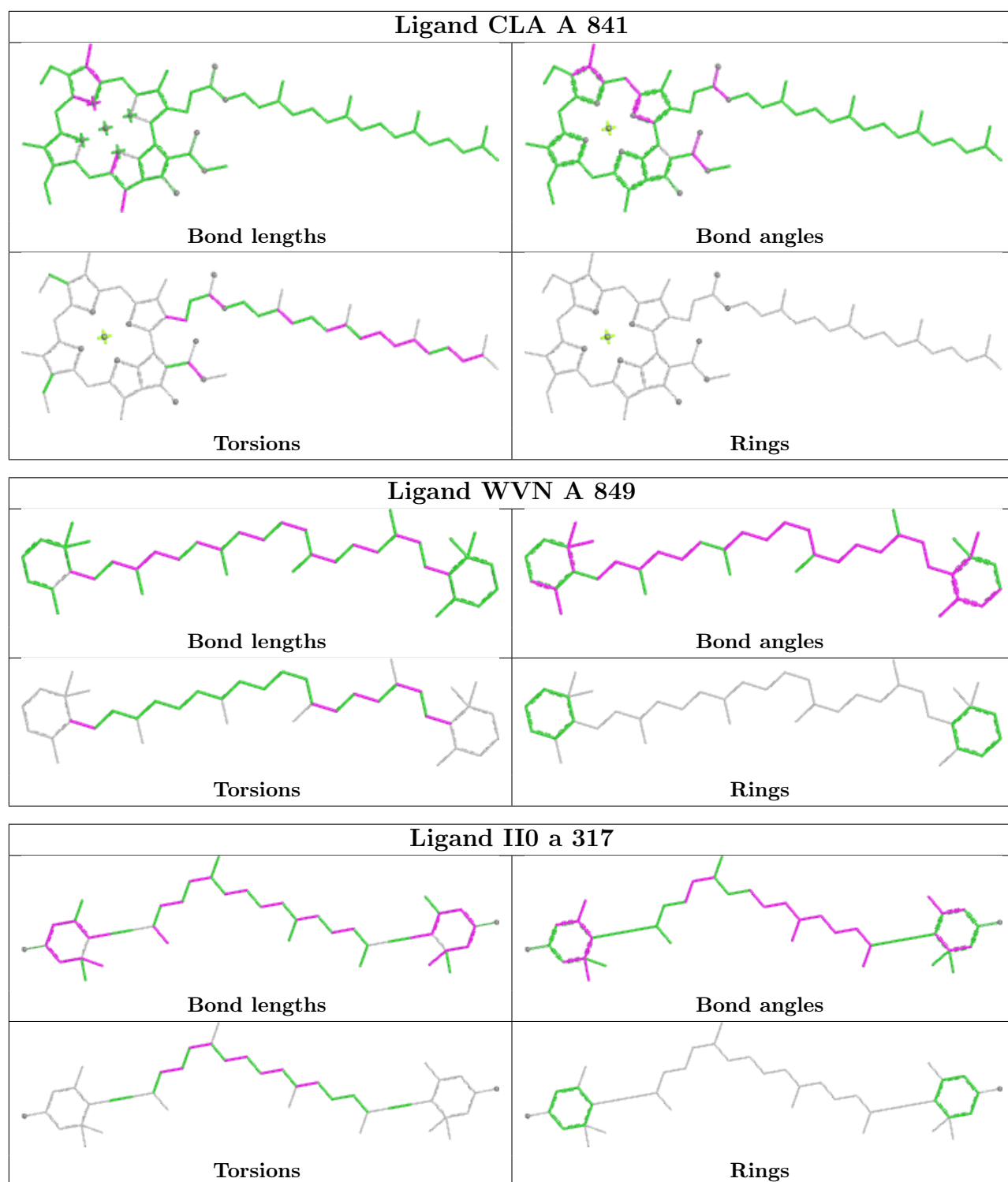
Bond angles

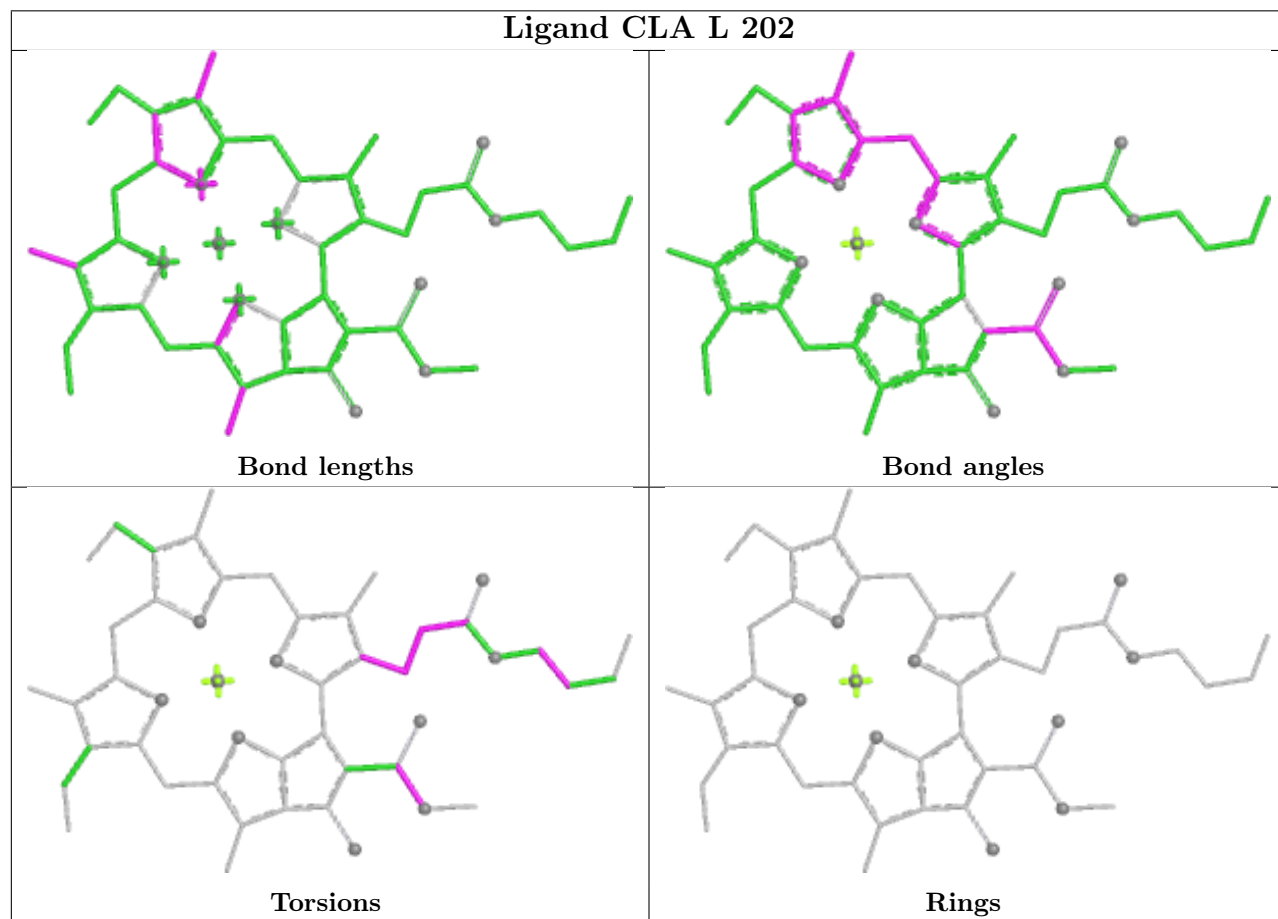
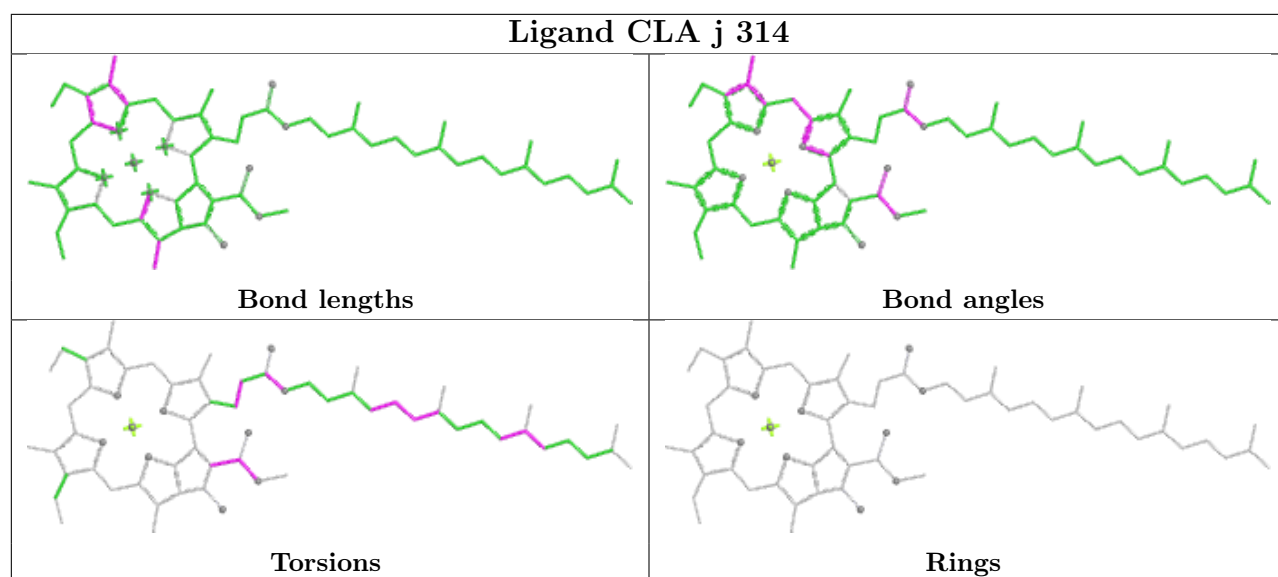


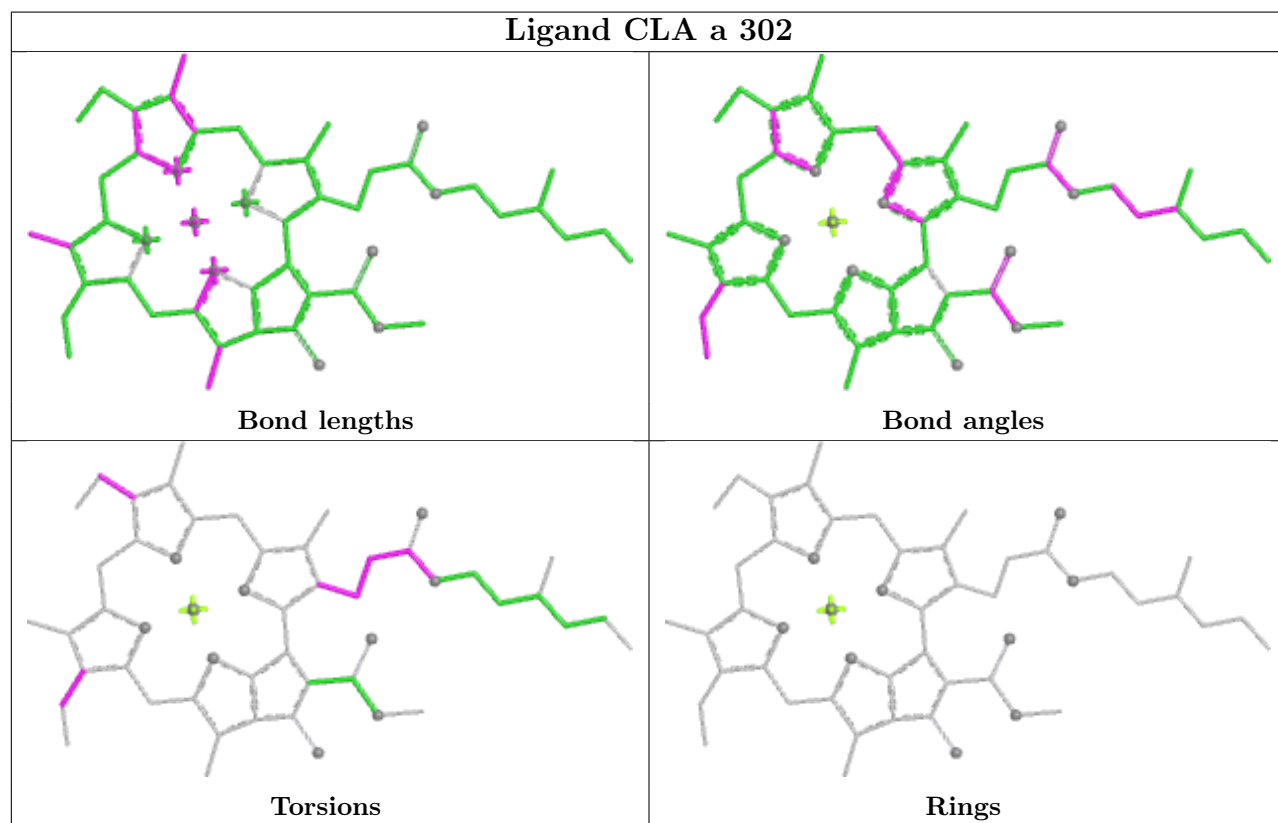
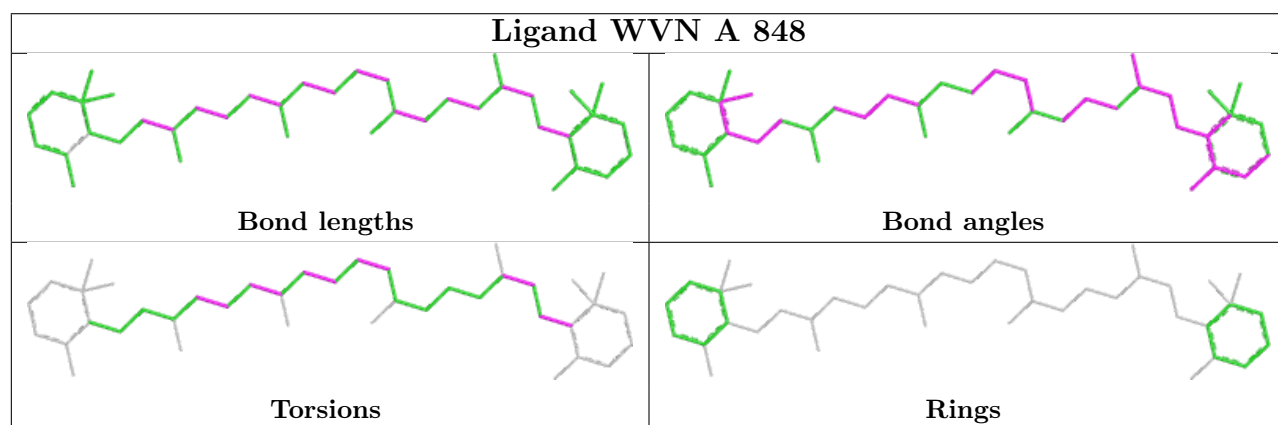
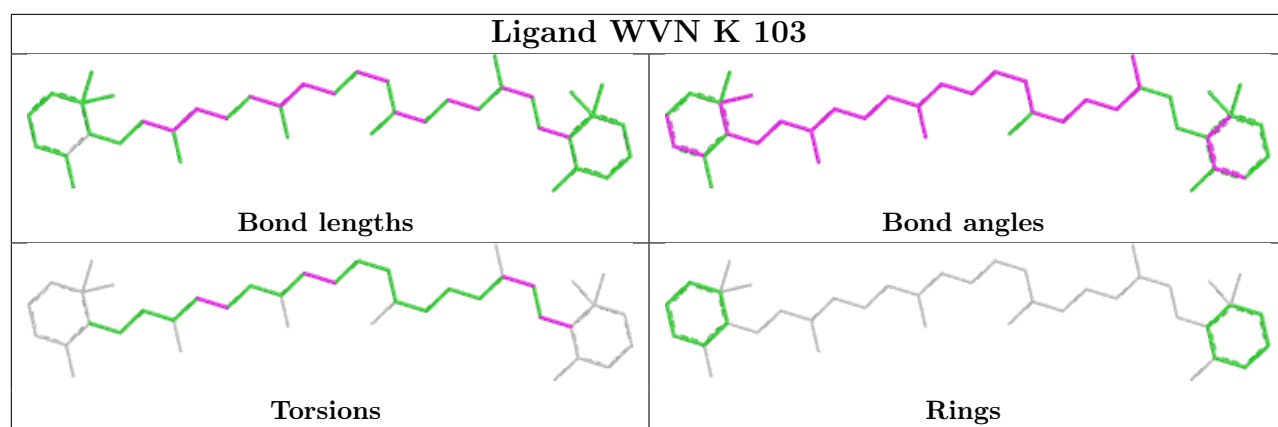
Torsions



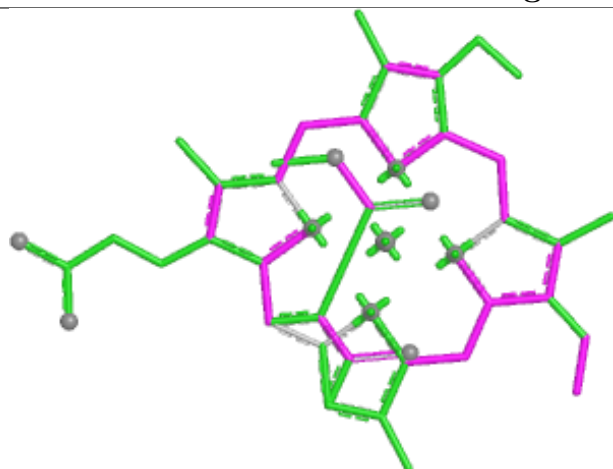
Rings



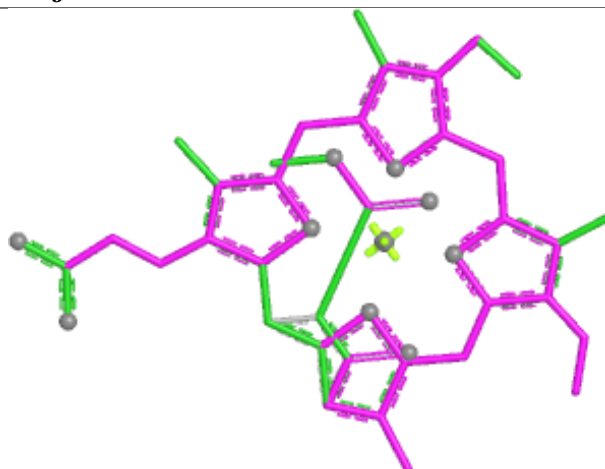




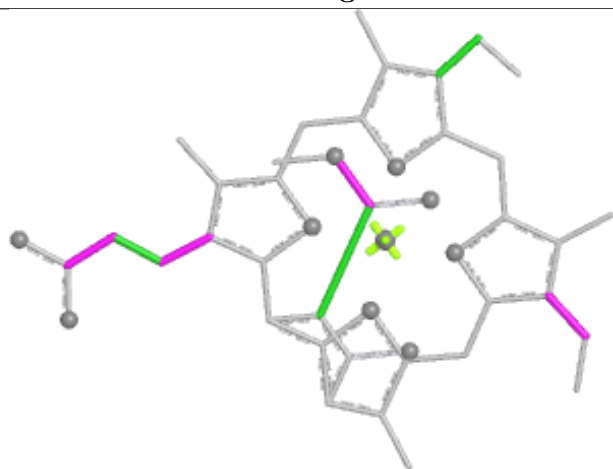
Ligand KC2 j 312



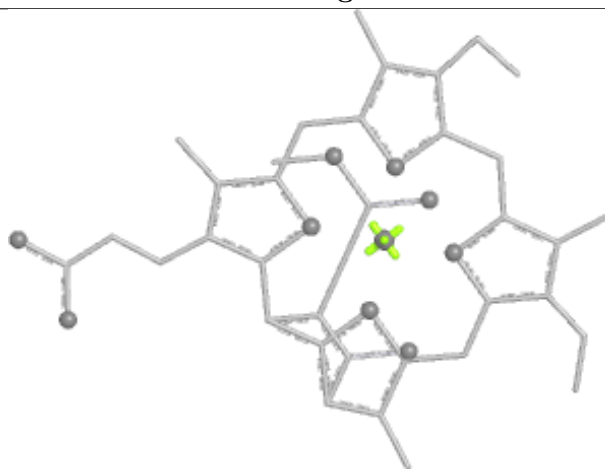
Bond lengths



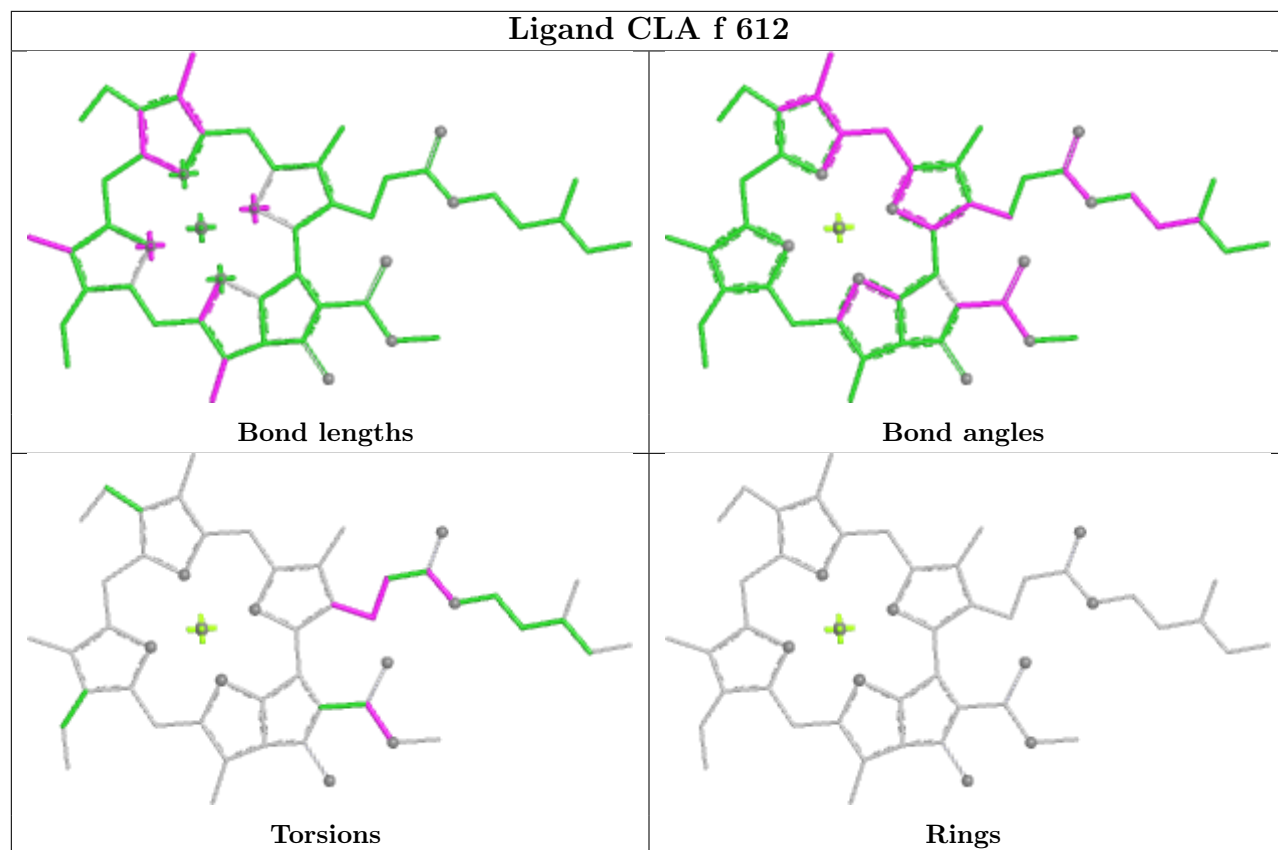
Bond angles



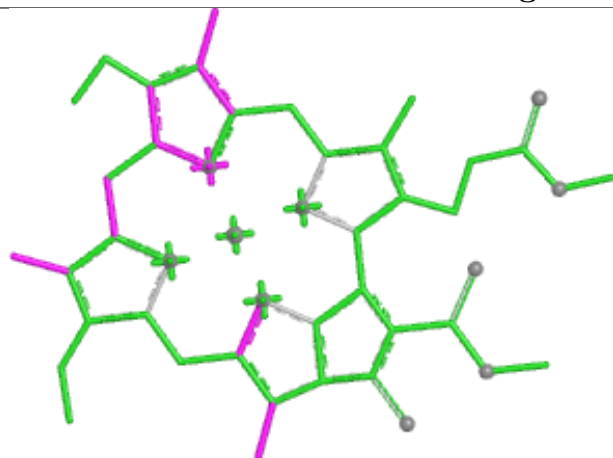
Torsions



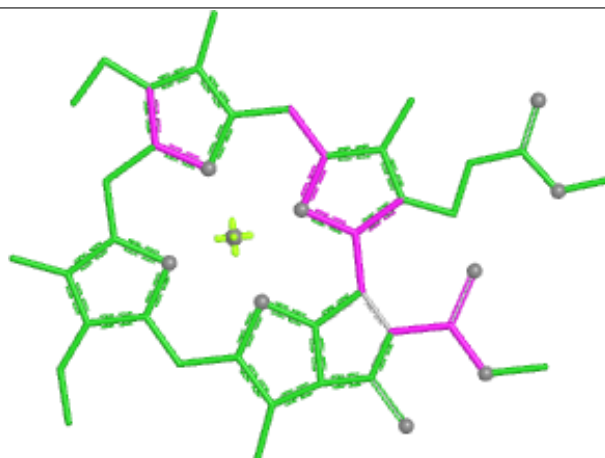
Rings



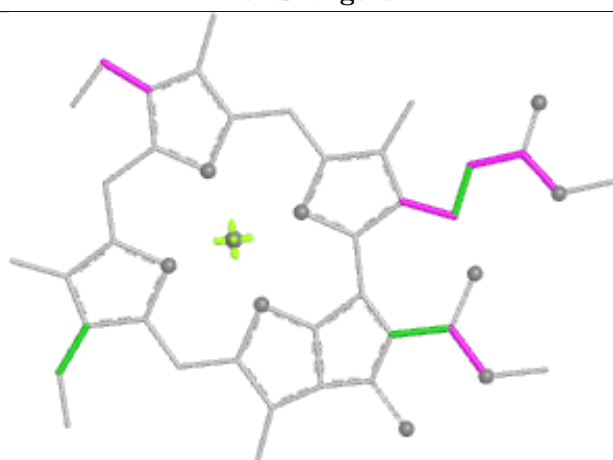
Ligand CLA e 608



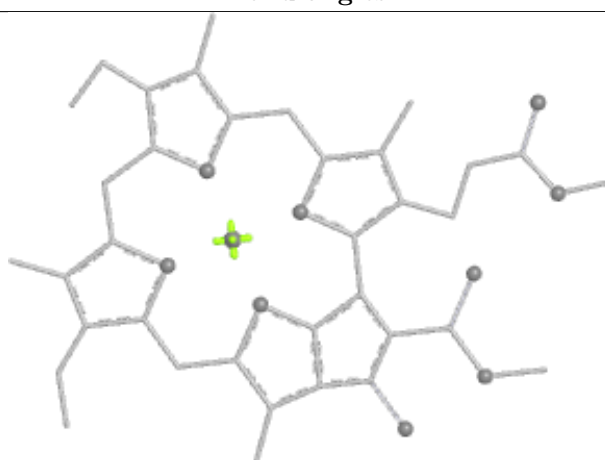
Bond lengths



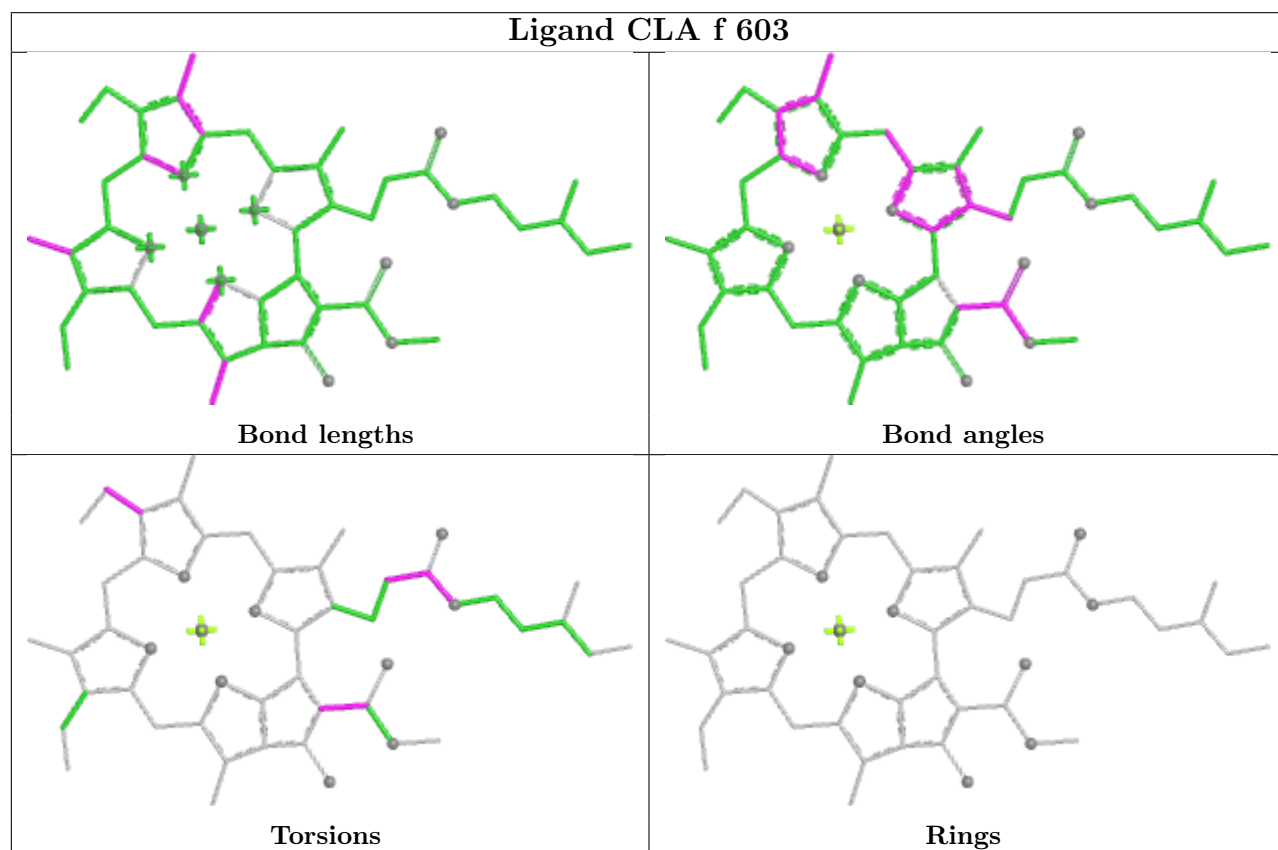
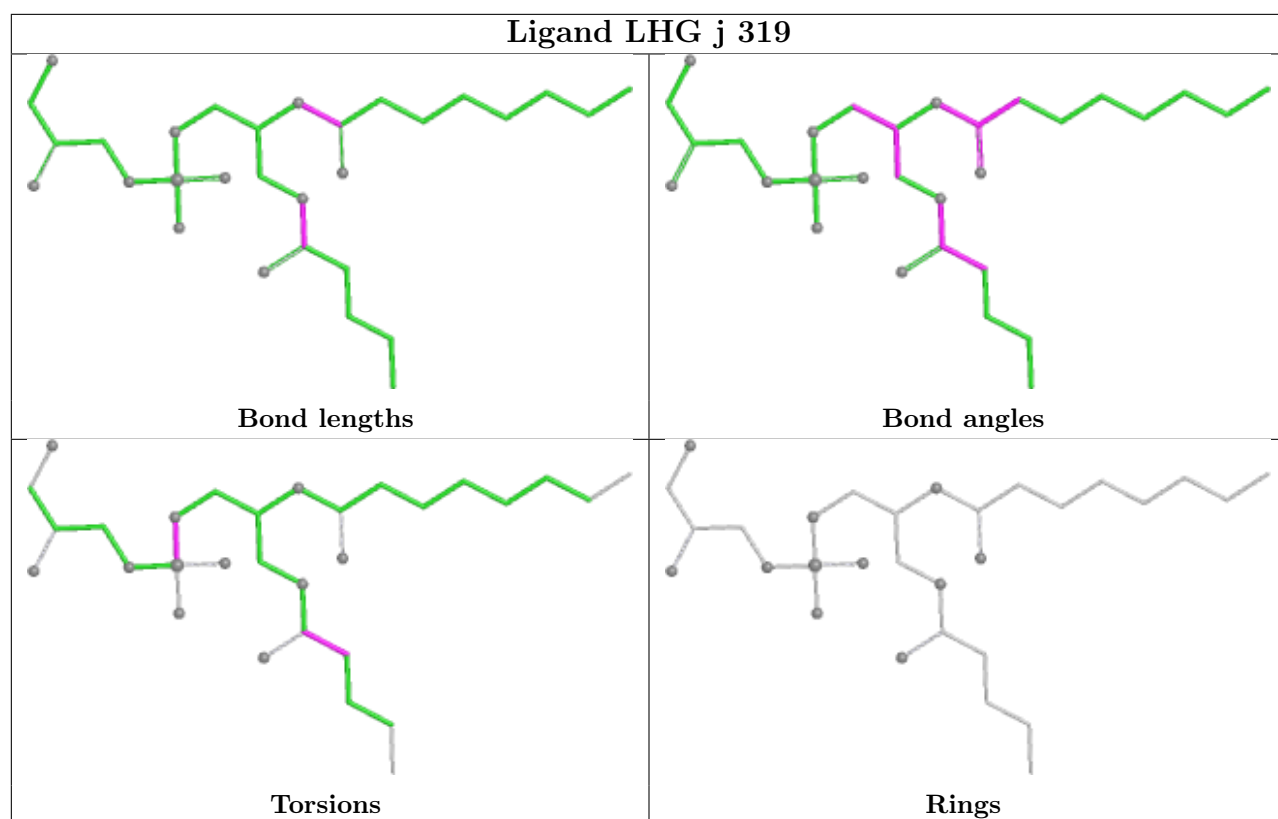
Bond angles

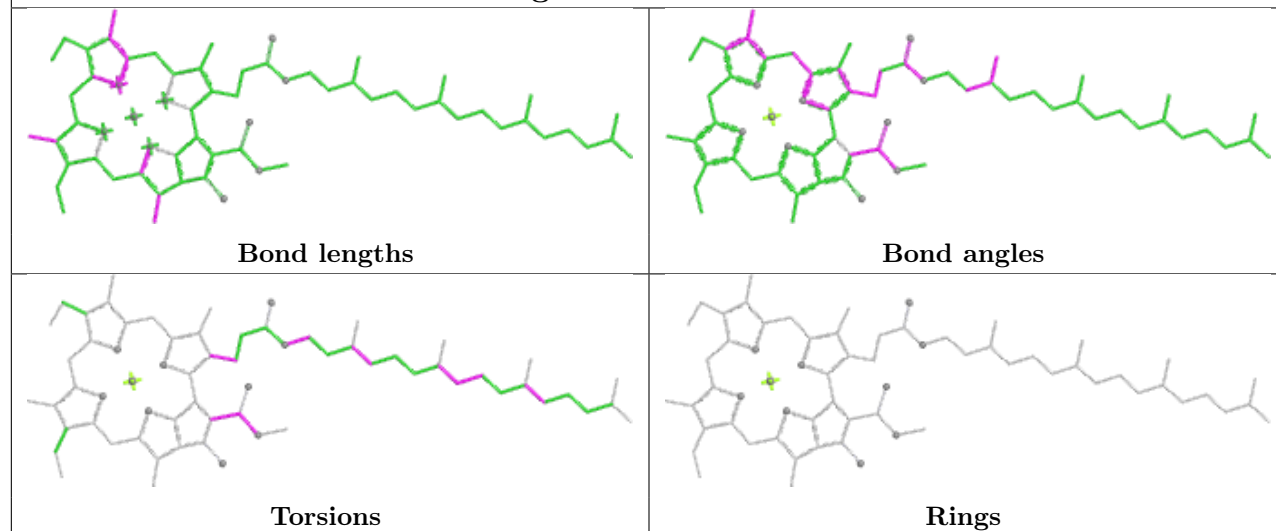
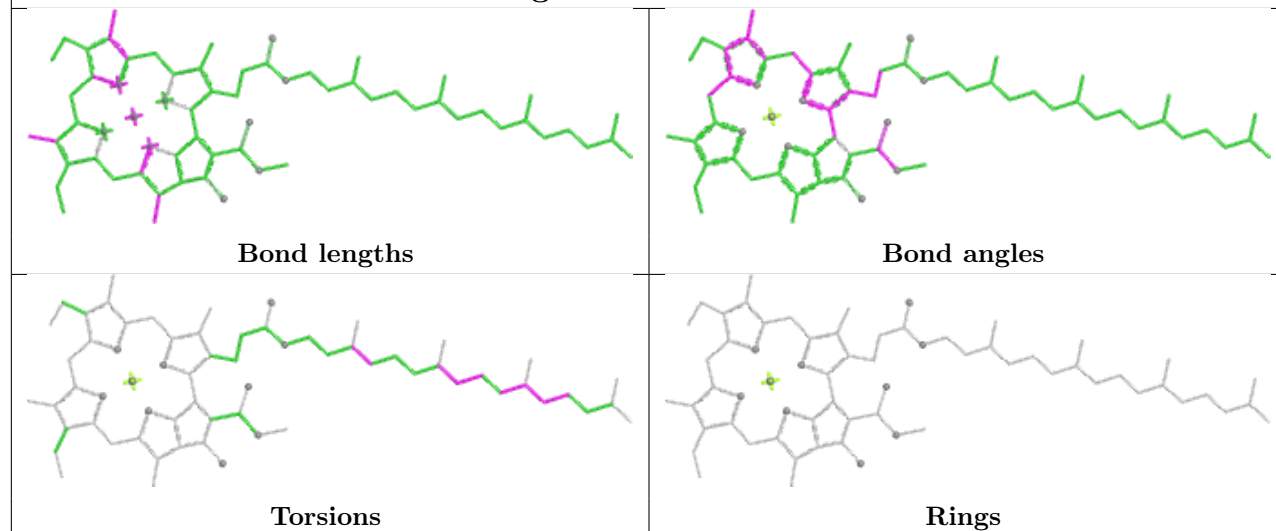


Torsions

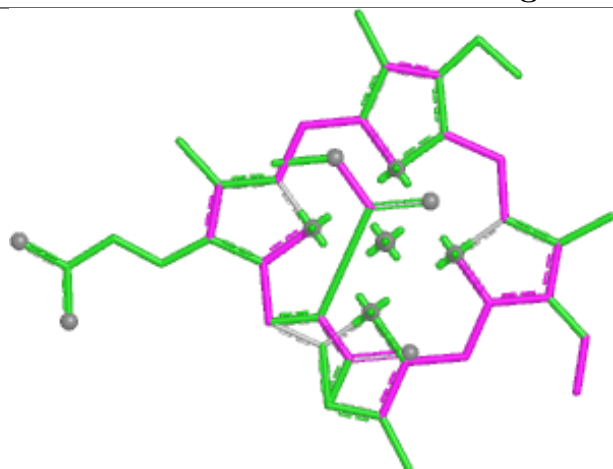


Rings

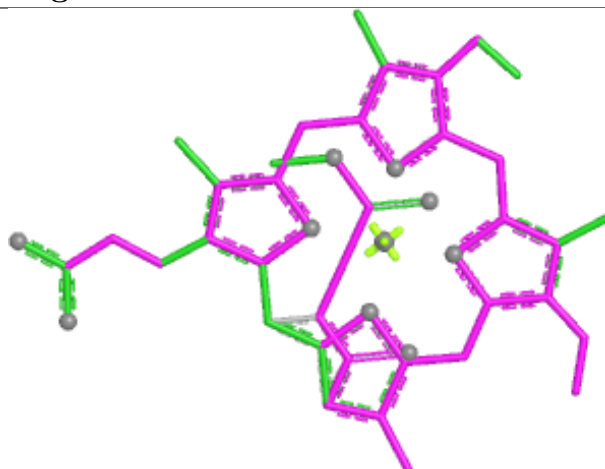


Ligand CLA A 816**Ligand CLA A 824**

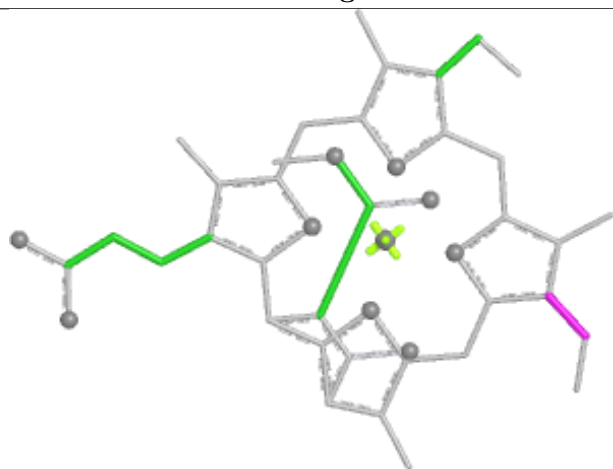
Ligand KC2 g 313



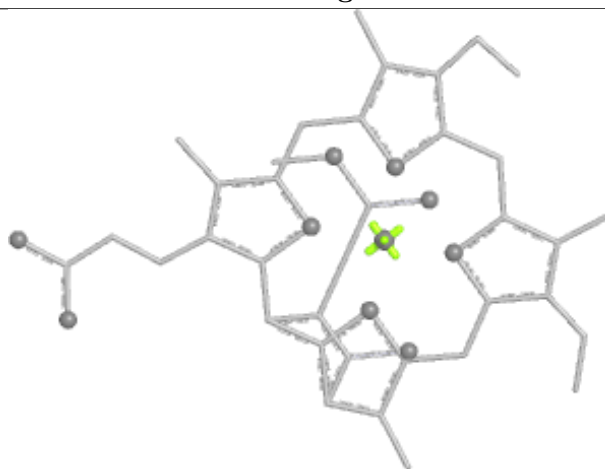
Bond lengths



Bond angles

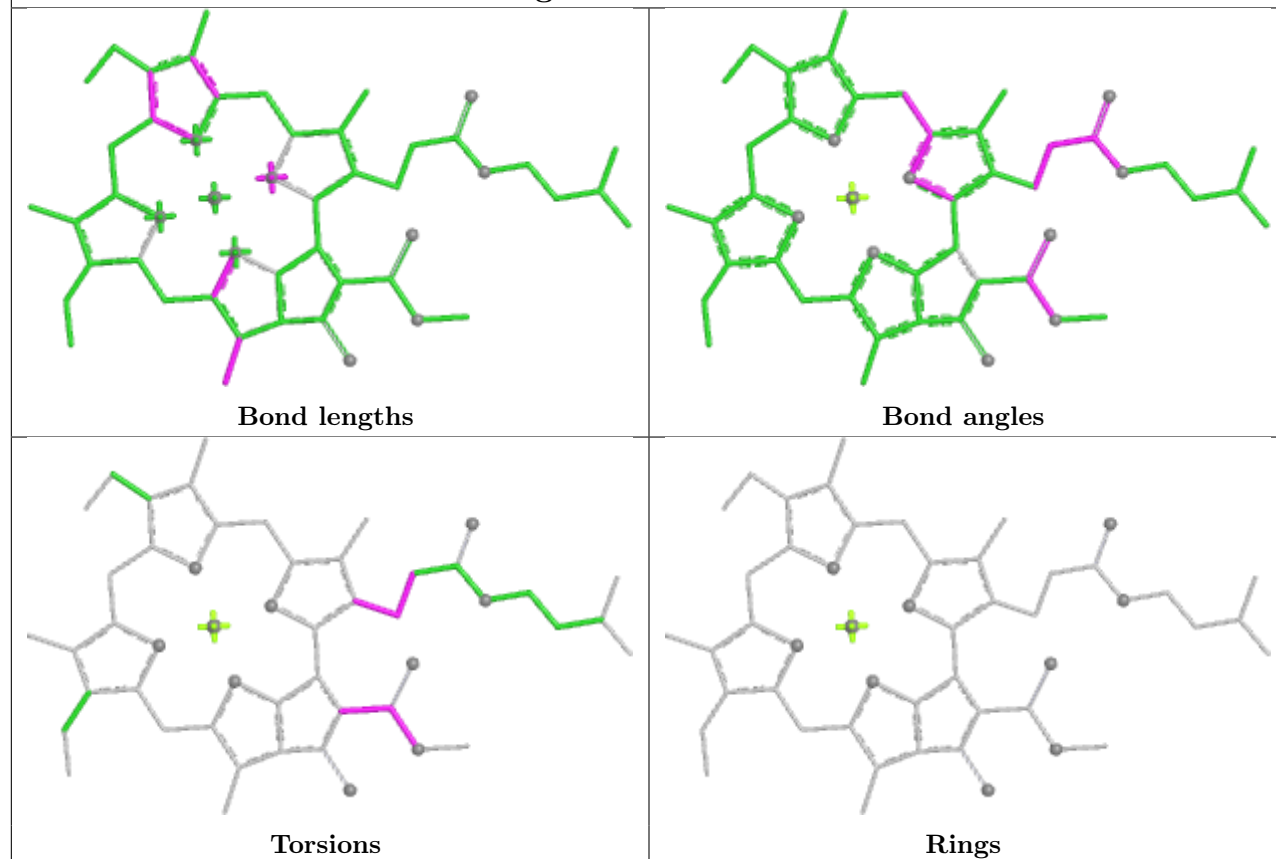


Torsions

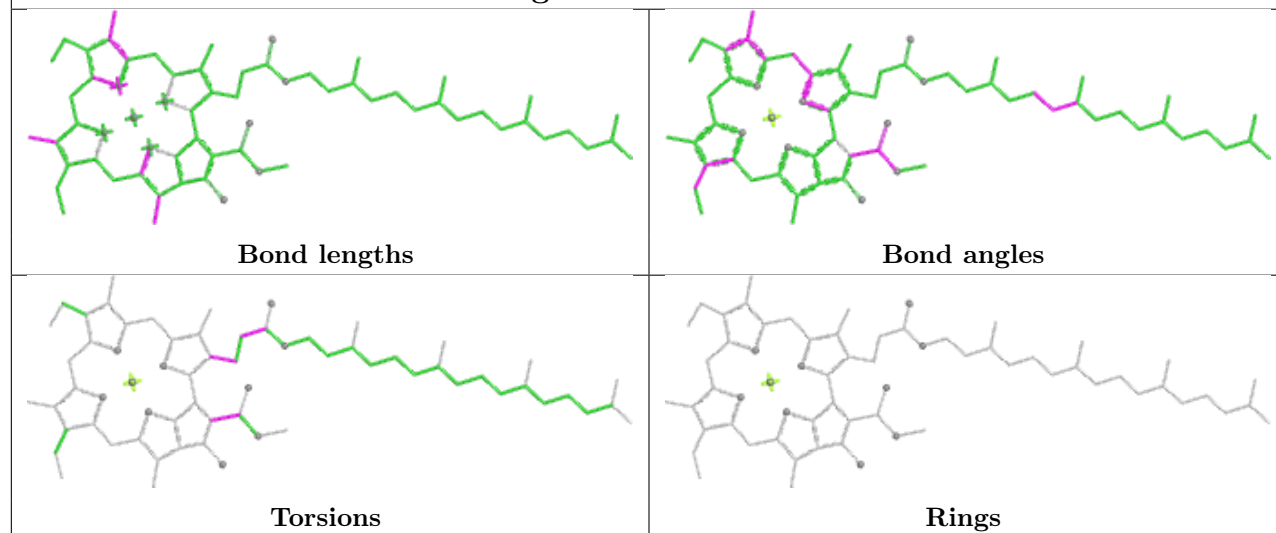


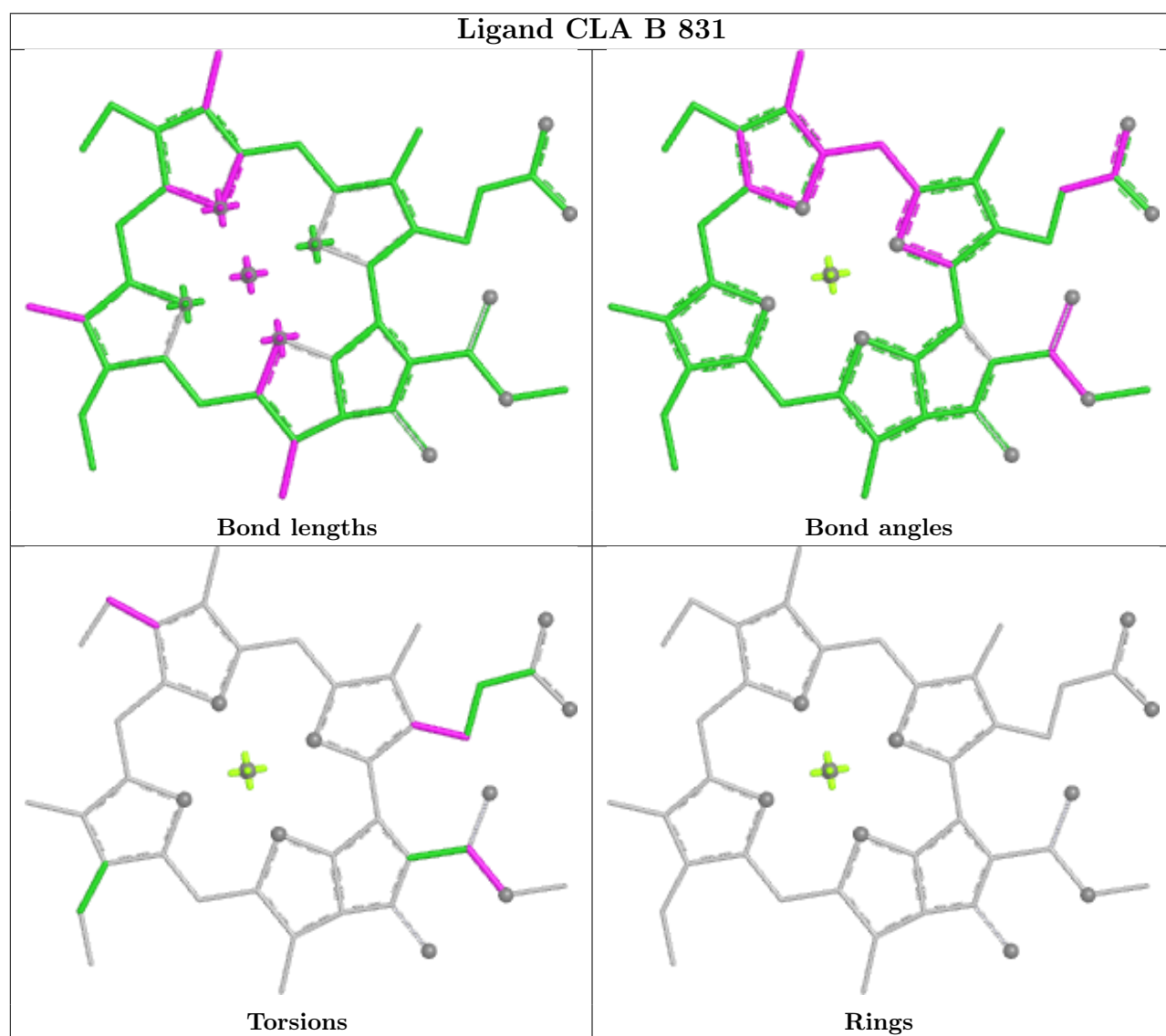
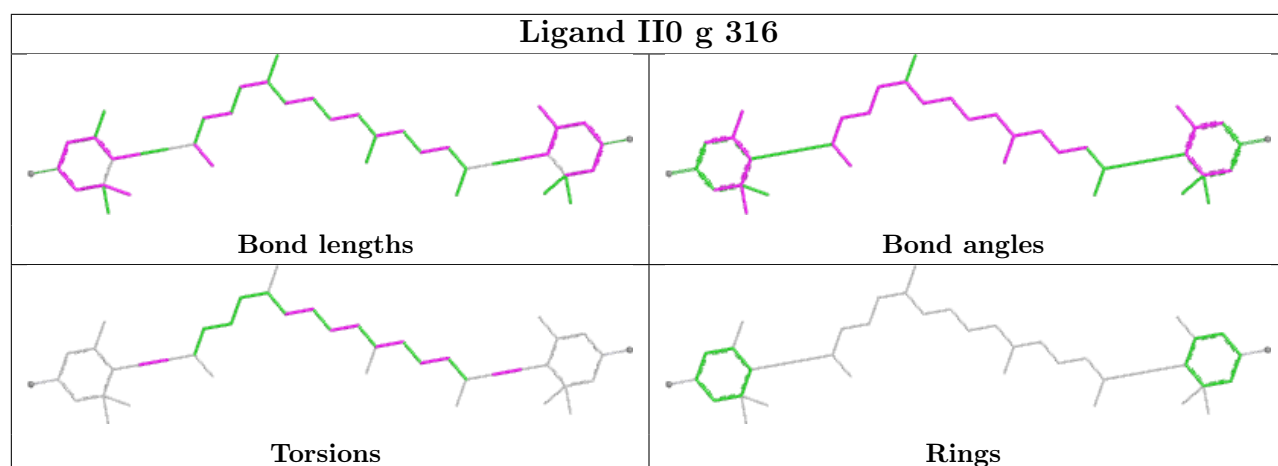
Rings

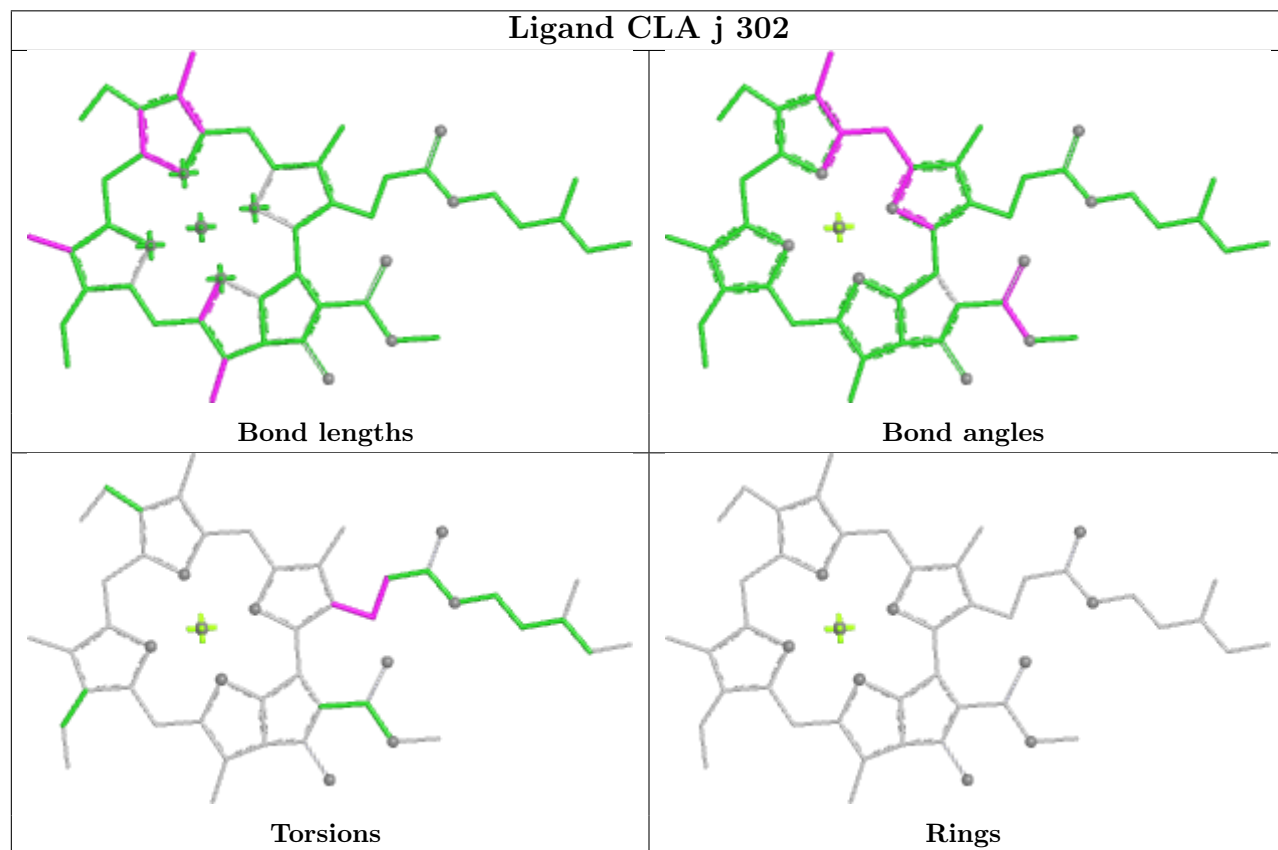
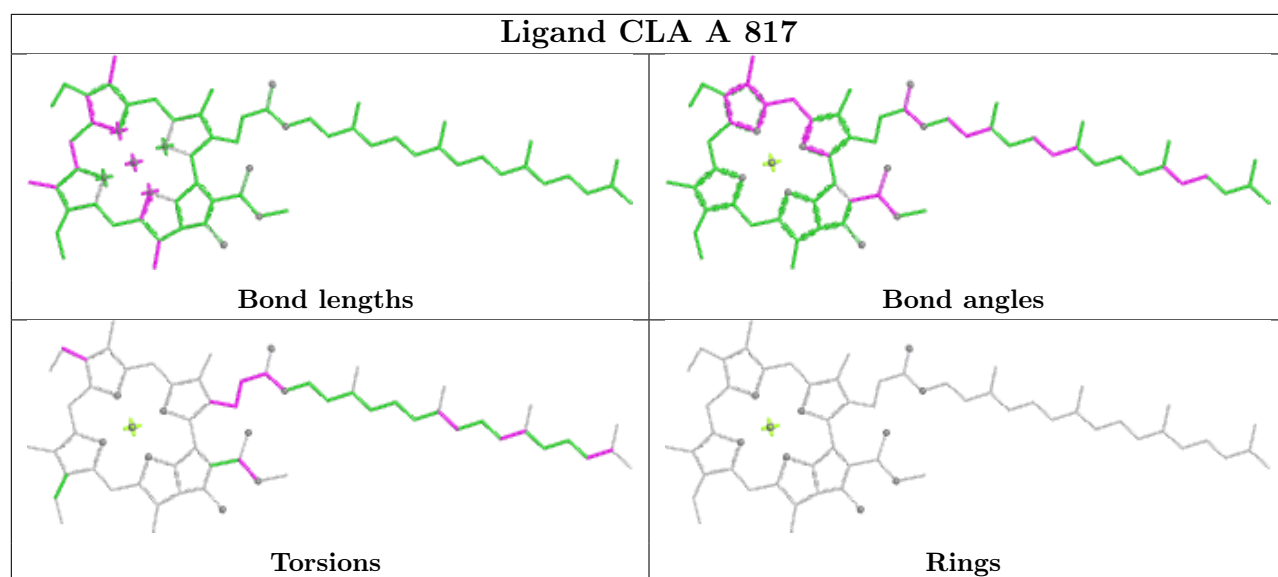
Ligand CLA d 301

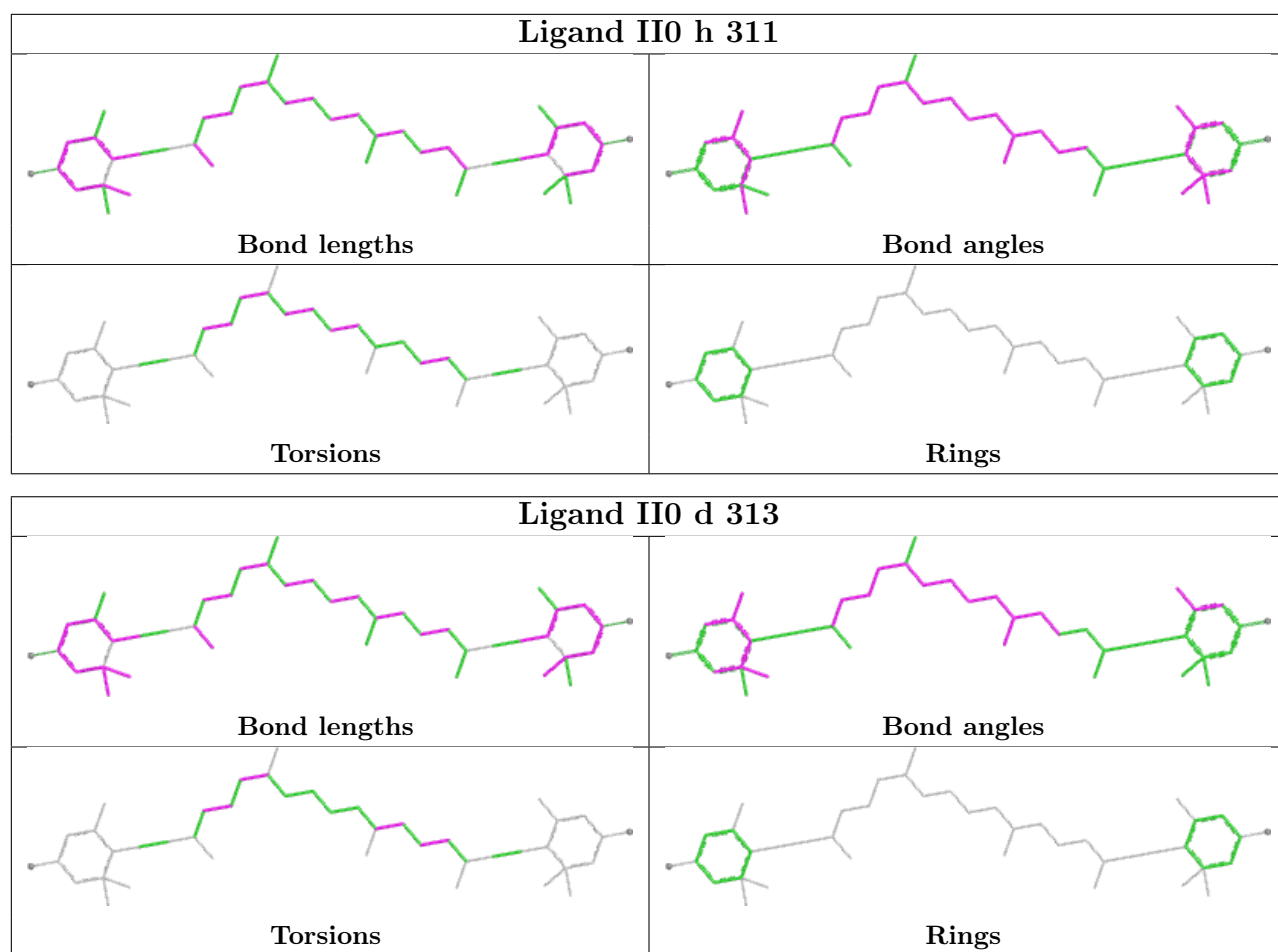


Ligand CLA A 804

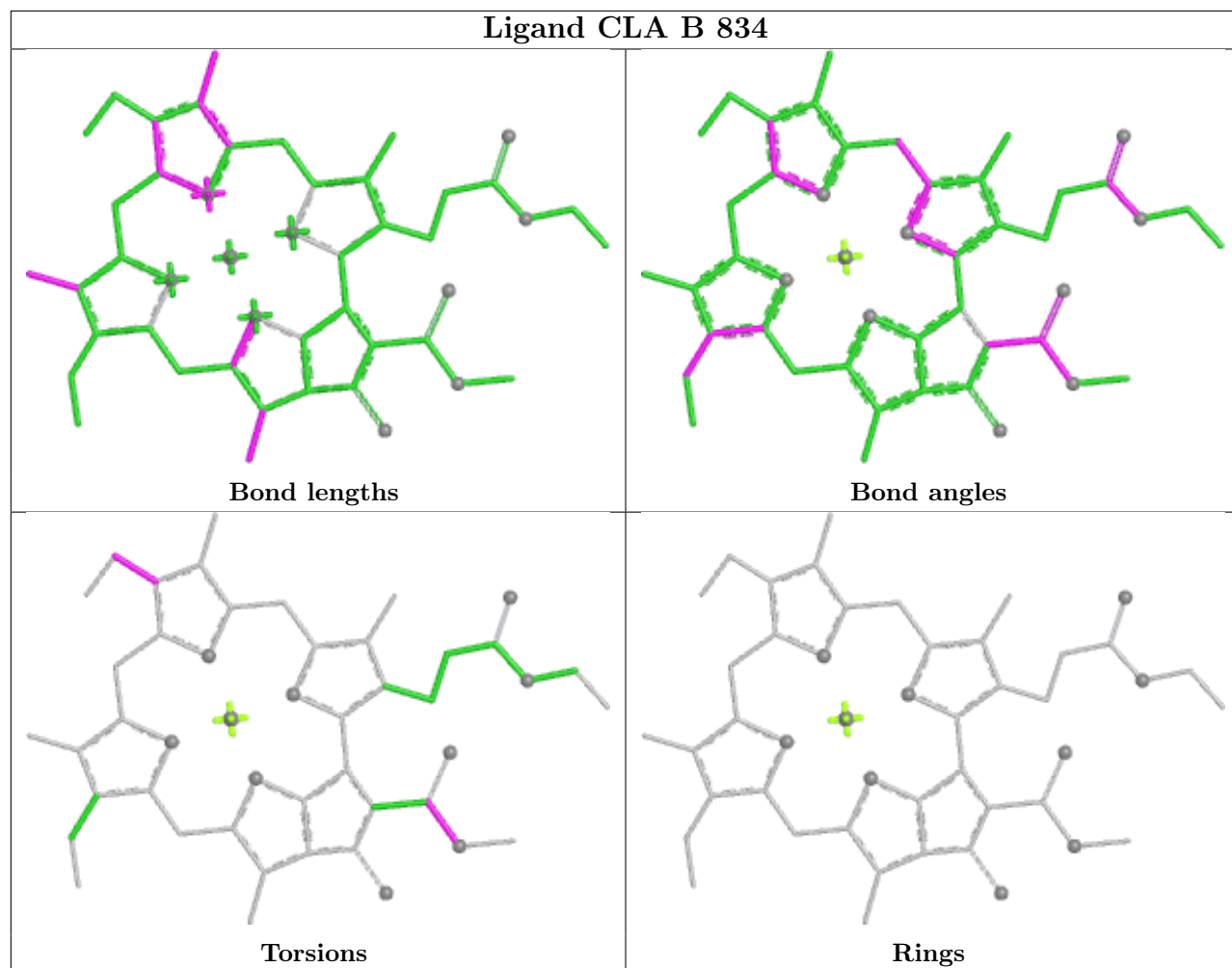


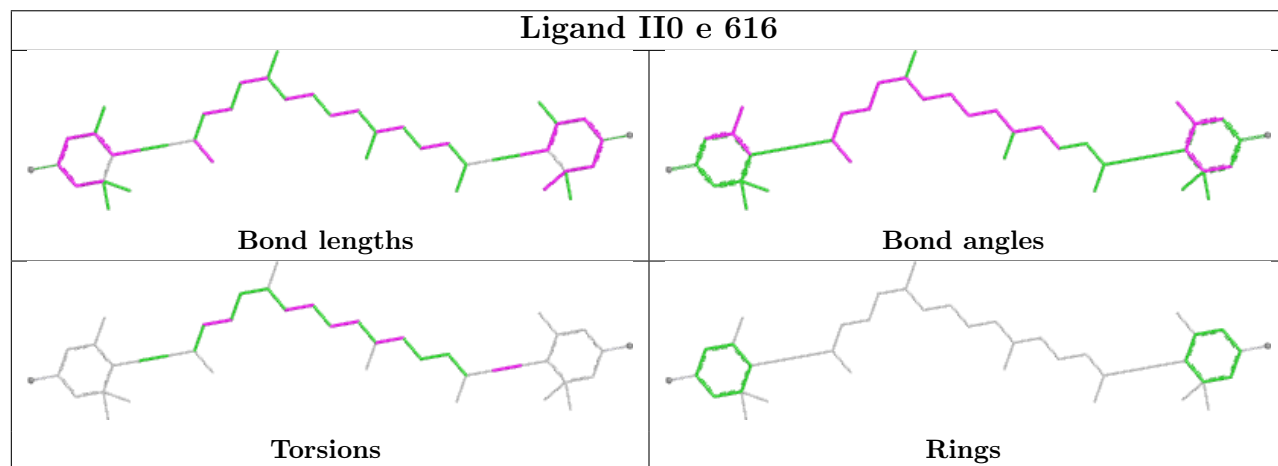
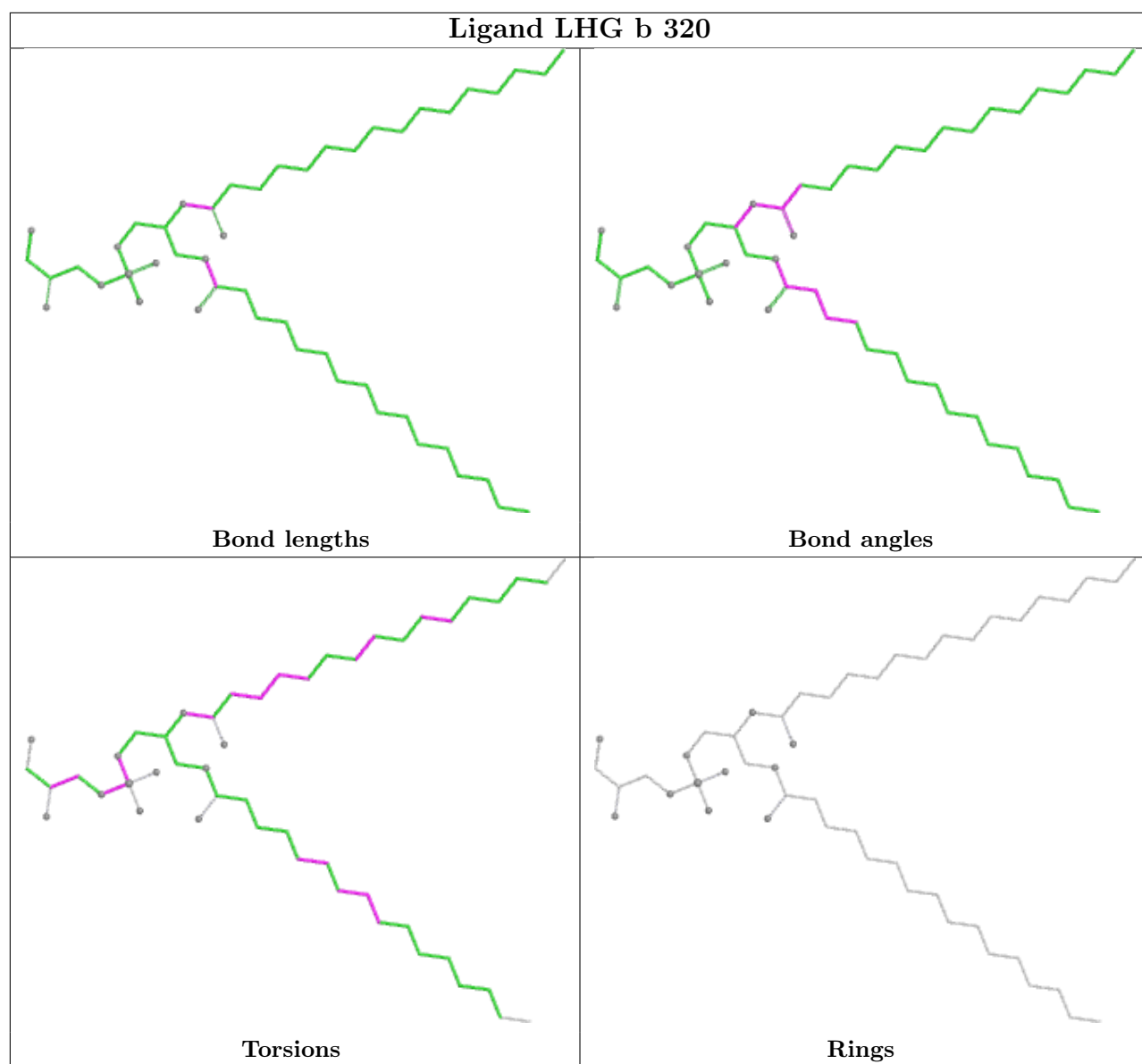


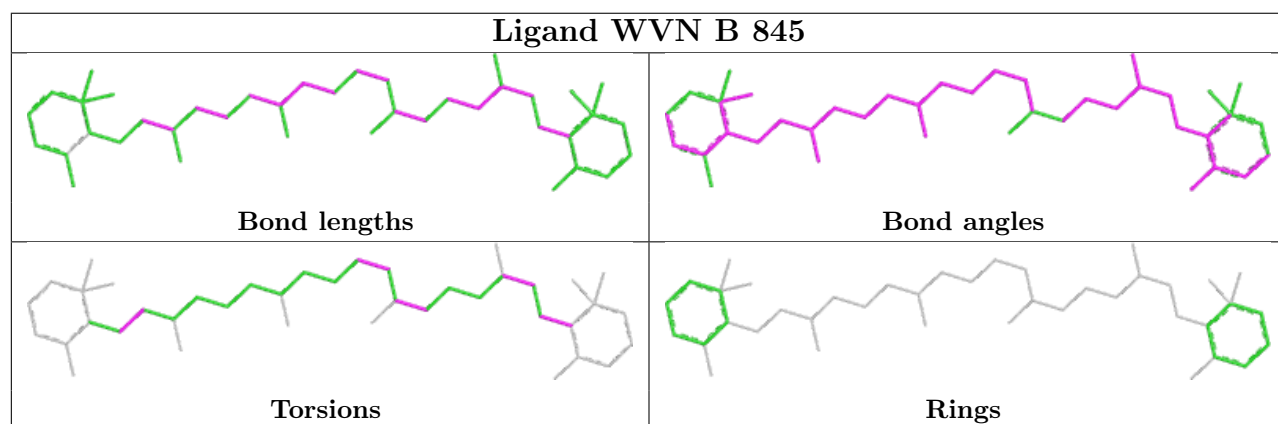
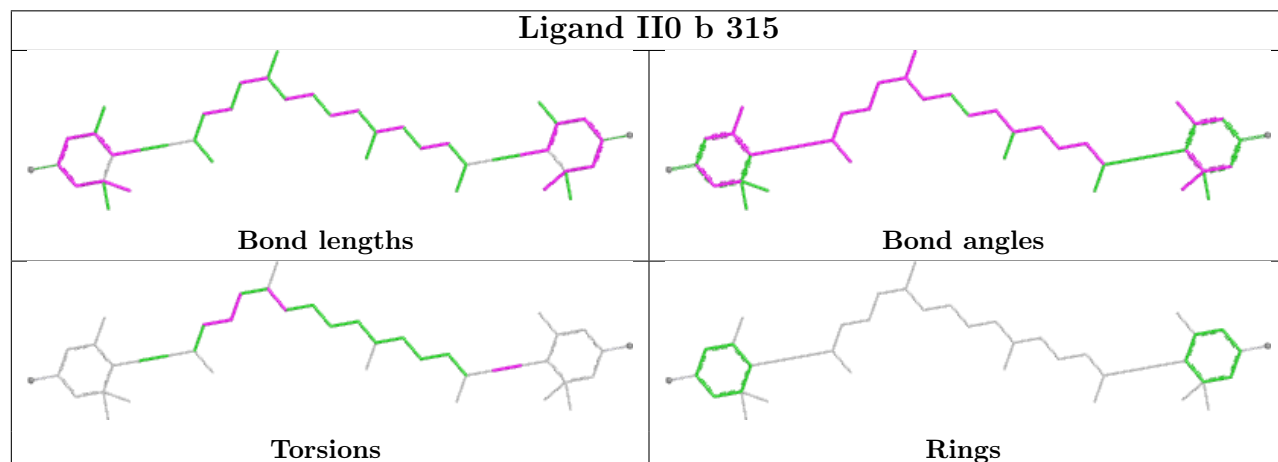
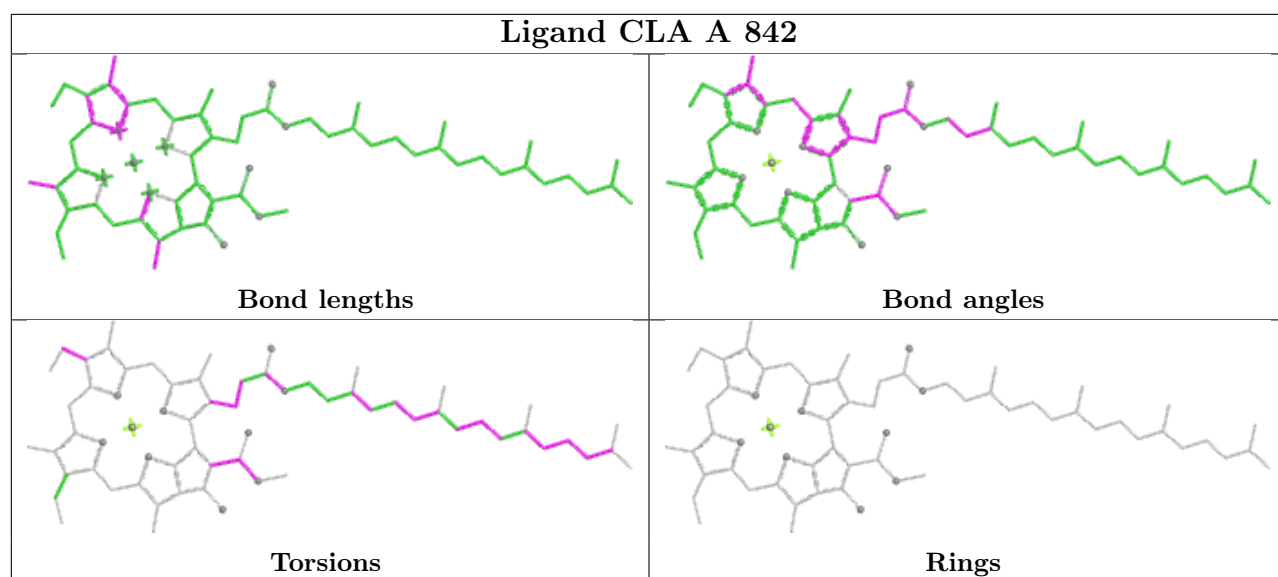


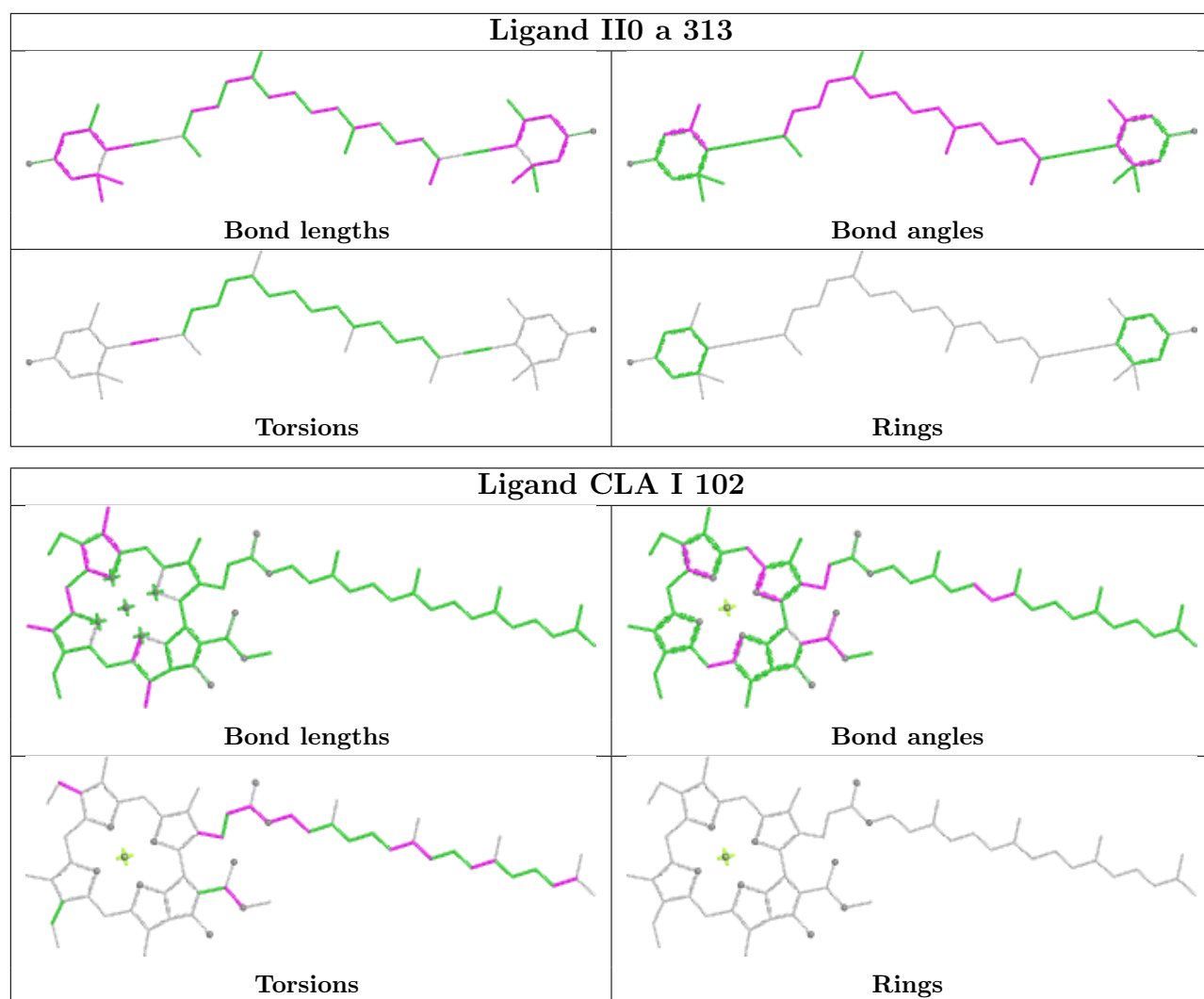


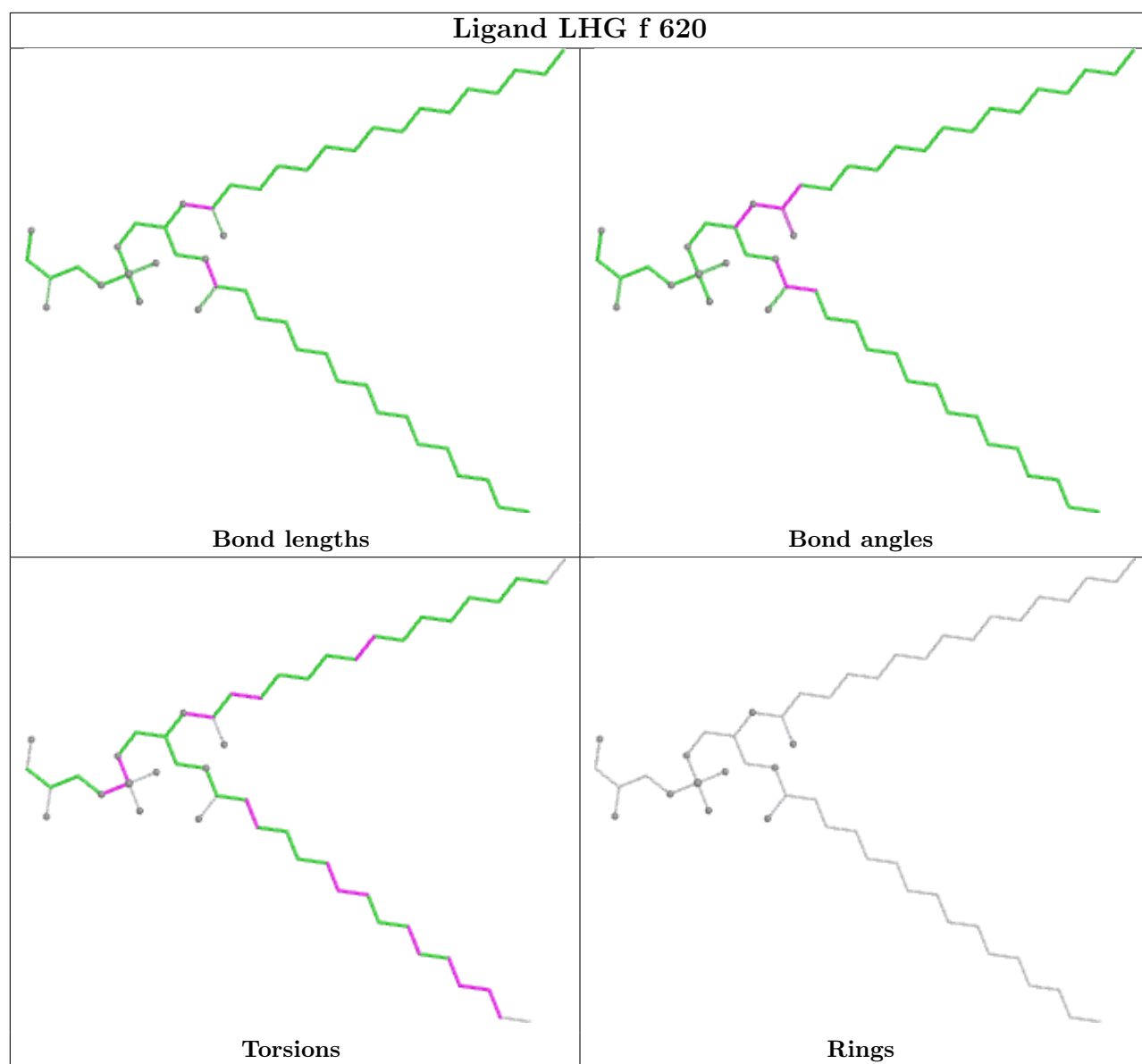
Ligand CLA B 834



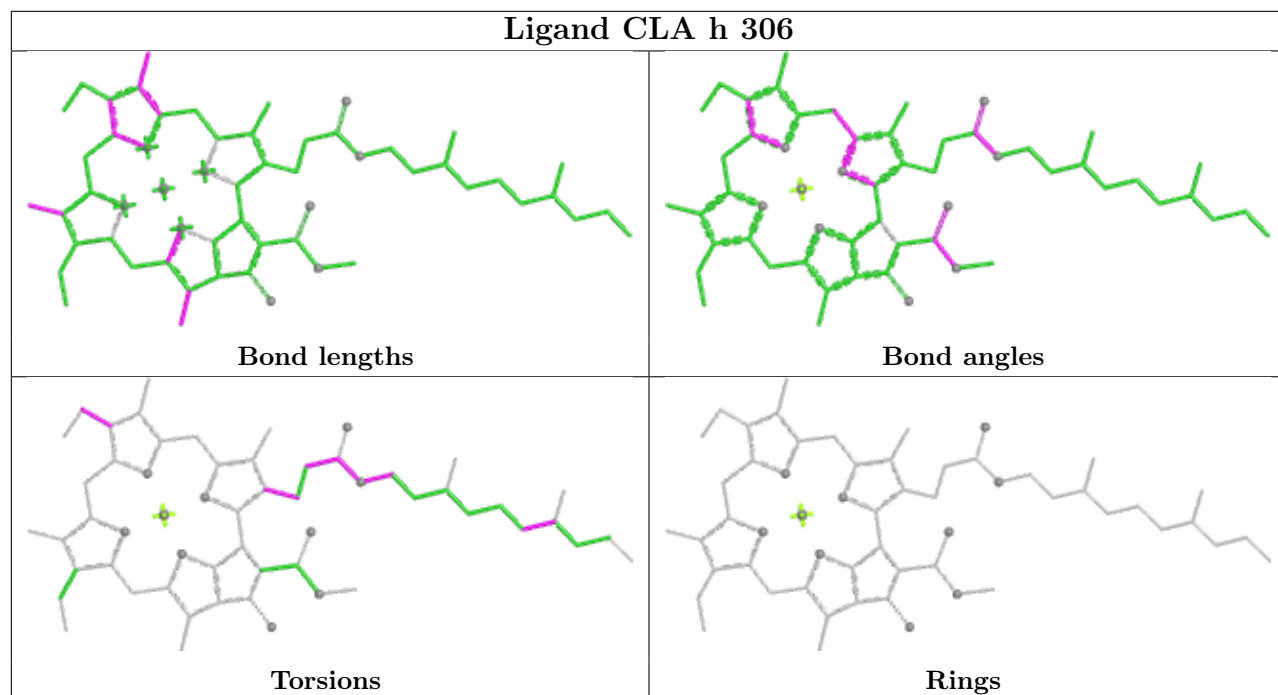




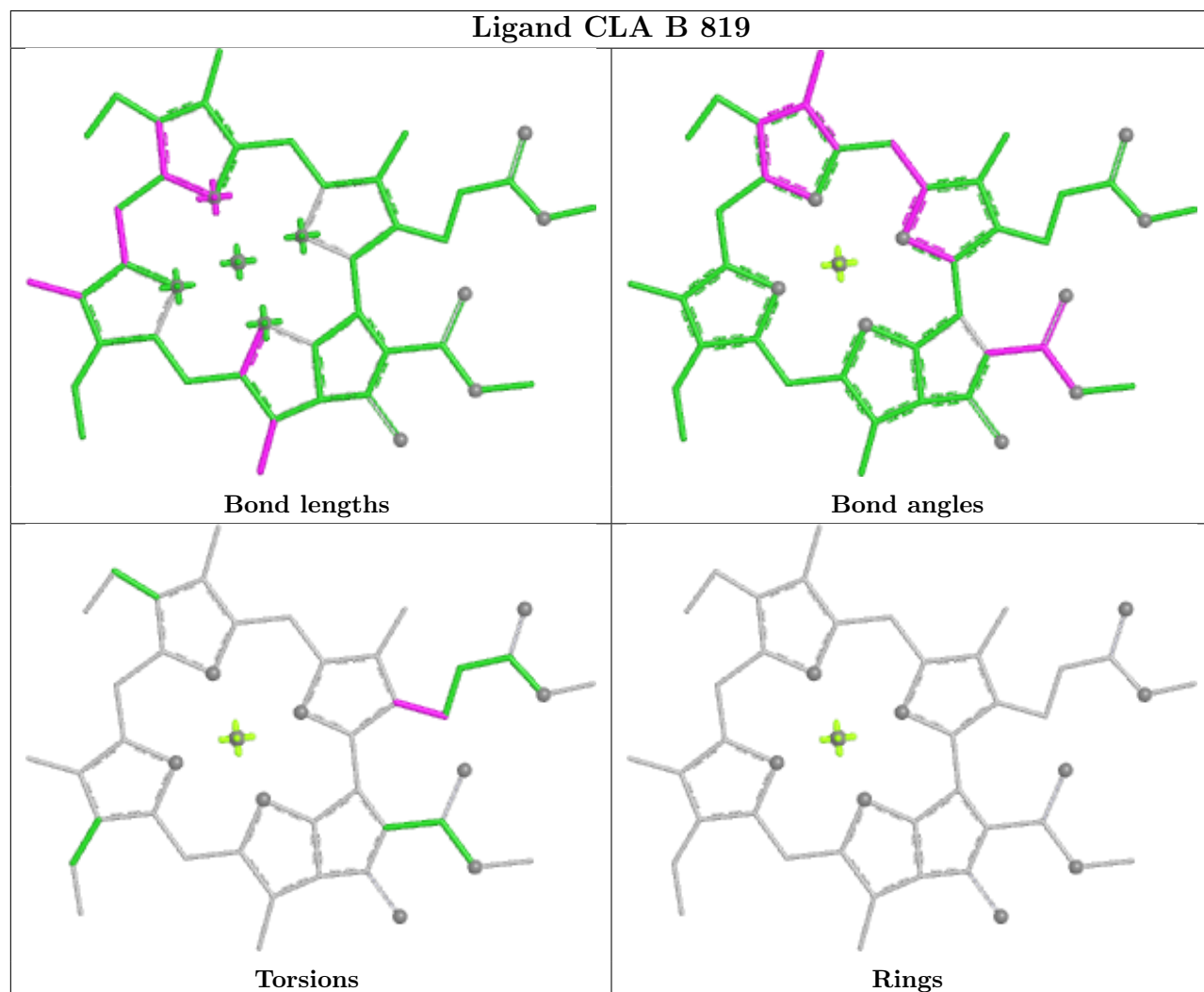


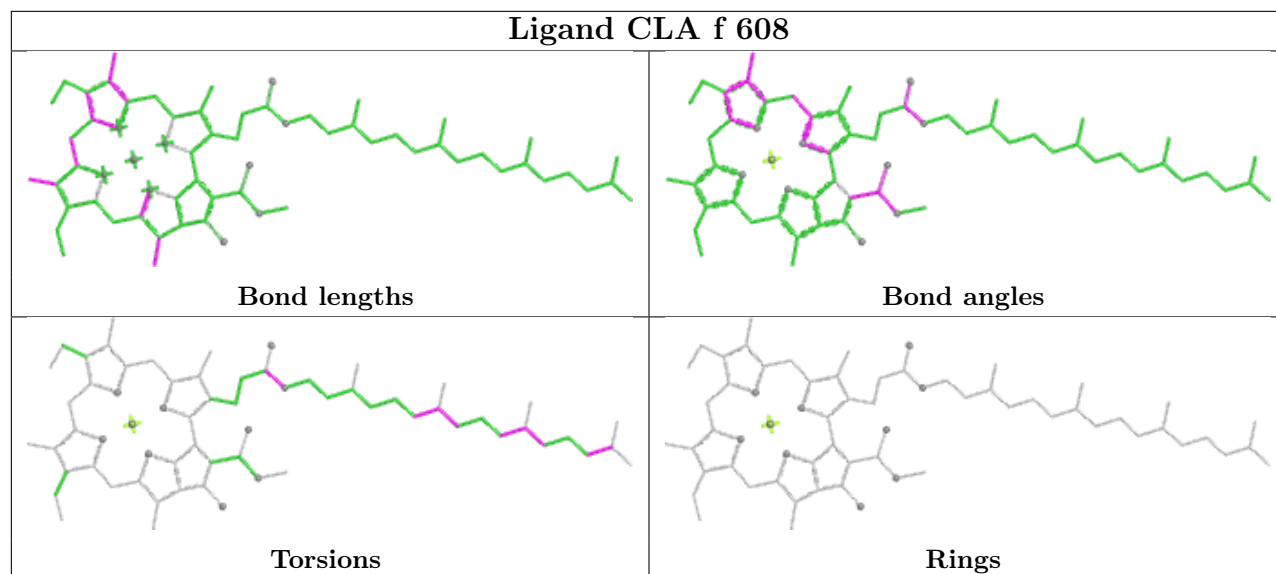
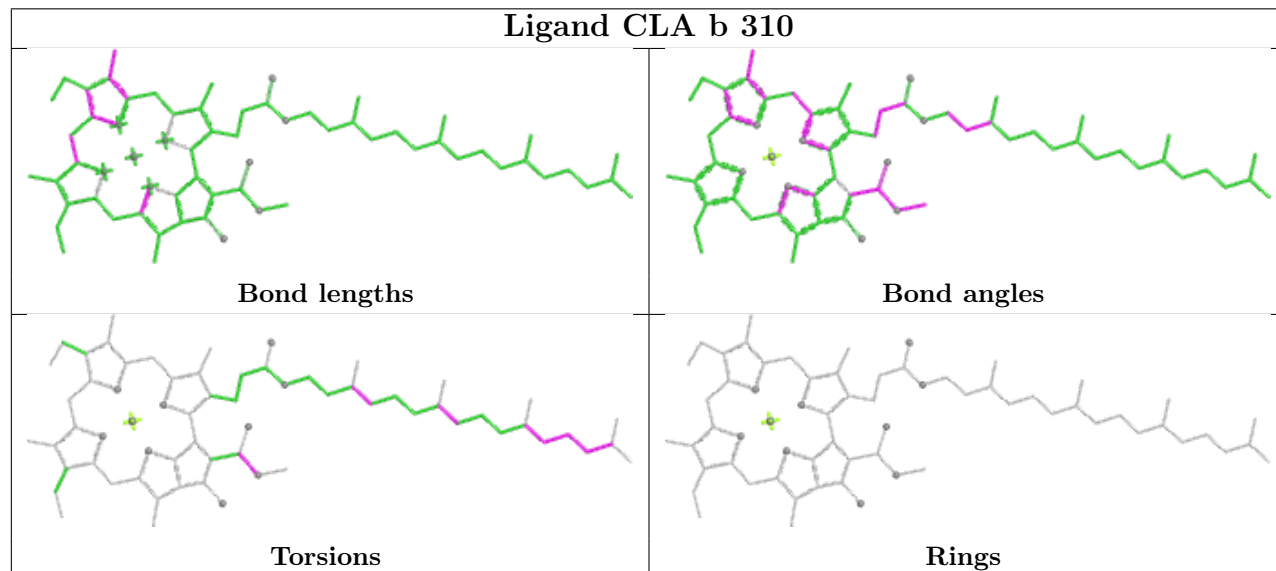


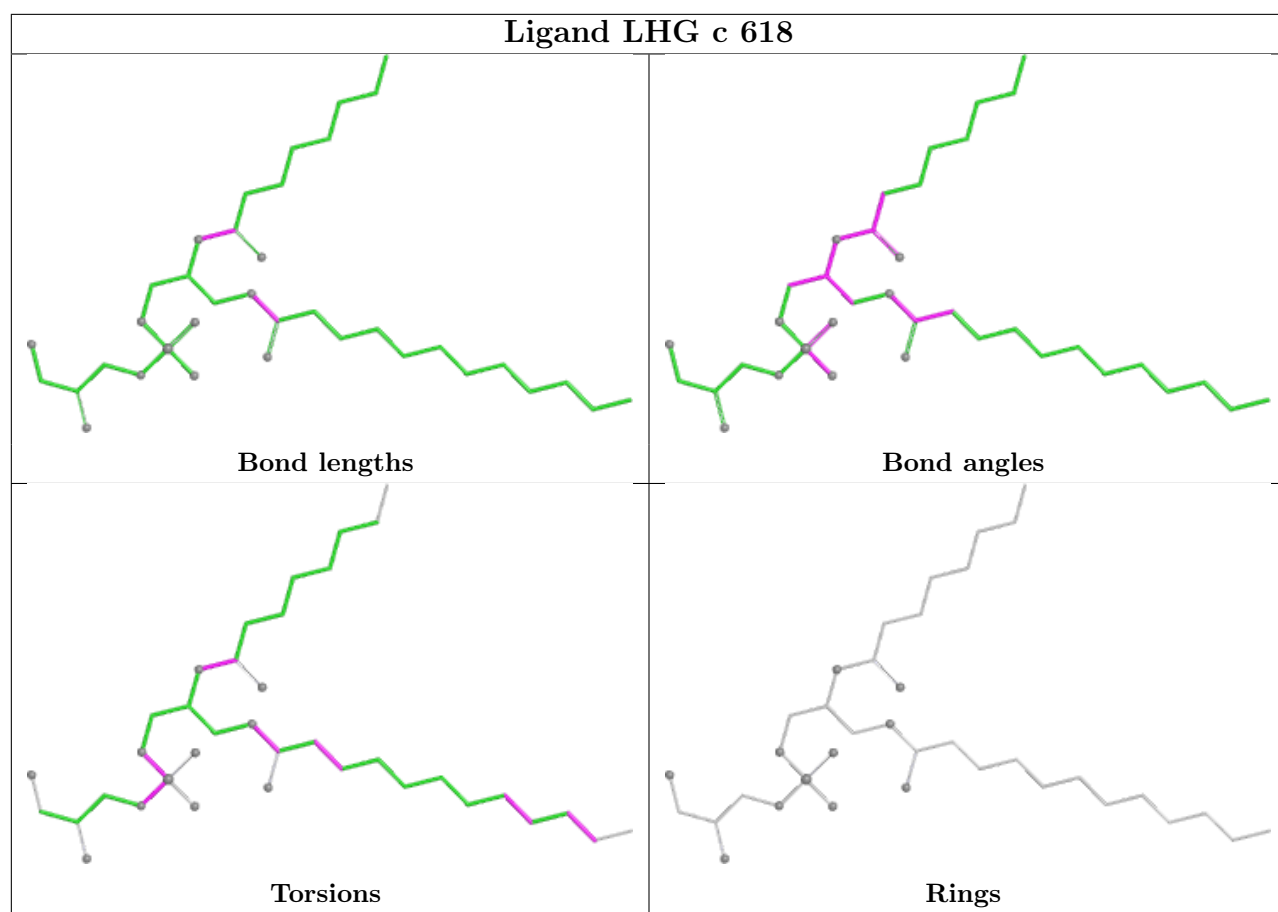
Ligand CLA h 306

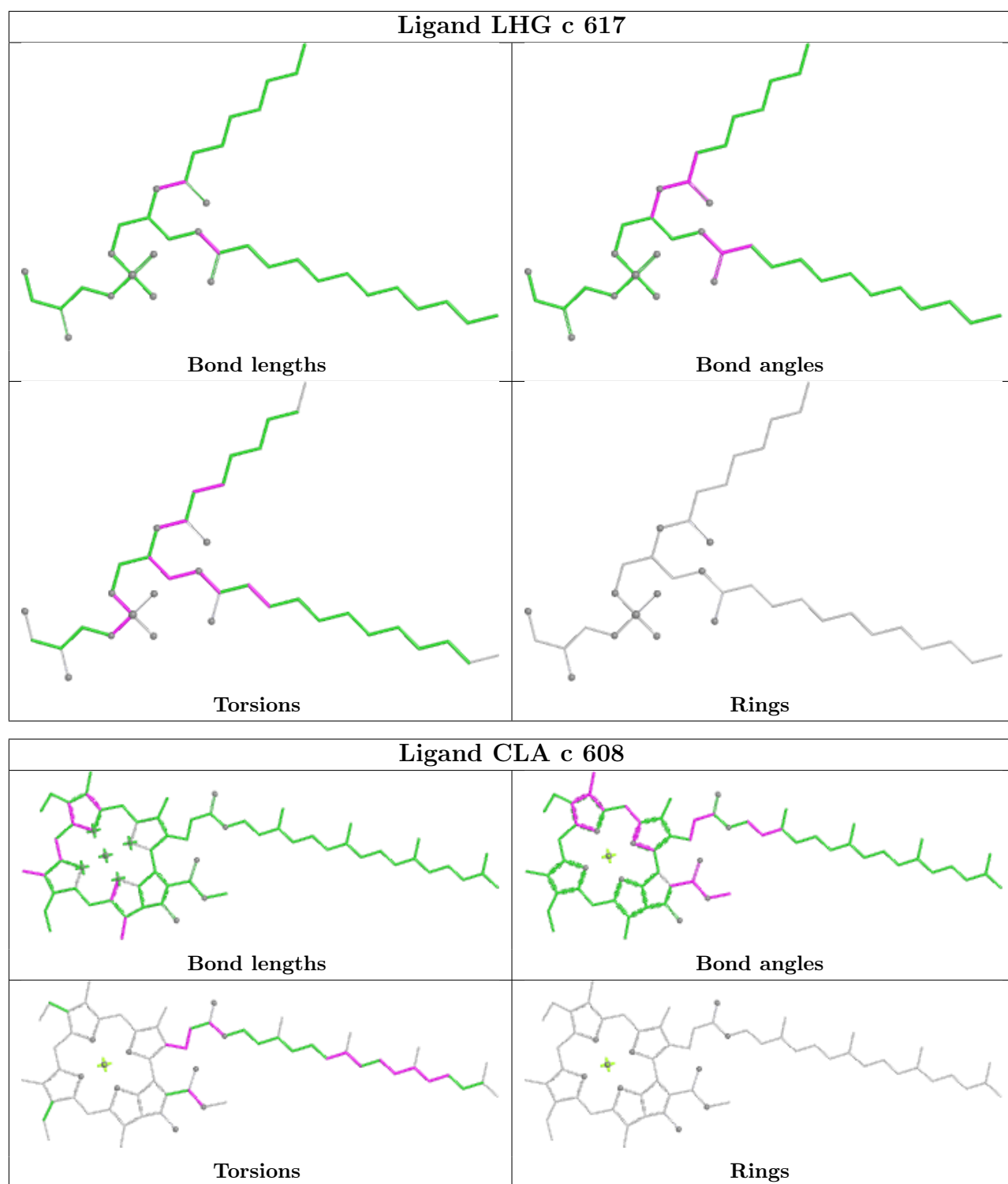


Ligand CLA B 819

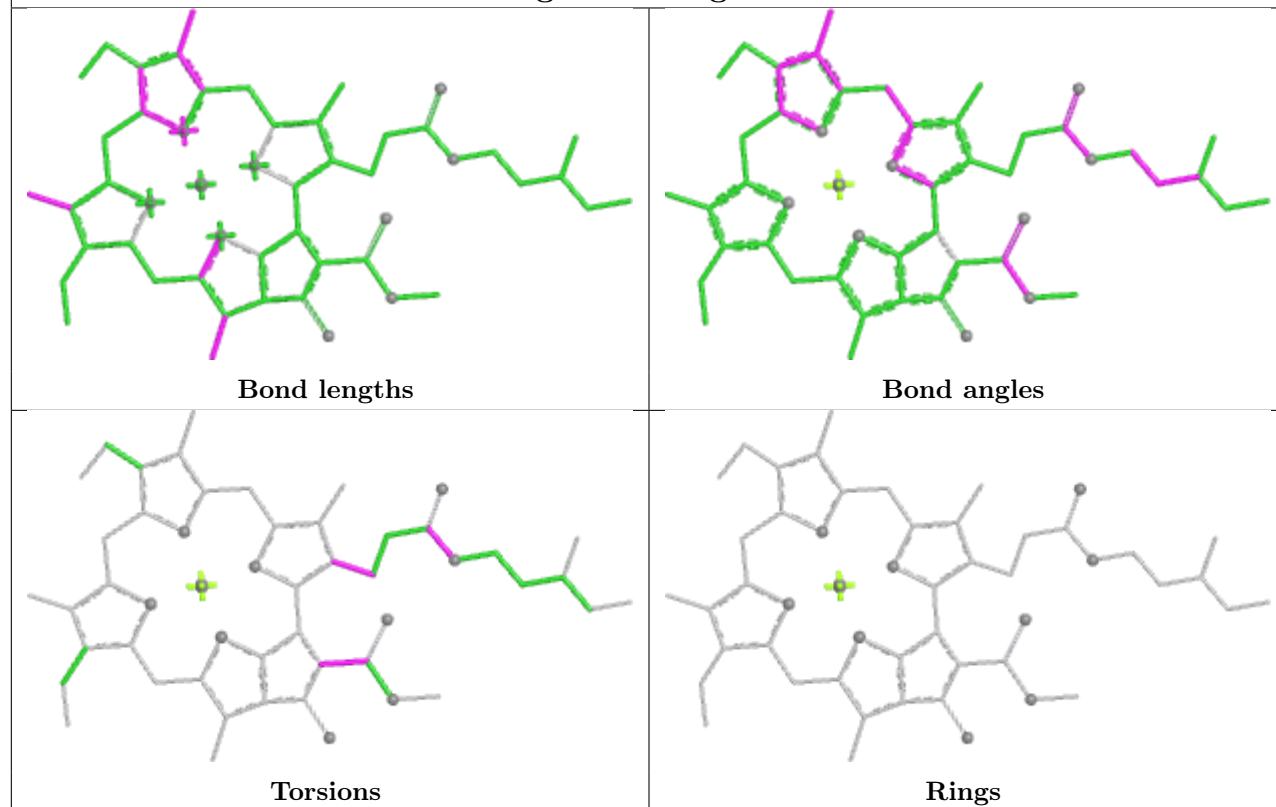


Ligand CLA f 608**Ligand CLA b 310**

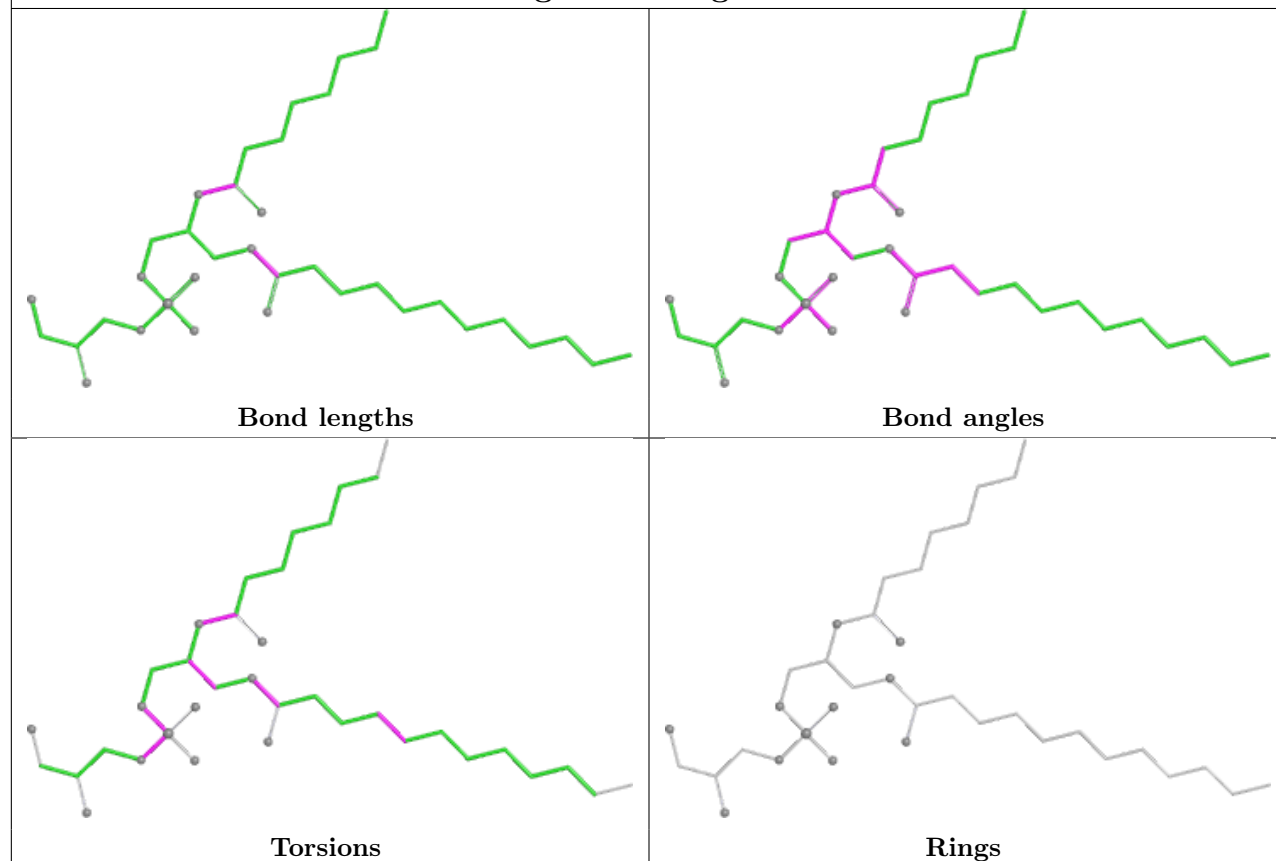


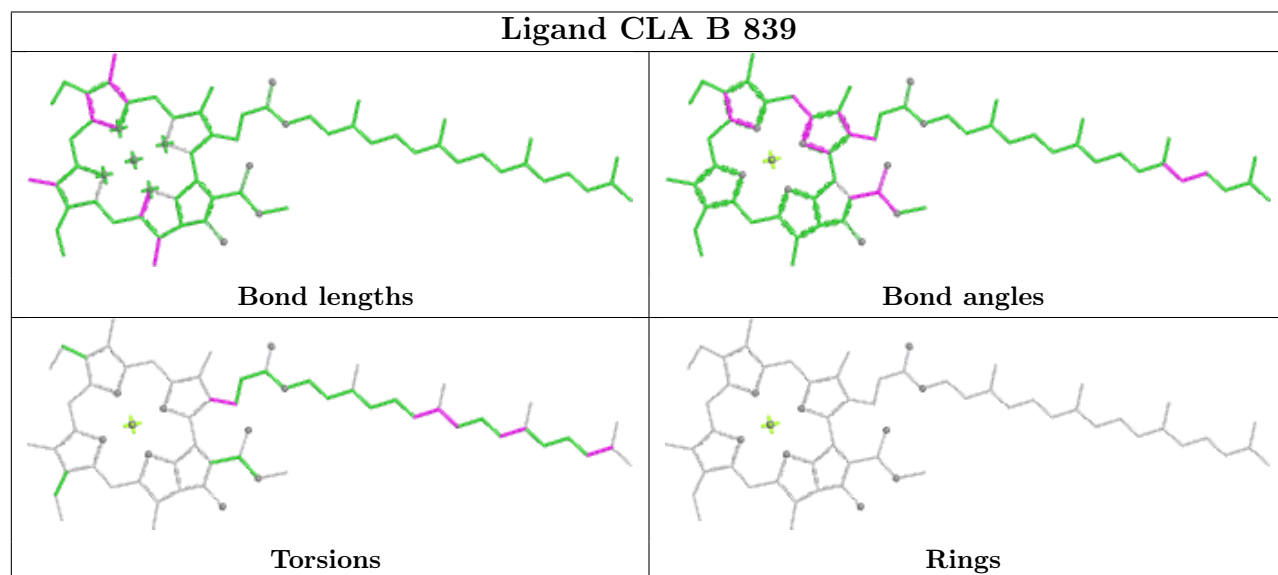
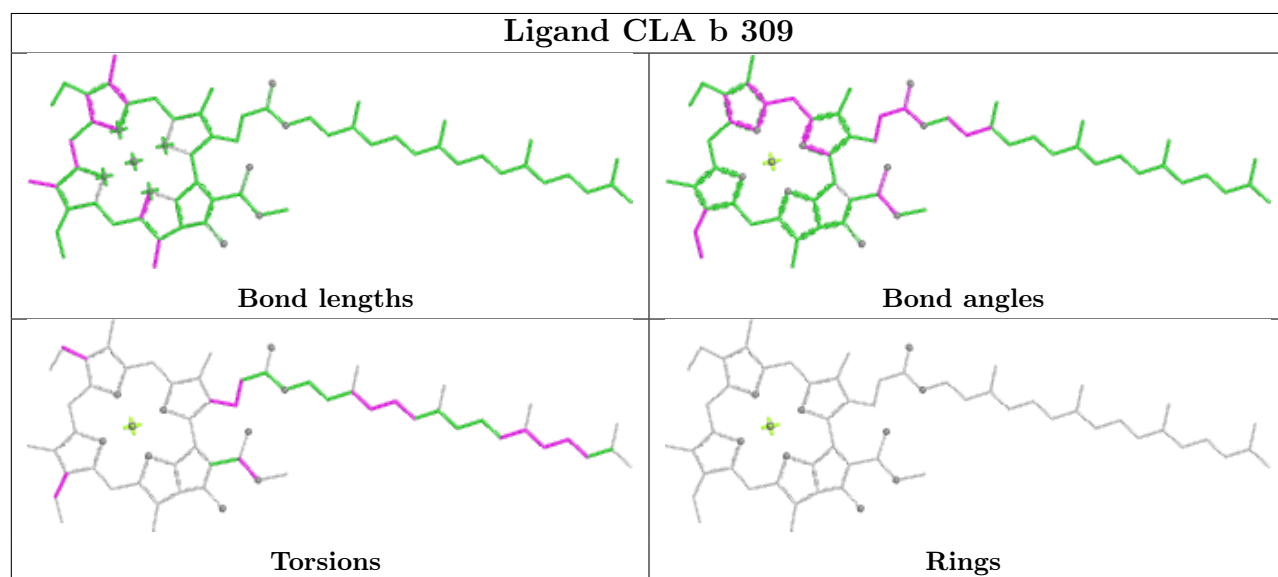
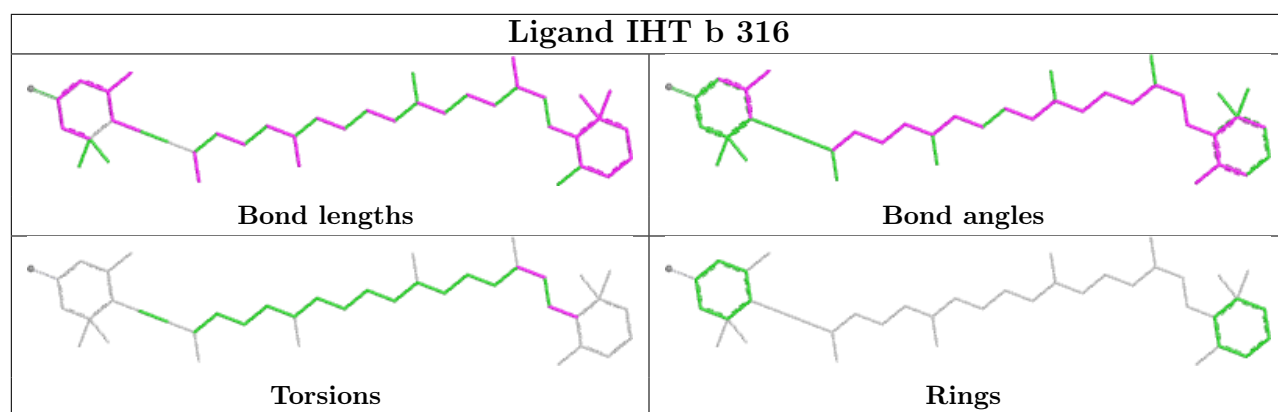


Ligand CLA g 310

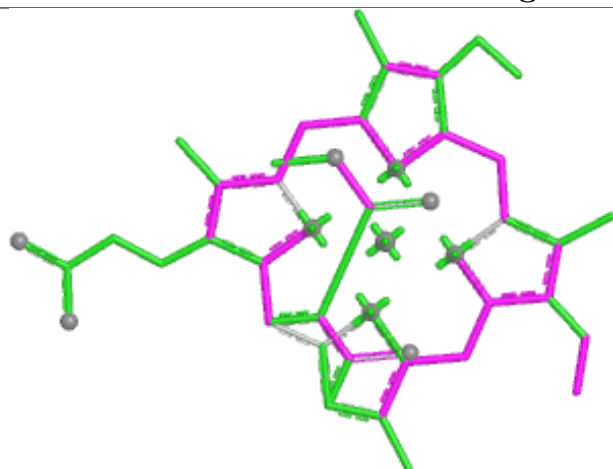


Ligand LHG g 321

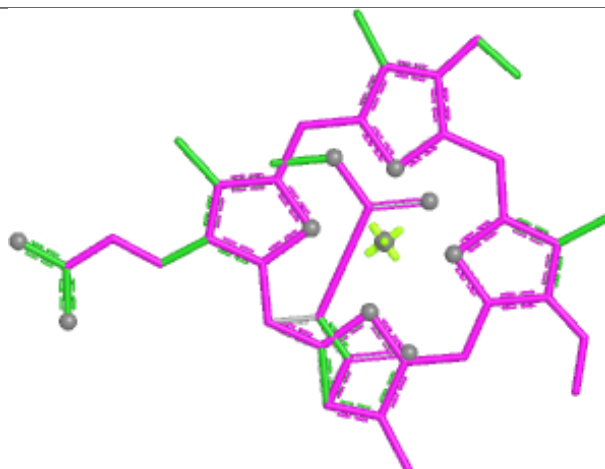




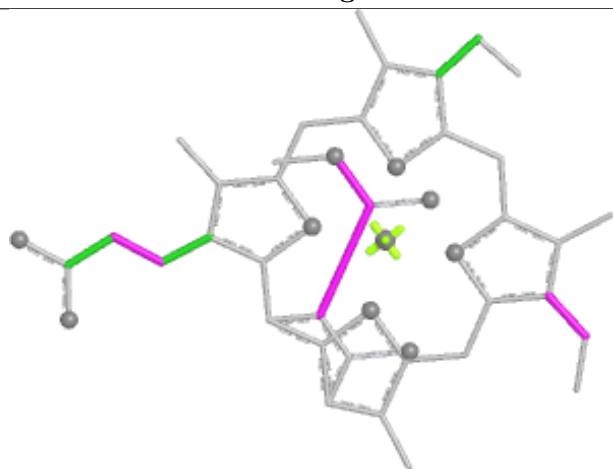
Ligand KC2 d 310



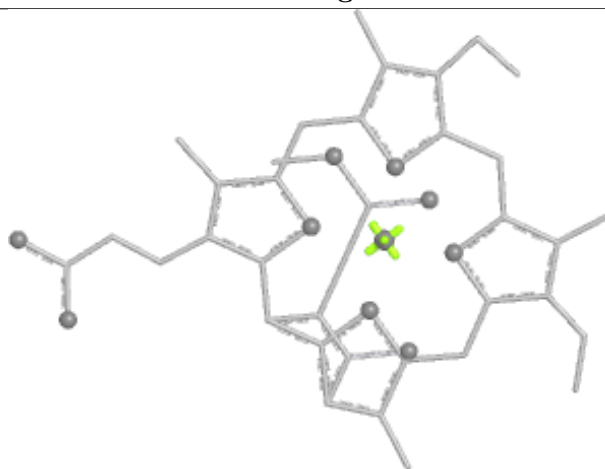
Bond lengths



Bond angles

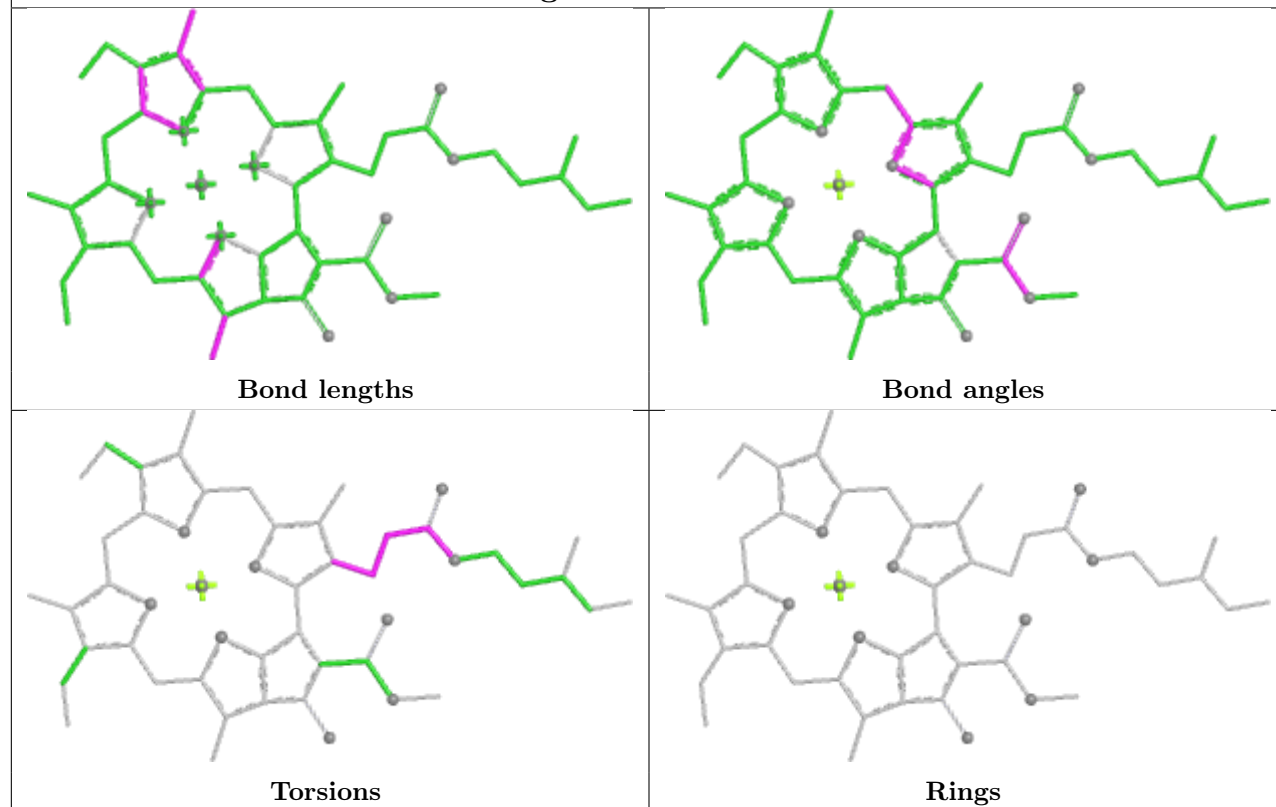


Torsions

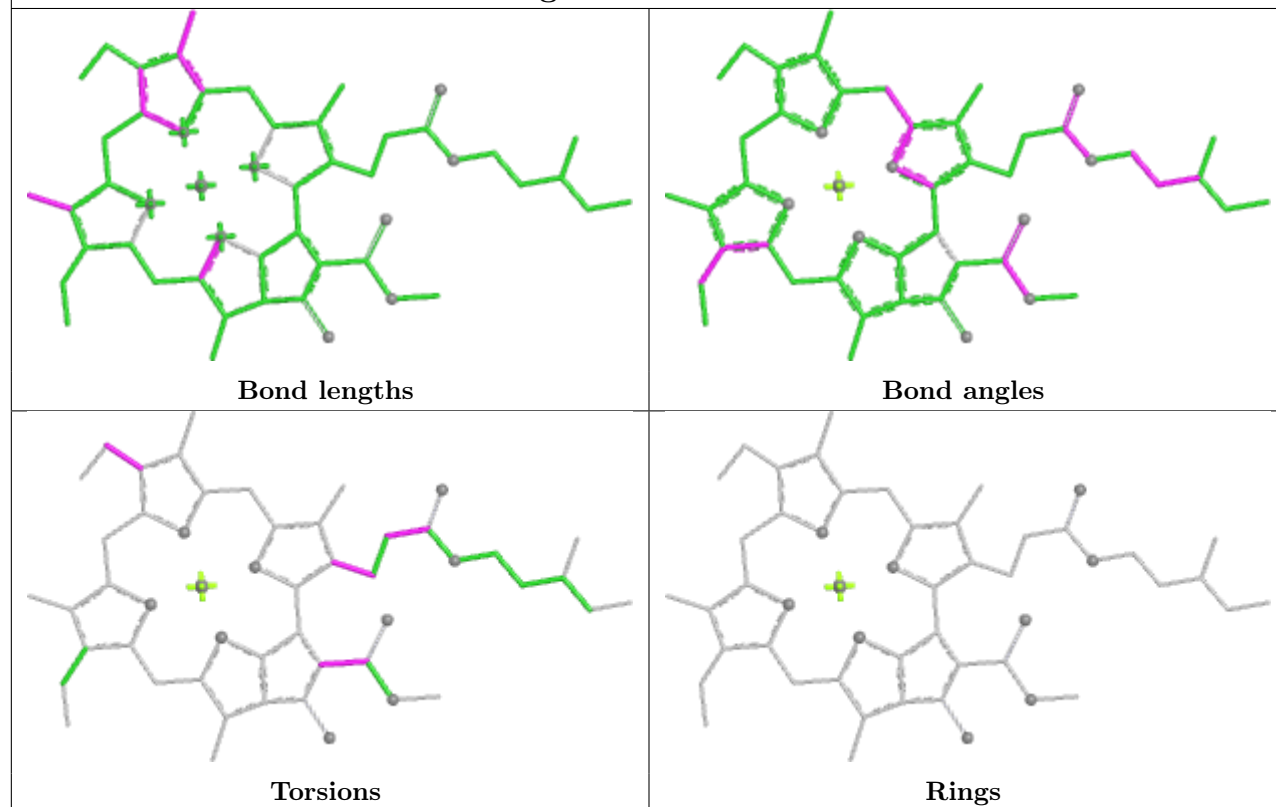


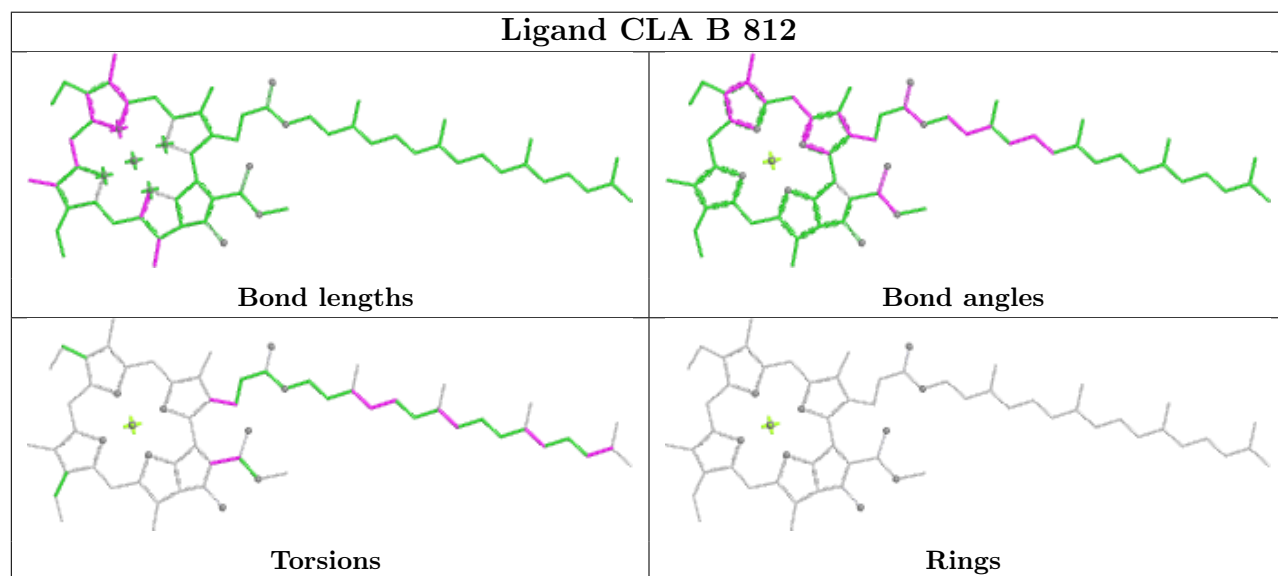
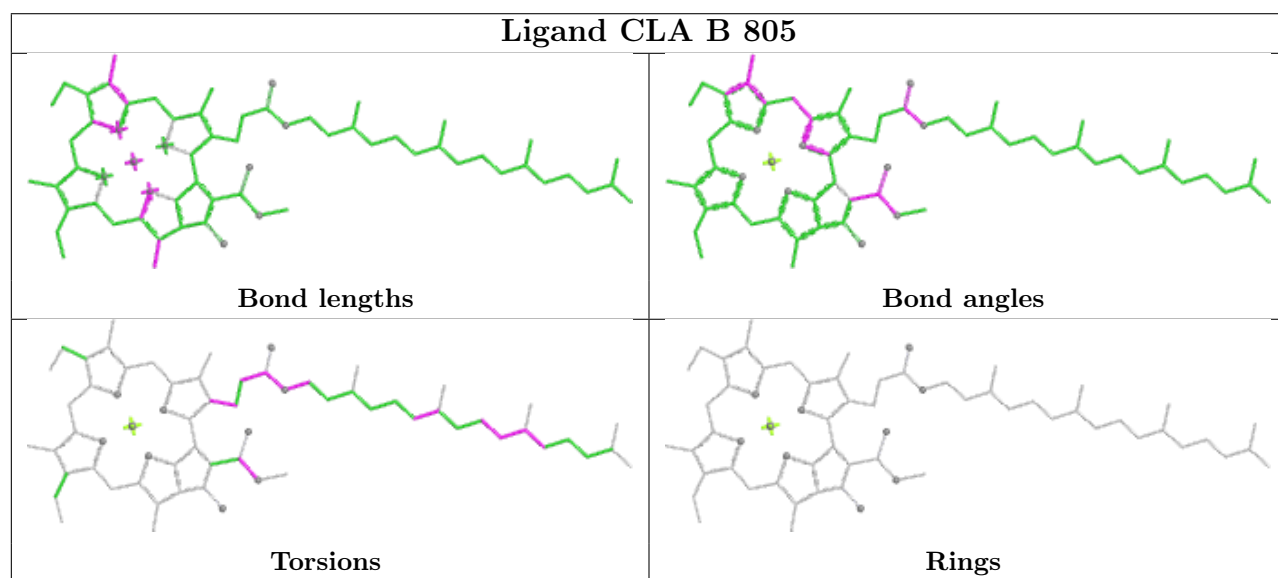
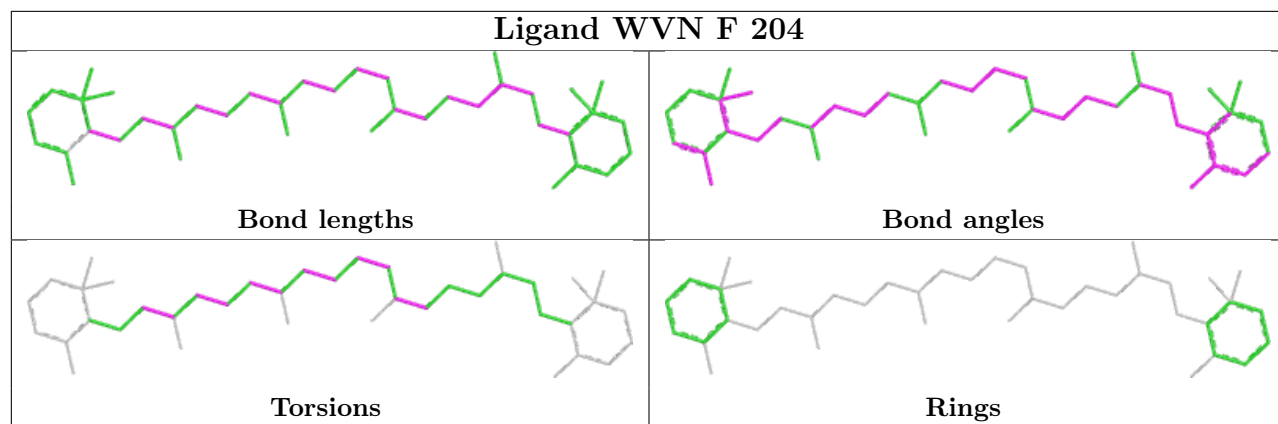
Rings

Ligand CLA i 601

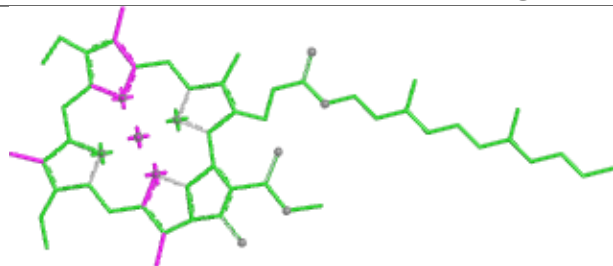


Ligand CLA f 606

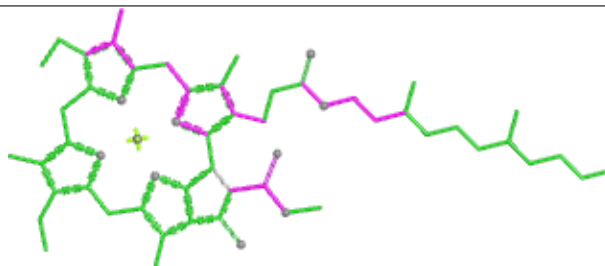




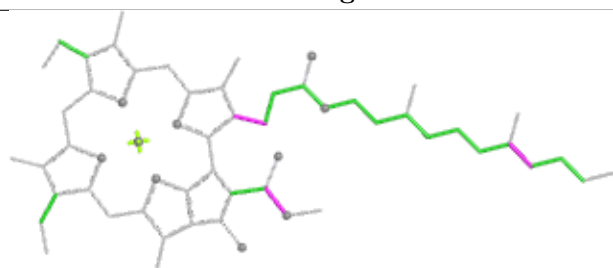
Ligand CLA B 832



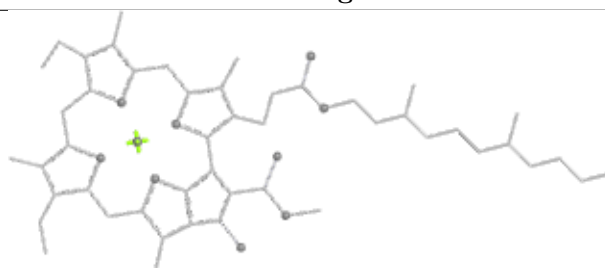
Bond lengths



Bond angles

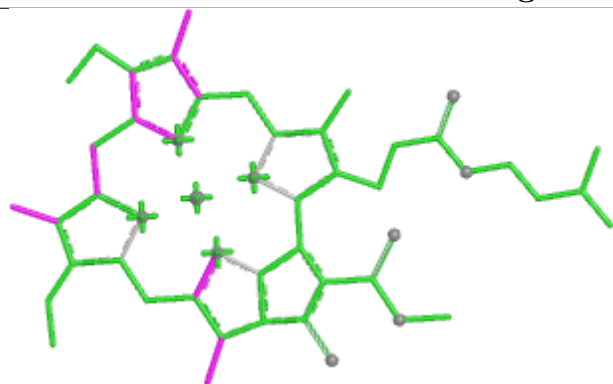


Torsions

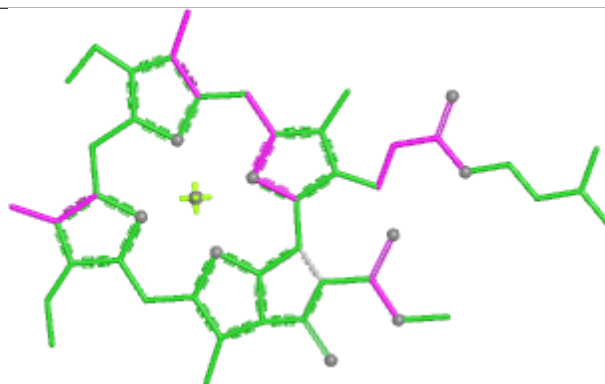


Rings

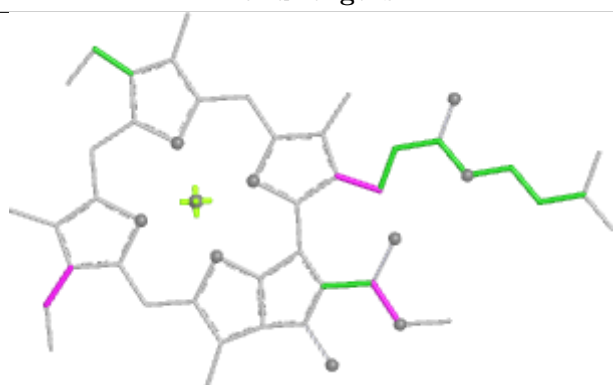
Ligand CLA k 602



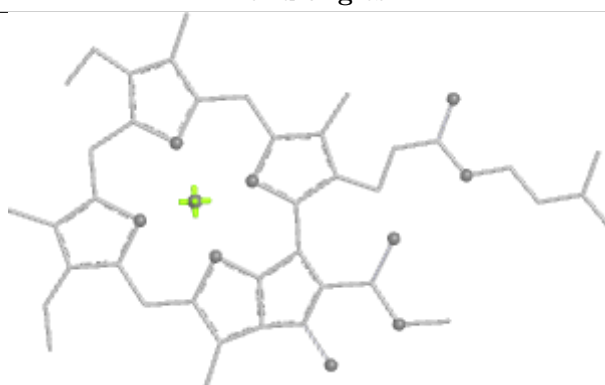
Bond lengths



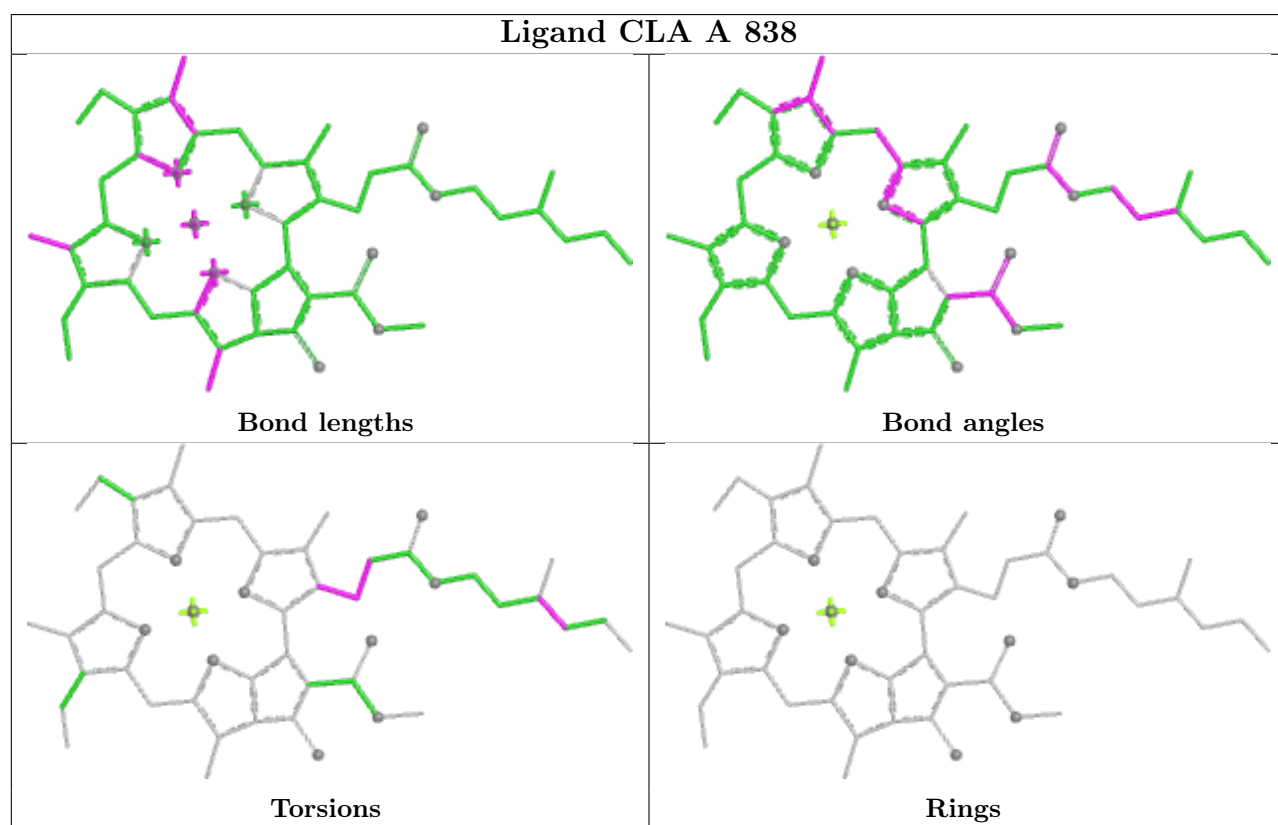
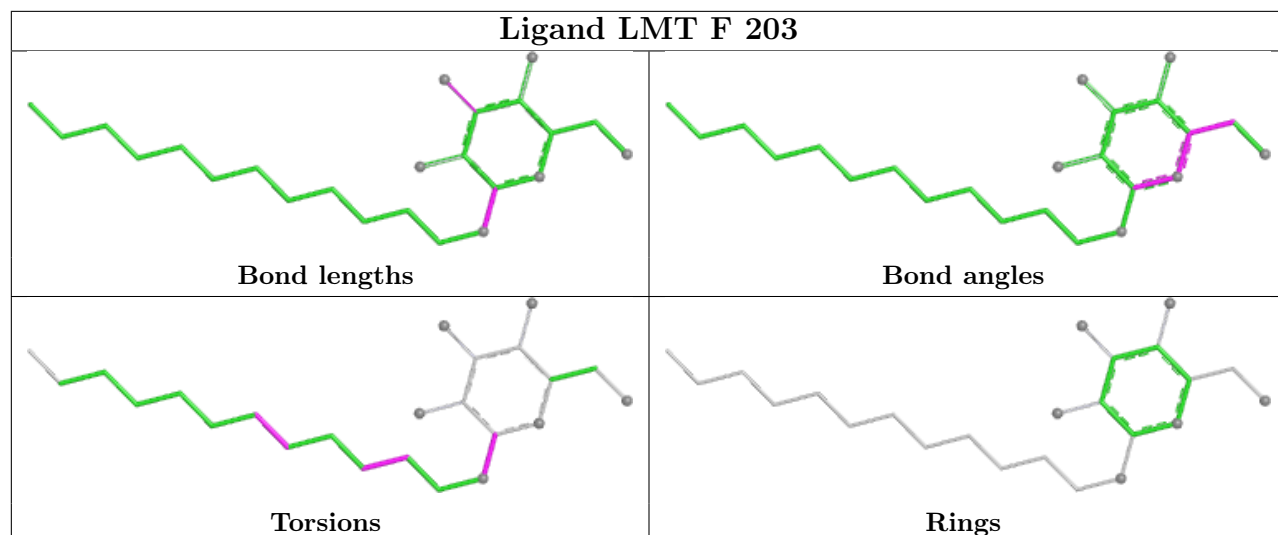
Bond angles

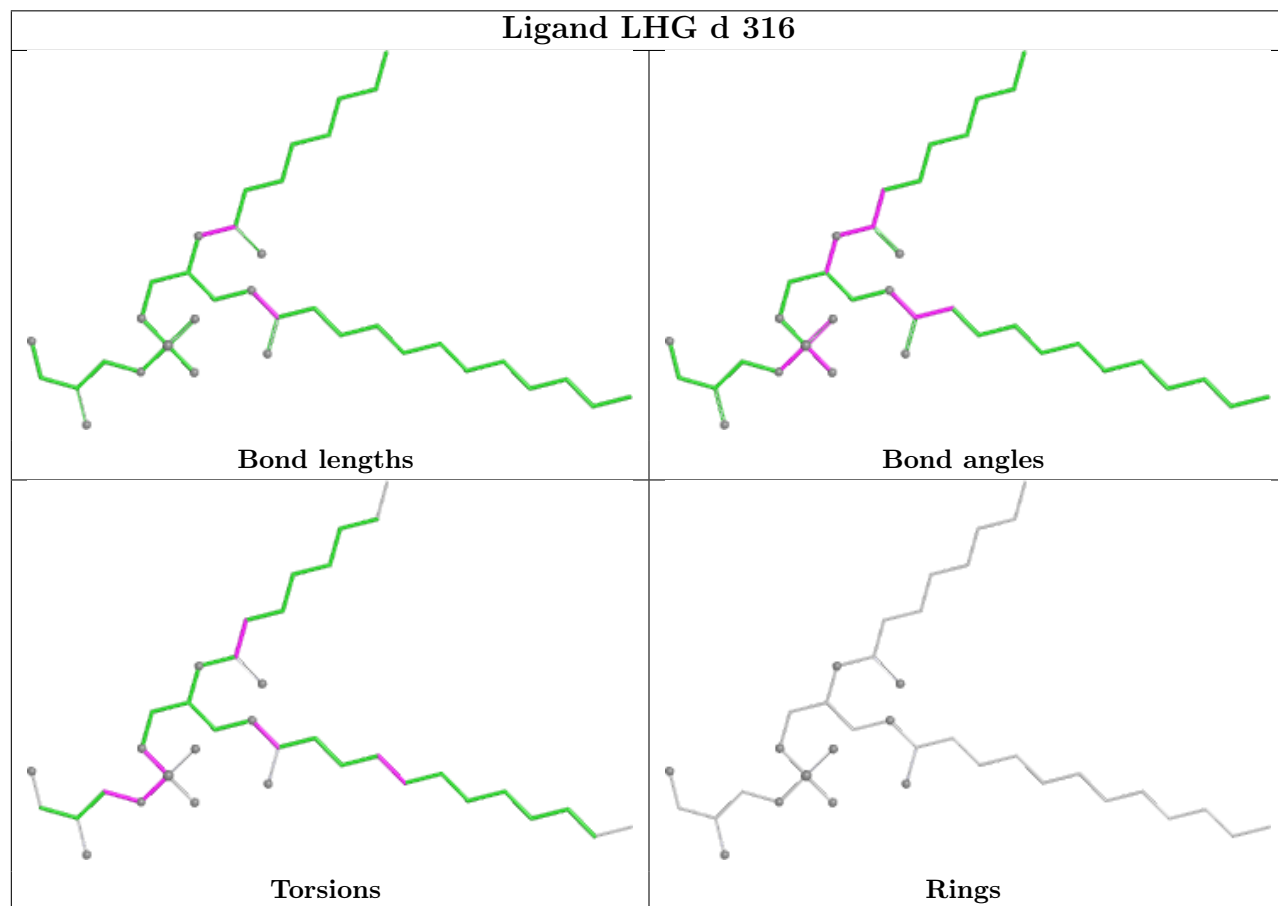
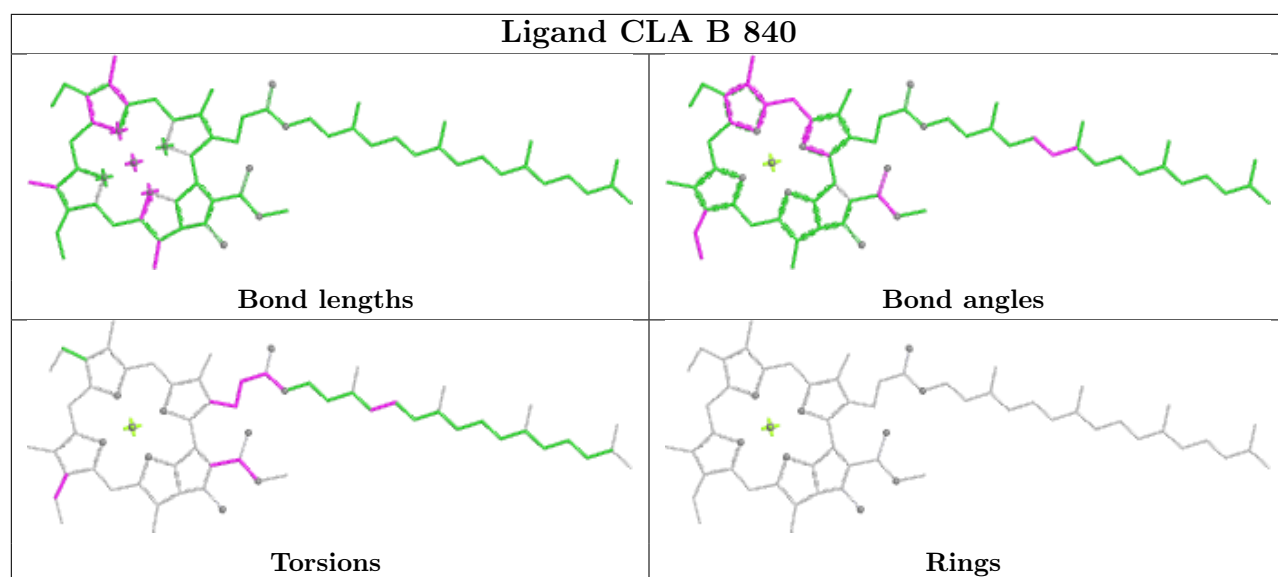


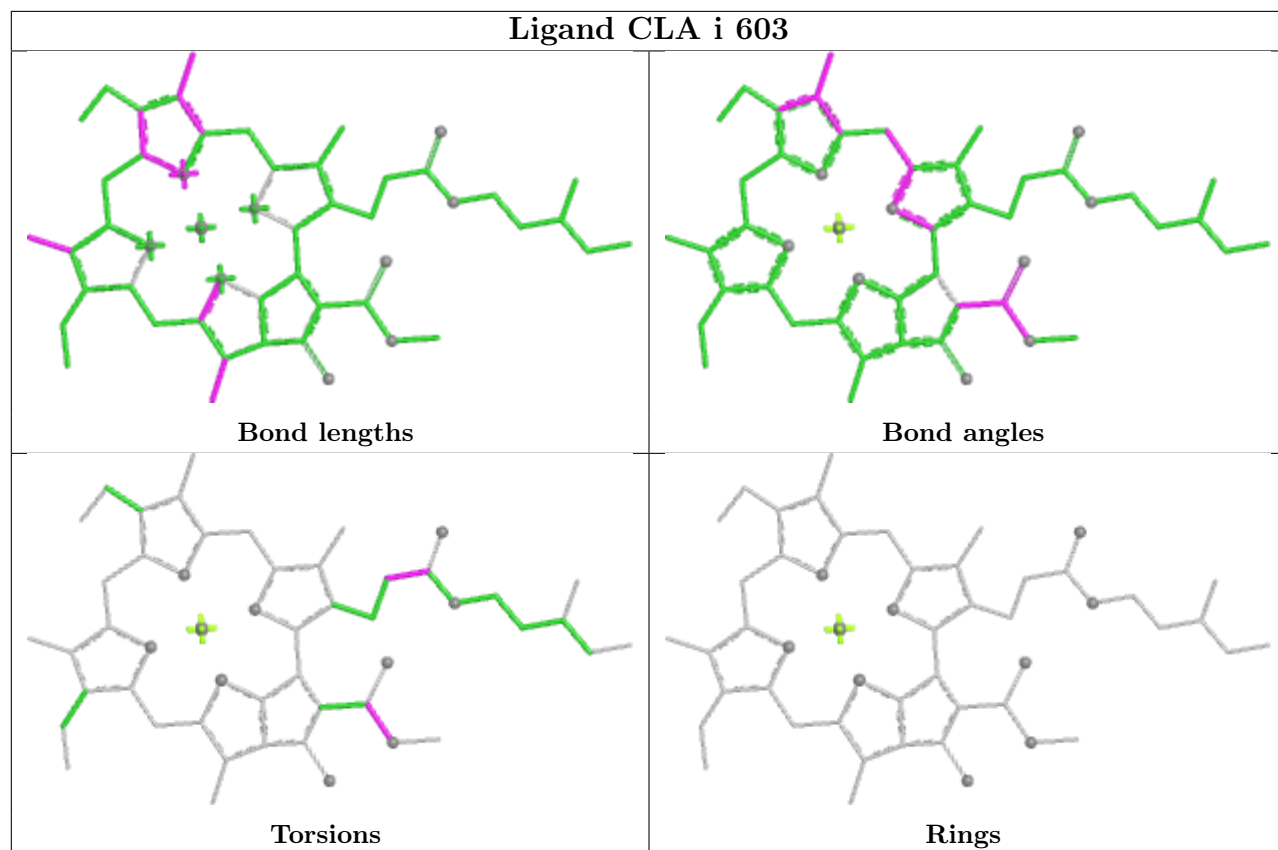
Torsions



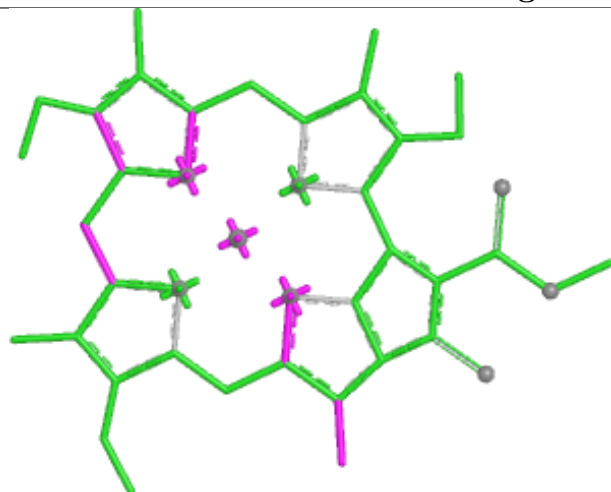
Rings







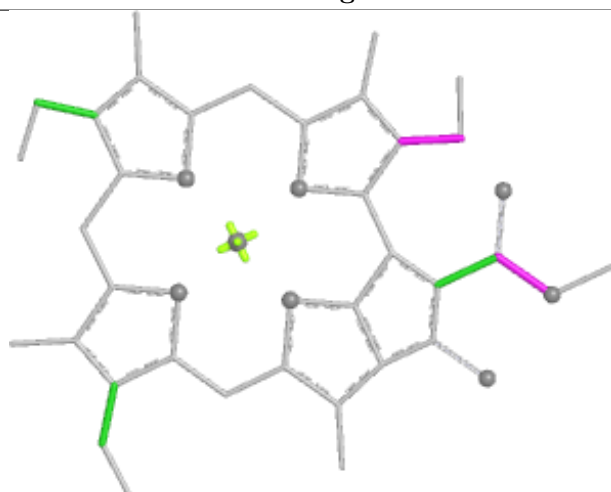
Ligand CLA J 103



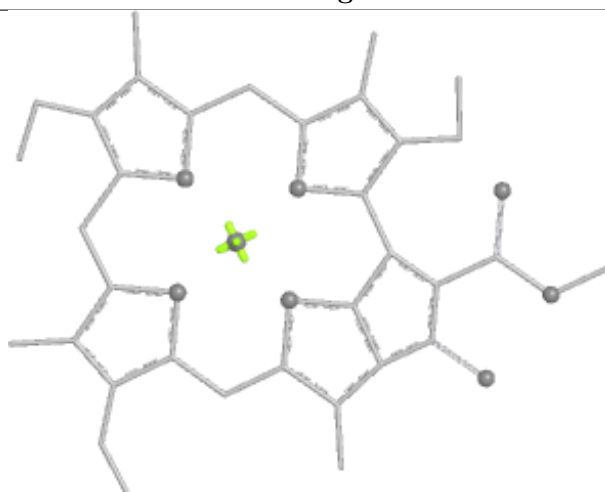
Bond lengths



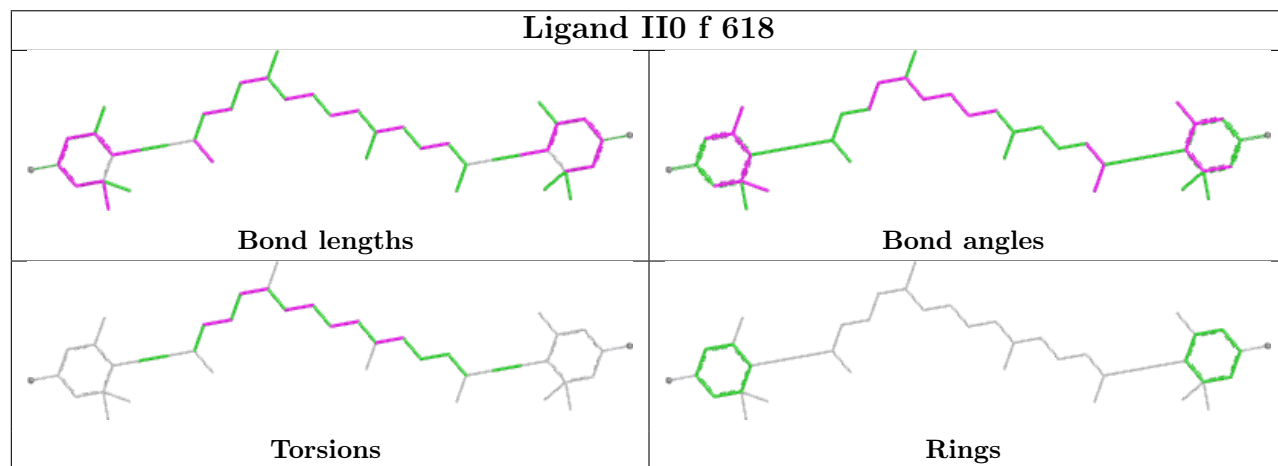
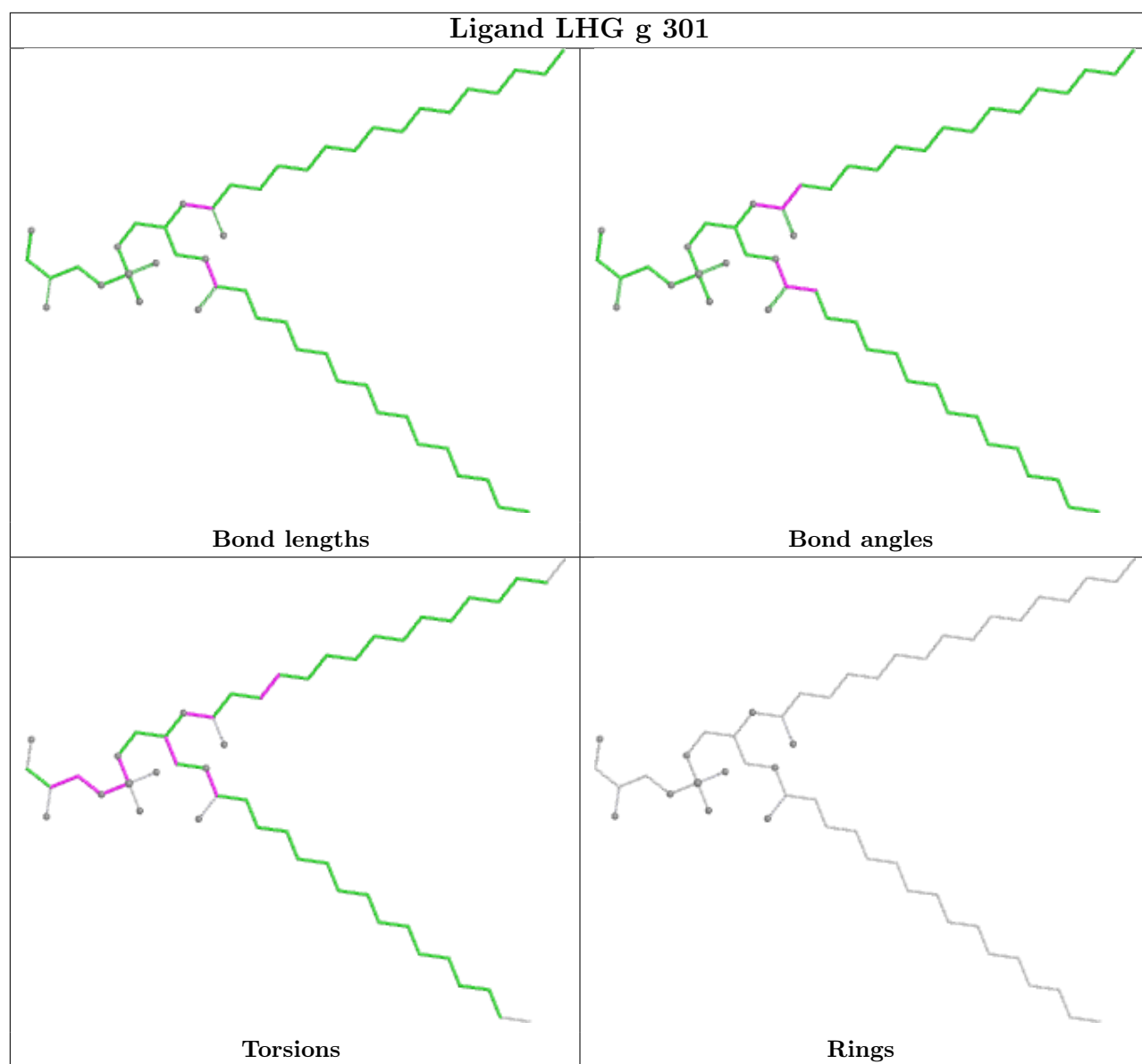
Bond angles



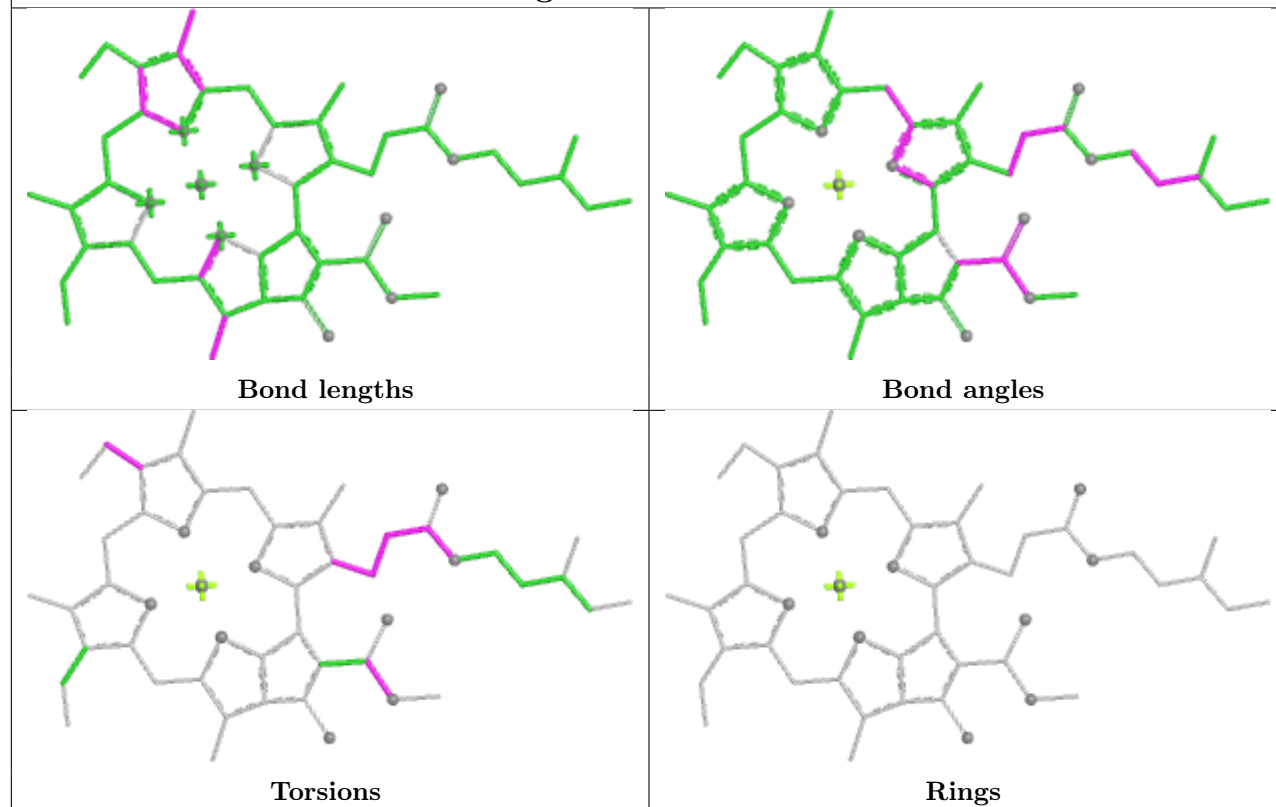
Torsions



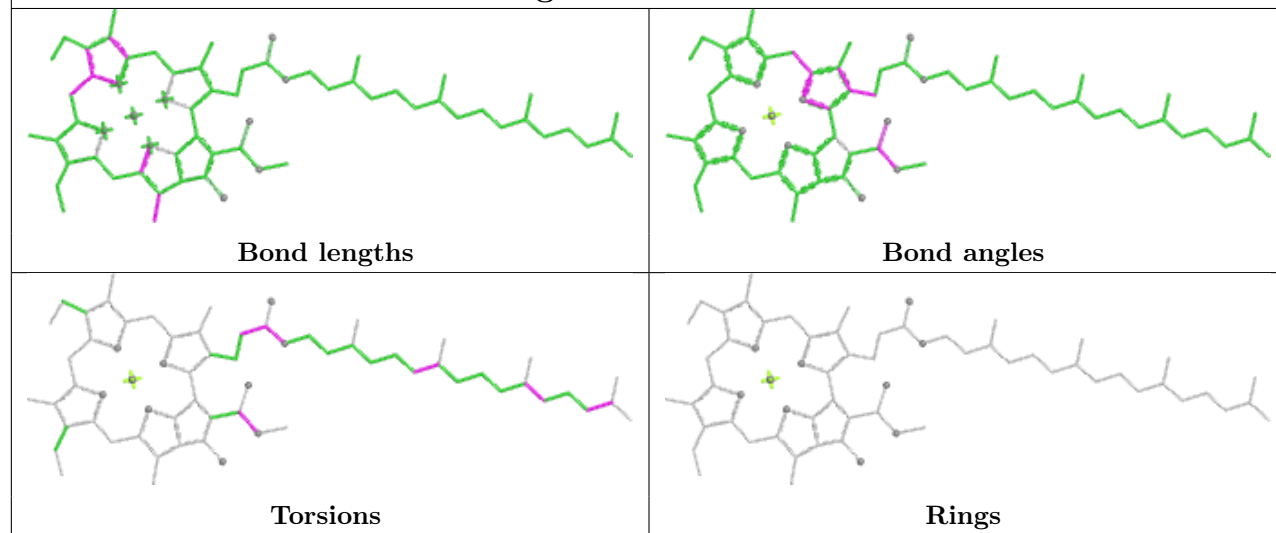
Rings



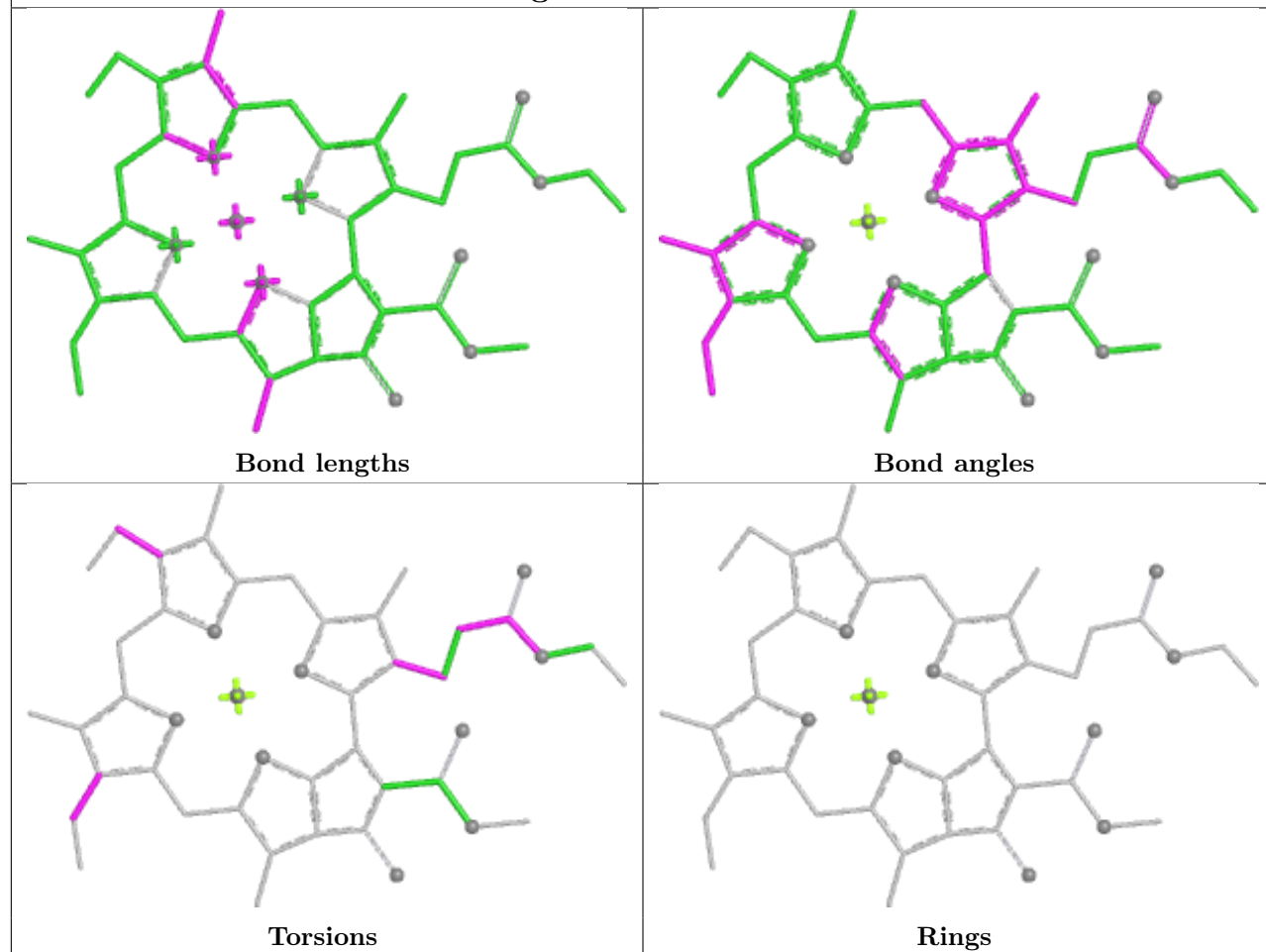
Ligand CLA k 610



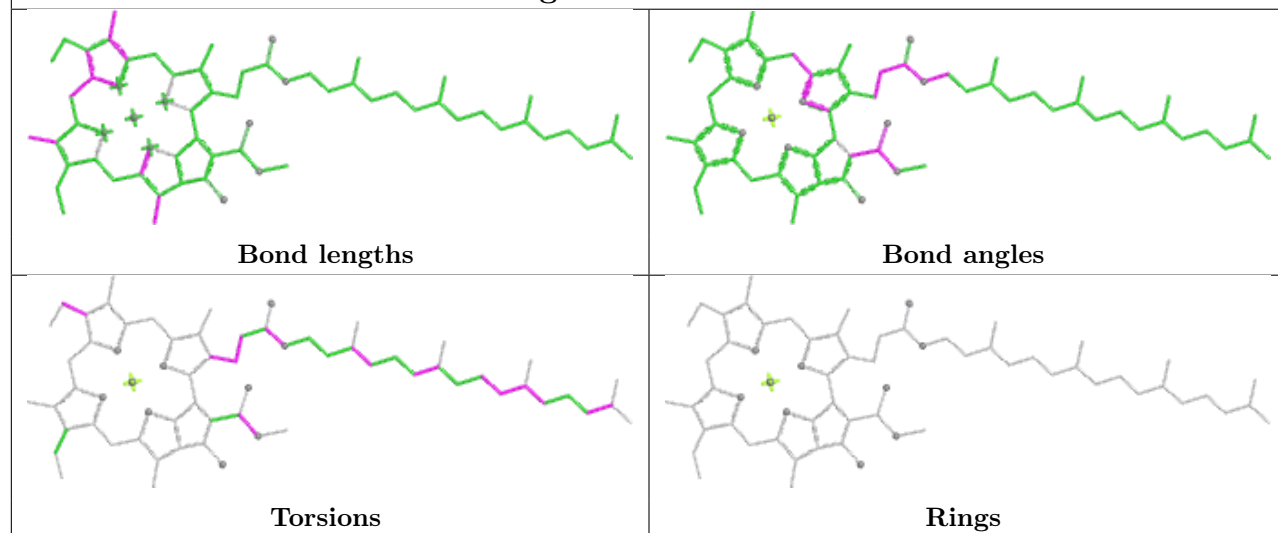
Ligand CLA a 310

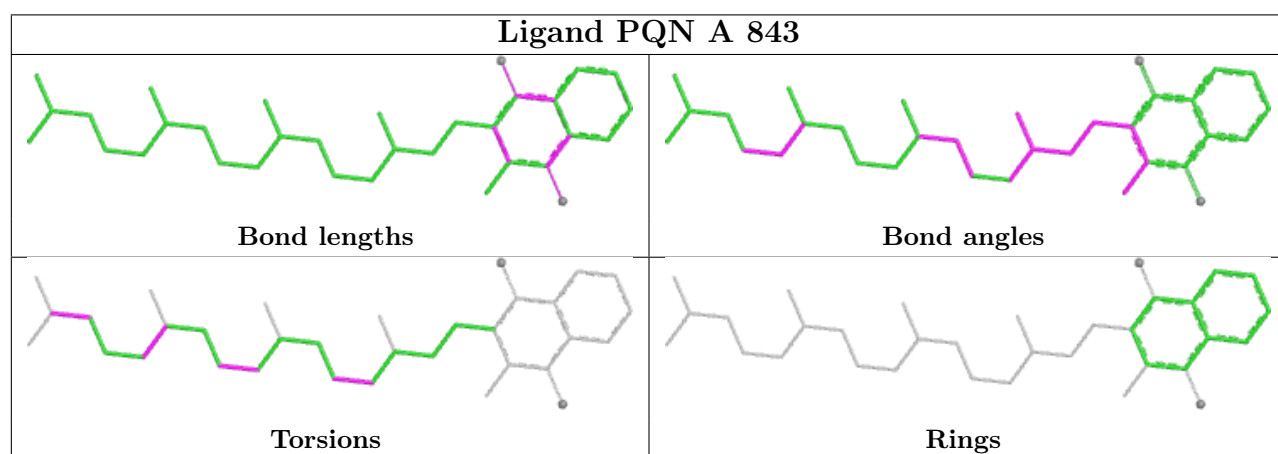
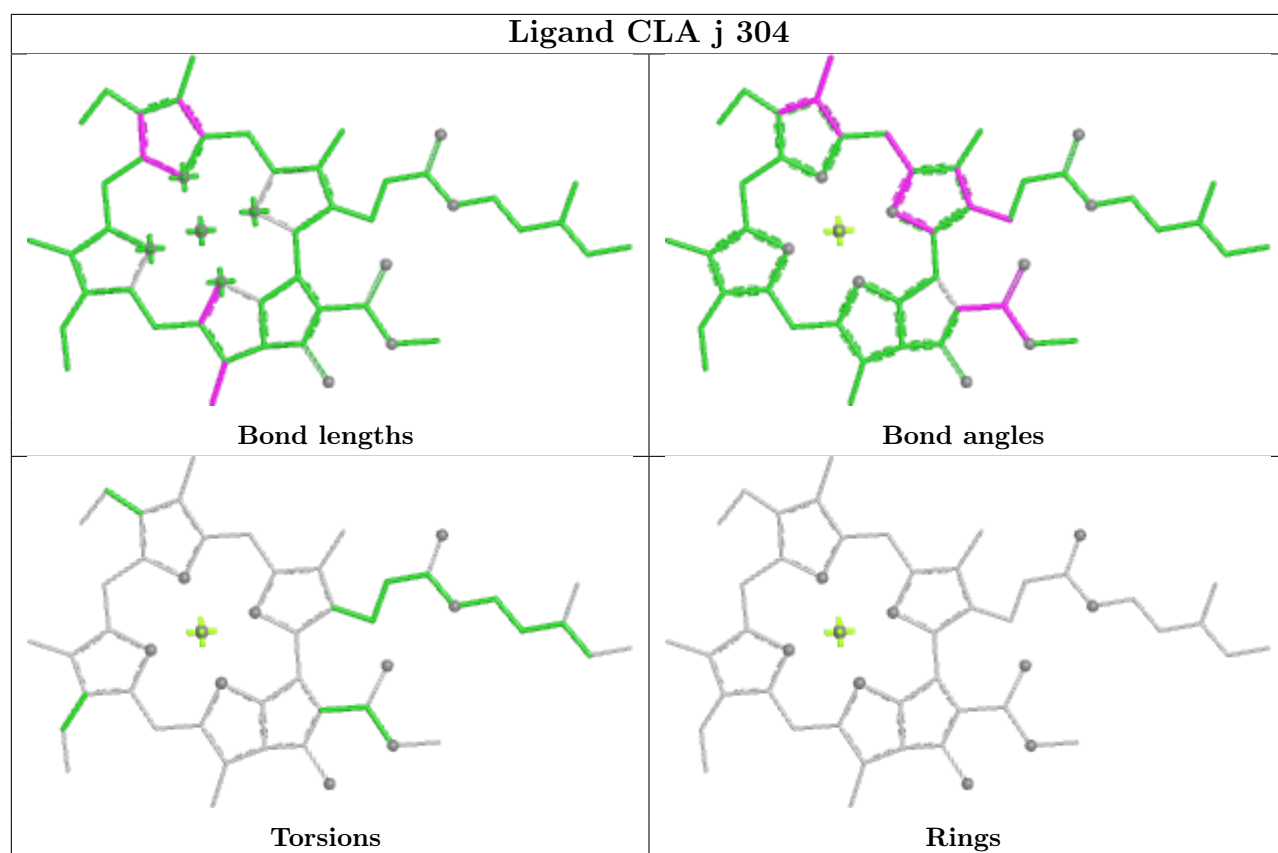


Ligand CLA a 311

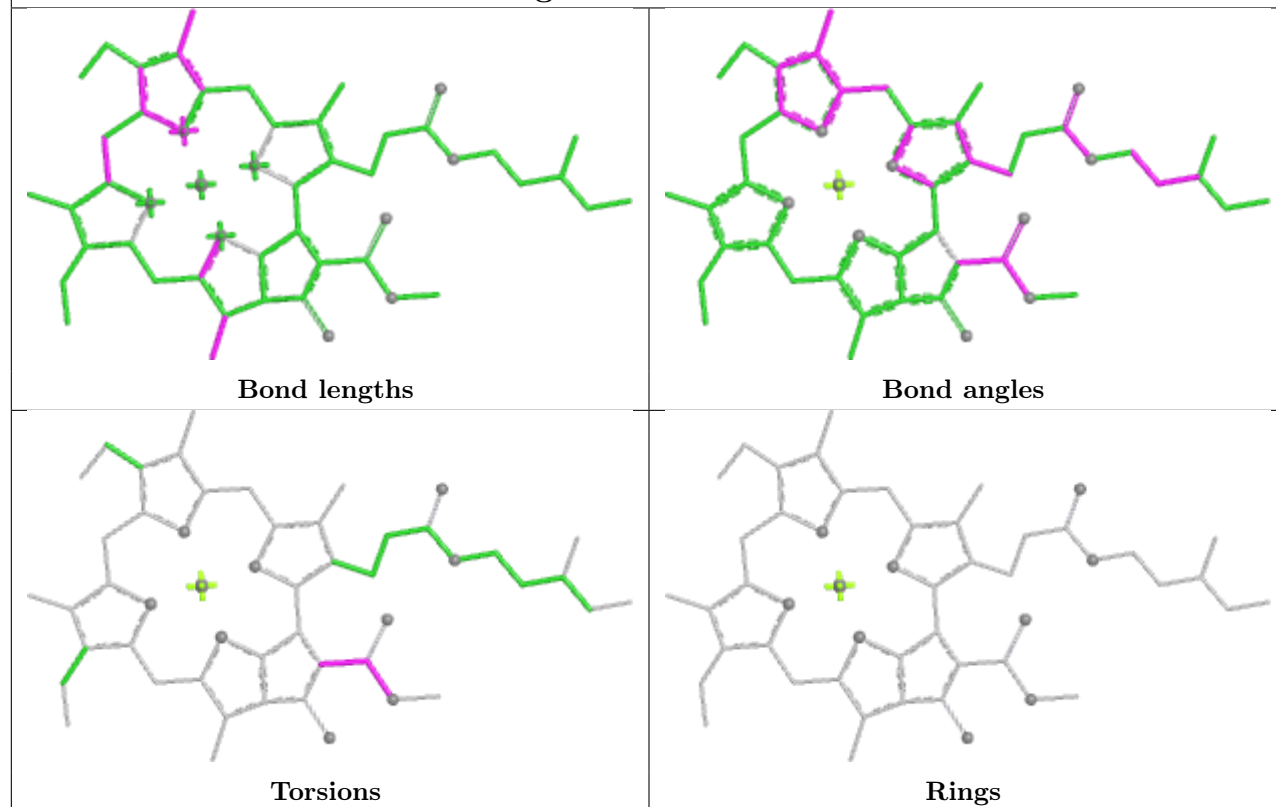


Ligand CLA f 607

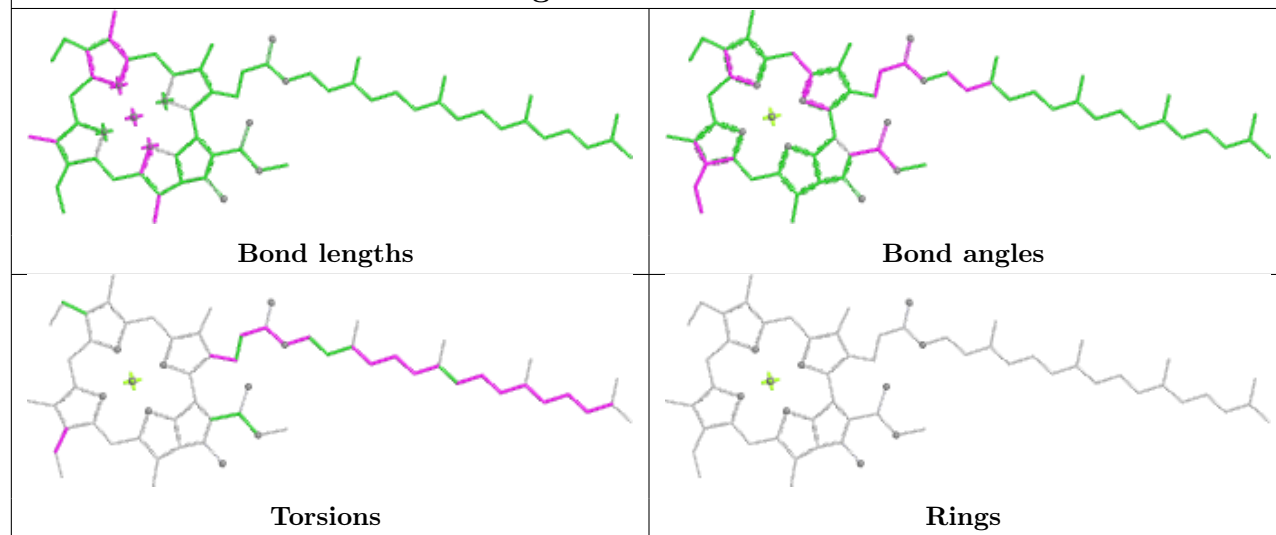


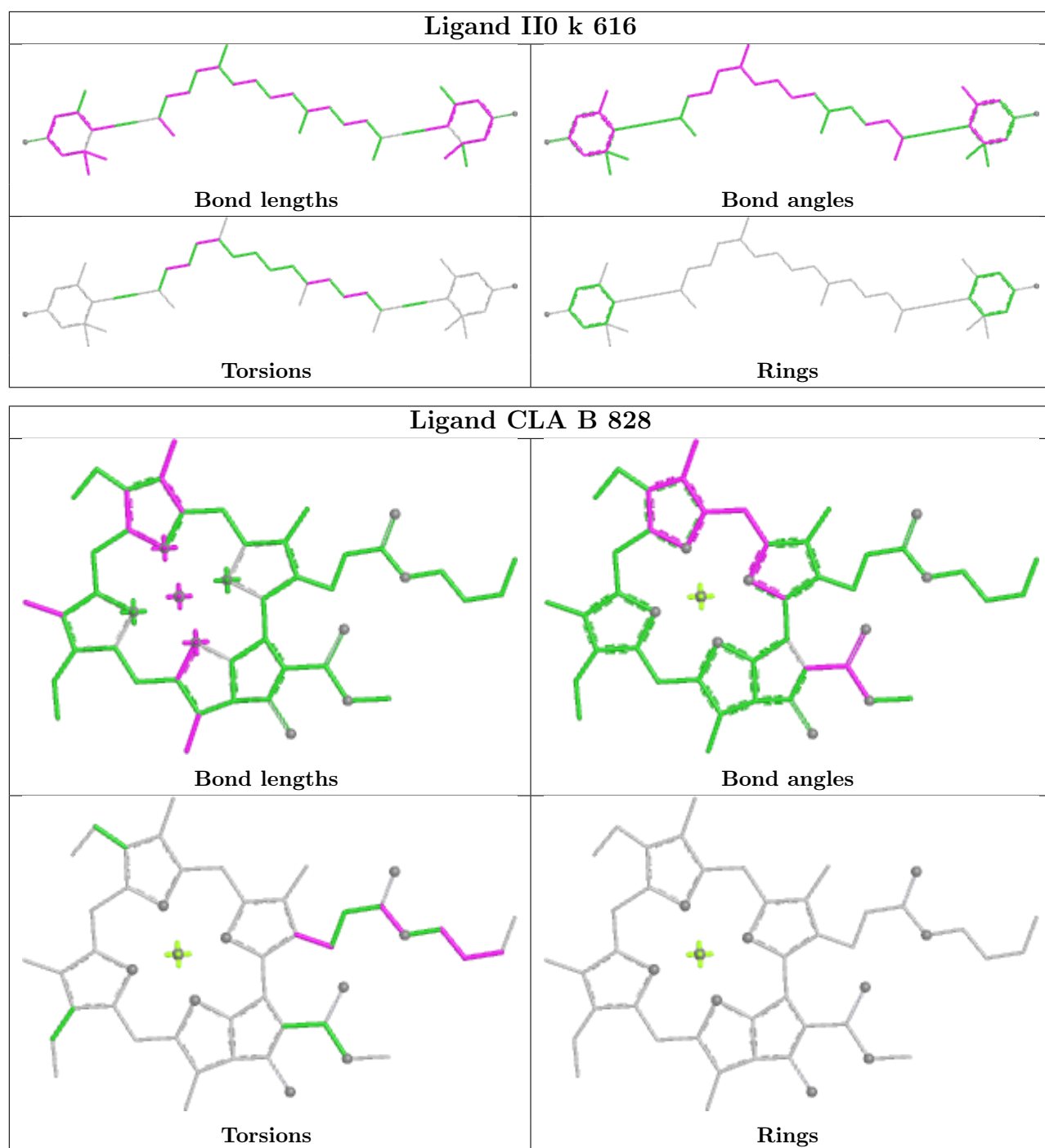


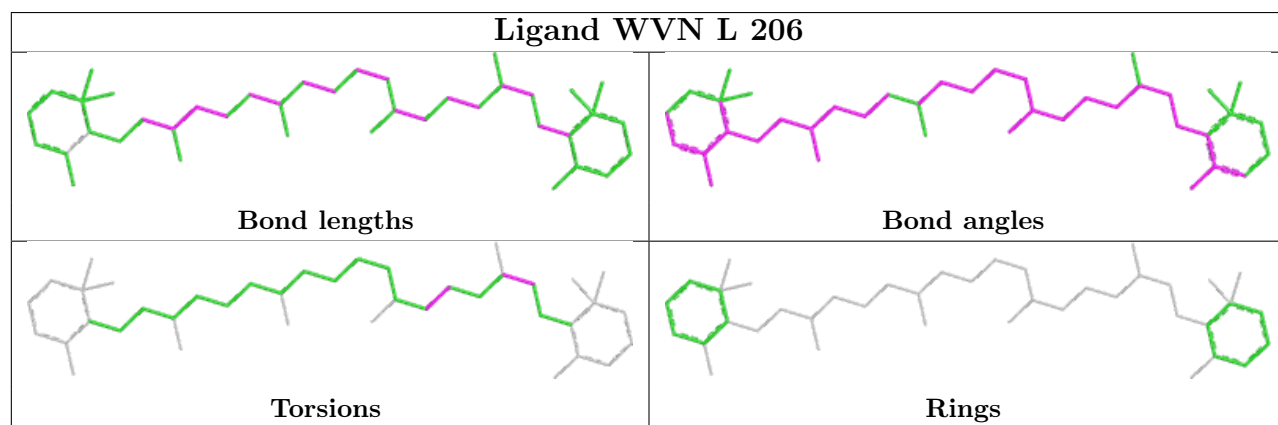
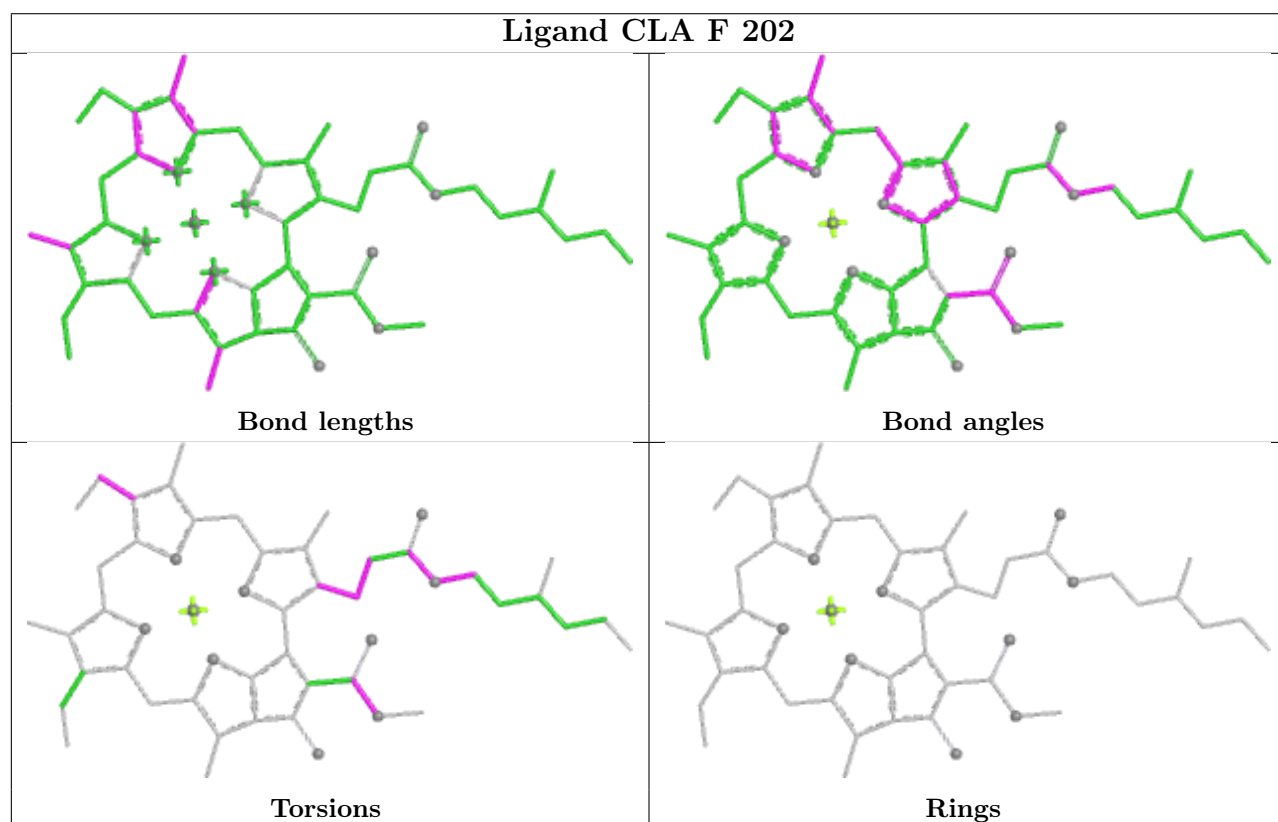
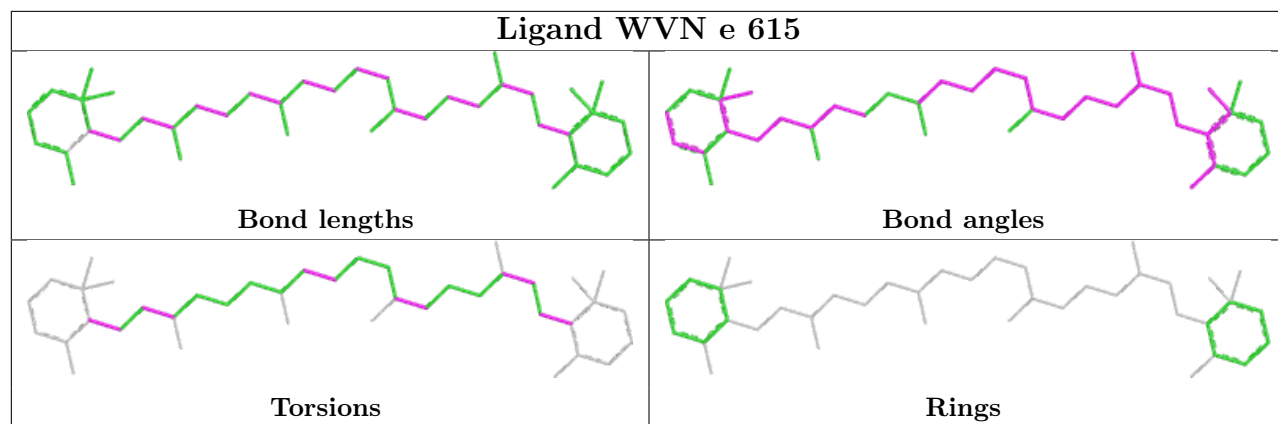
Ligand CLA d 302



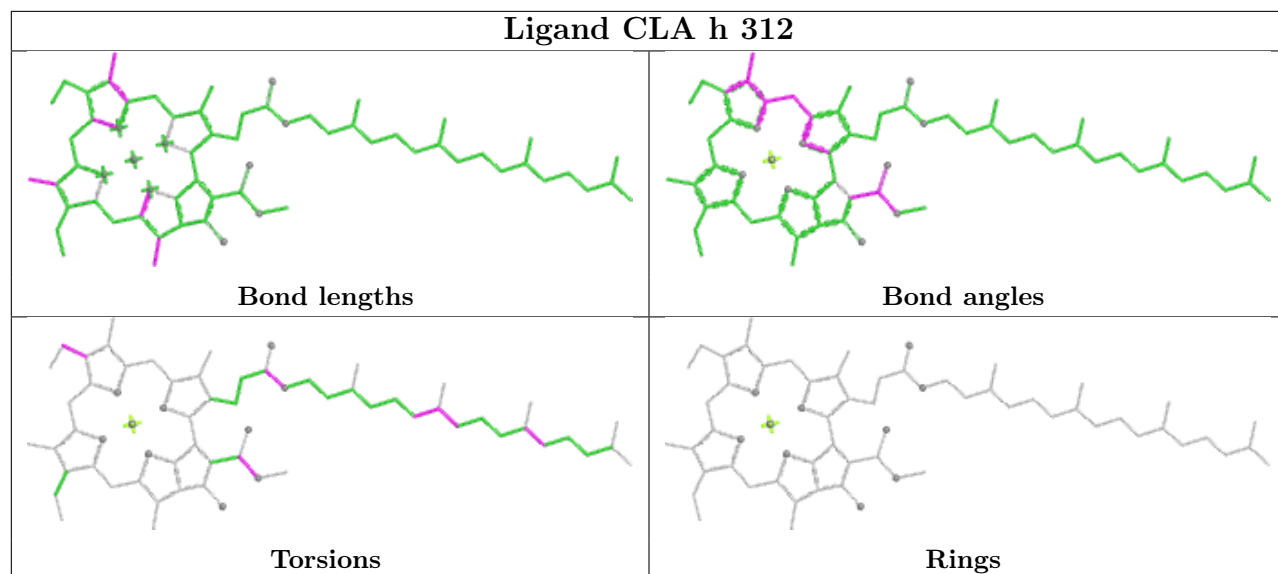
Ligand CLA B 836



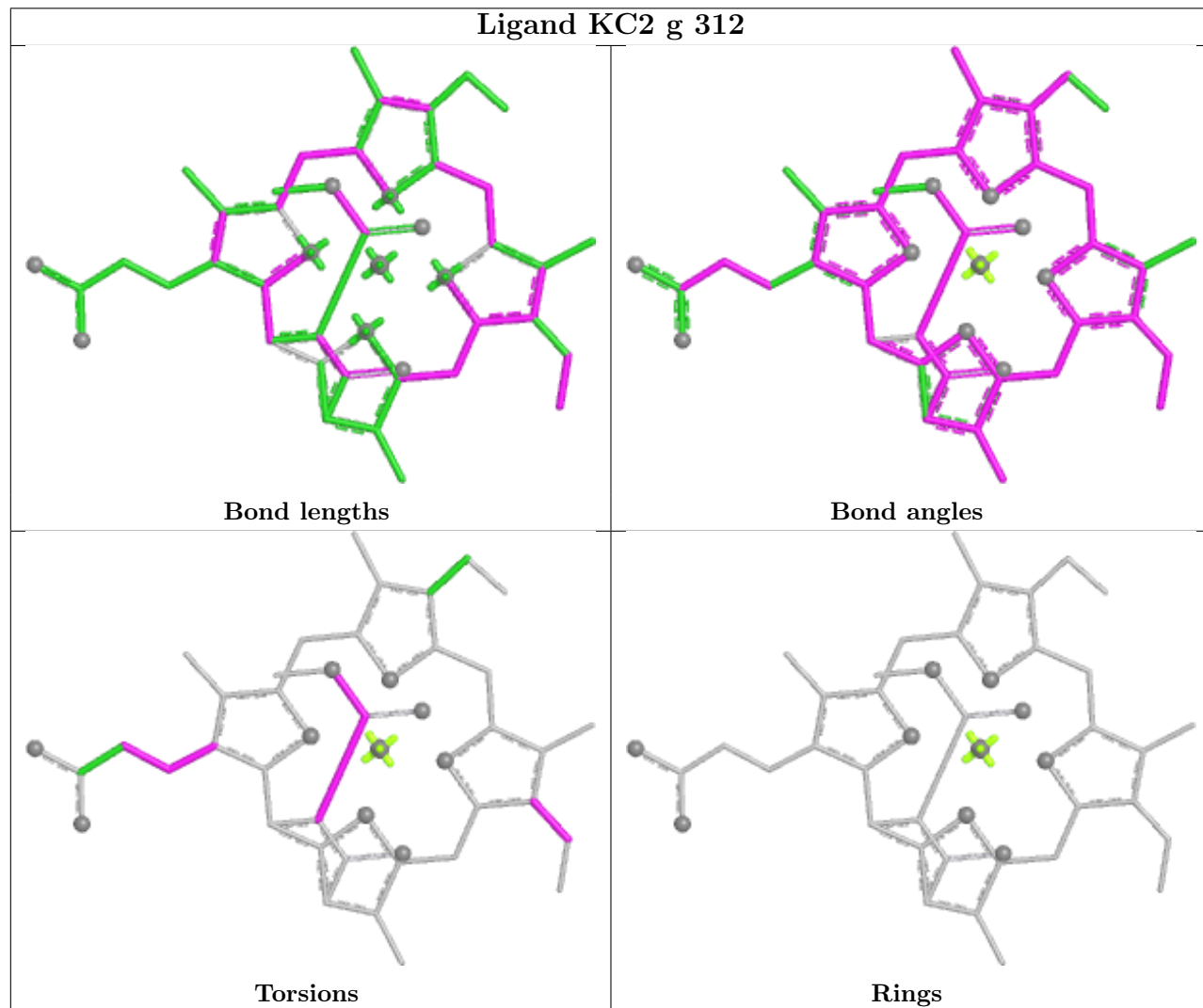


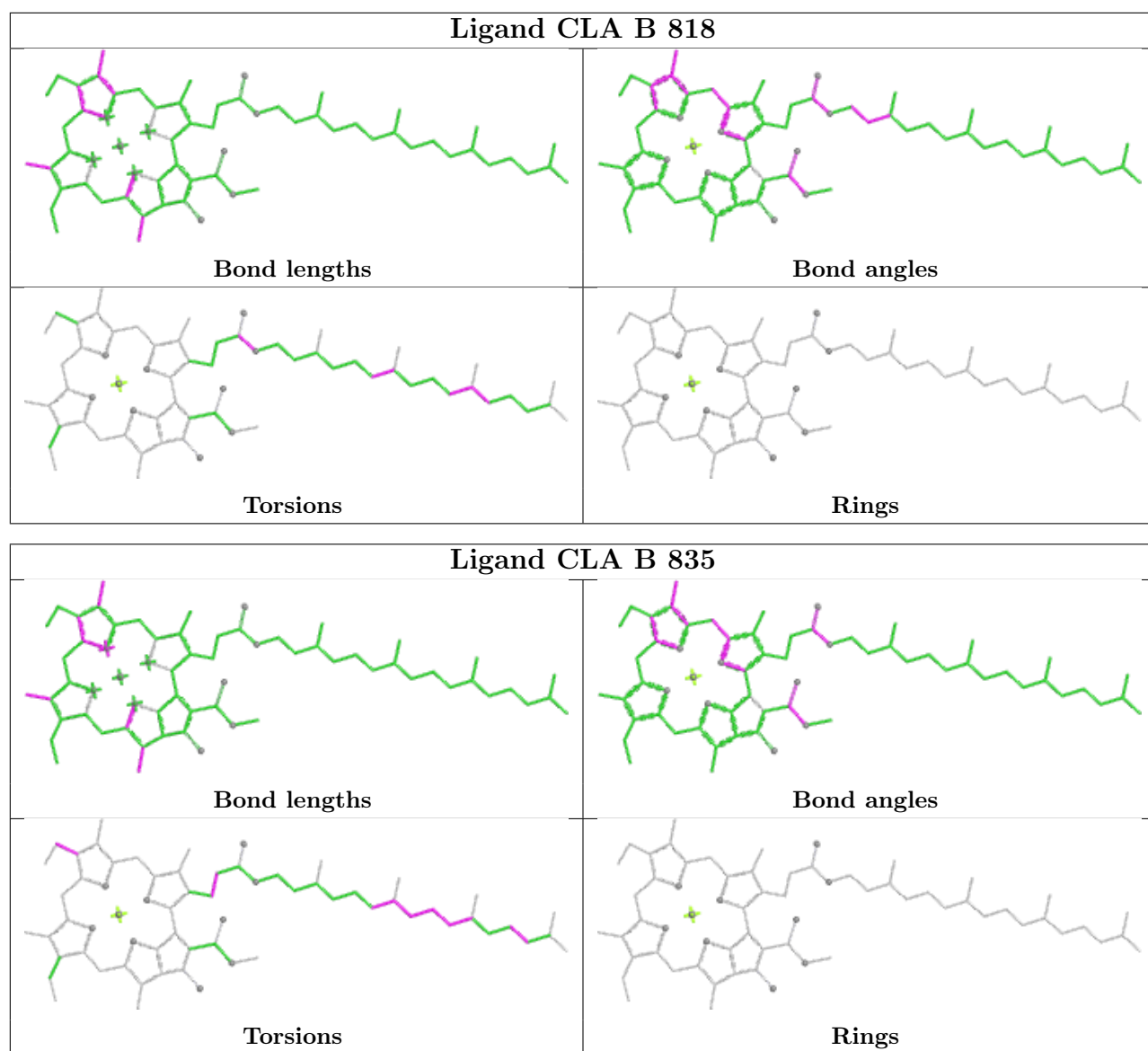


Ligand CLA h 312

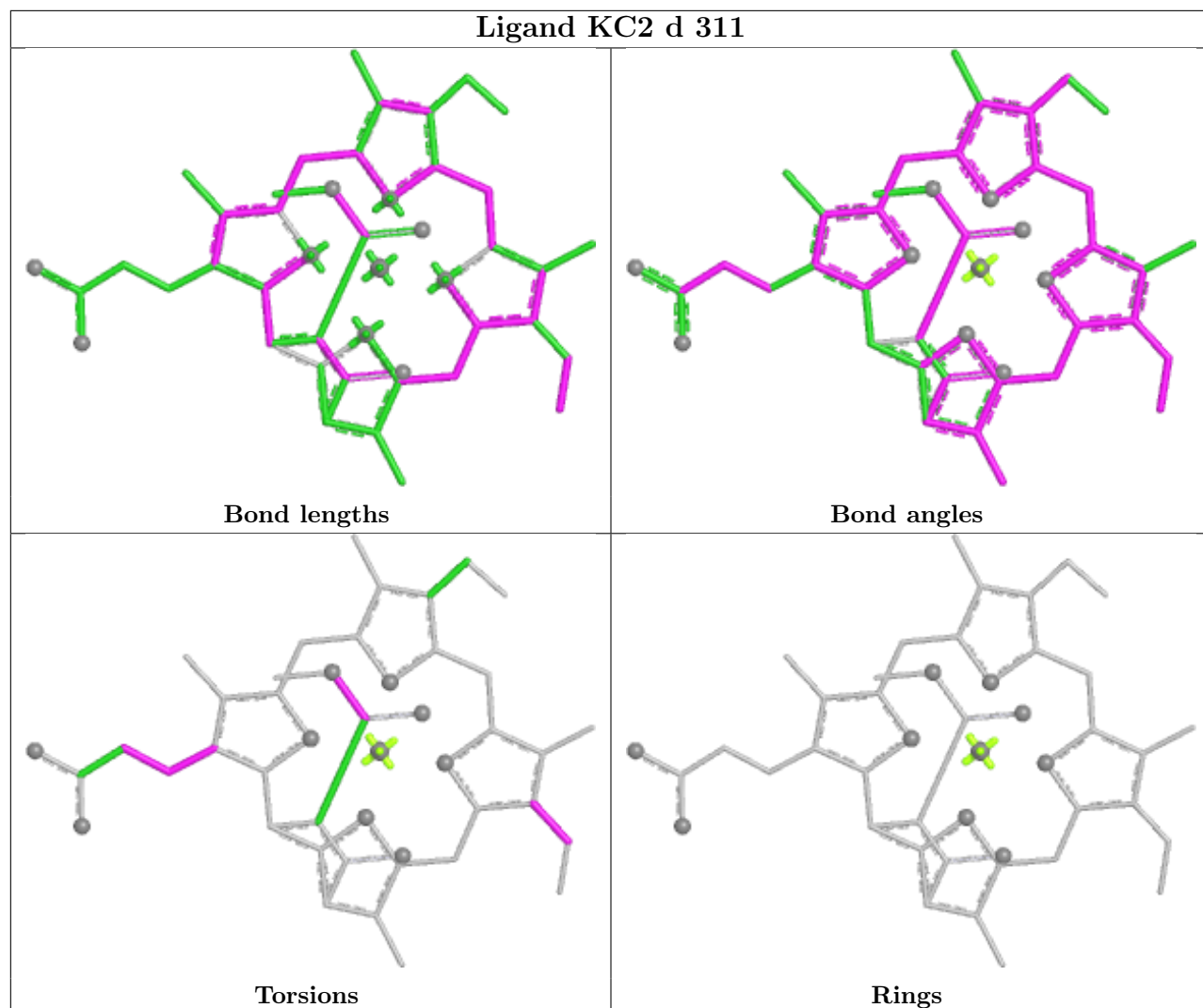


Ligand KC2 g 312

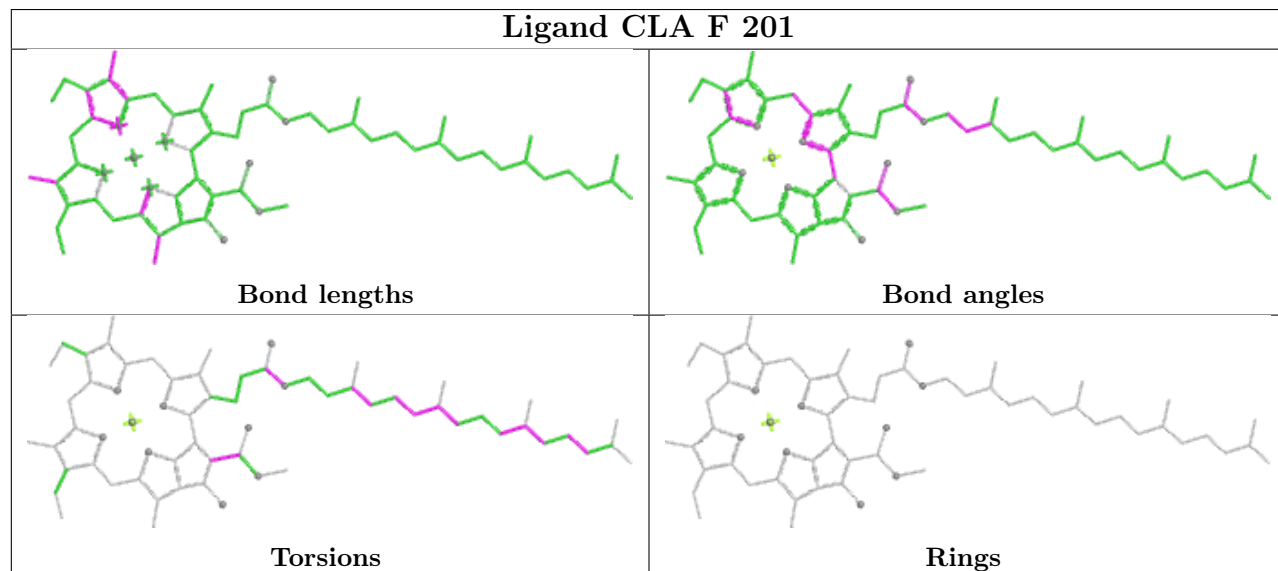


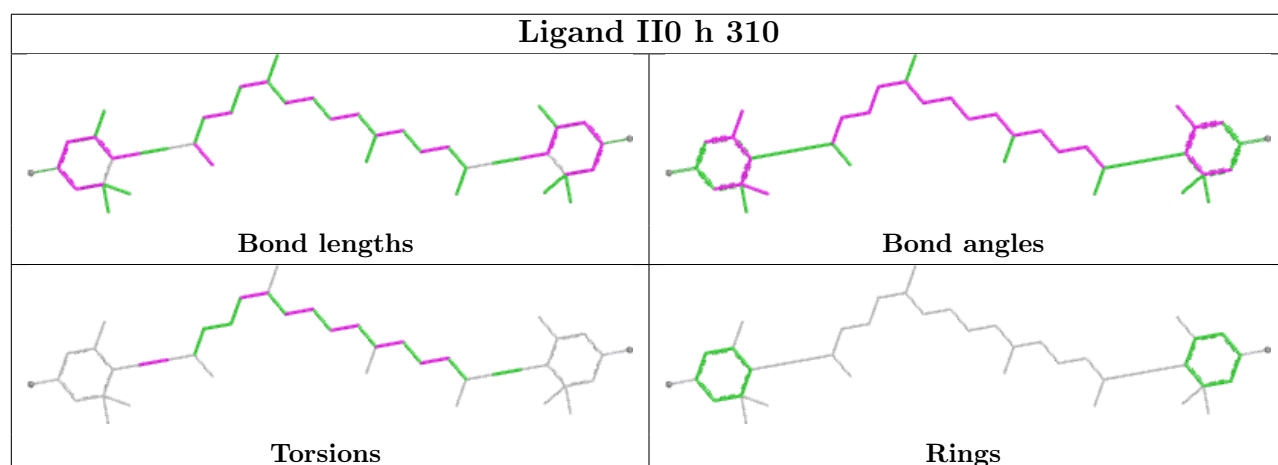
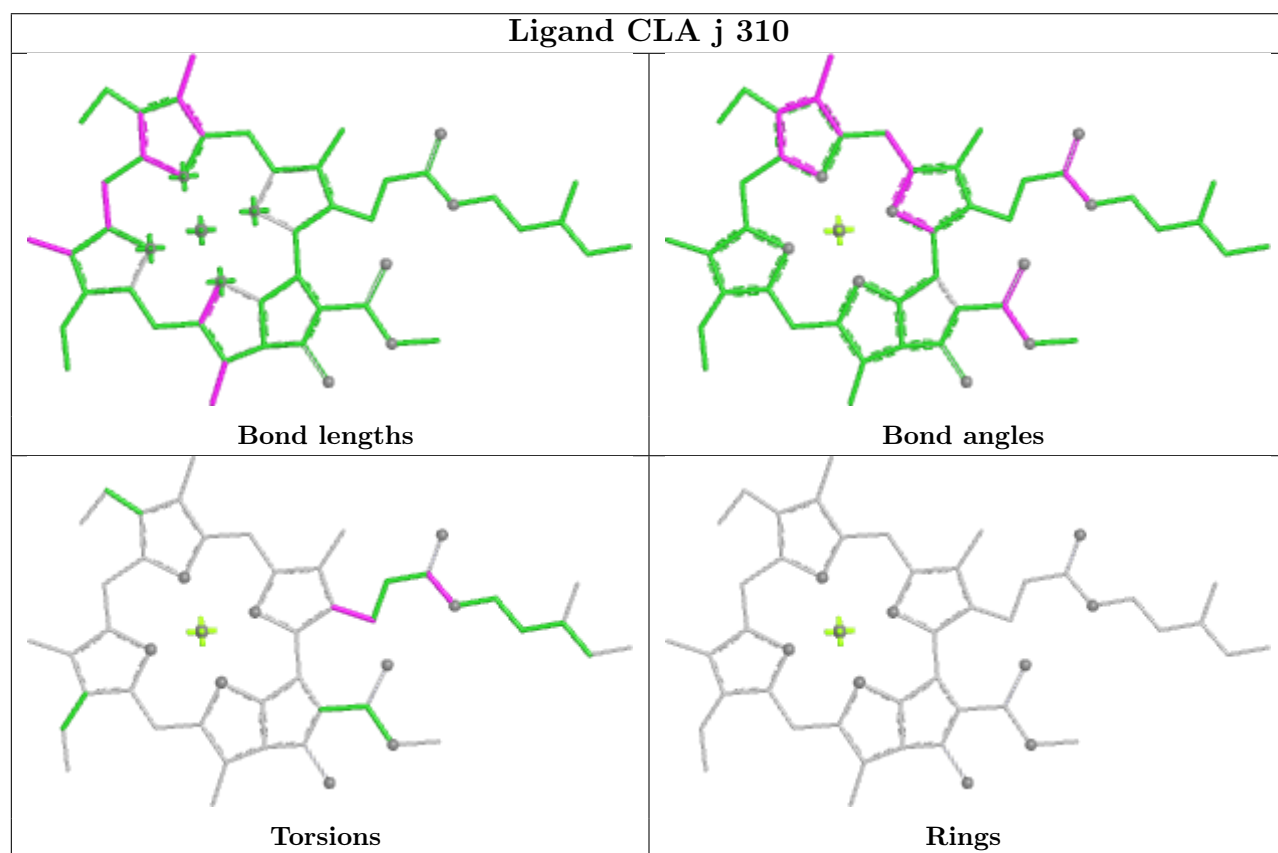
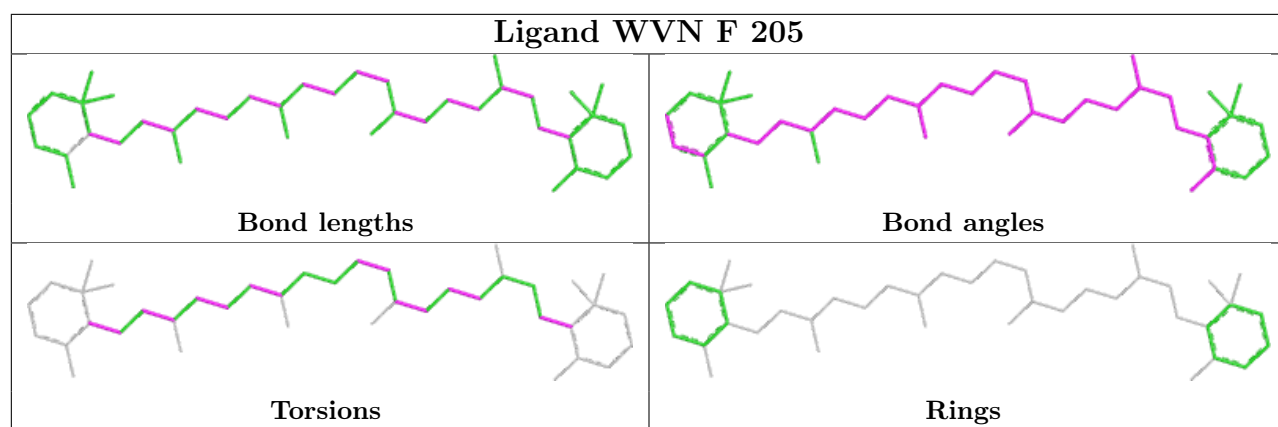


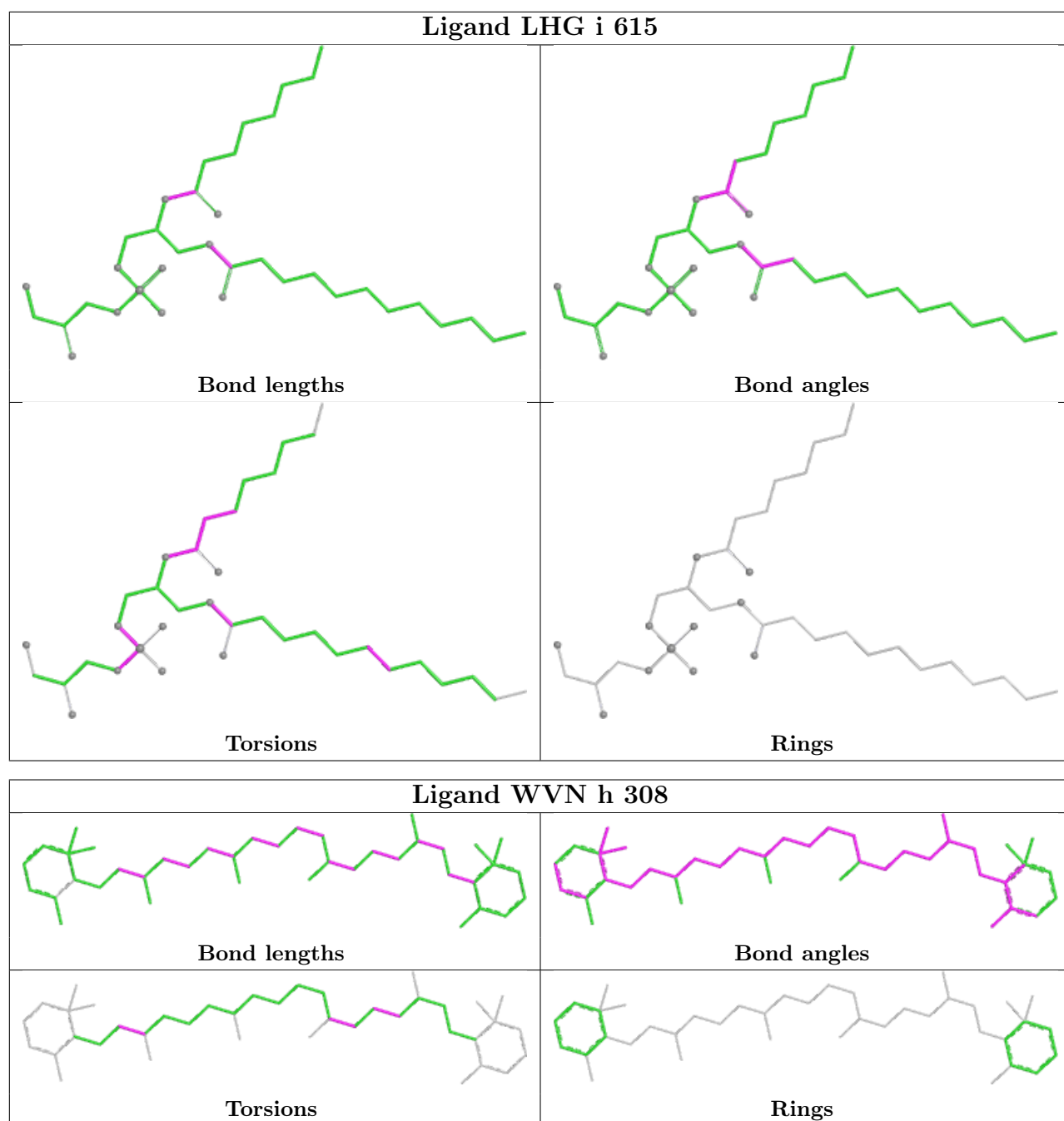
Ligand KC2 d 311

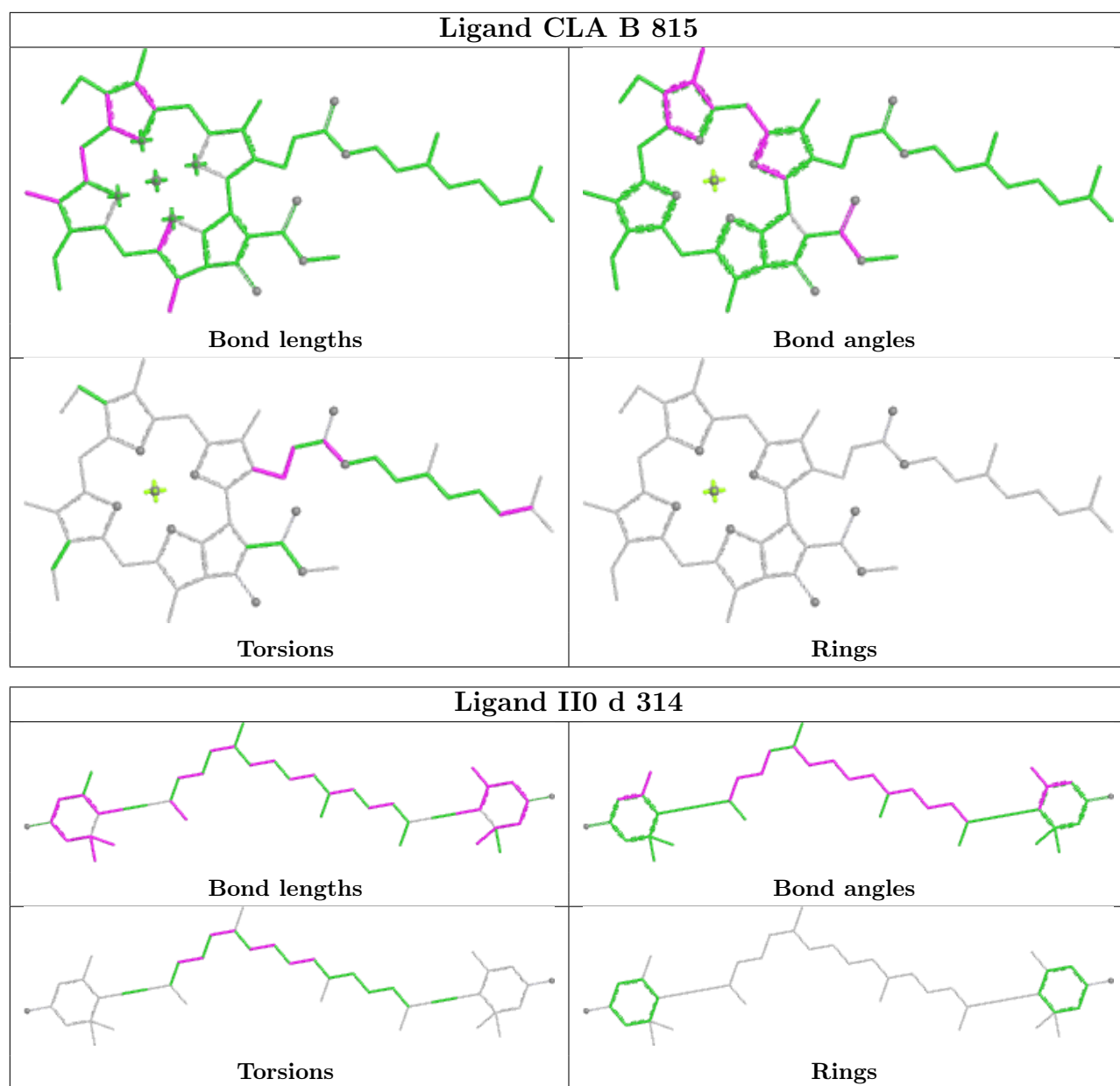


Ligand CLA F 201

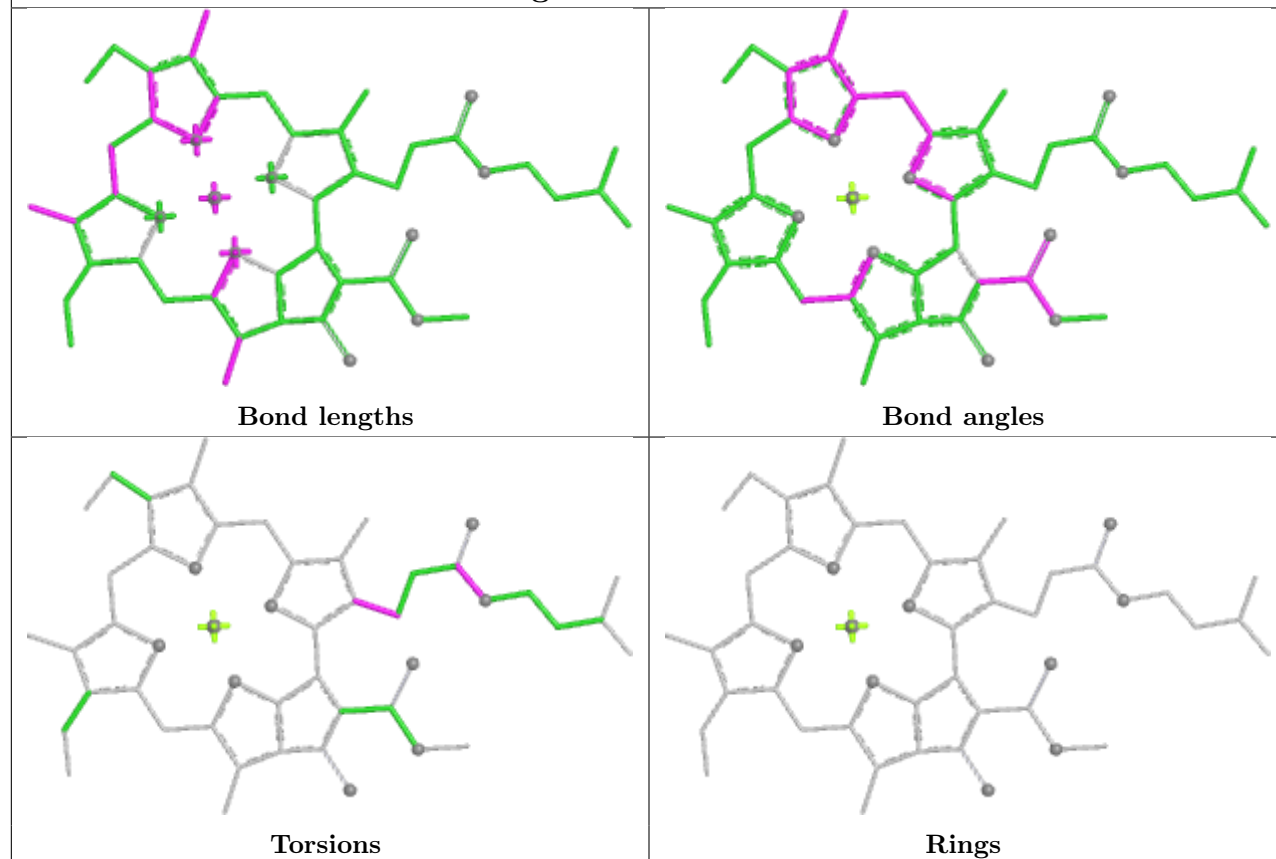




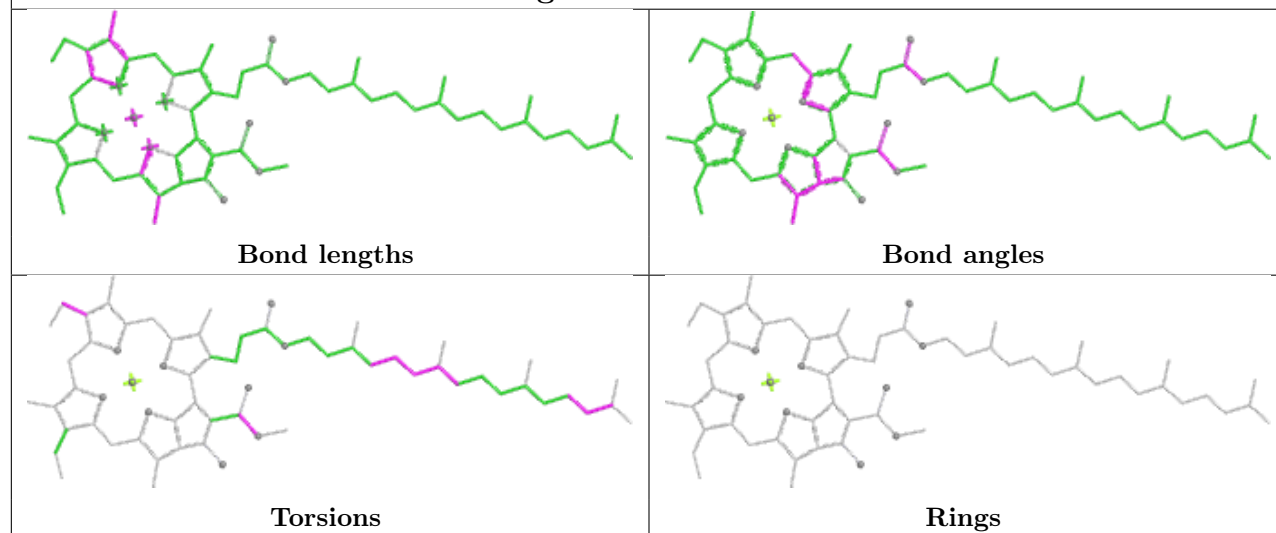




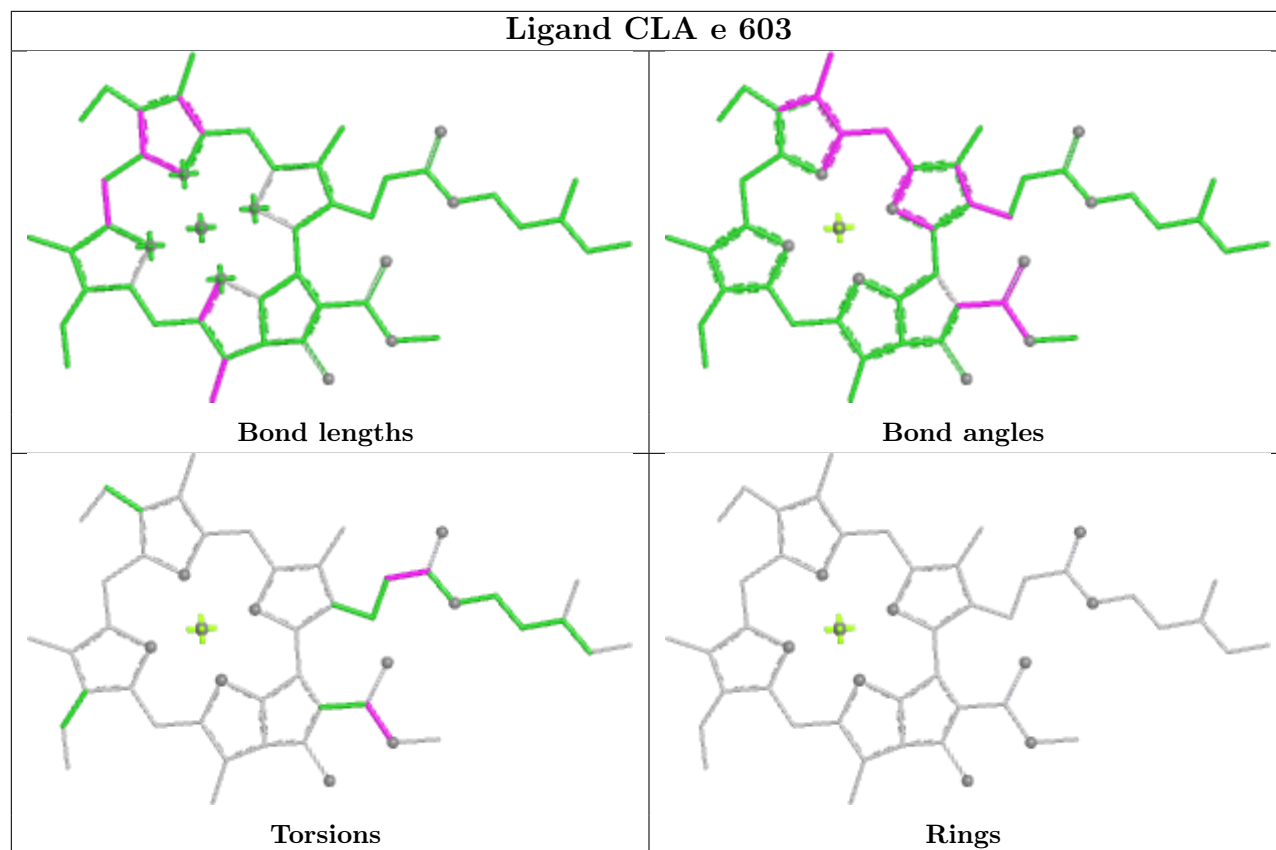
Ligand CLA A 830



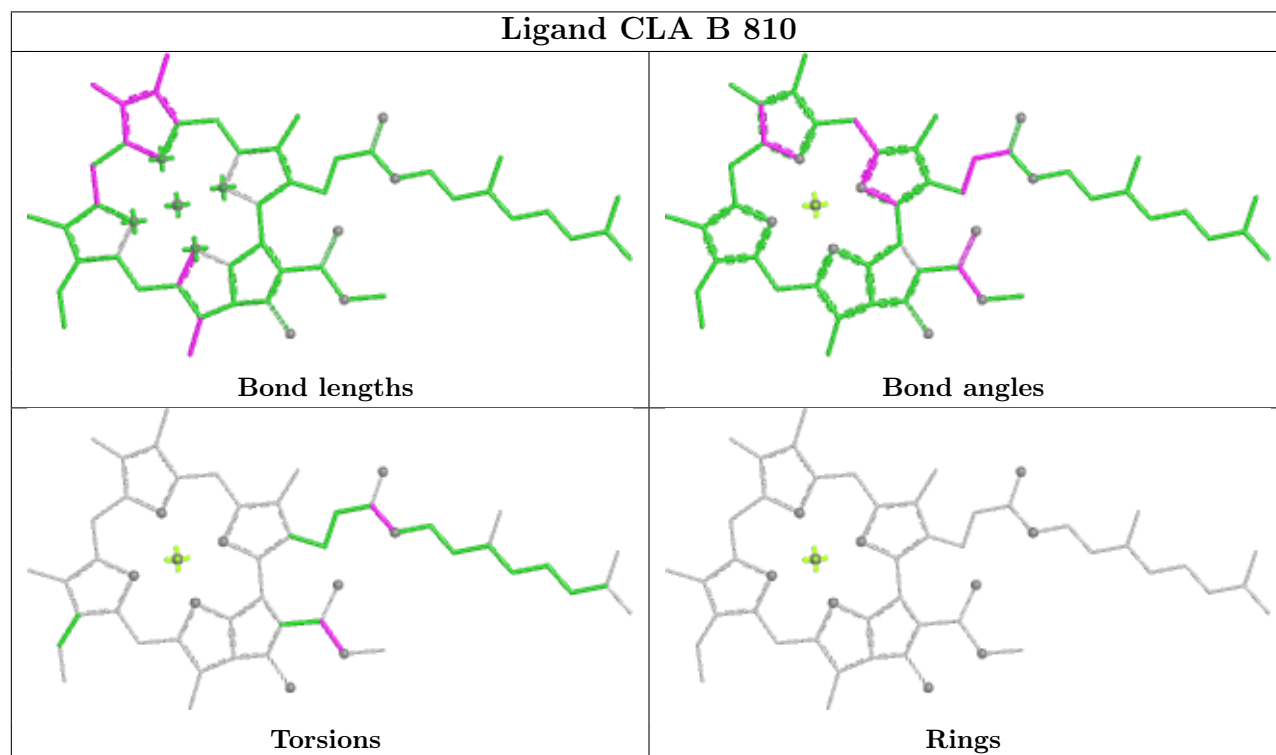
Ligand CLA e 605



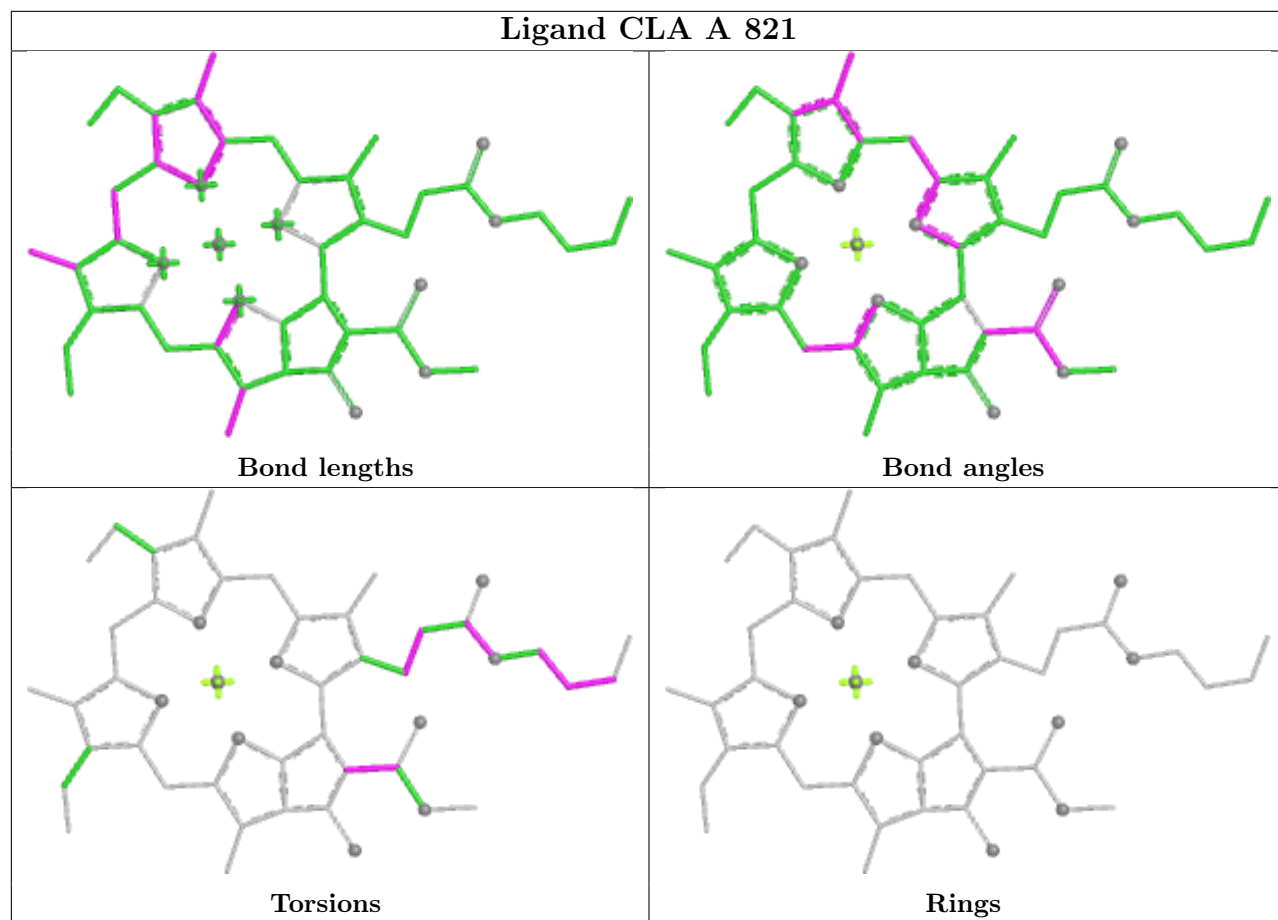
Ligand CLA e 603

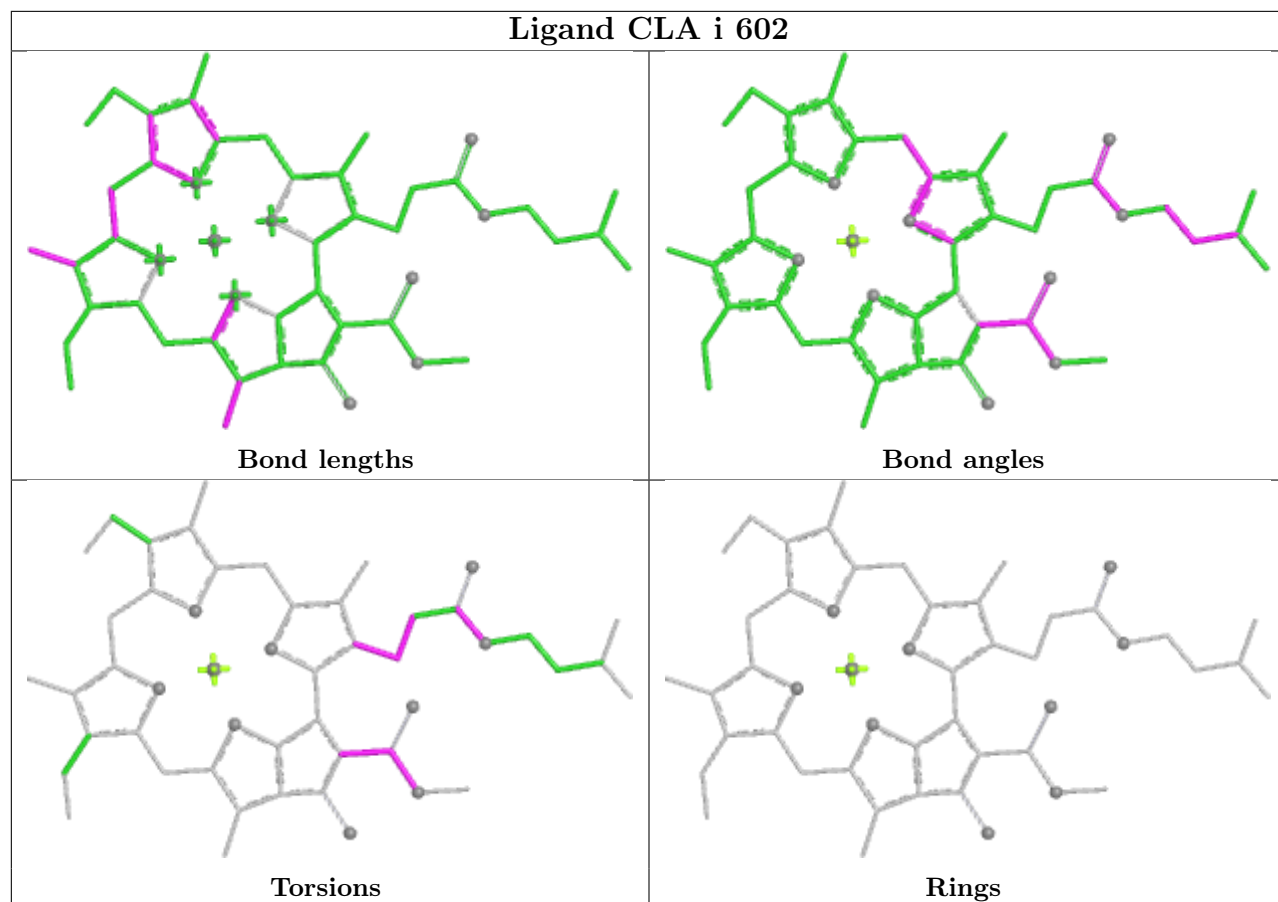


Ligand CLA B 810

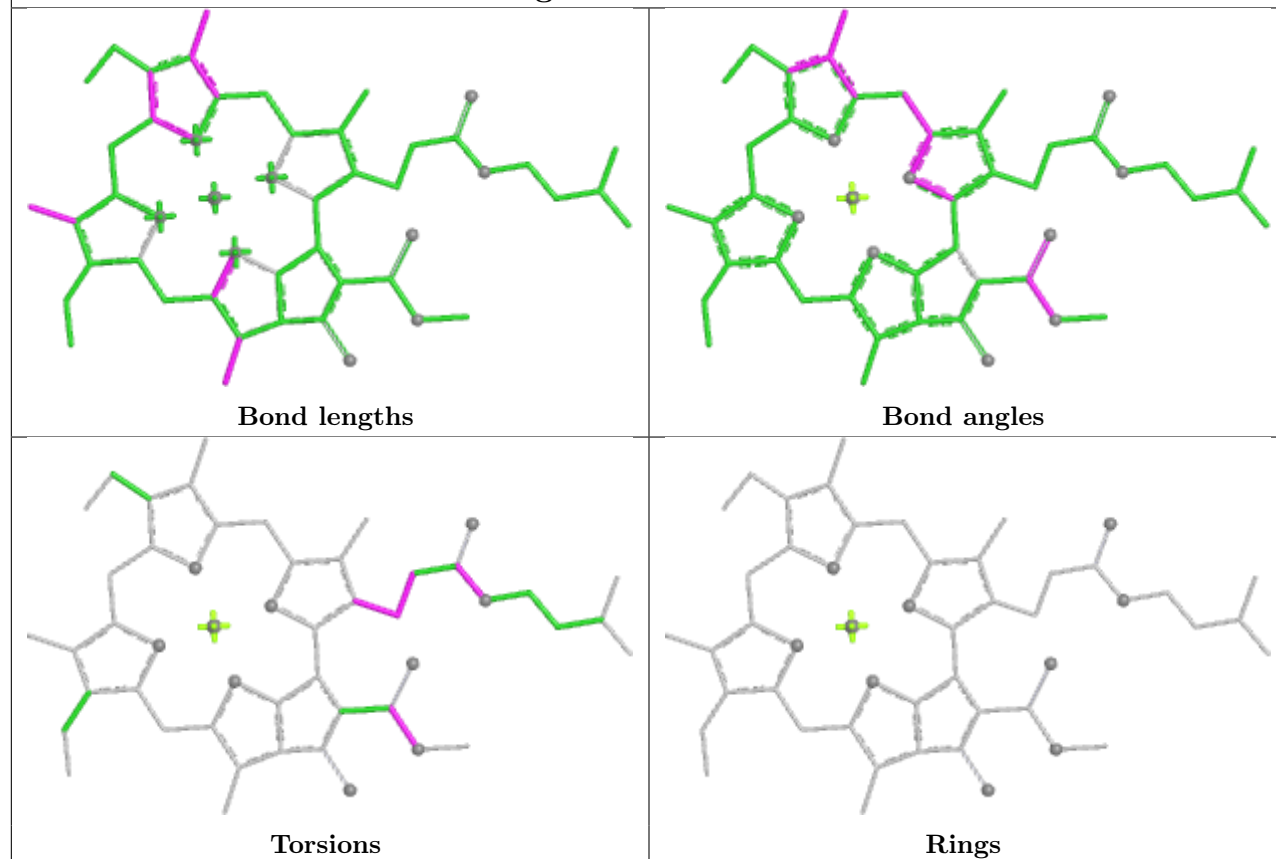


Ligand CLA A 821

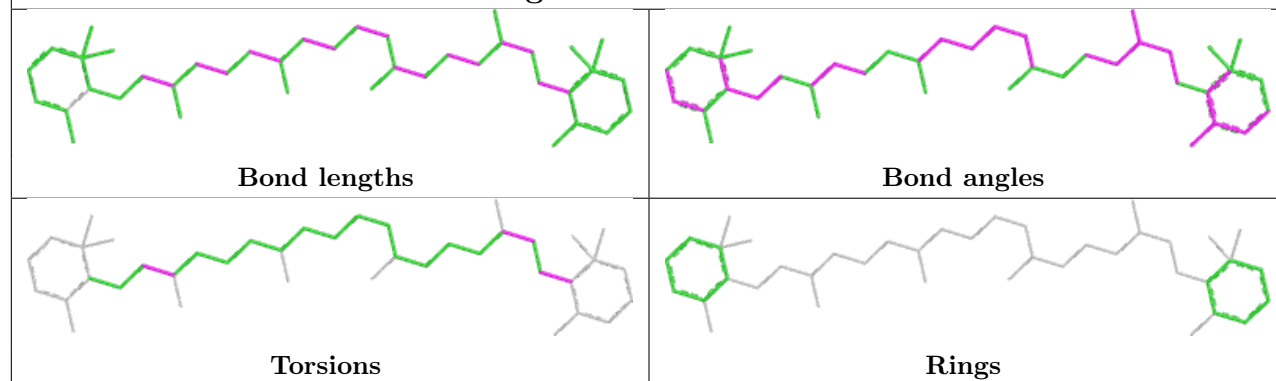


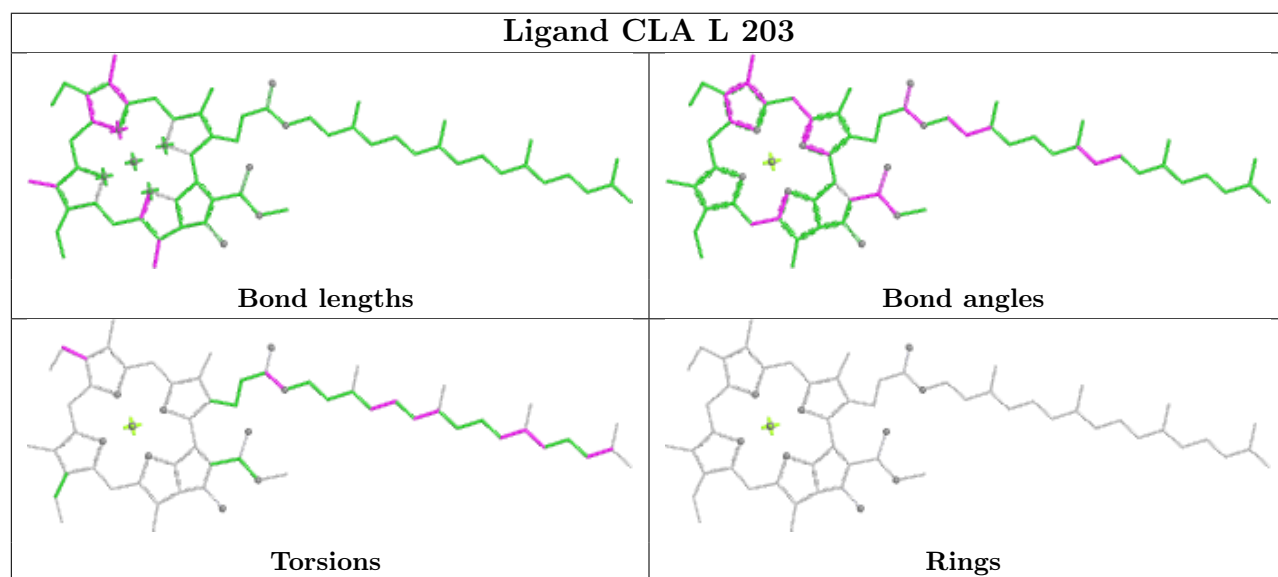
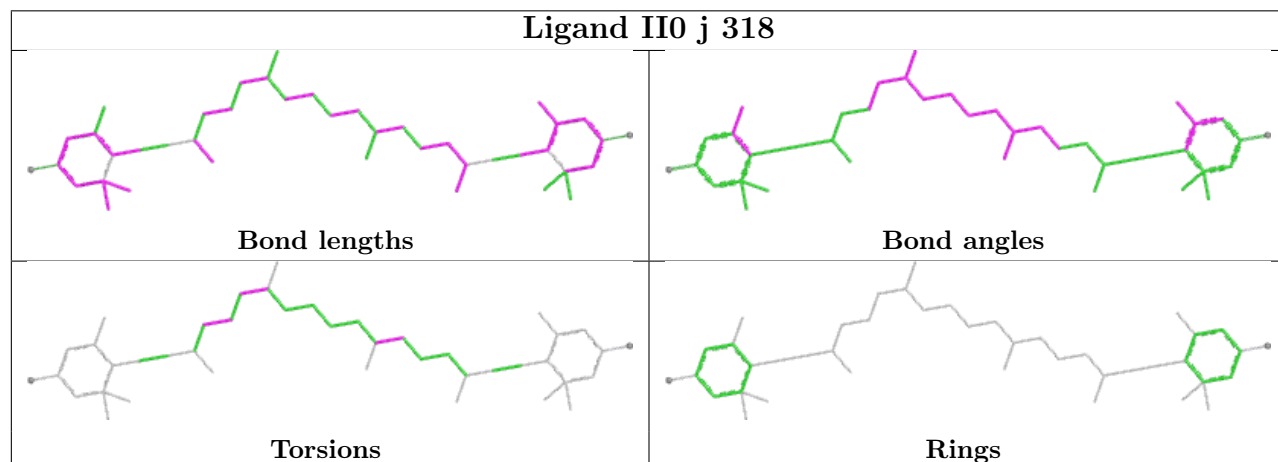
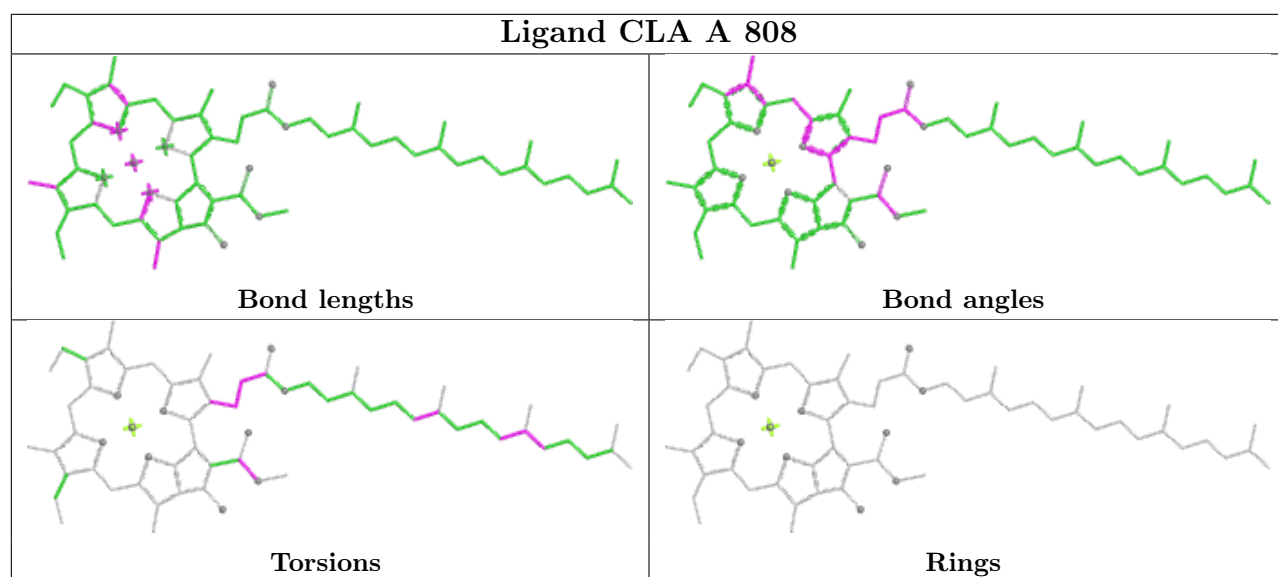


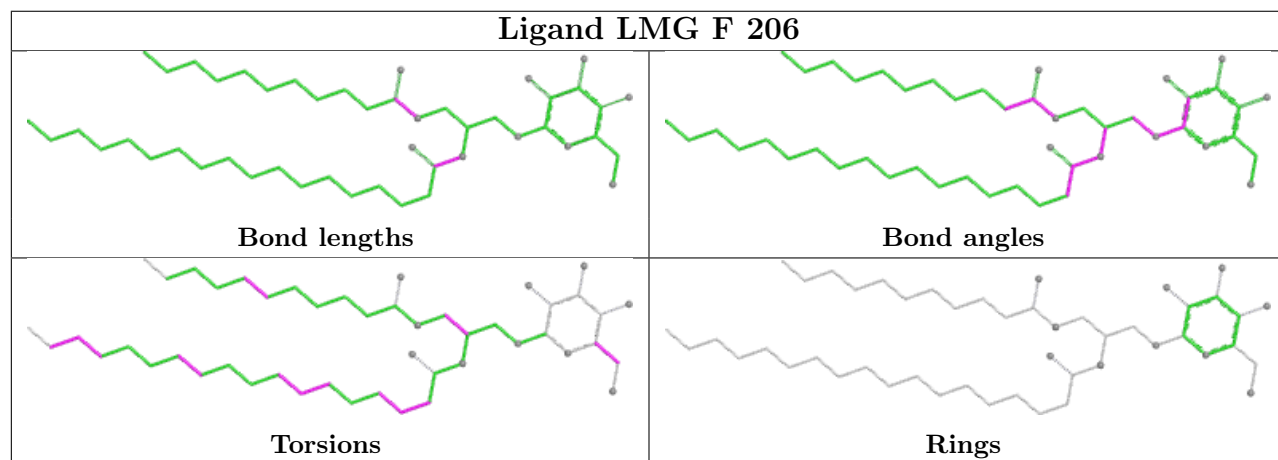
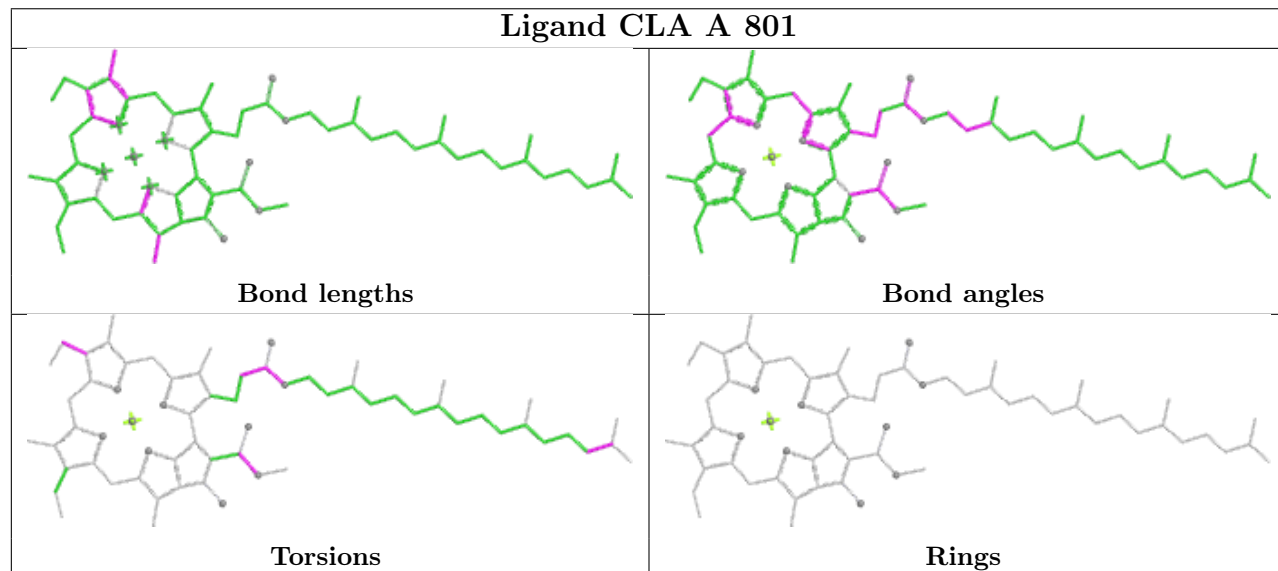
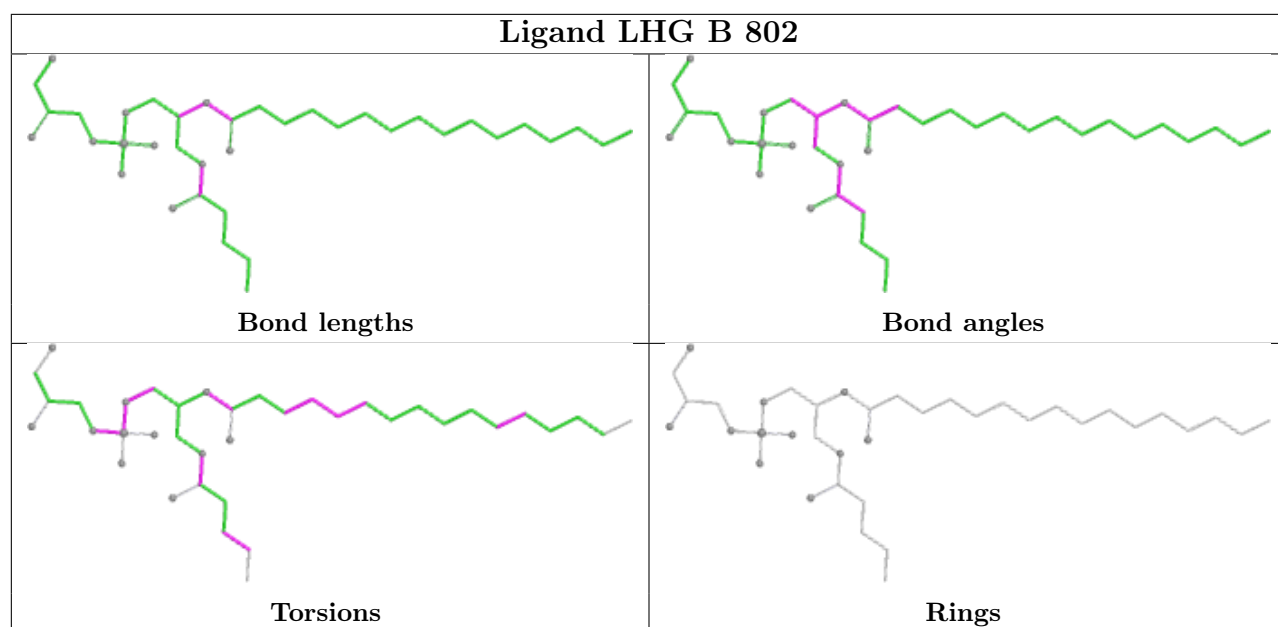
Ligand CLA h 301

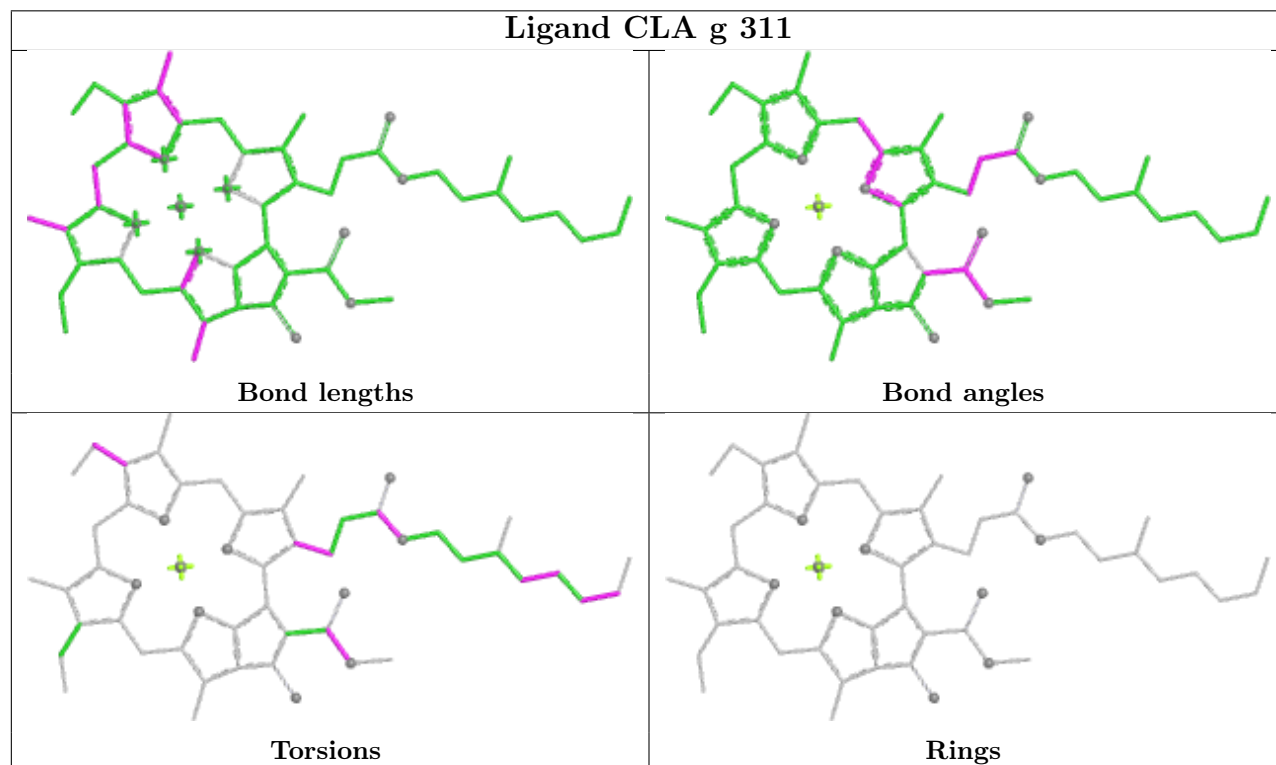
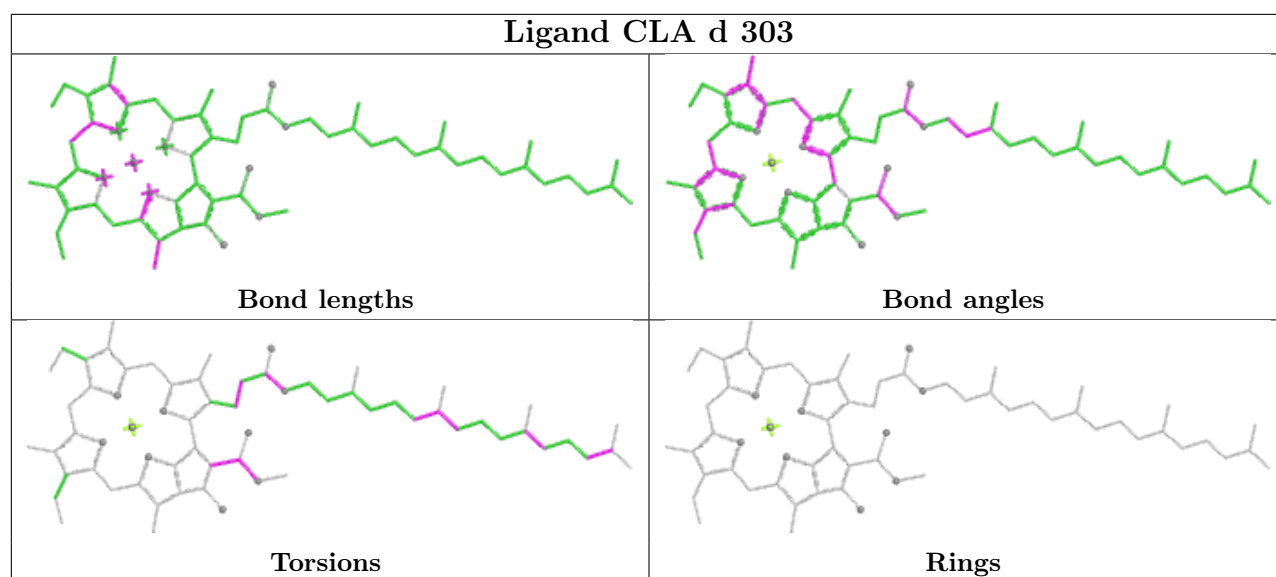


Ligand WVN L 205

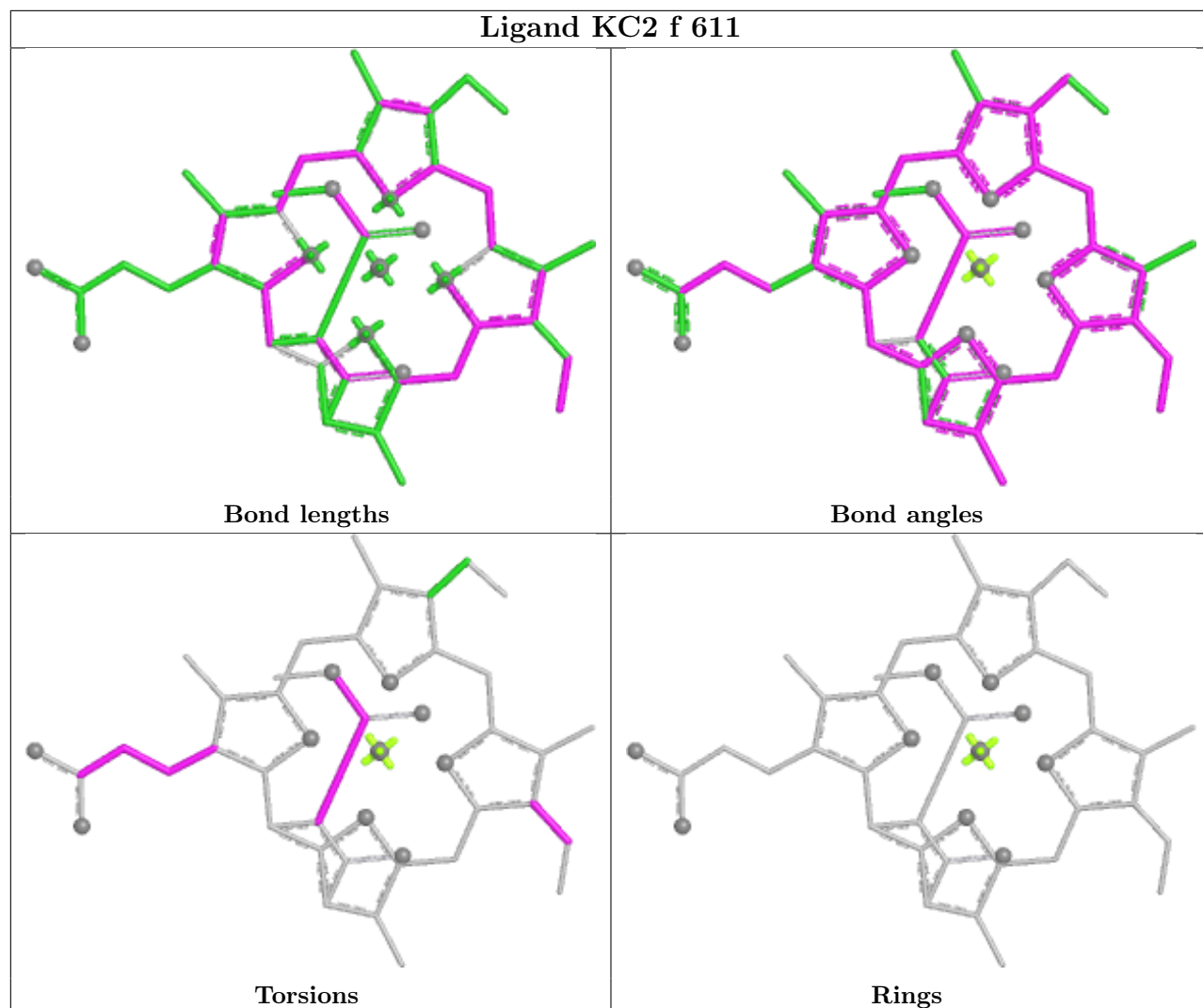




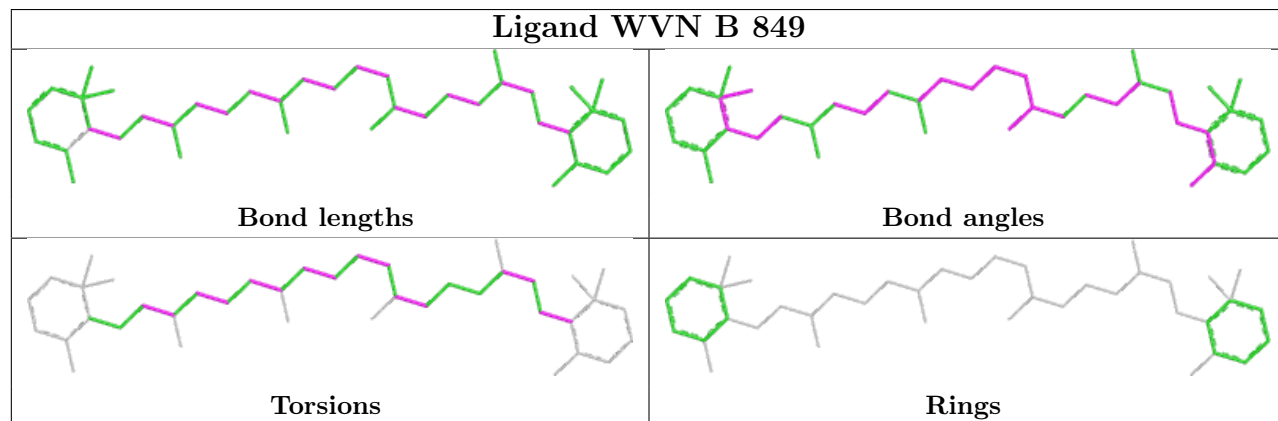




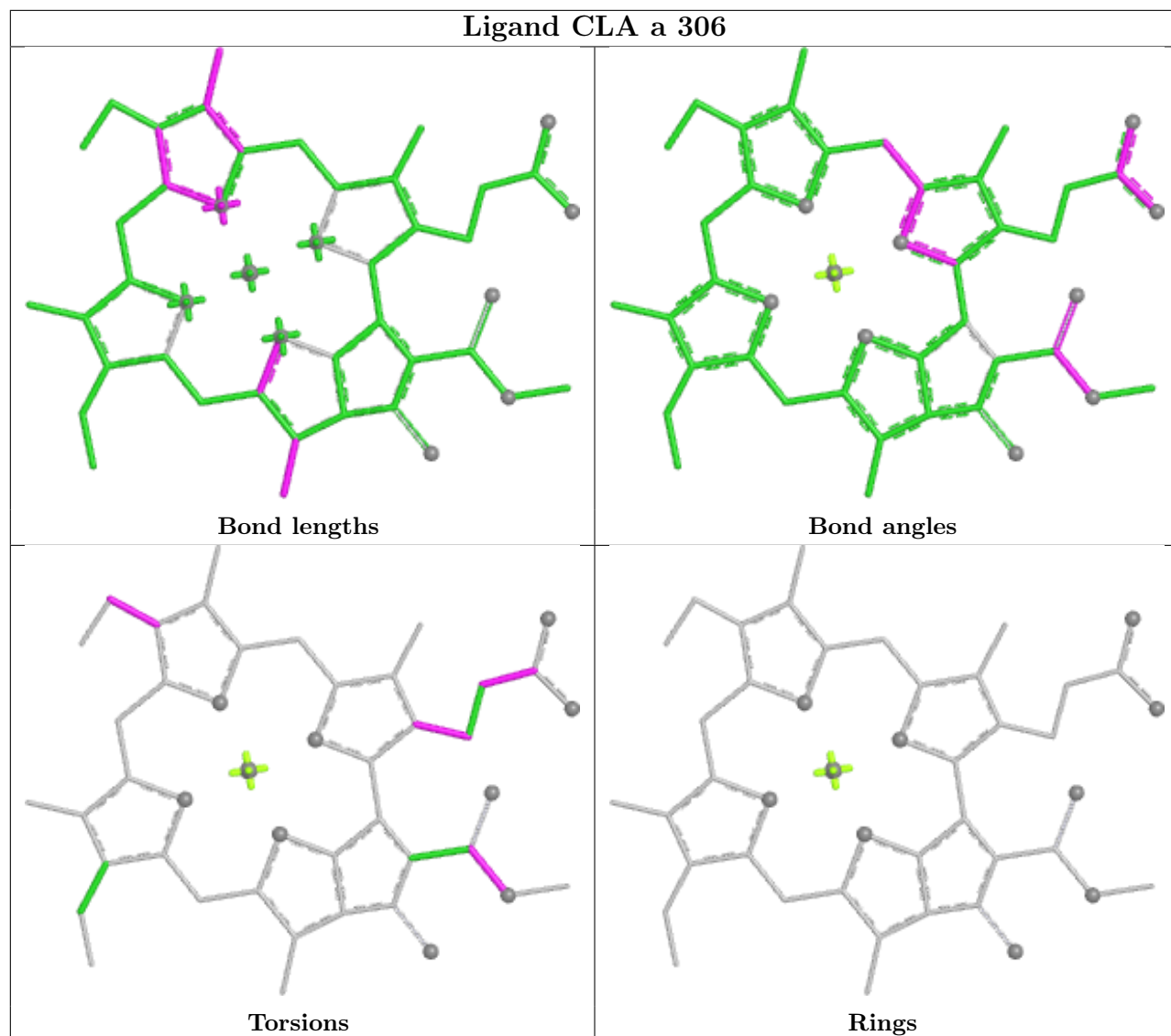
Ligand KC2 f 611



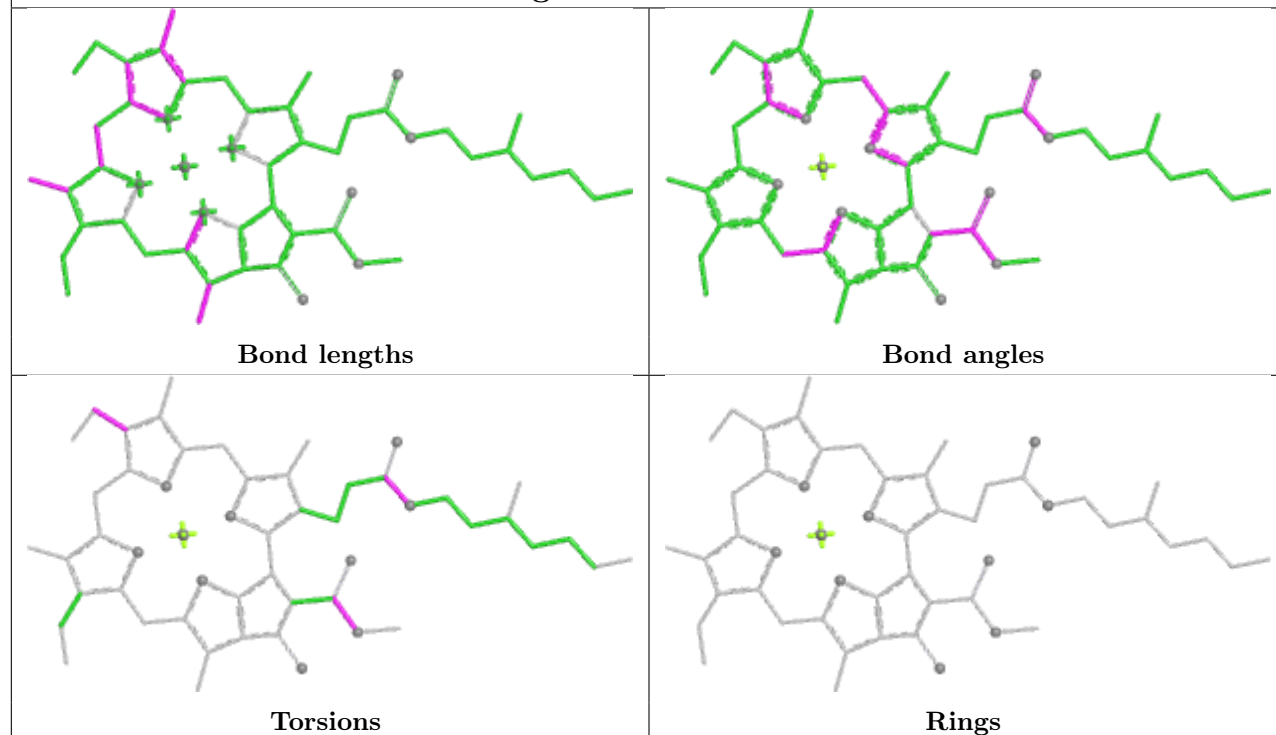
Ligand WVN B 849



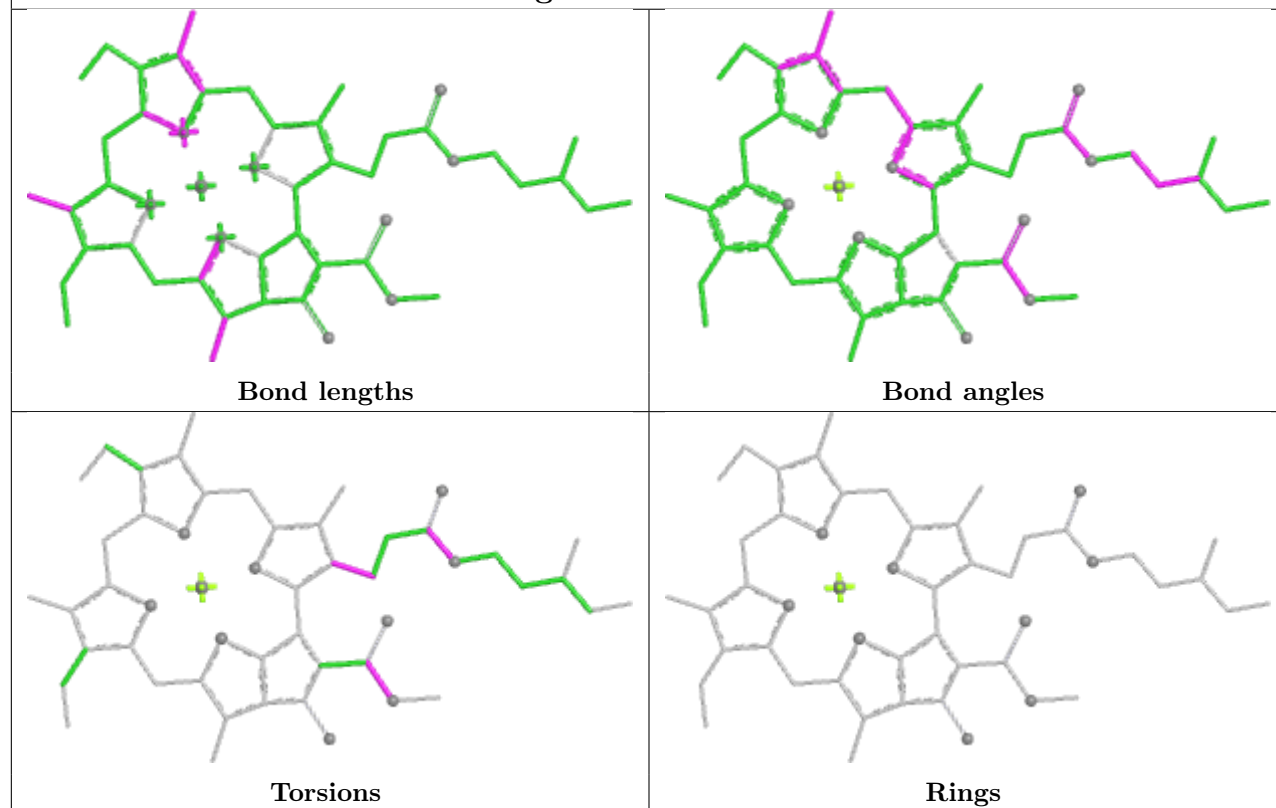
Ligand CLA a 306

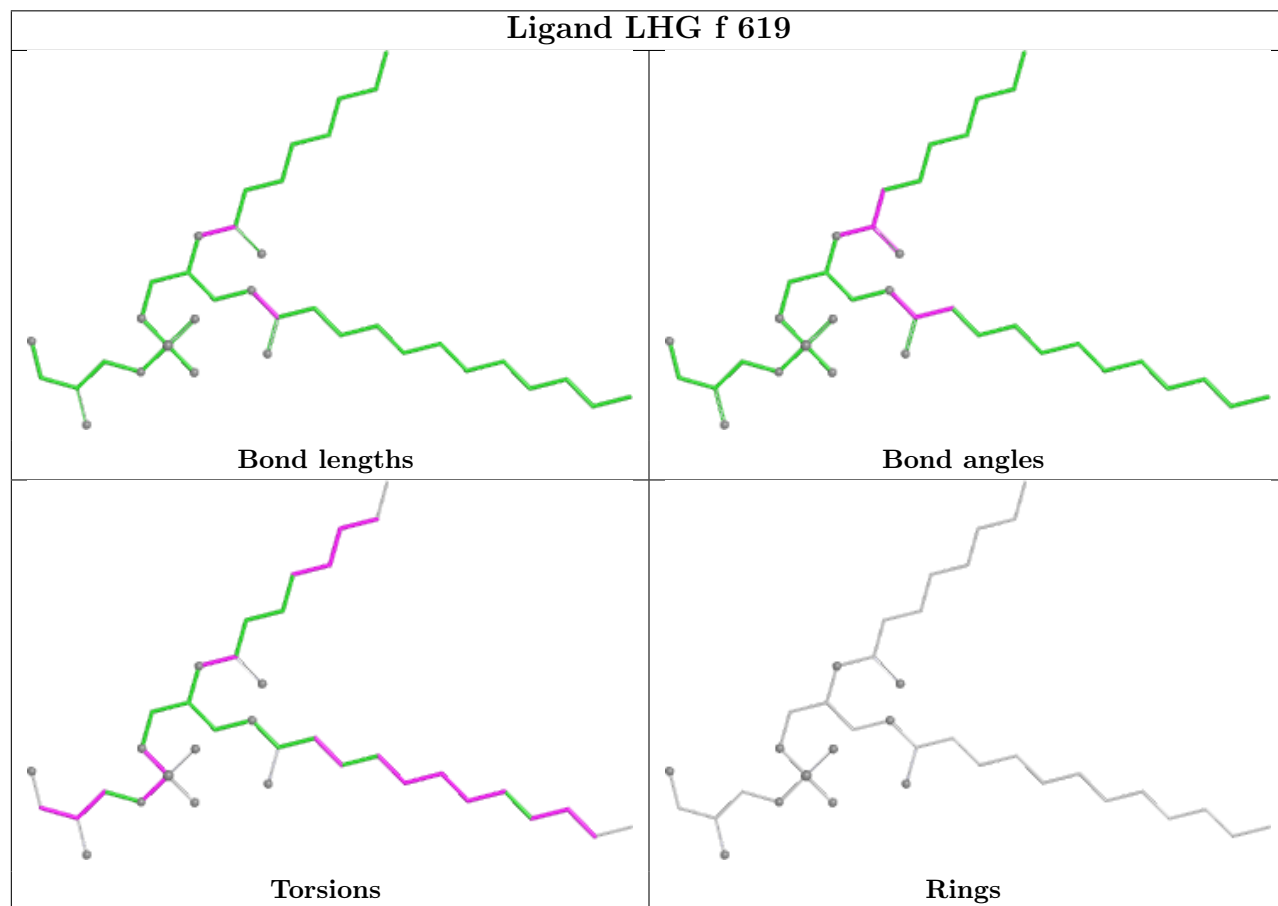
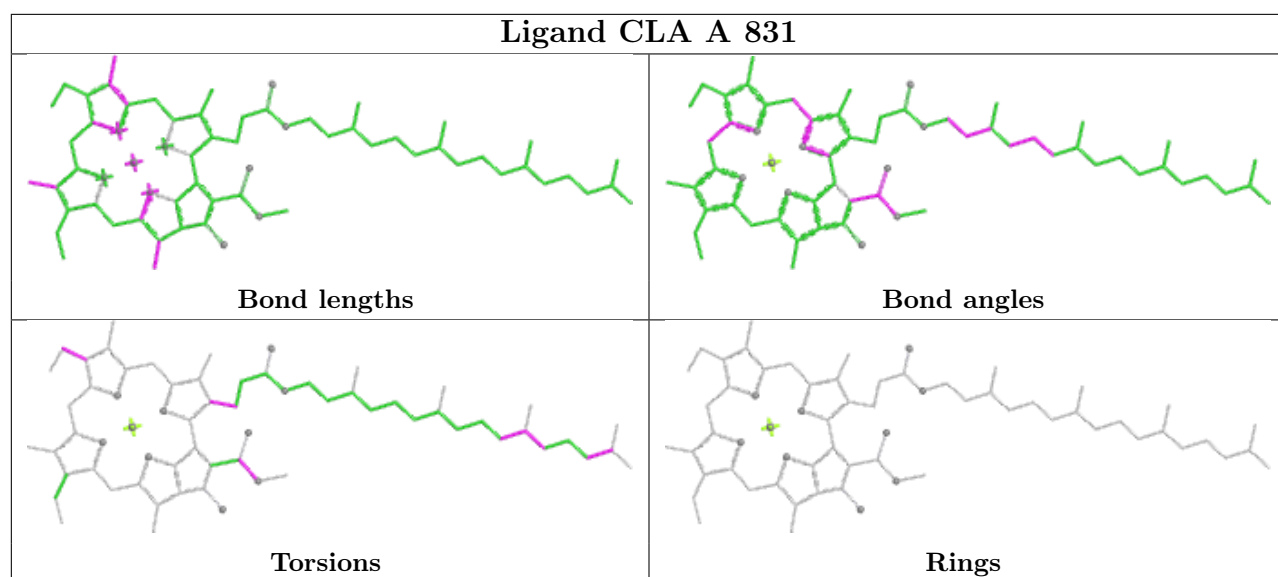


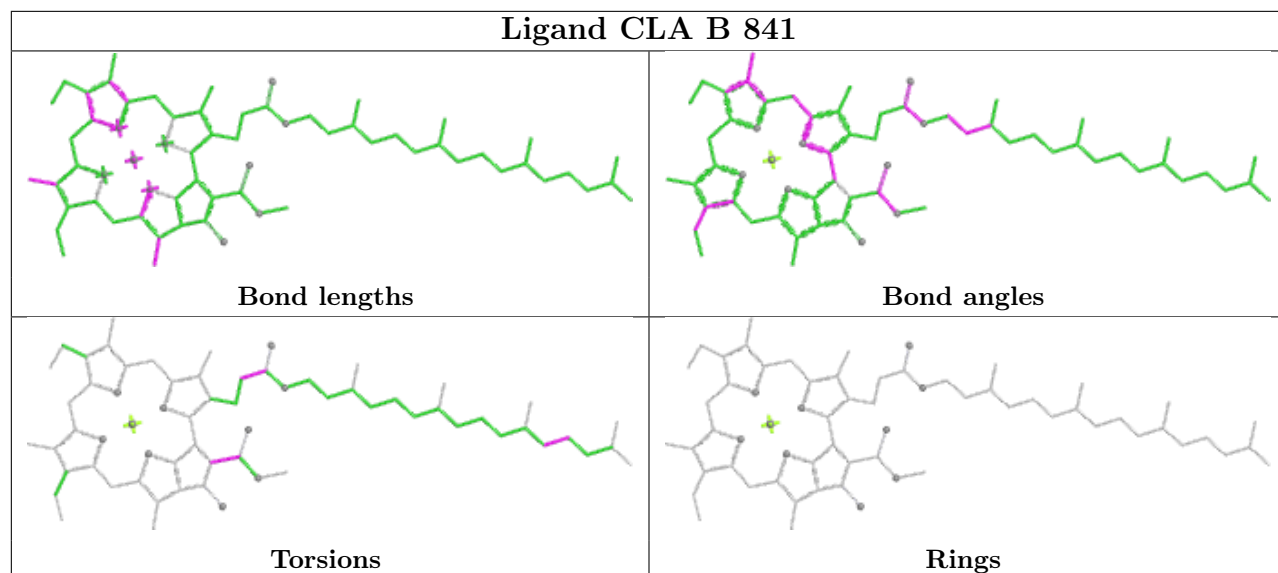
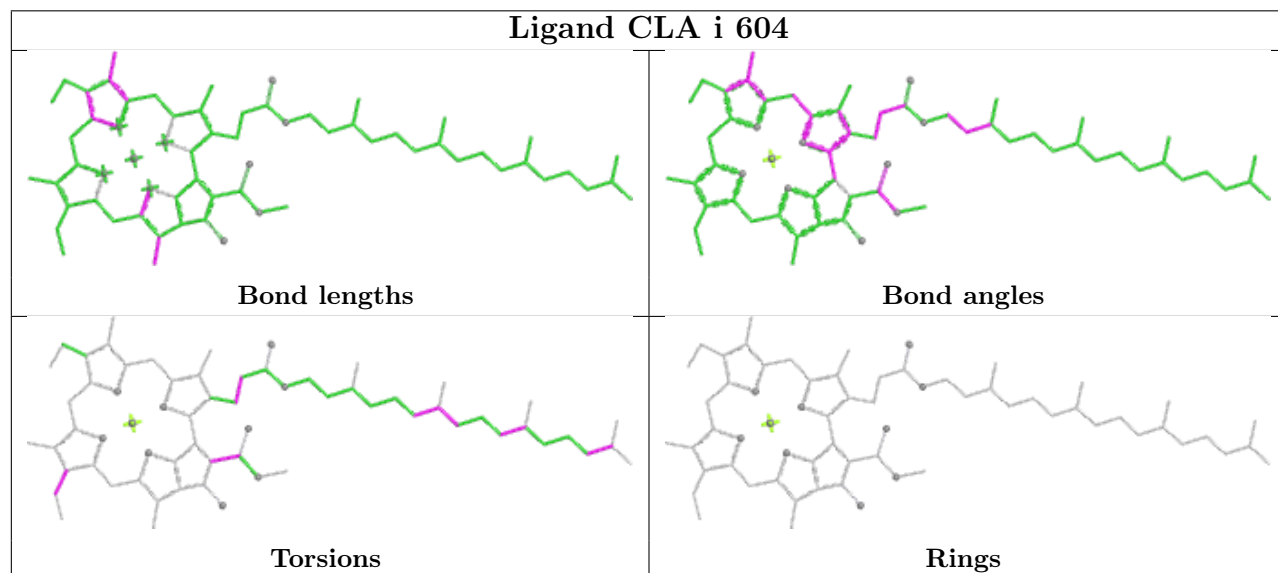
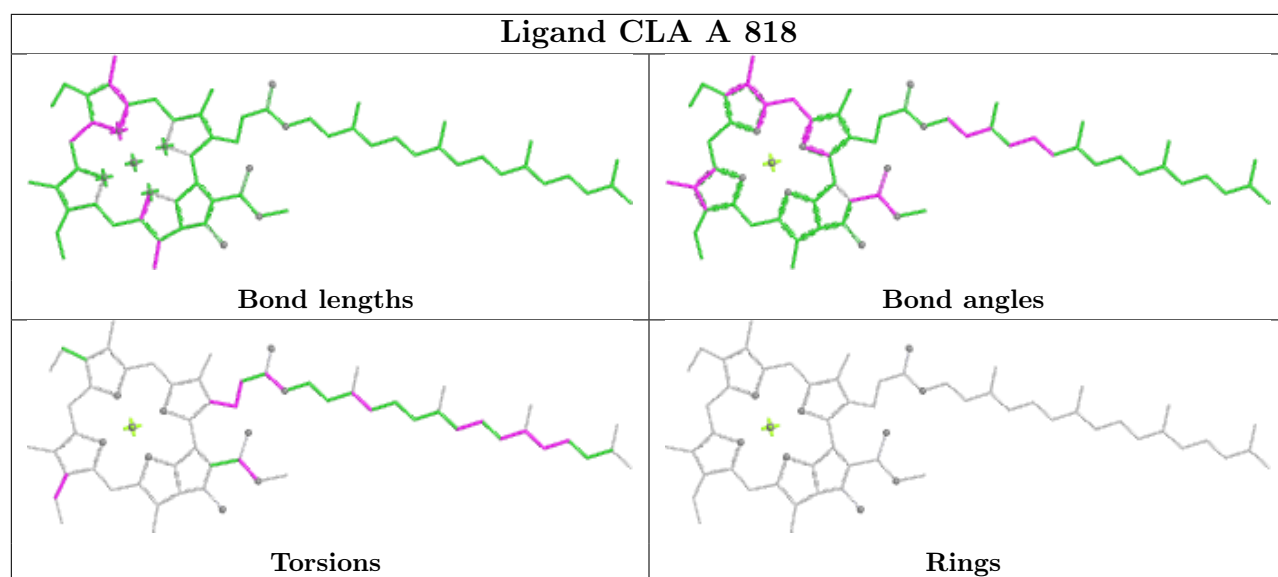
Ligand CLA B 821

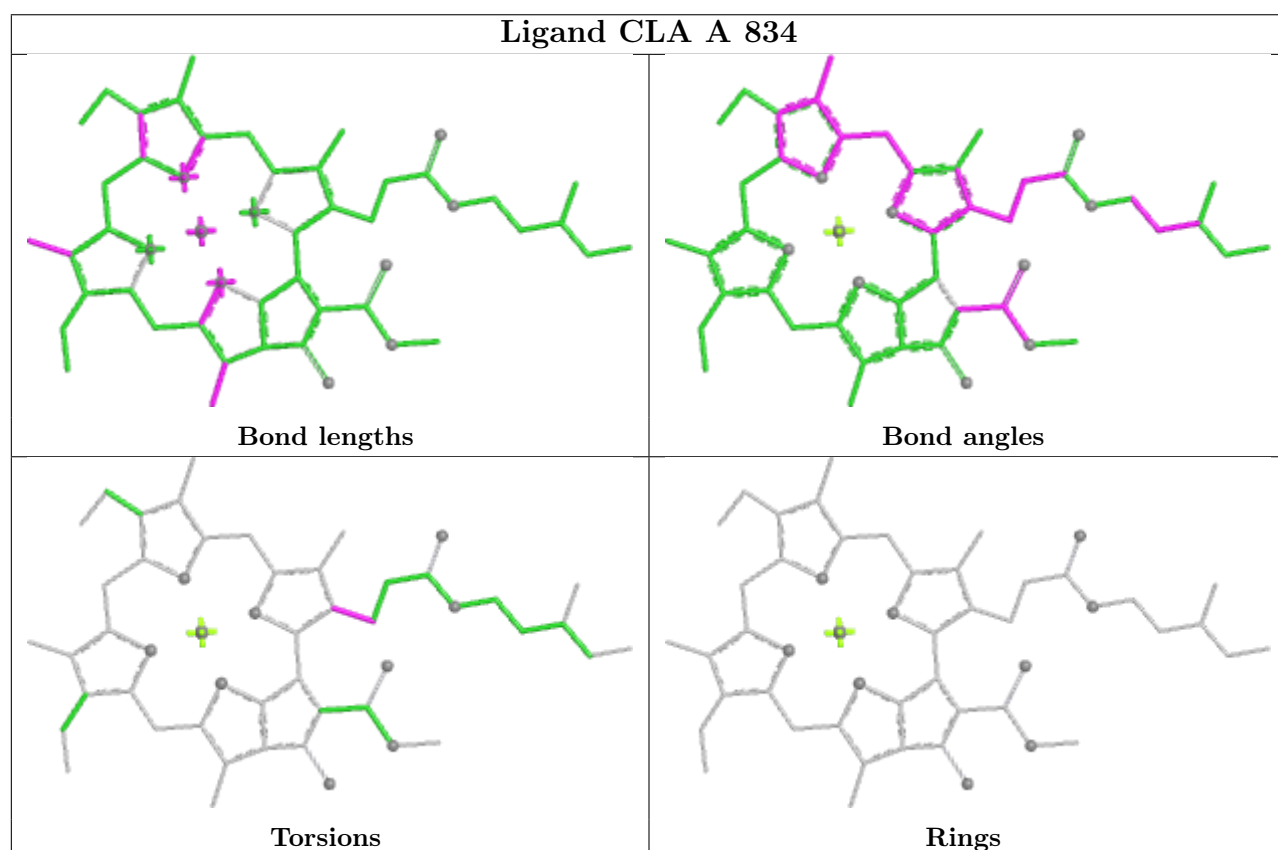
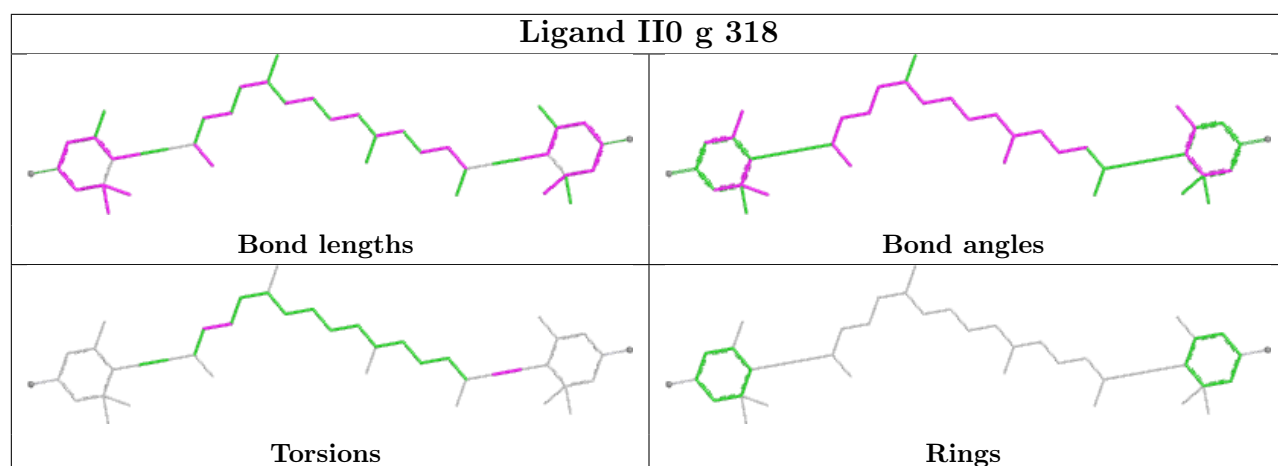


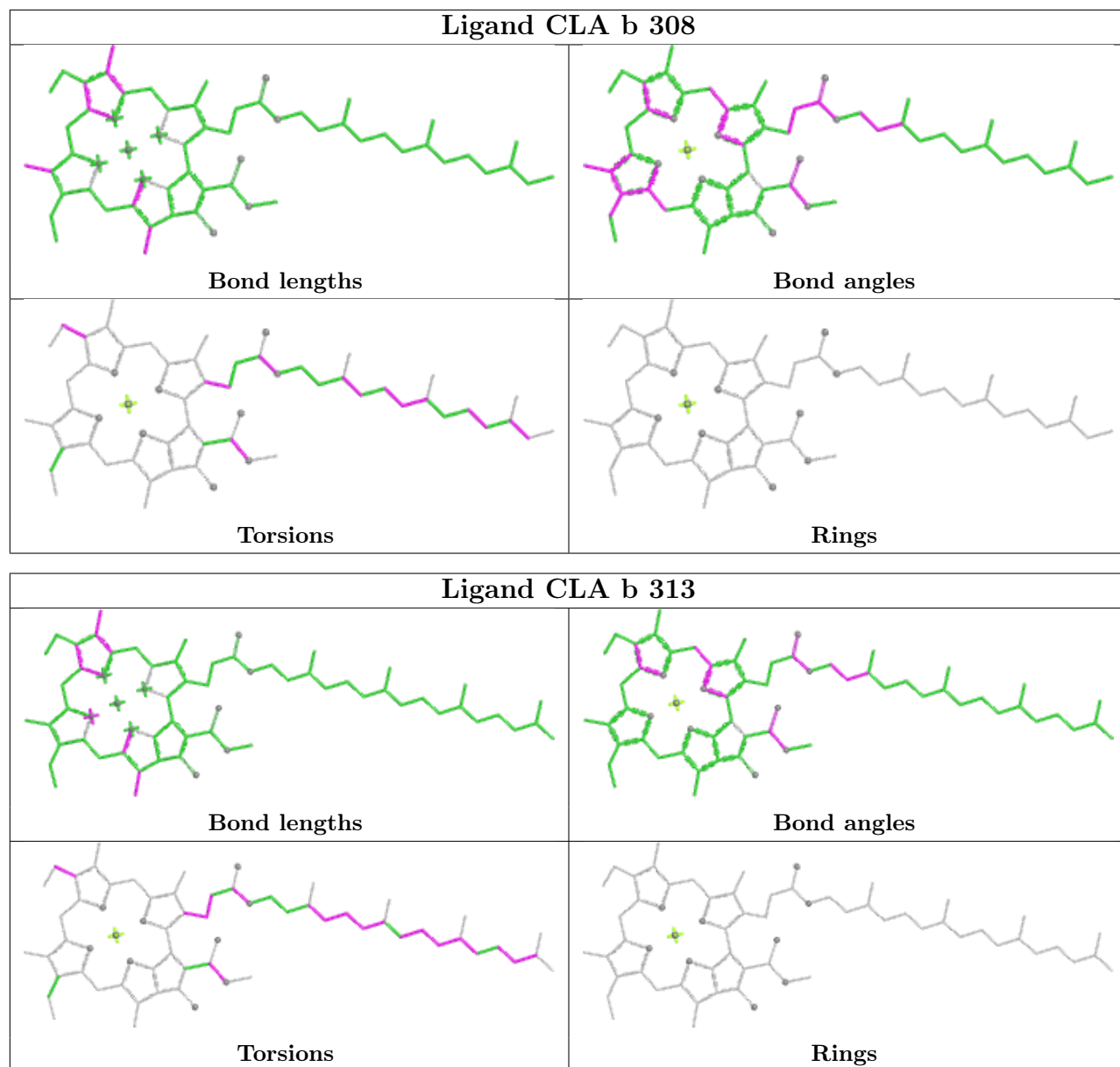
Ligand CLA h 304



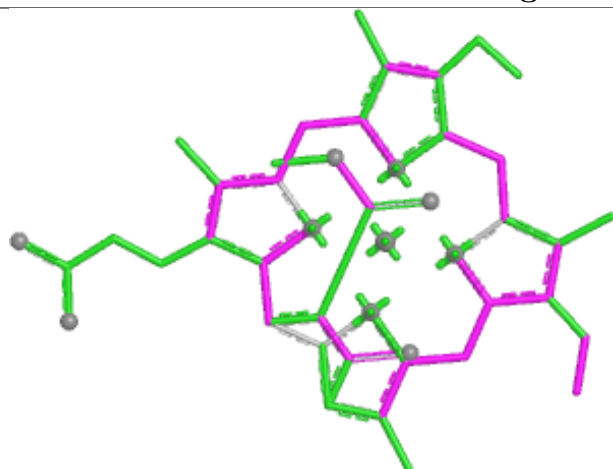




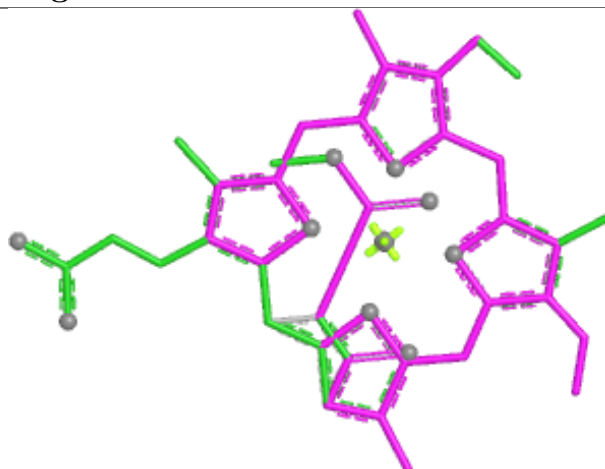




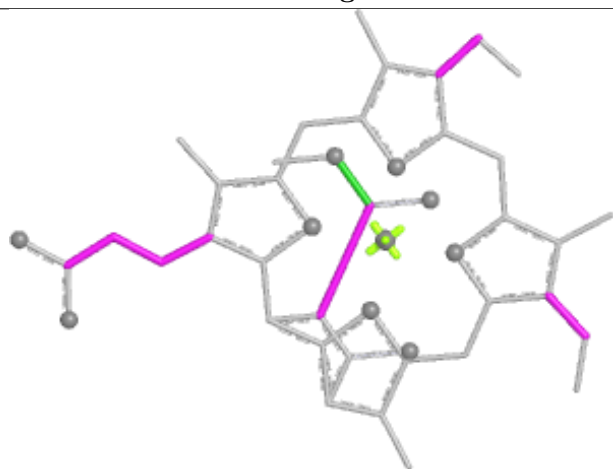
Ligand KC2 g 314



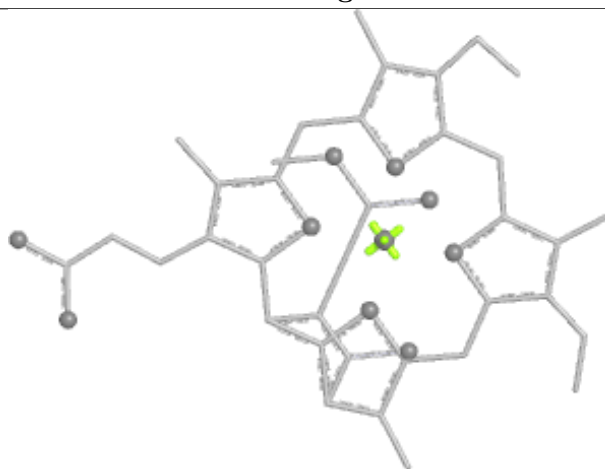
Bond lengths



Bond angles

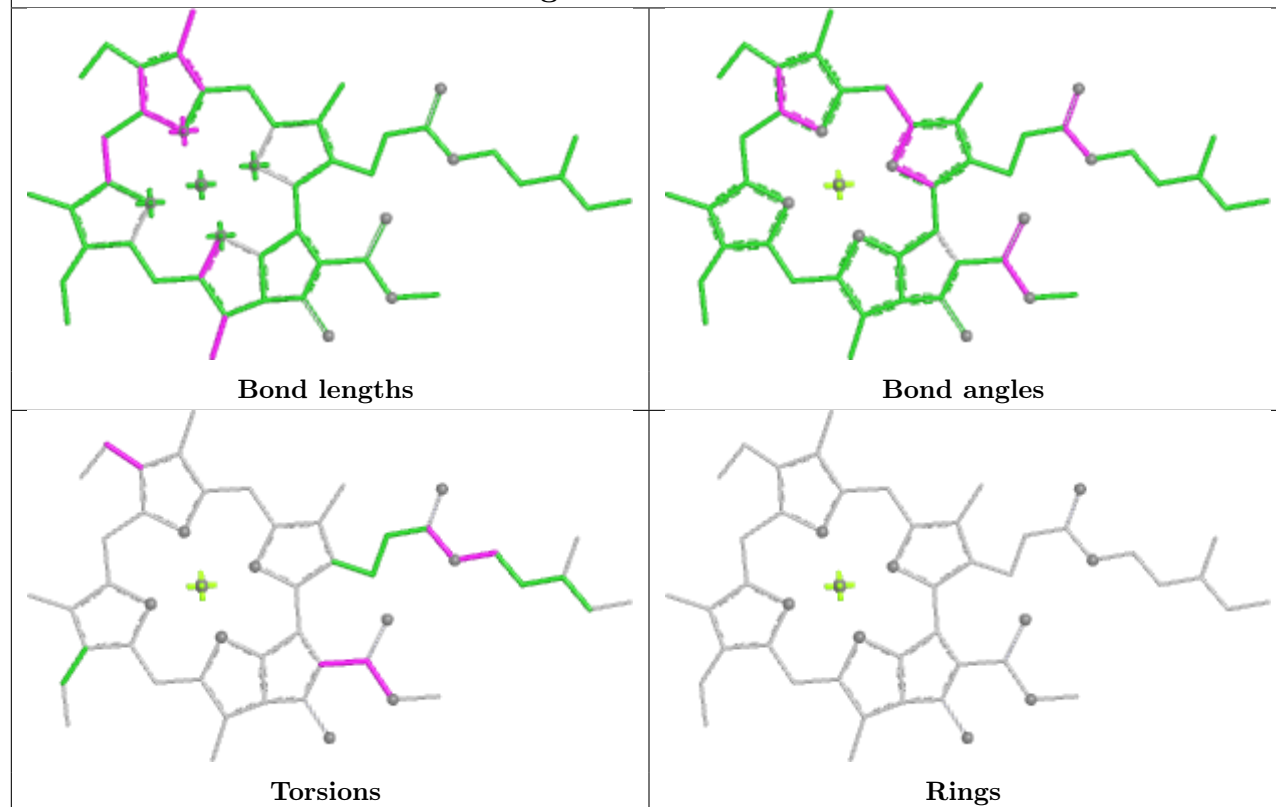


Torsions

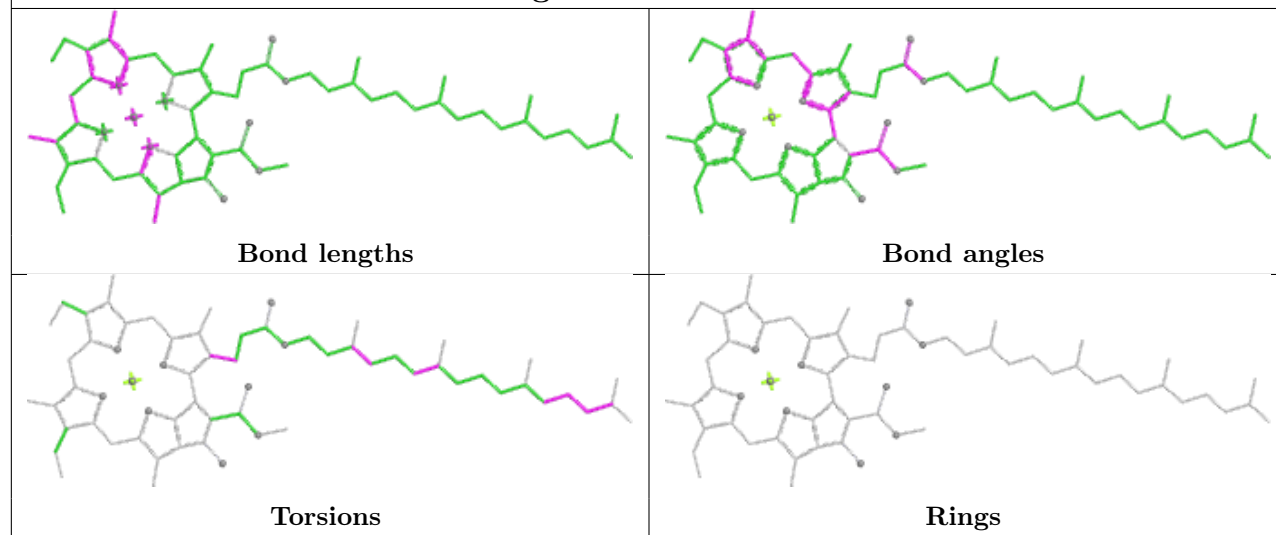


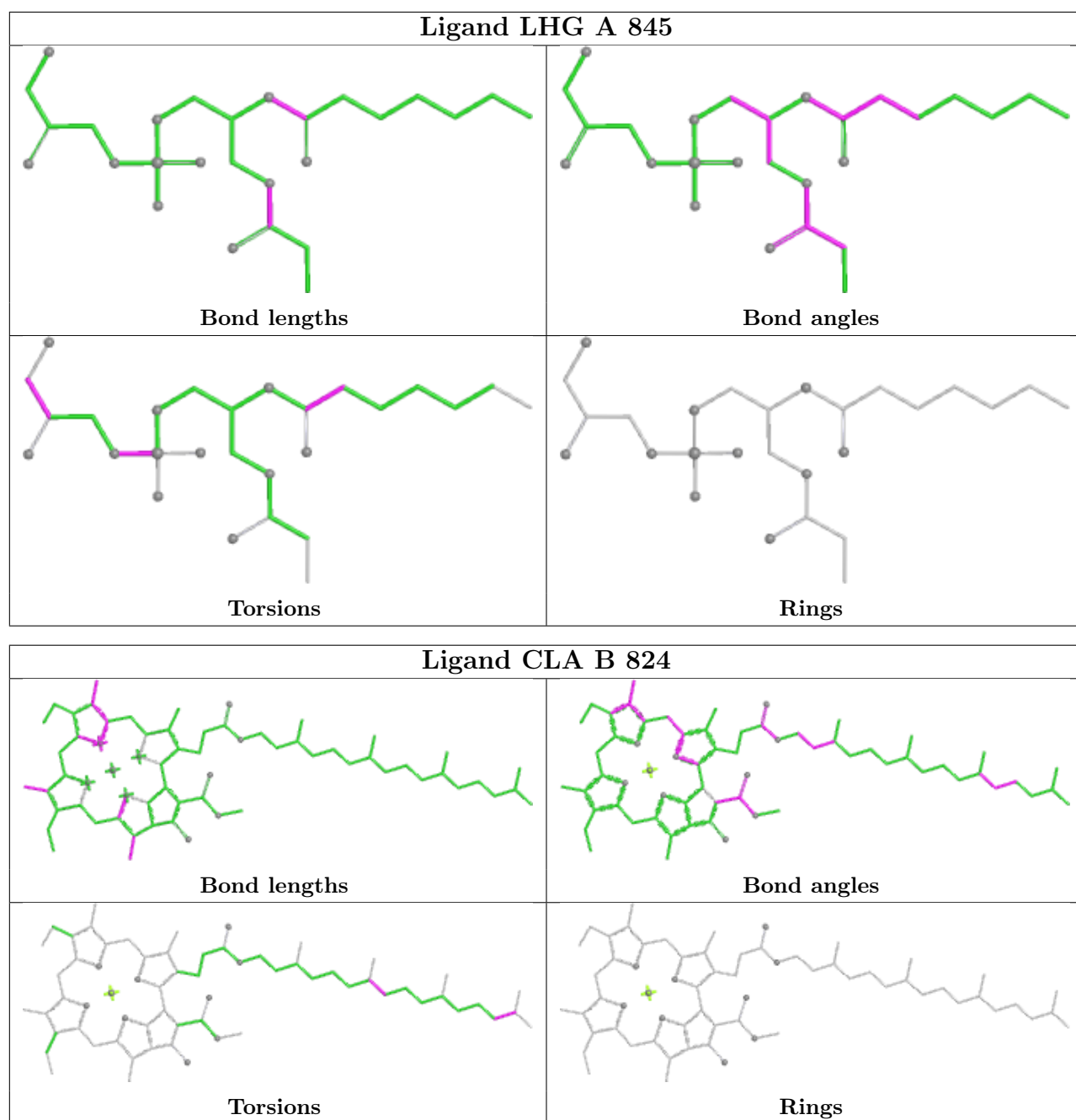
Rings

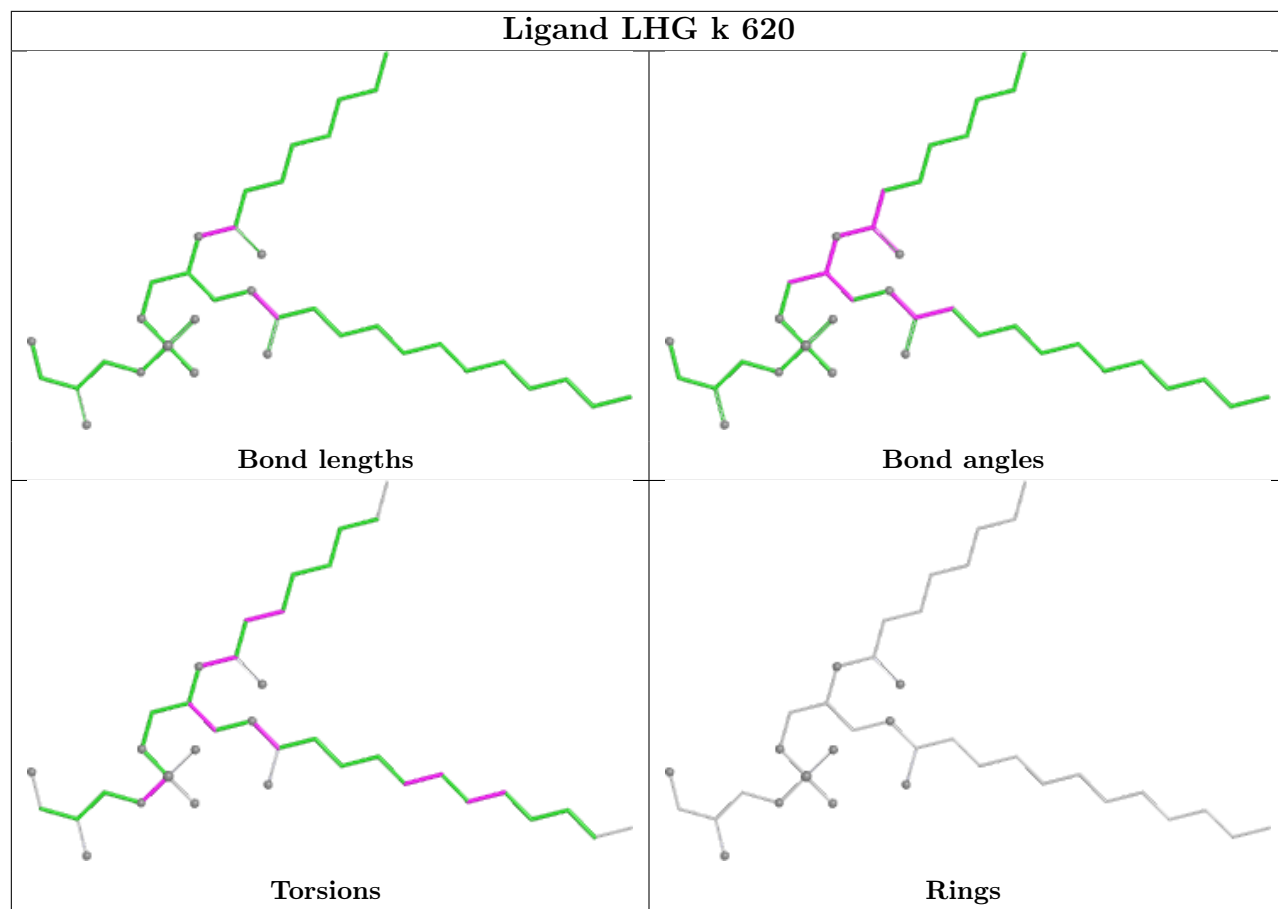
Ligand CLA i 605



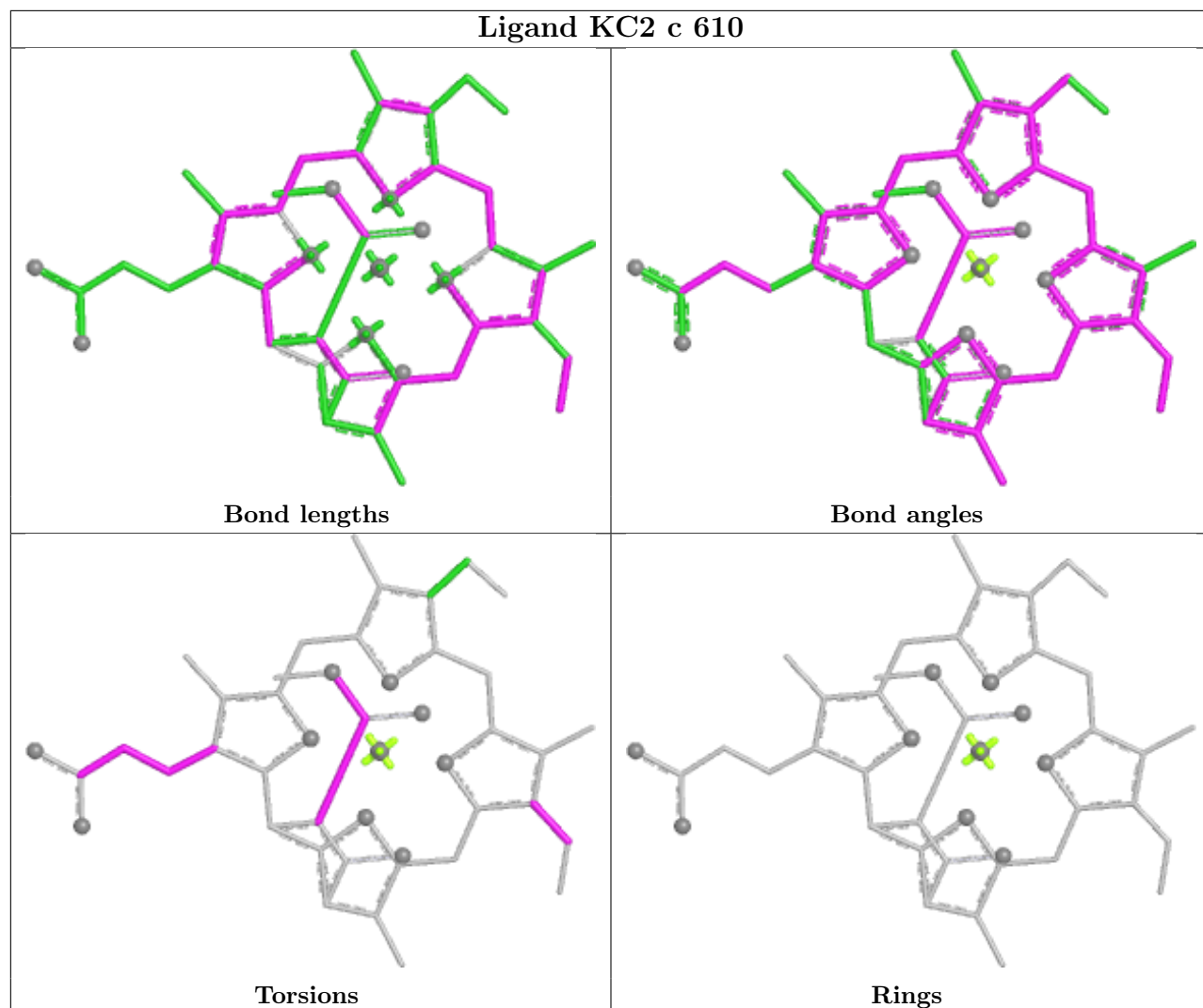
Ligand CLA B 825



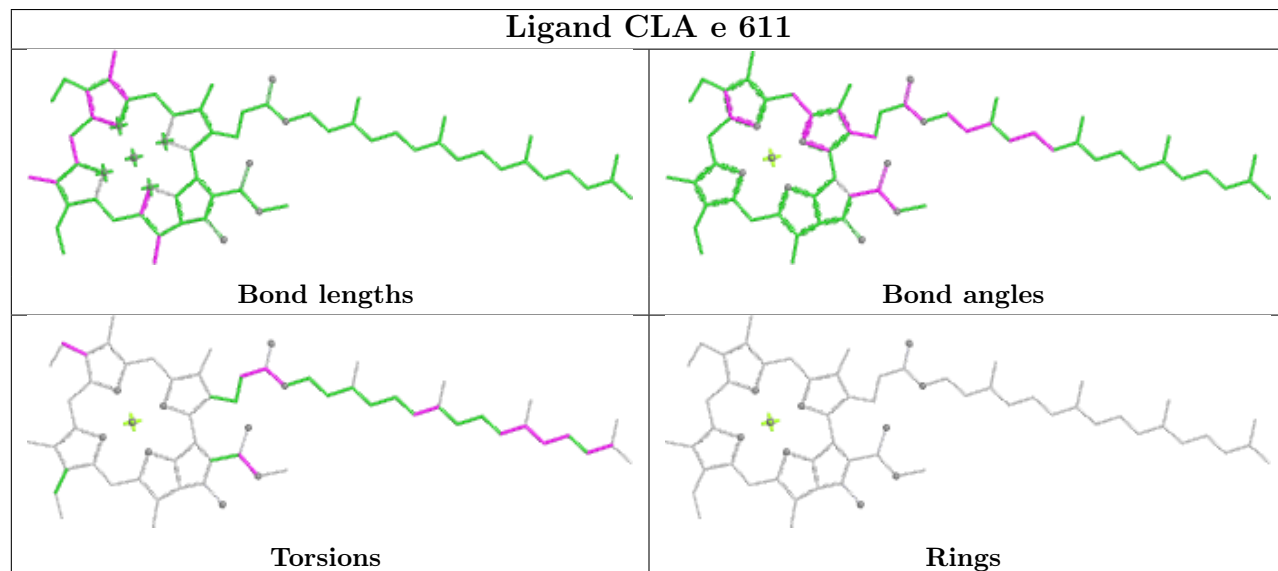




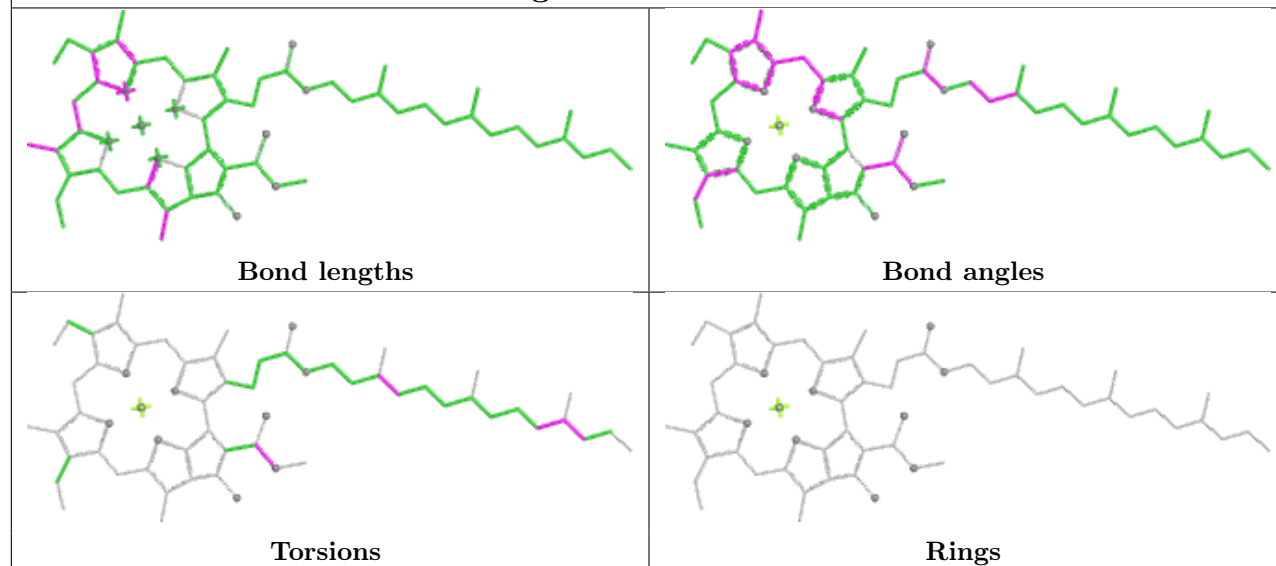
Ligand KC2 c 610



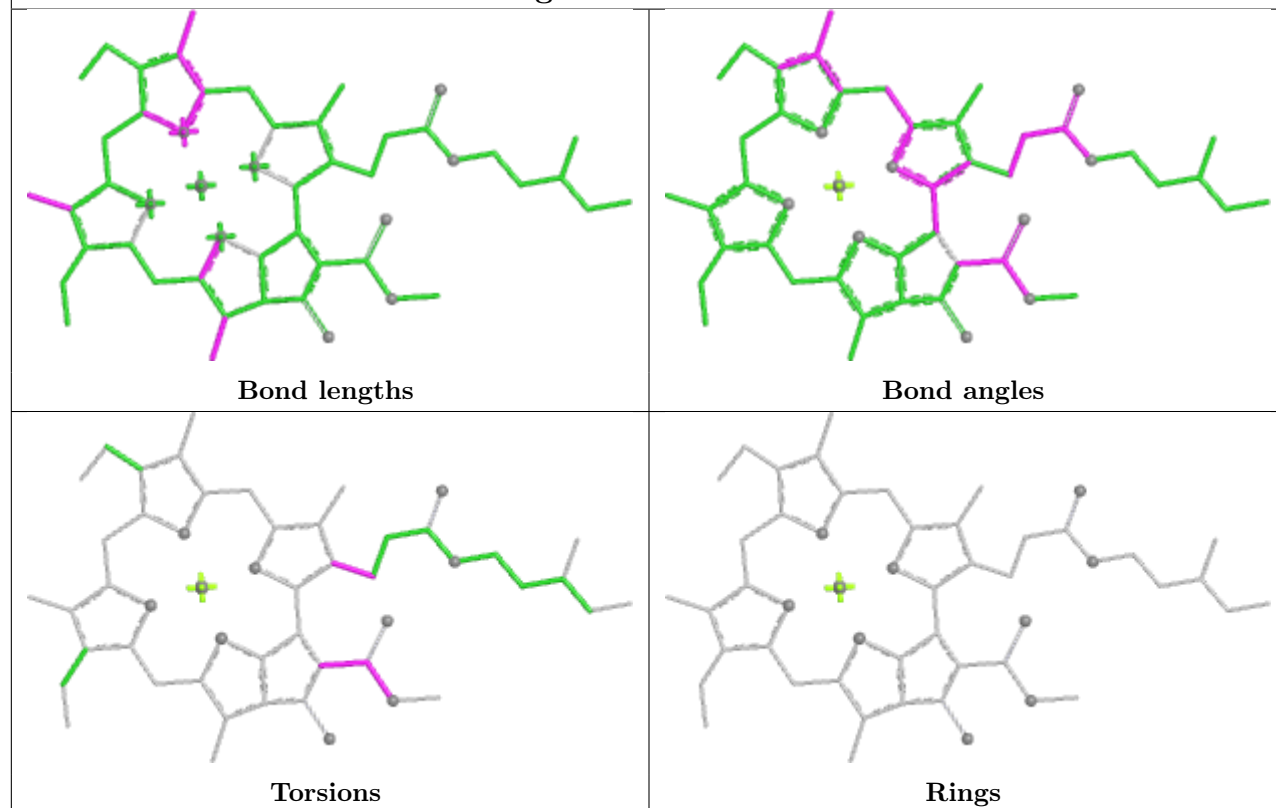
Ligand CLA e 611

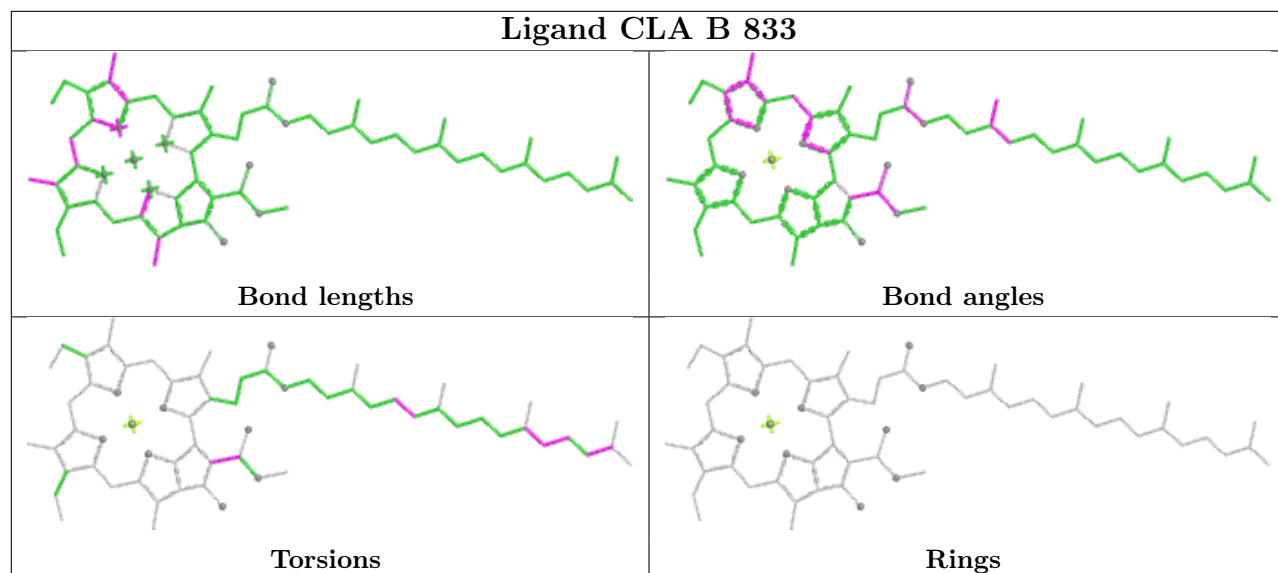
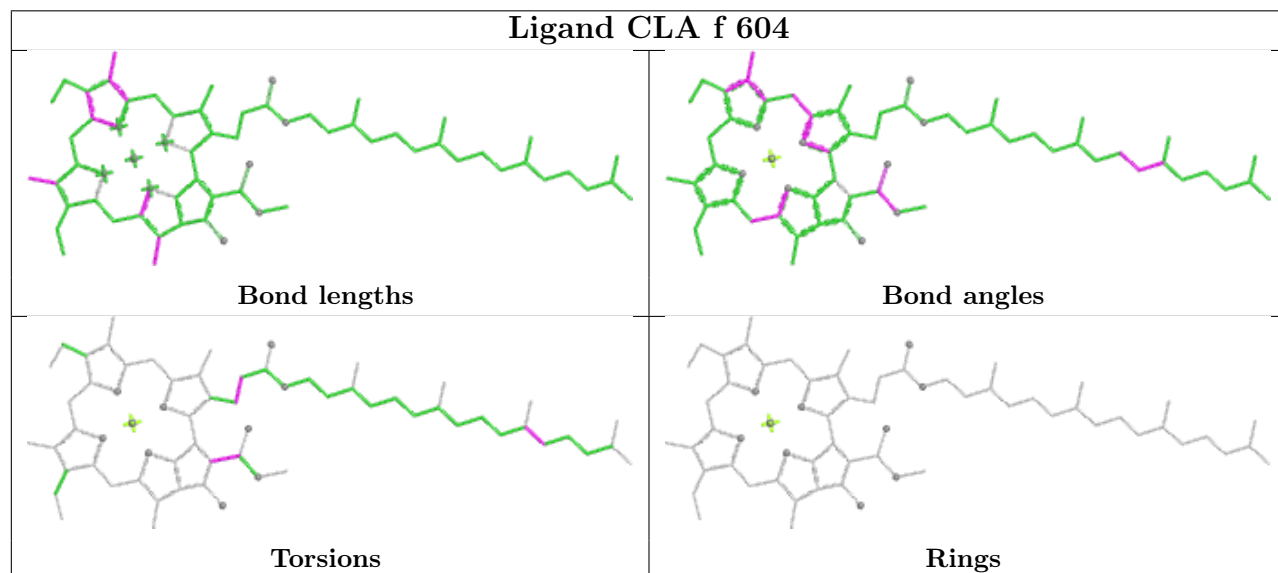
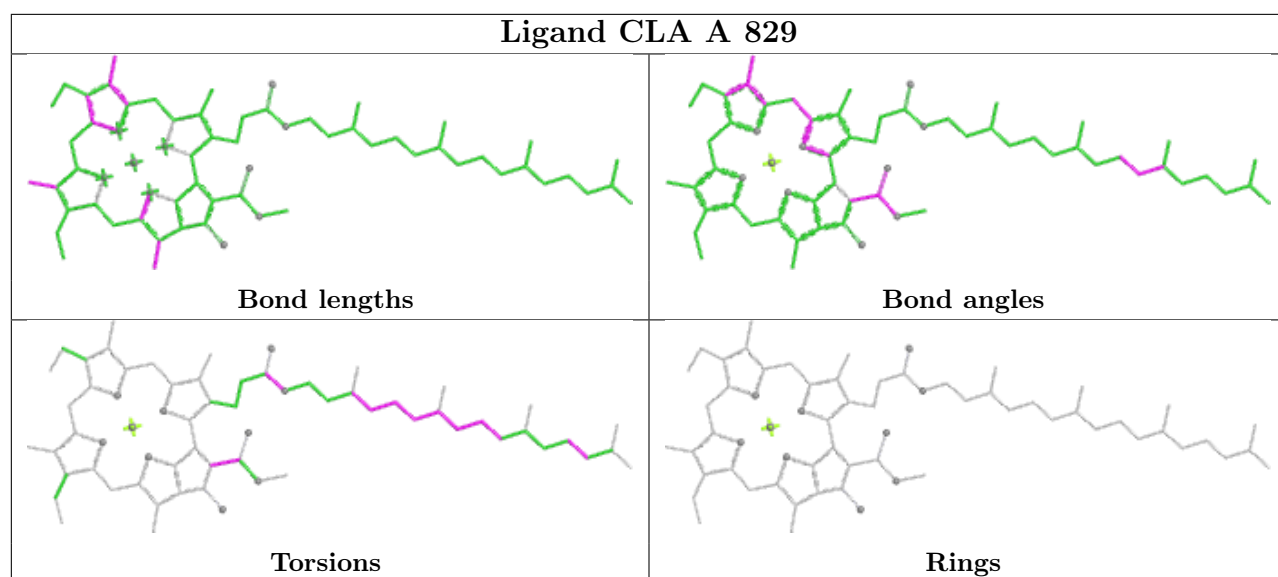


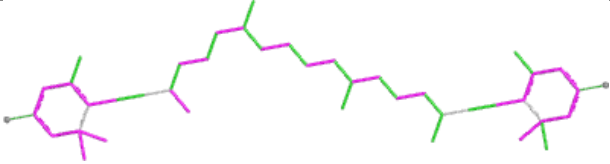
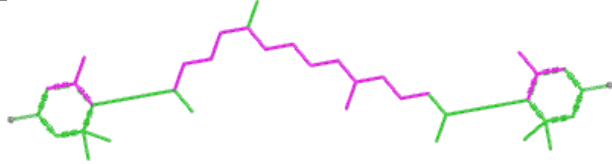
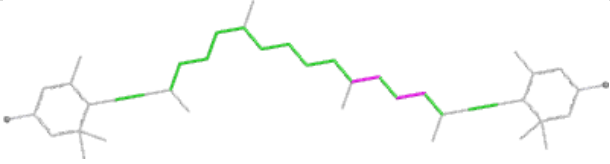
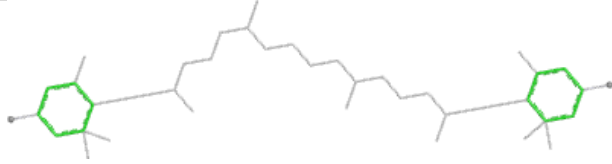
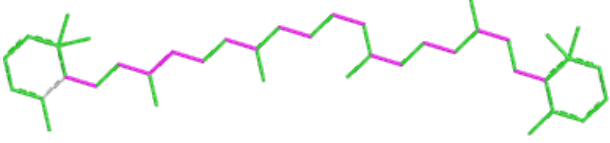
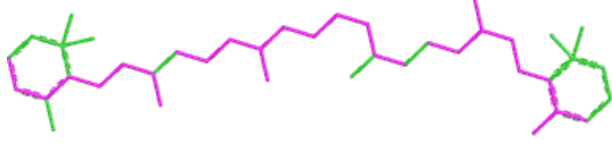
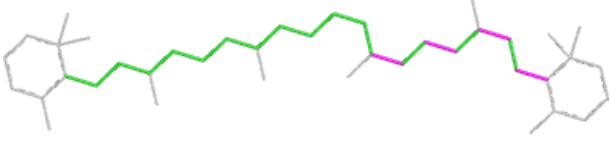
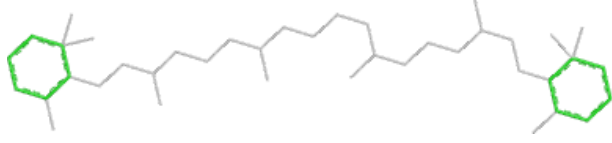
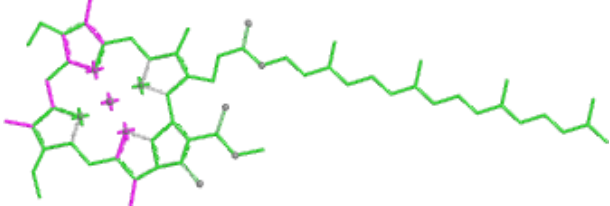
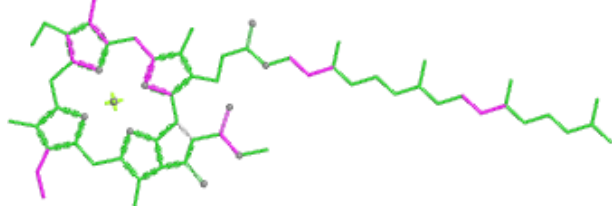
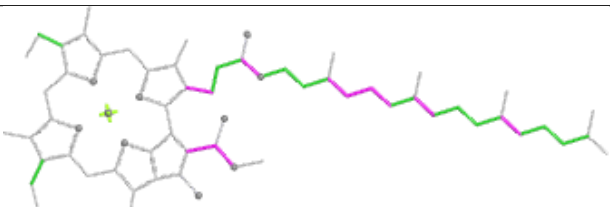
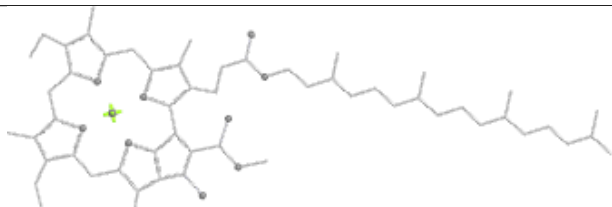
Ligand CLA A 827

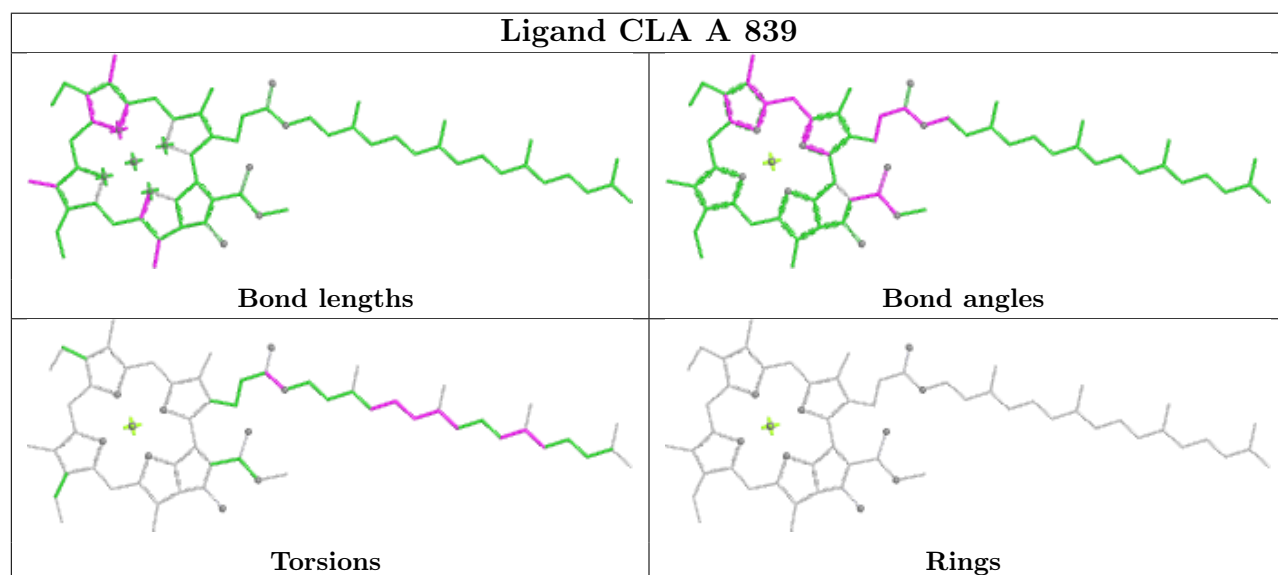
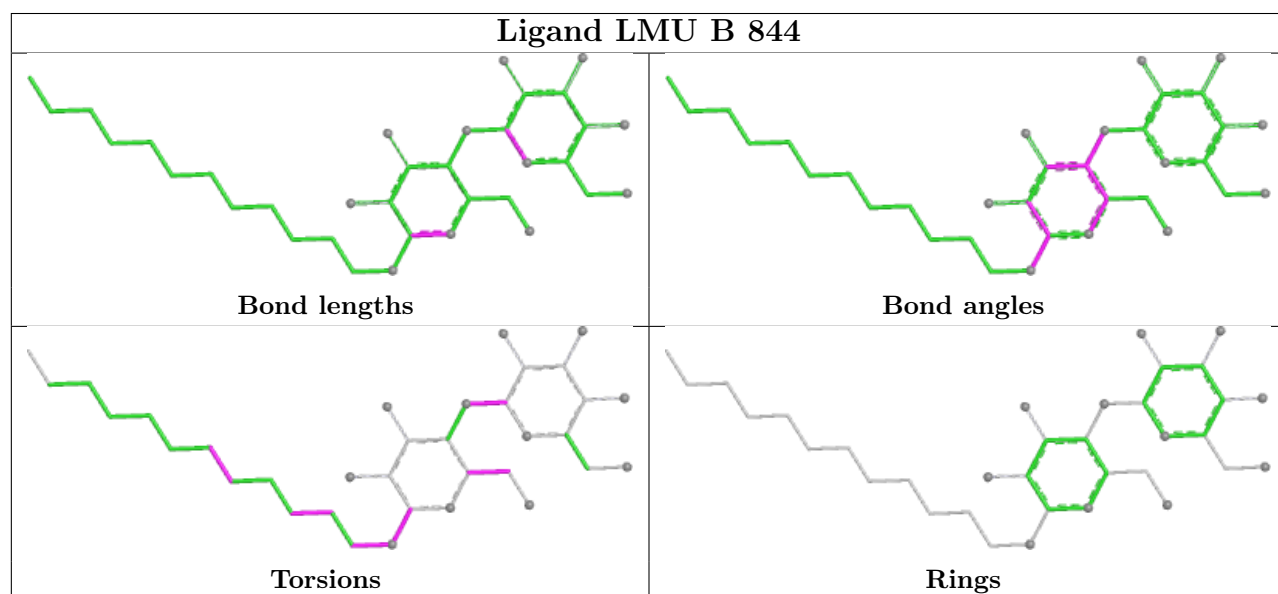
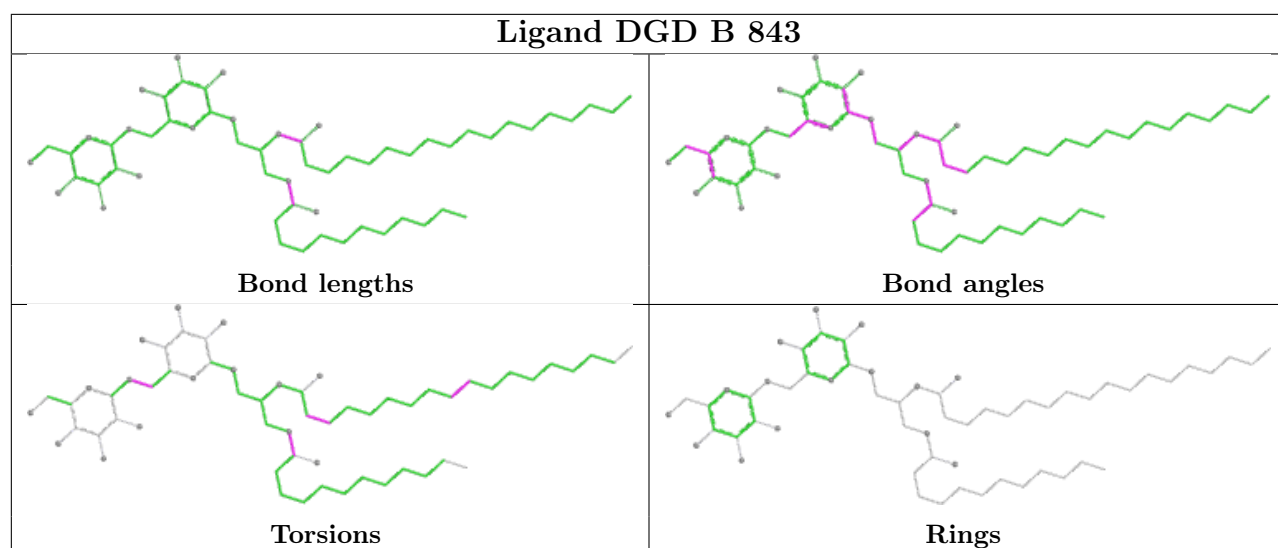


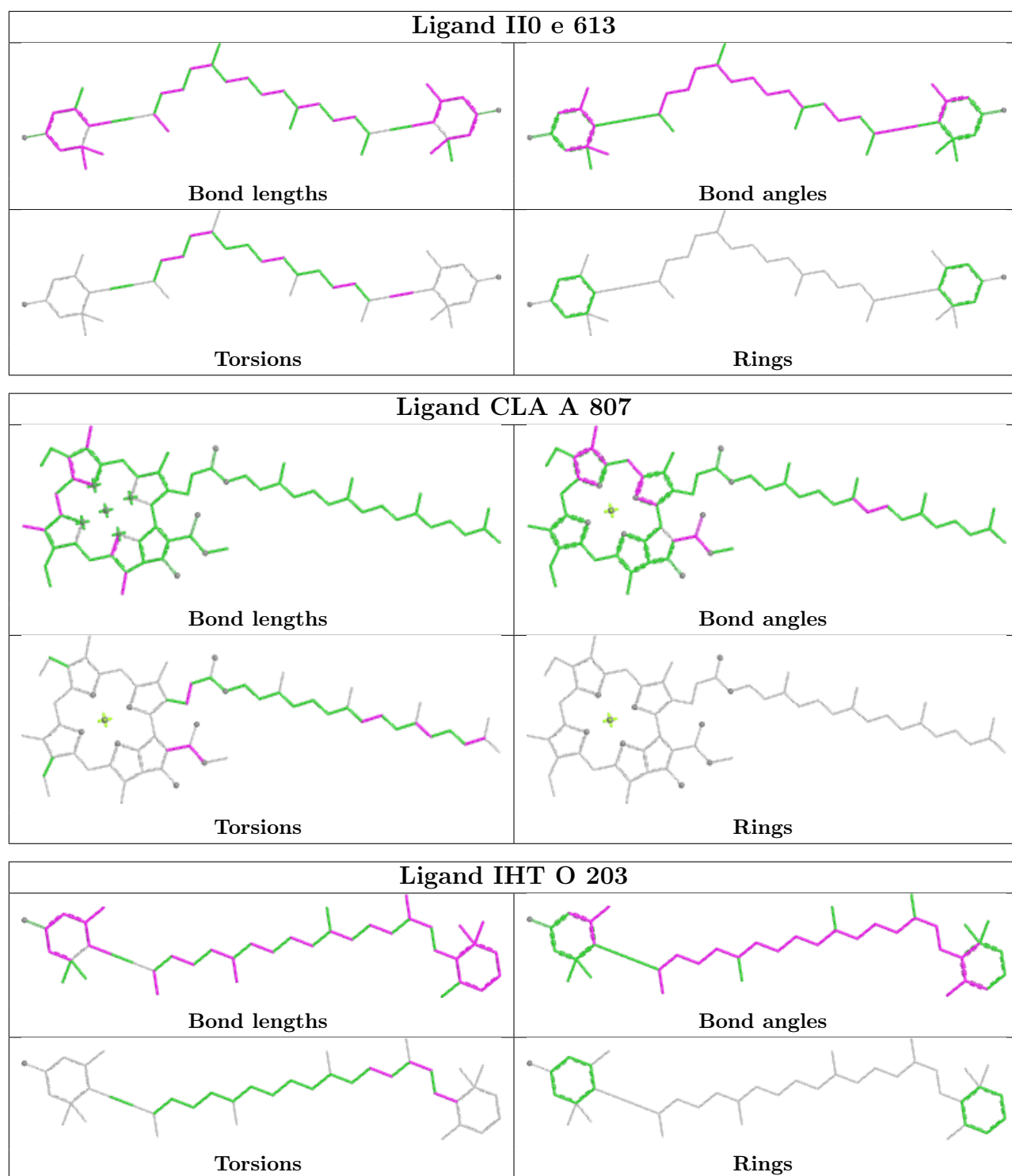
Ligand CLA h 303

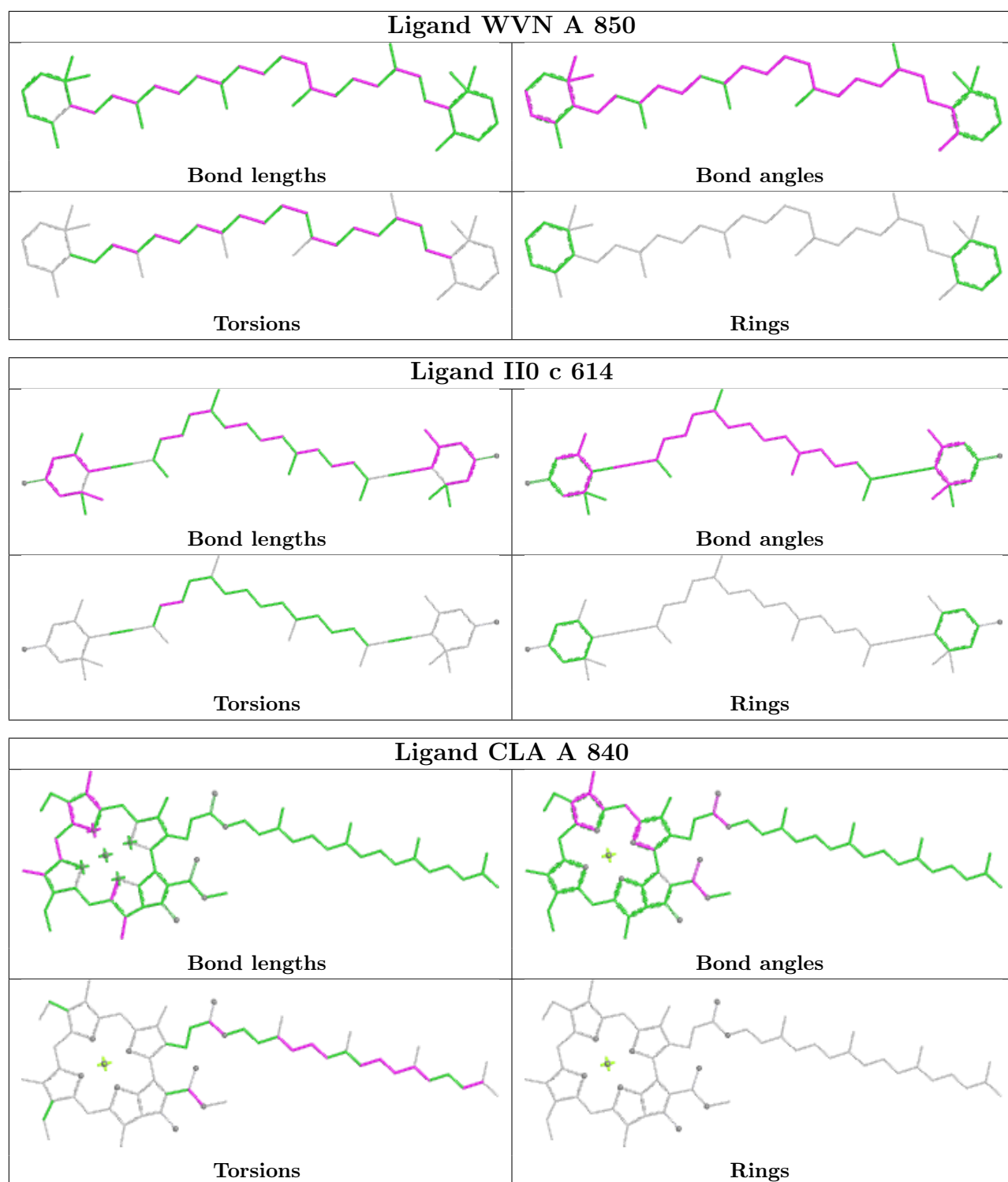




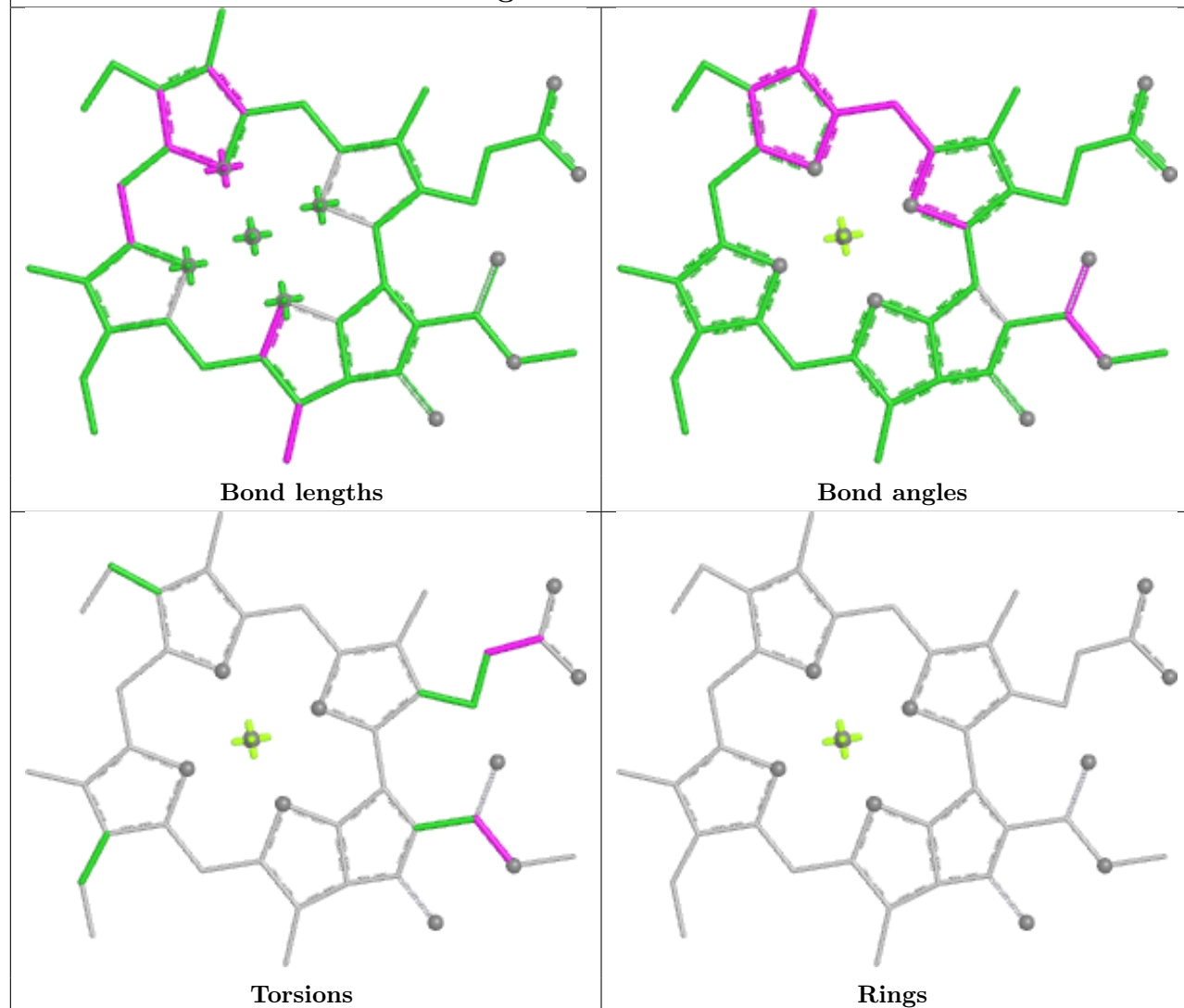
Ligand II0 c 613	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand WVN B 848	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA O 201	
 Bond lengths	 Bond angles
 Torsions	 Rings



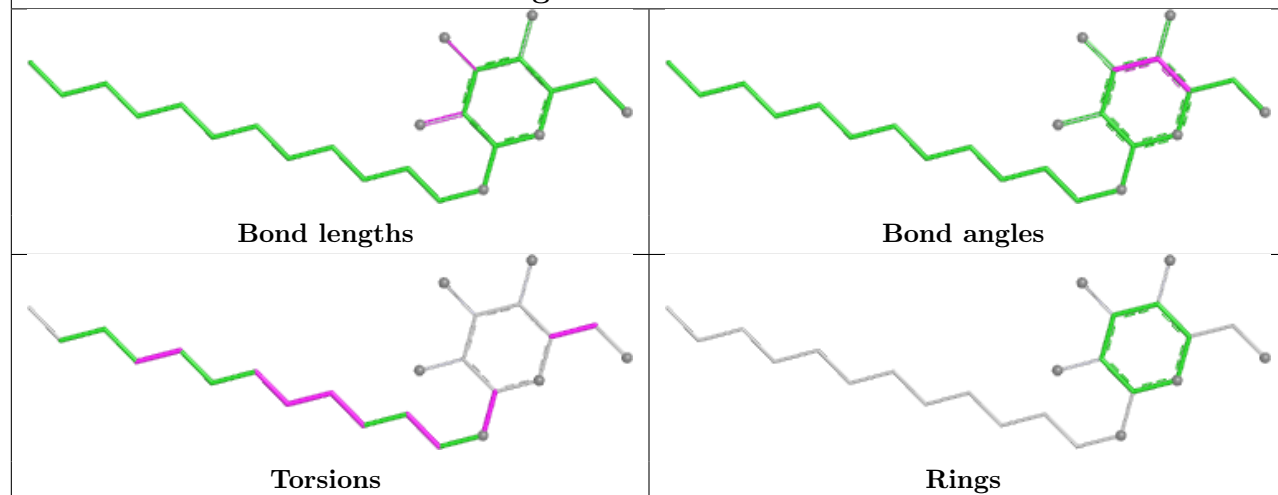




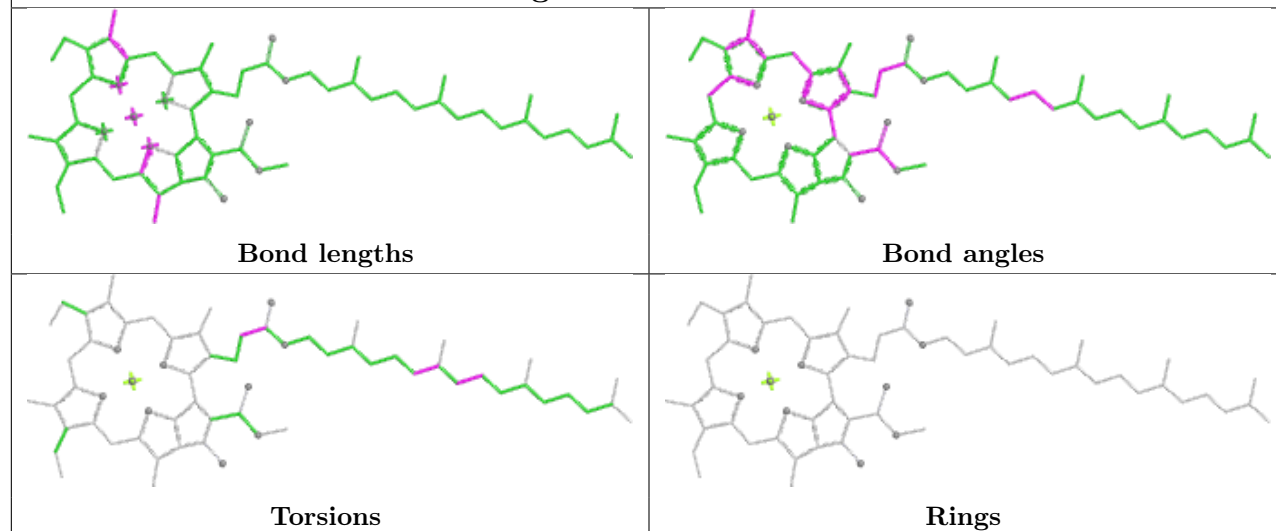
Ligand CLA c 609



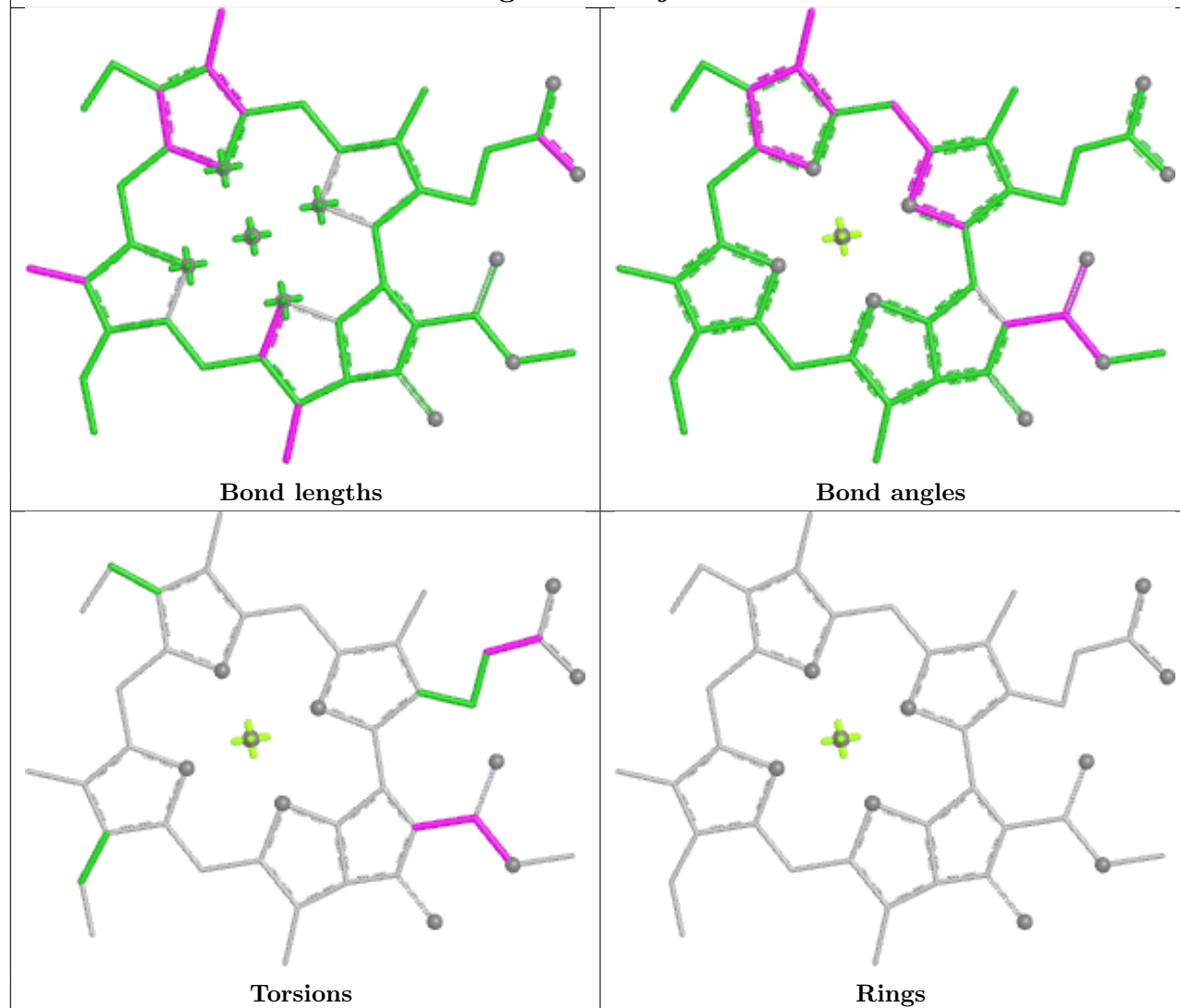
Ligand LMT b 319

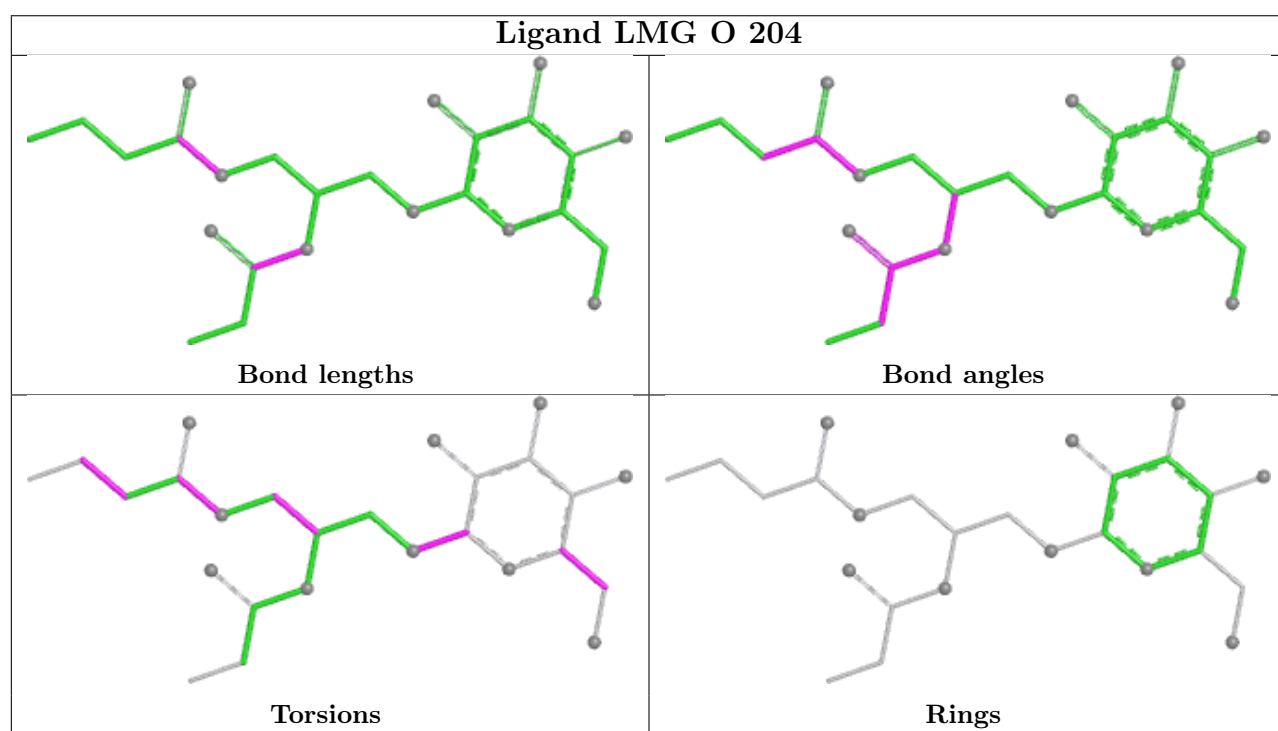
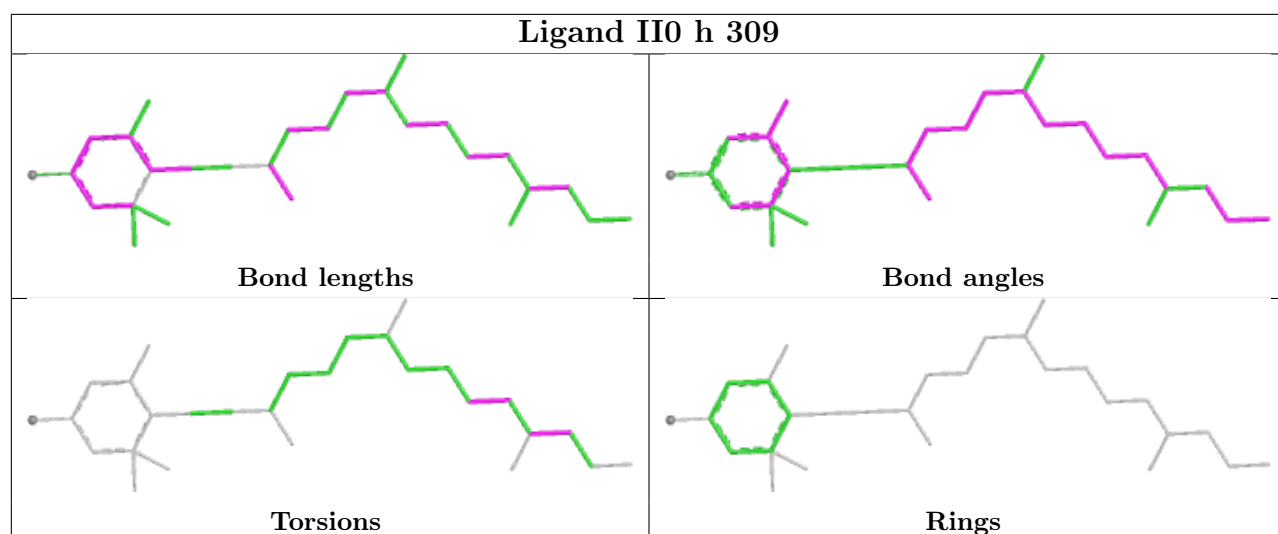


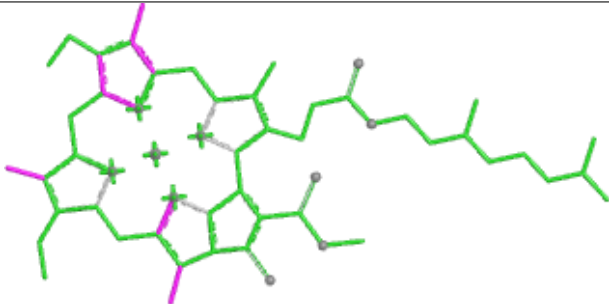
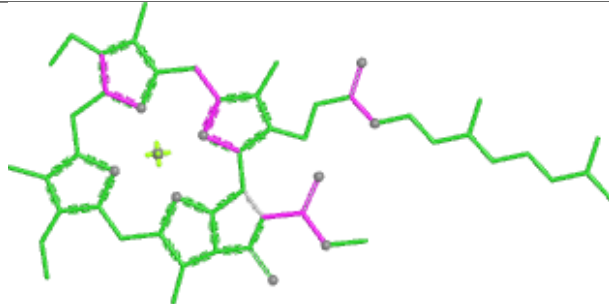
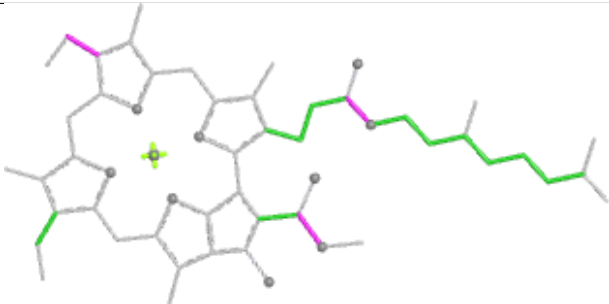
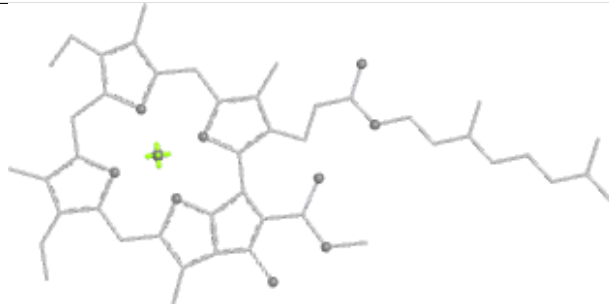
Ligand CLA A 836

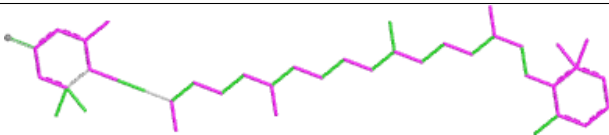
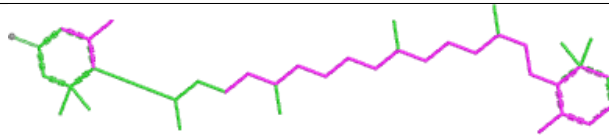
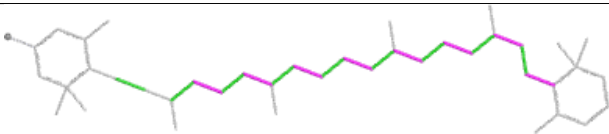
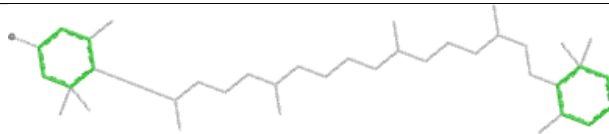


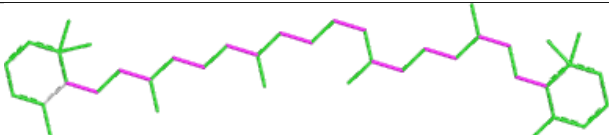
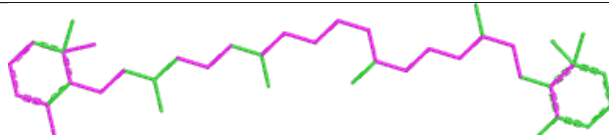
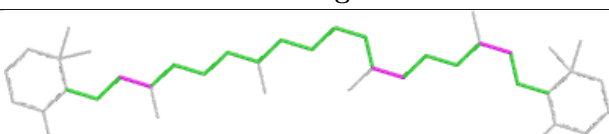
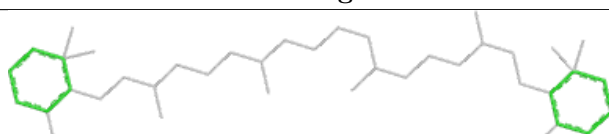
Ligand CLA j 309

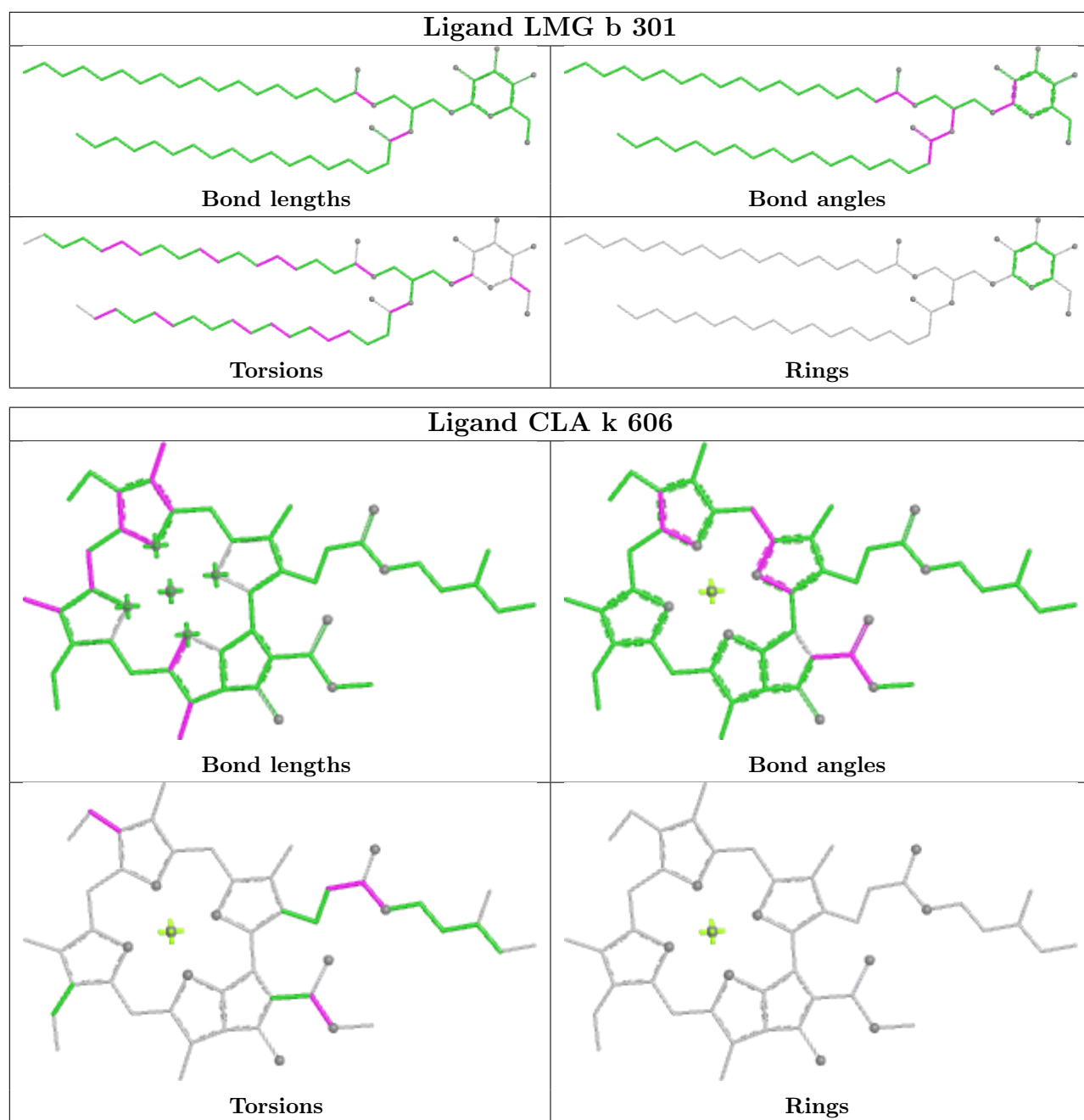




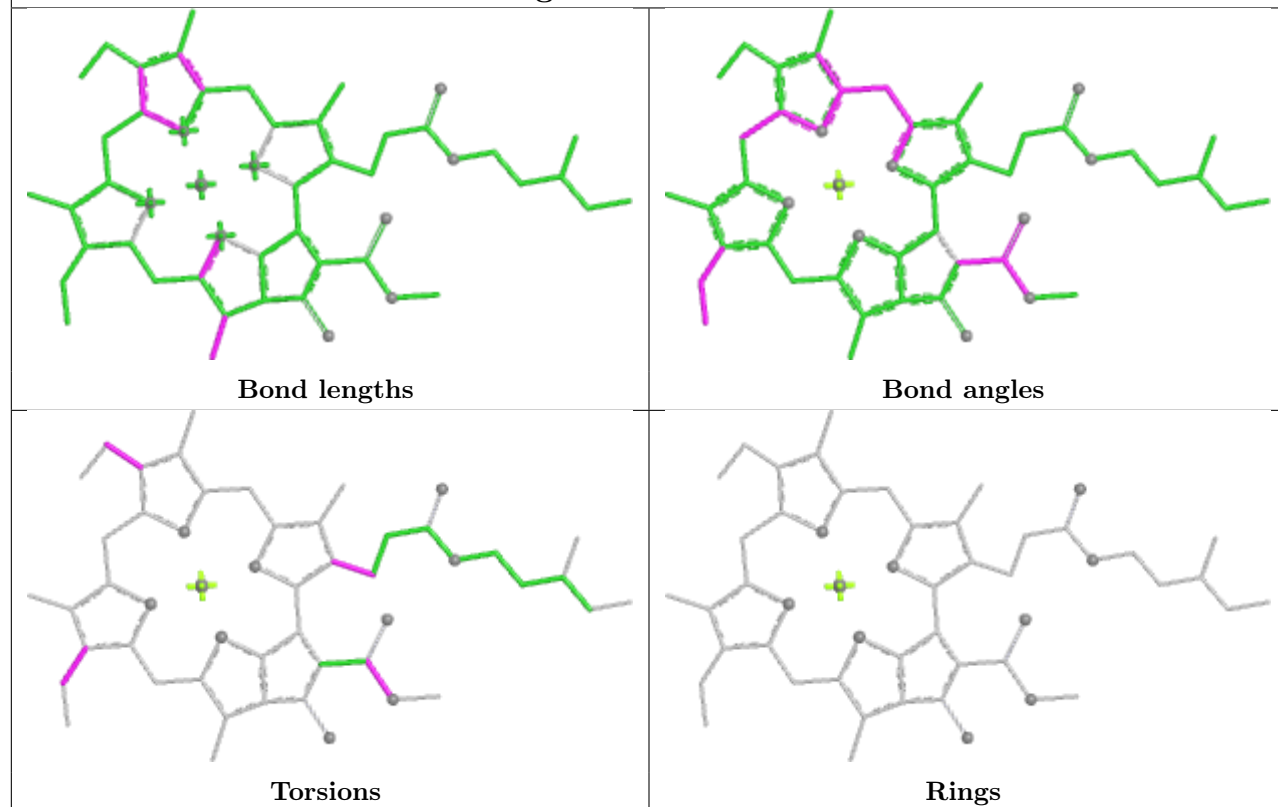
Ligand CLA A 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand IHT g 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

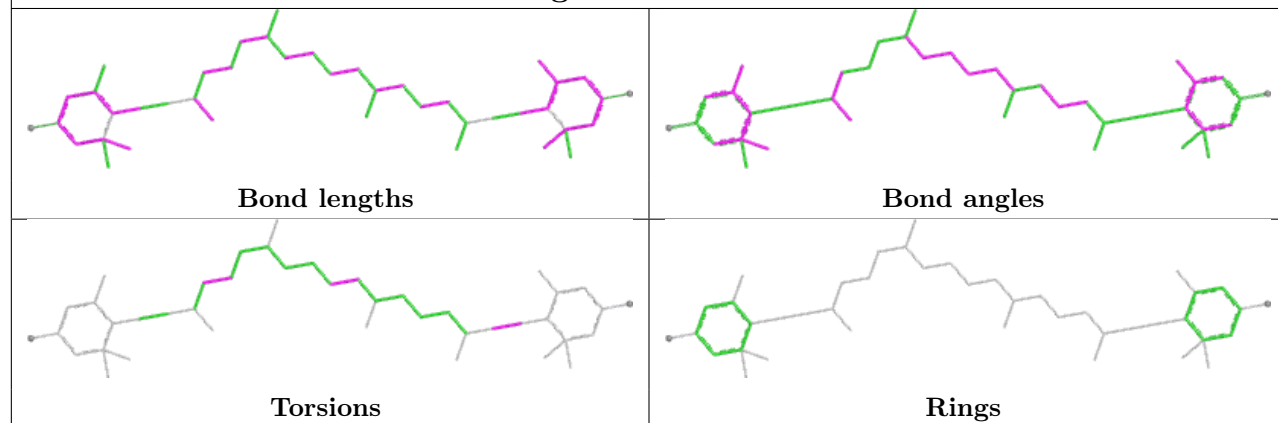
Ligand WVN R 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

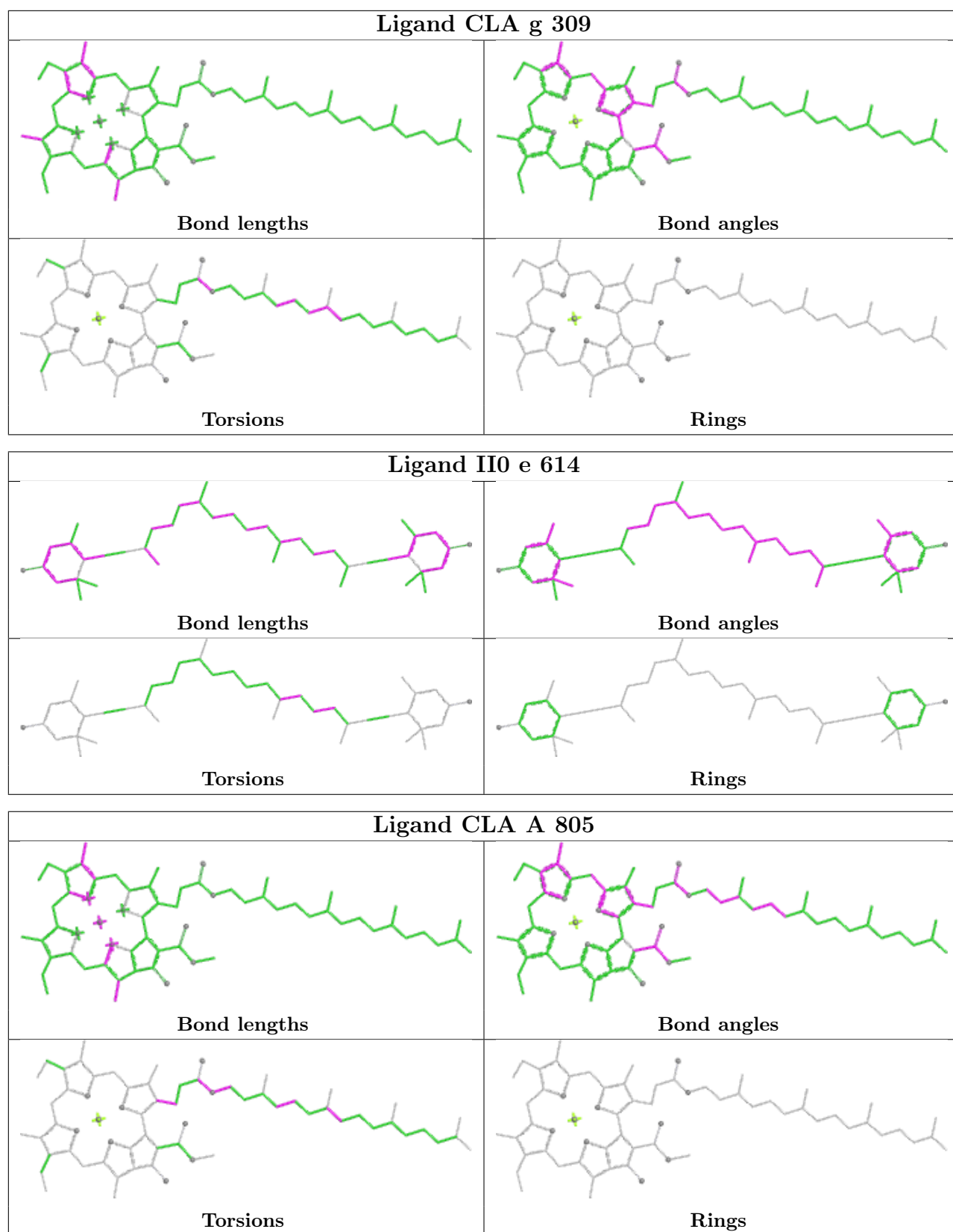


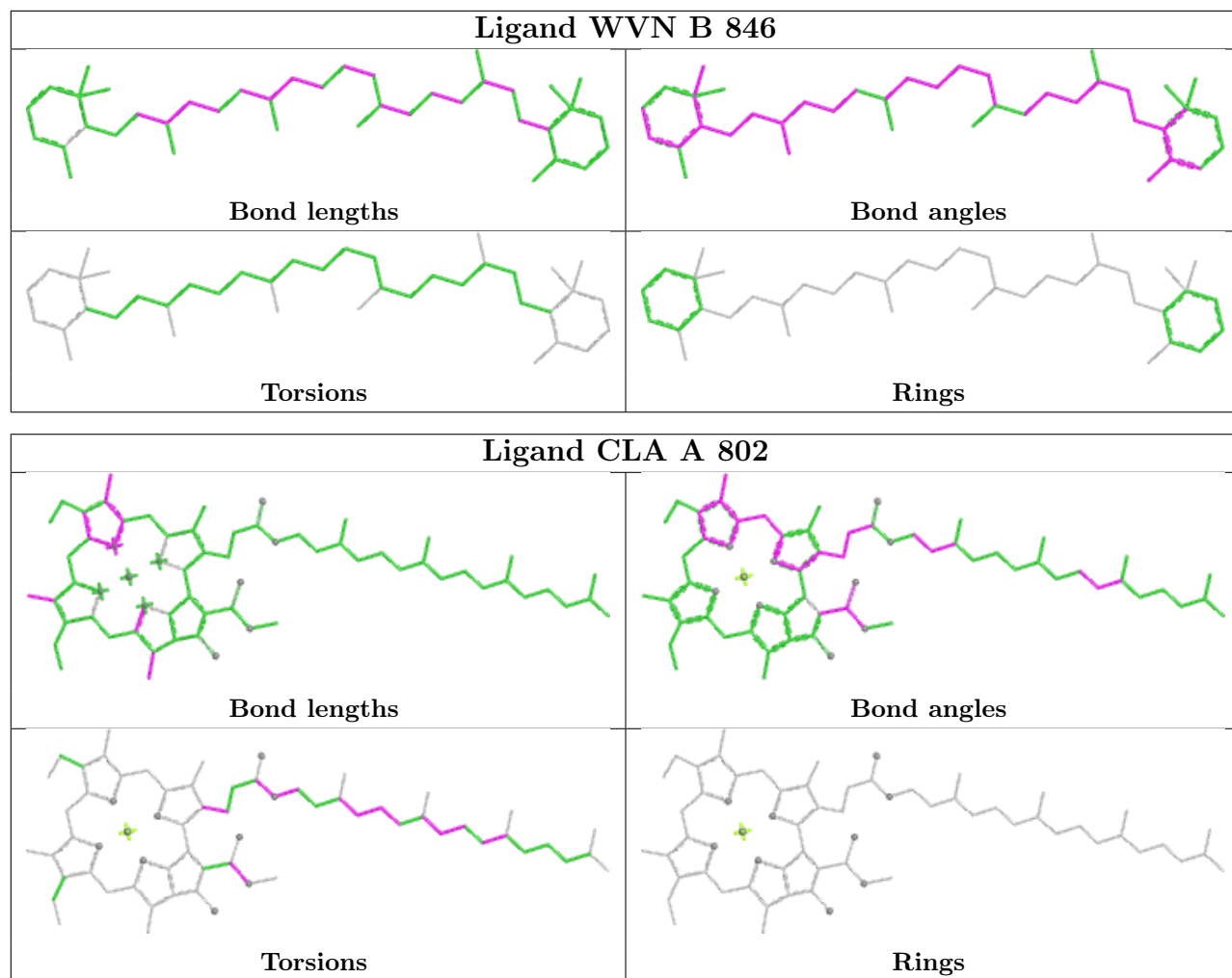
Ligand CLA k 614



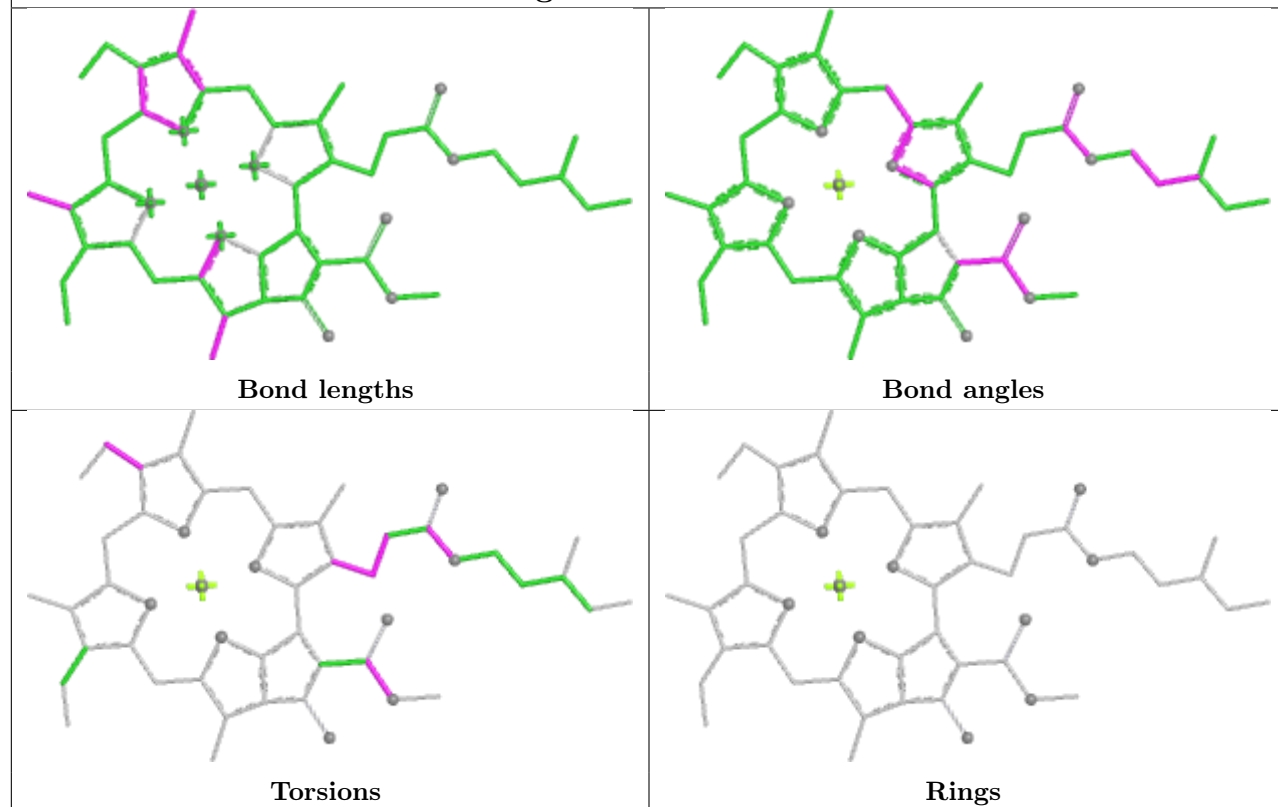
Ligand II0 a 315



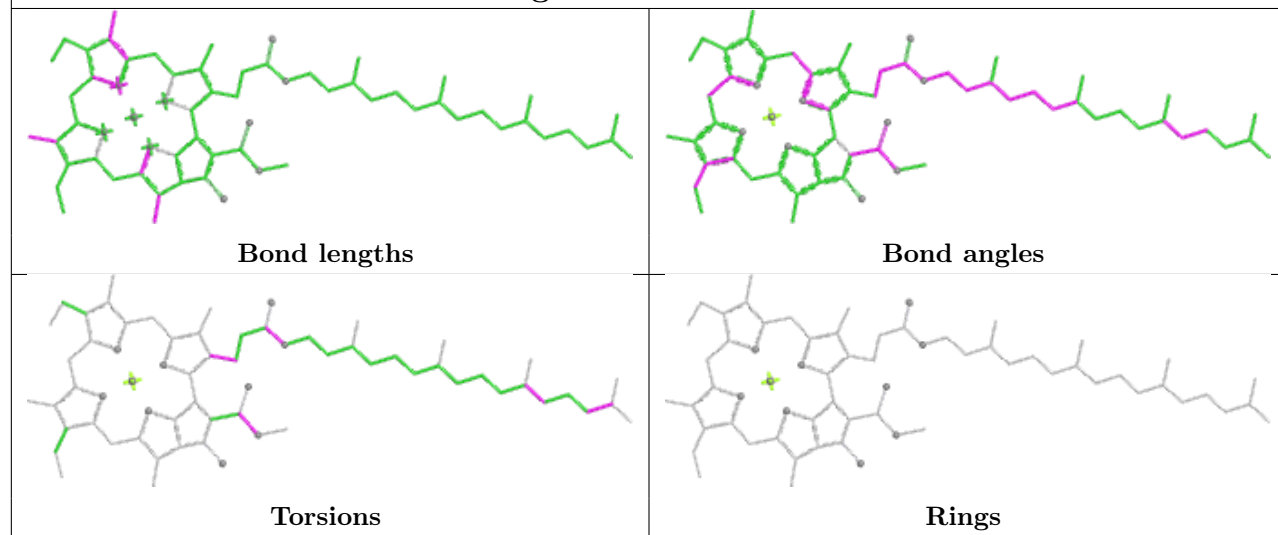


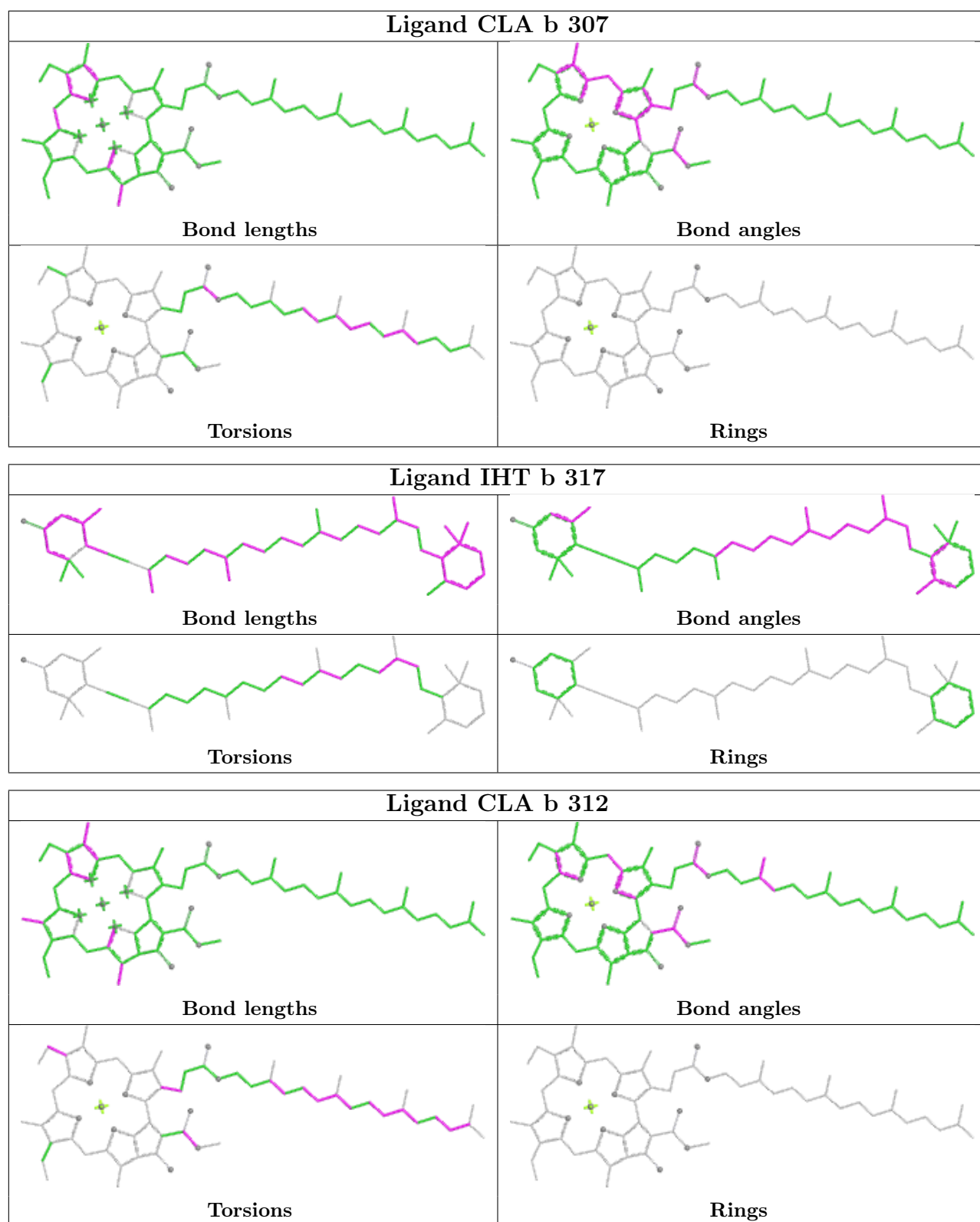


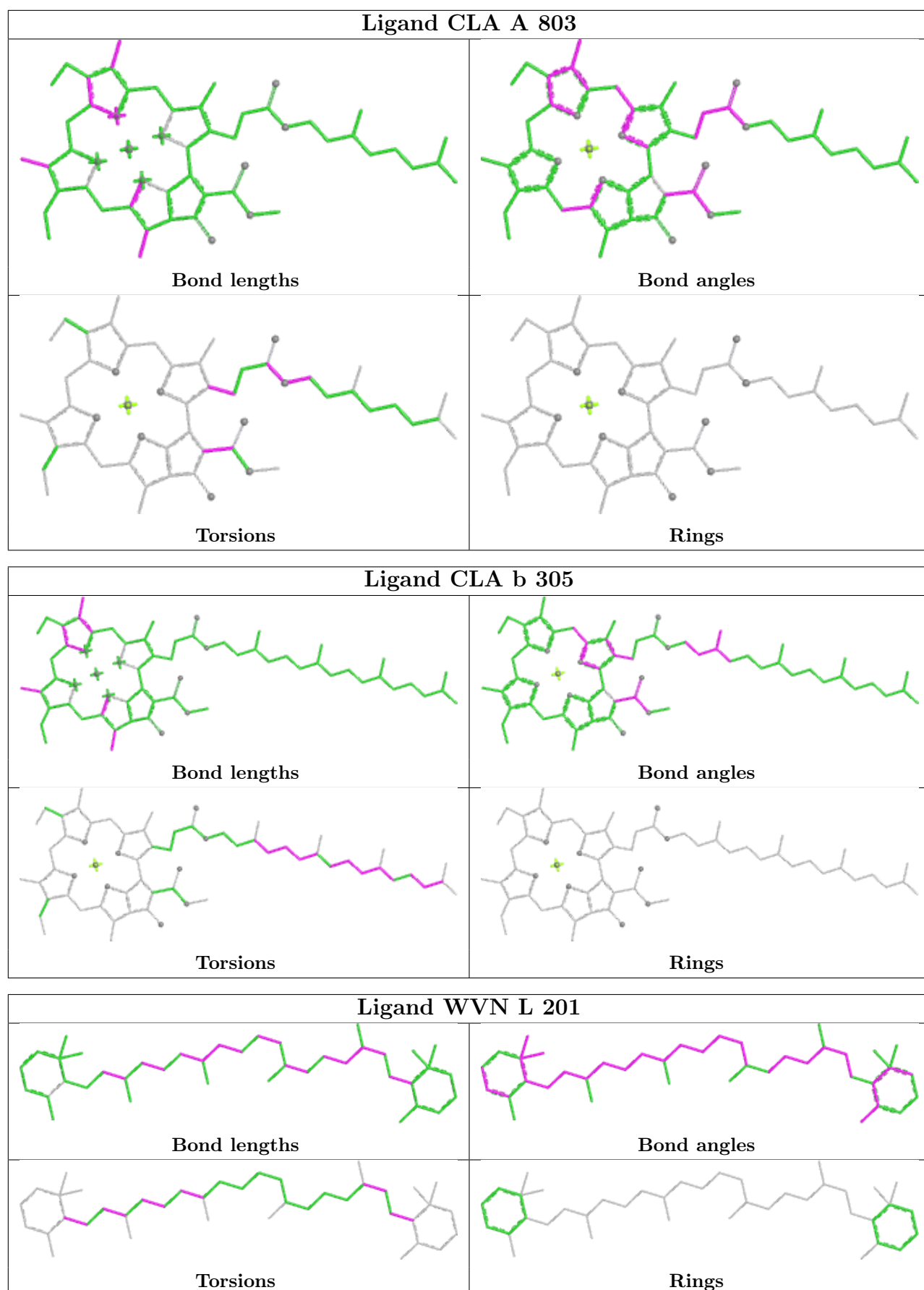
Ligand CLA k 607

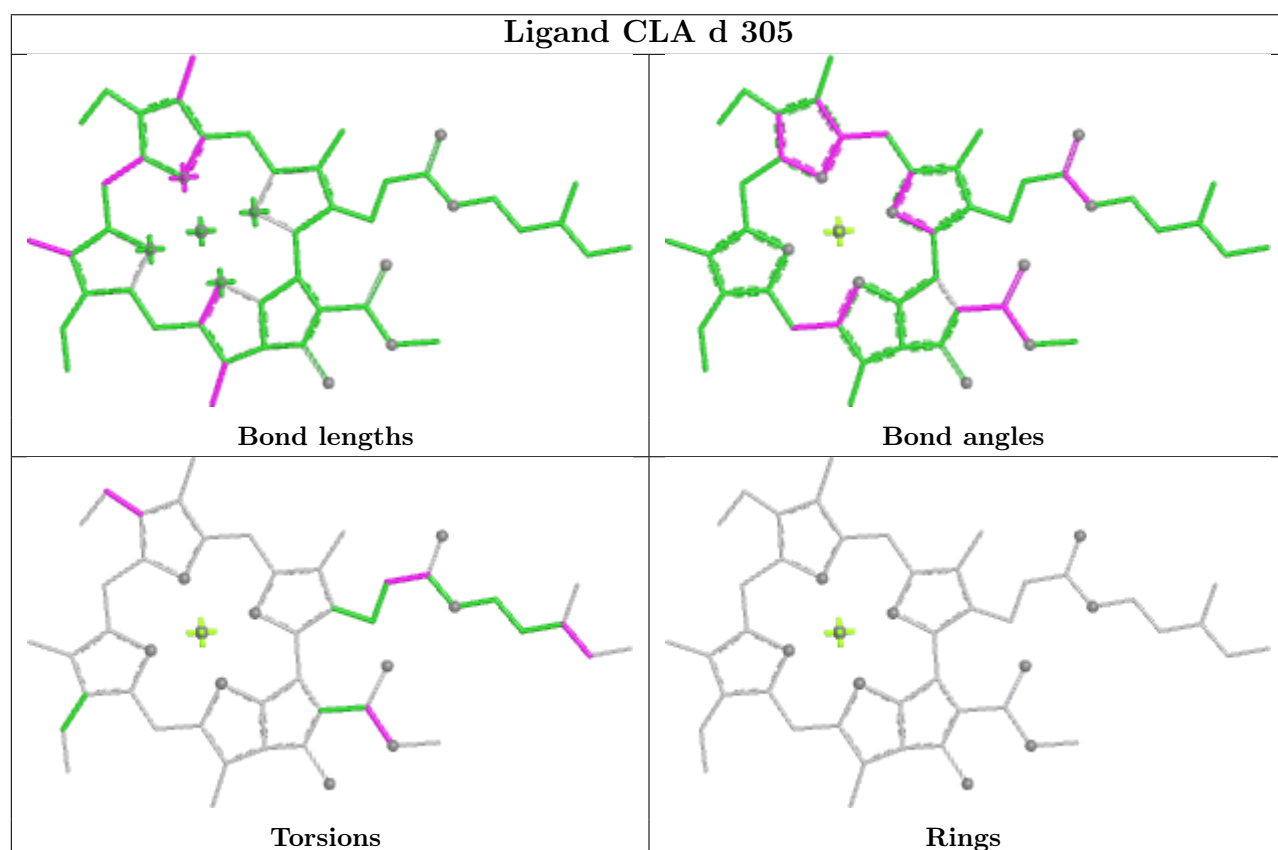
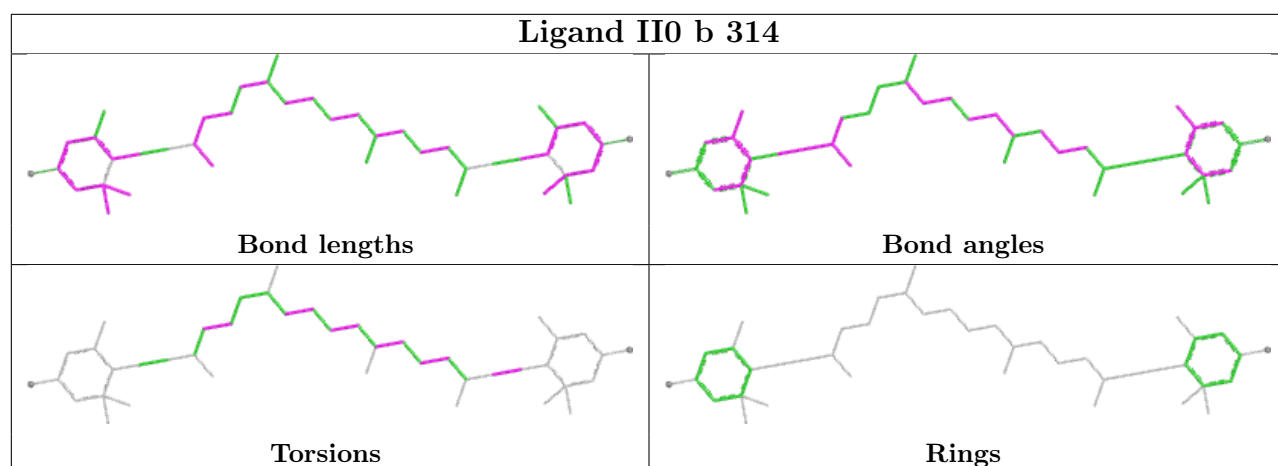


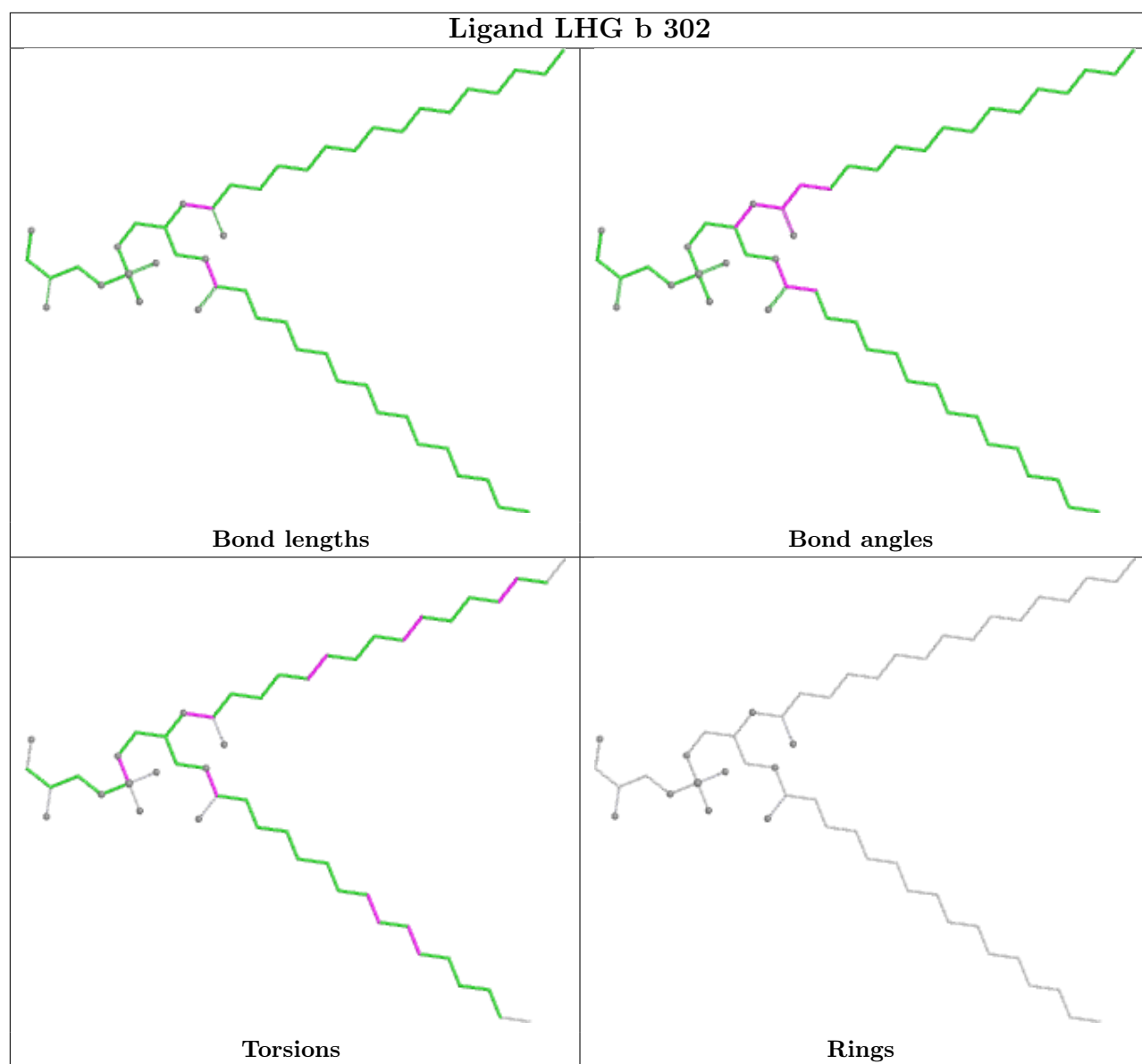
Ligand CLA A 837

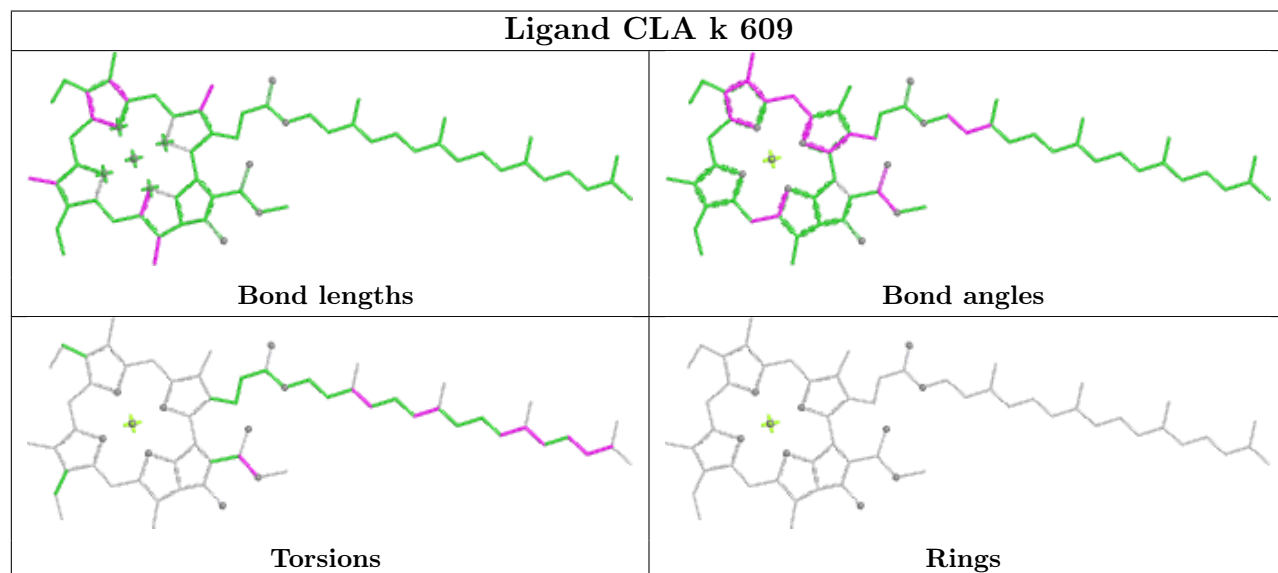
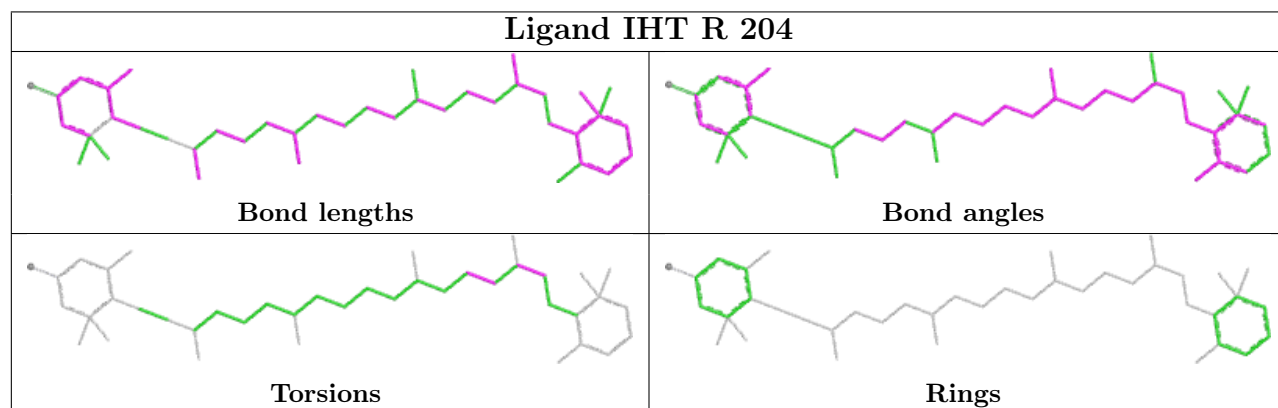
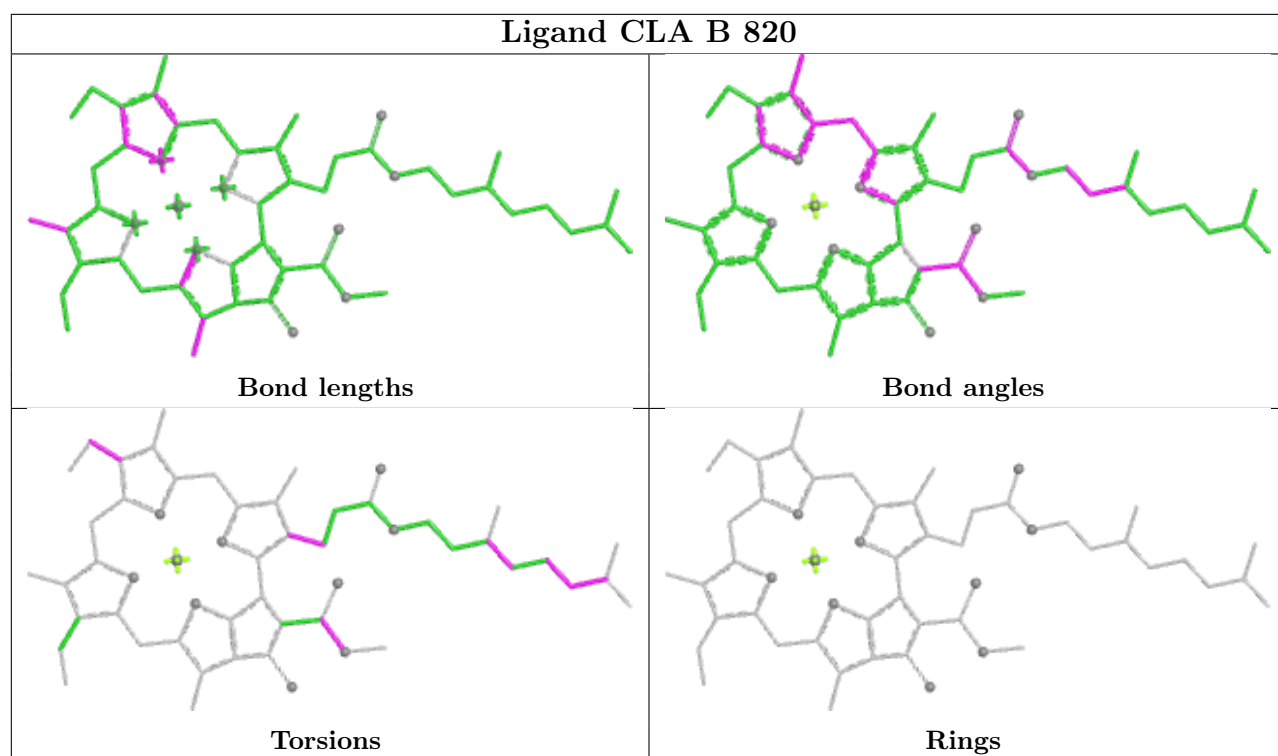


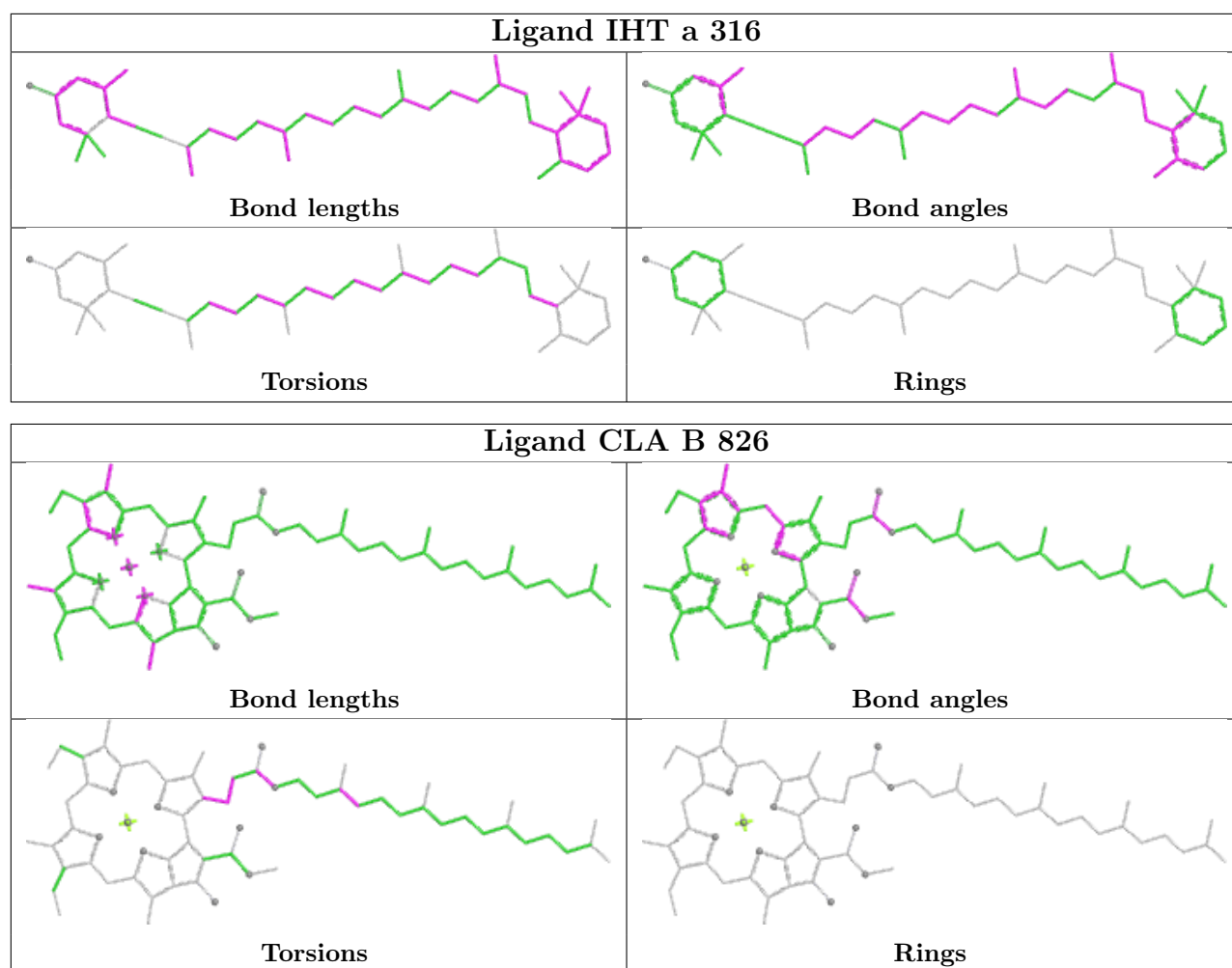




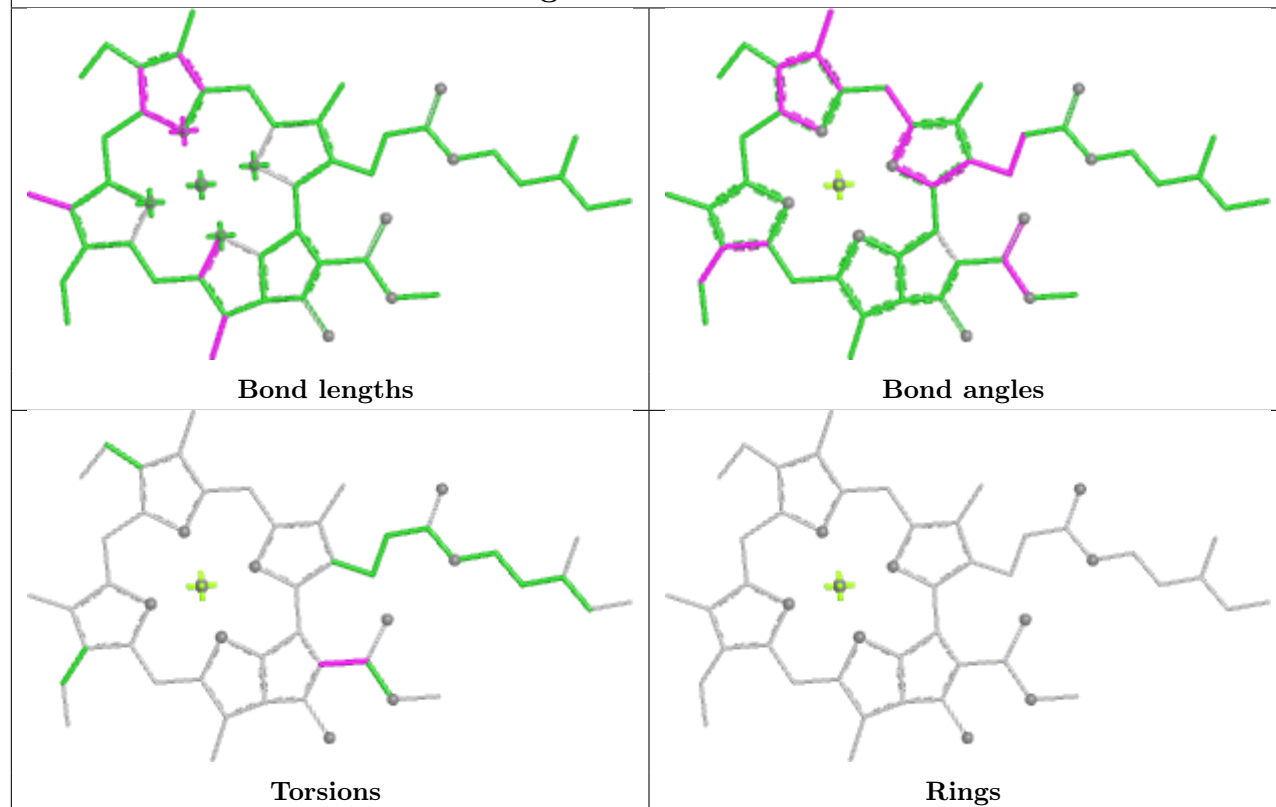




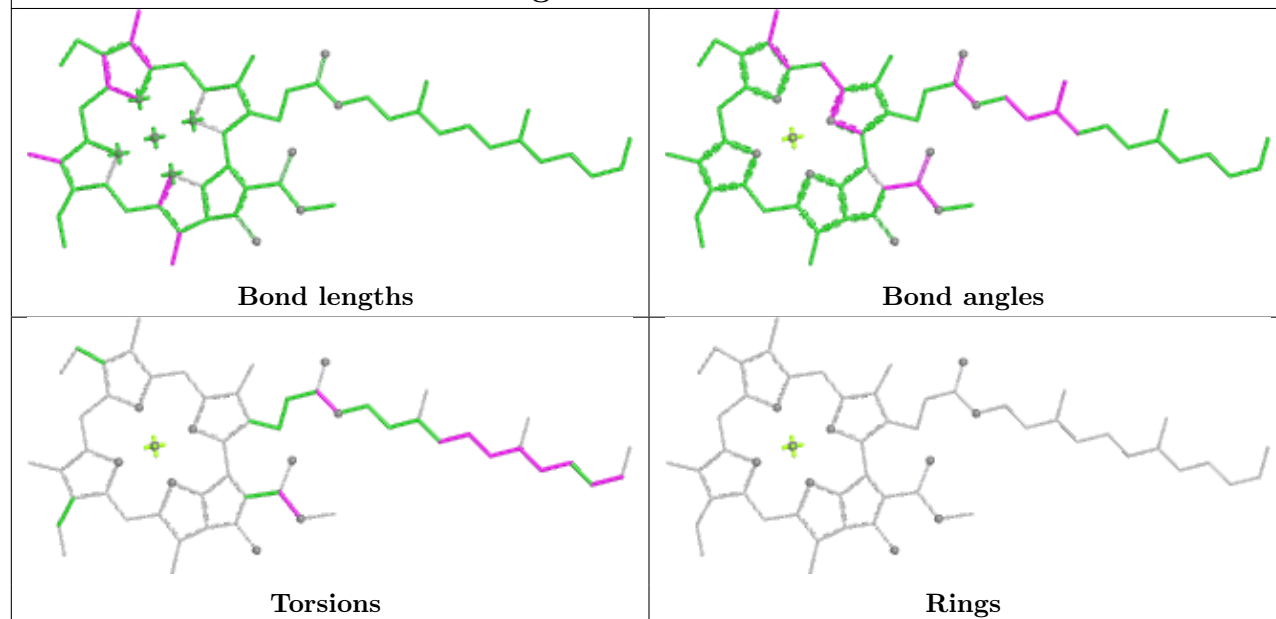


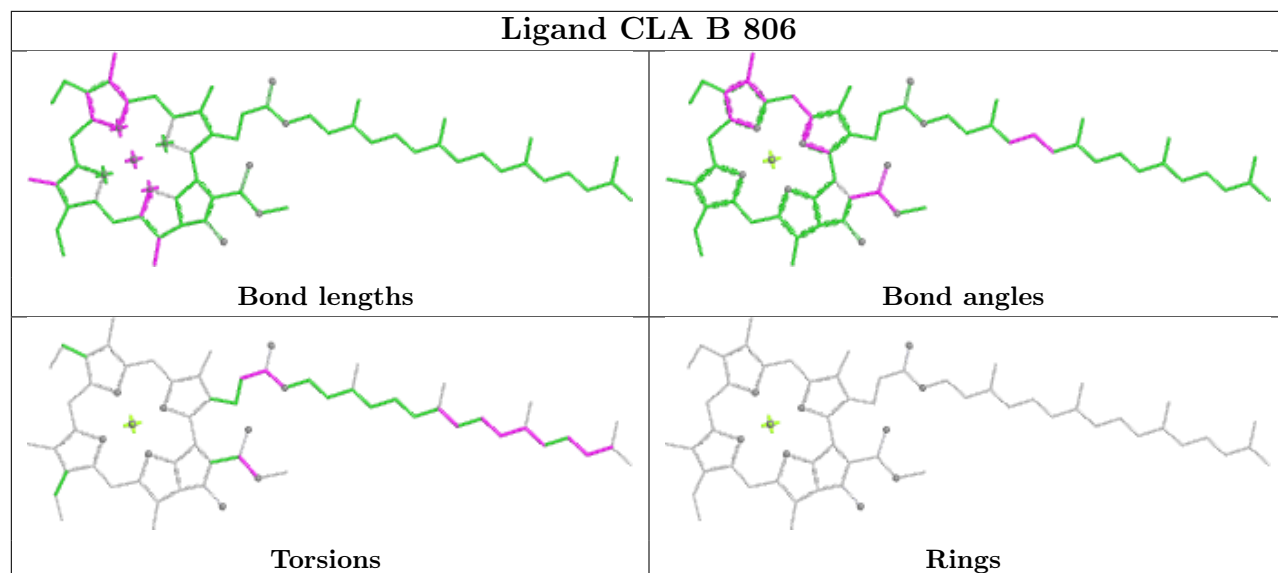
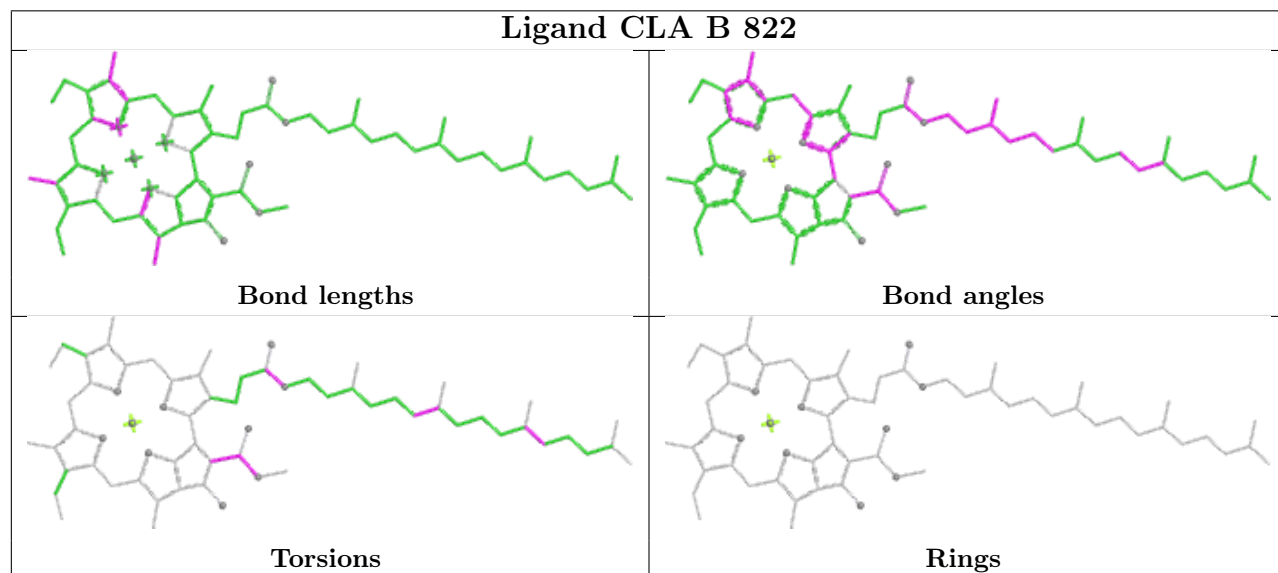
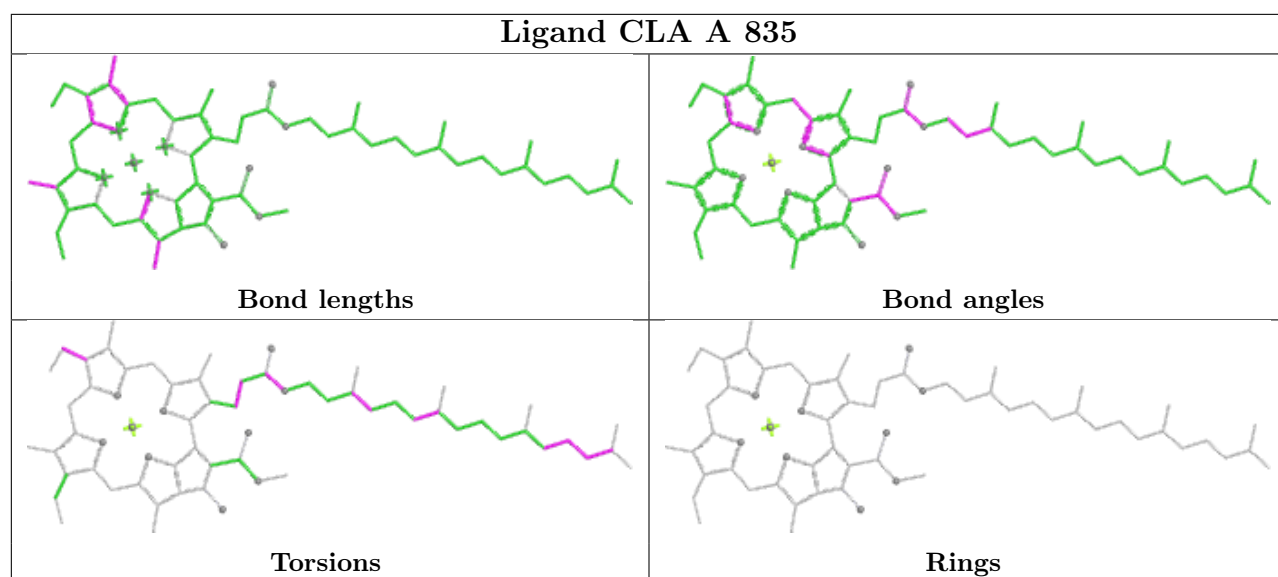


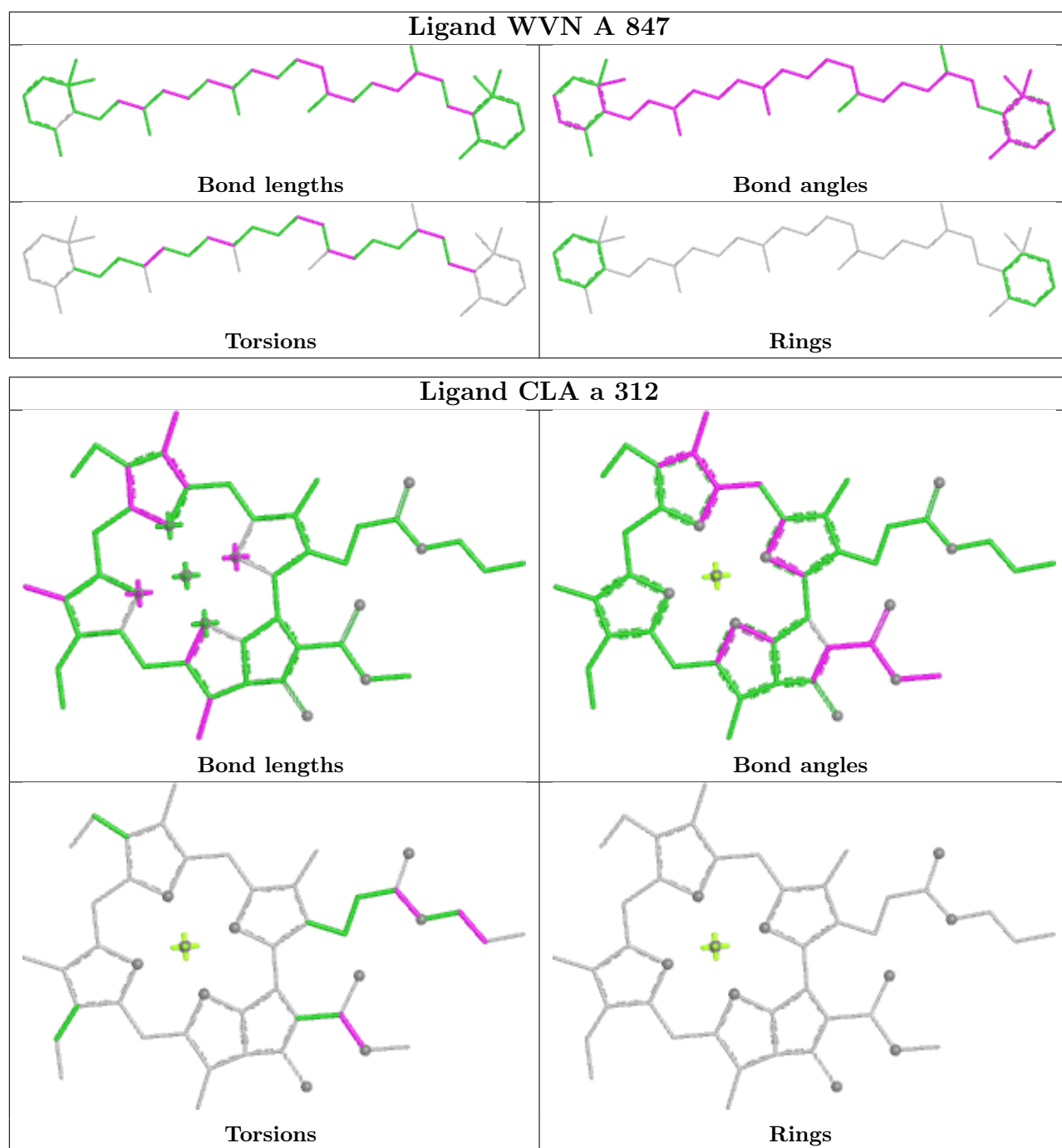
Ligand CLA i 607



Ligand CLA B 814







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.

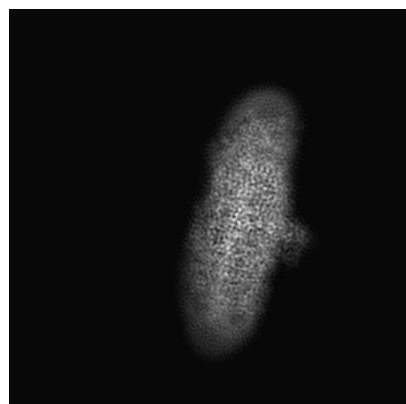
6 Map visualisation [i](#)

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.

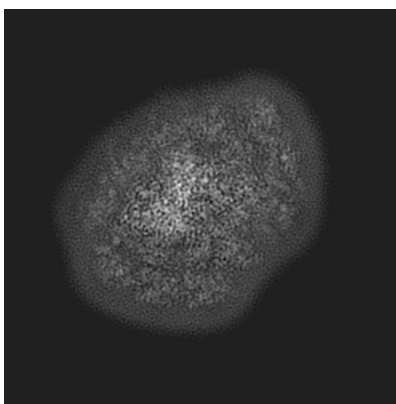
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

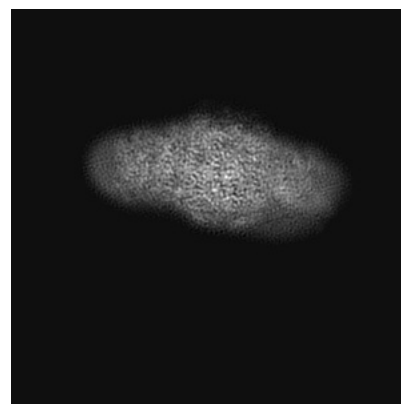
6.1.1 Primary map



X

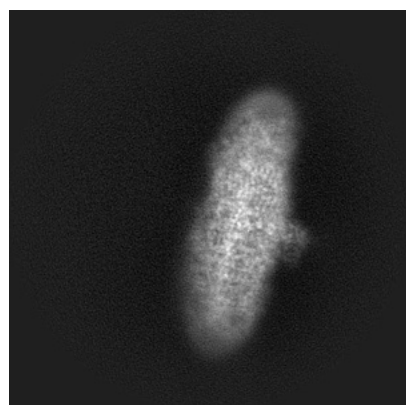


Y

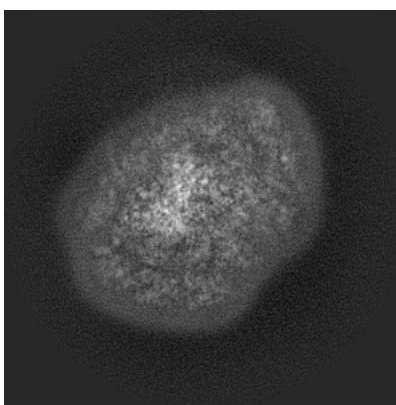


Z

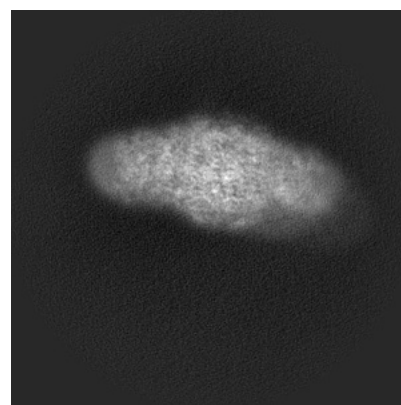
6.1.2 Raw map



X



Y

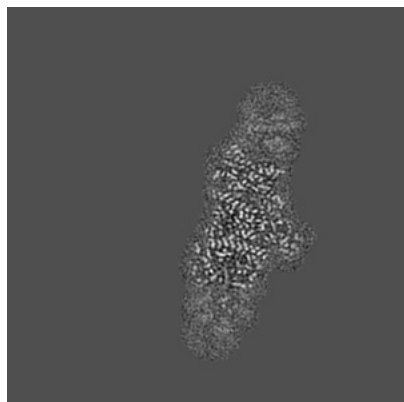


Z

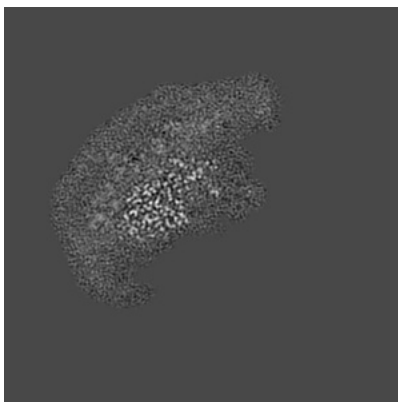
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

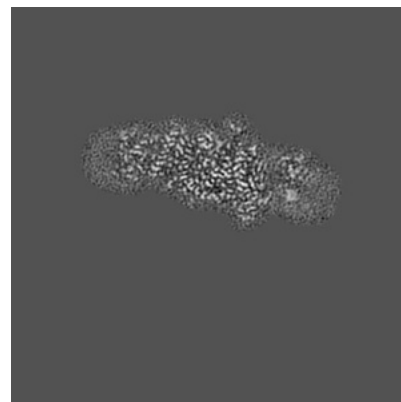
6.2.1 Primary map



X Index: 160

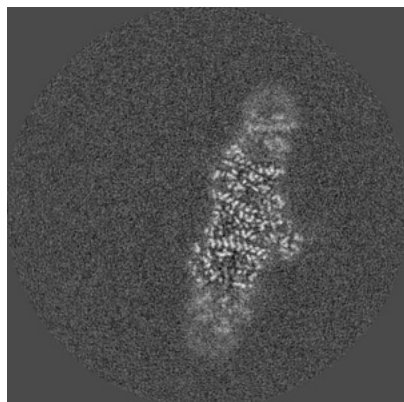


Y Index: 160

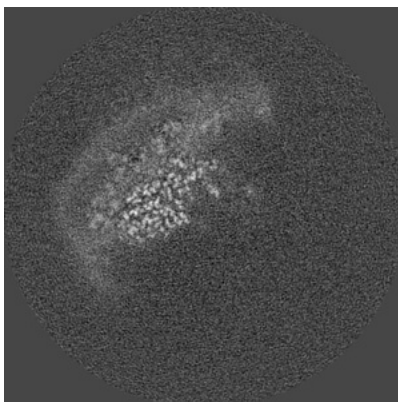


Z Index: 160

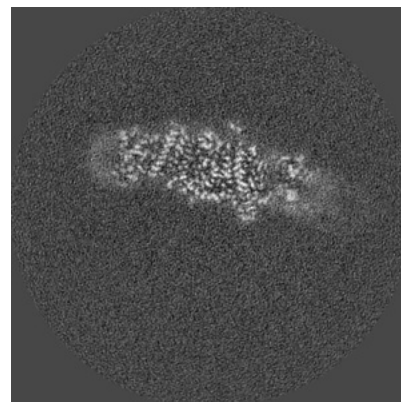
6.2.2 Raw map



X Index: 160



Y Index: 160

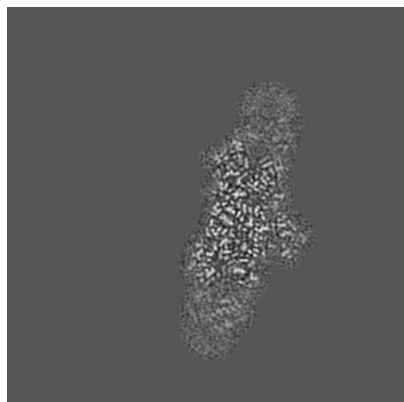


Z Index: 160

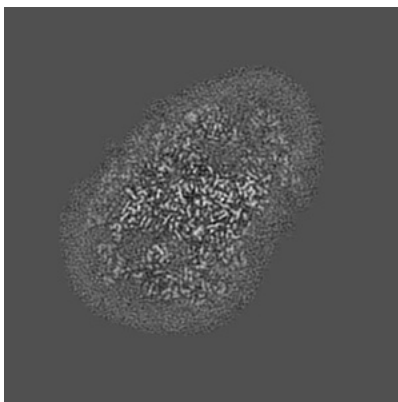
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

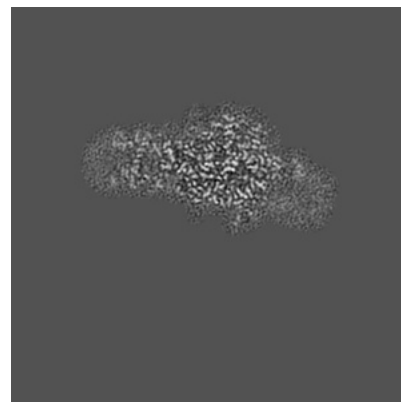
6.3.1 Primary map



X Index: 164

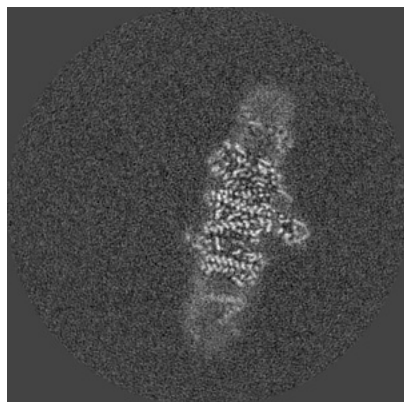


Y Index: 185

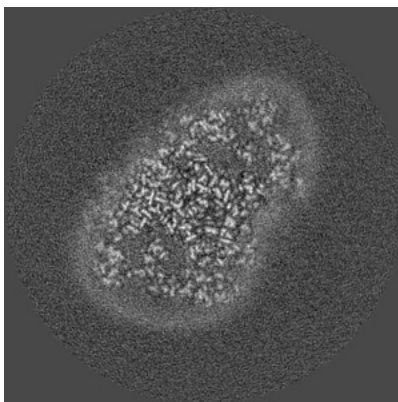


Z Index: 148

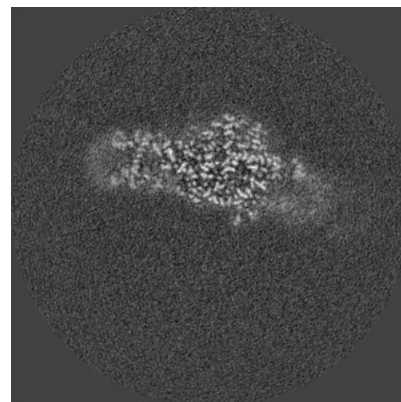
6.3.2 Raw map



X Index: 173



Y Index: 189

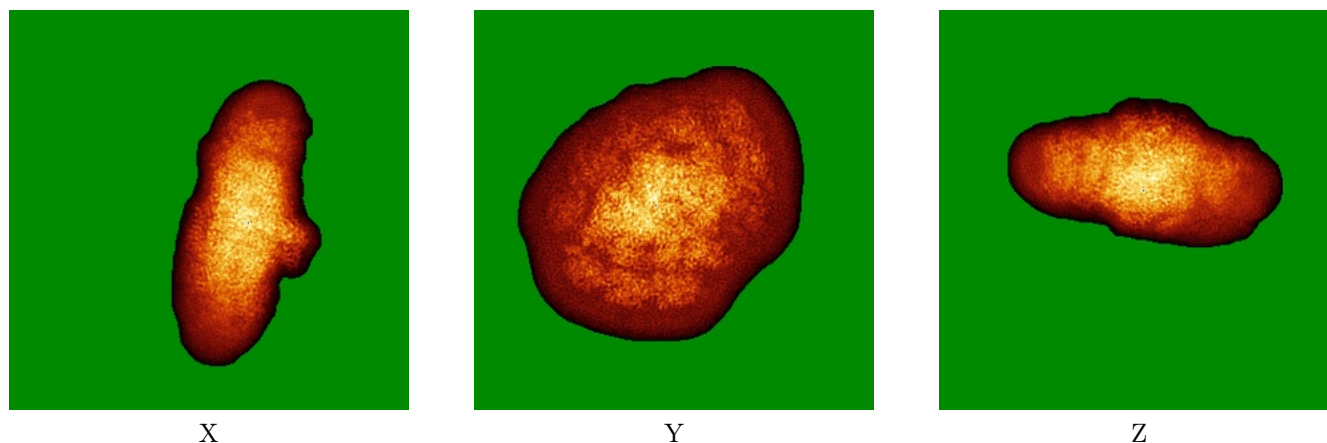


Z Index: 148

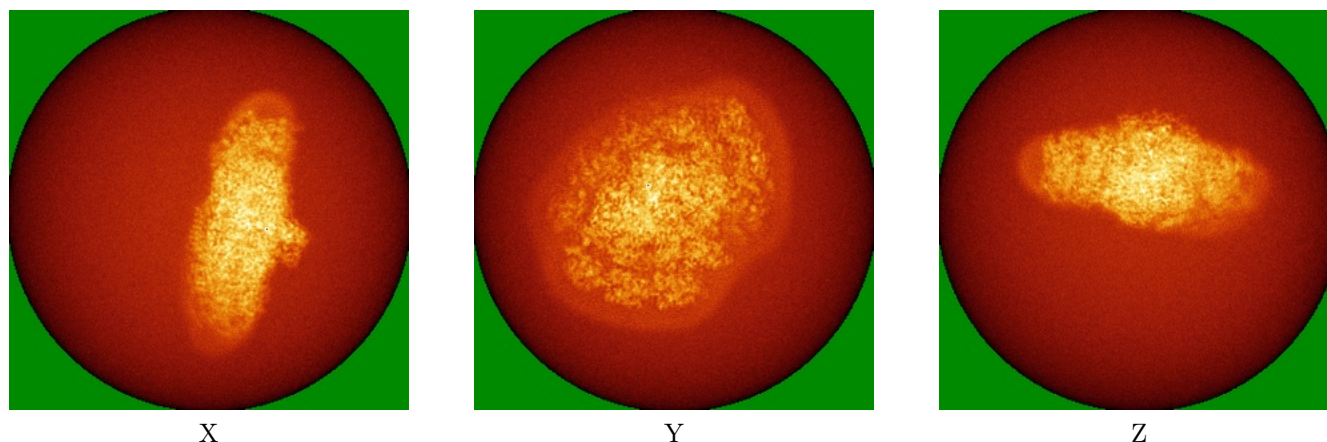
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

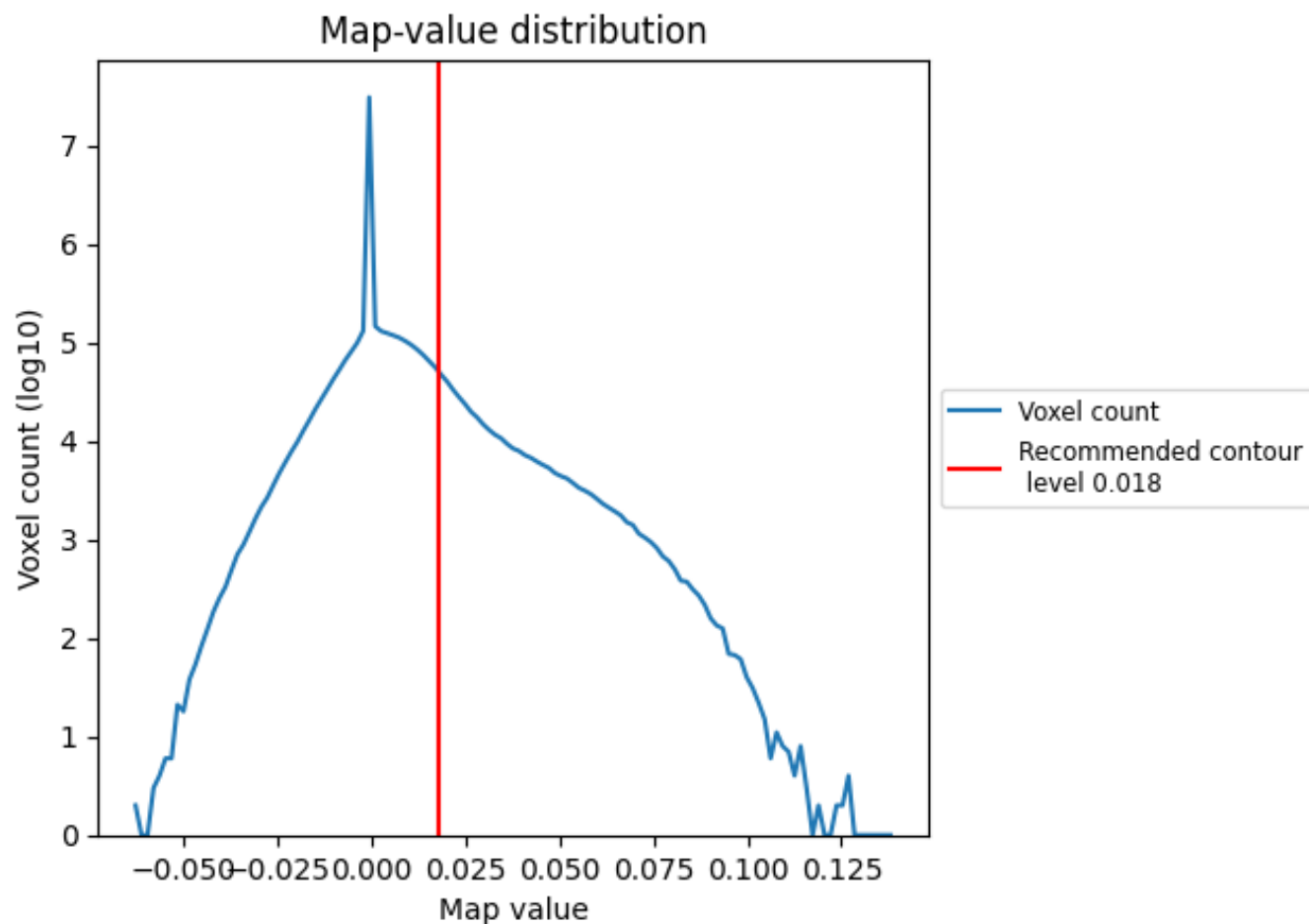
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

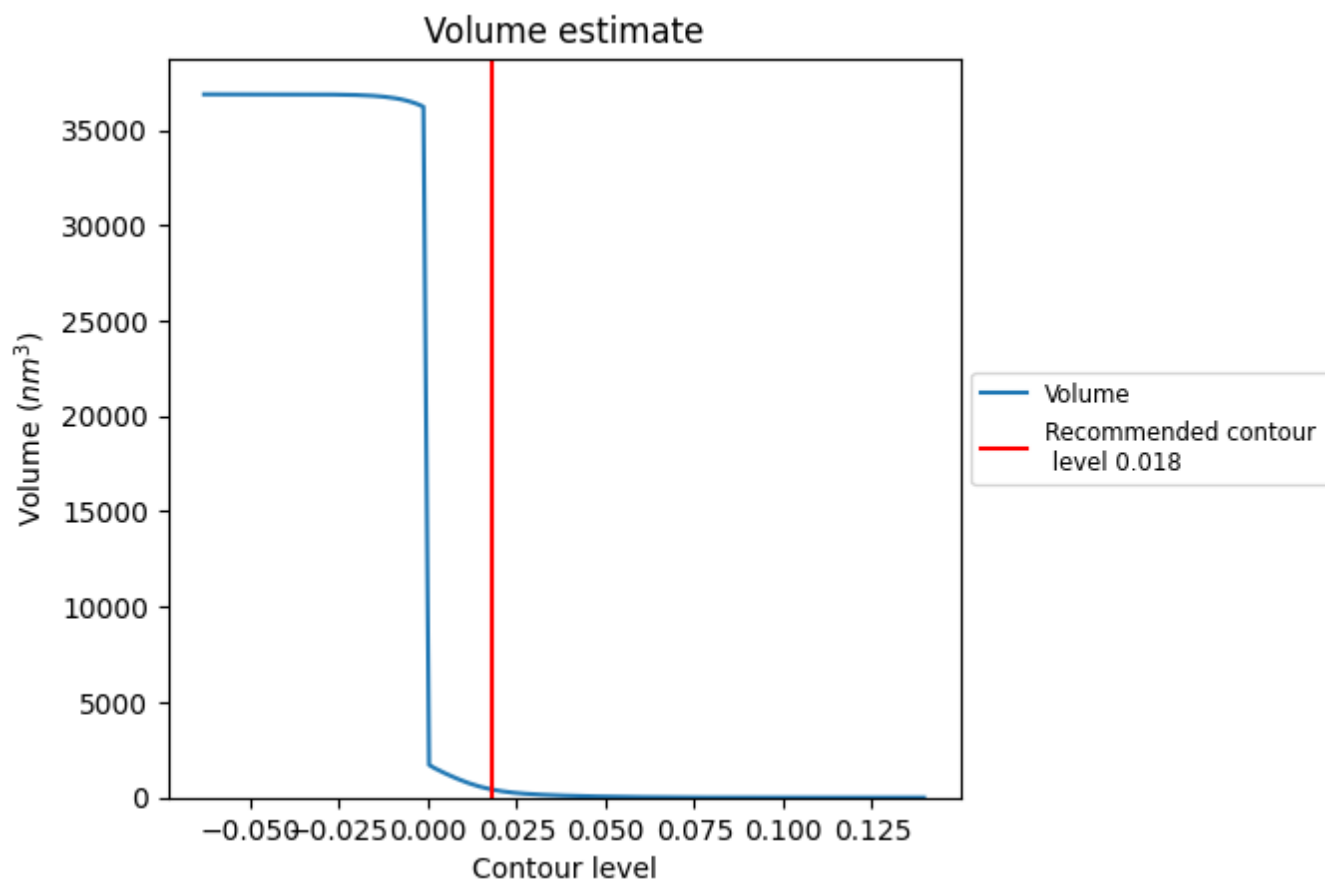
This section contains the results of statistical analysis of the map.

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.

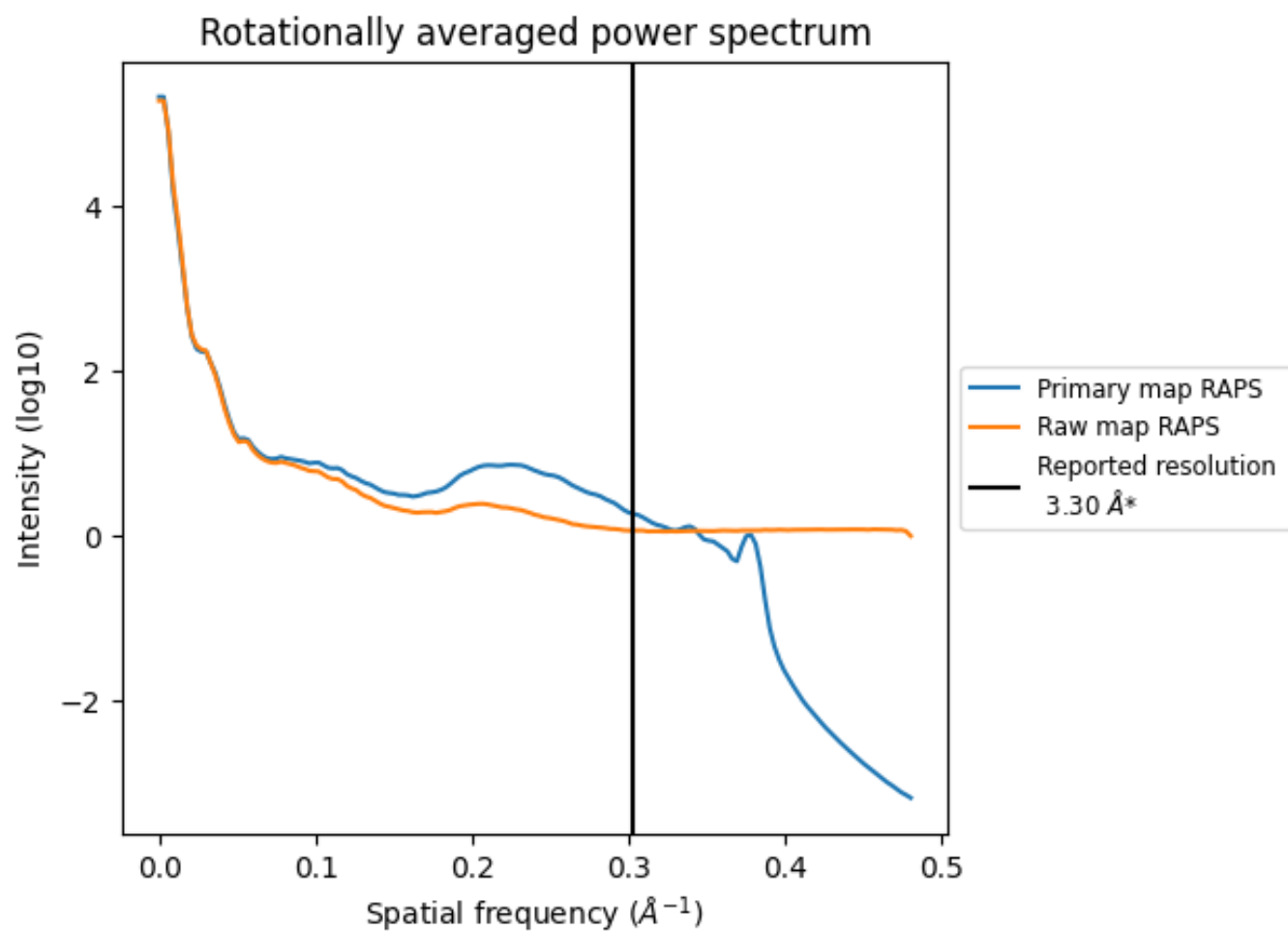
7.2 Volume estimate [i](#)



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 ⓘ

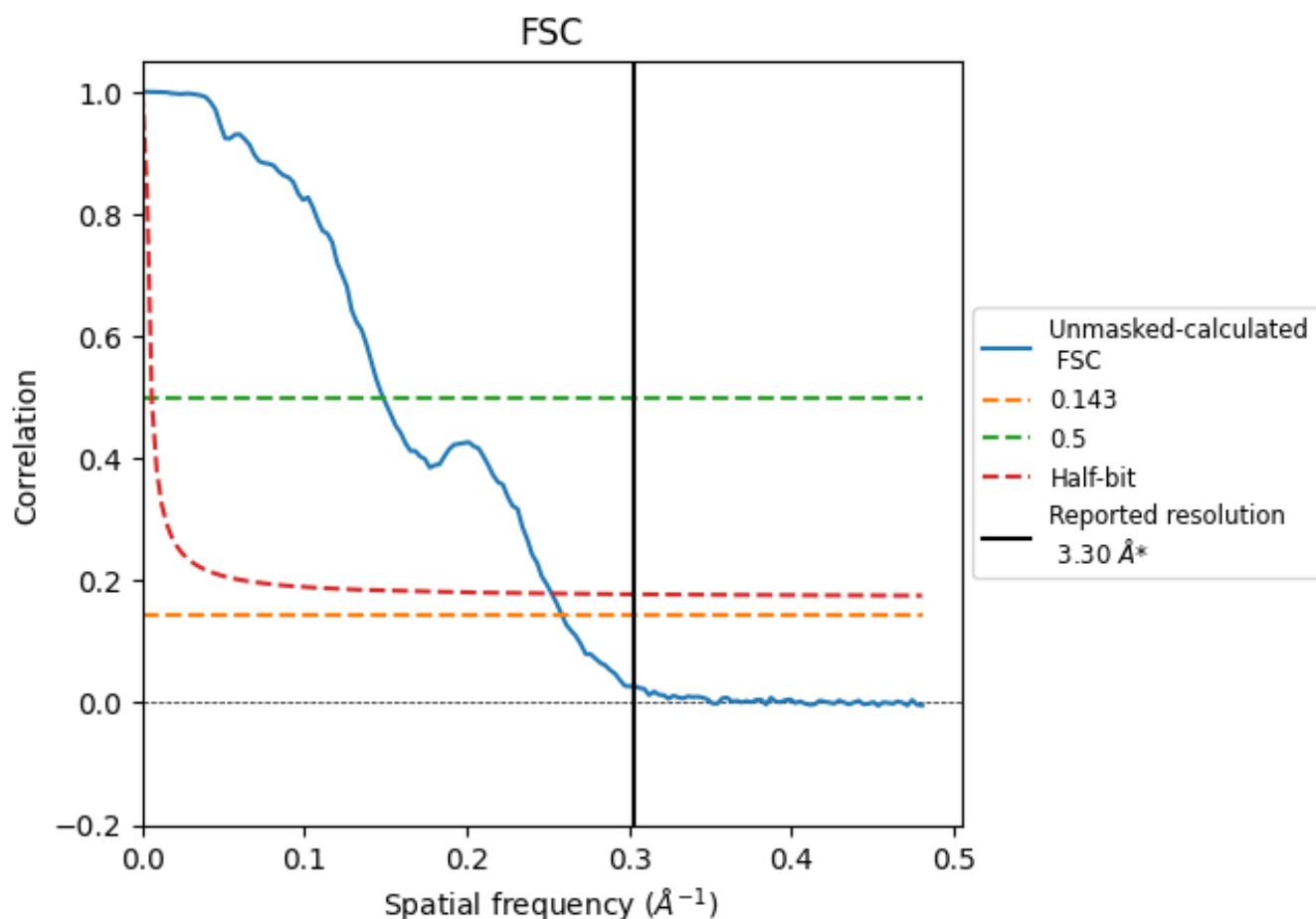


*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

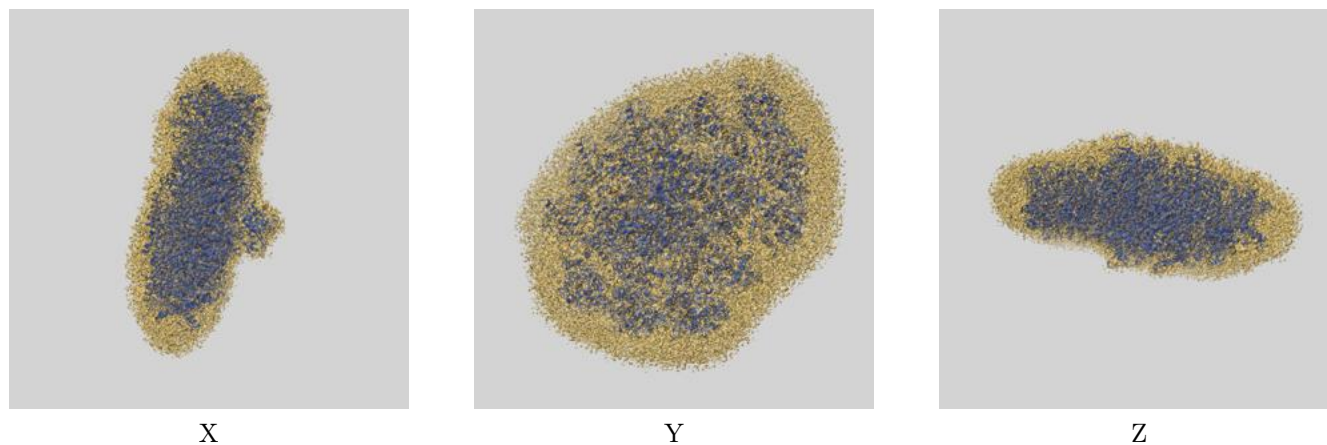
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	6.73	3.96

*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](#)

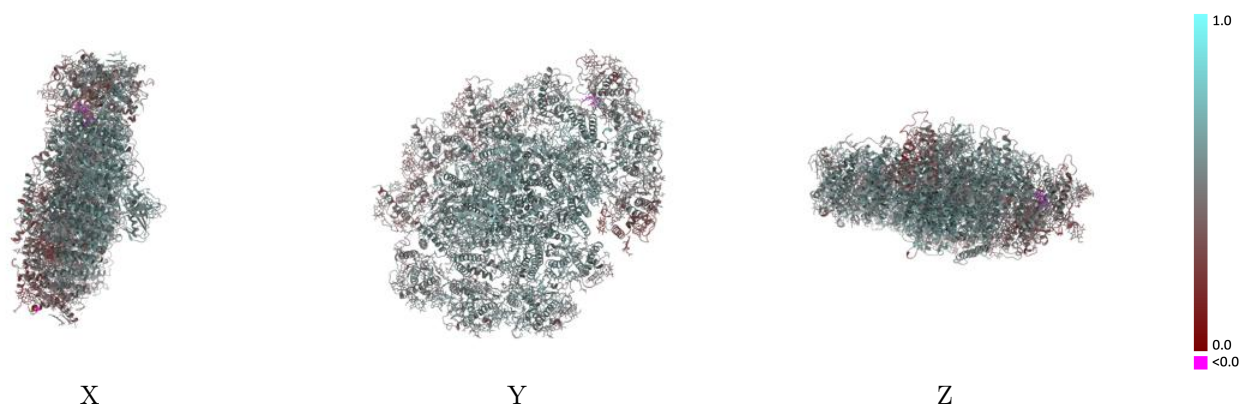
This section contains information regarding the fit between EMDB map EMD-37660 and PDB model 8WMW. Per-residue inclusion information can be found in section [3](#) on page [36](#).

9.1 Map-model overlay [i](#)



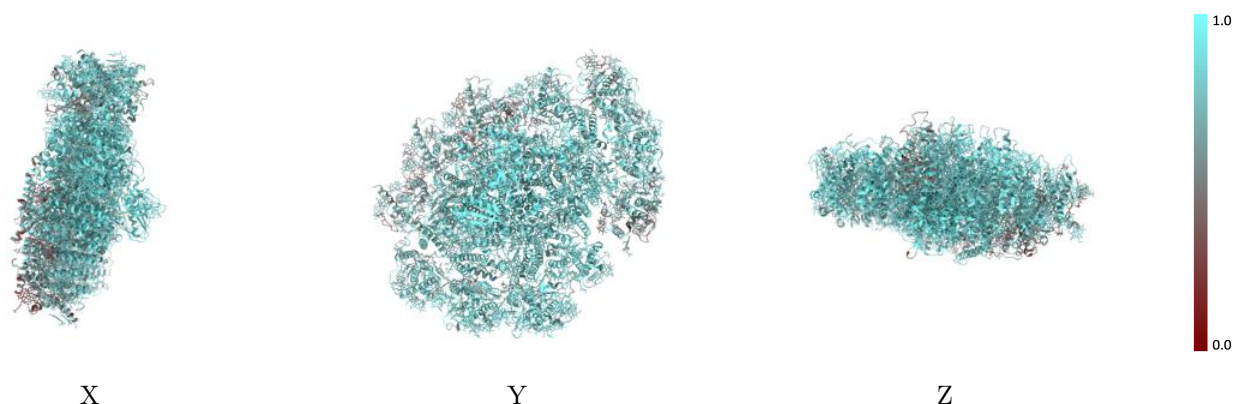
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



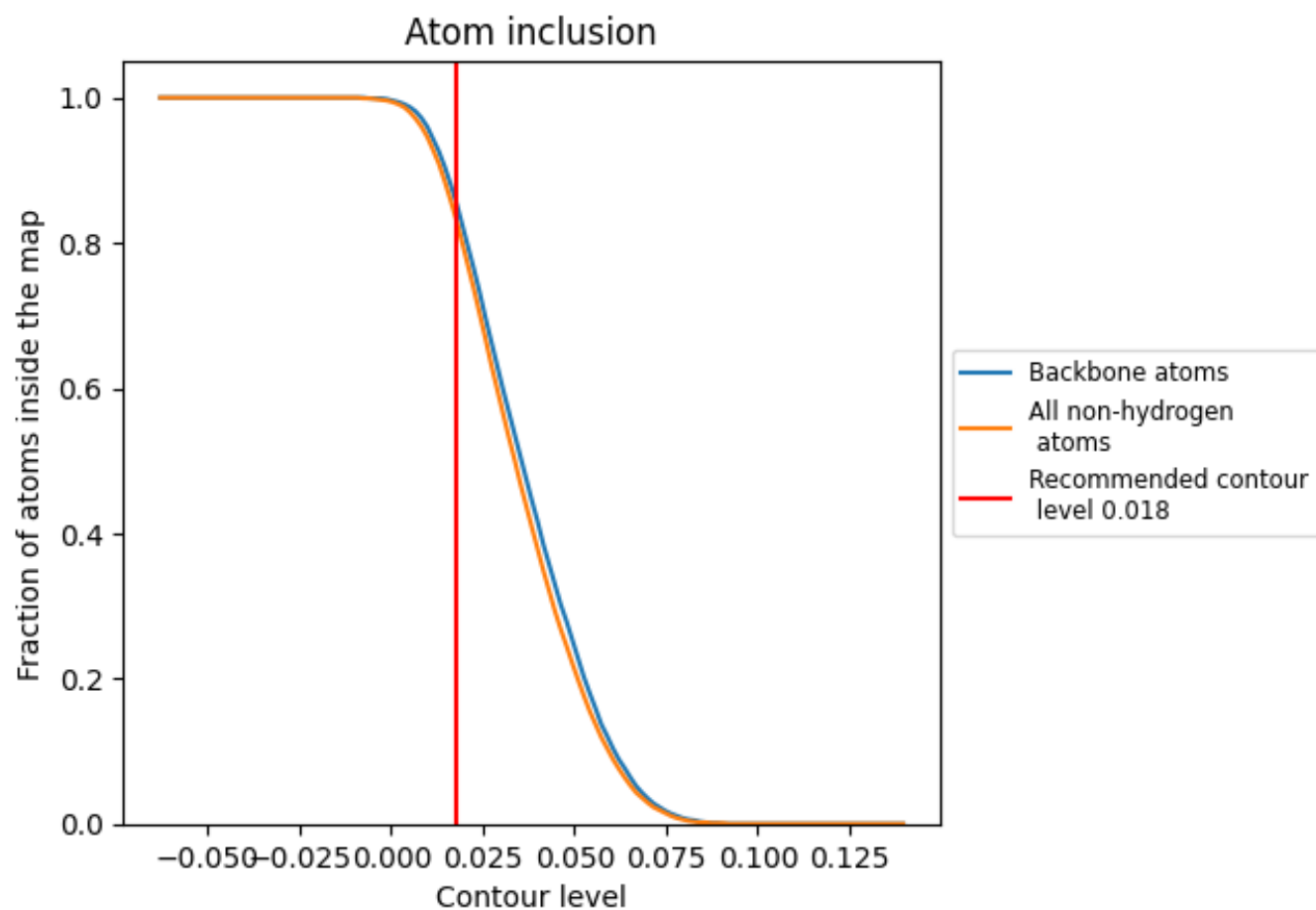
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

