



wwPDB EM Validation Summary Report ⓘ

Aug 7, 2026 – 01:56 AM JST

PDB ID : 9KZ9 / pdb_00009kz9
EMDB ID : EMD-62656
Title : Cryo-EM structure of PSI-ACPI from Rhodomonas sp. NIES-2332 at 2.08 angstroms resolution
Authors : Zhang, W.Y.; Akita, F.; Shen, J.R.
Deposited on : 2024-12-10
Resolution : 2.08 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

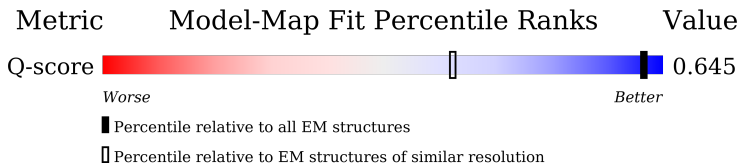
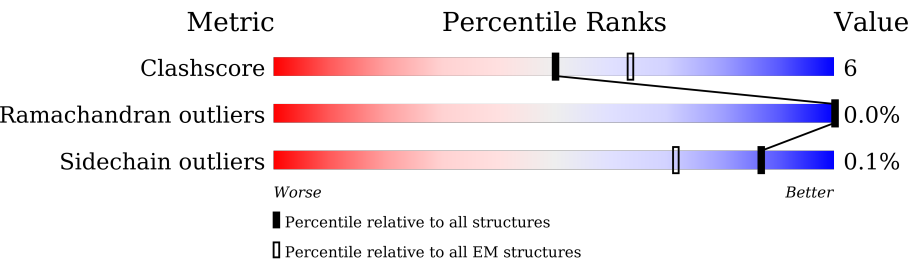
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.08 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.



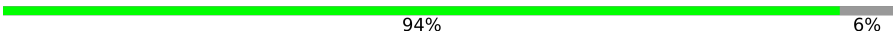
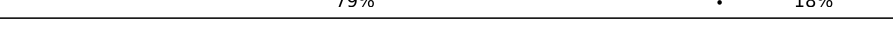
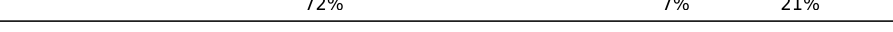
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1976 (1.58 - 2.58)

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% 11% .
3	C	81	91% 7% .
4	D	141	87% 11% .

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Mol	Chain	Length	Quality of chain
5	E	64	 94% 6%
6	F	188	 79% 7% 14%
7	I	33	 91% 9%
8	J	42	 79% 21%
9	L	153	 89% 9% ..
10	M	30	 90% 10%
11	O	153	 56% 5% • 38%
12	K	86	 70% 9% 21%
13	s	302	 49% • 49%
14	c	215	 67% 12% 21%
15	a	217	 71% 8% 21%
16	b	236	 65% 10% 25%
17	h	229	 66% • 29%
18	f	212	 76% 6% 18%
18	j	212	 70% 11% 18%
18	m	212	 79% • 18%
19	e	210	 72% 7% 21%
20	l	175	 87% 13%
21	k	232	 72% 9% 19%
22	i	200	 78% 11% 10%
23	d	219	 67% 9% 24%
24	g	216	 86% 14%
25	R	135	 61% 6% 33%
26	n	220	 70% 13% 18%
27	Q	233	 59% • 39%

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
32	WVN	A	844	-	X	-	-
32	WVN	A	845	-	X	-	-
32	WVN	A	846	-	X	-	-
32	WVN	A	847	-	X	-	-
32	WVN	A	854	-	X	-	-
32	WVN	B	847	-	X	-	-
32	WVN	B	848	-	X	-	-
32	WVN	B	849	-	X	-	-
32	WVN	F	204	-	X	-	-
32	WVN	F	205	-	X	-	-
32	WVN	F	207	-	X	-	-
32	WVN	I	101	-	X	-	-
32	WVN	J	101	-	X	-	-
32	WVN	K	103	-	X	-	-
32	WVN	L	201	-	X	-	-
32	WVN	L	205	-	X	-	-
32	WVN	L	206	-	X	-	-
32	WVN	M	101	-	X	-	-
32	WVN	R	201	-	X	-	-
32	WVN	R	202	-	X	-	-
32	WVN	e	315	-	X	-	-
32	WVN	h	308	-	X	-	-
32	WVN	i	315	-	X	-	-
32	WVN	l	302	-	X	-	-
32	WVN	l	316	-	X	-	-
32	WVN	s	407	-	X	-	-
38	II0	h	309	-	X	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 61938 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5826	3805	994	999	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	2	0
			5832	3849	982	987	14		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1075	687	185	200	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	161	Total	C	N	O	S	0	0
			1257	818	213	224	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	33	Total	C	N	O	S	0	0
			255	177	34	42	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	151	Total	C	N	O	S	1	0
			1158	763	183	209	3		

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

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

- Molecule 11 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	95	Total	C	N	O	S	0	0
			714	480	107	124	3		

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

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

- Molecule 13 is a protein called ACPI-s.

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

- Molecule 14 is a protein called ACPI-c.

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

- Molecule 15 is a protein called ACPI-a.

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

- Molecule 16 is a protein called ACPI-b.

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

- Molecule 17 is a protein called ACPI-h.

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

- Molecule 18 is a protein called ACPI-m,f,j.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	m	174	Total	C	N	O	S	0	0
			1313	850	217	238	8		
18	f	174	Total	C	N	O	S	0	0
			1306	846	215	237	8		
18	j	173	Total	C	N	O	S	0	0
			1302	841	216	237	8		

- Molecule 19 is a protein called ACPI-e.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	166	Total	C	N	O	S	0	0
			1268	822	209	228	9		

- Molecule 20 is a protein called ACPI-l.

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

- Molecule 21 is a protein called ACPI-k.

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

- Molecule 22 is a protein called ACPI-i.

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

- Molecule 23 is a protein called ACPI-d.

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

- Molecule 24 is a protein called ACPI-g.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	g	216	Total	C	N	O	S	0	0
			1608	1047	265	285	11		

- Molecule 25 is a protein called PsaR.

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

- Molecule 26 is a protein called ACPI-n.

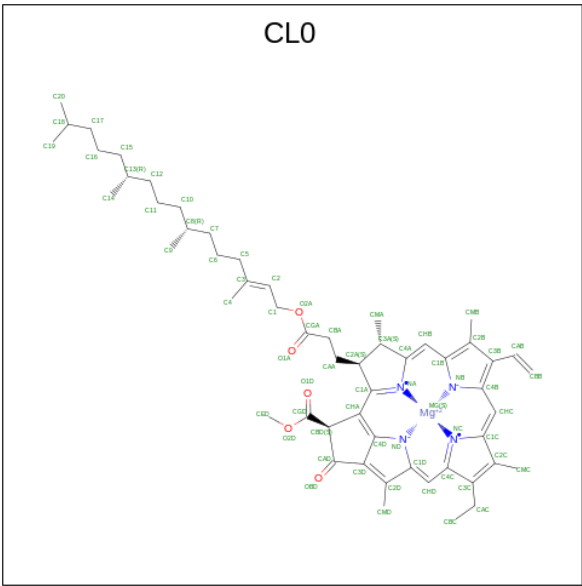
Mol	Chain	Residues	Atoms					AltConf	Trace
26	n	181	Total	C	N	O	S	0	0
			1343	862	226	245	10		

- Molecule 27 is a protein called PsaQ.

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

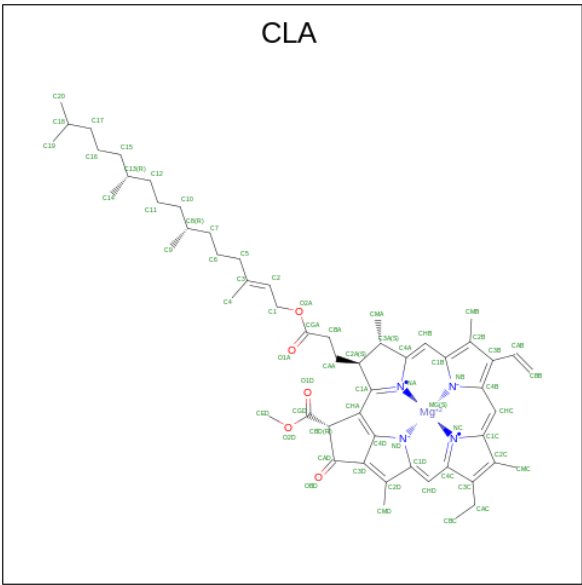
- Molecule 28 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅)

(labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	F	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	L	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
29	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 61	C 51	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	h	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	m	1	Total 59	C 49	Mg 1	N 4	O 5	0
29	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	m	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	m	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	m	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	e	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	l	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	l	1	Total 61	C 51	Mg 1	N 4	O 5	0
29	l	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	k	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	f	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	f	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	f	1	Total 51	C 41	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
29	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	j	1	Total 61	C 51	Mg 1	N 4	O 5	0
29	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	d	1	Total 62	C 52	Mg 1	N 4	O 5	0
29	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	d	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0

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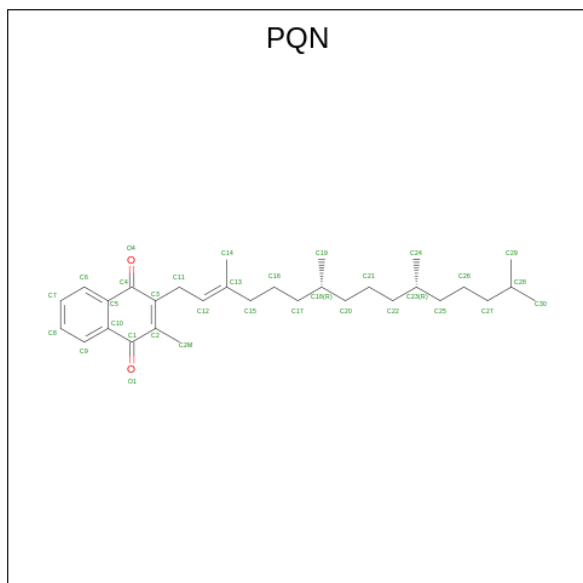
Mol	Chain	Residues	Atoms					AltConf
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 54	C 44	Mg 1	N 4	O 5	0
29	g	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	n	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	n	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	n	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 60	C 50	Mg 1	N 4	O 5	0

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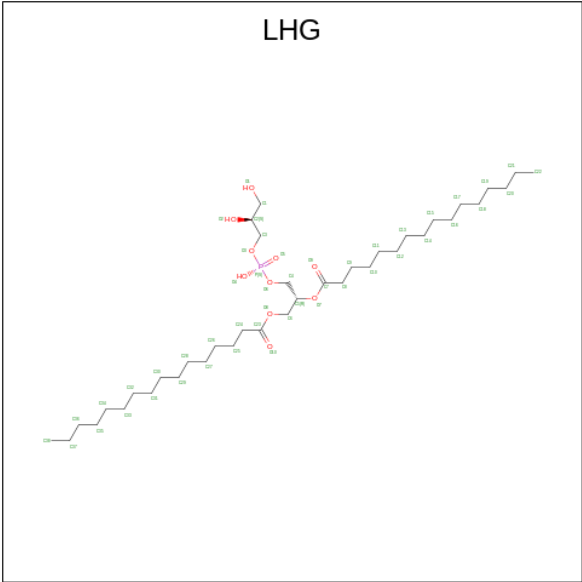
Mol	Chain	Residues	Atoms					AltConf
29	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 30 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



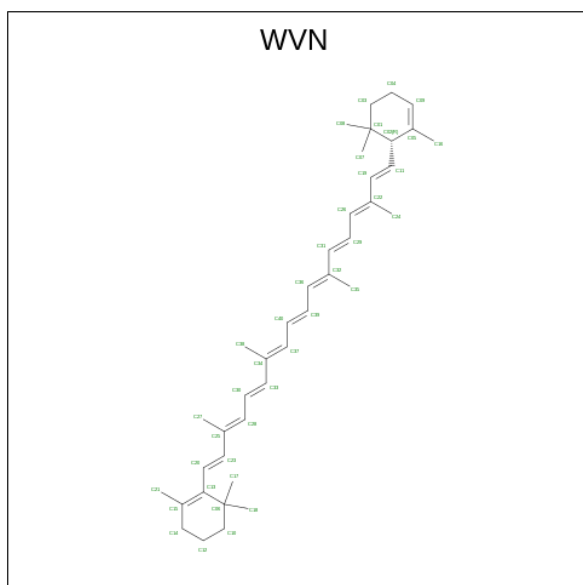
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	P	0
			48	37	10	1	
31	A	1	Total	C	O	P	0
			27	16	10	1	
31	A	1	Total	C	O	P	0
			27	20	6	1	
31	J	1	Total	C	O	P	0
			33	22	10	1	
31	L	1	Total	C	O	P	0
			47	36	10	1	
31	L	1	Total	C	O	P	0
			36	25	10	1	
31	s	1	Total	C	O	P	0
			33	24	8	1	
31	c	1	Total	C	O	P	0
			37	26	10	1	
31	c	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			49	38	10	1	
31	b	1	Total	C	O	P	0
			49	38	10	1	
31	m	1	Total	C	O	P	0
			37	26	10	1	
31	e	1	Total	C	O	P	0
			37	26	10	1	

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Mol	Chain	Residues	Atoms				AltConf
31	l	1	Total	C	O	P	0
			32	21	10	1	
31	f	1	Total	C	O	P	0
			49	38	10	1	
31	f	1	Total	C	O	P	0
			37	26	10	1	
31	i	1	Total	C	O	P	0
			37	26	10	1	
31	j	1	Total	C	O	P	0
			30	19	10	1	
31	g	1	Total	C	O	P	0
			45	34	10	1	
31	g	1	Total	C	O	P	0
			37	26	10	1	
31	n	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 32 is 1,3,3-trimethyl-2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-[(1R)-2,6,6-trimethylcyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohexene (CCD ID: WVN) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	C	0
			40	40	
32	A	1	Total	C	0
			40	40	

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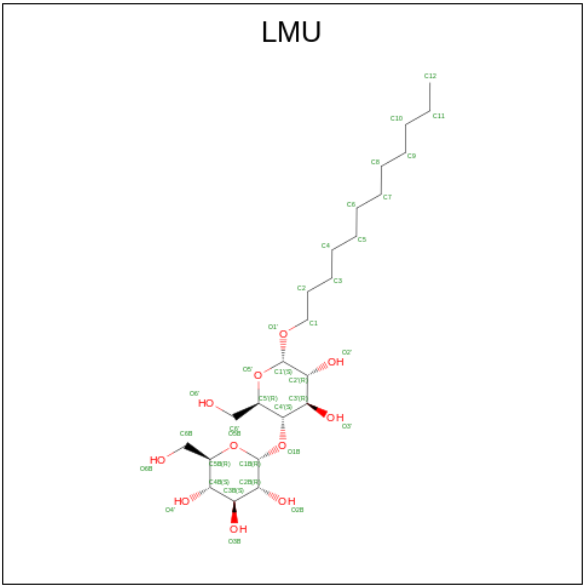
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	F	1	Total C 40 40	0
32	F	1	Total C 40 40	0
32	F	1	Total C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

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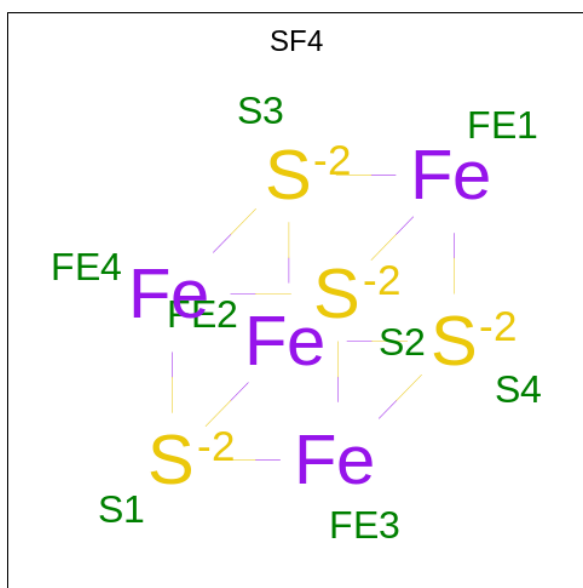
Mol	Chain	Residues	Atoms	AltConf
32	e	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	i	1	Total C 40 40	0
32	R	1	Total C 40 40	0
32	R	1	Total C 40 40	0

- Molecule 33 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



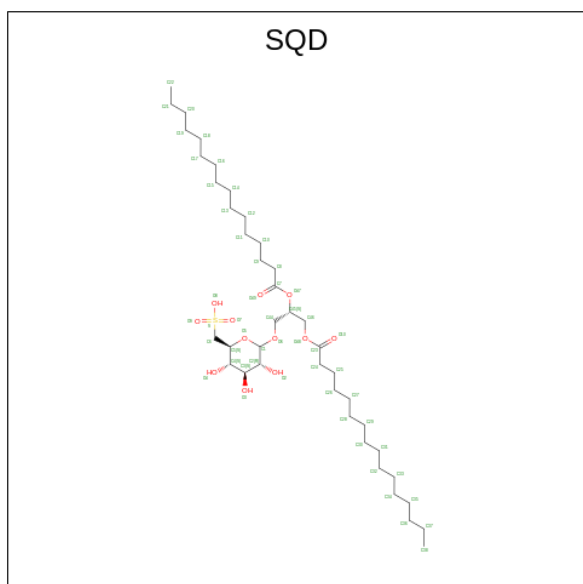
Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C O 35 24 11	0
33	A	1	Total C O 34 23 11	0
33	B	1	Total C O 35 24 11	0
33	a	1	Total C O 35 24 11	0
33	i	1	Total C O 35 24 11	0

- Molecule 34 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



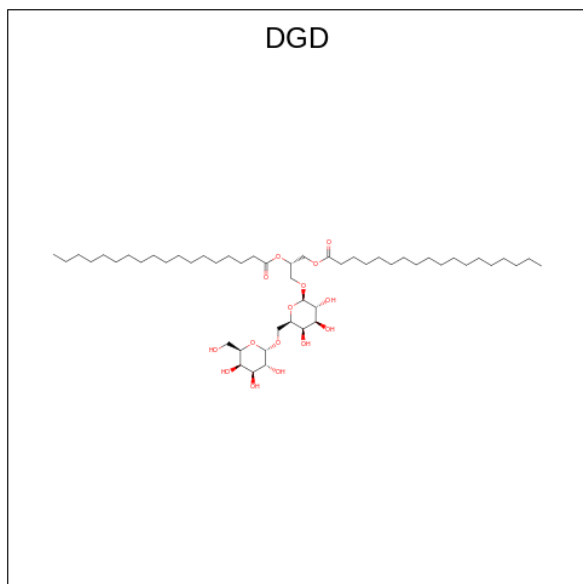
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	Fe	S	0
			8	4	4	
34	C	1	Total	Fe	S	0
			8	4	4	
34	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$) (labeled as "Ligand of Interest" by depositor).



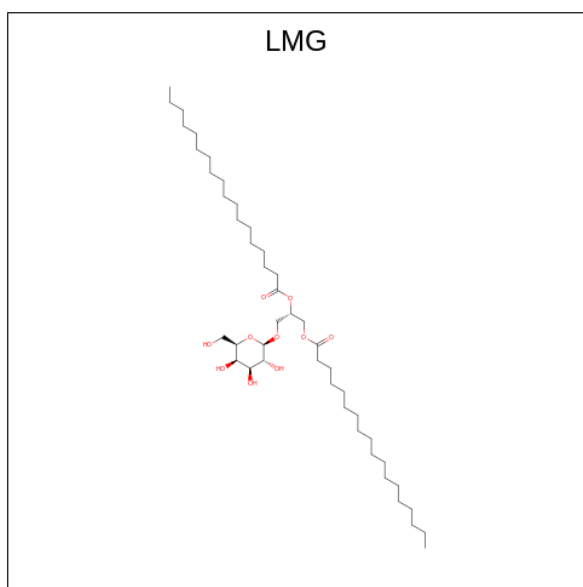
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



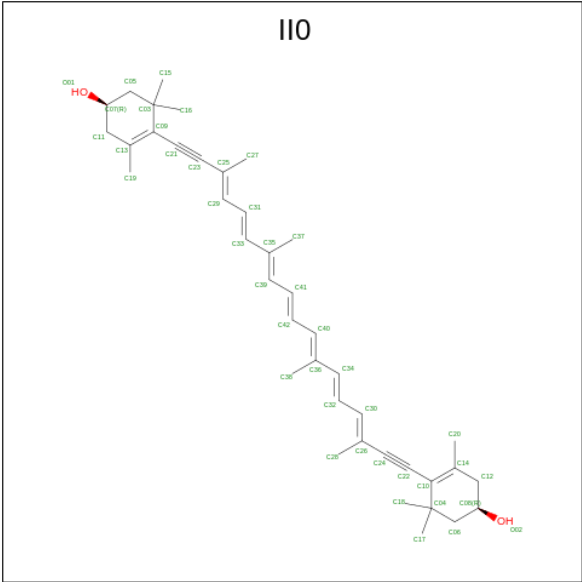
Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			66	51	15	
36	j	1	Total	C	O	0
			62	47	15	

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
37	F	1	Total	C	O	0
			53	43	10	
37	F	1	Total	C	O	0
			41	31	10	
37	L	1	Total	C	O	0
			45	35	10	
37	O	1	Total	C	O	0
			26	16	10	
37	c	1	Total	C	O	0
			55	45	10	
37	c	1	Total	C	O	0
			43	33	10	
37	b	1	Total	C	O	0
			42	32	10	
37	n	1	Total	C	O	0
			51	41	10	
37	Q	1	Total	C	O	0
			38	28	10	

- Molecule 38 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
38	J	1	Total	C	O	0
			42	40	2	
38	O	1	Total	C	O	0
			42	40	2	
38	c	1	Total	C	O	0
			42	40	2	
38	c	1	Total	C	O	0
			42	40	2	
38	a	1	Total	C	O	0
			42	40	2	
38	a	1	Total	C	O	0
			42	40	2	
38	a	1	Total	C	O	0
			42	40	2	
38	a	1	Total	C	O	0
			42	40	2	
38	b	1	Total	C	O	0
			42	40	2	
38	b	1	Total	C	O	0
			42	40	2	
38	b	1	Total	C	O	0
			42	40	2	
38	b	1	Total	C	O	0
			42	40	2	
38	h	1	Total	C	O	0
			28	27	1	
38	h	1	Total	C	O	0
			42	40	2	

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

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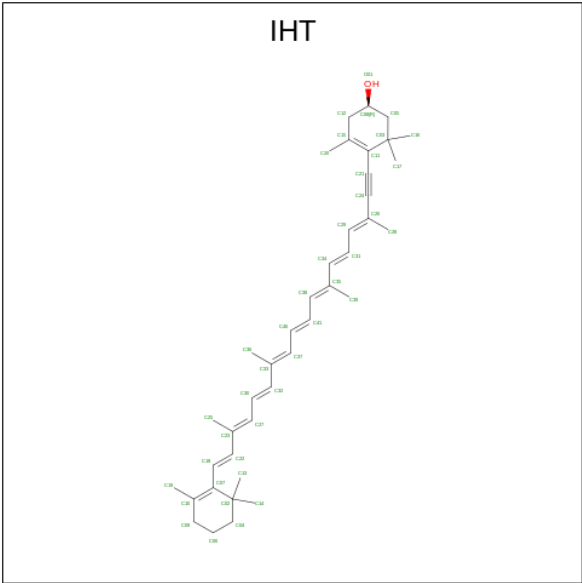
Mol	Chain	Residues	Atoms			AltConf
38	f	1	Total 42	C 40	O 2	0
38	f	1	Total 42	C 40	O 2	0
38	i	1	Total 42	C 40	O 2	0
38	i	1	Total 42	C 40	O 2	0
38	i	1	Total 42	C 40	O 2	0
38	i	1	Total 42	C 40	O 2	0
38	j	1	Total 42	C 40	O 2	0
38	j	1	Total 42	C 40	O 2	0
38	j	1	Total 42	C 40	O 2	0
38	d	1	Total 42	C 40	O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

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

- Molecule 39 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: C₄₀H₅₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
39	O	1	Total	C	O	0
			41	40	1	
39	c	1	Total	C	O	0
			41	40	1	
39	c	1	Total	C	O	0
			41	40	1	
39	a	1	Total	C	O	0
			41	40	1	
39	b	1	Total	C	O	0
			41	40	1	
39	m	1	Total	C	O	0
			41	40	1	
39	f	1	Total	C	O	0
			41	40	1	
39	j	1	Total	C	O	0
			41	40	1	

Continued on next page...

Mol	Chain	Residues	Atoms			AltConf
39	g	1	Total 41	C 40	O 1	0
39	g	1	Total 41	C 40	O 1	0
39	R	1	Total 41	C 40	O 1	0
39	n	1	Total 41	C 40	O 1	0

- ## KC2

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



WORLDWIDE
PDB
PROTEIN DATA BANK

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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	A	126	Total 126	O 126	0
41	B	150	Total 150	O 150	0
41	C	22	Total 22	O 22	0
41	D	15	Total 15	O 15	0
41	E	6	Total 6	O 6	0
41	F	14	Total 14	O 14	0

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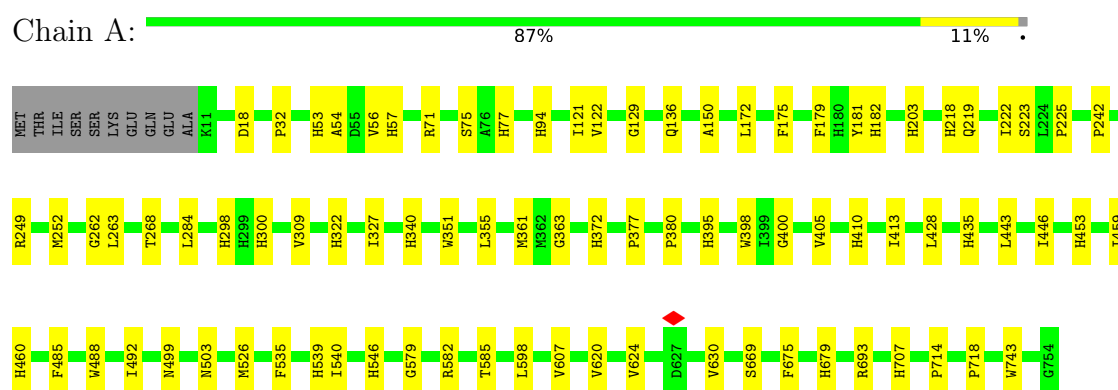
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Mol	Chain	Residues	Atoms		AltConf
41	J	2	Total 2	O 2	0
41	L	15	Total 15	O 15	0
41	M	2	Total 2	O 2	0
41	O	5	Total 5	O 5	0
41	K	2	Total 2	O 2	0
41	s	7	Total 7	O 7	0
41	c	2	Total 2	O 2	0
41	a	16	Total 16	O 16	0
41	b	21	Total 21	O 21	0
41	h	9	Total 9	O 9	0
41	m	1	Total 1	O 1	0
41	e	3	Total 3	O 3	0
41	f	1	Total 1	O 1	0
41	g	1	Total 1	O 1	0
41	R	1	Total 1	O 1	0
41	n	1	Total 1	O 1	0

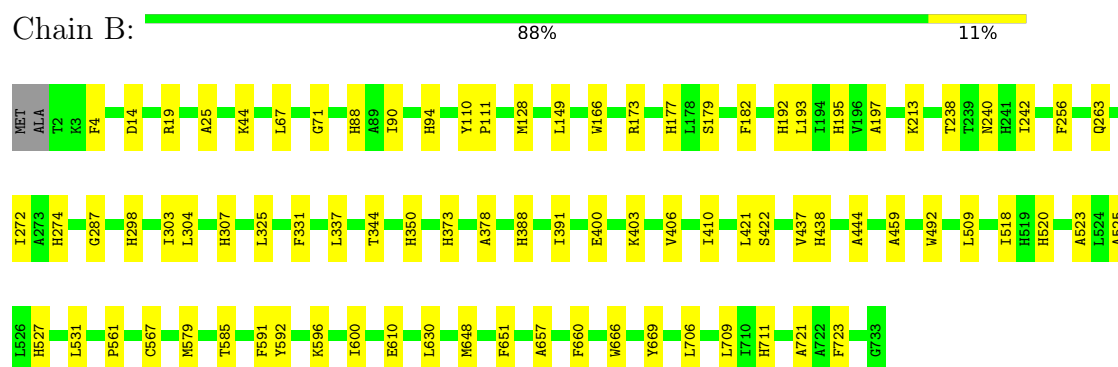
3 Residue-property plots

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

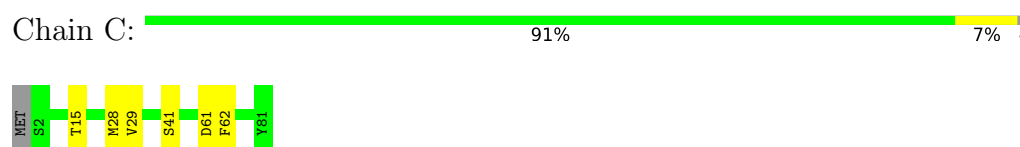
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II





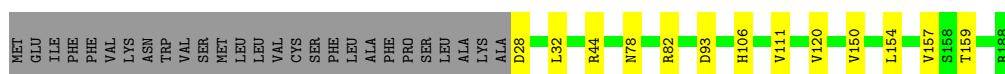
- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 94% 6%



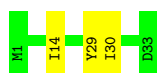
- Molecule 6: Photosystem I reaction center subunit III

Chain F: 79% 7% 14%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 91% 9%



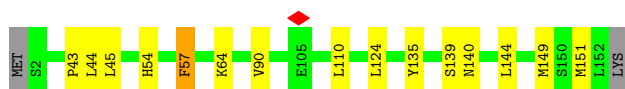
- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 79% 21%



- Molecule 9: Photosystem I reaction center subunit XI

Chain L: 89% 9% ..



- Molecule 10: Photosystem I reaction center subunit XII

Chain M: 90% 10%

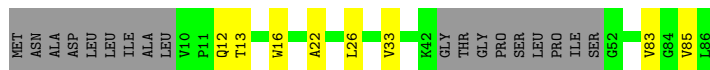


- Molecule 11: PsaO

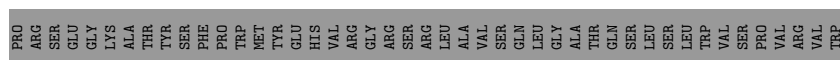
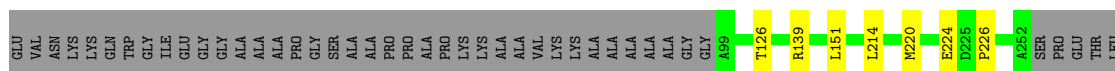
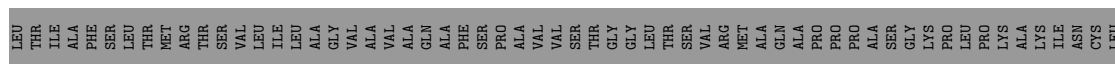
Chain O: 56% 5% 38%



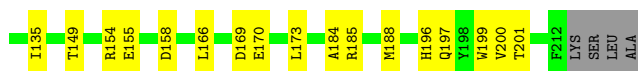
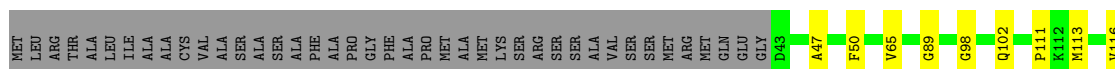
- Molecule 12: Photosystem I reaction center subunit PsaK



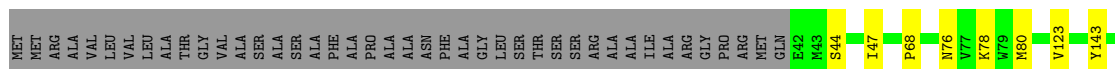
- Molecule 13: ACPI-s



- Molecule 14: ACPI-c

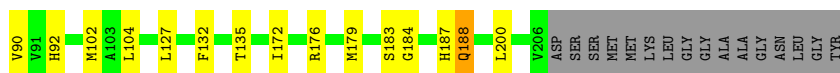


- Molecule 15: ACPI-a



- Molecule 16: ACPI-b

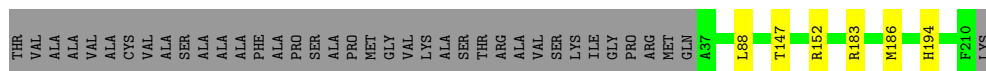


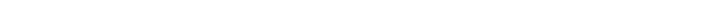


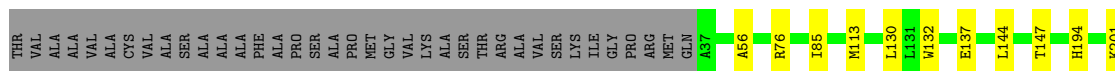
Chain h: 66% . 29%

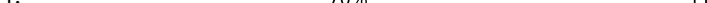


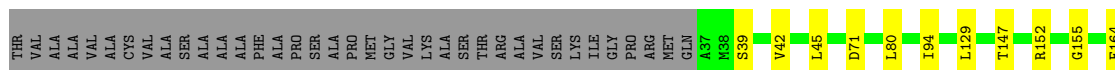
Chain m: 79% . 18%



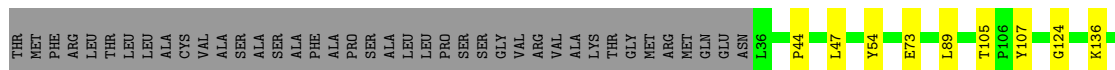
Chain f:  76% 6% 18%

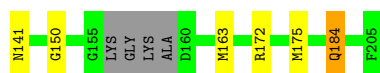


Chain j:  70% 11% 18%



Chain e:  72% 7% 21%





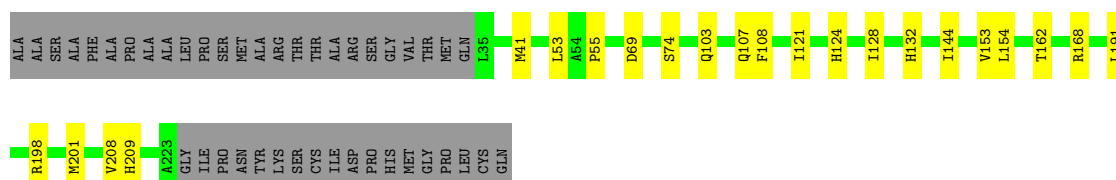
- Molecule 20: ACPI-I

Chain l: 87% 13%



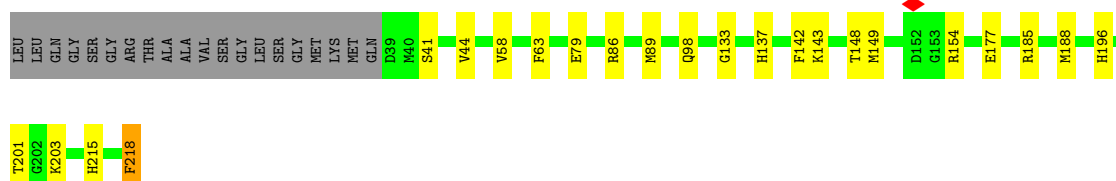
- Molecule 21: ACPI-k

Chain k: 72% 9% 19%



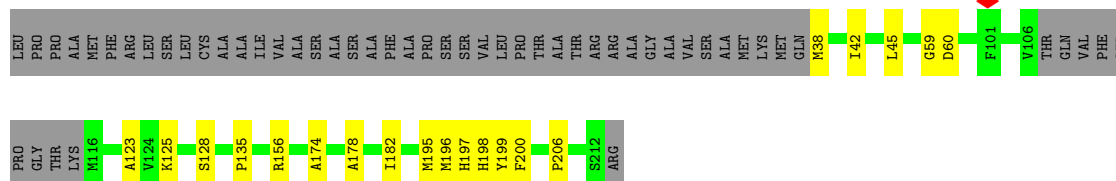
- Molecule 22: ACPI-i

Chain i: 78% 11% 10%



- Molecule 23: ACPI-d

Chain d: 67% 9% 24%



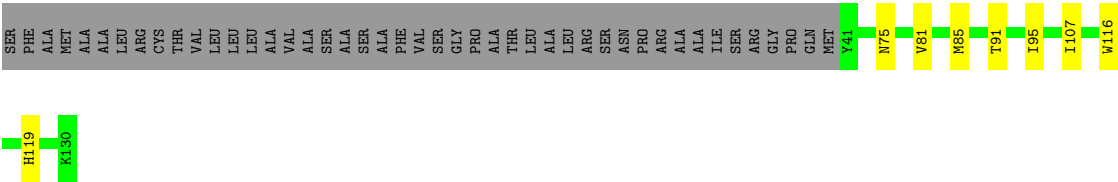
- Molecule 24: ACPI-g

Chain g: 86% 14%



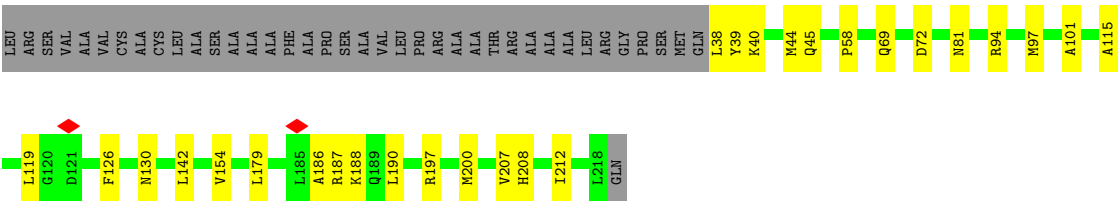
- Molecule 25: PsaR

Chain R: 61% 6% 33%



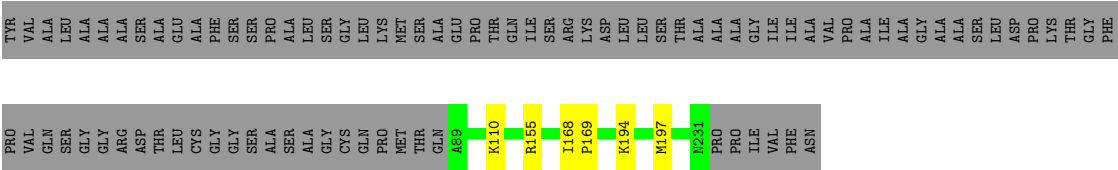
• Molecule 26: ACPI-n

Chain n: 70% 13% 18%



• Molecule 27: PsaQ

Chain Q: 59% 39%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38563	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.439	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, CLA, LMU, LHG, SQD, II0, SF4, WVN, LMG, CL0, PQN, IHT, KC2

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	0.24	0/6020	0.46	0/8205
2	B	0.25	0/6055	0.50	0/8266
3	C	0.17	0/601	0.48	0/813
4	D	0.16	0/1100	0.43	0/1488
5	E	0.16	0/492	0.34	0/666
6	F	0.22	0/1291	0.43	0/1750
7	I	0.25	0/262	0.55	0/358
8	J	0.21	0/364	0.48	0/495
9	L	0.22	0/1188	0.46	0/1616
10	M	0.17	0/233	0.37	0/315
11	O	0.23	0/741	0.49	0/1016
12	K	0.22	0/489	0.48	0/664
13	s	0.17	0/1177	0.42	0/1591
14	c	0.23	0/1401	0.48	0/1896
15	a	0.22	0/1372	0.42	0/1858
16	b	0.27	0/1360	0.49	0/1834
17	h	0.20	0/1228	0.44	0/1671
18	f	0.24	0/1334	0.51	1/1797 (0.1%)
18	j	0.24	0/1329	0.49	0/1789
18	m	0.21	0/1341	0.44	0/1805
19	e	0.20	0/1303	0.48	0/1764
20	l	0.21	0/1365	0.44	0/1845
21	k	0.24	0/1445	0.55	0/1954
22	i	0.28	0/1400	0.56	0/1891
23	d	0.27	0/1259	0.57	0/1700
24	g	0.25	0/1650	0.51	0/2238
25	R	0.22	0/687	0.49	0/940
26	n	0.21	0/1371	0.52	0/1847
27	Q	0.21	0/1053	0.46	0/1418
All	All	0.23	0/40911	0.48	1/55490 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	1
11	O	0	1
16	b	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	f	113	MET	CB-CA-C	-5.69	109.49	117.23

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	666	TRP	Peptide
3	C	61	ASP	Peptide
11	O	86	PHE	Peptide
16	b	188	GLN	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5826	0	5682	74	0
2	B	5832	0	5643	71	0
3	C	592	0	567	3	0
4	D	1075	0	1074	9	0
5	E	484	0	486	0	0
6	F	1257	0	1266	11	0
7	I	255	0	270	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	351	0	344	8	0
9	L	1158	0	1170	13	0
10	M	232	0	265	4	0
11	O	714	0	703	6	0
12	K	482	0	511	6	0
13	s	1146	0	1095	6	0
14	c	1362	0	1338	17	0
15	a	1331	0	1284	13	0
16	b	1332	0	1336	21	0
17	h	1201	0	1228	7	0
18	f	1306	0	1311	9	0
18	j	1302	0	1316	17	0
18	m	1313	0	1326	6	0
19	e	1268	0	1244	12	0
20	l	1333	0	1311	17	0
21	k	1412	0	1429	17	0
22	i	1363	0	1322	16	0
23	d	1231	0	1237	14	0
24	g	1608	0	1638	21	0
25	R	666	0	655	6	0
26	n	1343	0	1356	22	0
27	Q	1041	0	1071	7	0
28	A	65	0	72	5	0
29	A	2533	0	2645	83	0
29	B	2592	0	2717	81	0
29	F	182	0	187	5	0
29	J	42	0	31	0	0
29	K	107	0	103	3	0
29	L	225	0	208	6	0
29	O	182	0	187	2	0
29	Q	65	0	72	1	0
29	R	55	0	49	5	0
29	a	638	0	629	19	0
29	b	724	0	735	30	0
29	c	607	0	560	15	0
29	d	529	0	417	7	0
29	e	587	0	588	15	0
29	f	700	0	695	14	0
29	g	765	0	763	22	0
29	h	454	0	429	10	0
29	i	608	0	622	10	0
29	j	669	0	623	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	k	603	0	548	12	0
29	l	597	0	601	11	0
29	m	680	0	655	20	0
29	n	614	0	570	22	0
29	s	195	0	216	4	0
30	A	33	0	46	4	0
30	B	33	0	46	1	0
31	A	102	0	128	3	0
31	J	33	0	36	3	0
31	L	83	0	108	2	0
31	a	98	0	148	3	0
31	b	49	0	72	1	0
31	c	86	0	118	4	0
31	e	37	0	44	0	0
31	f	86	0	118	3	0
31	g	82	0	104	1	0
31	i	37	0	44	2	0
31	j	30	0	28	0	0
31	l	32	0	34	0	0
31	m	37	0	44	1	0
31	n	43	0	59	3	0
31	s	33	0	40	3	0
32	A	200	0	0	0	0
32	B	200	0	0	1	0
32	F	120	0	0	0	0
32	I	40	0	0	0	0
32	J	40	0	0	0	0
32	K	40	0	0	0	0
32	L	120	0	0	0	0
32	M	40	0	0	0	0
32	R	80	0	0	0	0
32	e	40	0	0	0	0
32	h	40	0	0	0	0
32	i	40	0	0	0	0
32	l	80	0	0	0	0
32	s	80	0	0	0	0
33	A	69	0	87	3	0
33	B	35	0	46	1	0
33	a	35	0	46	0	0
33	i	35	0	46	0	0
34	A	8	0	0	0	0
34	C	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	54	0	78	0	0
36	B	66	0	96	4	0
36	j	62	0	84	3	0
37	F	94	0	134	4	0
37	L	45	0	61	0	0
37	O	26	0	22	0	0
37	Q	38	0	46	4	0
37	b	42	0	54	2	0
37	c	98	0	141	4	0
37	n	51	0	75	2	0
38	J	42	0	0	0	0
38	O	42	0	0	0	0
38	a	168	0	0	0	0
38	b	168	0	0	2	0
38	c	84	0	0	0	0
38	d	252	0	0	0	0
38	e	168	0	0	0	0
38	f	168	0	0	0	0
38	g	168	0	0	2	0
38	h	112	0	0	0	0
38	i	168	0	0	0	0
38	j	126	0	0	0	0
38	k	252	0	0	1	0
38	l	168	0	0	0	0
38	m	168	0	0	0	0
38	n	168	0	0	4	0
39	O	41	0	0	0	0
39	R	41	0	0	0	0
39	a	41	0	0	0	0
39	b	41	0	0	1	0
39	c	82	0	0	0	0
39	f	41	0	0	0	0
39	g	82	0	0	5	0
39	j	41	0	0	0	0
39	m	41	0	0	0	0
39	n	41	0	0	1	0
40	c	45	0	0	0	0
40	d	90	0	0	1	0
40	e	45	0	0	0	0
40	f	45	0	0	1	0
40	g	135	0	0	5	0
40	i	90	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	j	45	0	0	0	0
40	k	135	0	0	0	0
40	l	45	0	0	3	0
40	m	45	0	0	0	0
40	n	90	0	0	1	0
40	s	90	0	0	2	0
41	A	126	0	0	1	0
41	B	150	0	0	1	0
41	C	22	0	0	0	0
41	D	15	0	0	0	0
41	E	6	0	0	0	0
41	F	14	0	0	0	0
41	J	2	0	0	0	0
41	K	2	0	0	0	0
41	L	15	0	0	0	0
41	M	2	0	0	0	0
41	O	5	0	0	0	0
41	R	1	0	0	0	0
41	a	16	0	0	1	0
41	b	21	0	0	0	0
41	c	2	0	0	0	0
41	e	3	0	0	0	0
41	f	1	0	0	0	0
41	g	1	0	0	0	0
41	h	9	0	0	0	0
41	m	1	0	0	0	0
41	n	1	0	0	0	0
41	s	7	0	0	0	0
All	All	61938	0	56633	661	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 661 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)
22:i:218:PHE:CE1	22:i:218:PHE:CE2	2.33	1.07
29:g:316:CLA:H111	39:g:324:IHT:C36	2.07	0.84
14:c:98:GLY:O	14:c:102:GLN:HB3	1.79	0.83
2:B:373:HIS:HE1	29:B:825:CLA:ND	1.77	0.81
1:A:410:HIS:HE1	29:A:829:CLA:NA	1.80	0.78

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%)	740 (100%)	0	0	100	100
2	B	732/734 (100%)	730 (100%)	2 (0%)	0	100	100
3	C	78/81 (96%)	77 (99%)	0	1 (1%)	9	5
4	D	136/141 (96%)	136 (100%)	0	0	100	100
5	E	58/64 (91%)	58 (100%)	0	0	100	100
6	F	159/188 (85%)	159 (100%)	0	0	100	100
7	I	31/33 (94%)	31 (100%)	0	0	100	100
8	J	40/42 (95%)	40 (100%)	0	0	100	100
9	L	150/153 (98%)	150 (100%)	0	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
11	O	93/153 (61%)	92 (99%)	0	1 (1%)	11	7
12	K	64/86 (74%)	64 (100%)	0	0	100	100
13	s	152/302 (50%)	151 (99%)	1 (1%)	0	100	100
14	c	168/215 (78%)	168 (100%)	0	0	100	100
15	a	170/217 (78%)	170 (100%)	0	0	100	100
16	b	176/236 (75%)	176 (100%)	0	0	100	100
17	h	160/229 (70%)	160 (100%)	0	0	100	100
18	f	172/212 (81%)	171 (99%)	1 (1%)	0	100	100
18	j	171/212 (81%)	170 (99%)	1 (1%)	0	100	100
18	m	172/212 (81%)	171 (99%)	1 (1%)	0	100	100
19	e	162/210 (77%)	162 (100%)	0	0	100	100
20	l	173/175 (99%)	173 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	k	187/232 (81%)	185 (99%)	2 (1%)	0	100	100
22	i	178/200 (89%)	177 (99%)	1 (1%)	0	100	100
23	d	162/219 (74%)	161 (99%)	1 (1%)	0	100	100
24	g	214/216 (99%)	214 (100%)	0	0	100	100
25	R	88/135 (65%)	88 (100%)	0	0	100	100
26	n	179/220 (81%)	179 (100%)	0	0	100	100
27	Q	141/233 (60%)	140 (99%)	1 (1%)	0	100	100
All	All	5134/6132 (84%)	5121 (100%)	11 (0%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	62	PHE
11	O	87	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	605/614 (98%)	605 (100%)	0	100	100
2	B	595/594 (100%)	595 (100%)	0	100	100
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	115/117 (98%)	115 (100%)	0	100	100
5	E	54/58 (93%)	54 (100%)	0	100	100
6	F	132/156 (85%)	132 (100%)	0	100	100
7	I	27/27 (100%)	27 (100%)	0	100	100
8	J	39/39 (100%)	39 (100%)	0	100	100
9	L	125/126 (99%)	123 (98%)	2 (2%)	55	62
10	M	25/25 (100%)	25 (100%)	0	100	100
11	O	74/117 (63%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	51/65 (78%)	51 (100%)	0	100	100
13	s	119/228 (52%)	119 (100%)	0	100	100
14	c	139/171 (81%)	139 (100%)	0	100	100
15	a	139/167 (83%)	139 (100%)	0	100	100
16	b	136/174 (78%)	136 (100%)	0	100	100
17	h	124/167 (74%)	124 (100%)	0	100	100
18	f	134/161 (83%)	134 (100%)	0	100	100
18	j	135/161 (84%)	135 (100%)	0	100	100
18	m	136/161 (84%)	136 (100%)	0	100	100
19	e	130/164 (79%)	129 (99%)	1 (1%)	73	80
20	l	136/137 (99%)	136 (100%)	0	100	100
21	k	143/178 (80%)	143 (100%)	0	100	100
22	i	142/156 (91%)	141 (99%)	1 (1%)	76	82
23	d	125/165 (76%)	125 (100%)	0	100	100
24	g	169/170 (99%)	169 (100%)	0	100	100
25	R	72/104 (69%)	72 (100%)	0	100	100
26	n	141/167 (84%)	141 (100%)	0	100	100
27	Q	106/169 (63%)	106 (100%)	0	100	100
All	All	4135/4806 (86%)	4131 (100%)	4 (0%)	87	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	L	57[A]	PHE
9	L	57[B]	PHE
19	e	184	GLN
22	i	218	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
26	n	50	ASN
26	n	195	ASN
27	Q	231	ASN
15	a	166	ASN

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Mol	Chain	Res	Type
13	s	240	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](#)

419 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	$\# Z > 2$
29	CLA	k	608	21	69,73,73	1.24	10 (14%)	83,113,113	1.24	5 (6%)
32	WVN	e	315	-	40,41,41	5.74	19 (47%)	50,56,56	6.26	31 (62%)
29	CLA	A	840	1	69,73,73	1.22	8 (11%)	83,113,113	1.35	8 (9%)
37	LMG	L	210	29	45,45,55	0.82	0	53,53,63	1.24	3 (5%)
38	II0	b	301	-	39,43,43	6.40	22 (56%)	50,60,60	6.77	29 (58%)
38	II0	i	314	-	39,43,43	6.60	22 (56%)	50,60,60	6.55	28 (56%)
29	CLA	B	810	2	69,73,73	1.23	7 (10%)	83,113,113	1.24	8 (9%)
32	WVN	I	101	-	40,41,41	5.69	19 (47%)	50,56,56	6.28	32 (64%)
29	CLA	d	309	23	45,49,73	1.50	8 (17%)	54,84,113	1.58	7 (12%)
40	KC2	n	612	26	49,53,53	1.57	9 (18%)	62,89,89	1.08	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	A	848	-	26,26,48	0.68	0	28,29,54	1.44	4 (14%)
29	CLA	B	826	2	69,73,73	1.24	9 (13%)	83,113,113	1.25	9 (10%)
29	CLA	a	304	15	55,59,73	1.38	7 (12%)	66,96,113	1.40	5 (7%)
29	CLA	L	204	9,41	64,68,73	1.30	9 (14%)	77,107,113	1.38	6 (7%)
40	KC2	i	310	22	49,53,53	3.07	21 (42%)	62,89,89	4.23	32 (51%)
38	II0	i	313	-	39,43,43	6.26	21 (53%)	50,60,60	7.02	30 (60%)
28	CL0	A	801	-	69,73,73	1.42	10 (14%)	83,113,113	0.81	3 (3%)
39	IHT	f	617	-	40,42,42	0.21	0	53,58,58	0.70	2 (3%)
33	LMU	B	850	-	36,36,36	0.21	0	47,47,47	0.40	0
29	CLA	h	305	17	69,73,73	1.25	9 (13%)	83,113,113	1.33	5 (6%)
38	II0	k	615	-	39,43,43	6.42	22 (56%)	50,60,60	6.71	31 (62%)
31	LHG	j	318	29	29,29,48	0.80	1 (3%)	32,35,54	1.28	3 (9%)
29	CLA	e	306	19	69,73,73	1.24	7 (10%)	83,113,113	1.24	7 (8%)
29	CLA	a	308	15	69,73,73	1.23	9 (13%)	83,113,113	1.32	7 (8%)
29	CLA	B	821	2	57,61,73	1.38	8 (14%)	68,98,113	1.36	6 (8%)
29	CLA	B	807	2	69,73,73	1.22	9 (13%)	83,113,113	1.30	4 (4%)
29	CLA	d	307	23	49,53,73	1.49	8 (16%)	59,89,113	1.43	7 (11%)
32	WVN	B	846	-	40,41,41	5.64	20 (50%)	50,56,56	6.25	29 (58%)
29	CLA	m	610	31	59,63,73	1.35	6 (10%)	71,101,113	1.37	5 (7%)
29	CLA	R	203	25	59,63,73	1.36	8 (13%)	71,101,113	1.53	10 (14%)
39	IHT	j	317	-	40,42,42	0.27	0	53,58,58	0.78	3 (5%)
29	CLA	B	814	2	69,73,73	1.22	8 (11%)	83,113,113	1.29	5 (6%)
29	CLA	a	311	15	69,73,73	1.25	9 (13%)	83,113,113	1.30	6 (7%)
29	CLA	B	813	2	64,68,73	1.29	8 (12%)	77,107,113	1.40	6 (7%)
38	II0	m	618	-	39,43,43	6.48	21 (53%)	50,60,60	6.77	30 (60%)
32	WVN	M	101	-	40,41,41	5.76	19 (47%)	50,56,56	6.44	33 (66%)
29	CLA	J	102	8	46,50,73	1.50	8 (17%)	55,85,113	1.50	6 (10%)
29	CLA	g	306	24	69,73,73	1.26	9 (13%)	83,113,113	1.57	13 (15%)
39	IHT	g	320	-	40,42,42	0.17	0	53,58,58	0.57	2 (3%)
31	LHG	c	316	29	36,36,48	0.73	1 (2%)	39,42,54	1.25	5 (12%)
29	CLA	n	608	26	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
29	CLA	c	304	14	66,70,73	1.26	8 (12%)	79,109,113	1.40	7 (8%)
36	DGD	B	844	-	67,67,67	0.89	4 (5%)	81,81,81	1.43	9 (11%)
39	IHT	R	204	-	40,42,42	0.21	0	53,58,58	0.52	1 (1%)
38	II0	n	616	-	39,43,43	6.27	21 (53%)	50,60,60	6.97	30 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	A	816	1	69,73,73	1.21	8 (11%)	83,113,113	1.44	8 (9%)
29	CLA	g	311	38,24	69,73,73	1.22	8 (11%)	83,113,113	1.43	10 (12%)
29	CLA	A	828	1	69,73,73	1.24	10 (14%)	83,113,113	1.28	6 (7%)
29	CLA	a	303	15	60,64,73	1.31	8 (13%)	72,102,113	1.36	7 (9%)
29	CLA	i	309	31	50,54,73	1.45	8 (16%)	60,90,113	1.47	4 (6%)
29	CLA	L	203	9	69,73,73	1.21	8 (11%)	83,113,113	1.37	9 (10%)
38	II0	n	614	-	39,43,43	0.28	0	50,60,60	0.88	3 (6%)
31	LHG	J	104	29	32,32,48	0.75	2 (6%)	35,38,54	1.24	3 (8%)
38	II0	k	619	-	39,43,43	6.21	22 (56%)	50,60,60	6.96	28 (56%)
29	CLA	A	833	1	69,73,73	1.23	7 (10%)	83,113,113	1.32	6 (7%)
29	CLA	m	601	18	46,50,73	1.51	8 (17%)	55,85,113	1.48	7 (12%)
40	KC2	k	612	21	49,53,53	1.58	8 (16%)	62,89,89	0.98	3 (4%)
29	CLA	l	306	20	69,73,73	1.24	9 (13%)	83,113,113	1.32	5 (6%)
37	LMG	n	620	-	51,51,55	0.87	2 (3%)	59,59,63	1.24	5 (8%)
29	CLA	c	303	14	55,59,73	1.39	9 (16%)	66,96,113	1.45	7 (10%)
29	CLA	O	202	41	69,73,73	1.24	9 (13%)	83,113,113	1.35	5 (6%)
40	KC2	g	315	40	49,53,53	3.06	21 (42%)	62,89,89	4.07	35 (56%)
38	II0	g	317	29	39,43,43	6.51	21 (53%)	50,60,60	6.92	29 (58%)
29	CLA	m	606	18	69,73,73	1.25	9 (13%)	83,113,113	1.30	6 (7%)
29	CLA	l	310	31	65,69,73	1.29	8 (12%)	78,108,113	1.31	5 (6%)
29	CLA	l	303	20	51,55,73	1.43	8 (15%)	61,91,113	1.42	5 (8%)
29	CLA	b	302	16	55,59,73	1.40	7 (12%)	66,96,113	1.44	5 (7%)
29	CLA	m	604	18	69,73,73	1.25	8 (11%)	83,113,113	1.36	7 (8%)
29	CLA	A	851	1	69,73,73	1.22	9 (13%)	83,113,113	1.34	7 (8%)
29	CLA	i	307	22	65,69,73	1.30	9 (13%)	78,108,113	1.21	6 (7%)
40	KC2	n	611	-	49,53,53	3.06	22 (44%)	62,89,89	4.18	33 (53%)
29	CLA	g	307	24	55,59,73	1.41	8 (14%)	66,96,113	1.45	6 (9%)
38	II0	k	620	-	39,43,43	6.13	21 (53%)	50,60,60	6.85	28 (56%)
38	II0	J	103	-	39,43,43	6.12	21 (53%)	50,60,60	6.85	30 (60%)
29	CLA	j	306	18	49,53,73	1.49	9 (18%)	59,89,113	1.60	6 (10%)
29	CLA	j	310	18	69,73,73	1.24	9 (13%)	83,113,113	1.31	4 (4%)
29	CLA	c	311	14	49,53,73	1.47	6 (12%)	59,89,113	1.57	5 (8%)
38	II0	l	317	-	39,43,43	0.21	0	50,60,60	0.40	0
39	IHT	n	617	-	40,42,42	0.18	0	53,58,58	0.58	0
29	CLA	B	841	2	69,73,73	1.28	8 (11%)	83,113,113	1.35	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	A	824	41	69,73,73	1.24	8 (11%)	83,113,113	1.34	10 (12%)
29	CLA	n	613	26	55,59,73	1.41	7 (12%)	66,96,113	1.31	7 (10%)
29	CLA	i	305	22	69,73,73	1.26	7 (10%)	83,113,113	1.36	7 (8%)
29	CLA	n	602	26	54,58,73	1.40	8 (14%)	65,95,113	1.45	8 (12%)
29	CLA	g	305	24,39	69,73,73	1.25	8 (11%)	83,113,113	1.32	5 (6%)
29	CLA	e	308	31	50,54,73	1.46	8 (16%)	60,90,113	1.42	4 (6%)
29	CLA	B	812	2	69,73,73	1.26	9 (13%)	83,113,113	1.32	9 (10%)
32	WVN	B	845	-	40,41,41	0.36	0	50,56,56	1.10	4 (8%)
39	IHT	a	316	-	40,42,42	0.20	0	53,58,58	0.51	0
37	LMG	F	208	-	41,41,55	0.89	0	49,49,63	1.26	3 (6%)
29	CLA	B	825	2	69,73,73	1.23	8 (11%)	83,113,113	1.30	9 (10%)
29	CLA	L	207	41	55,59,73	1.40	9 (16%)	66,96,113	1.39	5 (7%)
29	CLA	c	308	14	69,73,73	1.24	8 (11%)	83,113,113	1.31	6 (7%)
38	II0	a	314	-	39,43,43	6.39	21 (53%)	50,60,60	6.58	27 (54%)
39	IHT	b	316	-	40,42,42	0.21	0	53,58,58	0.78	1 (1%)
29	CLA	F	201	41	69,73,73	1.26	9 (13%)	83,113,113	1.27	6 (7%)
29	CLA	B	809	2	69,73,73	1.28	9 (13%)	83,113,113	1.37	6 (7%)
29	CLA	A	822	1	60,64,73	1.33	9 (15%)	72,102,113	1.38	7 (9%)
29	CLA	i	306	22	55,59,73	1.41	7 (12%)	66,96,113	1.44	5 (7%)
38	II0	i	316	-	39,43,43	6.26	21 (53%)	50,60,60	6.93	30 (60%)
29	CLA	i	302	22	69,73,73	1.24	7 (10%)	83,113,113	1.33	6 (7%)
29	CLA	j	303	18	58,62,73	1.34	8 (13%)	69,99,113	1.41	8 (11%)
29	CLA	A	802	-	69,73,73	1.22	10 (14%)	83,113,113	1.36	9 (10%)
38	II0	j	301	-	39,43,43	6.34	21 (53%)	50,60,60	6.89	28 (56%)
37	LMG	c	317	-	55,55,55	0.72	0	63,63,63	1.41	7 (11%)
29	CLA	d	310	23	45,49,73	1.53	8 (17%)	54,84,113	1.53	6 (11%)
29	CLA	n	609	26	69,73,73	1.24	10 (14%)	83,113,113	1.30	6 (7%)
39	IHT	g	324	29	40,42,42	0.17	0	53,58,58	0.79	2 (3%)
29	CLA	d	303	23	55,59,73	1.38	9 (16%)	66,96,113	1.48	8 (12%)
29	CLA	h	301	41	69,73,73	1.26	9 (13%)	83,113,113	3.23	8 (9%)
32	WVN	F	207	-	40,41,41	5.72	20 (50%)	50,56,56	6.18	29 (58%)
30	PQN	B	843	-	34,34,34	2.81	9 (26%)	42,45,45	1.94	4 (9%)
29	CLA	B	822	41	69,73,73	1.26	10 (14%)	83,113,113	1.52	10 (12%)
29	CLA	K	102	12	46,50,73	1.54	7 (15%)	55,85,113	1.57	9 (16%)
29	CLA	B	805	2	69,73,73	1.21	6 (8%)	83,113,113	1.37	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMU	i	301	-	36,36,36	1.75	12 (33%)	47,47,47	0.93	1 (2%)
37	LMG	Q	301	-	38,38,55	0.88	0	46,46,63	1.22	3 (6%)
29	CLA	B	804	-	69,73,73	1.23	9 (13%)	83,113,113	1.54	9 (10%)
29	CLA	A	811	1	58,62,73	1.38	9 (15%)	69,99,113	1.34	5 (7%)
29	CLA	B	827	2	55,59,73	1.41	10 (18%)	66,96,113	1.51	8 (12%)
29	CLA	l	308	20	69,73,73	1.24	8 (11%)	83,113,113	1.27	7 (8%)
29	CLA	b	313	31	55,59,73	1.40	8 (14%)	66,96,113	1.51	9 (13%)
33	LMU	A	855	-	35,35,36	0.17	0	46,46,47	0.29	0
29	CLA	B	820	2	69,73,73	1.23	8 (11%)	83,113,113	1.28	6 (7%)
33	LMU	a	319	-	36,36,36	0.15	0	47,47,47	0.25	0
32	WVN	B	848	-	40,41,41	5.58	19 (47%)	50,56,56	6.31	34 (68%)
33	LMU	A	849	-	36,36,36	1.75	11 (30%)	47,47,47	1.02	4 (8%)
32	WVN	L	205	-	40,41,41	5.72	19 (47%)	50,56,56	6.10	31 (62%)
38	II0	b	314	-	39,43,43	6.12	19 (48%)	50,60,60	6.77	29 (58%)
29	CLA	l	312	20	60,64,73	1.34	10 (16%)	72,102,113	1.38	5 (6%)
32	WVN	A	854	-	40,41,41	5.69	19 (47%)	50,56,56	6.32	33 (66%)
38	II0	a	317	-	39,43,43	6.38	20 (51%)	50,60,60	6.83	31 (62%)
29	CLA	c	309	31	49,53,73	1.48	8 (16%)	59,89,113	1.44	5 (8%)
29	CLA	a	309	31	52,56,73	1.43	10 (19%)	62,92,113	1.44	4 (6%)
29	CLA	c	302	14	64,68,73	1.29	8 (12%)	77,107,113	1.33	6 (7%)
29	CLA	j	308	18	55,59,73	1.36	8 (14%)	66,96,113	1.47	9 (13%)
38	II0	k	617	-	39,43,43	0.27	0	50,60,60	0.77	2 (4%)
29	CLA	B	837	2	69,73,73	1.23	7 (10%)	83,113,113	1.31	5 (6%)
29	CLA	b	303	16	59,63,73	1.32	9 (15%)	71,101,113	1.46	9 (12%)
31	LHG	s	408	29	32,32,48	0.80	2 (6%)	36,37,54	1.61	4 (11%)
38	II0	n	618	-	39,43,43	6.47	22 (56%)	50,60,60	6.73	33 (66%)
40	KC2	c	310	14	49,53,53	2.99	21 (42%)	62,89,89	4.22	33 (53%)
29	CLA	s	403	13	69,73,73	1.25	9 (13%)	83,113,113	1.39	6 (7%)
34	SF4	A	852	2,1	0,12,12	-	-	-	-	-
29	CLA	B	802	41	69,73,73	1.22	7 (10%)	83,113,113	1.29	8 (9%)
29	CLA	m	602	18	64,68,73	1.30	9 (14%)	77,107,113	1.52	15 (19%)
29	CLA	n	607	26	69,73,73	1.24	9 (13%)	83,113,113	1.23	8 (9%)
31	LHG	L	208	-	46,46,48	0.66	2 (4%)	49,52,54	1.35	7 (14%)
32	WVN	s	407	-	40,41,41	5.72	19 (47%)	50,56,56	6.53	32 (64%)
29	CLA	h	312	41	69,73,73	1.25	9 (13%)	83,113,113	1.27	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	m	603	18	63,67,73	1.28	8 (12%)	75,105,113	1.36	6 (8%)
32	WVN	B	849	-	40,41,41	5.67	20 (50%)	50,56,56	6.02	31 (62%)
29	CLA	B	836	41	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
29	CLA	c	307	14	50,54,73	1.45	8 (16%)	60,90,113	1.41	7 (11%)
29	CLA	f	609	18	69,73,73	1.23	10 (14%)	83,113,113	1.35	7 (8%)
29	CLA	B	829	2	69,73,73	1.24	8 (11%)	83,113,113	1.35	9 (10%)
40	KC2	s	404	-	49,53,53	3.04	20 (40%)	62,89,89	3.98	32 (51%)
29	CLA	h	307	17	55,59,73	1.40	8 (14%)	66,96,113	1.45	7 (10%)
38	II0	f	616	-	39,43,43	6.35	20 (51%)	50,60,60	6.73	28 (56%)
29	CLA	l	304	20	69,73,73	1.22	7 (10%)	83,113,113	1.40	9 (10%)
29	CLA	A	823	1	59,63,73	1.35	7 (11%)	71,101,113	1.46	7 (9%)
32	WVN	L	201	-	40,41,41	5.71	19 (47%)	50,56,56	6.23	32 (64%)
29	CLA	A	817	1	69,73,73	1.25	10 (14%)	83,113,113	1.34	9 (10%)
29	CLA	m	612	41	55,59,73	1.39	9 (16%)	66,96,113	1.47	8 (12%)
29	CLA	k	602	21	69,73,73	1.24	10 (14%)	83,113,113	1.30	5 (6%)
29	CLA	n	601	26	49,53,73	1.47	8 (16%)	59,89,113	1.44	4 (6%)
29	CLA	d	308	23	50,54,73	1.44	8 (16%)	60,90,113	1.38	4 (6%)
29	CLA	k	603	21	55,59,73	1.39	9 (16%)	66,96,113	1.41	8 (12%)
38	II0	e	313	-	39,43,43	6.27	21 (53%)	50,60,60	6.65	30 (60%)
38	II0	e	312	-	39,43,43	6.22	22 (56%)	50,60,60	6.80	30 (60%)
29	CLA	A	810	1	69,73,73	1.23	8 (11%)	83,113,113	1.22	5 (6%)
38	II0	l	313	-	39,43,43	6.31	21 (53%)	50,60,60	6.85	30 (60%)
39	IHT	O	204	-	40,42,42	0.22	0	53,58,58	0.31	0
29	CLA	A	815	41	49,53,73	1.45	8 (16%)	59,89,113	1.63	9 (15%)
29	CLA	g	323	31	59,63,73	1.37	9 (15%)	71,101,113	1.48	8 (11%)
29	CLA	O	201	31	56,60,73	1.37	10 (17%)	67,97,113	1.39	8 (11%)
29	CLA	b	306	41	69,73,73	1.24	8 (11%)	83,113,113	1.36	8 (9%)
31	LHG	c	320	-	48,48,48	0.59	0	51,54,54	1.25	6 (11%)
31	LHG	b	318	29	48,48,48	0.64	1 (2%)	51,54,54	1.25	6 (11%)
29	CLA	k	605	21	49,53,73	1.48	6 (12%)	59,89,113	1.57	6 (10%)
29	CLA	k	614	21	55,59,73	1.42	7 (12%)	66,96,113	1.46	8 (12%)
29	CLA	j	309	18	49,53,73	1.49	8 (16%)	59,89,113	1.45	6 (10%)
38	II0	b	317	-	39,43,43	0.22	0	50,60,60	0.91	2 (4%)
29	CLA	h	302	17	54,58,73	1.40	9 (16%)	65,95,113	1.47	7 (10%)
29	CLA	B	842	31	69,73,73	1.25	8 (11%)	83,113,113	1.33	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	g	310	24	69,73,73	1.25	9 (13%)	83,113,113	1.29	5 (6%)
29	CLA	Q	302	-	69,73,73	1.24	8 (11%)	83,113,113	1.28	4 (4%)
29	CLA	m	605	18	46,50,73	1.51	7 (15%)	55,85,113	1.56	6 (10%)
40	KC2	g	313	-	49,53,53	3.03	21 (42%)	62,89,89	4.09	35 (56%)
29	CLA	B	835	2	51,55,73	1.45	8 (15%)	61,91,113	1.39	6 (9%)
29	CLA	e	302	19	69,73,73	1.23	8 (11%)	83,113,113	1.30	8 (9%)
29	CLA	g	303	24	46,50,73	1.51	9 (19%)	55,85,113	1.46	5 (9%)
29	CLA	i	311	-	64,68,73	1.29	8 (12%)	77,107,113	1.32	5 (6%)
38	II0	l	315	-	39,43,43	6.55	22 (56%)	50,60,60	6.79	33 (66%)
38	II0	m	615	-	39,43,43	6.44	21 (53%)	50,60,60	6.66	33 (66%)
31	LHG	a	301	29	48,48,48	0.61	0	51,54,54	1.23	6 (11%)
29	CLA	A	830	1	64,68,73	1.30	8 (12%)	77,107,113	1.37	8 (10%)
29	CLA	O	206	11	69,73,73	1.25	10 (14%)	83,113,113	1.33	4 (4%)
38	II0	g	318	-	39,43,43	6.34	21 (53%)	50,60,60	6.66	30 (60%)
31	LHG	g	301	29	44,44,48	0.63	0	47,50,54	1.25	5 (10%)
29	CLA	k	610	-	55,59,73	1.41	8 (14%)	66,96,113	1.47	8 (12%)
38	II0	c	314	-	39,43,43	0.21	0	50,60,60	0.55	1 (2%)
29	CLA	n	606	26	55,59,73	1.40	8 (14%)	66,96,113	1.41	5 (7%)
29	CLA	j	304	18	55,59,73	1.39	9 (16%)	66,96,113	1.46	6 (9%)
35	SQD	A	853	-	53,54,54	0.92	4 (7%)	62,65,65	1.74	12 (19%)
29	CLA	j	313	-	55,59,73	1.39	9 (16%)	66,96,113	1.42	5 (7%)
29	CLA	A	832	1	69,73,73	1.22	6 (8%)	83,113,113	1.31	9 (10%)
40	KC2	f	611	-	49,53,53	2.98	20 (40%)	62,89,89	4.14	35 (56%)
37	LMG	O	205	-	26,26,55	1.07	1 (3%)	34,34,63	1.30	6 (17%)
29	CLA	A	829	1	69,73,73	1.28	10 (14%)	83,113,113	1.31	9 (10%)
38	II0	d	314	-	39,43,43	0.21	0	50,60,60	0.72	1 (2%)
29	CLA	A	834	1	64,68,73	1.29	8 (12%)	77,107,113	1.36	7 (9%)
29	CLA	B	808	2	69,73,73	1.22	7 (10%)	83,113,113	1.42	8 (9%)
29	CLA	i	303	22	69,73,73	1.24	8 (11%)	83,113,113	1.34	6 (7%)
29	CLA	B	803	2	69,73,73	1.22	9 (13%)	83,113,113	1.29	6 (7%)
29	CLA	i	308	22	69,73,73	1.22	7 (10%)	83,113,113	1.31	6 (7%)
29	CLA	k	606	21	55,59,73	1.40	9 (16%)	66,96,113	1.38	6 (9%)
29	CLA	A	807	1	69,73,73	1.22	8 (11%)	83,113,113	1.33	7 (8%)
29	CLA	s	406	41	69,73,73	1.26	9 (13%)	83,113,113	1.37	10 (12%)
37	LMG	F	206	-	53,53,55	0.75	0	61,61,63	1.33	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	KC2	d	311	-	49,53,53	3.07	22 (44%)	62,89,89	4.18	36 (58%)
38	II0	k	618	-	39,43,43	0.27	0	50,60,60	0.76	1 (2%)
29	CLA	a	312	15	52,56,73	1.42	7 (13%)	62,92,113	1.40	4 (6%)
29	CLA	A	838	1	69,73,73	1.26	8 (11%)	83,113,113	1.32	7 (8%)
29	CLA	f	612	41	55,59,73	1.37	8 (14%)	66,96,113	1.45	5 (7%)
29	CLA	s	402	13	69,73,73	1.27	9 (13%)	83,113,113	1.33	10 (12%)
32	WVN	K	103	-	40,41,41	5.63	19 (47%)	50,56,56	6.57	33 (66%)
29	CLA	k	609	21	61,65,73	1.35	10 (16%)	73,103,113	1.36	5 (6%)
31	LHG	A	843	29	26,26,48	0.89	1 (3%)	29,32,54	1.32	3 (10%)
29	CLA	A	839	1	64,68,73	1.29	8 (12%)	77,107,113	1.35	9 (11%)
29	CLA	b	309	37	69,73,73	1.24	8 (11%)	83,113,113	1.30	4 (4%)
29	CLA	e	305	19	69,73,73	1.26	9 (13%)	83,113,113	1.28	5 (6%)
29	CLA	m	613	18	69,73,73	1.24	8 (11%)	83,113,113	1.27	5 (6%)
29	CLA	e	310	41	59,63,73	1.34	8 (13%)	71,101,113	1.43	6 (8%)
30	PQN	A	841	-	34,34,34	2.80	10 (29%)	42,45,45	1.98	5 (11%)
32	WVN	l	302	-	40,41,41	5.67	19 (47%)	50,56,56	6.11	31 (62%)
29	CLA	g	308	24	55,59,73	1.40	7 (12%)	66,96,113	1.36	7 (10%)
38	II0	f	618	-	39,43,43	6.44	20 (51%)	50,60,60	6.82	32 (64%)
31	LHG	n	619	-	42,42,48	0.65	0	45,48,54	1.20	4 (8%)
29	CLA	A	806	1	64,68,73	1.31	7 (10%)	77,107,113	1.33	7 (9%)
29	CLA	m	608	18	69,73,73	1.26	9 (13%)	83,113,113	1.28	5 (6%)
29	CLA	F	202	41	69,73,73	1.27	9 (13%)	83,113,113	1.24	5 (6%)
29	CLA	A	831	1	69,73,73	1.25	8 (11%)	83,113,113	1.31	6 (7%)
29	CLA	e	307	19	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
32	WVN	h	308	-	40,41,41	5.77	20 (50%)	50,56,56	6.26	34 (68%)
38	II0	e	316	-	39,43,43	0.22	0	50,60,60	0.78	2 (4%)
32	WVN	B	847	-	40,41,41	5.69	20 (50%)	50,56,56	6.11	31 (62%)
31	LHG	e	317	29	36,36,48	0.71	1 (2%)	39,42,54	1.21	4 (10%)
29	CLA	e	304	-	69,73,73	1.24	9 (13%)	83,113,113	1.38	6 (7%)
38	II0	b	315	-	39,43,43	6.18	19 (48%)	50,60,60	6.52	27 (54%)
29	CLA	c	312	14	69,73,73	1.25	8 (11%)	83,113,113	1.26	4 (4%)
29	CLA	k	604	21	69,73,73	1.25	9 (13%)	83,113,113	1.35	7 (8%)
37	LMG	c	318	29	43,43,55	0.91	0	51,51,63	1.23	5 (9%)
29	CLA	B	801	41	69,73,73	1.26	9 (13%)	83,113,113	1.28	6 (7%)
29	CLA	f	607	18	69,73,73	1.27	8 (11%)	83,113,113	1.22	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	II0	f	614	-	39,43,43	6.26	22 (56%)	50,60,60	6.82	28 (56%)
40	KC2	i	318	22	49,53,53	3.13	23 (46%)	62,89,89	4.08	34 (54%)
29	CLA	a	306	15	49,53,73	1.48	9 (18%)	59,89,113	1.56	8 (13%)
29	CLA	f	610	31	69,73,73	1.25	9 (13%)	83,113,113	1.28	5 (6%)
29	CLA	f	601	18	51,55,73	1.44	9 (17%)	61,91,113	1.46	4 (6%)
38	II0	d	315	-	39,43,43	6.50	22 (56%)	50,60,60	6.45	29 (58%)
29	CLA	d	302	23	66,70,73	1.27	8 (12%)	79,109,113	1.33	7 (8%)
29	CLA	g	302	-	69,73,73	1.26	7 (10%)	83,113,113	1.33	7 (8%)
29	CLA	j	311	31	65,69,73	1.29	8 (12%)	78,108,113	1.32	5 (6%)
31	LHG	a	318	29	48,48,48	0.63	0	51,54,54	1.25	6 (11%)
29	CLA	e	303	19	55,59,73	1.38	8 (14%)	66,96,113	1.45	6 (9%)
32	WVN	s	405	-	40,41,41	5.67	19 (47%)	50,56,56	6.29	29 (58%)
40	KC2	k	613	-	49,53,53	1.56	9 (18%)	62,89,89	0.99	0
29	CLA	B	816	2	69,73,73	1.24	9 (13%)	83,113,113	1.40	12 (14%)
29	CLA	k	601	21	55,59,73	1.41	8 (14%)	66,96,113	1.47	7 (10%)
31	LHG	L	209	-	35,35,48	0.68	0	38,41,54	1.27	4 (10%)
29	CLA	B	833	2	59,63,73	1.35	8 (13%)	71,101,113	1.38	7 (9%)
32	WVN	A	845	-	40,41,41	5.63	20 (50%)	50,56,56	6.71	32 (64%)
29	CLA	m	609	18	64,68,73	1.27	8 (12%)	77,107,113	1.35	6 (7%)
37	LMG	b	319	-	42,42,55	0.89	2 (4%)	50,50,63	1.21	4 (8%)
29	CLA	L	202	9	53,57,73	1.42	8 (15%)	62,93,113	1.45	5 (8%)
29	CLA	g	304	24	69,73,73	1.25	9 (13%)	83,113,113	1.29	5 (6%)
29	CLA	A	805	1	69,73,73	1.24	8 (11%)	83,113,113	1.32	6 (7%)
29	CLA	A	819	1	69,73,73	1.25	9 (13%)	83,113,113	1.37	13 (15%)
38	II0	m	616	-	39,43,43	6.40	22 (56%)	50,60,60	6.76	31 (62%)
32	WVN	F	204	-	40,41,41	5.61	19 (47%)	50,56,56	6.18	33 (66%)
29	CLA	B	818	41	69,73,73	1.26	9 (13%)	83,113,113	1.31	7 (8%)
40	KC2	j	312	18	49,53,53	3.02	20 (40%)	62,89,89	4.16	36 (58%)
29	CLA	A	821	1	53,57,73	1.41	6 (11%)	62,93,113	1.46	7 (11%)
29	CLA	e	311	19	69,73,73	1.26	8 (11%)	83,113,113	1.29	8 (9%)
29	CLA	A	825	41	69,73,73	1.25	8 (11%)	83,113,113	1.31	11 (13%)
29	CLA	f	613	18	69,73,73	1.24	8 (11%)	83,113,113	1.36	7 (8%)
38	II0	m	614	-	39,43,43	6.42	22 (56%)	50,60,60	6.79	28 (56%)
31	LHG	f	619	-	48,48,48	0.60	0	51,54,54	1.23	6 (11%)
29	CLA	A	850	41	69,73,73	1.26	9 (13%)	83,113,113	1.26	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	m	607	18,31	55,59,73	1.40	7 (12%)	66,96,113	1.35	7 (10%)
31	LHG	A	842	-	47,47,48	0.66	1 (2%)	50,53,54	1.25	5 (10%)
29	CLA	A	814	1	54,58,73	1.38	7 (12%)	65,95,113	1.44	6 (9%)
29	CLA	h	303	17,37	54,58,73	1.41	9 (16%)	65,95,113	1.47	7 (10%)
32	WVN	i	315	-	40,41,41	5.77	20 (50%)	50,56,56	6.06	31 (62%)
38	II0	d	316	-	39,43,43	6.43	22 (56%)	50,60,60	6.81	30 (60%)
29	CLA	n	610	-	64,68,73	1.31	8 (12%)	77,107,113	1.37	7 (9%)
38	II0	i	319	-	39,43,43	6.38	21 (53%)	50,60,60	6.55	30 (60%)
29	CLA	A	837	1	69,73,73	1.26	7 (10%)	83,113,113	1.26	5 (6%)
29	CLA	i	304	22	69,73,73	1.23	7 (10%)	83,113,113	1.32	4 (4%)
29	CLA	A	804	1	69,73,73	1.22	8 (11%)	83,113,113	1.42	10 (12%)
31	LHG	f	620	29	36,36,48	0.70	1 (2%)	39,42,54	1.19	4 (10%)
29	CLA	n	603	26	55,59,73	1.39	9 (16%)	66,96,113	1.37	6 (9%)
29	CLA	A	827	1	66,70,73	1.26	7 (10%)	79,109,113	1.39	8 (10%)
32	WVN	R	202	-	40,41,41	5.74	19 (47%)	50,56,56	6.39	32 (64%)
29	CLA	A	820	41	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)
29	CLA	d	318	-	49,53,73	1.49	7 (14%)	59,89,113	1.51	6 (10%)
29	CLA	d	313	23	55,59,73	1.39	8 (14%)	66,96,113	1.47	10 (15%)
29	CLA	h	306	17	61,65,73	1.33	6 (9%)	73,103,113	1.38	6 (8%)
29	CLA	j	302	18,31	69,73,73	1.25	8 (11%)	83,113,113	1.31	4 (4%)
29	CLA	e	301	19	49,53,73	1.48	8 (16%)	59,89,113	1.46	4 (6%)
39	IHT	c	319	-	40,42,42	0.20	0	53,58,58	0.69	1 (1%)
29	CLA	c	301	14	55,59,73	1.40	5 (9%)	66,96,113	1.43	4 (6%)
31	LHG	l	318	29	31,31,48	0.76	0	34,37,54	1.27	4 (11%)
38	II0	g	321	-	39,43,43	0.23	0	50,60,60	0.47	0
29	CLA	A	826	1	69,73,73	1.24	9 (13%)	83,113,113	1.32	6 (7%)
29	CLA	B	830	2	54,58,73	1.38	7 (12%)	65,95,113	1.47	8 (12%)
39	IHT	c	315	-	40,42,42	0.20	0	53,58,58	0.79	2 (3%)
29	CLA	B	832	41	49,53,73	1.48	8 (16%)	59,89,113	1.50	5 (8%)
38	II0	j	316	-	39,43,43	6.31	22 (56%)	50,60,60	6.74	30 (60%)
29	CLA	a	307	15	69,73,73	1.25	8 (11%)	83,113,113	1.33	7 (8%)
38	II0	g	319	-	39,43,43	6.12	22 (56%)	50,60,60	6.94	29 (58%)
38	II0	e	314	-	39,43,43	6.43	22 (56%)	50,60,60	6.92	30 (60%)
38	II0	l	314	-	39,43,43	6.44	22 (56%)	50,60,60	6.69	26 (52%)
38	II0	a	315	-	39,43,43	6.15	21 (53%)	50,60,60	7.01	31 (62%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	824	2	69,73,73	1.23	8 (11%)	83,113,113	1.31	6 (7%)
29	CLA	K	101	41	69,73,73	1.23	7 (10%)	83,113,113	1.39	8 (9%)
32	WVN	R	201	-	40,41,41	5.60	19 (47%)	50,56,56	6.21	34 (68%)
29	CLA	n	605	26	55,59,73	1.40	8 (14%)	66,96,113	1.46	5 (7%)
29	CLA	A	836	1	69,73,73	1.25	8 (11%)	83,113,113	1.39	7 (8%)
29	CLA	B	839	2	61,65,73	1.33	8 (13%)	73,103,113	1.33	5 (6%)
29	CLA	g	316	24	61,65,73	1.35	7 (11%)	73,103,113	1.29	5 (6%)
29	CLA	b	310	16	69,73,73	1.25	8 (11%)	83,113,113	1.24	6 (7%)
38	II0	n	615	-	39,43,43	6.32	22 (56%)	50,60,60	6.86	28 (56%)
32	WVN	L	206	-	40,41,41	5.58	20 (50%)	50,56,56	6.50	31 (62%)
38	II0	k	616	-	39,43,43	6.42	22 (56%)	50,60,60	6.80	30 (60%)
29	CLA	g	309	24	69,73,73	1.22	8 (11%)	83,113,113	1.37	7 (8%)
29	CLA	f	603	18	55,59,73	1.37	9 (16%)	66,96,113	1.46	7 (10%)
40	KC2	e	309	-	49,53,53	3.08	22 (44%)	62,89,89	4.09	34 (54%)
29	CLA	B	806	2	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
31	LHG	m	619	29	36,36,48	0.70	0	39,42,54	1.22	4 (10%)
38	II0	O	203	-	39,43,43	0.19	0	50,60,60	1.05	4 (8%)
29	CLA	B	831	41	69,73,73	1.24	8 (11%)	83,113,113	1.28	6 (7%)
29	CLA	A	813	1	60,64,73	1.34	9 (15%)	72,102,113	1.43	11 (15%)
29	CLA	d	305	23	55,59,73	1.42	7 (12%)	66,96,113	1.42	7 (10%)
29	CLA	j	314	18	69,73,73	1.25	8 (11%)	83,113,113	1.28	8 (9%)
34	SF4	C	101	3	0,12,12	-	-	-	-	-
38	II0	h	311	-	39,43,43	6.31	22 (56%)	50,60,60	6.75	27 (54%)
31	LHG	i	317	29	36,36,48	0.66	0	39,42,54	1.22	4 (10%)
29	CLA	B	811	2	59,63,73	1.35	9 (15%)	71,101,113	1.35	6 (8%)
29	CLA	i	312	22	69,73,73	1.25	7 (10%)	83,113,113	1.39	7 (8%)
29	CLA	A	812	1	69,73,73	1.24	10 (14%)	83,113,113	1.30	5 (6%)
29	CLA	l	309	20	61,65,73	1.32	9 (14%)	73,103,113	1.38	5 (6%)
29	CLA	g	312	31	58,62,73	1.36	8 (13%)	69,99,113	1.38	4 (5%)
40	KC2	k	611	-	49,53,53	3.10	22 (44%)	62,89,89	4.14	35 (56%)
32	WVN	l	316	-	40,41,41	5.84	19 (47%)	50,56,56	6.14	31 (62%)
40	KC2	m	611	18	49,53,53	3.03	20 (40%)	62,89,89	4.18	34 (54%)
29	CLA	b	308	16	69,73,73	1.22	8 (11%)	83,113,113	1.33	8 (9%)
29	CLA	B	823	41	68,72,73	1.24	8 (11%)	81,111,113	1.33	8 (9%)
32	WVN	J	101	-	40,41,41	5.70	19 (47%)	50,56,56	6.24	29 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	II0	j	315	-	39,43,43	6.20	22 (56%)	50,60,60	6.96	30 (60%)
29	CLA	F	203	6	56,60,73	1.40	8 (14%)	67,97,113	1.39	6 (8%)
31	LHG	g	322	29	36,36,48	0.73	1 (2%)	39,42,54	1.23	4 (10%)
40	KC2	l	311	-	49,53,53	3.09	21 (42%)	62,89,89	3.97	32 (51%)
29	CLA	f	604	18	69,73,73	1.26	7 (10%)	83,113,113	1.46	8 (9%)
40	KC2	s	401	13	49,53,53	2.96	20 (40%)	62,89,89	4.03	35 (56%)
29	CLA	f	605	18	49,53,73	1.50	8 (16%)	59,89,113	1.51	7 (11%)
32	WVN	A	847	-	40,41,41	5.79	19 (47%)	50,56,56	5.80	32 (64%)
29	CLA	l	307	20	69,73,73	1.26	7 (10%)	83,113,113	1.34	6 (7%)
39	IHT	m	617	-	40,42,42	0.18	0	53,58,58	0.43	1 (1%)
38	II0	f	615	-	39,43,43	6.35	22 (56%)	50,60,60	6.70	29 (58%)
32	WVN	A	844	-	40,41,41	5.76	20 (50%)	50,56,56	6.18	33 (66%)
29	CLA	B	840	2	69,73,73	1.24	9 (13%)	83,113,113	1.37	7 (8%)
38	II0	d	317	-	39,43,43	6.40	21 (53%)	50,60,60	6.75	27 (54%)
29	CLA	B	815	2	59,63,73	1.32	9 (15%)	71,101,113	1.40	8 (11%)
29	CLA	A	808	29,1	69,73,73	1.25	9 (13%)	83,113,113	1.32	6 (7%)
29	CLA	B	834	2	69,73,73	1.24	9 (13%)	83,113,113	1.38	6 (7%)
29	CLA	l	301	20	69,73,73	1.25	7 (10%)	83,113,113	1.32	7 (8%)
29	CLA	A	803	29,1	59,63,73	1.37	8 (13%)	71,101,113	1.35	9 (12%)
29	CLA	b	304	16	56,60,73	1.38	8 (14%)	67,97,113	1.44	8 (11%)
29	CLA	b	307	16	65,69,73	1.28	9 (13%)	78,108,113	1.30	6 (7%)
40	KC2	d	312	23	49,53,53	1.58	8 (16%)	62,89,89	1.17	4 (6%)
29	CLA	A	835	1	69,73,73	1.24	8 (11%)	83,113,113	1.32	6 (7%)
29	CLA	b	312	16	69,73,73	1.25	6 (8%)	83,113,113	1.23	5 (6%)
29	CLA	A	809	1	60,64,73	1.32	8 (13%)	72,102,113	1.31	5 (6%)
29	CLA	d	306	23	55,59,73	1.40	9 (16%)	66,96,113	1.41	6 (9%)
40	KC2	g	314	24,40	49,53,53	3.07	21 (42%)	62,89,89	3.89	33 (53%)
29	CLA	a	310	15	69,73,73	1.24	10 (14%)	83,113,113	1.31	4 (4%)
29	CLA	j	307	18	55,59,73	1.40	8 (14%)	66,96,113	1.42	5 (7%)
29	CLA	b	305	16	69,73,73	1.24	7 (10%)	83,113,113	1.32	5 (6%)
32	WVN	F	205	-	40,41,41	5.26	16 (40%)	50,56,56	6.25	36 (72%)
29	CLA	l	305	20	55,59,73	1.38	8 (14%)	66,96,113	1.49	6 (9%)
29	CLA	B	819	2	69,73,73	1.31	9 (13%)	83,113,113	1.53	11 (13%)
29	CLA	c	305	14	69,73,73	1.27	8 (11%)	83,113,113	1.28	4 (4%)
36	DGD	j	319	18	63,63,67	1.01	5 (7%)	77,77,81	1.57	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	828	2	54,58,73	1.40	9 (16%)	65,95,113	1.39	7 (10%)
38	II0	d	319	-	39,43,43	0.21	0	50,60,60	0.76	1 (2%)
29	CLA	B	838	2	69,73,73	1.23	8 (11%)	83,113,113	1.32	7 (8%)
29	CLA	d	304	23	49,53,73	1.49	7 (14%)	59,89,113	1.59	5 (8%)
29	CLA	n	604	26	64,68,73	1.29	8 (12%)	77,107,113	1.49	10 (12%)
38	II0	h	310	-	39,43,43	6.09	21 (53%)	50,60,60	6.91	29 (58%)
29	CLA	a	302	15	69,73,73	1.25	9 (13%)	83,113,113	1.39	6 (7%)
29	CLA	f	606	18	55,59,73	1.39	7 (12%)	66,96,113	1.39	6 (9%)
38	II0	h	309	-	26,28,43	6.25	13 (50%)	31,37,60	6.82	19 (61%)
34	SF4	C	102	3	0,12,12	-	-	-	-	-
29	CLA	f	608	18	69,73,73	1.26	7 (10%)	83,113,113	1.36	7 (8%)
29	CLA	b	311	16	68,72,73	1.26	6 (8%)	81,111,113	1.55	6 (7%)
29	CLA	j	305	18	69,73,73	1.25	7 (10%)	83,113,113	1.37	10 (12%)
29	CLA	h	304	17	55,59,73	1.36	6 (10%)	66,96,113	1.43	6 (9%)
29	CLA	c	306	14	56,60,73	1.38	9 (16%)	67,97,113	1.35	6 (8%)
38	II0	d	301	-	39,43,43	6.16	22 (56%)	50,60,60	6.99	29 (58%)
29	CLA	k	607	21	55,59,73	1.39	7 (12%)	66,96,113	1.45	9 (13%)
38	II0	c	313	-	39,43,43	6.30	21 (53%)	50,60,60	6.91	29 (58%)
38	II0	a	313	-	39,43,43	6.29	21 (53%)	50,60,60	6.71	29 (58%)
32	WVN	A	846	-	40,41,41	5.64	19 (47%)	50,56,56	6.45	32 (64%)
29	CLA	f	602	18	69,73,73	1.22	9 (13%)	83,113,113	1.38	7 (8%)
29	CLA	A	818	1	69,73,73	1.26	9 (13%)	83,113,113	1.41	9 (10%)
29	CLA	a	305	41	69,73,73	1.24	9 (13%)	83,113,113	1.35	9 (10%)
29	CLA	B	817	2	69,73,73	1.24	9 (13%)	83,113,113	1.25	8 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	k	608	21	-	11/39/115/115	-
32	WVN	e	315	-	-	16/29/63/63	0/2/2/2
29	CLA	A	840	1	-	16/39/115/115	-
37	LMG	L	210	29	-	20/40/60/70	0/1/1/1
38	II0	b	301	-	-	13/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	II0	i	314	-	-	10/21/67/67	0/2/2/2
29	CLA	B	810	2	-	10/39/115/115	-
32	WVN	I	101	-	-	18/29/63/63	0/2/2/2
29	CLA	d	309	23	-	4/10/86/115	-
40	KC2	n	612	26	-	12/15/71/71	-
31	LHG	A	848	-	-	14/27/27/53	-
29	CLA	B	826	2	-	9/39/115/115	-
29	CLA	a	304	15	-	2/23/99/115	-
29	CLA	L	204	9,41	-	4/33/109/115	-
40	KC2	i	310	22	-	10/15/71/71	-
38	II0	i	313	-	-	11/21/67/67	0/2/2/2
28	CL0	A	801	-	-	11/39/115/115	-
39	IHT	f	617	-	-	2/25/65/65	0/2/2/2
33	LMU	B	850	-	-	4/21/61/61	0/2/2/2
29	CLA	h	305	17	-	12/39/115/115	-
38	II0	k	615	-	-	14/21/67/67	0/2/2/2
31	LHG	j	318	29	-	13/34/34/53	-
29	CLA	e	306	19	-	16/39/115/115	-
29	CLA	a	308	15	-	11/39/115/115	-
29	CLA	B	821	2	-	7/25/101/115	-
29	CLA	B	807	2	-	8/39/115/115	-
29	CLA	d	307	23	-	8/15/91/115	-
32	WVN	B	846	-	-	15/29/63/63	0/2/2/2
29	CLA	m	610	31	-	18/27/103/115	-
29	CLA	R	203	25	-	7/27/103/115	-
39	IHT	j	317	-	-	2/25/65/65	0/2/2/2
29	CLA	B	814	2	-	10/39/115/115	-
29	CLA	a	311	15	-	13/39/115/115	-
29	CLA	B	813	2	-	13/33/109/115	-
38	II0	m	618	-	-	13/21/67/67	0/2/2/2
32	WVN	M	101	-	-	17/29/63/63	0/2/2/2
29	CLA	J	102	8	-	5/12/88/115	-
29	CLA	g	306	24	-	12/39/115/115	-
39	IHT	g	320	-	-	5/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	c	316	29	-	19/41/41/53	-
29	CLA	n	608	26	-	18/39/115/115	-
29	CLA	c	304	14	-	16/36/112/115	-
36	DGD	B	844	-	-	28/55/95/95	0/2/2/2
39	IHT	R	204	-	-	1/25/65/65	0/2/2/2
38	II0	n	616	-	-	10/21/67/67	0/2/2/2
29	CLA	A	816	1	-	16/39/115/115	-
29	CLA	g	311	38,24	-	19/39/115/115	-
29	CLA	A	828	1	-	9/39/115/115	-
29	CLA	a	303	15	-	6/29/105/115	-
29	CLA	i	309	31	-	8/17/93/115	-
29	CLA	L	203	9	-	6/39/115/115	-
38	II0	n	614	-	-	10/21/67/67	0/2/2/2
31	LHG	J	104	29	-	16/37/37/53	-
38	II0	k	619	-	-	11/21/67/67	0/2/2/2
29	CLA	A	833	1	-	14/39/115/115	-
29	CLA	m	601	18	-	6/12/88/115	-
40	KC2	k	612	21	-	9/15/71/71	-
29	CLA	l	306	20	-	19/39/115/115	-
37	LMG	n	620	-	-	18/46/66/70	0/1/1/1
29	CLA	c	303	14	-	6/23/99/115	-
29	CLA	O	202	41	-	10/39/115/115	-
40	KC2	g	315	40	-	7/15/71/71	-
38	II0	g	317	29	-	9/21/67/67	0/2/2/2
29	CLA	m	606	18	-	17/39/115/115	-
29	CLA	l	310	31	-	14/35/111/115	-
29	CLA	l	303	20	-	8/18/94/115	-
29	CLA	b	302	16	-	6/23/99/115	-
29	CLA	m	604	18	-	12/39/115/115	-
29	CLA	A	851	1	-	14/39/115/115	-
29	CLA	i	307	22	-	10/35/111/115	-
40	KC2	n	611	-	-	5/15/71/71	-
29	CLA	g	307	24	-	13/23/99/115	-
38	II0	k	620	-	-	13/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	II0	J	103	-	-	14/21/67/67	0/2/2/2
29	CLA	j	306	18	-	10/15/91/115	-
29	CLA	j	310	18	-	15/39/115/115	-
29	CLA	c	311	14	-	9/15/91/115	-
38	II0	l	317	-	-	1/21/67/67	0/2/2/2
39	IHT	n	617	-	-	6/25/65/65	0/2/2/2
29	CLA	B	841	2	-	20/39/115/115	-
29	CLA	A	824	41	-	10/39/115/115	-
29	CLA	n	613	26	-	10/23/99/115	-
29	CLA	i	305	22	-	15/39/115/115	-
29	CLA	n	602	26	-	5/21/97/115	-
29	CLA	g	305	24,39	-	5/39/115/115	-
29	CLA	e	308	31	-	3/17/93/115	-
29	CLA	B	812	2	-	13/39/115/115	-
32	WVN	B	845	-	-	6/29/63/63	0/2/2/2
39	IHT	a	316	-	-	5/25/65/65	0/2/2/2
37	LMG	F	208	-	-	13/36/56/70	0/1/1/1
29	CLA	B	825	2	-	18/39/115/115	-
29	CLA	L	207	41	-	10/23/99/115	-
29	CLA	c	308	14	-	15/39/115/115	-
38	II0	a	314	-	-	10/21/67/67	0/2/2/2
39	IHT	b	316	-	-	8/25/65/65	0/2/2/2
29	CLA	F	201	41	-	16/39/115/115	-
29	CLA	B	809	2	-	9/39/115/115	-
29	CLA	A	822	1	-	15/29/105/115	-
29	CLA	i	306	22	-	9/23/99/115	-
38	II0	i	316	-	-	12/21/67/67	0/2/2/2
29	CLA	i	302	22	-	20/39/115/115	-
29	CLA	j	303	18	-	9/26/102/115	-
29	CLA	A	802	-	-	10/39/115/115	-
38	II0	j	301	-	-	14/21/67/67	0/2/2/2
37	LMG	c	317	-	-	21/50/70/70	0/1/1/1
29	CLA	d	310	23	-	6/10/86/115	-
29	CLA	n	609	26	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	IHT	g	324	29	-	7/25/65/65	0/2/2/2
29	CLA	d	303	23	-	7/23/99/115	-
29	CLA	h	301	41	-	11/39/115/115	-
32	WVN	F	207	-	-	18/29/63/63	0/2/2/2
30	PQN	B	843	-	-	8/23/43/43	0/2/2/2
29	CLA	B	822	41	-	18/39/115/115	-
29	CLA	K	102	12	-	6/12/88/115	-
29	CLA	B	805	2	-	13/39/115/115	-
33	LMU	i	301	-	-	13/21/61/61	0/2/2/2
37	LMG	Q	301	-	-	16/33/53/70	0/1/1/1
29	CLA	B	804	-	-	10/39/115/115	-
29	CLA	A	811	1	-	7/26/102/115	-
29	CLA	B	827	2	-	5/23/99/115	-
29	CLA	l	308	20	-	6/39/115/115	-
29	CLA	b	313	31	-	7/23/99/115	-
33	LMU	A	855	-	-	17/20/60/61	0/2/2/2
29	CLA	B	820	2	-	13/39/115/115	-
33	LMU	a	319	-	-	13/21/61/61	0/2/2/2
32	WVN	B	848	-	-	15/29/63/63	0/2/2/2
33	LMU	A	849	-	-	16/21/61/61	0/2/2/2
32	WVN	L	205	-	-	16/29/63/63	0/2/2/2
38	II0	b	314	-	-	13/21/67/67	0/2/2/2
29	CLA	l	312	20	-	10/29/105/115	-
32	WVN	A	854	-	-	19/29/63/63	0/2/2/2
38	II0	a	317	-	-	13/21/67/67	0/2/2/2
29	CLA	c	309	31	-	6/15/91/115	-
29	CLA	a	309	31	-	7/19/95/115	-
29	CLA	c	302	14	-	16/33/109/115	-
29	CLA	j	308	18	-	9/23/99/115	-
38	II0	k	617	-	-	4/21/67/67	0/2/2/2
29	CLA	B	837	2	-	17/39/115/115	-
29	CLA	b	303	16	-	11/27/103/115	-
31	LHG	s	408	29	-	12/34/34/53	-
38	II0	n	618	-	-	10/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	KC2	c	310	14	-	10/15/71/71	-
29	CLA	s	403	13	-	10/39/115/115	-
34	SF4	A	852	2,1	-	-	0/6/5/5
29	CLA	B	802	41	-	12/39/115/115	-
29	CLA	m	602	18	-	13/33/109/115	-
29	CLA	n	607	26	-	12/39/115/115	-
31	LHG	L	208	-	-	19/51/51/53	-
32	WVN	s	407	-	-	14/29/63/63	0/2/2/2
29	CLA	h	312	41	-	8/39/115/115	-
29	CLA	m	603	18	-	7/32/108/115	-
32	WVN	B	849	-	-	14/29/63/63	0/2/2/2
29	CLA	B	836	41	-	15/39/115/115	-
29	CLA	c	307	14	-	9/17/93/115	-
29	CLA	f	609	18	-	11/39/115/115	-
29	CLA	B	829	2	-	8/39/115/115	-
40	KC2	s	404	-	-	2/15/71/71	-
29	CLA	h	307	17	-	7/23/99/115	-
38	II0	f	616	-	-	12/21/67/67	0/2/2/2
29	CLA	l	304	20	-	14/39/115/115	-
29	CLA	A	823	1	-	11/27/103/115	-
32	WVN	L	201	-	-	22/29/63/63	0/2/2/2
29	CLA	A	817	1	-	12/39/115/115	-
29	CLA	m	612	41	-	11/23/99/115	-
29	CLA	k	602	21	-	19/39/115/115	-
29	CLA	n	601	26	-	7/15/91/115	-
29	CLA	d	308	23	-	9/17/93/115	-
29	CLA	k	603	21	-	0/23/99/115	-
38	II0	e	313	-	-	13/21/67/67	0/2/2/2
38	II0	e	312	-	-	14/21/67/67	0/2/2/2
29	CLA	A	810	1	-	19/39/115/115	-
38	II0	l	313	-	-	12/21/67/67	0/2/2/2
39	IHT	O	204	-	-	4/25/65/65	0/2/2/2
29	CLA	A	815	41	-	7/15/91/115	-
29	CLA	g	323	31	-	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	O	201	31	-	9/24/100/115	-
29	CLA	b	306	41	-	15/39/115/115	-
31	LHG	c	320	-	-	23/53/53/53	-
31	LHG	b	318	29	-	27/53/53/53	-
29	CLA	k	605	21	-	7/15/91/115	-
29	CLA	k	614	21	-	13/23/99/115	-
29	CLA	j	309	18	-	6/15/91/115	-
38	II0	b	317	-	-	9/21/67/67	0/2/2/2
29	CLA	h	302	17	-	6/21/97/115	-
29	CLA	B	842	31	-	7/39/115/115	-
29	CLA	g	310	24	-	16/39/115/115	-
29	CLA	Q	302	-	-	21/39/115/115	-
29	CLA	m	605	18	-	7/12/88/115	-
40	KC2	g	313	-	-	8/15/71/71	-
29	CLA	B	835	2	-	3/18/94/115	-
29	CLA	e	302	19	-	17/39/115/115	-
29	CLA	g	303	24	-	7/12/88/115	-
29	CLA	i	311	-	-	13/33/109/115	-
38	II0	l	315	-	-	11/21/67/67	0/2/2/2
38	II0	m	615	-	-	12/21/67/67	0/2/2/2
31	LHG	a	301	29	-	22/53/53/53	-
29	CLA	A	830	1	-	7/33/109/115	-
29	CLA	O	206	11	-	11/39/115/115	-
38	II0	g	318	-	-	13/21/67/67	0/2/2/2
31	LHG	g	301	29	-	24/49/49/53	-
29	CLA	k	610	-	-	10/23/99/115	-
38	II0	c	314	-	-	4/21/67/67	0/2/2/2
29	CLA	n	606	26	-	5/23/99/115	-
29	CLA	j	304	18	-	7/23/99/115	-
35	SQD	A	853	-	-	19/49/69/69	0/1/1/1
29	CLA	j	313	-	-	12/23/99/115	-
29	CLA	A	832	1	-	8/39/115/115	-
40	KC2	f	611	-	-	8/15/71/71	-
37	LMG	O	205	-	-	10/21/41/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	829	1	-	8/39/115/115	-
38	II0	d	314	-	-	3/21/67/67	0/2/2/2
29	CLA	A	834	1	-	8/33/109/115	-
29	CLA	B	808	2	-	7/39/115/115	-
29	CLA	i	303	22	-	18/39/115/115	-
29	CLA	B	803	2	-	17/39/115/115	-
29	CLA	i	308	22	-	19/39/115/115	-
29	CLA	k	606	21	-	7/23/99/115	-
29	CLA	A	807	1	-	7/39/115/115	-
29	CLA	s	406	41	-	12/39/115/115	-
37	LMG	F	206	-	-	31/48/68/70	0/1/1/1
40	KC2	d	311	-	-	12/15/71/71	-
38	II0	k	618	-	-	5/21/67/67	0/2/2/2
29	CLA	a	312	15	-	8/19/95/115	-
29	CLA	A	838	1	-	11/39/115/115	-
29	CLA	f	612	41	-	12/23/99/115	-
29	CLA	s	402	13	-	23/39/115/115	-
32	WVN	K	103	-	-	14/29/63/63	0/2/2/2
29	CLA	k	609	21	-	10/30/106/115	-
31	LHG	A	843	29	-	6/31/31/53	-
29	CLA	A	839	1	-	3/33/109/115	-
29	CLA	b	309	37	-	5/39/115/115	-
29	CLA	e	305	19	-	10/39/115/115	-
29	CLA	m	613	18	-	17/39/115/115	-
29	CLA	e	310	41	-	9/27/103/115	-
30	PQN	A	841	-	-	10/23/43/43	0/2/2/2
32	WVN	l	302	-	-	16/29/63/63	0/2/2/2
29	CLA	g	308	24	-	7/23/99/115	-
38	II0	f	618	-	-	12/21/67/67	0/2/2/2
31	LHG	n	619	-	-	20/47/47/53	-
29	CLA	A	806	1	-	5/33/109/115	-
29	CLA	m	608	18	-	12/39/115/115	-
29	CLA	F	202	41	-	15/39/115/115	-
29	CLA	A	831	1	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	e	307	19	-	15/39/115/115	-
32	WVN	h	308	-	-	18/29/63/63	0/2/2/2
38	II0	e	316	-	-	13/21/67/67	0/2/2/2
32	WVN	B	847	-	-	14/29/63/63	0/2/2/2
31	LHG	e	317	29	-	21/41/41/53	-
29	CLA	e	304	-	-	16/39/115/115	-
38	II0	b	315	-	-	10/21/67/67	0/2/2/2
29	CLA	c	312	14	-	12/39/115/115	-
29	CLA	k	604	21	-	12/39/115/115	-
37	LMG	c	318	29	-	21/38/58/70	0/1/1/1
29	CLA	B	801	41	-	17/39/115/115	-
29	CLA	f	607	18	-	15/39/115/115	-
38	II0	f	614	-	-	11/21/67/67	0/2/2/2
40	KC2	i	318	22	-	8/15/71/71	-
29	CLA	a	306	15	-	9/15/91/115	-
29	CLA	f	610	31	-	12/39/115/115	-
29	CLA	f	601	18	-	6/18/94/115	-
38	II0	d	315	-	-	11/21/67/67	0/2/2/2
29	CLA	d	302	23	-	17/36/112/115	-
29	CLA	g	302	-	-	17/39/115/115	-
29	CLA	j	311	31	-	15/35/111/115	-
31	LHG	a	318	29	-	27/53/53/53	-
29	CLA	e	303	19	-	6/23/99/115	-
32	WVN	s	405	-	-	14/29/63/63	0/2/2/2
40	KC2	k	613	-	-	9/15/71/71	-
29	CLA	B	816	2	-	17/39/115/115	-
29	CLA	k	601	21	-	7/23/99/115	-
31	LHG	L	209	-	-	23/40/40/53	-
29	CLA	B	833	2	-	5/27/103/115	-
32	WVN	A	845	-	-	17/29/63/63	0/2/2/2
29	CLA	m	609	18	-	17/33/109/115	-
37	LMG	b	319	-	-	17/37/57/70	0/1/1/1
29	CLA	L	202	9	-	8/20/96/115	-
29	CLA	g	304	24	-	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	805	1	-	10/39/115/115	-
29	CLA	A	819	1	-	19/39/115/115	-
38	II0	m	616	-	-	11/21/67/67	0/2/2/2
32	WVN	F	204	-	-	14/29/63/63	0/2/2/2
29	CLA	B	818	41	-	14/39/115/115	-
40	KC2	j	312	18	-	8/15/71/71	-
29	CLA	A	821	1	-	6/20/96/115	-
29	CLA	e	311	19	-	18/39/115/115	-
29	CLA	A	825	41	-	6/39/115/115	-
29	CLA	f	613	18	-	16/39/115/115	-
38	II0	m	614	-	-	13/21/67/67	0/2/2/2
31	LHG	f	619	-	-	18/53/53/53	-
29	CLA	A	850	41	-	3/39/115/115	-
29	CLA	m	607	18,31	-	3/23/99/115	-
31	LHG	A	842	-	-	23/52/52/53	-
29	CLA	A	814	1	-	8/21/97/115	-
29	CLA	h	303	17,37	-	8/21/97/115	-
32	WVN	i	315	-	-	18/29/63/63	0/2/2/2
38	II0	d	316	-	-	11/21/67/67	0/2/2/2
29	CLA	n	610	-	-	16/33/109/115	-
38	II0	i	319	-	-	12/21/67/67	0/2/2/2
29	CLA	A	837	1	-	13/39/115/115	-
29	CLA	i	304	22	-	7/39/115/115	-
29	CLA	A	804	1	-	5/39/115/115	-
31	LHG	f	620	29	-	21/41/41/53	-
29	CLA	n	603	26	-	11/23/99/115	-
29	CLA	A	827	1	-	7/36/112/115	-
32	WVN	R	202	-	-	15/29/63/63	0/2/2/2
29	CLA	A	820	41	-	7/39/115/115	-
29	CLA	d	318	-	-	8/15/91/115	-
29	CLA	d	313	23	-	10/23/99/115	-
29	CLA	h	306	17	-	12/30/106/115	-
29	CLA	j	302	18,31	-	16/39/115/115	-
29	CLA	e	301	19	-	10/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	IHT	c	319	-	-	8/25/65/65	0/2/2/2
29	CLA	c	301	14	-	11/23/99/115	-
31	LHG	l	318	29	-	12/36/36/53	-
38	II0	g	321	-	-	3/21/67/67	0/2/2/2
29	CLA	A	826	1	-	9/39/115/115	-
29	CLA	B	830	2	-	7/21/97/115	-
39	IHT	c	315	-	-	6/25/65/65	0/2/2/2
29	CLA	B	832	41	-	4/15/91/115	-
38	II0	j	316	-	-	13/21/67/67	0/2/2/2
29	CLA	a	307	15	-	15/39/115/115	-
38	II0	g	319	-	-	13/21/67/67	0/2/2/2
38	II0	e	314	-	-	11/21/67/67	0/2/2/2
38	II0	l	314	-	-	11/21/67/67	0/2/2/2
38	II0	a	315	-	-	11/21/67/67	0/2/2/2
29	CLA	B	824	2	-	3/39/115/115	-
29	CLA	K	101	41	-	19/39/115/115	-
32	WVN	R	201	-	-	18/29/63/63	0/2/2/2
29	CLA	n	605	26	-	11/23/99/115	-
29	CLA	A	836	1	-	10/39/115/115	-
29	CLA	B	839	2	-	10/30/106/115	-
29	CLA	g	316	24	-	10/30/106/115	-
29	CLA	b	310	16	-	13/39/115/115	-
38	II0	n	615	-	-	12/21/67/67	0/2/2/2
32	WVN	L	206	-	-	17/29/63/63	0/2/2/2
38	II0	k	616	-	-	12/21/67/67	0/2/2/2
29	CLA	g	309	24	-	12/39/115/115	-
29	CLA	f	603	18	-	6/23/99/115	-
40	KC2	e	309	-	-	9/15/71/71	-
29	CLA	B	806	2	-	16/39/115/115	-
31	LHG	m	619	29	-	13/41/41/53	-
38	II0	O	203	-	-	4/21/67/67	0/2/2/2
29	CLA	B	831	41	-	9/39/115/115	-
29	CLA	A	813	1	-	9/29/105/115	-
29	CLA	d	305	23	-	5/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	j	314	18	-	12/39/115/115	-
38	II0	h	311	-	-	12/21/67/67	0/2/2/2
34	SF4	C	101	3	-	-	0/6/5/5
31	LHG	i	317	29	-	16/41/41/53	-
29	CLA	B	811	2	-	3/27/103/115	-
29	CLA	i	312	22	-	16/39/115/115	-
29	CLA	A	812	1	-	10/39/115/115	-
29	CLA	l	309	20	-	10/30/106/115	-
29	CLA	g	312	31	-	5/26/102/115	-
40	KC2	k	611	-	-	8/15/71/71	-
32	WVN	l	316	-	-	19/29/63/63	0/2/2/2
40	KC2	m	611	18	-	7/15/71/71	-
29	CLA	b	308	16	-	11/39/115/115	-
29	CLA	B	823	41	-	8/38/114/115	-
32	WVN	J	101	-	-	17/29/63/63	0/2/2/2
38	II0	j	315	-	-	11/21/67/67	0/2/2/2
29	CLA	F	203	6	-	10/24/100/115	-
31	LHG	g	322	29	-	17/41/41/53	-
40	KC2	l	311	-	-	6/15/71/71	-
29	CLA	f	604	18	-	13/39/115/115	-
40	KC2	s	401	13	-	7/15/71/71	-
29	CLA	f	605	18	-	6/15/91/115	-
32	WVN	A	847	-	-	18/29/63/63	0/2/2/2
29	CLA	l	307	20	-	7/39/115/115	-
39	IHT	m	617	-	-	2/25/65/65	0/2/2/2
38	II0	f	615	-	-	12/21/67/67	0/2/2/2
32	WVN	A	844	-	-	18/29/63/63	0/2/2/2
29	CLA	B	840	2	-	7/39/115/115	-
38	II0	d	317	-	-	13/21/67/67	0/2/2/2
29	CLA	B	815	2	-	3/27/103/115	-
29	CLA	A	808	29,1	-	10/39/115/115	-
29	CLA	B	834	2	-	11/39/115/115	-
29	CLA	l	301	20	-	11/39/115/115	-
29	CLA	A	803	29,1	-	8/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	304	16	-	2/24/100/115	-
29	CLA	b	307	16	-	8/35/111/115	-
40	KC2	d	312	23	-	12/15/71/71	-
29	CLA	A	835	1	-	14/39/115/115	-
29	CLA	b	312	16	-	17/39/115/115	-
29	CLA	A	809	1	-	11/29/105/115	-
29	CLA	d	306	23	-	8/23/99/115	-
40	KC2	g	314	24,40	-	10/15/71/71	-
29	CLA	a	310	15	-	11/39/115/115	-
29	CLA	j	307	18	-	5/23/99/115	-
29	CLA	b	305	16	-	15/39/115/115	-
32	WVN	F	205	-	-	21/29/63/63	0/2/2/2
29	CLA	l	305	20	-	0/23/99/115	-
29	CLA	B	819	2	-	18/39/115/115	-
29	CLA	c	305	14	-	7/39/115/115	-
36	DGD	j	319	18	-	23/51/91/95	0/2/2/2
29	CLA	B	828	2	-	10/21/97/115	-
38	II0	d	319	-	-	7/21/67/67	0/2/2/2
29	CLA	B	838	2	-	13/39/115/115	-
29	CLA	d	304	23	-	10/15/91/115	-
29	CLA	n	604	26	-	13/33/109/115	-
38	II0	h	310	-	-	11/21/67/67	0/2/2/2
29	CLA	a	302	15	-	11/39/115/115	-
29	CLA	f	606	18	-	6/23/99/115	-
38	II0	h	309	-	-	12/17/40/67	0/1/1/2
34	SF4	C	102	3	-	-	0/6/5/5
29	CLA	f	608	18	-	7/39/115/115	-
29	CLA	b	311	16	-	14/38/114/115	-
29	CLA	j	305	18	-	12/39/115/115	-
29	CLA	h	304	17	-	6/23/99/115	-
29	CLA	c	306	14	-	9/24/100/115	-
38	II0	d	301	-	-	14/21/67/67	0/2/2/2
29	CLA	k	607	21	-	8/23/99/115	-
38	II0	c	313	-	-	12/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	II0	a	313	-	-	12/21/67/67	0/2/2/2
32	WVN	A	846	-	-	15/29/63/63	0/2/2/2
29	CLA	f	602	18	-	18/39/115/115	-
29	CLA	A	818	1	-	15/39/115/115	-
29	CLA	a	305	41	-	8/39/115/115	-
29	CLA	B	817	2	-	13/39/115/115	-

The worst 5 of 4074 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	k	615	II0	C14-C10	20.53	1.57	1.34
38	g	317	II0	C13-C09	20.15	1.57	1.34
38	l	315	II0	C13-C09	20.10	1.57	1.34
38	d	315	II0	C14-C10	19.87	1.57	1.34
38	e	314	II0	C13-C09	19.81	1.57	1.34

The worst 5 of 4755 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	e	314	II0	C24-C22-C10	-25.41	111.10	175.43
38	i	313	II0	C24-C22-C10	-25.20	111.61	175.43
38	m	615	II0	C23-C21-C09	-24.97	112.20	175.43
38	m	616	II0	C23-C21-C09	-24.96	112.23	175.43
38	m	615	II0	C24-C22-C10	-24.96	112.24	175.43

There are no chirality outliers.

5 of 4748 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	801	CL0	C2B-C3B-CAB-CBB
28	A	801	CL0	C4B-C3B-CAB-CBB
29	A	804	CLA	CHA-CBD-CGD-O1D
29	A	804	CLA	CHA-CBD-CGD-O2D
29	A	805	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

249 monomers are involved in 448 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	k	608	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	840	CLA	5	0
29	B	810	CLA	1	0
31	A	848	LHG	1	0
29	B	826	CLA	1	0
29	L	204	CLA	1	0
28	A	801	CL0	5	0
33	B	850	LMU	1	0
29	h	305	CLA	3	0
29	e	306	CLA	2	0
29	a	308	CLA	2	0
29	B	821	CLA	2	0
29	B	807	CLA	3	0
29	d	307	CLA	1	0
29	m	610	CLA	2	0
29	R	203	CLA	5	0
29	B	814	CLA	3	0
29	a	311	CLA	2	0
29	B	813	CLA	3	0
29	g	306	CLA	1	0
39	g	320	IHT	1	0
31	c	316	LHG	1	0
29	n	608	CLA	4	0
36	B	844	DGD	4	0
38	n	616	II0	1	0
29	A	816	CLA	3	0
29	g	311	CLA	2	0
29	A	828	CLA	1	0
29	a	303	CLA	1	0
29	L	203	CLA	4	0
38	n	614	II0	3	0
31	J	104	LHG	3	0
29	A	833	CLA	3	0
29	l	306	CLA	1	0
37	n	620	LMG	2	0
29	c	303	CLA	2	0
29	O	202	CLA	1	0
40	g	315	KC2	3	0
38	g	317	II0	1	0
29	l	310	CLA	1	0
29	b	302	CLA	2	0
29	m	604	CLA	1	0
29	A	851	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	i	307	CLA	2	0
40	n	611	KC2	1	0
29	j	306	CLA	1	0
29	j	310	CLA	2	0
29	c	311	CLA	2	0
39	n	617	IHT	1	0
29	B	841	CLA	2	0
29	A	824	CLA	2	0
29	n	613	CLA	2	0
29	i	305	CLA	1	0
29	n	602	CLA	1	0
29	g	305	CLA	3	0
29	B	812	CLA	3	0
32	B	845	WVN	1	0
37	F	208	LMG	1	0
29	B	825	CLA	5	0
29	L	207	CLA	1	0
29	c	308	CLA	5	0
39	b	316	IHT	1	0
29	F	201	CLA	2	0
29	B	809	CLA	1	0
29	A	822	CLA	3	0
29	i	306	CLA	1	0
29	i	302	CLA	3	0
29	A	802	CLA	1	0
37	c	317	LMG	1	0
29	n	609	CLA	4	0
39	g	324	IHT	4	0
29	h	301	CLA	3	0
30	B	843	PQN	1	0
29	B	822	CLA	3	0
29	B	805	CLA	1	0
37	Q	301	LMG	4	0
29	B	804	CLA	2	0
29	A	811	CLA	1	0
29	B	827	CLA	2	0
29	l	308	CLA	2	0
29	b	313	CLA	3	0
33	A	855	LMU	3	0
29	B	820	CLA	3	0
38	b	314	II0	1	0
29	l	312	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	309	CLA	2	0
29	c	302	CLA	1	0
29	j	308	CLA	1	0
29	B	837	CLA	1	0
29	b	303	CLA	1	0
31	s	408	LHG	3	0
29	s	403	CLA	1	0
29	m	602	CLA	6	0
29	n	607	CLA	4	0
31	L	208	LHG	1	0
29	h	312	CLA	1	0
29	m	603	CLA	2	0
29	c	307	CLA	1	0
29	B	829	CLA	2	0
40	s	404	KC2	2	0
29	h	307	CLA	1	0
29	l	304	CLA	1	0
29	A	823	CLA	4	0
29	A	817	CLA	2	0
29	k	602	CLA	3	0
29	k	603	CLA	1	0
29	A	810	CLA	3	0
29	g	323	CLA	1	0
29	O	201	CLA	1	0
29	b	306	CLA	4	0
31	c	320	LHG	3	0
31	b	318	LHG	1	0
29	k	614	CLA	1	0
29	j	309	CLA	3	0
38	b	317	II0	1	0
29	B	842	CLA	3	0
29	g	310	CLA	1	0
29	Q	302	CLA	1	0
40	g	313	KC2	1	0
29	B	835	CLA	3	0
29	e	302	CLA	4	0
31	a	301	LHG	3	0
29	A	830	CLA	1	0
31	g	301	LHG	1	0
29	k	610	CLA	1	0
29	j	304	CLA	2	0
29	j	313	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	832	CLA	4	0
40	f	611	KC2	1	0
29	A	829	CLA	4	0
29	A	834	CLA	1	0
29	B	808	CLA	3	0
29	B	803	CLA	2	0
29	i	308	CLA	1	0
29	s	406	CLA	1	0
37	F	206	LMG	3	0
38	k	618	II0	1	0
29	a	312	CLA	1	0
29	A	838	CLA	4	0
29	s	402	CLA	2	0
29	k	609	CLA	1	0
31	A	843	LHG	1	0
29	b	309	CLA	3	0
29	e	305	CLA	2	0
29	m	613	CLA	4	0
30	A	841	PQN	4	0
31	n	619	LHG	3	0
29	A	806	CLA	2	0
29	m	608	CLA	1	0
29	F	202	CLA	2	0
29	A	831	CLA	1	0
29	e	307	CLA	3	0
29	e	304	CLA	1	0
29	c	312	CLA	2	0
29	k	604	CLA	2	0
37	c	318	LMG	3	0
29	B	801	CLA	1	0
29	f	607	CLA	1	0
40	i	318	KC2	2	0
29	f	610	CLA	2	0
29	f	601	CLA	1	0
29	d	302	CLA	2	0
29	g	302	CLA	3	0
29	j	311	CLA	1	0
29	B	816	CLA	2	0
31	L	209	LHG	1	0
29	B	833	CLA	1	0
37	b	319	LMG	2	0
29	L	202	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	g	304	CLA	6	0
29	A	819	CLA	1	0
29	e	311	CLA	2	0
29	f	613	CLA	3	0
31	f	619	LHG	3	0
29	A	850	CLA	2	0
29	m	607	CLA	4	0
31	A	842	LHG	1	0
29	A	814	CLA	3	0
29	n	610	CLA	4	0
29	A	837	CLA	3	0
29	i	304	CLA	1	0
29	A	804	CLA	4	0
29	n	603	CLA	1	0
29	A	827	CLA	6	0
29	A	820	CLA	1	0
29	d	313	CLA	3	0
29	h	306	CLA	2	0
29	j	302	CLA	1	0
29	e	301	CLA	1	0
29	c	301	CLA	1	0
38	g	321	II0	1	0
29	A	826	CLA	2	0
29	B	830	CLA	4	0
29	B	832	CLA	1	0
29	a	307	CLA	6	0
29	B	824	CLA	2	0
29	K	101	CLA	3	0
29	n	605	CLA	1	0
29	A	836	CLA	3	0
29	g	316	CLA	4	0
29	b	310	CLA	3	0
29	g	309	CLA	1	0
29	B	806	CLA	2	0
31	m	619	LHG	1	0
29	B	831	CLA	3	0
29	A	813	CLA	1	0
29	j	314	CLA	3	0
31	i	317	LHG	2	0
29	i	312	CLA	2	0
29	A	812	CLA	1	0
29	l	309	CLA	1	0

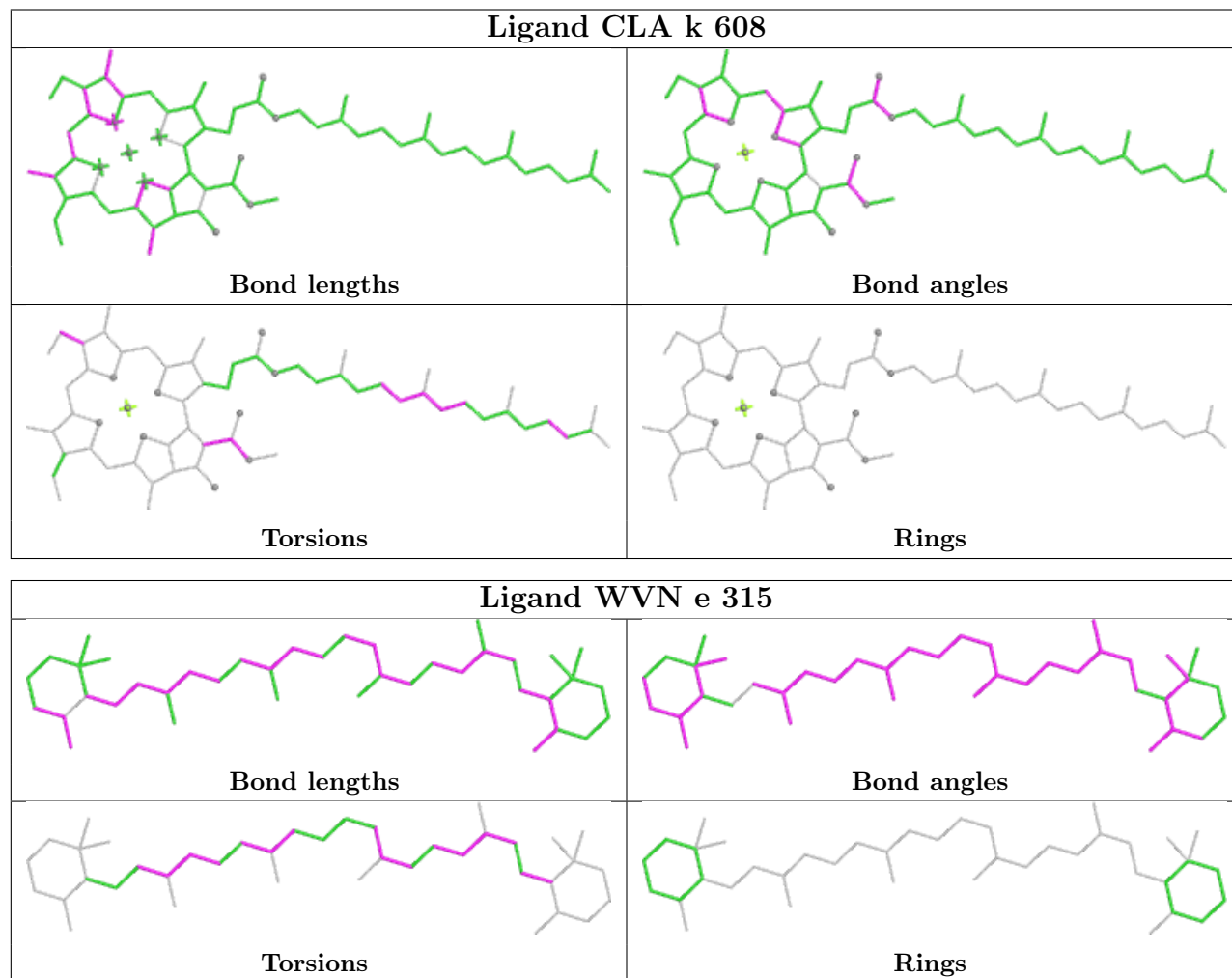
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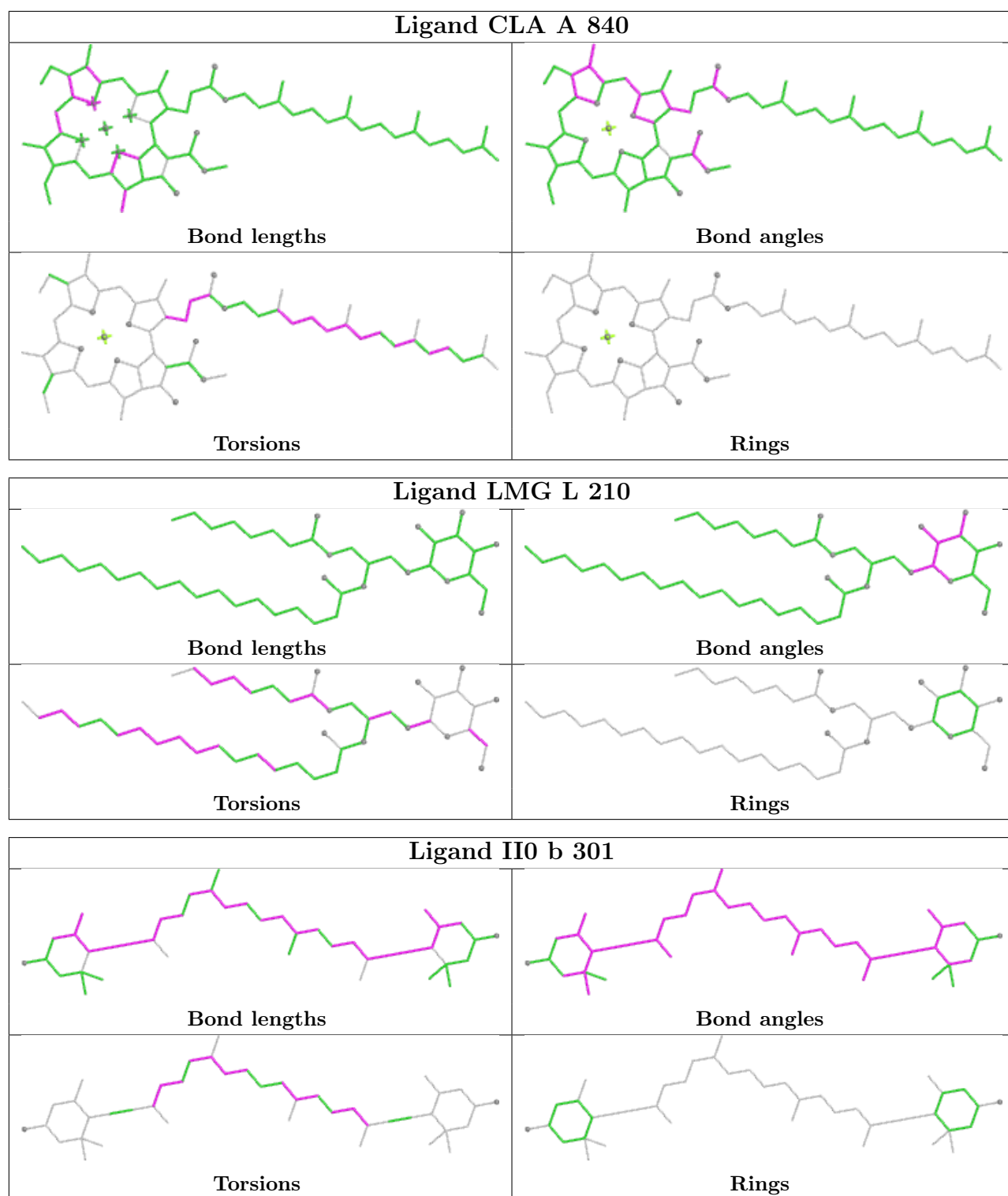
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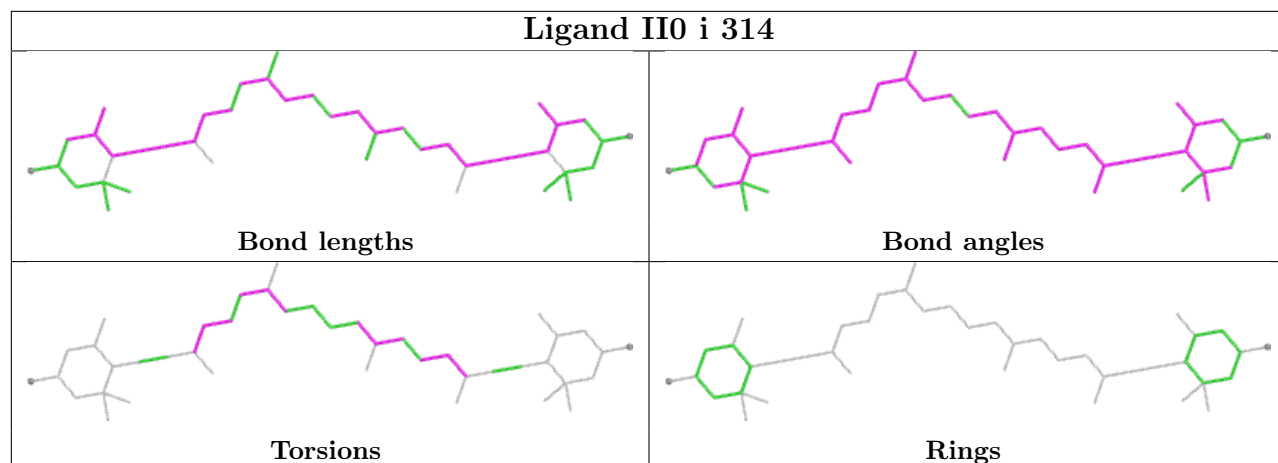
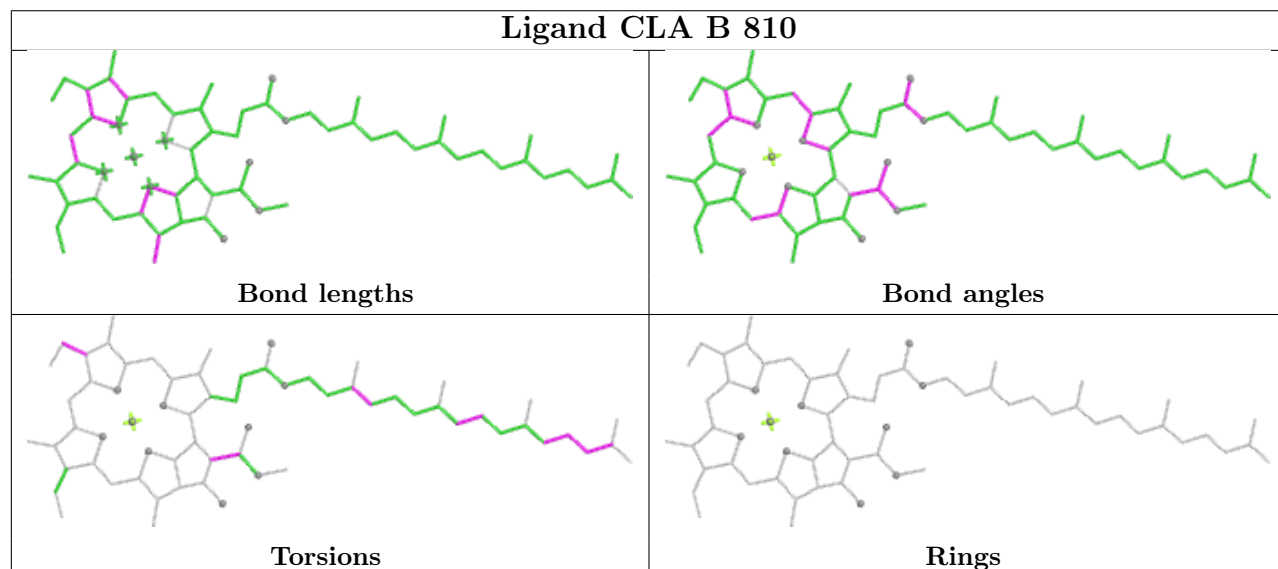
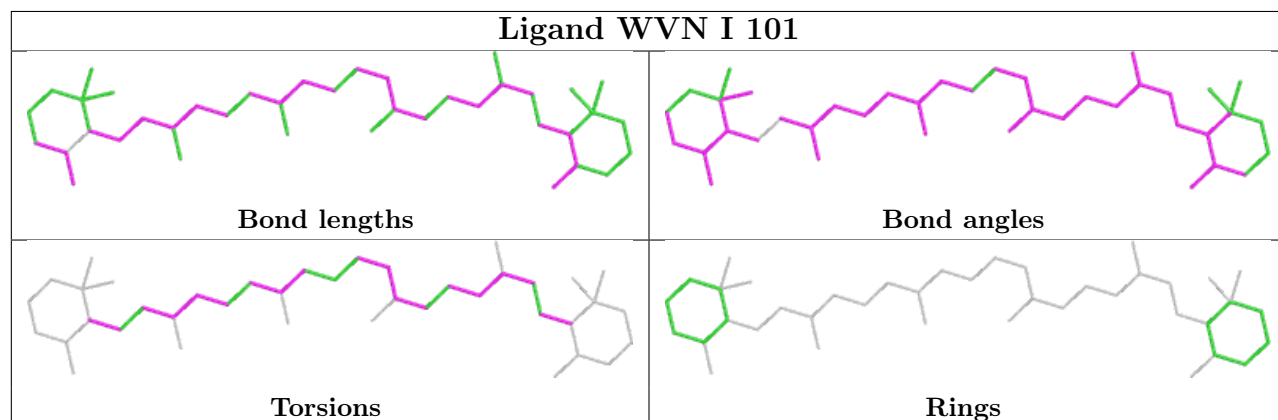
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	g	312	CLA	2	0
29	B	823	CLA	1	0
29	F	203	CLA	1	0
40	l	311	KC2	3	0
40	s	401	KC2	1	0
29	B	840	CLA	5	0
29	B	815	CLA	2	0
29	A	808	CLA	1	0
29	B	834	CLA	4	0
29	l	301	CLA	3	0
29	A	803	CLA	5	0
29	b	307	CLA	1	0
40	d	312	KC2	1	0
29	A	835	CLA	6	0
29	b	312	CLA	6	0
29	d	306	CLA	1	0
40	g	314	KC2	2	0
29	a	310	CLA	1	0
29	b	305	CLA	5	0
29	l	305	CLA	1	0
29	B	819	CLA	5	0
29	c	305	CLA	1	0
36	j	319	DGD	3	0
29	B	828	CLA	2	0
29	B	838	CLA	2	0
29	d	304	CLA	1	0
29	n	604	CLA	2	0
29	a	302	CLA	4	0
29	f	606	CLA	2	0
29	f	608	CLA	3	0
29	b	311	CLA	4	0
29	h	304	CLA	2	0
29	c	306	CLA	1	0
29	k	607	CLA	2	0
29	f	602	CLA	2	0
29	A	818	CLA	3	0
29	a	305	CLA	2	0
29	B	817	CLA	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

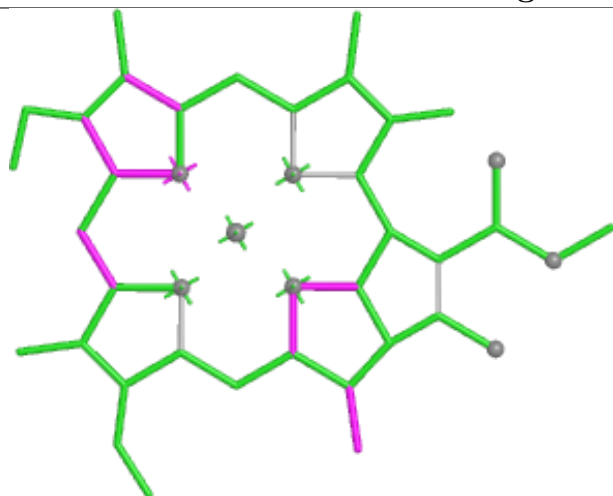
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



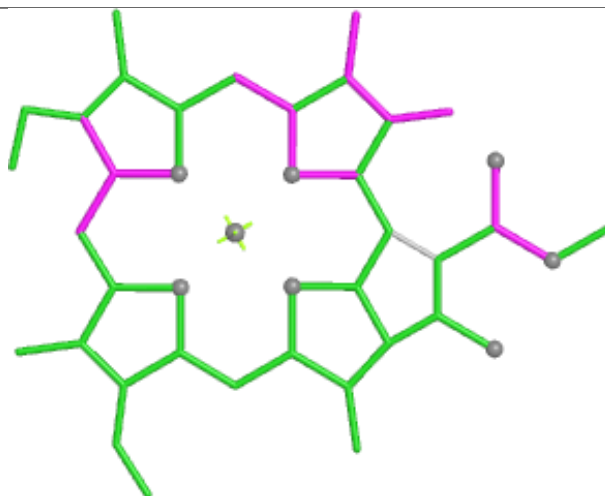


Ligand II0 i 314**Ligand CLA B 810****Ligand WVN I 101**

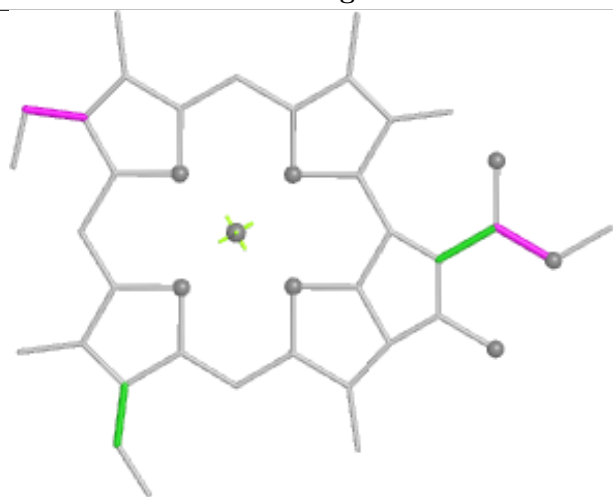
Ligand CLA d 309



Bond lengths



Bond angles

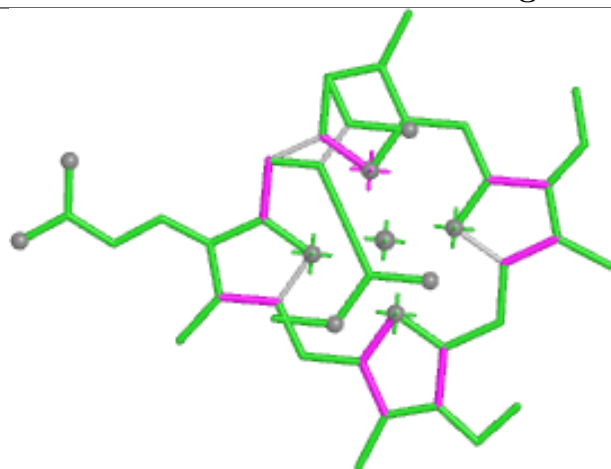


Torsions

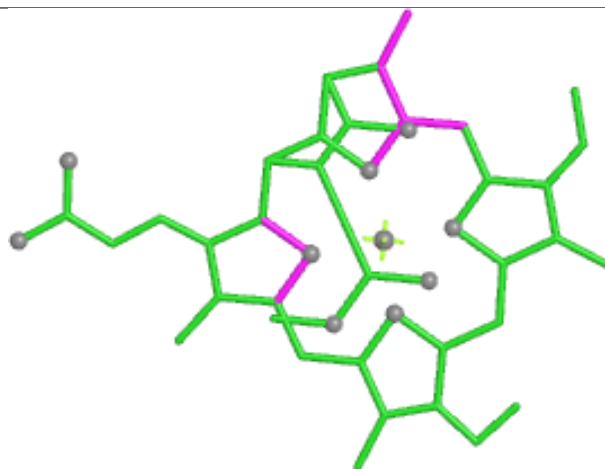


Rings

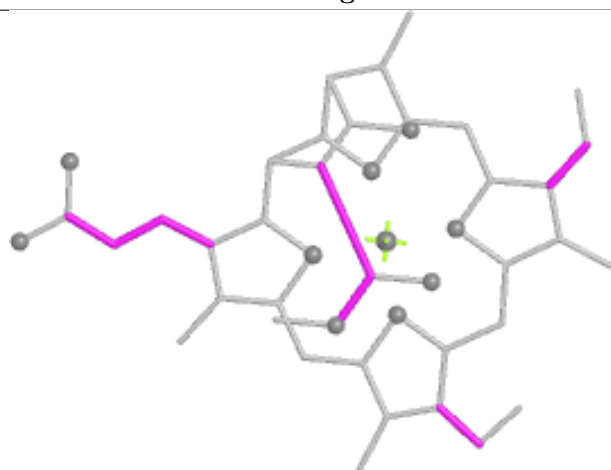
Ligand KC2 n 612



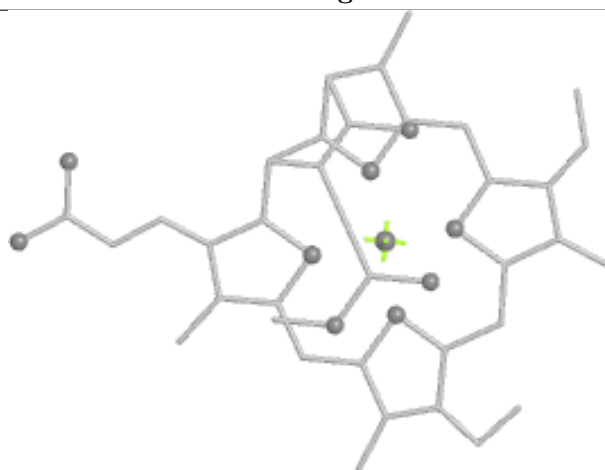
Bond lengths



Bond angles

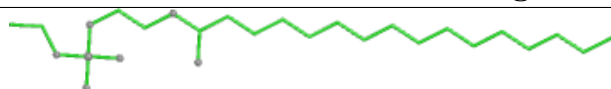


Torsions

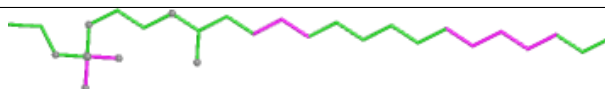


Rings

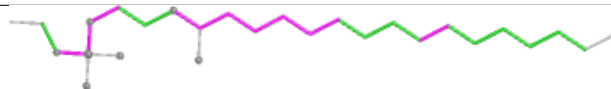
Ligand LHG A 848



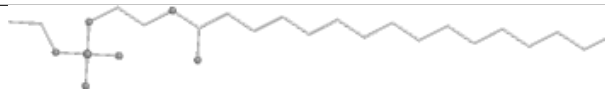
Bond lengths



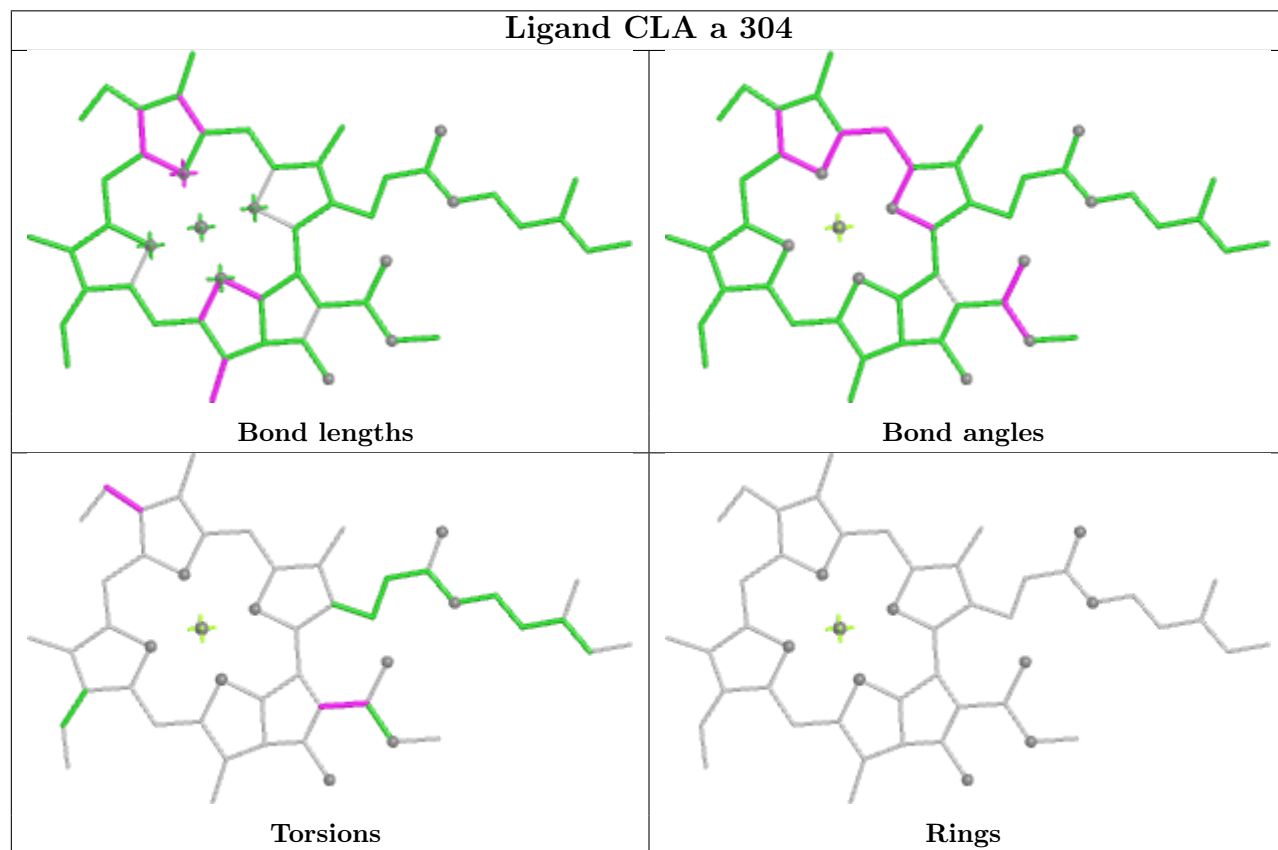
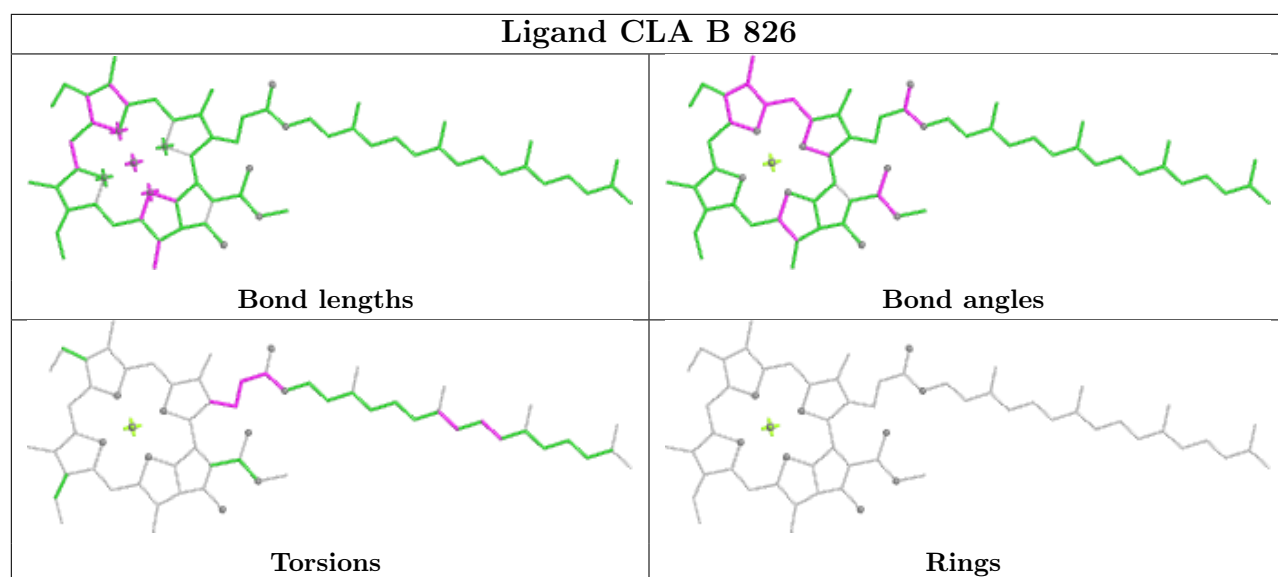
Bond angles



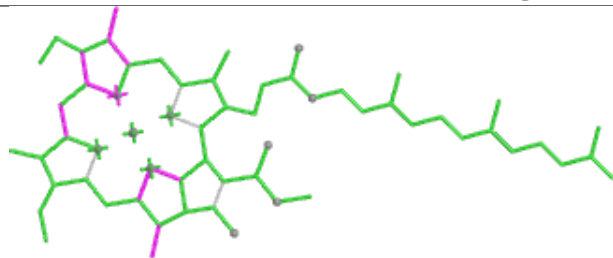
Torsions



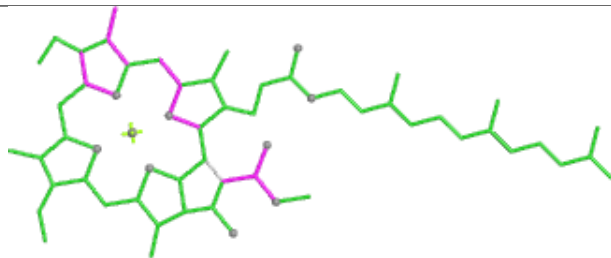
Rings



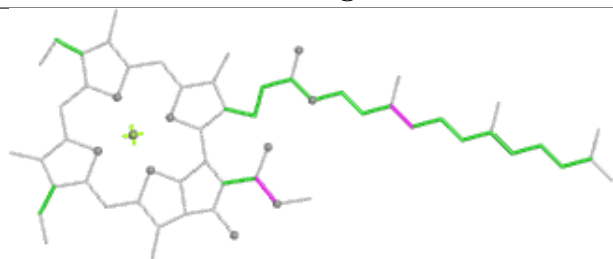
Ligand CLA L 204



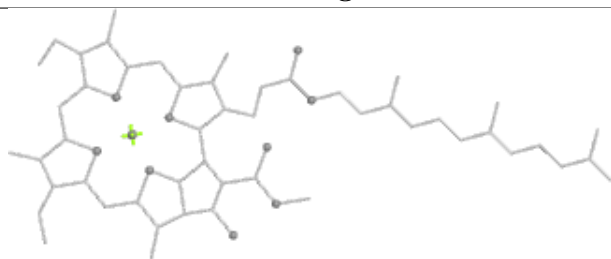
Bond lengths



Bond angles

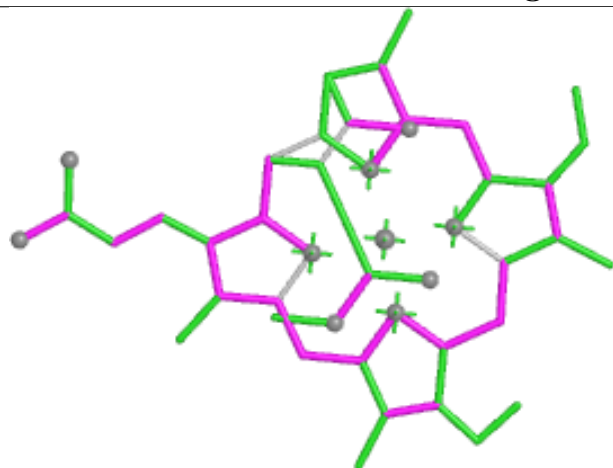


Torsions

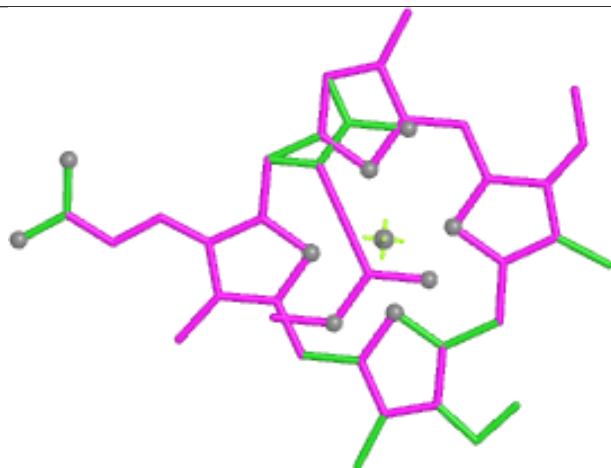


Rings

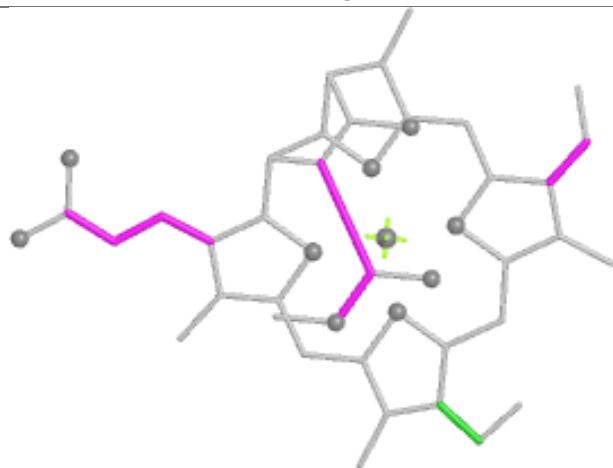
Ligand KC2 i 310



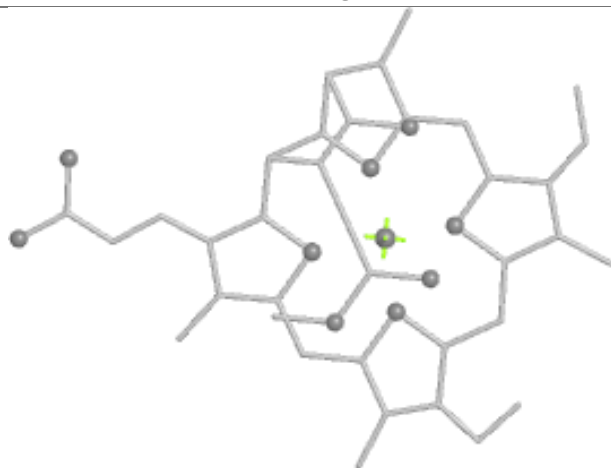
Bond lengths



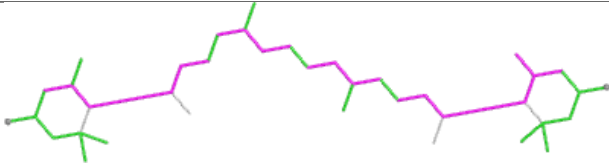
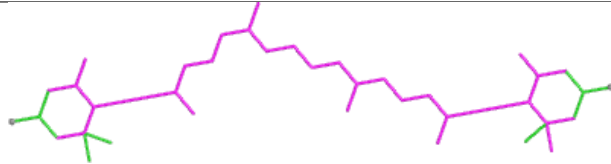
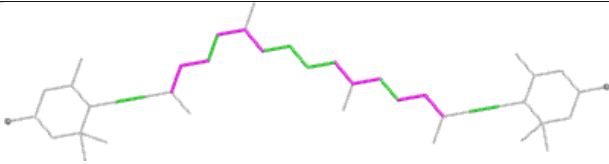
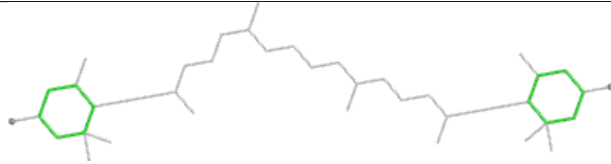
Bond angles

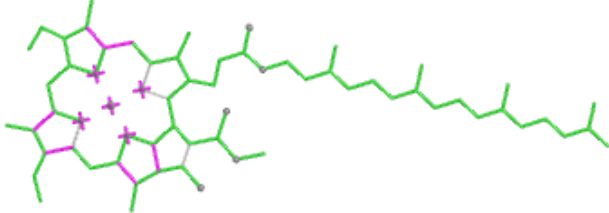
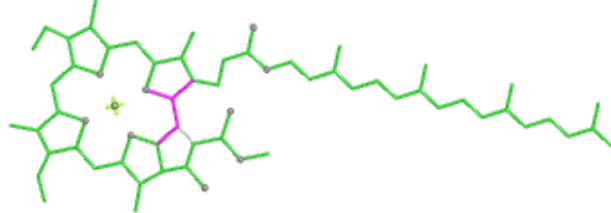
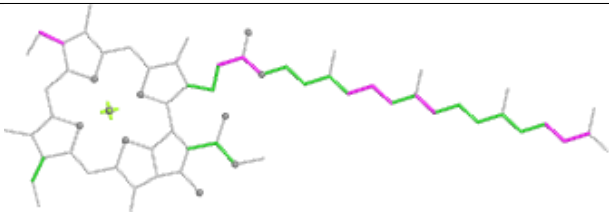
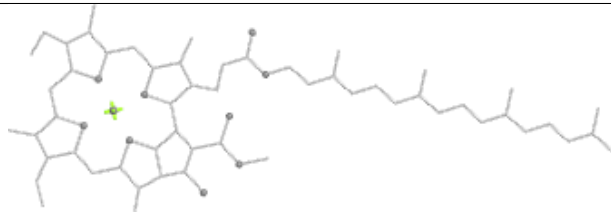


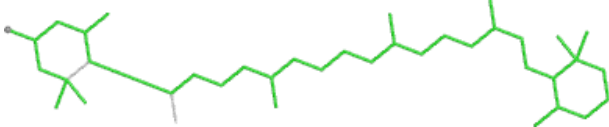
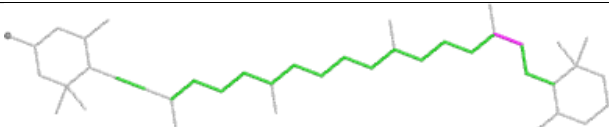
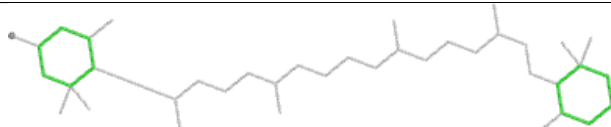
Torsions

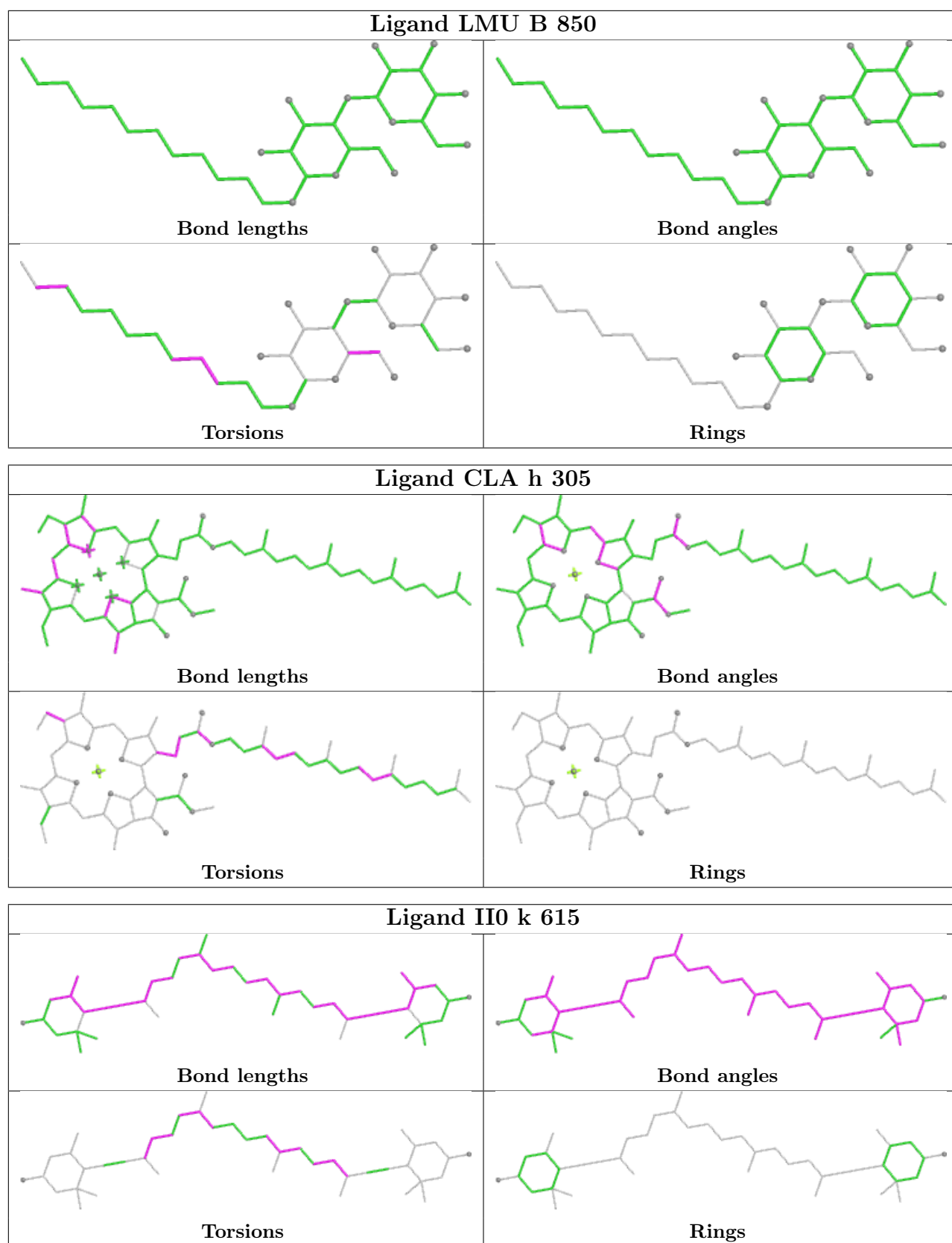


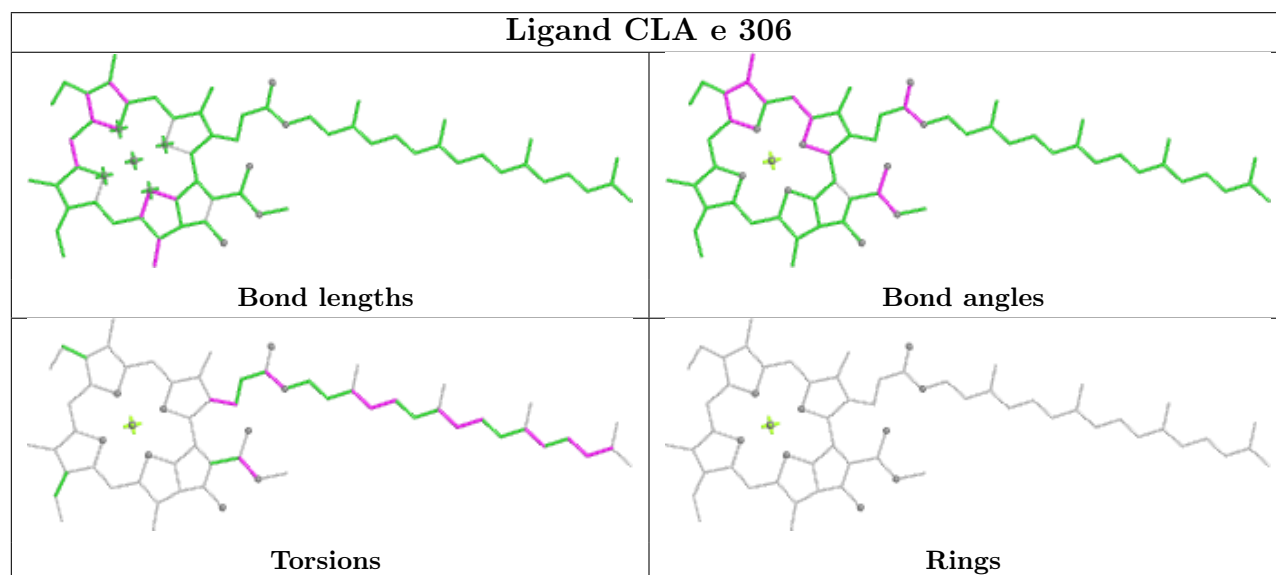
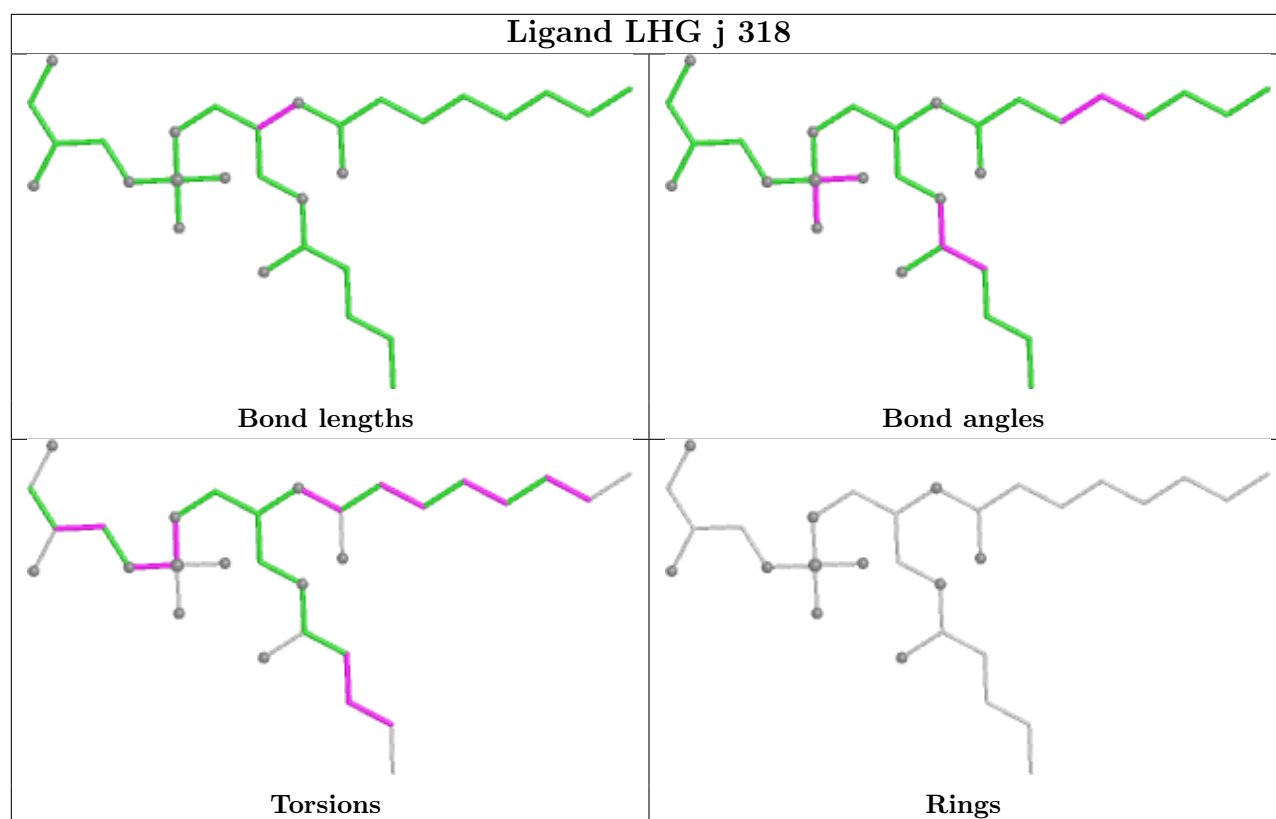
Rings

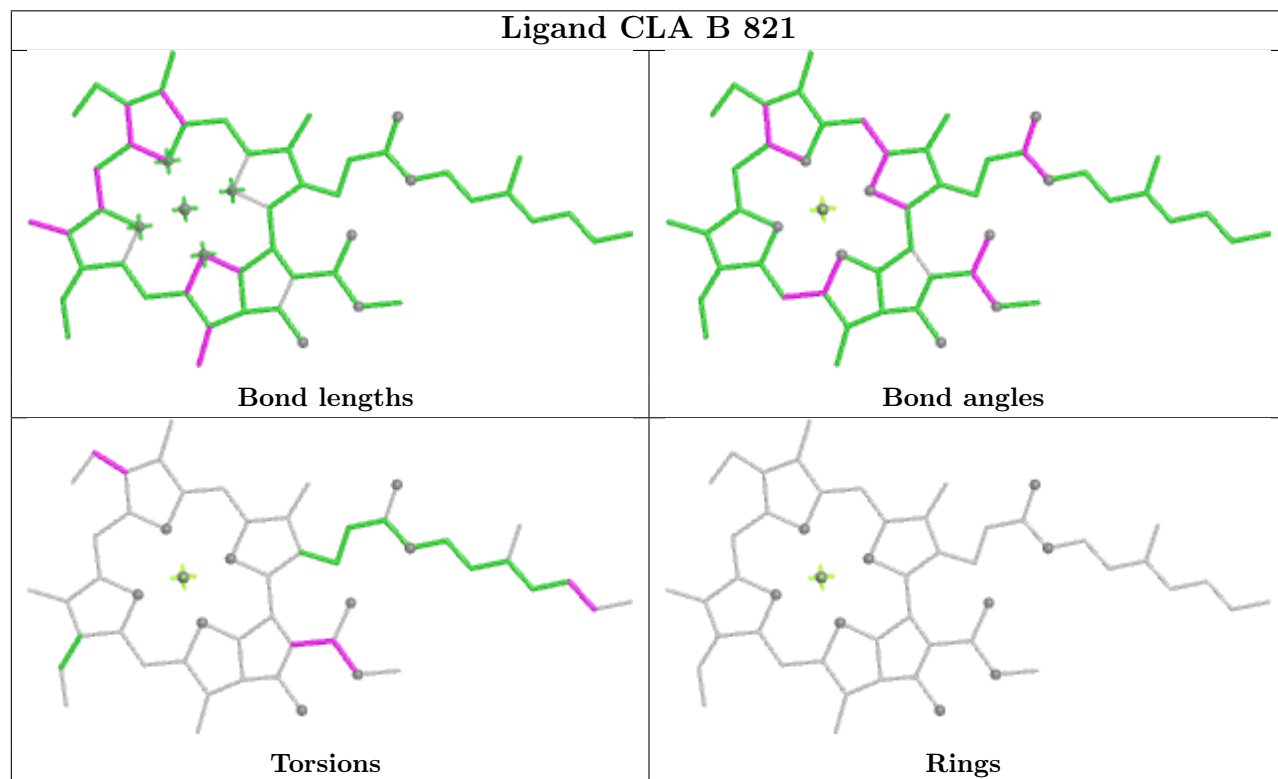
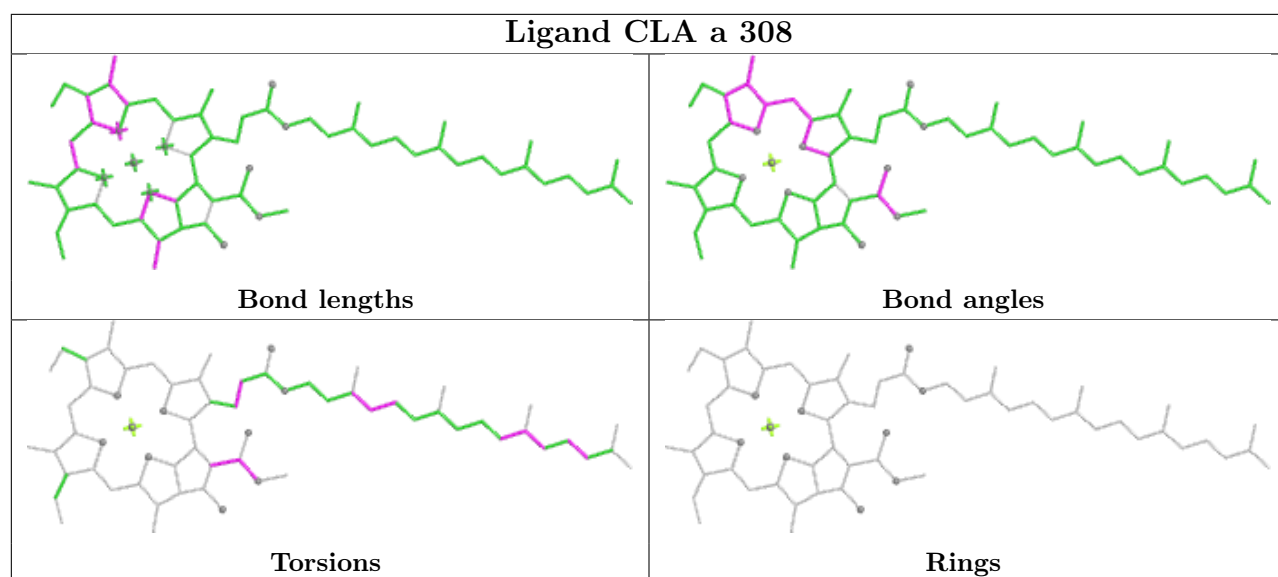
Ligand II0 i 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CL0 A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

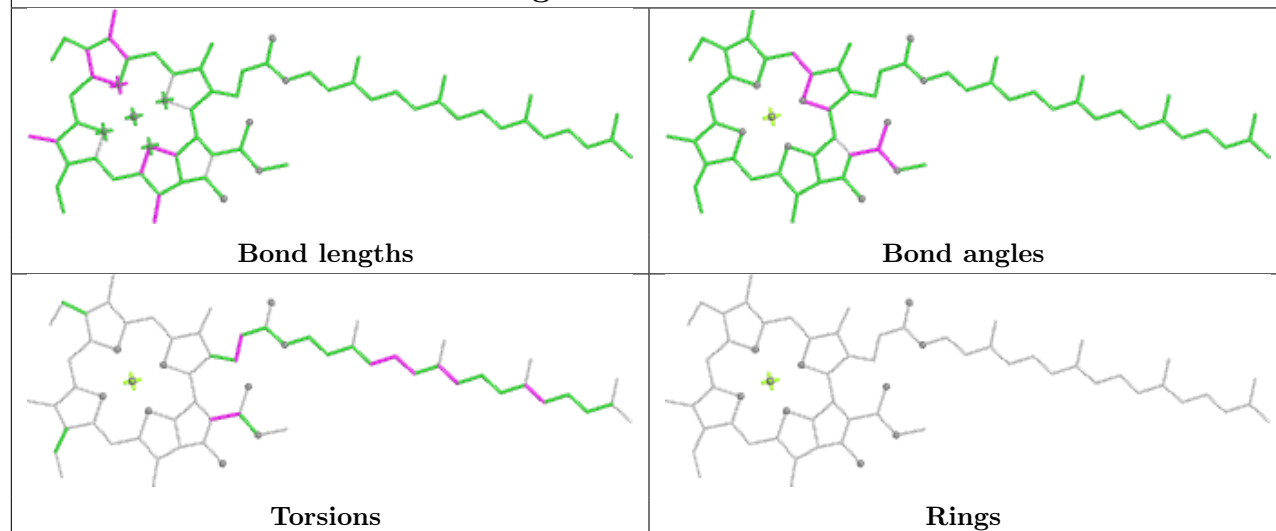
Ligand IHT f 617	
	
Bond lengths	Bond angles
	
Torsions	Rings



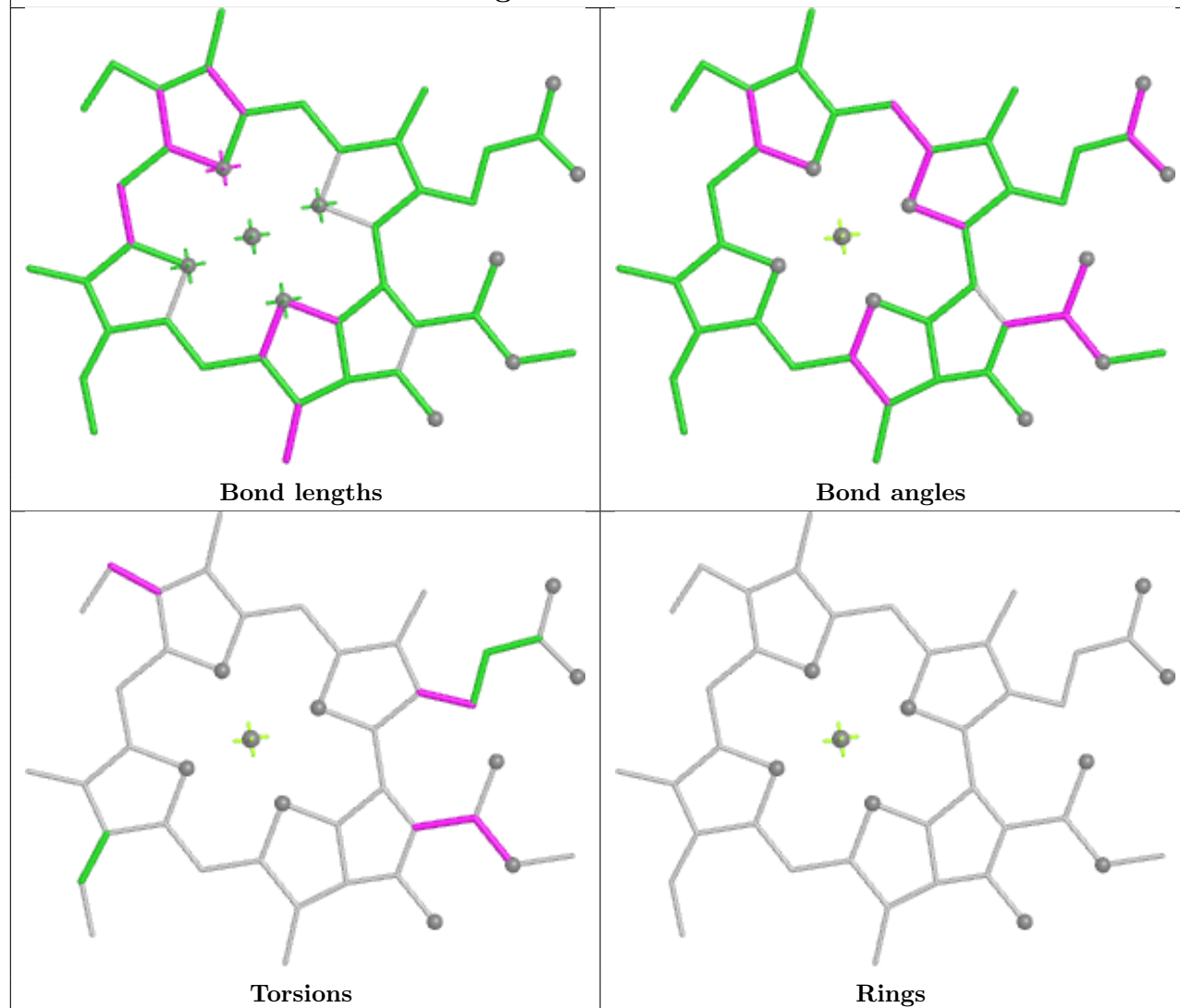


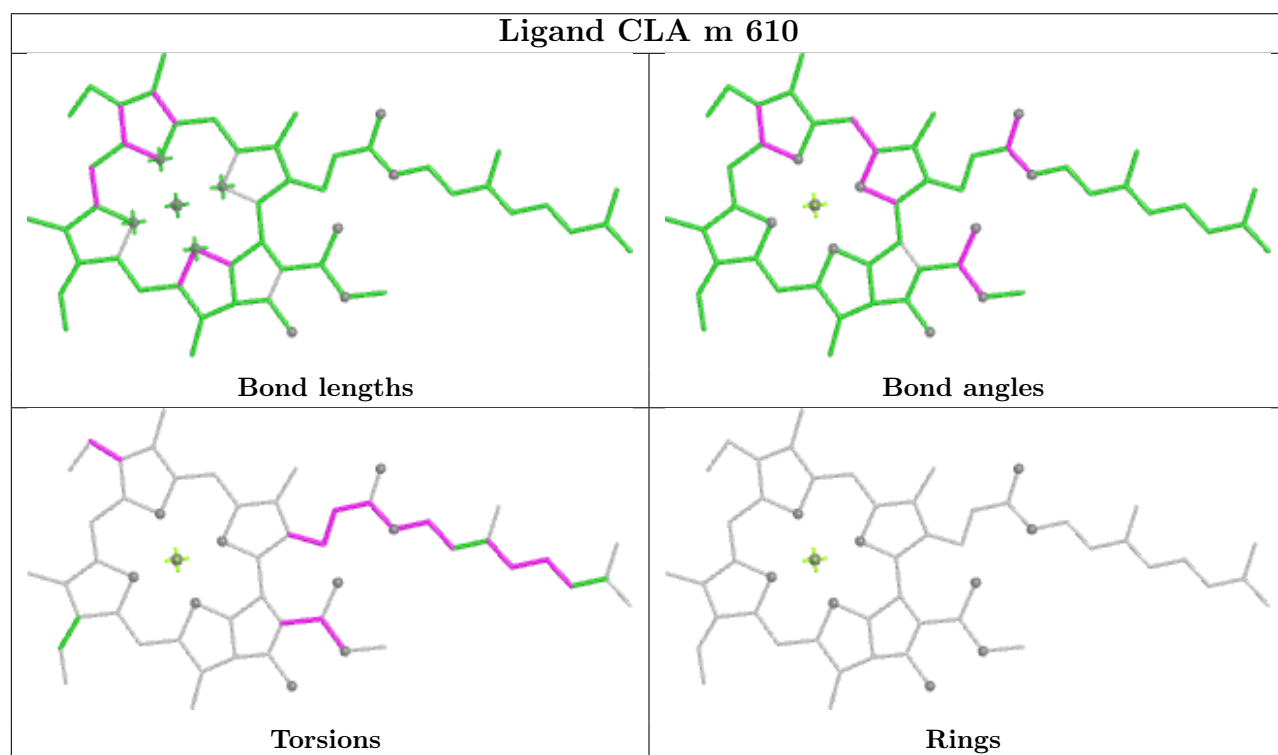
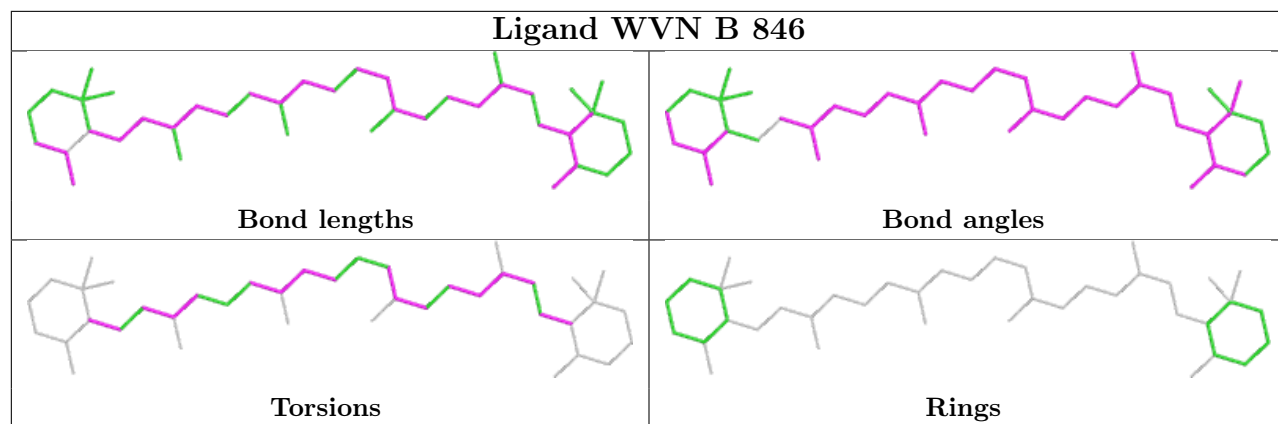


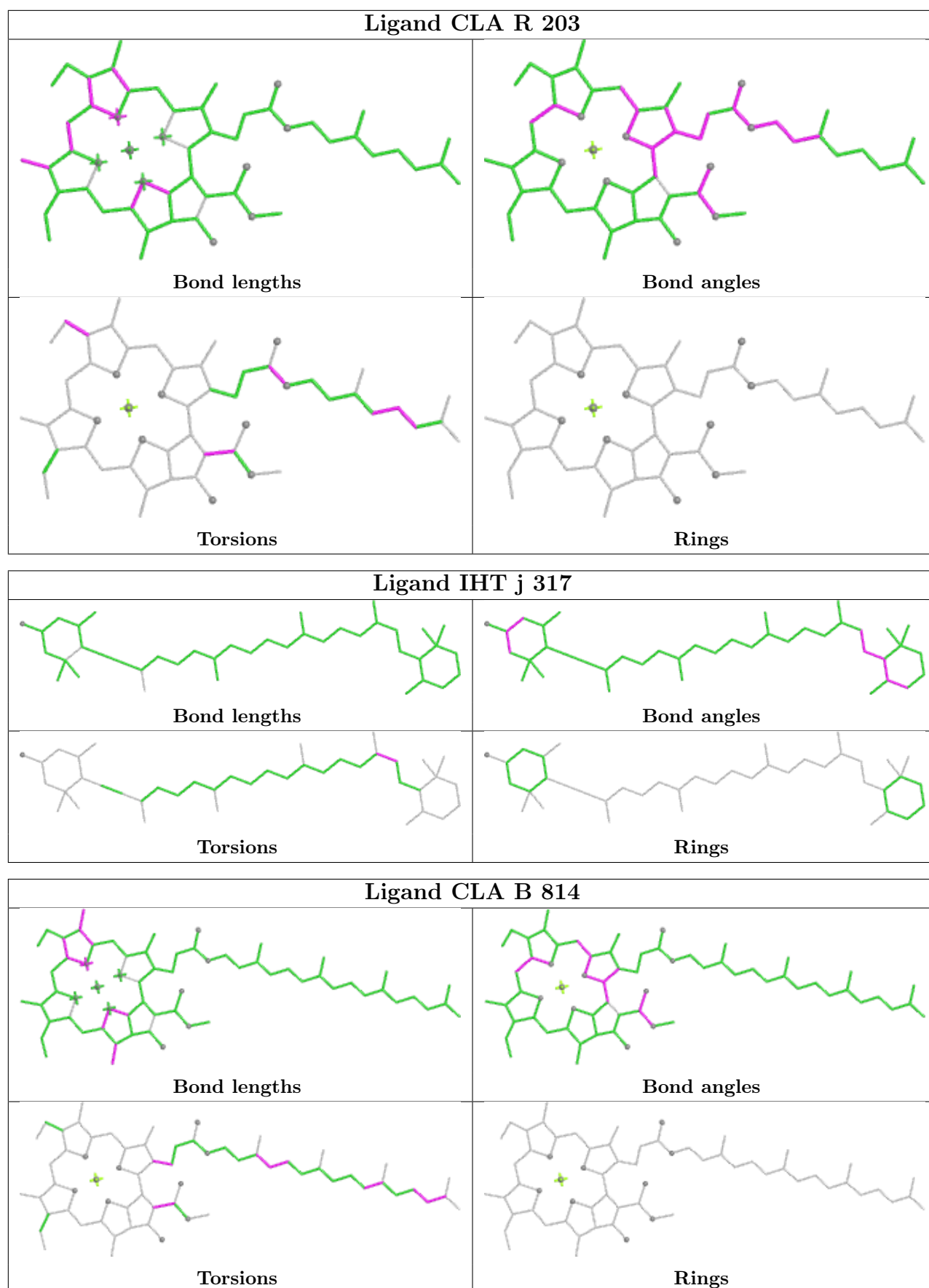
Ligand CLA B 807

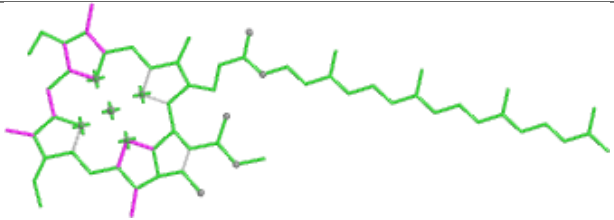
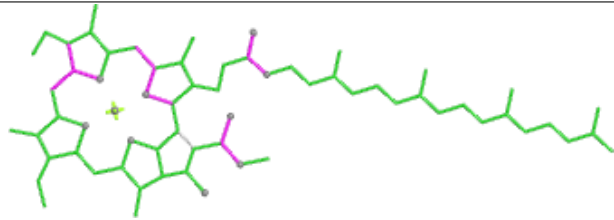
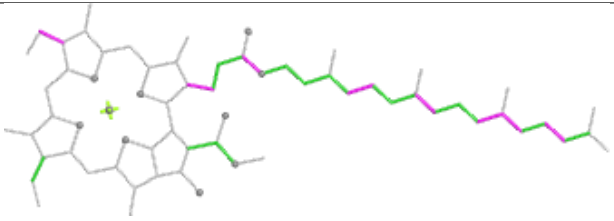
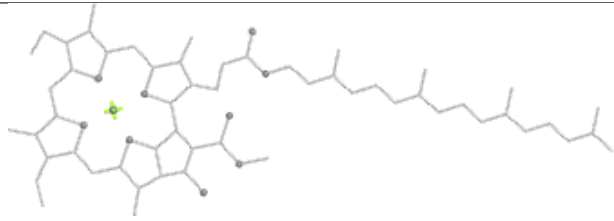


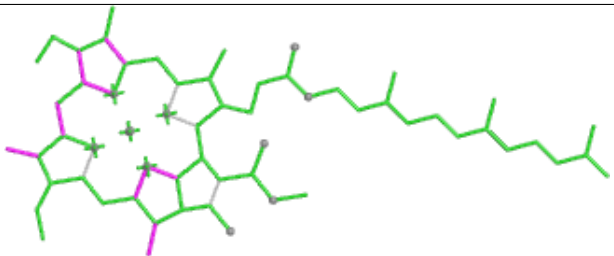
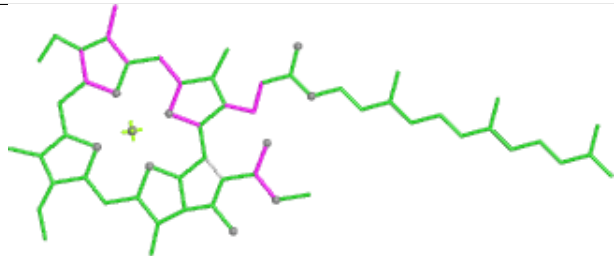
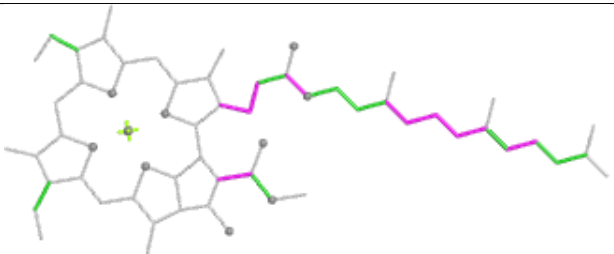
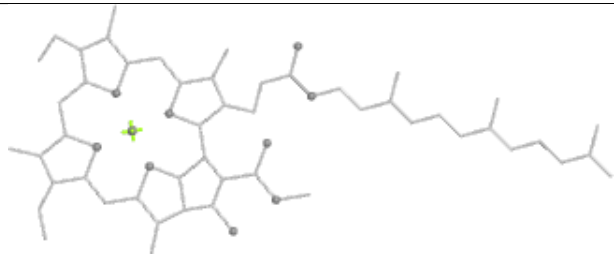
Ligand CLA d 307

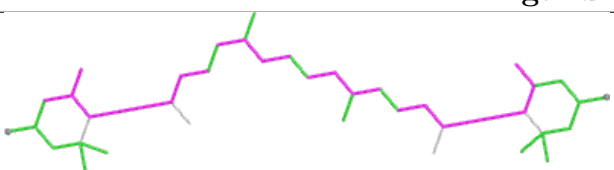
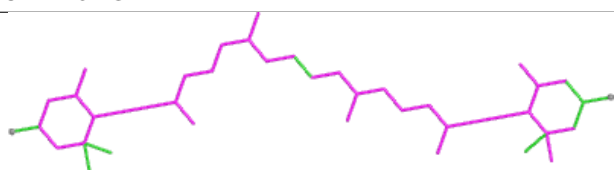
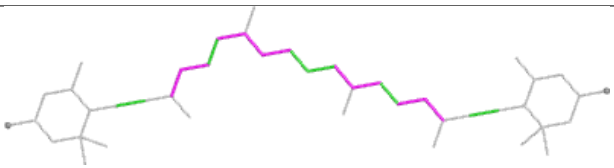
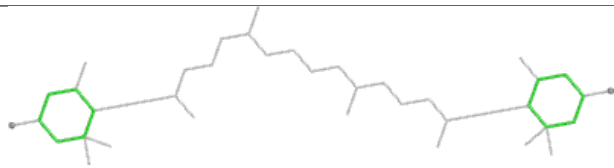




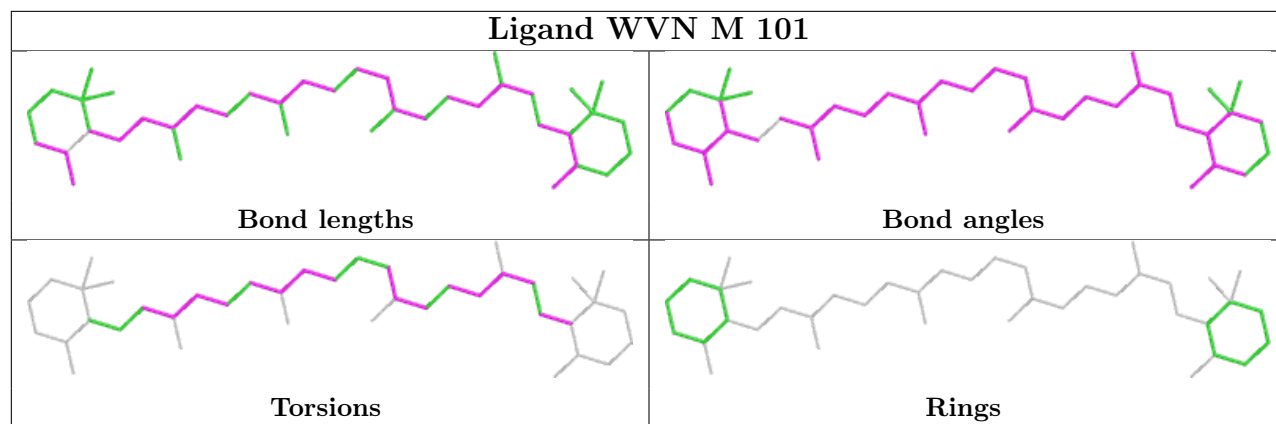


Ligand CLA a 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

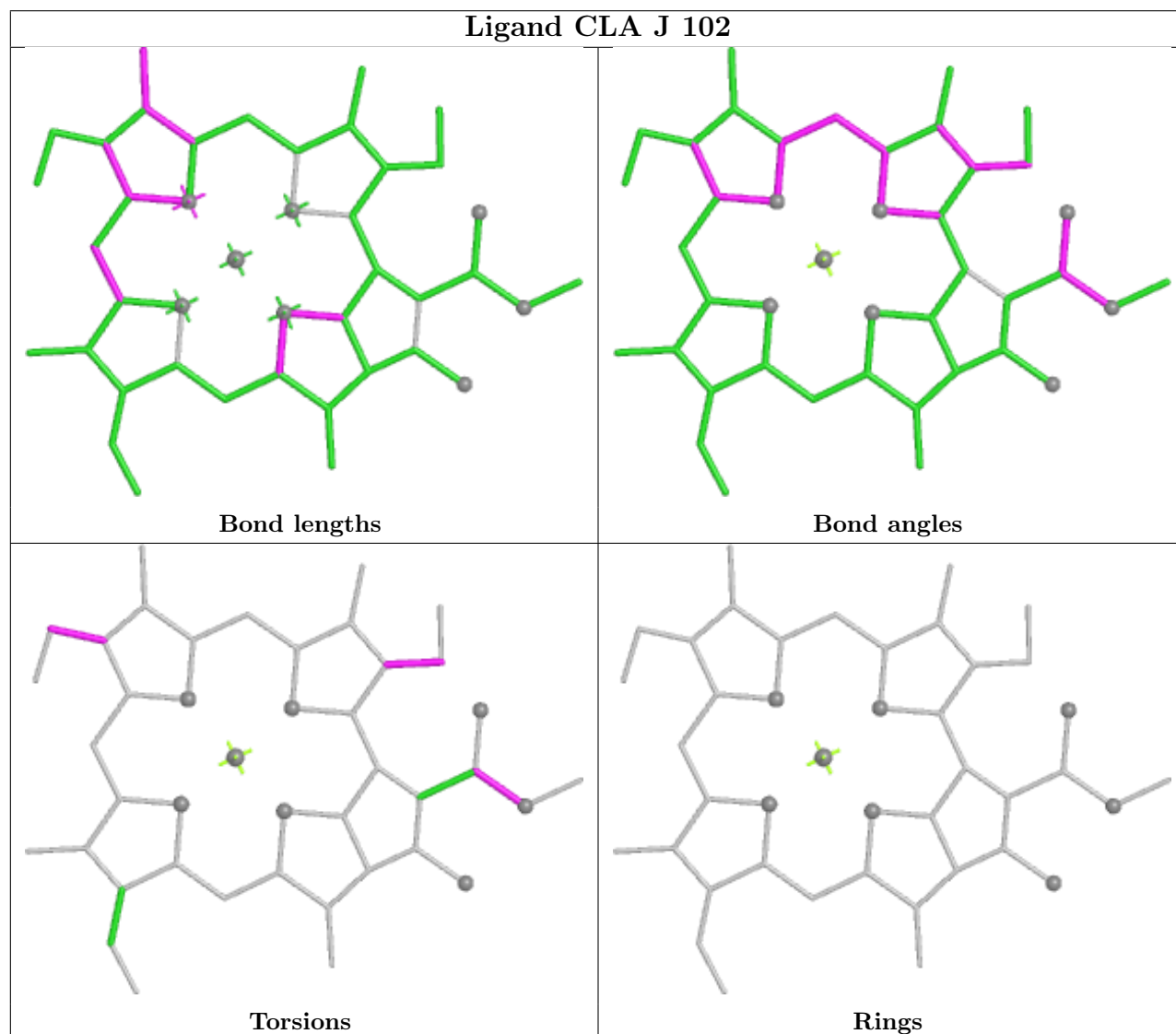
Ligand CLA B 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

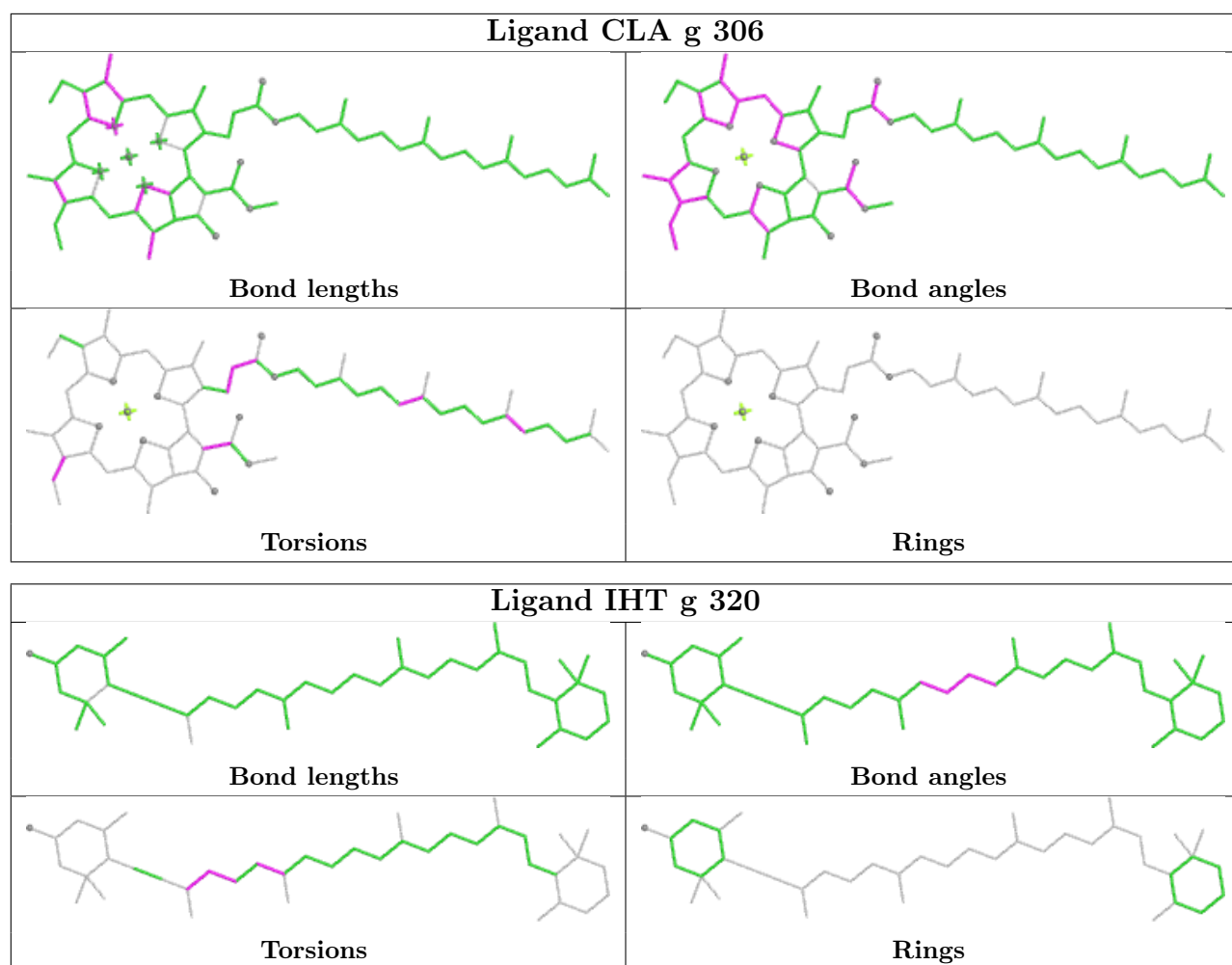
Ligand II0 m 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

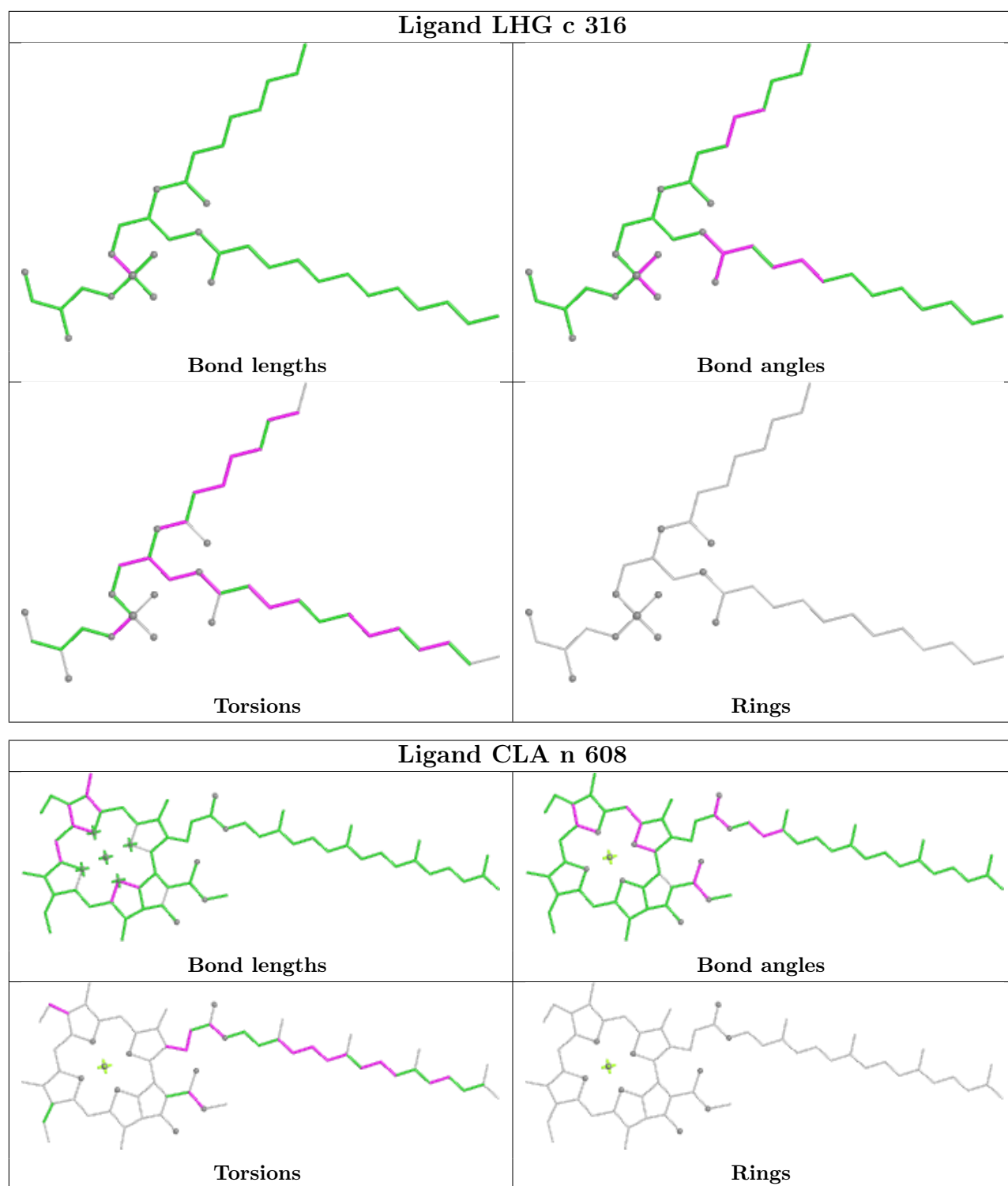
Ligand WVN M 101

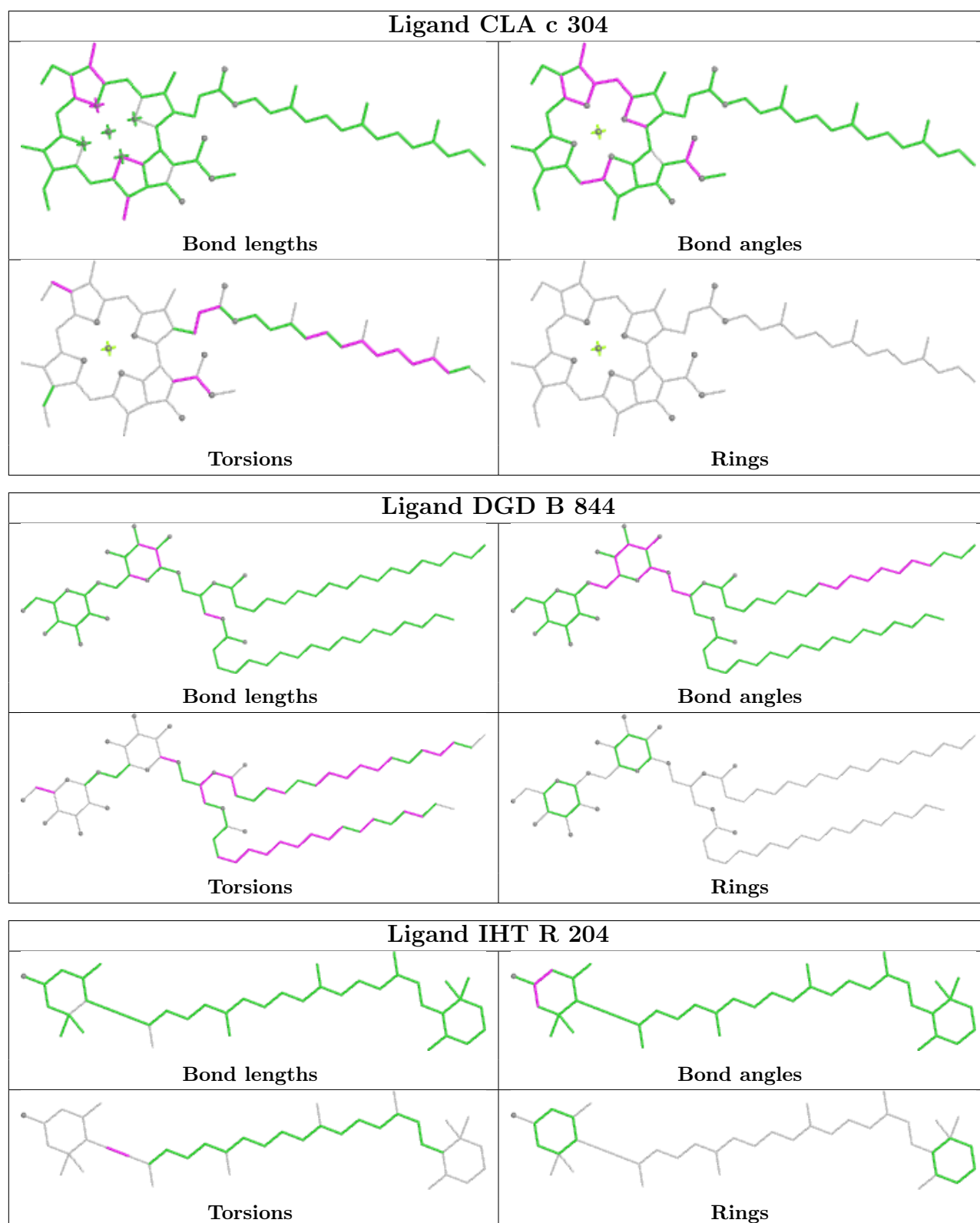


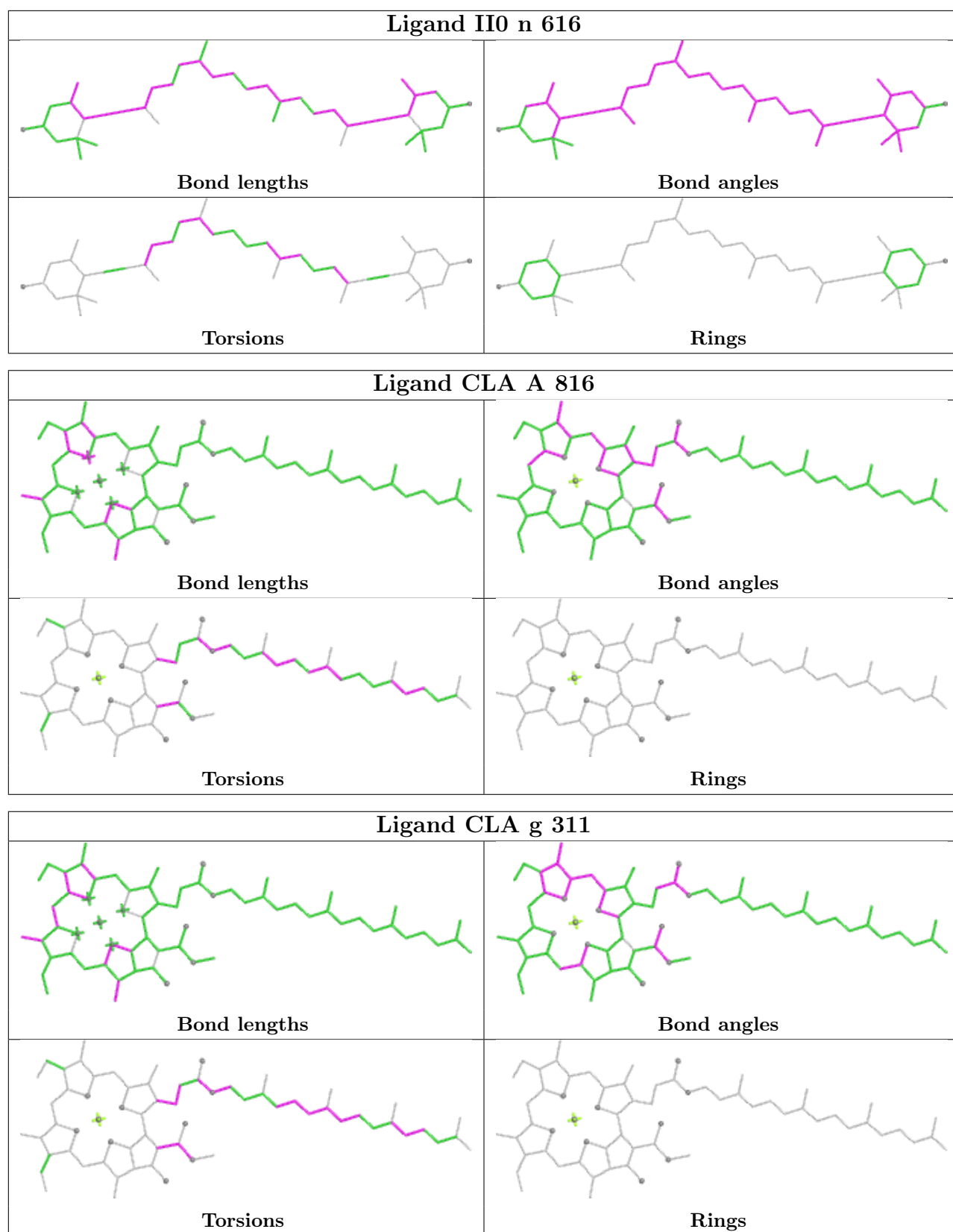
Ligand CLA J 102

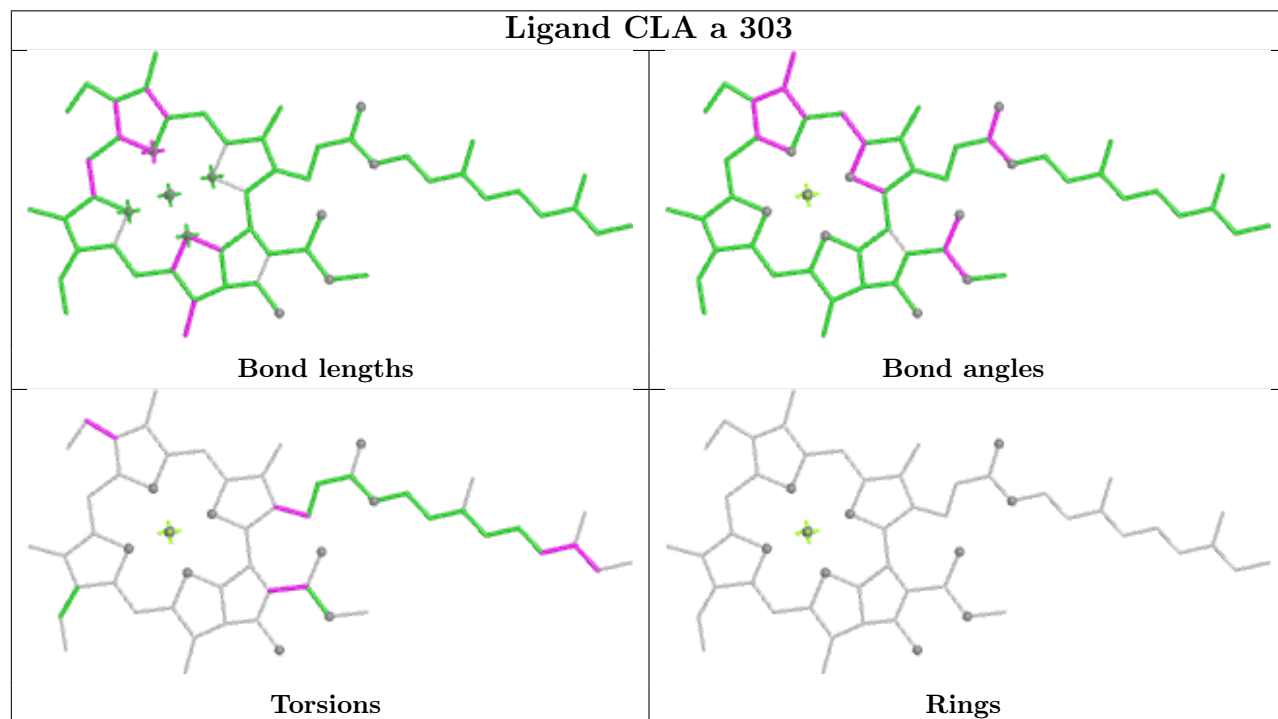
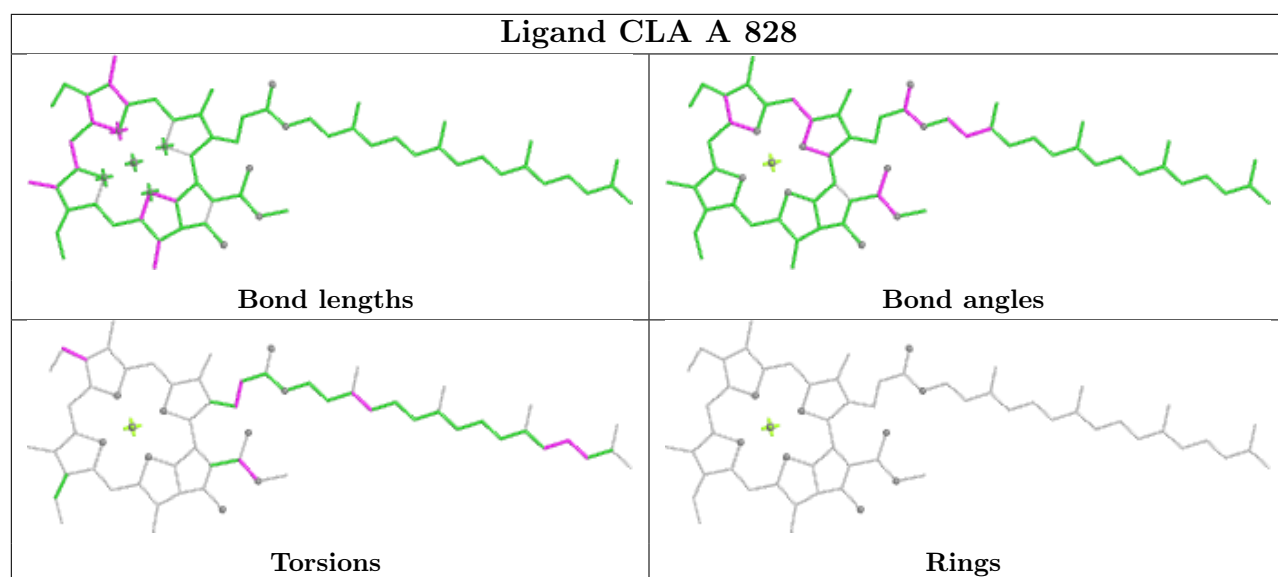




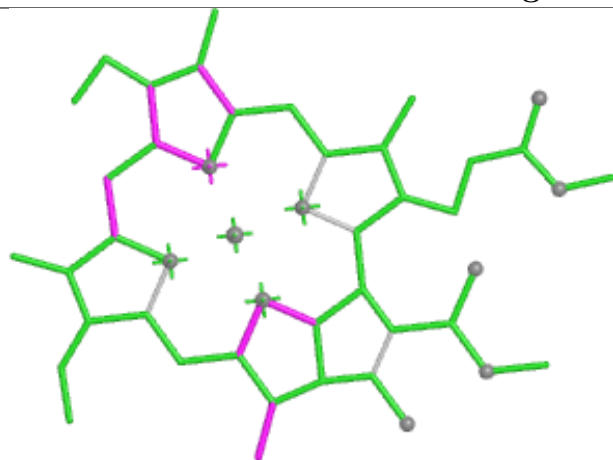




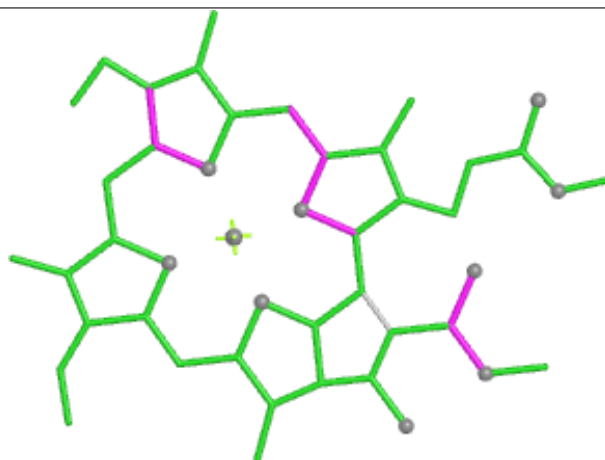




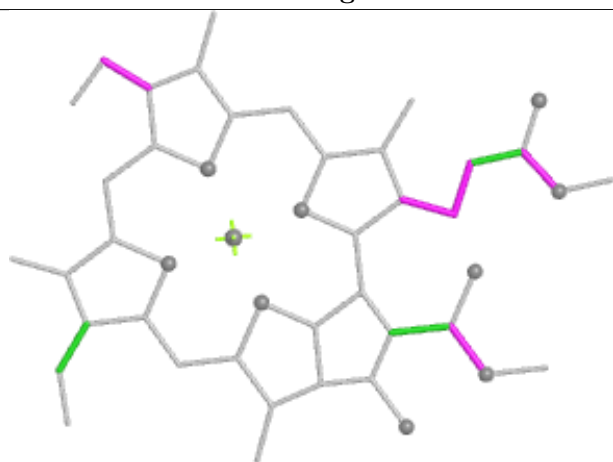
Ligand CLA i 309



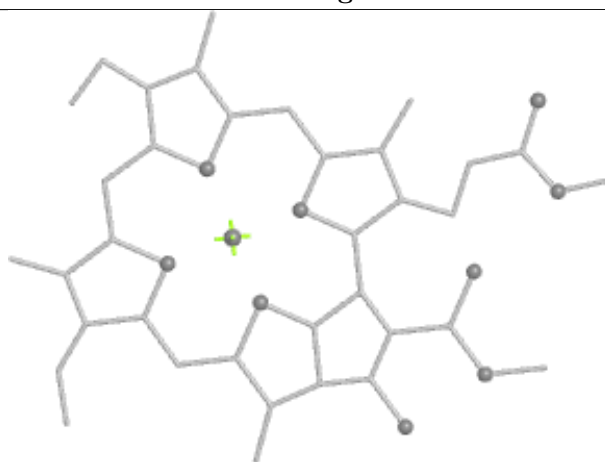
Bond lengths



Bond angles

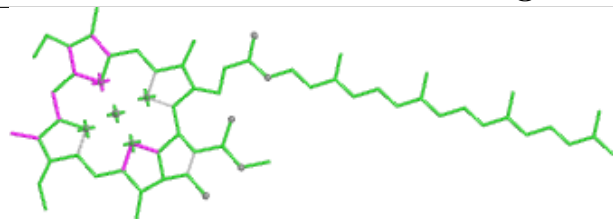


Torsions

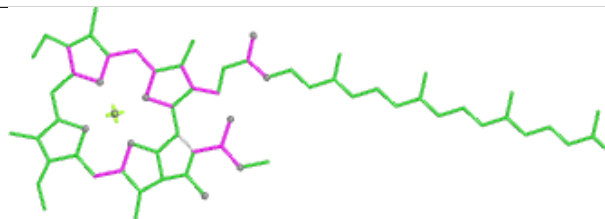


Rings

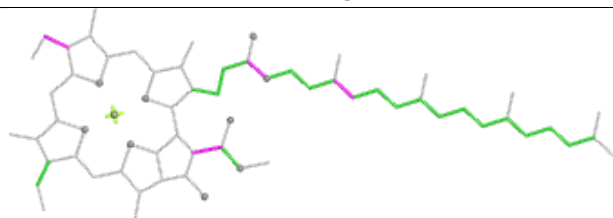
Ligand CLA L 203



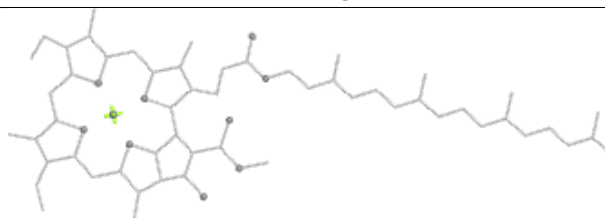
Bond lengths



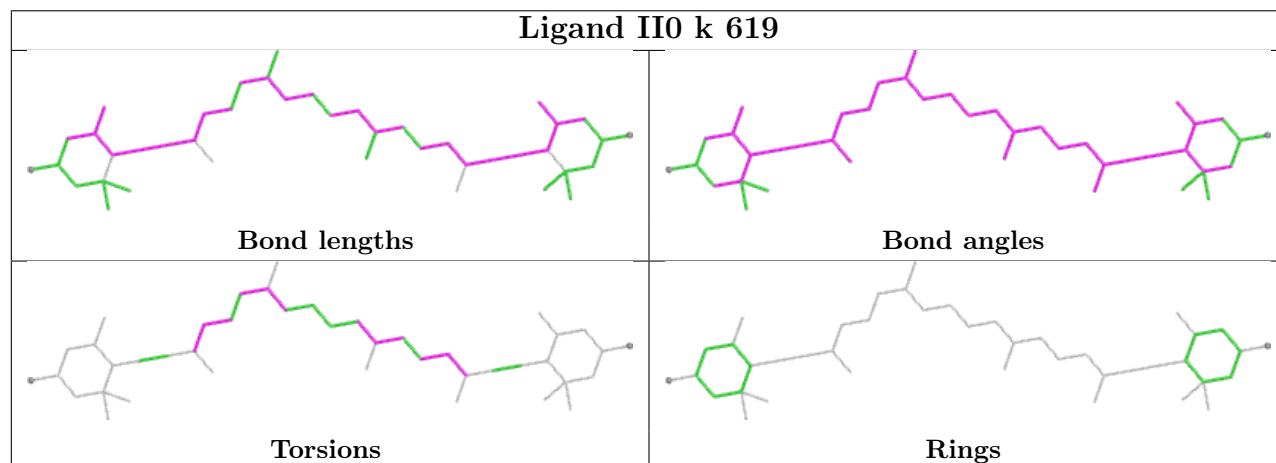
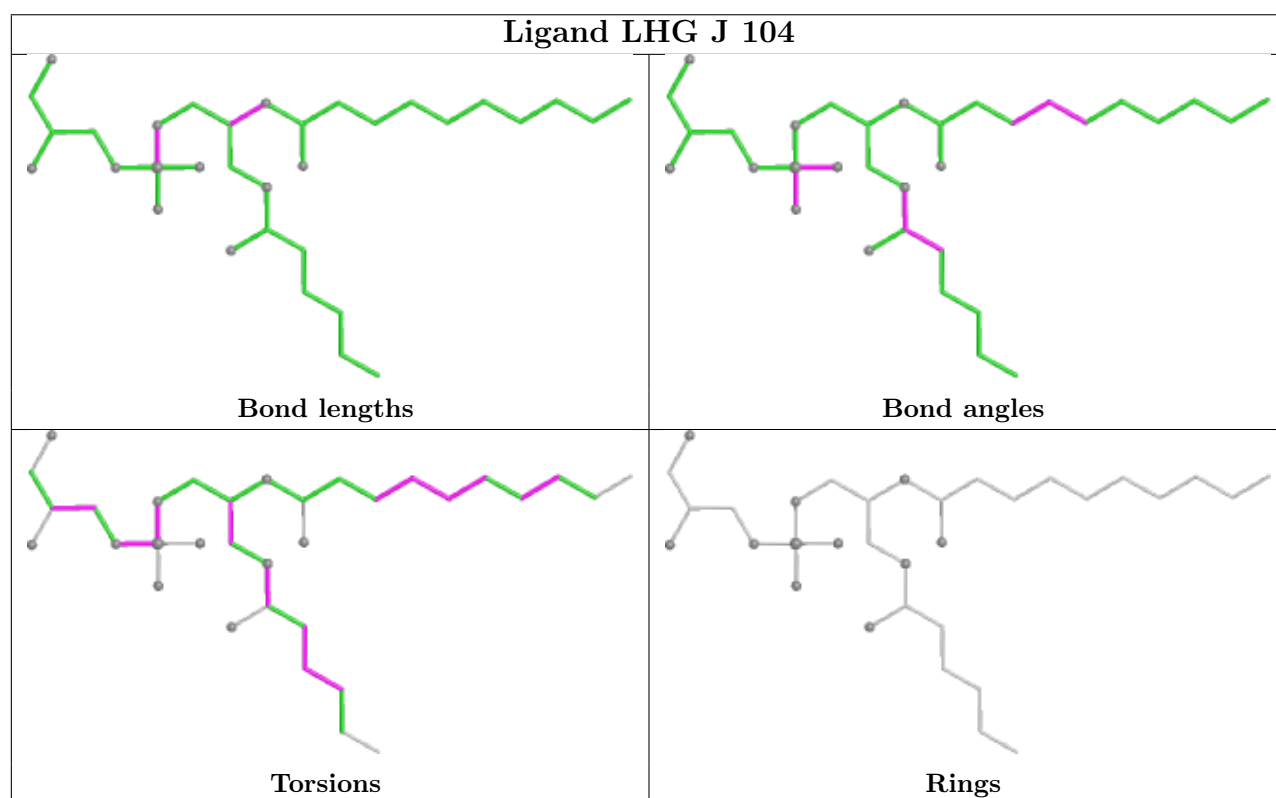
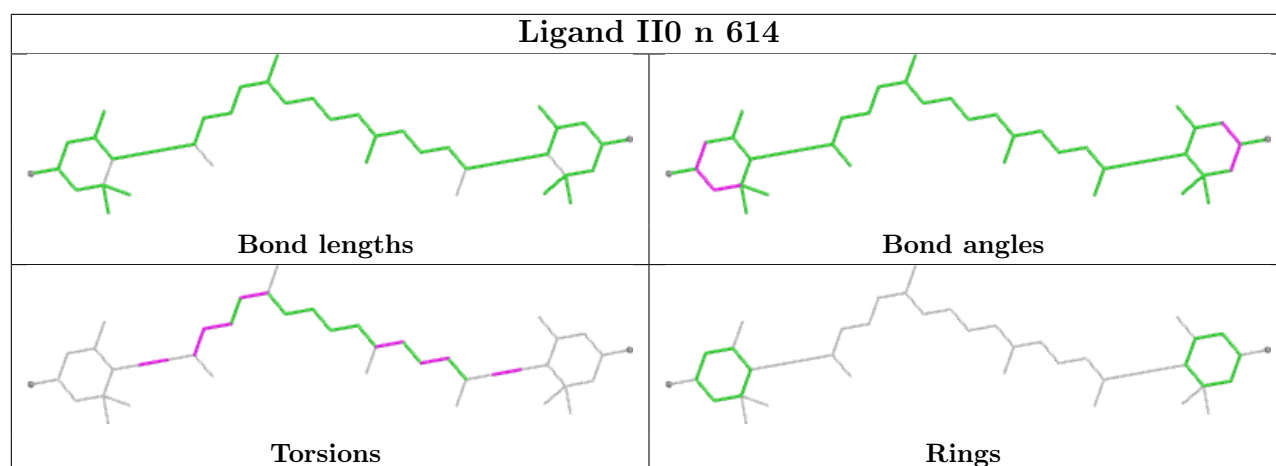
Bond angles



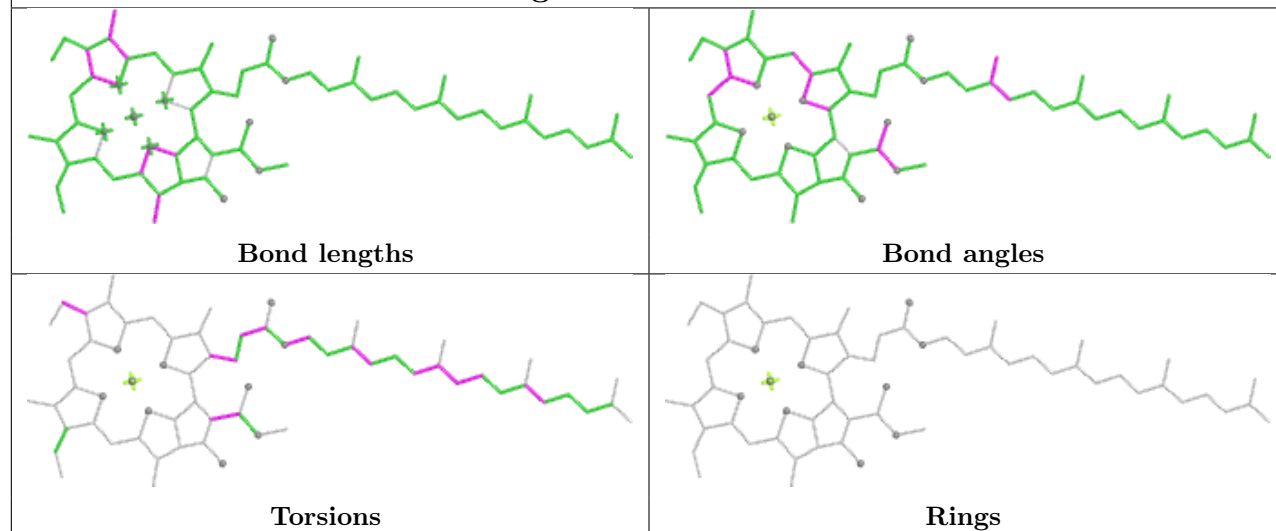
Torsions



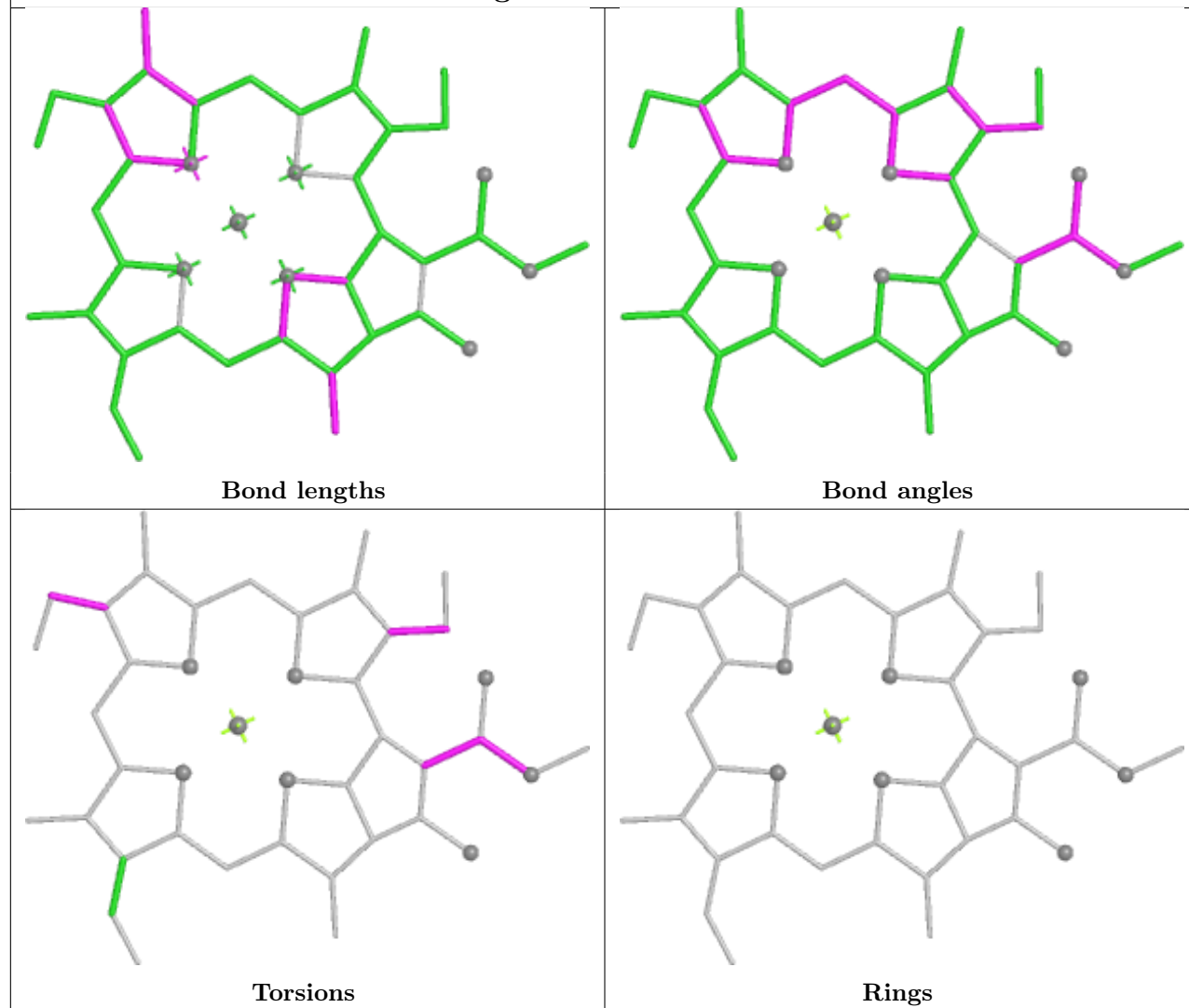
Rings



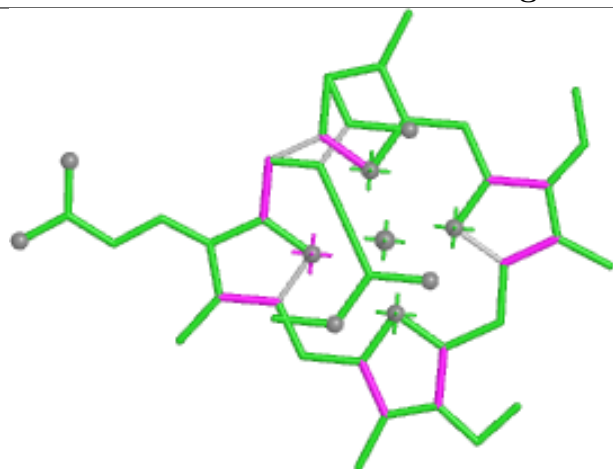
Ligand CLA A 833



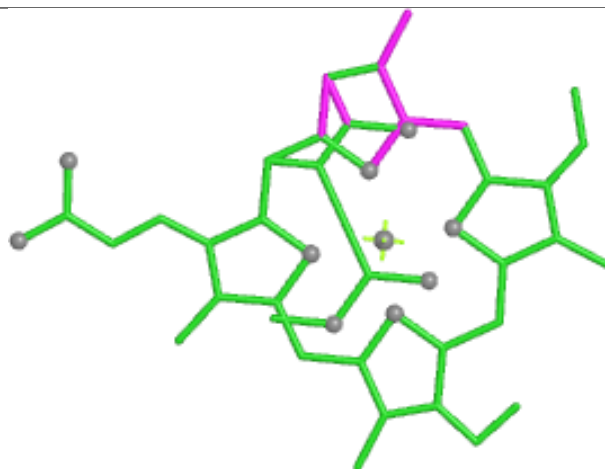
Ligand CLA m 601



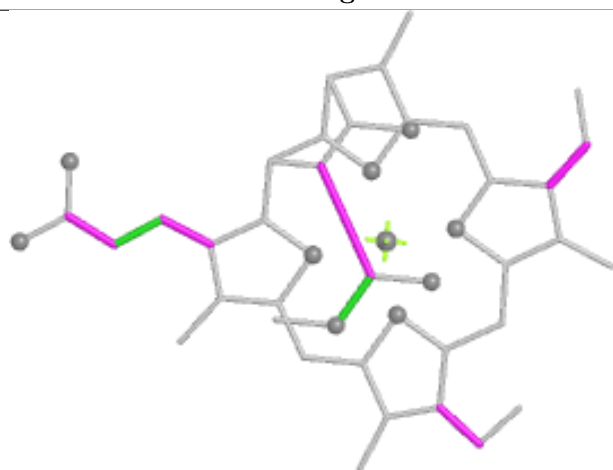
Ligand KC2 k 612



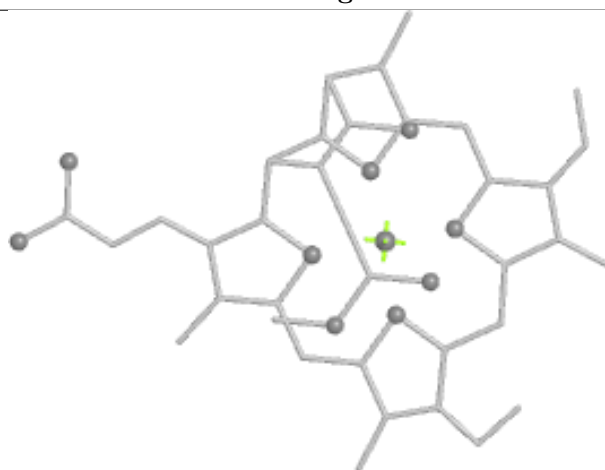
Bond lengths



Bond angles

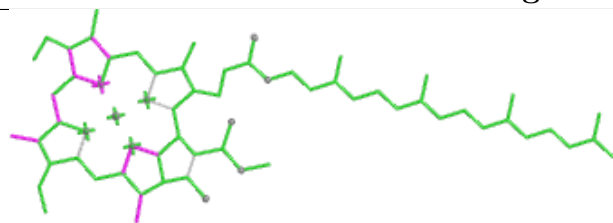


Torsions

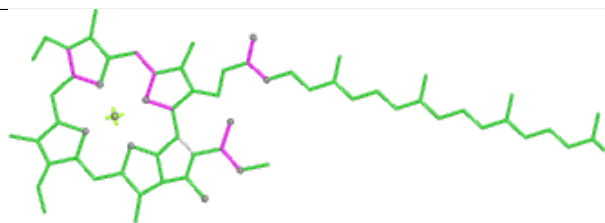


Rings

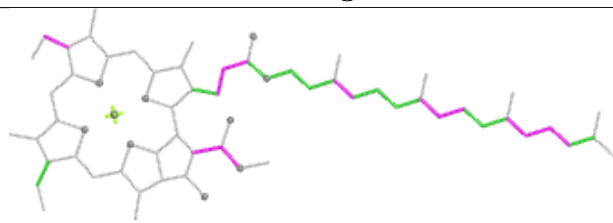
Ligand CLA l 306



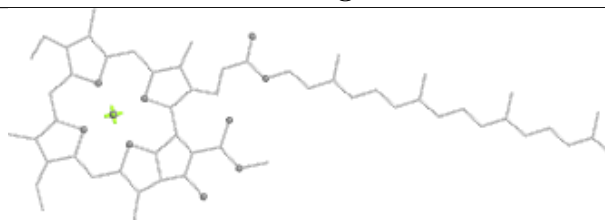
Bond lengths



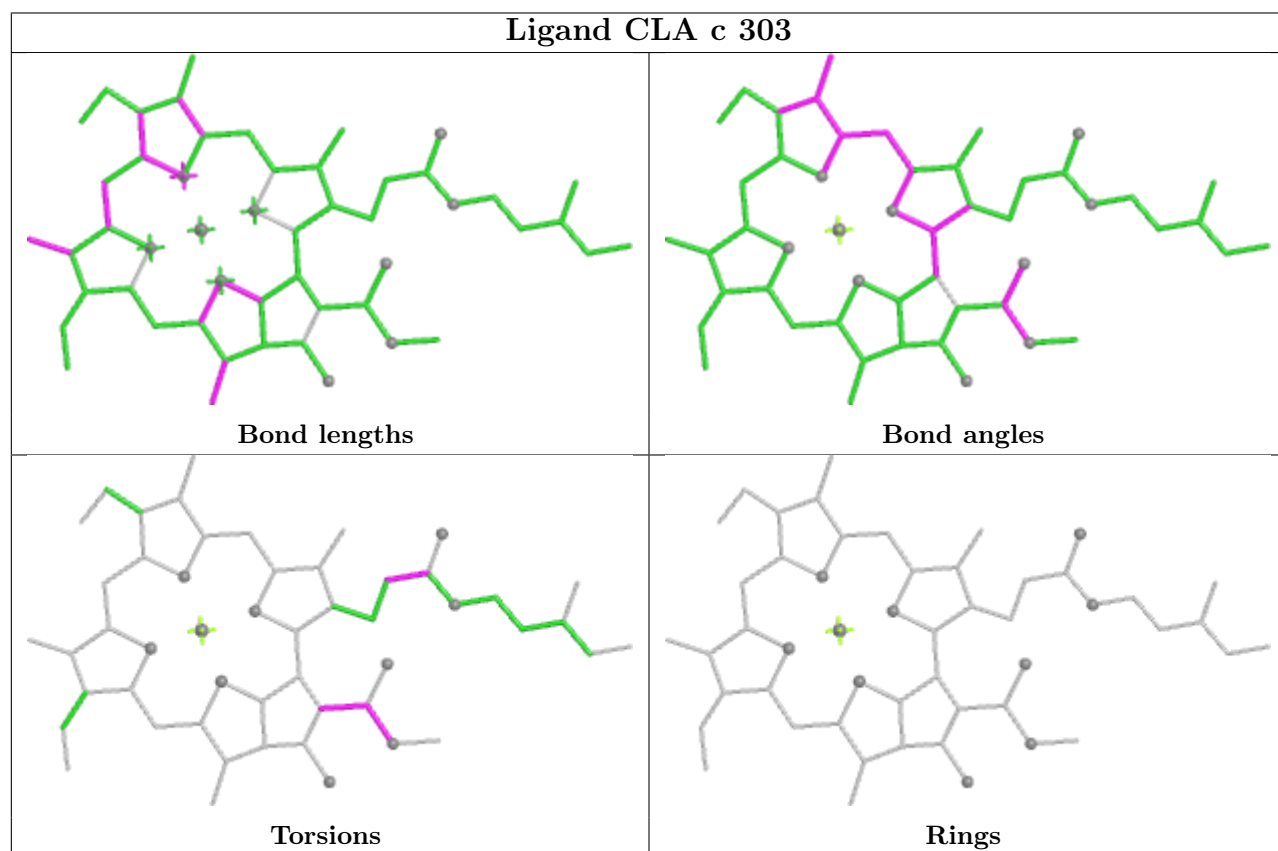
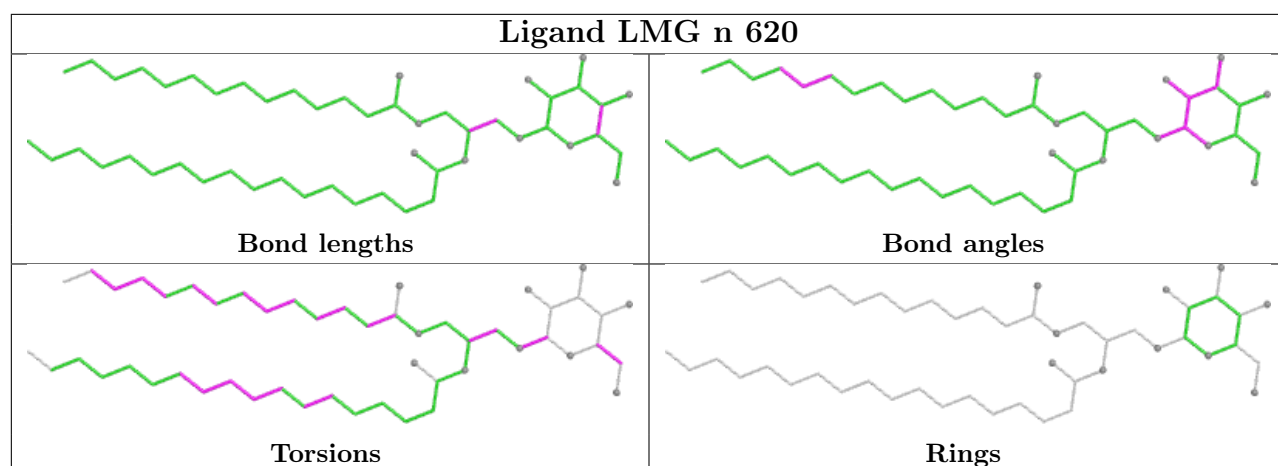
Bond angles



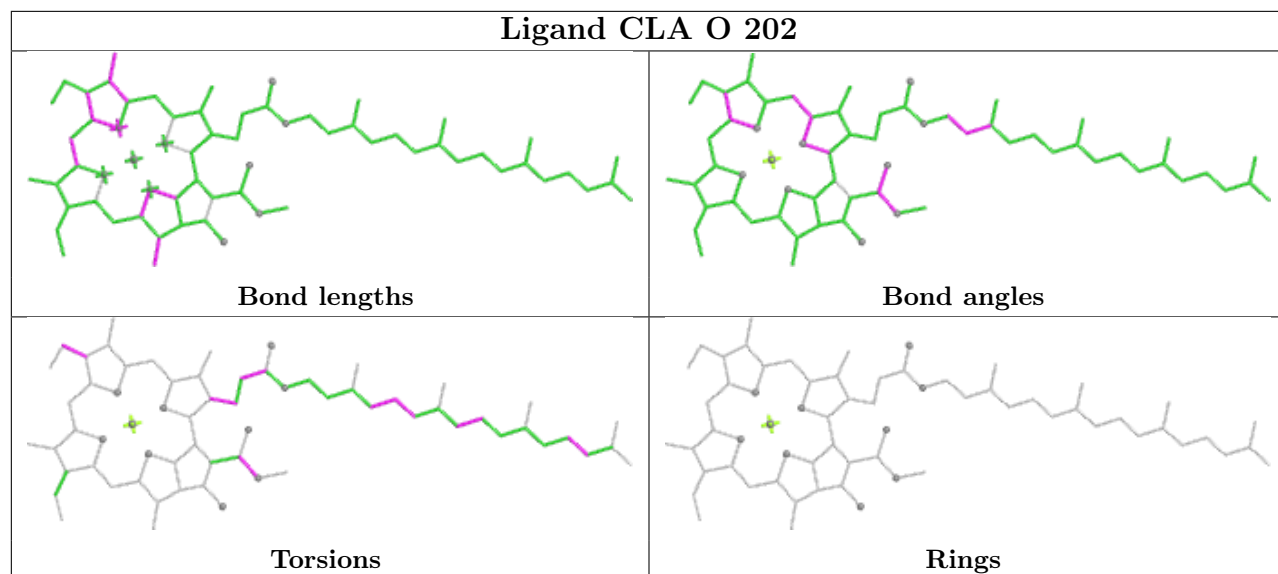
Torsions



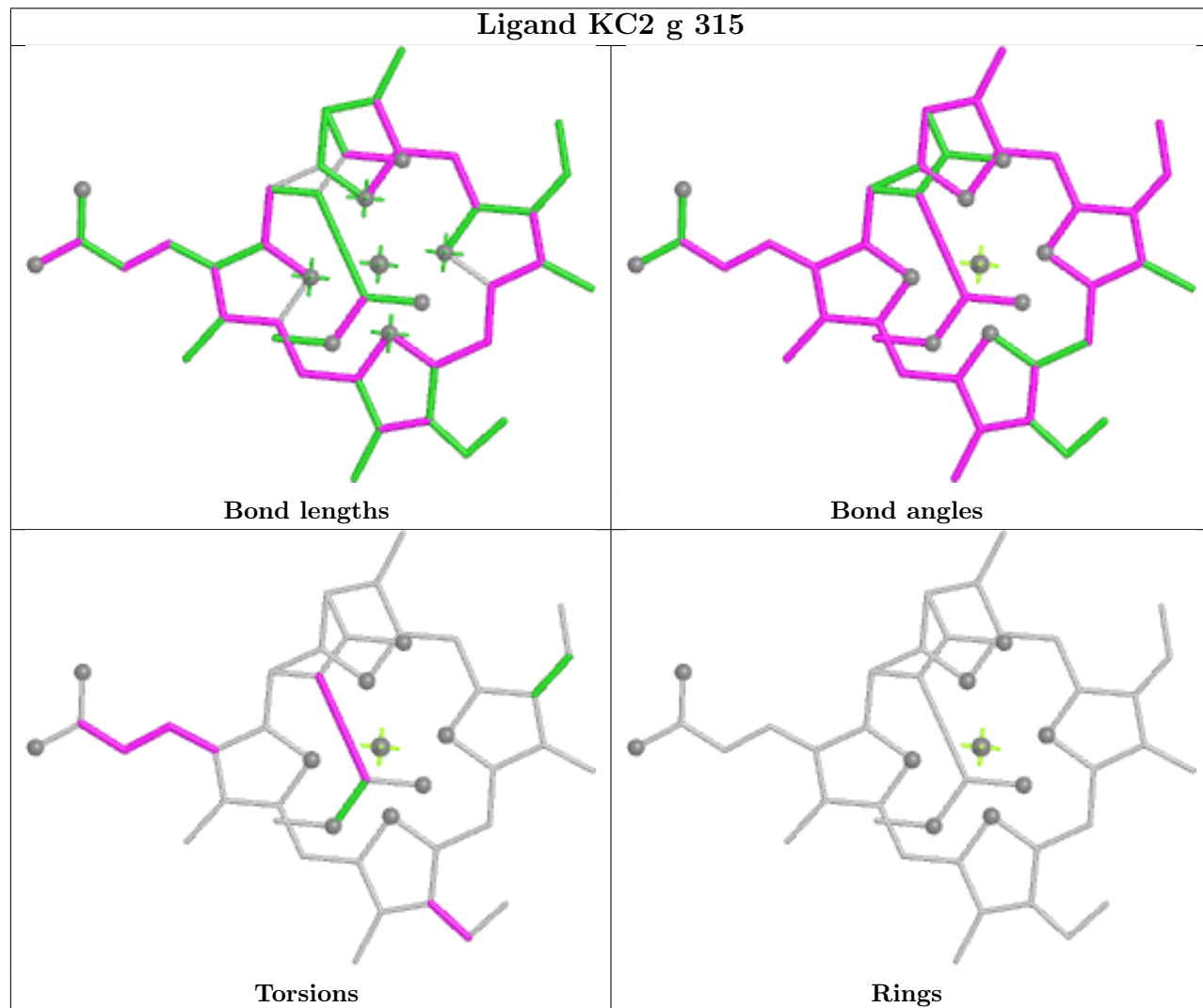
Rings

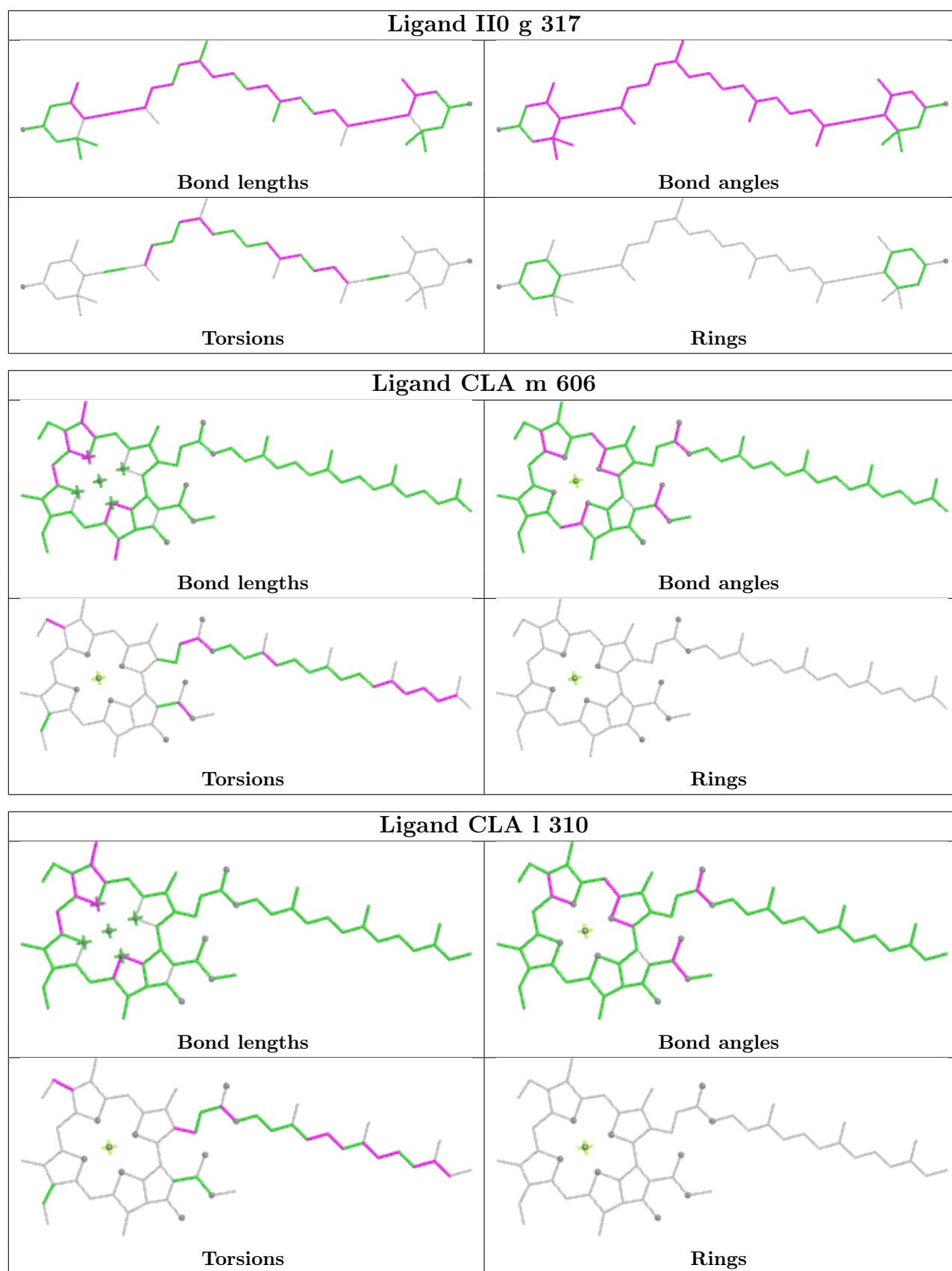


Ligand CLA O 202

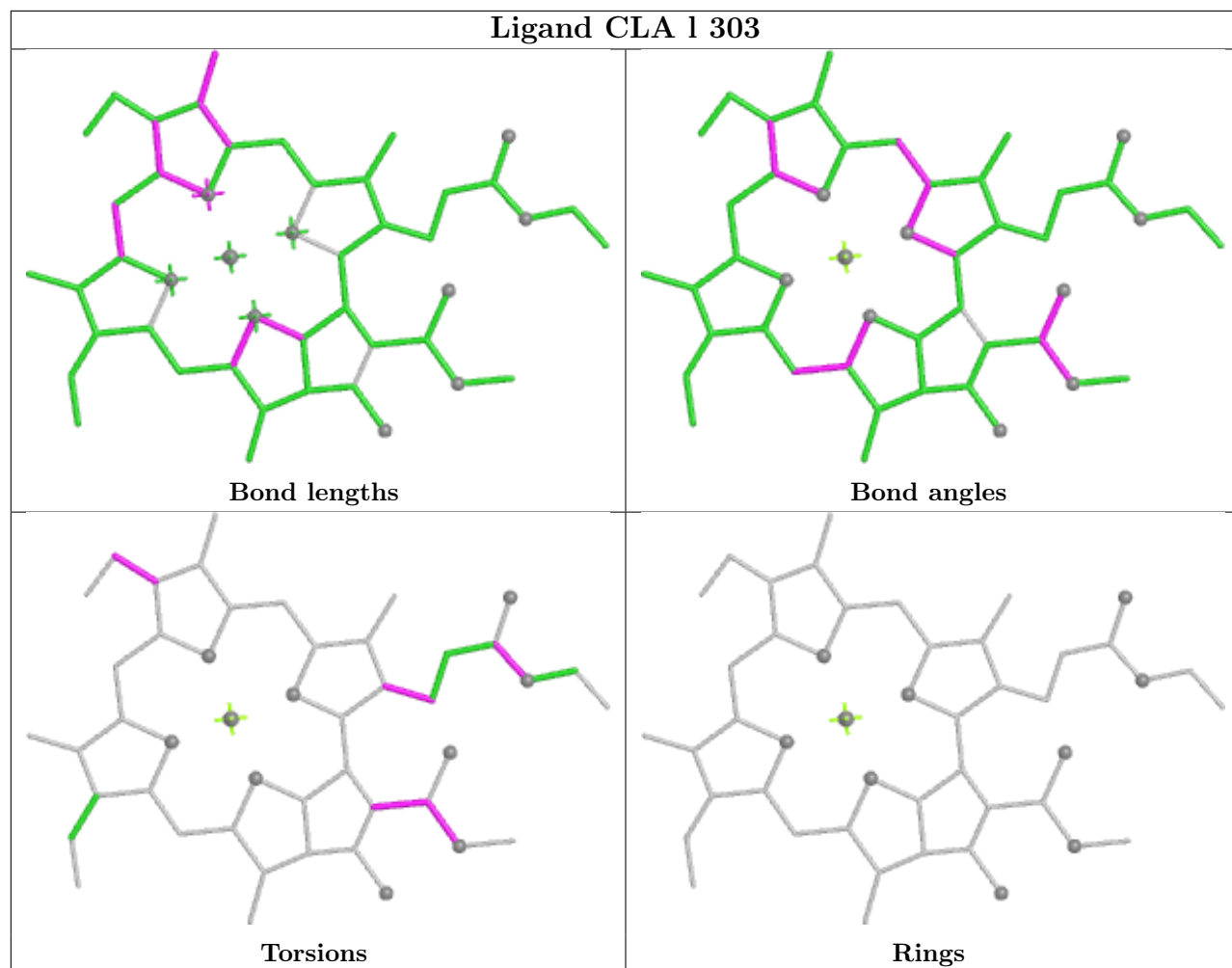


Ligand KC2 g 315

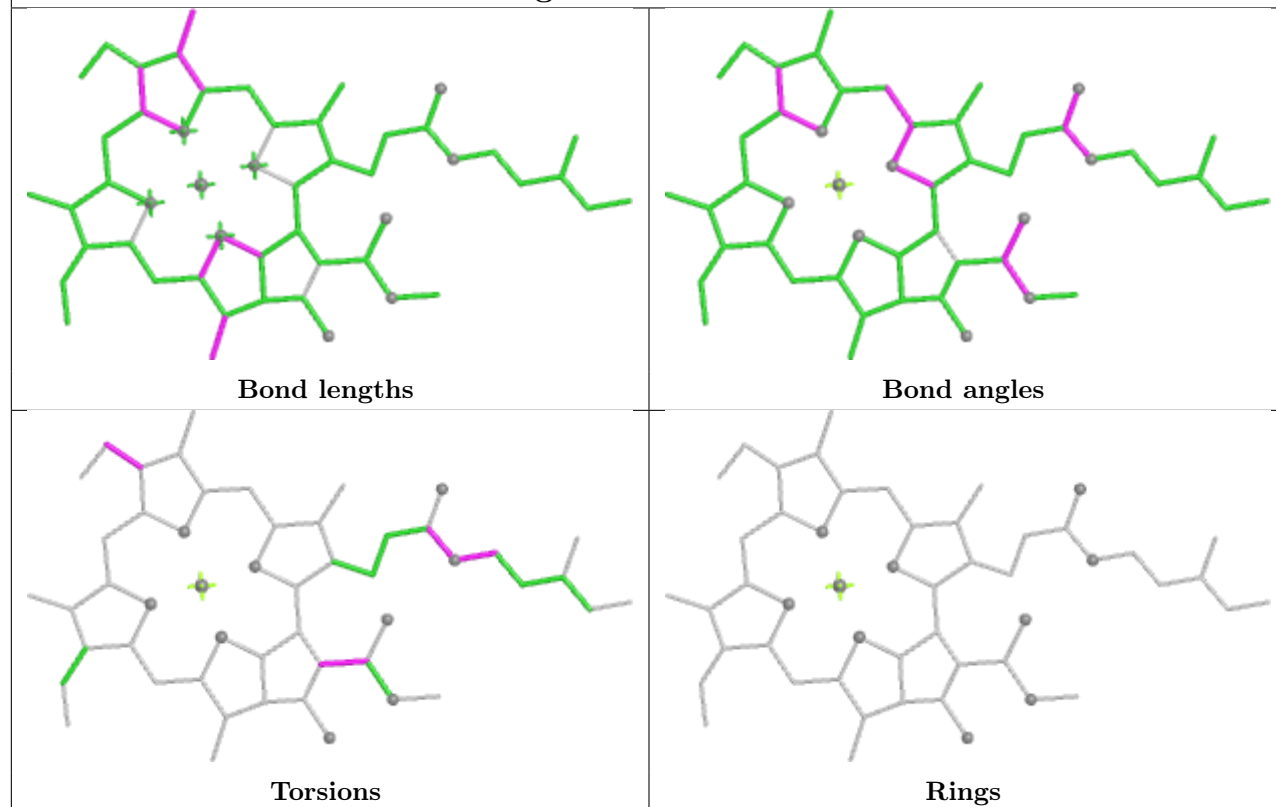




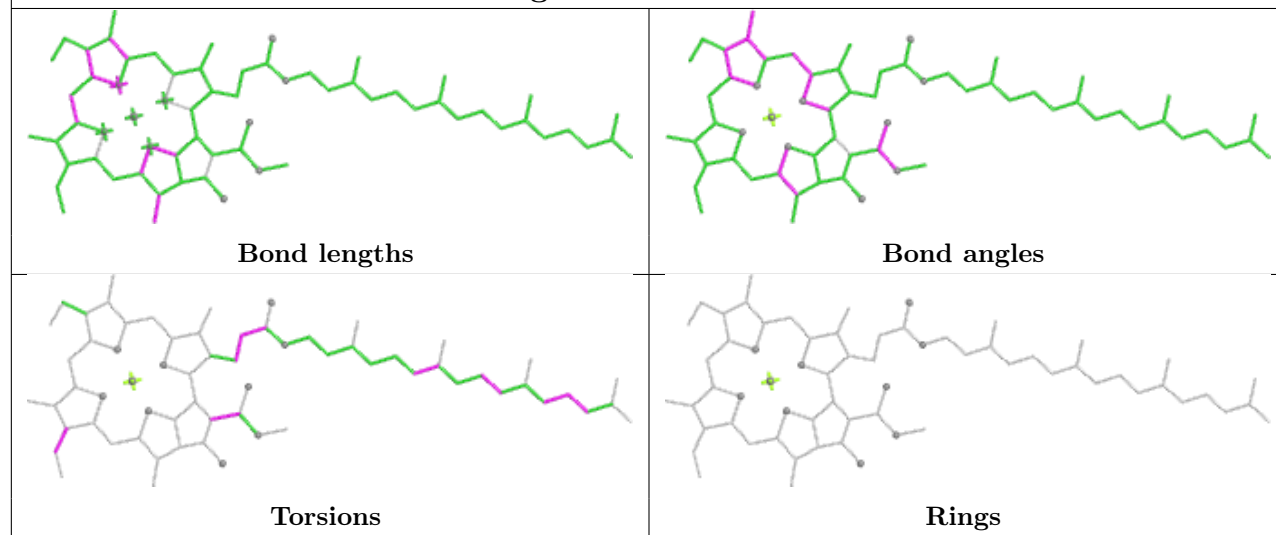
Ligand CLA 1 303

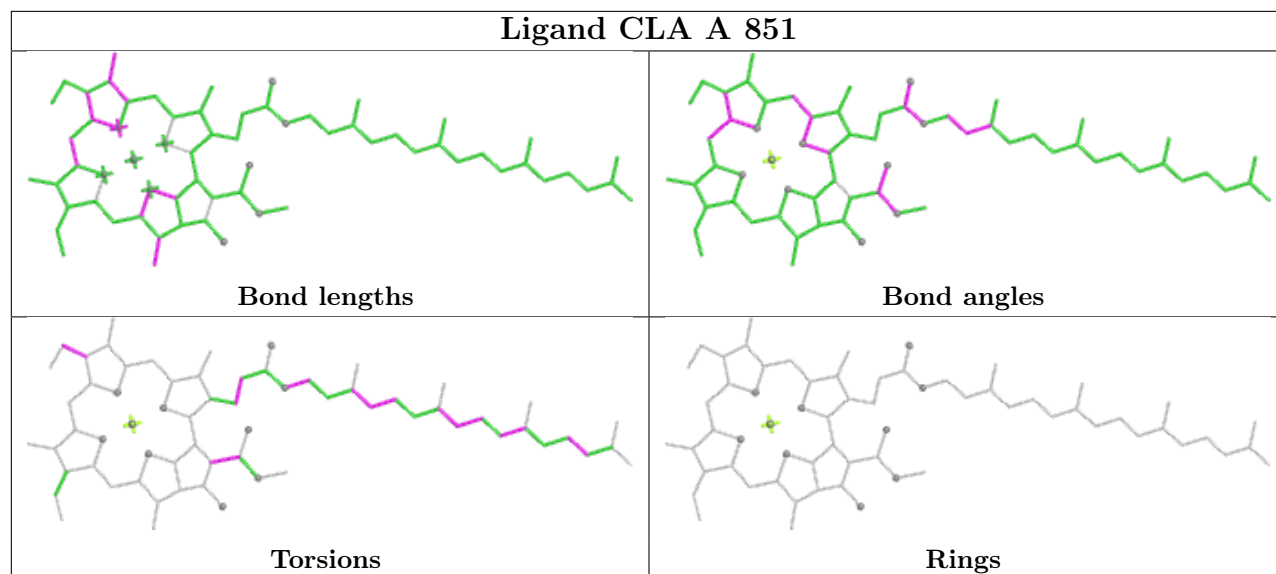
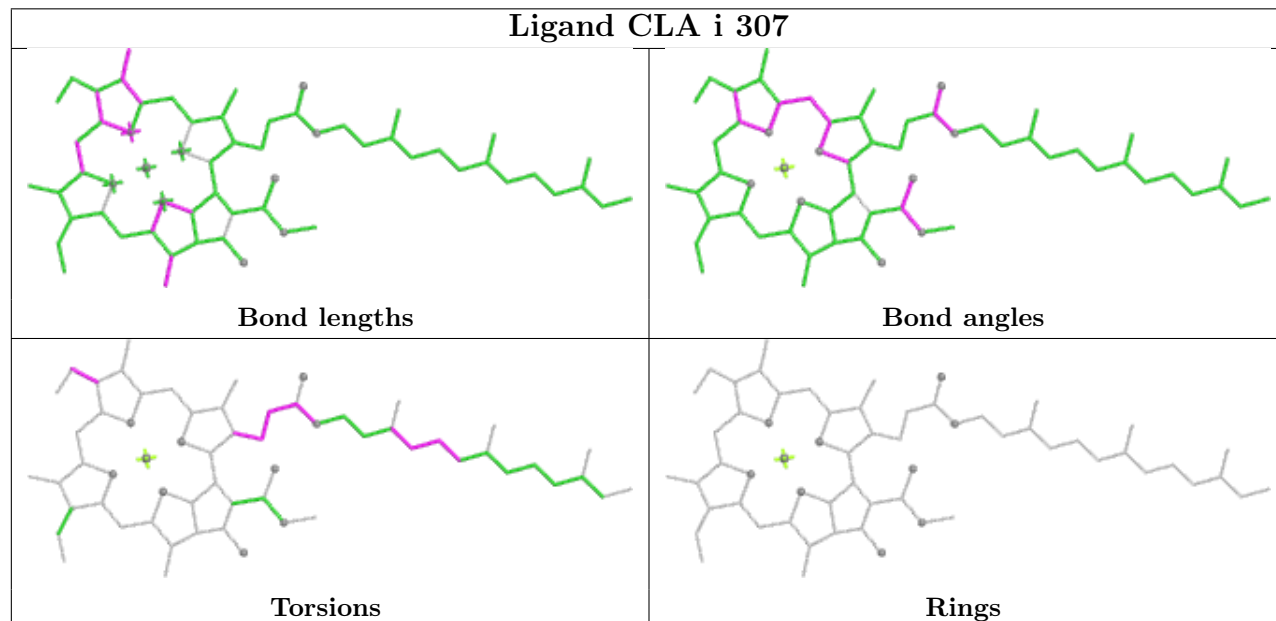


Ligand CLA b 302

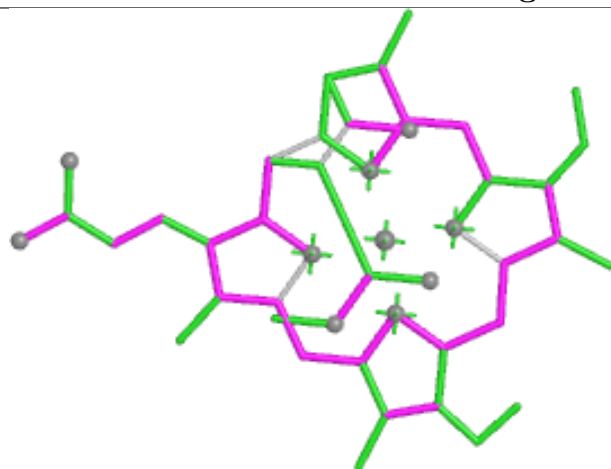


Ligand CLA m 604

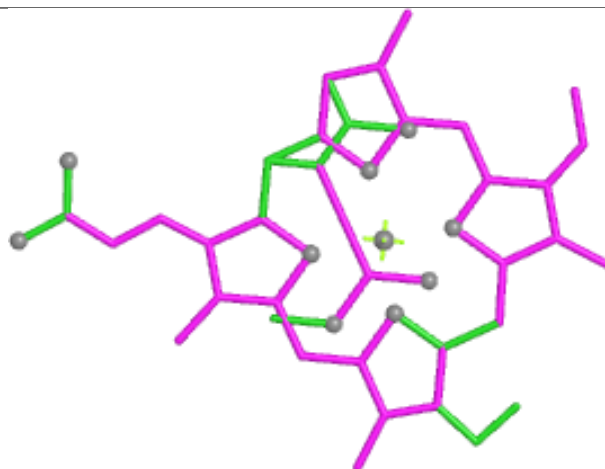


Ligand CLA A 851**Ligand CLA i 307**

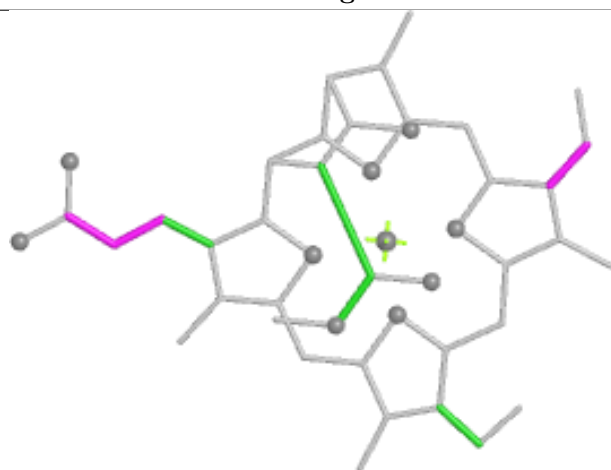
Ligand KC2 n 611



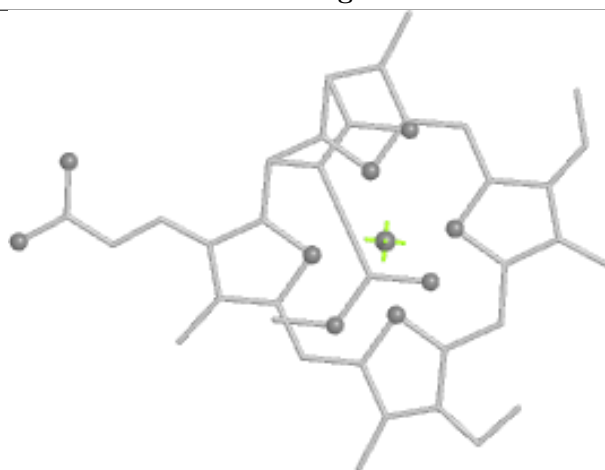
Bond lengths



Bond angles

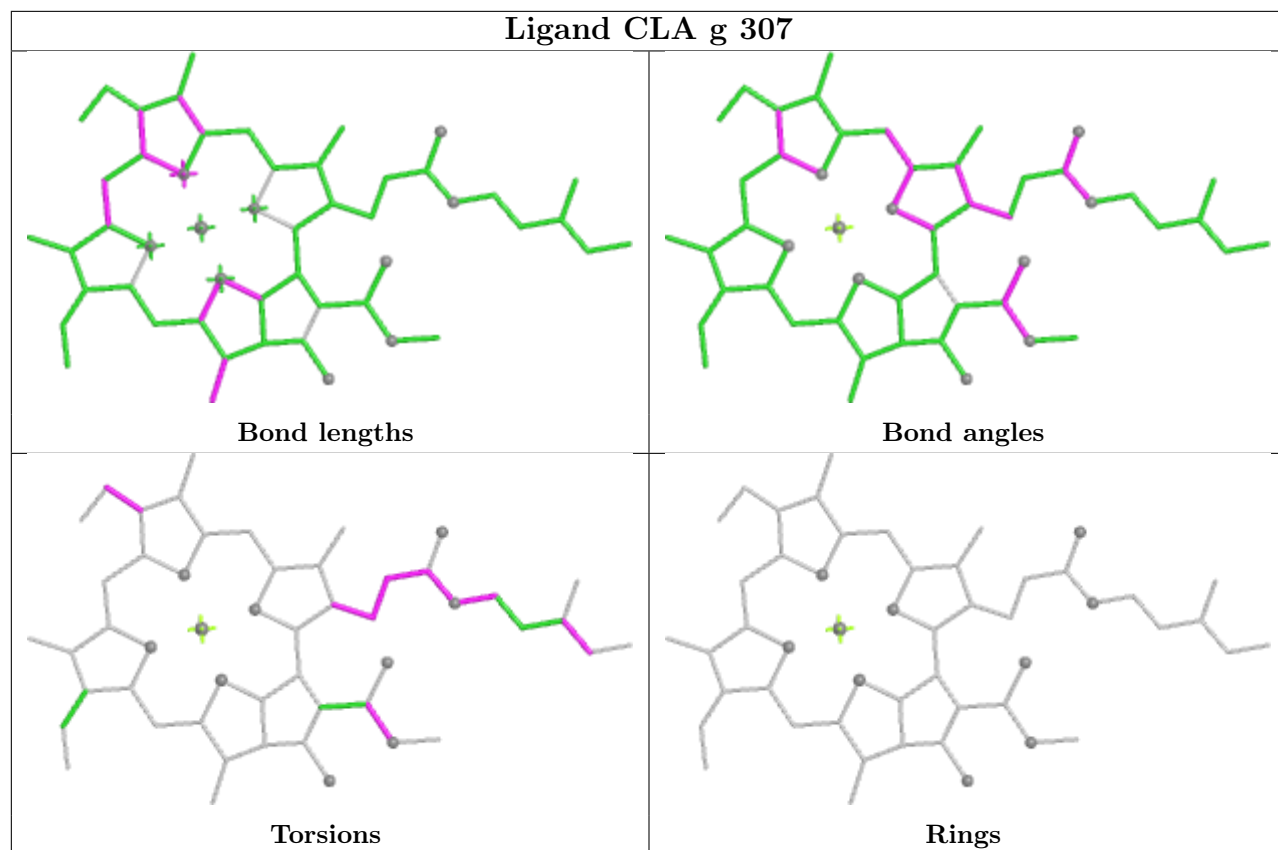


Torsions

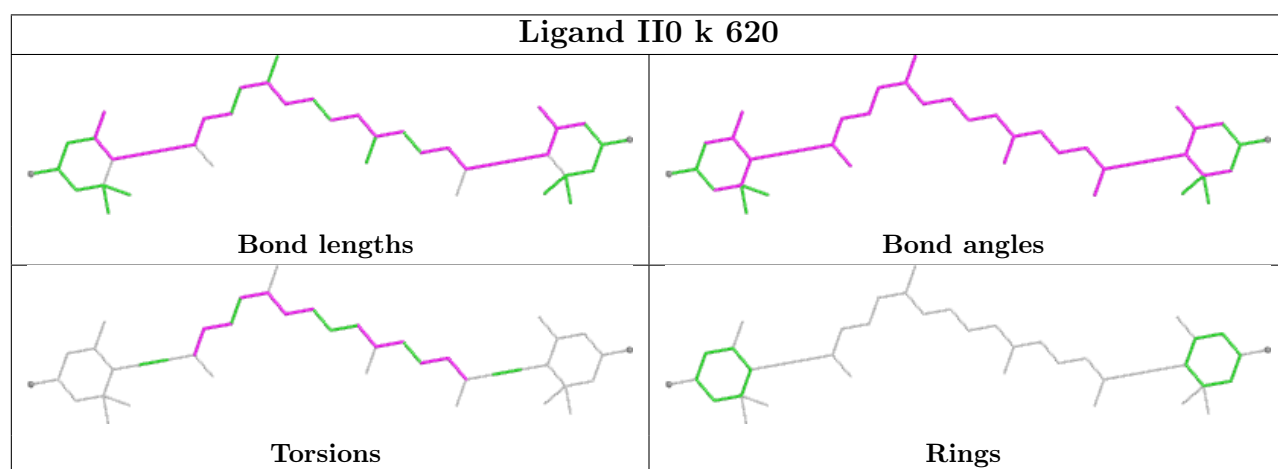


Rings

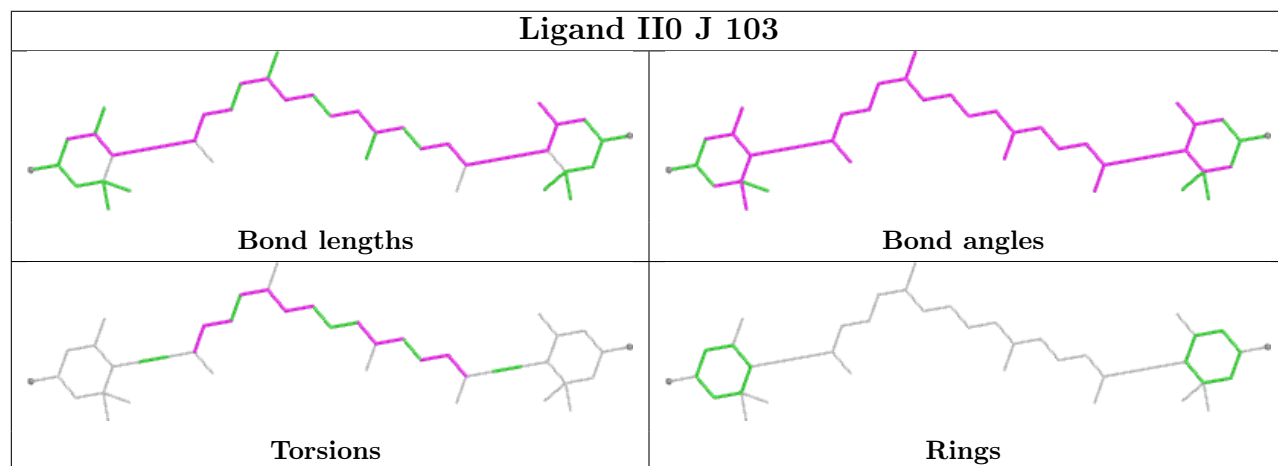
Ligand CLA g 307



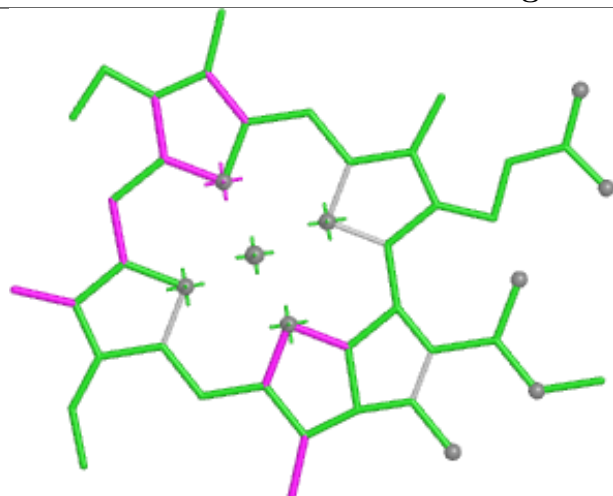
Ligand II0 k 620



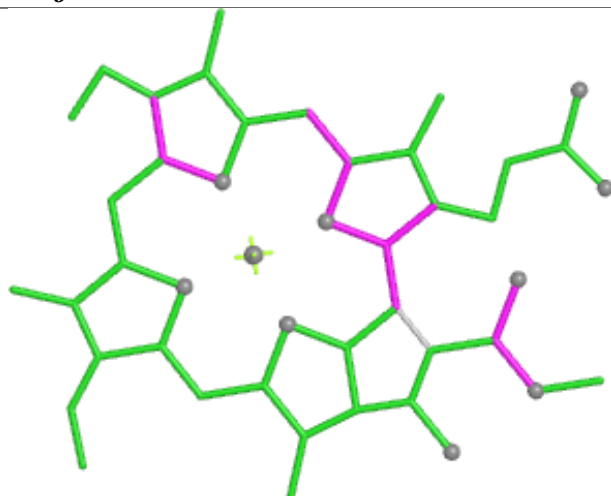
Ligand II0 J 103



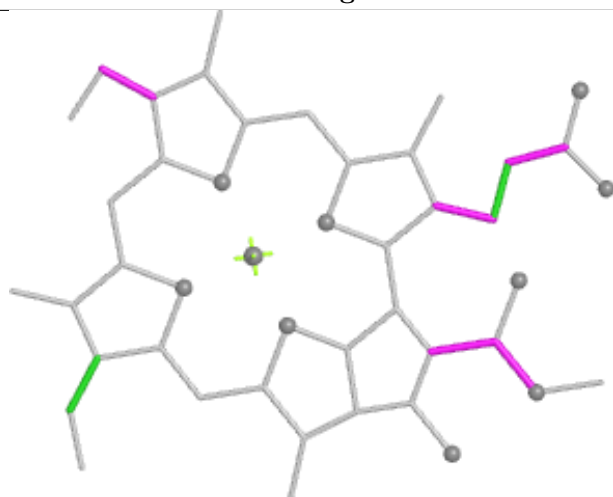
Ligand CLA j 306



Bond lengths



Bond angles

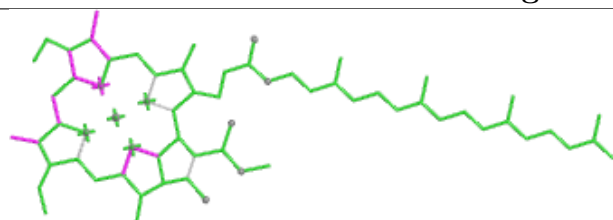


Torsions

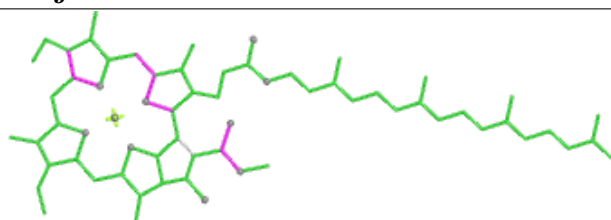


Rings

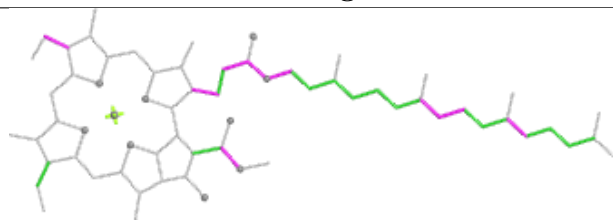
Ligand CLA j 310



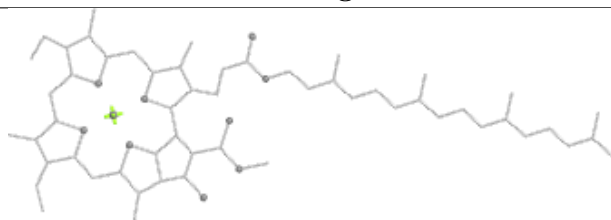
Bond lengths



Bond angles

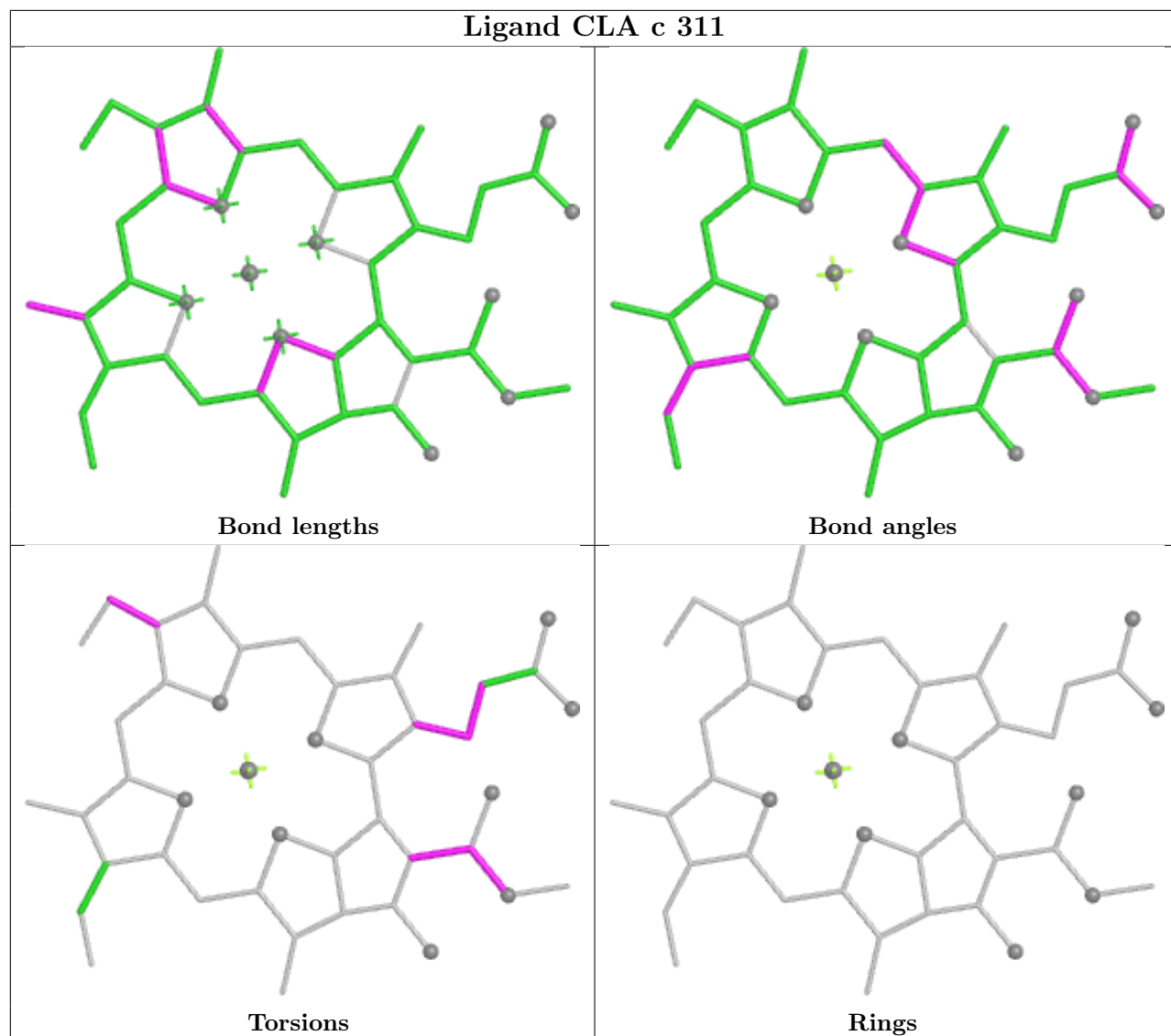


Torsions

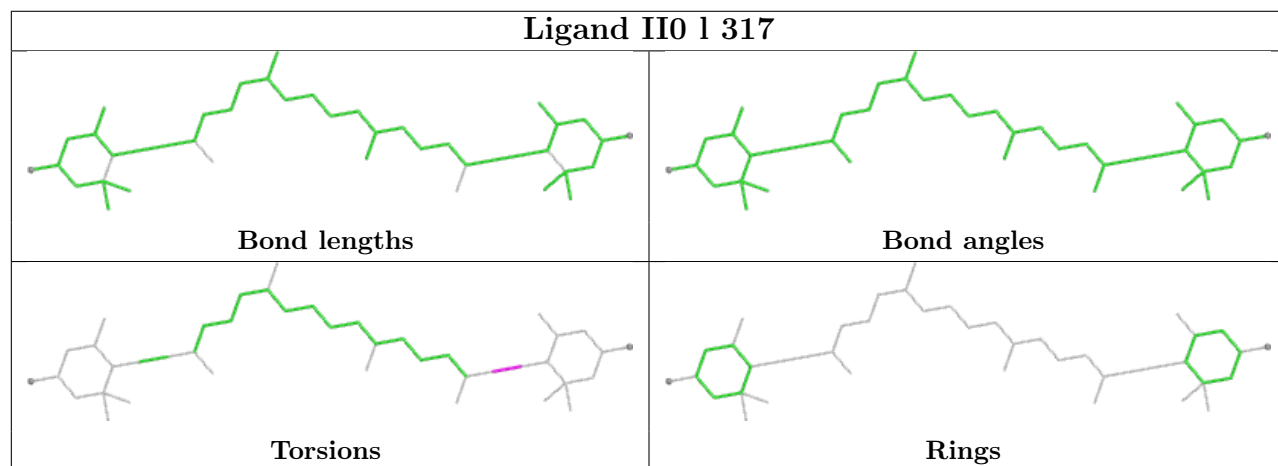


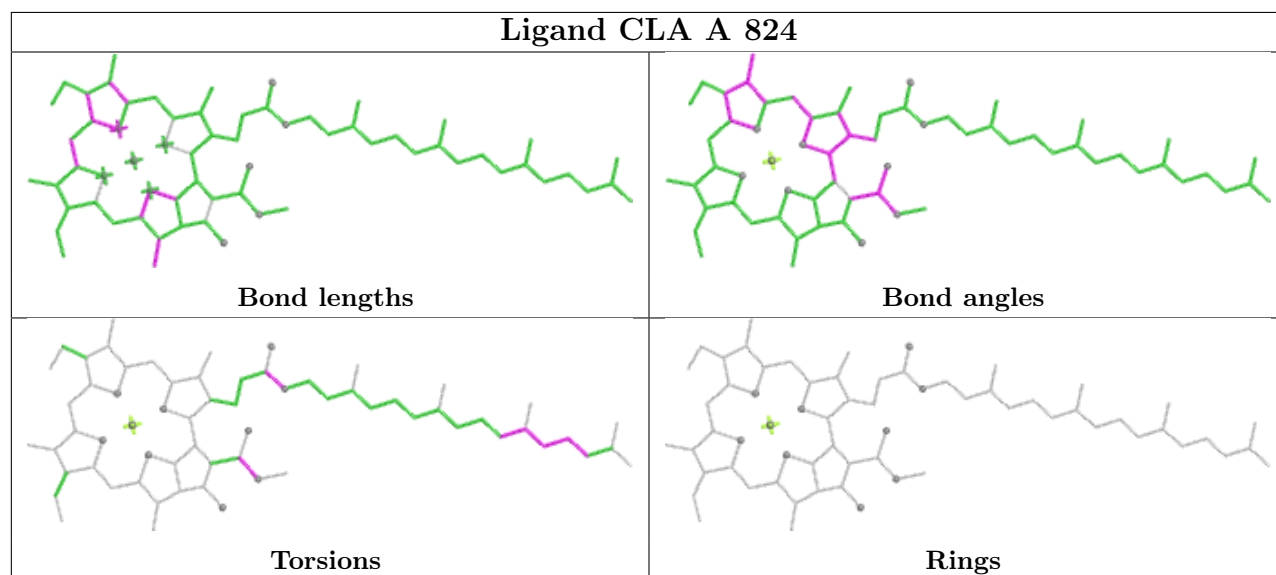
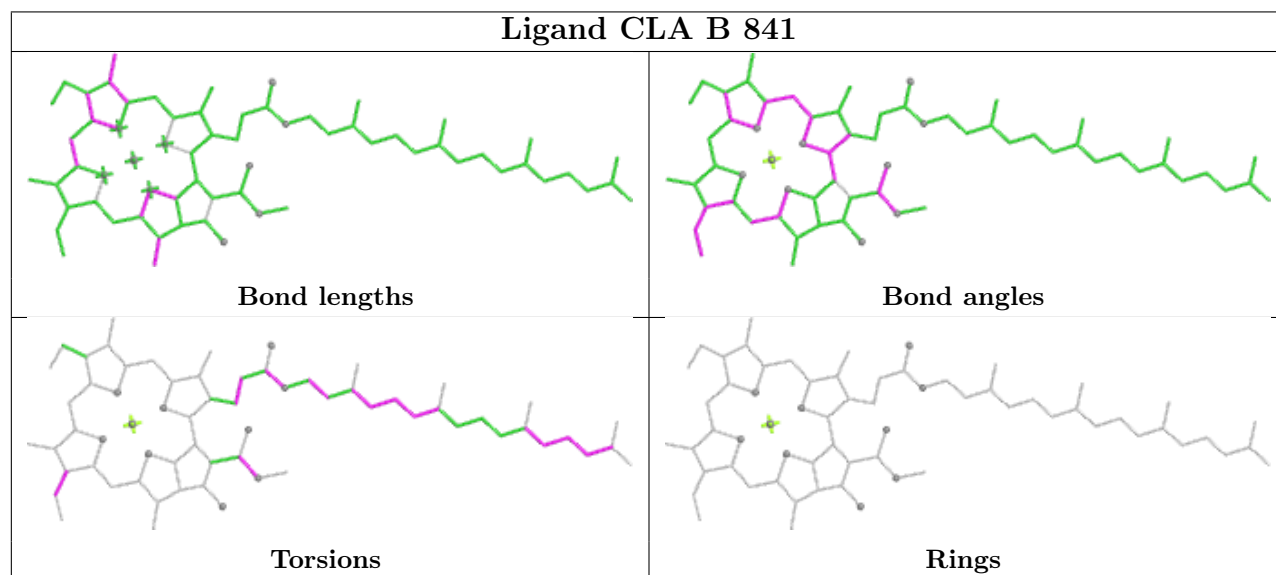
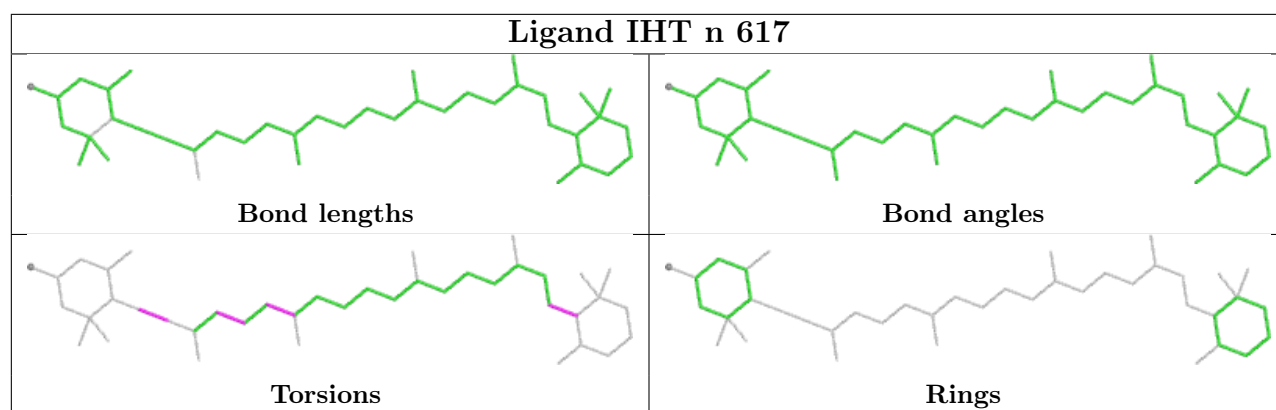
Rings

Ligand CLA c 311

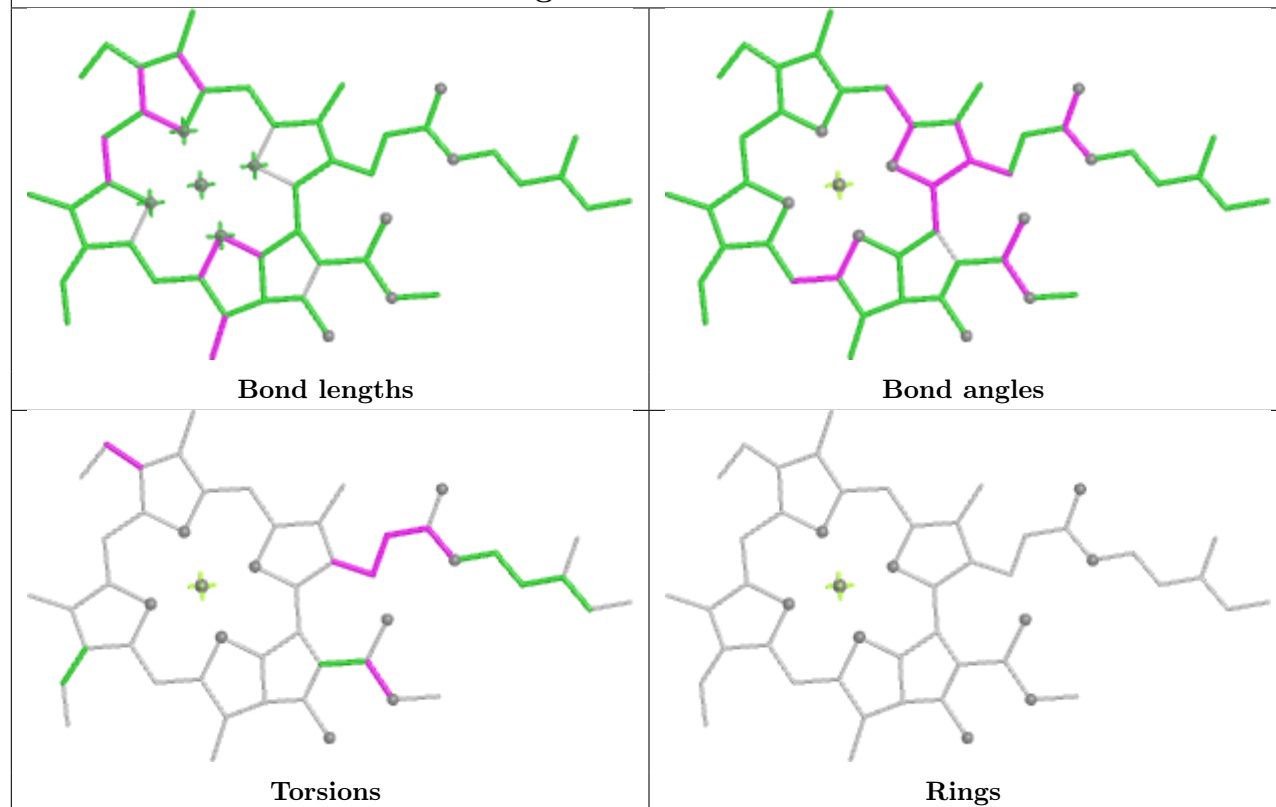


Ligand II0 l 317

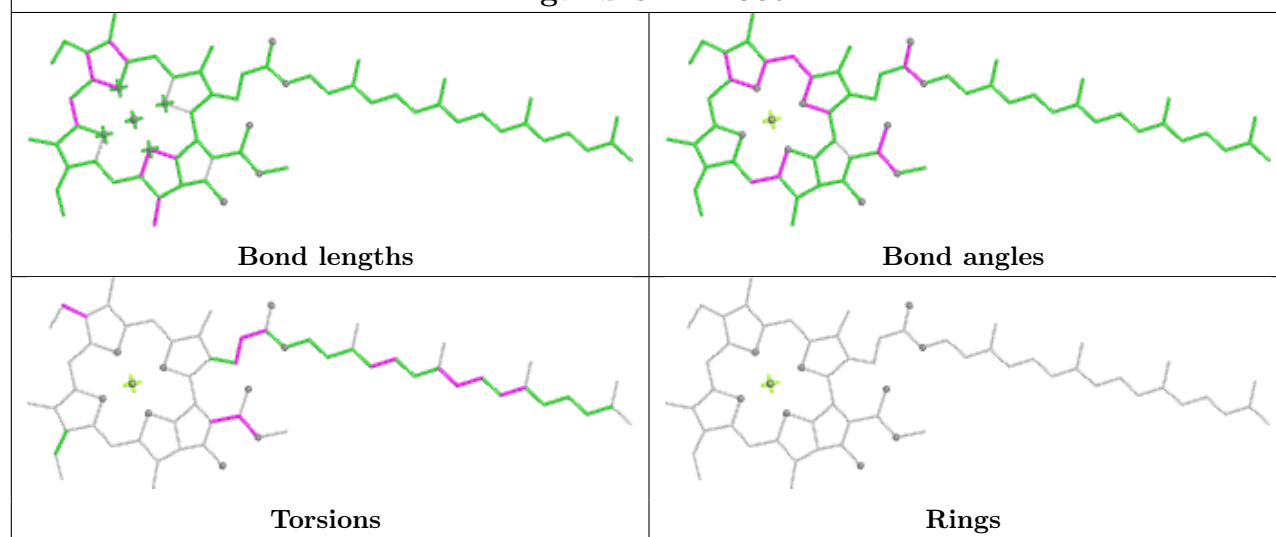




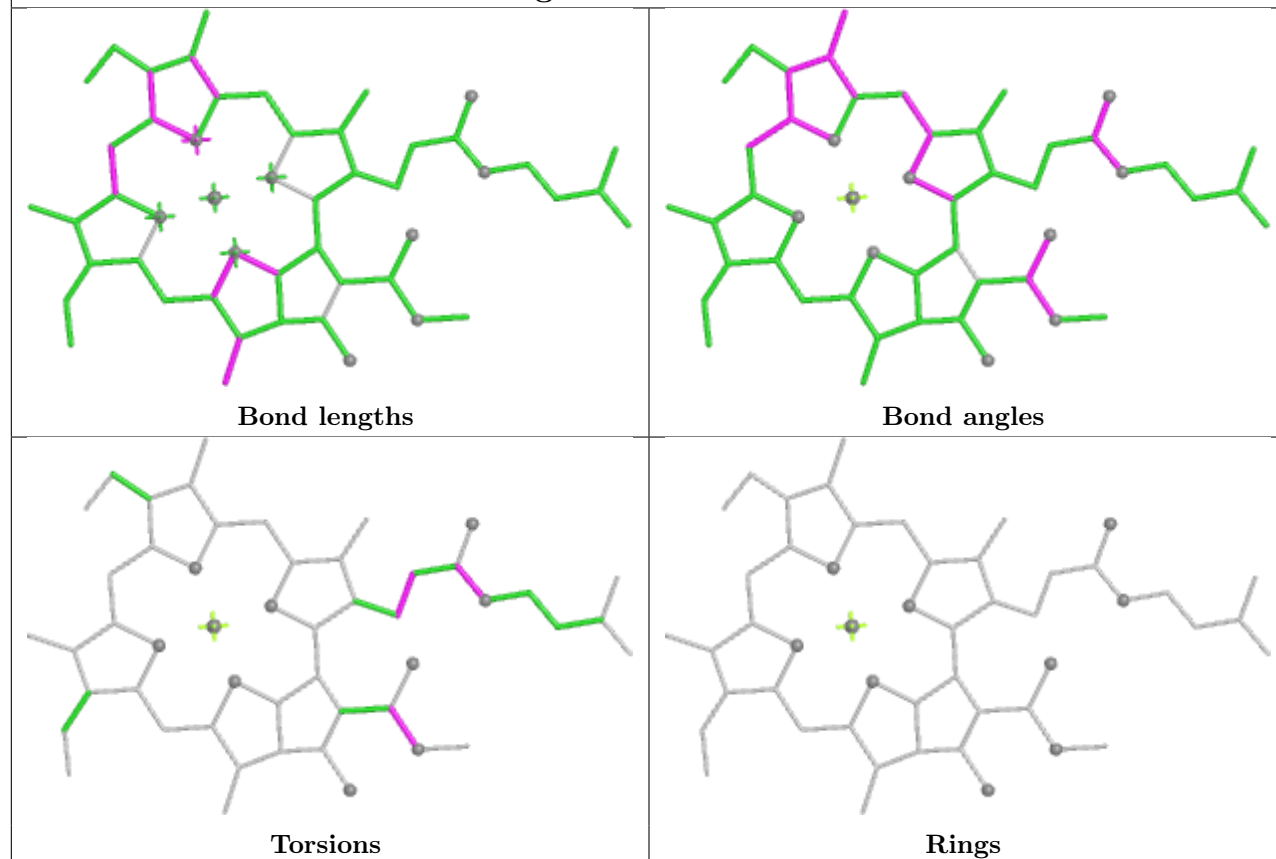
Ligand CLA n 613



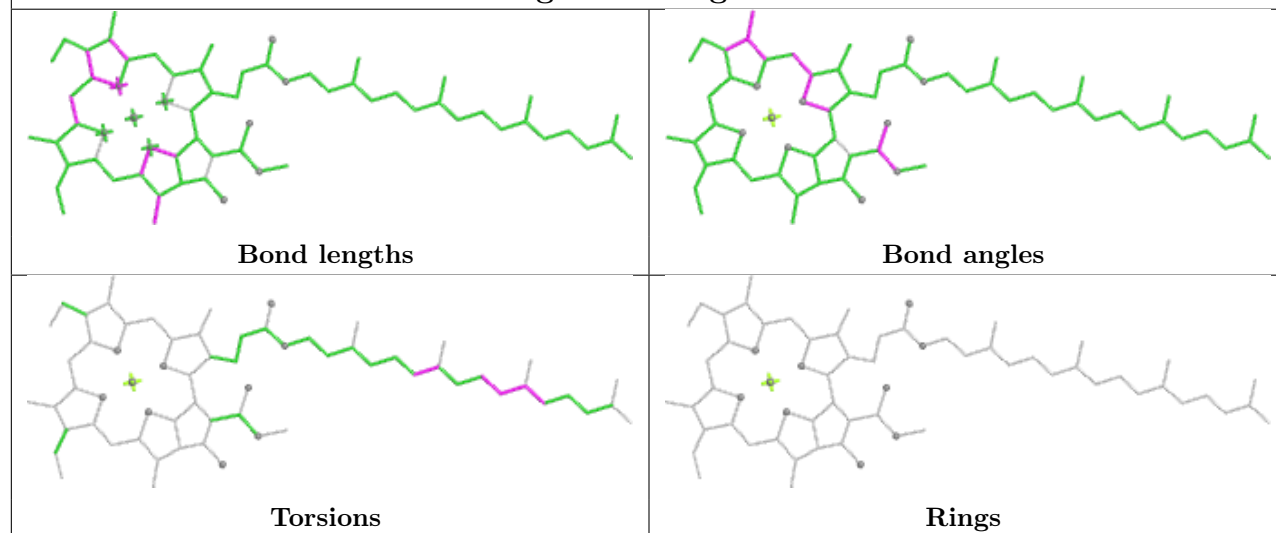
Ligand CLA i 305



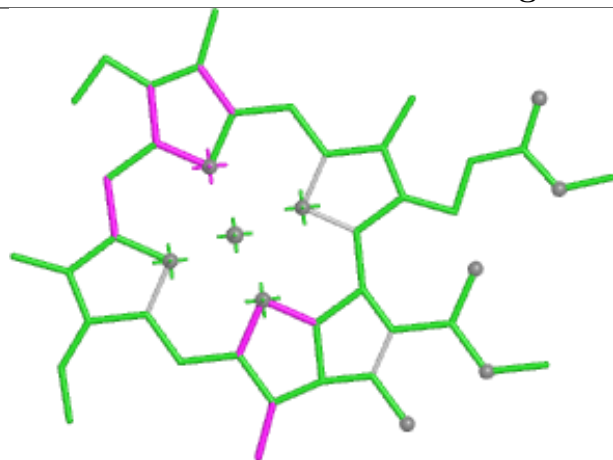
Ligand CLA n 602



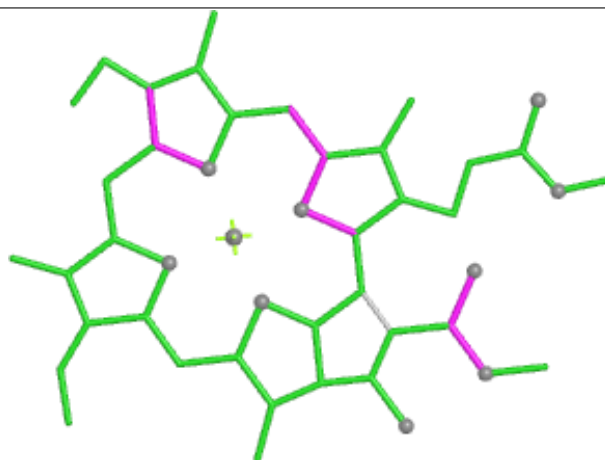
Ligand CLA g 305



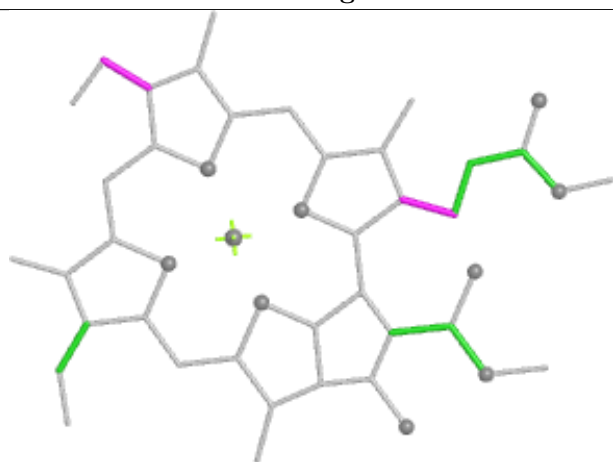
Ligand CLA e 308



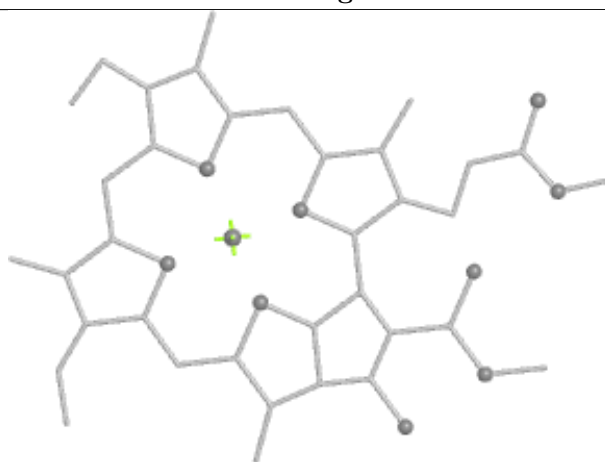
Bond lengths



Bond angles

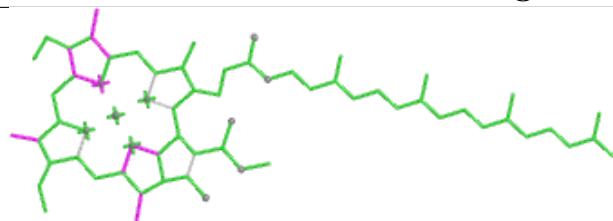


Torsions

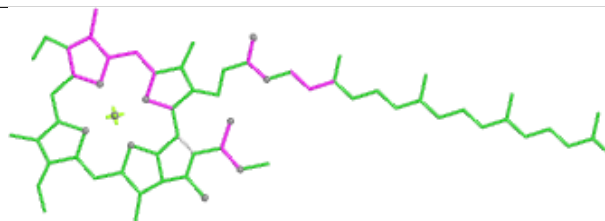


Rings

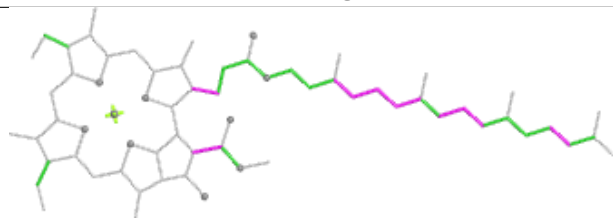
Ligand CLA B 812



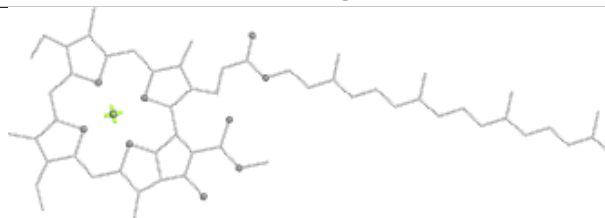
Bond lengths



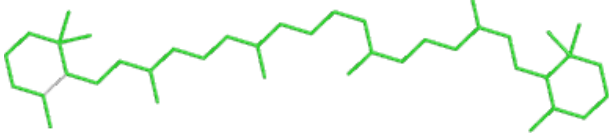
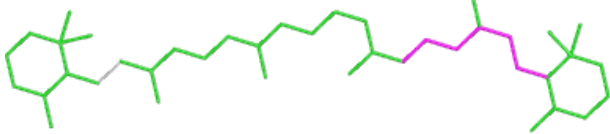
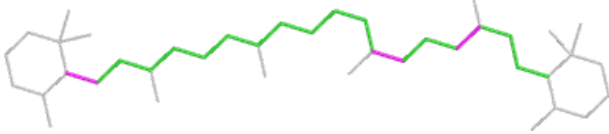
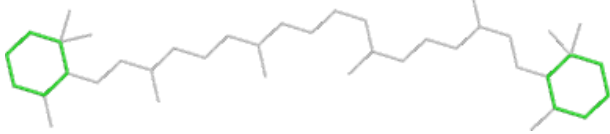
Bond angles

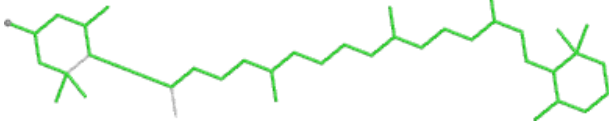
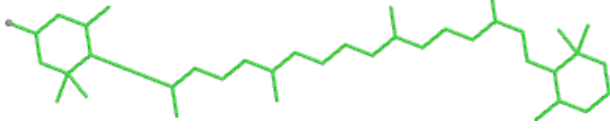
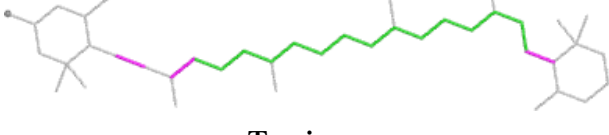
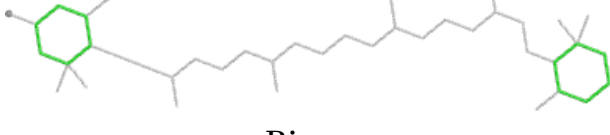


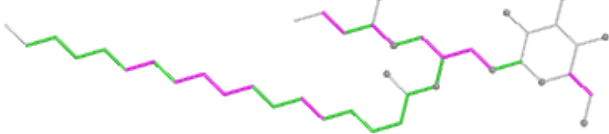
Torsions

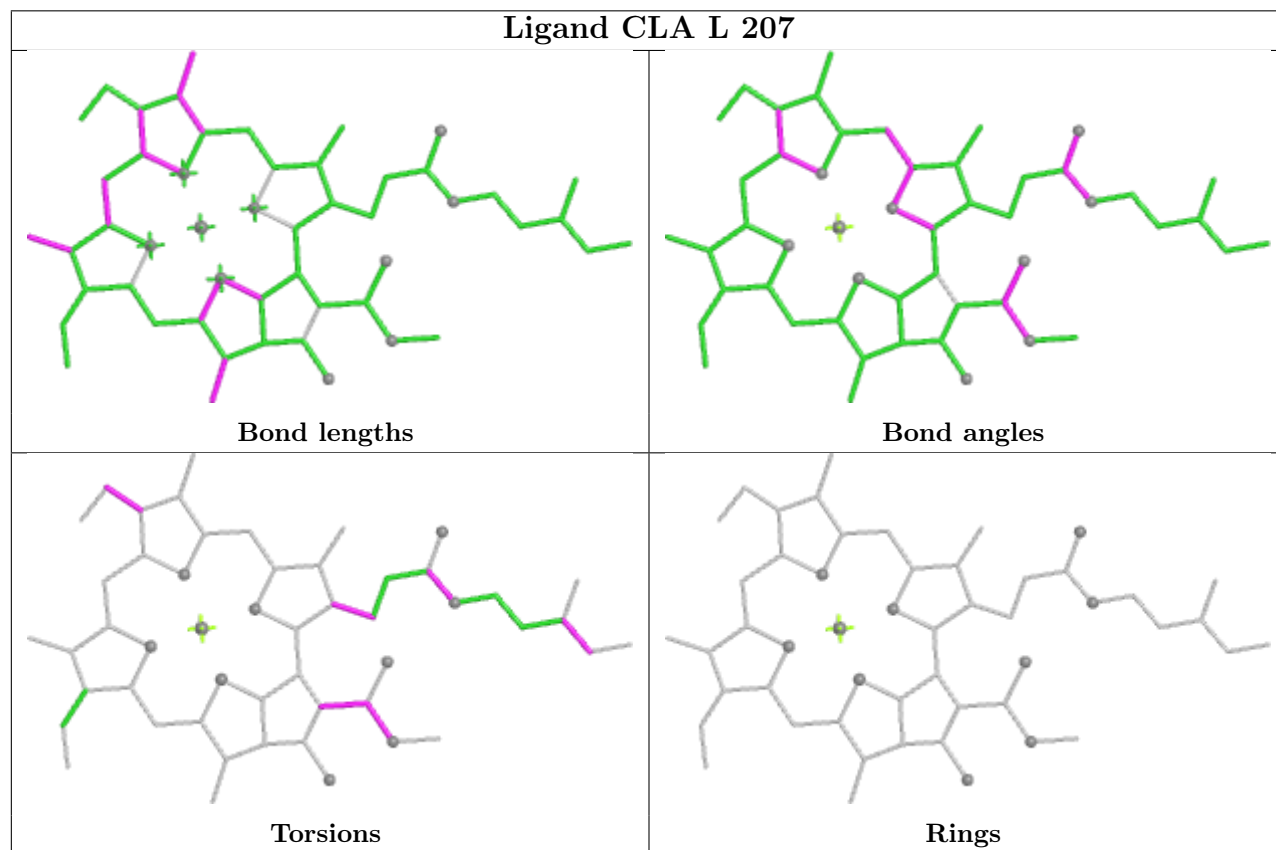
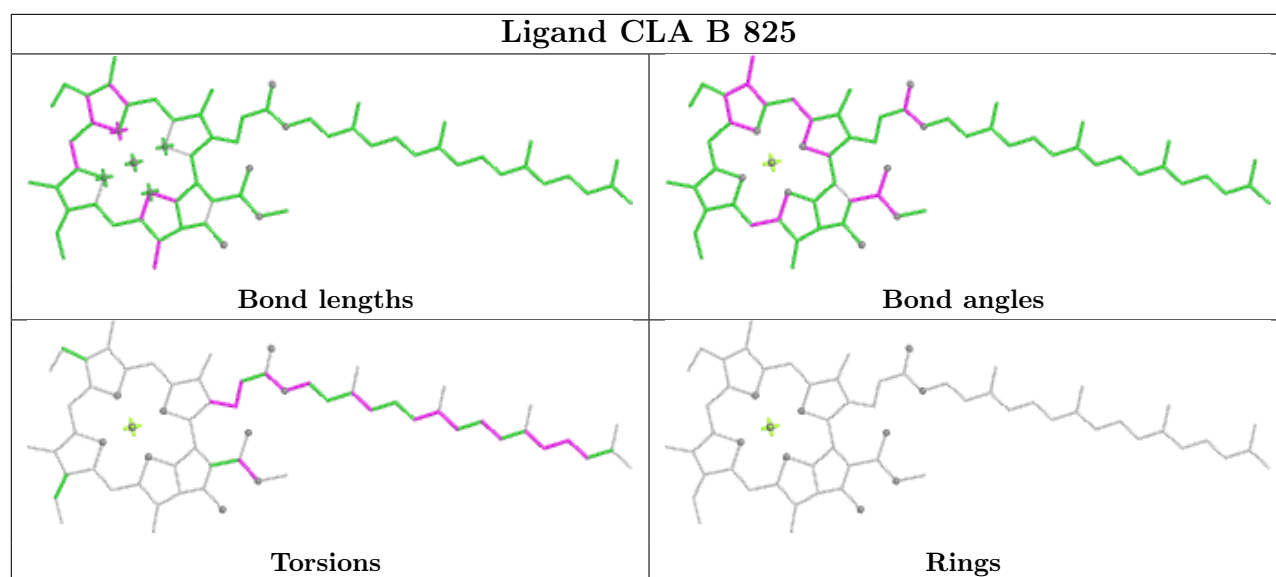


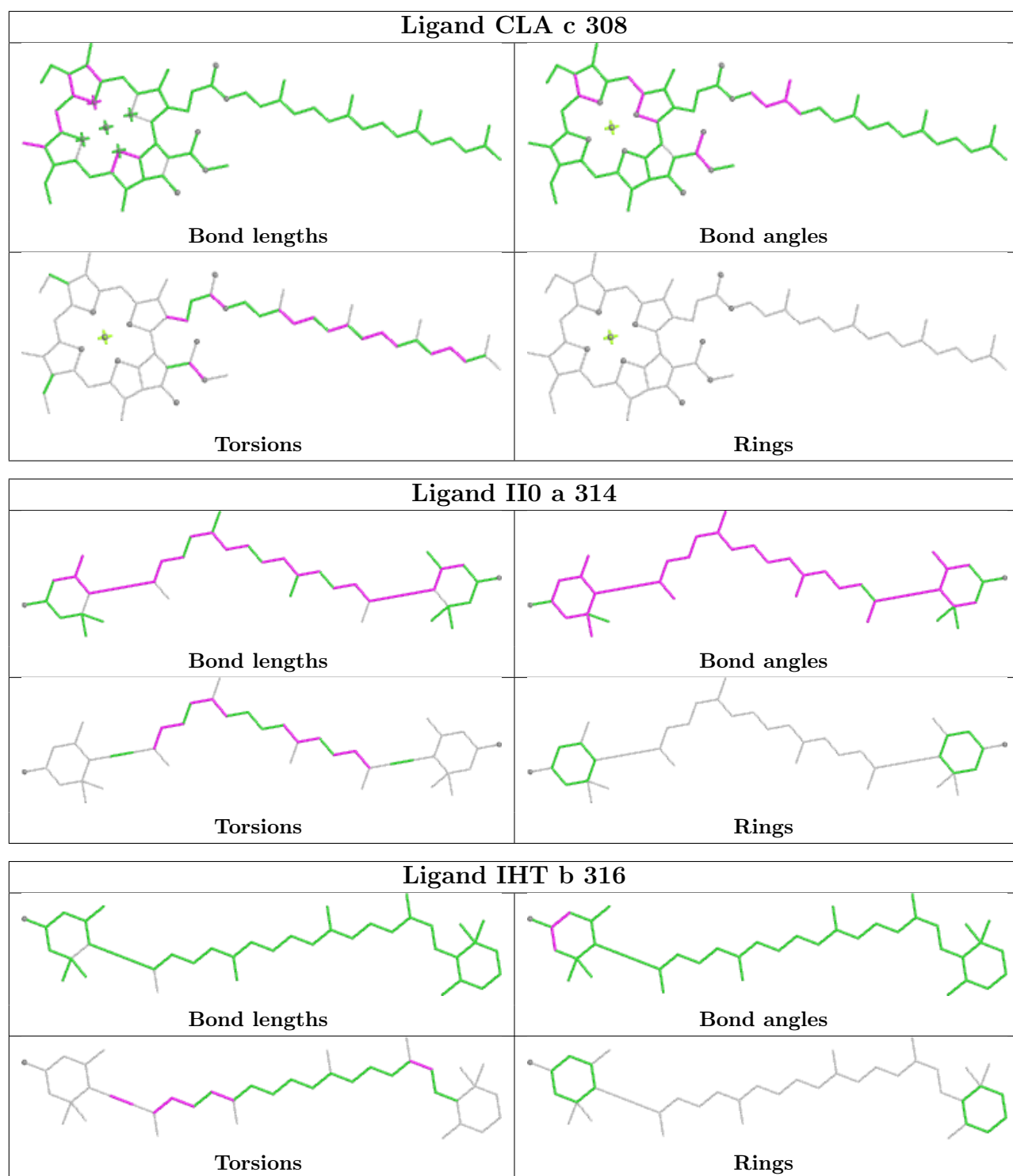
Rings

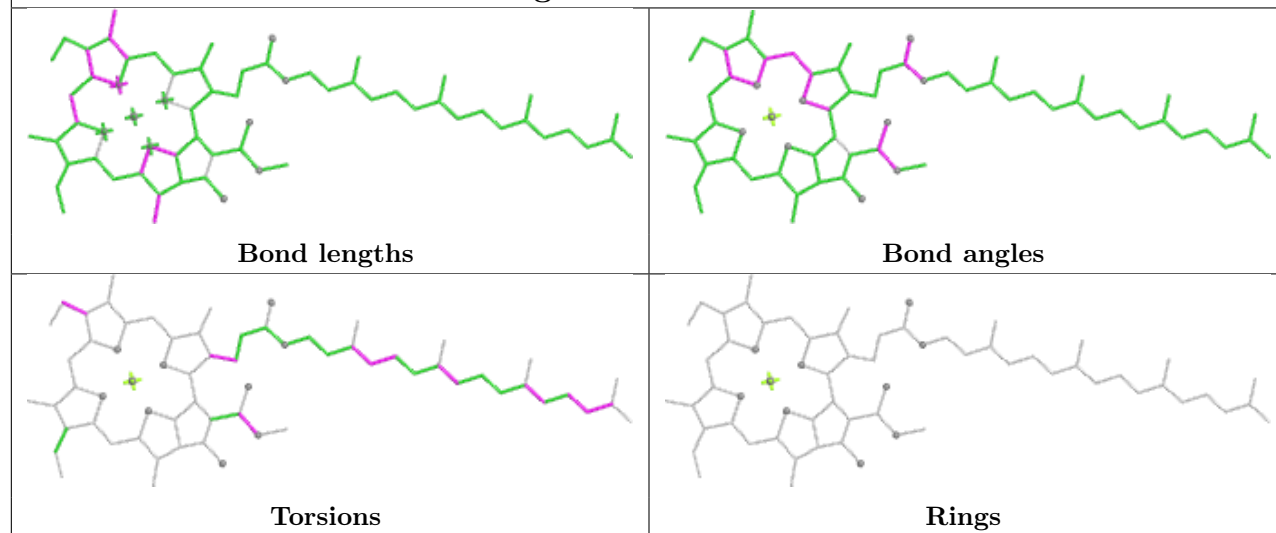
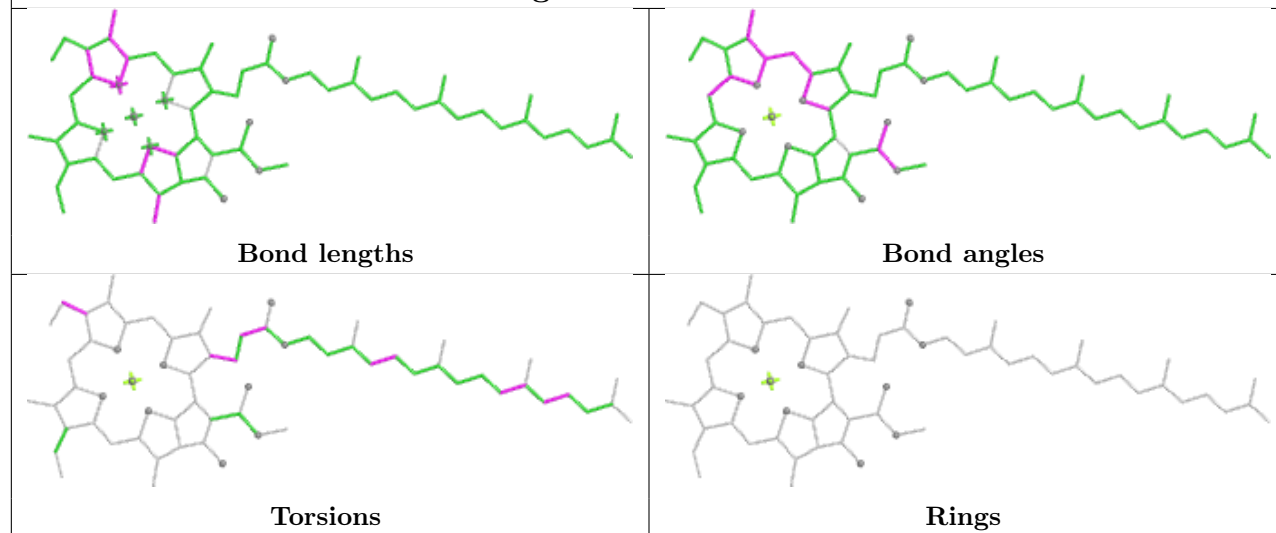
Ligand WVN B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand IHT a 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

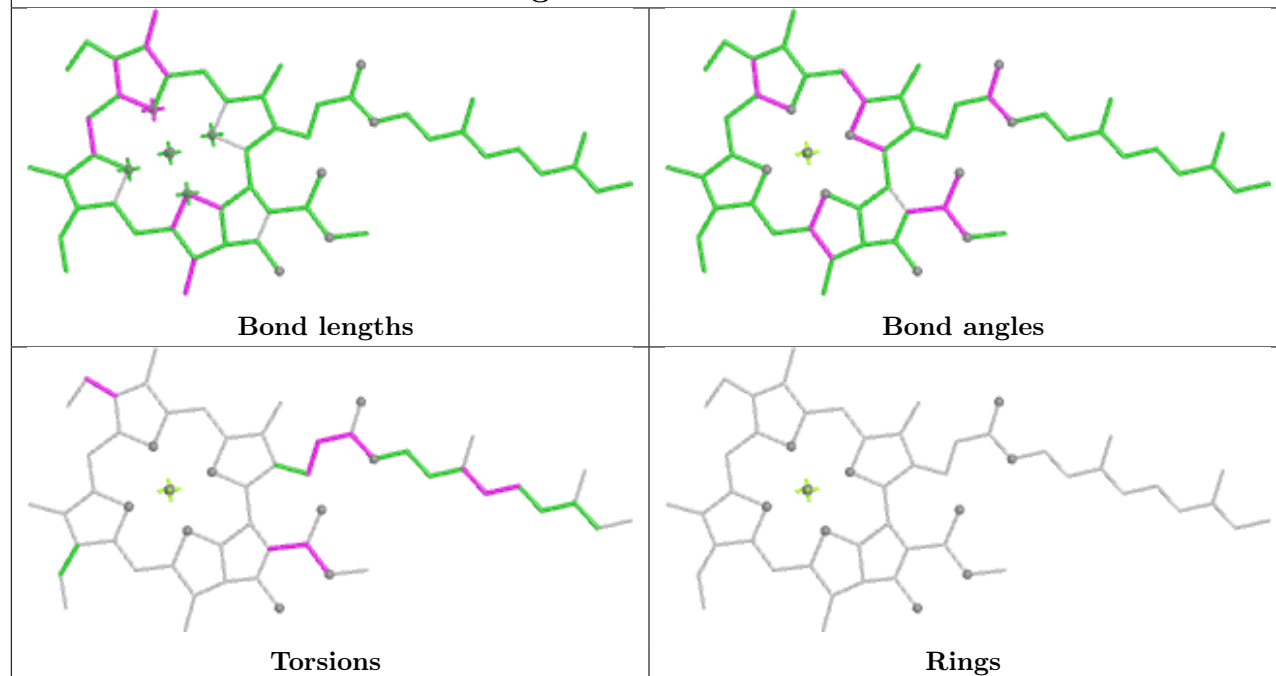
Ligand LMG F 208	
	
Bond lengths	Bond angles
	
Torsions	Rings



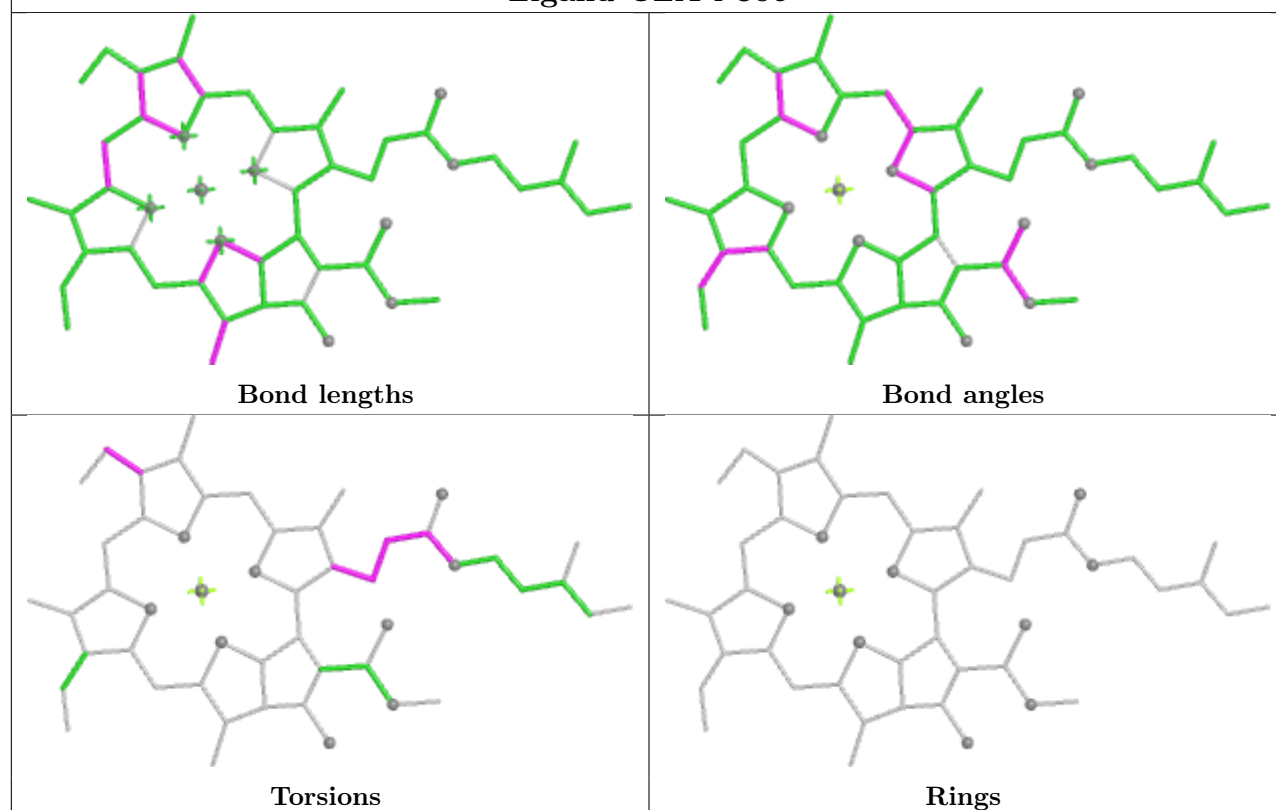


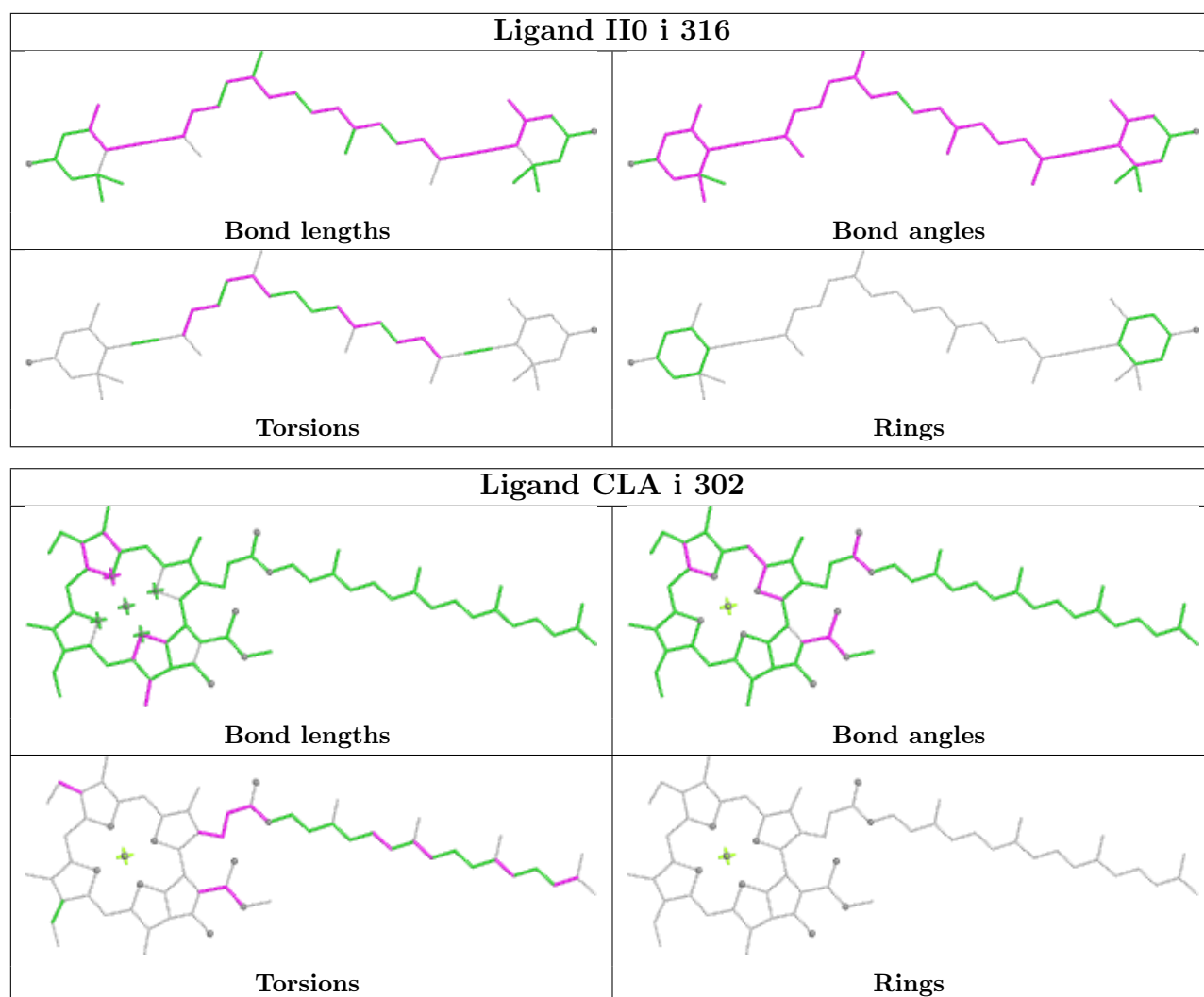
Ligand CLA F 201**Ligand CLA B 809**

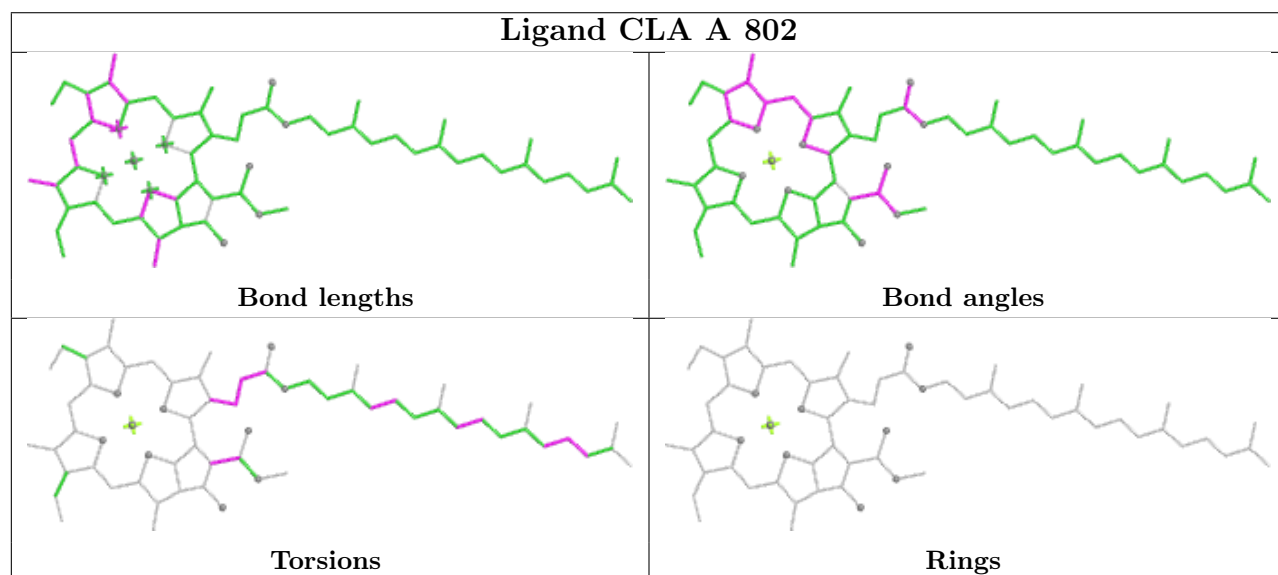
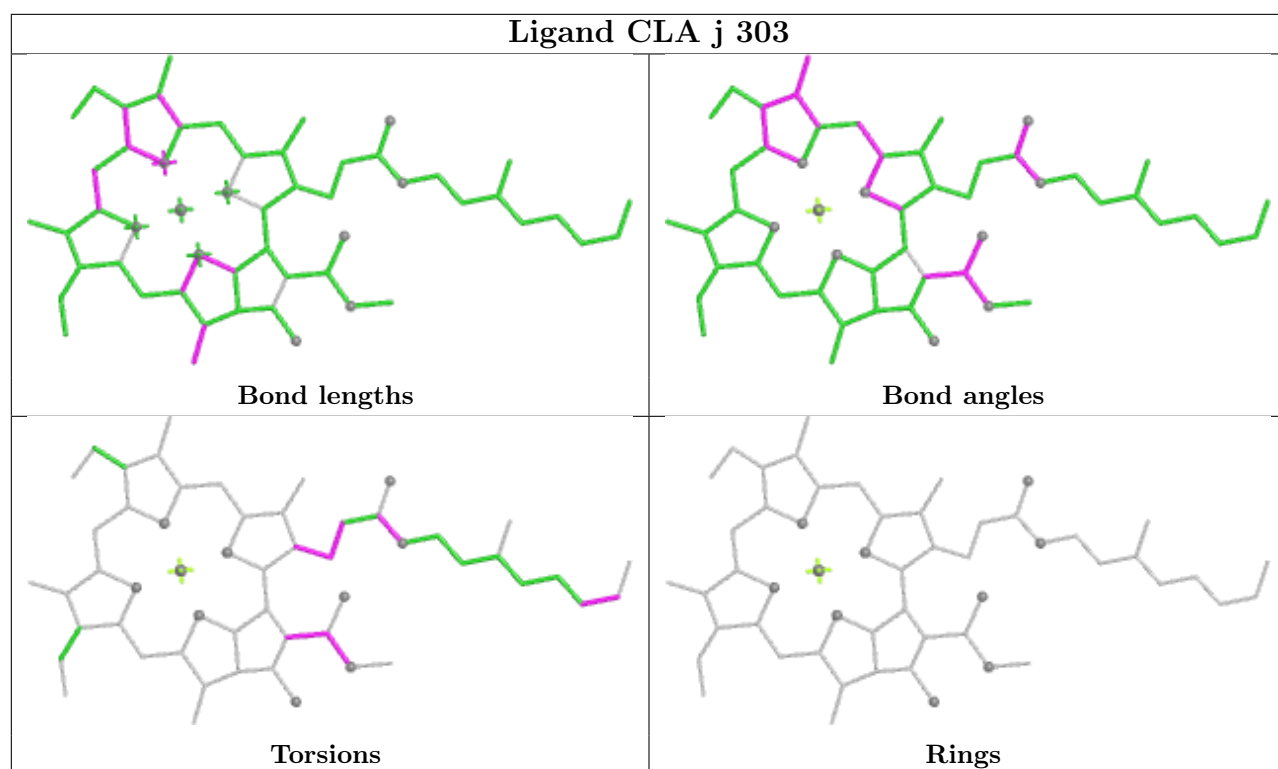
Ligand CLA A 822

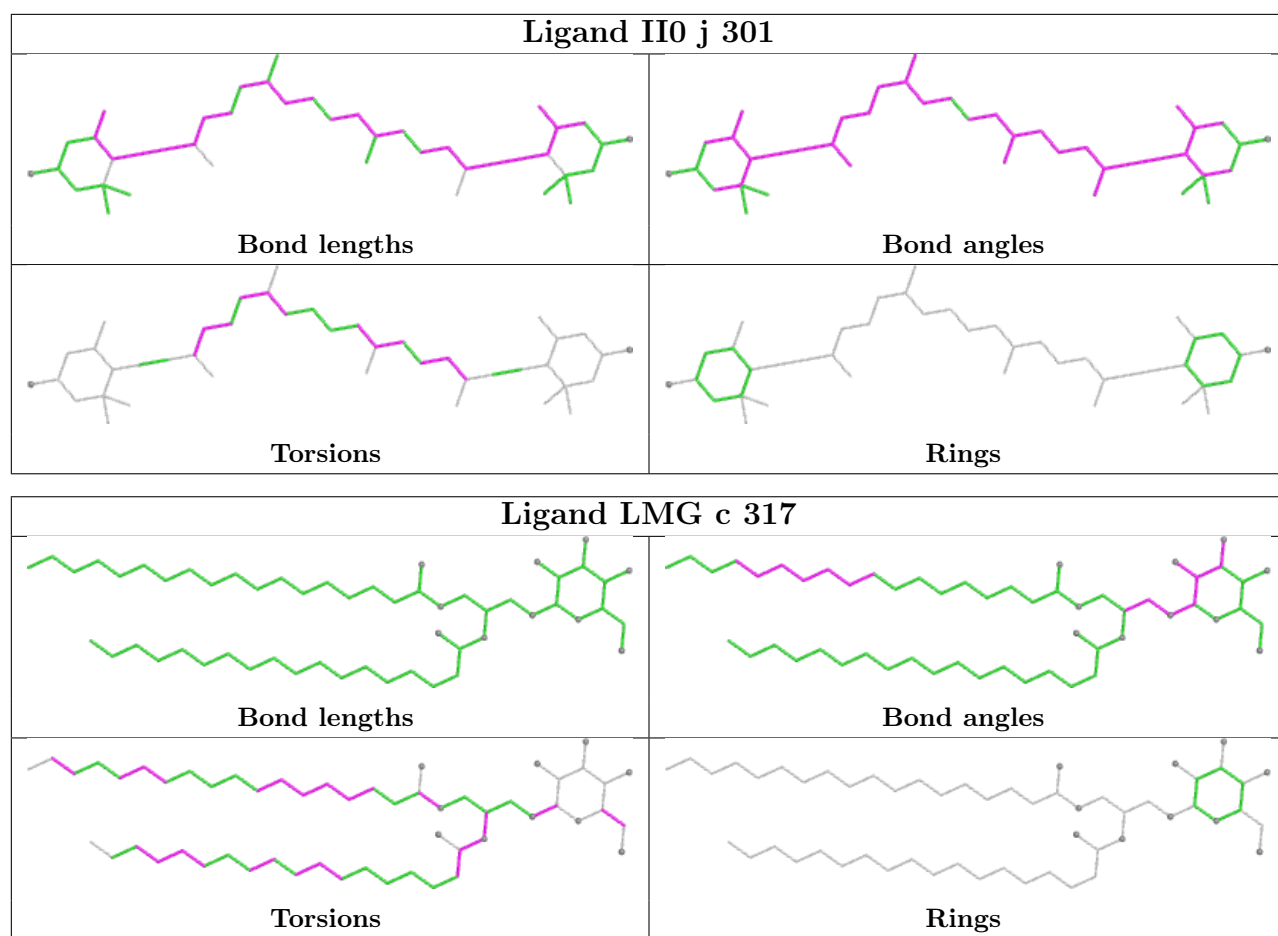


Ligand CLA i 306

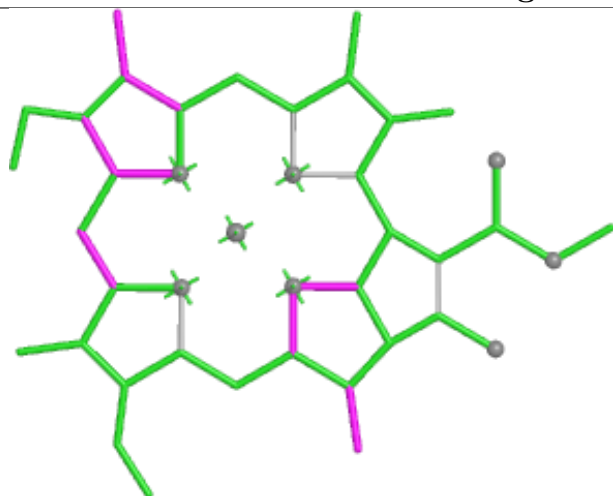








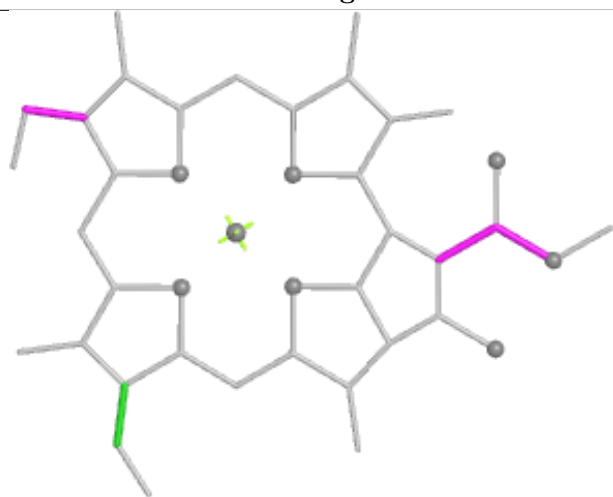
Ligand CLA d 310



Bond lengths



Bond angles

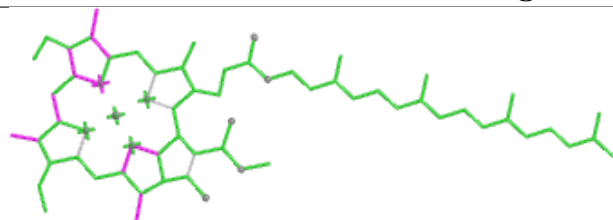


Torsions

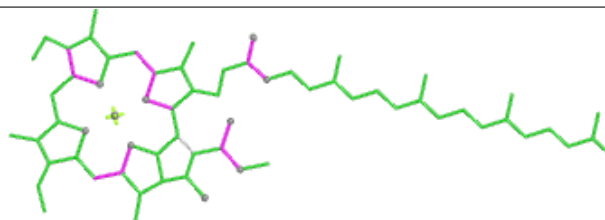


Rings

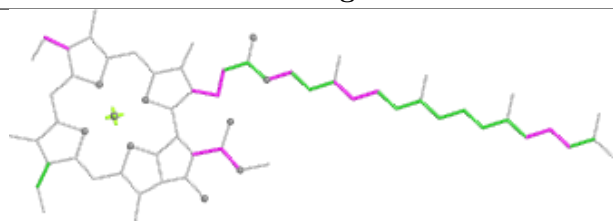
Ligand CLA n 609



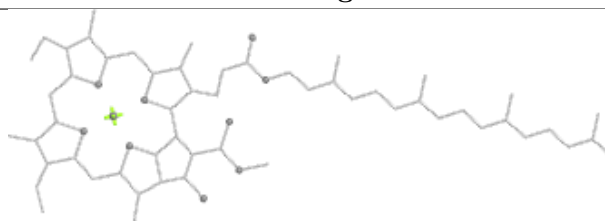
Bond lengths



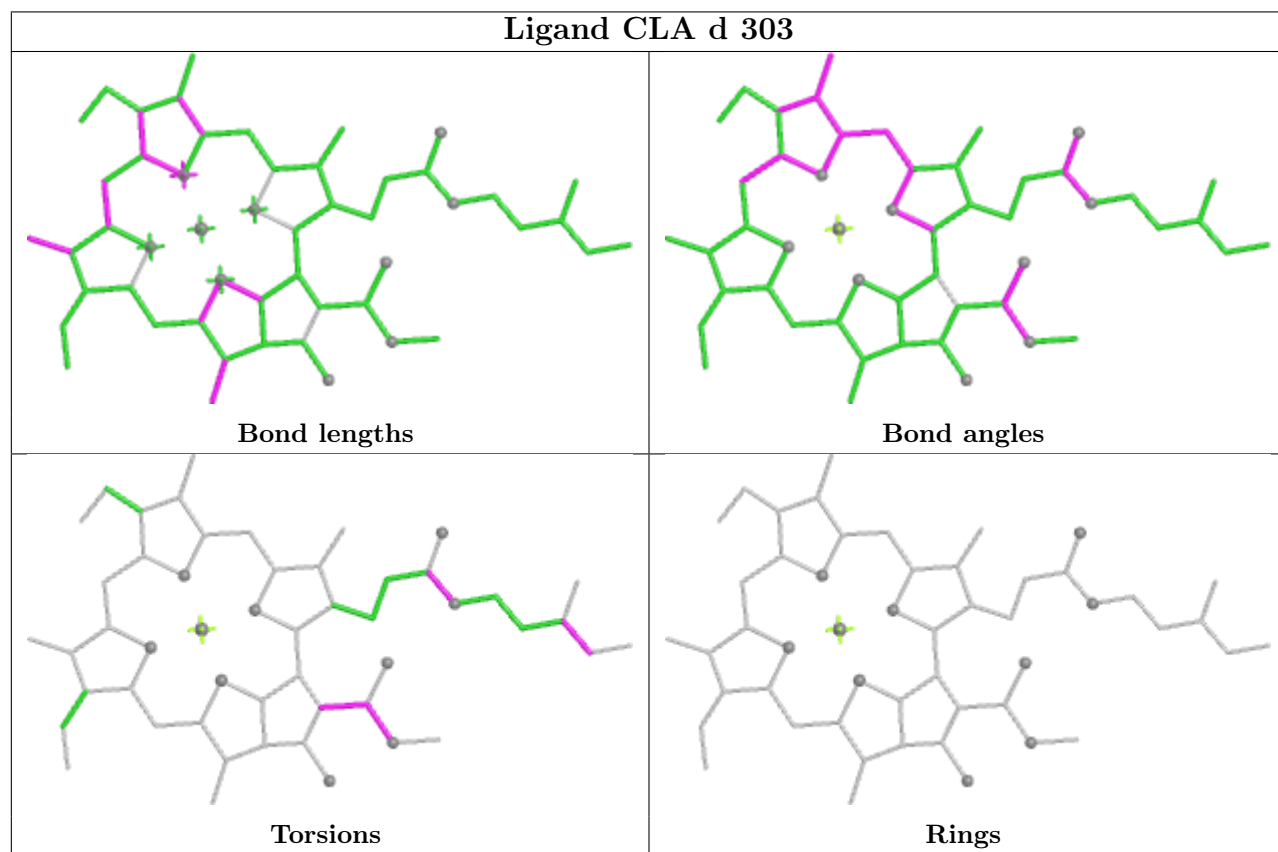
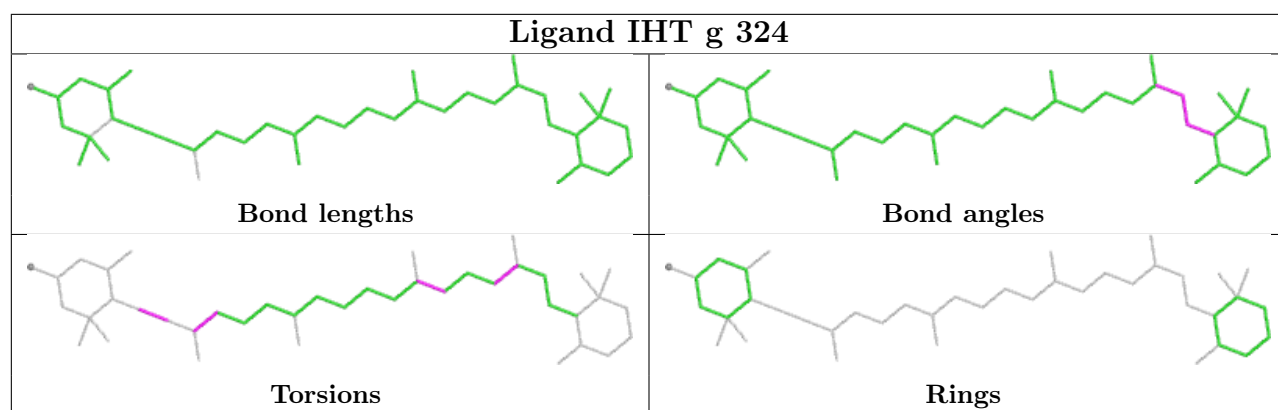
Bond angles

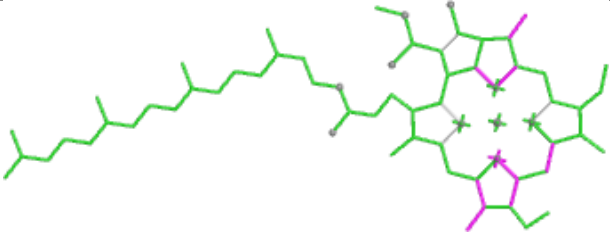
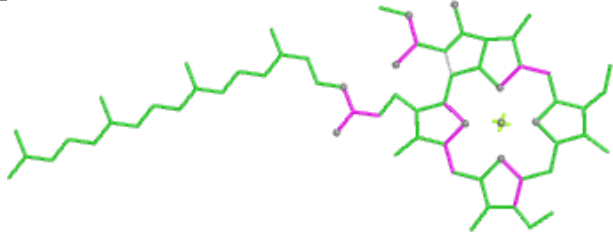
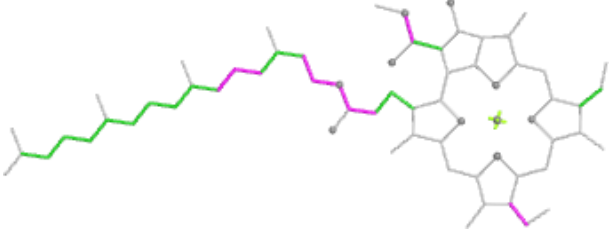
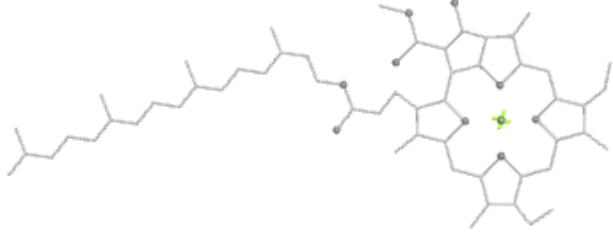
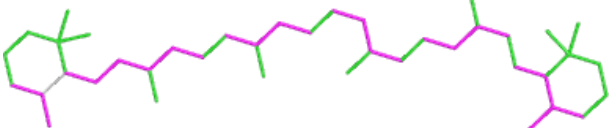
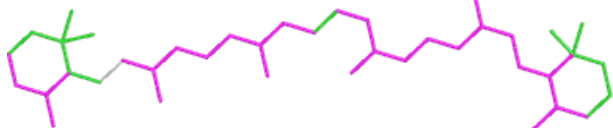
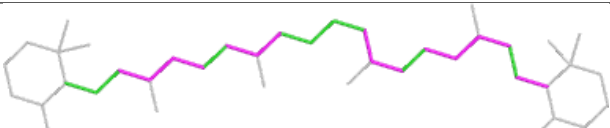
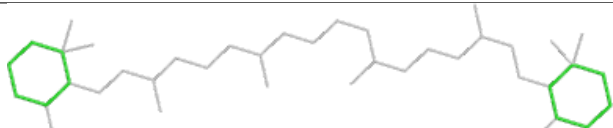
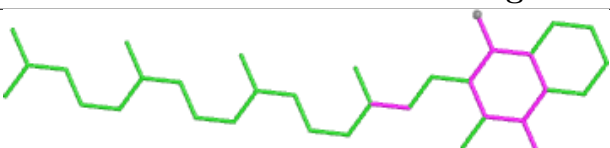
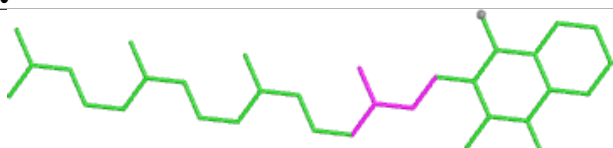
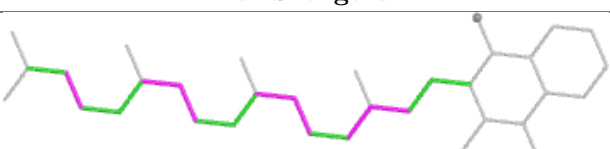
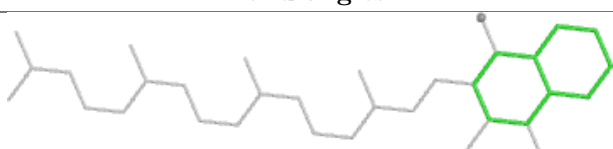


Torsions

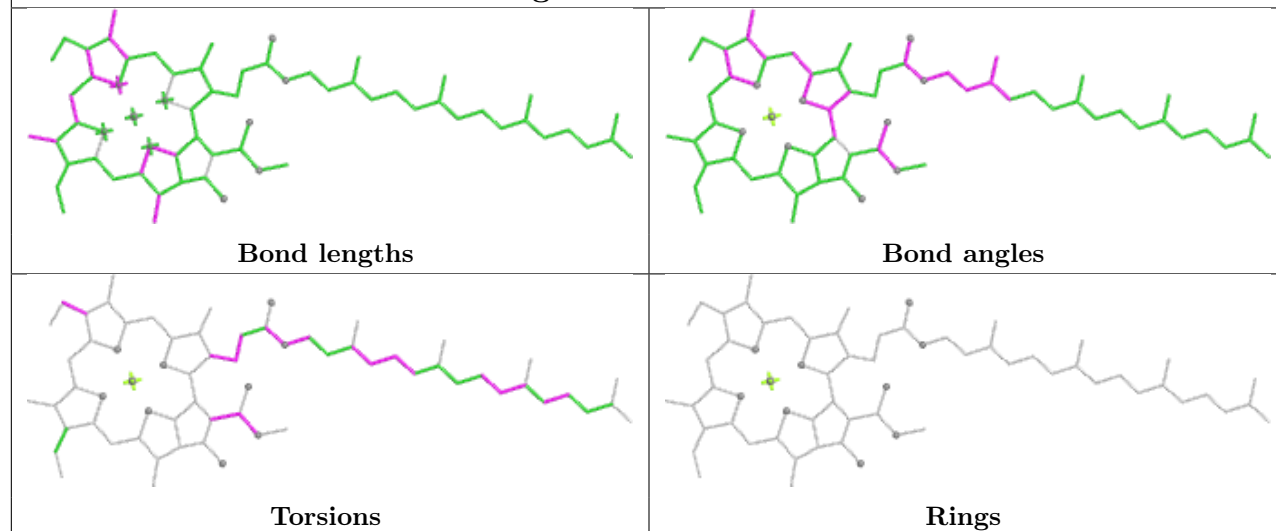


Rings

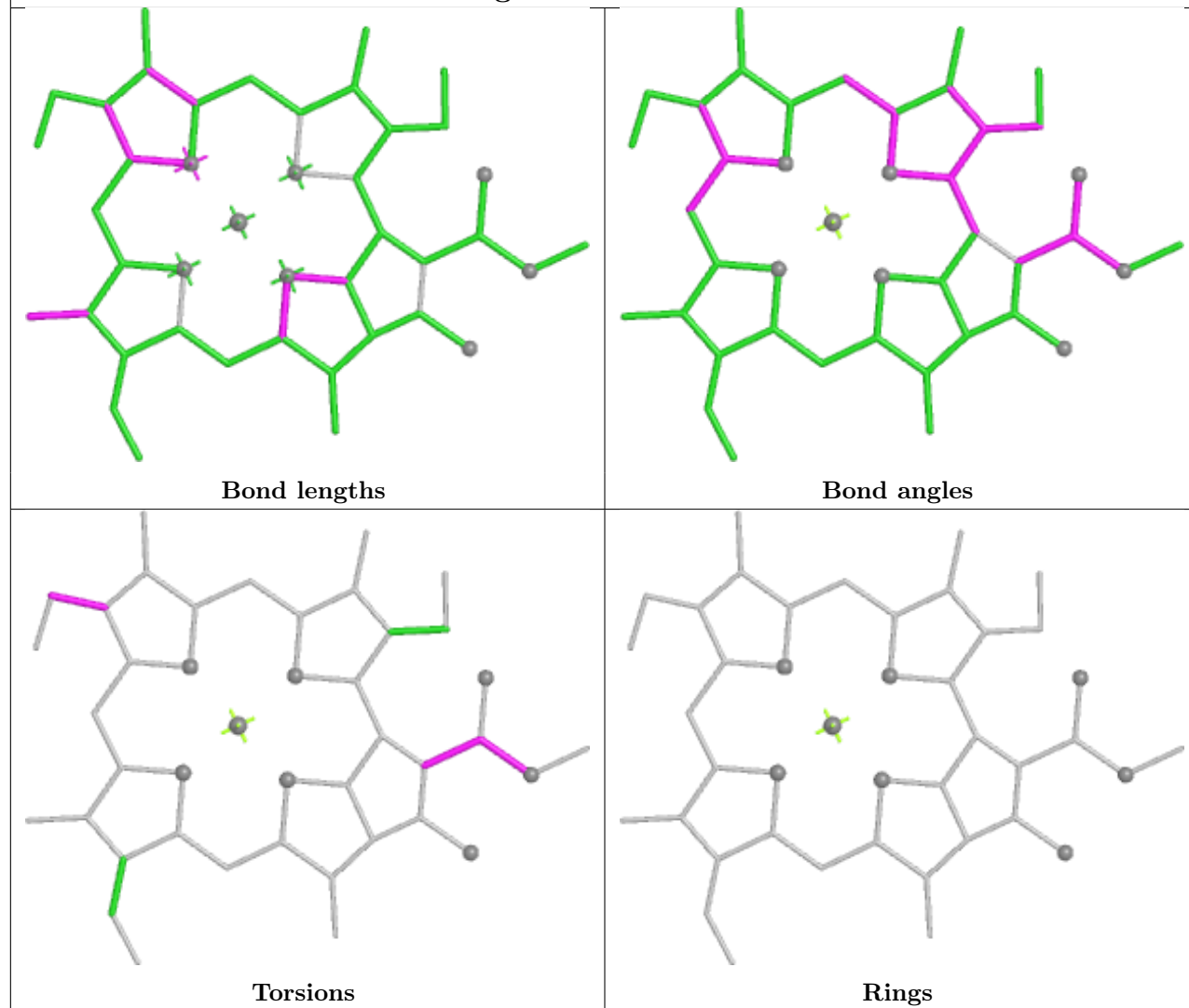


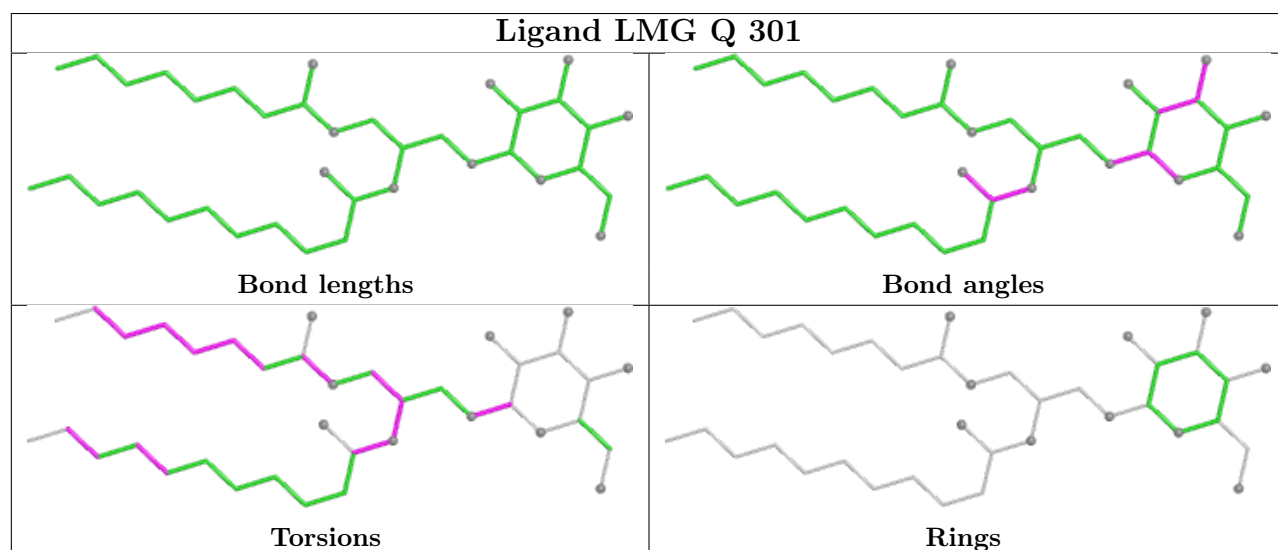
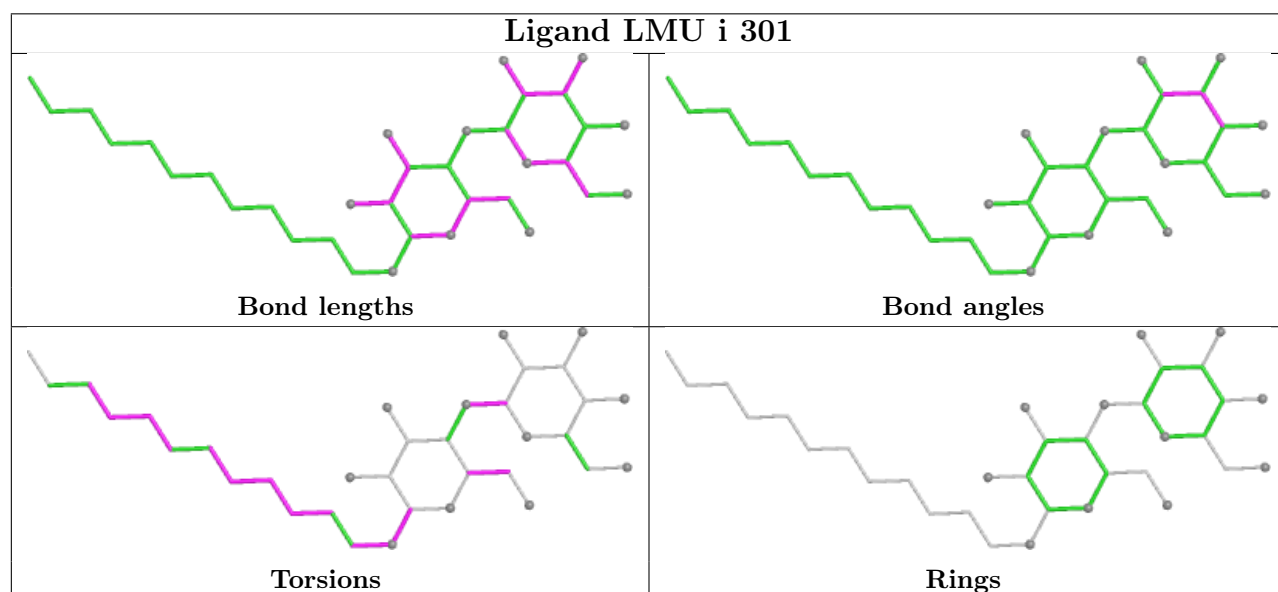
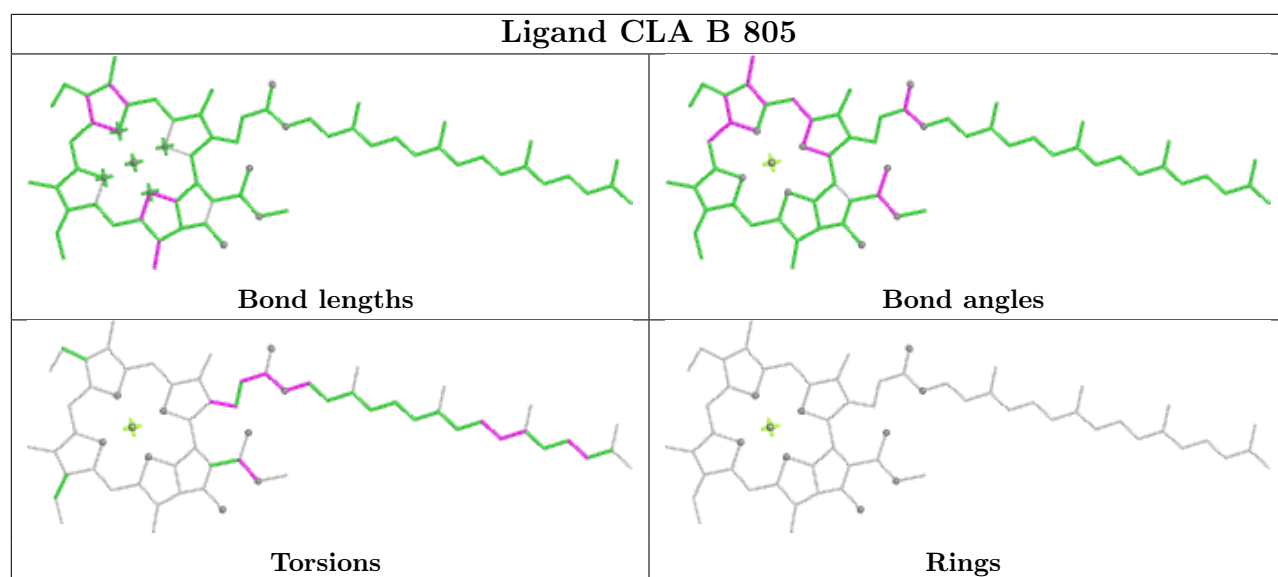
Ligand CLA h 301	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand WVN F 207	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand PQN B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

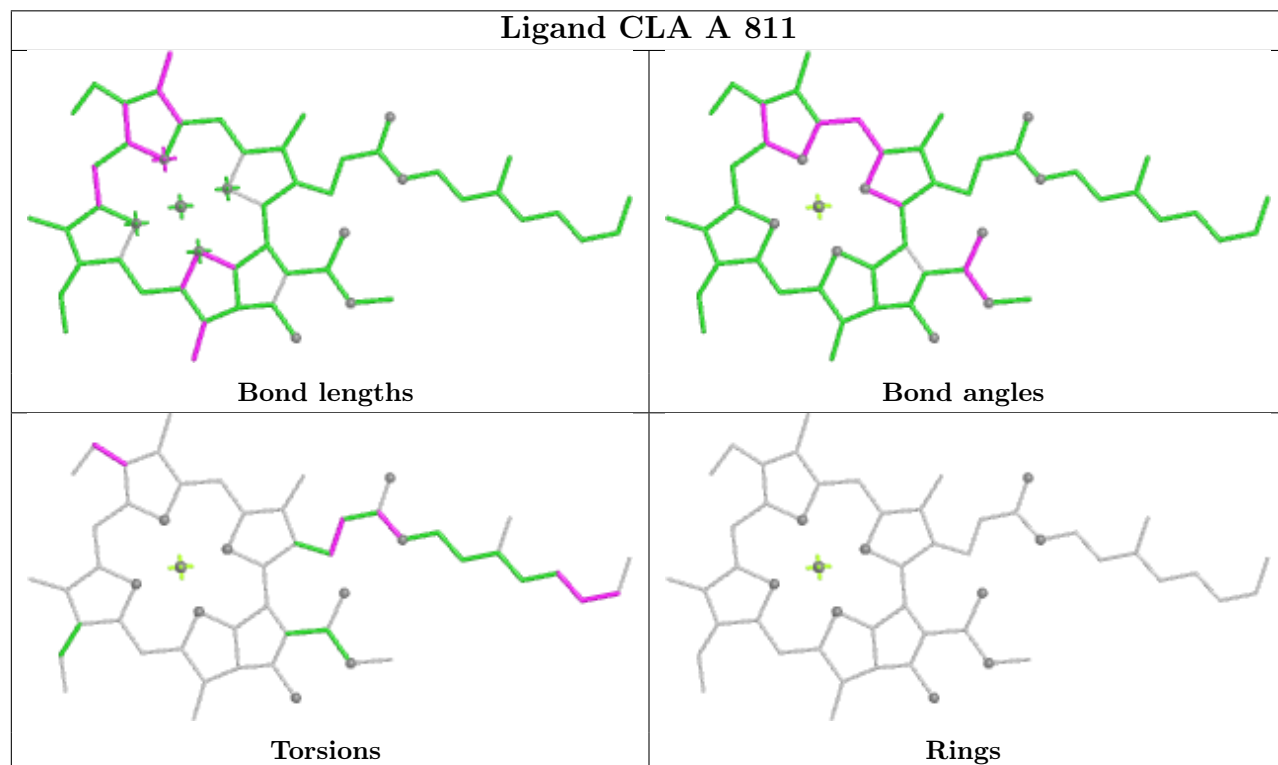
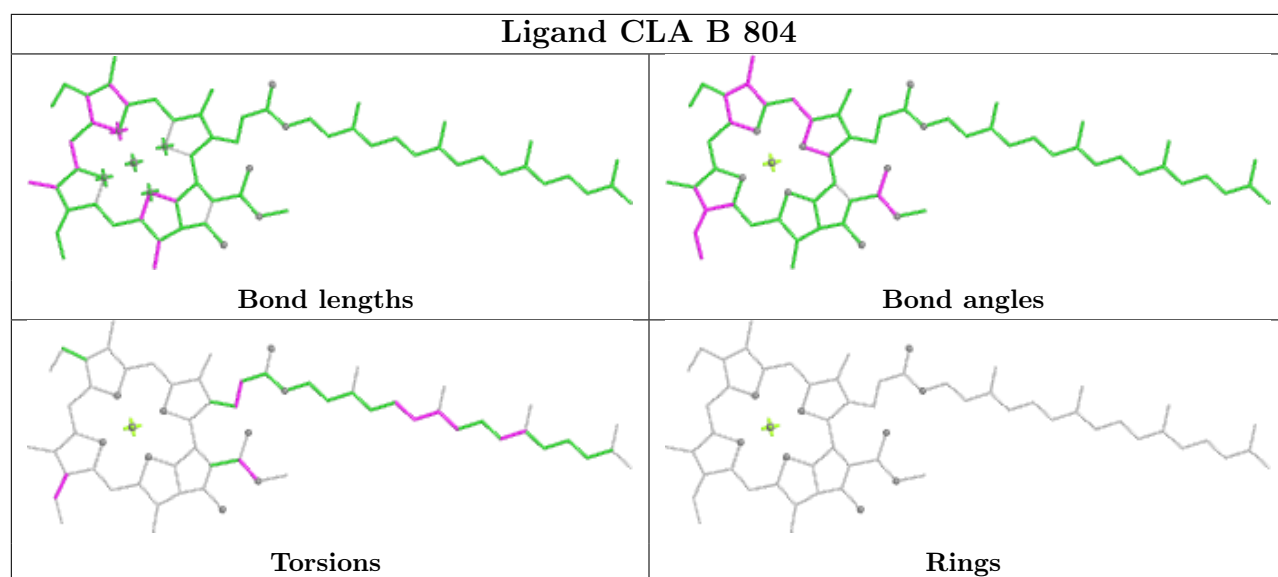
Ligand CLA B 822



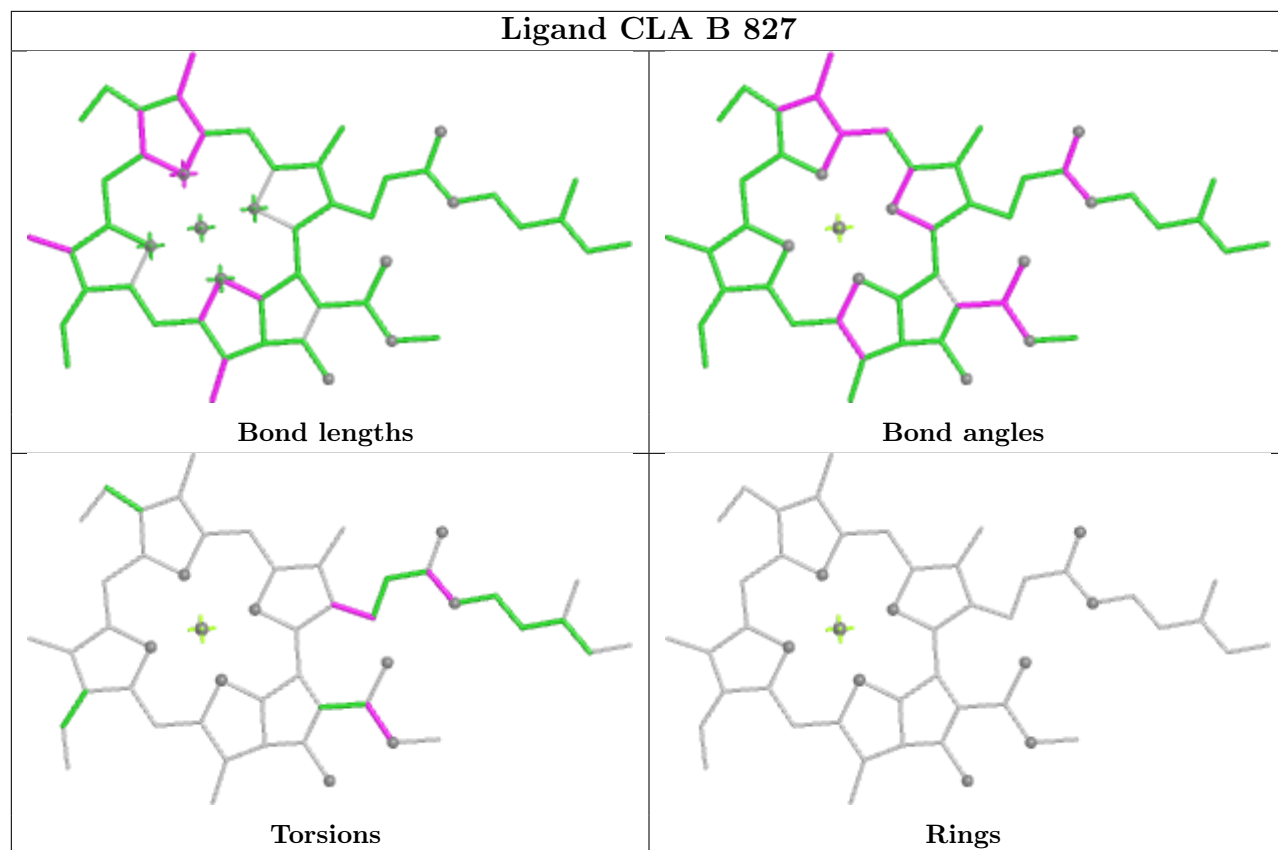
Ligand CLA K 102



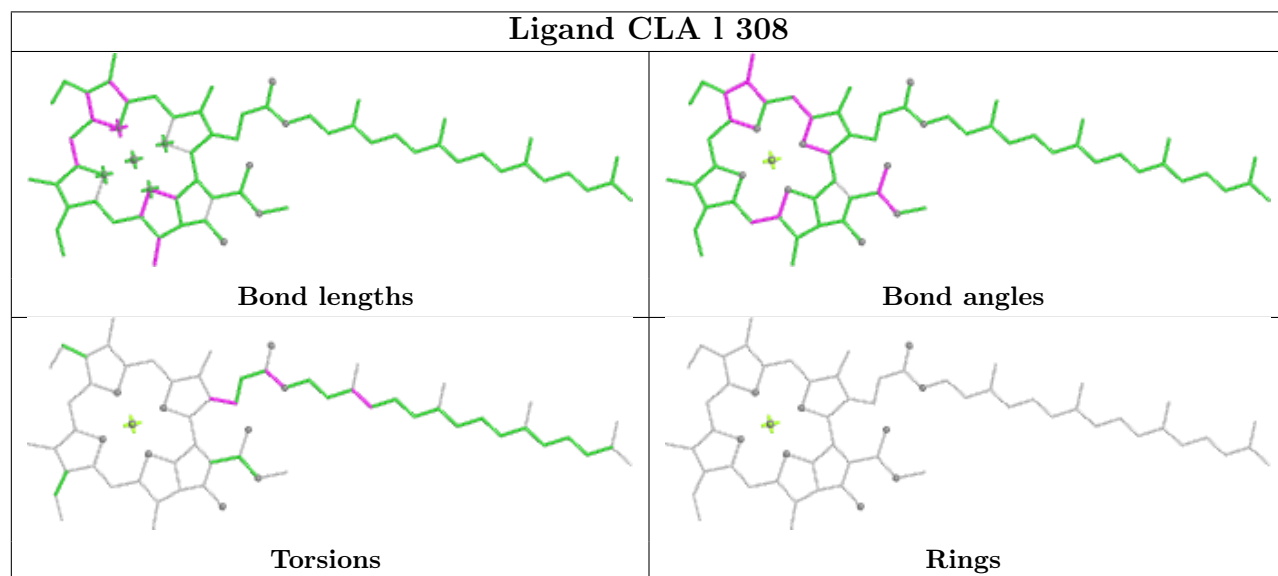




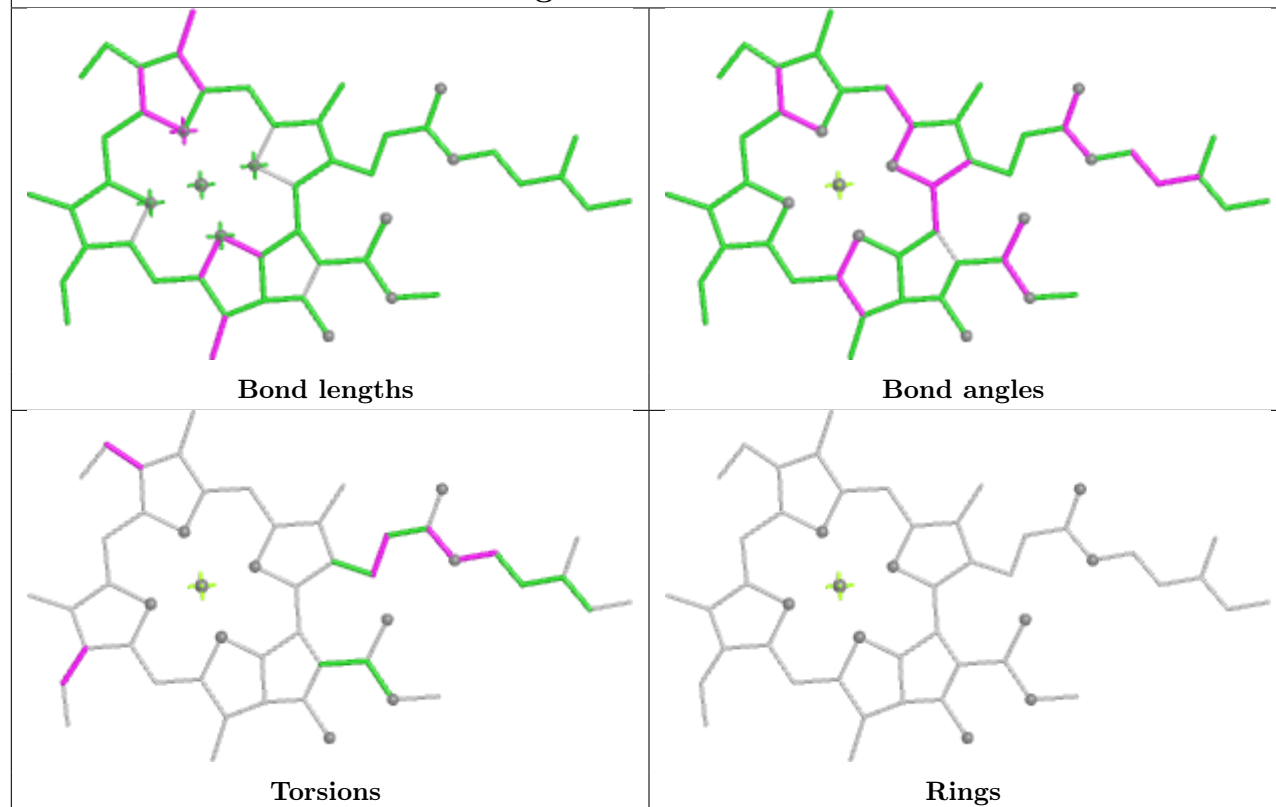
Ligand CLA B 827



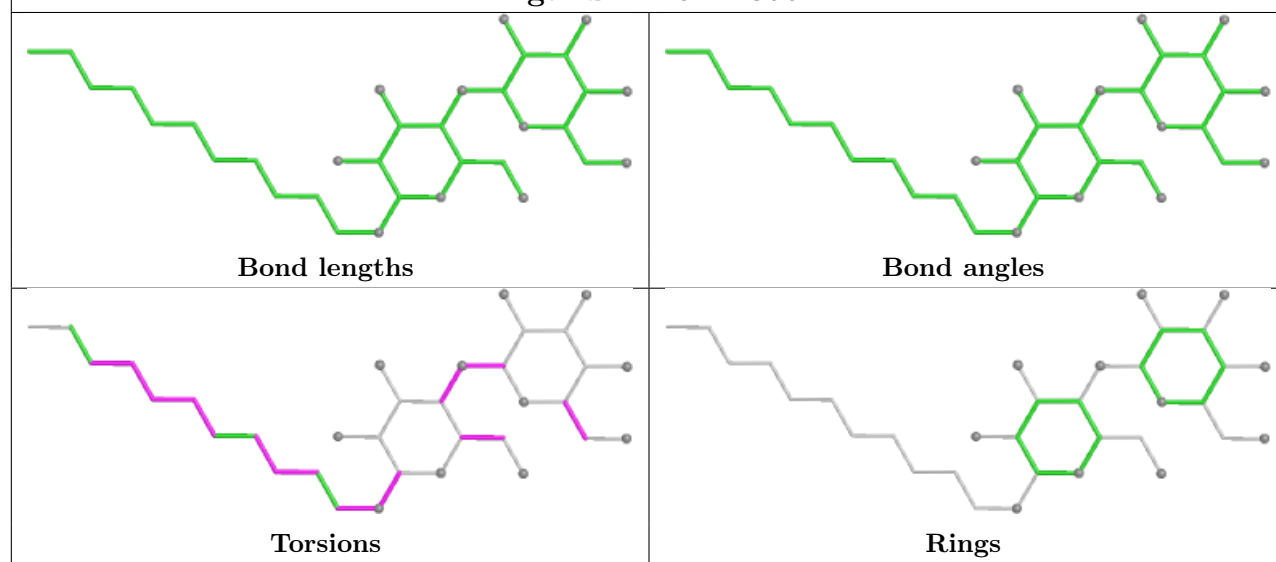
Ligand CLA I 308

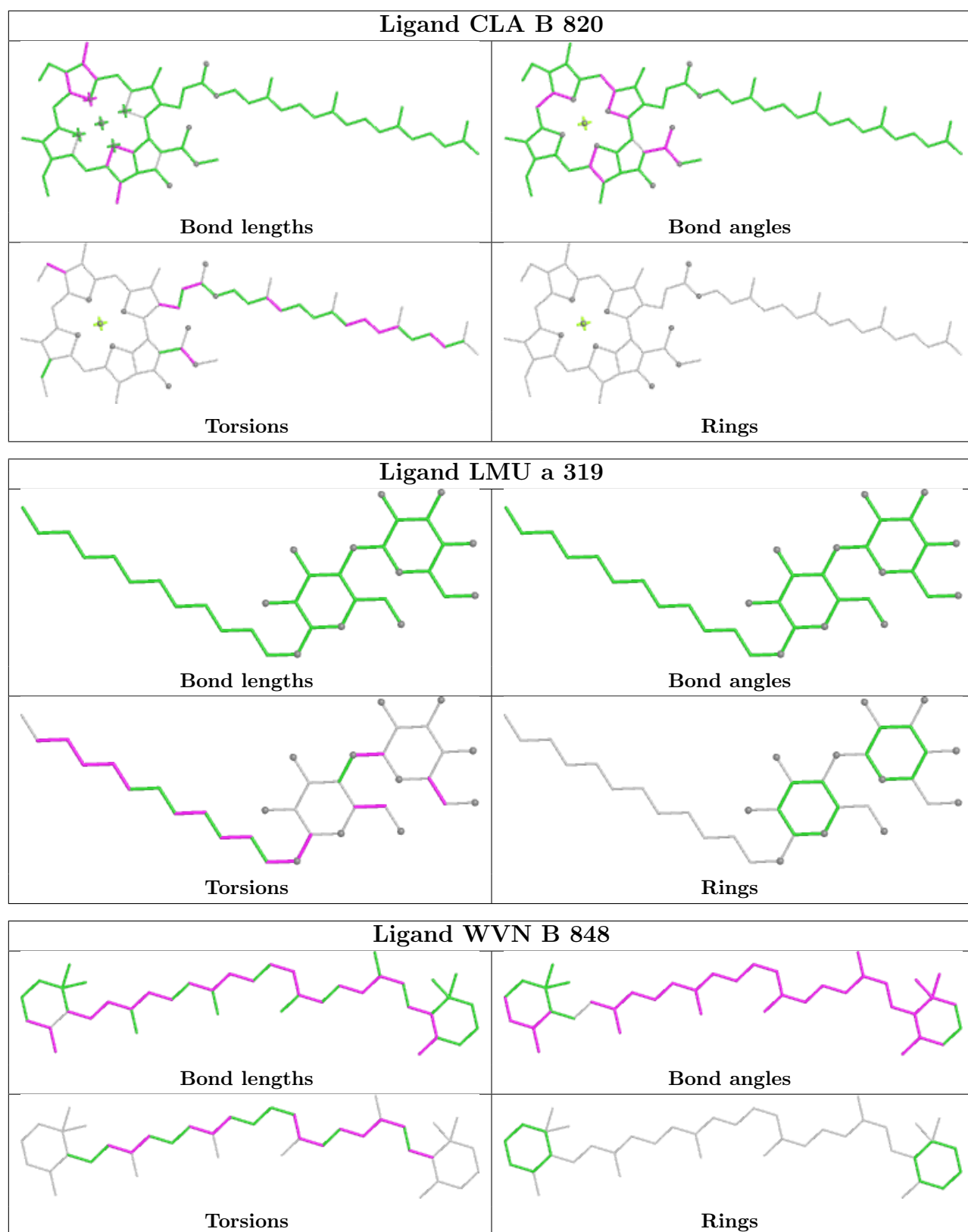


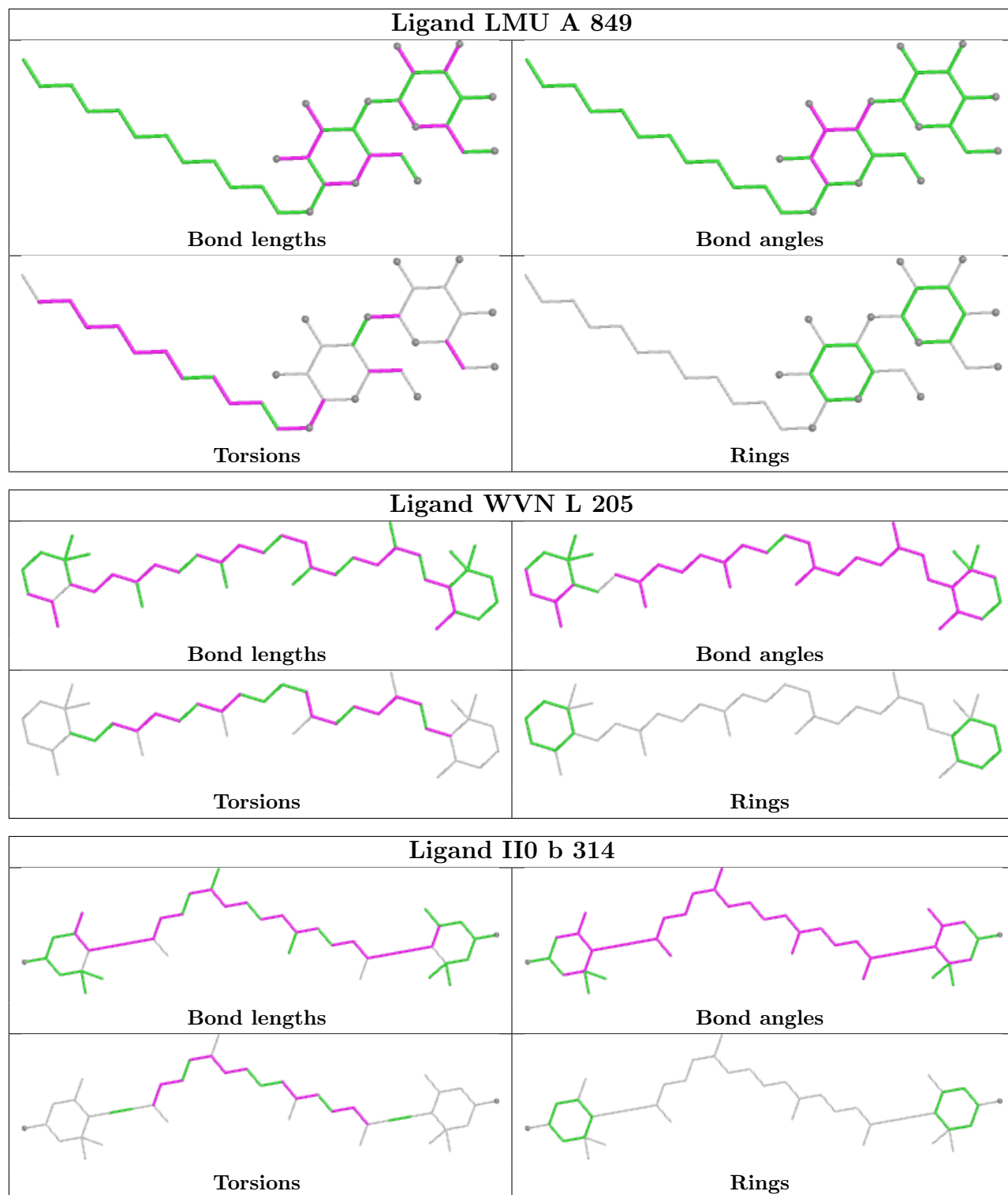
Ligand CLA b 313

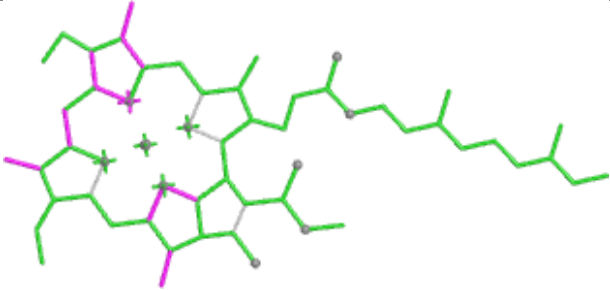
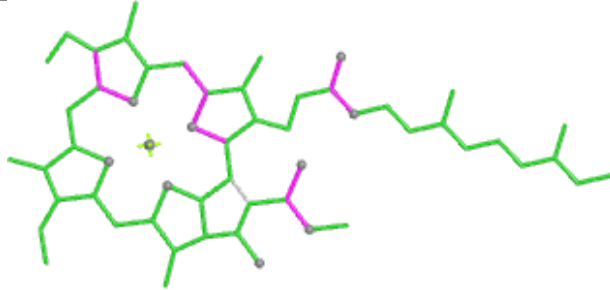
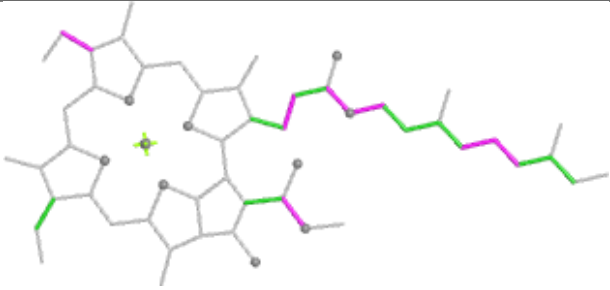
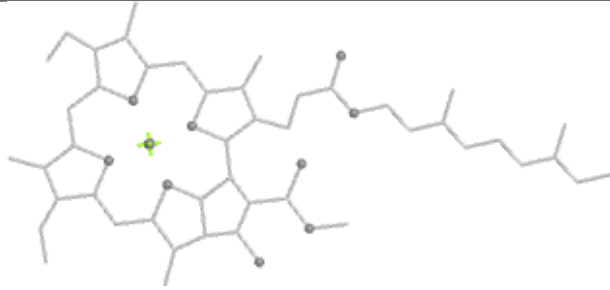
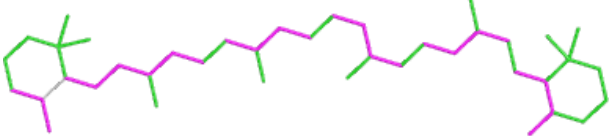
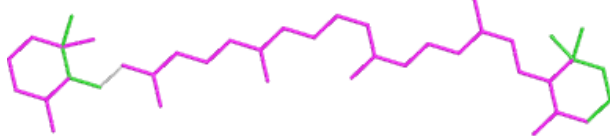
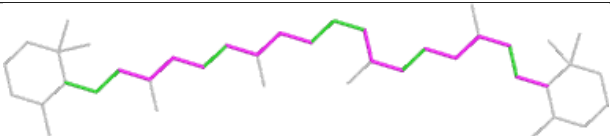
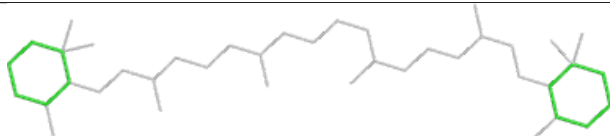
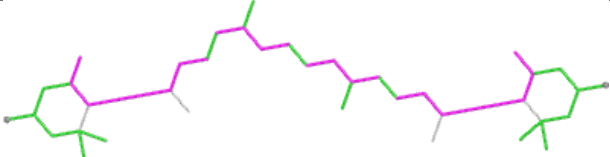
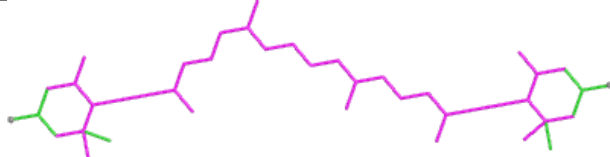
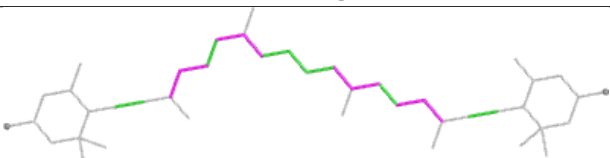
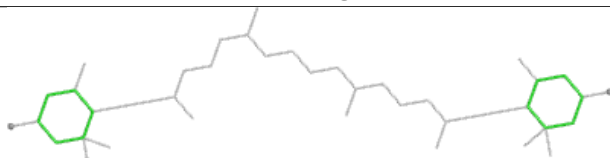


Ligand LMU A 855

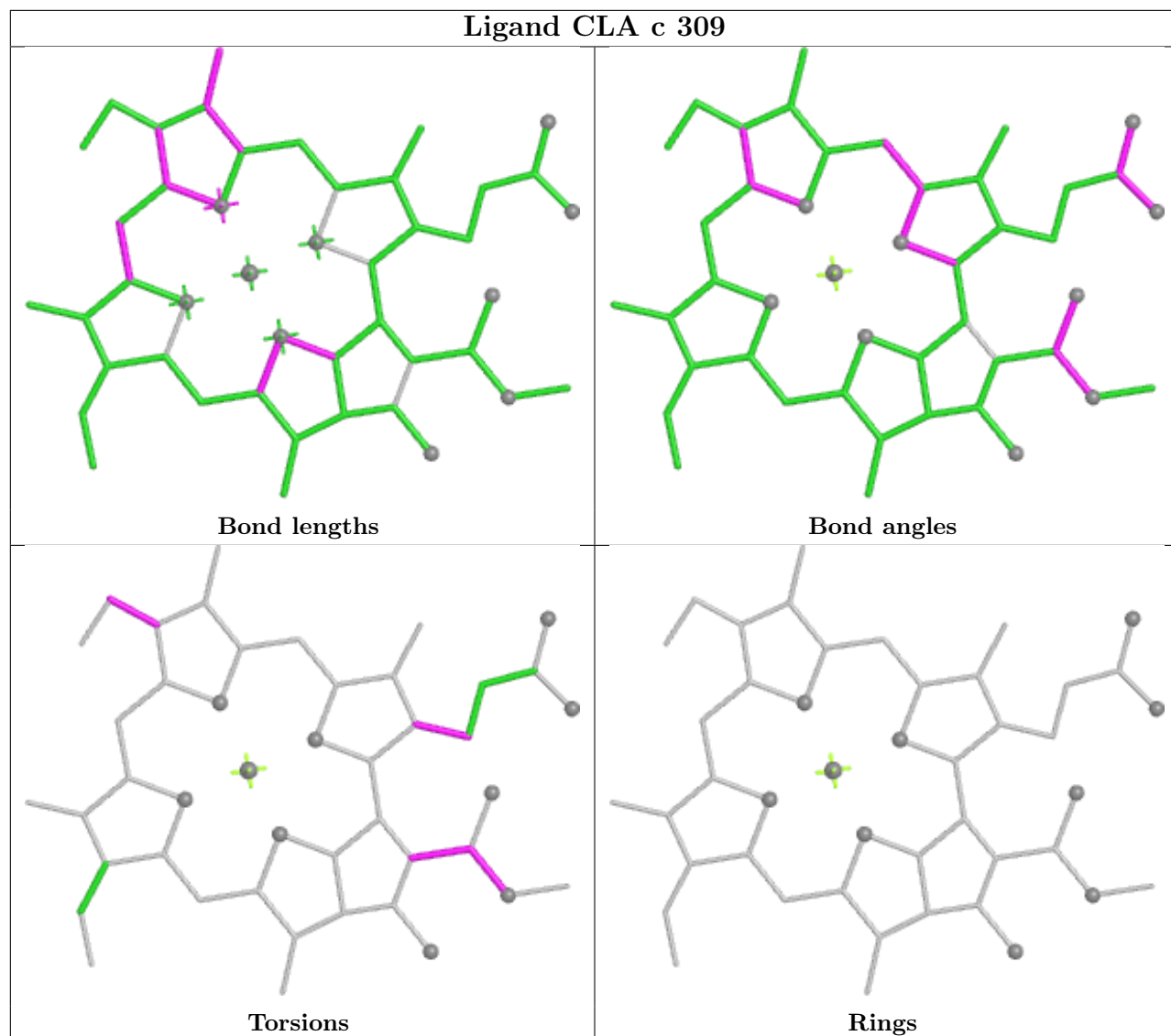




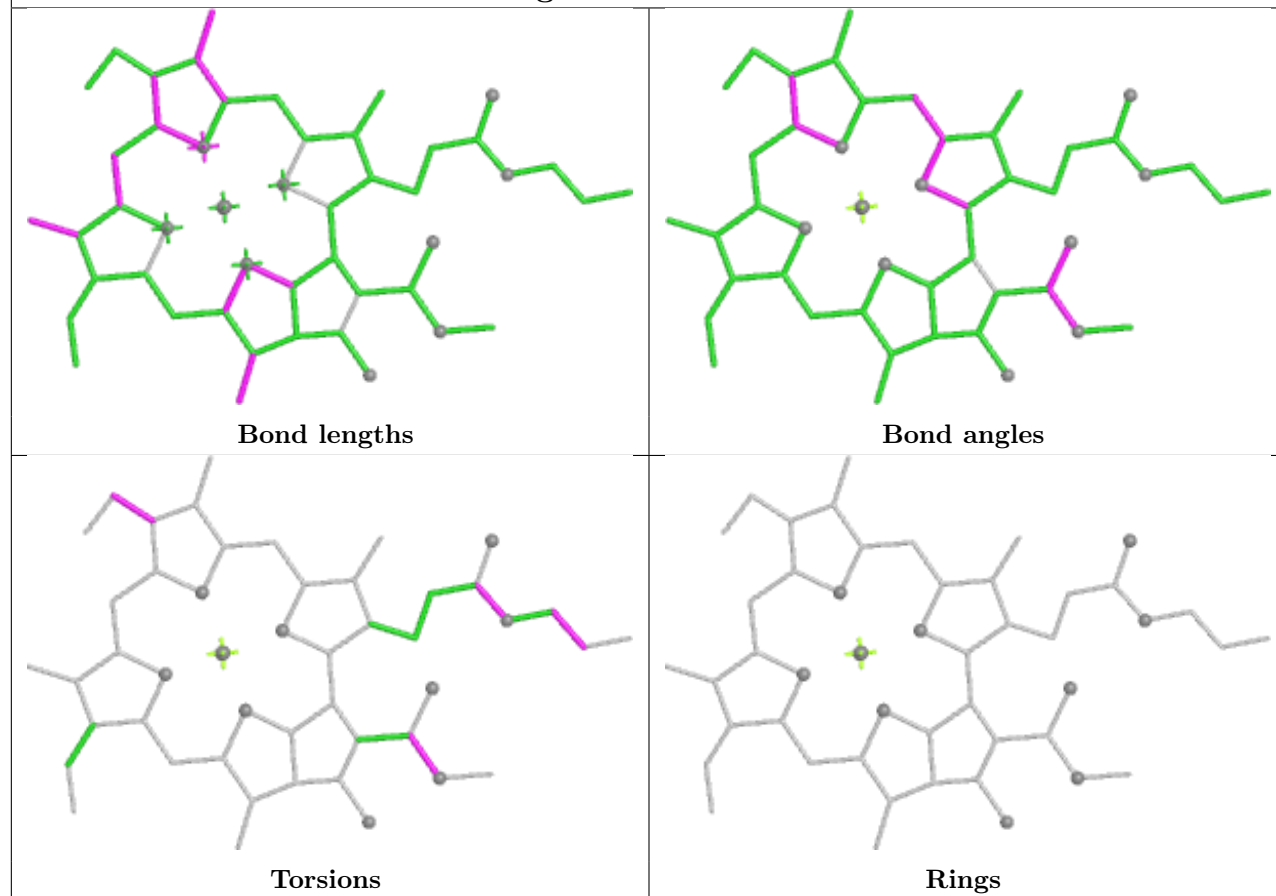


Ligand CLA l 312	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand WVN A 854	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand II0 a 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

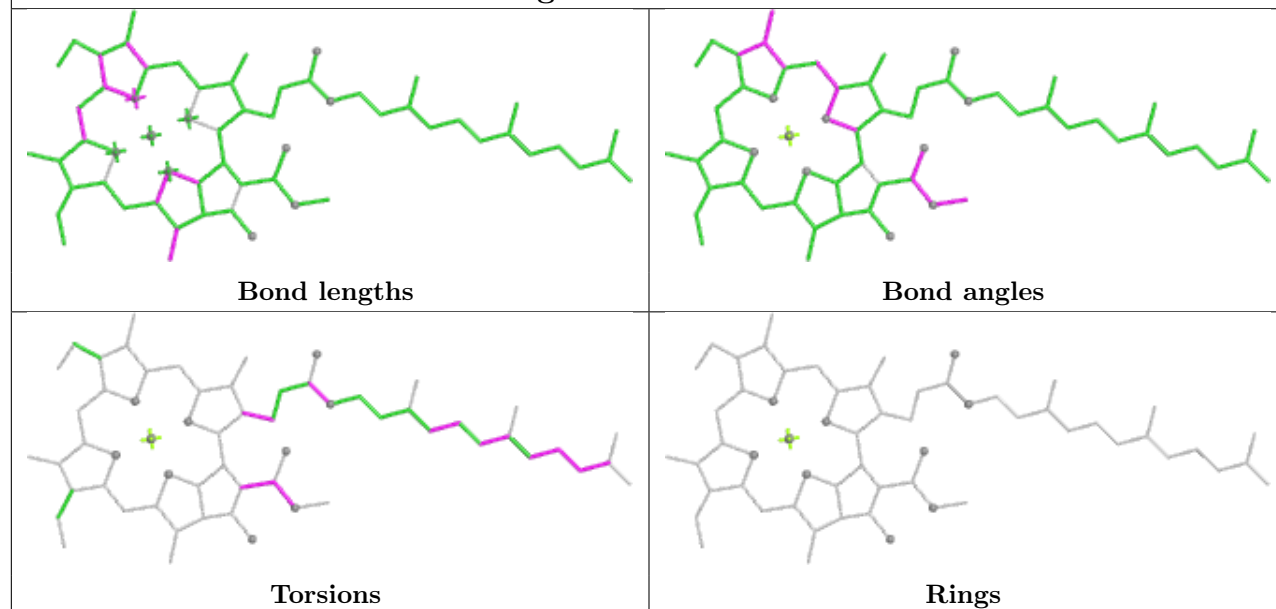
Ligand CLA c 309



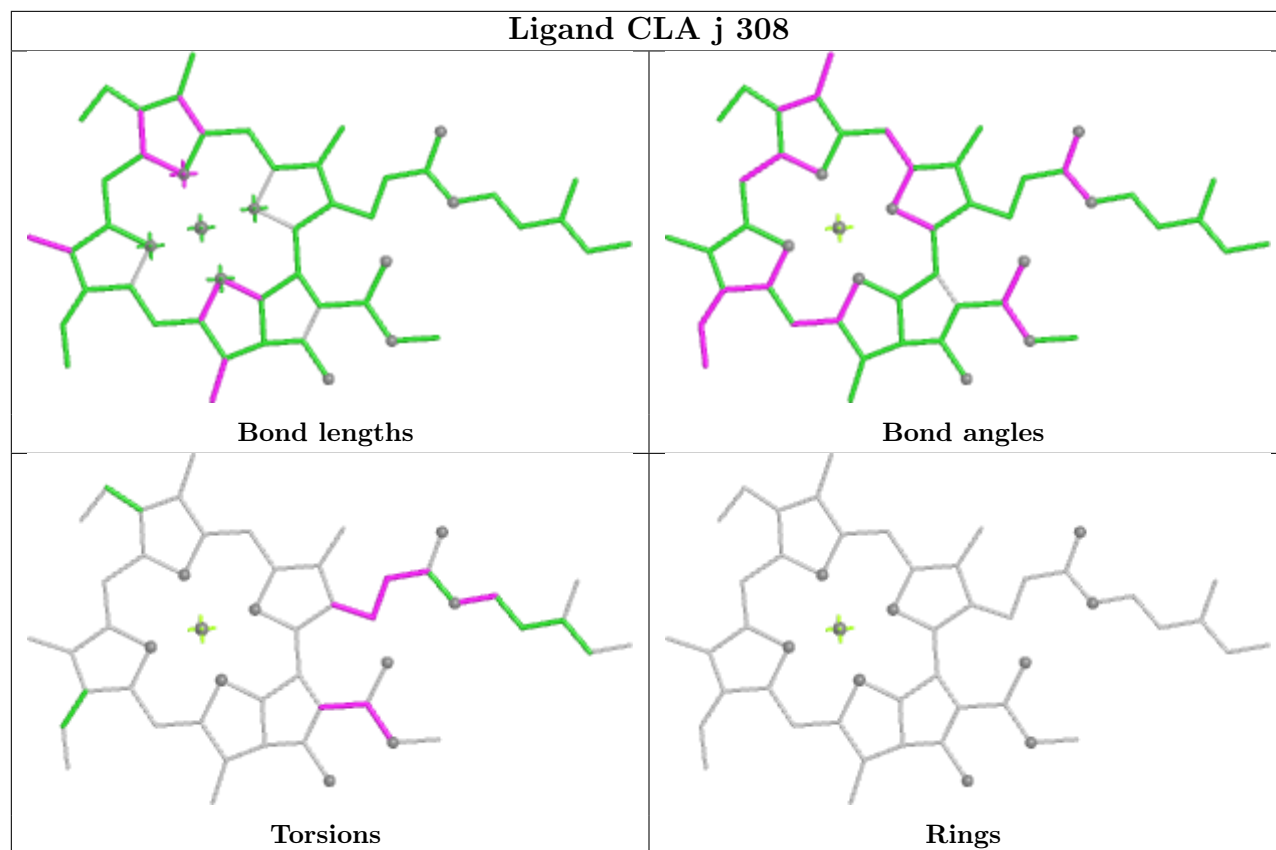
Ligand CLA a 309



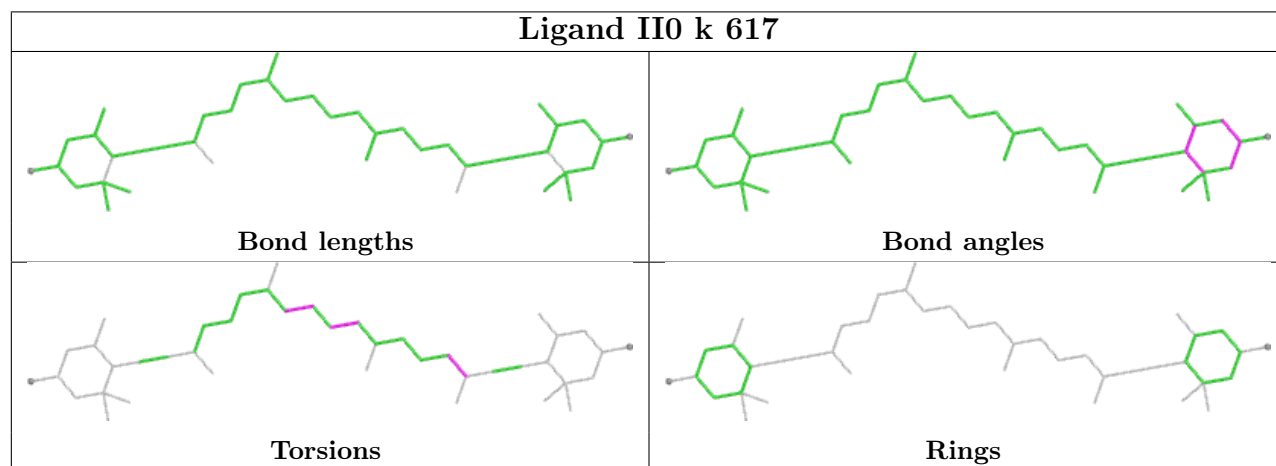
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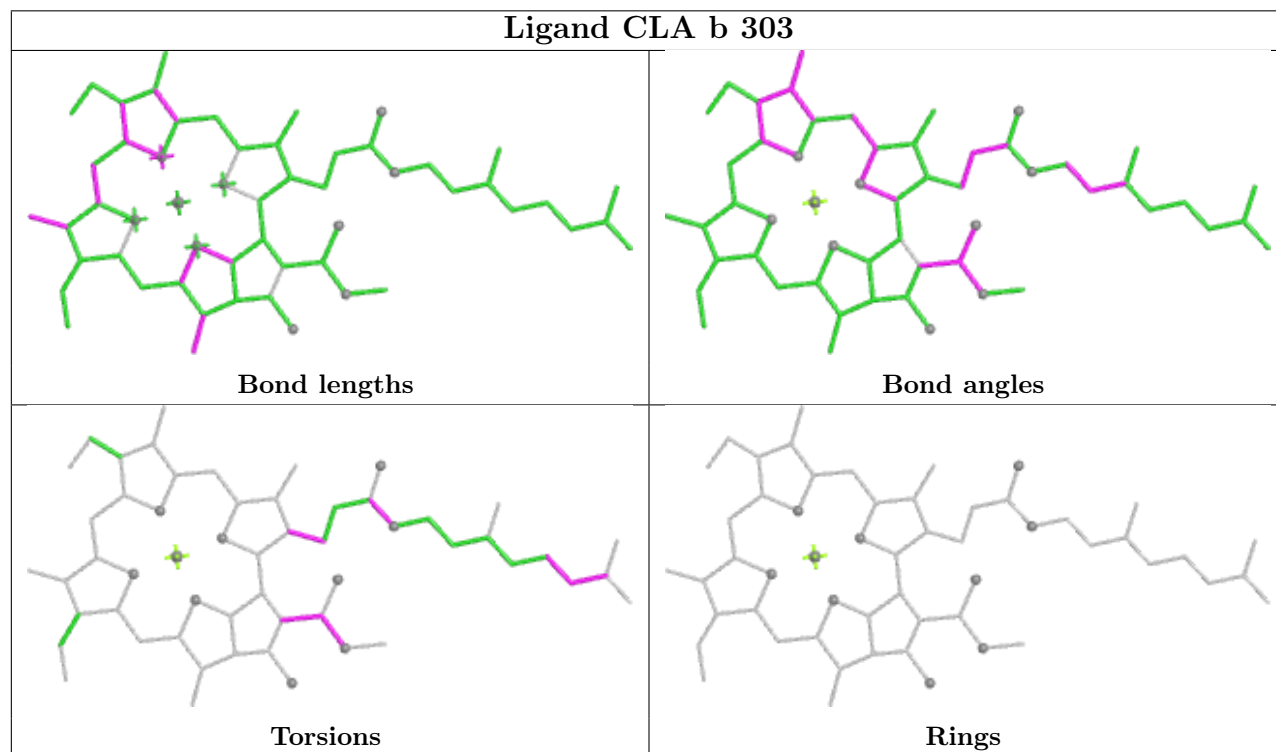
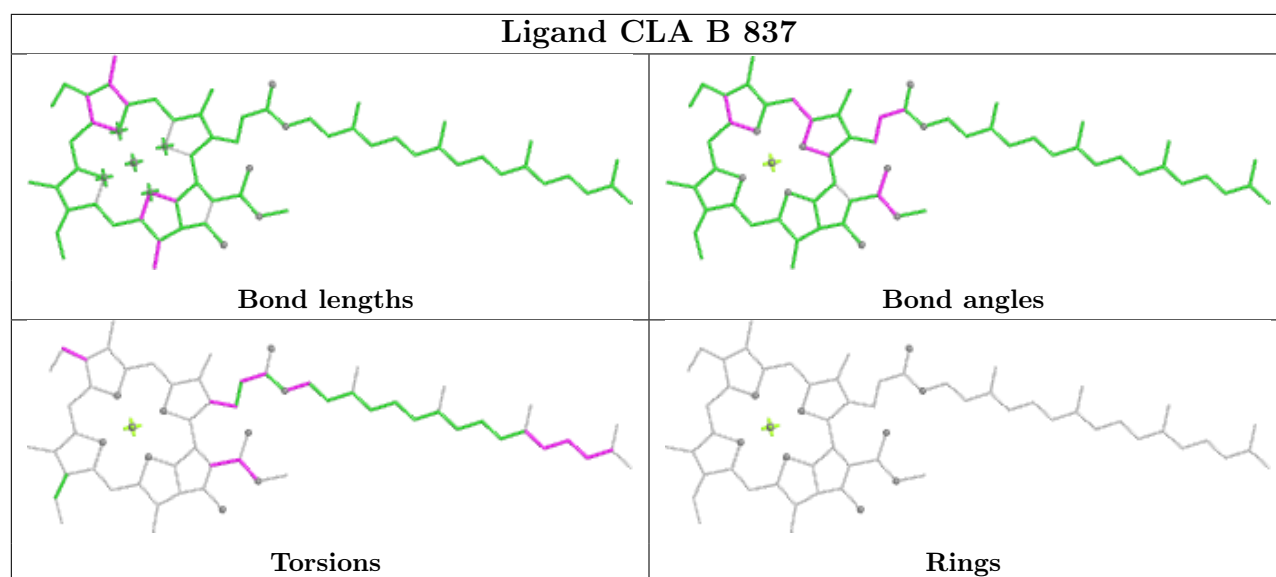


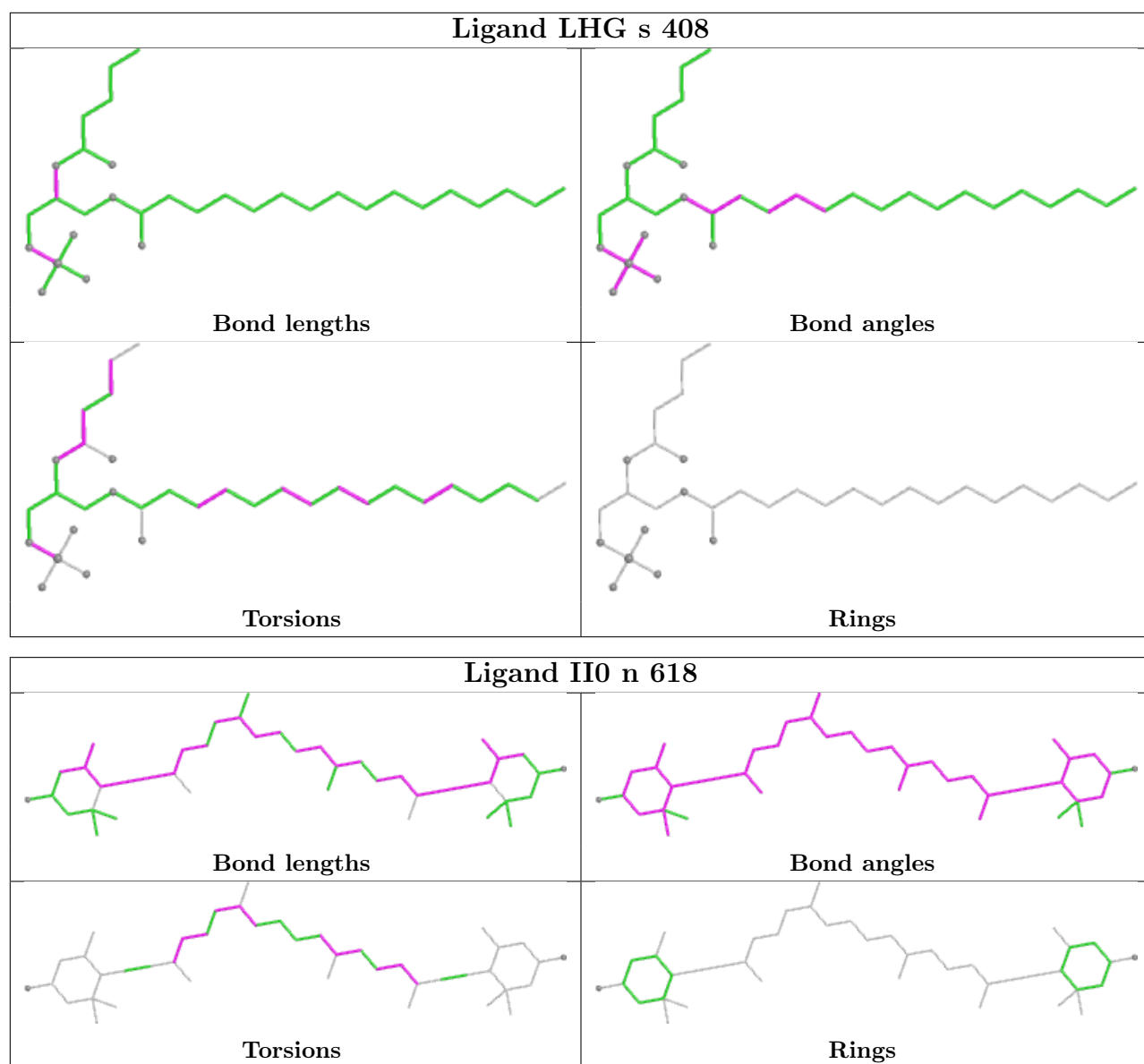
Ligand CLA j 308



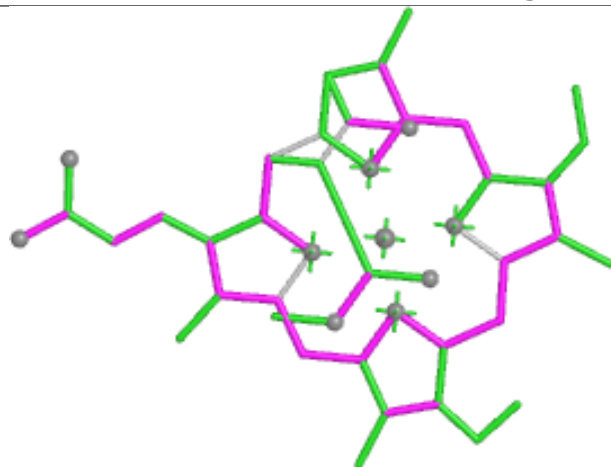
Ligand II0 k 617



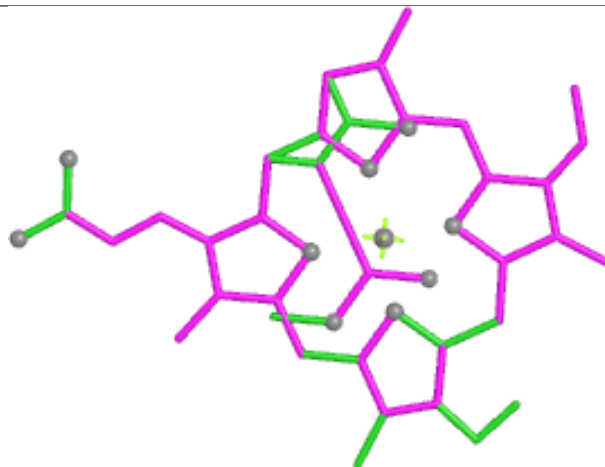




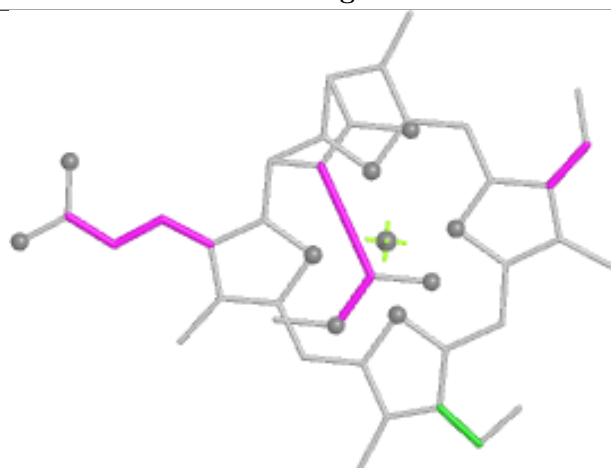
Ligand KC2 c 310



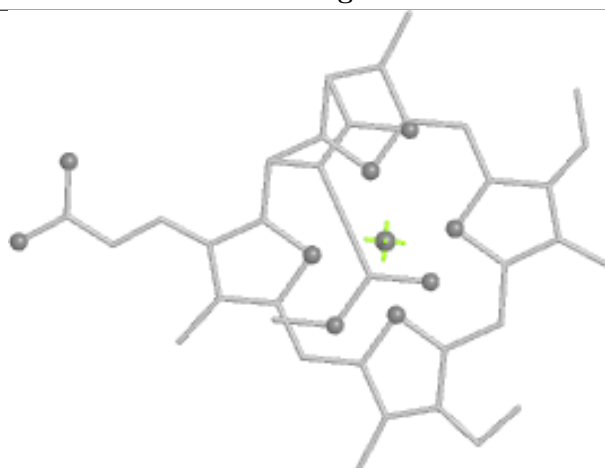
Bond lengths



Bond angles

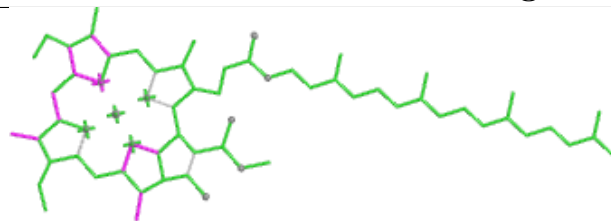


Torsions

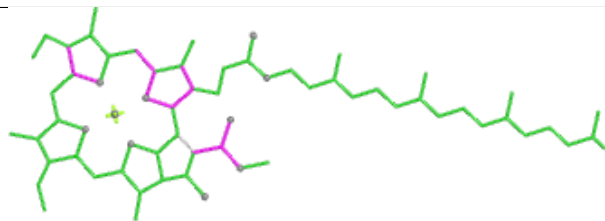


Rings

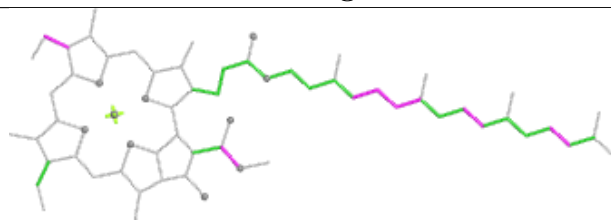
Ligand CLA s 403



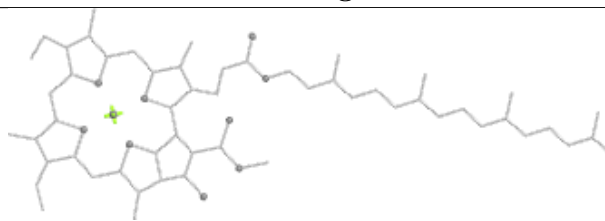
Bond lengths



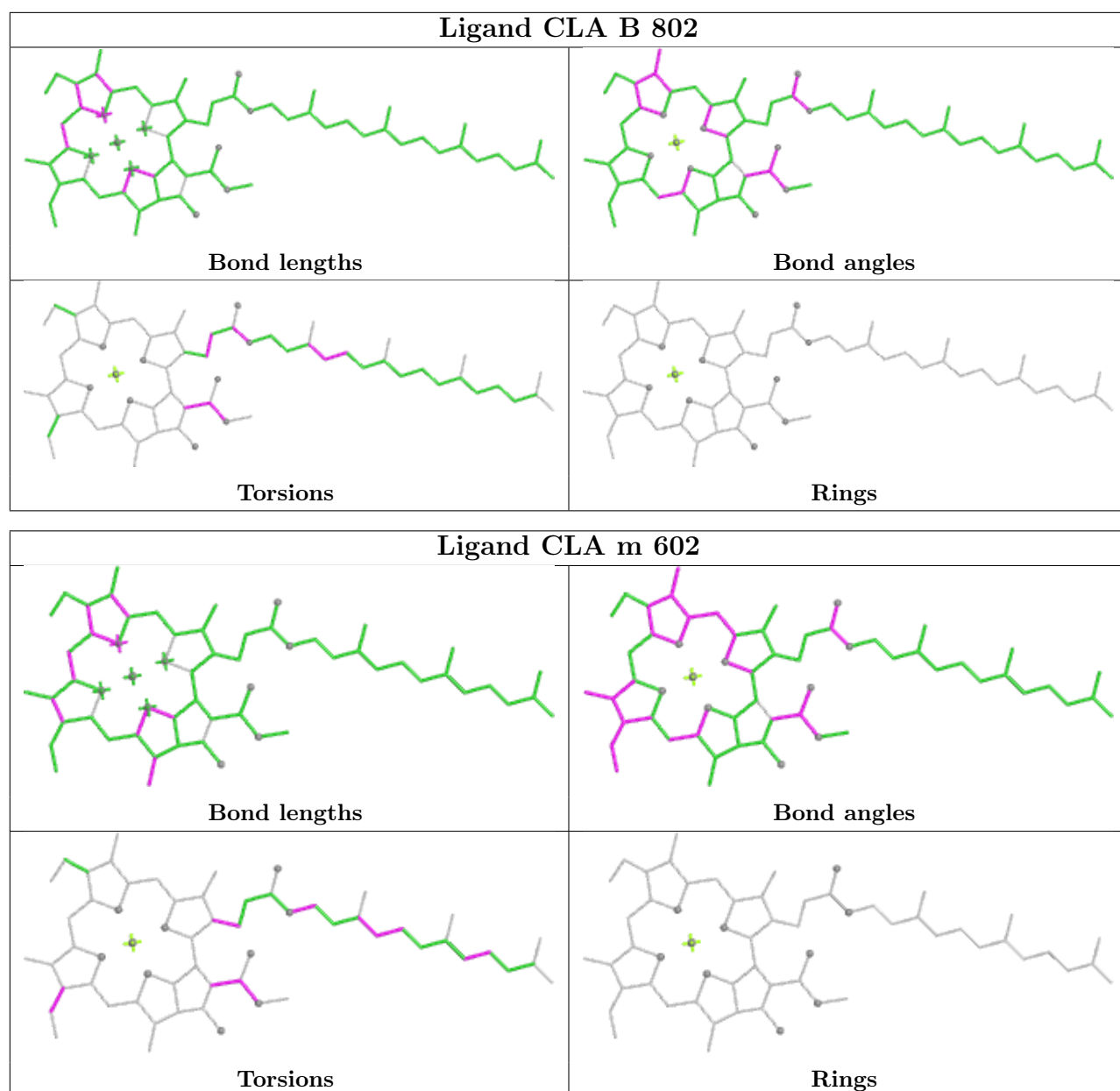
Bond angles

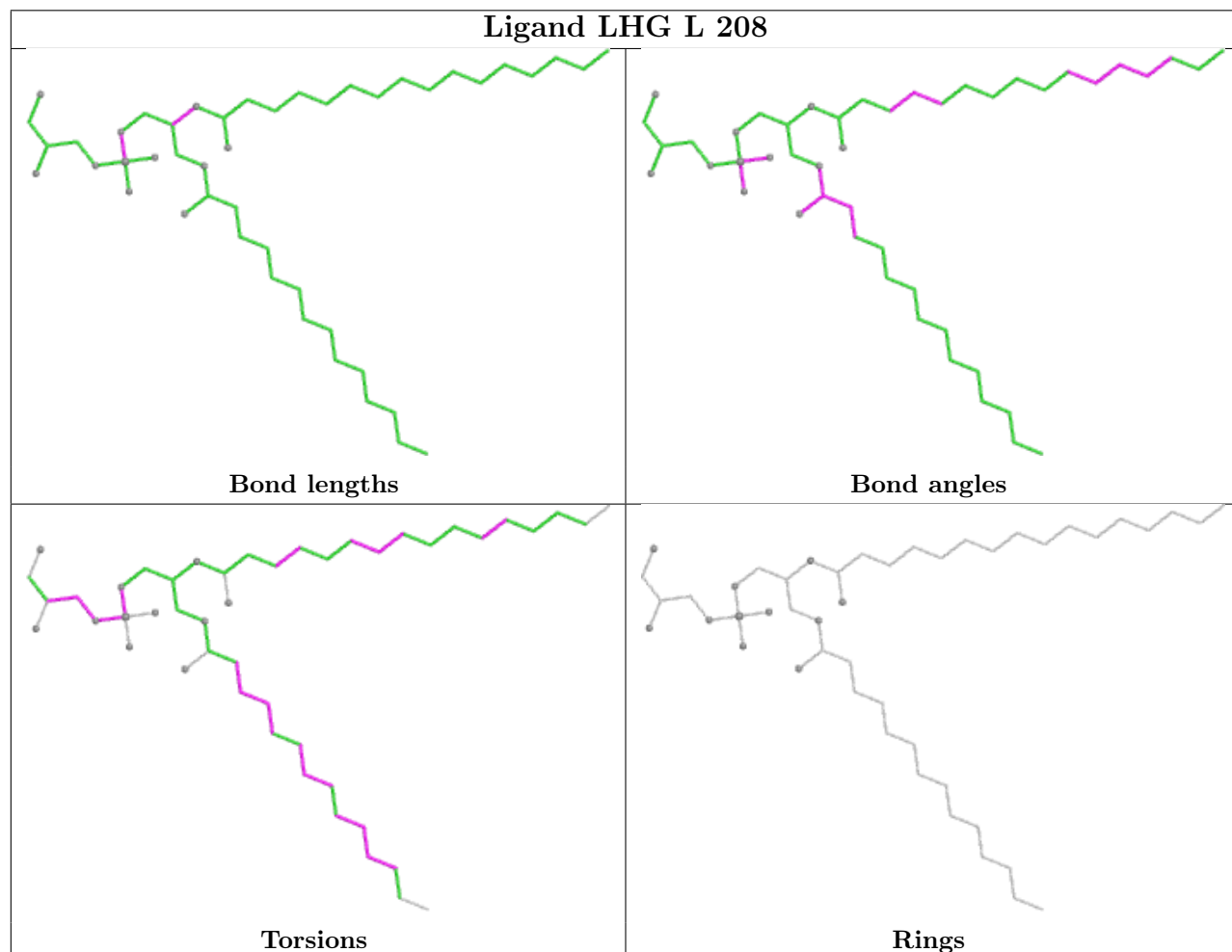
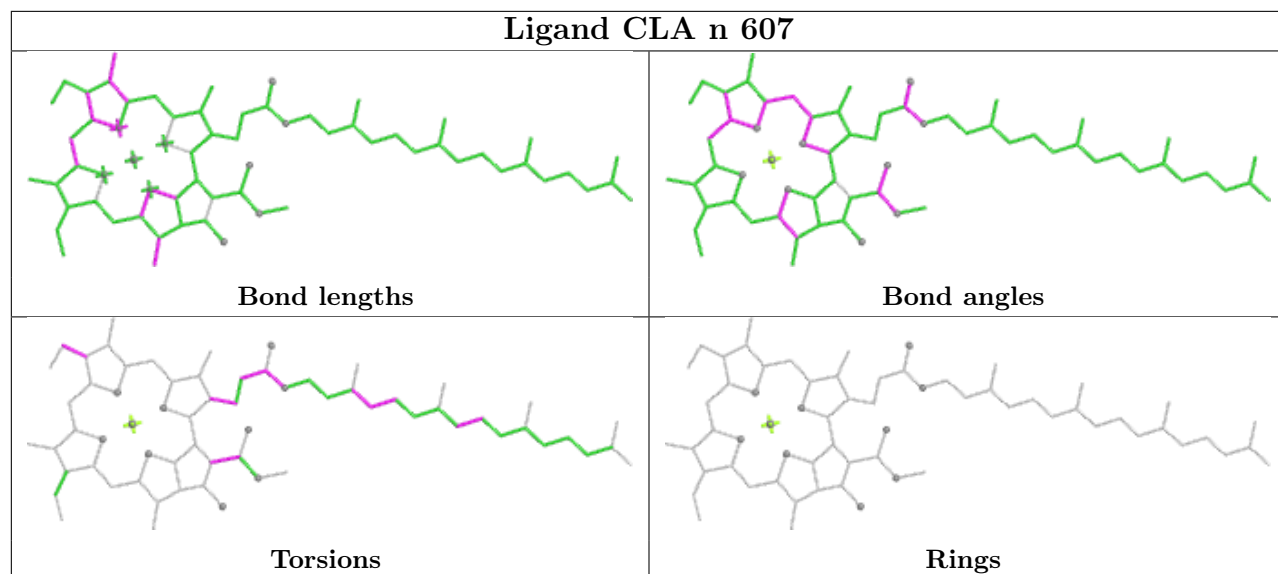


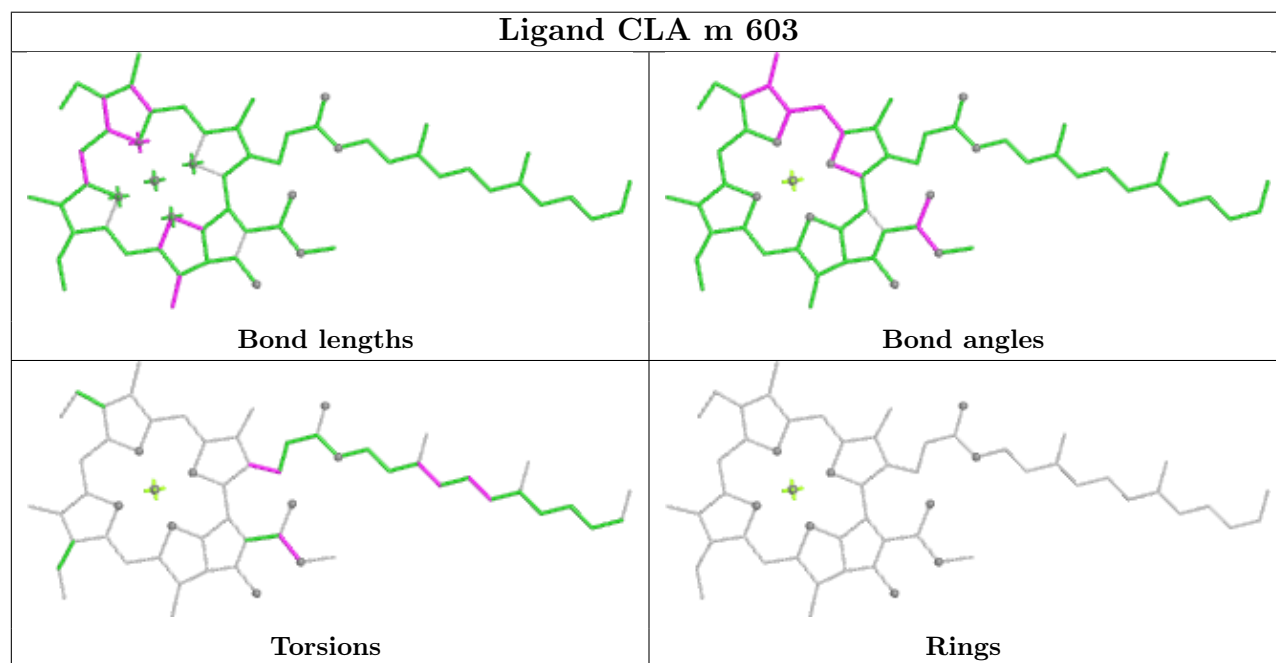
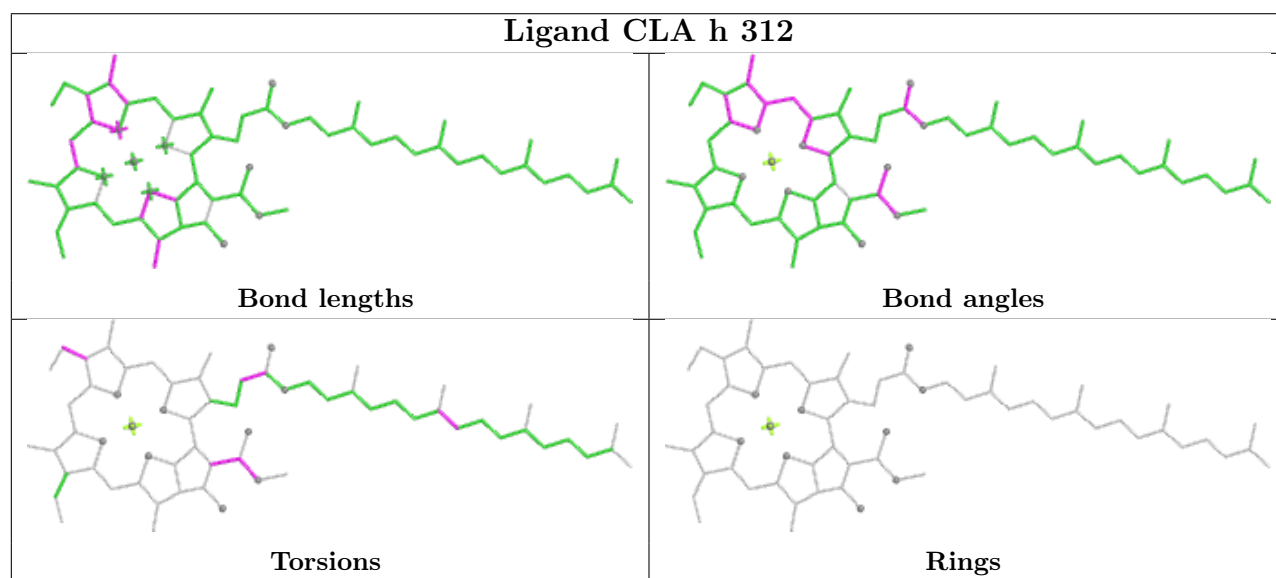
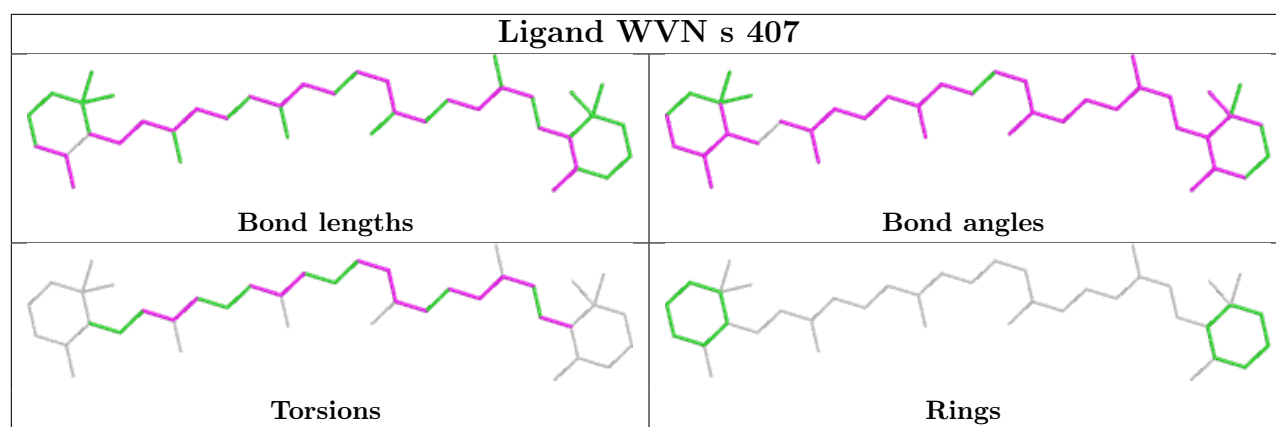
Torsions

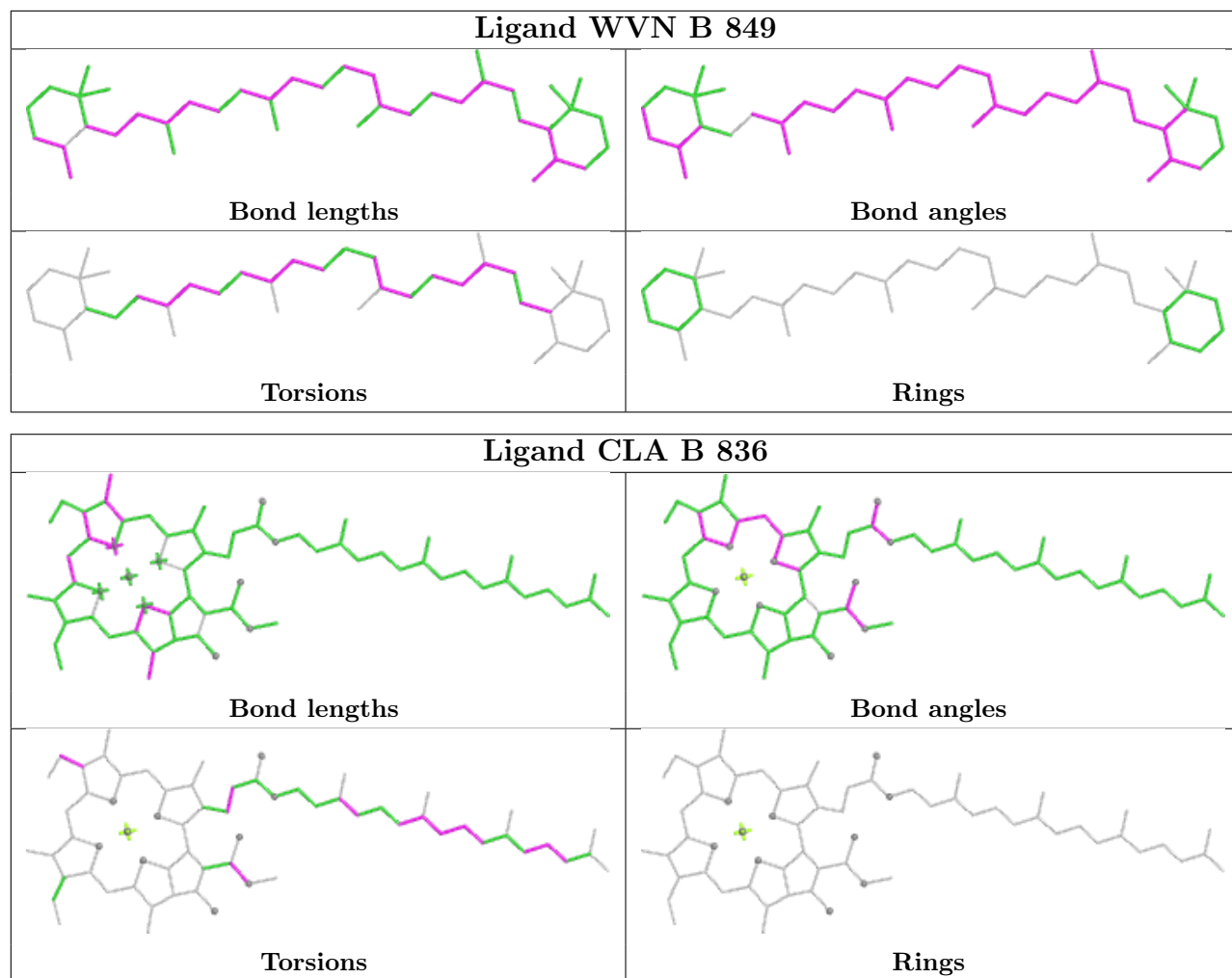


Rings

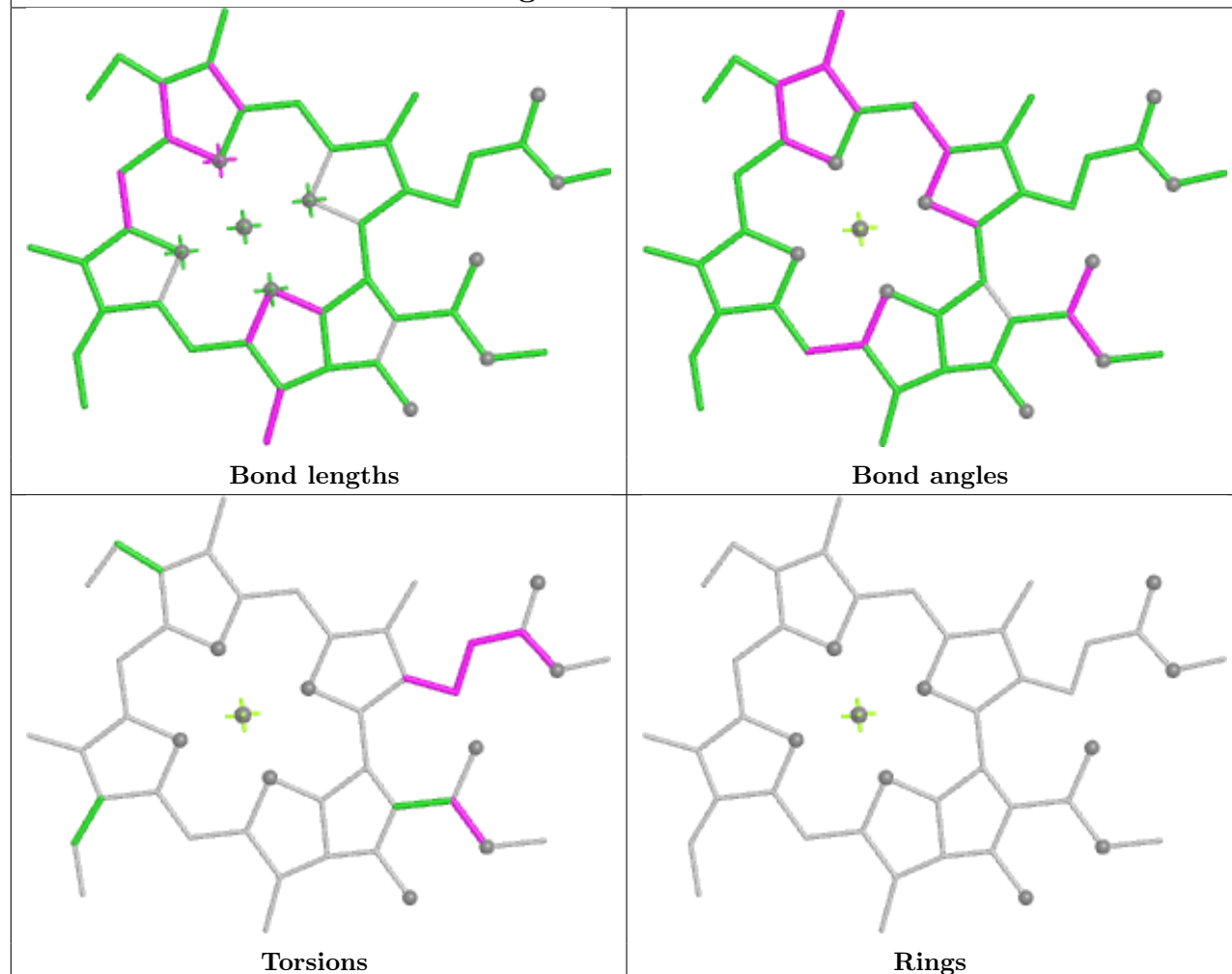




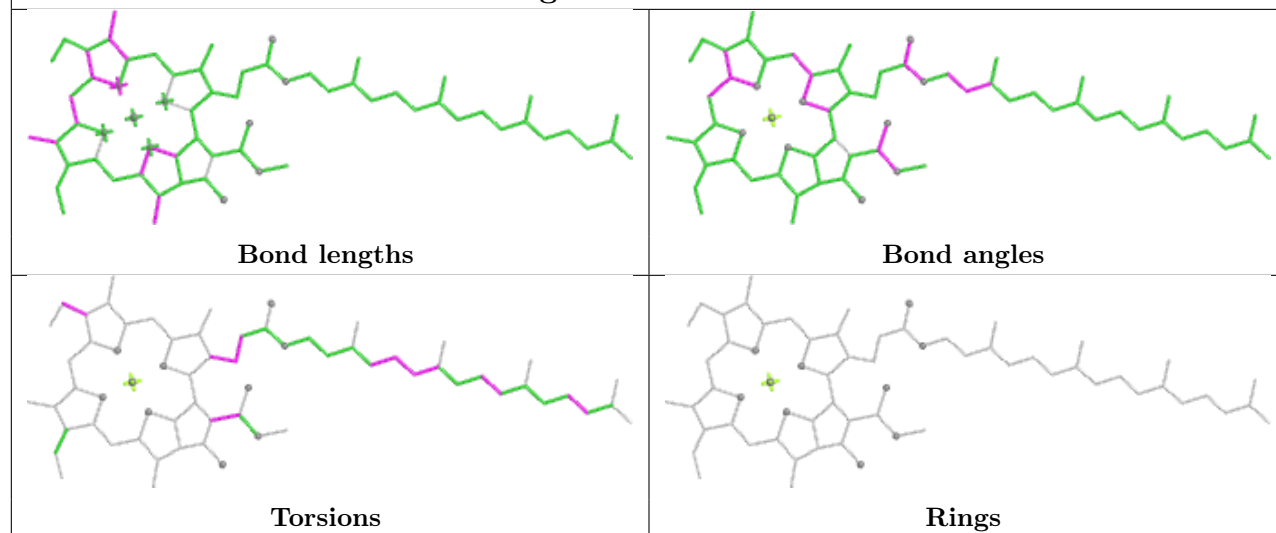




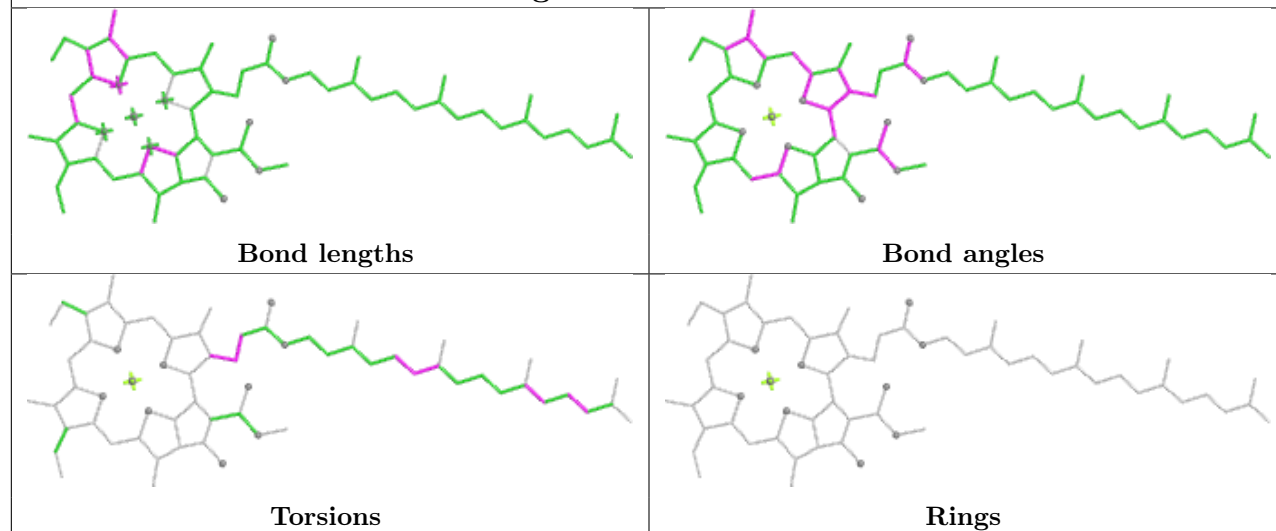
Ligand CLA c 307



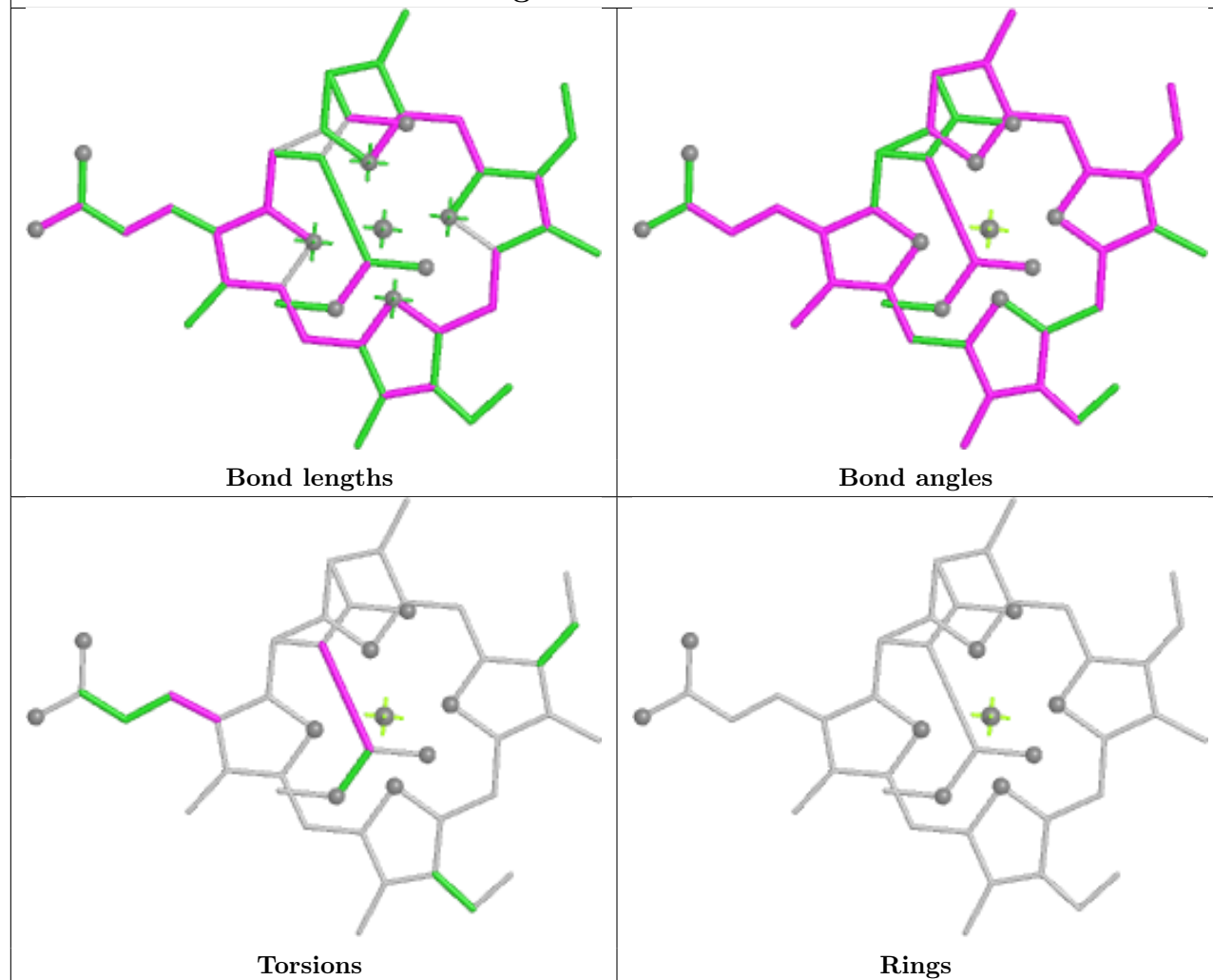
Ligand CLA f 609



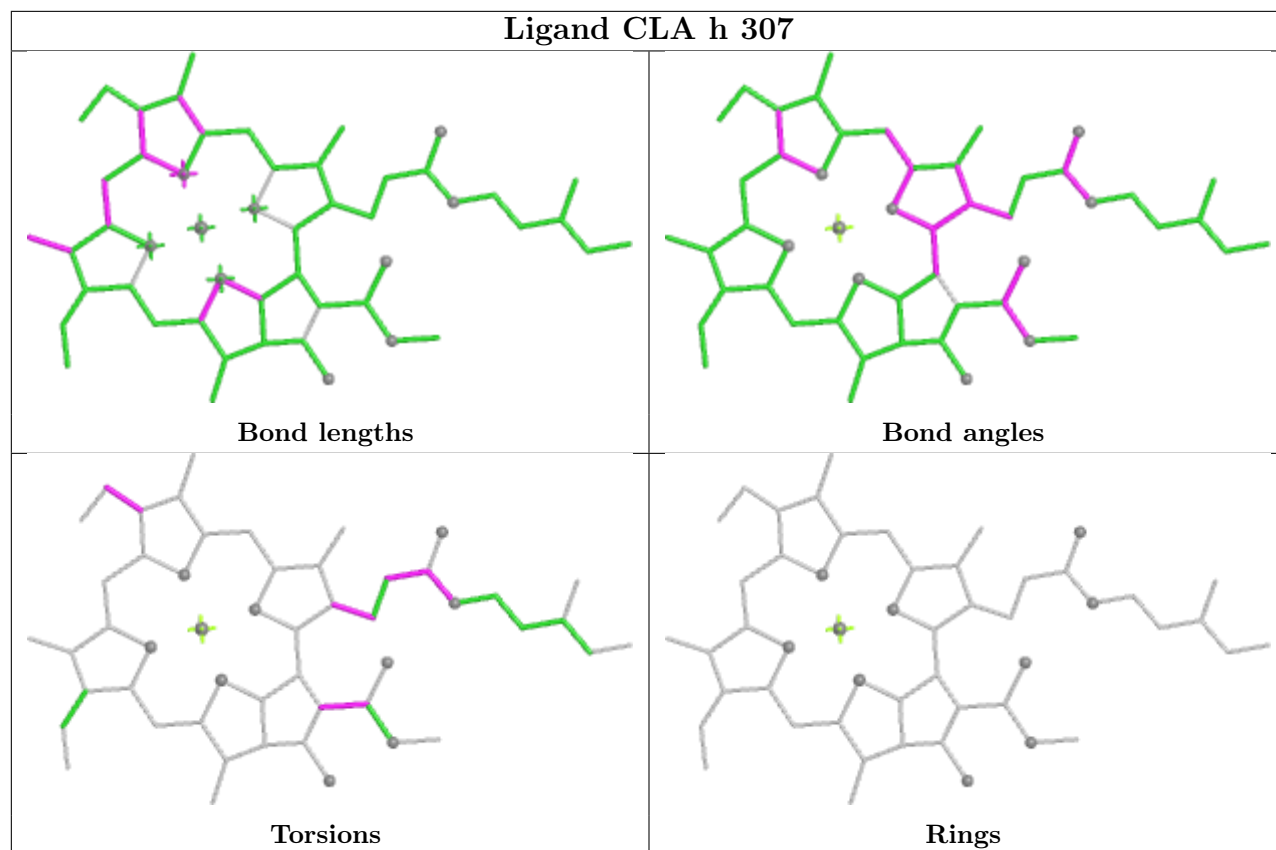
Ligand CLA B 829



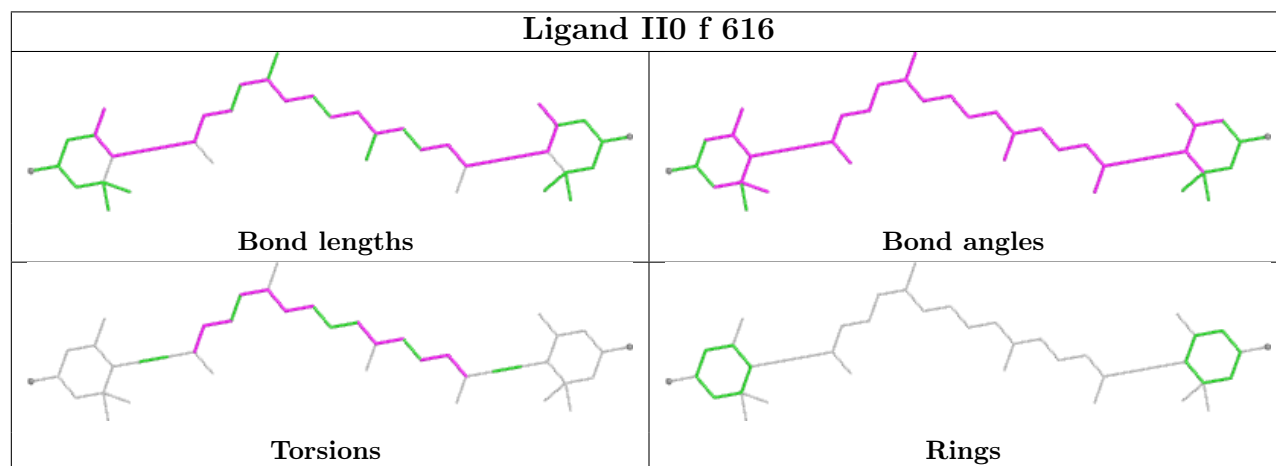
Ligand KC2 s 404

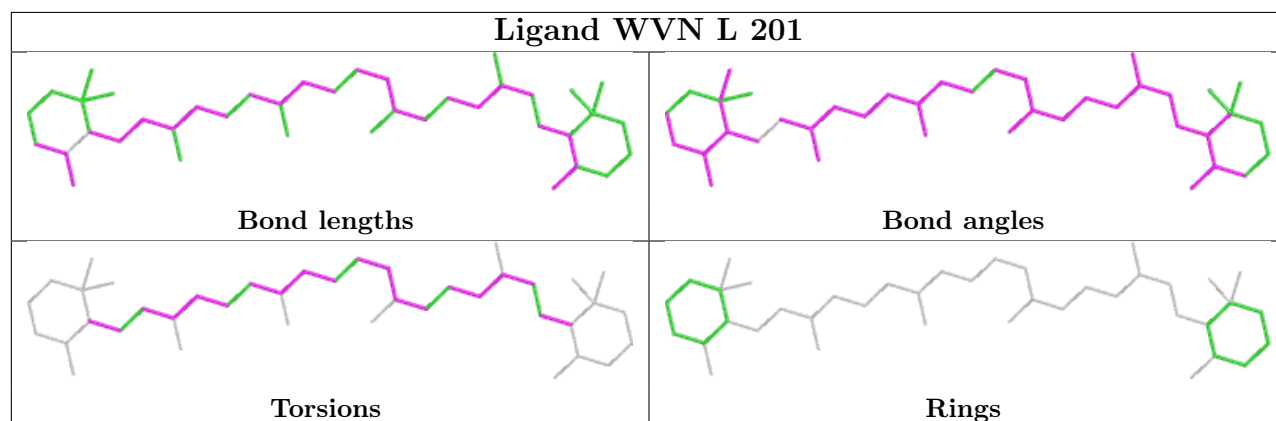
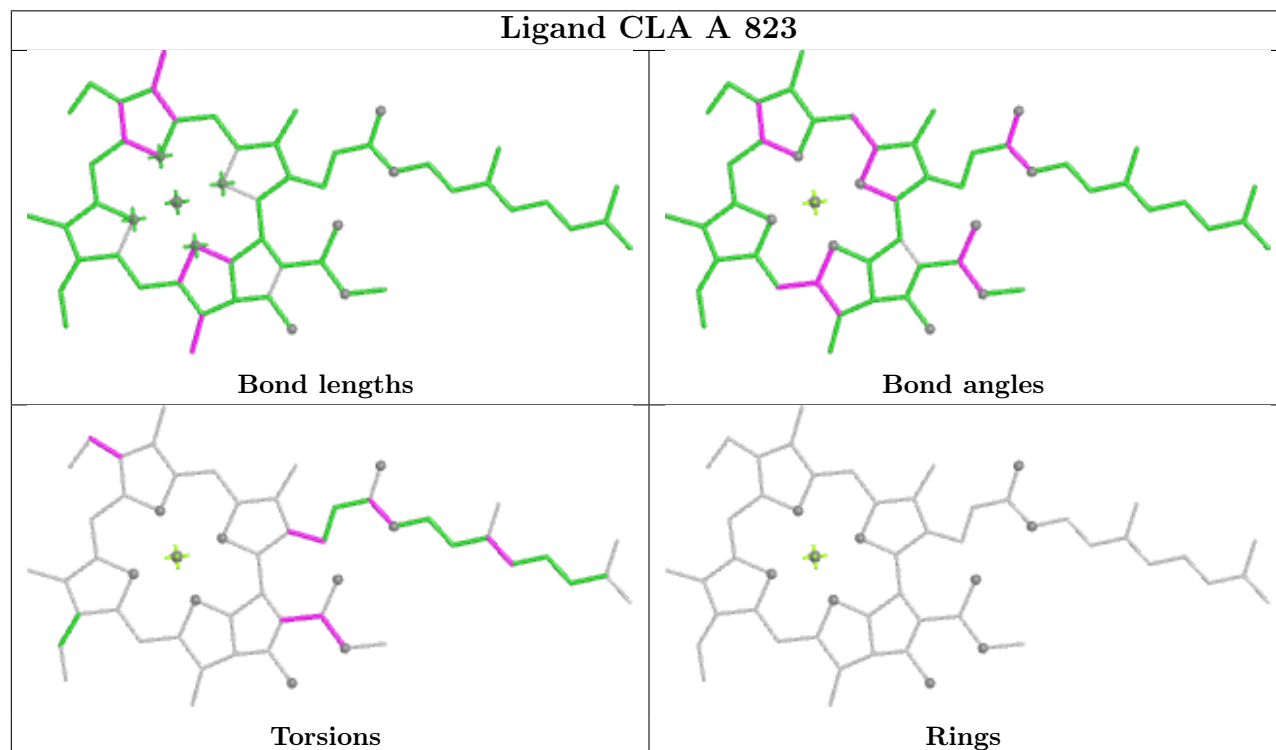
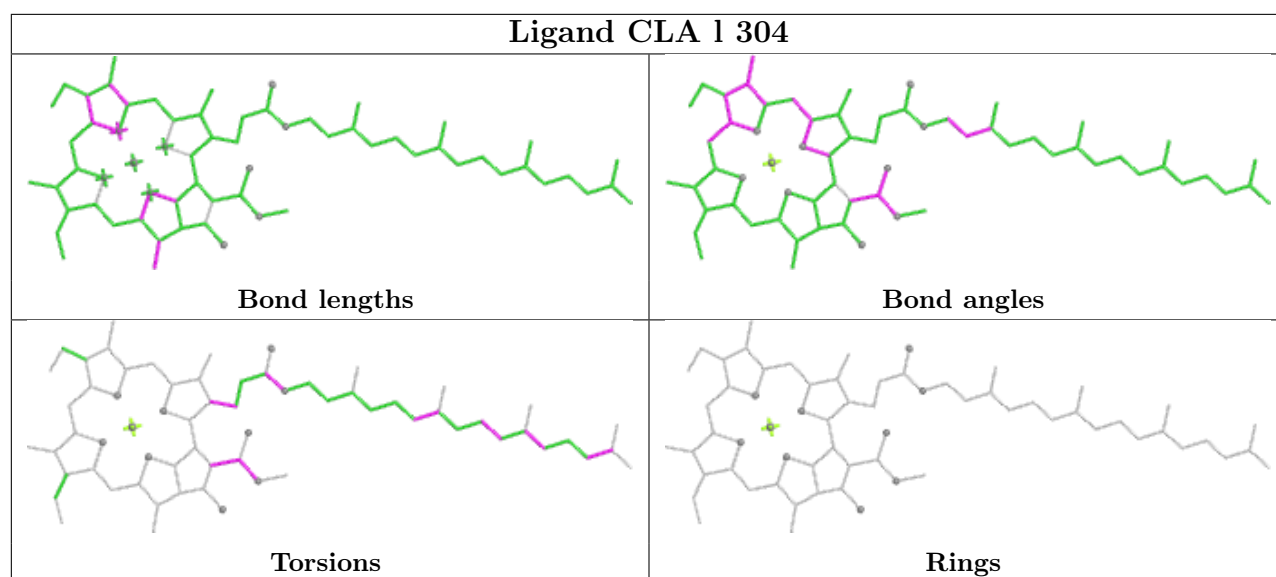


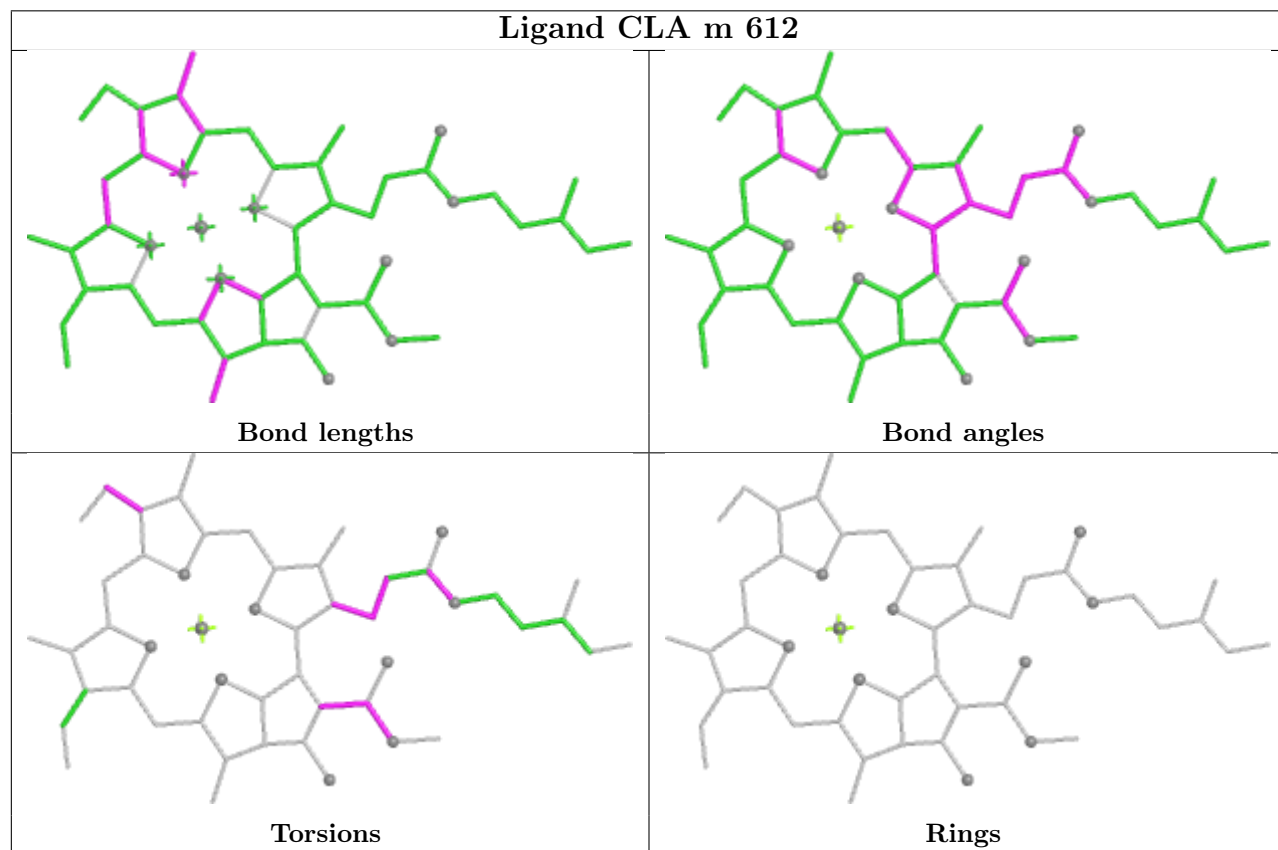
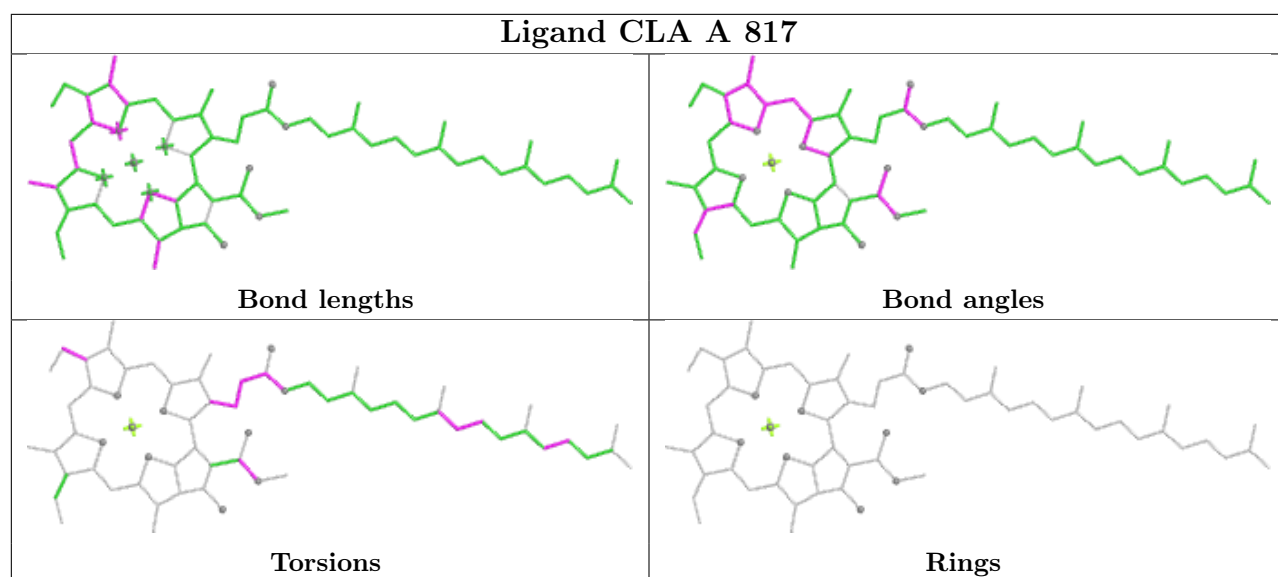
Ligand CLA h 307

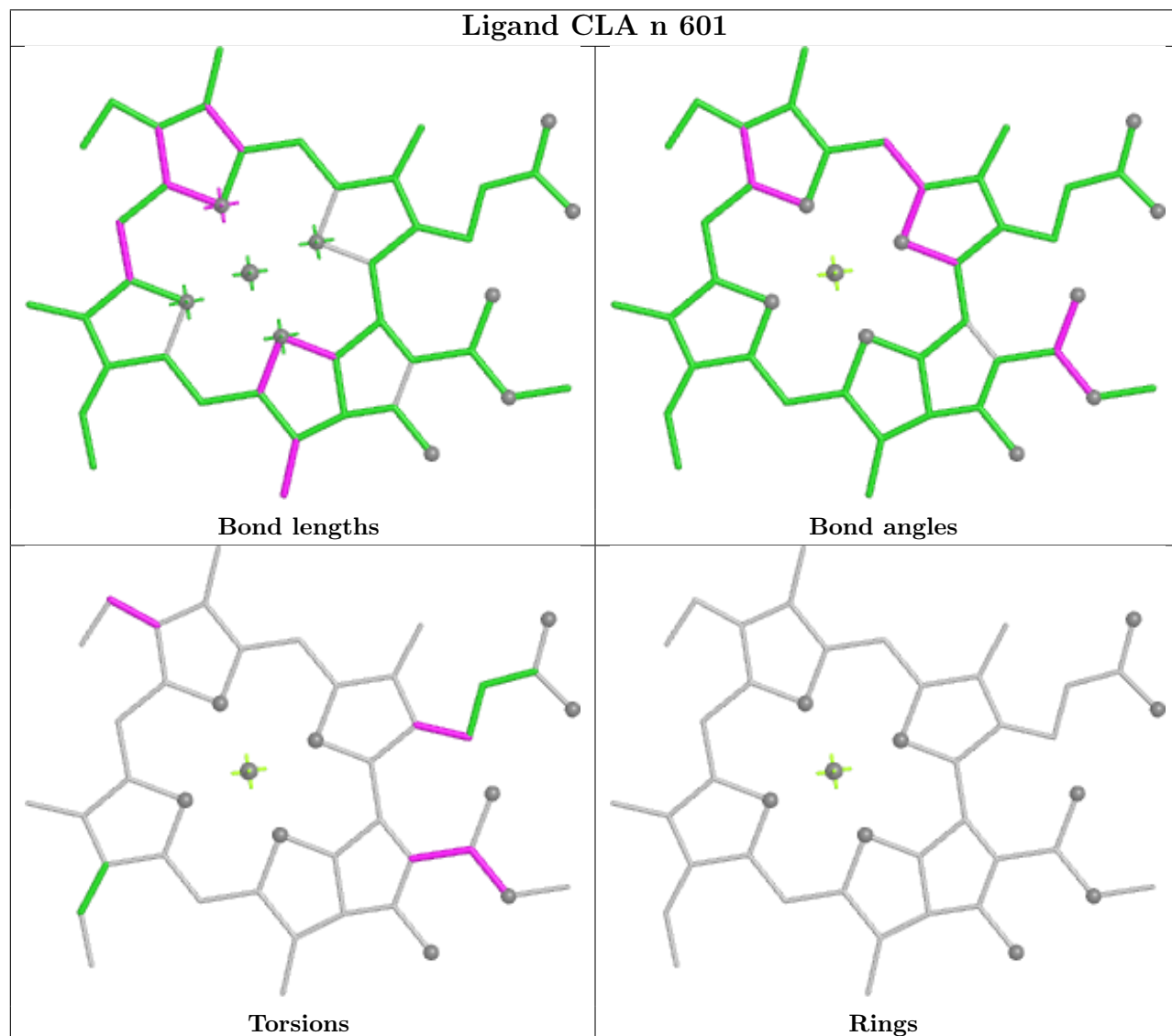
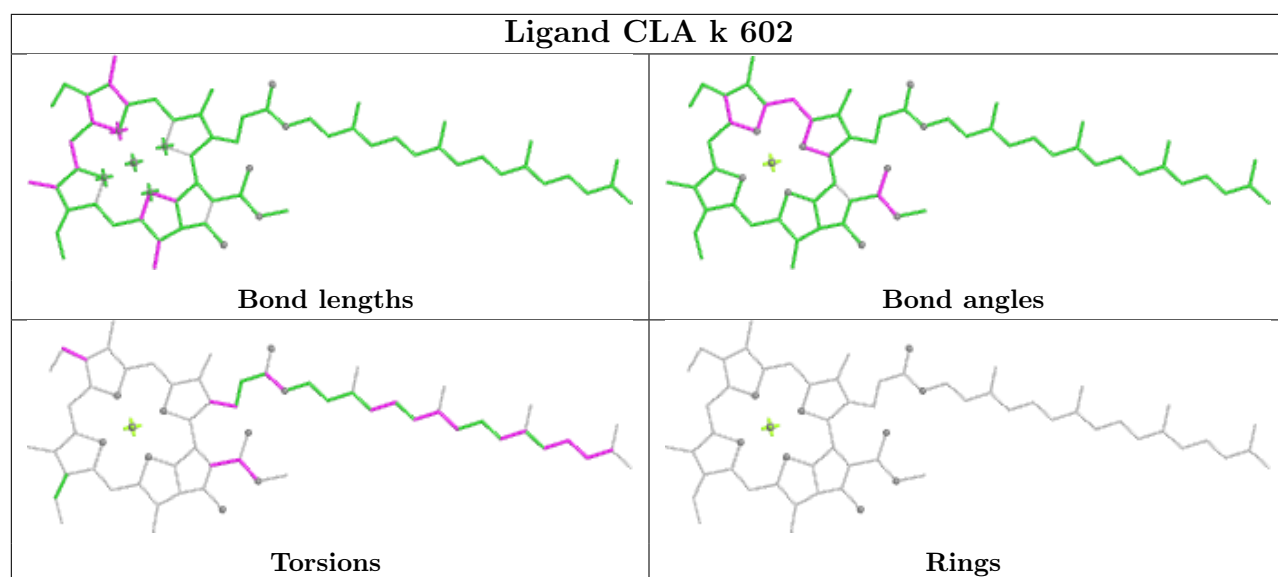


Ligand II0 f 616

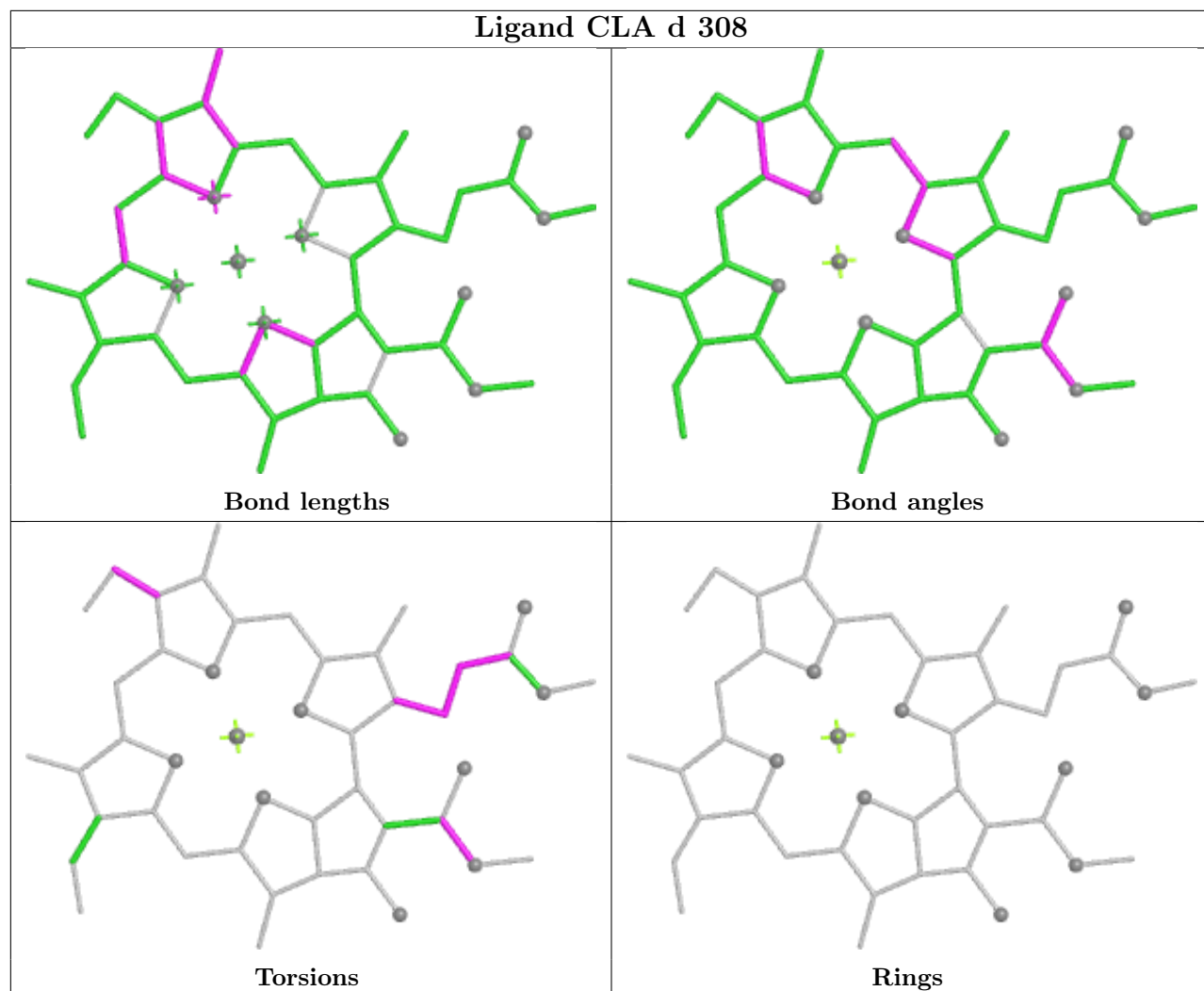


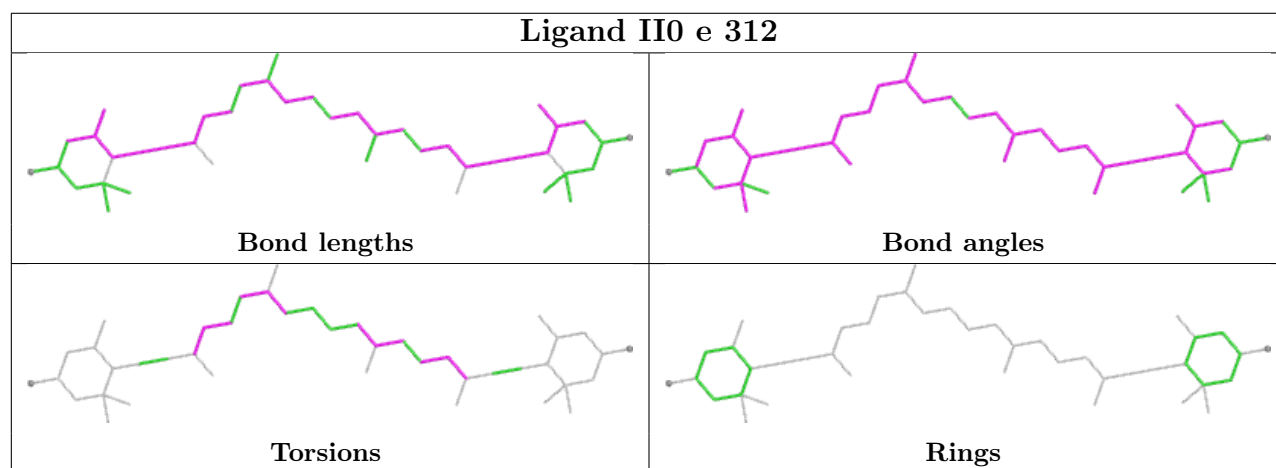
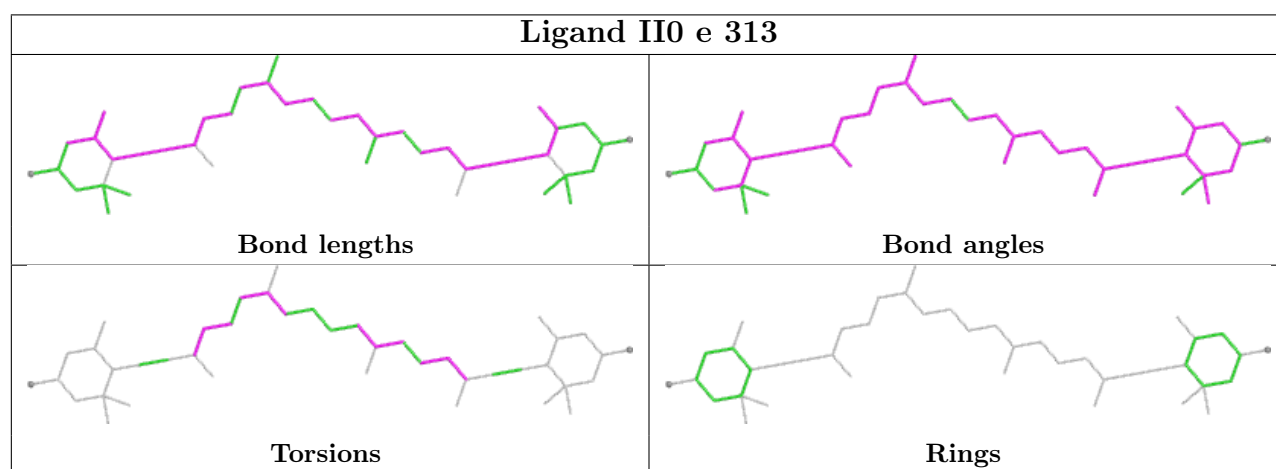
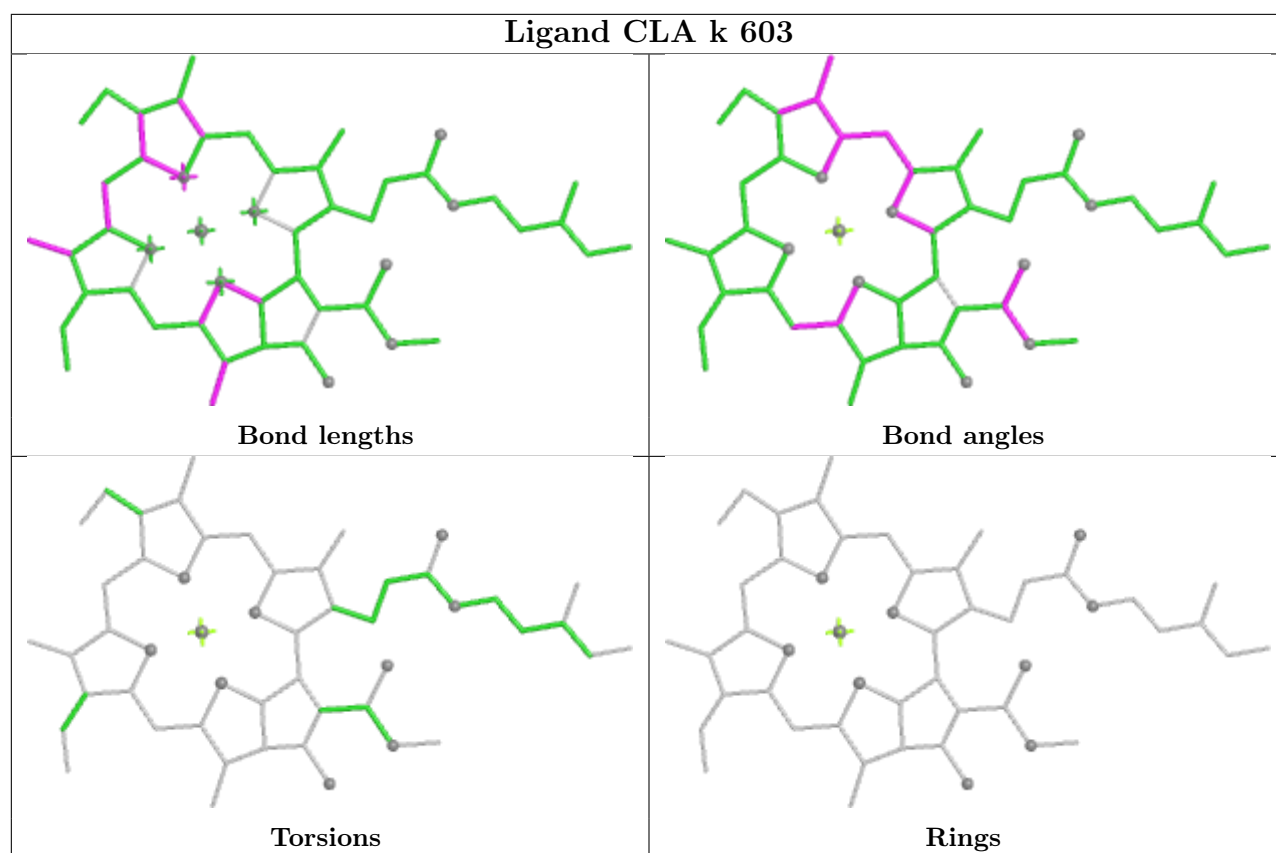


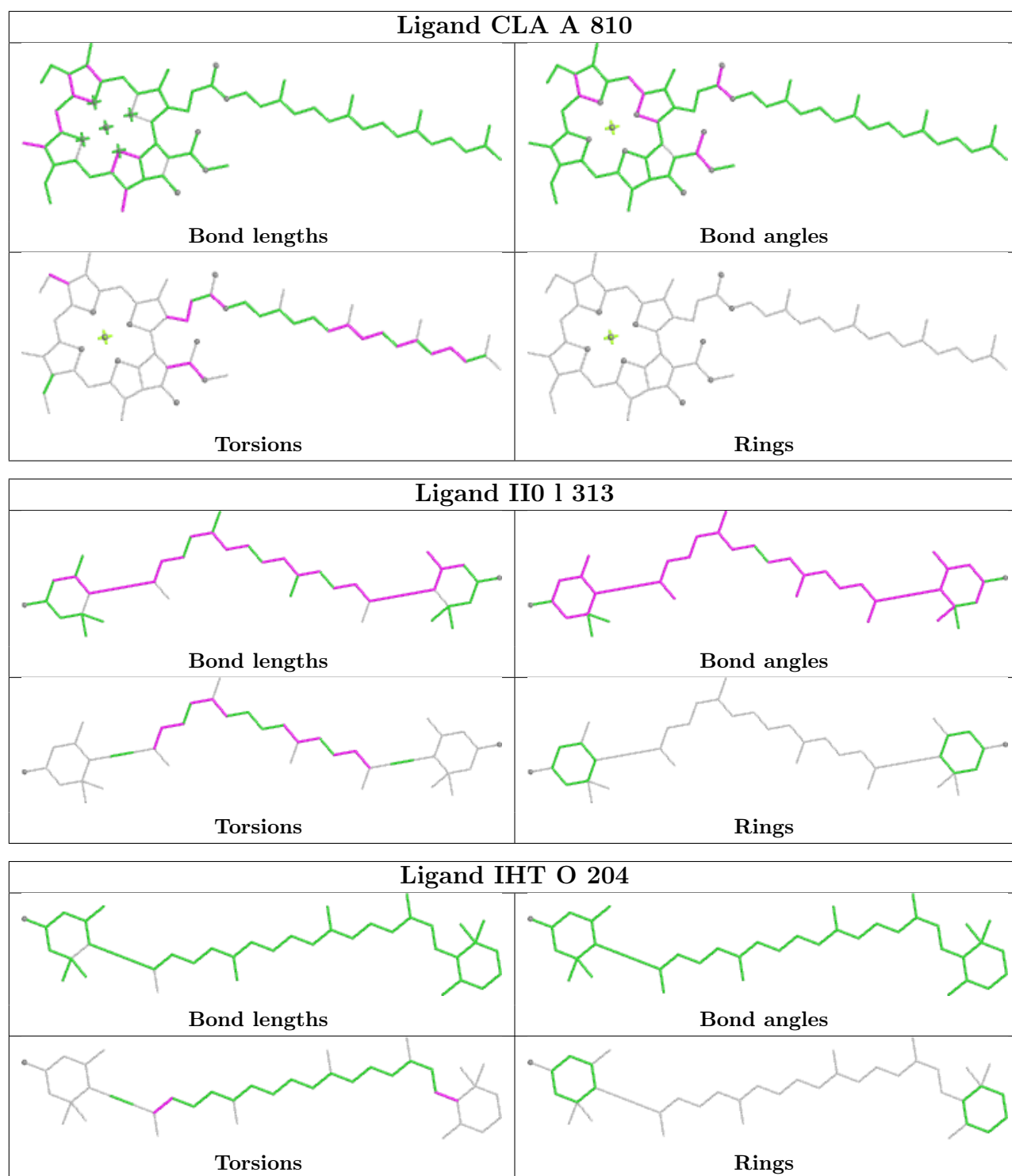




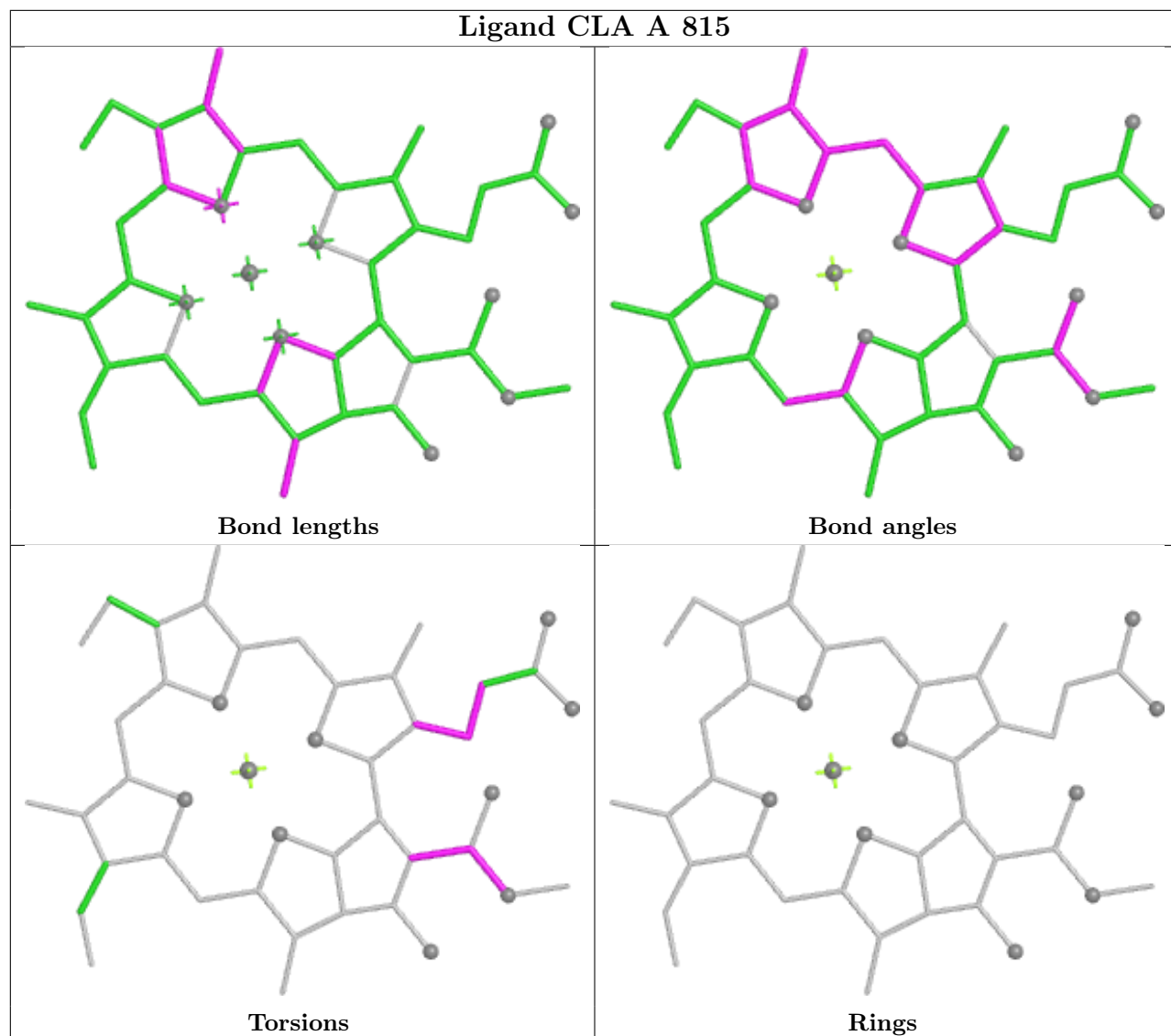
Ligand CLA d 308



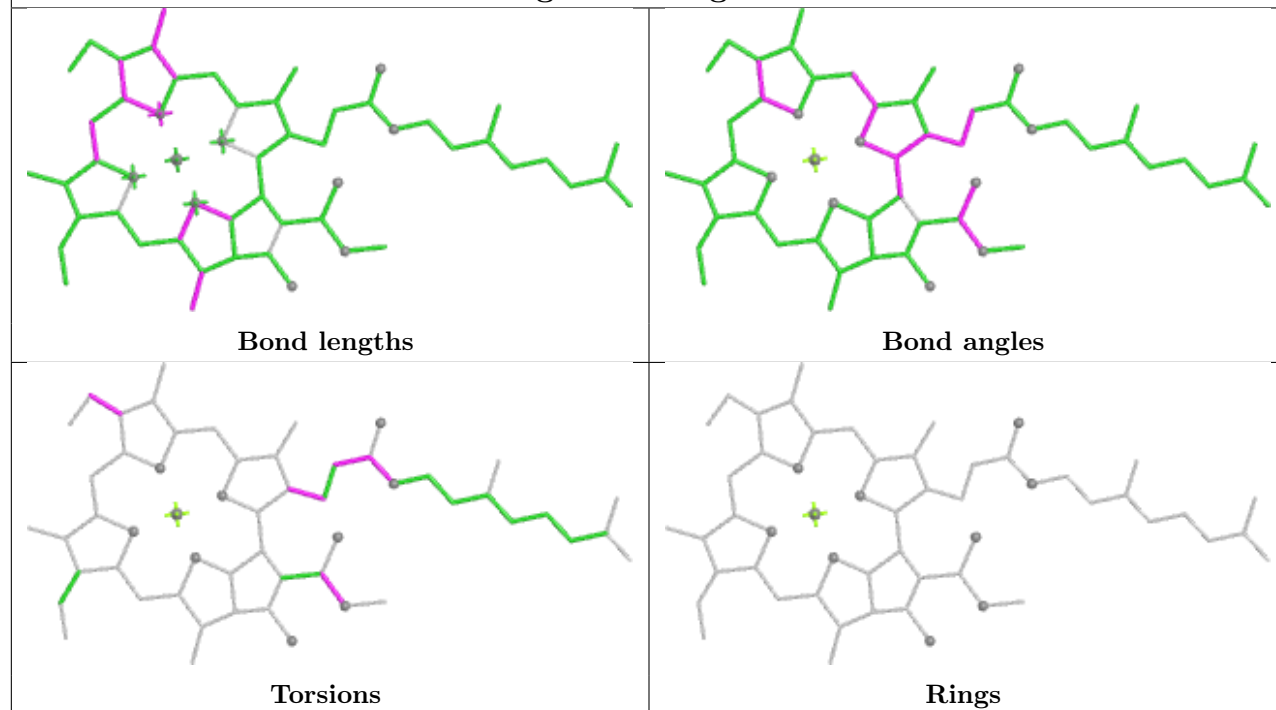




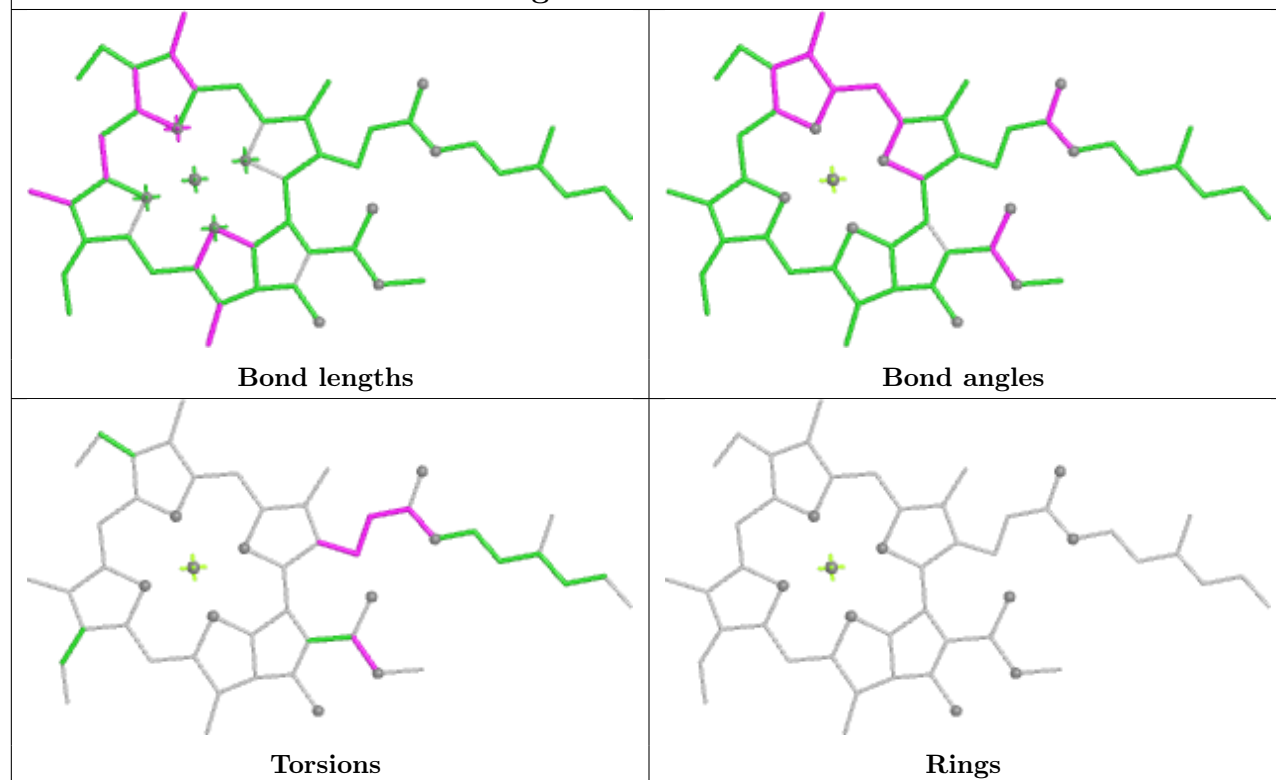
Ligand CLA A 815

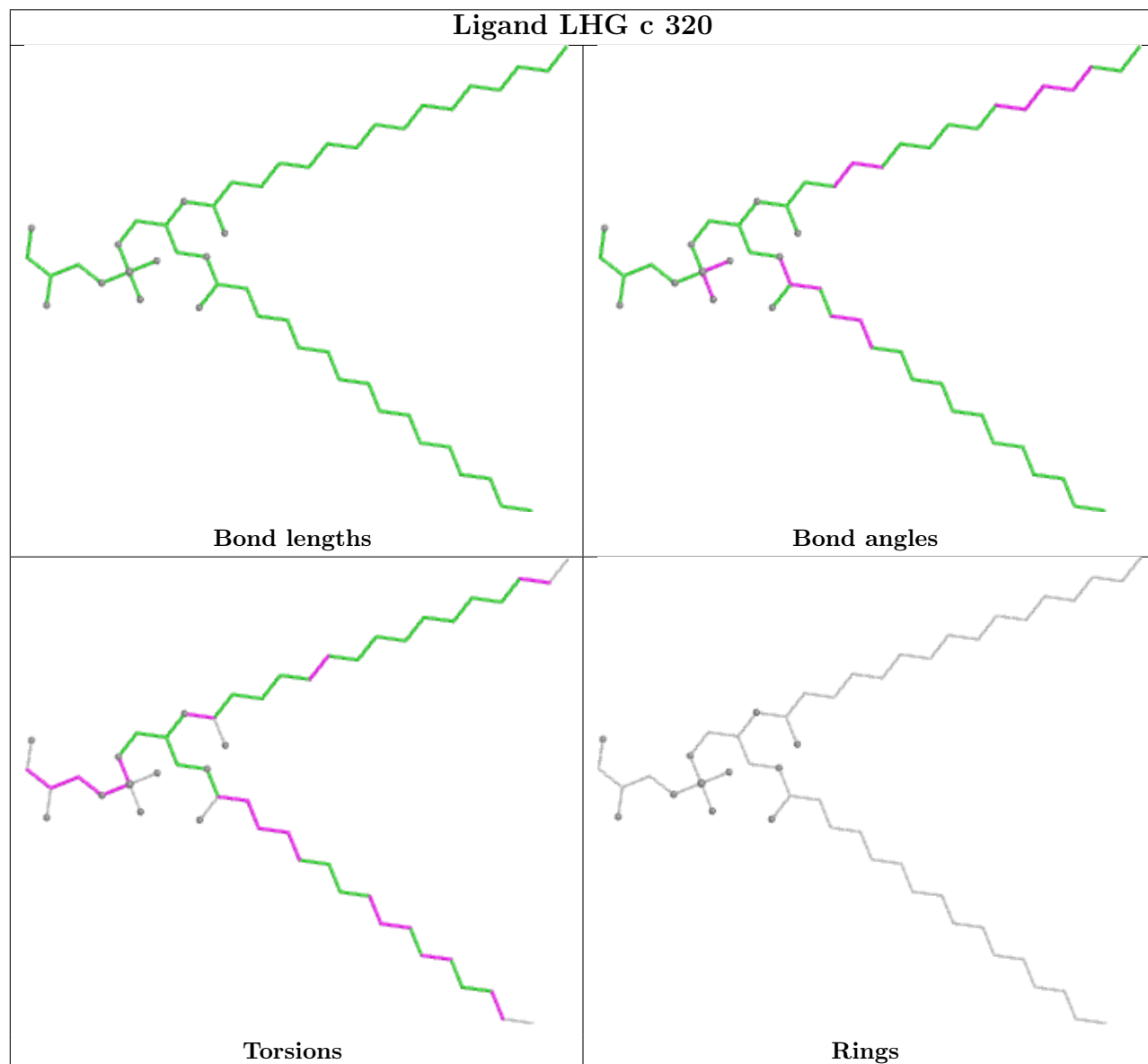
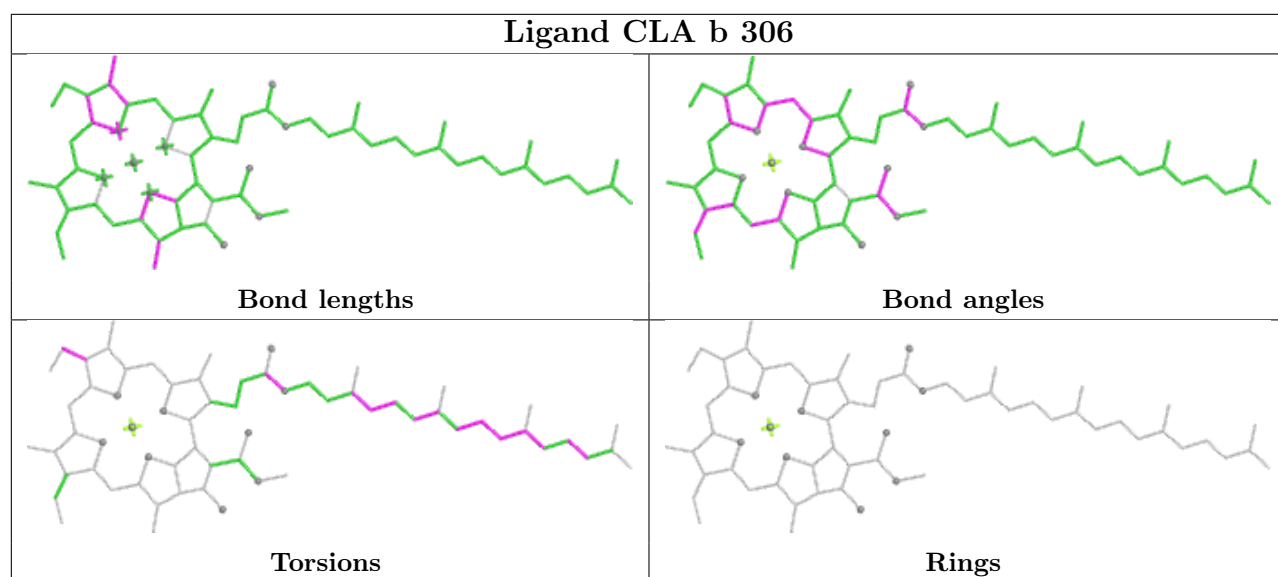


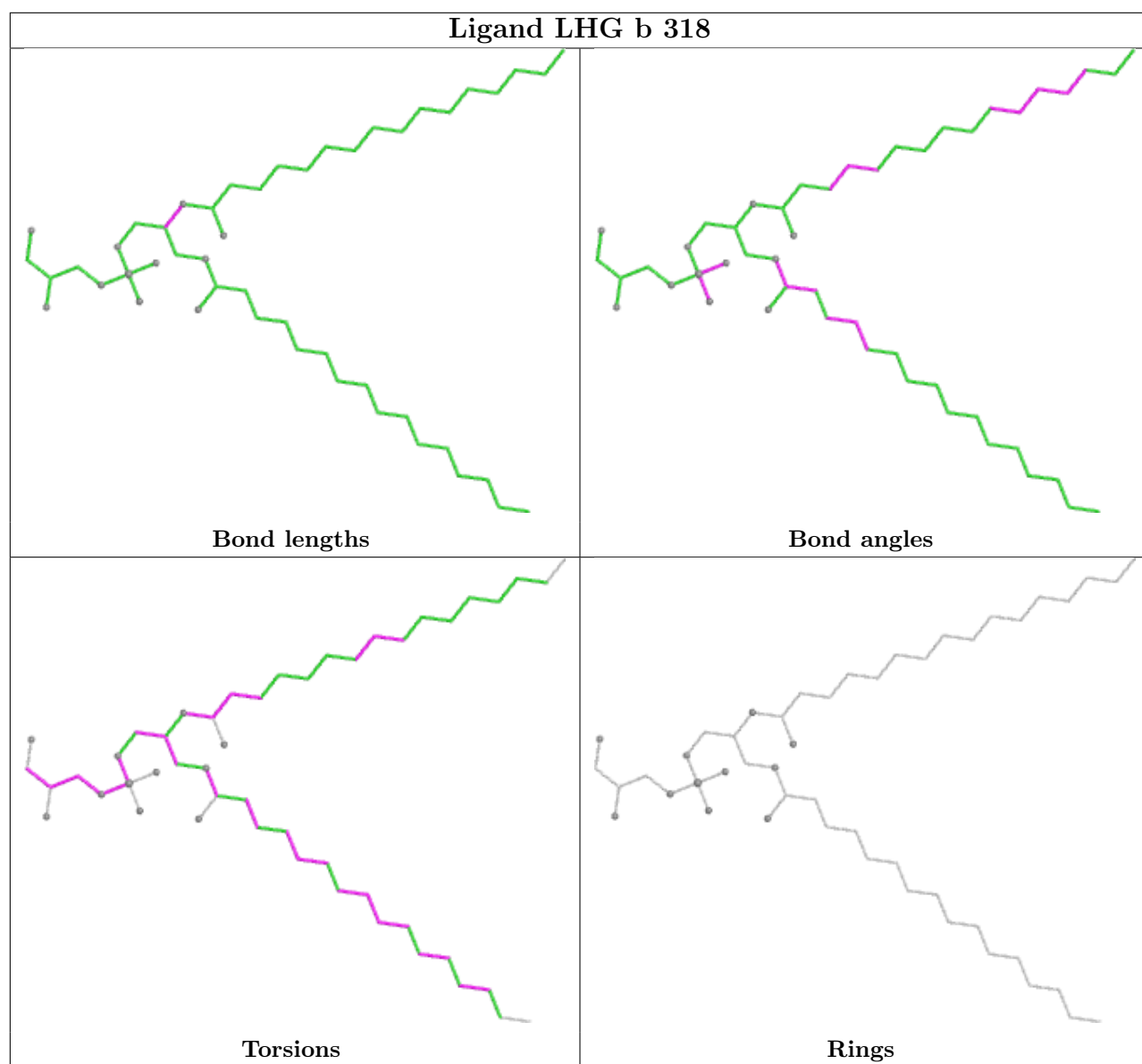
Ligand CLA g 323



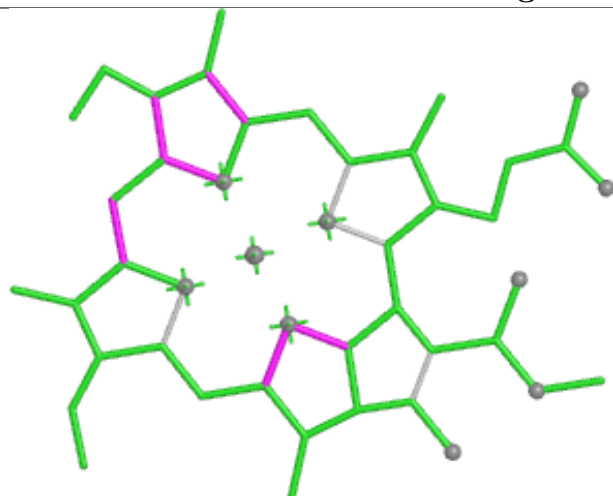
Ligand CLA O 201



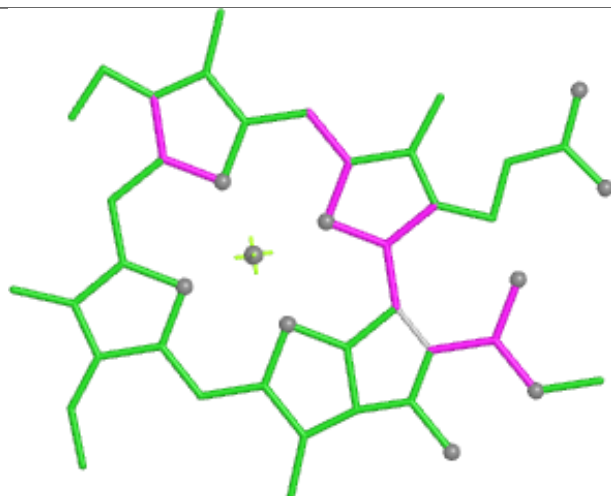




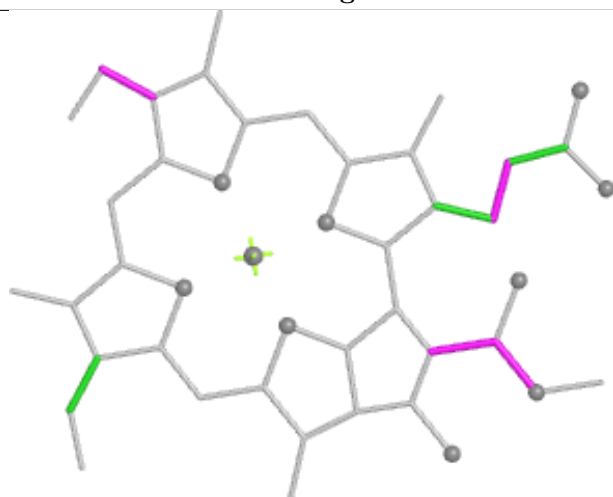
Ligand CLA k 605



Bond lengths



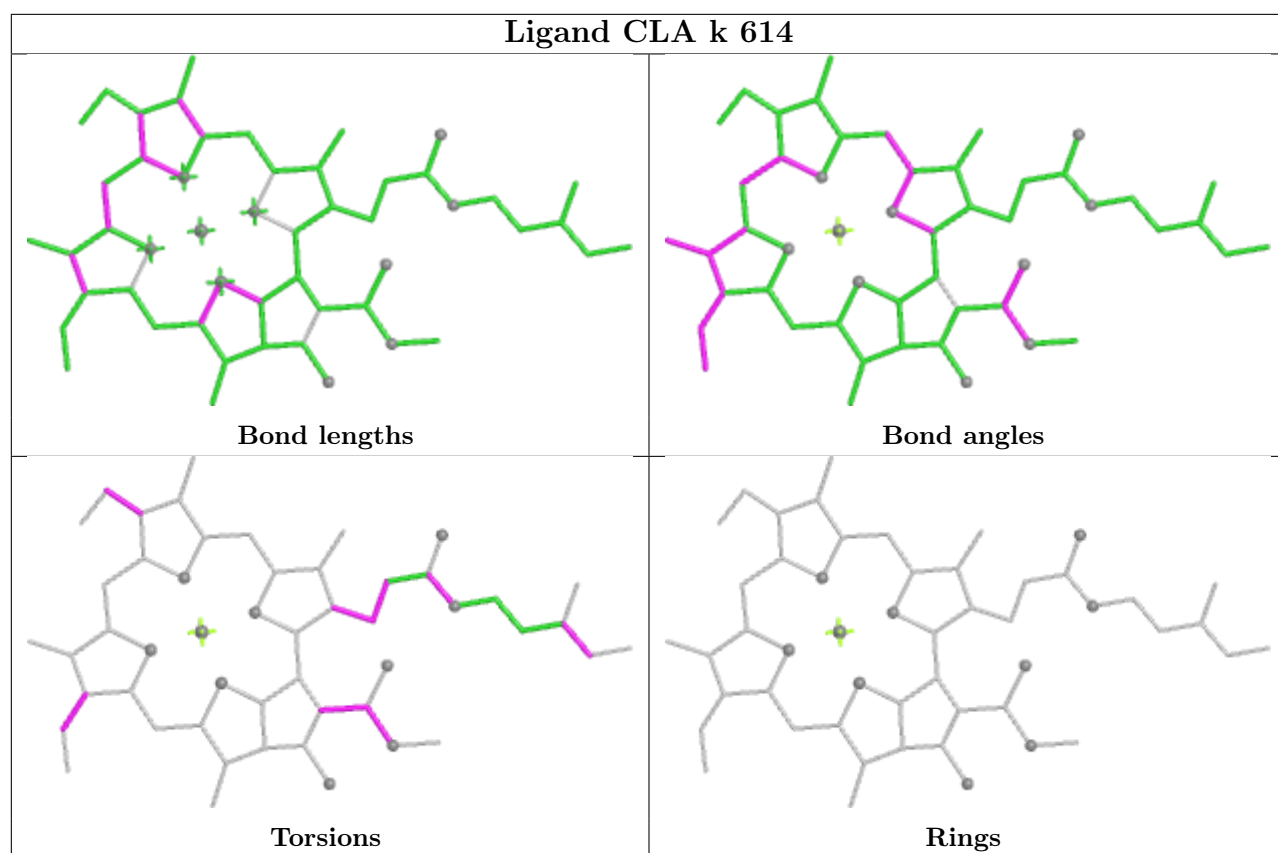
Bond angles



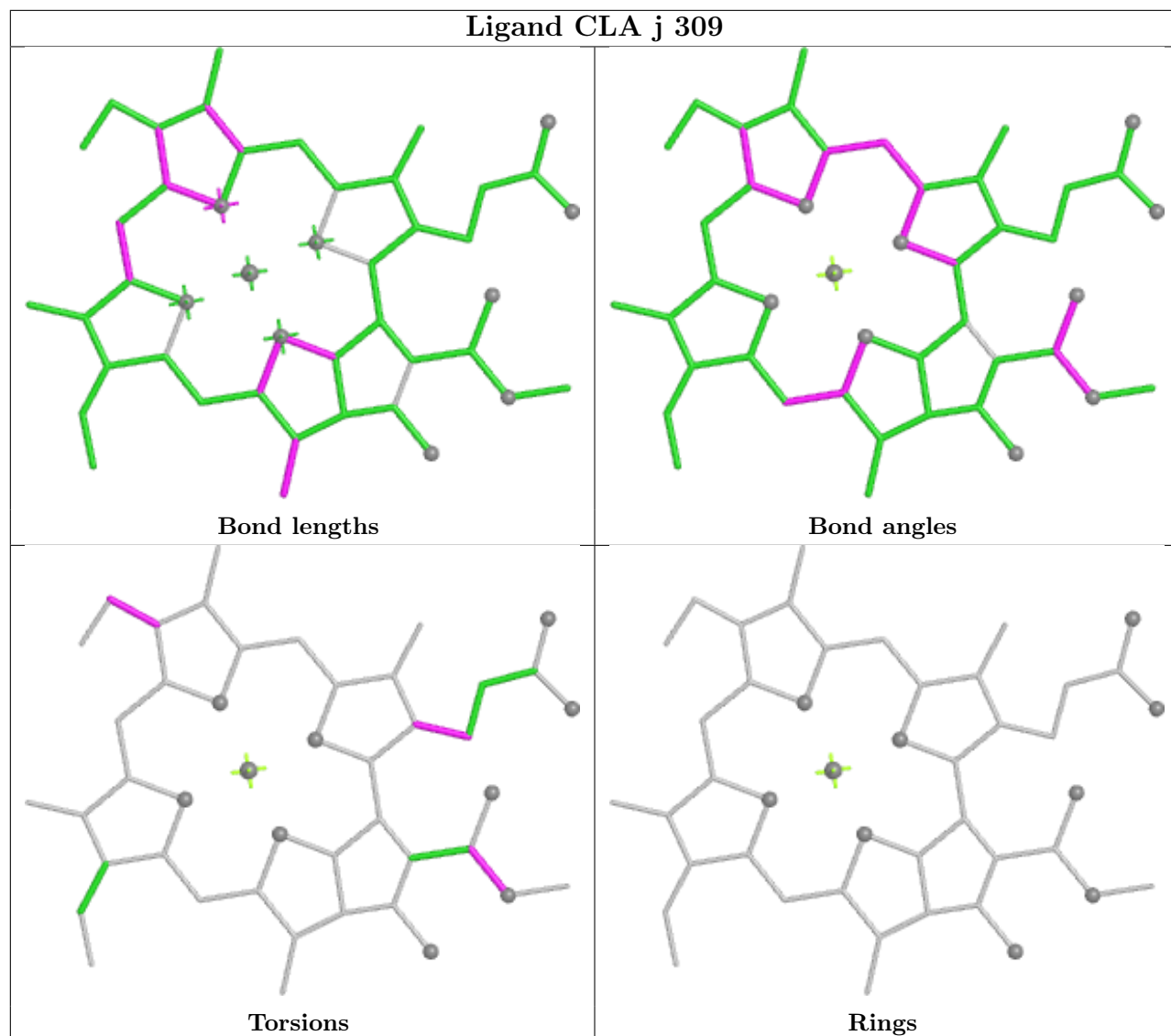
Torsions



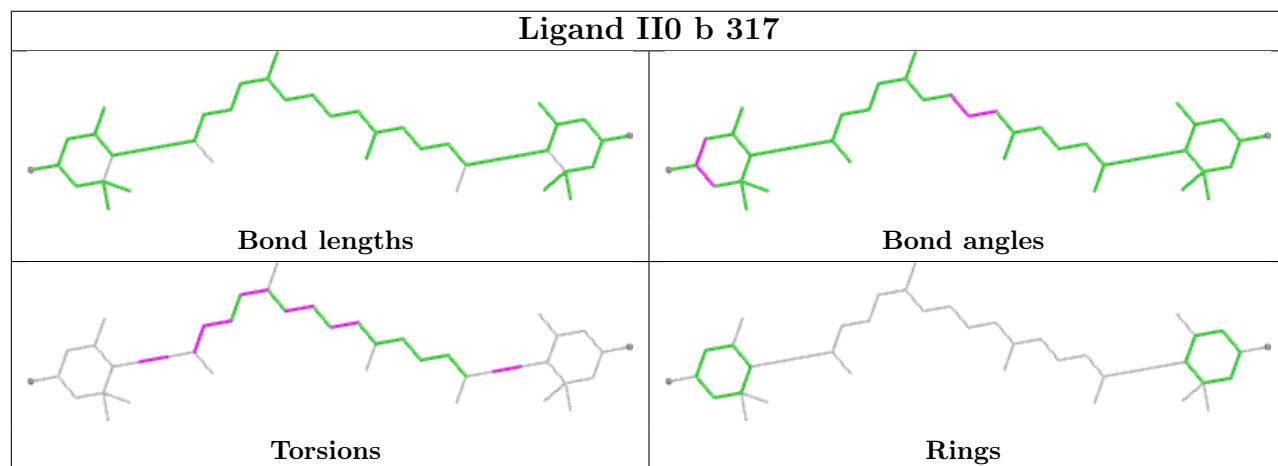
Rings



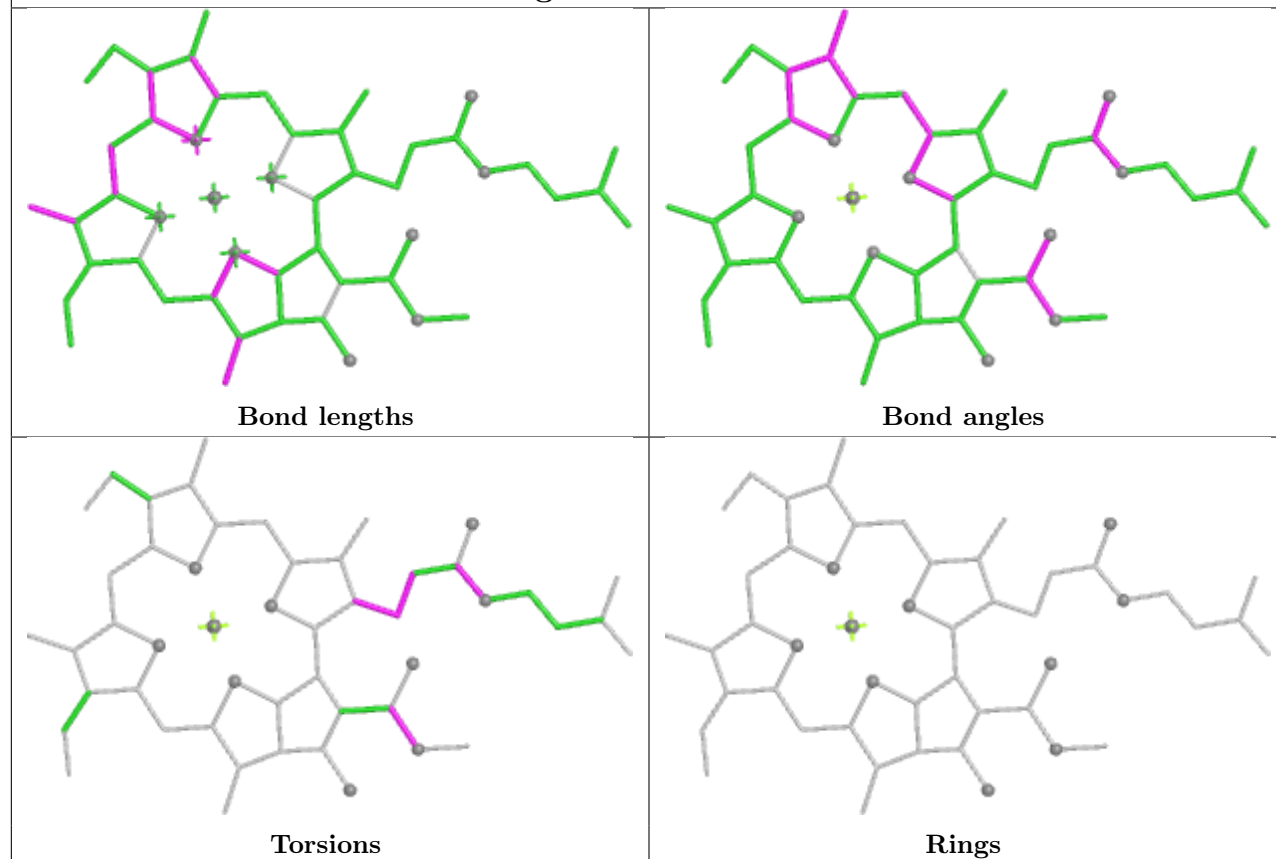
Ligand CLA j 309



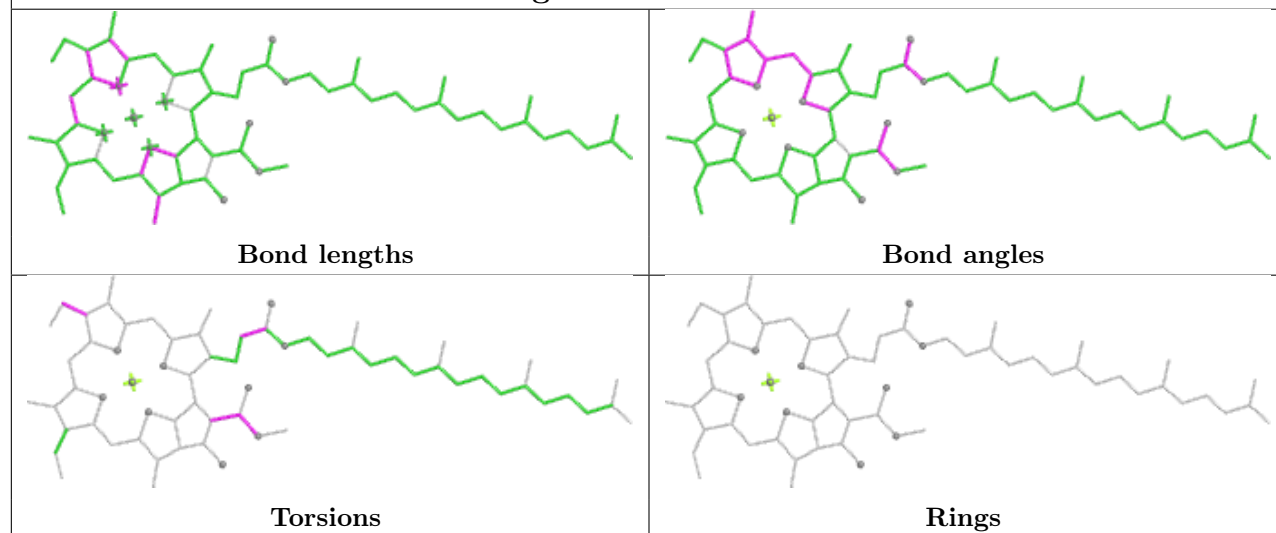
Ligand II0 b 317

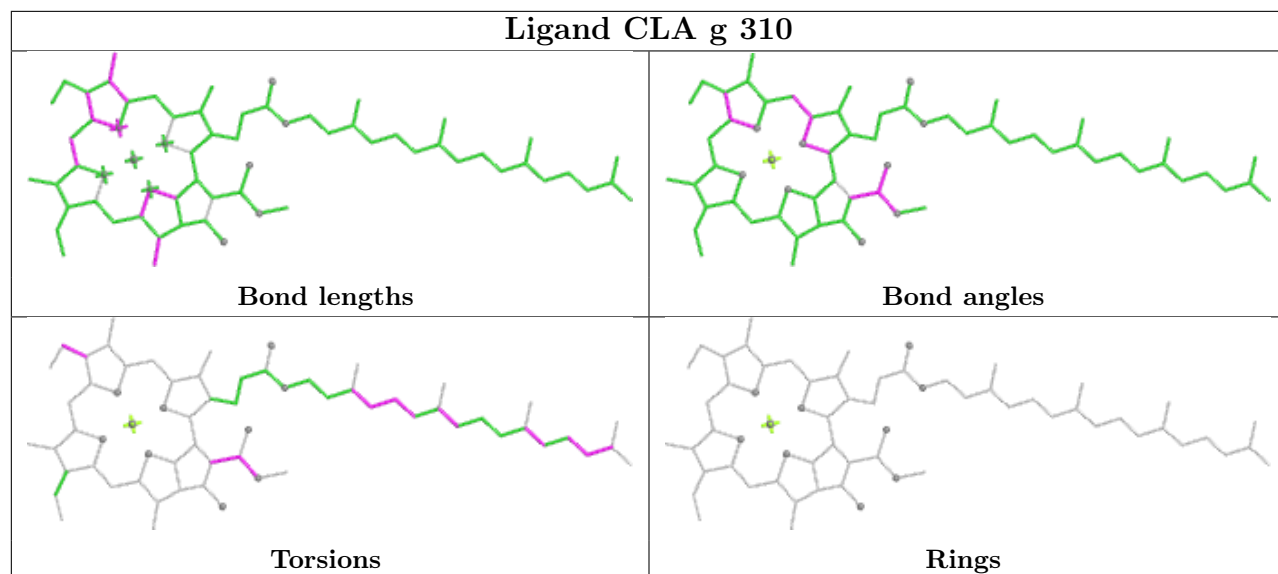
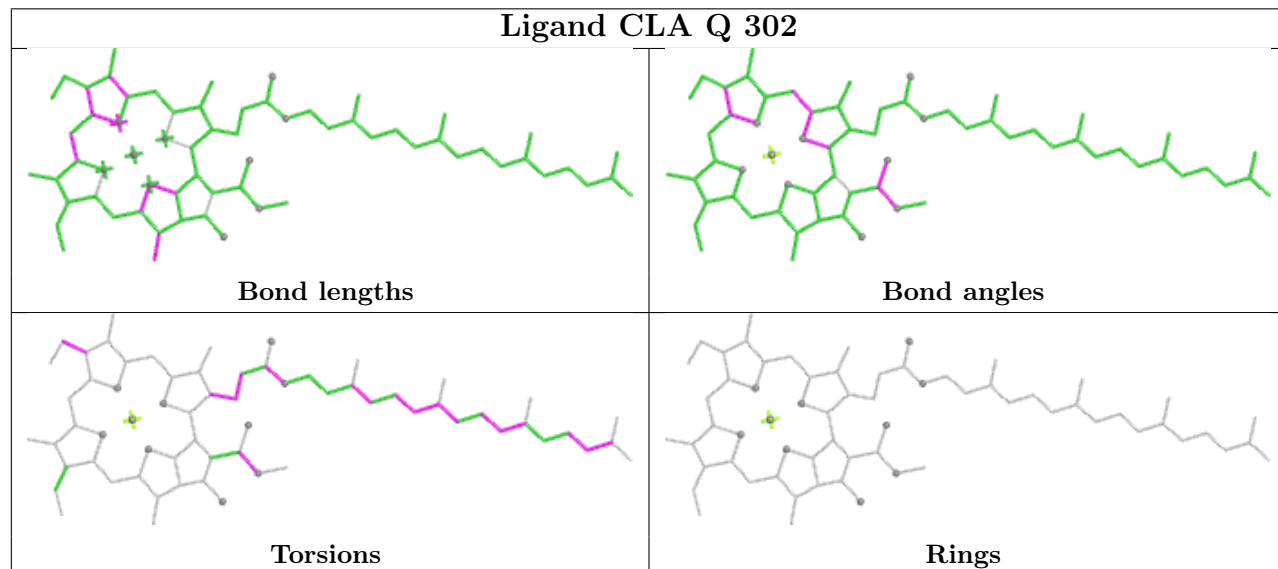


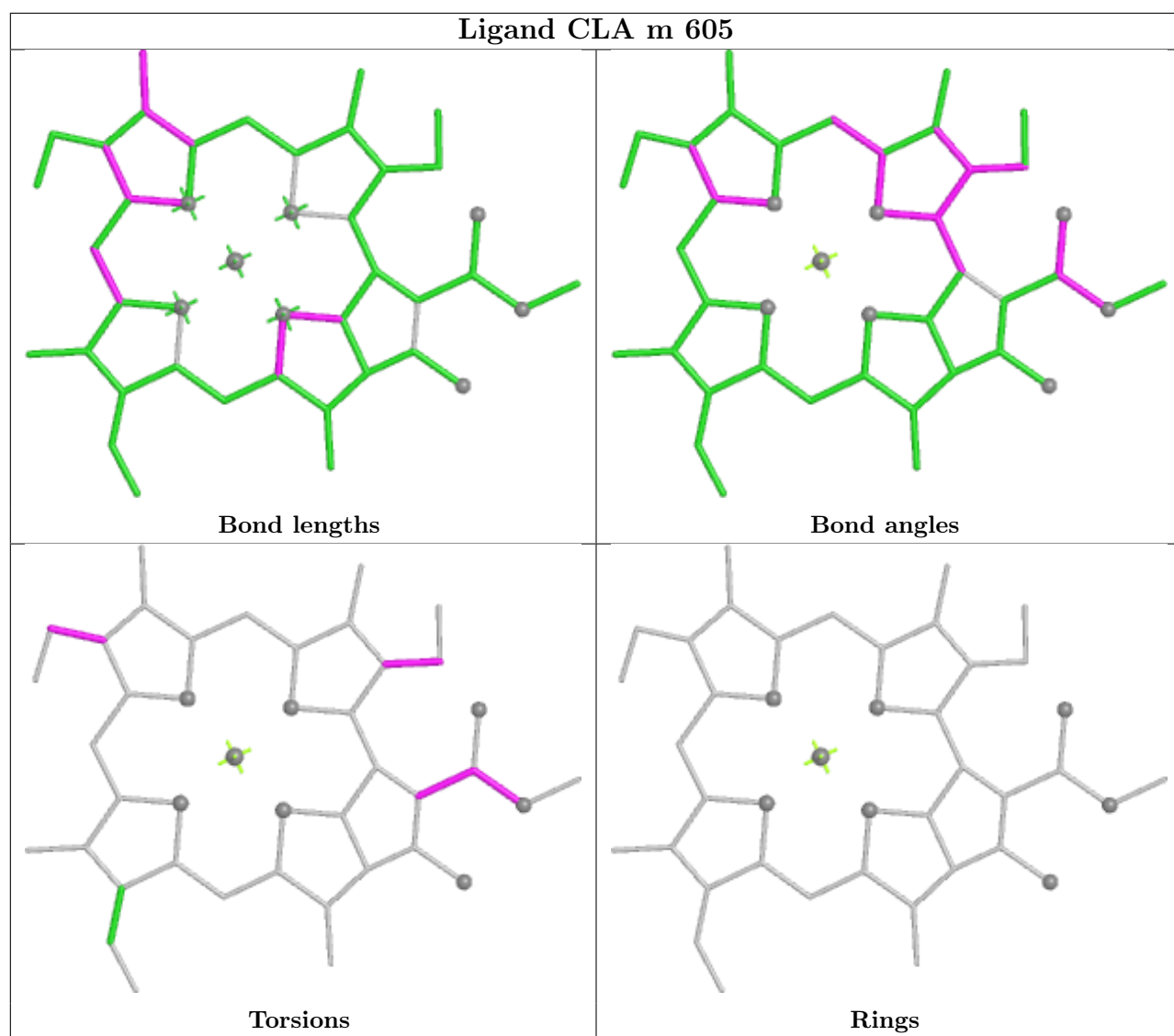
Ligand CLA h 302



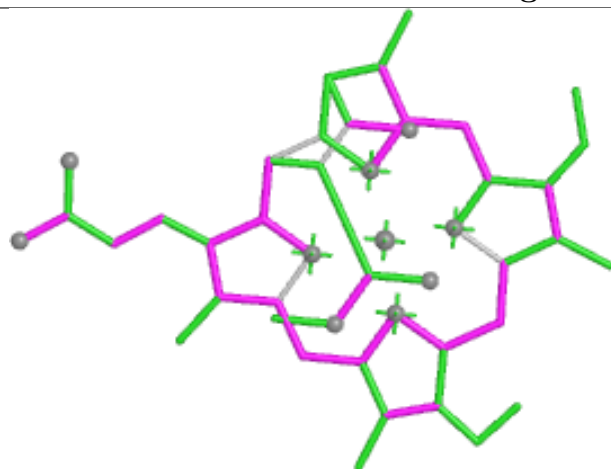
Ligand CLA B 842



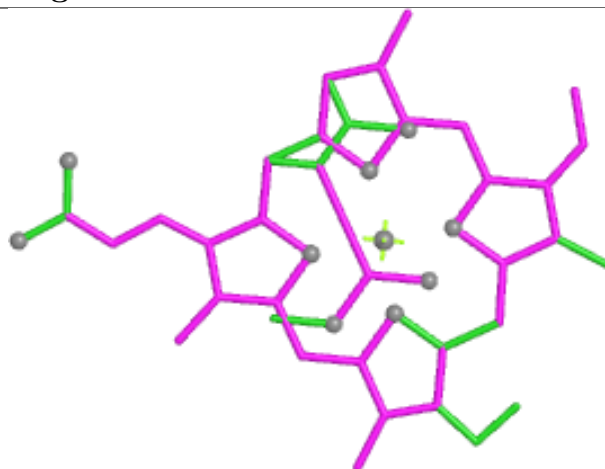
Ligand CLA g 310**Ligand CLA Q 302**



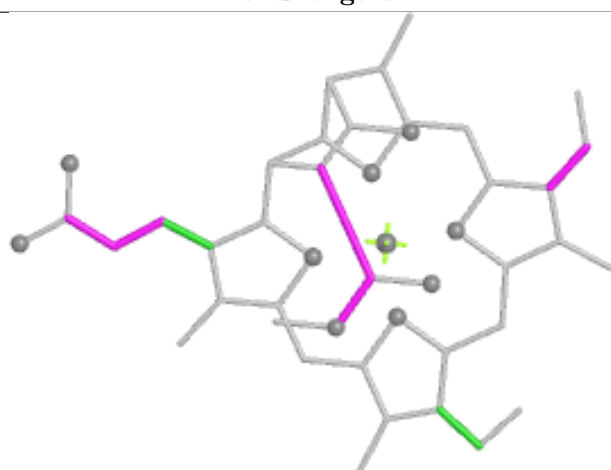
Ligand KC2 g 313



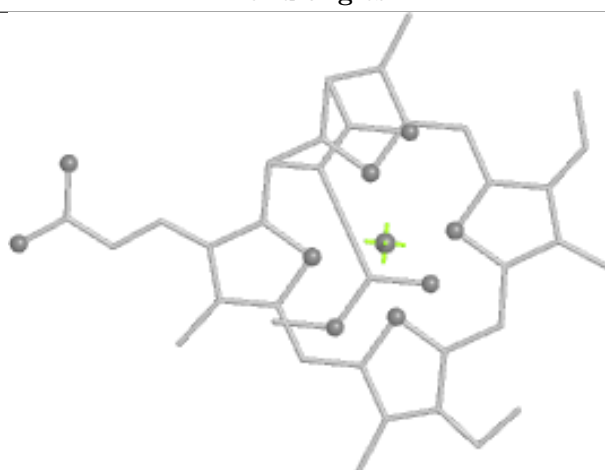
Bond lengths



Bond angles

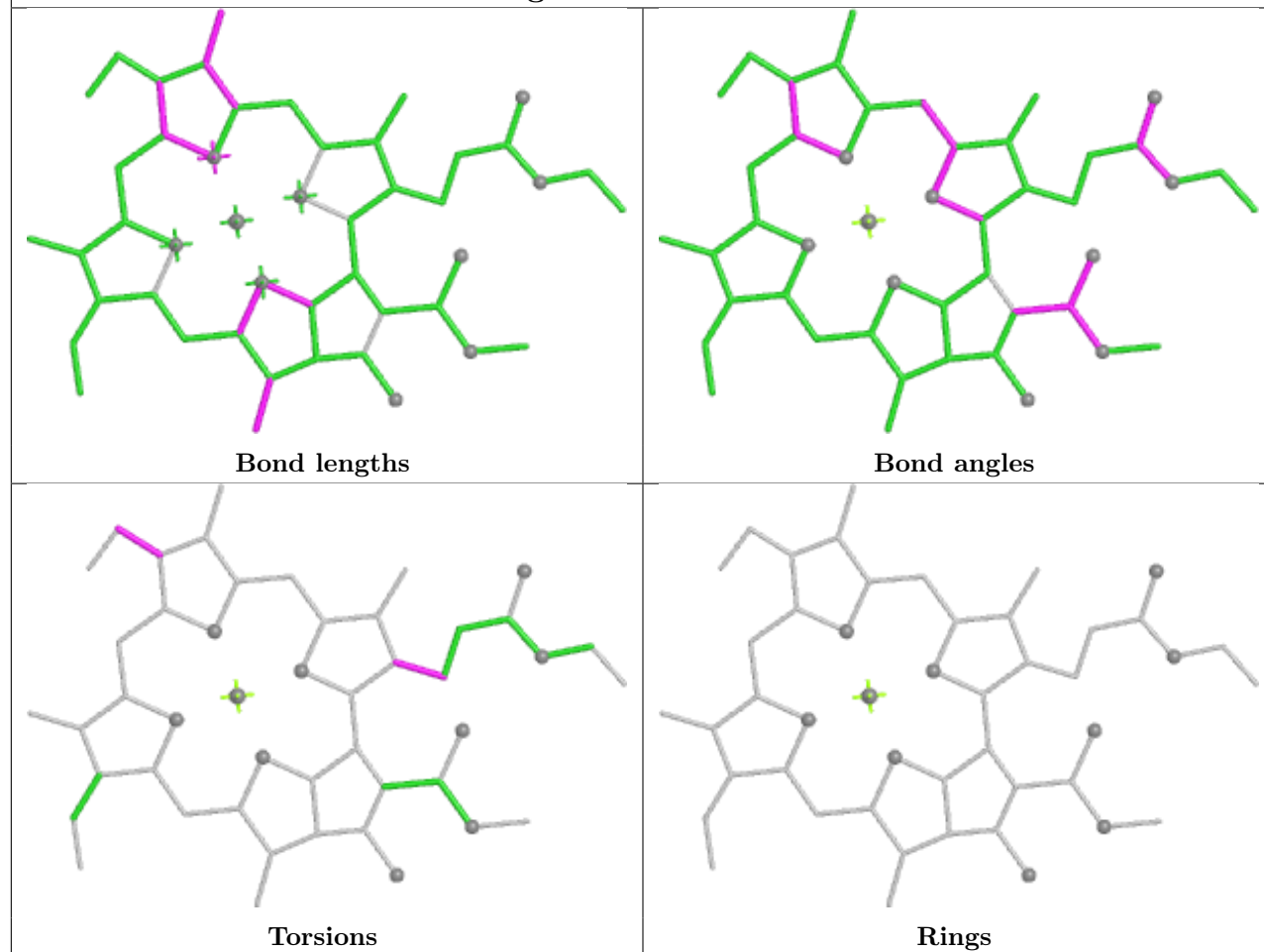


Torsions

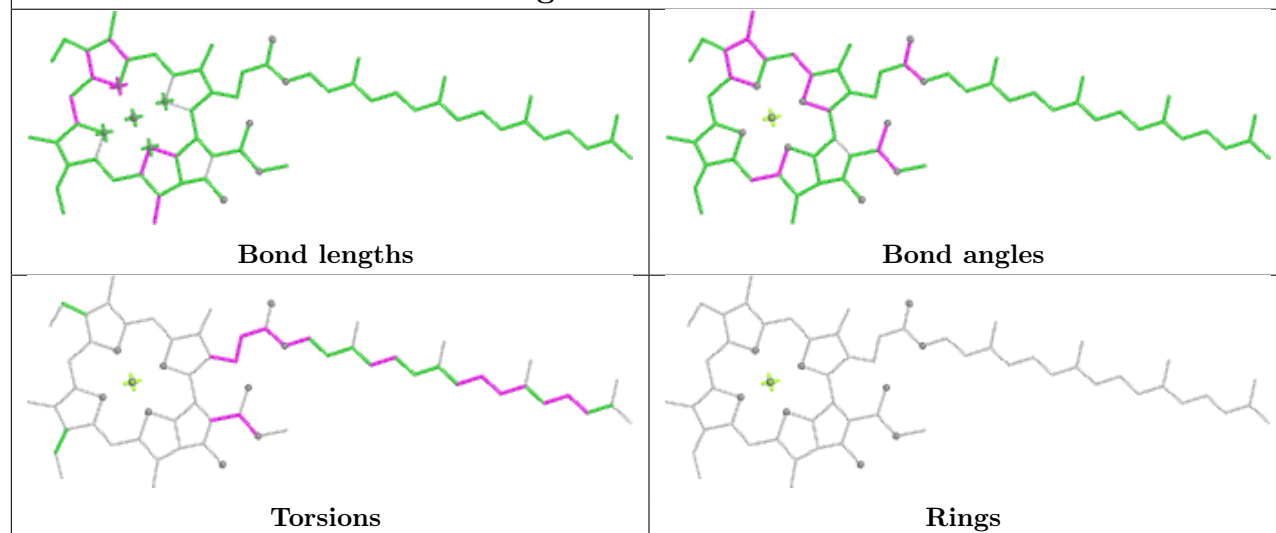


Rings

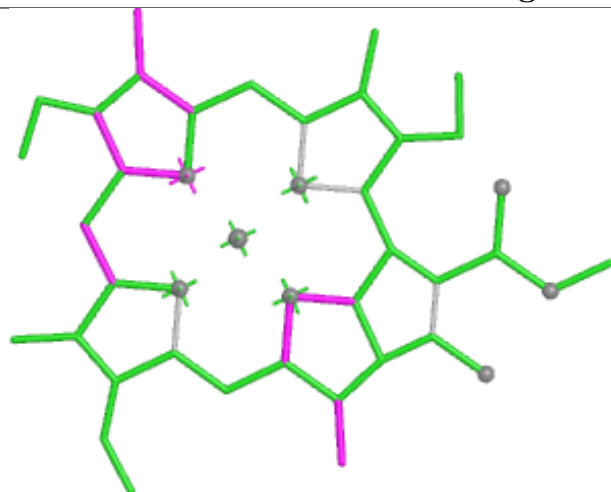
Ligand CLA B 835



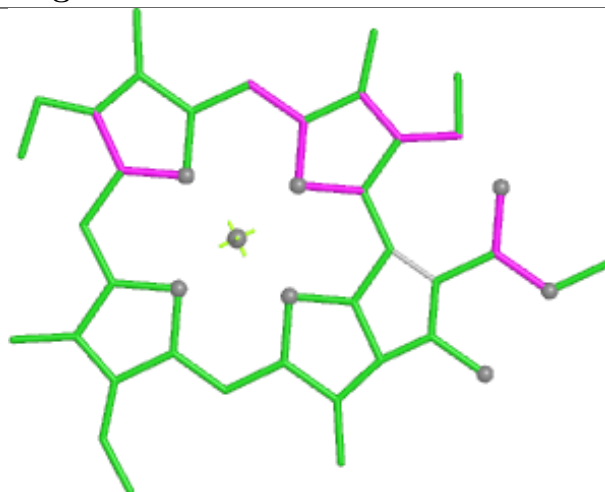
Ligand CLA e 302



Ligand CLA g 303



Bond lengths



Bond angles

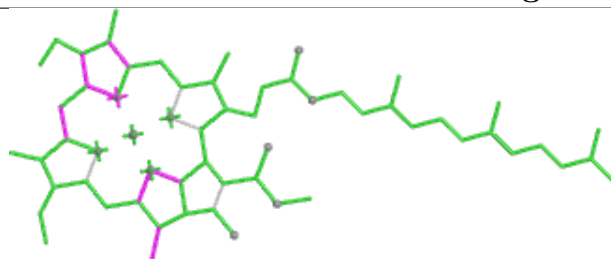


Torsions

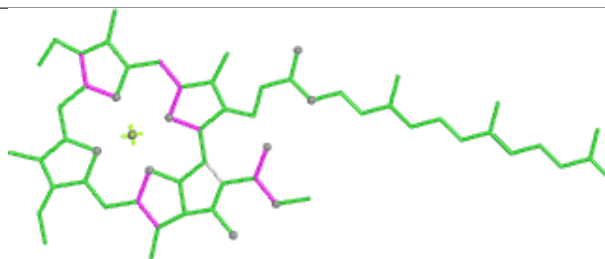


Rings

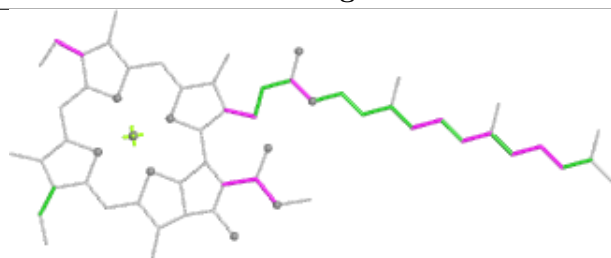
Ligand CLA i 311



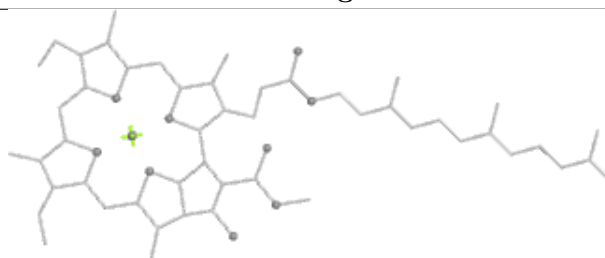
Bond lengths



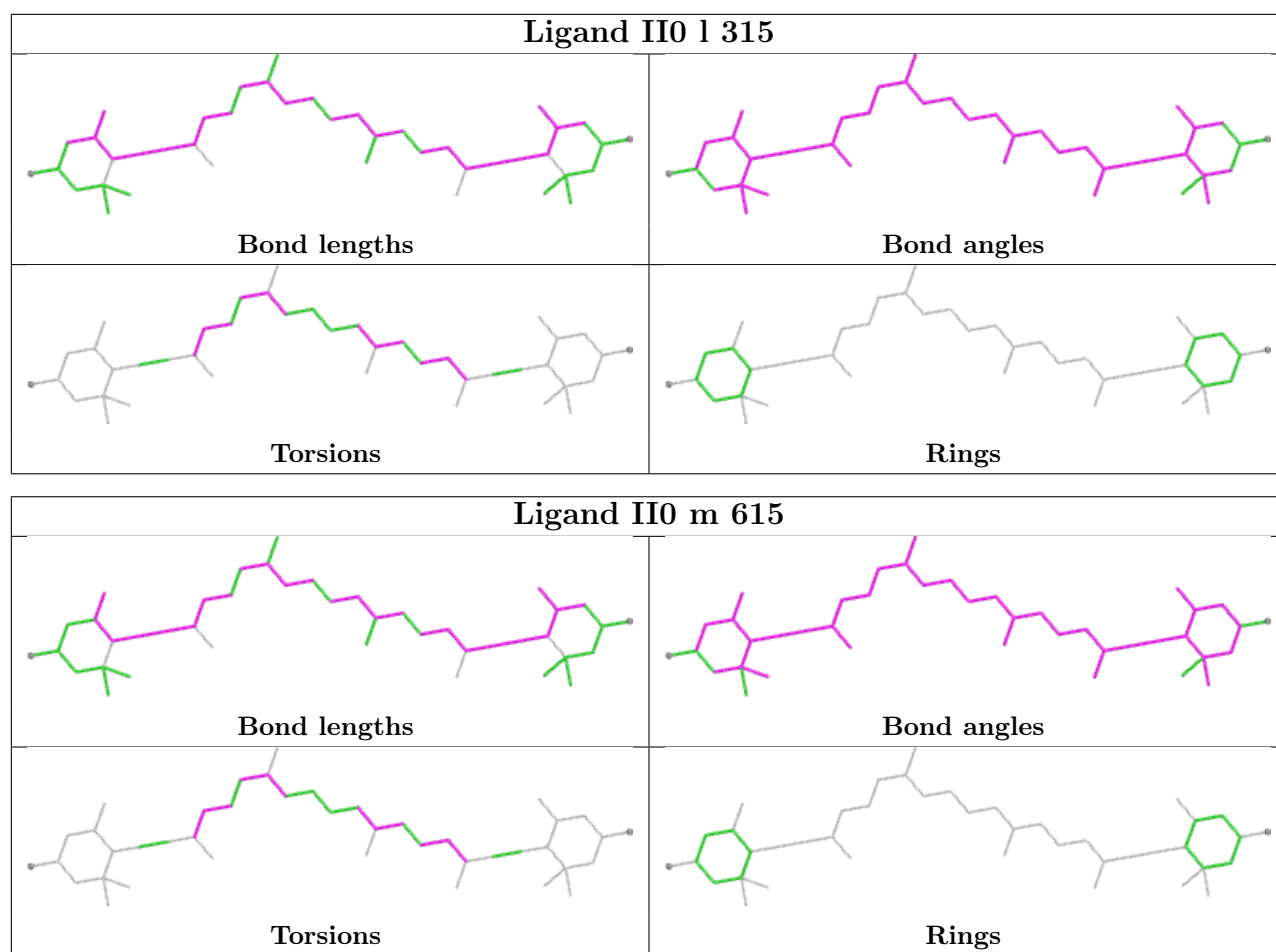
Bond angles

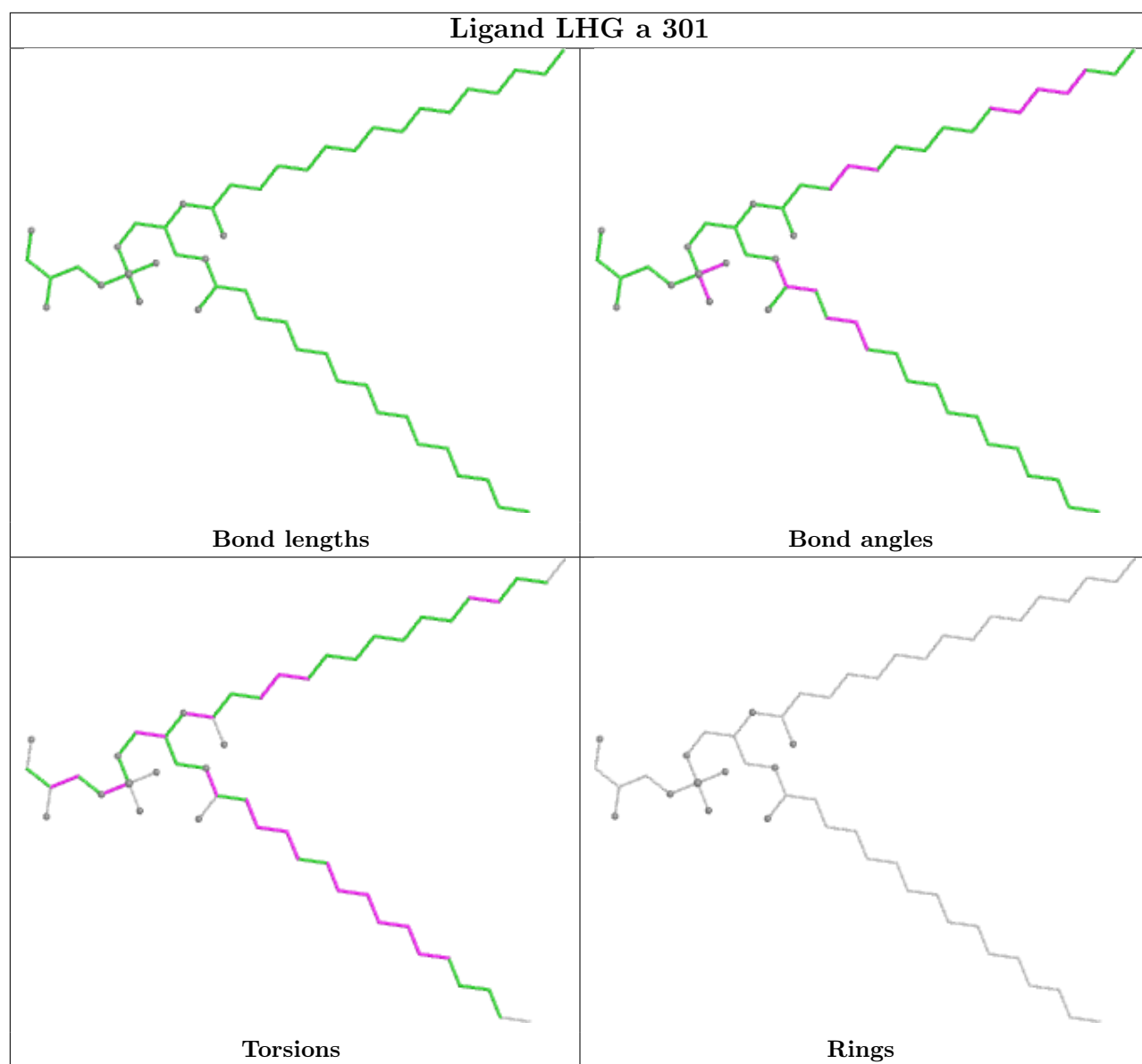


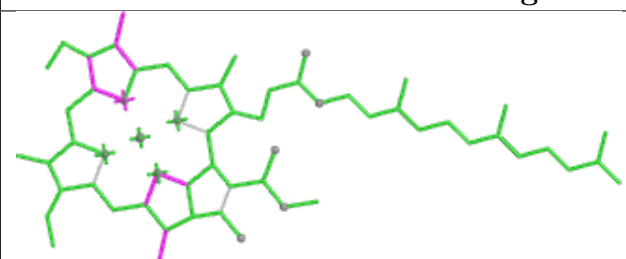
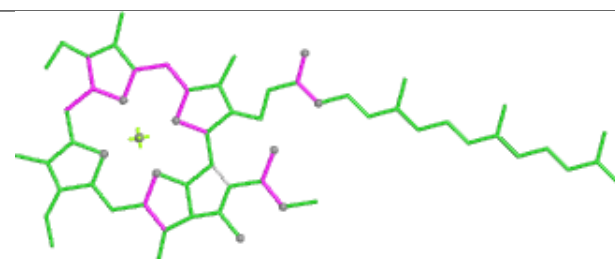
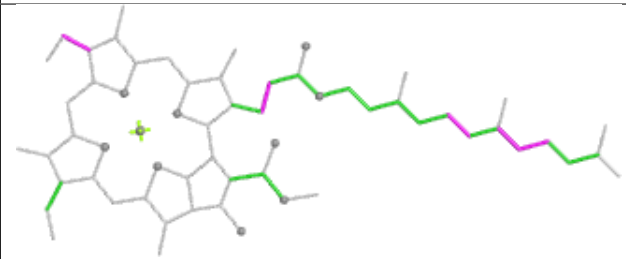
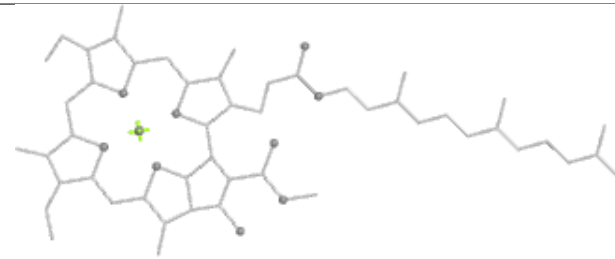
Torsions

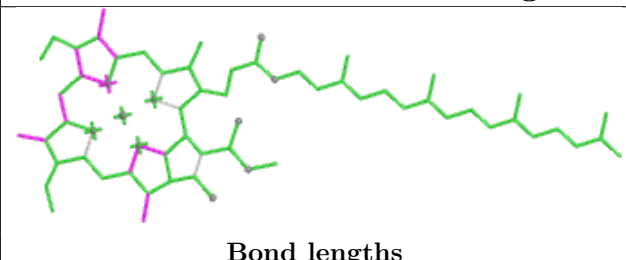
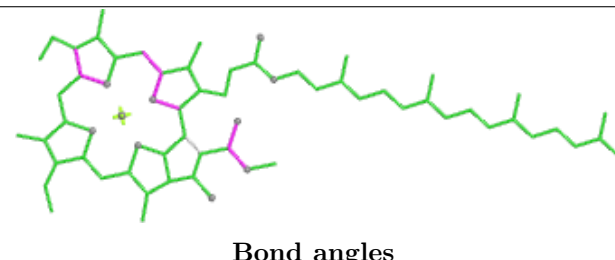
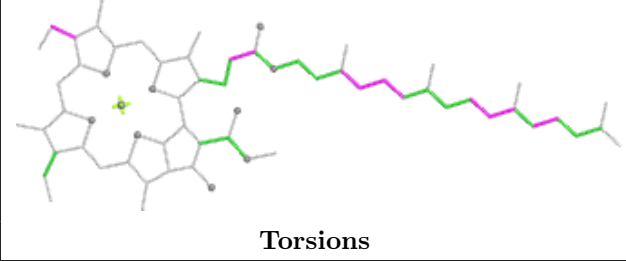
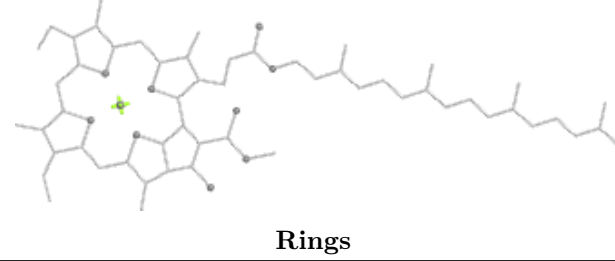


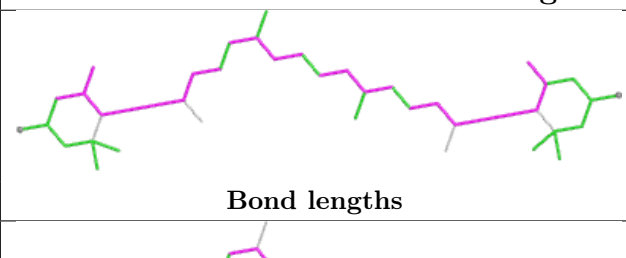
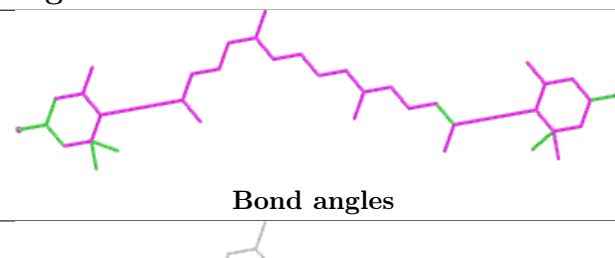
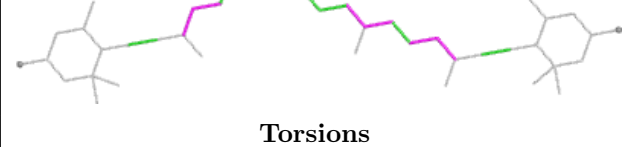
Rings

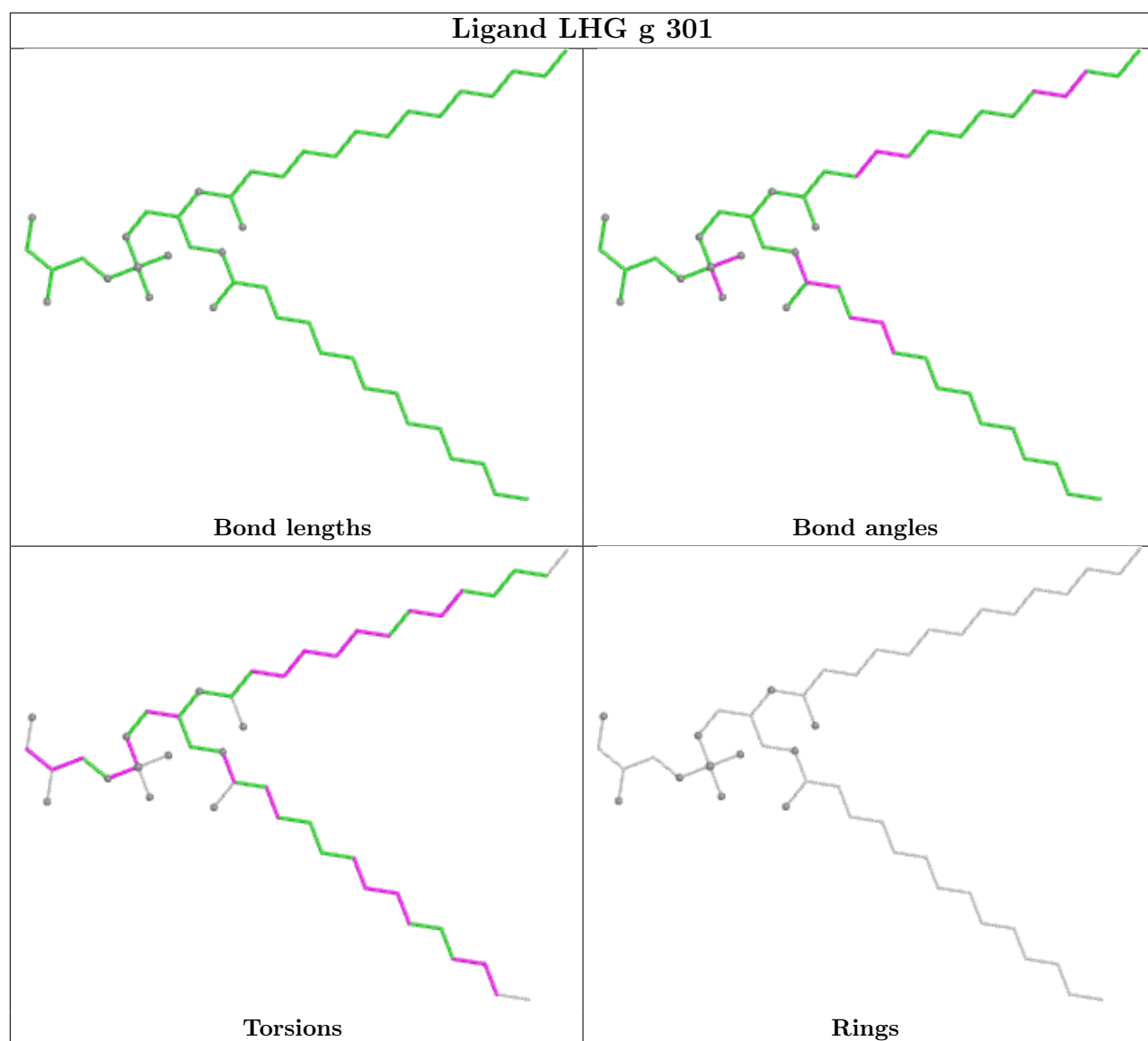




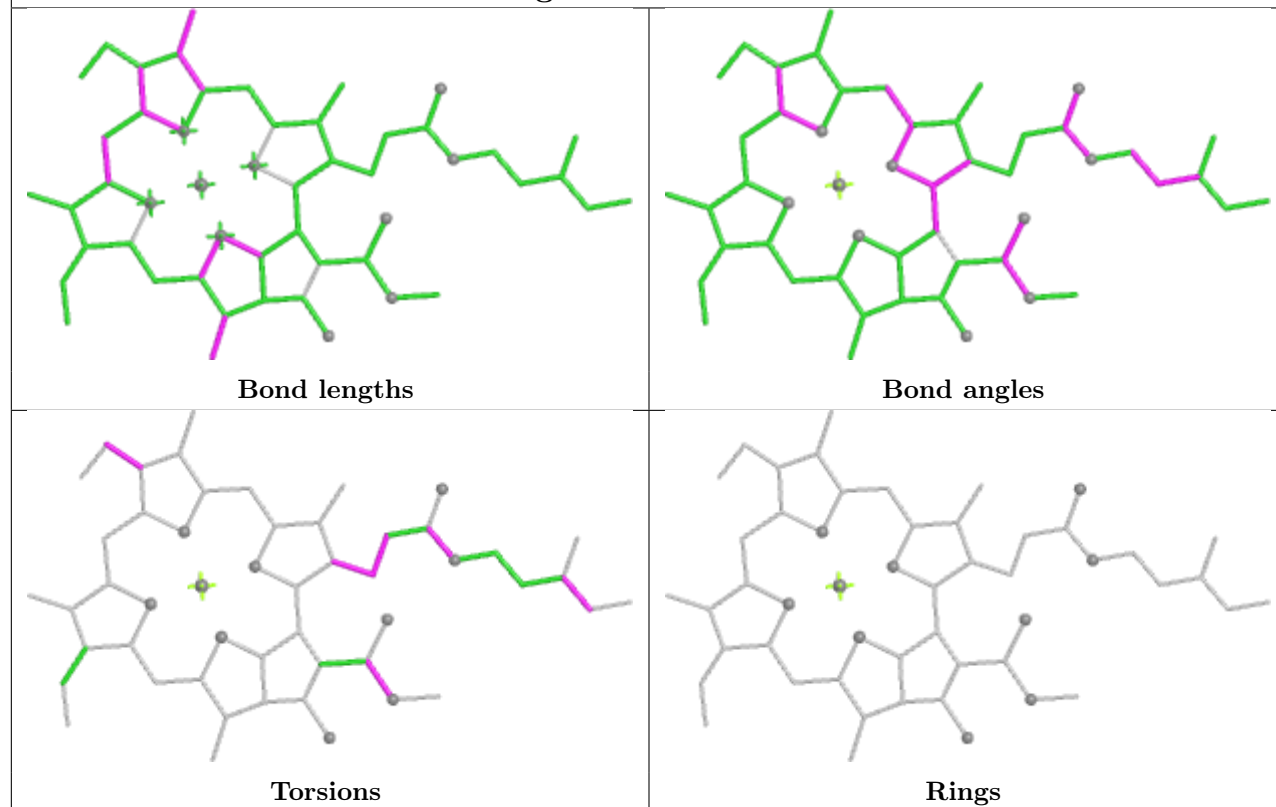
Ligand CLA A 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA O 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

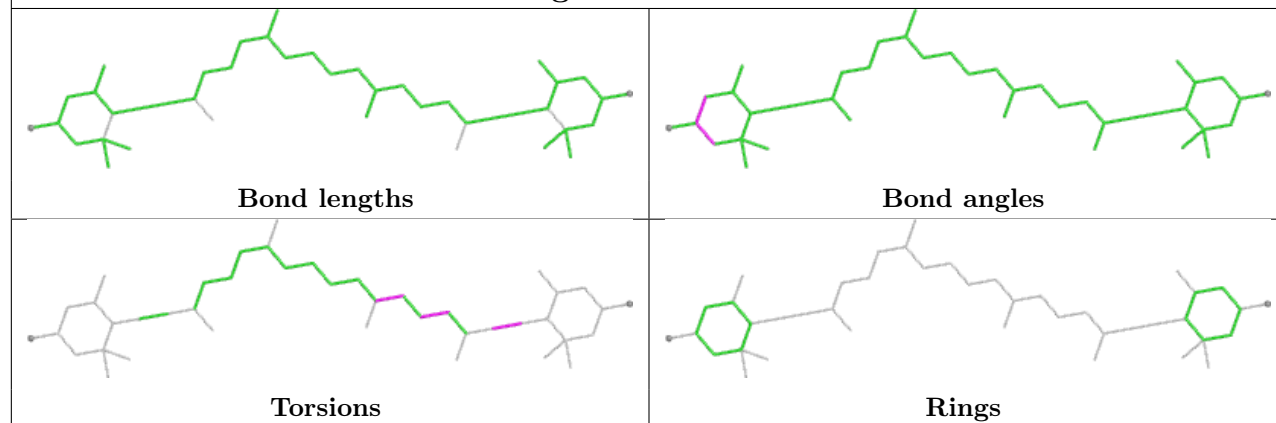
Ligand II0 g 318	
	
Bond lengths	Bond angles
	
Torsions	Rings



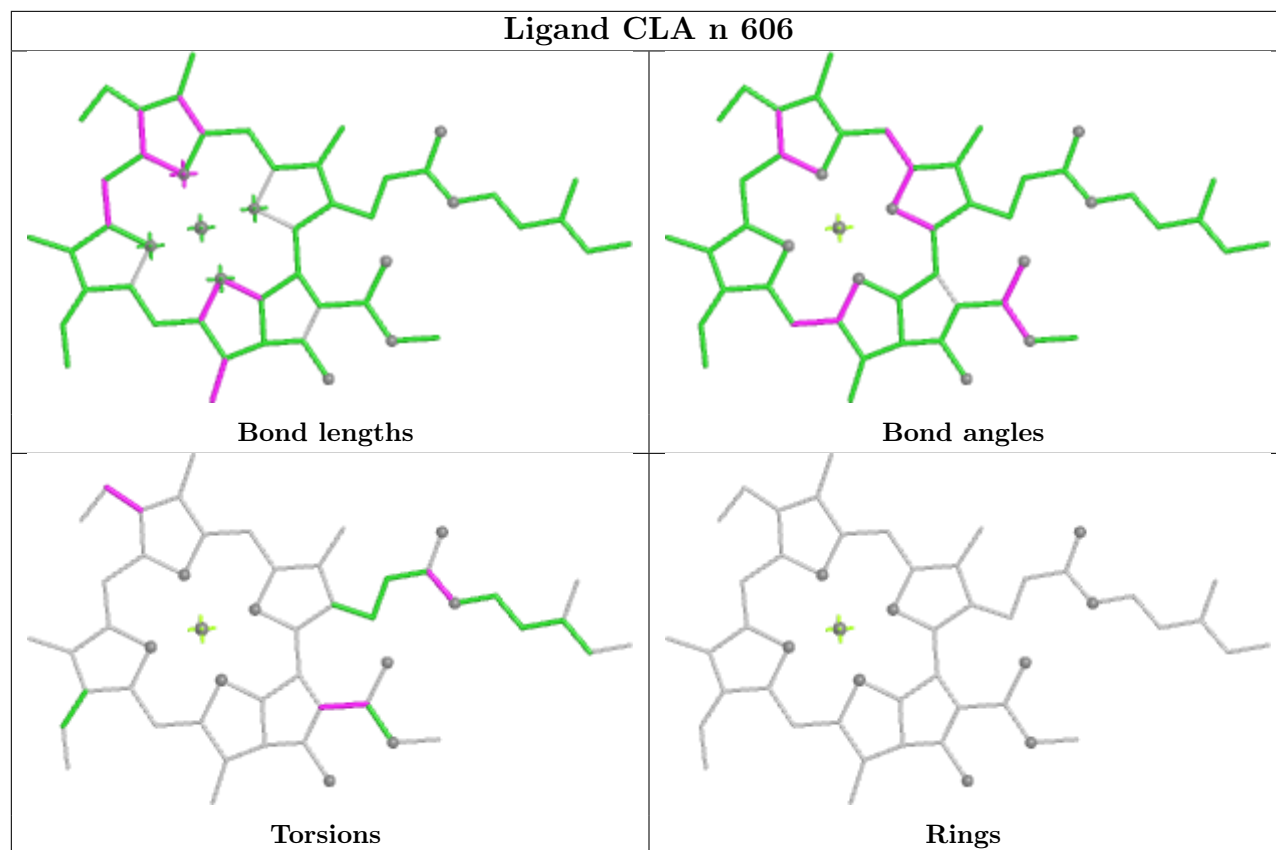
Ligand CLA k 610



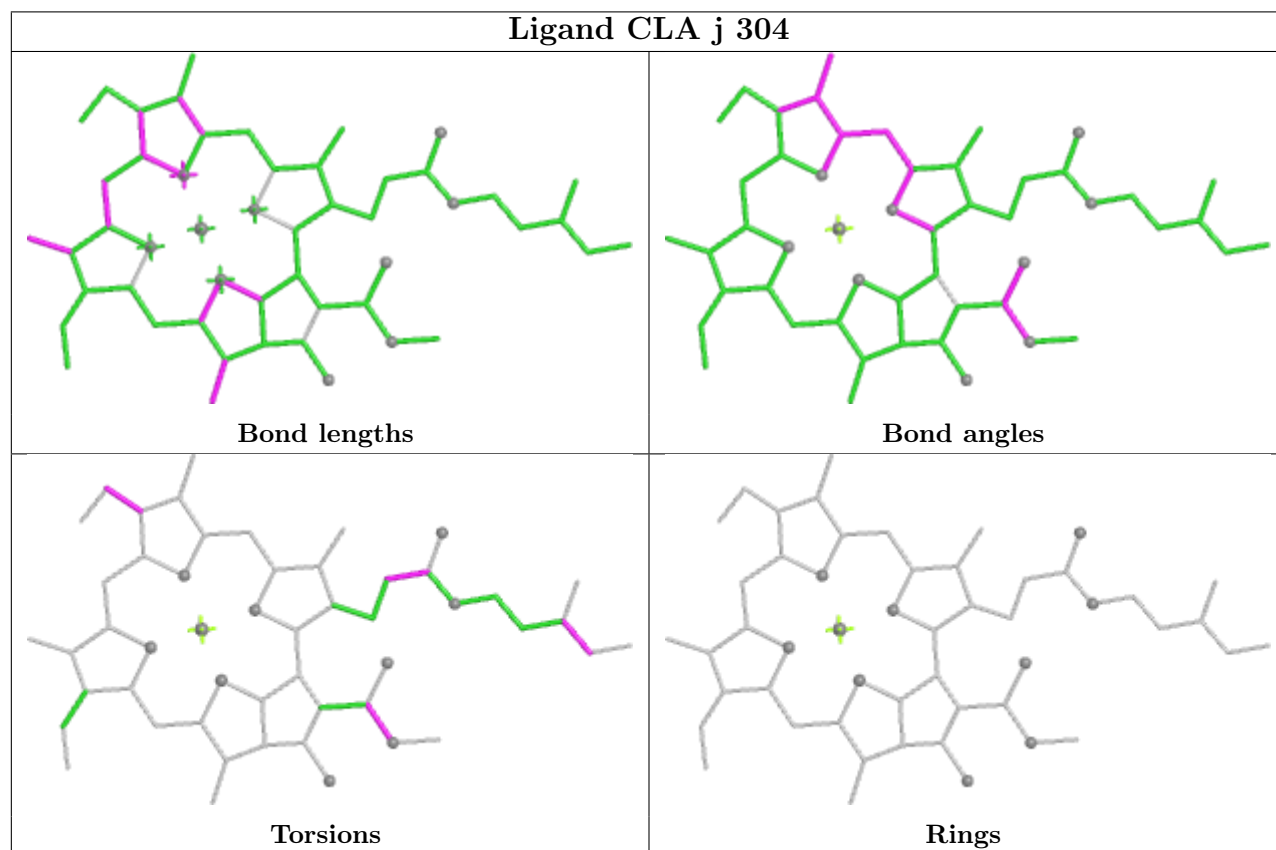
Ligand II0 c 314

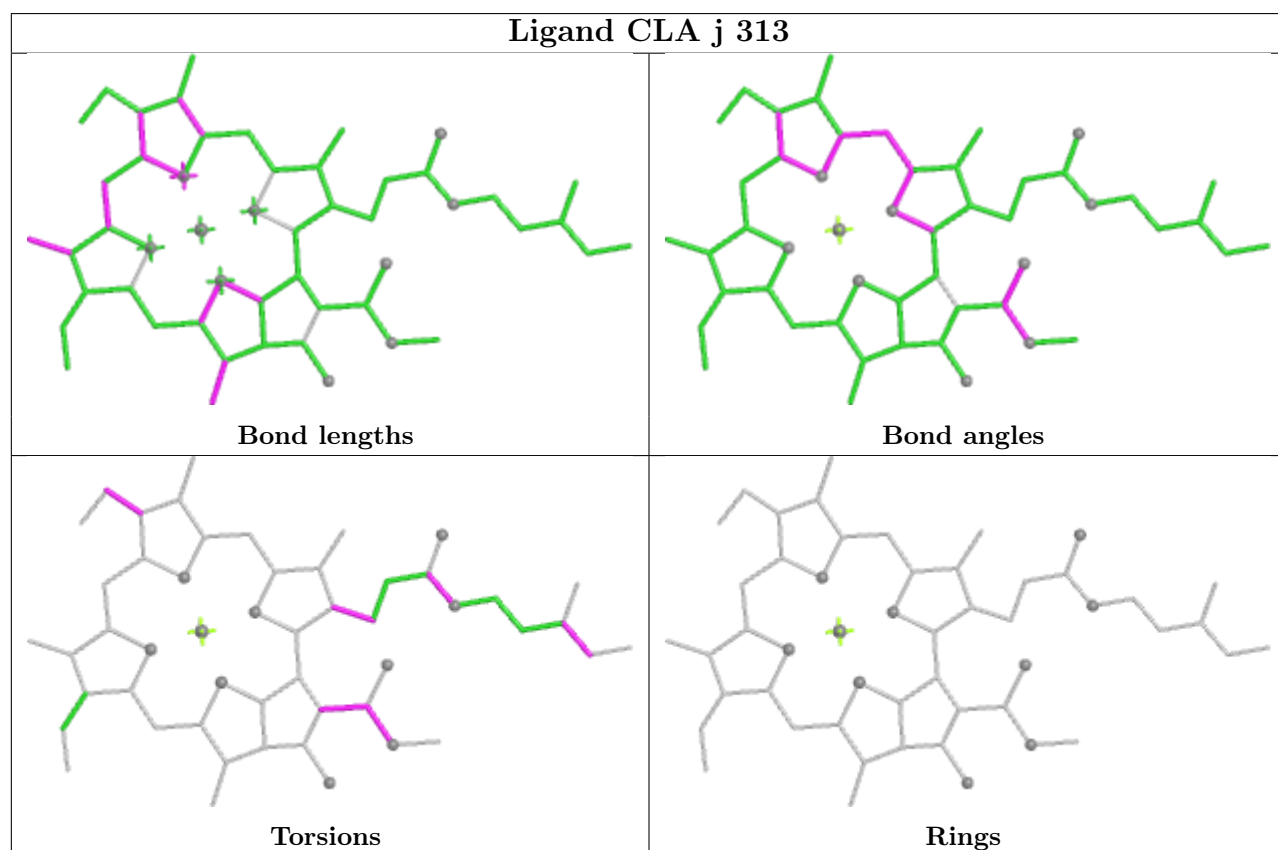
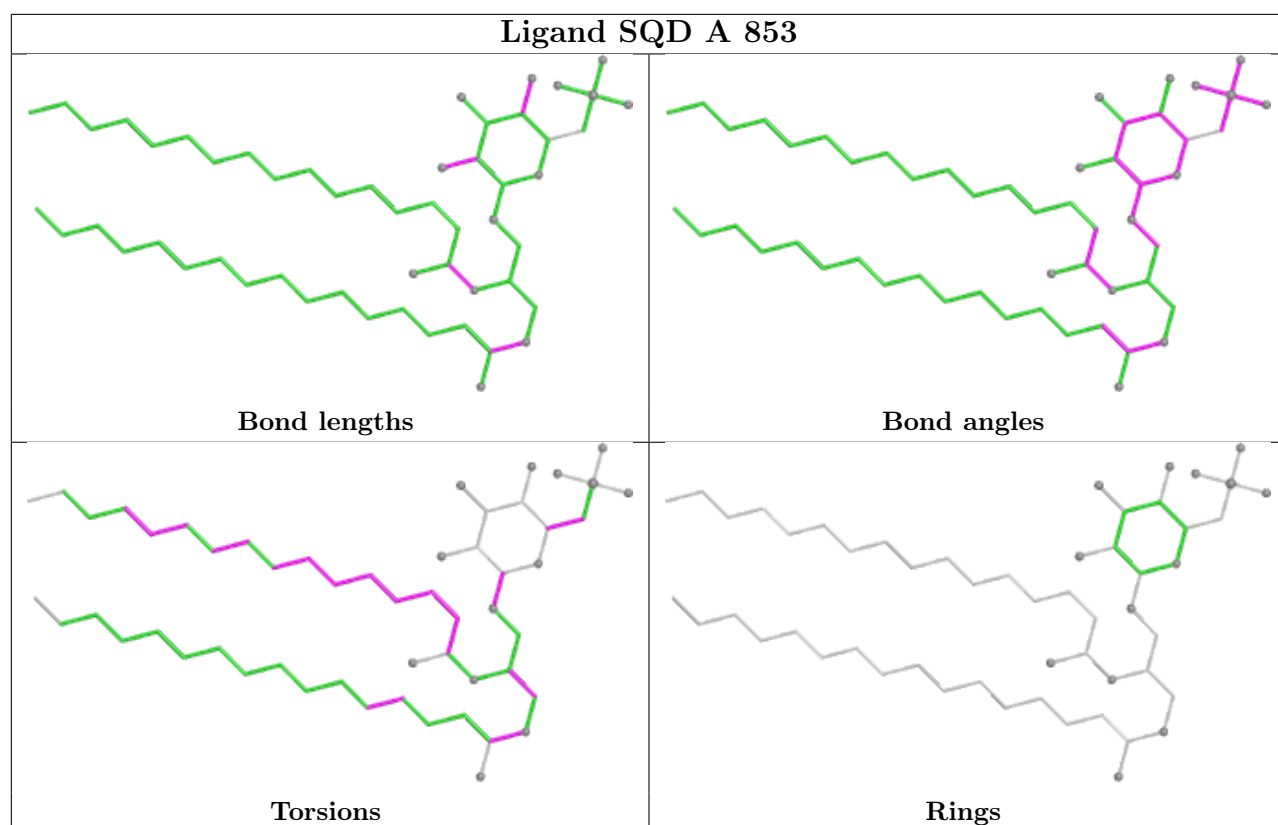


Ligand CLA n 606

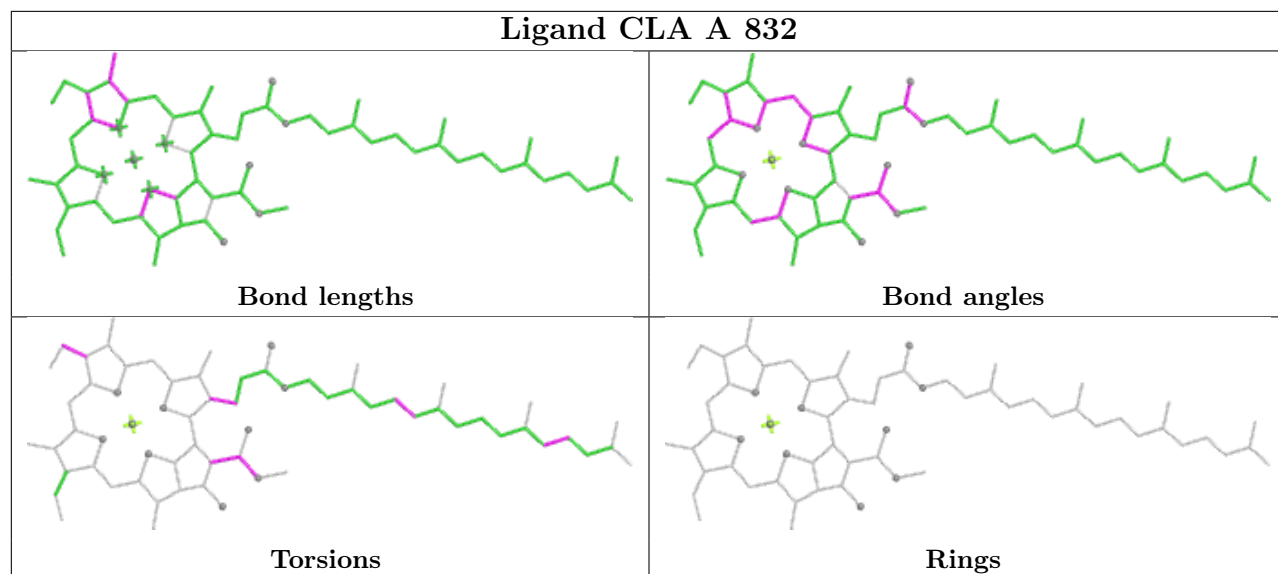


Ligand CLA j 304

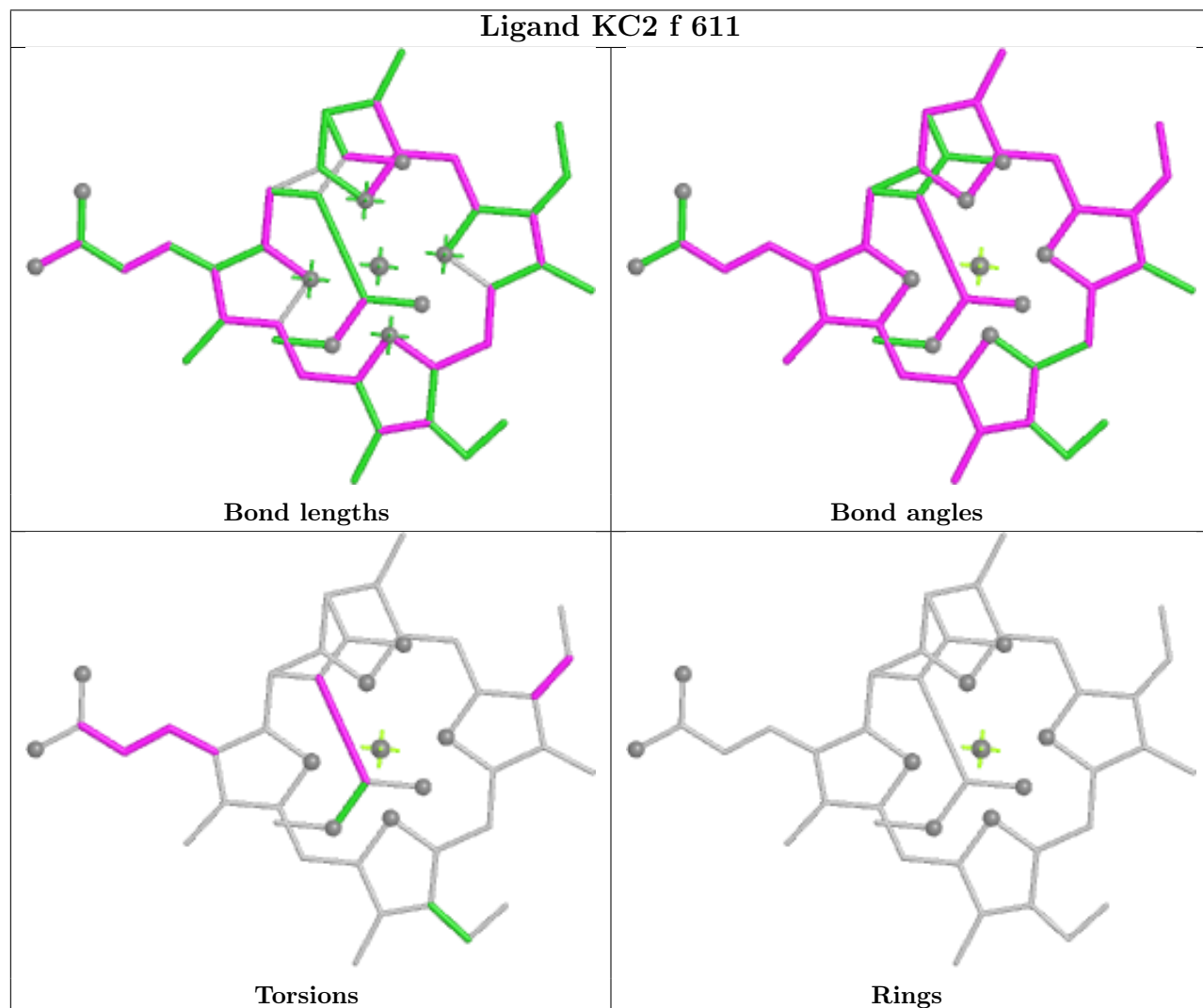


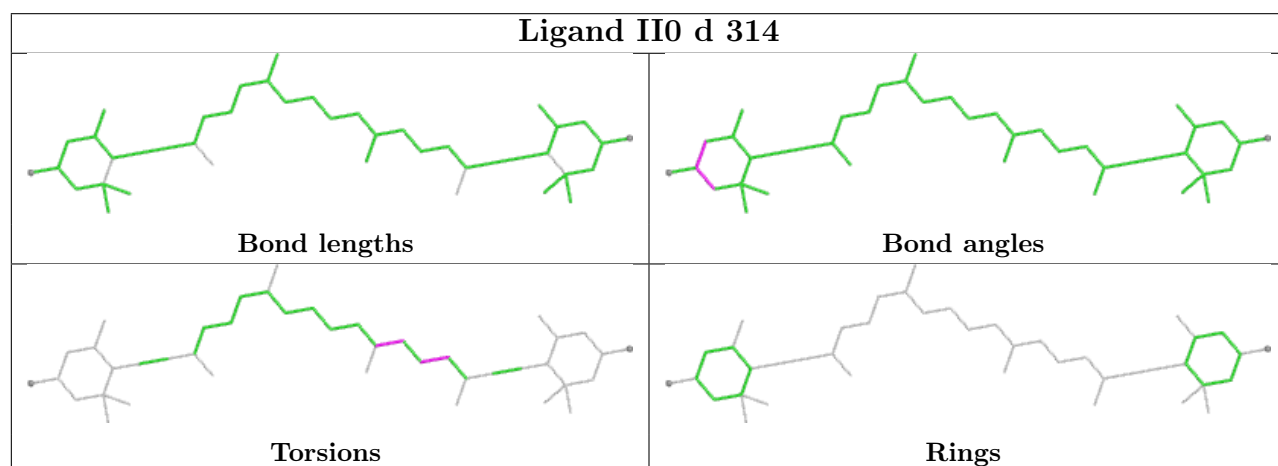
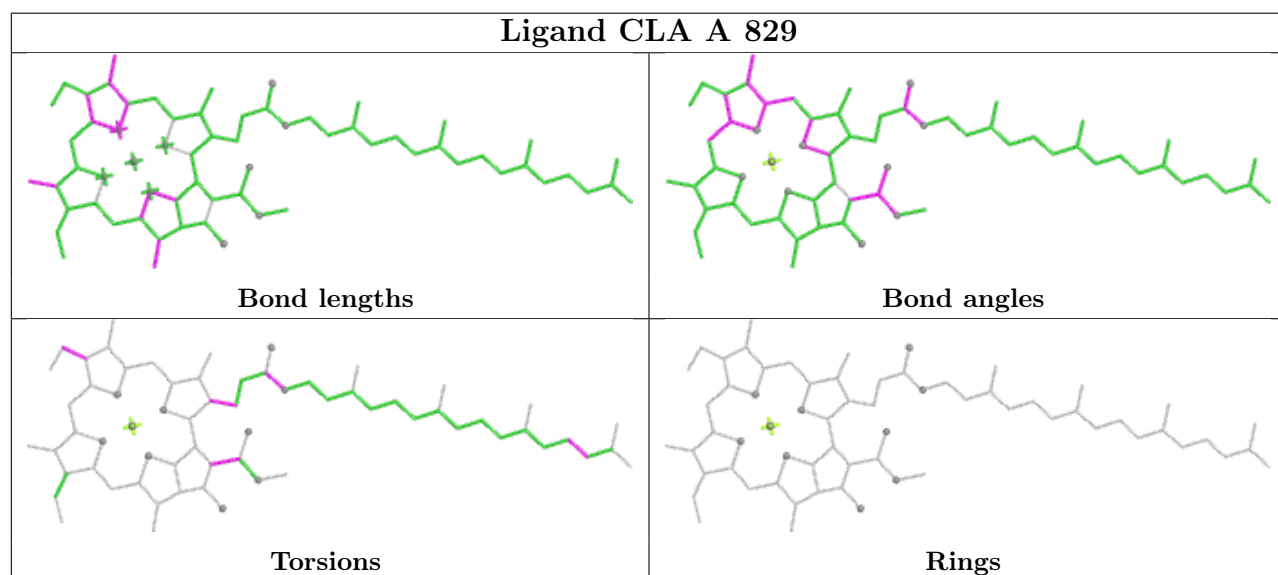
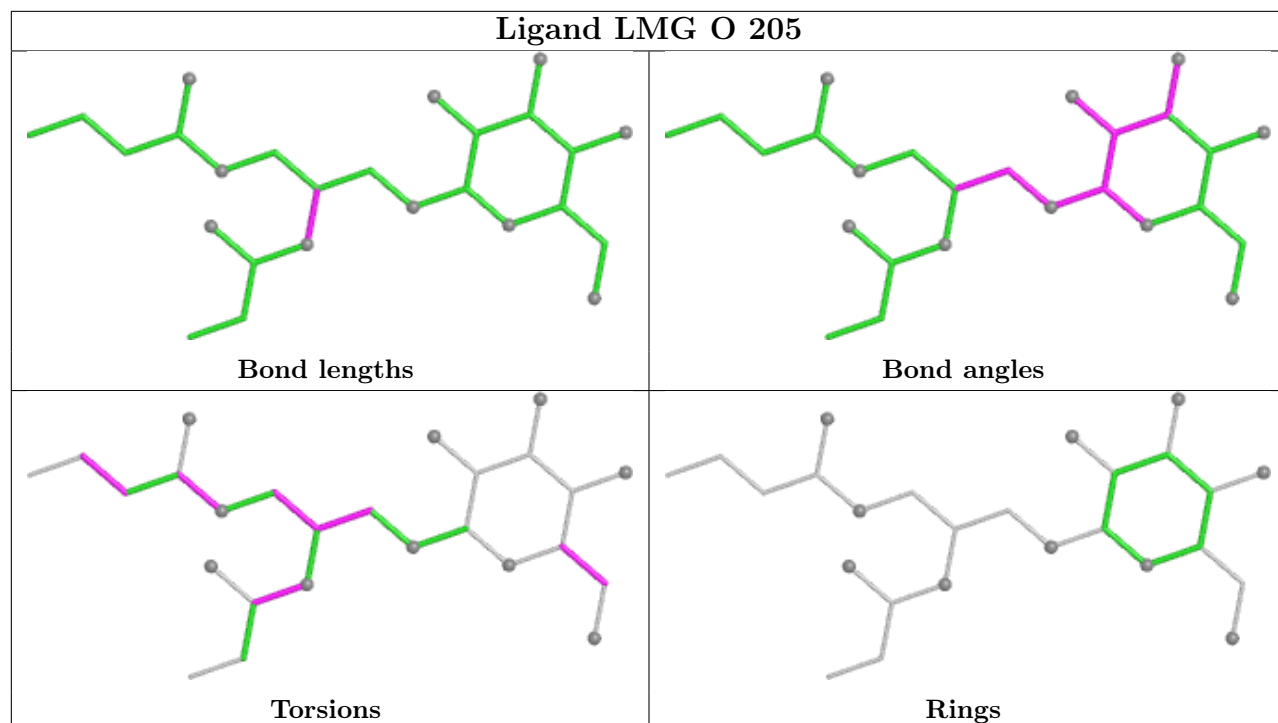


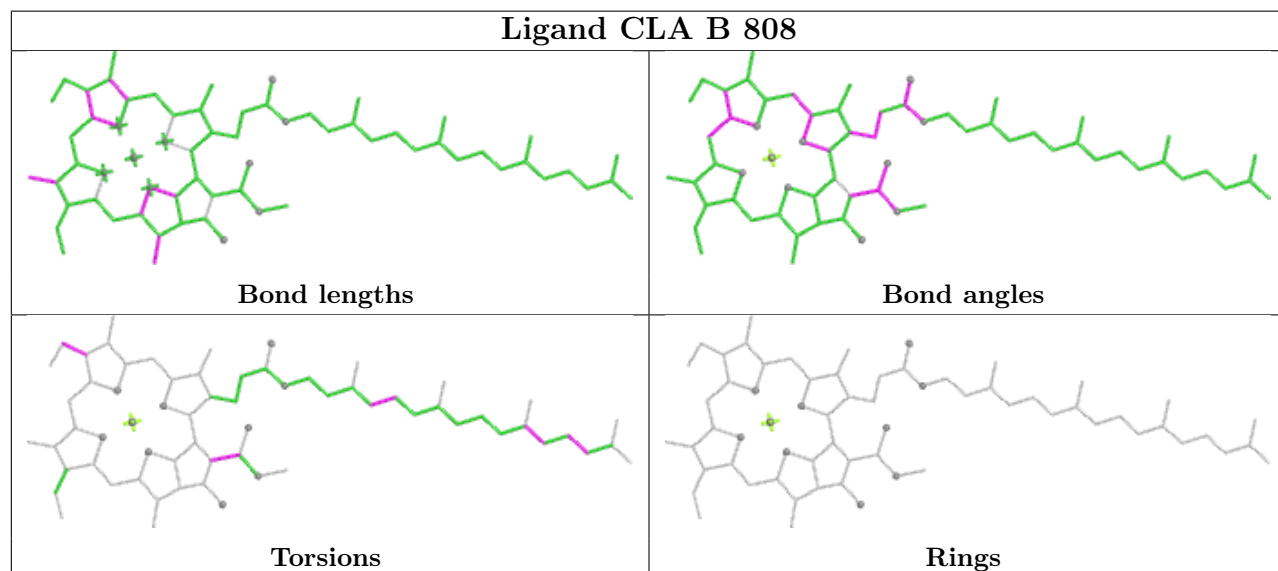
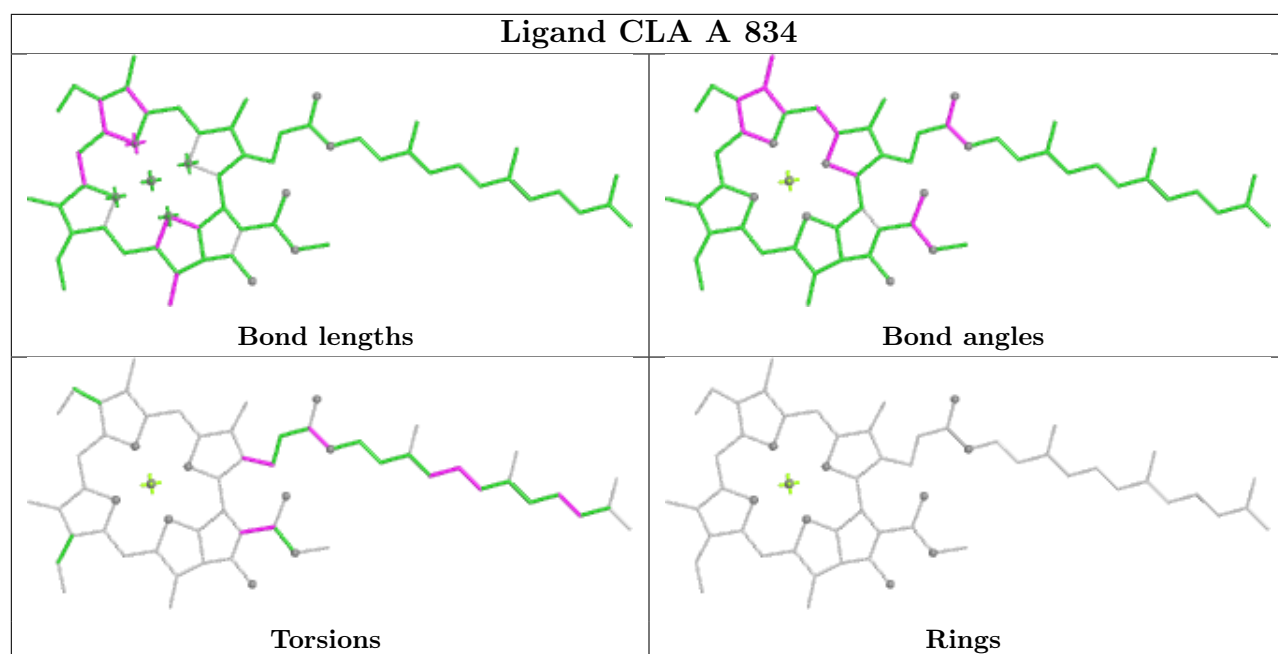
Ligand CLA A 832

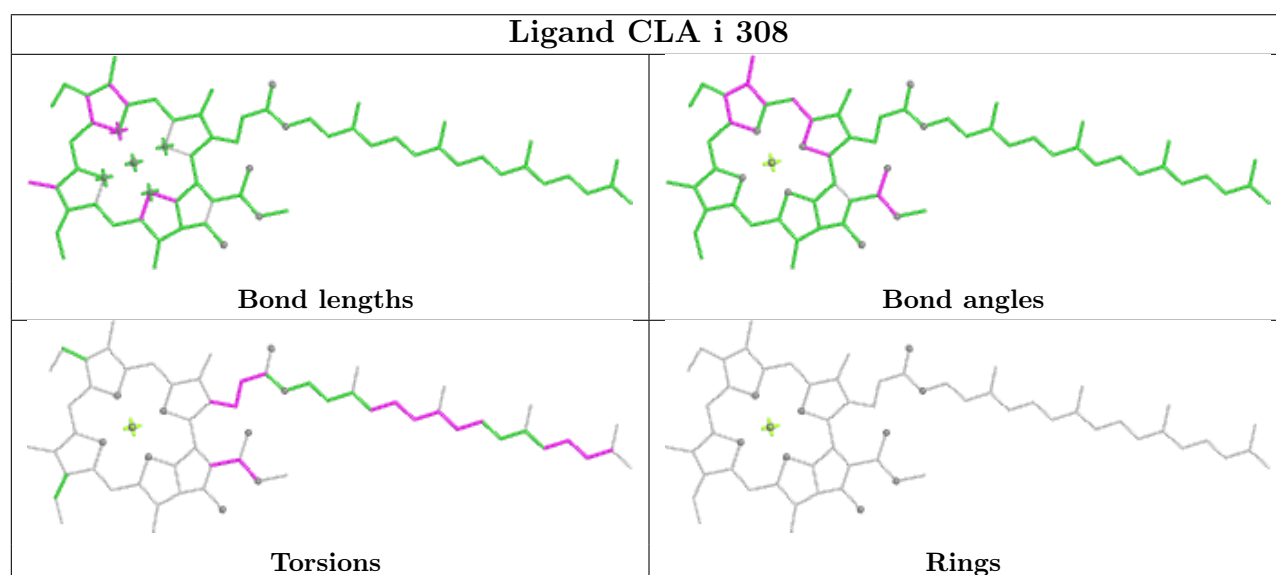
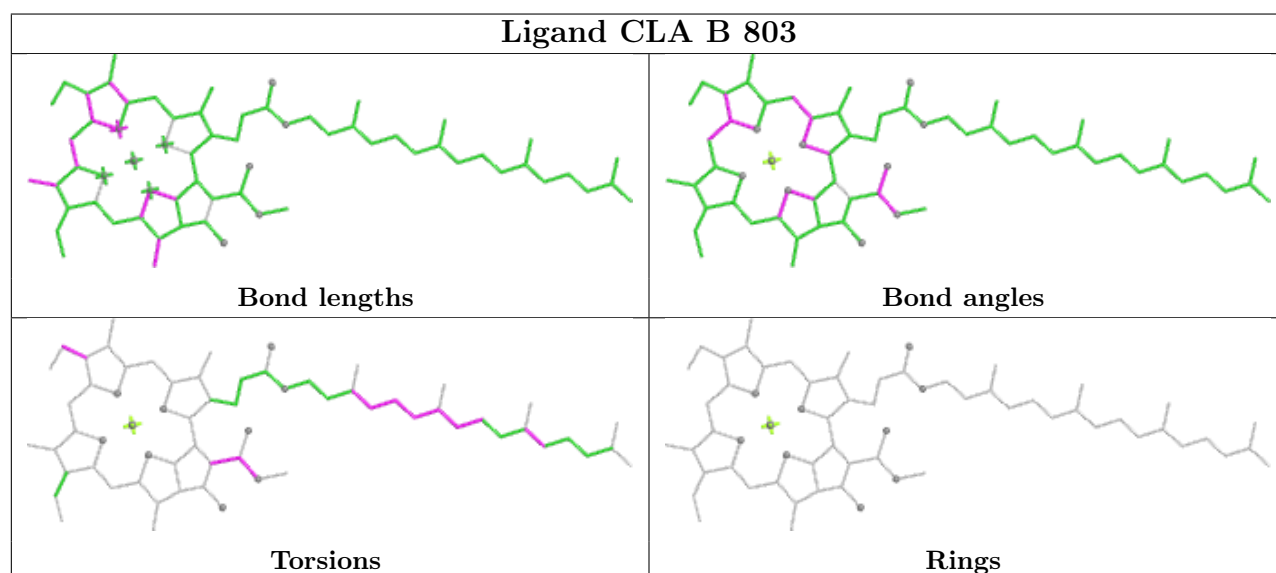
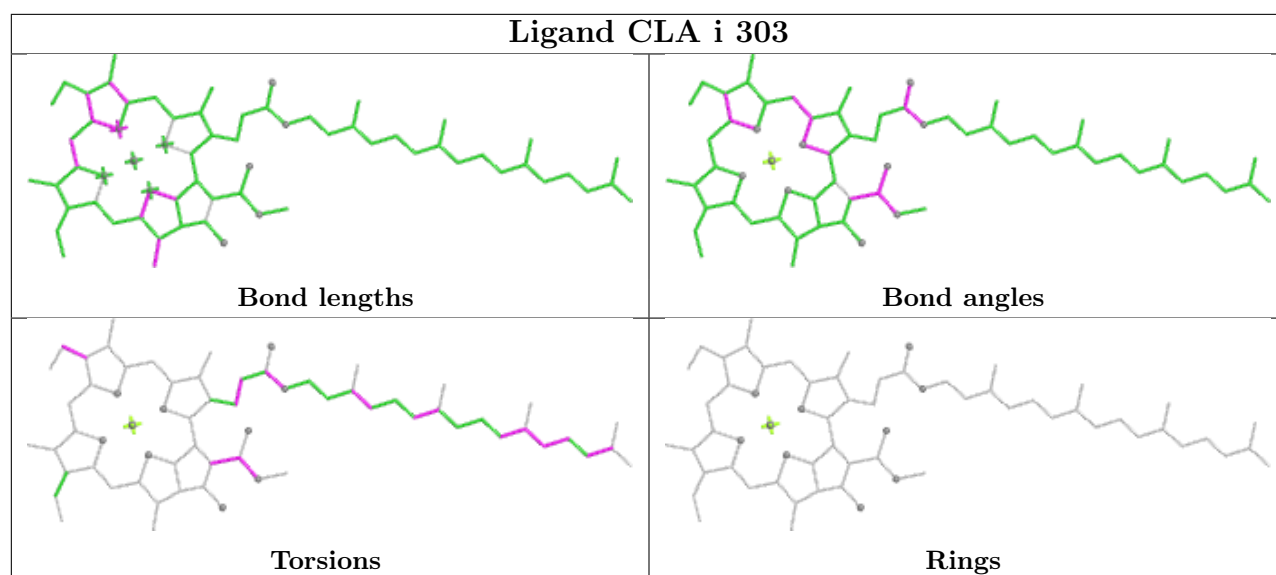


Ligand KC2 f 611

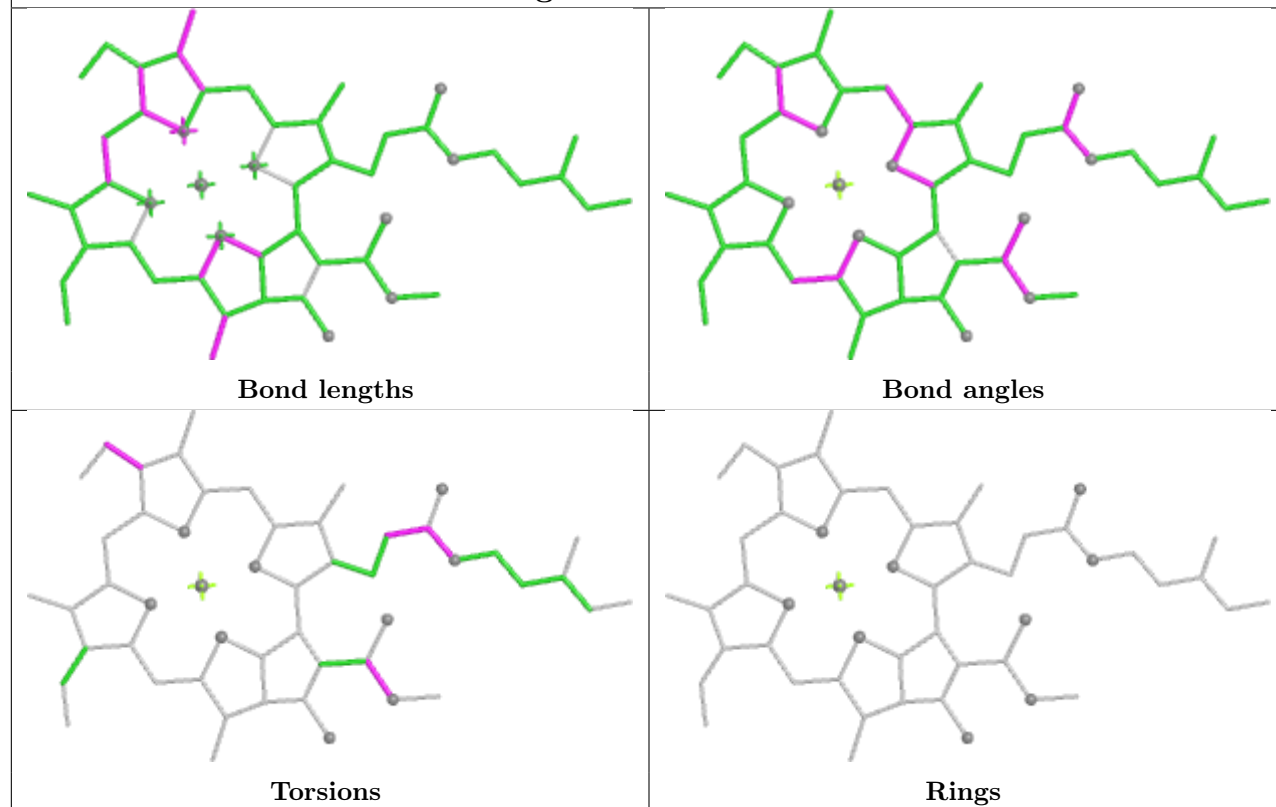




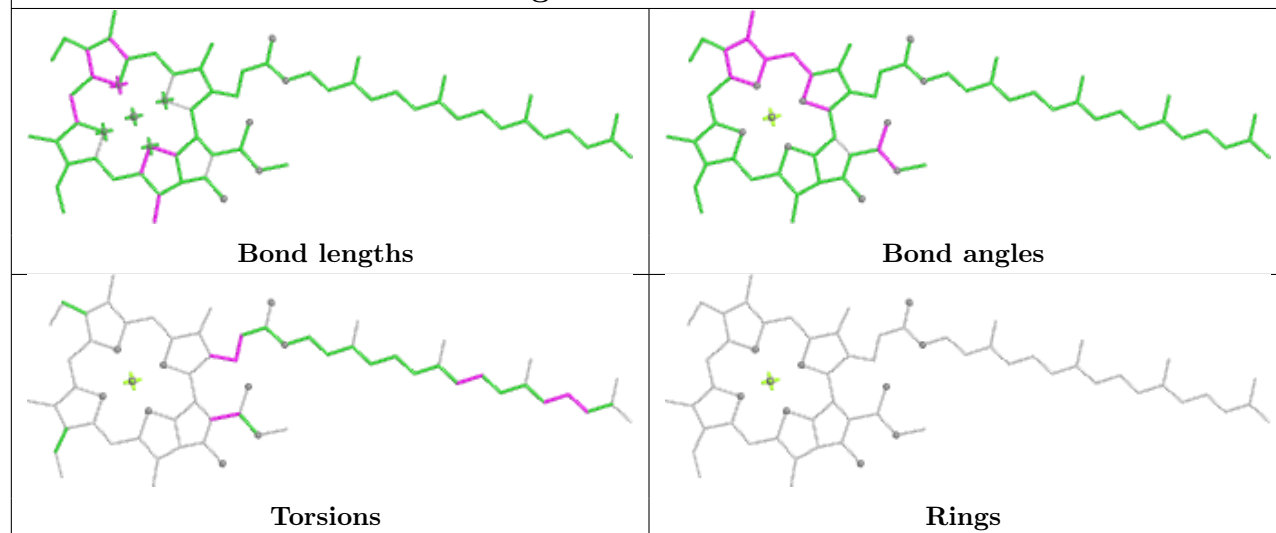


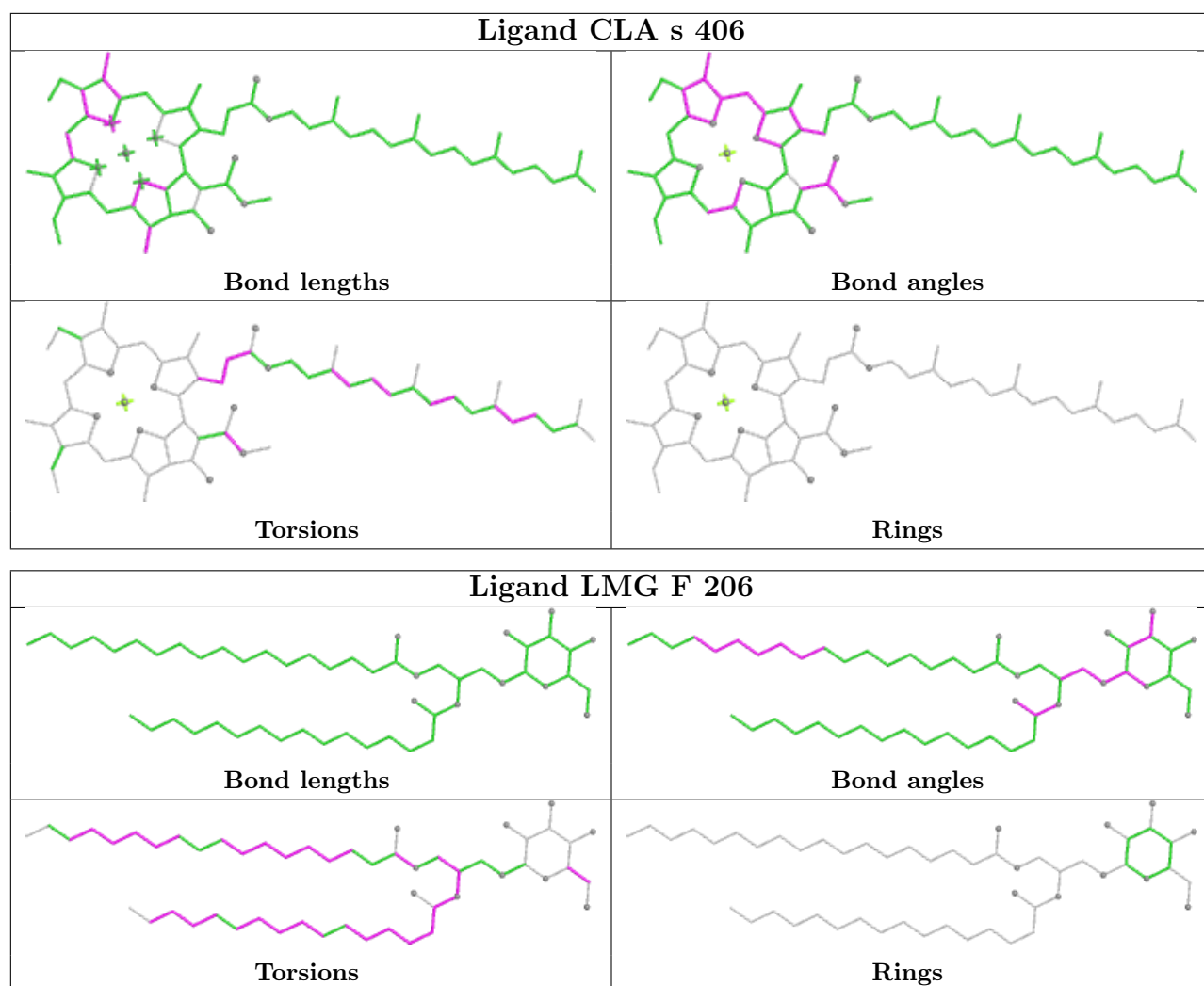


Ligand CLA k 606

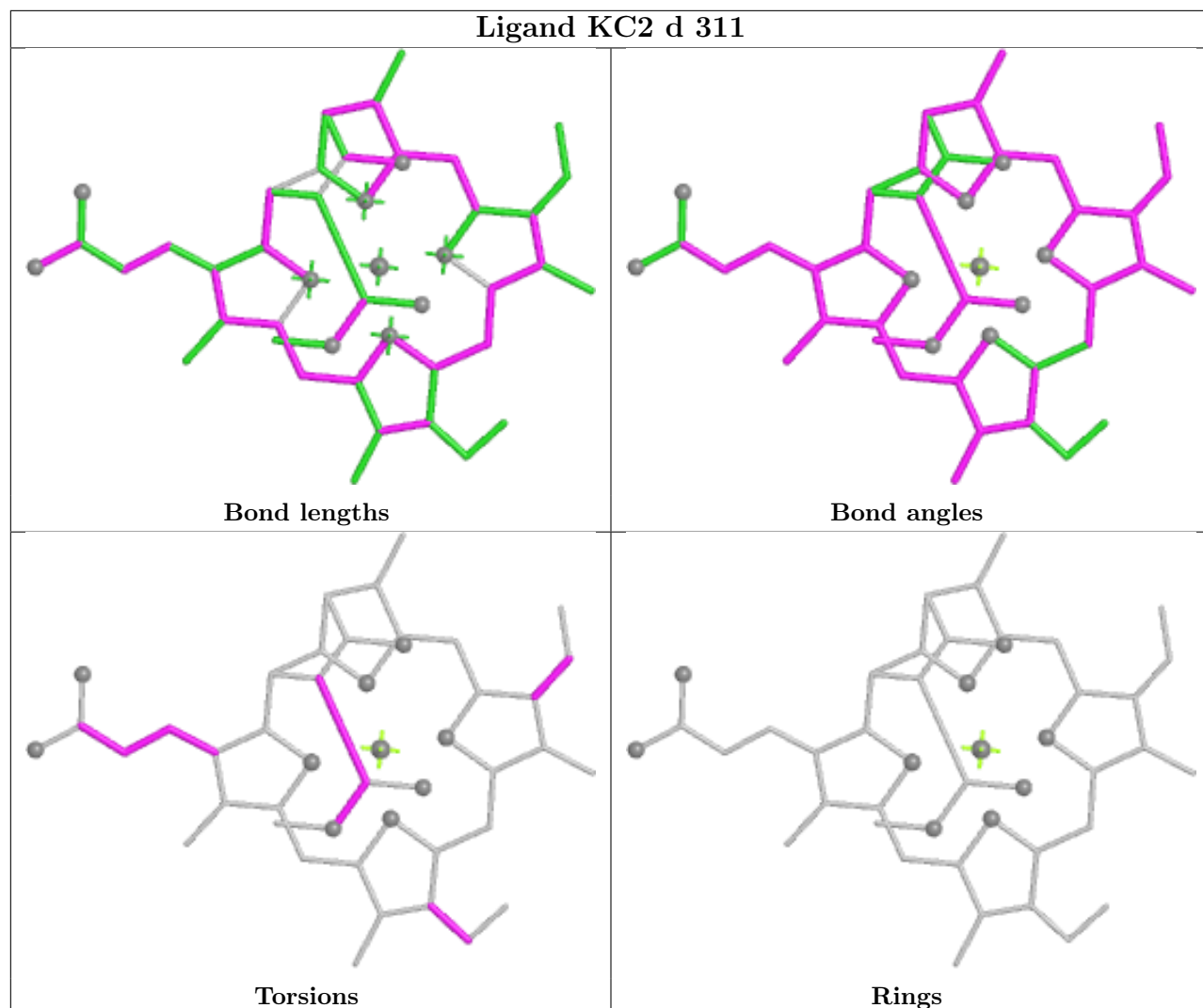


Ligand CLA A 807

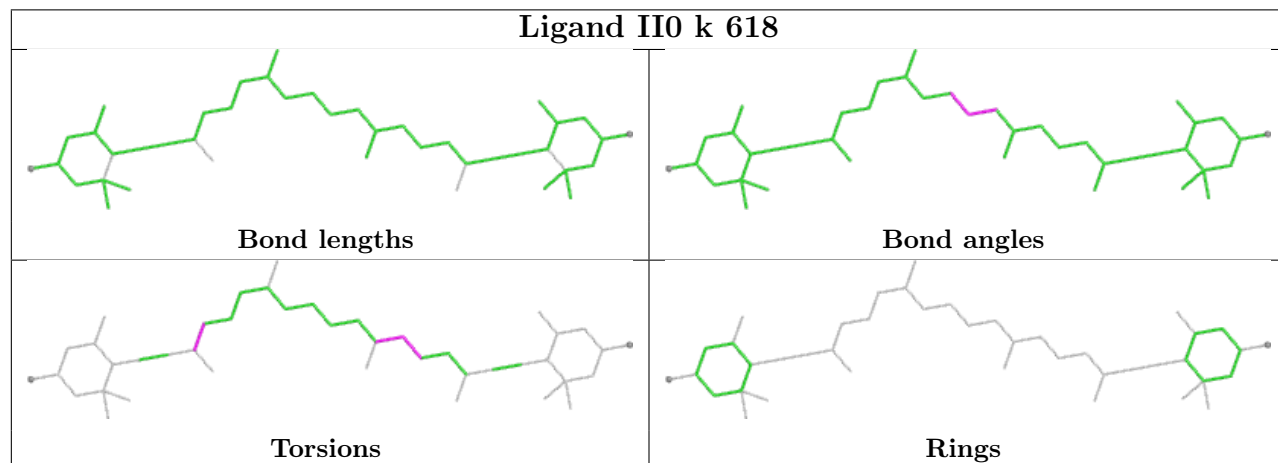




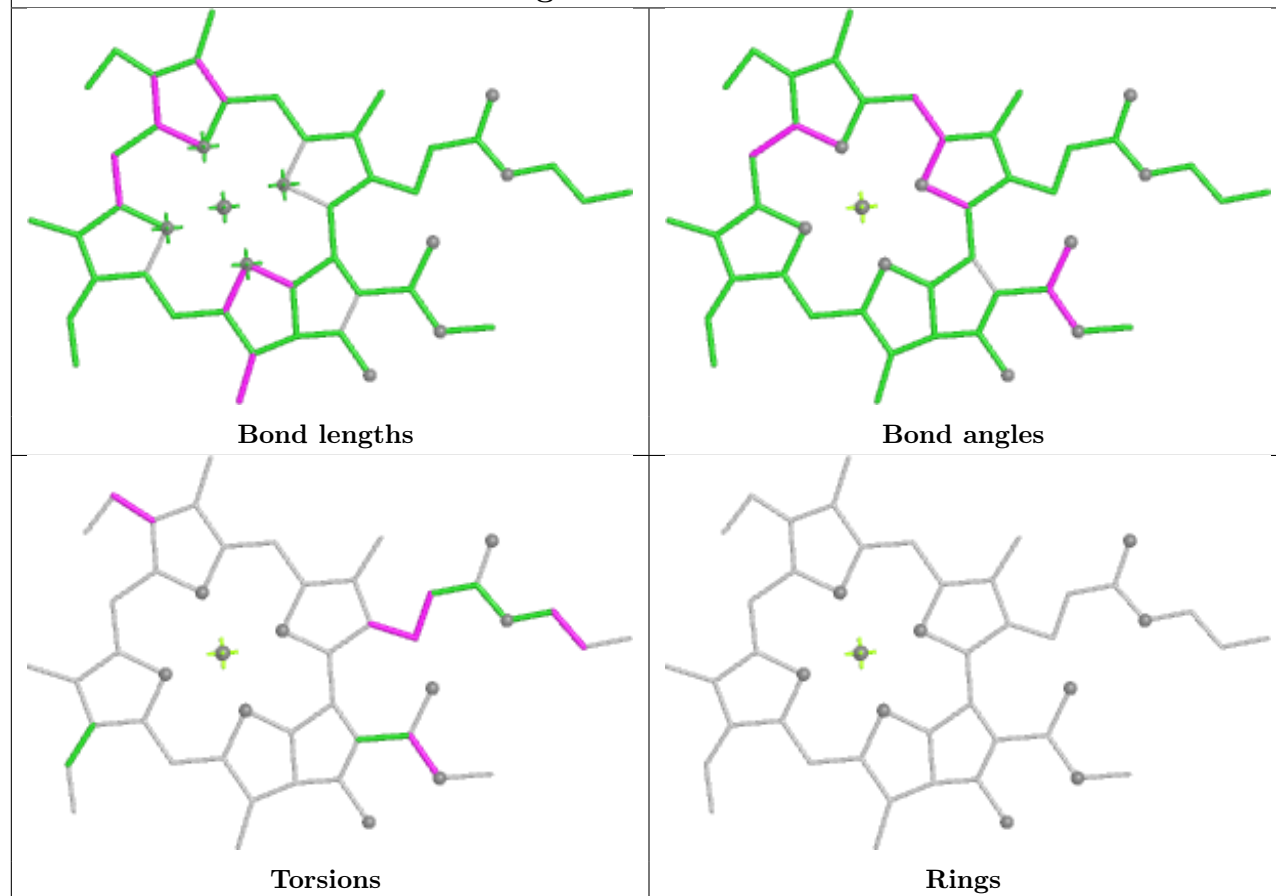
Ligand KC2 d 311



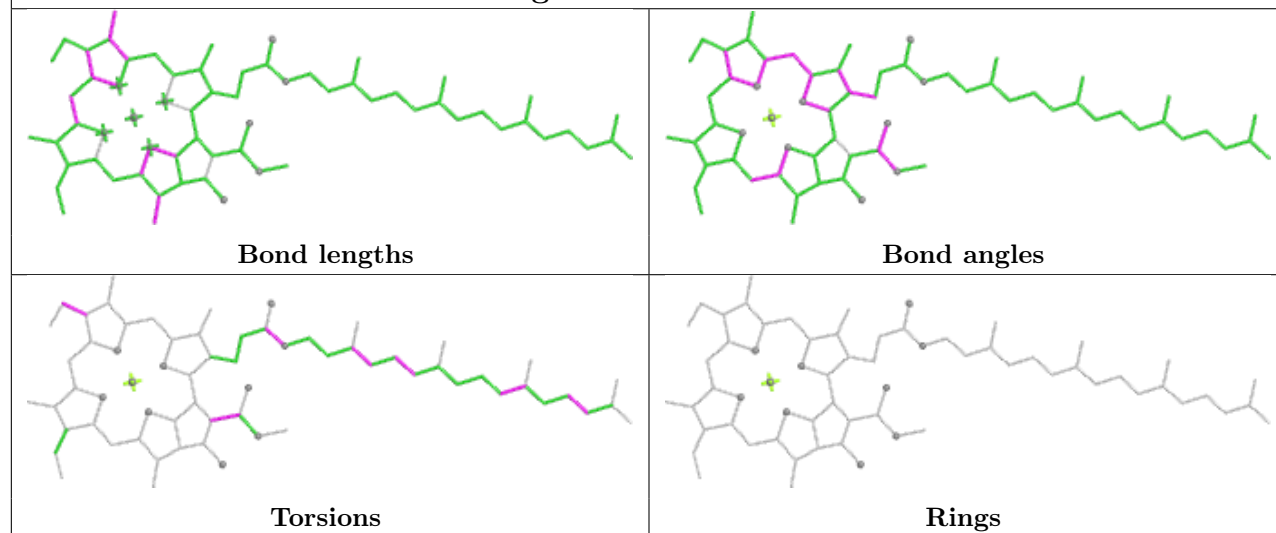
Ligand II0 k 618

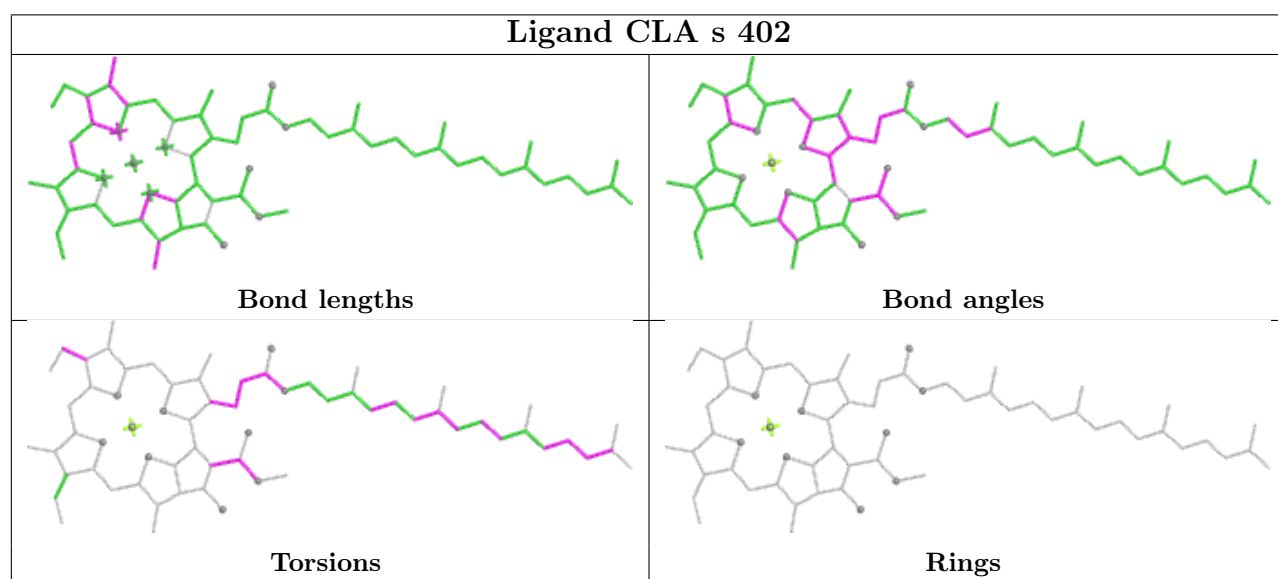
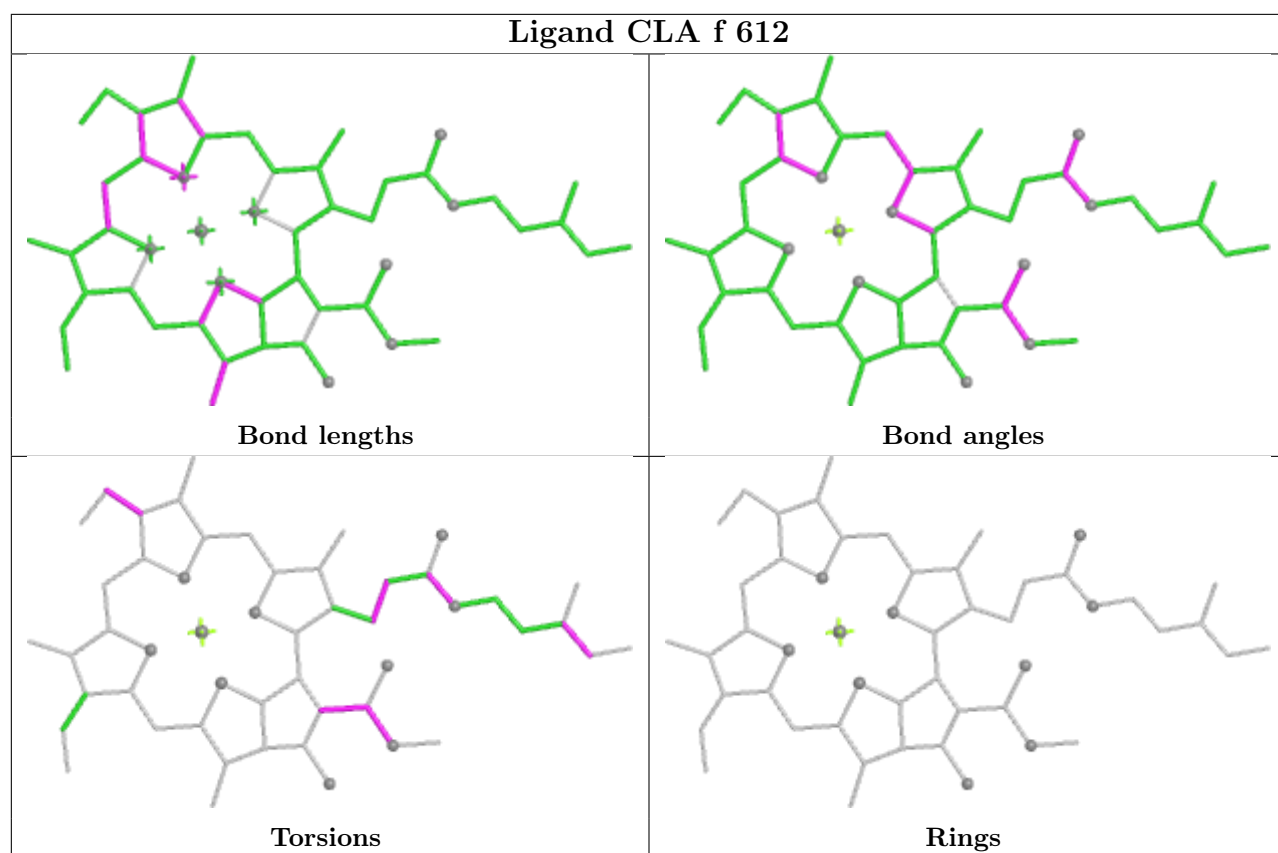


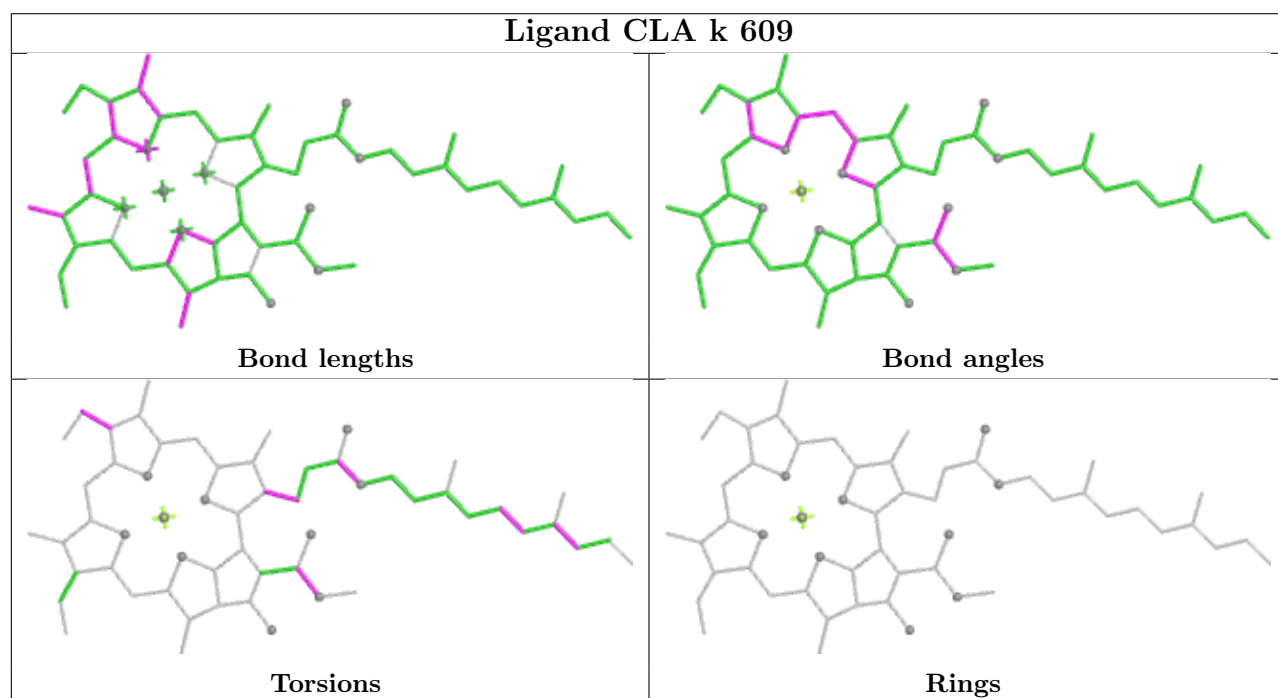
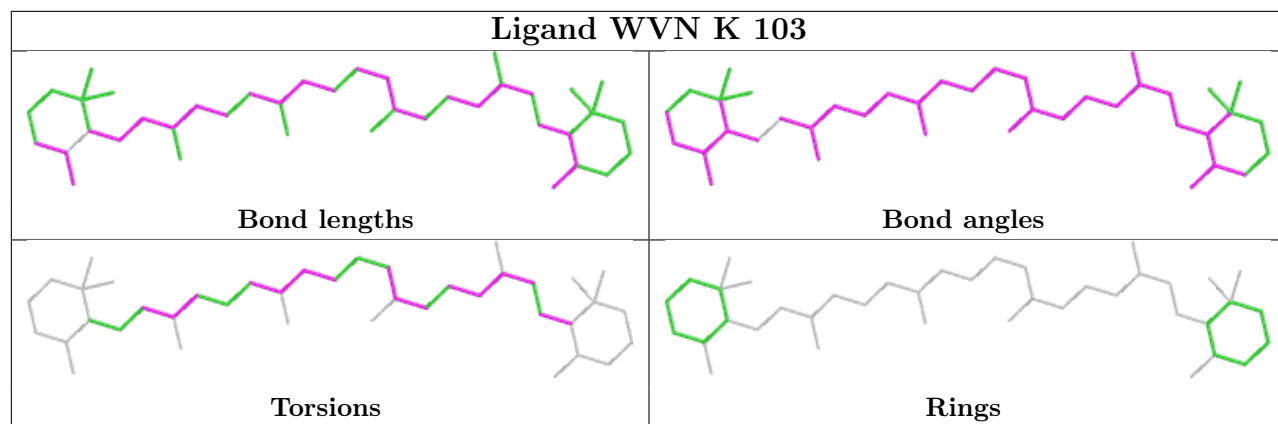
Ligand CLA a 312

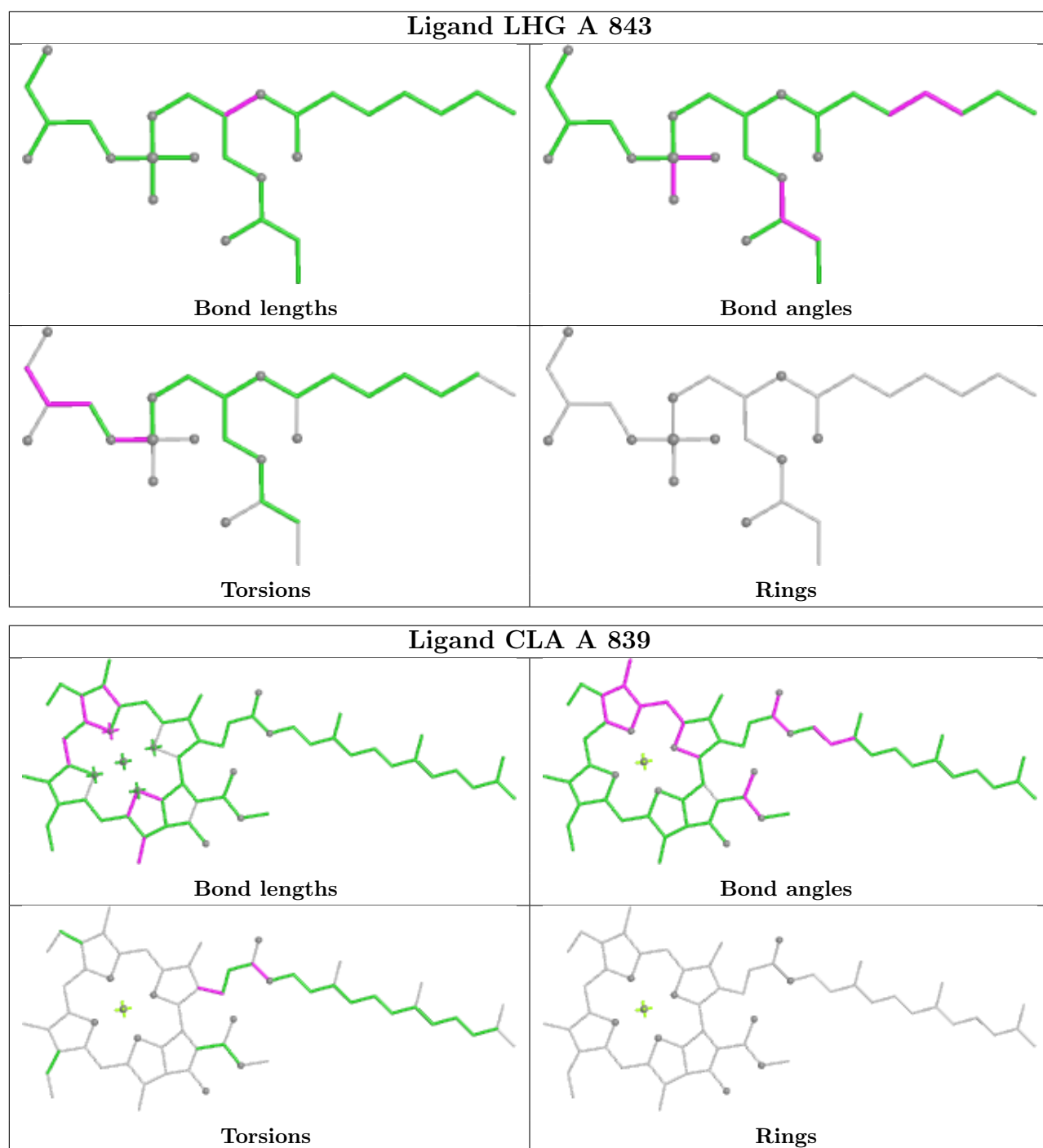


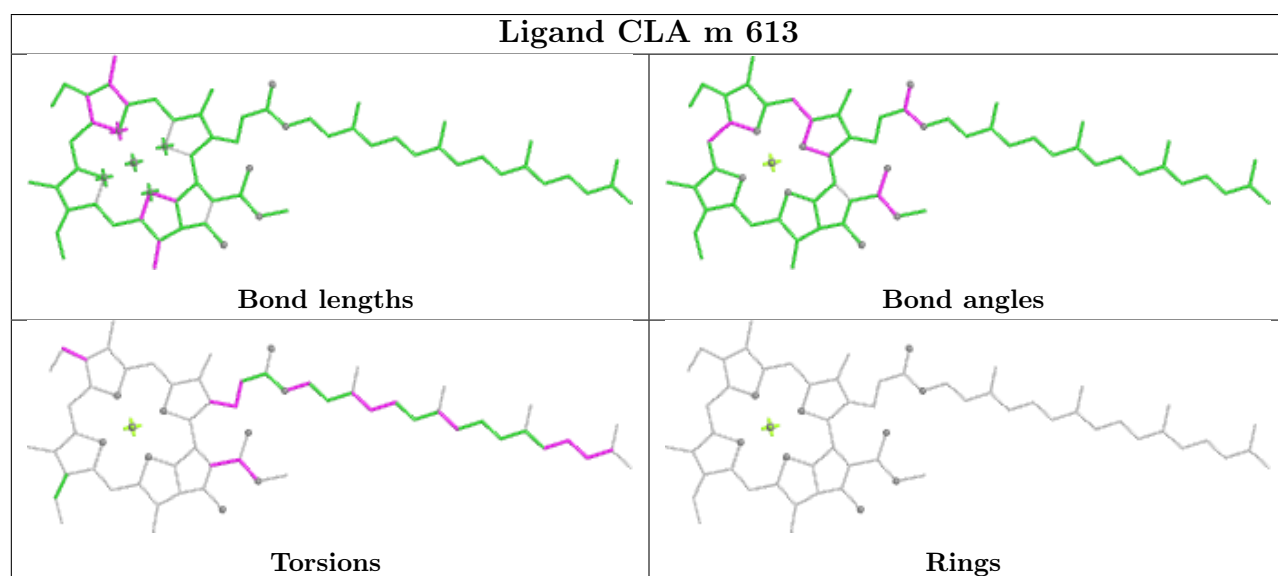
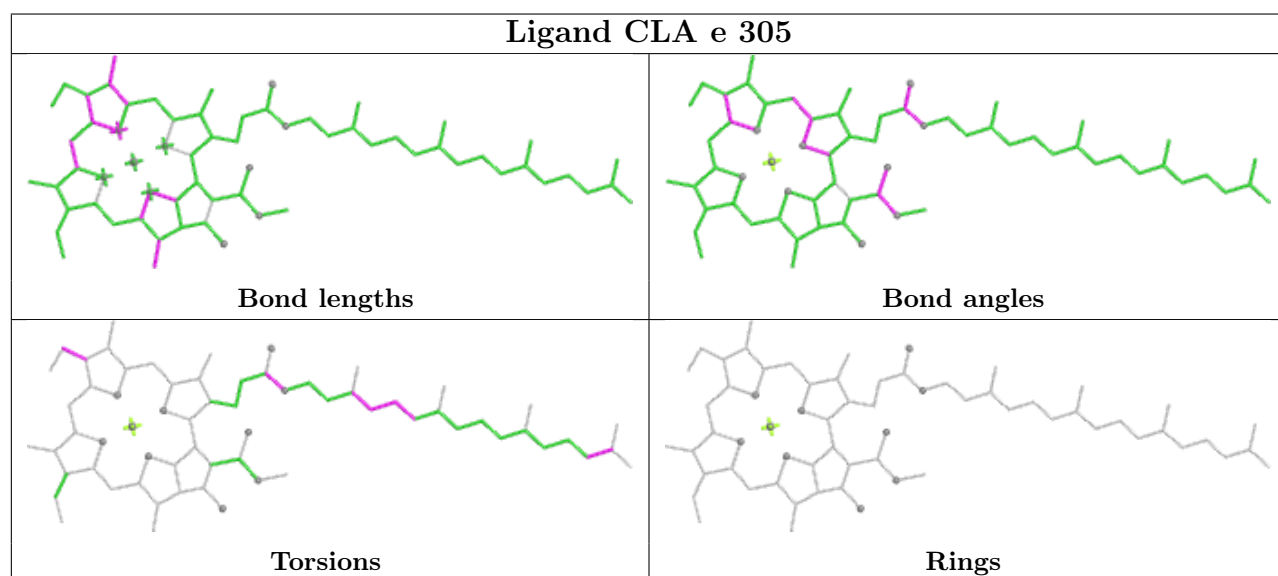
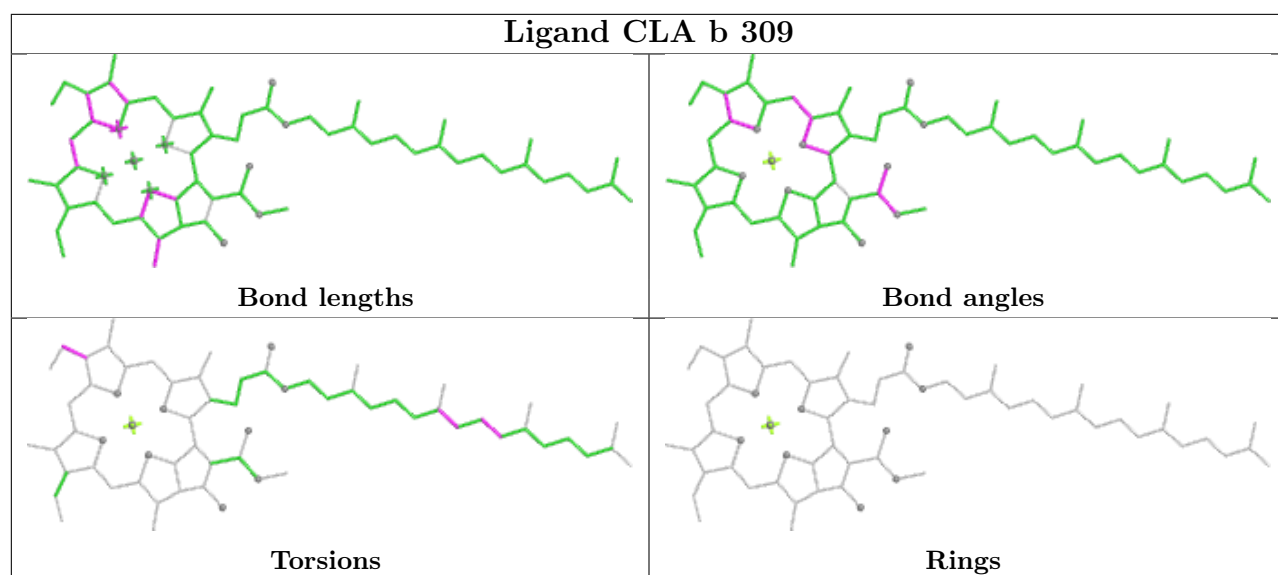
Ligand CLA A 838

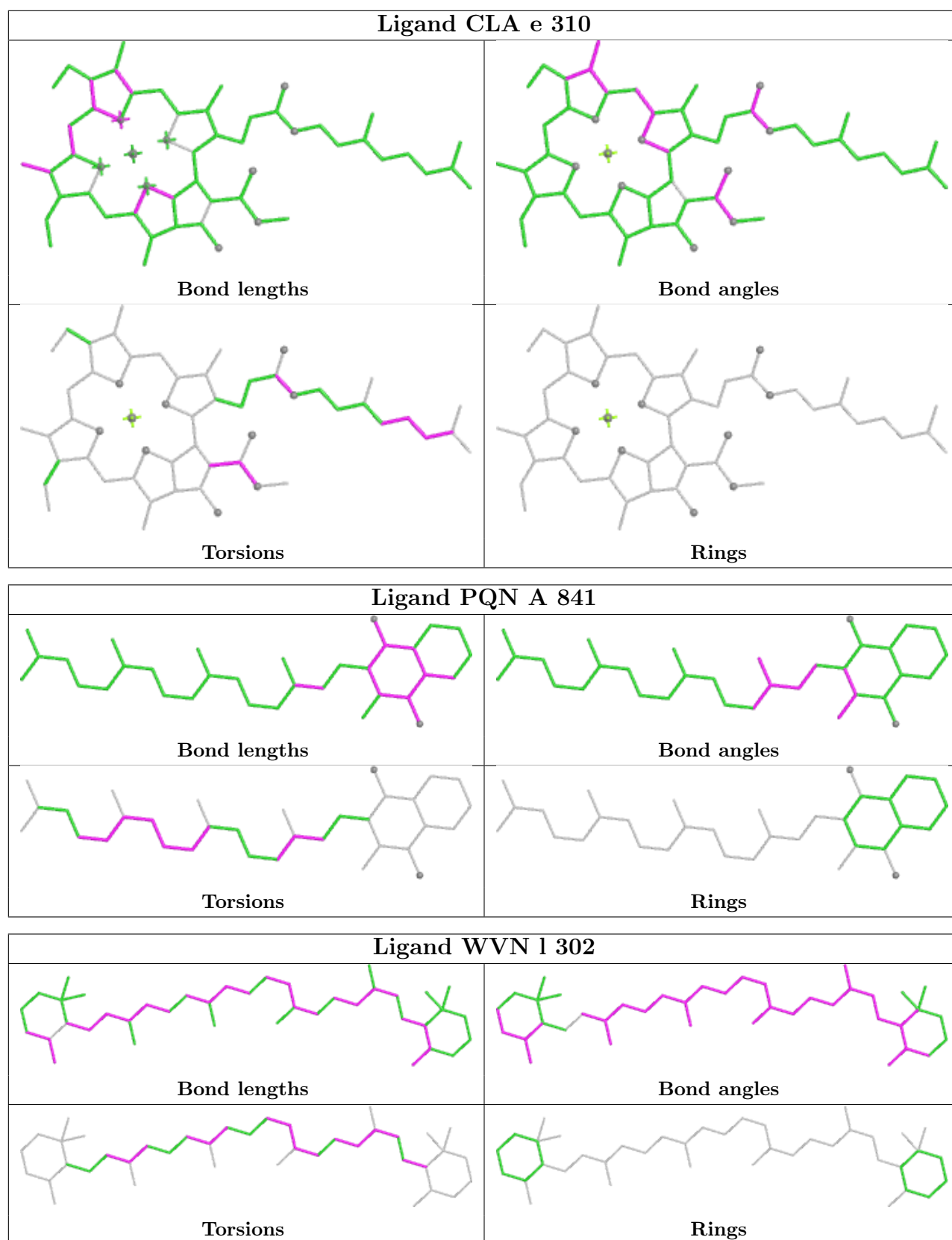


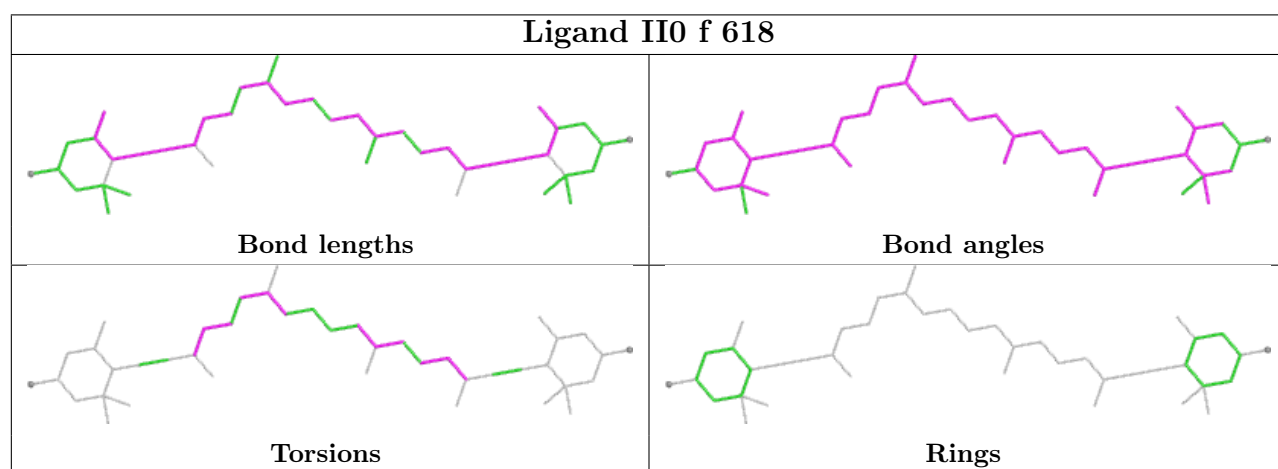
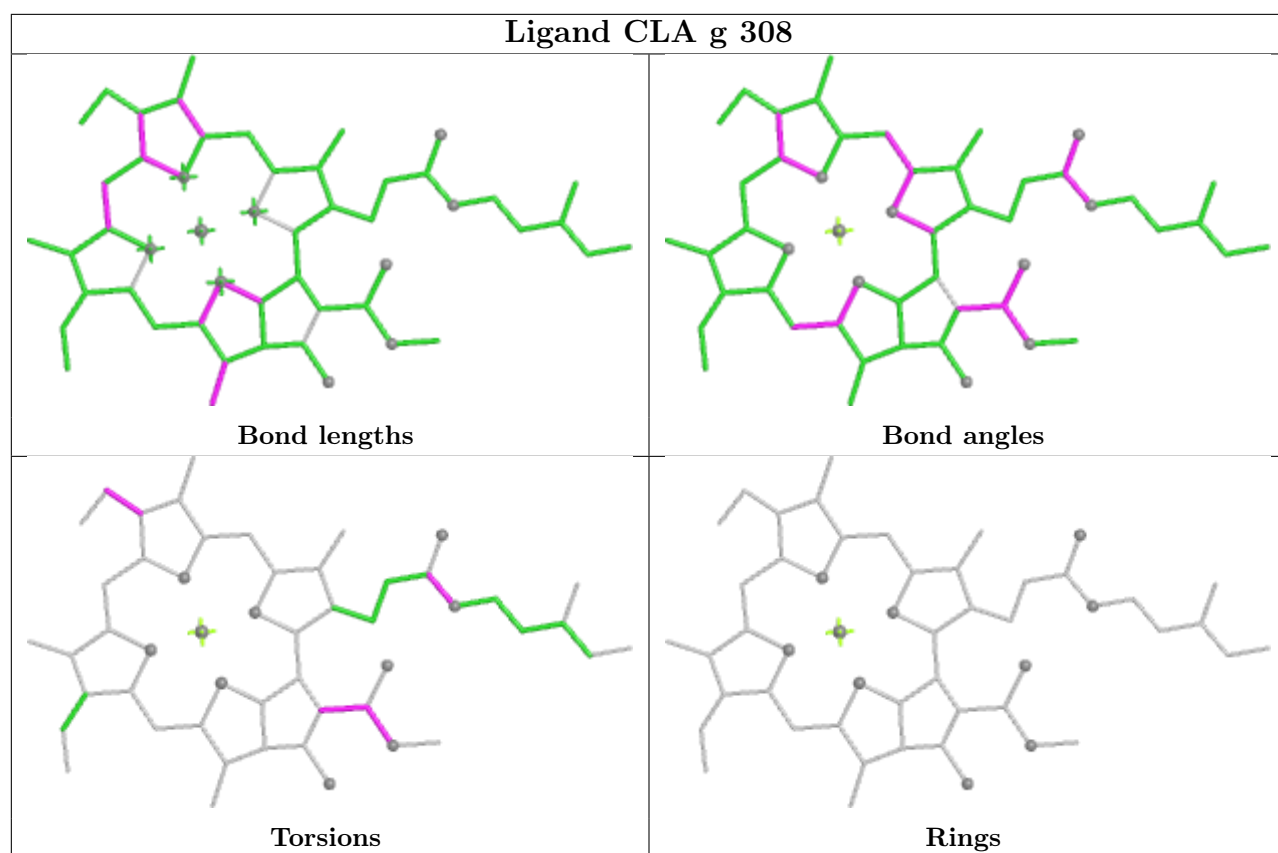




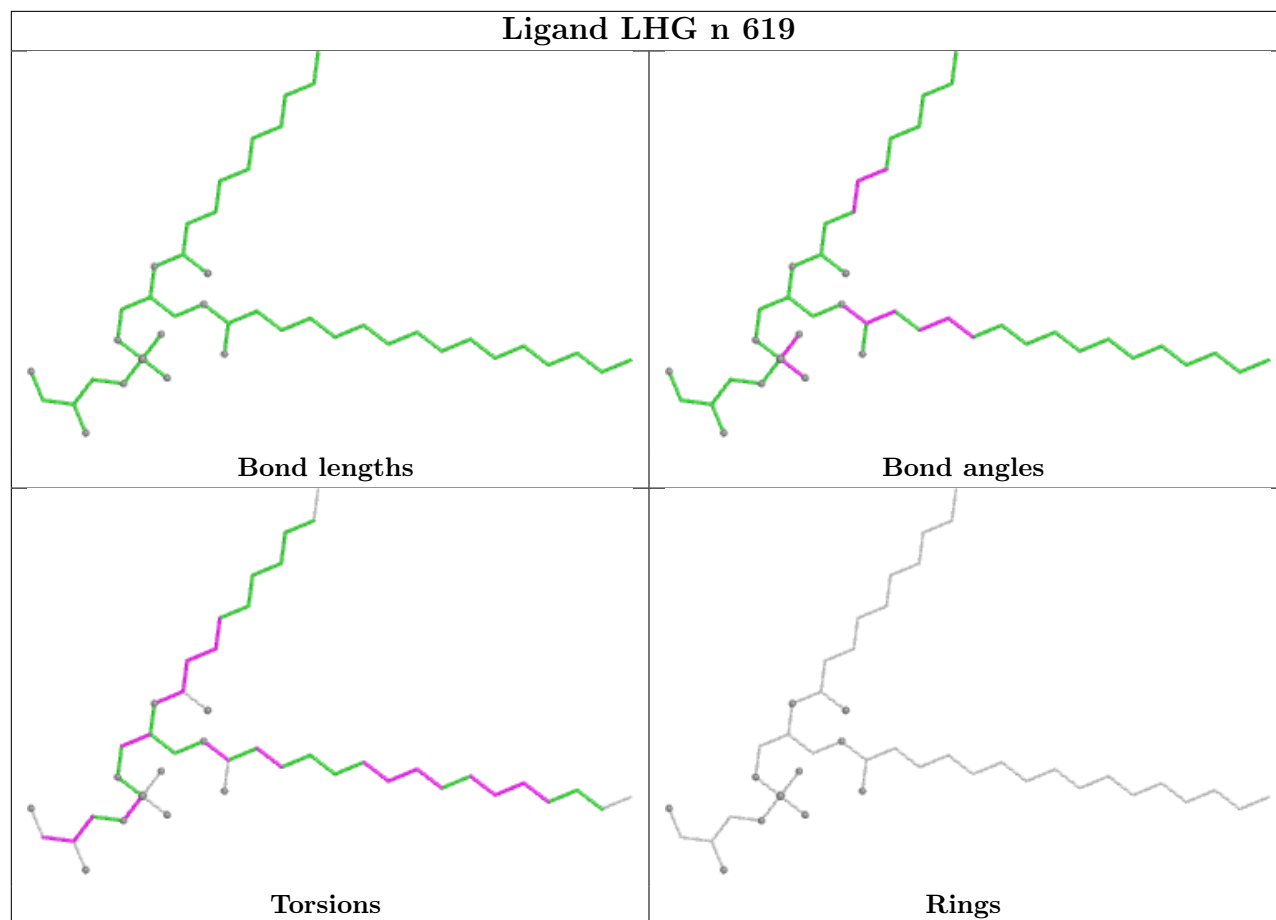




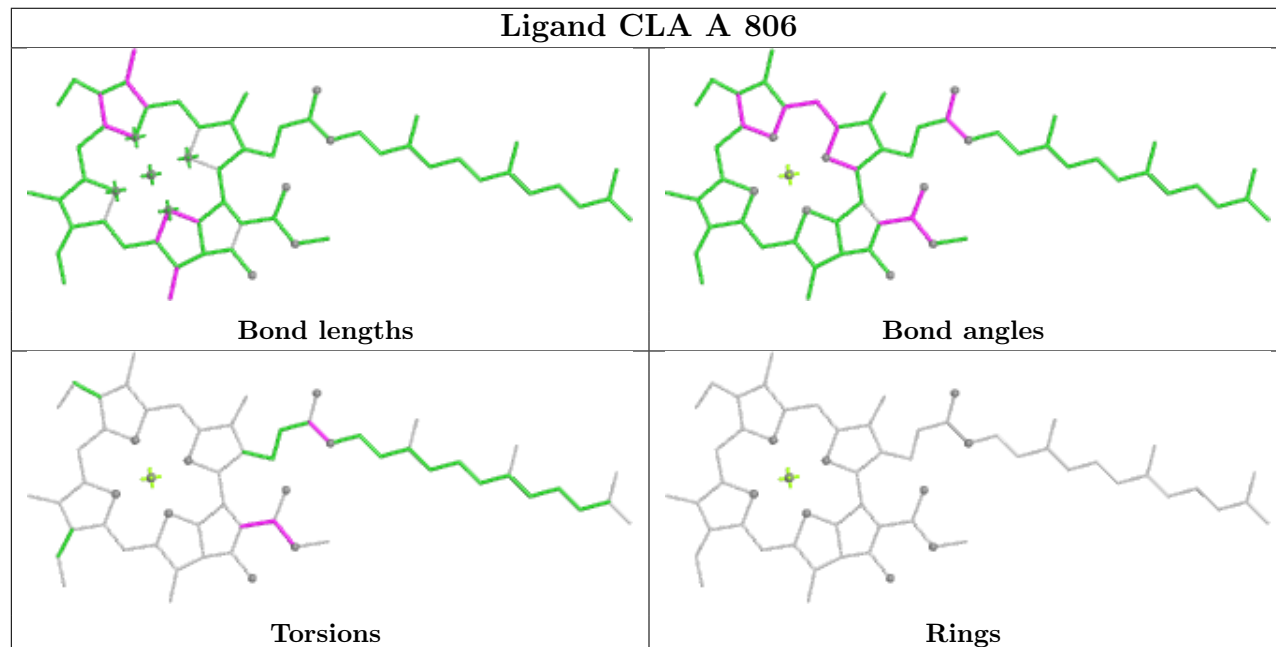


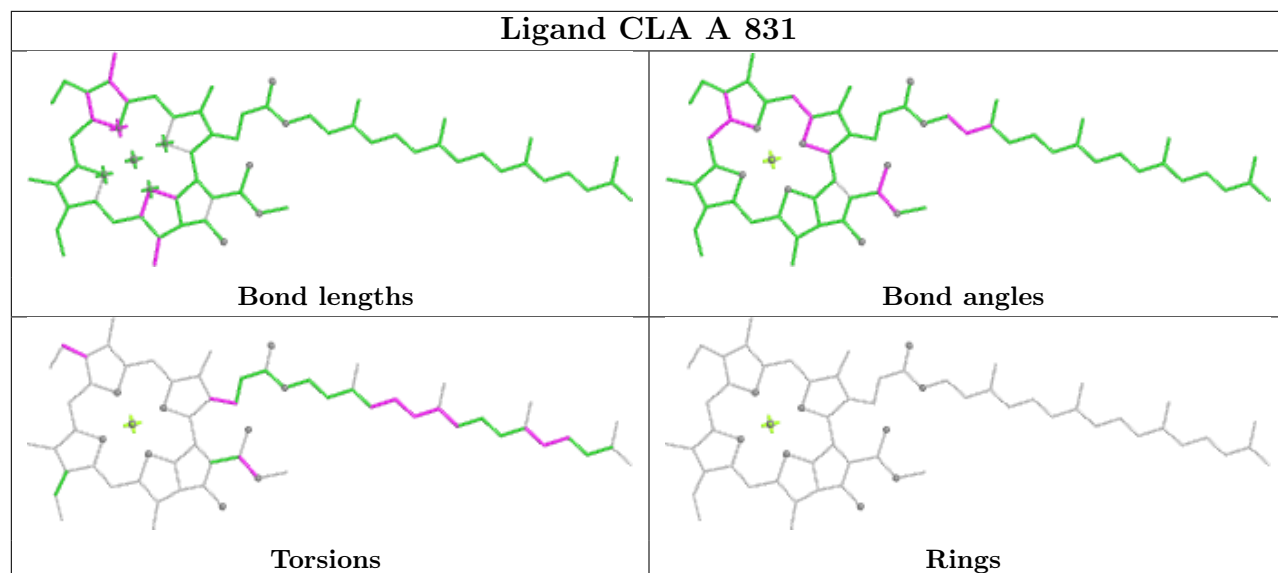
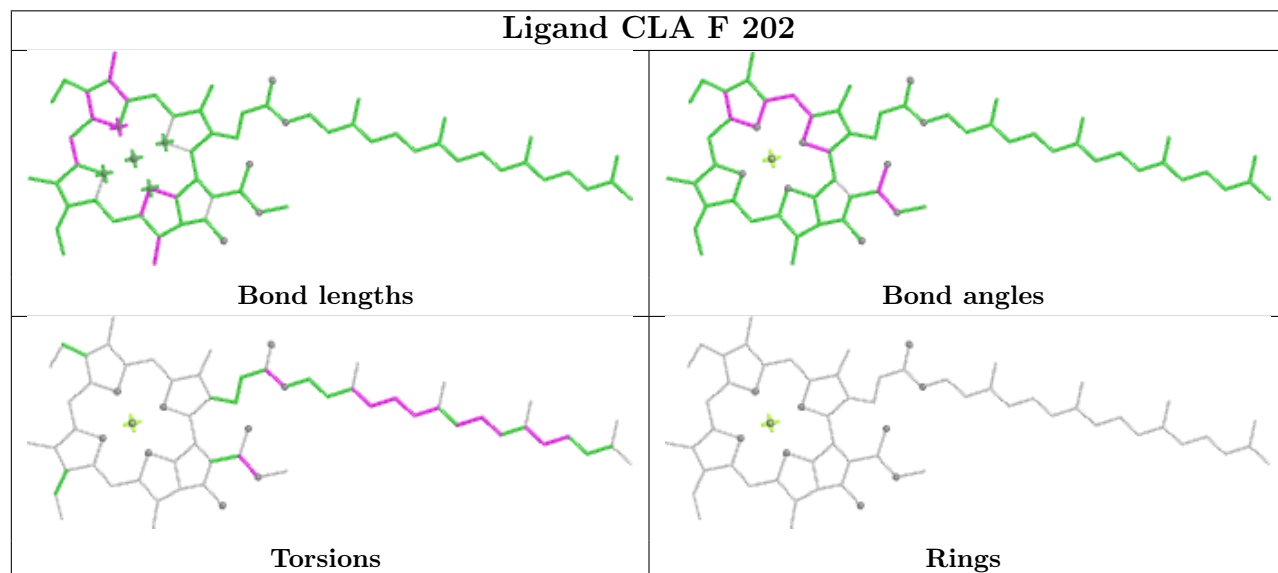
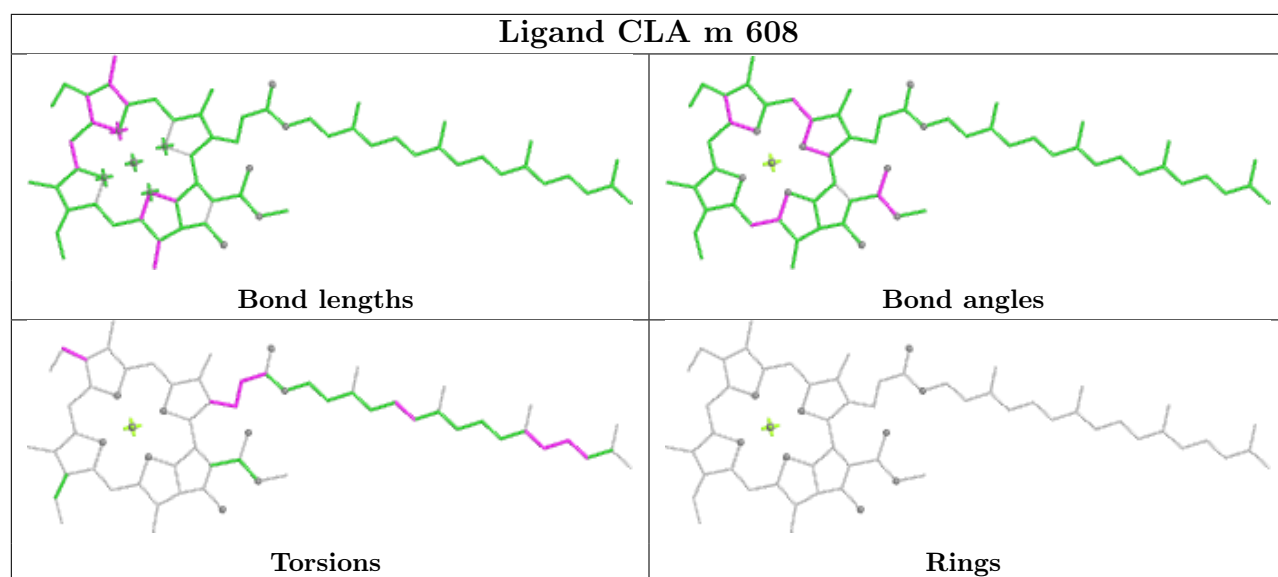


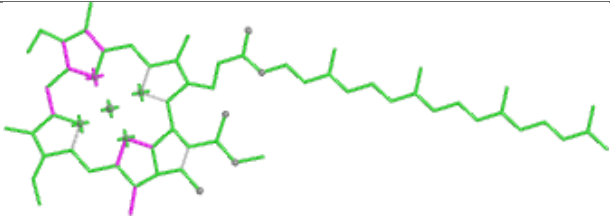
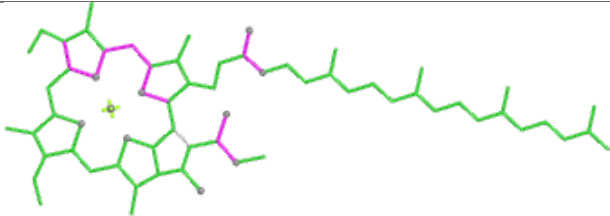
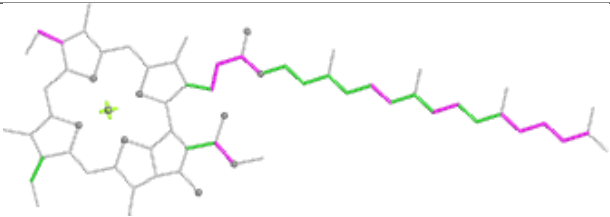
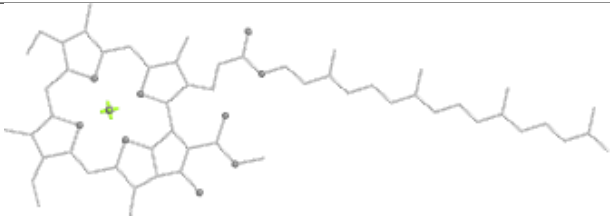
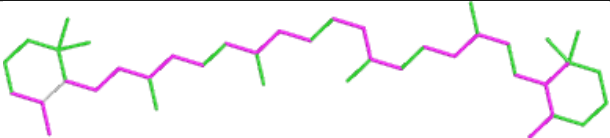
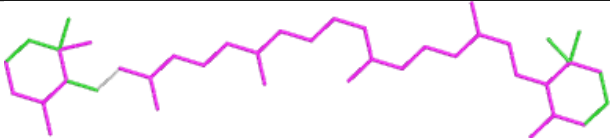
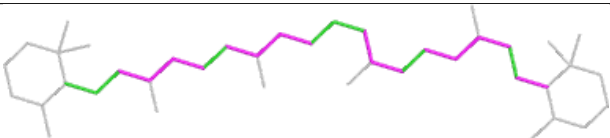
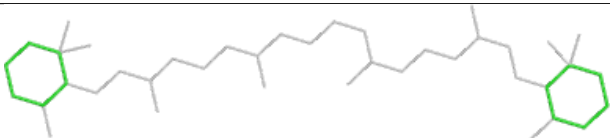
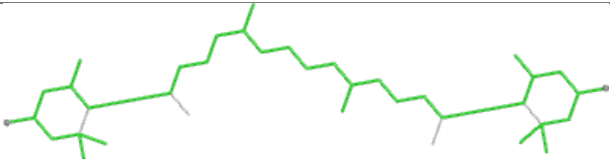
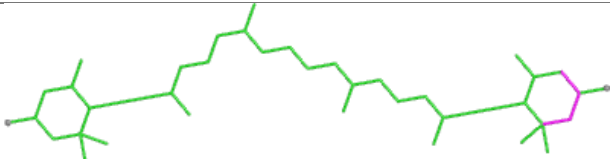
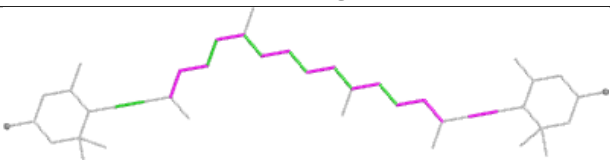
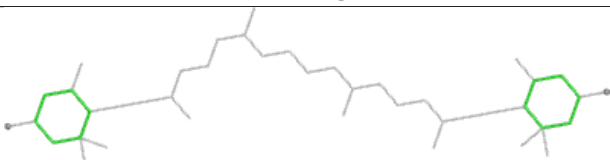
Ligand LHG n 619

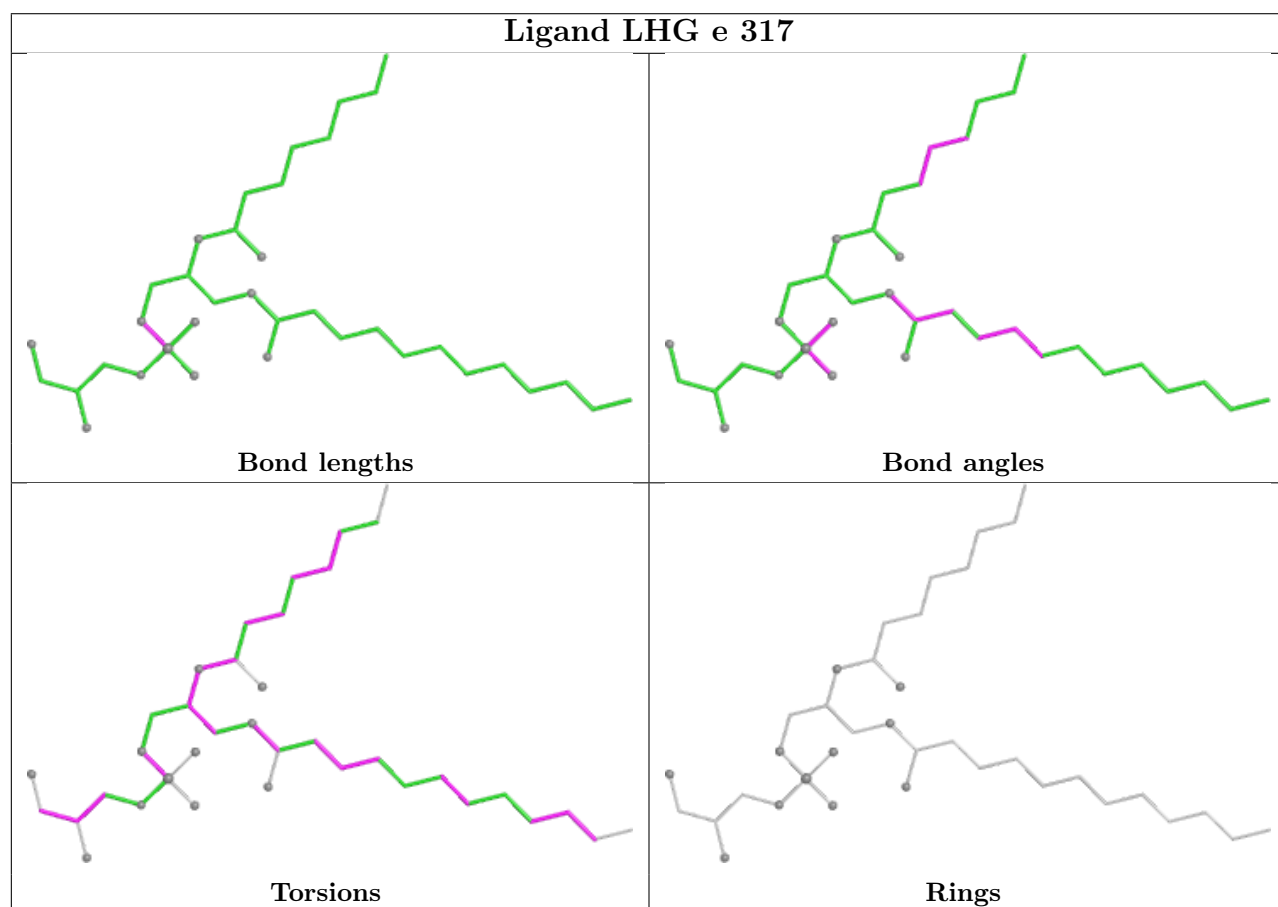
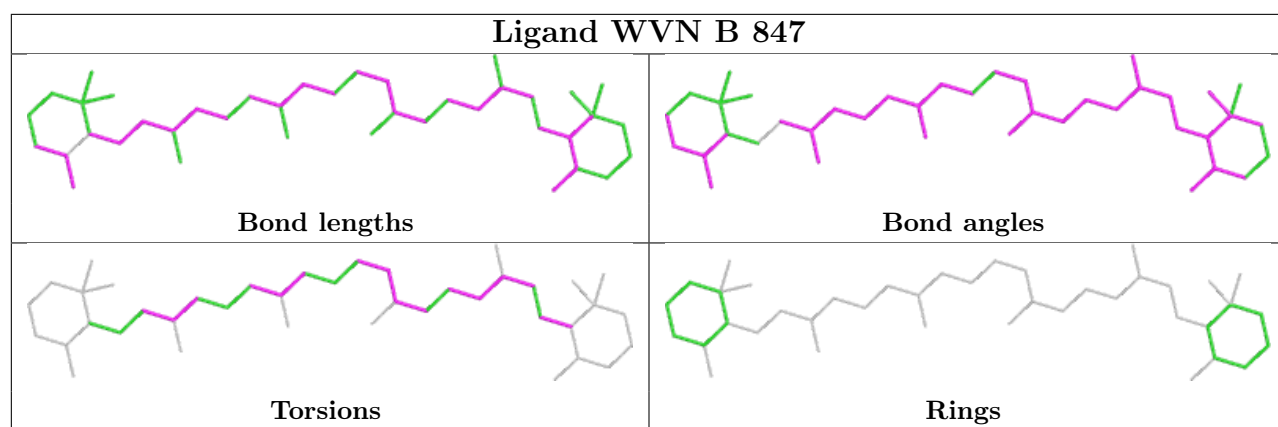


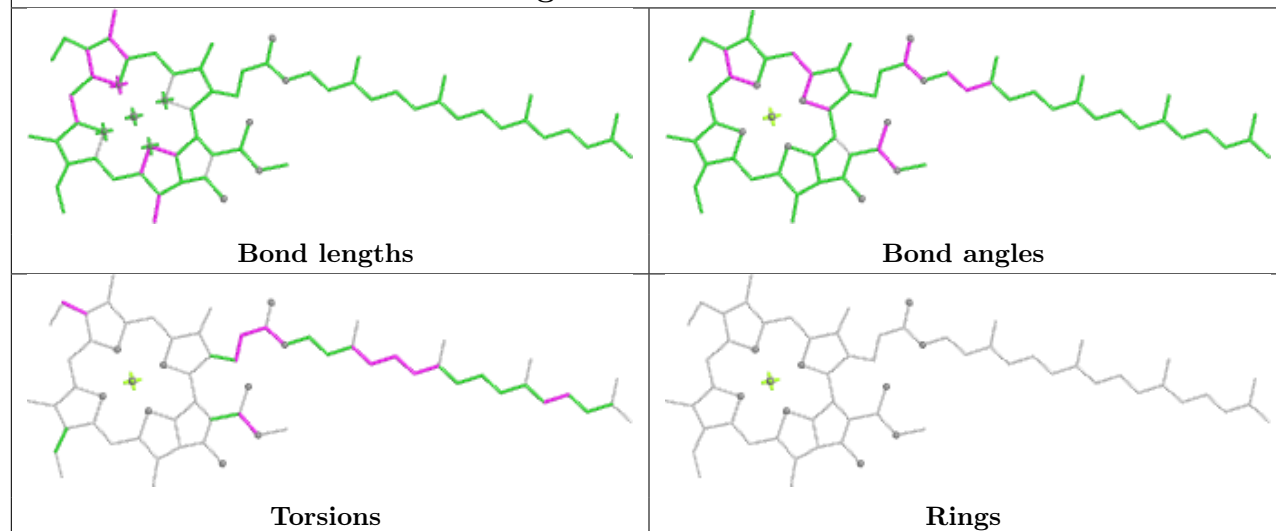
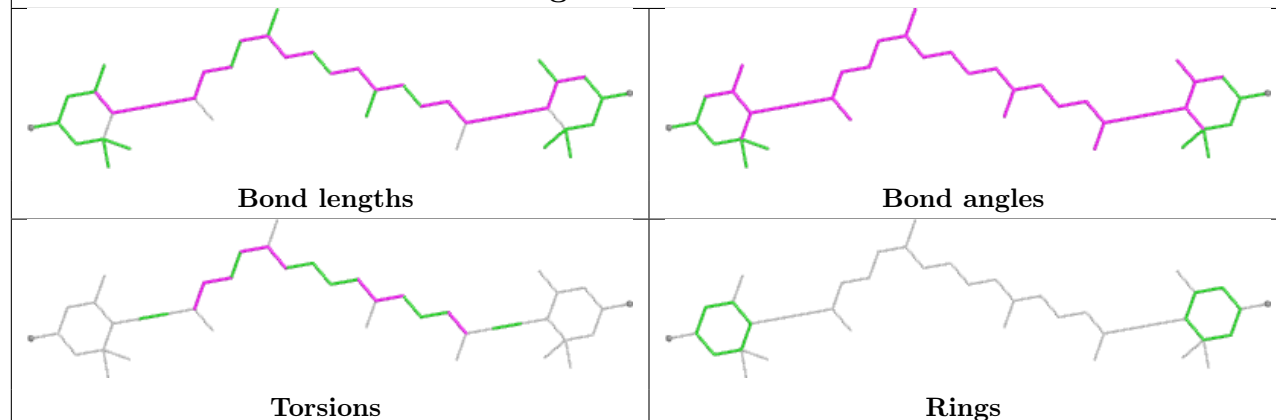
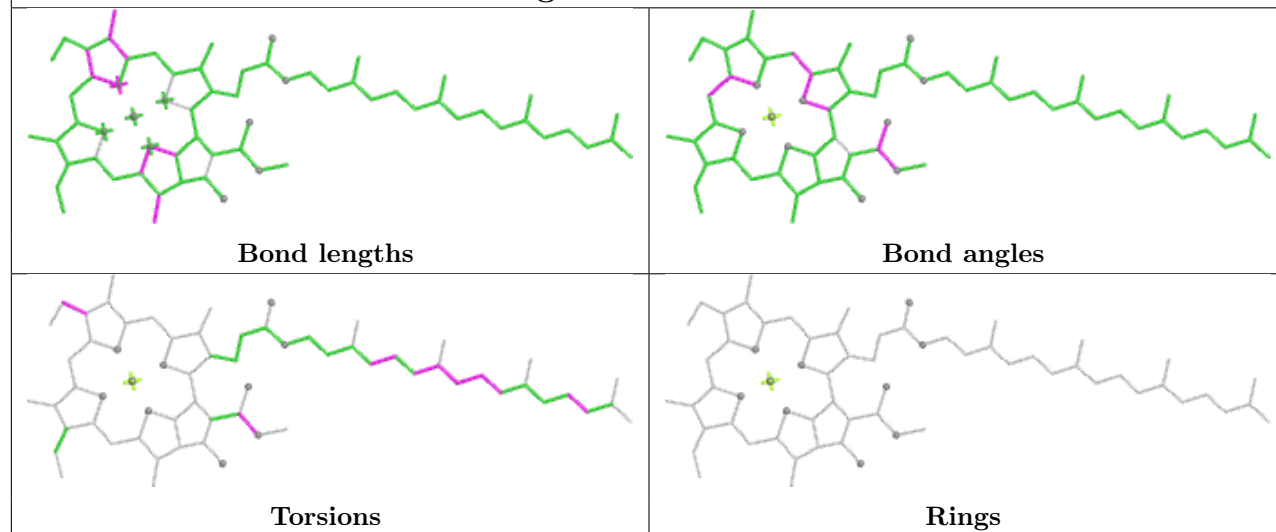
Ligand CLA A 806

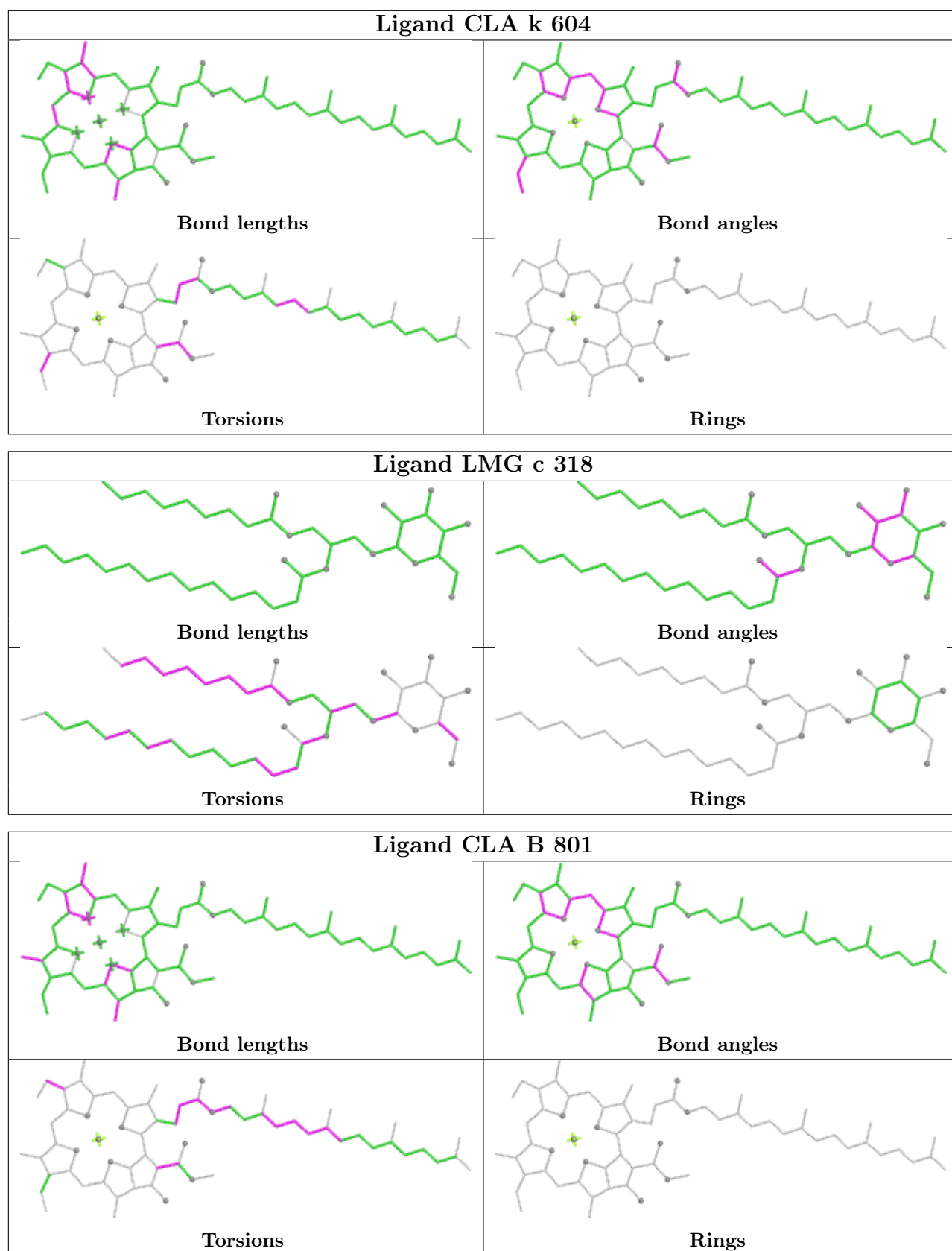


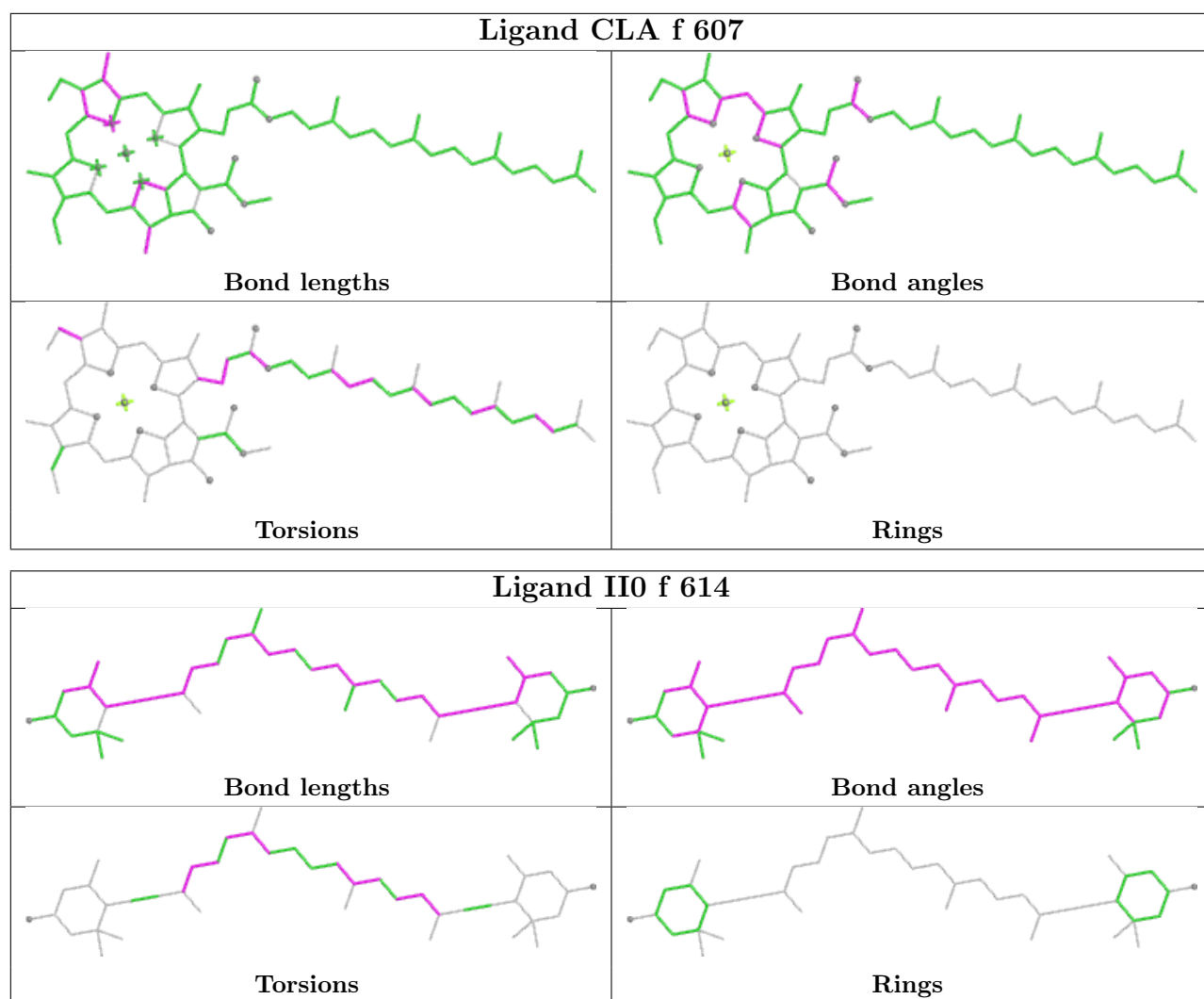


Ligand CLA e 307	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand WVN h 308	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand II0 e 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

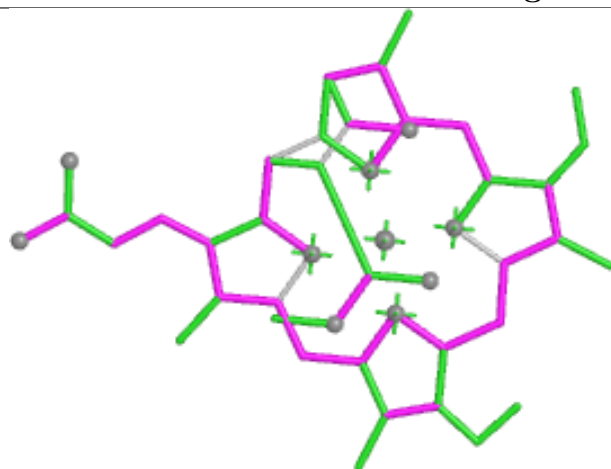


Ligand CLA e 304**Ligand II0 b 315****Ligand CLA c 312**

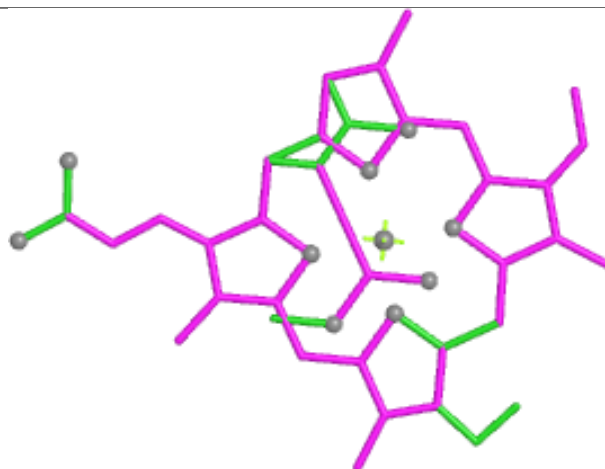




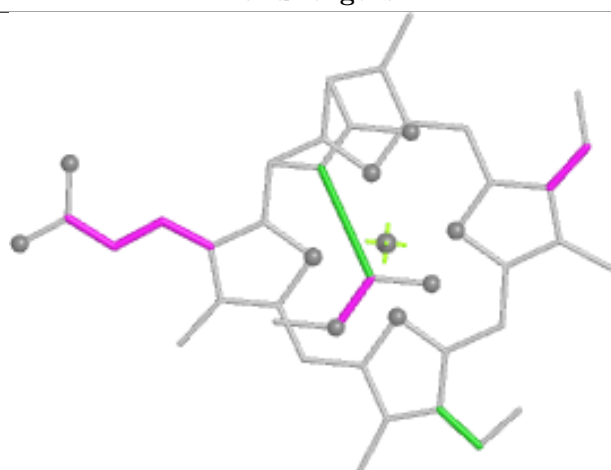
Ligand KC2 i 318



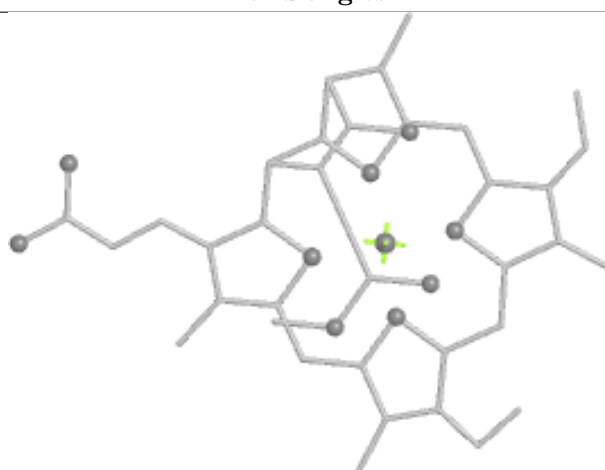
Bond lengths



Bond angles

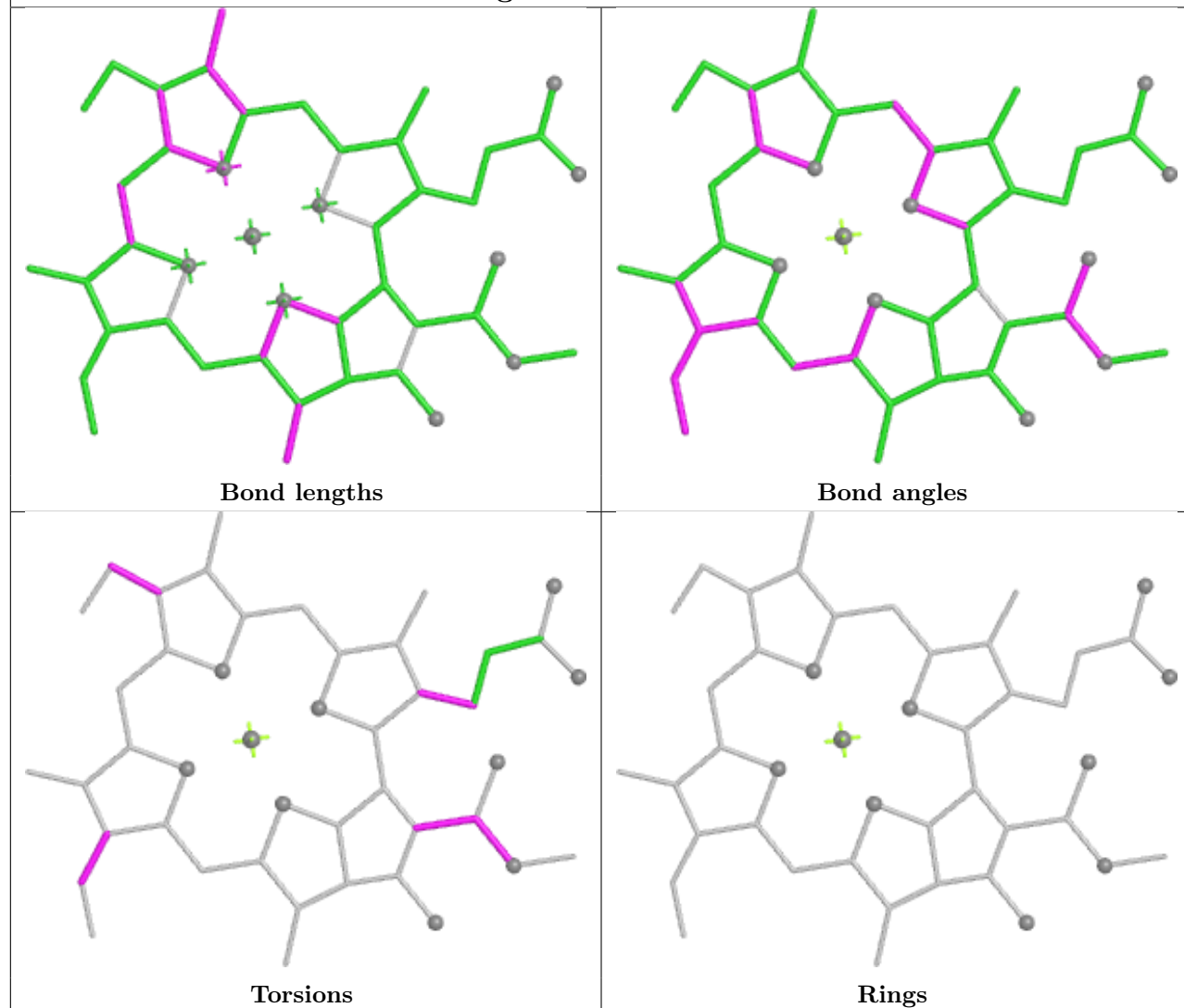


Torsions

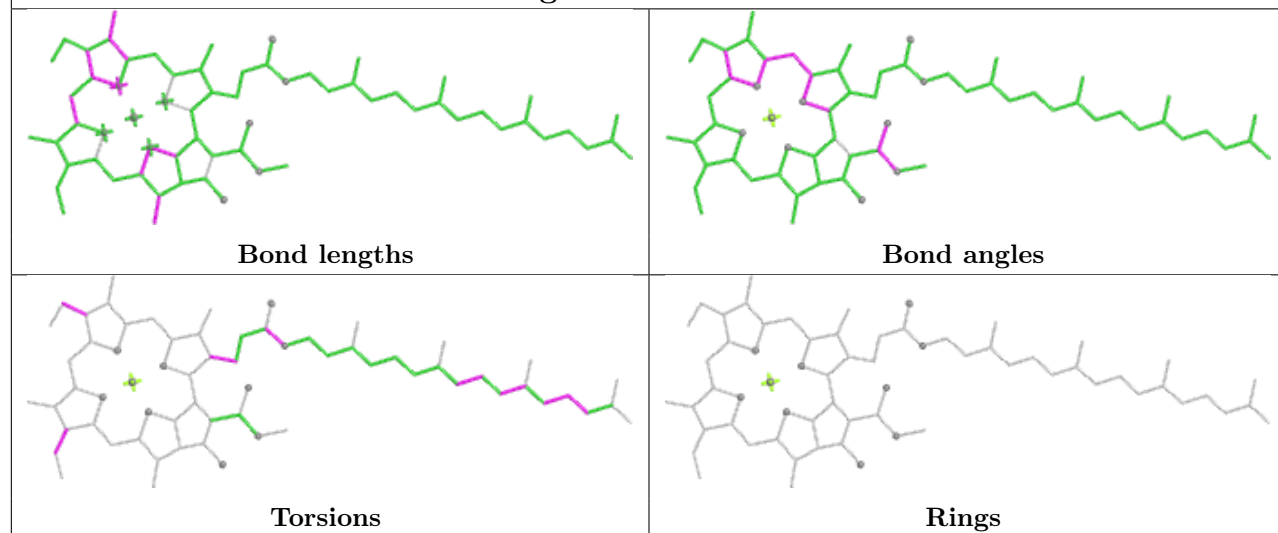


Rings

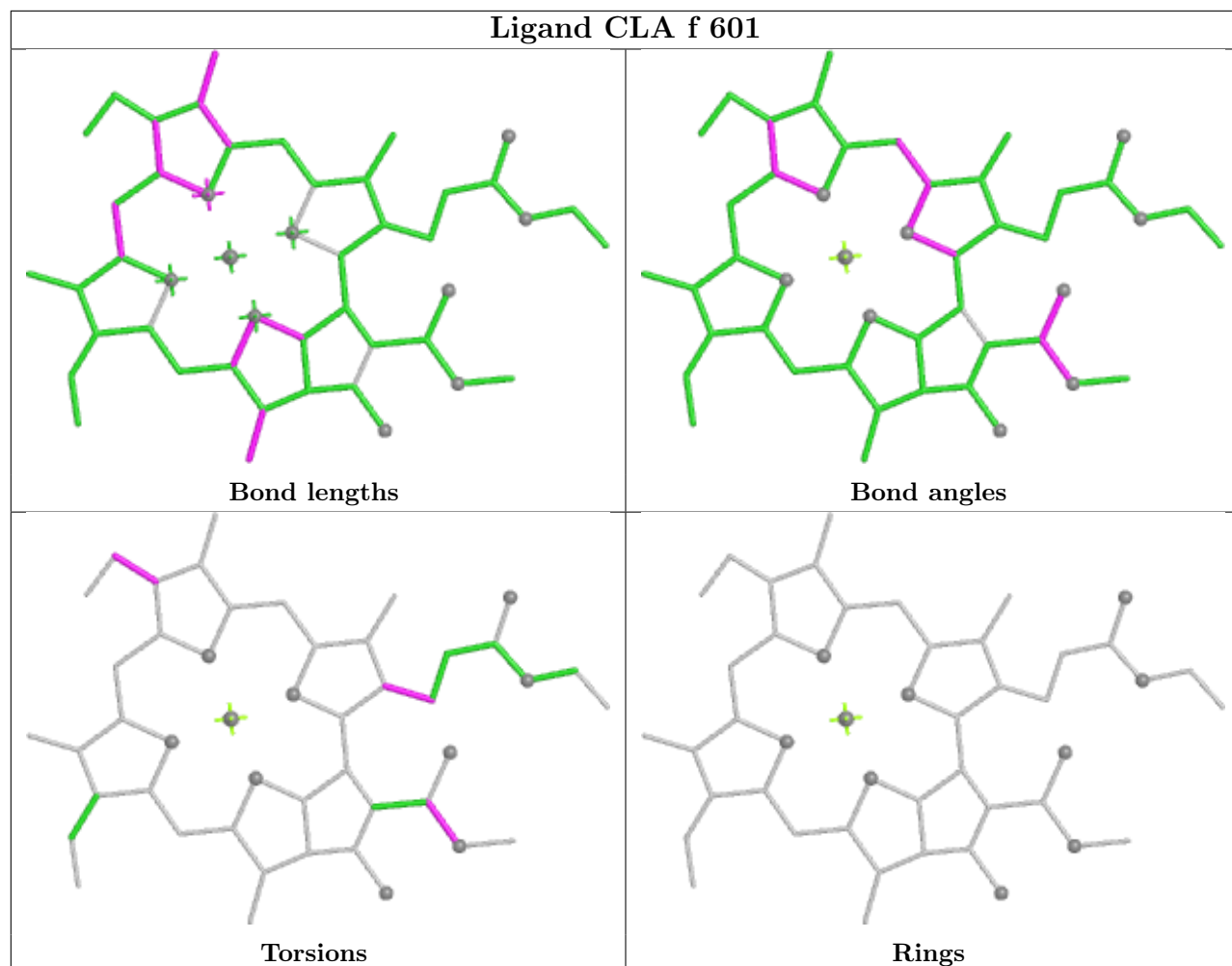
Ligand CLA a 306



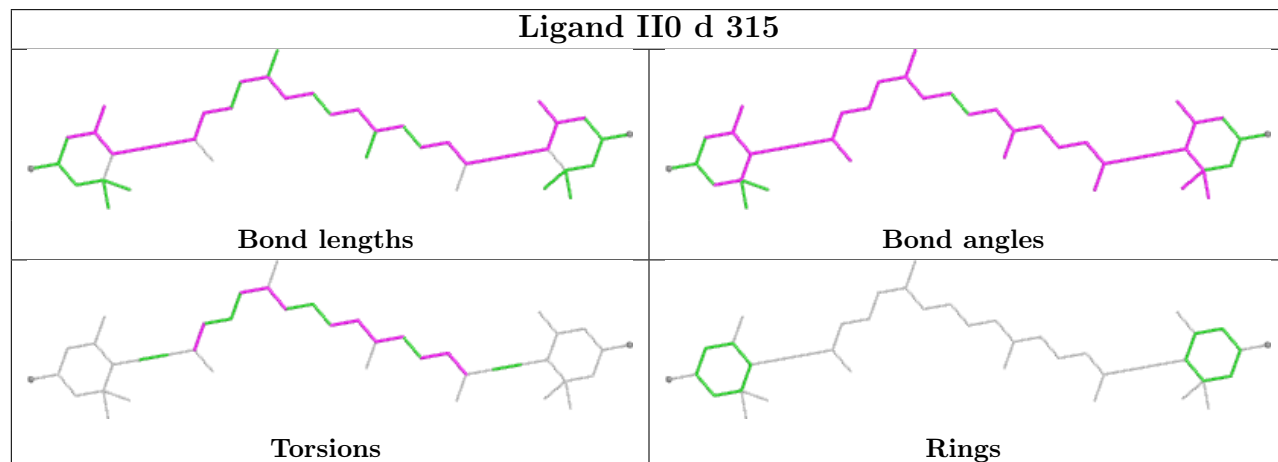
Ligand CLA f 610

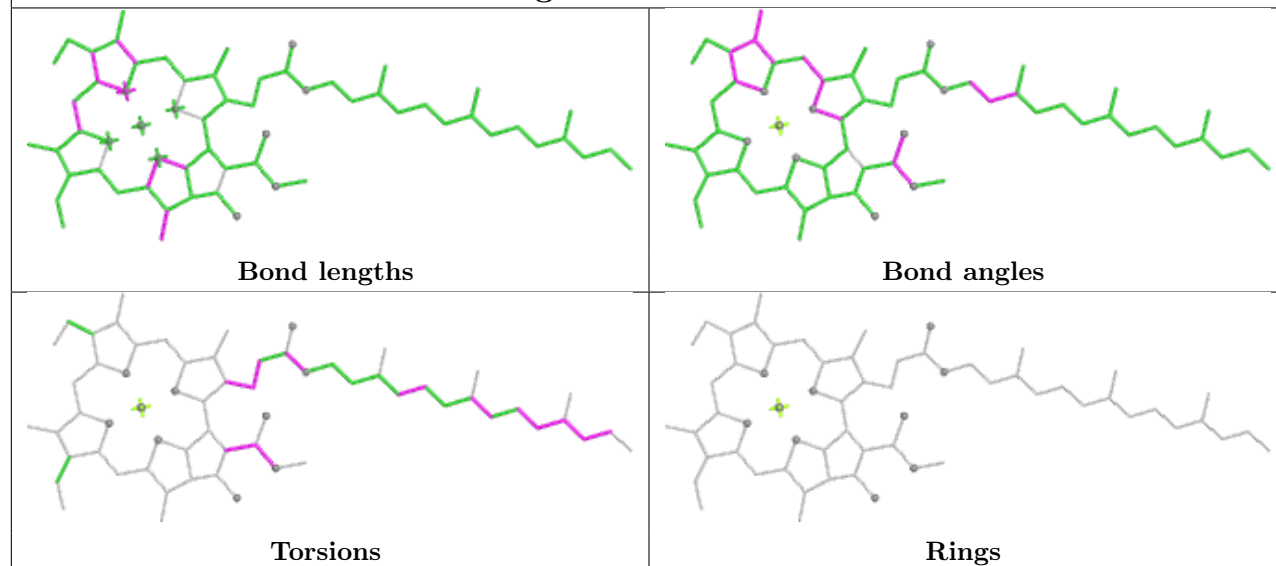
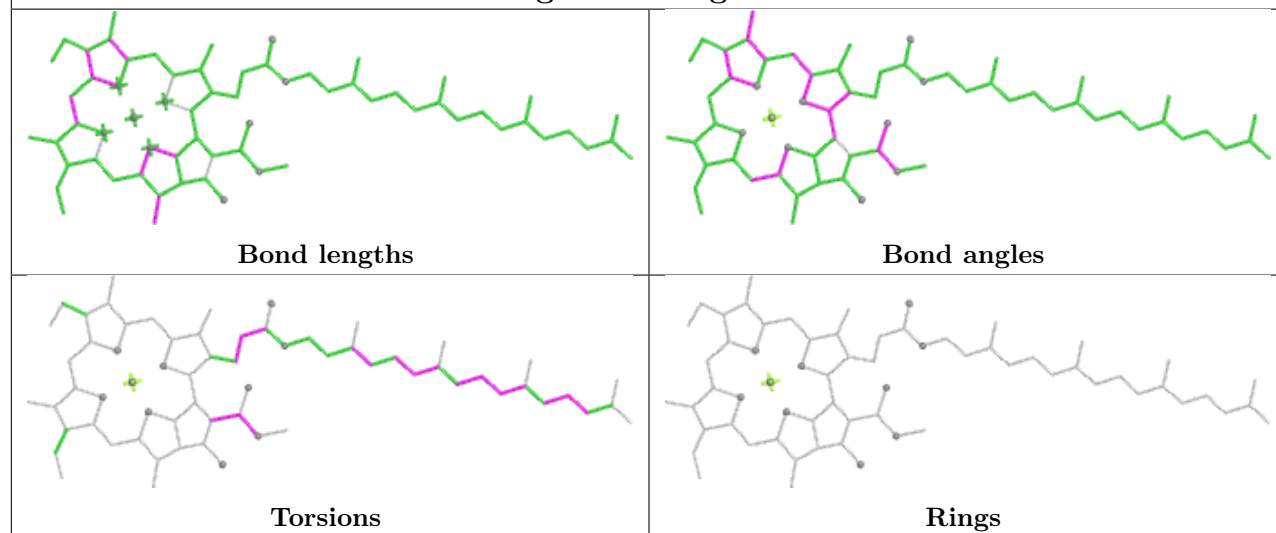


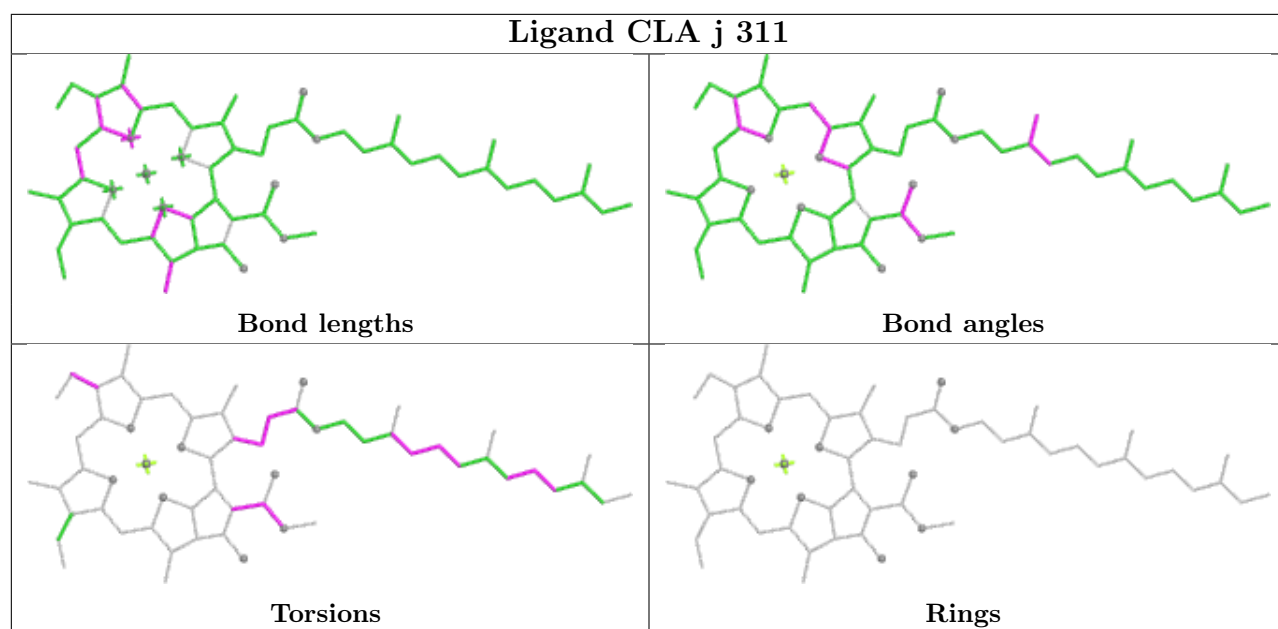
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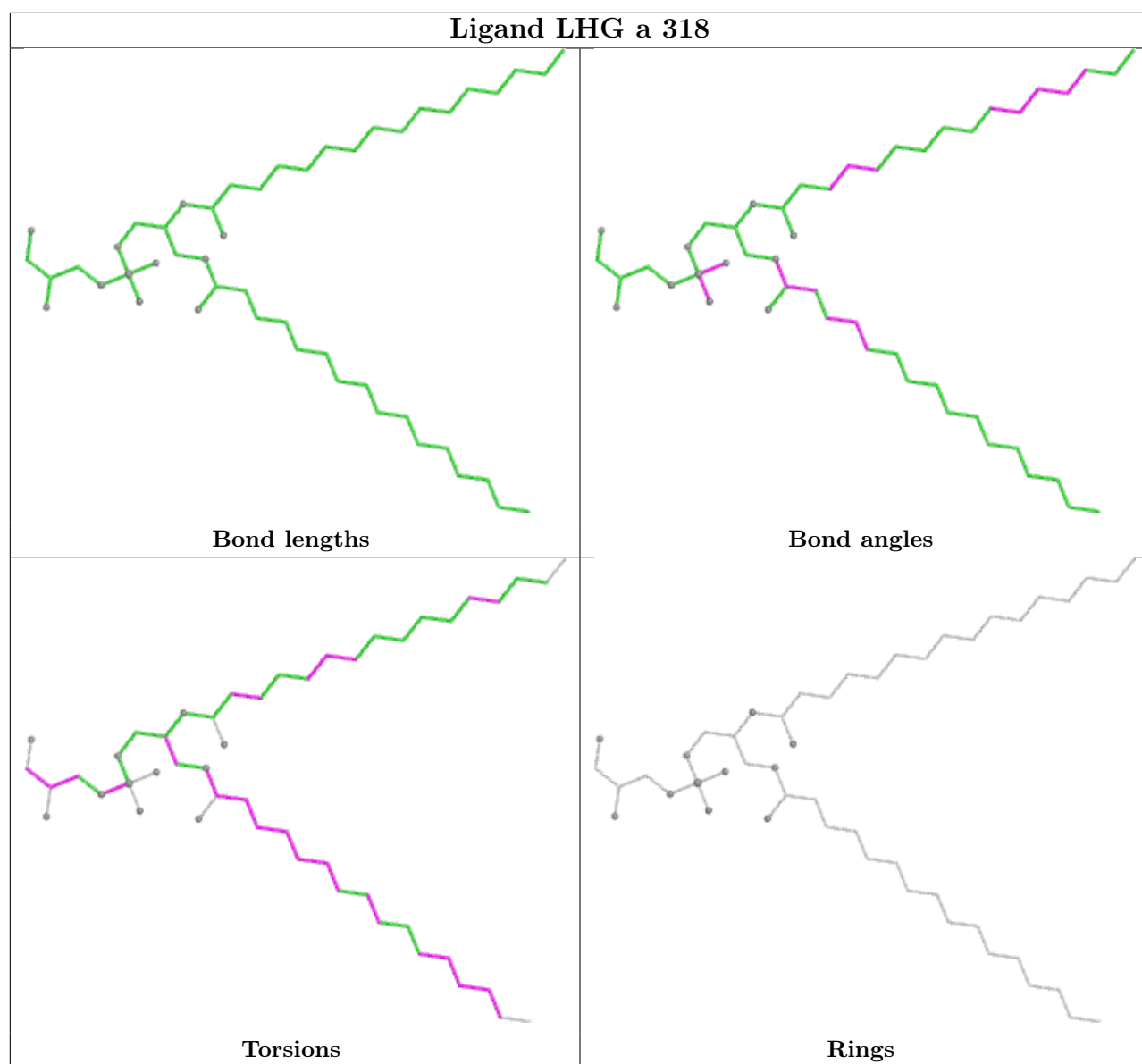


Ligand II0 d 315

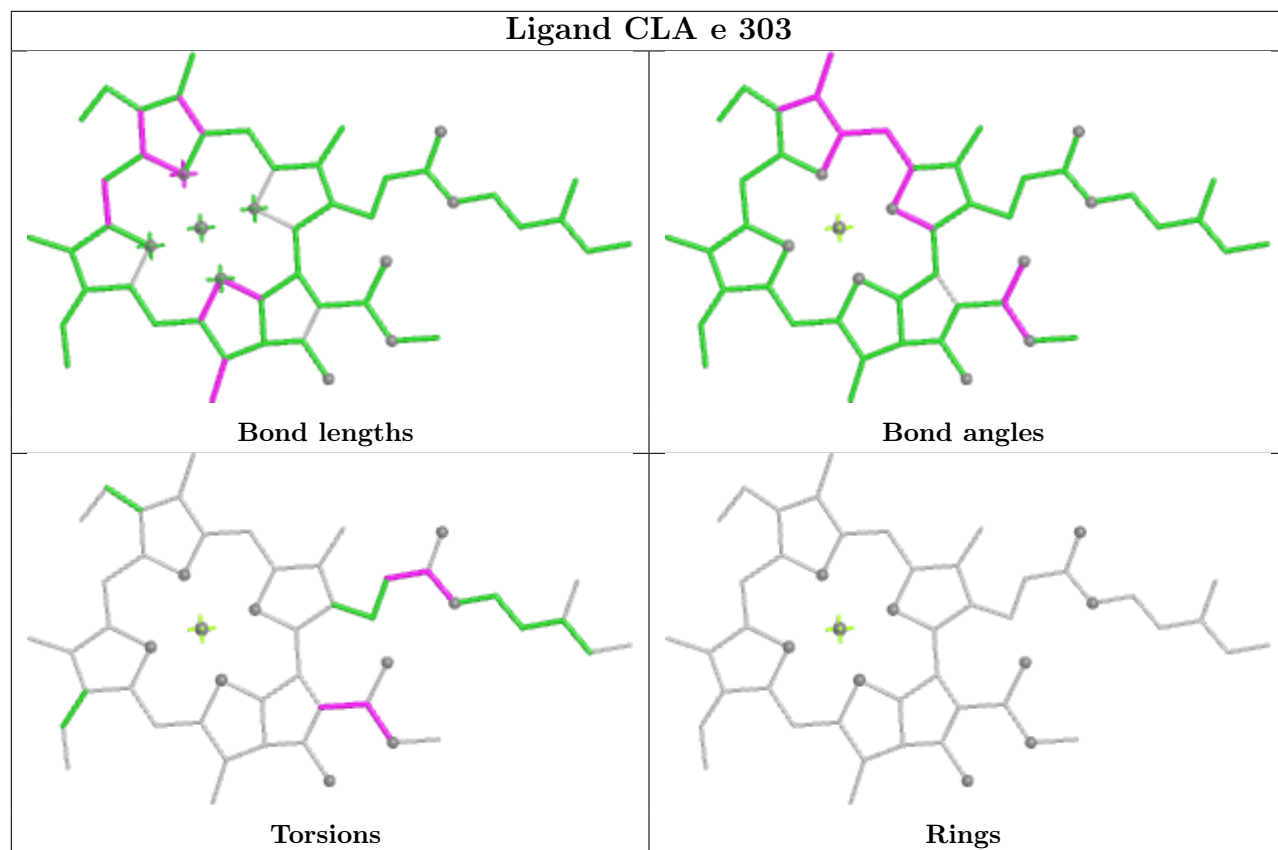


Ligand CLA d 302**Ligand CLA g 302**

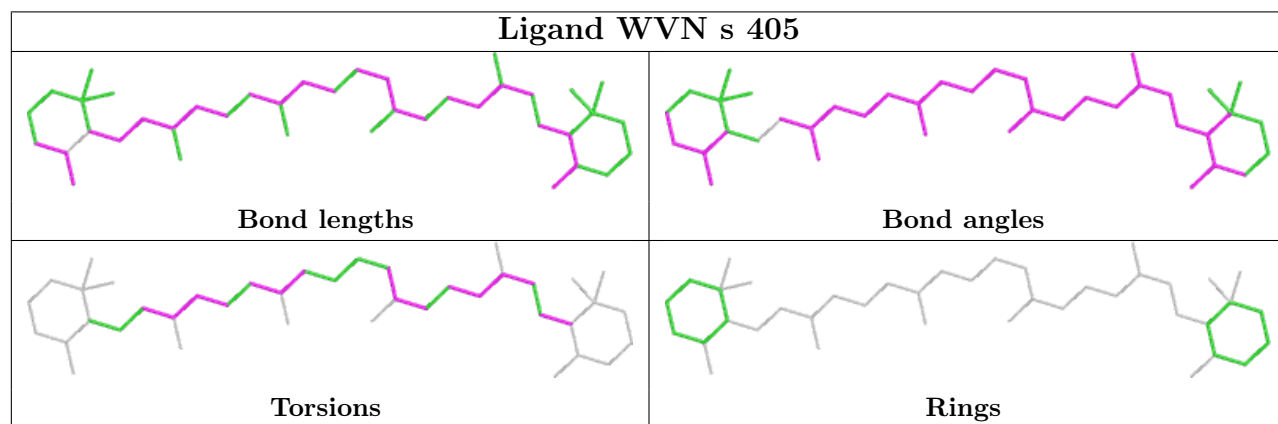




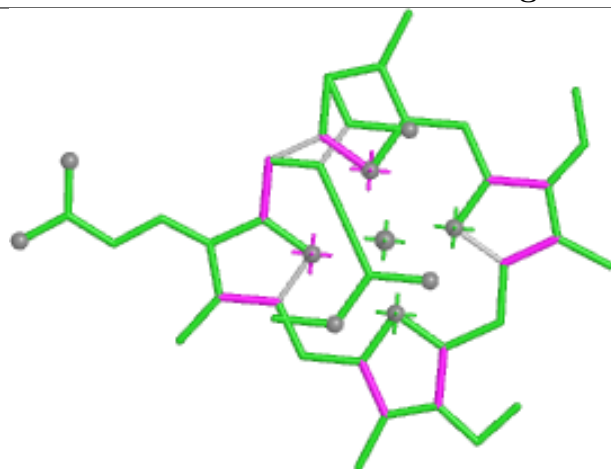
Ligand CLA e 303



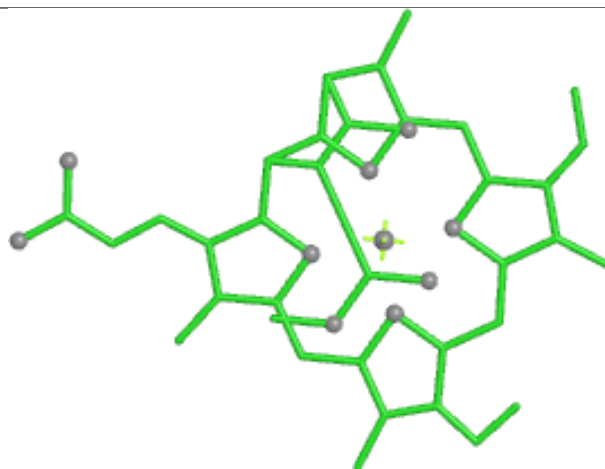
Ligand WVN s 405



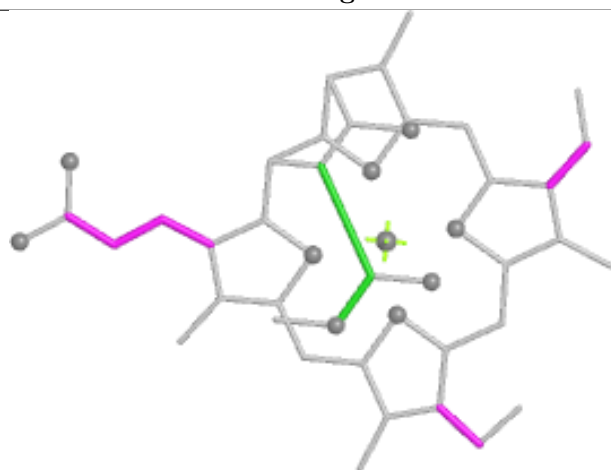
Ligand KC2 k 613



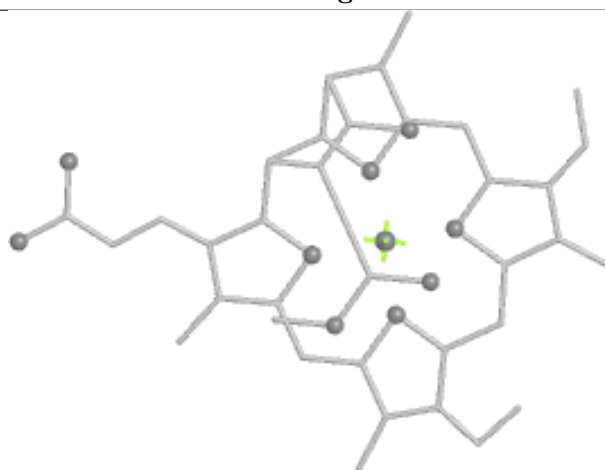
Bond lengths



Bond angles

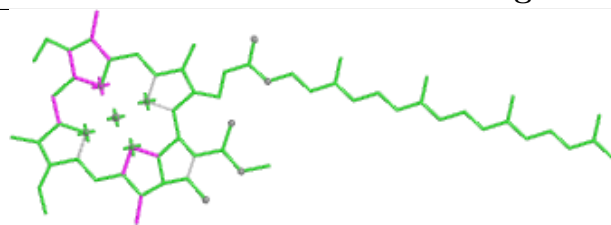


Torsions

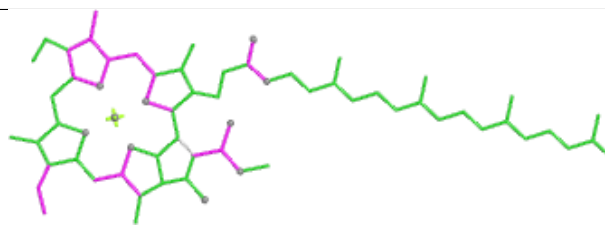


Rings

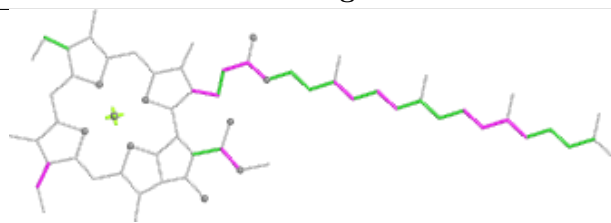
Ligand CLA B 816



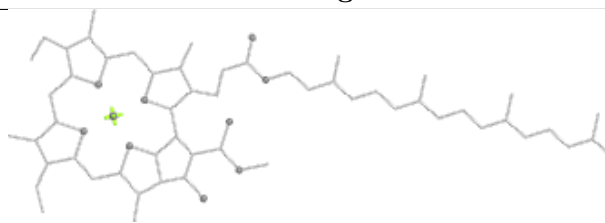
Bond lengths



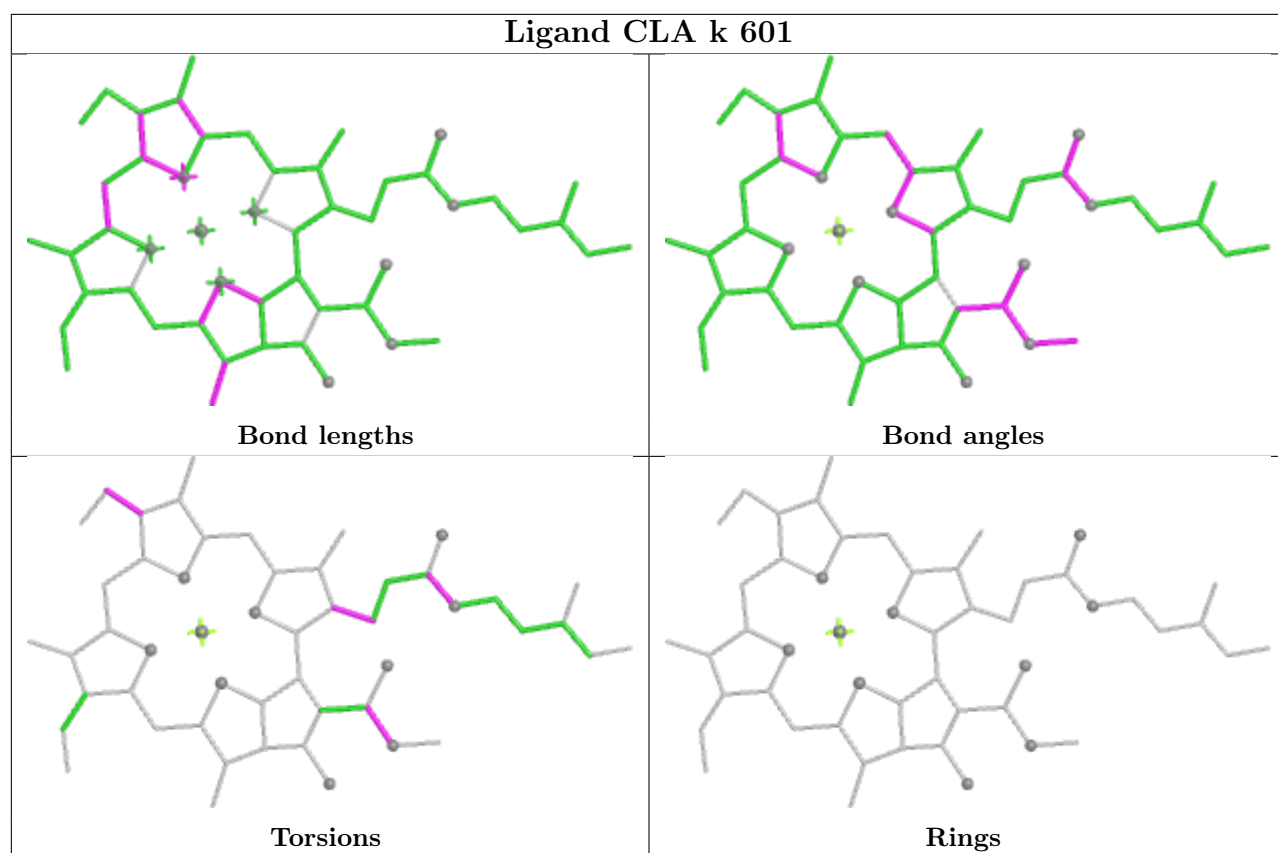
Bond angles

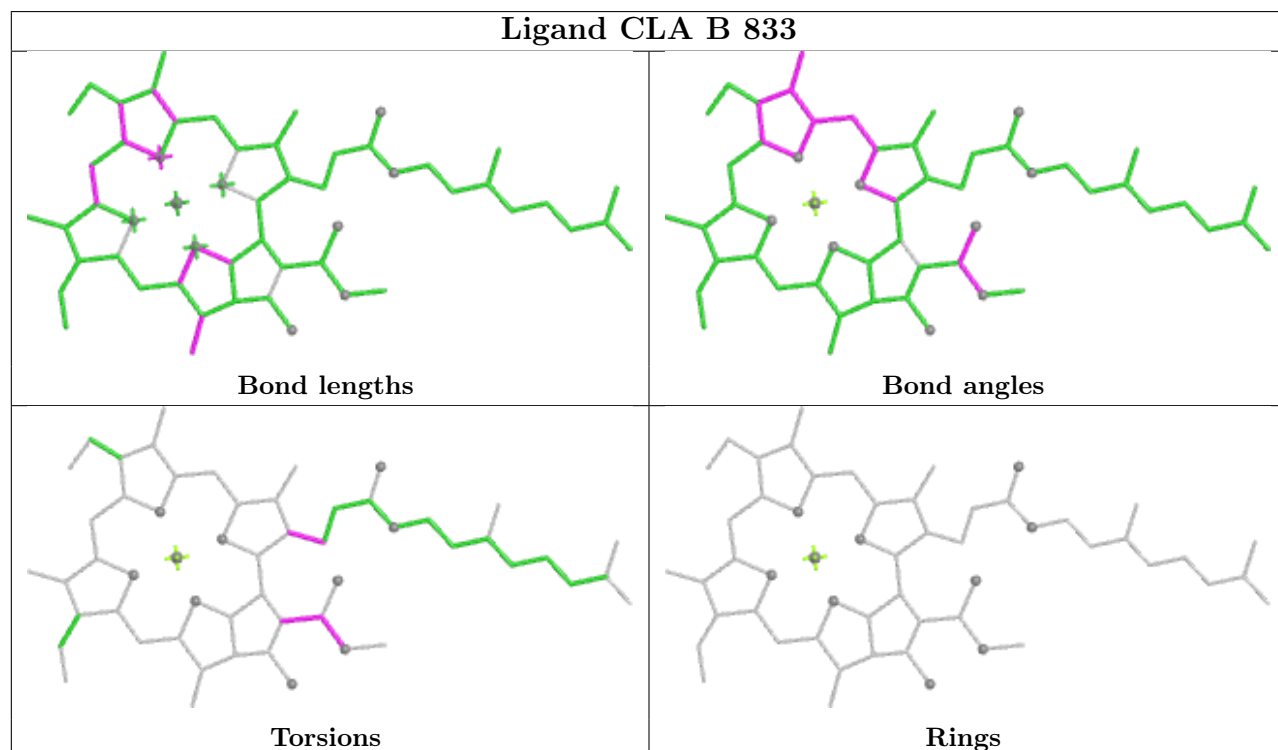
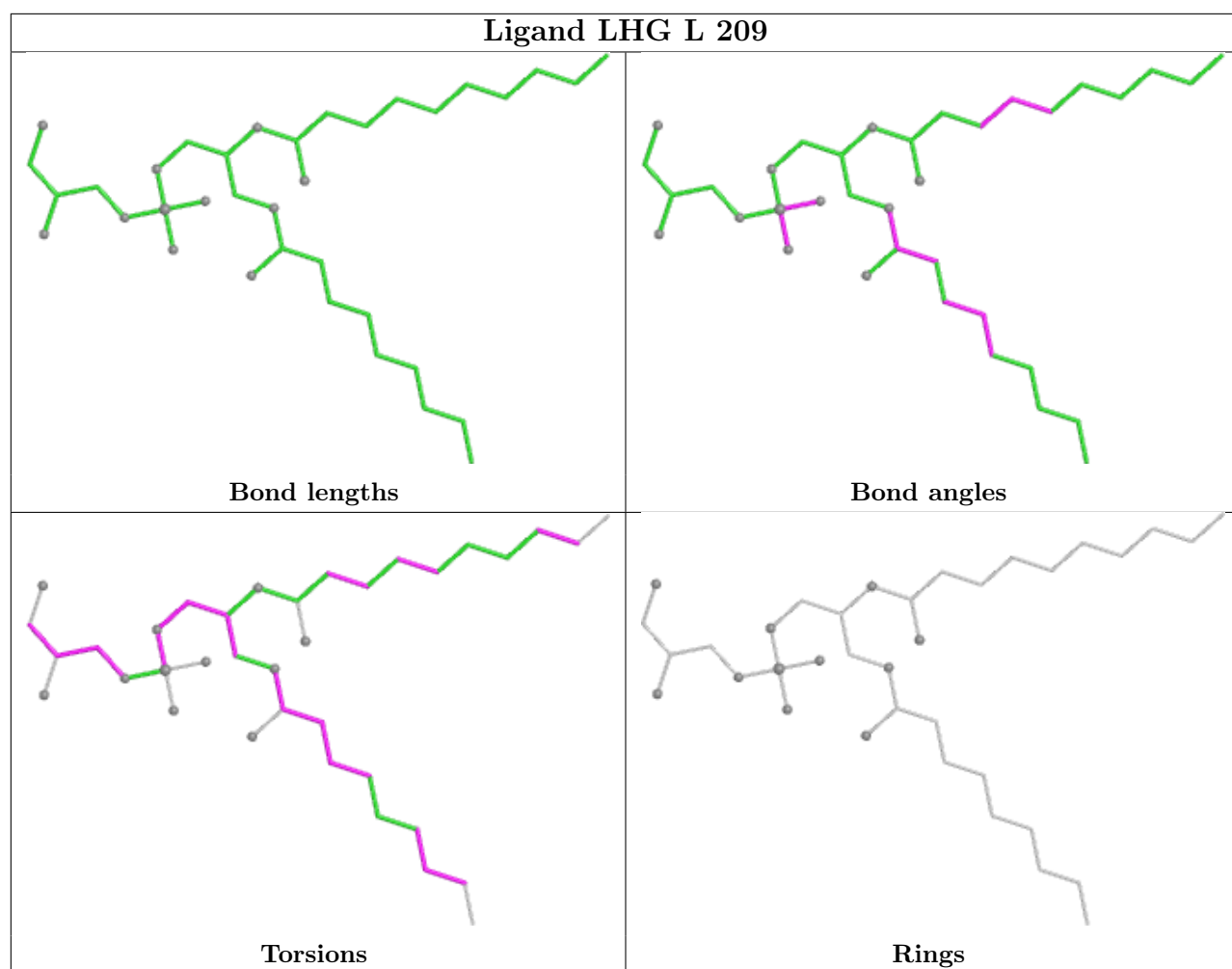


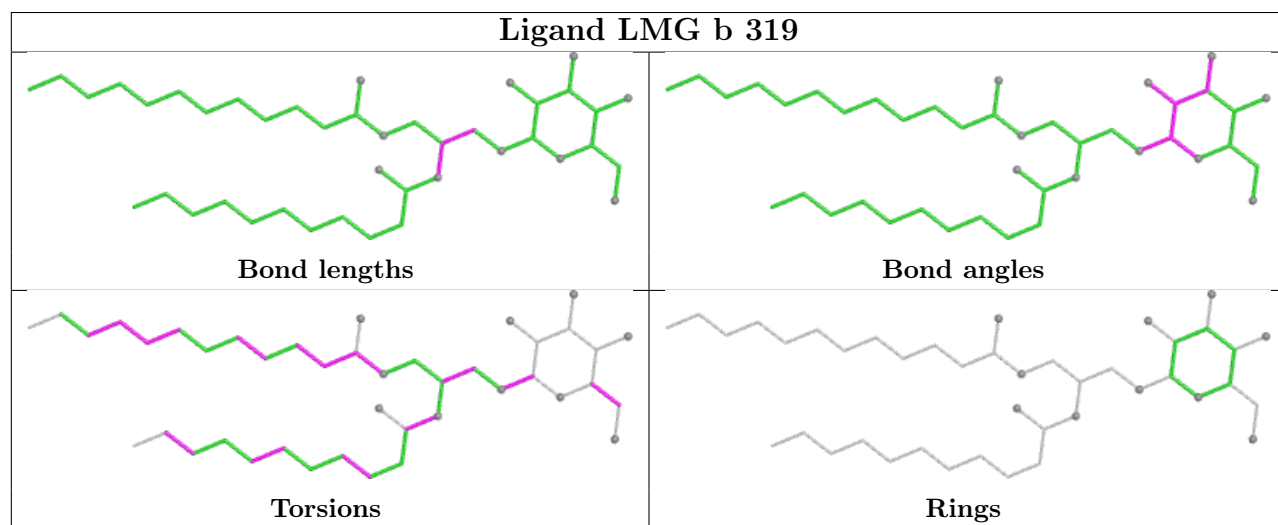
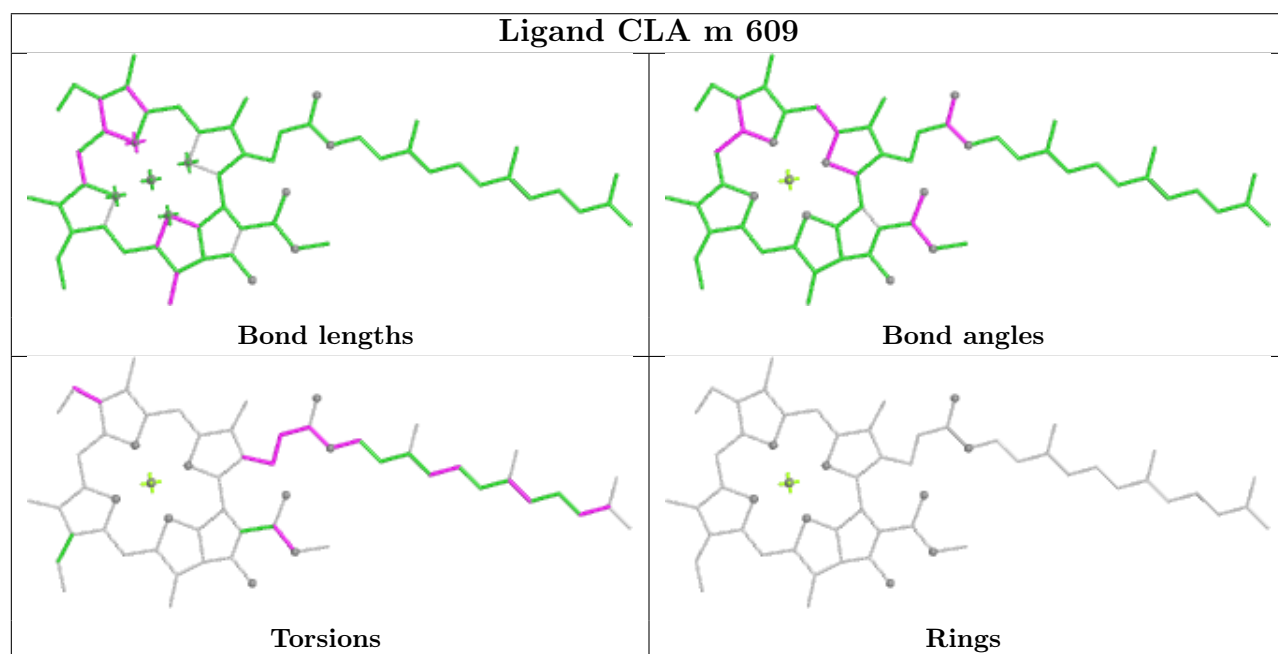
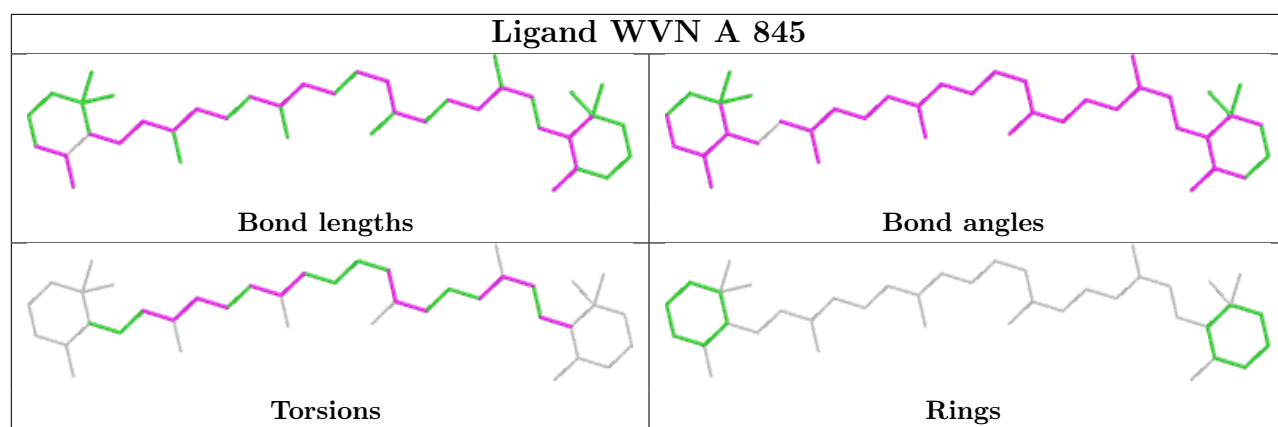
Torsions



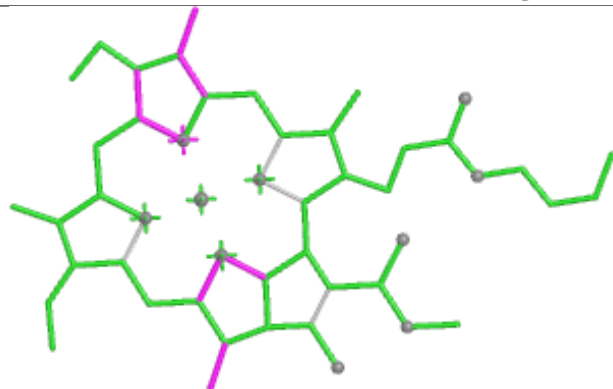
Rings



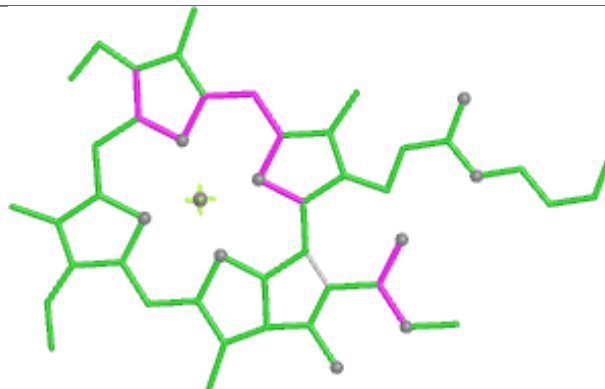




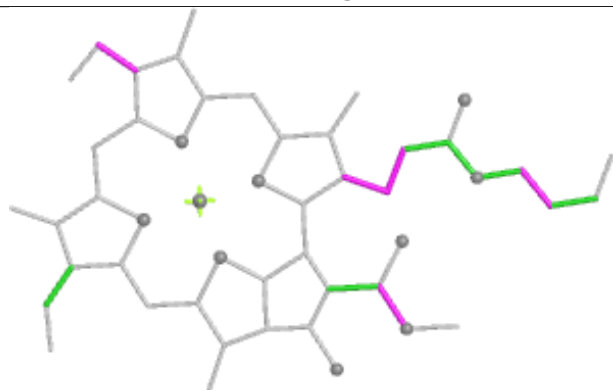
Ligand CLA L 202



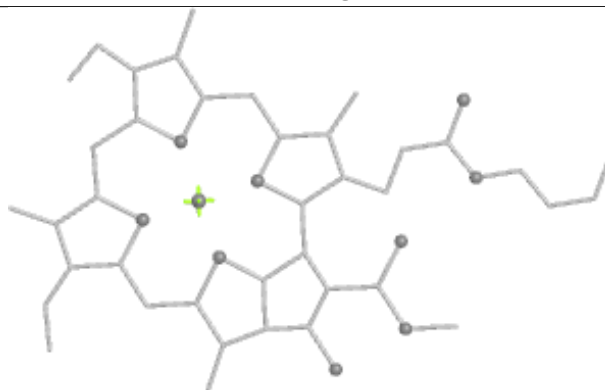
Bond lengths



Bond angles

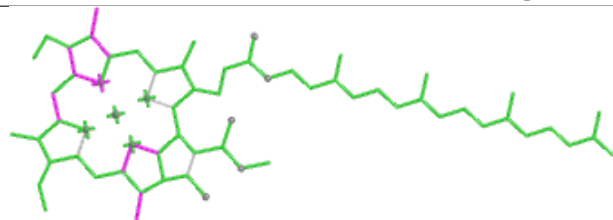


Torsions

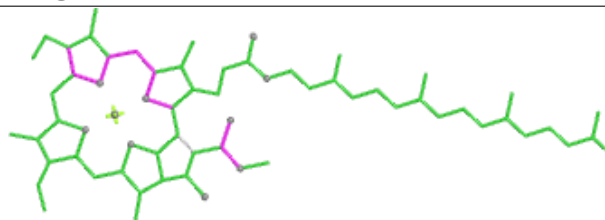


Rings

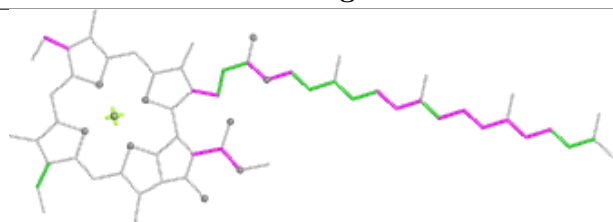
Ligand CLA g 304



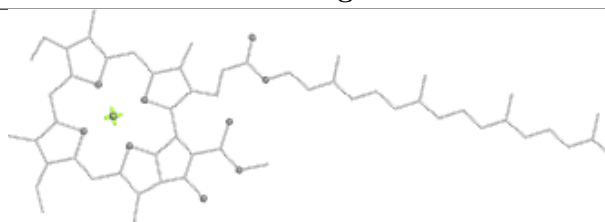
Bond lengths



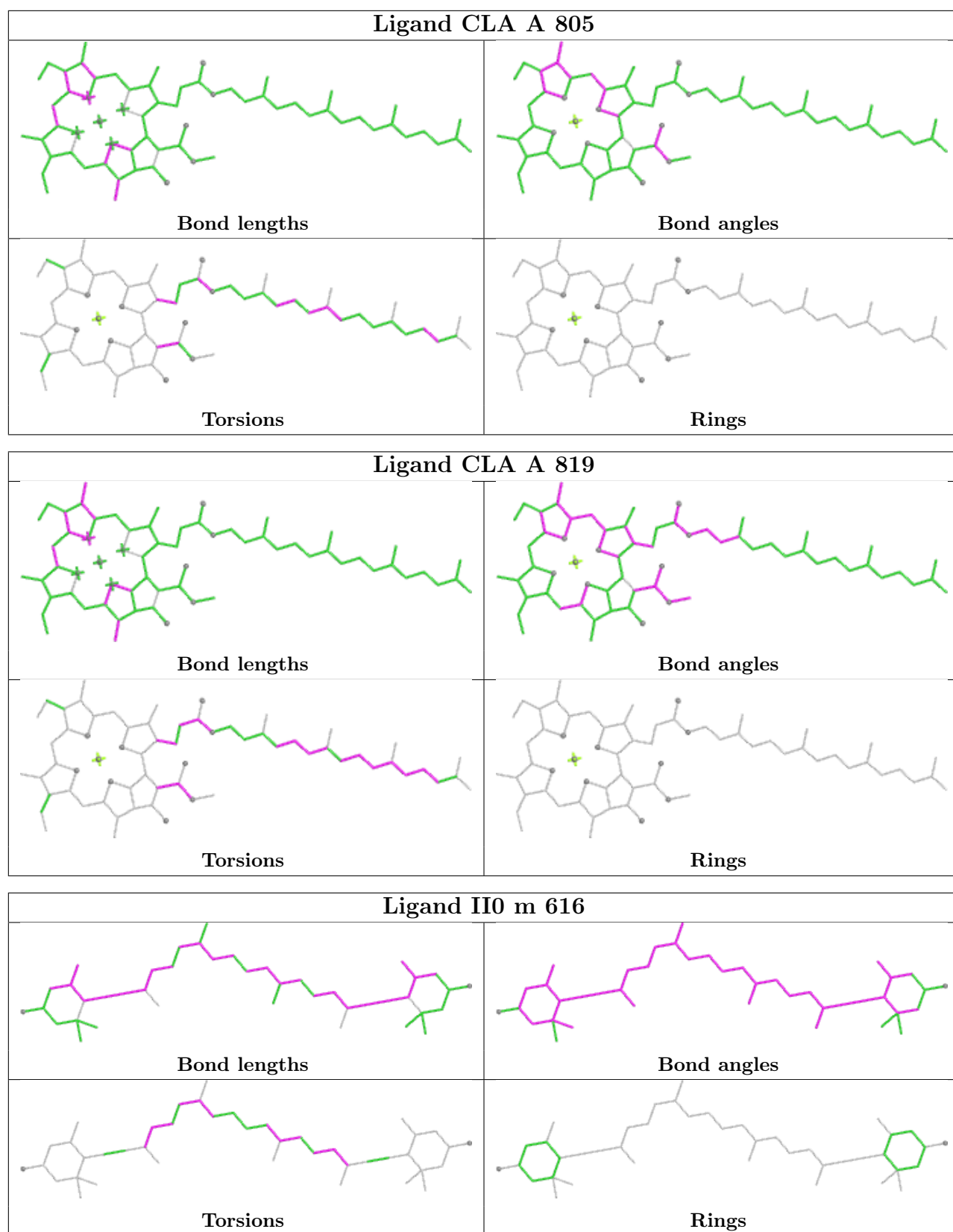
Bond angles

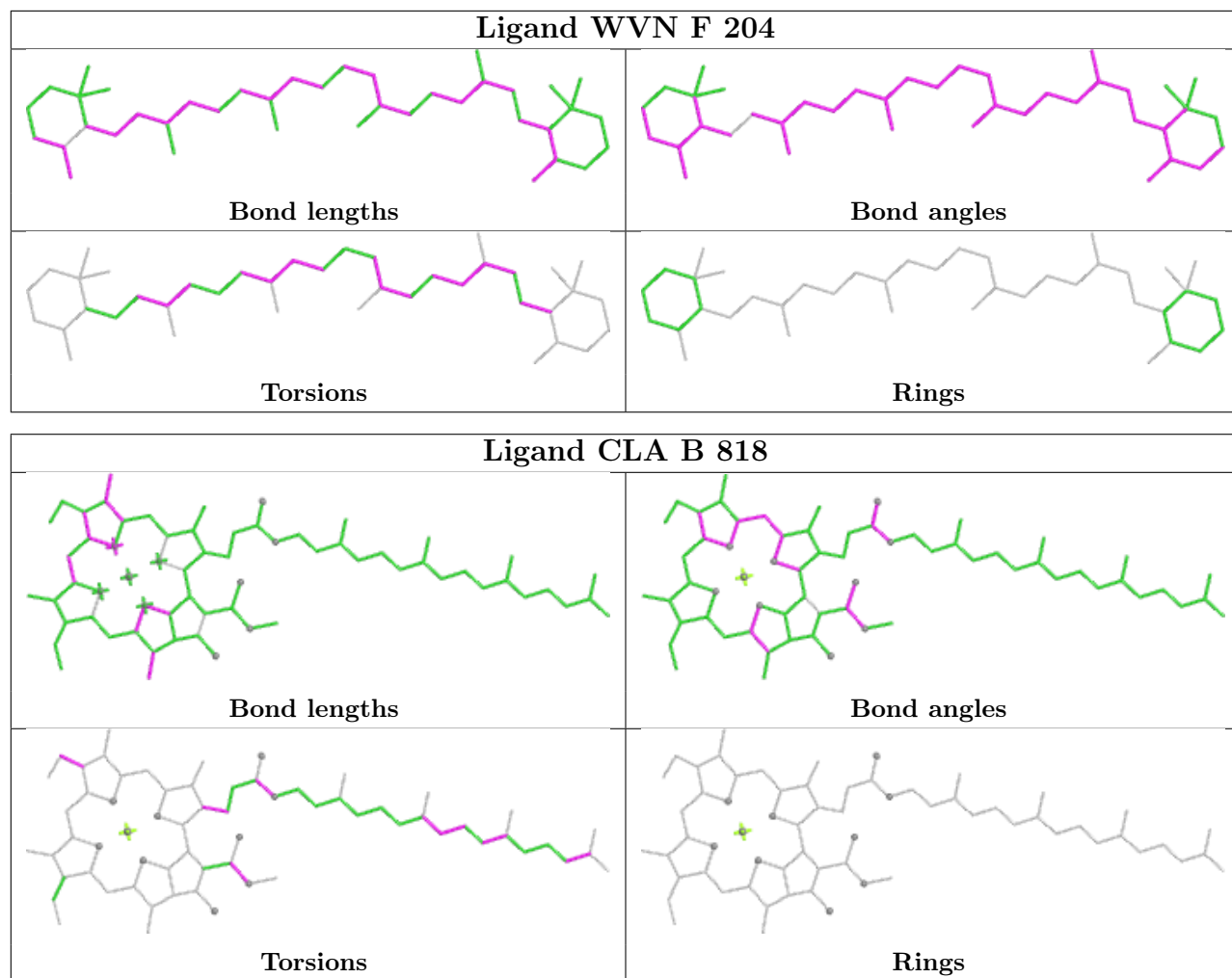


Torsions

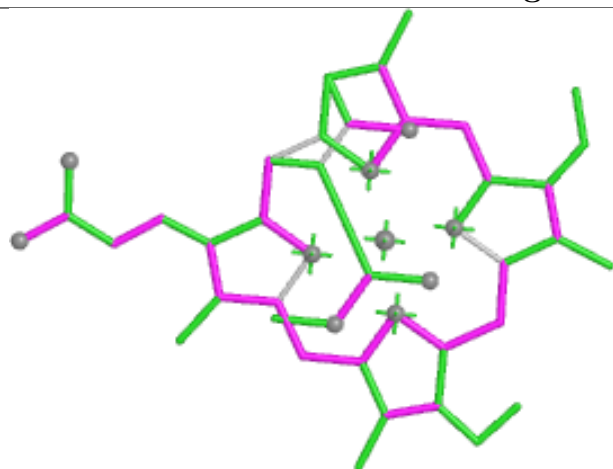


Rings

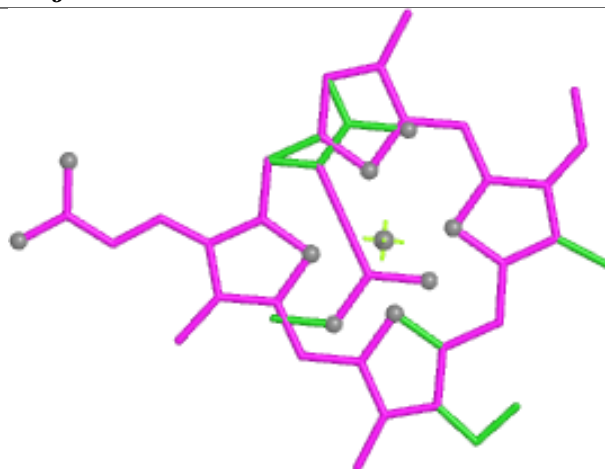




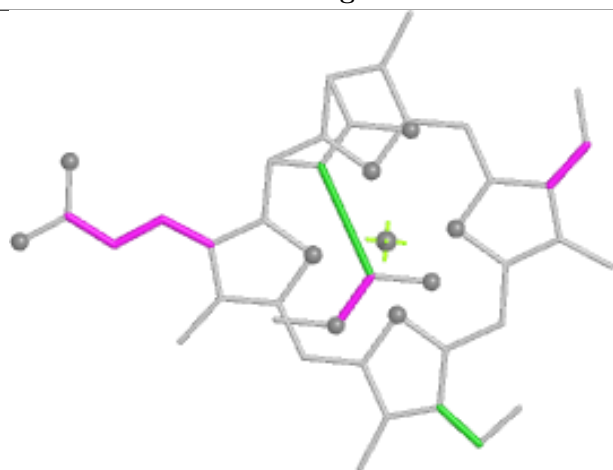
Ligand KC2 j 312



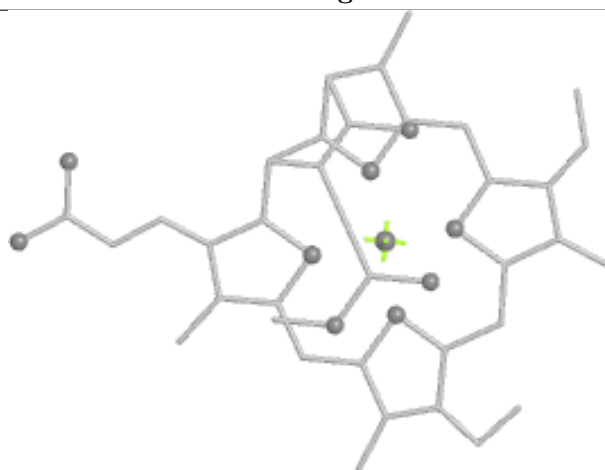
Bond lengths



Bond angles

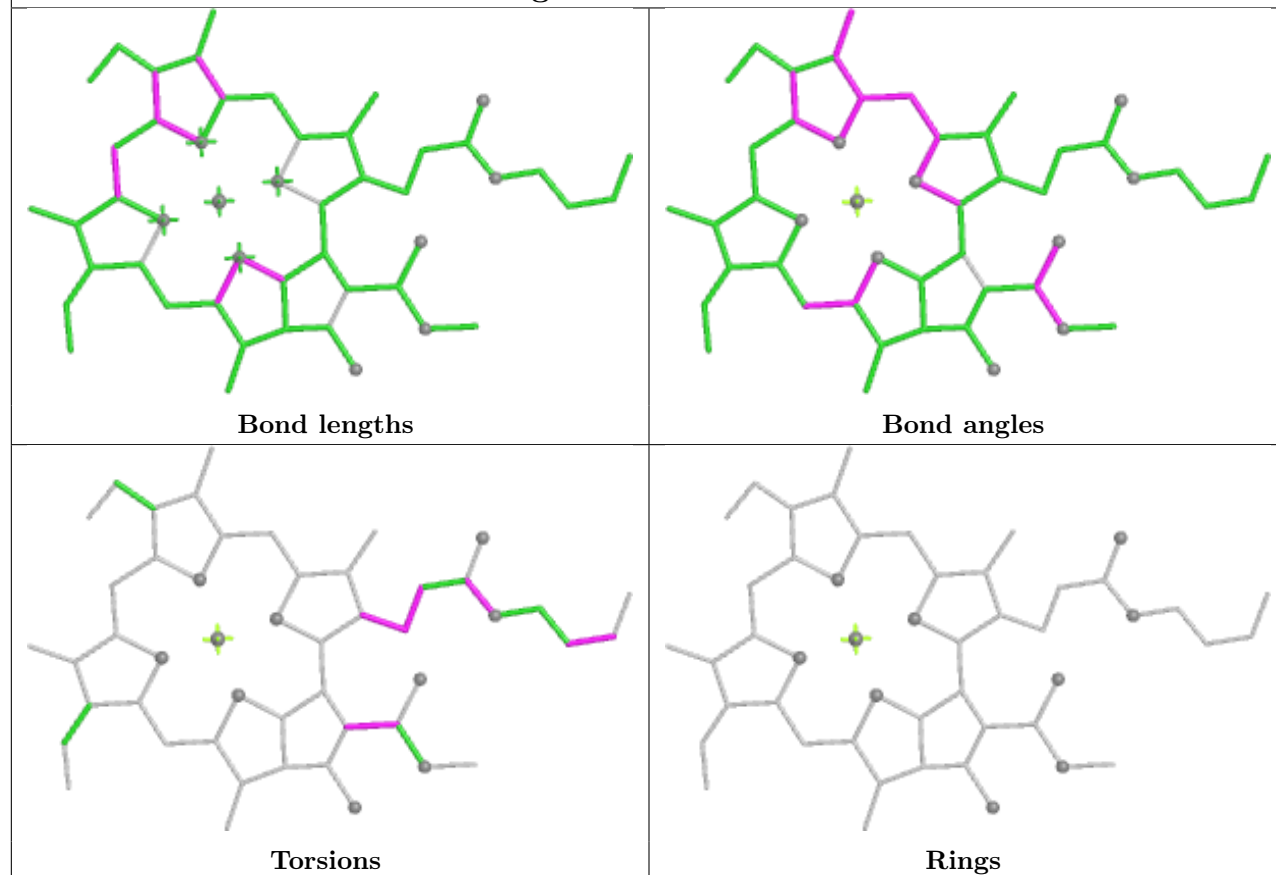


Torsions

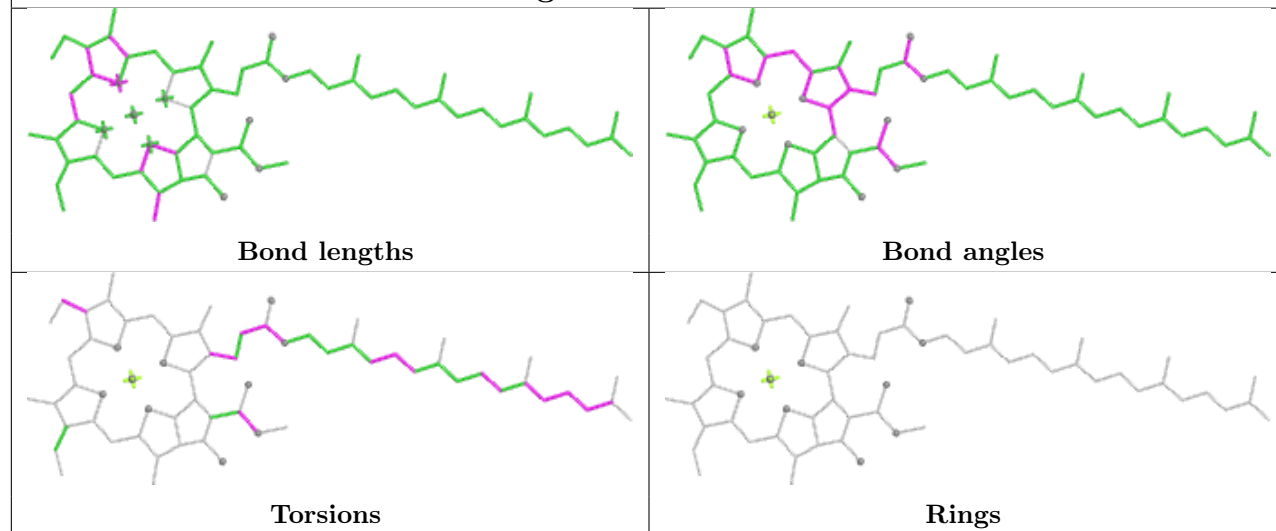


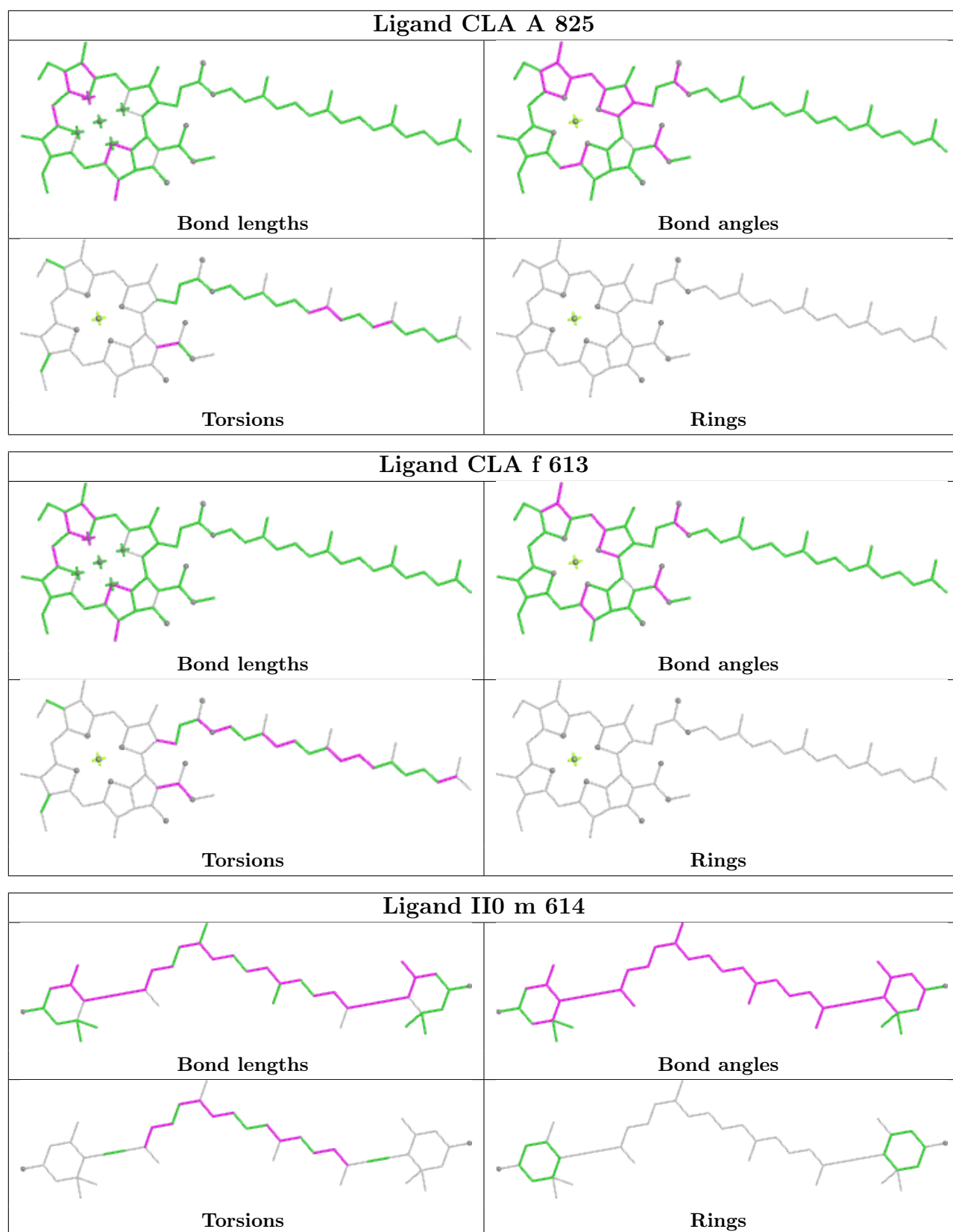
Rings

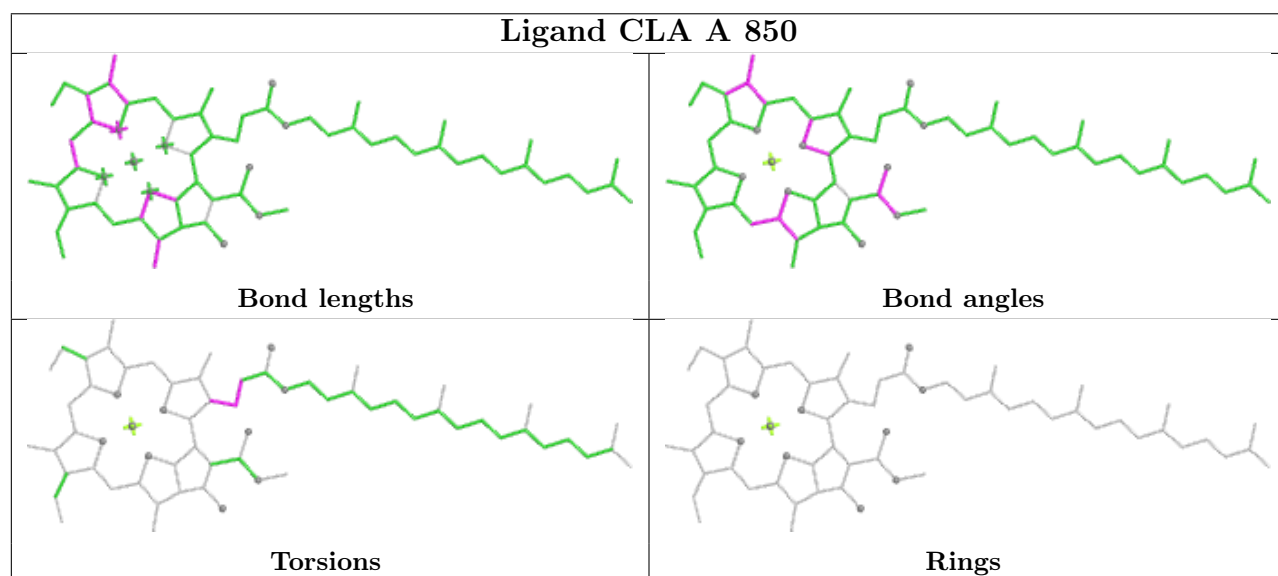
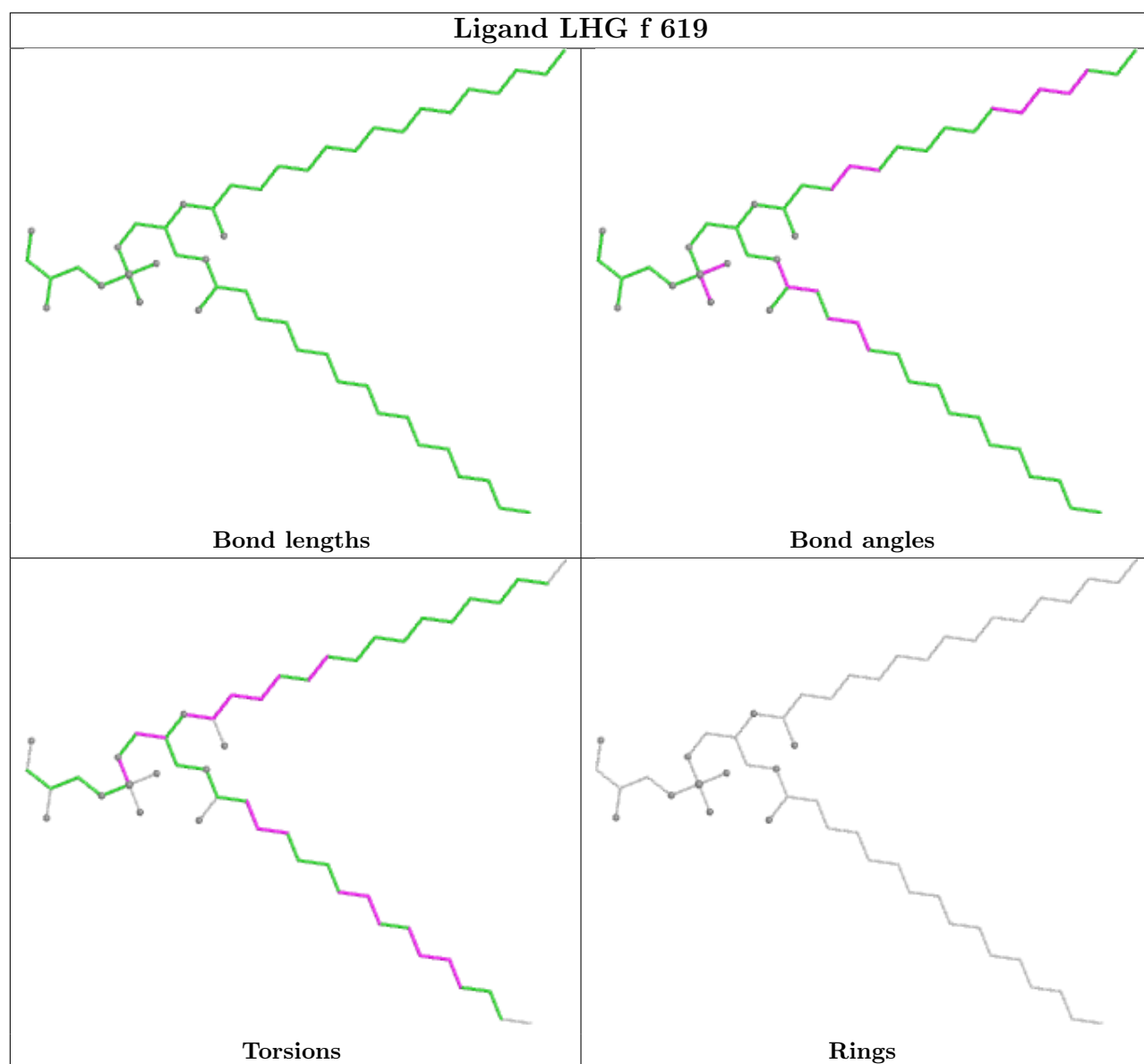
Ligand CLA A 821

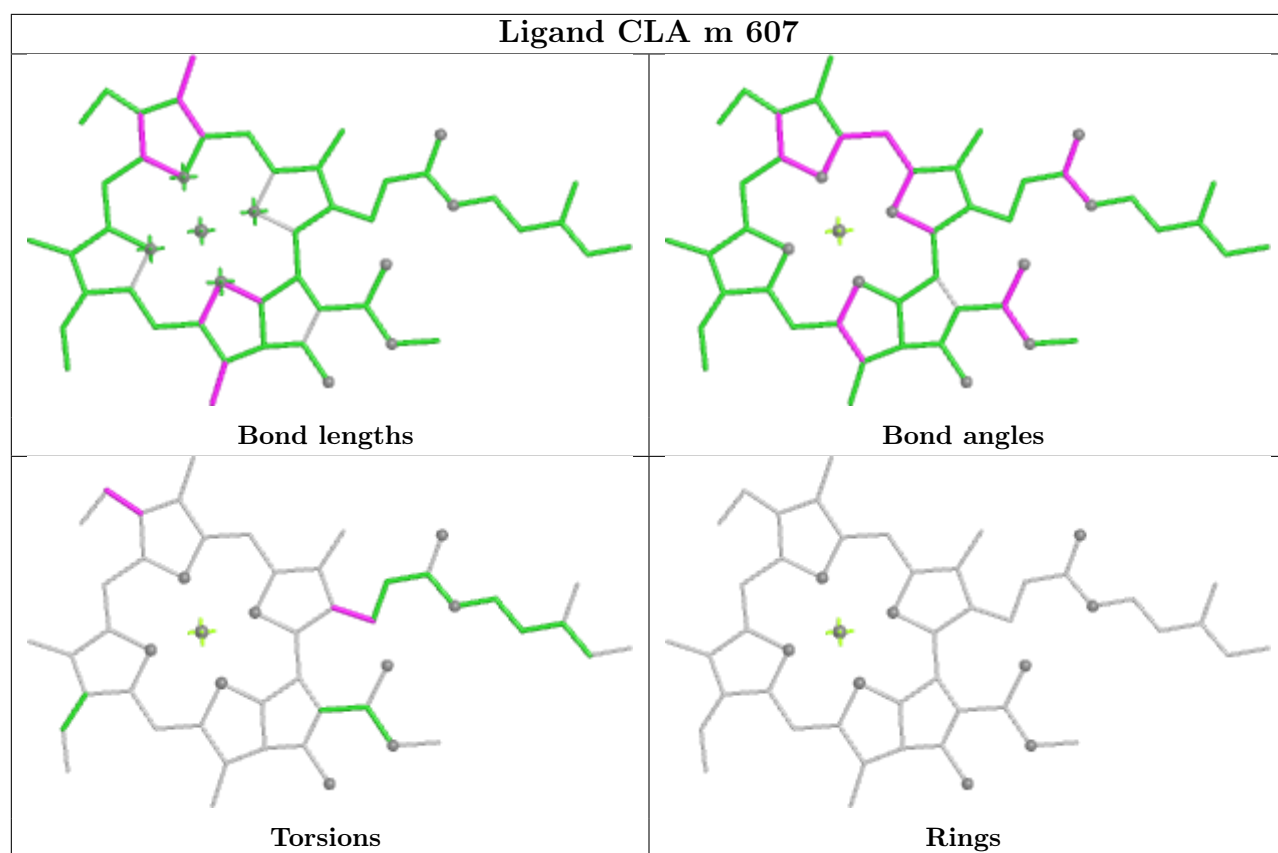


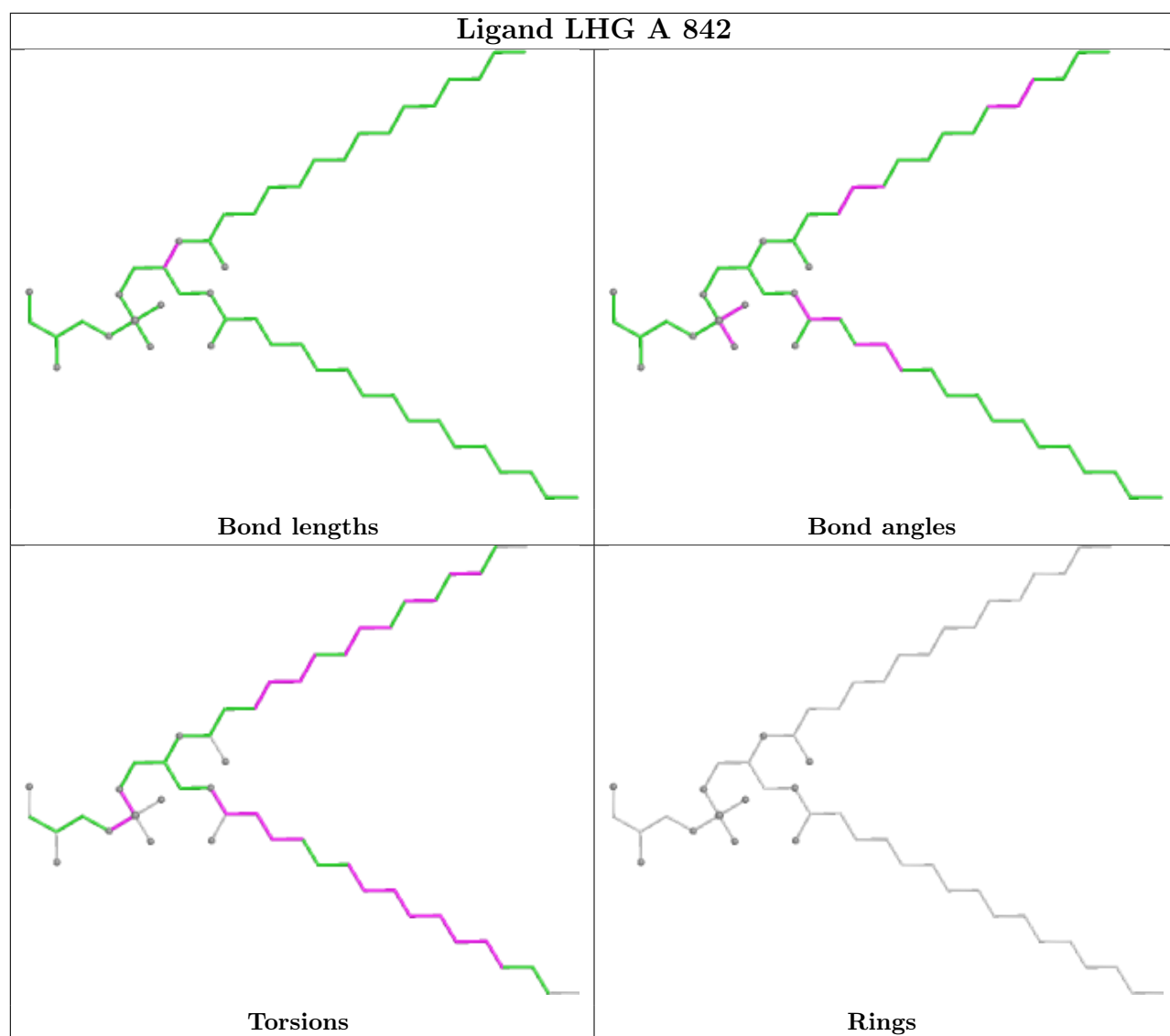
Ligand CLA e 311

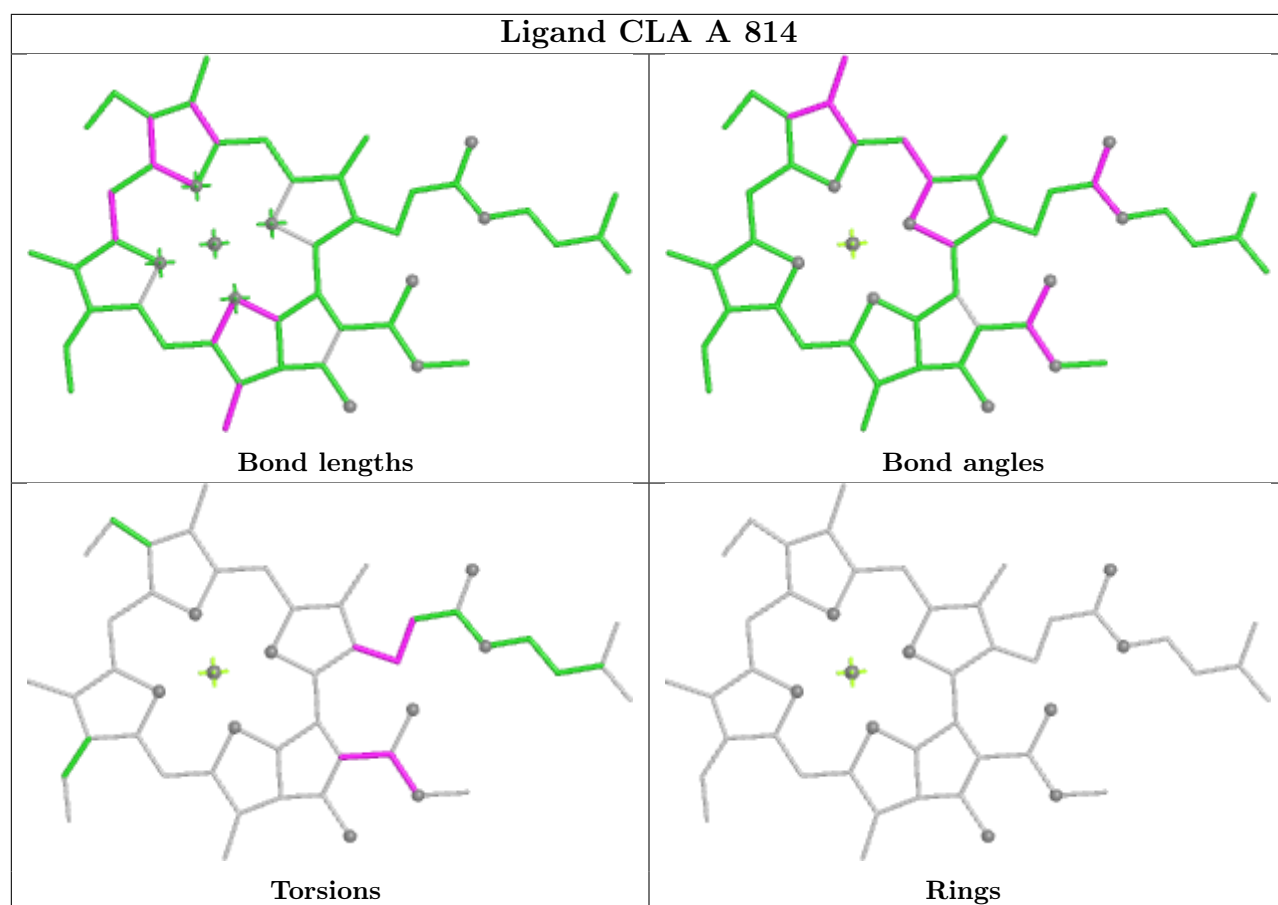


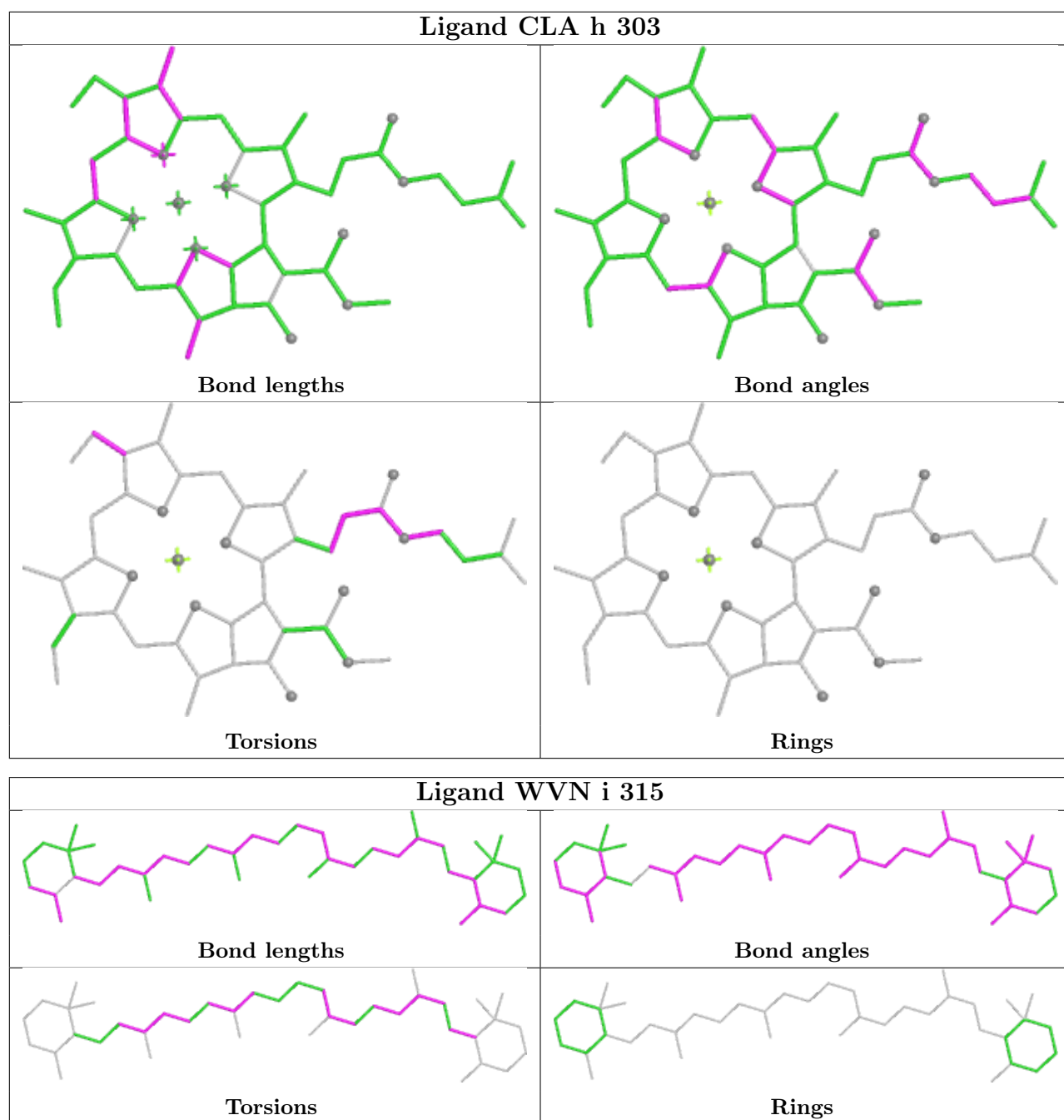


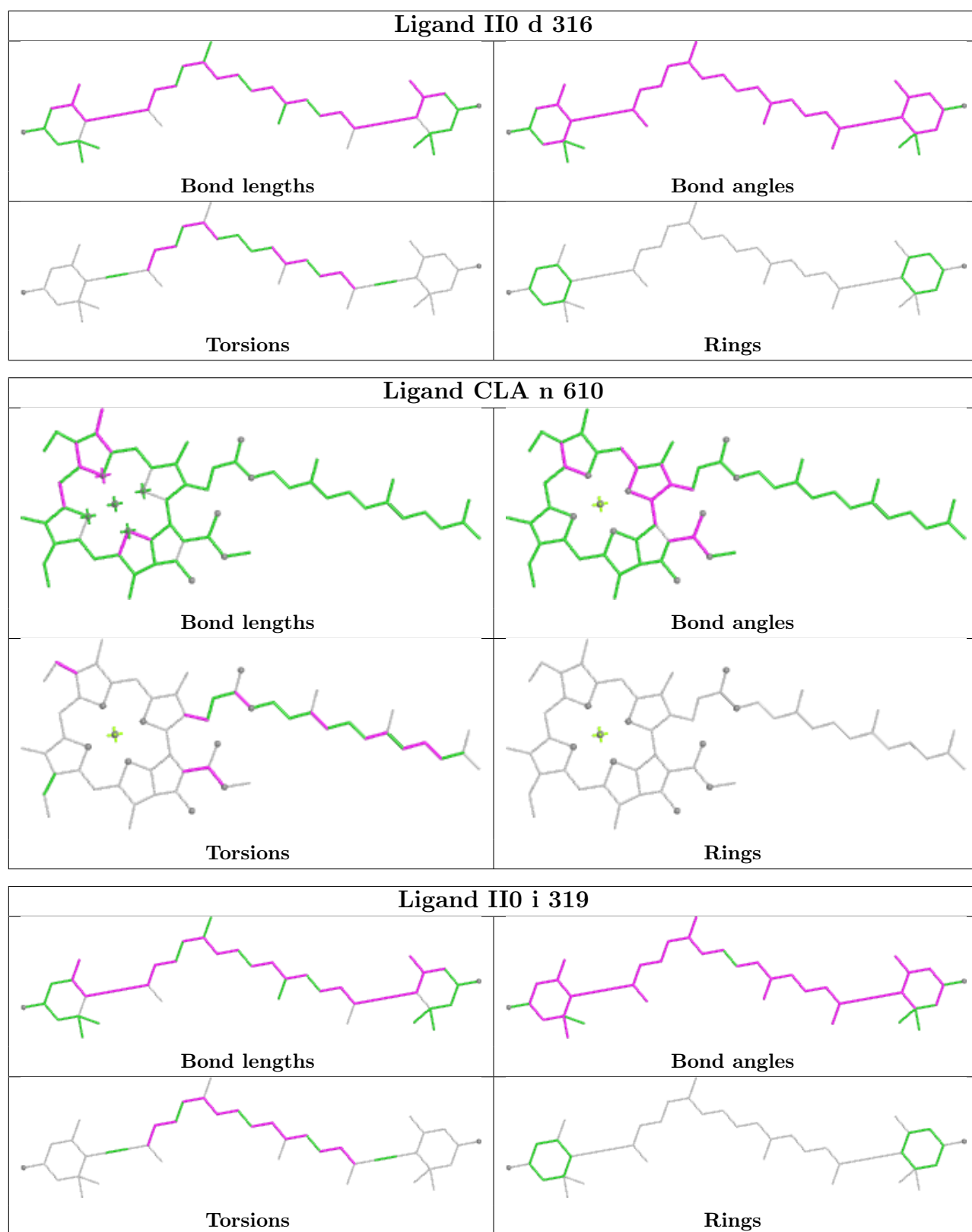


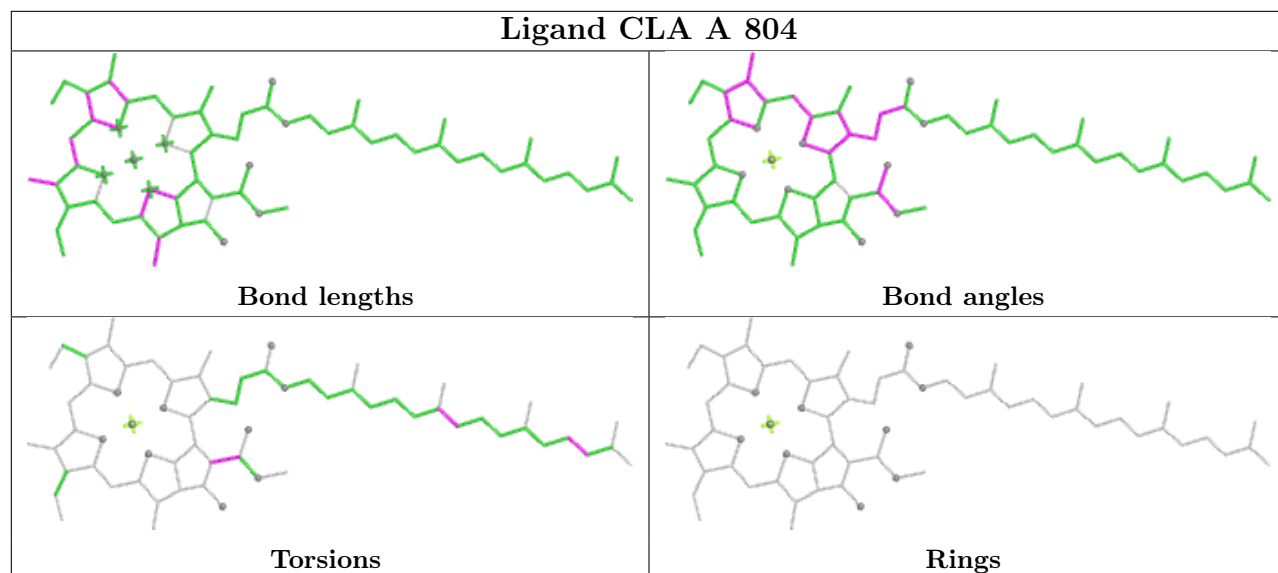
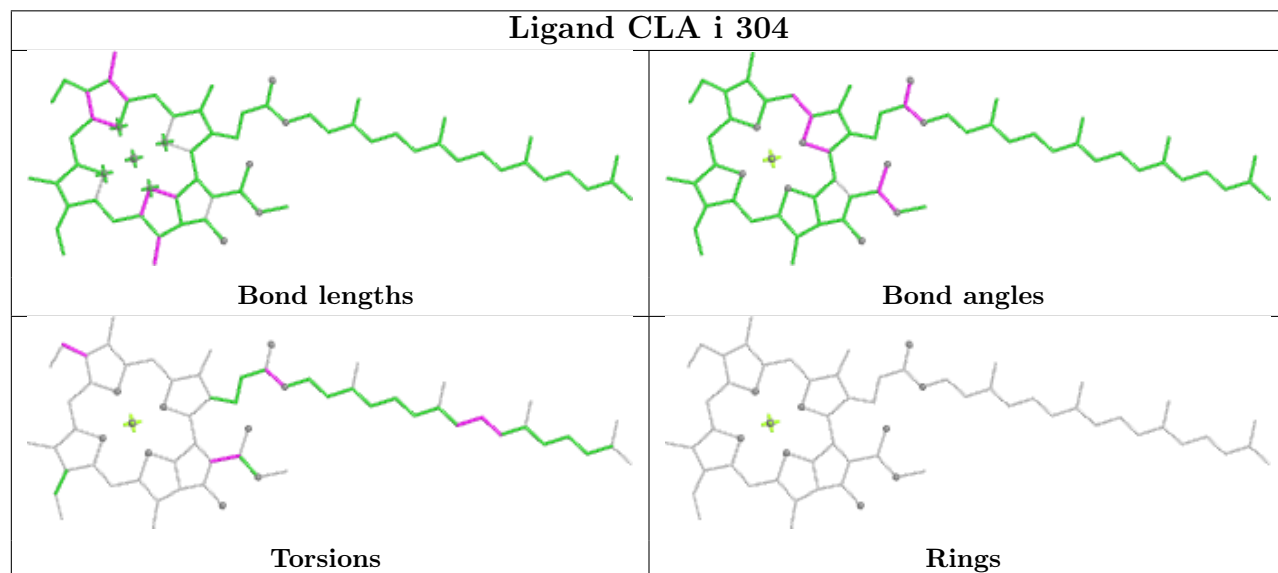
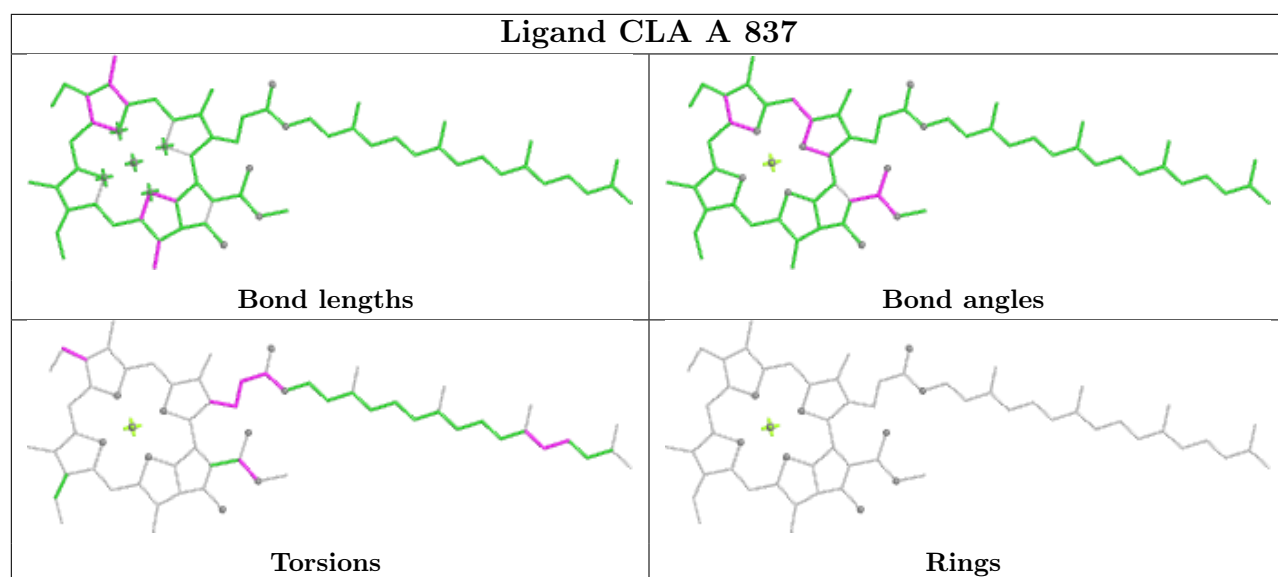


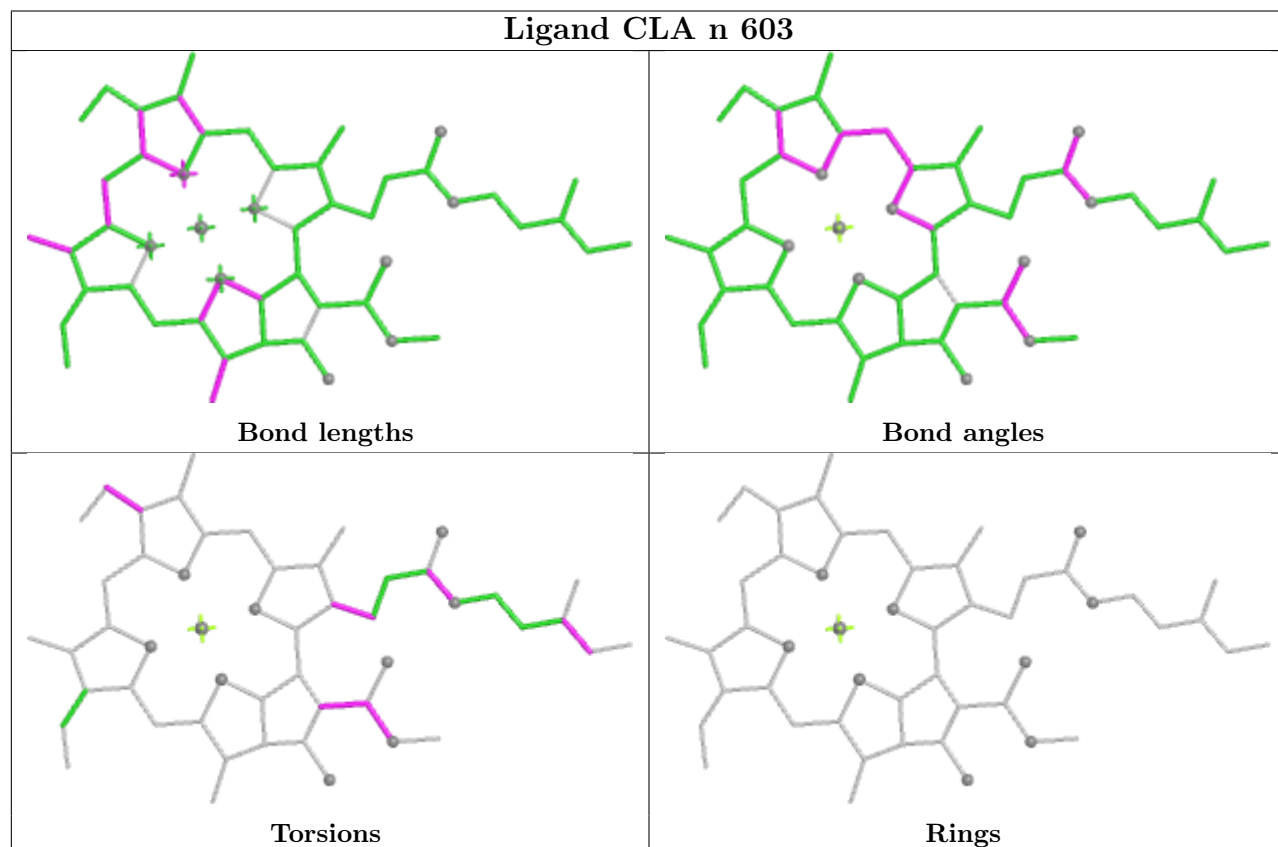
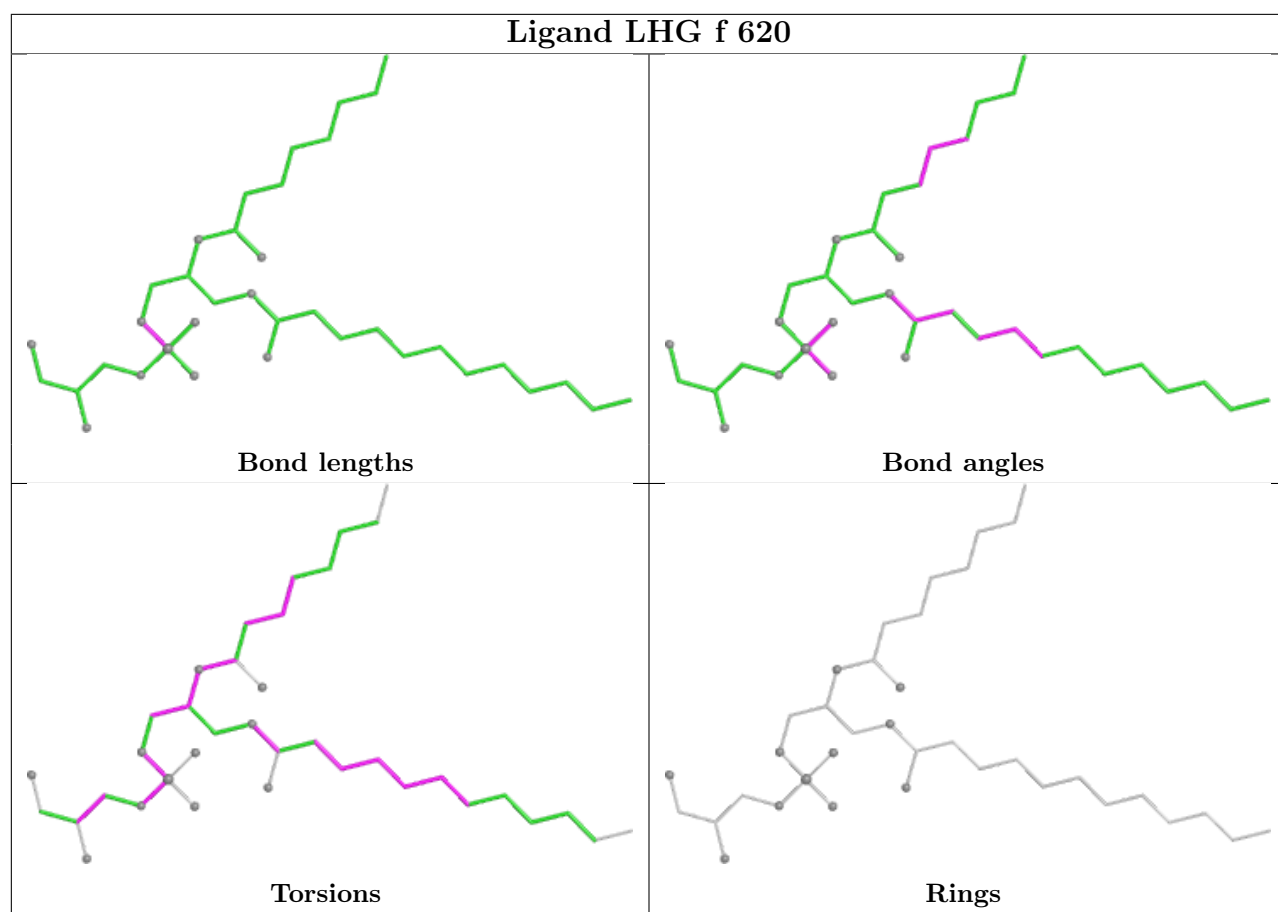


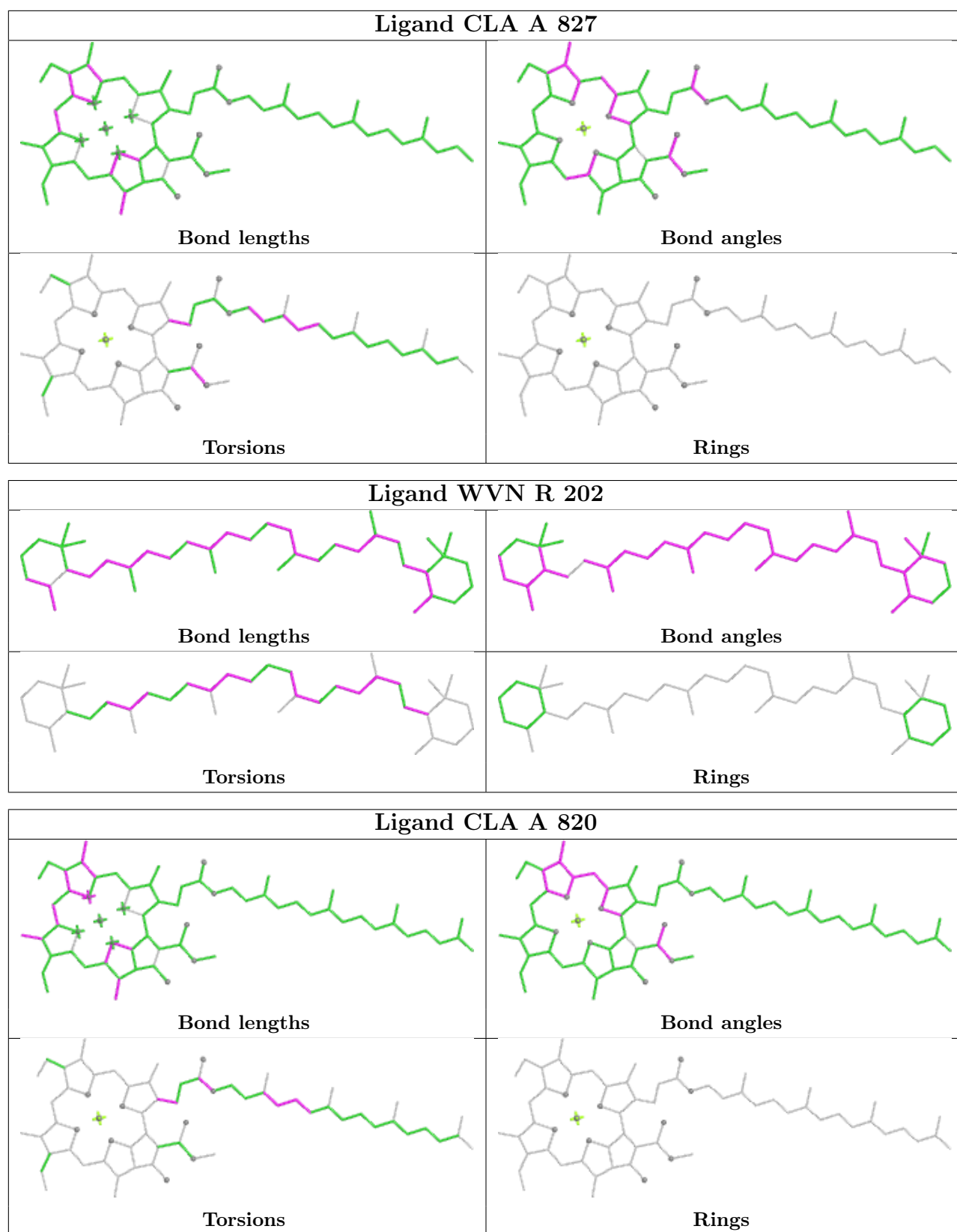




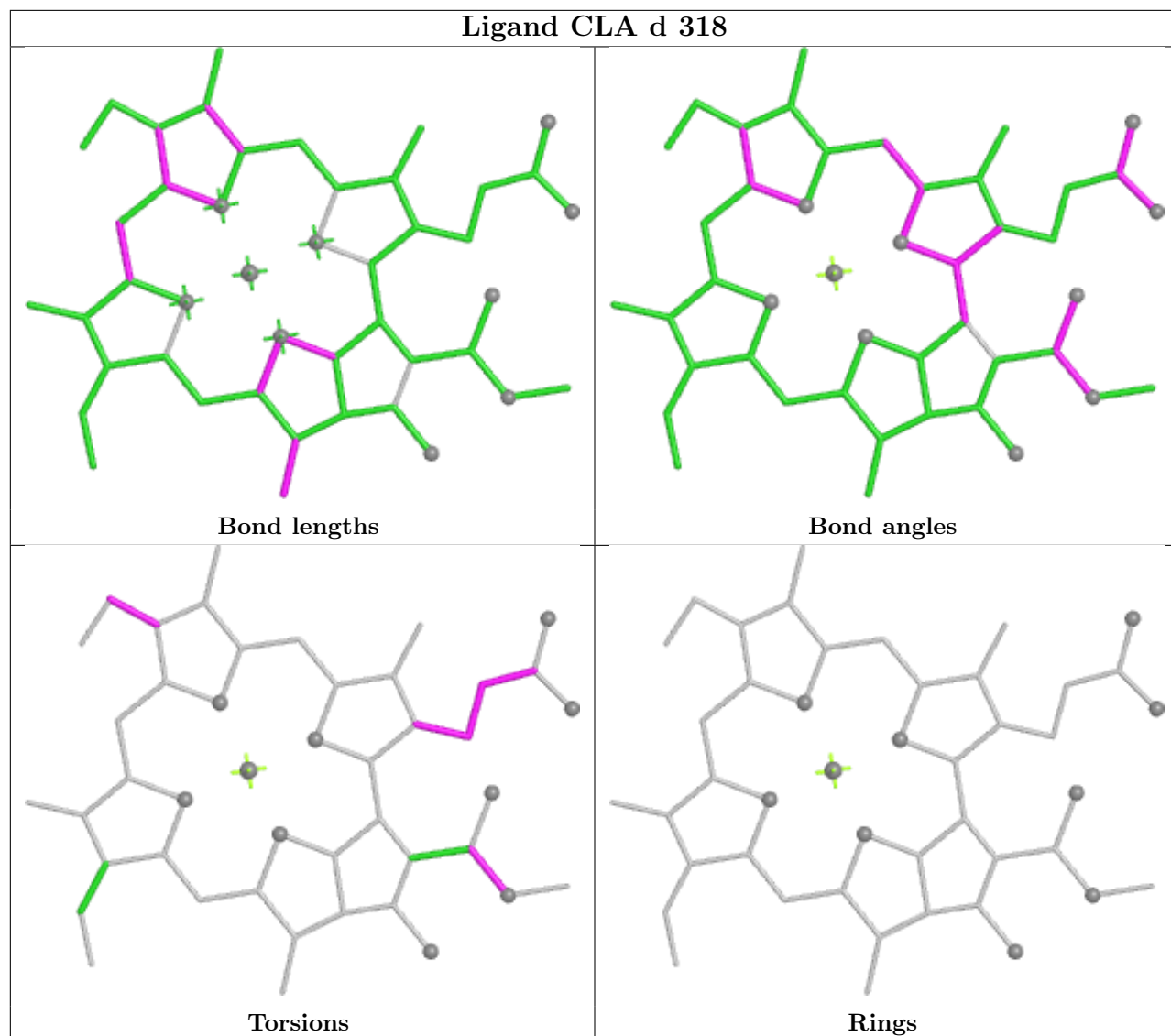




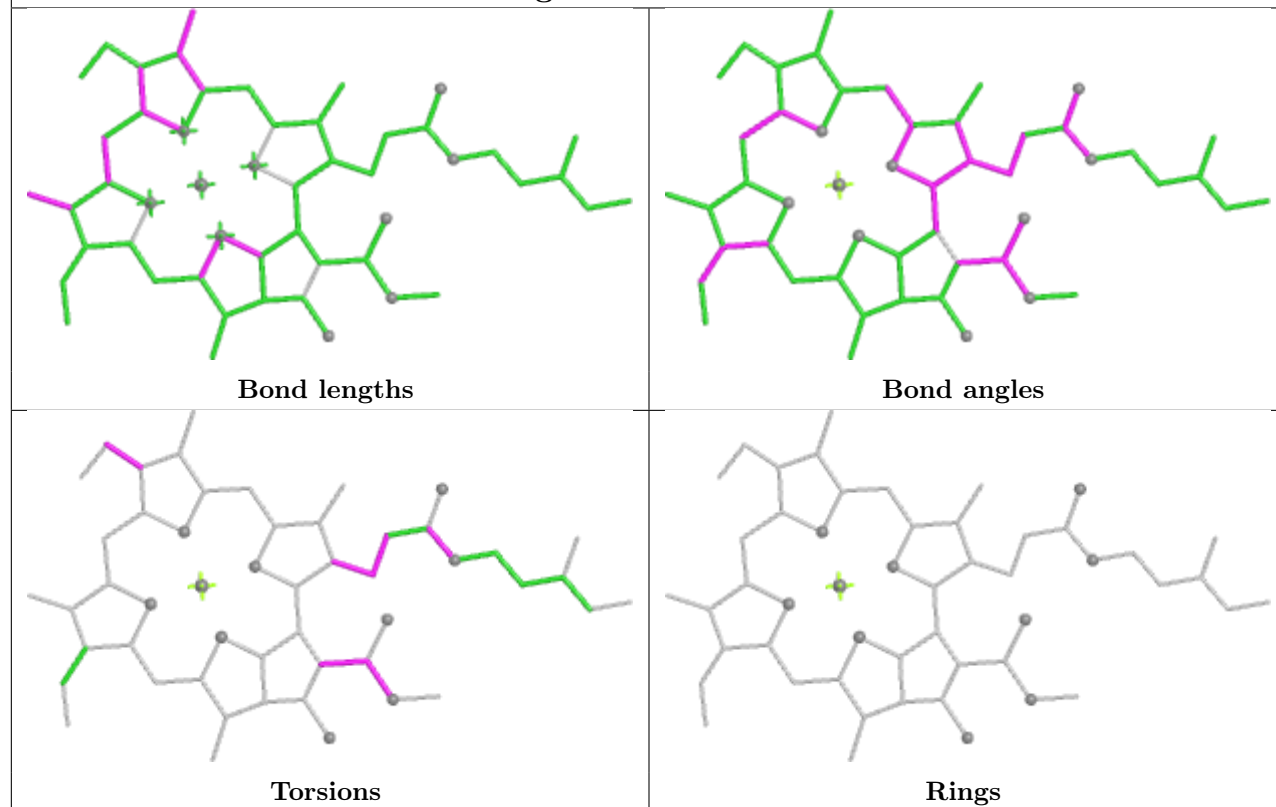




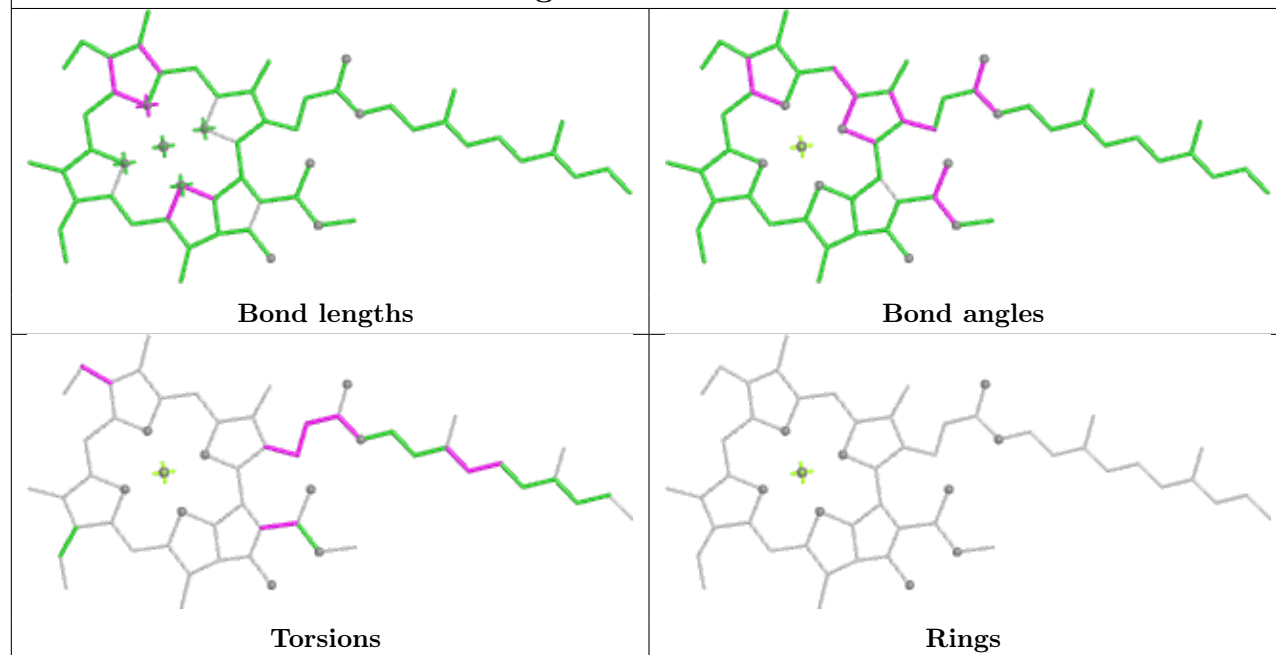
Ligand CLA d 318



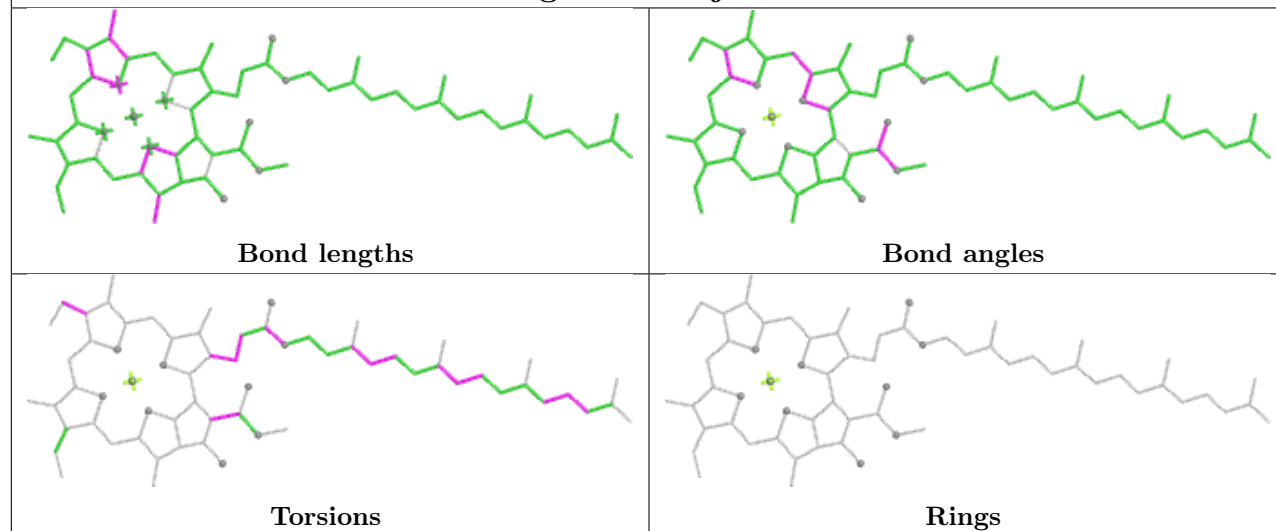
Ligand CLA d 313



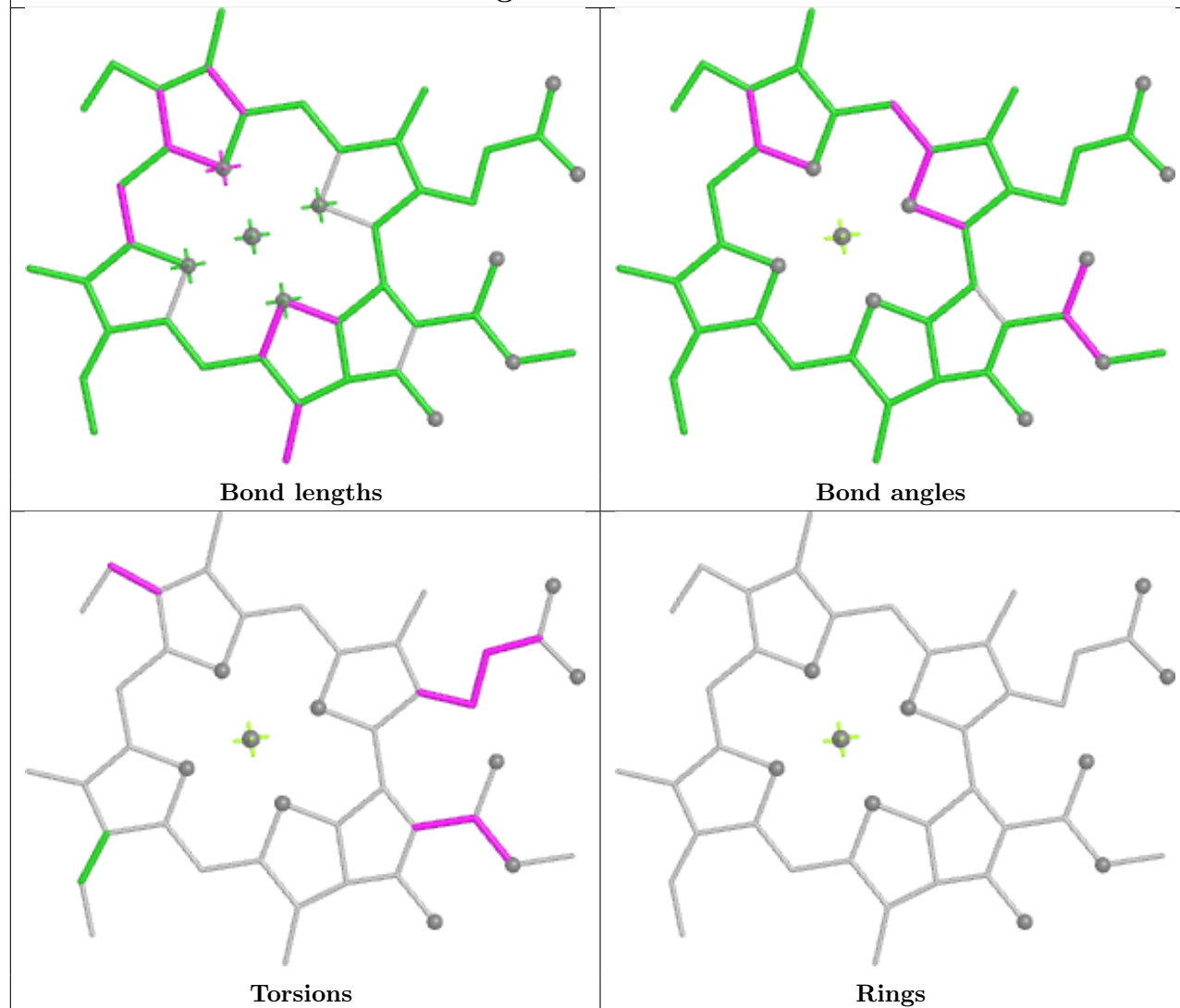
Ligand CLA h 306

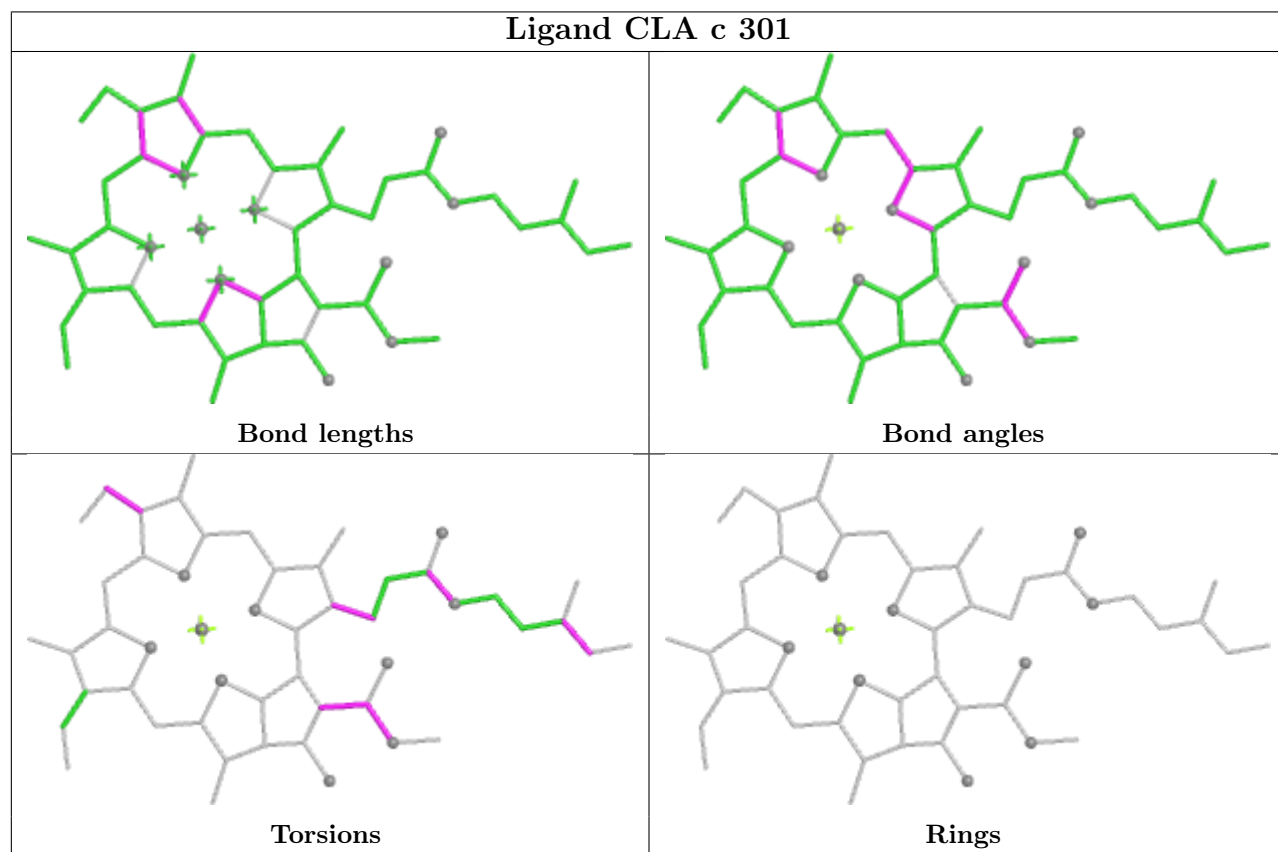
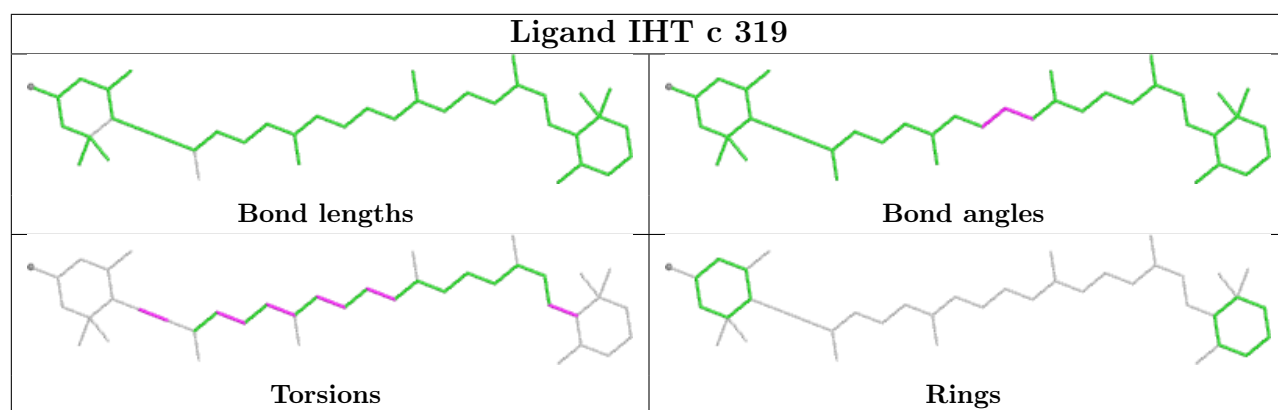


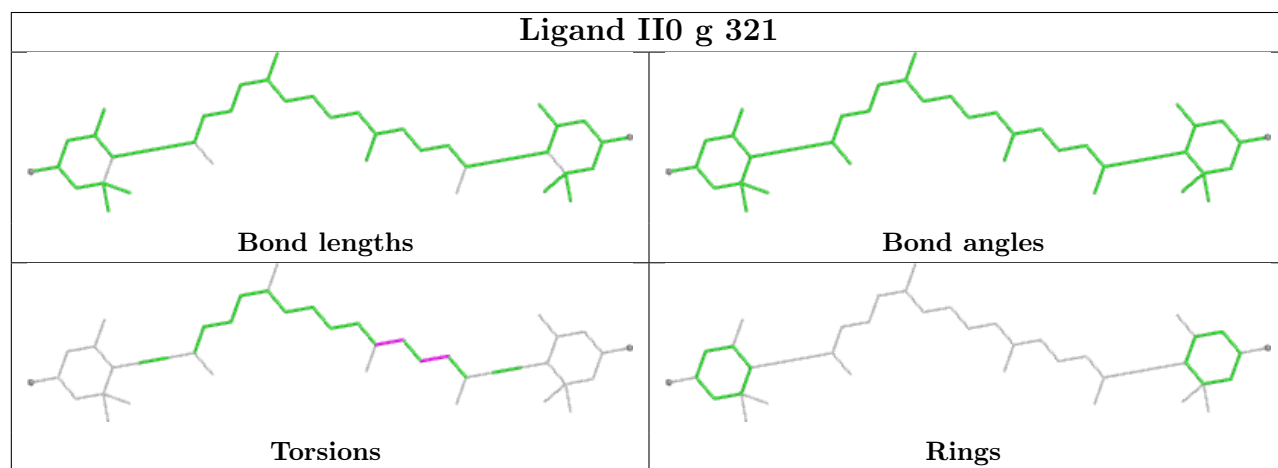
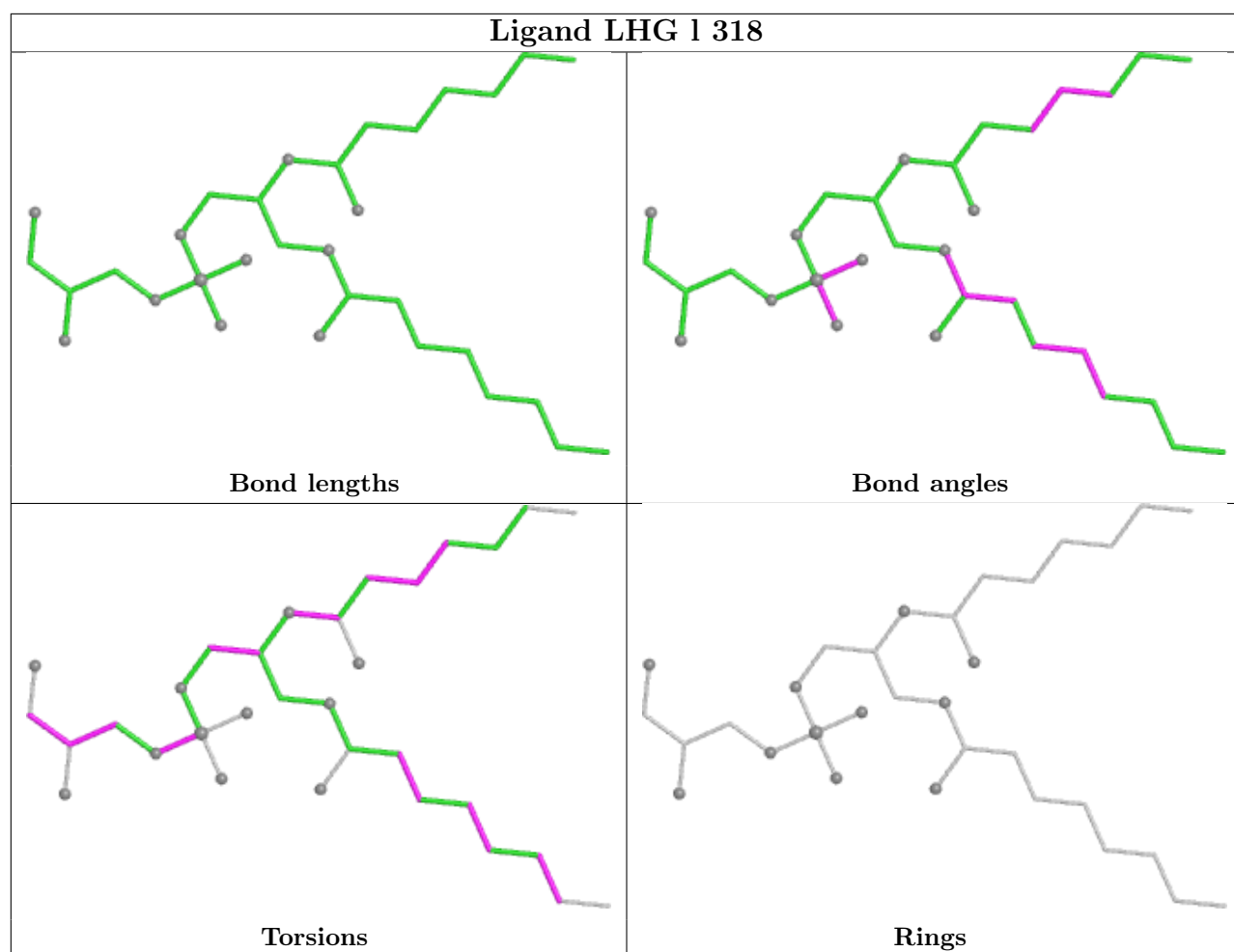
Ligand CLA j 302

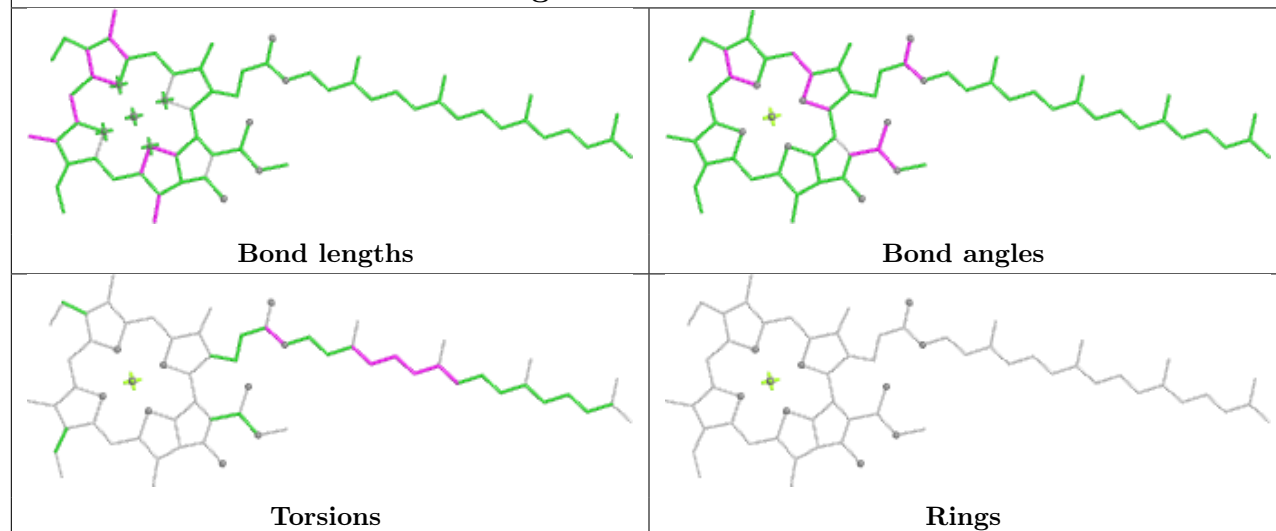
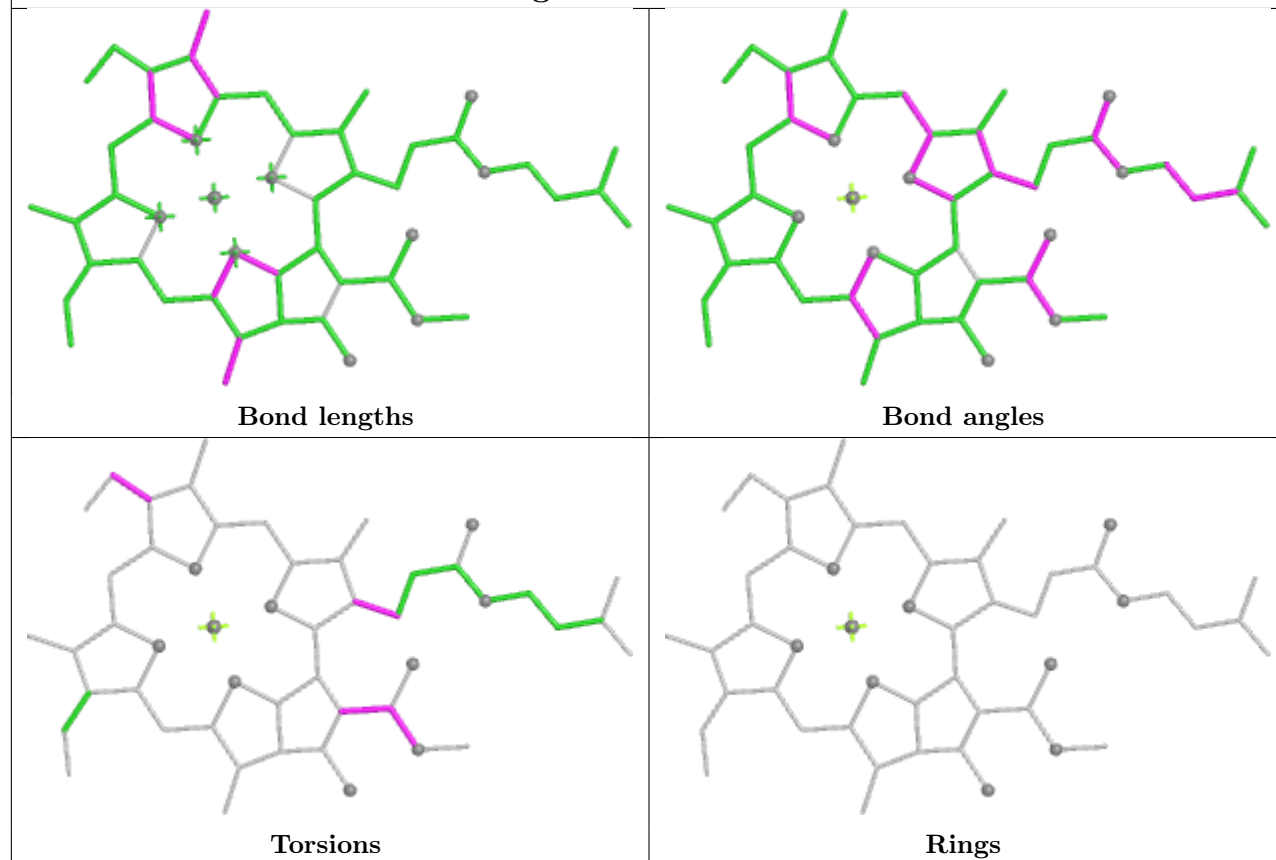


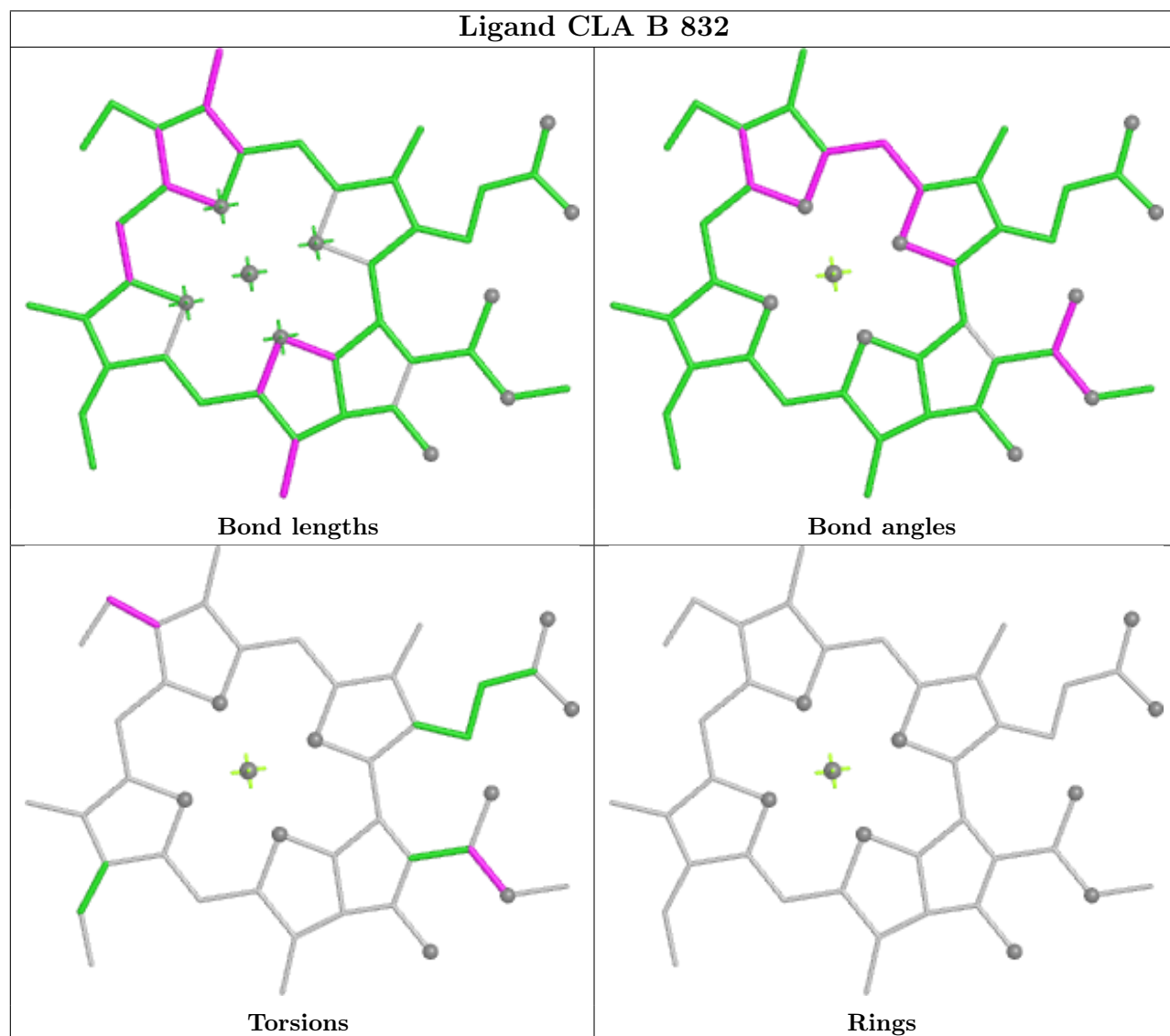
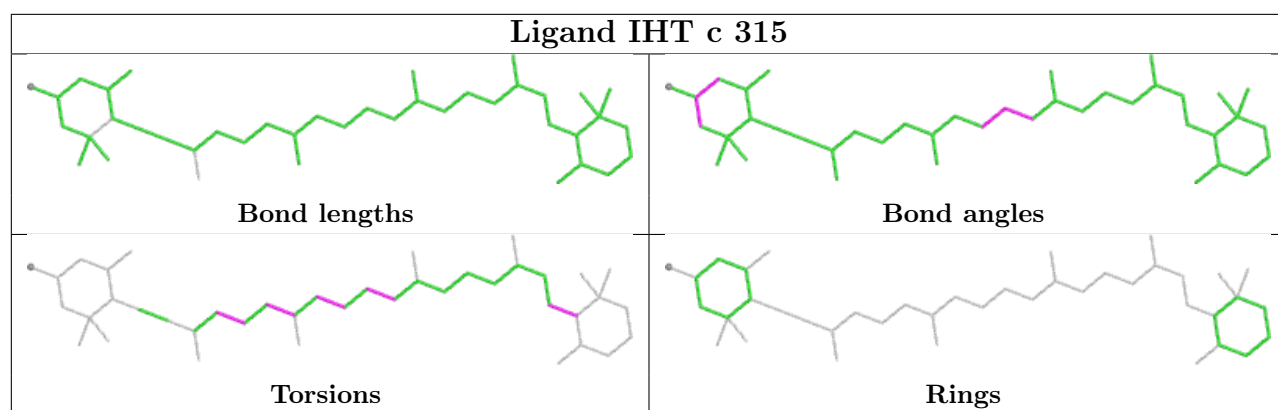
Ligand CLA e 301



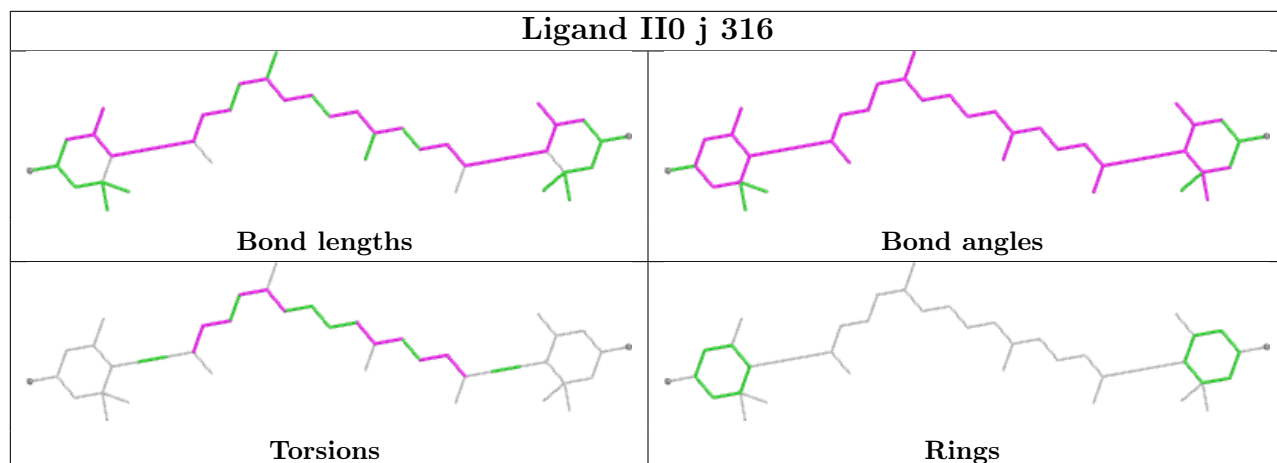




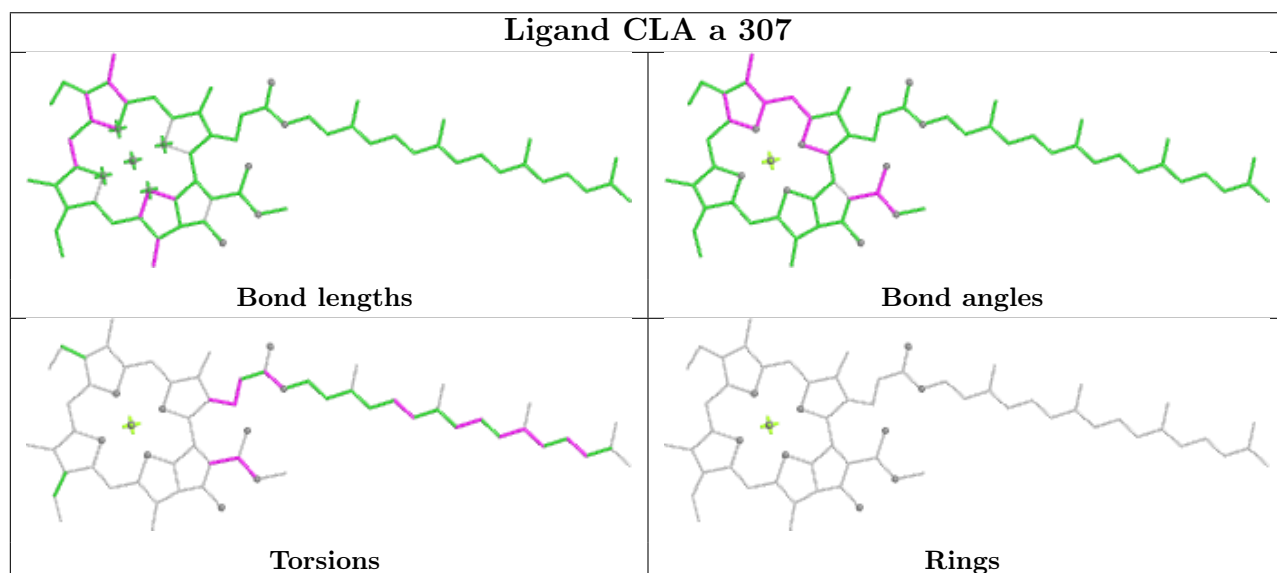
Ligand CLA A 826**Ligand CLA B 830**



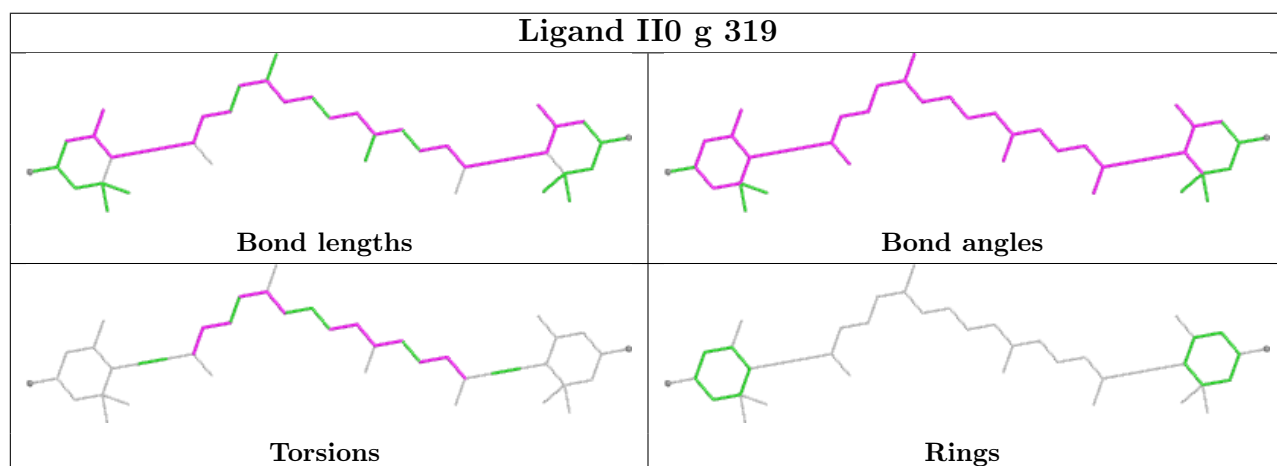
Ligand II0 j 316

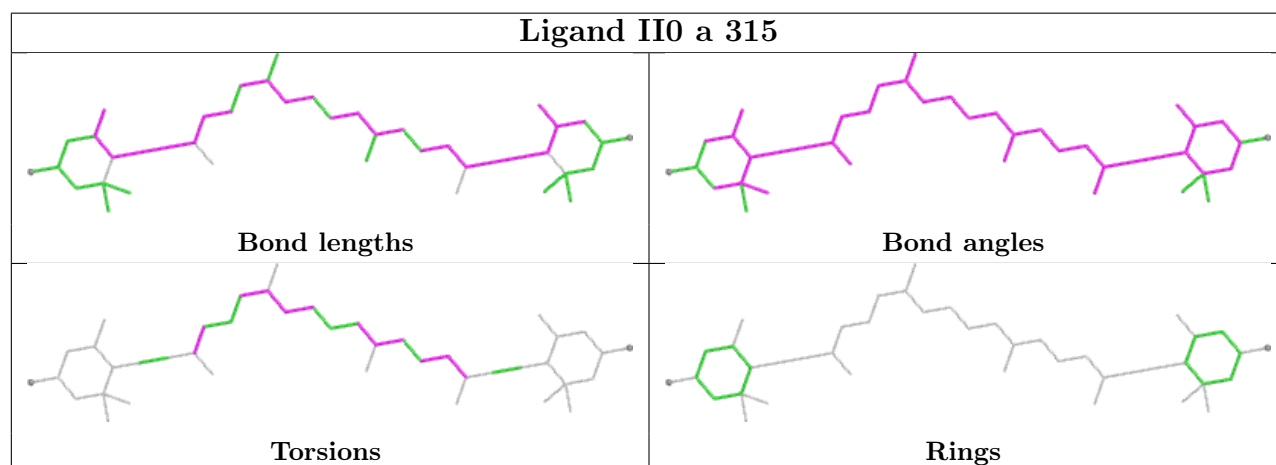
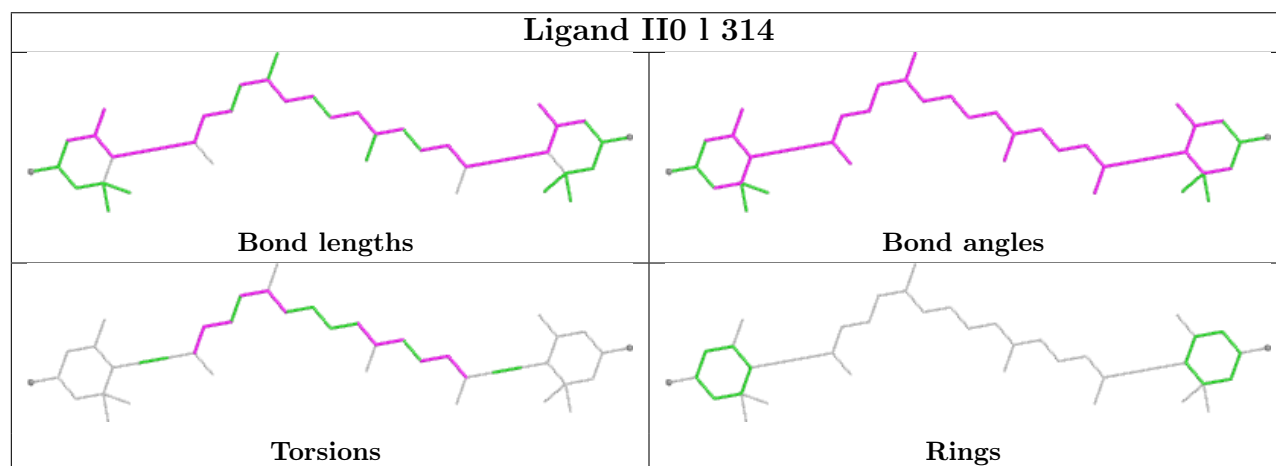
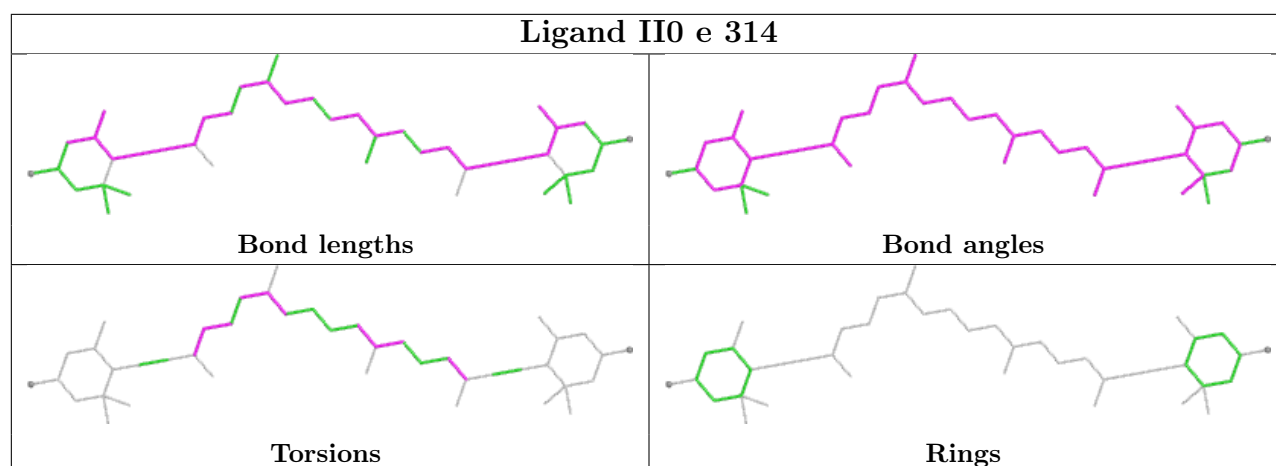


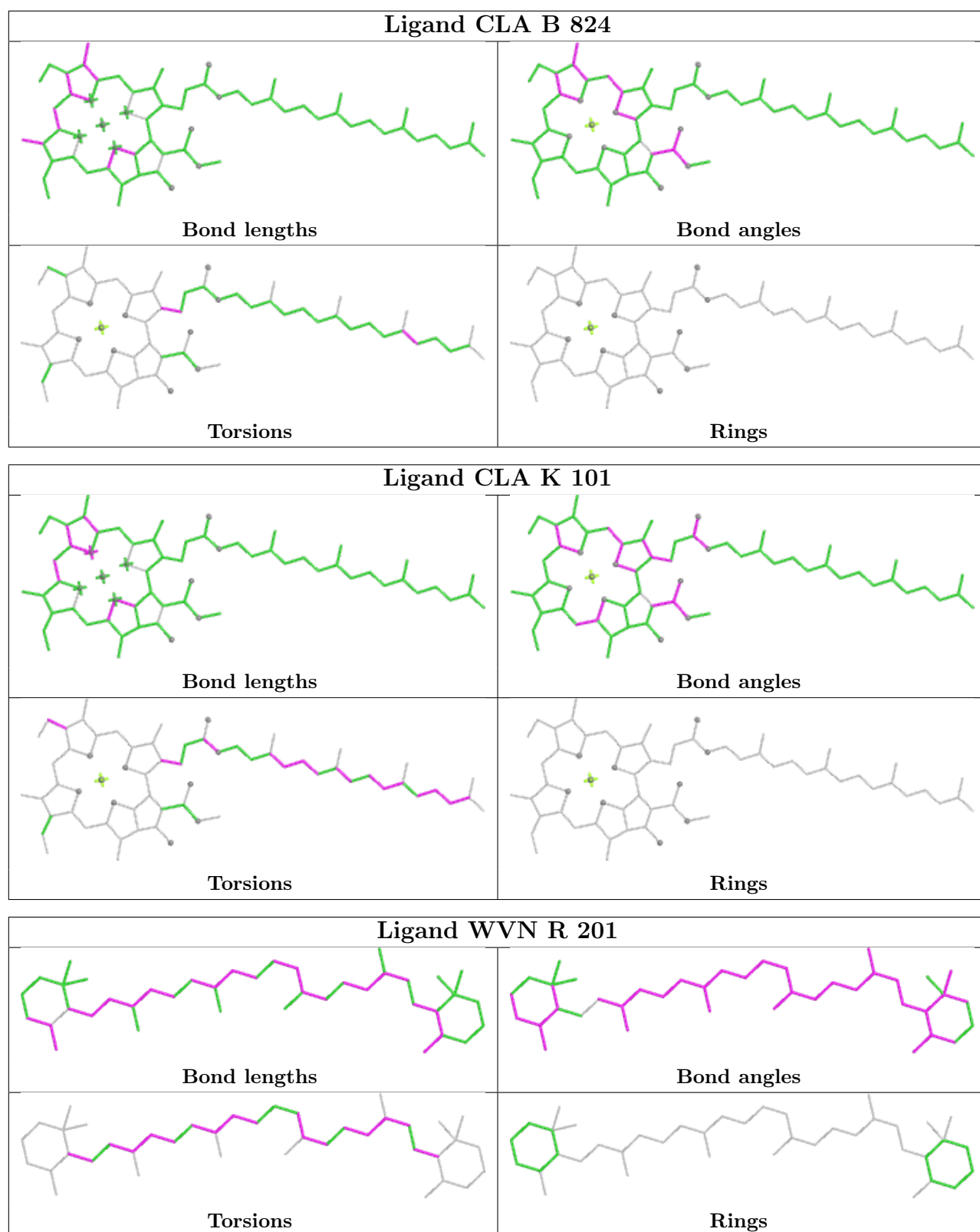
Ligand CLA a 307

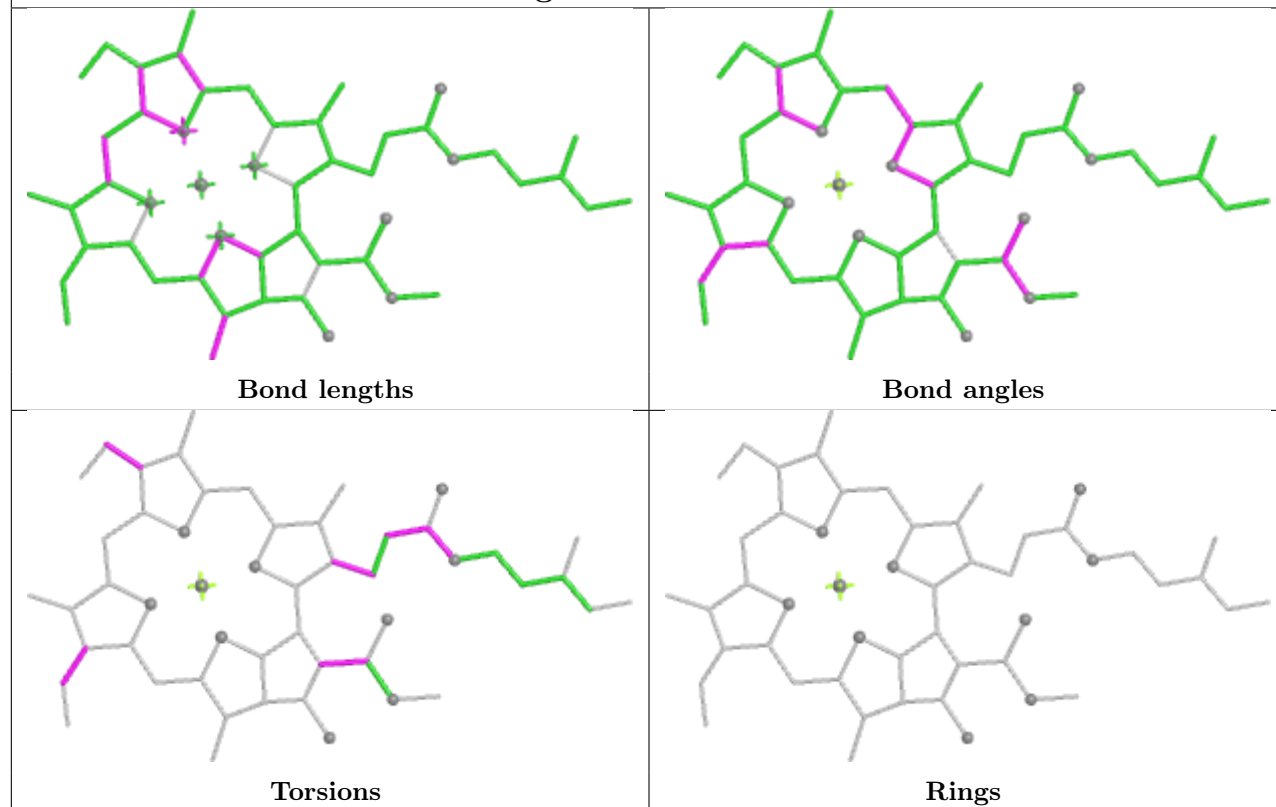
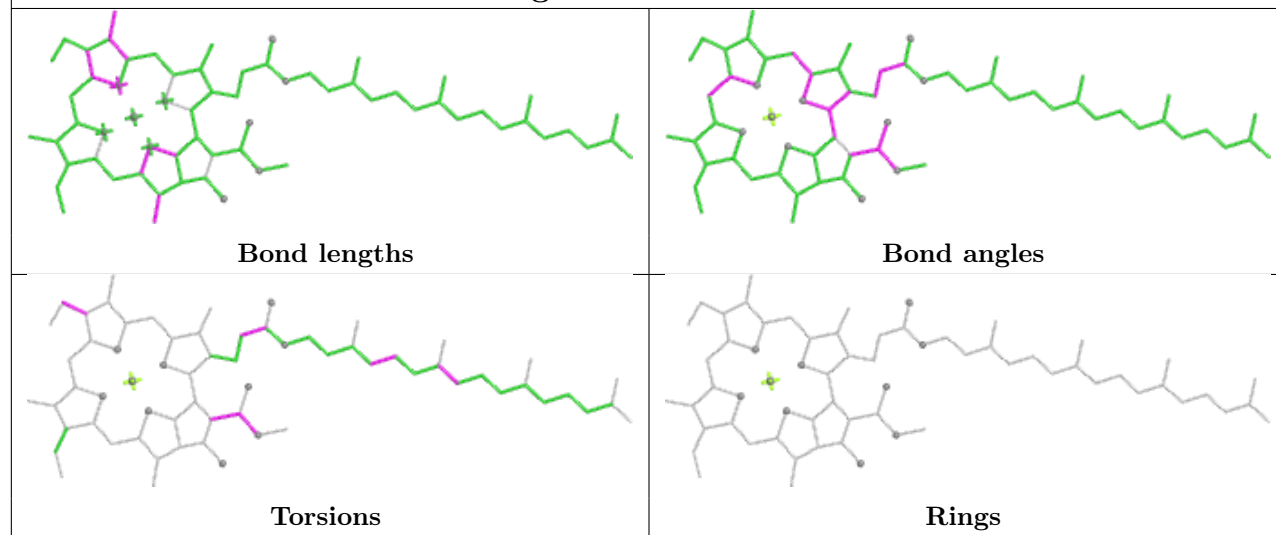


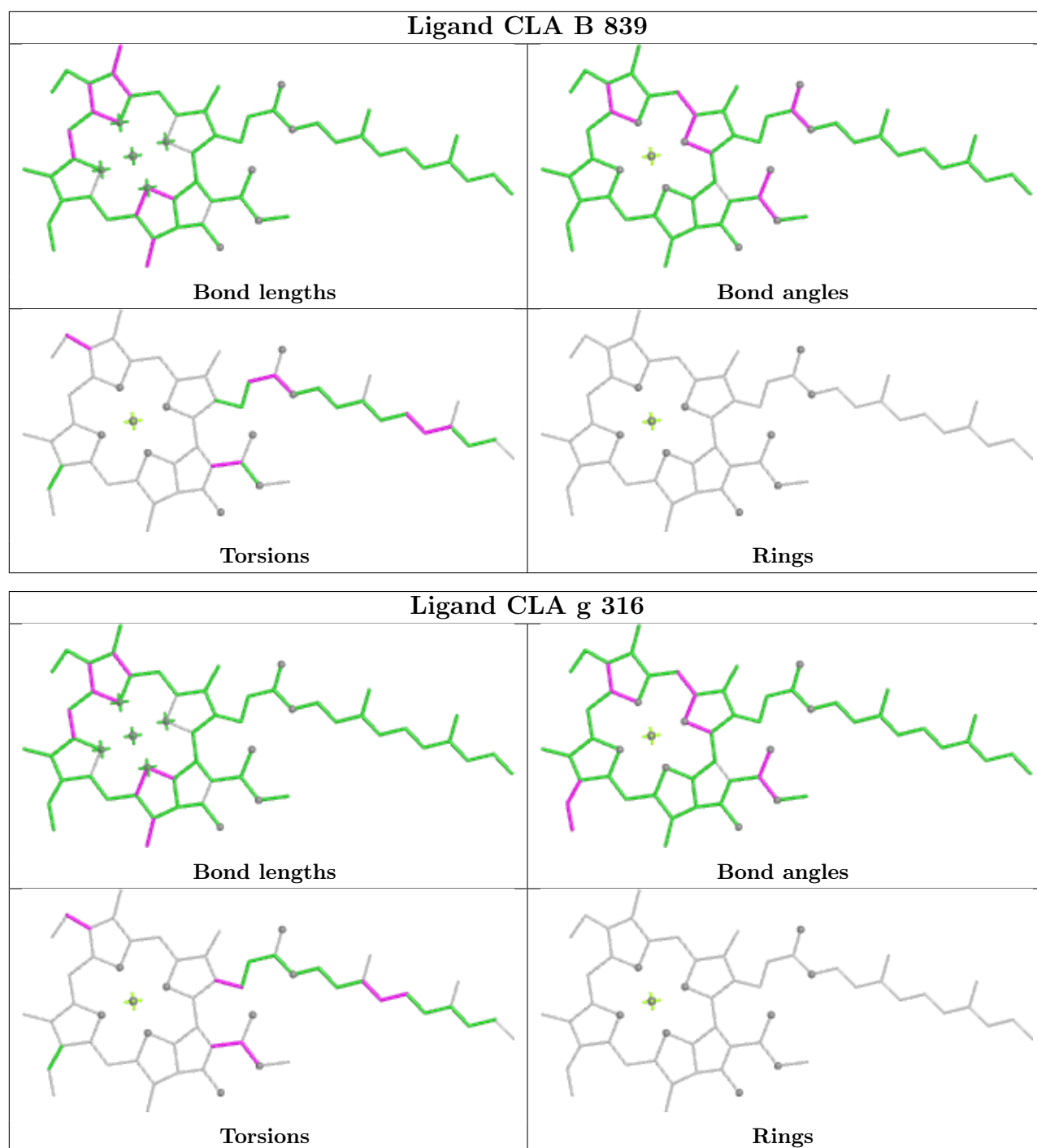
Ligand II0 g 319

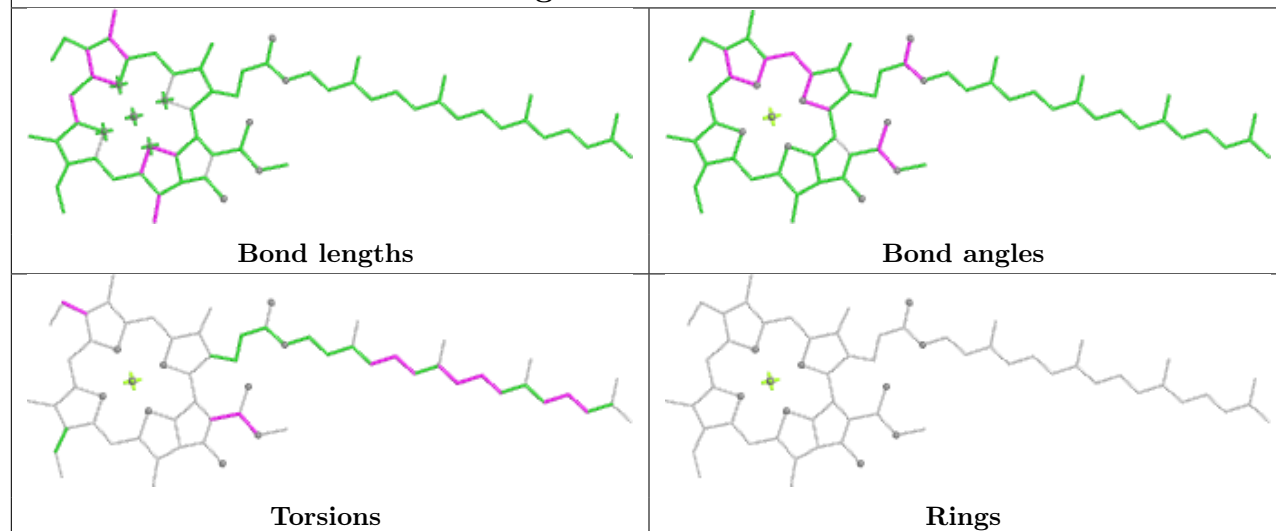
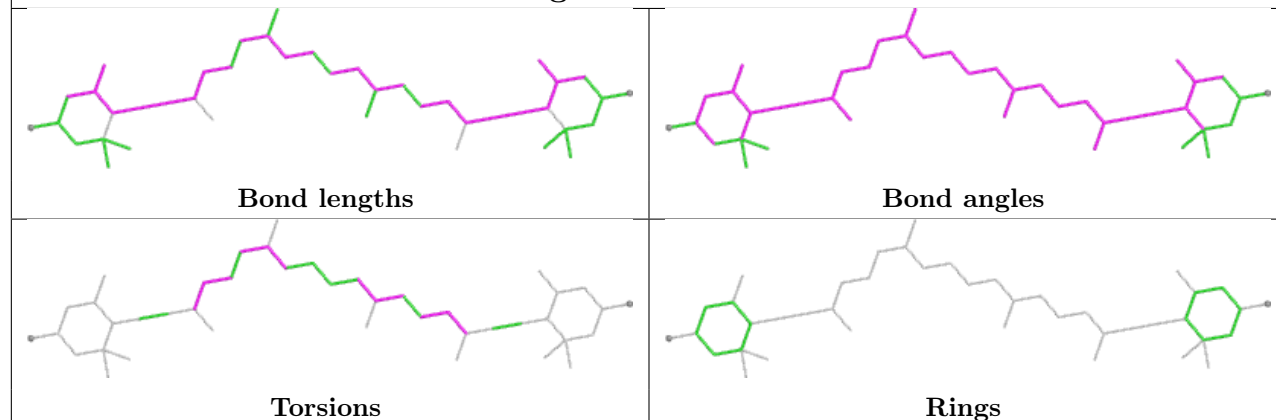
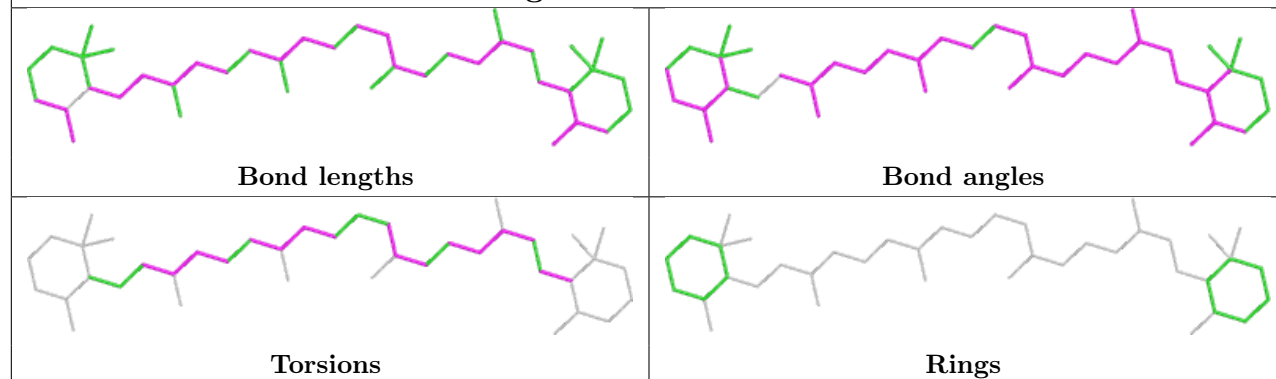


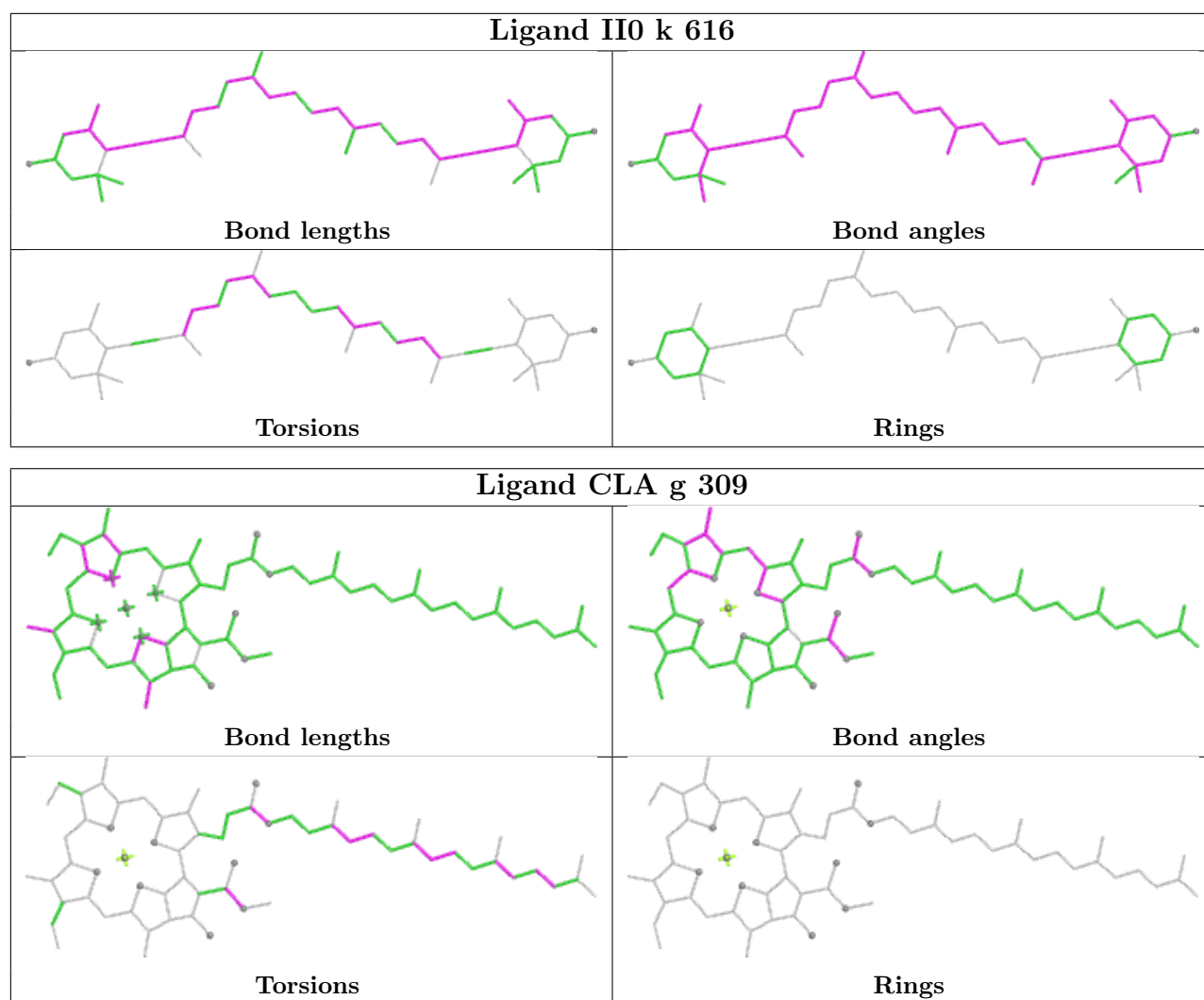


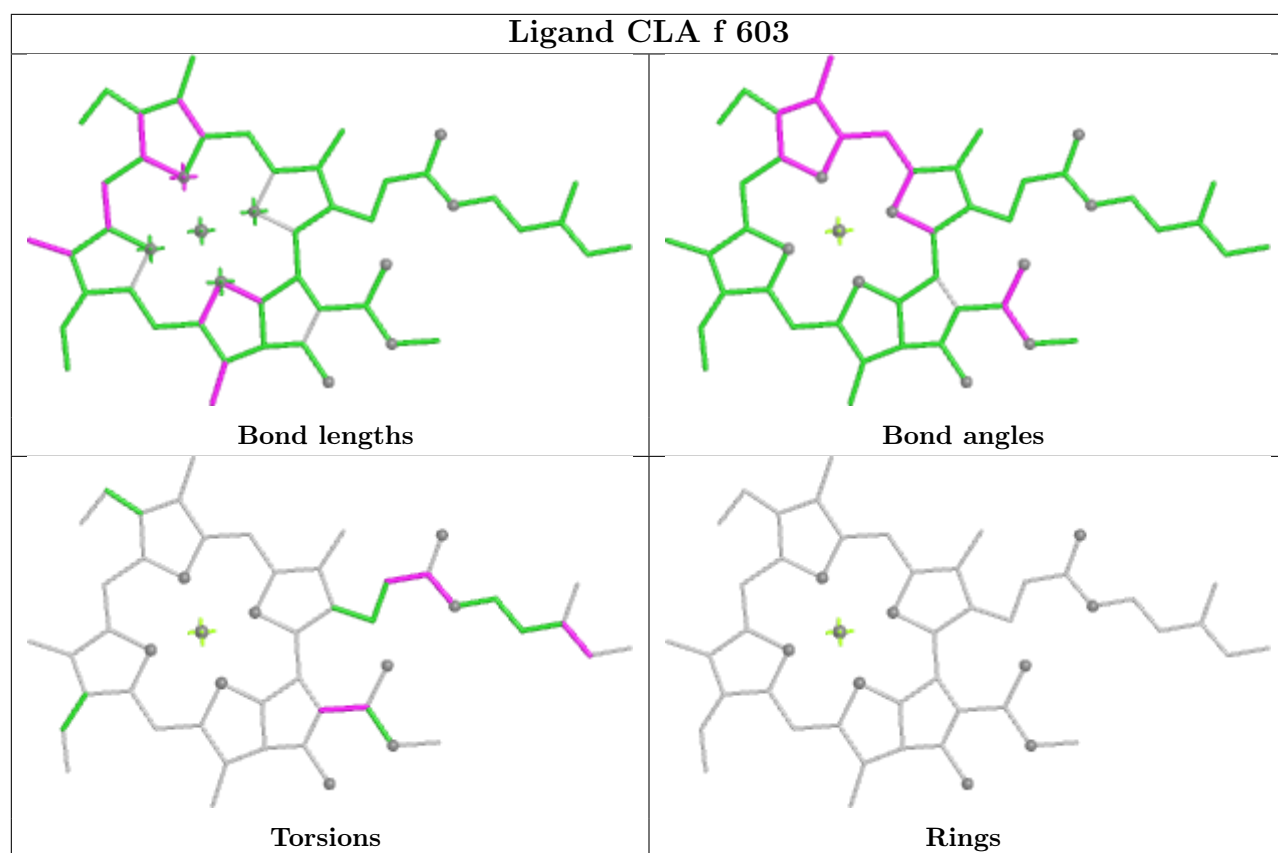


Ligand CLA n 605**Ligand CLA A 836**

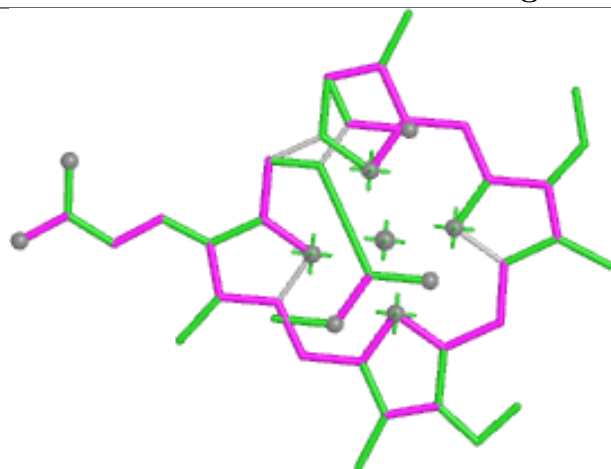


Ligand CLA b 310**Ligand II0 n 615****Ligand WVN L 206**

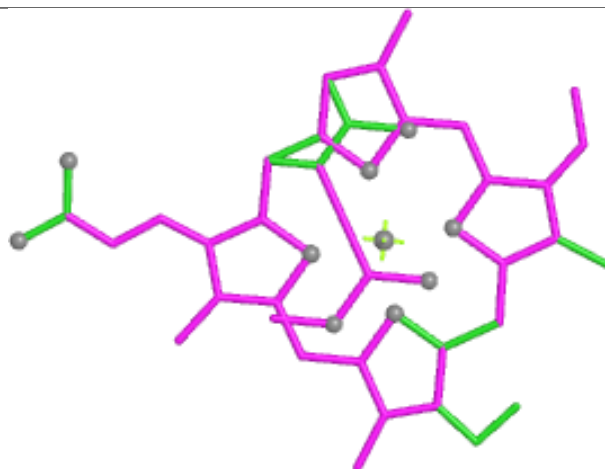




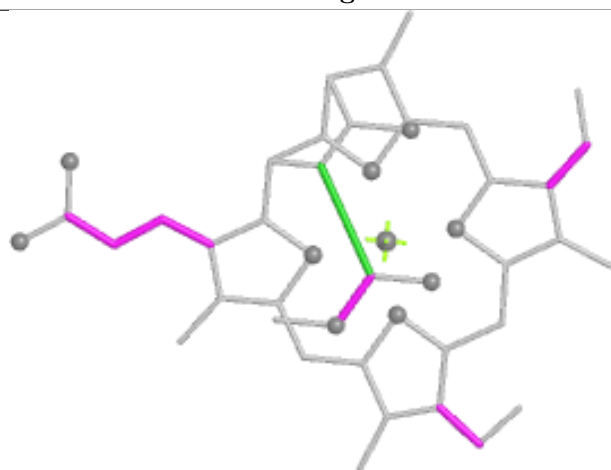
Ligand KC2 e 309



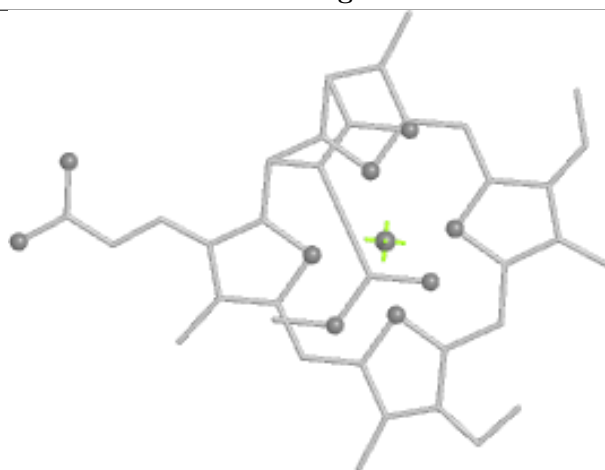
Bond lengths



Bond angles

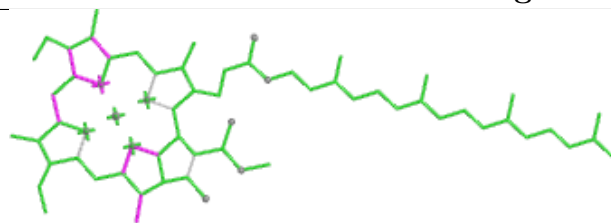


Torsions

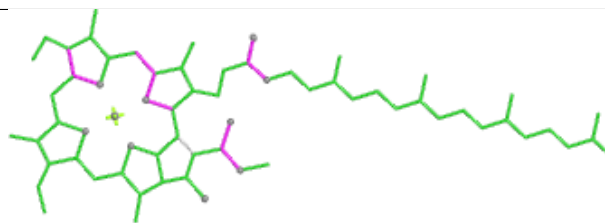


Rings

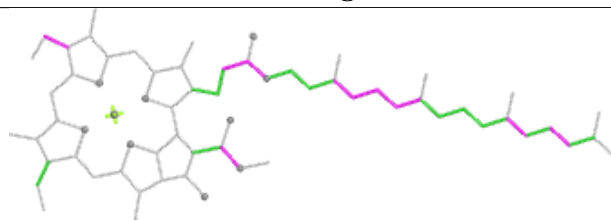
Ligand CLA B 806



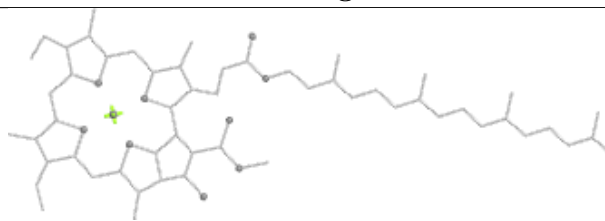
Bond lengths



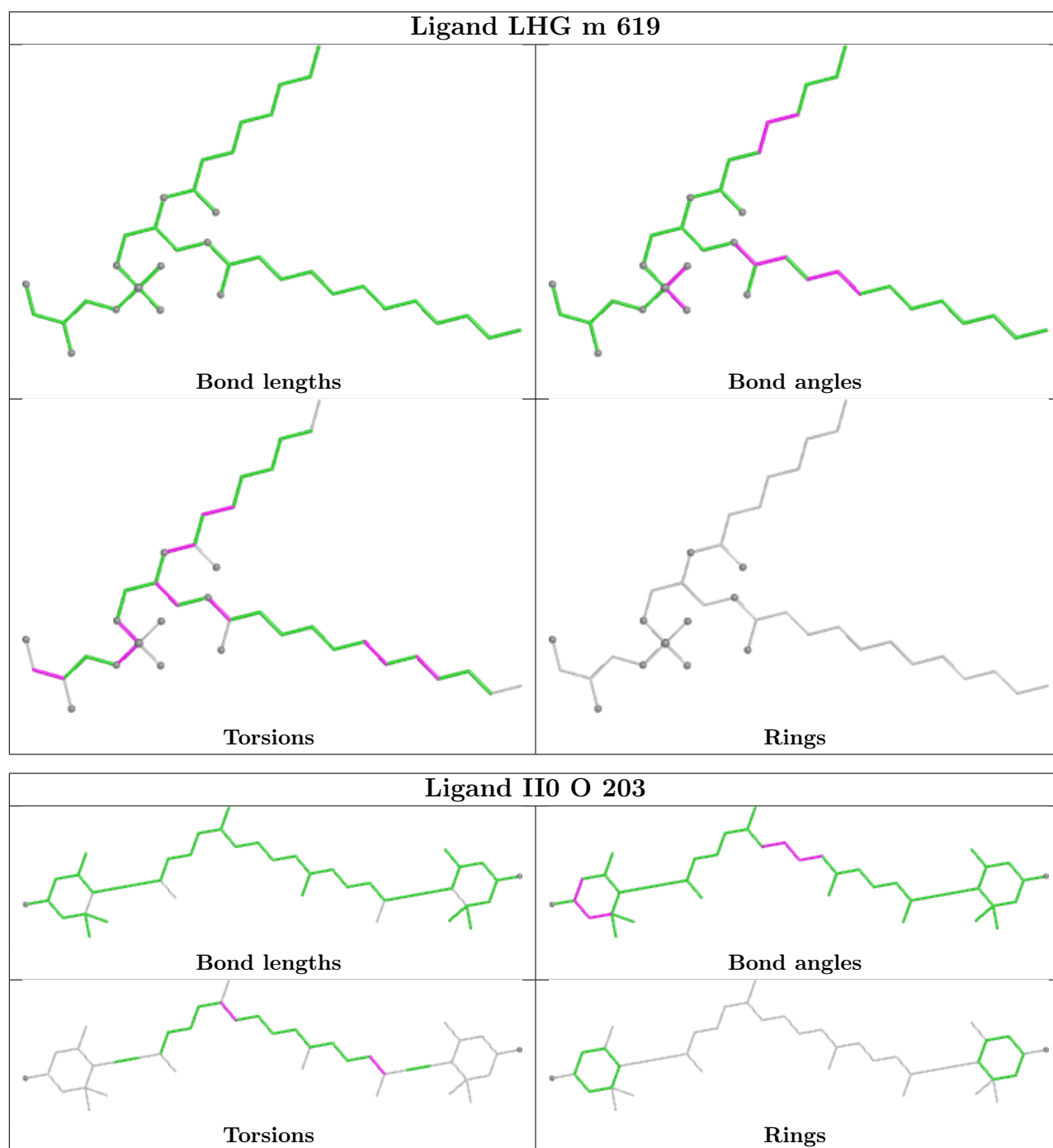
Bond angles

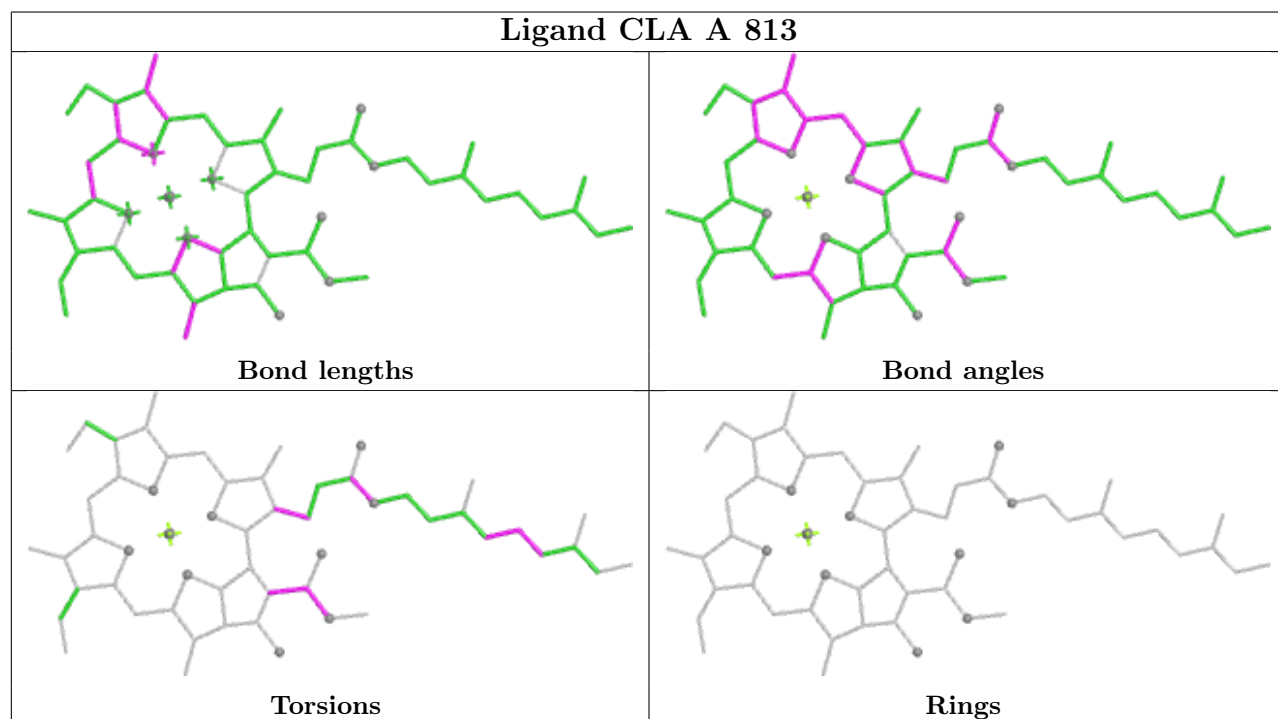
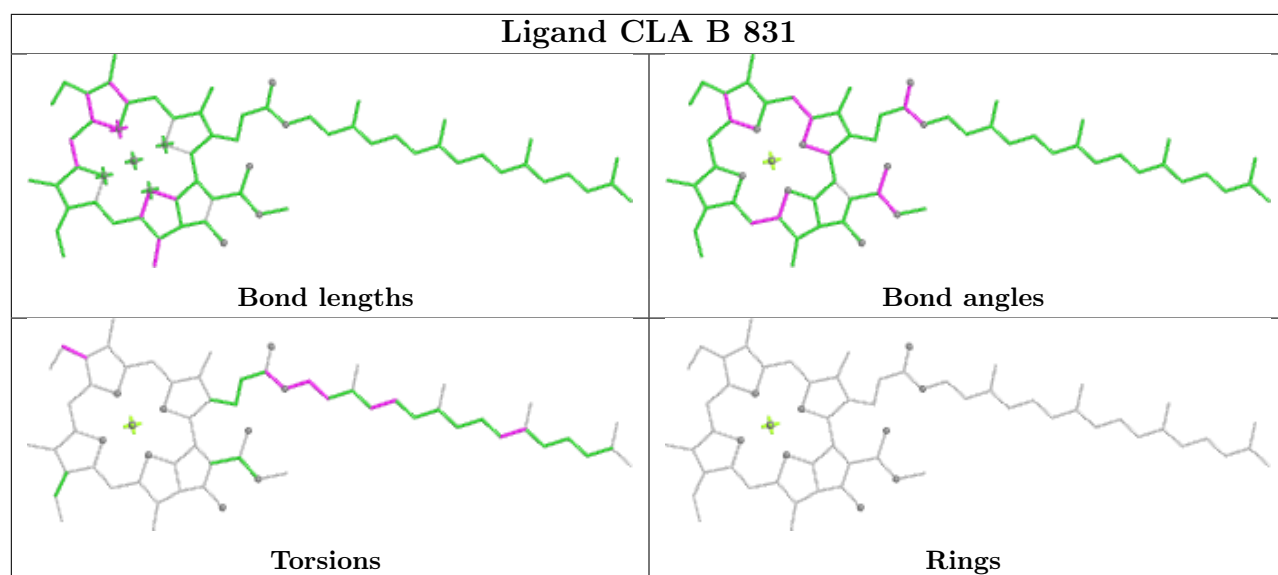


Torsions

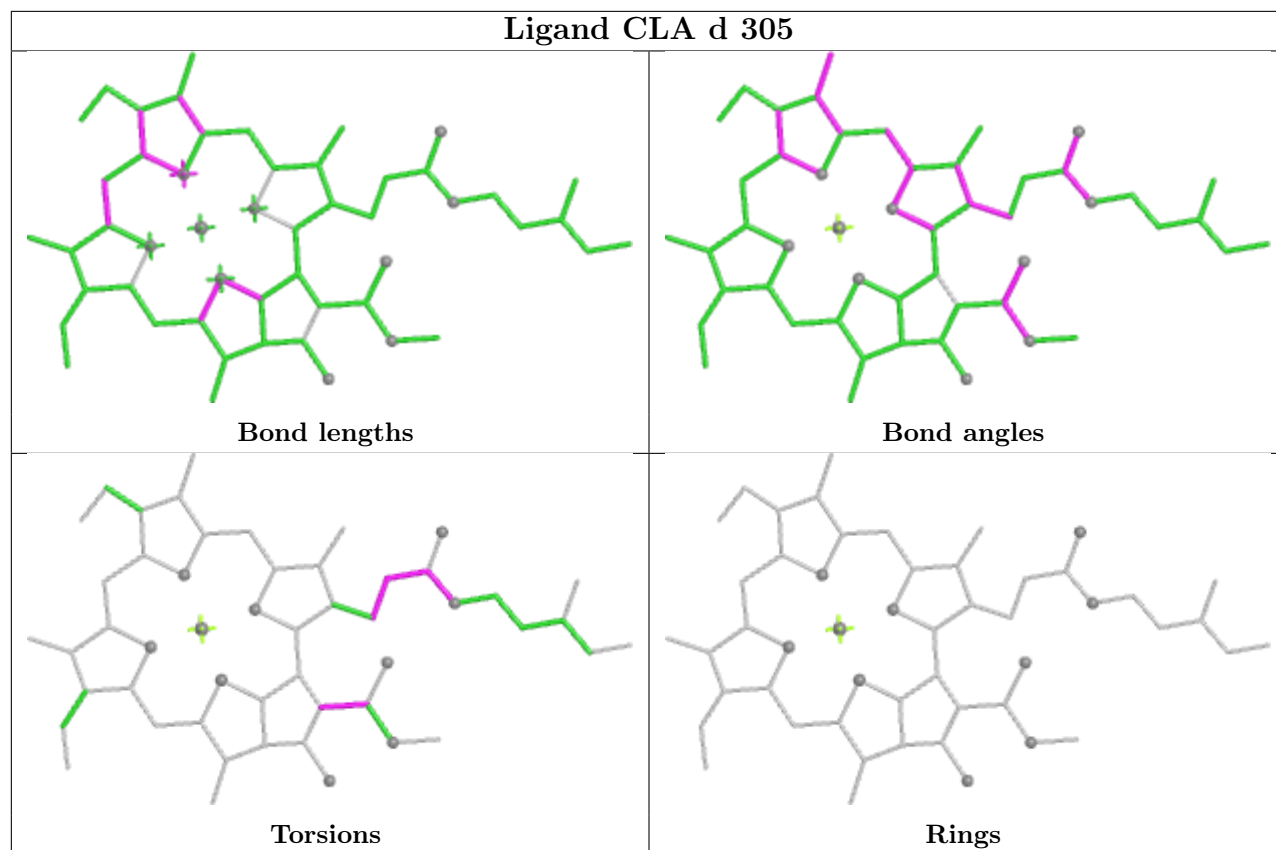


Rings

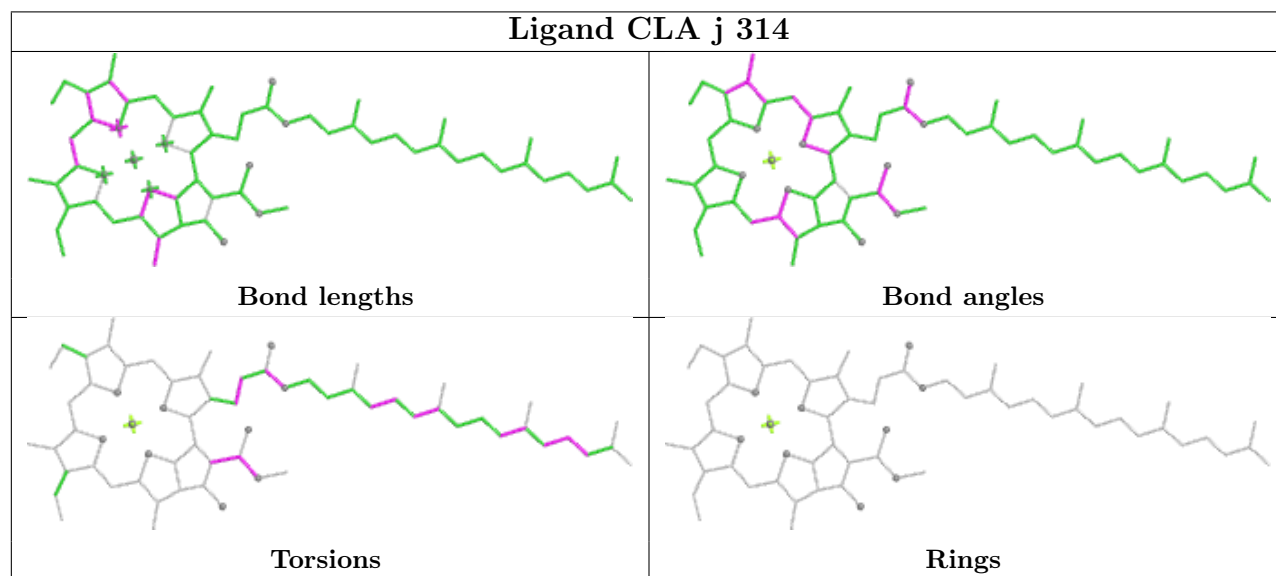


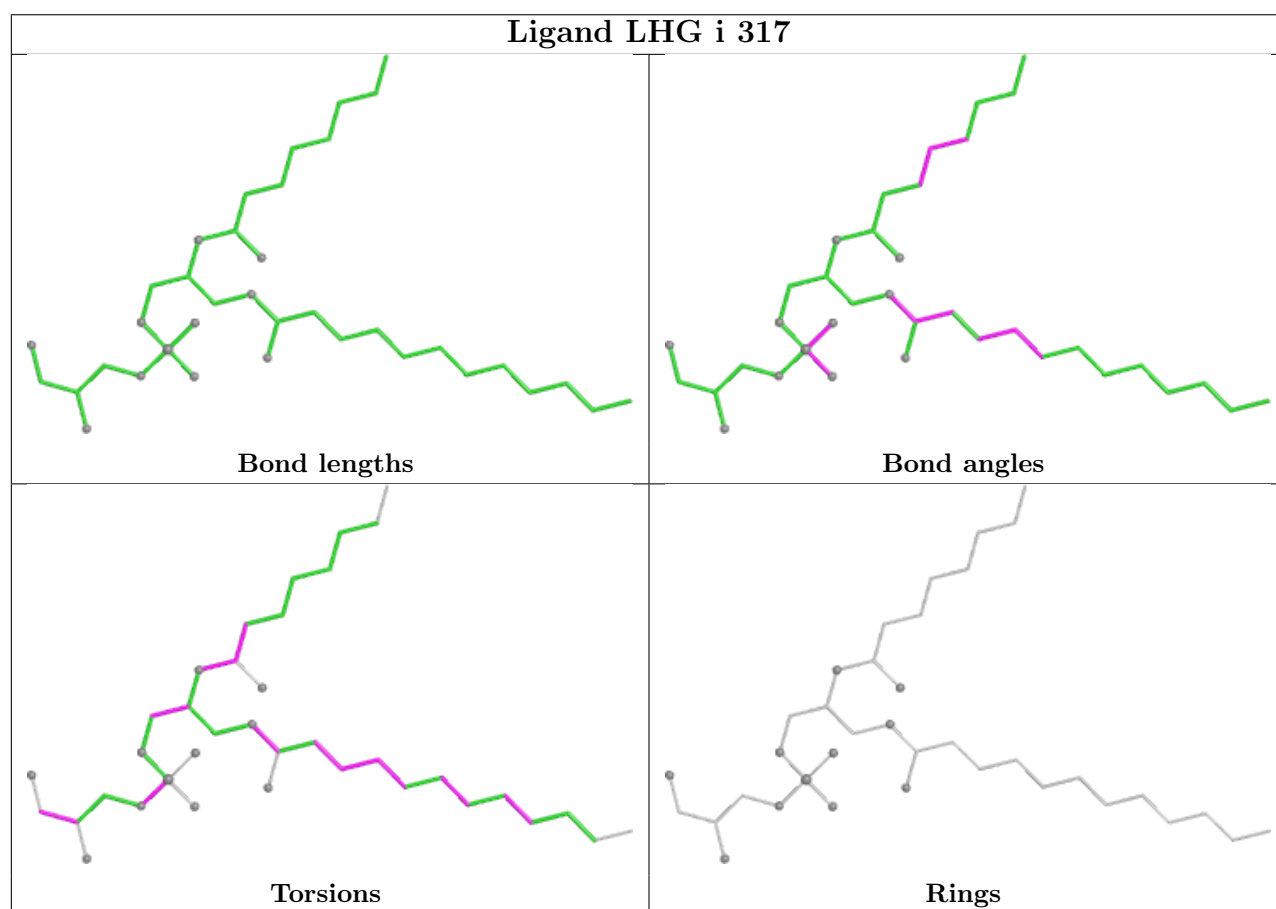
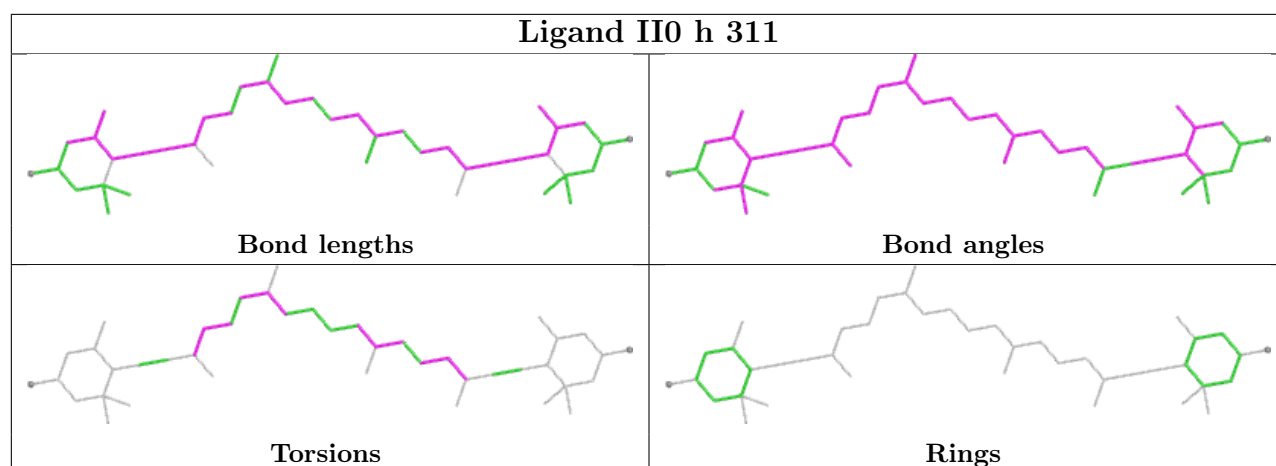


Ligand CLA d 305

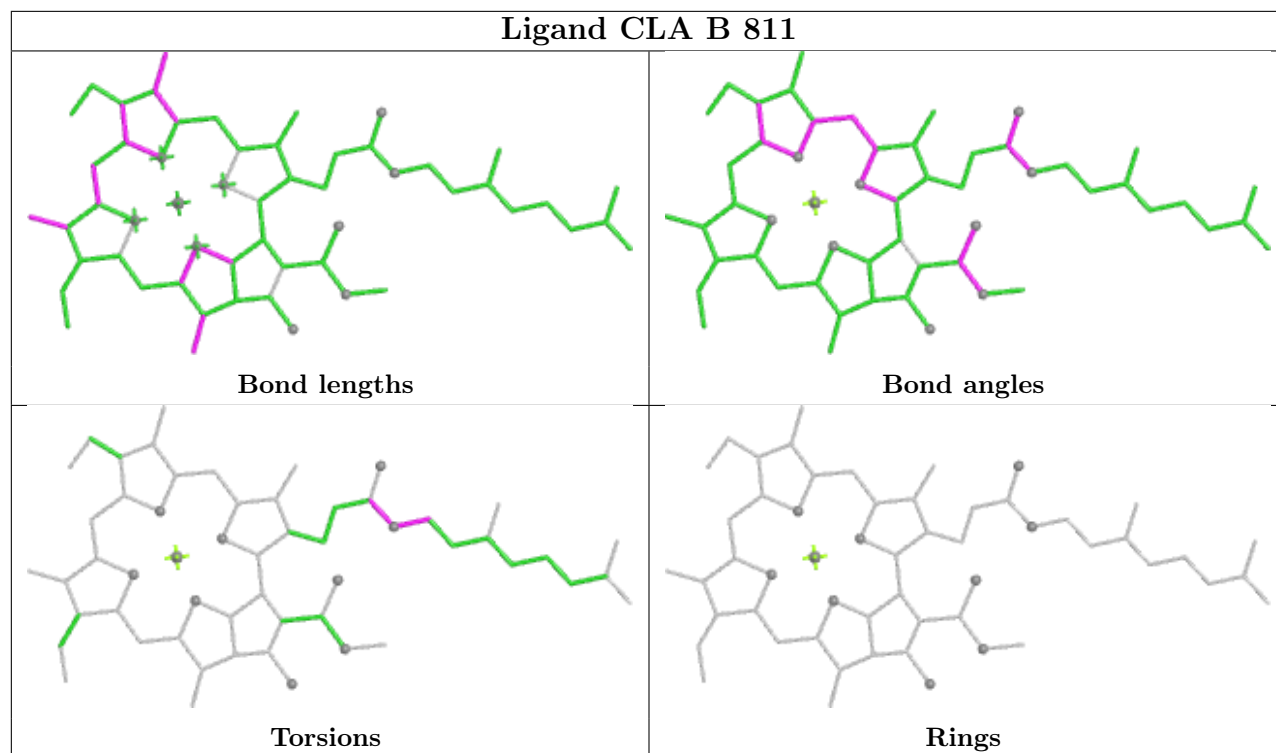


Ligand CLA j 314

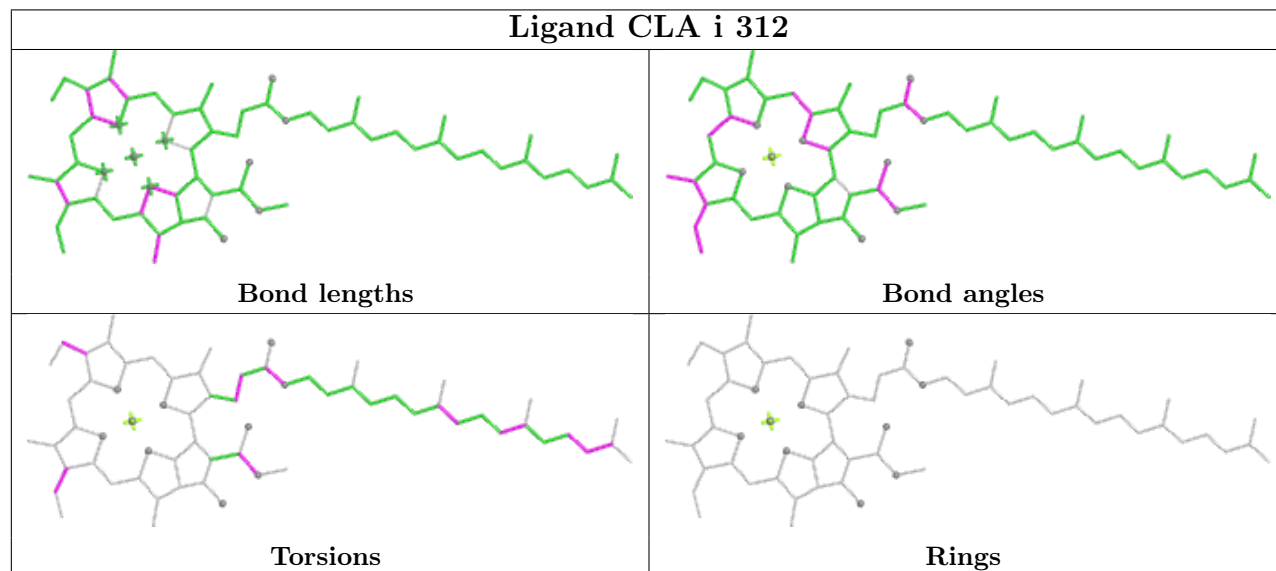


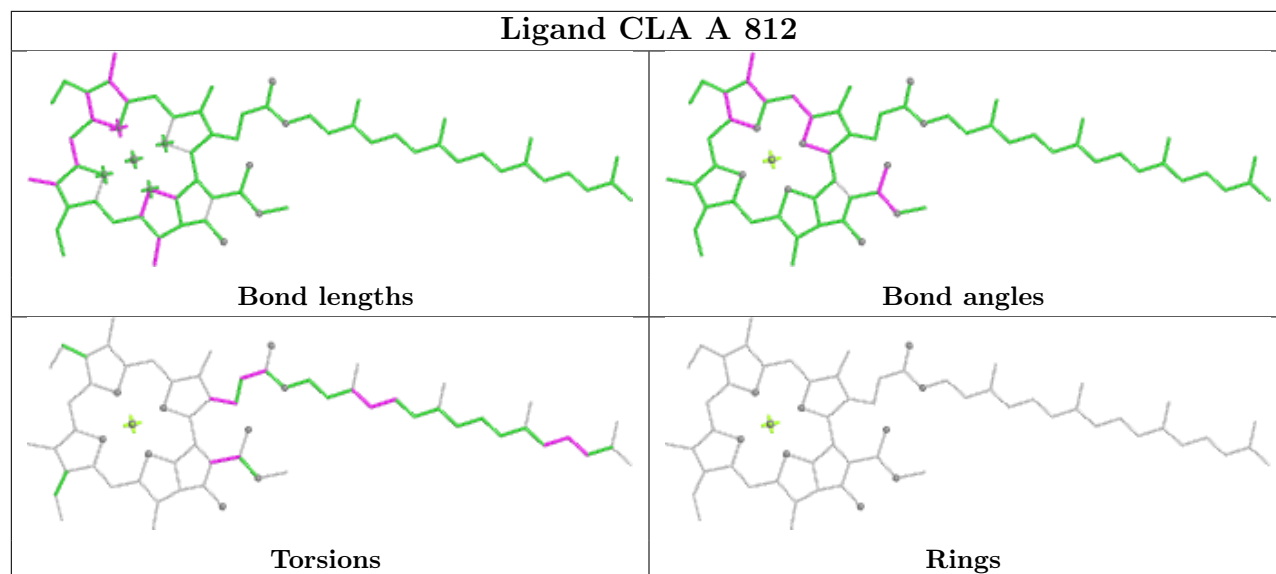
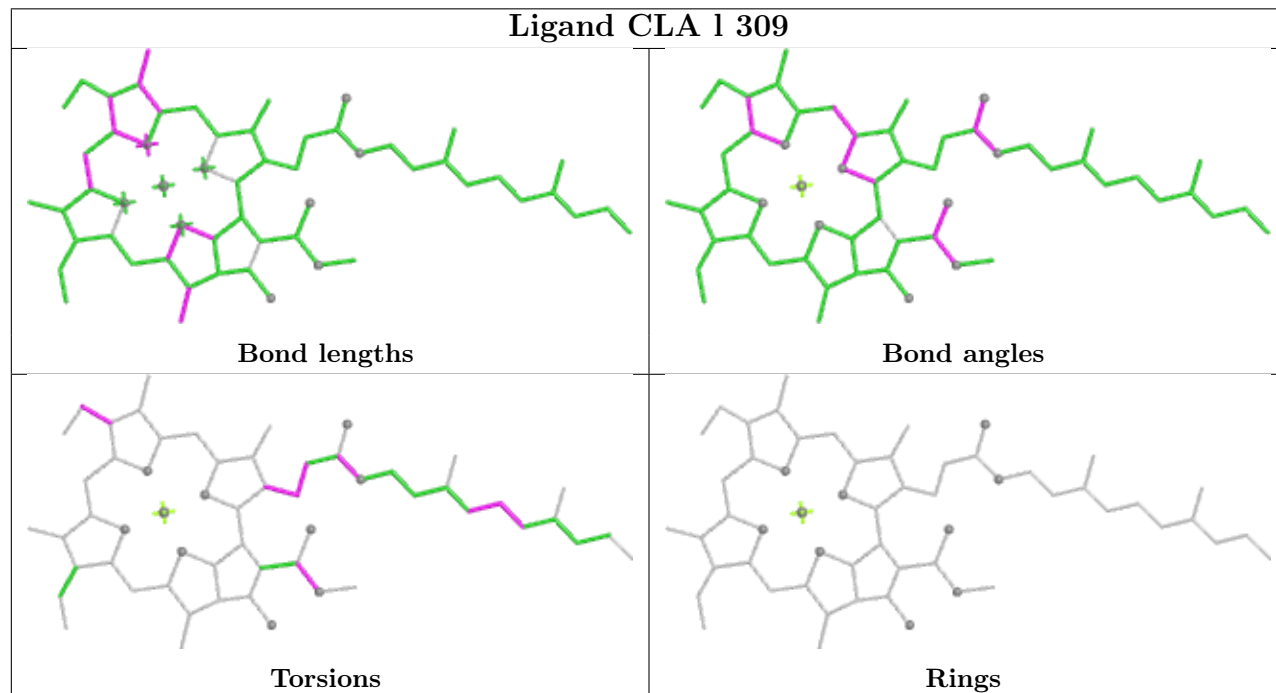


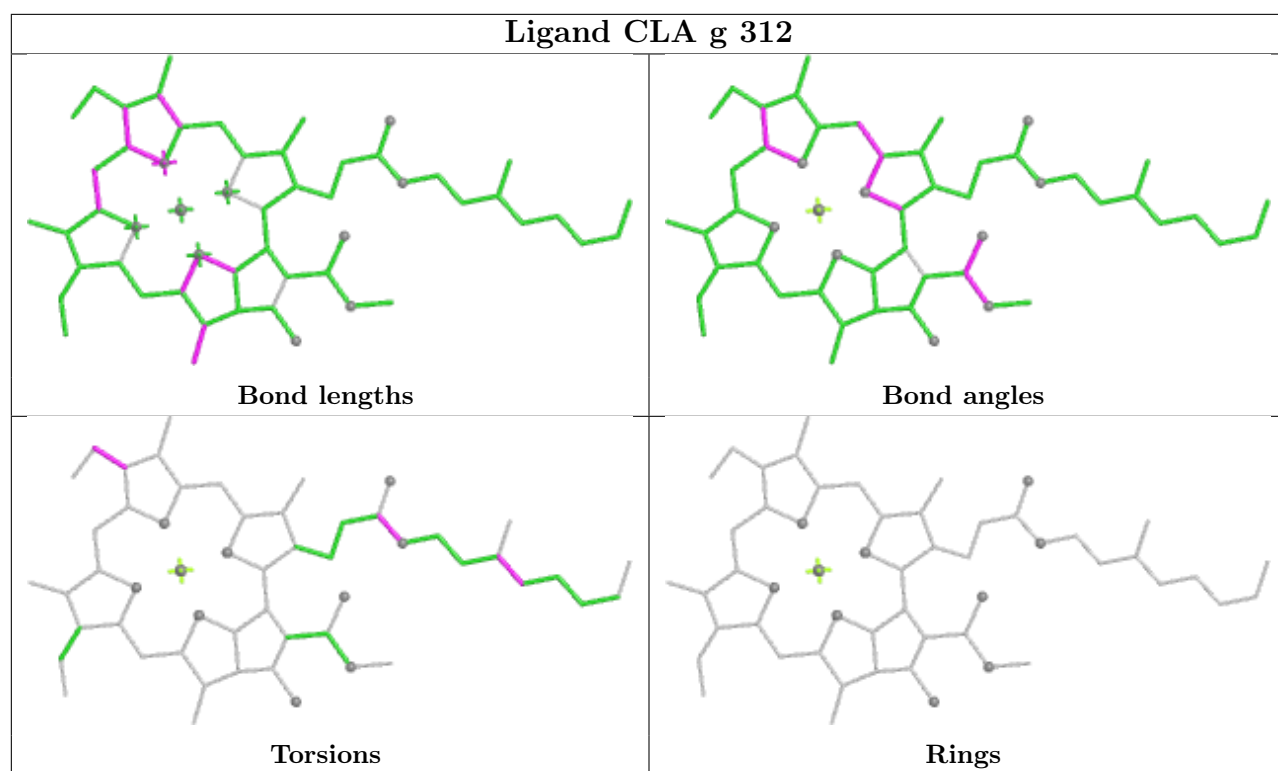
Ligand CLA B 811



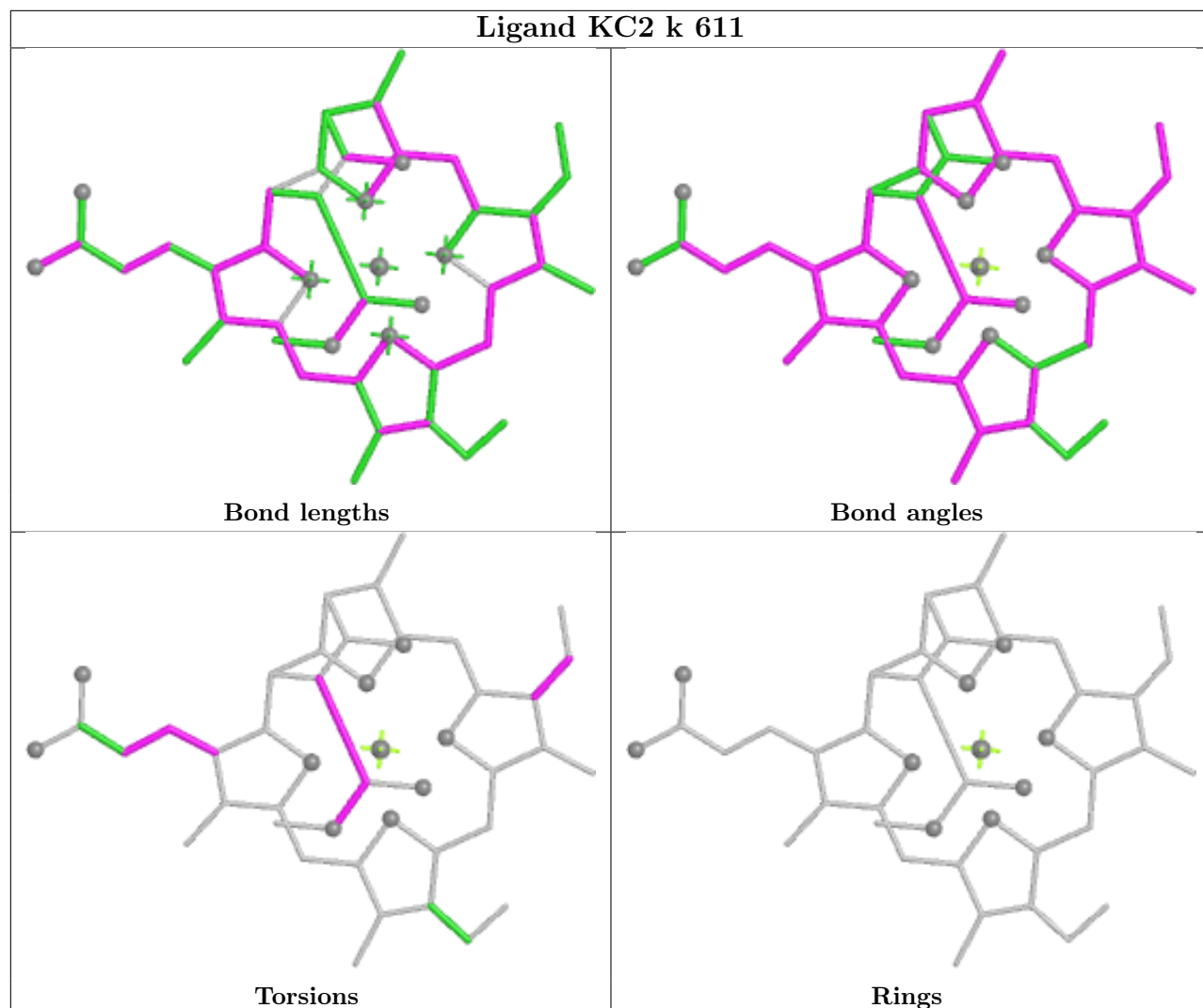
Ligand CLA i 312



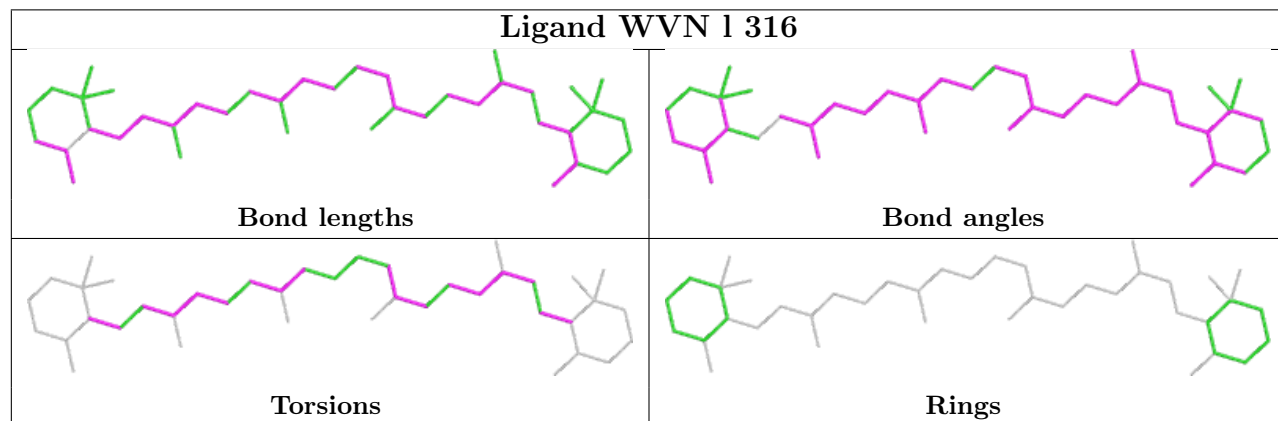
Ligand CLA A 812**Ligand CLA I 309**



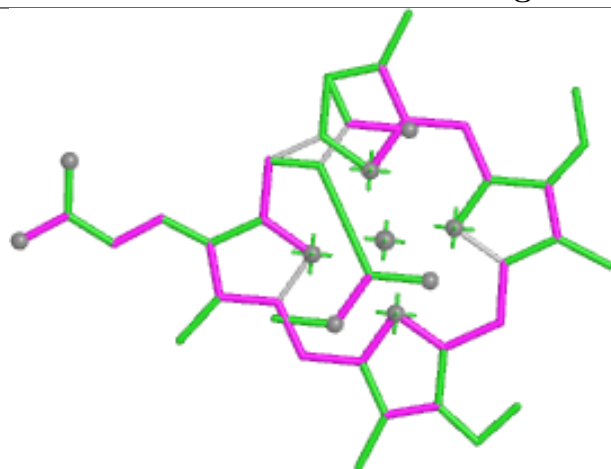
Ligand KC2 k 611



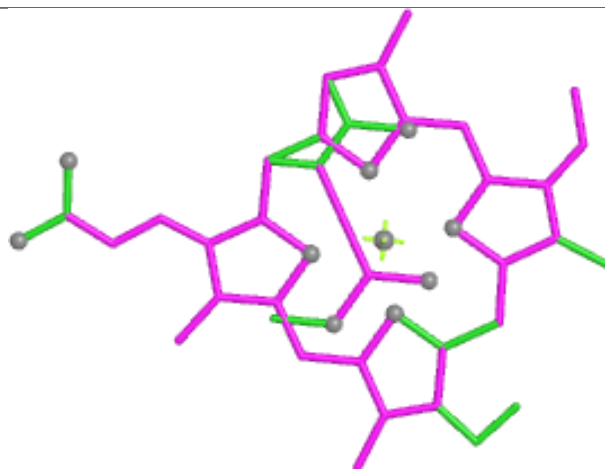
Ligand WVN l 316



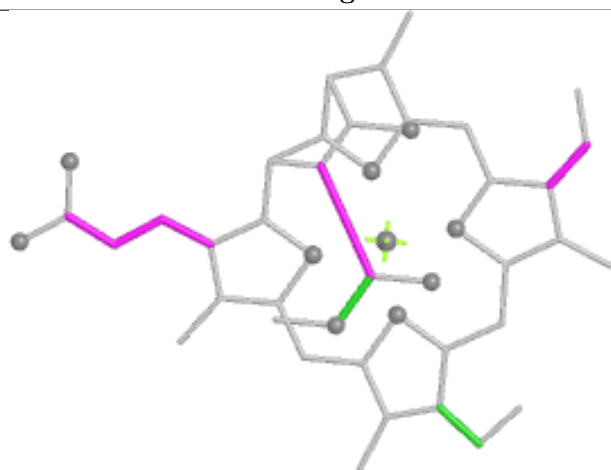
Ligand KC2 m 611



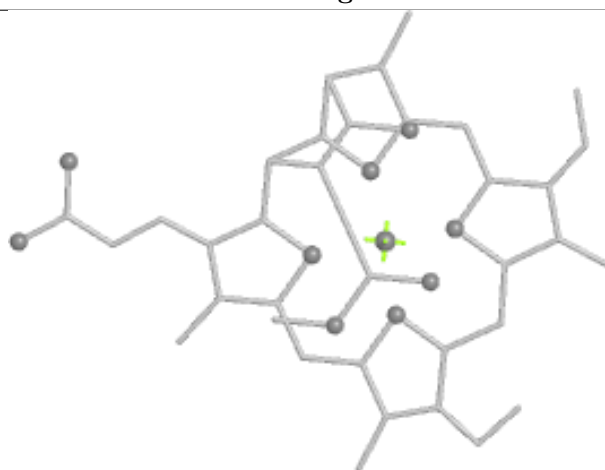
Bond lengths



Bond angles

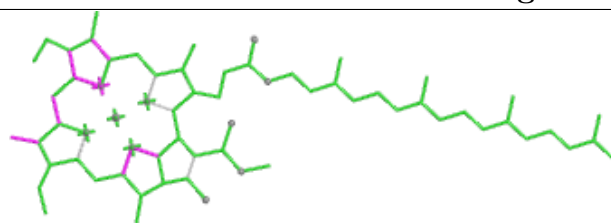


Torsions

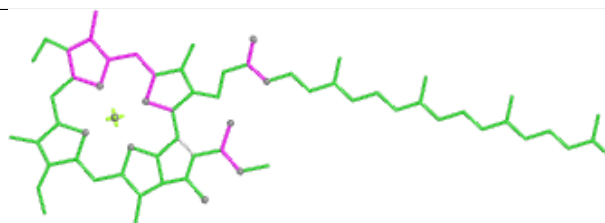


Rings

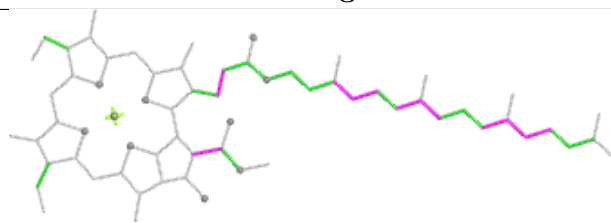
Ligand CLA b 308



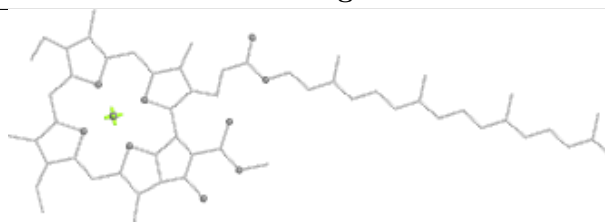
Bond lengths



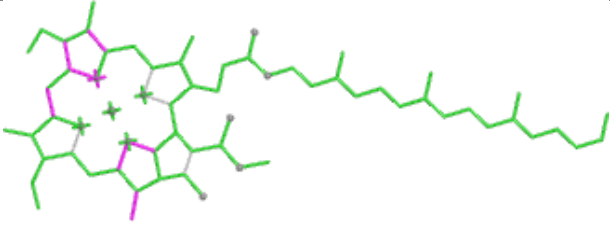
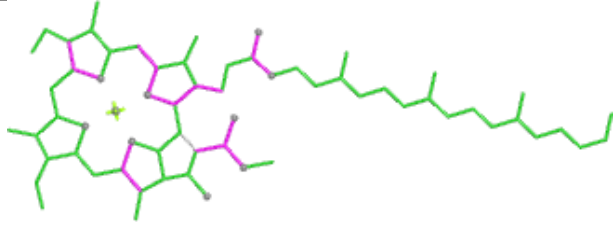
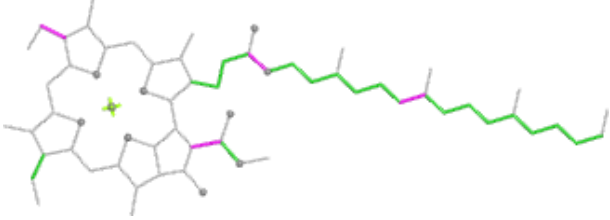
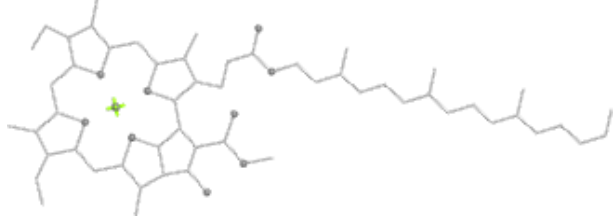
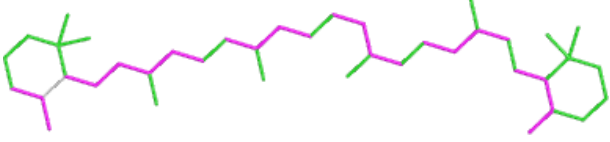
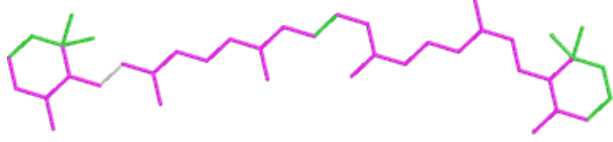
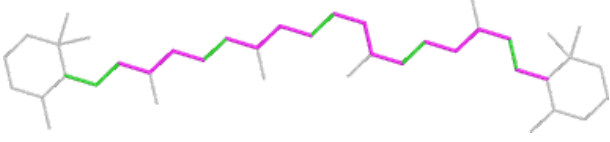
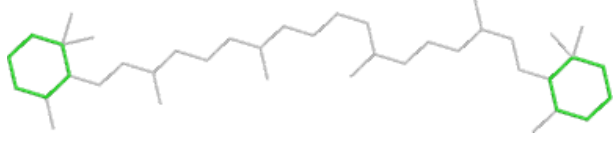
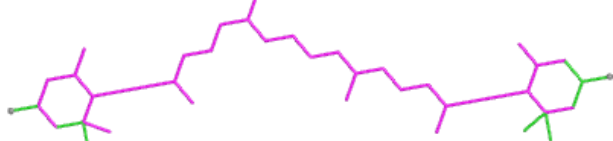
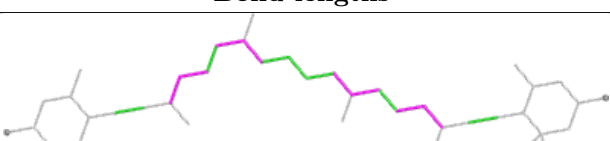
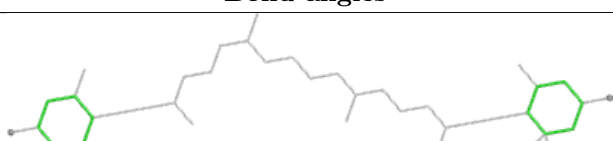
Bond angles



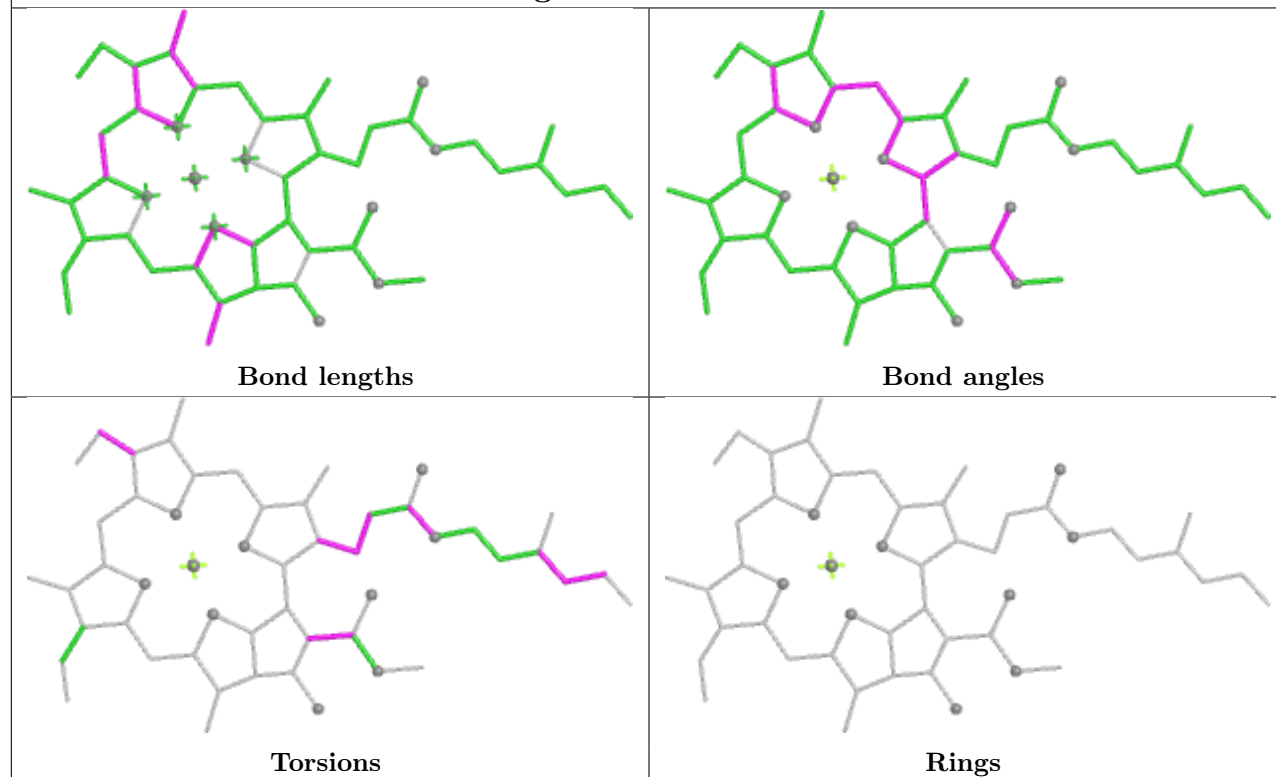
Torsions



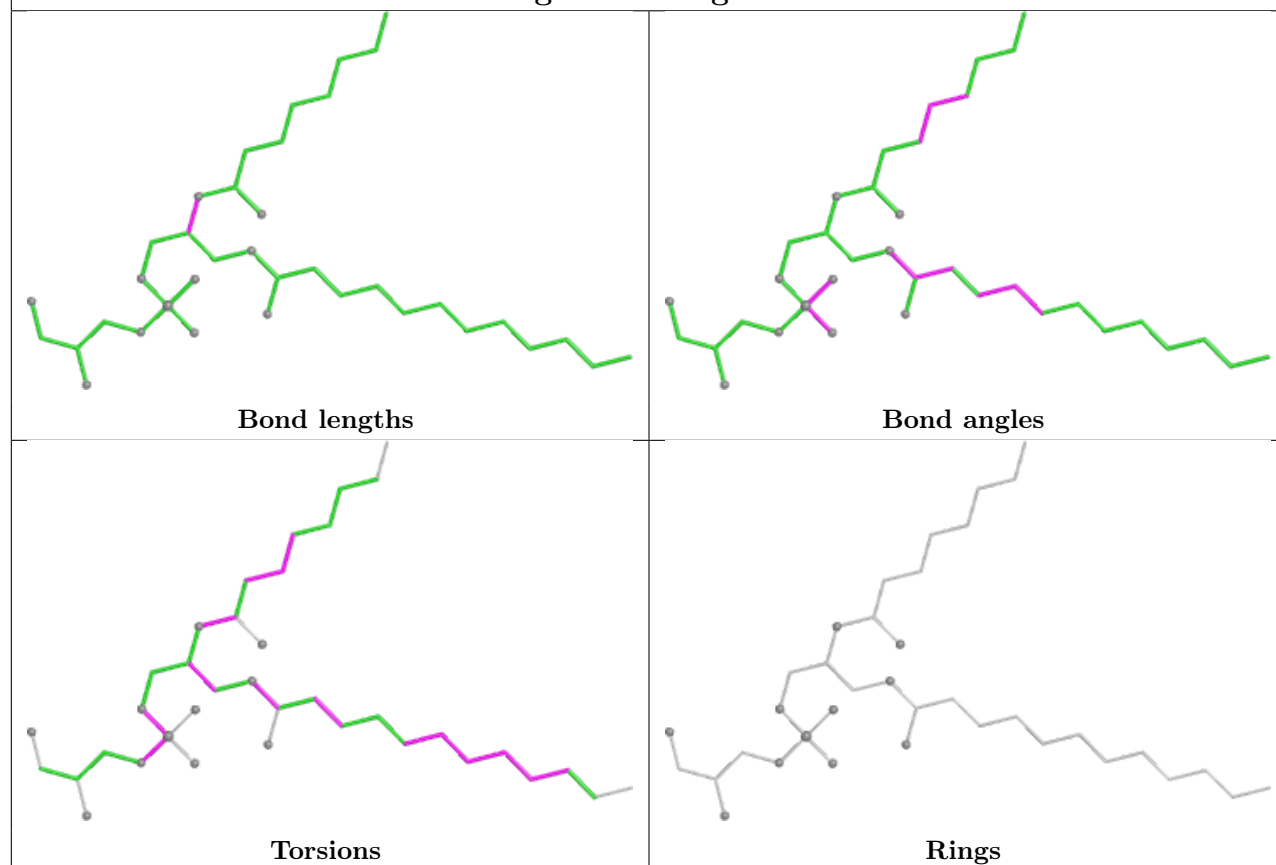
Rings

Ligand CLA B 823	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand WVN J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand II0 j 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

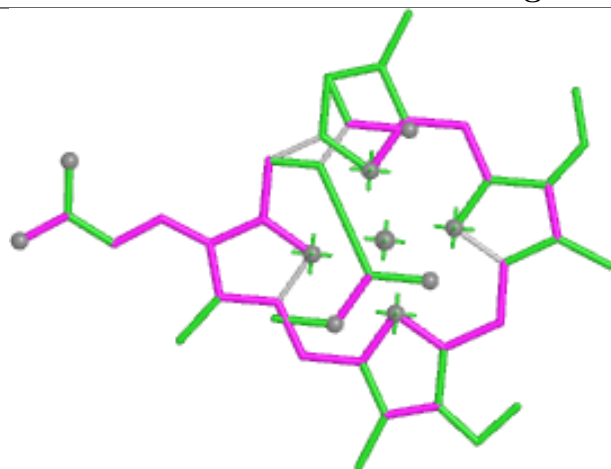
Ligand CLA F 203



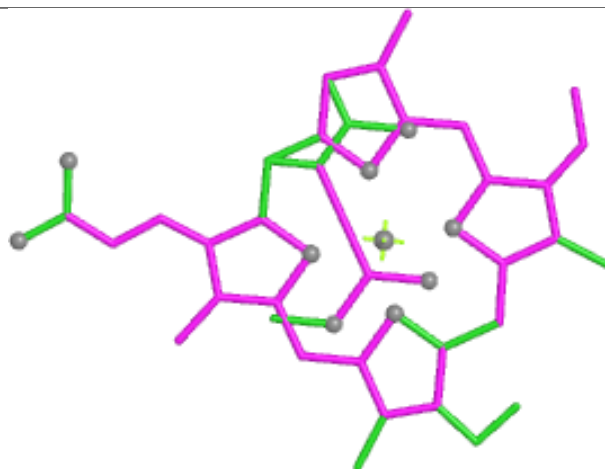
Ligand LHG g 322



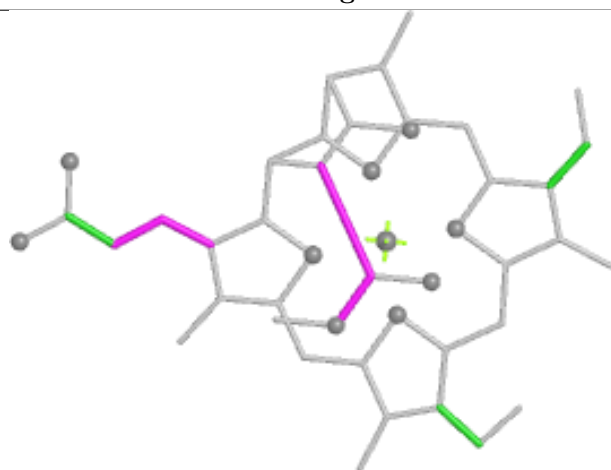
Ligand KC2 l 311



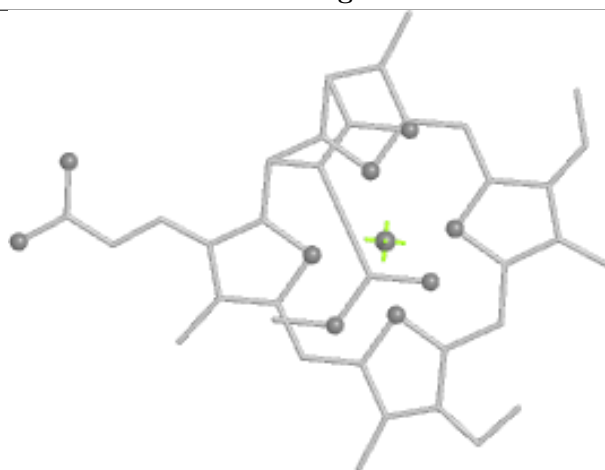
Bond lengths



Bond angles

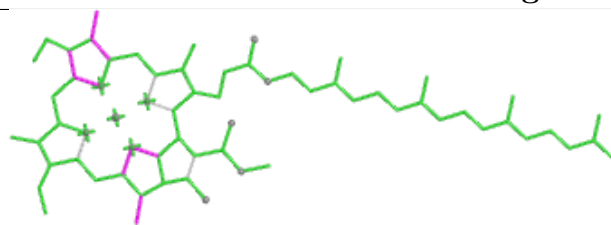


Torsions

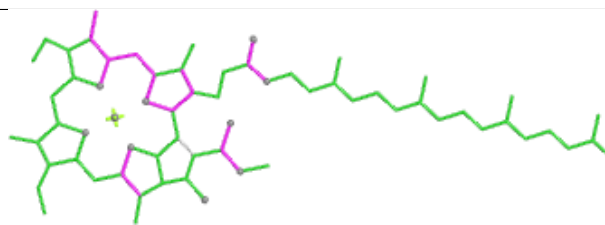


Rings

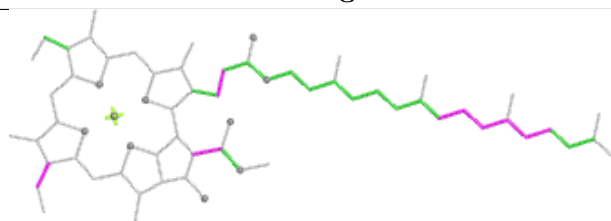
Ligand CLA f 604



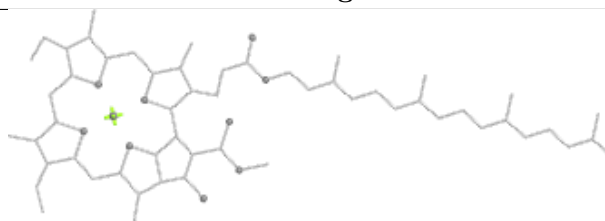
Bond lengths



Bond angles

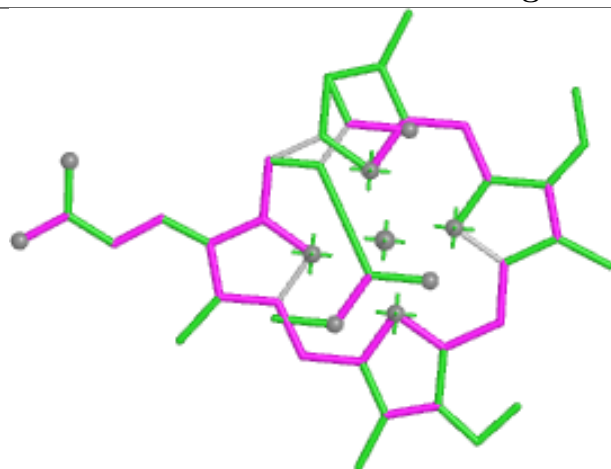


Torsions

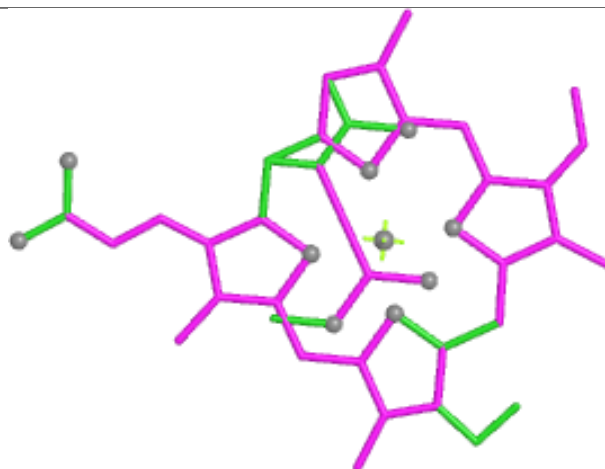


Rings

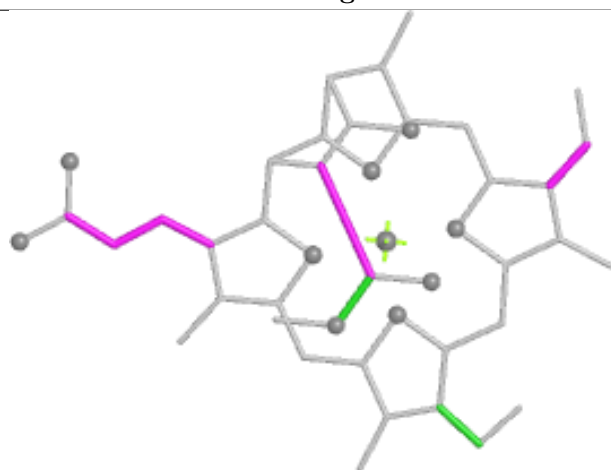
Ligand KC2 s 401



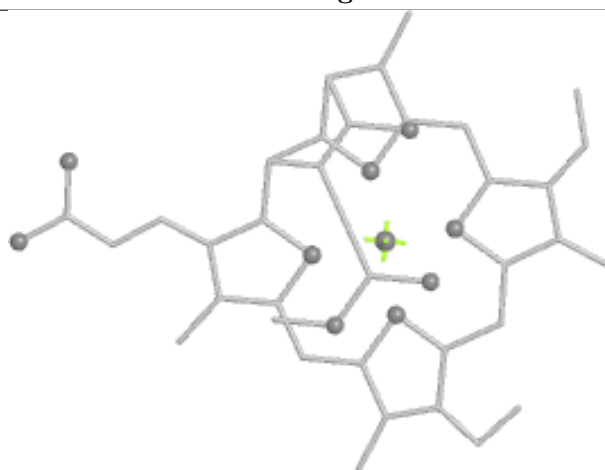
Bond lengths



Bond angles

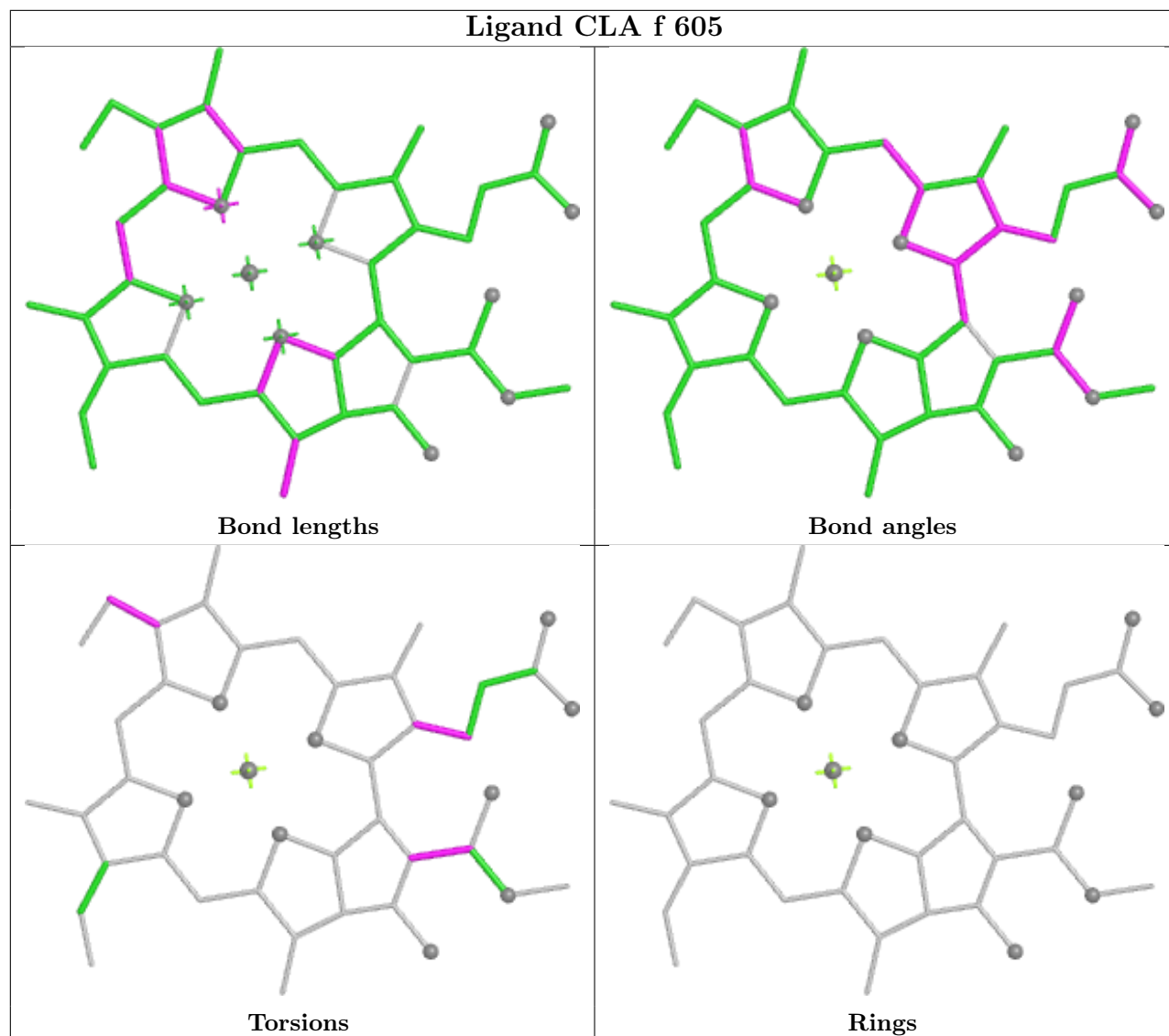


Torsions

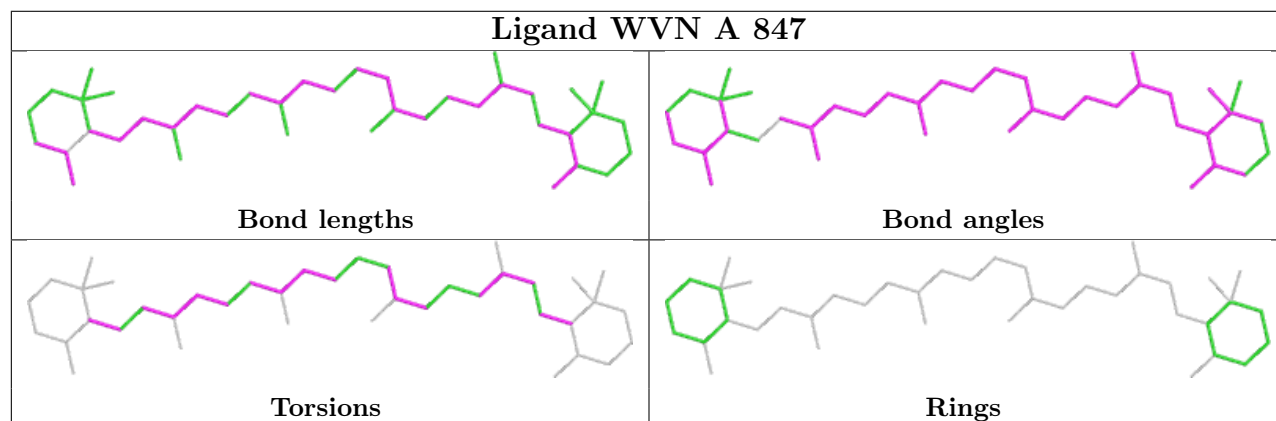


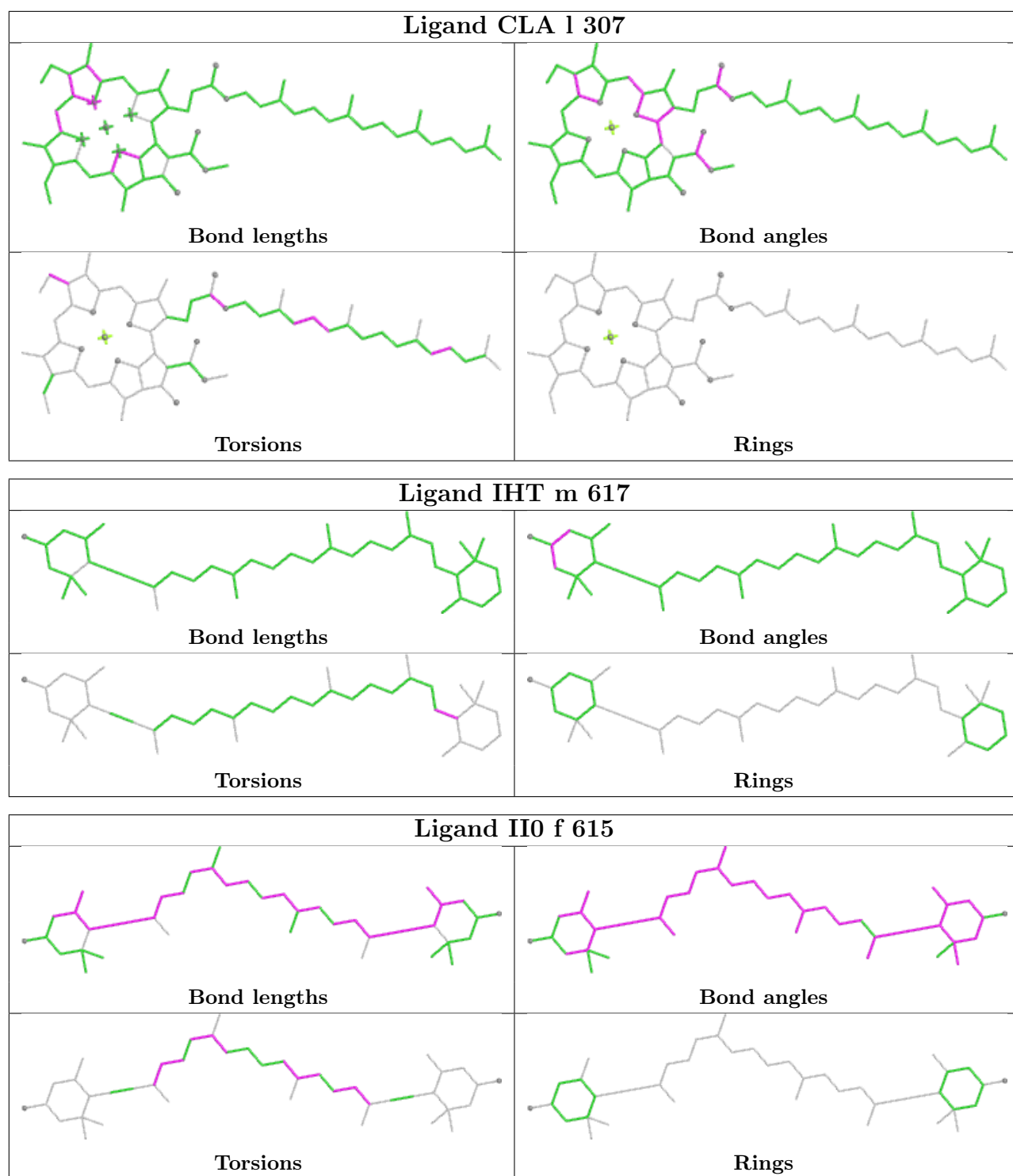
Rings

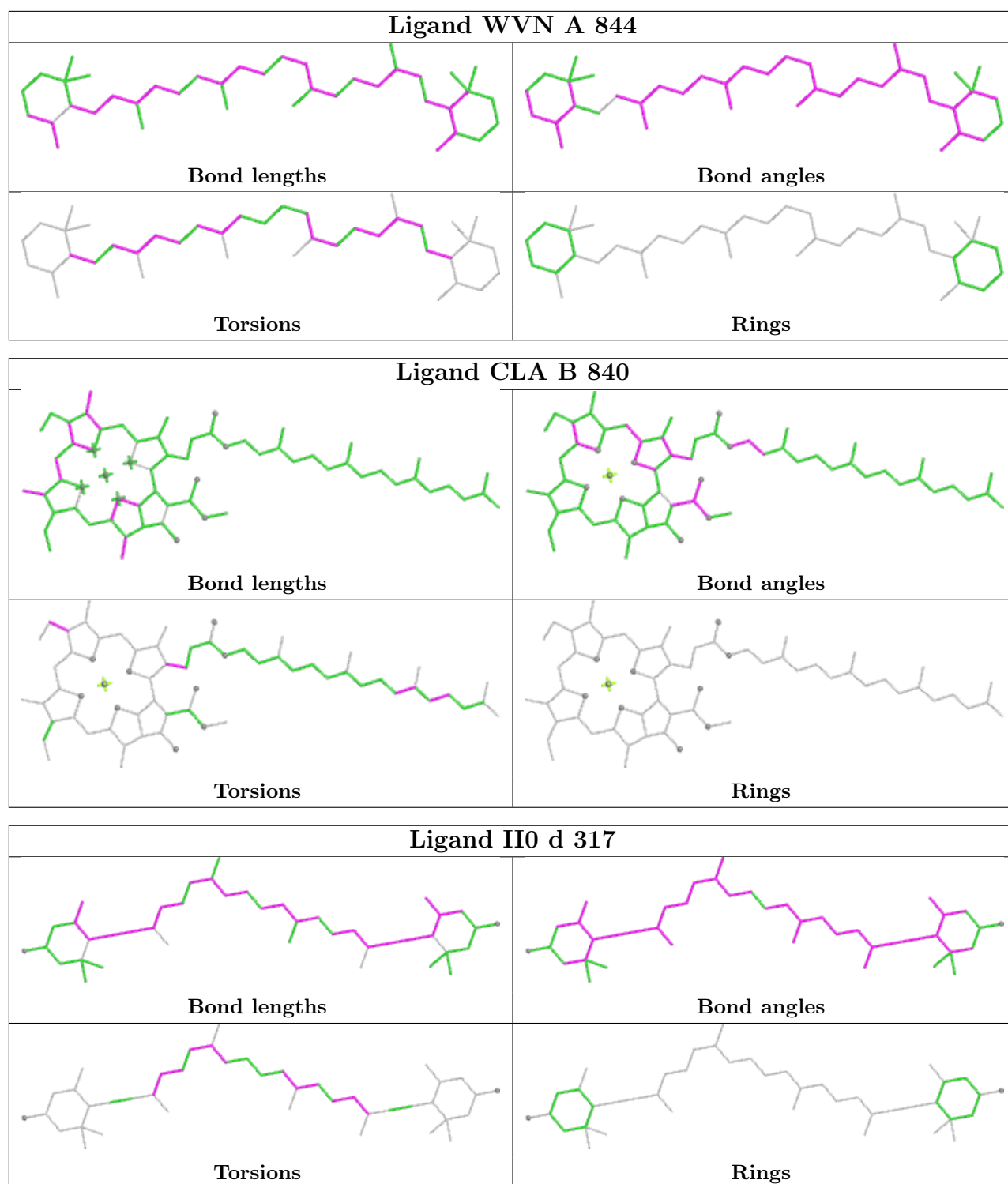
Ligand CLA f 605

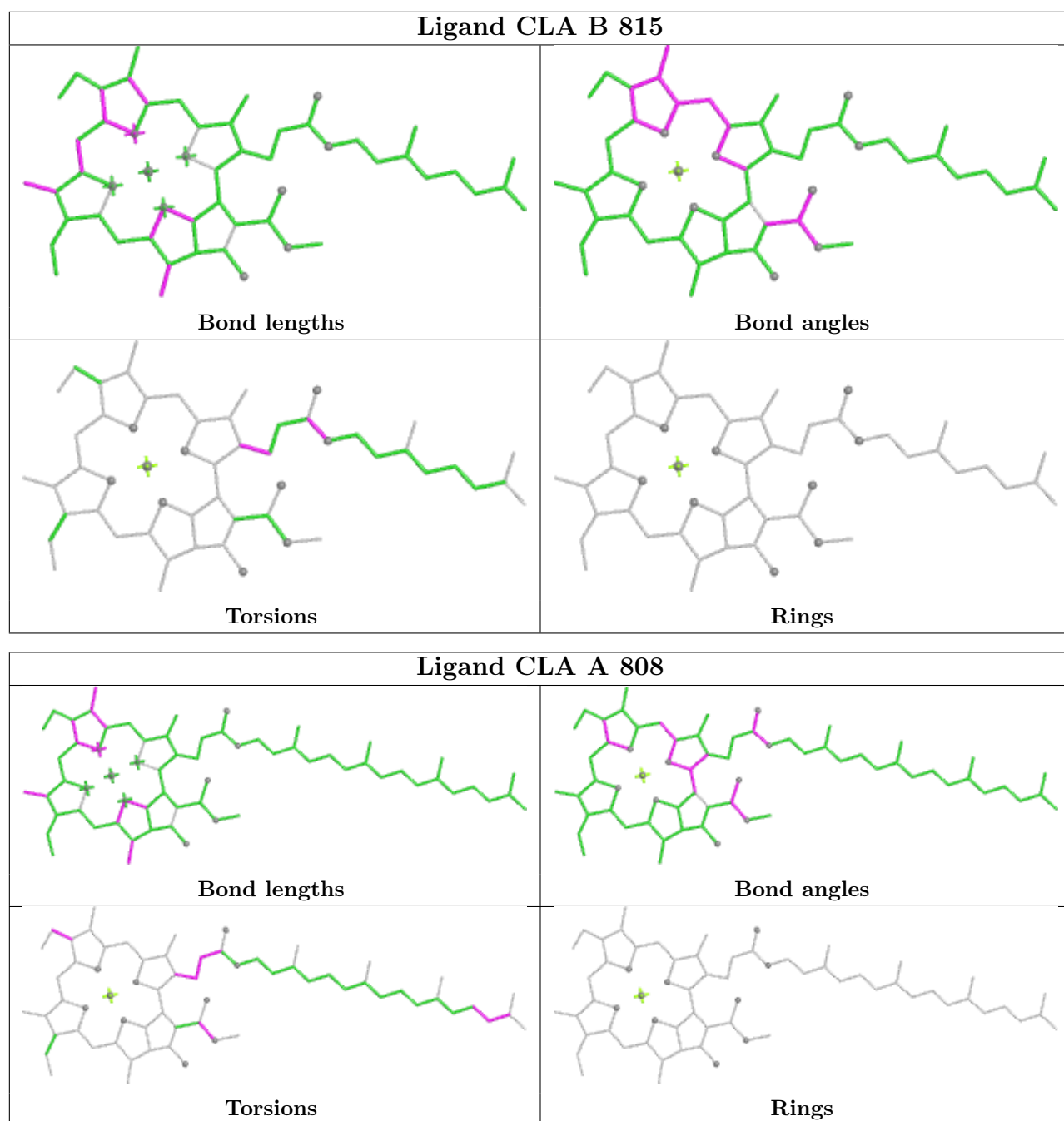


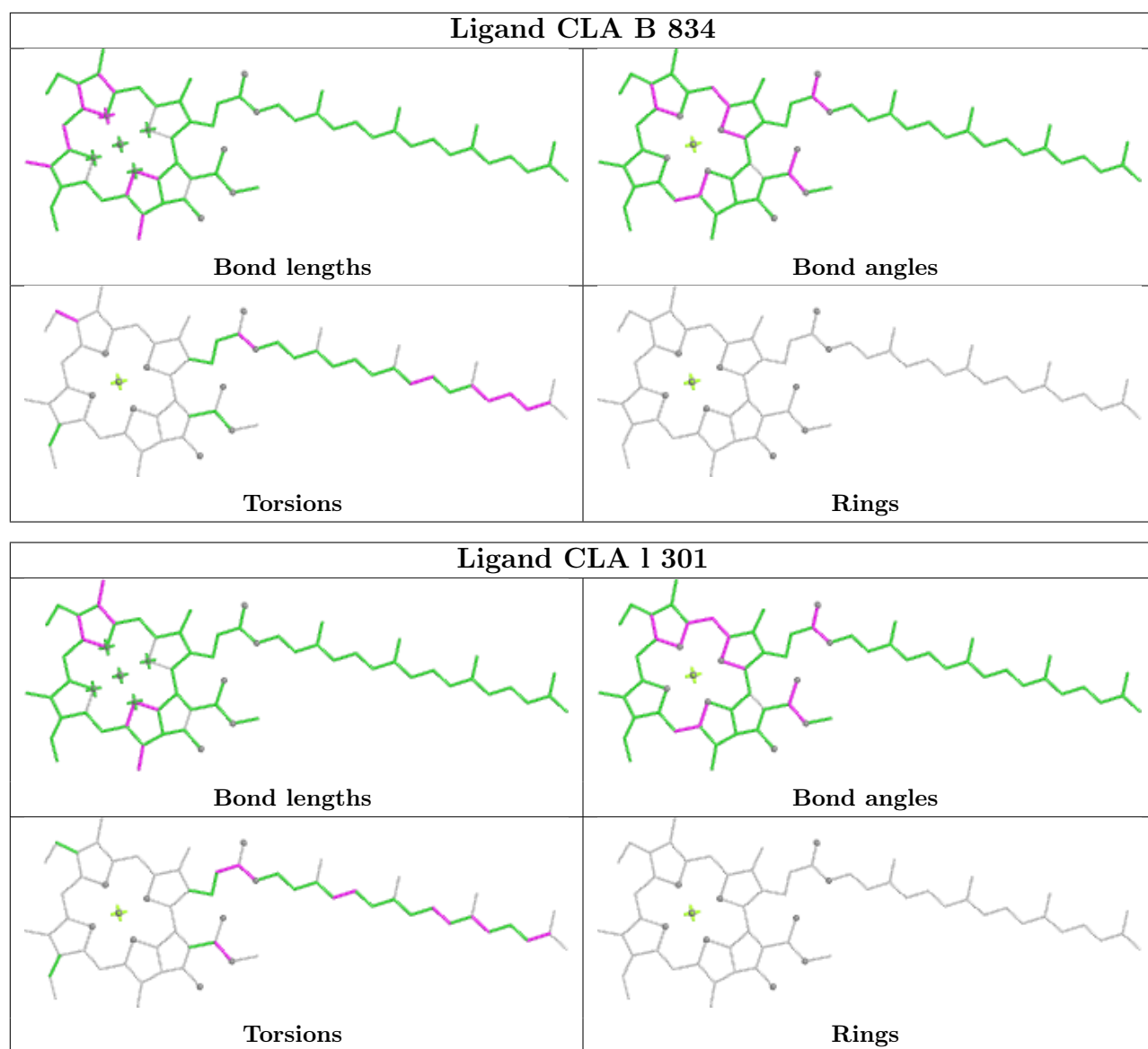
Ligand WVN A 847



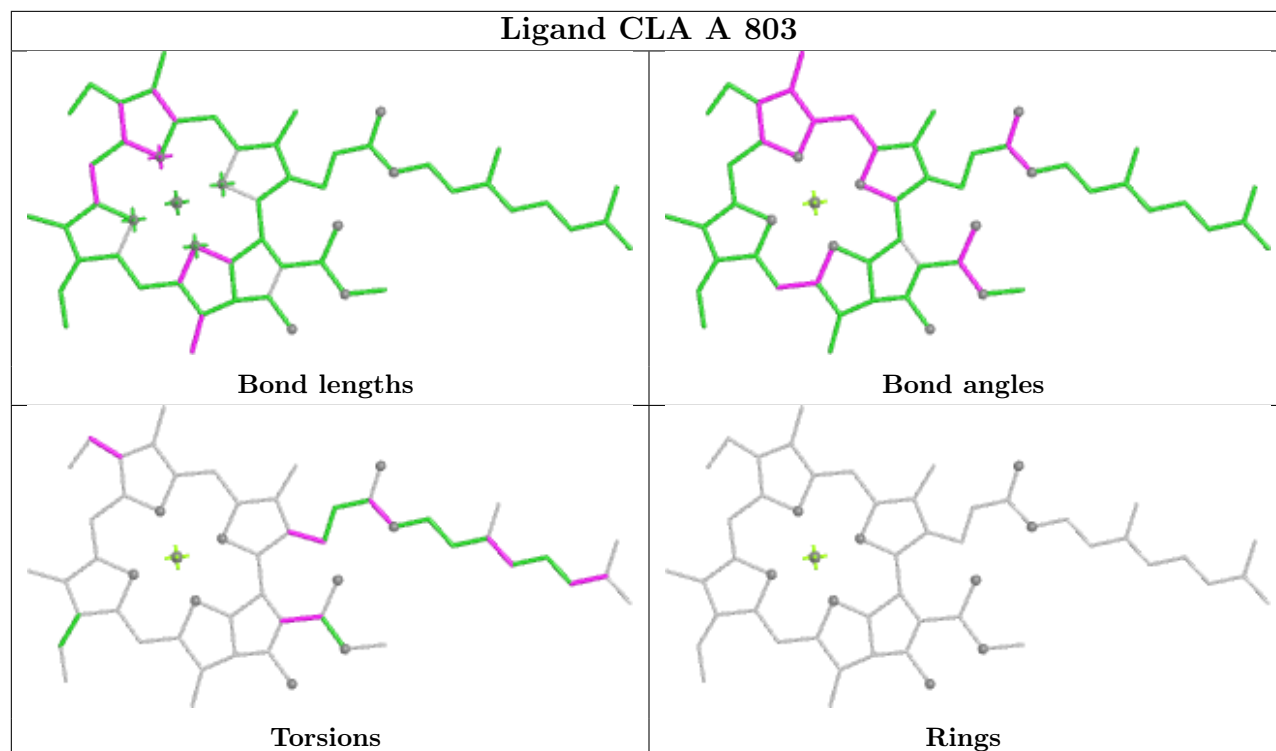




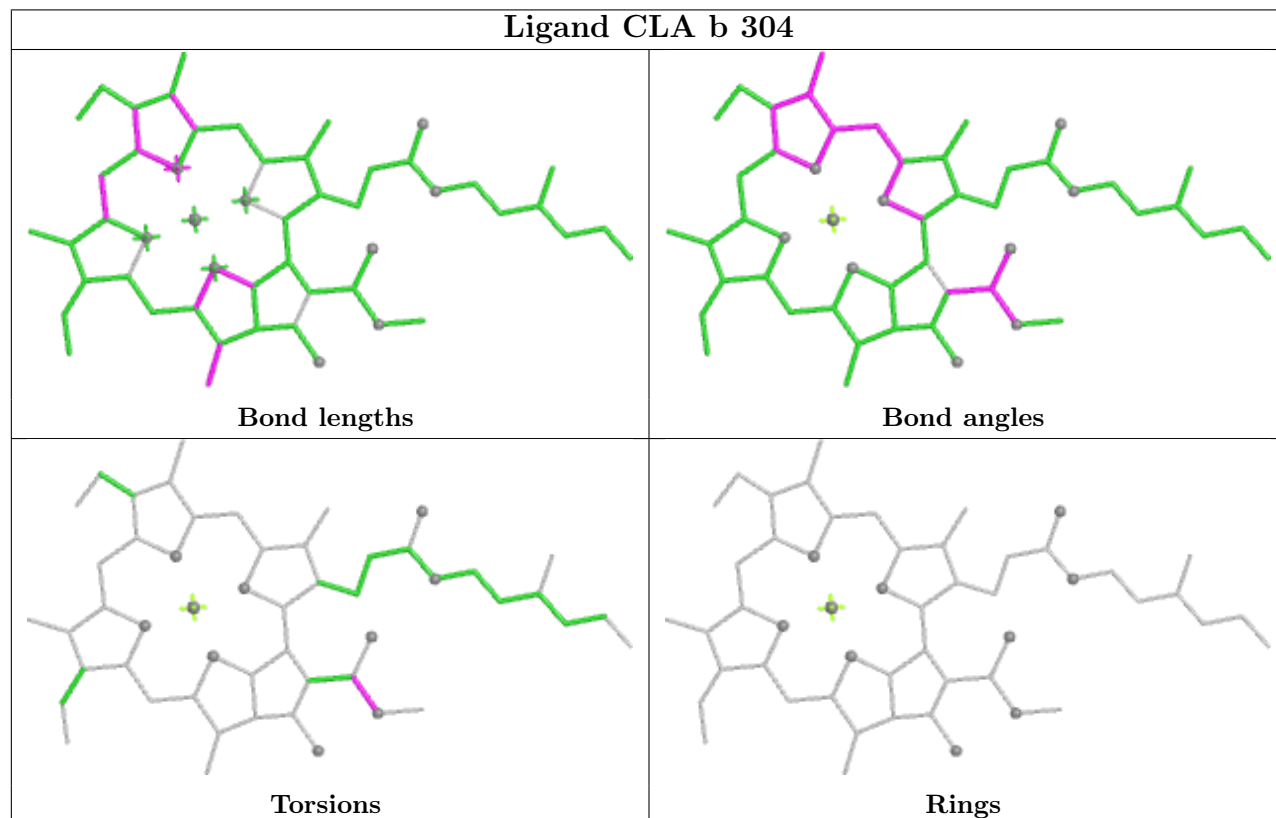




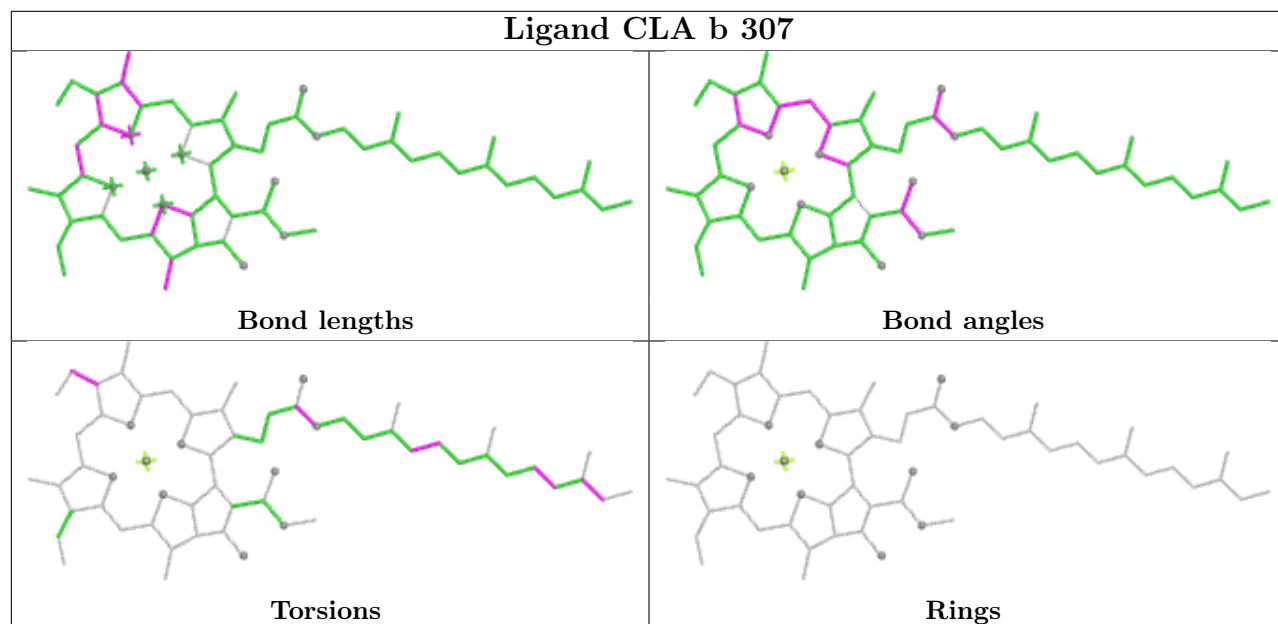
Ligand CLA A 803



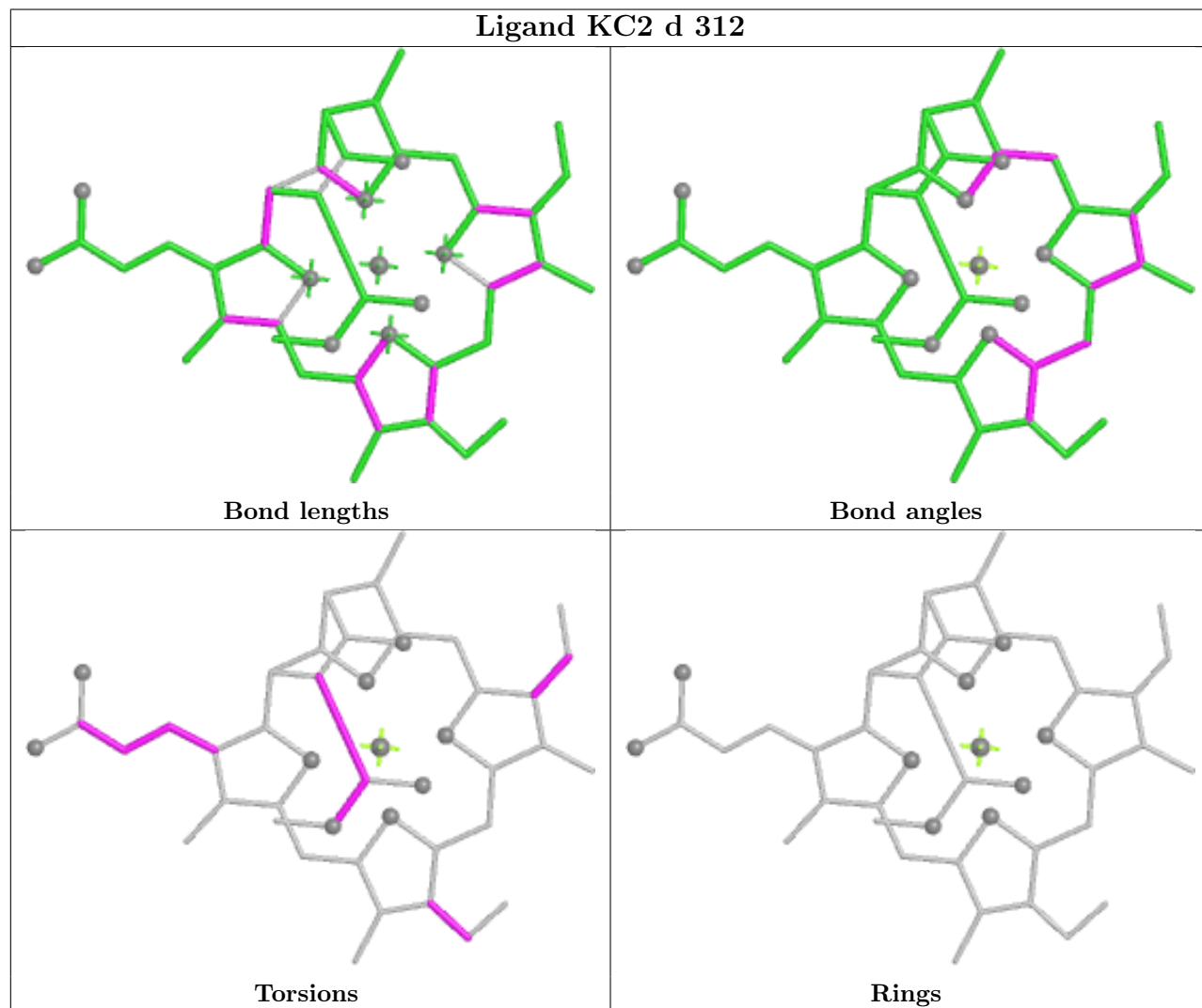
Ligand CLA b 304

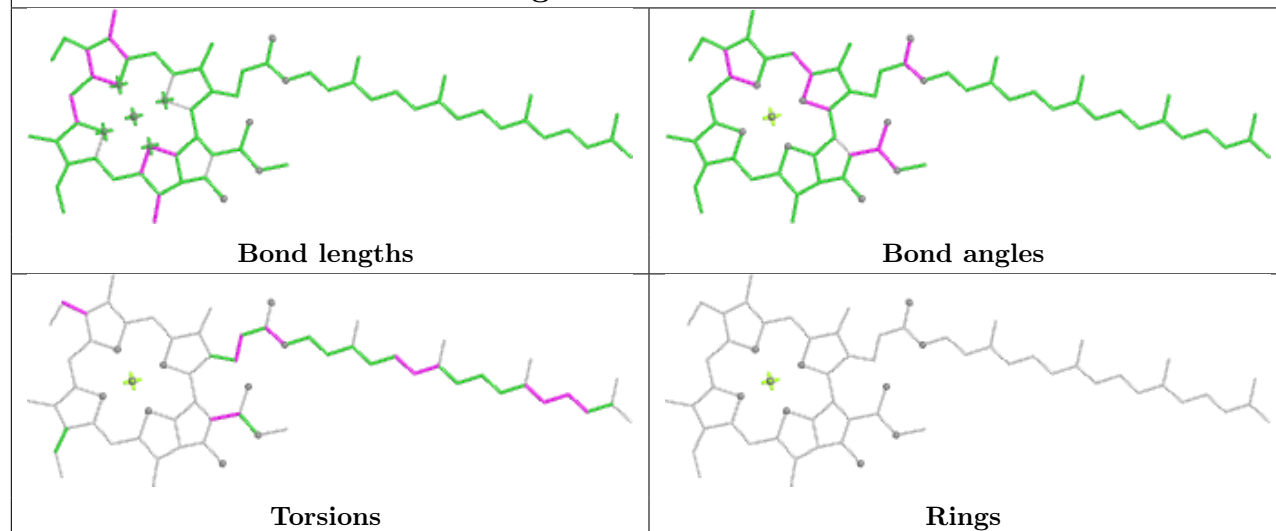
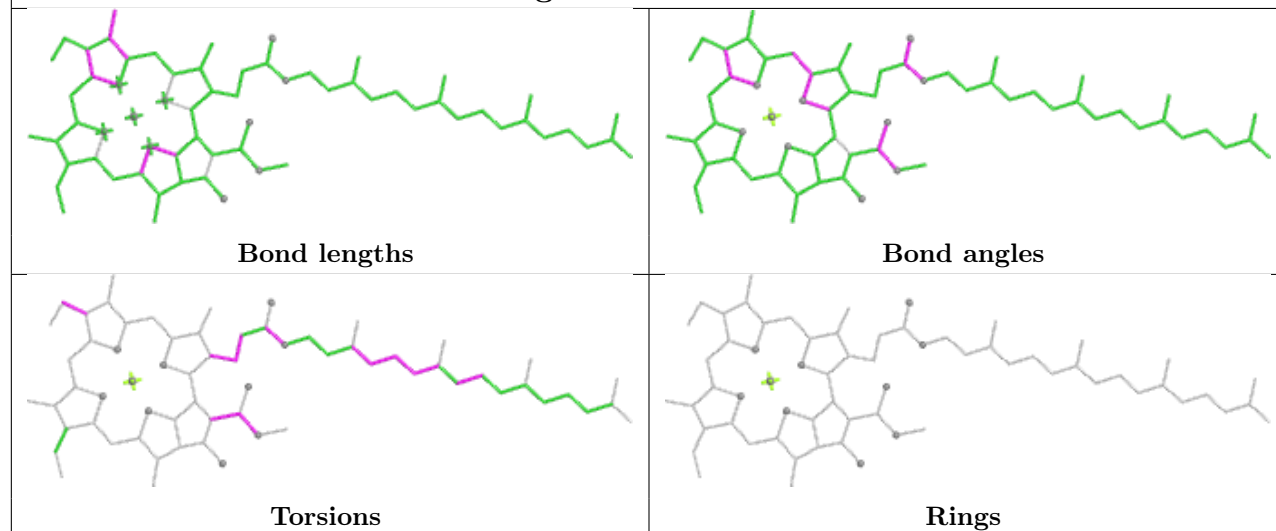


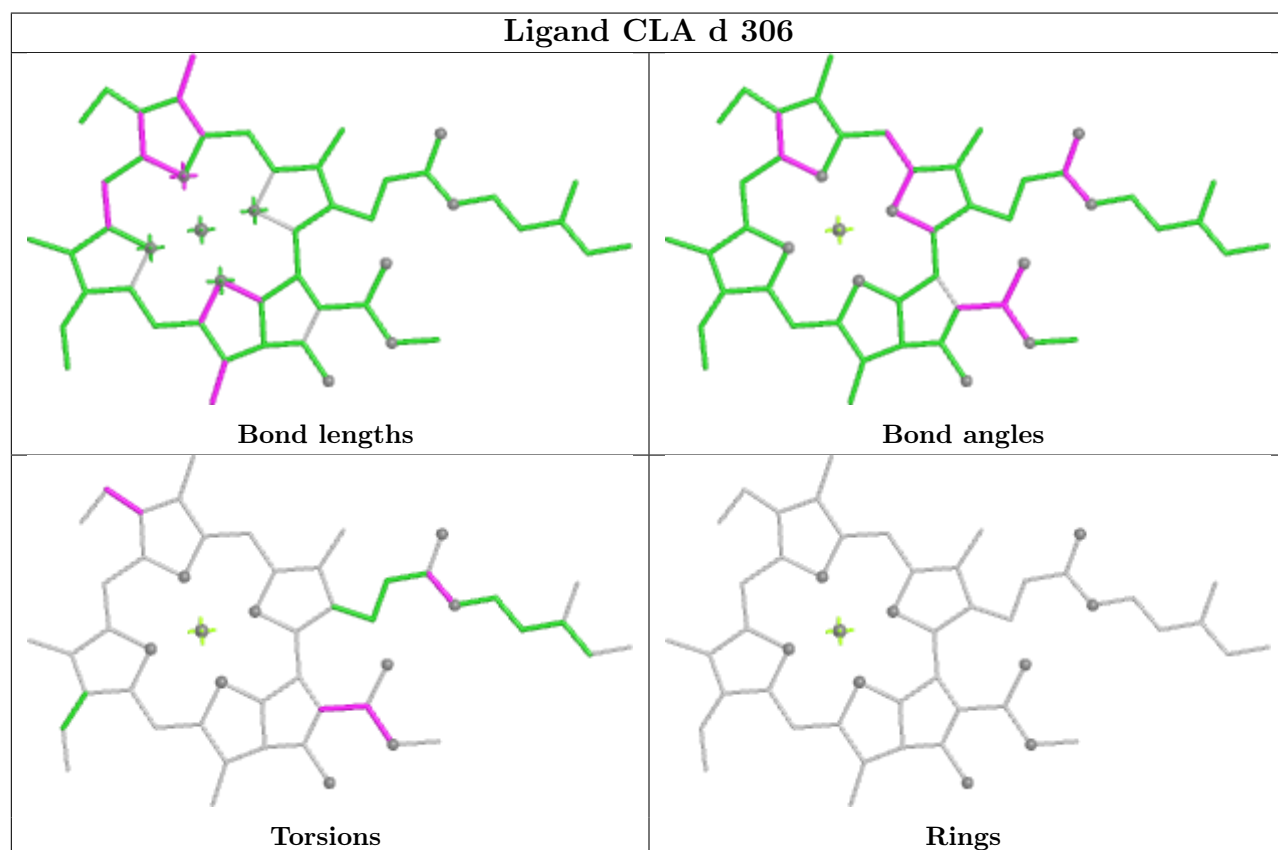
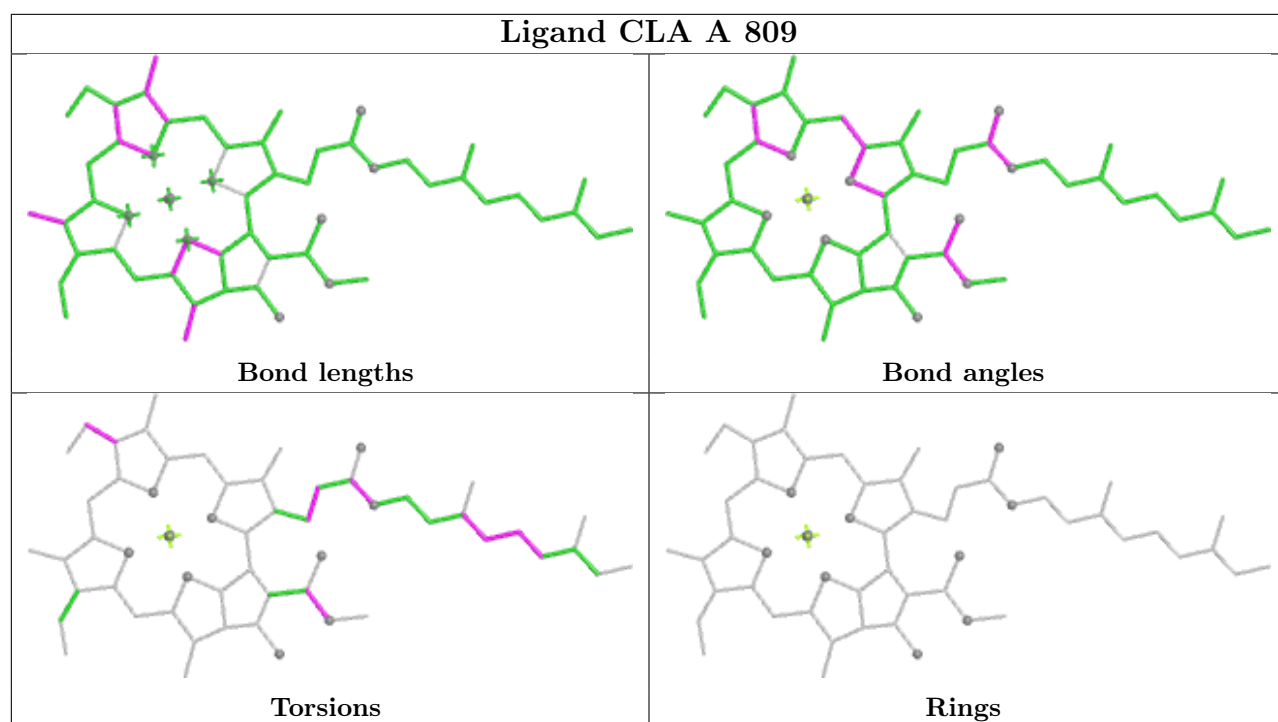
Ligand CLA b 307



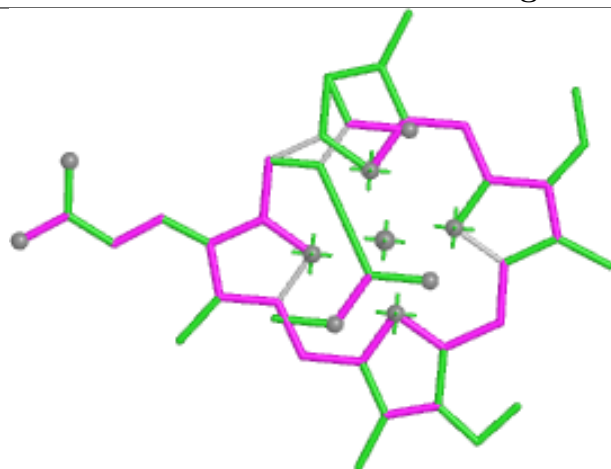
Ligand KC2 d 312



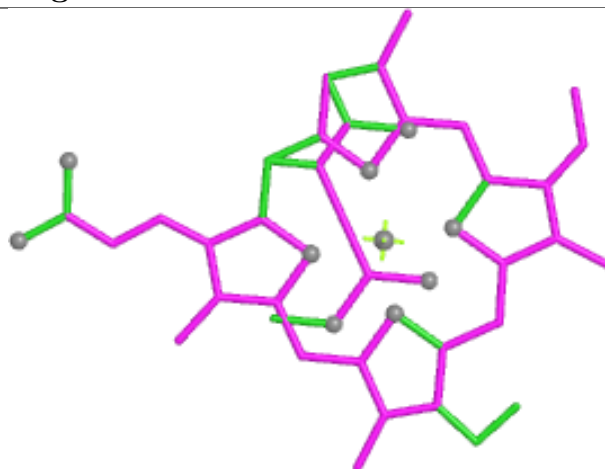
Ligand CLA A 835**Ligand CLA b 312**



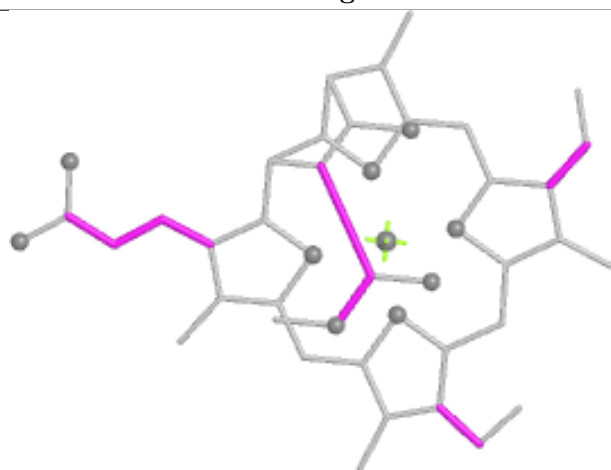
Ligand KC2 g 314



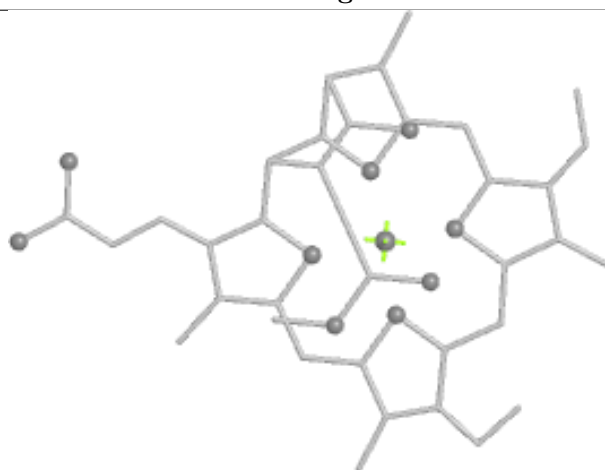
Bond lengths



Bond angles

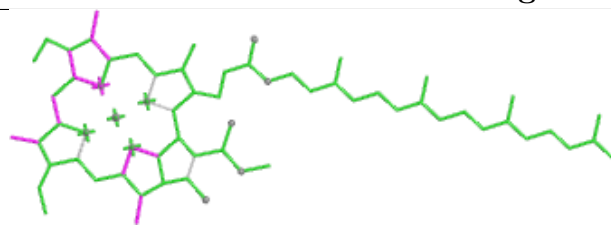


Torsions

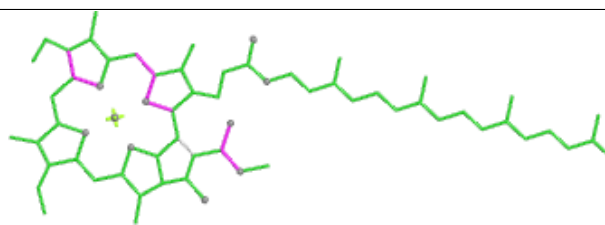


Rings

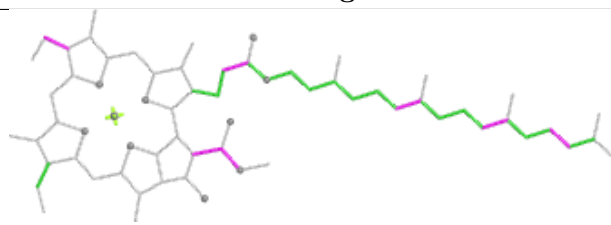
Ligand CLA a 310



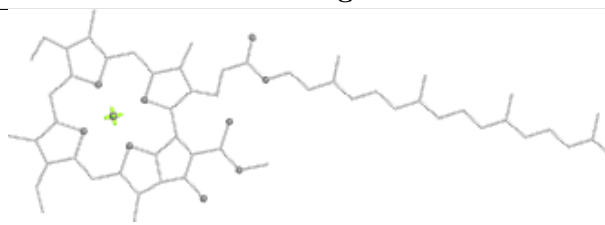
Bond lengths



Bond angles

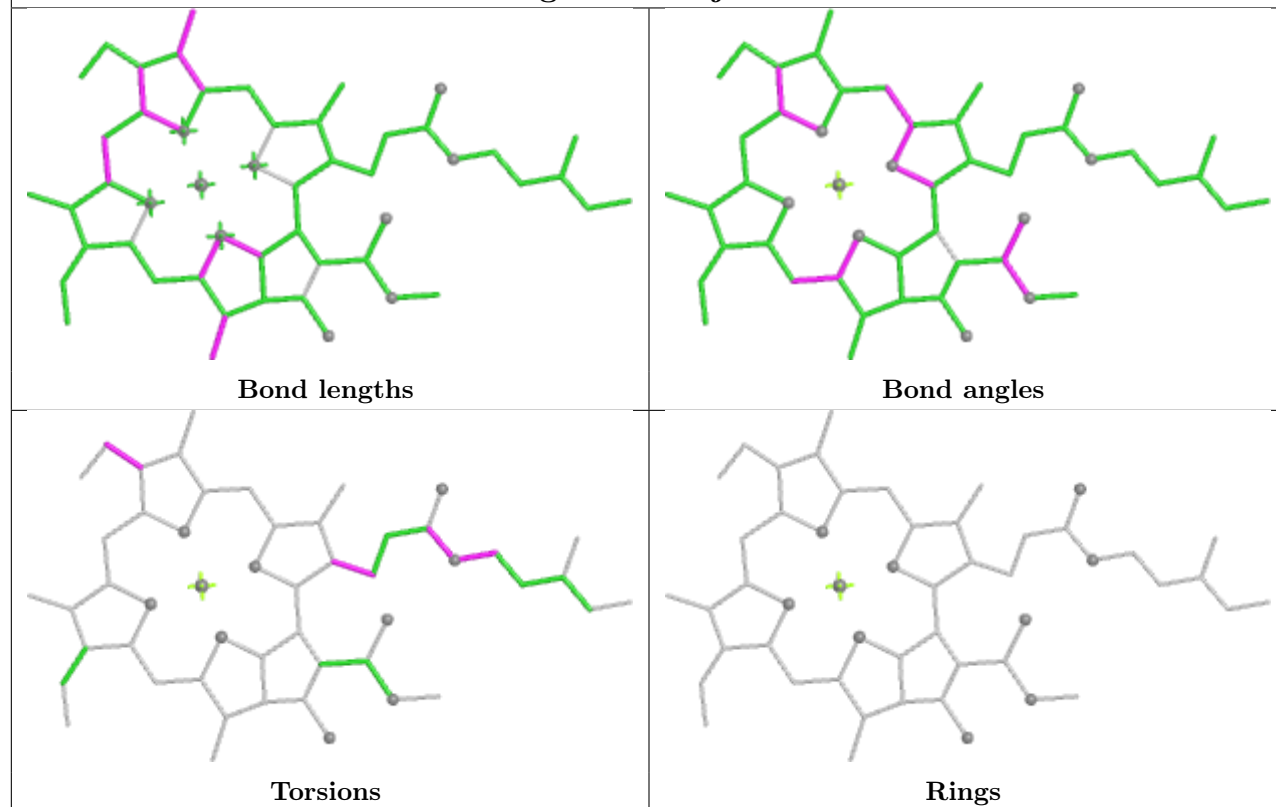


Torsions

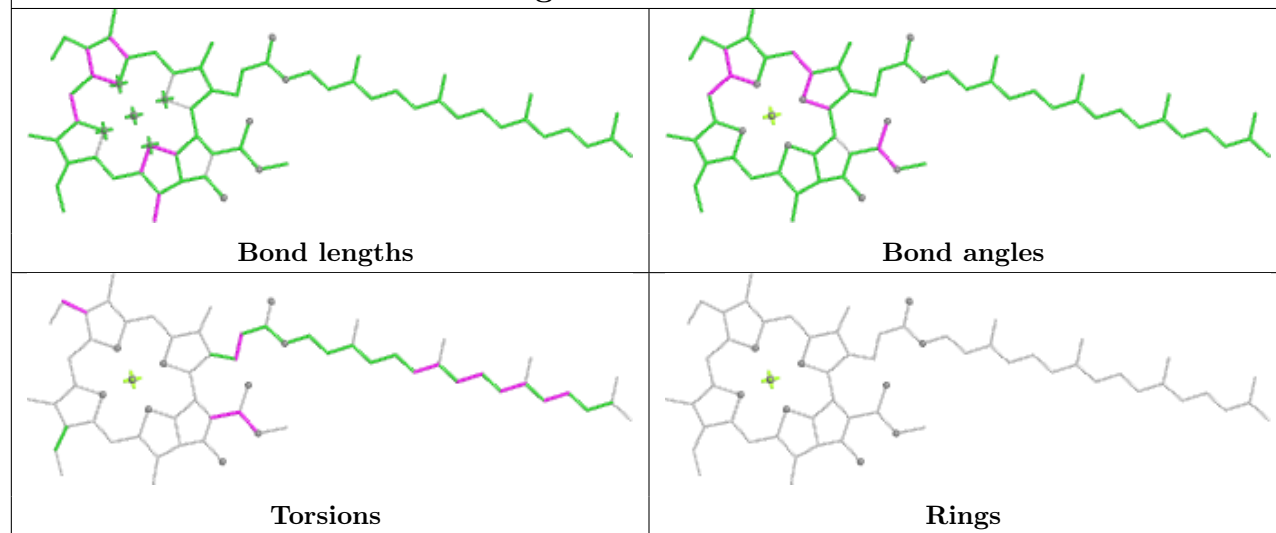


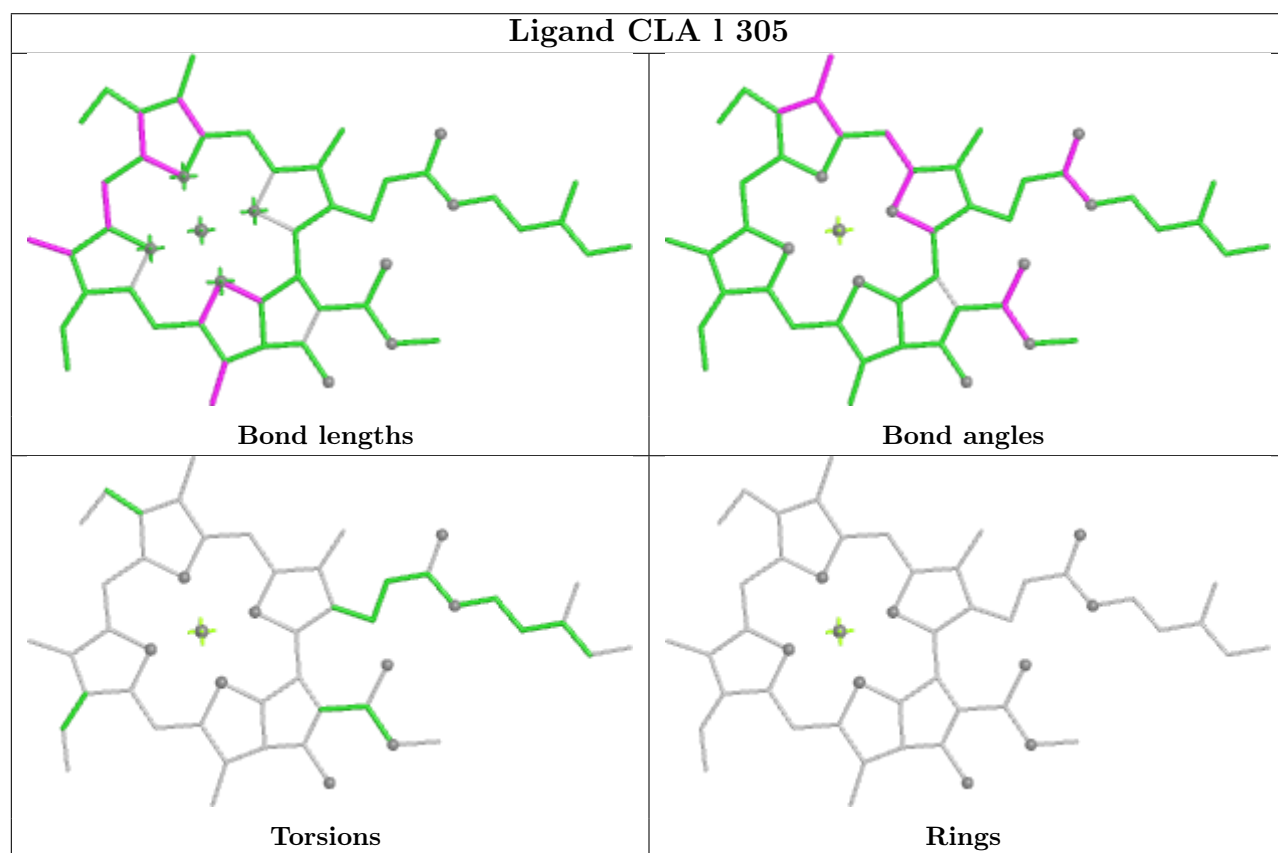
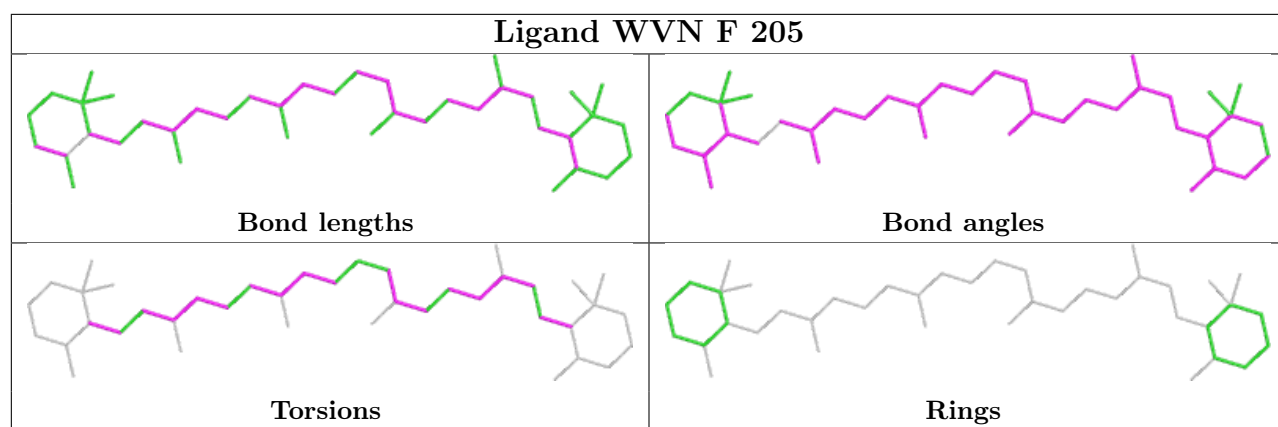
Rings

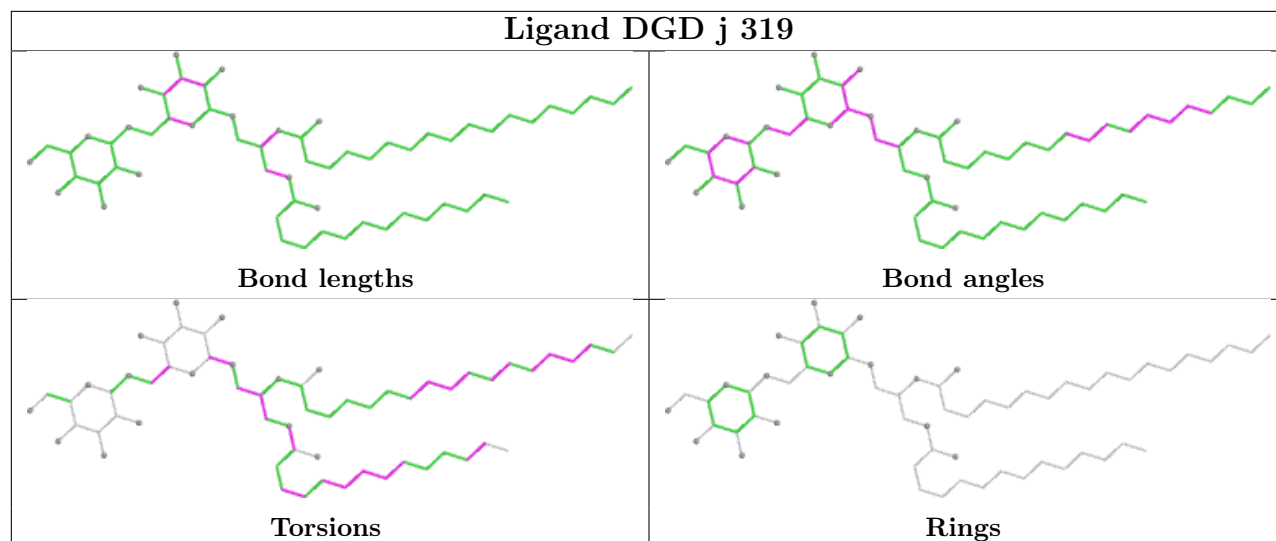
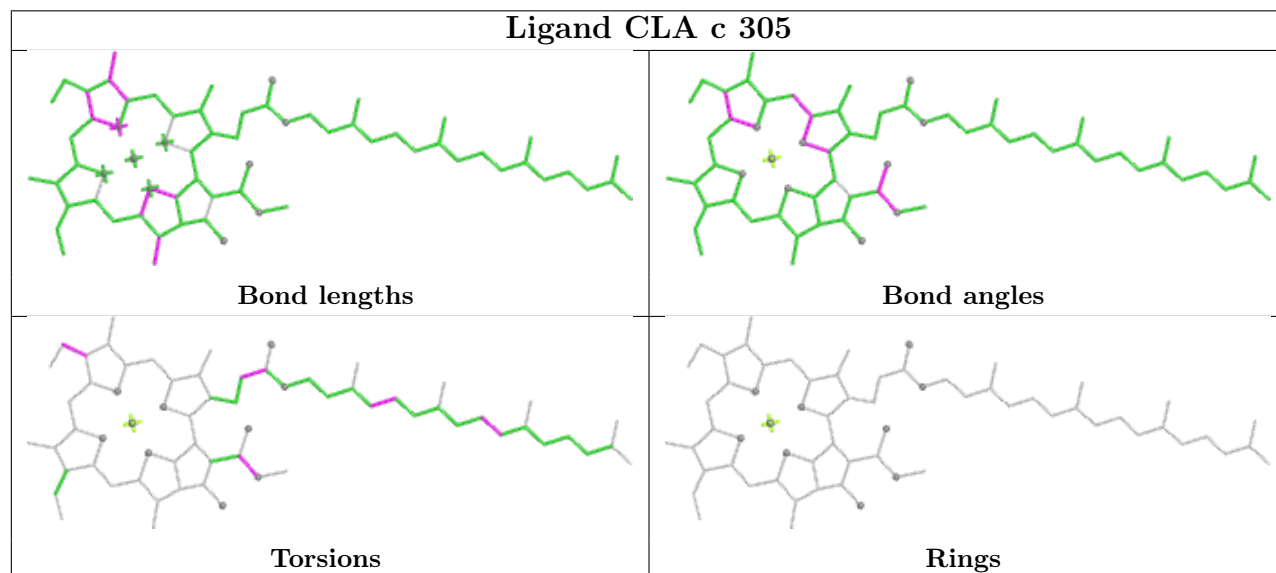
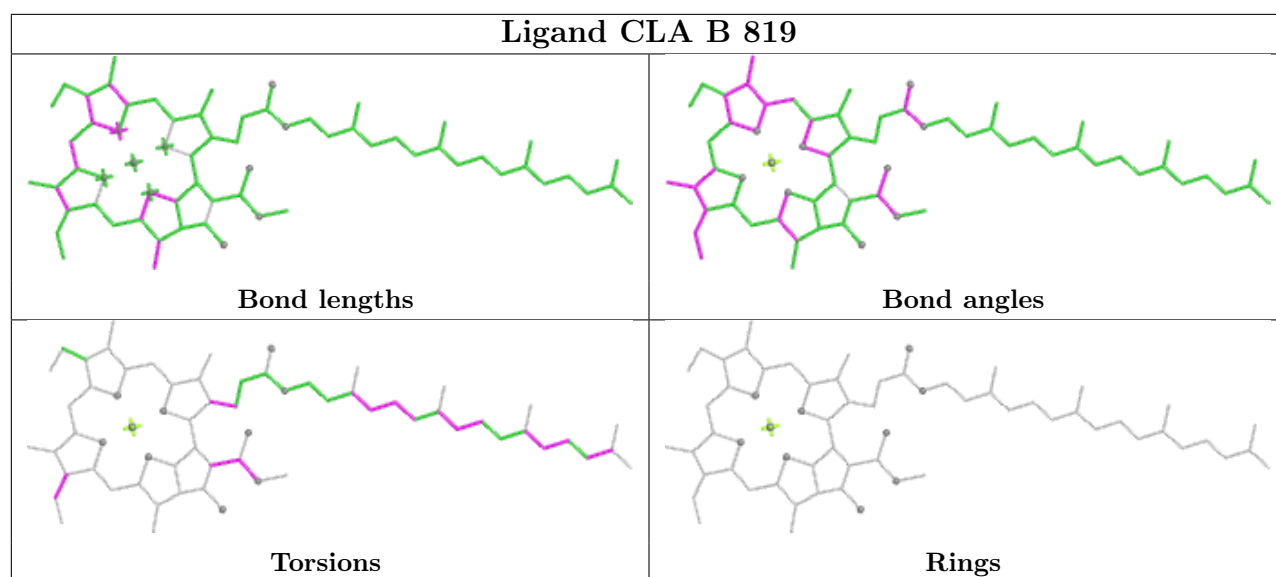
Ligand CLA j 307



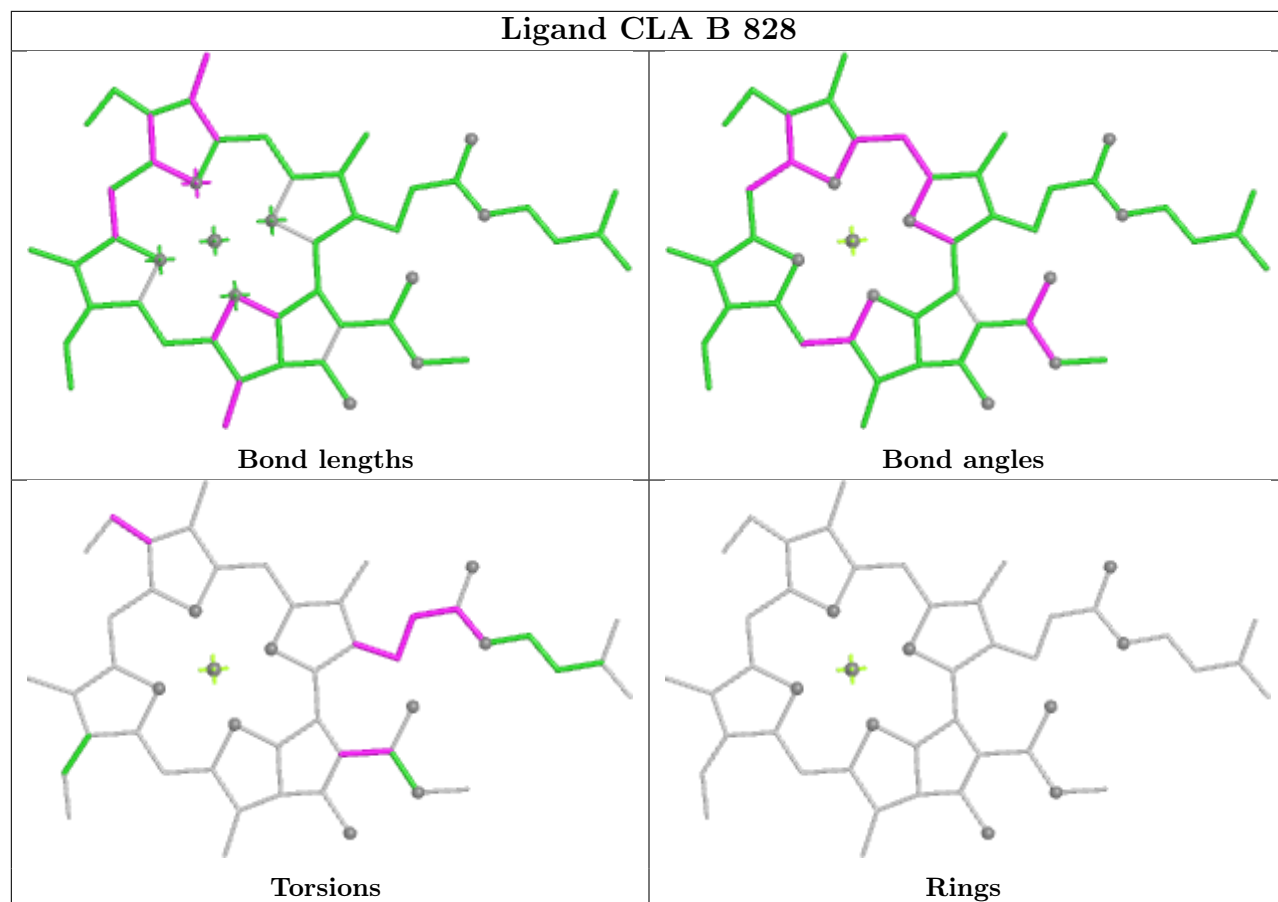
Ligand CLA b 305



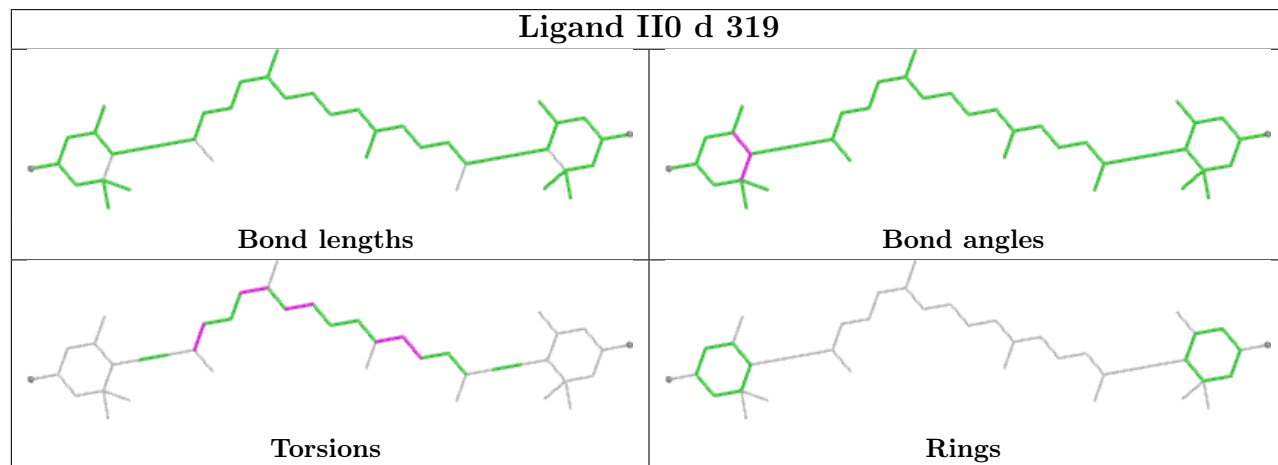




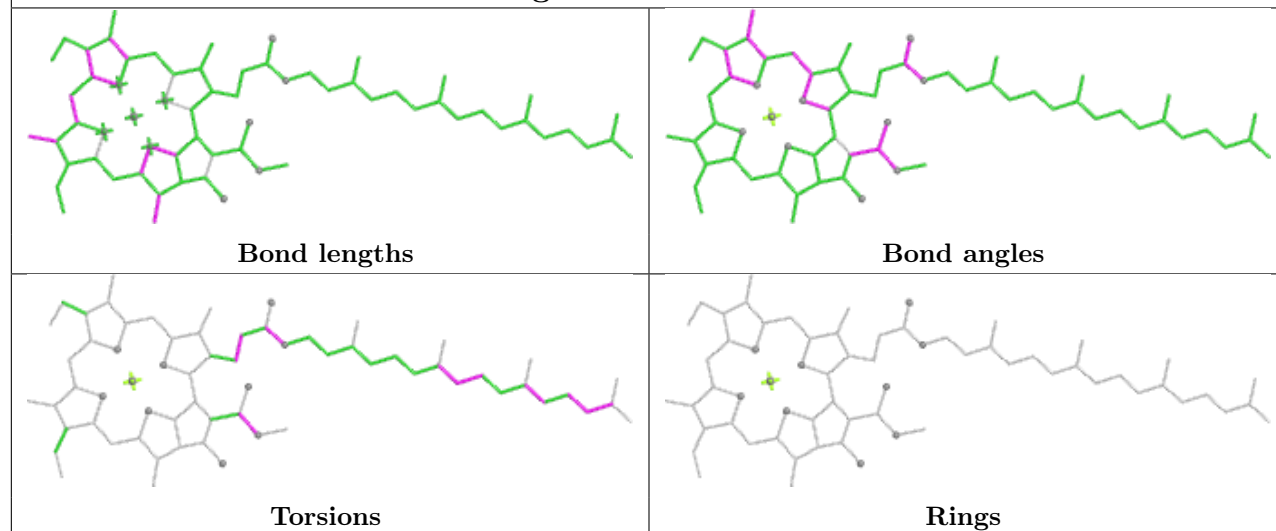
Ligand CLA B 828



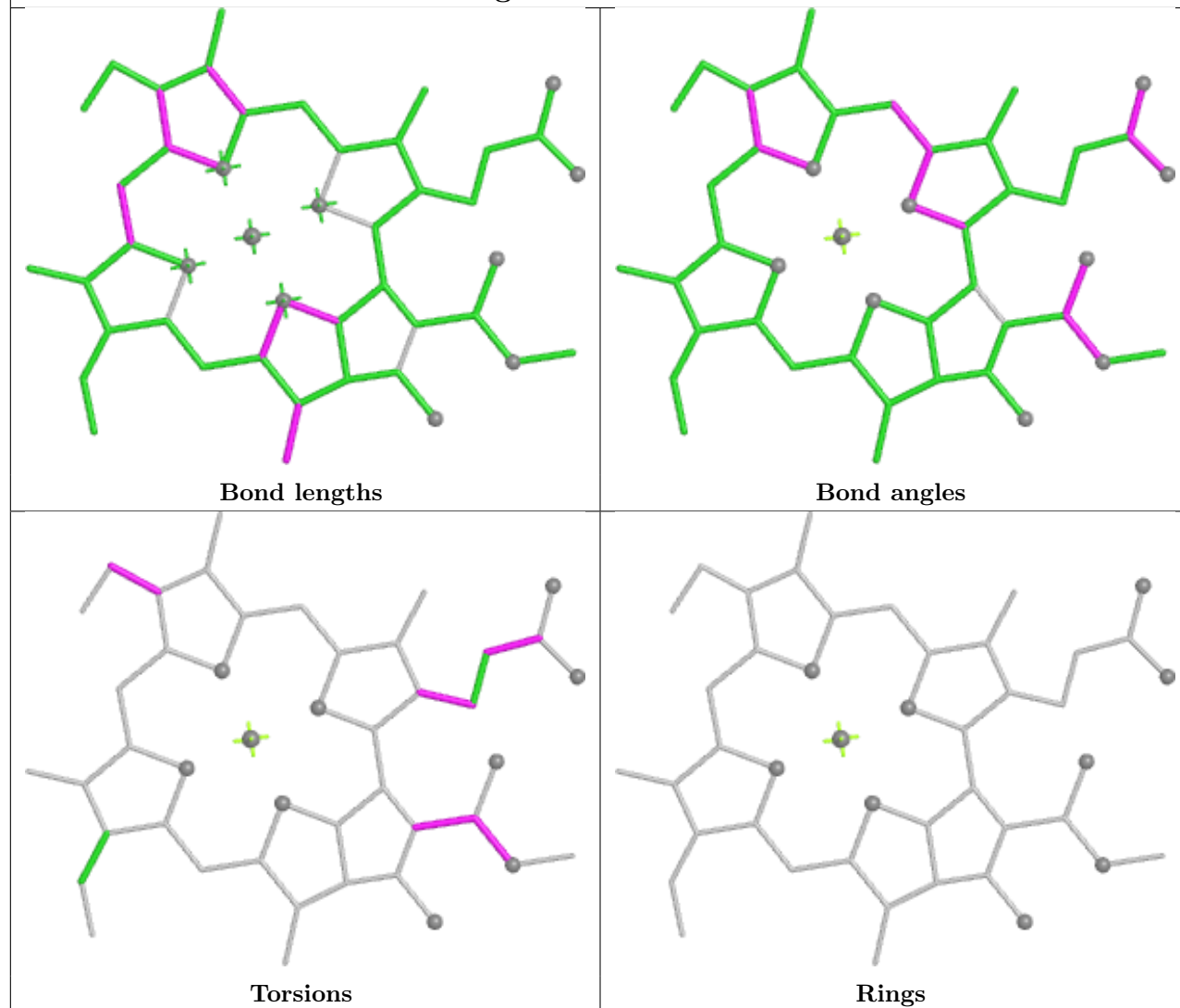
Ligand II0 d 319

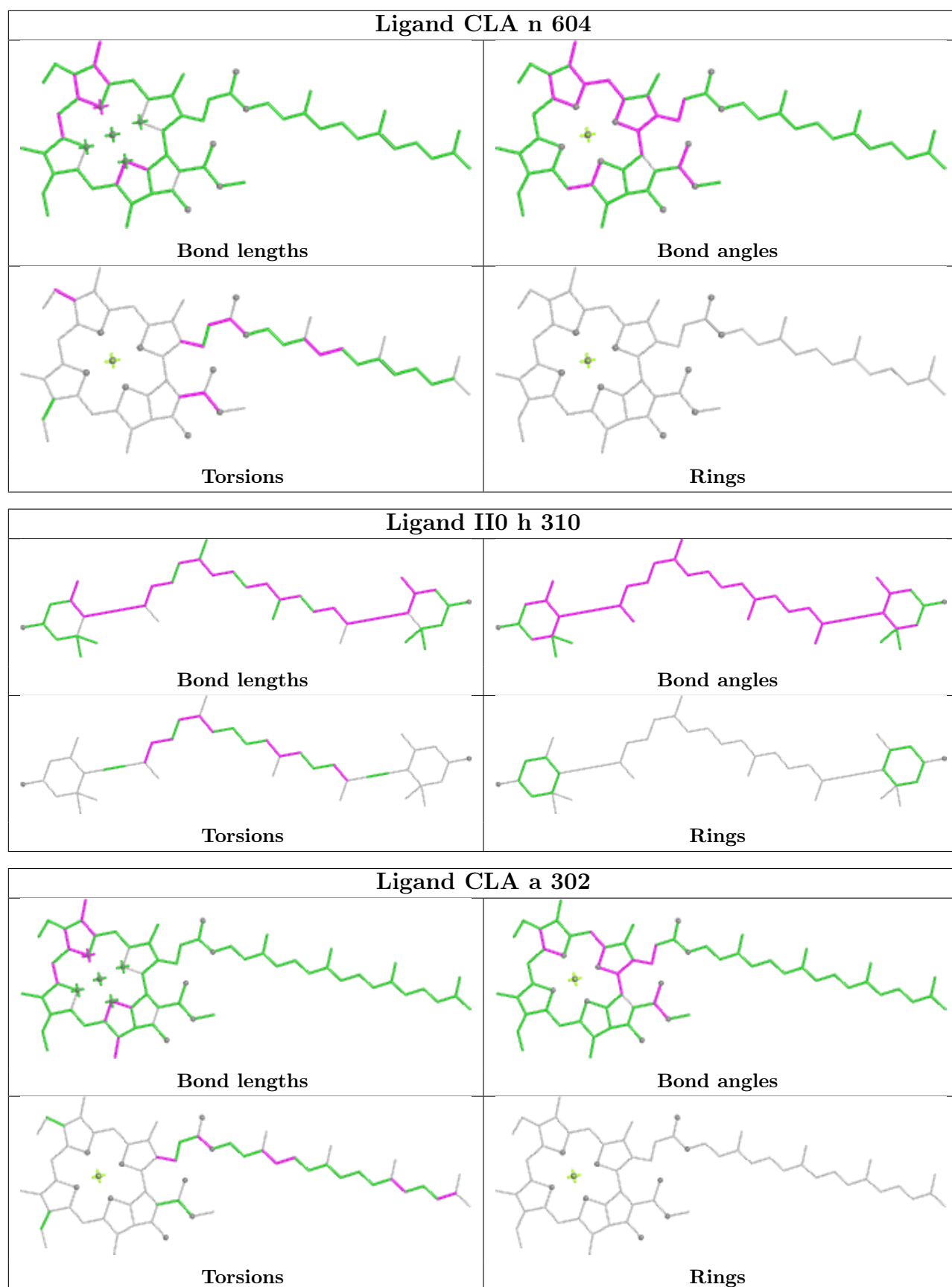


Ligand CLA B 838

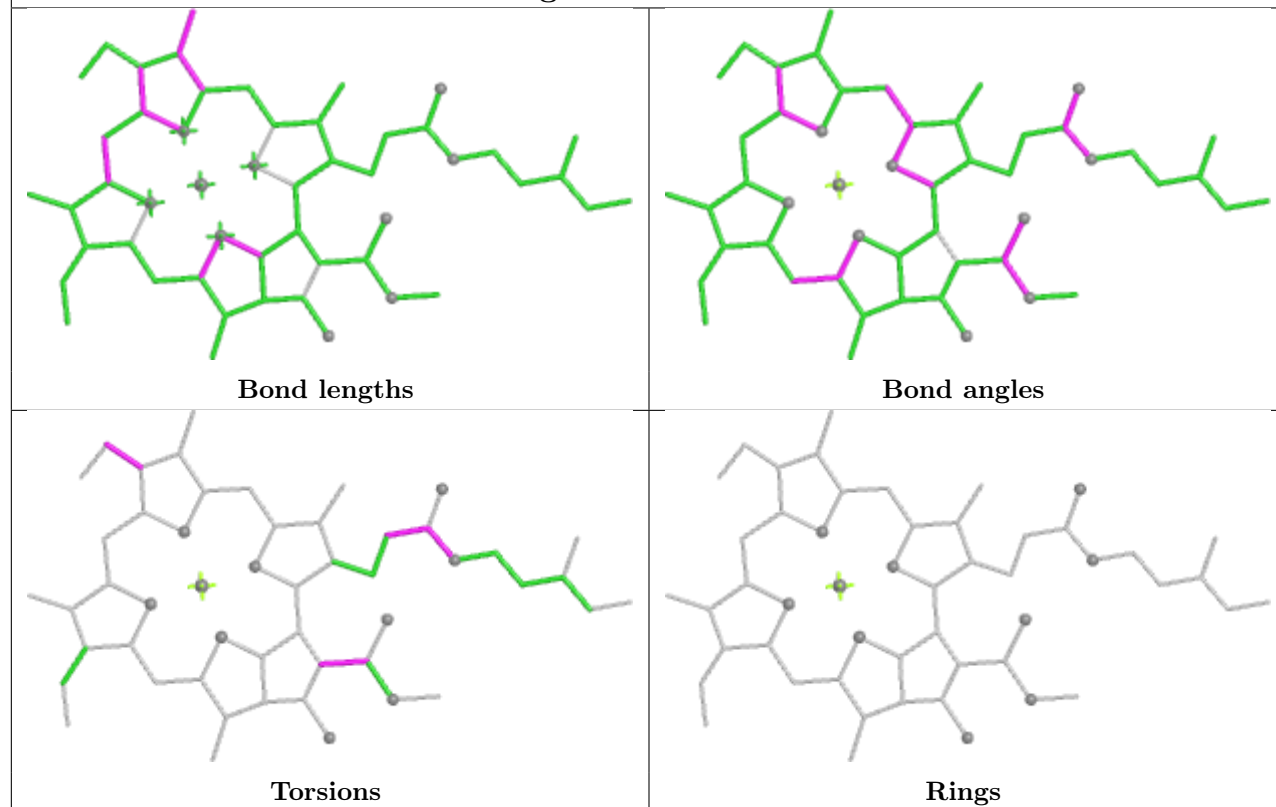


Ligand CLA d 304

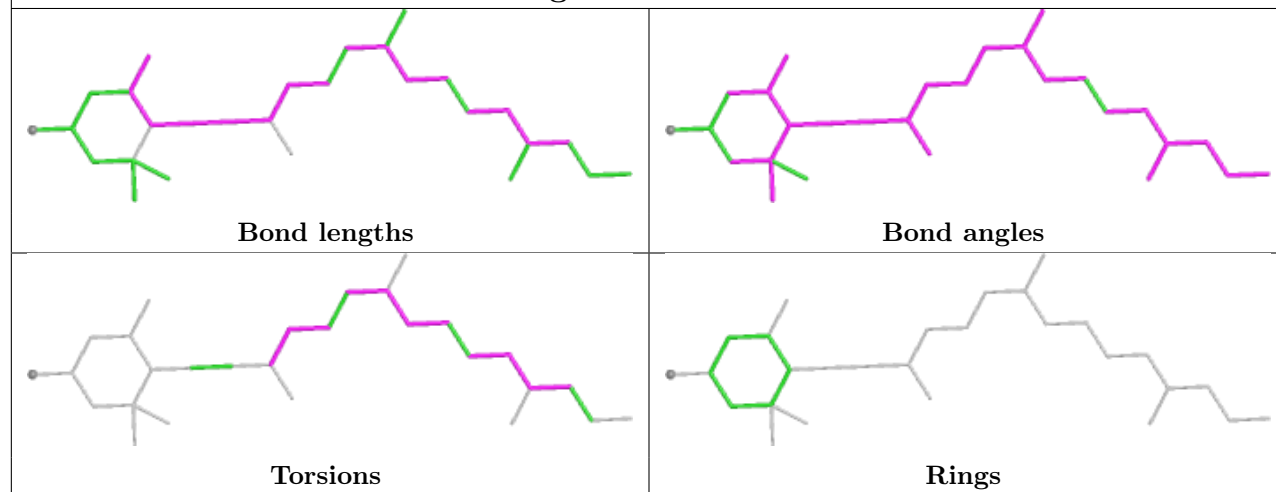


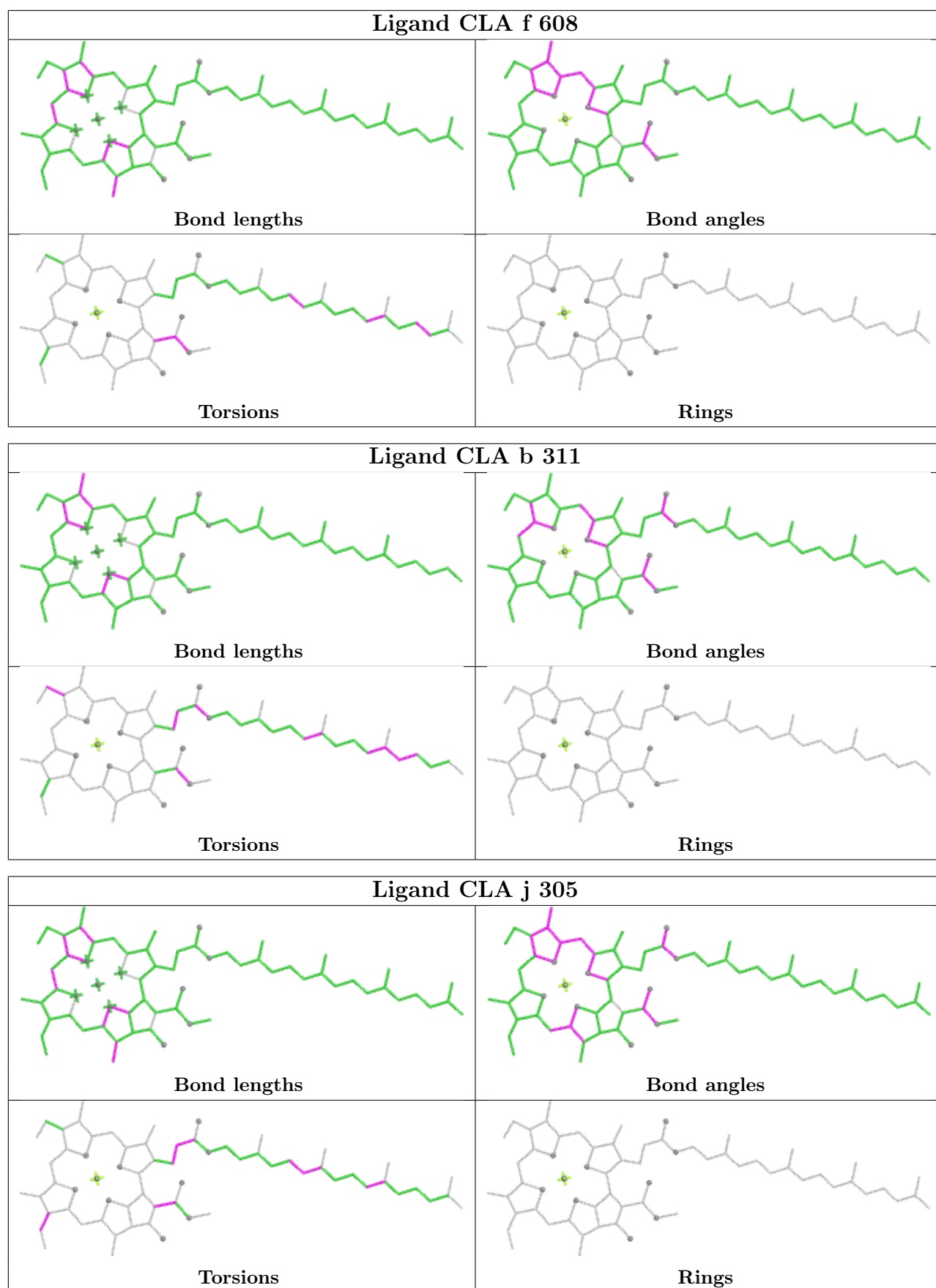


Ligand CLA f 606

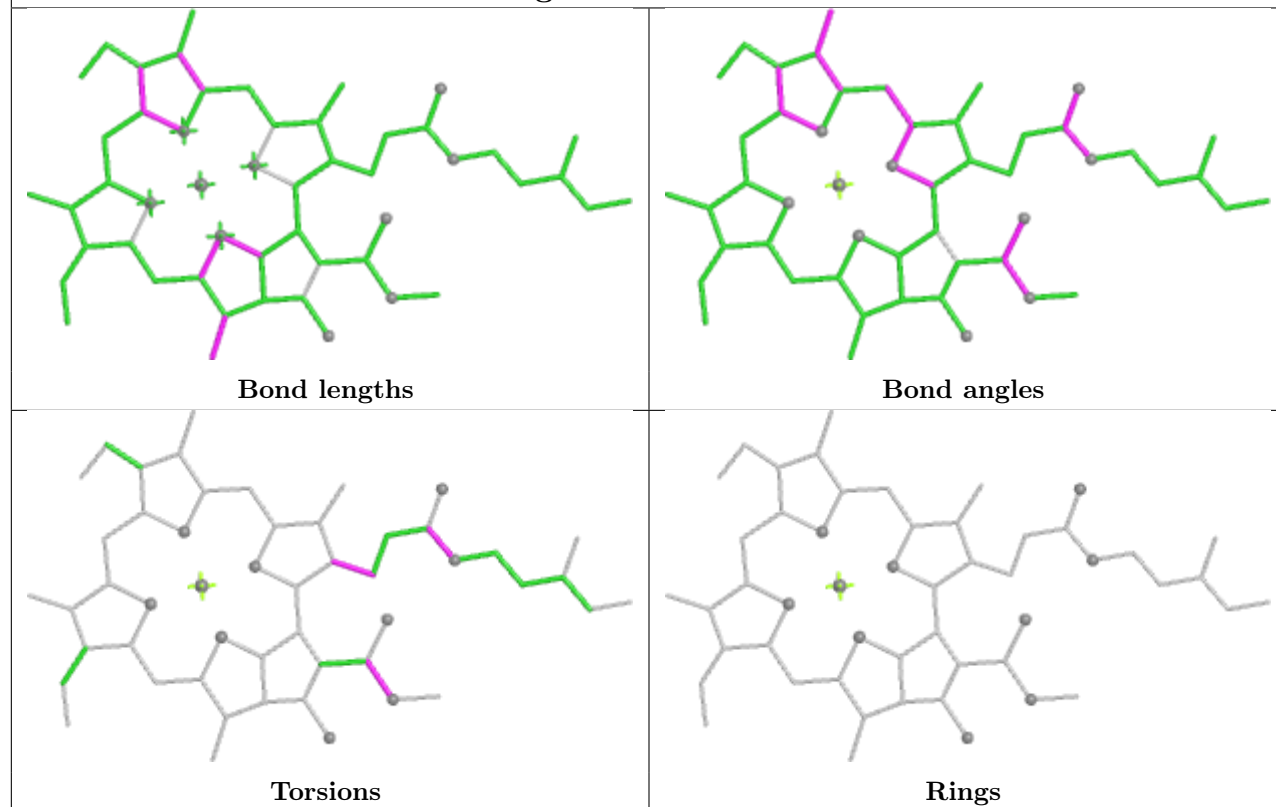


Ligand II0 h 309

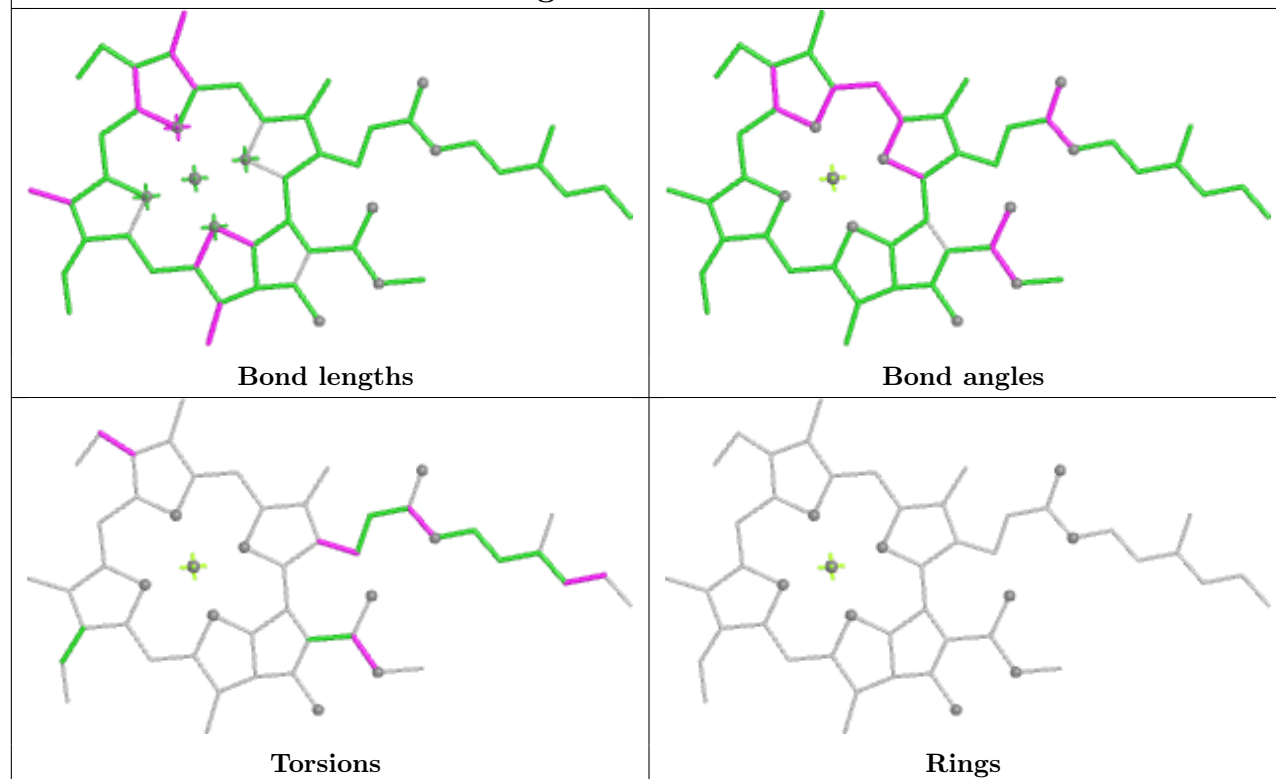




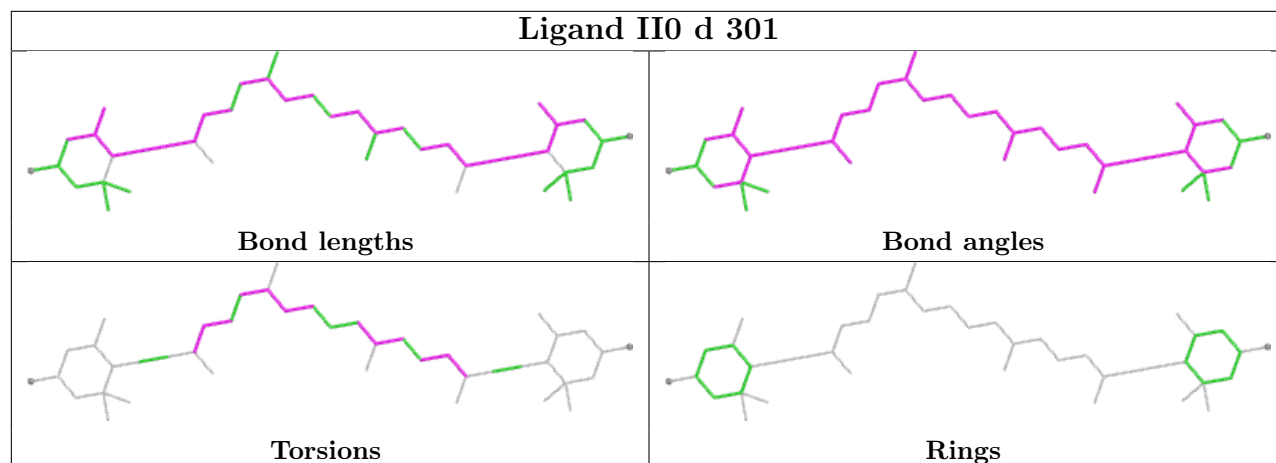
Ligand CLA h 304



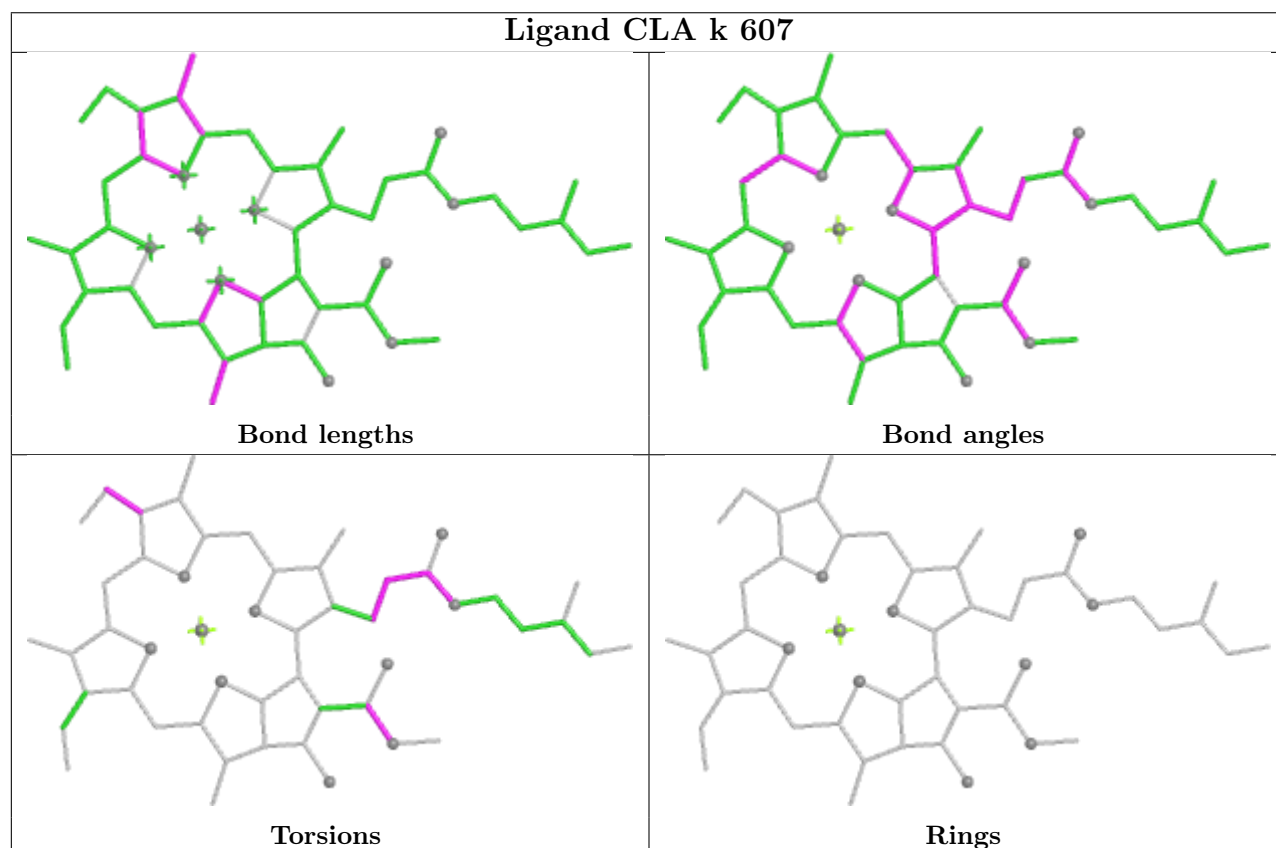
Ligand CLA c 306



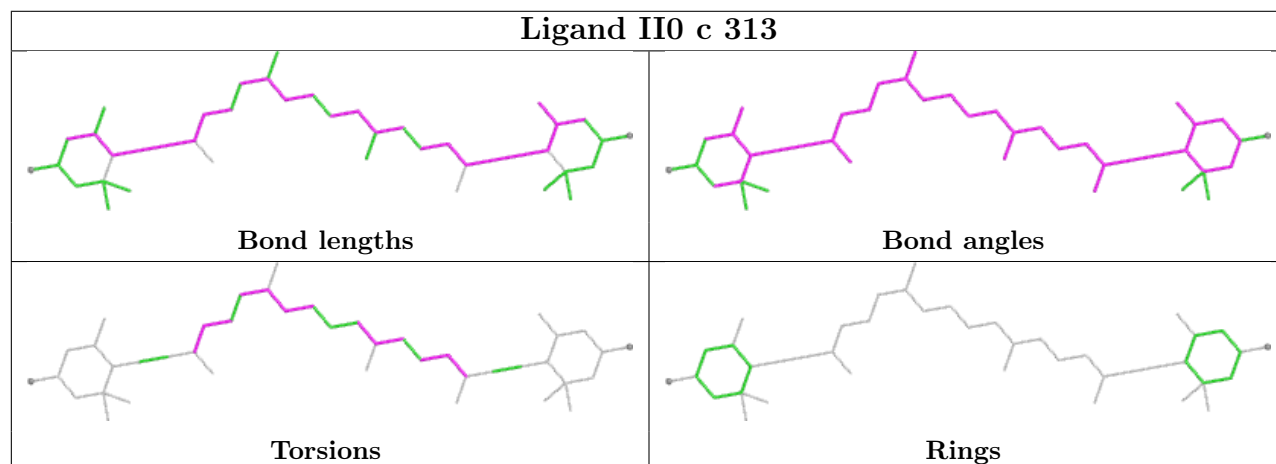
Ligand II0 d 301

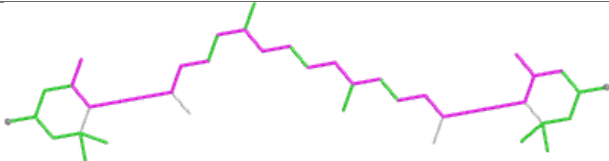
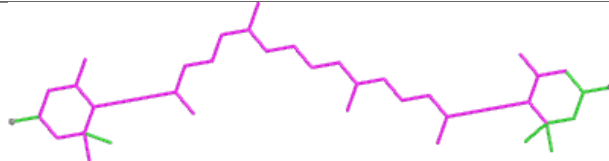
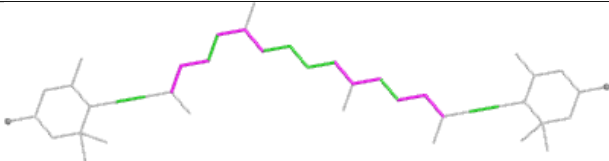
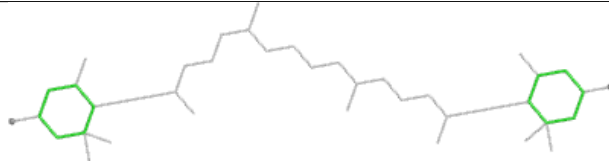


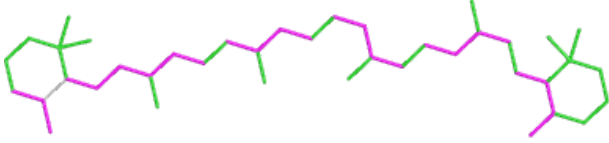
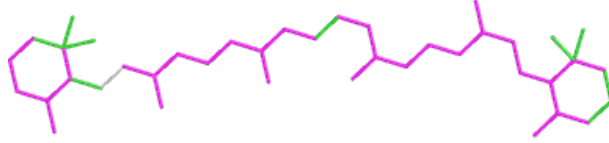
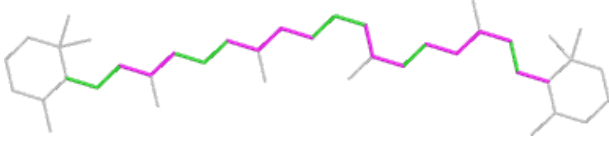
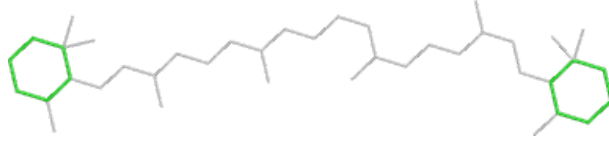
Ligand CLA k 607

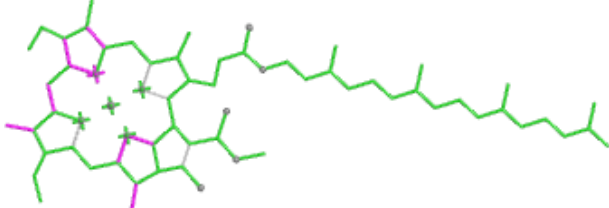
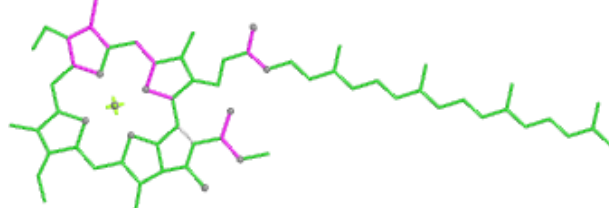
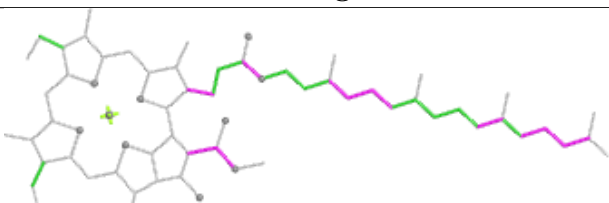
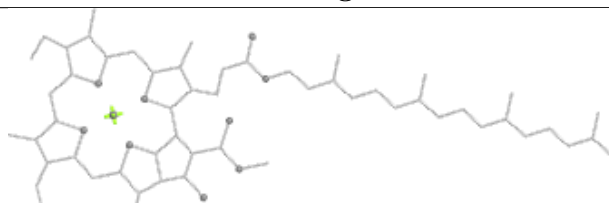


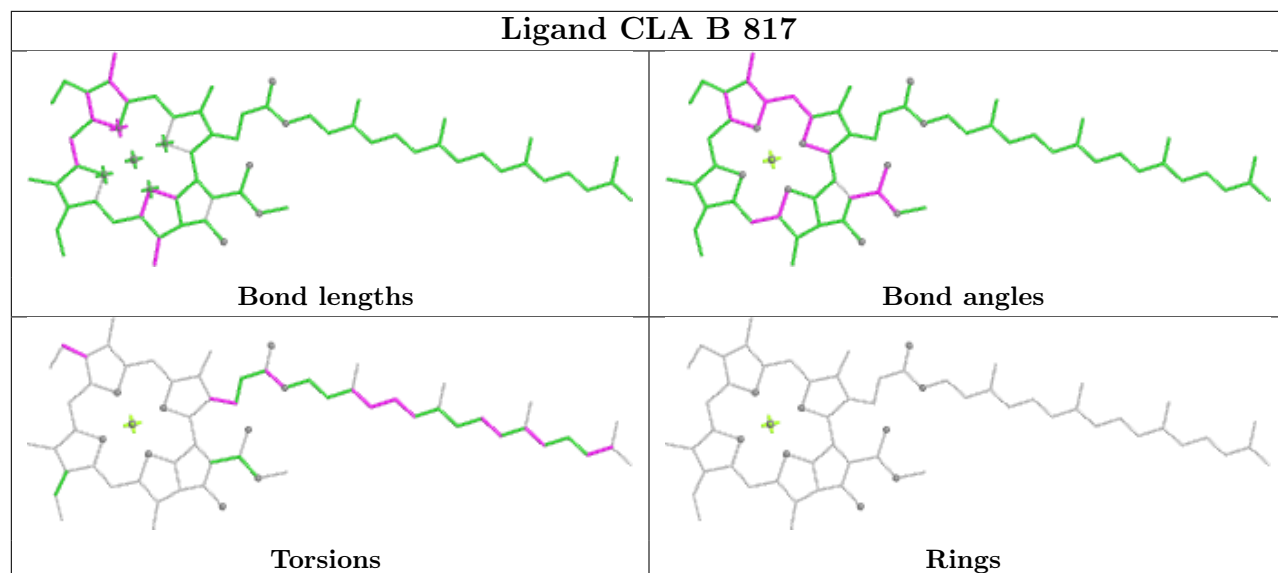
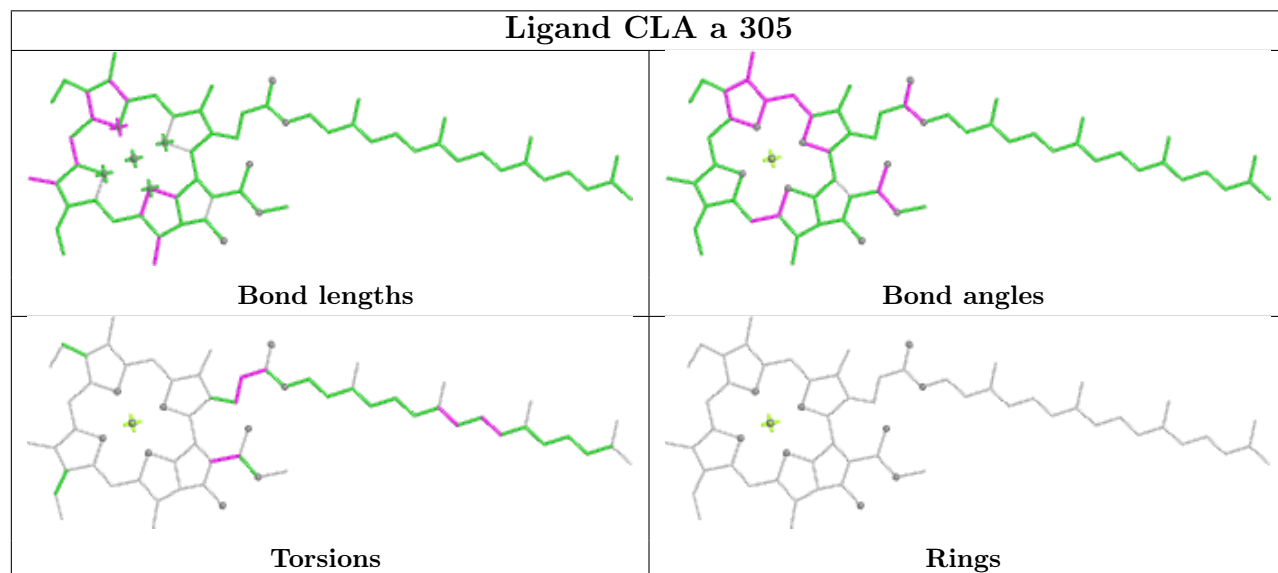
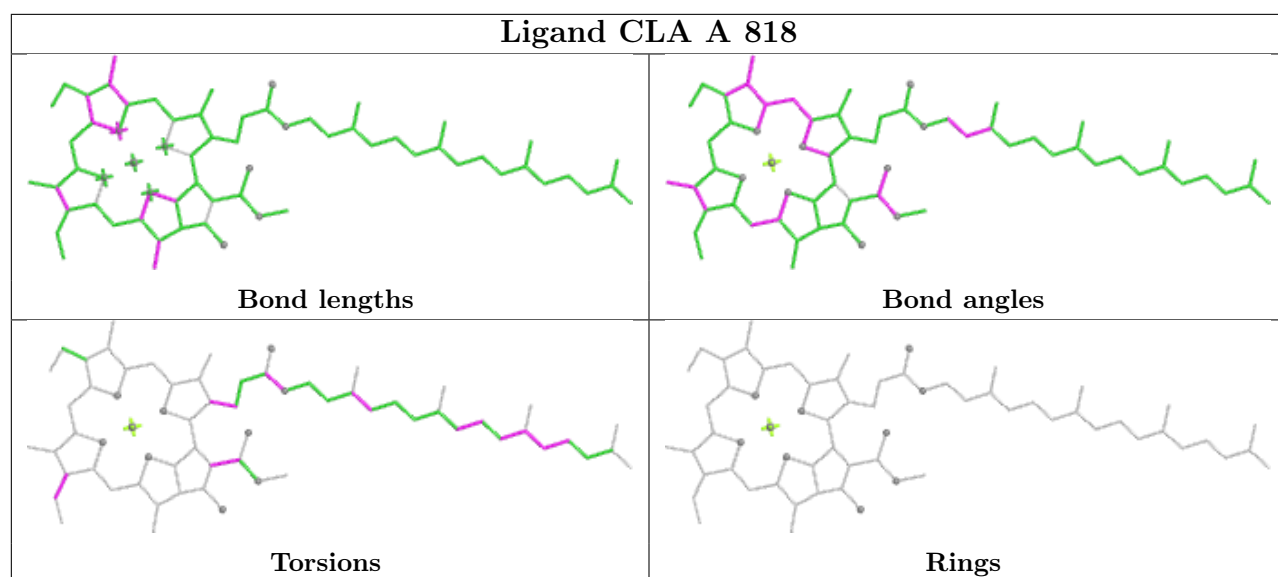
Ligand II0 c 313



Ligand II0 a 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand WVN A 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA f 602	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

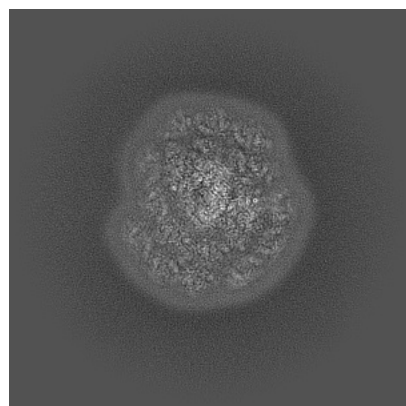
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62656. These allow visual inspection of the internal detail of the map and identification of artifacts.

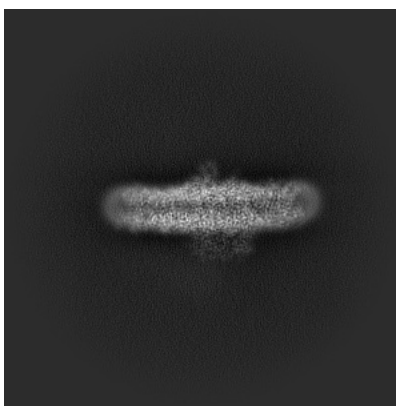
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

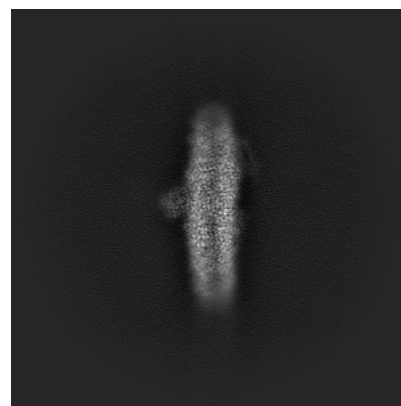
6.1.1 Primary map



X

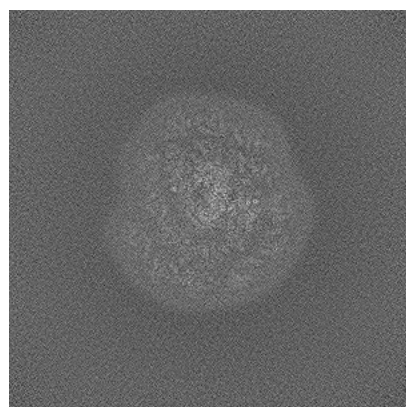


Y

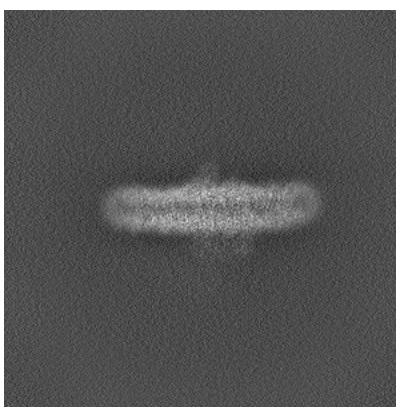


Z

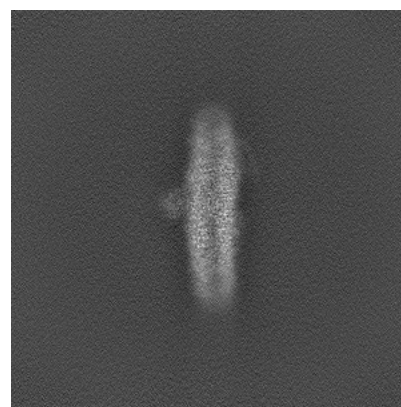
6.1.2 Raw map



X



Y

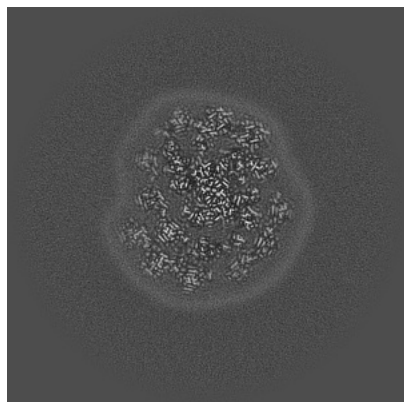


Z

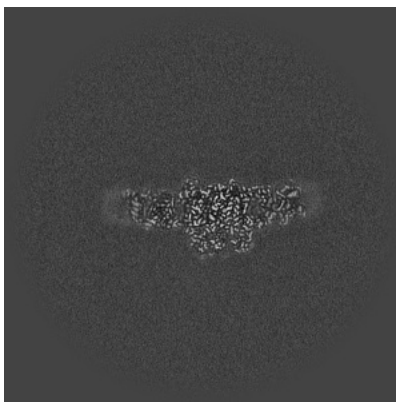
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

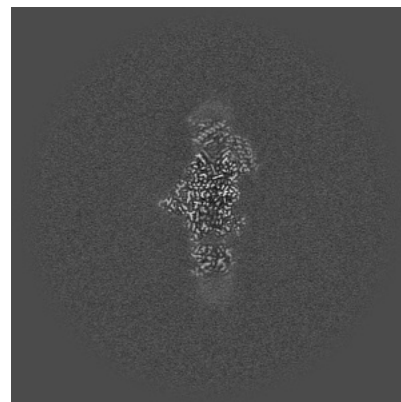
6.2.1 Primary map



X Index: 300

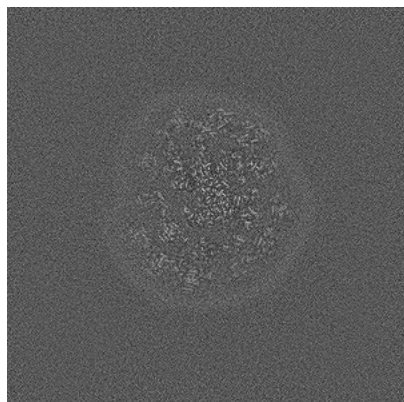


Y Index: 300

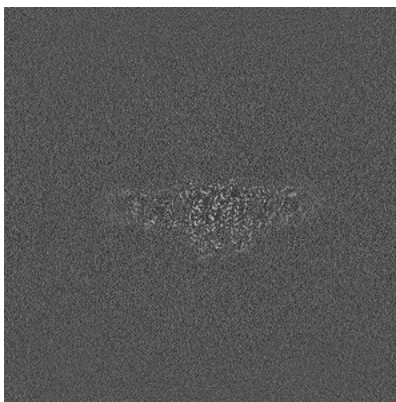


Z Index: 300

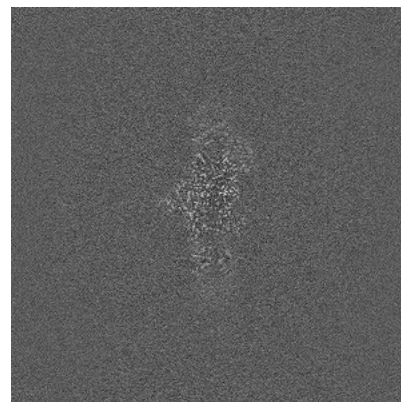
6.2.2 Raw map



X Index: 300



Y Index: 300

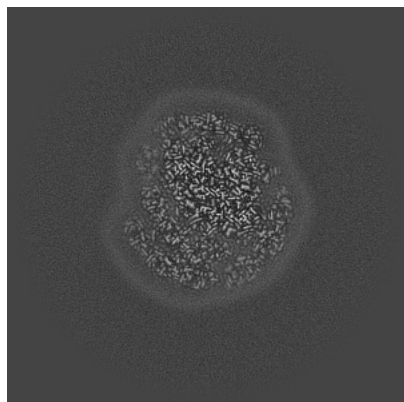


Z Index: 300

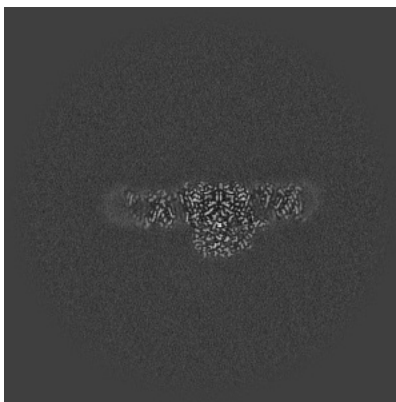
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

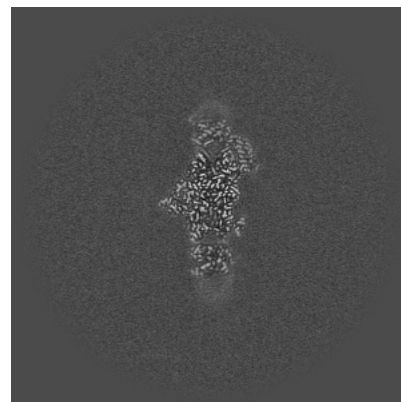
6.3.1 Primary map



X Index: 315

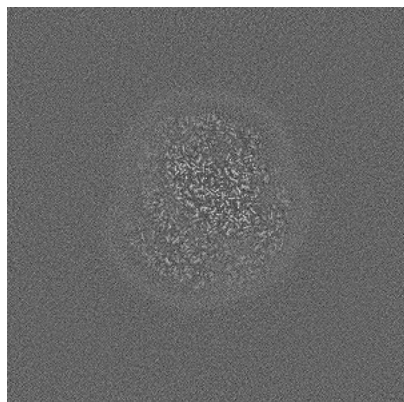


Y Index: 308

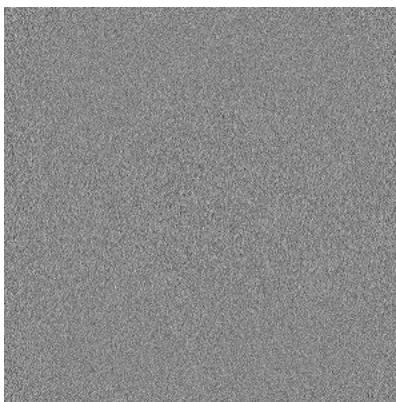


Z Index: 301

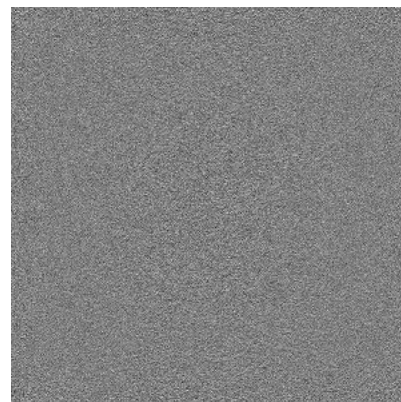
6.3.2 Raw map



X Index: 315



Y Index: 0

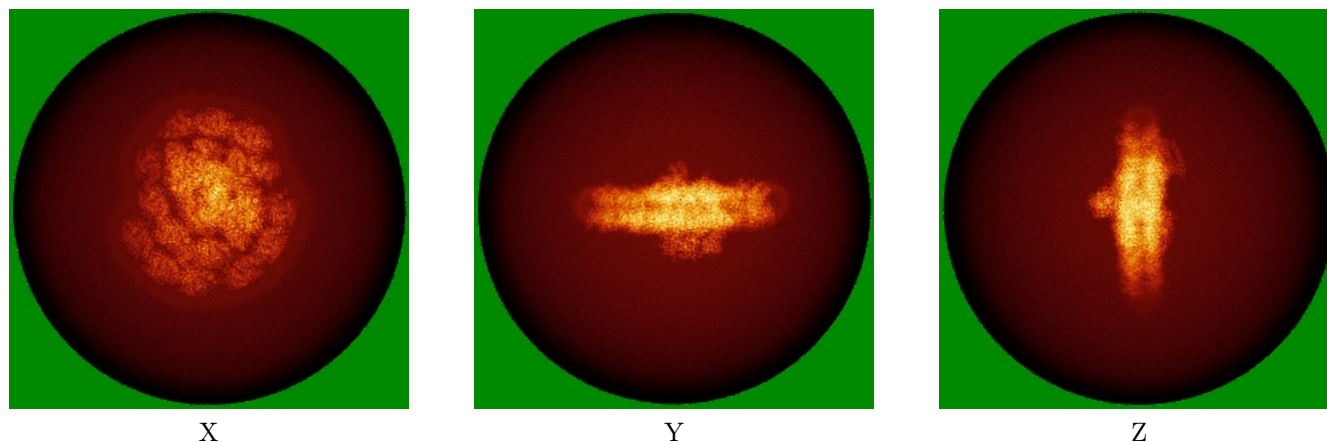


Z Index: 0

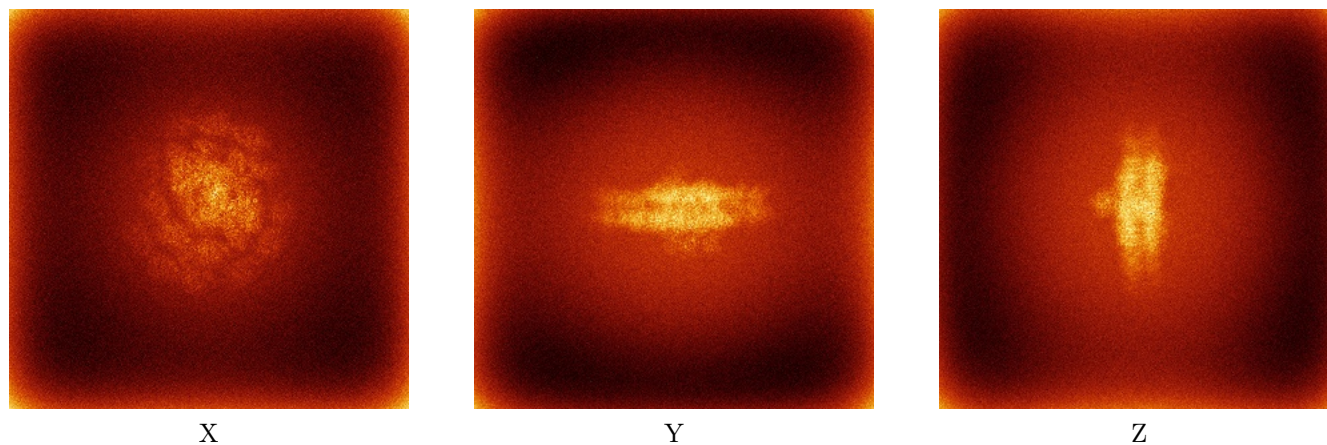
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



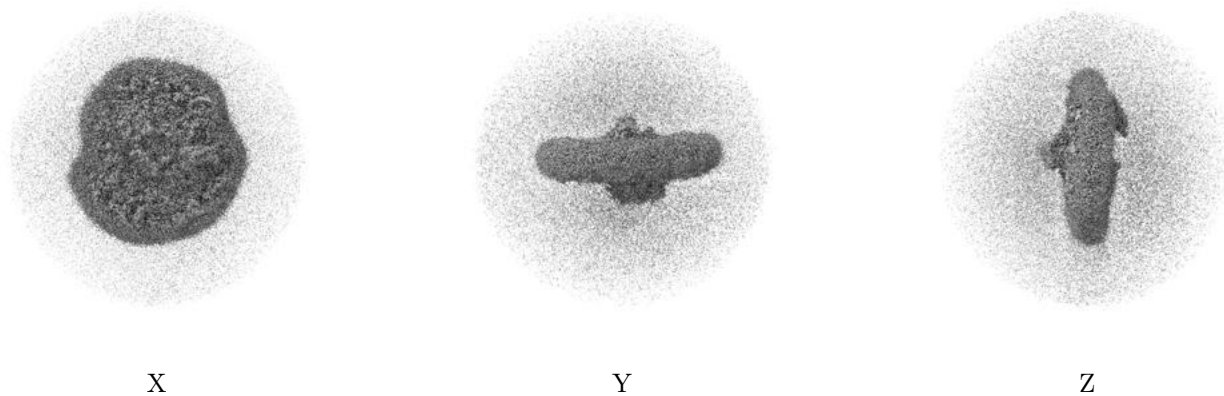
6.4.2 Raw map



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.

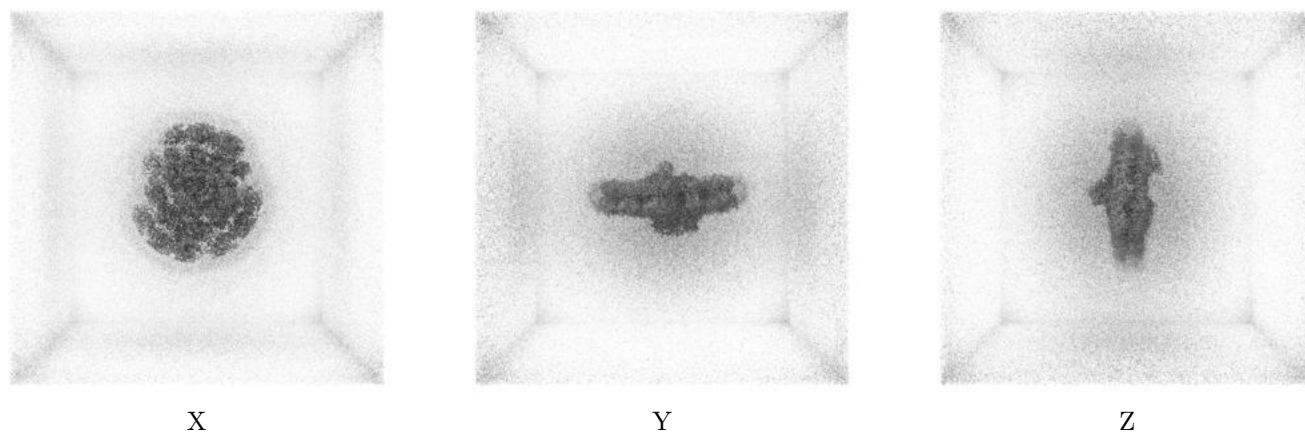
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

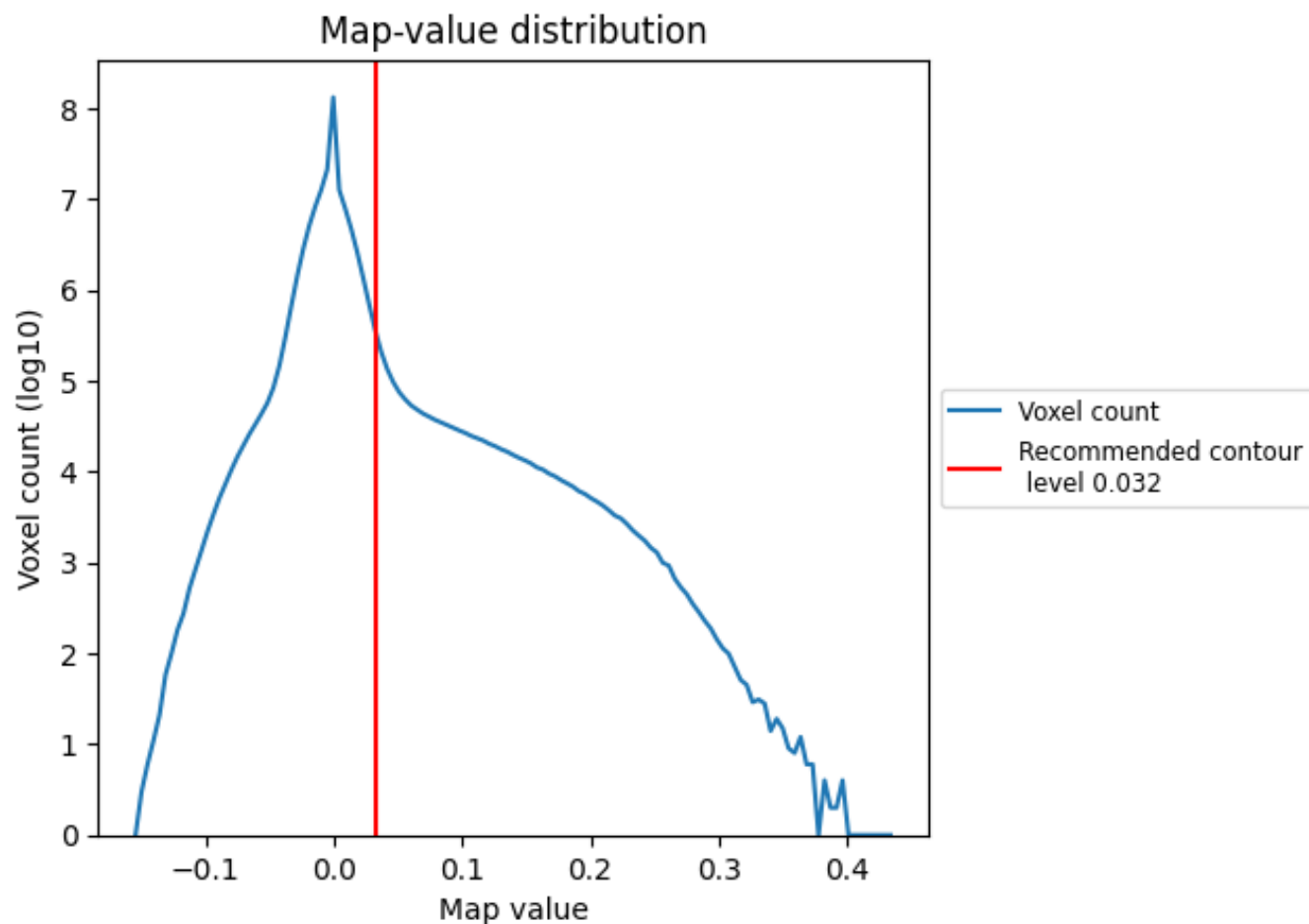
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

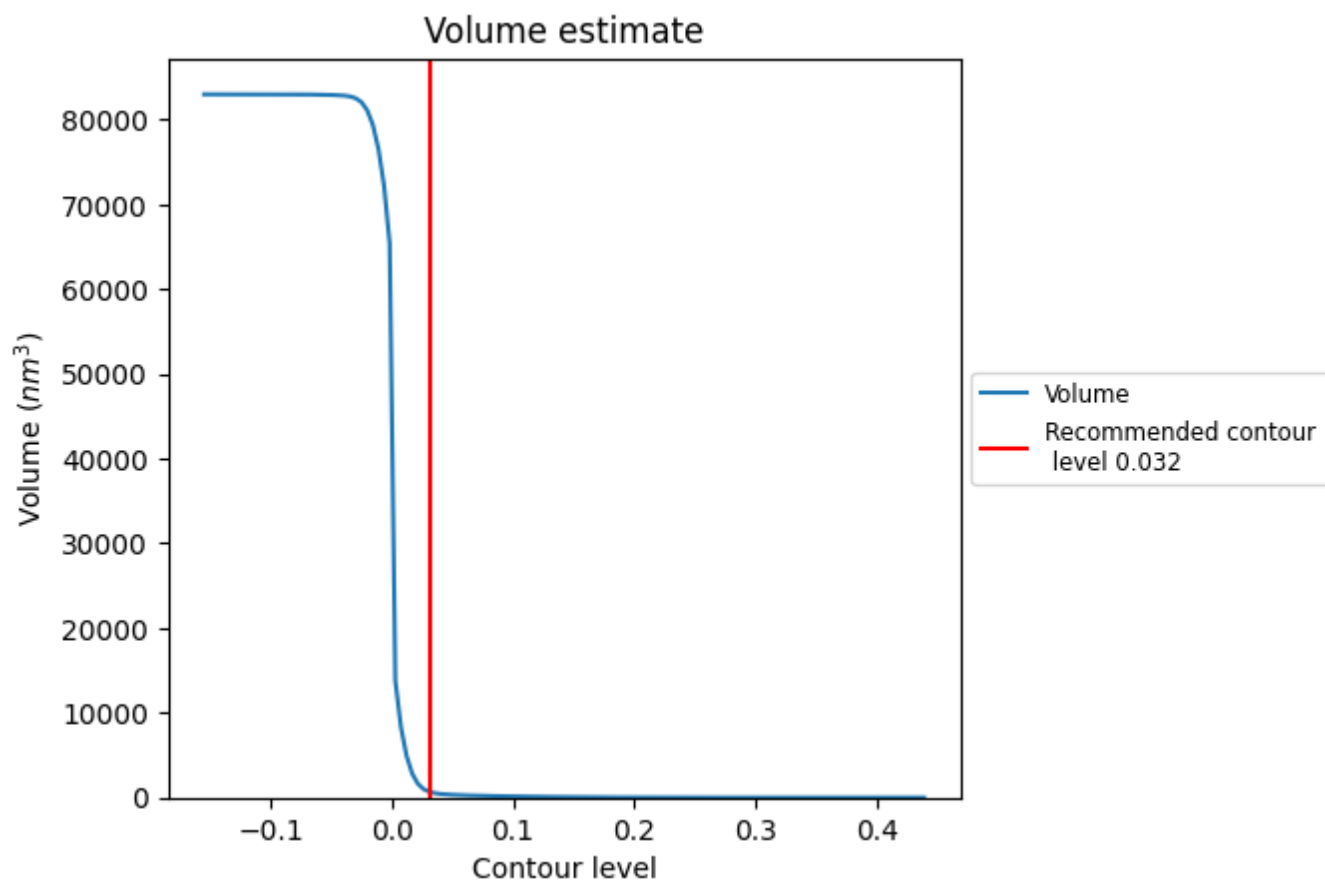
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

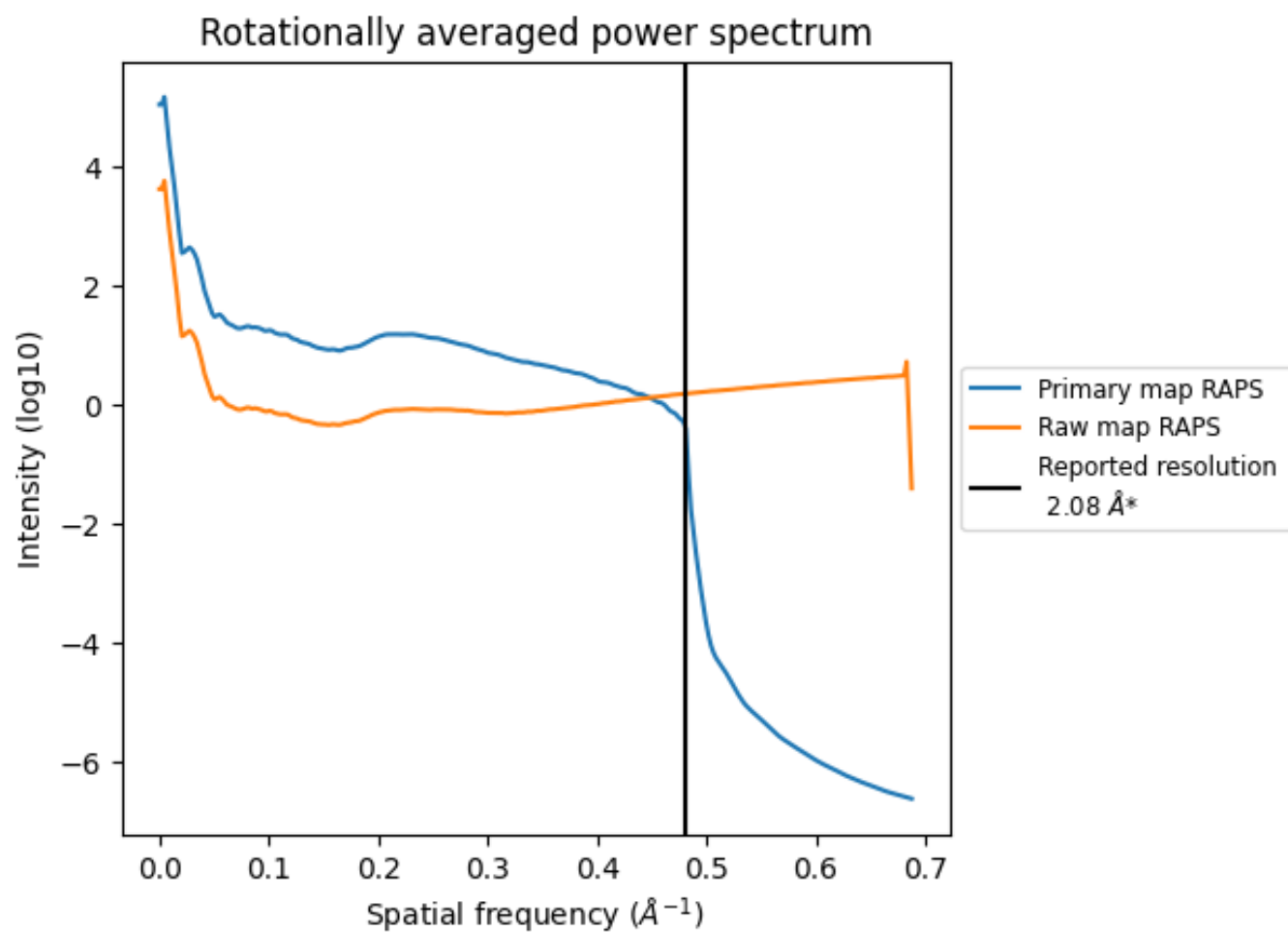
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 646 nm³; this corresponds to an approximate mass of 583 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 ⓘ

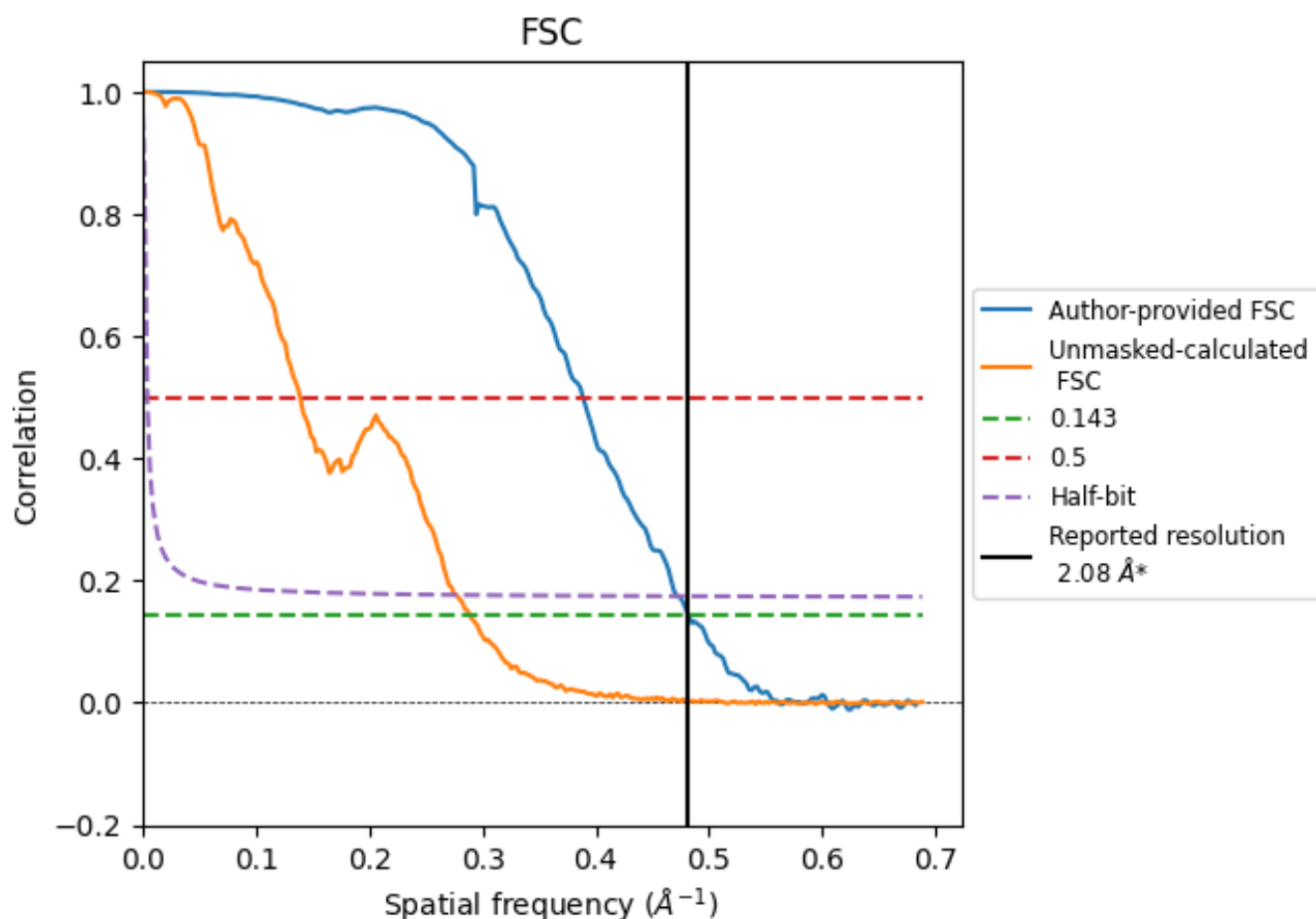


*Reported resolution corresponds to spatial frequency of 0.481 $\text{\AA}^{-1}$

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 0.481 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

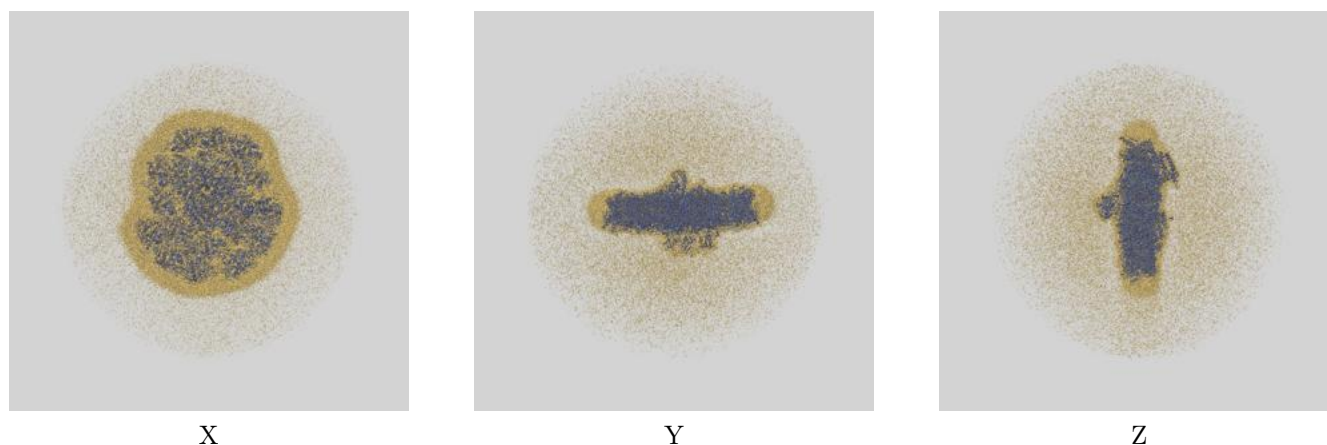
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.08	-	-
Author-provided FSC curve	2.08	2.57	2.12
Unmasked-calculated*	3.46	7.18	3.61

*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 3.46 differs from the reported value 2.08 by more than 10 %

9 Map-model fit [i](#)

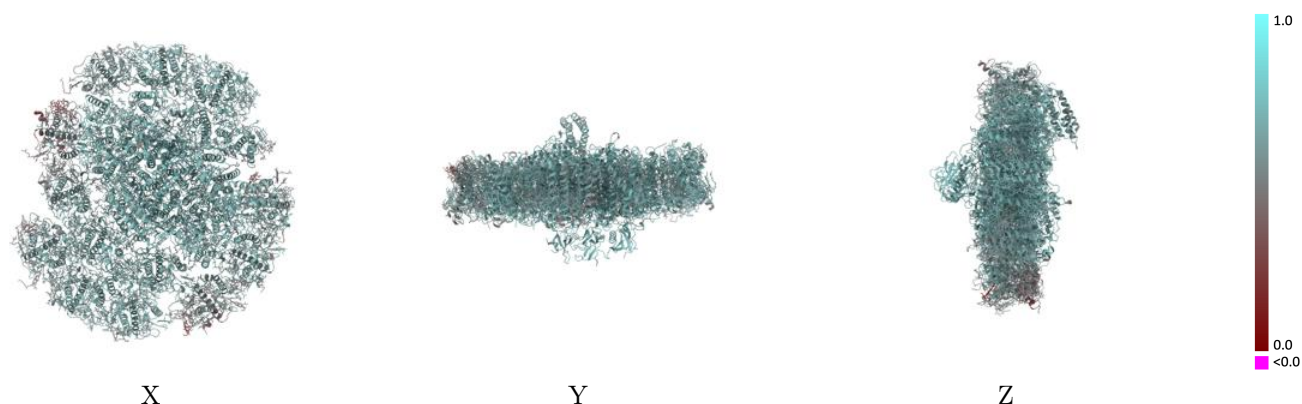
This section contains information regarding the fit between EMDB map EMD-62656 and PDB model 9KZ9. Per-residue inclusion information can be found in section [3](#) on page [37](#).

9.1 Map-model overlay [i](#)



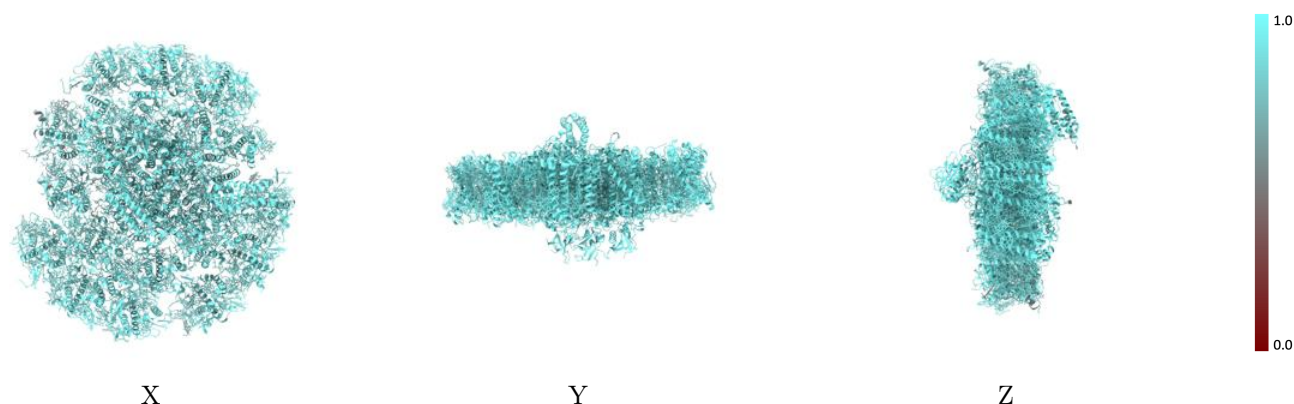
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



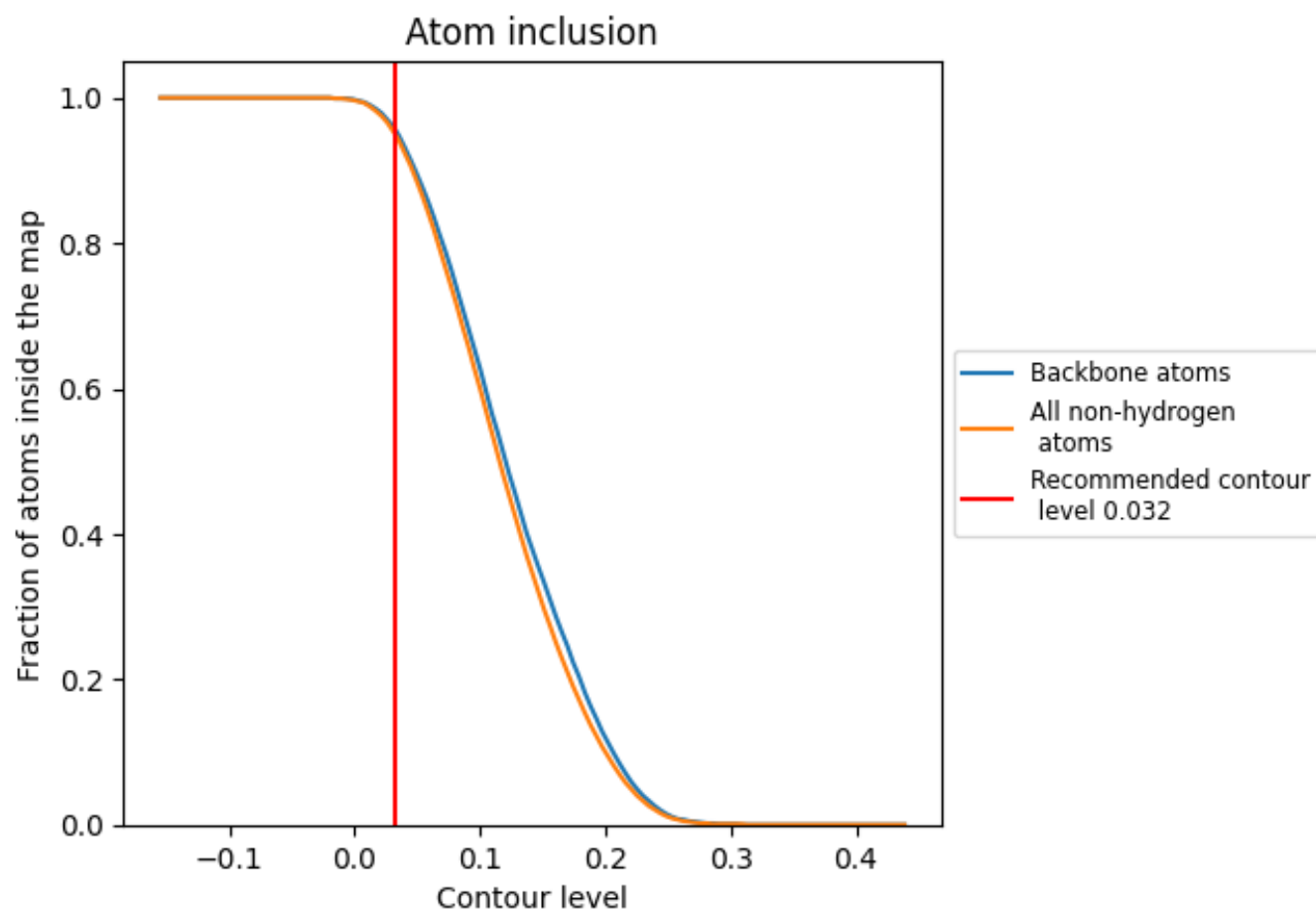
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.9510	 0.6450
A	 0.9820	 0.6990
B	 0.9830	 0.7020
C	 0.9970	 0.7120
D	 0.9870	 0.6910
E	 0.9680	 0.6680
F	 0.9680	 0.6800
I	 0.9860	 0.6850
J	 0.9720	 0.6720
K	 0.9610	 0.6620
L	 0.9650	 0.6740
M	 0.9550	 0.6570
O	 0.9670	 0.6720
Q	 0.9120	 0.6040
R	 0.9710	 0.6650
a	 0.9690	 0.6670
b	 0.9690	 0.6700
c	 0.9210	 0.6110
d	 0.8310	 0.5040
e	 0.9040	 0.5680
f	 0.9540	 0.6410
g	 0.9500	 0.6330
h	 0.9470	 0.6400
i	 0.9080	 0.5650
j	 0.9220	 0.6080
k	 0.8970	 0.5460
l	 0.9540	 0.6250
m	 0.9390	 0.6290
n	 0.8970	 0.5760
s	 0.9520	 0.6460

