



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:38 AM UTC

PDB ID : 9VJS / pdb_00009vjs
EMDB ID : EMD-65121
Title : Cryo-EM structure of Euglenophyte photosystem I
Authors : Zhao, L.S.; Qin, B.Y.; Li, K.; Liu, L.N.; Zhang, Y.Z.
Deposited on : 2025-06-21
Resolution : 2.72 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

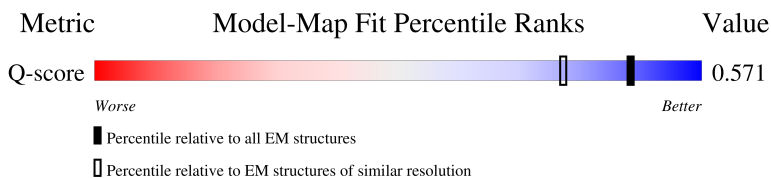
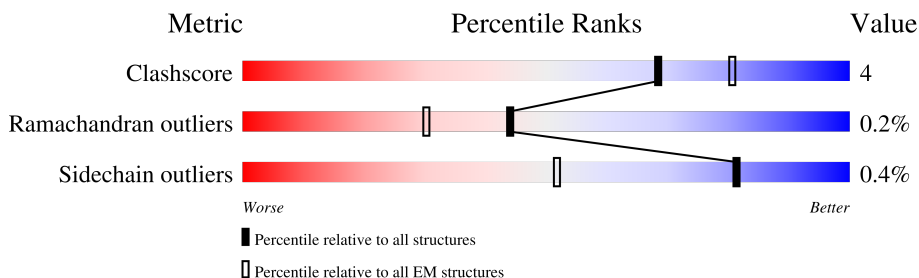
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.72 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.




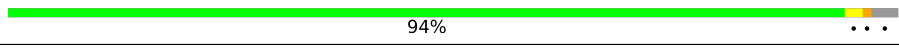
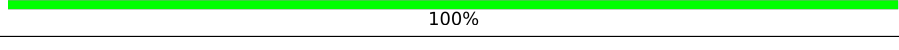

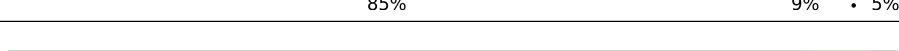

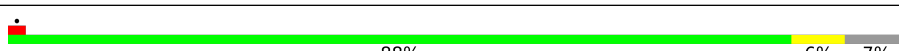


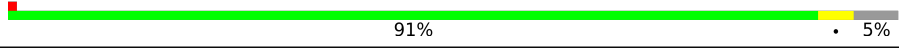

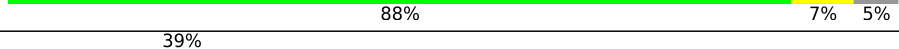
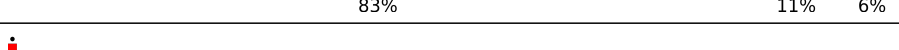





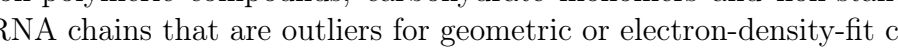
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10355 (2.22 - 3.22)

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	751	
2	B	733	
3	C	81	
4	D	203	

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Mol	Chain	Length	Quality of chain
5	E	99	
6	F	172	
7	J	37	
8	M	31	
9	a	209	
10	b	225	
11	c	230	
12	d	184	
13	e	177	
14	f	185	
15	g	191	
15	j	191	
16	h	188	
16	o	188	
17	i	185	
18	k	174	
18	l	174	
18	m	174	
18	n	174	

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
19	CLA	A	801	X	-	-	-
19	CLA	A	802	X	-	-	-
19	CLA	A	803	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	-	-
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	810	X	-	-	-
19	CLA	A	811	X	-	-	-
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-
19	CLA	A	815	X	-	-	-
19	CLA	A	816	X	-	-	-
19	CLA	A	817	X	-	-	-
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	820	X	-	-	-
19	CLA	A	821	X	-	-	-
19	CLA	A	822	X	-	-	-
19	CLA	A	823	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	825	X	-	-	-
19	CLA	A	826	X	-	-	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	839	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	841	X	-	-	-
19	CLA	A	842	X	-	-	-
19	CLA	A	843	X	-	-	-
19	CLA	A	844	X	-	-	-
19	CLA	A	845	X	-	-	-
19	CLA	A	846	X	-	-	-
19	CLA	A	847	X	-	-	-
19	CLA	A	848	X	-	-	-
19	CLA	A	849	X	-	-	-
19	CLA	A	850	X	-	-	-
19	CLA	A	852	X	-	-	-
19	CLA	A	853	X	-	-	-
19	CLA	B	801	X	-	-	-
19	CLA	B	803	X	-	-	-
19	CLA	B	804	X	-	-	-
19	CLA	B	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	806	X	-	-	-
19	CLA	B	807	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	813	X	-	-	-
19	CLA	B	814	X	-	-	-
19	CLA	B	815	X	-	-	-
19	CLA	B	816	X	-	-	-
19	CLA	B	817	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	820	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	838	X	-	-	-
19	CLA	B	839	X	-	-	-
19	CLA	B	840	X	-	-	-
19	CLA	B	841	X	-	-	-
19	CLA	B	842	X	-	-	-
19	CLA	B	843	X	-	-	-
19	CLA	B	844	X	-	-	-
19	CLA	B	845	X	-	-	-
19	CLA	B	846	X	-	-	-
19	CLA	B	847	X	-	-	-
19	CLA	B	848	X	-	-	-
19	CLA	B	849	X	-	-	-
19	CLA	D	301	X	-	-	-
19	CLA	F	201	X	-	-	-
19	CLA	F	202	X	-	-	-
19	CLA	F	203	X	-	-	-
19	CLA	F	204	X	-	-	-
19	CLA	J	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	a	302	X	-	-	-
19	CLA	a	303	X	-	-	-
19	CLA	a	304	X	-	-	-
19	CLA	a	305	X	-	-	-
19	CLA	a	306	X	-	-	-
19	CLA	a	307	X	-	-	-
19	CLA	a	308	X	-	-	-
19	CLA	a	309	X	-	-	-
19	CLA	a	310	X	-	-	-
19	CLA	a	314	X	-	-	-
19	CLA	b	302	X	-	-	-
19	CLA	b	303	X	-	-	-
19	CLA	b	304	X	-	-	-
19	CLA	b	305	X	-	-	-
19	CLA	b	306	X	-	-	-
19	CLA	b	307	X	-	-	-
19	CLA	b	308	X	-	-	-
19	CLA	b	309	X	-	-	-
19	CLA	b	313	X	-	-	-
19	CLA	b	315	X	-	-	-
19	CLA	c	302	X	-	-	-
19	CLA	c	303	X	-	-	-
19	CLA	c	304	X	-	-	-
19	CLA	c	306	X	-	-	-
19	CLA	c	307	X	-	-	-
19	CLA	c	308	X	-	-	-
19	CLA	c	309	X	-	-	-
19	CLA	c	310	X	-	-	-
19	CLA	c	311	X	-	-	-
19	CLA	c	314	X	-	-	-
19	CLA	c	315	X	-	-	-
19	CLA	c	316	X	-	-	-
19	CLA	d	201	X	-	-	-
19	CLA	d	203	X	-	-	-
19	CLA	d	204	X	-	-	-
19	CLA	d	206	X	-	-	-
19	CLA	d	207	X	-	-	-
19	CLA	d	208	X	-	-	-
19	CLA	d	209	X	-	-	-
19	CLA	d	210	X	-	-	-
19	CLA	d	211	X	-	-	-
19	CLA	d	212	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	e	302	X	-	-	-
19	CLA	e	303	X	-	-	-
19	CLA	e	305	X	-	-	-
19	CLA	e	306	X	-	-	-
19	CLA	e	307	X	-	-	-
19	CLA	e	308	X	-	-	-
19	CLA	e	309	X	-	-	-
19	CLA	e	310	X	-	-	-
19	CLA	e	311	X	-	-	-
19	CLA	f	302	X	-	-	-
19	CLA	f	303	X	-	-	-
19	CLA	f	305	X	-	-	-
19	CLA	f	306	X	-	-	-
19	CLA	f	307	X	-	-	-
19	CLA	f	308	X	-	-	-
19	CLA	f	309	X	-	-	-
19	CLA	f	310	X	-	-	-
19	CLA	f	311	X	-	-	-
19	CLA	f	312	X	-	-	-
19	CLA	f	314	X	-	-	-
19	CLA	g	301	X	-	-	-
19	CLA	g	302	X	-	-	-
19	CLA	g	304	X	-	-	-
19	CLA	g	305	X	-	-	-
19	CLA	g	307	X	-	-	-
19	CLA	g	308	X	-	-	-
19	CLA	g	309	X	-	-	-
19	CLA	g	311	X	-	-	-
19	CLA	h	201	X	-	-	-
19	CLA	h	203	X	-	-	-
19	CLA	h	204	X	-	-	-
19	CLA	h	205	X	-	-	-
19	CLA	h	206	X	-	-	-
19	CLA	h	207	X	-	-	-
19	CLA	h	208	X	-	-	-
19	CLA	h	209	X	-	-	-
19	CLA	h	210	X	-	-	-
19	CLA	h	211	X	-	-	-
19	CLA	h	212	X	-	-	-
19	CLA	h	213	X	-	-	-
19	CLA	i	302	X	-	-	-
19	CLA	i	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	i	305	X	-	-	-
19	CLA	i	306	X	-	-	-
19	CLA	i	307	X	-	-	-
19	CLA	i	308	X	-	-	-
19	CLA	i	309	X	-	-	-
19	CLA	i	310	X	-	-	-
19	CLA	i	311	X	-	-	-
19	CLA	i	312	X	-	-	-
19	CLA	i	313	X	-	-	-
19	CLA	j	301	X	-	-	-
19	CLA	j	302	X	-	-	-
19	CLA	j	303	X	-	-	-
19	CLA	j	304	X	-	-	-
19	CLA	j	305	X	-	-	-
19	CLA	j	306	X	-	-	-
19	CLA	j	307	X	-	-	-
19	CLA	j	308	X	-	-	-
19	CLA	j	309	X	-	-	-
19	CLA	j	310	X	-	-	-
19	CLA	j	311	X	-	-	-
19	CLA	j	312	X	-	-	-
19	CLA	j	313	X	-	-	-
19	CLA	k	302	X	-	-	-
19	CLA	k	303	X	-	-	-
19	CLA	k	304	X	-	-	-
19	CLA	k	305	X	-	-	-
19	CLA	k	306	X	-	-	-
19	CLA	k	307	X	-	-	-
19	CLA	k	308	X	-	-	-
19	CLA	k	309	X	-	-	-
19	CLA	k	310	X	-	-	-
19	CLA	k	311	X	-	-	-
19	CLA	l	201	X	-	-	-
19	CLA	l	202	X	-	-	-
19	CLA	l	203	X	-	-	-
19	CLA	l	204	X	-	-	-
19	CLA	l	205	X	-	-	-
19	CLA	l	206	X	-	-	-
19	CLA	l	207	X	-	-	-
19	CLA	l	208	X	-	-	-
19	CLA	l	209	X	-	-	-
19	CLA	m	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	m	303	X	-	-	-
19	CLA	m	304	X	-	-	-
19	CLA	m	305	X	-	-	-
19	CLA	m	306	X	-	-	-
19	CLA	m	307	X	-	-	-
19	CLA	m	308	X	-	-	-
19	CLA	m	309	X	-	-	-
19	CLA	m	310	X	-	-	-
19	CLA	m	311	X	-	-	-
19	CLA	n	201	X	-	-	-
19	CLA	n	202	X	-	-	-
19	CLA	n	203	X	-	-	-
19	CLA	n	204	X	-	-	-
19	CLA	n	205	X	-	-	-
19	CLA	n	206	X	-	-	-
19	CLA	n	207	X	-	-	-
19	CLA	n	208	X	-	-	-
19	CLA	n	209	X	-	-	-
19	CLA	o	302	X	-	-	-
19	CLA	o	303	X	-	-	-
19	CLA	o	304	X	-	-	-
19	CLA	o	305	X	-	-	-
19	CLA	o	306	X	-	-	-
19	CLA	o	307	X	-	-	-
19	CLA	o	308	X	-	-	-
19	CLA	o	309	X	-	-	-
19	CLA	o	310	X	-	-	-
19	CLA	o	311	X	-	-	-
19	CLA	o	312	X	-	-	-
28	CHL	a	311	X	-	-	-
28	CHL	a	312	X	-	-	-
28	CHL	a	313	X	-	-	-
28	CHL	a	315	X	-	-	-
28	CHL	b	301	X	-	-	-
28	CHL	b	310	X	-	-	-
28	CHL	b	311	X	-	-	-
28	CHL	b	312	X	-	-	-
28	CHL	b	314	X	-	-	-
28	CHL	c	305	X	-	-	-
28	CHL	c	312	X	-	-	-
28	CHL	c	313	X	-	-	-
28	CHL	d	202	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CHL	d	205	X	-	-	-
28	CHL	e	301	X	-	-	-
28	CHL	e	304	X	-	-	-
28	CHL	f	301	X	-	-	-
28	CHL	f	304	X	-	-	-
28	CHL	g	303	X	-	-	-
28	CHL	g	306	X	-	-	-
28	CHL	g	310	X	-	-	-
28	CHL	h	202	X	-	-	-
28	CHL	i	301	X	-	-	-
28	CHL	i	304	X	-	-	-
28	CHL	k	301	X	-	-	-
28	CHL	m	301	X	-	-	-
28	CHL	o	301	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 54391 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	740	Total	C	N	O	S	0	0
			5871	3854	992	1004	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	SER	THR	conflict	UNP P19430

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	730	Total	C	N	O	S	0	0
			5856	3853	983	1005	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			595	363	104	117	11		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	187	Total	C	N	O	S	0	0
			1462	935	248	277	2		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	63	Total	C	N	O	0	0
			510	324	86	100		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	166	Total	C	N	O	S	0	0
			1267	813	213	239	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	37	Total	C	N	O	S	0	0
			304	209	43	51	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	31	Total	C	N	O	S	0	0
			242	162	37	42	1		

- Molecule 9 is a protein called LHC-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	199	Total	C	N	O	S	0	0
			1514	977	258	273	6		

- Molecule 10 is a protein called Light harvesting chlorophyll a /b binding protein of PSII.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	219	Total	C	N	O	S	0	0
			1665	1086	274	301	4		

- Molecule 11 is a protein called LHC-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	222	Total	C	N	O	S	0	0
			1683	1090	283	305	5		

- Molecule 12 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	172	Total	C	N	O	S	0	0
			1327	858	219	246	4		

- Molecule 13 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	166	Total	C	N	O	S	0	0
			1274	819	220	228	7		

- Molecule 14 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	172	Total	C	N	O	S	0	0
			1338	860	232	241	5		

- Molecule 15 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	182	Total	C	N	O	S	0	0
			1441	939	245	251	6		
15	j	180	Total	C	N	O	S	0	0
			1420	924	242	248	6		

- Molecule 16 is a protein called LHC-10, 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	178	Total	C	N	O	S	0	0
			1361	870	243	244	4		
16	o	177	Total	C	N	O	S	0	0
			1356	867	242	243	4		

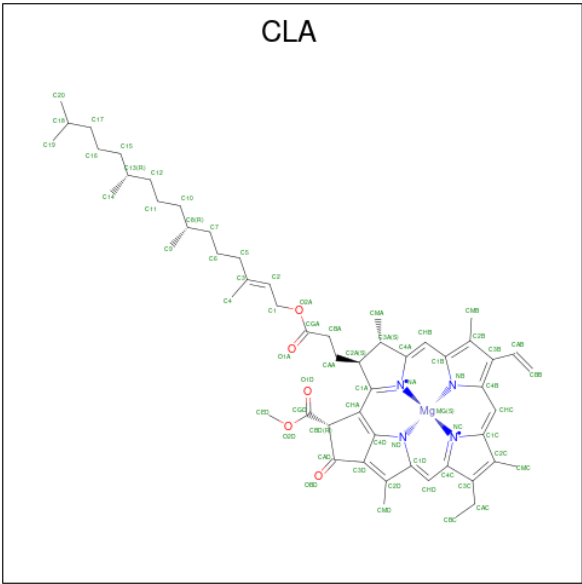
- Molecule 17 is a protein called LHC-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	172	Total	C	N	O	S	0	0
			1342	861	231	245	5		

- Molecule 18 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	k	168	Total	C	N	O	S	0	0
			1260	813	215	228	4		
18	l	167	Total	C	N	O	S	0	0
			1253	808	214	227	4		
18	m	168	Total	C	N	O	S	0	0
			1260	813	215	228	4		
18	n	156	Total	C	N	O	S	0	0
			1170	754	199	213	4		

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
19	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
19	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
19	B	1	Total 64	C 54	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
19	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
19	D	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	F	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	a	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	a	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	c	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	c	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	c	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	c	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	c	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	c	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	c	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	c	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	c	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	d	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	d	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	d	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	d	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	d	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	d	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	d	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	d	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	d	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	d	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	e	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	e	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	e	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	e	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	f	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	f	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	f	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	f	1	Total 54	C 44	Mg 1	N 4	O 5	0
19	f	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	f	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	f	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	f	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	g	1	Total 48	C 38	Mg 1	N 4	O 5	0
19	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	g	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	g	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	g	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	g	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	h	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	i	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	i	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	j	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	j	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	j	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	j	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	j	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	j	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	j	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	j	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	j	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	j	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	j	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	j	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	j	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	k	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	k	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	k	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	k	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	k	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	k	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	k	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	k	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	k	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	l	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	l	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	l	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	l	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	l	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	l	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	l	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	l	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	l	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	l	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	m	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	m	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	m	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	m	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	m	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	m	1	Total 47	C 37	Mg 1	N 4	O 5	0

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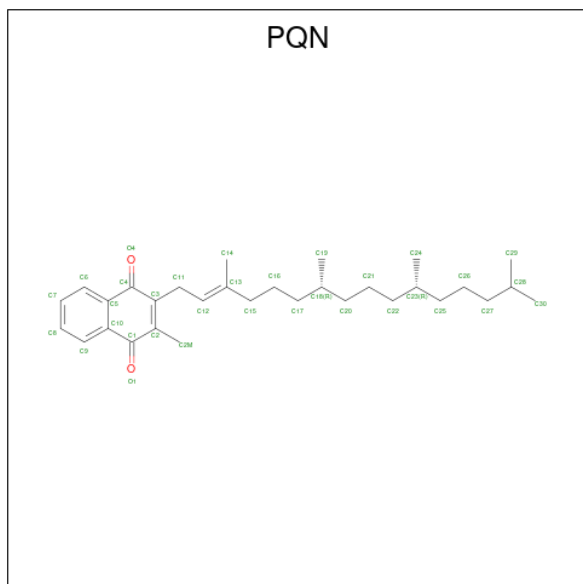
Mol	Chain	Residues	Atoms					AltConf
19	m	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	m	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	n	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	n	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	n	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	n	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	n	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	n	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	n	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	n	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	o	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	o	1	Total 48	C 38	Mg 1	N 4	O 5	0
19	o	1	Total 54	C 44	Mg 1	N 4	O 5	0
19	o	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	o	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	o	1	Total 53	C 43	Mg 1	N 4	O 5	0
19	o	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	o	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	o	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	o	1	47	37	1	4	5	0

- Molecule 20 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 22 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total 43	C 40	O 3	0
22	A	1	Total 43	C 40	O 3	0

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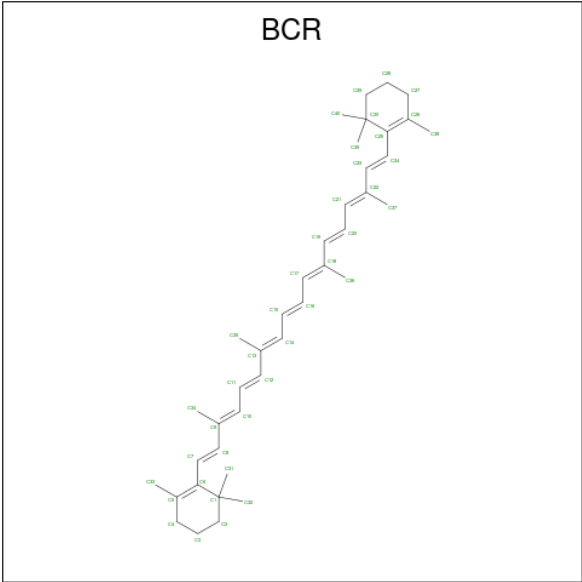
Mol	Chain	Residues	Atoms			AltConf
22	F	1	Total 43	C 40	O 3	0
22	J	1	Total 43	C 40	O 3	0
22	J	1	Total 43	C 40	O 3	0
22	a	1	Total 43	C 40	O 3	0
22	a	1	Total 43	C 40	O 3	0
22	b	1	Total 43	C 40	O 3	0
22	b	1	Total 43	C 40	O 3	0
22	b	1	Total 43	C 40	O 3	0
22	c	1	Total 43	C 40	O 3	0
22	c	1	Total 43	C 40	O 3	0
22	c	1	Total 43	C 40	O 3	0
22	d	1	Total 43	C 40	O 3	0
22	d	1	Total 43	C 40	O 3	0
22	e	1	Total 43	C 40	O 3	0
22	e	1	Total 43	C 40	O 3	0
22	f	1	Total 43	C 40	O 3	0
22	f	1	Total 43	C 40	O 3	0
22	g	1	Total 43	C 40	O 3	0
22	g	1	Total 43	C 40	O 3	0
22	h	1	Total 43	C 40	O 3	0
22	h	1	Total 43	C 40	O 3	0

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Mol	Chain	Residues	Atoms			AltConf
22	i	1	Total	C	O	0
			43	40	3	
22	i	1	Total	C	O	0
			43	40	3	
22	j	1	Total	C	O	0
			43	40	3	
22	j	1	Total	C	O	0
			43	40	3	
22	k	1	Total	C	O	0
			43	40	3	
22	k	1	Total	C	O	0
			43	40	3	
22	l	1	Total	C	O	0
			43	40	3	
22	l	1	Total	C	O	0
			43	40	3	
22	m	1	Total	C	O	0
			43	40	3	
22	m	1	Total	C	O	0
			43	40	3	
22	n	1	Total	C	O	0
			43	40	3	
22	n	1	Total	C	O	0
			43	40	3	
22	o	1	Total	C	O	0
			43	40	3	
22	o	1	Total	C	O	0
			43	40	3	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			39	39	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	J	1	Total	C	0
			40	40	
23	M	1	Total	C	0
			40	40	

- Molecule 24 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



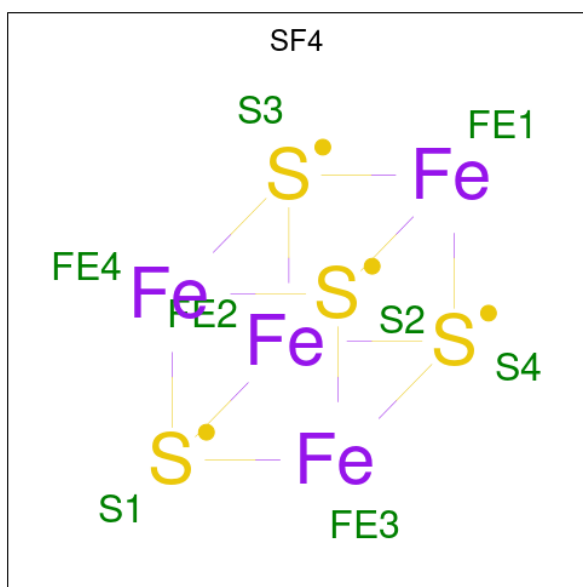
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total 34	C 24	O 10	0
24	a	1	Total 34	C 24	O 10	0
24	c	1	Total 34	C 24	O 10	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



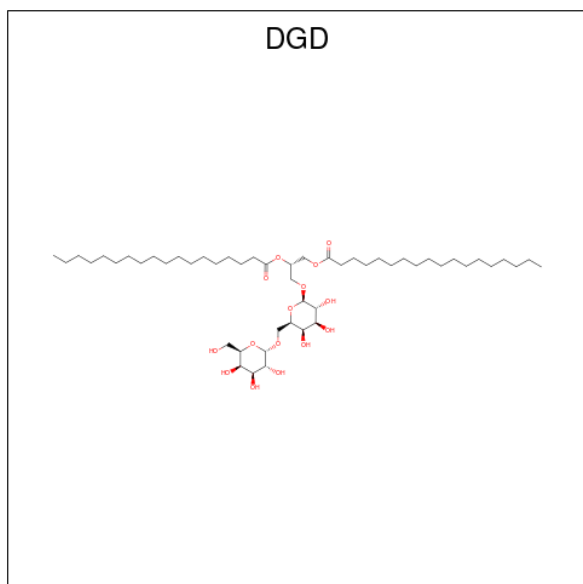
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			34	24	10	
25	a	1	Total	C	O	0
			40	30	10	
25	a	1	Total	C	O	0
			27	17	10	
25	a	1	Total	C	O	0
			40	30	10	
25	b	1	Total	C	O	0
			42	32	10	
25	c	1	Total	C	O	0
			38	28	10	
25	d	1	Total	C	O	0
			31	21	10	
25	e	1	Total	C	O	0
			44	34	10	
25	f	1	Total	C	O	0
			26	16	10	
25	g	1	Total	C	O	0
			37	27	10	
25	g	1	Total	C	O	0
			33	23	10	
25	g	1	Total	C	O	0
			44	34	10	
25	h	1	Total	C	O	0
			35	25	10	
25	i	1	Total	C	O	0
			41	31	10	
25	j	1	Total	C	O	0
			37	27	10	
25	k	1	Total	C	O	0
			37	27	10	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



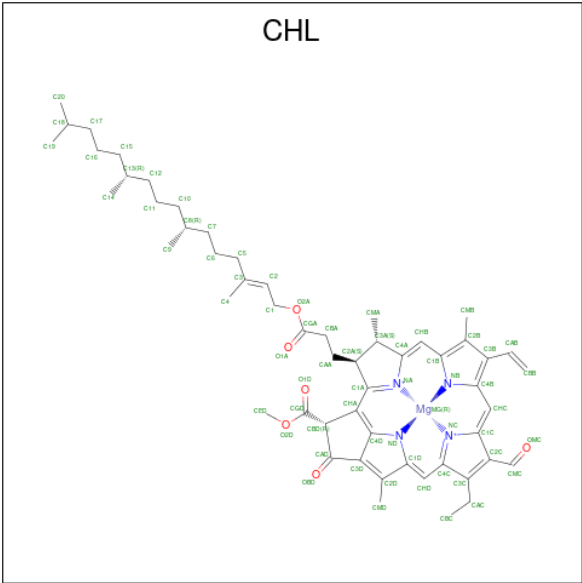
Mol	Chain	Residues	Atoms			AltConf
26	B	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			62	47	15	

- Molecule 28 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



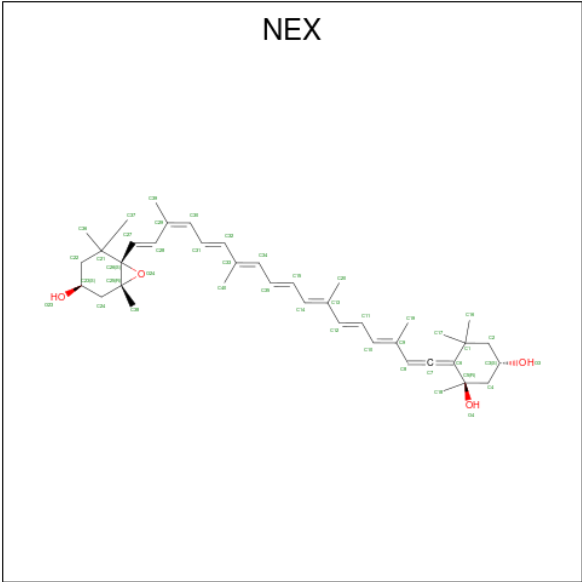
Mol	Chain	Residues	Atoms						AltConf
28	a	1	Total	C	Mg	N	O	0	
			48	37	1	4	6		
28	a	1	Total	C	Mg	N	O	0	
			48	37	1	4	6		
28	a	1	Total	C	Mg	N	O	0	
			48	37	1	4	6		
28	a	1	Total	C	Mg	N	O	0	
			48	37	1	4	6		
28	b	1	Total	C	Mg	N	O	0	
			56	45	1	4	6		
28	b	1	Total	C	Mg	N	O	0	
			48	37	1	4	6		
28	b	1	Total	C	Mg	N	O	0	
			48	37	1	4	6		
28	b	1	Total	C	Mg	N	O	0	
			53	42	1	4	6		
28	b	1	Total	C	Mg	N	O	0	
			52	41	1	4	6		
28	c	1	Total	C	Mg	N	O	0	
			61	50	1	4	6		

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Mol	Chain	Residues	Atoms					AltConf
28	c	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	c	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	d	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	d	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	e	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
28	e	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
28	f	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	f	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	g	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	g	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	g	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
28	h	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	i	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	i	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	k	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	m	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	o	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

- Molecule 29 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).

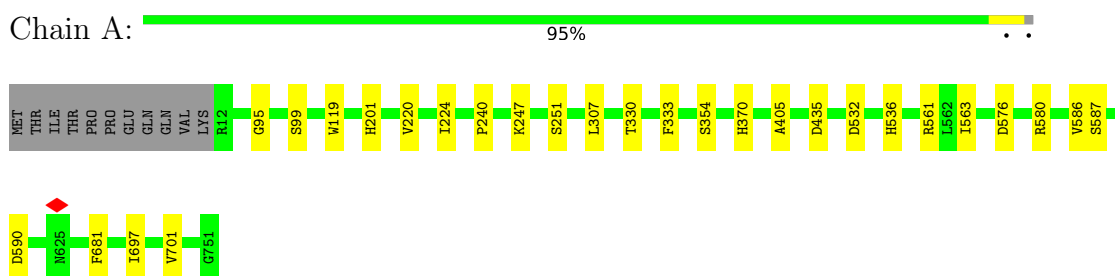


Mol	Chain	Residues	Atoms			AltConf
29	a	1	Total	C	O	0
			44	40	4	

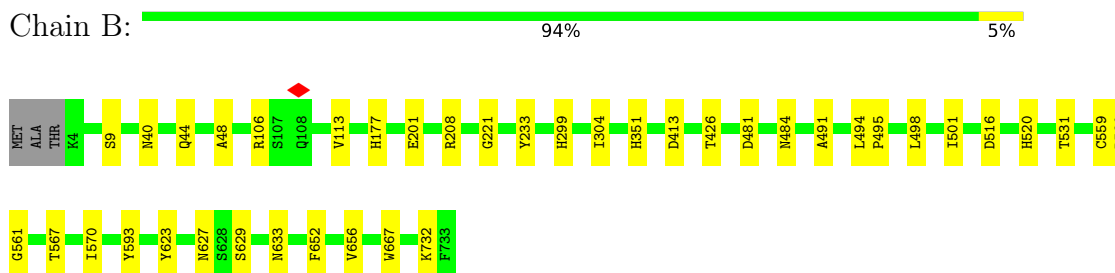
3 Residue-property plots

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.

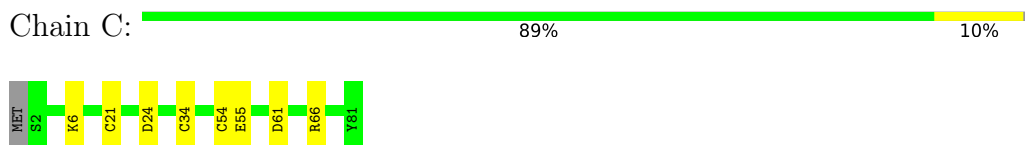
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



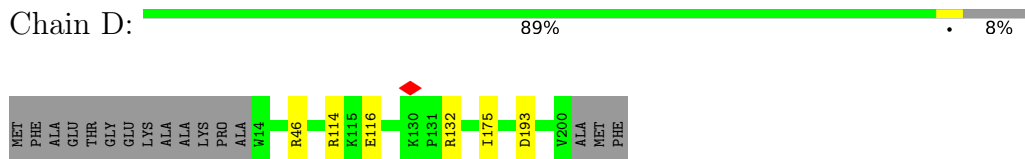
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



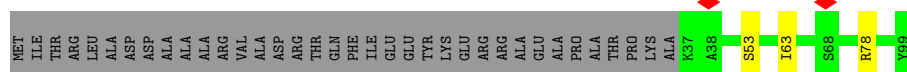
- Molecule 3: Photosystem I iron-sulfur center



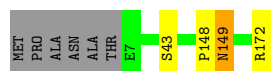
- Molecule 4: PsaD



- Molecule 5: PsaE



- Molecule 6: PsaF

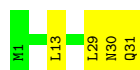
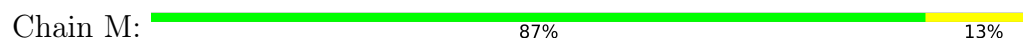


- Molecule 7: Photosystem I reaction center subunit IX

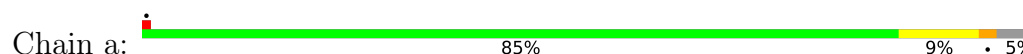


There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem I reaction center subunit XII



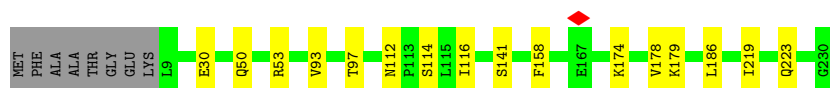
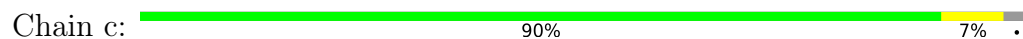
- Molecule 9: LHC-1



- Molecule 10: Light harvesting chlorophyll a /b binding protein of PSII



- Molecule 11: LHC-3

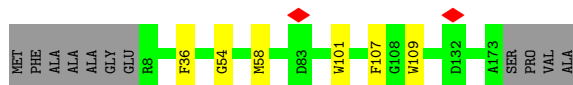
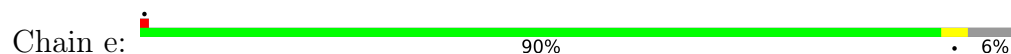


- Molecule 12: Chloroplast light-harvesting complex I protein

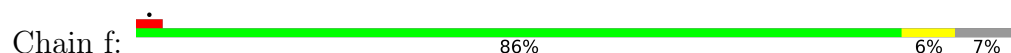




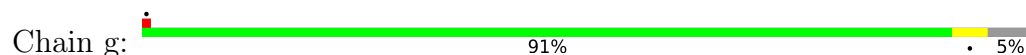
- Molecule 13: Chloroplast light-harvesting complex I protein



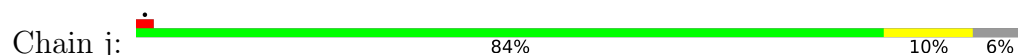
- Molecule 14: Chloroplast light-harvesting complex I protein



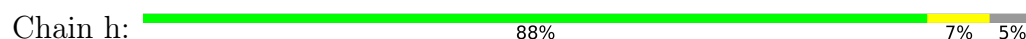
- Molecule 15: Chloroplast light-harvesting complex I protein



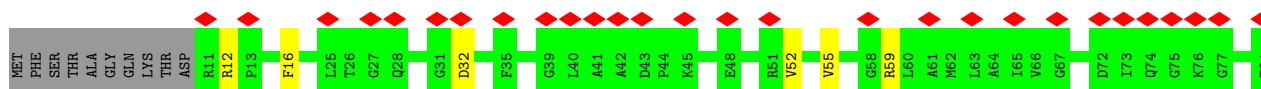
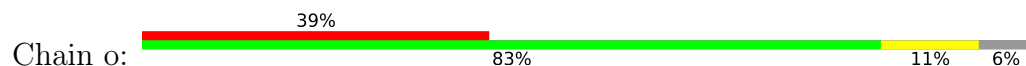
- Molecule 15: Chloroplast light-harvesting complex I protein

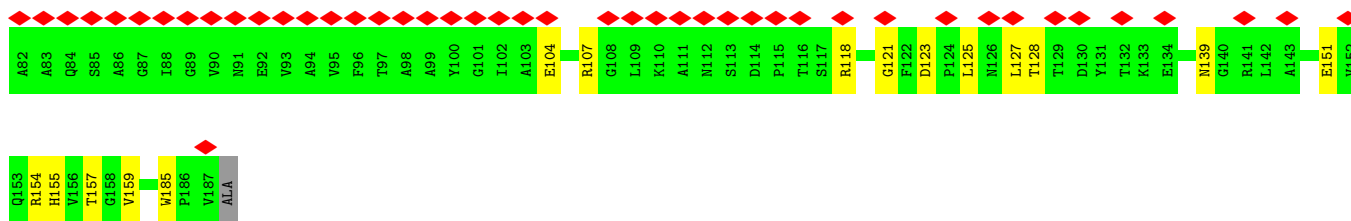


- Molecule 16: LHC-10, 15

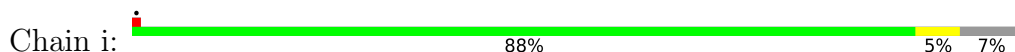


- Molecule 16: LHC-10, 15





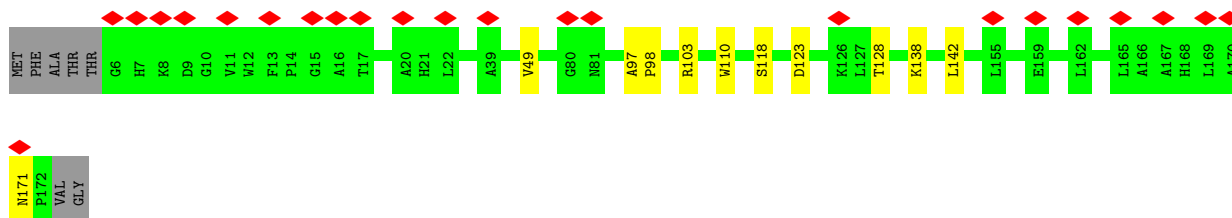
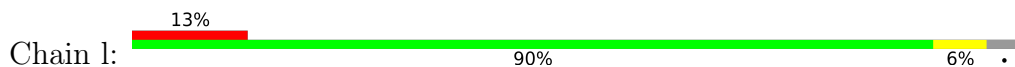
• Molecule 17: LHC-11



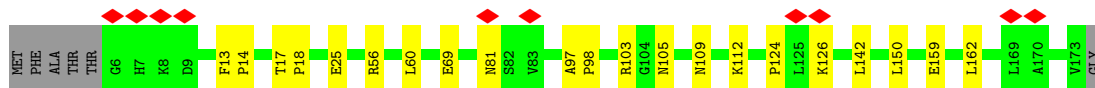
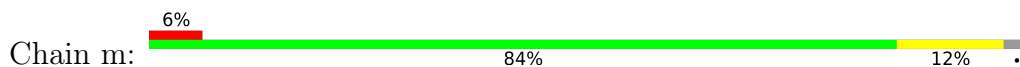
• Molecule 18: Chloroplast light-harvesting complex I protein



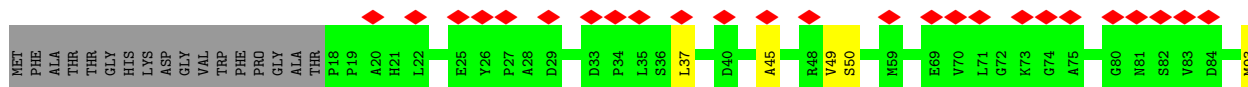
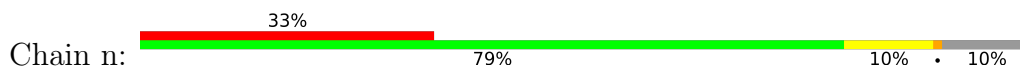
• Molecule 18: Chloroplast light-harvesting complex I protein

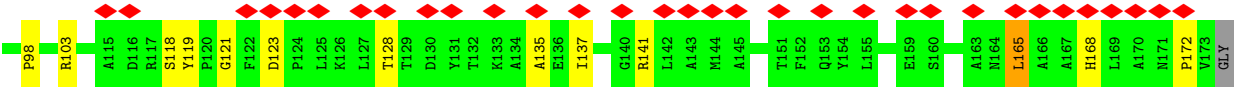


• Molecule 18: Chloroplast light-harvesting complex I protein



• Molecule 18: Chloroplast light-harvesting complex I protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78124	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.443	Depositor
Minimum map value	-0.463	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.22	Depositor
Map size (\AA)	417.2, 417.2, 417.2	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8344, 0.8344, 0.8344	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: PQN, LMG, LMU, DGD, LHG, DD6, CLA, SF4, BCR, NEX, CHL

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	0.16	0/6071	0.33	0/8276
2	B	0.17	0/6066	0.36	0/8272
3	C	0.48	0/605	0.47	0/819
4	D	0.18	0/1498	0.38	0/2030
5	E	0.18	0/522	0.38	0/707
6	F	0.24	0/1293	0.39	0/1751
7	J	0.18	0/313	0.34	0/429
8	M	0.32	0/246	0.42	0/332
9	a	0.45	0/1562	0.55	1/2135 (0.0%)
10	b	0.28	1/1715 (0.1%)	0.38	0/2338
11	c	0.20	0/1725	0.33	0/2341
12	d	0.17	0/1370	0.37	0/1865
13	e	0.19	0/1311	0.40	0/1772
14	f	0.21	0/1377	0.42	0/1871
15	g	0.17	0/1490	0.36	0/2033
15	j	0.20	0/1468	0.39	0/2004
16	h	0.17	0/1399	0.35	0/1907
16	o	0.23	0/1394	0.47	0/1900
17	i	0.19	0/1380	0.41	0/1876
18	k	0.21	0/1297	0.41	0/1768
18	l	0.22	0/1290	0.41	0/1758
18	m	0.26	0/1297	0.44	0/1768
18	n	0.21	0/1202	0.46	0/1637
All	All	0.22	1/37891 (0.0%)	0.39	1/51589 (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
16	h	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	b	135	THR	CA-C	-5.67	1.45	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	126	ARG	N-CA-C	-5.73	105.12	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	667	TRP	Peptide
16	h	185	TRP	Peptide

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	5871	0	5731	19	0
2	B	5856	0	5659	30	0
3	C	595	0	579	5	0
4	D	1462	0	1450	5	0
5	E	510	0	489	3	0
6	F	1267	0	1299	3	0
7	J	304	0	317	0	0
8	M	242	0	258	6	0
9	a	1514	0	1466	13	0
10	b	1665	0	1645	13	0
11	c	1683	0	1680	9	0
12	d	1327	0	1271	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	e	1274	0	1233	4	0
14	f	1338	0	1313	10	0
15	g	1441	0	1393	7	0
15	j	1420	0	1371	14	0
16	h	1361	0	1339	9	0
16	o	1356	0	1334	17	0
17	i	1342	0	1316	6	0
18	k	1260	0	1234	9	0
18	l	1253	0	1225	10	0
18	m	1260	0	1234	13	0
18	n	1170	0	1155	16	0
19	A	2506	0	2465	17	0
19	B	2277	0	2172	19	0
19	D	52	0	43	1	0
19	F	229	0	219	2	0
19	J	47	0	35	1	0
19	a	529	0	454	7	0
19	b	528	0	452	10	0
19	c	634	0	547	1	0
19	d	523	0	446	7	0
19	e	480	0	415	4	0
19	f	565	0	468	4	0
19	g	419	0	355	2	0
19	h	634	0	545	4	0
19	i	559	0	458	2	0
19	j	687	0	589	22	0
19	k	529	0	456	4	0
19	l	458	0	379	11	0
19	m	507	0	416	4	0
19	n	458	0	379	24	0
19	o	555	0	451	18	0
20	A	33	0	46	0	0
20	B	33	0	46	0	0
21	A	49	0	74	0	0
22	A	86	0	0	0	0
22	F	43	0	0	0	0
22	J	86	0	0	1	0
22	a	86	0	0	5	0
22	b	129	0	0	2	0
22	c	129	0	0	2	0
22	d	86	0	0	0	0
22	e	86	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	f	86	0	0	2	0
22	g	86	0	0	5	0
22	h	86	0	0	0	0
22	i	86	0	0	1	0
22	j	86	0	0	11	0
22	k	86	0	0	0	0
22	l	86	0	0	5	0
22	m	86	0	0	1	0
22	n	86	0	0	10	0
22	o	86	0	0	6	0
23	A	159	0	221	3	0
23	B	280	0	392	6	0
23	J	40	0	56	6	0
23	M	40	0	56	7	0
24	A	34	0	44	1	0
24	a	34	0	44	0	0
24	c	34	0	44	3	0
25	A	34	0	38	0	0
25	a	107	0	124	6	0
25	b	42	0	54	2	0
25	c	38	0	46	6	0
25	d	31	0	32	1	0
25	e	44	0	61	0	0
25	f	26	0	22	1	0
25	g	114	0	141	1	0
25	h	35	0	40	2	0
25	i	41	0	52	7	0
25	j	37	0	44	0	0
25	k	37	0	44	2	0
26	B	8	0	0	0	0
26	C	16	0	0	0	0
27	B	62	0	85	2	0
28	a	192	0	132	11	0
28	b	257	0	193	10	0
28	c	173	0	151	12	0
28	d	104	0	80	5	0
28	e	112	0	94	12	0
28	f	104	0	80	5	0
28	g	163	0	131	8	0
28	h	48	0	33	2	0
28	i	104	0	80	2	0
28	k	48	0	33	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	m	48	0	33	2	0
28	o	48	0	33	2	0
29	a	44	0	56	0	0
All	All	54391	0	50670	391	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 4.

The worst 5 of 391 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)
19:j:306:CLA:HBB1	22:j:316:DD6:C1	1.69	1.22
28:e:304:CHL:H93	22:e:313:DD6:C10	1.72	1.19
19:n:206:CLA:HMB1	22:n:210:DD6:C23	1.95	0.95
19:n:206:CLA:CMB	22:n:210:DD6:C23	2.45	0.94
19:l:201:CLA:CBB	22:l:210:DD6:C10	2.49	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/751 (66%)	483 (97%)	14 (3%)	0	100	100
2	B	610/733 (83%)	593 (97%)	17 (3%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	185/203 (91%)	175 (95%)	9 (5%)	1 (0%)	24	46
5	E	61/99 (62%)	56 (92%)	5 (8%)	0	100	100
6	F	164/172 (95%)	158 (96%)	5 (3%)	1 (1%)	21	42
7	J	35/37 (95%)	34 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	M	29/31 (94%)	29 (100%)	0	0	100	100
9	a	197/209 (94%)	189 (96%)	5 (2%)	3 (2%)	8	20
10	b	217/225 (96%)	211 (97%)	6 (3%)	0	100	100
11	c	220/230 (96%)	213 (97%)	5 (2%)	2 (1%)	14	33
12	d	170/184 (92%)	160 (94%)	10 (6%)	0	100	100
13	e	164/177 (93%)	155 (94%)	9 (6%)	0	100	100
14	f	170/185 (92%)	166 (98%)	4 (2%)	0	100	100
15	g	180/191 (94%)	179 (99%)	1 (1%)	0	100	100
15	j	178/191 (93%)	168 (94%)	9 (5%)	1 (1%)	21	42
16	h	176/188 (94%)	171 (97%)	5 (3%)	0	100	100
16	o	175/188 (93%)	168 (96%)	7 (4%)	0	100	100
17	i	170/185 (92%)	164 (96%)	6 (4%)	0	100	100
18	k	166/174 (95%)	158 (95%)	8 (5%)	0	100	100
18	l	165/174 (95%)	158 (96%)	7 (4%)	0	100	100
18	m	166/174 (95%)	158 (95%)	7 (4%)	1 (1%)	21	42
18	n	154/174 (88%)	145 (94%)	9 (6%)	0	100	100
All	All	4327/4956 (87%)	4165 (96%)	153 (4%)	9 (0%)	44	66

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	a	136	LYS
9	a	107	ASN
11	c	30	GLU
18	m	25	GLU
6	F	43	SER

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	620/632 (98%)	620 (100%)	0	100	100
2	B	607/609 (100%)	606 (100%)	1 (0%)	87	95
3	C	69/70 (99%)	68 (99%)	1 (1%)	59	80
4	D	154/164 (94%)	154 (100%)	0	100	100
5	E	54/81 (67%)	54 (100%)	0	100	100
6	F	132/136 (97%)	131 (99%)	1 (1%)	73	87
7	J	34/34 (100%)	34 (100%)	0	100	100
8	M	26/26 (100%)	25 (96%)	1 (4%)	29	56
9	a	152/159 (96%)	146 (96%)	6 (4%)	28	56
10	b	167/170 (98%)	166 (99%)	1 (1%)	78	90
11	c	172/178 (97%)	172 (100%)	0	100	100
12	d	133/142 (94%)	133 (100%)	0	100	100
13	e	125/131 (95%)	124 (99%)	1 (1%)	73	87
14	f	141/147 (96%)	141 (100%)	0	100	100
15	g	144/151 (95%)	144 (100%)	0	100	100
15	j	142/151 (94%)	141 (99%)	1 (1%)	76	89
16	h	137/145 (94%)	136 (99%)	1 (1%)	76	89
16	o	137/145 (94%)	137 (100%)	0	100	100
17	i	142/148 (96%)	141 (99%)	1 (1%)	76	89
18	k	122/126 (97%)	122 (100%)	0	100	100
18	l	121/126 (96%)	121 (100%)	0	100	100
18	m	122/126 (97%)	122 (100%)	0	100	100
18	n	114/126 (90%)	113 (99%)	1 (1%)	70	86
All	All	3767/3923 (96%)	3751 (100%)	16 (0%)	81	92

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	j	111	TRP
17	i	176	ASN
9	a	128	ASN
16	h	127	LEU
9	a	119	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26

such sidechains are listed below:

Mol	Chain	Res	Type
15	g	170	HIS
17	i	153	GLN
18	n	105	ASN
17	i	129	ASN
15	j	82	ASN

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](#)

348 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	$\# Z > 2$
19	CLA	B	808	-	69,73,73	1.69	9 (13%)	82,113,113	1.36	7 (8%)
19	CLA	j	312	-	51,55,73	2.04	9 (17%)	60,91,113	1.64	8 (13%)
22	DD6	j	316	-	40,45,45	0.20	0	51,67,67	0.87	1 (1%)
22	DD6	n	210	-	40,45,45	0.19	0	51,67,67	1.34	4 (7%)
19	CLA	i	307	17	58,62,73	1.87	9 (15%)	68,99,113	1.43	7 (10%)
19	CLA	h	204	16	52,56,73	1.98	9 (17%)	61,92,113	1.49	6 (9%)
19	CLA	d	211	-	64,68,73	1.74	9 (14%)	76,107,113	1.29	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LMG	d	213	-	31,31,55	1.14	1 (3%)	39,39,63	1.29	5 (12%)
23	BCR	B	826	-	41,41,41	0.21	0	56,56,56	0.46	0
19	CLA	f	310	-	51,55,73	1.98	9 (17%)	60,91,113	1.48	6 (10%)
28	CHL	m	301	18	42,56,74	2.15	11 (26%)	36,92,114	3.04	16 (44%)
19	CLA	A	817	-	69,73,73	1.71	9 (13%)	82,113,113	1.48	10 (12%)
19	CLA	A	822	-	69,73,73	1.66	9 (13%)	82,113,113	1.24	7 (8%)
19	CLA	A	816	-	63,67,73	1.74	9 (14%)	74,105,113	1.36	9 (12%)
19	CLA	c	316	11	69,73,73	1.69	9 (13%)	82,113,113	1.24	6 (7%)
19	CLA	d	207	-	51,55,73	2.01	9 (17%)	60,91,113	1.53	6 (10%)
24	LMU	a	319	-	35,35,36	0.42	0	44,45,47	0.71	1 (2%)
19	CLA	B	822	-	69,73,73	1.70	9 (13%)	82,113,113	1.32	6 (7%)
19	CLA	B	820	2	65,69,73	1.76	9 (13%)	77,108,113	1.35	6 (7%)
19	CLA	A	825	-	54,58,73	1.95	9 (16%)	64,95,113	1.56	7 (10%)
19	CLA	f	311	-	56,60,73	1.94	9 (16%)	65,97,113	1.65	8 (12%)
19	CLA	A	840	1	69,73,73	1.70	9 (13%)	82,113,113	1.28	6 (7%)
19	CLA	o	304	16	58,62,73	1.88	9 (15%)	68,99,113	1.54	10 (14%)
19	CLA	f	307	14	58,62,73	1.89	9 (15%)	68,99,113	1.51	8 (11%)
19	CLA	m	302	-	51,55,73	2.00	10 (19%)	60,91,113	1.57	9 (15%)
19	CLA	h	210	-	51,55,73	2.00	9 (17%)	60,91,113	1.48	5 (8%)
19	CLA	a	314	-	51,55,73	2.01	9 (17%)	60,91,113	1.63	9 (15%)
19	CLA	h	209	16	64,68,73	1.78	9 (14%)	76,107,113	1.32	6 (7%)
28	CHL	a	313	-	42,56,74	2.08	11 (26%)	36,92,114	3.13	19 (52%)
23	BCR	B	827	-	41,41,41	0.17	0	56,56,56	0.44	0
28	CHL	b	310	-	42,56,74	2.19	11 (26%)	36,92,114	2.99	15 (41%)
19	CLA	A	846	1	51,55,73	1.94	9 (17%)	60,91,113	1.49	7 (11%)
19	CLA	A	807	1	69,73,73	1.69	9 (13%)	82,113,113	1.29	6 (7%)
19	CLA	m	306	18	51,55,73	2.01	9 (17%)	60,91,113	1.58	7 (11%)
19	CLA	g	309	-	60,64,73	1.81	9 (15%)	71,102,113	1.35	6 (8%)
22	DD6	d	214	-	40,45,45	0.17	0	51,67,67	0.92	3 (5%)
25	LMG	k	312	19	37,37,55	0.91	0	45,45,63	1.13	4 (8%)
19	CLA	o	305	-	51,55,73	1.99	9 (17%)	60,91,113	1.53	10 (16%)
22	DD6	a	321	-	40,45,45	0.22	0	51,67,67	0.70	2 (3%)
19	CLA	e	307	13	64,68,73	1.79	9 (14%)	76,107,113	1.43	7 (9%)
22	DD6	b	318	-	40,45,45	0.20	0	51,67,67	0.76	1 (1%)
22	DD6	a	320	-	40,45,45	0.21	0	51,67,67	1.07	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	a	303	-	59,63,73	1.85	9 (15%)	70,101,113	1.48	9 (12%)
19	CLA	m	304	-	51,55,73	2.13	9 (17%)	60,91,113	1.96	12 (20%)
19	CLA	A	810	1	54,58,73	1.92	9 (16%)	64,95,113	1.42	7 (10%)
26	SF4	B	802	-	0,12,12	-	-	-	-	-
19	CLA	n	203	18	64,68,73	1.80	9 (14%)	76,107,113	1.53	8 (10%)
19	CLA	f	309	-	64,68,73	1.80	9 (14%)	76,107,113	1.43	7 (9%)
19	CLA	a	302	9	51,55,73	1.99	9 (17%)	60,91,113	1.60	9 (15%)
22	DD6	l	211	-	40,45,45	0.16	0	51,67,67	0.82	1 (1%)
23	BCR	A	836	-	41,41,41	0.15	0	56,56,56	0.48	0
19	CLA	c	315	11	51,55,73	1.97	9 (17%)	60,91,113	1.46	7 (11%)
19	CLA	n	209	-	51,55,73	2.07	9 (17%)	60,91,113	1.48	9 (15%)
19	CLA	m	307	18	64,68,73	1.78	9 (14%)	76,107,113	1.37	6 (7%)
19	CLA	c	311	-	51,55,73	1.98	9 (17%)	60,91,113	1.46	6 (10%)
19	CLA	o	308	-	57,61,73	1.89	9 (15%)	67,98,113	1.42	6 (8%)
28	CHL	a	315	9	42,56,74	2.09	11 (26%)	36,92,114	3.21	16 (44%)
22	DD6	f	315	-	40,45,45	0.17	0	51,67,67	0.89	2 (3%)
19	CLA	h	203	-	59,63,73	1.85	9 (15%)	70,101,113	1.37	5 (7%)
19	CLA	d	201	-	51,55,73	1.97	9 (17%)	60,91,113	1.48	6 (10%)
25	LMG	g	313	-	33,33,55	0.96	1 (3%)	41,41,63	1.22	6 (14%)
19	CLA	n	207	-	51,55,73	1.99	9 (17%)	60,91,113	1.56	6 (10%)
19	CLA	B	817	-	66,70,73	1.71	9 (13%)	78,109,113	1.36	9 (11%)
29	NEX	a	317	-	40,46,46	0.37	1 (2%)	50,70,70	1.16	2 (4%)
19	CLA	e	308	13	60,64,73	1.94	9 (15%)	71,102,113	1.64	12 (16%)
19	CLA	h	212	-	60,64,73	1.81	9 (15%)	71,102,113	1.36	7 (9%)
19	CLA	l	203	18	64,68,73	1.81	9 (14%)	76,107,113	1.43	8 (10%)
19	CLA	b	308	10	60,64,73	1.83	9 (15%)	71,102,113	1.36	7 (9%)
22	DD6	h	214	-	40,45,45	0.16	0	51,67,67	0.94	2 (3%)
19	CLA	m	310	-	59,63,73	1.85	9 (15%)	70,101,113	1.35	6 (8%)
19	CLA	j	309	-	60,64,73	1.83	9 (15%)	71,102,113	1.31	5 (7%)
28	CHL	c	305	11	55,69,74	1.90	13 (23%)	52,108,114	2.75	19 (36%)
22	DD6	f	316	-	40,45,45	0.16	0	51,67,67	0.65	3 (5%)
19	CLA	A	847	1	51,55,73	2.00	9 (17%)	60,91,113	1.54	7 (11%)
19	CLA	B	833	2	60,64,73	1.84	9 (15%)	71,102,113	1.40	6 (8%)
25	LMG	c	320	-	38,38,55	0.87	0	46,46,63	1.24	2 (4%)
19	CLA	b	302	25	59,63,73	1.87	9 (15%)	70,101,113	1.39	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	o	306	-	51,55,73	2.01	9 (17%)	60,91,113	1.52	6 (10%)
19	CLA	B	809	2	58,62,73	1.84	9 (15%)	68,99,113	1.35	7 (10%)
19	CLA	B	848	-	51,55,73	2.02	9 (17%)	60,91,113	1.55	8 (13%)
19	CLA	e	302	-	59,63,73	1.85	9 (15%)	70,101,113	1.37	6 (8%)
19	CLA	A	824	-	69,73,73	1.69	9 (13%)	82,113,113	1.22	5 (6%)
19	CLA	D	301	15	56,60,73	1.89	9 (16%)	65,97,113	1.40	7 (10%)
19	CLA	B	805	2	69,73,73	1.70	9 (13%)	82,113,113	1.35	8 (9%)
19	CLA	l	209	-	51,55,73	2.01	9 (17%)	60,91,113	1.67	10 (16%)
22	DD6	A	832	-	40,45,45	0.24	0	51,67,67	0.98	3 (5%)
25	LMG	e	312	-	44,44,55	0.83	1 (2%)	52,52,63	1.14	3 (5%)
19	CLA	F	202	-	61,65,73	1.81	9 (14%)	72,103,113	1.29	6 (8%)
23	BCR	B	825	-	41,41,41	0.20	0	56,56,56	0.38	0
19	CLA	B	839	2	69,73,73	1.69	9 (13%)	82,113,113	1.25	6 (7%)
25	LMG	g	316	-	44,44,55	0.75	0	52,52,63	1.29	6 (11%)
19	CLA	c	309	11	60,64,73	1.82	9 (15%)	71,102,113	1.35	6 (8%)
22	DD6	i	315	-	40,45,45	0.17	0	51,67,67	0.85	2 (3%)
19	CLA	A	809	-	69,73,73	1.71	9 (13%)	82,113,113	1.26	7 (8%)
28	CHL	g	303	15	50,64,74	1.89	11 (22%)	46,102,114	2.81	19 (41%)
19	CLA	n	201	-	51,55,73	1.96	9 (17%)	60,91,113	1.40	7 (11%)
19	CLA	A	844	-	69,73,73	1.69	9 (13%)	82,113,113	1.31	7 (8%)
19	CLA	d	210	-	64,68,73	1.80	9 (14%)	76,107,113	1.37	6 (7%)
21	LHG	A	831	-	48,48,48	0.64	0	51,54,54	1.21	5 (9%)
19	CLA	f	314	14	59,63,73	1.89	9 (15%)	70,101,113	1.58	8 (11%)
19	CLA	i	312	17	51,55,73	1.98	9 (17%)	60,91,113	1.52	6 (10%)
19	CLA	d	209	12	60,64,73	1.80	9 (15%)	71,102,113	1.34	5 (7%)
19	CLA	o	311	-	54,58,73	1.91	9 (16%)	64,95,113	1.36	8 (12%)
19	CLA	A	805	19,1	56,60,73	1.88	9 (16%)	65,97,113	1.54	8 (12%)
19	CLA	c	308	-	61,65,73	1.82	9 (14%)	72,103,113	1.42	7 (9%)
19	CLA	g	308	-	60,64,73	1.84	9 (15%)	71,102,113	1.41	7 (9%)
22	DD6	n	211	-	40,45,45	0.14	0	51,67,67	0.69	1 (1%)
19	CLA	c	310	-	54,58,73	1.91	9 (16%)	64,95,113	1.38	5 (7%)
19	CLA	l	201	-	51,55,73	1.95	9 (17%)	60,91,113	1.40	11 (18%)
19	CLA	B	814	-	63,67,73	1.79	9 (14%)	74,105,113	1.41	7 (9%)
19	CLA	A	802	-	69,73,73	1.68	9 (13%)	82,113,113	1.27	8 (9%)
22	DD6	m	313	-	40,45,45	0.15	0	51,67,67	0.72	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CHL	b	314	-	46,60,74	2.03	12 (26%)	40,97,114	3.03	21 (52%)
19	CLA	A	828	-	69,73,73	1.71	9 (13%)	82,113,113	1.30	8 (9%)
19	CLA	k	307	18	64,68,73	1.78	9 (14%)	76,107,113	1.38	7 (9%)
19	CLA	A	804	1	69,73,73	1.71	9 (13%)	82,113,113	1.30	8 (9%)
19	CLA	f	302	-	59,63,73	1.85	9 (15%)	70,101,113	1.36	5 (7%)
19	CLA	m	303	-	51,55,73	2.00	9 (17%)	60,91,113	1.57	6 (10%)
19	CLA	i	311	-	56,60,73	1.94	9 (16%)	65,97,113	1.63	9 (13%)
19	CLA	h	208	-	64,68,73	1.79	9 (14%)	76,107,113	1.40	6 (7%)
19	CLA	A	811	19	65,69,73	1.77	9 (13%)	77,108,113	1.34	7 (9%)
19	CLA	B	830	2	62,66,73	1.81	9 (14%)	73,104,113	1.35	6 (8%)
19	CLA	F	204	-	51,55,73	1.97	9 (17%)	60,91,113	1.44	7 (11%)
28	CHL	i	304	17	50,64,74	2.02	12 (24%)	46,102,114	2.85	19 (41%)
19	CLA	A	829	-	69,73,73	1.71	9 (13%)	82,113,113	1.28	6 (7%)
19	CLA	A	853	-	51,55,73	1.99	9 (17%)	60,91,113	1.54	9 (15%)
19	CLA	a	308	9	64,68,73	1.79	9 (14%)	76,107,113	1.46	7 (9%)
19	CLA	g	301	15	52,56,73	1.91	9 (17%)	61,92,113	1.44	9 (14%)
19	CLA	k	303	-	51,55,73	2.00	9 (17%)	60,91,113	1.48	6 (10%)
19	CLA	g	307	15	64,68,73	1.76	9 (14%)	76,107,113	1.28	5 (6%)
23	BCR	B	831	-	41,41,41	0.24	0	56,56,56	0.35	0
19	CLA	g	305	15	51,55,73	2.01	9 (17%)	60,91,113	1.55	9 (15%)
19	CLA	A	823	-	69,73,73	1.66	9 (13%)	82,113,113	1.26	7 (8%)
22	DD6	F	205	-	40,45,45	0.19	0	51,67,67	0.83	3 (5%)
19	CLA	B	815	-	64,68,73	1.74	9 (14%)	76,107,113	1.40	8 (10%)
19	CLA	B	842	-	51,55,73	1.99	9 (17%)	60,91,113	1.50	9 (15%)
22	DD6	i	314	-	40,45,45	0.18	0	51,67,67	0.69	2 (3%)
19	CLA	i	308	17	55,59,73	1.92	9 (16%)	64,96,113	1.42	6 (9%)
19	CLA	B	837	-	54,58,73	1.95	9 (16%)	64,95,113	1.48	9 (14%)
19	CLA	f	306	14	51,55,73	1.99	9 (17%)	60,91,113	1.45	6 (10%)
22	DD6	c	319	-	40,45,45	0.19	0	51,67,67	0.88	3 (5%)
23	BCR	B	850	-	41,41,41	0.32	0	56,56,56	0.62	1 (1%)
19	CLA	a	304	-	51,55,73	1.98	9 (17%)	60,91,113	1.49	6 (10%)
28	CHL	a	311	-	42,56,74	2.11	12 (28%)	36,92,114	3.39	18 (50%)
19	CLA	B	849	-	65,69,73	1.76	9 (13%)	77,108,113	1.41	9 (11%)
22	DD6	J	802	-	40,45,45	0.22	0	51,67,67	0.84	3 (5%)
19	CLA	B	806	-	69,73,73	1.69	9 (13%)	82,113,113	1.26	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	DD6	k	313	-	40,45,45	0.18	0	51,67,67	0.91	2 (3%)
19	CLA	o	312	16	51,55,73	2.02	9 (17%)	60,91,113	1.57	6 (10%)
19	CLA	a	306	9	56,60,73	1.87	9 (16%)	65,97,113	1.50	9 (13%)
22	DD6	h	215	-	40,45,45	0.21	0	51,67,67	0.65	1 (1%)
19	CLA	c	307	-	59,63,73	1.85	9 (15%)	70,101,113	1.35	8 (11%)
19	CLA	B	841	-	51,55,73	1.95	9 (17%)	60,91,113	1.48	8 (13%)
19	CLA	g	311	-	51,55,73	2.05	9 (17%)	60,91,113	1.61	7 (11%)
19	CLA	n	202	18	51,55,73	2.05	9 (17%)	60,91,113	1.87	14 (23%)
19	CLA	B	818	-	69,73,73	1.69	9 (13%)	82,113,113	1.31	9 (10%)
19	CLA	j	308	15	64,68,73	1.77	9 (14%)	76,107,113	1.35	7 (9%)
19	CLA	B	832	2	54,58,73	1.89	9 (16%)	64,95,113	1.55	9 (14%)
19	CLA	o	310	-	51,55,73	2.00	9 (17%)	60,91,113	1.51	7 (11%)
19	CLA	A	821	1	67,71,73	1.73	9 (13%)	79,110,113	1.29	6 (7%)
19	CLA	A	826	1	54,58,73	1.91	9 (16%)	64,95,113	1.40	6 (9%)
19	CLA	a	305	9	64,68,73	1.78	9 (14%)	76,107,113	1.32	8 (10%)
19	CLA	A	839	-	52,56,73	1.94	9 (17%)	61,92,113	1.43	7 (11%)
26	SF4	C	801	-	0,12,12	-	-	-	-	-
19	CLA	B	836	-	68,72,73	1.70	9 (13%)	80,111,113	1.22	7 (8%)
19	CLA	A	808	1	54,58,73	1.92	9 (16%)	64,95,113	1.45	6 (9%)
25	LMG	f	313	-	26,26,55	0.95	0	34,34,63	1.23	4 (11%)
19	CLA	B	811	2	62,66,73	1.80	9 (14%)	73,104,113	1.39	7 (9%)
28	CHL	k	301	18	42,56,74	2.05	12 (28%)	36,92,114	3.22	17 (47%)
19	CLA	j	305	15	54,58,73	1.85	9 (16%)	64,95,113	1.46	9 (14%)
19	CLA	m	305	18	64,68,73	1.74	9 (14%)	76,107,113	1.37	7 (9%)
25	LMG	a	316	-	27,27,55	0.95	0	35,35,63	1.22	6 (17%)
22	DD6	J	801	-	40,45,45	0.29	0	51,67,67	0.98	1 (1%)
22	DD6	g	315	-	40,45,45	0.18	0	51,67,67	0.86	2 (3%)
28	CHL	b	301	10	50,64,74	1.99	12 (24%)	46,102,114	2.90	20 (43%)
19	CLA	i	313	17	56,60,73	1.95	9 (16%)	65,97,113	1.64	8 (12%)
22	DD6	e	314	-	40,45,45	0.16	0	51,67,67	0.56	1 (1%)
19	CLA	k	308	18	54,58,73	1.94	9 (16%)	64,95,113	1.46	7 (10%)
19	CLA	e	310	-	59,63,73	1.83	9 (15%)	70,101,113	1.48	9 (12%)
19	CLA	e	303	-	51,55,73	1.96	9 (17%)	60,91,113	1.46	7 (11%)
19	CLA	g	302	-	59,63,73	1.85	9 (15%)	70,101,113	1.35	6 (8%)
19	CLA	l	202	-	51,55,73	2.06	9 (17%)	60,91,113	1.66	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	j	311	-	54,58,73	1.90	9 (16%)	64,95,113	1.45	12 (18%)
28	CHL	e	304	13	55,69,74	1.90	14 (25%)	52,108,114	2.78	18 (34%)
19	CLA	A	841	1	69,73,73	1.70	9 (13%)	82,113,113	1.28	7 (8%)
19	CLA	a	307	9	59,63,73	1.87	9 (15%)	70,101,113	1.45	7 (10%)
22	DD6	l	210	-	40,45,45	0.24	0	51,67,67	0.77	1 (1%)
19	CLA	c	314	-	51,55,73	2.00	9 (17%)	60,91,113	1.55	6 (10%)
19	CLA	A	827	1	55,59,73	1.93	9 (16%)	64,96,113	1.48	6 (9%)
19	CLA	b	303	-	55,59,73	1.90	9 (16%)	64,96,113	1.42	6 (9%)
19	CLA	A	812	1	60,64,73	1.83	9 (15%)	71,102,113	1.34	6 (8%)
19	CLA	k	302	25	60,64,73	1.84	9 (15%)	71,102,113	1.44	9 (12%)
19	CLA	a	310	-	54,58,73	1.90	9 (16%)	64,95,113	1.42	8 (12%)
19	CLA	j	307	15	64,68,73	1.80	9 (14%)	76,107,113	1.46	8 (10%)
25	LMG	h	216	-	35,35,55	0.97	0	43,43,63	1.26	3 (6%)
19	CLA	i	302	-	59,63,73	1.87	9 (15%)	70,101,113	1.38	6 (8%)
28	CHL	a	312	-	42,56,74	2.13	12 (28%)	36,92,114	3.13	18 (50%)
22	DD6	m	312	-	40,45,45	0.19	0	51,67,67	0.95	2 (3%)
19	CLA	B	835	-	60,64,73	1.83	9 (15%)	71,102,113	1.44	7 (9%)
22	DD6	c	317	-	40,45,45	0.14	0	51,67,67	0.81	2 (3%)
19	CLA	j	310	-	51,55,73	1.95	9 (17%)	60,91,113	1.44	8 (13%)
19	CLA	B	846	2	51,55,73	1.97	9 (17%)	60,91,113	1.31	9 (15%)
19	CLA	j	306	15	51,55,73	2.08	9 (17%)	60,91,113	1.58	9 (15%)
22	DD6	b	317	-	40,45,45	0.21	0	51,67,67	1.12	3 (5%)
19	CLA	J	803	-	51,55,73	1.95	9 (17%)	60,91,113	1.44	5 (8%)
28	CHL	b	311	-	42,56,74	2.10	11 (26%)	36,92,114	3.13	16 (44%)
22	DD6	j	315	-	40,45,45	0.20	0	51,67,67	0.90	2 (3%)
19	CLA	B	801	-	68,72,73	1.69	9 (13%)	80,111,113	1.33	7 (8%)
23	BCR	B	834	-	41,41,41	0.17	0	56,56,56	0.37	0
19	CLA	f	303	14	51,55,73	1.97	9 (17%)	60,91,113	1.47	6 (10%)
19	CLA	l	206	-	51,55,73	2.13	9 (17%)	60,91,113	1.58	9 (15%)
22	DD6	o	313	-	40,45,45	0.20	0	51,67,67	0.70	2 (3%)
25	LMG	j	314	-	37,37,55	0.99	1 (2%)	45,45,63	1.47	5 (11%)
19	CLA	o	307	-	64,68,73	1.84	9 (14%)	76,107,113	1.66	12 (15%)
19	CLA	o	302	-	59,63,73	1.96	9 (15%)	70,101,113	1.64	9 (12%)
19	CLA	A	813	-	64,68,73	1.81	9 (14%)	76,107,113	1.39	7 (9%)
19	CLA	B	845	2	51,55,73	1.99	9 (17%)	60,91,113	1.50	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	B	828	-	41,41,41	0.14	0	56,56,56	0.46	0
25	LMG	g	312	-	37,37,55	0.91	1 (2%)	45,45,63	1.27	5 (11%)
19	CLA	n	205	18	64,68,73	1.81	9 (14%)	76,107,113	1.43	8 (10%)
27	DGD	B	829	-	63,63,67	0.91	1 (1%)	77,77,81	1.29	4 (5%)
19	CLA	B	804	-	69,73,73	1.73	9 (13%)	82,113,113	1.25	8 (9%)
19	CLA	B	807	2	69,73,73	1.67	9 (13%)	82,113,113	1.31	6 (7%)
20	PQN	A	830	-	34,34,34	0.41	0	43,45,45	0.72	1 (2%)
28	CHL	g	306	15	50,64,74	2.00	12 (24%)	46,102,114	2.91	19 (41%)
19	CLA	c	303	-	59,63,73	1.87	9 (15%)	70,101,113	1.38	6 (8%)
19	CLA	B	823	-	51,55,73	1.97	9 (17%)	60,91,113	1.58	6 (10%)
19	CLA	d	208	-	64,68,73	1.73	9 (14%)	76,107,113	1.41	9 (11%)
19	CLA	A	815	-	55,59,73	1.92	9 (16%)	64,96,113	1.42	6 (9%)
24	LMU	A	838	-	35,35,36	0.37	0	44,45,47	0.93	1 (2%)
19	CLA	A	842	1	69,73,73	1.69	9 (13%)	82,113,113	1.32	10 (12%)
19	CLA	d	206	-	51,55,73	1.95	9 (17%)	60,91,113	1.44	7 (11%)
23	BCR	A	834	-	41,41,41	0.13	0	56,56,56	0.38	0
19	CLA	c	302	11	51,55,73	1.96	9 (17%)	60,91,113	1.53	9 (15%)
19	CLA	B	821	-	60,64,73	1.85	9 (15%)	71,102,113	1.39	5 (7%)
19	CLA	B	844	2	51,55,73	2.00	9 (17%)	60,91,113	1.56	8 (13%)
19	CLA	b	315	-	51,55,73	2.07	9 (17%)	60,91,113	1.70	10 (16%)
19	CLA	h	205	16	64,68,73	1.80	9 (14%)	76,107,113	1.37	9 (11%)
22	DD6	o	314	-	40,45,45	0.15	0	51,67,67	0.84	3 (5%)
19	CLA	b	307	10	64,68,73	1.77	9 (14%)	76,107,113	1.36	7 (9%)
19	CLA	l	208	-	51,55,73	1.99	9 (17%)	60,91,113	1.48	6 (10%)
19	CLA	d	212	-	51,55,73	1.95	9 (17%)	60,91,113	1.41	6 (10%)
19	CLA	A	848	1	54,58,73	1.90	9 (16%)	64,95,113	1.44	6 (9%)
28	CHL	g	310	-	45,59,74	2.08	13 (28%)	40,96,114	3.01	19 (47%)
19	CLA	B	810	-	56,61,73	1.93	9 (16%)	68,99,113	1.45	6 (8%)
25	LMG	a	318	-	40,40,55	0.81	0	48,48,63	1.29	5 (10%)
28	CHL	i	301	17	42,56,74	2.05	10 (23%)	36,92,114	3.11	17 (47%)
19	CLA	A	852	-	59,63,73	1.84	9 (15%)	70,101,113	1.34	5 (7%)
19	CLA	B	838	-	54,58,73	1.99	9 (16%)	64,95,113	1.57	8 (12%)
22	DD6	k	314	-	40,45,45	0.19	0	51,67,67	1.24	4 (7%)
28	CHL	b	312	-	47,61,74	2.07	12 (25%)	41,98,114	3.03	18 (43%)
19	CLA	j	304	15	64,68,73	1.78	9 (14%)	76,107,113	1.37	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	814	-	51,55,73	1.96	9 (17%)	60,91,113	1.45	6 (10%)
19	CLA	o	303	16	52,56,73	2.00	9 (17%)	61,92,113	1.58	8 (13%)
19	CLA	e	305	13	54,58,73	1.96	9 (16%)	64,95,113	1.51	8 (12%)
19	CLA	h	213	-	51,55,73	2.00	9 (17%)	60,91,113	1.57	7 (11%)
19	CLA	F	203	-	69,73,73	1.71	9 (13%)	82,113,113	1.34	8 (9%)
20	PQN	B	824	-	34,34,34	0.41	0	43,45,45	0.68	1 (2%)
19	CLA	B	819	-	69,73,73	1.70	9 (13%)	82,113,113	1.27	5 (6%)
19	CLA	l	205	-	64,68,73	1.78	9 (14%)	76,107,113	1.37	7 (9%)
23	BCR	A	835	-	40,40,41	0.21	0	54,54,56	0.52	1 (1%)
26	SF4	C	802	-	0,12,12	-	-	-	-	-
19	CLA	k	305	18	64,68,73	1.75	9 (14%)	76,107,113	1.29	7 (9%)
19	CLA	i	303	-	51,55,73	1.99	9 (17%)	60,91,113	1.47	6 (10%)
19	CLA	b	305	10	51,55,73	1.93	9 (17%)	60,91,113	1.42	8 (13%)
25	LMG	b	316	19	42,42,55	0.85	1 (2%)	50,50,63	1.24	5 (10%)
19	CLA	i	305	-	51,55,73	2.03	9 (17%)	60,91,113	1.55	7 (11%)
19	CLA	B	803	-	69,73,73	1.66	9 (13%)	82,113,113	1.22	7 (8%)
19	CLA	g	304	15	54,58,73	1.86	9 (16%)	64,95,113	1.40	9 (14%)
19	CLA	c	304	11	56,60,73	1.88	9 (16%)	65,97,113	1.38	7 (10%)
19	CLA	k	304	-	64,68,73	1.82	9 (14%)	76,107,113	1.40	8 (10%)
19	CLA	A	806	1	69,73,73	1.72	9 (13%)	82,113,113	1.41	8 (9%)
28	CHL	o	301	16	42,56,74	2.16	11 (26%)	36,92,114	3.16	18 (50%)
22	DD6	d	215	-	40,45,45	0.26	0	51,67,67	0.73	1 (1%)
19	CLA	k	311	-	51,55,73	2.00	9 (17%)	60,91,113	1.53	6 (10%)
28	CHL	h	202	16	42,56,74	2.03	10 (23%)	36,92,114	3.24	17 (47%)
23	BCR	A	837	-	41,41,41	0.20	0	56,56,56	0.50	0
24	LMU	c	301	-	35,35,36	0.43	0	44,45,47	0.88	1 (2%)
28	CHL	d	202	12	42,56,74	2.19	11 (26%)	36,92,114	3.05	17 (47%)
19	CLA	h	207	-	51,55,73	1.99	9 (17%)	60,91,113	1.45	6 (10%)
19	CLA	A	819	-	68,72,73	1.73	9 (13%)	80,111,113	1.29	8 (10%)
19	CLA	i	309	-	64,68,73	1.77	9 (14%)	76,107,113	1.27	6 (7%)
19	CLA	B	847	-	69,73,73	1.75	9 (13%)	82,113,113	1.43	7 (8%)
28	CHL	e	301	13	45,59,74	2.06	13 (28%)	40,96,114	2.86	18 (45%)
19	CLA	m	311	-	51,55,73	2.00	9 (17%)	60,91,113	1.54	6 (10%)
19	CLA	e	309	-	51,55,73	1.99	9 (17%)	60,91,113	1.53	6 (10%)
28	CHL	c	313	-	50,64,74	1.92	13 (26%)	46,102,114	2.93	19 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	845	1	51,55,73	2.03	9 (17%)	60,91,113	1.48	6 (10%)
19	CLA	o	309	-	51,55,73	2.02	9 (17%)	60,91,113	1.52	8 (13%)
19	CLA	l	207	-	51,55,73	1.98	9 (17%)	60,91,113	1.52	6 (10%)
19	CLA	B	840	2	51,55,73	2.07	9 (17%)	60,91,113	1.67	8 (13%)
19	CLA	j	301	-	51,55,73	2.01	9 (17%)	60,91,113	1.60	7 (11%)
19	CLA	A	820	-	59,63,73	1.89	9 (15%)	70,101,113	1.46	6 (8%)
19	CLA	B	813	-	58,62,73	1.89	9 (15%)	68,99,113	1.39	5 (7%)
19	CLA	j	313	15	60,64,73	1.85	9 (15%)	71,102,113	1.42	7 (9%)
19	CLA	i	310	17	51,55,73	1.95	9 (17%)	60,91,113	1.47	9 (15%)
19	CLA	i	306	17	51,55,73	1.99	9 (17%)	60,91,113	1.49	7 (11%)
19	CLA	f	305	-	54,58,73	1.96	9 (16%)	64,95,113	1.58	9 (14%)
19	CLA	f	312	-	51,55,73	2.00	9 (17%)	60,91,113	1.49	5 (8%)
22	DD6	e	313	-	40,45,45	0.19	0	51,67,67	0.95	3 (5%)
22	DD6	g	314	-	40,45,45	0.19	0	51,67,67	0.96	1 (1%)
19	CLA	d	203	-	51,55,73	2.01	9 (17%)	60,91,113	1.56	8 (13%)
19	CLA	d	204	-	56,60,73	1.91	9 (16%)	65,97,113	1.49	8 (12%)
22	DD6	A	833	-	40,45,45	0.18	0	51,67,67	0.79	2 (3%)
28	CHL	d	205	12	50,64,74	1.96	11 (22%)	46,102,114	2.91	20 (43%)
19	CLA	B	816	-	53,57,73	1.95	9 (16%)	61,93,113	1.54	6 (9%)
19	CLA	b	313	-	51,55,73	2.00	9 (17%)	60,91,113	1.59	11 (18%)
22	DD6	c	318	-	40,45,45	0.19	0	51,67,67	0.67	2 (3%)
23	BCR	J	804	-	41,41,41	0.18	0	56,56,56	0.37	0
19	CLA	k	306	18	51,55,73	1.97	9 (17%)	60,91,113	1.52	8 (13%)
19	CLA	n	208	-	51,55,73	1.98	9 (17%)	60,91,113	1.51	10 (16%)
19	CLA	n	206	18	51,55,73	2.14	9 (17%)	60,91,113	1.45	8 (13%)
19	CLA	c	306	11	60,64,73	1.88	8 (13%)	71,102,113	1.41	6 (8%)
23	BCR	M	801	-	41,41,41	0.13	0	56,56,56	0.35	0
19	CLA	B	812	2	68,72,73	1.72	9 (13%)	80,111,113	1.28	6 (7%)
19	CLA	j	303	15	56,60,73	1.87	9 (16%)	65,97,113	1.41	7 (10%)
19	CLA	j	302	-	59,63,73	1.87	9 (15%)	70,101,113	1.38	6 (8%)
19	CLA	n	204	-	60,64,73	1.91	9 (15%)	71,102,113	1.48	7 (9%)
25	LMG	A	851	-	34,34,55	0.83	1 (2%)	42,42,63	1.29	6 (14%)
19	CLA	m	309	-	51,55,73	1.98	9 (17%)	60,91,113	1.55	8 (13%)
19	CLA	A	849	1	51,55,73	1.99	9 (17%)	60,91,113	1.48	6 (10%)
22	DD6	b	319	-	40,45,45	0.16	0	51,67,67	0.60	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	h	211	-	55,59,73	1.89	9 (16%)	64,96,113	1.46	7 (10%)
19	CLA	A	850	1	69,73,73	1.73	9 (13%)	82,113,113	1.29	6 (7%)
19	CLA	k	310	-	59,63,73	1.84	9 (15%)	70,101,113	1.37	6 (8%)
19	CLA	e	306	13	59,63,73	1.85	9 (15%)	70,101,113	1.40	7 (10%)
19	CLA	A	801	-	69,73,73	1.67	8 (11%)	82,113,113	1.21	8 (9%)
25	LMG	a	301	-	40,40,55	0.87	2 (5%)	48,48,63	1.27	6 (12%)
28	CHL	c	312	-	50,64,74	1.99	12 (24%)	46,102,114	2.92	18 (39%)
28	CHL	f	301	14	42,56,74	2.03	12 (28%)	36,92,114	3.08	19 (52%)
19	CLA	h	201	-	60,64,73	1.84	9 (15%)	71,102,113	1.37	6 (8%)
19	CLA	e	311	13	59,63,73	1.86	9 (15%)	70,101,113	1.38	7 (10%)
19	CLA	A	803	-	69,73,73	1.76	10 (14%)	82,113,113	1.35	8 (9%)
25	LMG	i	316	-	41,41,55	0.90	1 (2%)	49,49,63	1.21	3 (6%)
19	CLA	f	308	14	55,59,73	1.90	9 (16%)	64,96,113	1.42	5 (7%)
19	CLA	A	818	-	68,72,73	1.73	9 (13%)	80,111,113	1.33	6 (7%)
19	CLA	b	306	10	64,68,73	1.78	9 (14%)	76,107,113	1.41	9 (11%)
19	CLA	a	309	-	60,64,73	1.83	9 (15%)	71,102,113	1.34	5 (7%)
28	CHL	f	304	14	50,64,74	1.93	12 (24%)	46,102,114	2.84	20 (43%)
19	CLA	m	308	18	54,58,73	1.95	9 (16%)	64,95,113	1.42	7 (10%)
19	CLA	b	309	-	54,58,73	1.90	9 (16%)	64,95,113	1.40	6 (9%)
19	CLA	A	843	-	69,73,73	1.78	9 (13%)	82,113,113	1.55	10 (12%)
19	CLA	B	843	-	51,55,73	1.99	9 (17%)	60,91,113	1.53	6 (10%)
19	CLA	k	309	-	51,55,73	2.06	9 (17%)	60,91,113	1.62	8 (13%)
19	CLA	b	304	-	59,63,73	1.78	9 (15%)	70,101,113	1.41	8 (11%)
19	CLA	F	201	-	64,68,73	1.74	9 (14%)	76,107,113	1.31	6 (7%)
19	CLA	l	204	18	60,64,73	1.84	9 (15%)	71,102,113	1.35	6 (8%)
19	CLA	h	206	16	51,55,73	1.99	9 (17%)	60,91,113	1.51	7 (11%)

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
19	CLA	B	808	-	1/1/15/20	8/39/115/115	-
19	CLA	j	312	-	1/1/11/20	4/18/94/115	-
22	DD6	j	316	-	-	0/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	DD6	n	210	-	-	2/26/80/80	0/3/3/3
19	CLA	i	307	17	1/1/12/20	6/26/102/115	-
19	CLA	h	204	16	1/1/11/20	2/19/95/115	-
19	CLA	d	211	-	1/1/14/20	5/33/109/115	-
25	LMG	d	213	-	-	9/26/46/70	0/1/1/1
23	BCR	B	826	-	-	8/29/63/63	0/2/2/2
19	CLA	f	310	-	1/1/11/20	2/18/94/115	-
28	CHL	m	301	18	3/3/16/26	8/18/116/137	-
19	CLA	A	817	-	1/1/15/20	7/39/115/115	-
19	CLA	A	822	-	1/1/15/20	12/39/115/115	-
19	CLA	A	816	-	1/1/13/20	7/32/108/115	-
19	CLA	c	316	11	1/1/15/20	7/39/115/115	-
19	CLA	d	207	-	1/1/11/20	2/18/94/115	-
24	LMU	a	319	-	-	9/21/57/61	0/2/2/2
19	CLA	B	822	-	1/1/15/20	10/39/115/115	-
19	CLA	B	820	2	1/1/14/20	7/35/111/115	-
19	CLA	A	825	-	1/1/12/20	2/21/97/115	-
19	CLA	f	311	-	1/1/12/20	5/24/100/115	-
19	CLA	A	840	1	1/1/15/20	9/39/115/115	-
19	CLA	o	304	16	1/1/12/20	14/26/102/115	-
19	CLA	f	307	14	1/1/12/20	4/26/102/115	-
19	CLA	m	302	-	1/1/11/20	9/18/94/115	-
19	CLA	h	210	-	1/1/11/20	0/18/94/115	-
19	CLA	a	314	-	1/1/11/20	8/18/94/115	-
19	CLA	h	209	16	1/1/14/20	7/33/109/115	-
28	CHL	a	313	-	3/3/16/26	9/18/116/137	-
23	BCR	B	827	-	-	1/29/63/63	0/2/2/2
28	CHL	b	310	-	3/3/16/26	5/18/116/137	-
19	CLA	A	846	1	1/1/11/20	3/18/94/115	-
19	CLA	A	807	1	1/1/15/20	10/39/115/115	-
19	CLA	m	306	18	1/1/11/20	1/18/94/115	-
19	CLA	g	309	-	1/1/13/20	6/29/105/115	-
22	DD6	d	214	-	-	0/26/80/80	0/3/3/3
25	LMG	k	312	19	-	10/32/52/70	0/1/1/1
19	CLA	o	305	-	1/1/11/20	7/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	DD6	a	321	-	-	0/26/80/80	0/3/3/3
19	CLA	e	307	13	1/1/14/20	4/33/109/115	-
22	DD6	b	318	-	-	0/26/80/80	0/3/3/3
22	DD6	a	320	-	-	0/26/80/80	0/3/3/3
19	CLA	a	303	-	1/1/13/20	12/27/103/115	-
19	CLA	m	304	-	1/1/11/20	5/18/94/115	-
19	CLA	A	810	1	1/1/12/20	4/21/97/115	-
26	SF4	B	802	-	-	-	0/6/5/5
19	CLA	n	203	18	1/1/14/20	11/33/109/115	-
19	CLA	f	309	-	1/1/14/20	8/33/109/115	-
19	CLA	a	302	9	1/1/11/20	9/18/94/115	-
22	DD6	l	211	-	-	0/26/80/80	0/3/3/3
23	BCR	A	836	-	-	2/29/63/63	0/2/2/2
19	CLA	c	315	11	1/1/11/20	3/18/94/115	-
19	CLA	n	209	-	1/1/11/20	10/18/94/115	-
19	CLA	m	307	18	1/1/14/20	6/33/109/115	-
19	CLA	c	311	-	1/1/11/20	3/18/94/115	-
19	CLA	o	308	-	1/1/12/20	4/25/101/115	-
28	CHL	a	315	9	2/2/16/26	11/18/116/137	-
22	DD6	f	315	-	-	0/26/80/80	0/3/3/3
19	CLA	h	203	-	1/1/13/20	2/27/103/115	-
19	CLA	d	201	-	1/1/11/20	1/18/94/115	-
25	LMG	g	313	-	-	11/28/48/70	0/1/1/1
19	CLA	n	207	-	1/1/11/20	2/18/94/115	-
19	CLA	B	817	-	1/1/14/20	12/36/112/115	-
29	NEX	a	317	-	-	6/27/83/83	0/3/3/3
19	CLA	e	308	13	1/1/13/20	6/29/105/115	-
19	CLA	h	212	-	1/1/13/20	7/29/105/115	-
19	CLA	l	203	18	1/1/14/20	11/33/109/115	-
19	CLA	b	308	10	1/1/13/20	4/29/105/115	-
22	DD6	h	214	-	-	0/26/80/80	0/3/3/3
19	CLA	m	310	-	1/1/13/20	8/27/103/115	-
19	CLA	j	309	-	1/1/13/20	4/29/105/115	-
28	CHL	c	305	11	3/3/19/26	13/33/131/137	-
22	DD6	f	316	-	-	1/26/80/80	0/3/3/3
19	CLA	A	847	1	1/1/11/20	6/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	833	2	1/1/13/20	6/29/105/115	-
25	LMG	c	320	-	-	19/33/53/70	0/1/1/1
19	CLA	b	302	25	1/1/13/20	7/27/103/115	-
19	CLA	o	306	-	1/1/11/20	6/18/94/115	-
19	CLA	B	809	2	1/1/12/20	3/26/102/115	-
19	CLA	B	848	-	1/1/11/20	6/18/94/115	-
19	CLA	e	302	-	1/1/13/20	4/27/103/115	-
19	CLA	A	824	-	1/1/15/20	5/39/115/115	-
19	CLA	D	301	15	1/1/12/20	4/24/100/115	-
19	CLA	B	805	2	1/1/15/20	10/39/115/115	-
19	CLA	l	209	-	1/1/11/20	4/18/94/115	-
22	DD6	A	832	-	-	2/26/80/80	0/3/3/3
25	LMG	e	312	-	-	18/39/59/70	0/1/1/1
19	CLA	F	202	-	1/1/13/20	8/30/106/115	-
23	BCR	B	825	-	-	0/29/63/63	0/2/2/2
19	CLA	B	839	2	1/1/15/20	9/39/115/115	-
25	LMG	g	316	-	-	30/39/59/70	0/1/1/1
19	CLA	c	309	11	1/1/13/20	2/29/105/115	-
22	DD6	i	315	-	-	1/26/80/80	0/3/3/3
19	CLA	A	809	-	1/1/15/20	5/39/115/115	-
28	CHL	g	303	15	3/3/18/26	8/27/125/137	-
19	CLA	n	201	-	1/1/11/20	6/18/94/115	-
19	CLA	A	844	-	1/1/15/20	5/39/115/115	-
19	CLA	d	210	-	1/1/14/20	5/33/109/115	-
21	LHG	A	831	-	-	18/53/53/53	-
19	CLA	f	314	14	1/1/13/20	8/27/103/115	-
19	CLA	i	312	17	1/1/11/20	1/18/94/115	-
19	CLA	d	209	12	1/1/13/20	6/29/105/115	-
19	CLA	o	311	-	1/1/12/20	7/21/97/115	-
19	CLA	A	805	19,1	1/1/12/20	3/24/100/115	-
19	CLA	c	308	-	1/1/13/20	2/30/106/115	-
19	CLA	g	308	-	1/1/13/20	3/29/105/115	-
22	DD6	n	211	-	-	0/26/80/80	0/3/3/3
19	CLA	c	310	-	1/1/12/20	2/21/97/115	-
19	CLA	l	201	-	1/1/11/20	3/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	814	-	1/1/13/20	6/32/108/115	-
19	CLA	A	802	-	1/1/15/20	12/39/115/115	-
22	DD6	m	313	-	-	0/26/80/80	0/3/3/3
28	CHL	b	314	-	3/3/17/26	9/23/121/137	-
19	CLA	A	828	-	1/1/15/20	5/39/115/115	-
19	CLA	k	307	18	1/1/14/20	2/33/109/115	-
19	CLA	A	804	1	1/1/15/20	8/39/115/115	-
19	CLA	f	302	-	1/1/13/20	4/27/103/115	-
19	CLA	m	303	-	1/1/11/20	4/18/94/115	-
19	CLA	i	311	-	1/1/12/20	5/24/100/115	-
19	CLA	h	208	-	1/1/14/20	1/33/109/115	-
19	CLA	A	811	19	1/1/14/20	7/35/111/115	-
19	CLA	B	830	2	1/1/13/20	13/31/107/115	-
19	CLA	F	204	-	1/1/11/20	2/18/94/115	-
28	CHL	i	304	17	3/3/18/26	10/27/125/137	-
19	CLA	A	829	-	1/1/15/20	4/39/115/115	-
19	CLA	A	853	-	1/1/11/20	4/18/94/115	-
19	CLA	a	308	9	1/1/14/20	1/33/109/115	-
19	CLA	g	301	15	1/1/11/20	3/19/95/115	-
19	CLA	k	303	-	1/1/11/20	2/18/94/115	-
19	CLA	g	307	15	1/1/14/20	3/33/109/115	-
23	BCR	B	831	-	-	6/29/63/63	0/2/2/2
19	CLA	g	305	15	1/1/11/20	7/18/94/115	-
19	CLA	A	823	-	1/1/15/20	4/39/115/115	-
22	DD6	F	205	-	-	2/26/80/80	0/3/3/3
19	CLA	B	815	-	1/1/14/20	8/33/109/115	-
19	CLA	B	842	-	1/1/11/20	4/18/94/115	-
22	DD6	i	314	-	-	0/26/80/80	0/3/3/3
19	CLA	i	308	17	1/1/12/20	6/23/99/115	-
19	CLA	B	837	-	1/1/12/20	9/21/97/115	-
19	CLA	f	306	14	1/1/11/20	3/18/94/115	-
22	DD6	c	319	-	-	0/26/80/80	0/3/3/3
23	BCR	B	850	-	-	5/29/63/63	0/2/2/2
19	CLA	a	304	-	1/1/11/20	5/18/94/115	-
28	CHL	a	311	-	3/3/16/26	5/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	849	-	1/1/14/20	14/35/111/115	-
22	DD6	J	802	-	-	2/26/80/80	0/3/3/3
19	CLA	B	806	-	1/1/15/20	9/39/115/115	-
22	DD6	k	313	-	-	1/26/80/80	0/3/3/3
19	CLA	o	312	16	1/1/11/20	2/18/94/115	-
19	CLA	a	306	9	1/1/12/20	10/24/100/115	-
22	DD6	h	215	-	-	1/26/80/80	0/3/3/3
19	CLA	c	307	-	1/1/13/20	9/27/103/115	-
19	CLA	B	841	-	1/1/11/20	6/18/94/115	-
19	CLA	g	311	-	1/1/11/20	5/18/94/115	-
19	CLA	n	202	18	1/1/11/20	7/18/94/115	-
19	CLA	B	818	-	1/1/15/20	8/39/115/115	-
19	CLA	j	308	15	1/1/14/20	6/33/109/115	-
19	CLA	B	832	2	1/1/12/20	6/21/97/115	-
19	CLA	o	310	-	1/1/11/20	4/18/94/115	-
19	CLA	A	821	1	1/1/14/20	3/37/113/115	-
19	CLA	A	826	1	1/1/12/20	2/21/97/115	-
19	CLA	a	305	9	1/1/14/20	8/33/109/115	-
19	CLA	A	839	-	1/1/11/20	2/19/95/115	-
26	SF4	C	801	-	-	-	0/6/5/5
19	CLA	B	836	-	1/1/14/20	4/38/114/115	-
19	CLA	A	808	1	1/1/12/20	1/21/97/115	-
25	LMG	f	313	-	-	10/20/40/70	0/1/1/1
19	CLA	B	811	2	1/1/13/20	12/31/107/115	-
28	CHL	k	301	18	2/2/16/26	12/18/116/137	-
19	CLA	j	305	15	1/1/12/20	12/21/97/115	-
19	CLA	m	305	18	1/1/14/20	6/33/109/115	-
25	LMG	a	316	-	-	9/21/41/70	0/1/1/1
28	CHL	b	301	10	2/2/18/26	16/27/125/137	-
22	DD6	J	801	-	-	2/26/80/80	0/3/3/3
22	DD6	g	315	-	-	0/26/80/80	0/3/3/3
19	CLA	i	313	17	1/1/12/20	8/24/100/115	-
22	DD6	e	314	-	-	0/26/80/80	0/3/3/3
19	CLA	k	308	18	1/1/12/20	2/21/97/115	-
19	CLA	e	310	-	1/1/13/20	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	e	303	-	1/1/11/20	3/18/94/115	-
19	CLA	g	302	-	1/1/13/20	6/27/103/115	-
19	CLA	l	202	-	1/1/11/20	2/18/94/115	-
19	CLA	j	311	-	1/1/12/20	4/21/97/115	-
28	CHL	e	304	13	2/2/19/26	18/33/131/137	-
19	CLA	A	841	1	1/1/15/20	9/39/115/115	-
19	CLA	a	307	9	1/1/13/20	2/27/103/115	-
22	DD6	l	210	-	-	1/26/80/80	0/3/3/3
19	CLA	c	314	-	1/1/11/20	5/18/94/115	-
19	CLA	A	827	1	1/1/12/20	6/23/99/115	-
19	CLA	b	303	-	1/1/12/20	6/23/99/115	-
19	CLA	A	812	1	1/1/13/20	2/29/105/115	-
19	CLA	k	302	25	1/1/13/20	8/29/105/115	-
19	CLA	a	310	-	1/1/12/20	1/21/97/115	-
19	CLA	j	307	15	1/1/14/20	6/33/109/115	-
25	LMG	h	216	-	-	10/30/50/70	0/1/1/1
19	CLA	i	302	-	1/1/13/20	4/27/103/115	-
28	CHL	a	312	-	3/3/16/26	4/18/116/137	-
22	DD6	m	312	-	-	1/26/80/80	0/3/3/3
19	CLA	B	835	-	1/1/13/20	9/29/105/115	-
22	DD6	c	317	-	-	1/26/80/80	0/3/3/3
19	CLA	j	310	-	1/1/11/20	7/18/94/115	-
19	CLA	B	846	2	1/1/11/20	6/18/94/115	-
19	CLA	j	306	15	1/1/11/20	7/18/94/115	-
22	DD6	b	317	-	-	2/26/80/80	0/3/3/3
19	CLA	J	803	-	1/1/11/20	0/18/94/115	-
28	CHL	b	311	-	3/3/16/26	8/18/116/137	-
22	DD6	j	315	-	-	0/26/80/80	0/3/3/3
19	CLA	B	801	-	1/1/14/20	11/38/114/115	-
23	BCR	B	834	-	-	3/29/63/63	0/2/2/2
19	CLA	f	303	14	1/1/11/20	3/18/94/115	-
19	CLA	l	206	-	1/1/11/20	5/18/94/115	-
22	DD6	o	313	-	-	0/26/80/80	0/3/3/3
25	LMG	j	314	-	-	11/32/52/70	0/1/1/1
19	CLA	o	307	-	1/1/14/20	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	o	302	-	1/1/13/20	16/27/103/115	-
19	CLA	A	813	-	1/1/14/20	6/33/109/115	-
19	CLA	B	845	2	1/1/11/20	2/18/94/115	-
23	BCR	B	828	-	-	0/29/63/63	0/2/2/2
25	LMG	g	312	-	-	13/32/52/70	0/1/1/1
19	CLA	n	205	18	1/1/14/20	6/33/109/115	-
27	DGD	B	829	-	-	26/51/91/95	0/2/2/2
19	CLA	B	804	-	1/1/15/20	6/39/115/115	-
19	CLA	B	807	2	1/1/15/20	11/39/115/115	-
20	PQN	A	830	-	-	11/23/43/43	0/2/2/2
28	CHL	g	306	15	3/3/18/26	7/27/125/137	-
19	CLA	c	303	-	1/1/13/20	3/27/103/115	-
19	CLA	B	823	-	1/1/11/20	2/18/94/115	-
19	CLA	d	208	-	1/1/14/20	13/33/109/115	-
19	CLA	A	815	-	1/1/12/20	4/23/99/115	-
24	LMU	A	838	-	-	7/21/57/61	0/2/2/2
19	CLA	A	842	1	1/1/15/20	20/39/115/115	-
19	CLA	d	206	-	1/1/11/20	3/18/94/115	-
23	BCR	A	834	-	-	0/29/63/63	0/2/2/2
19	CLA	c	302	11	1/1/11/20	4/18/94/115	-
19	CLA	B	821	-	1/1/13/20	7/29/105/115	-
19	CLA	B	844	2	1/1/11/20	4/18/94/115	-
19	CLA	b	315	-	1/1/11/20	9/18/94/115	-
19	CLA	h	205	16	1/1/14/20	3/33/109/115	-
22	DD6	o	314	-	-	1/26/80/80	0/3/3/3
19	CLA	b	307	10	1/1/14/20	2/33/109/115	-
19	CLA	l	208	-	1/1/11/20	4/18/94/115	-
19	CLA	d	212	-	1/1/11/20	2/18/94/115	-
19	CLA	A	848	1	1/1/12/20	6/21/97/115	-
28	CHL	g	310	-	3/3/17/26	9/21/119/137	-
19	CLA	B	810	-	1/1/13/20	7/23/99/115	-
28	CHL	i	301	17	3/3/16/26	7/18/116/137	-
25	LMG	a	318	-	-	20/35/55/70	0/1/1/1
19	CLA	A	852	-	1/1/13/20	6/27/103/115	-
19	CLA	B	838	-	1/1/12/20	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CHL	b	312	-	3/3/17/26	13/24/122/137	-
22	DD6	k	314	-	-	0/26/80/80	0/3/3/3
19	CLA	j	304	15	1/1/14/20	14/33/109/115	-
19	CLA	A	814	-	1/1/11/20	2/18/94/115	-
19	CLA	o	303	16	1/1/11/20	11/19/95/115	-
19	CLA	e	305	13	1/1/12/20	1/21/97/115	-
19	CLA	h	213	-	1/1/11/20	4/18/94/115	-
19	CLA	F	203	-	1/1/15/20	20/39/115/115	-
20	PQN	B	824	-	-	5/23/43/43	0/2/2/2
19	CLA	B	819	-	1/1/15/20	3/39/115/115	-
19	CLA	l	205	-	1/1/14/20	2/33/109/115	-
23	BCR	A	835	-	-	5/27/61/63	0/2/2/2
26	SF4	C	802	-	-	-	0/6/5/5
19	CLA	k	305	18	1/1/14/20	6/33/109/115	-
19	CLA	i	303	-	1/1/11/20	5/18/94/115	-
19	CLA	b	305	10	1/1/11/20	3/18/94/115	-
25	LMG	b	316	19	-	13/37/57/70	0/1/1/1
19	CLA	i	305	-	1/1/11/20	3/18/94/115	-
19	CLA	B	803	-	1/1/15/20	7/39/115/115	-
19	CLA	g	304	15	1/1/12/20	4/21/97/115	-
19	CLA	c	304	11	1/1/12/20	6/24/100/115	-
19	CLA	k	304	-	1/1/14/20	9/33/109/115	-
19	CLA	A	806	1	1/1/15/20	16/39/115/115	-
28	CHL	o	301	16	3/3/16/26	5/18/116/137	-
22	DD6	d	215	-	-	0/26/80/80	0/3/3/3
19	CLA	k	311	-	1/1/11/20	3/18/94/115	-
28	CHL	h	202	16	2/2/16/26	10/18/116/137	-
23	BCR	A	837	-	-	6/29/63/63	0/2/2/2
24	LMU	c	301	-	-	3/21/57/61	0/2/2/2
28	CHL	d	202	12	3/3/16/26	11/18/116/137	-
19	CLA	h	207	-	1/1/11/20	4/18/94/115	-
19	CLA	A	819	-	1/1/14/20	5/37/113/115	-
19	CLA	i	309	-	1/1/14/20	14/33/109/115	-
19	CLA	B	847	-	1/1/15/20	6/39/115/115	-
28	CHL	e	301	13	3/3/17/26	9/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	m	311	-	1/1/11/20	7/18/94/115	-
19	CLA	e	309	-	1/1/11/20	2/18/94/115	-
28	CHL	c	313	-	3/3/18/26	8/27/125/137	-
19	CLA	A	845	1	1/1/11/20	0/18/94/115	-
19	CLA	o	309	-	1/1/11/20	7/18/94/115	-
19	CLA	l	207	-	1/1/11/20	2/18/94/115	-
19	CLA	B	840	2	1/1/11/20	6/18/94/115	-
19	CLA	j	301	-	1/1/11/20	2/18/94/115	-
19	CLA	A	820	-	1/1/13/20	7/27/103/115	-
19	CLA	B	813	-	1/1/12/20	4/25/101/115	-
19	CLA	j	313	15	1/1/13/20	4/29/105/115	-
19	CLA	i	310	17	1/1/11/20	11/18/94/115	-
19	CLA	i	306	17	1/1/11/20	3/18/94/115	-
19	CLA	f	305	-	1/1/12/20	2/21/97/115	-
19	CLA	f	312	-	1/1/11/20	5/18/94/115	-
22	DD6	e	313	-	-	1/26/80/80	0/3/3/3
22	DD6	g	314	-	-	1/26/80/80	0/3/3/3
19	CLA	d	203	-	1/1/11/20	4/18/94/115	-
19	CLA	d	204	-	1/1/12/20	4/24/100/115	-
22	DD6	A	833	-	-	1/26/80/80	0/3/3/3
28	CHL	d	205	12	3/3/18/26	16/27/125/137	-
19	CLA	B	816	-	1/1/11/20	3/20/96/115	-
19	CLA	b	313	-	1/1/11/20	6/18/94/115	-
22	DD6	c	318	-	-	1/26/80/80	0/3/3/3
23	BCR	J	804	-	-	0/29/63/63	0/2/2/2
19	CLA	k	306	18	1/1/11/20	4/18/94/115	-
19	CLA	n	208	-	1/1/11/20	9/18/94/115	-
19	CLA	n	206	18	1/1/11/20	6/18/94/115	-
19	CLA	c	306	11	1/1/13/20	9/29/105/115	-
23	BCR	M	801	-	-	2/29/63/63	0/2/2/2
19	CLA	B	812	2	1/1/14/20	4/38/114/115	-
19	CLA	j	303	15	1/1/12/20	3/24/100/115	-
19	CLA	j	302	-	1/1/13/20	6/27/103/115	-
19	CLA	n	204	-	1/1/13/20	7/29/105/115	-
25	LMG	A	851	-	-	13/29/49/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	m	309	-	1/1/11/20	10/18/94/115	-
19	CLA	A	849	1	1/1/11/20	2/18/94/115	-
22	DD6	b	319	-	-	0/26/80/80	0/3/3/3
19	CLA	h	211	-	1/1/12/20	6/23/99/115	-
19	CLA	A	850	1	1/1/15/20	8/39/115/115	-
19	CLA	k	310	-	1/1/13/20	5/27/103/115	-
19	CLA	e	306	13	1/1/13/20	7/27/103/115	-
19	CLA	A	801	-	1/1/15/20	9/39/115/115	-
28	CHL	c	312	-	3/3/18/26	21/27/125/137	-
25	LMG	a	301	-	-	18/35/55/70	0/1/1/1
28	CHL	f	301	14	2/2/16/26	9/18/116/137	-
19	CLA	h	201	-	1/1/13/20	6/29/105/115	-
19	CLA	e	311	13	1/1/13/20	5/27/103/115	-
19	CLA	A	803	-	1/1/15/20	5/39/115/115	-
25	LMG	i	316	-	-	21/36/56/70	0/1/1/1
19	CLA	f	308	14	1/1/12/20	4/23/99/115	-
19	CLA	A	818	-	1/1/14/20	3/38/114/115	-
19	CLA	b	306	10	1/1/14/20	16/33/109/115	-
19	CLA	a	309	-	1/1/13/20	1/29/105/115	-
28	CHL	f	304	14	3/3/18/26	10/27/125/137	-
19	CLA	m	308	18	1/1/12/20	4/21/97/115	-
19	CLA	b	309	-	1/1/12/20	0/21/97/115	-
19	CLA	A	843	-	1/1/15/20	10/39/115/115	-
19	CLA	B	843	-	1/1/11/20	2/18/94/115	-
19	CLA	k	309	-	1/1/11/20	2/18/94/115	-
19	CLA	b	304	-	1/1/13/20	8/27/103/115	-
19	CLA	F	201	-	1/1/14/20	6/33/109/115	-
19	CLA	l	204	18	1/1/13/20	5/29/105/115	-
19	CLA	h	206	16	1/1/11/20	2/18/94/115	-

The worst 5 of 2525 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	o	311	CLA	C1D-ND	7.20	1.47	1.37
19	A	819	CLA	C1D-ND	7.16	1.47	1.37
19	k	311	CLA	C1D-ND	7.12	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	842	CLA	C1D-ND	7.09	1.47	1.37
19	B	830	CLA	C1D-ND	7.06	1.47	1.37

The worst 5 of 2428 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	311	CHL	C1B-CHB-C4A	13.22	129.82	121.32
28	c	312	CHL	C1B-CHB-C4A	12.35	129.27	121.32
28	h	202	CHL	C1B-CHB-C4A	12.30	129.24	121.32
28	d	205	CHL	C1B-CHB-C4A	12.29	129.23	121.32
28	b	301	CHL	C1B-CHB-C4A	12.25	129.20	121.32

5 of 319 chirality outliers are listed below:

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

5 of 2054 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	804	CLA	CHA-CBD-CGD-O1D
19	A	804	CLA	CHA-CBD-CGD-O2D
19	A	804	CLA	C14-C13-C15-C16
19	A	805	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

152 monomers are involved in 270 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	j	316	DD6	11	0
22	n	210	DD6	10	0
19	i	307	CLA	1	0
25	d	213	LMG	1	0
23	B	826	BCR	3	0
28	m	301	CHL	2	0
19	A	822	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	816	CLA	1	0
19	d	207	CLA	1	0
19	f	311	CLA	1	0
19	o	304	CLA	5	0
19	m	302	CLA	1	0
19	a	314	CLA	1	0
28	b	310	CHL	3	0
25	k	312	LMG	2	0
22	a	321	DD6	5	0
22	b	318	DD6	2	0
19	A	810	CLA	3	0
19	n	203	CLA	4	0
19	a	302	CLA	1	0
23	A	836	BCR	1	0
19	n	209	CLA	1	0
19	m	307	CLA	1	0
28	a	315	CHL	4	0
22	f	315	DD6	2	0
19	h	203	CLA	2	0
19	e	308	CLA	1	0
19	l	203	CLA	1	0
28	c	305	CHL	4	0
19	B	833	CLA	2	0
25	c	320	LMG	6	0
19	b	302	CLA	1	0
19	B	848	CLA	1	0
19	D	301	CLA	1	0
19	A	809	CLA	1	0
28	g	303	CHL	1	0
19	n	201	CLA	1	0
19	d	210	CLA	1	0
19	f	314	CLA	1	0
19	d	209	CLA	1	0
19	l	201	CLA	9	0
19	B	814	CLA	1	0
19	A	802	CLA	1	0
22	m	313	DD6	1	0
19	A	804	CLA	1	0
19	f	302	CLA	1	0
19	m	303	CLA	1	0
19	F	204	CLA	1	0
28	i	304	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	829	CLA	1	0
19	A	853	CLA	3	0
19	g	301	CLA	1	0
23	B	831	BCR	1	0
22	i	314	DD6	1	0
19	B	837	CLA	2	0
23	B	850	BCR	2	0
28	a	311	CHL	1	0
19	B	849	CLA	2	0
22	J	802	DD6	1	0
19	a	306	CLA	5	0
19	B	841	CLA	1	0
19	n	202	CLA	3	0
19	j	308	CLA	1	0
19	B	832	CLA	1	0
19	o	310	CLA	2	0
19	A	808	CLA	1	0
25	f	313	LMG	1	0
28	k	301	CHL	3	0
19	j	305	CLA	3	0
19	m	305	CLA	1	0
25	a	316	LMG	1	0
22	g	315	DD6	1	0
28	b	301	CHL	2	0
19	e	310	CLA	3	0
19	l	202	CLA	1	0
28	e	304	CHL	12	0
19	A	841	CLA	1	0
22	l	210	DD6	5	0
19	k	302	CLA	2	0
19	j	307	CLA	1	0
25	h	216	LMG	2	0
28	a	312	CHL	6	0
19	j	310	CLA	1	0
19	j	306	CLA	12	0
19	J	803	CLA	1	0
28	b	311	CHL	1	0
19	B	801	CLA	2	0
19	f	303	CLA	1	0
22	o	313	DD6	6	0
19	o	307	CLA	1	0
19	o	302	CLA	3	0

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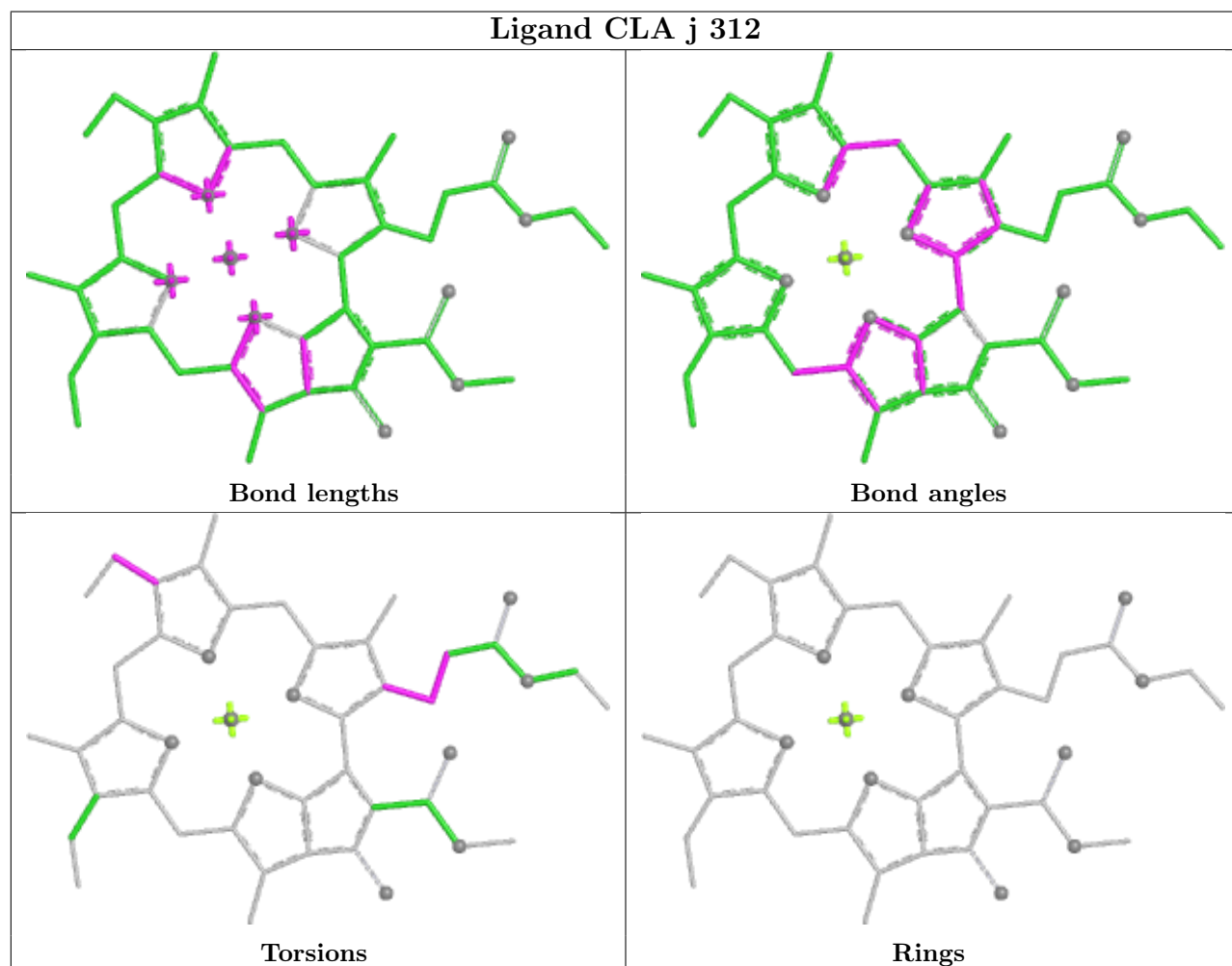
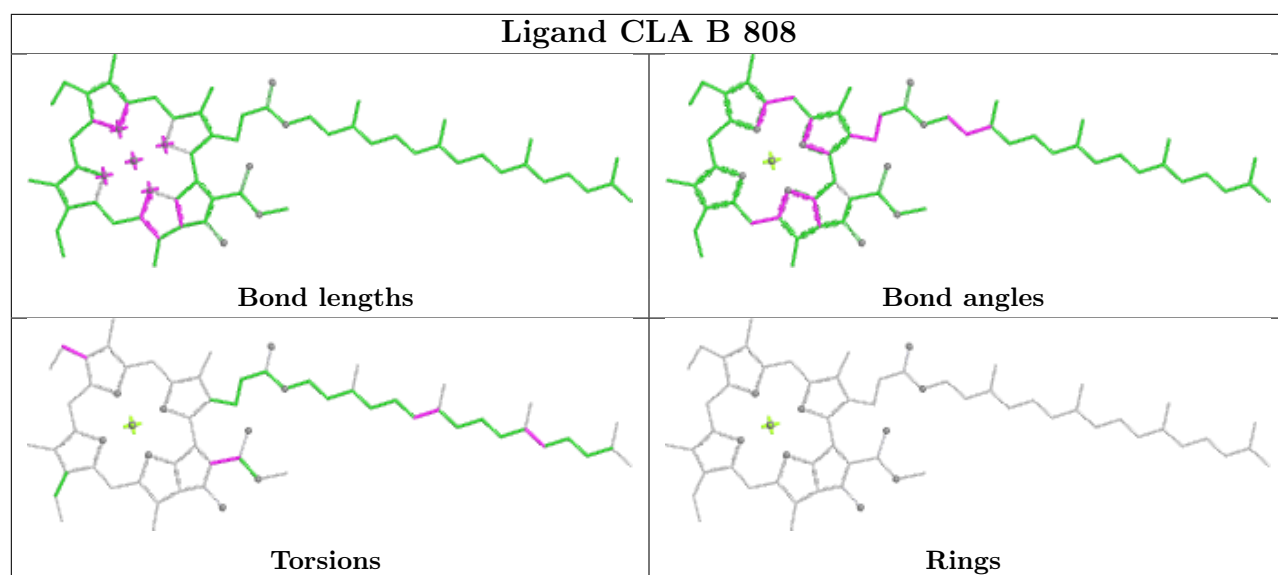
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	845	CLA	1	0
25	g	312	LMG	1	0
19	n	205	CLA	2	0
27	B	829	DGD	2	0
19	B	807	CLA	1	0
28	g	306	CHL	1	0
19	c	303	CLA	1	0
19	B	823	CLA	1	0
19	d	208	CLA	3	0
24	A	838	LMU	1	0
19	A	842	CLA	2	0
19	B	844	CLA	1	0
19	b	315	CLA	1	0
28	g	310	CHL	6	0
25	a	318	LMG	2	0
28	i	301	CHL	1	0
19	B	838	CLA	2	0
28	b	312	CHL	4	0
19	j	304	CLA	2	0
19	o	303	CLA	8	0
23	A	835	BCR	1	0
19	k	305	CLA	1	0
19	b	305	CLA	3	0
25	b	316	LMG	2	0
19	B	803	CLA	1	0
19	g	304	CLA	1	0
19	k	304	CLA	1	0
28	o	301	CHL	2	0
28	h	202	CHL	2	0
23	A	837	BCR	1	0
24	c	301	LMU	3	0
28	d	202	CHL	2	0
19	A	819	CLA	1	0
19	i	309	CLA	1	0
28	c	313	CHL	3	0
19	A	845	CLA	1	0
19	o	309	CLA	1	0
19	B	840	CLA	1	0
19	j	313	CLA	1	0
22	e	313	DD6	10	0
22	g	314	DD6	4	0
19	d	203	CLA	1	0

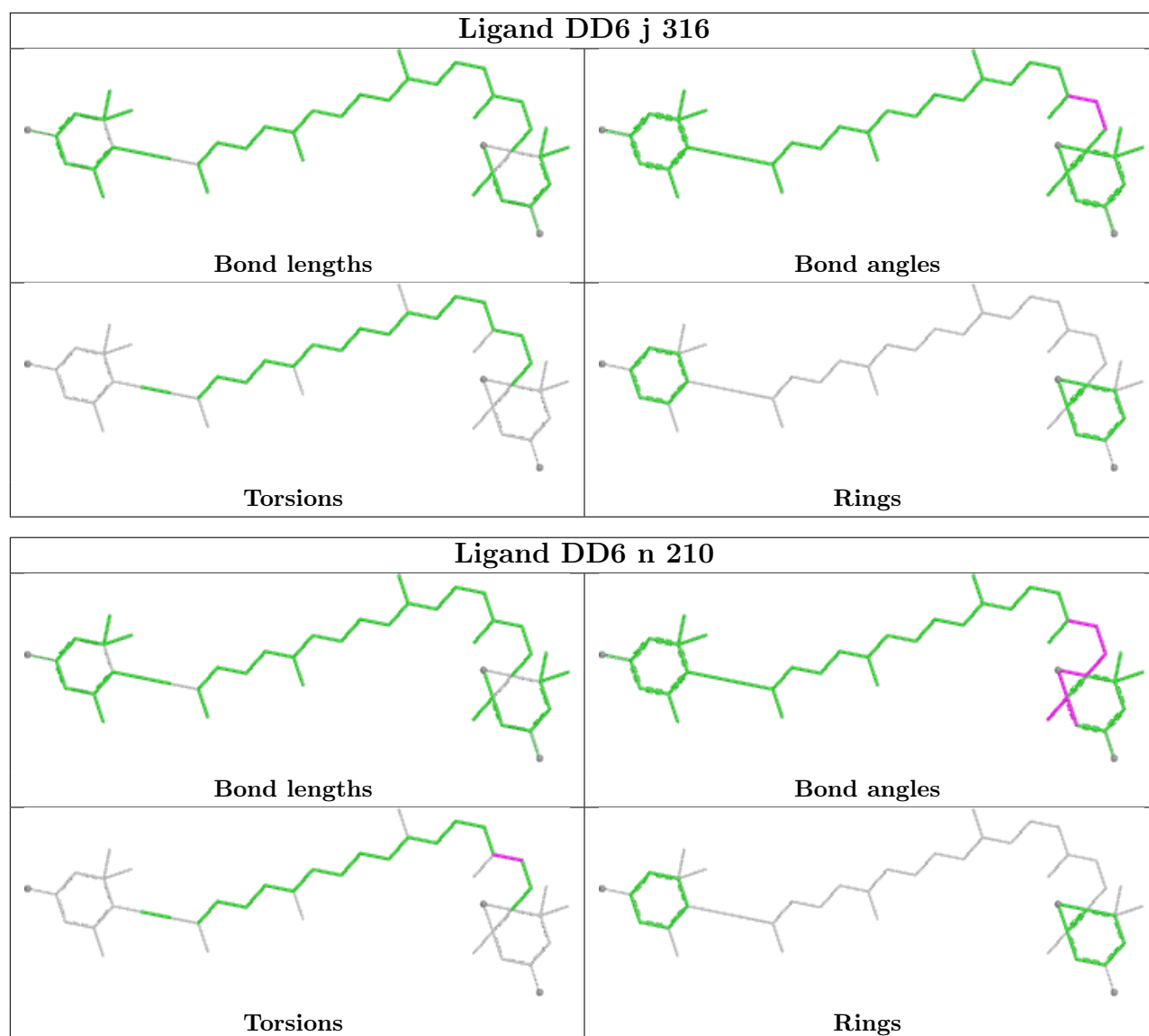
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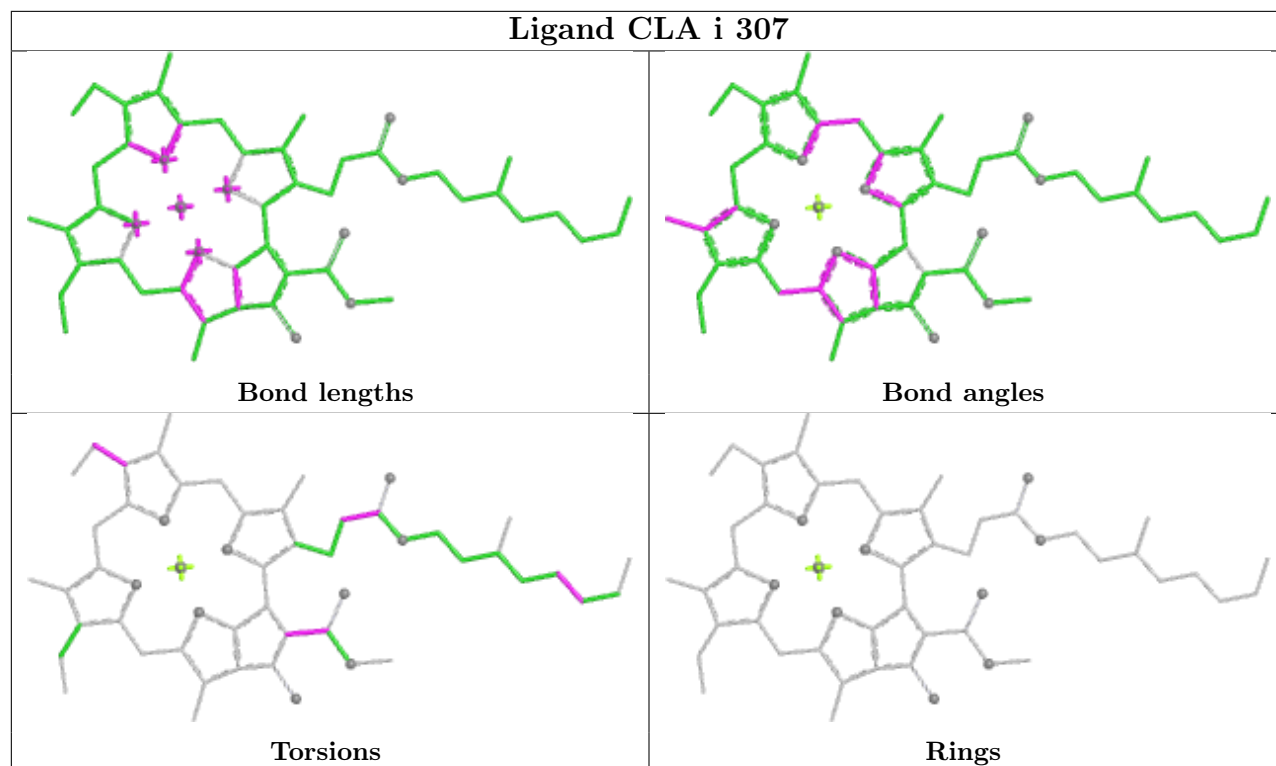
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	d	205	CHL	3	0
22	c	318	DD6	2	0
23	J	804	BCR	6	0
19	n	206	CLA	13	0
23	M	801	BCR	7	0
19	B	812	CLA	1	0
19	j	302	CLA	1	0
19	n	204	CLA	2	0
25	a	301	LMG	3	0
28	c	312	CHL	5	0
28	f	301	CHL	2	0
19	h	201	CLA	2	0
19	A	803	CLA	1	0
25	i	316	LMG	7	0
19	b	306	CLA	4	0
28	f	304	CHL	3	0
19	b	309	CLA	1	0
19	B	843	CLA	1	0
19	F	201	CLA	1	0

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

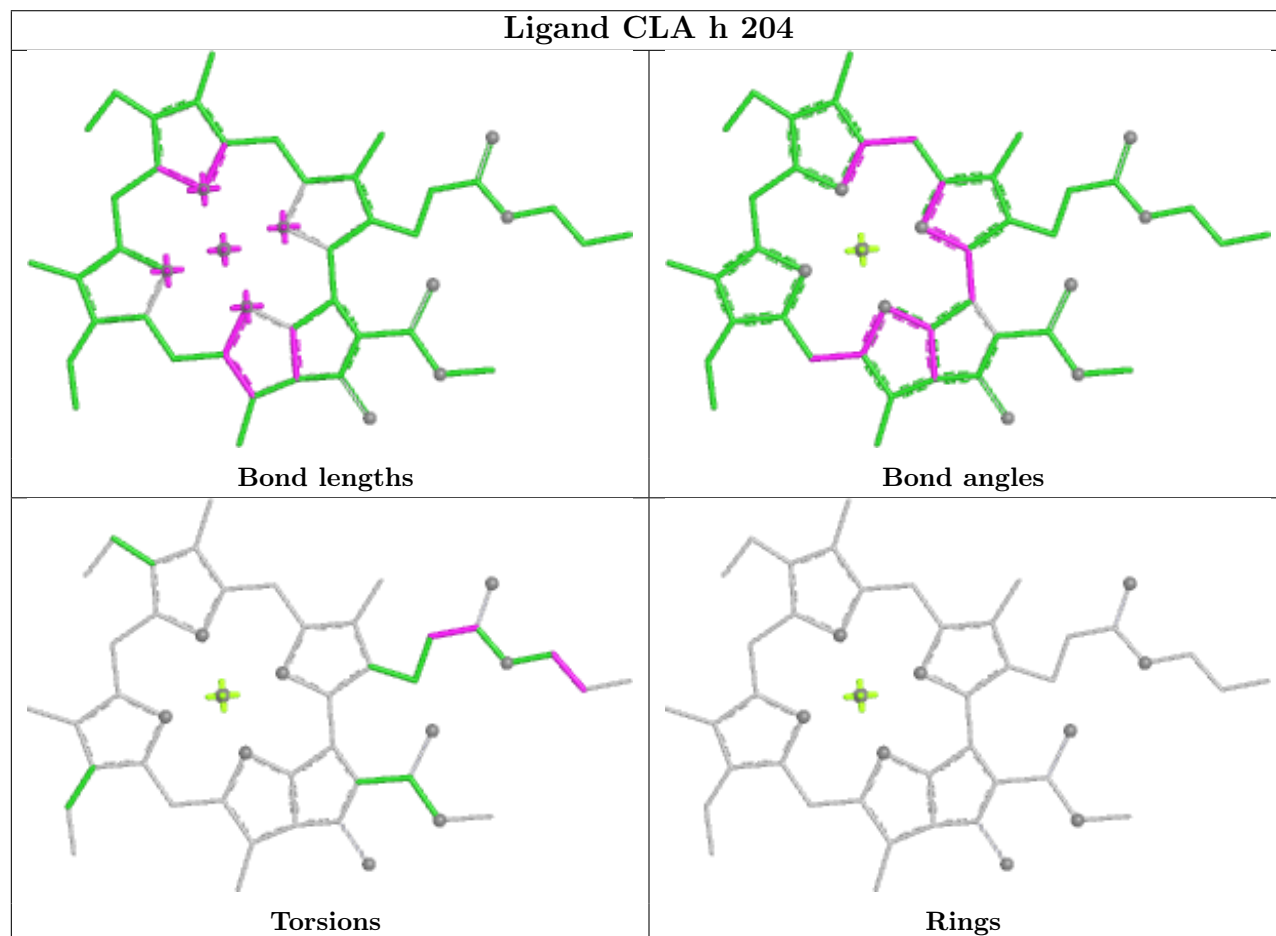


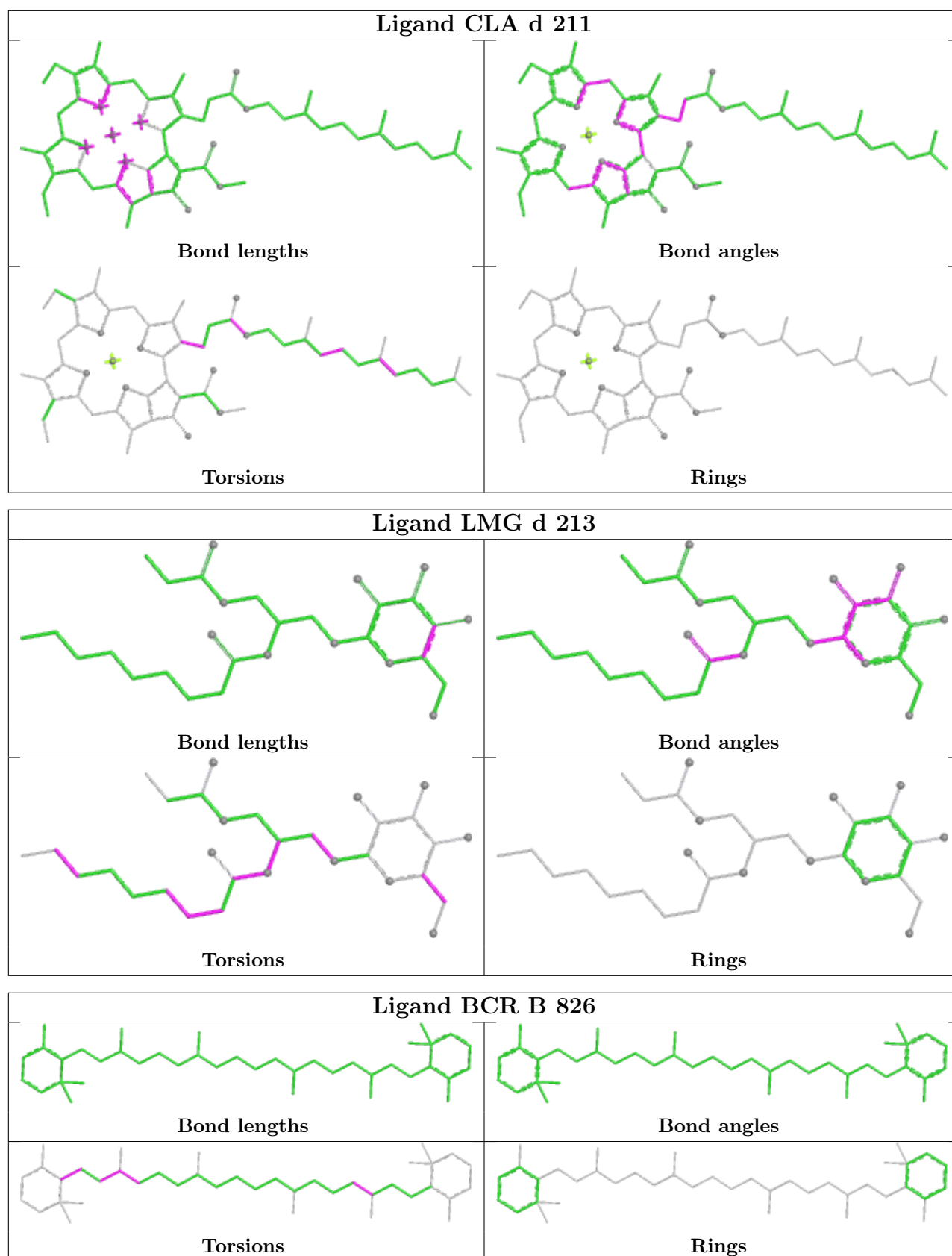


Ligand CLA i 307

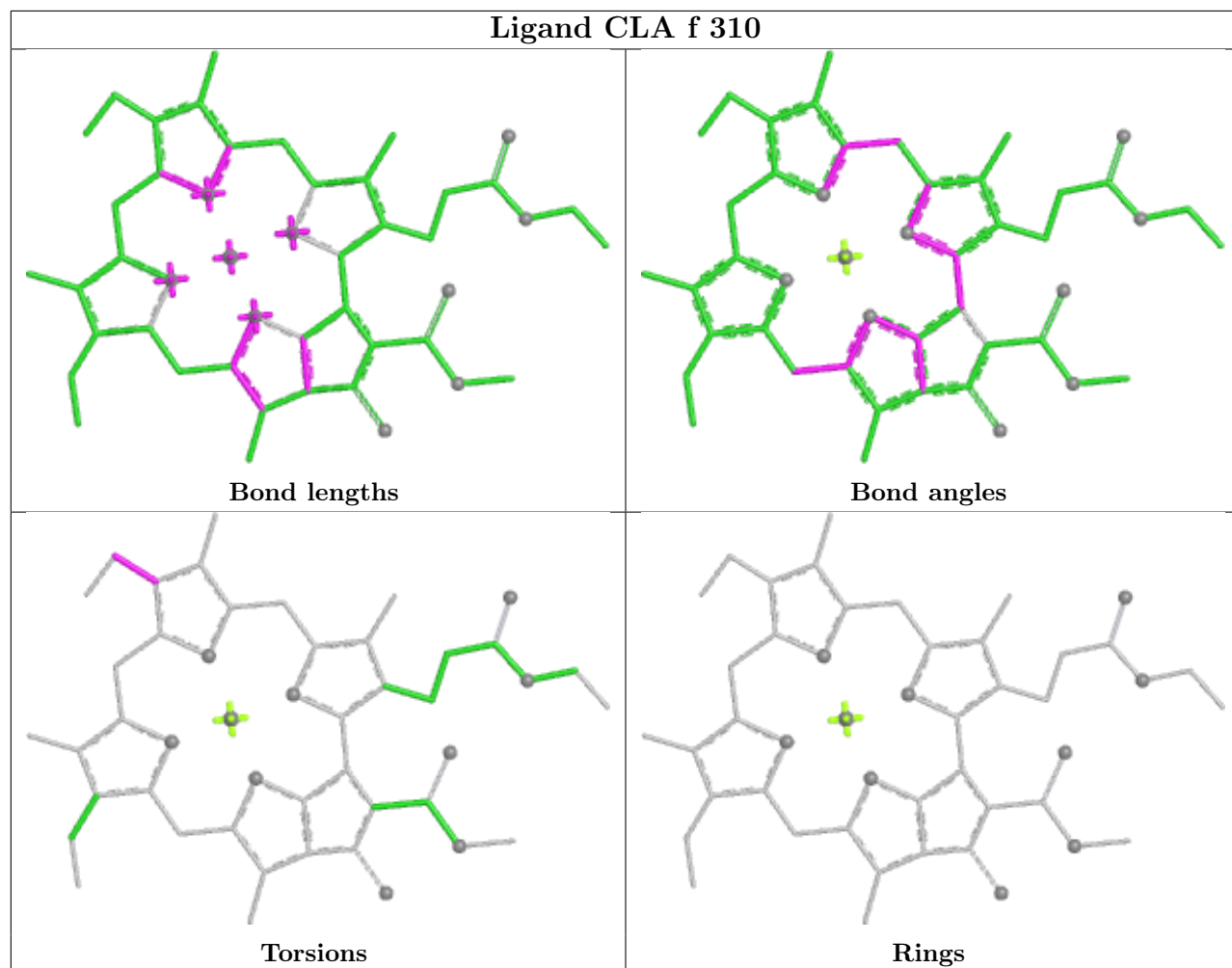


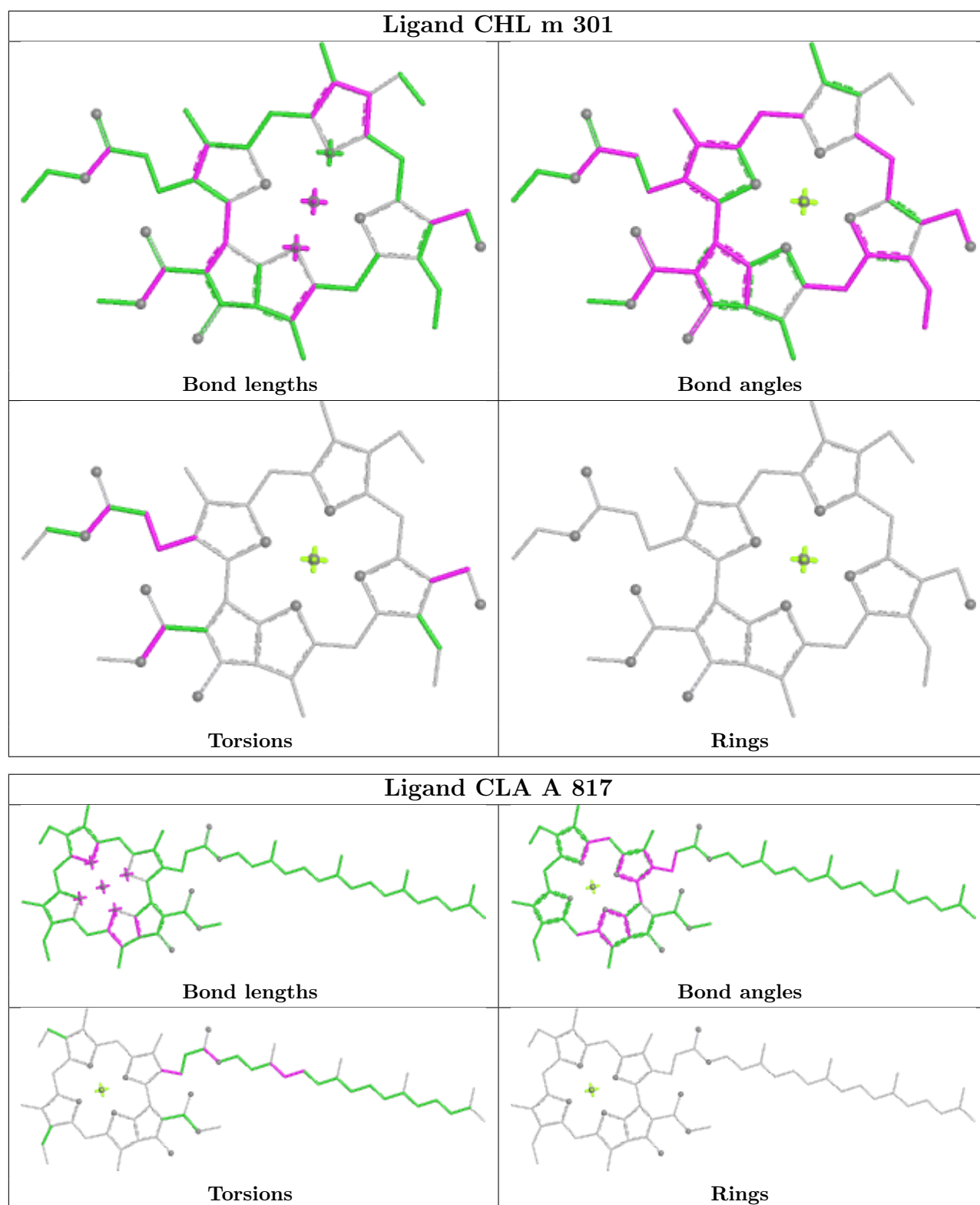
Ligand CLA h 204

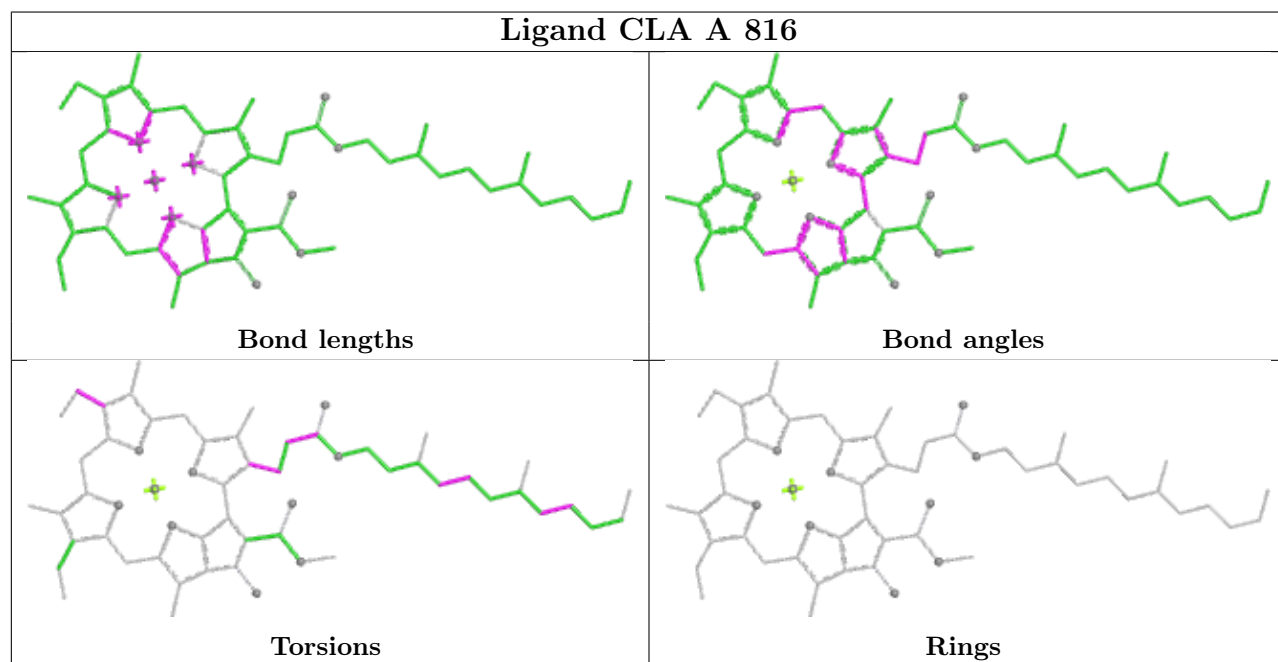
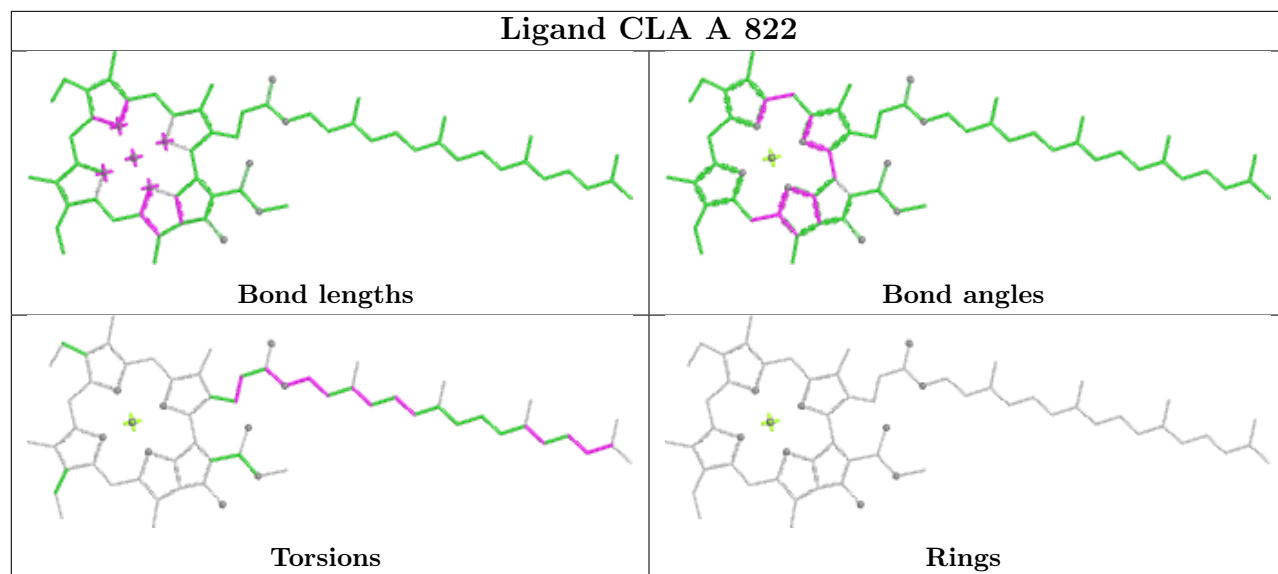




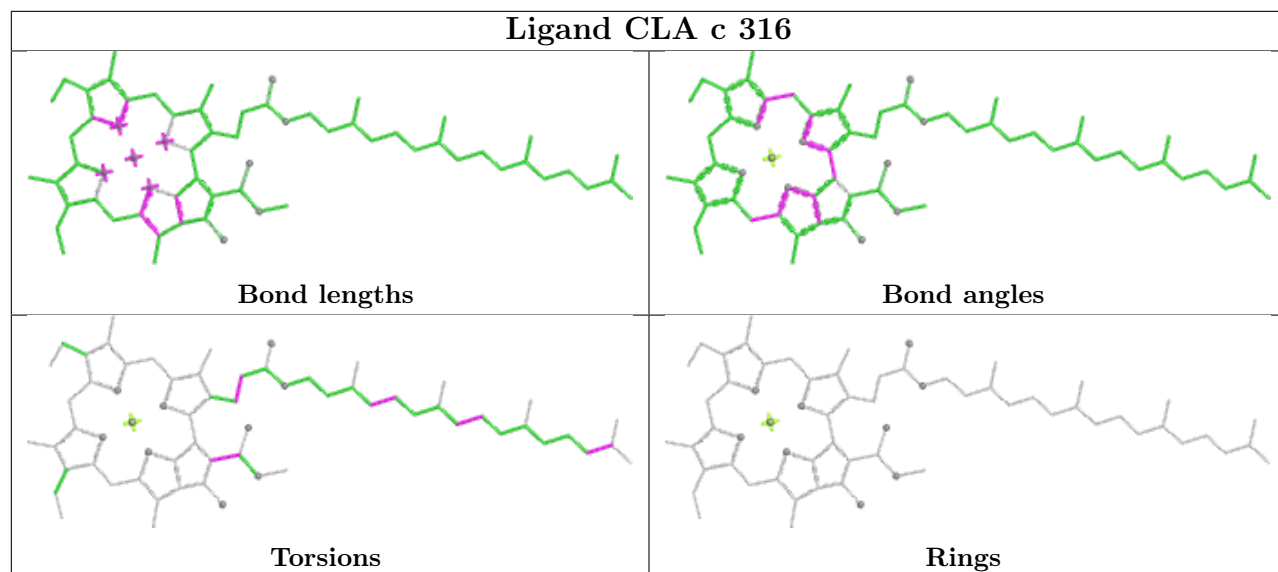
Ligand CLA f 310



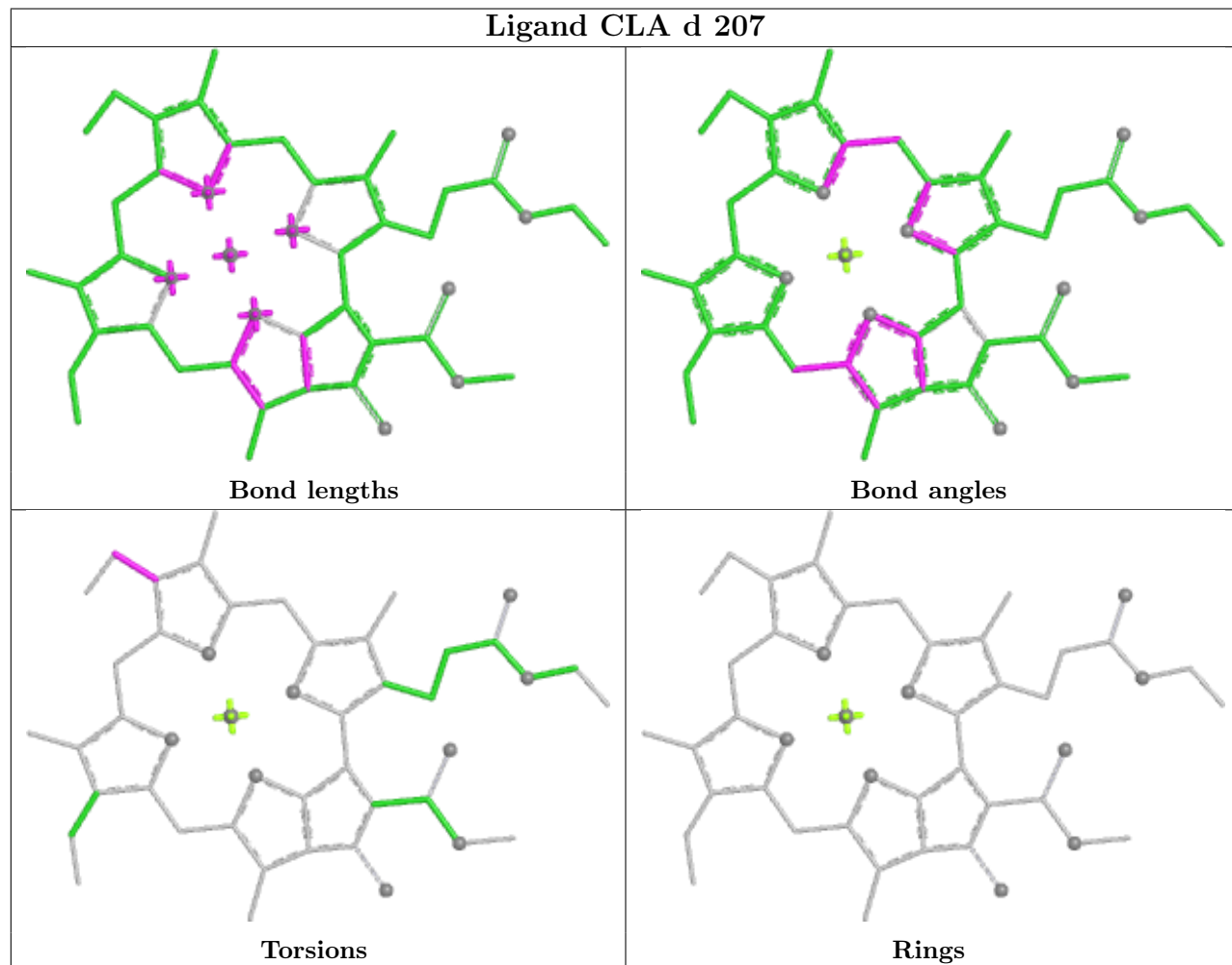


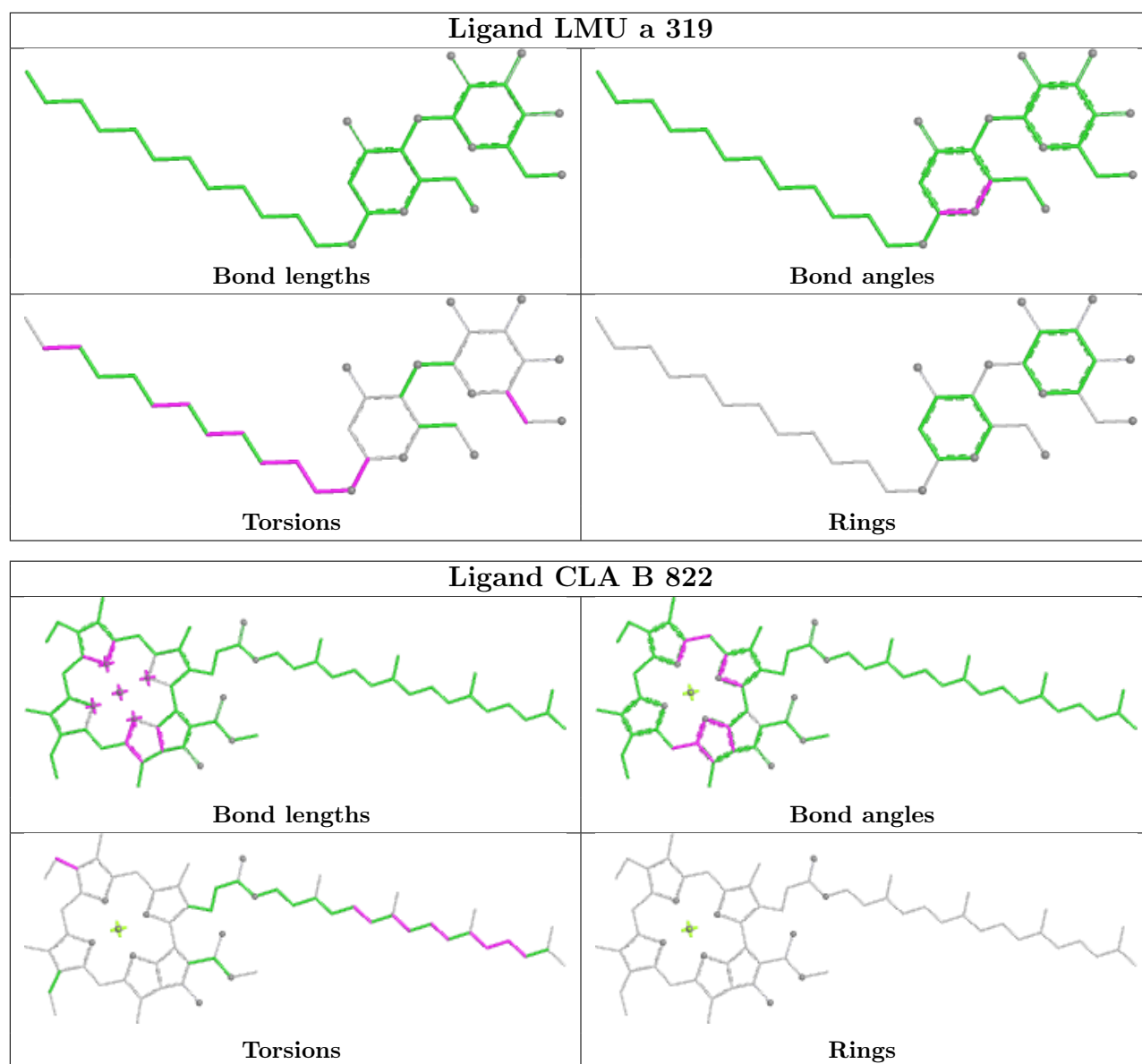


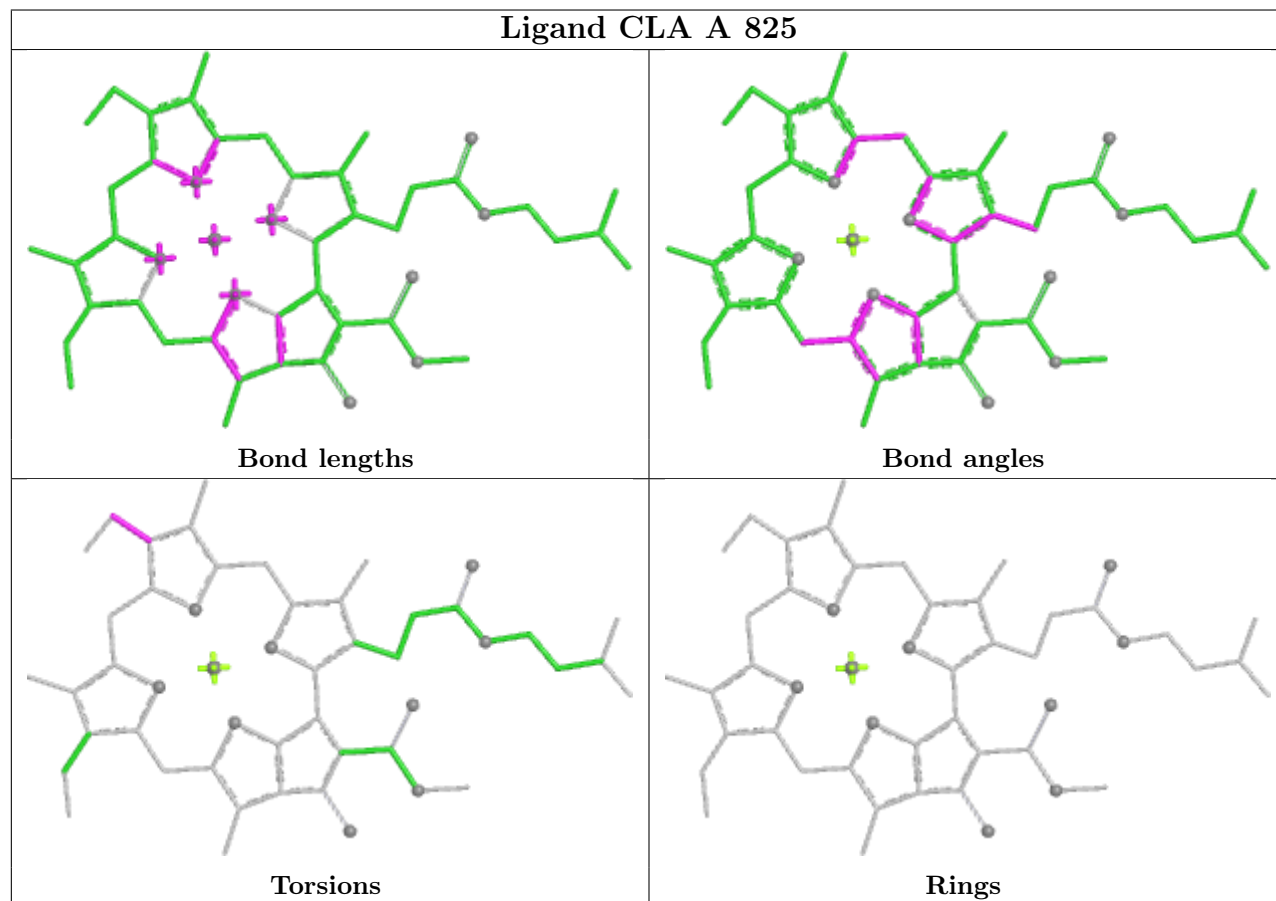
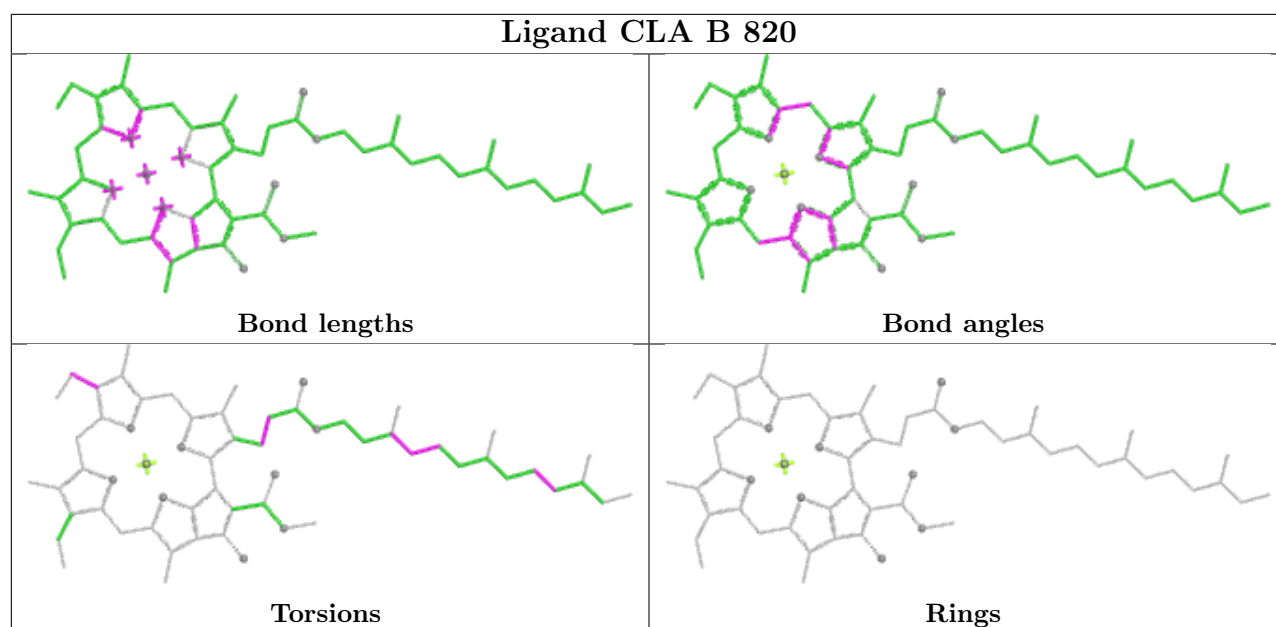
Ligand CLA c 316

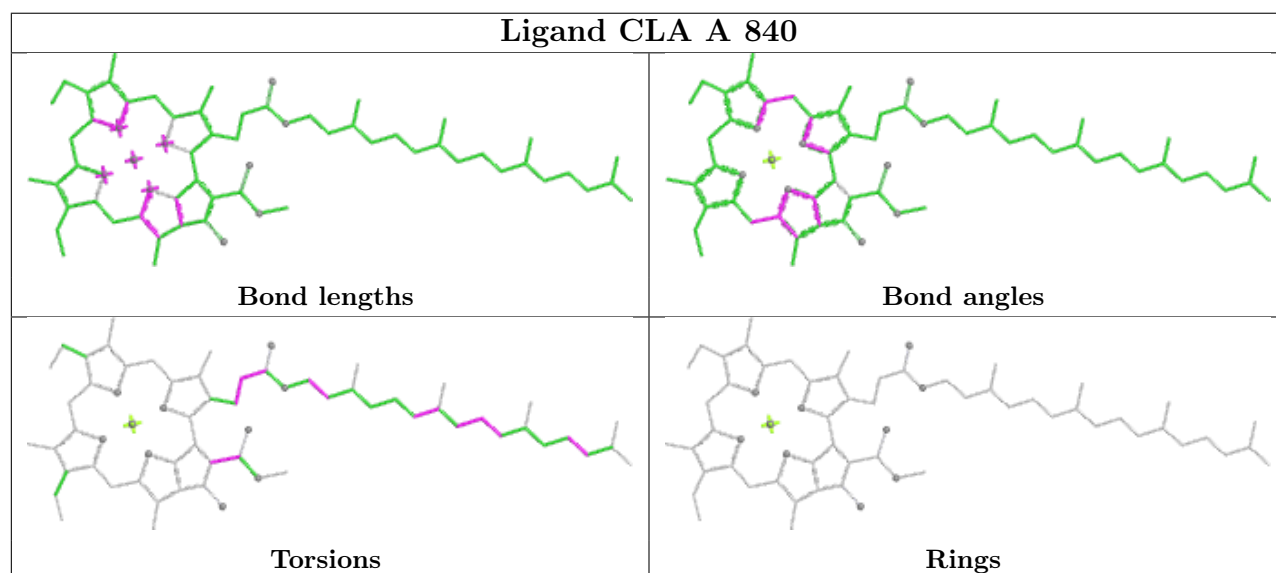
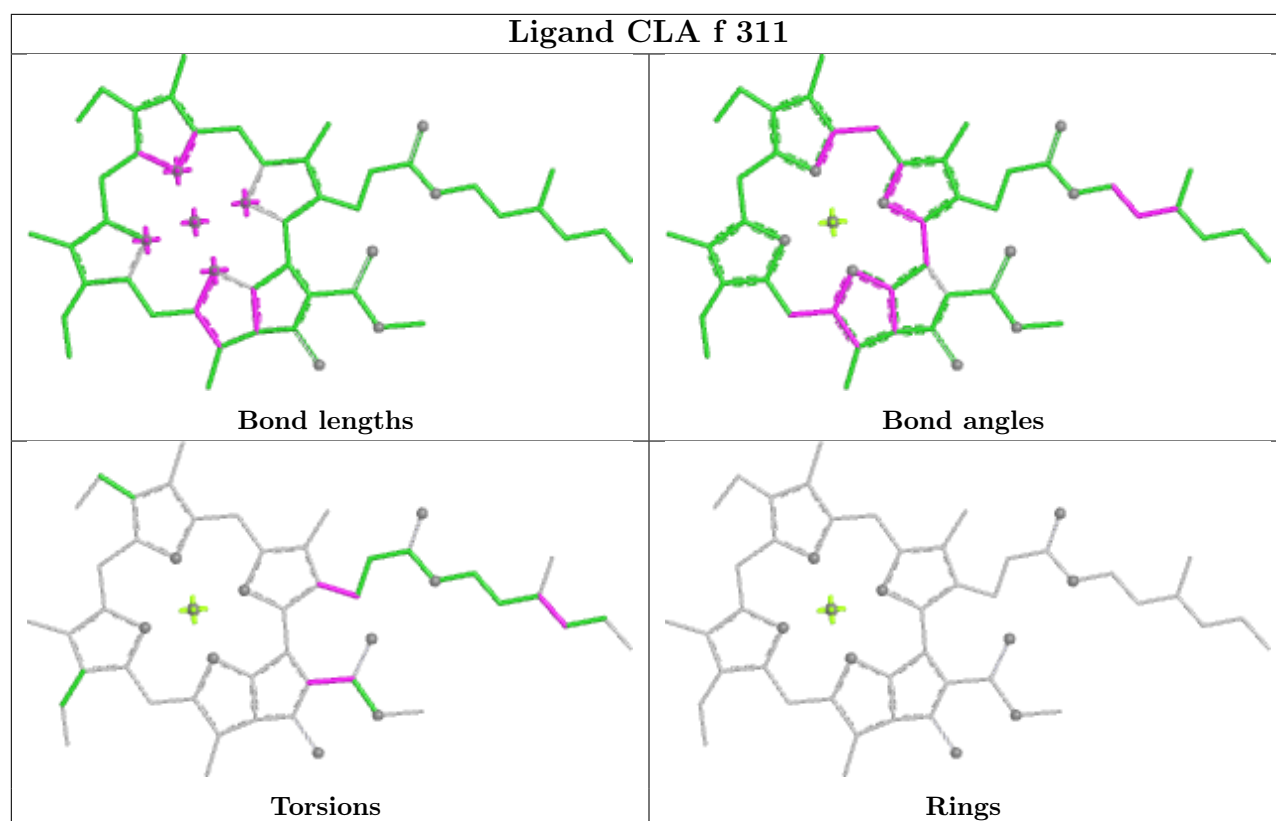


Ligand CLA d 207

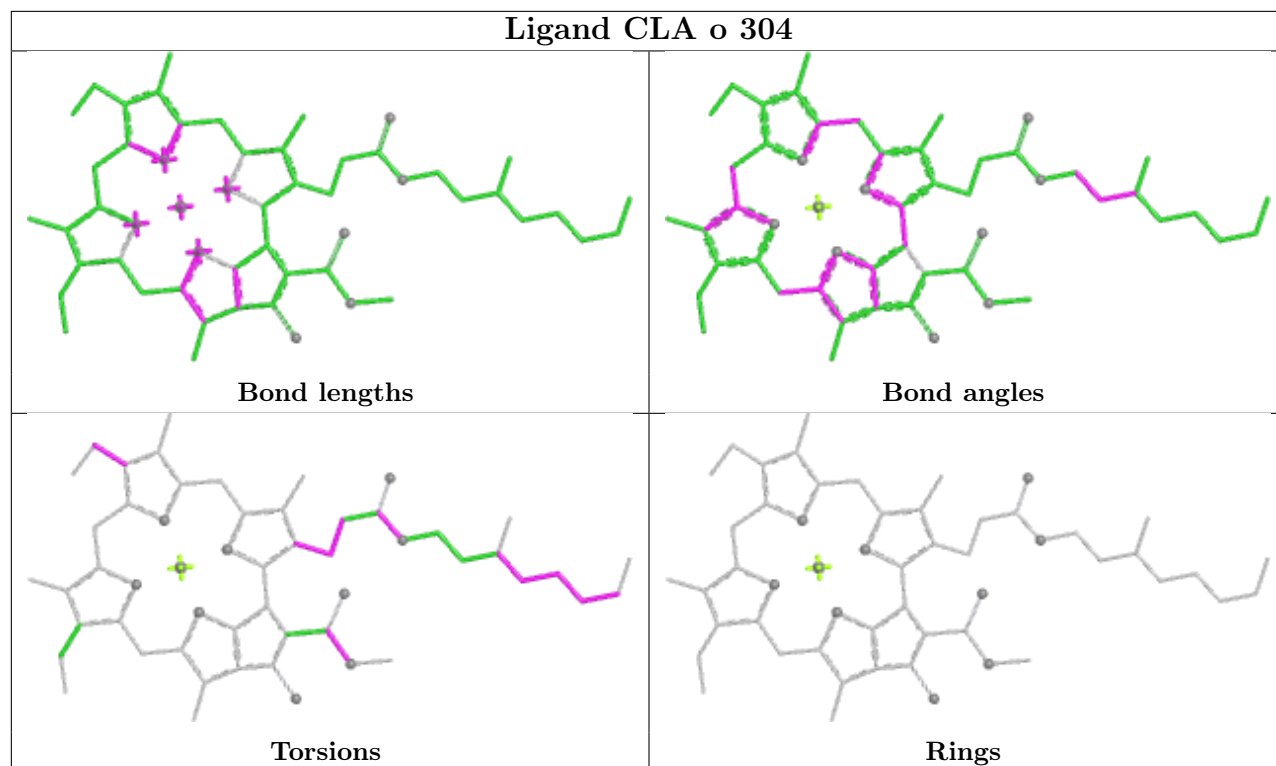




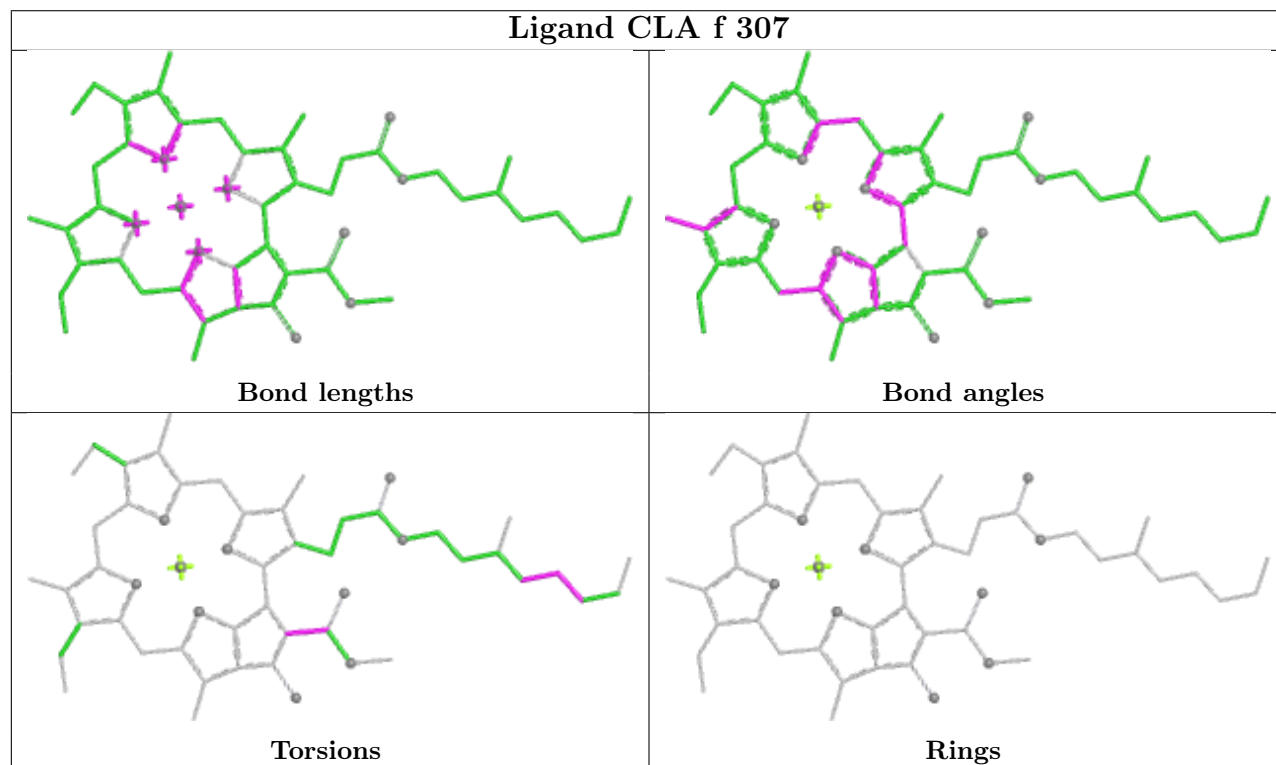


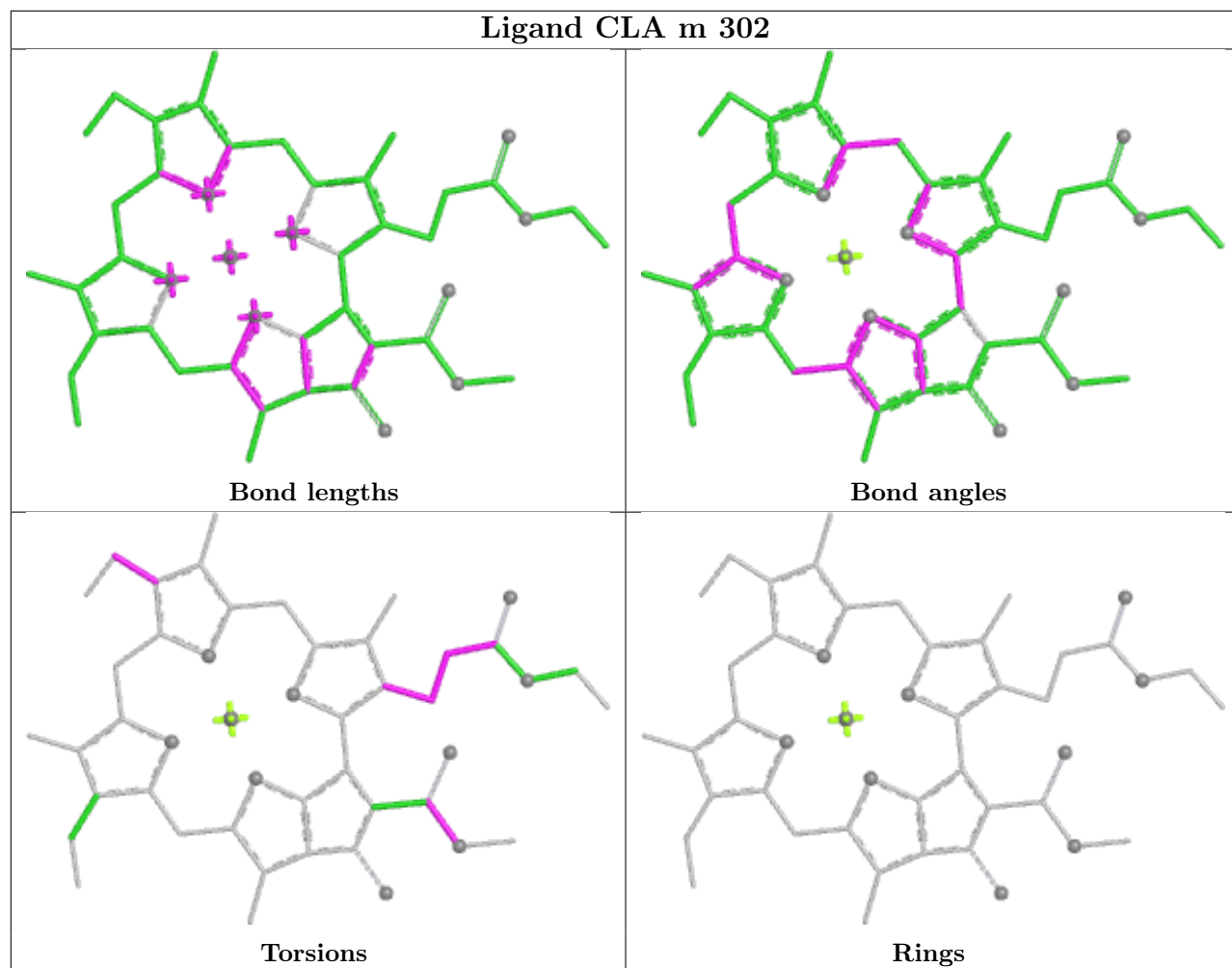


Ligand CLA o 304

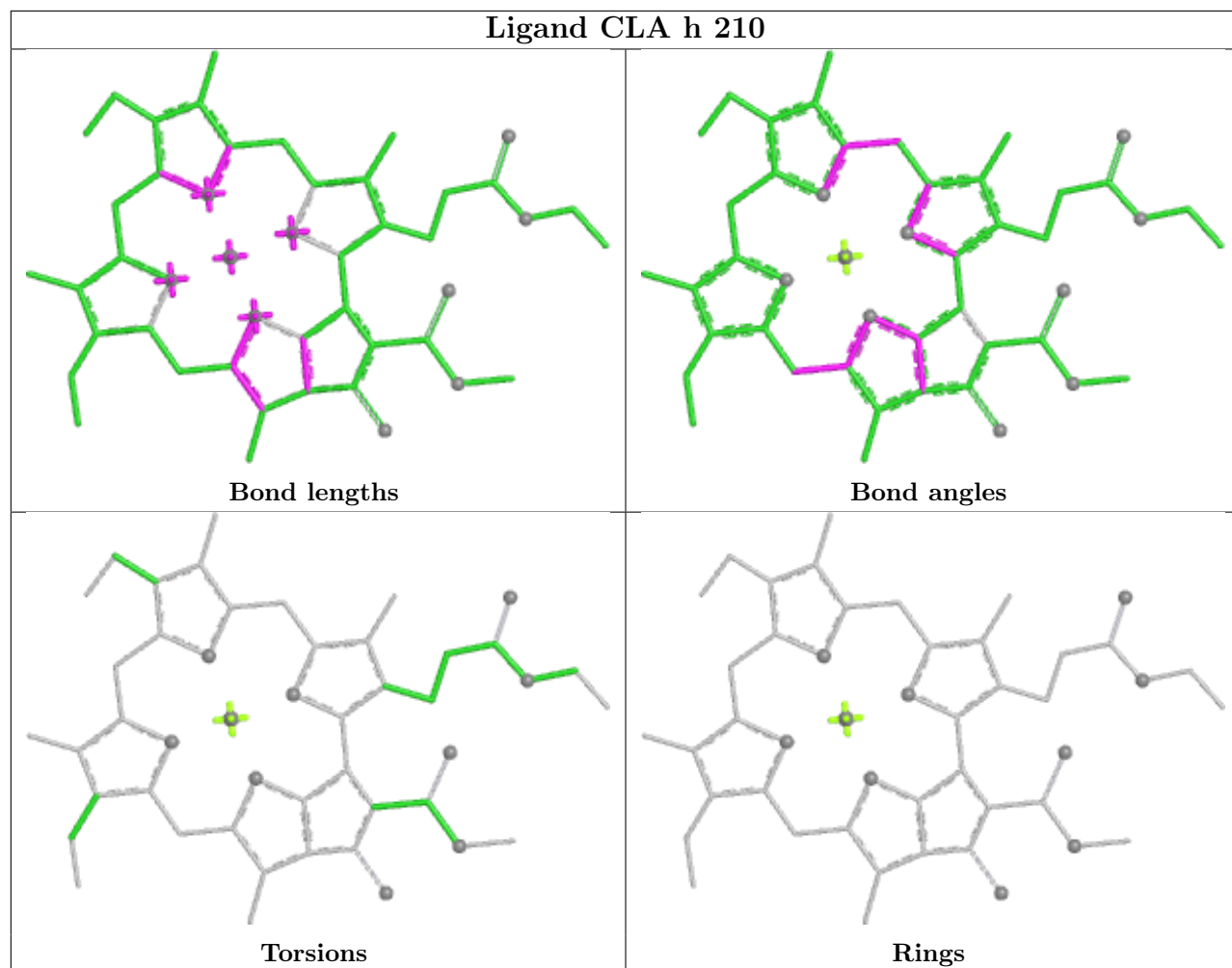


Ligand CLA f 307

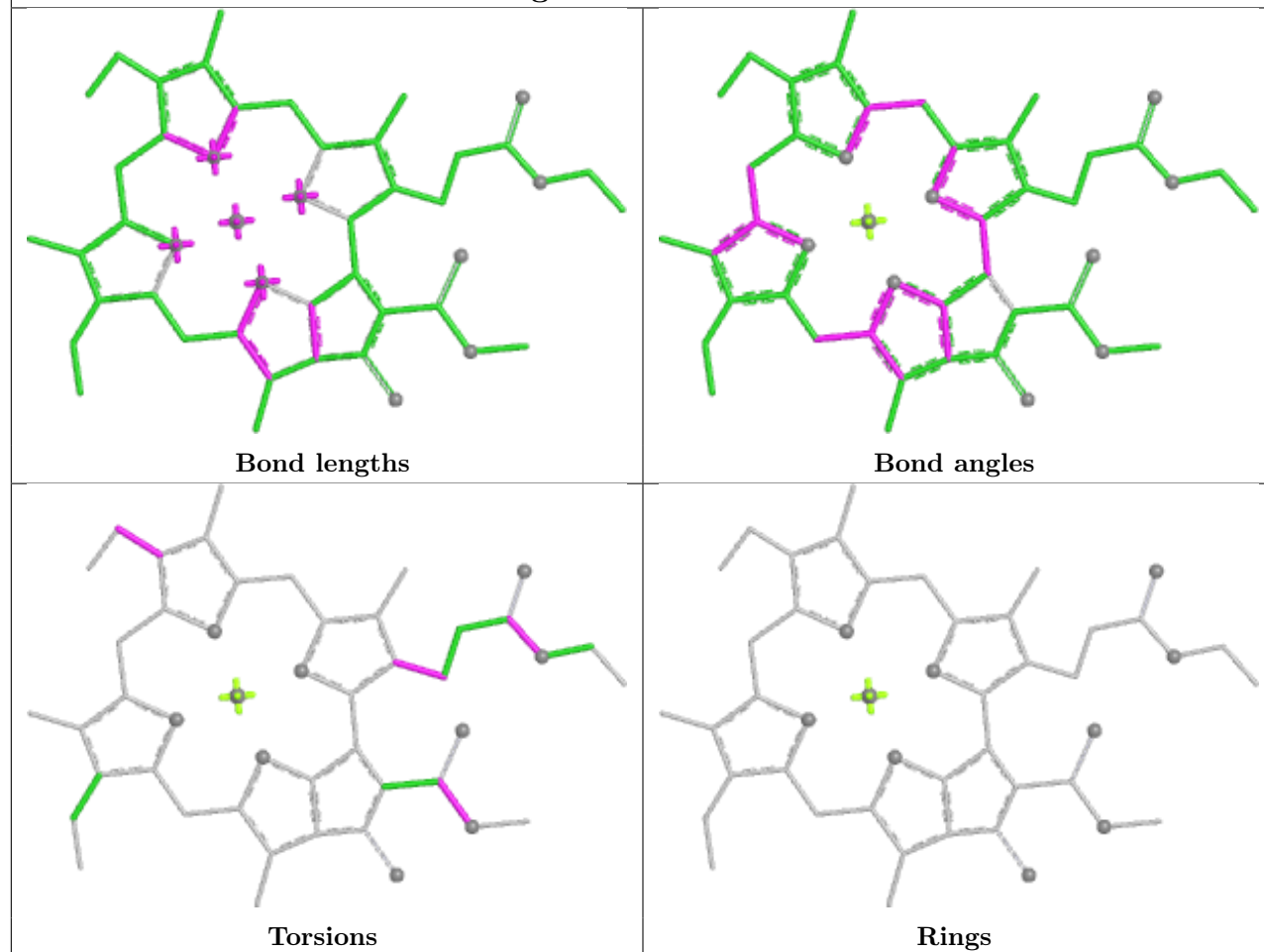




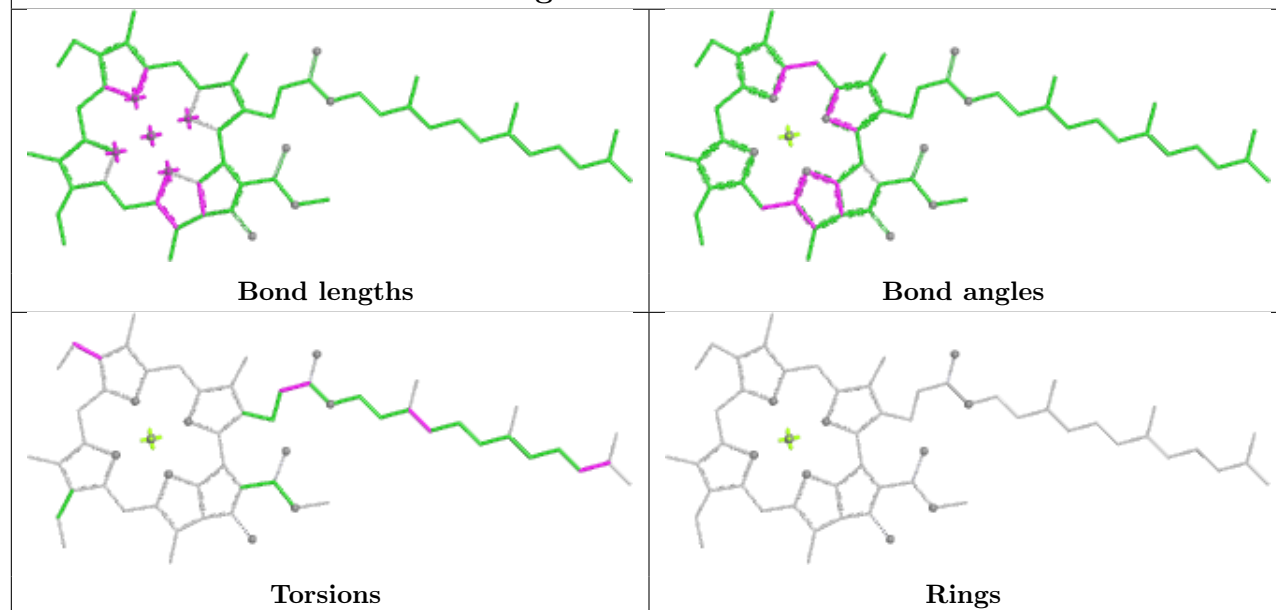
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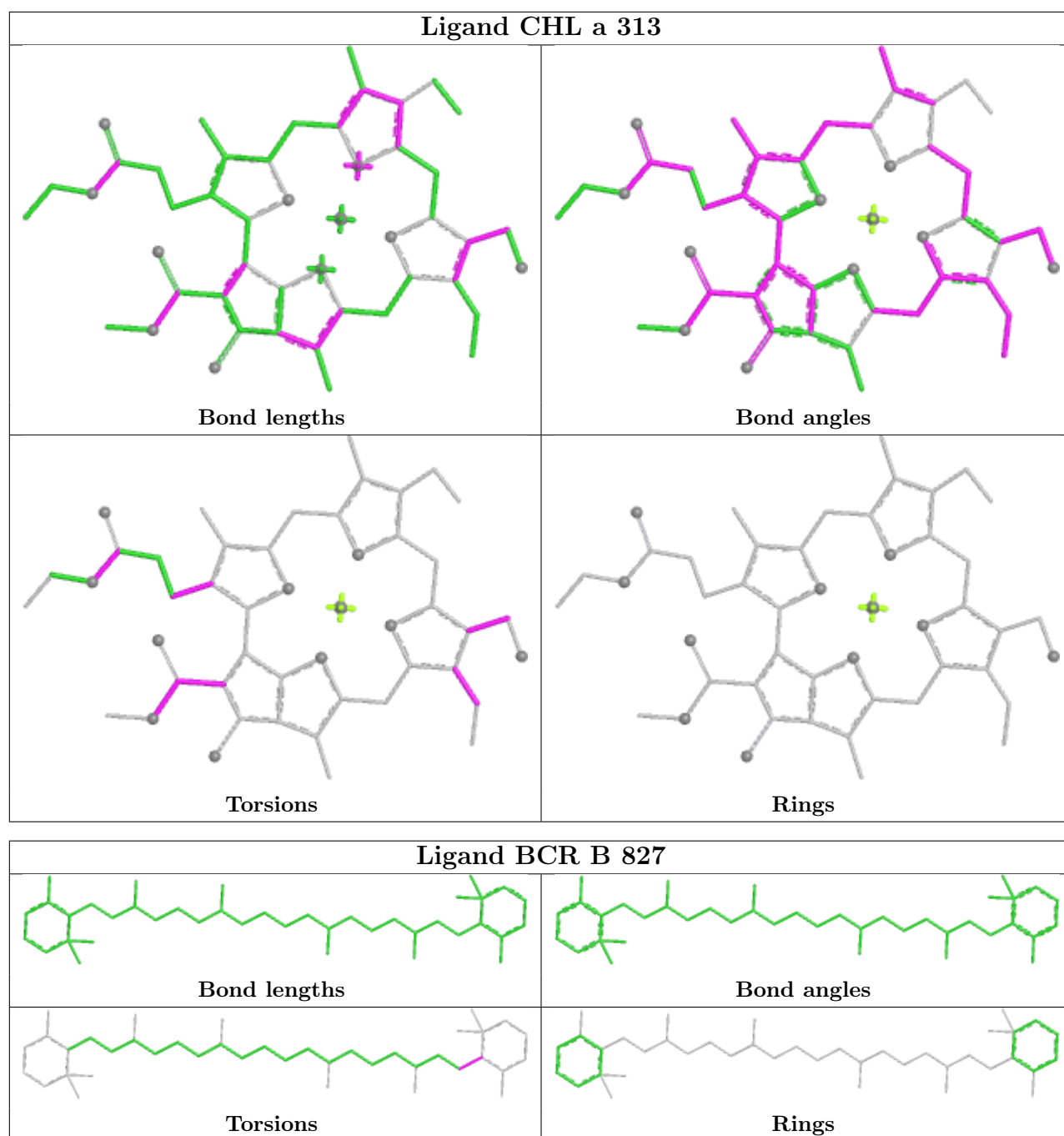


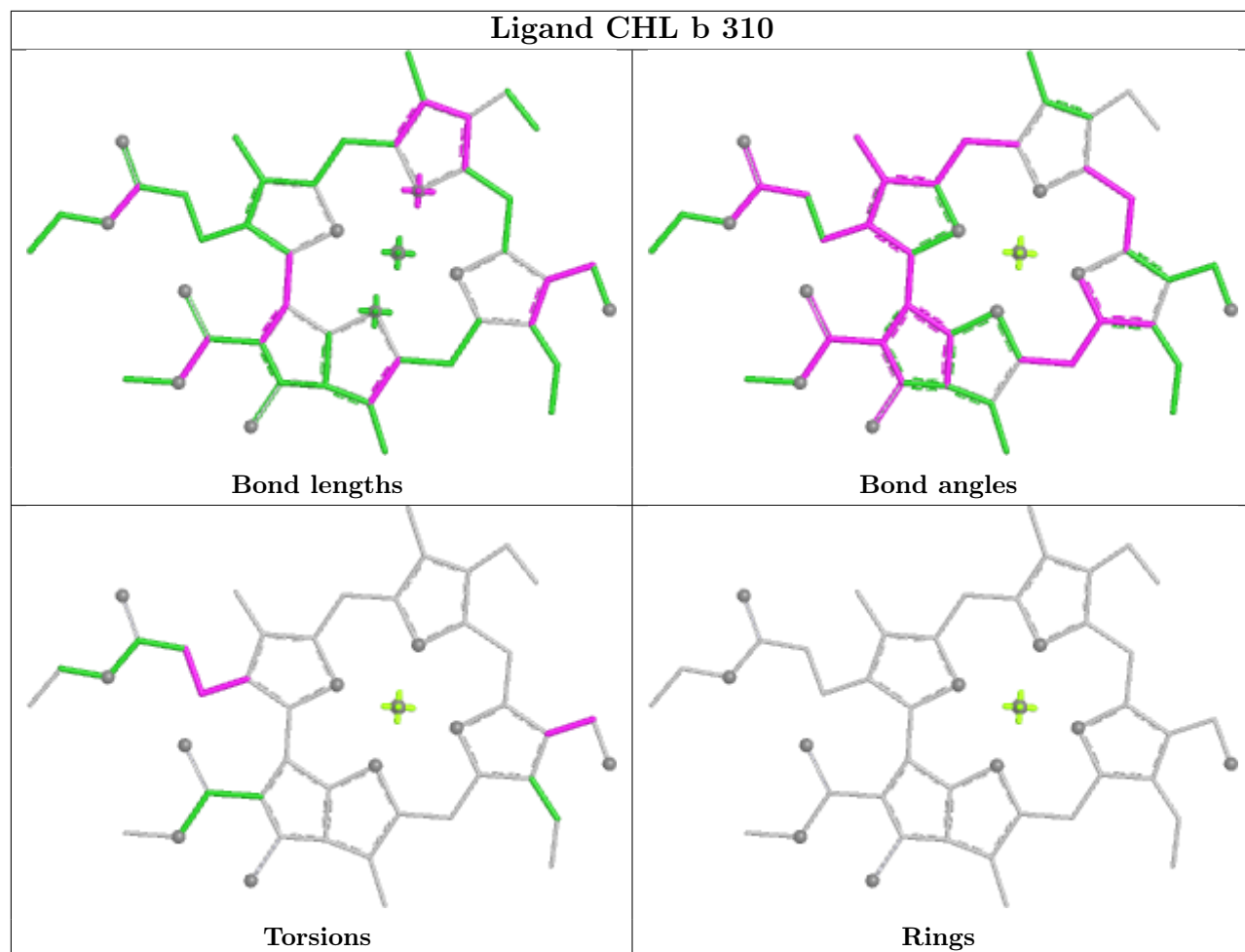
Ligand CLA a 314



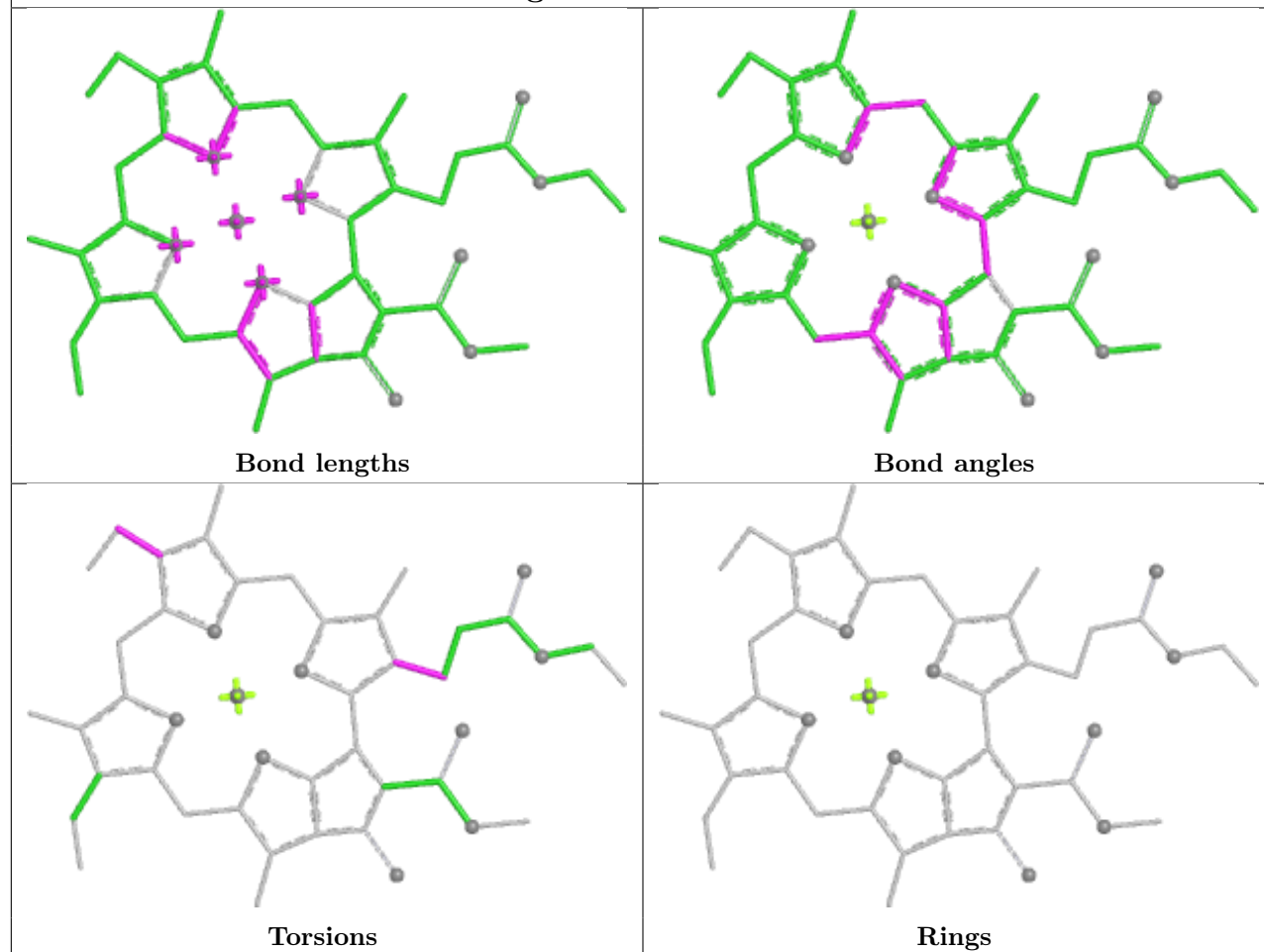
Ligand CLA h 209



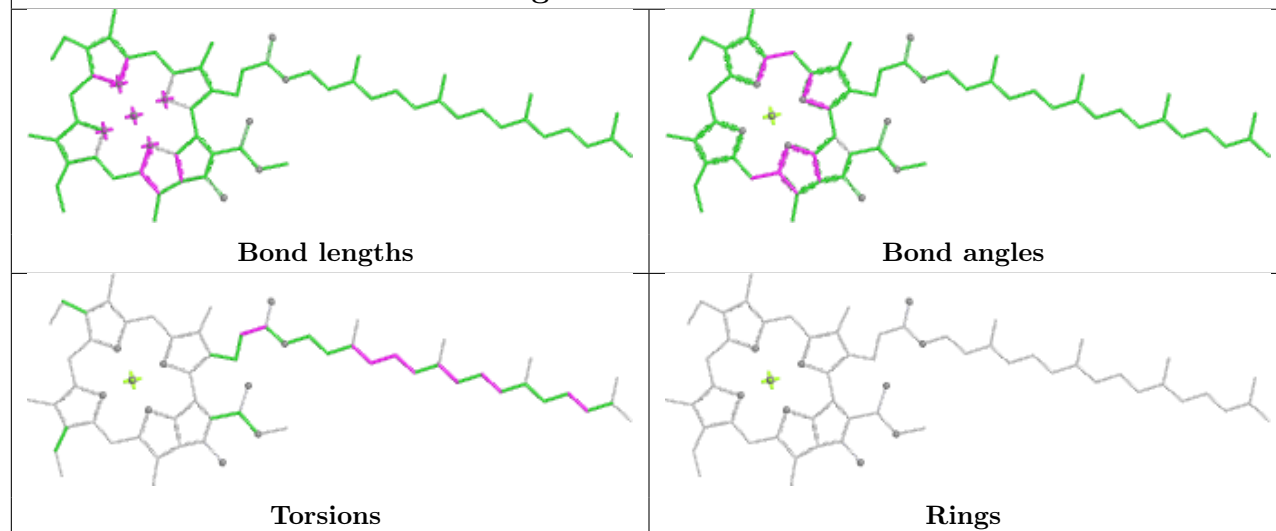


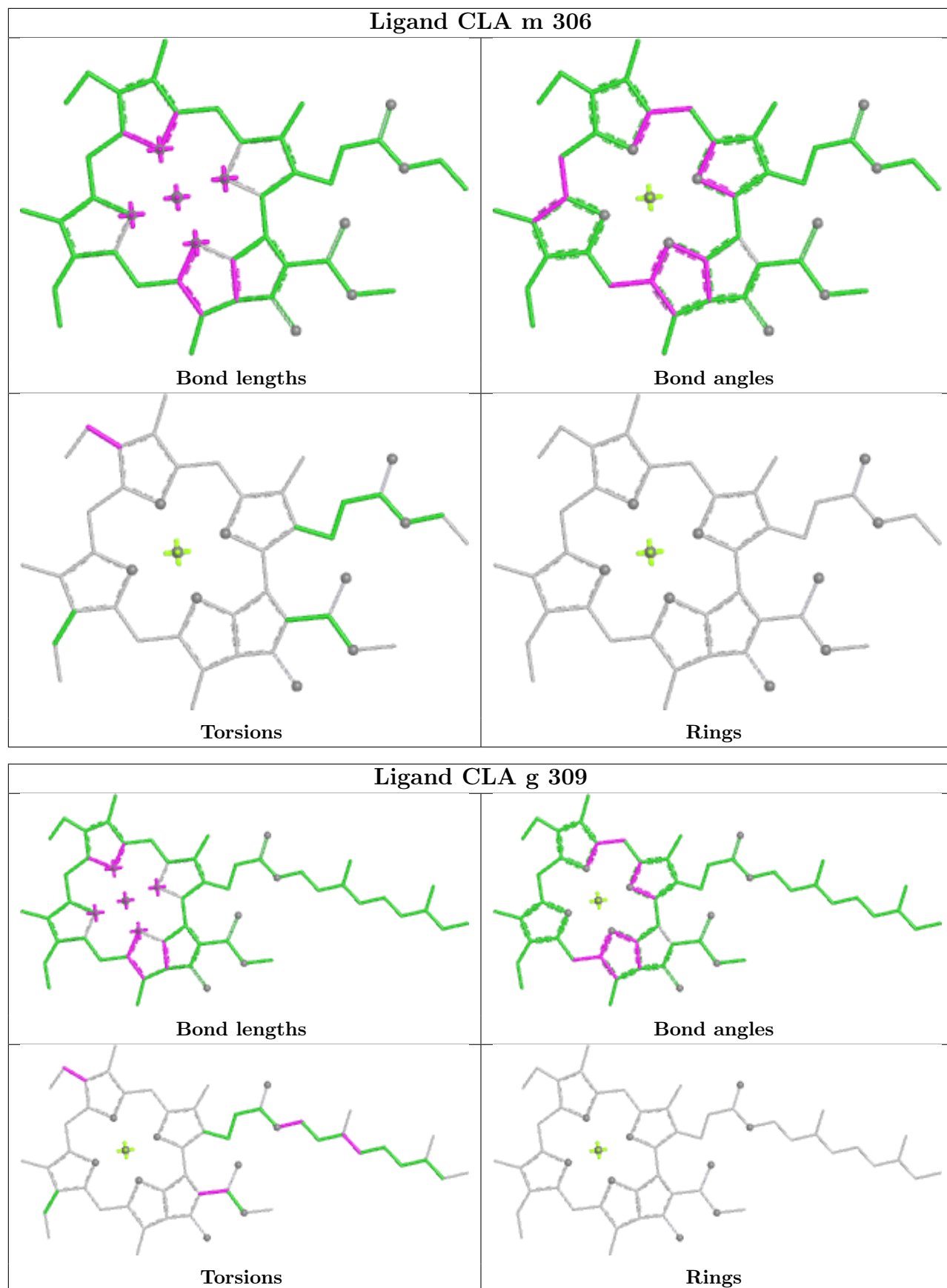


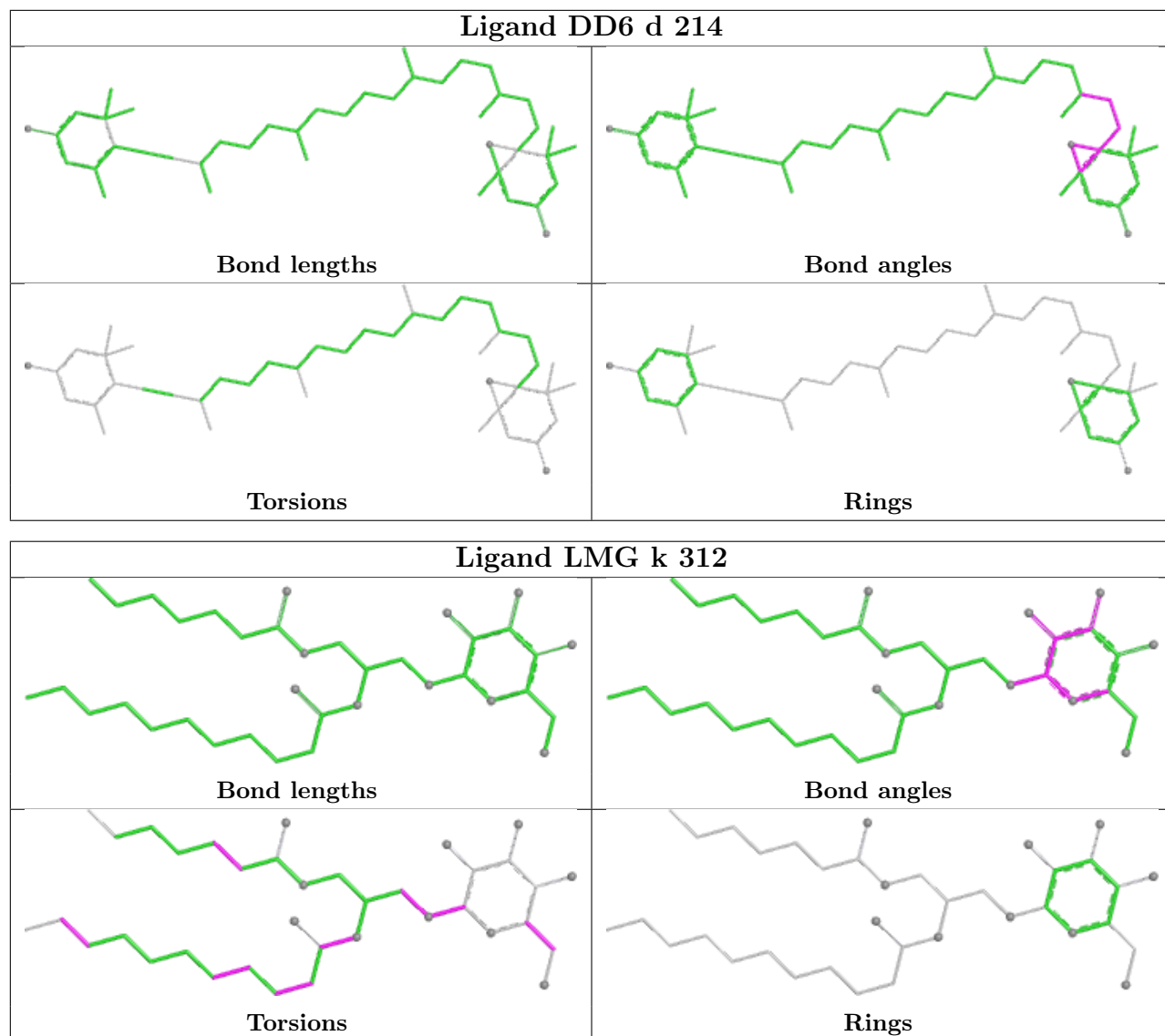
Ligand CLA A 846



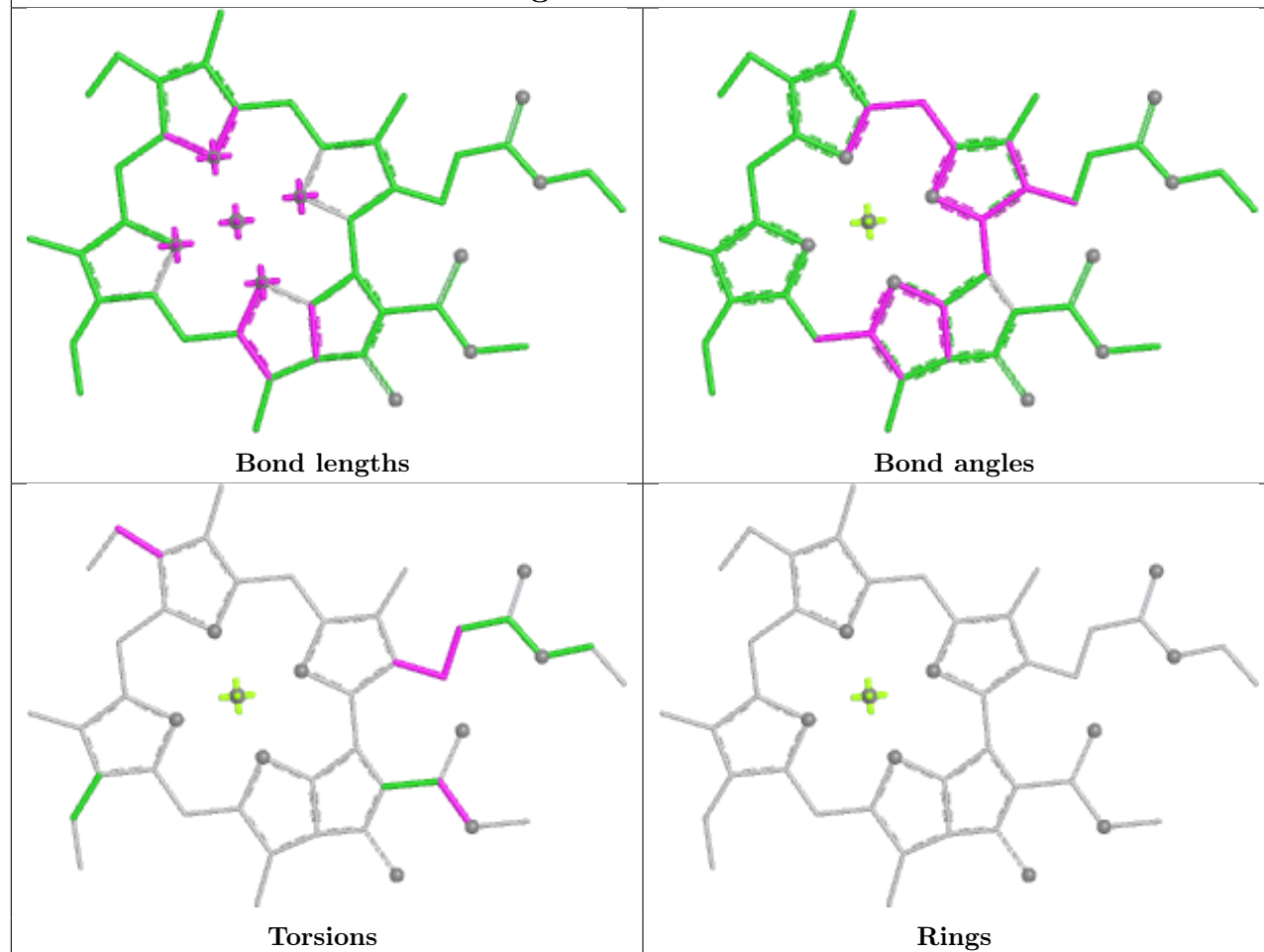
Ligand CLA A 807



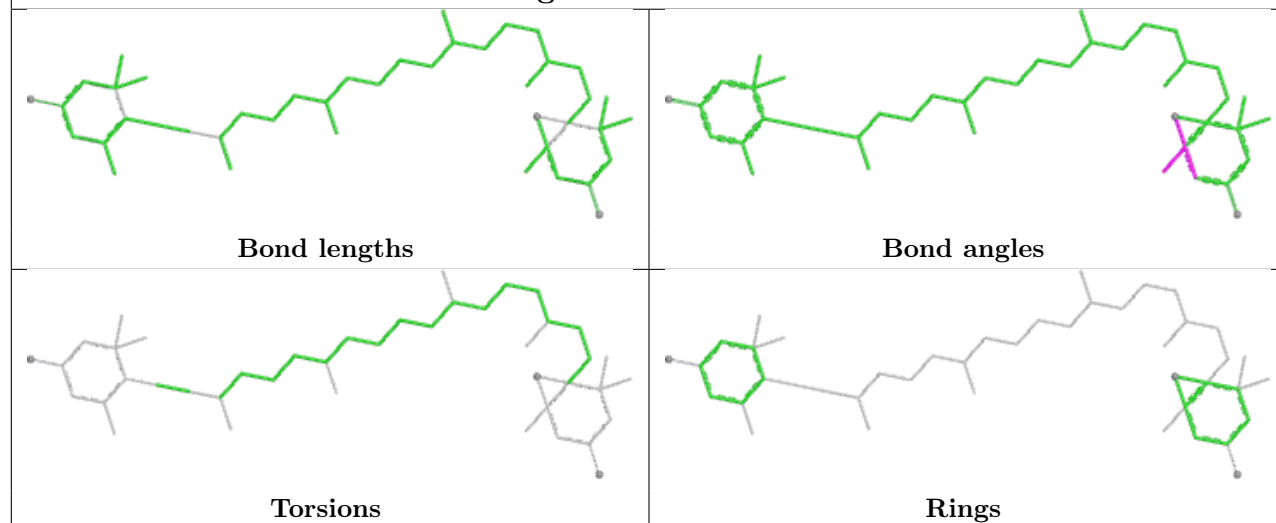


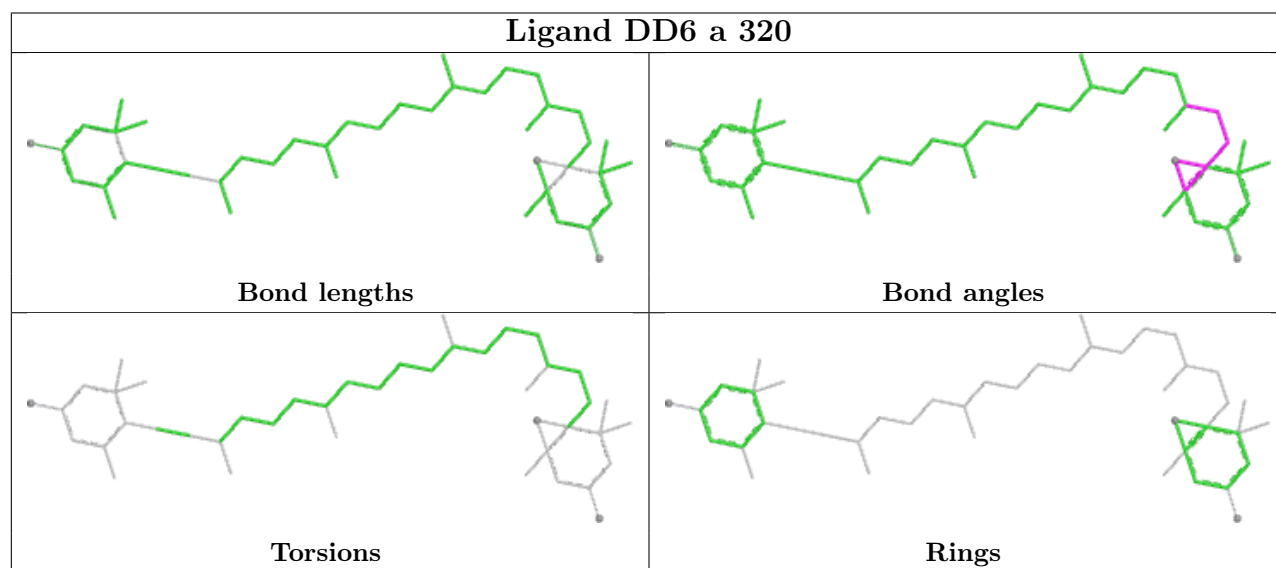
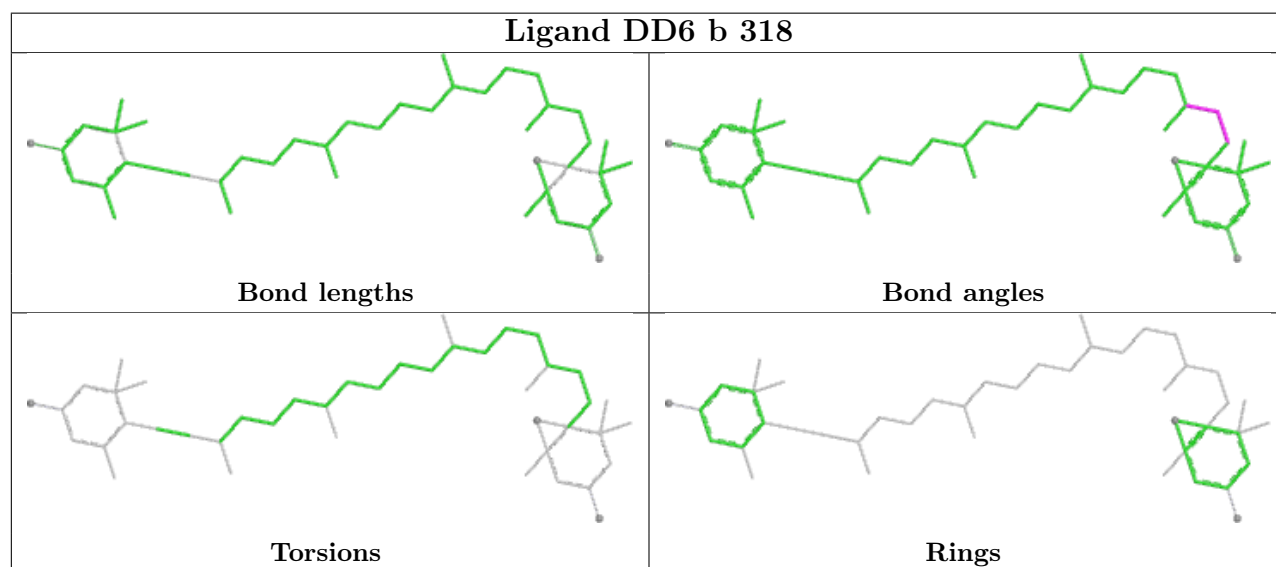
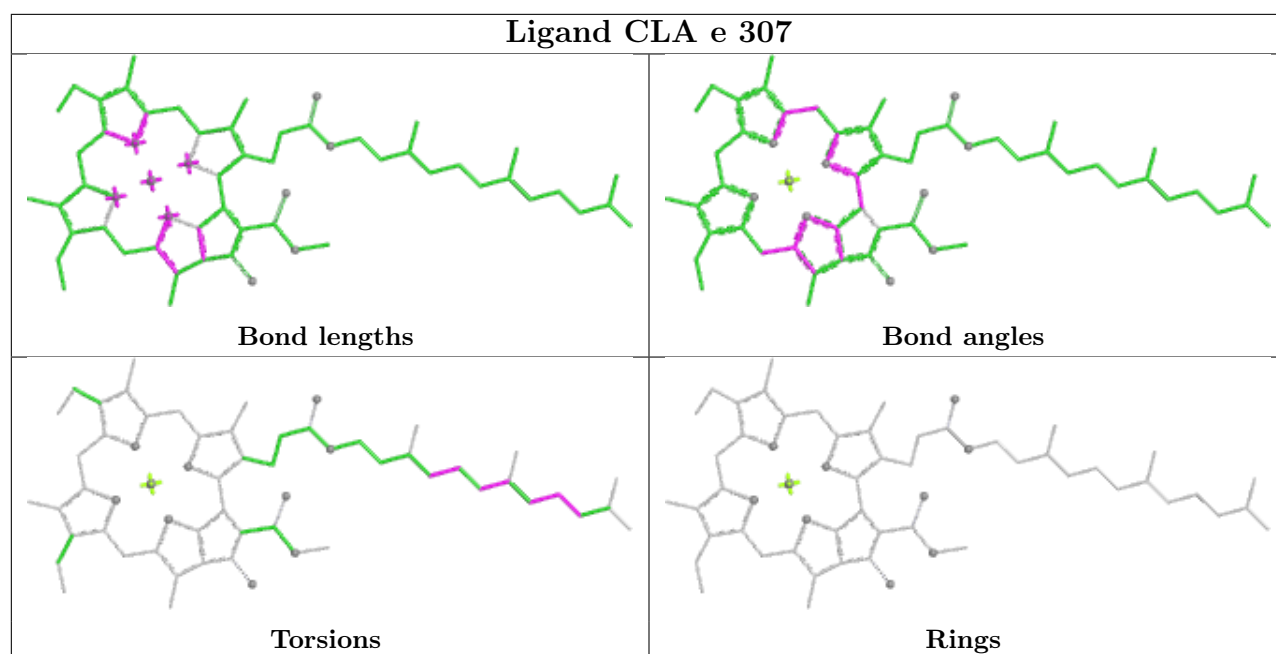


Ligand CLA o 305

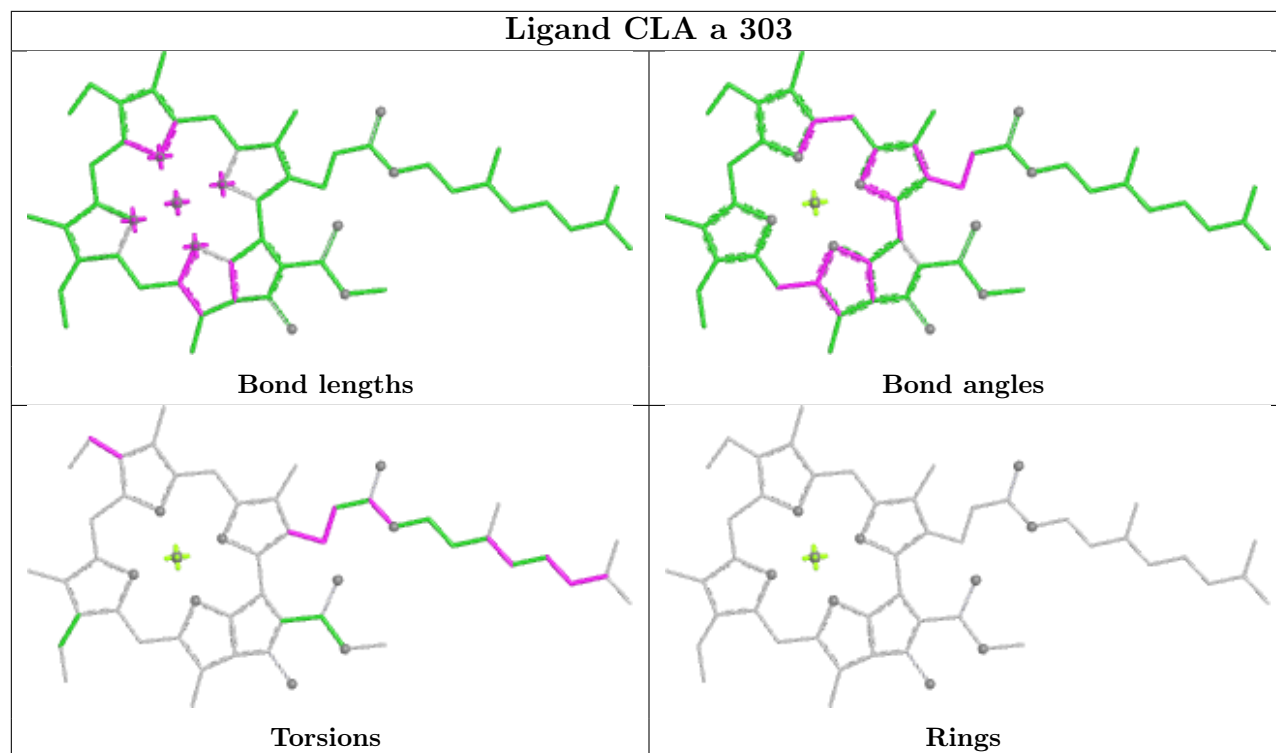


Ligand DD6 a 321

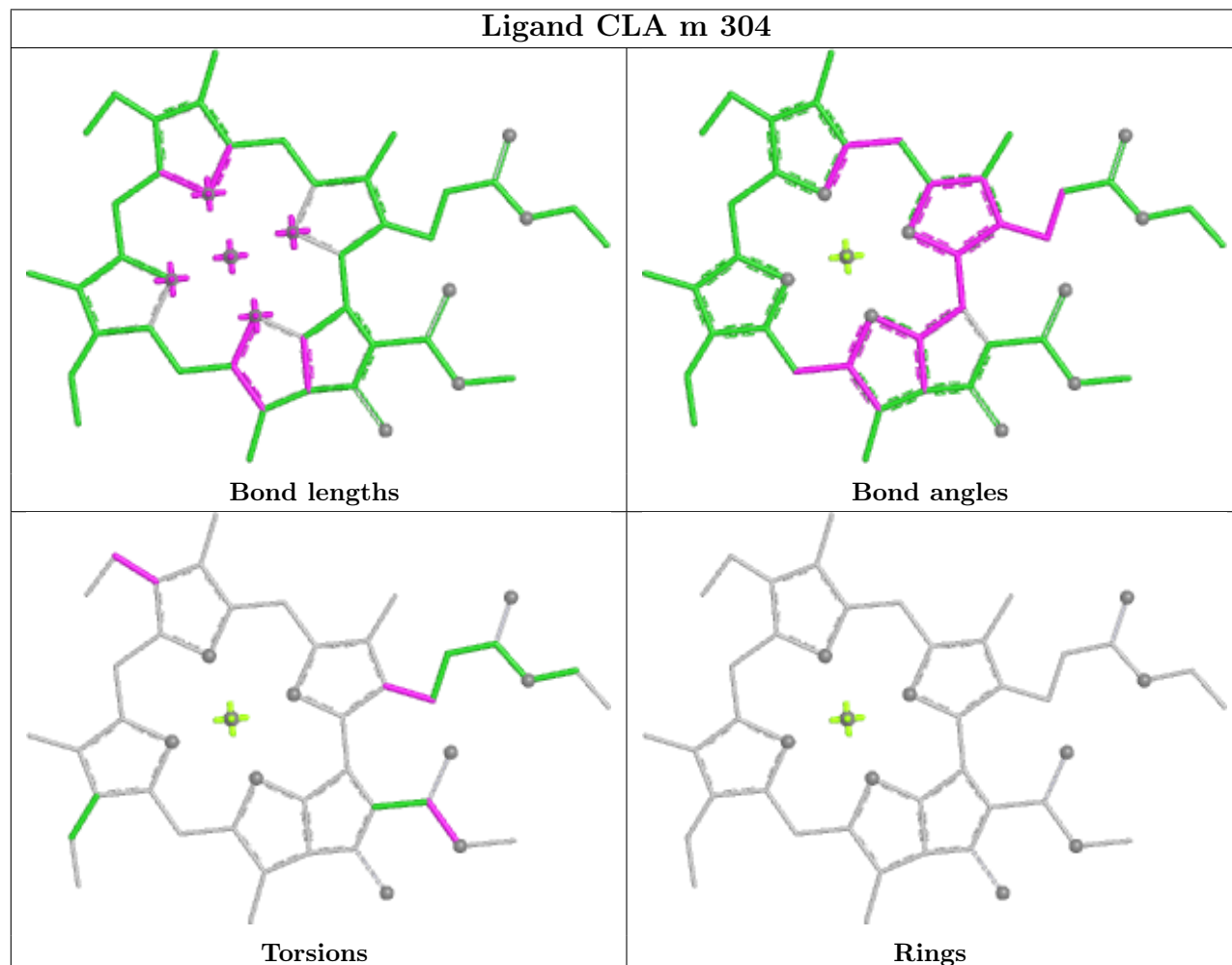




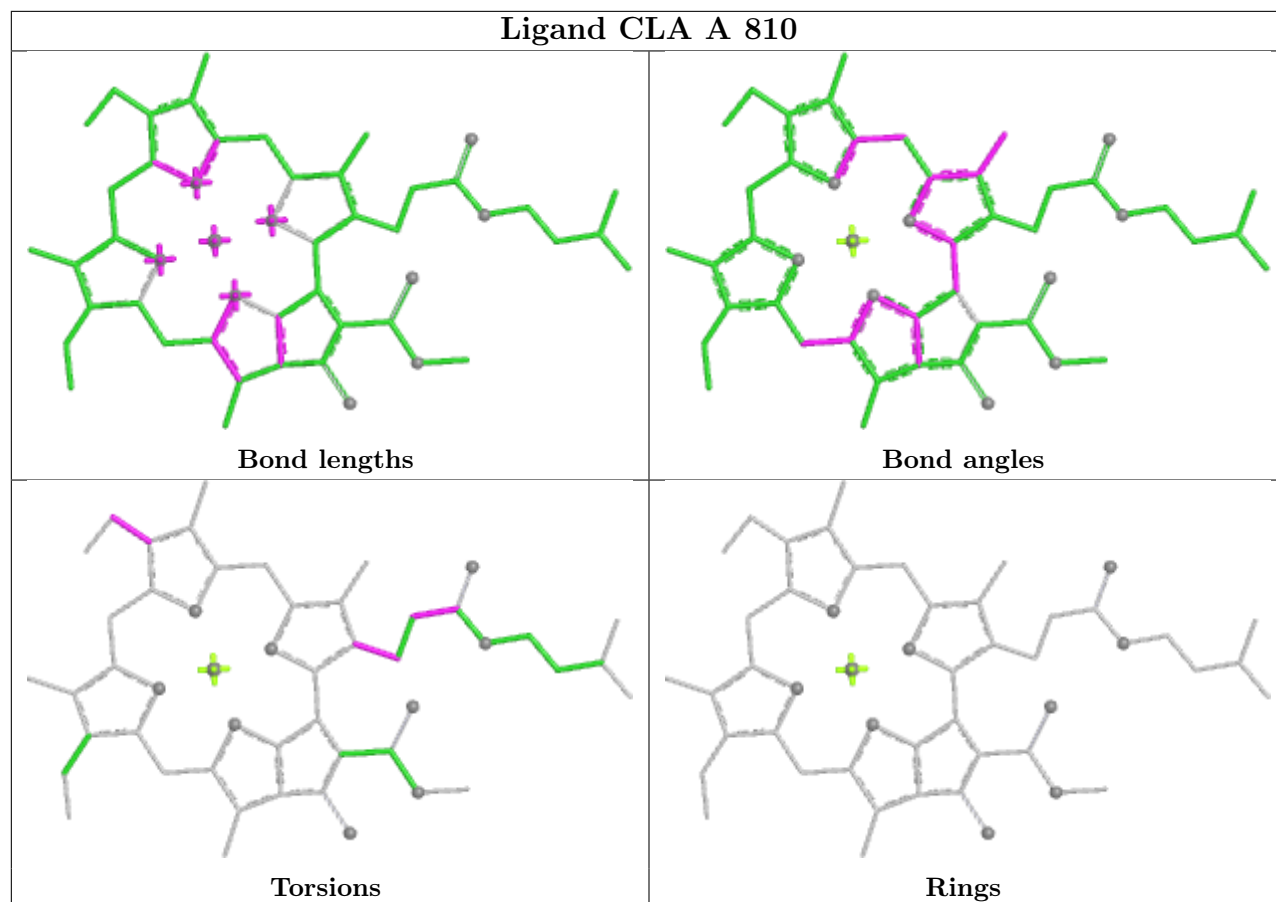
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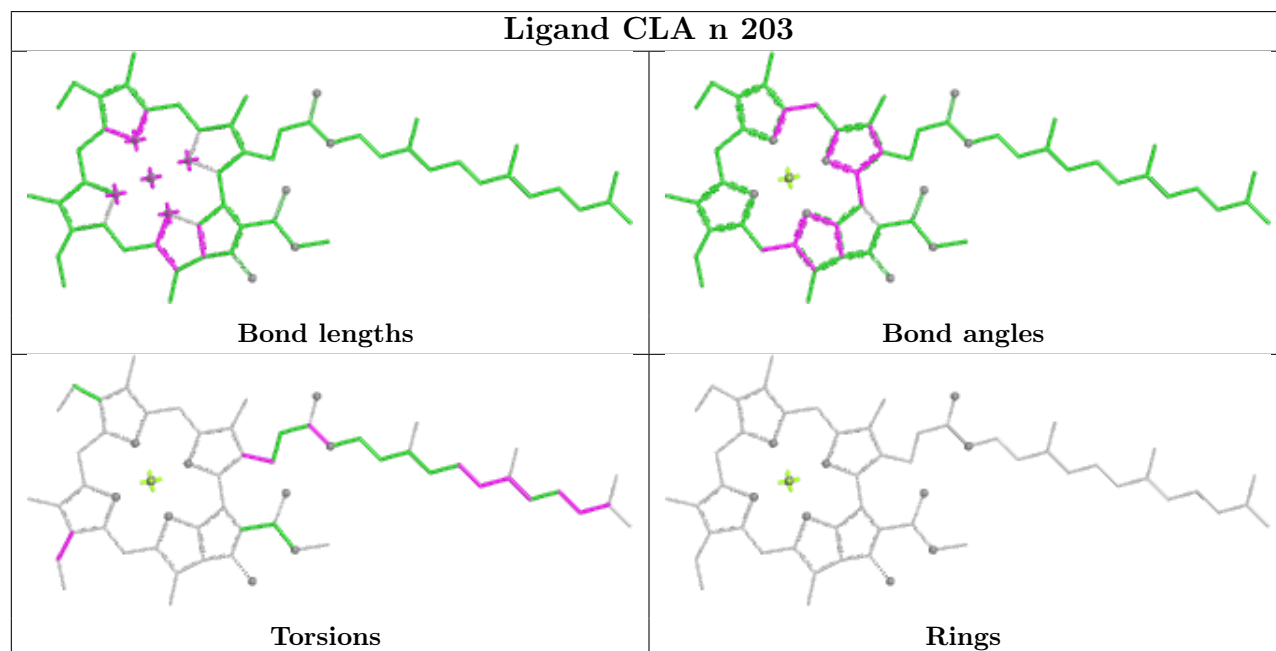
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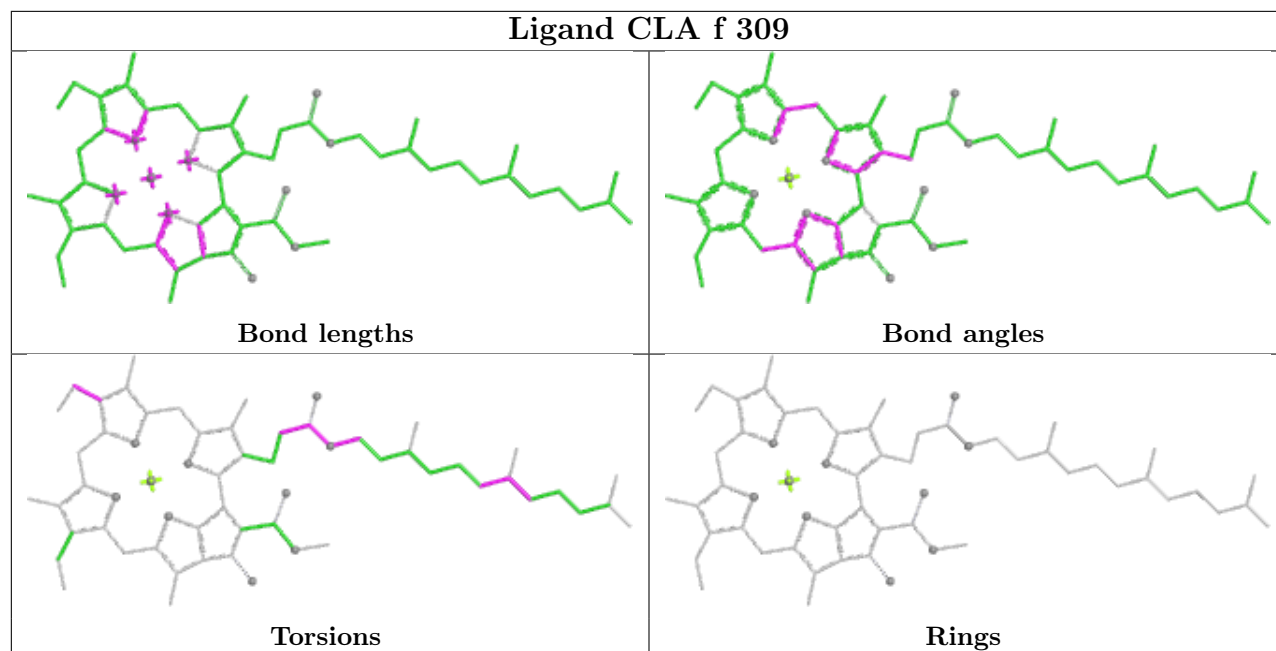
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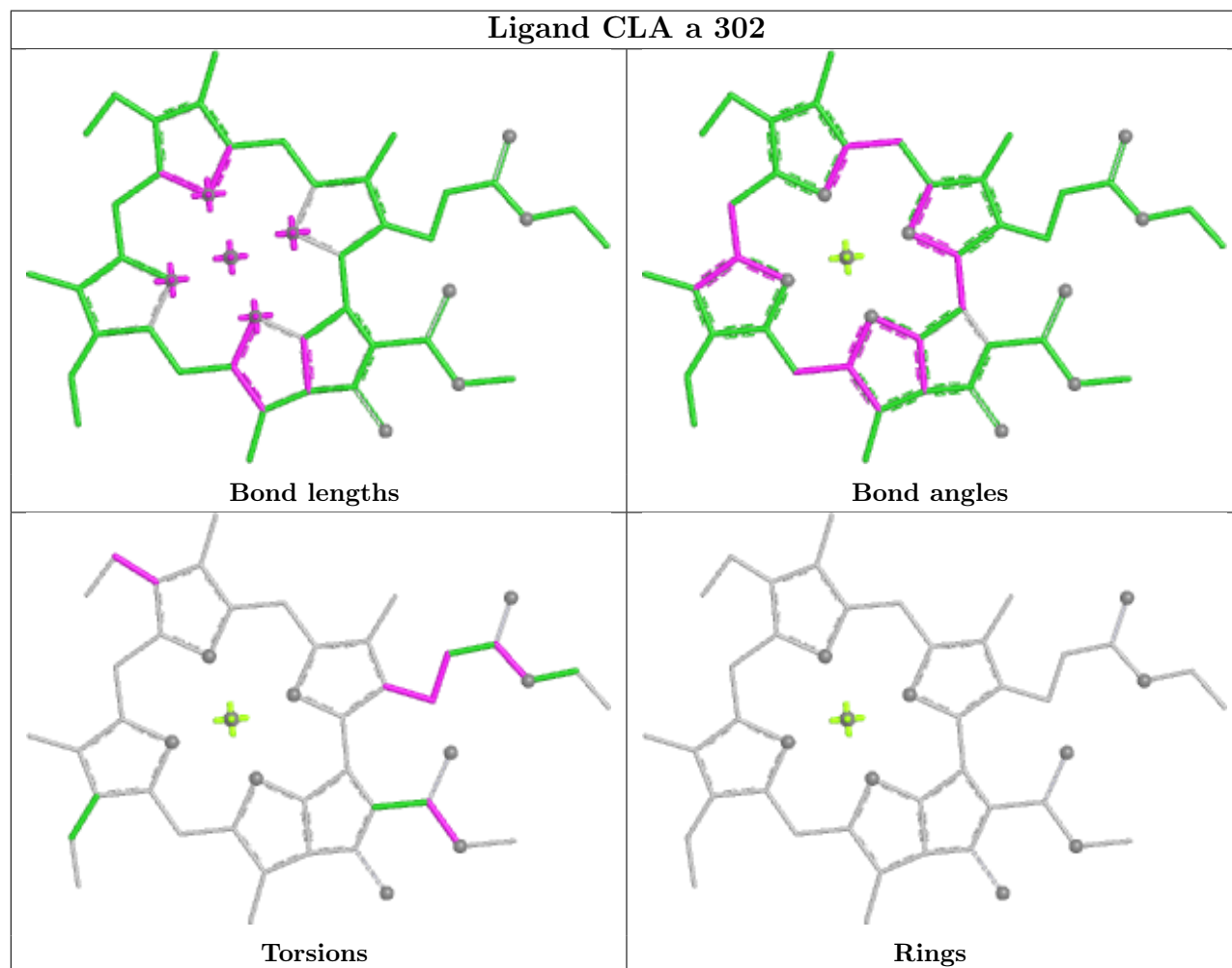
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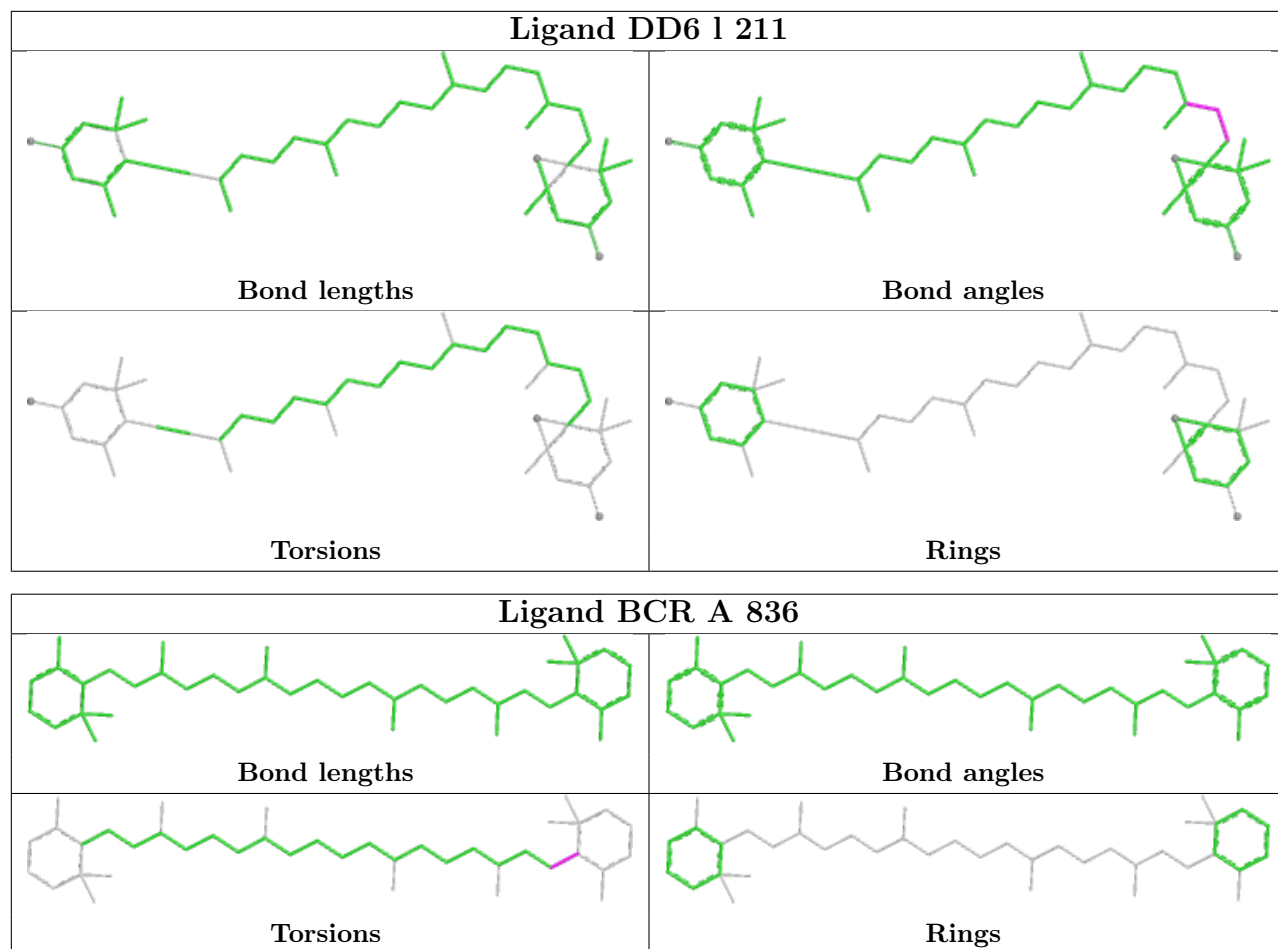


Ligand CLA f 309

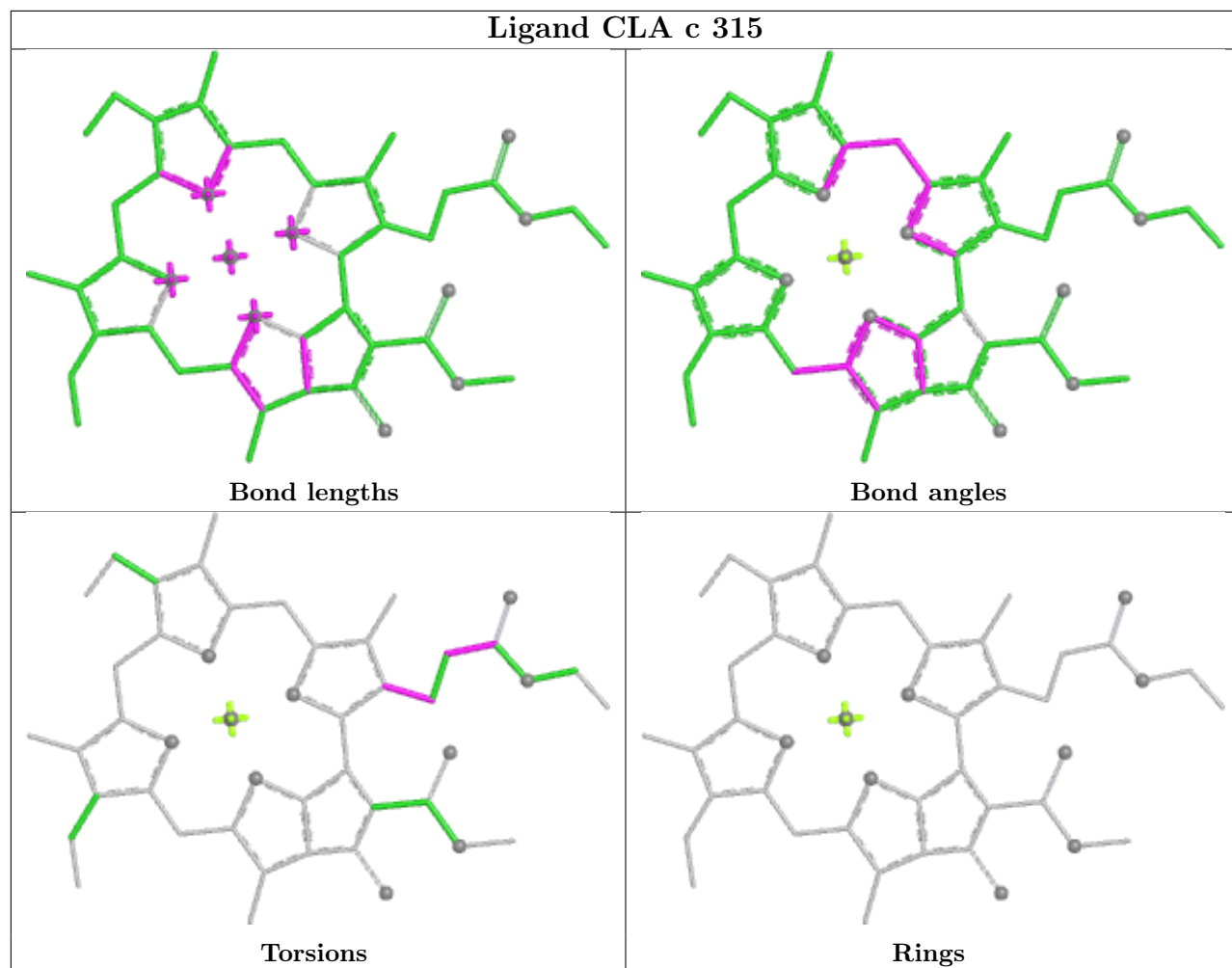


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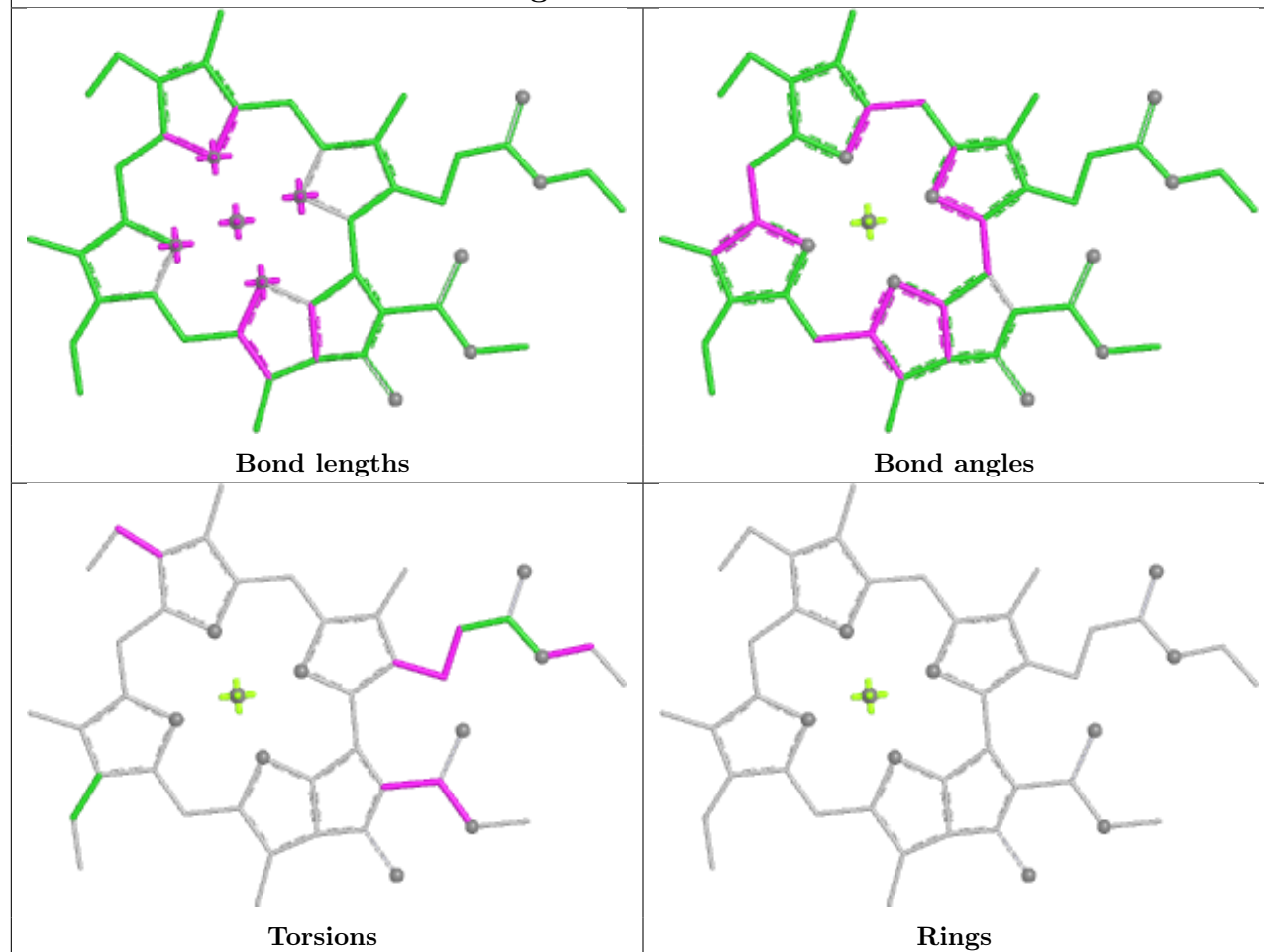




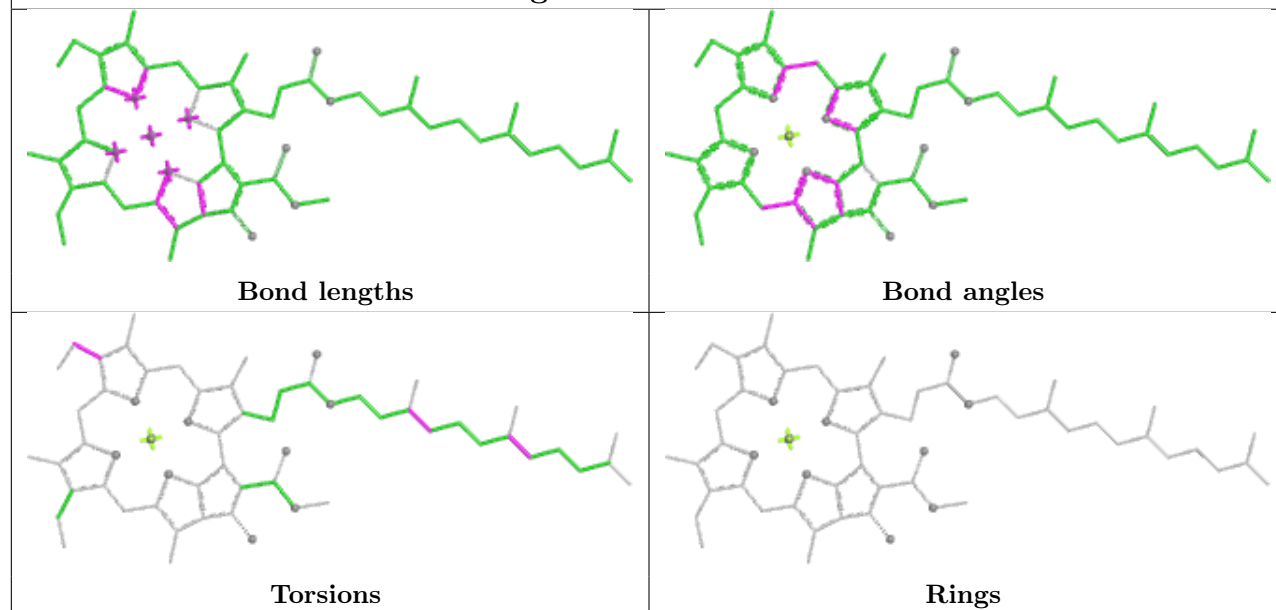
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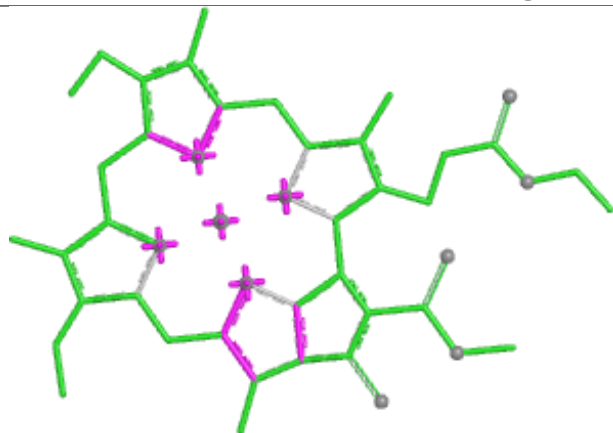
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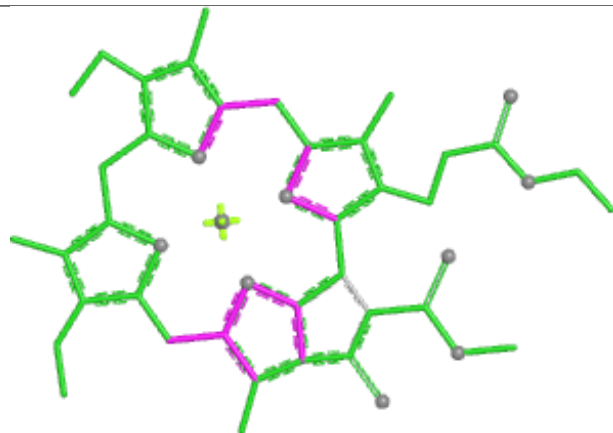
Ligand CLA m 307



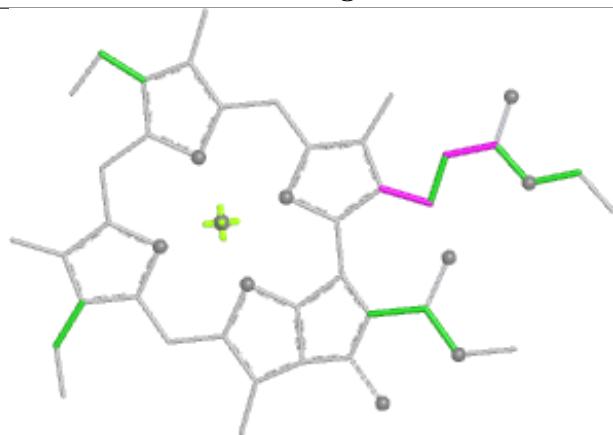
Ligand CLA c 311



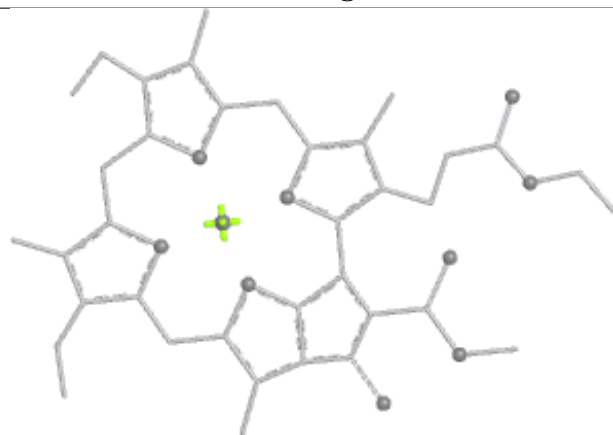
Bond lengths



Bond angles

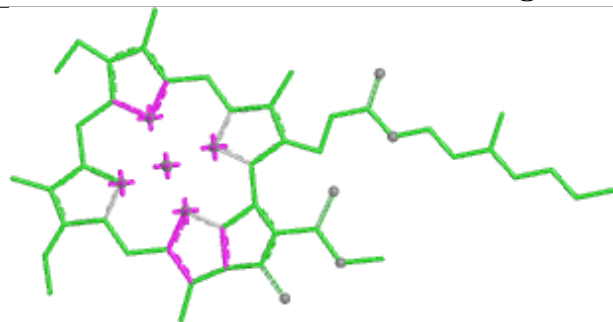


Torsions

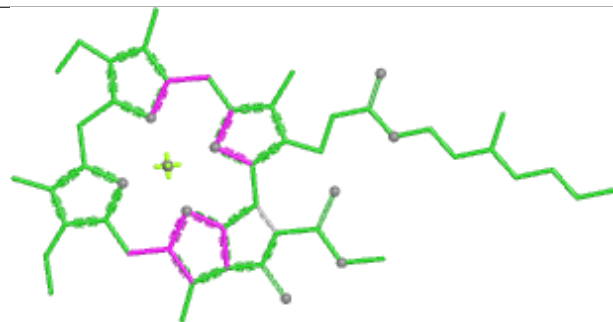


Rings

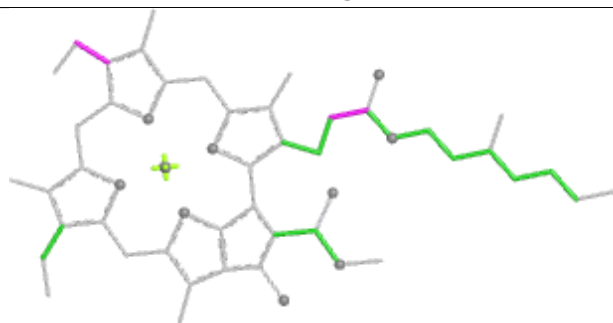
Ligand CLA o 308



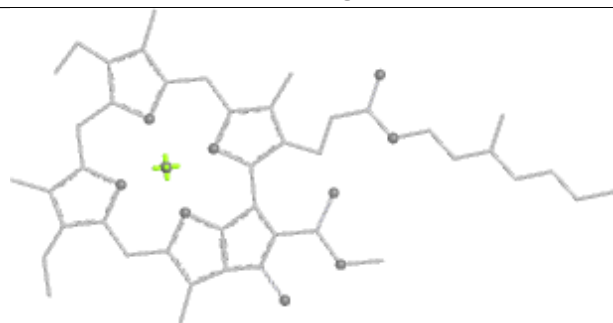
Bond lengths



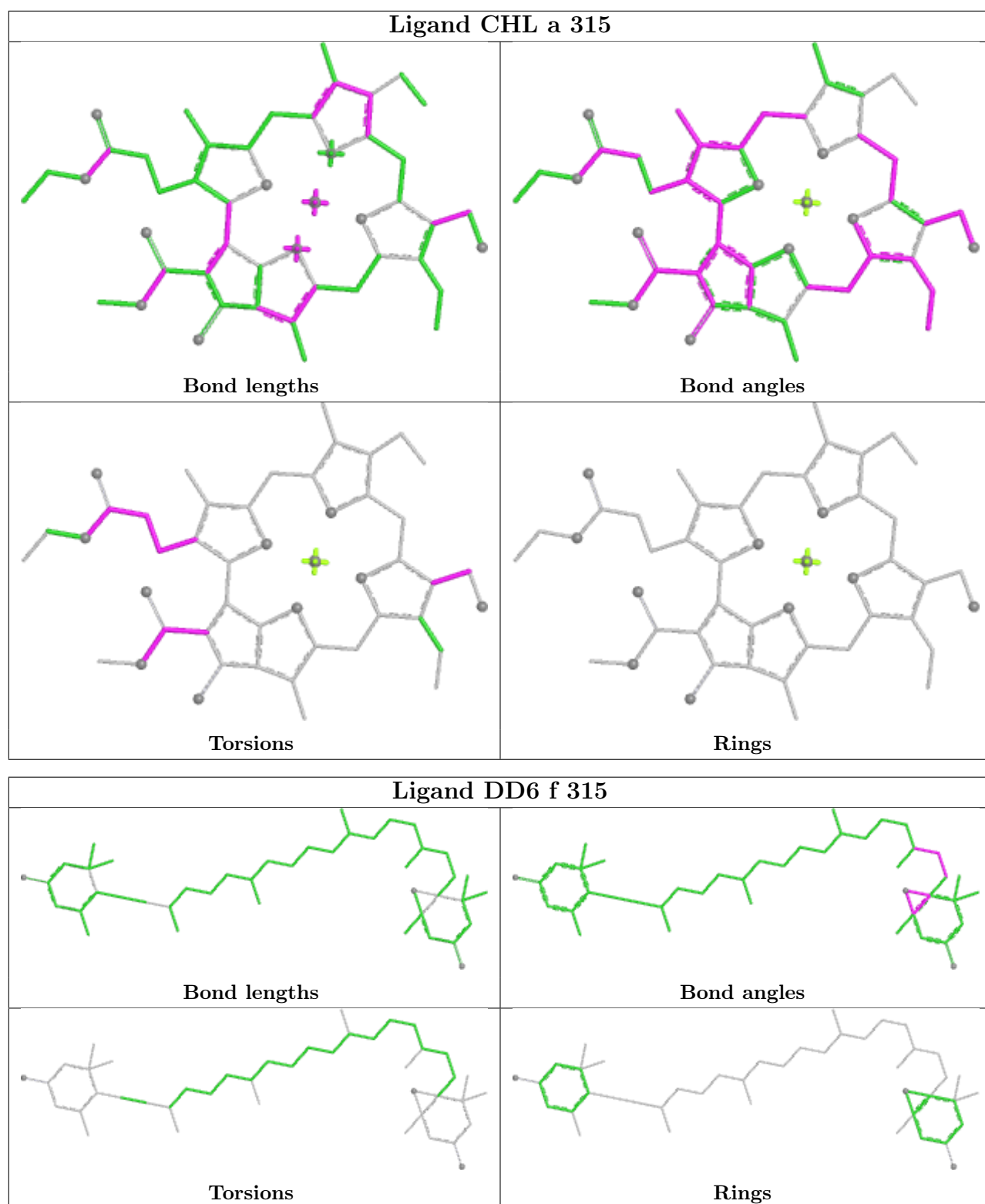
Bond angles



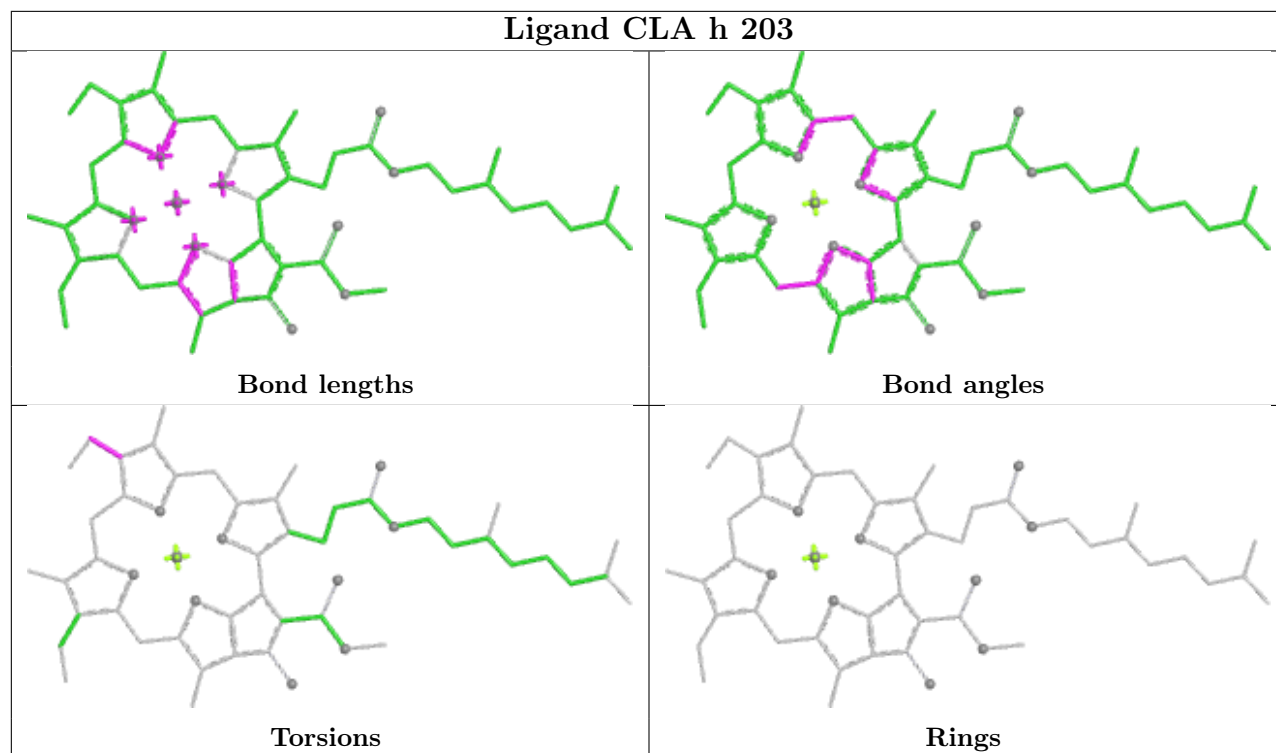
Torsions



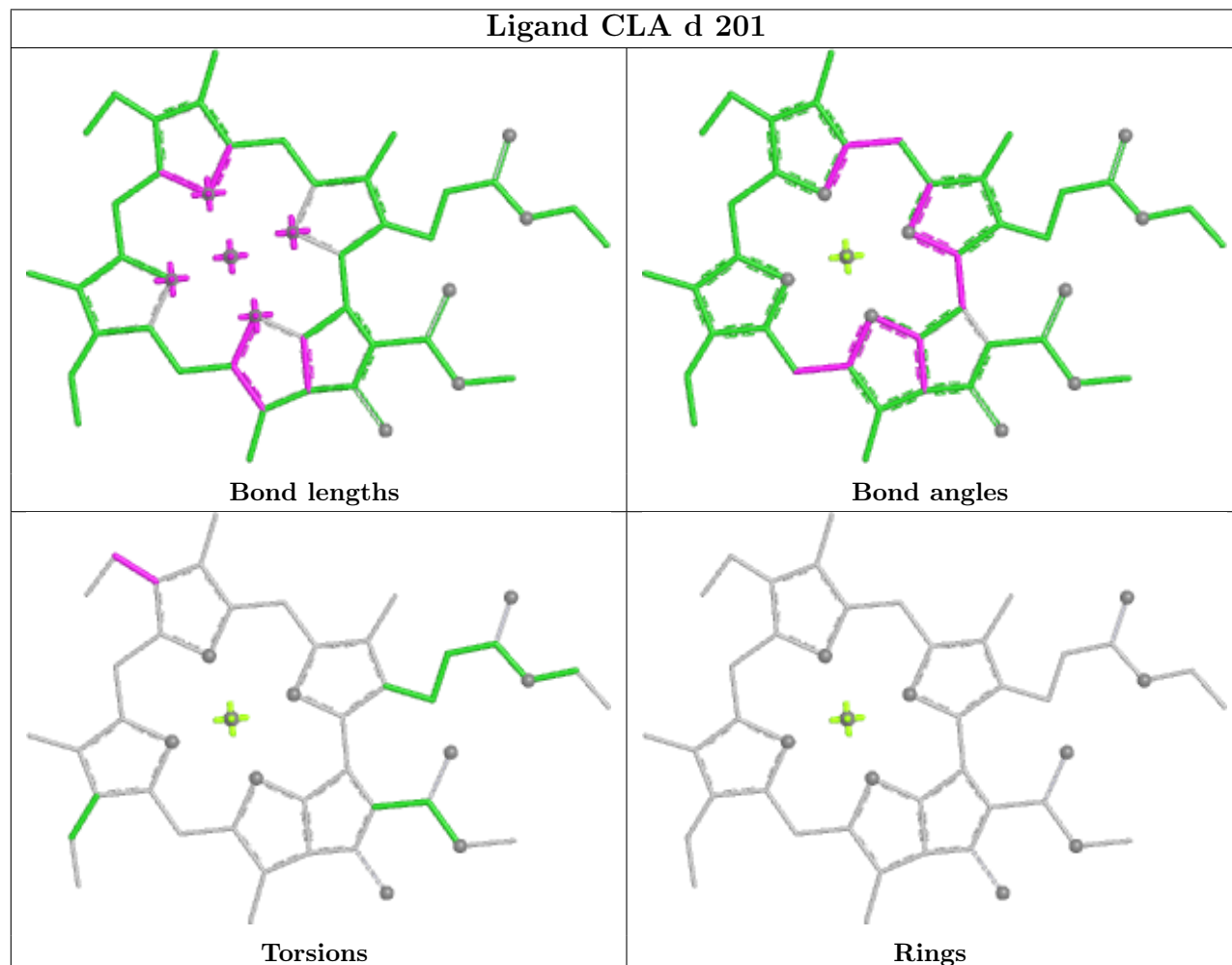
Rings

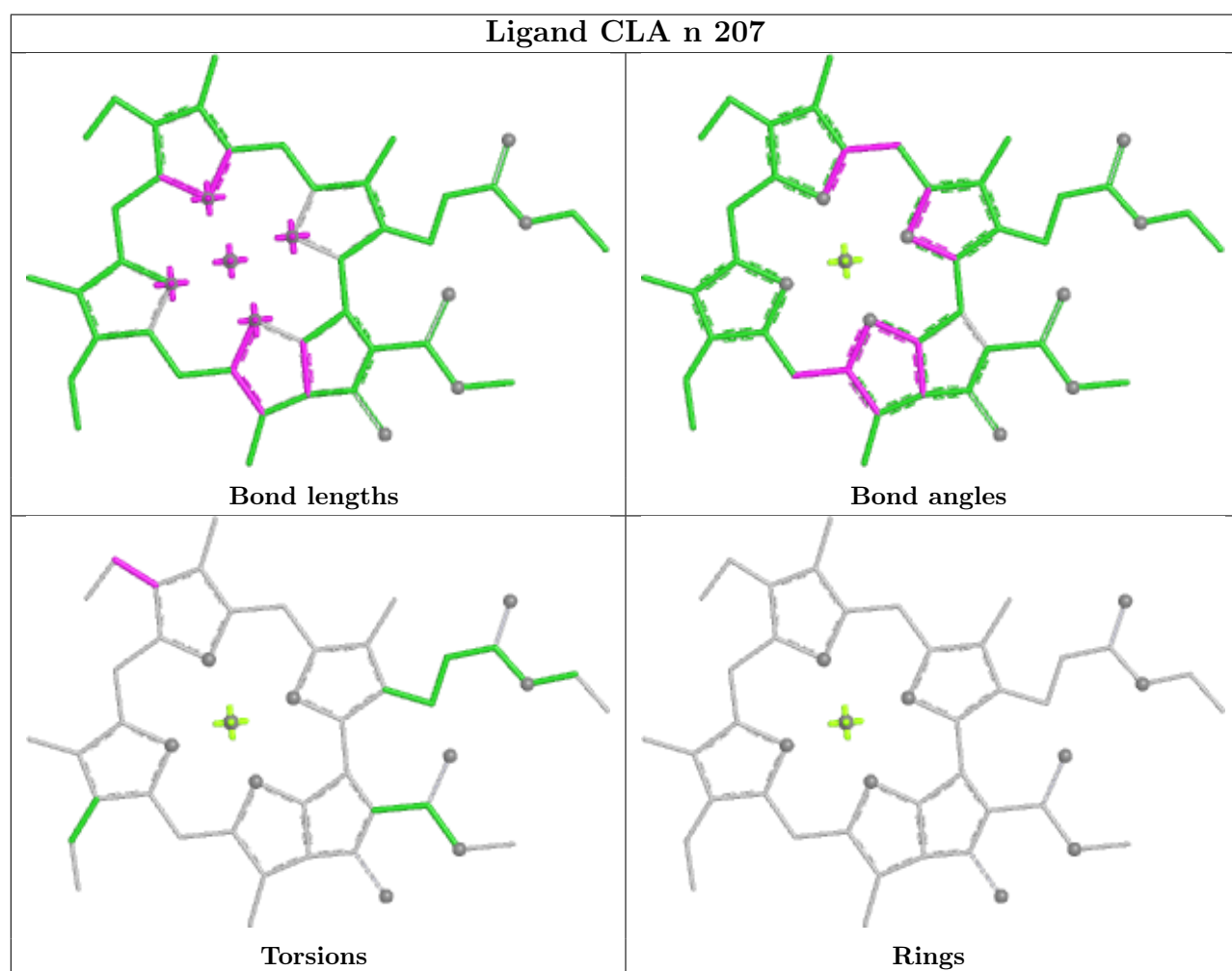
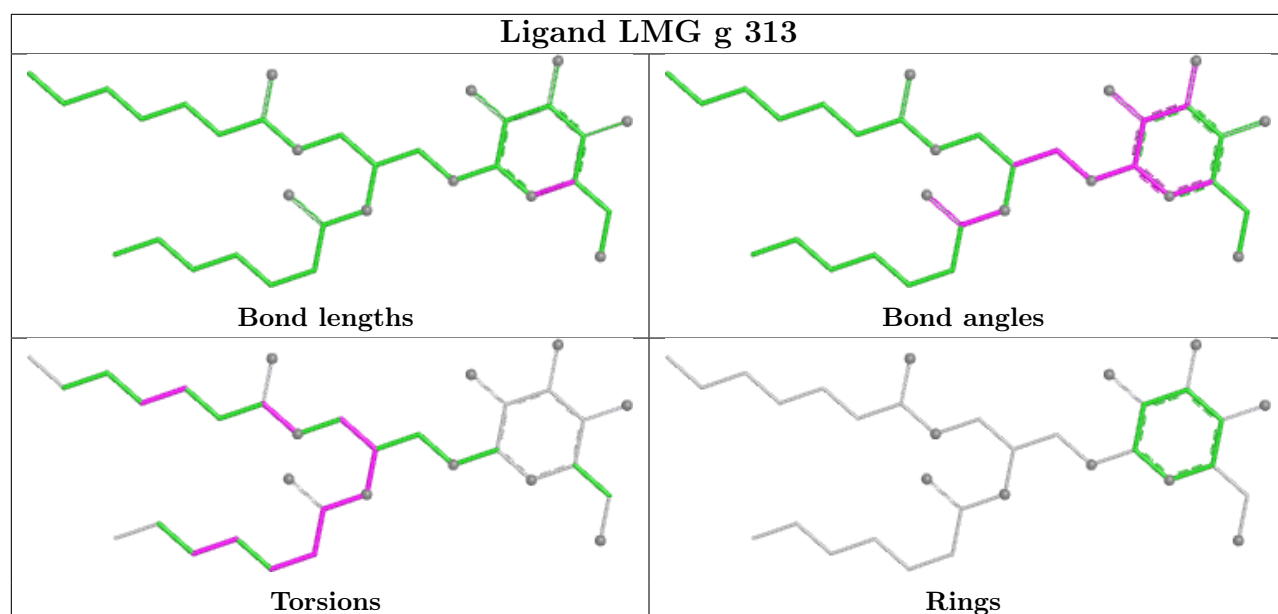


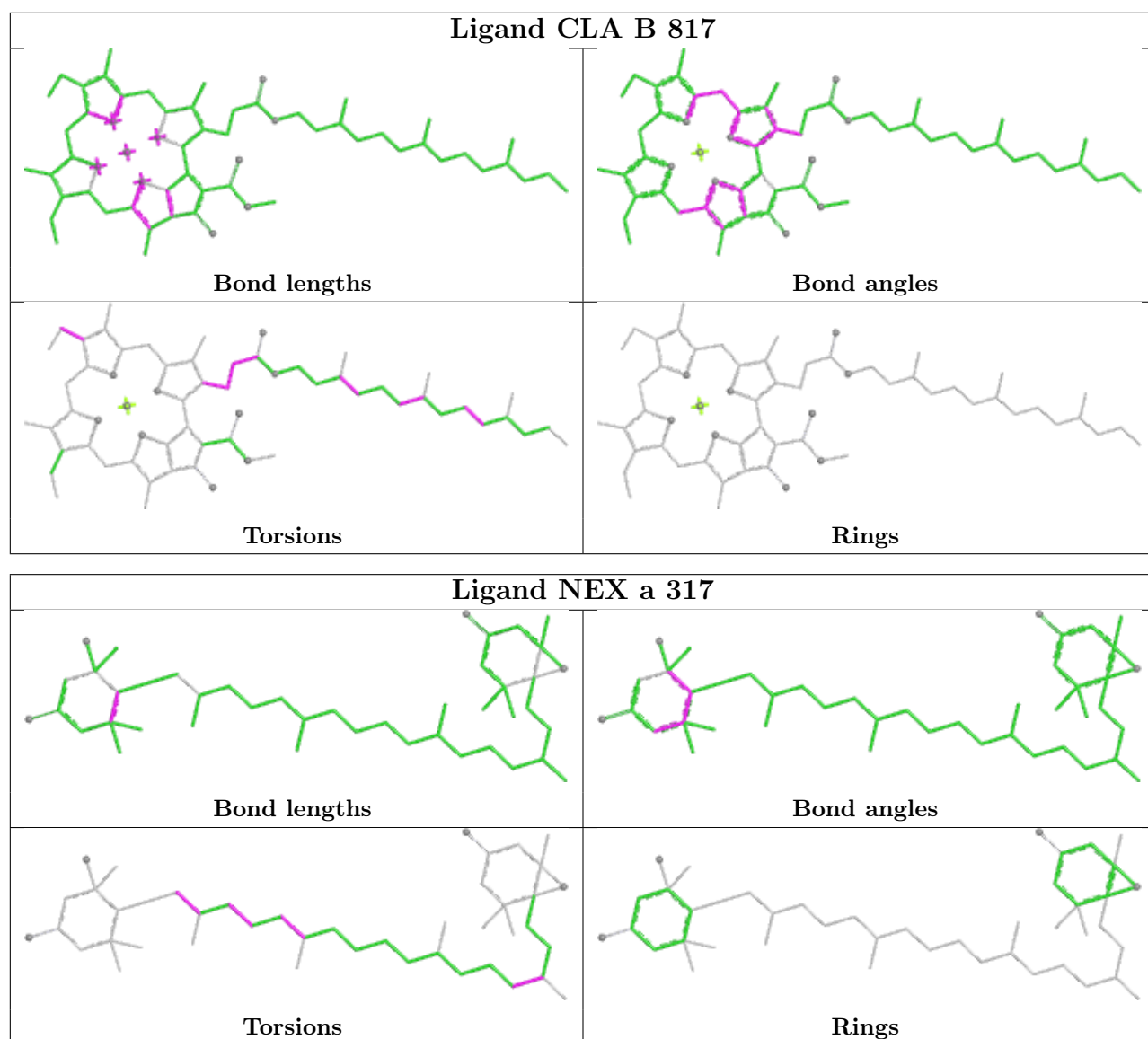
Ligand CLA h 203



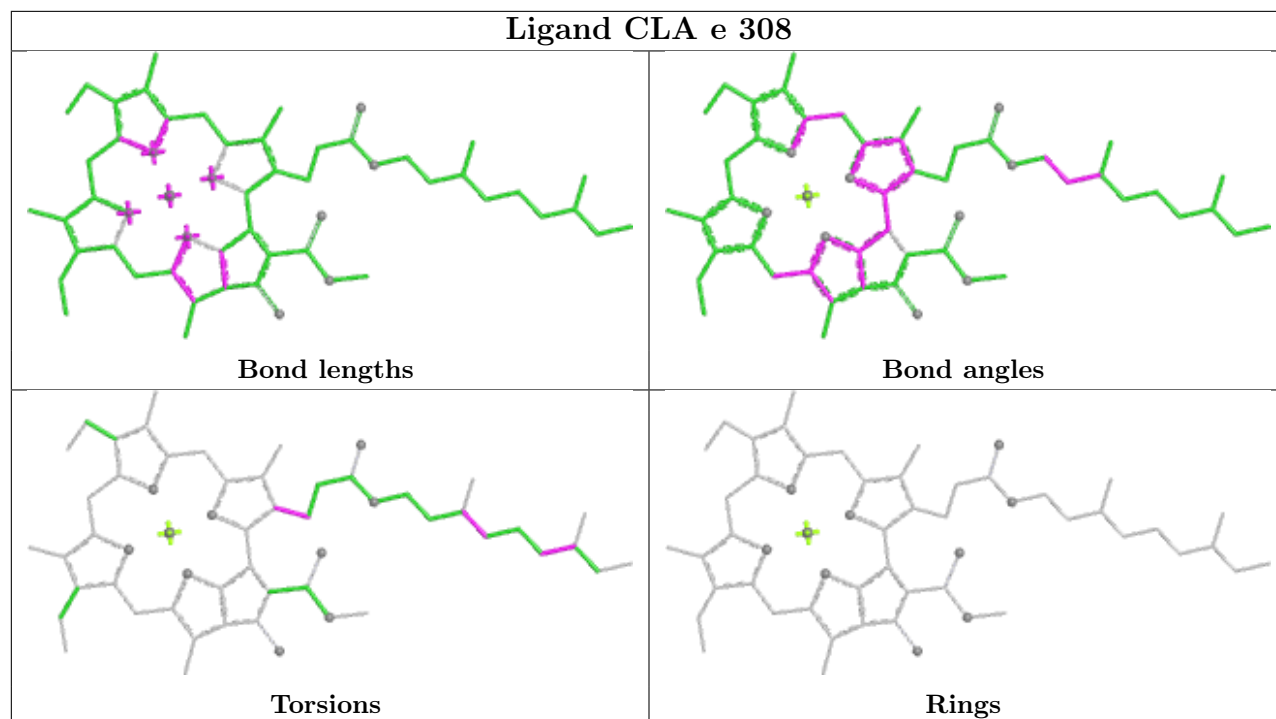
Ligand CLA d 201



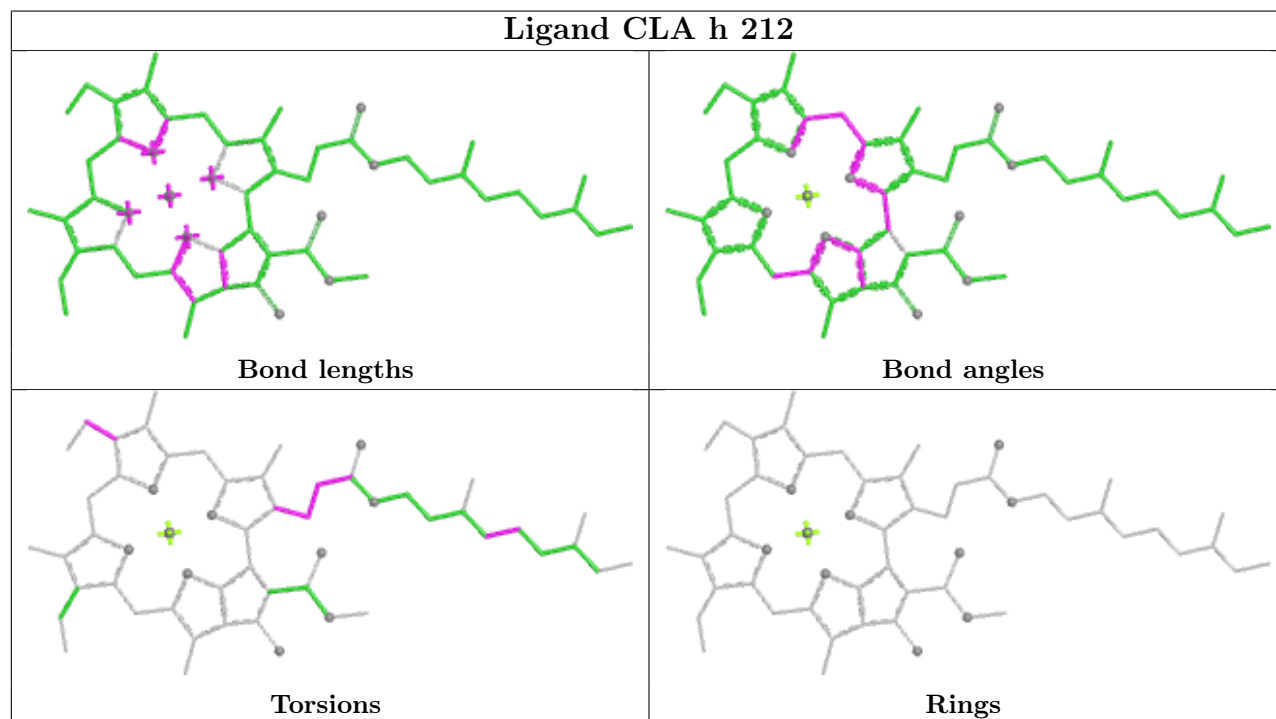


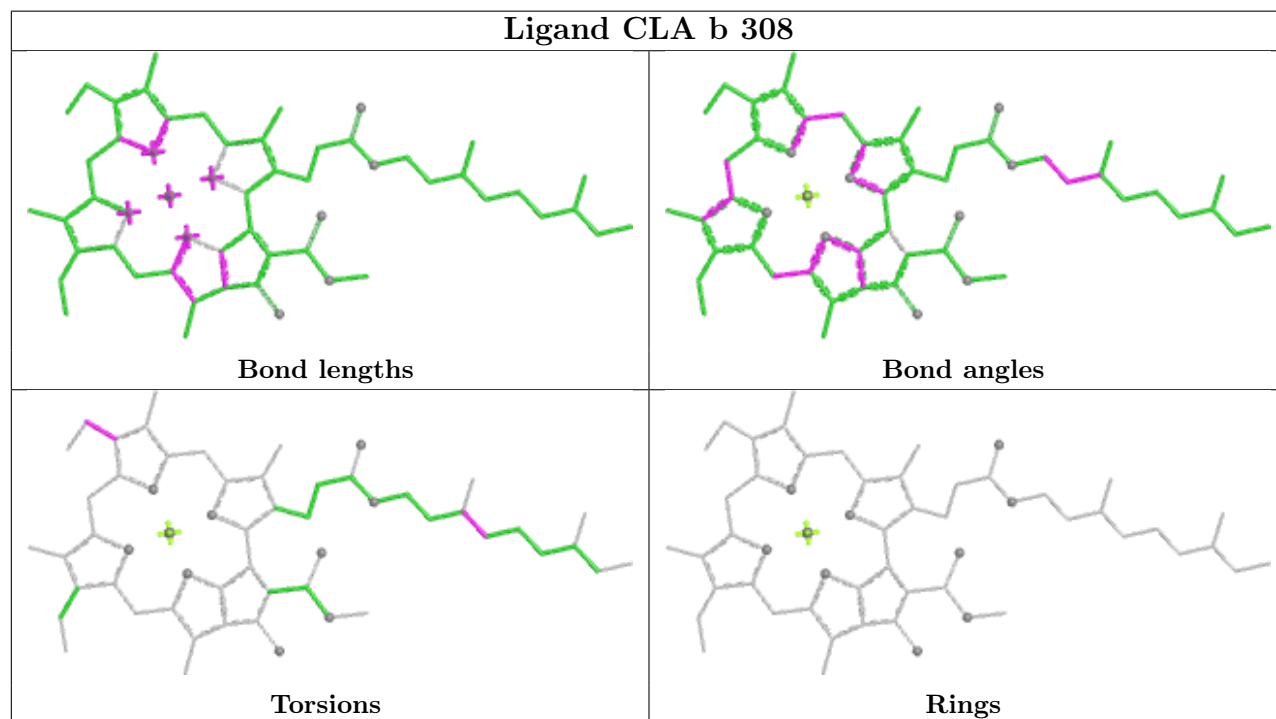
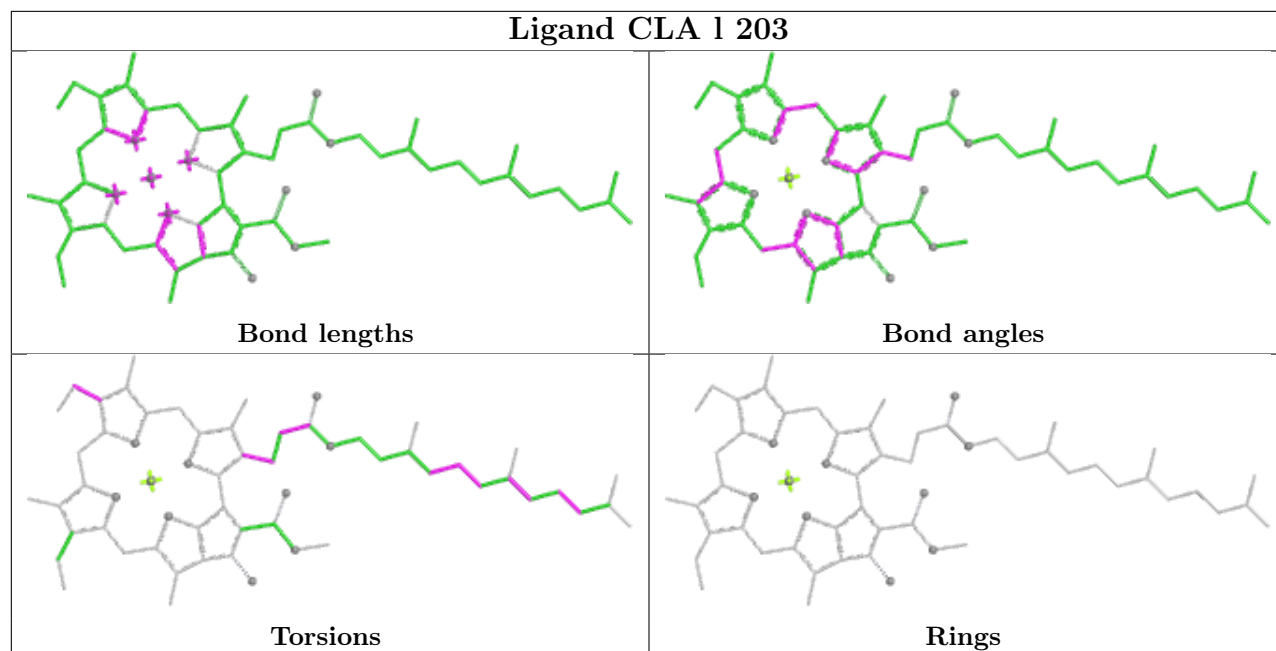


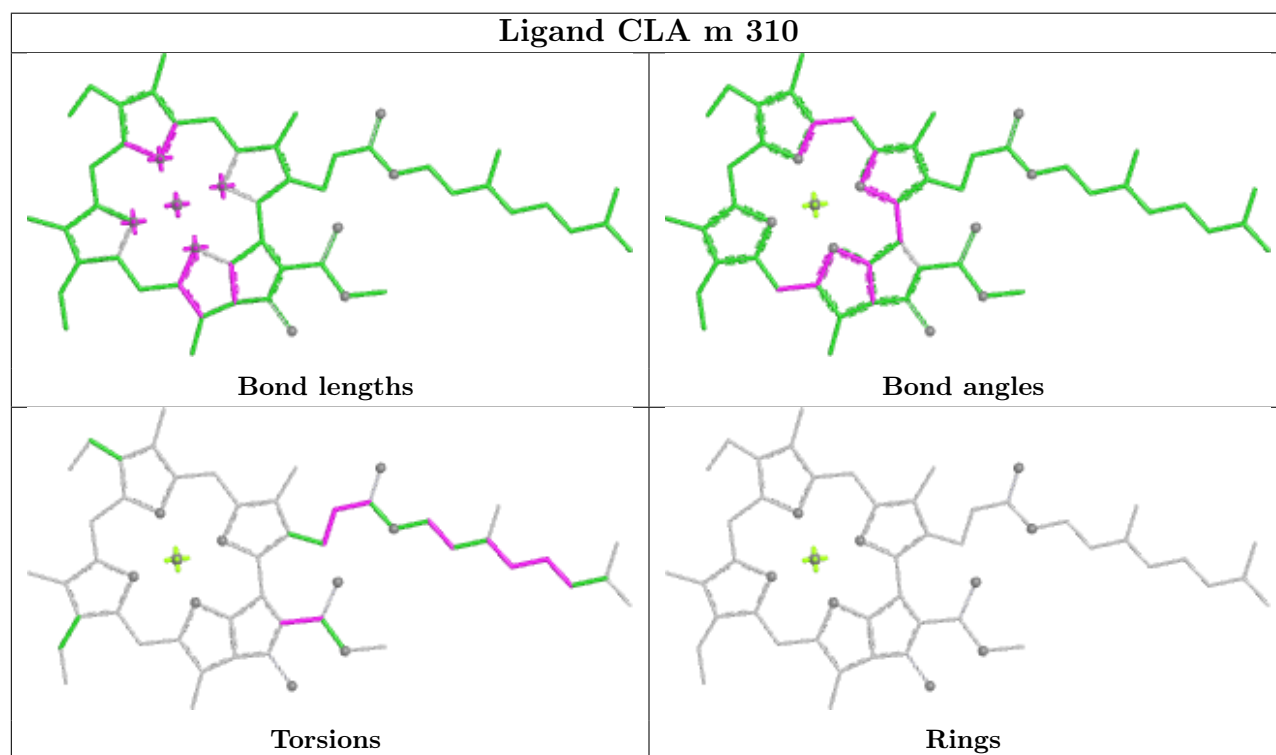
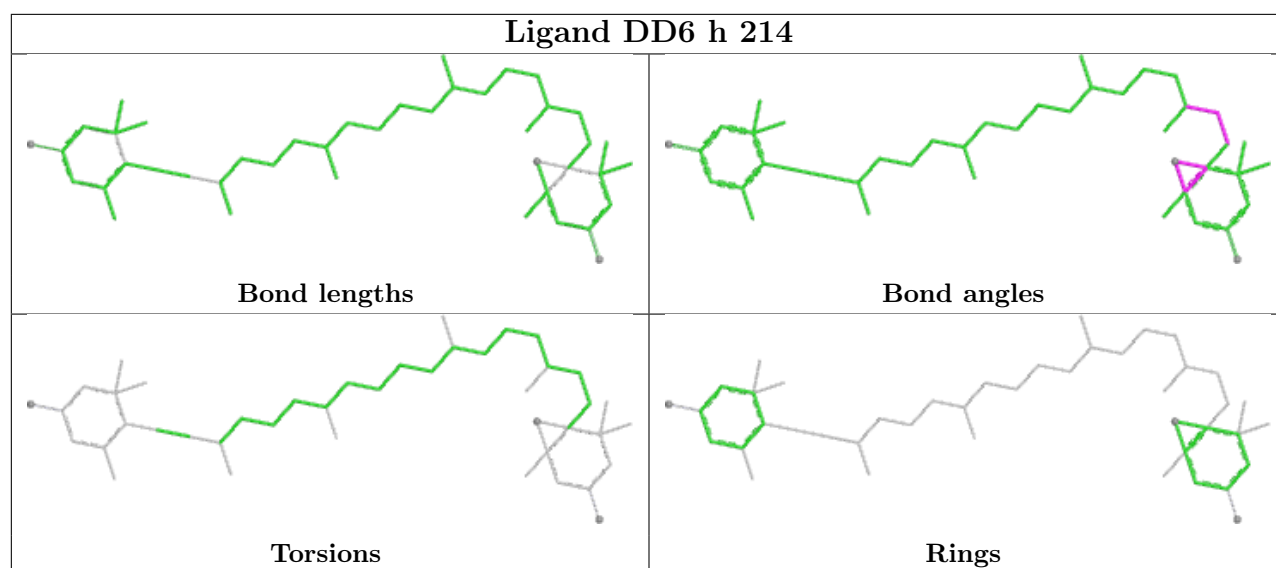
Ligand CLA e 308



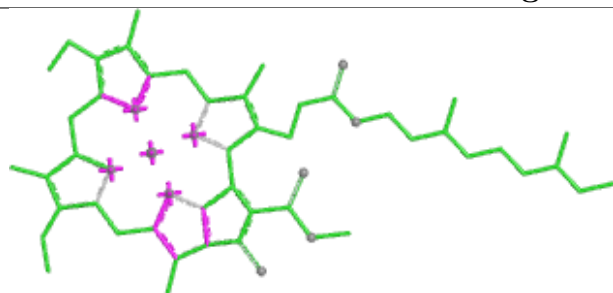
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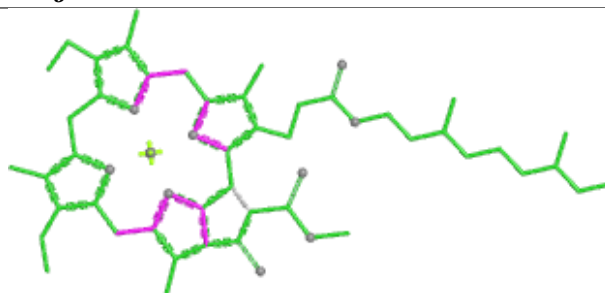




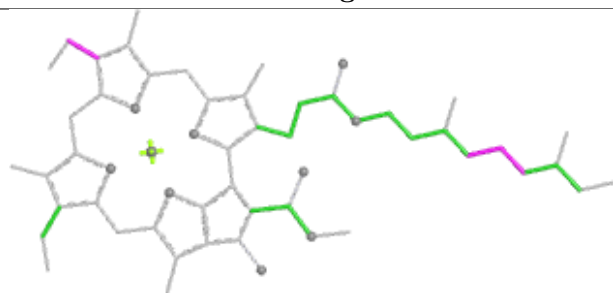
Ligand CLA j 309



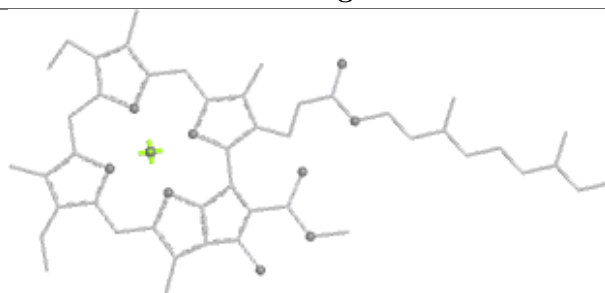
Bond lengths



Bond angles

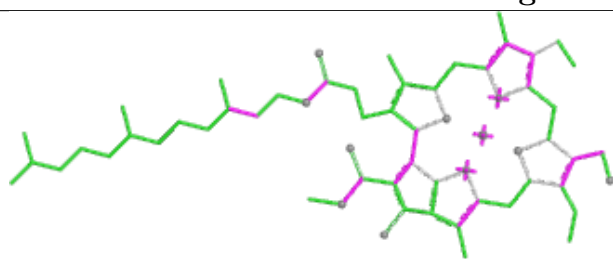


Torsions

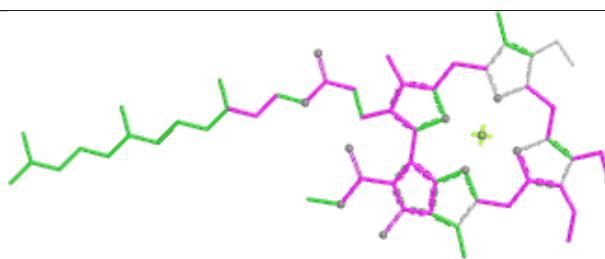


Rings

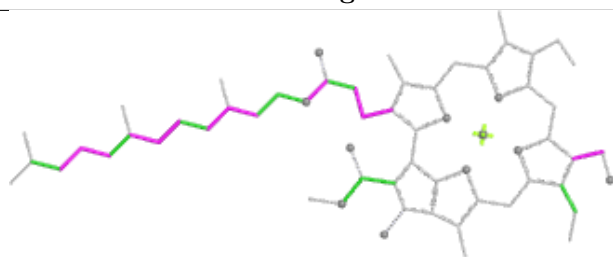
Ligand CHL c 305



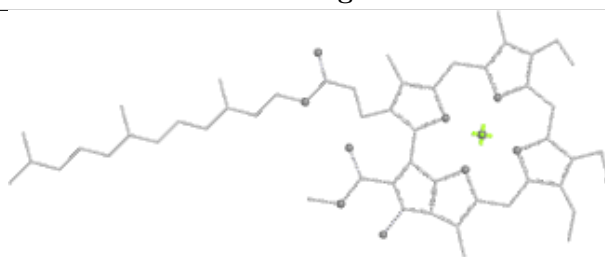
Bond lengths



Bond angles

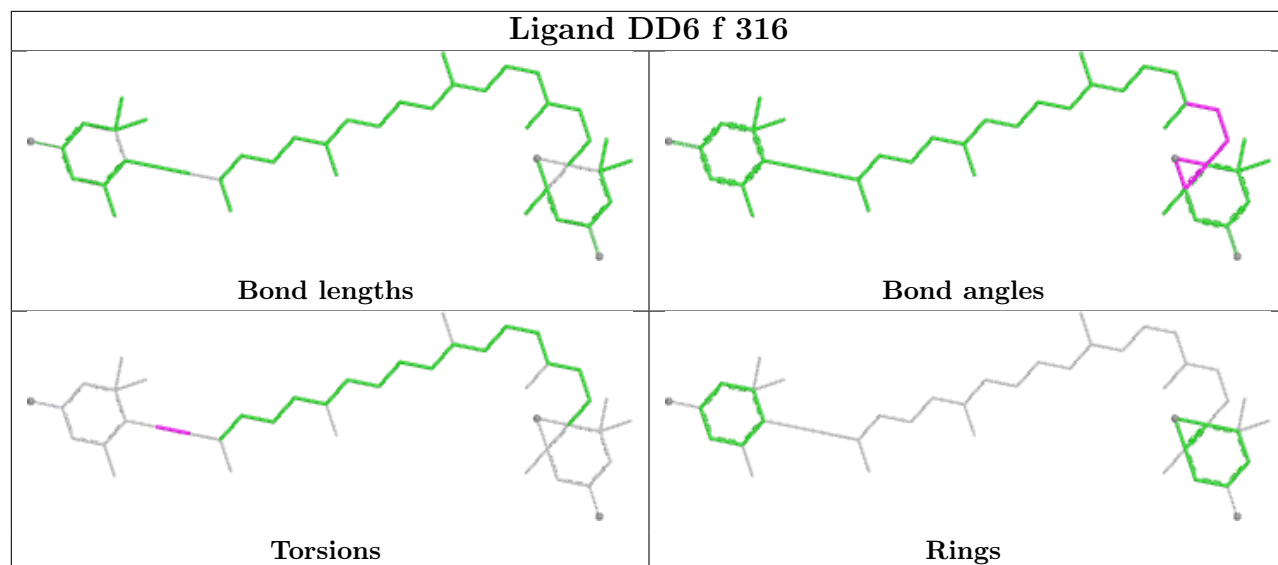


Torsions

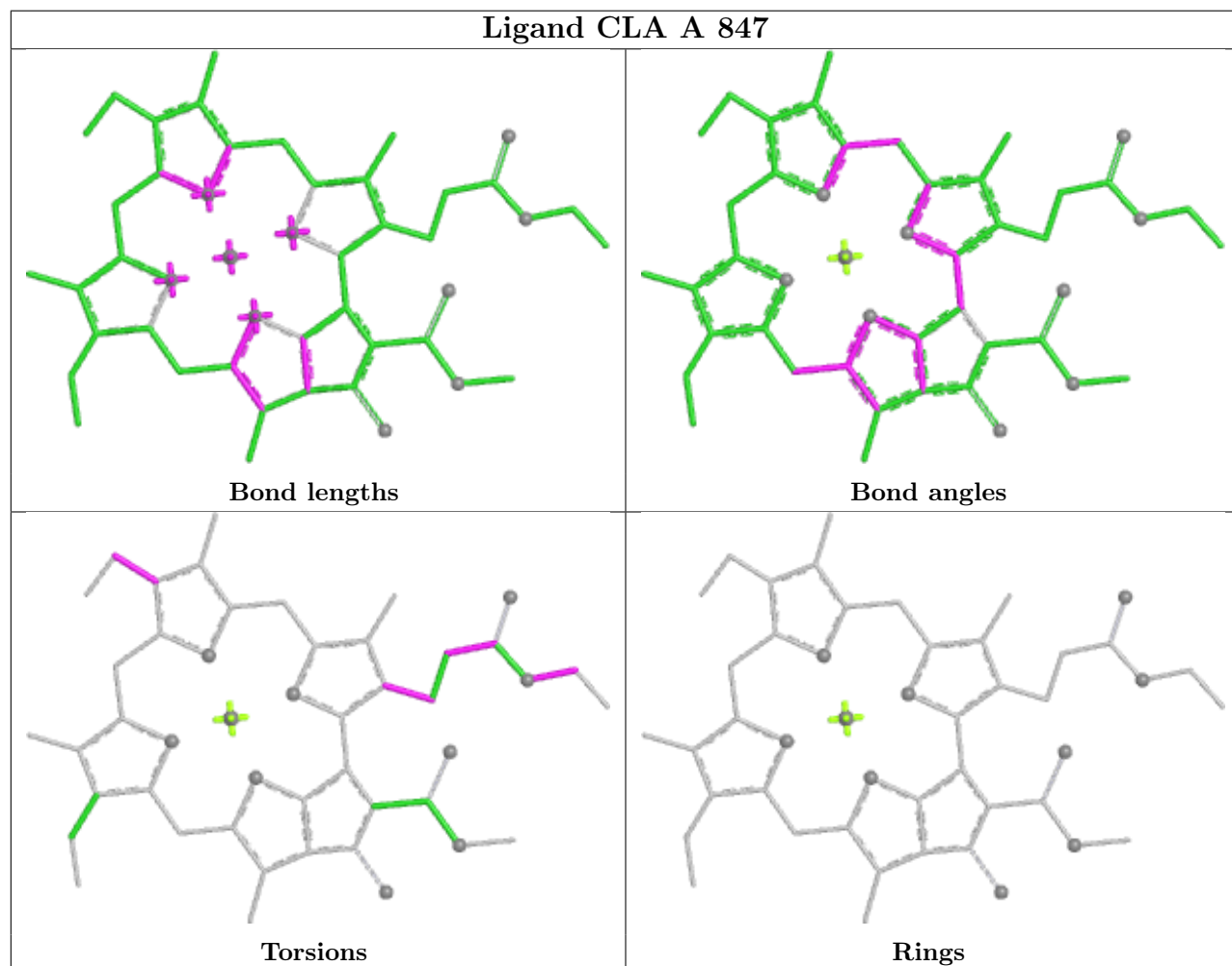


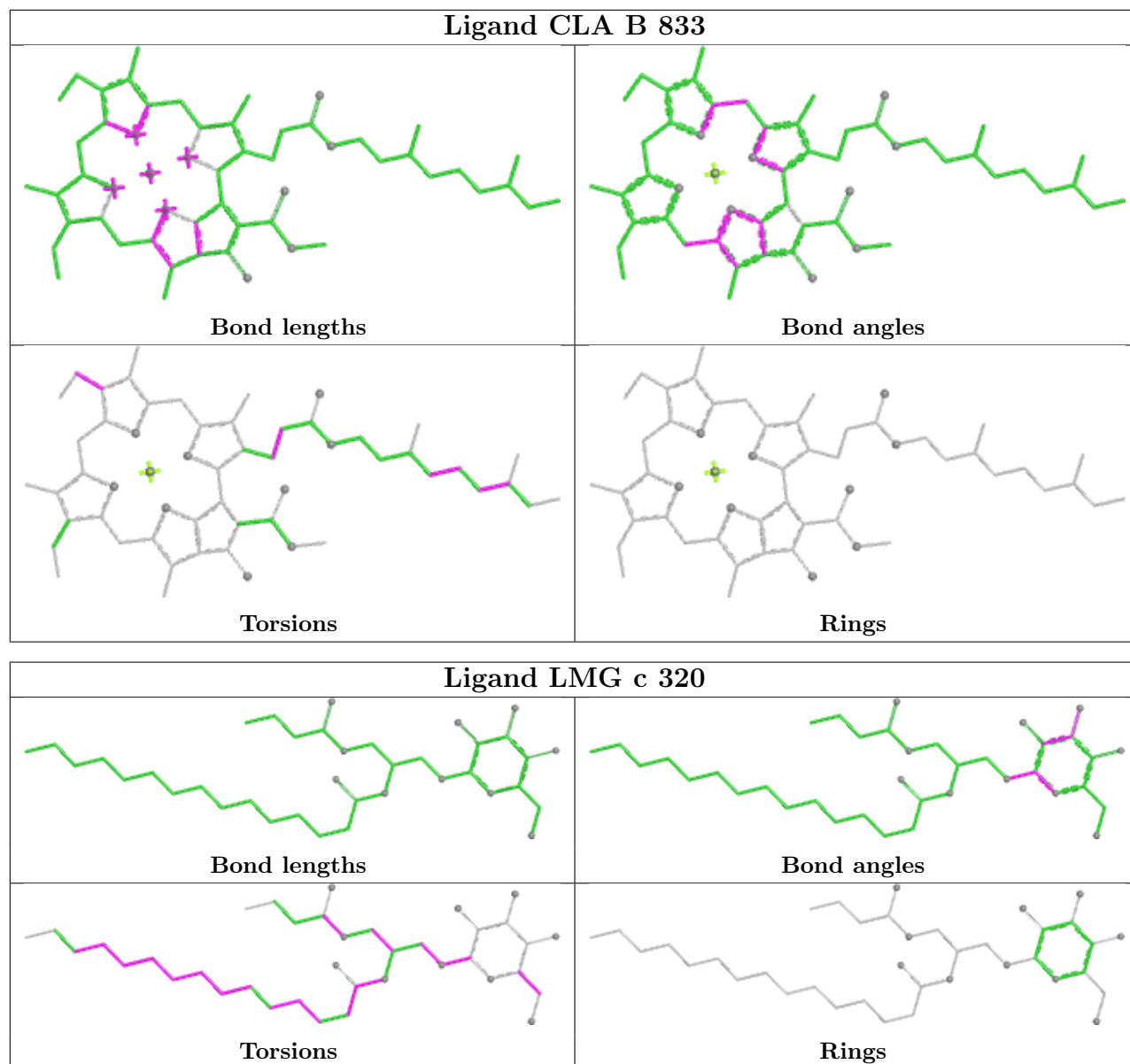
Rings

Ligand DD6 f 316

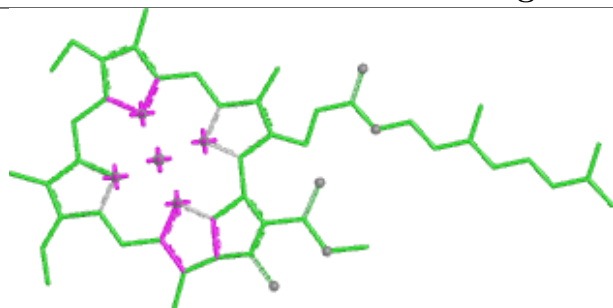


Ligand CLA A 847

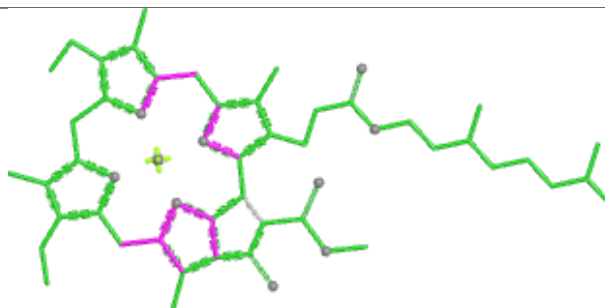




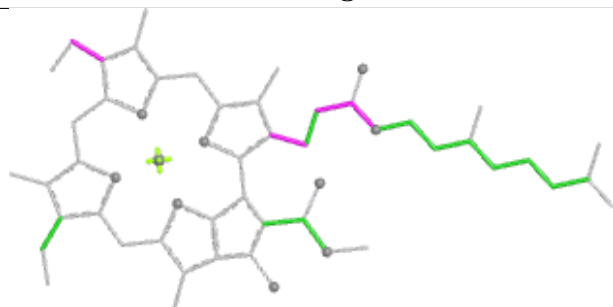
Ligand CLA b 302



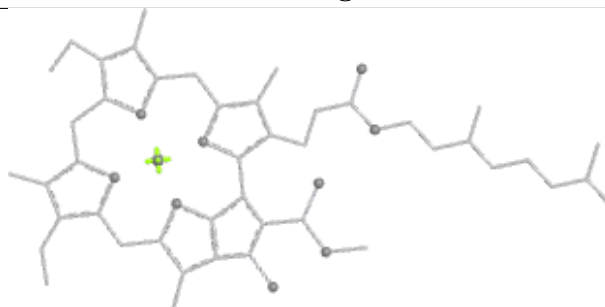
Bond lengths



Bond angles

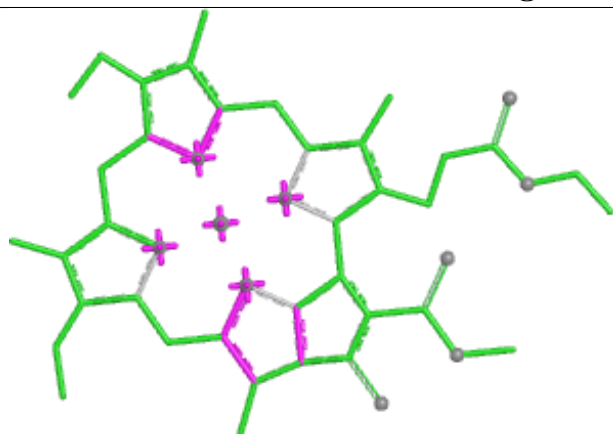


Torsions

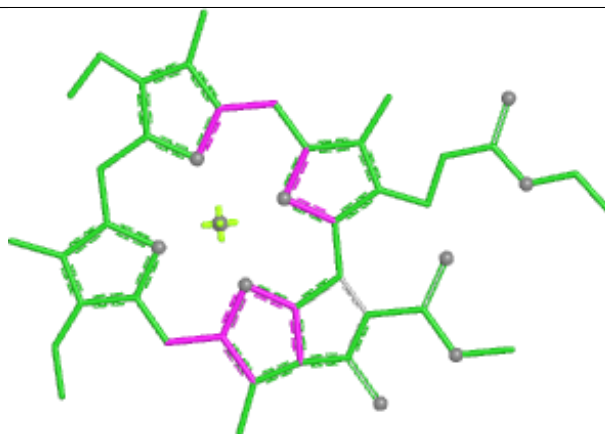


Rings

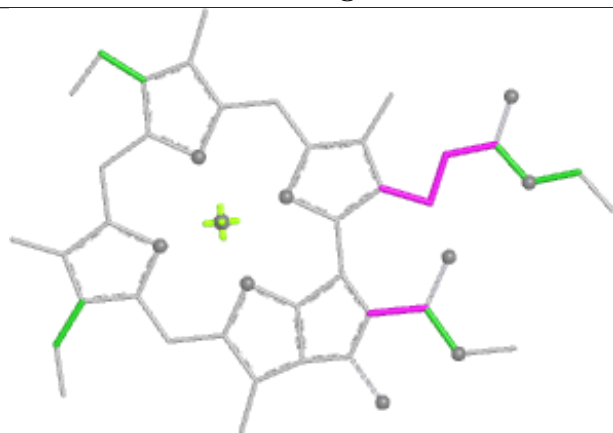
Ligand CLA o 306



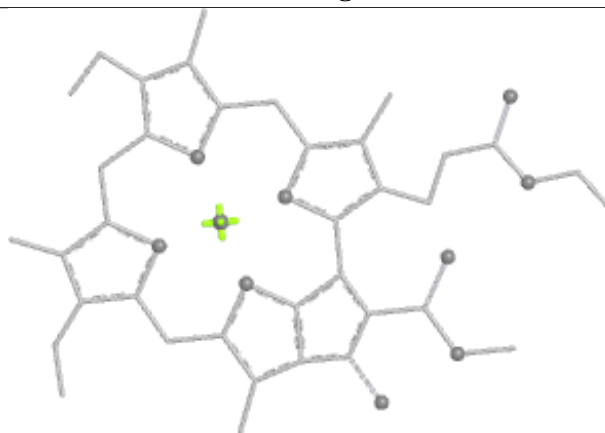
Bond lengths



Bond angles

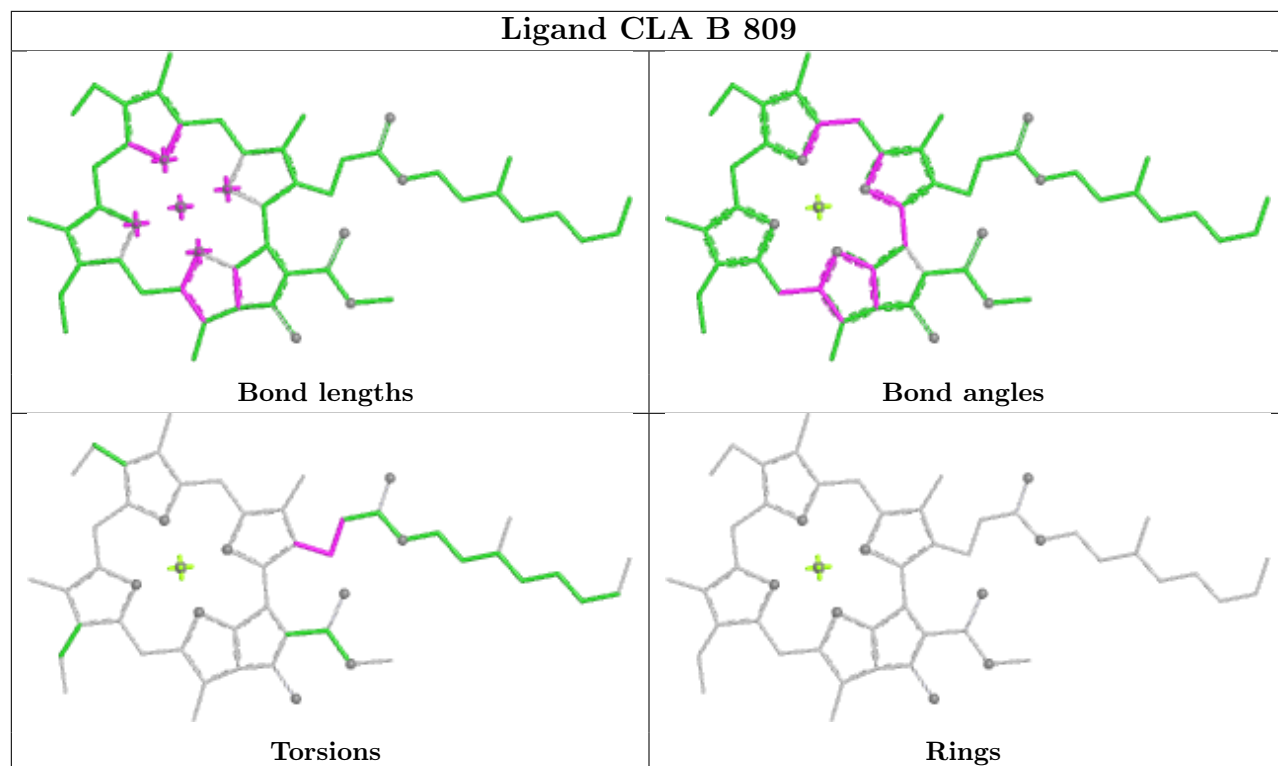


Torsions

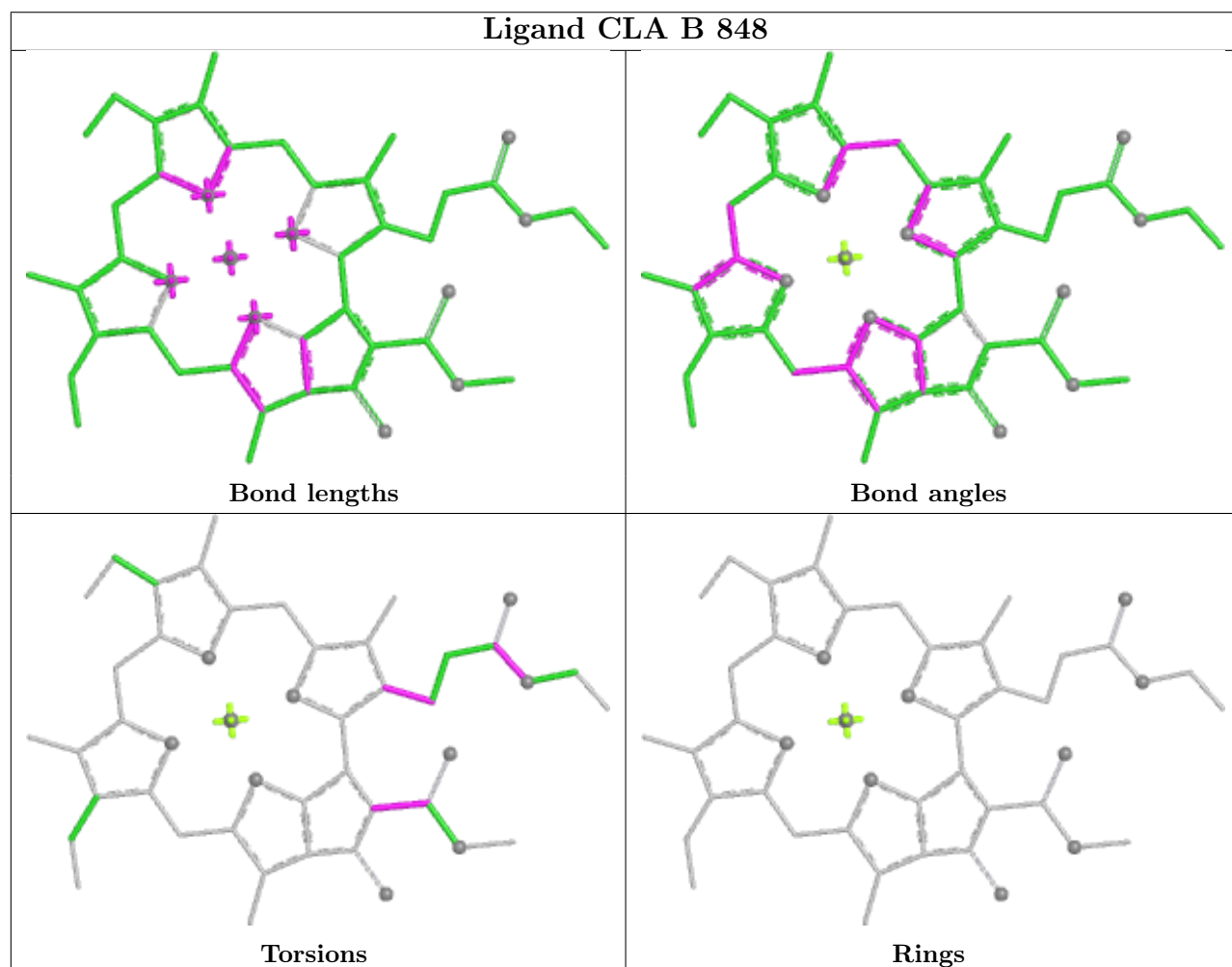


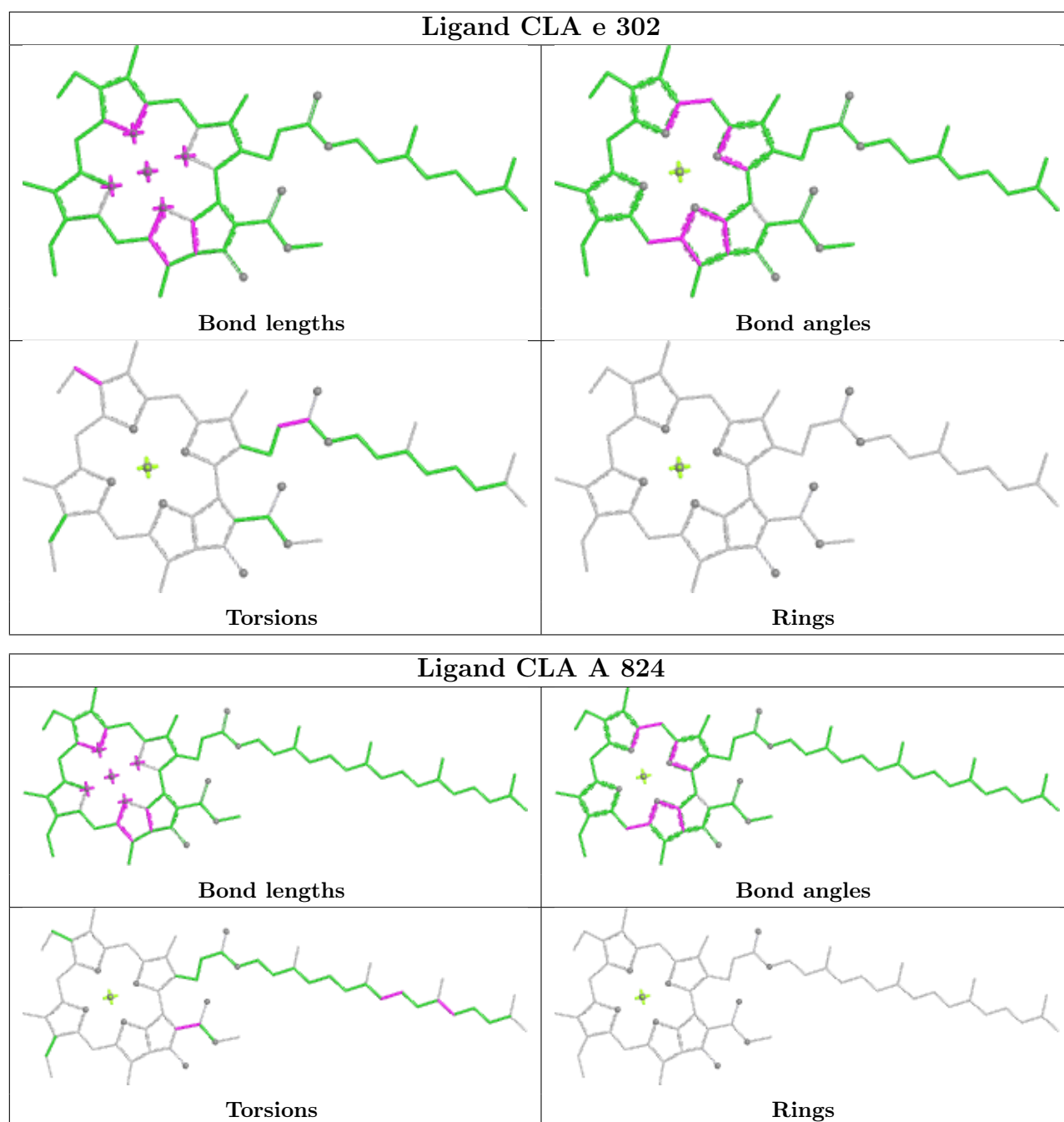
Rings

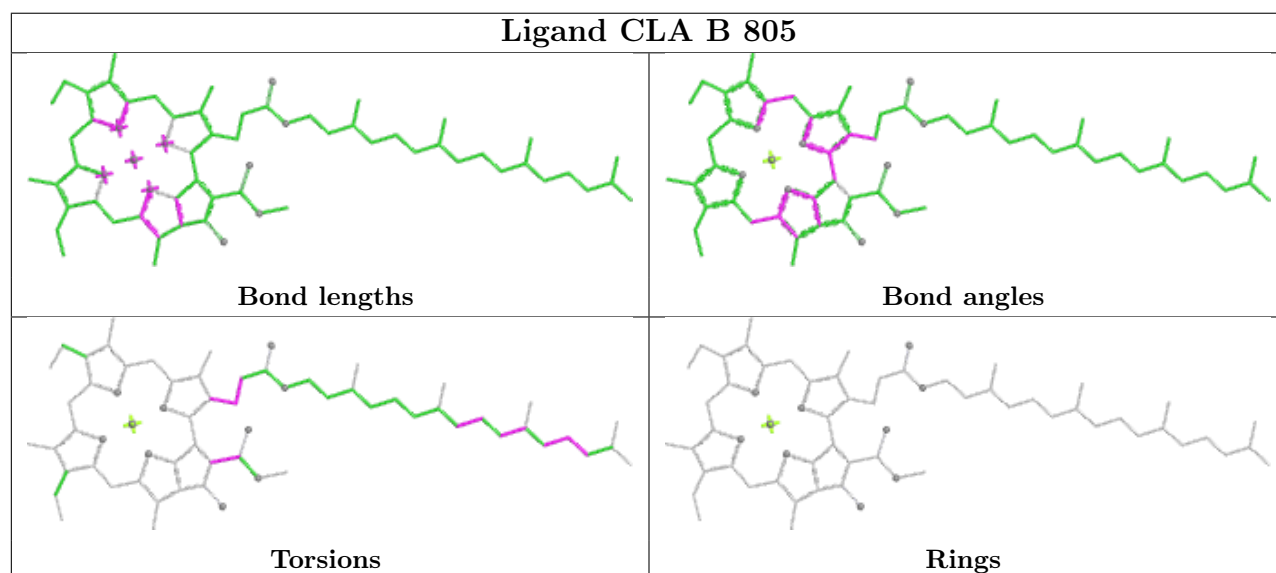
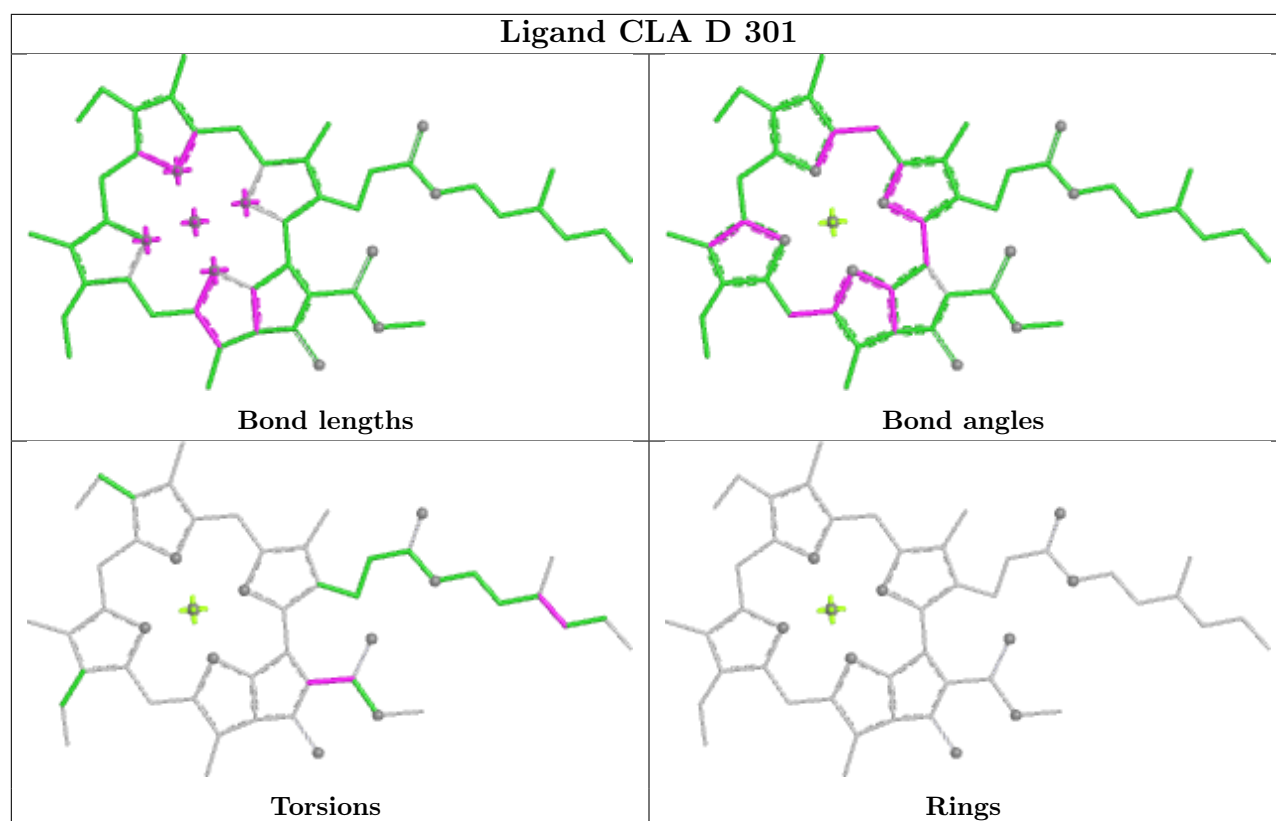
Ligand CLA B 809



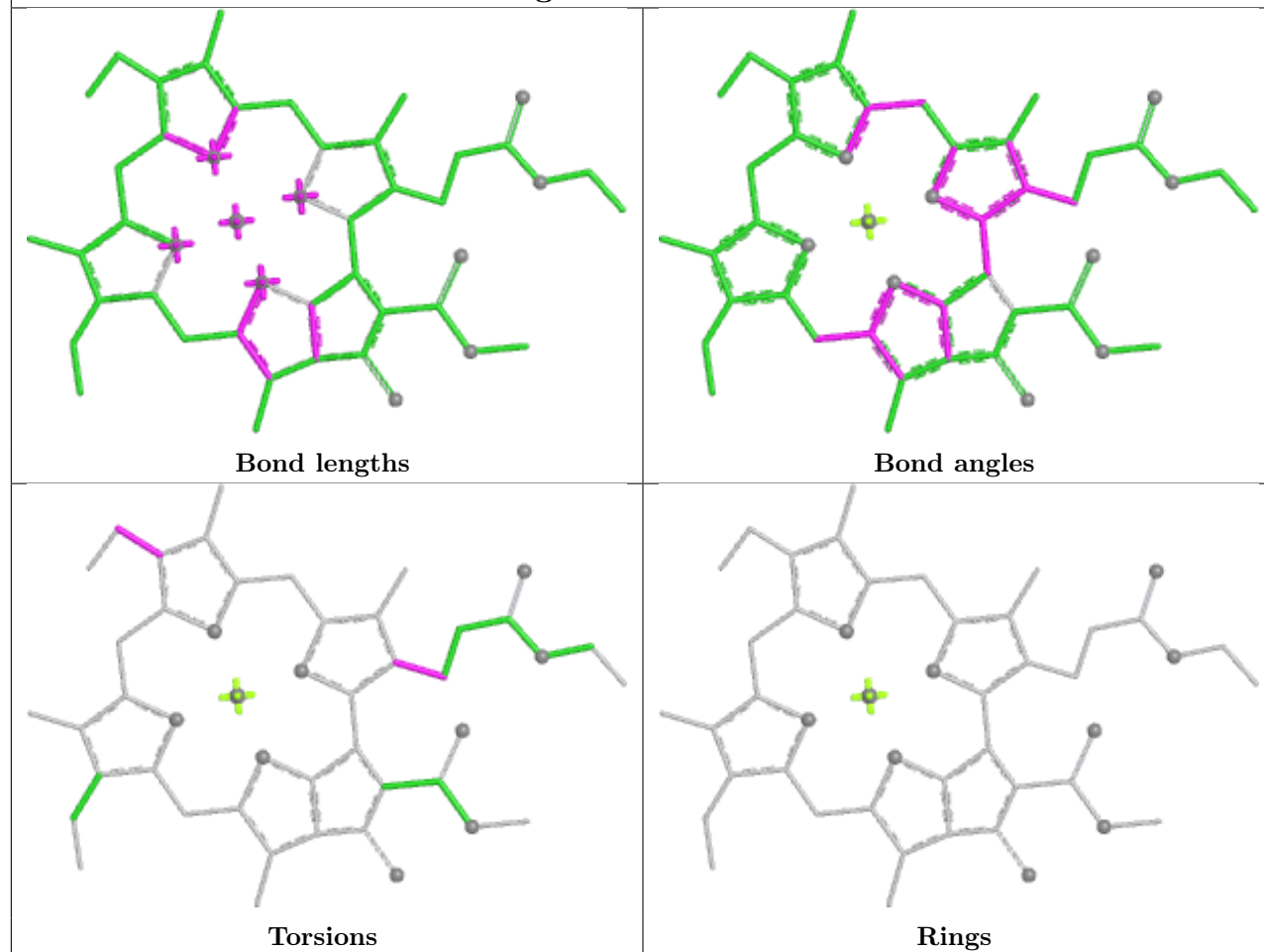
Ligand CLA B 848



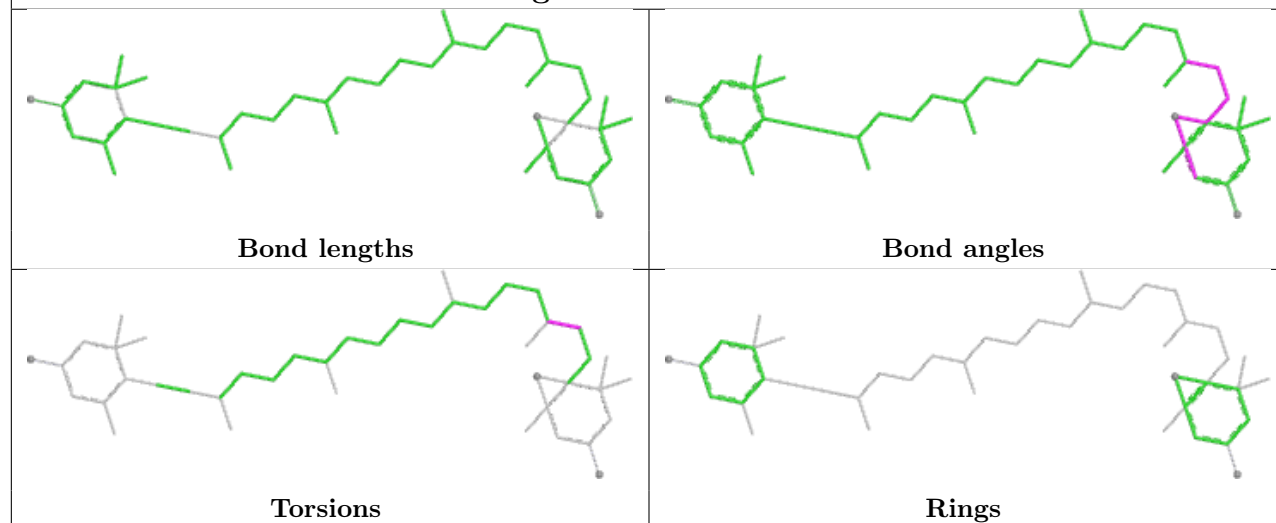


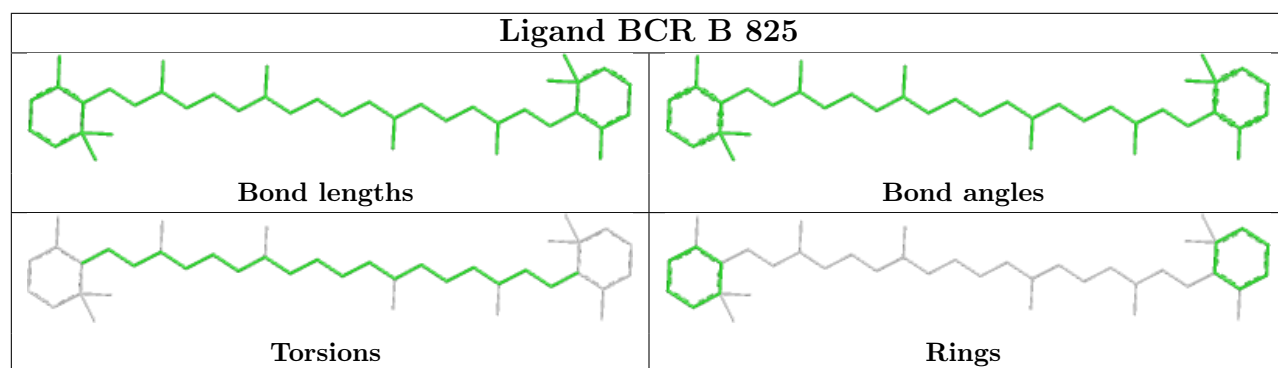
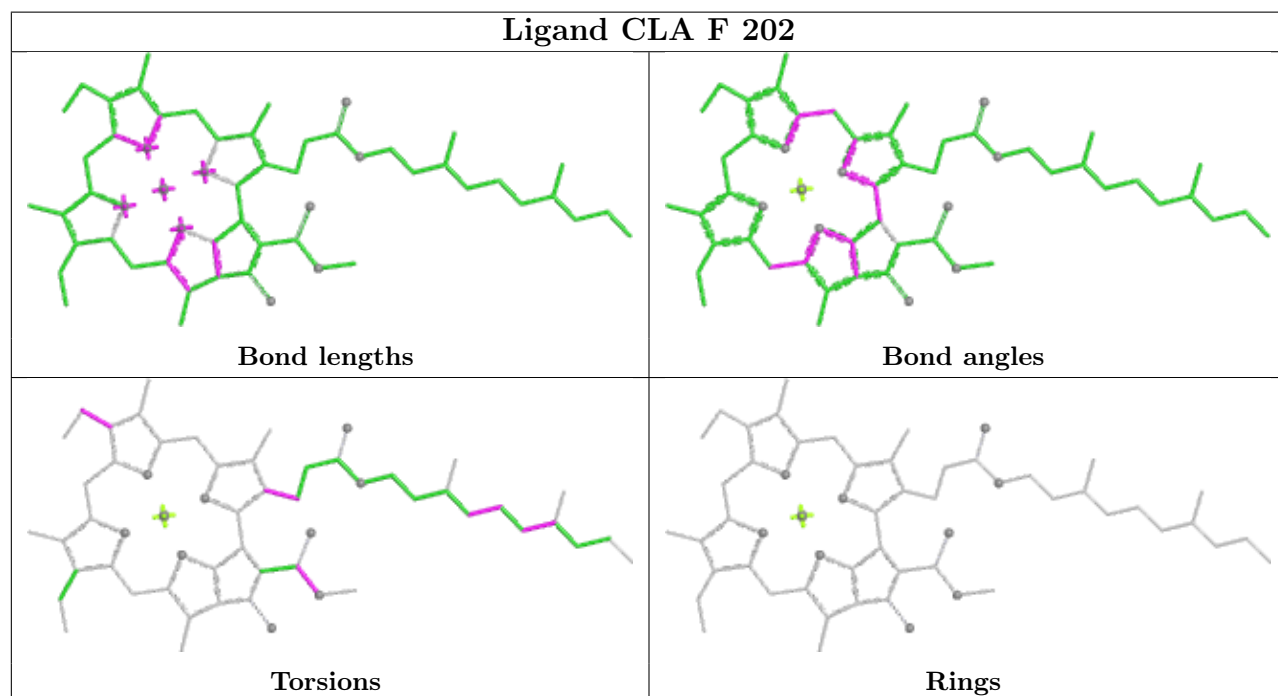
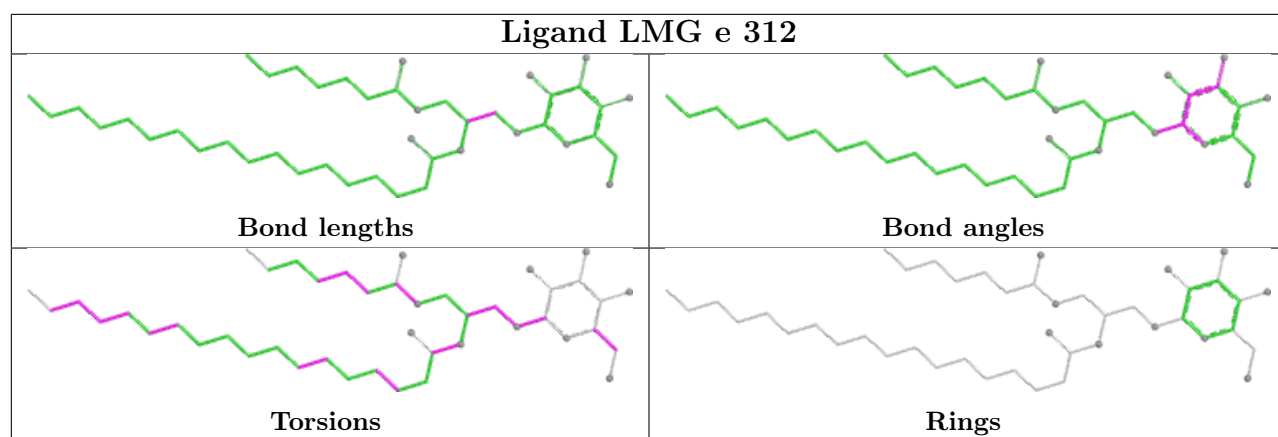


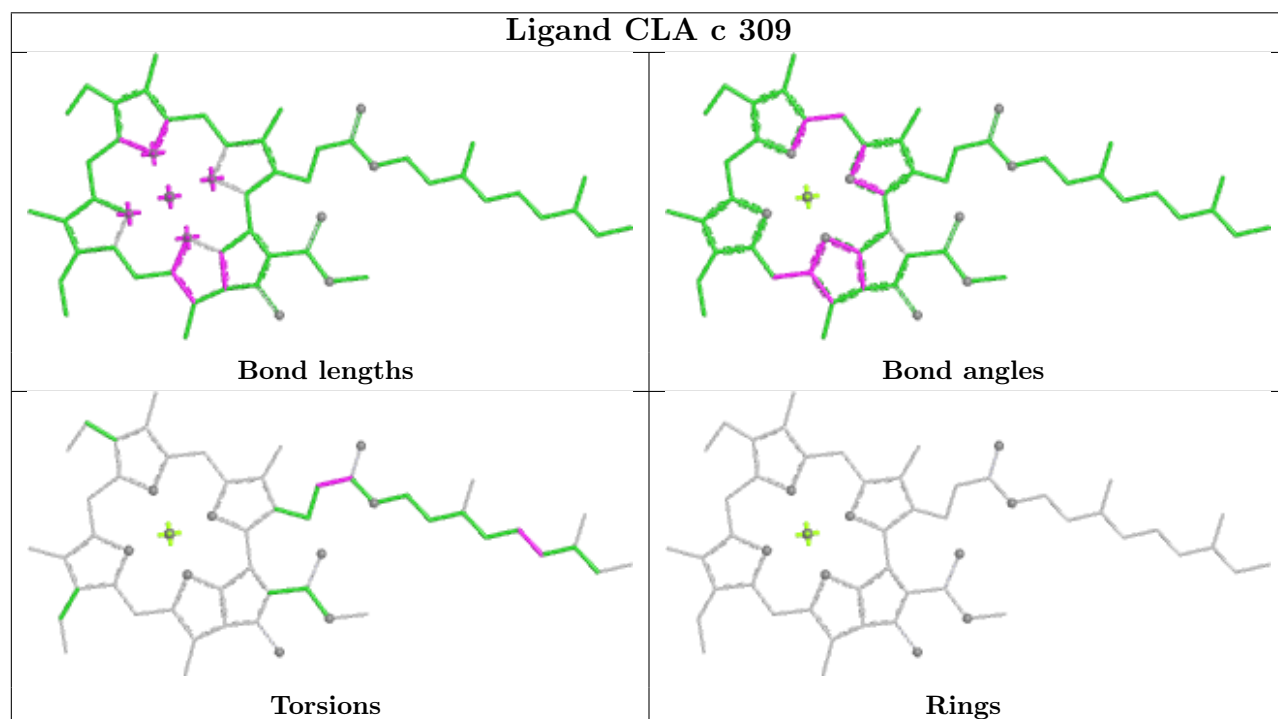
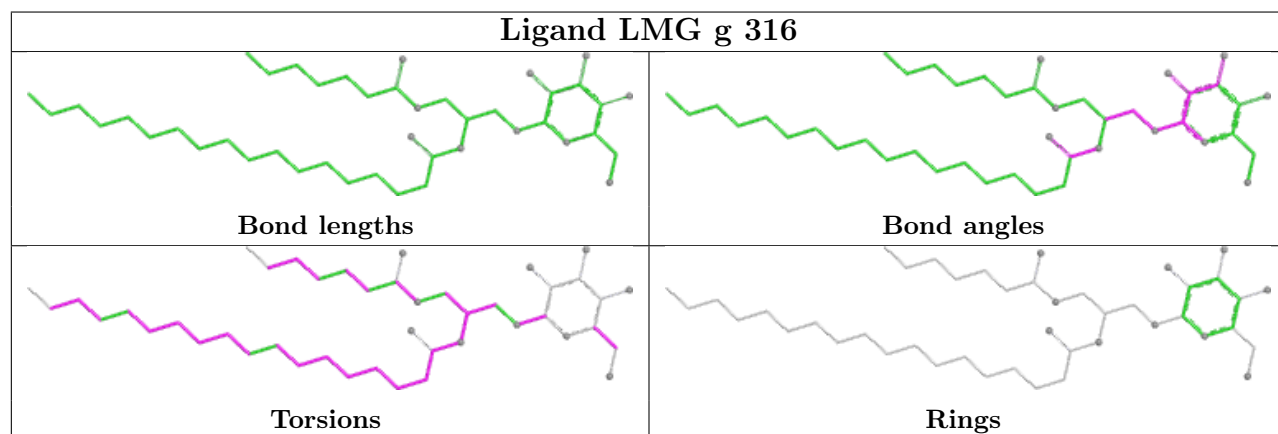
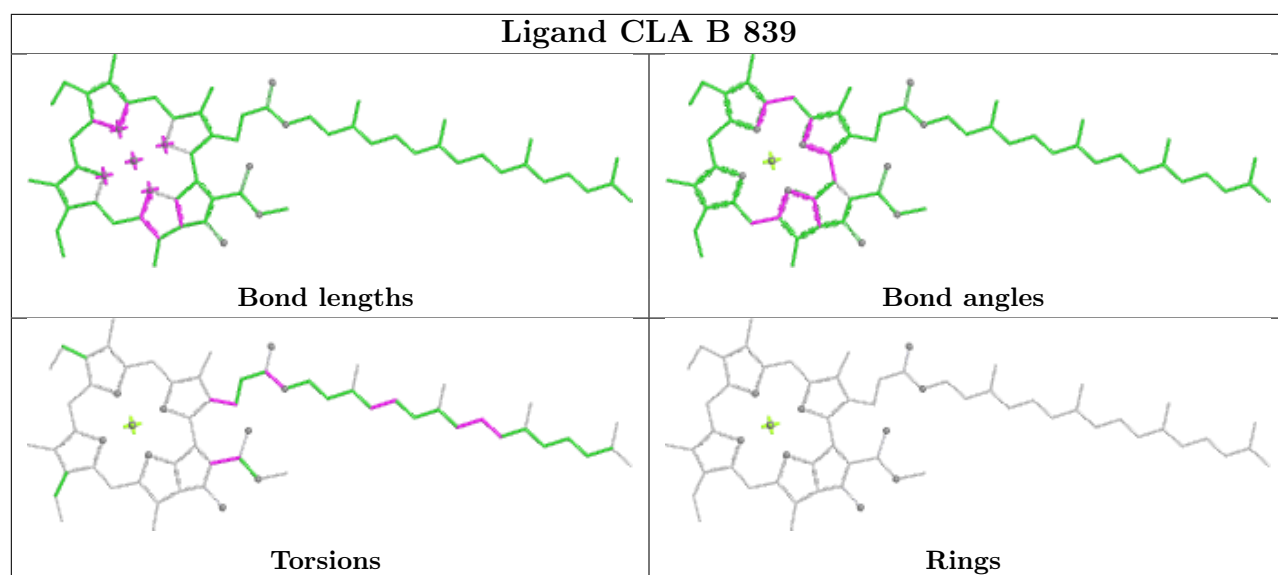
Ligand CLA 1 209

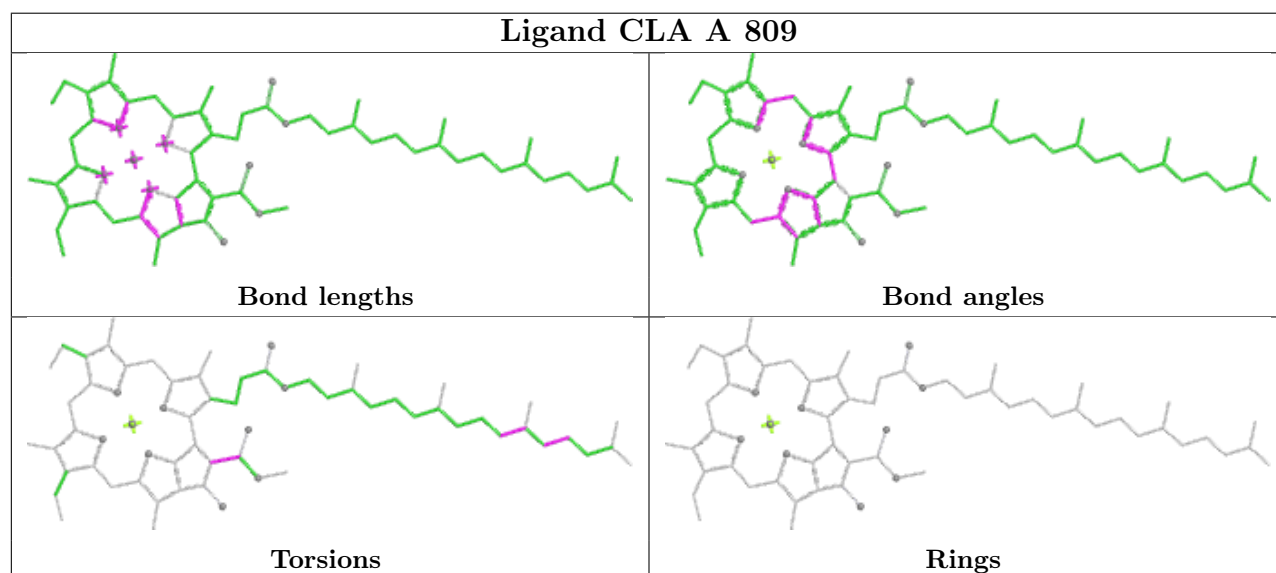
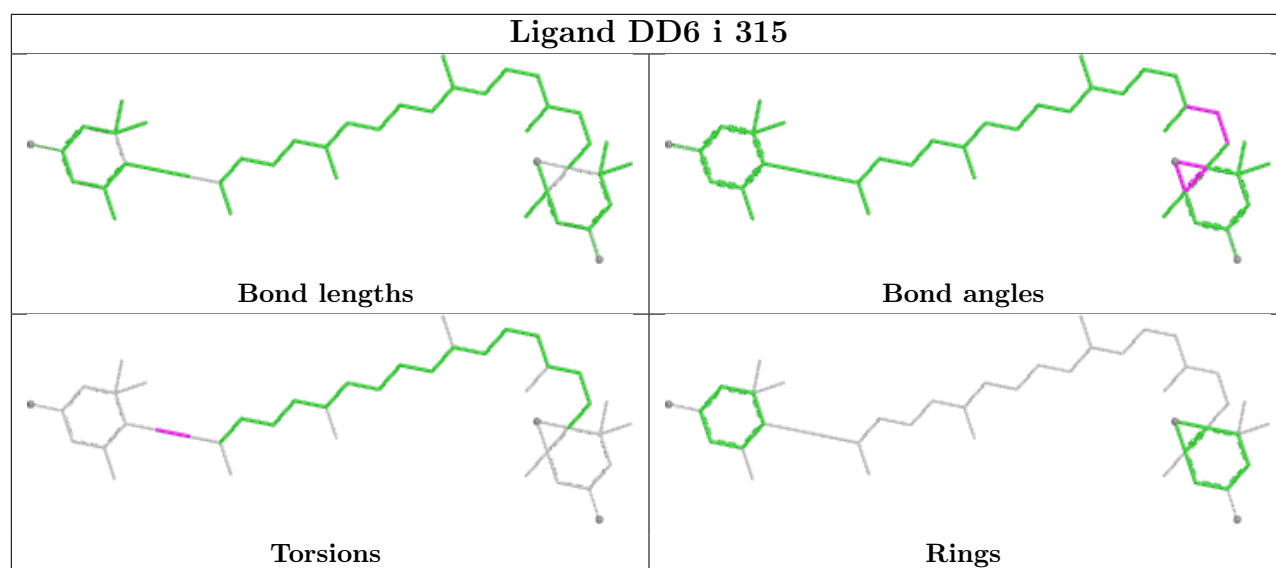


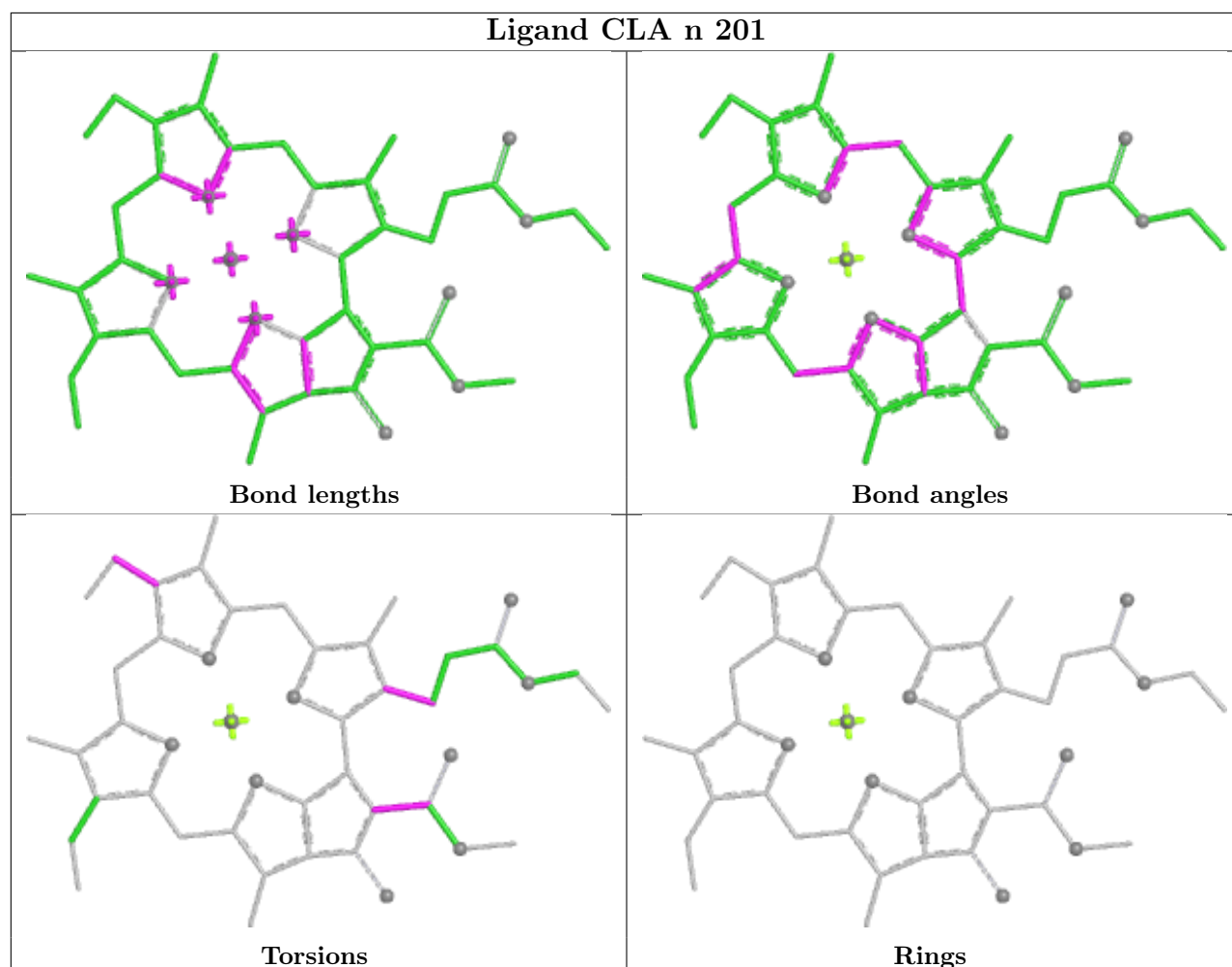
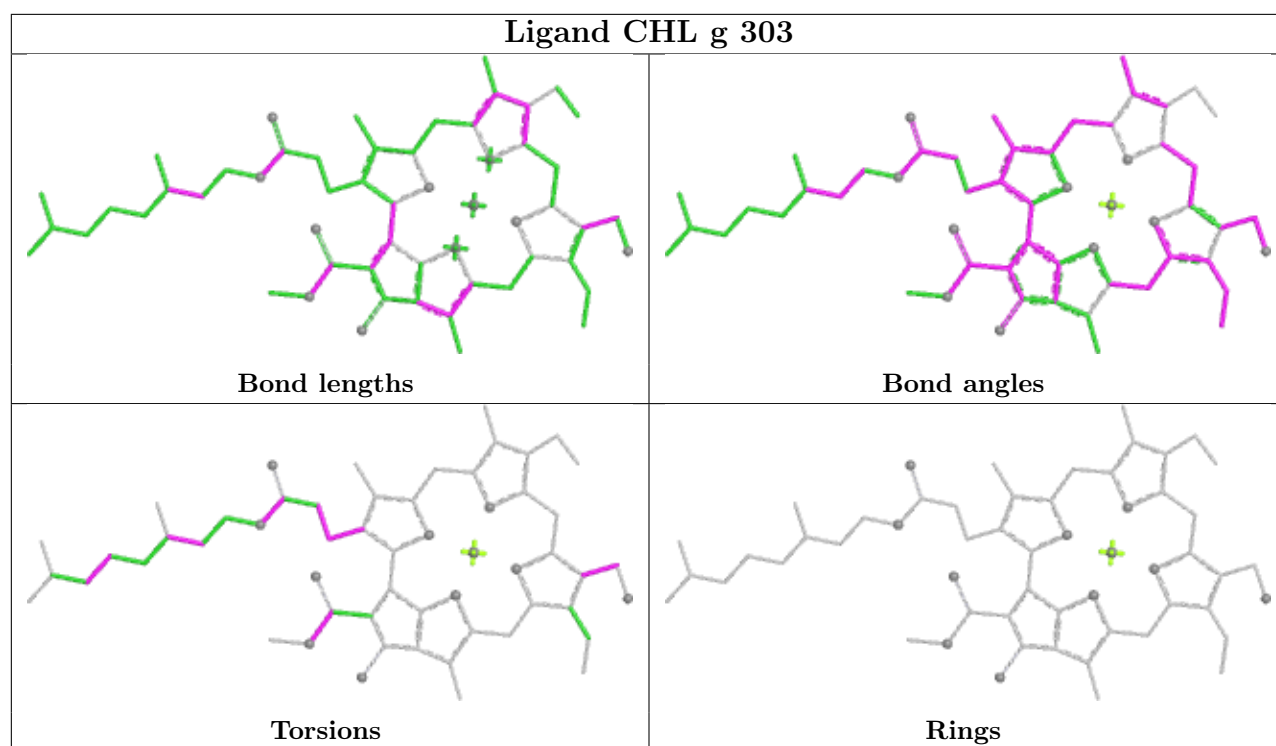
Ligand DD6 A 832

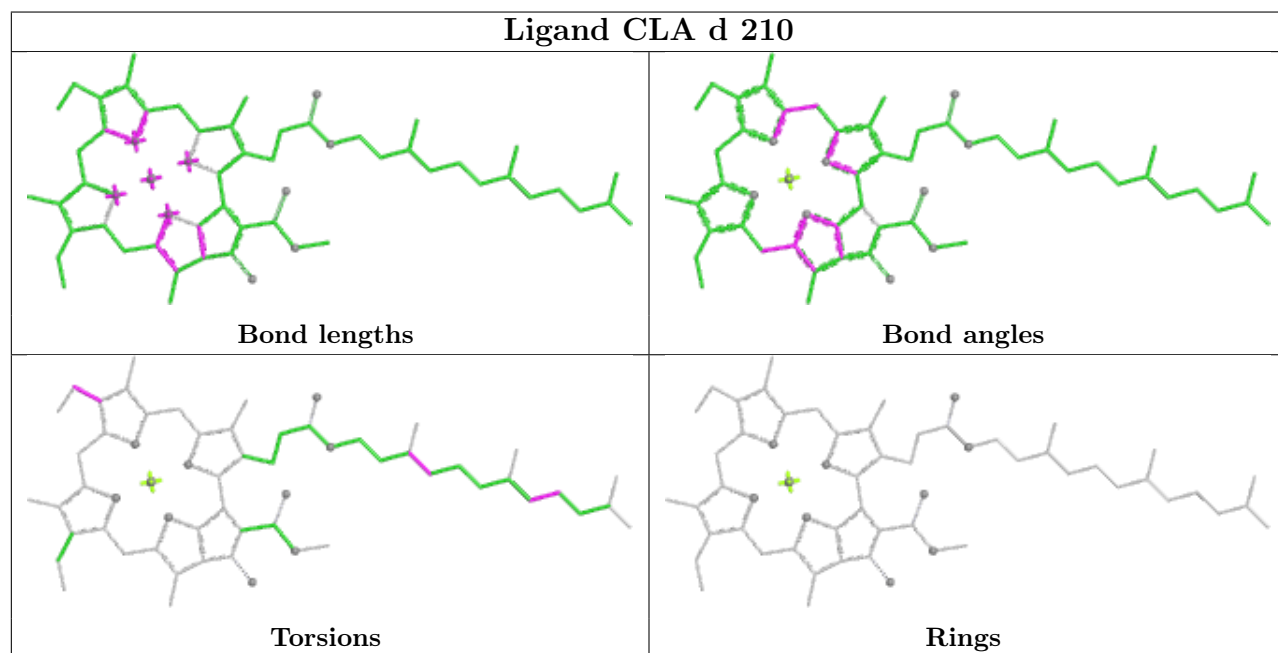
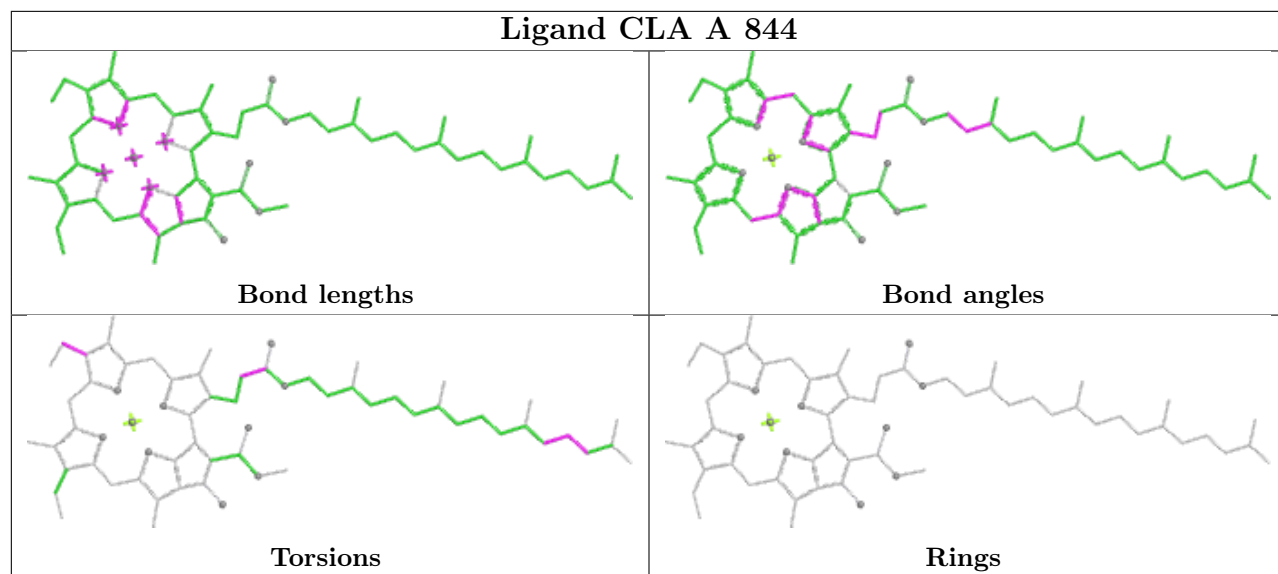


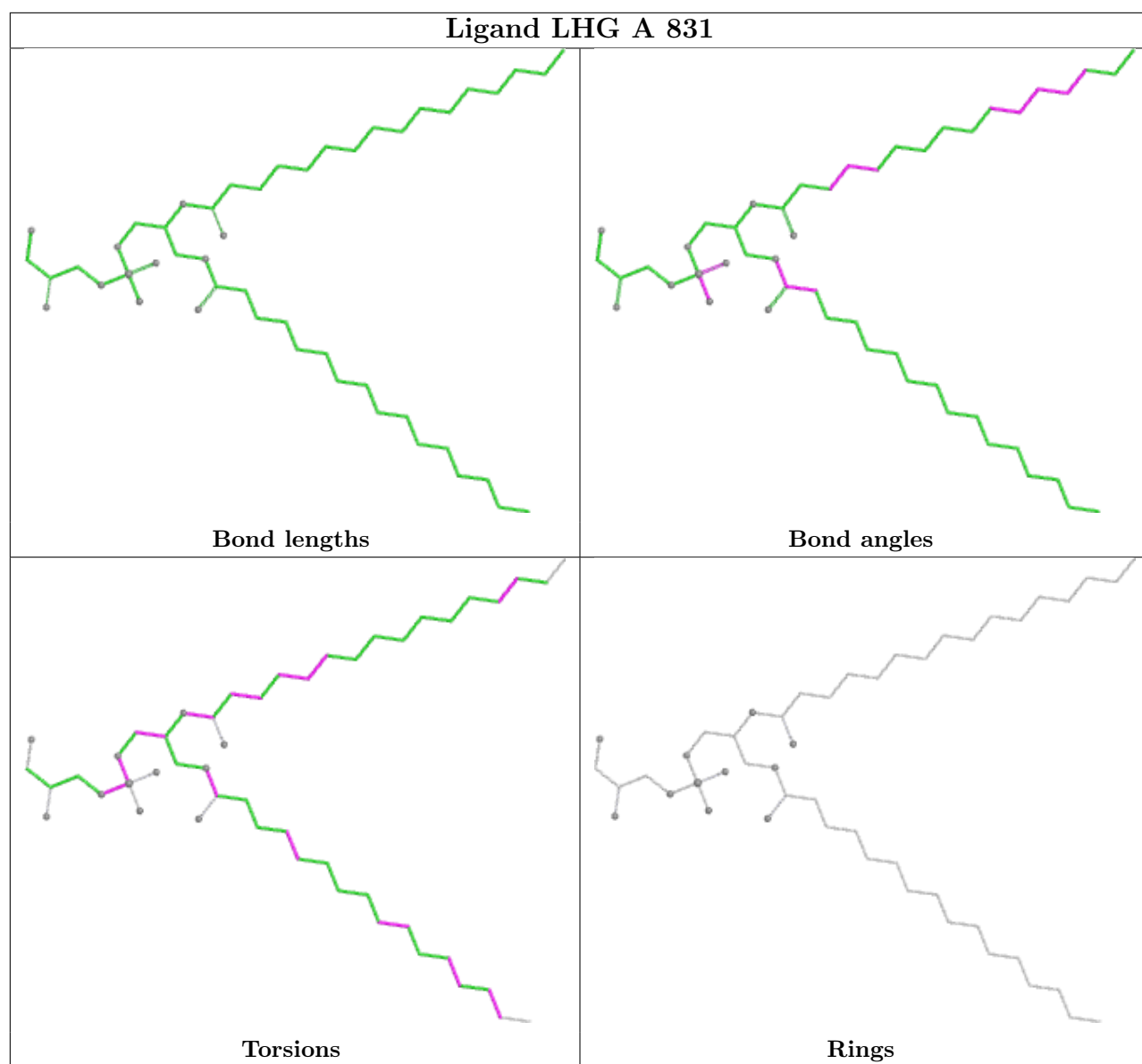




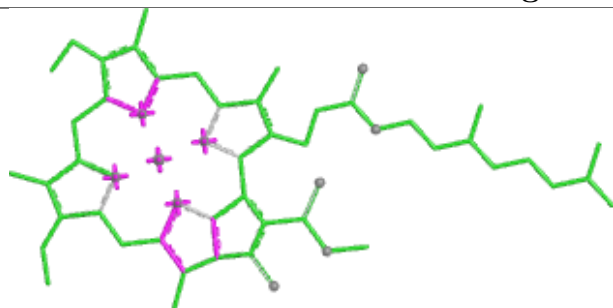




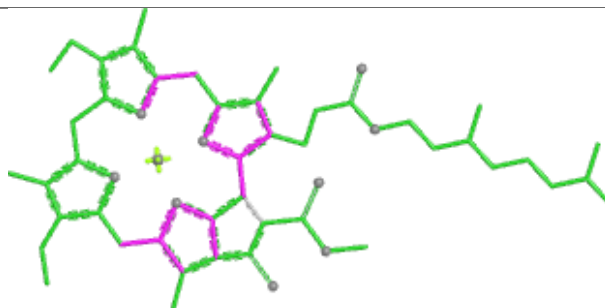




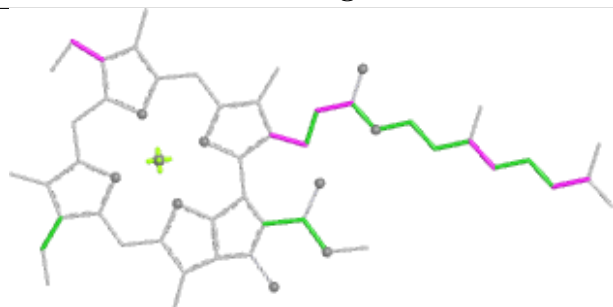
Ligand CLA f 314



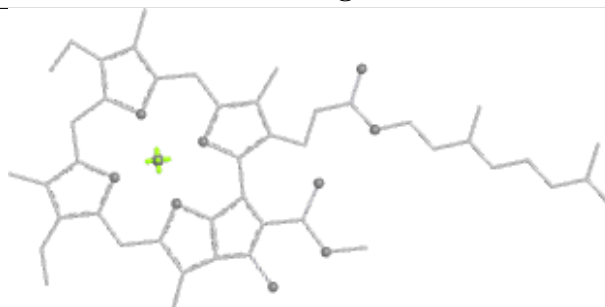
Bond lengths



Bond angles

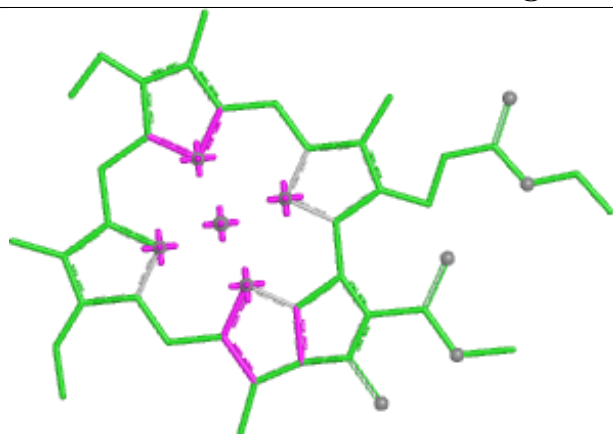


Torsions

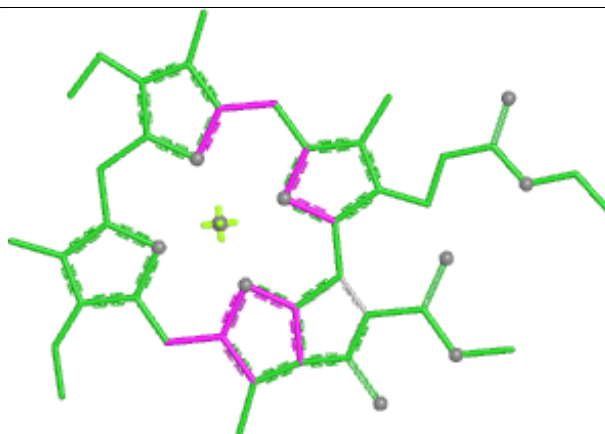


Rings

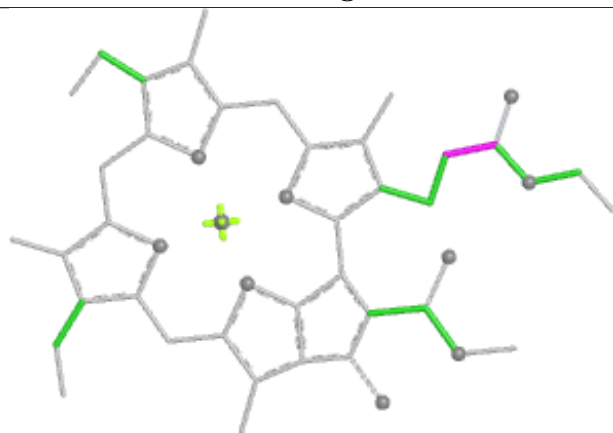
Ligand CLA i 312



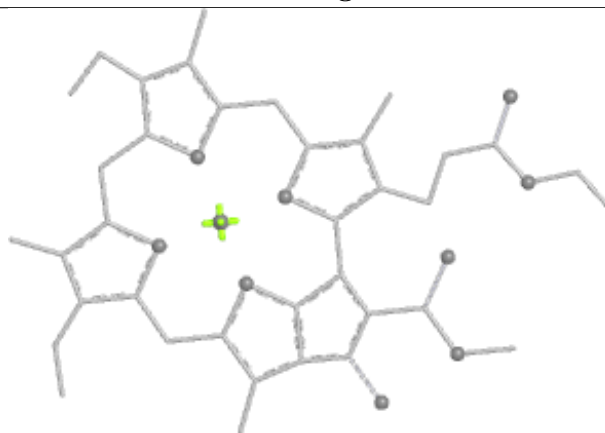
Bond lengths



Bond angles

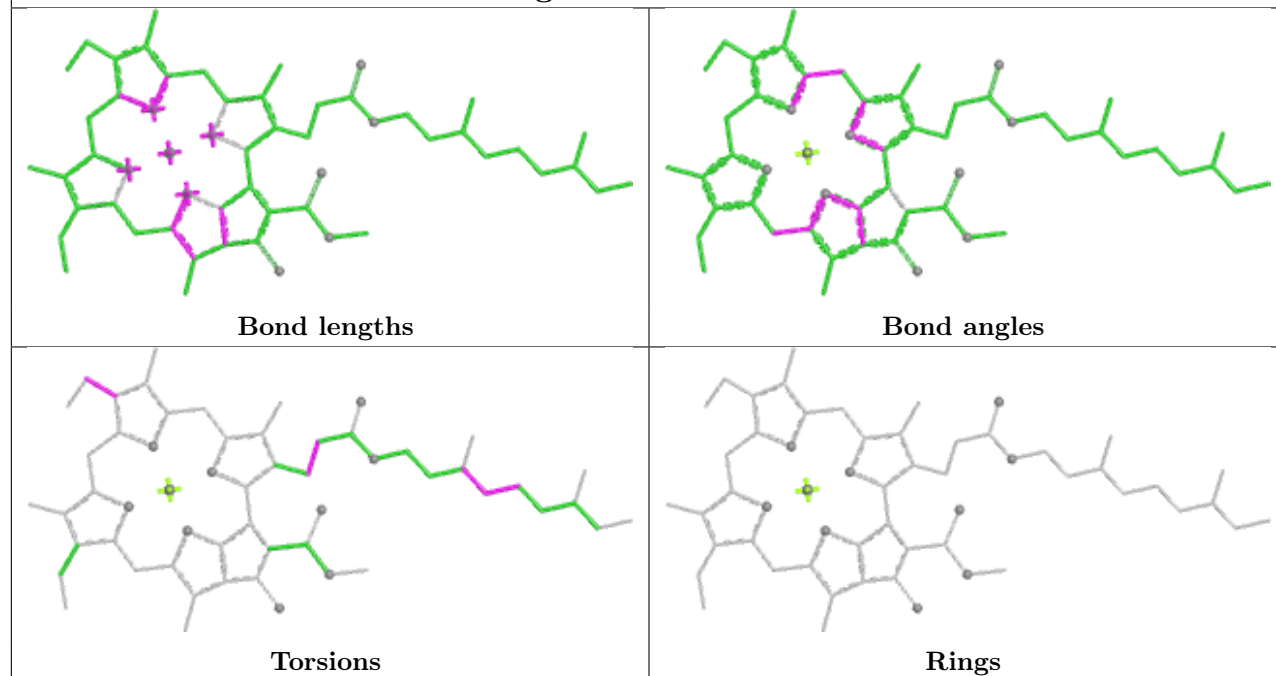


Torsions

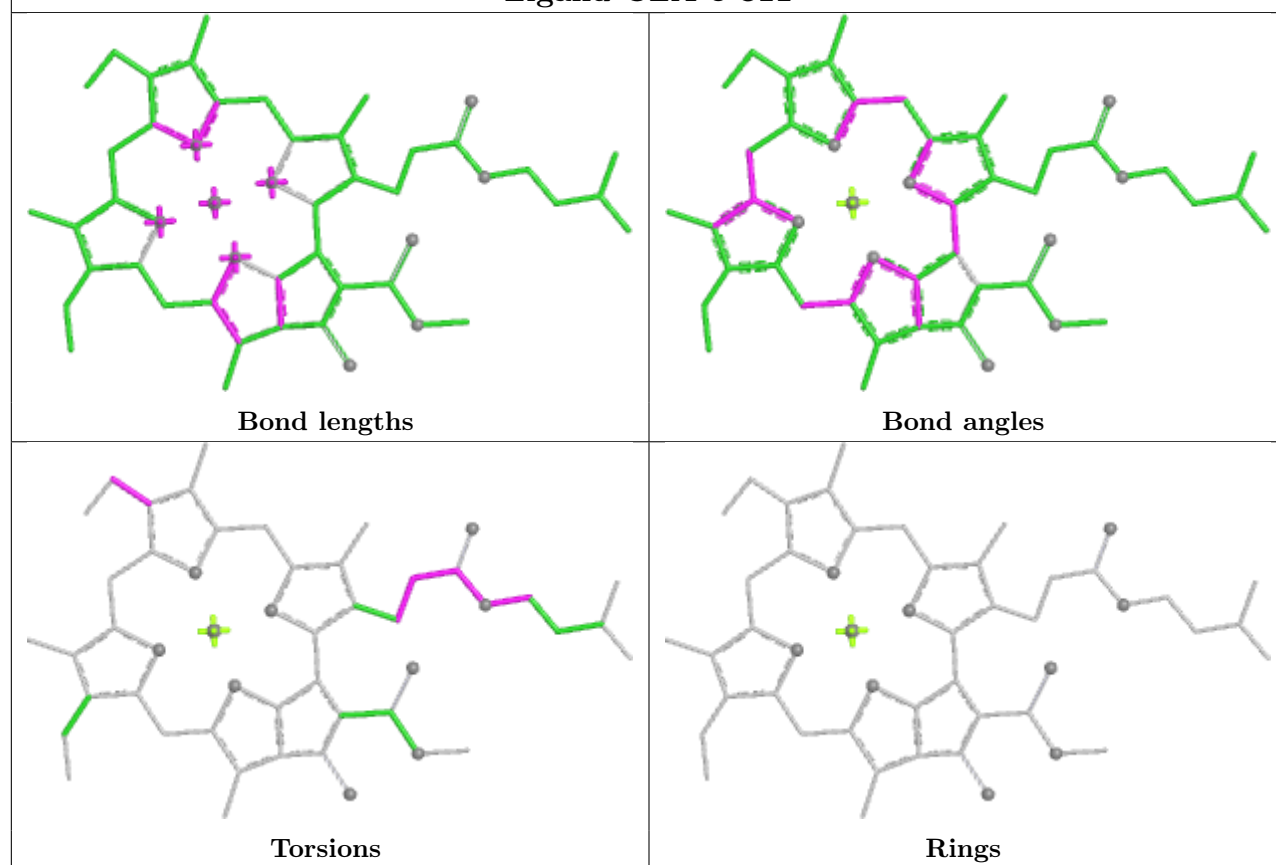


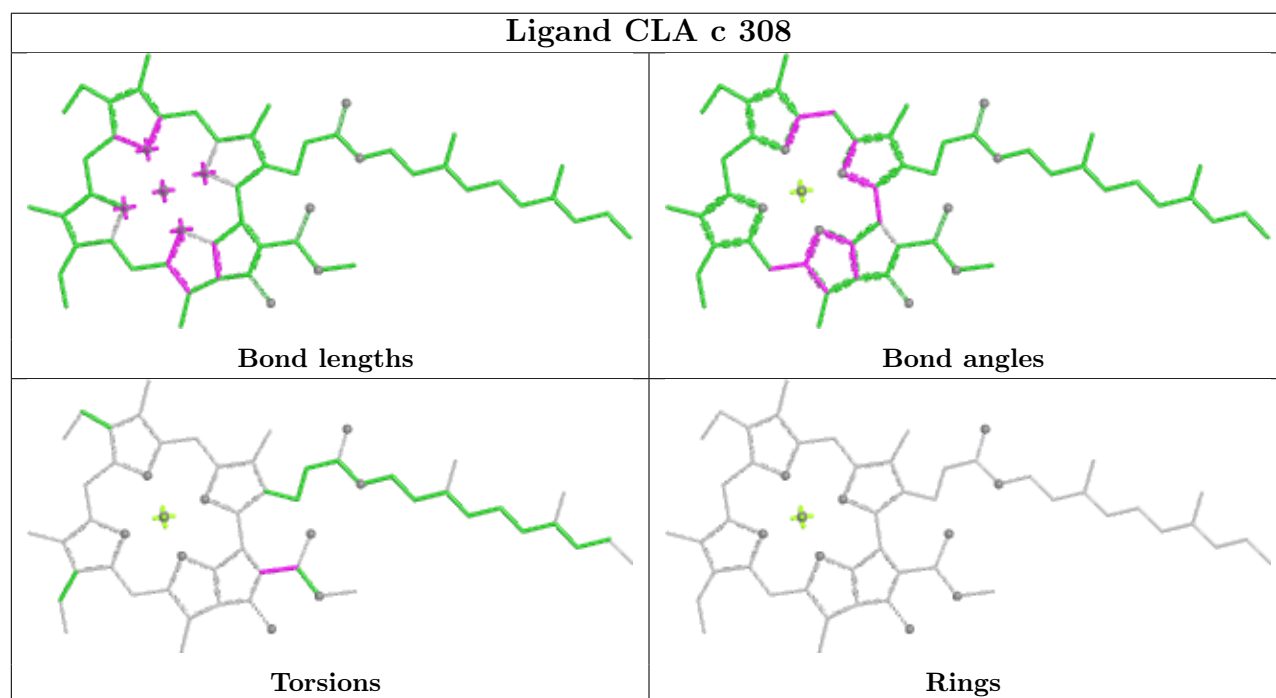
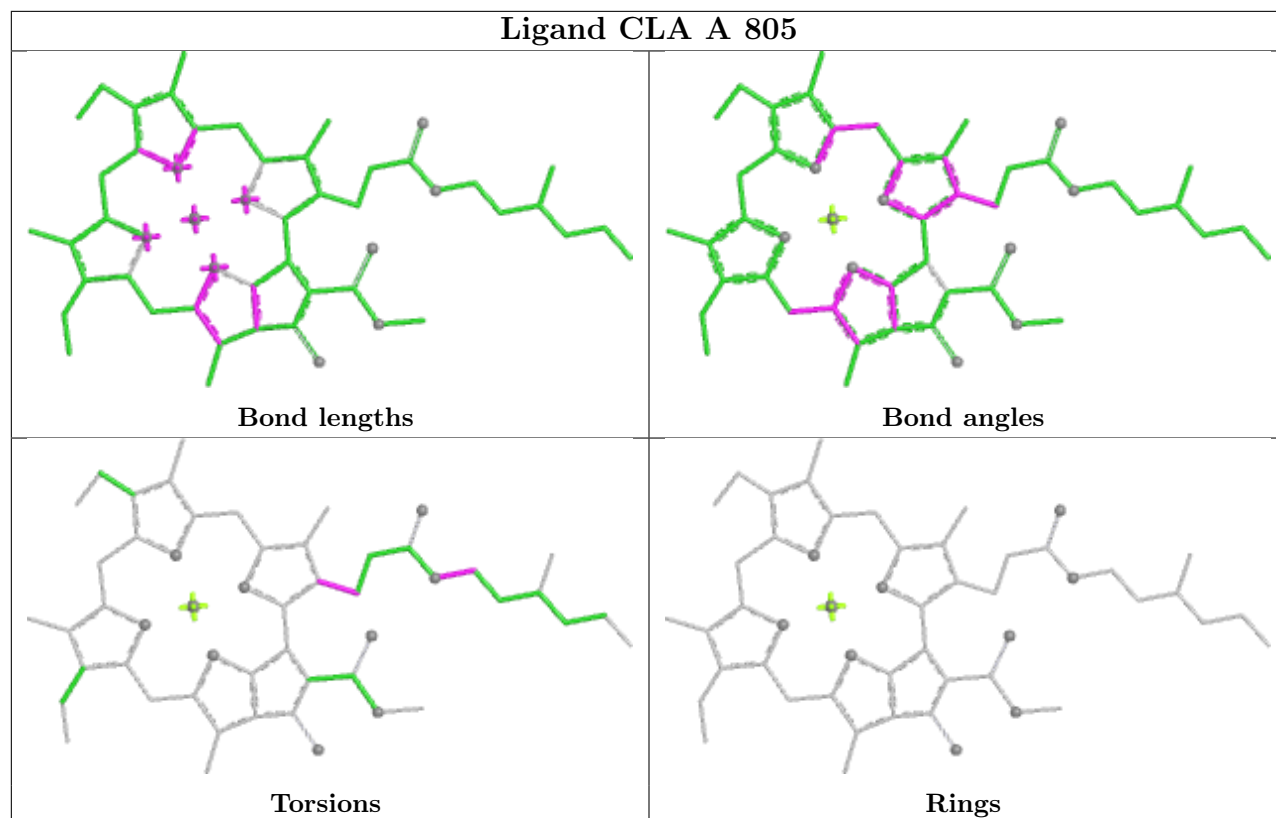
Rings

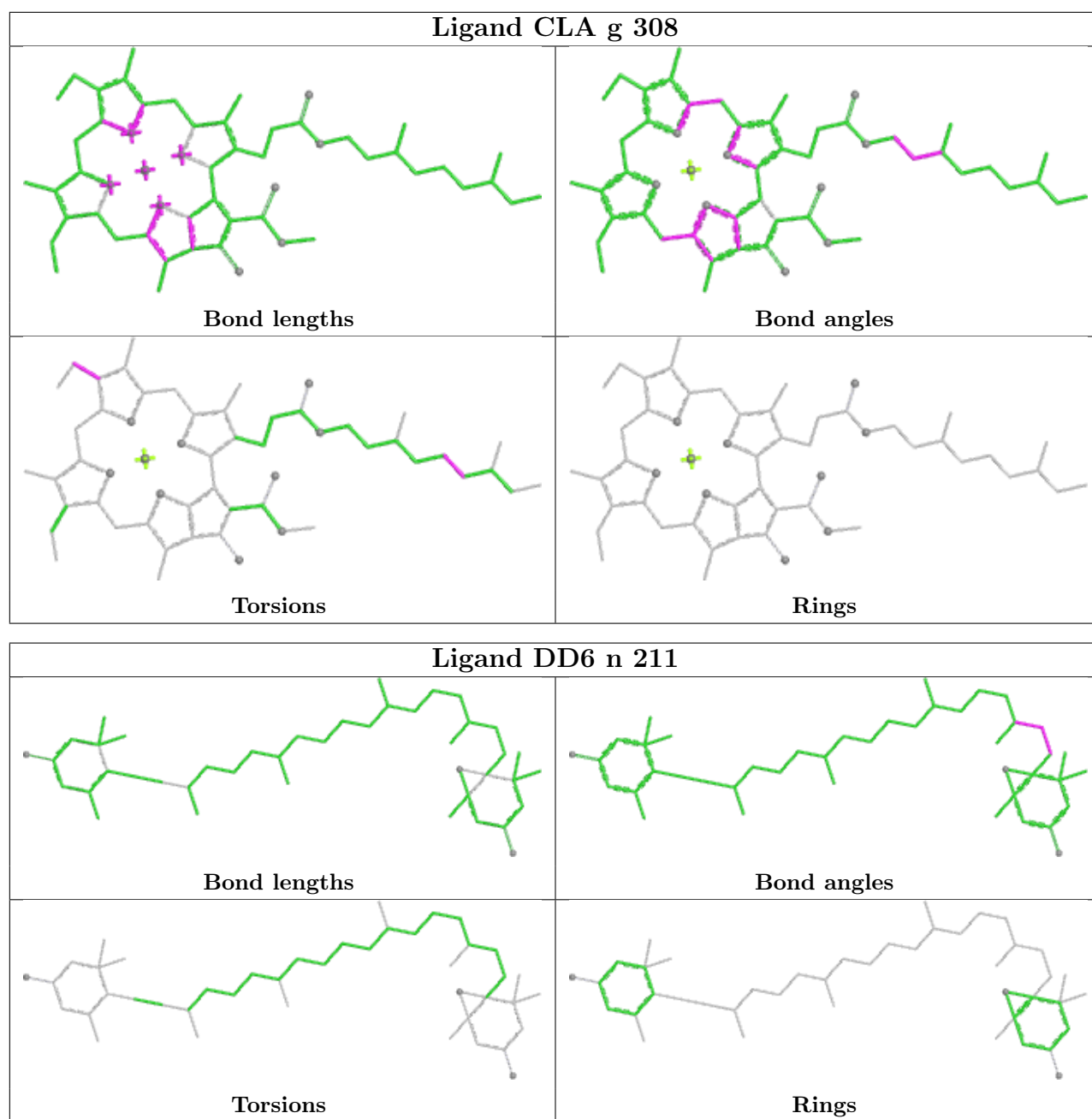
Ligand CLA d 209



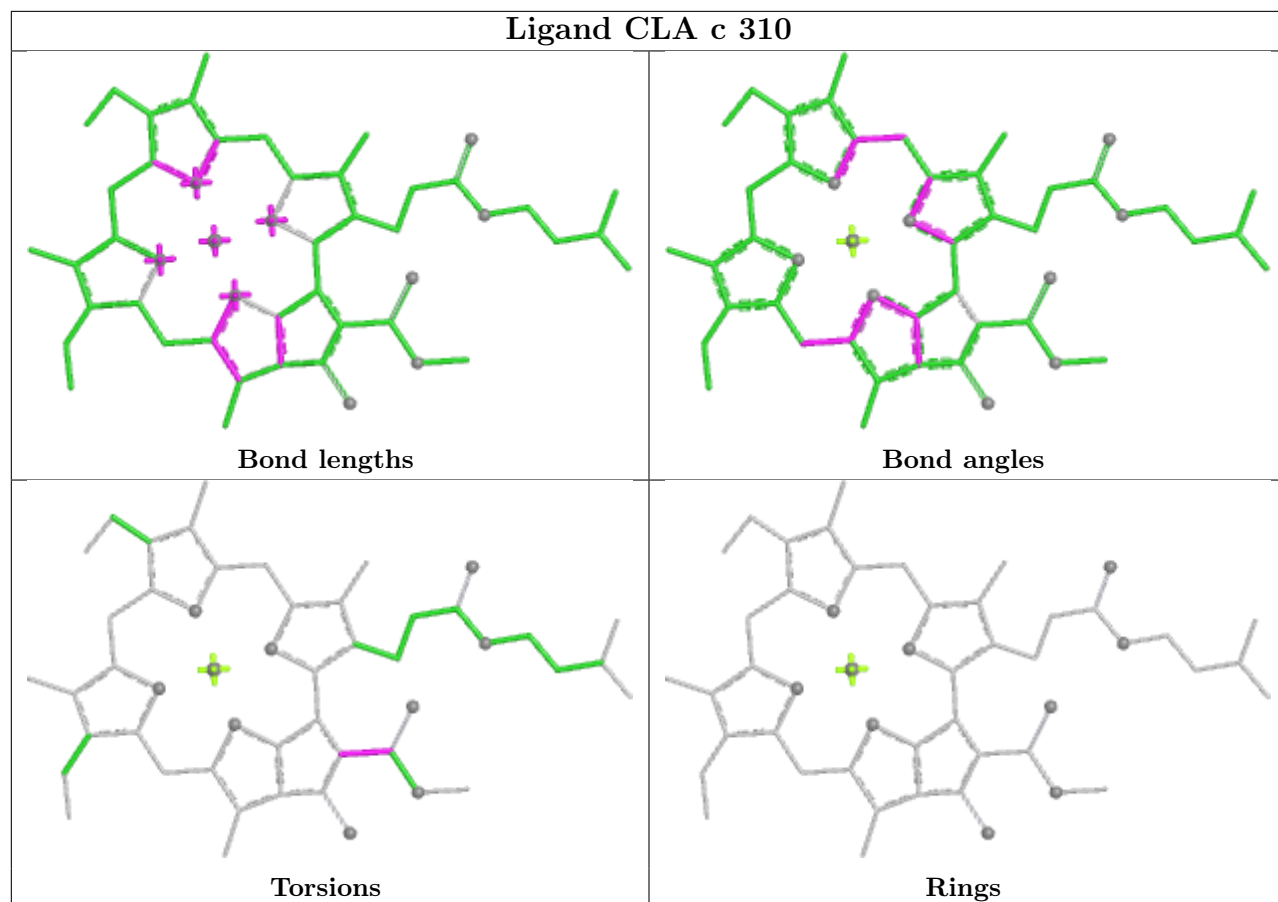
Ligand CLA o 311



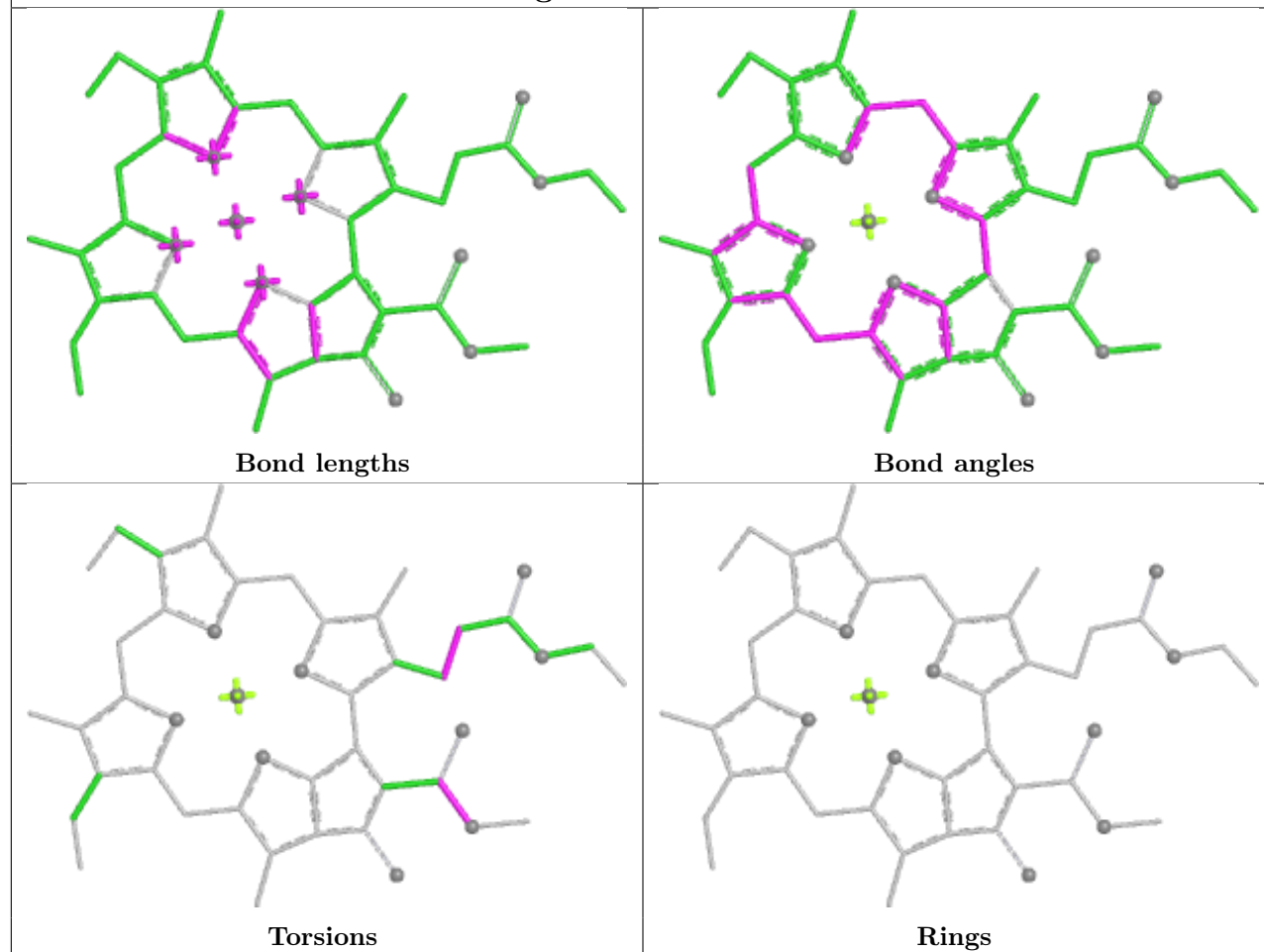




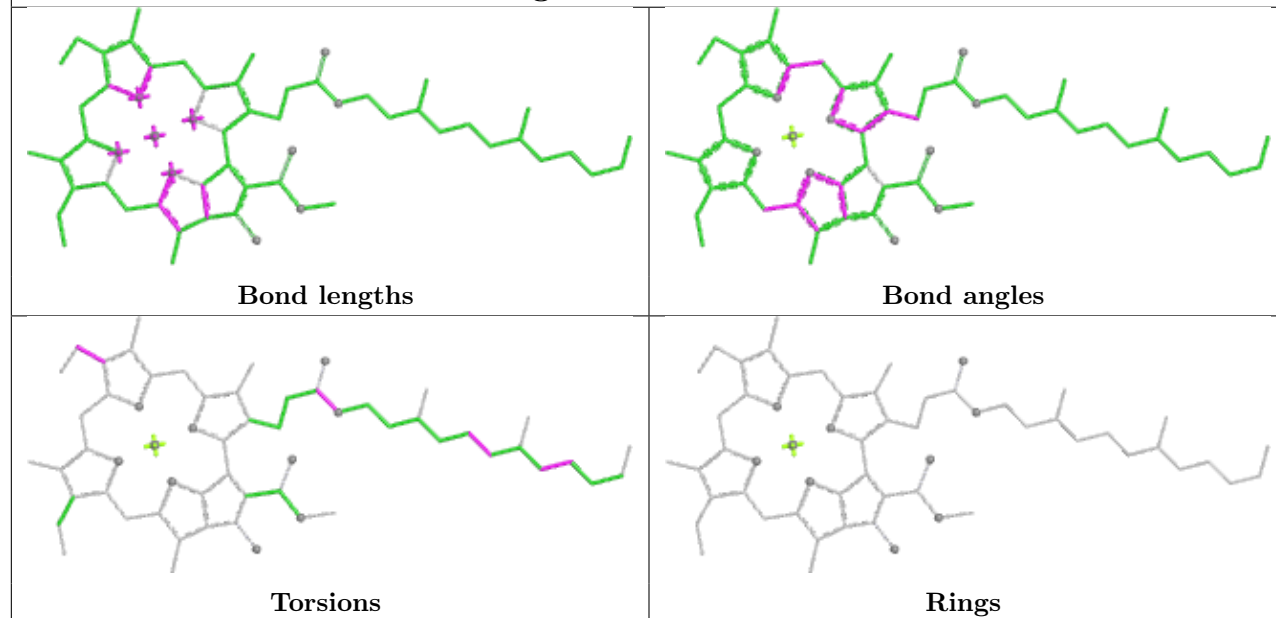
Ligand CLA c 310

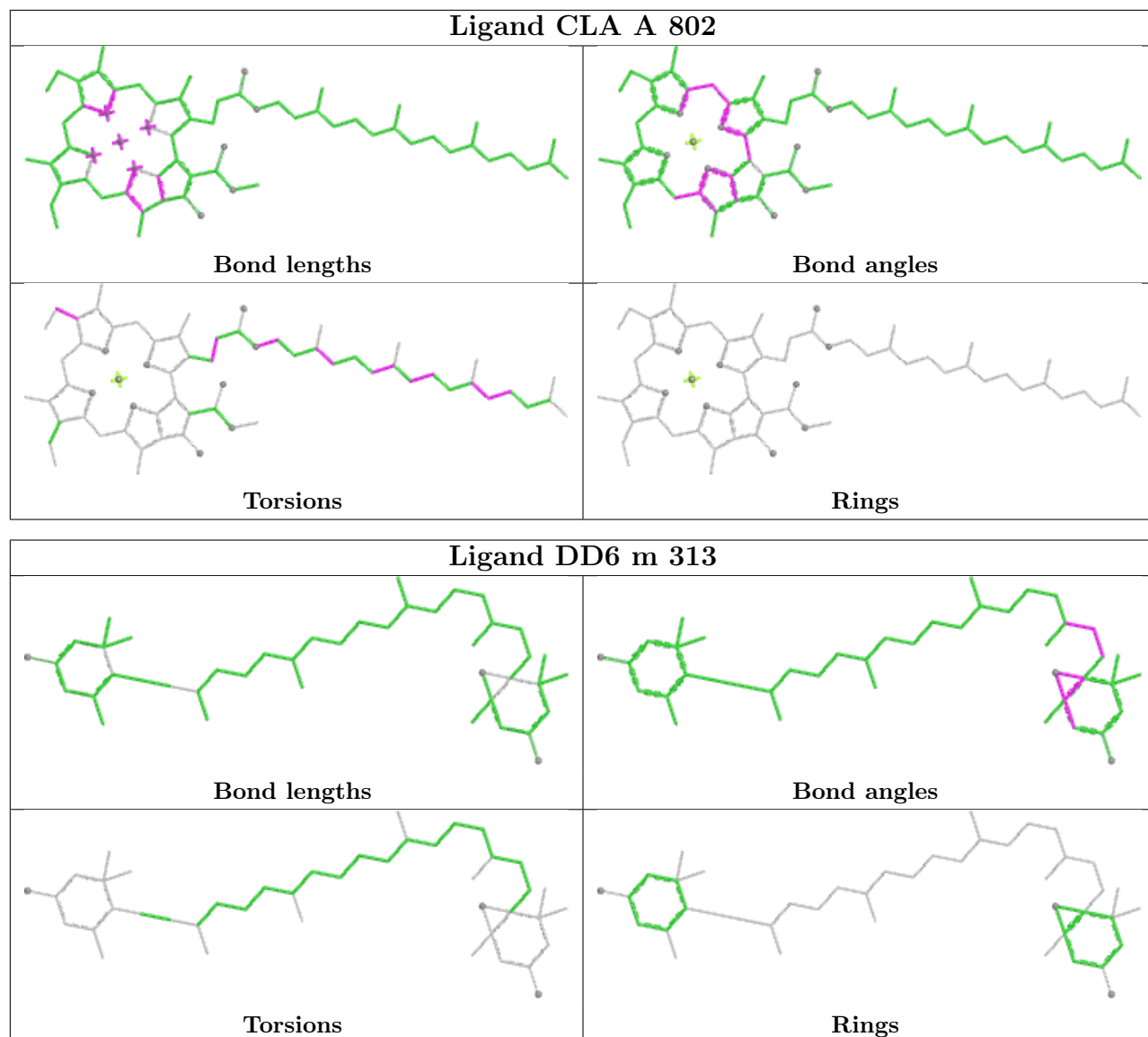


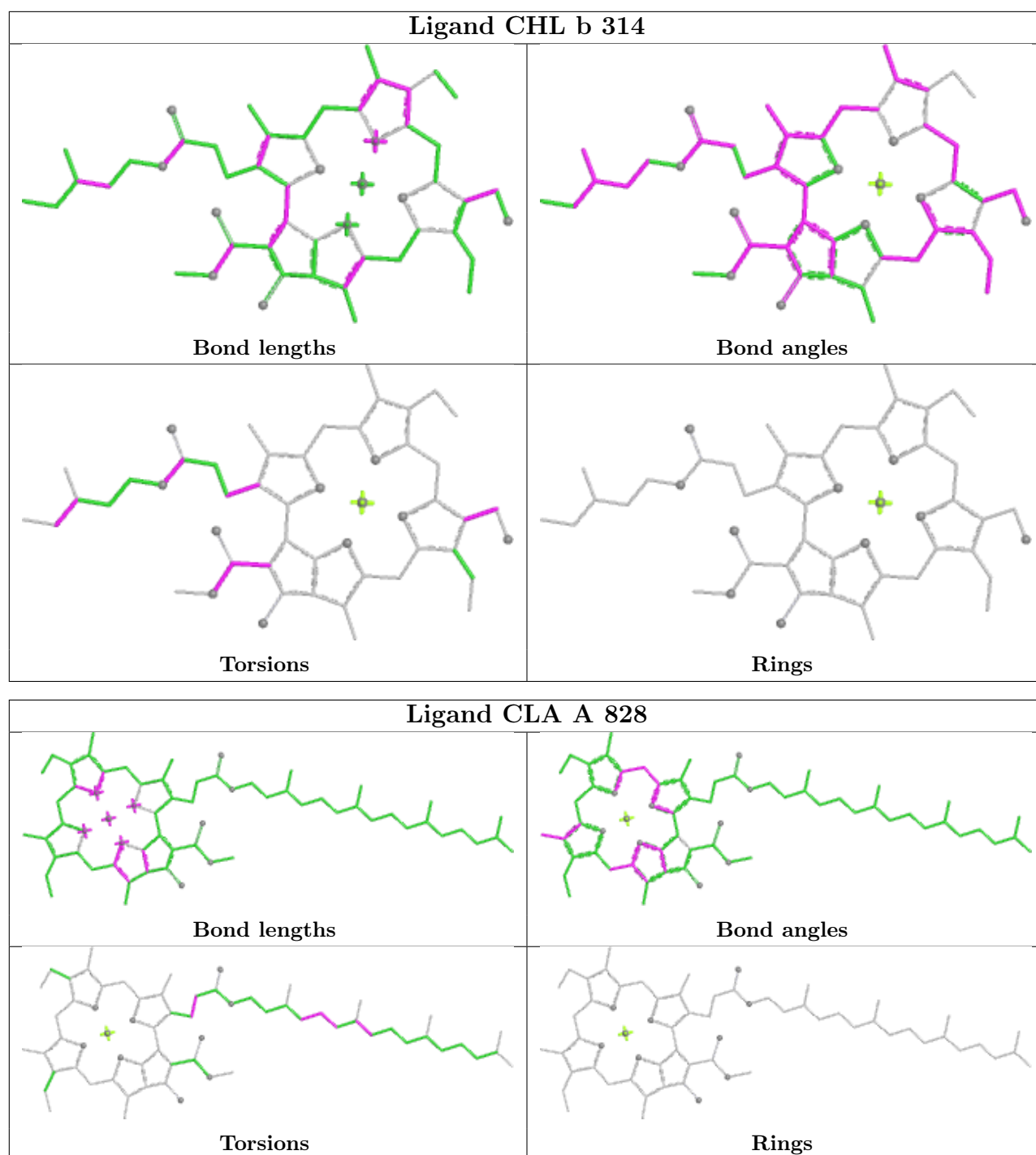
Ligand CLA I 201



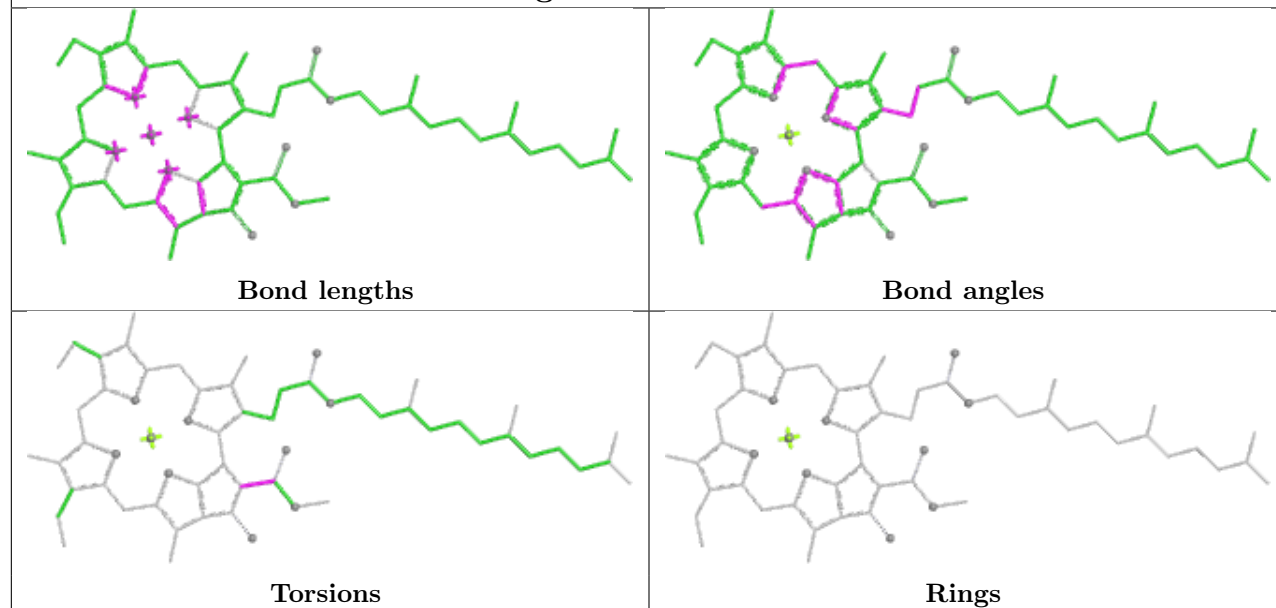
Ligand CLA B 814



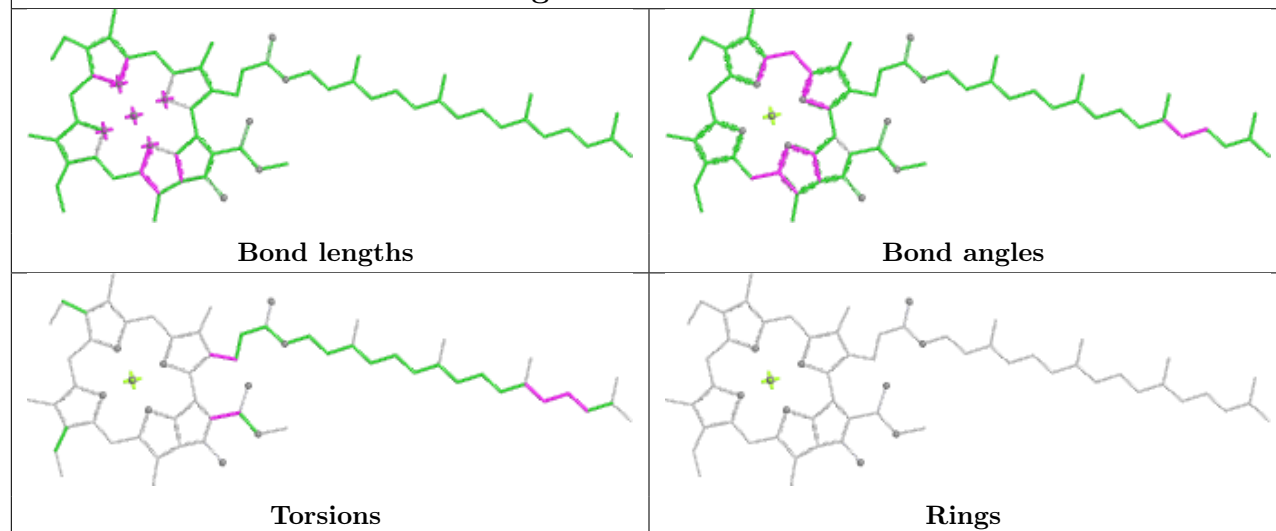




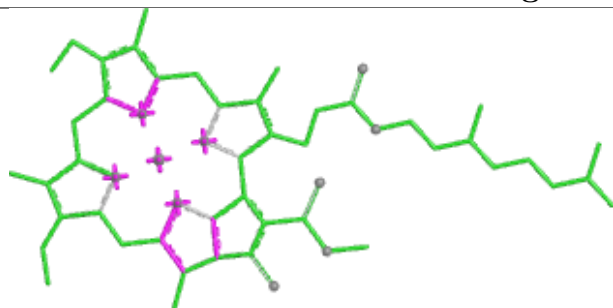
Ligand CLA k 307



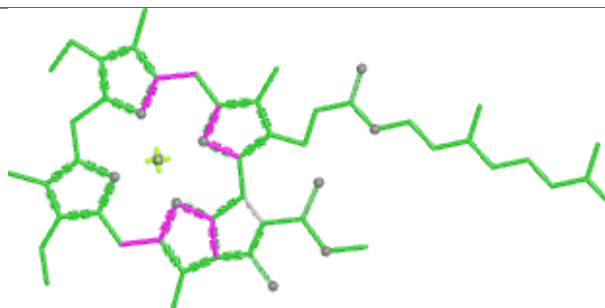
Ligand CLA A 804



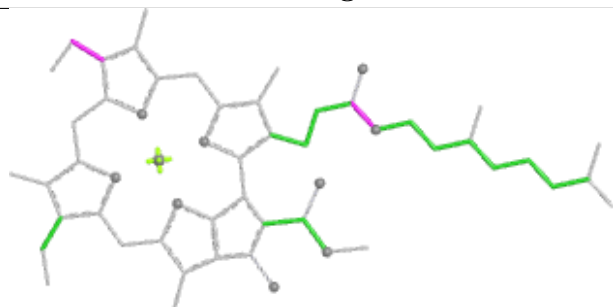
Ligand CLA f 302



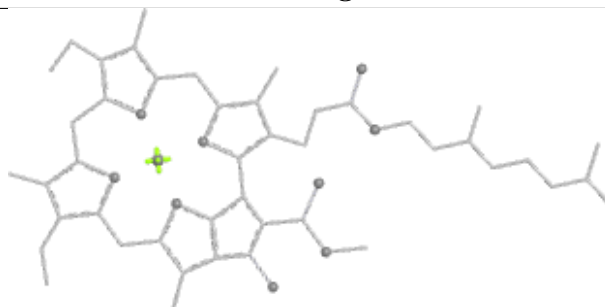
Bond lengths



Bond angles

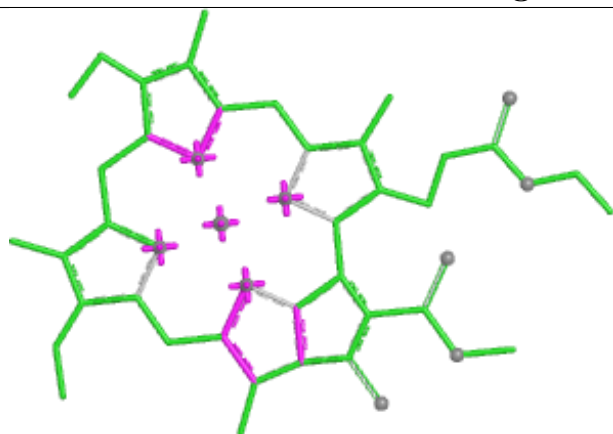


Torsions

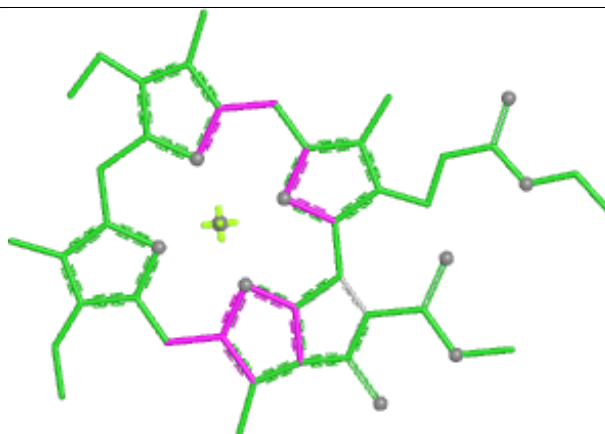


Rings

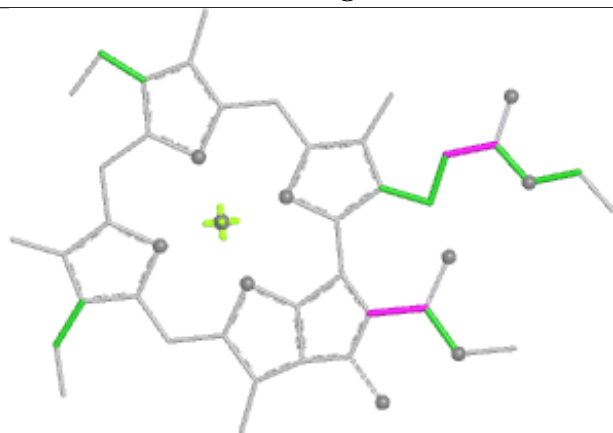
Ligand CLA m 303



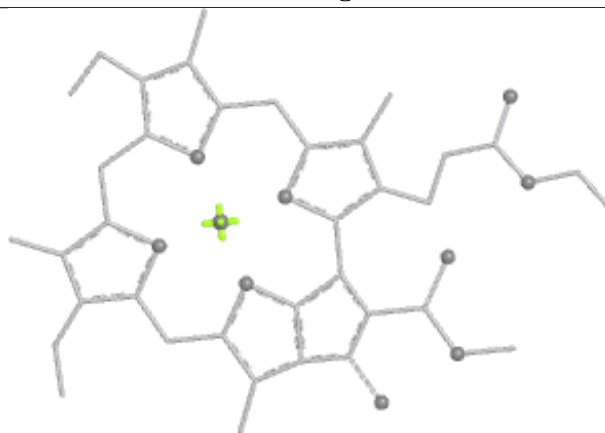
Bond lengths



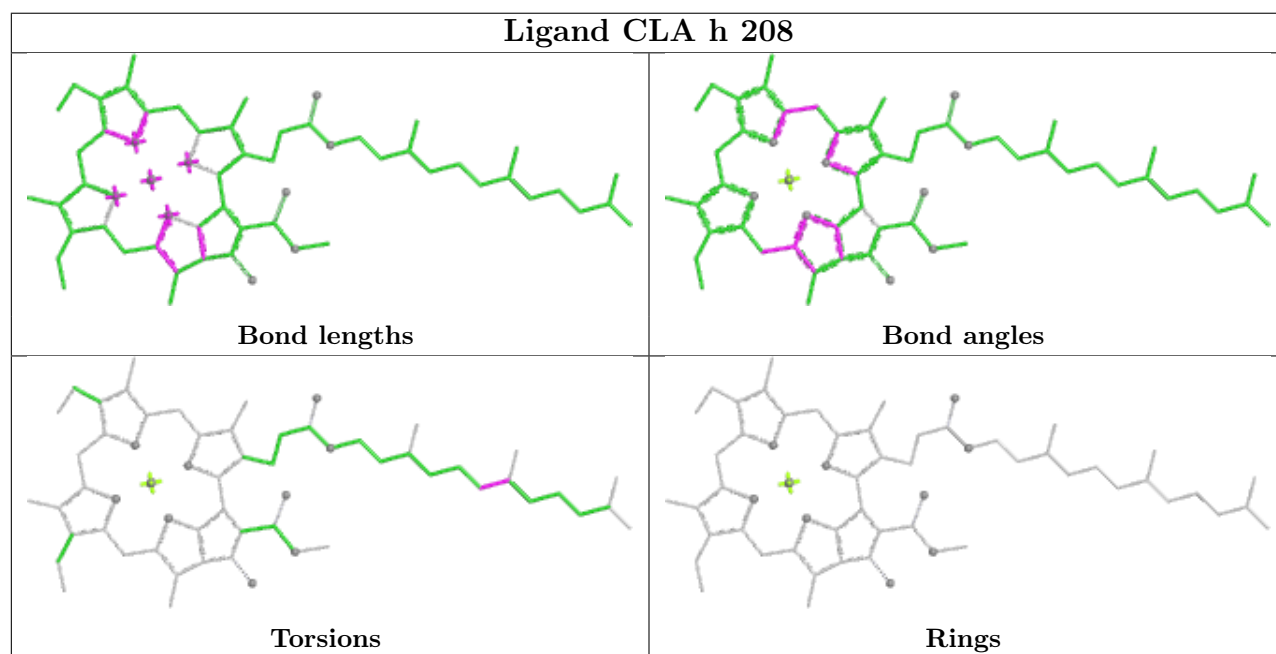
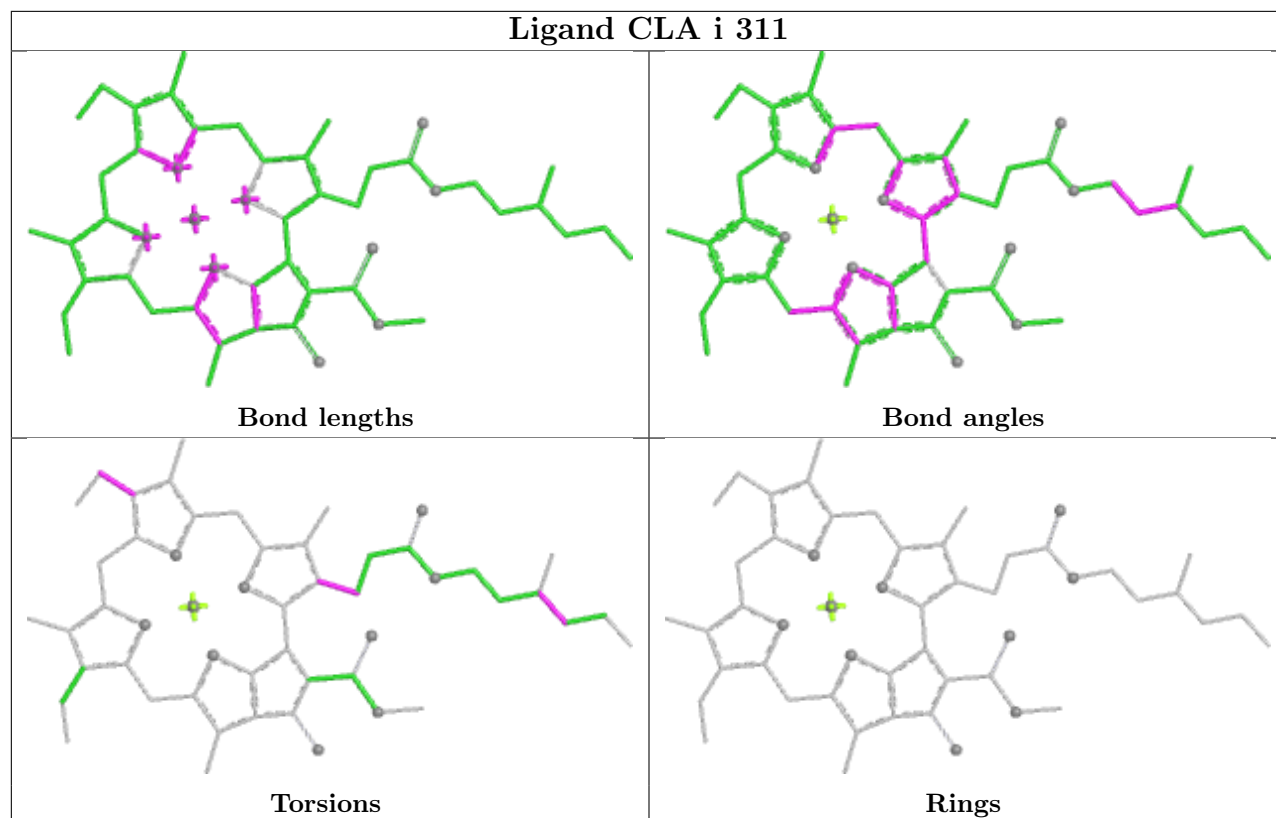
Bond angles

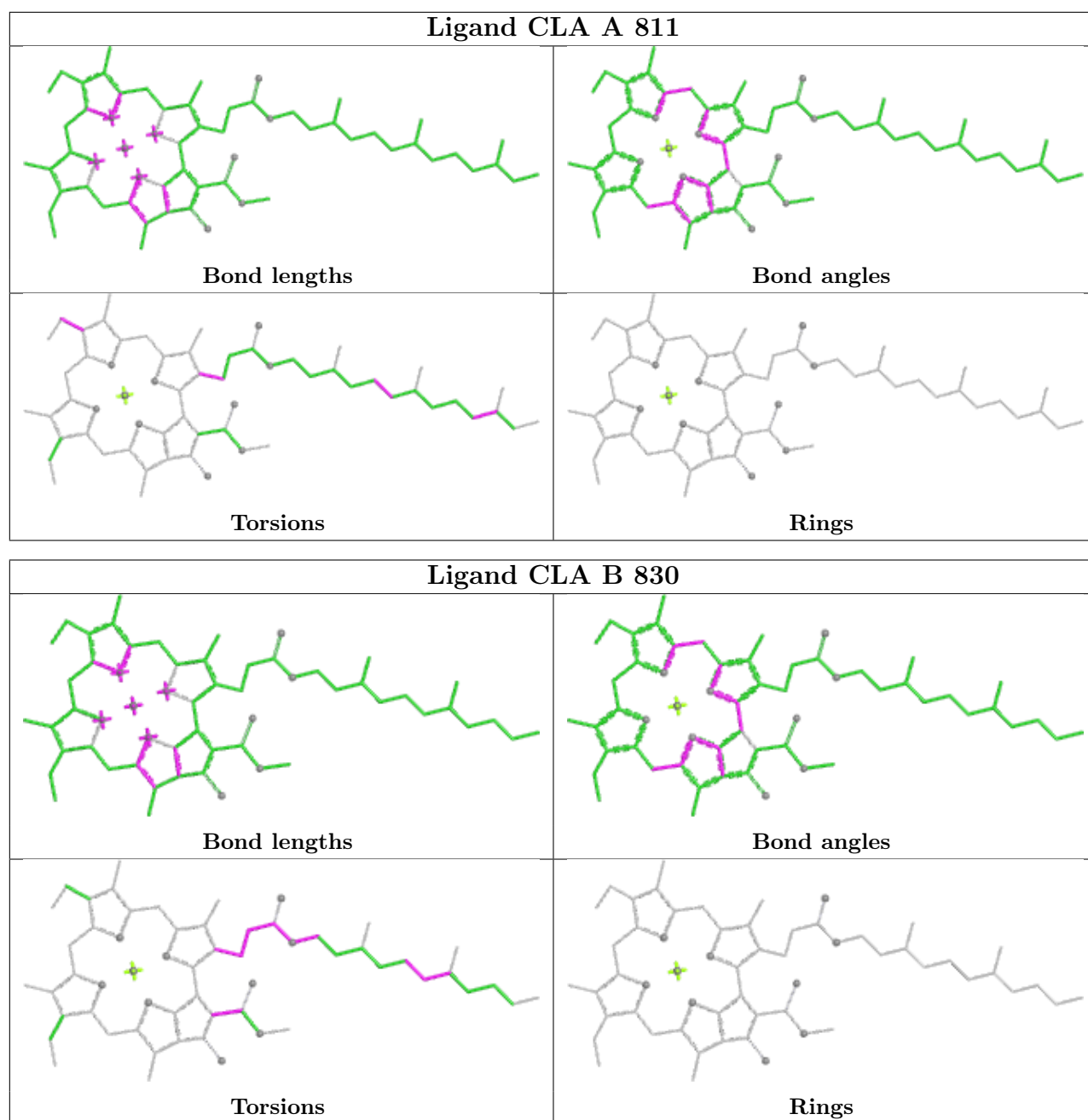


Torsions

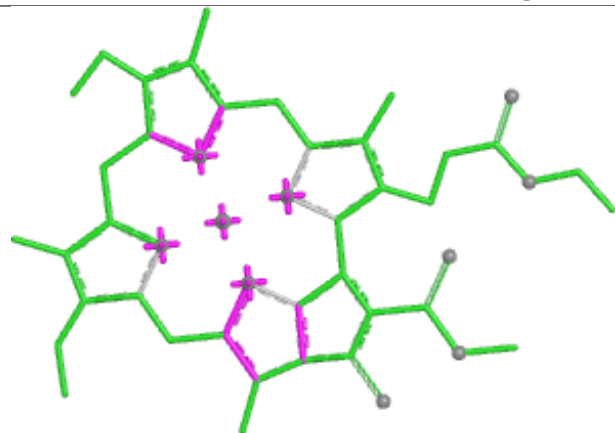


Rings

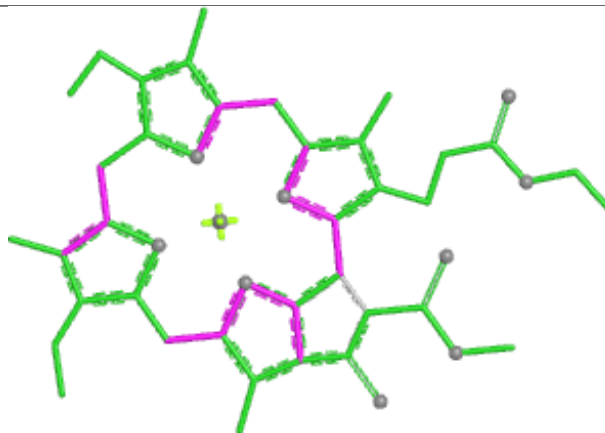




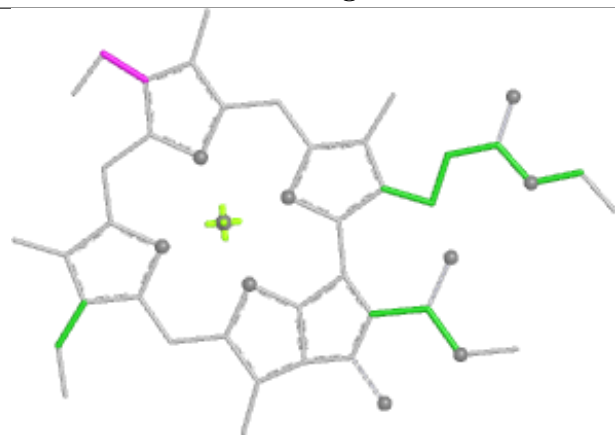
Ligand CLA F 204



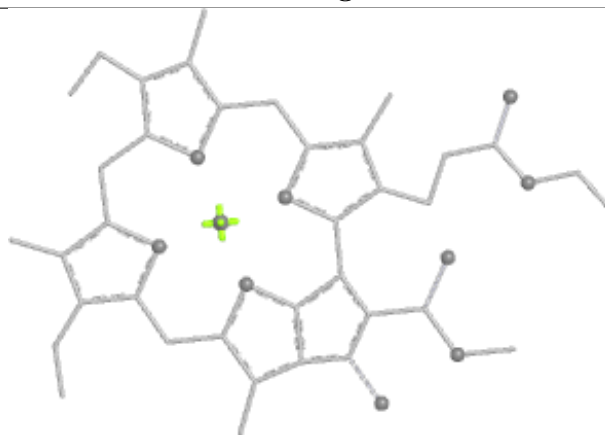
Bond lengths



Bond angles

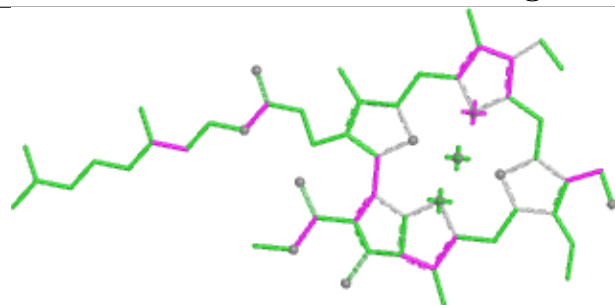


Torsions

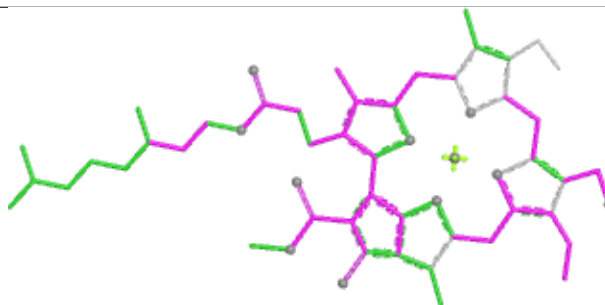


Rings

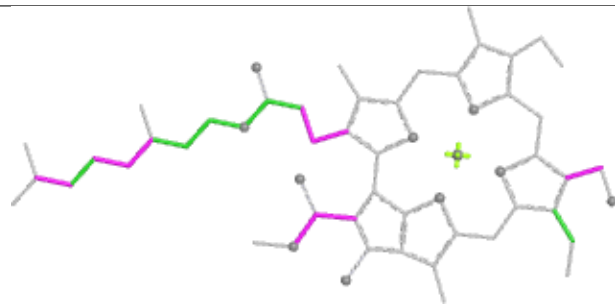
Ligand CHL i 304



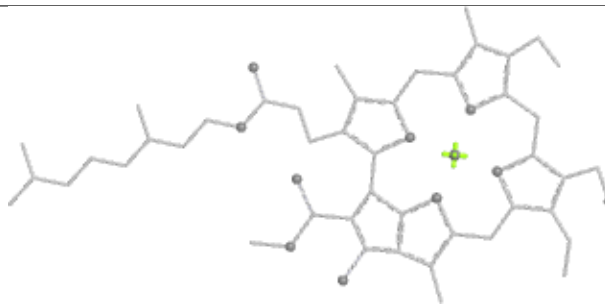
Bond lengths



Bond angles

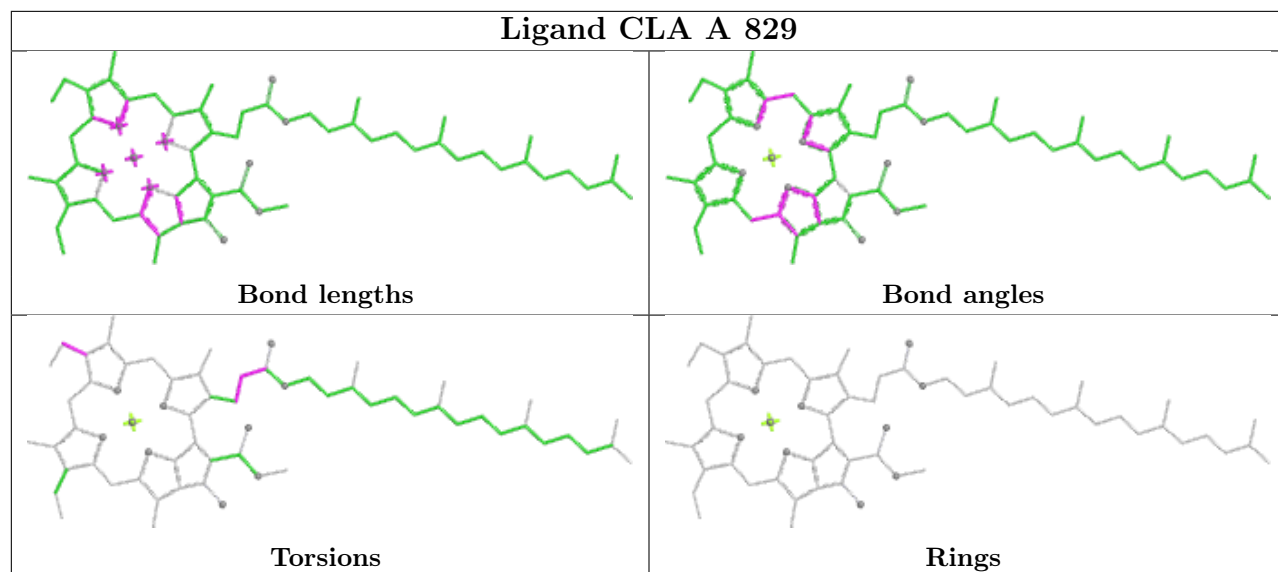


Torsions

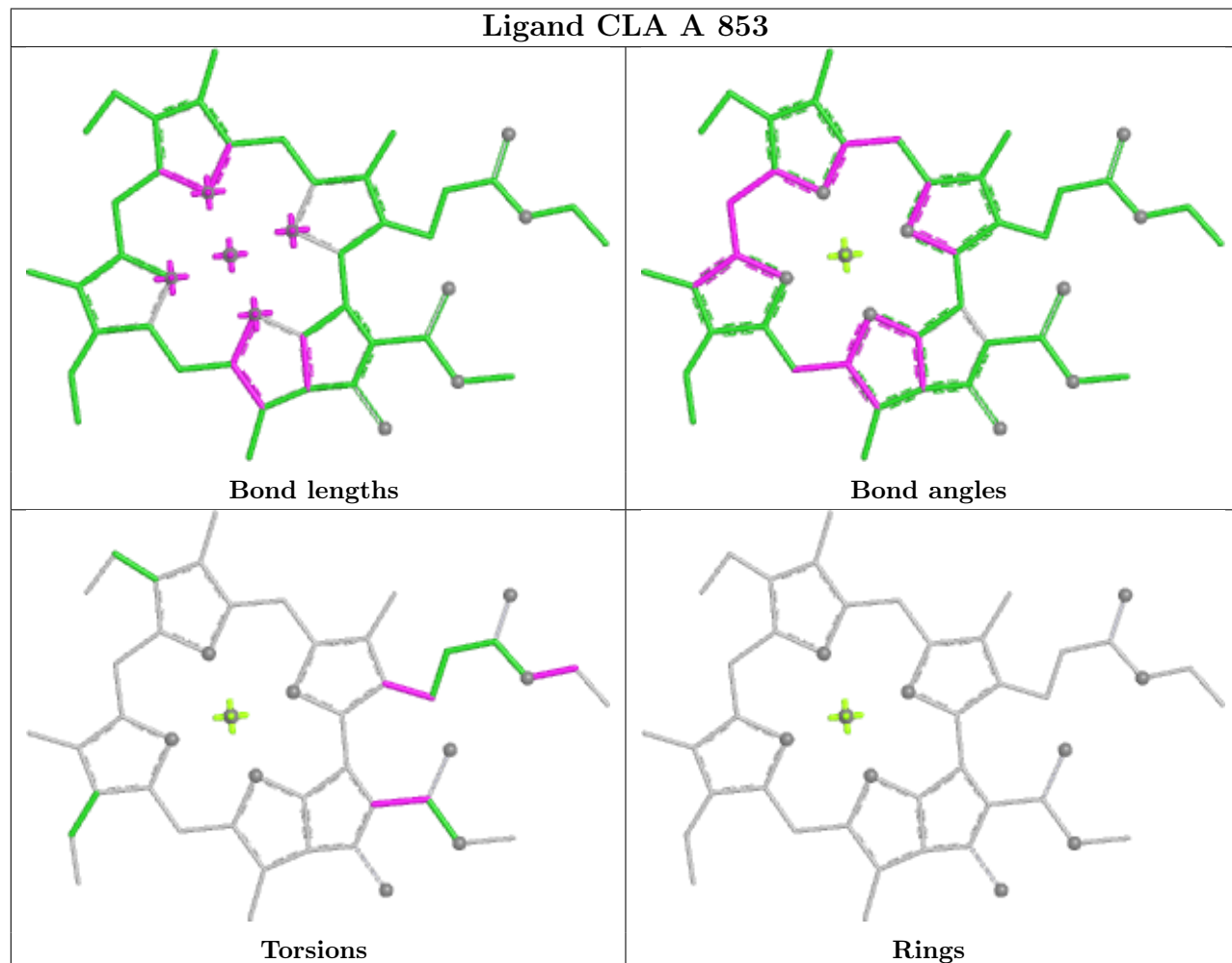


Rings

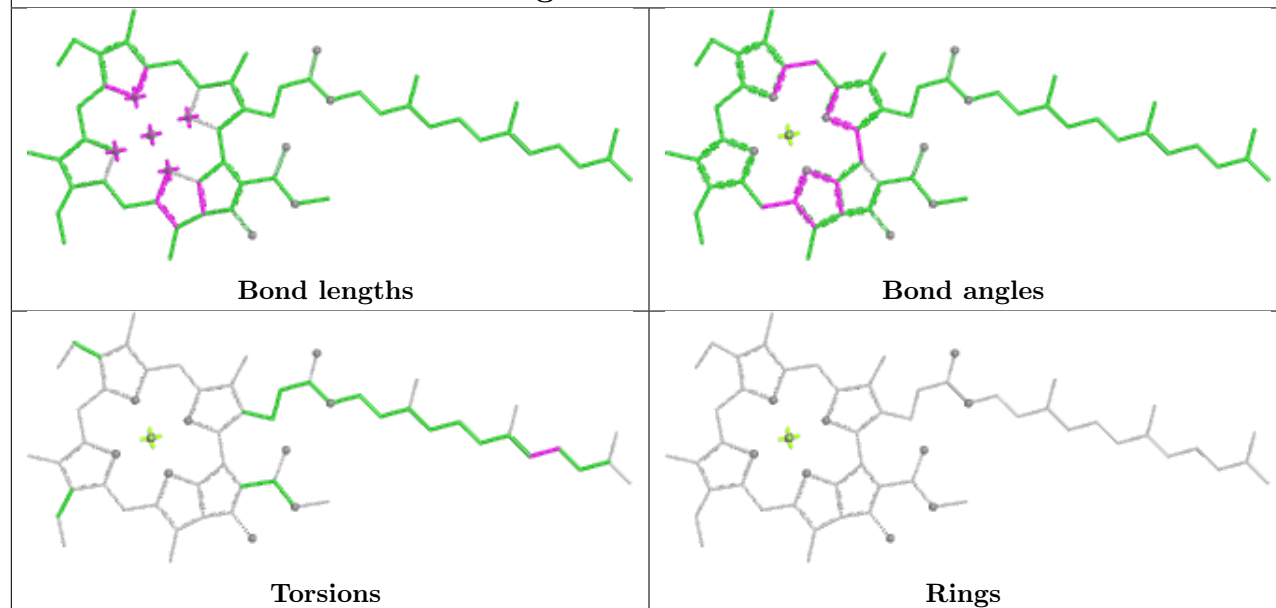
Ligand CLA A 829



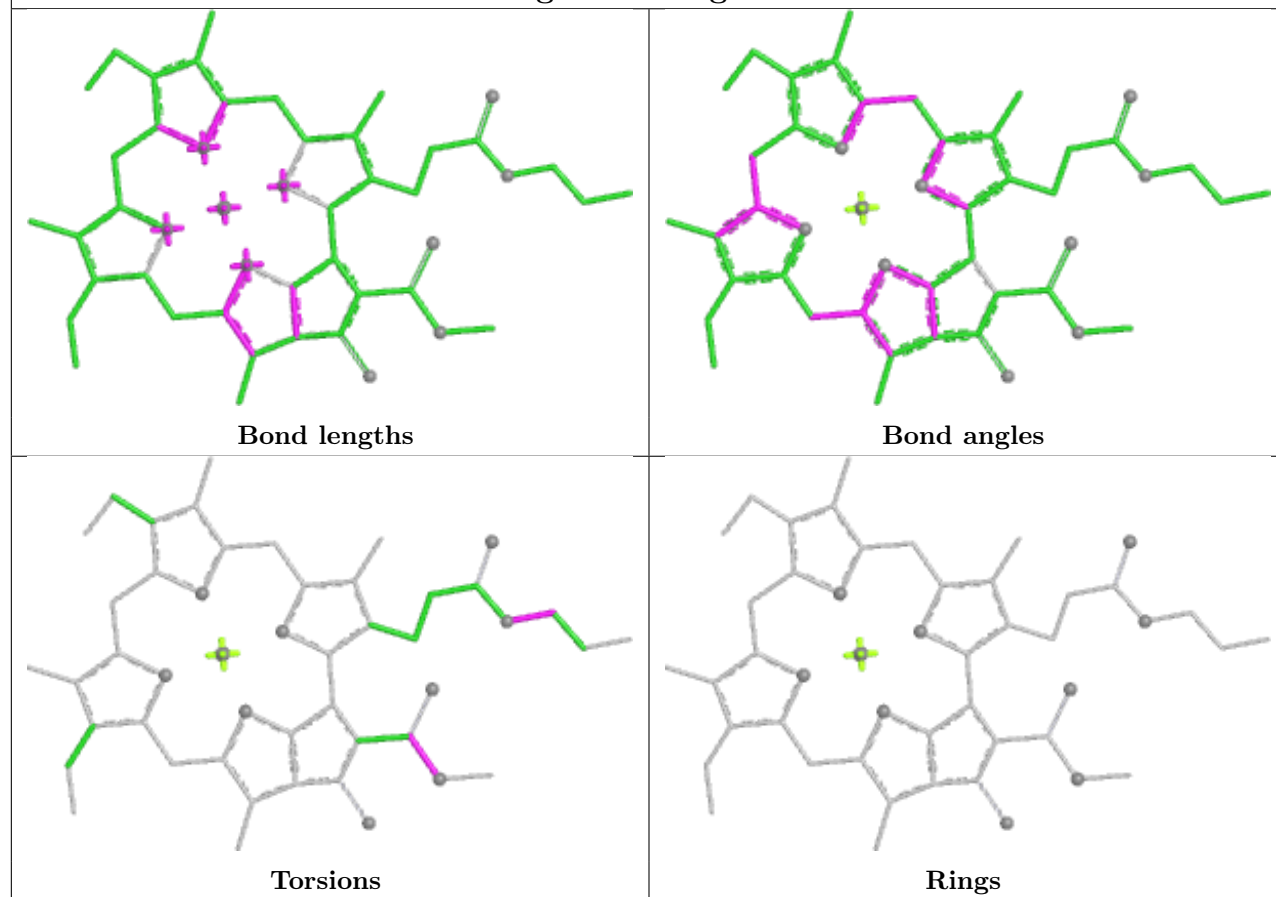
Ligand CLA A 853



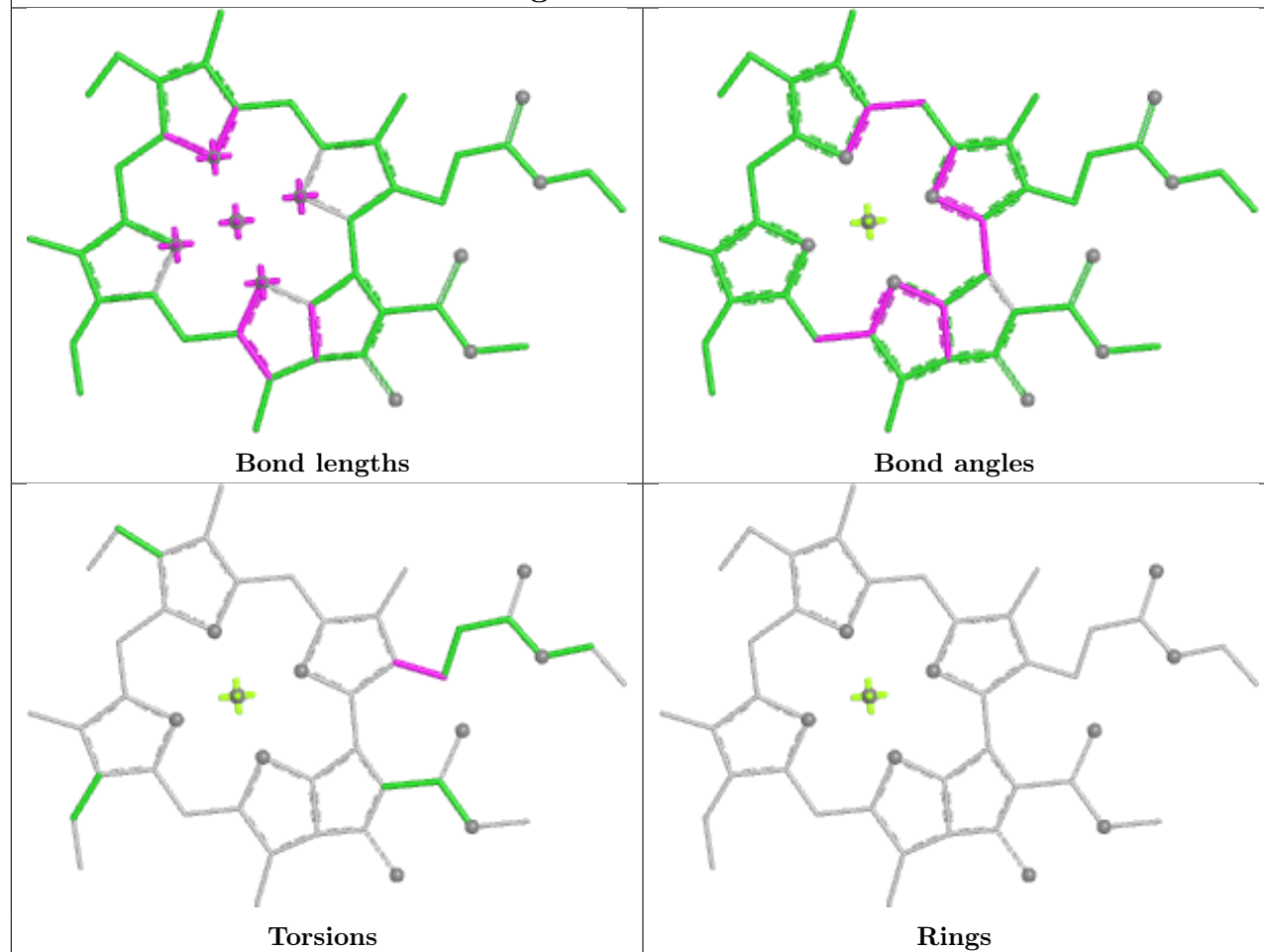
Ligand CLA a 308



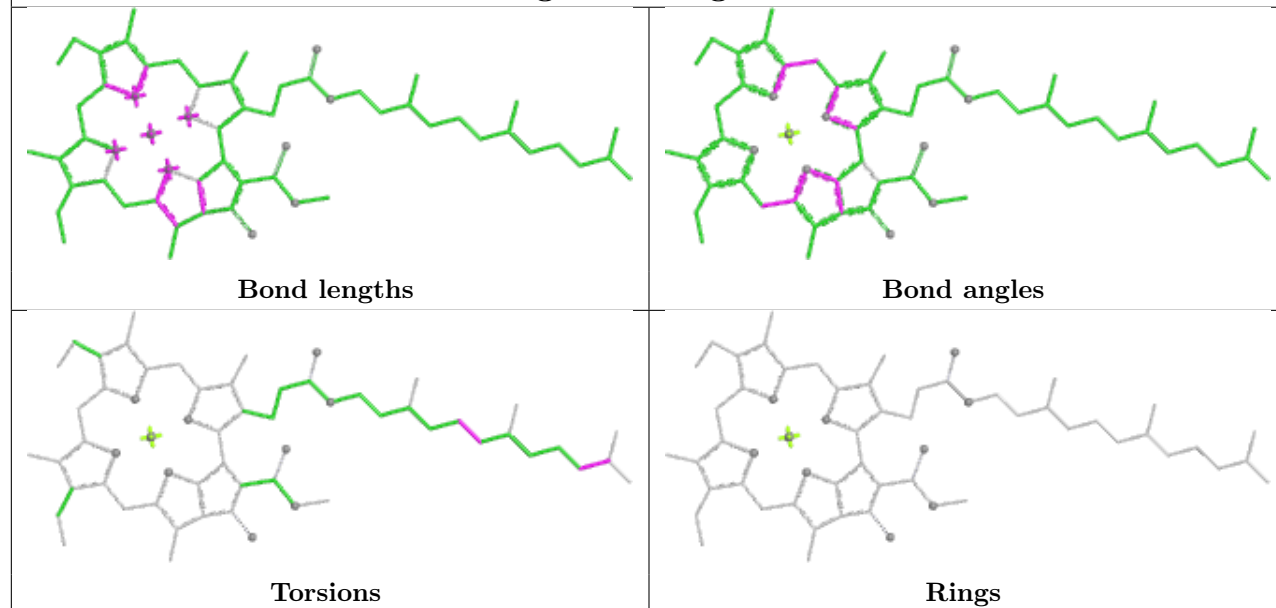
Ligand CLA g 301

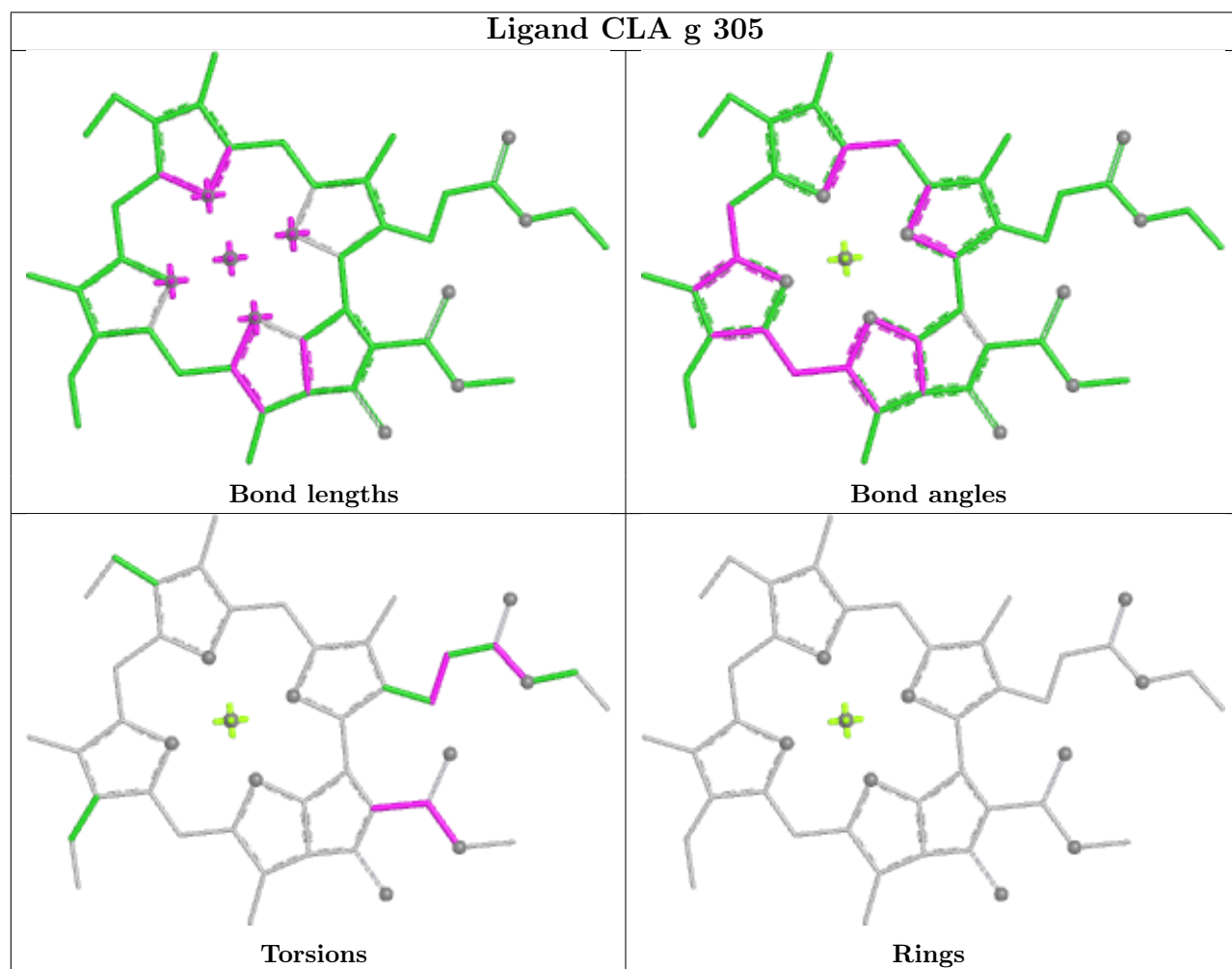
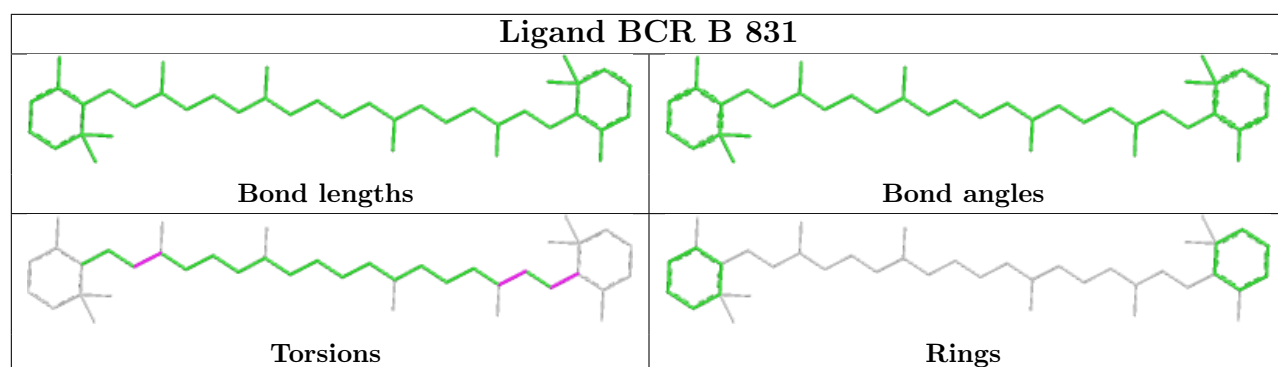


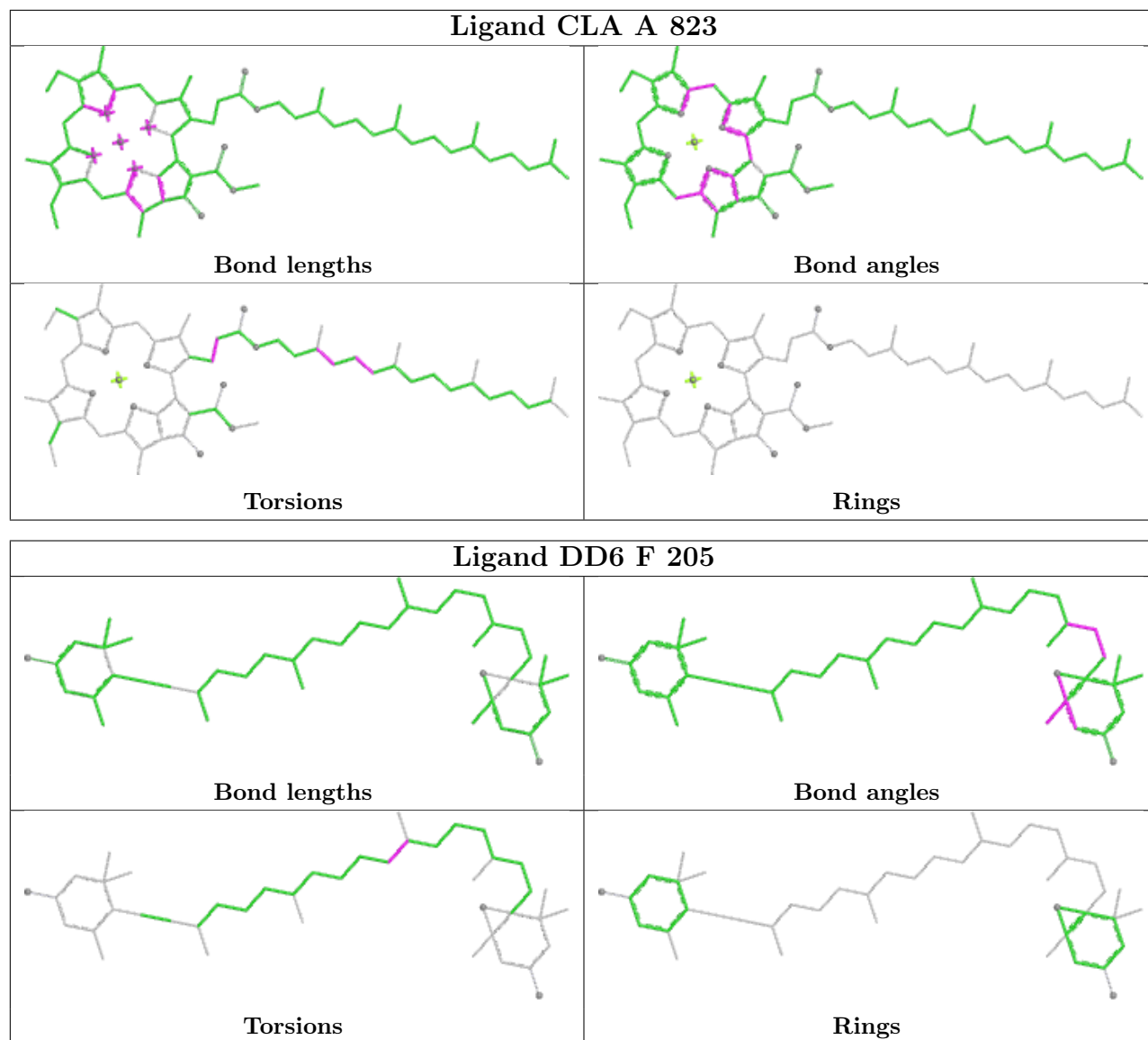
Ligand CLA k 303



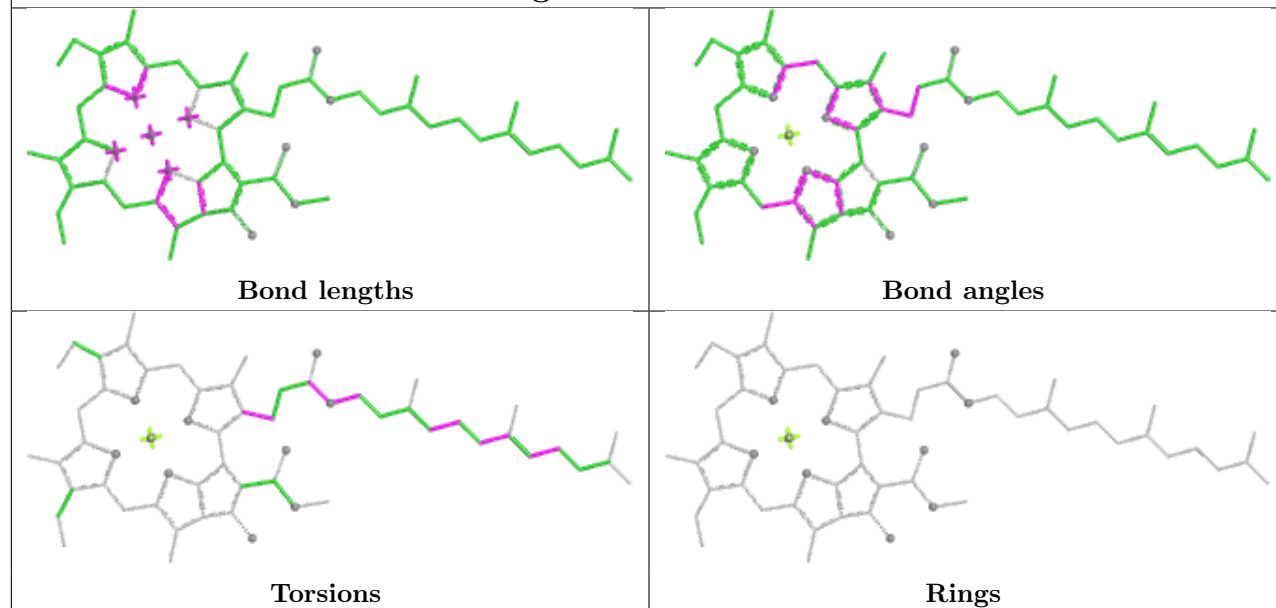
Ligand CLA g 307



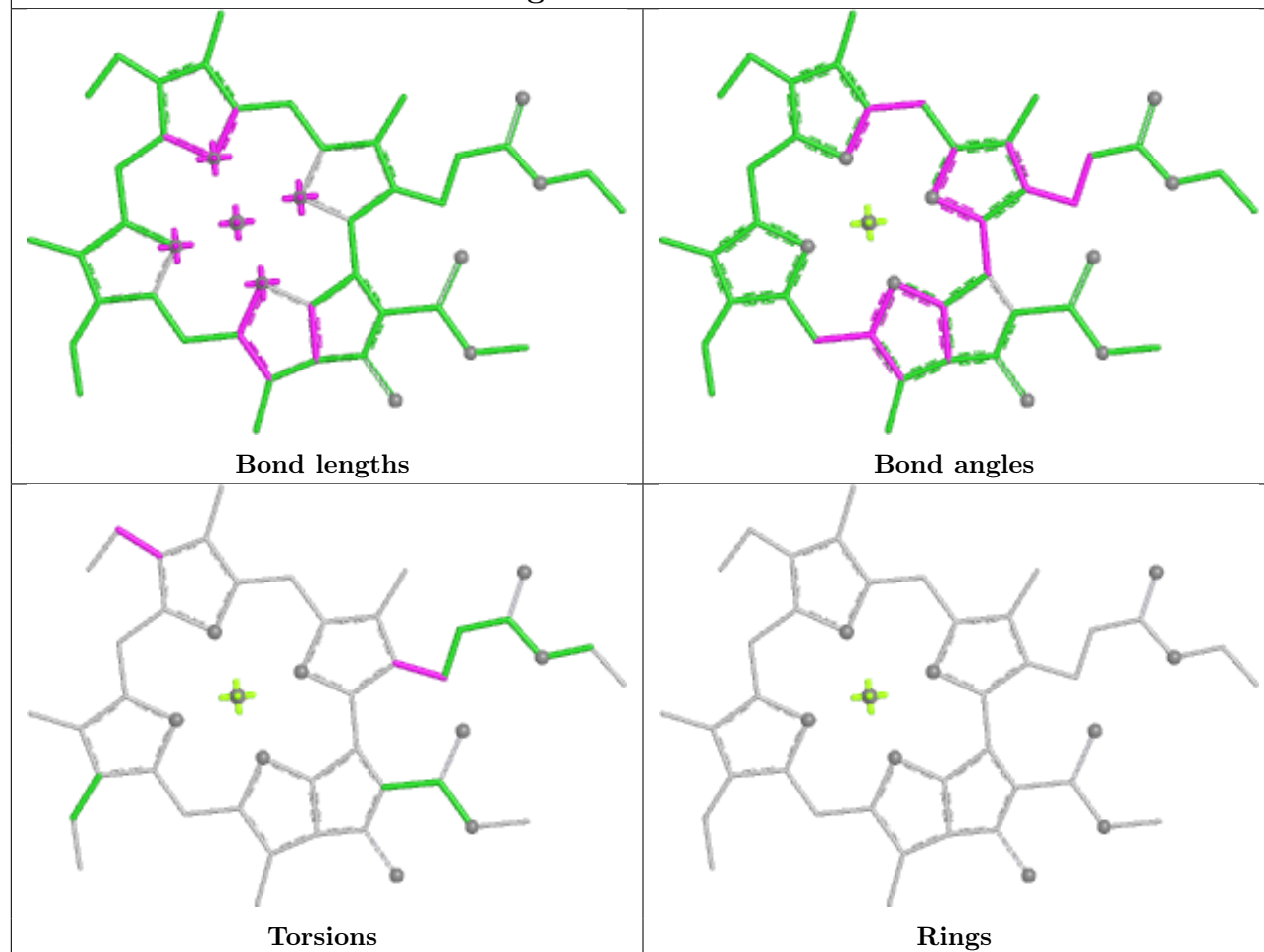


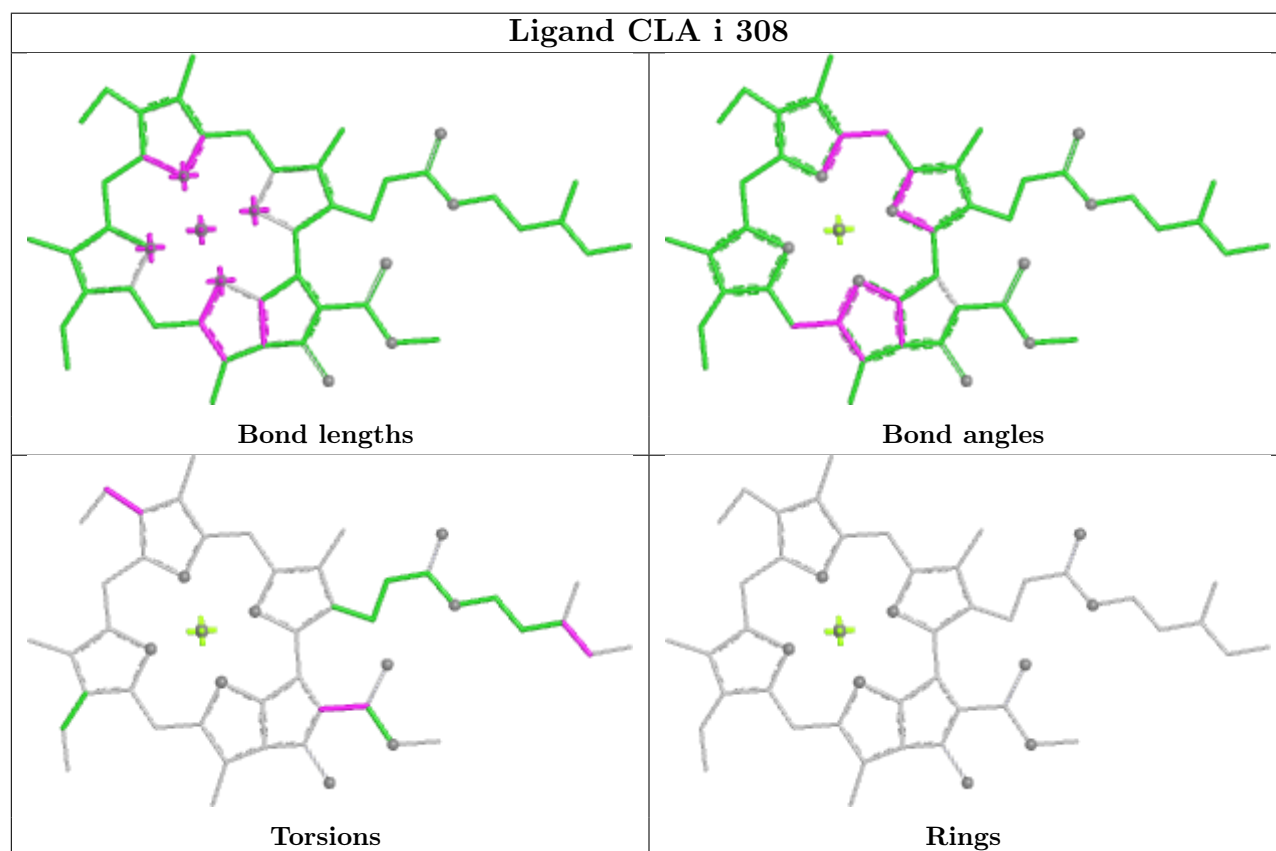
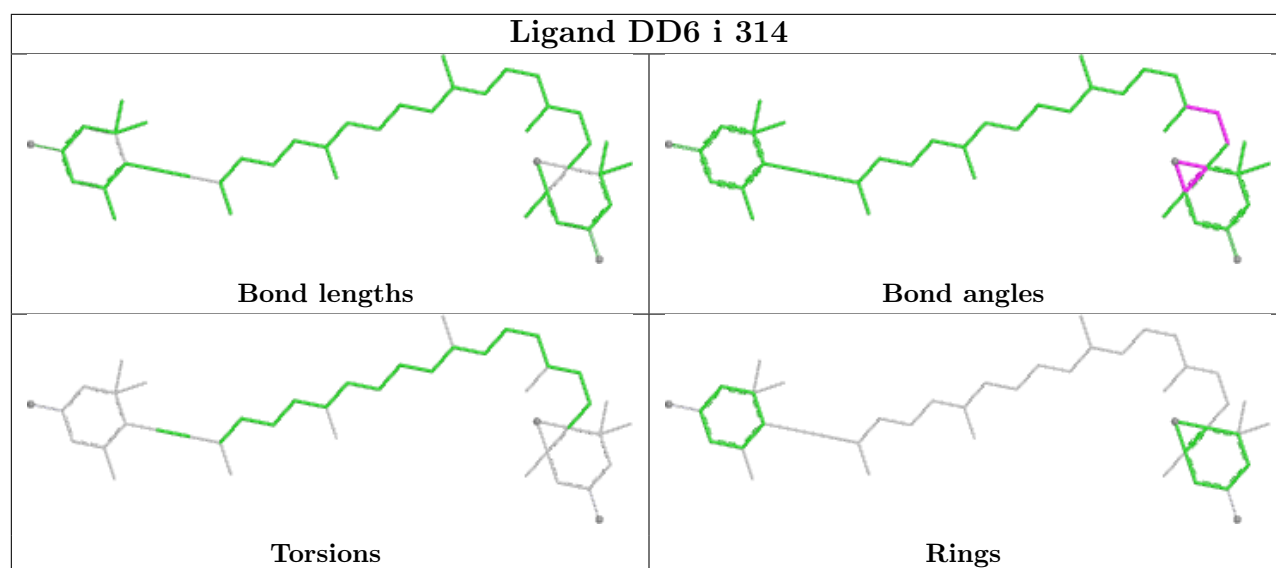


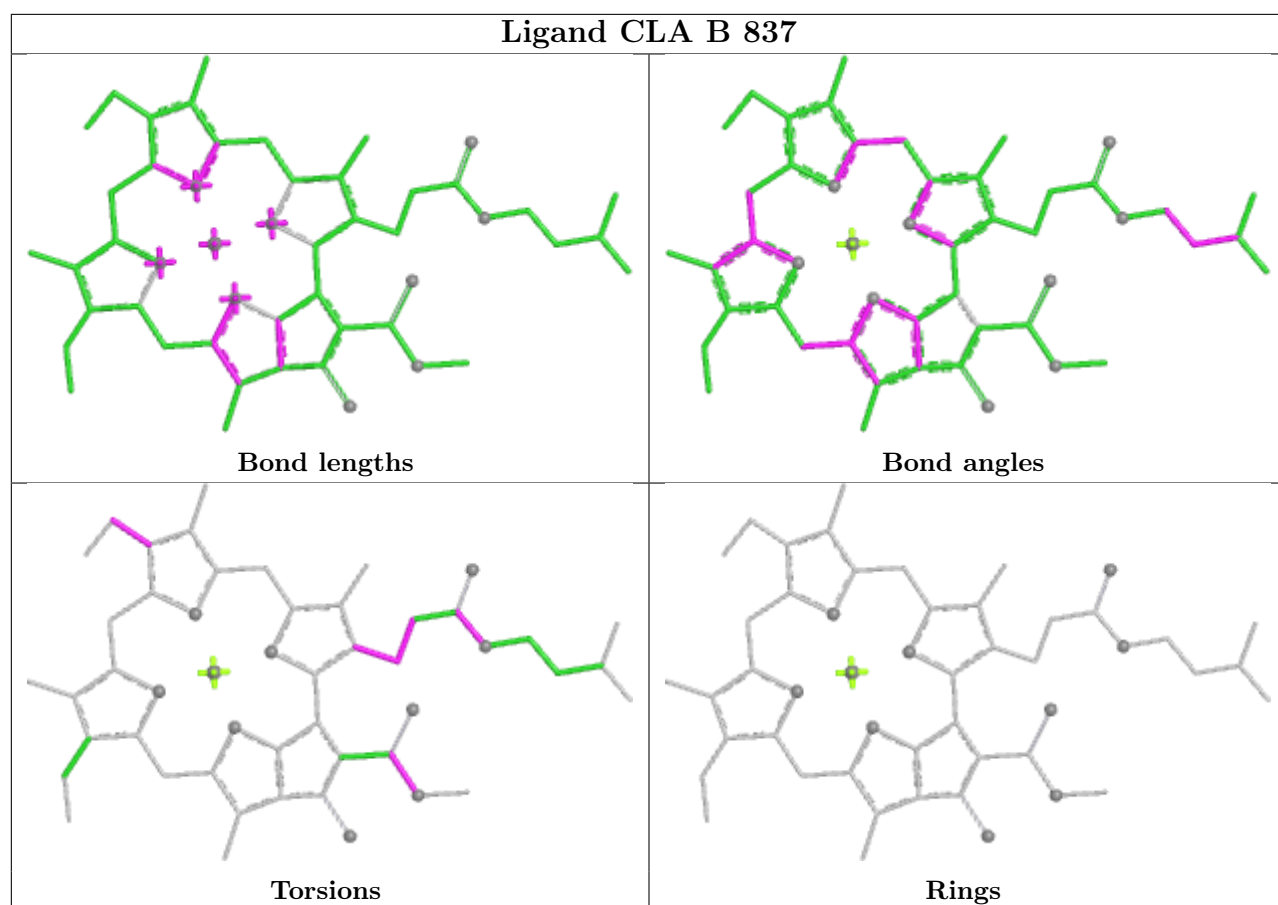
Ligand CLA B 815



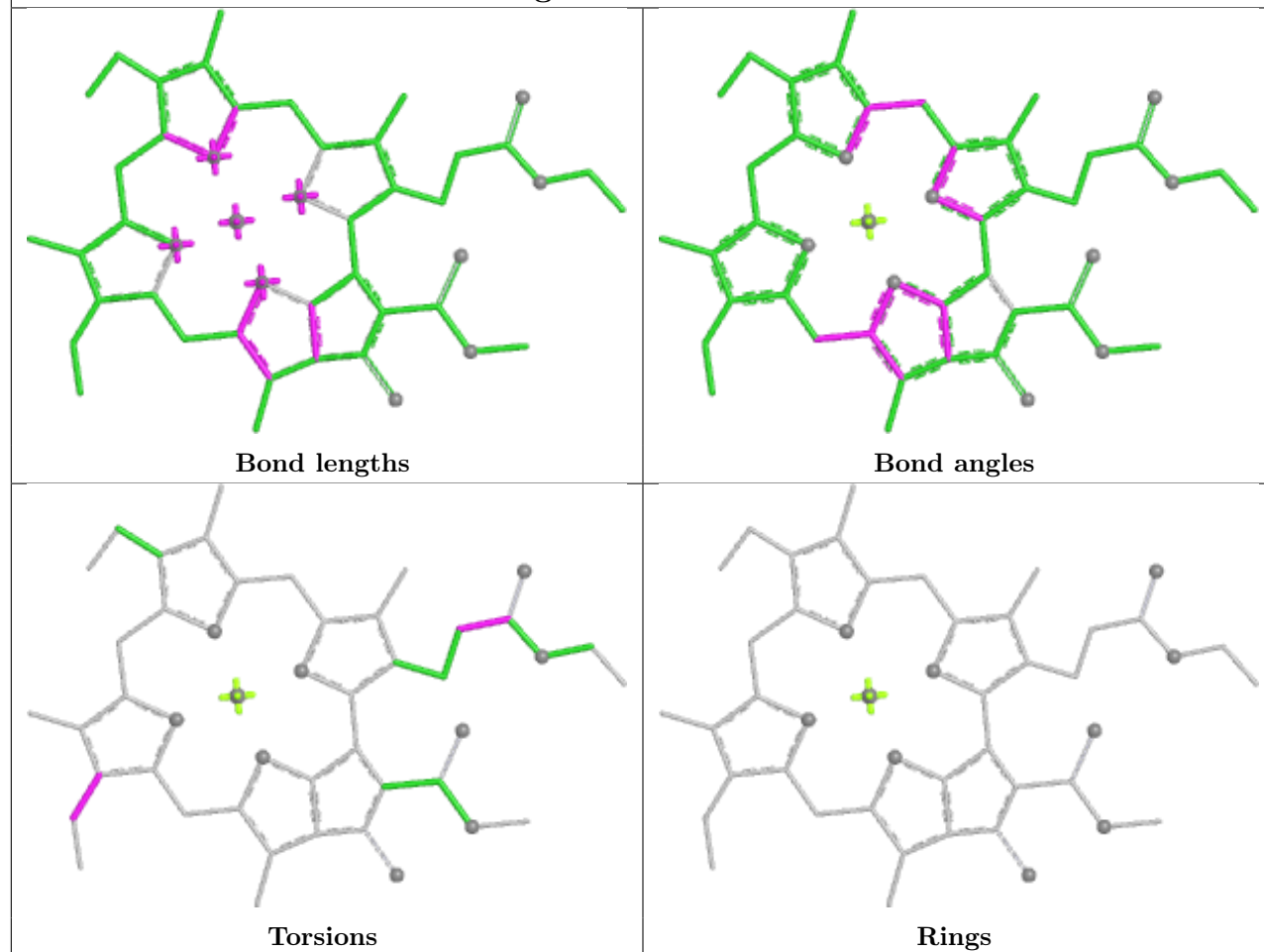
Ligand CLA B 842



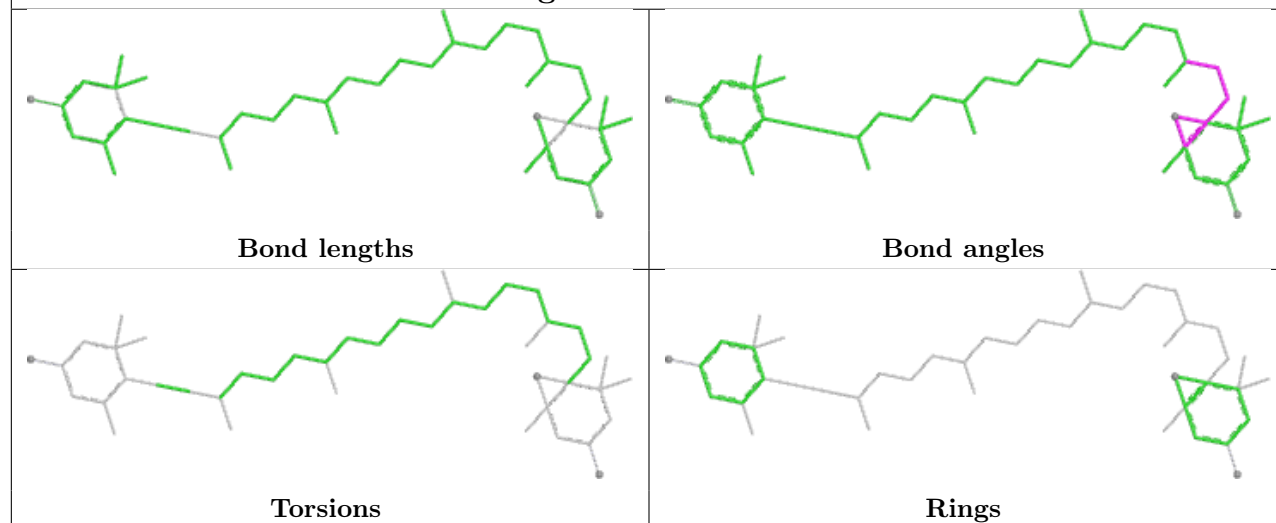


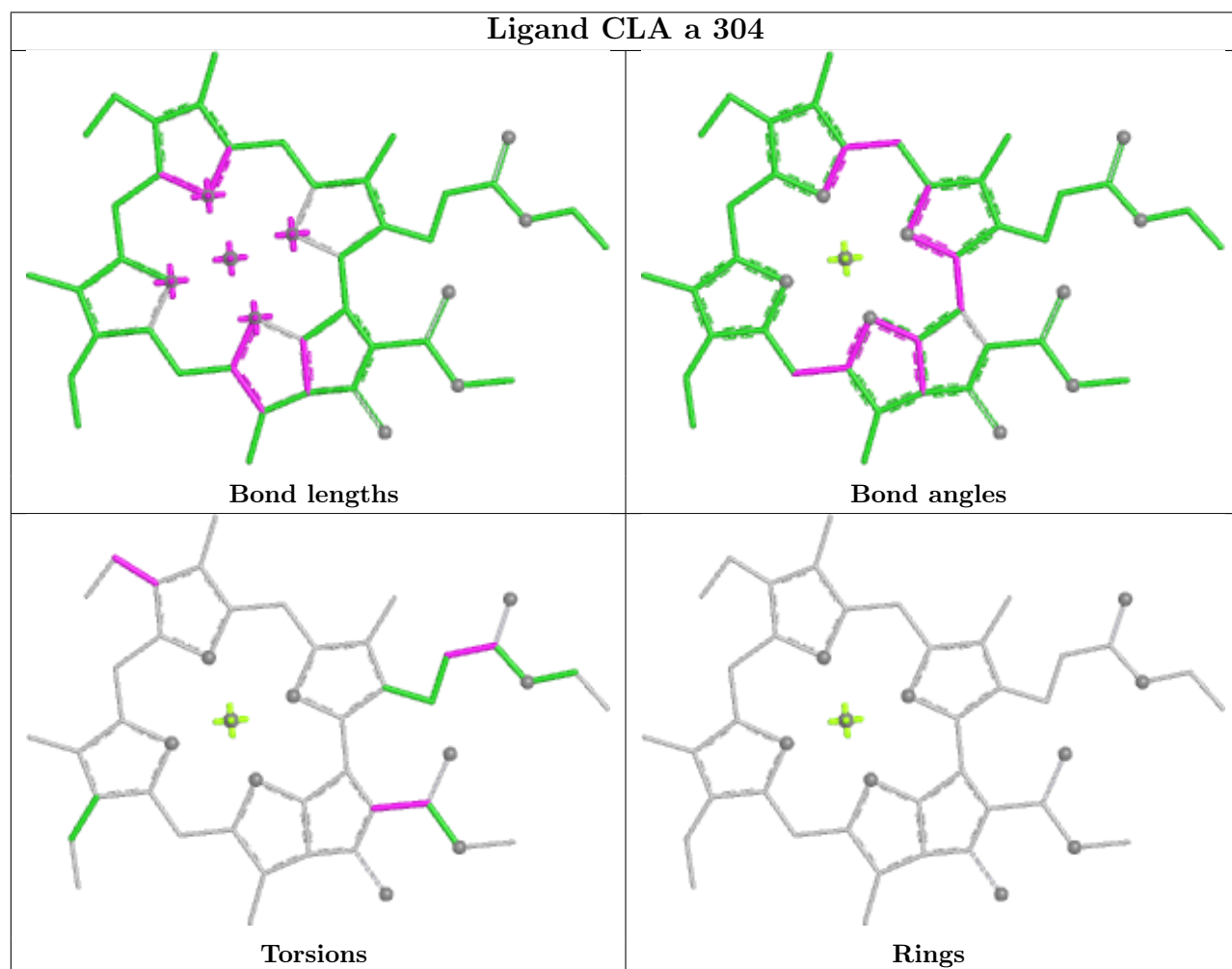
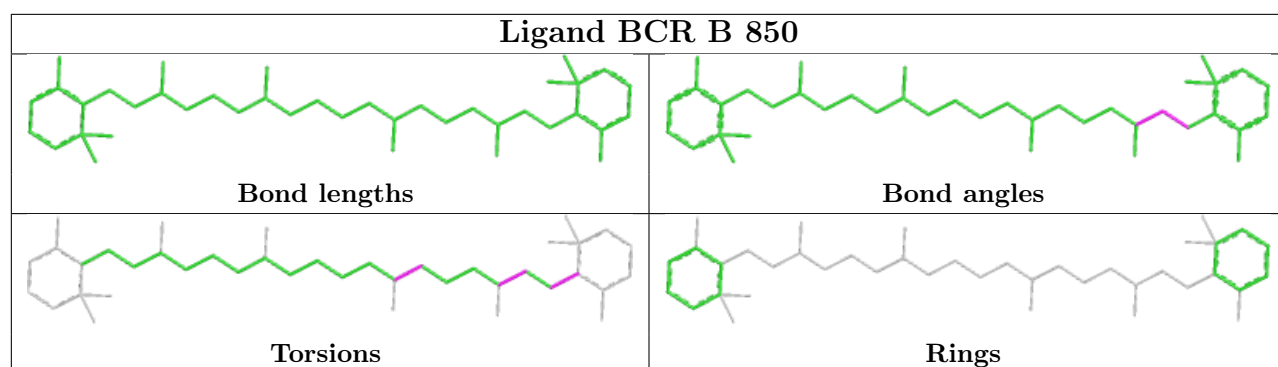


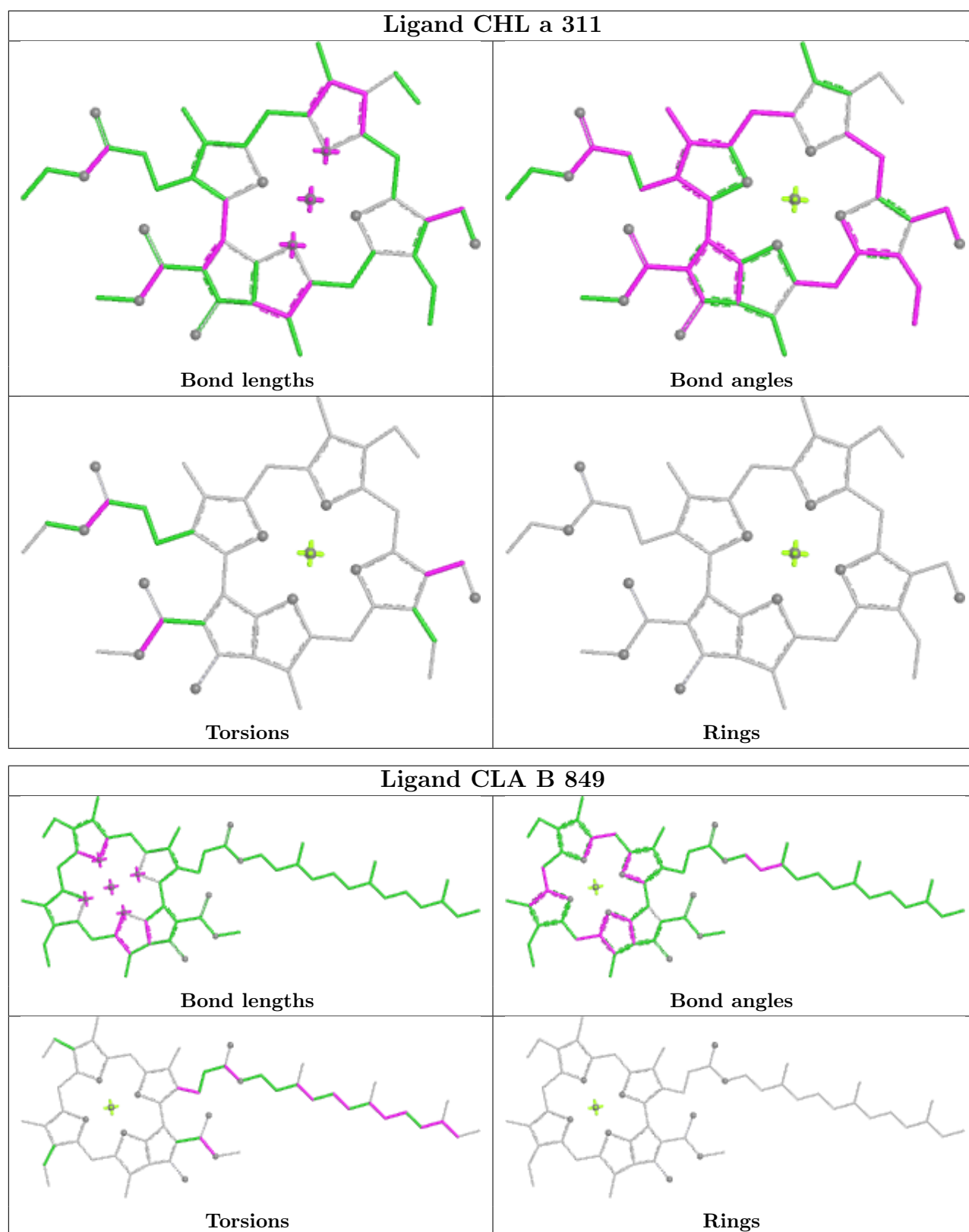
Ligand CLA f 306

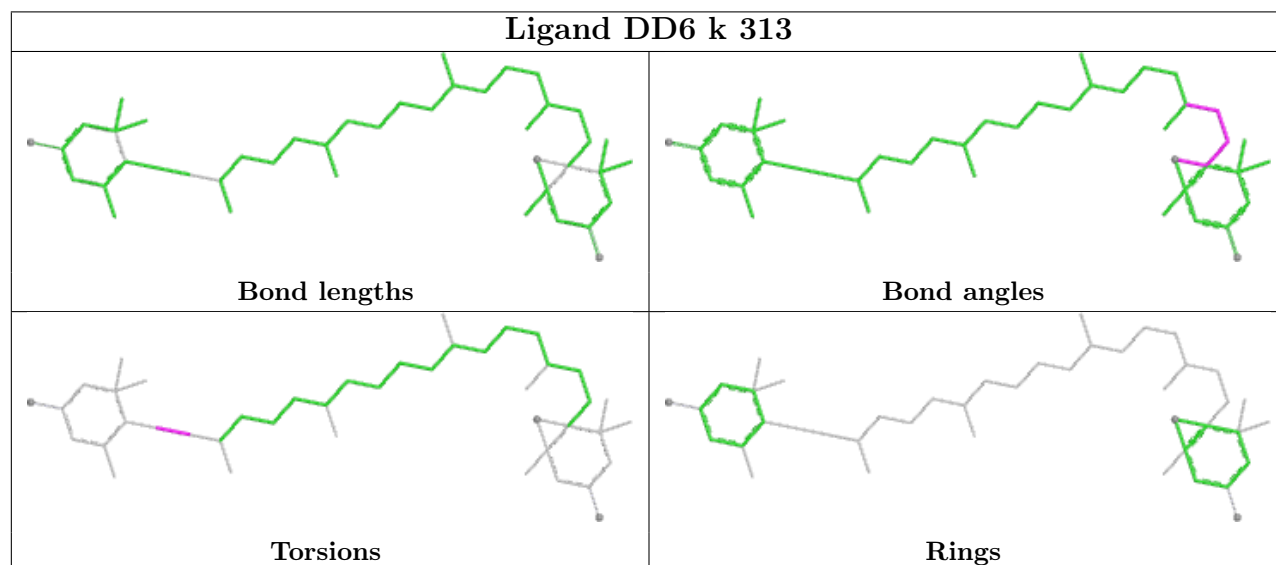
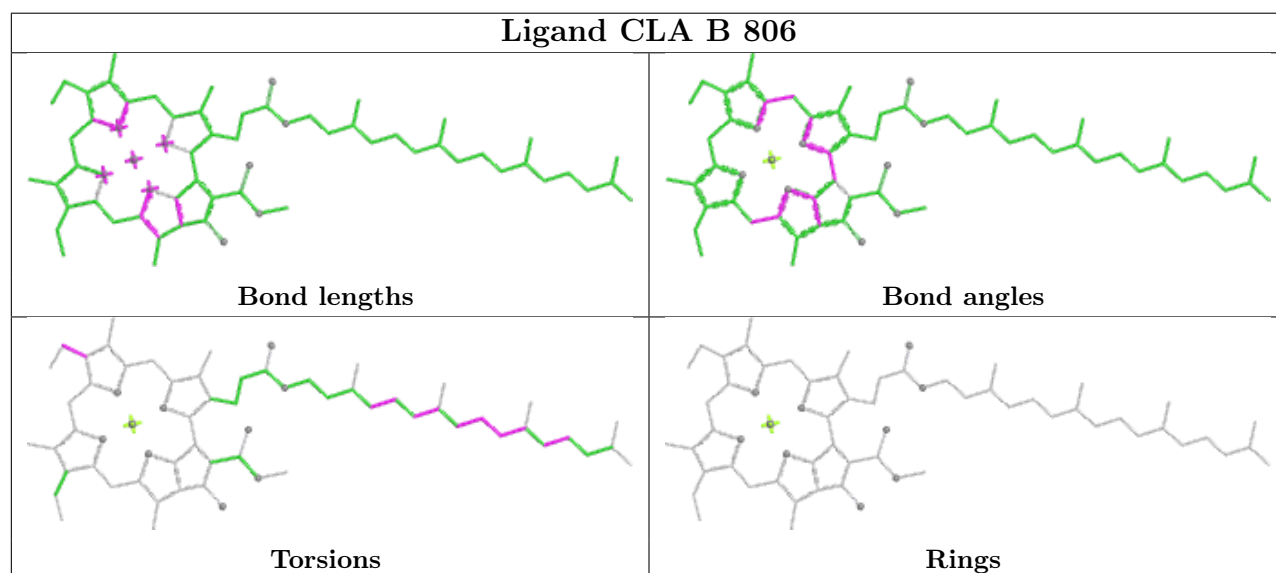
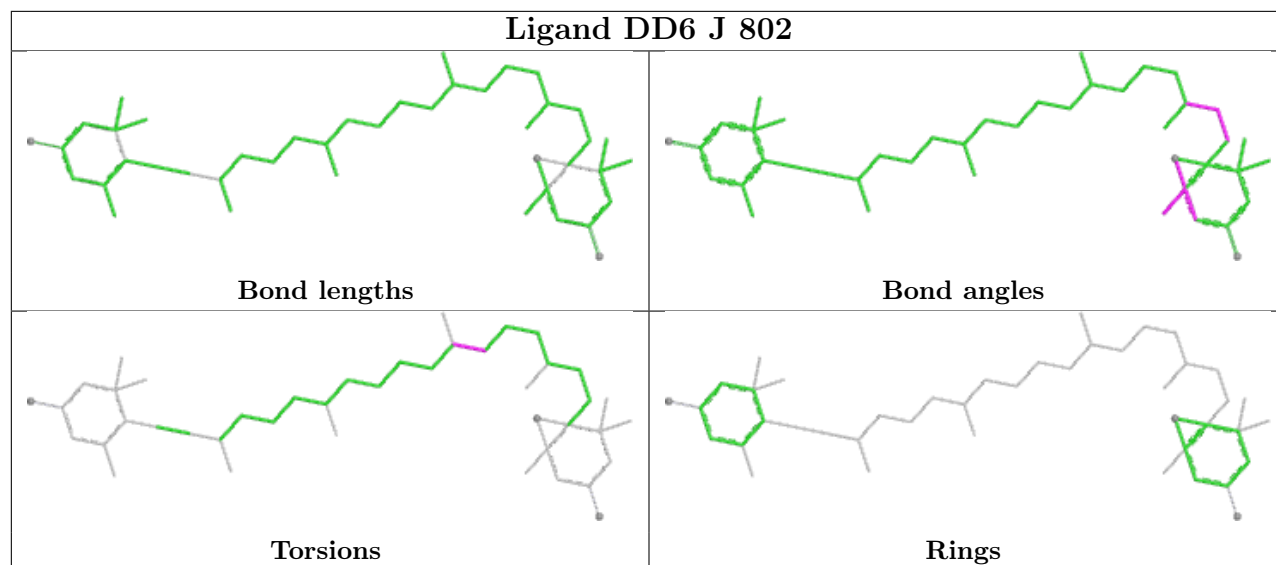


Ligand DD6 c 319

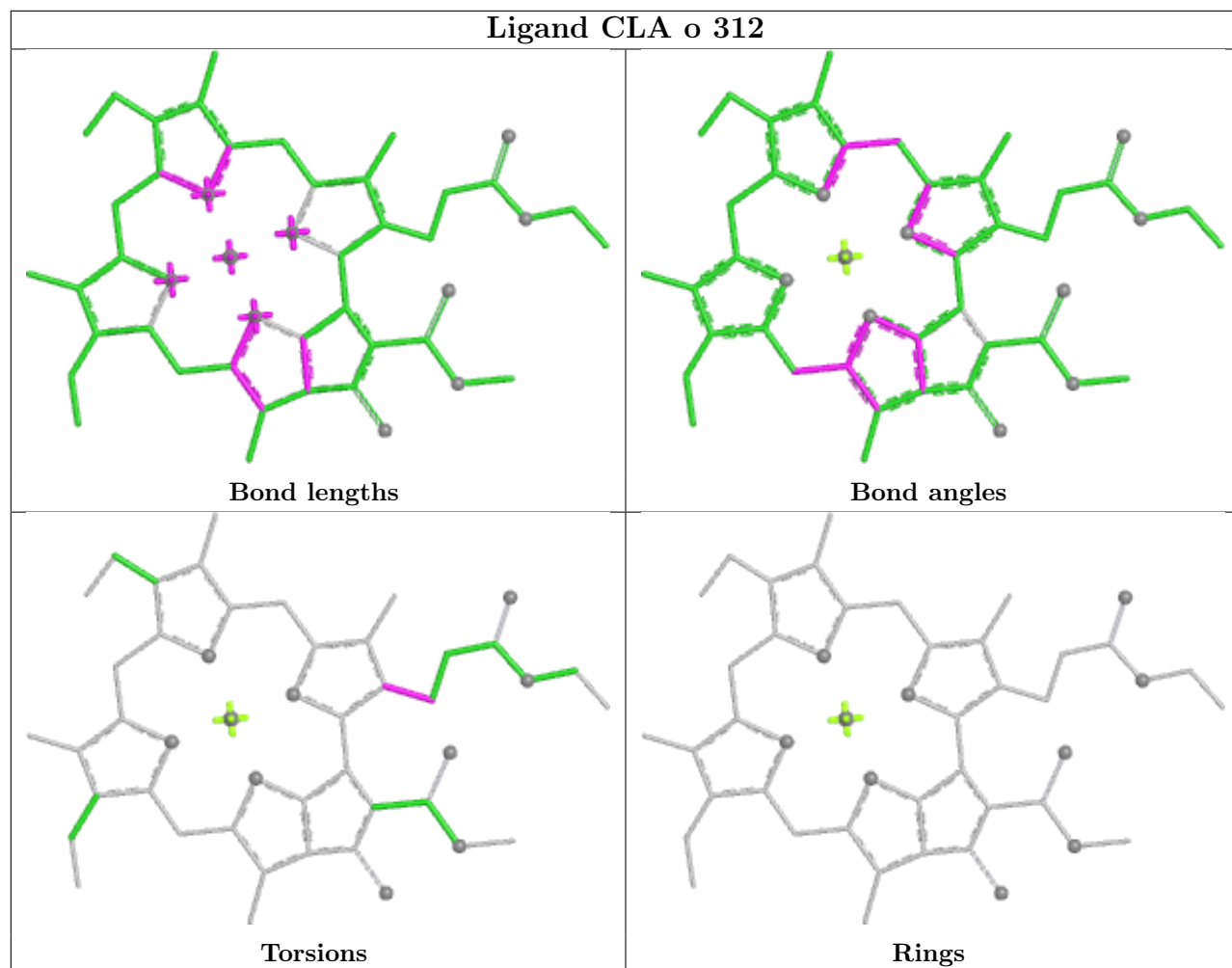


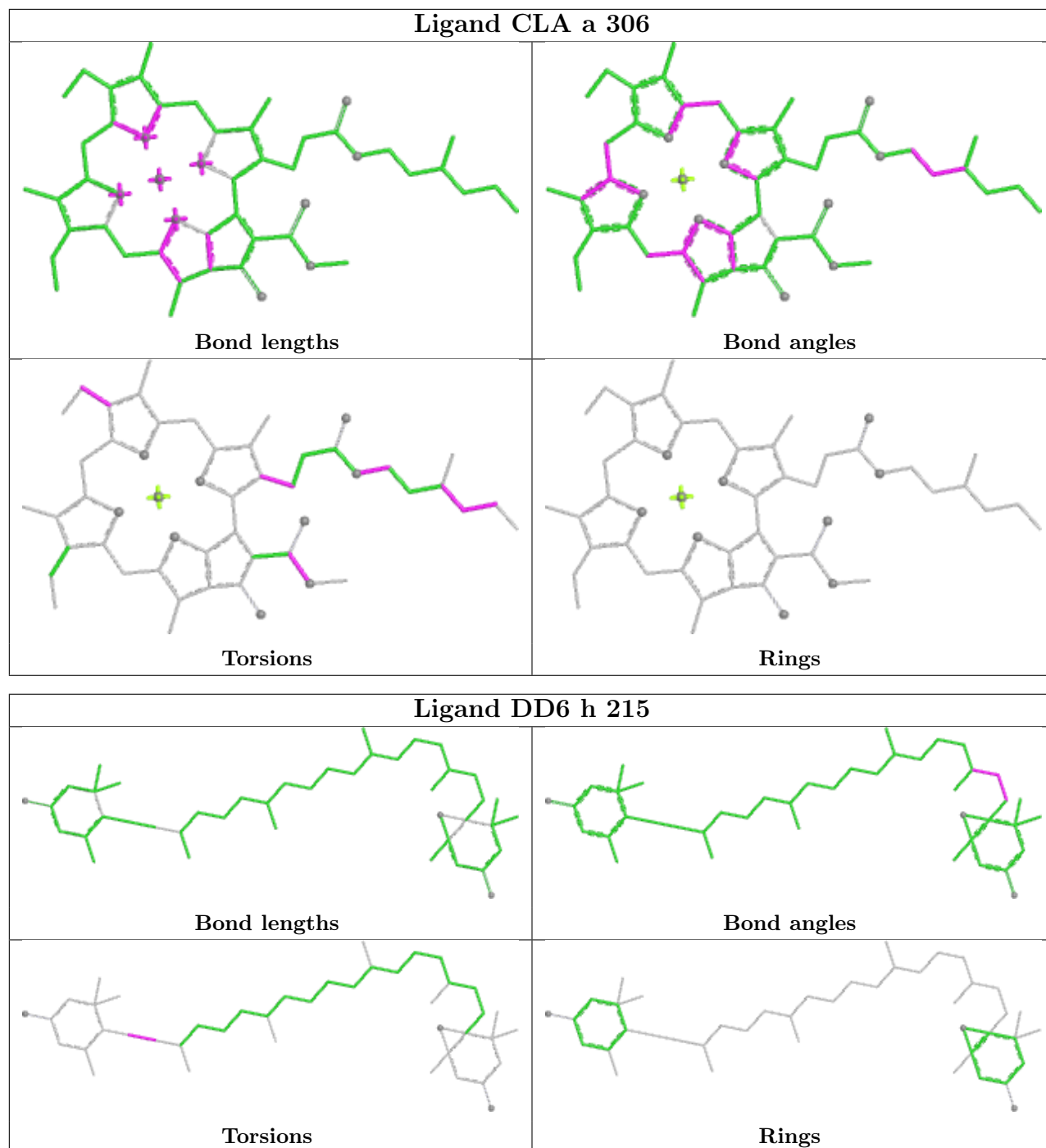




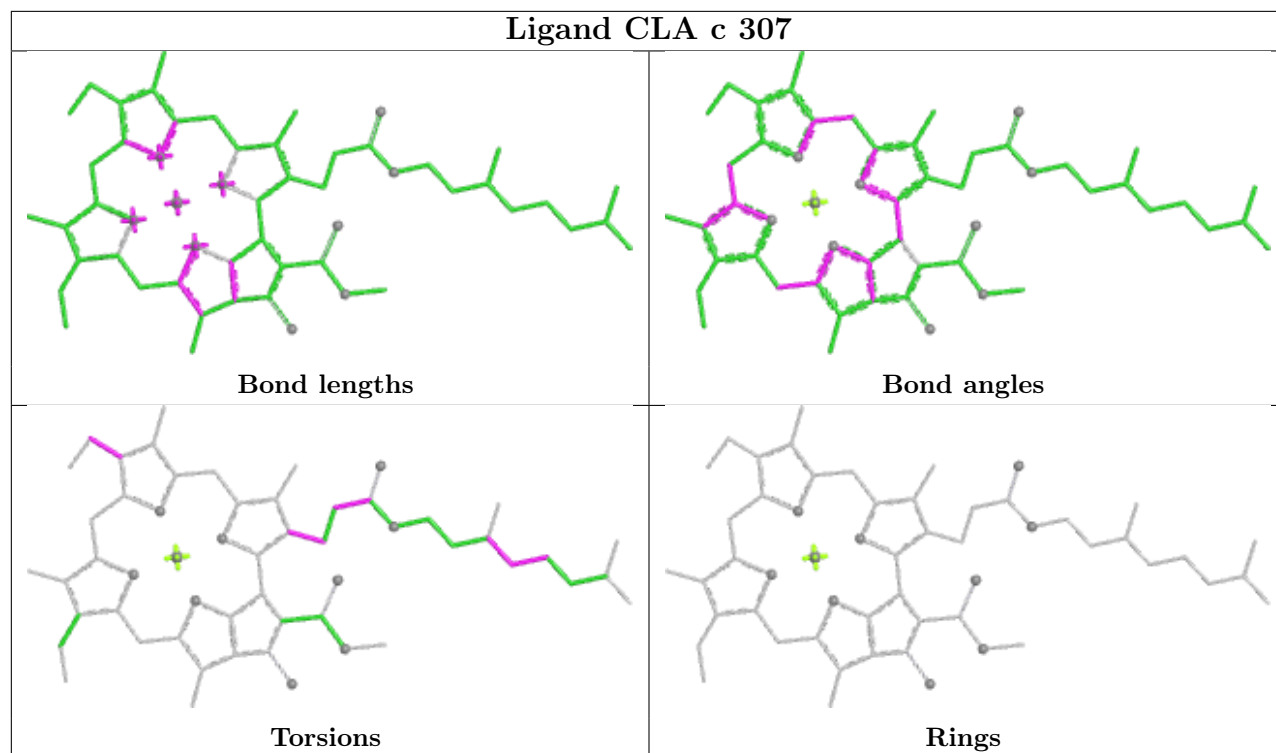


Ligand CLA o 312

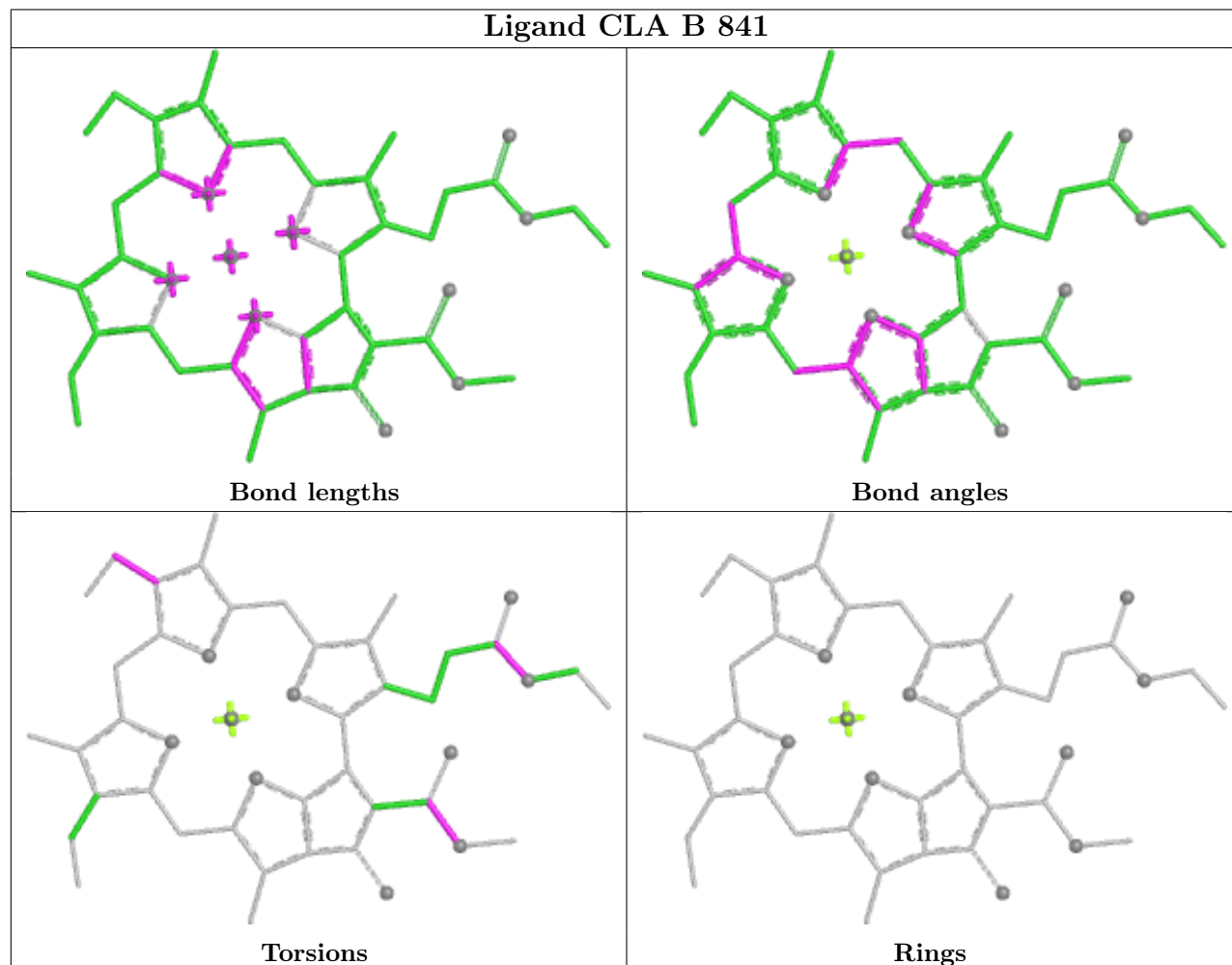




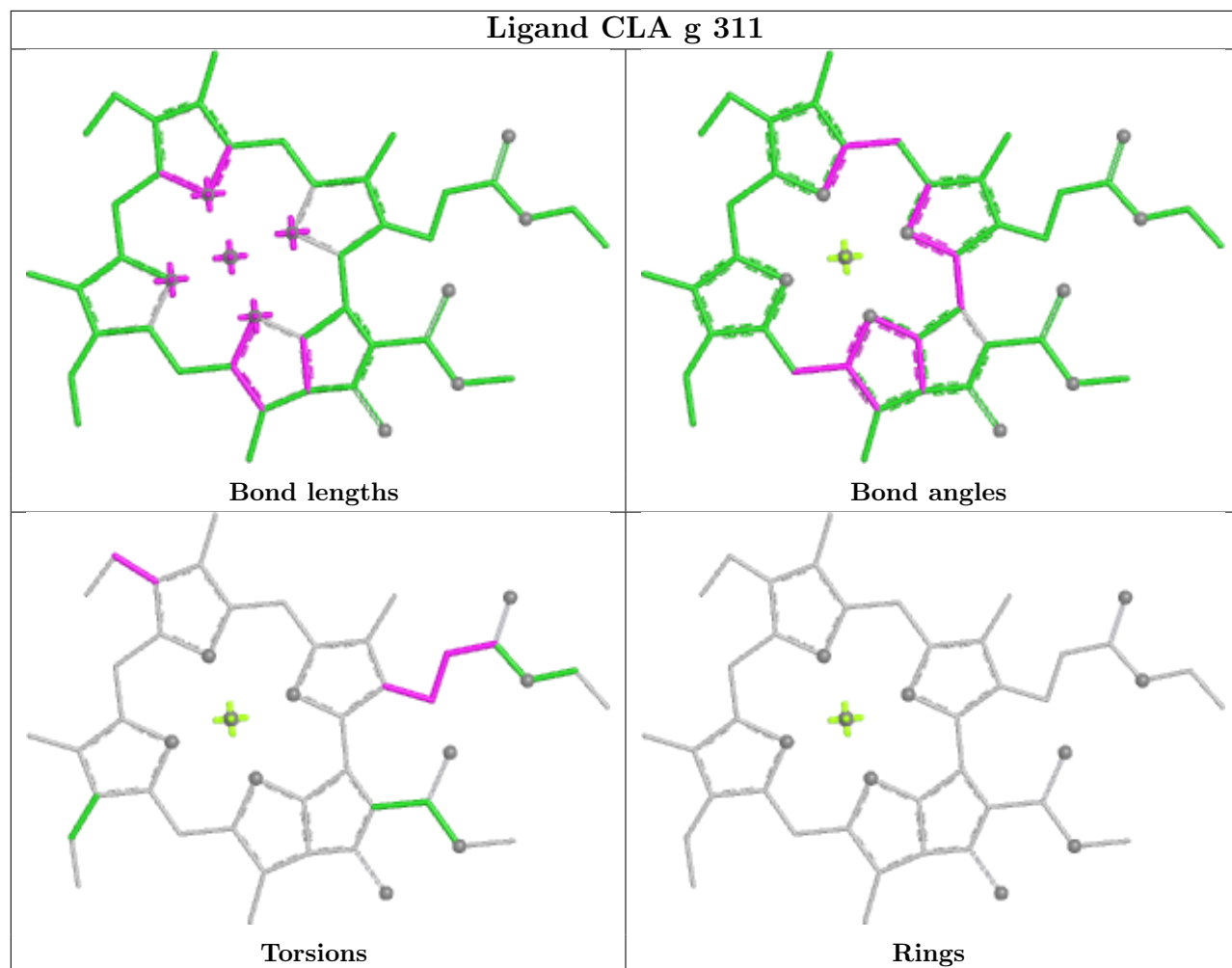
Ligand CLA c 307



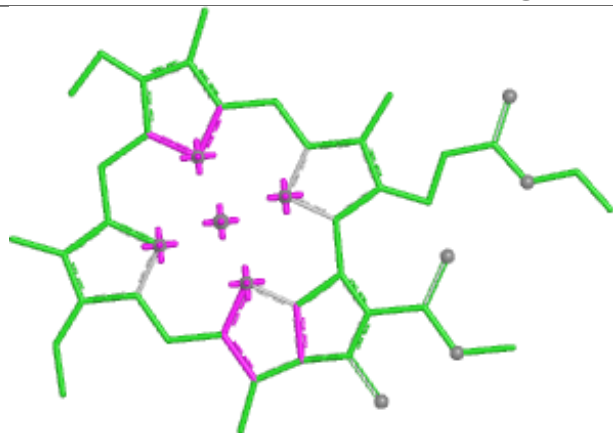
Ligand CLA B 841



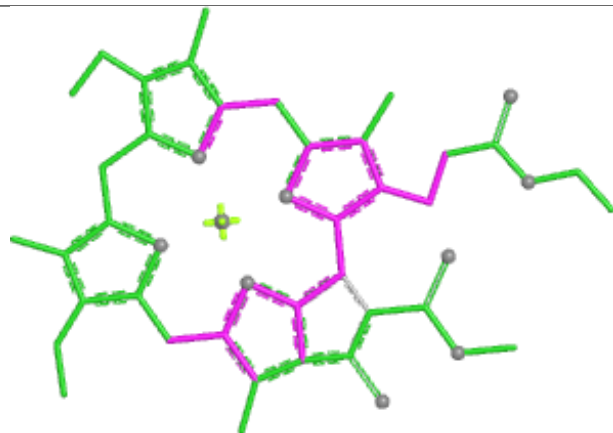
Ligand CLA g 311



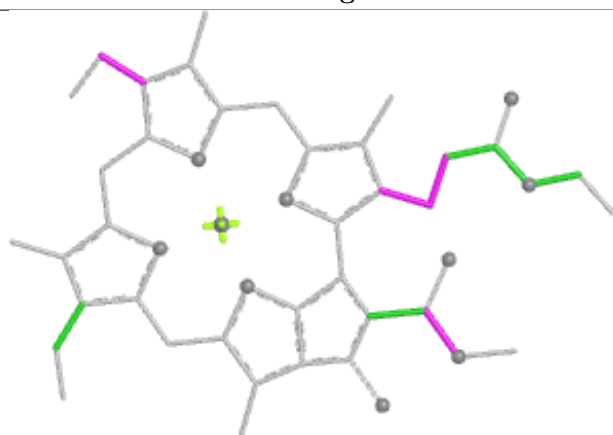
Ligand CLA n 202



Bond lengths



Bond angles

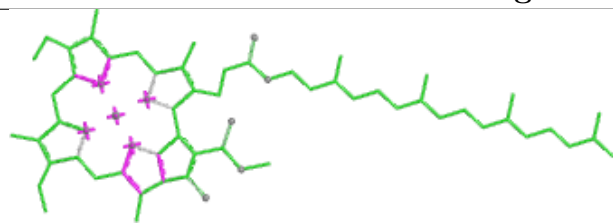


Torsions

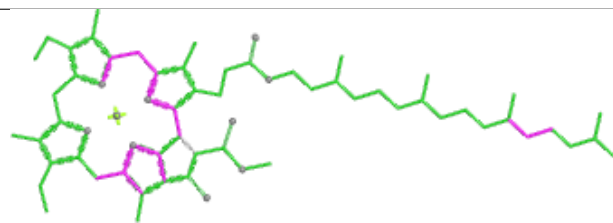


Rings

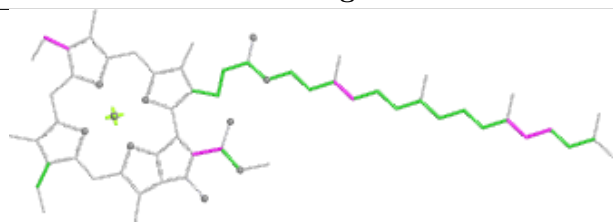
Ligand CLA B 818



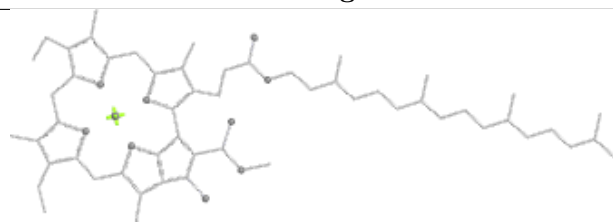
Bond lengths



Bond angles

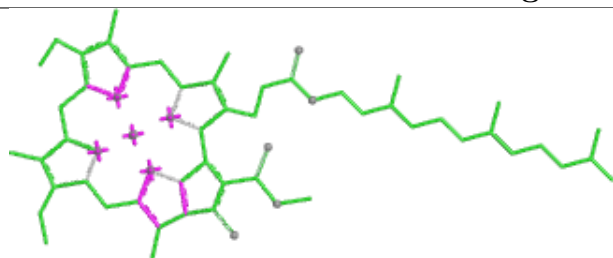


Torsions

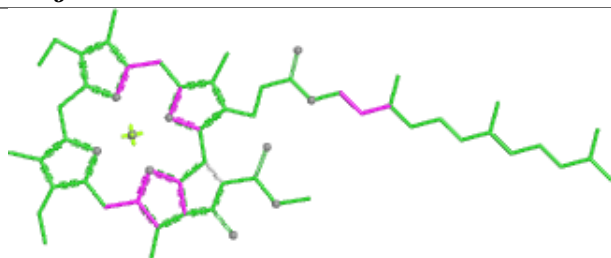


Rings

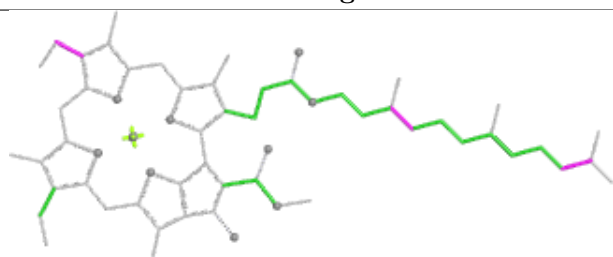
Ligand CLA j 308



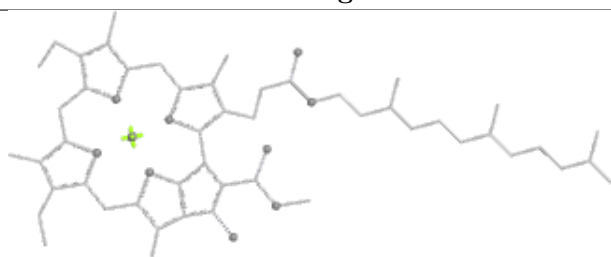
Bond lengths



Bond angles

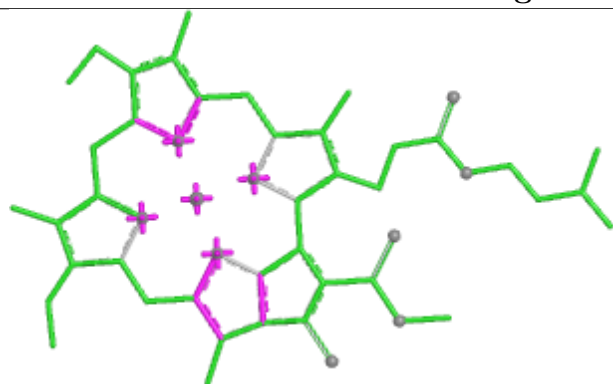


Torsions

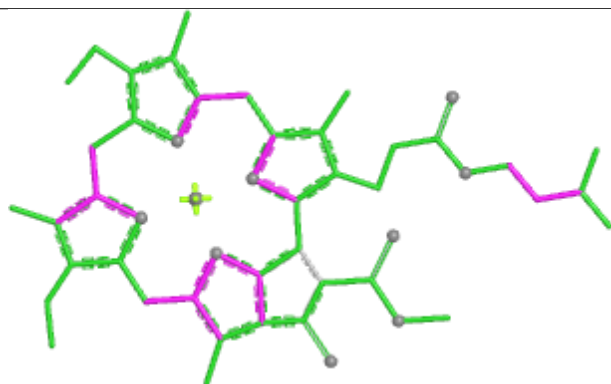


Rings

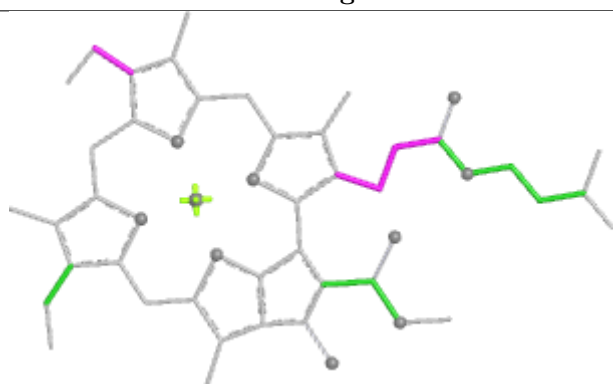
Ligand CLA B 832



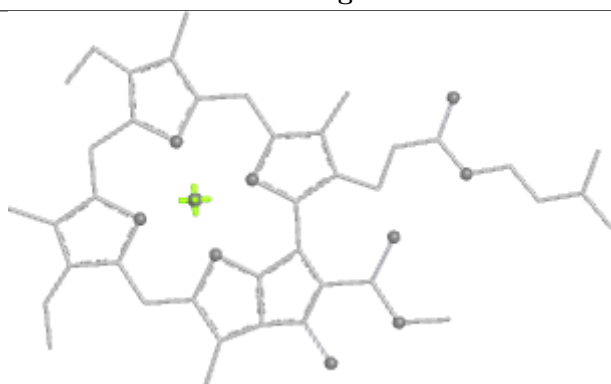
Bond lengths



Bond angles

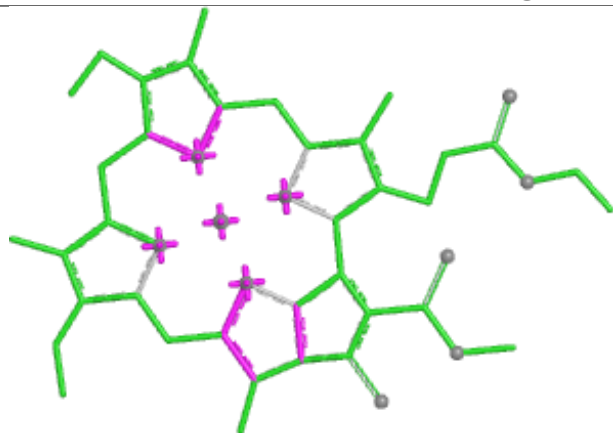


Torsions

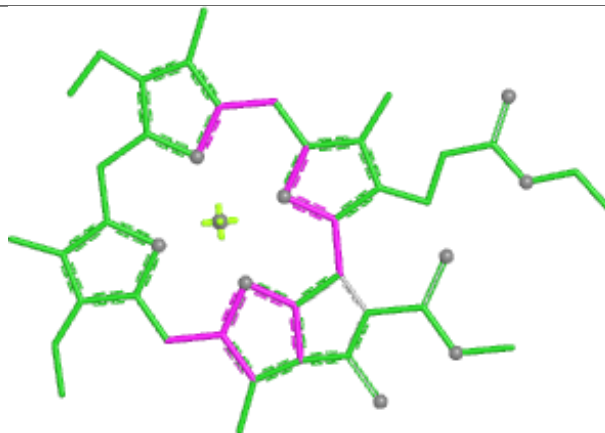


Rings

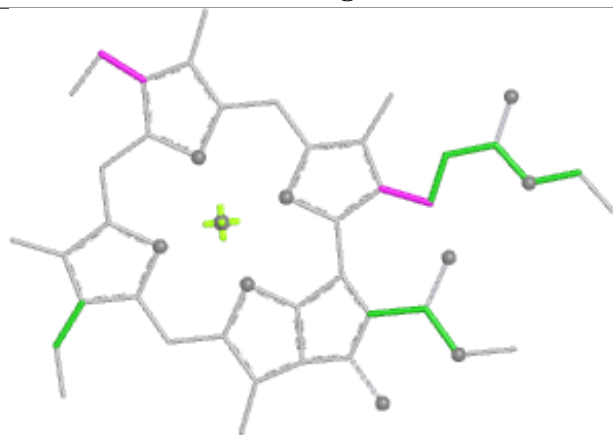
Ligand CLA o 310



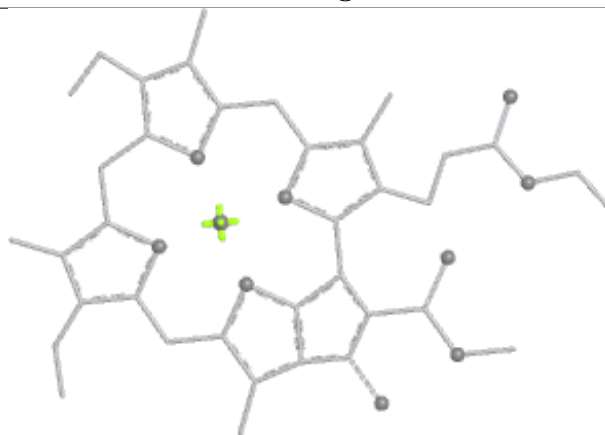
Bond lengths



Bond angles

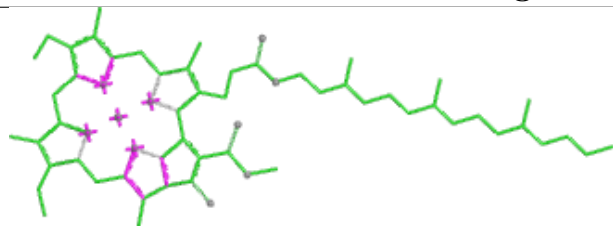


Torsions

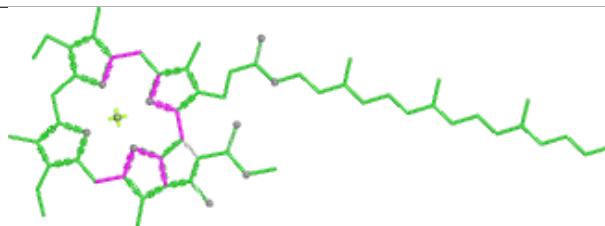


Rings

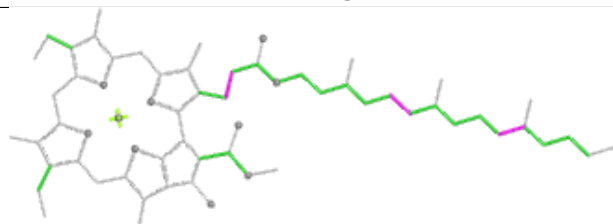
Ligand CLA A 821



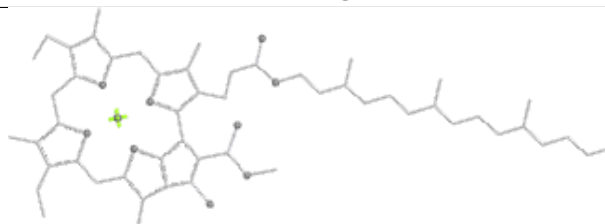
Bond lengths



Bond angles

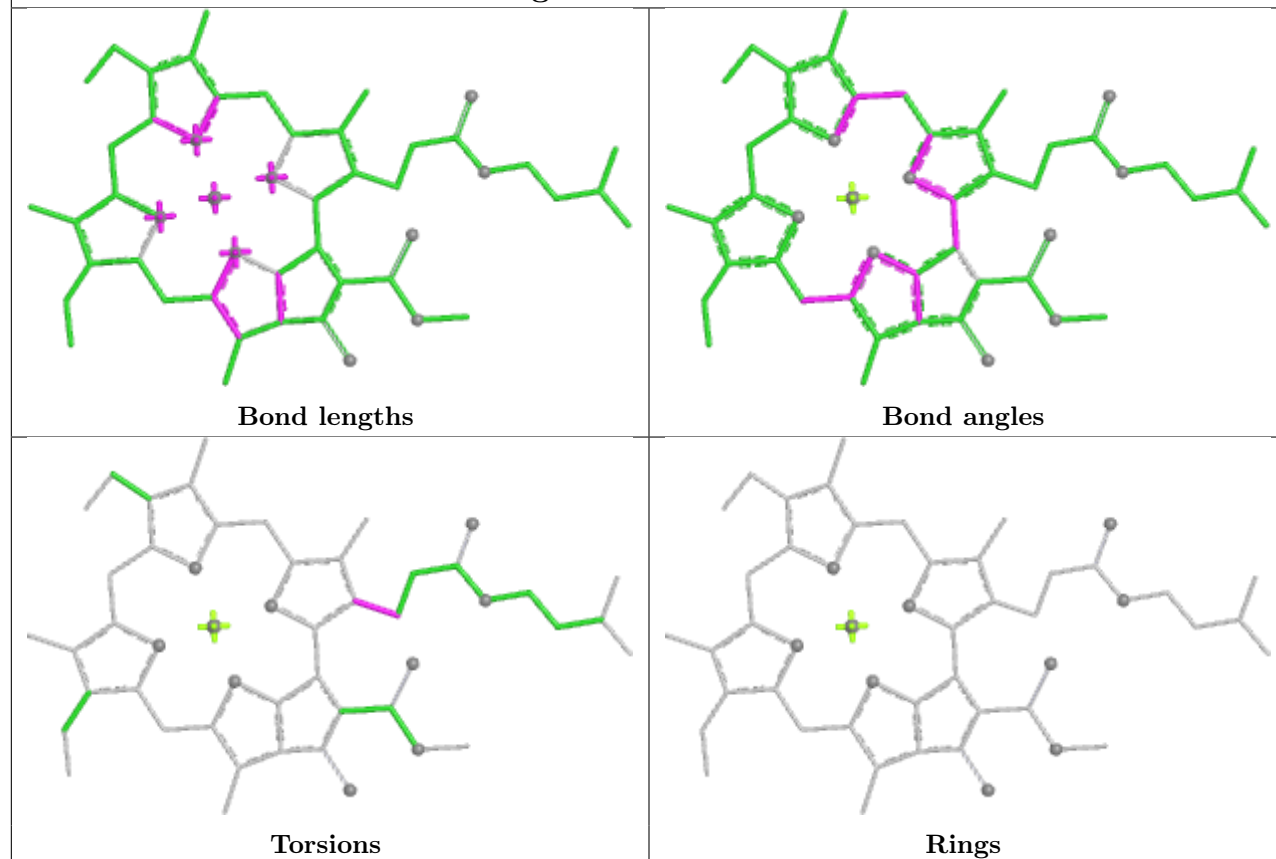


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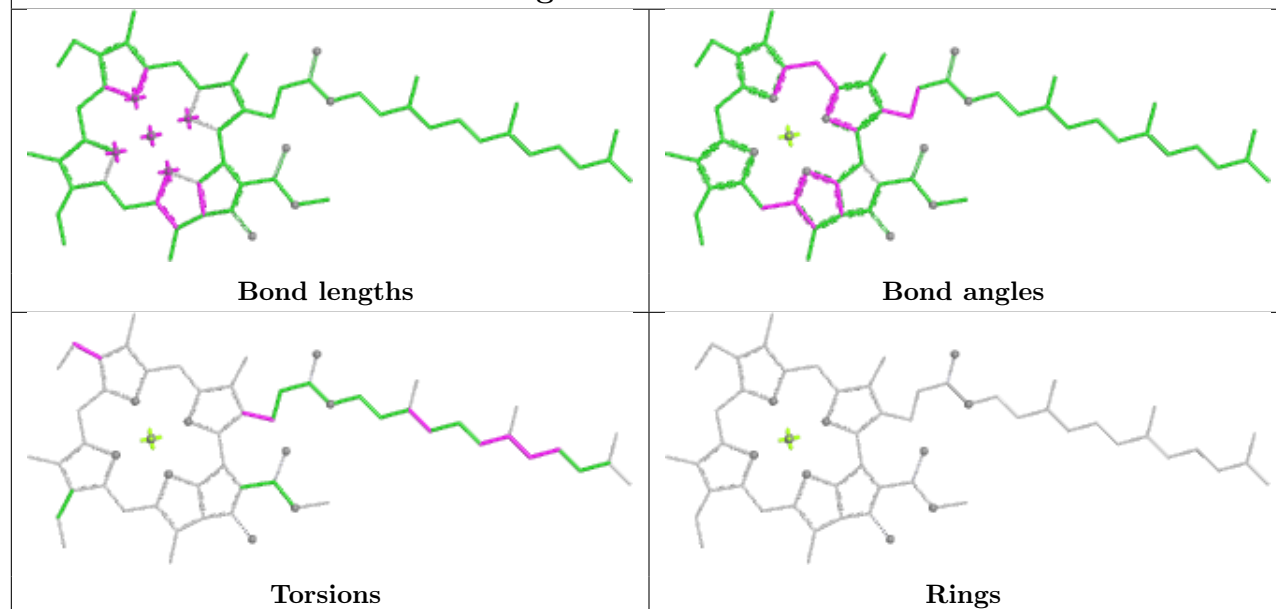


Rings

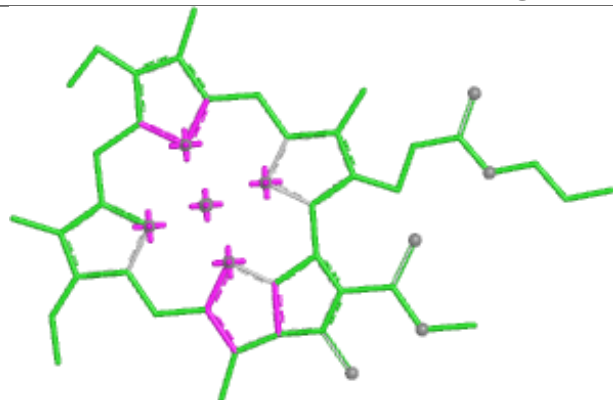
Ligand CLA A 826



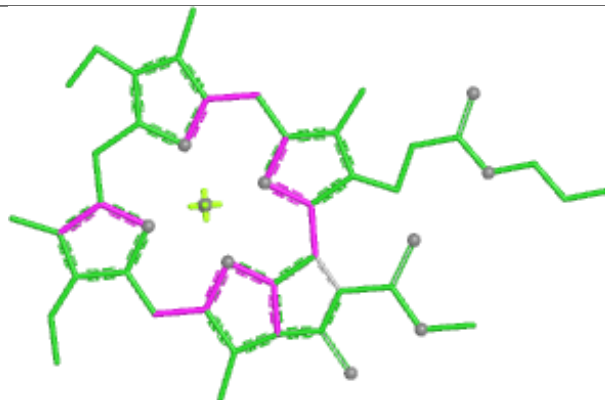
Ligand CLA a 305



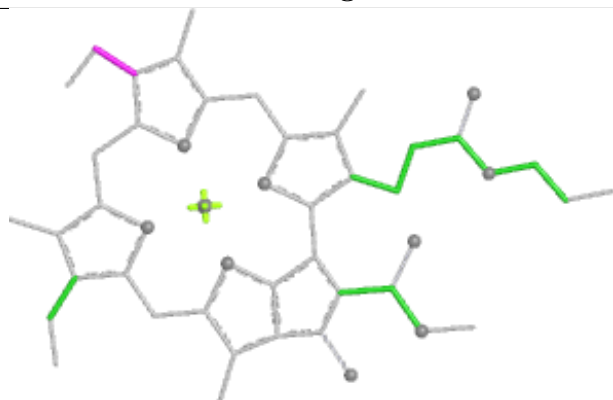
Ligand CLA A 839



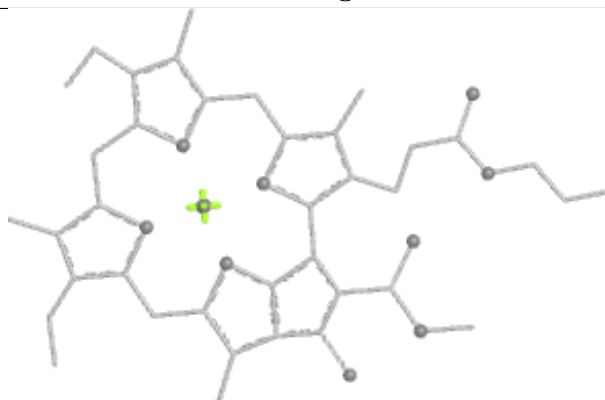
Bond lengths



Bond angles

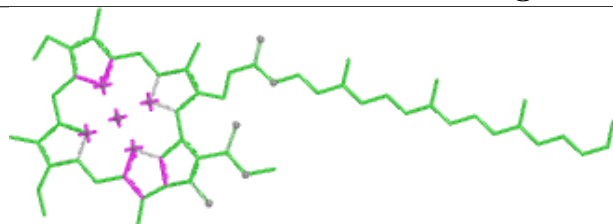


Torsions

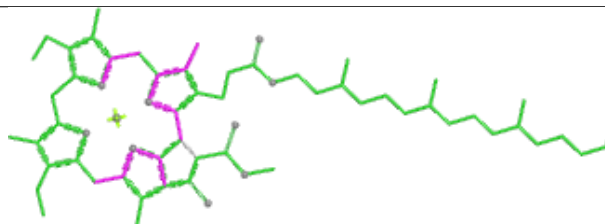


Rings

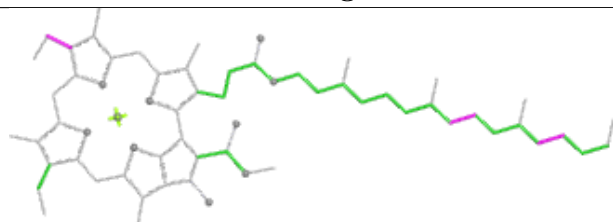
Ligand CLA B 836



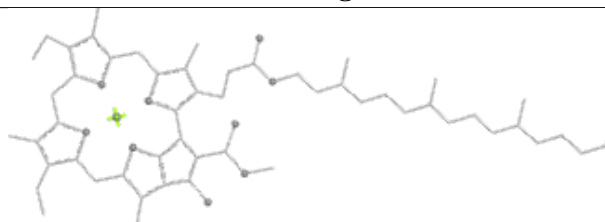
Bond lengths



Bond angles

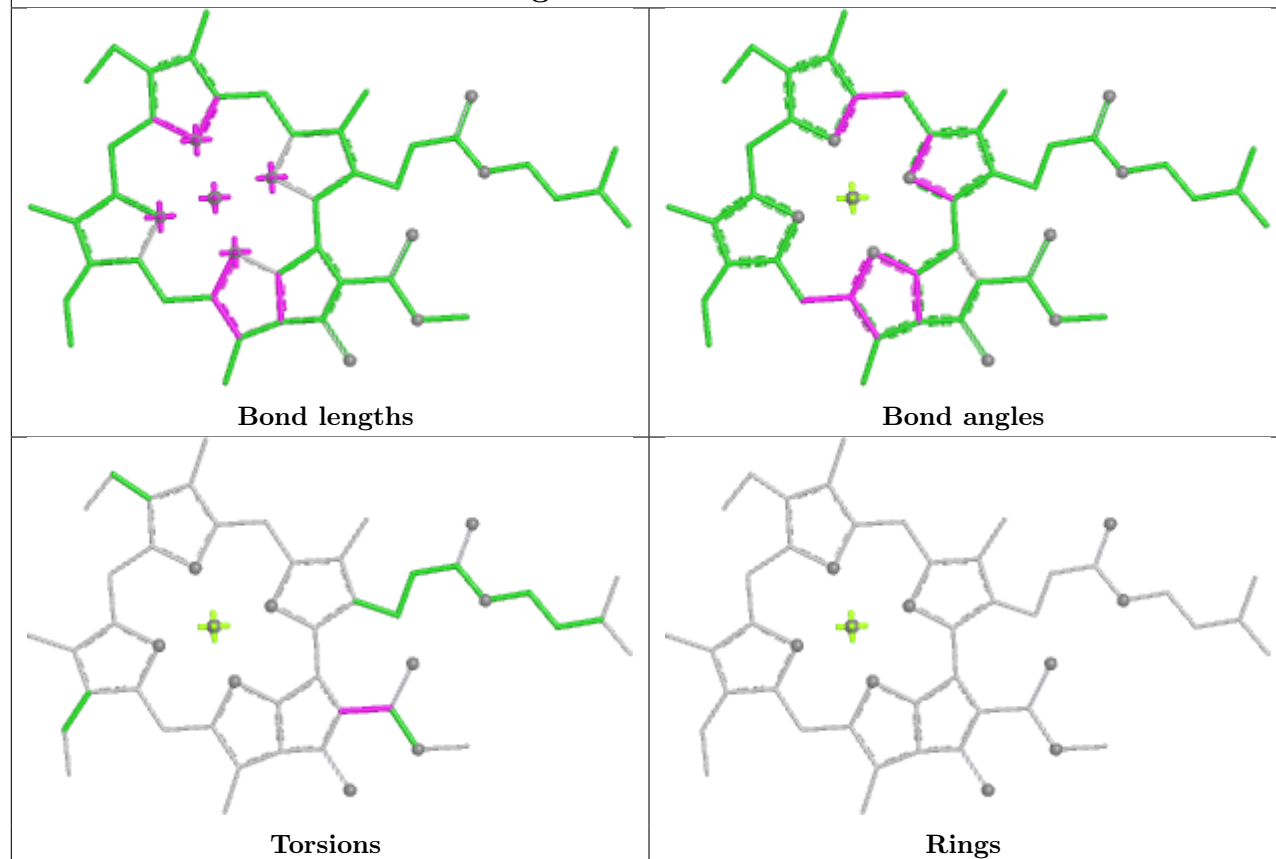


Torsions

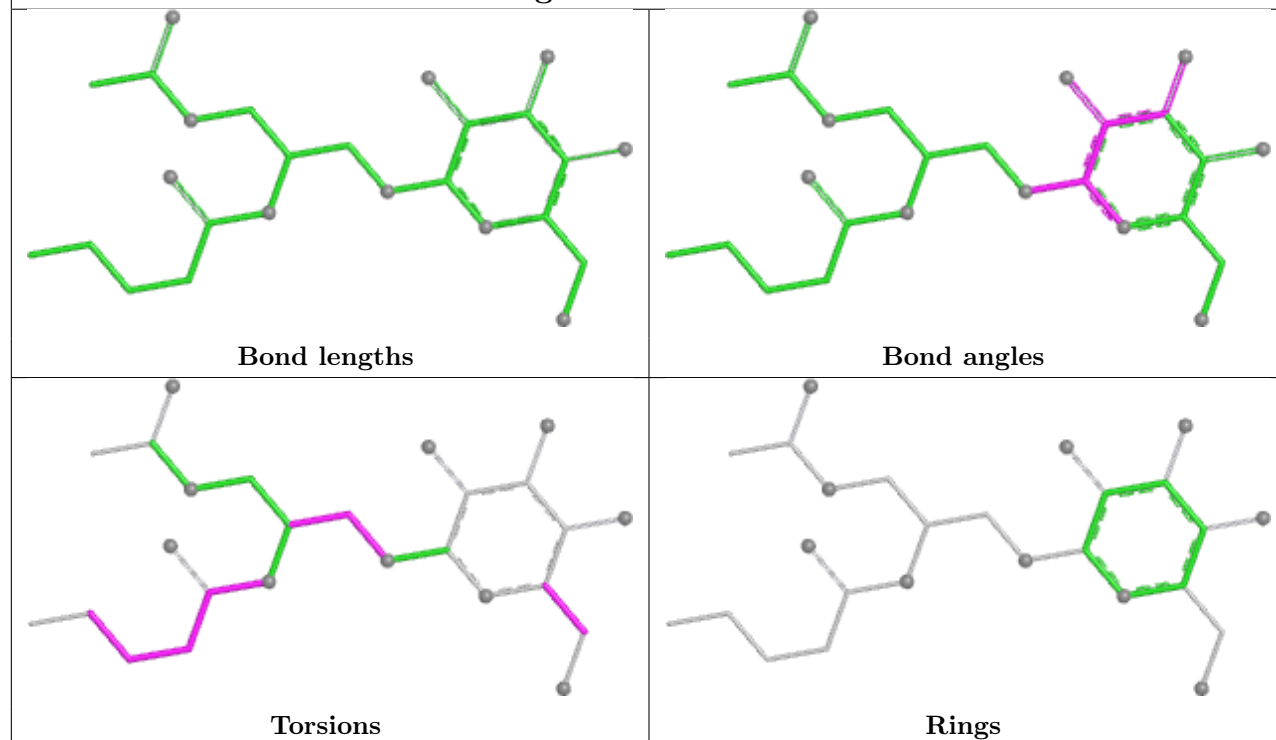


Rings

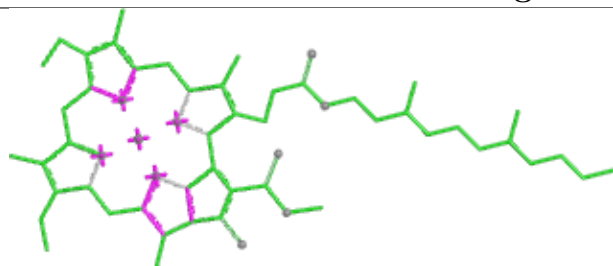
Ligand CLA A 808



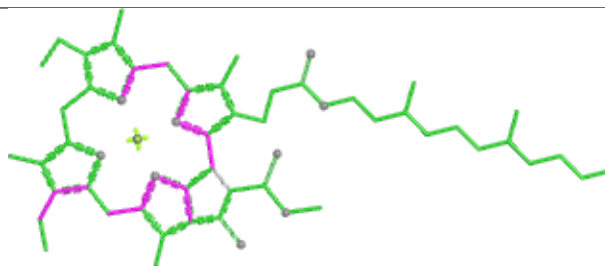
Ligand LMG f 313



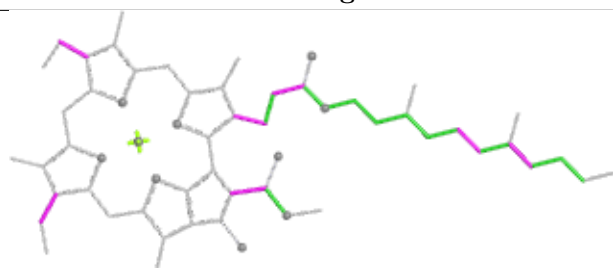
Ligand CLA B 811



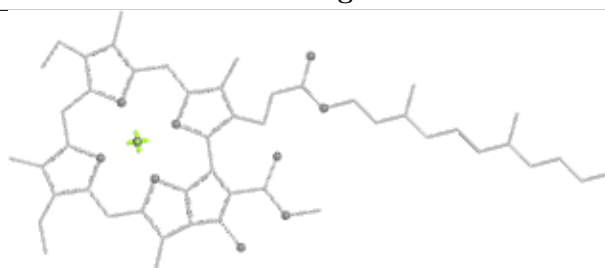
Bond lengths



Bond angles

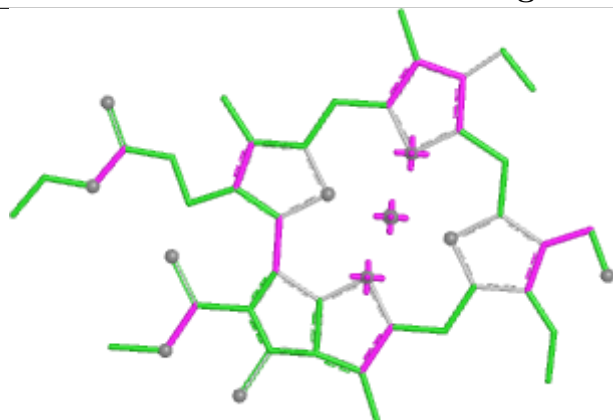


Torsions

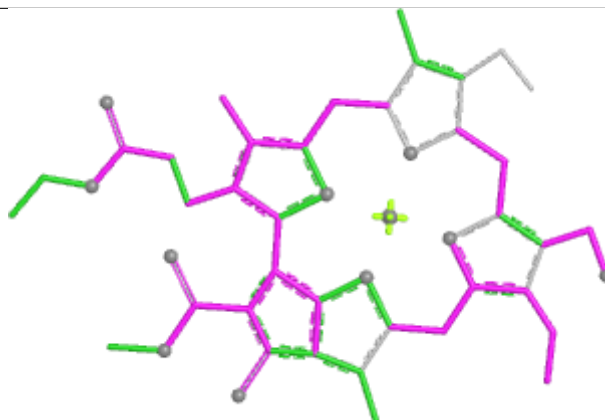


Rings

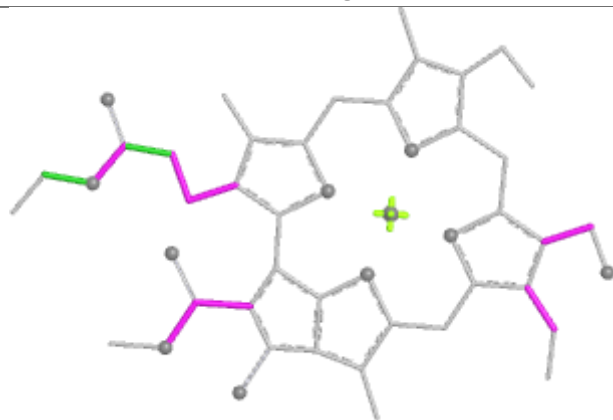
Ligand CHL k 301



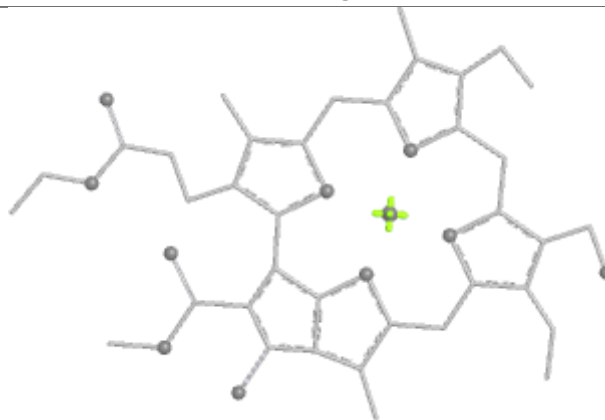
Bond lengths



Bond angles

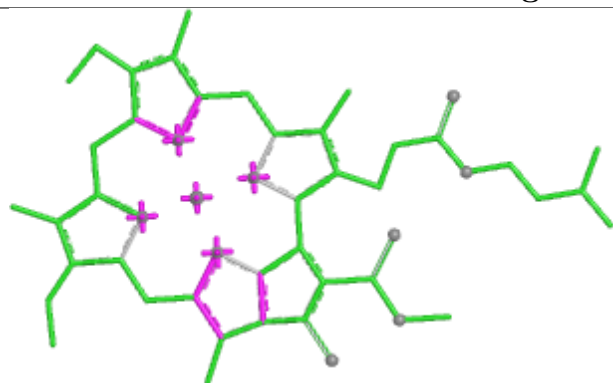


Torsions

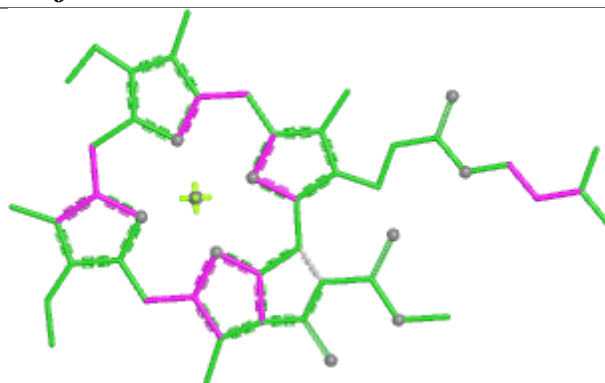


Rings

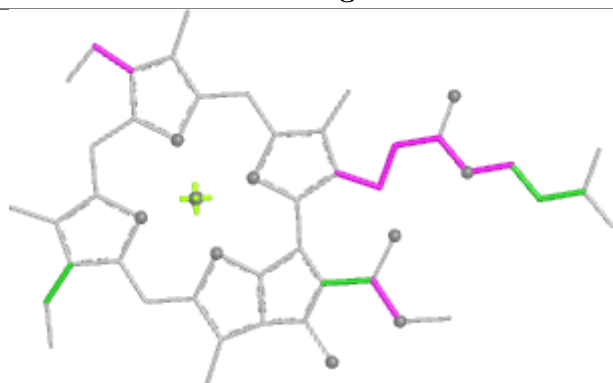
Ligand CLA j 305



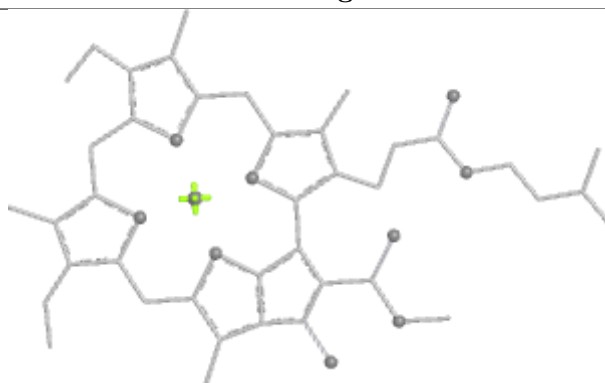
Bond lengths



Bond angles

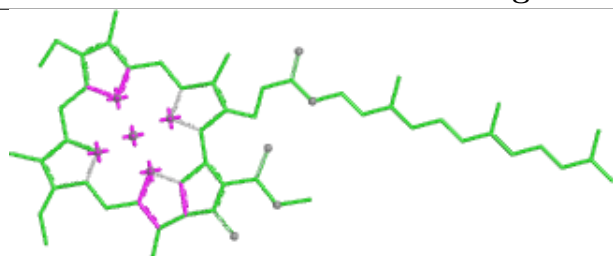


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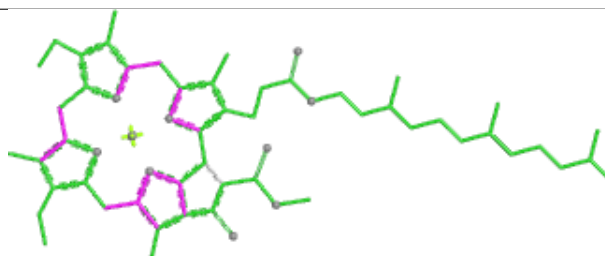


Rings

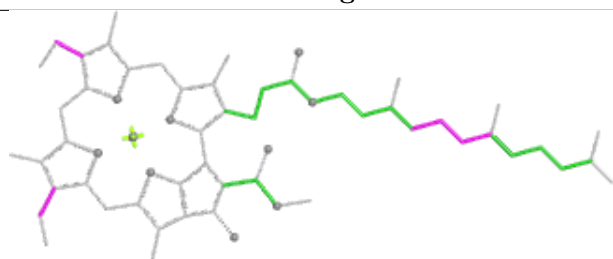
Ligand CLA m 305



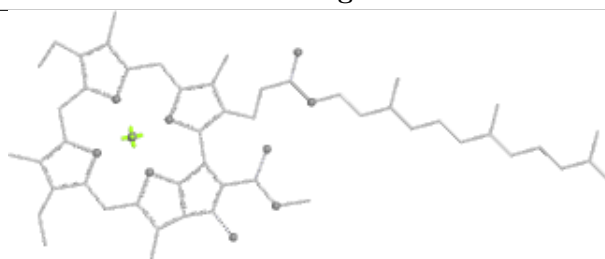
Bond lengths



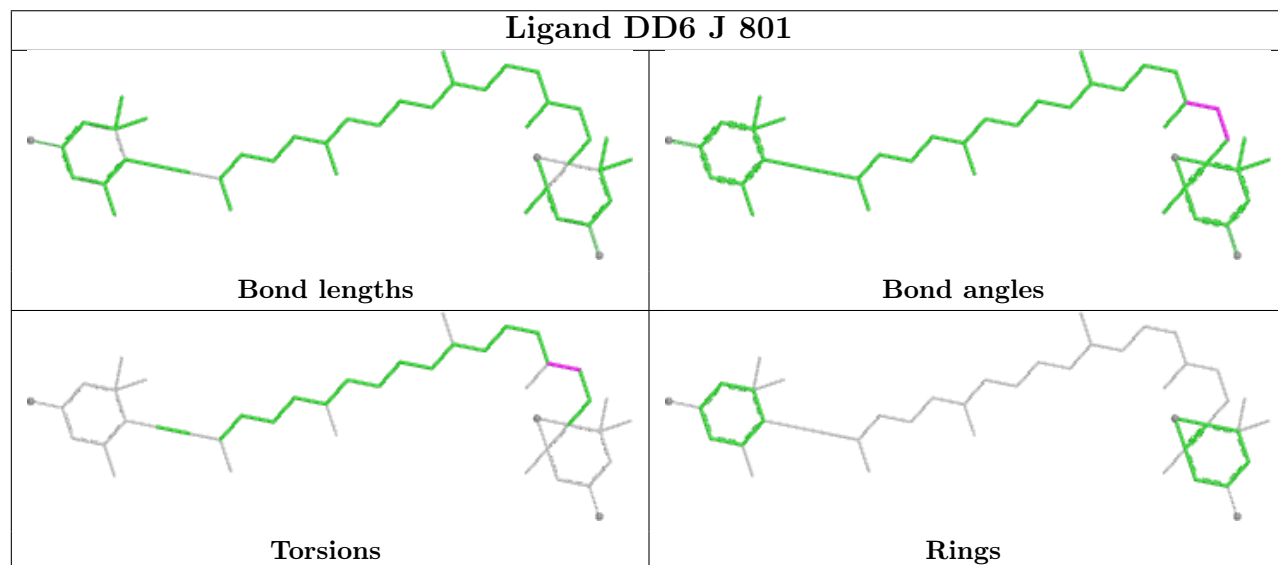
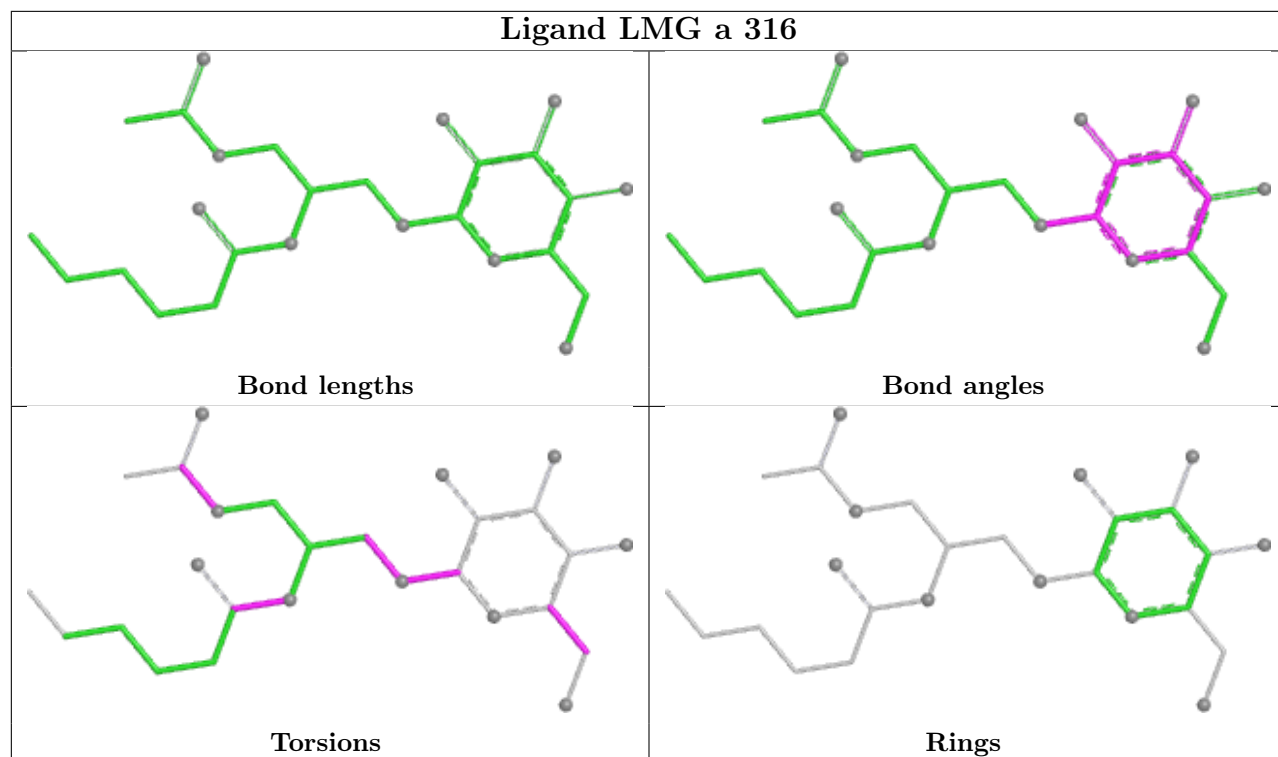
Bond angles

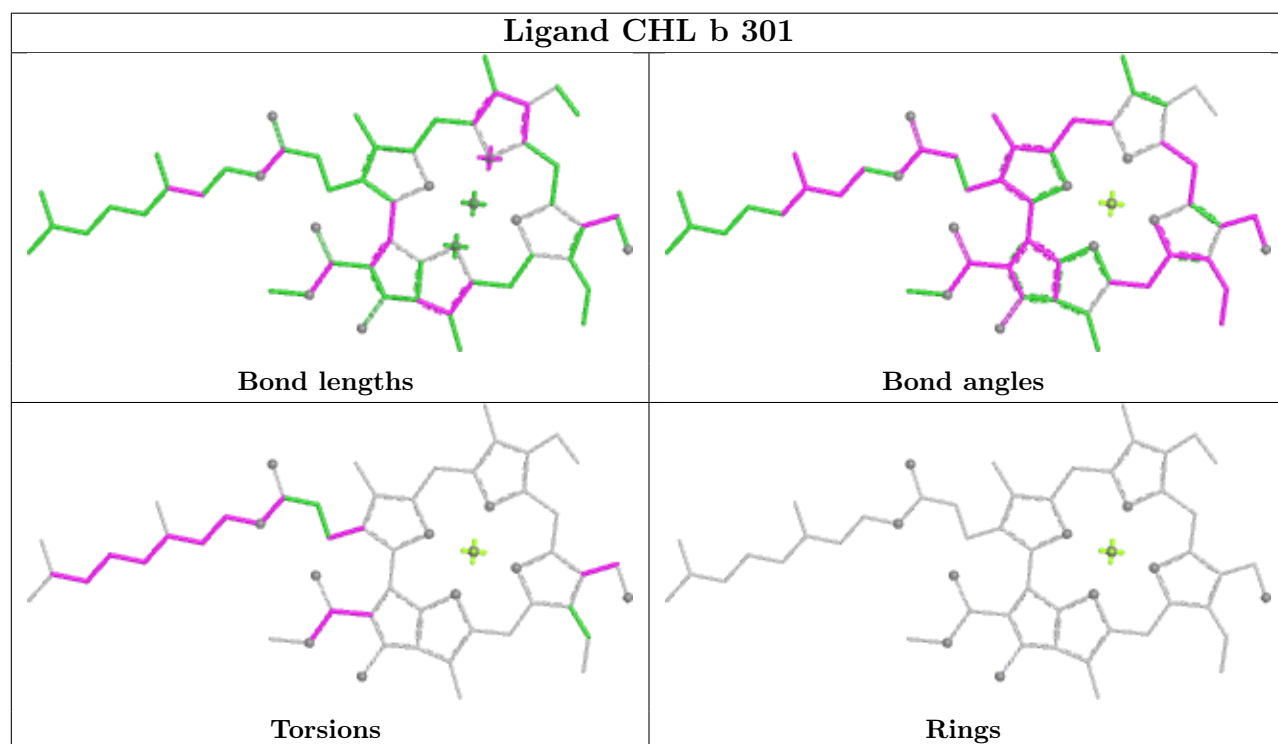
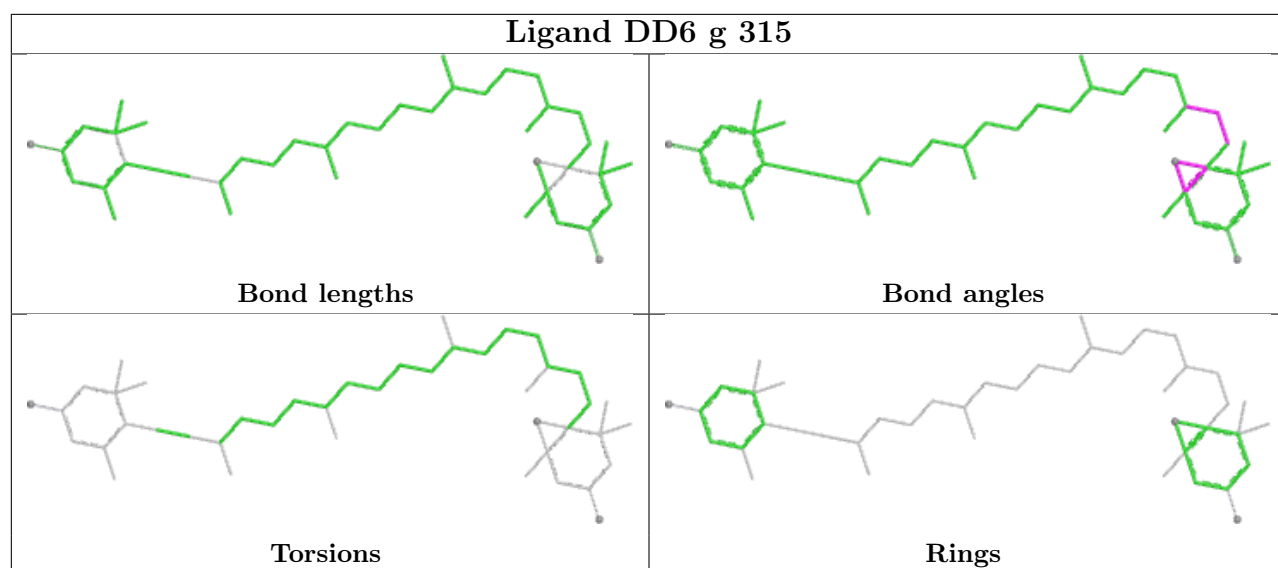


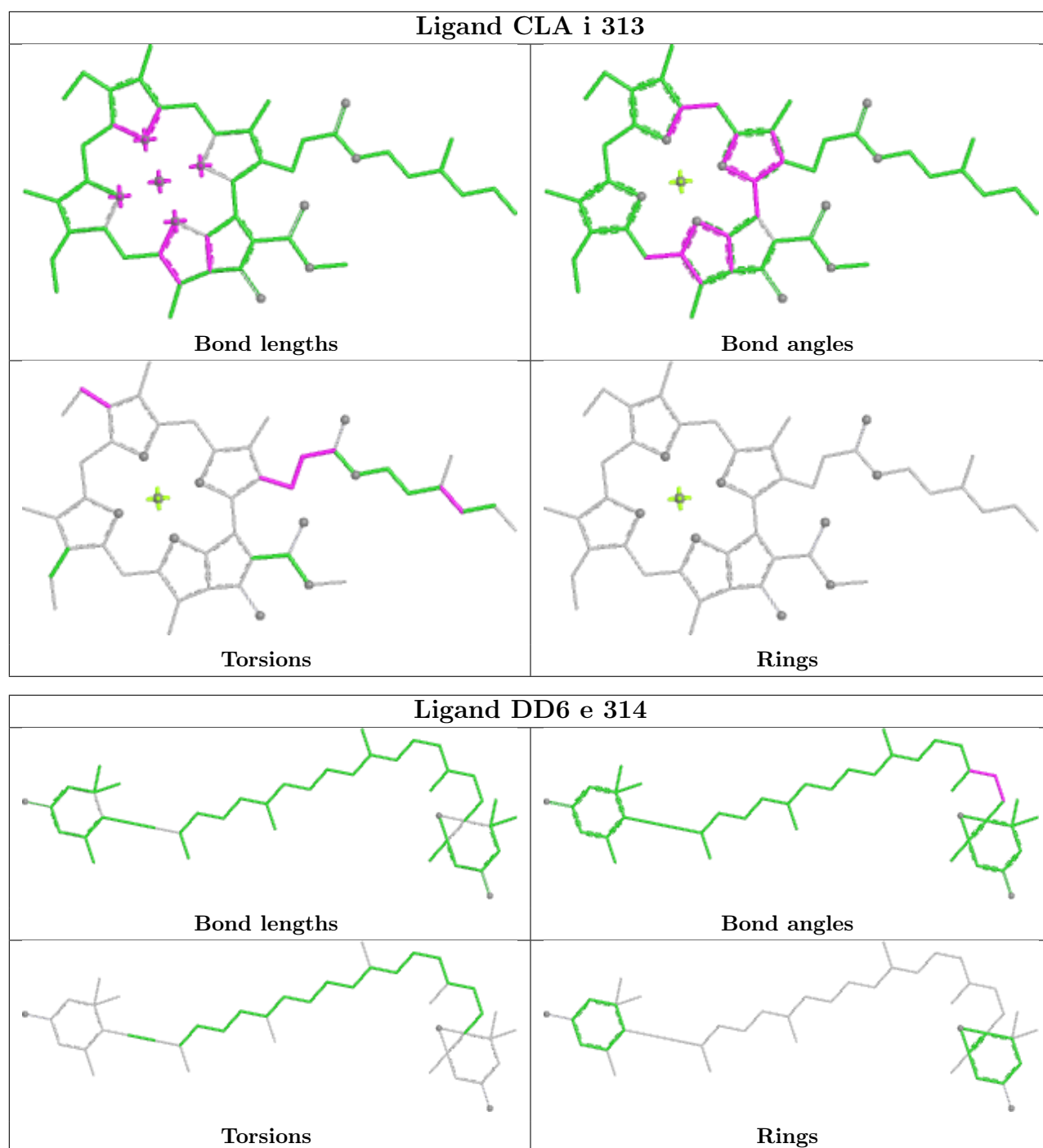
Torsions



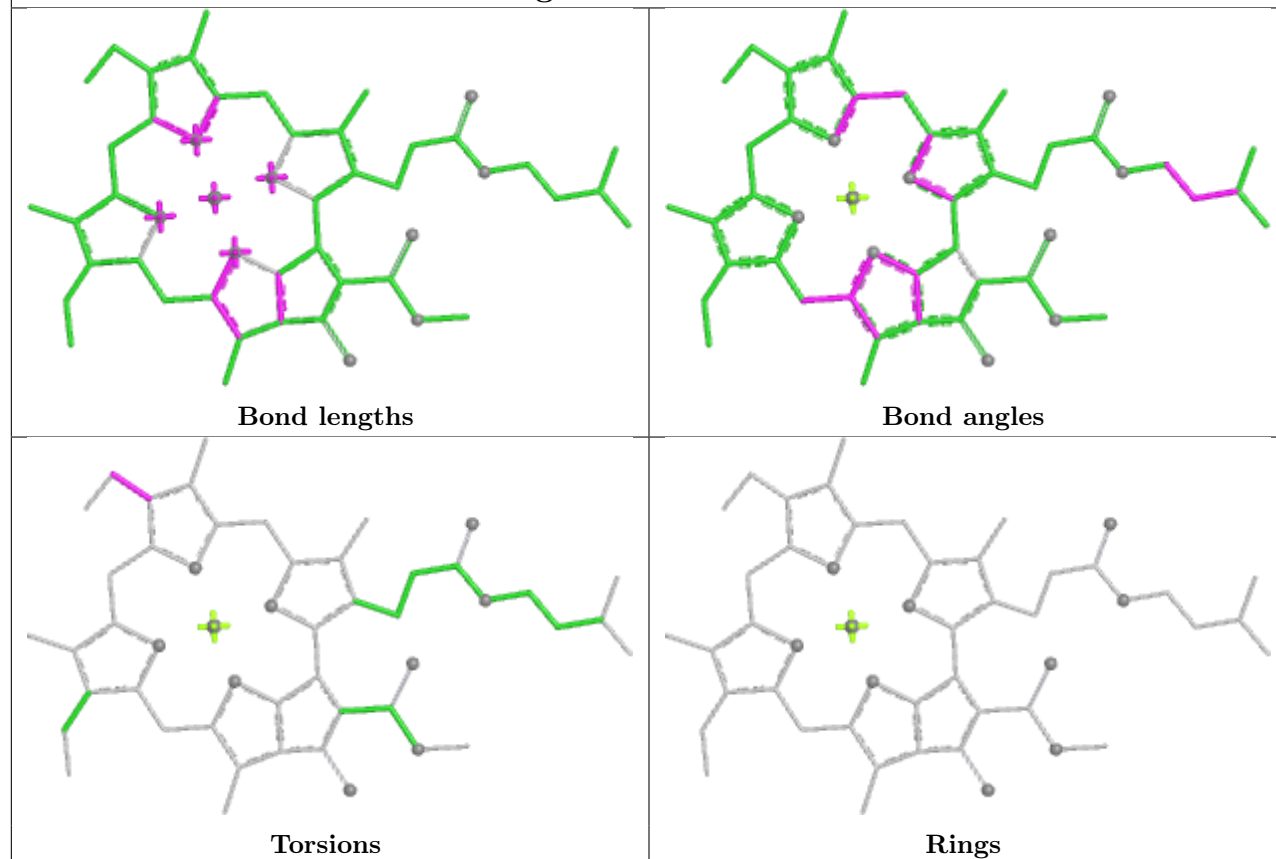
Rings



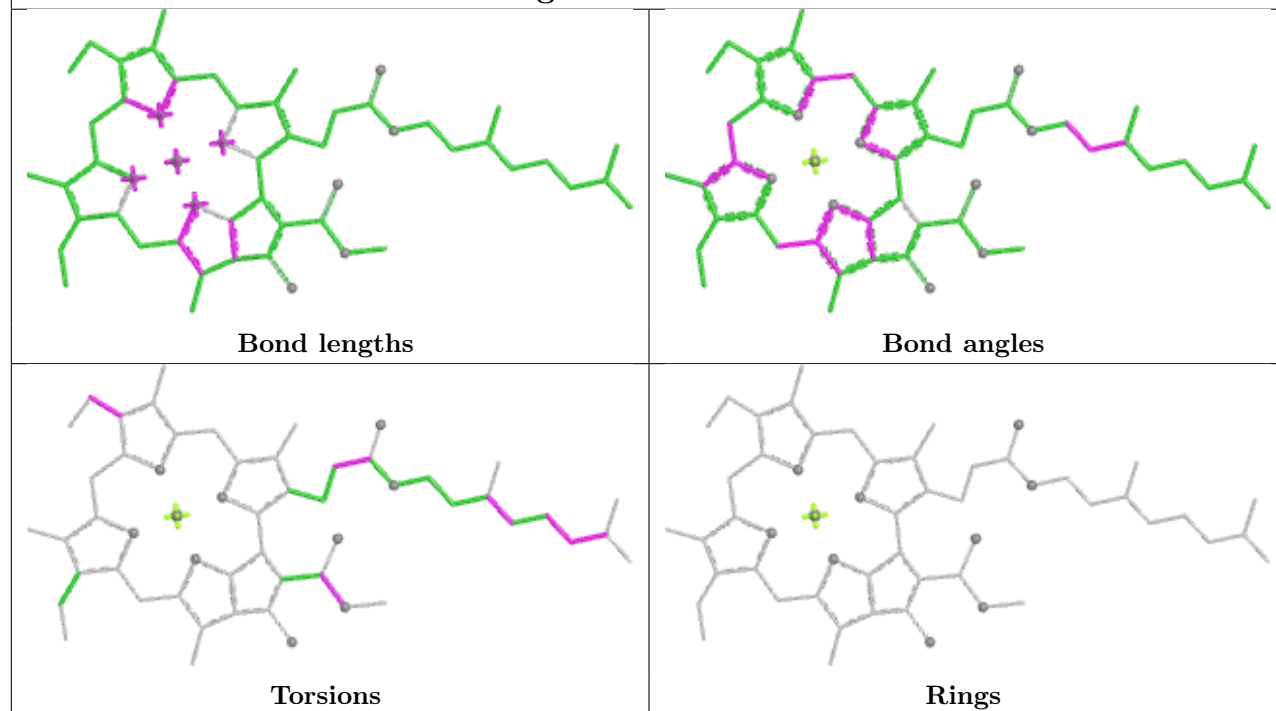




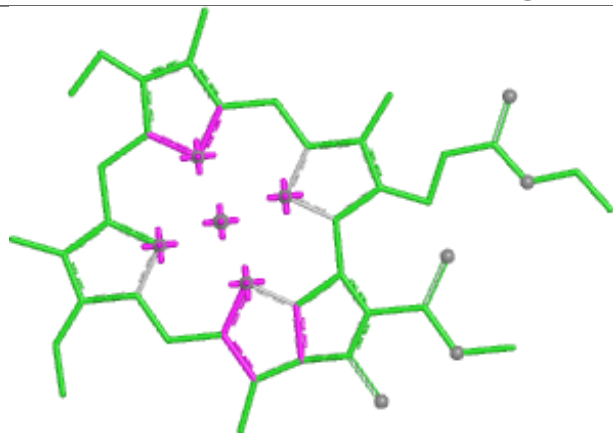
Ligand CLA k 308



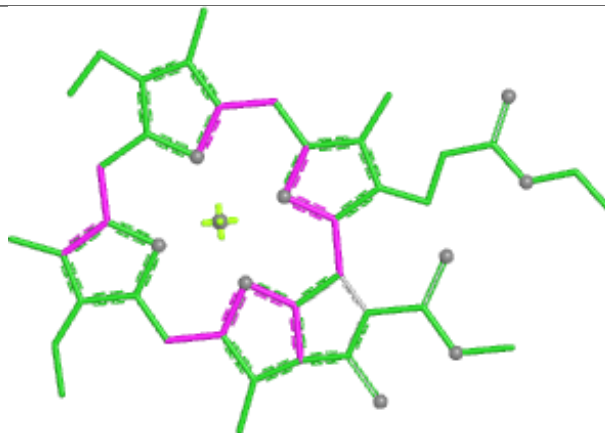
Ligand CLA e 310



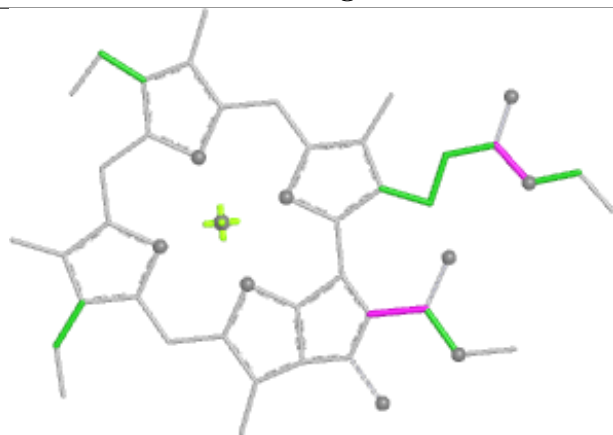
Ligand CLA e 303



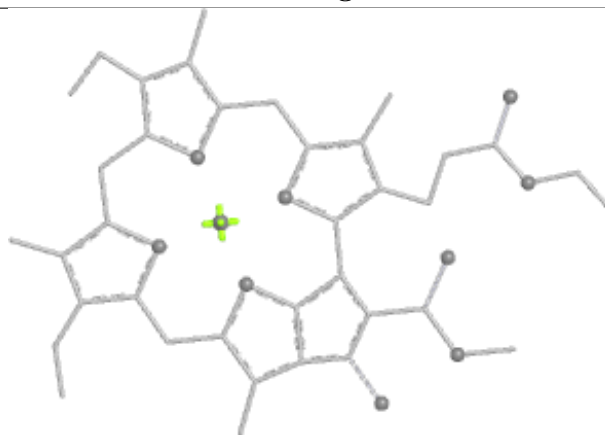
Bond lengths



Bond angles

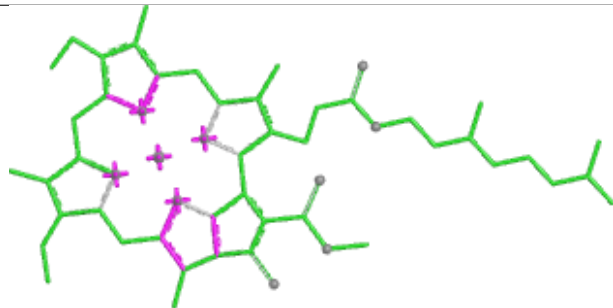


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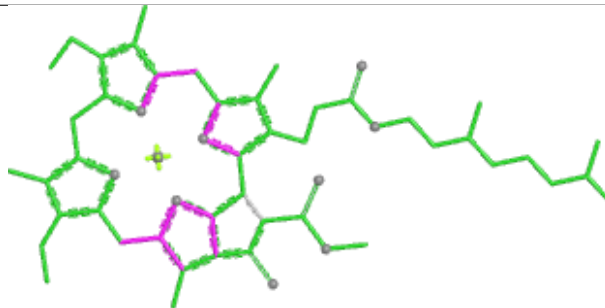


Rings

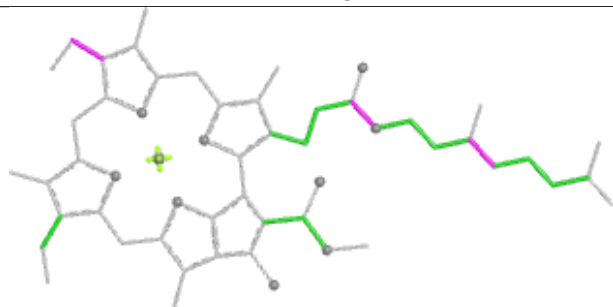
Ligand CLA g 302



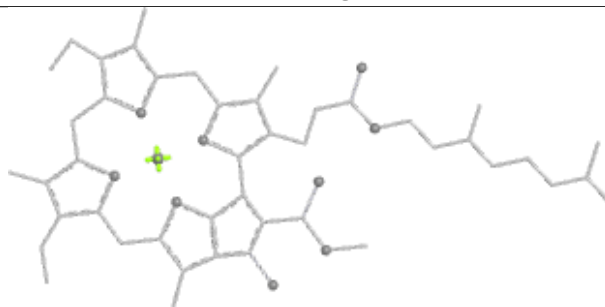
Bond lengths



Bond angles

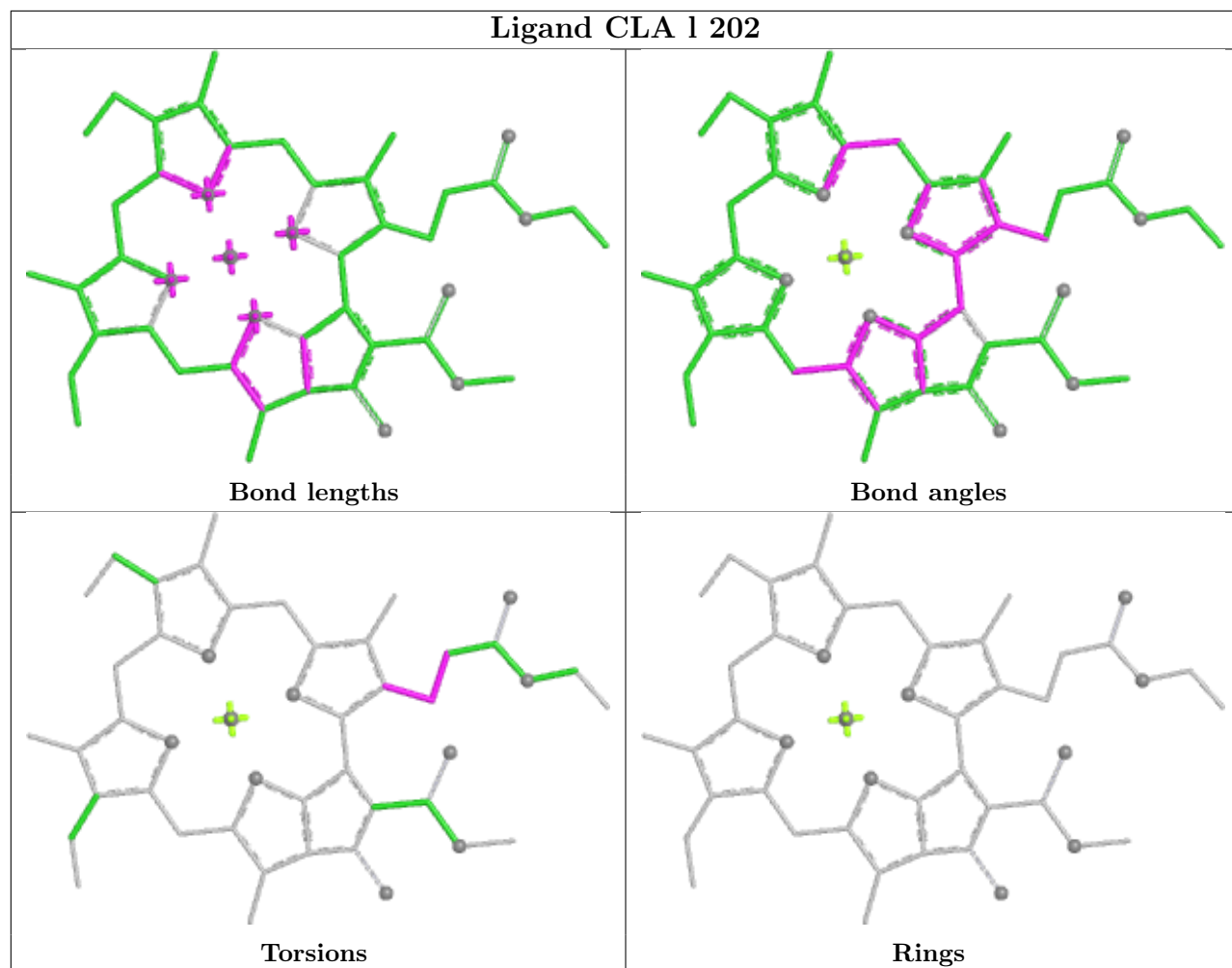


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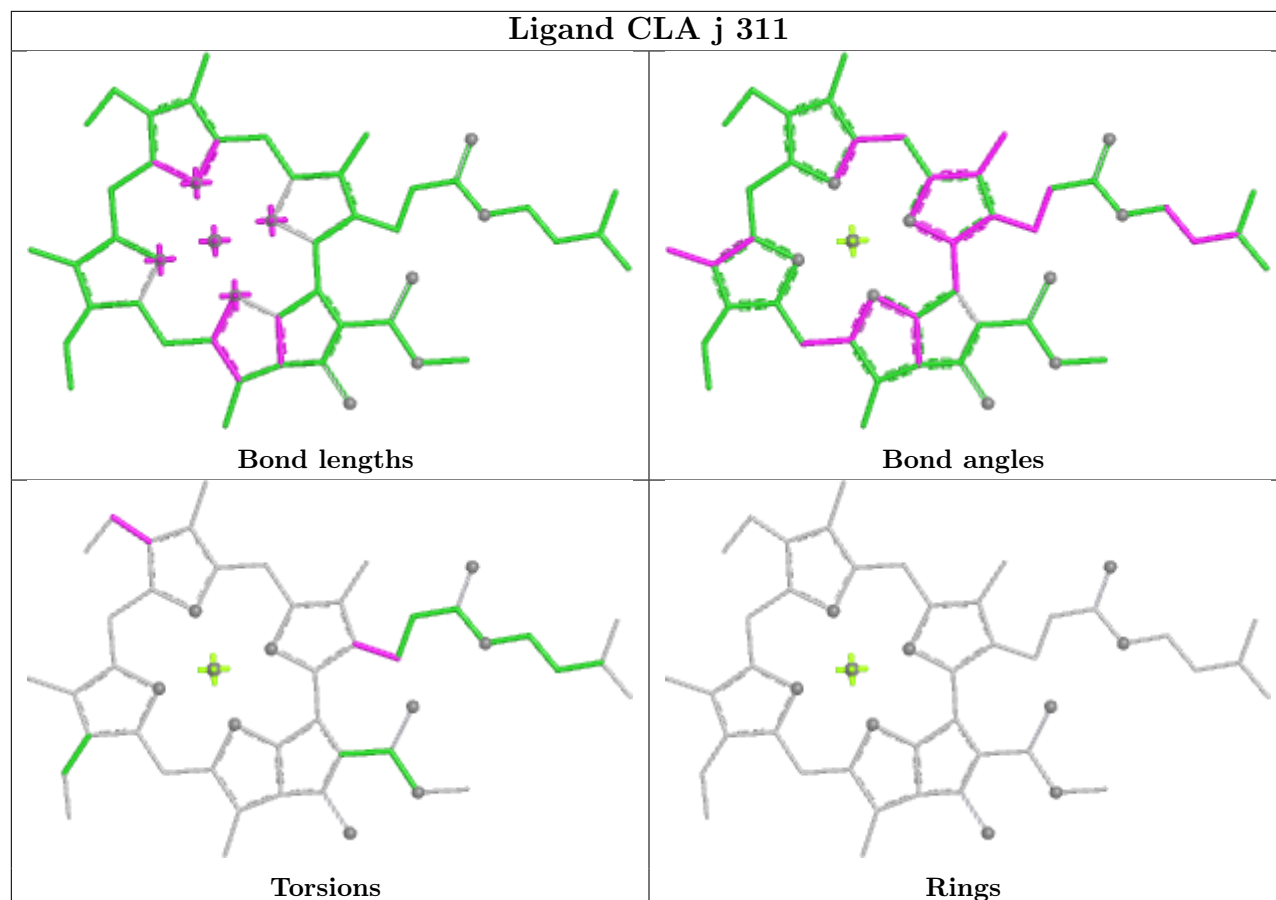


Rings

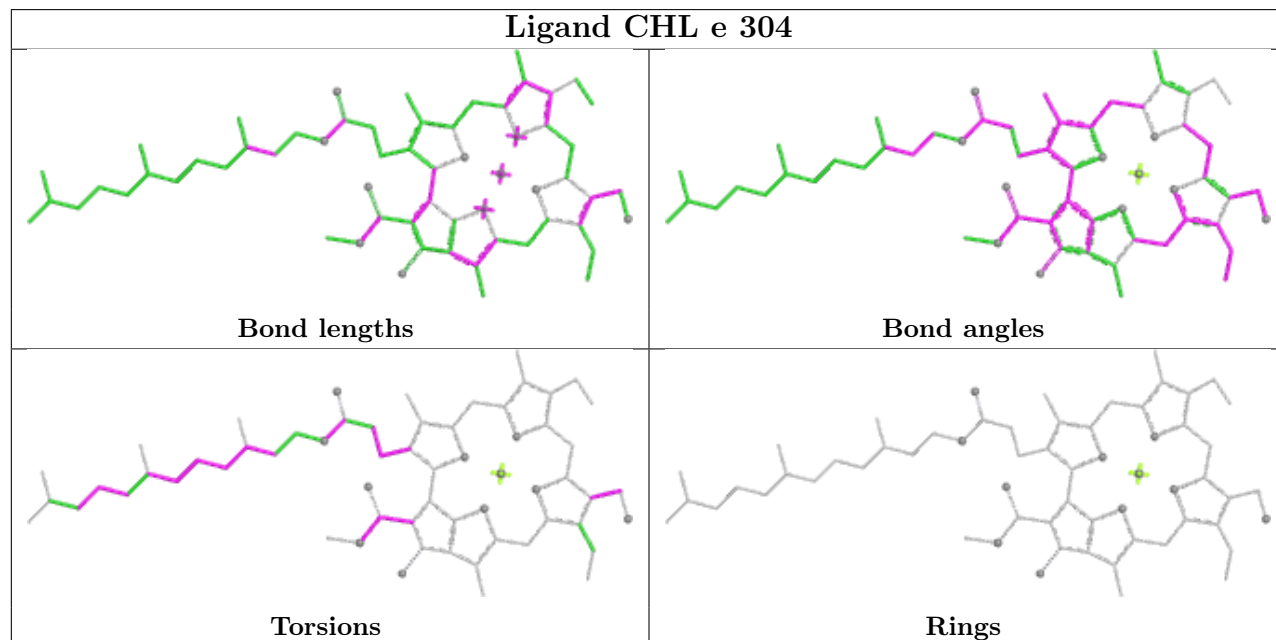
Ligand CLA 1 202

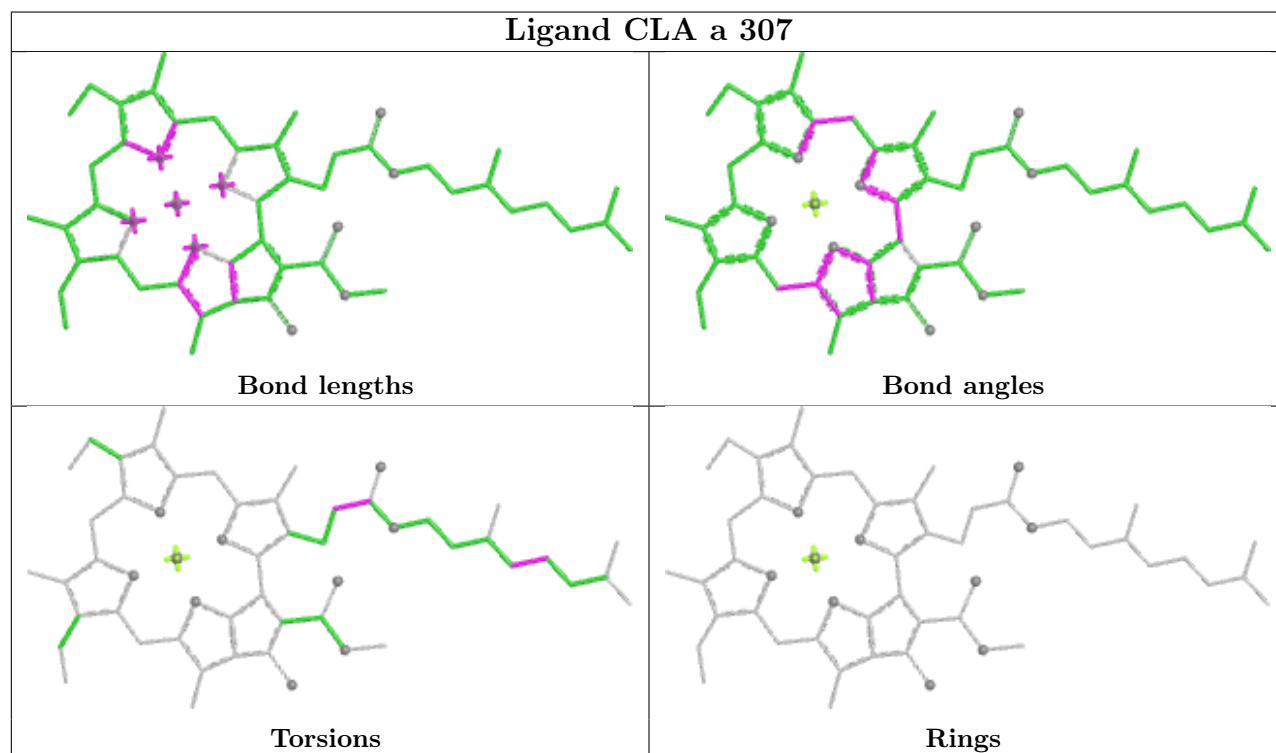
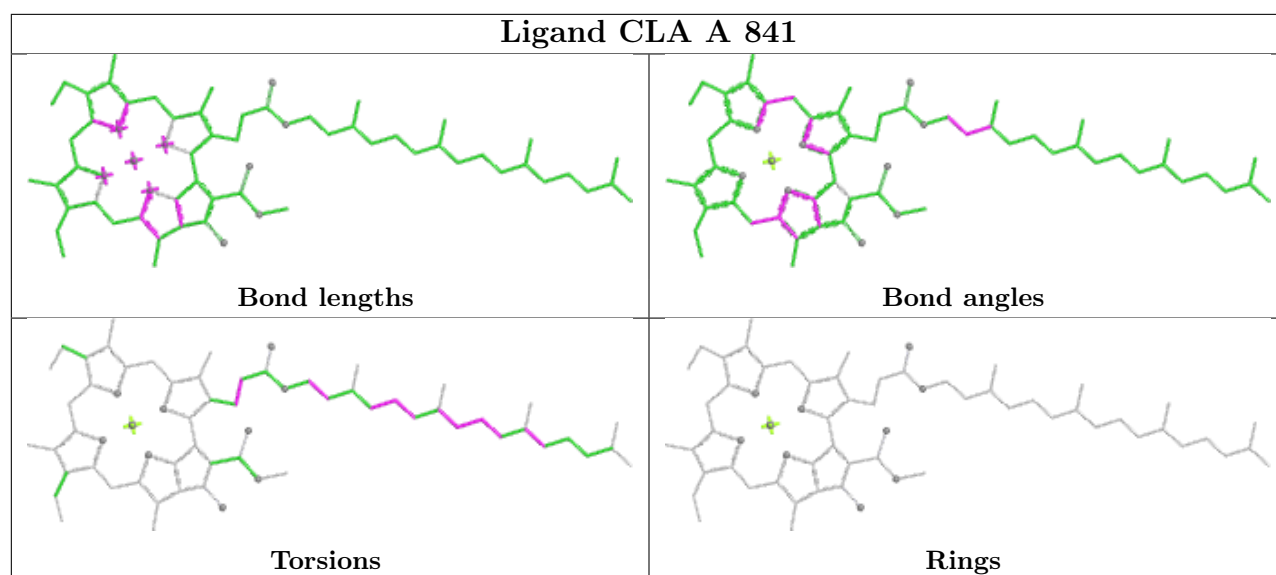


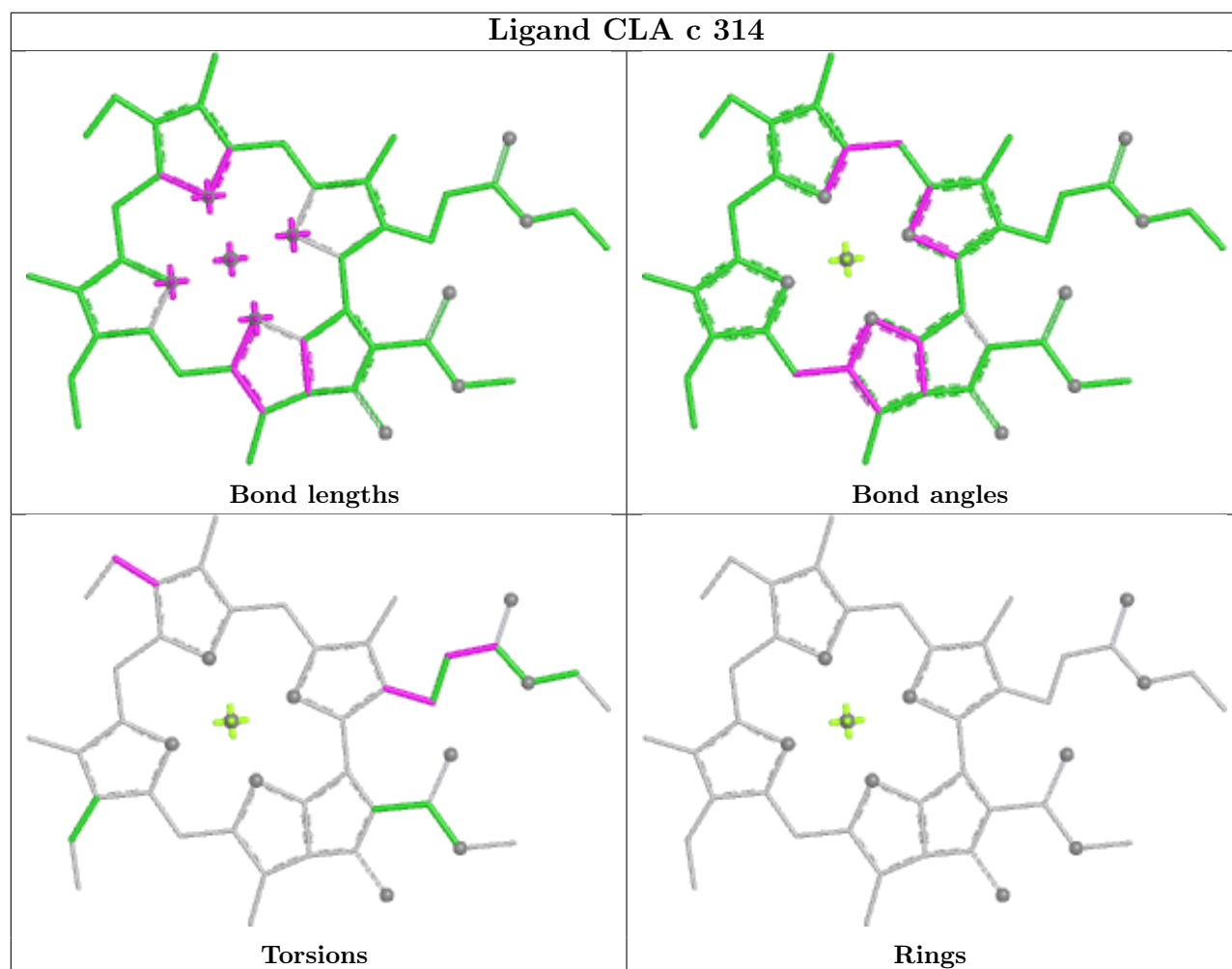
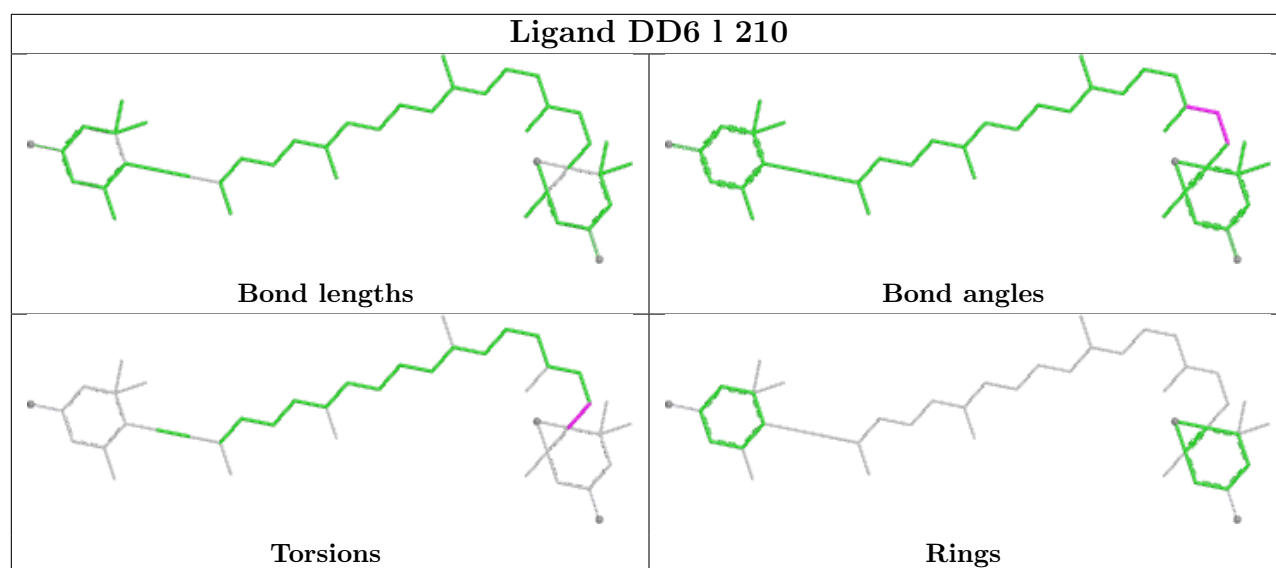
Ligand CLA j 311



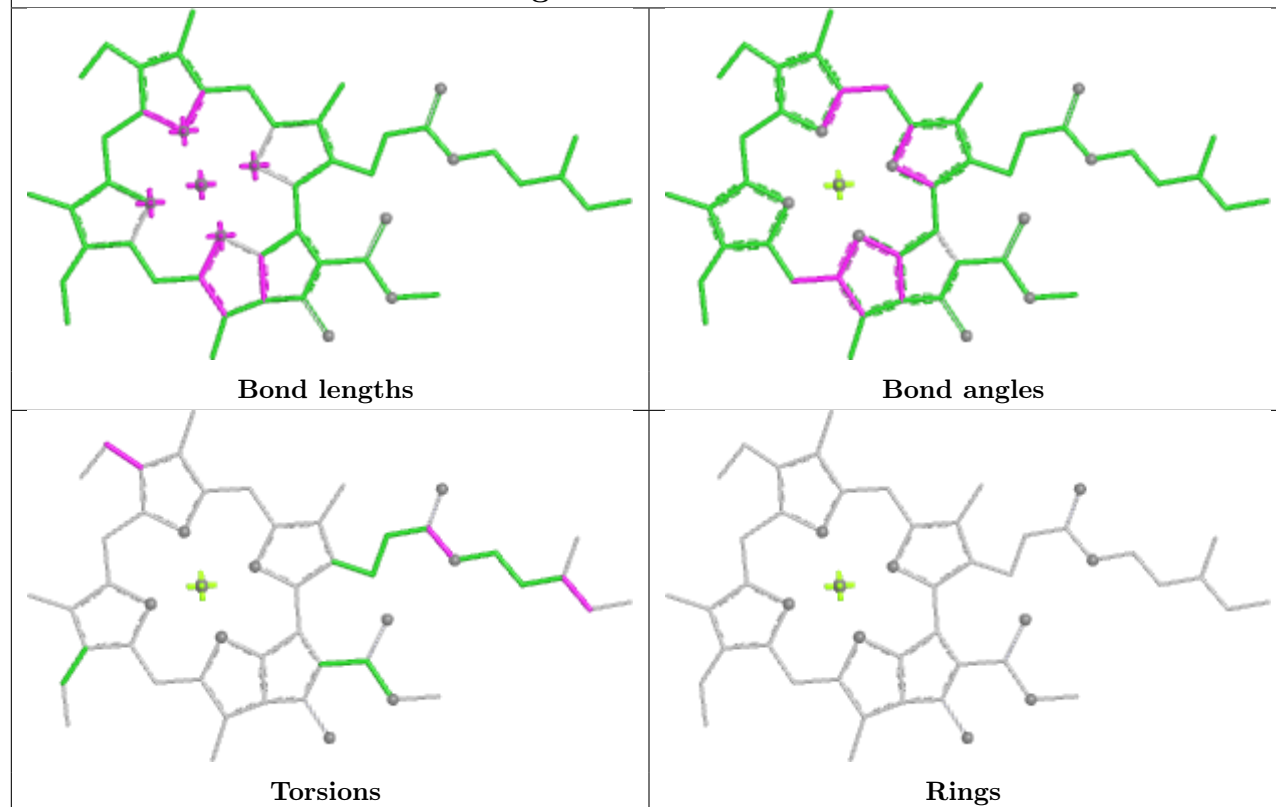
Ligand CHL e 304



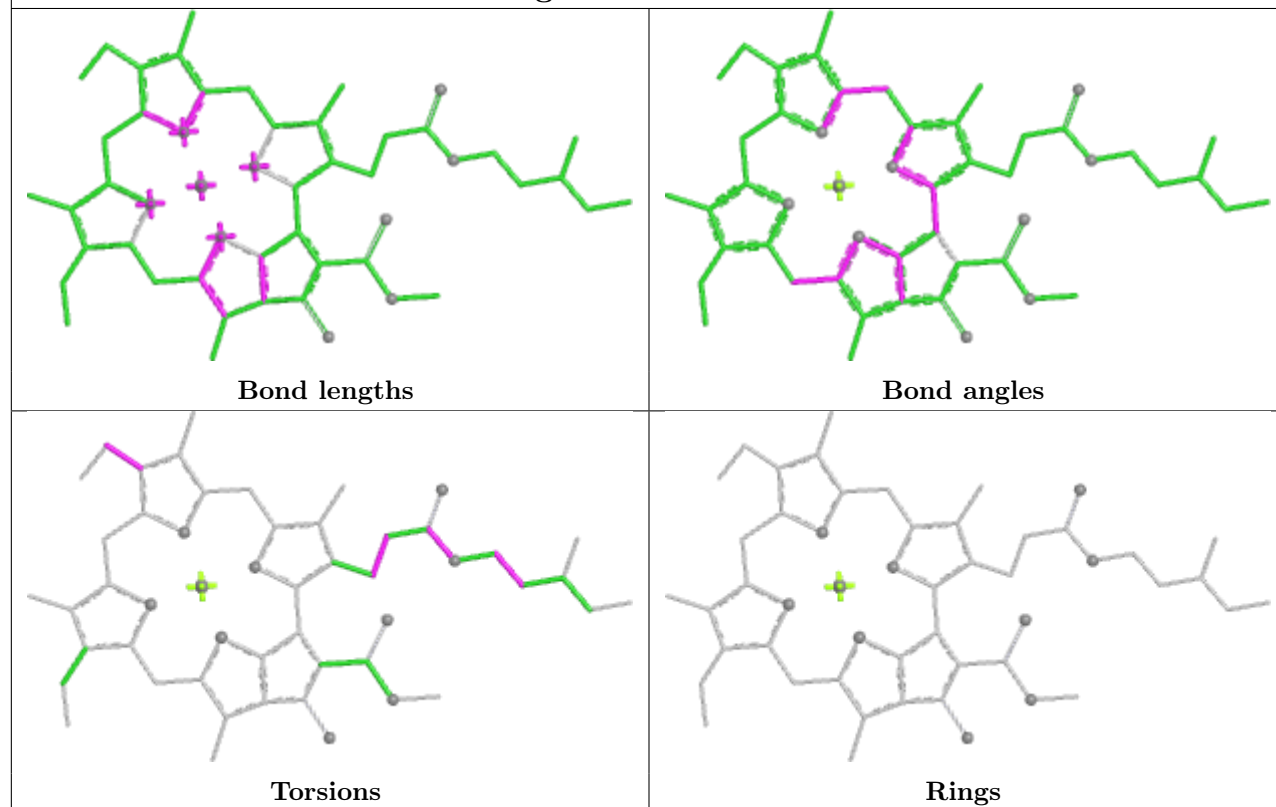


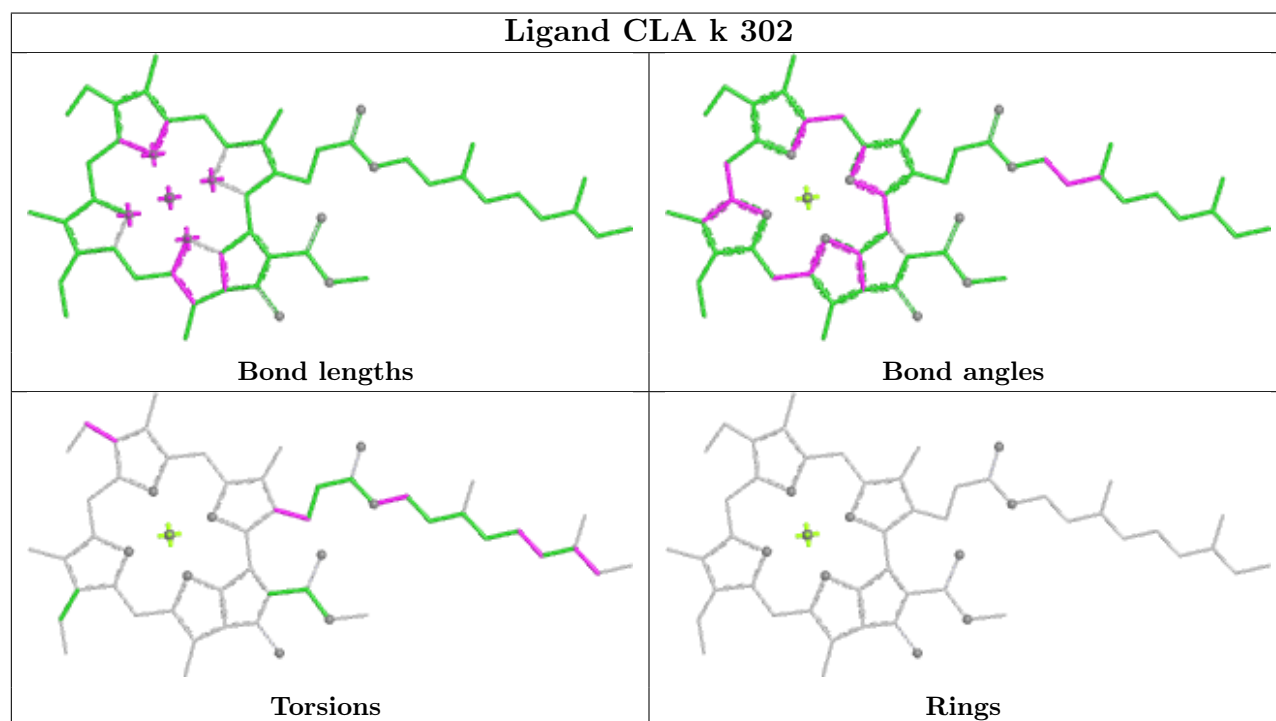
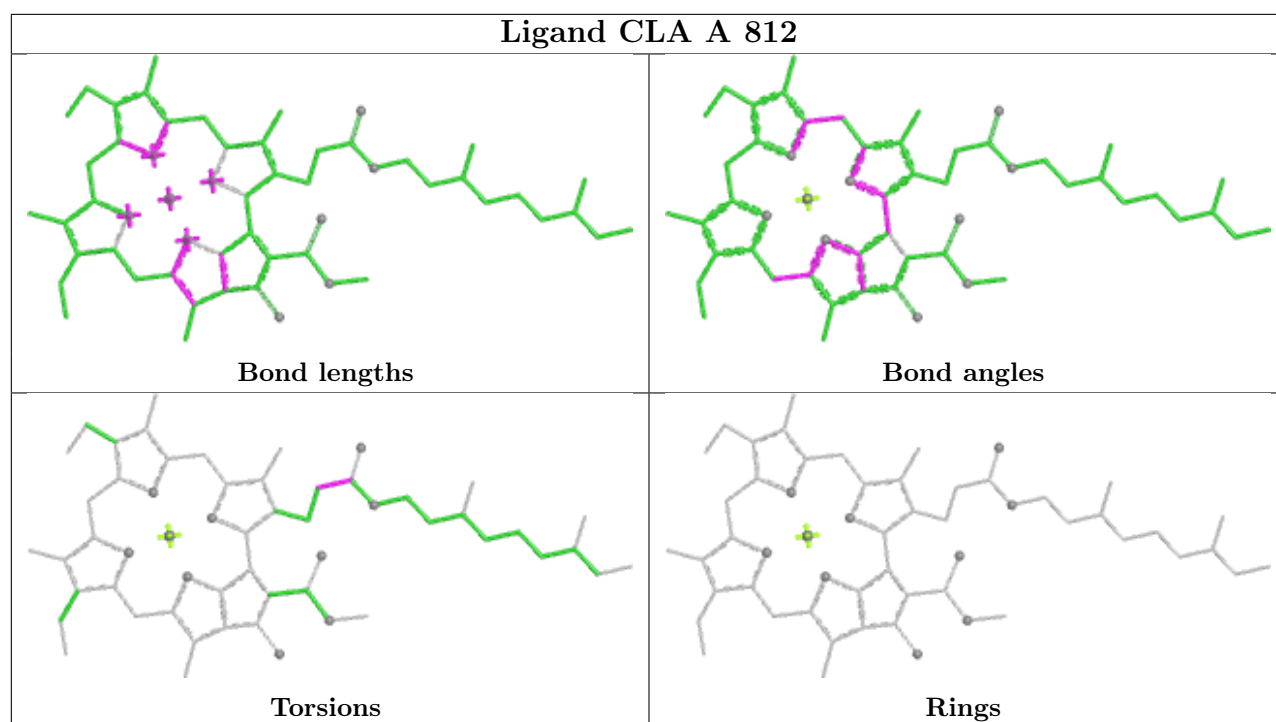


Ligand CLA A 827

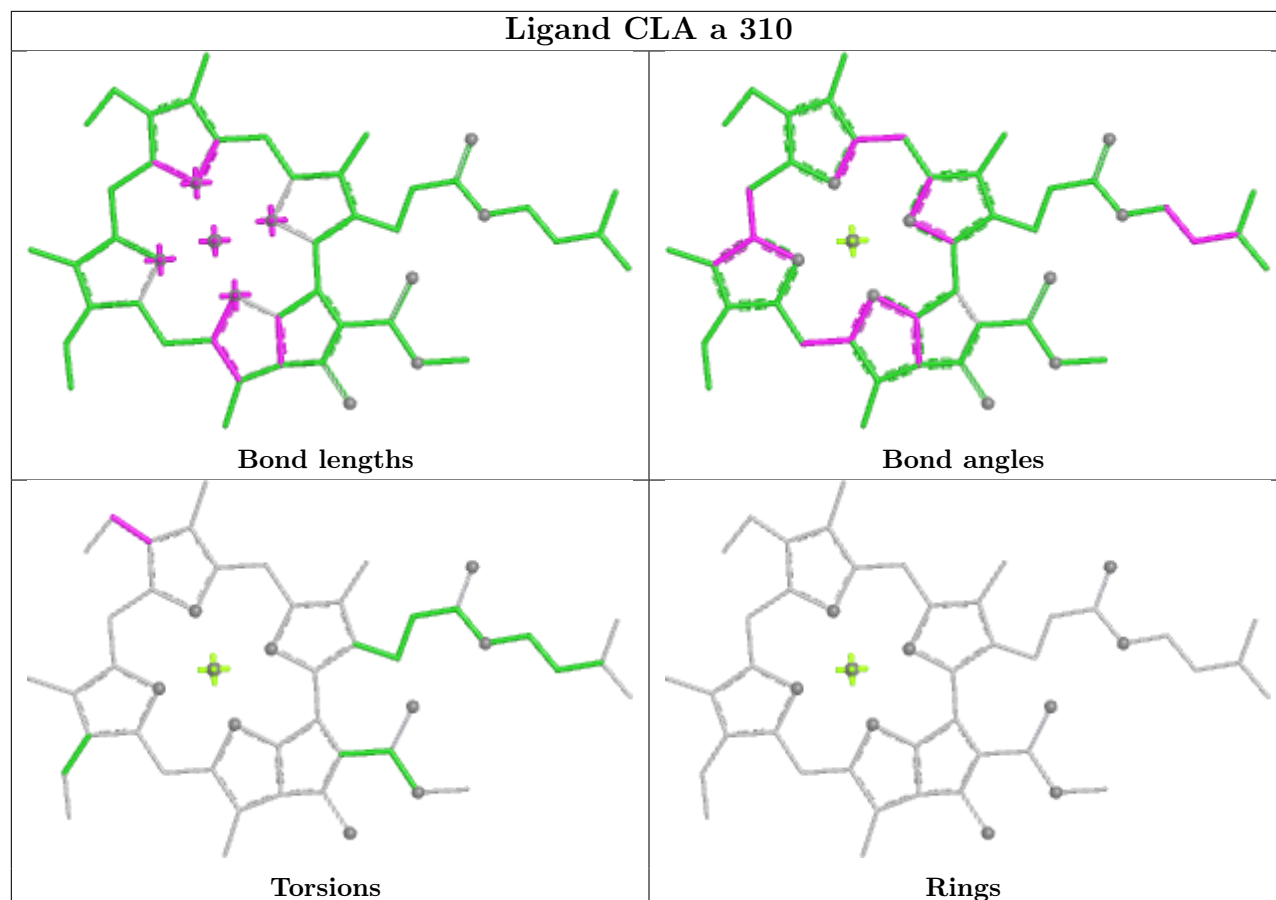


Ligand CLA b 303

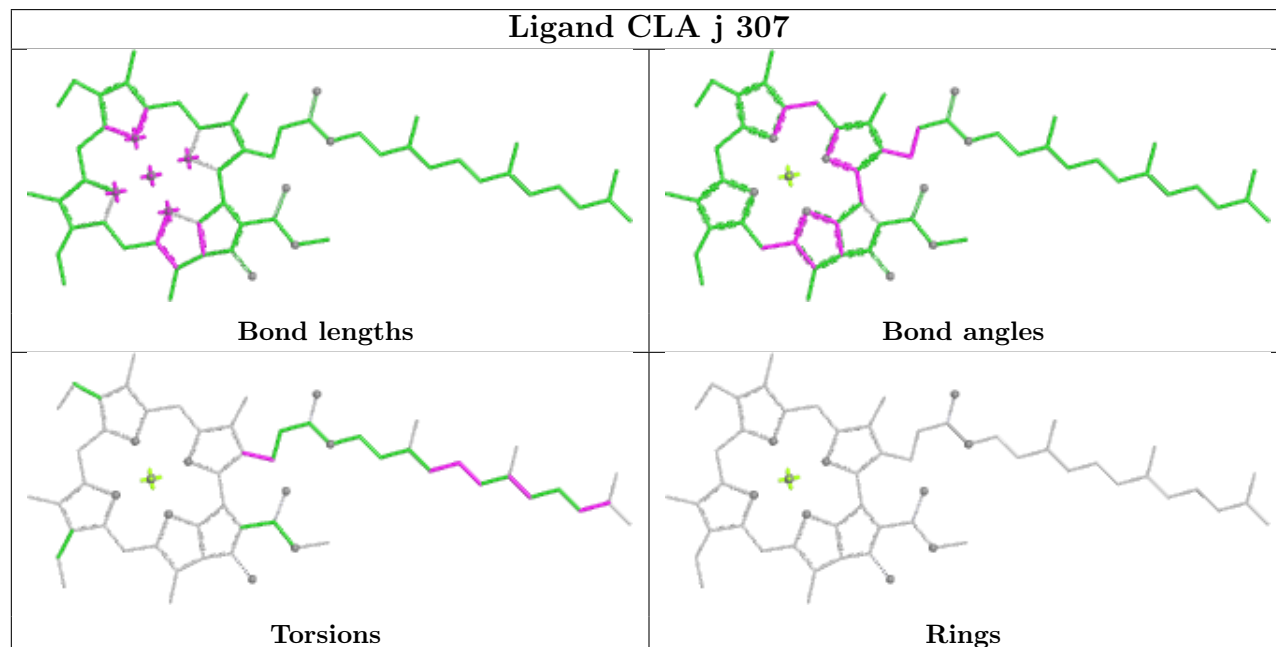


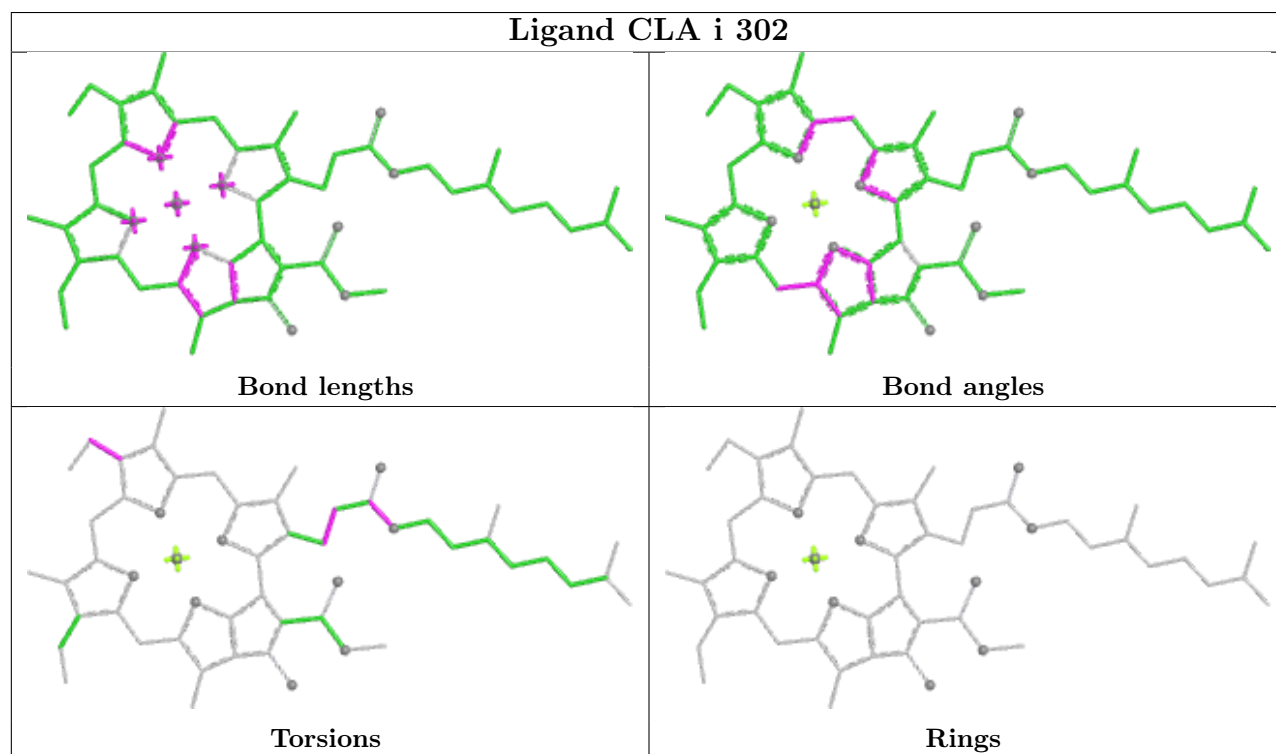
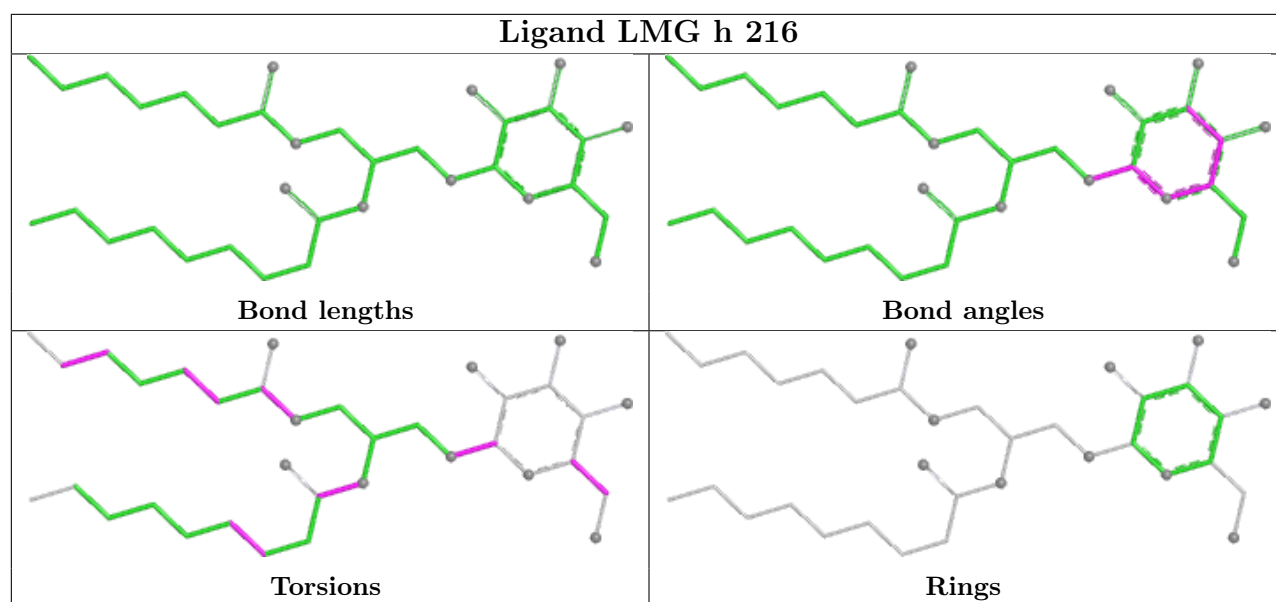


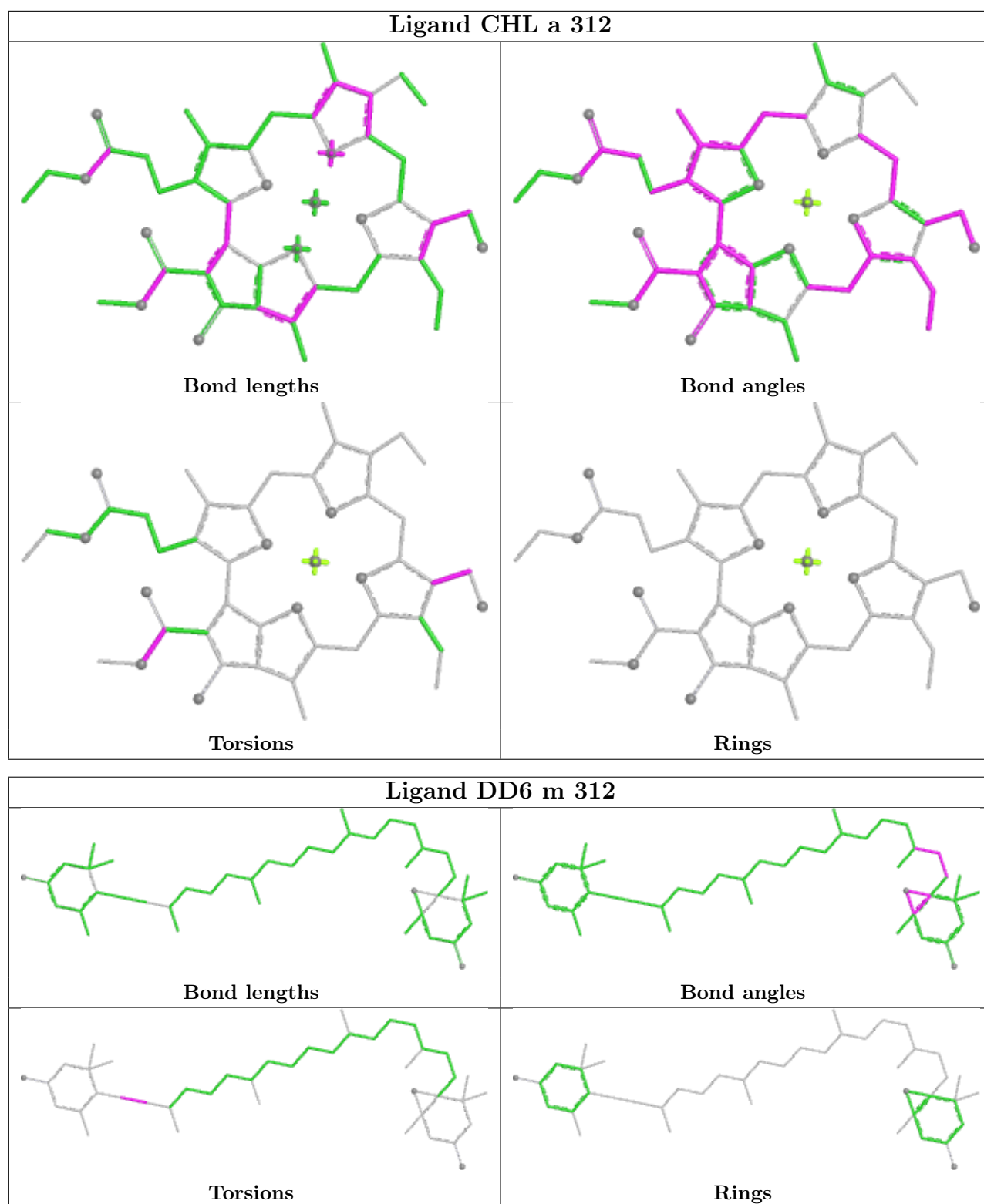
Ligand CLA a 310

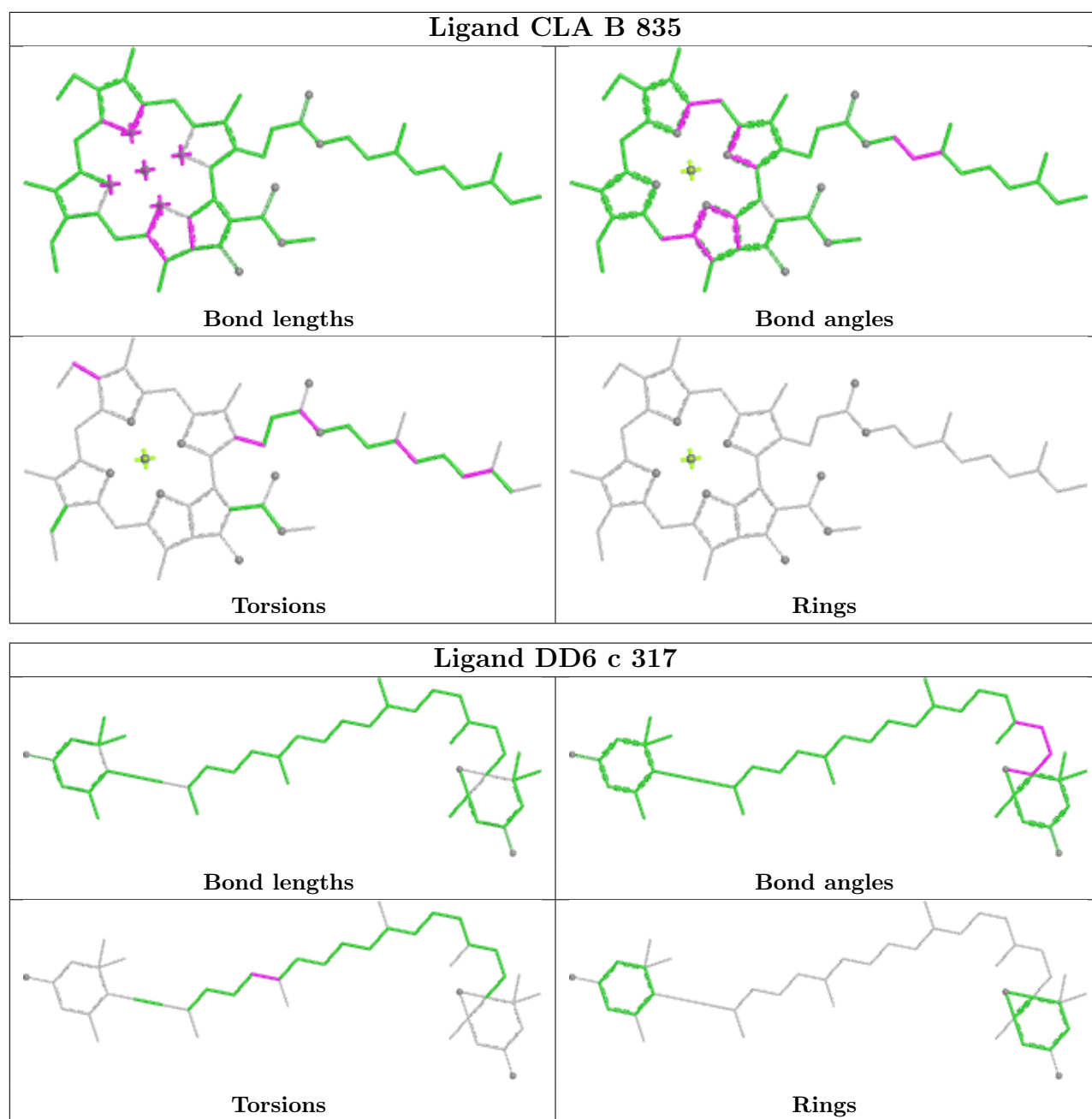


Ligand CLA j 307

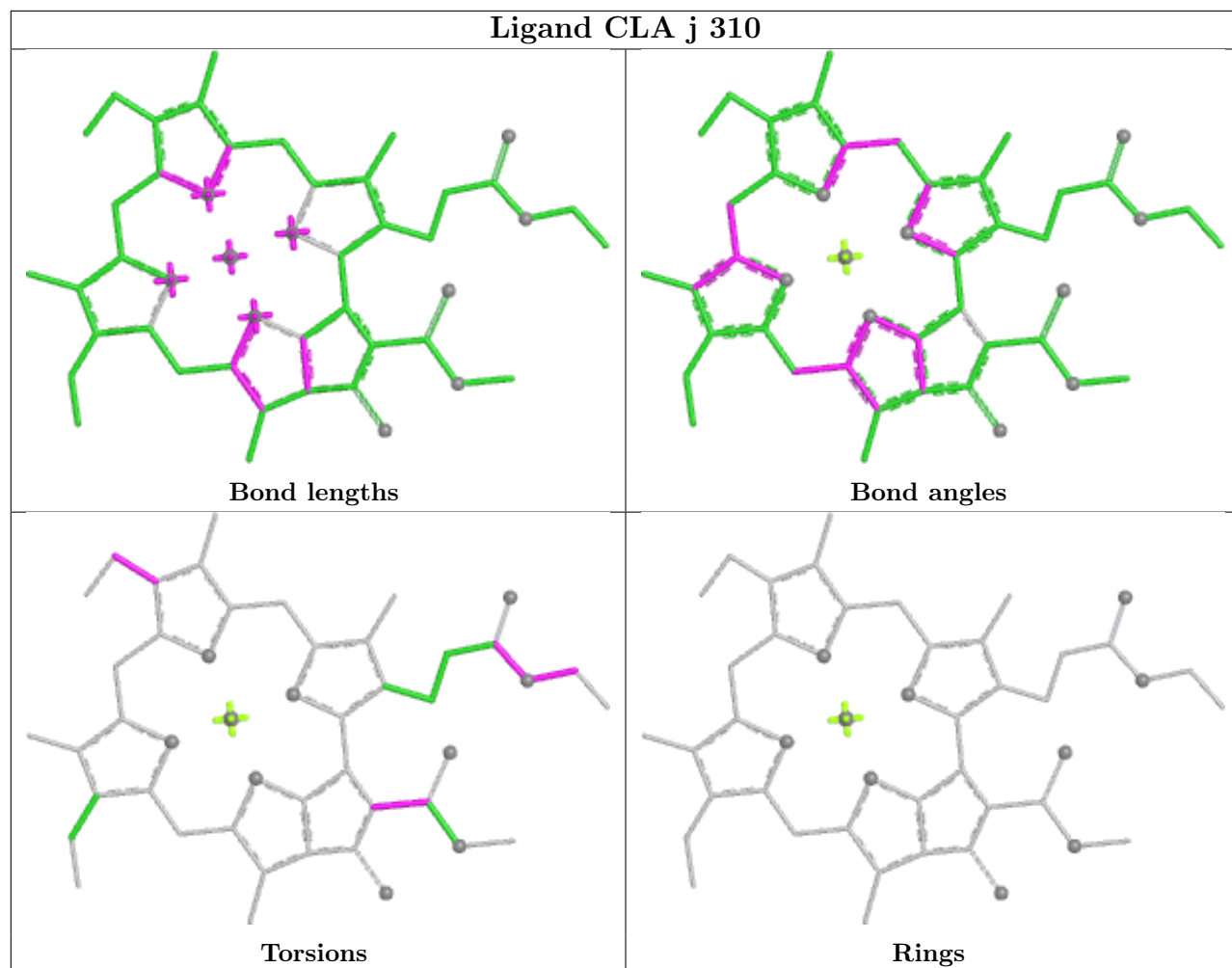




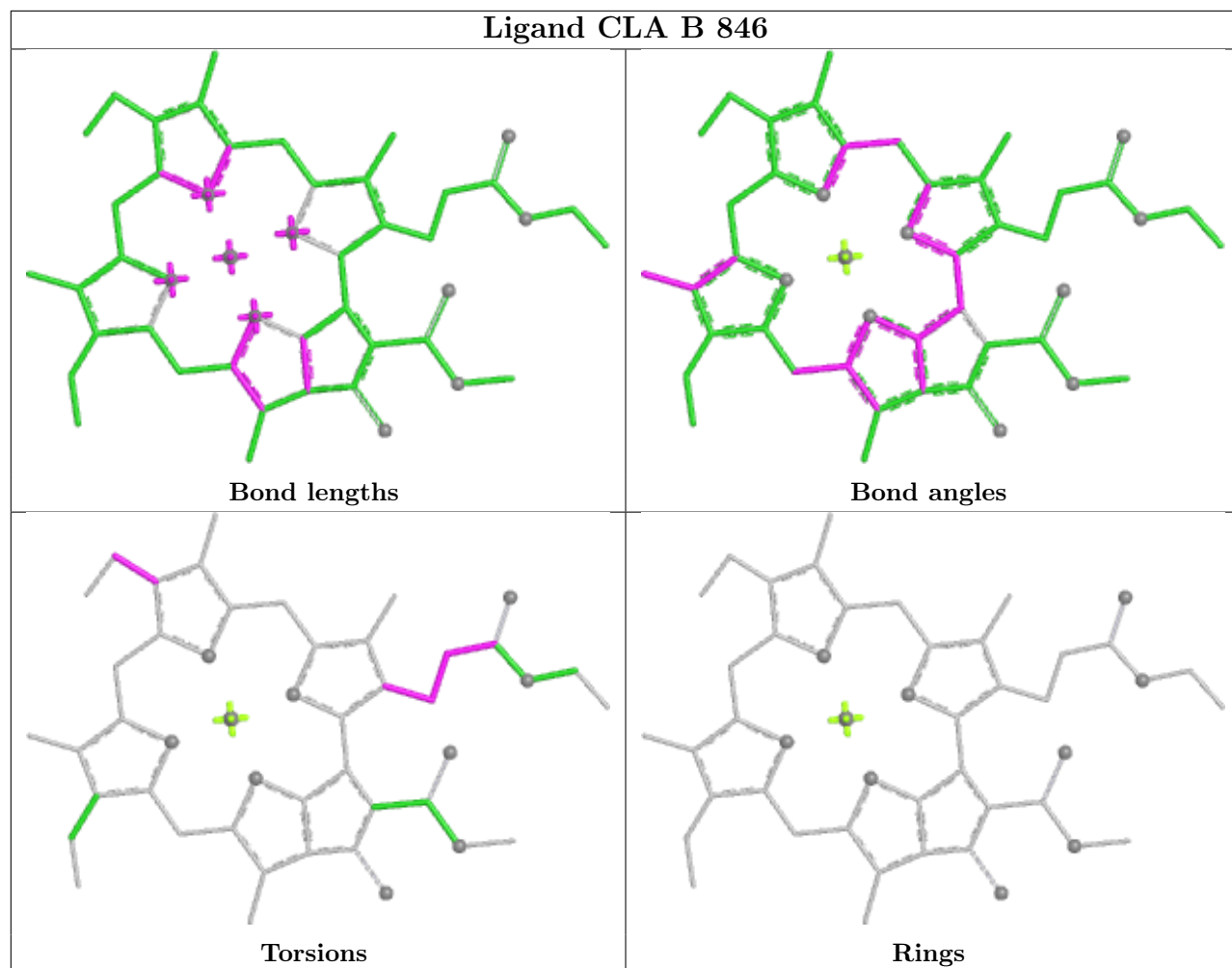




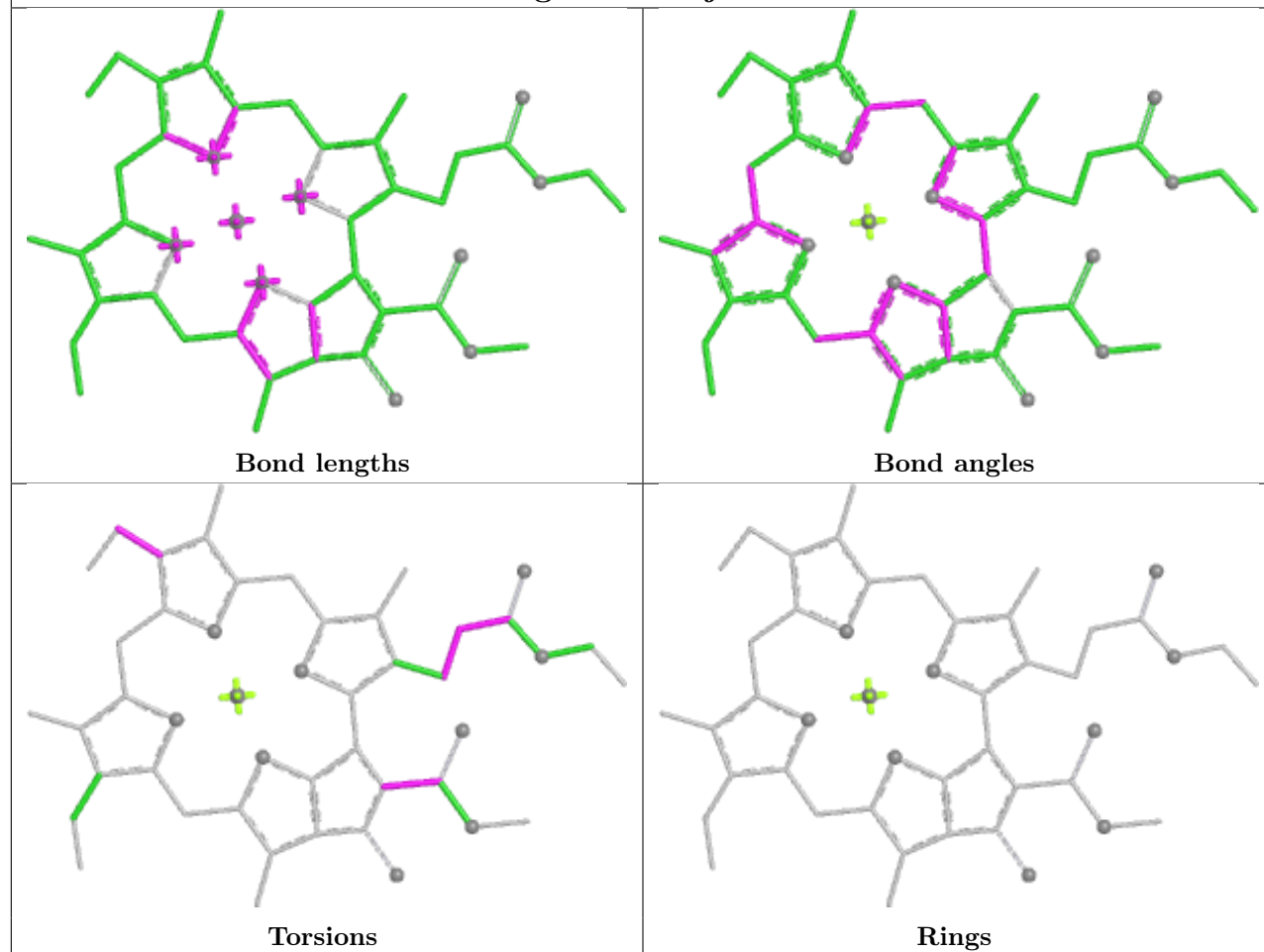
Ligand CLA j 310



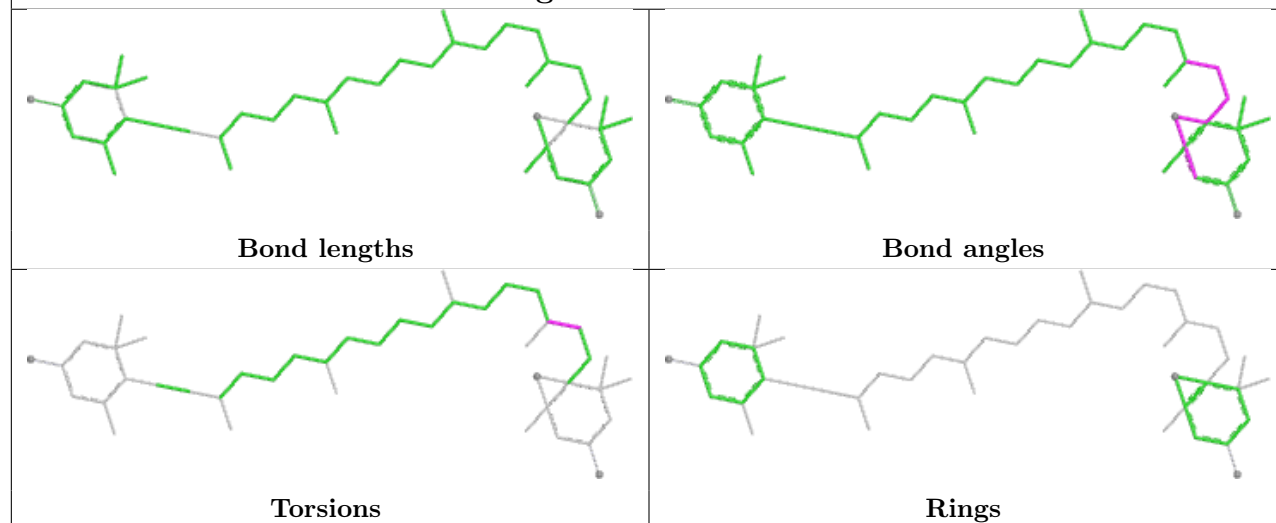
Ligand CLA B 846



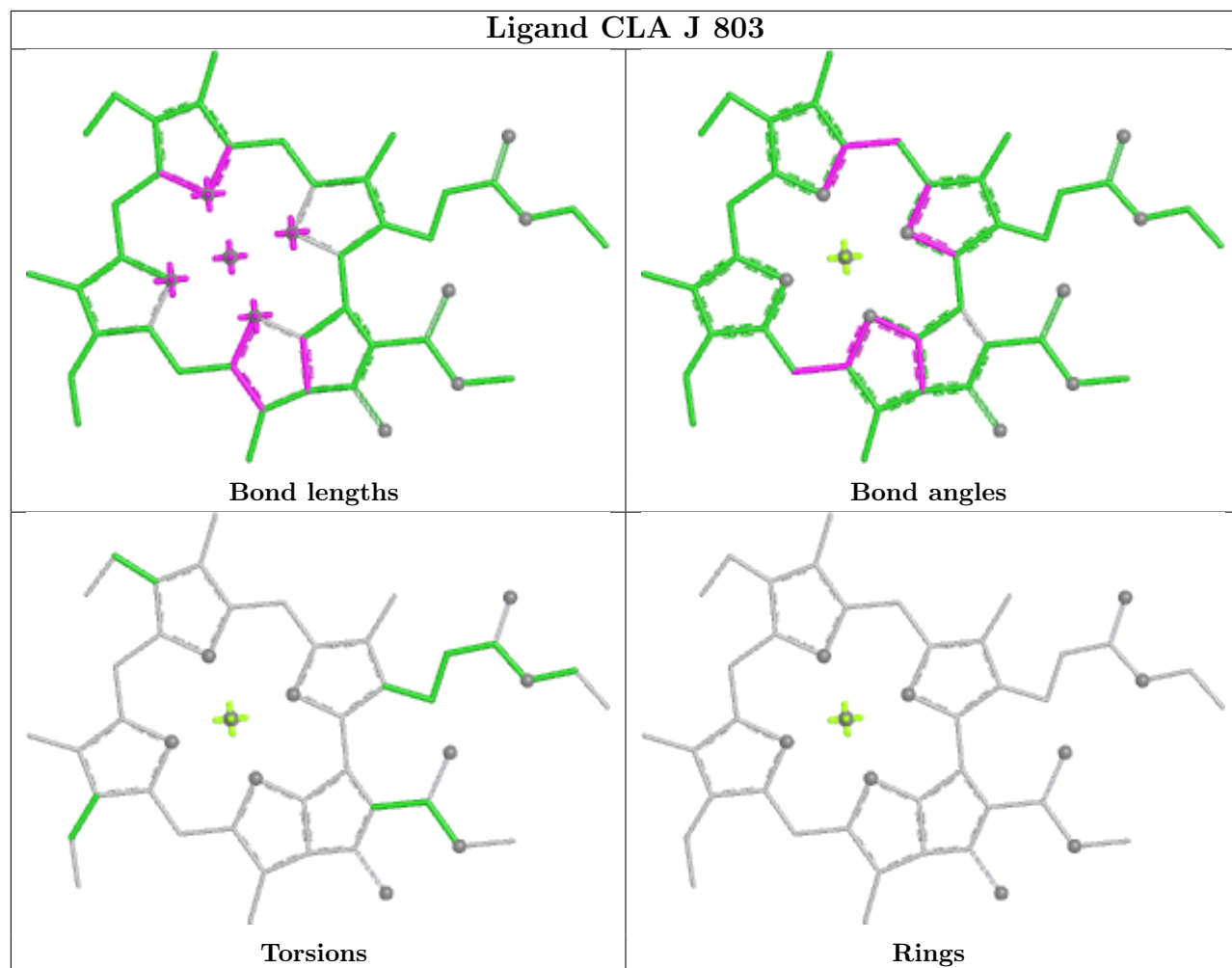
Ligand CLA j 306

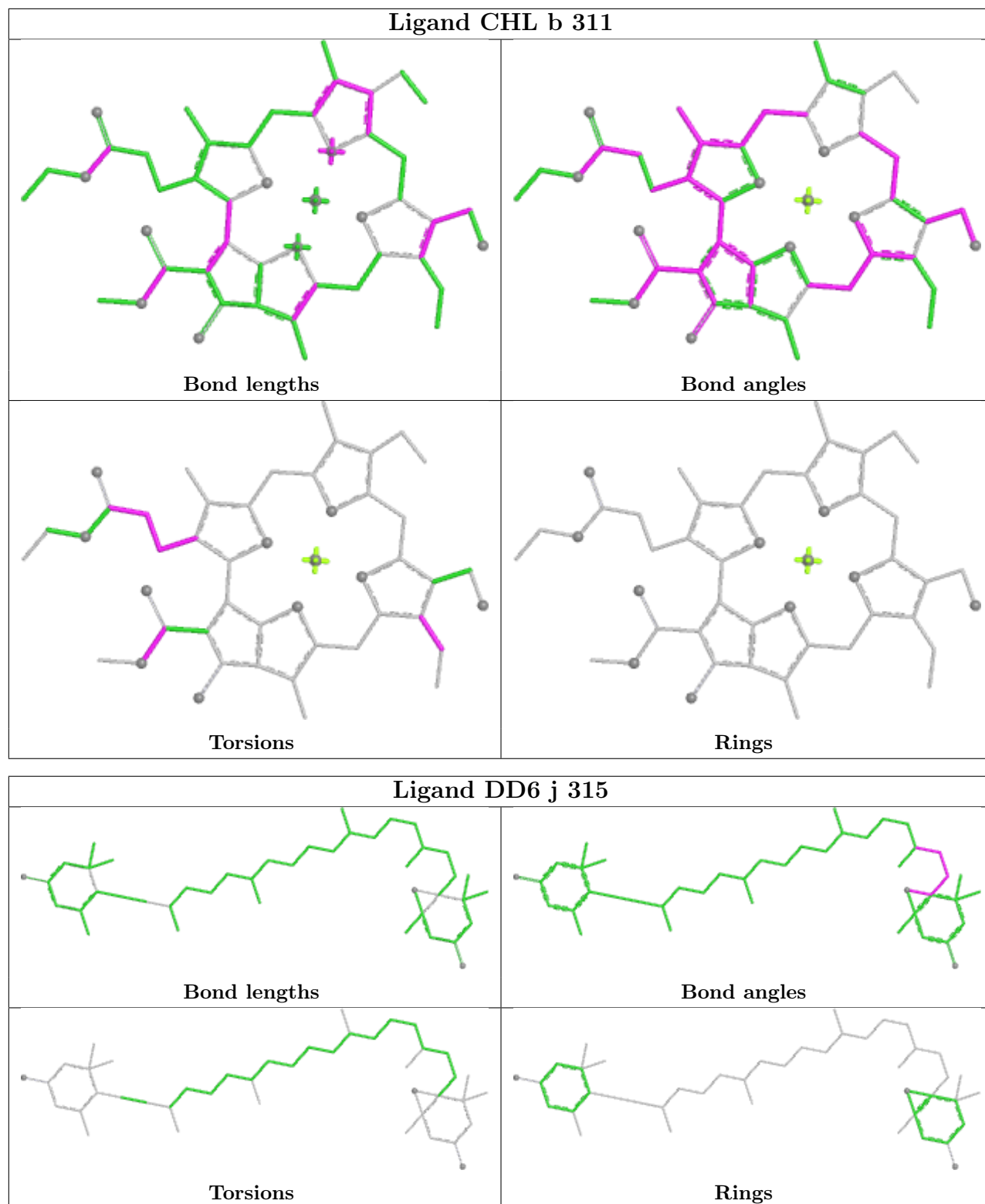


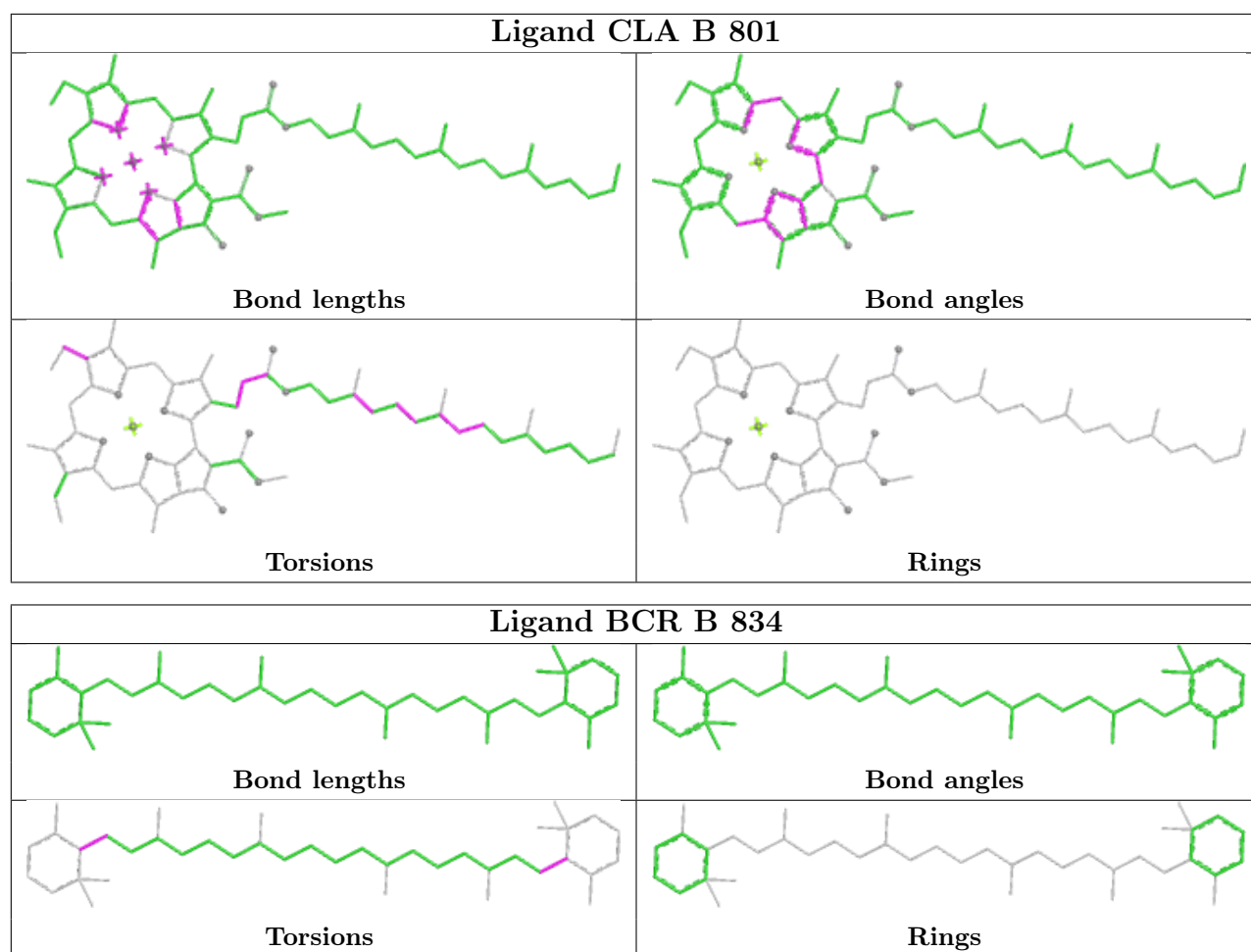
Ligand DD6 b 317



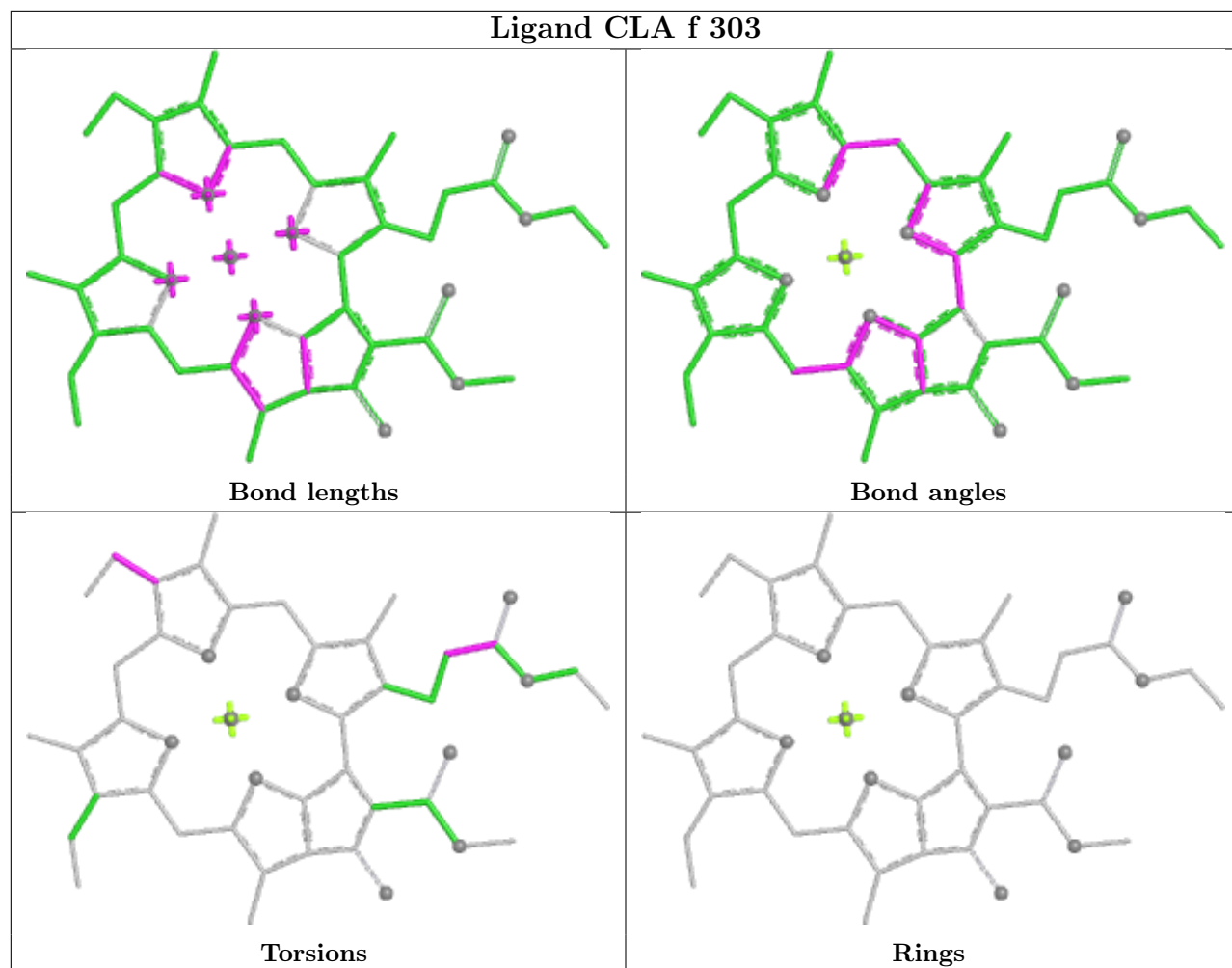
Ligand CLA J 803



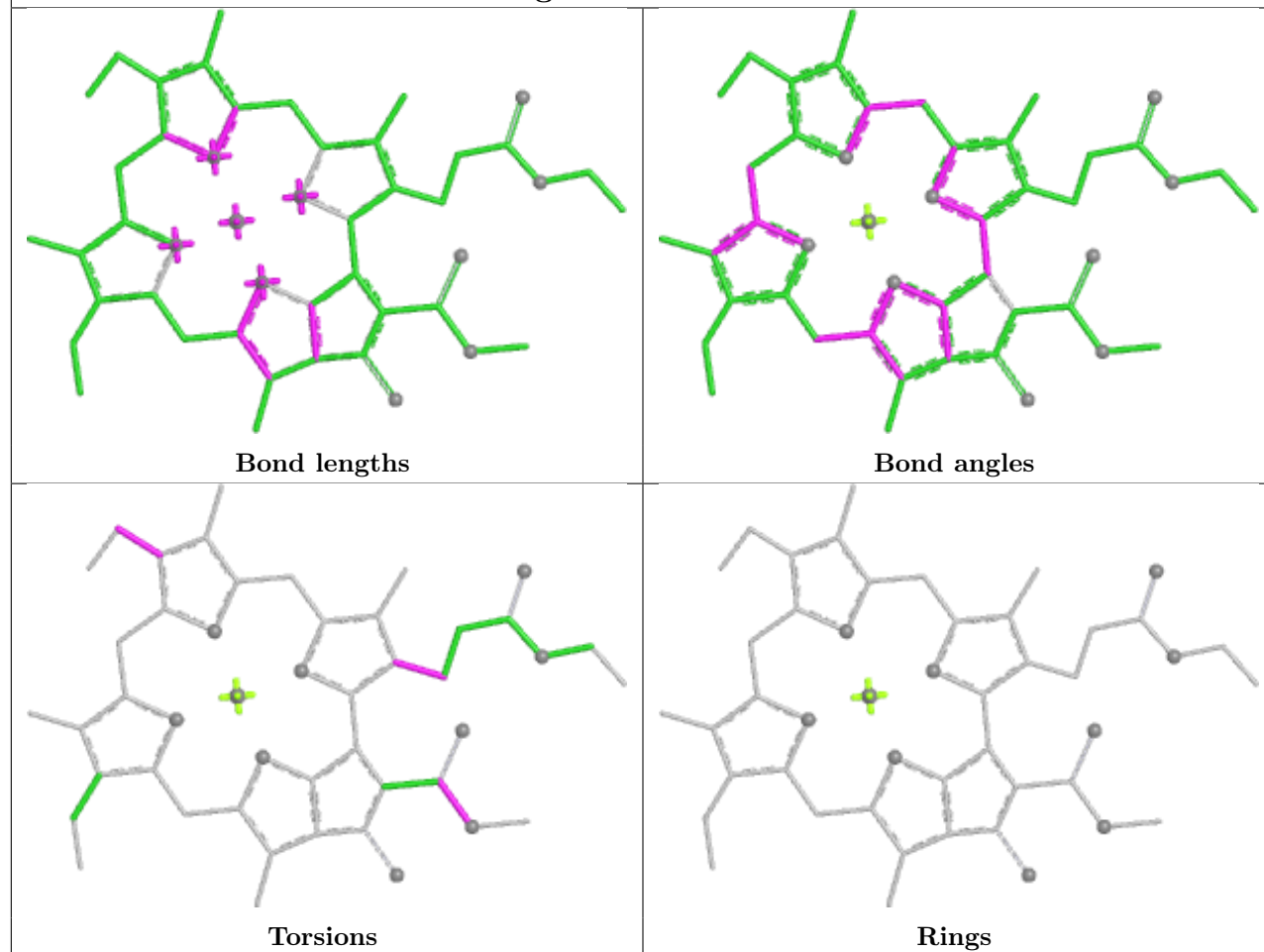




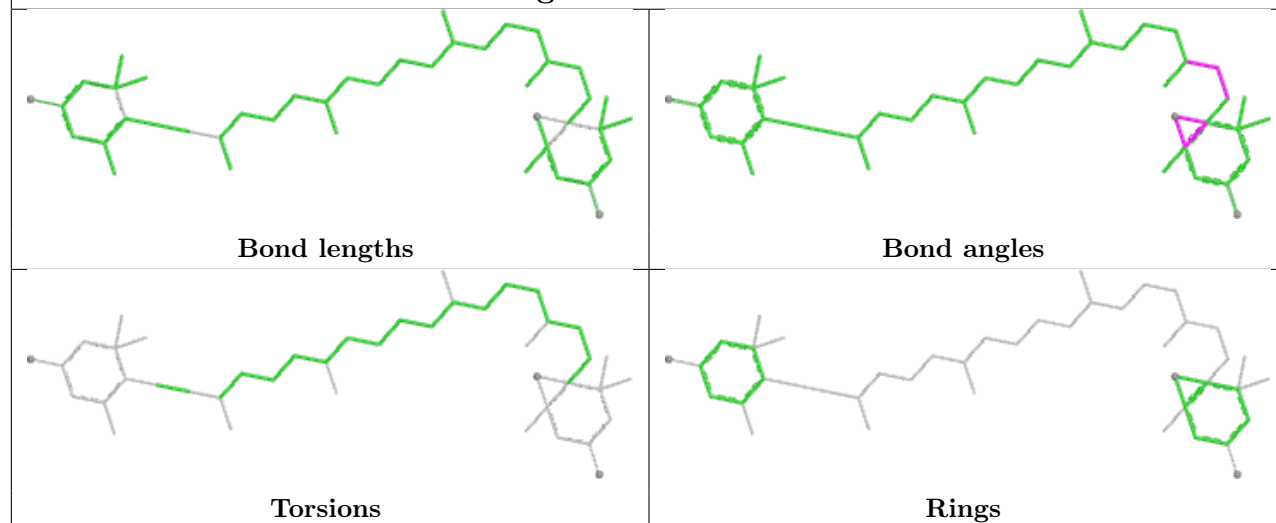
Ligand CLA f 303

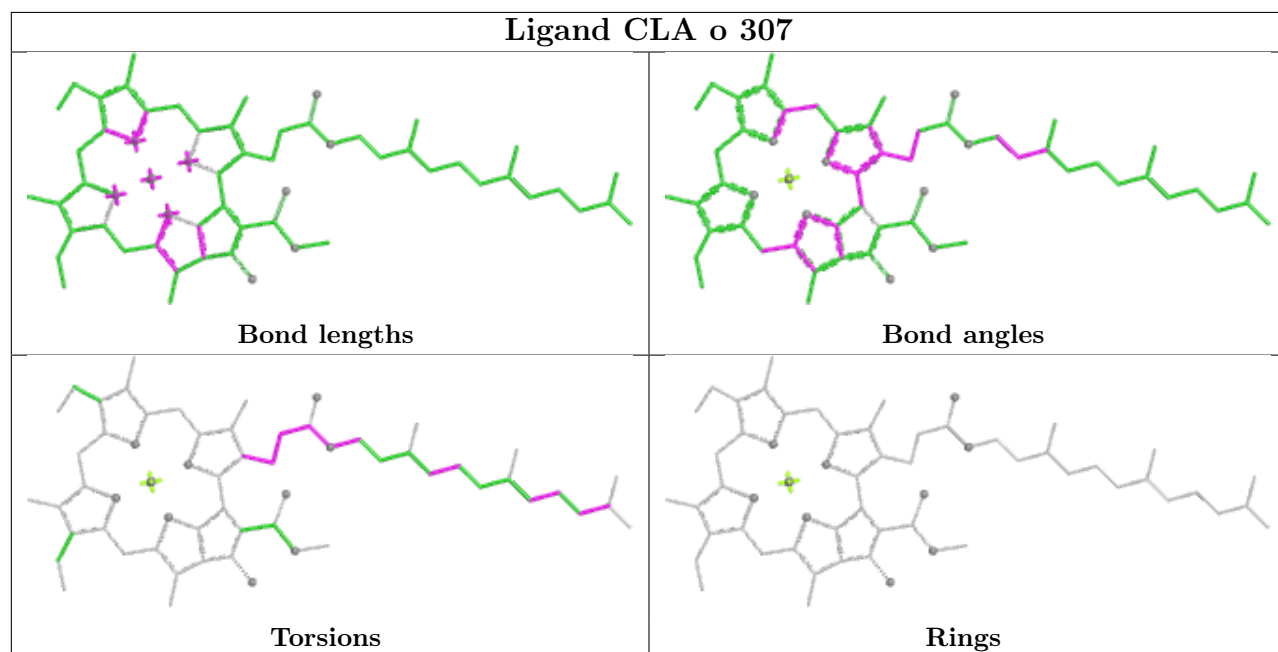
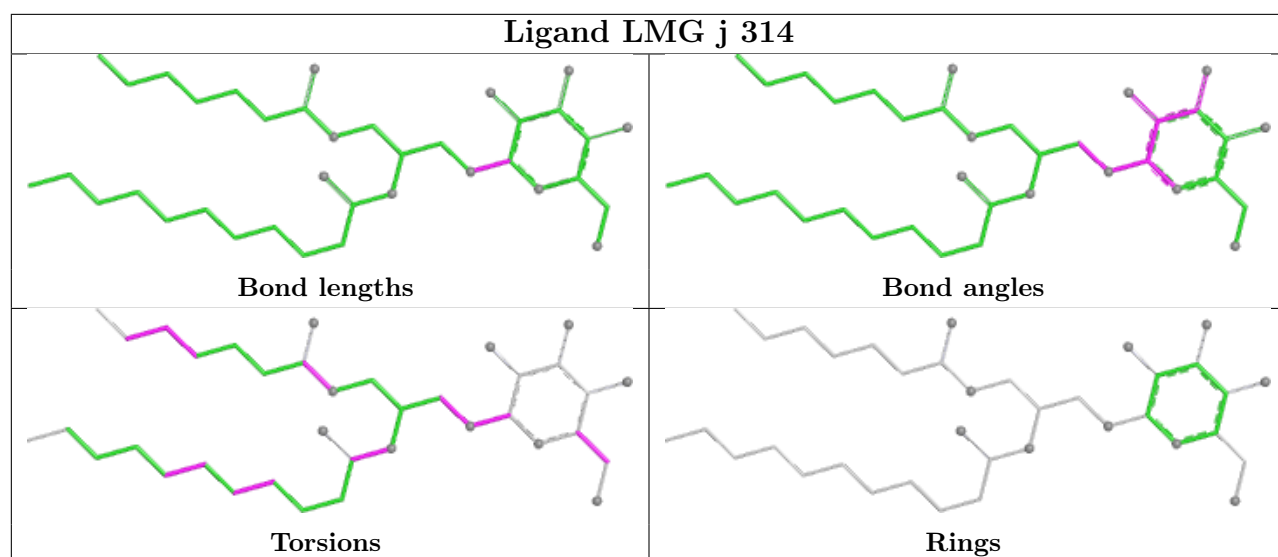


Ligand CLA 1 206

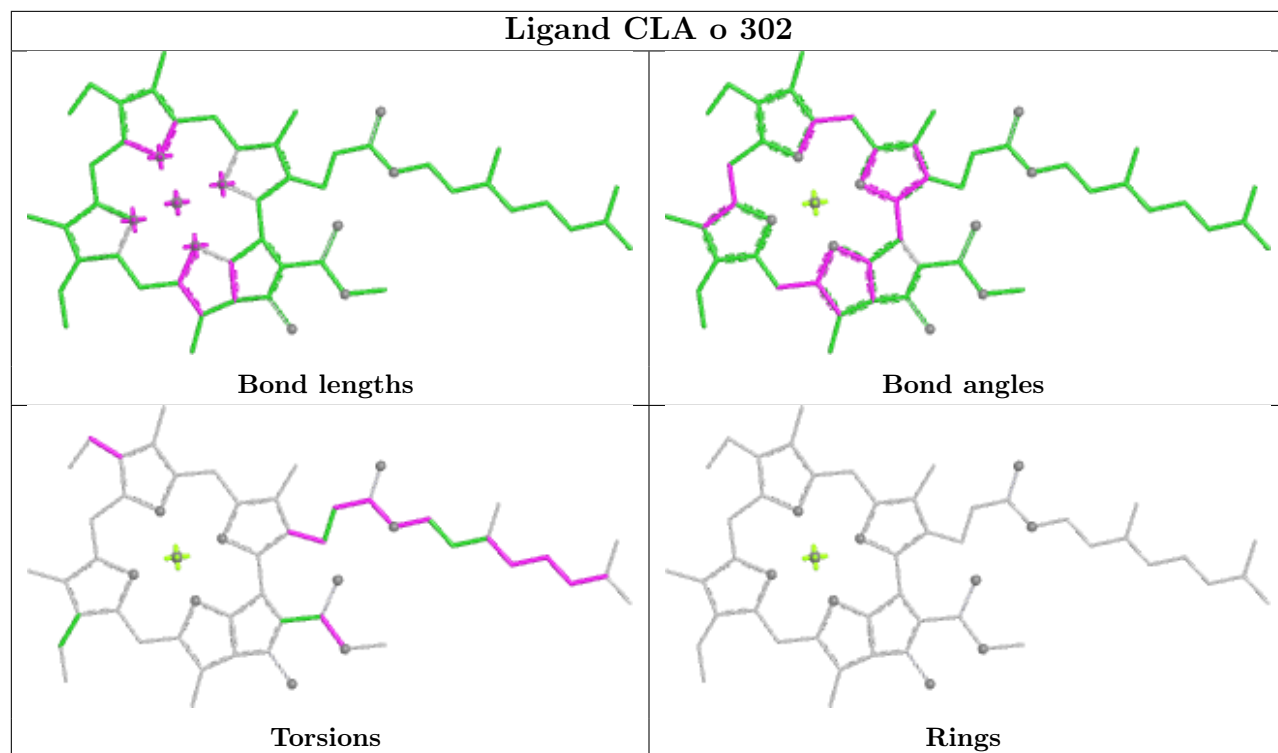


Ligand DD6 o 313

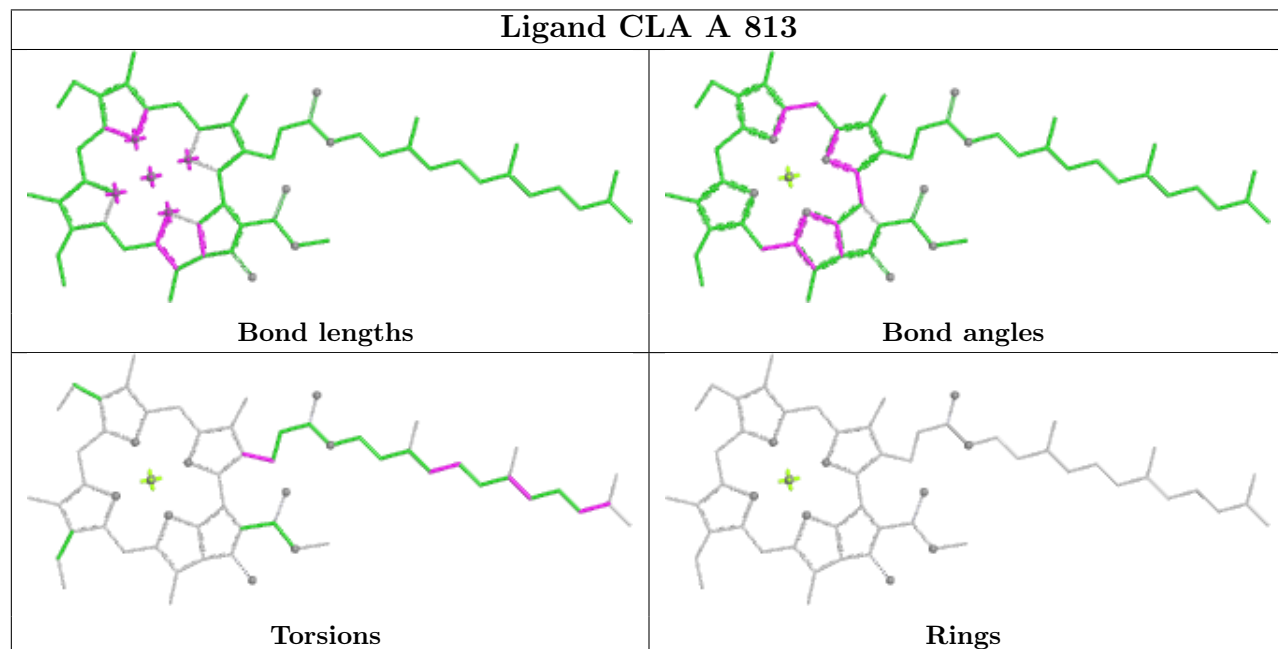




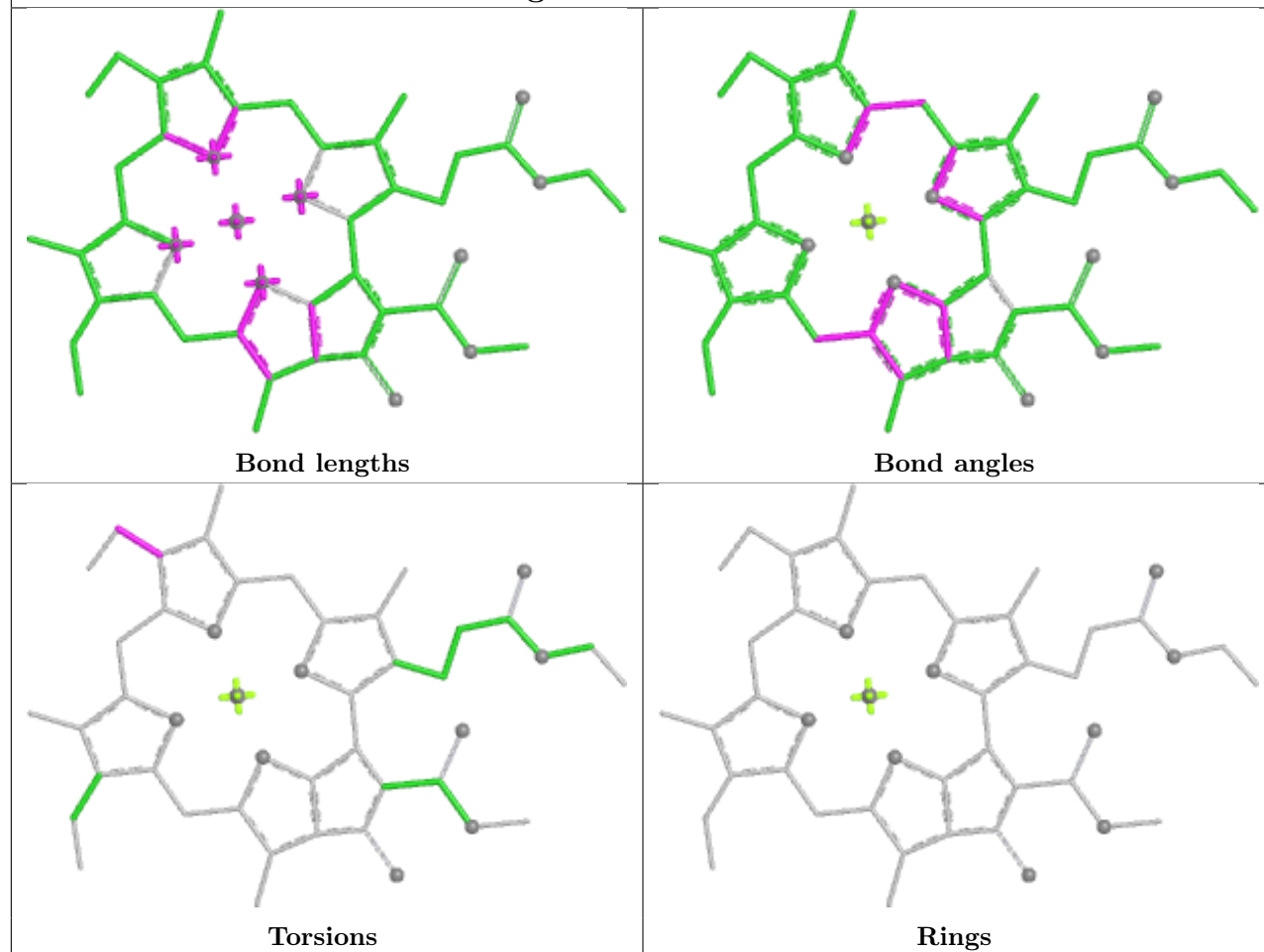
Ligand CLA o 302



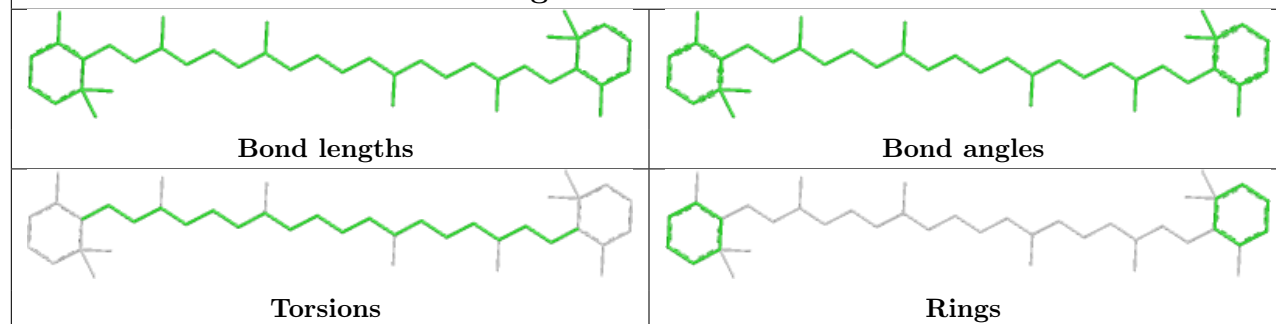
Ligand CLA A 813

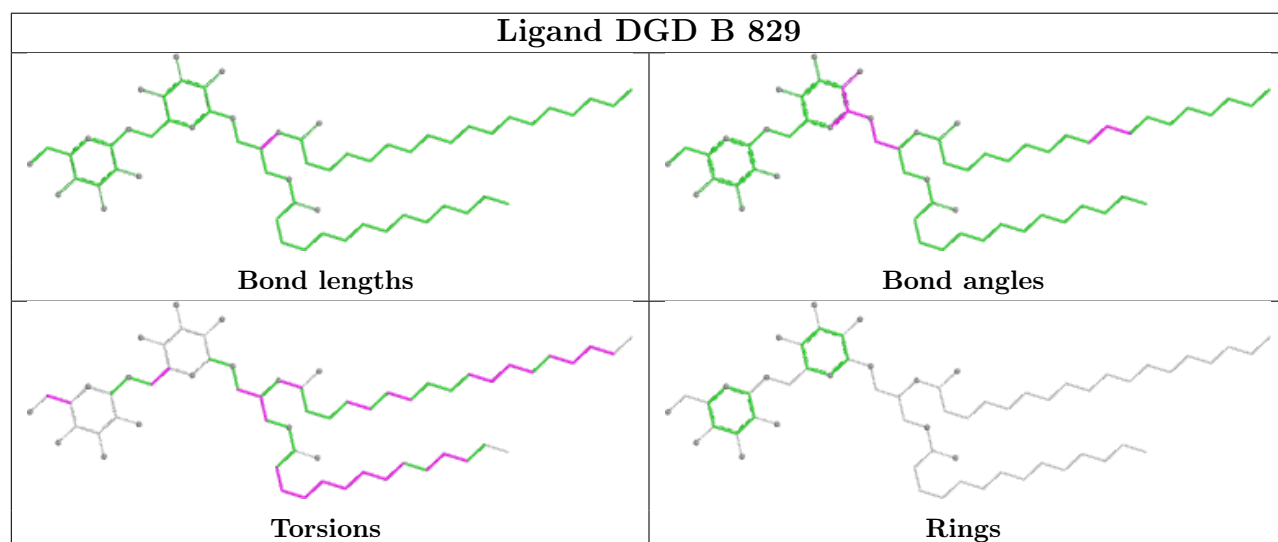
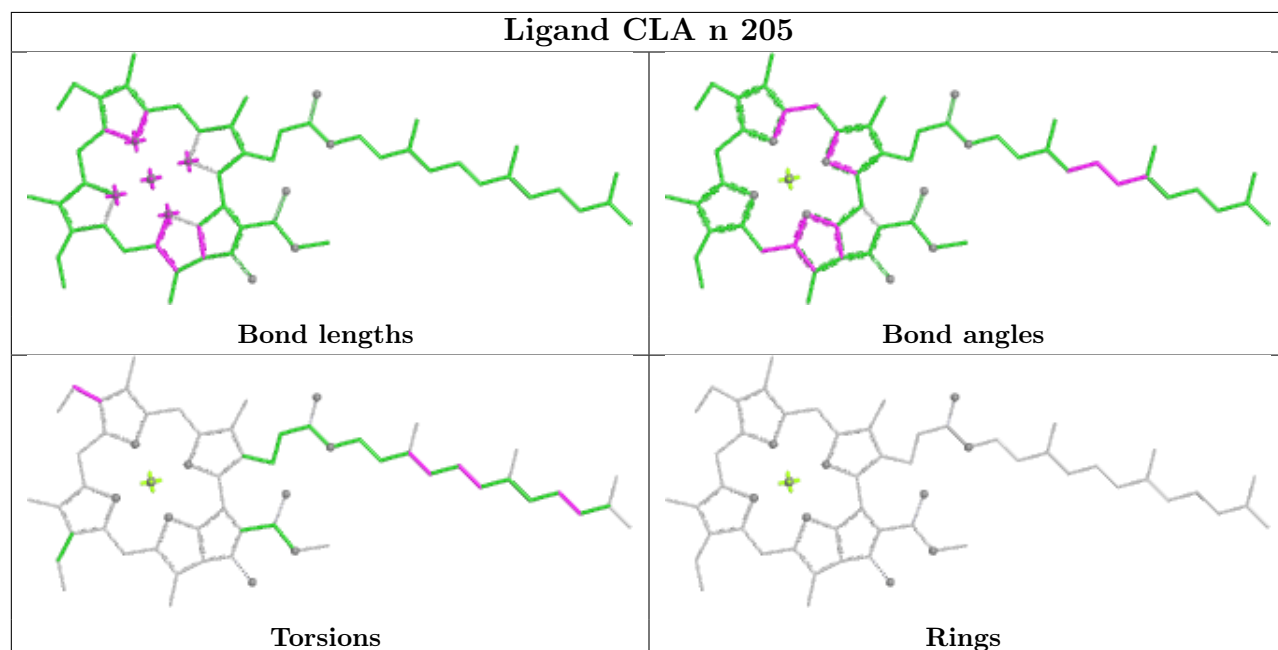
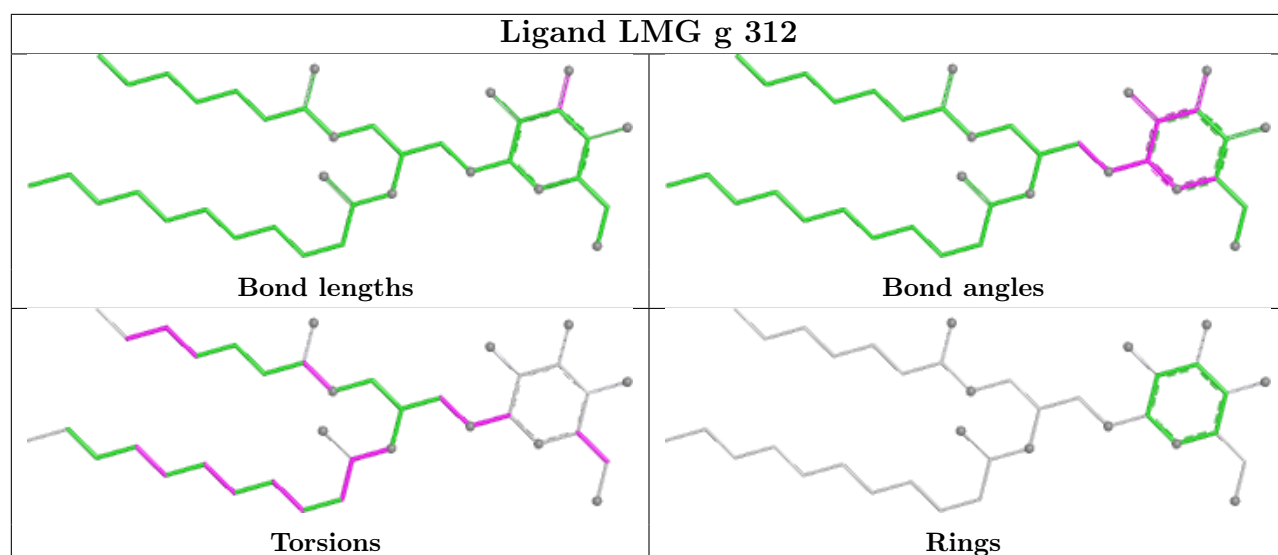


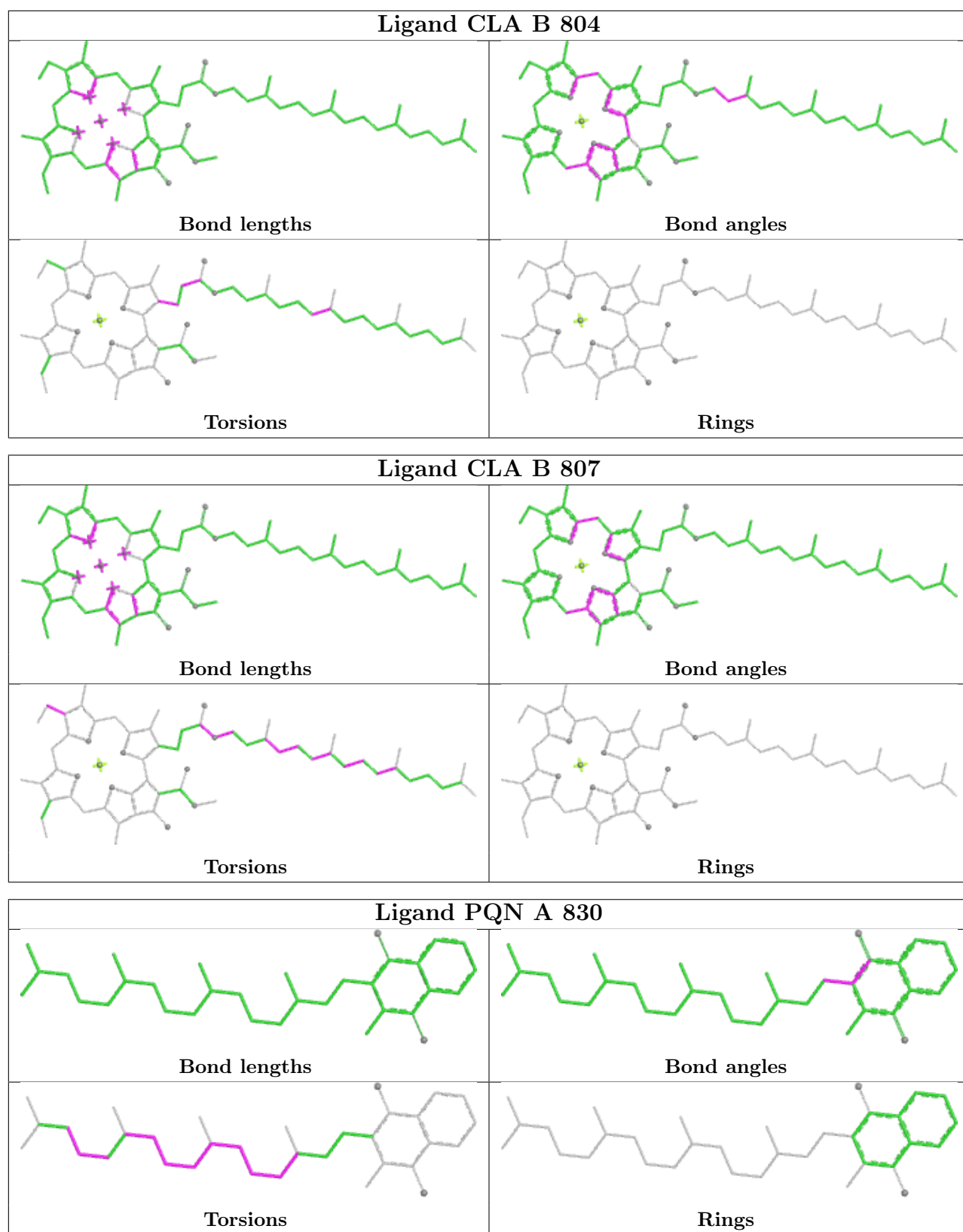
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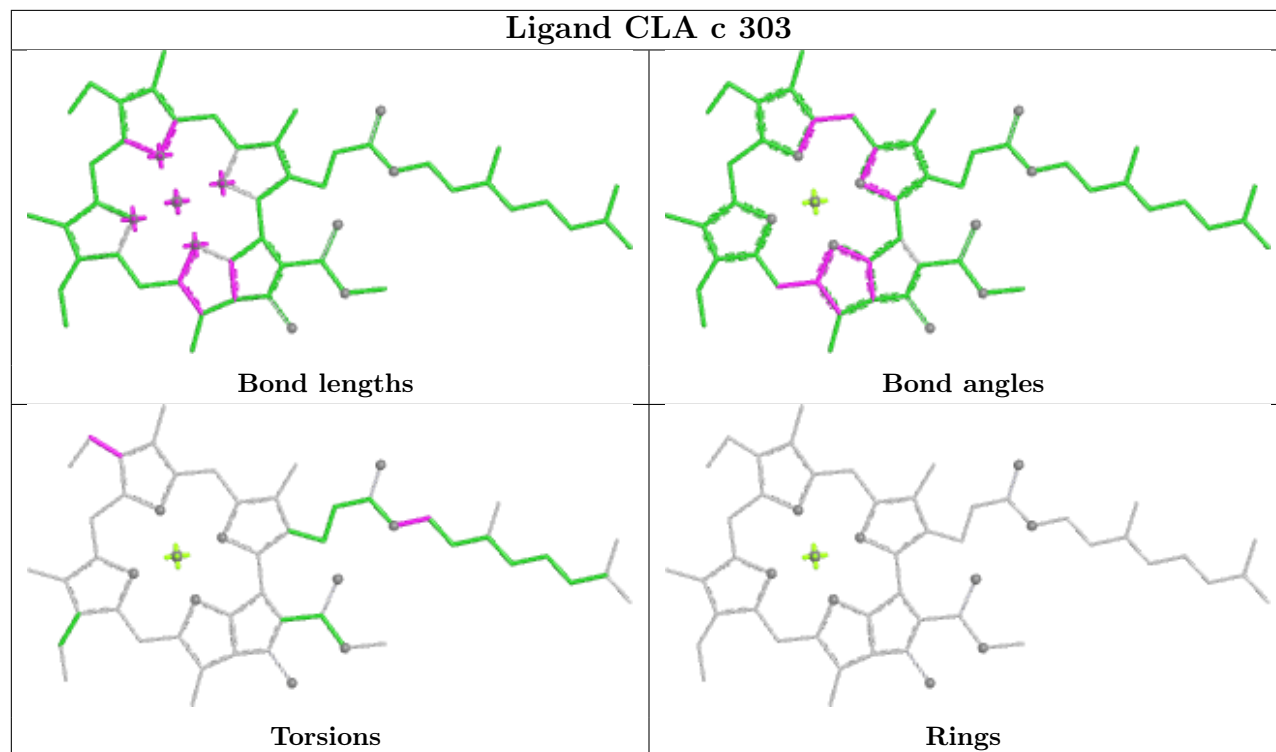
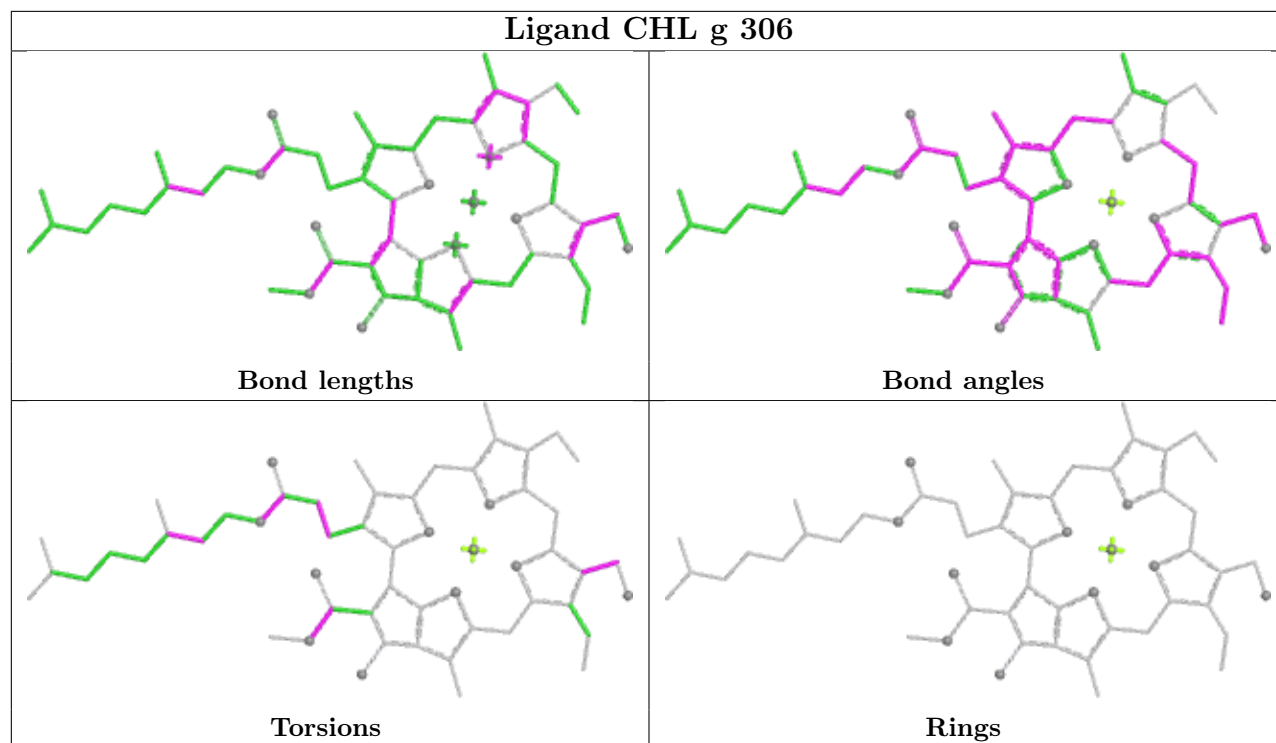


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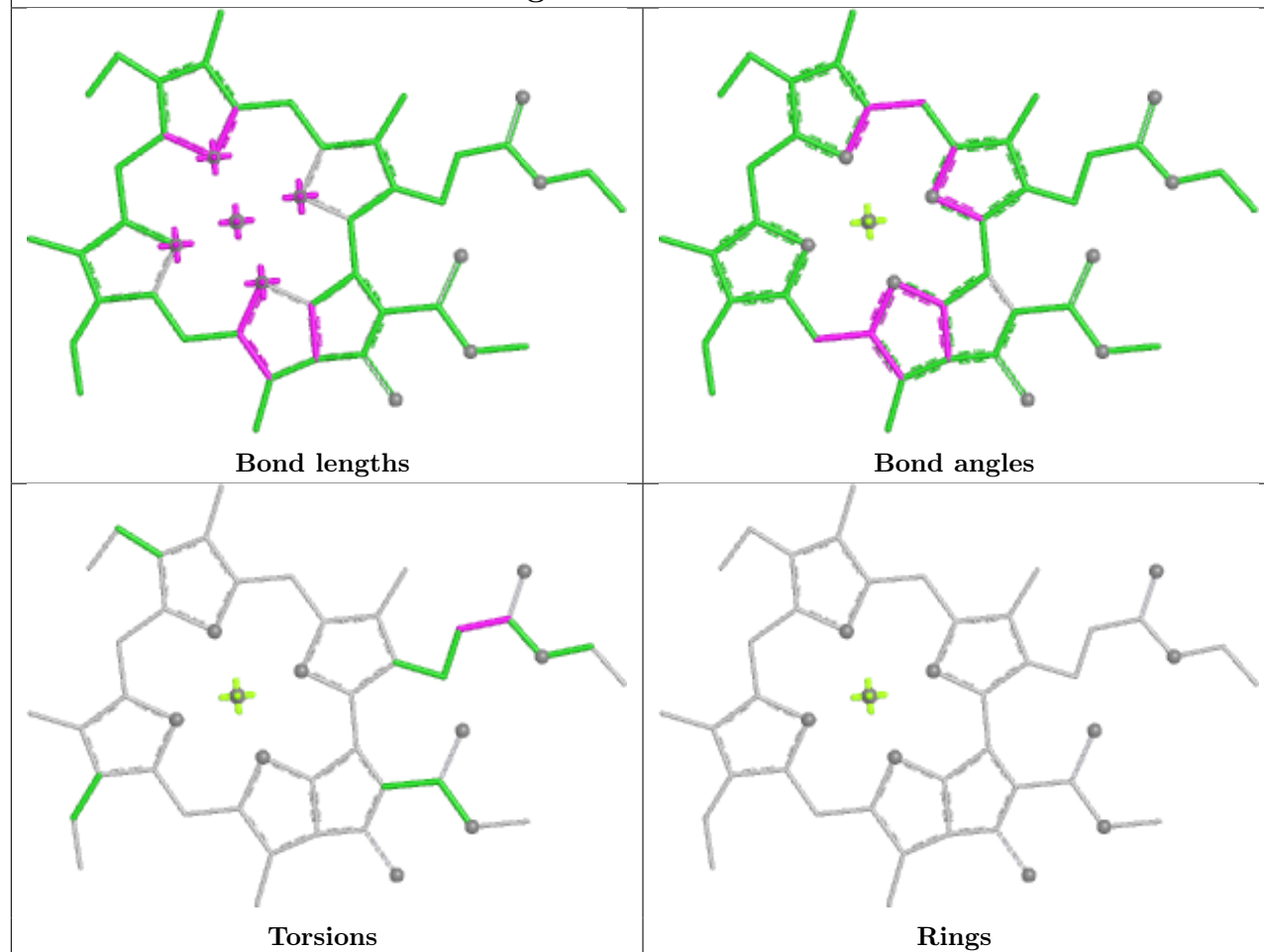




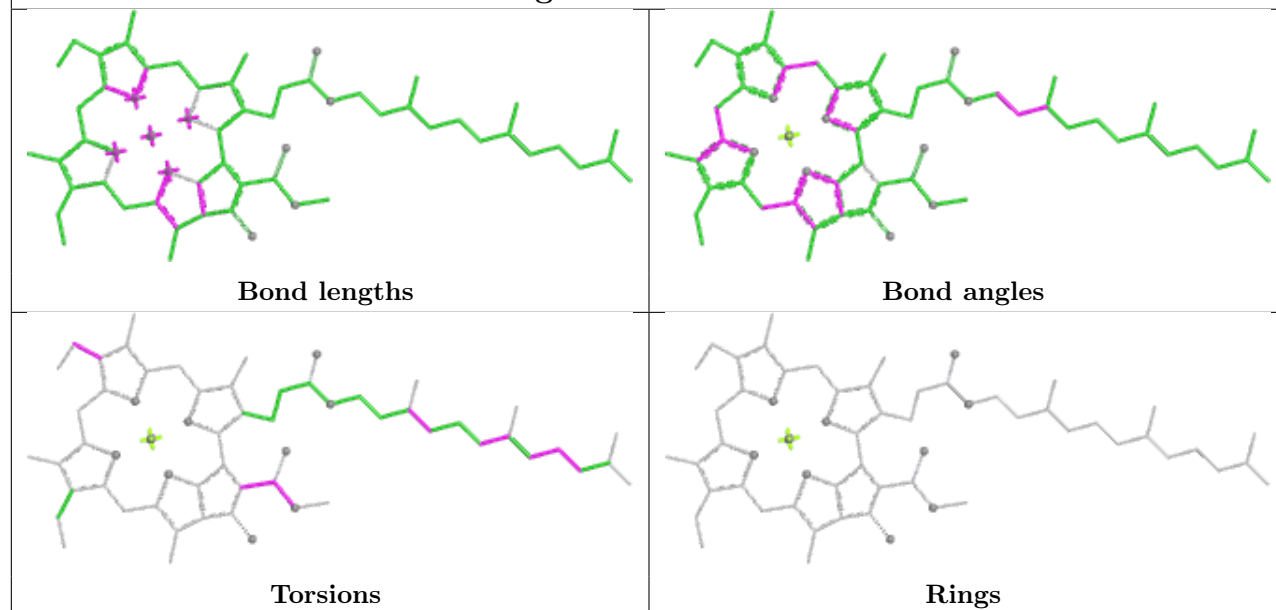


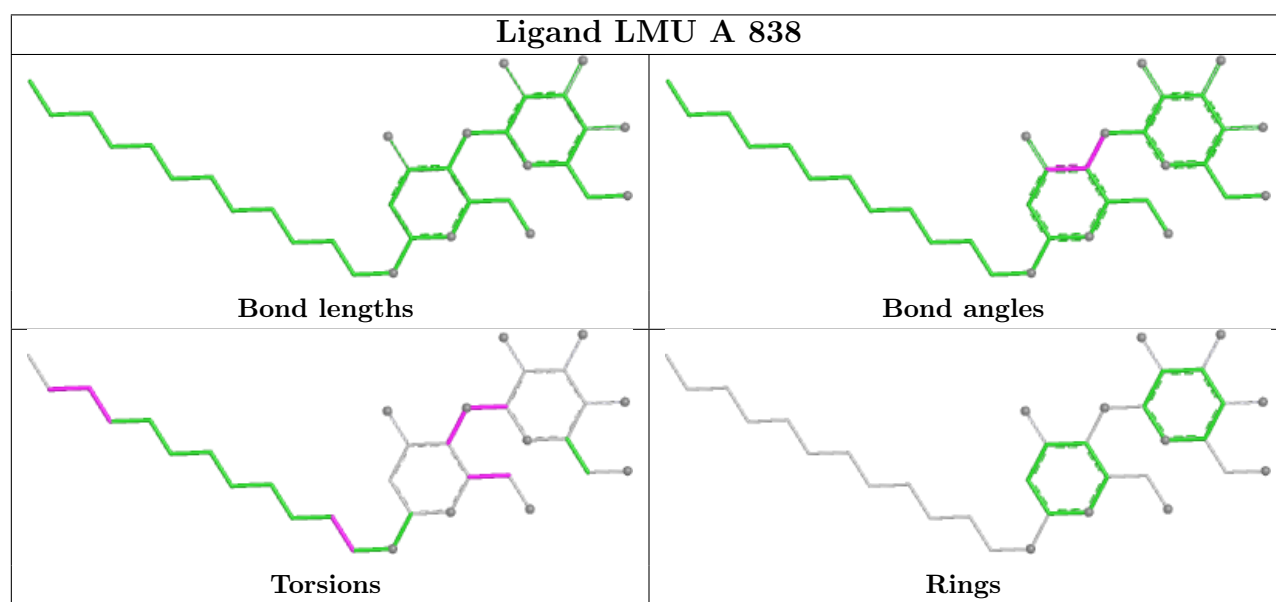
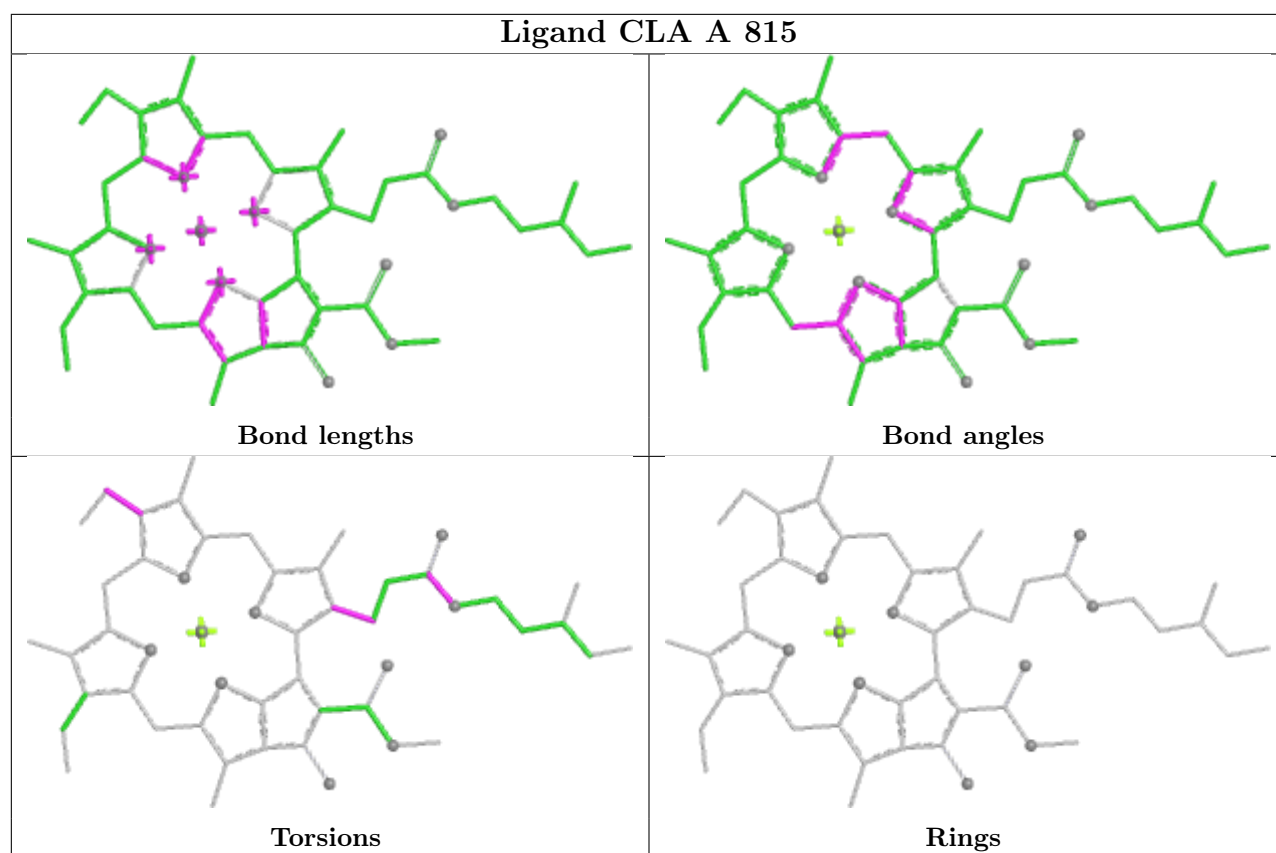


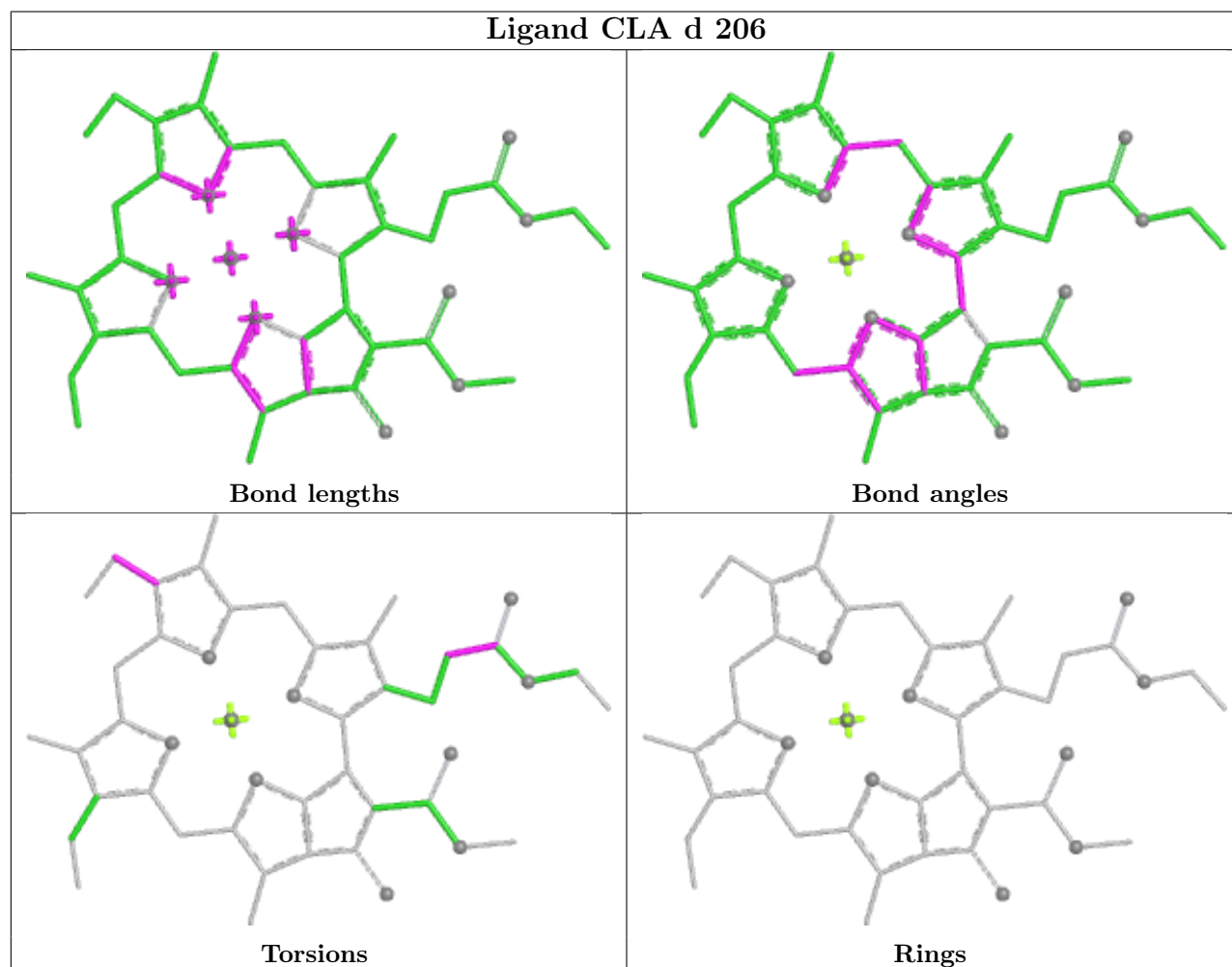
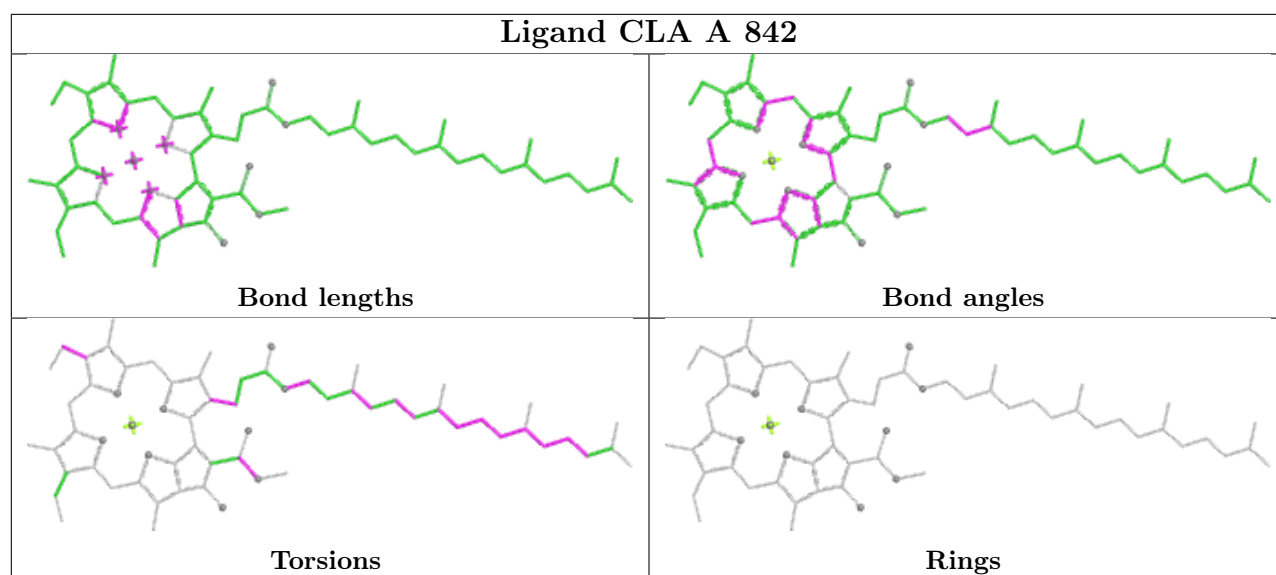
Ligand CLA B 823

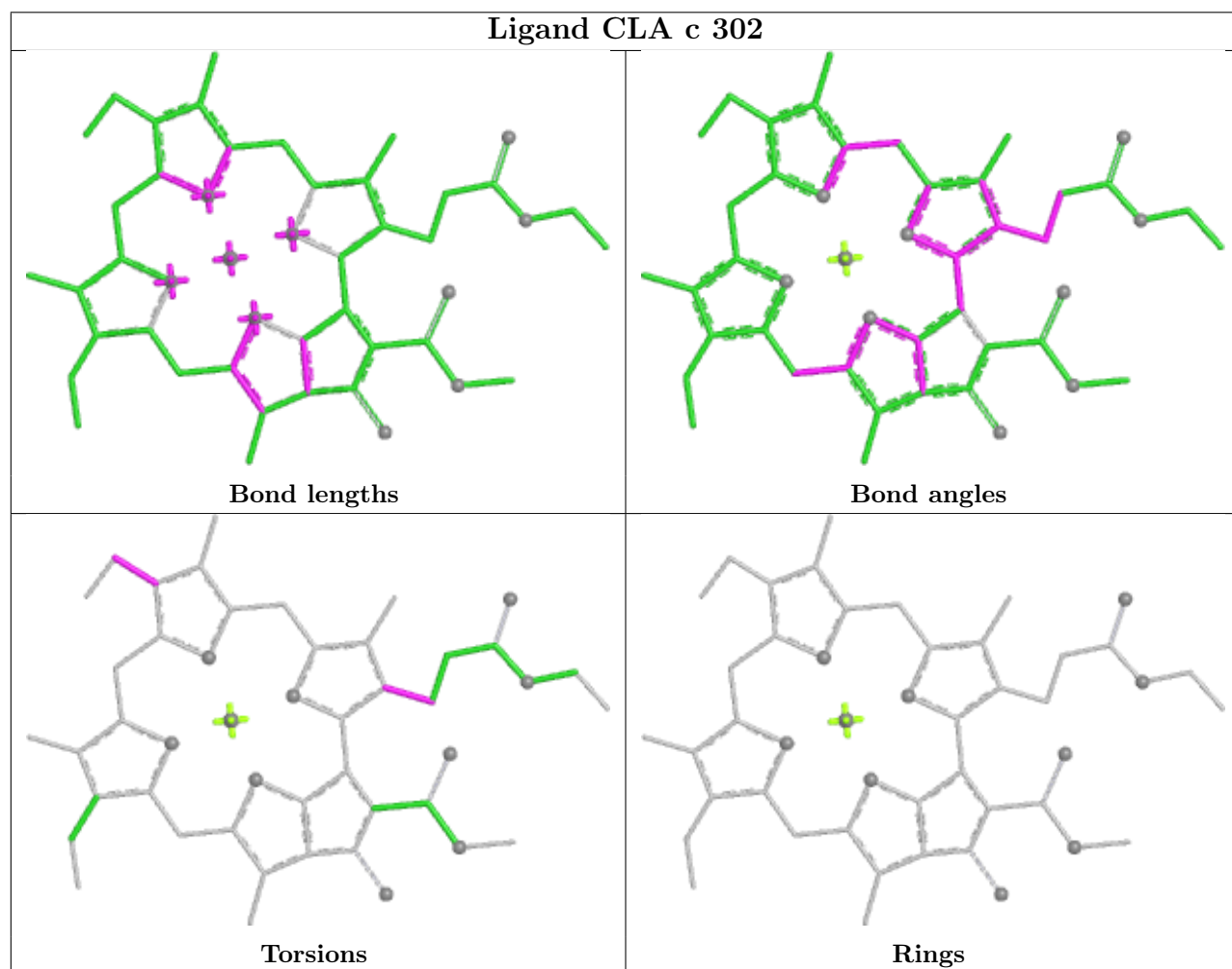
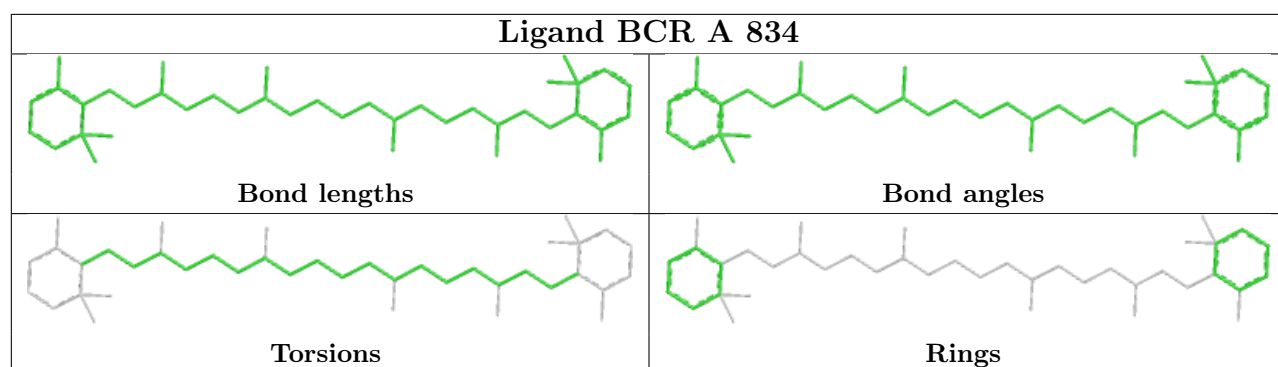


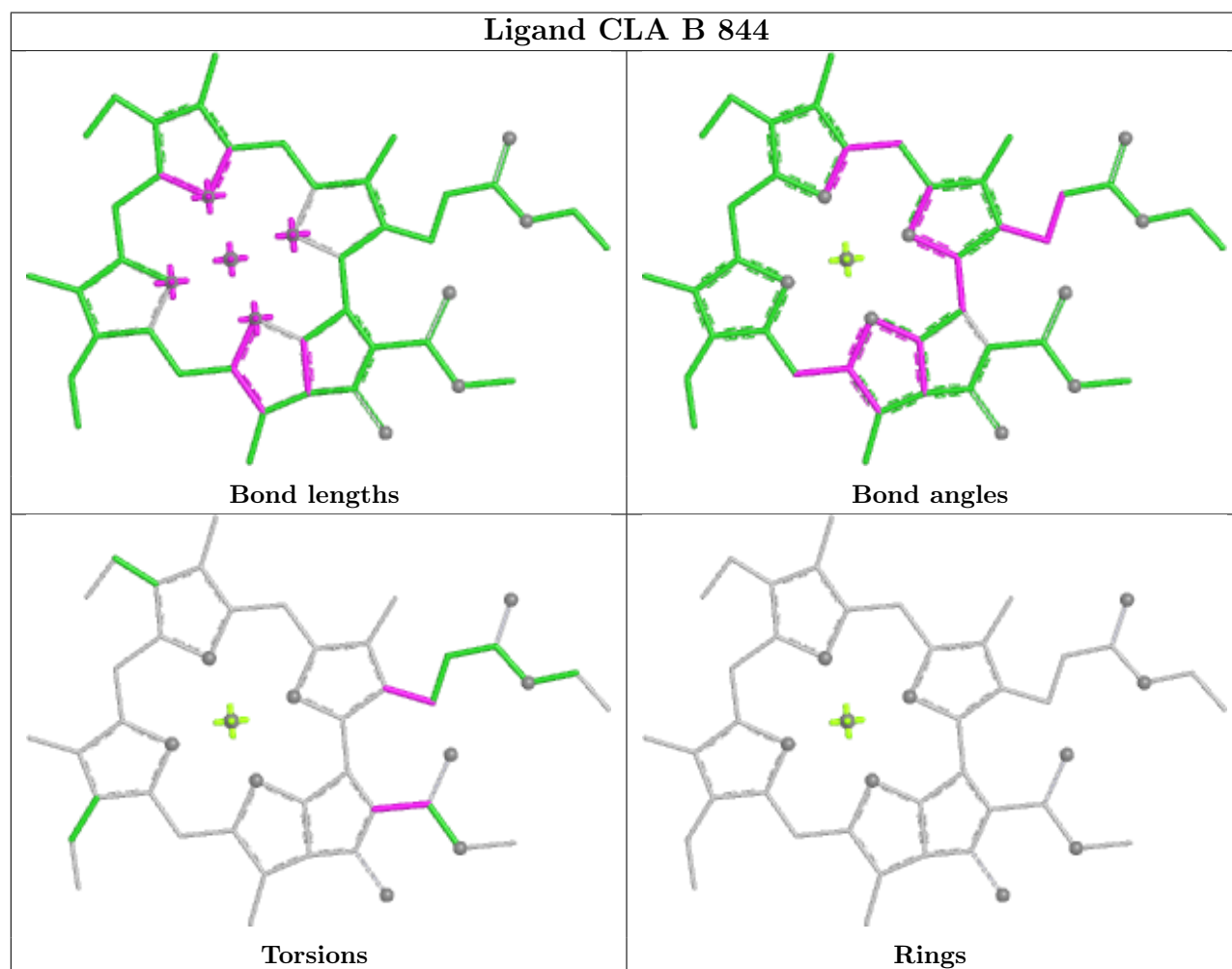
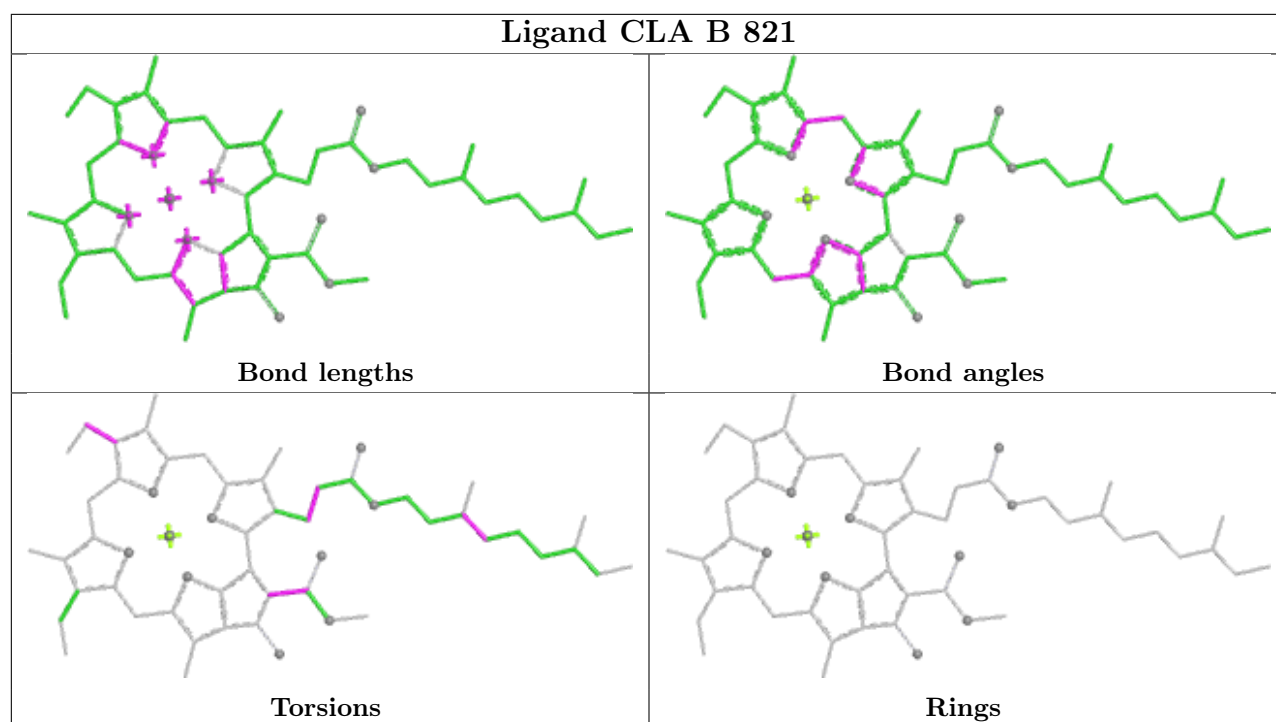
Ligand CLA d 208



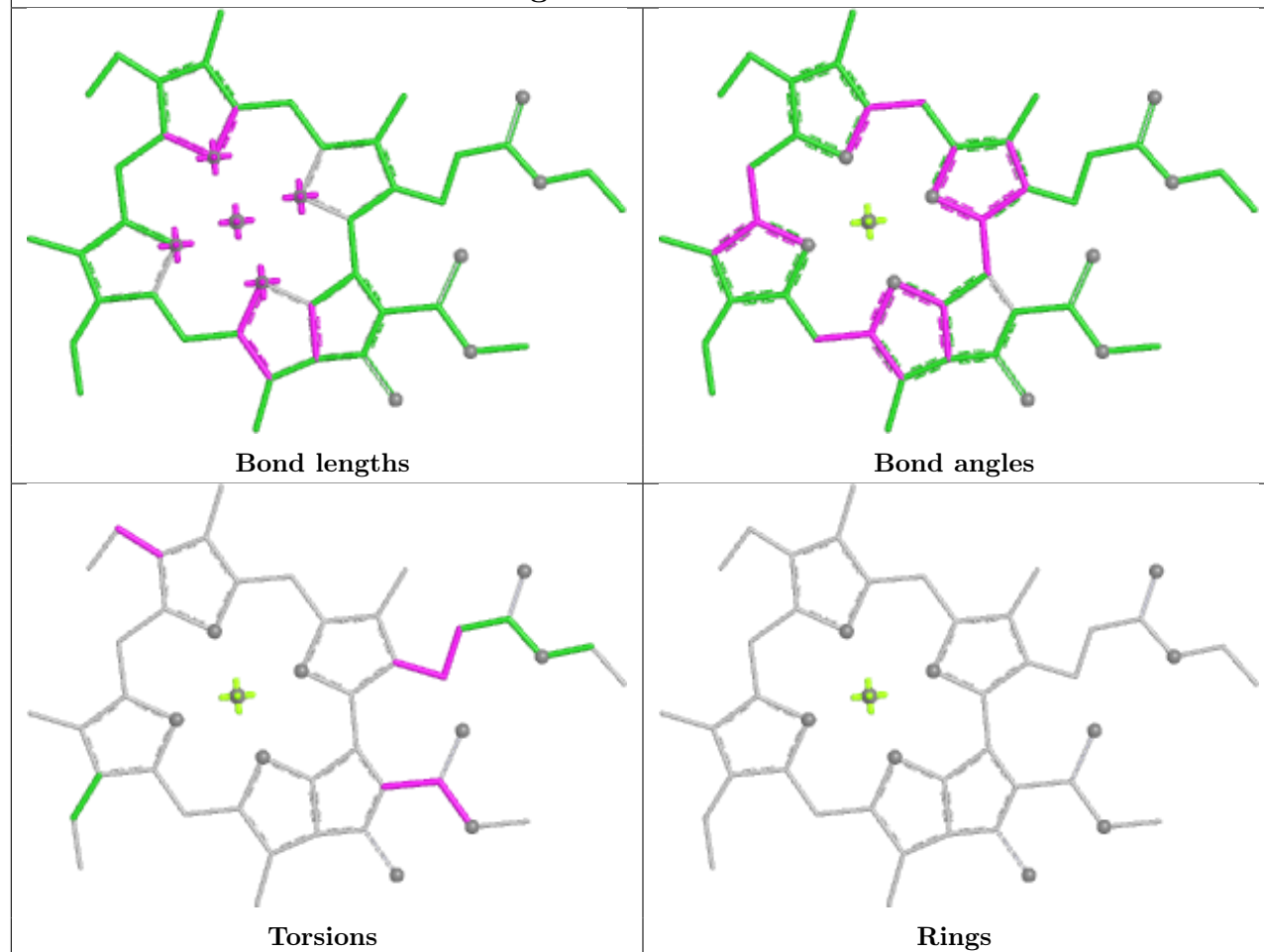




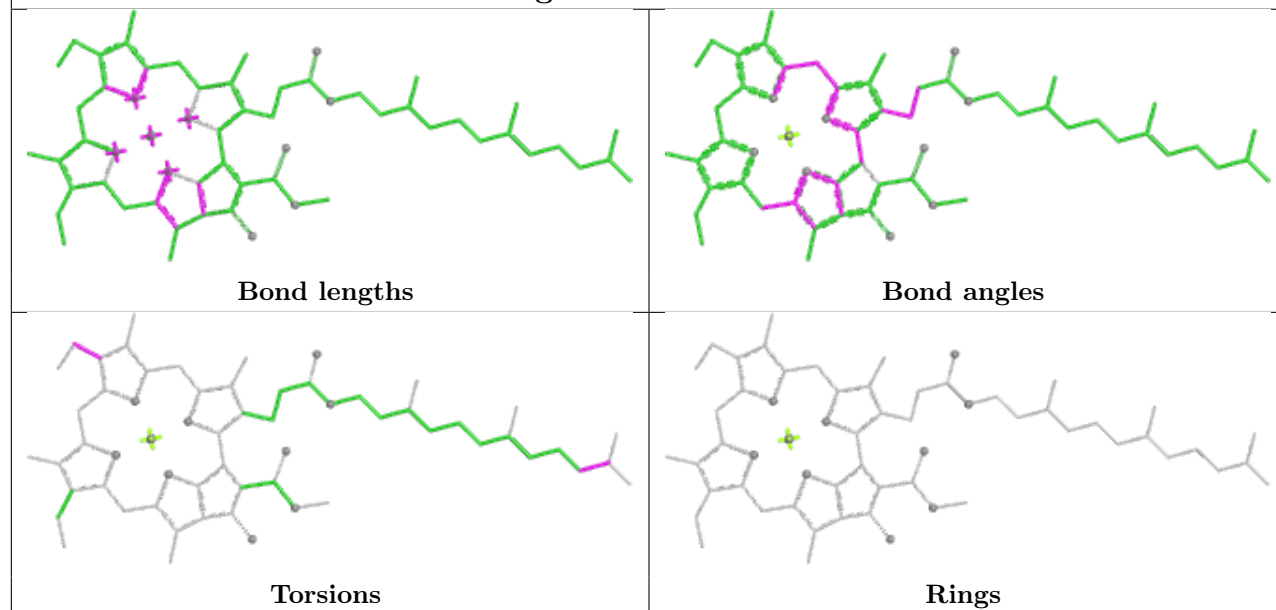


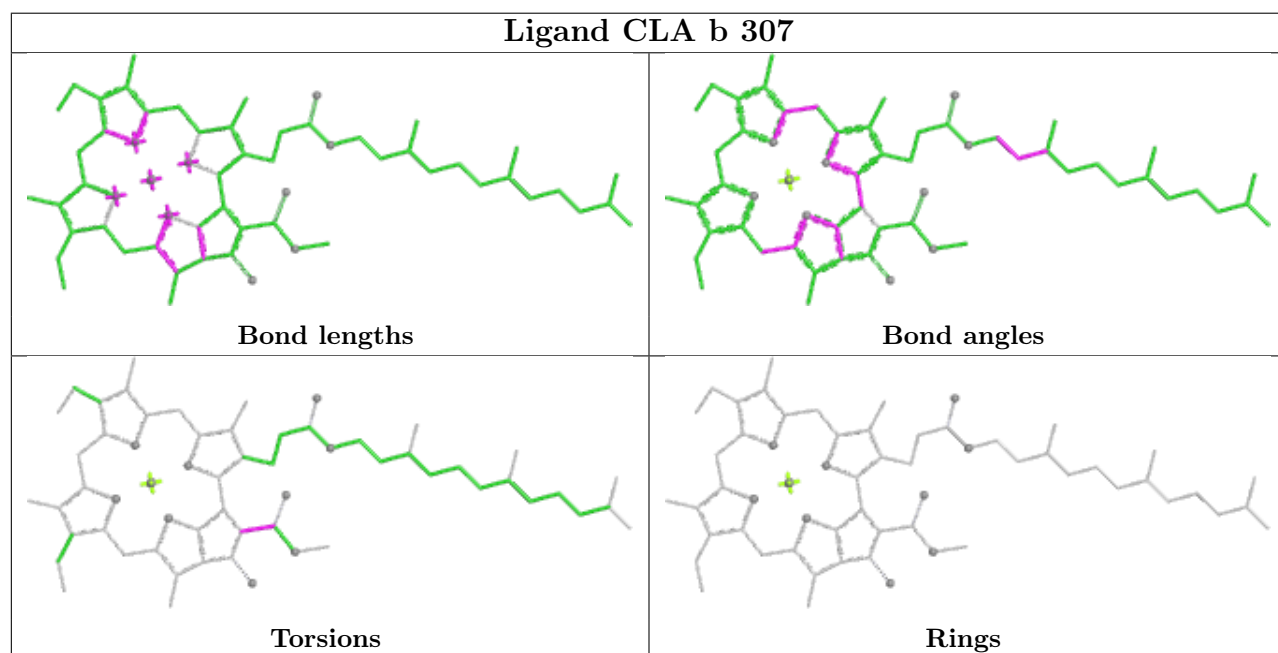
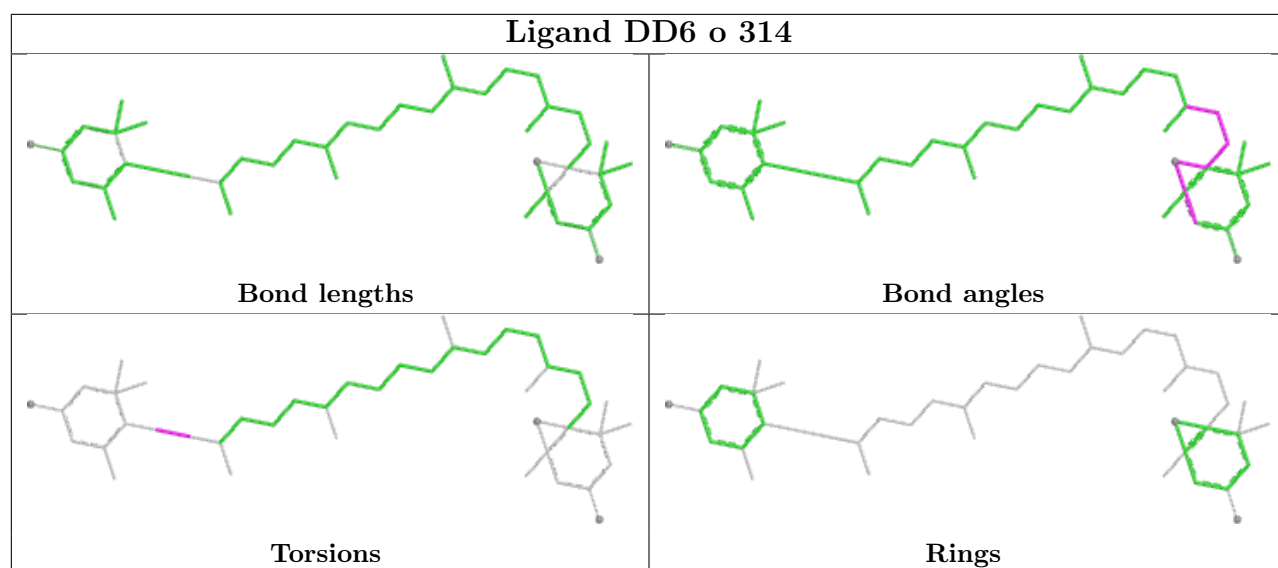


Ligand CLA b 315

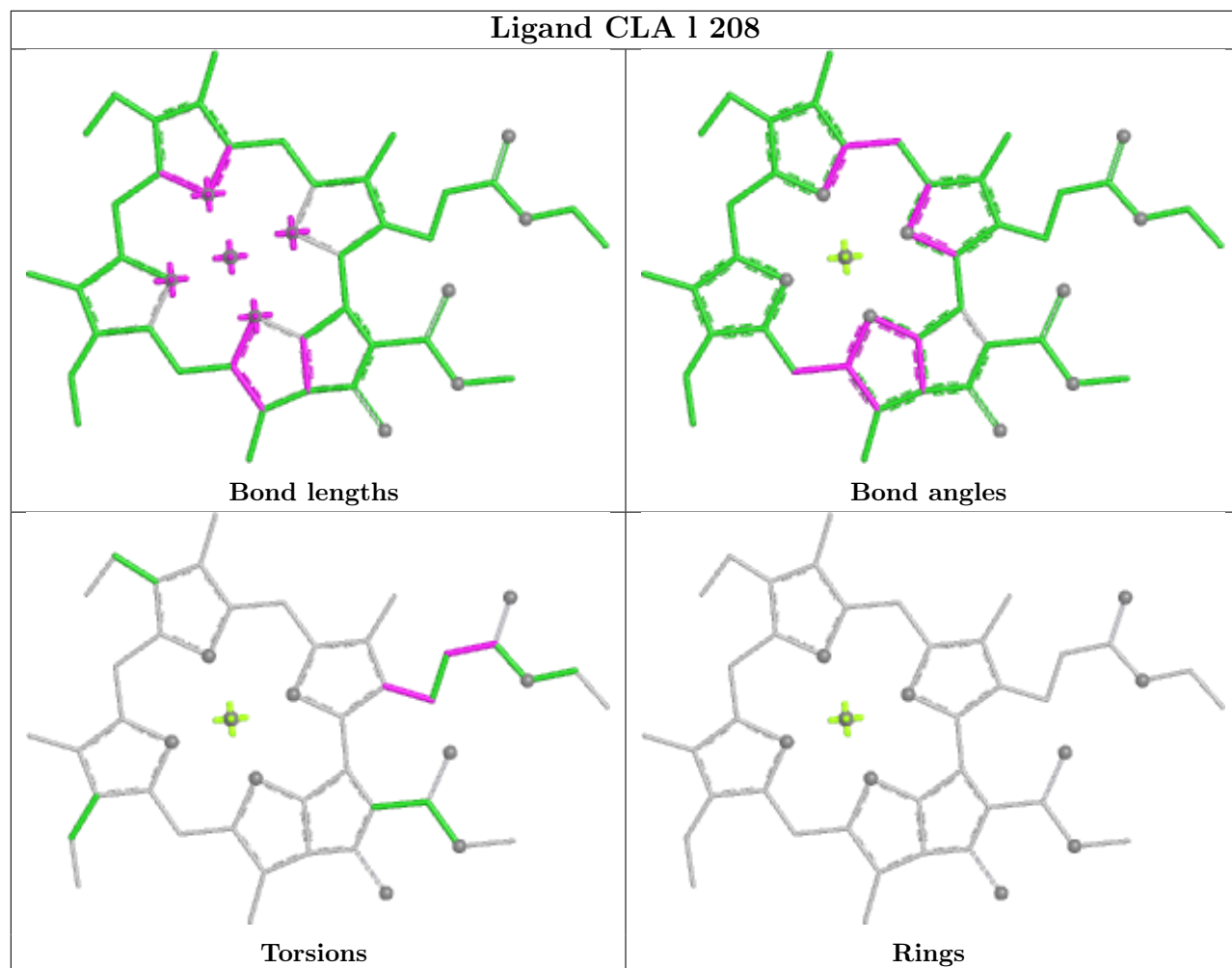


Ligand CLA h 205

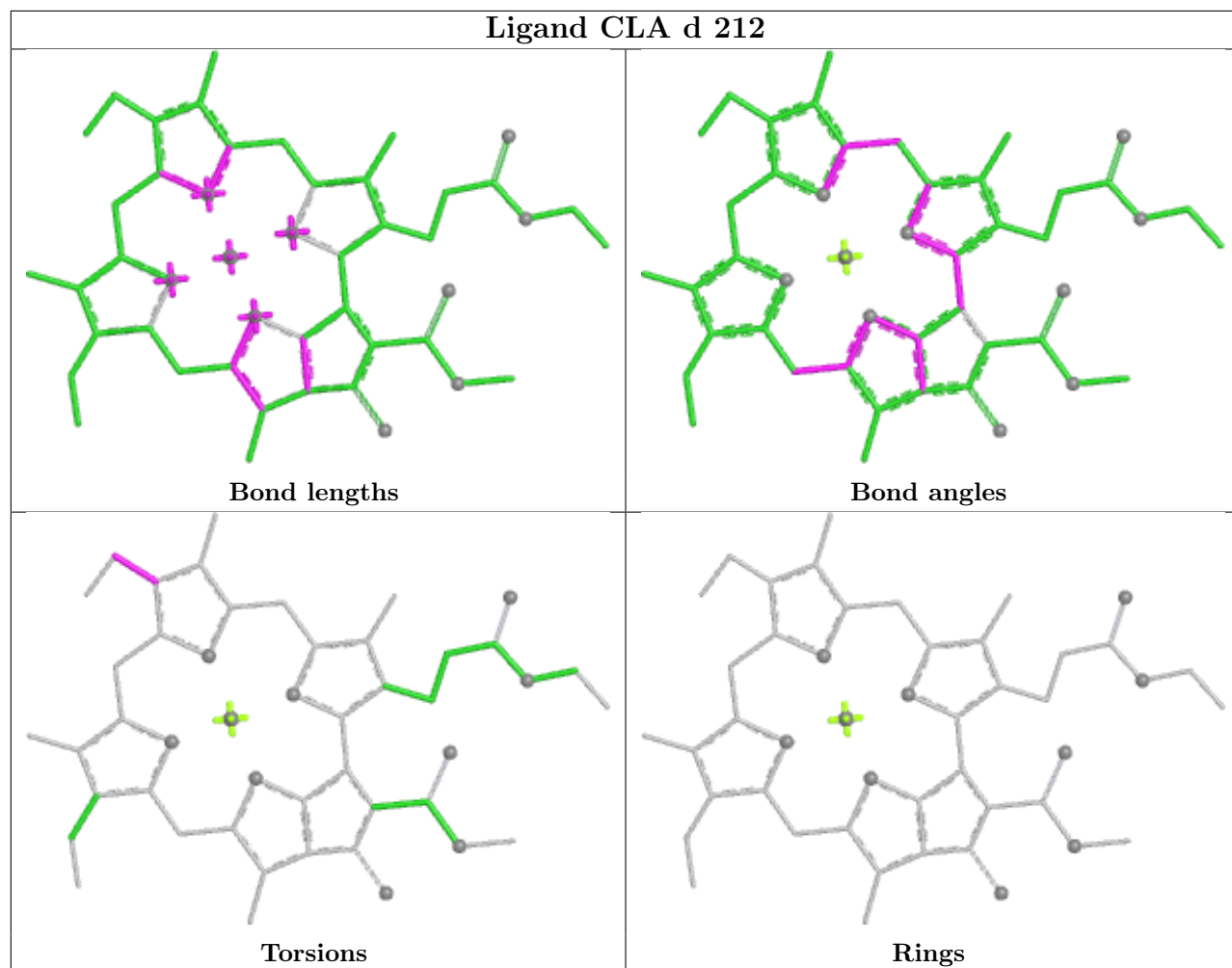




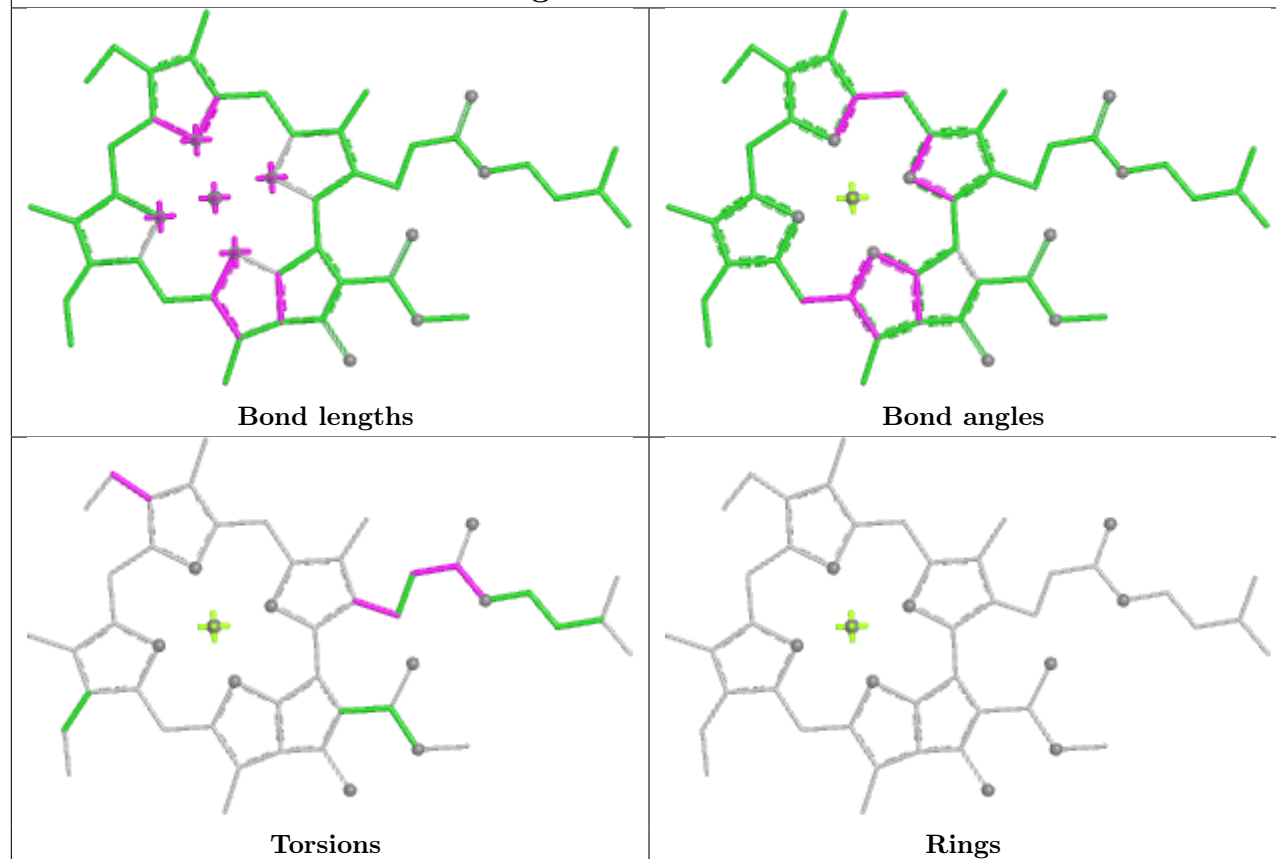
Ligand CLA 1 208



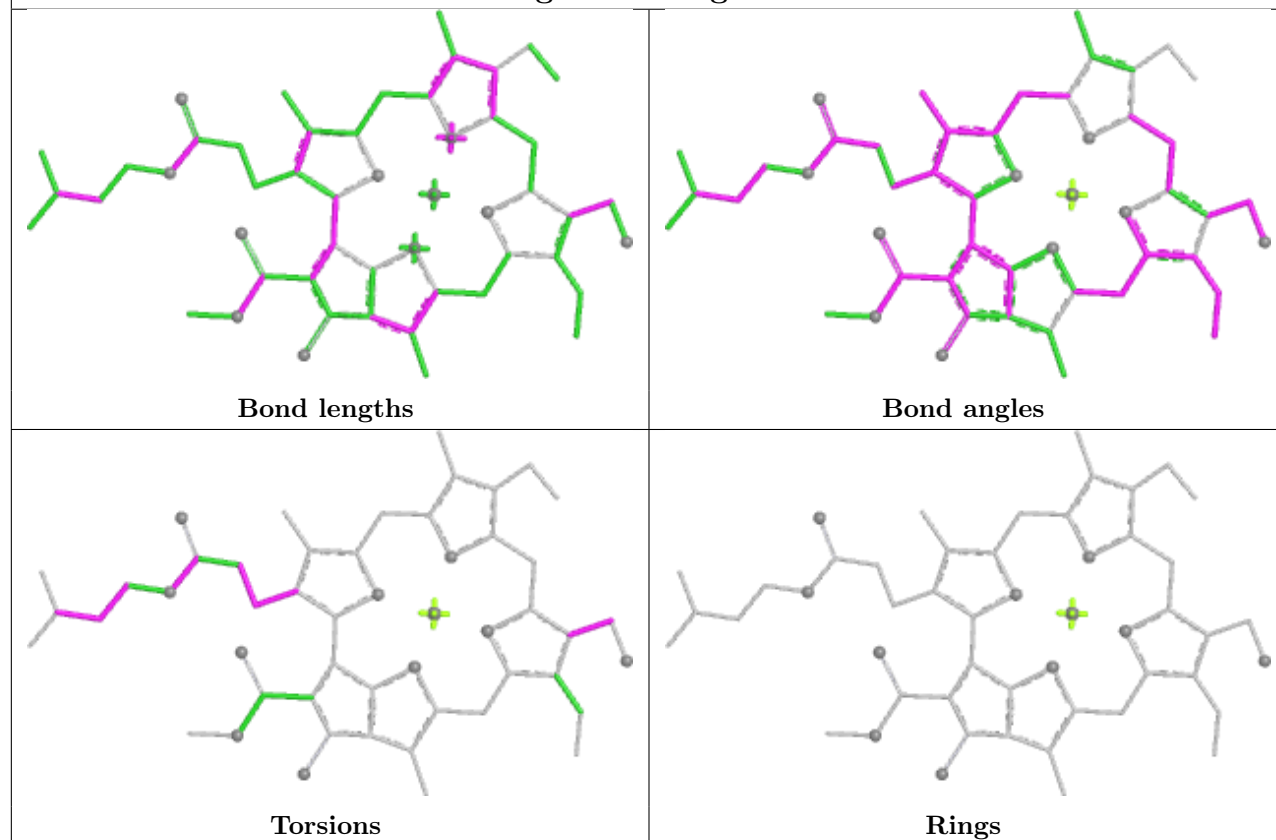
Ligand CLA d 212

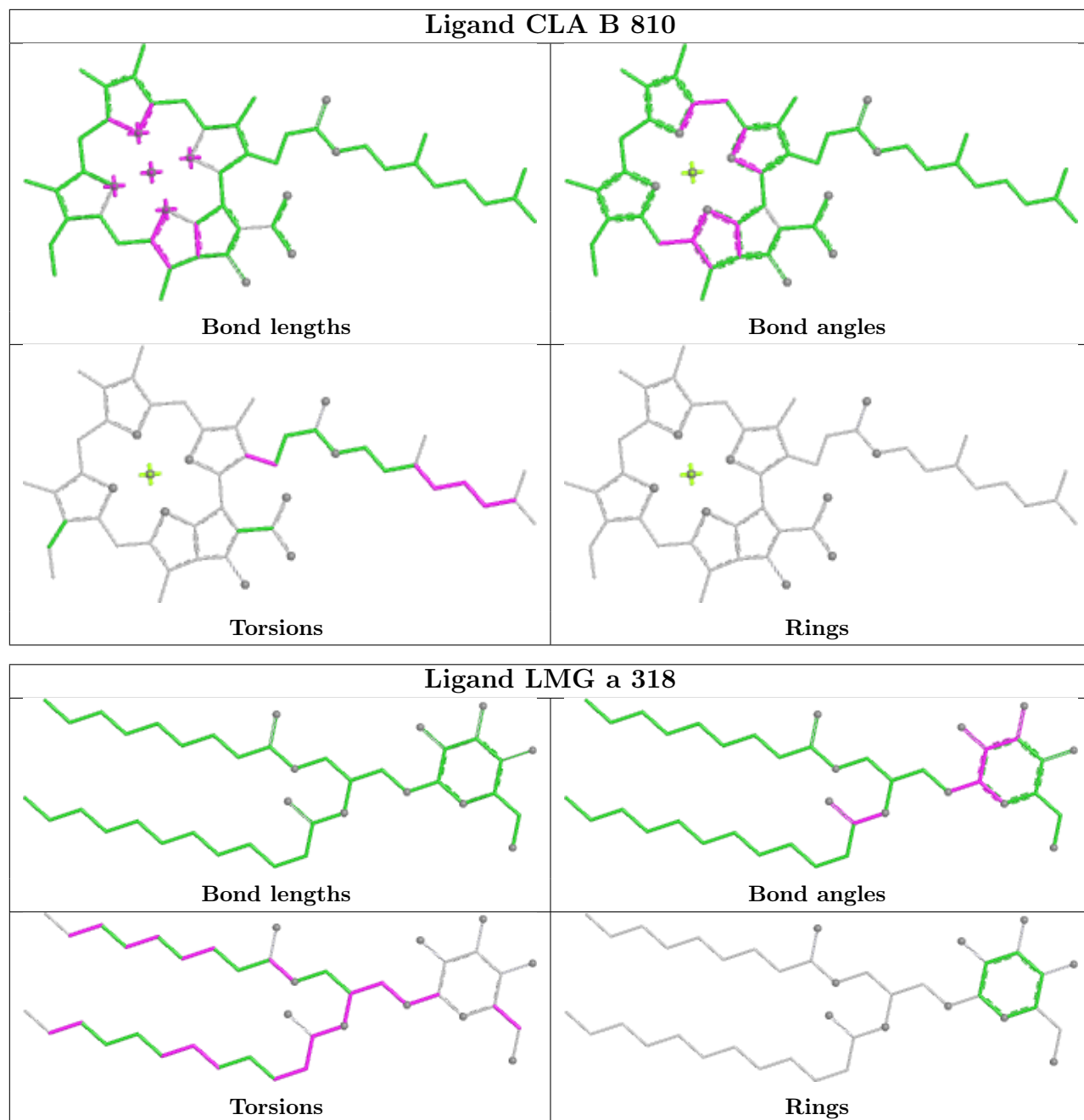


Ligand CLA A 848

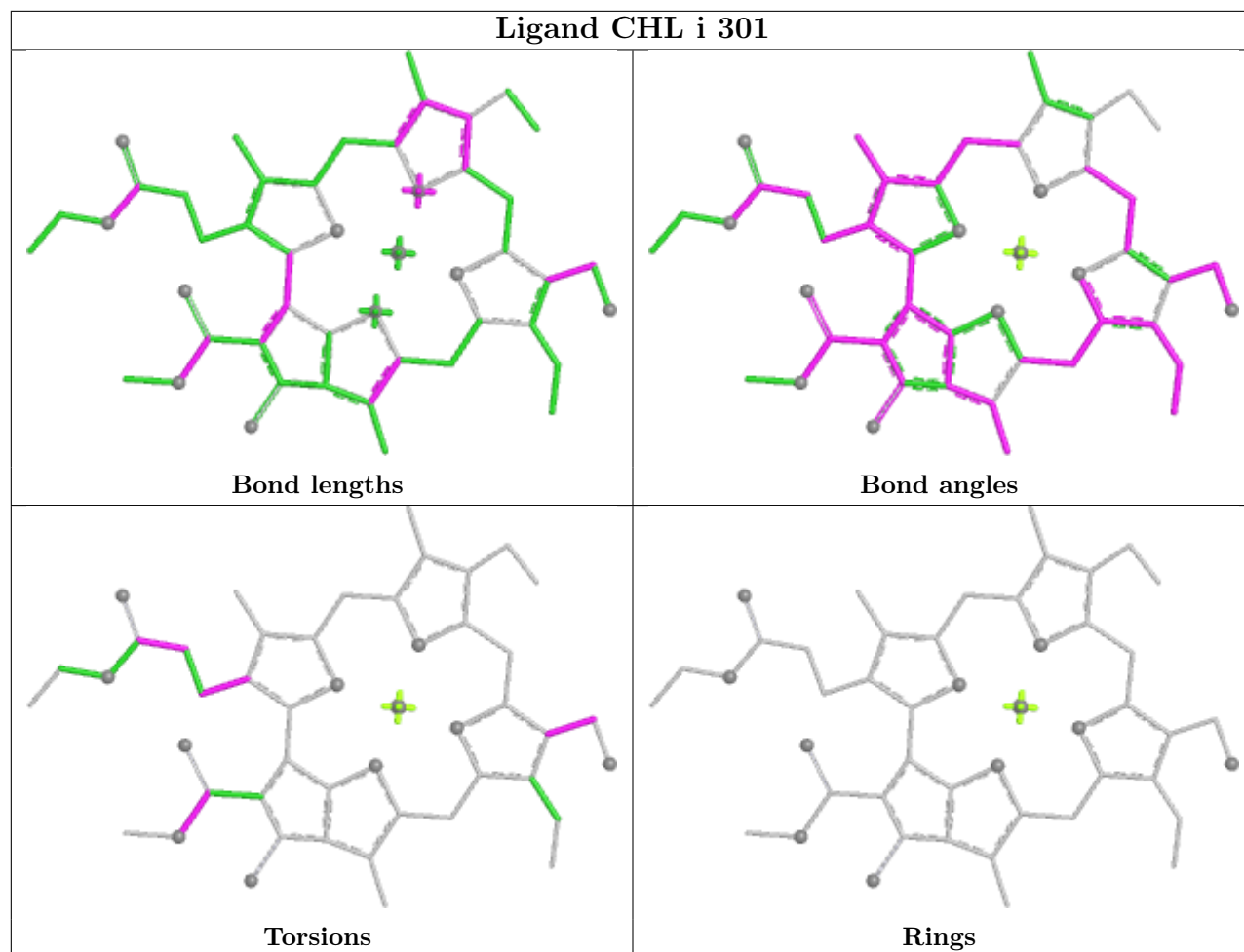


Ligand CHL g 310

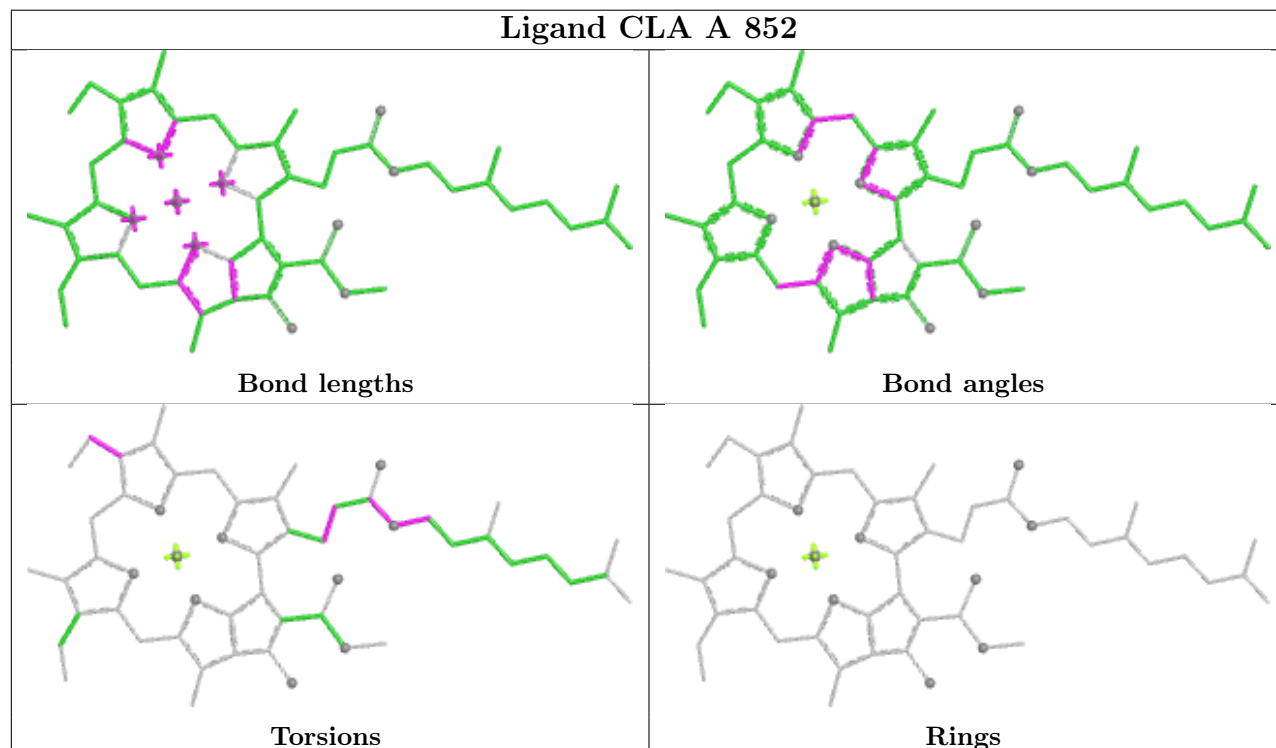




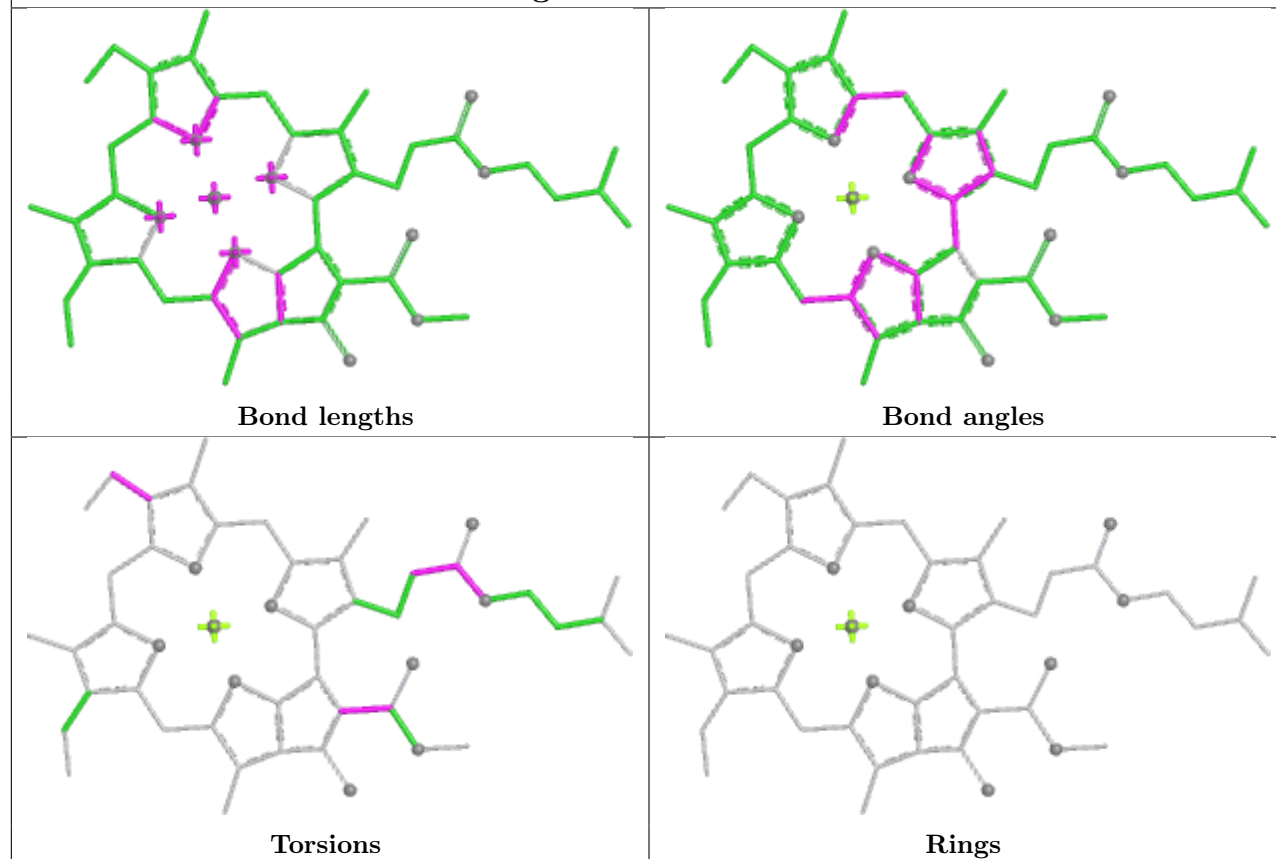
Ligand CHL i 301



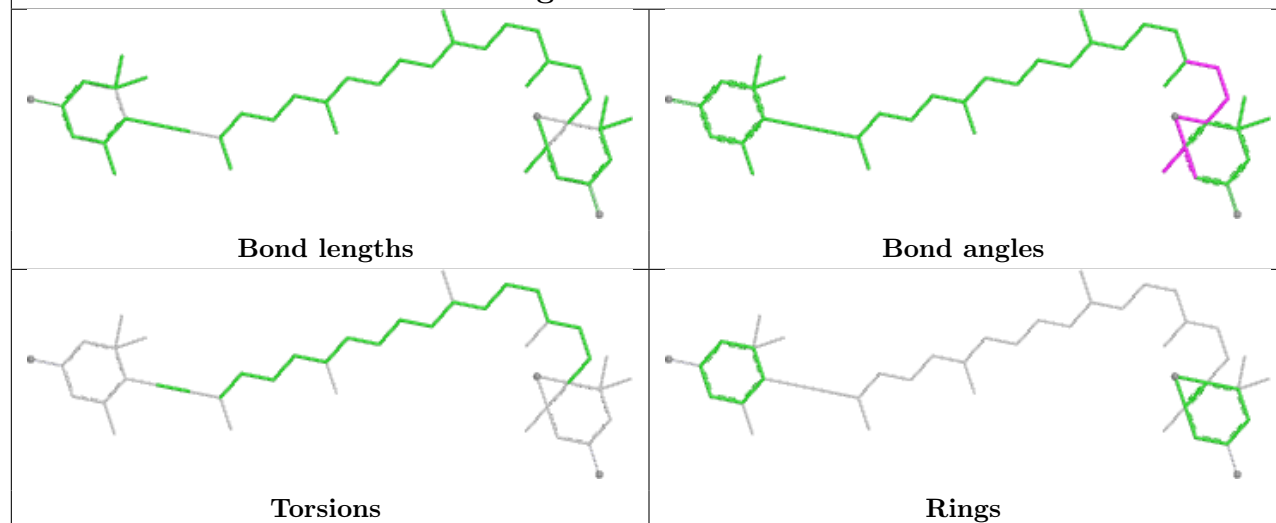
Ligand CLA A 852



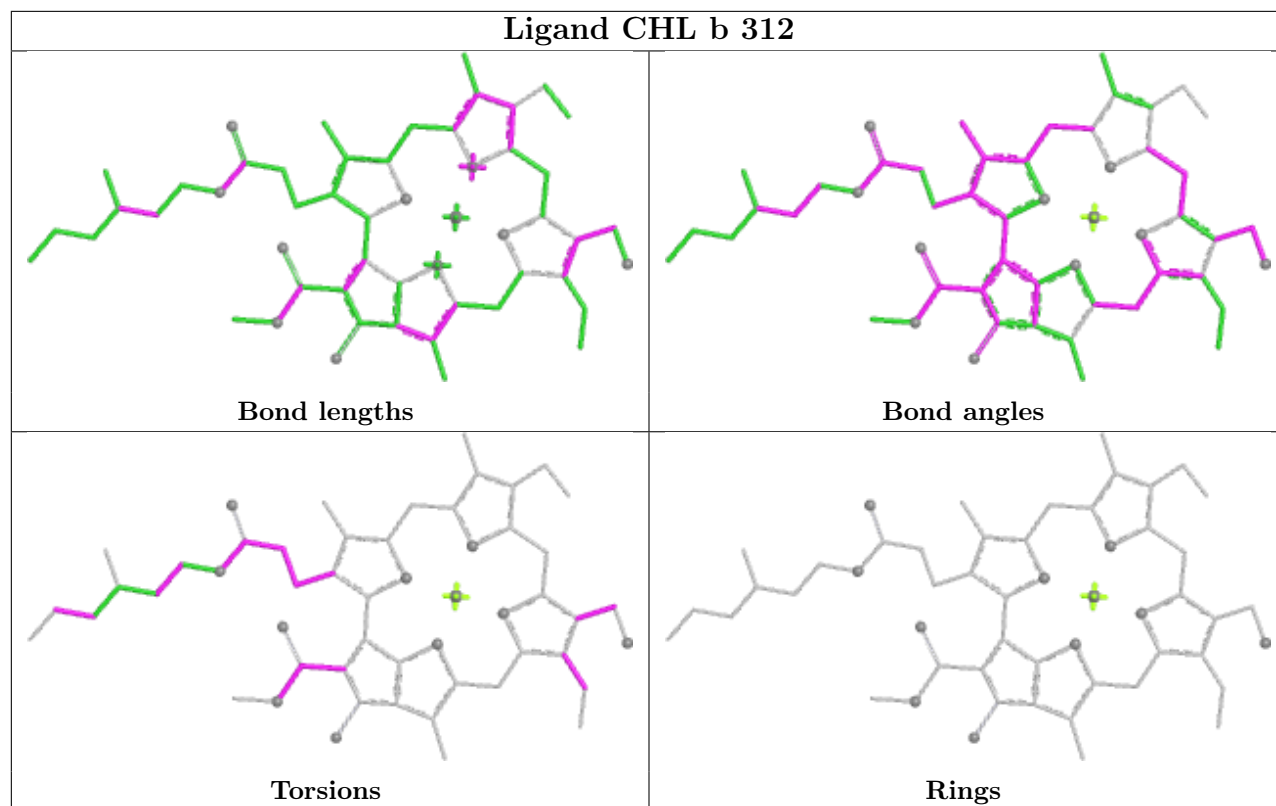
Ligand CLA B 838



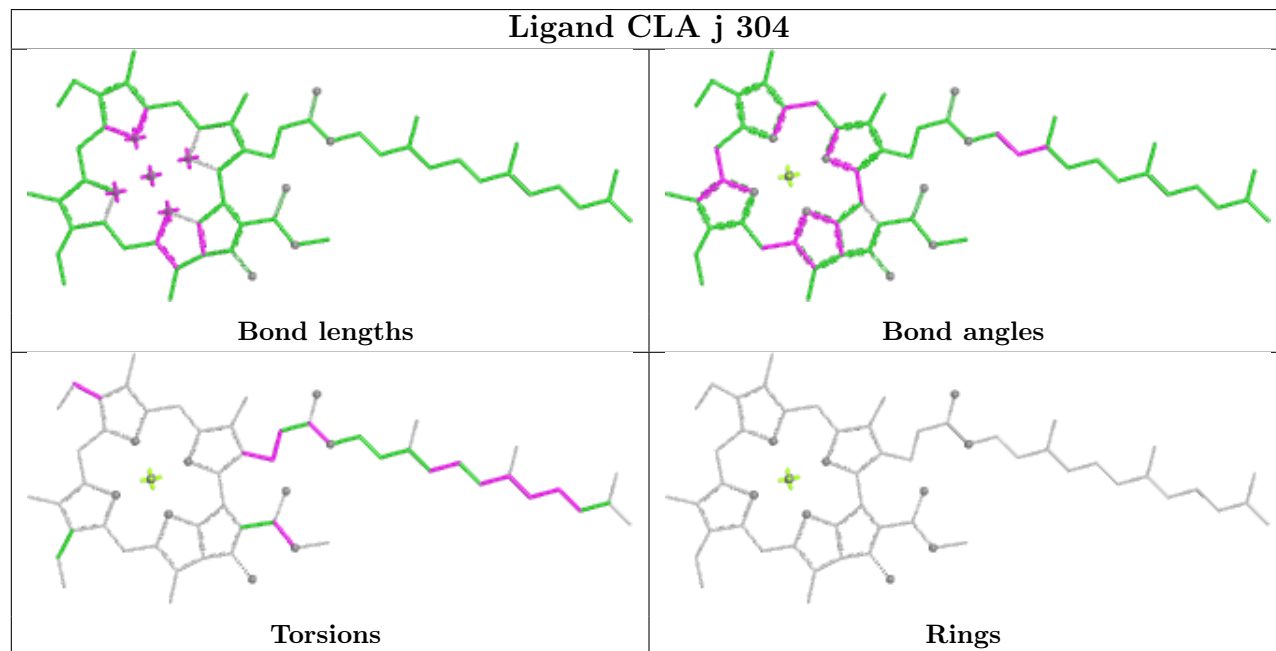
Ligand DD6 k 314



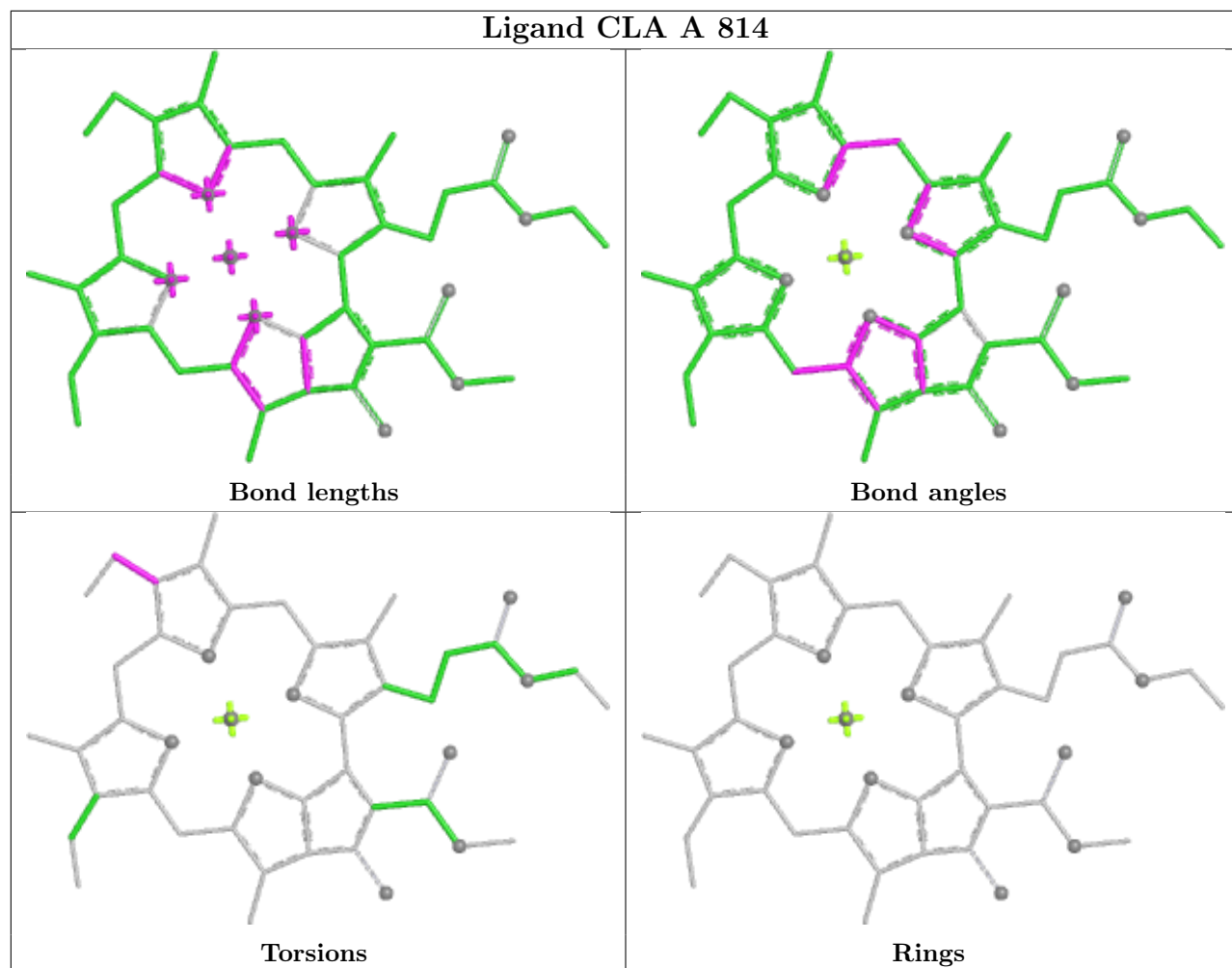
Ligand CHL b 312

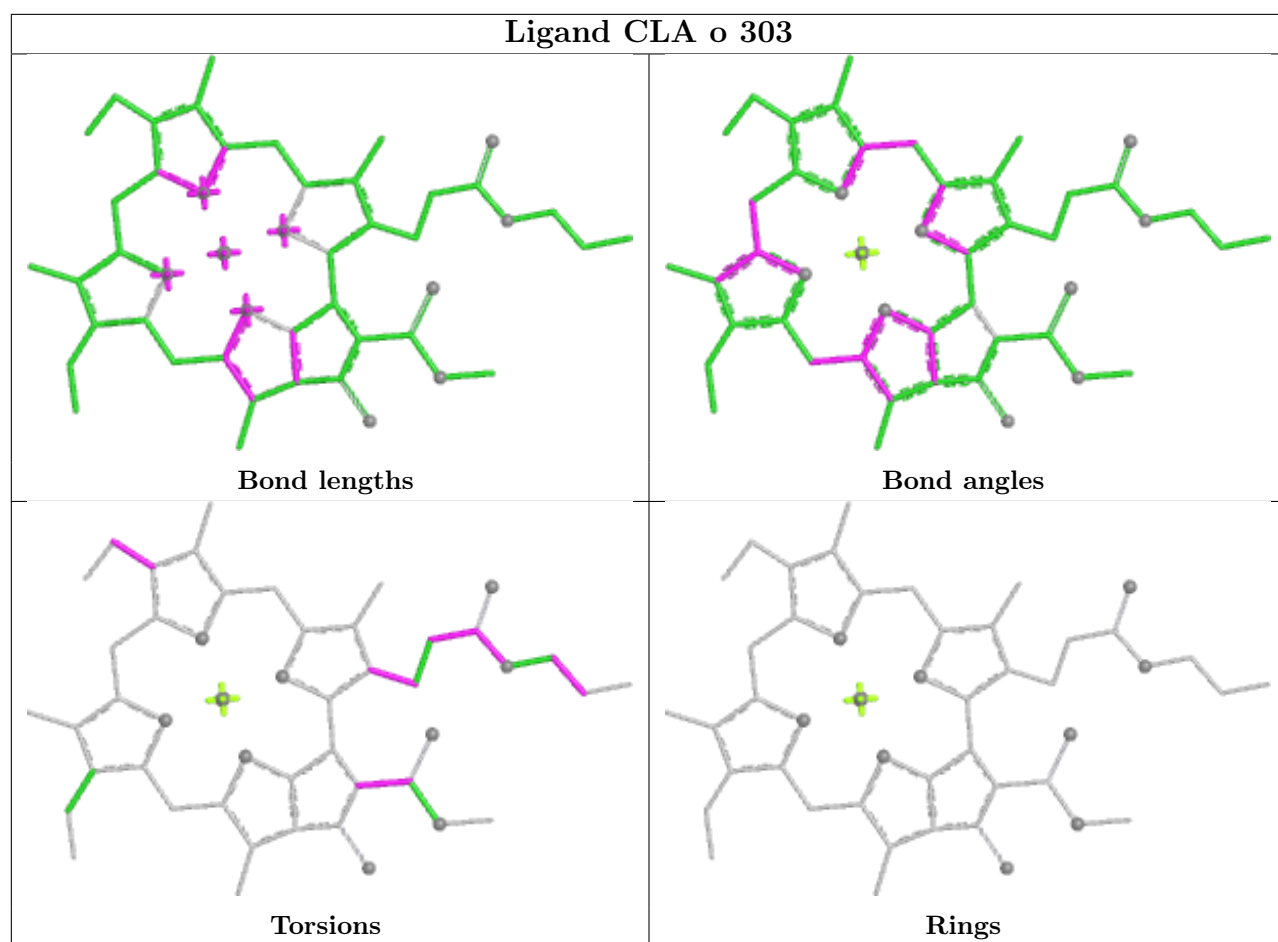


Ligand CLA j 304

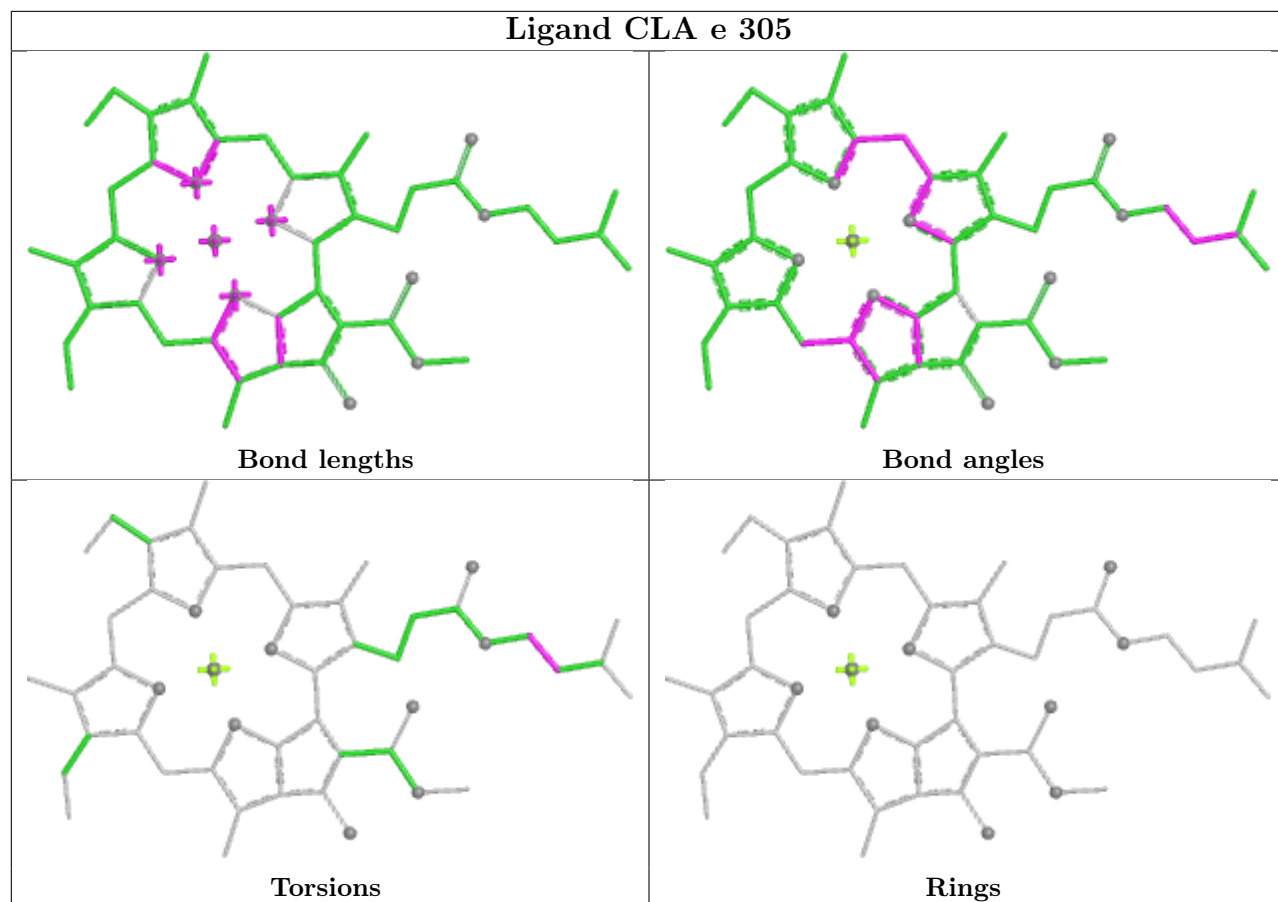


Ligand CLA A 814

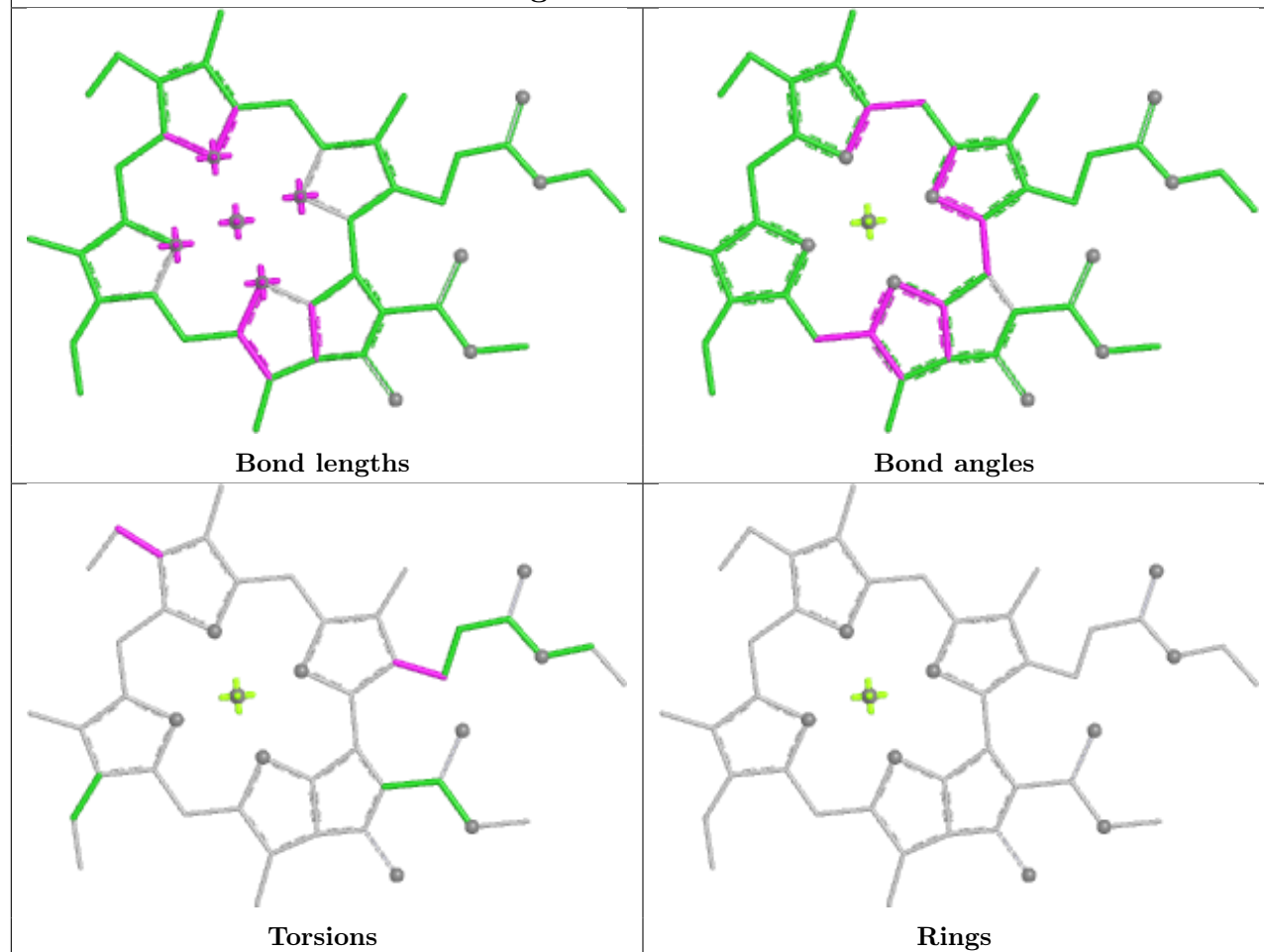




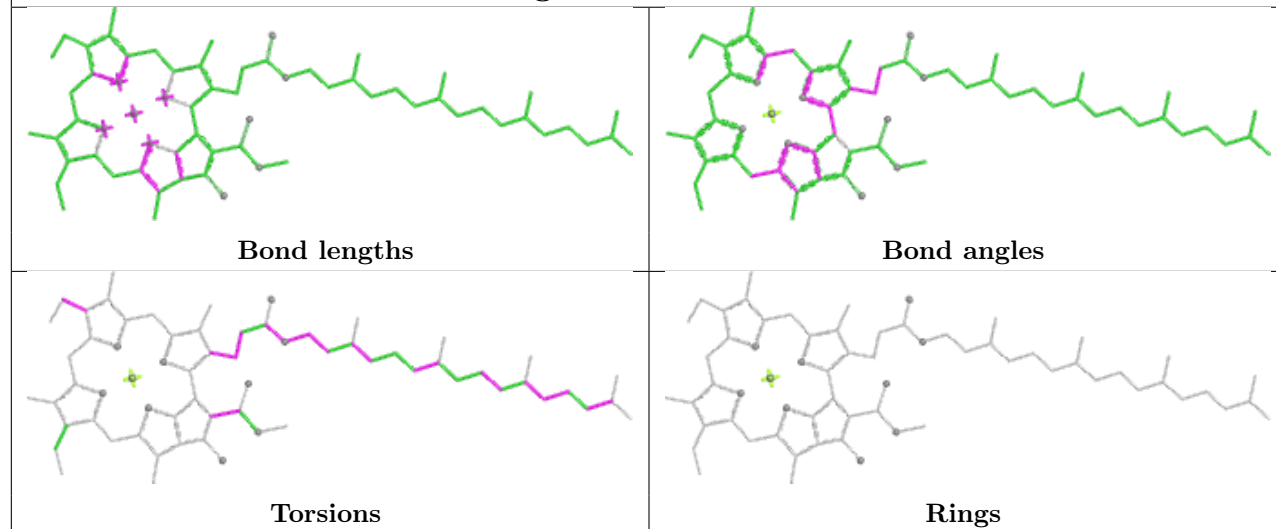
Ligand CLA e 305

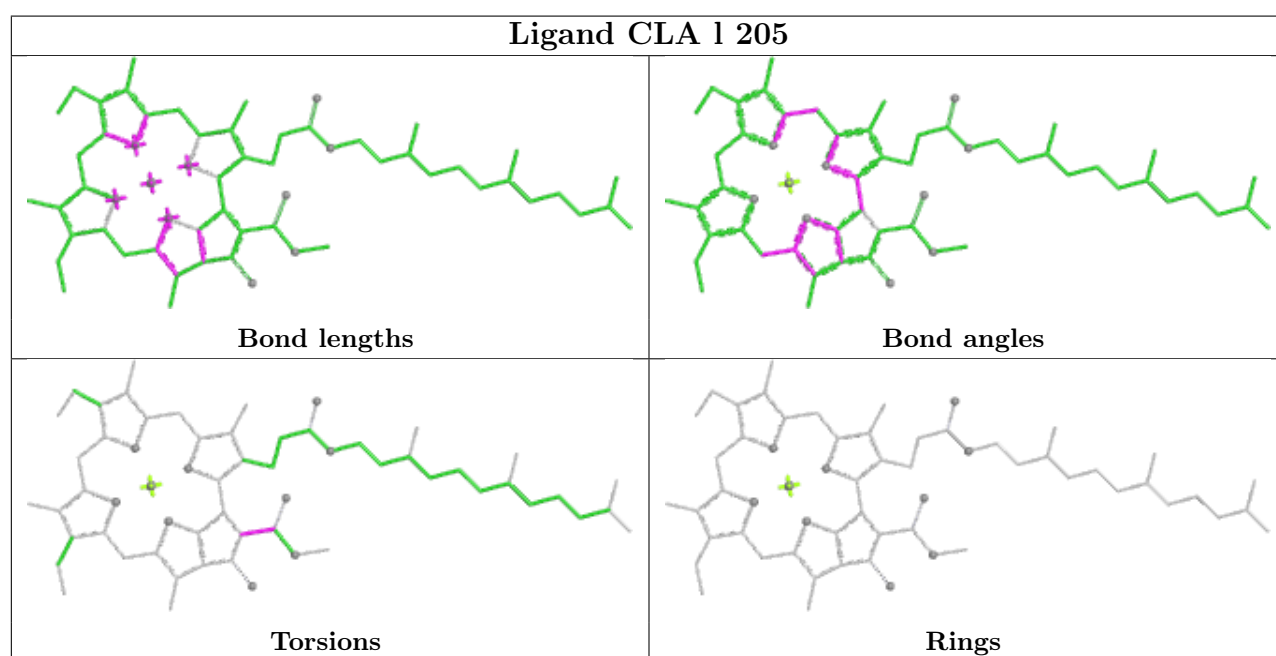
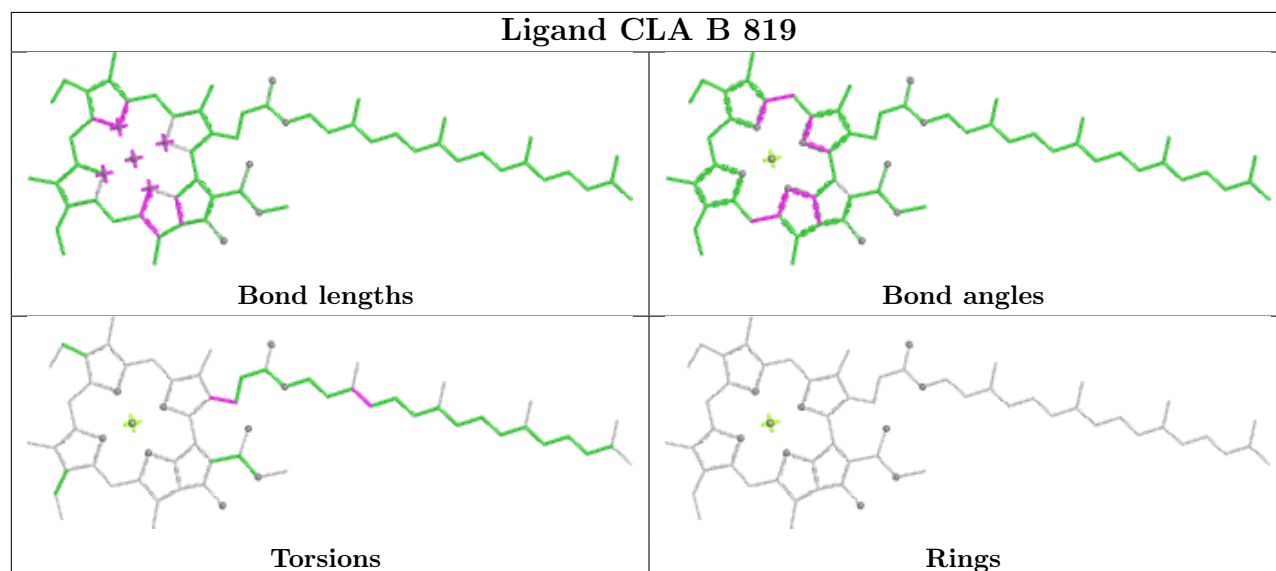
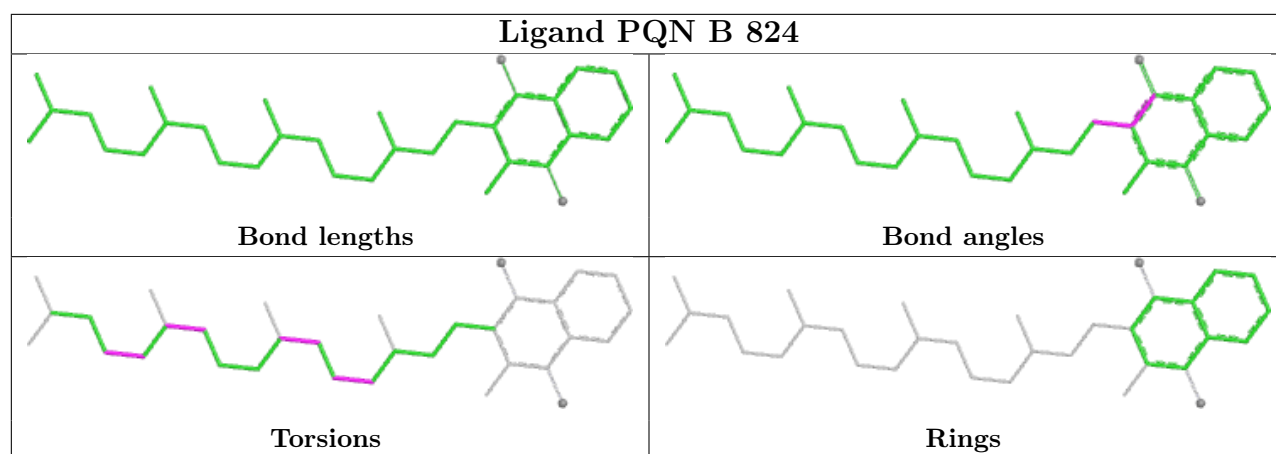


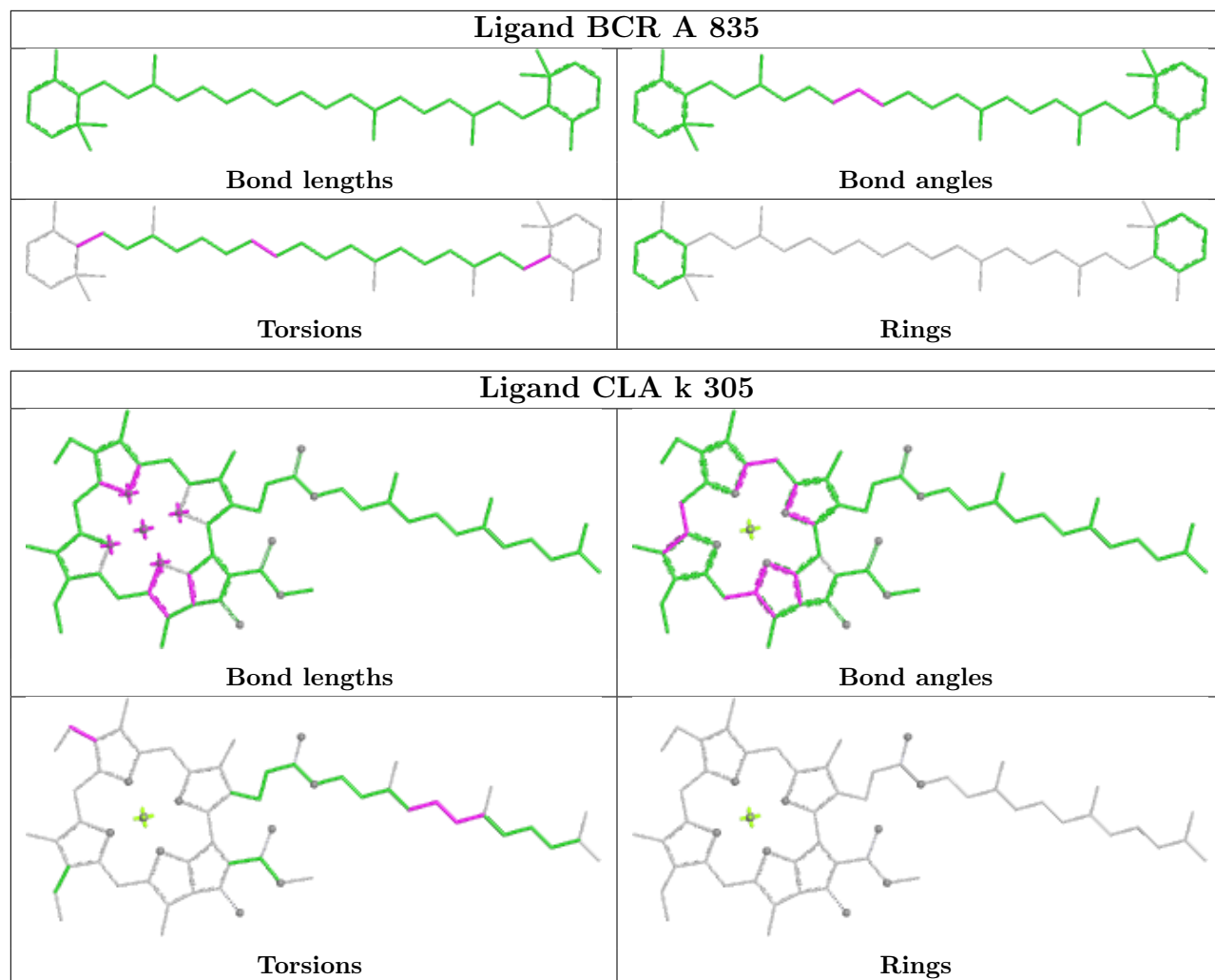
Ligand CLA h 213



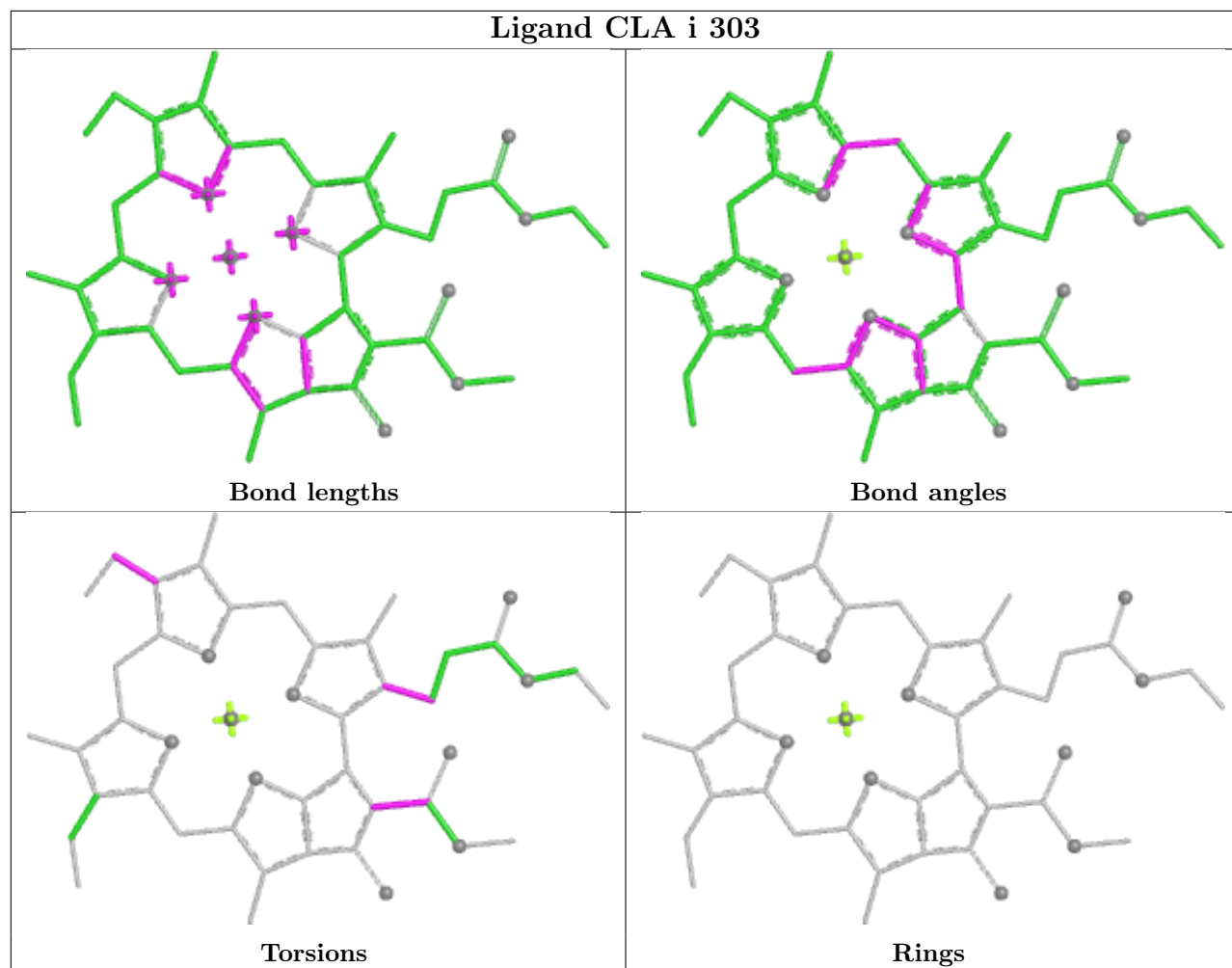
Ligand CLA F 203



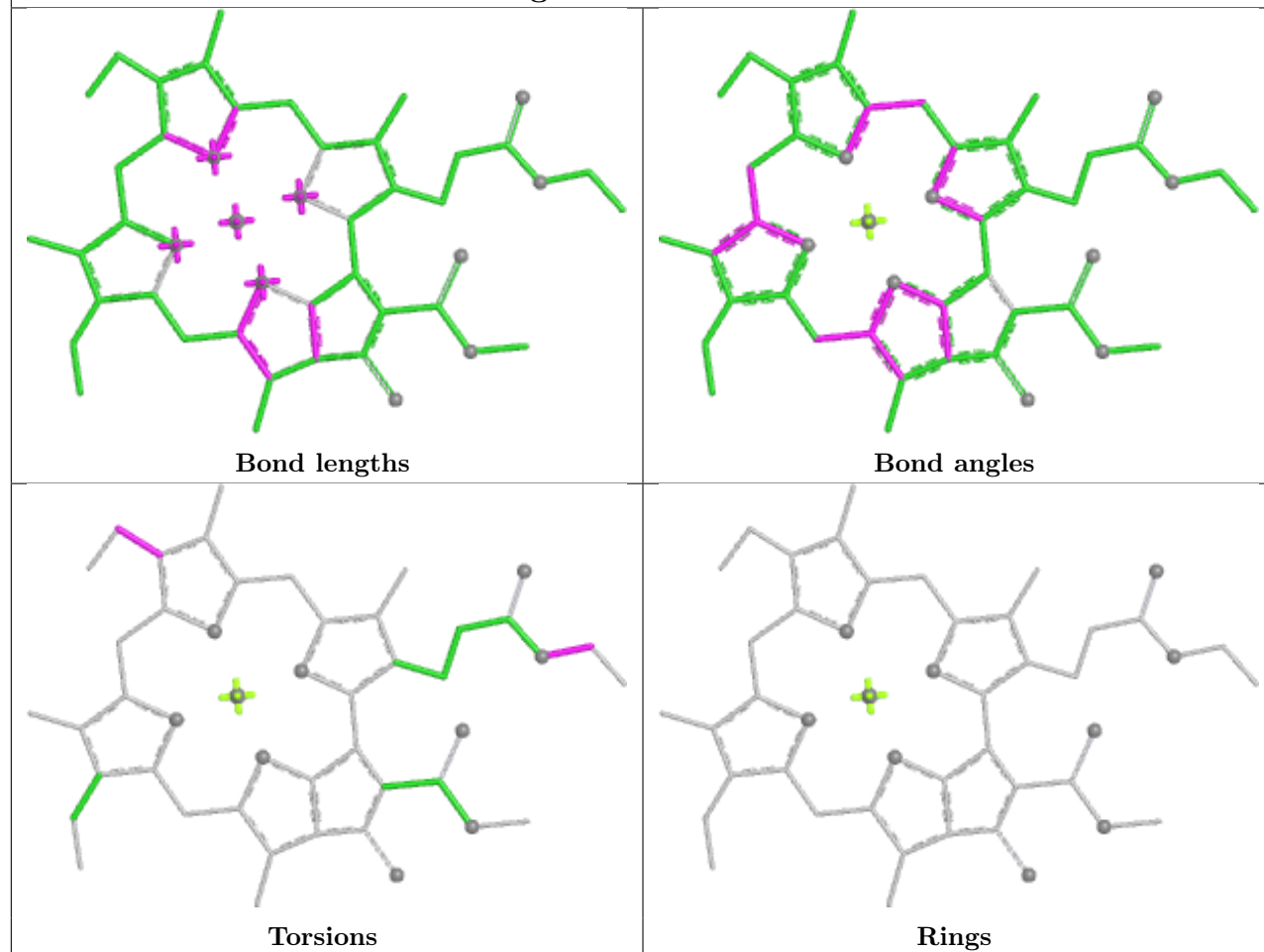




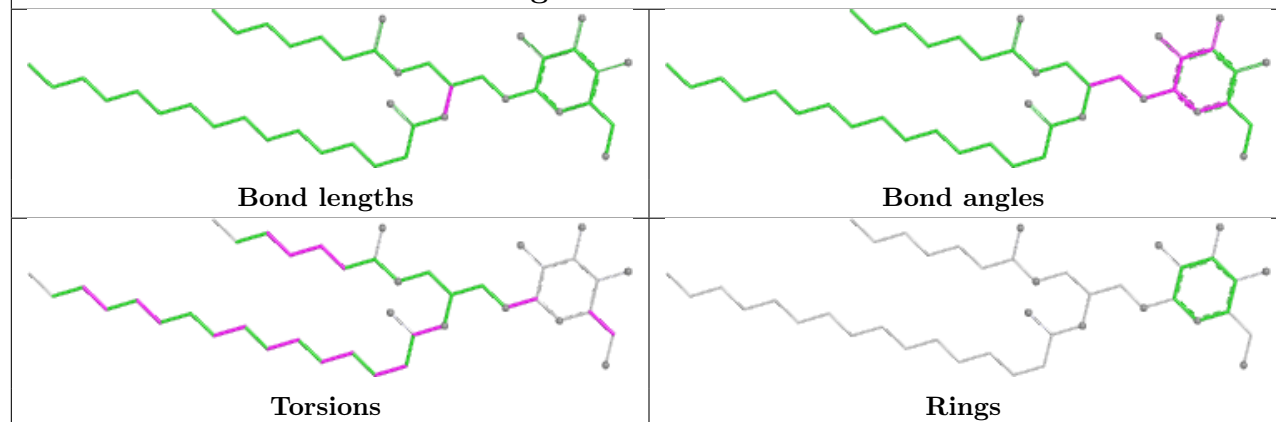
Ligand CLA i 303



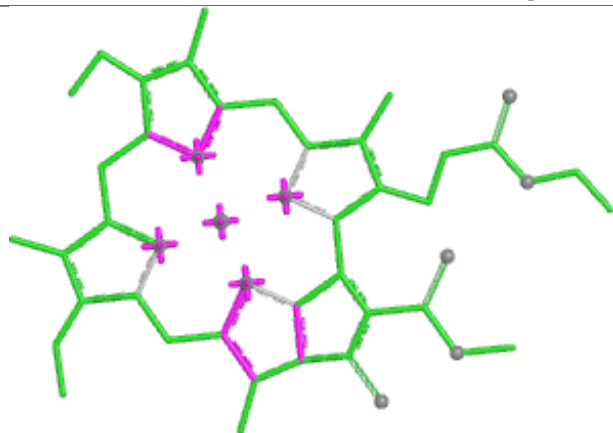
Ligand CLA b 305



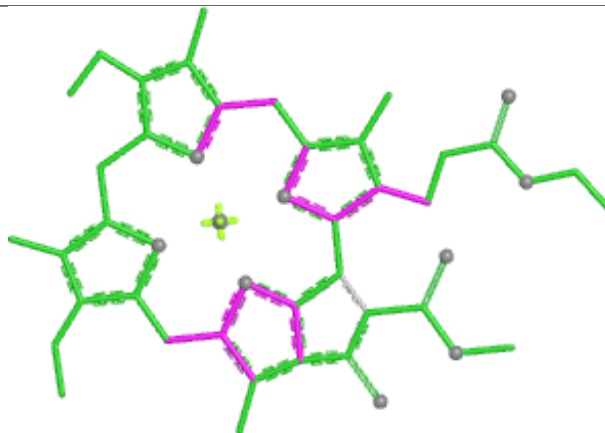
Ligand LMG b 316



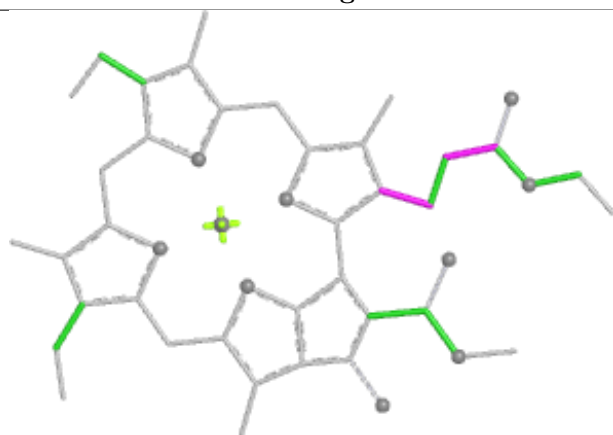
Ligand CLA i 305



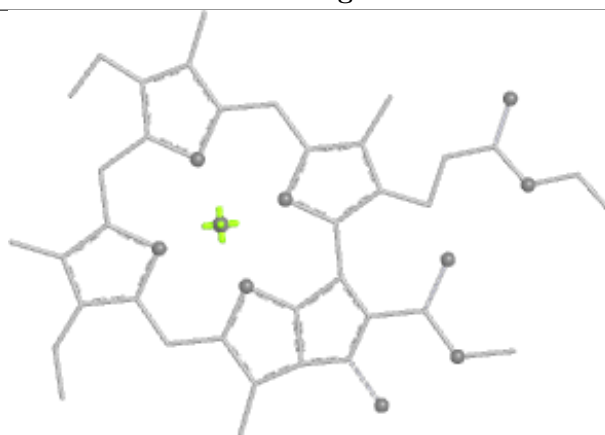
Bond lengths



Bond angles

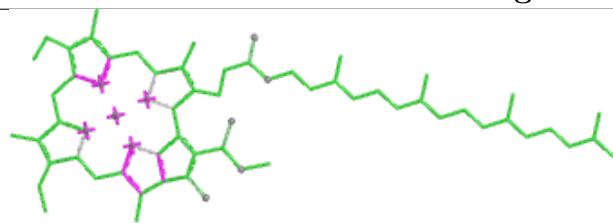


Torsions

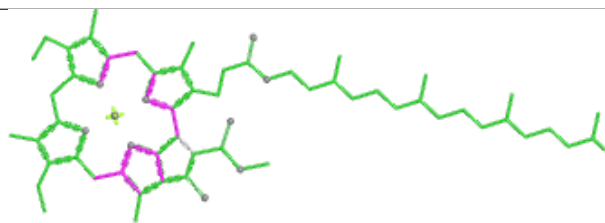


Rings

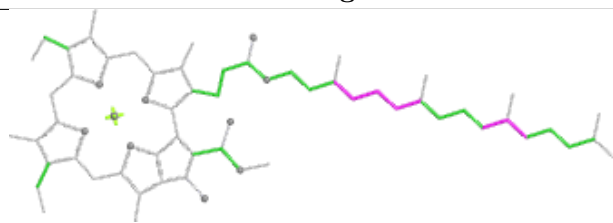
Ligand CLA B 803



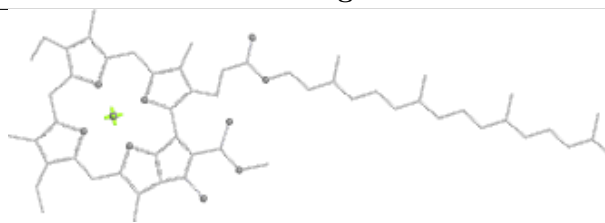
Bond lengths



Bond angles

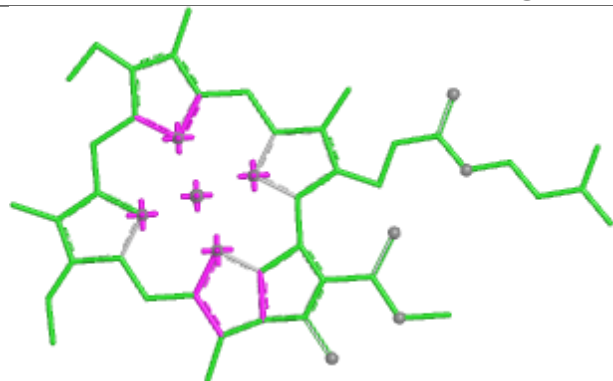


Torsions

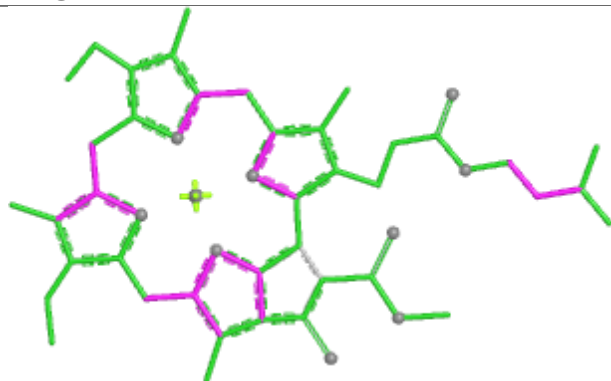


Rings

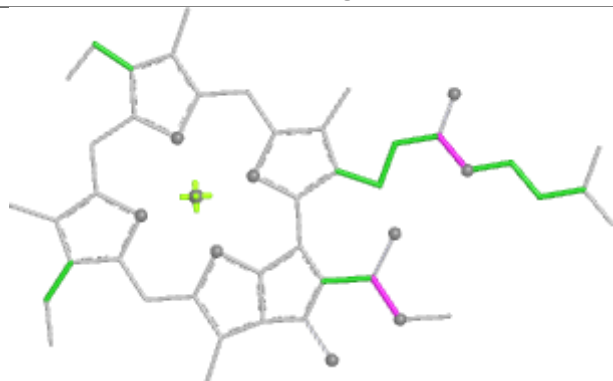
Ligand CLA g 304



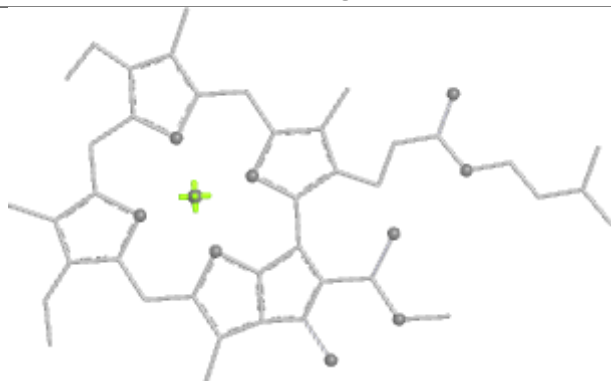
Bond lengths



Bond angles

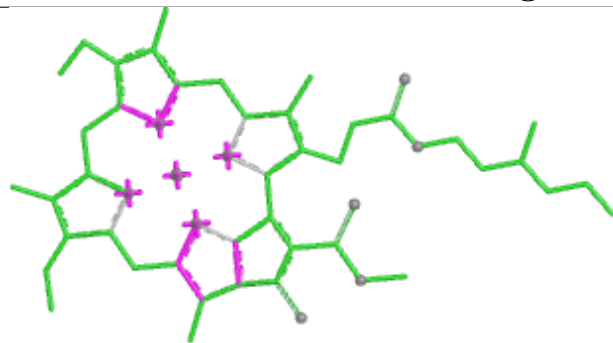


Torsions

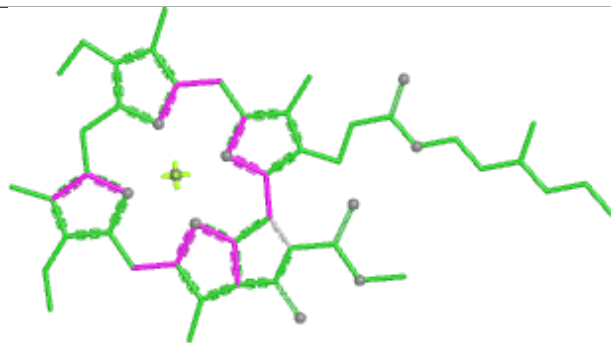


Rings

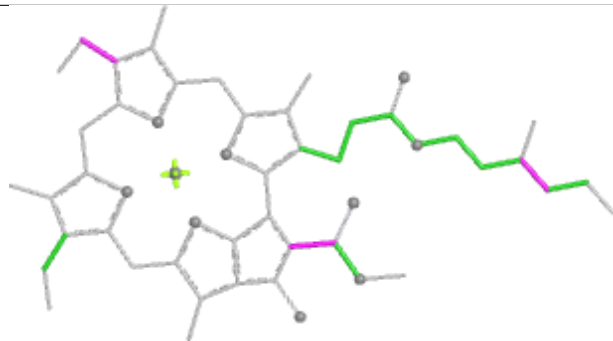
Ligand CLA c 304



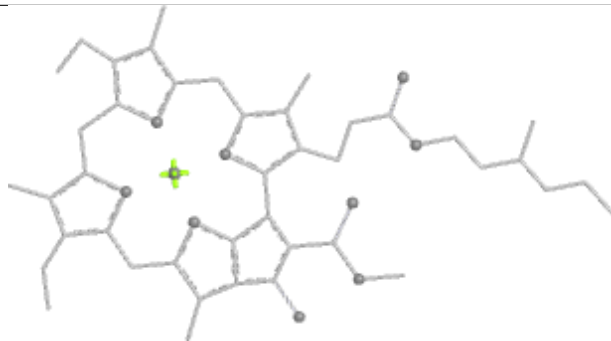
Bond lengths



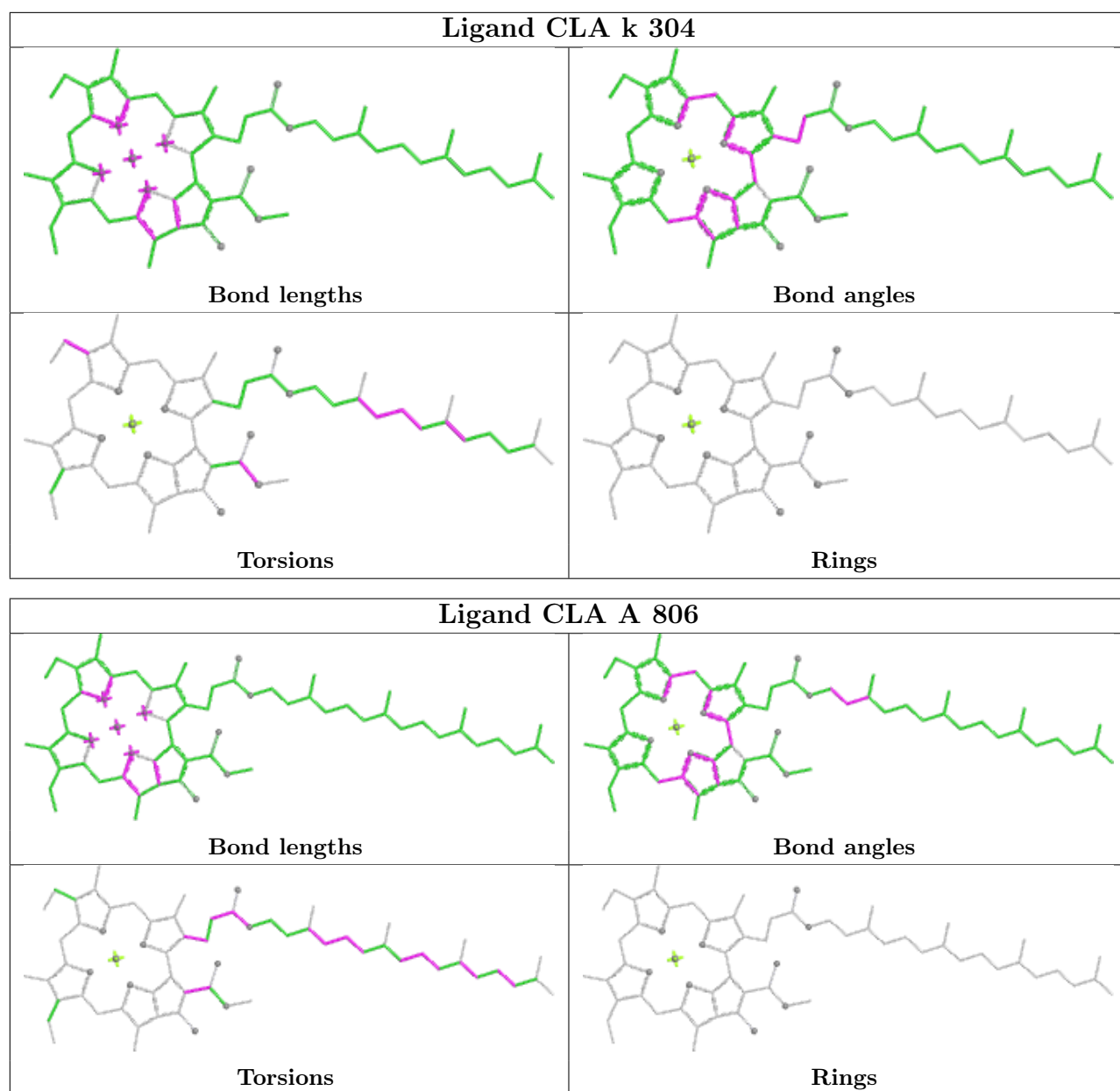
Bond angles

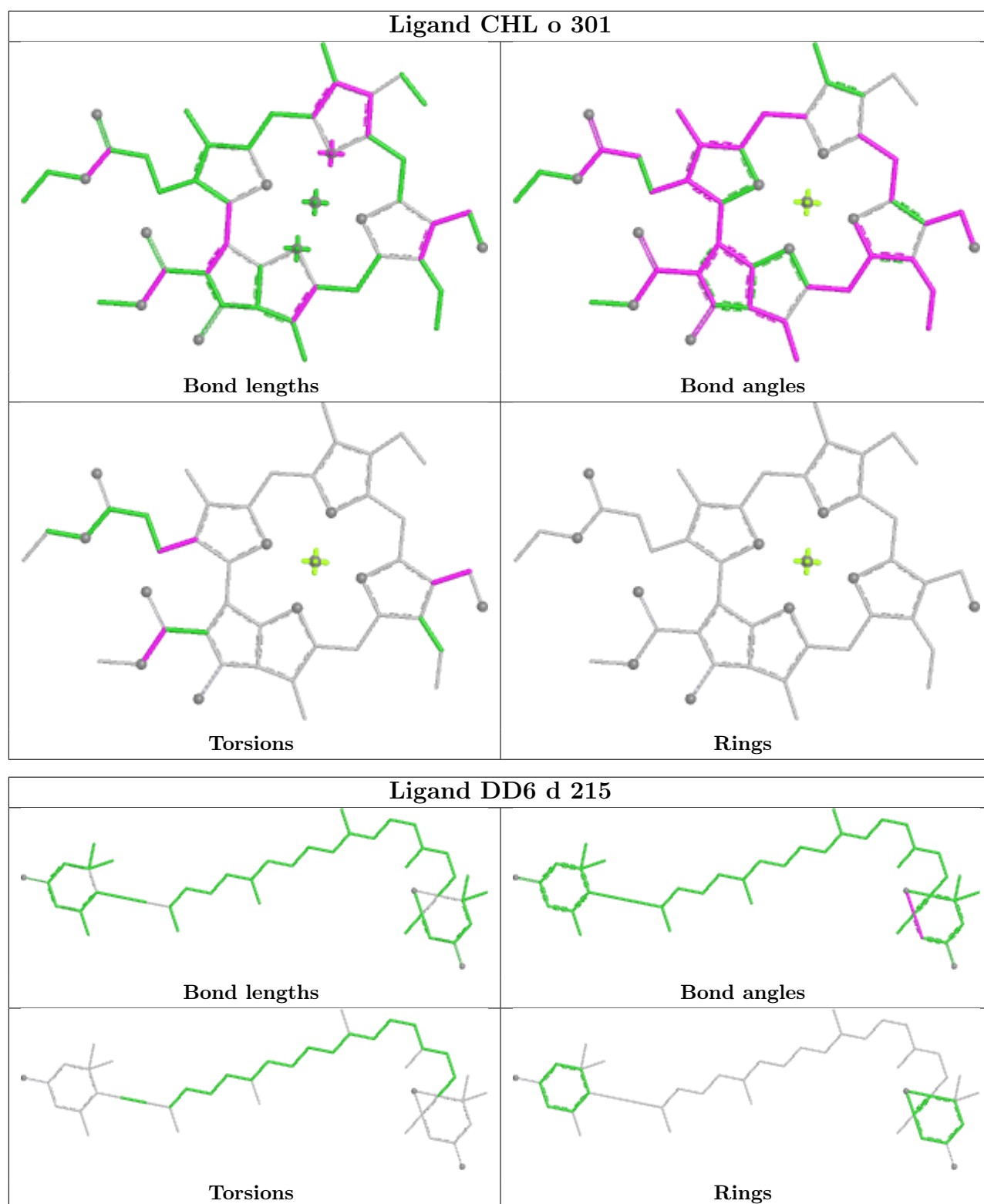


Torsions

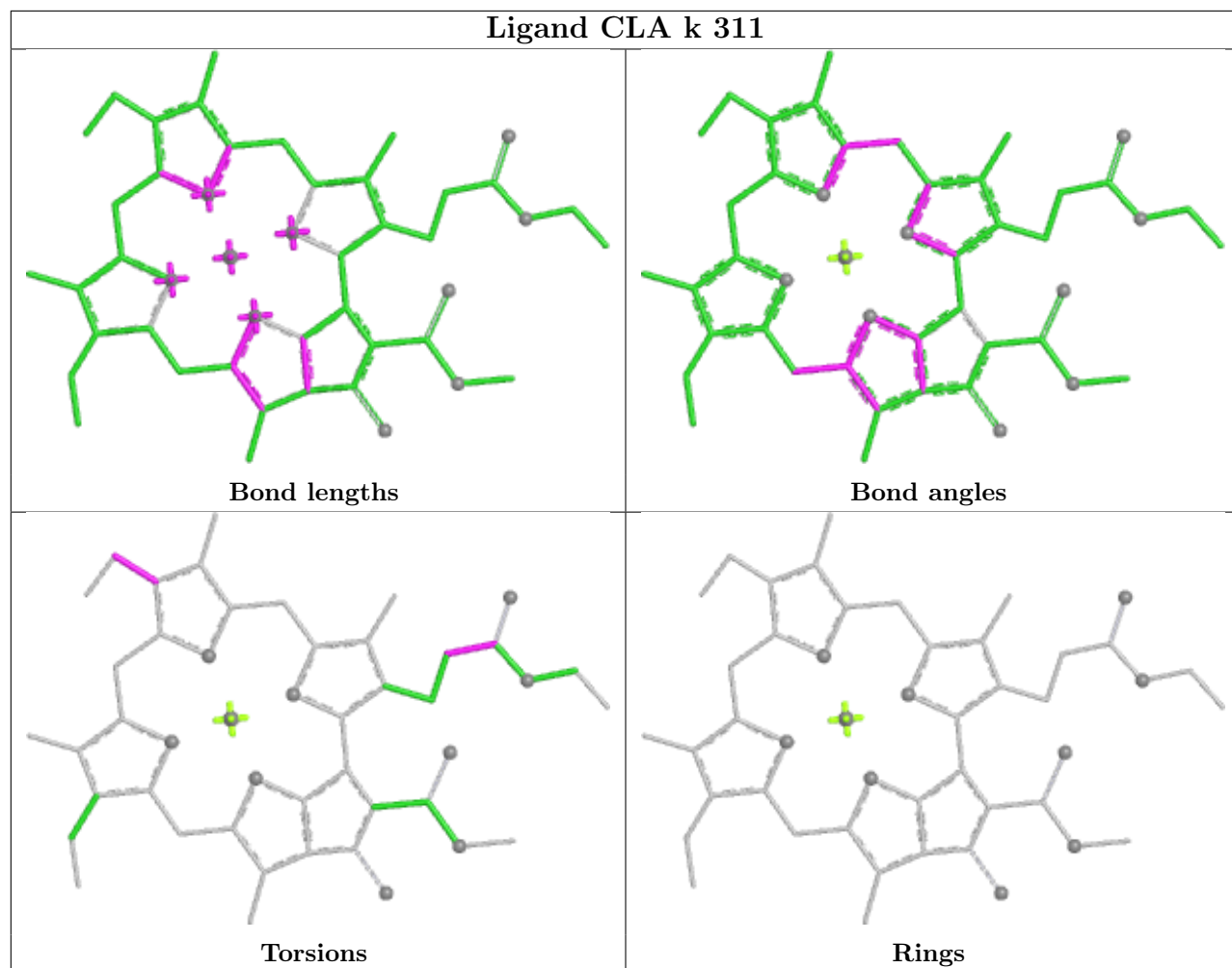


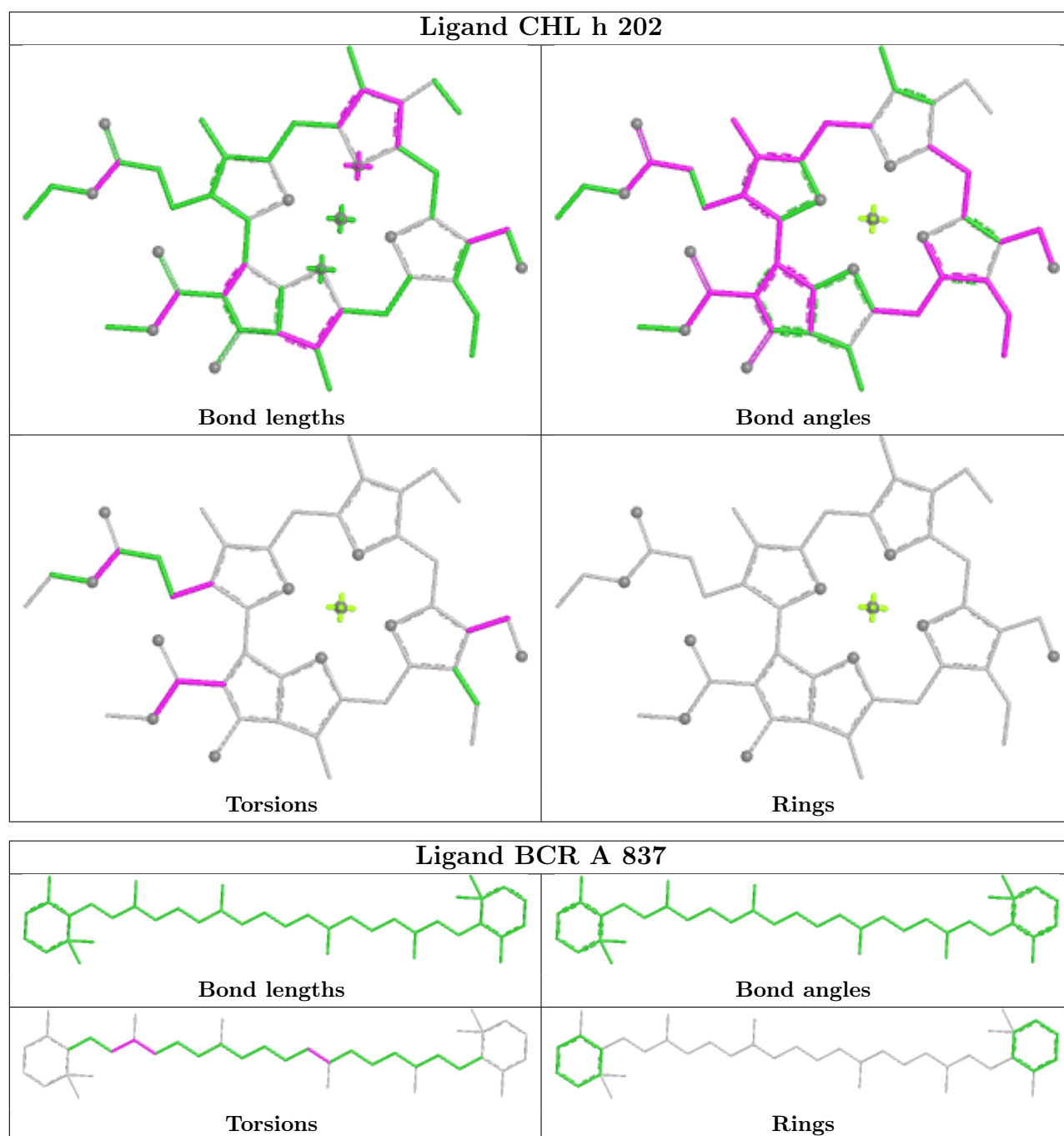
Rings

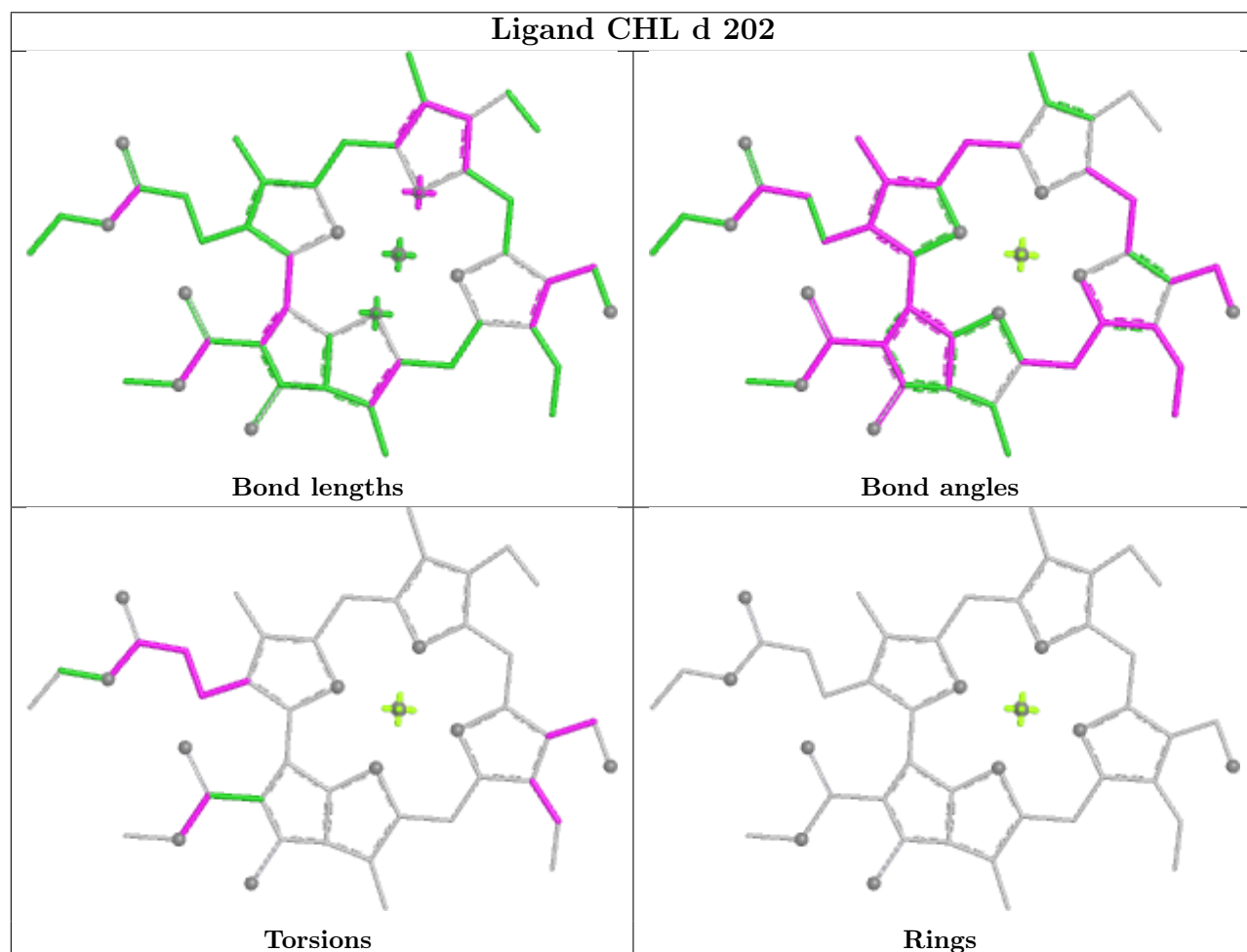
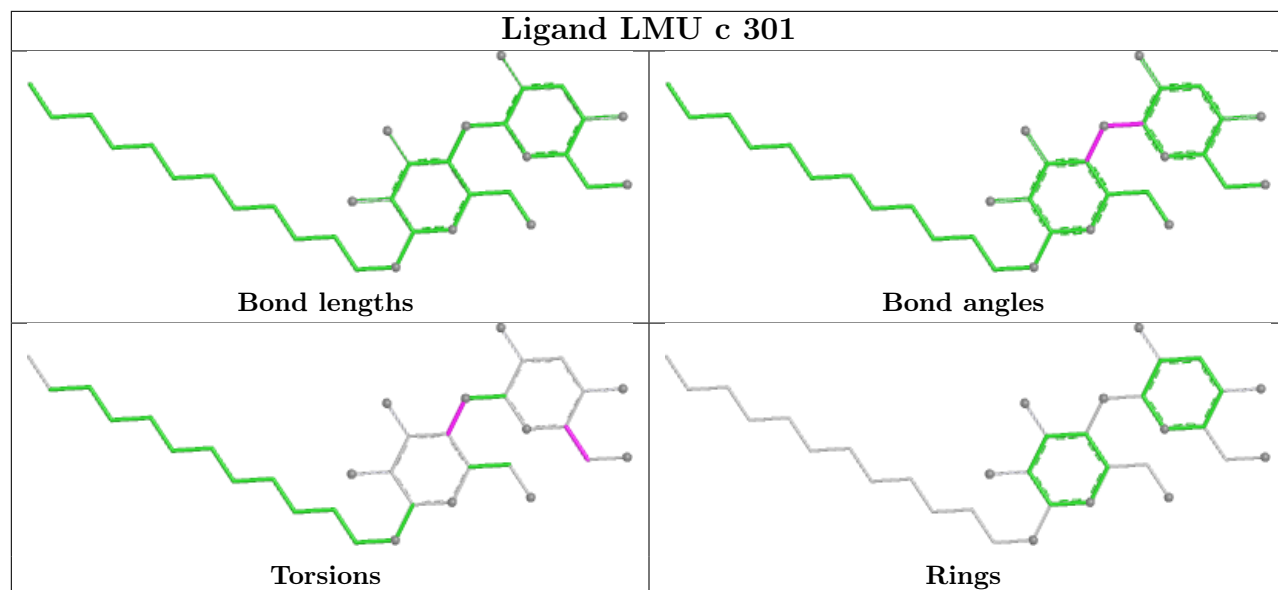




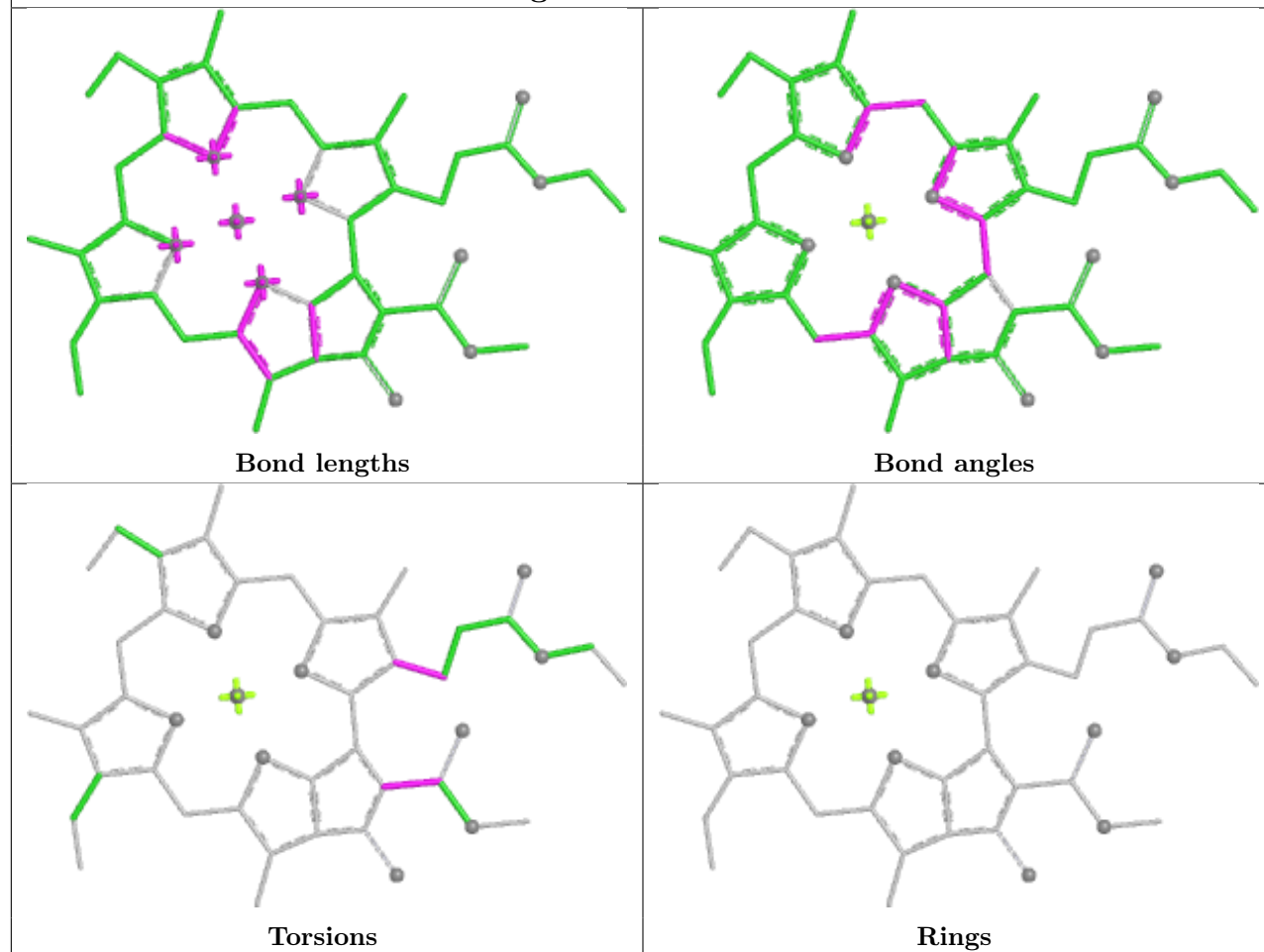
Ligand CLA k 311



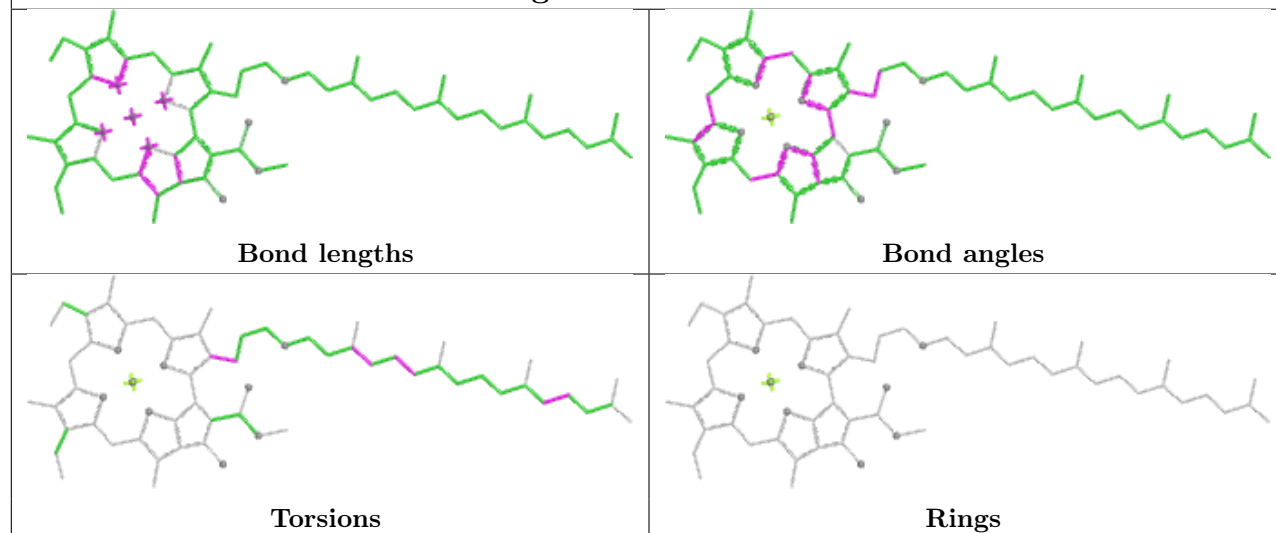


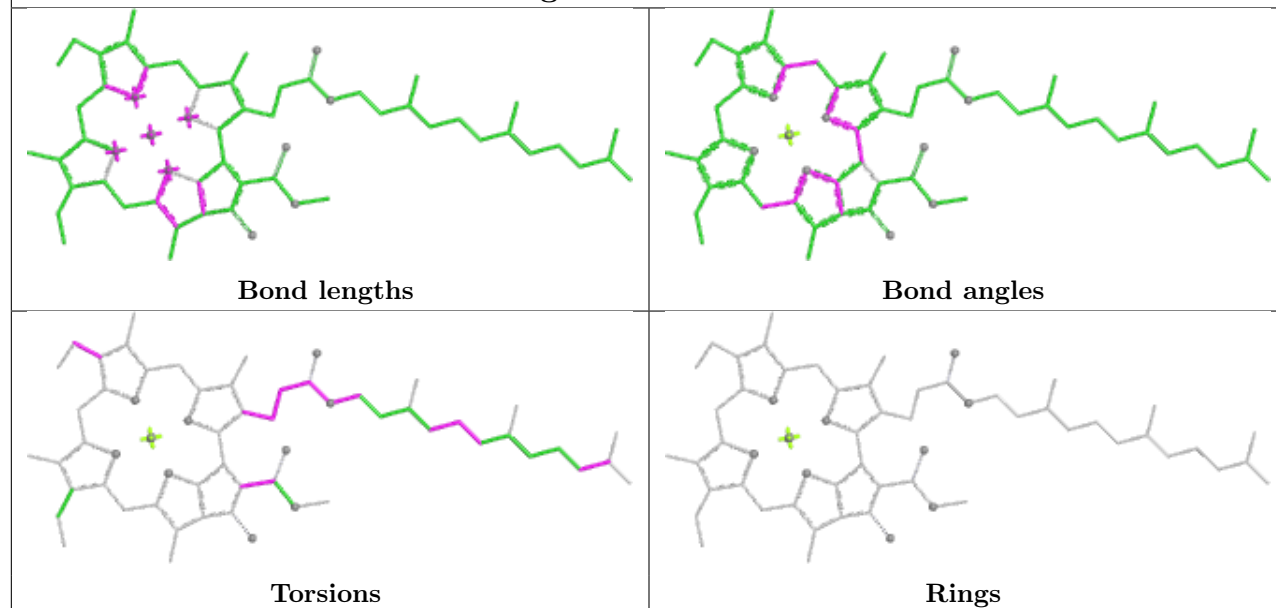
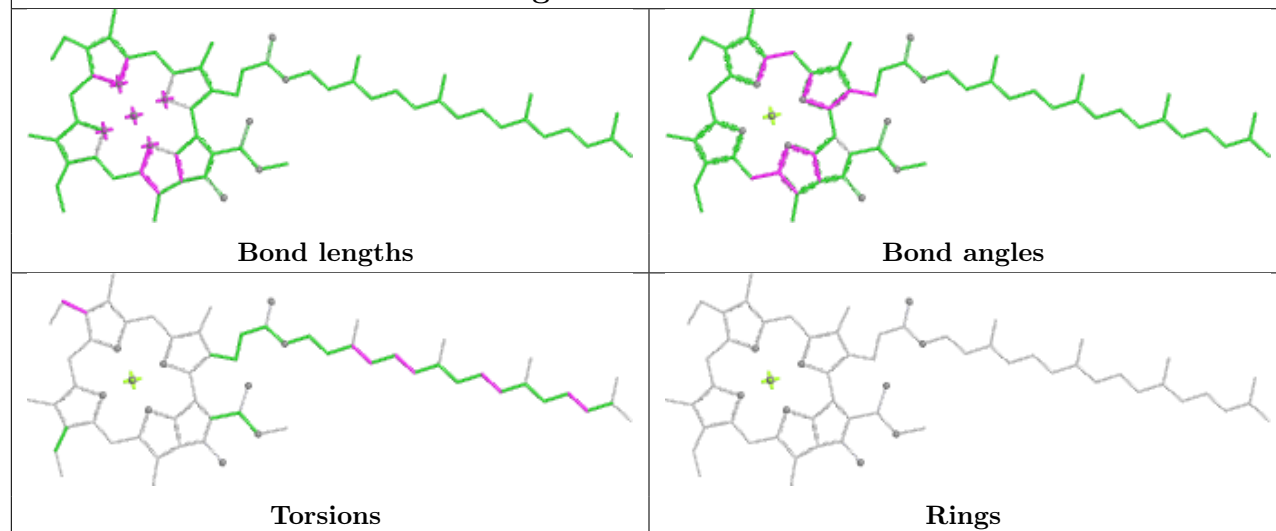


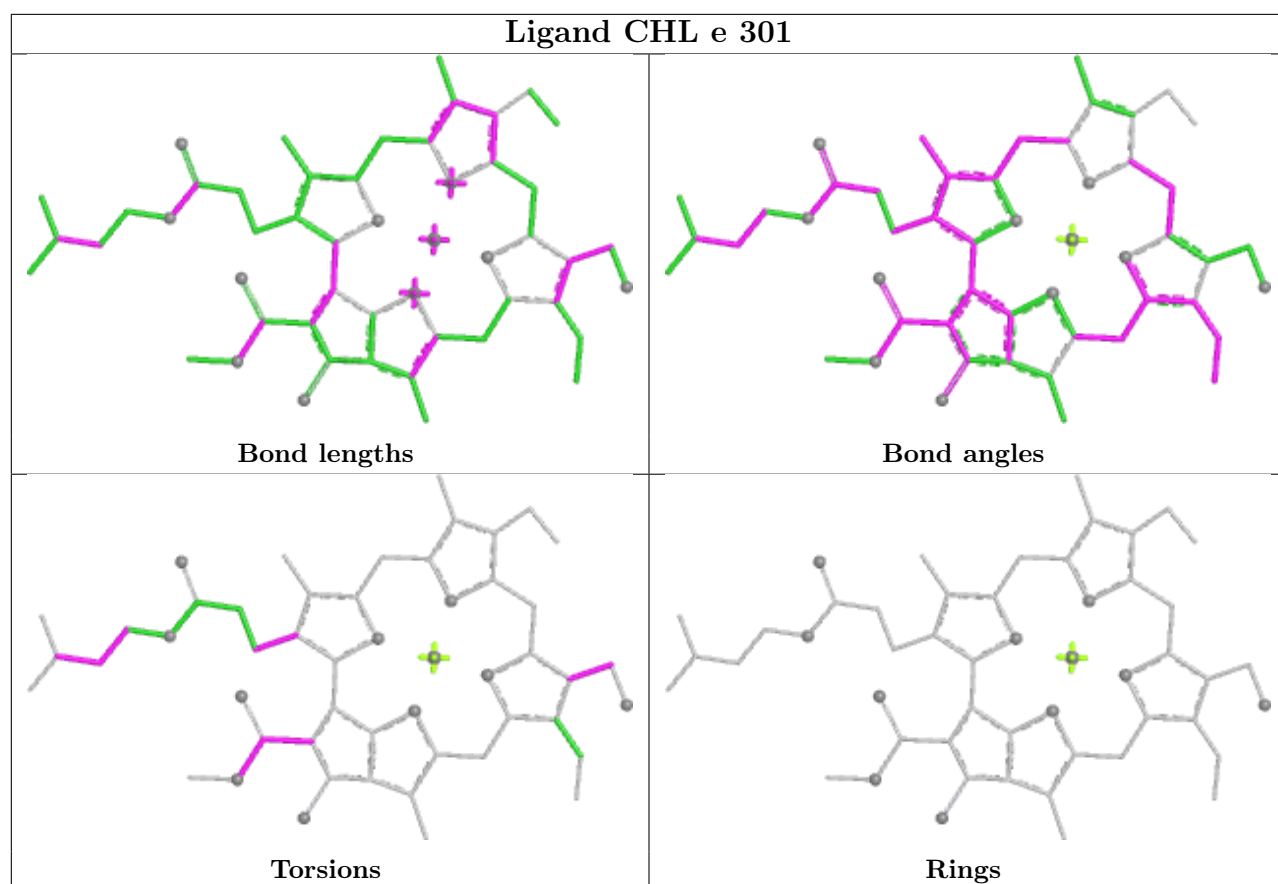
Ligand CLA h 207

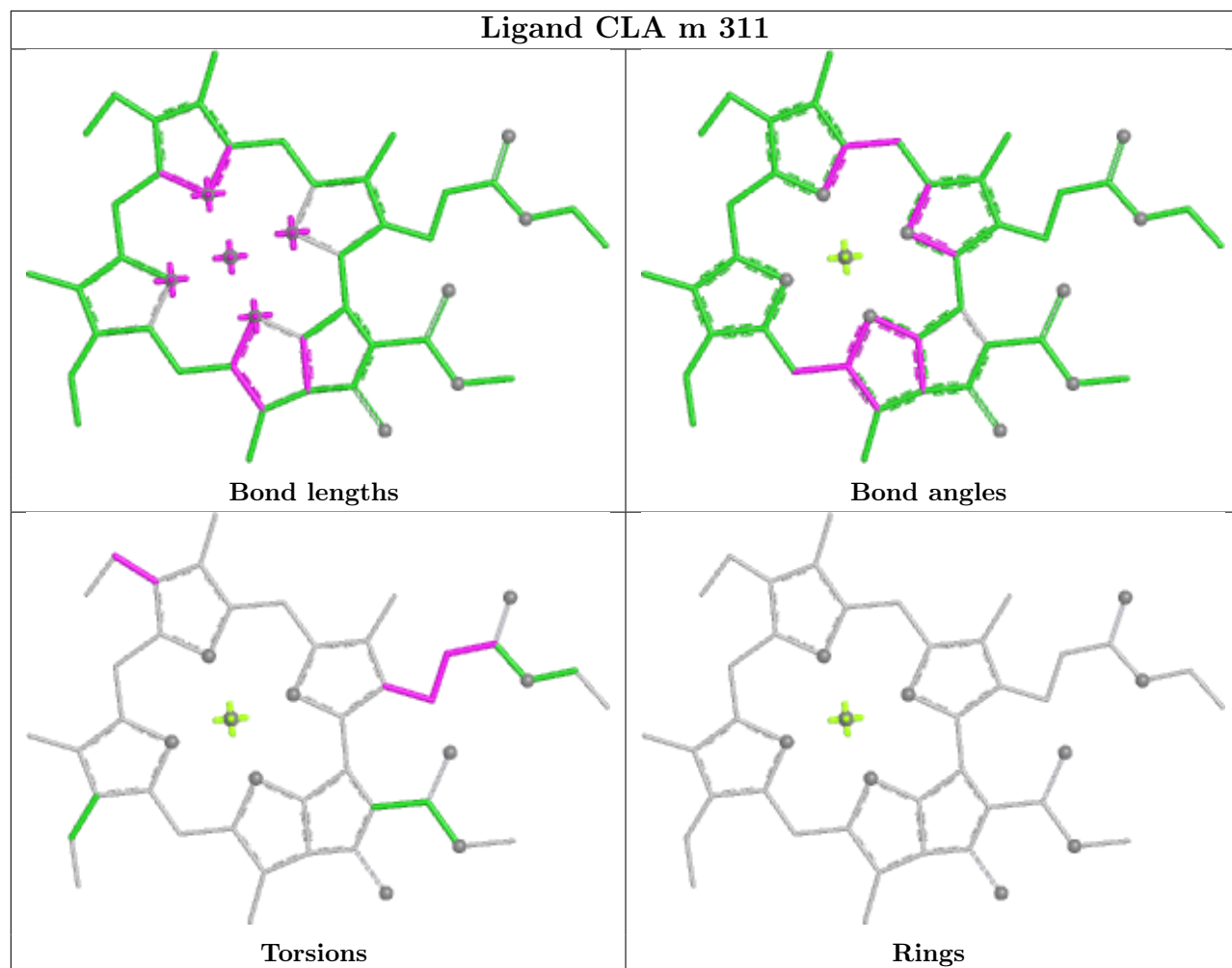


Ligand CLA A 819

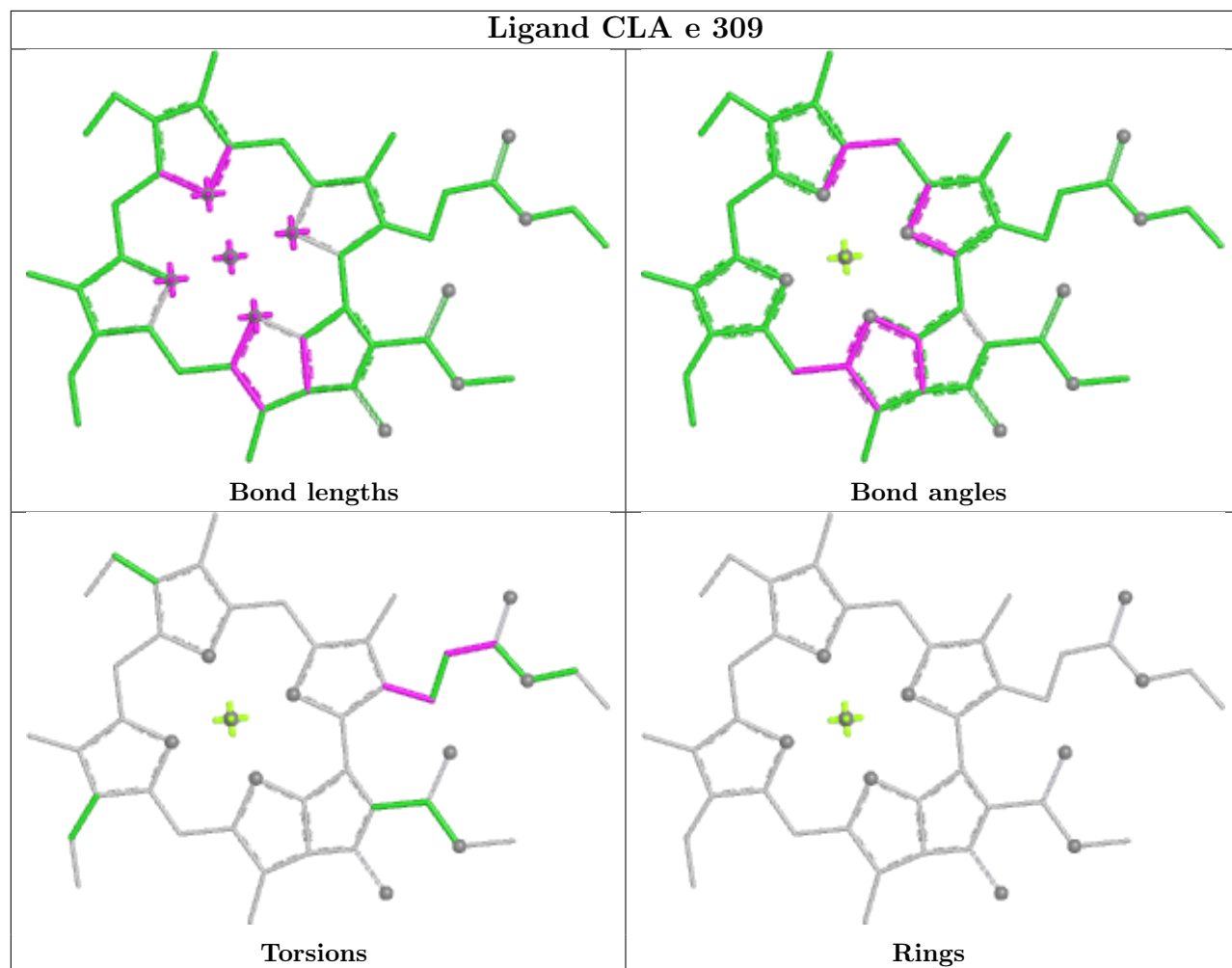


Ligand CLA i 309**Ligand CLA B 847**

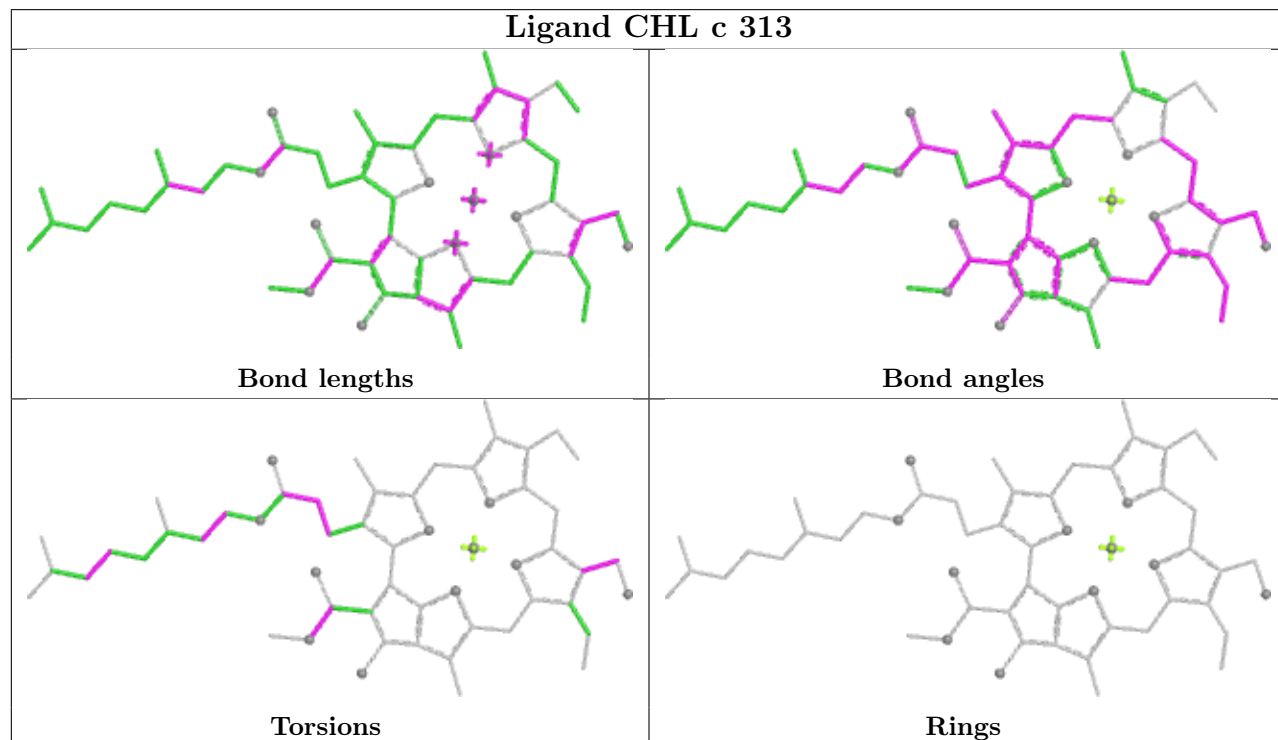




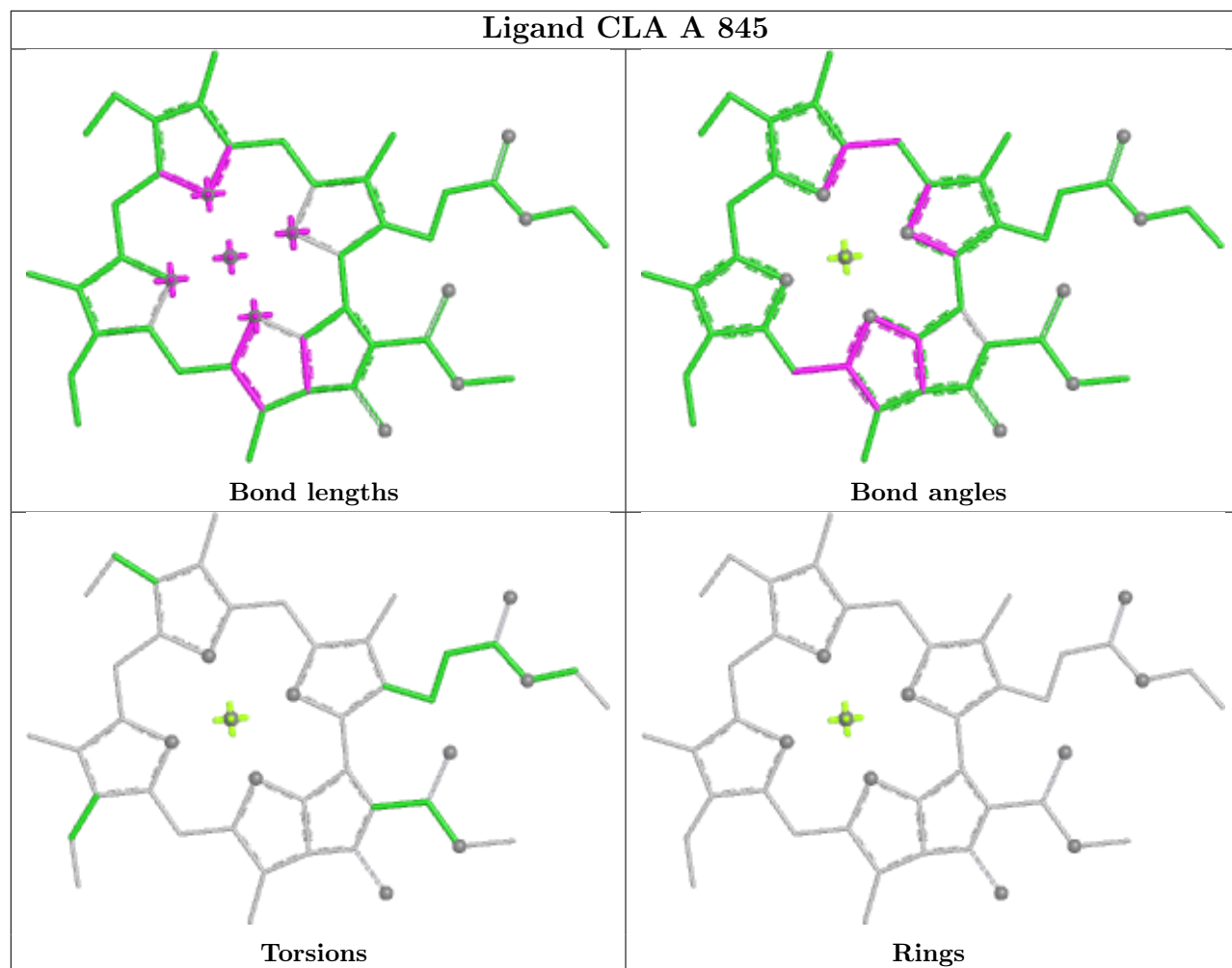
Ligand CLA e 309



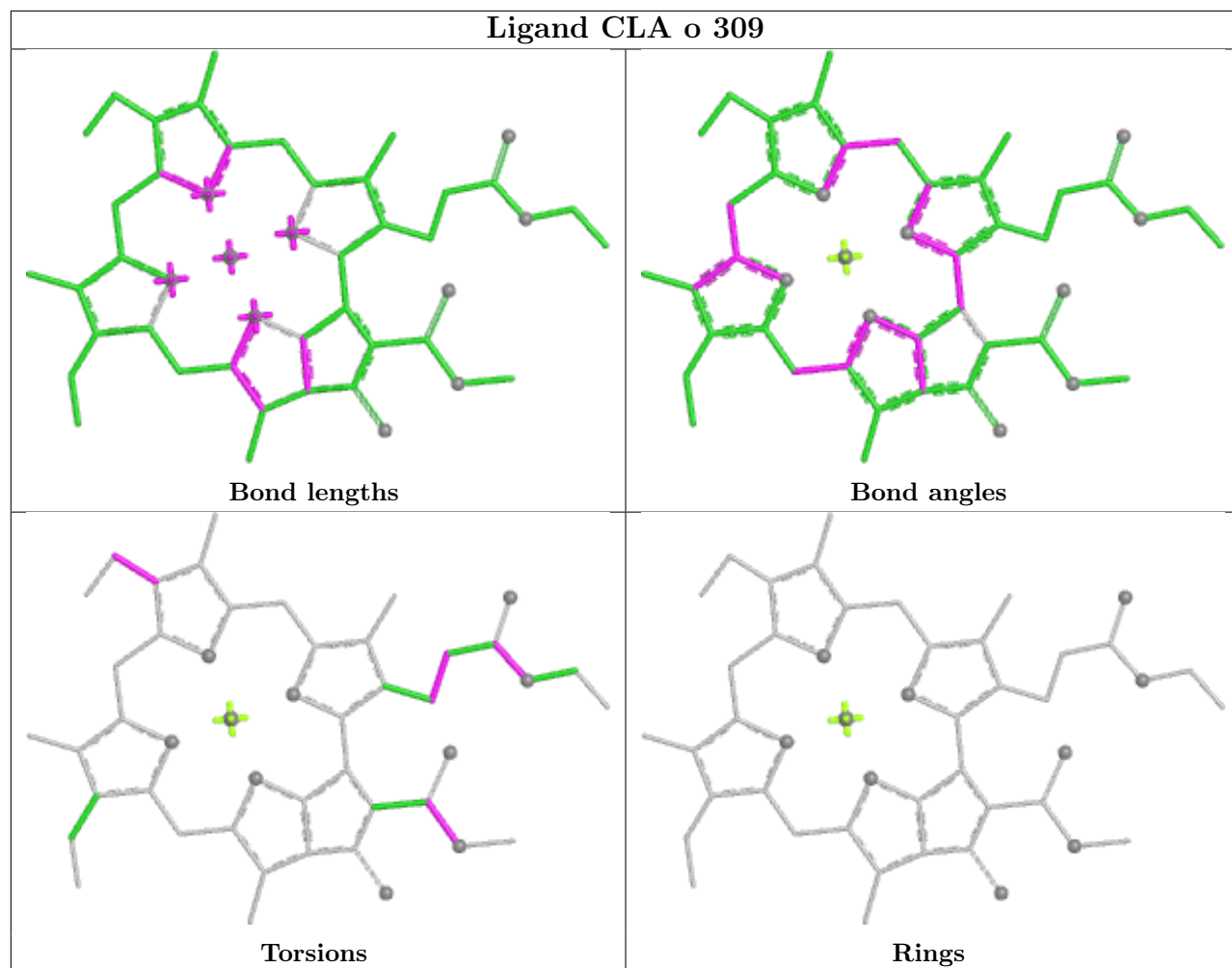
Ligand CHL c 313



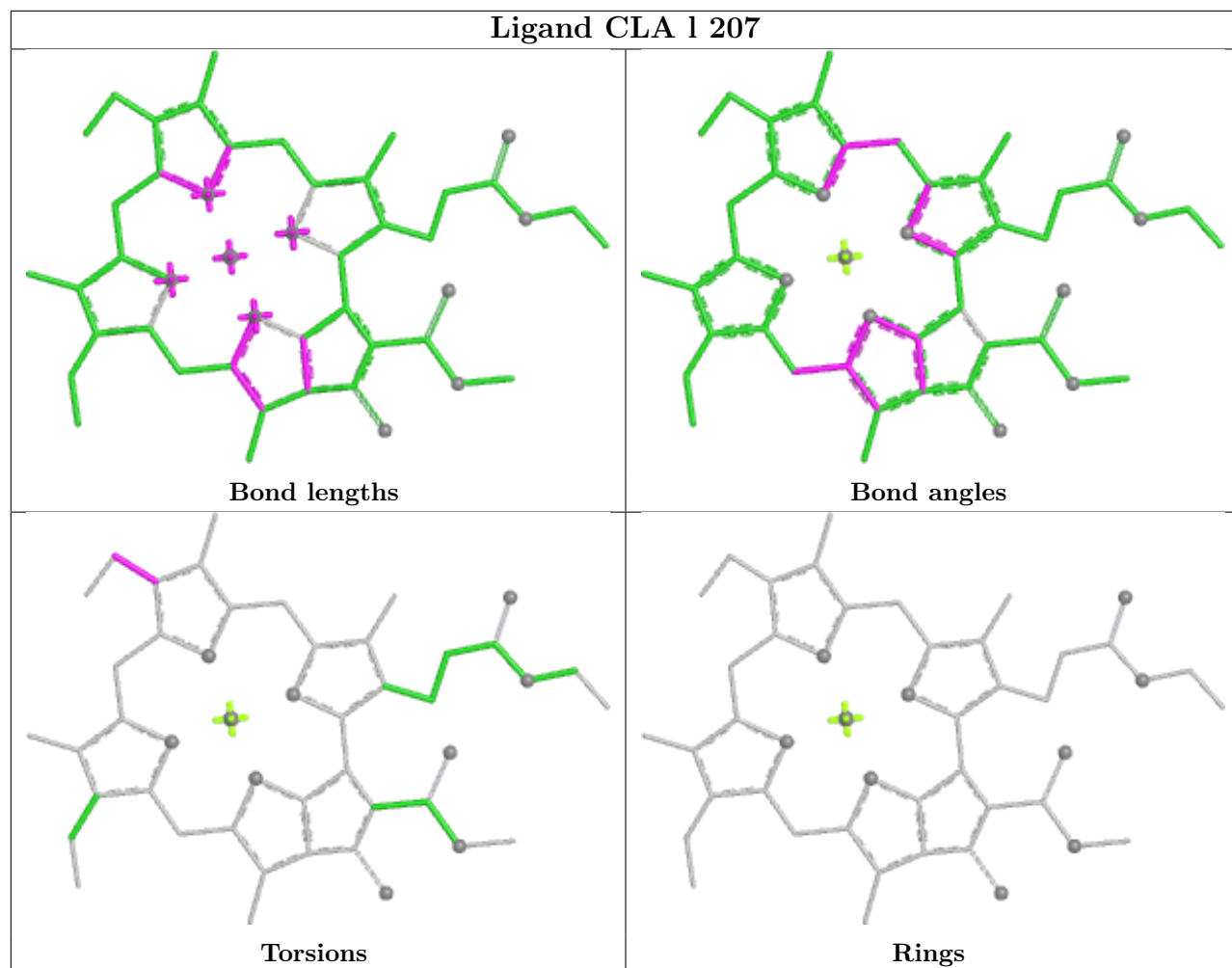
Ligand CLA A 845



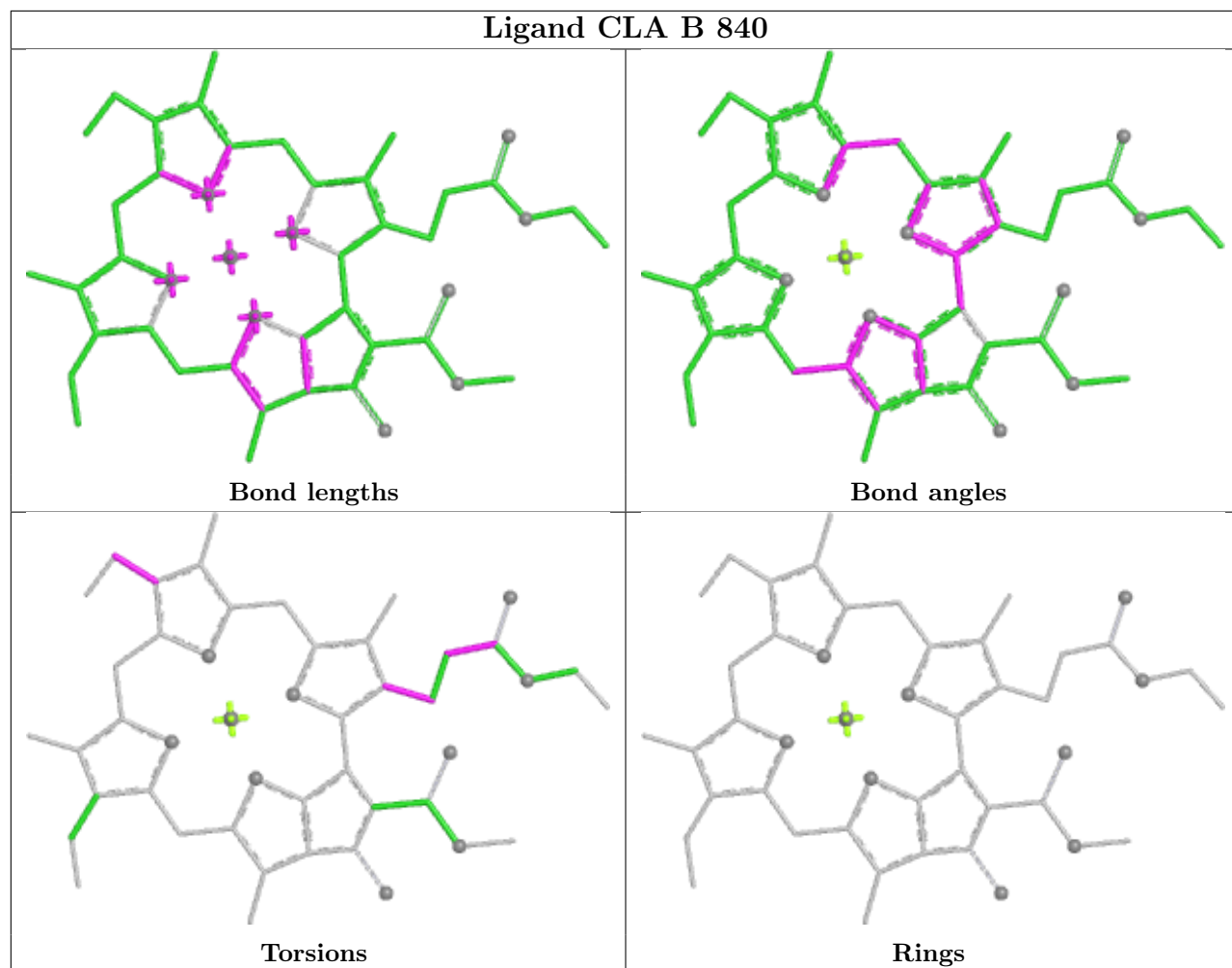
Ligand CLA o 309



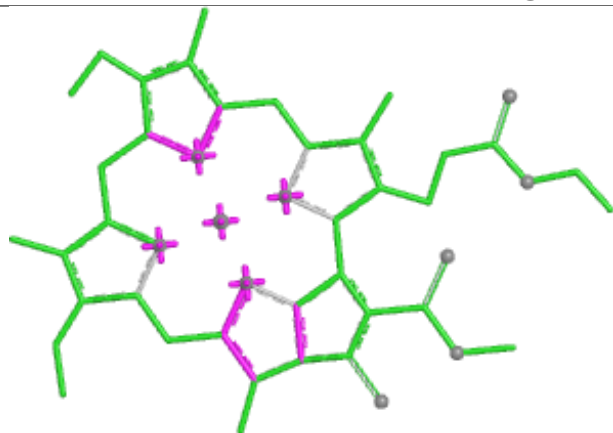
Ligand CLA 1 207



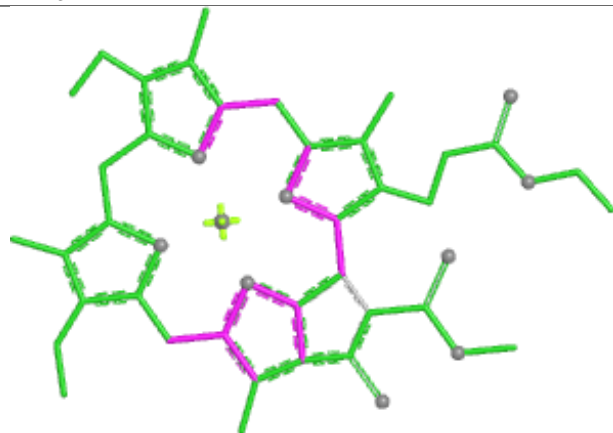
Ligand CLA B 840



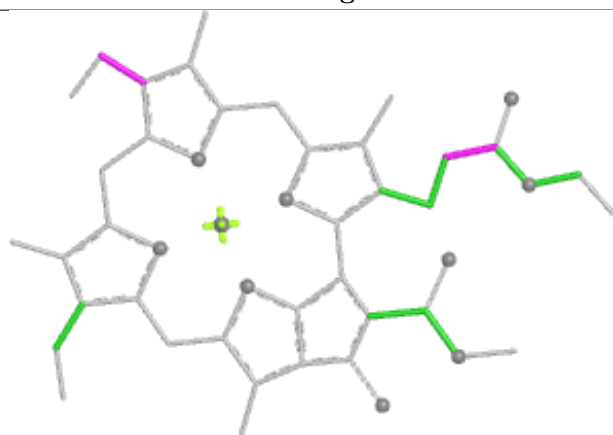
Ligand CLA j 301



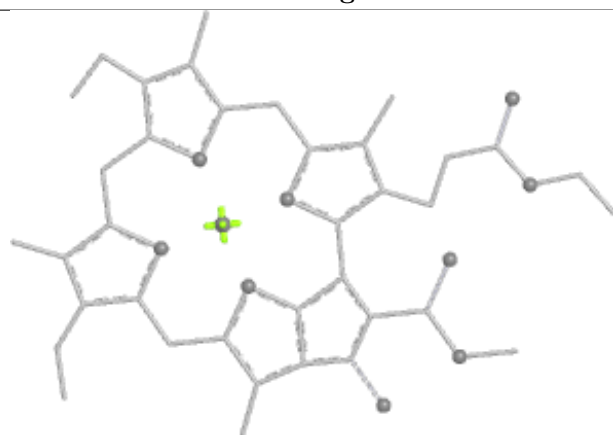
Bond lengths



Bond angles

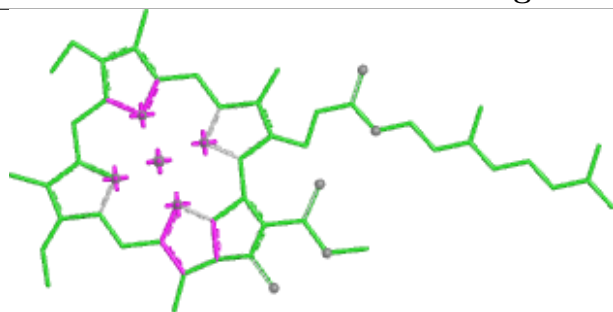


Torsions

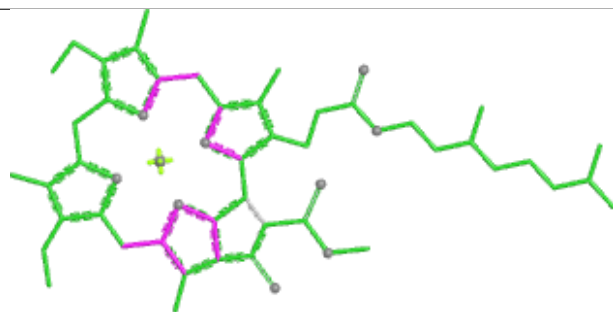


Rings

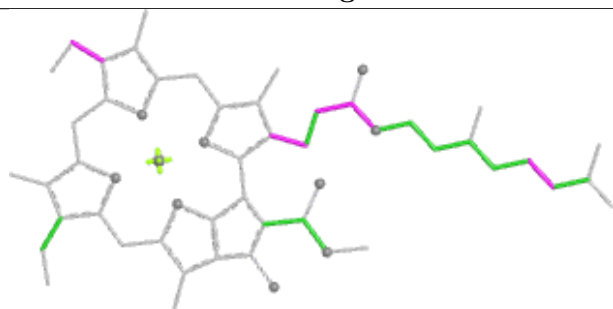
Ligand CLA A 820



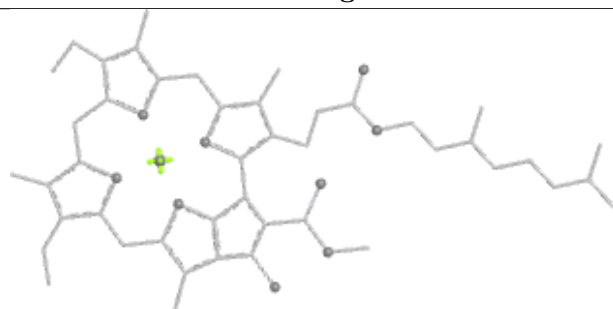
Bond lengths



Bond angles

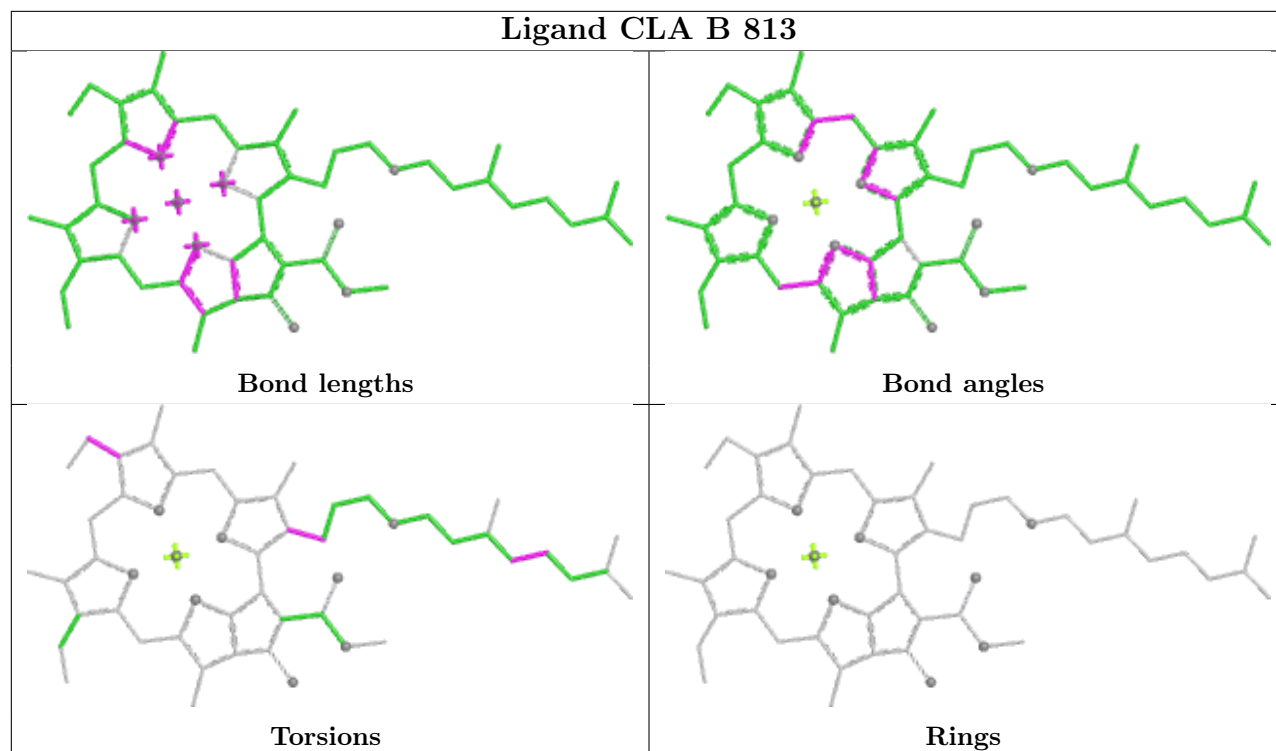


Torsions

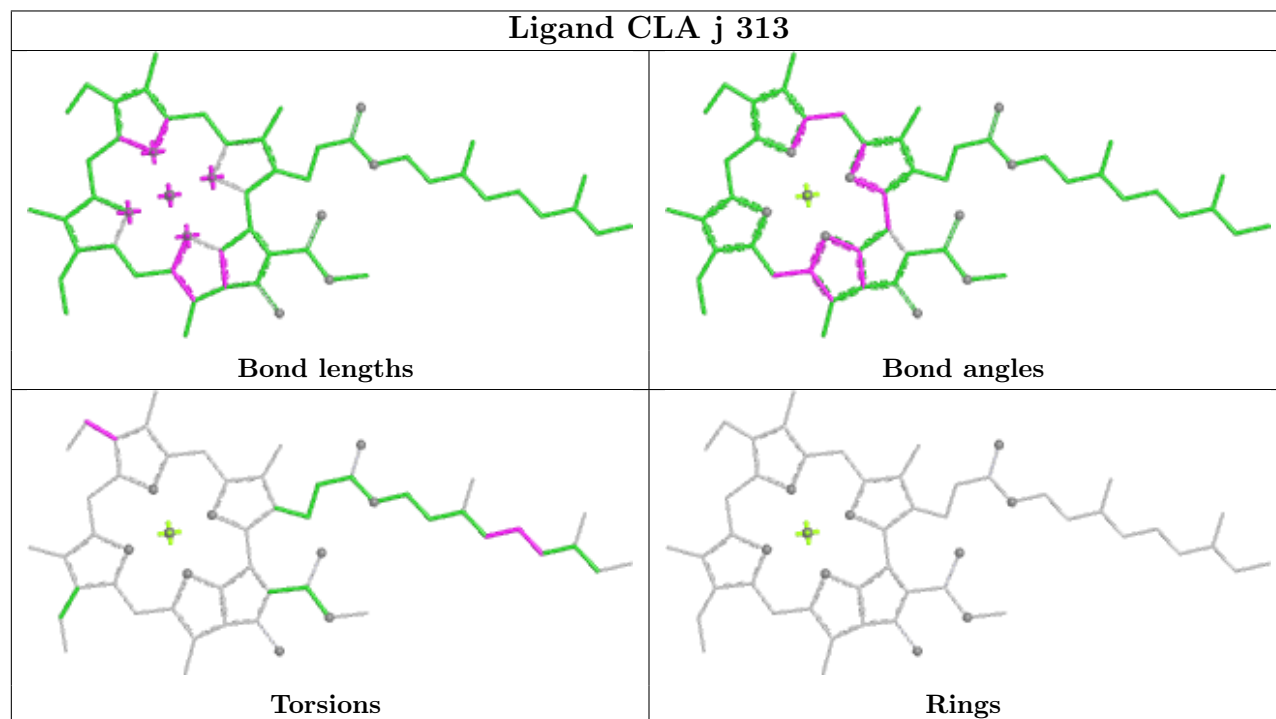


Rings

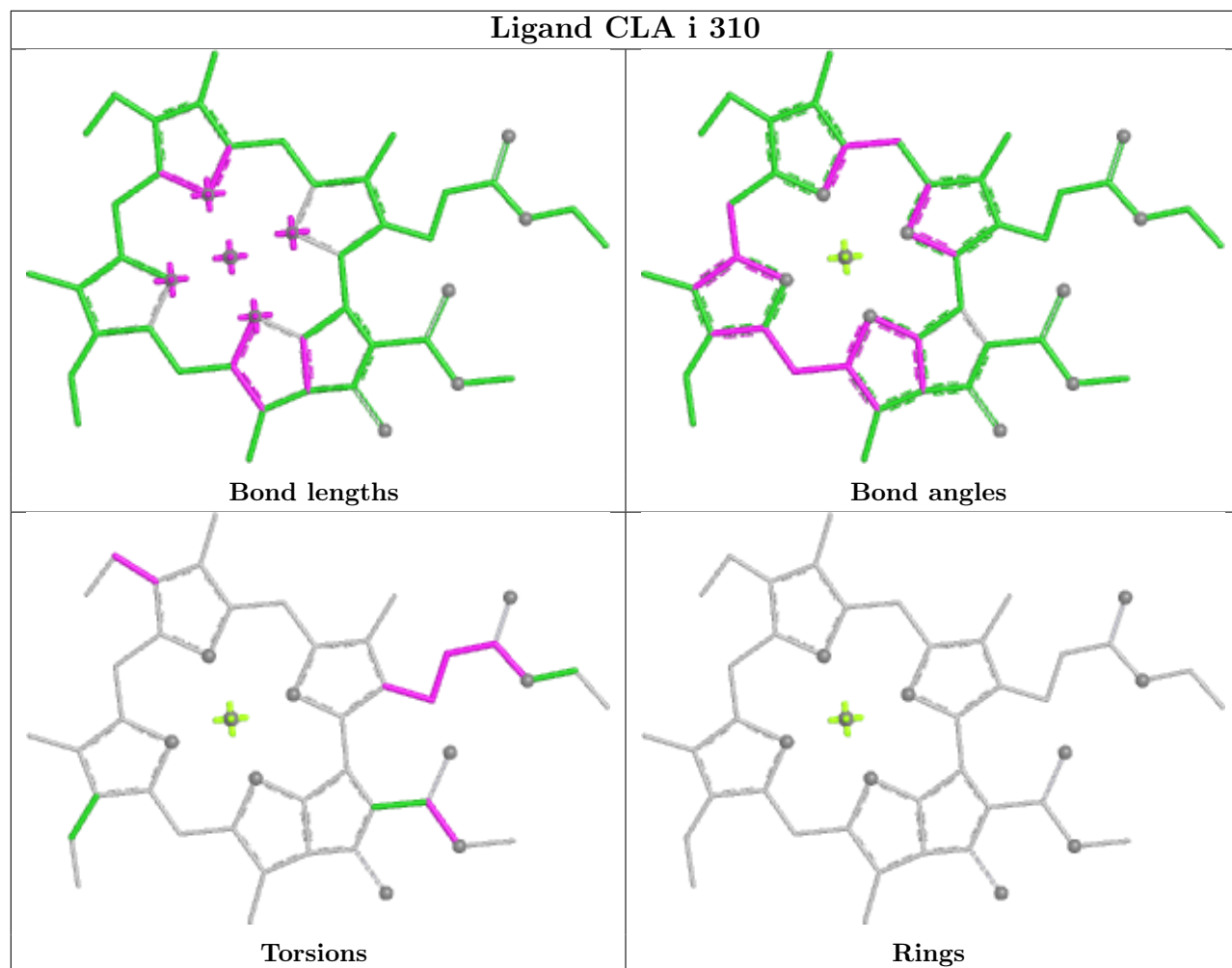
Ligand CLA B 813



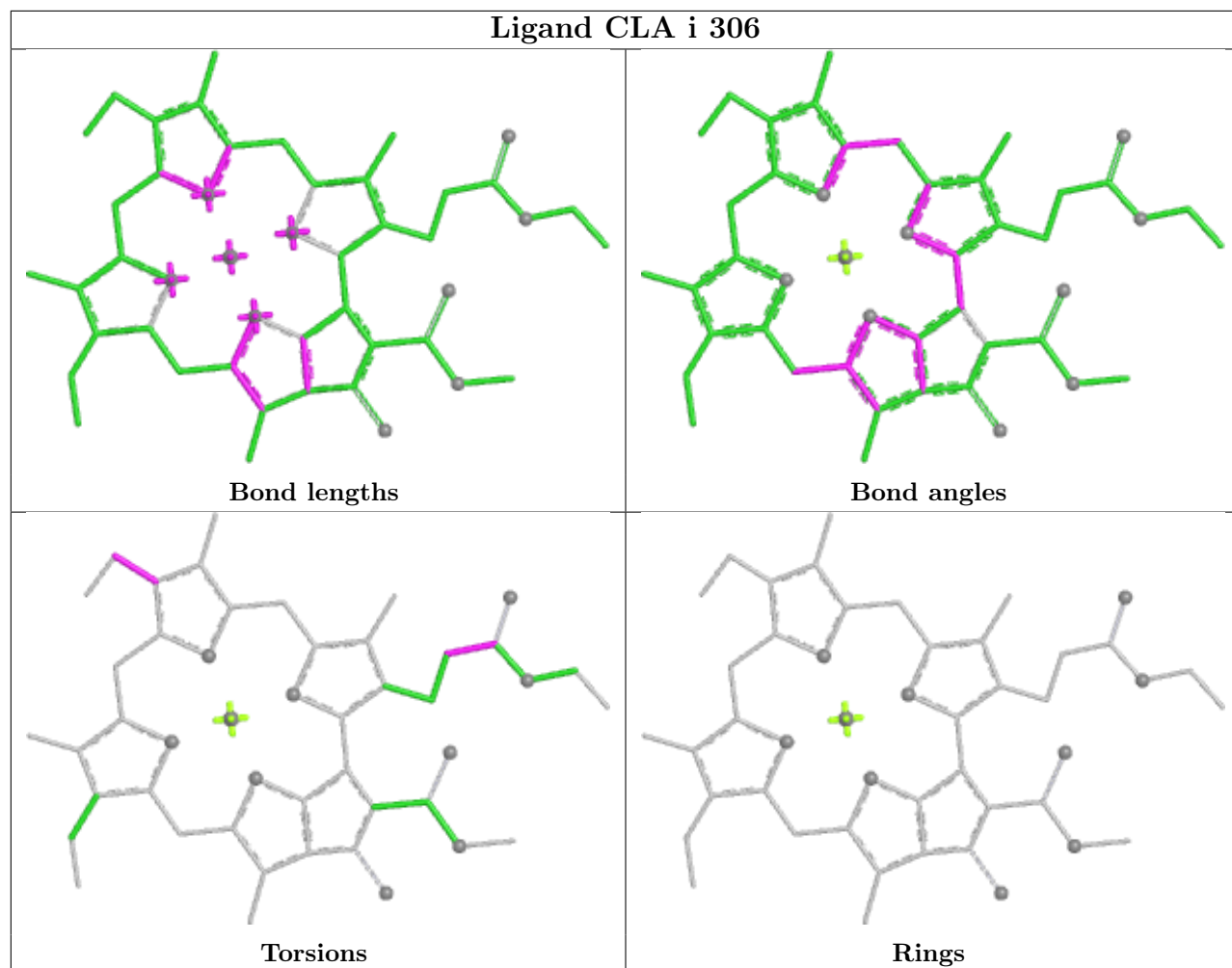
Ligand CLA j 313



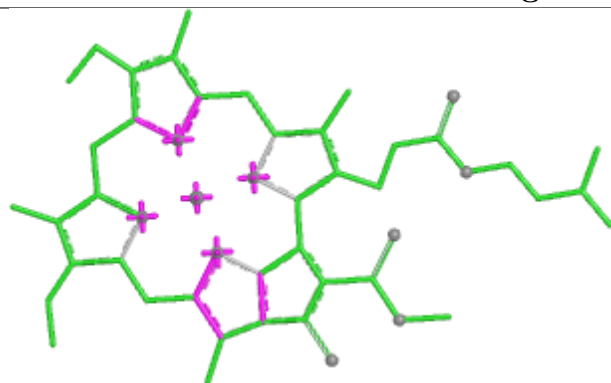
Ligand CLA i 310



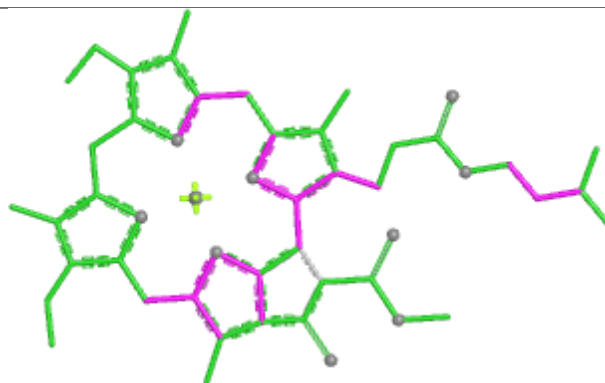
Ligand CLA i 306



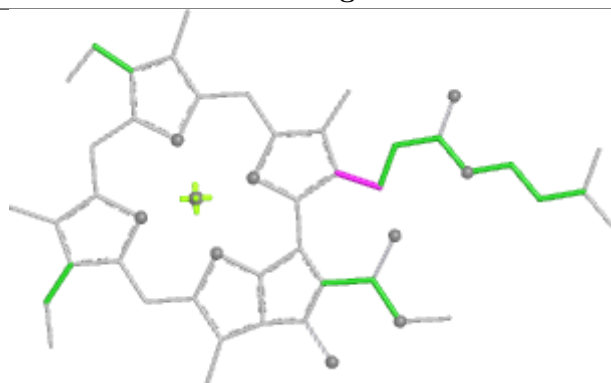
Ligand CLA f 305



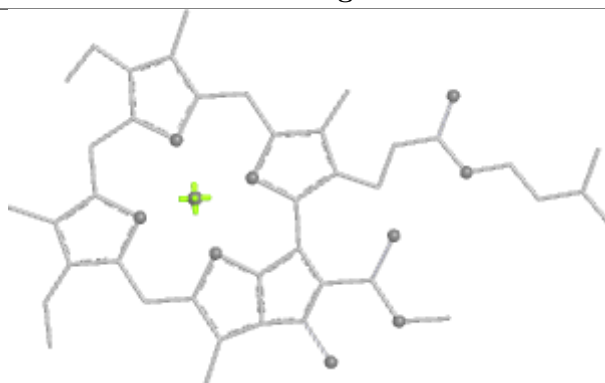
Bond lengths



Bond angles

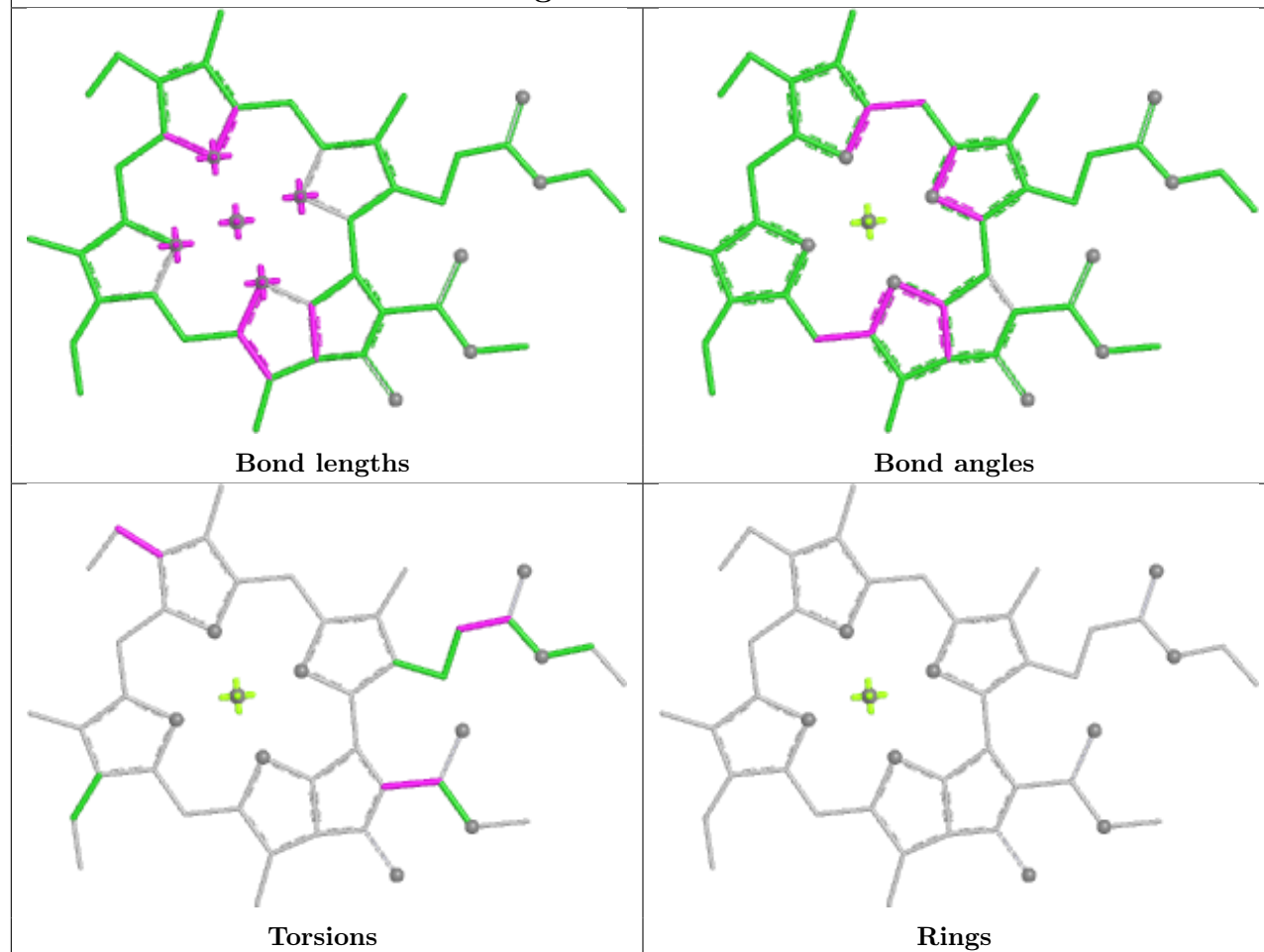


Torsions

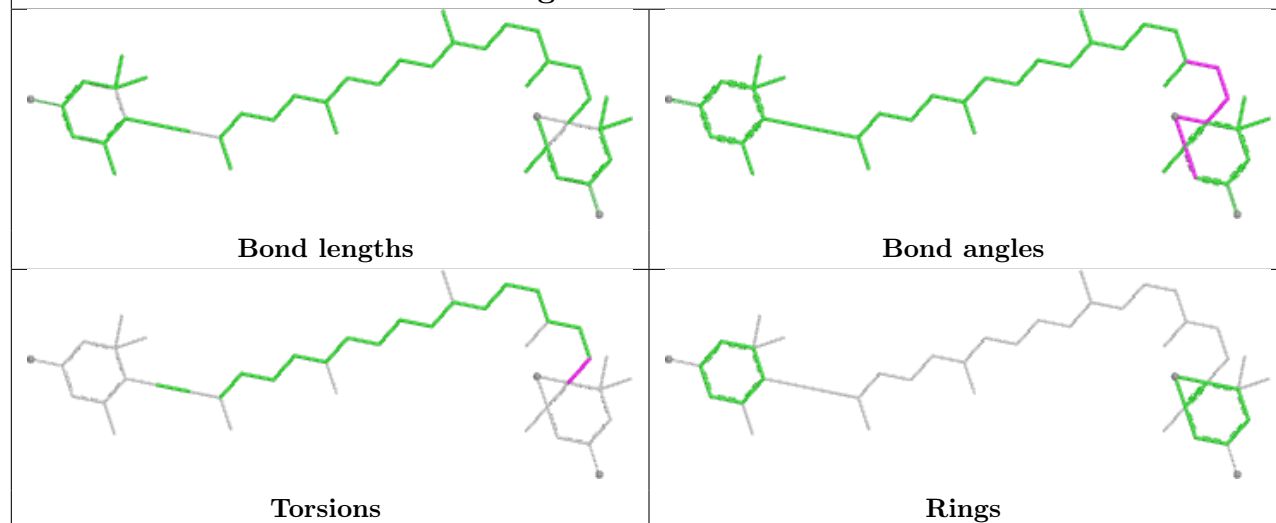


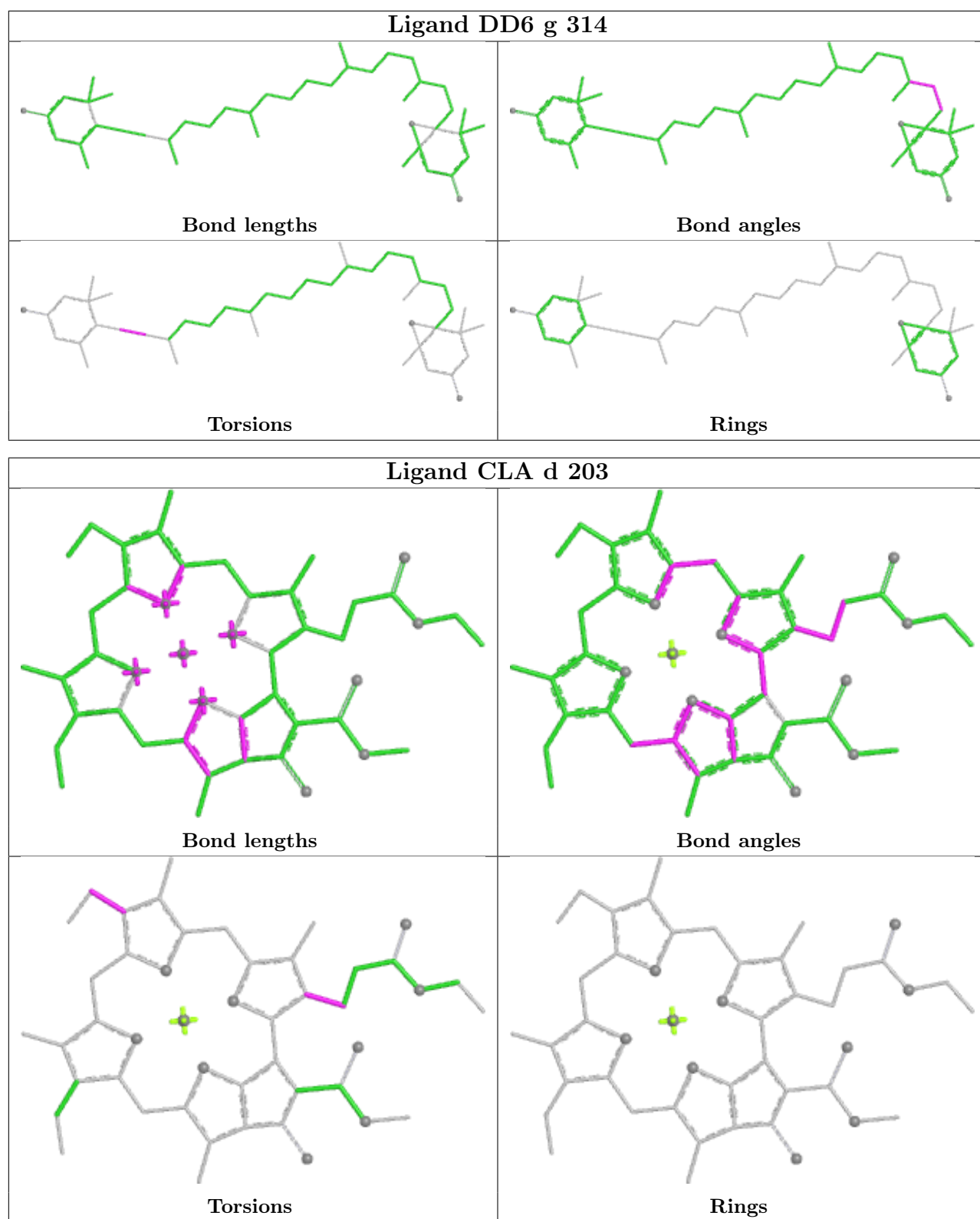
Rings

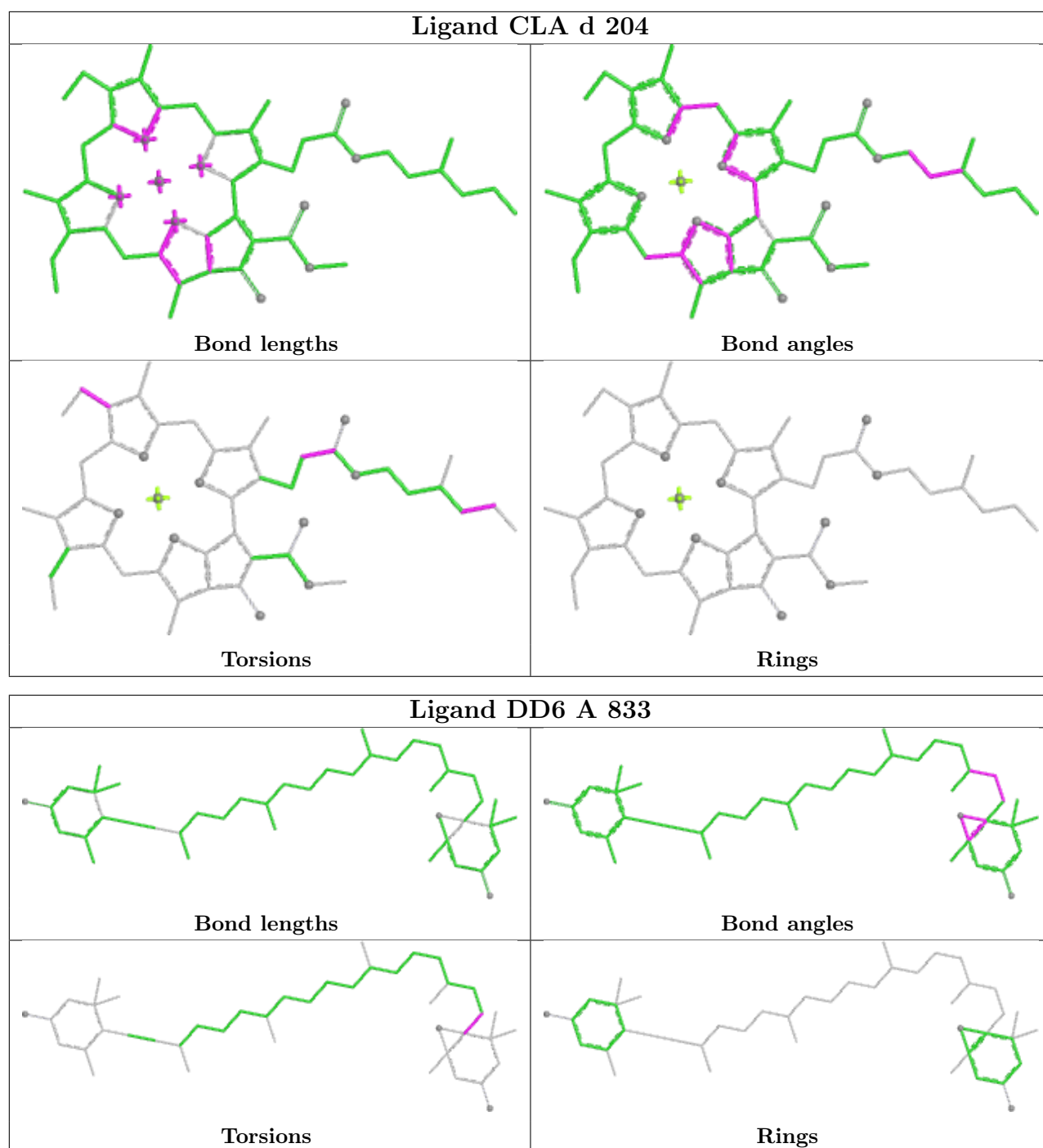
Ligand CLA f 312



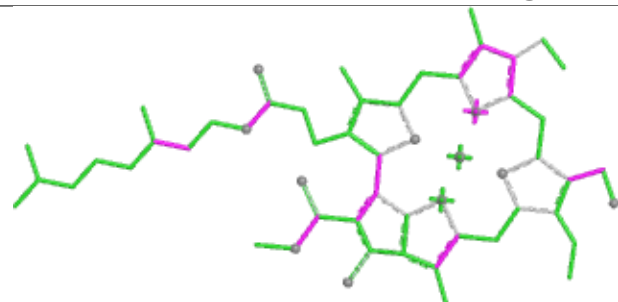
Ligand DD6 e 313



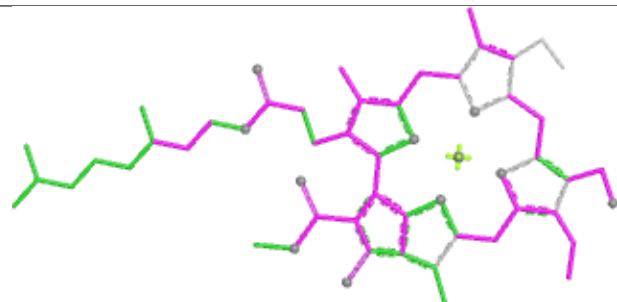




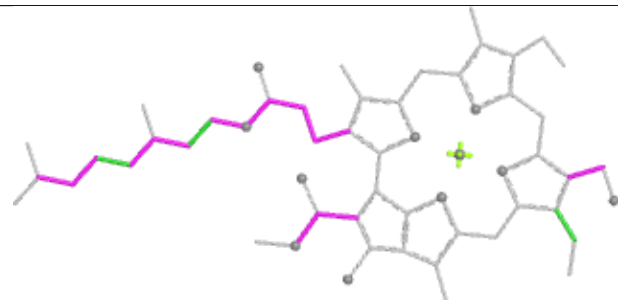
Ligand CHL d 205



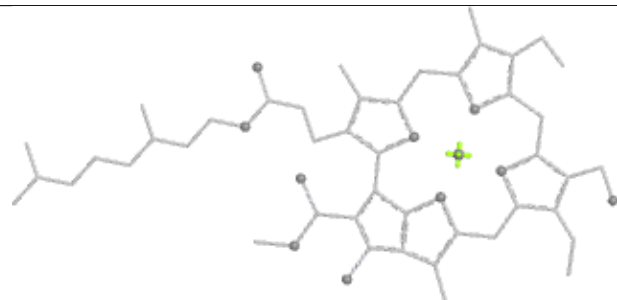
Bond lengths



Bond angles

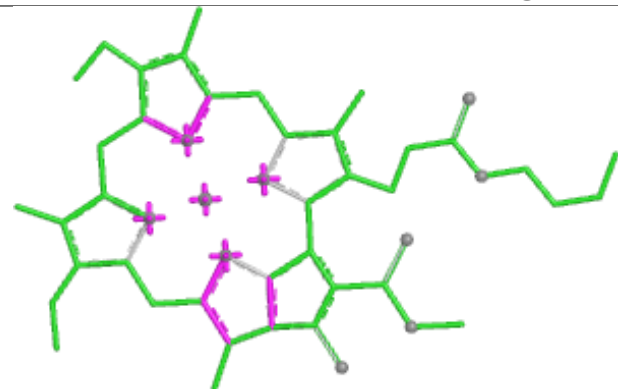


Torsions

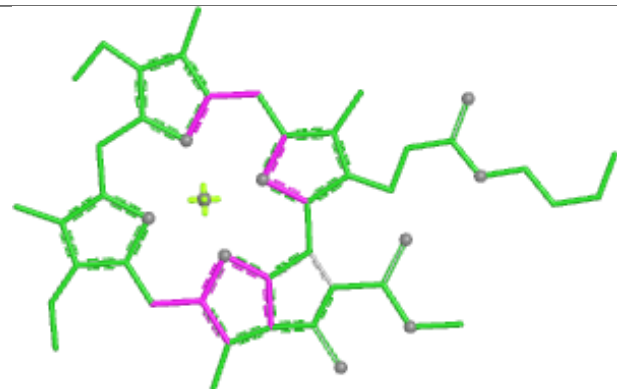


Rings

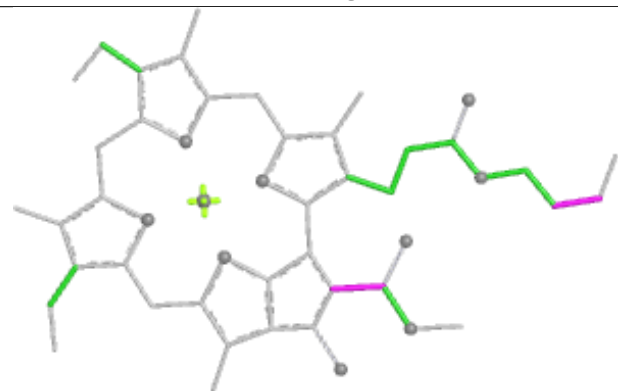
Ligand CLA B 816



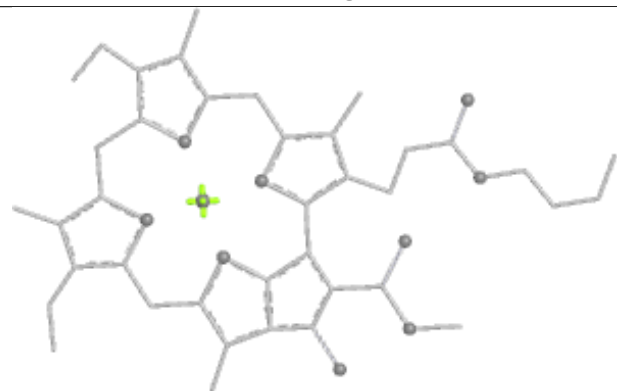
Bond lengths



Bond angles

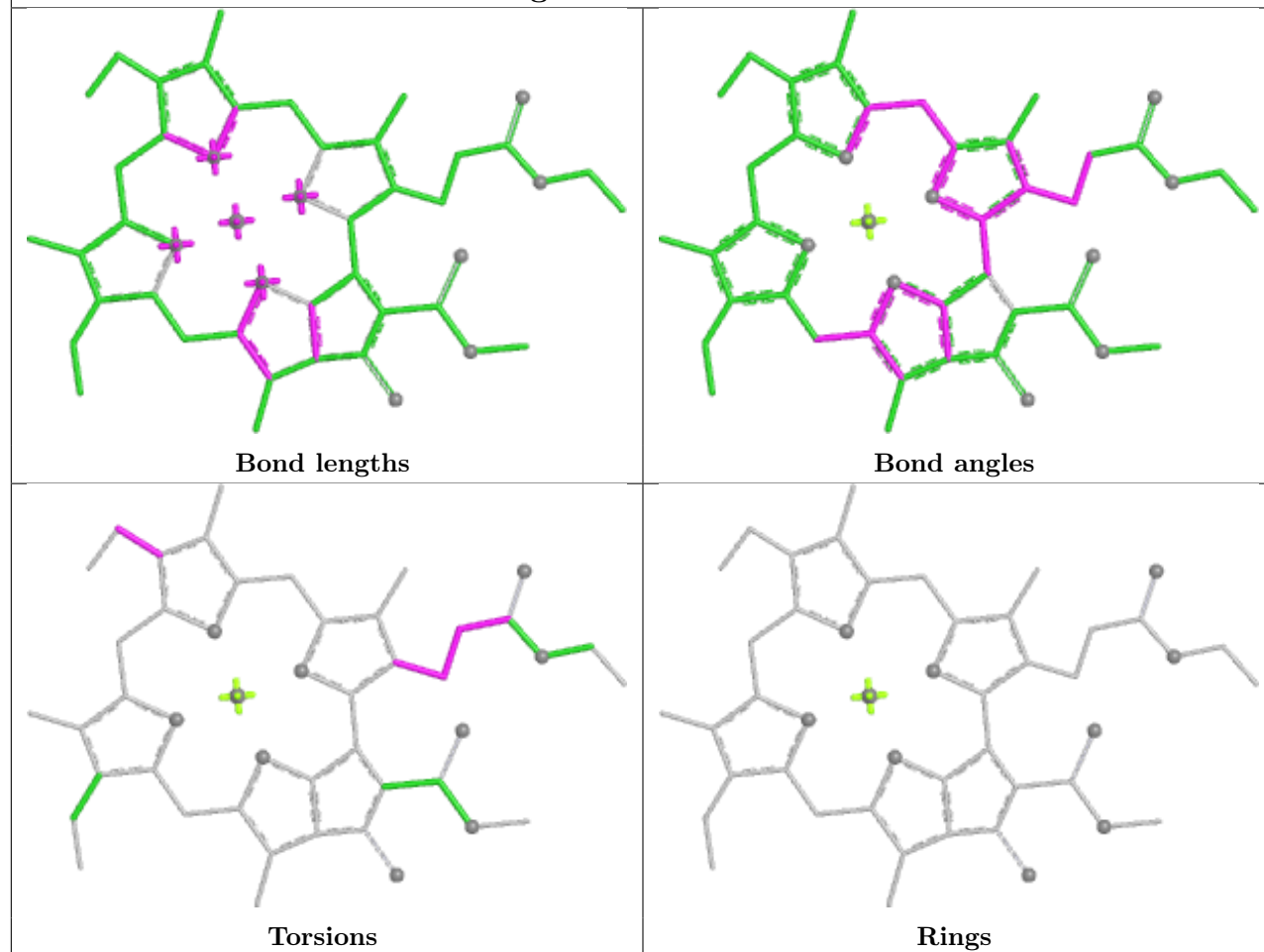


Torsions

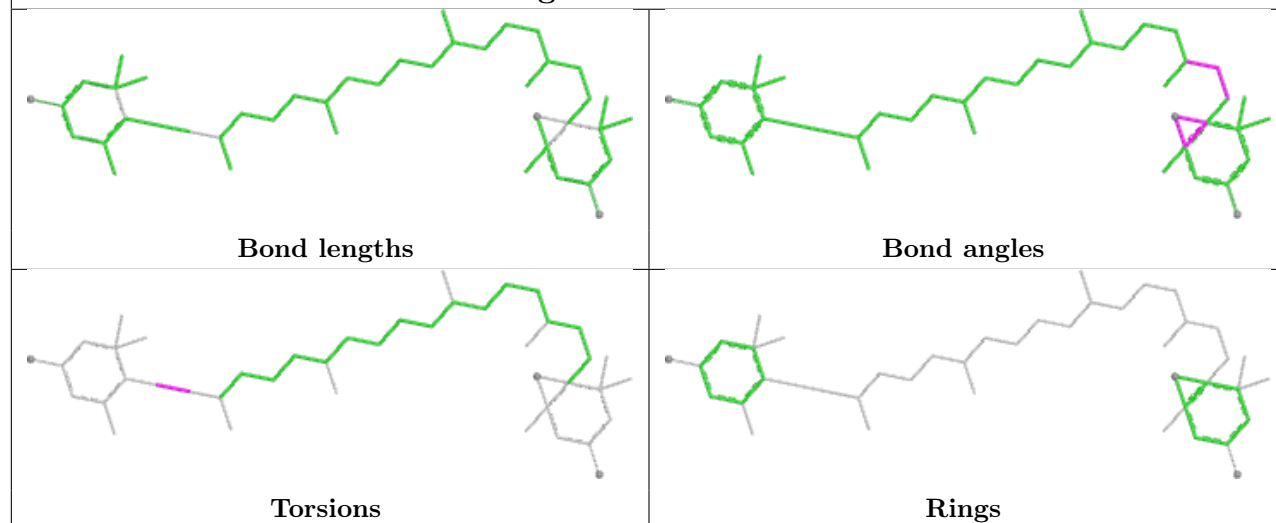


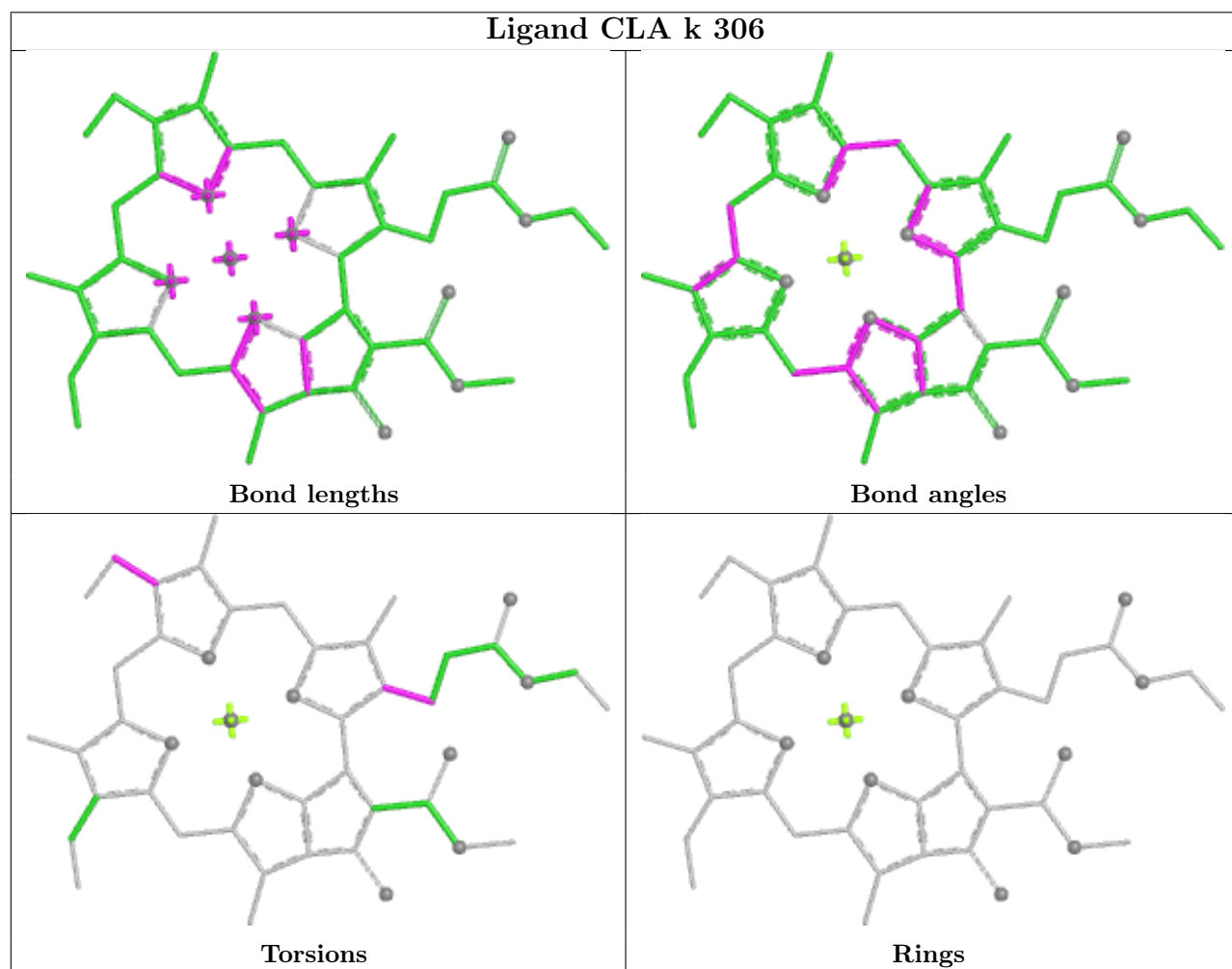
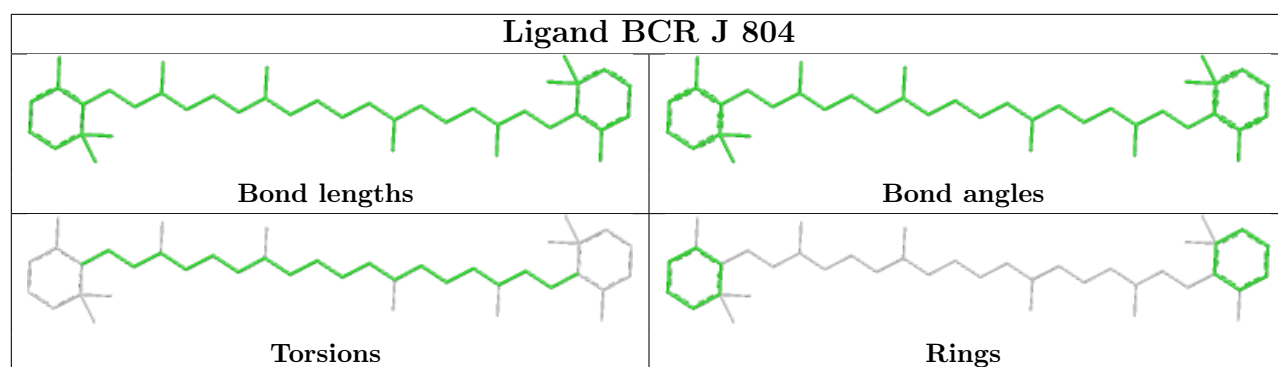
Rings

Ligand CLA b 313

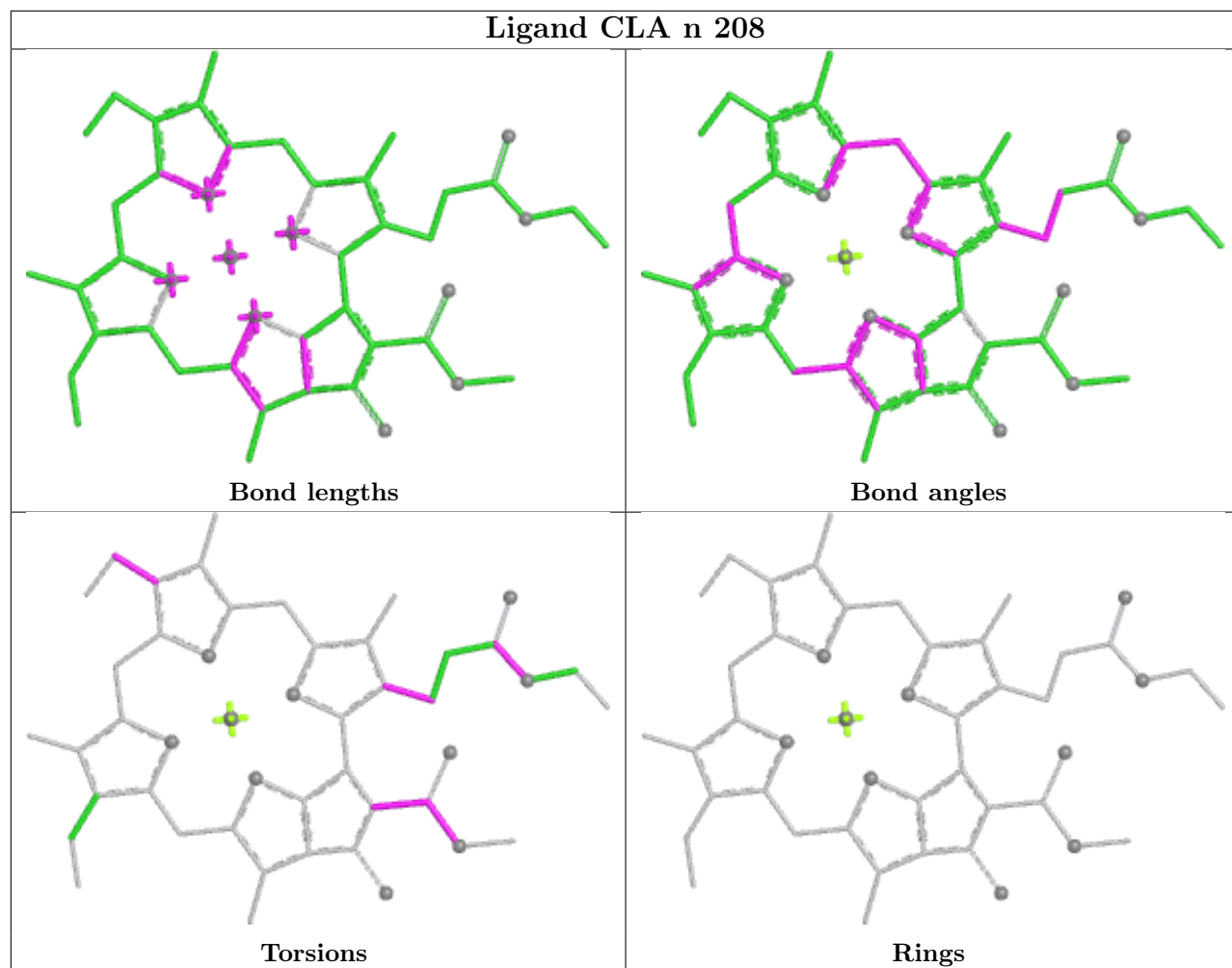


Ligand DD6 c 318

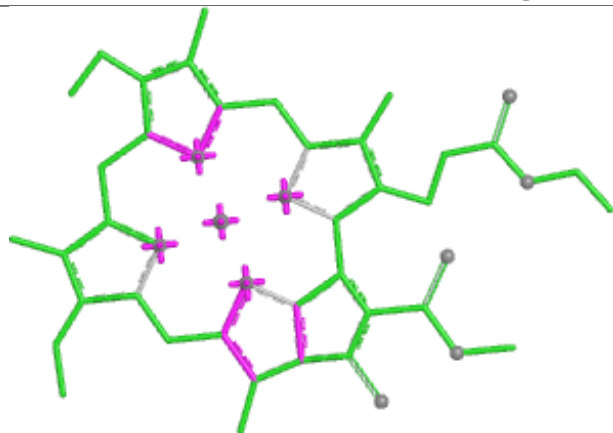




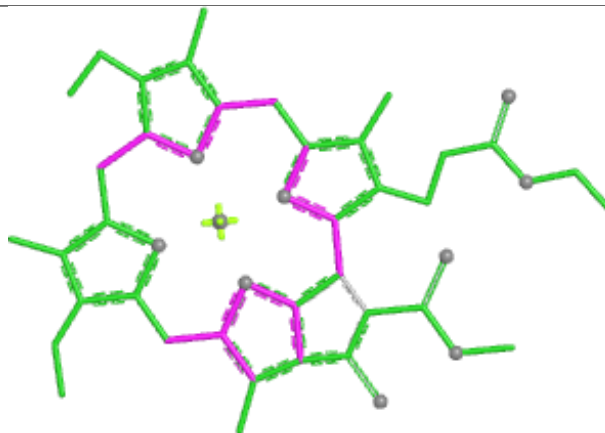
Ligand CLA n 208



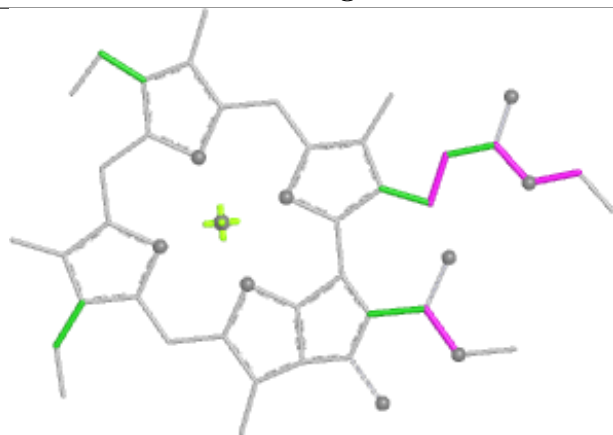
Ligand CLA n 206



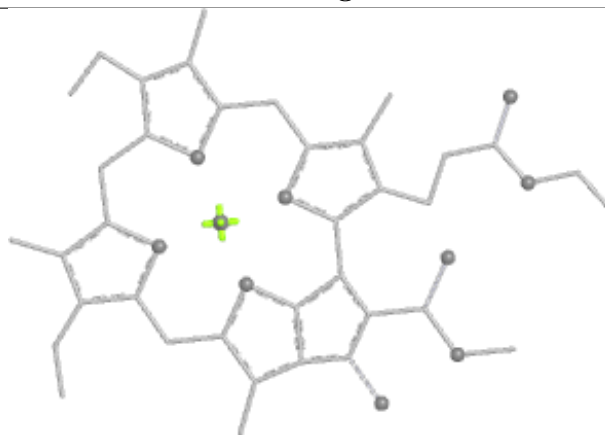
Bond lengths



Bond angles

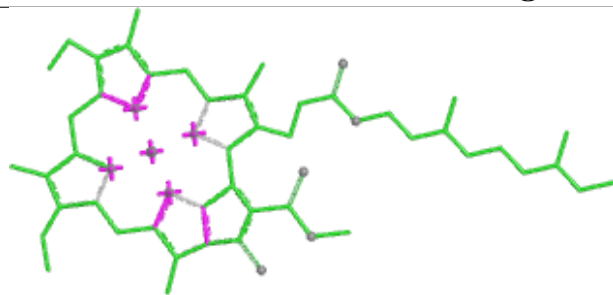


Torsions

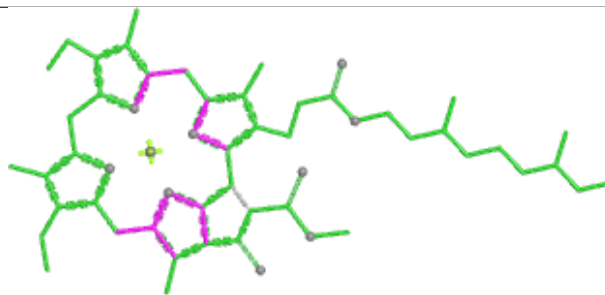


Rings

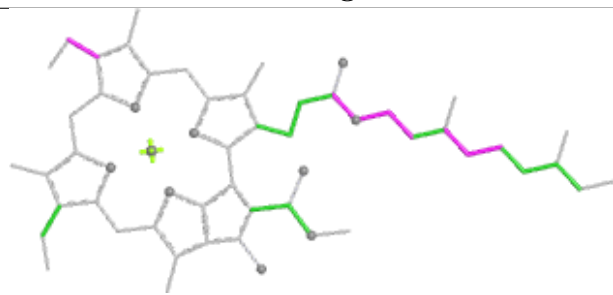
Ligand CLA c 306



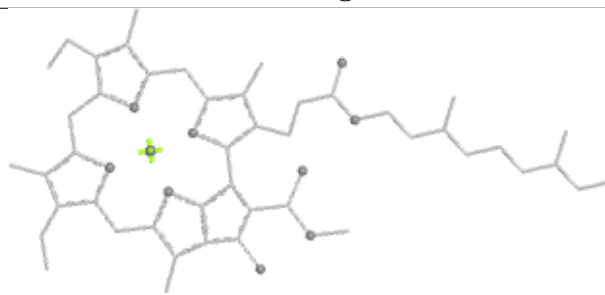
Bond lengths



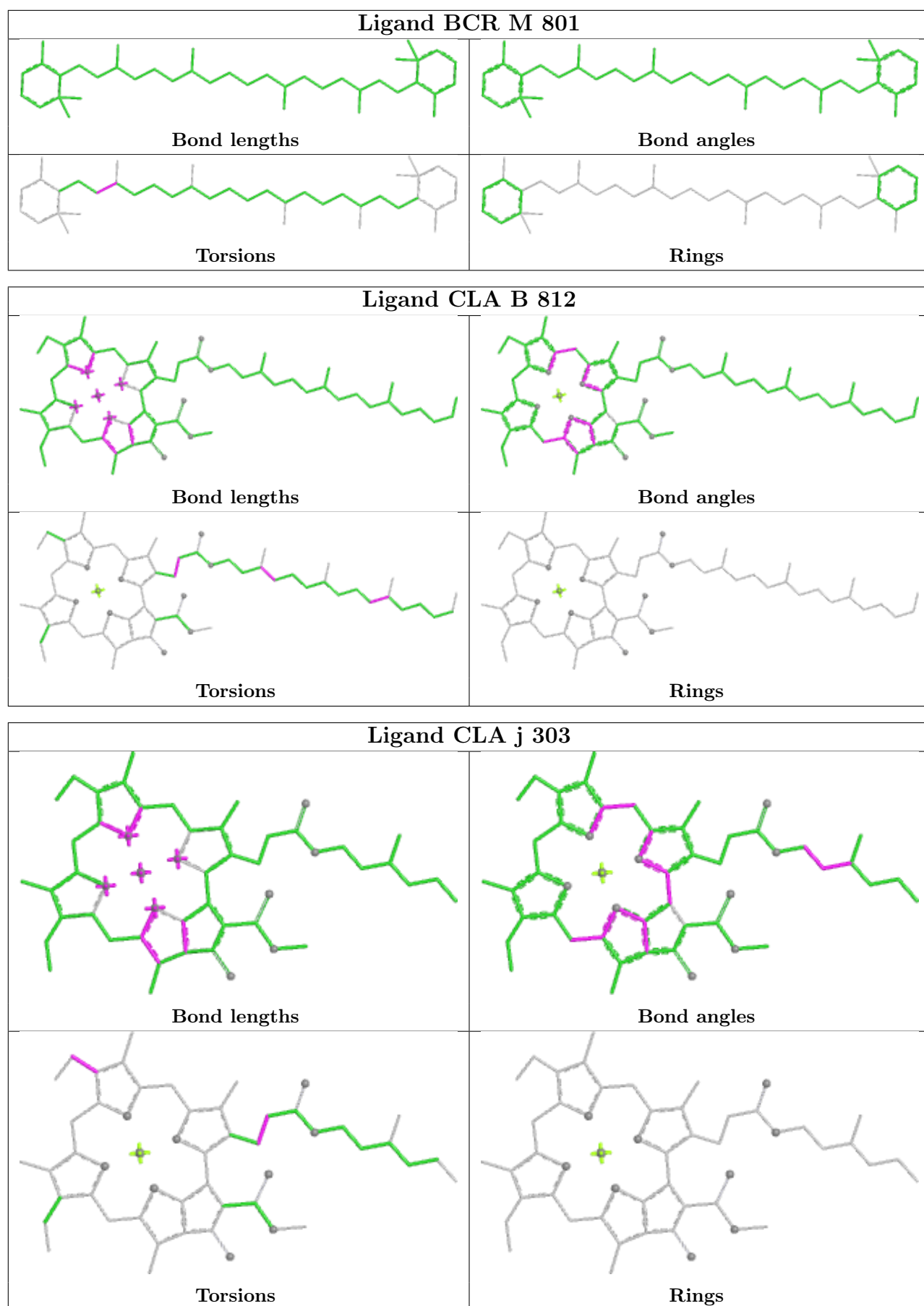
Bond angles



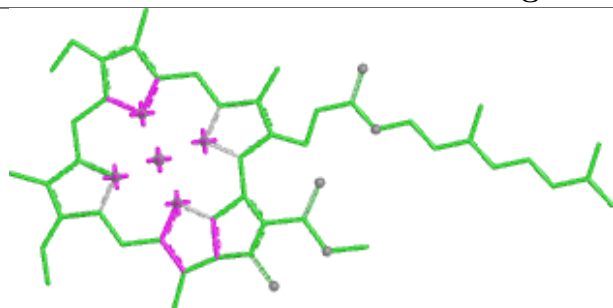
Torsions



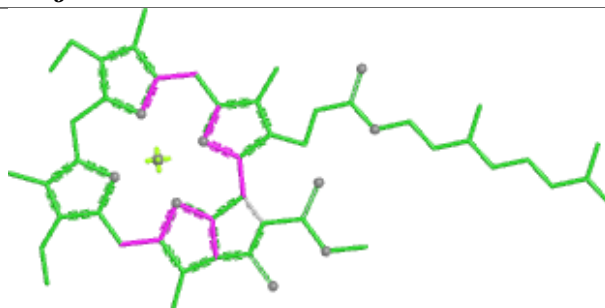
Rings



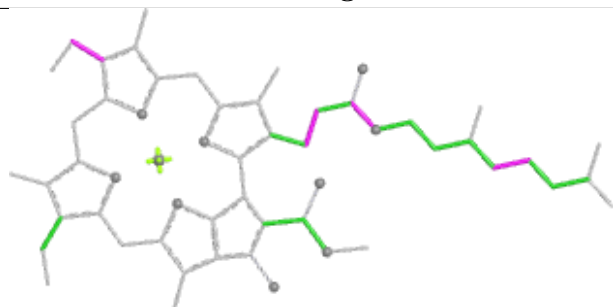
Ligand CLA j 302



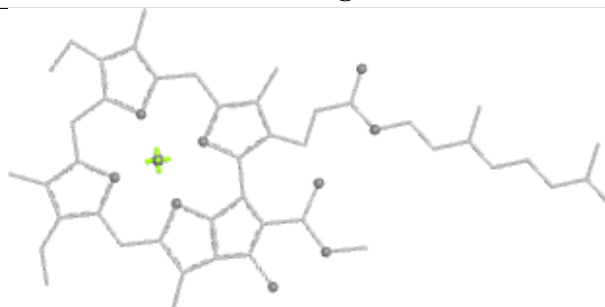
Bond lengths



Bond angles

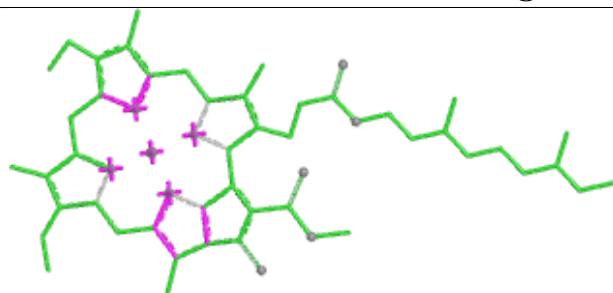


Torsions

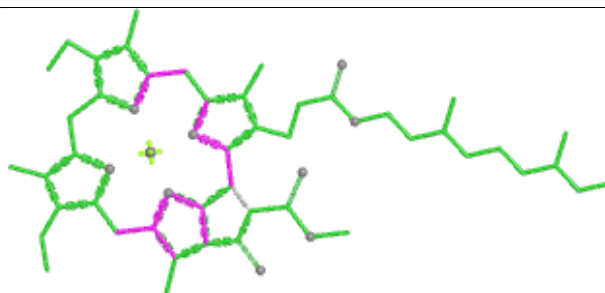


Rings

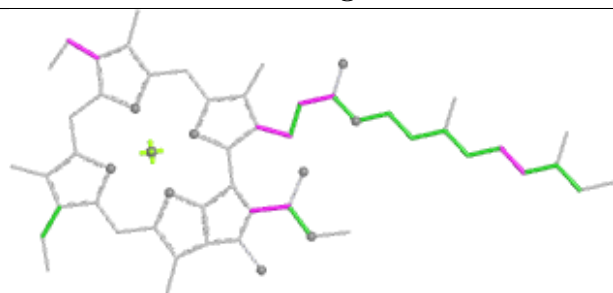
Ligand CLA n 204



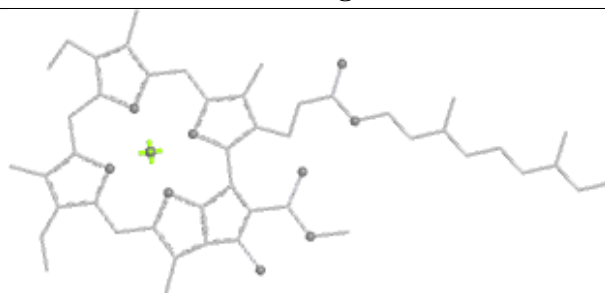
Bond lengths



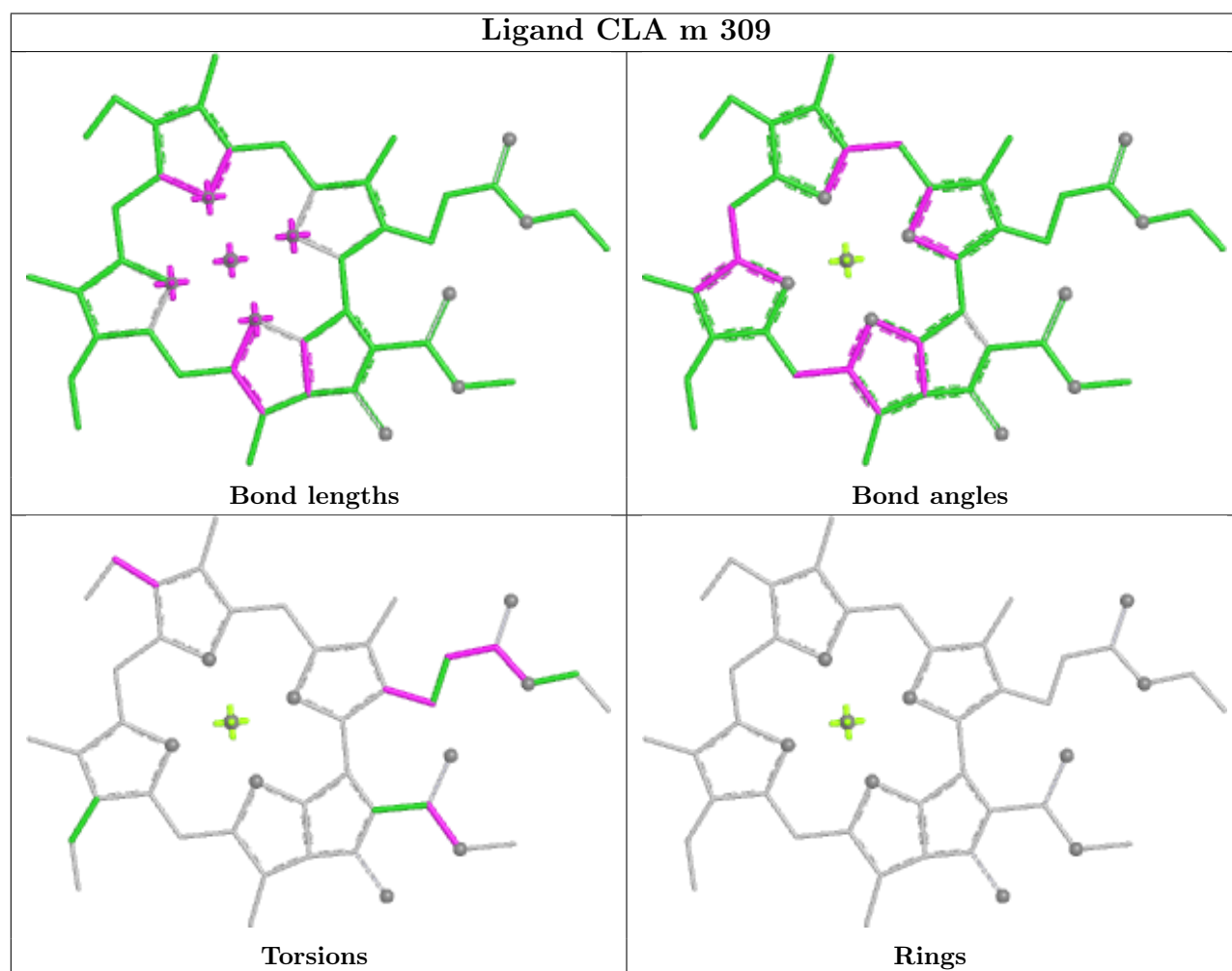
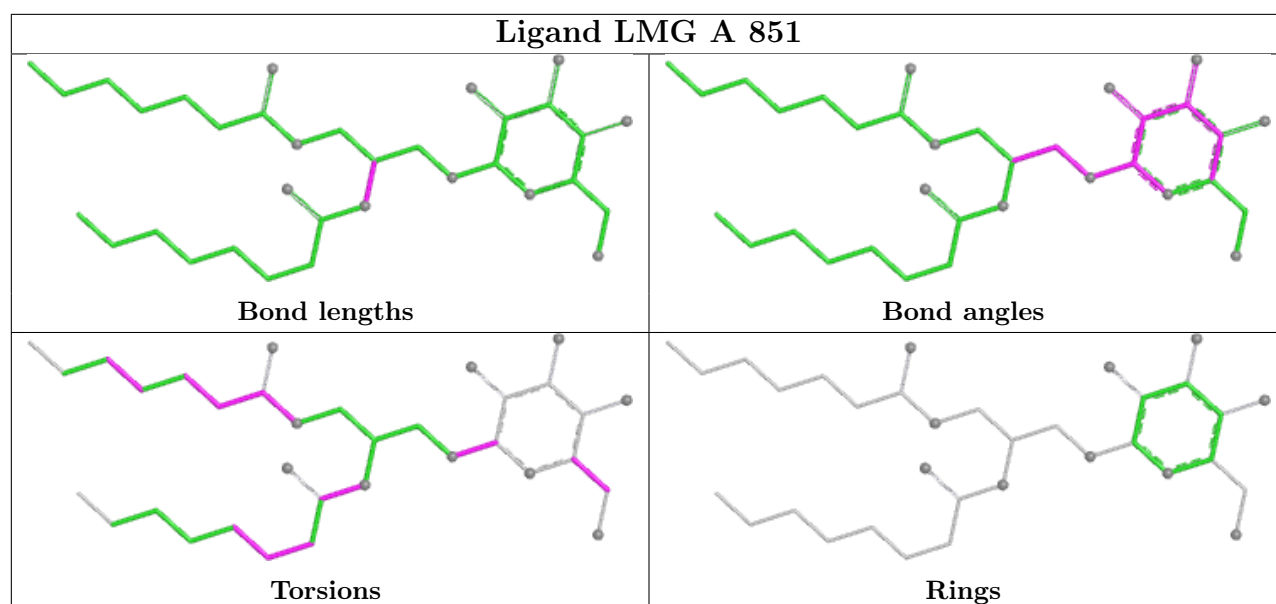
Bond angles



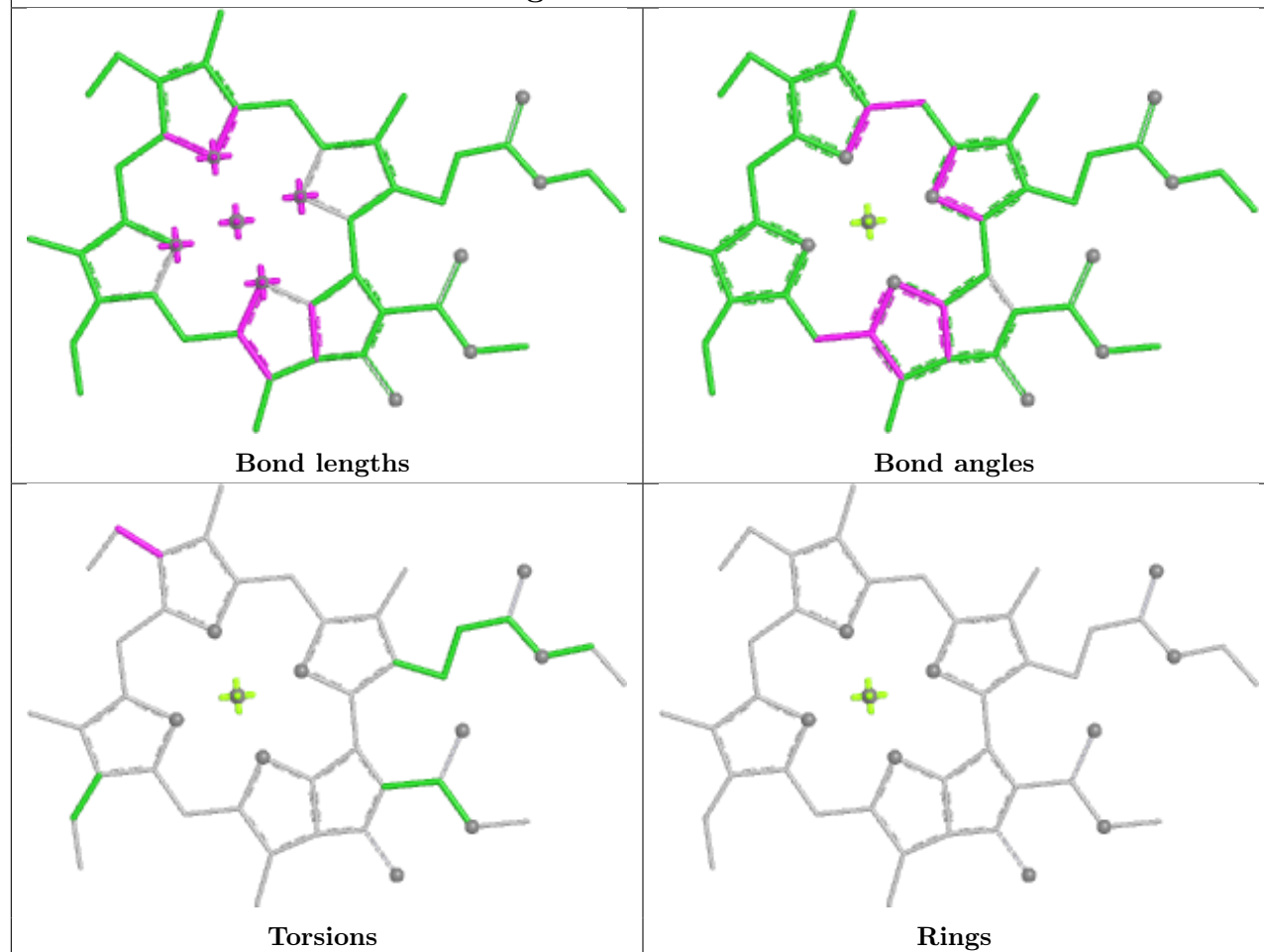
Torsions



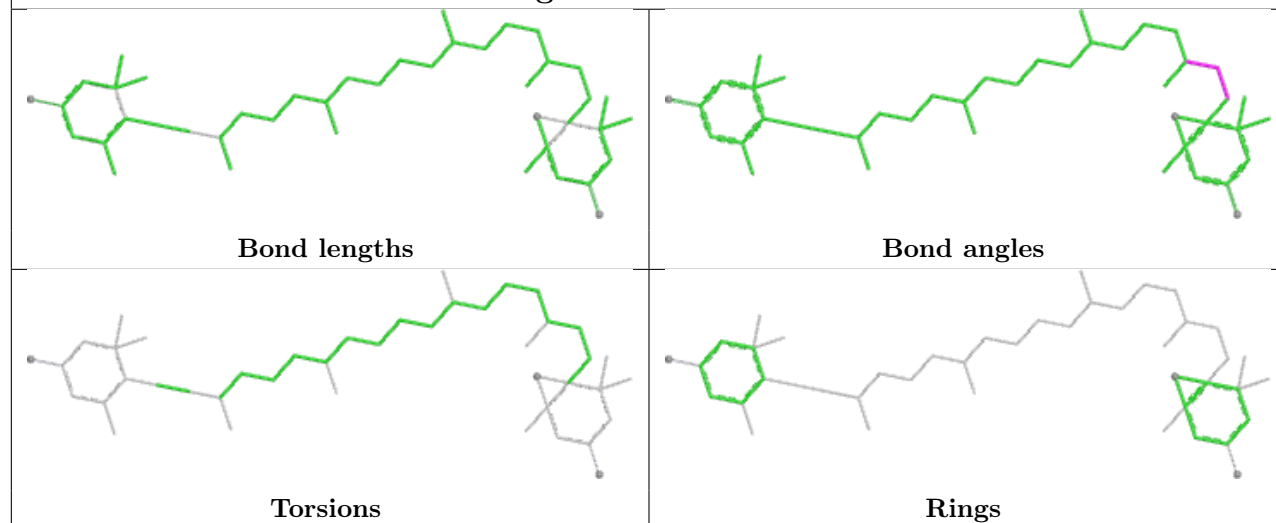
Rings



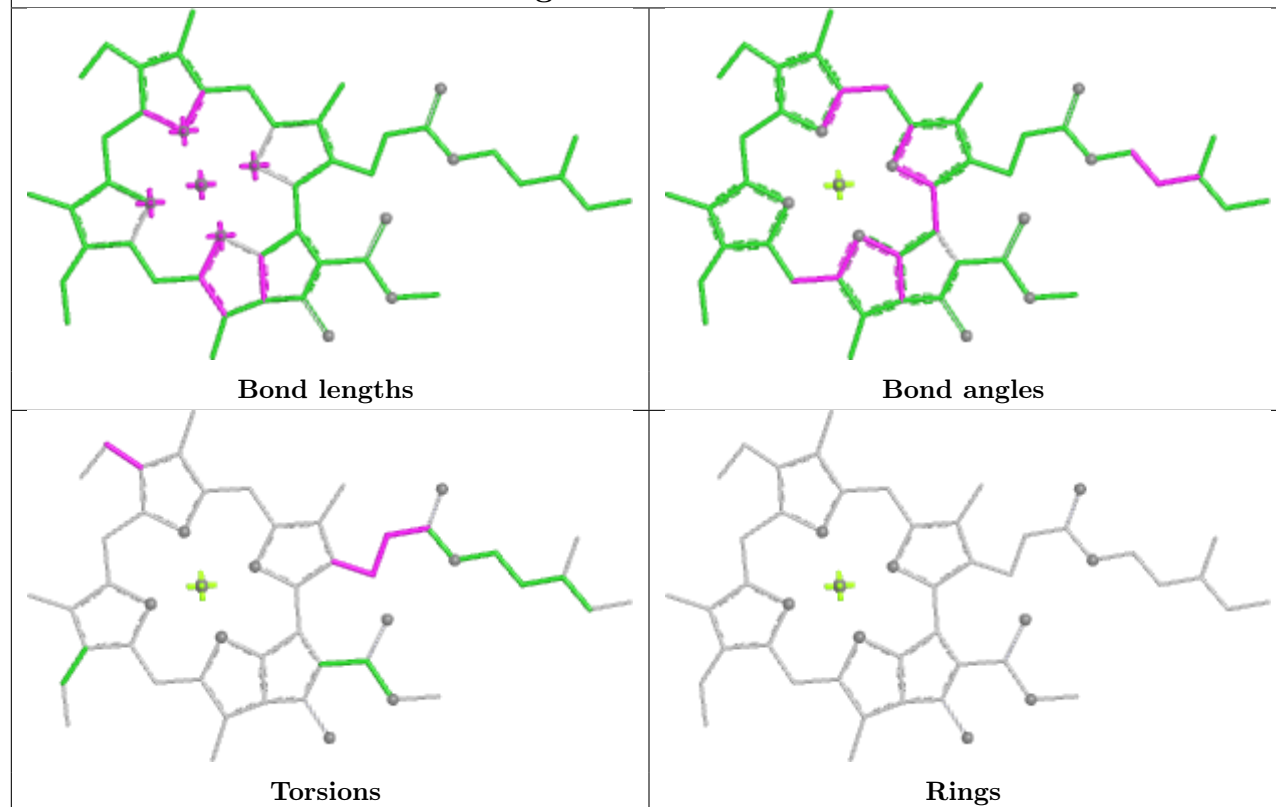
Ligand CLA A 849



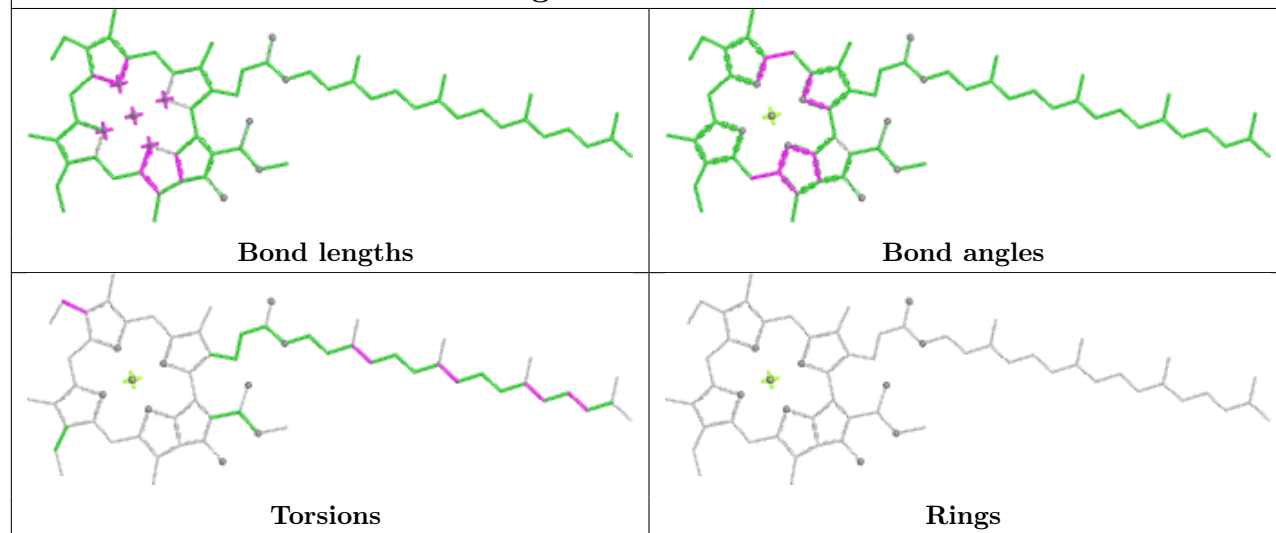
Ligand DD6 b 319



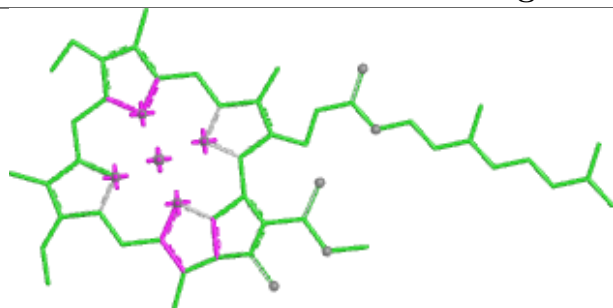
Ligand CLA h 211



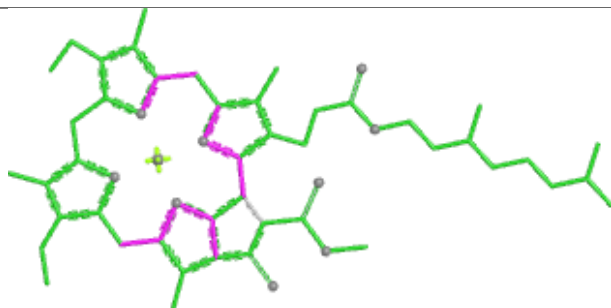
Ligand CLA A 850



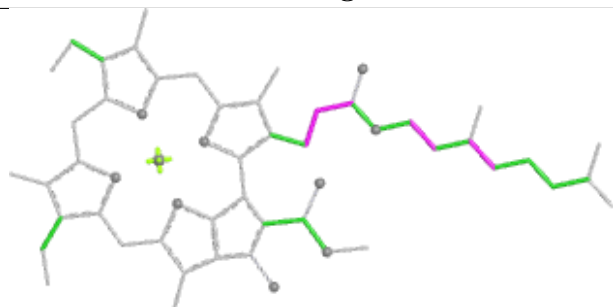
Ligand CLA k 310



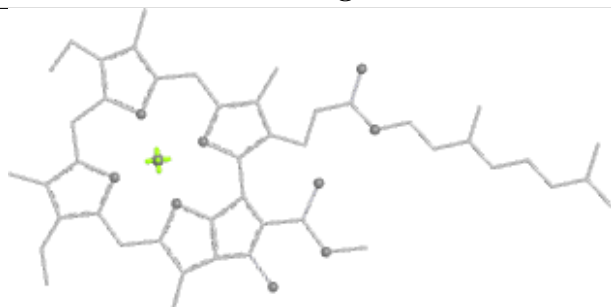
Bond lengths



Bond angles

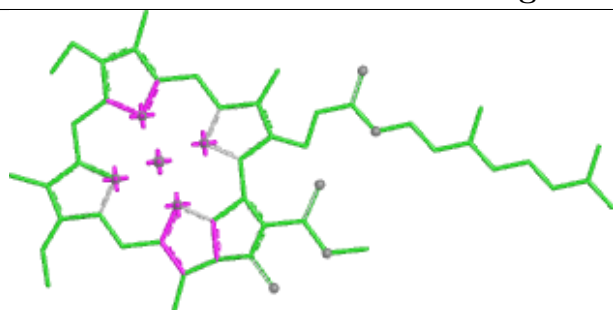


Torsions

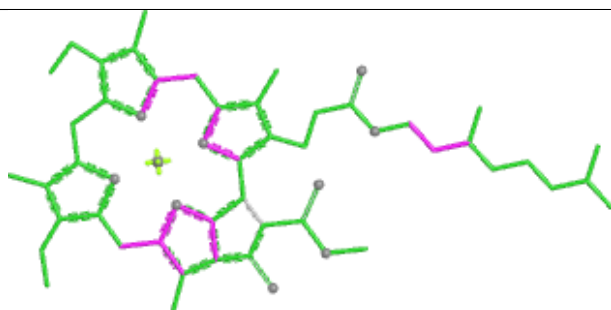


Rings

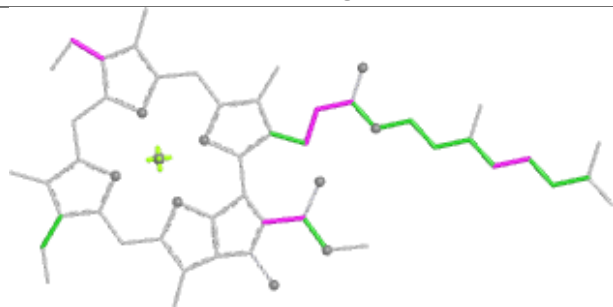
Ligand CLA e 306



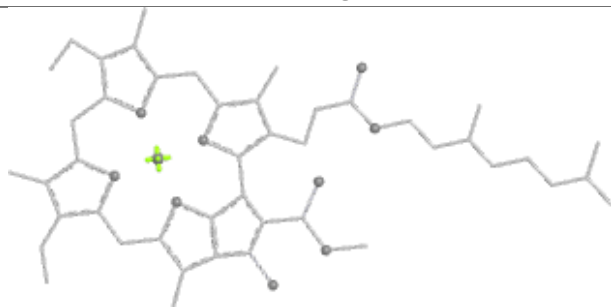
Bond lengths



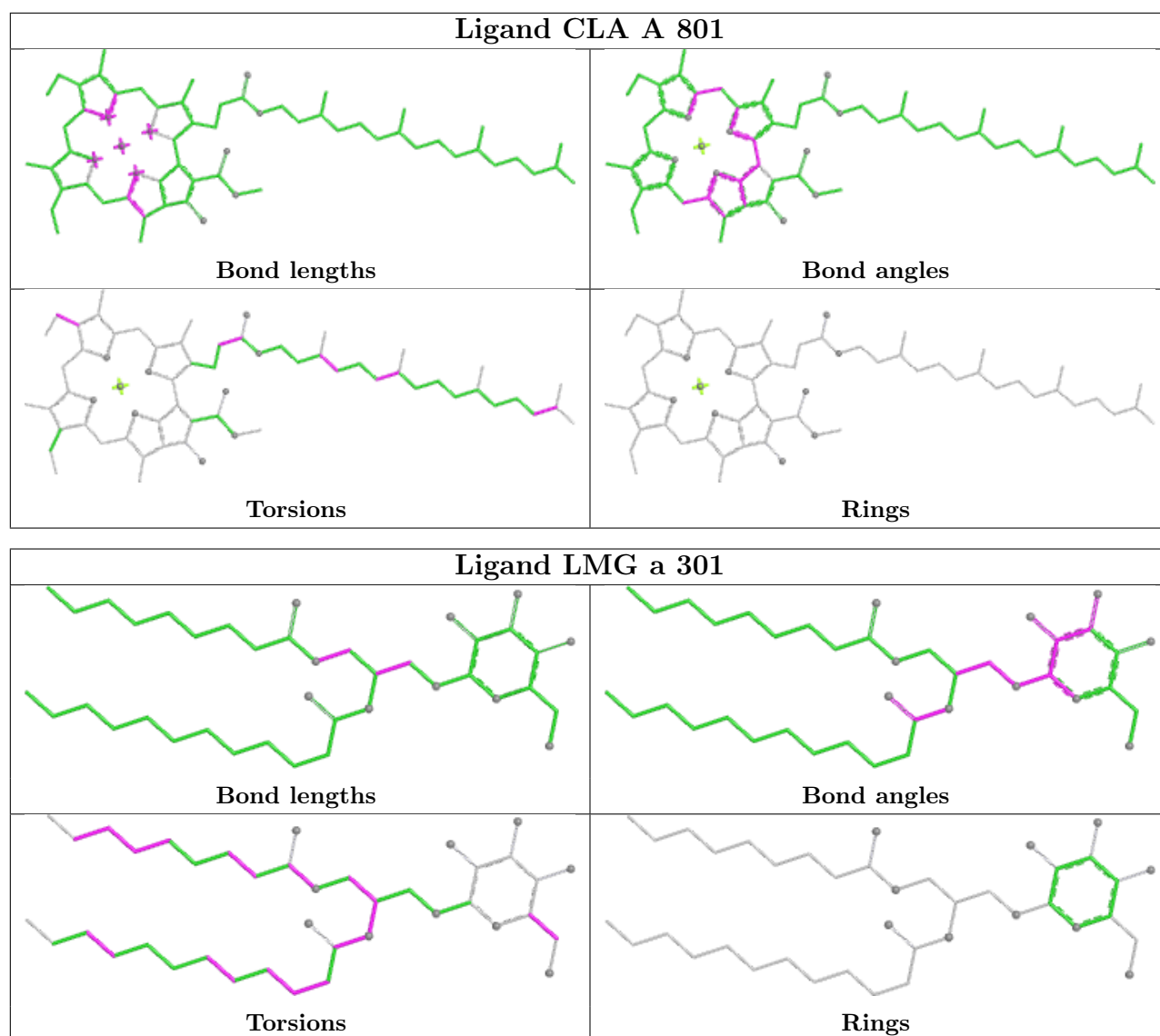
Bond angles



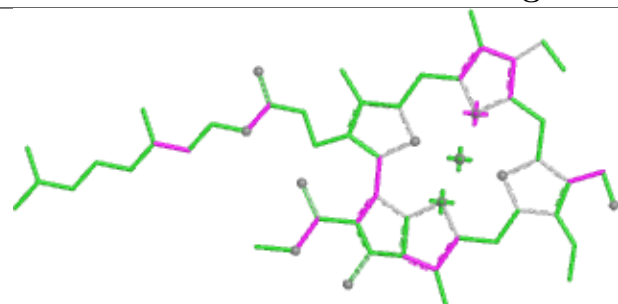
Torsions



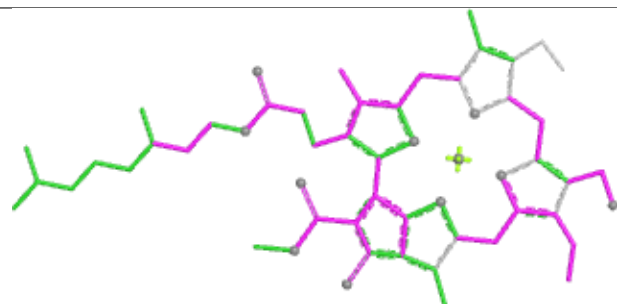
Rings



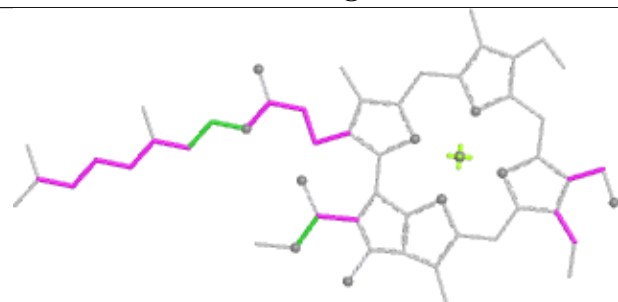
Ligand CHL c 312



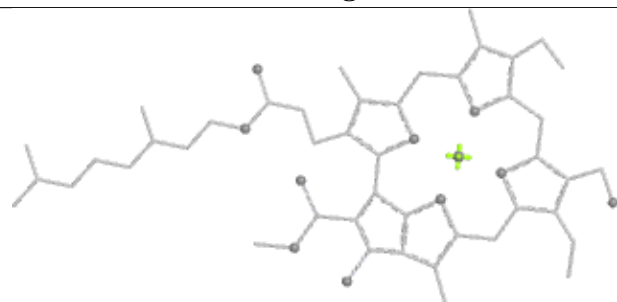
Bond lengths



Bond angles

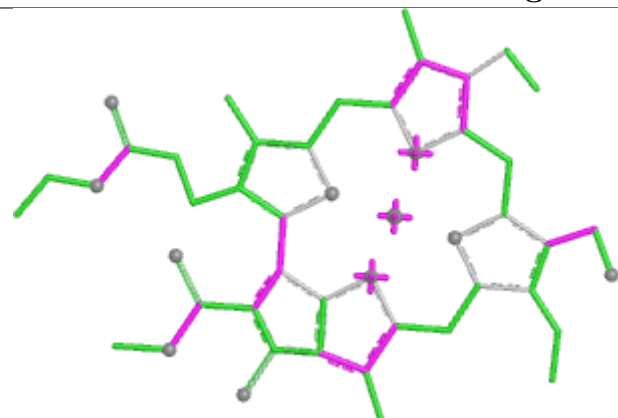


Torsions

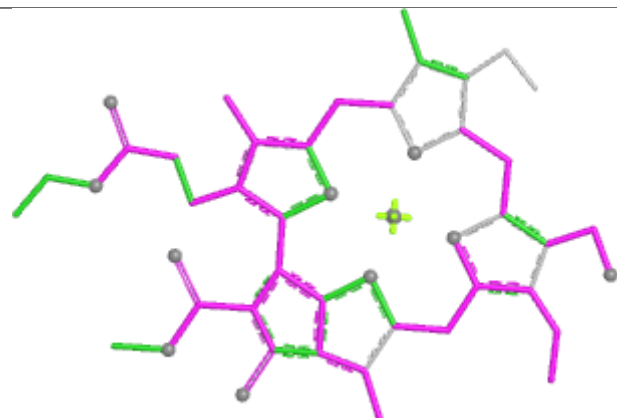


Rings

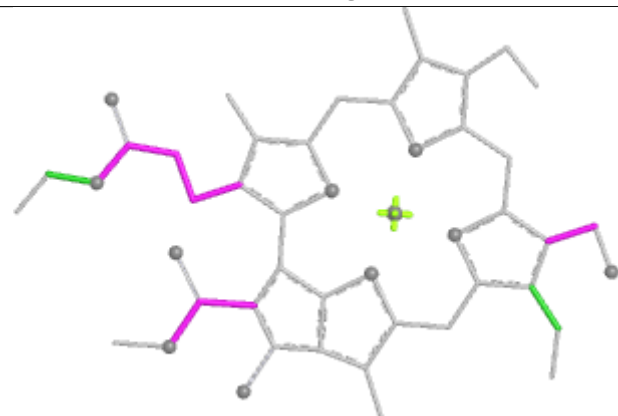
Ligand CHL f 301



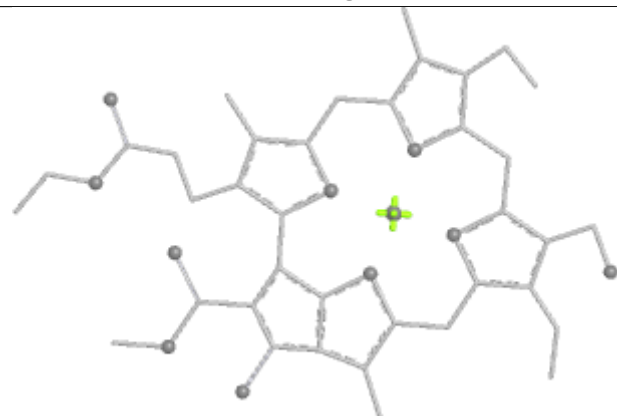
Bond lengths



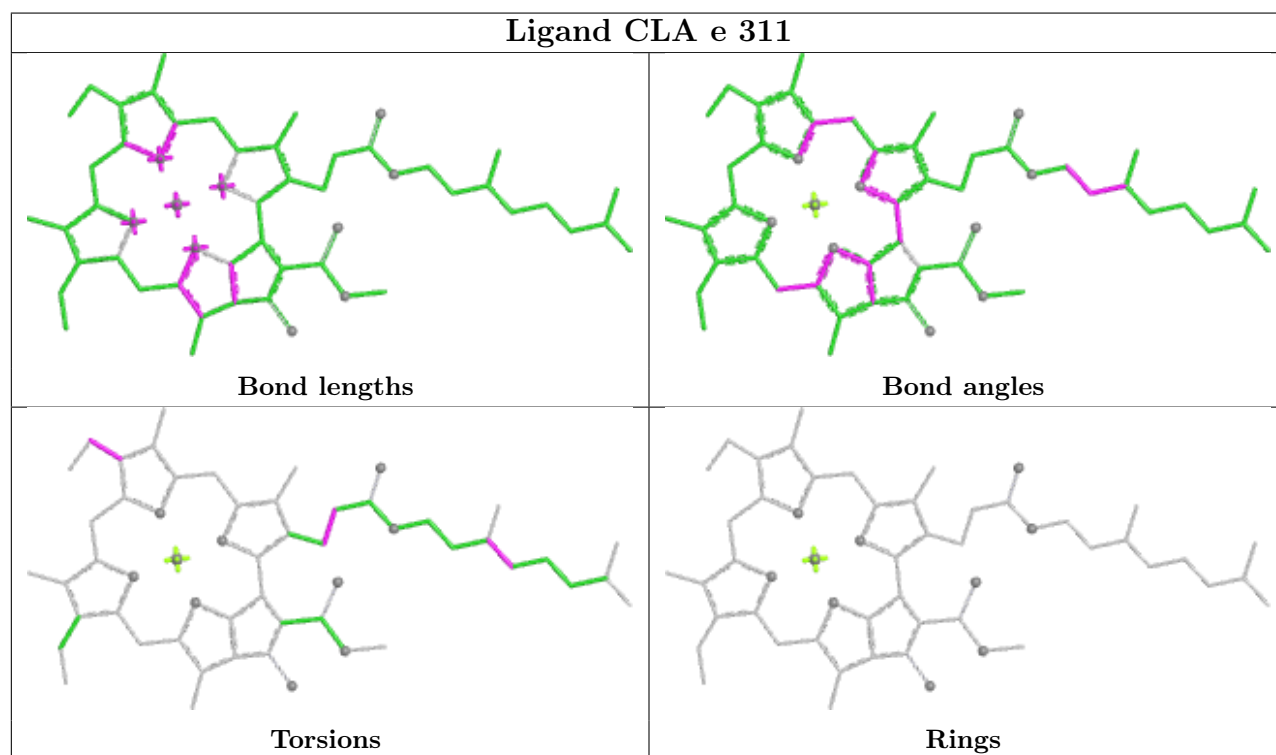
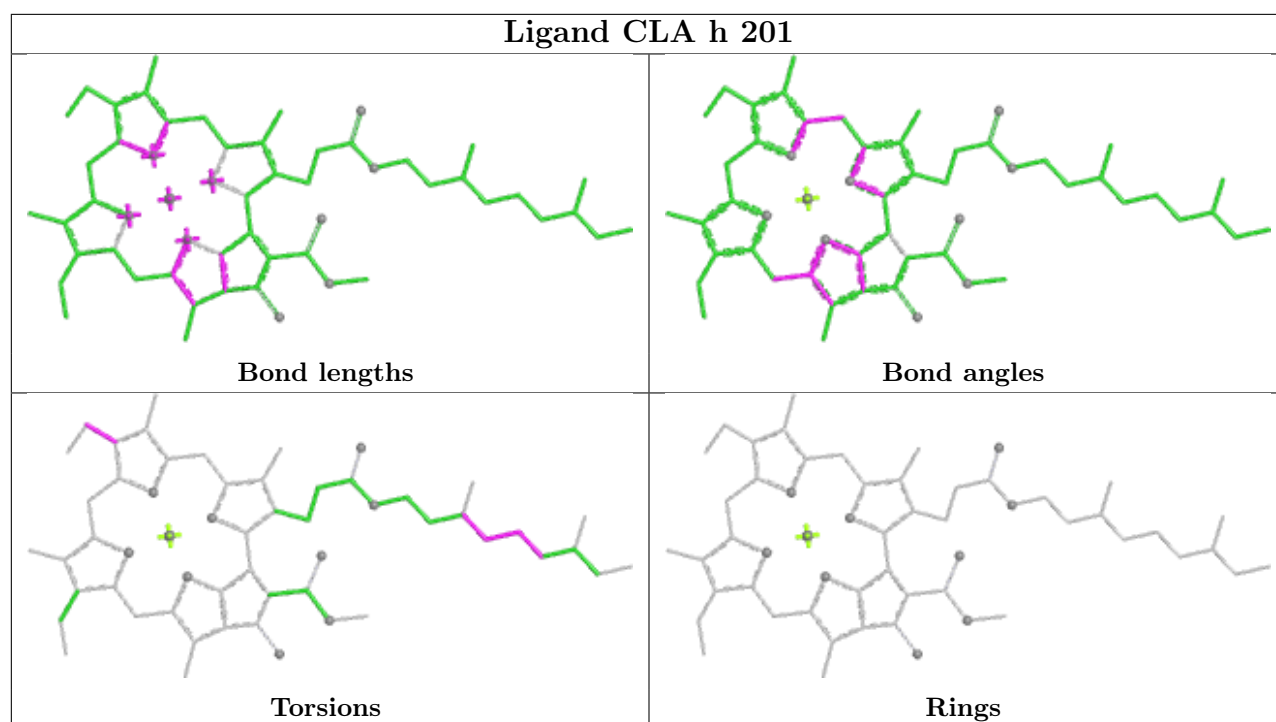
Bond angles

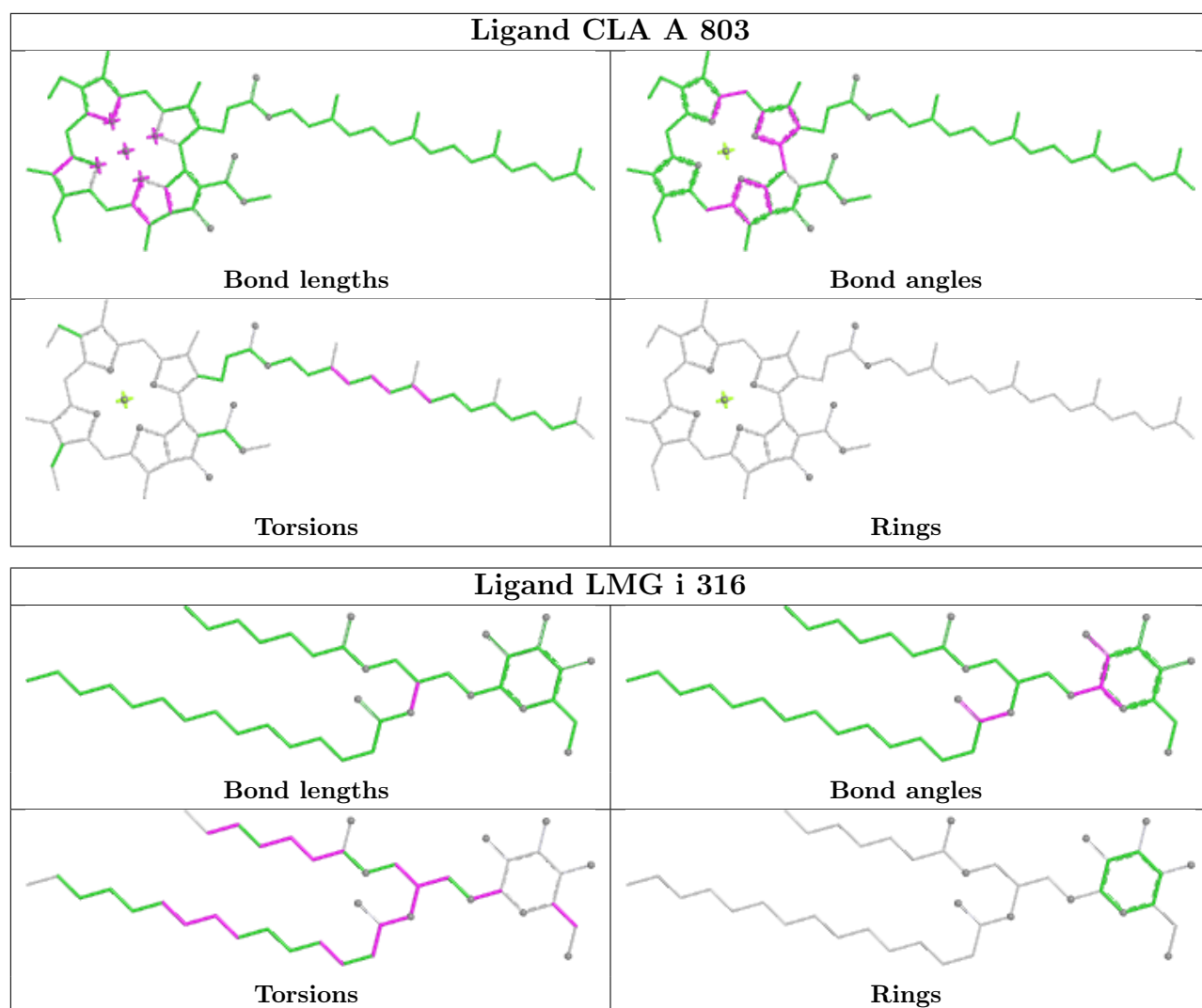


Torsions

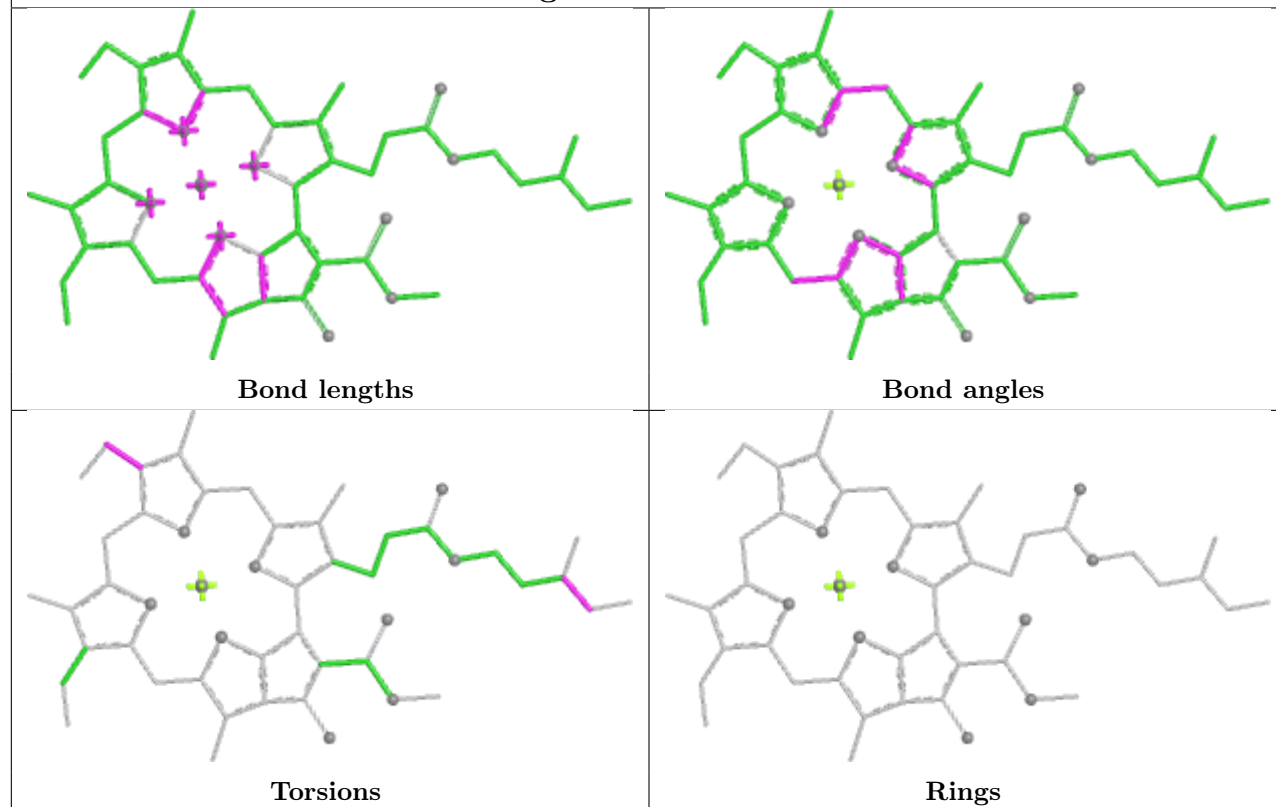


Rings

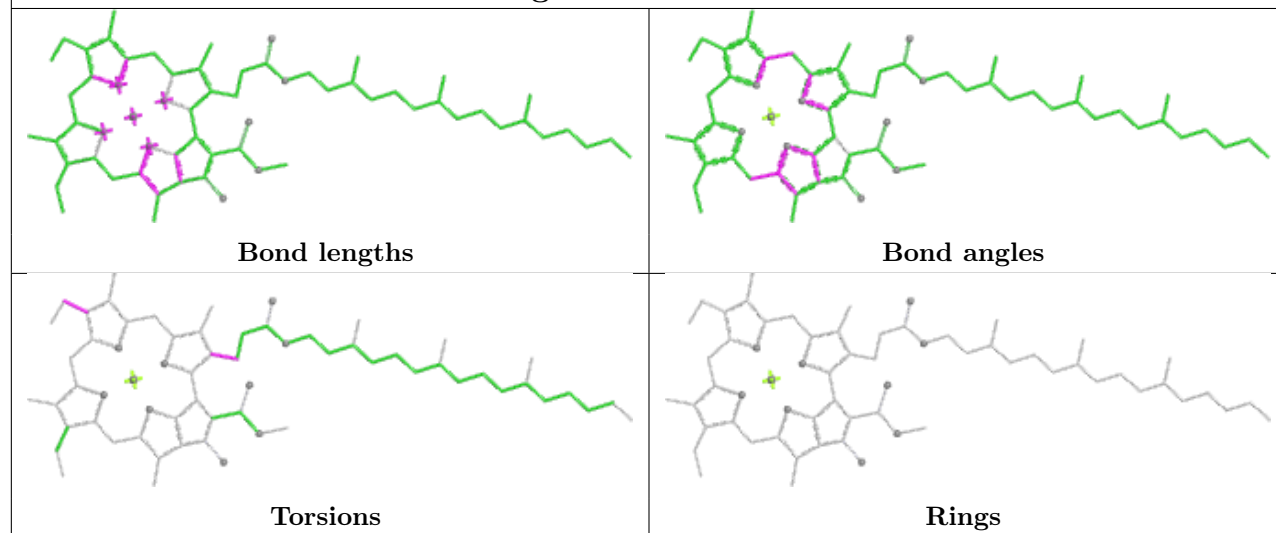


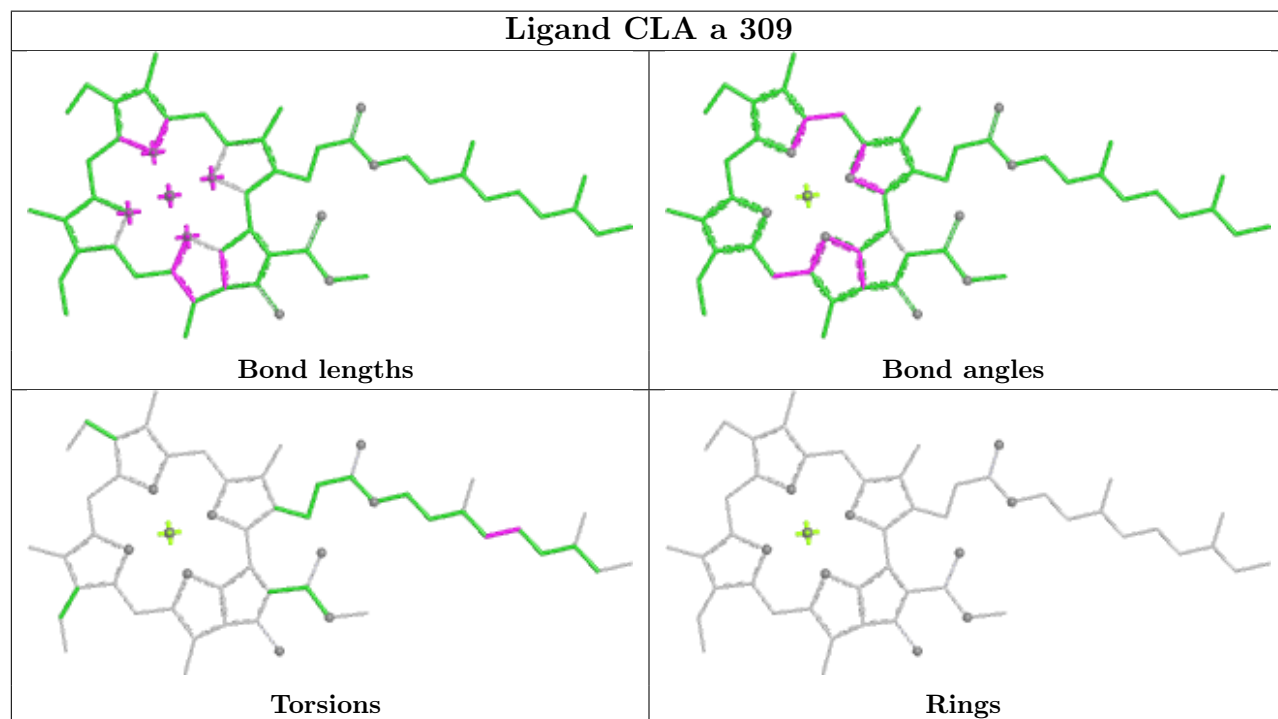
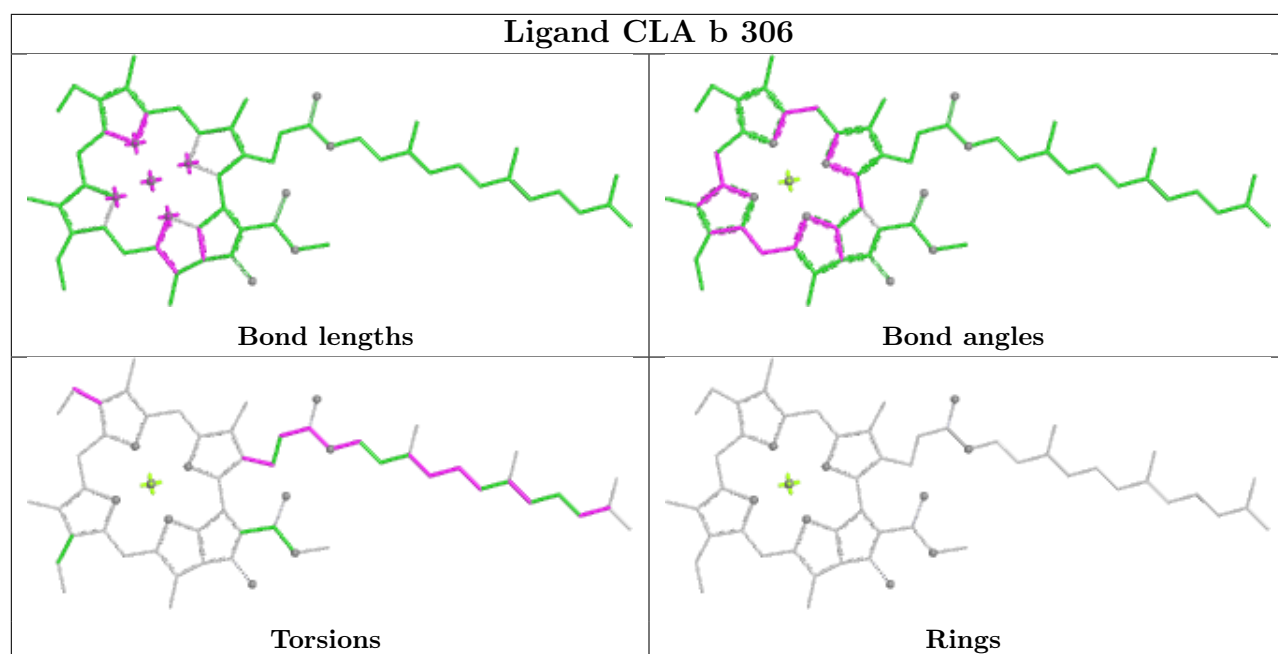


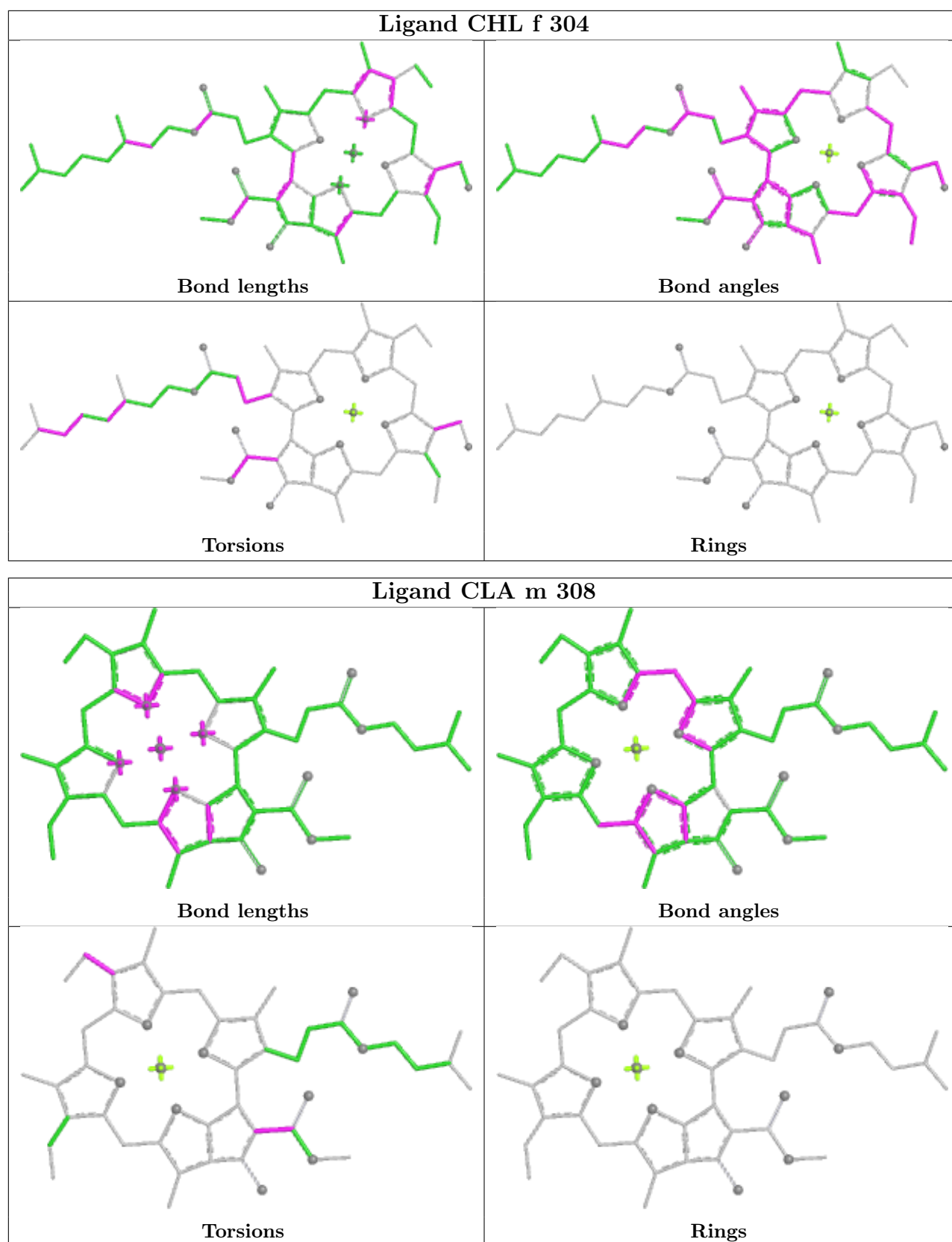
Ligand CLA f 308



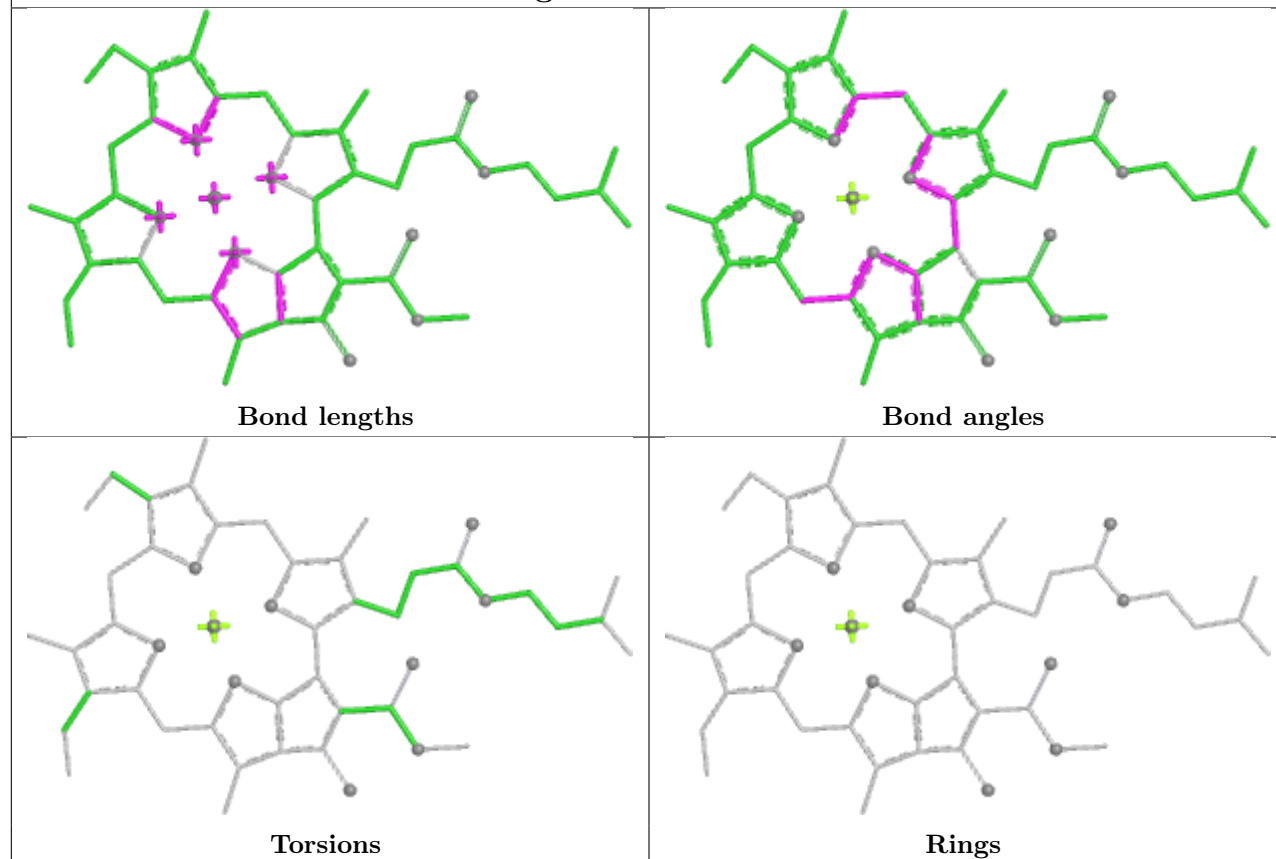
Ligand CLA A 818



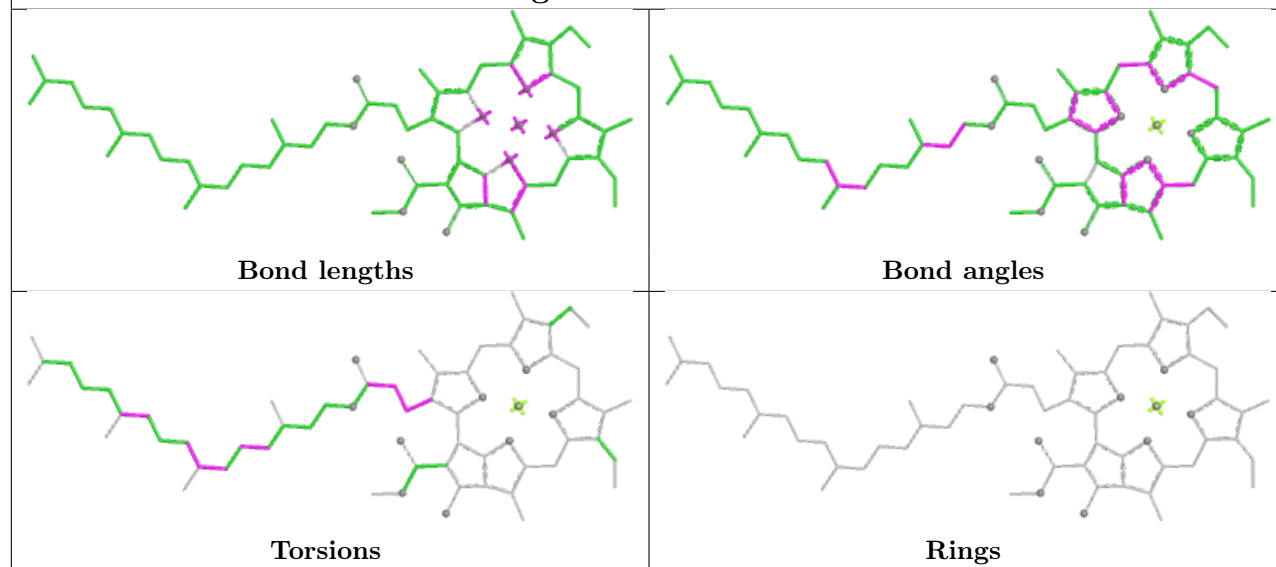




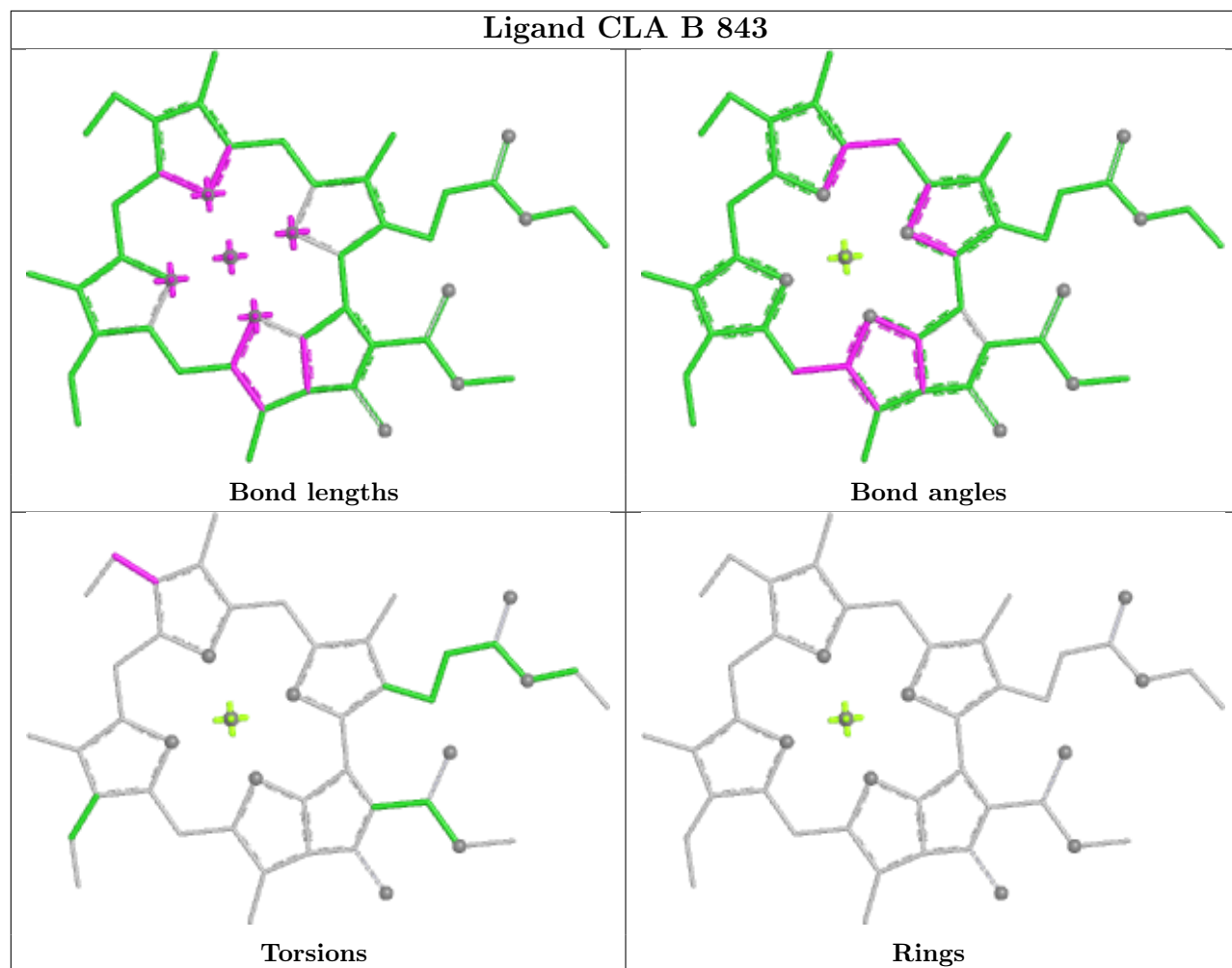
Ligand CLA b 309



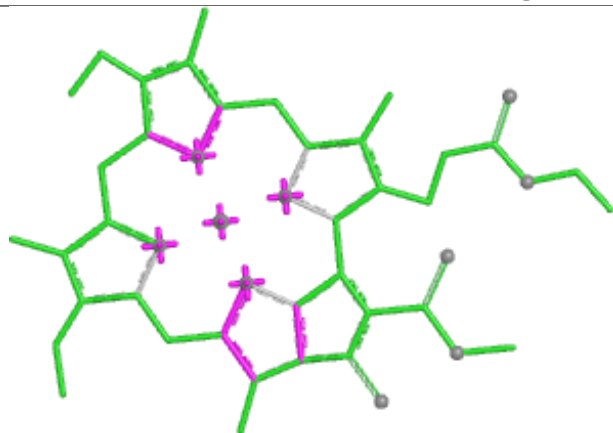
Ligand CLA A 843



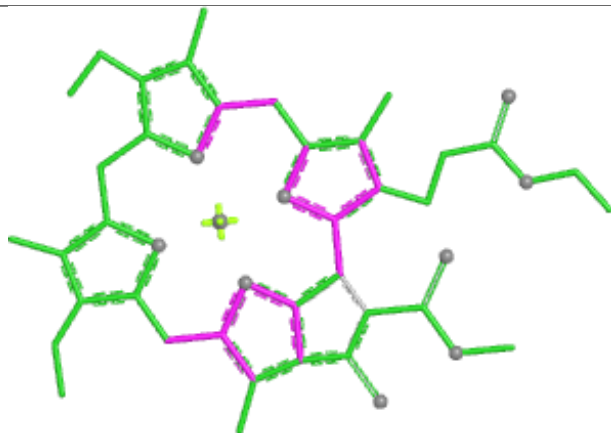
Ligand CLA B 843



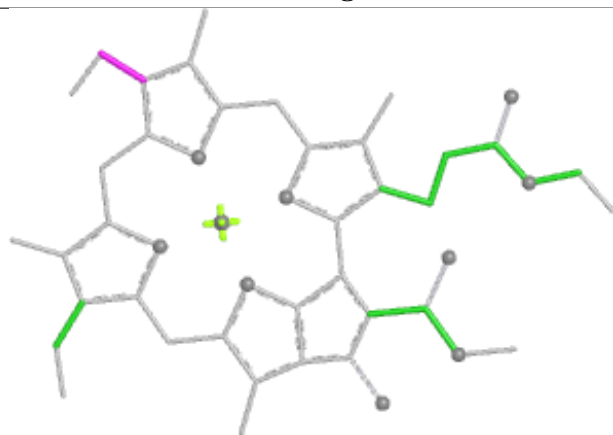
Ligand CLA k 309



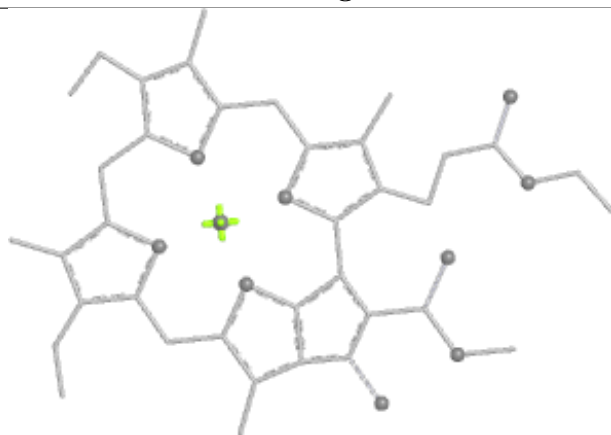
Bond lengths



Bond angles

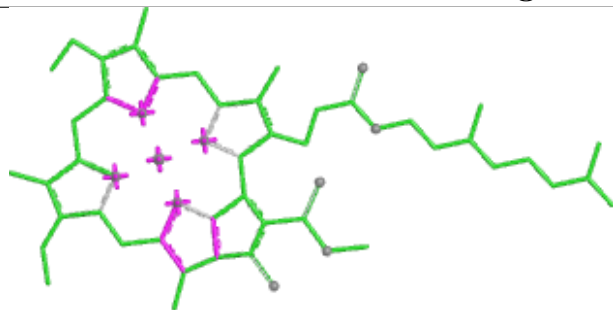


Torsions

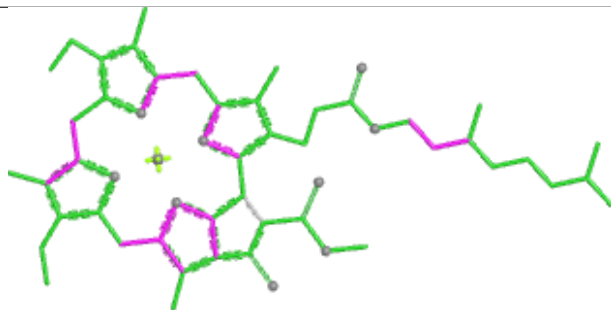


Rings

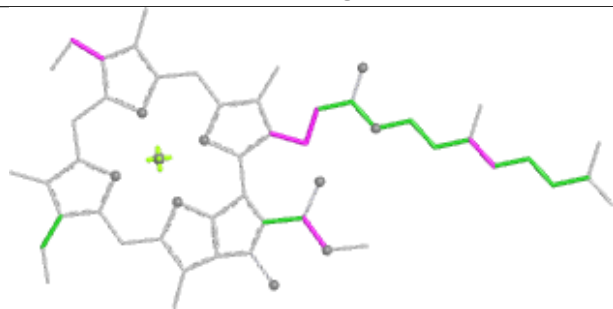
Ligand CLA b 304



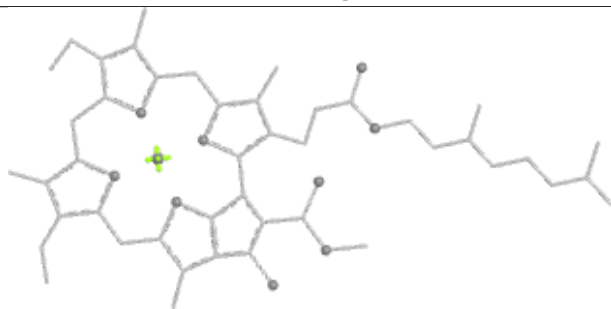
Bond lengths



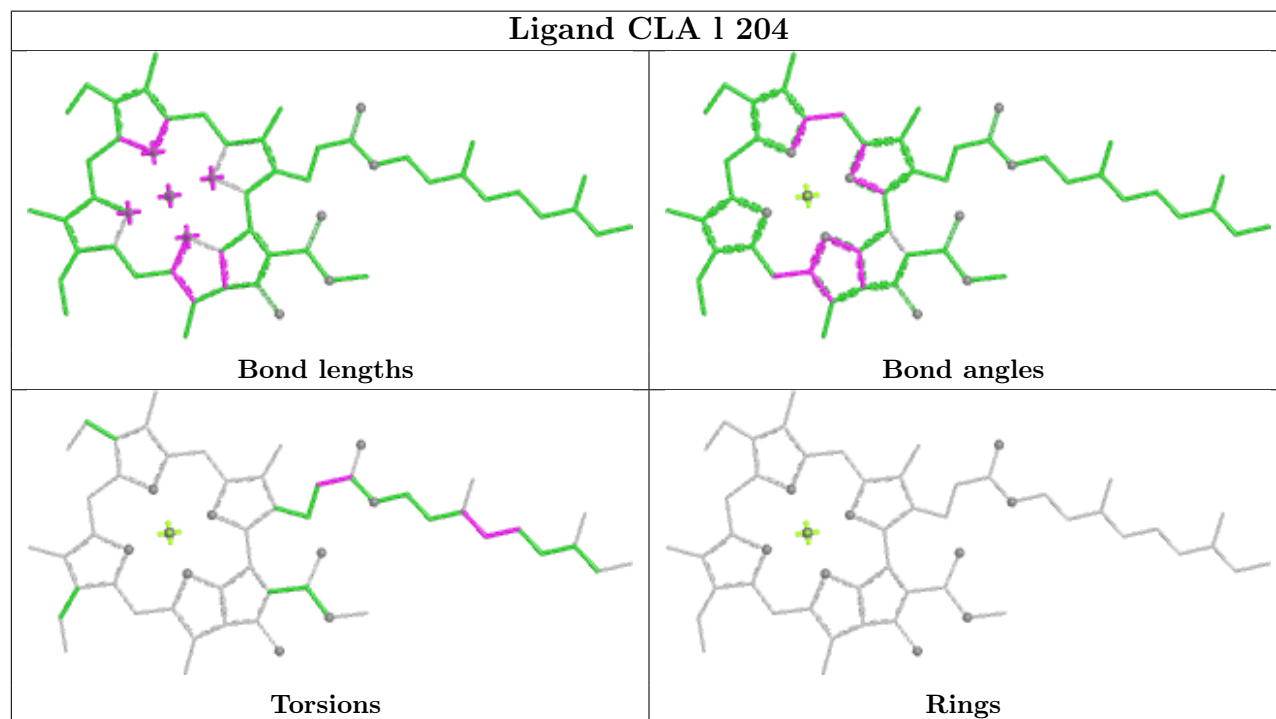
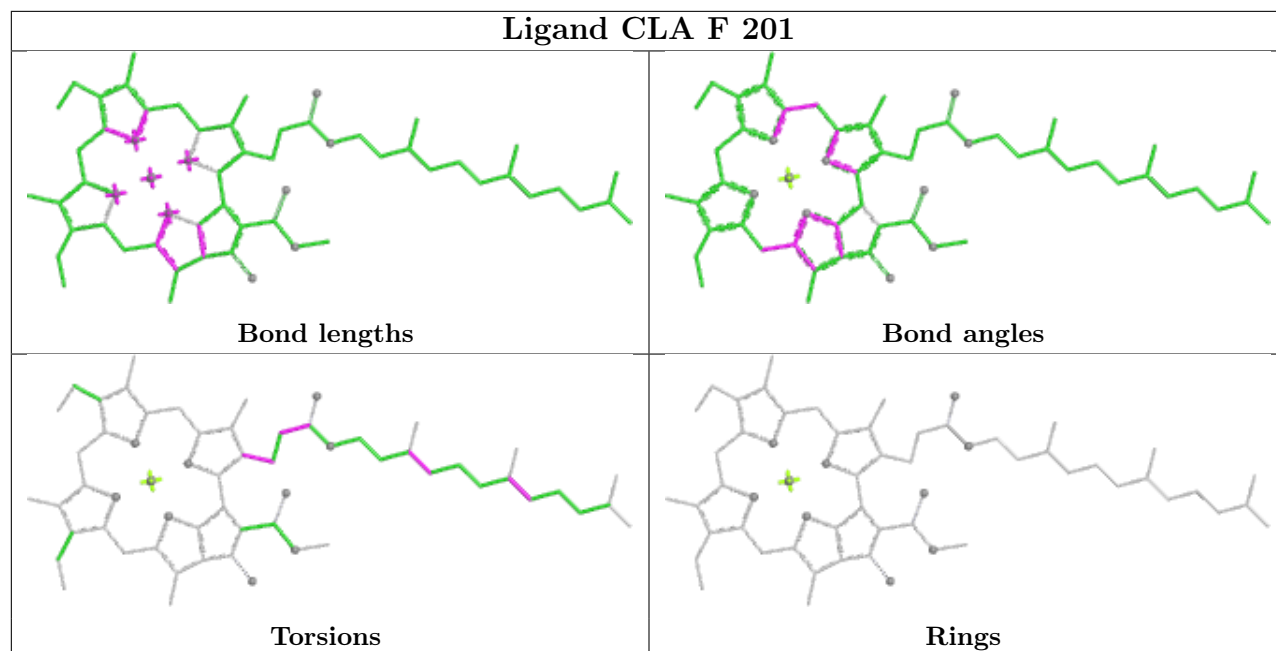
Bond angles

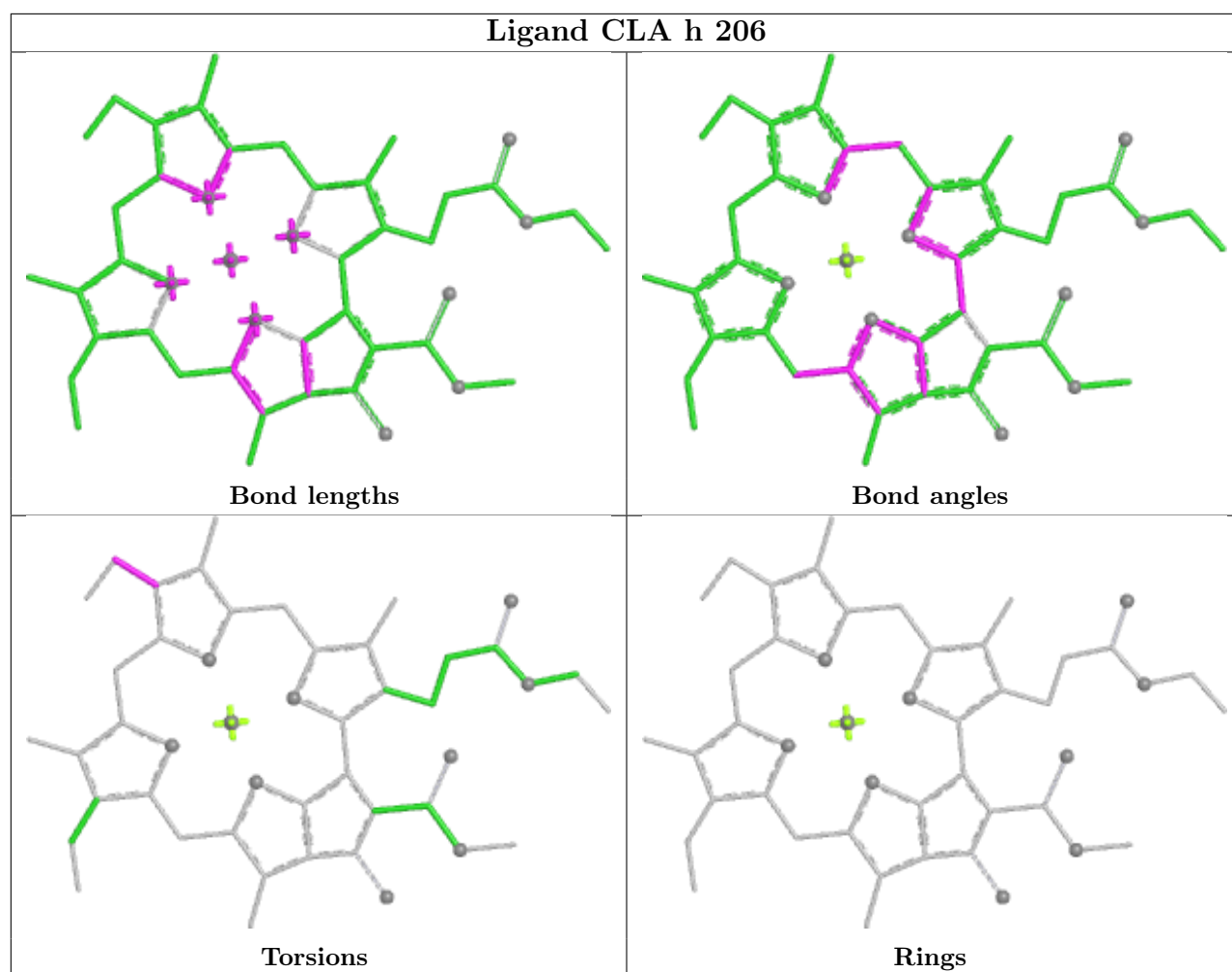


Torsions



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.

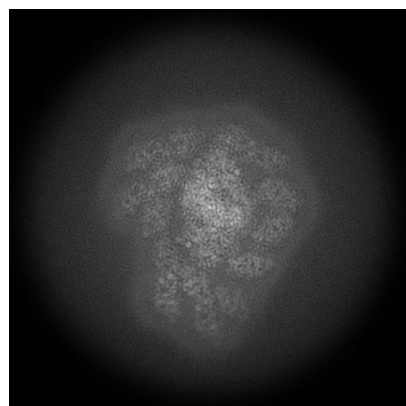
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65121. These allow visual inspection of the internal detail of the map and identification of artifacts.

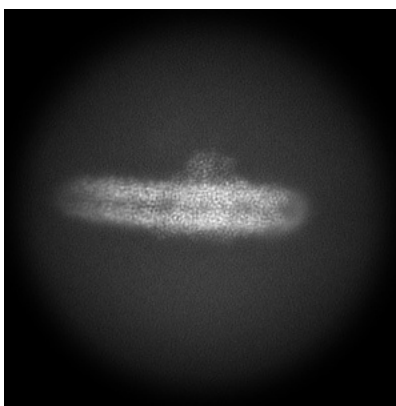
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

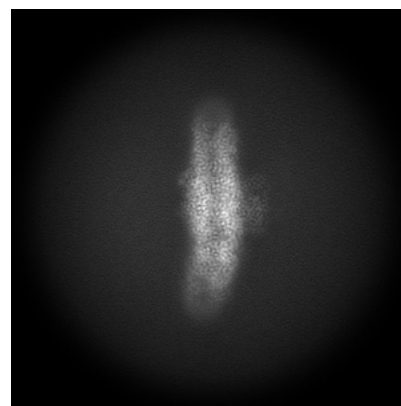
6.1.1 Primary map



X

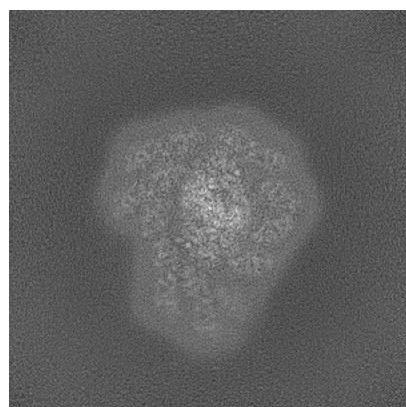


Y

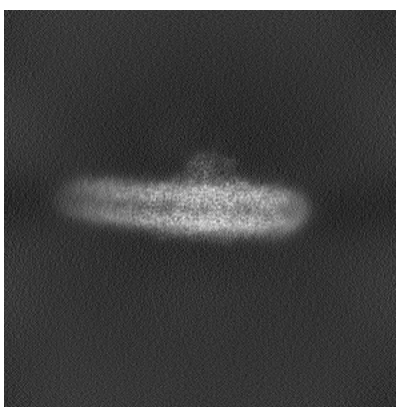


Z

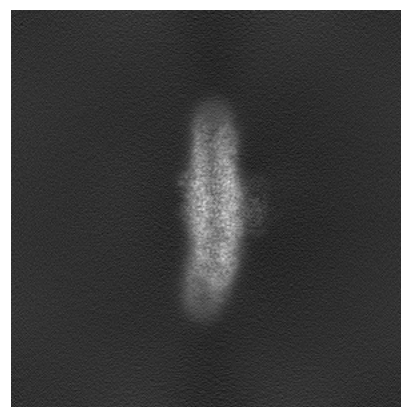
6.1.2 Raw map



X



Y

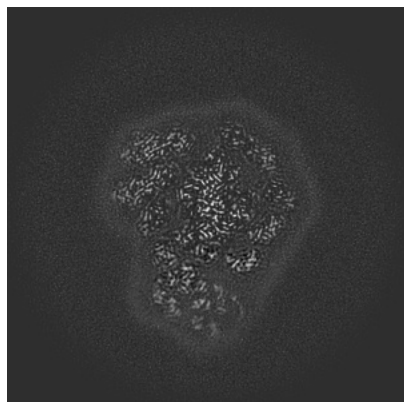


Z

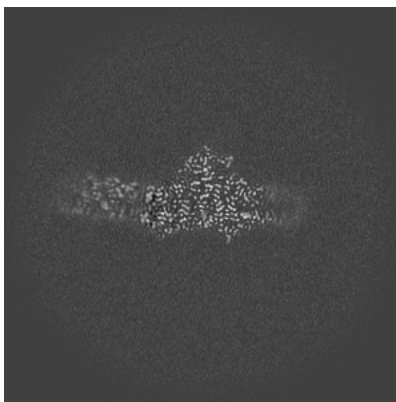
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

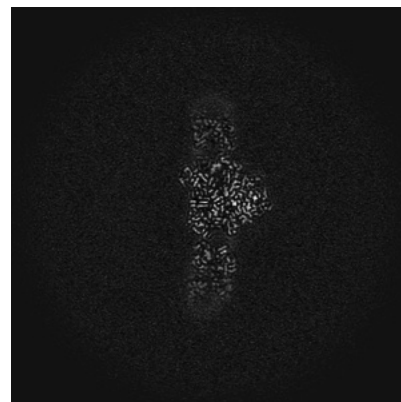
6.2.1 Primary map



X Index: 250

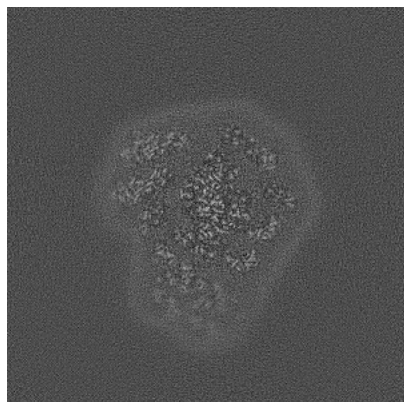


Y Index: 250

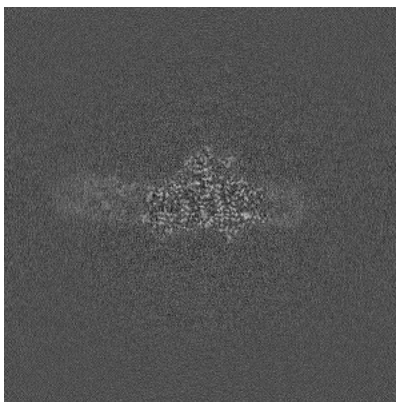


Z Index: 250

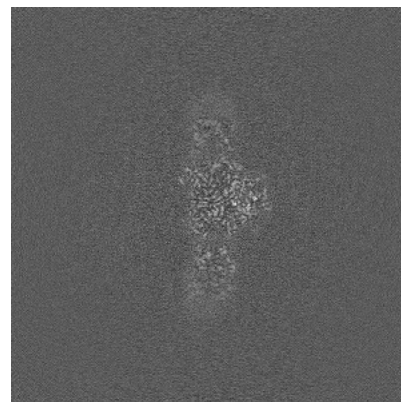
6.2.2 Raw map



X Index: 250



Y Index: 250

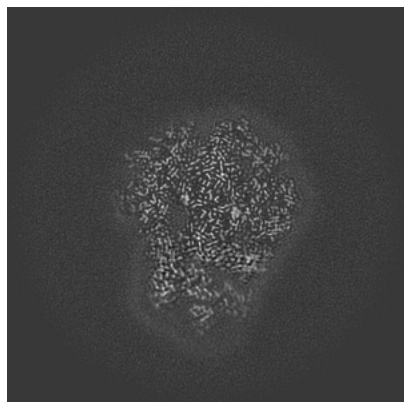


Z Index: 250

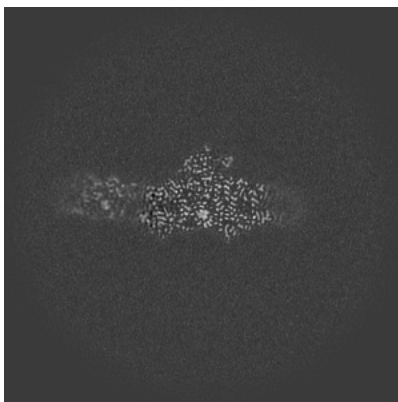
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

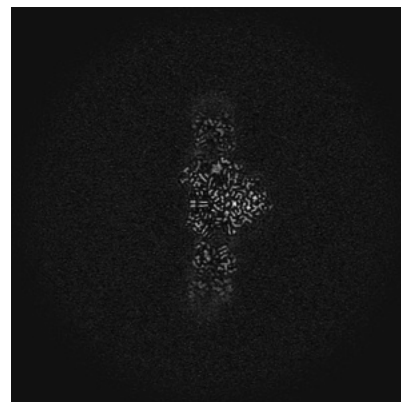
6.3.1 Primary map



X Index: 267

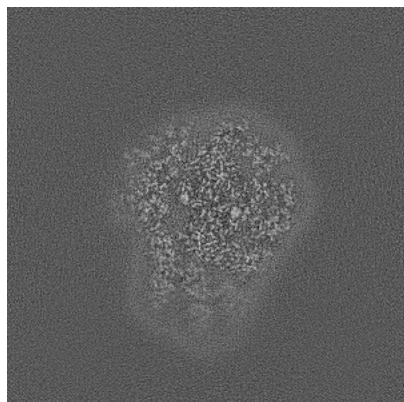


Y Index: 251

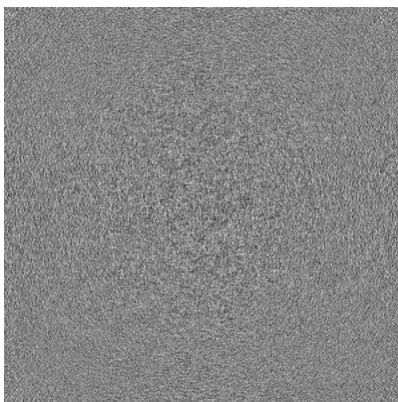


Z Index: 251

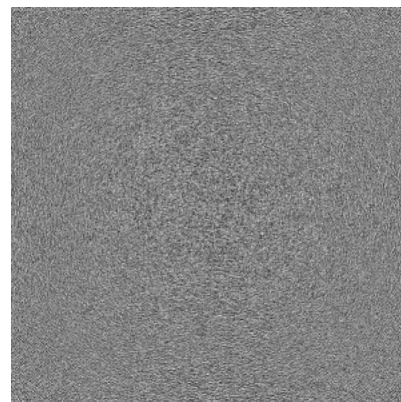
6.3.2 Raw map



X Index: 267



Y Index: 0

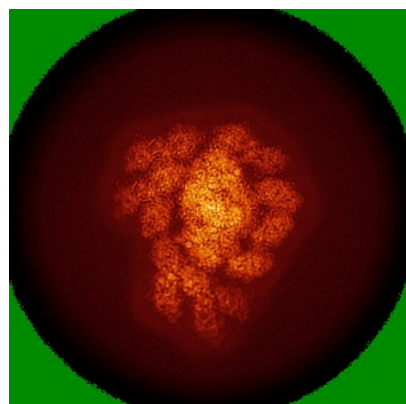


Z Index: 499

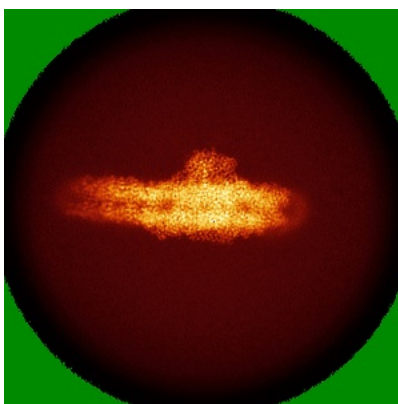
The images above show the largest variance slices of the map in three orthogonal directions.

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

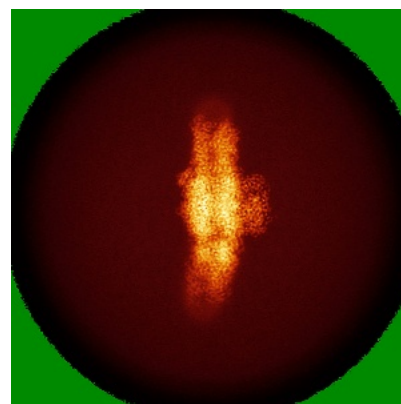
6.4.1 Primary map



X

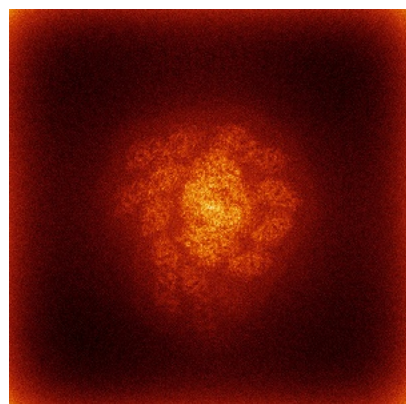


Y

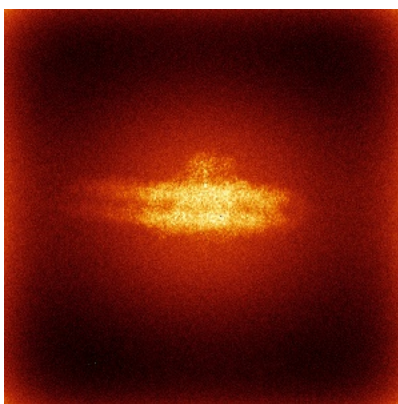


Z

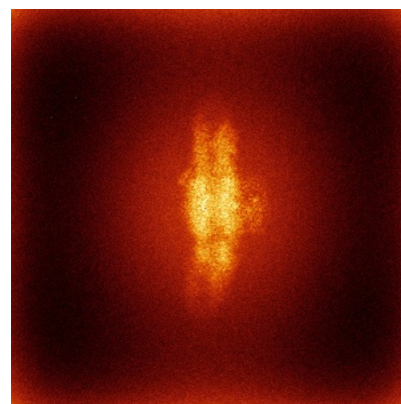
6.4.2 Raw map



X



Y

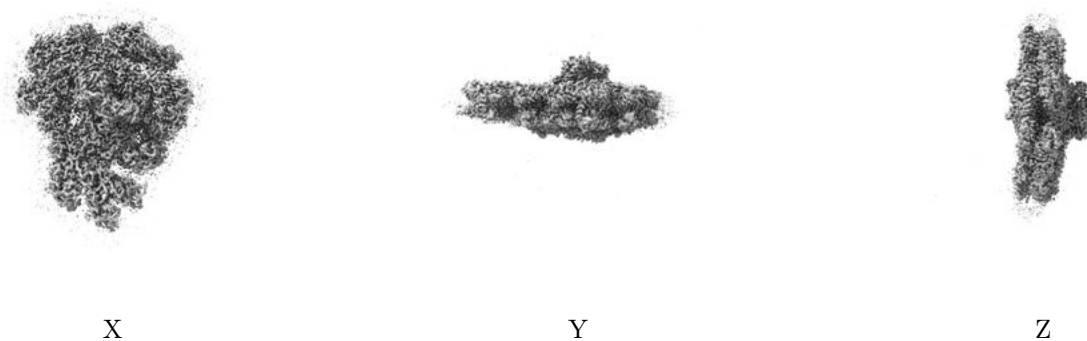


Z

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

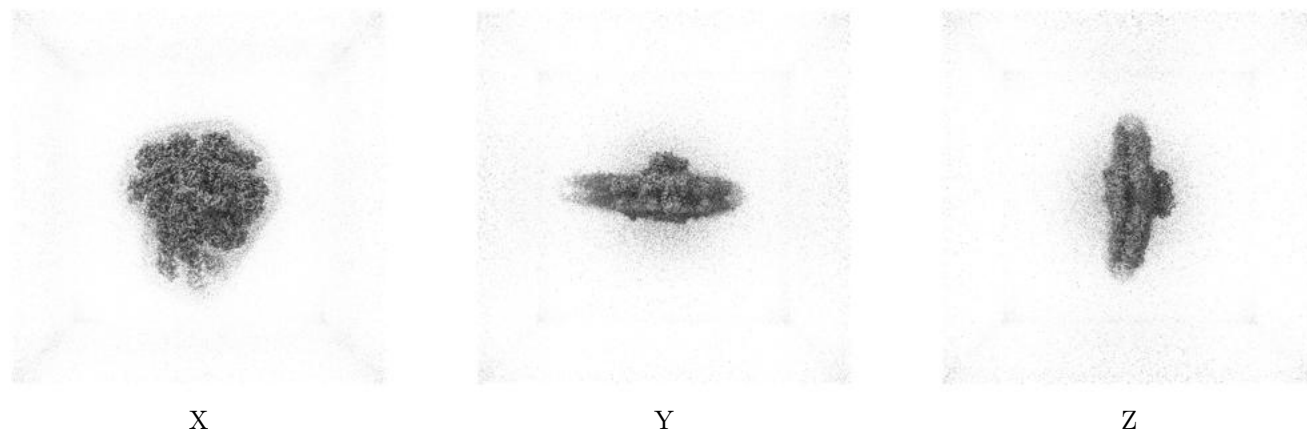
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. 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.

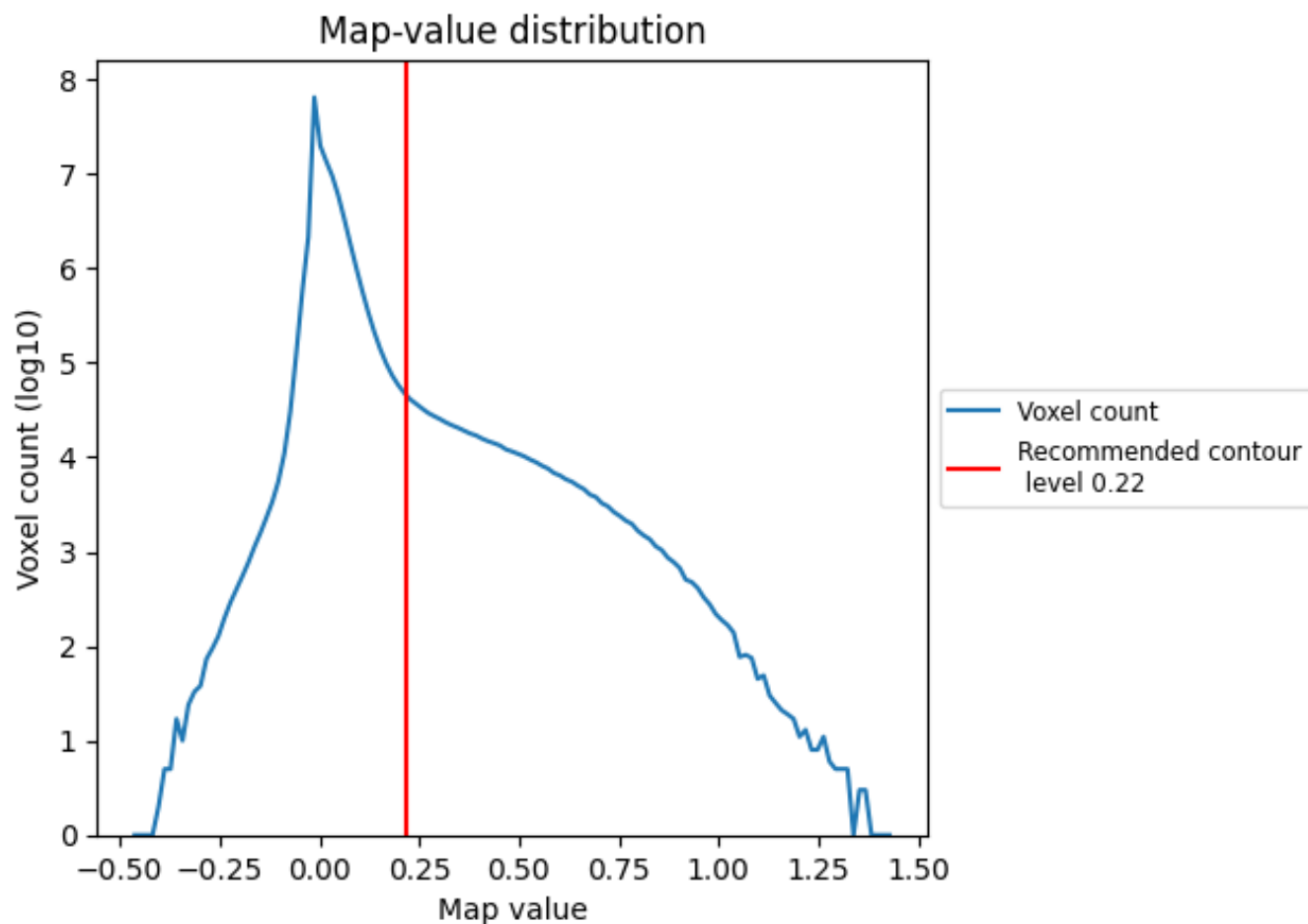
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

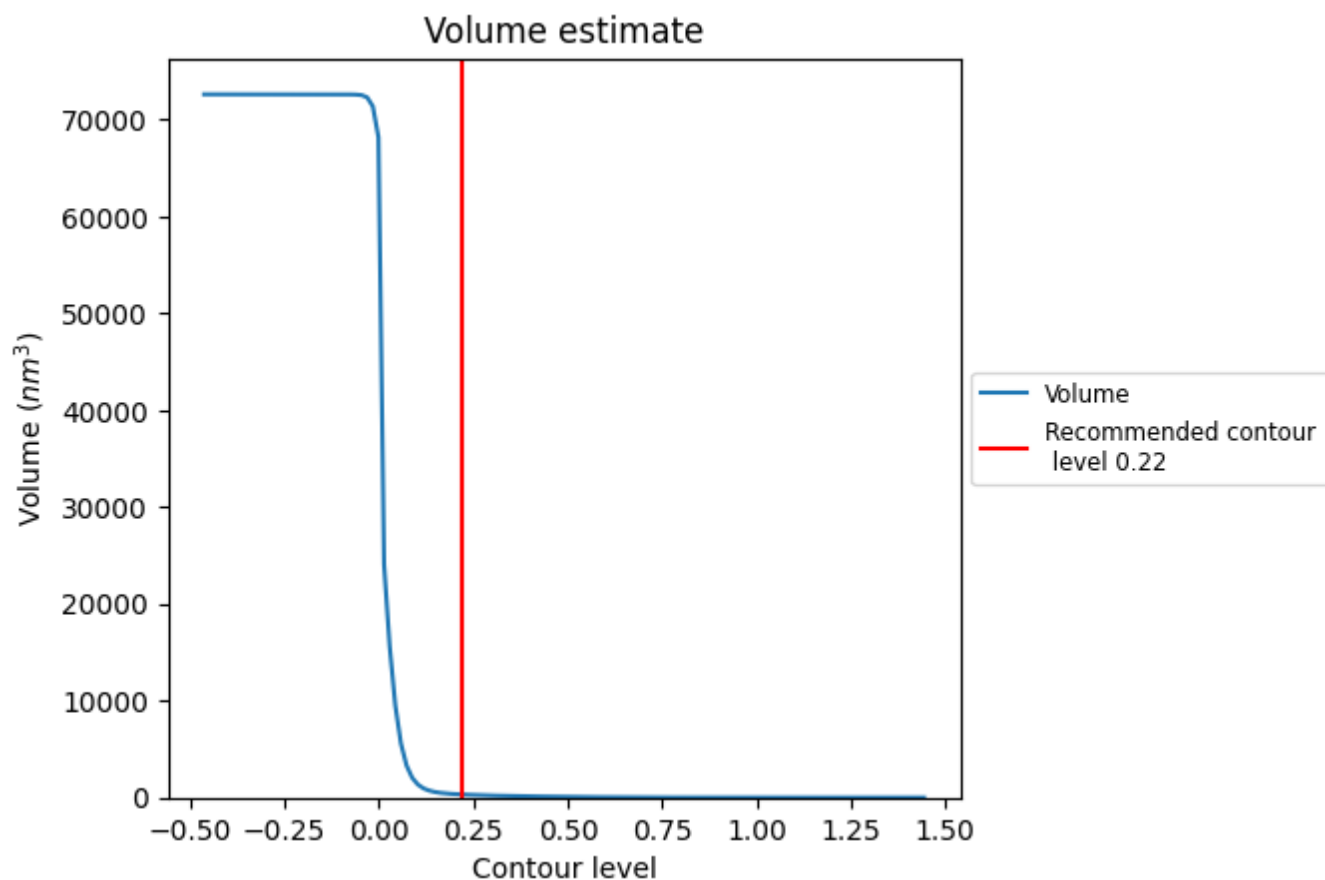
This section contains the results of statistical analysis of the map.

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.

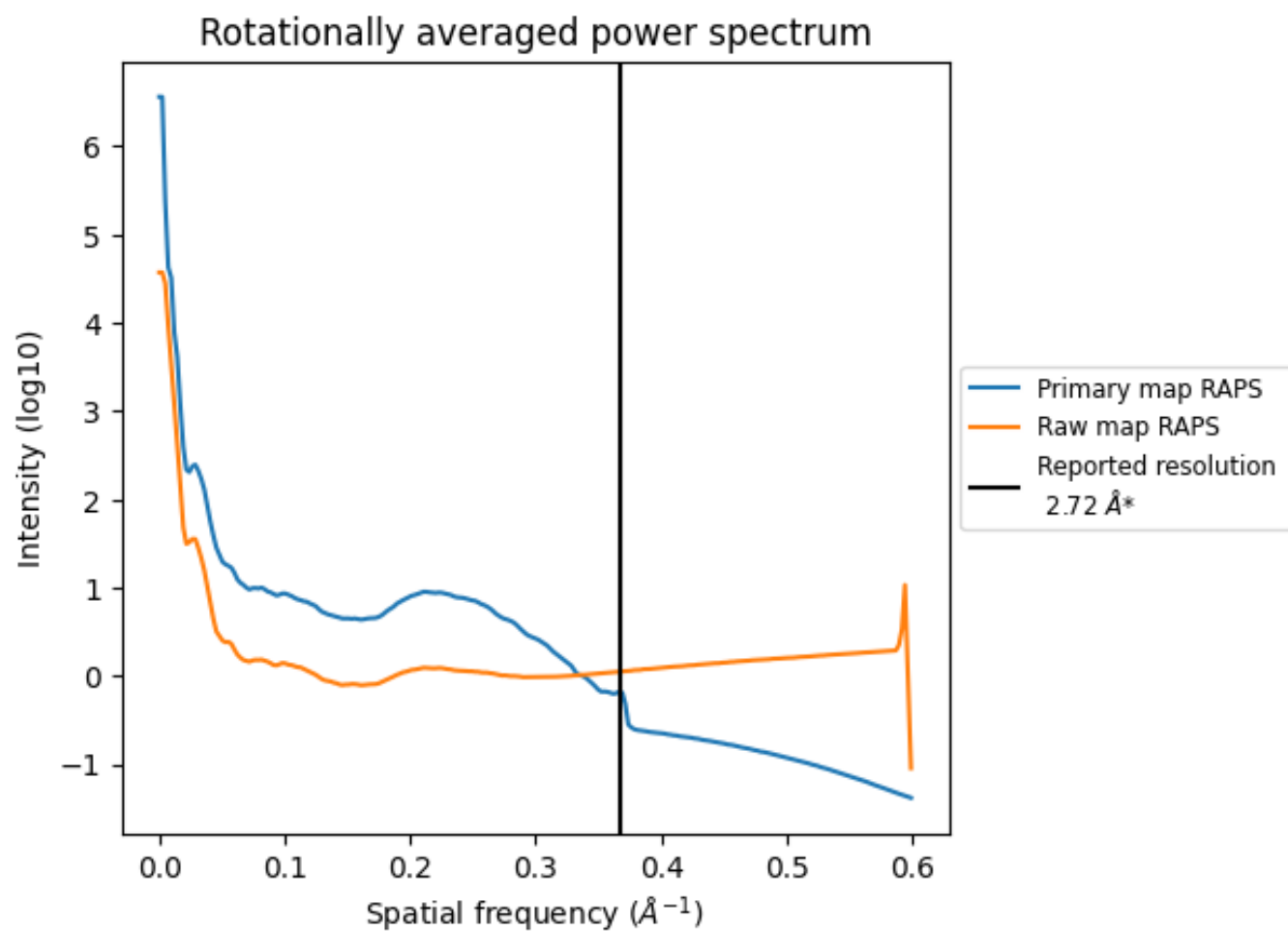
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 315 nm³; this corresponds to an approximate mass of 285 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 ⓘ

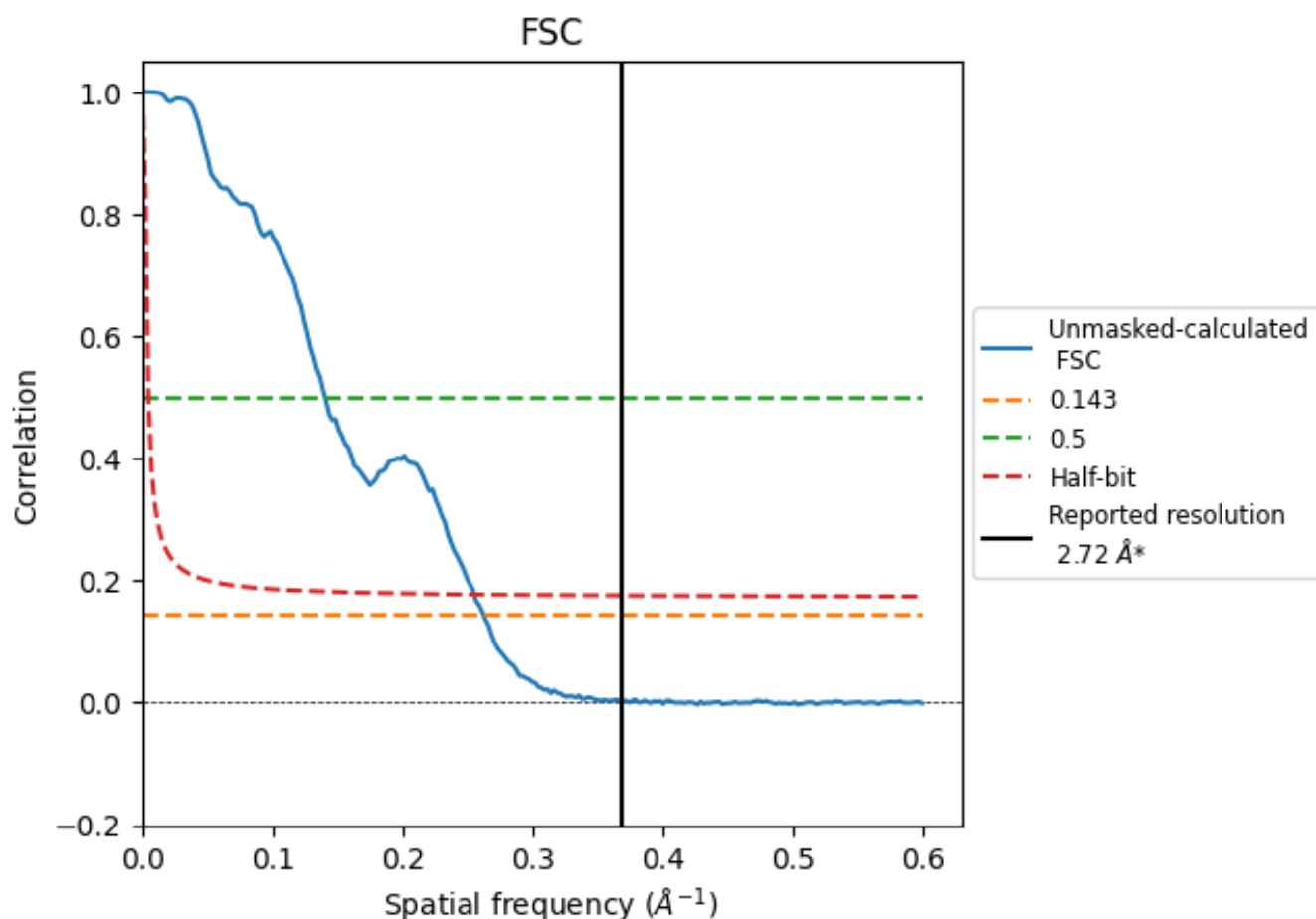


*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.81	7.12	3.92

*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 3.81 differs from the reported value 2.72 by more than 10 %

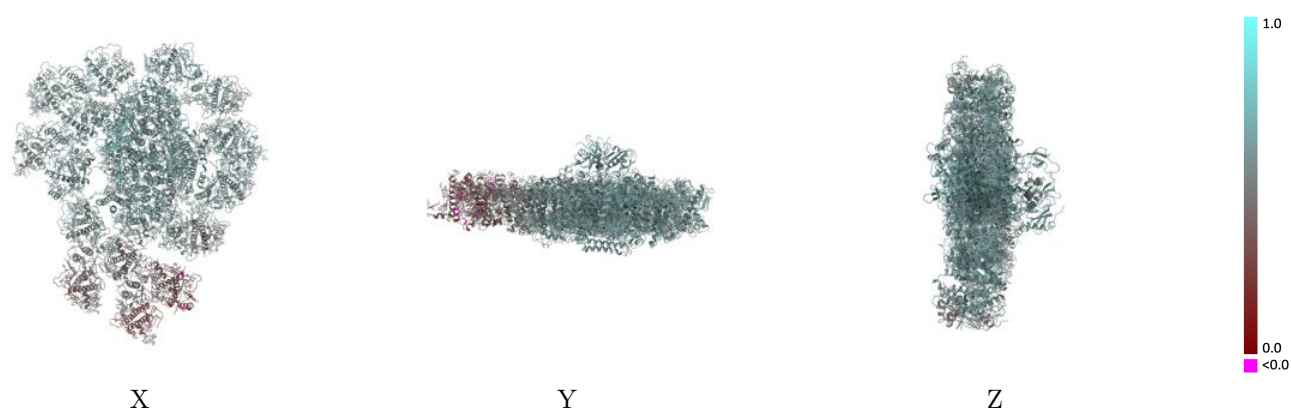
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65121 and PDB model 9VJS. Per-residue inclusion information can be found in section 3 on page 37.

9.1 Map-model overlay [i](#)

This section was not generated.

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

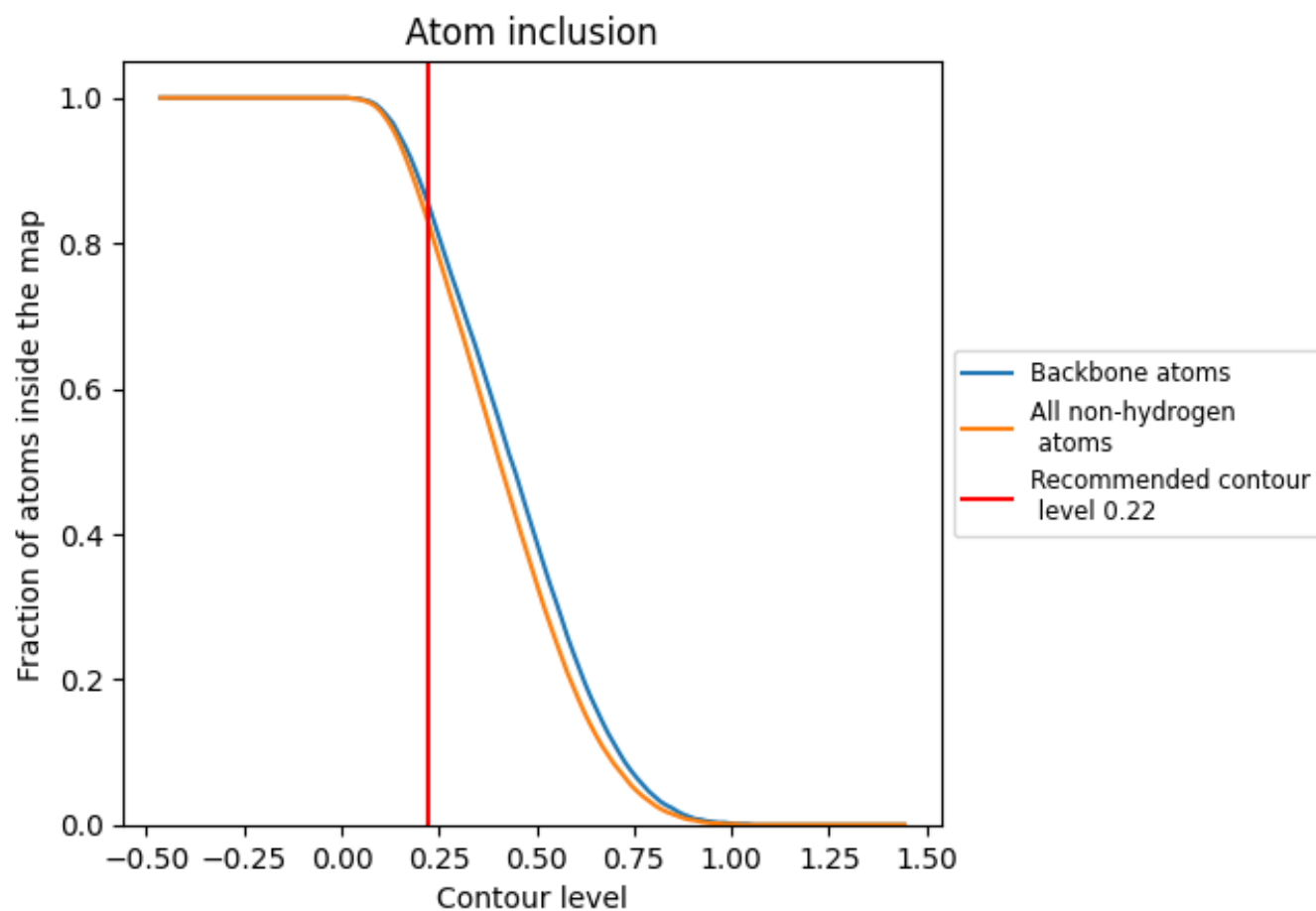


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8330	<div></div> 0.5710
A	<div></div> 0.9380	<div></div> 0.6360
B	<div></div> 0.9210	<div></div> 0.6160
C	<div></div> 0.9430	<div></div> 0.6200
D	<div></div> 0.8720	<div></div> 0.6140
E	<div></div> 0.8550	<div></div> 0.6040
F	<div></div> 0.8690	<div></div> 0.6070
J	<div></div> 0.8970	<div></div> 0.6150
M	<div></div> 0.8400	<div></div> 0.5830
a	<div></div> 0.8230	<div></div> 0.5250
b	<div></div> 0.8560	<div></div> 0.5880
c	<div></div> 0.8400	<div></div> 0.5980
d	<div></div> 0.7760	<div></div> 0.5790
e	<div></div> 0.8250	<div></div> 0.5930
f	<div></div> 0.8350	<div></div> 0.5860
g	<div></div> 0.9040	<div></div> 0.6140
h	<div></div> 0.8640	<div></div> 0.5950
i	<div></div> 0.8280	<div></div> 0.5570
j	<div></div> 0.7880	<div></div> 0.4850
k	<div></div> 0.7750	<div></div> 0.5630
l	<div></div> 0.6880	<div></div> 0.5250
m	<div></div> 0.7010	<div></div> 0.4350
n	<div></div> 0.4940	<div></div> 0.3690
o	<div></div> 0.4690	<div></div> 0.3550

