



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 11:20 AM UTC

PDB ID : 8ZEH / pdb_00008zeh
EMDB ID : EMD-60032
Title : PSI-FCPI-L in Thalassiosira pseudonana
Authors : Feng, Y.; Li, Z.; Wang, W.; Shen, J.R.
Deposited on : 2024-05-06
Resolution : 2.78 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

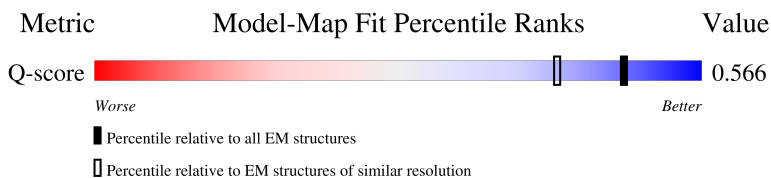
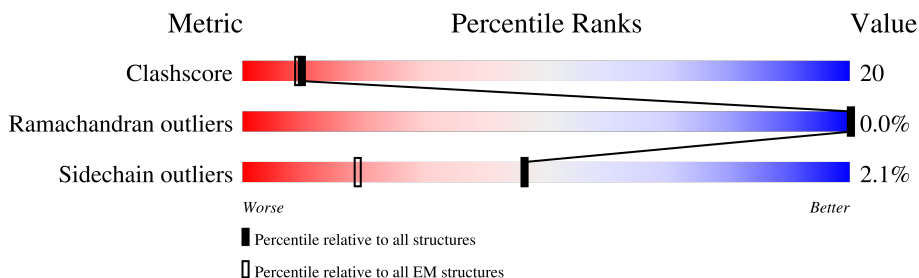
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 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.



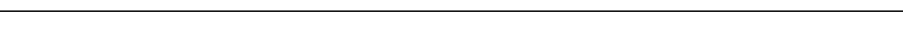
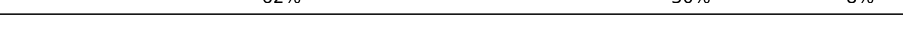
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10754 (2.28 - 3.28)

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	148	
2	B	165	
3	C	170	
4	E	185	

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Mol	Chain	Length	Quality of chain
5	F	170	
6	G	174	
7	H	168	
8	I	172	
9	J	183	
10	K	176	
11	L	217	
12	M	171	
13	a	743	
14	d	132	
15	e	62	
16	f	160	
17	g	131	
18	i	33	
19	j	40	
20	l	146	
21	m	29	
22	r	89	
23	D	164	
24	b	732	
25	c	80	

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
27	CLA	A	203	X	-	-	-
27	CLA	A	204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	A	205	X	-	-	-
27	CLA	A	206	X	-	-	-
27	CLA	A	207	X	-	-	-
27	CLA	A	208	X	-	-	-
27	CLA	A	210	X	-	-	-
27	CLA	A	211	X	-	-	-
27	CLA	B	306	X	-	-	-
27	CLA	B	307	X	-	-	-
27	CLA	B	308	X	-	-	-
27	CLA	B	309	X	-	-	-
27	CLA	B	310	X	-	-	-
27	CLA	B	311	X	-	-	-
27	CLA	B	312	X	-	-	-
27	CLA	B	314	X	-	-	-
27	CLA	C	306	X	-	-	-
27	CLA	C	307	X	-	-	-
27	CLA	C	309	X	-	-	-
27	CLA	C	310	X	-	-	-
27	CLA	C	311	X	-	-	-
27	CLA	C	312	X	-	-	-
27	CLA	C	314	X	-	-	-
27	CLA	C	315	X	-	-	-
27	CLA	C	316	X	-	-	-
27	CLA	C	317	X	-	-	-
27	CLA	C	318	X	-	-	-
27	CLA	D	207	X	-	-	-
27	CLA	D	208	X	-	-	-
27	CLA	D	209	X	-	-	-
27	CLA	D	210	X	-	-	-
27	CLA	D	211	X	-	-	-
27	CLA	D	212	X	-	-	-
27	CLA	D	213	X	-	-	-
27	CLA	D	214	X	-	-	-
27	CLA	D	215	X	-	-	-
27	CLA	D	216	X	-	-	-
27	CLA	D	217	X	-	-	-
27	CLA	E	308	X	-	-	-
27	CLA	E	309	X	-	-	-
27	CLA	E	310	X	-	-	-
27	CLA	E	311	X	-	-	-
27	CLA	E	312	X	-	-	-
27	CLA	E	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	E	314	X	-	-	-
27	CLA	E	315	X	-	-	-
27	CLA	F	305	X	-	X	-
27	CLA	F	306	X	-	-	-
27	CLA	F	307	X	-	-	-
27	CLA	F	308	X	-	-	-
27	CLA	F	309	X	-	X	-
27	CLA	F	310	X	-	-	-
27	CLA	F	311	X	-	-	-
27	CLA	F	313	X	-	-	-
27	CLA	F	314	X	-	-	-
27	CLA	F	315	X	-	-	-
27	CLA	F	316	X	-	-	-
27	CLA	F	317	X	-	-	-
27	CLA	G	306	X	-	-	-
27	CLA	G	307	X	-	-	-
27	CLA	G	308	X	-	-	-
27	CLA	G	309	X	-	-	-
27	CLA	G	310	X	-	-	-
27	CLA	G	311	X	-	-	-
27	CLA	G	312	X	-	-	-
27	CLA	G	314	X	-	-	-
27	CLA	G	315	X	-	-	-
27	CLA	G	316	X	-	-	-
27	CLA	G	317	X	-	-	-
27	CLA	H	204	X	-	-	-
27	CLA	H	205	X	-	-	-
27	CLA	H	206	X	-	-	-
27	CLA	H	207	X	-	-	-
27	CLA	H	208	X	-	-	-
27	CLA	H	209	X	-	-	-
27	CLA	H	210	X	-	-	-
27	CLA	H	212	X	-	-	-
27	CLA	H	213	X	-	-	-
27	CLA	H	214	X	-	-	-
27	CLA	I	305	X	-	-	-
27	CLA	I	306	X	-	-	-
27	CLA	I	307	X	-	-	-
27	CLA	I	308	X	-	-	-
27	CLA	I	309	X	-	-	-
27	CLA	I	310	X	-	-	-
27	CLA	I	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	I	313	X	-	-	-
27	CLA	I	314	X	-	-	-
27	CLA	I	315	X	-	-	-
27	CLA	I	316	X	-	-	-
27	CLA	I	317	X	-	-	-
27	CLA	J	307	X	-	-	-
27	CLA	J	308	X	-	-	-
27	CLA	J	309	X	-	-	-
27	CLA	J	310	X	-	-	-
27	CLA	J	311	X	-	-	-
27	CLA	J	312	X	-	-	-
27	CLA	J	313	X	-	-	-
27	CLA	J	314	X	-	-	-
27	CLA	J	315	X	-	-	-
27	CLA	K	309	X	-	-	-
27	CLA	K	310	X	-	-	-
27	CLA	K	311	X	-	-	-
27	CLA	K	312	X	-	-	-
27	CLA	K	313	X	-	-	-
27	CLA	K	314	X	-	-	-
27	CLA	K	316	X	-	-	-
27	CLA	K	317	X	-	-	-
27	CLA	K	318	X	-	-	-
27	CLA	K	319	X	-	-	-
27	CLA	L	307	X	-	-	-
27	CLA	L	308	X	-	-	-
27	CLA	L	309	X	-	-	-
27	CLA	L	310	X	-	-	-
27	CLA	L	311	X	-	-	-
27	CLA	L	312	X	-	-	-
27	CLA	L	313	X	-	-	-
27	CLA	L	315	X	-	X	-
27	CLA	L	316	X	-	-	-
27	CLA	L	317	X	-	-	-
27	CLA	L	318	X	-	-	-
27	CLA	L	319	X	-	-	-
27	CLA	L	321	X	-	-	-
27	CLA	M	307	X	-	-	-
27	CLA	M	308	X	-	-	-
27	CLA	M	309	X	-	-	-
27	CLA	M	310	X	-	-	-
27	CLA	M	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	M	312	X	-	-	-
27	CLA	M	313	X	-	-	-
27	CLA	M	315	X	-	-	-
27	CLA	M	316	X	-	-	-
27	CLA	M	318	X	-	-	-
27	CLA	M	319	X	-	-	-
27	CLA	a	803	X	-	-	-
27	CLA	a	804	X	-	-	-
27	CLA	a	805	X	-	-	-
27	CLA	a	806	X	-	-	-
27	CLA	a	807	X	-	-	-
27	CLA	a	808	X	-	-	-
27	CLA	a	809	X	-	-	-
27	CLA	a	810	X	-	-	-
27	CLA	a	811	X	-	-	-
27	CLA	a	812	X	-	-	-
27	CLA	a	813	X	-	-	-
27	CLA	a	814	X	-	-	-
27	CLA	a	815	X	-	-	-
27	CLA	a	816	X	-	-	-
27	CLA	a	817	X	-	-	-
27	CLA	a	818	X	-	-	-
27	CLA	a	819	X	-	-	-
27	CLA	a	820	X	-	-	-
27	CLA	a	821	X	-	-	-
27	CLA	a	822	X	-	-	-
27	CLA	a	823	X	-	-	-
27	CLA	a	824	X	-	-	-
27	CLA	a	825	X	-	-	-
27	CLA	a	826	X	-	-	-
27	CLA	a	827	X	-	-	-
27	CLA	a	828	X	-	-	-
27	CLA	a	829	X	-	-	-
27	CLA	a	830	X	-	-	-
27	CLA	a	832	X	-	-	-
27	CLA	a	838	X	-	-	-
27	CLA	a	839	X	-	-	-
27	CLA	a	840	X	-	-	-
27	CLA	a	841	X	-	-	-
27	CLA	a	842	X	-	-	-
27	CLA	a	843	X	-	-	-
27	CLA	a	844	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	a	845	X	-	-	-
27	CLA	a	846	X	-	-	-
27	CLA	a	848	X	-	-	-
27	CLA	a	849	X	-	-	-
27	CLA	a	850	X	-	-	-
27	CLA	a	854	X	-	-	-
27	CLA	a	855	X	-	-	-
27	CLA	a	856	X	-	-	-
27	CLA	b	801	X	-	-	-
27	CLA	b	803	X	-	-	-
27	CLA	b	804	X	-	-	-
27	CLA	b	805	X	-	-	-
27	CLA	b	806	X	-	-	-
27	CLA	b	807	X	-	-	-
27	CLA	b	808	X	-	-	-
27	CLA	b	809	X	-	-	-
27	CLA	b	810	X	-	-	-
27	CLA	b	811	X	-	-	-
27	CLA	b	812	X	-	-	-
27	CLA	b	813	X	-	-	-
27	CLA	b	814	X	-	-	-
27	CLA	b	815	X	-	-	-
27	CLA	b	816	X	-	-	-
27	CLA	b	817	X	-	-	-
27	CLA	b	818	X	-	-	-
27	CLA	b	819	X	-	-	-
27	CLA	b	820	X	-	-	-
27	CLA	b	821	X	-	-	-
27	CLA	b	822	X	-	-	-
27	CLA	b	823	X	-	-	-
27	CLA	b	824	X	-	-	-
27	CLA	b	825	X	-	-	-
27	CLA	b	826	X	-	-	-
27	CLA	b	827	X	-	-	-
27	CLA	b	828	X	-	-	-
27	CLA	b	829	X	-	-	-
27	CLA	b	830	X	-	-	-
27	CLA	b	831	X	-	-	-
27	CLA	b	838	X	-	-	-
27	CLA	b	839	X	-	-	-
27	CLA	b	841	X	-	-	-
27	CLA	b	842	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	b	843	X	-	-	-
27	CLA	b	844	X	-	-	-
27	CLA	b	845	X	-	-	-
27	CLA	b	846	X	-	-	-
27	CLA	b	847	X	-	-	-
27	CLA	b	849	X	-	-	-
27	CLA	b	850	X	-	-	-
27	CLA	f	301	X	-	-	-
27	CLA	f	302	X	-	-	-
27	CLA	f	303	X	-	-	-
27	CLA	i	101	X	-	-	-
27	CLA	j	104	X	-	-	-
27	CLA	l	203	X	-	-	-
27	CLA	l	204	X	-	-	-
27	CLA	l	206	X	-	-	-
27	CLA	r	201	X	-	-	-
29	LMG	L	323	-	-	X	-
36	SF4	b	802	-	-	X	-
36	SF4	c	101	-	-	X	-
36	SF4	c	102	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 54849 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 Tp-Lhcr18.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	148	Total	C	N	O	S	0	0
			1172	760	194	212	6		

- Molecule 2 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	165	Total	C	N	O	S	0	0
			1285	833	204	240	8		

- Molecule 3 is a protein called Fucoxanthin chl a/c light-harvesting protein, major type.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	170	Total	C	N	O	S	0	0
			1302	841	213	240	8		

- Molecule 4 is a protein called Tp-RedCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	185	Total	C	N	O	S	0	0
			1413	902	235	262	14		

- Molecule 5 is a protein called Tp-Lhcr20.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	170	Total	C	N	O	S	0	0
			1299	830	221	236	12		

- Molecule 6 is a protein called Fucoxanthin chl a/c light-harvesting protein, lhcr type.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	174	Total	C	N	O	S	0	0
			1320	837	218	250	15		

- Molecule 7 is a protein called Fucoxanthin chl a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	168	Total	C	N	O	S	0	0
			1300	834	214	242	10		

- Molecule 8 is a protein called Fucoxanthin chl a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	172	Total	C	N	O	S	0	0
			1315	850	212	243	10		

- Molecule 9 is a protein called Fucoxanthin chl a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	183	Total	C	N	O	S	0	0
			1389	887	233	258	11		

- Molecule 10 is a protein called Fucoxanthin chlorophyll a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	176	Total	C	N	O	S	0	0
			1332	853	223	242	14		

- Molecule 11 is a protein called Fucoxanthin chlorophyll a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	217	Total	C	N	O	S	0	0
			1669	1074	274	306	15		

- Molecule 12 is a protein called Fucoxanthin chlorophyll a/c light-harvesting protein, lhcr type.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	171	Total	C	N	O	S	0	0
			1308	847	214	237	10		

- Molecule 13 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	743	Total	C	N	O	S	0	0
			5852	3822	992	1009	29		

- Molecule 14 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	132	Total	C	N	O	S	0	0
			1040	665	177	195	3		

- Molecule 15 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	62	Total	C	N	O	S	0	0
			503	317	89	96	1		

- Molecule 16 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	160	Total	C	N	O	S	0	0
			1242	795	211	233	3		

- Molecule 17 is a protein called Photosystem I reaction center subunit Psa29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	131	Total	C	N	O	S	0	0
			981	619	154	204	4		

- Molecule 18 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	i	33	Total	C	N	O	S	0	0
			256	177	34	44	1		

- Molecule 19 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	j	40	Total	C	N	O	S	0	0
			332	224	48	57	3		

- Molecule 20 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	146	Total	C	N	O	S	0	0
			1095	722	178	193	2		

- Molecule 21 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	29	Total	C	N	O	S	0	0
			220	147	33	38	2		

- Molecule 22 is a protein called Tp-PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	89	Total	C	N	O	S	0	0
			683	443	112	121	7		

- Molecule 23 is a protein called Pt17531-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D	164	Total	C	N	O	S	0	0
			1271	819	208	234	10		

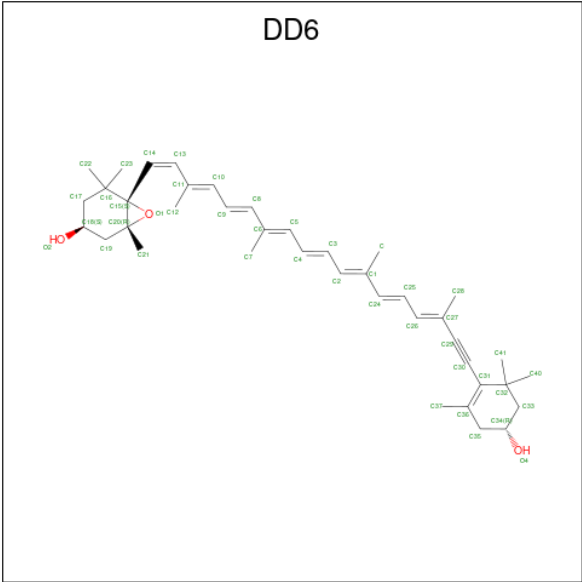
- Molecule 24 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	732	Total	C	N	O	S	0	0
			5824	3827	982	996	19		

- Molecule 25 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	80	Total	C	N	O	S	0	0
			599	368	103	118	10		

- Molecule 26 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).



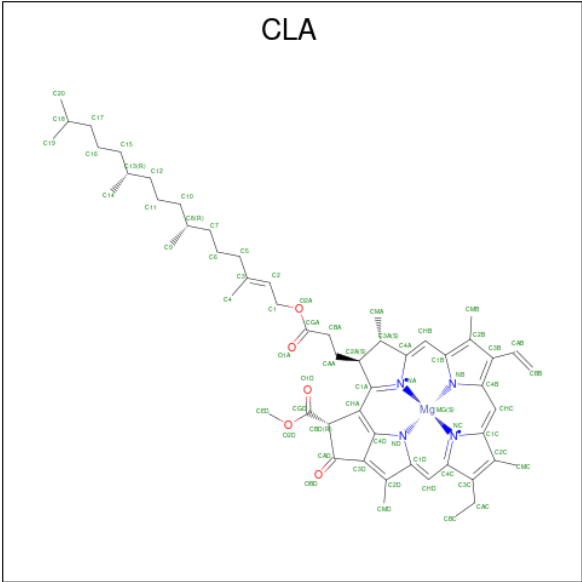
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			43	40	3	
26	A	1	Total	C	O	0
			43	40	3	
26	B	1	Total	C	O	0
			43	40	3	
26	C	1	Total	C	O	0
			43	40	3	
26	E	1	Total	C	O	0
			43	40	3	
26	E	1	Total	C	O	0
			43	40	3	
26	E	1	Total	C	O	0
			43	40	3	
26	E	1	Total	C	O	0
			43	40	3	
26	F	1	Total	C	O	0
			43	40	3	
26	F	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
26	H	1	Total	C	O	0
			43	40	3	
26	I	1	Total	C	O	0
			43	40	3	
26	I	1	Total	C	O	0
			43	40	3	
26	J	1	Total	C	O	0
			43	40	3	
26	J	1	Total	C	O	0
			43	40	3	
26	J	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	L	1	Total	C	O	0
			43	40	3	
26	L	1	Total	C	O	0
			43	40	3	
26	M	1	Total	C	O	0
			43	40	3	
26	M	1	Total	C	O	0
			43	40	3	
26	M	1	Total	C	O	0
			43	40	3	
26	D	1	Total	C	O	0
			43	40	3	

- Molecule 27 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	B	1	Total	C	Mg	N	O	0
			57	49	1	4	3	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 62	C 52	Mg 1	N 4	O 5	0
27	C	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	C	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	C	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	C	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	E	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	E	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	E	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	F	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	F	1	Total 59	C 49	Mg 1	N 4	O 5	0
27	F	1	Total 62	C 52	Mg 1	N 4	O 5	0
27	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	F	1	Total 58	C 48	Mg 1	N 4	O 5	0
27	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	G	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	G	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	G	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
27	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	H	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	H	1	Total 57	C 47	Mg 1	N 4	O 5	0
27	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	I	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	I	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	I	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	I	1	Total 49	C 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	I	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	J	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	J	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	K	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	K	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	K	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	K	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	L	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	L	1	Total 40	C 32	Mg 1	N 4	O 3	0
27	L	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	L	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	L	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	L	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	M	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	M	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	M	1	Total 59	C 49	Mg 1	N 4	O 5	0
27	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	M	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	M	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	M	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	i	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	j	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	l	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	l	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	D	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	D	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	D	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	D	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	D	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	D	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	D	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	D	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
27	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 46	C 36	Mg 1	N 4	O 5	0

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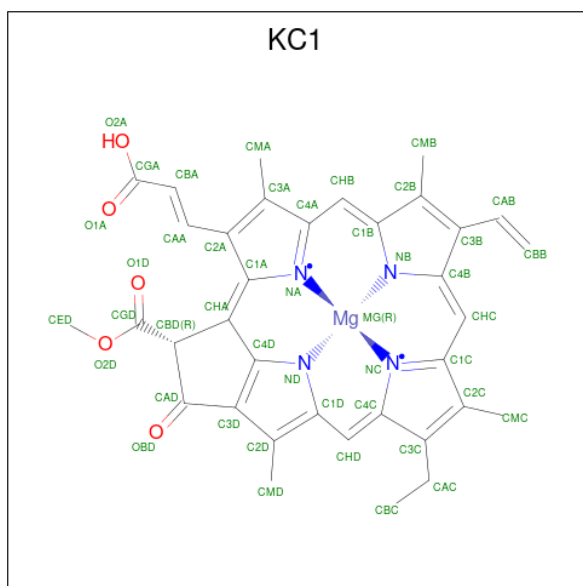
Mol	Chain	Residues	Atoms					AltConf
27	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 28 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



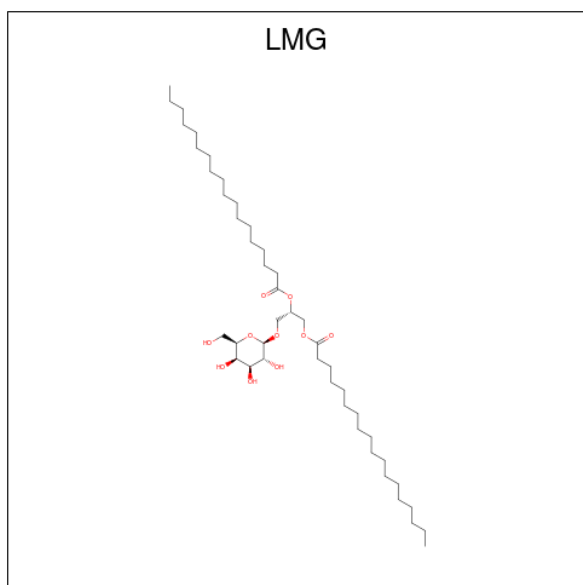
Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



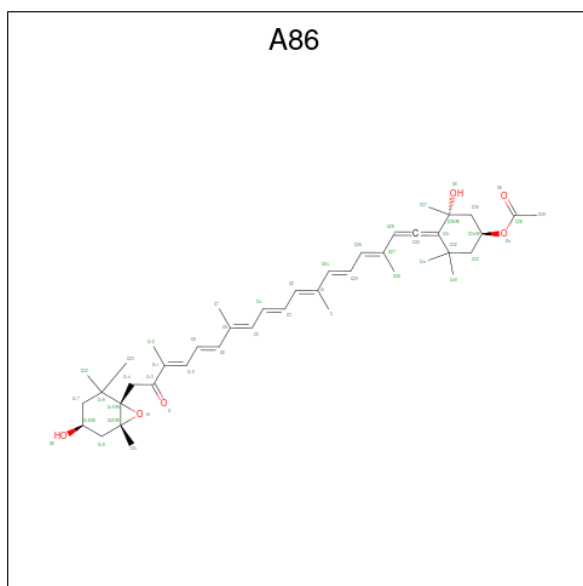
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			51	41	10	
29	A	1	Total	C	O	0
			41	31	10	

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Mol	Chain	Residues	Atoms			AltConf
29	C	1	Total	C	O	0
			31	21	10	
29	C	1	Total	C	O	0
			44	34	10	
29	E	1	Total	C	O	0
			43	33	10	
29	I	1	Total	C	O	0
			37	27	10	
29	J	1	Total	C	O	0
			51	41	10	
29	L	1	Total	C	O	0
			46	36	10	
29	M	1	Total	C	O	0
			42	32	10	
29	a	1	Total	C	O	0
			33	23	10	
29	j	1	Total	C	O	0
			37	27	10	
29	l	1	Total	C	O	0
			40	30	10	
29	D	1	Total	C	O	0
			46	36	10	

- Molecule 30 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆) (labeled as "Ligand of Interest" by depositor).



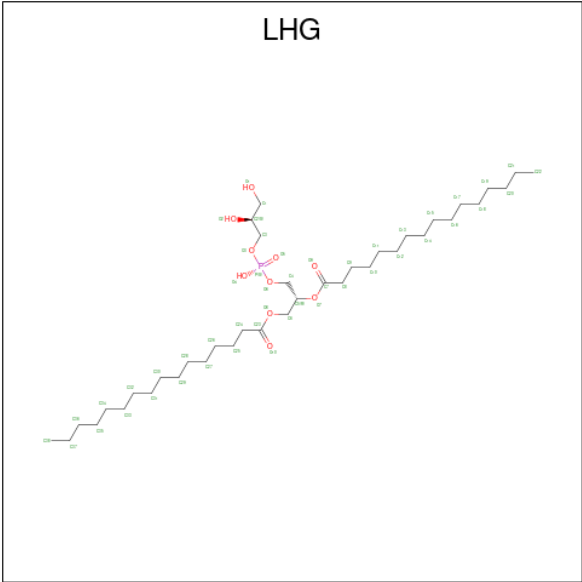
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			48	42	6	
30	B	1	Total	C	O	0
			48	42	6	
30	B	1	Total	C	O	0
			48	42	6	
30	B	1	Total	C	O	0
			48	42	6	
30	B	1	Total	C	O	0
			48	42	6	
30	C	1	Total	C	O	0
			48	42	6	
30	C	1	Total	C	O	0
			48	42	6	
30	C	1	Total	C	O	0
			48	42	6	
30	E	1	Total	C	O	0
			48	42	6	
30	F	1	Total	C	O	0
			48	42	6	
30	F	1	Total	C	O	0
			48	42	6	
30	G	1	Total	C	O	0
			48	42	6	
30	H	1	Total	C	O	0
			48	42	6	
30	H	1	Total	C	O	0
			48	42	6	
30	I	1	Total	C	O	0
			48	42	6	
30	I	1	Total	C	O	0
			48	42	6	
30	J	1	Total	C	O	0
			48	42	6	
30	J	1	Total	C	O	0
			48	42	6	
30	J	1	Total	C	O	0
			48	42	6	
30	K	1	Total	C	O	0
			48	42	6	
30	K	1	Total	C	O	0
			48	42	6	
30	K	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
30	K	1	Total	C	O	0
			48	42	6	
30	K	1	Total	C	O	0
			48	42	6	
30	K	1	Total	C	O	0
			48	42	6	
30	L	1	Total	C	O	0
			48	42	6	
30	L	1	Total	C	O	0
			48	42	6	
30	L	1	Total	C	O	0
			48	42	6	
30	L	1	Total	C	O	0
			48	42	6	
30	M	1	Total	C	O	0
			48	42	6	
30	M	1	Total	C	O	0
			48	42	6	
30	M	1	Total	C	O	0
			48	42	6	
30	m	1	Total	C	O	0
			48	42	6	
30	r	1	Total	C	O	0
			48	42	6	
30	D	1	Total	C	O	0
			48	42	6	
30	D	1	Total	C	O	0
			48	42	6	
30	D	1	Total	C	O	0
			48	42	6	
30	b	1	Total	C	O	0
			48	42	6	

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



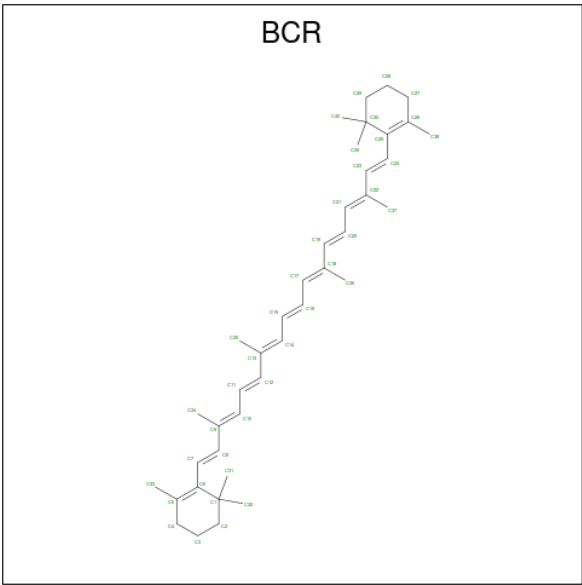
Mol	Chain	Residues	Atoms				AltConf
31	B	1	Total	C	O	P	0
			42	31	10	1	
31	E	1	Total	C	O	P	0
			42	31	10	1	
31	E	1	Total	C	O	P	0
			49	38	10	1	
31	H	1	Total	C	O	P	0
			35	24	10	1	
31	I	1	Total	C	O	P	0
			35	24	10	1	
31	K	1	Total	C	O	P	0
			33	24	8	1	
31	M	1	Total	C	O	P	0
			47	36	10	1	
31	a	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			27	16	10	1	
31	a	1	Total	C	O	P	0
			33	22	10	1	
31	j	1	Total	C	O	P	0
			49	38	10	1	
31	D	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
31	b	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 32 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



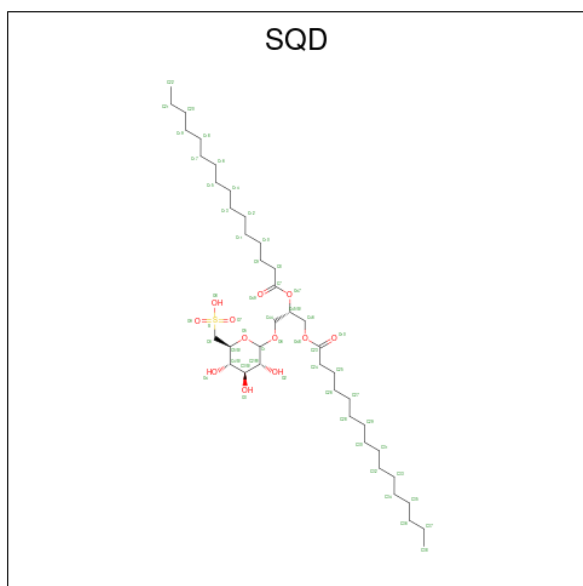
Mol	Chain	Residues	Atoms		AltConf
32	E	1	Total	C	0
			40	40	
32	E	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	f	1	Total	C	0
			40	40	
32	f	1	Total	C	0
			40	40	
32	i	1	Total	C	0
			40	40	

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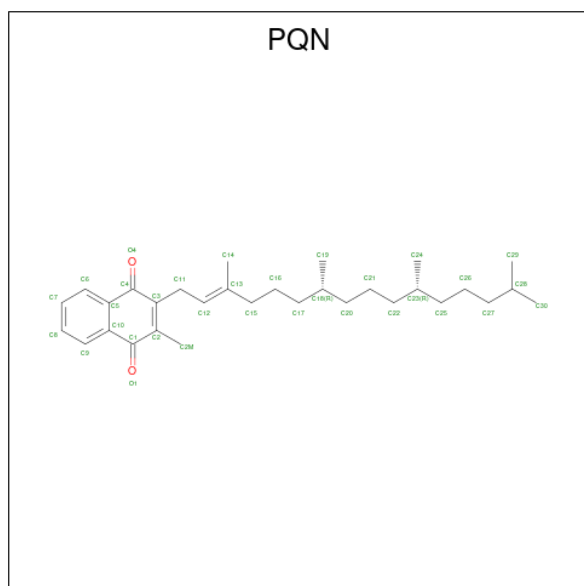
Mol	Chain	Residues	Atoms	AltConf
32	i	1	Total C 40 40	0
32	j	1	Total C 40 40	0
32	j	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	m	1	Total C 40 40	0
32	r	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



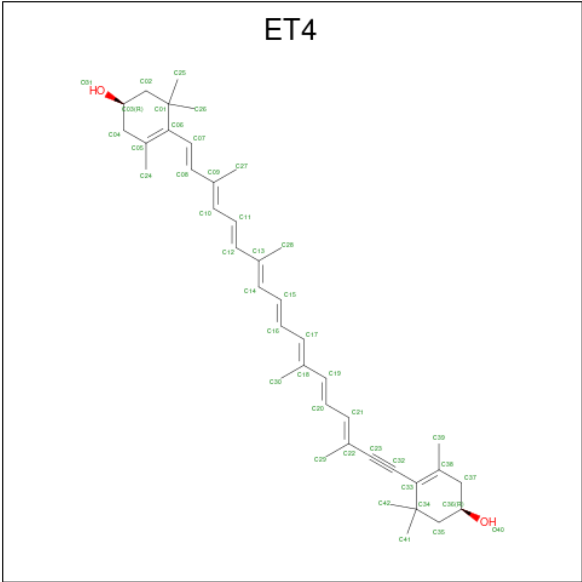
Mol	Chain	Residues	Atoms				AltConf
33	J	1	Total	C	O	S	0
			33	23	9	1	

- Molecule 34 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



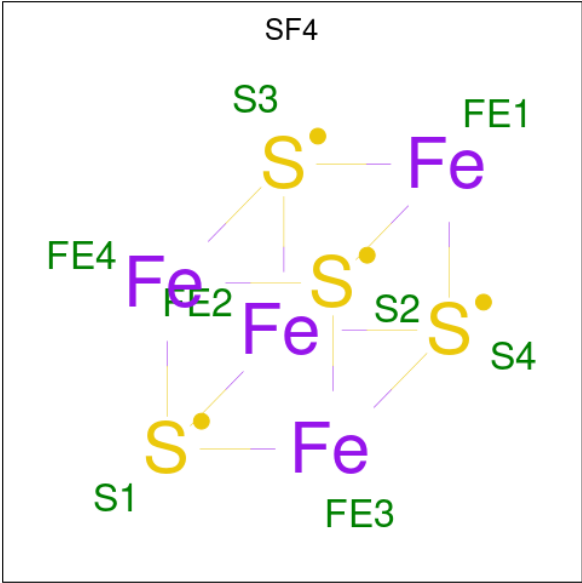
Mol	Chain	Residues	Atoms				AltConf
34	a	1	Total	C	O		0
			33	31	2		
34	b	1	Total	C	O		0
			33	31	2		

- Molecule 35 is (1 {R})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15-octaen-17-ynyl]cyclohex-3-en-1-ol (CCD ID: ET4) (formula: $C_{40}H_{54}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
35	1	1	Total	C	O	0
			42	40	2	

- Molecule 36 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



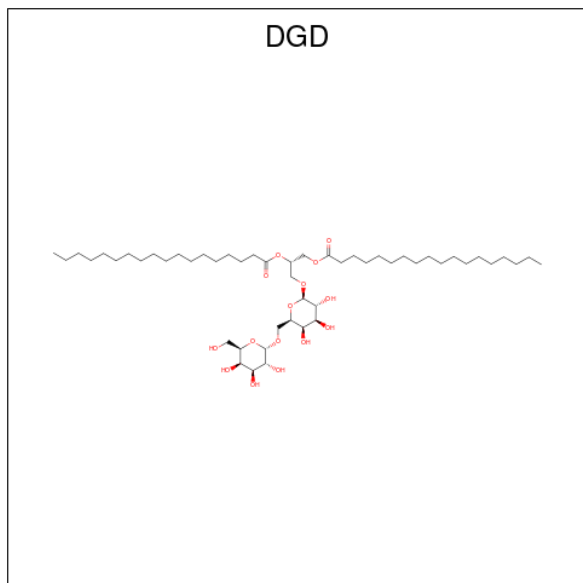
Mol	Chain	Residues	Atoms			AltConf
36	b	1	Total	Fe	S	0
			8	4	4	
36	c	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
36	c	1	8	4	4	0

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

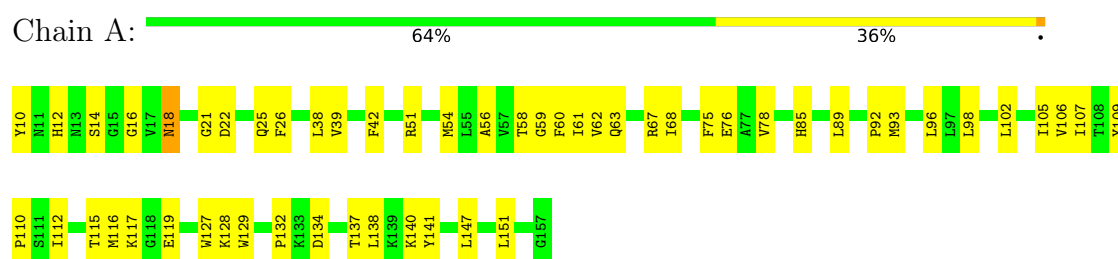


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
37	b	1	60	45	15	0

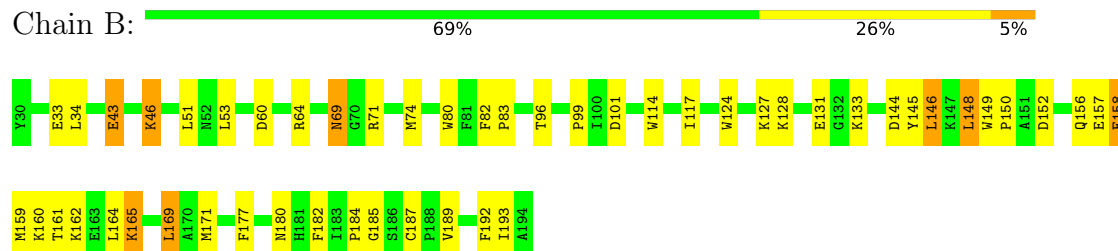
3 Residue-property plots [i](#)

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.

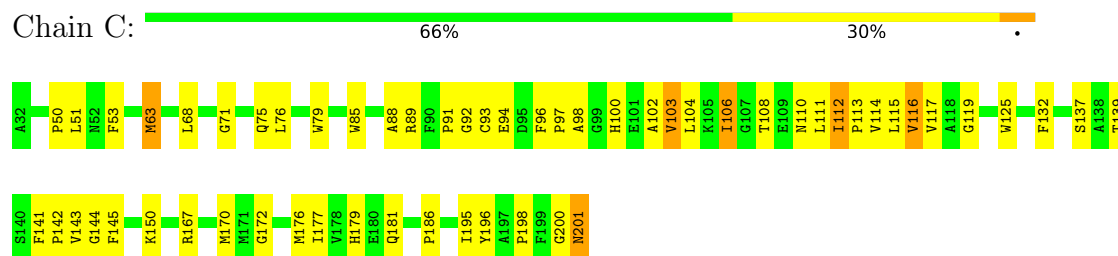
• Molecule 1: Tp-Lhcr18



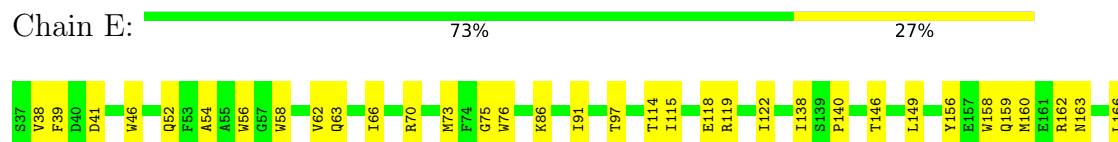
• Molecule 2: Fucoxanthin chlorophyll a/c-binding protein Lhcq8

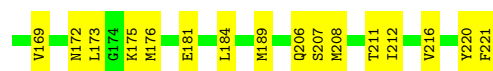


• Molecule 3: Fucoxanthin chl a/c light-harvesting protein, major type



• Molecule 4: Tp-RedCAP





• Molecule 5: Tp-Lhcr20



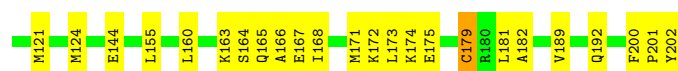
• Molecule 6: Fucoxanthin chl a/c light-harvesting protein, lhcr type



• Molecule 7: Fucoxanthin chl a/c light-harvesting protein

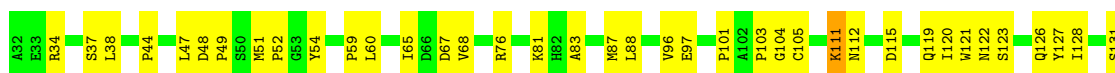


• Molecule 8: Fucoxanthin chl a/c light-harvesting protein



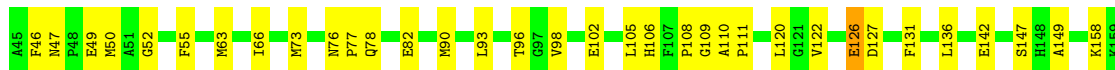
• Molecule 9: Fucoxanthin chl a/c light-harvesting protein





- Molecule 10: Fucoxanthin chlorophyll a/c light-harvesting protein

Chain K: 73% 26% .



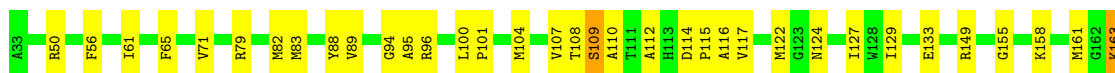
- Molecule 11: Fucoxanthin chlorophyll a/c light-harvesting protein

Chain L: 58% 40% .



- Molecule 12: Fucoxanthin chlorophyll a/c light-harvesting protein, lhcr type

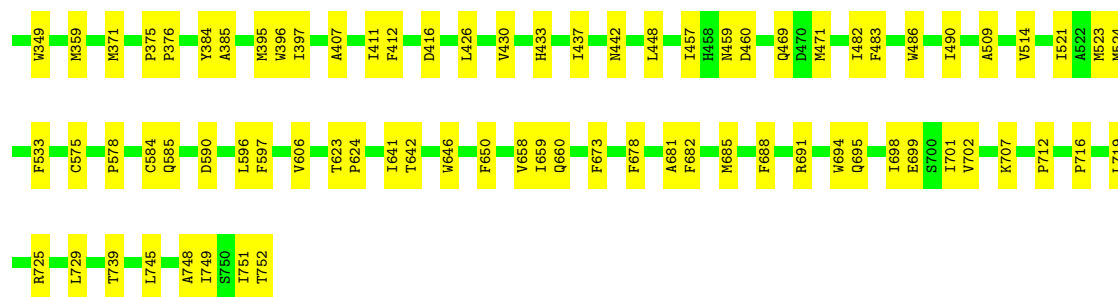
Chain M: 70% 27% .



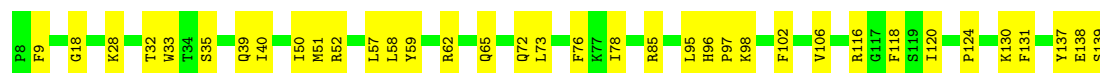
- Molecule 13: Photosystem I P700 chlorophyll a apoprotein A1

Chain a: 80% 19%





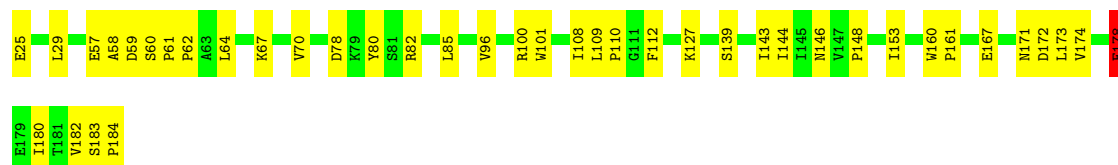
• Molecule 14: Photosystem I reaction center subunit II



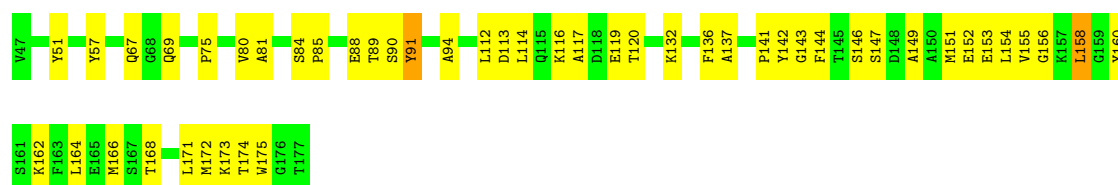
• Molecule 15: Photosystem I reaction center subunit IV



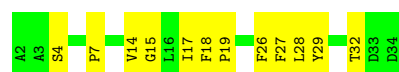
• Molecule 16: Photosystem I reaction center subunit III



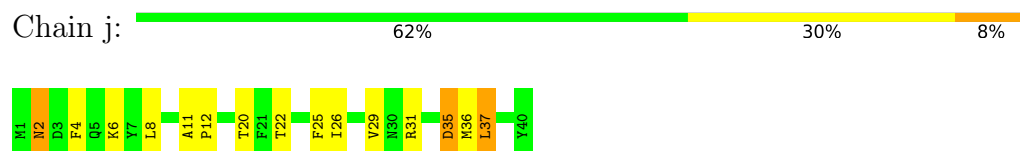
• Molecule 17: Photosystem I reaction center subunit Psa29



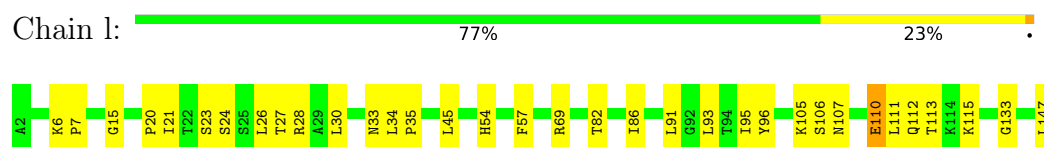
• Molecule 18: Photosystem I reaction center subunit VIII



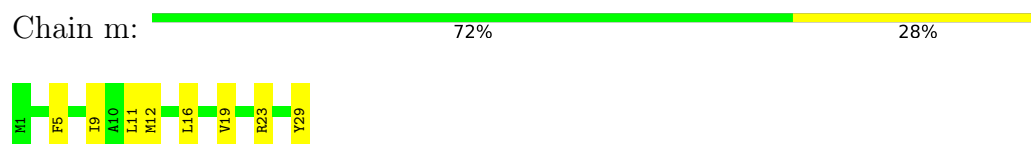
- Molecule 19: Photosystem I reaction center subunit IX



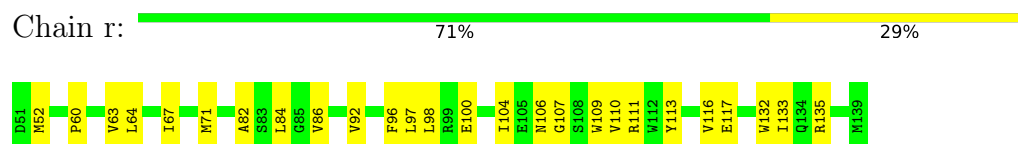
- Molecule 20: Photosystem I reaction center subunit XI



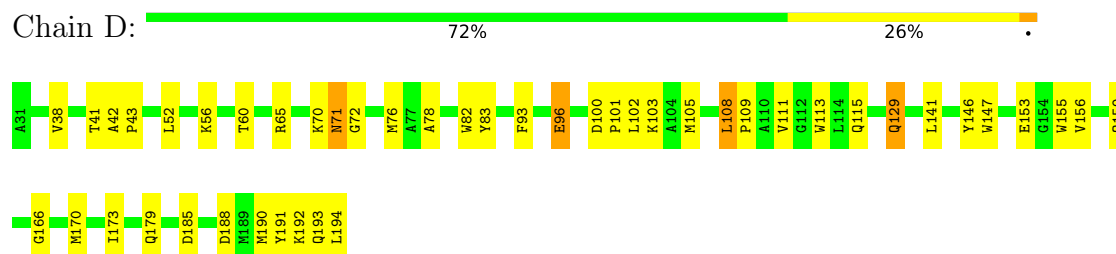
- Molecule 21: Photosystem I reaction center subunit XII



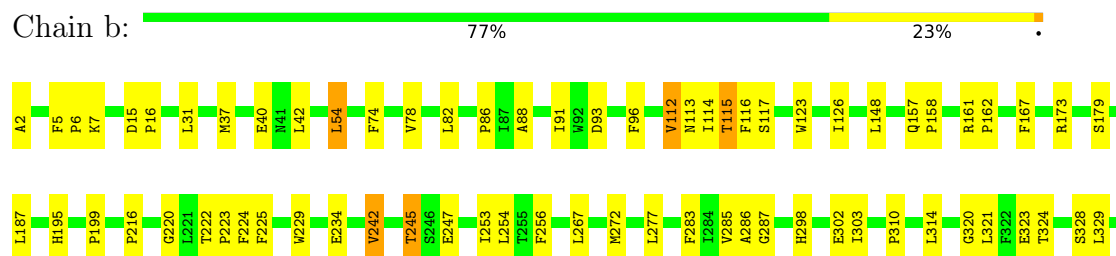
- Molecule 22: Tp-PsaR

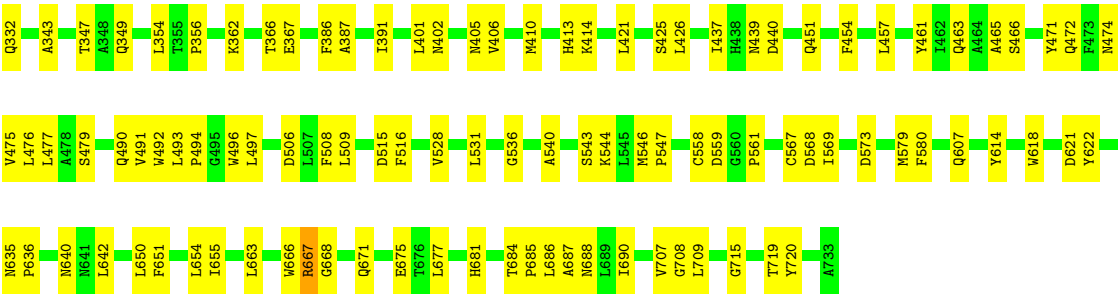


- Molecule 23: Pt17531-like protein

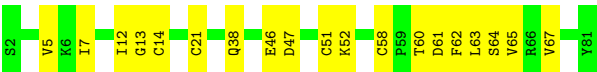


- Molecule 24: Photosystem I P700 chlorophyll a apoprotein A2





● Molecule 25: Photosystem I iron-sulfur center



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129097	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.719	Depositor
Minimum map value	-0.472	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.088	Depositor
Map size ($\text{\AA}$)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KC1, LMG, PQN, LHG, BCR, DD6, A86, SQD, ET4, SF4, DGD, CLA

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	0.46	0/1206	0.70	0/1637
2	B	0.53	0/1324	0.65	0/1804
3	C	0.50	0/1339	0.68	1/1813 (0.1%)
4	E	0.52	0/1450	0.67	0/1974
5	F	0.49	0/1330	0.71	1/1794 (0.1%)
6	G	0.49	0/1348	0.74	2/1815 (0.1%)
7	H	0.51	0/1334	0.65	1/1809 (0.1%)
8	I	0.53	0/1348	0.68	0/1820
9	J	0.50	0/1426	0.69	0/1931
10	K	0.53	0/1368	0.67	0/1845
11	L	0.43	0/1716	0.67	0/2327
12	M	0.50	0/1345	0.72	3/1823 (0.2%)
13	a	0.53	0/6049	0.67	2/8234 (0.0%)
14	d	0.47	0/1067	0.72	0/1441
15	e	0.43	0/511	0.72	0/690
16	f	0.53	0/1271	0.73	3/1727 (0.2%)
17	g	0.43	0/1003	0.68	1/1354 (0.1%)
18	i	0.51	0/264	0.73	0/360
19	j	0.52	0/342	0.78	2/463 (0.4%)
20	l	0.54	0/1123	0.67	1/1523 (0.1%)
21	m	0.56	0/222	0.56	0/300
22	r	0.48	0/704	0.59	0/957
23	D	0.51	0/1304	0.64	0/1771
24	b	0.52	0/6034	0.66	1/8236 (0.0%)
25	c	0.51	0/609	0.80	1/826 (0.1%)
All	All	0.51	0/37037	0.68	19/50274 (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
14	d	0	1

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	667	ARG	N-CA-C	8.64	120.32	111.07
17	g	156	GLY	N-CA-C	-8.10	103.10	112.50
6	G	46	THR	N-CA-C	-6.81	103.28	112.26
16	f	58	ALA	CB-CA-C	-6.30	109.29	116.54
13	a	266	GLY	N-CA-C	-6.29	102.72	112.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	d	96	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1172	0	1144	54	0
2	B	1285	0	1239	61	0
3	C	1302	0	1243	69	0
4	E	1413	0	1365	44	0
5	F	1299	0	1281	115	0
6	G	1320	0	1285	60	0
7	H	1300	0	1262	45	0
8	I	1315	0	1281	66	0
9	J	1389	0	1341	79	0
10	K	1332	0	1301	44	0
11	L	1669	0	1619	104	0
12	M	1308	0	1278	69	0
13	a	5852	0	5682	116	0
14	d	1040	0	1027	26	0
15	e	503	0	500	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	f	1242	0	1239	36	0
17	g	981	0	922	39	0
18	i	256	0	259	12	0
19	j	332	0	331	20	0
20	l	1095	0	1116	35	0
21	m	220	0	241	7	0
22	r	683	0	675	27	0
23	D	1271	0	1227	44	0
24	b	5824	0	5643	152	0
25	c	599	0	582	20	0
26	A	86	0	0	8	0
26	B	43	0	0	0	0
26	C	43	0	0	1	0
26	D	43	0	0	3	0
26	E	172	0	0	3	0
26	F	86	0	0	2	0
26	G	172	0	0	2	0
26	H	43	0	0	3	0
26	I	86	0	0	4	0
26	J	129	0	0	3	0
26	K	43	0	0	1	0
26	L	86	0	0	9	0
26	M	129	0	0	2	0
27	A	442	0	419	38	0
27	B	469	0	479	35	0
27	C	547	0	472	61	0
27	D	568	0	501	36	0
27	E	462	0	454	21	0
27	F	637	0	565	98	0
27	G	571	0	497	42	0
27	H	587	0	583	56	0
27	I	624	0	549	52	0
27	J	522	0	516	49	0
27	K	553	0	520	68	0
27	L	684	0	621	90	0
27	M	634	0	563	70	0
27	a	2671	0	2759	146	0
27	b	2492	0	2569	142	0
27	f	175	0	177	4	0
27	i	60	0	59	2	0
27	j	41	0	29	1	0
27	l	159	0	144	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	r	45	0	33	1	0
28	A	45	0	0	0	0
28	B	45	0	0	4	0
28	C	90	0	0	5	0
28	F	45	0	0	5	0
28	G	45	0	0	0	0
28	H	45	0	0	1	0
28	I	45	0	0	2	0
28	J	45	0	0	1	0
28	K	90	0	0	4	0
28	L	135	0	0	10	0
28	M	45	0	0	3	0
29	A	92	0	121	9	0
29	C	75	0	88	1	0
29	D	46	0	61	1	0
29	E	43	0	55	6	0
29	I	37	0	43	2	0
29	J	51	0	71	5	0
29	L	46	0	60	26	0
29	M	42	0	54	2	0
29	a	33	0	33	2	0
29	j	37	0	42	1	0
29	l	40	0	49	1	0
30	A	48	0	0	0	0
30	B	192	0	0	7	0
30	C	144	0	0	5	0
30	D	144	0	0	4	0
30	E	48	0	0	0	0
30	F	96	0	0	8	0
30	G	48	0	0	6	0
30	H	96	0	0	17	0
30	I	96	0	0	2	0
30	J	144	0	0	10	0
30	K	288	0	0	13	0
30	L	192	0	0	22	0
30	M	144	0	0	10	0
30	b	48	0	0	4	0
30	m	48	0	0	5	0
30	r	48	0	0	2	0
31	B	42	0	54	3	0
31	D	49	0	74	7	0
31	E	91	0	131	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	H	35	0	43	0	0
31	I	35	0	40	3	0
31	K	33	0	42	1	0
31	M	47	0	67	5	0
31	a	207	0	282	21	0
31	b	49	0	74	6	0
31	j	49	0	74	5	0
32	E	80	0	112	8	0
32	a	200	0	280	34	0
32	b	160	0	224	18	0
32	f	80	0	112	8	0
32	i	80	0	112	13	0
32	j	80	0	112	17	0
32	l	80	0	112	10	0
32	m	40	0	56	4	0
32	r	40	0	56	1	0
33	J	33	0	39	7	0
34	a	33	0	46	1	0
34	b	33	0	46	4	0
35	l	42	0	0	0	0
36	b	8	0	0	2	0
36	c	16	0	0	8	0
37	b	60	0	81	1	0
All	All	54849	0	50538	2076	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 20.

The worst 5 of 2076 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)
29:L:323:LMG:O6	29:L:323:LMG:C1	1.69	1.39
30:K:301:A86:C37	27:K:316:CLA:H42	1.61	1.29
29:L:323:LMG:H351	29:L:323:LMG:C11	1.65	1.24
27:I:317:CLA:HED2	27:I:317:CLA:O1A	1.35	1.22
26:A:201:DD6:C2	27:A:206:CLA:HMD1	1.68	1.21

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
2	B	163/165 (99%)	157 (96%)	6 (4%)	0	100	100
3	C	168/170 (99%)	165 (98%)	3 (2%)	0	100	100
4	E	183/185 (99%)	180 (98%)	3 (2%)	0	100	100
5	F	168/170 (99%)	152 (90%)	15 (9%)	1 (1%)	21	47
6	G	172/174 (99%)	169 (98%)	3 (2%)	0	100	100
7	H	166/168 (99%)	162 (98%)	4 (2%)	0	100	100
8	I	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
9	J	181/183 (99%)	172 (95%)	9 (5%)	0	100	100
10	K	174/176 (99%)	172 (99%)	1 (1%)	1 (1%)	21	47
11	L	215/217 (99%)	211 (98%)	4 (2%)	0	100	100
12	M	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
13	a	741/743 (100%)	723 (98%)	18 (2%)	0	100	100
14	d	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
15	e	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
16	f	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
17	g	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
18	i	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
19	j	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
20	l	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
21	m	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
22	r	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
23	D	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
24	b	730/732 (100%)	713 (98%)	17 (2%)	0	100	100
25	c	78/80 (98%)	74 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4590/4640 (99%)	4449 (97%)	139 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	192	MET
10	K	212	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	122/122 (100%)	120 (98%)	2 (2%)	55	81
2	B	133/133 (100%)	124 (93%)	9 (7%)	14	38
3	C	129/130 (99%)	123 (95%)	6 (5%)	23	54
4	E	144/144 (100%)	144 (100%)	0	100	100
5	F	133/133 (100%)	125 (94%)	8 (6%)	17	43
6	G	139/139 (100%)	137 (99%)	2 (1%)	59	82
7	H	136/136 (100%)	135 (99%)	1 (1%)	76	90
8	I	136/136 (100%)	133 (98%)	3 (2%)	45	75
9	J	139/139 (100%)	132 (95%)	7 (5%)	22	51
10	K	134/134 (100%)	130 (97%)	4 (3%)	36	69
11	L	173/173 (100%)	167 (96%)	6 (4%)	32	64
12	M	133/133 (100%)	129 (97%)	4 (3%)	36	69
13	a	603/603 (100%)	598 (99%)	5 (1%)	73	89
14	d	111/111 (100%)	111 (100%)	0	100	100
15	e	55/55 (100%)	52 (94%)	3 (6%)	19	47
16	f	132/132 (100%)	130 (98%)	2 (2%)	57	81
17	g	98/98 (100%)	95 (97%)	3 (3%)	35	68
18	i	28/28 (100%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	j	36/36 (100%)	34 (94%)	2 (6%)	19	46
20	l	113/113 (100%)	113 (100%)	0	100	100
21	m	22/22 (100%)	22 (100%)	0	100	100
22	r	72/72 (100%)	72 (100%)	0	100	100
23	D	128/128 (100%)	124 (97%)	4 (3%)	35	68
24	b	597/597 (100%)	591 (99%)	6 (1%)	68	86
25	c	69/69 (100%)	68 (99%)	1 (1%)	59	82
All	All	3715/3716 (100%)	3637 (98%)	78 (2%)	46	76

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	e	14	GLU
24	b	54	LEU
15	e	59	VAL
19	j	2	ASN
24	b	245	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
24	b	113	ASN
24	b	293	ASN
24	b	703	GLN
9	J	183	ASN
9	J	122	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

366 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
27	CLA	a	840	13	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
26	DD6	M	306	-	40,45,45	2.04	8 (20%)	51,67,67	2.87	15 (29%)
27	CLA	F	316	-	45,49,73	1.42	8 (17%)	54,84,113	1.43	6 (11%)
27	CLA	G	310	6	50,54,73	1.36	8 (16%)	59,90,113	1.38	4 (6%)
27	CLA	a	824	13	54,58,73	1.30	7 (12%)	64,95,113	1.42	6 (9%)
30	A86	E	301	-	47,50,50	1.68	9 (19%)	51,76,76	3.04	24 (47%)
27	CLA	a	841	13	69,73,73	1.15	9 (13%)	82,113,113	1.29	5 (6%)
27	CLA	a	817	13	69,73,73	1.16	8 (11%)	82,113,113	1.26	7 (8%)
32	BCR	b	833	-	41,41,41	0.69	0	56,56,56	1.93	14 (25%)
27	CLA	L	317	11	49,53,73	1.38	8 (16%)	58,89,113	1.41	4 (6%)
27	CLA	A	205	1	69,73,73	1.15	8 (11%)	82,113,113	1.31	7 (8%)
27	CLA	B	307	2	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
30	A86	D	204	-	47,50,50	1.73	10 (21%)	51,76,76	3.96	24 (47%)
26	DD6	J	302	-	40,45,45	1.61	1 (2%)	51,67,67	2.22	17 (33%)
28	KC1	C	313	-	49,53,53	1.36	6 (12%)	61,89,89	1.75	13 (21%)
36	SF4	c	101	25	0,12,12	-	-	-	-	-
29	LMG	C	301	-	31,31,55	1.60	6 (19%)	39,39,63	3.05	7 (17%)
27	CLA	a	844	-	69,73,73	1.17	7 (10%)	82,113,113	1.39	6 (7%)
28	KC1	H	211	7	49,53,53	1.63	8 (16%)	61,89,89	1.79	13 (21%)
27	CLA	E	314	4	69,73,73	1.18	9 (13%)	82,113,113	1.29	5 (6%)
26	DD6	G	304	-	40,45,45	1.54	2 (5%)	51,67,67	1.87	14 (27%)
27	CLA	b	814	24	59,63,73	1.25	8 (13%)	70,101,113	1.35	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	E	311	4	69,73,73	1.22	9 (13%)	82,113,113	1.33	7 (8%)
27	CLA	b	810	24	59,63,73	1.27	9 (15%)	70,101,113	1.35	5 (7%)
29	LMG	D	202	-	46,46,55	1.79	7 (15%)	54,54,63	1.37	5 (9%)
26	DD6	E	307	-	40,45,45	1.54	2 (5%)	51,67,67	1.77	12 (23%)
27	CLA	a	849	13	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
27	CLA	j	104	19	45,49,73	1.41	8 (17%)	54,84,113	1.50	5 (9%)
27	CLA	D	210	-	60,64,73	1.24	8 (13%)	71,102,113	1.41	6 (8%)
27	CLA	a	813	13	54,58,73	1.30	8 (14%)	64,95,113	1.45	7 (10%)
30	A86	J	301	-	47,50,50	1.63	7 (14%)	51,76,76	3.16	22 (43%)
27	CLA	b	845	24	66,70,73	1.18	8 (12%)	78,109,113	1.32	5 (6%)
27	CLA	a	826	13	55,59,73	1.30	8 (14%)	64,96,113	1.42	7 (10%)
27	CLA	I	317	-	50,54,73	1.33	9 (18%)	59,90,113	1.44	4 (6%)
29	LMG	L	323	-	46,46,55	1.97	6 (13%)	54,54,63	2.21	8 (14%)
37	DGD	b	835	-	61,61,67	0.85	2 (3%)	75,75,81	1.11	4 (5%)
27	CLA	b	805	24	49,53,73	1.39	9 (18%)	58,89,113	1.53	6 (10%)
27	CLA	M	307	29	65,69,73	1.19	9 (13%)	77,108,113	1.41	7 (9%)
32	BCR	f	304	-	41,41,41	0.71	0	56,56,56	1.96	15 (26%)
27	CLA	a	820	13	55,59,73	1.31	9 (16%)	64,96,113	1.55	7 (10%)
26	DD6	L	301	-	40,45,45	1.59	2 (5%)	51,67,67	2.16	16 (31%)
27	CLA	I	307	8	59,63,73	1.25	8 (13%)	70,101,113	1.41	5 (7%)
27	CLA	F	313	-	45,49,73	1.40	9 (20%)	54,84,113	1.52	6 (11%)
27	CLA	M	309	12	69,73,73	1.17	9 (13%)	82,113,113	1.37	6 (7%)
27	CLA	K	309	10	69,73,73	1.16	8 (11%)	82,113,113	1.36	6 (7%)
27	CLA	M	317	-	49,53,73	1.34	8 (16%)	58,89,113	1.54	8 (13%)
27	CLA	H	213	7	69,73,73	1.17	9 (13%)	82,113,113	1.39	8 (9%)
31	LHG	E	318	-	48,48,48	1.15	6 (12%)	51,54,54	1.05	3 (5%)
32	BCR	f	305	-	41,41,41	0.94	2 (4%)	56,56,56	1.94	18 (32%)
27	CLA	D	216	23	50,54,73	1.34	8 (16%)	59,90,113	1.41	4 (6%)
27	CLA	D	215	-	45,49,73	1.41	9 (20%)	54,84,113	1.46	5 (9%)
27	CLA	r	201	22	49,53,73	1.37	8 (16%)	58,89,113	1.41	5 (8%)
30	A86	L	304	-	47,50,50	1.48	6 (12%)	51,76,76	2.80	22 (43%)
27	CLA	a	839	13	64,68,73	1.26	8 (12%)	76,107,113	1.52	8 (10%)
27	CLA	b	801	-	69,73,73	1.19	10 (14%)	82,113,113	1.45	7 (8%)
27	CLA	G	308	6	58,62,73	1.28	9 (15%)	68,99,113	1.34	5 (7%)
29	LMG	A	212	-	51,51,55	1.15	5 (9%)	59,59,63	1.57	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	i	101	-	64,68,73	1.21	8 (12%)	76,107,113	1.32	7 (9%)
27	CLA	a	854	13	59,63,73	1.27	8 (13%)	70,101,113	1.38	6 (8%)
29	LMG	E	317	-	43,43,55	2.01	7 (16%)	51,51,63	1.99	8 (15%)
28	KC1	J	306	-	49,53,53	1.52	7 (14%)	61,89,89	1.76	14 (22%)
27	CLA	G	315	6	46,50,73	1.40	8 (17%)	53,85,113	1.43	4 (7%)
27	CLA	I	315	-	59,63,73	1.25	9 (15%)	70,101,113	1.42	6 (8%)
27	CLA	J	307	9	69,73,73	1.17	8 (11%)	82,113,113	1.33	6 (7%)
27	CLA	b	807	24	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
27	CLA	M	308	12	64,68,73	1.22	8 (12%)	76,107,113	1.35	6 (7%)
27	CLA	b	816	24	50,54,73	1.35	9 (18%)	59,90,113	1.45	4 (6%)
30	A86	F	301	-	47,50,50	1.44	7 (14%)	51,76,76	2.73	13 (25%)
30	A86	H	201	-	47,50,50	1.81	10 (21%)	51,76,76	3.57	24 (47%)
30	A86	H	203	-	47,50,50	1.71	10 (21%)	51,76,76	3.21	24 (47%)
28	KC1	A	209	-	49,53,53	1.45	7 (14%)	61,89,89	1.77	13 (21%)
27	CLA	K	317	10	45,49,73	1.38	7 (15%)	54,84,113	1.62	7 (12%)
26	DD6	L	303	-	40,45,45	1.92	6 (15%)	51,67,67	2.04	16 (31%)
27	CLA	M	315	12	45,49,73	1.41	8 (17%)	54,84,113	1.52	5 (9%)
27	CLA	I	306	8	69,73,73	1.16	9 (13%)	82,113,113	1.25	6 (7%)
32	BCR	b	837	-	41,41,41	0.73	0	56,56,56	2.00	17 (30%)
27	CLA	J	315	9	53,57,73	1.29	9 (16%)	61,93,113	1.39	5 (8%)
27	CLA	b	822	24	54,58,73	1.31	9 (16%)	64,95,113	1.37	6 (9%)
27	CLA	C	318	3	46,50,73	1.38	8 (17%)	53,85,113	1.48	3 (5%)
31	LHG	D	201	-	48,48,48	1.12	4 (8%)	51,54,54	1.05	2 (3%)
26	DD6	E	303	-	40,45,45	2.18	8 (20%)	51,67,67	3.33	15 (29%)
35	ET4	l	207	-	41,43,43	1.45	8 (19%)	52,60,60	2.23	18 (34%)
27	CLA	F	317	-	51,55,73	1.31	7 (13%)	60,91,113	1.42	4 (6%)
27	CLA	D	214	23	60,64,73	1.25	9 (15%)	71,102,113	1.38	6 (8%)
30	A86	I	303	-	47,50,50	1.70	8 (17%)	51,76,76	3.27	25 (49%)
27	CLA	B	310	2	50,54,73	1.36	9 (18%)	59,90,113	1.38	4 (6%)
27	CLA	b	849	24	58,62,73	1.27	8 (13%)	68,99,113	1.31	5 (7%)
30	A86	K	301	-	47,50,50	1.53	5 (10%)	51,76,76	2.58	18 (35%)
27	CLA	A	208	1	58,62,73	1.26	9 (15%)	68,99,113	1.42	6 (8%)
26	DD6	G	305	-	40,45,45	1.57	3 (7%)	51,67,67	1.89	15 (29%)
31	LHG	j	102	-	48,48,48	1.15	6 (12%)	51,54,54	0.93	2 (3%)
27	CLA	b	812	24	64,68,73	1.20	8 (12%)	76,107,113	1.40	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	J	310	9	50,54,73	1.32	8 (16%)	59,90,113	1.40	5 (8%)
27	CLA	H	207	7	69,73,73	1.17	9 (13%)	82,113,113	1.43	7 (8%)
29	LMG	a	852	-	33,33,55	1.59	5 (15%)	41,41,63	3.67	8 (19%)
26	DD6	G	303	-	40,45,45	1.55	2 (5%)	51,67,67	1.82	15 (29%)
27	CLA	H	206	7	69,73,73	1.18	8 (11%)	82,113,113	1.49	12 (14%)
31	LHG	a	833	-	48,48,48	1.16	3 (6%)	51,54,54	1.01	3 (5%)
27	CLA	H	210	7	61,65,73	1.24	8 (13%)	72,103,113	1.41	6 (8%)
32	BCR	j	101	-	41,41,41	0.69	0	56,56,56	2.06	13 (23%)
30	A86	D	203	-	47,50,50	1.58	7 (14%)	51,76,76	3.57	20 (39%)
27	CLA	b	842	24	69,73,73	1.17	9 (13%)	82,113,113	1.26	6 (7%)
27	CLA	L	319	-	49,53,73	1.37	9 (18%)	58,89,113	1.53	6 (10%)
33	SQD	J	318	-	31,32,54	3.13	8 (25%)	33,36,65	2.79	8 (24%)
27	CLA	I	313	8	45,49,73	1.38	8 (17%)	54,84,113	1.53	7 (12%)
27	CLA	F	308	-	66,70,73	1.20	9 (13%)	78,109,113	1.32	6 (7%)
27	CLA	J	309	-	69,73,73	1.15	8 (11%)	82,113,113	1.34	6 (7%)
32	BCR	j	105	-	41,41,41	0.73	0	56,56,56	2.09	11 (19%)
32	BCR	a	836	-	41,41,41	0.70	0	56,56,56	1.97	15 (26%)
27	CLA	D	217	-	45,49,73	1.39	8 (17%)	54,84,113	1.47	6 (11%)
26	DD6	M	304	-	40,45,45	2.00	6 (15%)	51,67,67	2.79	13 (25%)
34	PQN	a	831	-	34,34,34	1.63	2 (5%)	43,45,45	1.09	2 (4%)
27	CLA	b	830	24	69,73,73	1.19	9 (13%)	82,113,113	1.44	8 (9%)
27	CLA	L	311	11	44,48,73	1.41	8 (18%)	51,82,113	1.53	6 (11%)
27	CLA	H	204	-	58,62,73	1.28	9 (15%)	68,99,113	1.49	6 (8%)
29	LMG	J	317	-	51,51,55	1.39	8 (15%)	59,59,63	1.28	7 (11%)
30	A86	K	307	-	47,50,50	1.54	7 (14%)	51,76,76	2.63	18 (35%)
27	CLA	G	306	-	50,54,73	1.36	8 (16%)	59,90,113	1.42	4 (6%)
27	CLA	l	206	-	49,53,73	1.38	8 (16%)	58,89,113	1.44	6 (10%)
30	A86	m	101	-	47,50,50	1.55	9 (19%)	51,76,76	3.33	25 (49%)
27	CLA	B	312	2	69,73,73	1.15	9 (13%)	82,113,113	1.28	4 (4%)
30	A86	K	304	27	47,50,50	1.49	5 (10%)	51,76,76	2.53	15 (29%)
29	LMG	I	319	-	37,37,55	2.05	7 (18%)	45,45,63	2.68	4 (8%)
27	CLA	a	830	13	69,73,73	1.15	8 (11%)	82,113,113	1.28	6 (7%)
26	DD6	E	306	-	40,45,45	1.71	3 (7%)	51,67,67	2.89	20 (39%)
27	CLA	C	311	3	64,68,73	1.22	10 (15%)	76,107,113	1.35	6 (7%)
27	CLA	F	307	5	63,67,73	1.23	7 (11%)	74,105,113	1.31	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	L	318	11	45,50,73	1.38	10 (22%)	52,85,113	1.44	6 (11%)
27	CLA	G	309	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
32	BCR	a	851	-	41,41,41	1.05	2 (4%)	56,56,56	1.80	11 (19%)
27	CLA	A	204	1	69,73,73	1.15	9 (13%)	82,113,113	1.38	6 (7%)
27	CLA	I	310	8	51,55,73	1.34	7 (13%)	60,91,113	1.38	5 (8%)
27	CLA	G	314	-	45,49,73	1.41	8 (17%)	54,84,113	1.51	5 (9%)
27	CLA	G	317	6	53,57,73	1.33	8 (15%)	61,93,113	1.41	5 (8%)
27	CLA	G	312	6	65,69,73	1.20	9 (13%)	77,108,113	1.32	6 (7%)
30	A86	r	202	-	47,50,50	1.78	10 (21%)	51,76,76	3.90	27 (52%)
30	A86	C	304	-	47,50,50	1.68	9 (19%)	51,76,76	2.84	16 (31%)
27	CLA	B	306	2	61,65,73	1.23	9 (14%)	73,102,113	1.24	3 (4%)
27	CLA	a	816	13	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
27	CLA	C	309	-	66,70,73	1.19	9 (13%)	78,109,113	1.49	8 (10%)
27	CLA	I	309	8	50,54,73	1.33	9 (18%)	59,90,113	1.44	6 (10%)
28	KC1	F	312	5	49,53,53	1.35	6 (12%)	61,89,89	1.73	12 (19%)
27	CLA	b	828	24	51,55,73	1.34	9 (17%)	60,91,113	1.38	5 (8%)
30	A86	B	304	-	47,50,50	1.70	9 (19%)	51,76,76	3.02	19 (37%)
27	CLA	b	804	24	69,73,73	1.22	10 (14%)	82,113,113	1.33	8 (9%)
27	CLA	B	309	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	5 (6%)
27	CLA	I	305	-	49,53,73	1.37	9 (18%)	58,89,113	1.47	5 (8%)
27	CLA	a	823	13	69,73,73	1.16	8 (11%)	82,113,113	1.27	5 (6%)
27	CLA	B	314	2	45,49,73	1.41	9 (20%)	54,84,113	1.48	7 (12%)
27	CLA	L	307	-	58,62,73	1.25	10 (17%)	68,99,113	1.35	5 (7%)
27	CLA	b	811	24	69,73,73	1.17	9 (13%)	82,113,113	1.29	5 (6%)
27	CLA	L	308	11	69,73,73	1.15	8 (11%)	82,113,113	1.27	7 (8%)
30	A86	K	302	-	47,50,50	1.52	6 (12%)	51,76,76	2.82	23 (45%)
27	CLA	M	311	-	50,54,73	1.36	9 (18%)	59,90,113	1.51	6 (10%)
30	A86	L	302	-	47,50,50	1.54	7 (14%)	51,76,76	2.81	14 (27%)
31	LHG	E	316	-	41,41,48	1.00	2 (4%)	44,47,54	1.22	5 (11%)
28	KC1	L	320	28	49,53,53	1.35	6 (12%)	61,89,89	1.73	13 (21%)
27	CLA	a	807	13	69,73,73	1.15	8 (11%)	82,113,113	1.32	6 (7%)
29	LMG	A	214	27	41,41,55	1.73	7 (17%)	49,49,63	1.60	4 (8%)
27	CLA	b	818	24	64,68,73	1.21	9 (14%)	76,107,113	1.29	5 (6%)
26	DD6	I	304	-	40,45,45	1.96	7 (17%)	51,67,67	2.44	18 (35%)
27	CLA	C	307	3	69,73,73	1.17	7 (10%)	82,113,113	1.34	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	a	829	13	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
27	CLA	H	214	7	49,53,73	1.38	9 (18%)	58,89,113	1.44	4 (6%)
27	CLA	a	812	13	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
27	CLA	a	803	13	69,73,73	1.22	9 (13%)	82,113,113	1.34	7 (8%)
31	LHG	b	836	27	48,48,48	1.14	3 (6%)	51,54,54	1.04	3 (5%)
27	CLA	b	847	24	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
27	CLA	b	843	24	69,73,73	1.17	8 (11%)	82,113,113	1.28	5 (6%)
27	CLA	B	308	2	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
27	CLA	F	306	5	59,63,73	1.26	8 (13%)	70,101,113	1.31	6 (8%)
27	CLA	D	213	23	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
30	A86	C	302	-	47,50,50	1.74	10 (21%)	51,76,76	3.28	24 (47%)
27	CLA	K	314	10,30	69,73,73	1.14	6 (8%)	82,113,113	1.65	16 (19%)
27	CLA	a	842	-	69,73,73	1.20	8 (11%)	82,113,113	1.36	6 (7%)
27	CLA	K	316	10	69,73,73	1.19	12 (17%)	82,113,113	1.41	8 (9%)
27	CLA	f	302	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	5 (6%)
27	CLA	a	827	13	64,68,73	1.24	10 (15%)	76,107,113	1.47	10 (13%)
27	CLA	a	822	13	69,73,73	1.17	8 (11%)	82,113,113	1.31	7 (8%)
27	CLA	D	207	-	65,69,73	1.20	9 (13%)	77,108,113	1.39	7 (9%)
27	CLA	G	316	6	59,63,73	1.26	9 (15%)	70,101,113	1.31	6 (8%)
27	CLA	a	832	31	56,60,73	1.30	9 (16%)	65,97,113	1.38	5 (7%)
27	CLA	K	311	-	56,60,73	1.28	8 (14%)	65,97,113	1.44	8 (12%)
27	CLA	a	843	-	69,73,73	1.20	9 (13%)	82,113,113	1.34	8 (9%)
27	CLA	a	828	13	69,73,73	1.18	8 (11%)	82,113,113	1.29	6 (7%)
31	LHG	K	320	-	32,32,48	1.31	7 (21%)	35,37,54	1.19	2 (5%)
27	CLA	a	806	27,13	59,63,73	1.27	9 (15%)	70,101,113	1.34	6 (8%)
31	LHG	a	834	27	26,26,48	1.30	5 (19%)	29,32,54	1.17	2 (6%)
27	CLA	C	316	3	45,49,73	1.40	10 (22%)	54,84,113	1.51	5 (9%)
28	KC1	L	314	-	49,53,53	1.51	7 (14%)	61,89,89	1.76	14 (22%)
27	CLA	J	313	-	50,54,73	1.33	10 (20%)	59,90,113	1.44	4 (6%)
27	CLA	F	311	5	64,68,73	1.22	9 (14%)	76,107,113	1.28	5 (6%)
26	DD6	B	303	-	40,45,45	2.06	6 (15%)	51,67,67	2.93	18 (35%)
27	CLA	b	838	24	64,68,73	1.20	8 (12%)	76,107,113	1.43	6 (7%)
27	CLA	E	313	4	49,53,73	1.38	11 (22%)	58,89,113	1.48	6 (10%)
26	DD6	E	302	-	40,45,45	1.53	2 (5%)	51,67,67	1.88	8 (15%)
27	CLA	K	318	10	50,54,73	1.31	7 (14%)	59,90,113	1.44	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	E	308	4	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)
27	CLA	E	315	-	60,64,73	1.25	8 (13%)	71,102,113	1.36	6 (8%)
27	CLA	C	315	3	46,50,73	1.41	9 (19%)	53,85,113	1.40	4 (7%)
27	CLA	I	311	8	69,73,73	1.16	9 (13%)	82,113,113	1.47	9 (10%)
27	CLA	A	210	1	50,54,73	1.32	7 (14%)	59,90,113	1.42	4 (6%)
30	A86	A	213	-	47,50,50	1.54	7 (14%)	51,76,76	2.56	19 (37%)
28	KC1	M	314	-	49,53,53	1.59	8 (16%)	61,89,89	1.90	15 (24%)
27	CLA	a	814	-	49,53,73	1.39	9 (18%)	58,89,113	1.44	4 (6%)
27	CLA	M	318	12	50,54,73	1.35	8 (16%)	59,90,113	1.45	5 (8%)
27	CLA	a	850	13	60,64,73	1.25	8 (13%)	71,102,113	1.32	5 (7%)
27	CLA	a	811	27,13	66,70,73	1.19	8 (12%)	78,109,113	1.27	6 (7%)
30	A86	L	306	-	47,50,50	1.50	5 (10%)	51,76,76	2.53	16 (31%)
27	CLA	M	319	12	50,54,73	1.34	7 (14%)	59,90,113	1.36	4 (6%)
28	KC1	C	308	3	49,53,53	1.36	6 (12%)	61,89,89	1.78	13 (21%)
27	CLA	M	316	12	58,62,73	1.31	9 (15%)	68,99,113	1.59	11 (16%)
28	KC1	I	312	8	49,53,53	1.57	7 (14%)	61,89,89	1.77	13 (21%)
27	CLA	K	319	10	50,54,73	1.32	7 (14%)	59,90,113	1.40	6 (10%)
32	BCR	b	834	-	41,41,41	0.69	0	56,56,56	3.34	20 (35%)
27	CLA	b	826	-	49,53,73	1.39	9 (18%)	58,89,113	1.42	5 (8%)
36	SF4	c	102	25	0,12,12	-	-	-	-	-
29	LMG	l	201	-	40,40,55	1.24	5 (12%)	48,48,63	1.79	4 (8%)
30	A86	B	301	-	47,50,50	1.50	6 (12%)	51,76,76	2.88	17 (33%)
27	CLA	b	806	24	69,73,73	1.16	8 (11%)	82,113,113	1.33	6 (7%)
27	CLA	D	208	23	69,73,73	1.19	11 (15%)	82,113,113	1.46	9 (10%)
27	CLA	C	312	3	65,69,73	1.21	9 (13%)	77,108,113	1.38	7 (9%)
27	CLA	L	310	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	5 (6%)
32	BCR	l	205	-	41,41,41	0.87	0	56,56,56	2.05	14 (25%)
27	CLA	b	821	24	69,73,73	1.16	8 (11%)	82,113,113	1.49	7 (8%)
29	LMG	j	103	-	37,37,55	1.56	5 (13%)	45,45,63	3.67	7 (15%)
27	CLA	K	313	10	56,60,73	1.27	8 (14%)	65,97,113	1.51	6 (9%)
28	KC1	K	308	-	49,53,53	1.51	7 (14%)	61,89,89	1.88	15 (24%)
27	CLA	b	825	-	69,73,73	1.21	9 (13%)	82,113,113	1.47	7 (8%)
27	CLA	H	205	7	69,73,73	1.17	8 (11%)	82,113,113	1.29	6 (7%)
27	CLA	J	308	9	60,64,73	1.26	8 (13%)	71,102,113	1.31	6 (8%)
27	CLA	C	306	29	49,53,73	1.38	8 (16%)	58,89,113	1.44	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	F	302	-	40,45,45	1.56	1 (2%)	51,67,67	1.99	12 (23%)
27	CLA	a	818	13	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
27	CLA	B	311	2	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
32	BCR	i	103	-	41,41,41	0.67	0	56,56,56	2.05	14 (25%)
30	A86	G	302	-	47,50,50	1.76	8 (17%)	51,76,76	3.96	30 (58%)
27	CLA	l	203	20	53,57,73	1.32	9 (16%)	61,93,113	1.49	8 (13%)
30	A86	b	848	-	47,50,50	1.63	9 (19%)	51,76,76	2.68	18 (35%)
27	CLA	b	809	24	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
27	CLA	a	838	13	69,73,73	1.15	8 (11%)	82,113,113	1.25	5 (6%)
31	LHG	a	802	-	48,48,48	1.12	5 (10%)	51,54,54	0.94	2 (3%)
27	CLA	H	209	-	64,68,73	1.20	8 (12%)	76,107,113	1.45	7 (9%)
30	A86	I	301	-	47,50,50	1.68	7 (14%)	51,76,76	3.27	24 (47%)
27	CLA	G	311	6	60,64,73	1.24	8 (13%)	71,102,113	1.32	5 (7%)
30	A86	D	206	-	47,50,50	1.70	9 (19%)	51,76,76	3.31	21 (41%)
27	CLA	A	206	1	50,54,73	1.35	8 (16%)	59,90,113	1.38	4 (6%)
27	CLA	D	211	23	50,54,73	1.36	9 (18%)	59,90,113	1.41	4 (6%)
36	SF4	b	802	24	0,12,12	-	-	-	-	-
27	CLA	b	819	24	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
27	CLA	E	310	4	50,54,73	1.36	8 (16%)	59,90,113	1.38	5 (8%)
27	CLA	E	312	4	59,63,73	1.26	9 (15%)	70,101,113	1.38	6 (8%)
32	BCR	E	305	-	41,41,41	0.70	0	56,56,56	2.02	15 (26%)
27	CLA	b	841	24	65,69,73	1.19	9 (13%)	77,108,113	1.34	6 (7%)
27	CLA	a	809	13	69,73,73	1.19	9 (13%)	82,113,113	1.46	9 (10%)
27	CLA	C	310	3	50,54,73	1.32	8 (16%)	59,90,113	1.41	5 (8%)
27	CLA	b	846	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
26	DD6	D	205	-	40,45,45	1.98	7 (17%)	51,67,67	3.21	24 (47%)
31	LHG	H	215	-	34,34,48	1.15	4 (11%)	37,40,54	0.99	2 (5%)
31	LHG	a	801	-	48,48,48	1.15	5 (10%)	51,54,54	0.98	2 (3%)
27	CLA	K	310	10	60,64,73	1.24	8 (13%)	71,102,113	1.48	7 (9%)
27	CLA	M	310	-	63,67,73	1.23	9 (14%)	74,105,113	1.34	5 (6%)
26	DD6	G	301	-	40,45,45	1.54	2 (5%)	51,67,67	1.83	12 (23%)
32	BCR	l	202	-	41,41,41	0.96	2 (4%)	56,56,56	2.04	16 (28%)
26	DD6	F	303	-	40,45,45	1.58	2 (5%)	51,67,67	2.02	15 (29%)
30	A86	M	305	-	47,50,50	1.55	6 (12%)	51,76,76	2.46	16 (31%)
27	CLA	b	850	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	L	315	11	45,49,73	1.39	10 (22%)	54,84,113	1.42	4 (7%)
31	LHG	I	318	-	34,34,48	1.34	5 (14%)	37,40,54	1.14	2 (5%)
27	CLA	M	312	12	50,54,73	1.33	8 (16%)	59,90,113	1.49	6 (10%)
32	BCR	b	840	-	41,41,41	1.02	2 (4%)	56,56,56	2.04	20 (35%)
27	CLA	H	212	7	69,73,73	1.17	9 (13%)	82,113,113	1.44	7 (8%)
26	DD6	M	301	-	40,45,45	1.69	2 (5%)	51,67,67	1.96	16 (31%)
30	A86	L	305	-	47,50,50	1.52	5 (10%)	51,76,76	2.44	16 (31%)
32	BCR	a	853	-	41,41,41	0.70	0	56,56,56	2.15	16 (28%)
32	BCR	m	102	-	41,41,41	0.66	0	56,56,56	2.14	15 (26%)
27	CLA	b	817	24	59,63,73	1.25	9 (15%)	70,101,113	1.31	4 (5%)
27	CLA	b	815	-	69,73,73	1.17	9 (13%)	82,113,113	1.29	7 (8%)
31	LHG	a	837	-	32,32,48	1.34	5 (15%)	35,38,54	1.20	2 (5%)
27	CLA	F	305	5	65,69,73	1.22	6 (9%)	77,108,113	1.28	6 (7%)
27	CLA	f	301	-	69,73,73	1.16	7 (10%)	82,113,113	1.31	7 (8%)
30	A86	B	302	-	47,50,50	1.81	10 (21%)	51,76,76	3.58	24 (47%)
30	A86	J	304	-	47,50,50	1.58	8 (17%)	51,76,76	3.02	21 (41%)
32	BCR	a	847	-	41,41,41	0.93	2 (4%)	56,56,56	1.97	19 (33%)
27	CLA	a	848	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
27	CLA	A	211	-	44,48,73	1.39	9 (20%)	51,82,113	1.56	6 (11%)
30	A86	F	304	-	47,50,50	1.47	6 (12%)	51,76,76	2.85	22 (43%)
28	KC1	L	322	28	49,53,53	1.60	8 (16%)	61,89,89	1.85	12 (19%)
26	DD6	J	303	-	40,45,45	1.67	3 (7%)	51,67,67	2.20	16 (31%)
27	CLA	A	203	1	65,69,73	1.20	8 (12%)	77,108,113	1.30	4 (5%)
27	CLA	G	307	6	60,64,73	1.24	8 (13%)	71,102,113	1.34	5 (7%)
30	A86	B	305	-	47,50,50	1.72	12 (25%)	51,76,76	3.43	27 (52%)
27	CLA	b	839	-	69,73,73	1.17	9 (13%)	82,113,113	1.29	5 (6%)
27	CLA	J	312	9	69,73,73	1.16	8 (11%)	82,113,113	1.32	6 (7%)
26	DD6	I	302	-	40,45,45	1.56	2 (5%)	51,67,67	1.77	14 (27%)
29	LMG	M	321	-	42,42,55	1.56	6 (14%)	50,50,63	1.38	5 (10%)
27	CLA	a	821	13	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
27	CLA	b	844	24	69,73,73	1.17	8 (11%)	82,113,113	1.35	6 (7%)
27	CLA	D	209	23	53,57,73	1.33	9 (16%)	61,93,113	1.41	5 (8%)
27	CLA	L	312	11	60,64,73	1.24	8 (13%)	71,102,113	1.36	6 (8%)
27	CLA	l	204	20	69,73,73	1.18	8 (11%)	82,113,113	1.46	7 (8%)
27	CLA	b	823	24	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	L	321	11	49,53,73	1.39	9 (18%)	58,89,113	1.41	5 (8%)
27	CLA	b	824	24	62,66,73	1.23	9 (14%)	73,104,113	1.36	6 (8%)
27	CLA	L	316	11	60,64,73	1.23	8 (13%)	71,102,113	1.43	5 (7%)
27	CLA	I	314	8	53,57,73	1.32	10 (18%)	61,93,113	1.37	5 (8%)
30	A86	M	302	-	47,50,50	1.74	10 (21%)	51,76,76	3.37	25 (49%)
27	CLA	b	813	24	63,67,73	1.21	9 (14%)	74,105,113	1.32	6 (8%)
30	A86	C	305	-	47,50,50	1.76	10 (21%)	51,76,76	3.40	26 (50%)
27	CLA	a	855	13	69,73,73	1.16	9 (13%)	82,113,113	1.31	7 (8%)
32	BCR	i	102	-	41,41,41	0.73	1 (2%)	56,56,56	1.95	17 (30%)
27	CLA	b	831	31	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
26	DD6	H	202	-	40,45,45	2.16	11 (27%)	51,67,67	2.44	18 (35%)
26	DD6	A	201	-	40,45,45	1.69	4 (10%)	51,67,67	2.06	14 (27%)
27	CLA	L	313	11	69,73,73	1.14	9 (13%)	82,113,113	1.35	5 (6%)
27	CLA	b	820	24	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
31	LHG	M	320	-	46,46,48	1.15	4 (8%)	49,52,54	1.07	3 (6%)
26	DD6	J	305	-	40,45,45	1.88	5 (12%)	51,67,67	2.74	14 (27%)
27	CLA	F	309	5	50,54,73	1.35	7 (14%)	59,90,113	1.43	4 (6%)
27	CLA	b	808	24	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
28	KC1	K	315	10	49,53,53	1.52	8 (16%)	61,89,89	1.74	12 (19%)
27	CLA	F	310	5	64,68,73	1.22	7 (10%)	76,107,113	1.29	5 (6%)
27	CLA	F	314	5	51,55,73	1.36	8 (15%)	60,91,113	1.39	5 (8%)
32	BCR	a	835	-	41,41,41	0.89	2 (4%)	56,56,56	1.93	21 (37%)
27	CLA	D	212	23	46,50,73	1.39	9 (19%)	53,85,113	1.40	4 (7%)
30	A86	K	306	-	47,50,50	1.60	7 (14%)	51,76,76	2.64	19 (37%)
26	DD6	C	303	-	40,45,45	1.70	3 (7%)	51,67,67	2.28	17 (33%)
34	PQN	b	832	-	34,34,34	1.61	2 (5%)	43,45,45	1.21	4 (9%)
27	CLA	I	316	8	49,53,73	1.38	9 (18%)	58,89,113	1.43	4 (6%)
27	CLA	a	808	13	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
27	CLA	a	825	13	49,53,73	1.38	8 (16%)	58,89,113	1.41	4 (6%)
27	CLA	A	207	1	69,73,73	1.15	9 (13%)	82,113,113	1.33	6 (7%)
27	CLA	b	827	24	64,68,73	1.21	8 (12%)	76,107,113	1.36	7 (9%)
27	CLA	a	810	13	69,73,73	1.17	9 (13%)	82,113,113	1.29	5 (6%)
27	CLA	E	309	4	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
27	CLA	f	303	16	49,53,73	1.38	9 (18%)	58,89,113	1.44	4 (6%)
27	CLA	C	317	-	46,50,73	1.44	8 (17%)	53,85,113	1.60	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	BCR	r	203	-	41,41,41	0.67	0	56,56,56	1.77	15 (26%)
27	CLA	a	805	13	69,73,73	1.18	9 (13%)	82,113,113	1.50	7 (8%)
27	CLA	J	314	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	6 (7%)
28	KC1	B	313	-	49,53,53	1.55	8 (16%)	61,89,89	1.89	13 (21%)
30	A86	M	303	-	47,50,50	1.62	8 (17%)	51,76,76	3.60	23 (45%)
26	DD6	K	303	-	40,45,45	2.00	7 (17%)	51,67,67	2.74	21 (41%)
27	CLA	a	845	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	7 (8%)
27	CLA	b	829	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
30	A86	K	305	-	47,50,50	1.52	7 (14%)	51,76,76	2.51	16 (31%)
26	DD6	A	202	-	40,45,45	1.98	6 (15%)	51,67,67	2.57	18 (35%)
29	LMG	C	319	27	44,44,55	1.32	7 (15%)	52,52,63	1.85	4 (7%)
27	CLA	J	311	9	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
27	CLA	b	803	24	69,73,73	1.16	8 (11%)	82,113,113	1.28	5 (6%)
27	CLA	I	308	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	7 (8%)
27	CLA	a	804	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
27	CLA	a	856	-	69,73,73	1.19	7 (10%)	82,113,113	1.44	6 (7%)
27	CLA	L	309	11	69,73,73	1.16	9 (13%)	82,113,113	1.30	7 (8%)
27	CLA	F	315	5	62,66,73	1.25	8 (12%)	73,104,113	1.30	6 (8%)
31	LHG	B	315	-	41,41,48	0.99	2 (4%)	44,47,54	1.10	3 (6%)
28	KC1	G	313	6	49,53,53	1.35	6 (12%)	61,89,89	1.72	12 (19%)
27	CLA	a	815	13	69,73,73	1.16	9 (13%)	82,113,113	1.48	10 (12%)
27	CLA	a	819	13	53,57,73	1.32	8 (15%)	61,93,113	1.42	5 (8%)
32	BCR	E	304	-	41,41,41	0.66	0	56,56,56	1.88	17 (30%)
27	CLA	a	846	13	69,73,73	1.17	8 (11%)	82,113,113	1.28	5 (6%)
27	CLA	M	313	12	69,73,73	1.18	8 (11%)	82,113,113	1.51	11 (13%)
27	CLA	H	208	7	50,54,73	1.35	8 (16%)	59,90,113	1.40	4 (6%)
27	CLA	C	314	3	45,49,73	1.40	11 (24%)	54,84,113	1.50	7 (12%)
30	A86	J	316	-	47,50,50	1.63	7 (14%)	51,76,76	3.84	26 (50%)
27	CLA	K	312	-	69,73,73	1.18	9 (13%)	82,113,113	1.32	6 (7%)

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
27	CLA	a	840	13	1/1/15/20	12/39/115/115	-
26	DD6	M	306	-	-	2/26/80/80	0/3/3/3
27	CLA	F	316	-	1/1/10/20	4/10/86/115	-
27	CLA	G	310	6	1/1/11/20	7/17/93/115	-
27	CLA	a	824	13	1/1/12/20	7/21/97/115	-
30	A86	E	301	-	-	5/34/90/90	0/3/3/3
27	CLA	a	841	13	1/1/15/20	11/39/115/115	-
27	CLA	a	817	13	1/1/15/20	15/39/115/115	-
32	BCR	b	833	-	-	0/29/63/63	0/2/2/2
27	CLA	L	317	11	1/1/11/20	6/15/91/115	-
27	CLA	A	205	1	1/1/15/20	20/39/115/115	-
27	CLA	B	307	2	1/1/15/20	8/39/115/115	-
30	A86	D	204	-	-	4/34/90/90	0/3/3/3
26	DD6	J	302	-	-	10/26/80/80	0/3/3/3
28	KC1	C	313	-	-	5/15/71/71	-
36	SF4	c	101	25	-	-	0/6/5/5
29	LMG	C	301	-	-	14/26/46/70	0/1/1/1
27	CLA	a	844	-	1/1/15/20	9/39/115/115	-
28	KC1	H	211	7	-	9/15/71/71	-
27	CLA	E	314	4	1/1/15/20	11/39/115/115	-
26	DD6	G	304	-	-	0/26/80/80	0/3/3/3
27	CLA	b	814	24	1/1/13/20	12/27/103/115	-
27	CLA	E	311	4	1/1/15/20	10/39/115/115	-
27	CLA	b	810	24	1/1/13/20	4/27/103/115	-
29	LMG	D	202	-	-	17/41/61/70	0/1/1/1
26	DD6	E	307	-	-	1/26/80/80	0/3/3/3
27	CLA	a	849	13	1/1/15/20	13/39/115/115	-
27	CLA	j	104	19	1/1/10/20	4/10/86/115	-
27	CLA	D	210	-	1/1/13/20	6/29/105/115	-
27	CLA	a	813	13	1/1/12/20	6/21/97/115	-
30	A86	J	301	-	-	7/34/90/90	0/3/3/3
27	CLA	b	845	24	1/1/14/20	10/36/112/115	-
27	CLA	a	826	13	1/1/12/20	9/23/99/115	-
27	CLA	I	317	-	1/1/11/20	6/17/93/115	-
29	LMG	L	323	-	-	23/41/61/70	0/1/1/1
37	DGD	b	835	-	-	28/49/89/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	b	805	24	1/1/11/20	3/15/91/115	-
27	CLA	M	307	29	1/1/14/20	13/35/111/115	-
32	BCR	f	304	-	-	2/29/63/63	0/2/2/2
27	CLA	a	820	13	1/1/12/20	4/23/99/115	-
26	DD6	L	301	-	-	8/26/80/80	0/3/3/3
27	CLA	I	307	8	1/1/13/20	6/27/103/115	-
27	CLA	F	313	-	1/1/10/20	3/10/86/115	-
27	CLA	M	309	12	1/1/15/20	10/39/115/115	-
27	CLA	K	309	10	1/1/15/20	17/39/115/115	-
27	CLA	M	317	-	-	6/15/91/115	-
27	CLA	H	213	7	1/1/15/20	12/39/115/115	-
31	LHG	E	318	-	-	33/53/53/53	-
32	BCR	f	305	-	-	8/29/63/63	0/2/2/2
27	CLA	D	216	23	1/1/11/20	5/17/93/115	-
27	CLA	D	215	-	1/1/10/20	4/10/86/115	-
27	CLA	r	201	22	1/1/11/20	11/15/91/115	-
30	A86	L	304	-	-	6/34/90/90	0/3/3/3
27	CLA	a	839	13	1/1/14/20	14/33/109/115	-
27	CLA	b	801	-	1/1/15/20	8/39/115/115	-
27	CLA	G	308	6	1/1/12/20	10/26/102/115	-
29	LMG	A	212	-	-	25/46/66/70	0/1/1/1
27	CLA	i	101	-	1/1/14/20	10/33/109/115	-
27	CLA	a	854	13	1/1/13/20	10/27/103/115	-
29	LMG	E	317	-	-	21/38/58/70	0/1/1/1
28	KC1	J	306	-	-	7/15/71/71	-
27	CLA	G	315	6	1/1/10/20	7/12/88/115	-
27	CLA	I	315	-	1/1/13/20	12/27/103/115	-
27	CLA	J	307	9	1/1/15/20	8/39/115/115	-
27	CLA	b	807	24	1/1/15/20	15/39/115/115	-
27	CLA	M	308	12	1/1/14/20	15/33/109/115	-
27	CLA	b	816	24	1/1/11/20	6/17/93/115	-
30	A86	F	301	-	-	8/34/90/90	0/3/3/3
30	A86	H	201	-	-	5/34/90/90	0/3/3/3
30	A86	H	203	-	-	4/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	KC1	A	209	-	-	9/15/71/71	-
27	CLA	K	317	10	1/1/10/20	7/10/86/115	-
27	CLA	M	315	12	1/1/10/20	4/10/86/115	-
26	DD6	L	303	-	-	0/26/80/80	0/3/3/3
27	CLA	I	306	8	1/1/15/20	11/39/115/115	-
32	BCR	b	837	-	-	5/29/63/63	0/2/2/2
27	CLA	J	315	9	1/1/11/20	10/20/96/115	-
27	CLA	b	822	24	1/1/12/20	9/21/97/115	-
27	CLA	C	318	3	1/1/10/20	6/12/88/115	-
31	LHG	D	201	-	-	32/53/53/53	-
26	DD6	E	303	-	-	6/26/80/80	0/3/3/3
35	ET4	l	207	-	-	3/25/67/67	0/2/2/2
27	CLA	F	317	-	1/1/11/20	9/18/94/115	-
27	CLA	D	214	23	1/1/13/20	9/29/105/115	-
30	A86	I	303	-	-	5/34/90/90	0/3/3/3
27	CLA	B	310	2	1/1/11/20	6/17/93/115	-
27	CLA	b	849	24	1/1/12/20	10/26/102/115	-
30	A86	K	301	-	-	8/34/90/90	0/3/3/3
27	CLA	A	208	1	1/1/12/20	12/26/102/115	-
26	DD6	G	305	-	-	2/26/80/80	0/3/3/3
31	LHG	j	102	-	-	18/53/53/53	-
27	CLA	b	812	24	1/1/14/20	8/33/109/115	-
27	CLA	J	310	9	1/1/11/20	11/17/93/115	-
27	CLA	H	207	7	1/1/15/20	10/39/115/115	-
29	LMG	a	852	-	-	16/28/48/70	0/1/1/1
26	DD6	G	303	-	-	0/26/80/80	0/3/3/3
27	CLA	H	206	7	1/1/15/20	15/39/115/115	-
31	LHG	a	833	-	-	25/53/53/53	-
27	CLA	H	210	7	1/1/13/20	8/30/106/115	-
32	BCR	j	101	-	-	2/29/63/63	0/2/2/2
30	A86	D	203	-	-	10/34/90/90	0/3/3/3
27	CLA	b	842	24	1/1/15/20	7/39/115/115	-
27	CLA	L	319	-	1/1/11/20	4/15/91/115	-
33	SQD	J	318	-	-	19/33/33/69	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	I	313	8	1/1/10/20	6/10/86/115	-
27	CLA	F	308	-	1/1/14/20	8/36/112/115	-
27	CLA	J	309	-	1/1/15/20	17/39/115/115	-
32	BCR	j	105	-	-	5/29/63/63	0/2/2/2
32	BCR	a	836	-	-	4/29/63/63	0/2/2/2
27	CLA	D	217	-	1/1/10/20	4/10/86/115	-
26	DD6	M	304	-	-	0/26/80/80	0/3/3/3
34	PQN	a	831	-	-	2/23/43/43	0/2/2/2
27	CLA	b	830	24	1/1/15/20	13/39/115/115	-
27	CLA	L	311	11	1/1/9/20	8/10/82/115	-
27	CLA	H	204	-	1/1/12/20	10/26/102/115	-
29	LMG	J	317	-	-	26/46/66/70	0/1/1/1
30	A86	K	307	-	-	3/34/90/90	1/3/3/3
27	CLA	G	306	-	1/1/11/20	10/17/93/115	-
27	CLA	l	206	-	1/1/11/20	3/15/91/115	-
30	A86	m	101	-	-	7/34/90/90	0/3/3/3
27	CLA	B	312	2	1/1/15/20	13/39/115/115	-
30	A86	K	304	27	-	3/34/90/90	0/3/3/3
29	LMG	I	319	-	-	13/32/52/70	0/1/1/1
27	CLA	a	830	13	1/1/15/20	10/39/115/115	-
26	DD6	E	306	-	-	11/26/80/80	0/3/3/3
27	CLA	C	311	3	1/1/14/20	13/33/109/115	-
27	CLA	F	307	5	1/1/13/20	11/32/108/115	-
27	CLA	L	318	11	1/1/10/20	3/11/87/115	-
27	CLA	G	309	-	1/1/15/20	23/39/115/115	-
32	BCR	a	851	-	-	4/29/63/63	0/2/2/2
27	CLA	A	204	1	1/1/15/20	19/39/115/115	-
27	CLA	I	310	8	1/1/11/20	8/18/94/115	-
27	CLA	G	314	-	1/1/10/20	4/10/86/115	-
27	CLA	G	317	6	1/1/11/20	9/20/96/115	-
27	CLA	G	312	6	1/1/14/20	12/35/111/115	-
30	A86	r	202	-	-	5/34/90/90	0/3/3/3
30	A86	C	304	-	-	4/34/90/90	0/3/3/3
27	CLA	B	306	2	1/1/12/20	18/29/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	816	13	1/1/15/20	8/39/115/115	-
27	CLA	C	309	-	1/1/14/20	14/36/112/115	-
27	CLA	I	309	8	1/1/11/20	6/17/93/115	-
28	KC1	F	312	5	-	6/15/71/71	-
27	CLA	b	828	24	1/1/11/20	5/18/94/115	-
30	A86	B	304	-	-	3/34/90/90	0/3/3/3
27	CLA	b	804	24	1/1/15/20	17/39/115/115	-
27	CLA	B	309	-	1/1/15/20	9/39/115/115	-
27	CLA	I	305	-	1/1/11/20	7/15/91/115	-
27	CLA	a	823	13	1/1/15/20	13/39/115/115	-
27	CLA	B	314	2	1/1/10/20	2/10/86/115	-
27	CLA	L	307	-	1/1/12/20	13/26/102/115	-
27	CLA	b	811	24	1/1/15/20	7/39/115/115	-
27	CLA	L	308	11	1/1/15/20	8/39/115/115	-
30	A86	K	302	-	-	8/34/90/90	0/3/3/3
27	CLA	M	311	-	1/1/11/20	7/17/93/115	-
30	A86	L	302	-	-	8/34/90/90	0/3/3/3
31	LHG	E	316	-	-	5/46/46/53	-
28	KC1	L	320	28	-	6/15/71/71	-
27	CLA	a	807	13	1/1/15/20	12/39/115/115	-
29	LMG	A	214	27	-	29/36/56/70	0/1/1/1
27	CLA	b	818	24	1/1/14/20	17/33/109/115	-
26	DD6	I	304	-	-	3/26/80/80	0/3/3/3
27	CLA	C	307	3	1/1/15/20	5/39/115/115	-
27	CLA	a	829	13	1/1/15/20	7/39/115/115	-
27	CLA	H	214	7	1/1/11/20	6/15/91/115	-
27	CLA	a	812	13	1/1/15/20	8/39/115/115	-
27	CLA	a	803	13	1/1/15/20	15/39/115/115	-
31	LHG	b	836	27	-	32/53/53/53	-
27	CLA	b	847	24	1/1/15/20	14/39/115/115	-
27	CLA	b	843	24	1/1/15/20	15/39/115/115	-
27	CLA	B	308	2	1/1/15/20	11/39/115/115	-
27	CLA	F	306	5	1/1/13/20	10/27/103/115	-
27	CLA	D	213	23	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	A86	C	302	-	-	5/34/90/90	0/3/3/3
27	CLA	K	314	10,30	1/1/15/20	19/39/115/115	-
27	CLA	a	842	-	1/1/15/20	13/39/115/115	-
27	CLA	K	316	10	1/1/15/20	16/39/115/115	-
27	CLA	f	302	-	1/1/15/20	11/39/115/115	-
27	CLA	a	827	13	1/1/14/20	13/33/109/115	-
27	CLA	a	822	13	1/1/15/20	8/39/115/115	-
27	CLA	D	207	-	1/1/14/20	11/35/111/115	-
27	CLA	G	316	6	1/1/13/20	7/27/103/115	-
27	CLA	a	832	31	1/1/12/20	6/24/100/115	-
27	CLA	K	311	-	1/1/12/20	11/24/100/115	-
27	CLA	a	843	-	1/1/15/20	20/39/115/115	-
27	CLA	a	828	13	1/1/15/20	11/39/115/115	-
31	LHG	K	320	-	-	24/34/34/53	-
27	CLA	a	806	27,13	1/1/13/20	5/27/103/115	-
31	LHG	a	834	27	-	13/31/31/53	-
27	CLA	C	316	3	1/1/10/20	4/10/86/115	-
28	KC1	L	314	-	-	11/15/71/71	-
27	CLA	J	313	-	1/1/11/20	11/17/93/115	-
27	CLA	F	311	5	1/1/14/20	15/33/109/115	-
26	DD6	B	303	-	-	0/26/80/80	0/3/3/3
27	CLA	b	838	24	1/1/14/20	13/33/109/115	-
27	CLA	E	313	4	1/1/11/20	4/15/91/115	-
26	DD6	E	302	-	-	3/26/80/80	0/3/3/3
27	CLA	K	318	10	1/1/11/20	5/17/93/115	-
27	CLA	E	308	4	1/1/15/20	13/39/115/115	-
27	CLA	E	315	-	1/1/13/20	4/29/105/115	-
27	CLA	C	315	3	1/1/10/20	6/12/88/115	-
27	CLA	I	311	8	1/1/15/20	19/39/115/115	-
27	CLA	A	210	1	1/1/11/20	6/17/93/115	-
30	A86	A	213	-	-	4/34/90/90	0/3/3/3
28	KC1	M	314	-	-	6/15/71/71	-
27	CLA	a	814	-	1/1/11/20	6/15/91/115	-
27	CLA	M	318	12	1/1/11/20	11/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	850	13	1/1/13/20	11/29/105/115	-
27	CLA	a	811	27,13	1/1/14/20	13/36/112/115	-
30	A86	L	306	-	-	6/34/90/90	0/3/3/3
27	CLA	M	319	12	1/1/11/20	9/17/93/115	-
28	KC1	C	308	3	-	7/15/71/71	-
27	CLA	M	316	12	1/1/12/20	8/26/102/115	-
28	KC1	I	312	8	-	6/15/71/71	-
27	CLA	K	319	10	1/1/11/20	10/17/93/115	-
32	BCR	b	834	-	-	6/29/63/63	0/2/2/2
27	CLA	b	826	-	1/1/11/20	4/15/91/115	-
36	SF4	c	102	25	-	-	0/6/5/5
29	LMG	l	201	-	-	16/35/55/70	0/1/1/1
30	A86	B	301	-	-	10/34/90/90	0/3/3/3
27	CLA	b	806	24	1/1/15/20	13/39/115/115	-
27	CLA	D	208	23	1/1/15/20	15/39/115/115	-
27	CLA	C	312	3	1/1/14/20	12/35/111/115	-
27	CLA	L	310	-	1/1/15/20	15/39/115/115	-
32	BCR	l	205	-	-	8/29/63/63	0/2/2/2
27	CLA	b	821	24	1/1/15/20	15/39/115/115	-
29	LMG	j	103	-	-	16/32/52/70	0/1/1/1
27	CLA	K	313	10	1/1/12/20	8/24/100/115	-
28	KC1	K	308	-	-	7/15/71/71	-
27	CLA	b	825	-	1/1/15/20	17/39/115/115	-
27	CLA	H	205	7	1/1/15/20	12/39/115/115	-
27	CLA	J	308	9	1/1/13/20	7/29/105/115	-
27	CLA	C	306	29	1/1/11/20	4/15/91/115	-
26	DD6	F	302	-	-	1/26/80/80	0/3/3/3
27	CLA	a	818	13	1/1/11/20	10/15/91/115	-
27	CLA	B	311	2	1/1/15/20	12/39/115/115	-
32	BCR	i	103	-	-	4/29/63/63	0/2/2/2
30	A86	G	302	-	-	13/34/90/90	0/3/3/3
27	CLA	l	203	20	1/1/11/20	7/20/96/115	-
30	A86	b	848	-	-	14/34/90/90	0/3/3/3
27	CLA	b	809	24	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	838	13	1/1/15/20	12/39/115/115	-
31	LHG	a	802	-	-	33/53/53/53	-
27	CLA	H	209	-	1/1/14/20	9/33/109/115	-
30	A86	I	301	-	-	10/34/90/90	0/3/3/3
27	CLA	G	311	6	1/1/13/20	8/29/105/115	-
30	A86	D	206	-	-	7/34/90/90	0/3/3/3
27	CLA	A	206	1	1/1/11/20	6/17/93/115	-
27	CLA	D	211	23	1/1/11/20	10/17/93/115	-
36	SF4	b	802	24	-	-	0/6/5/5
27	CLA	b	819	24	1/1/15/20	7/39/115/115	-
27	CLA	E	310	4	1/1/11/20	6/17/93/115	-
27	CLA	E	312	4	1/1/13/20	9/27/103/115	-
32	BCR	E	305	-	-	0/29/63/63	0/2/2/2
27	CLA	b	841	24	1/1/14/20	12/35/111/115	-
27	CLA	a	809	13	1/1/15/20	9/39/115/115	-
27	CLA	C	310	3	1/1/11/20	8/17/93/115	-
27	CLA	b	846	-	1/1/15/20	13/39/115/115	-
26	DD6	D	205	-	-	3/26/80/80	0/3/3/3
31	LHG	H	215	-	-	19/38/38/53	-
31	LHG	a	801	-	-	28/53/53/53	-
27	CLA	K	310	10	1/1/13/20	15/29/105/115	-
27	CLA	M	310	-	1/1/13/20	13/32/108/115	-
26	DD6	G	301	-	-	3/26/80/80	0/3/3/3
32	BCR	l	202	-	-	4/29/63/63	0/2/2/2
26	DD6	F	303	-	-	5/26/80/80	0/3/3/3
30	A86	M	305	-	-	6/34/90/90	0/3/3/3
27	CLA	b	850	-	1/1/15/20	16/39/115/115	-
27	CLA	L	315	11	1/1/10/20	4/10/86/115	-
31	LHG	I	318	-	-	15/39/39/53	-
27	CLA	M	312	12	1/1/11/20	7/17/93/115	-
32	BCR	b	840	-	-	6/29/63/63	0/2/2/2
27	CLA	H	212	7	1/1/15/20	18/39/115/115	-
26	DD6	M	301	-	-	2/26/80/80	0/3/3/3
30	A86	L	305	-	-	7/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	BCR	a	853	-	-	8/29/63/63	0/2/2/2
32	BCR	m	102	-	-	7/29/63/63	0/2/2/2
27	CLA	b	817	24	1/1/13/20	6/27/103/115	-
27	CLA	b	815	-	1/1/15/20	11/39/115/115	-
31	LHG	a	837	-	-	19/36/36/53	-
27	CLA	F	305	5	1/1/14/20	13/35/111/115	-
27	CLA	f	301	-	1/1/15/20	7/39/115/115	-
30	A86	B	302	-	-	5/34/90/90	0/3/3/3
30	A86	J	304	-	-	4/34/90/90	0/3/3/3
32	BCR	a	847	-	-	2/29/63/63	0/2/2/2
27	CLA	a	848	-	1/1/15/20	8/39/115/115	-
27	CLA	A	211	-	1/1/9/20	2/10/82/115	-
30	A86	F	304	-	-	5/34/90/90	0/3/3/3
28	KC1	L	322	28	-	7/15/71/71	-
26	DD6	J	303	-	-	4/26/80/80	0/3/3/3
27	CLA	A	203	1	1/1/14/20	4/35/111/115	-
27	CLA	G	307	6	1/1/13/20	4/29/105/115	-
30	A86	B	305	-	-	4/34/90/90	0/3/3/3
27	CLA	b	839	-	1/1/15/20	8/39/115/115	-
27	CLA	J	312	9	1/1/15/20	16/39/115/115	-
26	DD6	I	302	-	-	1/26/80/80	0/3/3/3
29	LMG	M	321	-	-	15/37/57/70	0/1/1/1
27	CLA	a	821	13	1/1/15/20	4/39/115/115	-
27	CLA	b	844	24	1/1/15/20	17/39/115/115	-
27	CLA	D	209	23	1/1/11/20	11/20/96/115	-
27	CLA	L	312	11	1/1/13/20	11/29/105/115	-
27	CLA	l	204	20	1/1/15/20	16/39/115/115	-
27	CLA	b	823	24	1/1/15/20	15/39/115/115	-
27	CLA	L	321	11	1/1/11/20	7/15/91/115	-
27	CLA	b	824	24	1/1/13/20	13/31/107/115	-
27	CLA	L	316	11	1/1/13/20	15/29/105/115	-
27	CLA	I	314	8	1/1/11/20	7/20/96/115	-
30	A86	M	302	-	-	5/34/90/90	0/3/3/3
27	CLA	b	813	24	1/1/13/20	9/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	A86	C	305	-	-	4/34/90/90	0/3/3/3
27	CLA	a	855	13	1/1/15/20	11/39/115/115	-
32	BCR	i	102	-	-	0/29/63/63	0/2/2/2
27	CLA	b	831	31	1/1/15/20	9/39/115/115	-
26	DD6	H	202	-	-	3/26/80/80	0/3/3/3
27	CLA	L	313	11	1/1/15/20	12/39/115/115	-
26	DD6	A	201	-	-	7/26/80/80	0/3/3/3
27	CLA	b	820	24	1/1/15/20	14/39/115/115	-
31	LHG	M	320	-	-	29/51/51/53	-
26	DD6	J	305	-	-	2/26/80/80	0/3/3/3
27	CLA	F	309	5	1/1/11/20	2/17/93/115	-
27	CLA	b	808	24	1/1/15/20	9/39/115/115	-
28	KC1	K	315	10	-	5/15/71/71	-
27	CLA	F	310	5	1/1/14/20	13/33/109/115	-
27	CLA	F	314	5	1/1/11/20	6/18/94/115	-
32	BCR	a	835	-	-	0/29/63/63	0/2/2/2
27	CLA	D	212	23	1/1/10/20	2/12/88/115	-
30	A86	K	306	-	-	5/34/90/90	0/3/3/3
26	DD6	C	303	-	-	5/26/80/80	0/3/3/3
34	PQN	b	832	-	-	3/23/43/43	0/2/2/2
27	CLA	I	316	8	1/1/11/20	4/15/91/115	-
27	CLA	a	808	13	1/1/15/20	13/39/115/115	-
27	CLA	a	825	13	1/1/11/20	9/15/91/115	-
27	CLA	A	207	1	1/1/15/20	18/39/115/115	-
27	CLA	b	827	24	1/1/14/20	9/33/109/115	-
27	CLA	a	810	13	1/1/15/20	12/39/115/115	-
27	CLA	E	309	4	1/1/15/20	13/39/115/115	-
27	CLA	f	303	16	1/1/11/20	5/15/91/115	-
27	CLA	C	317	-	1/1/10/20	8/12/88/115	-
32	BCR	r	203	-	-	4/29/63/63	0/2/2/2
27	CLA	a	805	13	1/1/15/20	12/39/115/115	-
27	CLA	J	314	-	1/1/15/20	16/39/115/115	-
28	KC1	B	313	-	-	6/15/71/71	-
30	A86	M	303	-	-	10/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DD6	K	303	-	-	6/26/80/80	0/3/3/3
27	CLA	a	845	-	1/1/15/20	10/39/115/115	-
27	CLA	b	829	-	1/1/15/20	10/39/115/115	-
30	A86	K	305	-	-	3/34/90/90	0/3/3/3
26	DD6	A	202	-	-	1/26/80/80	0/3/3/3
29	LMG	C	319	27	-	20/39/59/70	0/1/1/1
27	CLA	J	311	9	1/1/15/20	13/39/115/115	-
27	CLA	b	803	24	1/1/15/20	12/39/115/115	-
27	CLA	I	308	-	1/1/15/20	14/39/115/115	-
27	CLA	a	804	-	1/1/15/20	8/39/115/115	-
27	CLA	a	856	-	1/1/15/20	16/39/115/115	-
27	CLA	L	309	11	1/1/15/20	15/39/115/115	-
27	CLA	F	315	5	1/1/13/20	19/31/107/115	-
31	LHG	B	315	-	-	25/46/46/53	-
28	KC1	G	313	6	-	5/15/71/71	-
27	CLA	a	815	13	1/1/15/20	24/39/115/115	-
27	CLA	a	819	13	1/1/11/20	11/20/96/115	-
32	BCR	E	304	-	-	2/29/63/63	0/2/2/2
27	CLA	a	846	13	1/1/15/20	16/39/115/115	-
27	CLA	M	313	12	1/1/15/20	21/39/115/115	-
27	CLA	H	208	7	1/1/11/20	9/17/93/115	-
27	CLA	C	314	3	1/1/10/20	4/10/86/115	-
30	A86	J	316	-	-	15/34/90/90	0/3/3/3
27	CLA	K	312	-	1/1/15/20	24/39/115/115	-

The worst 5 of 2644 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	318	SQD	C6-S	-12.68	1.59	1.77
29	L	323	LMG	O6-C1	10.77	1.69	1.41
29	E	317	LMG	O2-C2	-10.23	1.17	1.43
29	I	319	LMG	O2-C2	-9.53	1.19	1.43
26	A	202	DD6	C30-C31	-9.03	1.24	1.42

The worst 5 of 3241 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j	103	LMG	O2-C2-C1	-21.73	58.28	110.08
29	a	852	LMG	O2-C2-C1	-19.20	64.32	110.08
26	E	303	DD6	C21-C20-C15	-16.47	95.19	122.30
29	C	301	LMG	O2-C2-C1	15.55	147.12	110.08
32	b	834	BCR	C32-C1-C6	-14.55	87.43	110.24

5 of 228 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	203	CLA	ND
27	A	204	CLA	ND
27	A	205	CLA	ND
27	A	206	CLA	ND
27	A	207	CLA	ND

5 of 3485 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	201	DD6	C12-C11-C13-C14
26	A	201	DD6	C1-C2-C3-C4
26	A	202	DD6	C13-C14-C15-C20
26	E	302	DD6	C10-C11-C13-C14
26	E	303	DD6	C13-C14-C15-C16

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	K	307	A86	C31-C32-C33-C34-C35-C36

321 monomers are involved in 1231 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	840	CLA	2	0
27	F	316	CLA	8	0
27	G	310	CLA	1	0
27	a	841	CLA	2	0
27	a	817	CLA	6	0
32	b	833	BCR	4	0
27	L	317	CLA	10	0
27	A	205	CLA	9	0
27	B	307	CLA	4	0
26	J	302	DD6	1	0
36	c	101	SF4	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	844	CLA	5	0
28	H	211	KC1	1	0
27	E	314	CLA	4	0
26	G	304	DD6	2	0
27	b	814	CLA	20	0
27	E	311	CLA	6	0
27	b	810	CLA	2	0
29	D	202	LMG	1	0
27	a	849	CLA	3	0
27	j	104	CLA	1	0
27	D	210	CLA	2	0
27	a	813	CLA	1	0
27	b	845	CLA	2	0
27	I	317	CLA	7	0
29	L	323	LMG	26	0
37	b	835	DGD	1	0
27	b	805	CLA	1	0
27	M	307	CLA	5	0
32	f	304	BCR	4	0
27	a	820	CLA	4	0
26	L	301	DD6	4	0
27	I	307	CLA	3	0
27	F	313	CLA	9	0
27	M	309	CLA	4	0
27	K	309	CLA	8	0
27	M	317	CLA	12	0
27	H	213	CLA	5	0
31	E	318	LHG	2	0
32	f	305	BCR	4	0
27	D	216	CLA	4	0
27	D	215	CLA	5	0
27	r	201	CLA	1	0
30	L	304	A86	1	0
27	a	839	CLA	6	0
27	b	801	CLA	11	0
27	G	308	CLA	1	0
29	A	212	LMG	7	0
27	i	101	CLA	2	0
29	E	317	LMG	6	0
28	J	306	KC1	1	0
27	I	315	CLA	4	0
27	J	307	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	807	CLA	3	0
27	M	308	CLA	4	0
27	b	816	CLA	2	0
30	F	301	A86	6	0
30	H	201	A86	17	0
27	K	317	CLA	6	0
26	L	303	DD6	5	0
27	M	315	CLA	3	0
27	I	306	CLA	1	0
32	b	837	BCR	3	0
27	J	315	CLA	5	0
27	b	822	CLA	3	0
27	C	318	CLA	10	0
31	D	201	LHG	7	0
26	E	303	DD6	1	0
27	F	317	CLA	4	0
27	D	214	CLA	6	0
30	I	303	A86	1	0
27	b	849	CLA	3	0
30	K	301	A86	10	0
27	A	208	CLA	3	0
31	j	102	LHG	5	0
27	b	812	CLA	2	0
27	J	310	CLA	8	0
27	H	207	CLA	3	0
29	a	852	LMG	2	0
27	H	206	CLA	4	0
31	a	833	LHG	2	0
27	H	210	CLA	5	0
32	j	101	BCR	7	0
30	D	203	A86	4	0
27	b	842	CLA	4	0
27	L	319	CLA	9	0
33	J	318	SQD	7	0
27	I	313	CLA	3	0
27	F	308	CLA	9	0
27	J	309	CLA	8	0
32	j	105	BCR	10	0
32	a	836	BCR	3	0
27	D	217	CLA	3	0
26	M	304	DD6	2	0
34	a	831	PQN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	830	CLA	6	0
27	L	311	CLA	4	0
27	H	204	CLA	3	0
29	J	317	LMG	5	0
27	G	306	CLA	1	0
30	m	101	A86	5	0
27	B	312	CLA	7	0
30	K	304	A86	3	0
29	I	319	LMG	2	0
27	a	830	CLA	2	0
26	E	306	DD6	2	0
27	C	311	CLA	8	0
27	F	307	CLA	1	0
27	L	318	CLA	2	0
27	G	309	CLA	12	0
32	a	851	BCR	3	0
27	A	204	CLA	6	0
27	I	310	CLA	2	0
27	G	317	CLA	4	0
27	G	312	CLA	5	0
30	r	202	A86	2	0
30	C	304	A86	1	0
27	B	306	CLA	14	0
27	a	816	CLA	3	0
27	C	309	CLA	5	0
27	I	309	CLA	2	0
28	F	312	KC1	5	0
27	b	828	CLA	2	0
30	B	304	A86	2	0
27	b	804	CLA	3	0
27	B	309	CLA	2	0
27	I	305	CLA	5	0
27	a	823	CLA	2	0
27	B	314	CLA	3	0
27	L	307	CLA	2	0
27	b	811	CLA	2	0
27	L	308	CLA	3	0
27	M	311	CLA	7	0
30	L	302	A86	4	0
31	E	316	LHG	3	0
28	L	320	KC1	1	0
27	a	807	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	214	LMG	2	0
27	b	818	CLA	6	0
26	I	304	DD6	2	0
27	C	307	CLA	6	0
27	a	829	CLA	3	0
27	a	812	CLA	2	0
27	a	803	CLA	2	0
31	b	836	LHG	6	0
27	b	847	CLA	1	0
27	b	843	CLA	6	0
27	B	308	CLA	1	0
27	D	213	CLA	2	0
27	K	314	CLA	6	0
27	a	842	CLA	3	0
27	K	316	CLA	15	0
27	f	302	CLA	1	0
27	a	827	CLA	4	0
27	a	822	CLA	2	0
27	D	207	CLA	3	0
27	G	316	CLA	15	0
27	a	832	CLA	4	0
27	K	311	CLA	7	0
27	a	843	CLA	7	0
27	a	828	CLA	1	0
31	K	320	LHG	1	0
27	a	806	CLA	9	0
31	a	834	LHG	3	0
27	C	316	CLA	11	0
28	L	314	KC1	7	0
27	J	313	CLA	4	0
27	F	311	CLA	5	0
27	b	838	CLA	2	0
27	K	318	CLA	2	0
27	E	308	CLA	5	0
27	E	315	CLA	5	0
27	C	315	CLA	2	0
27	I	311	CLA	18	0
27	A	210	CLA	6	0
28	M	314	KC1	3	0
27	M	318	CLA	2	0
27	a	850	CLA	5	0
27	a	811	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	L	306	A86	1	0
27	M	319	CLA	10	0
28	C	308	KC1	5	0
27	M	316	CLA	4	0
28	I	312	KC1	2	0
27	K	319	CLA	11	0
32	b	834	BCR	3	0
27	b	826	CLA	3	0
36	c	102	SF4	5	0
29	l	201	LMG	1	0
30	B	301	A86	2	0
27	b	806	CLA	4	0
27	D	208	CLA	10	0
27	C	312	CLA	11	0
27	L	310	CLA	11	0
32	l	205	BCR	8	0
27	b	821	CLA	4	0
29	j	103	LMG	1	0
27	K	313	CLA	6	0
28	K	308	KC1	2	0
27	b	825	CLA	5	0
27	H	205	CLA	8	0
26	F	302	DD6	1	0
27	a	818	CLA	3	0
27	B	311	CLA	5	0
32	i	103	BCR	6	0
30	G	302	A86	6	0
27	l	203	CLA	3	0
30	b	848	A86	4	0
27	b	809	CLA	2	0
27	a	838	CLA	4	0
31	a	802	LHG	11	0
27	H	209	CLA	4	0
30	I	301	A86	1	0
27	A	206	CLA	3	0
27	D	211	CLA	2	0
36	b	802	SF4	2	0
27	b	819	CLA	3	0
27	E	310	CLA	1	0
27	E	312	CLA	1	0
32	E	305	BCR	7	0
27	b	841	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	809	CLA	15	0
27	C	310	CLA	3	0
27	b	846	CLA	7	0
26	D	205	DD6	3	0
31	a	801	LHG	4	0
27	K	310	CLA	3	0
27	M	310	CLA	5	0
32	l	202	BCR	2	0
26	F	303	DD6	1	0
30	M	305	A86	7	0
27	b	850	CLA	6	0
27	L	315	CLA	27	0
31	I	318	LHG	3	0
27	M	312	CLA	4	0
32	b	840	BCR	8	0
27	H	212	CLA	9	0
30	L	305	A86	16	0
32	a	853	BCR	16	0
32	m	102	BCR	4	0
27	b	815	CLA	6	0
31	a	837	LHG	1	0
27	F	305	CLA	27	0
27	f	301	CLA	1	0
30	B	302	A86	3	0
30	J	304	A86	3	0
32	a	847	BCR	4	0
27	A	211	CLA	3	0
30	F	304	A86	2	0
28	L	322	KC1	2	0
26	J	303	DD6	2	0
27	A	203	CLA	6	0
27	G	307	CLA	4	0
27	b	839	CLA	4	0
27	J	312	CLA	11	0
26	I	302	DD6	2	0
29	M	321	LMG	2	0
27	a	821	CLA	1	0
27	b	844	CLA	5	0
27	D	209	CLA	2	0
27	L	312	CLA	3	0
27	l	204	CLA	6	0
27	b	823	CLA	2	0

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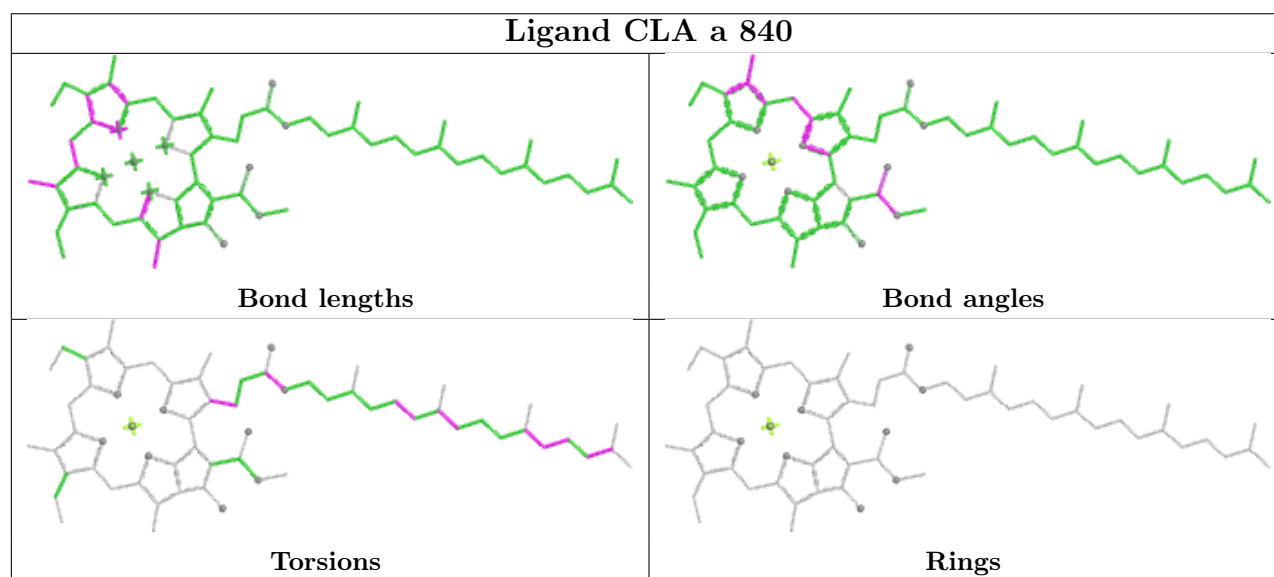
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	L	321	CLA	1	0
27	b	824	CLA	7	0
27	L	316	CLA	2	0
27	I	314	CLA	2	0
30	M	302	A86	1	0
27	b	813	CLA	3	0
30	C	305	A86	4	0
27	a	855	CLA	5	0
32	i	102	BCR	7	0
27	b	831	CLA	1	0
26	H	202	DD6	3	0
26	A	201	DD6	4	0
27	L	313	CLA	17	0
27	b	820	CLA	5	0
31	M	320	LHG	5	0
27	F	309	CLA	27	0
27	b	808	CLA	3	0
28	K	315	KC1	2	0
27	F	310	CLA	2	0
27	F	314	CLA	1	0
32	a	835	BCR	20	0
27	D	212	CLA	1	0
26	C	303	DD6	1	0
34	b	832	PQN	4	0
27	I	316	CLA	2	0
27	a	808	CLA	3	0
27	a	825	CLA	1	0
27	A	207	CLA	5	0
27	a	810	CLA	6	0
27	E	309	CLA	2	0
27	f	303	CLA	2	0
27	C	317	CLA	8	0
32	r	203	BCR	1	0
27	a	805	CLA	13	0
27	J	314	CLA	2	0
28	B	313	KC1	4	0
30	M	303	A86	2	0
26	K	303	DD6	1	0
27	a	845	CLA	1	0
26	A	202	DD6	4	0
29	C	319	LMG	1	0
27	J	311	CLA	9	0

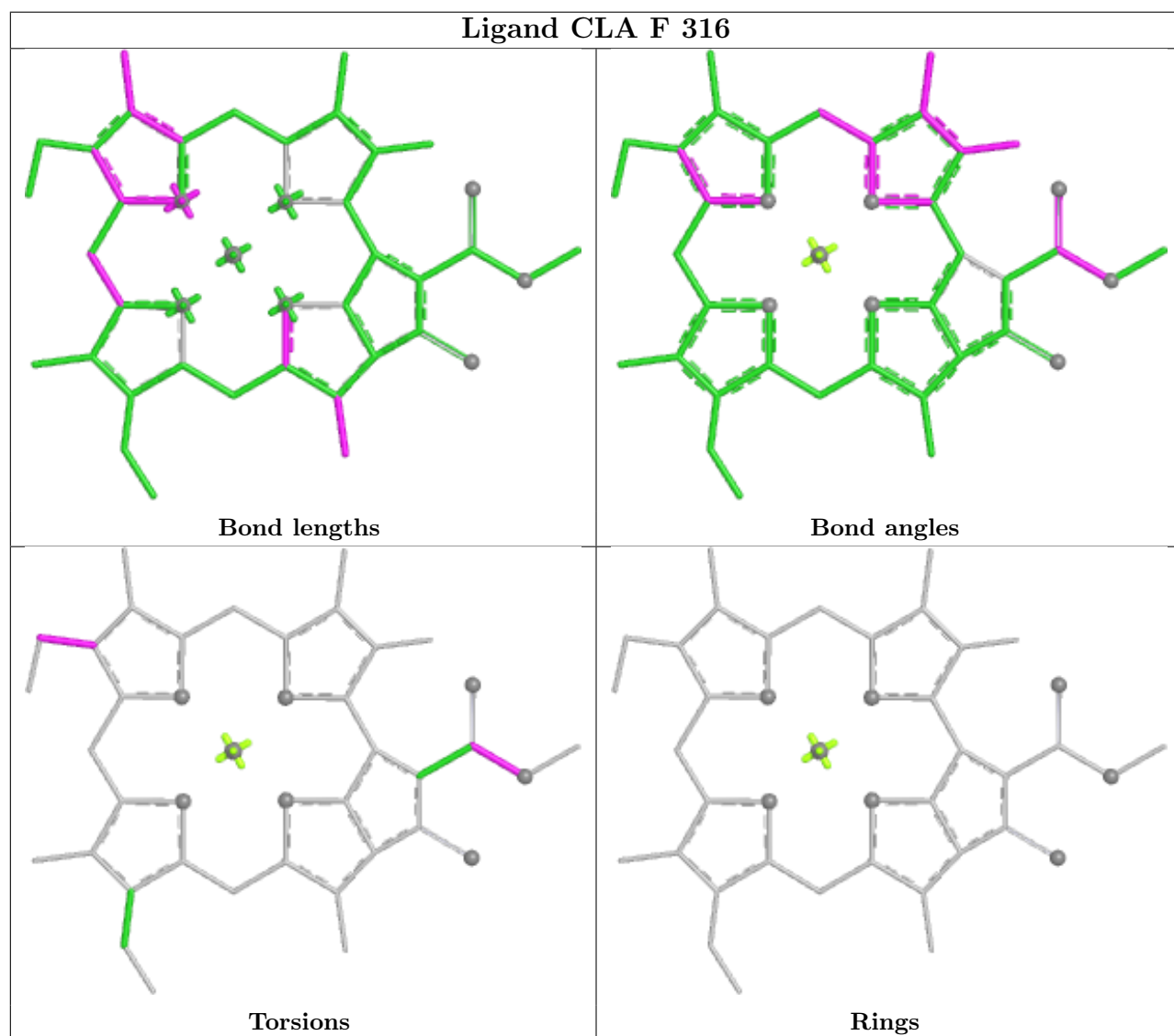
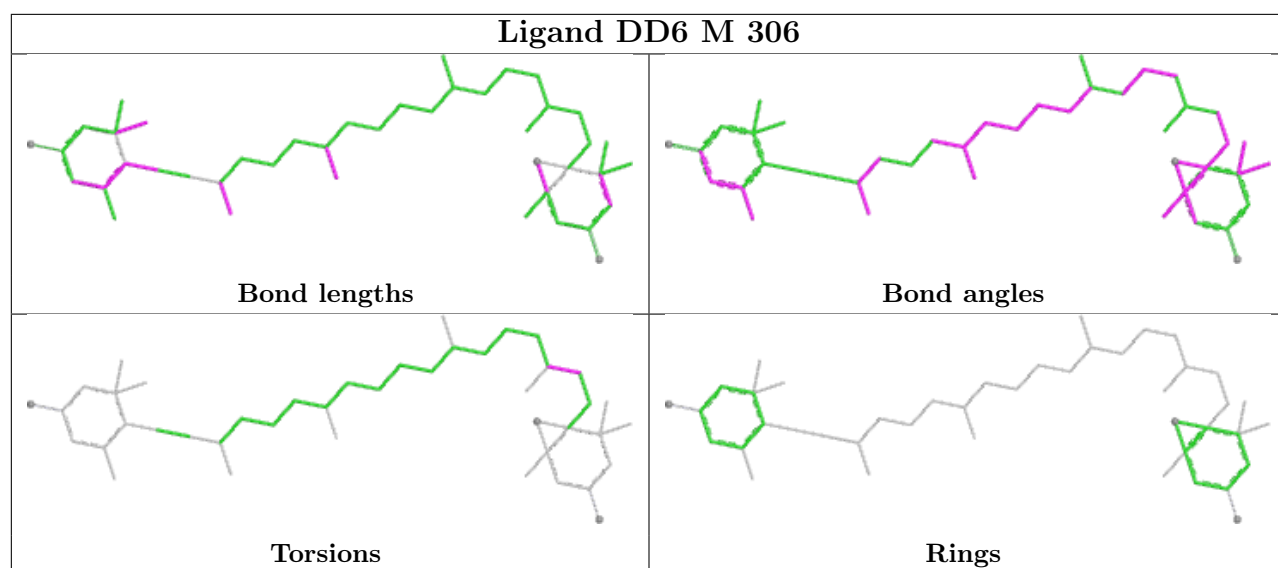
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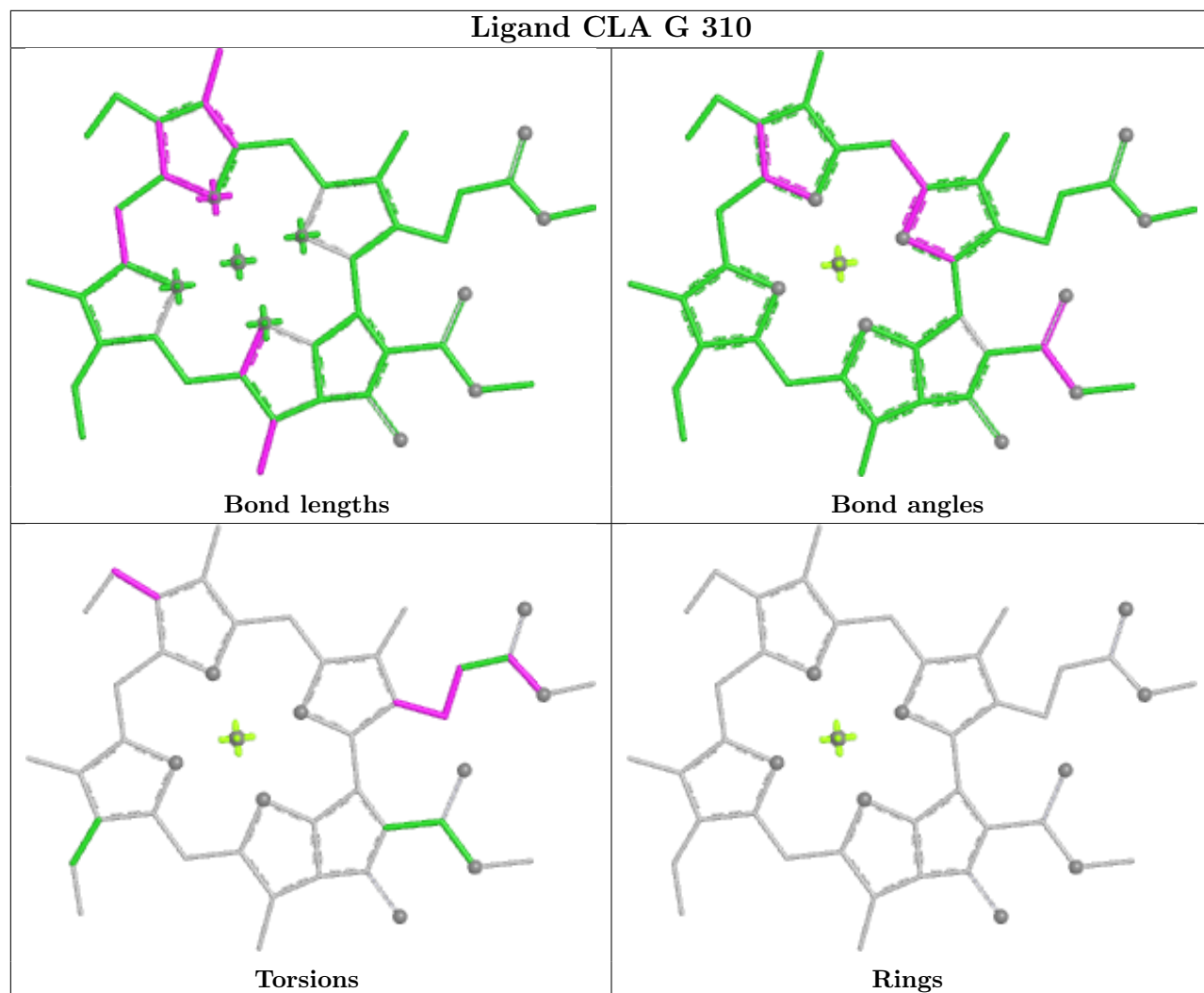
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	803	CLA	7	0
27	I	308	CLA	3	0
27	a	804	CLA	12	0
27	a	856	CLA	3	0
27	L	309	CLA	3	0
27	F	315	CLA	11	0
31	B	315	LHG	3	0
27	a	815	CLA	7	0
27	a	819	CLA	1	0
32	E	304	BCR	1	0
27	a	846	CLA	6	0
27	M	313	CLA	11	0
27	H	208	CLA	16	0
27	C	314	CLA	3	0
30	J	316	A86	7	0
27	K	312	CLA	6	0

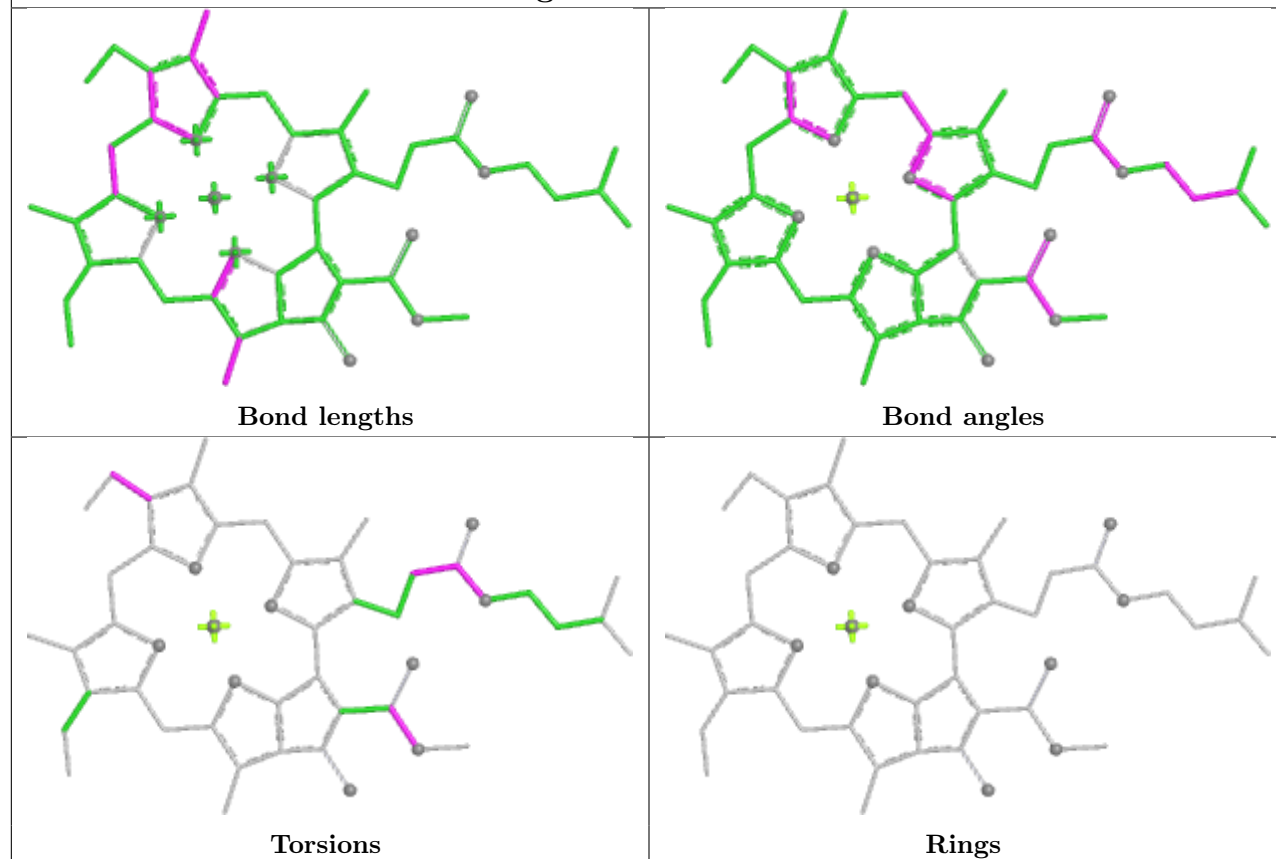
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



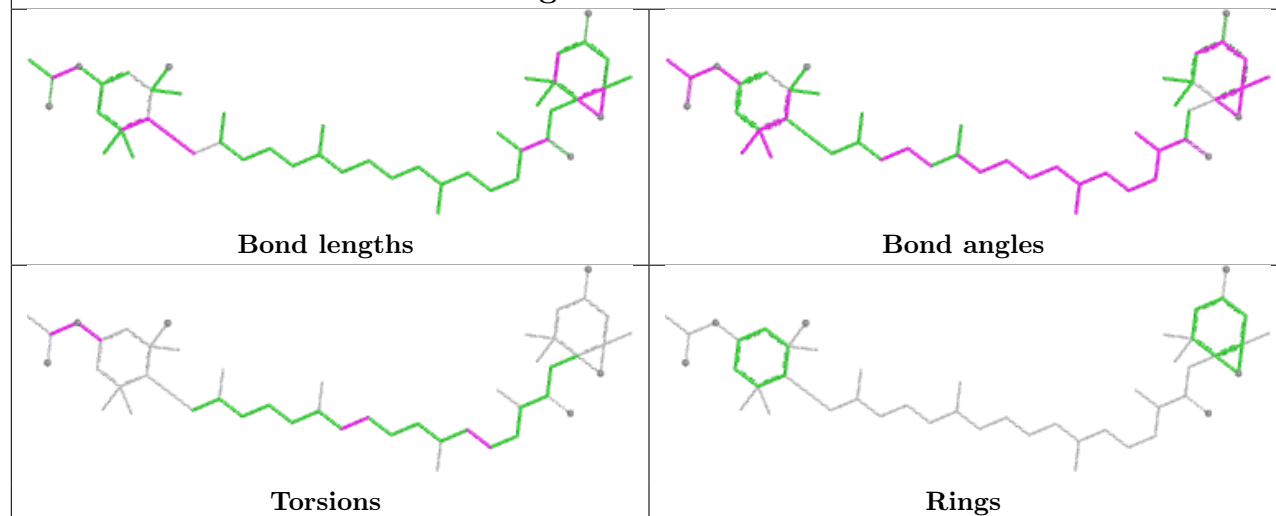


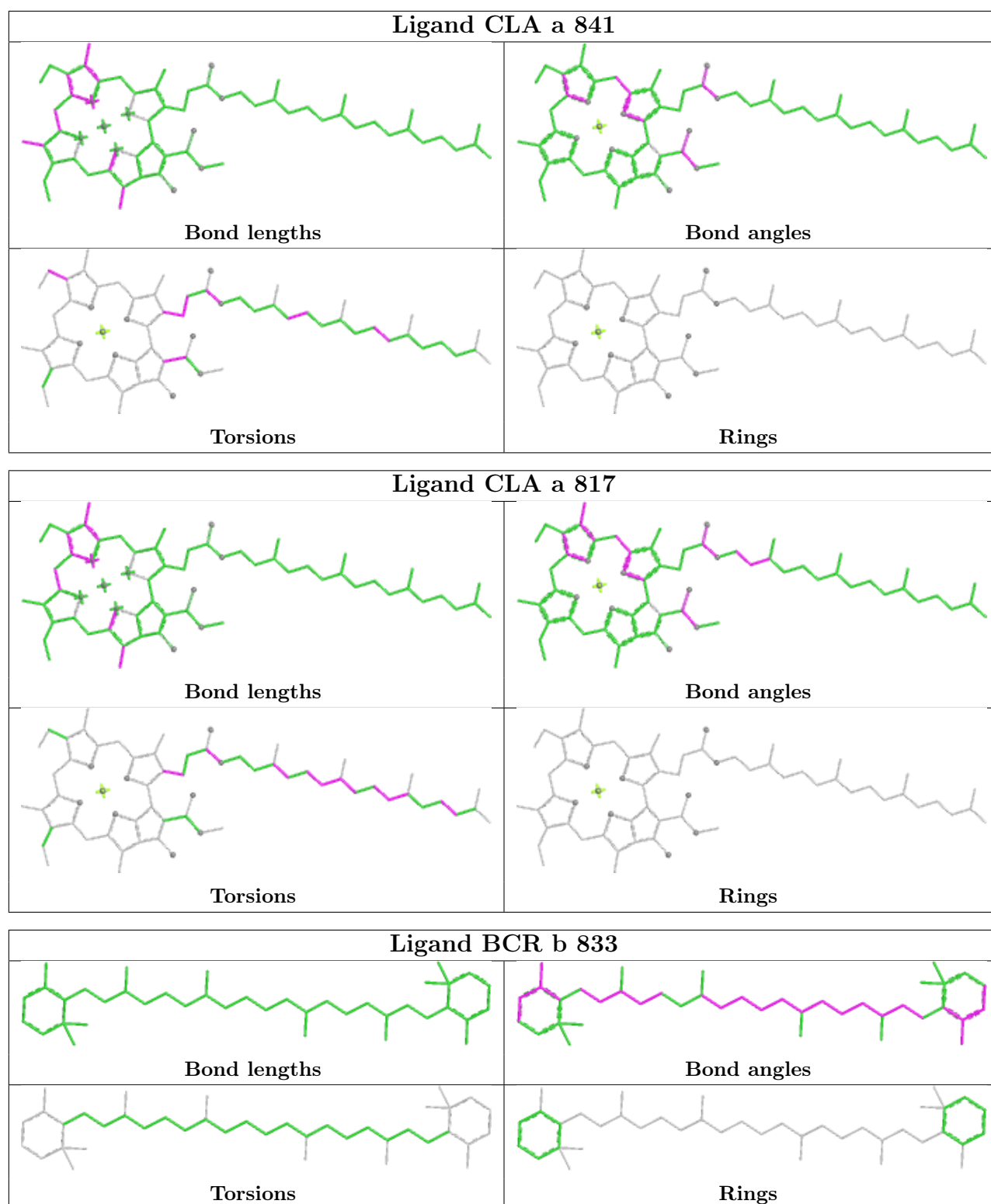


Ligand CLA a 824

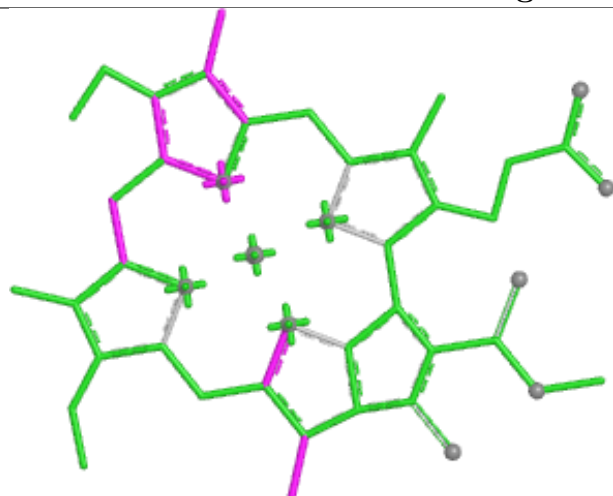


Ligand A86 E 301

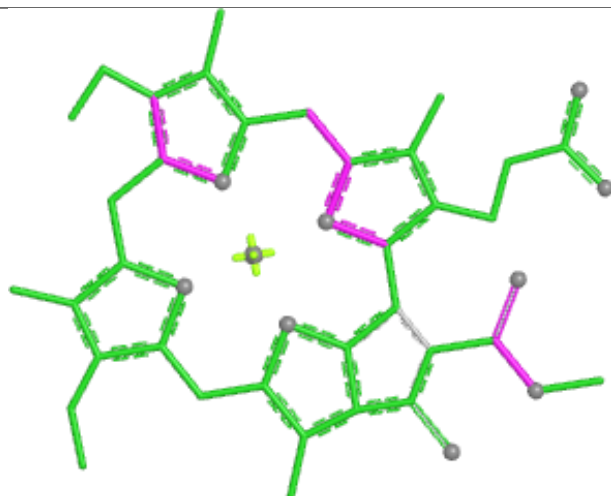




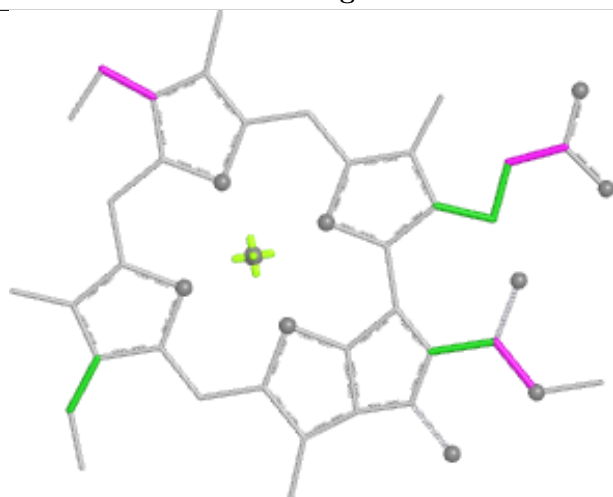
Ligand CLA L 317



Bond lengths



Bond angles

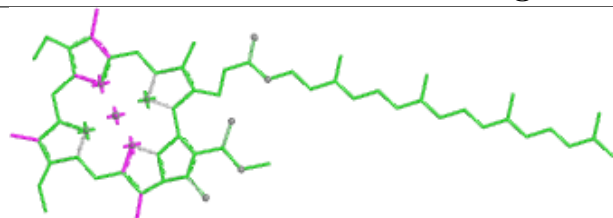


Torsions

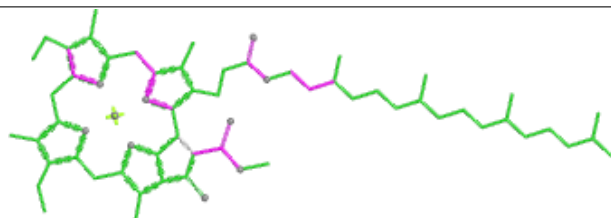


Rings

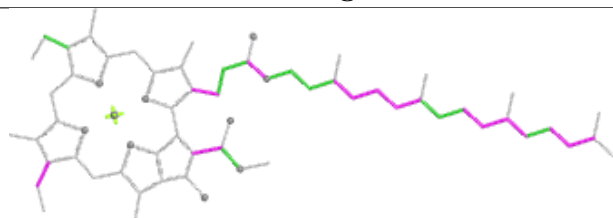
Ligand CLA A 205



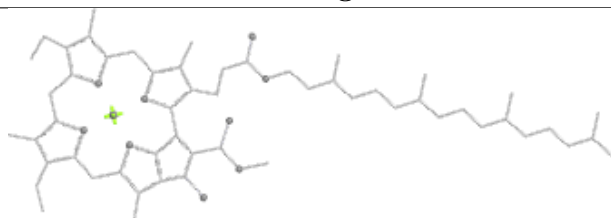
Bond lengths



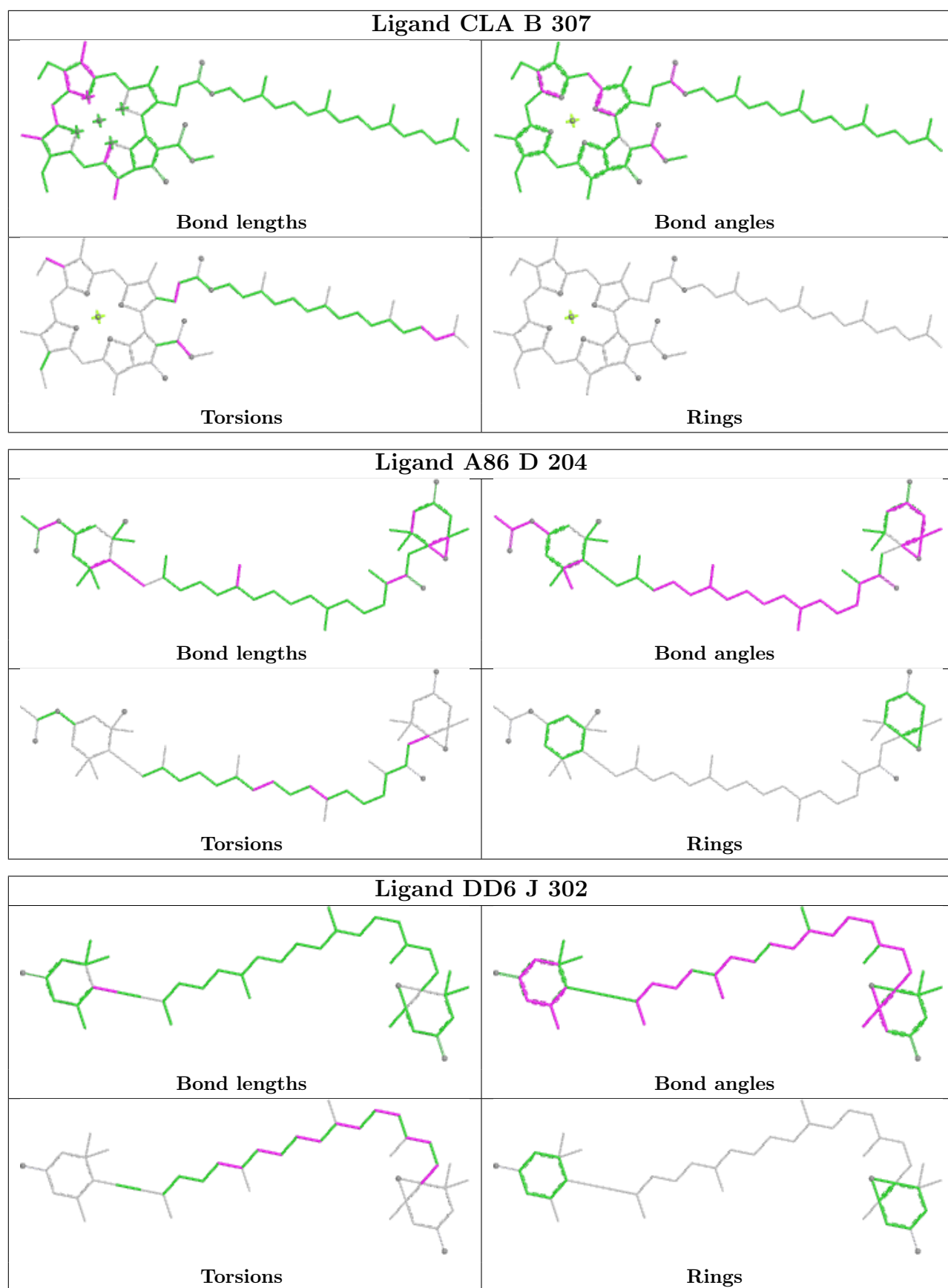
Bond angles



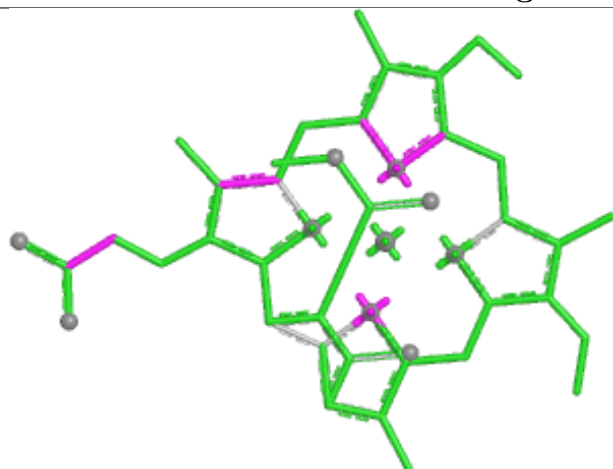
Torsions



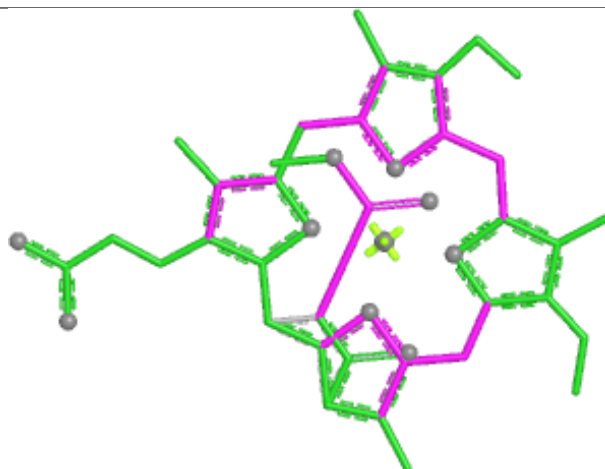
Rings



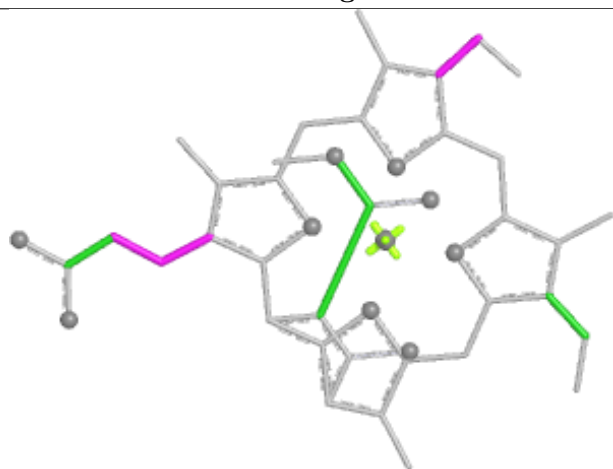
Ligand KC1 C 313



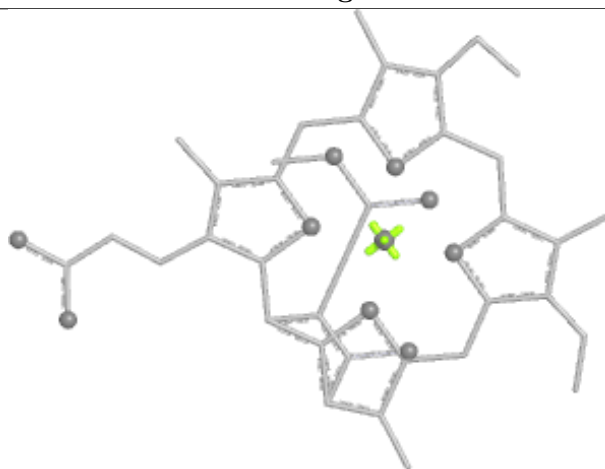
Bond lengths



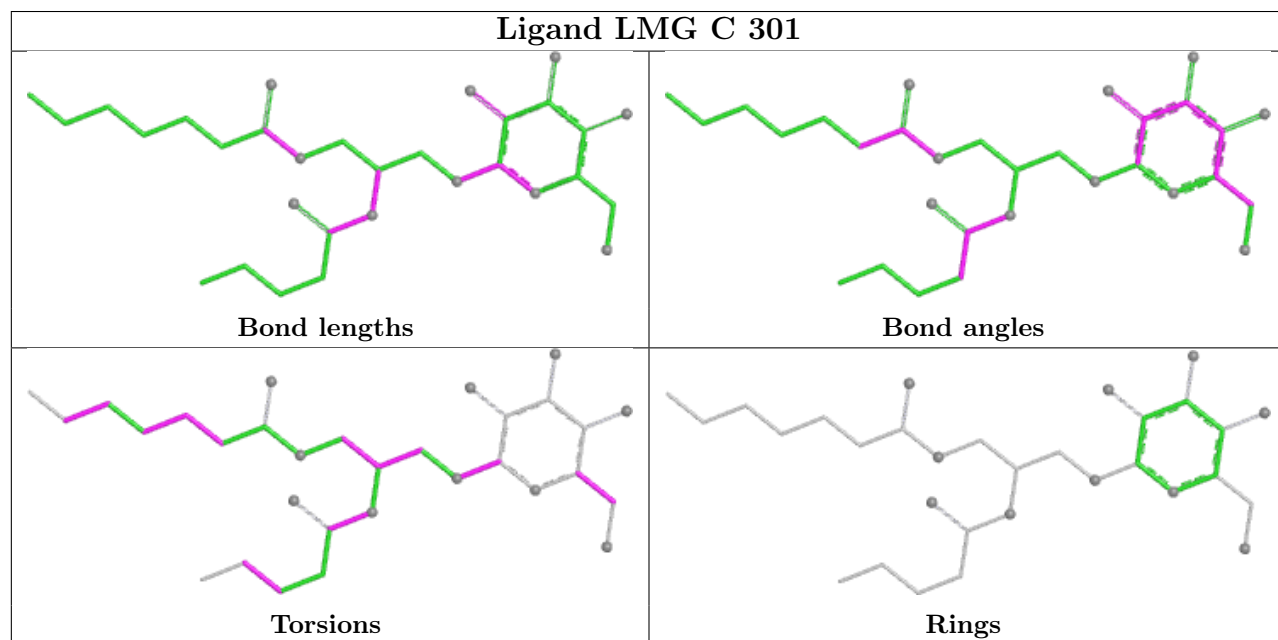
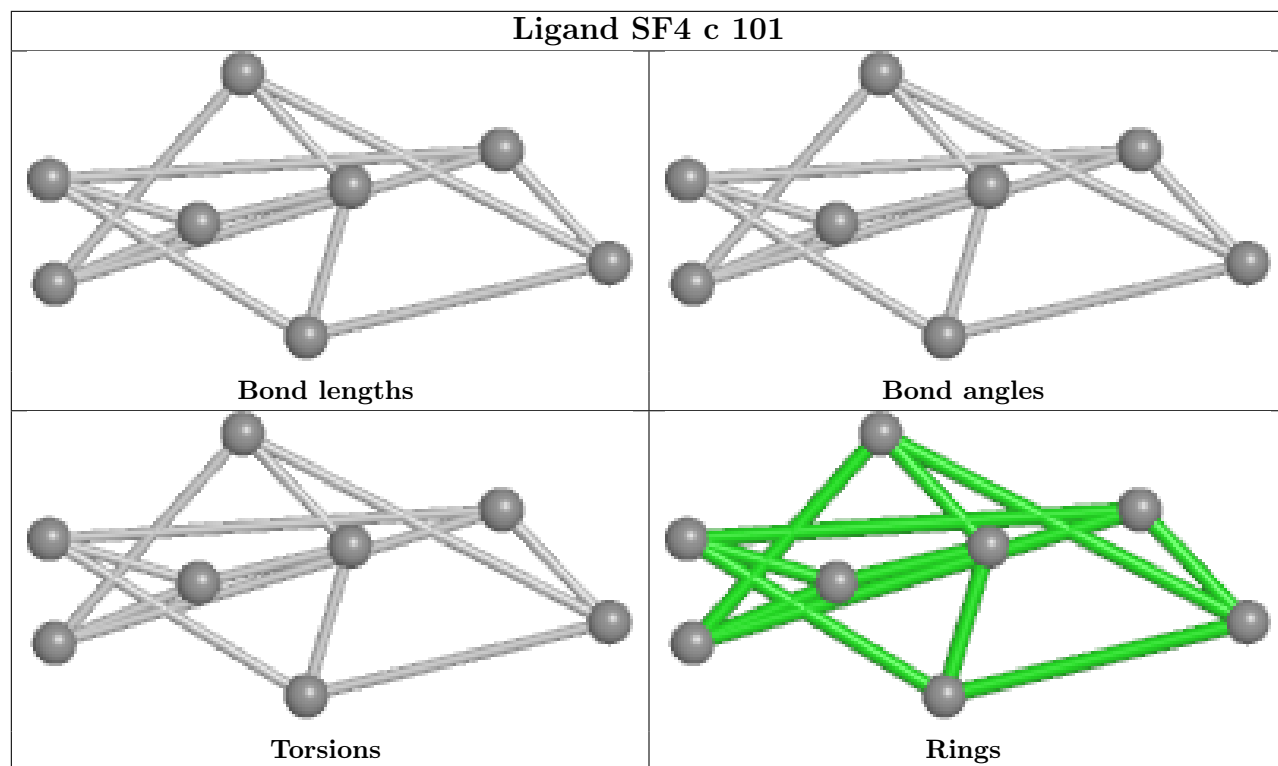
Bond angles



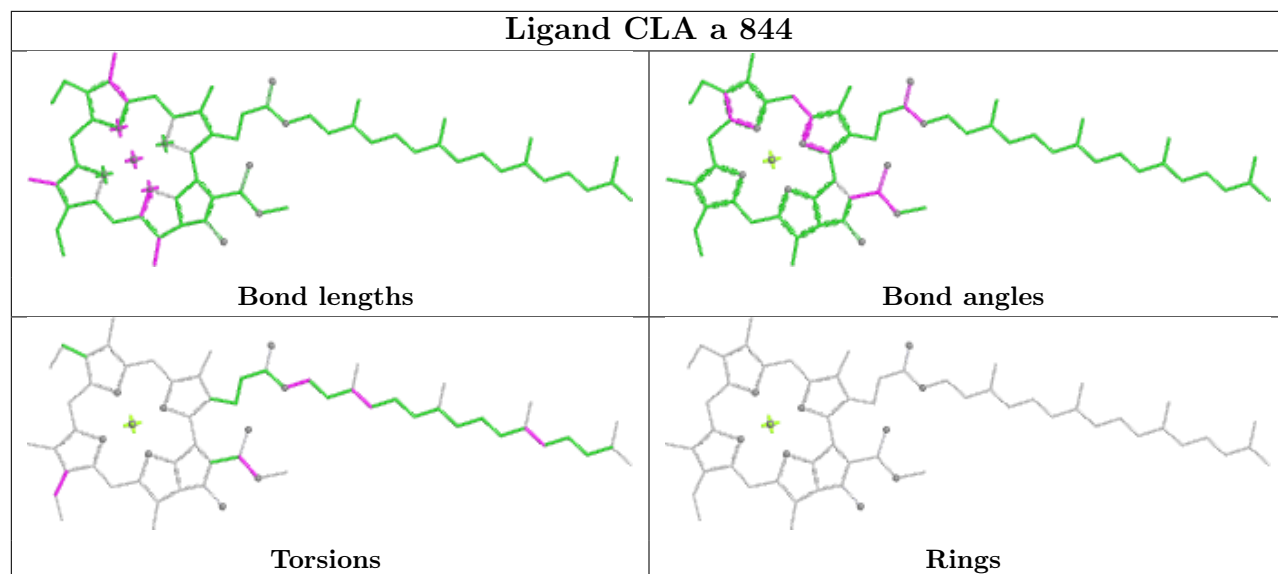
Torsions



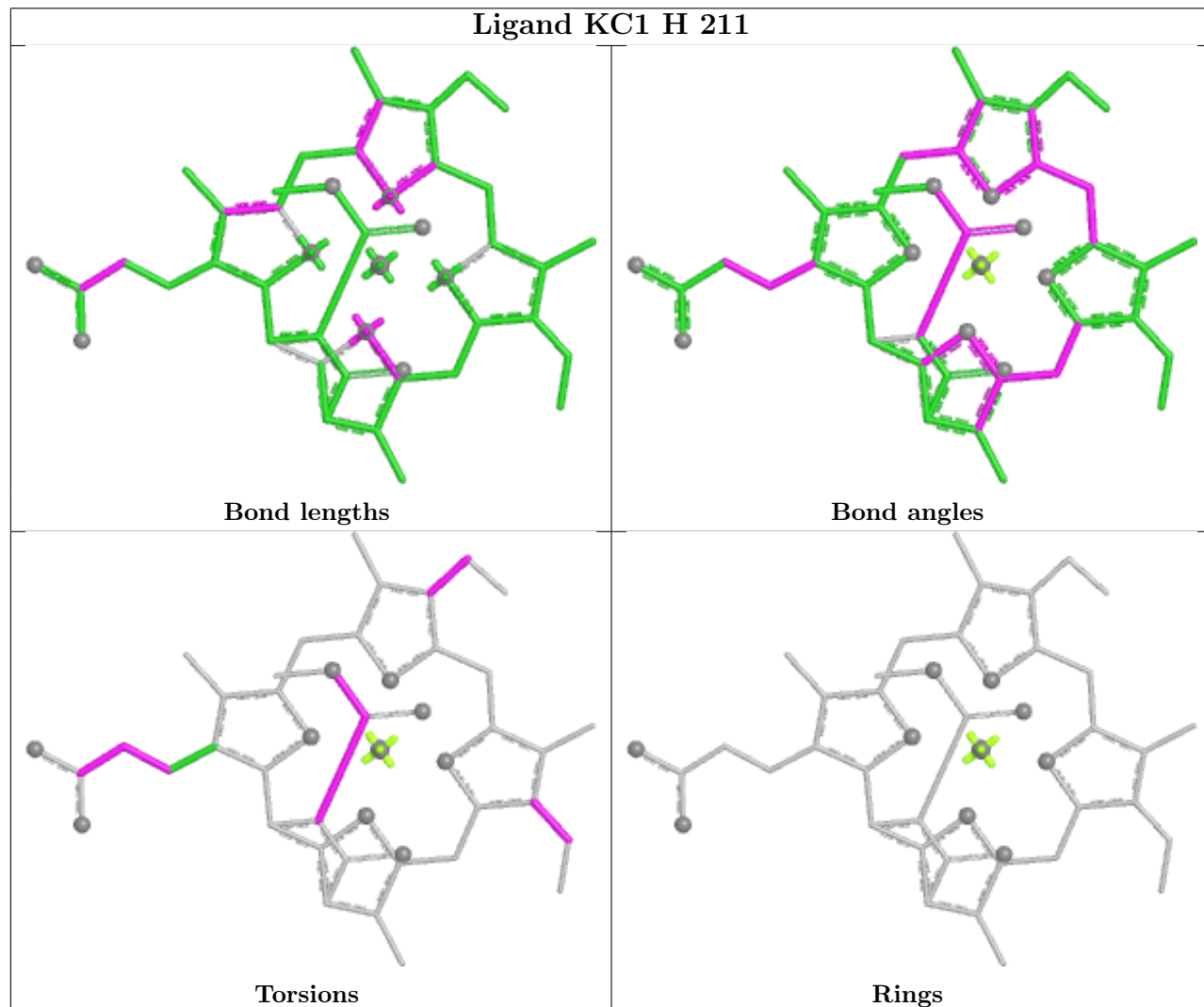
Rings

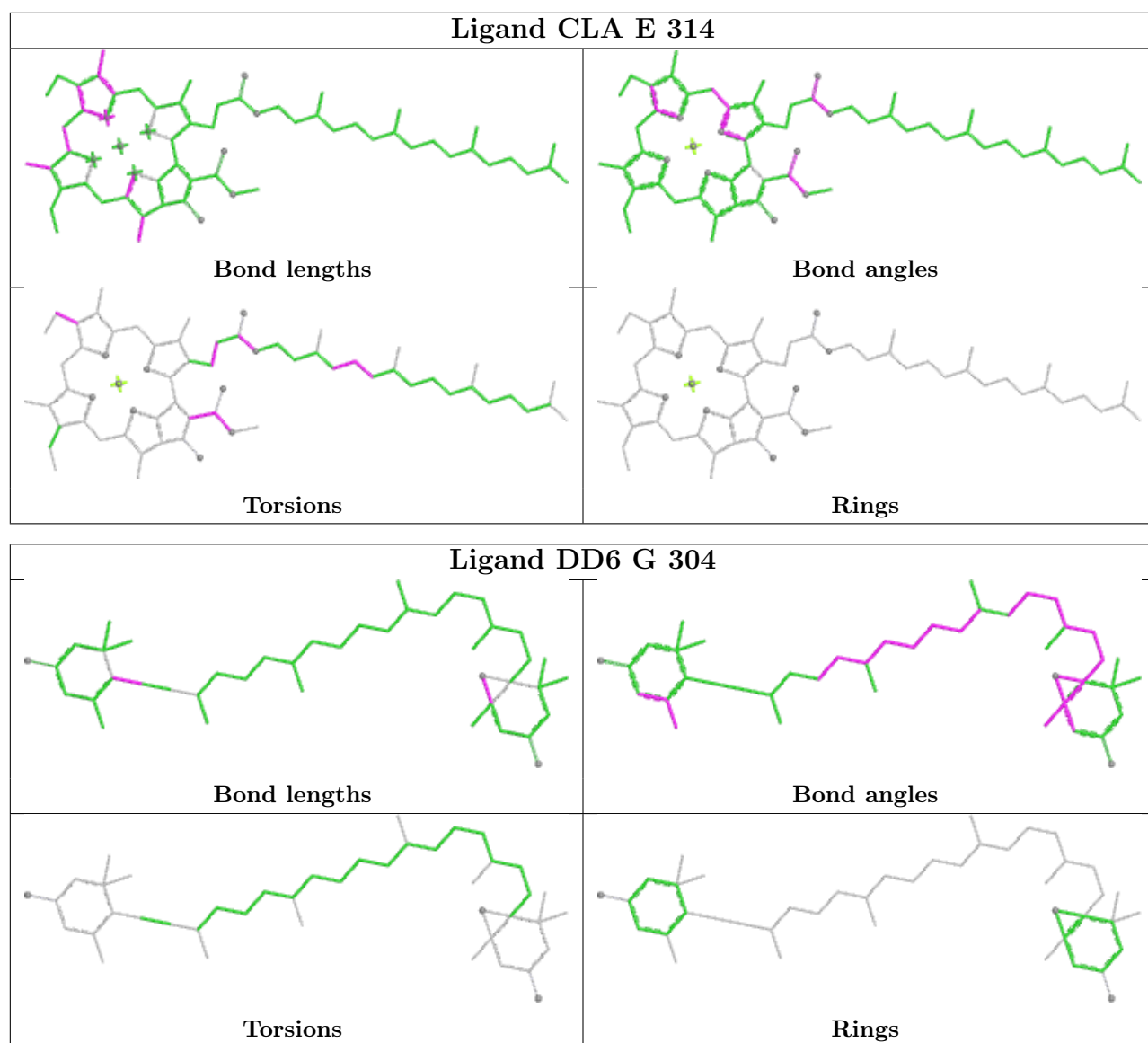


Ligand CLA a 844

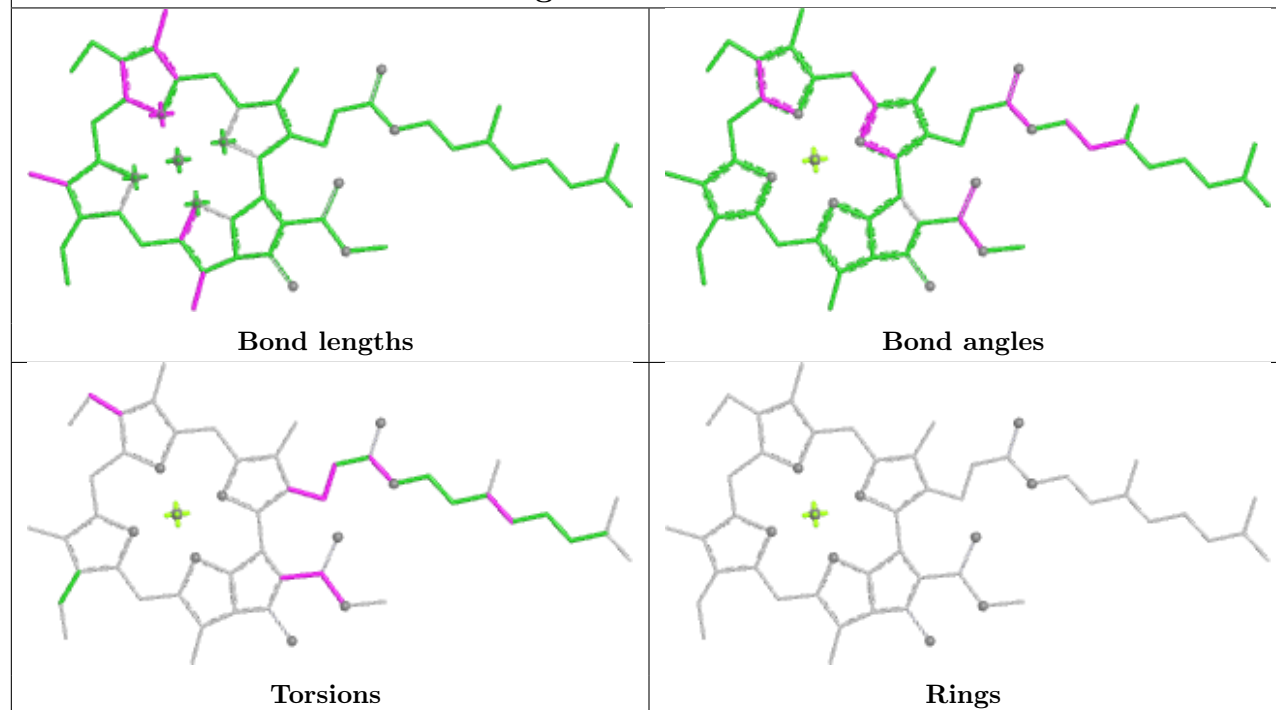


Ligand KC1 H 211

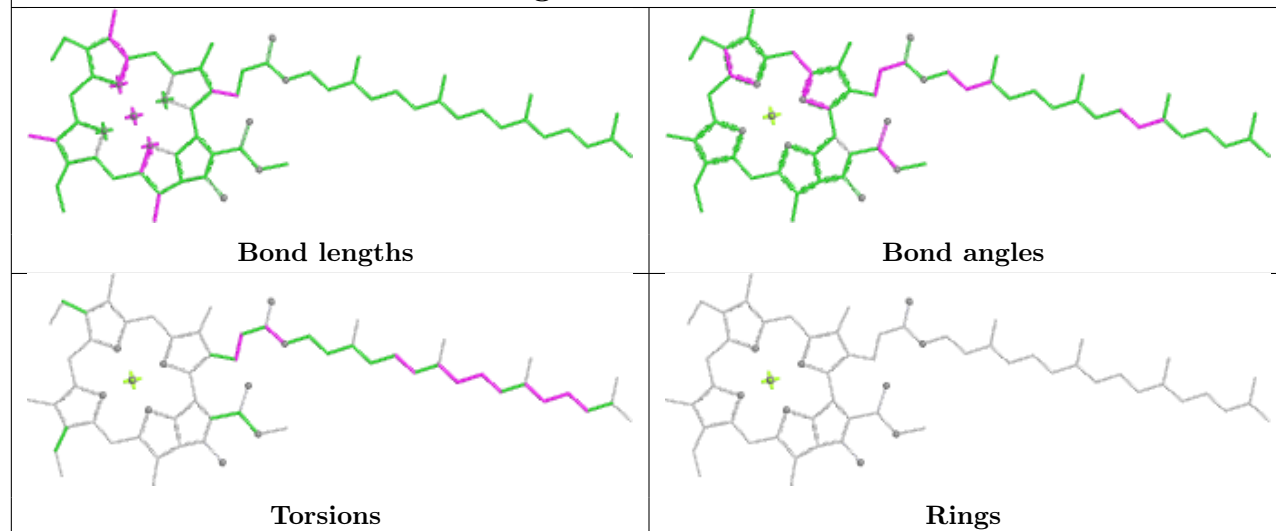




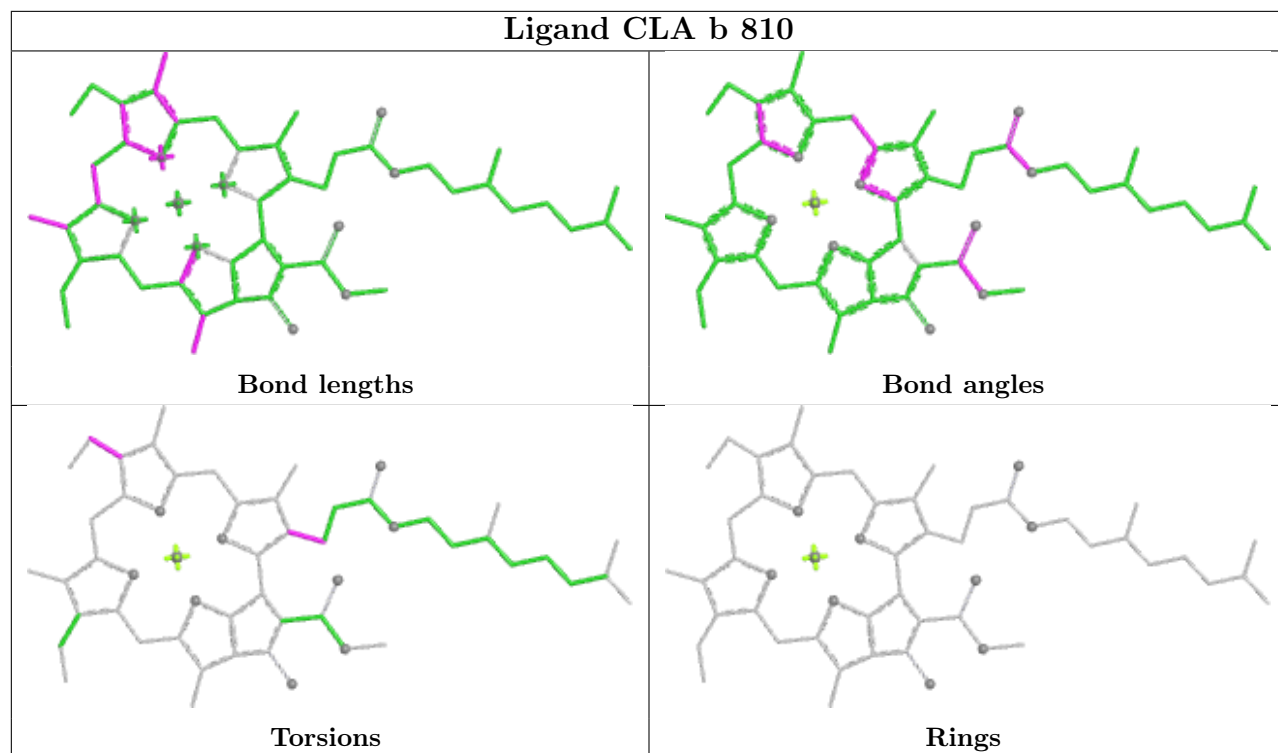
Ligand CLA b 814



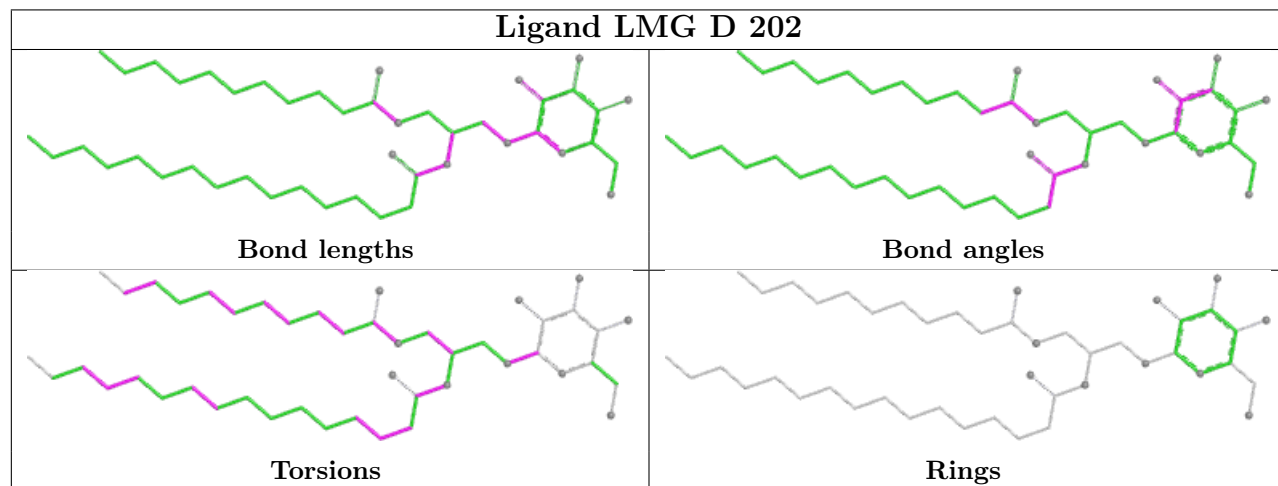
Ligand CLA E 311

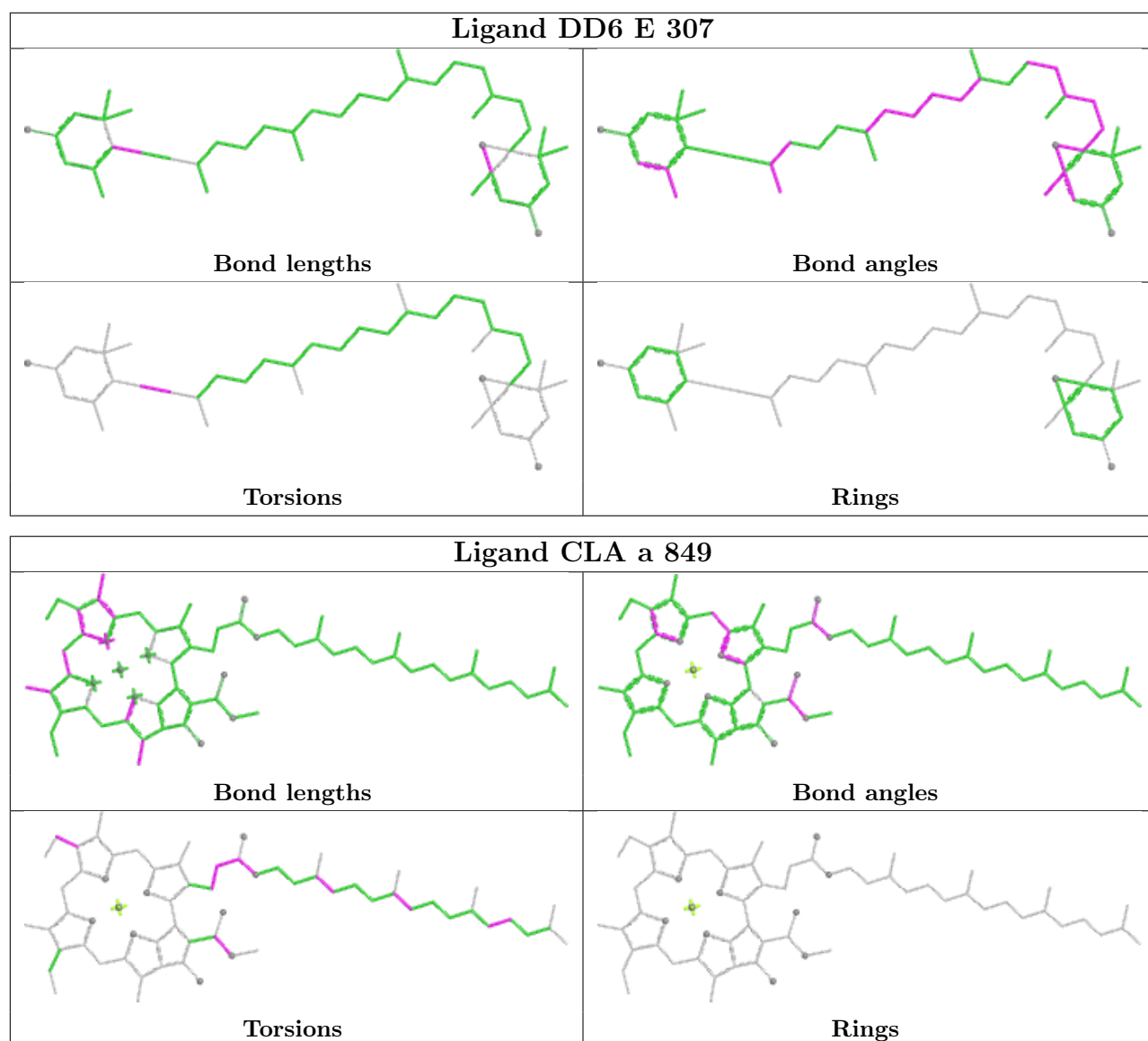


Ligand CLA b 810

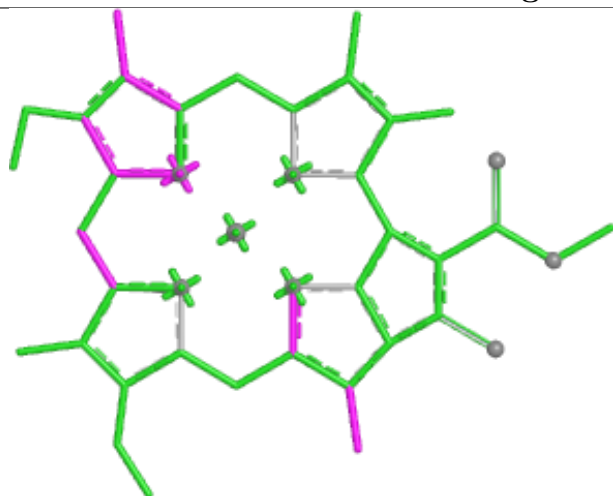


Ligand LMG D 202

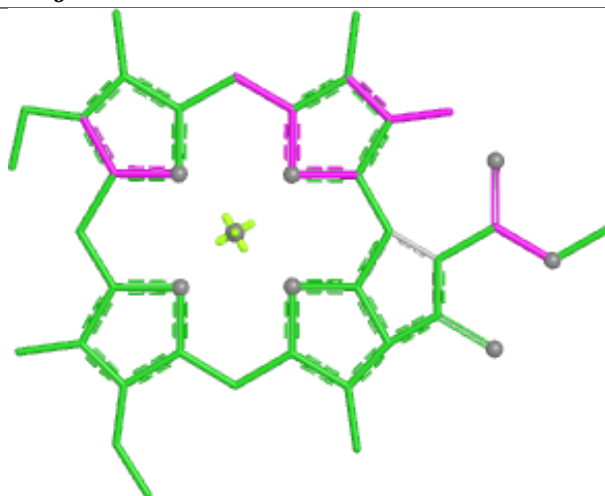




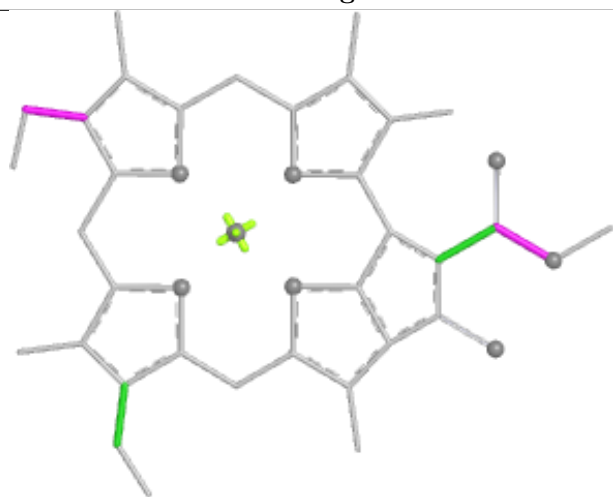
Ligand CLA j 104



Bond lengths



Bond angles

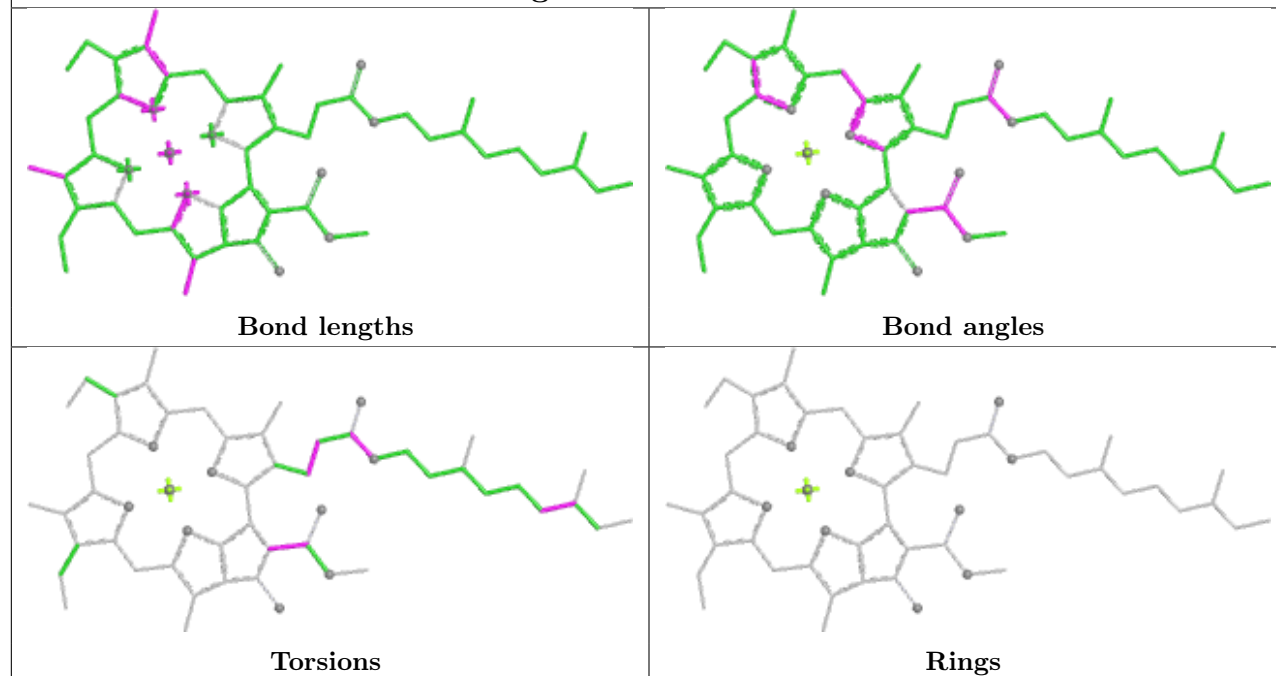


Torsions

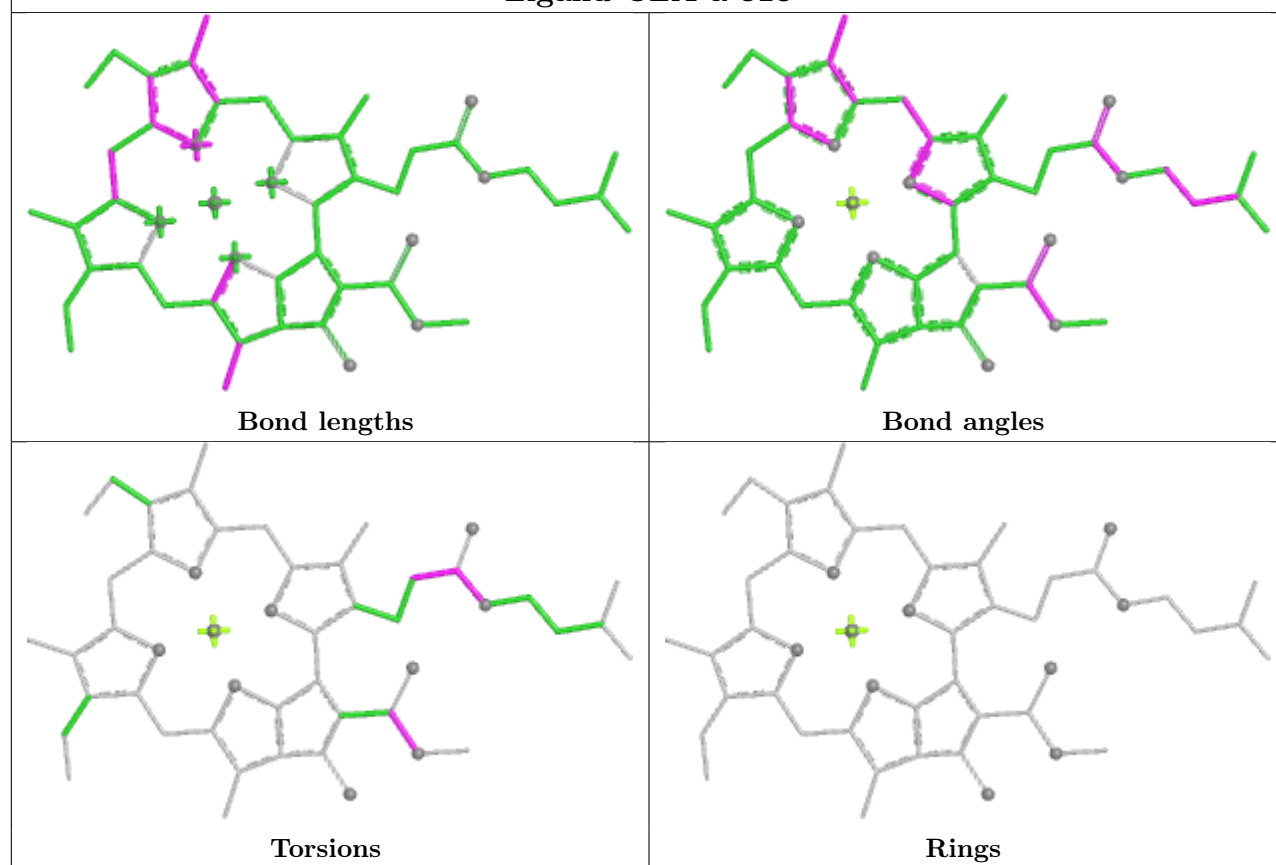


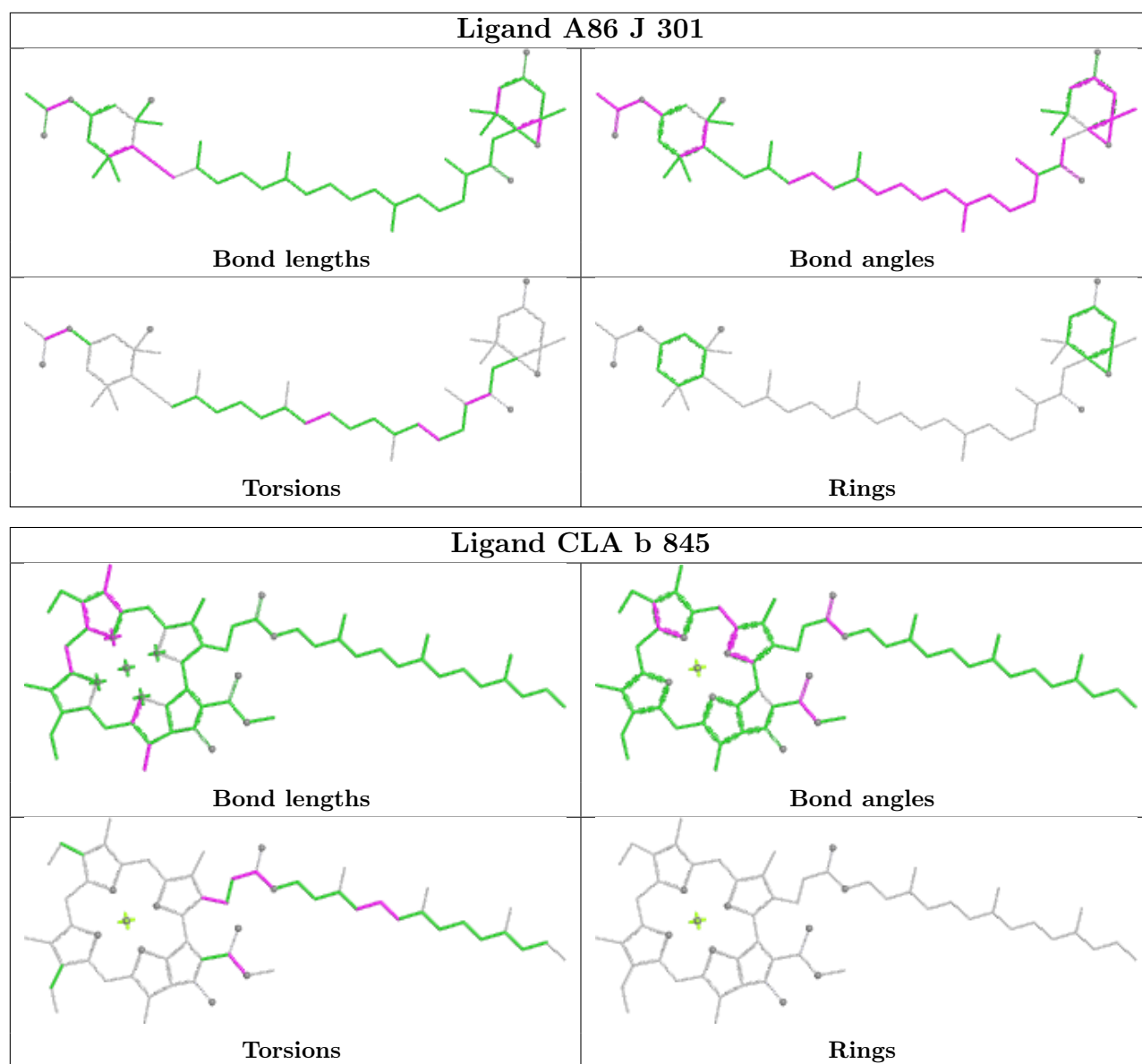
Rings

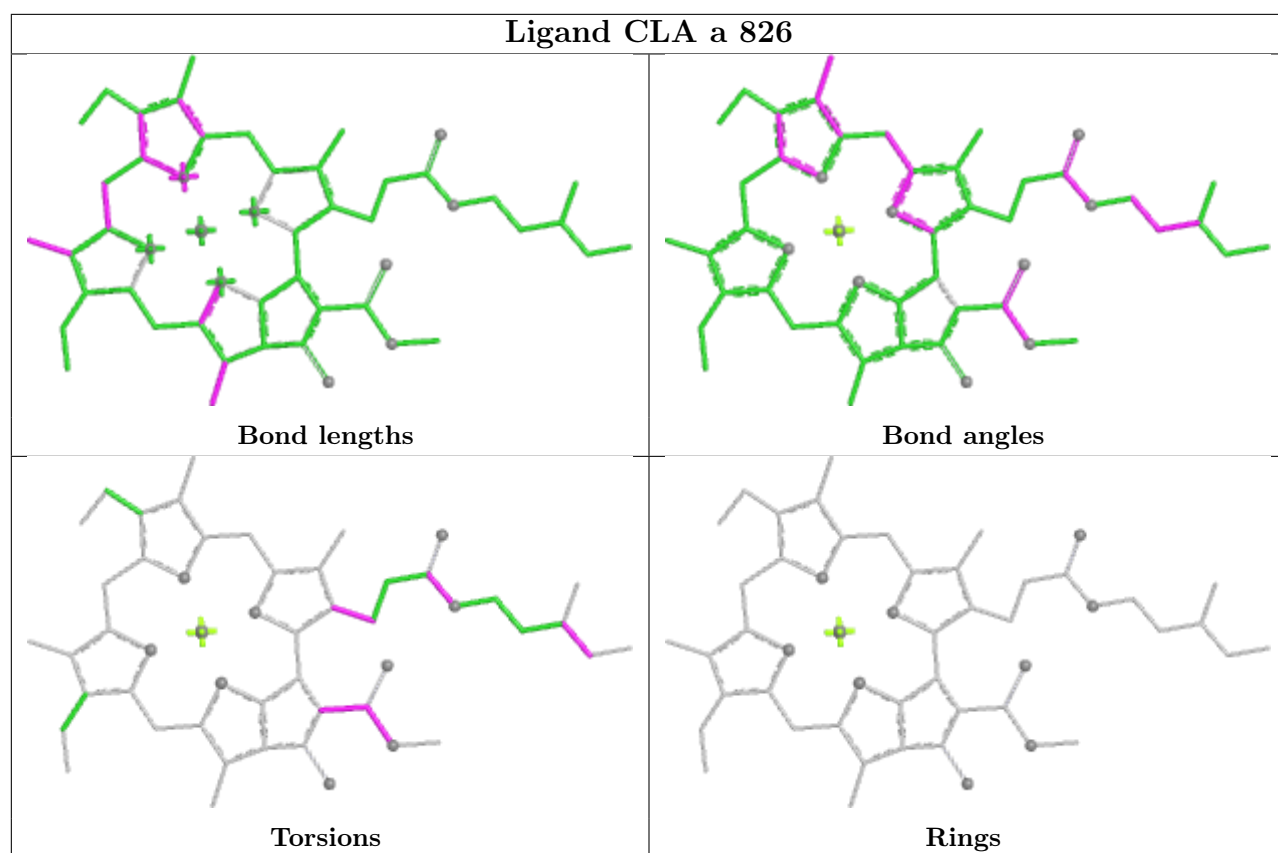
Ligand CLA D 210



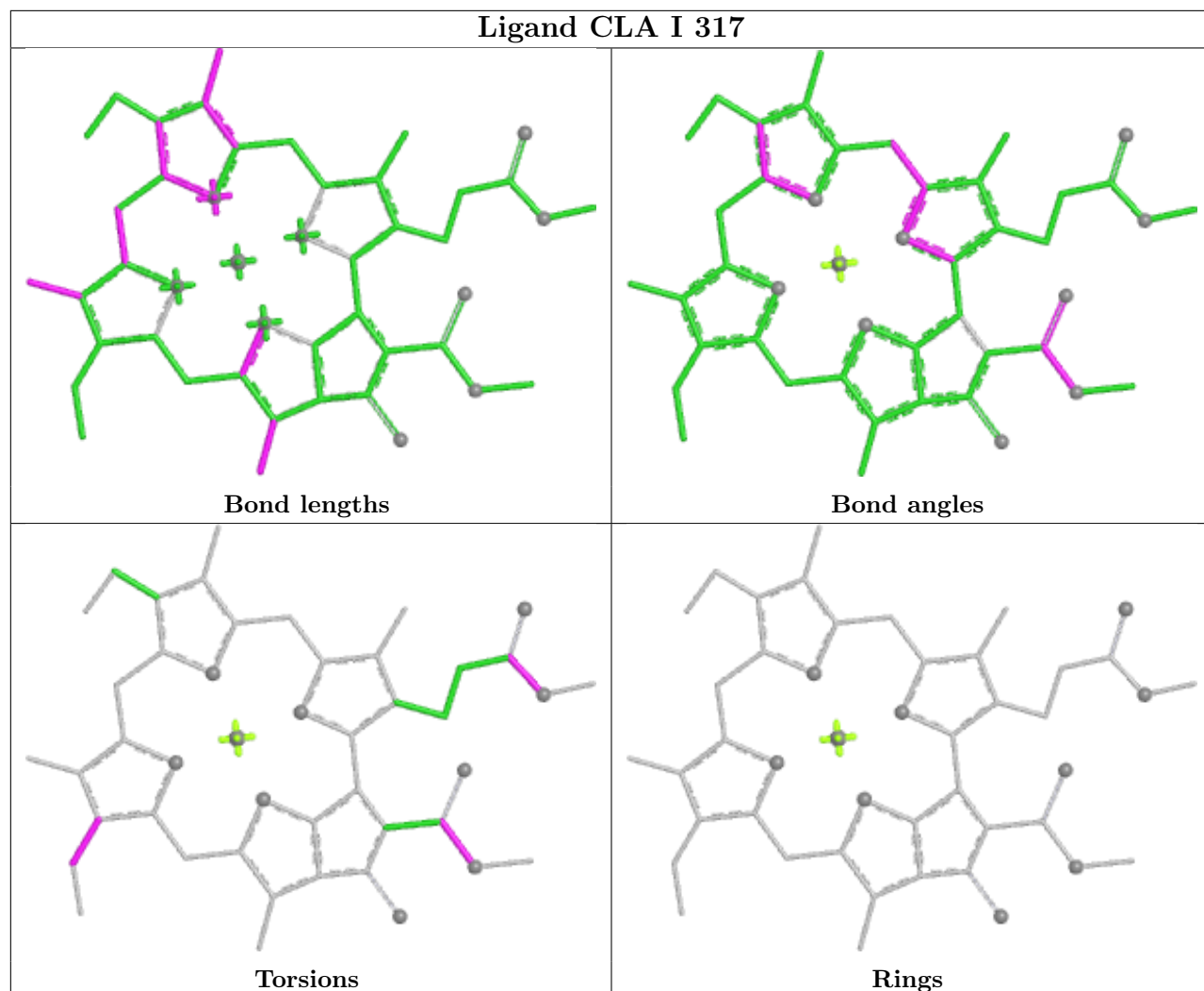
Ligand CLA a 813



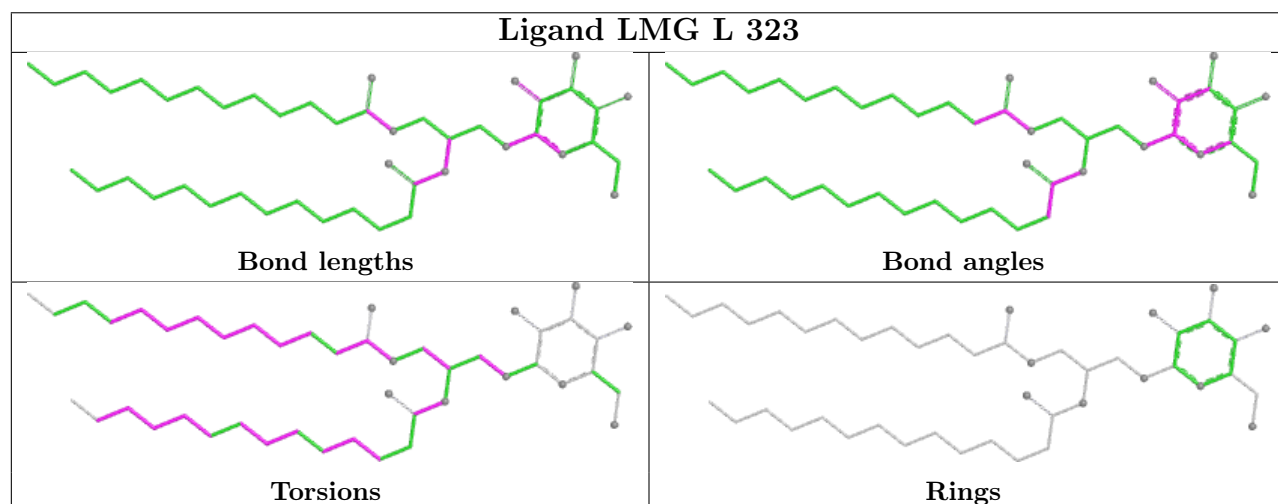


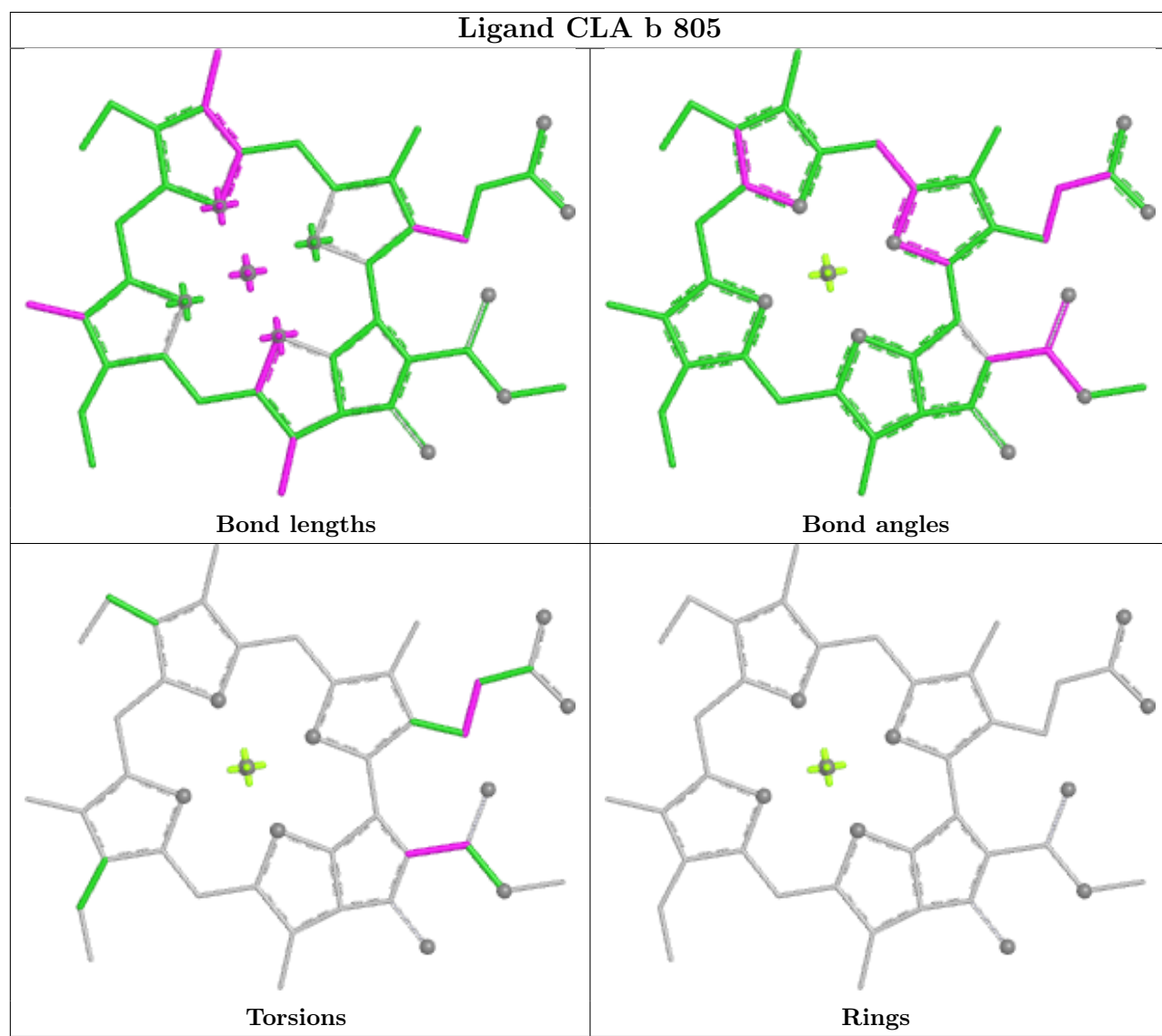
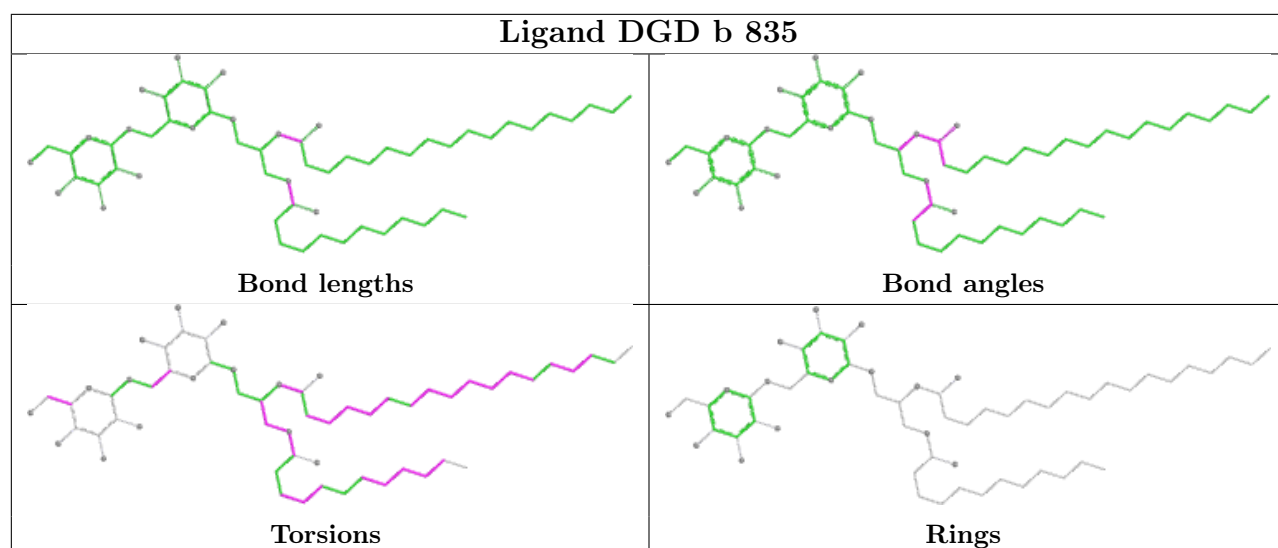


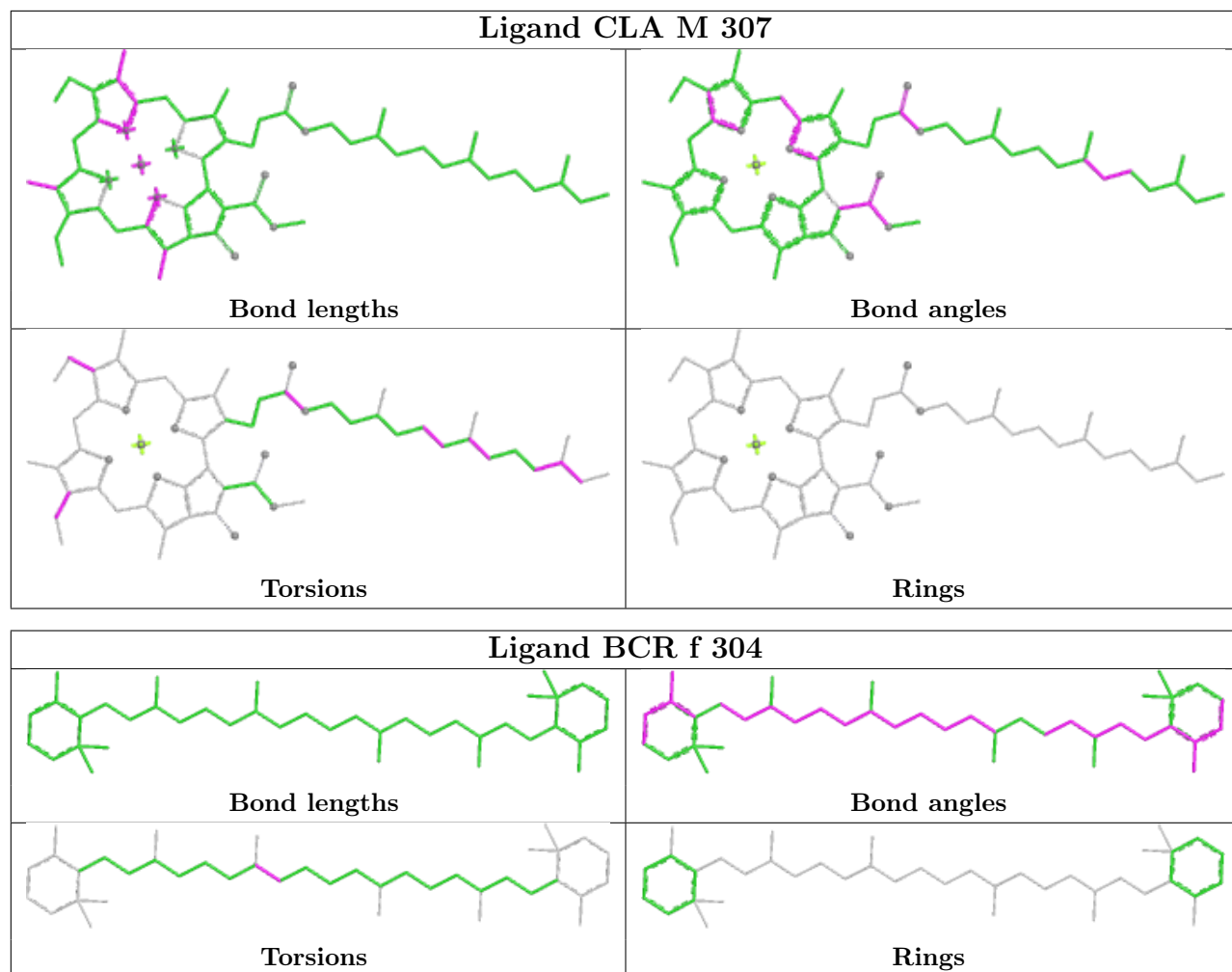
Ligand CLA I 317

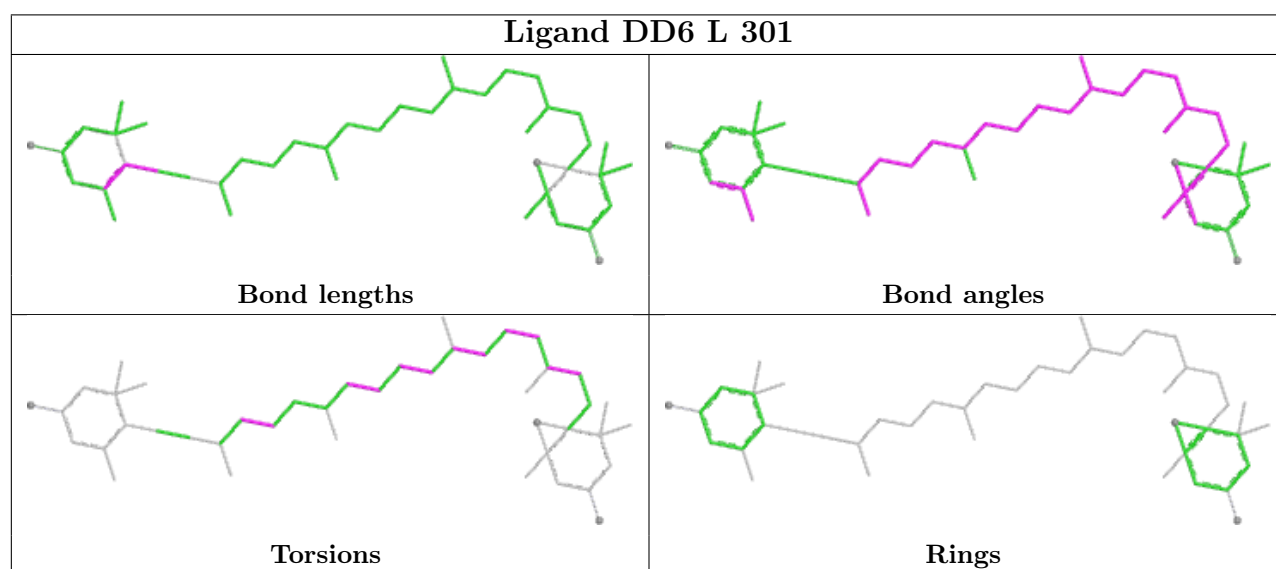
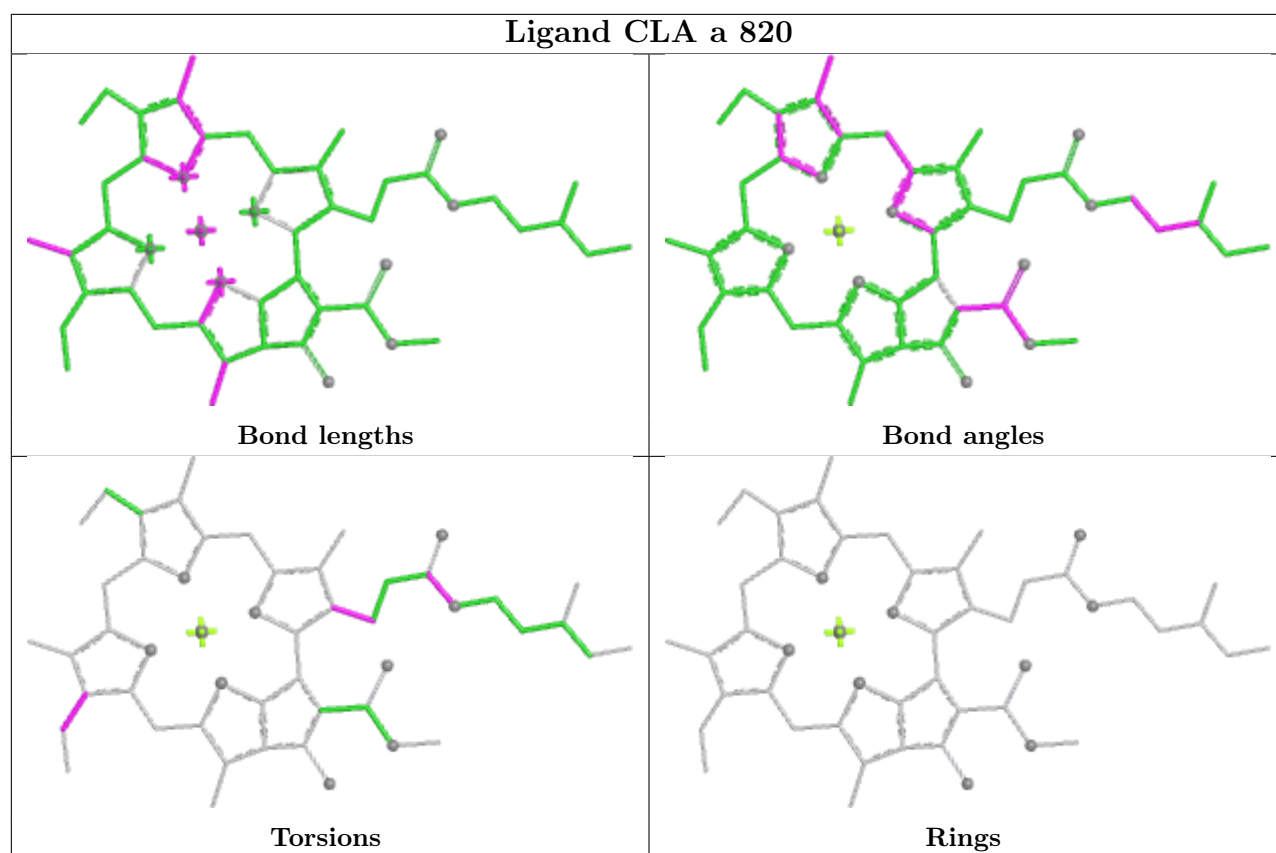


Ligand LMG L 323

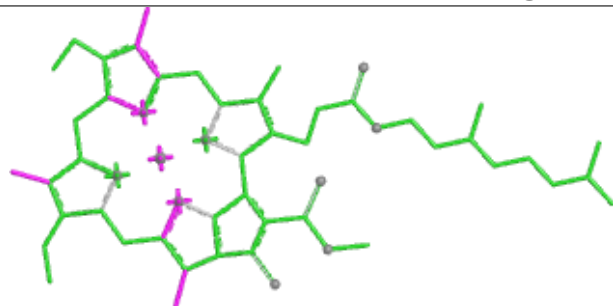




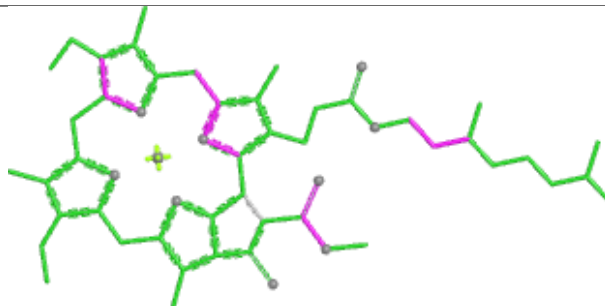




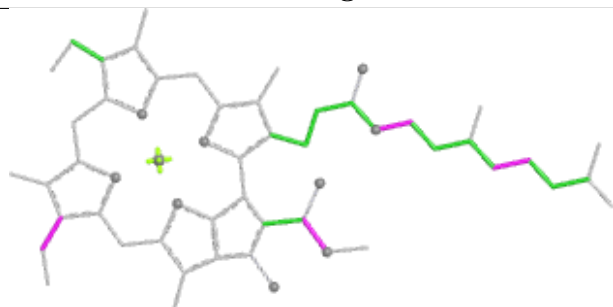
Ligand CLA I 307



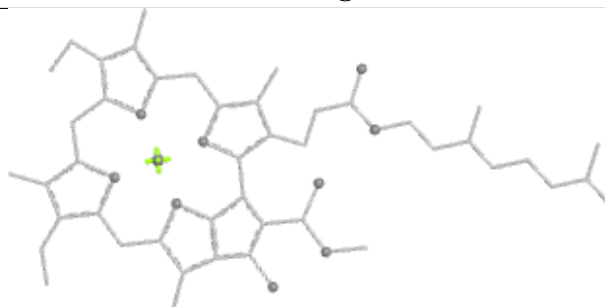
Bond lengths



Bond angles

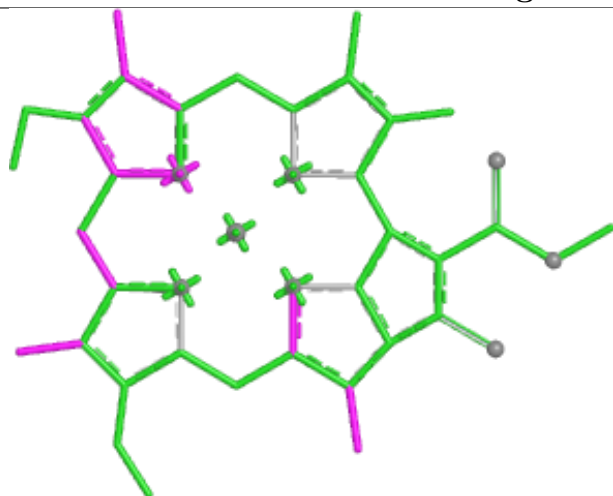


Torsions

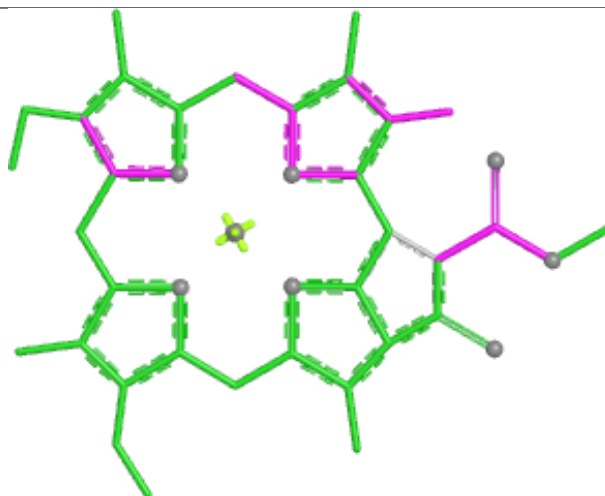


Rings

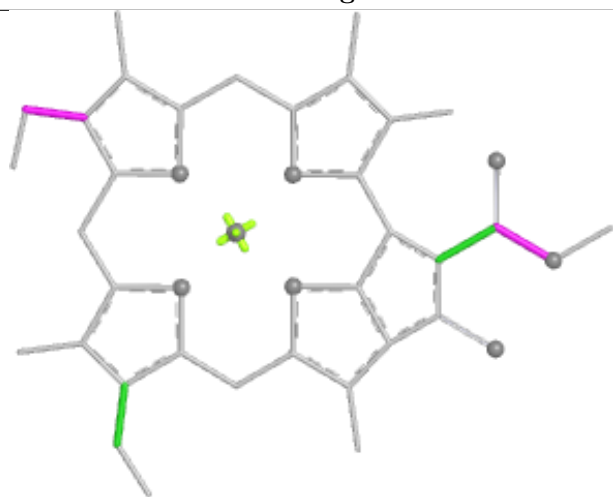
Ligand CLA F 313



Bond lengths



Bond angles

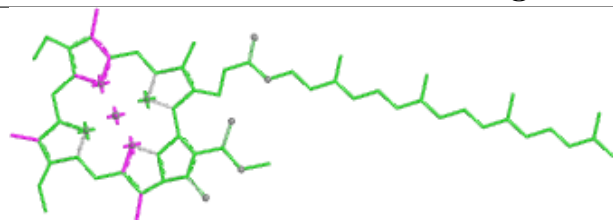


Torsions

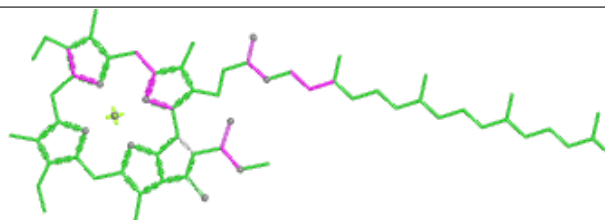


Rings

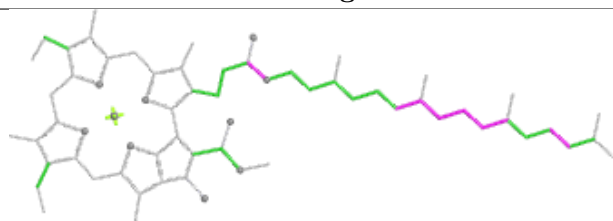
Ligand CLA M 309



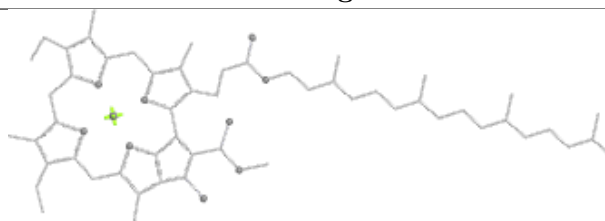
Bond lengths



Bond angles

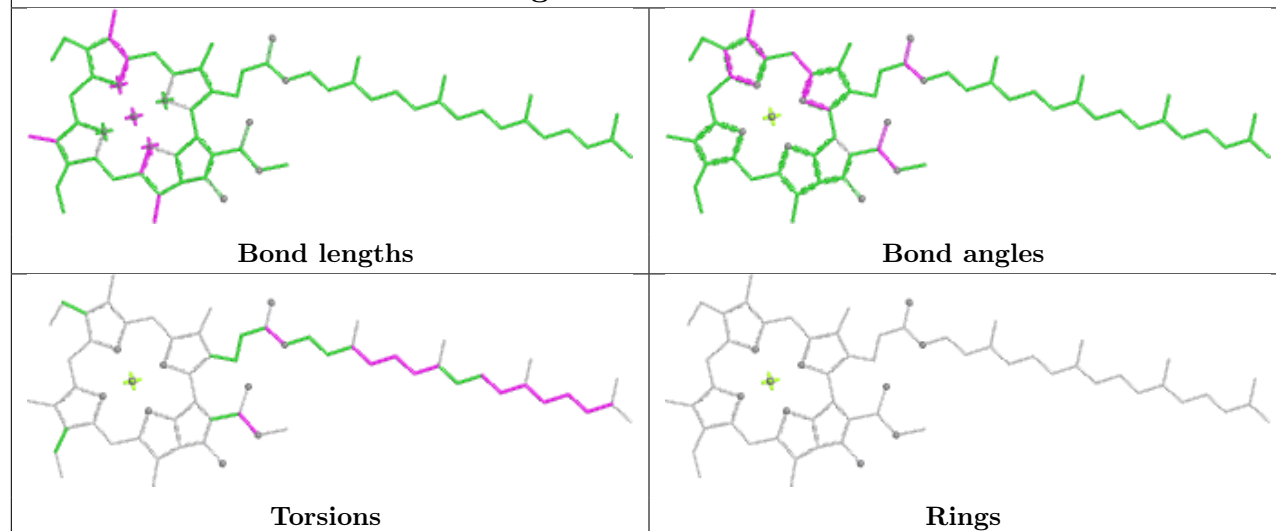


Torsions

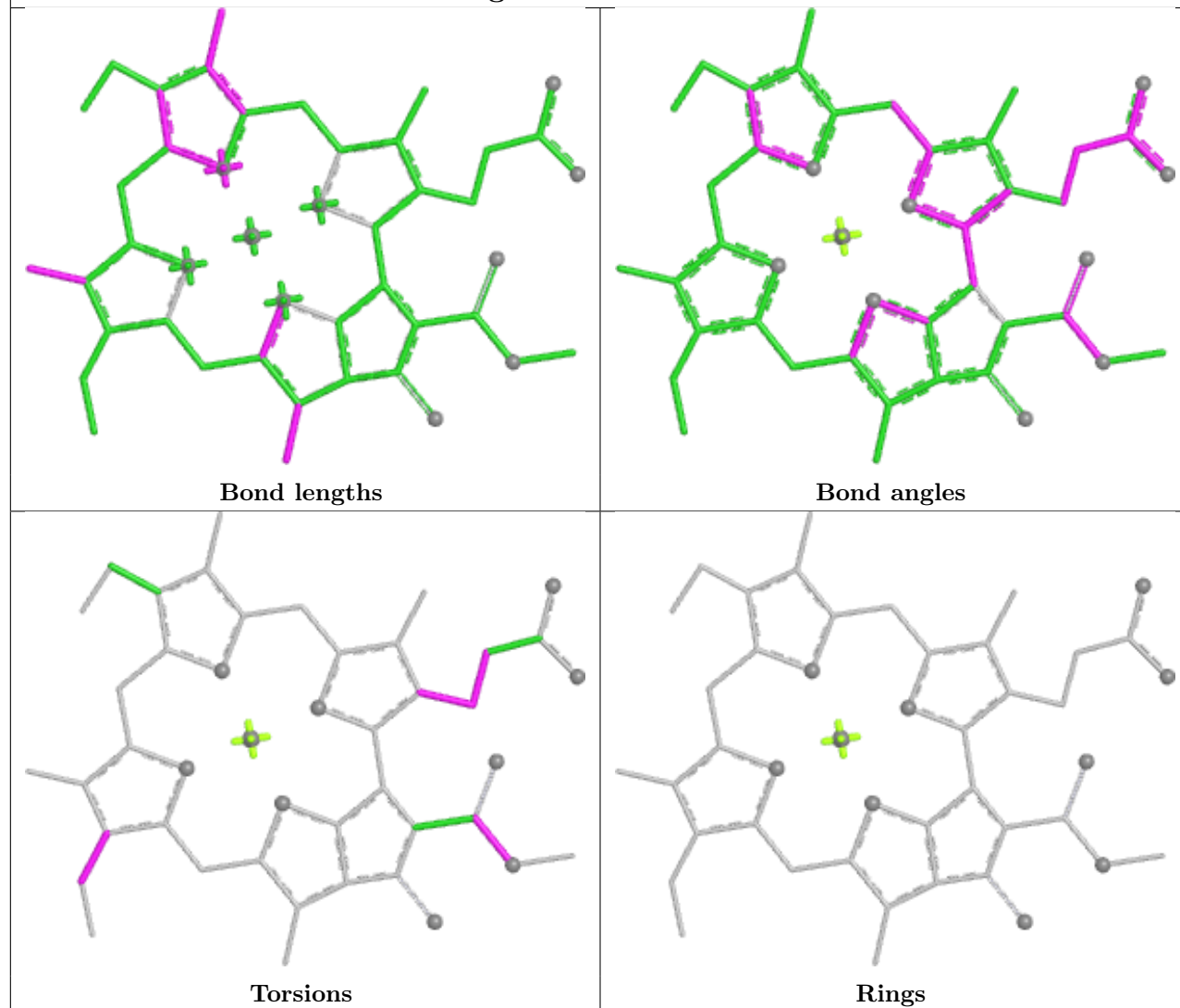


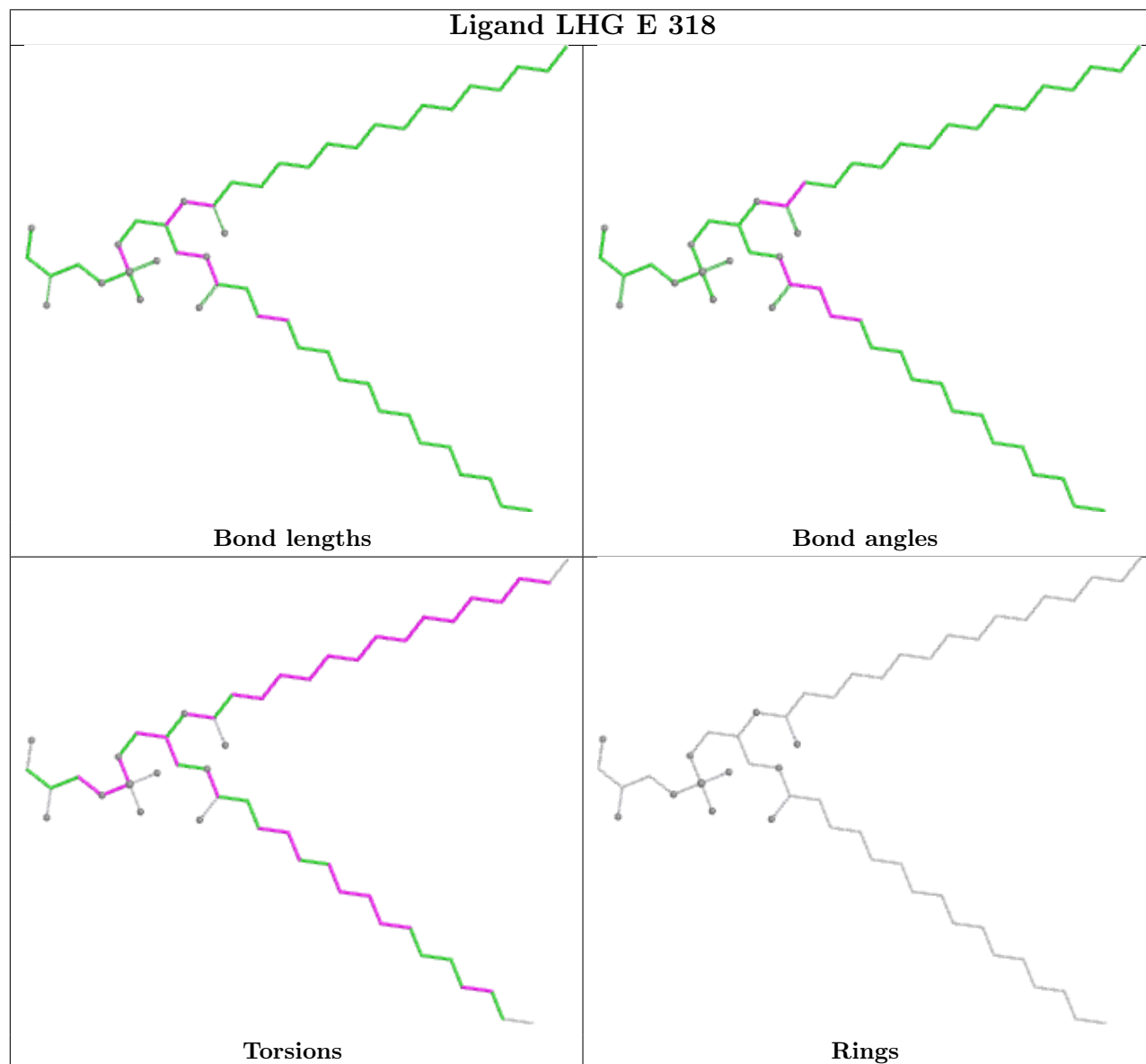
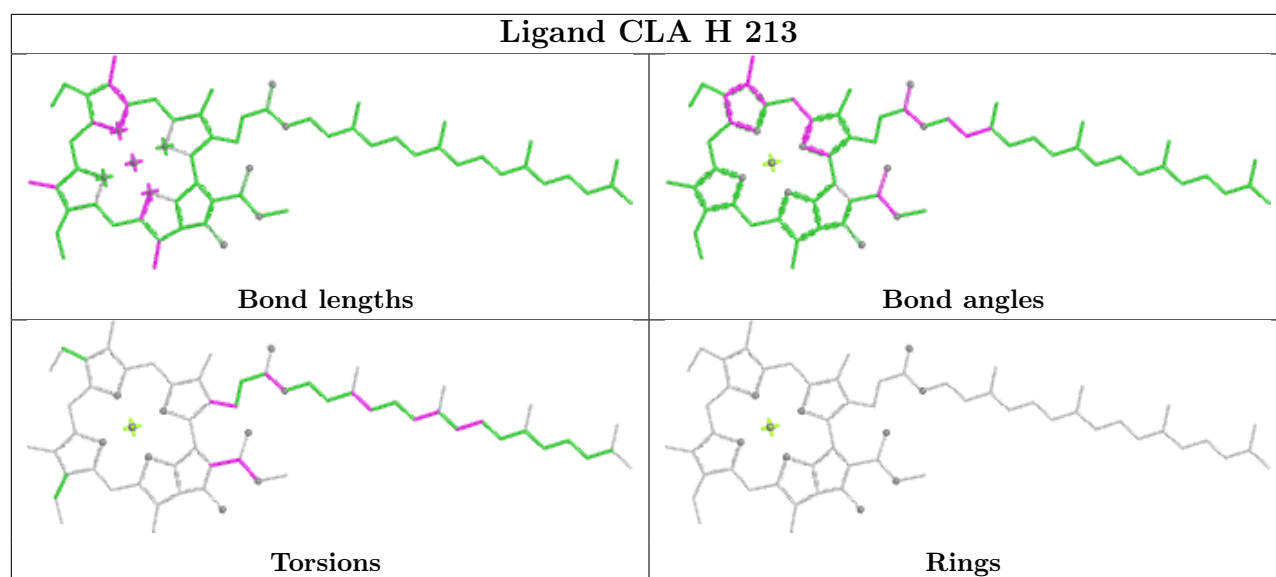
Rings

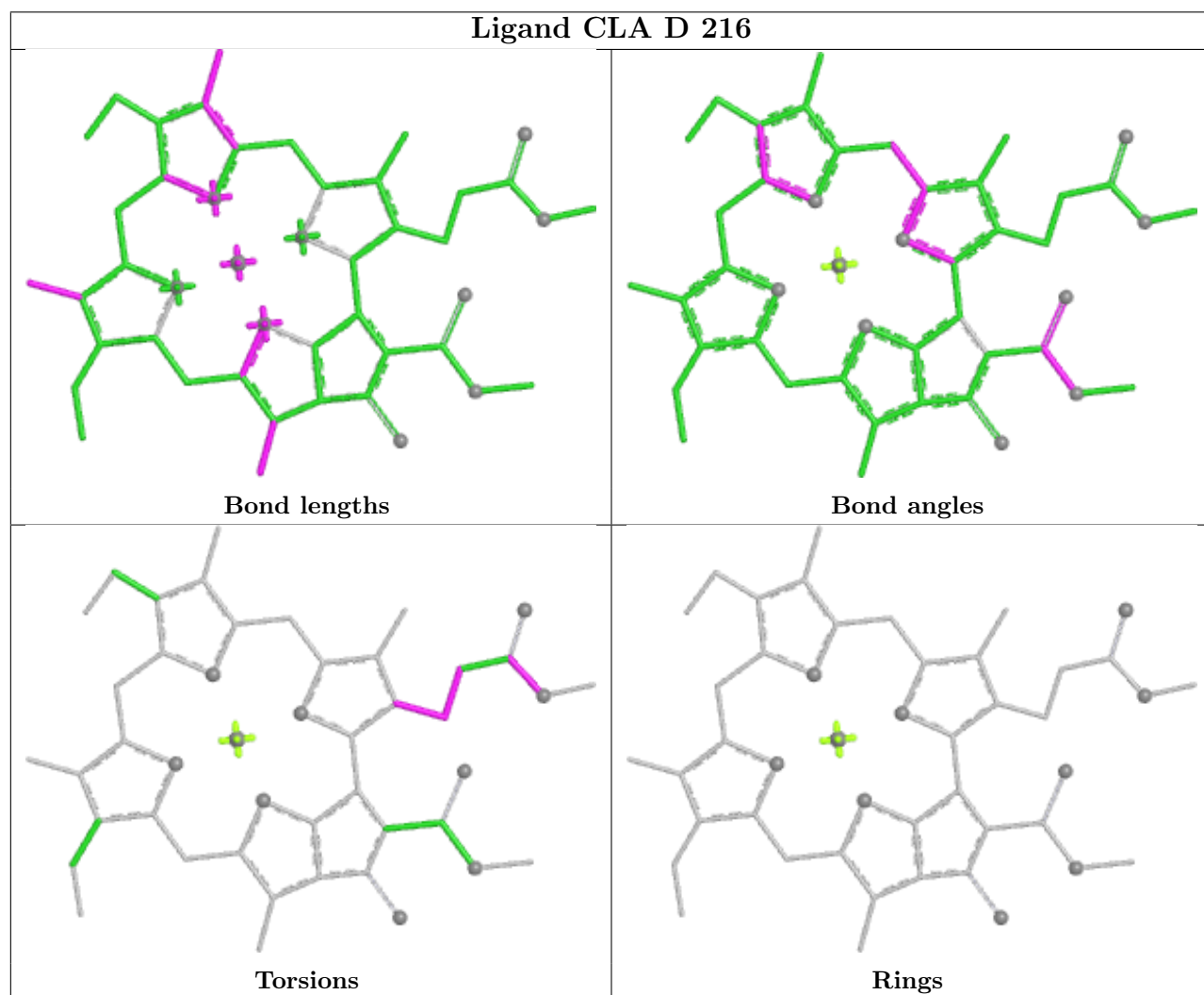
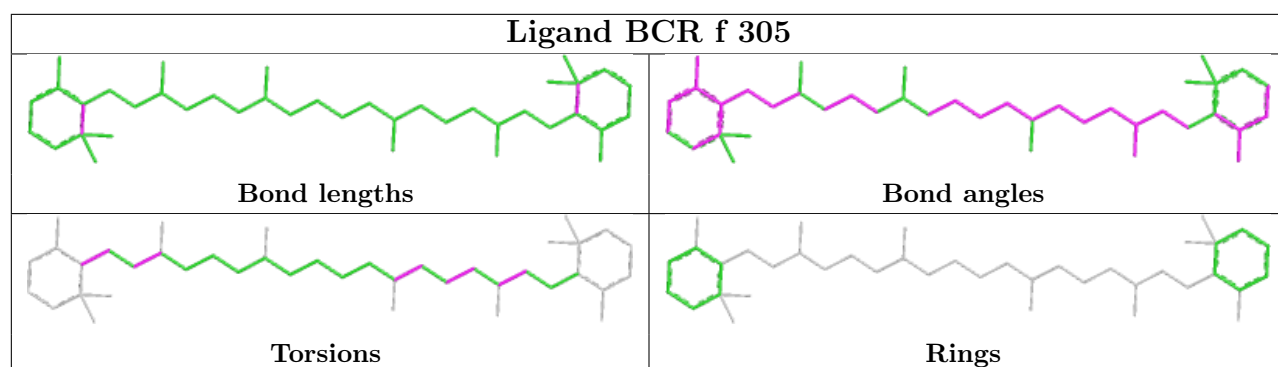
Ligand CLA K 309



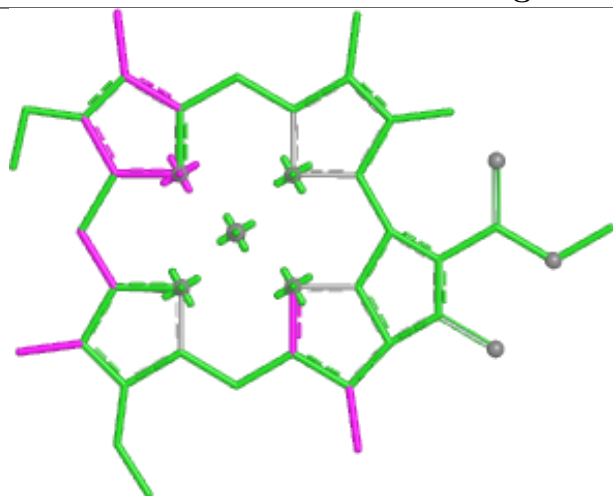
Ligand CLA M 317



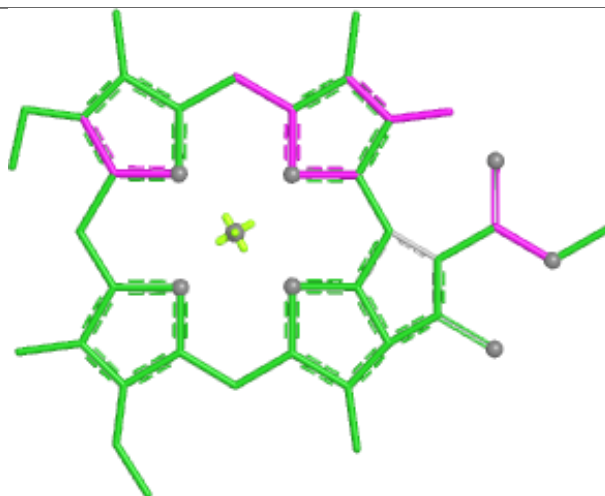




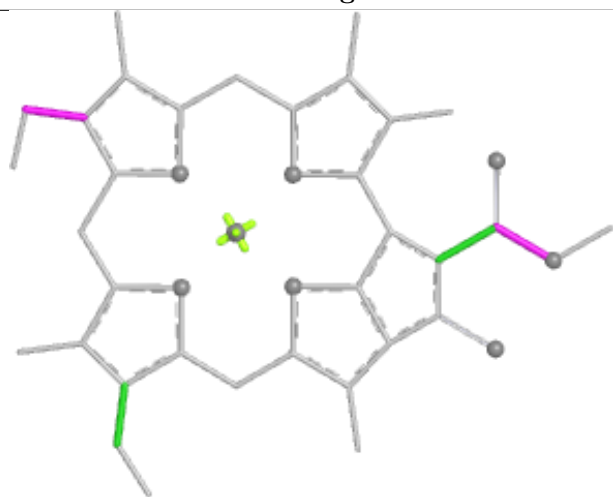
Ligand CLA D 215



Bond lengths



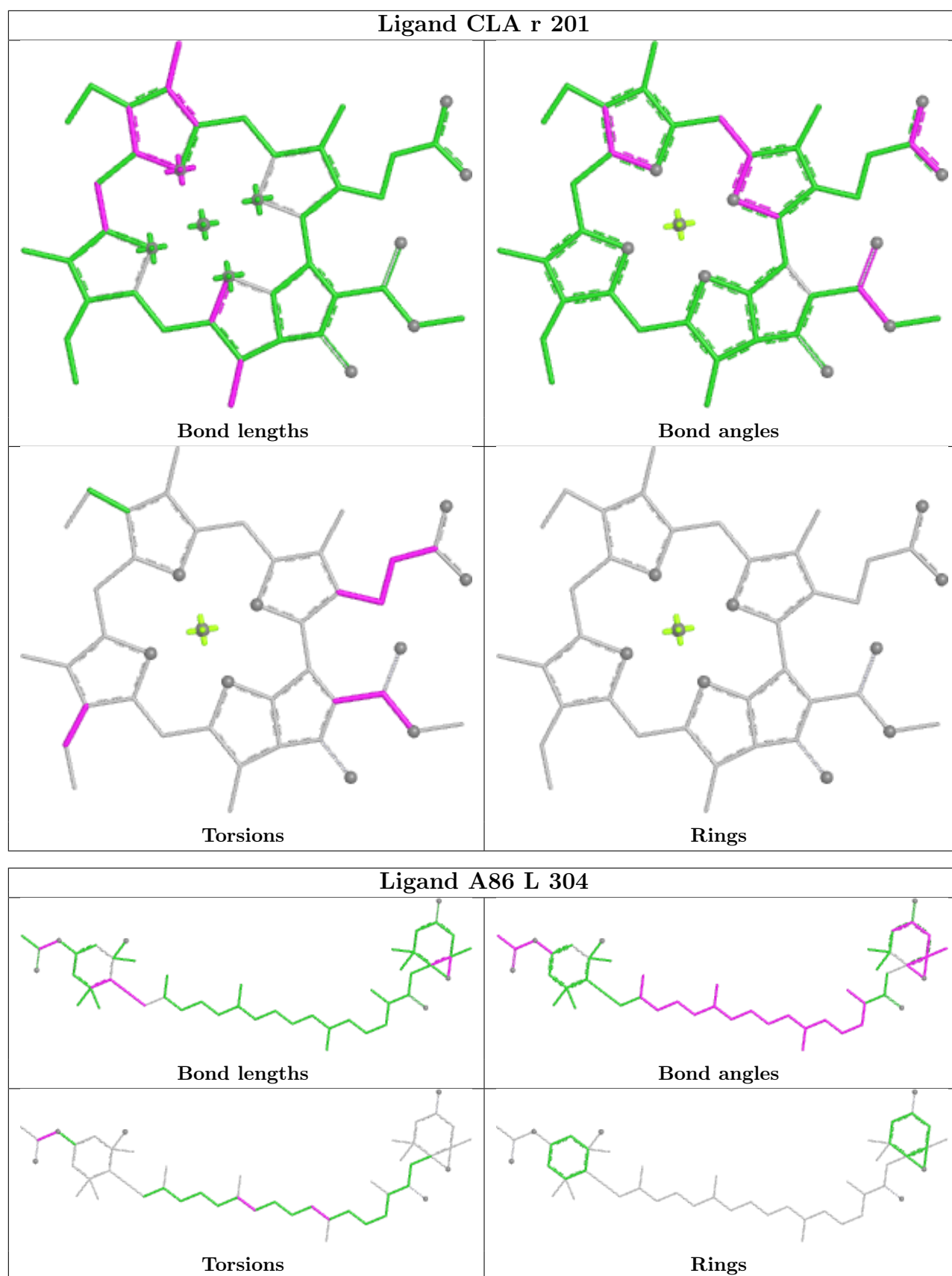
Bond angles

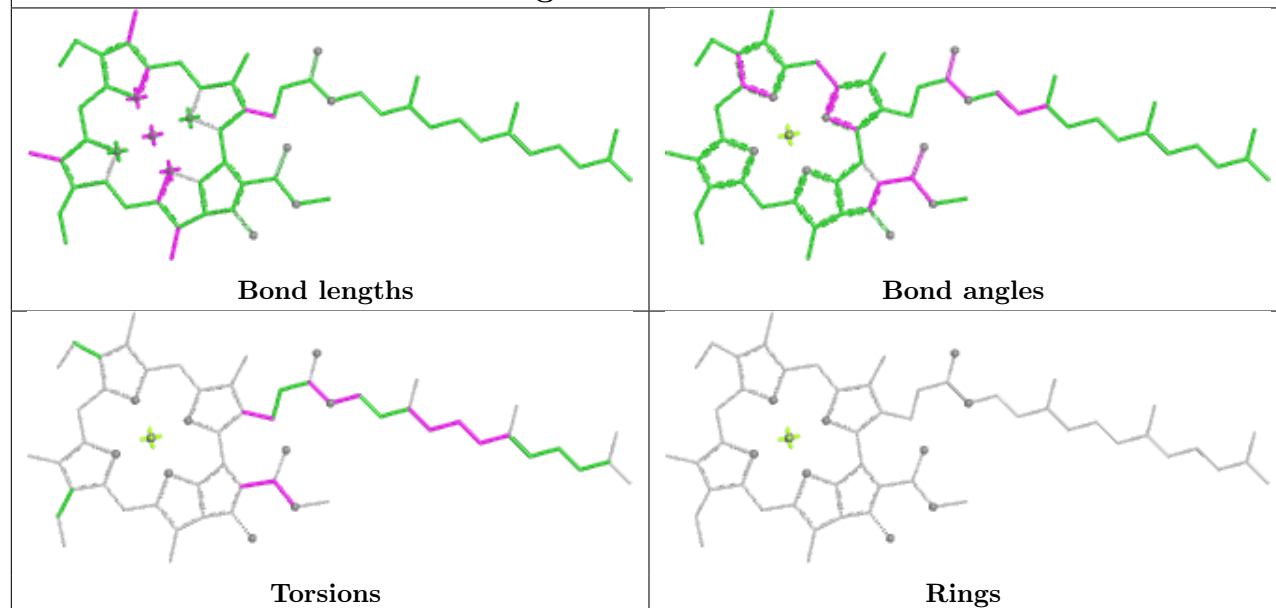
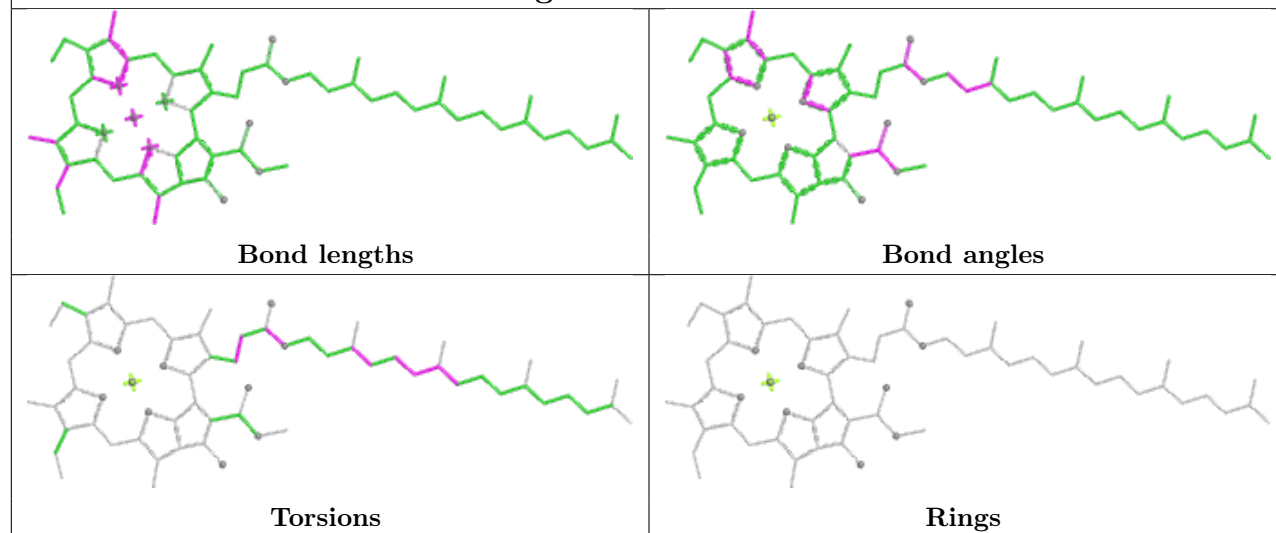


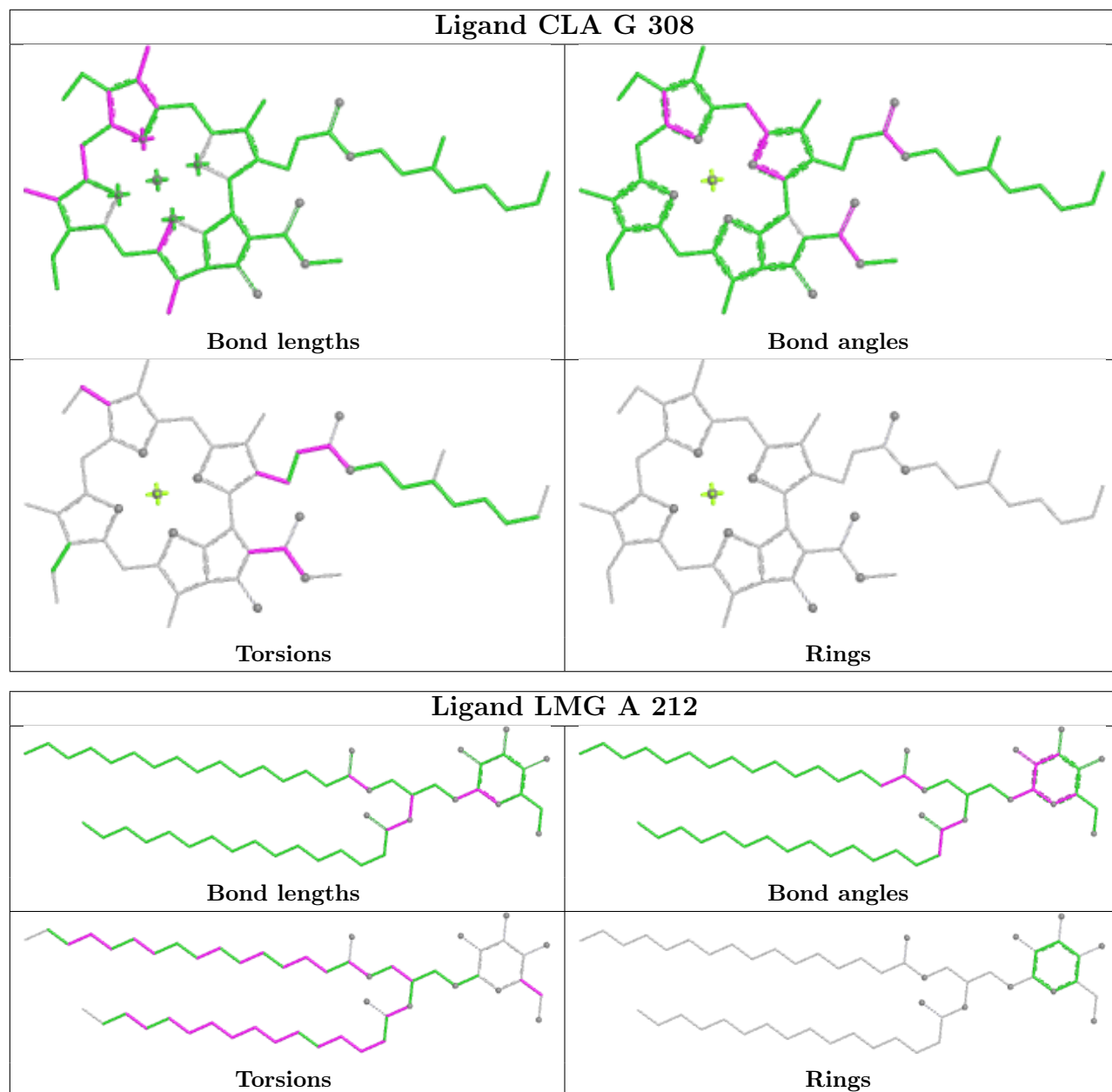
Torsions

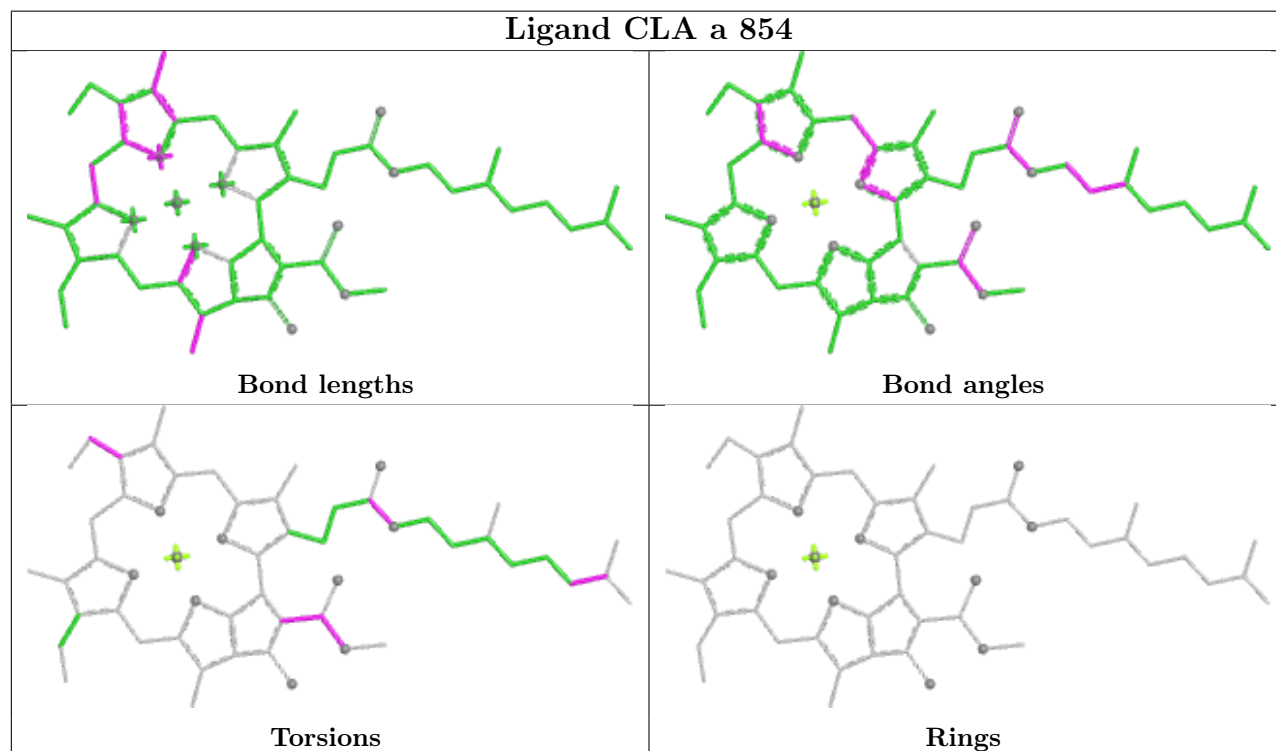
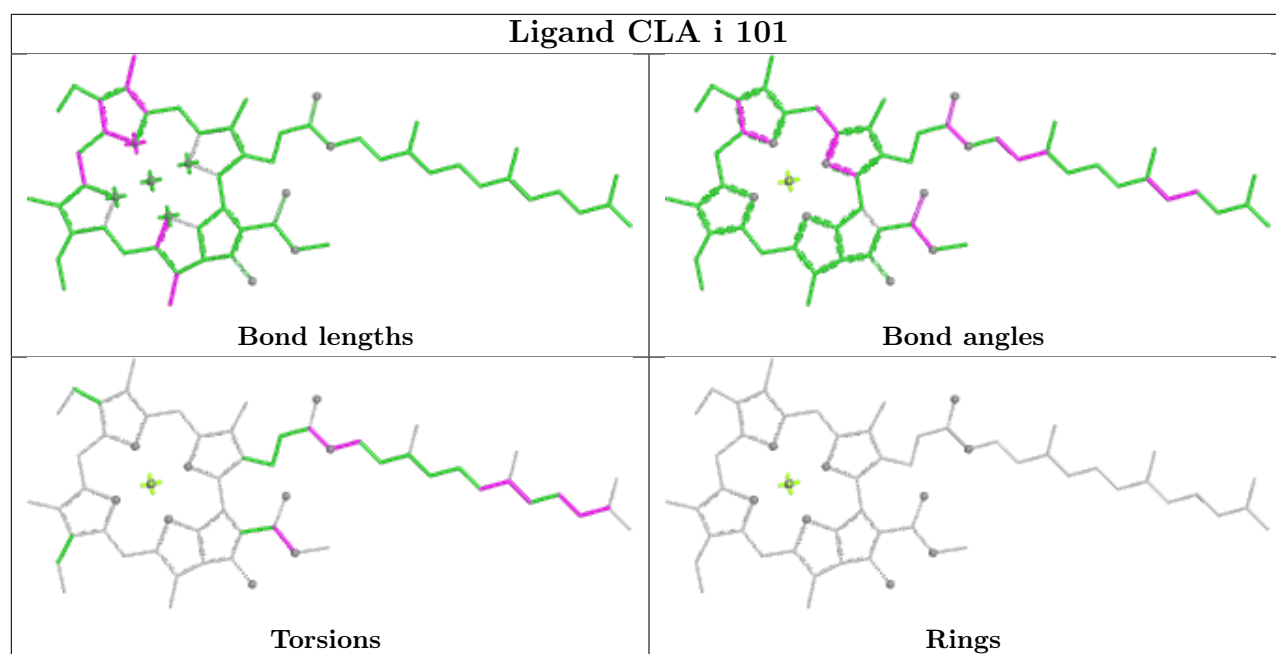


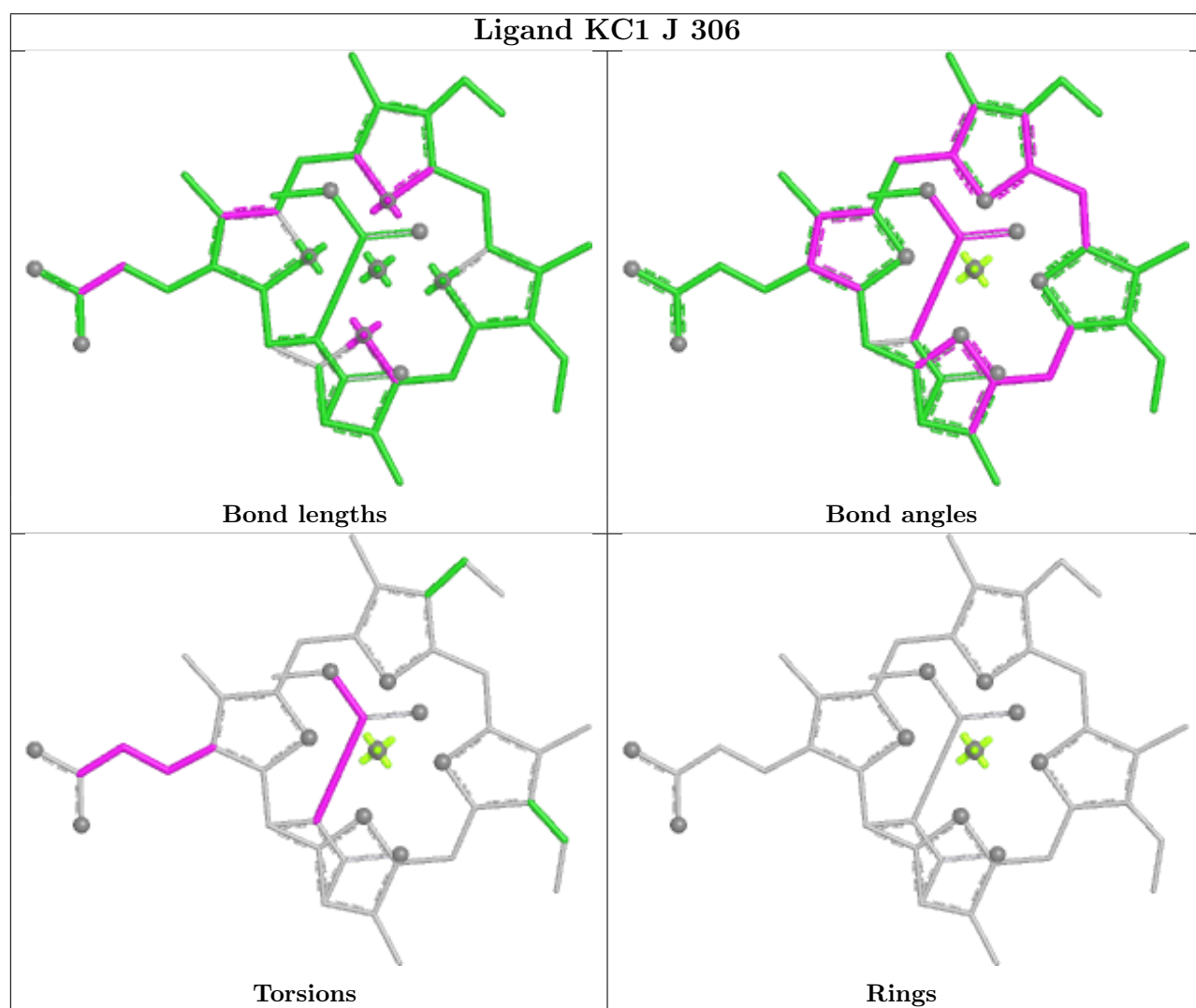
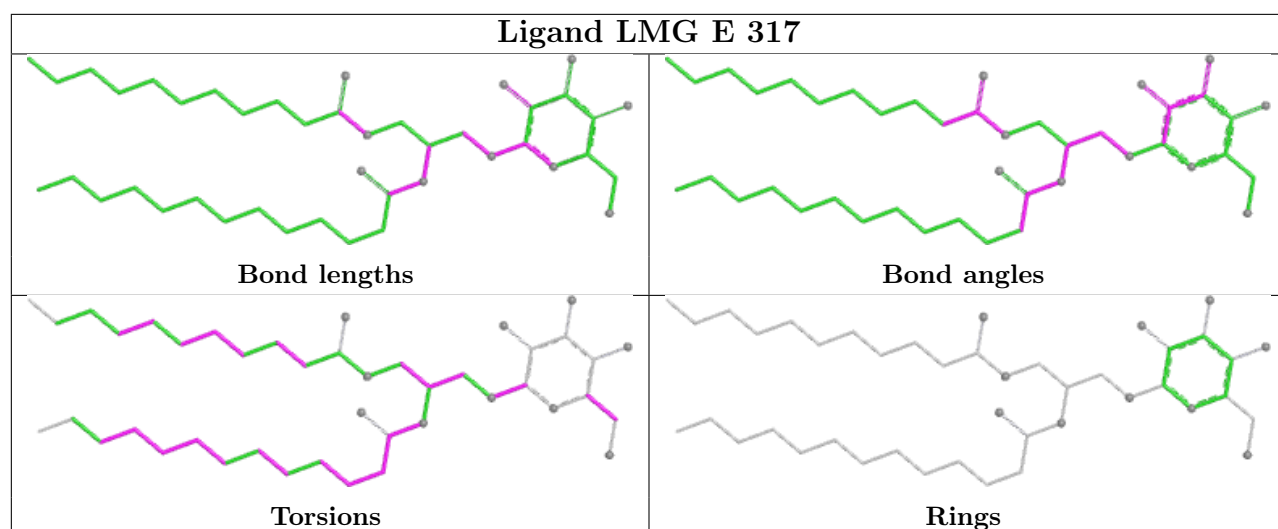
Rings

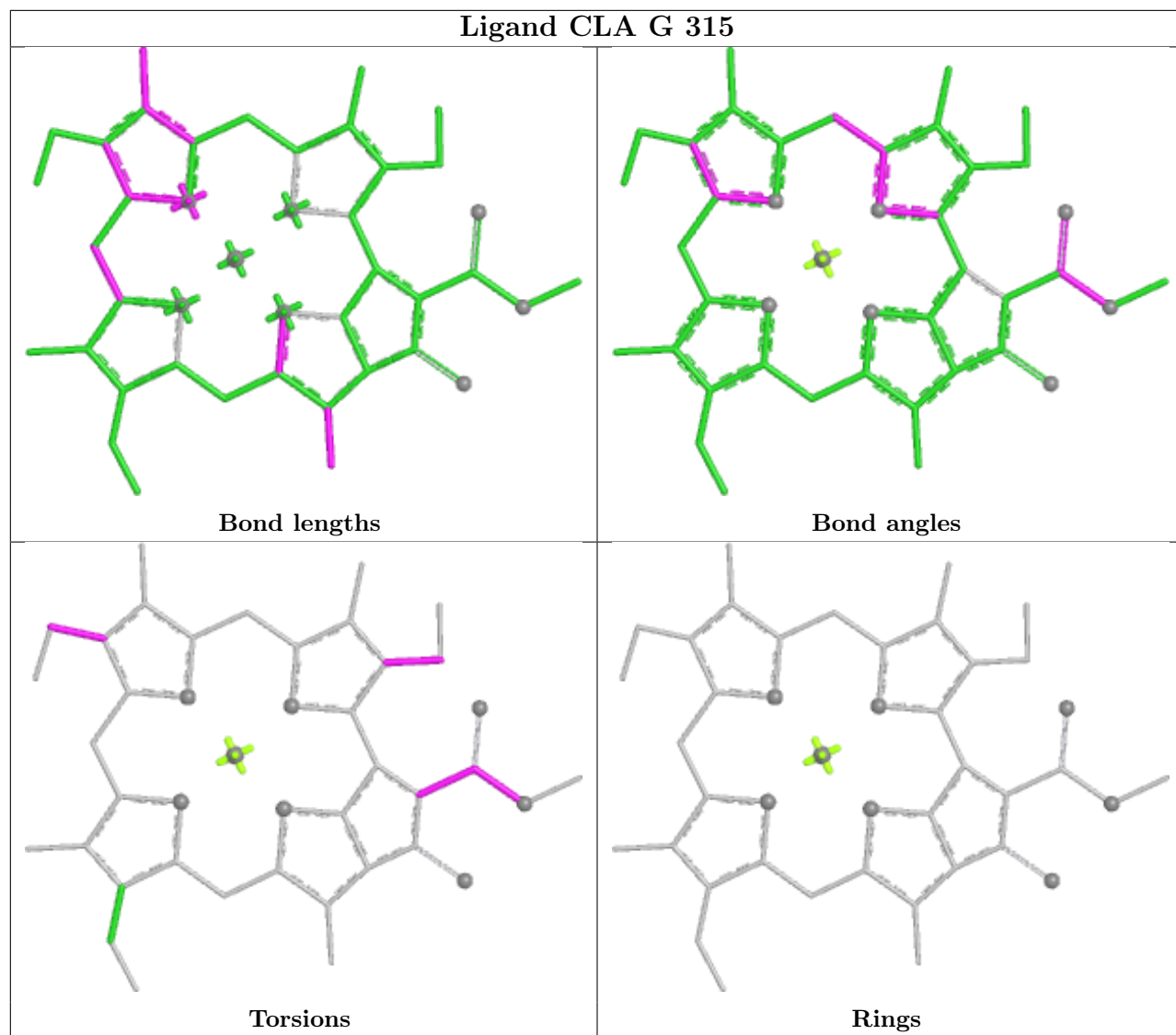


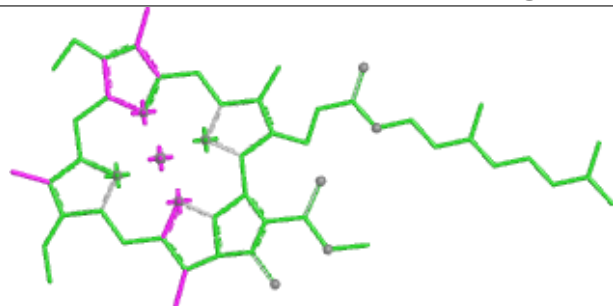
Ligand CLA a 839**Ligand CLA b 801**



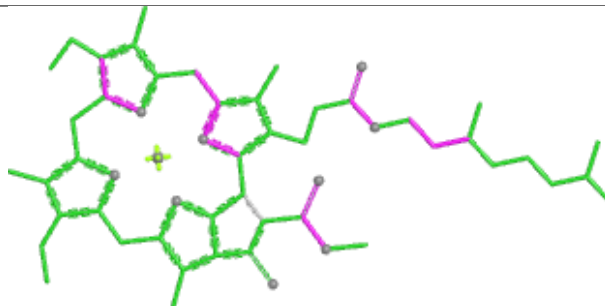




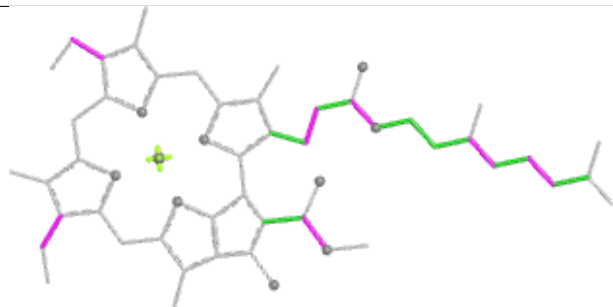


Ligand CLA I 315

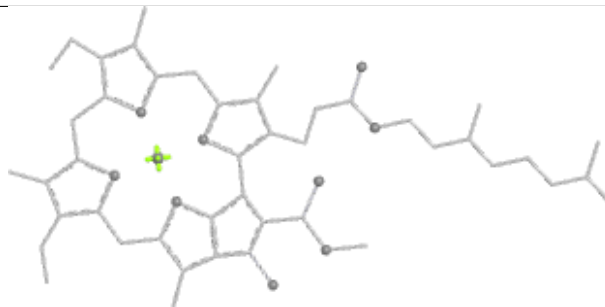
Bond lengths



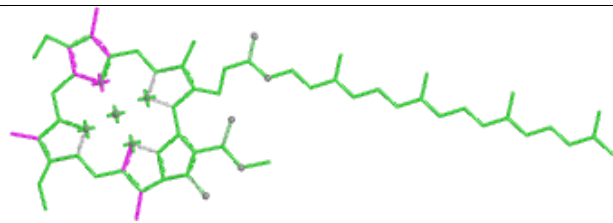
Bond angles



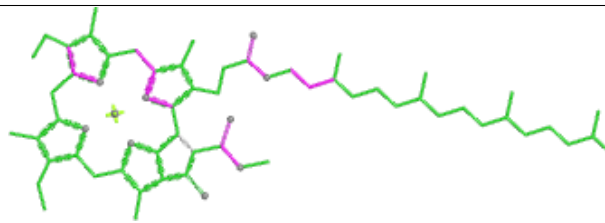
Torsions



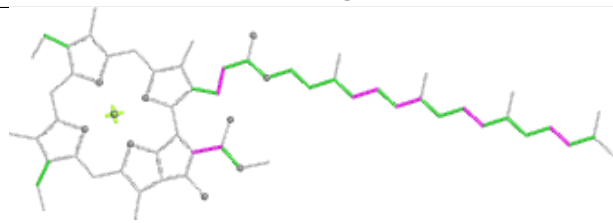
Rings

Ligand CLA J 307

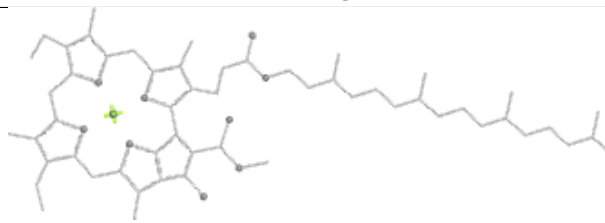
Bond lengths



Bond angles

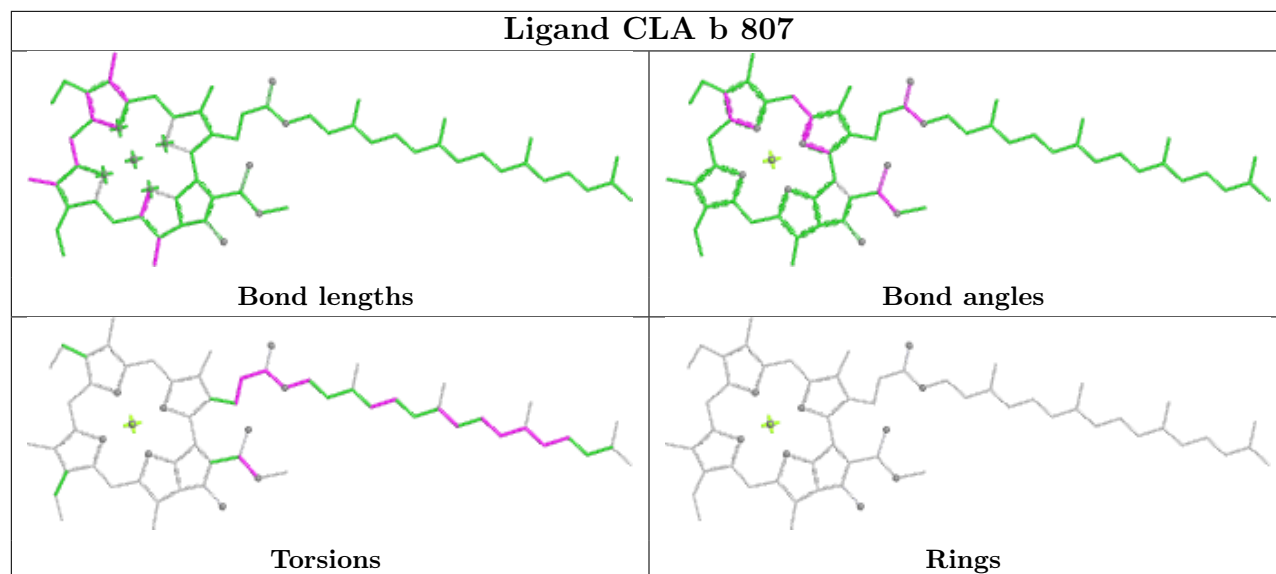


Torsions

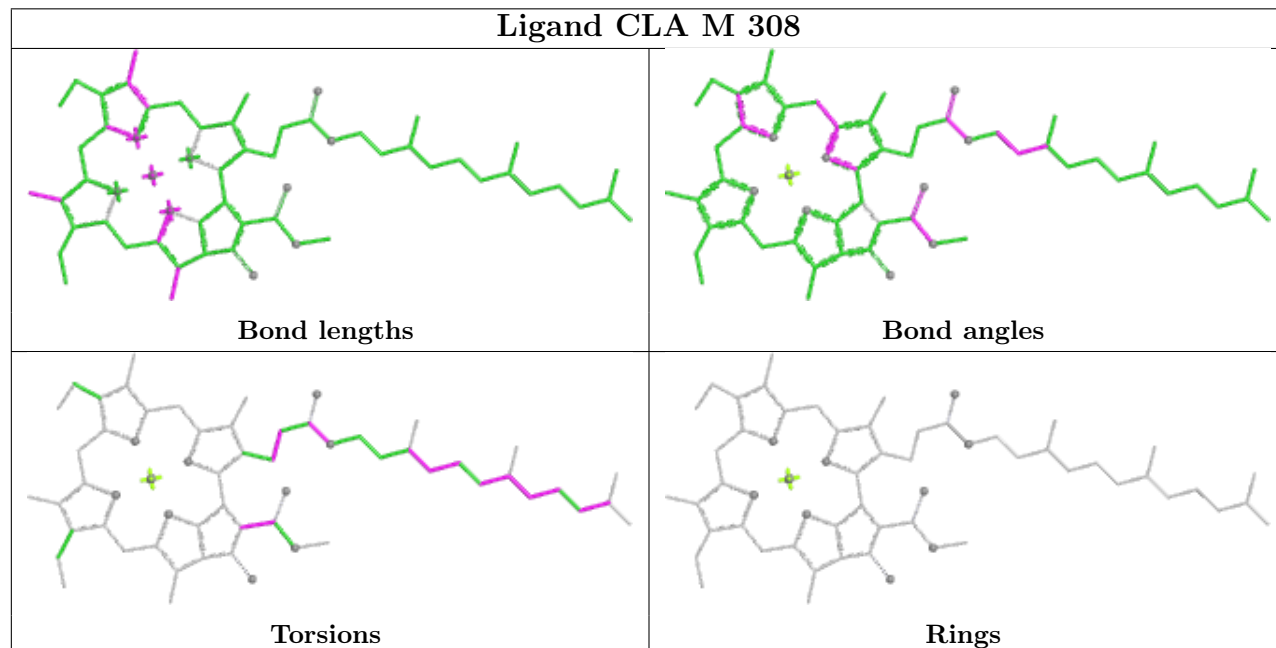


Rings

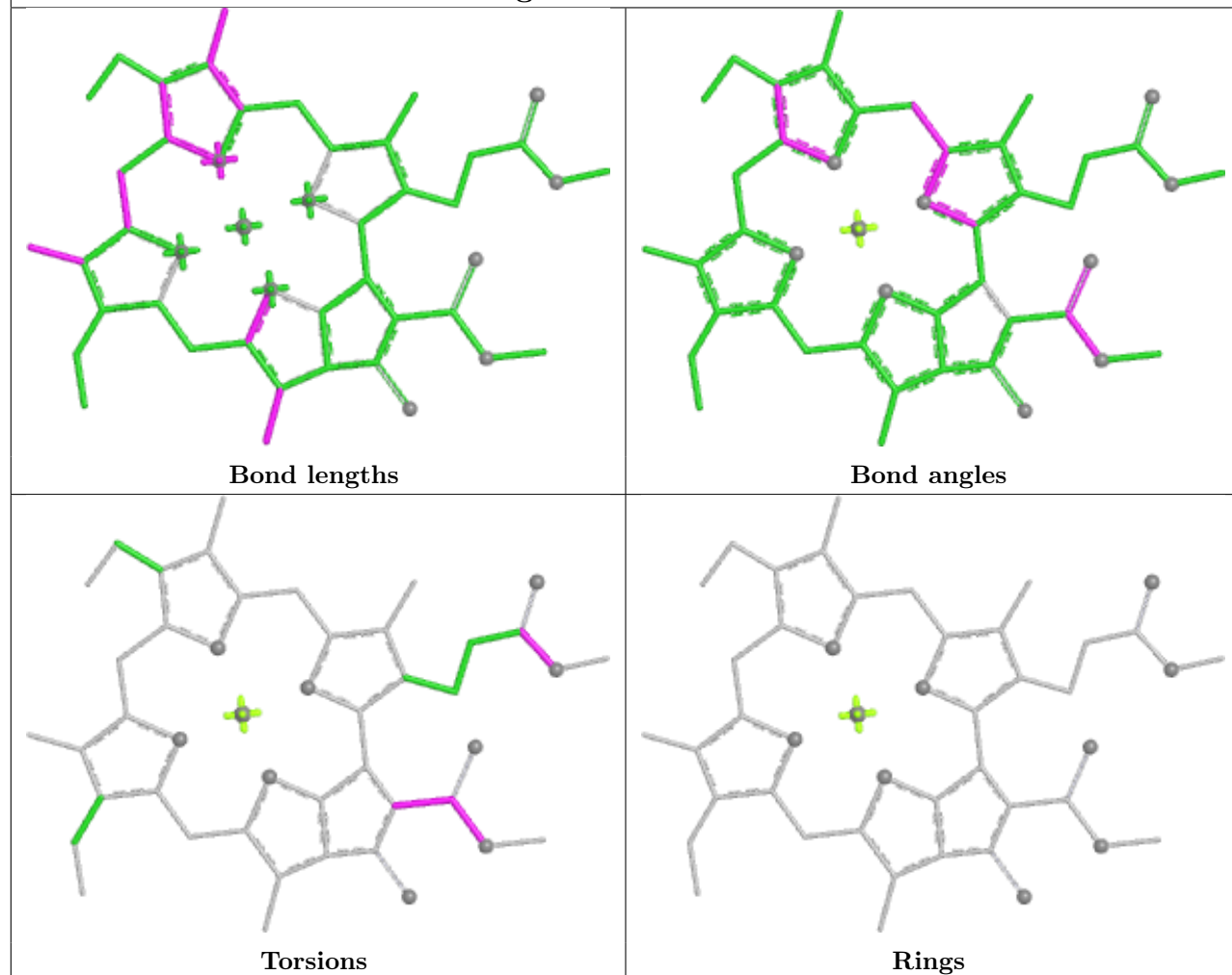
Ligand CLA b 807



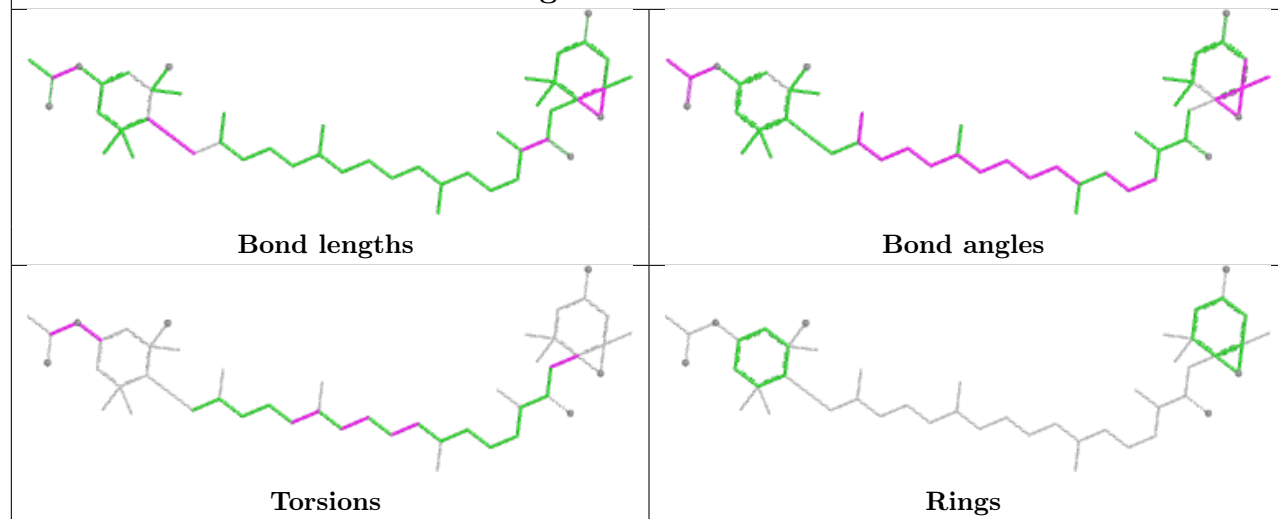
Ligand CLA M 308

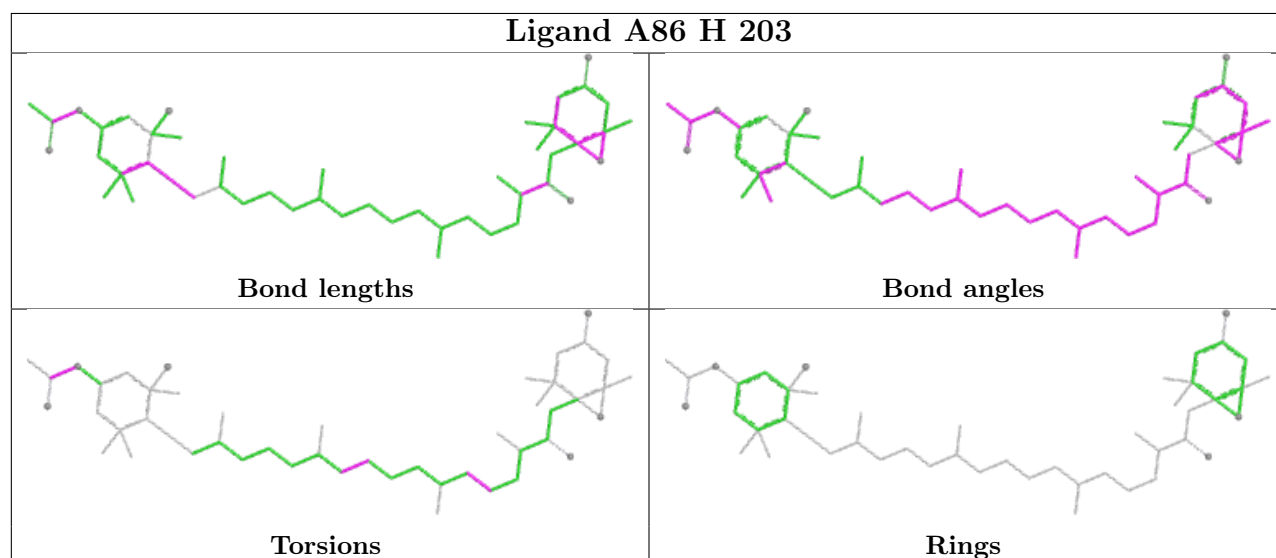
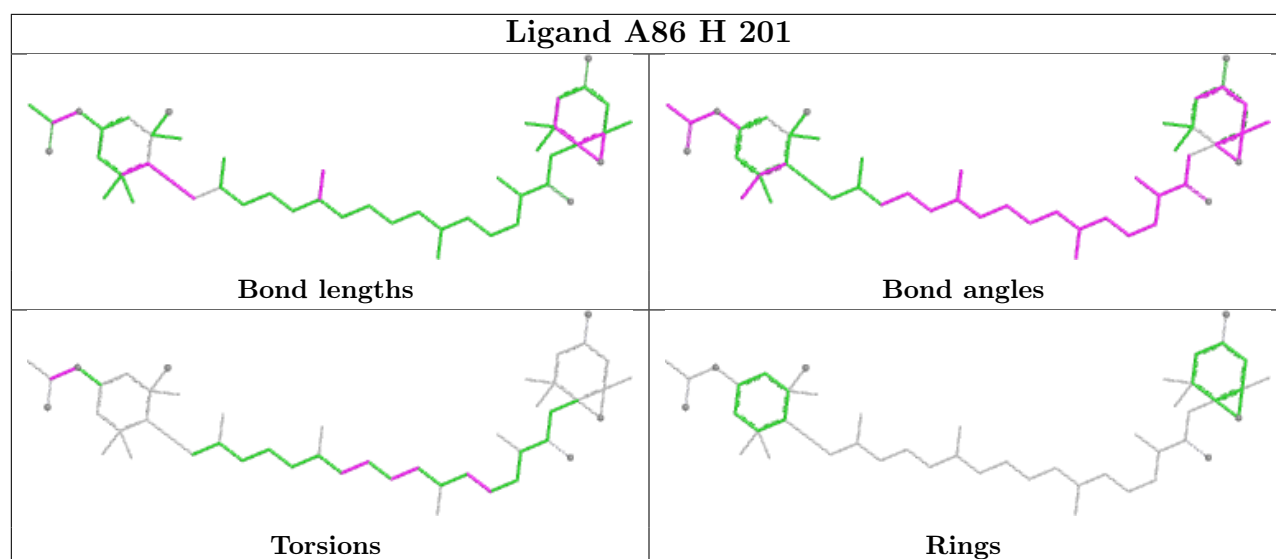


Ligand CLA b 816

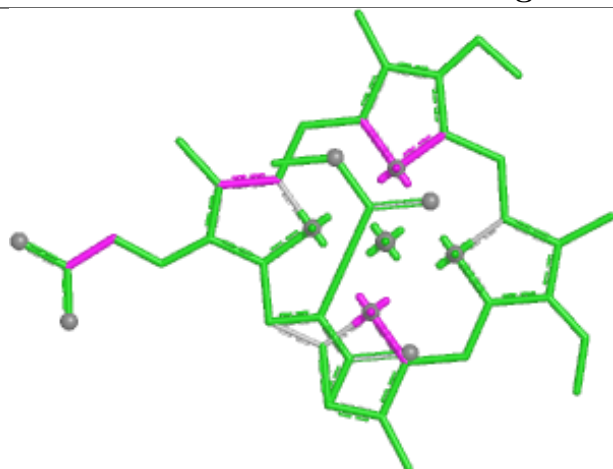


Ligand A86 F 301

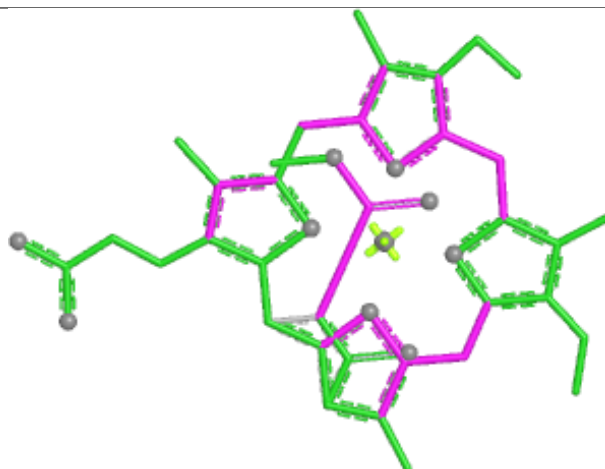




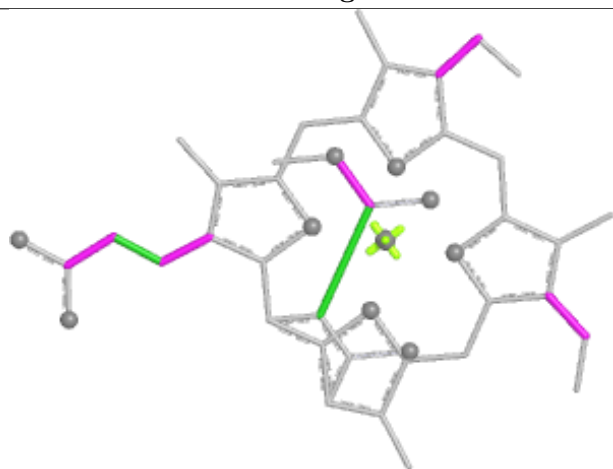
Ligand KC1 A 209



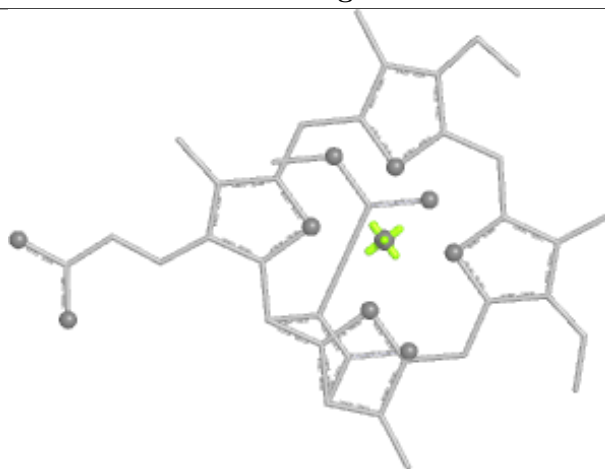
Bond lengths



Bond angles

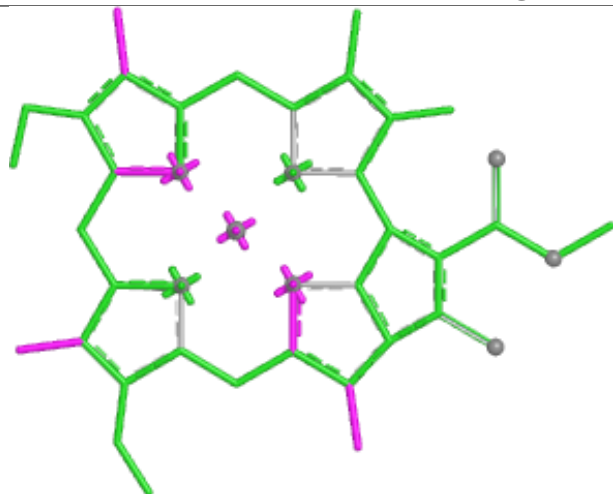


Torsions

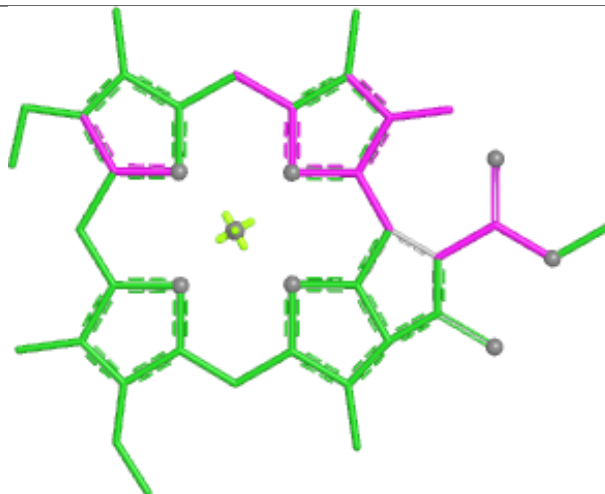


Rings

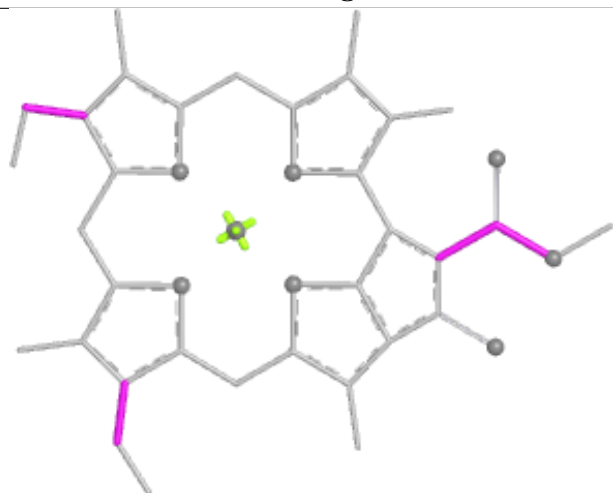
Ligand CLA K 317



Bond lengths



Bond angles

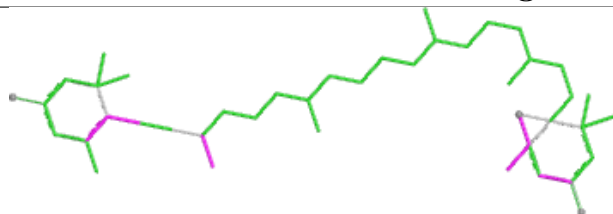


Torsions

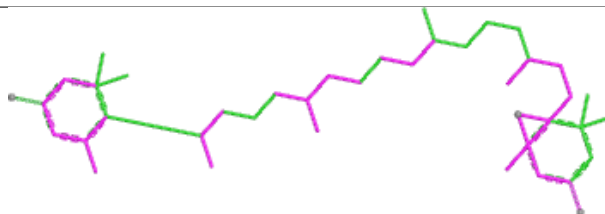


Rings

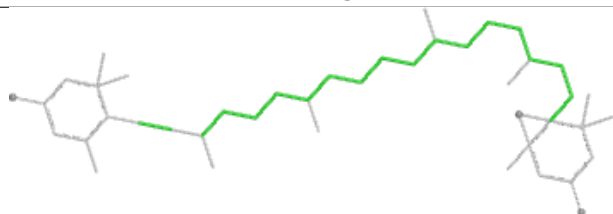
Ligand DD6 L 303



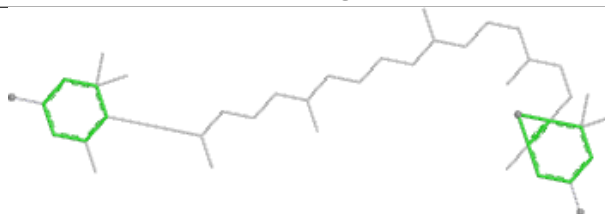
Bond lengths



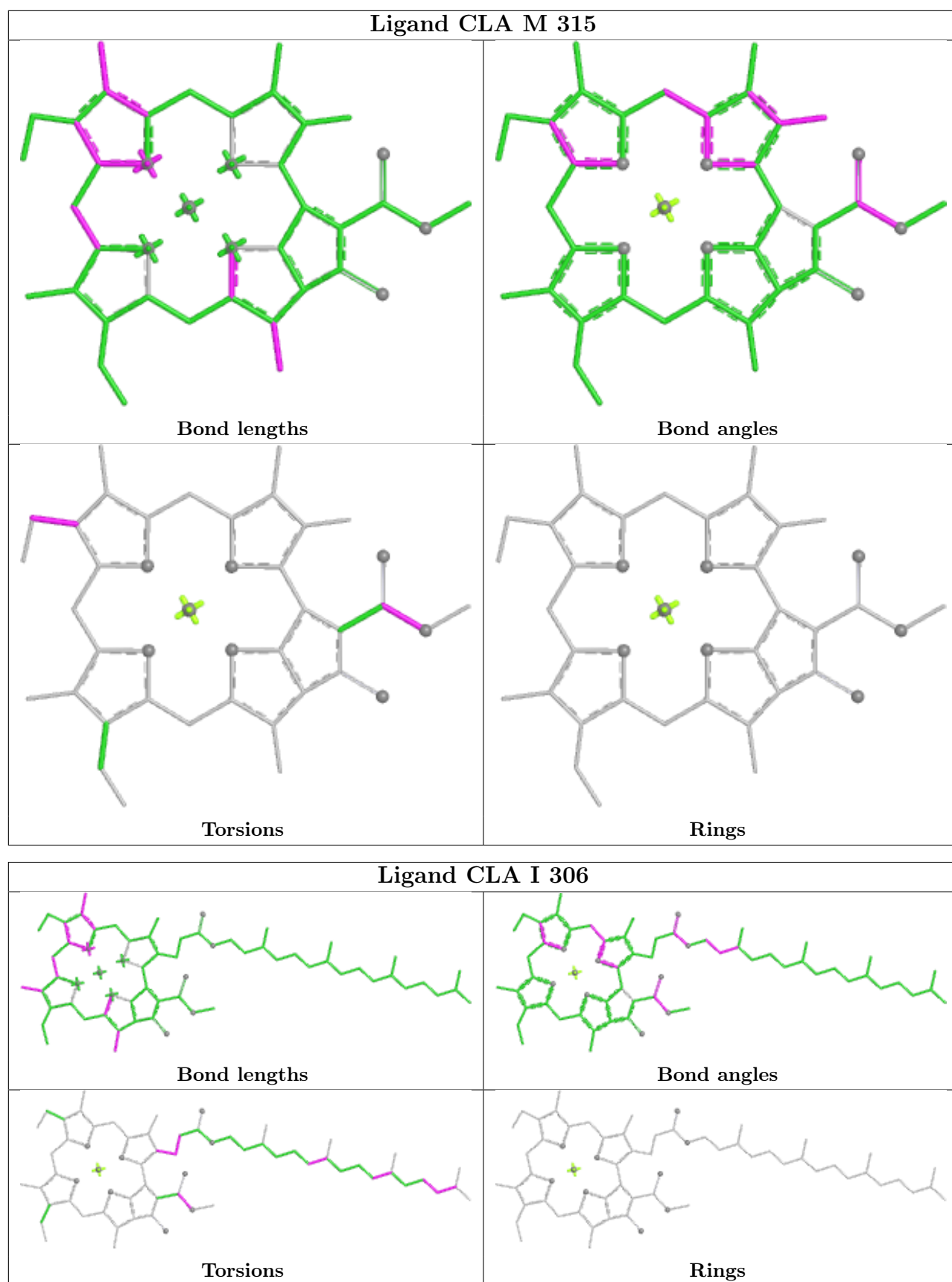
Bond angles

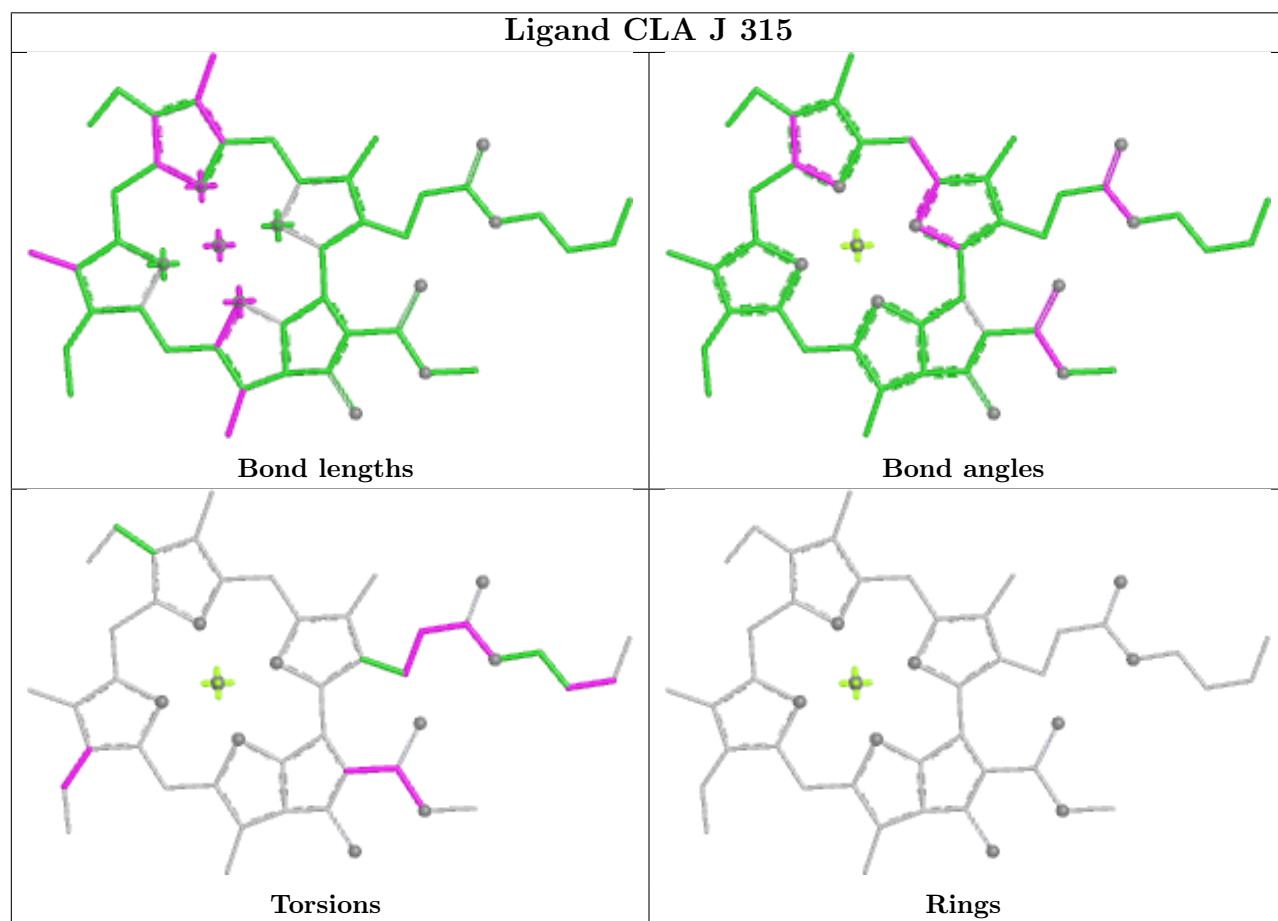
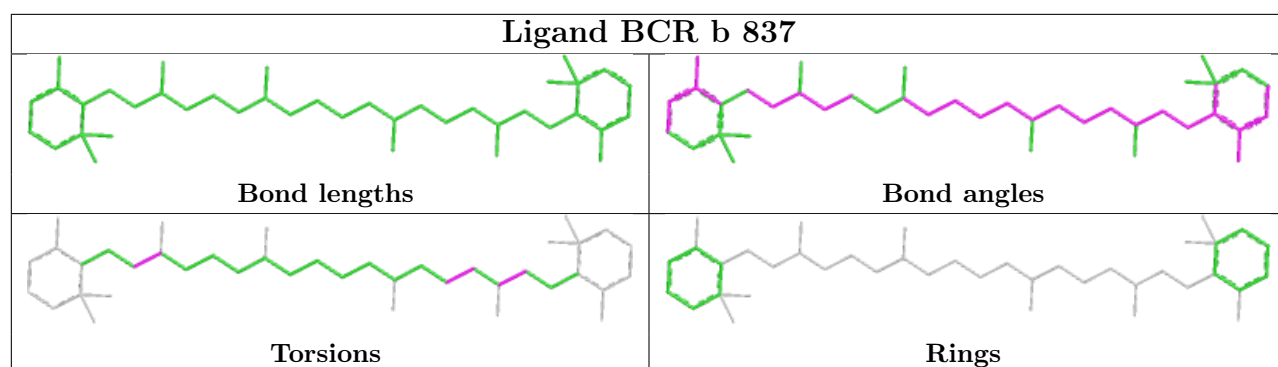


Torsions

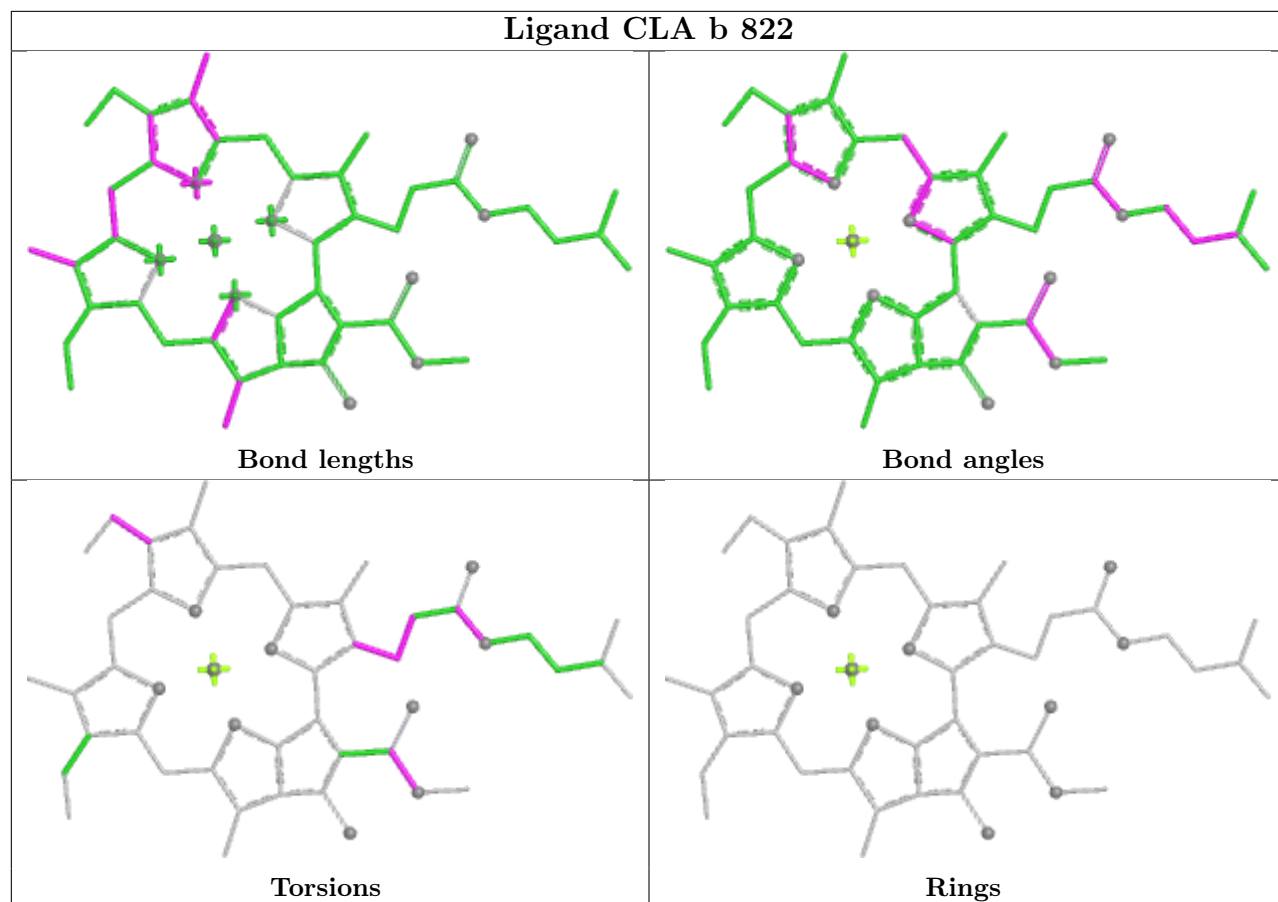


Rings

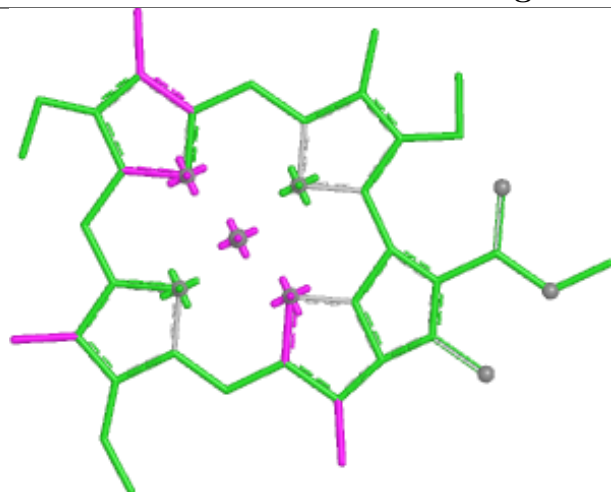




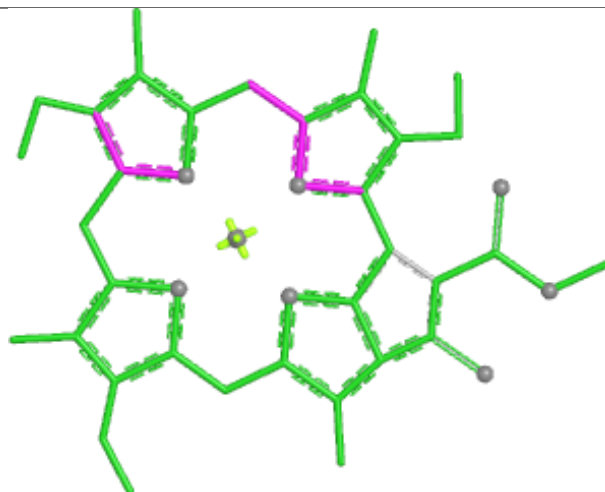
Ligand CLA b 822



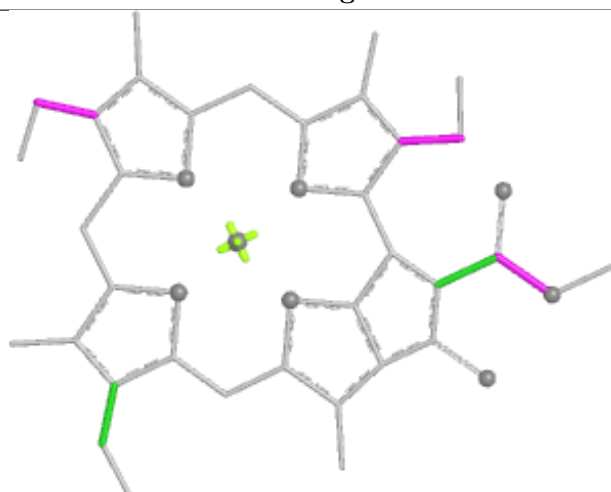
Ligand CLA C 318



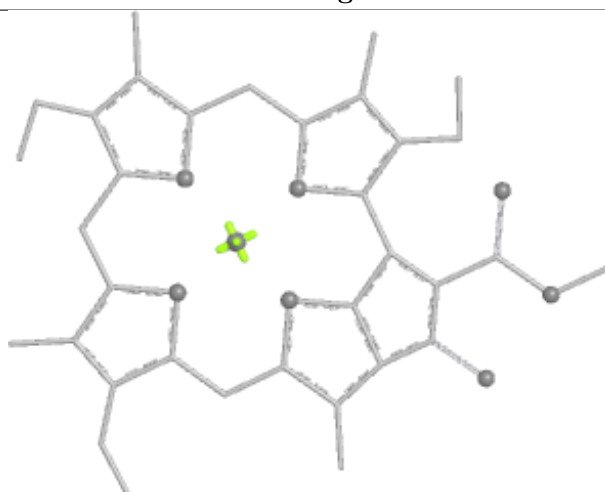
Bond lengths



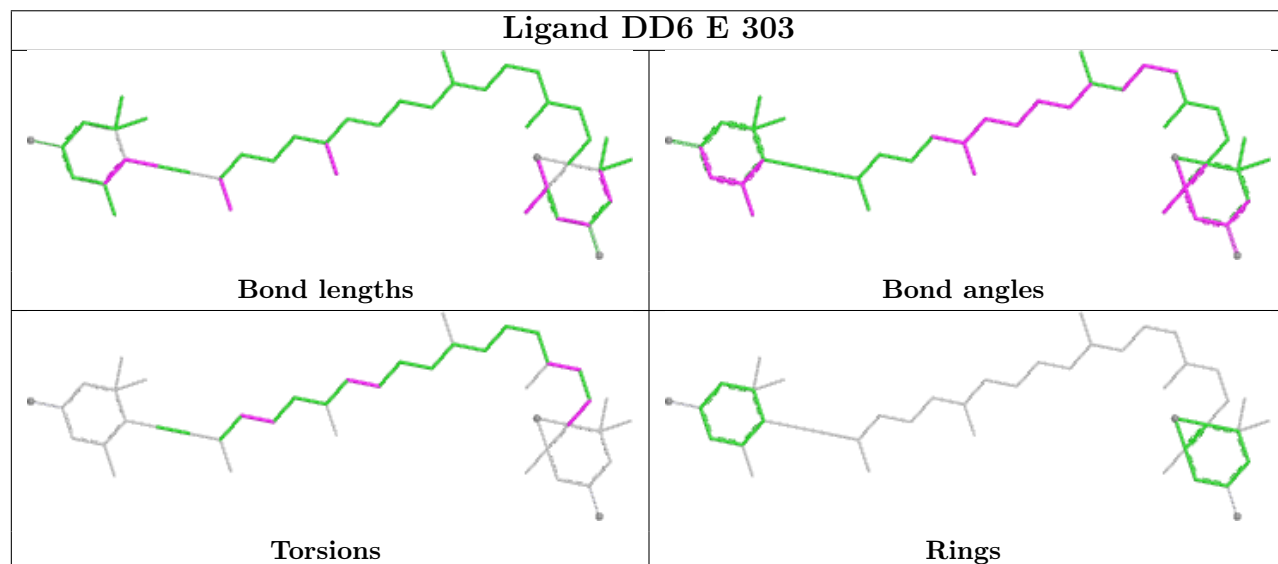
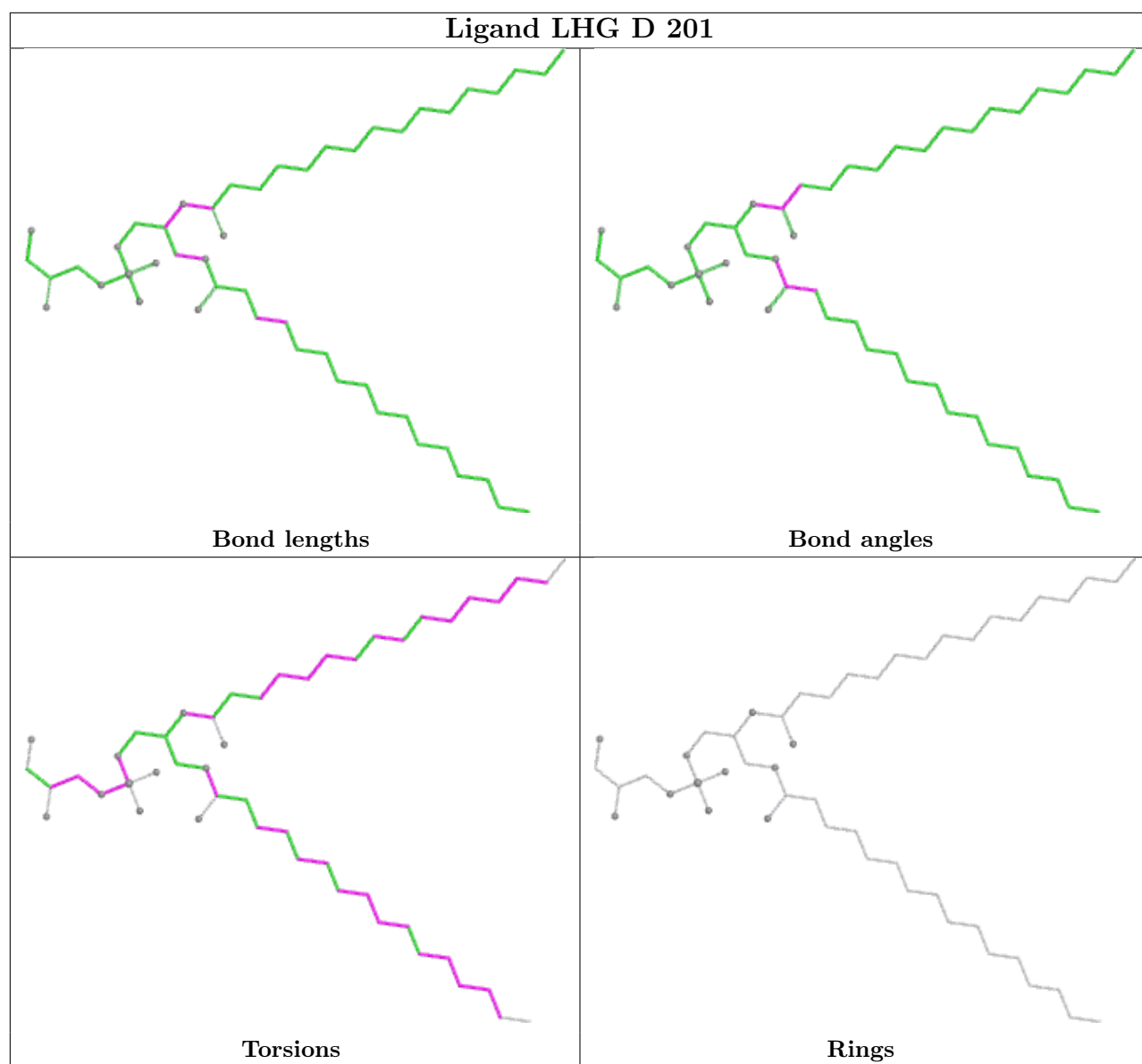
Bond angles

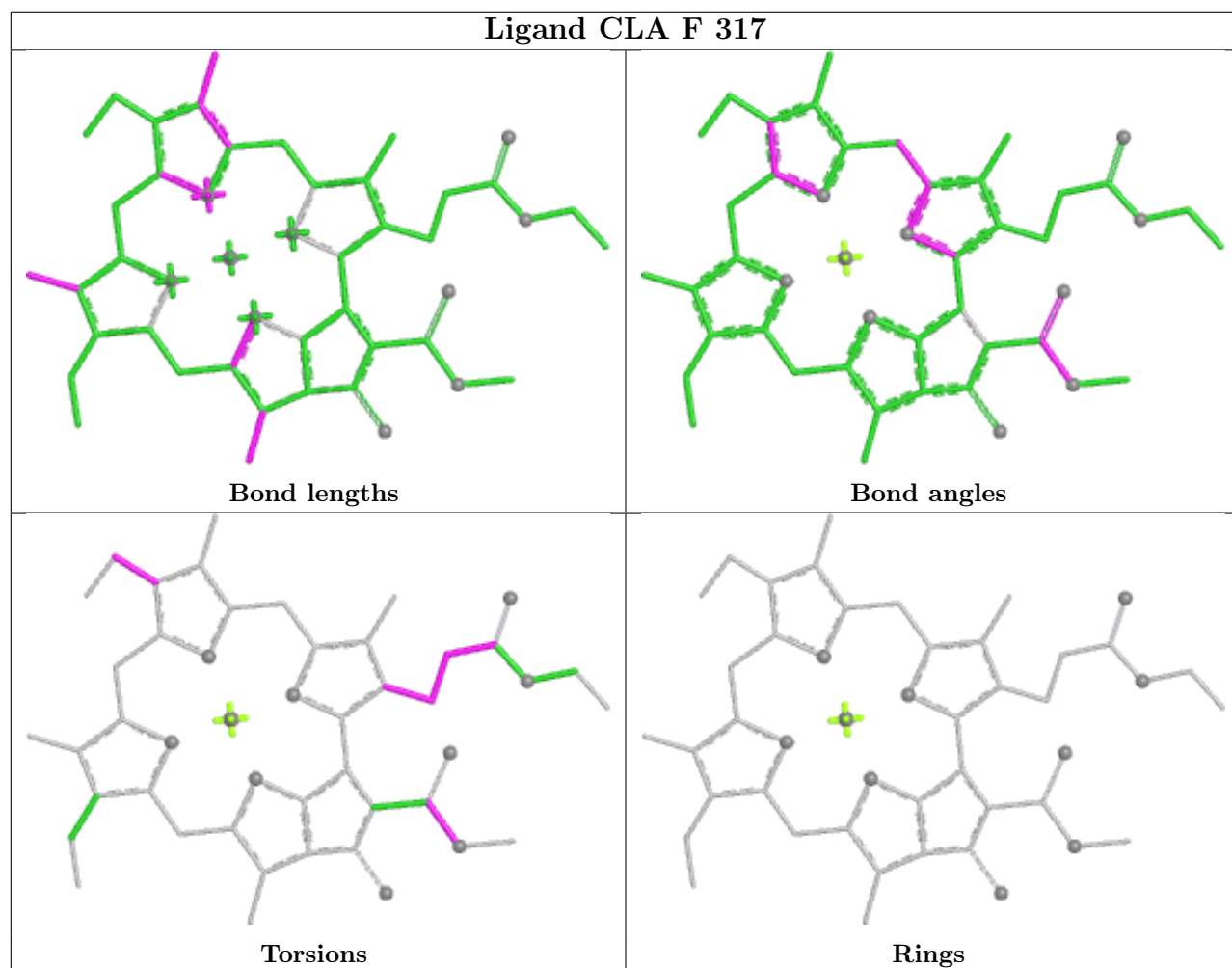
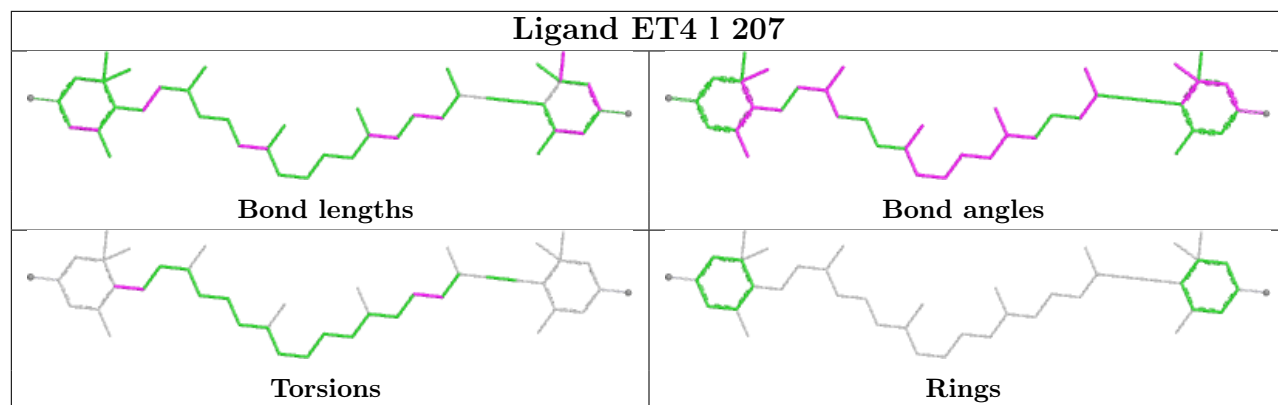


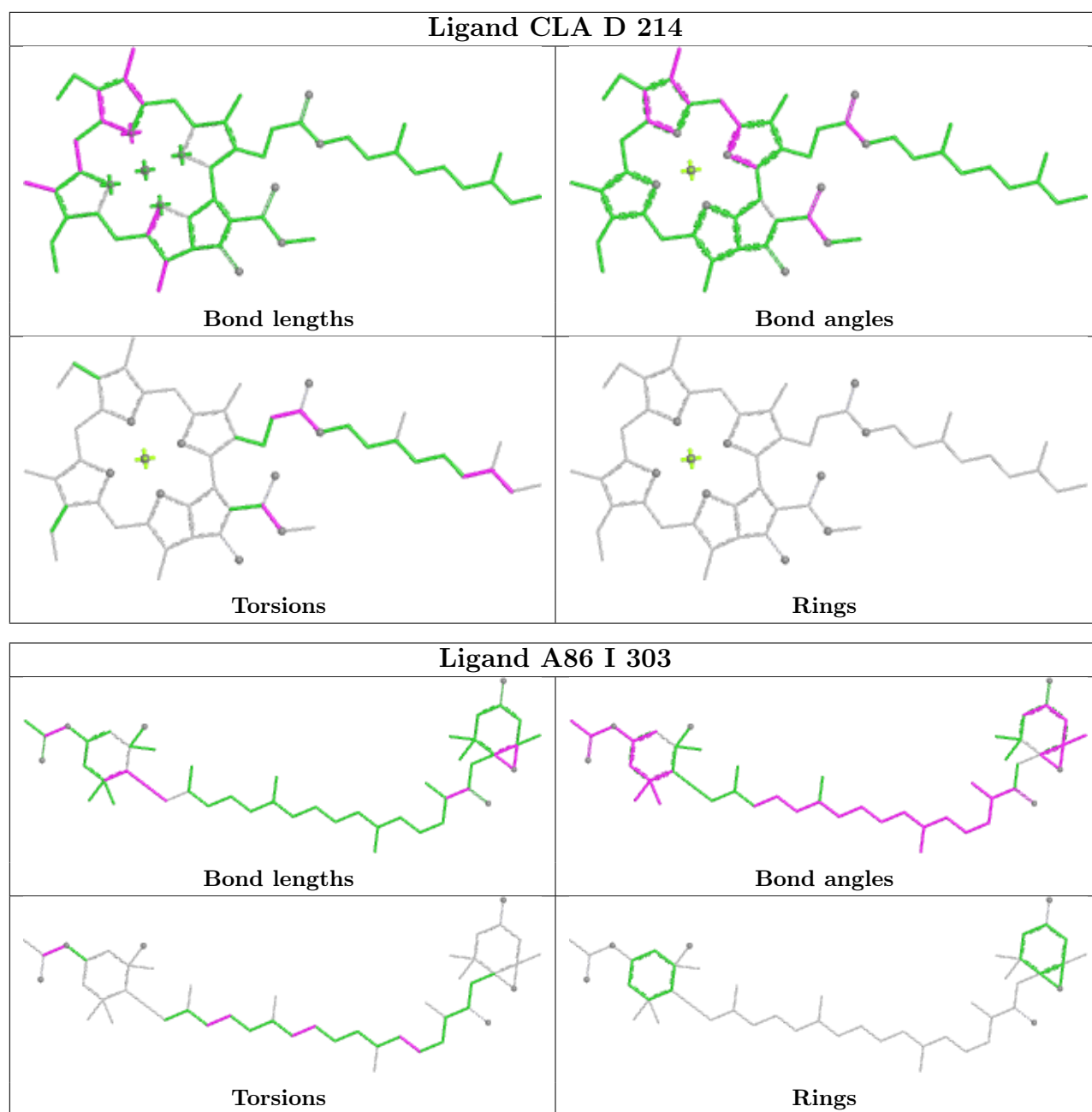
Torsions



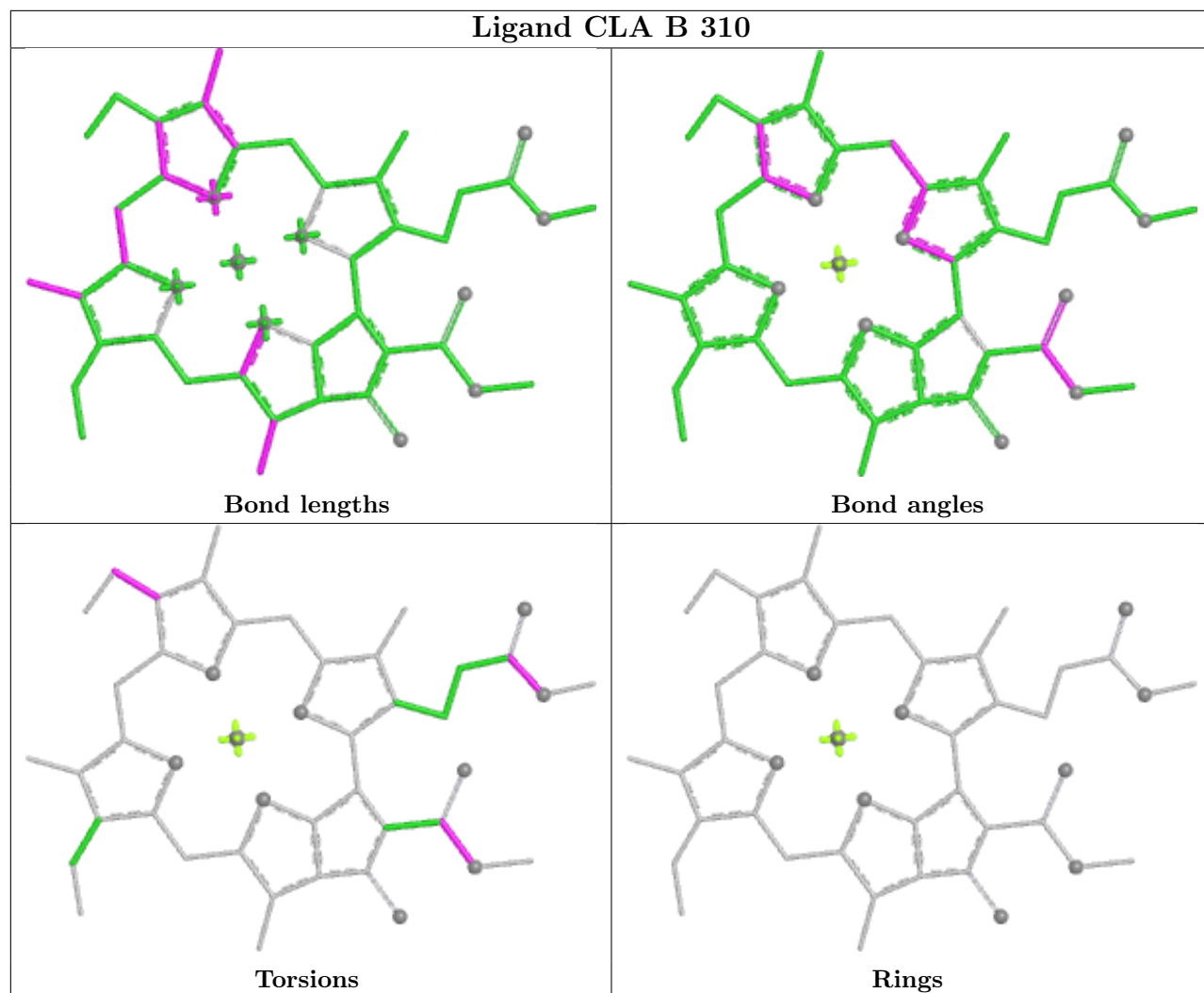
Rings

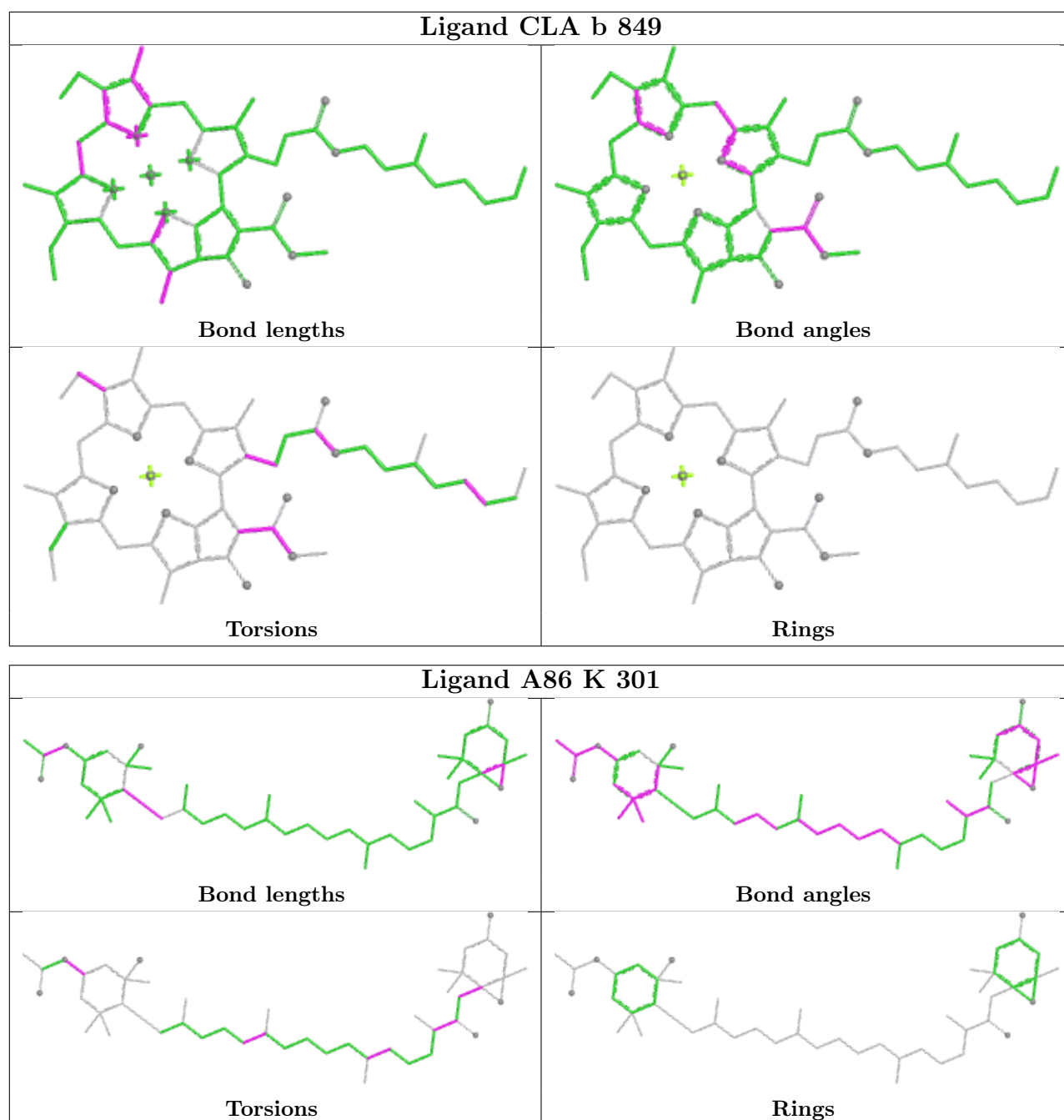


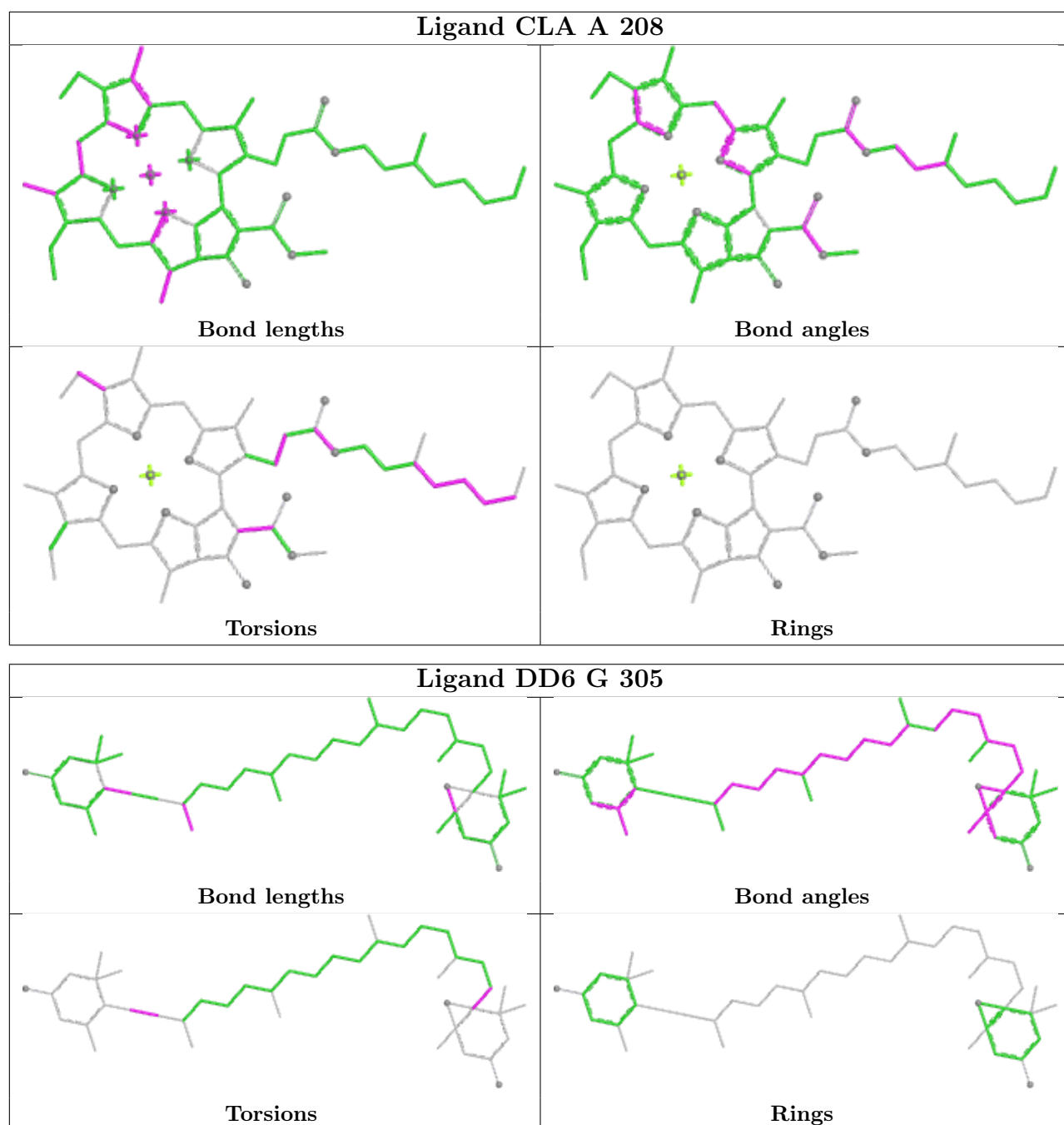


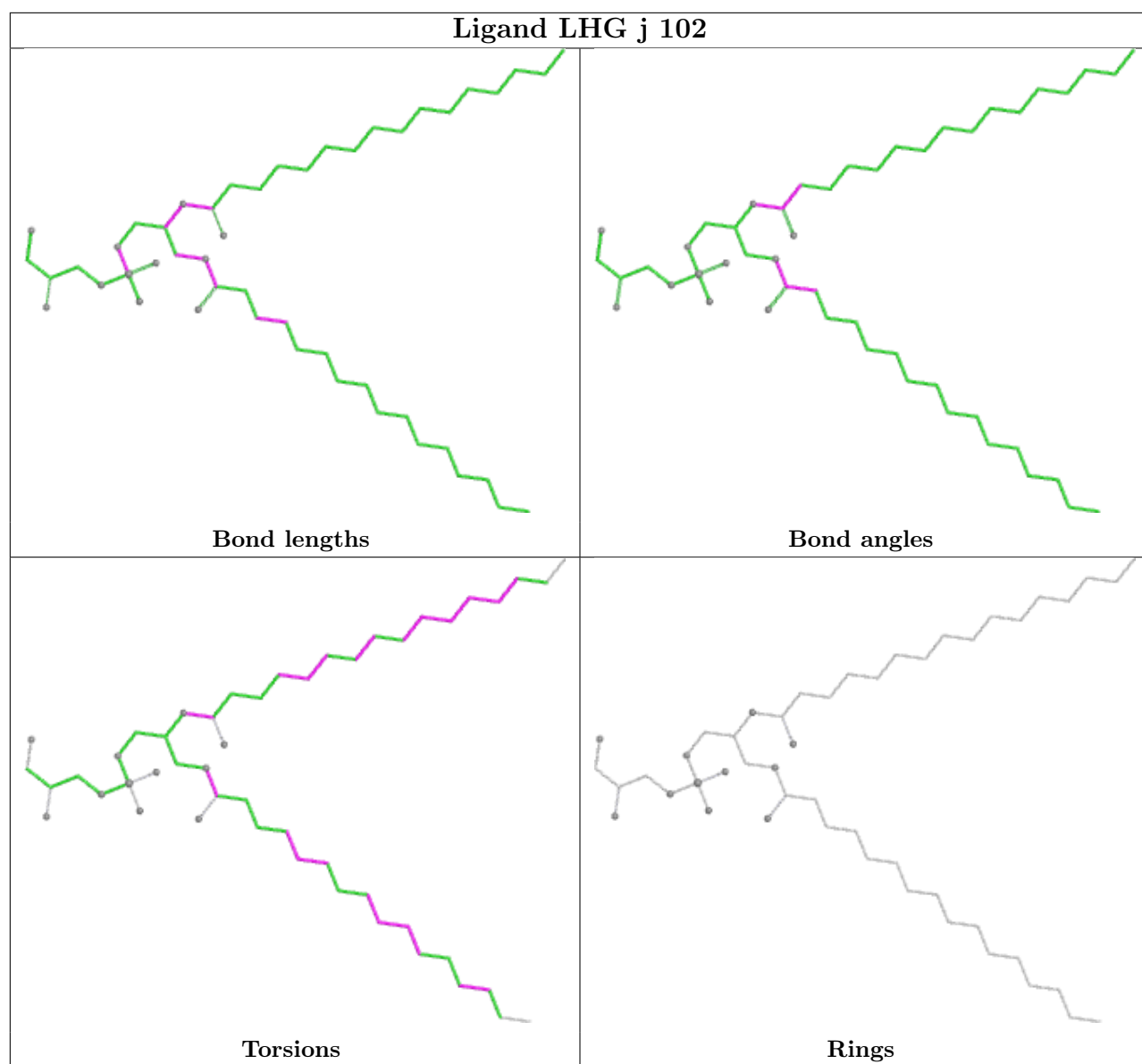


Ligand CLA B 310

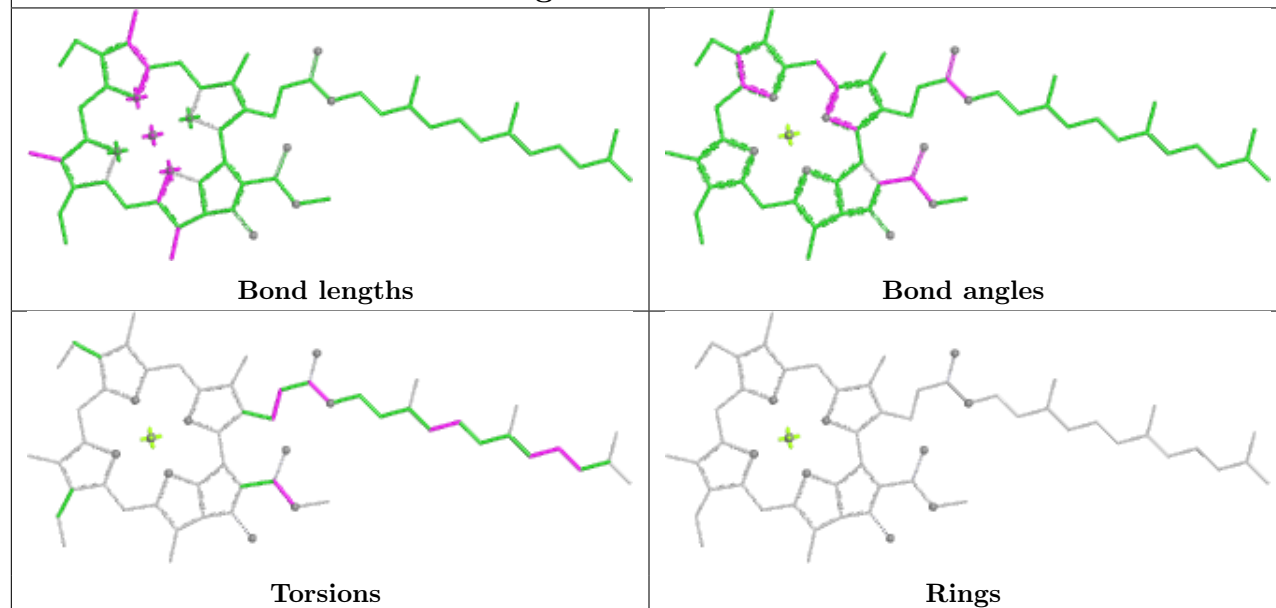




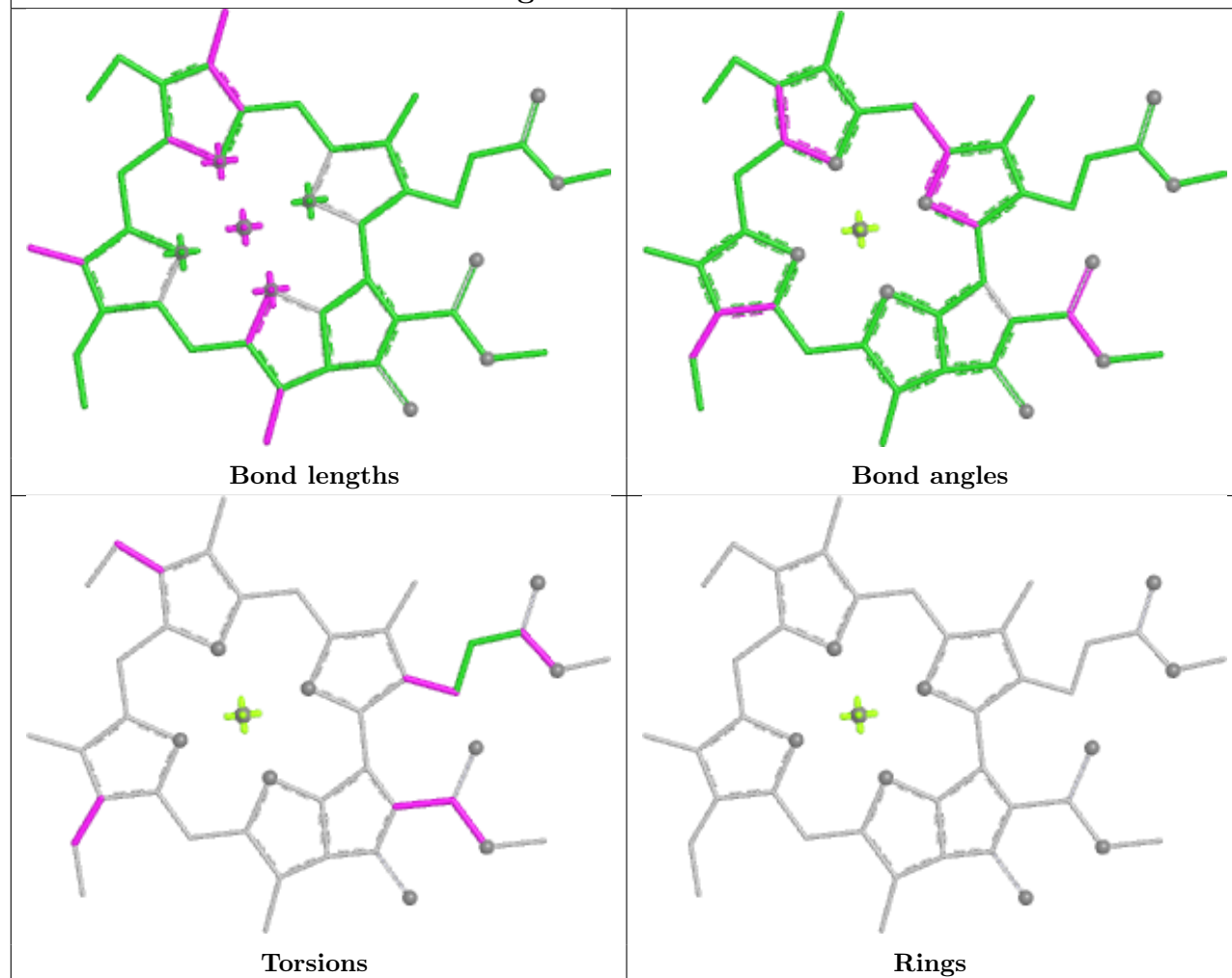


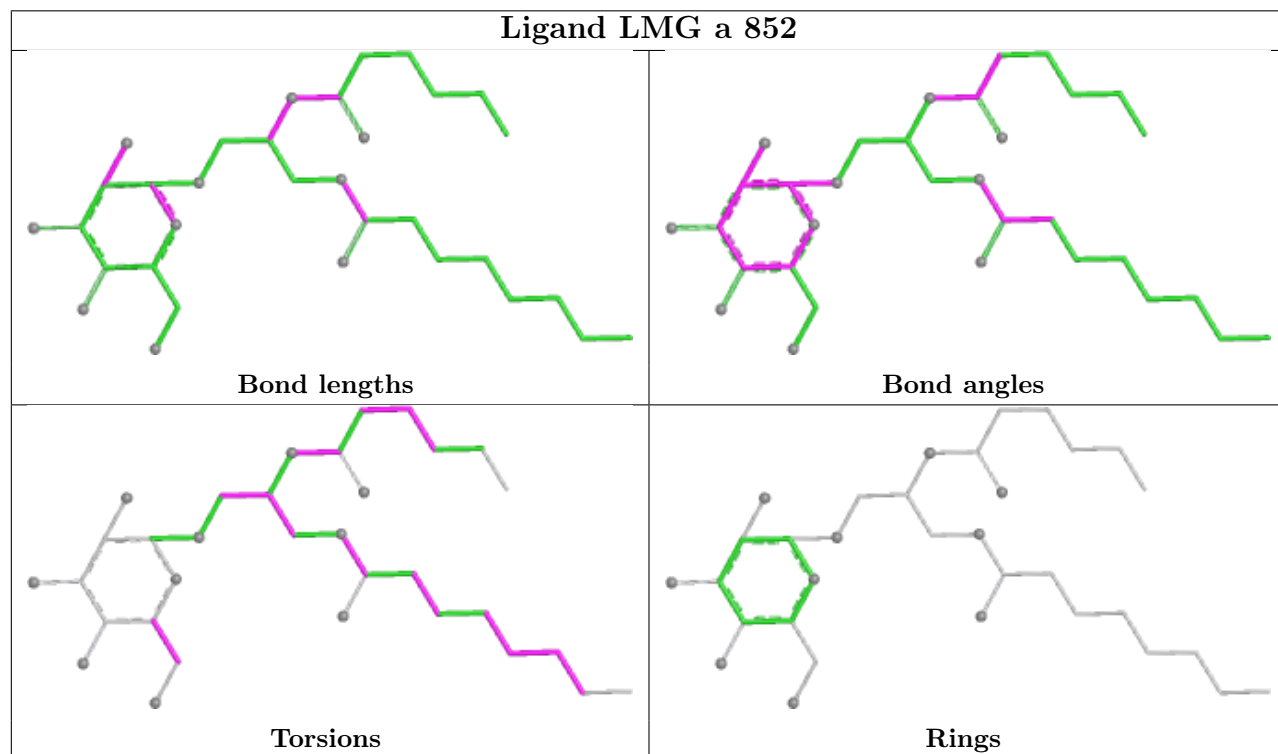
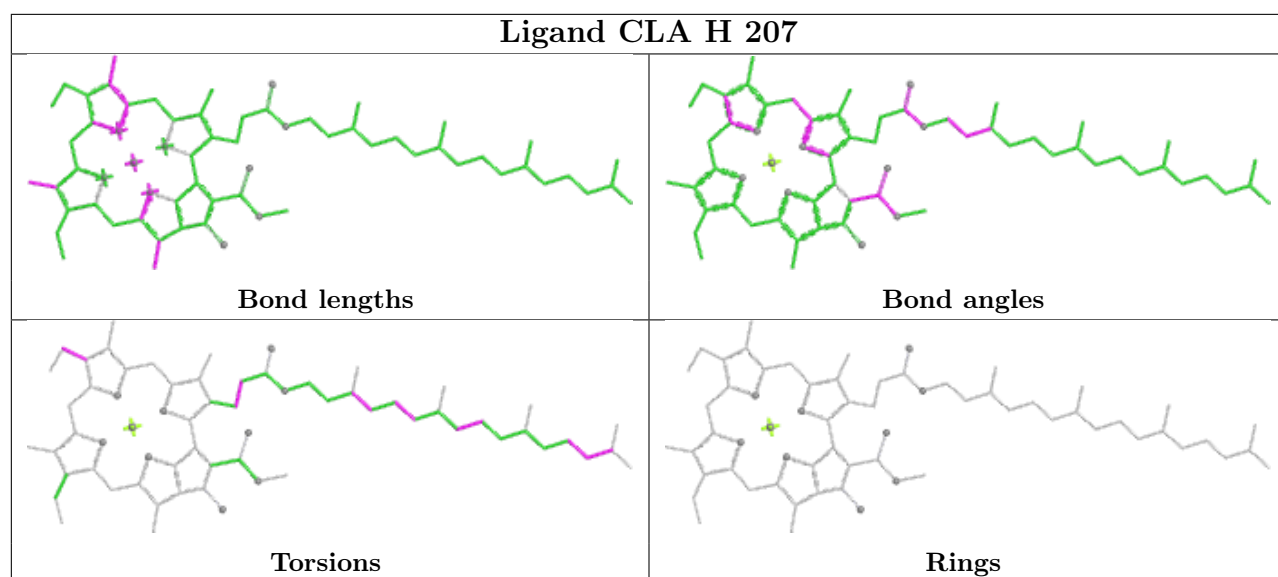


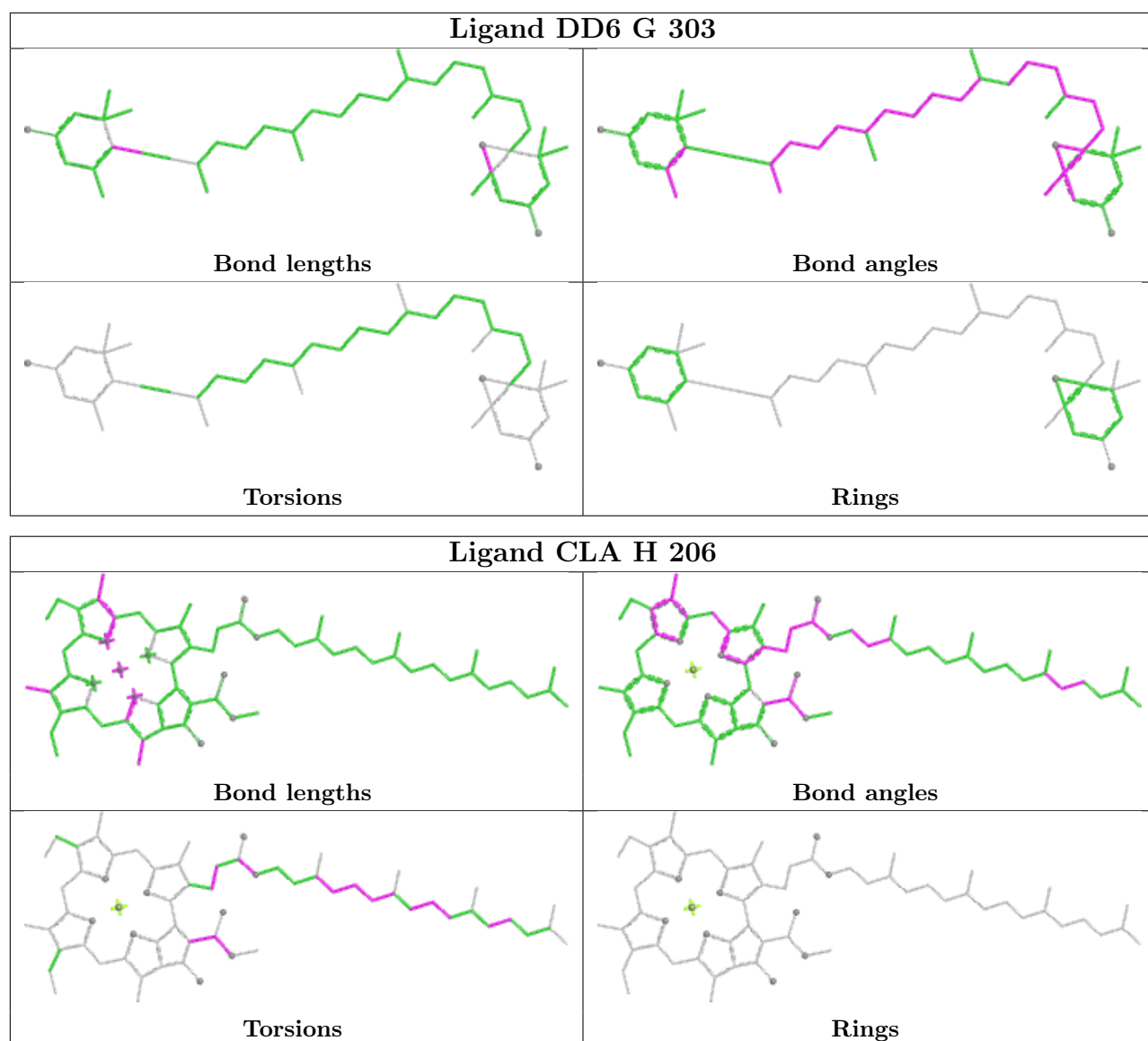
Ligand CLA b 812

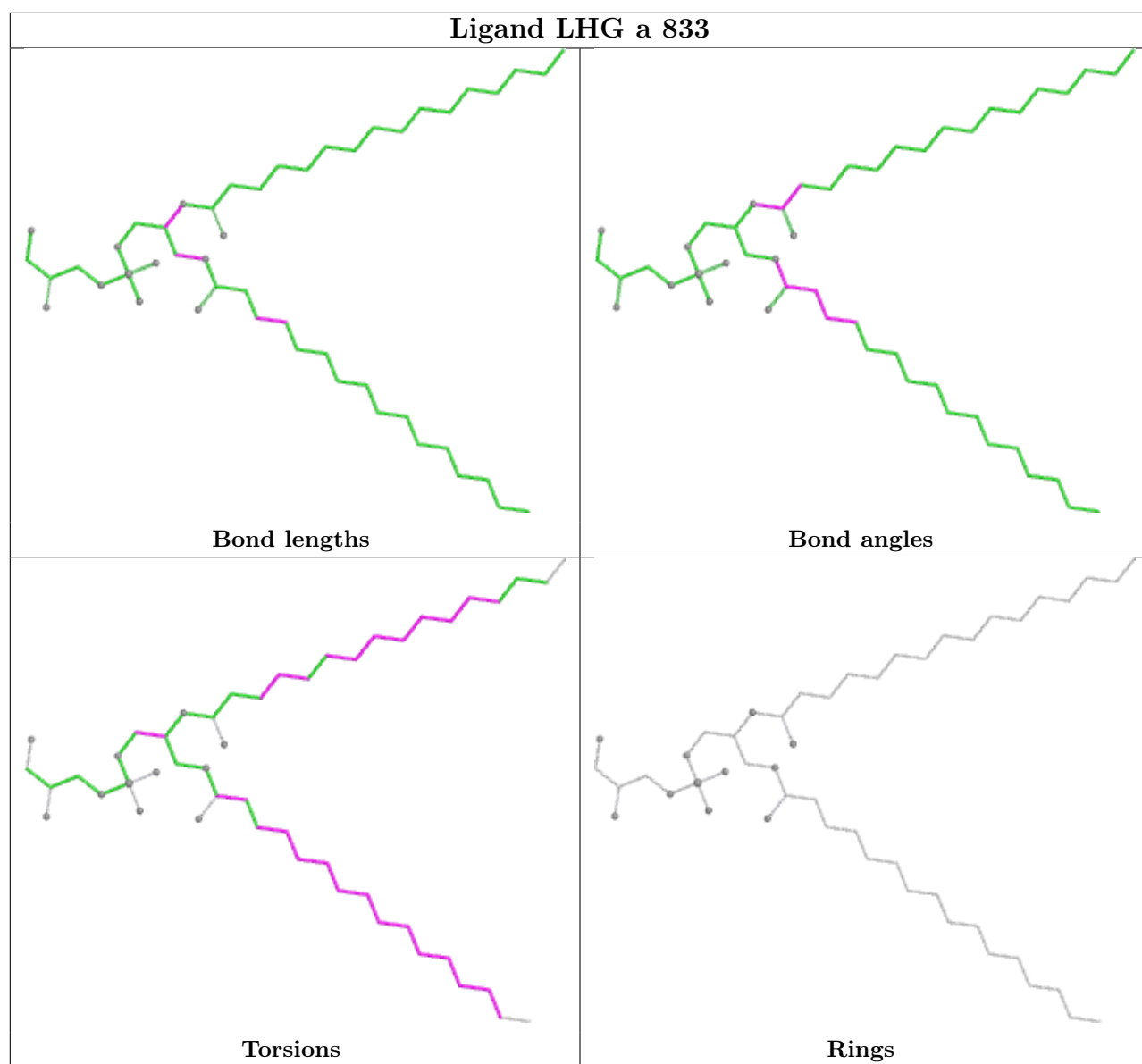


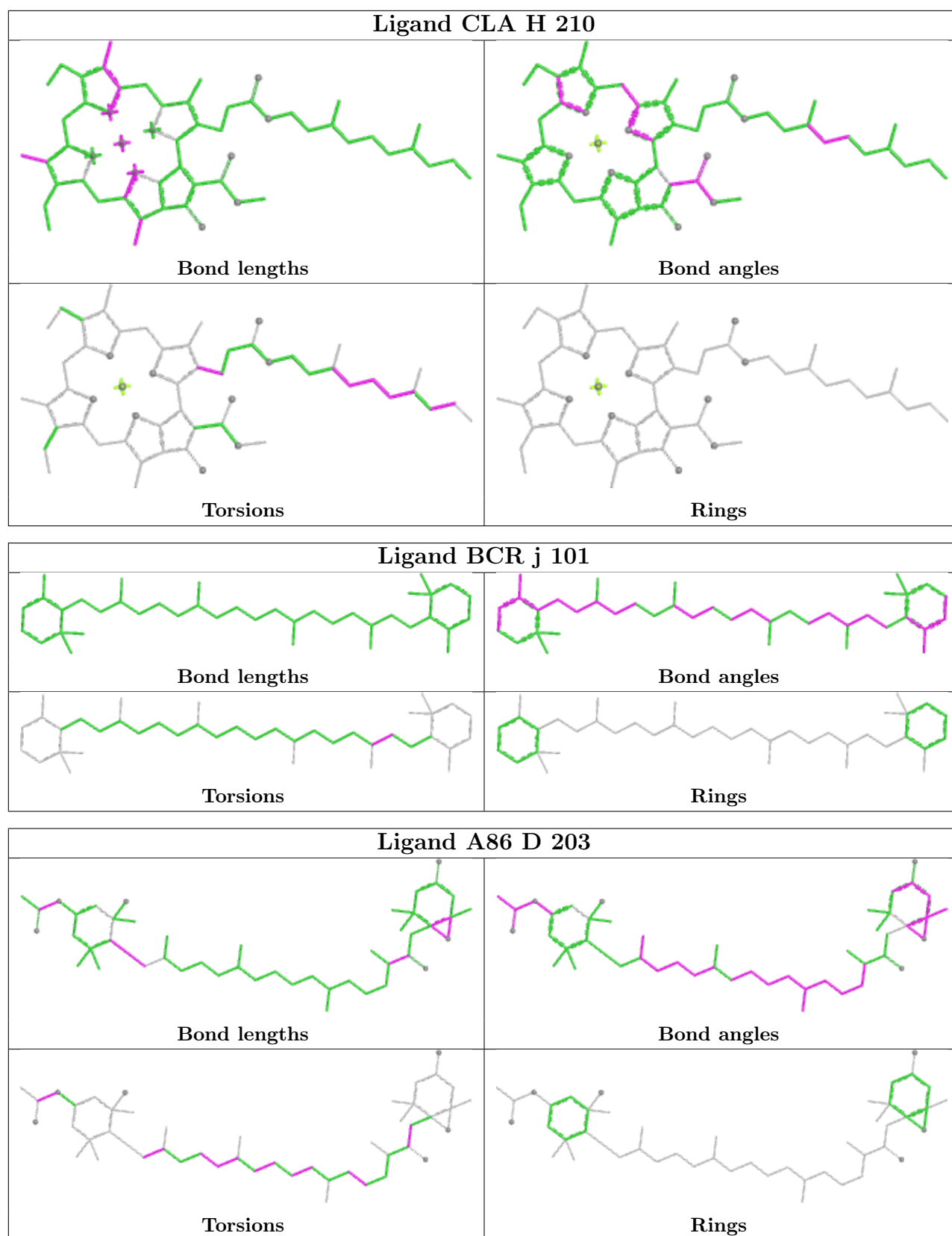
Ligand CLA J 310



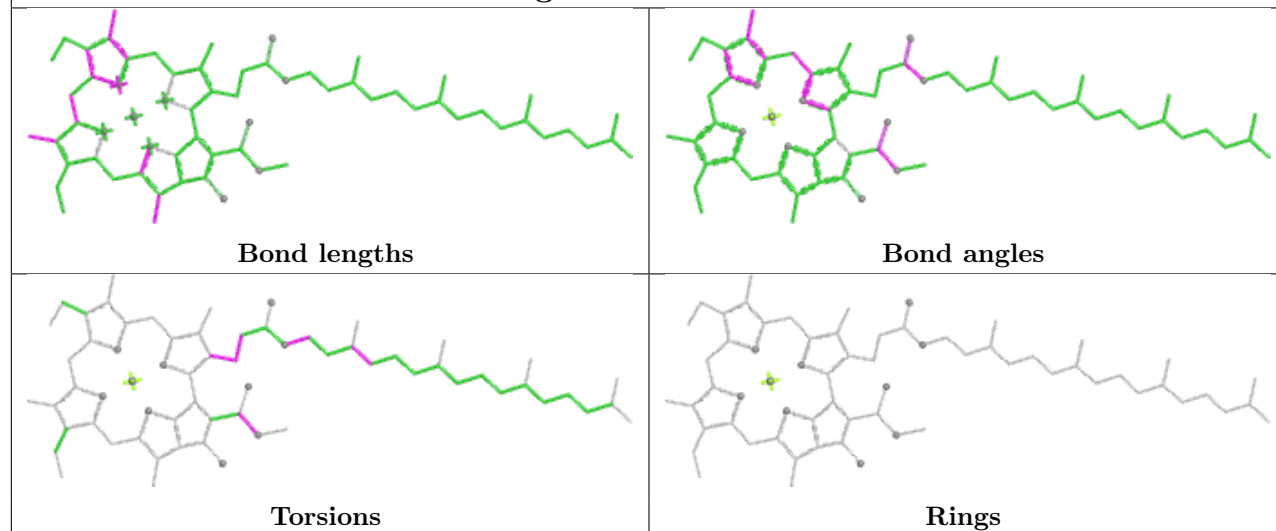




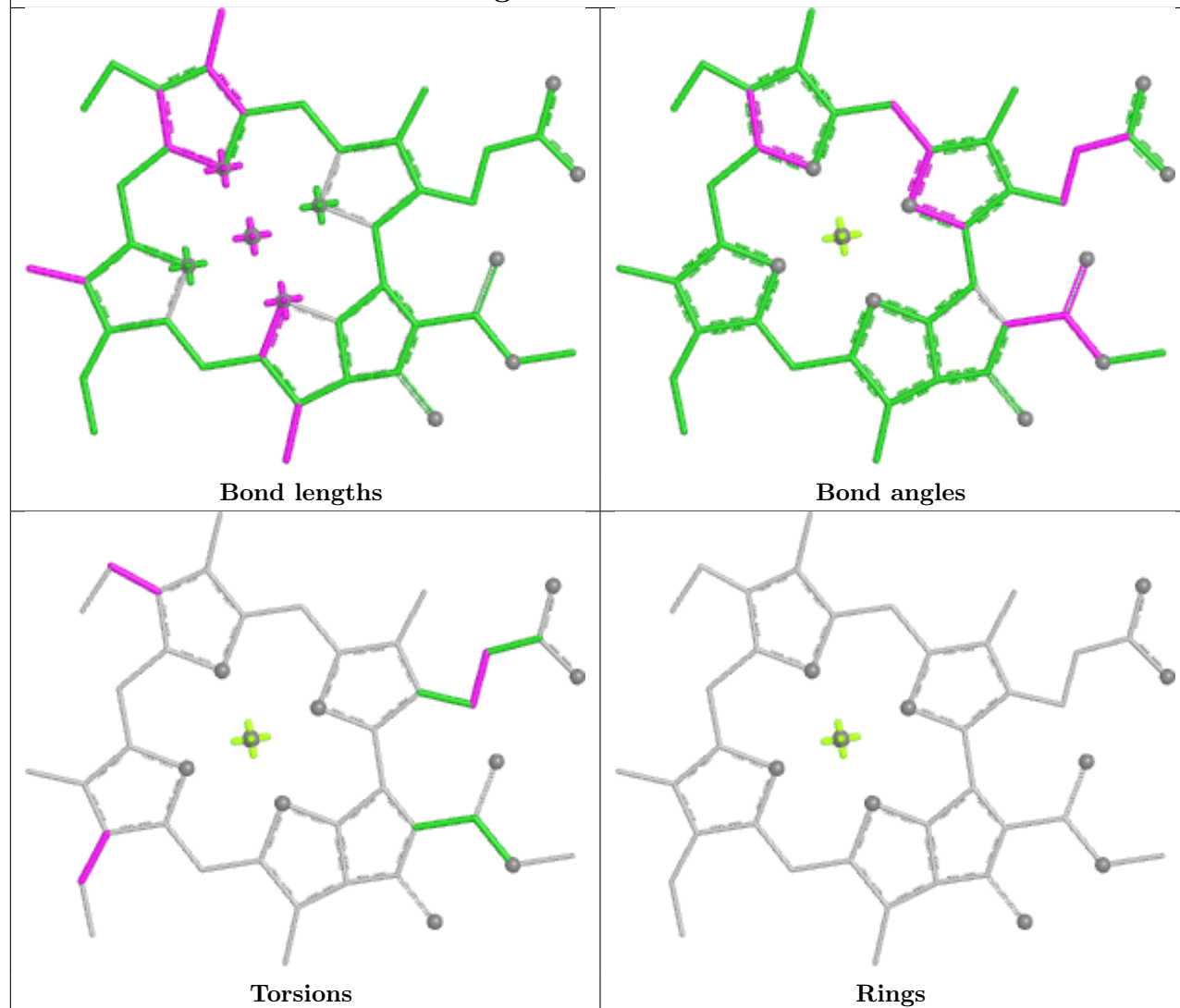


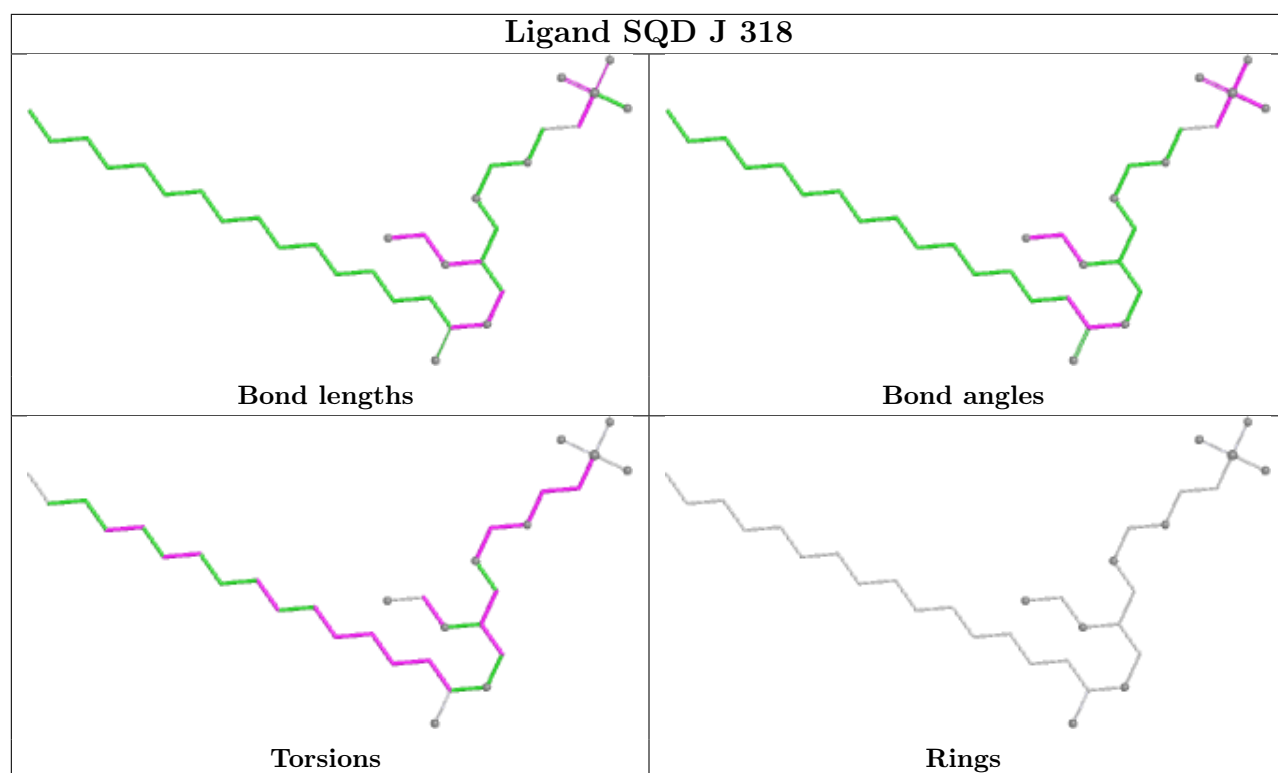


Ligand CLA b 842

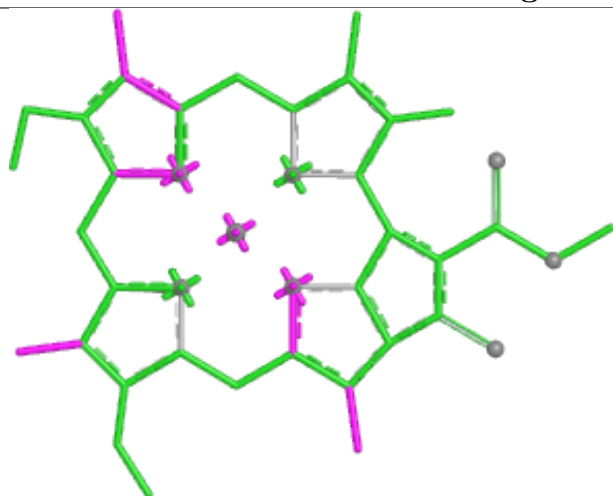


Ligand CLA L 319

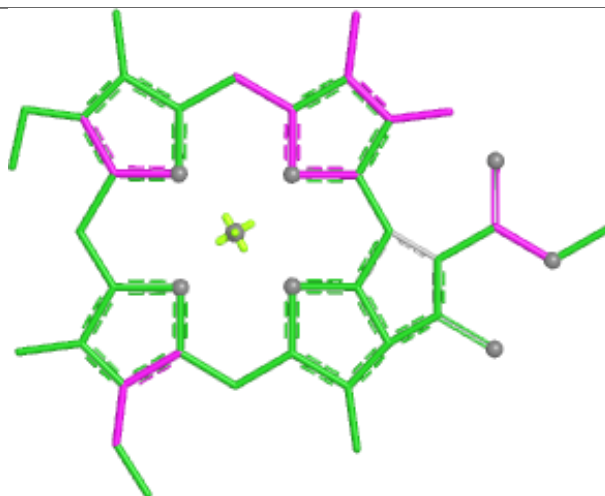




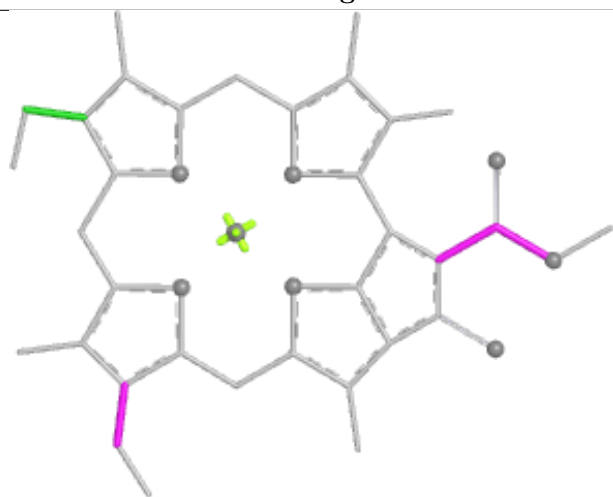
Ligand CLA I 313



Bond lengths



Bond angles

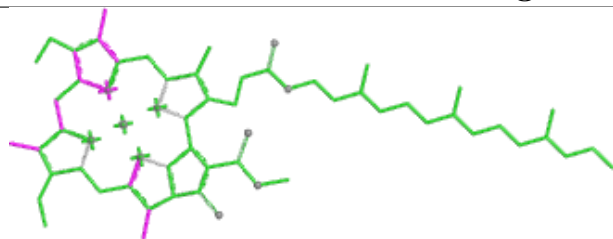


Torsions

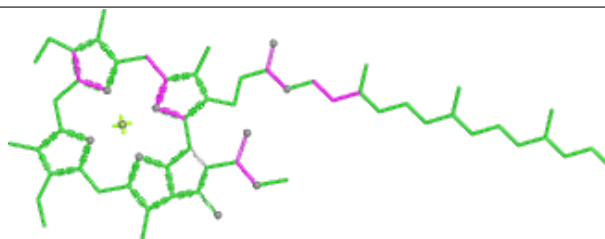


Rings

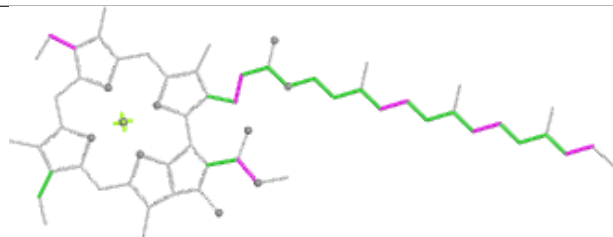
Ligand CLA F 308



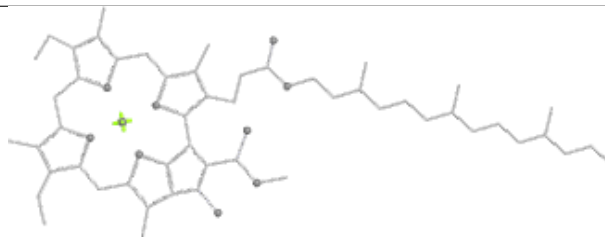
Bond lengths



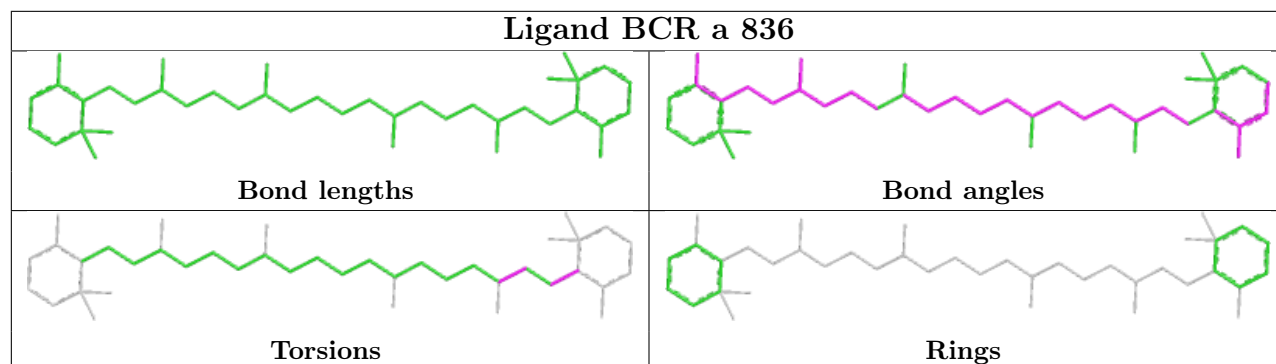
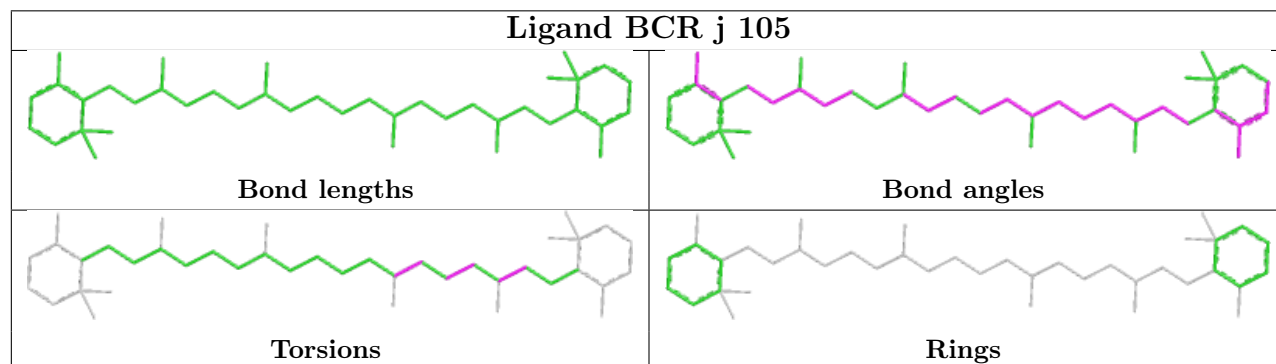
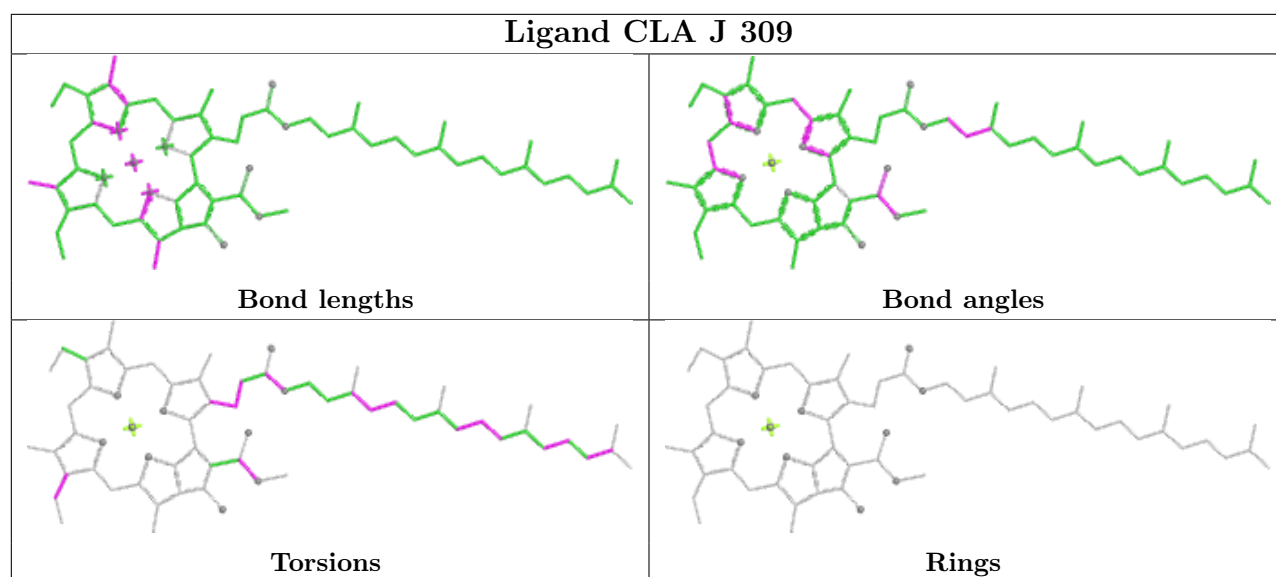
Bond angles



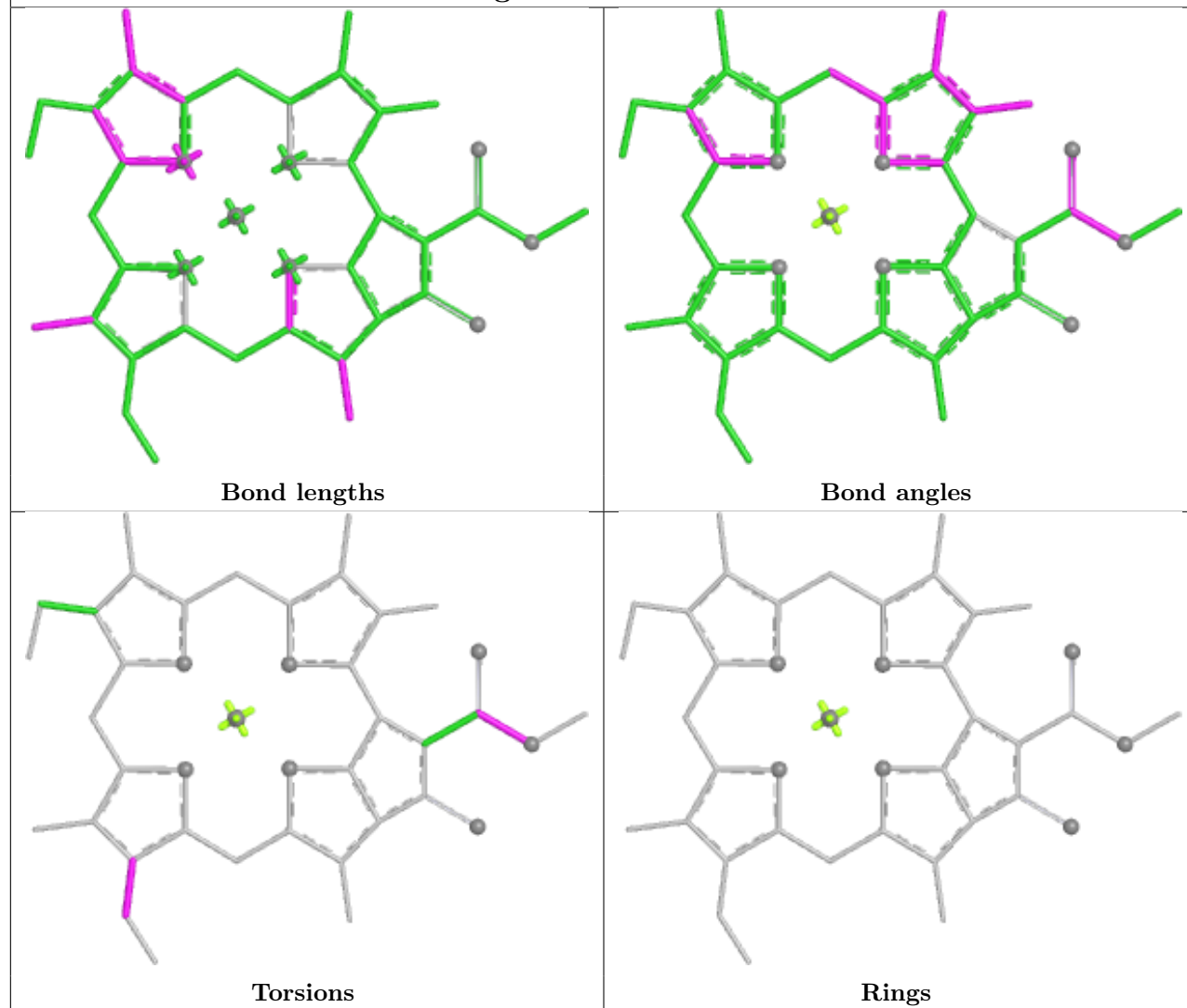
Torsions



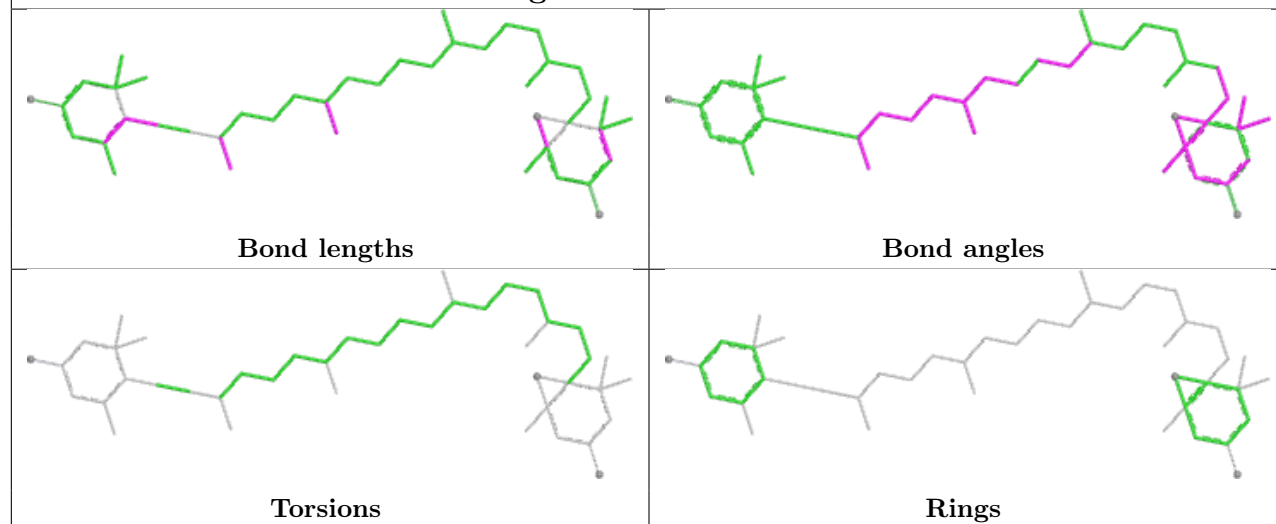
Rings

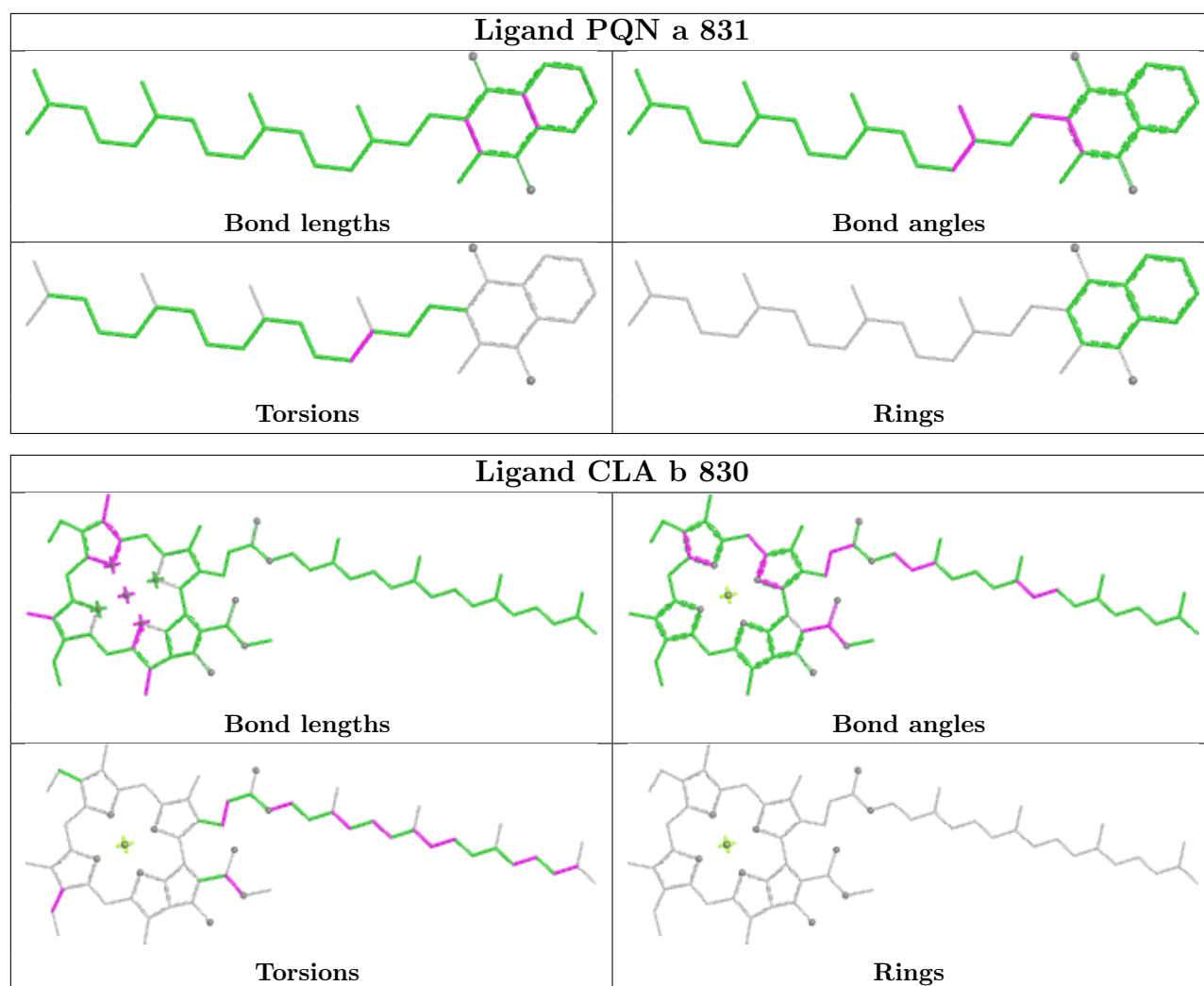


Ligand CLA D 217

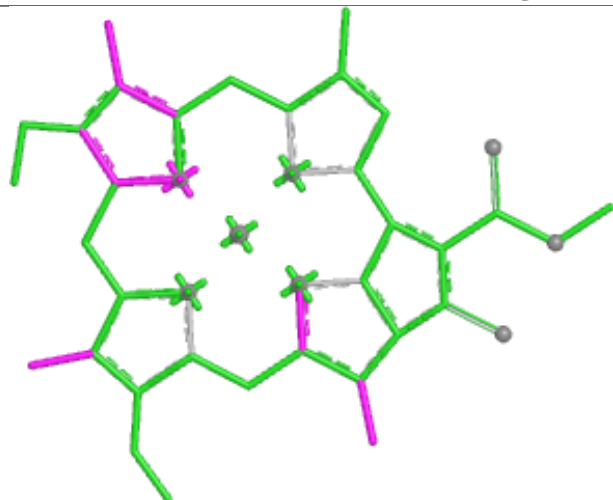


Ligand DD6 M 304

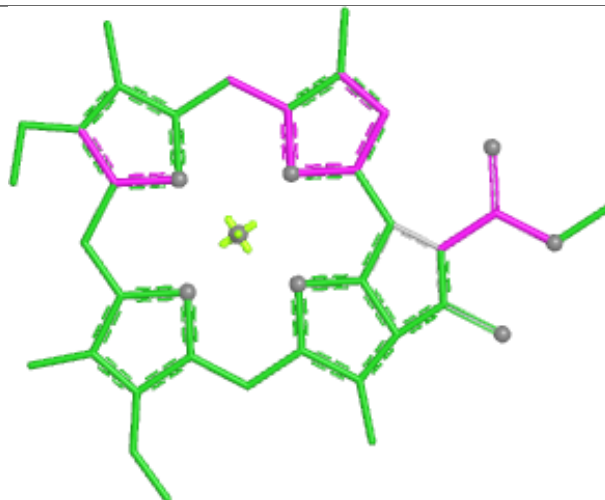




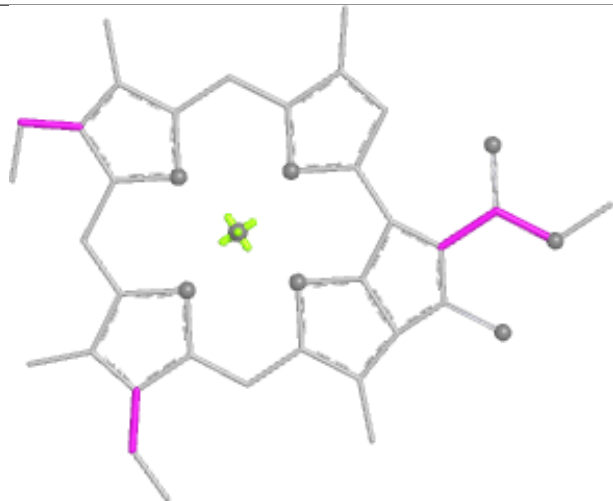
Ligand CLA L 311



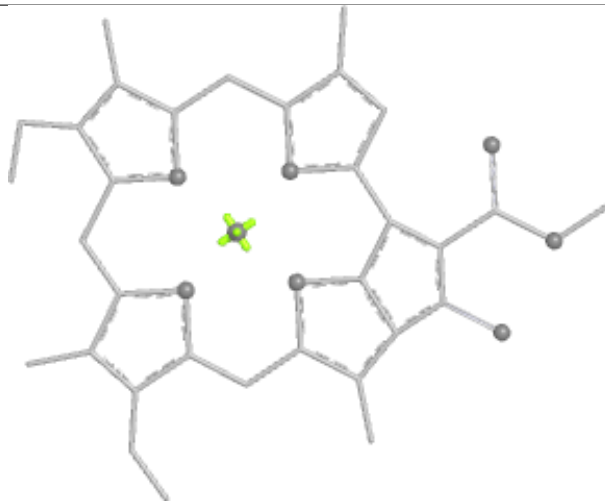
Bond lengths



Bond angles

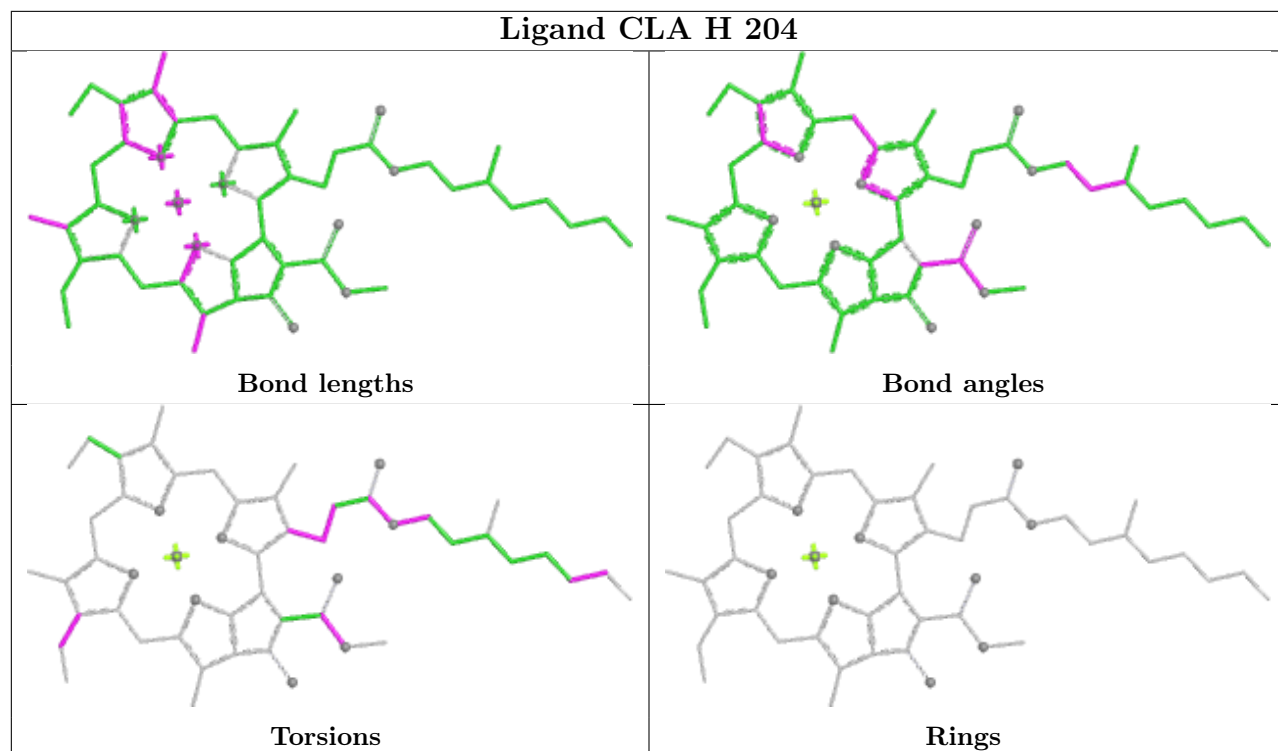


Torsions

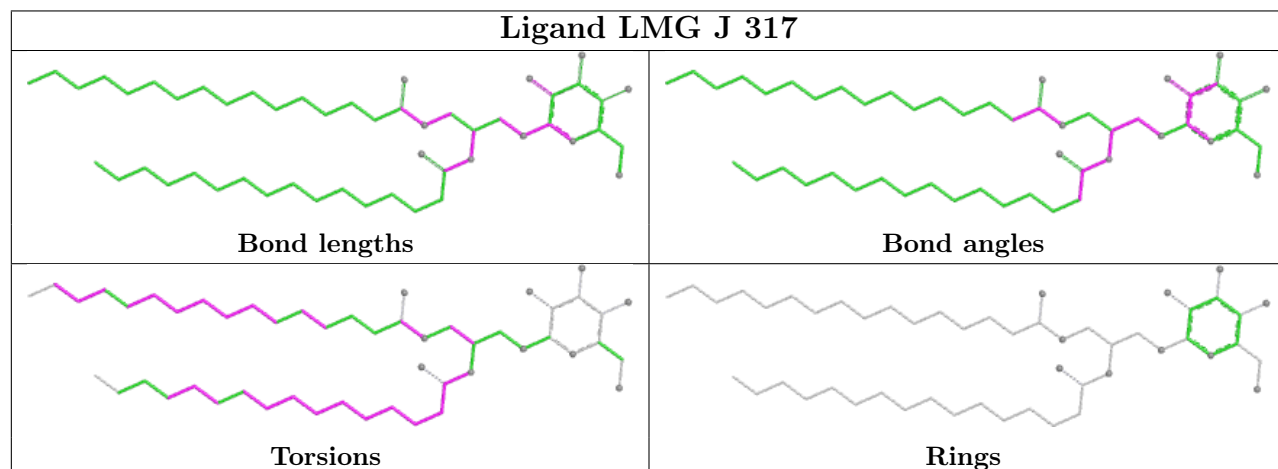


Rings

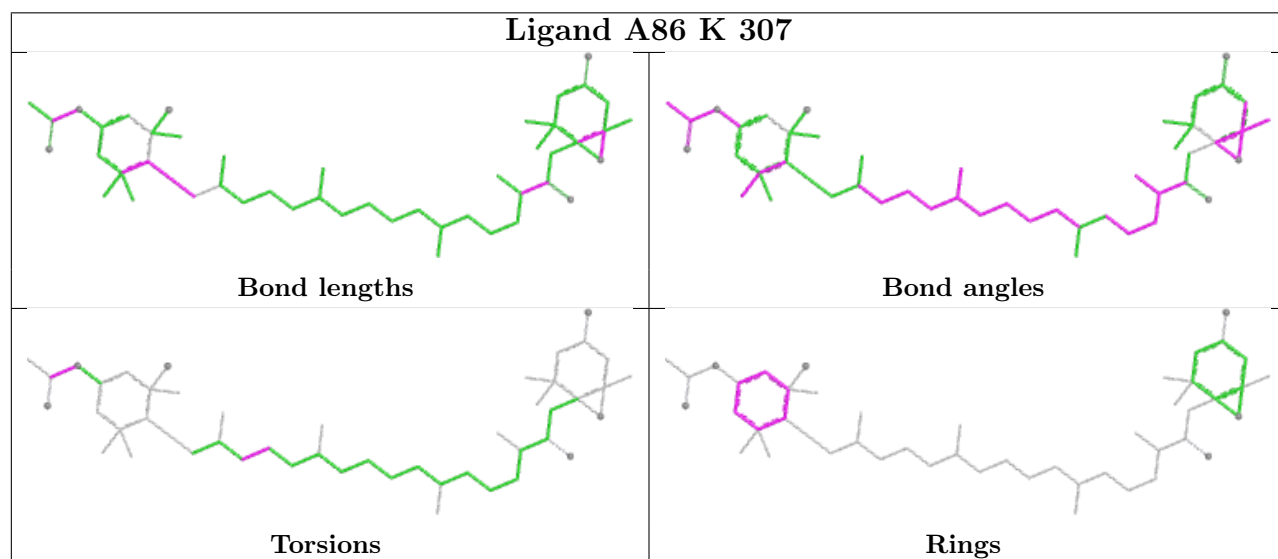
Ligand CLA H 204



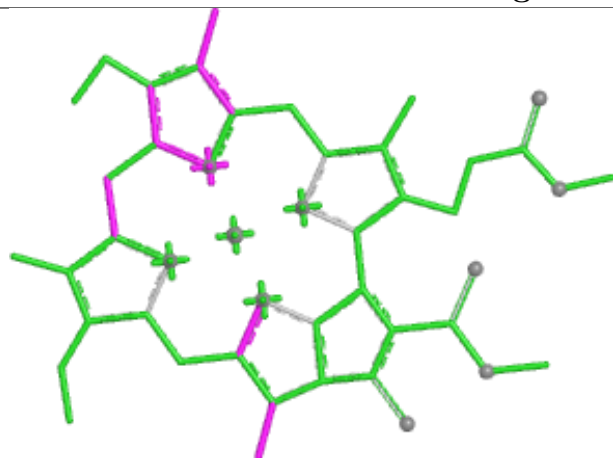
Ligand LMG J 317



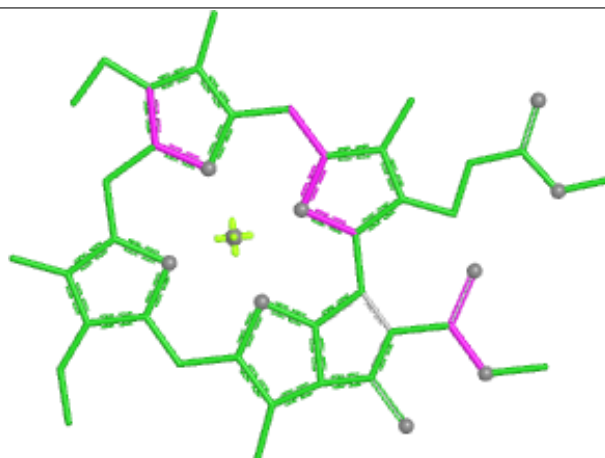
Ligand A86 K 307



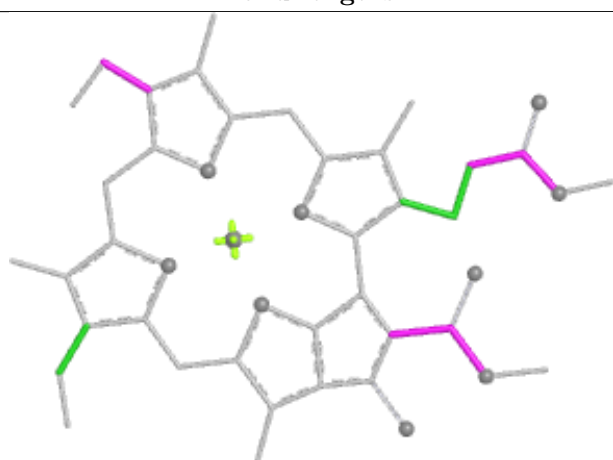
Ligand CLA G 306



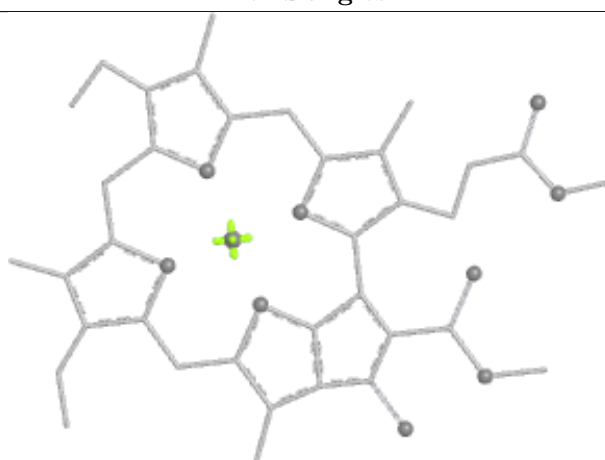
Bond lengths



Bond angles

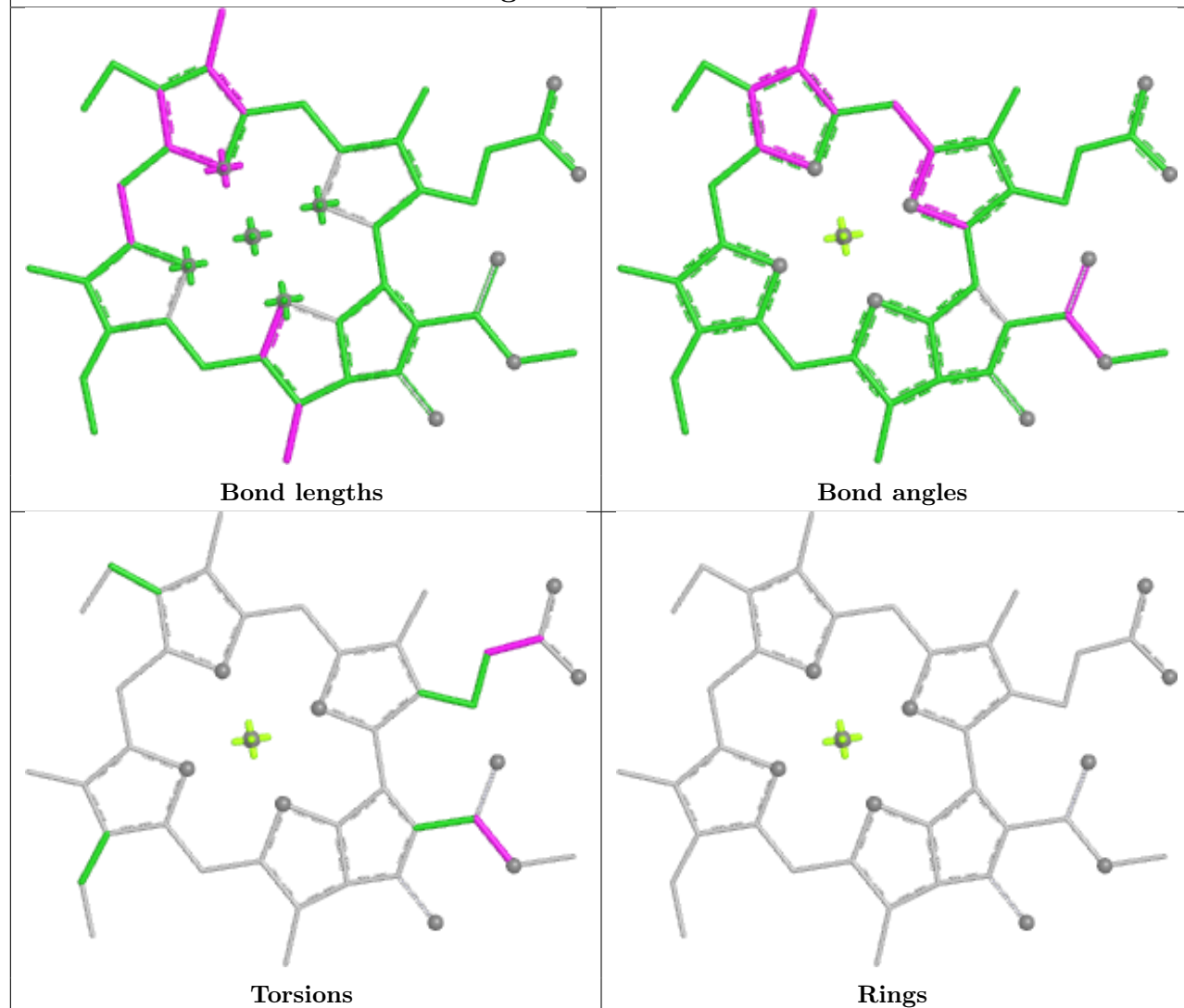


Torsions

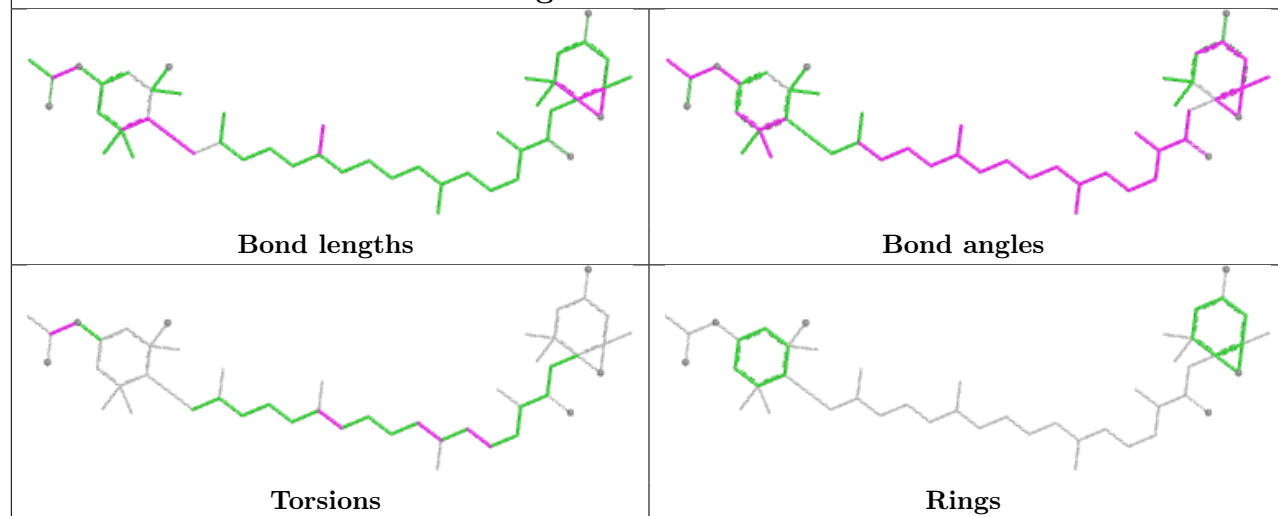


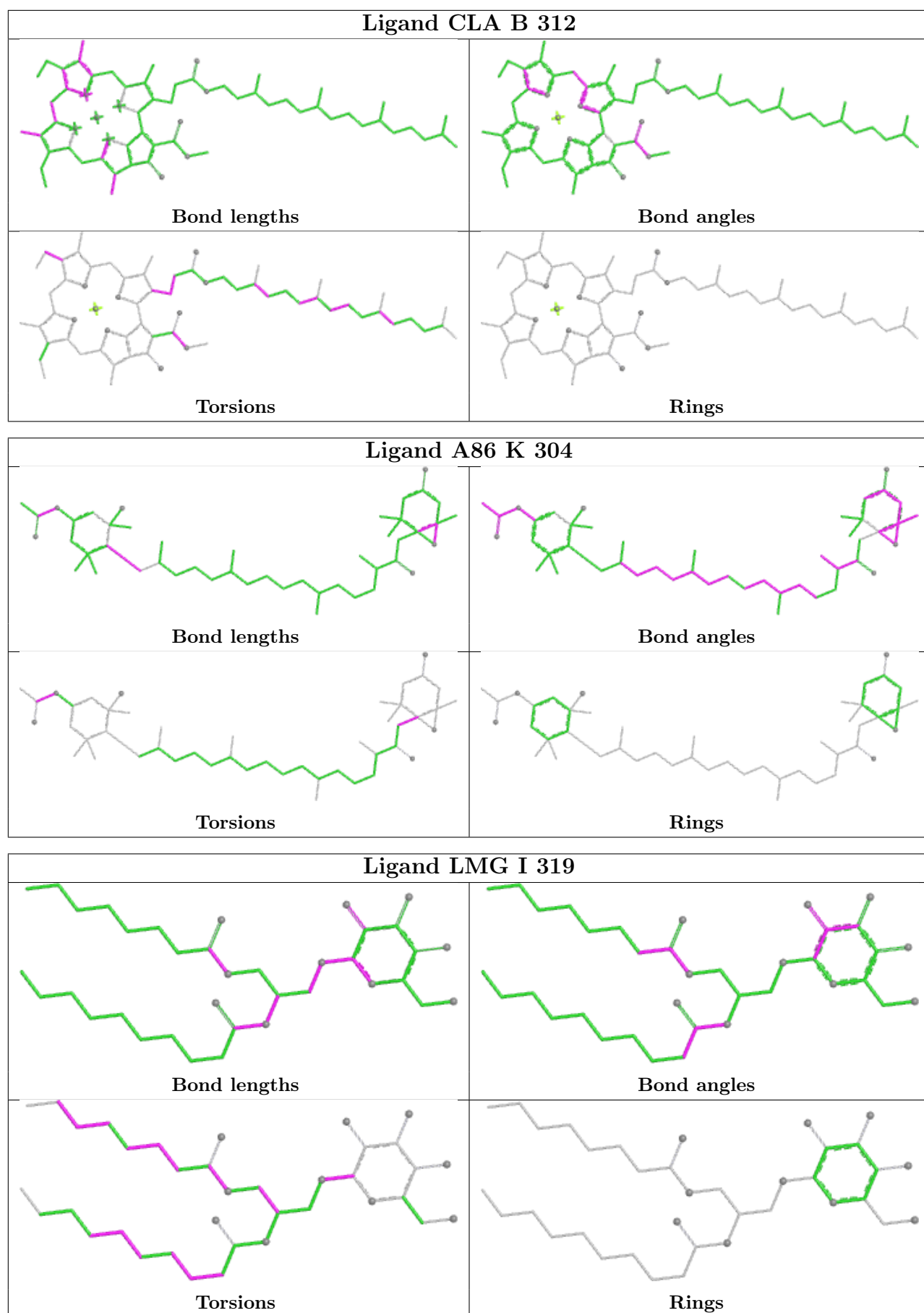
Rings

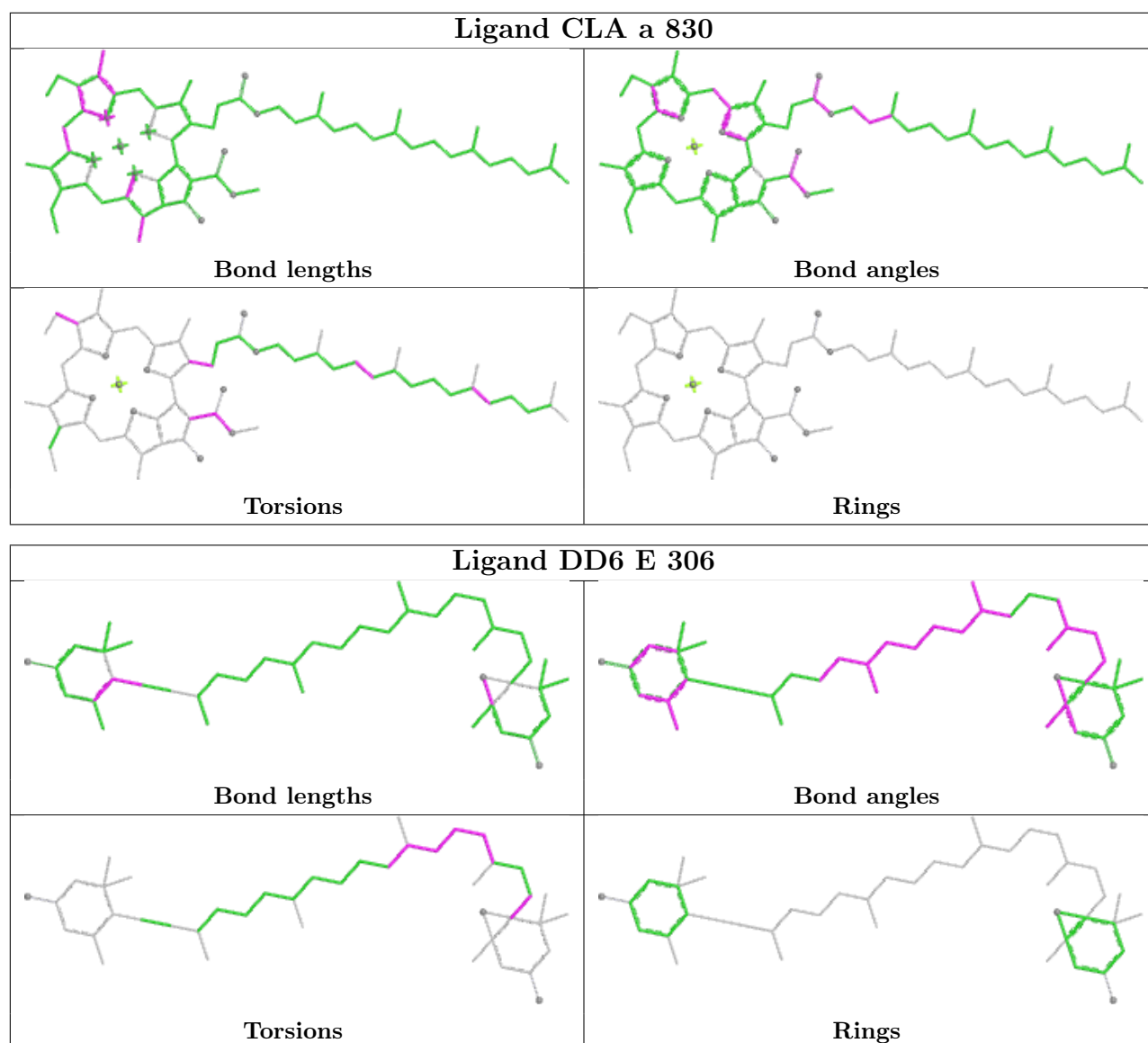
Ligand CLA 1 206



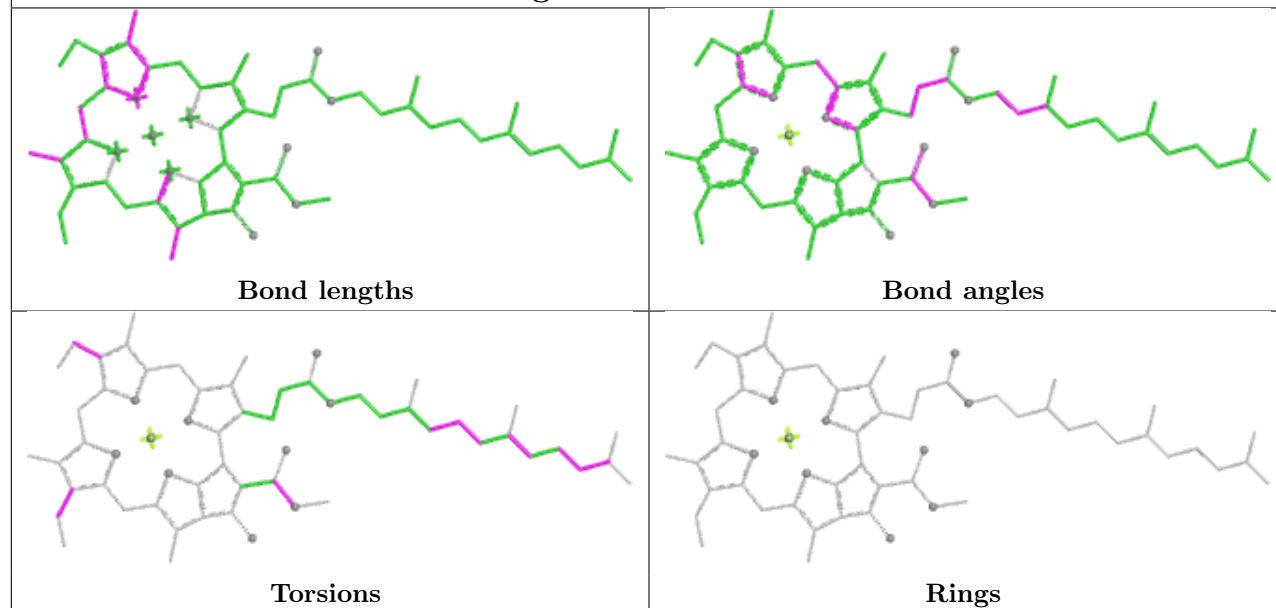
Ligand A86 m 101



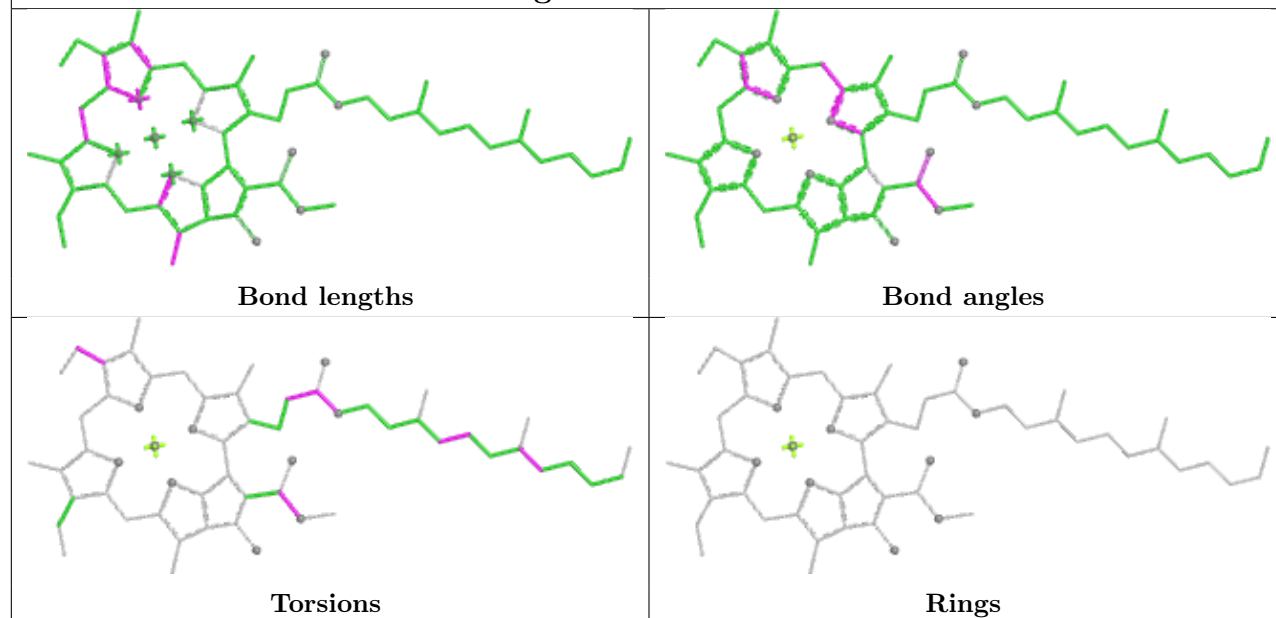




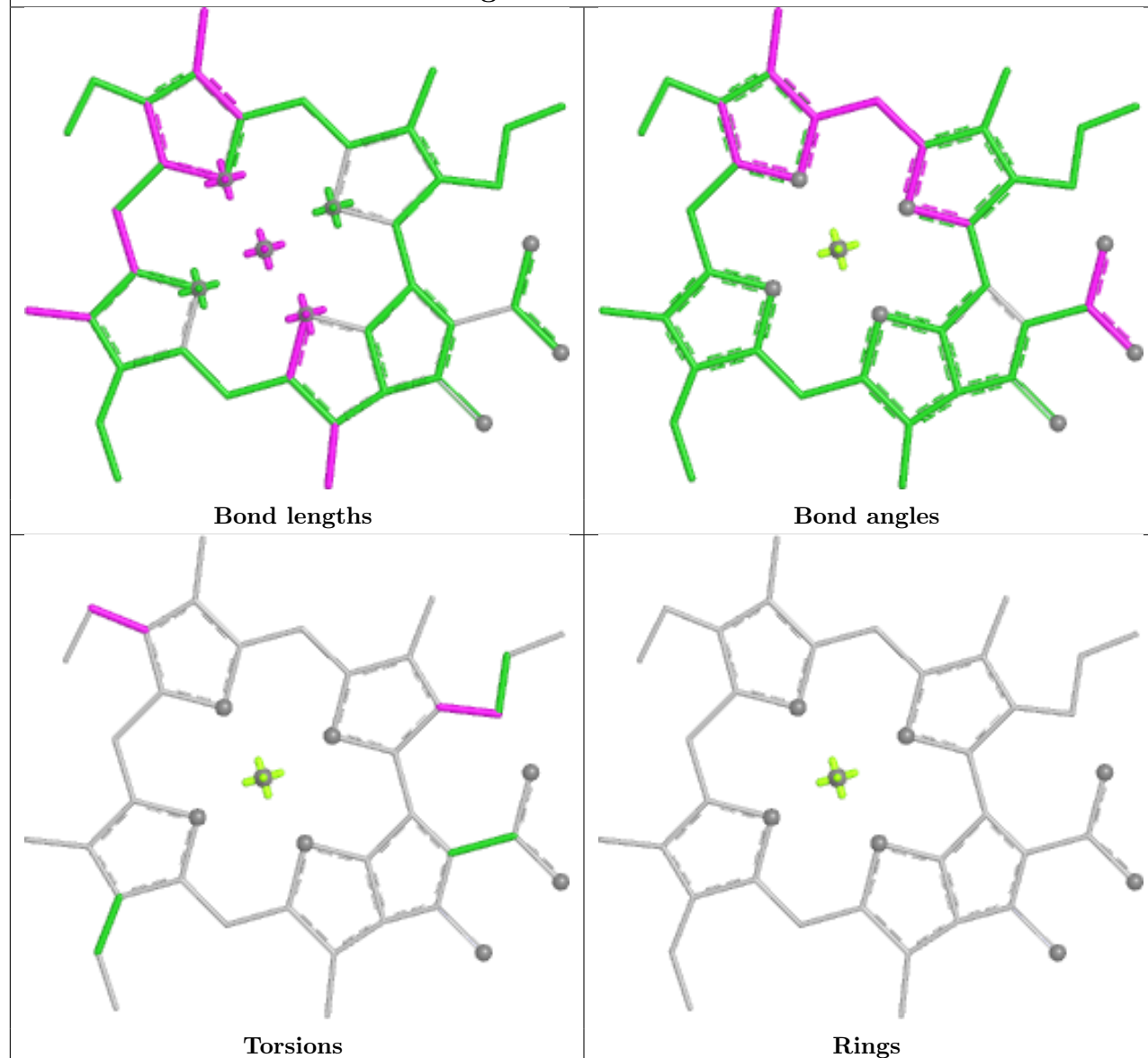
Ligand CLA C 311



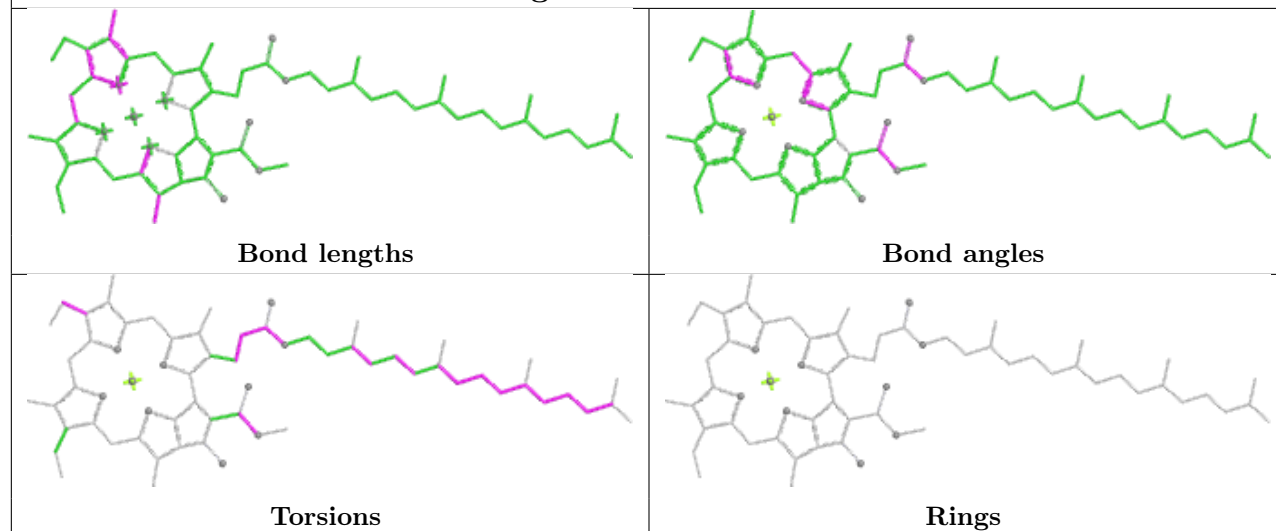
Ligand CLA F 307

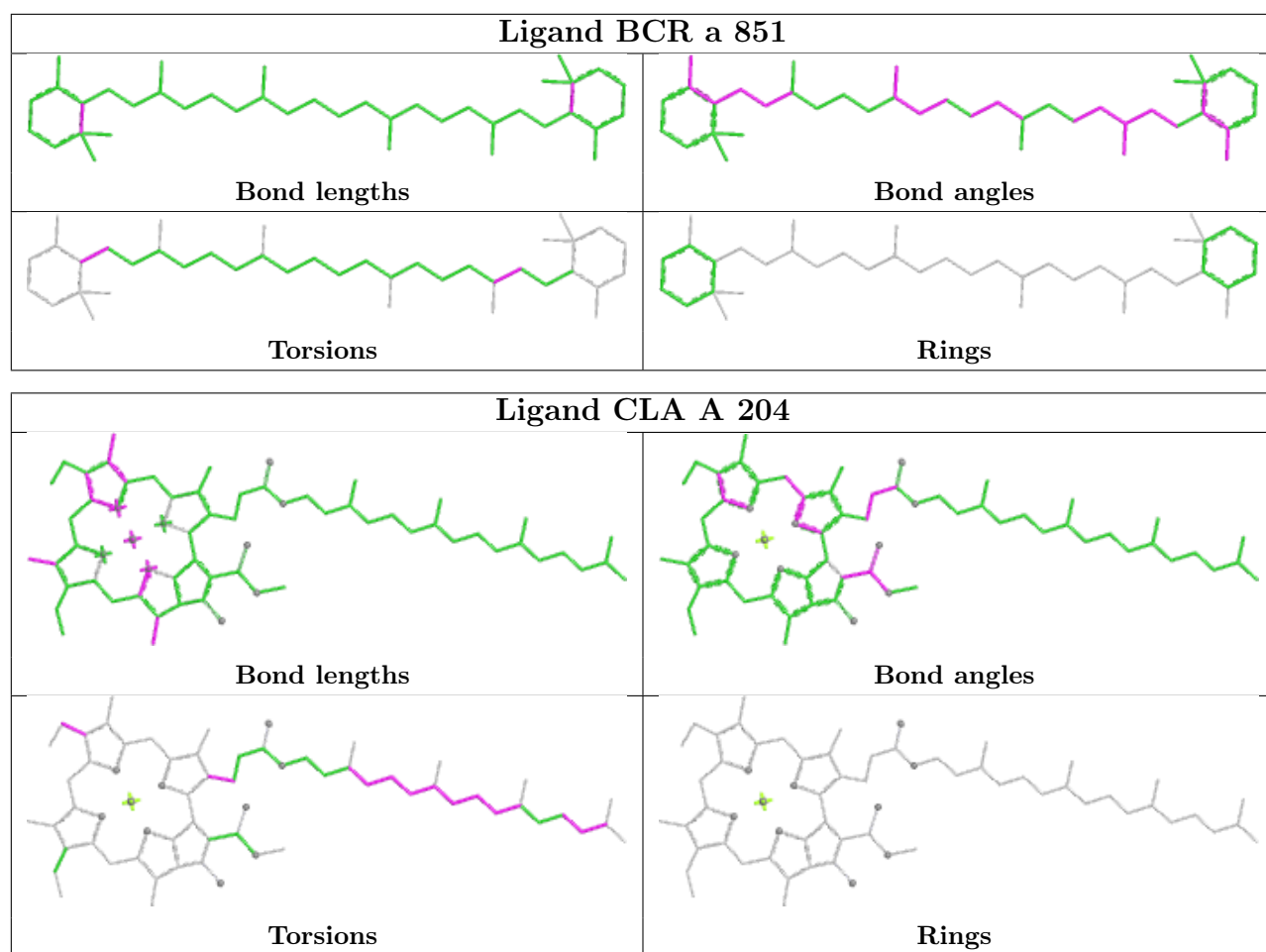


Ligand CLA L 318

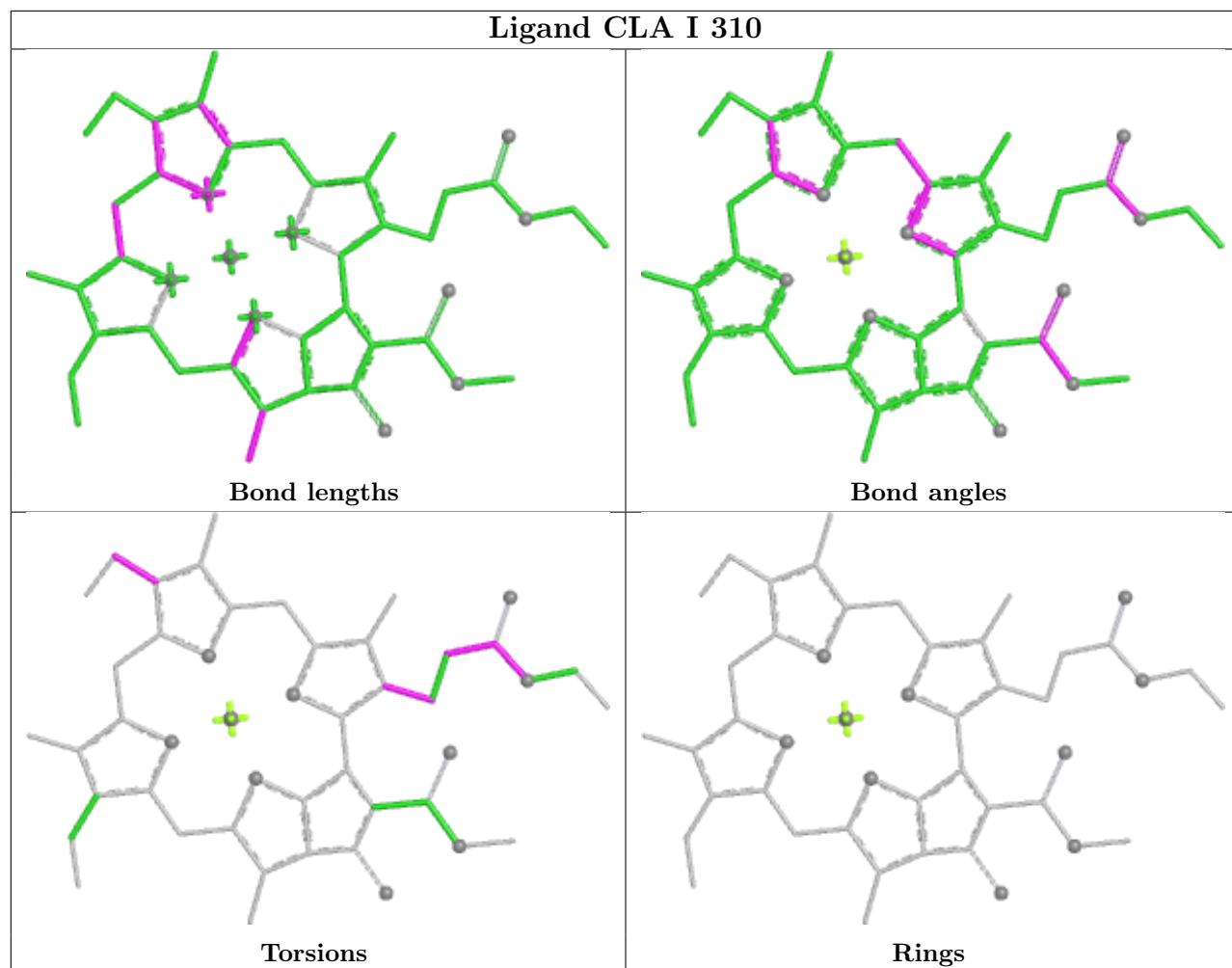


Ligand CLA G 309

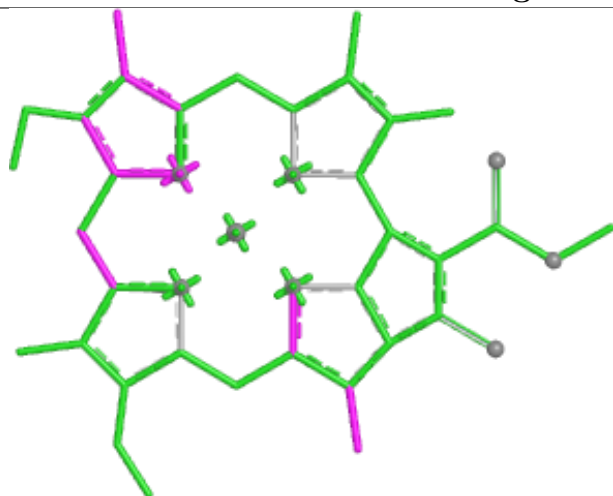




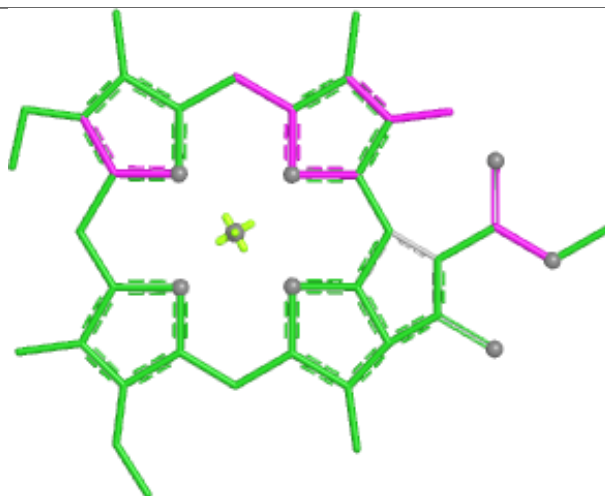
Ligand CLA I 310



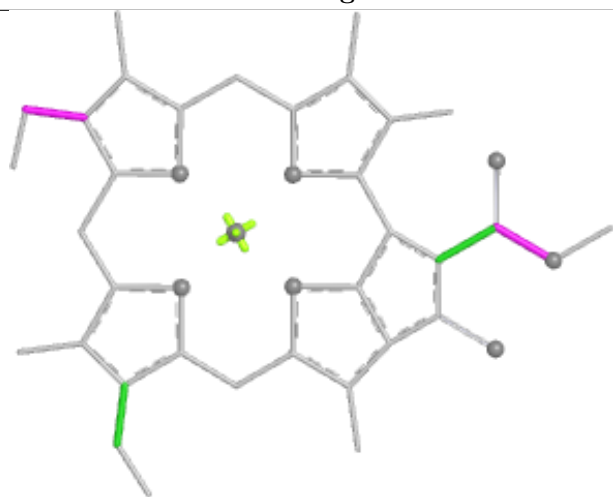
Ligand CLA G 314



Bond lengths



Bond angles

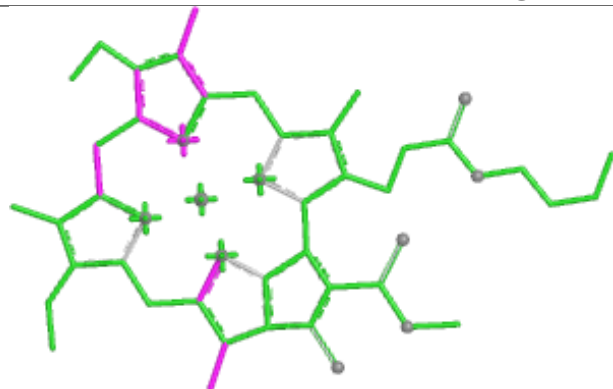


Torsions

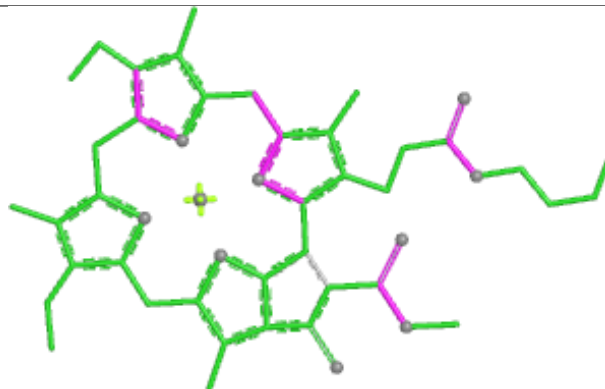


Rings

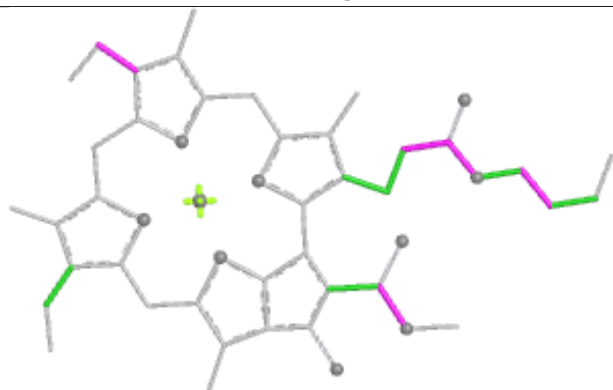
Ligand CLA G 317



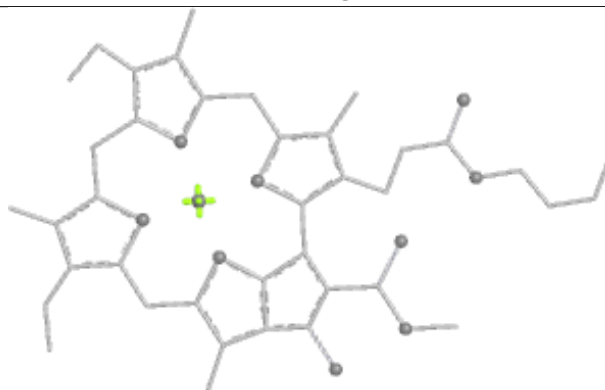
Bond lengths



Bond angles

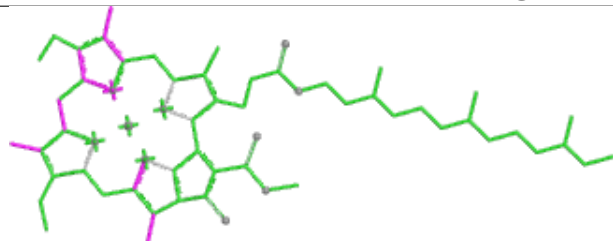


Torsions

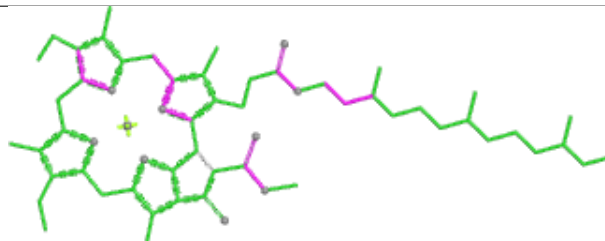


Rings

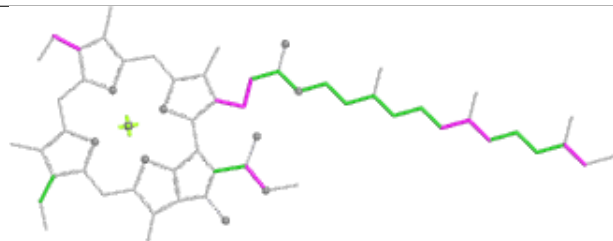
Ligand CLA G 312



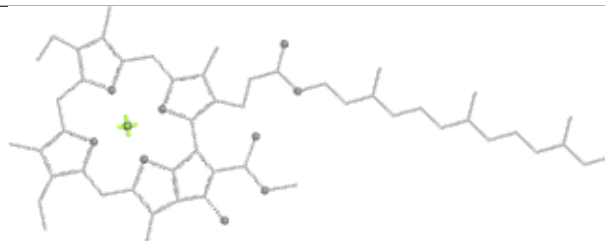
Bond lengths



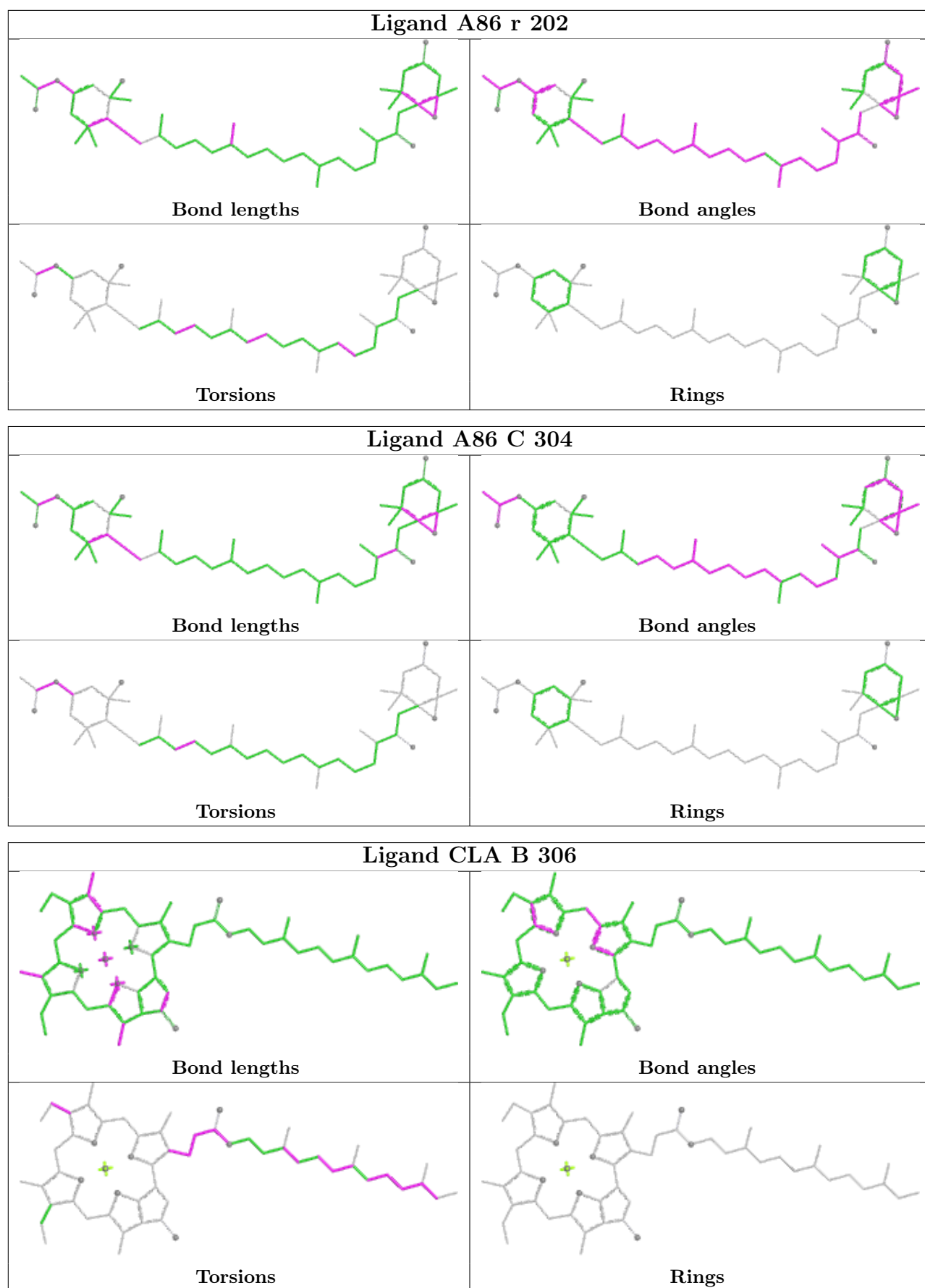
Bond angles

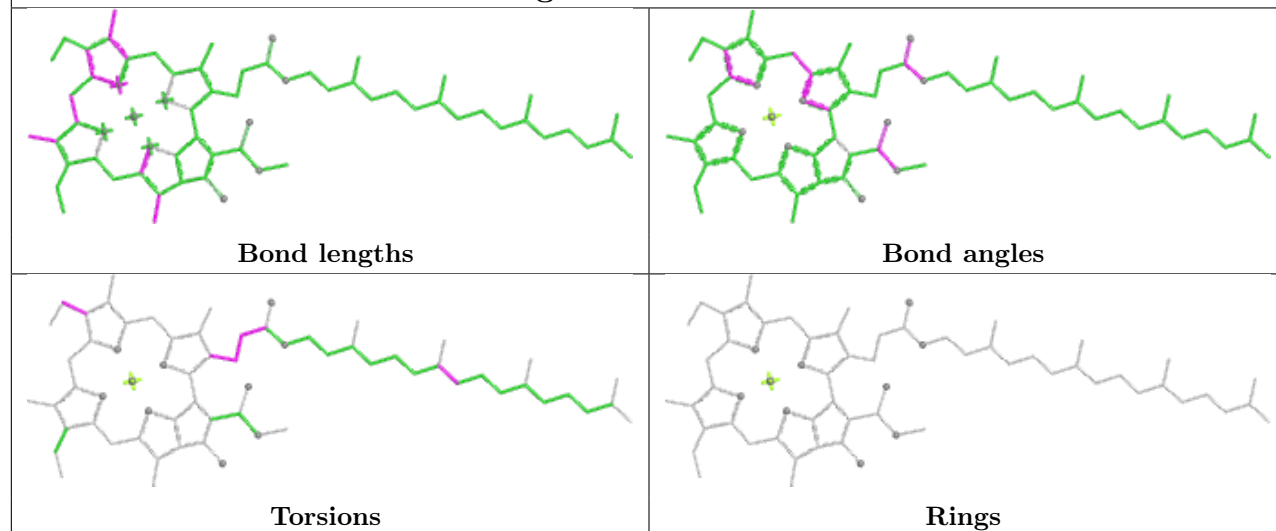
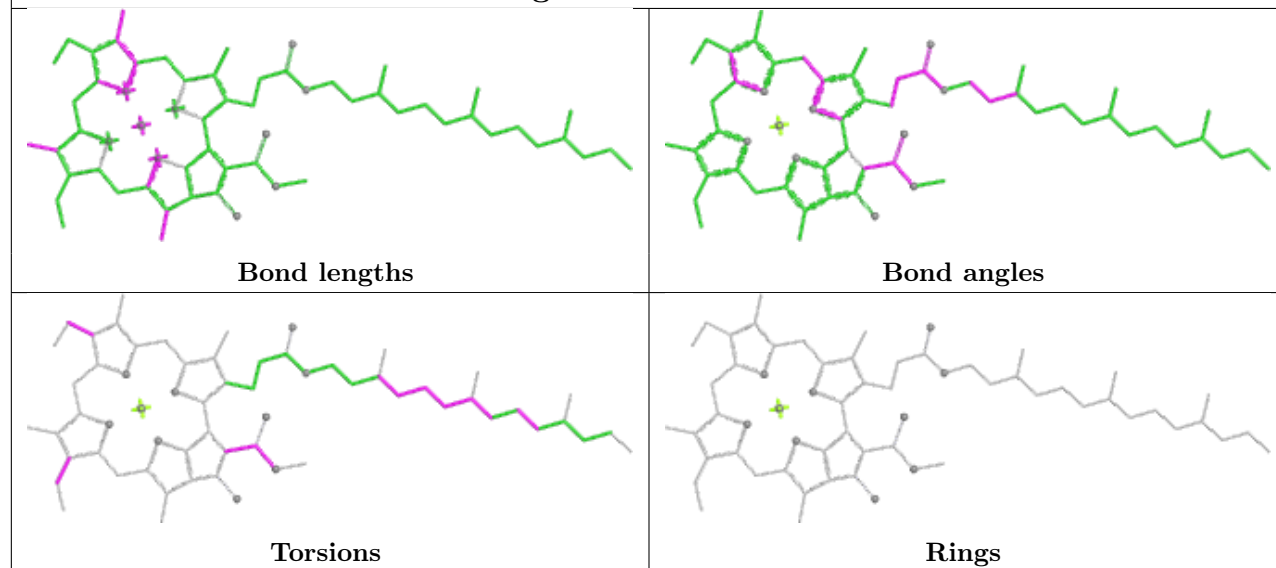


Torsions

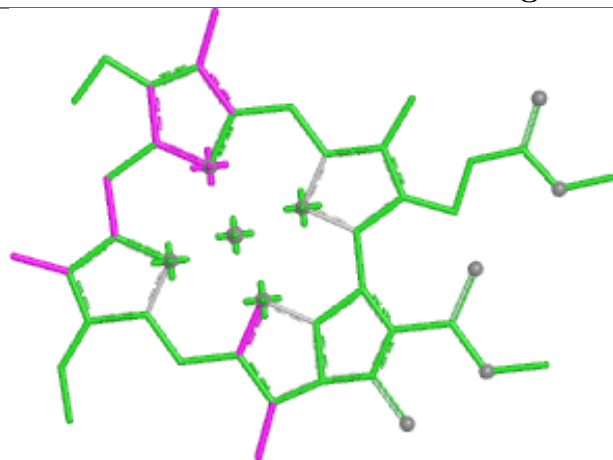


Rings

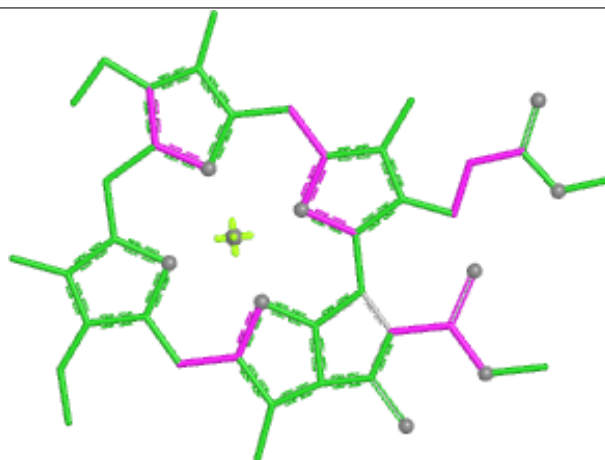


Ligand CLA a 816**Ligand CLA C 309**

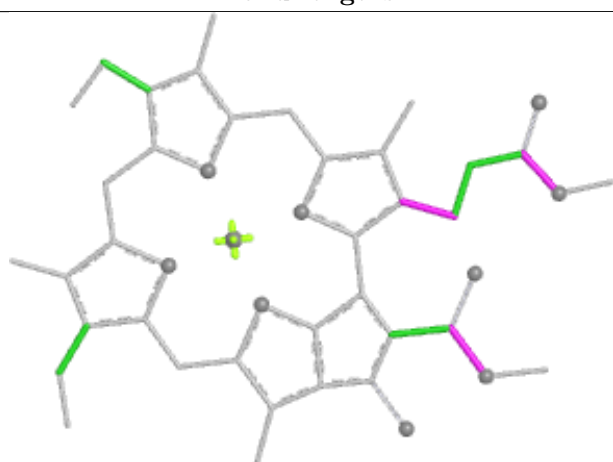
Ligand CLA I 309



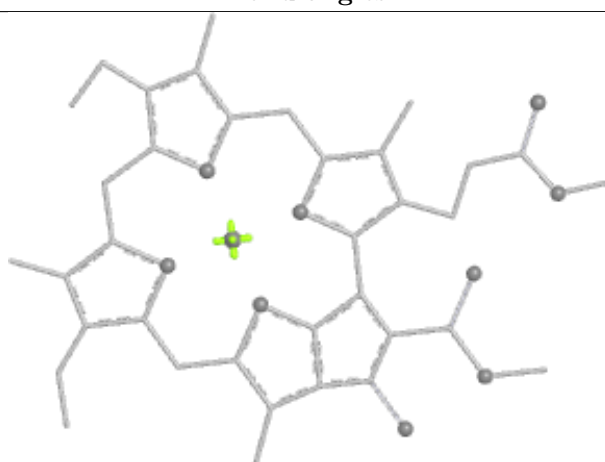
Bond lengths



Bond angles

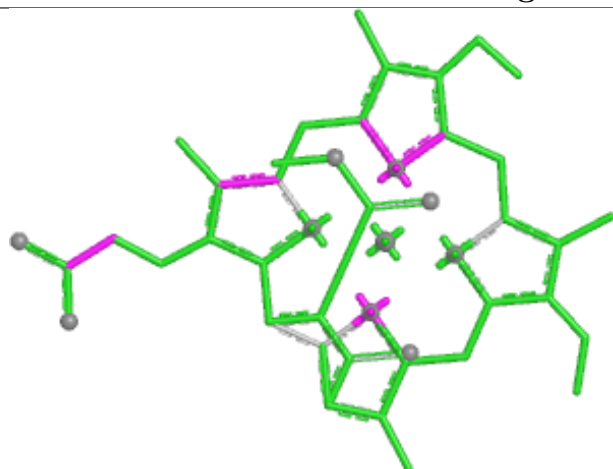


Torsions

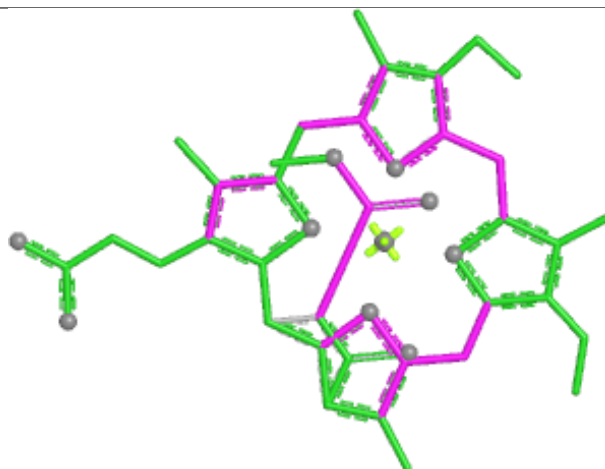


Rings

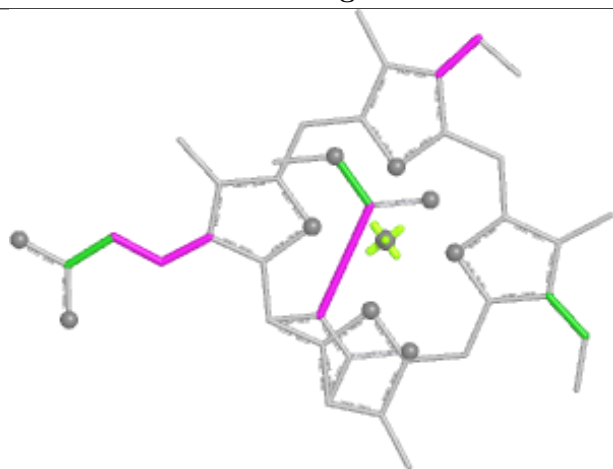
Ligand KC1 F 312



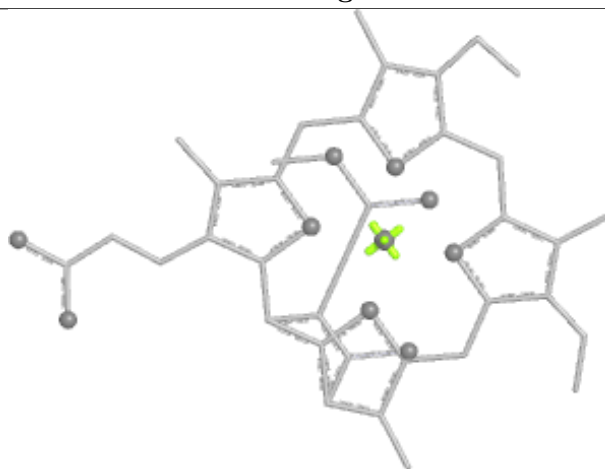
Bond lengths



Bond angles

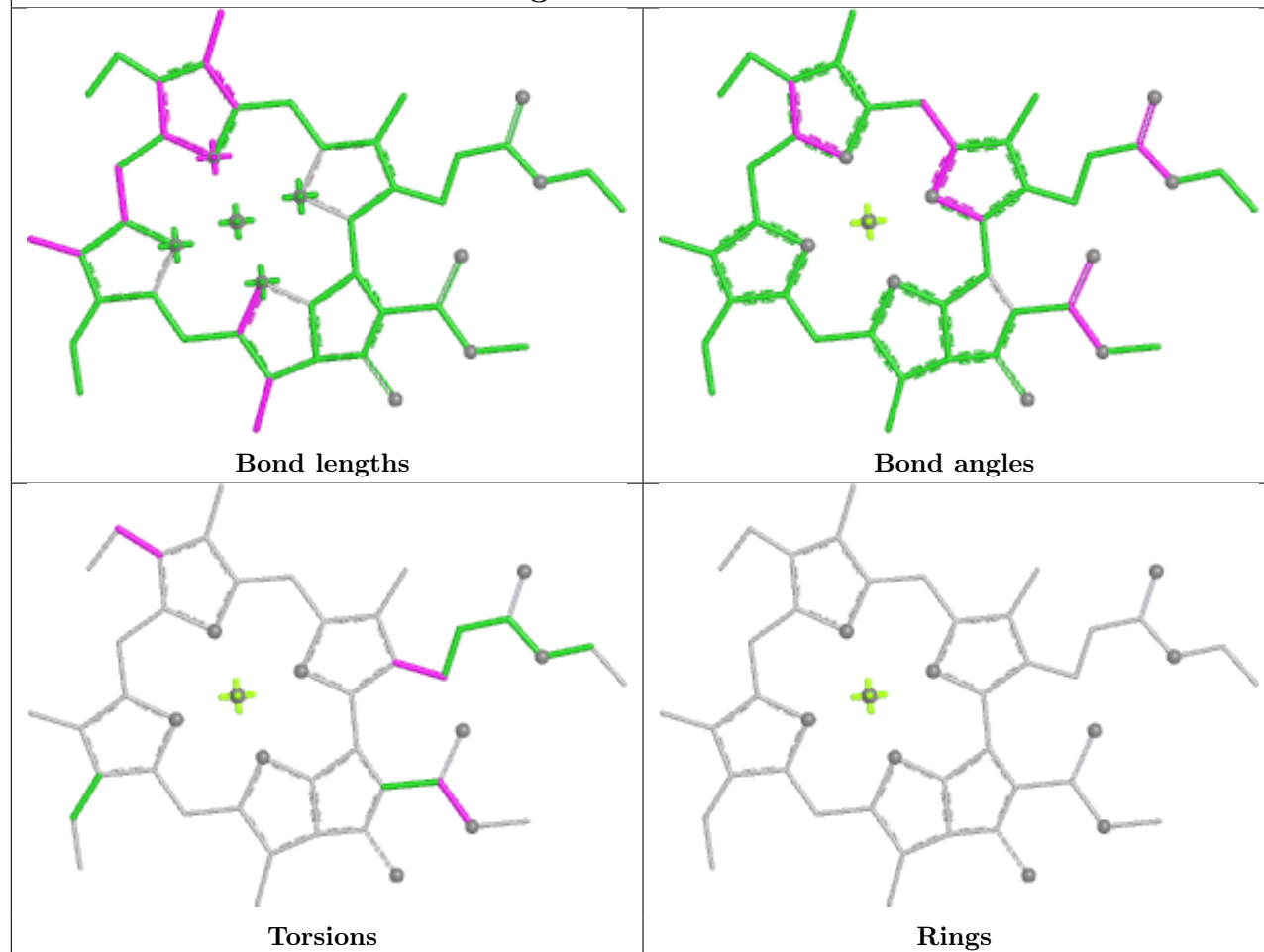


Torsions

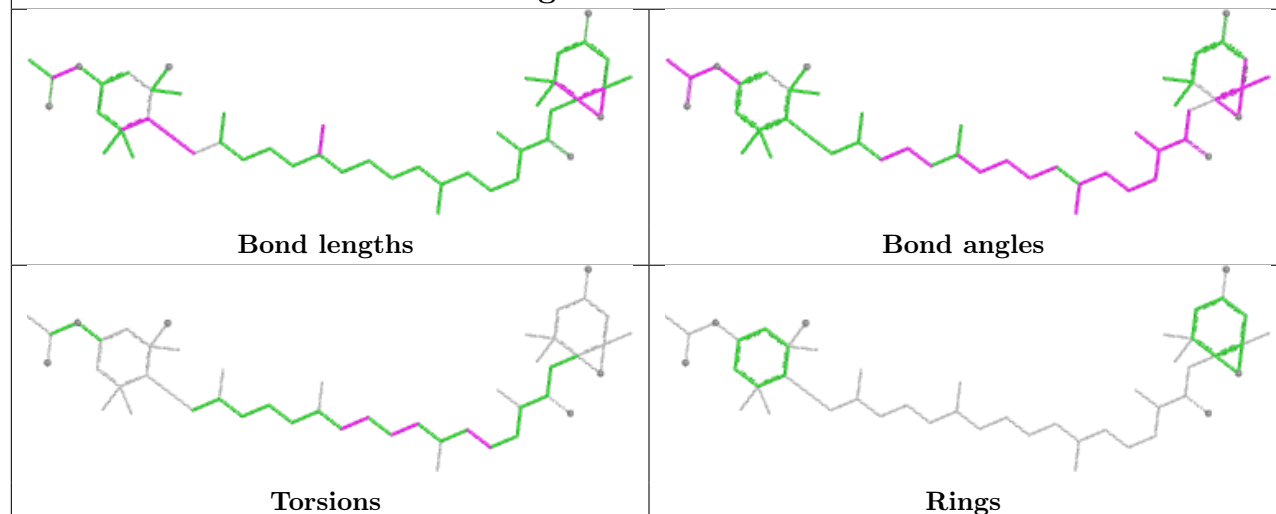


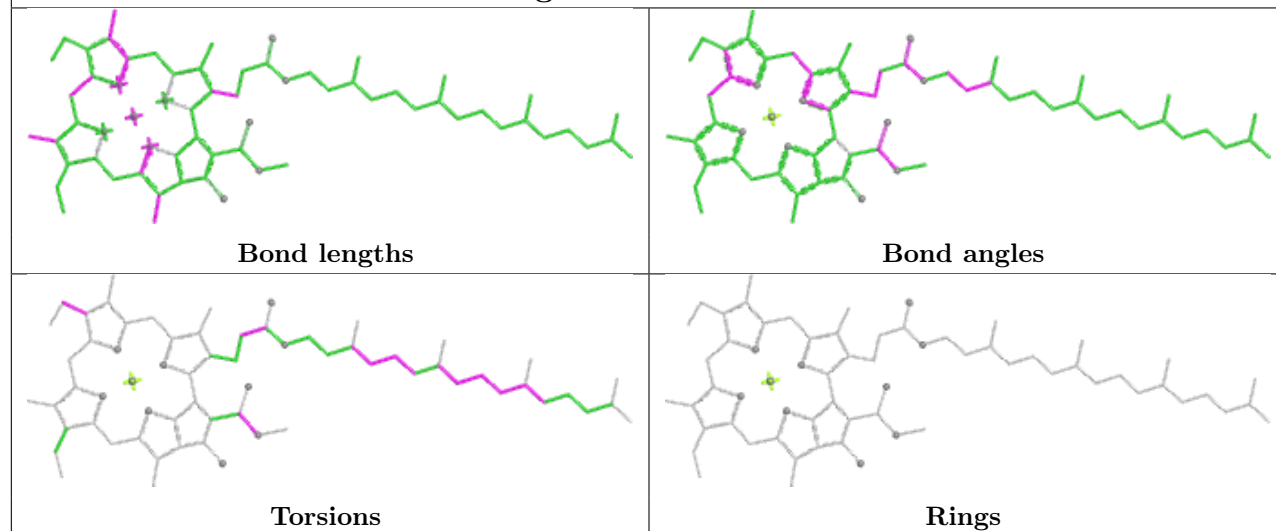
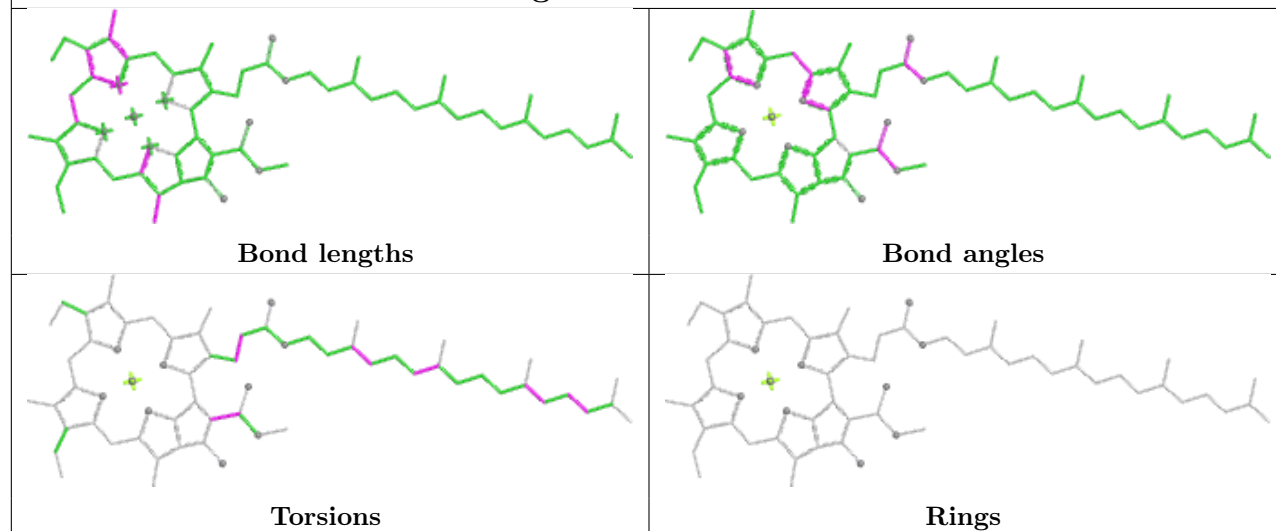
Rings

Ligand CLA b 828

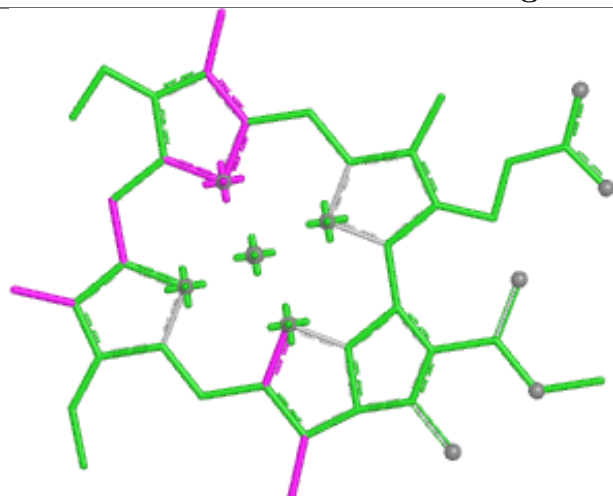


Ligand A86 B 304

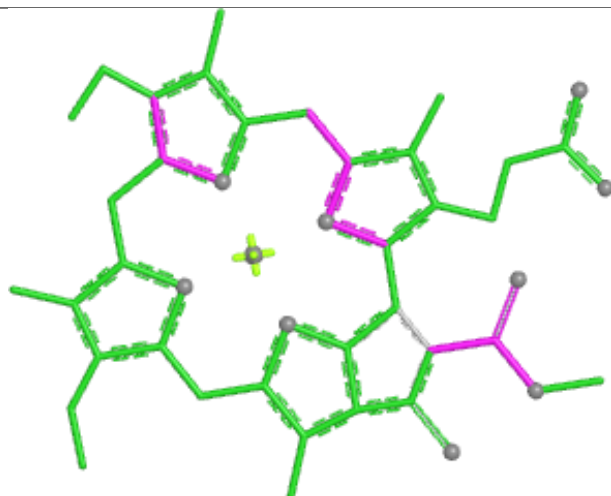


Ligand CLA b 804**Ligand CLA B 309**

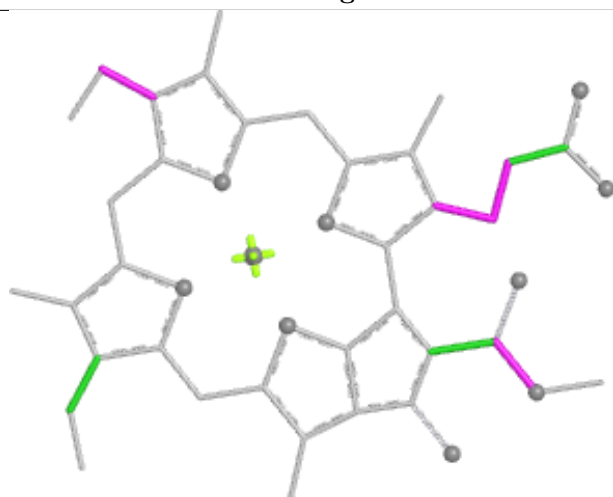
Ligand CLA I 305



Bond lengths



Bond angles

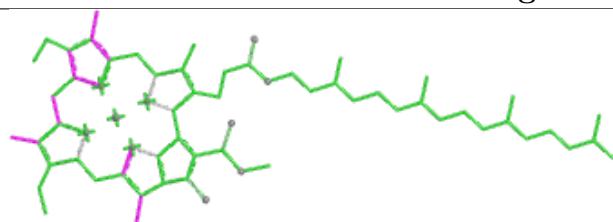


Torsions

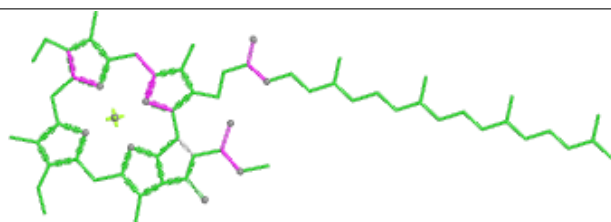


Rings

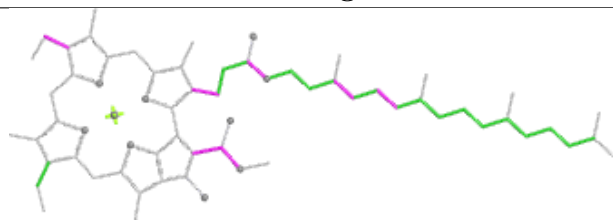
Ligand CLA a 823



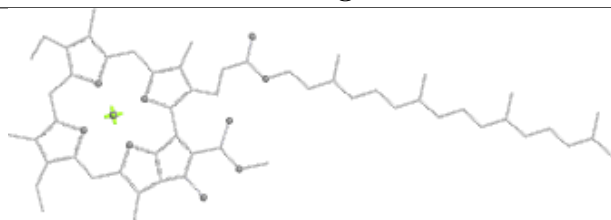
Bond lengths



Bond angles

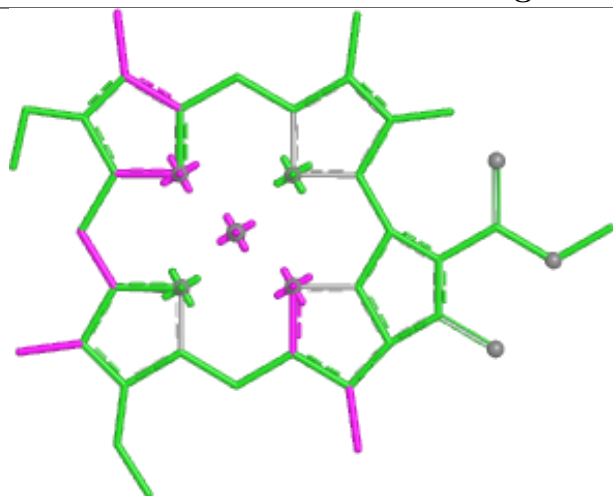


Torsions

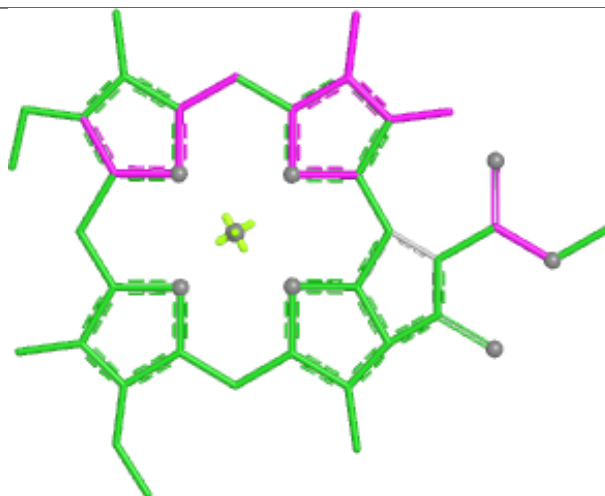


Rings

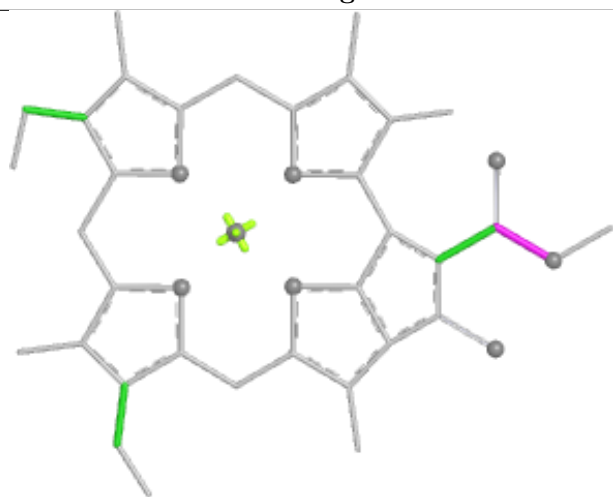
Ligand CLA B 314



Bond lengths



Bond angles

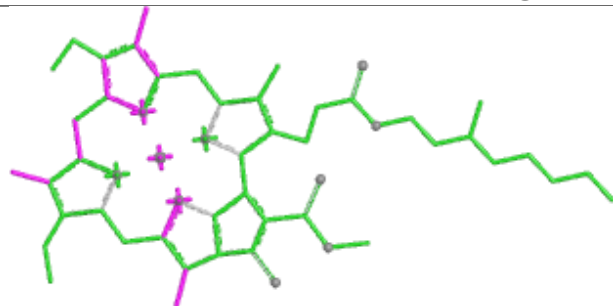


Torsions

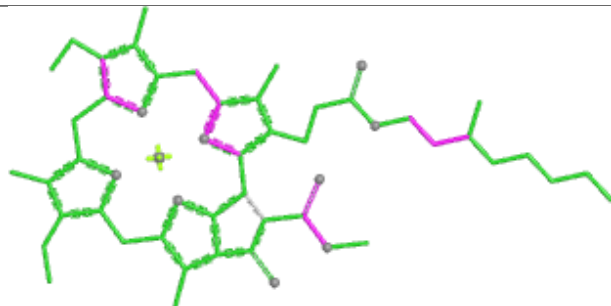


Rings

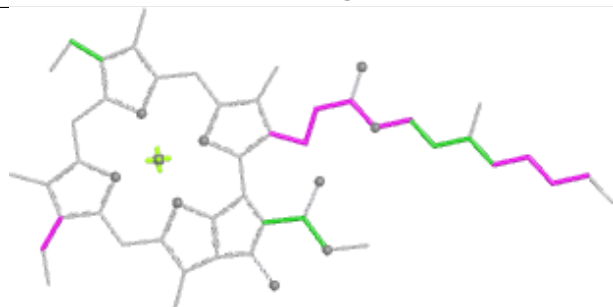
Ligand CLA L 307



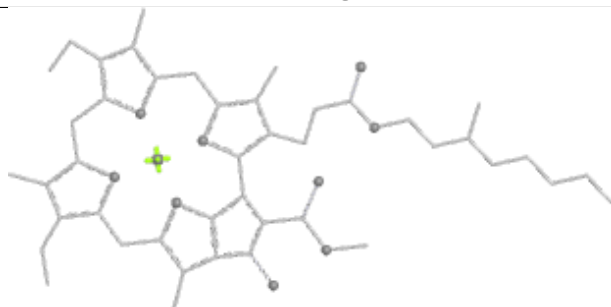
Bond lengths



Bond angles

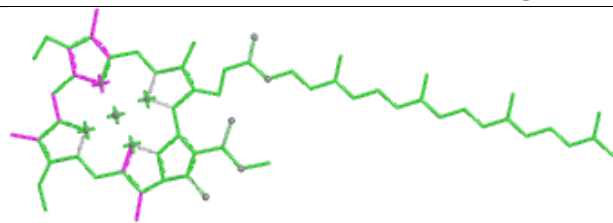


Torsions

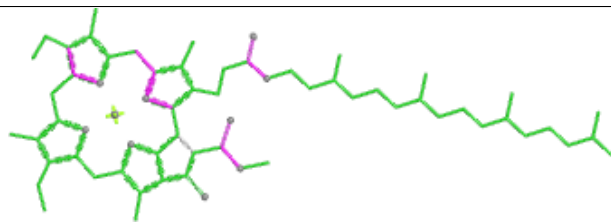


Rings

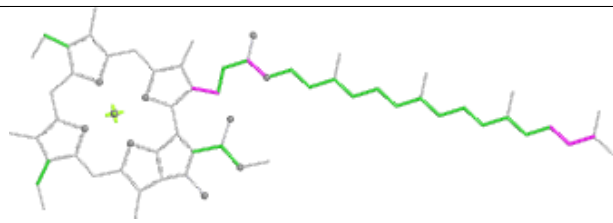
Ligand CLA b 811



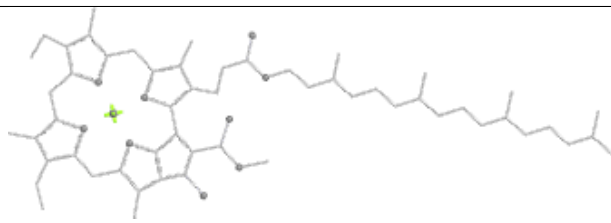
Bond lengths



Bond angles

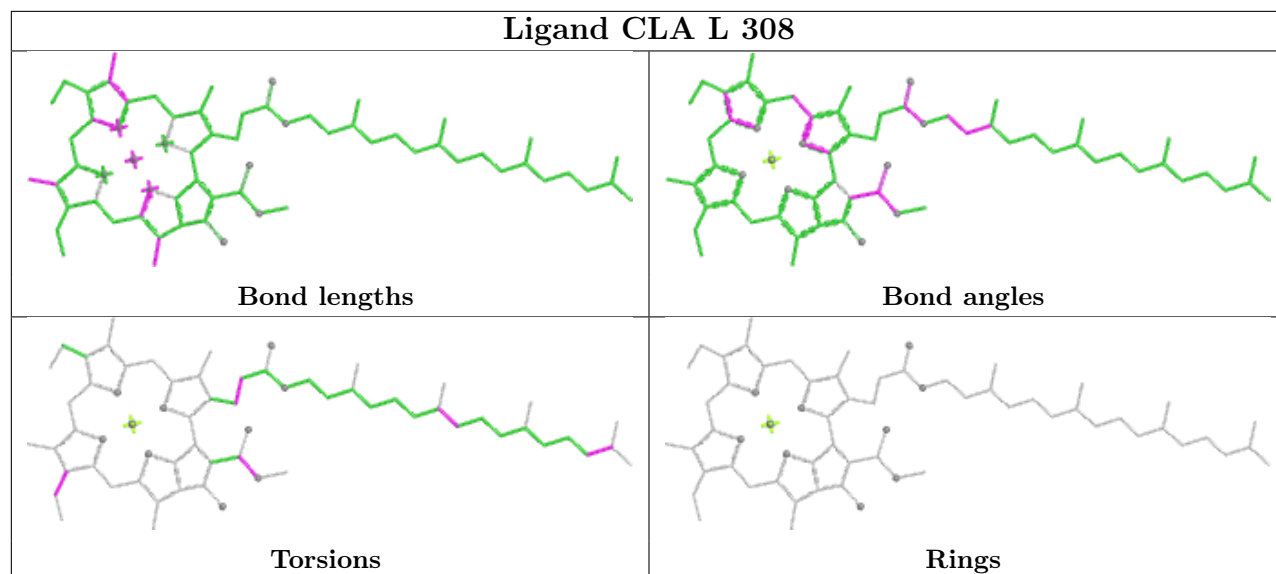


Torsions

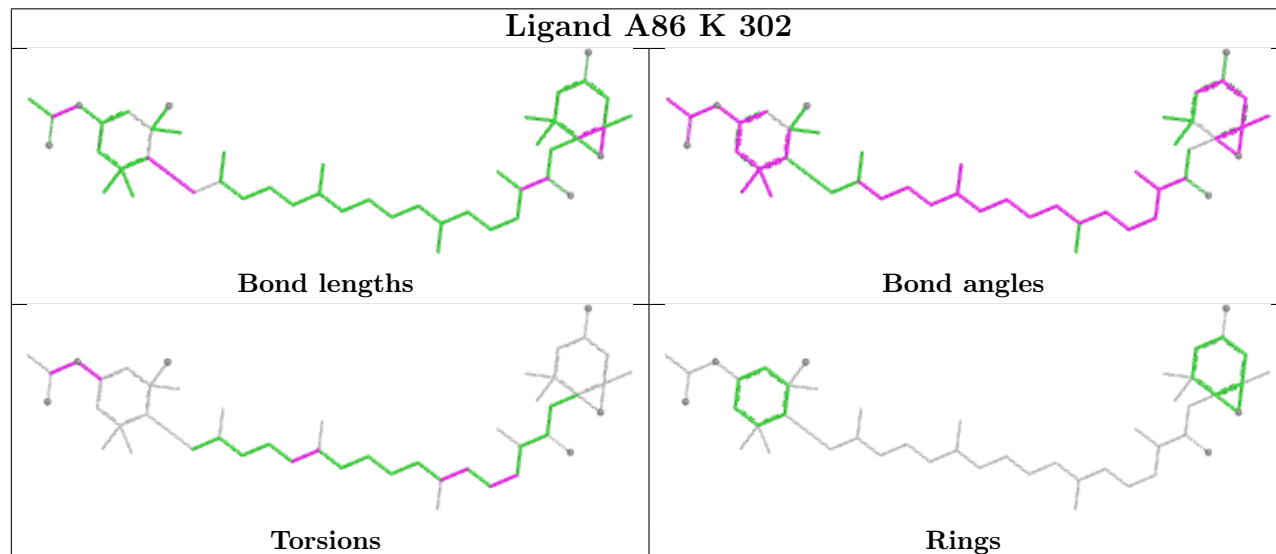


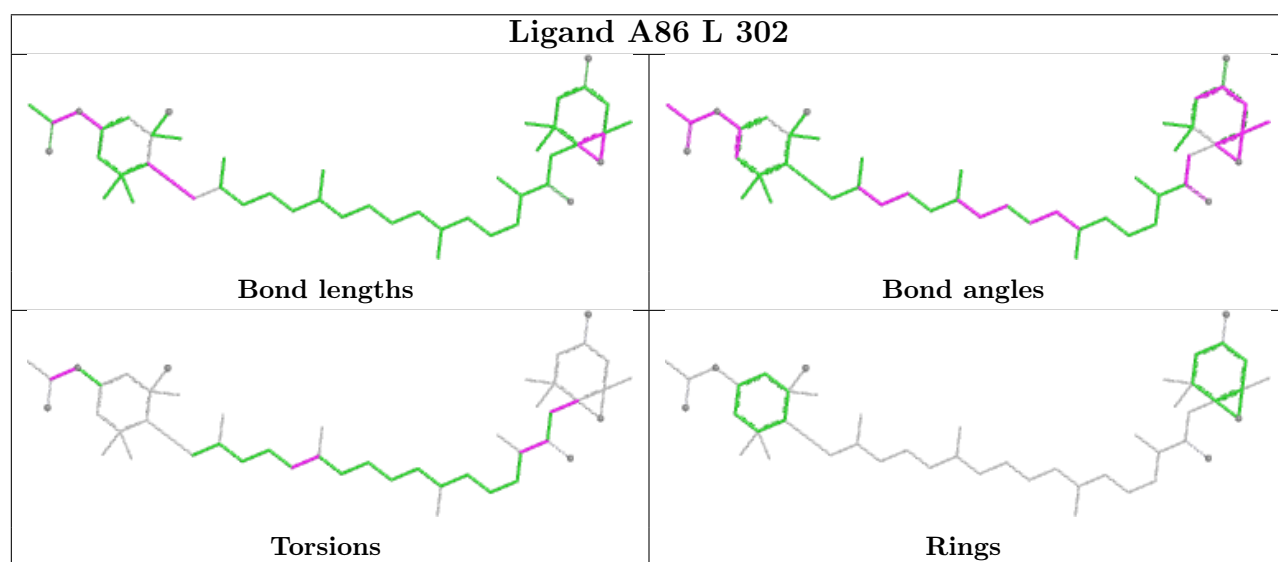
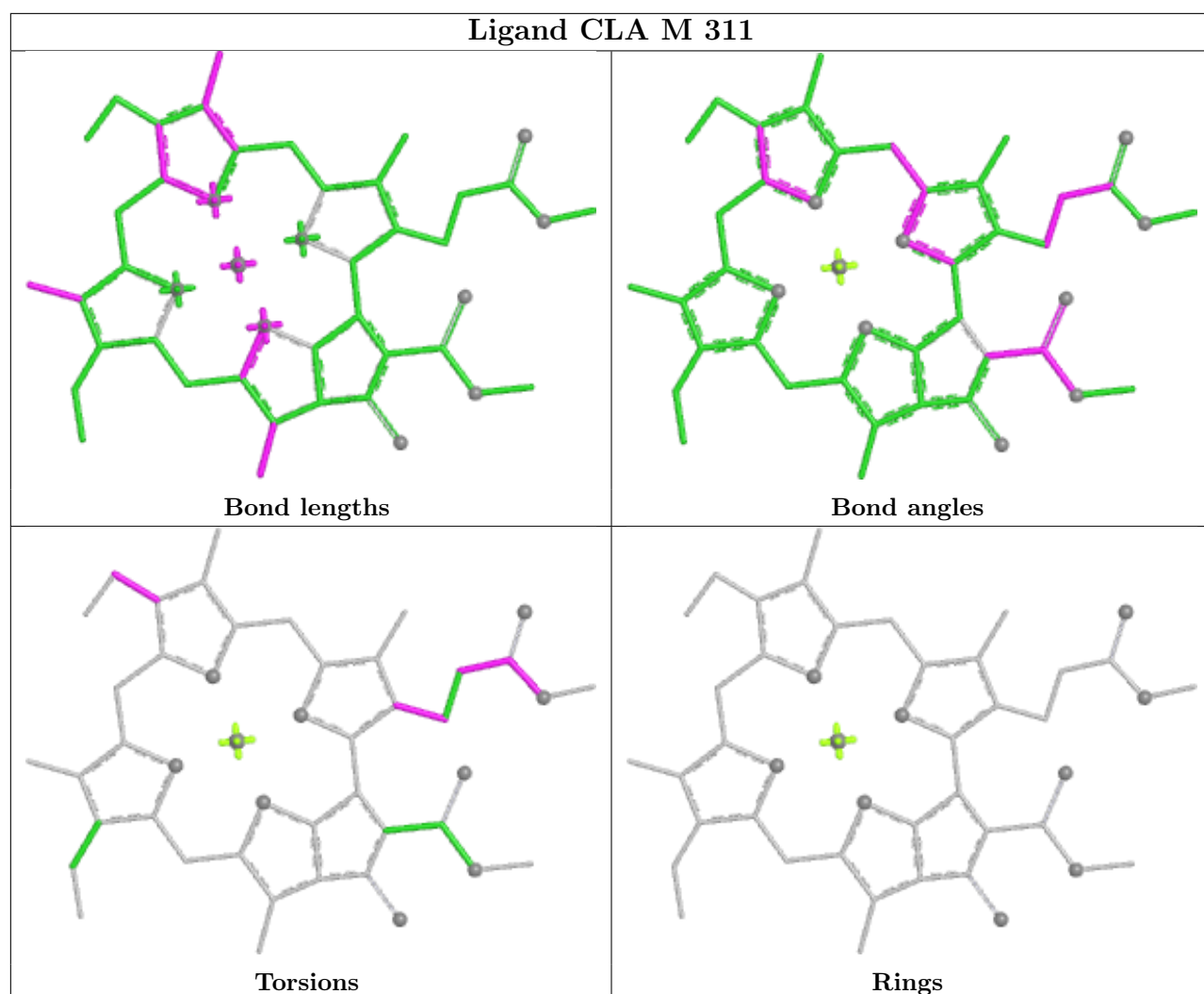
Rings

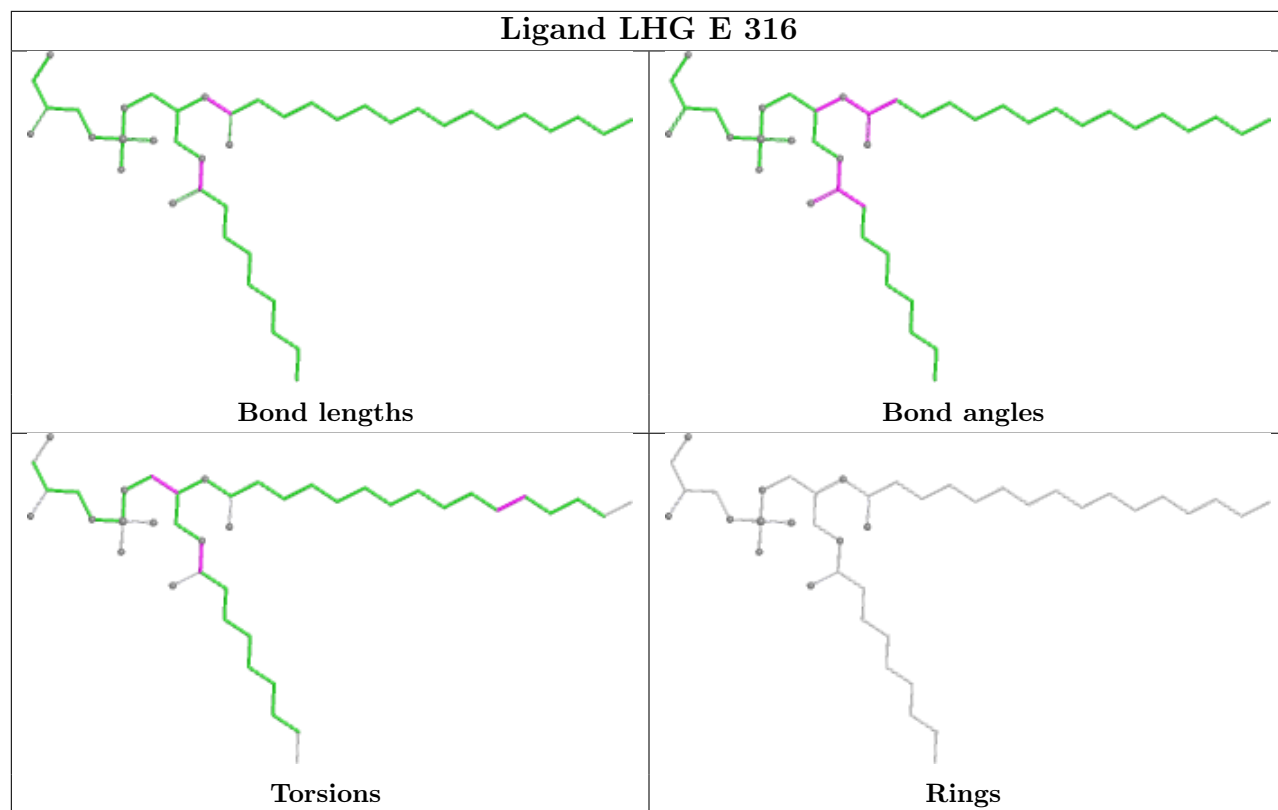
Ligand CLA L 308



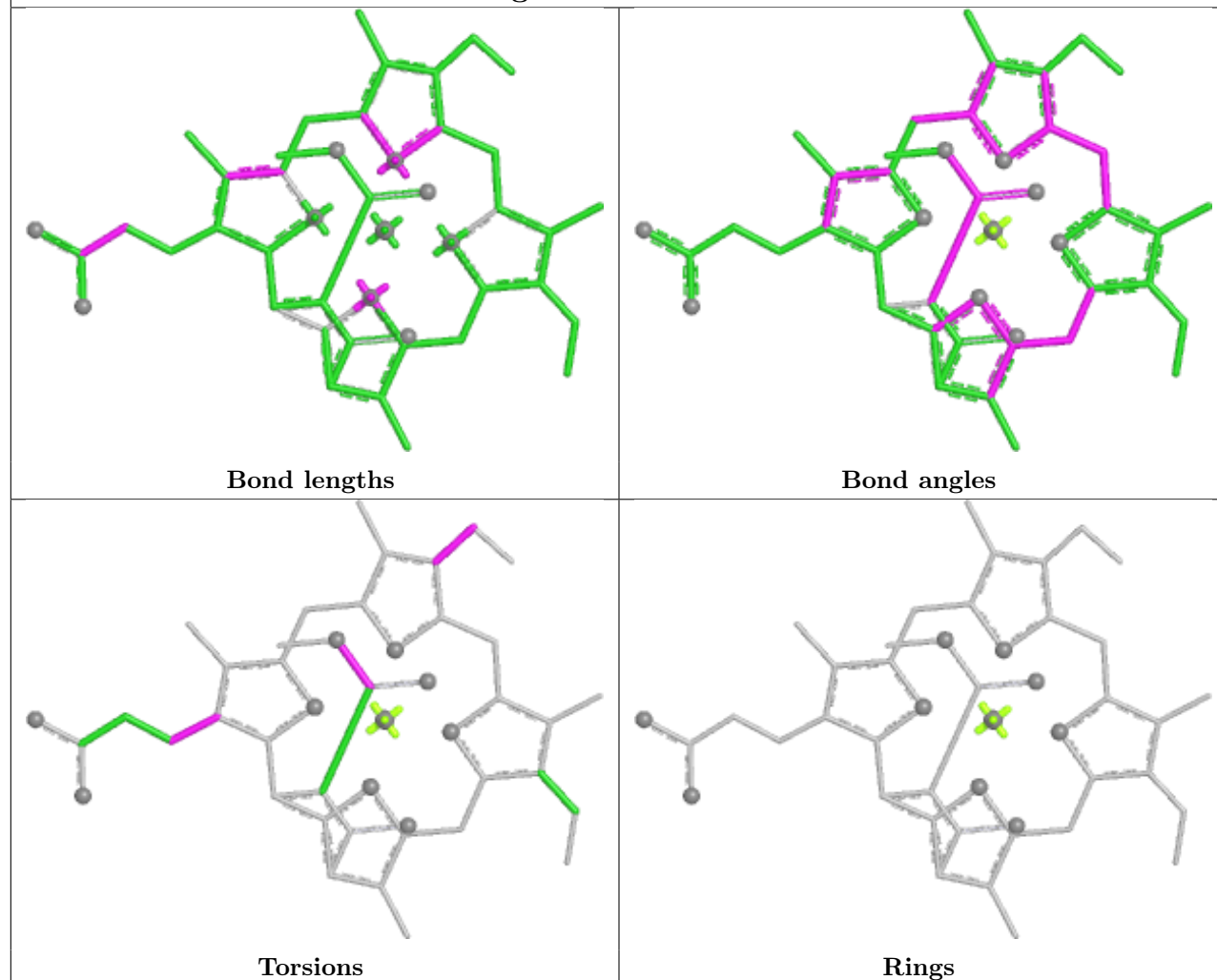
Ligand A86 K 302



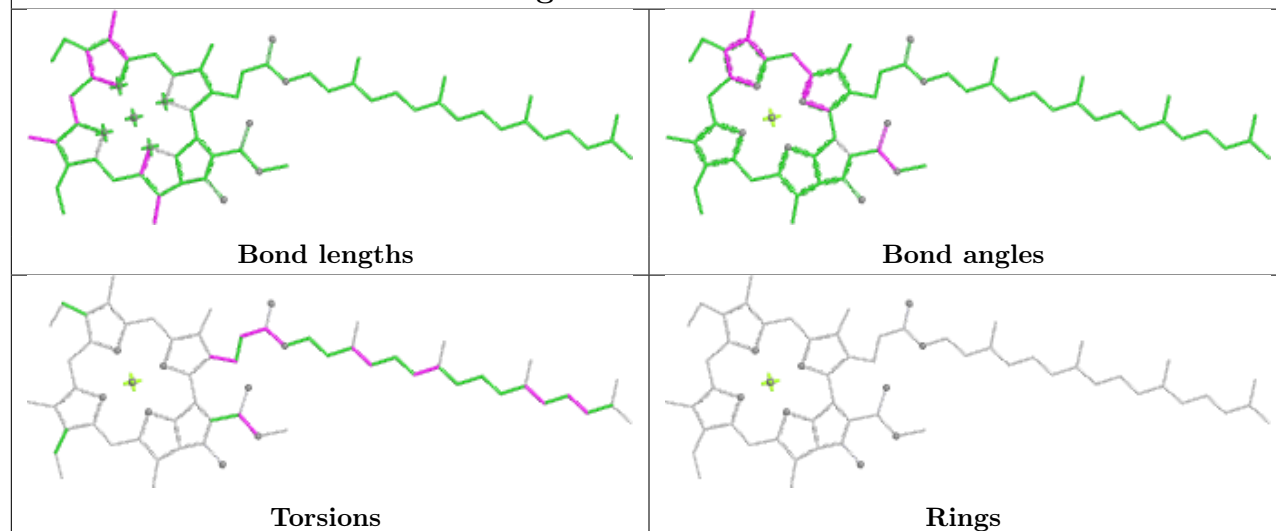


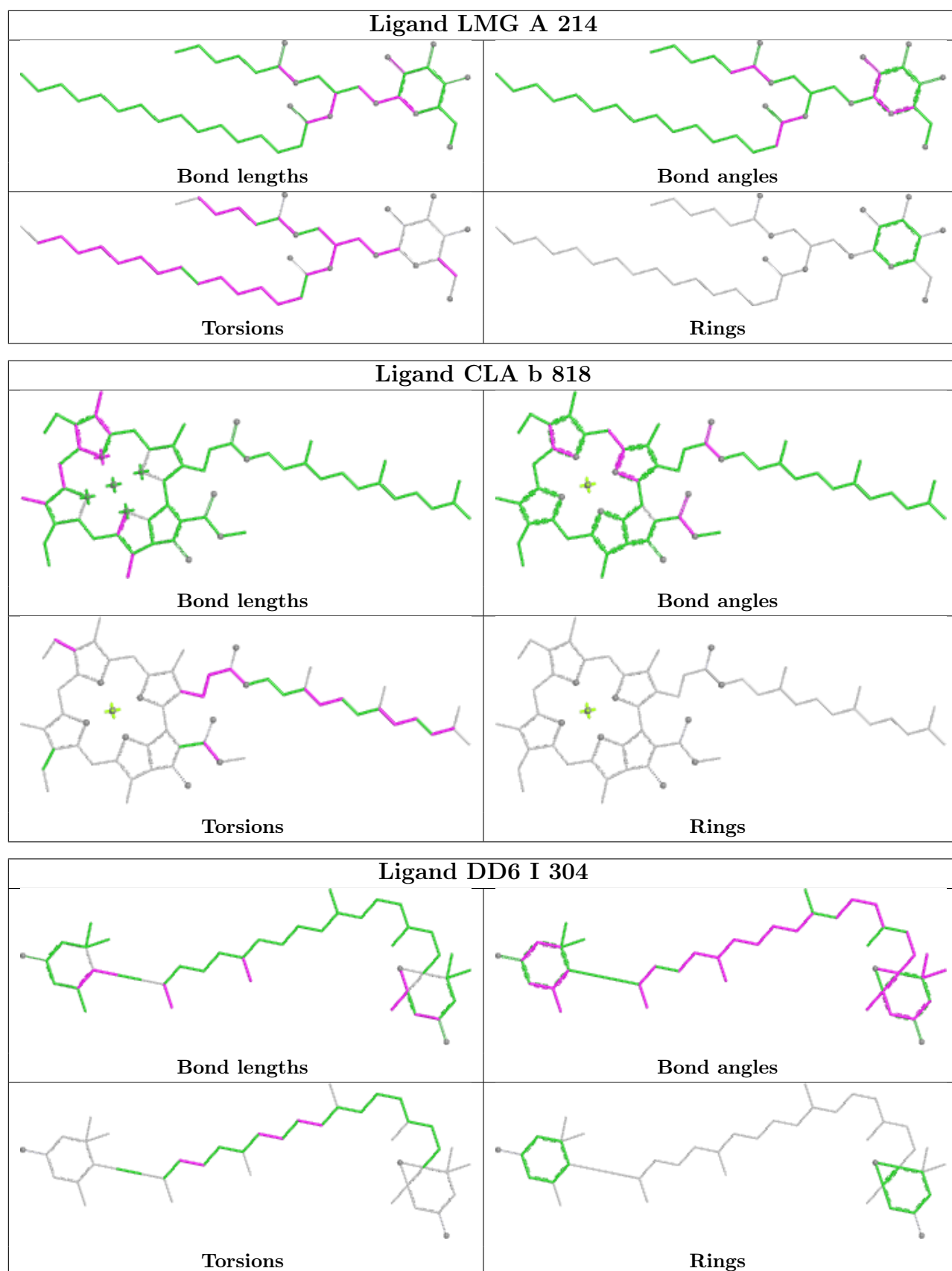


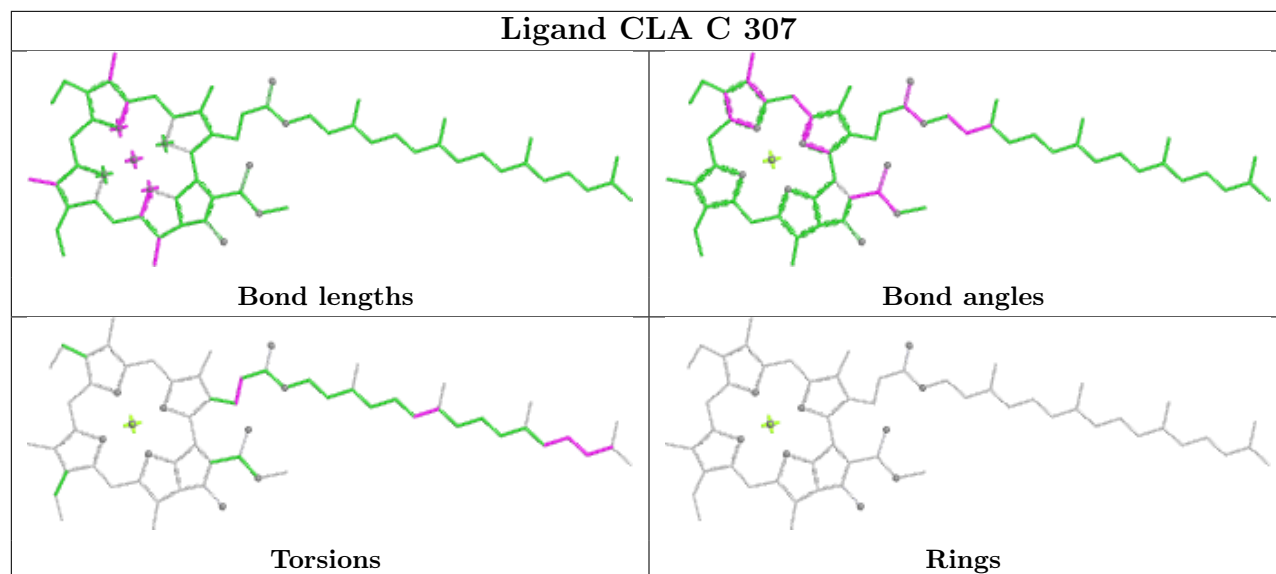
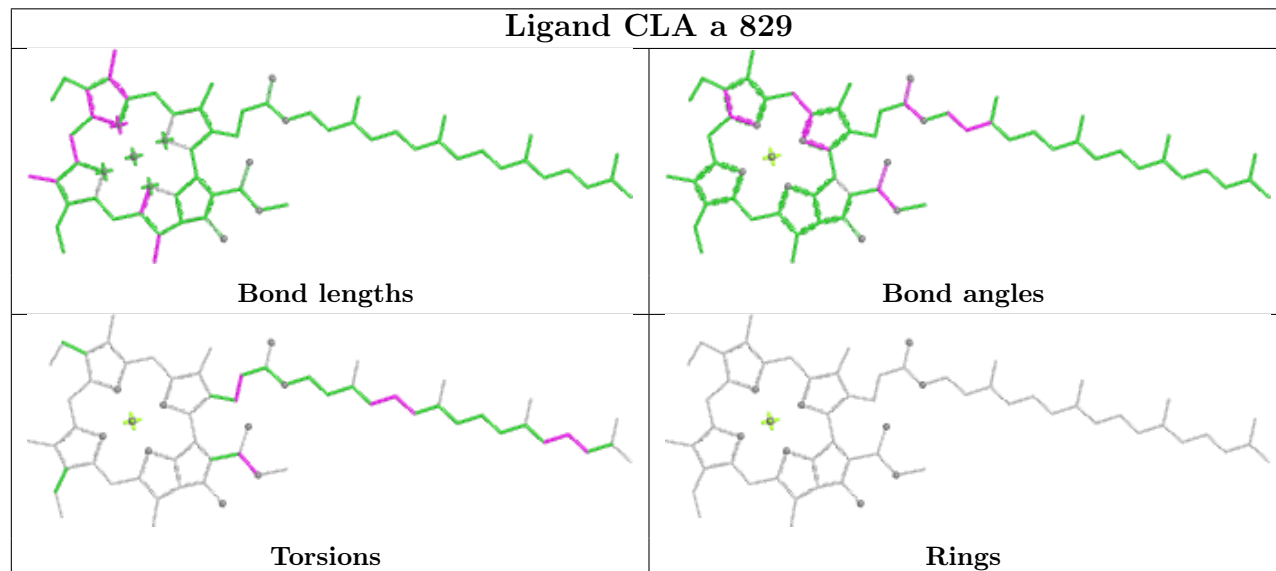
Ligand KC1 L 320



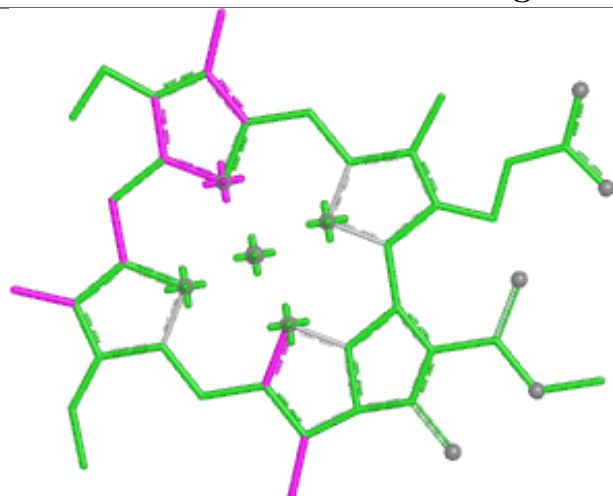
Ligand CLA a 807



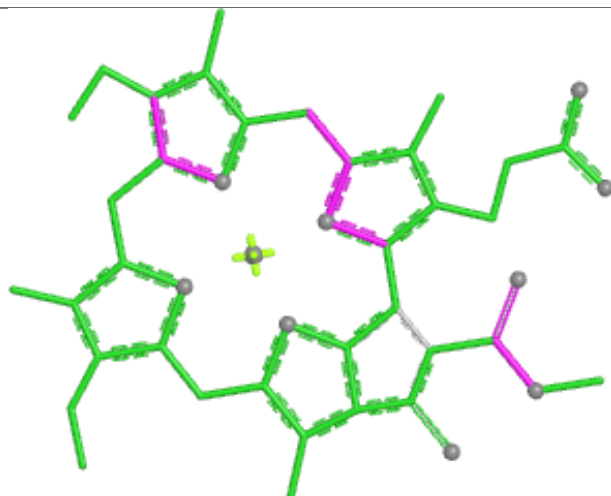


Ligand CLA C 307**Ligand CLA a 829**

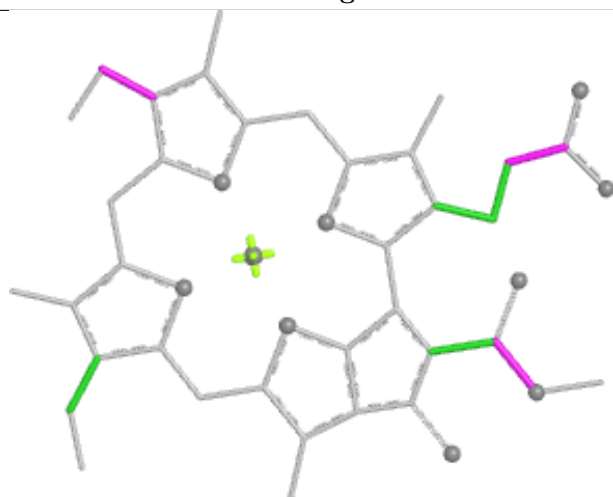
Ligand CLA H 214



Bond lengths



Bond angles

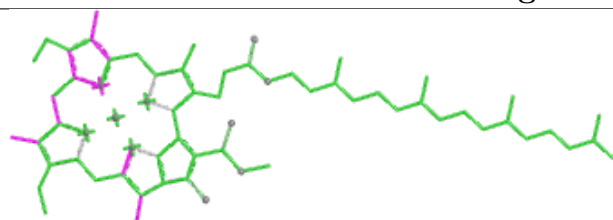


Torsions

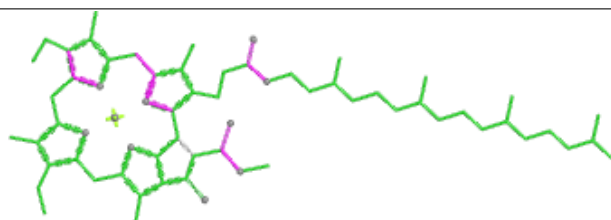


Rings

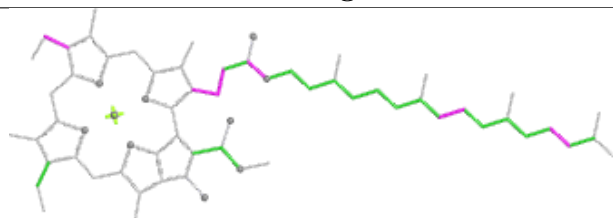
Ligand CLA a 812



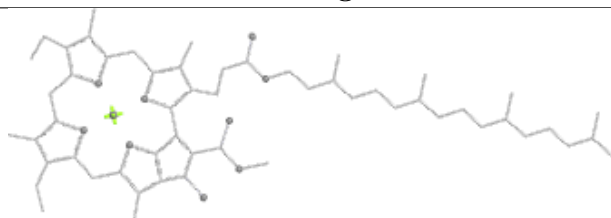
Bond lengths



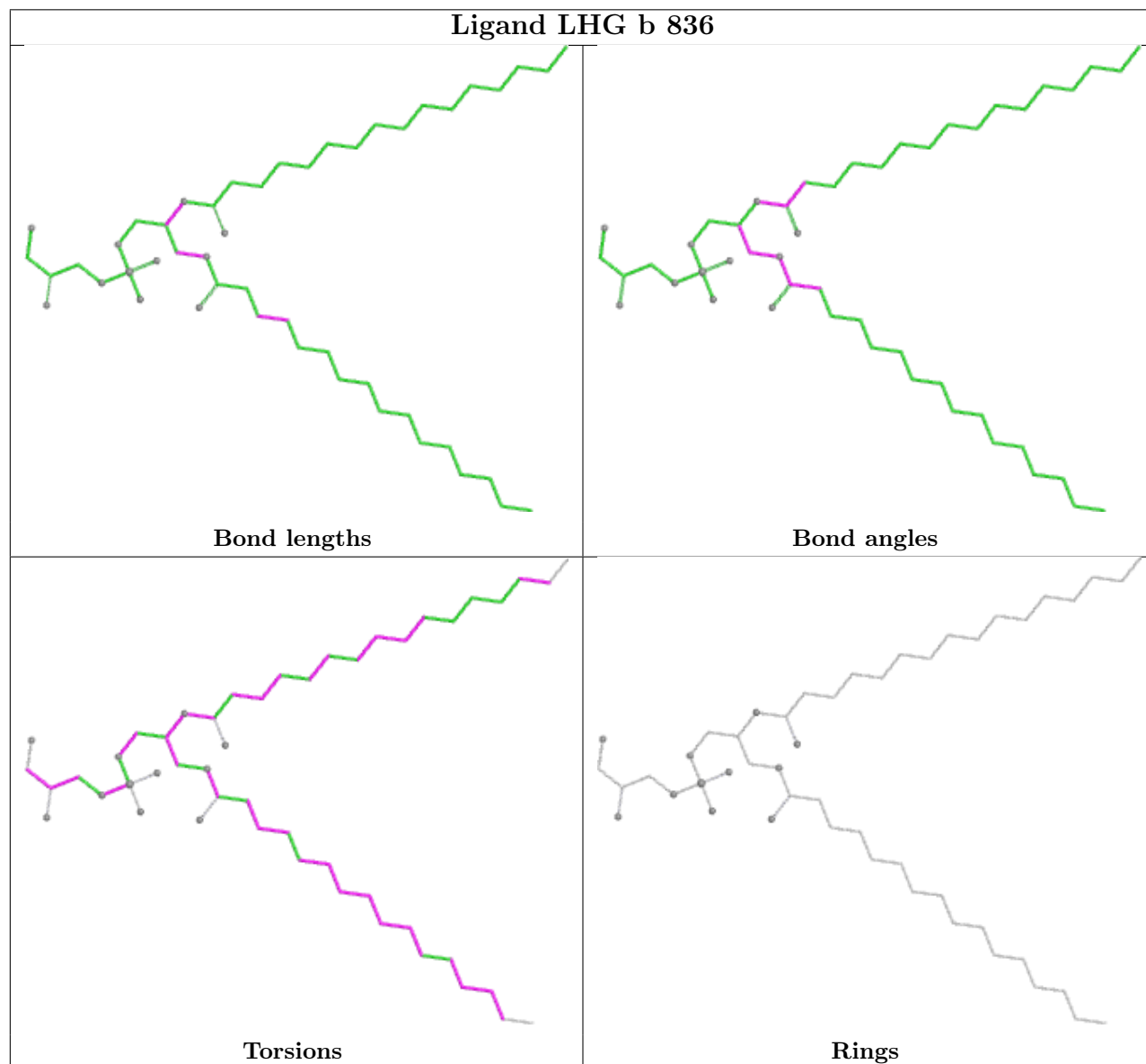
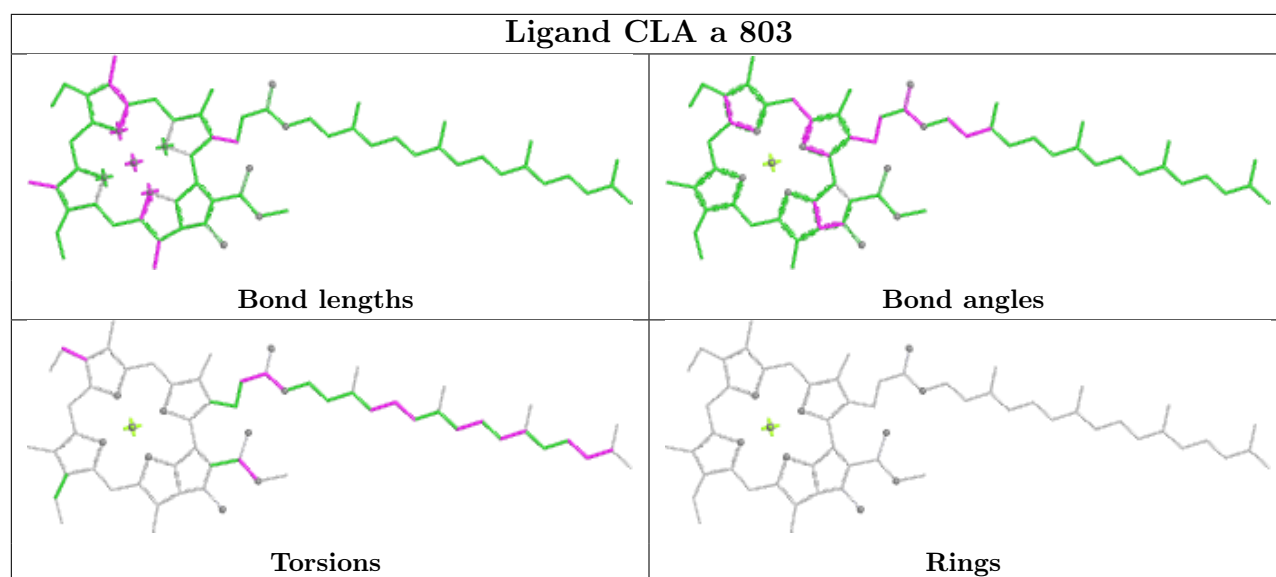
Bond angles

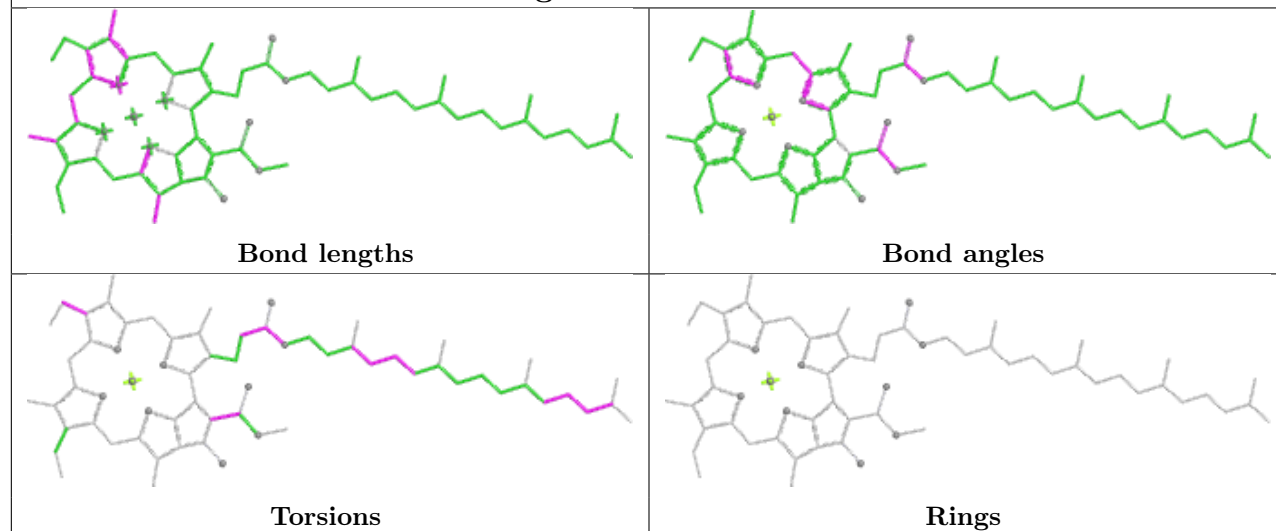
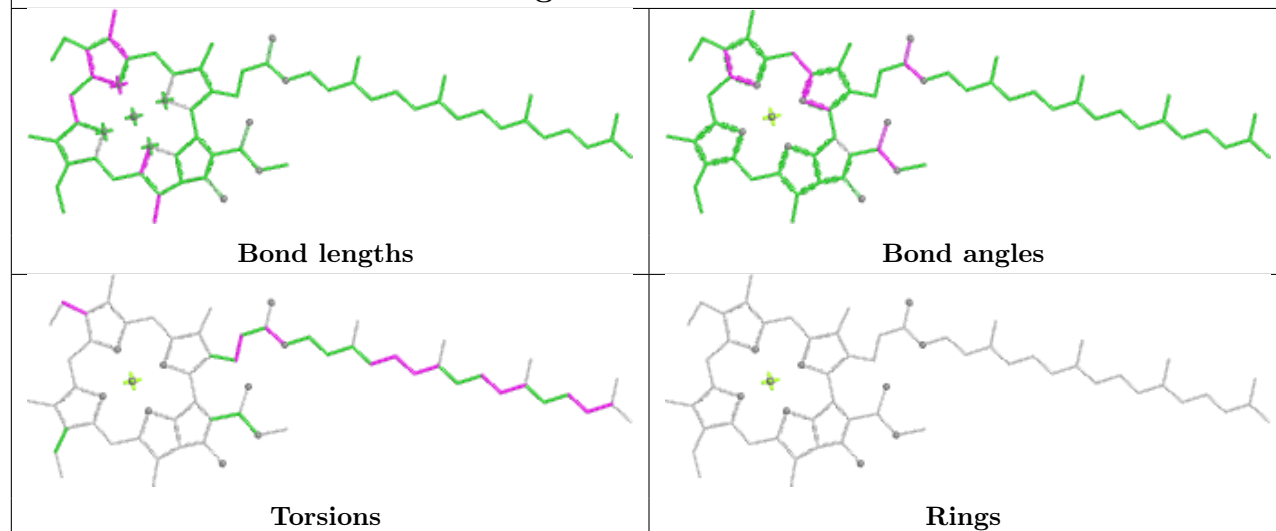
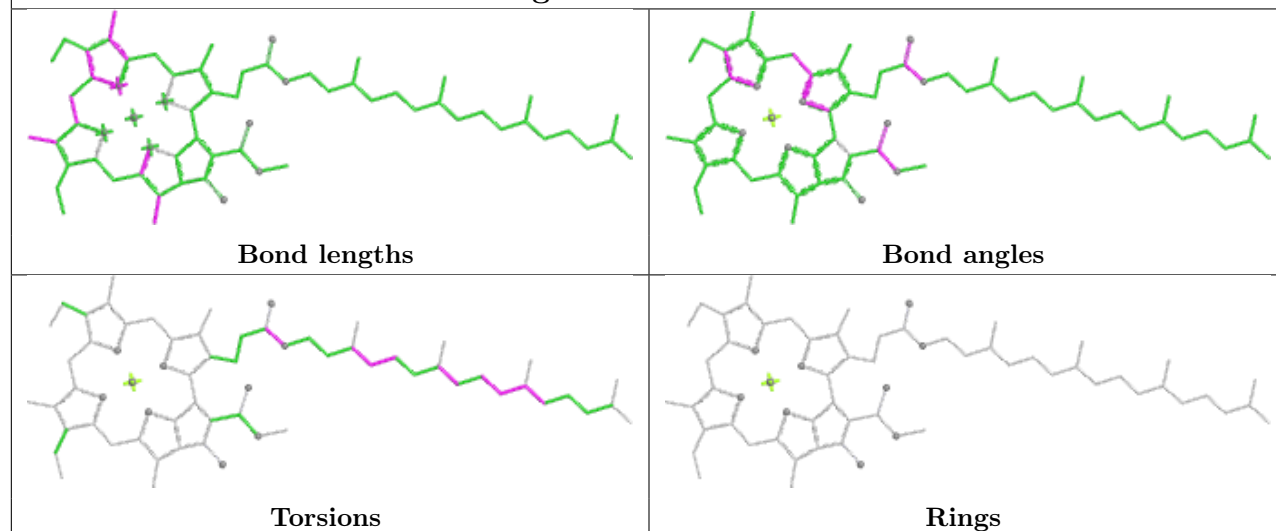


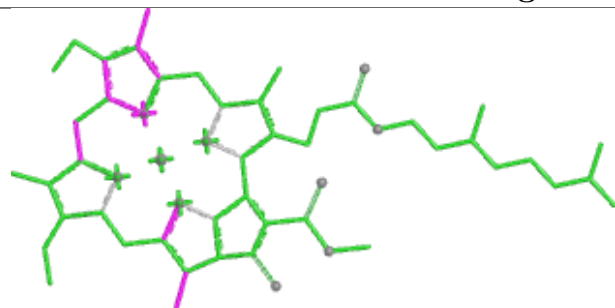
Torsions



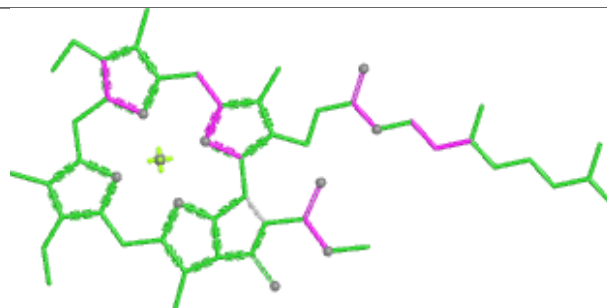
Rings



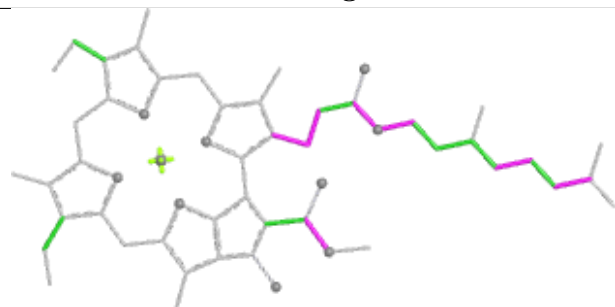
Ligand CLA b 847**Ligand CLA b 843****Ligand CLA B 308**

Ligand CLA F 306

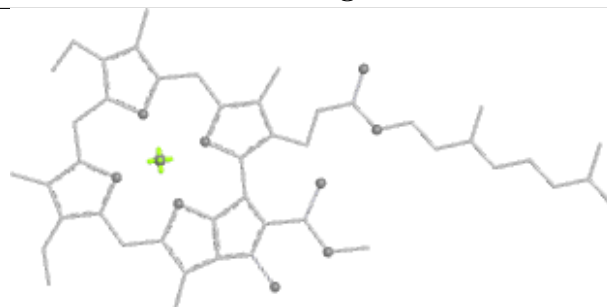
Bond lengths



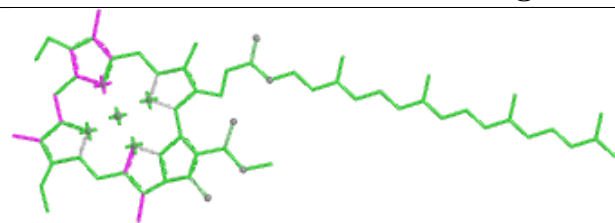
Bond angles



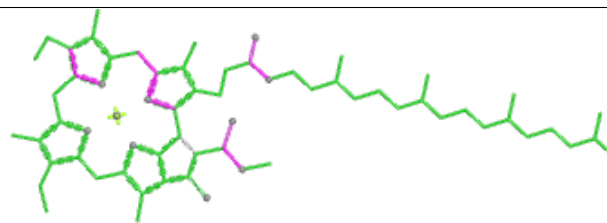
Torsions



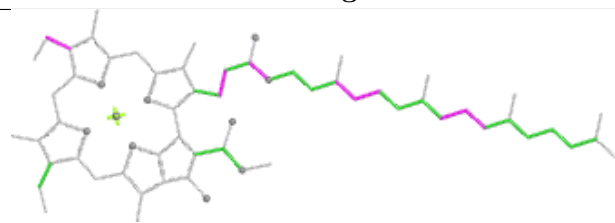
Rings

Ligand CLA D 213

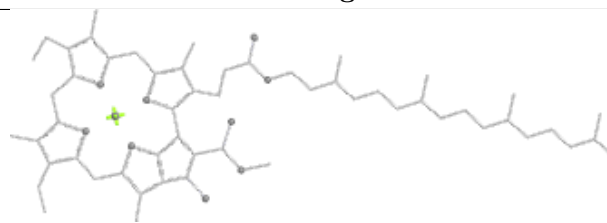
Bond lengths



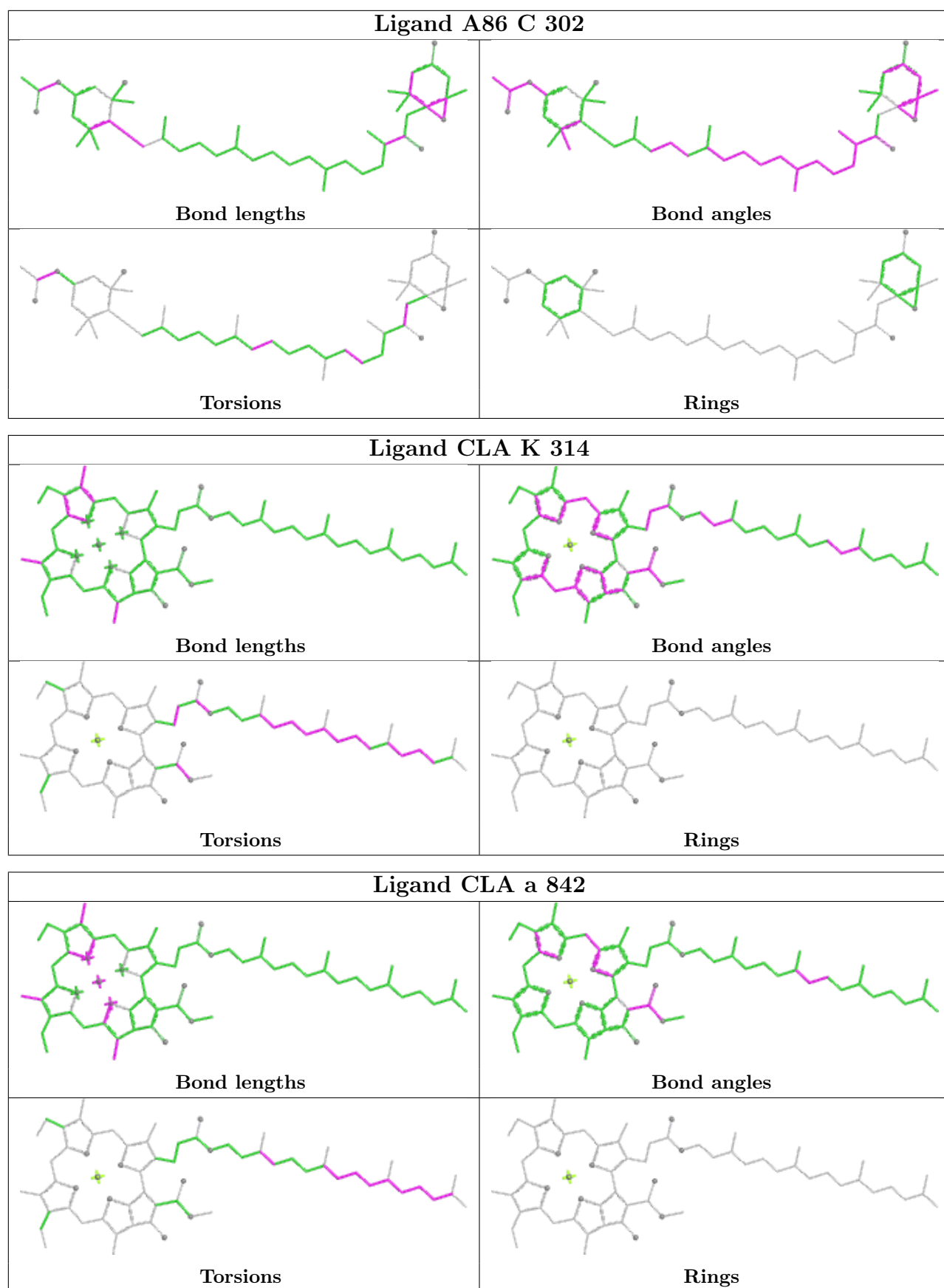
Bond angles

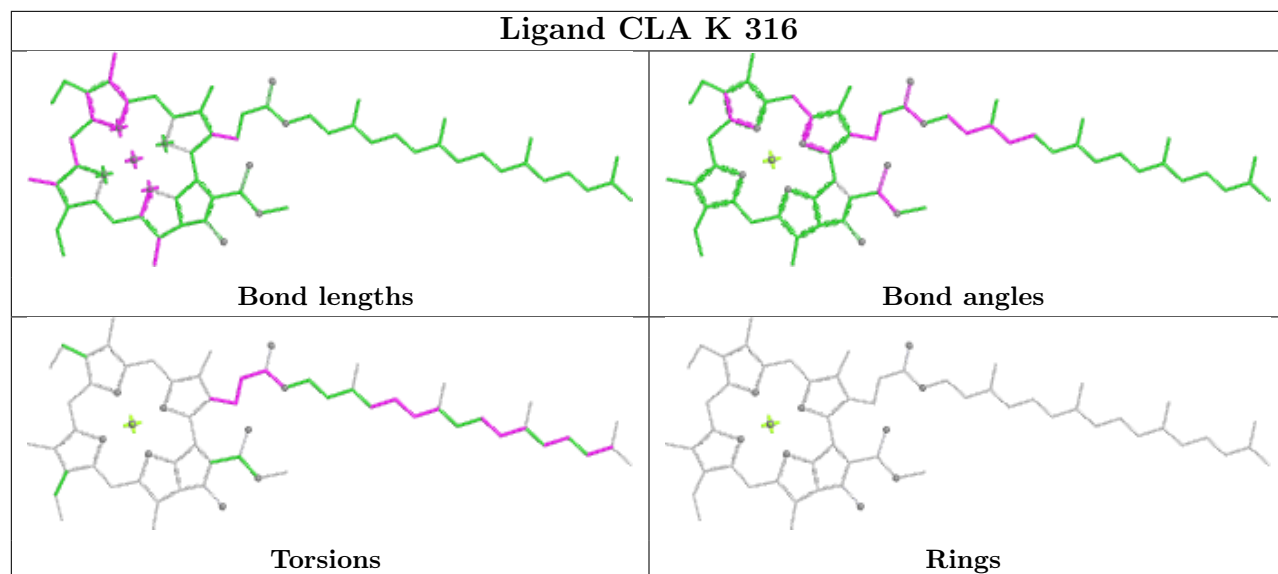
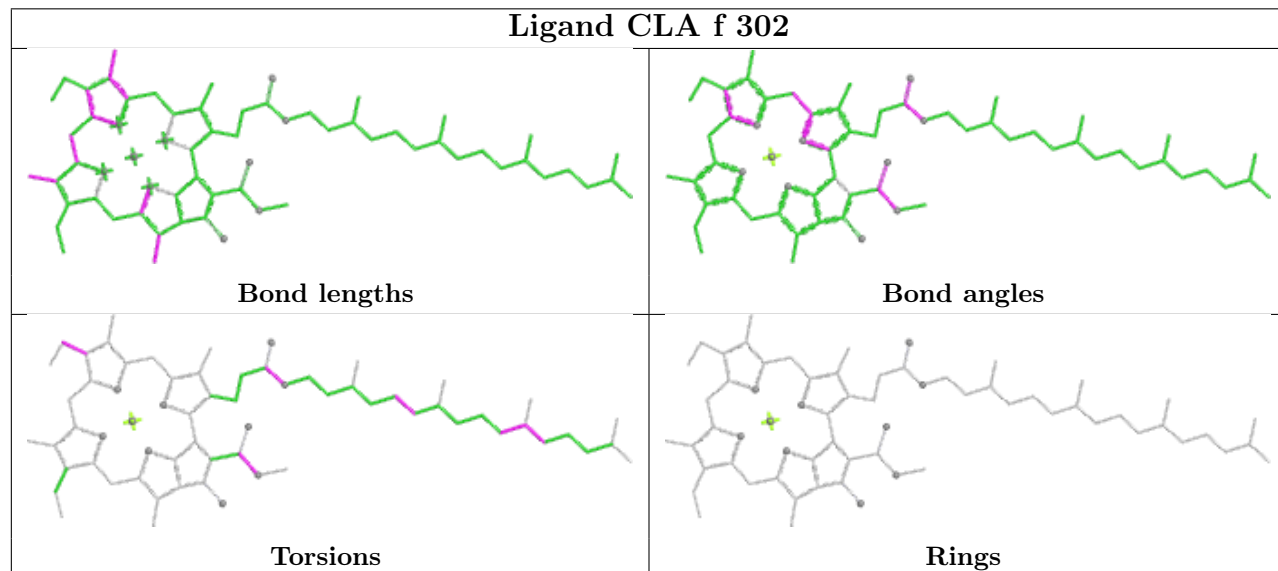


Torsions

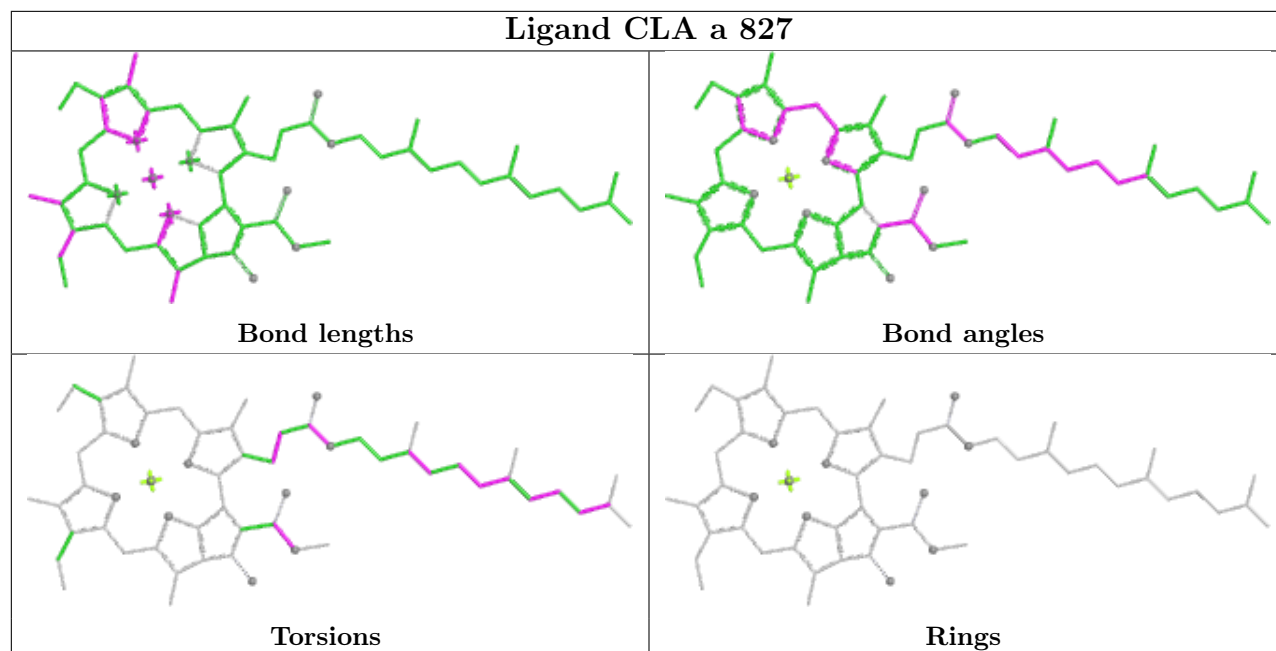


Rings

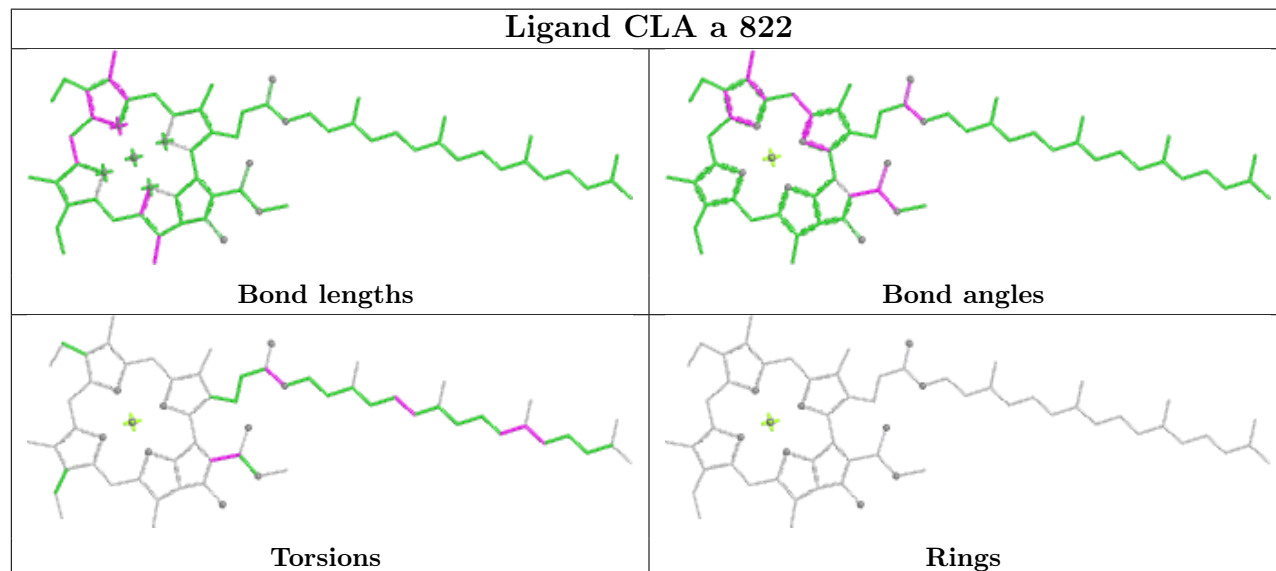


Ligand CLA K 316**Ligand CLA f 302**

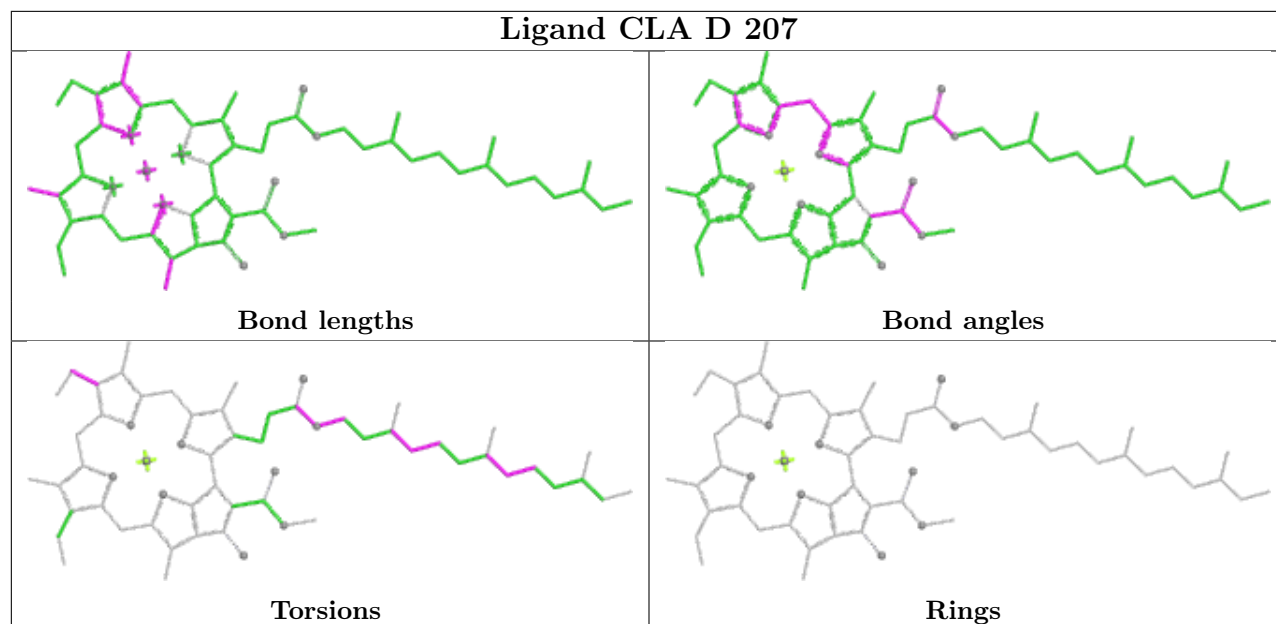
Ligand CLA a 827



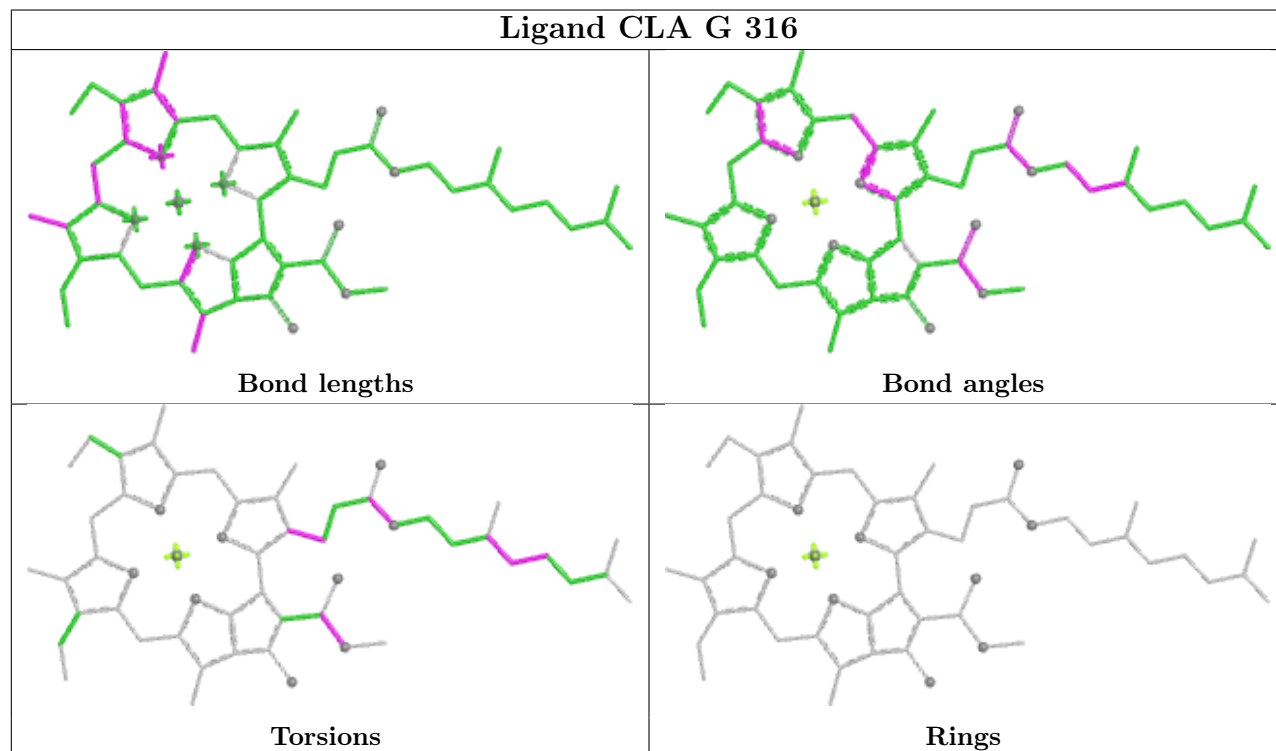
Ligand CLA a 822



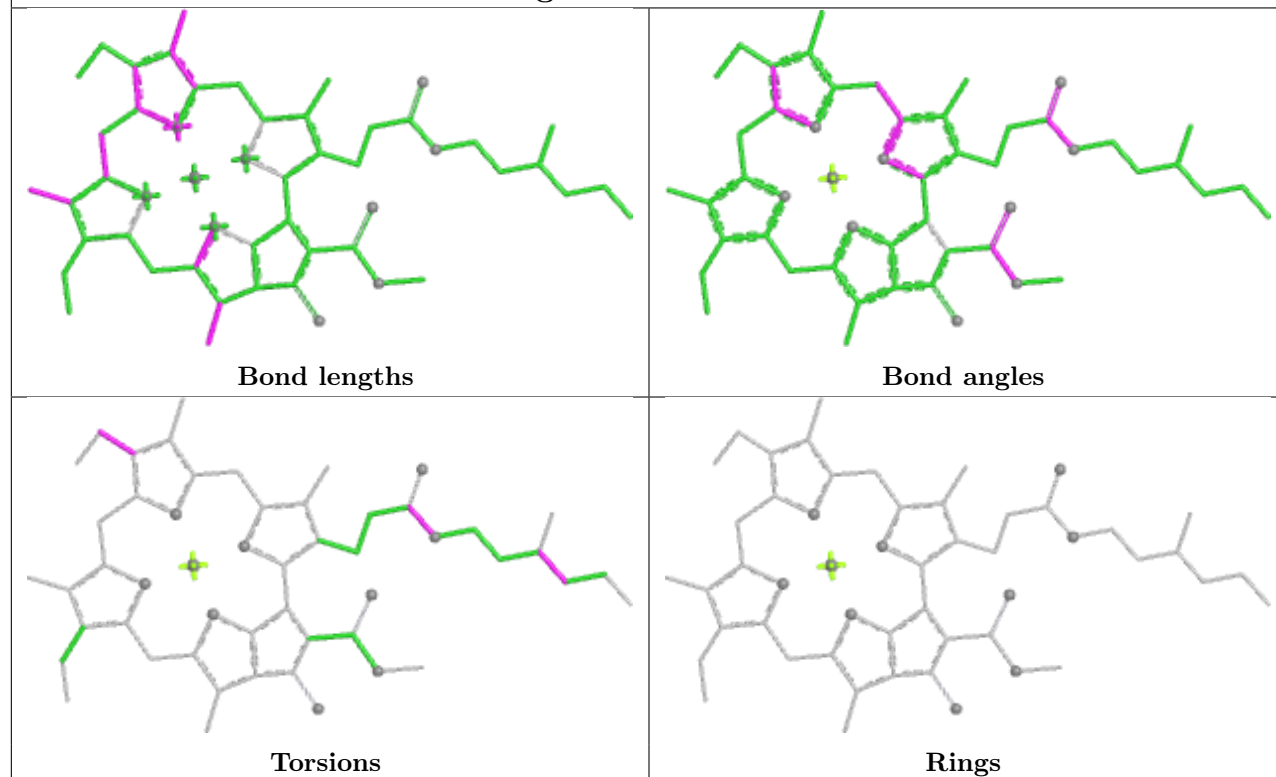
Ligand CLA D 207



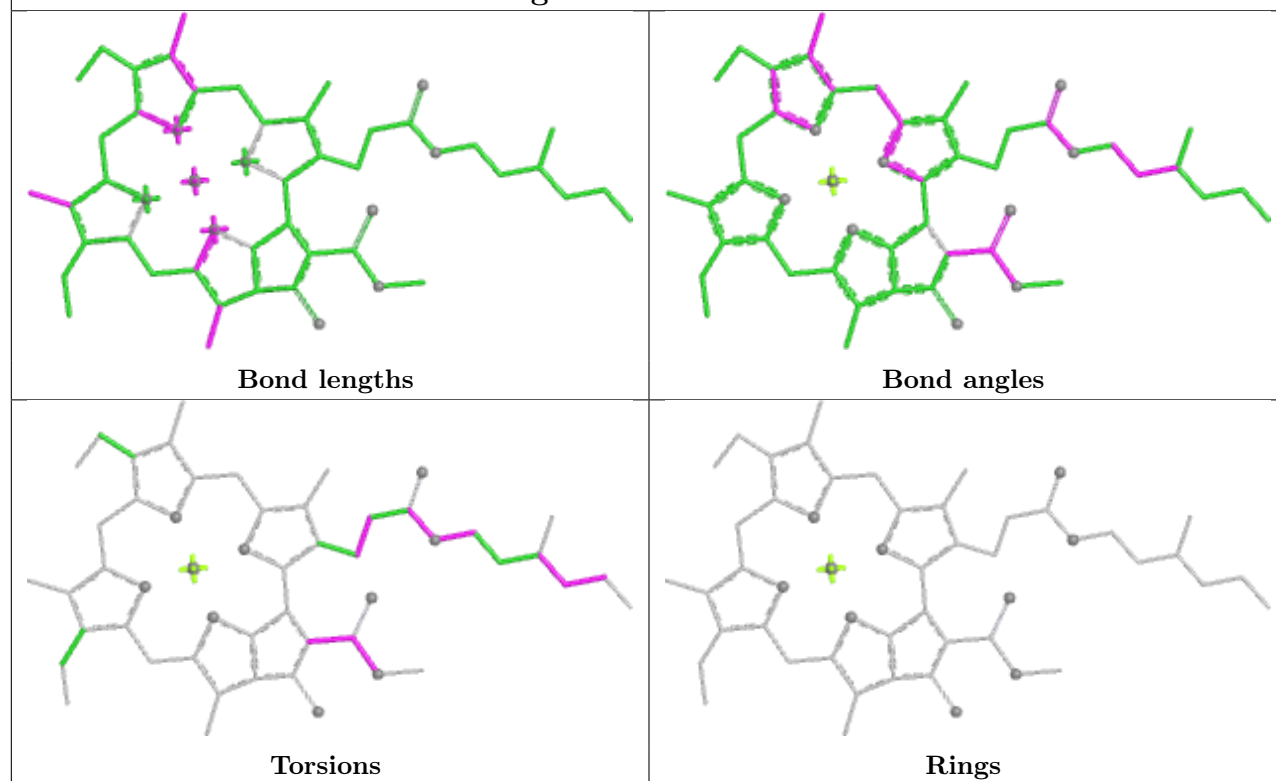
Ligand CLA G 316

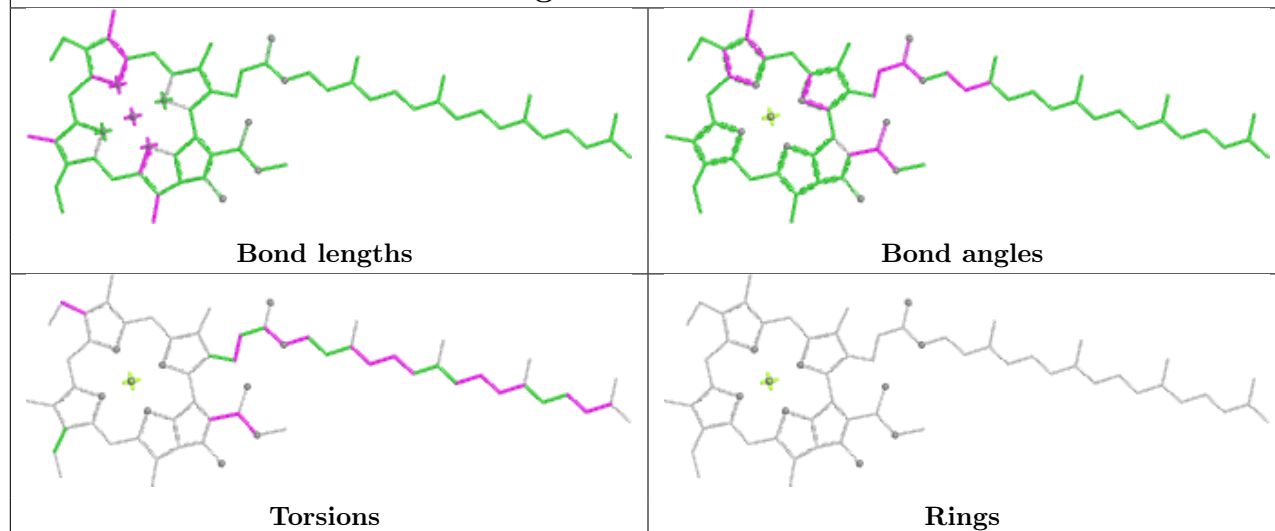
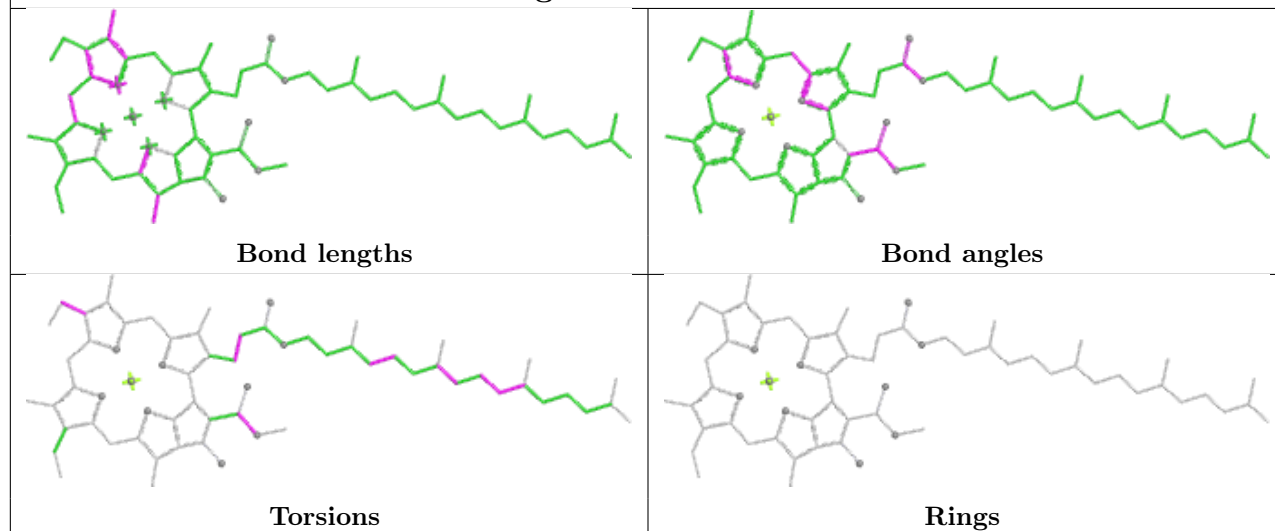
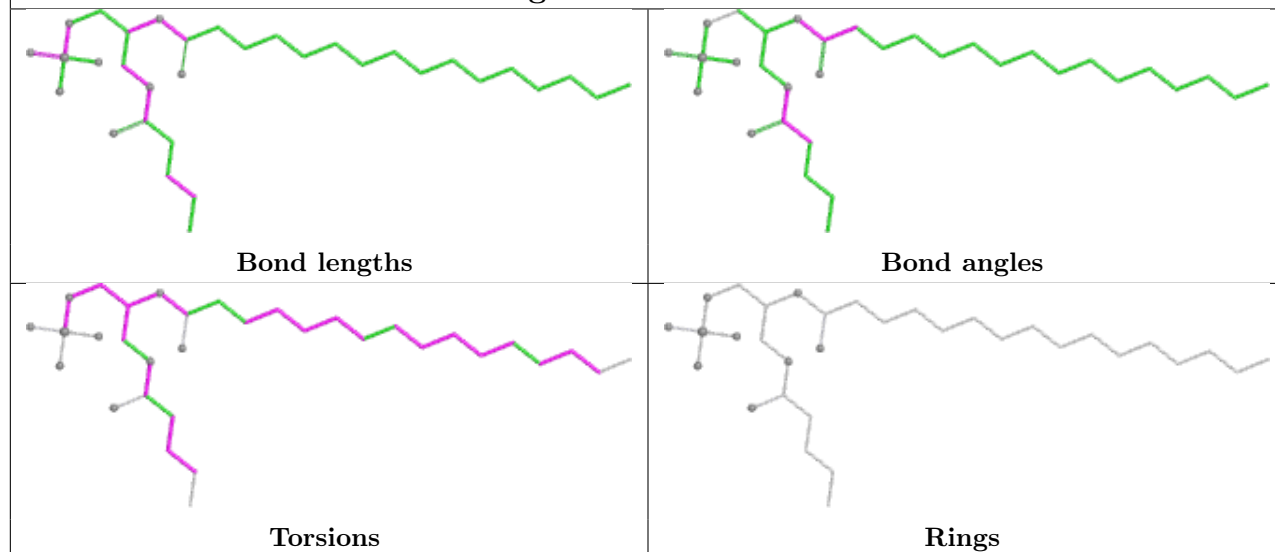


Ligand CLA a 832

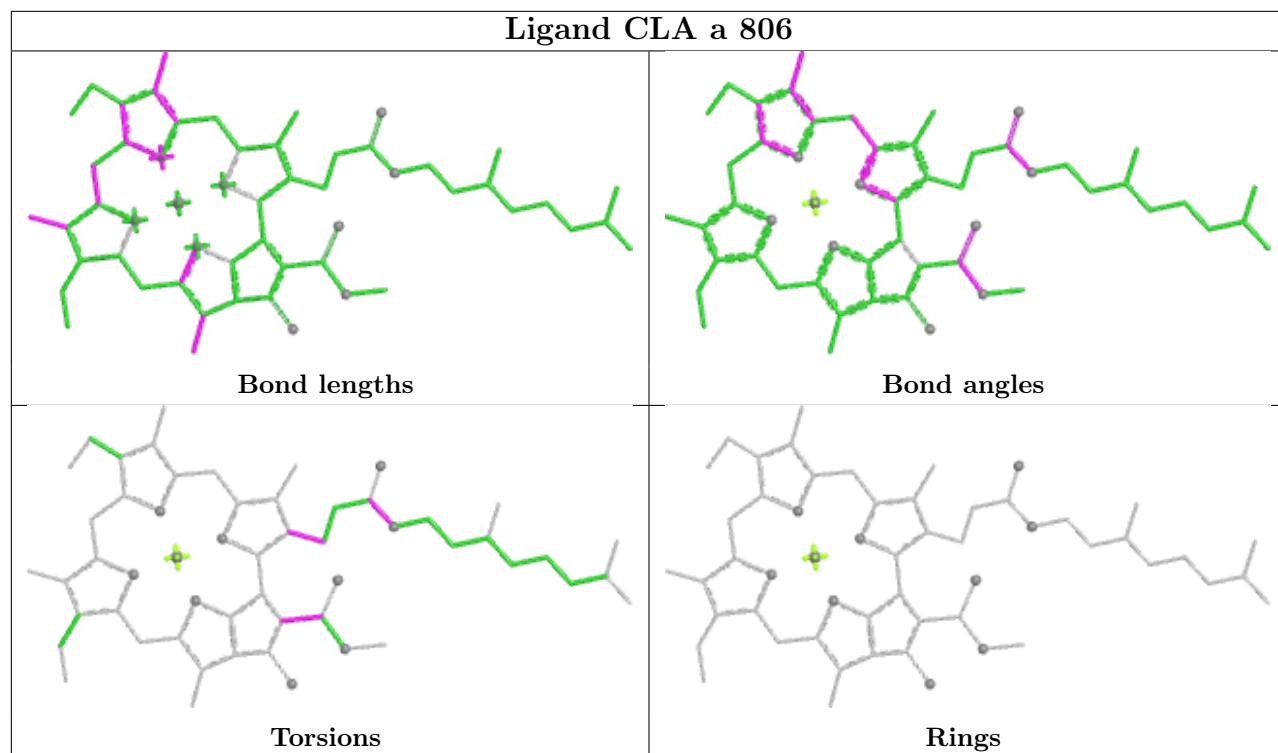


Ligand CLA K 311

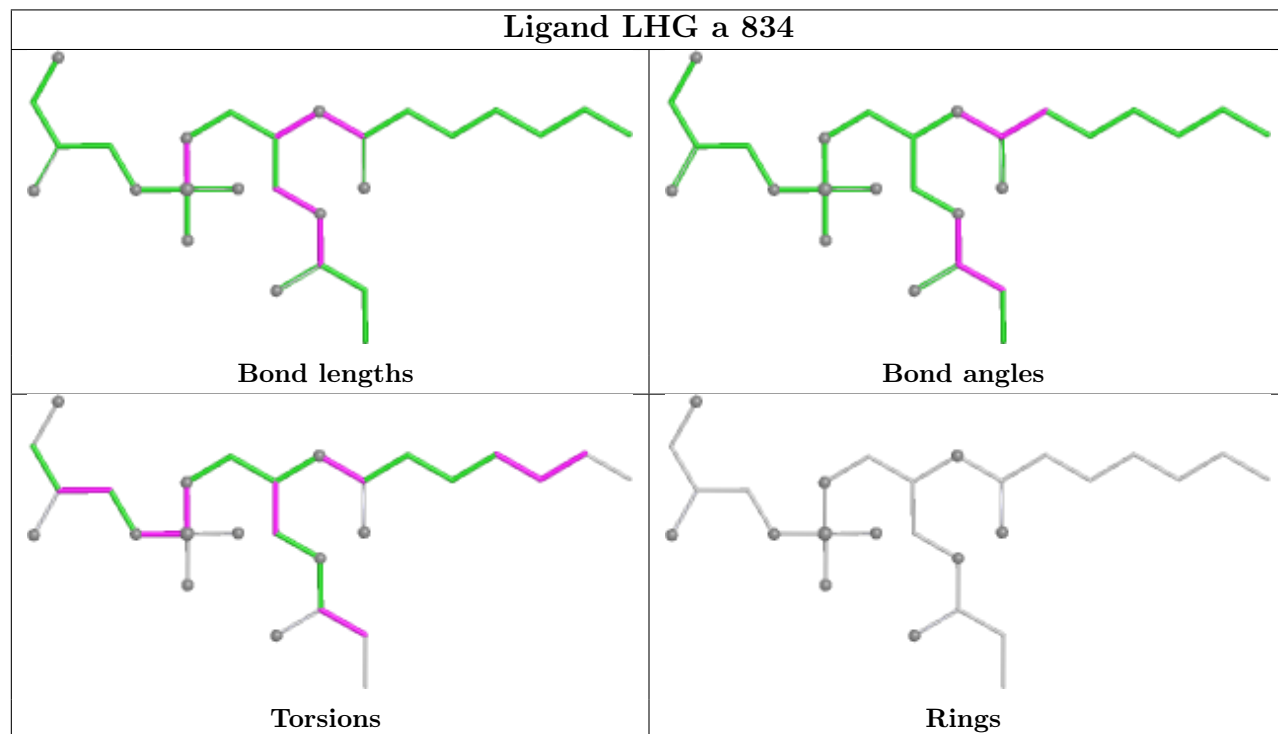


Ligand CLA a 843**Ligand CLA a 828****Ligand LHG K 320**

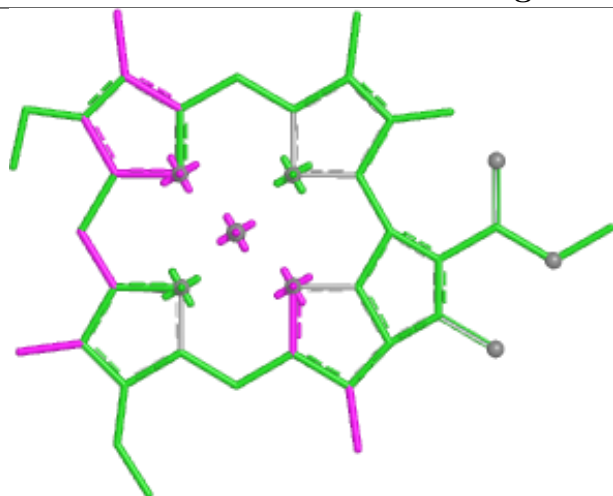
Ligand CLA a 806



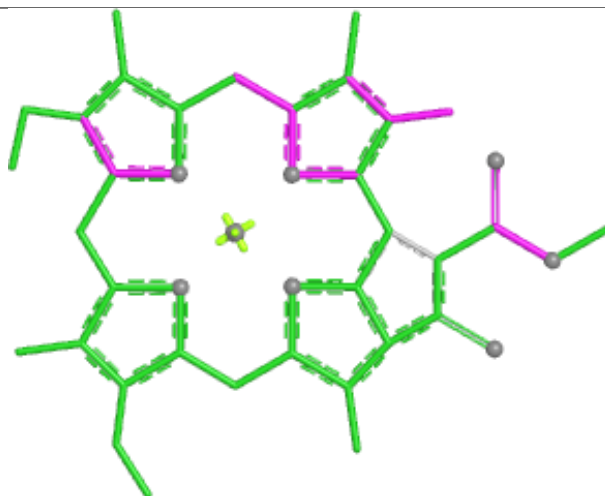
Ligand LHG a 834



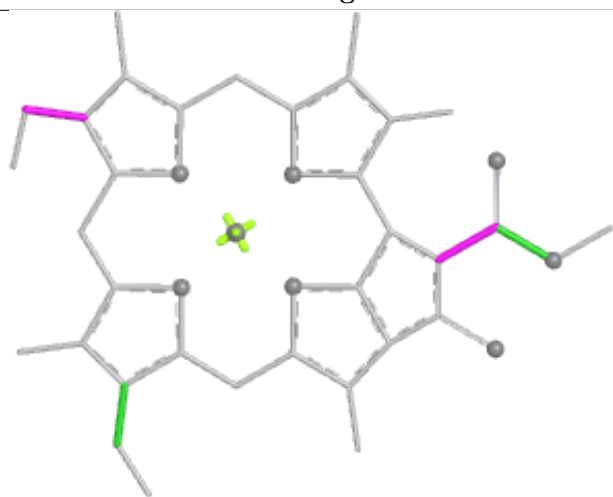
Ligand CLA C 316



Bond lengths



Bond angles

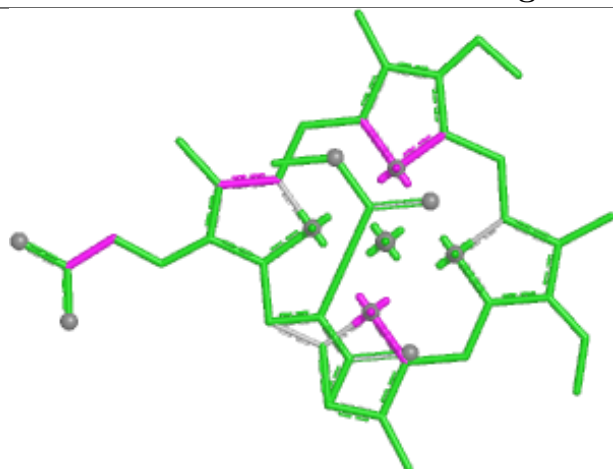


Torsions

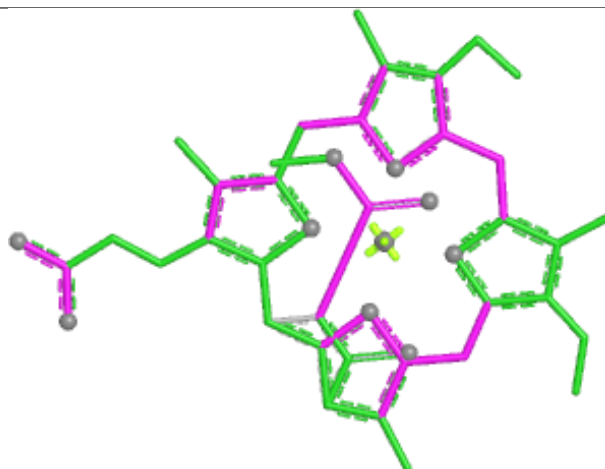


Rings

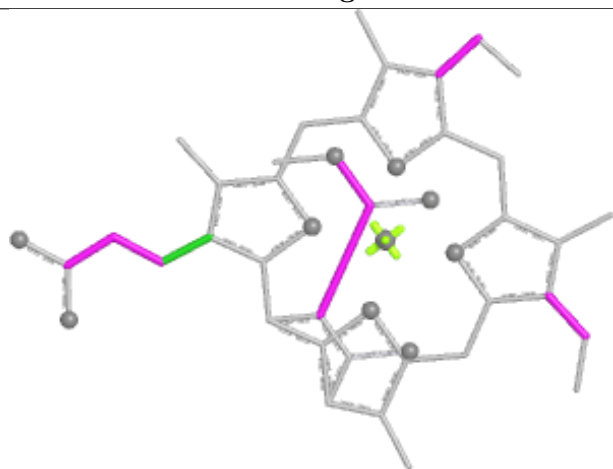
Ligand KC1 L 314



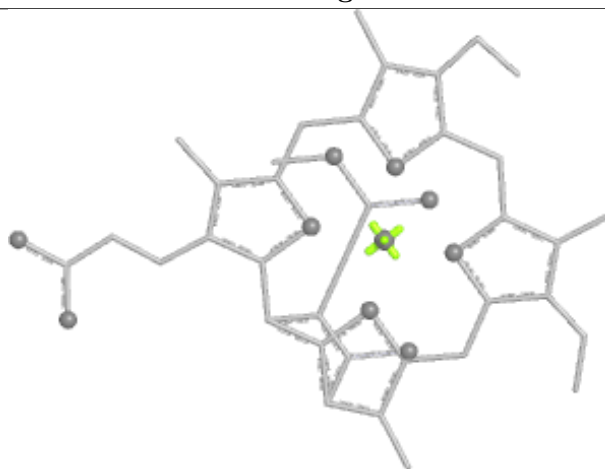
Bond lengths



Bond angles

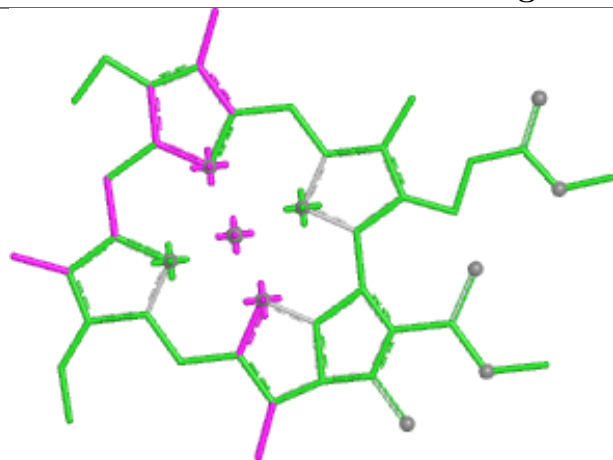


Torsions

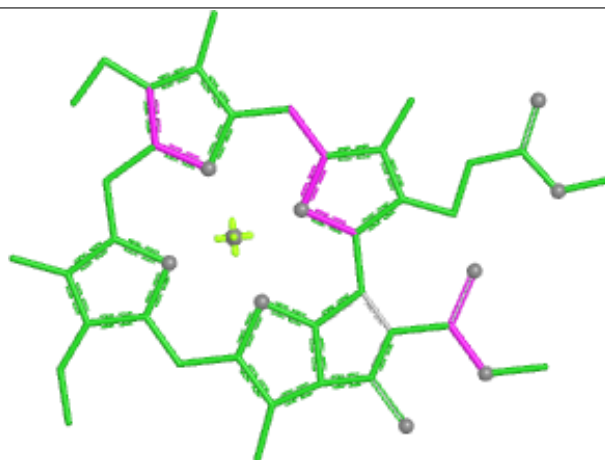


Rings

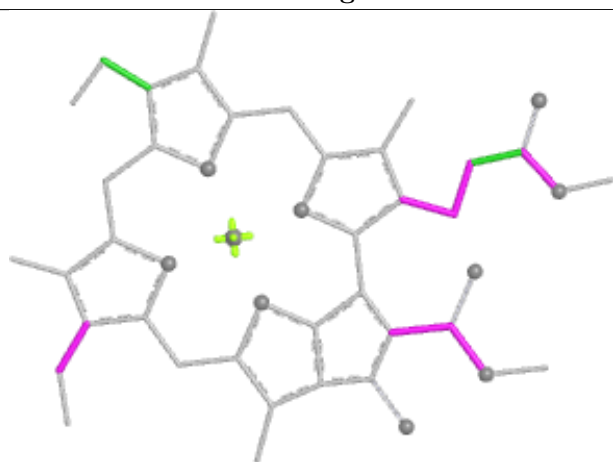
Ligand CLA J 313



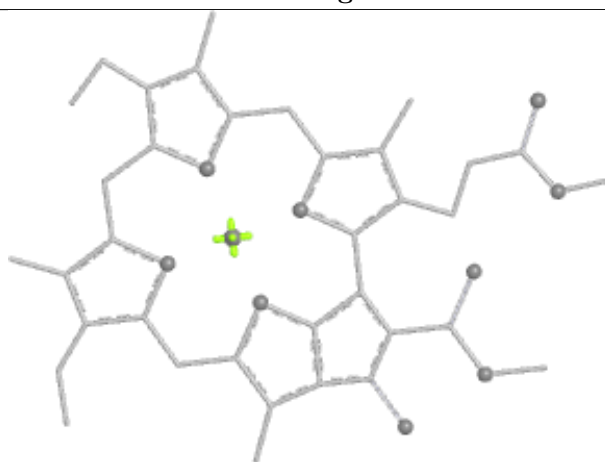
Bond lengths



Bond angles

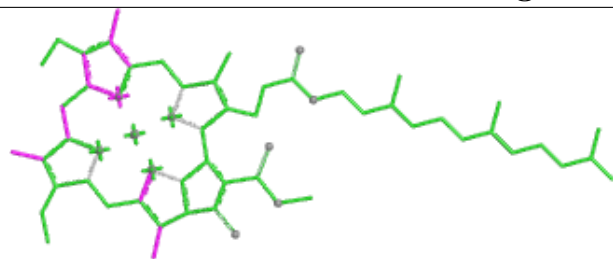


Torsions

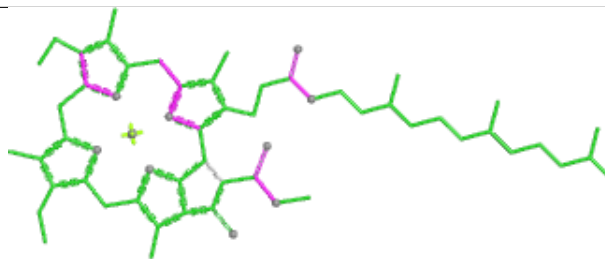


Rings

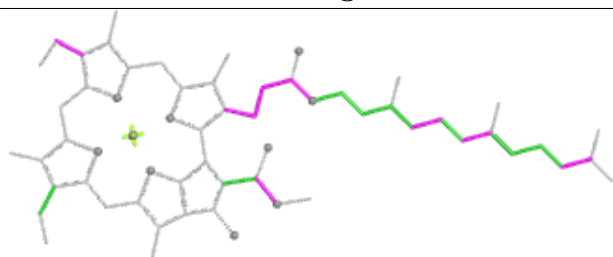
Ligand CLA F 311



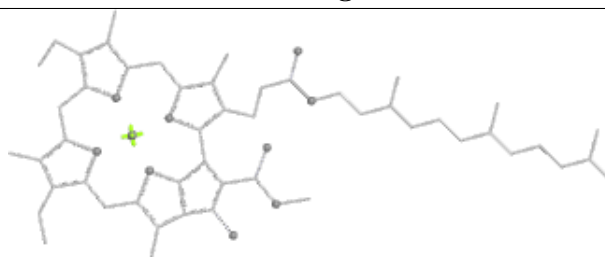
Bond lengths



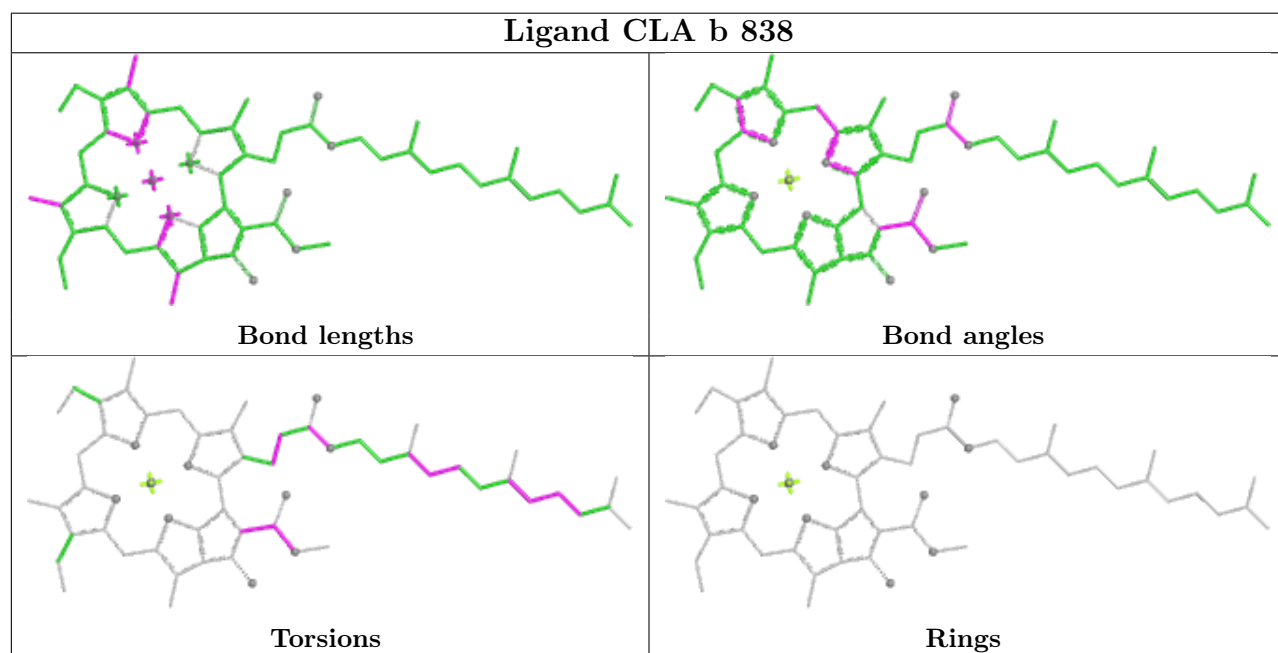
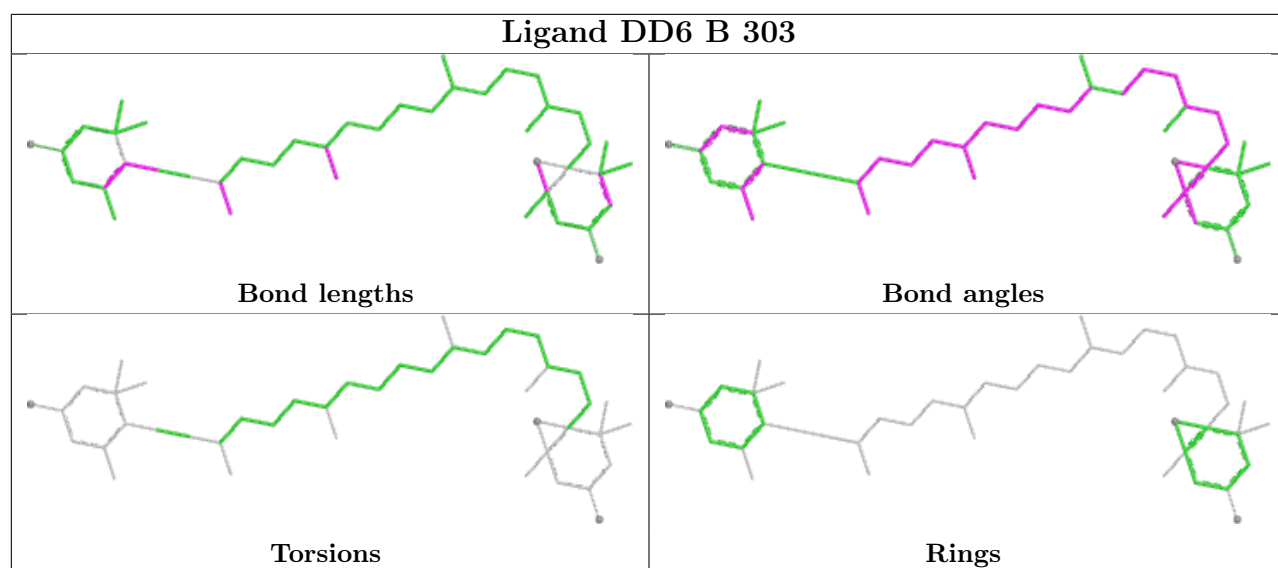
Bond angles



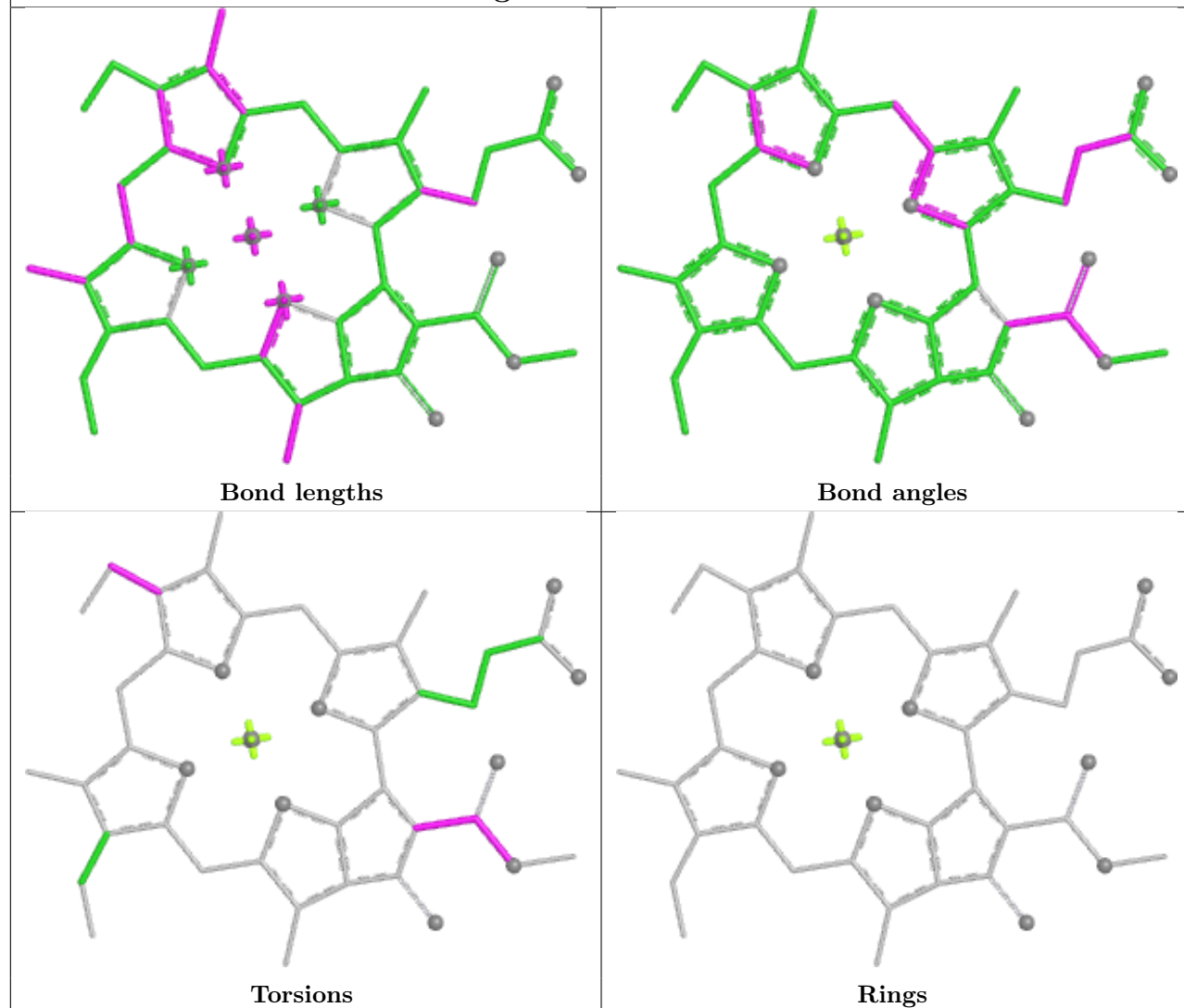
Torsions



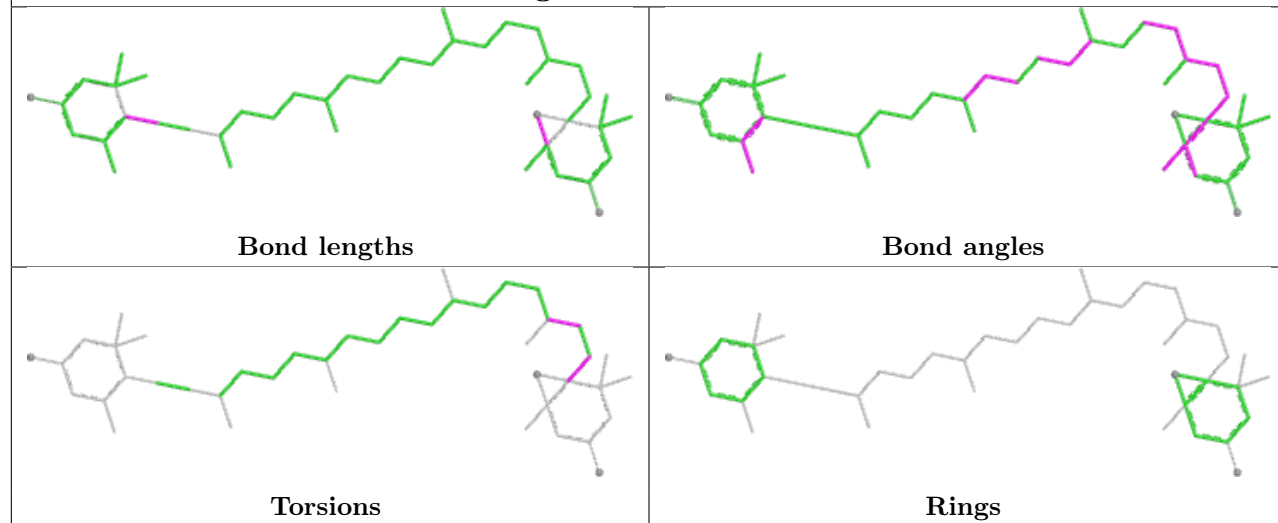
Rings



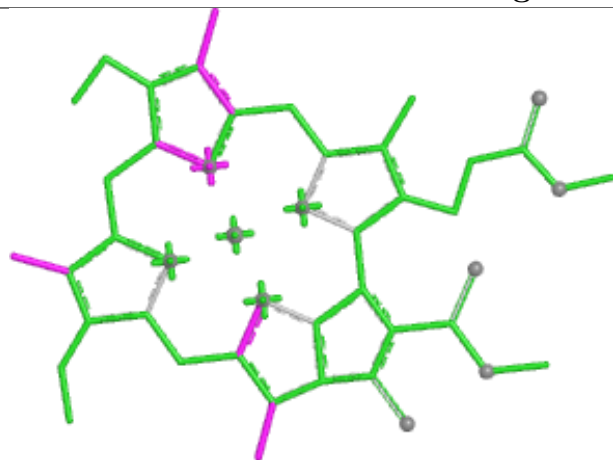
Ligand CLA E 313



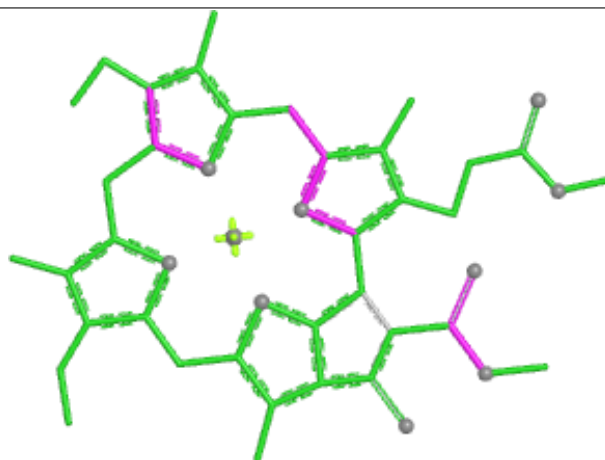
Ligand DD6 E 302



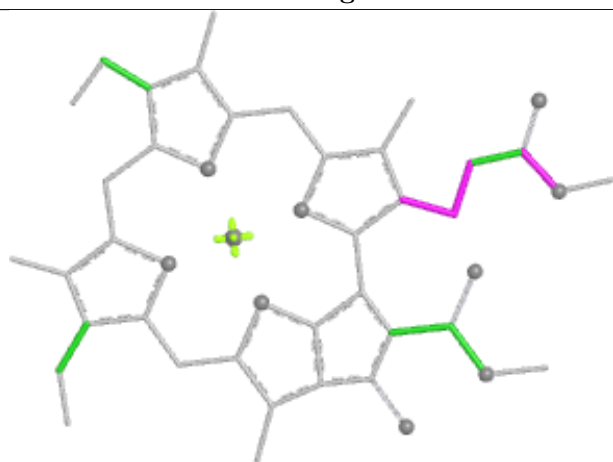
Ligand CLA K 318



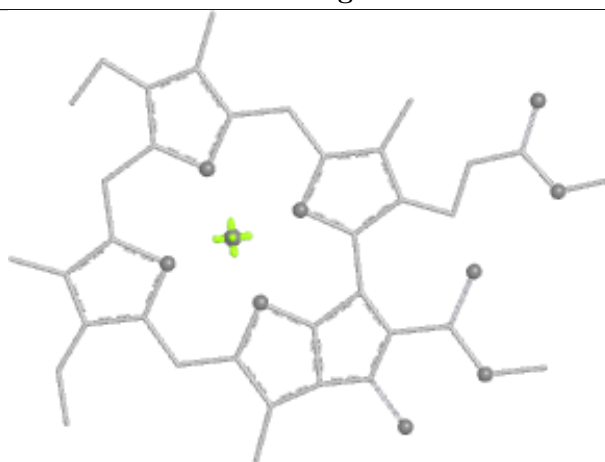
Bond lengths



Bond angles

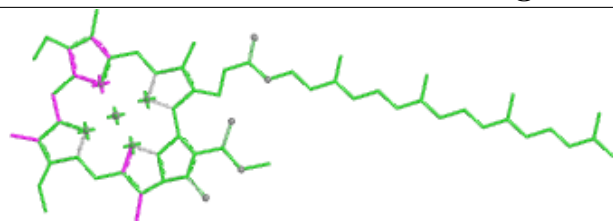


Torsions

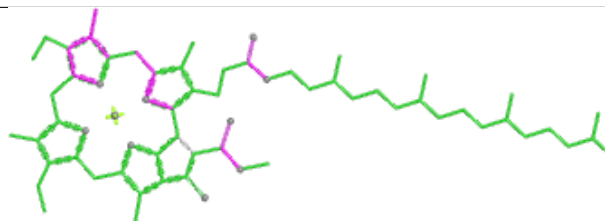


Rings

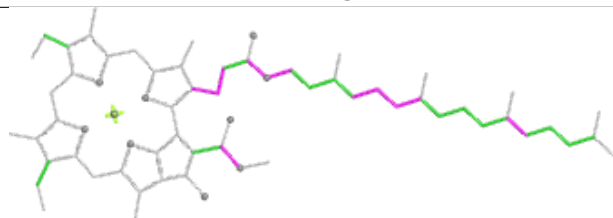
Ligand CLA E 308



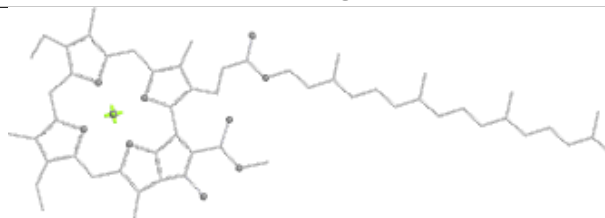
Bond lengths



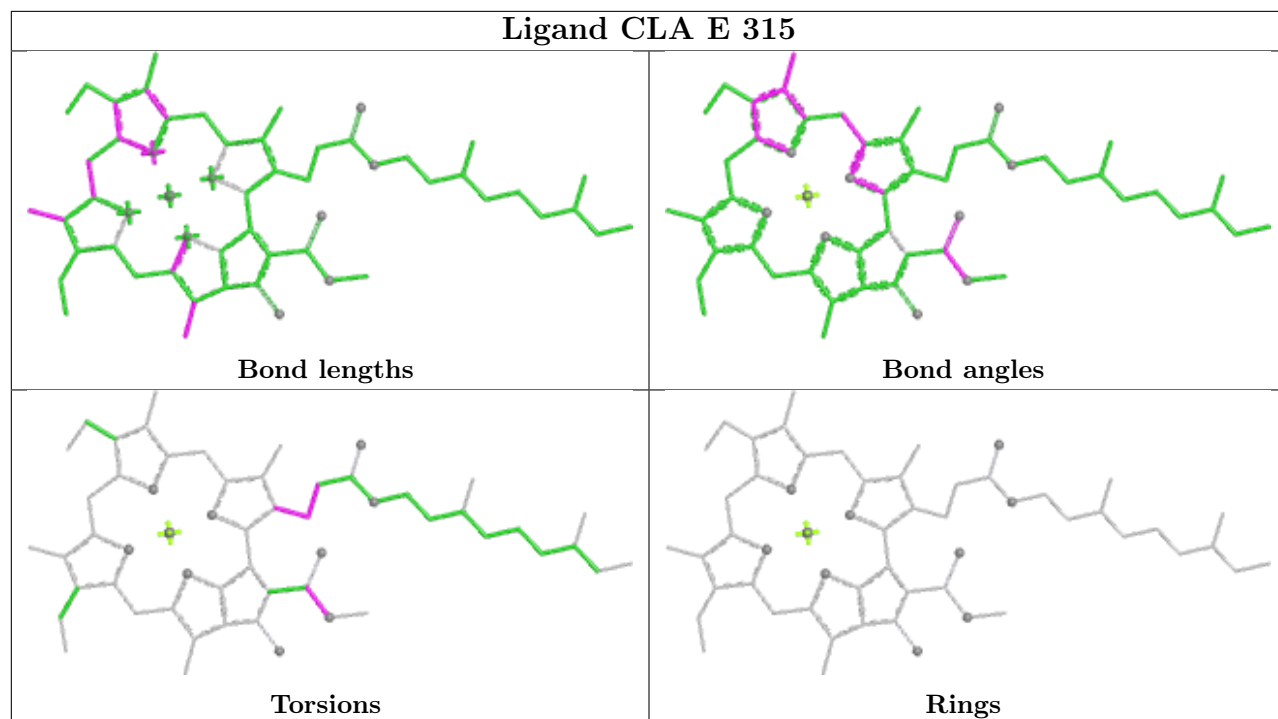
Bond angles



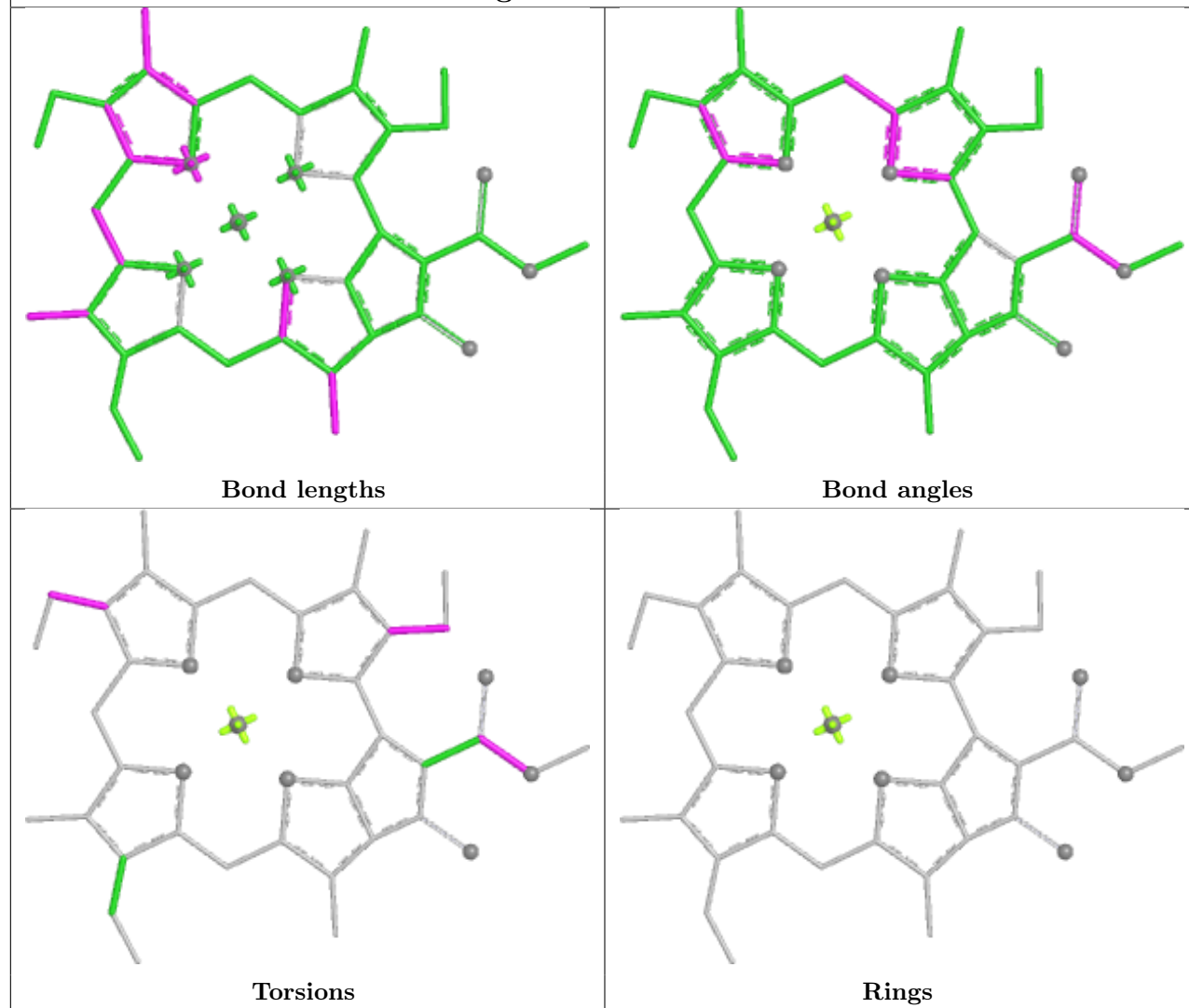
Torsions



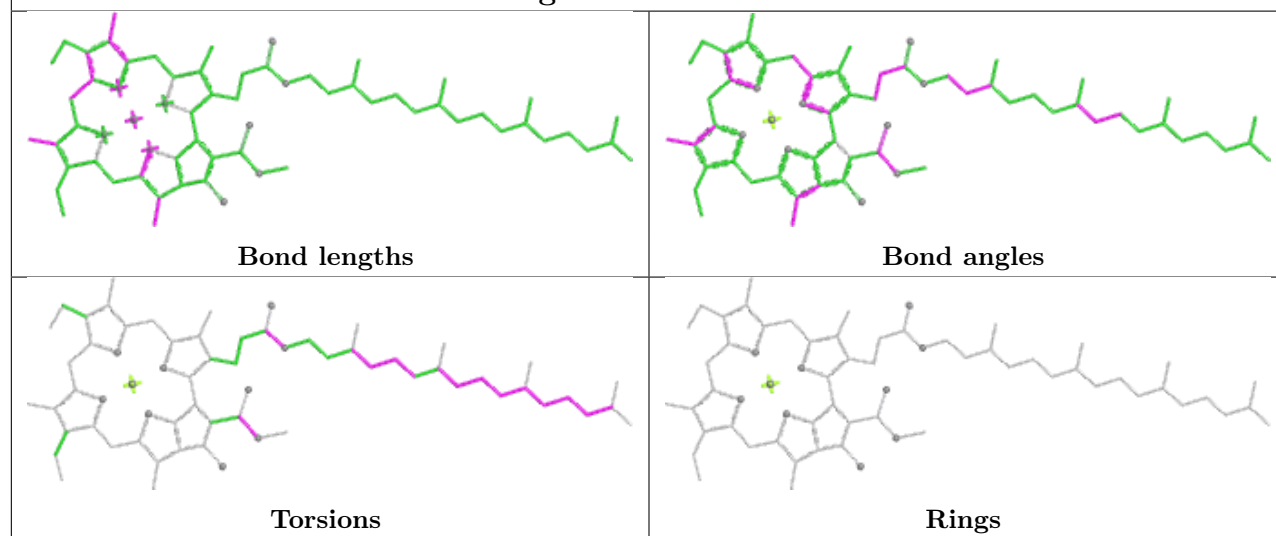
Rings



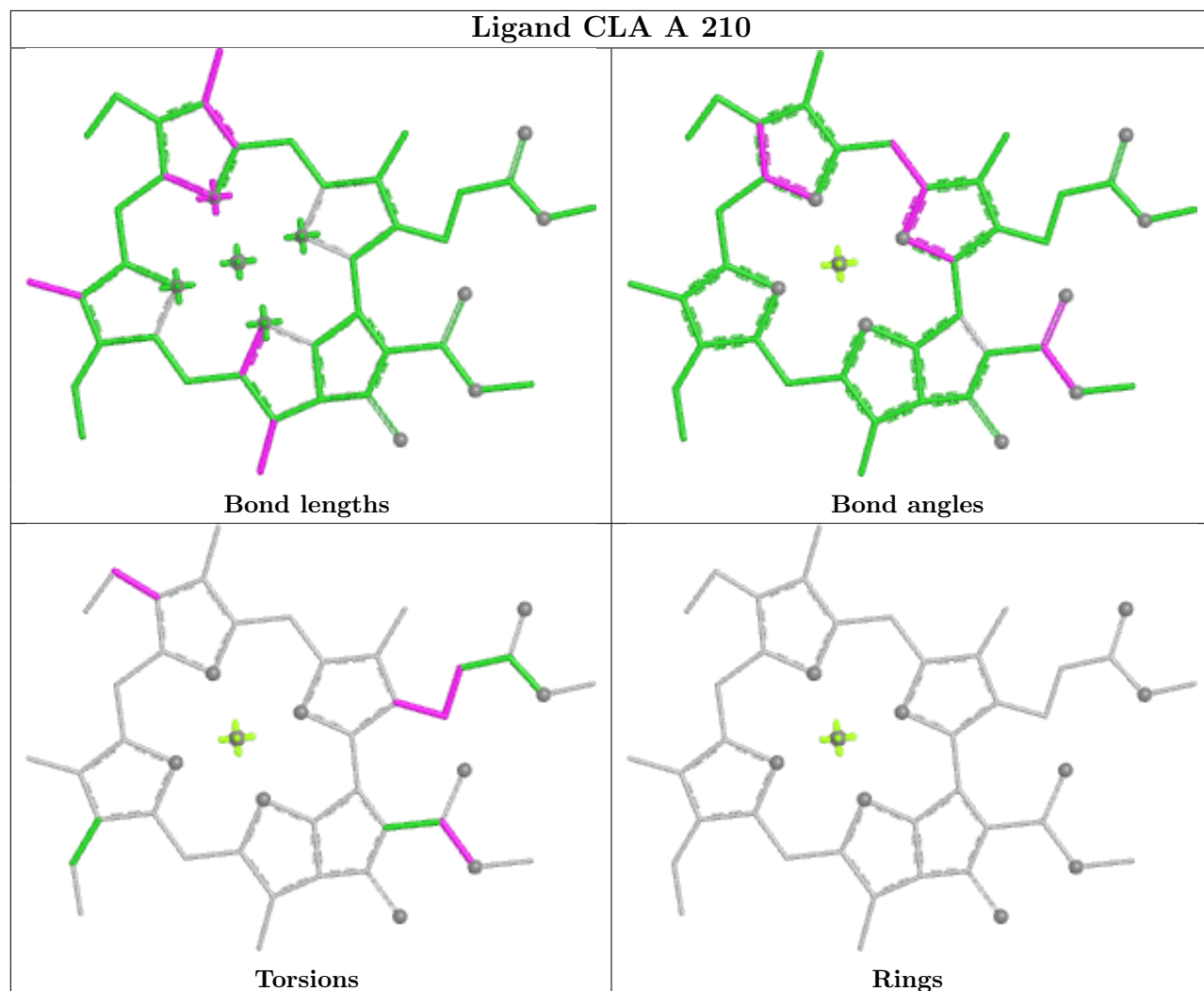
Ligand CLA C 315



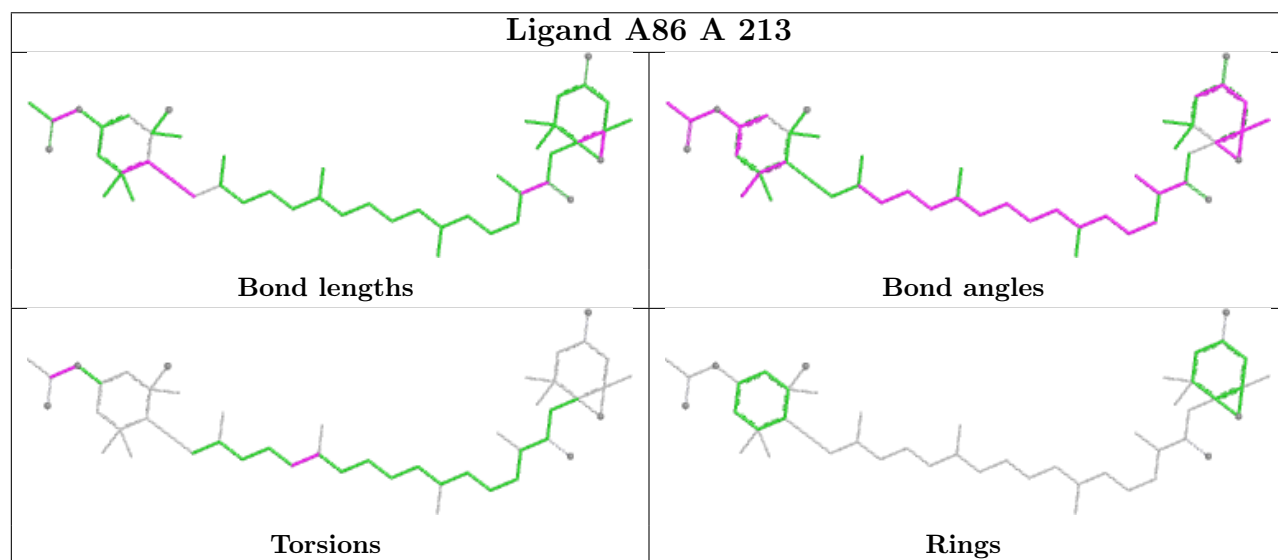
Ligand CLA I 311

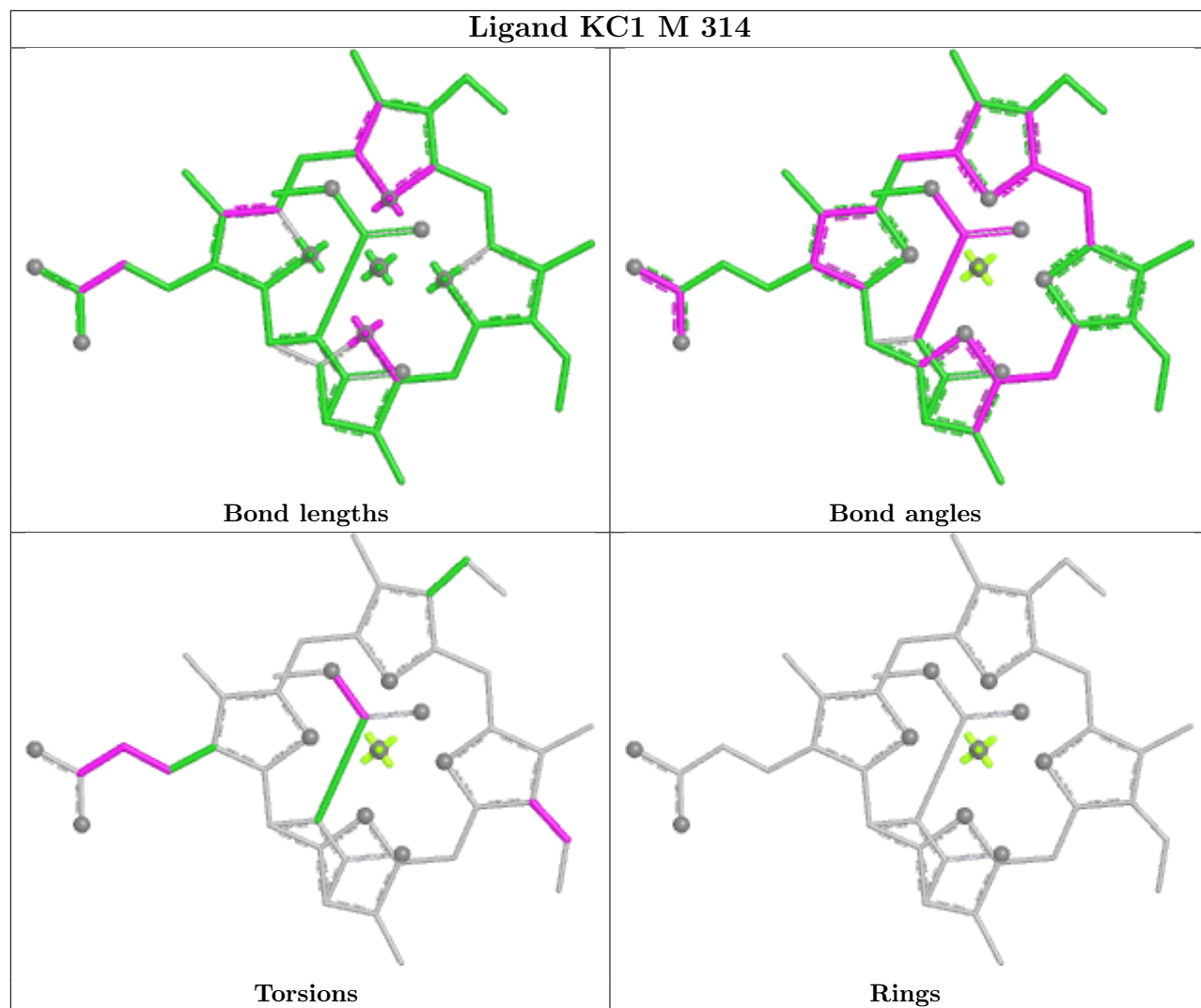


Ligand CLA A 210

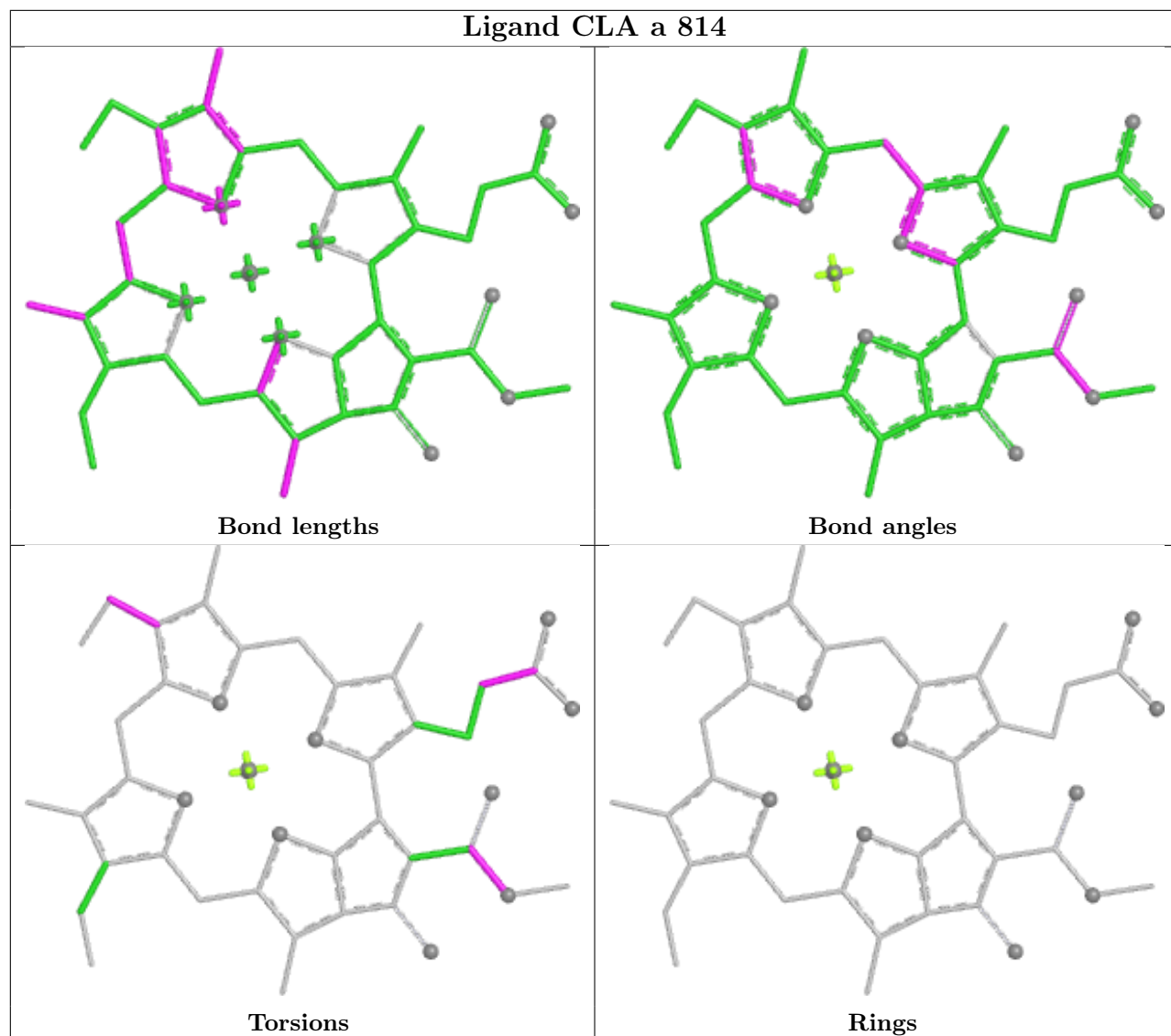


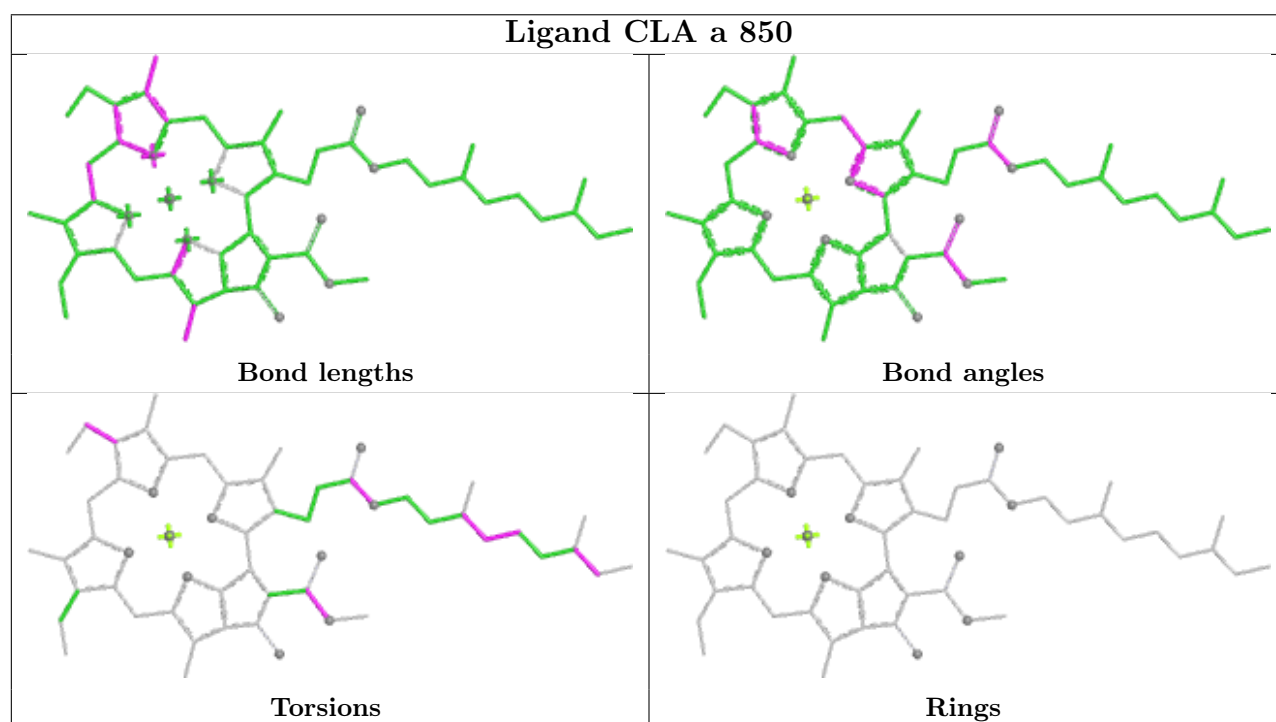
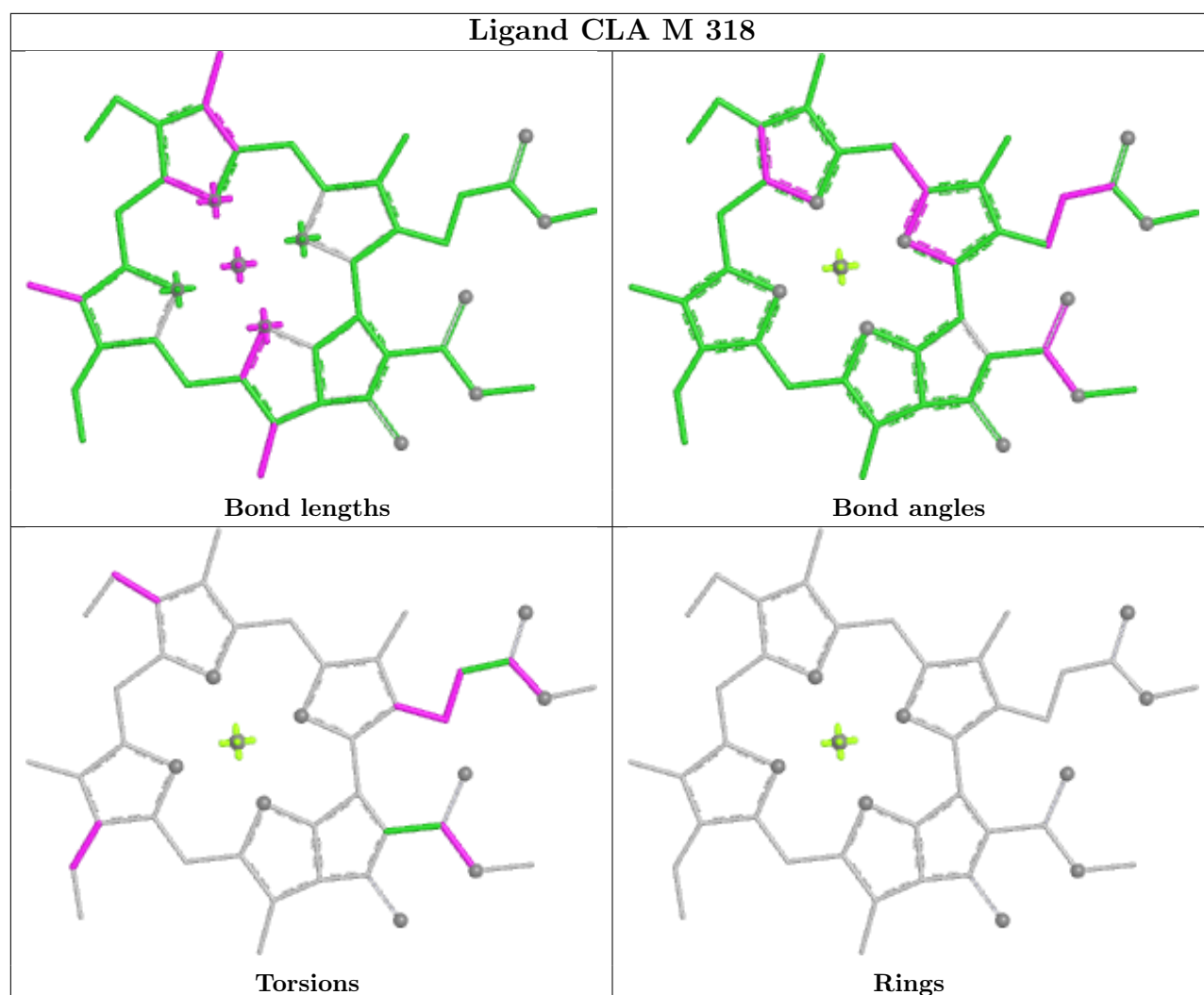
Ligand A86 A 213

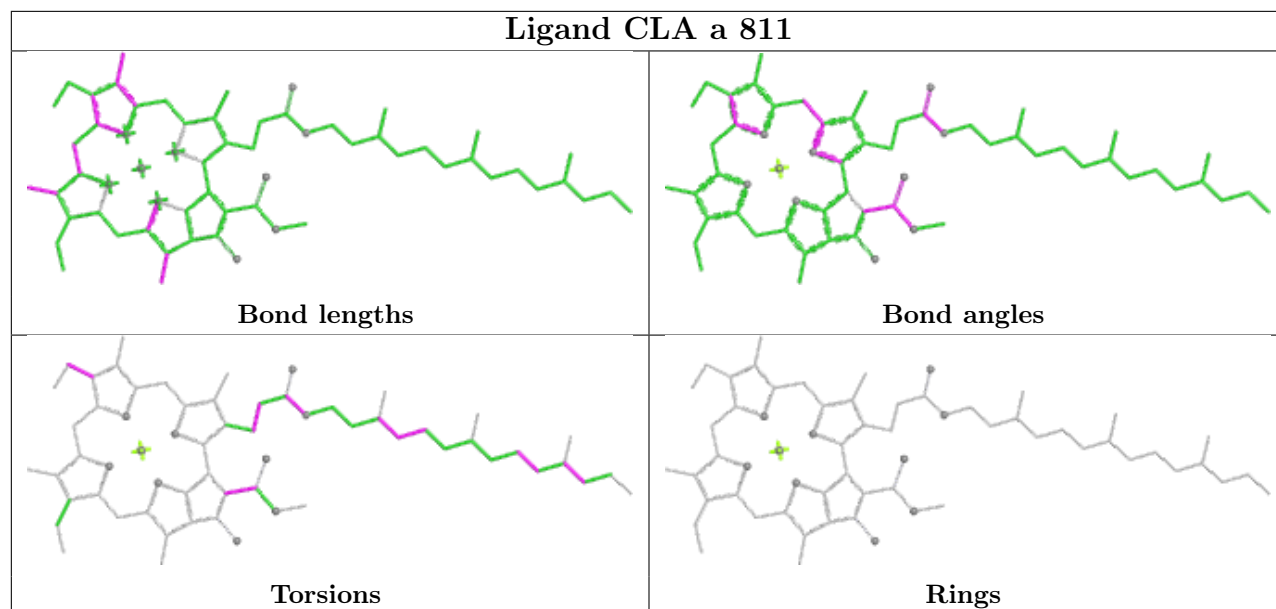
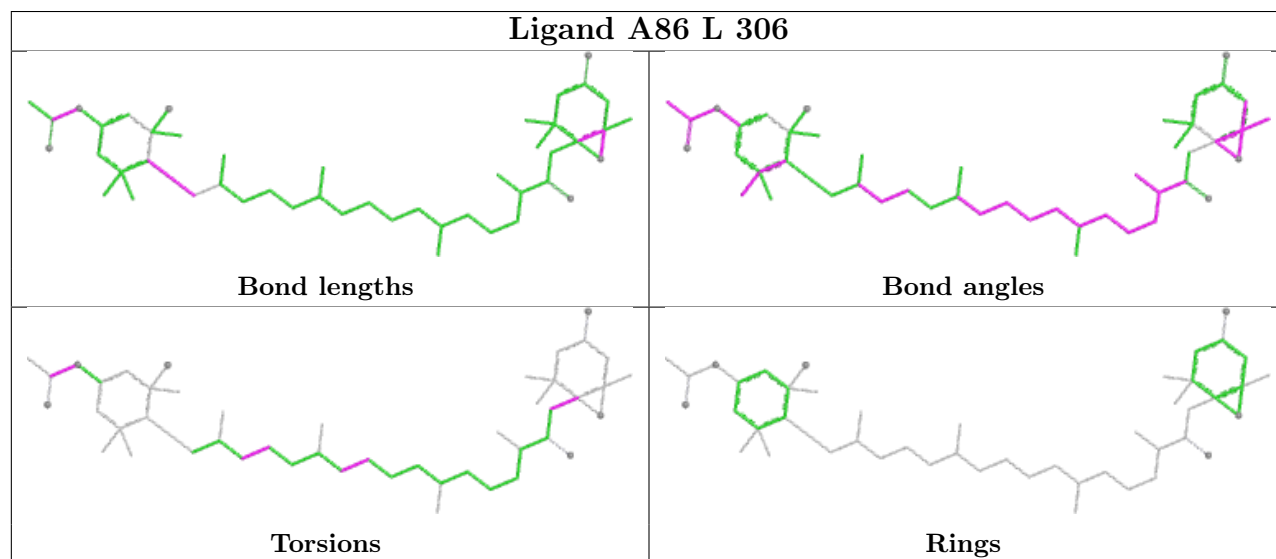


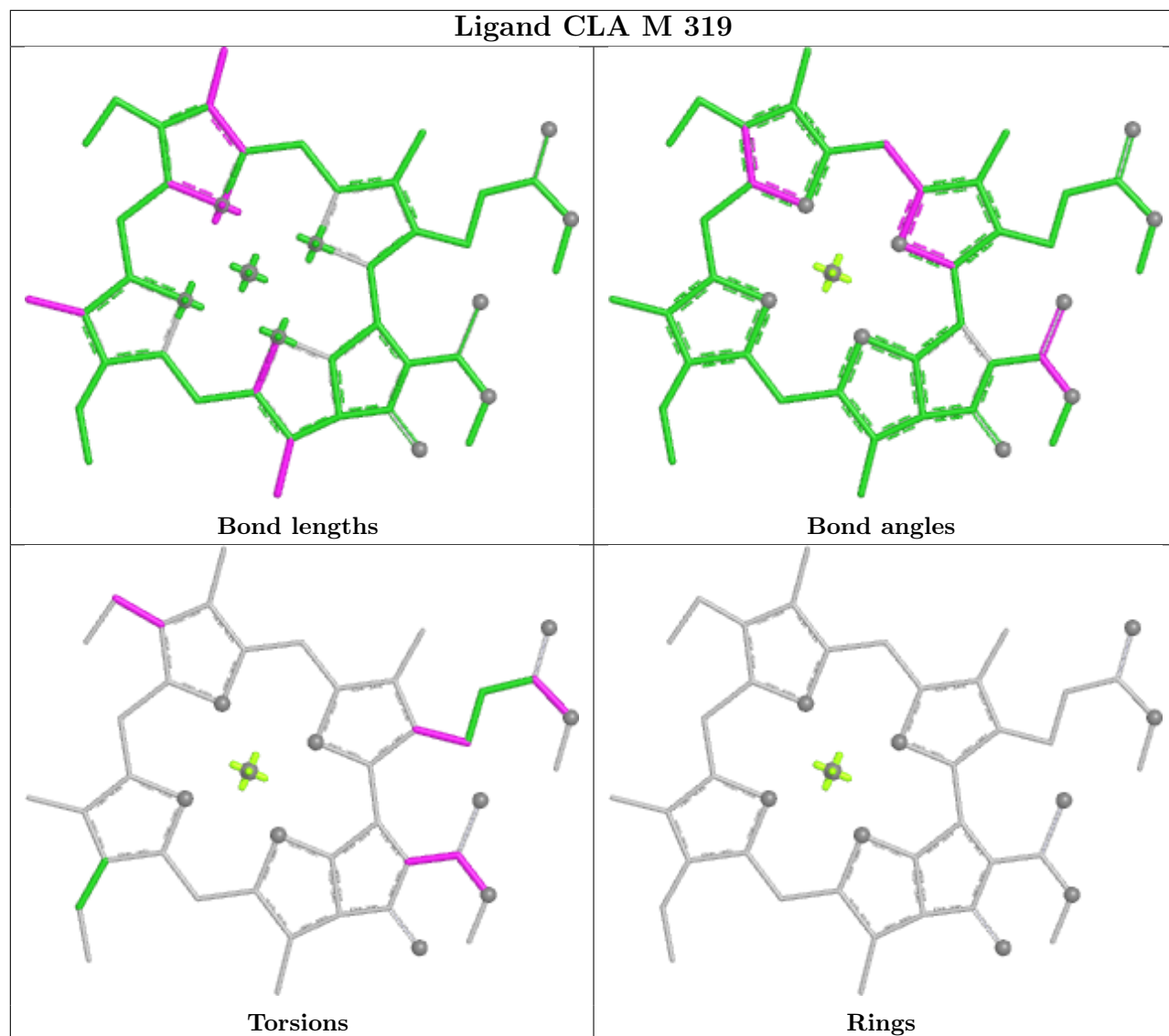


Ligand CLA a 814

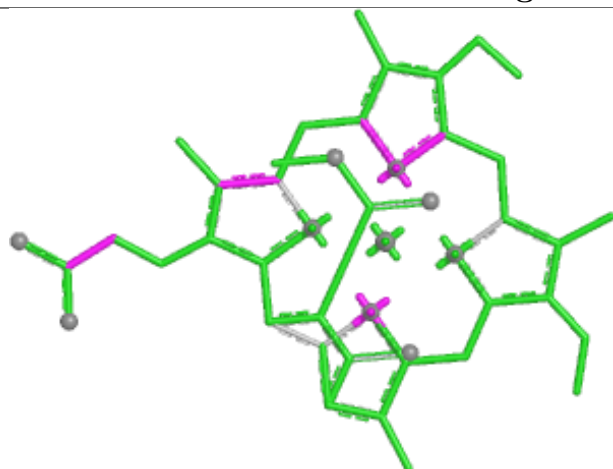




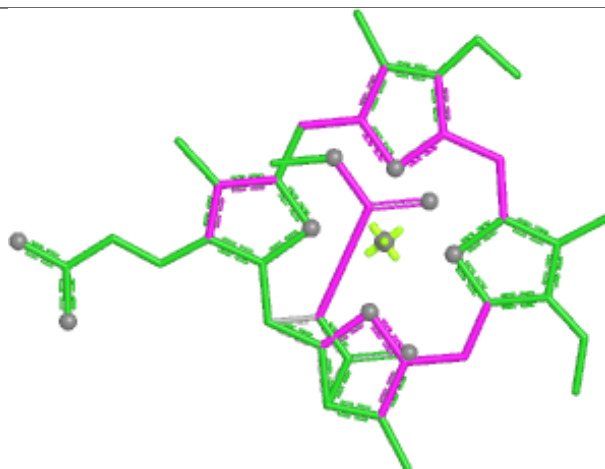
Ligand CLA a 811**Ligand A86 L 306**



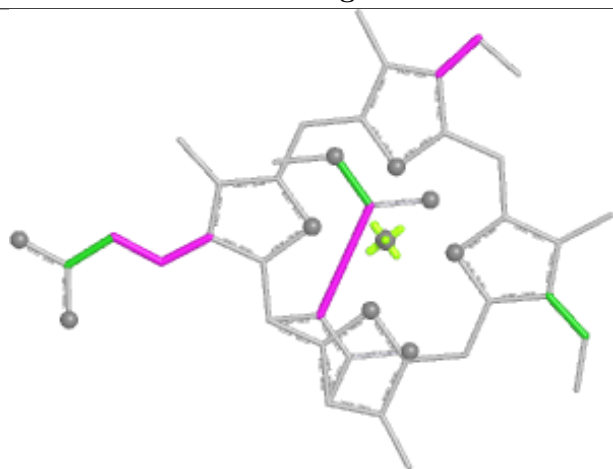
Ligand KC1 C 308



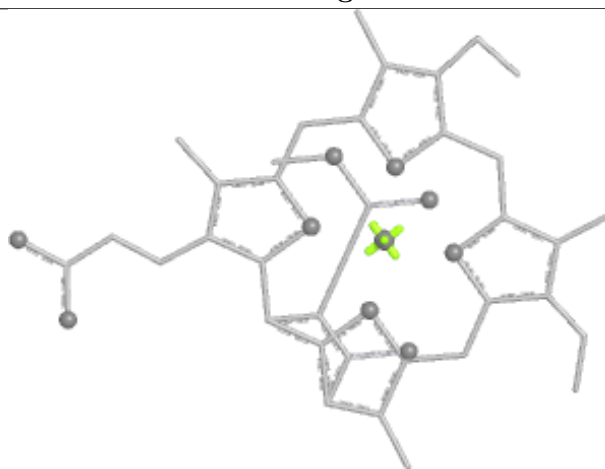
Bond lengths



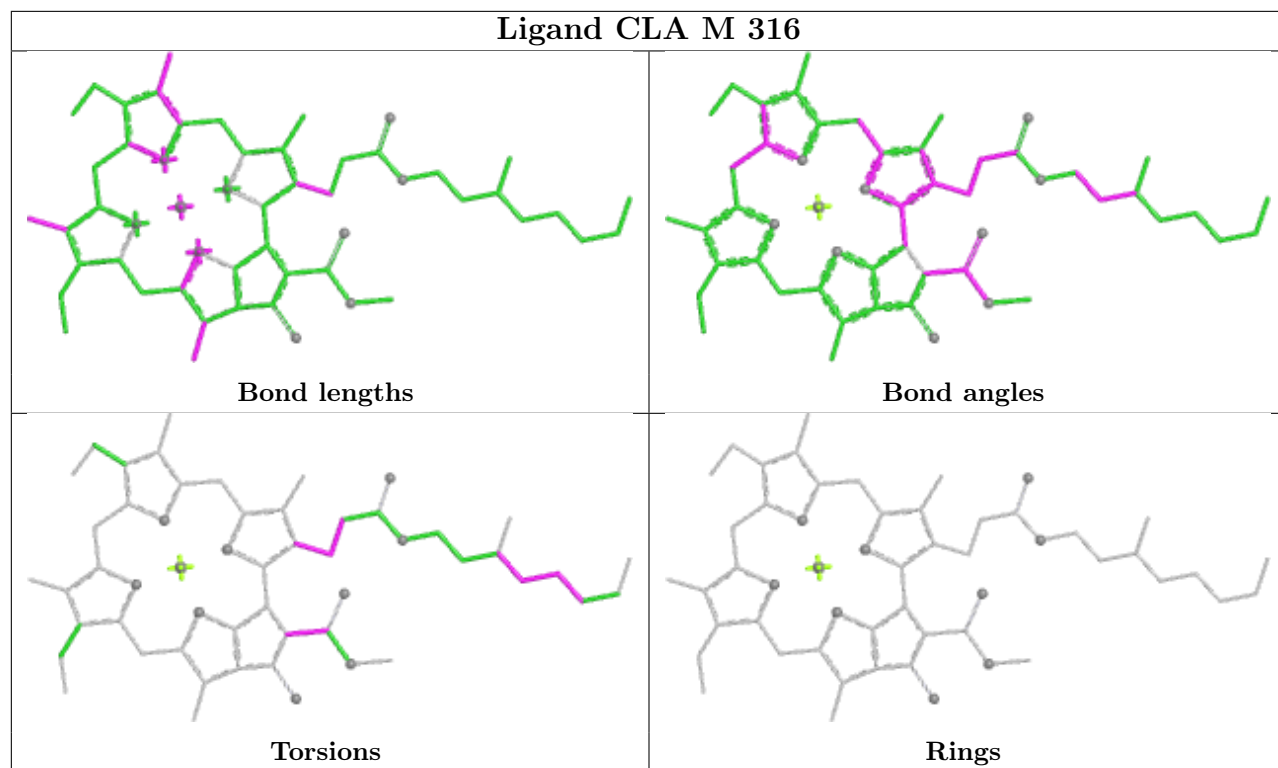
Bond angles



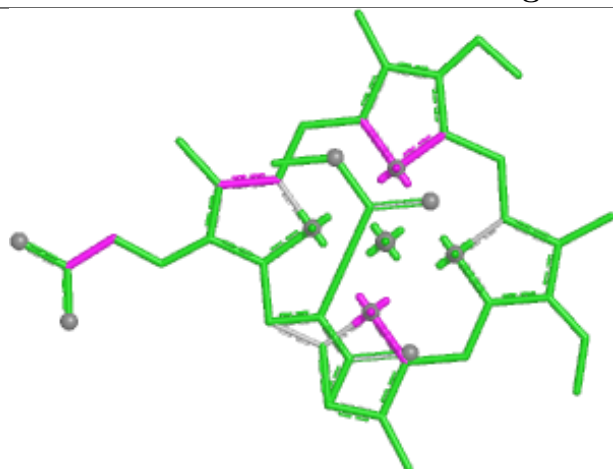
Torsions



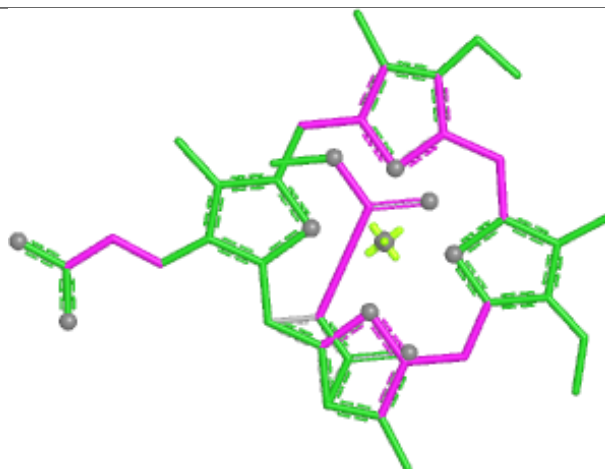
Rings



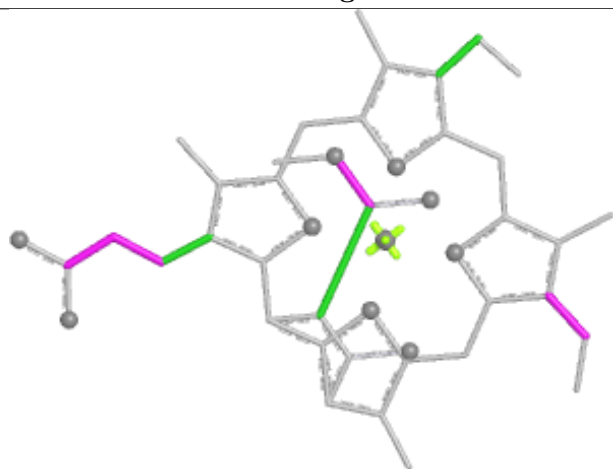
Ligand KC1 I 312



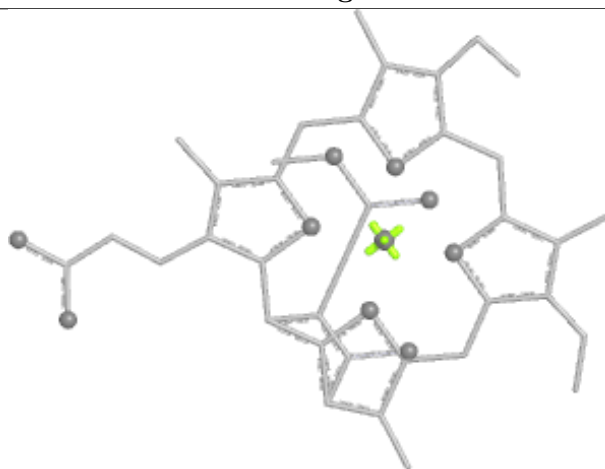
Bond lengths



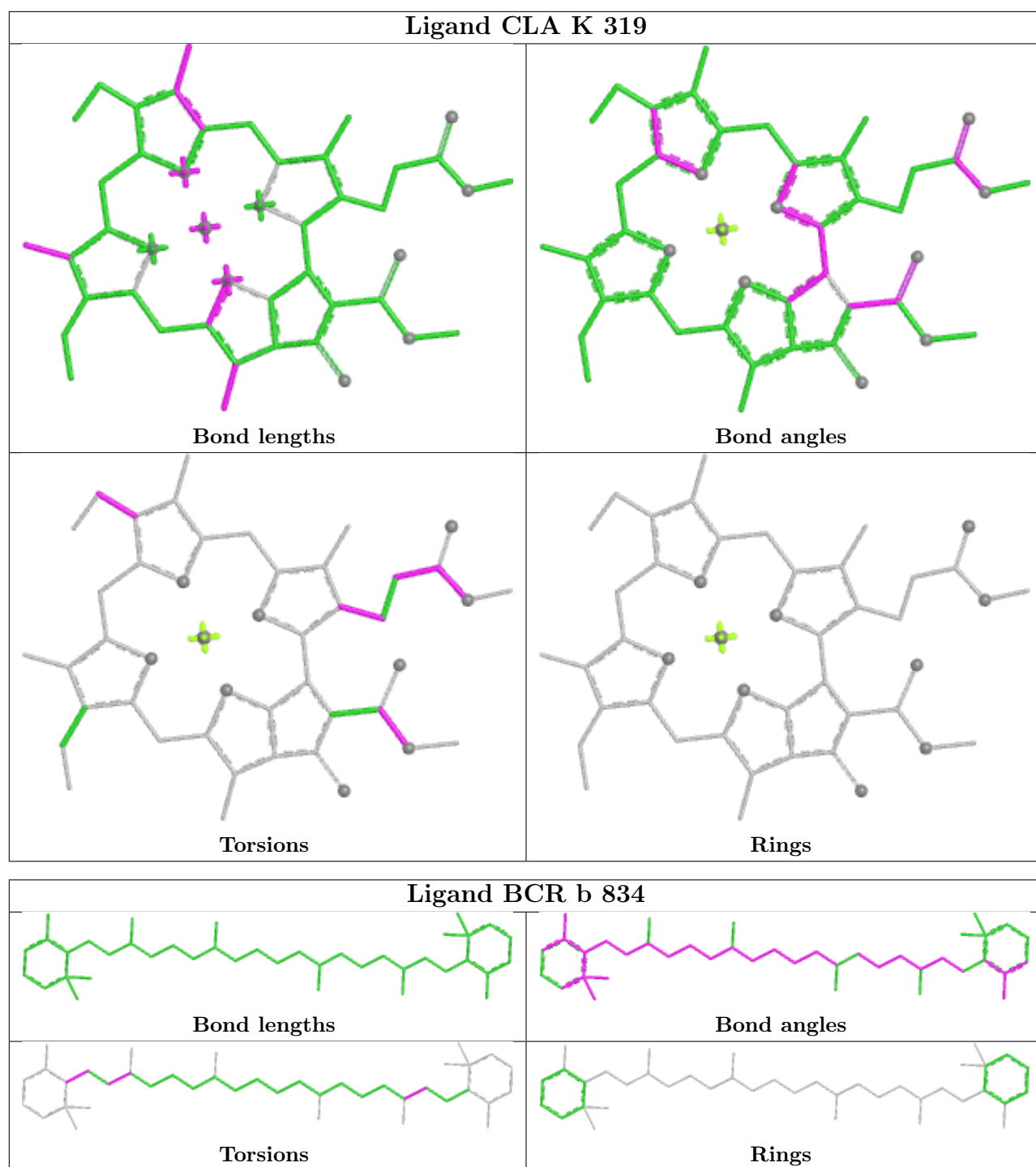
Bond angles



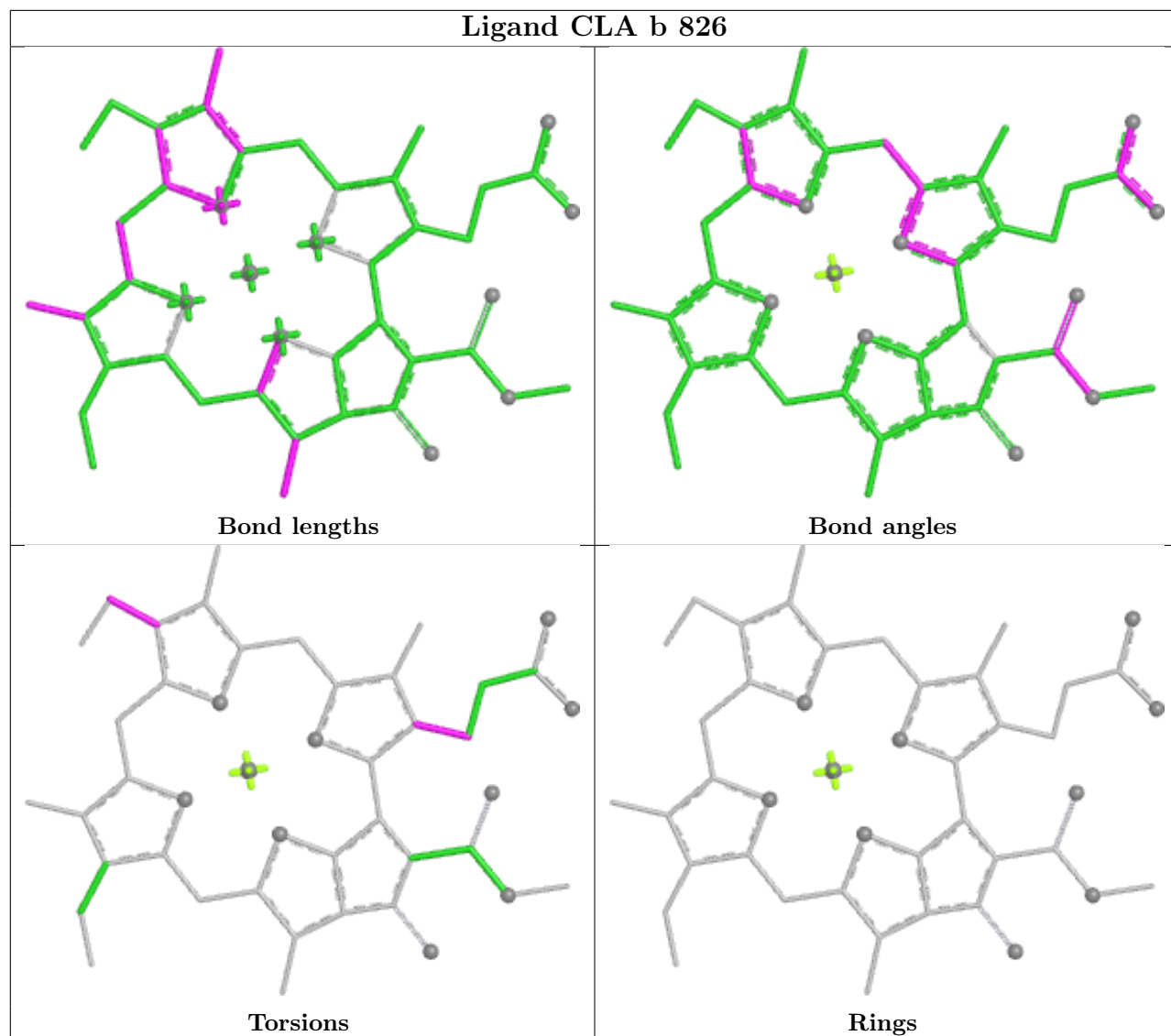
Torsions

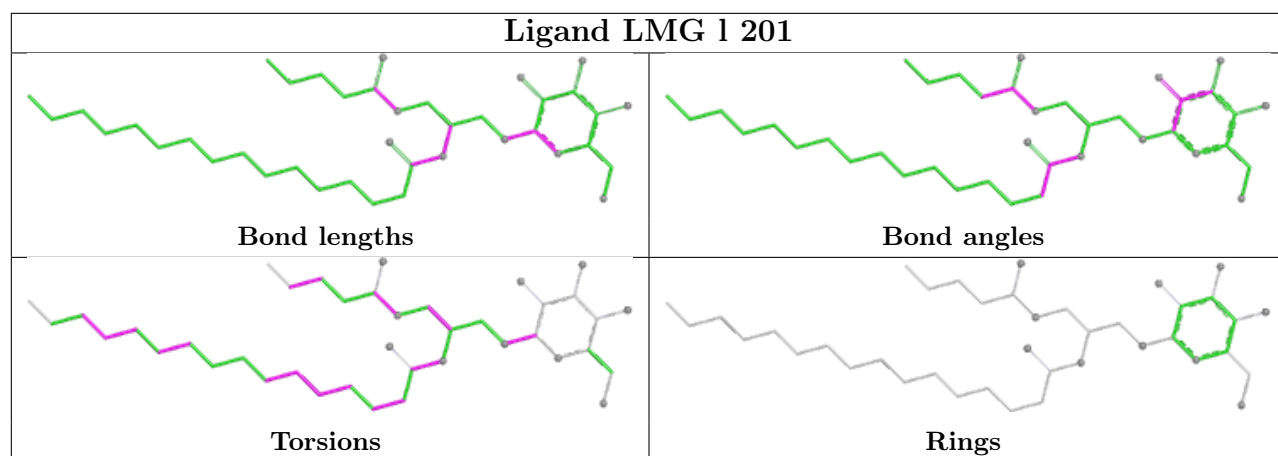
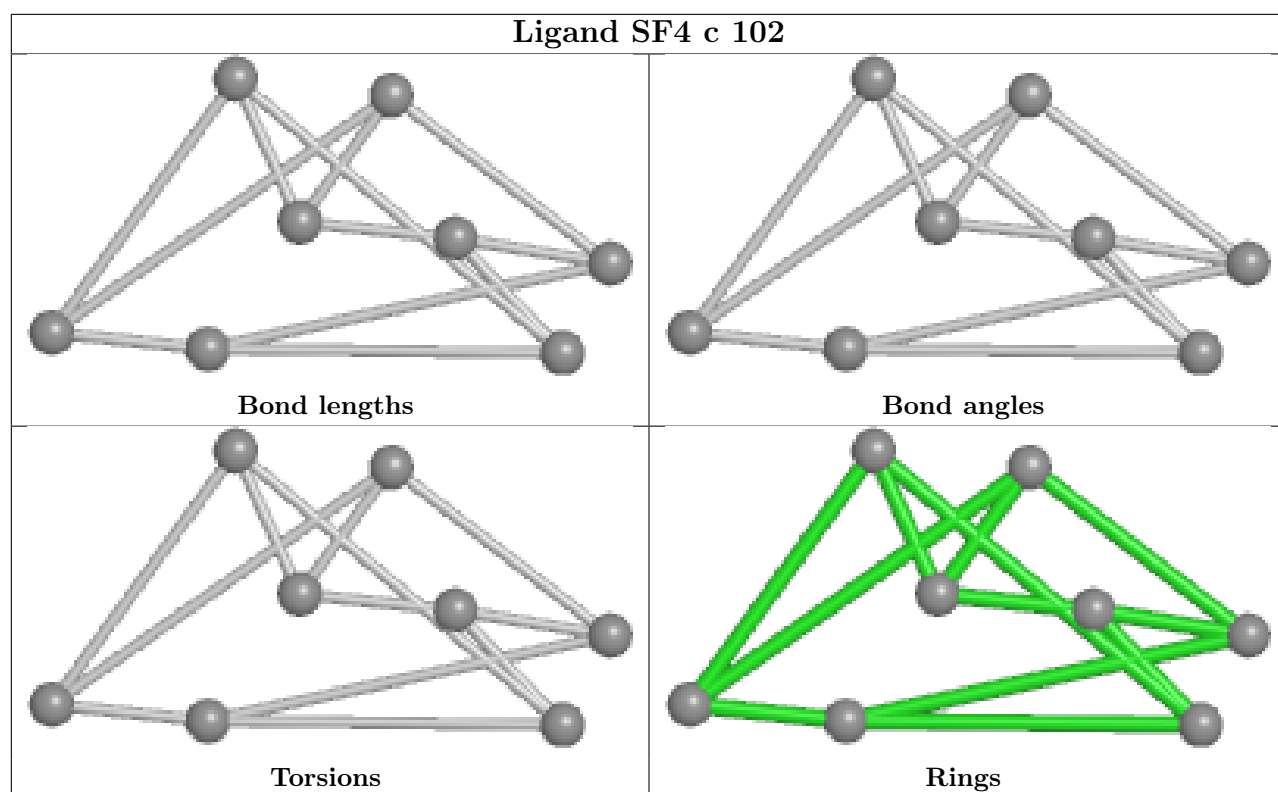


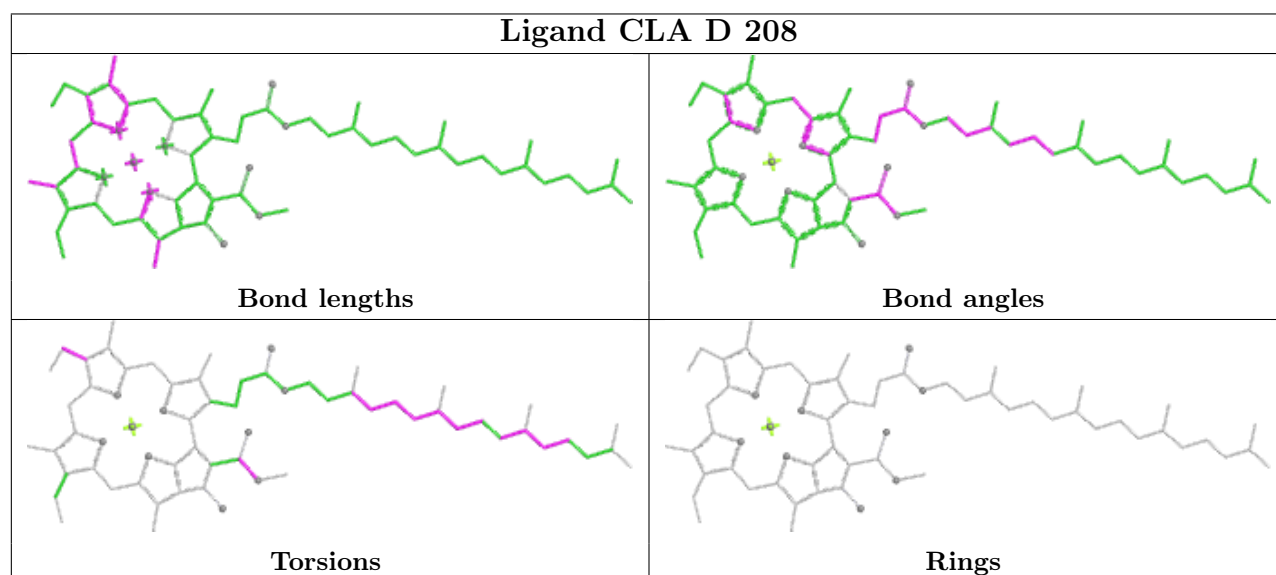
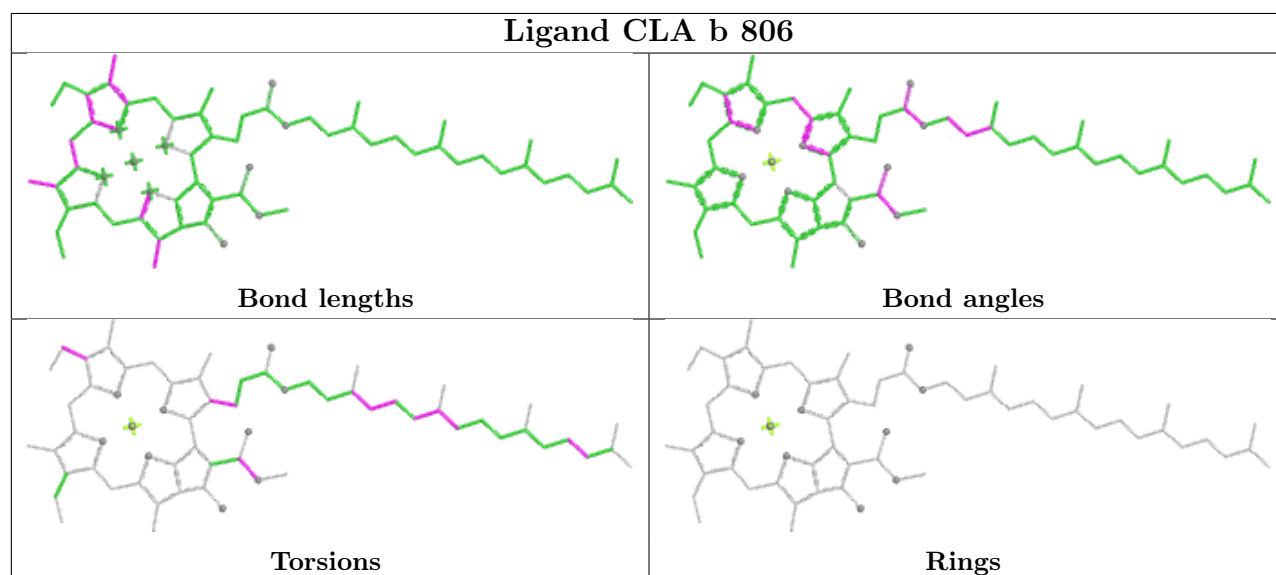
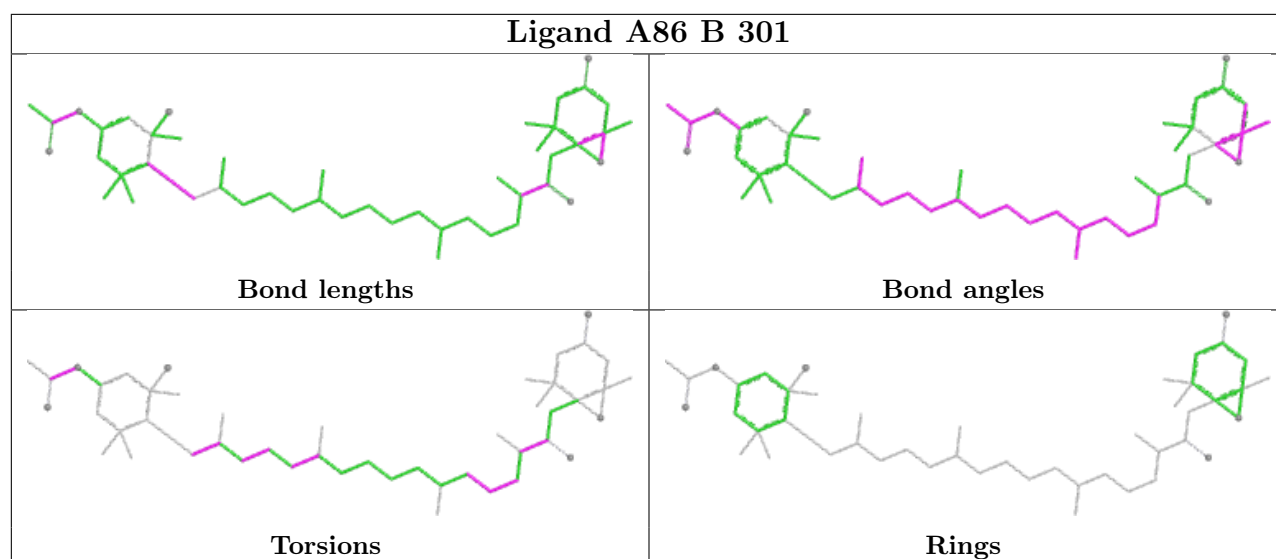
Rings

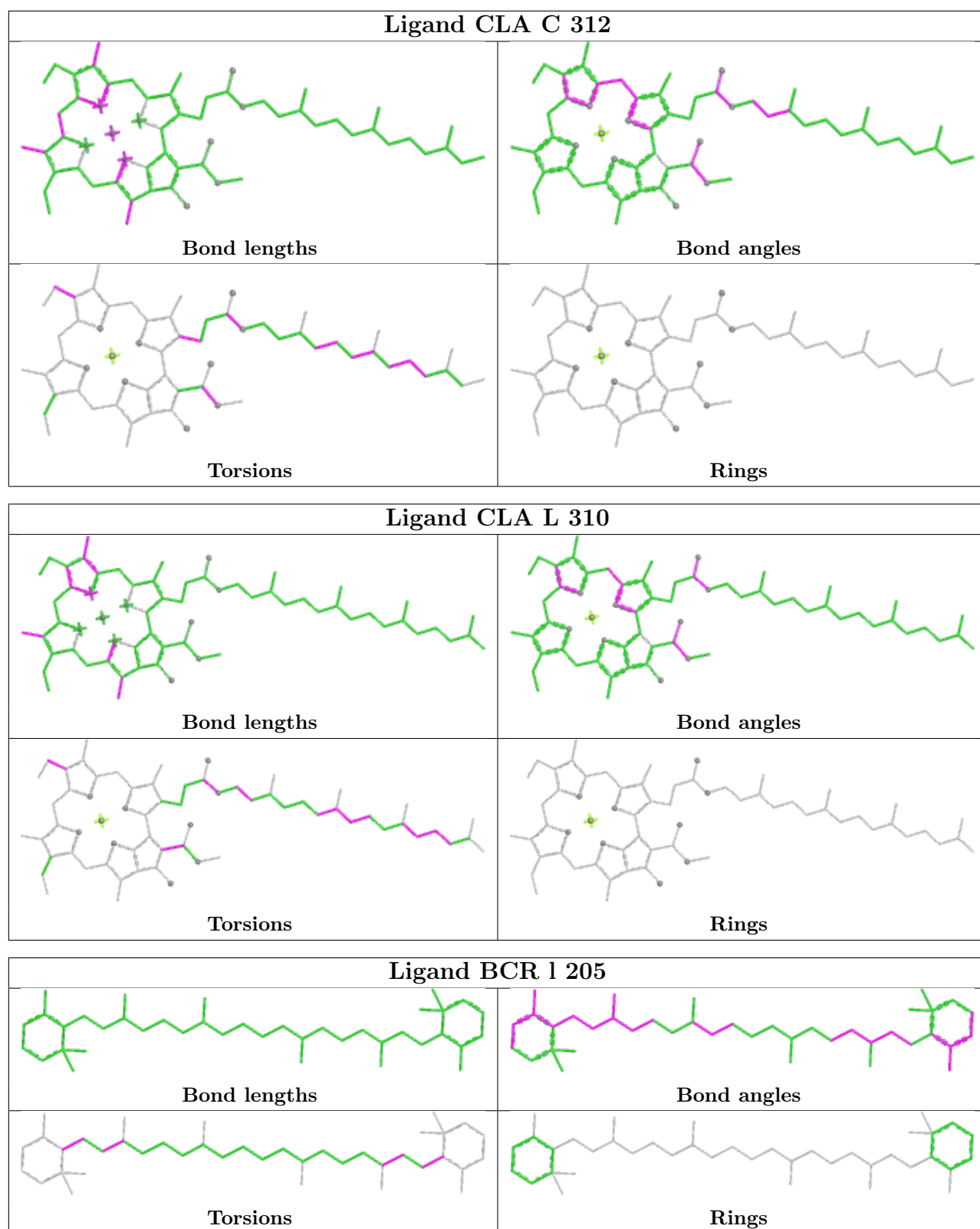


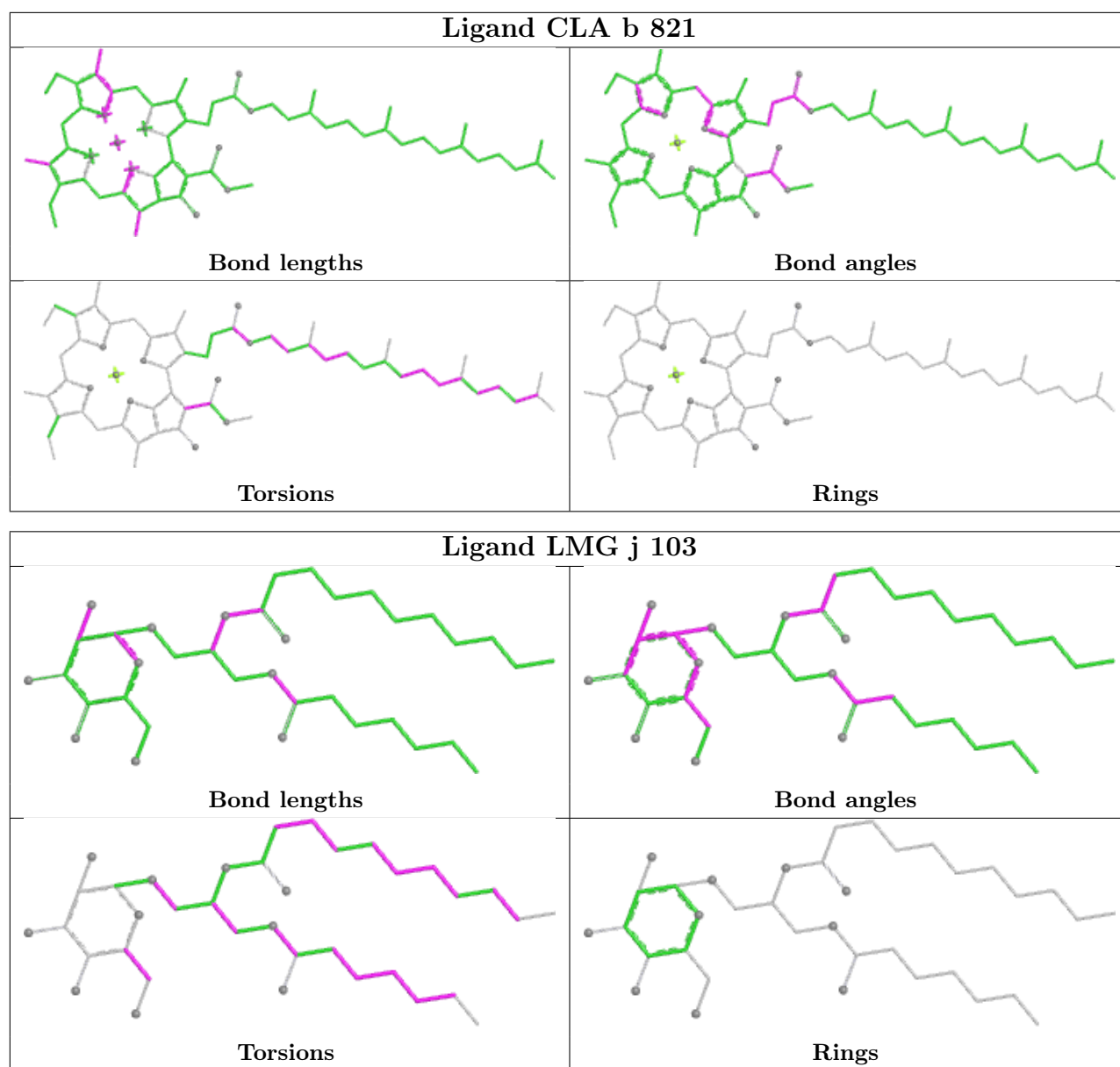
Ligand CLA b 826

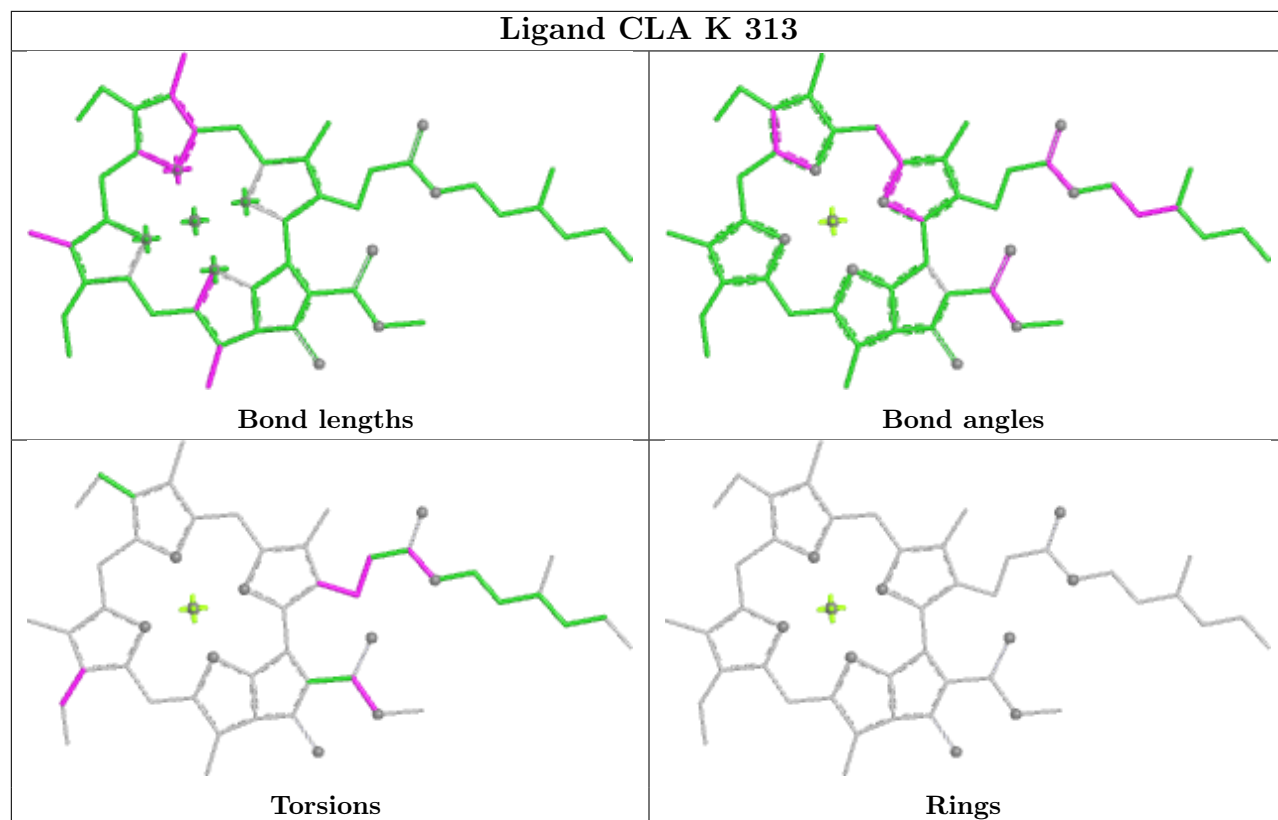




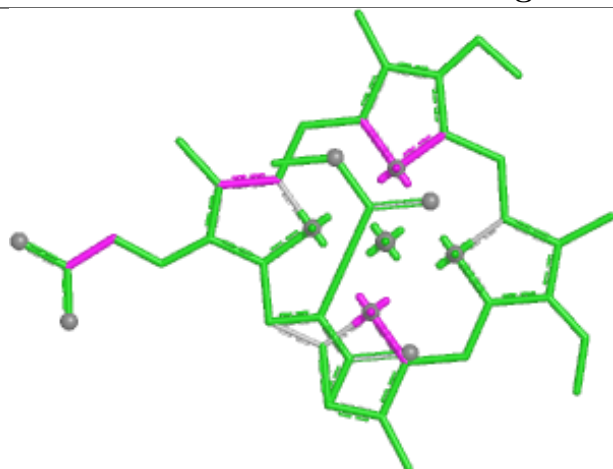




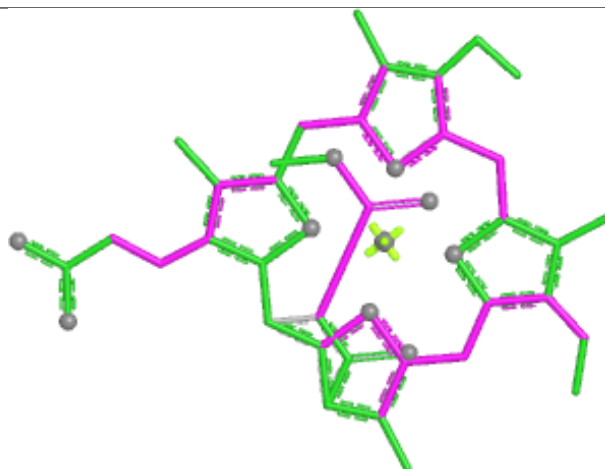




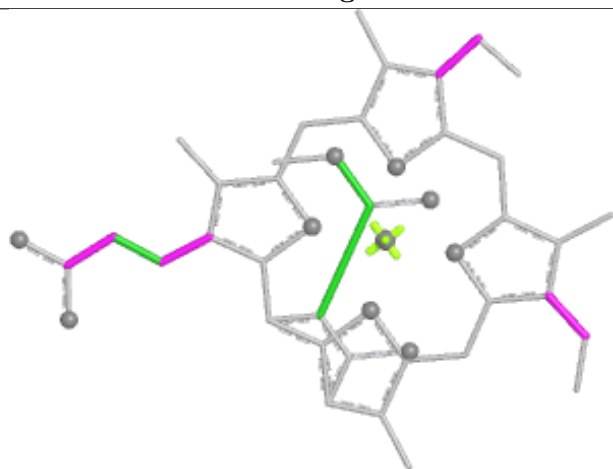
Ligand KC1 K 308



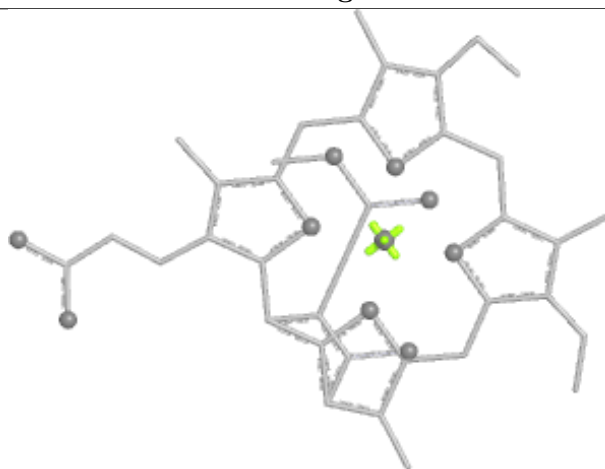
Bond lengths



Bond angles

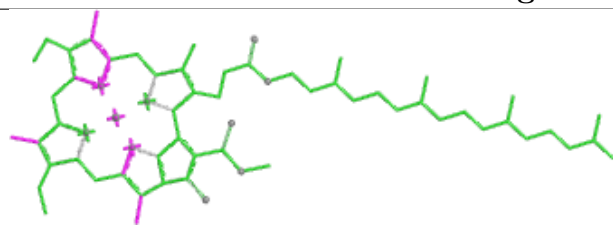


Torsions

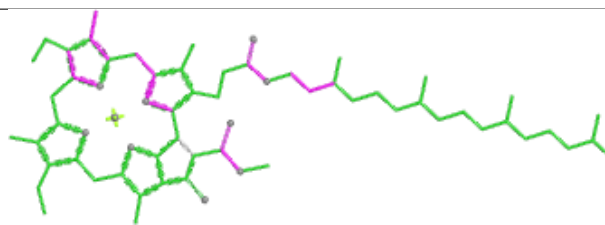


Rings

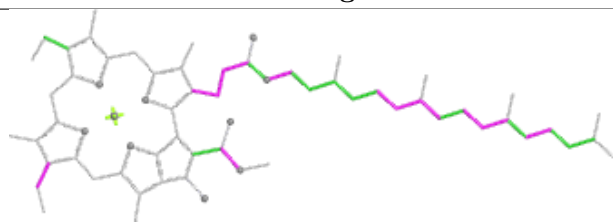
Ligand CLA b 825



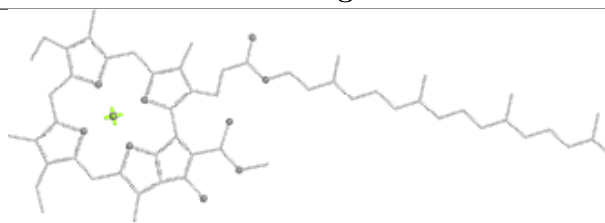
Bond lengths



Bond angles

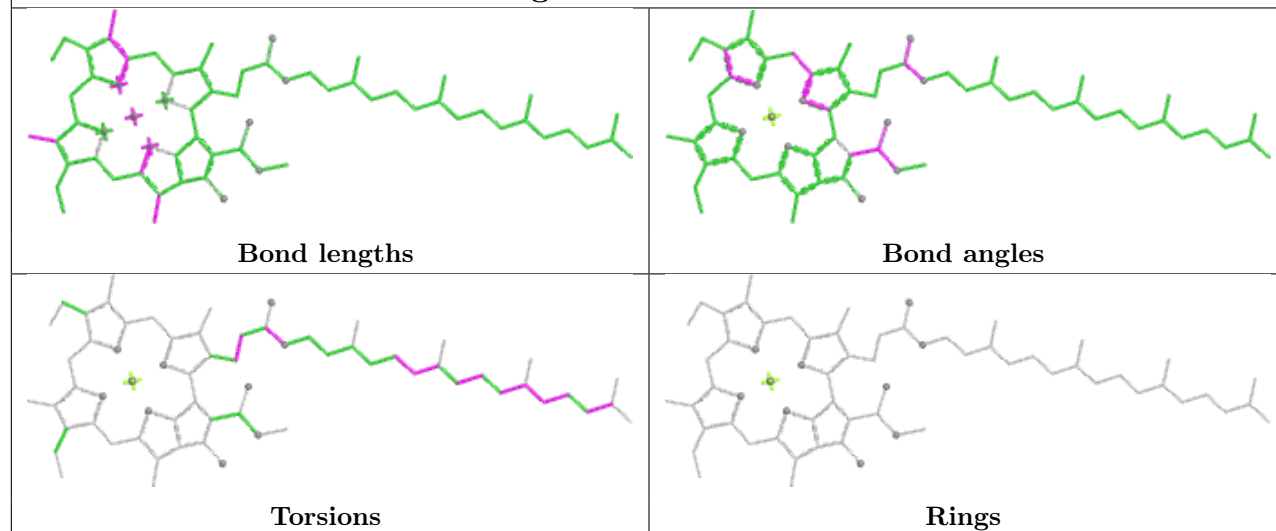


Torsions

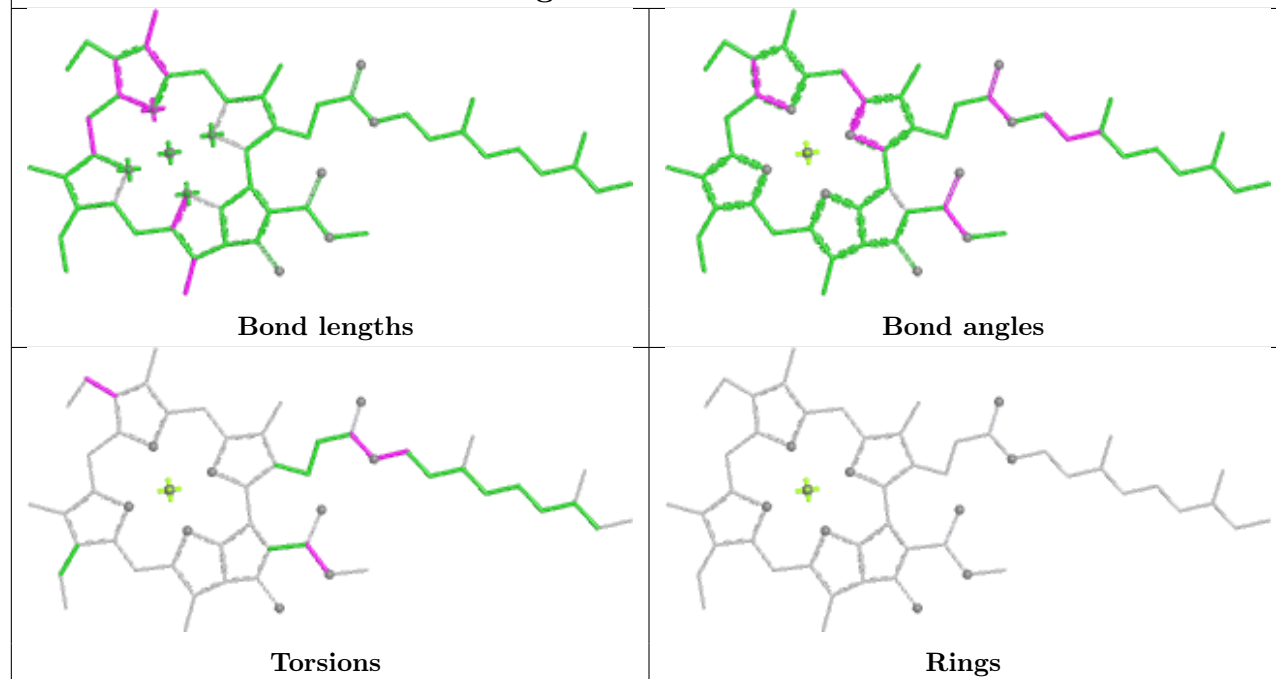


Rings

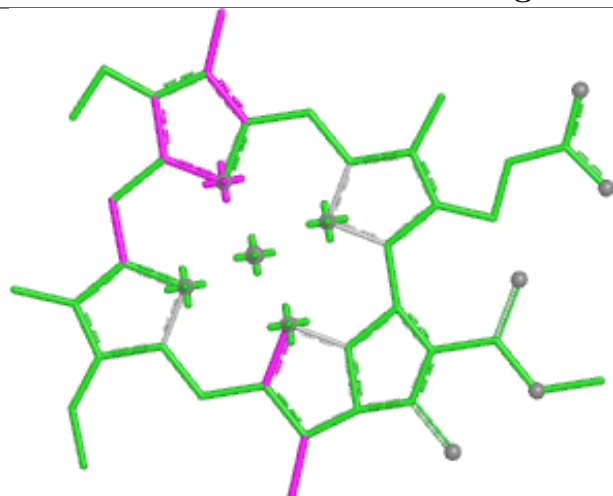
Ligand CLA H 205



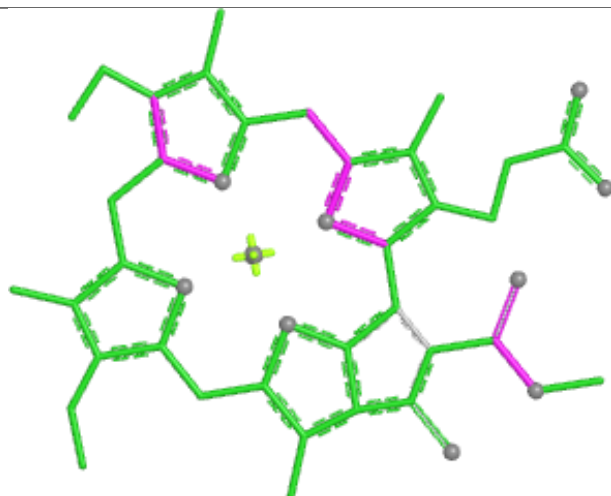
Ligand CLA J 308



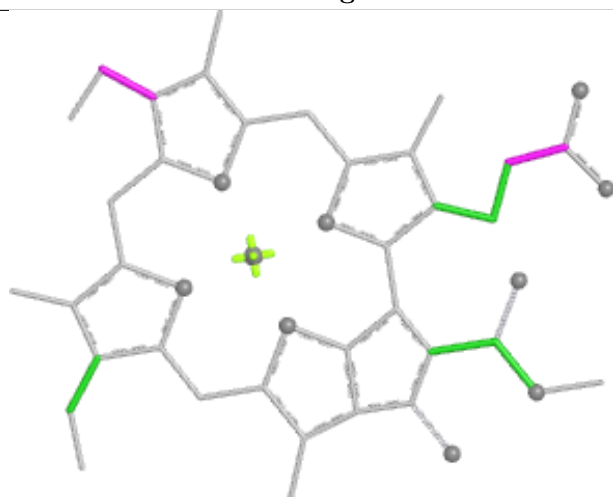
Ligand CLA C 306



Bond lengths



Bond angles

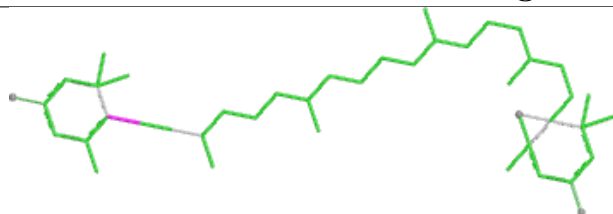


Torsions

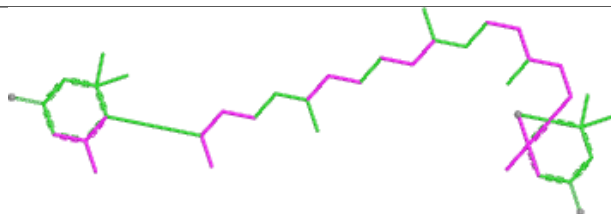


Rings

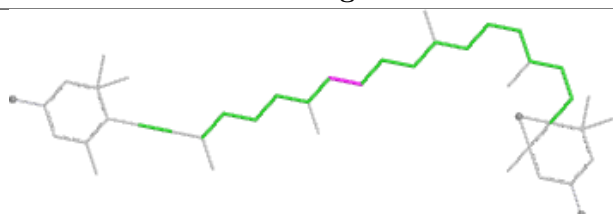
Ligand DD6 F 302



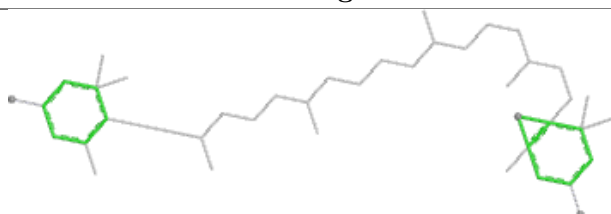
Bond lengths



Bond angles

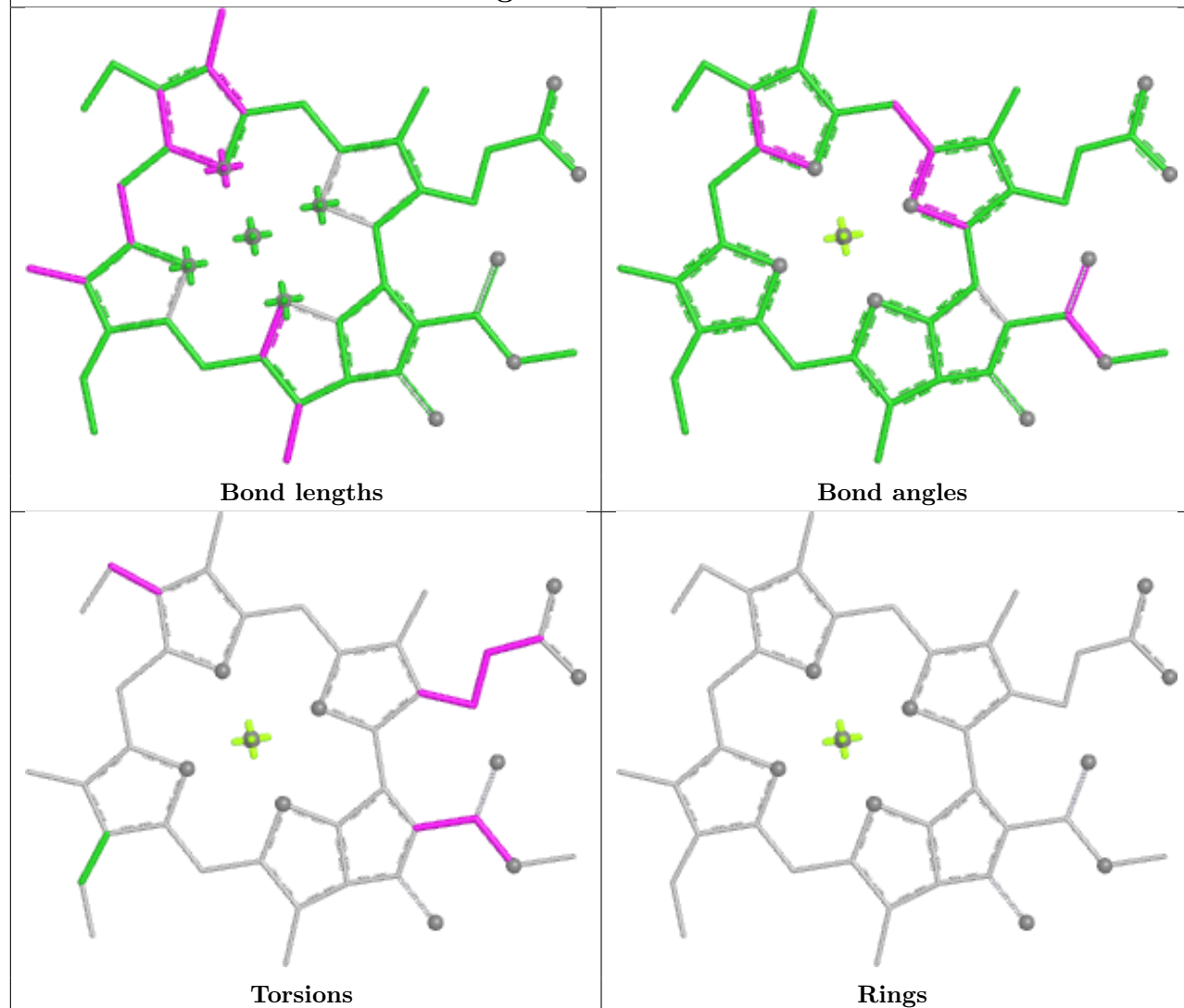


Torsions

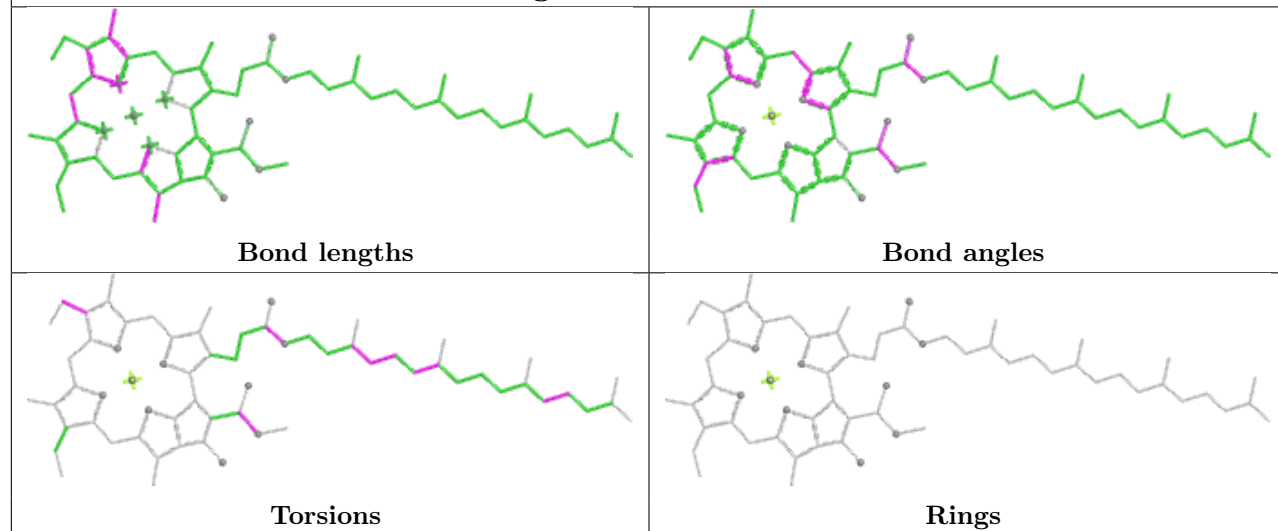


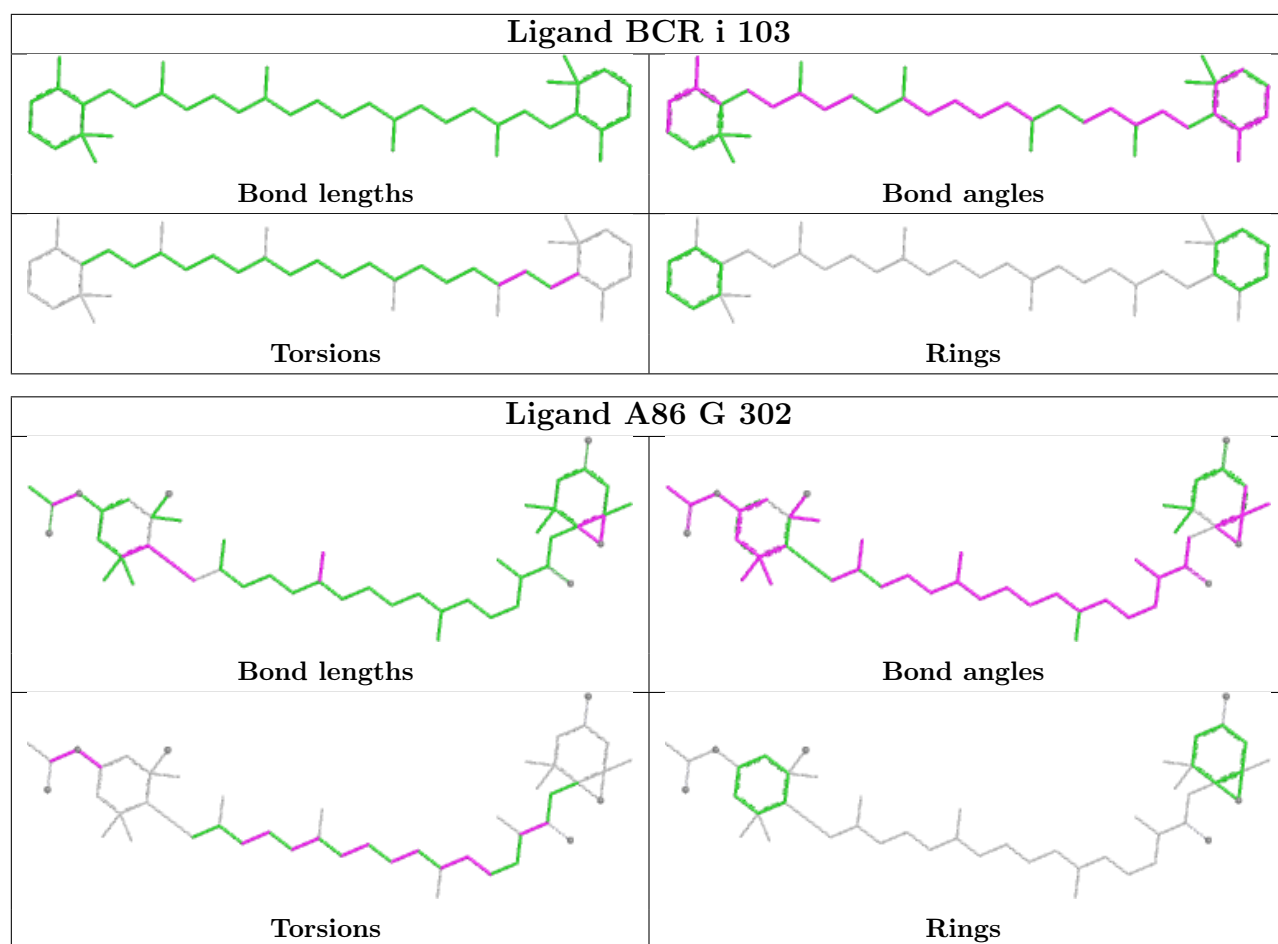
Rings

Ligand CLA a 818

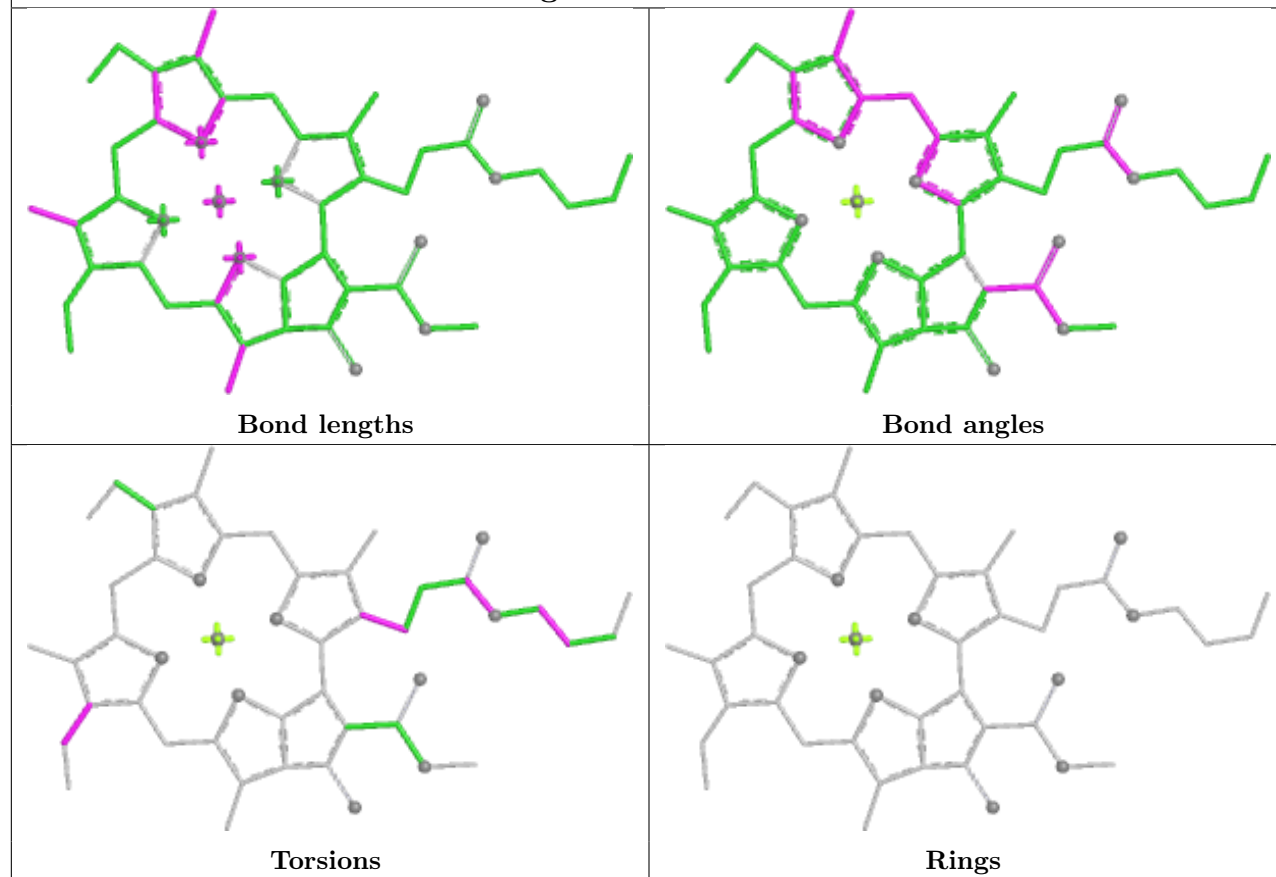


Ligand CLA B 311

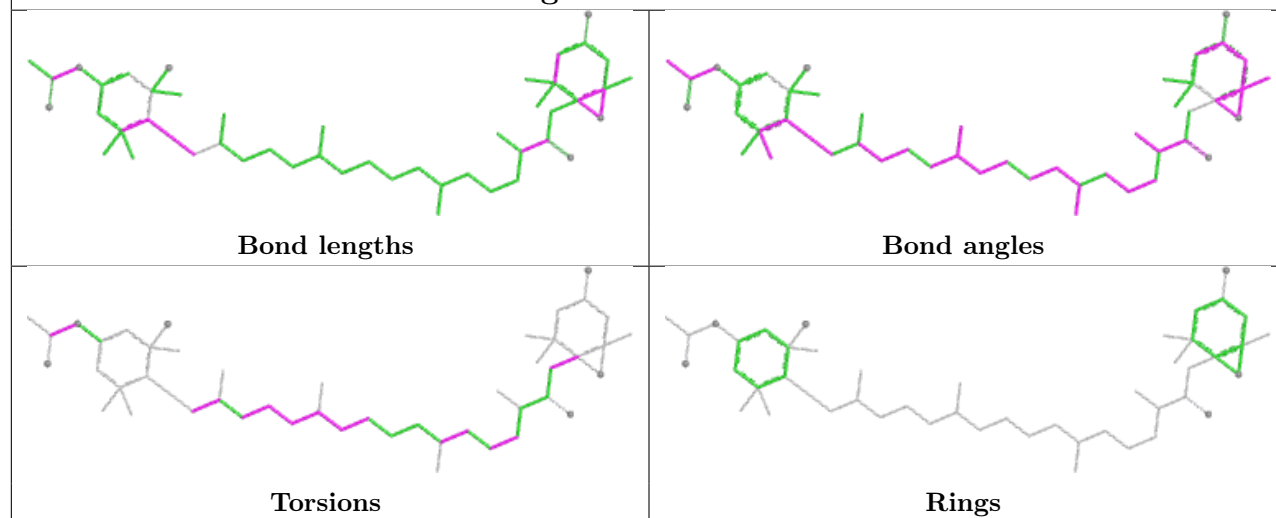


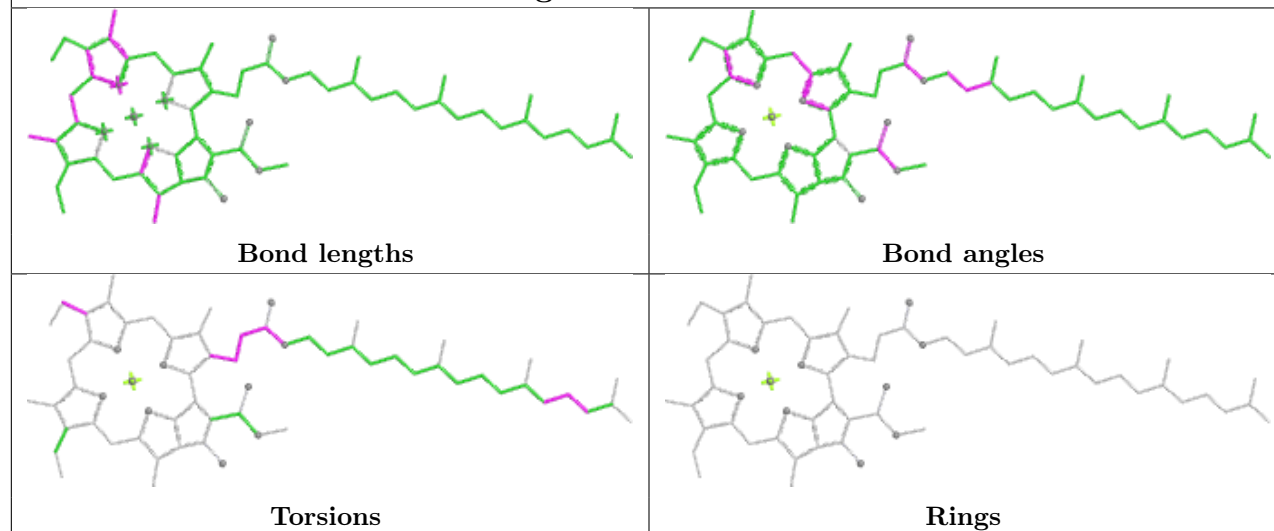
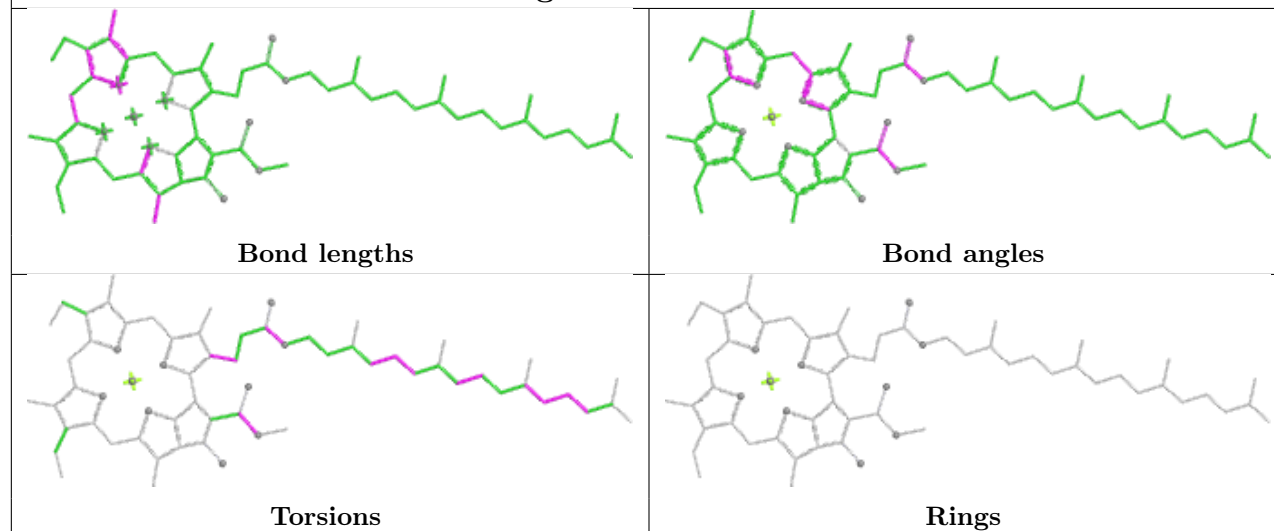


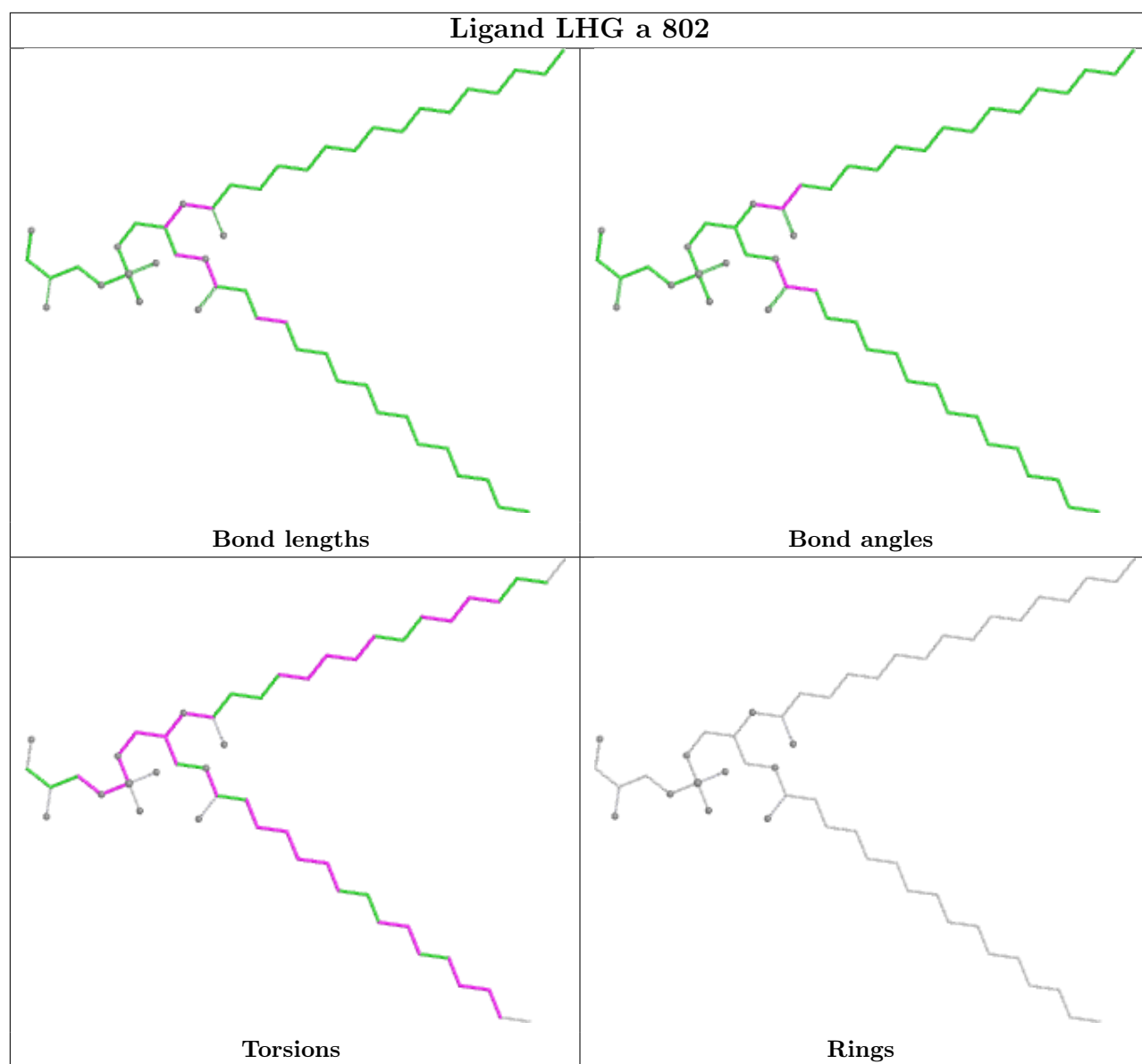
Ligand CLA 1 203

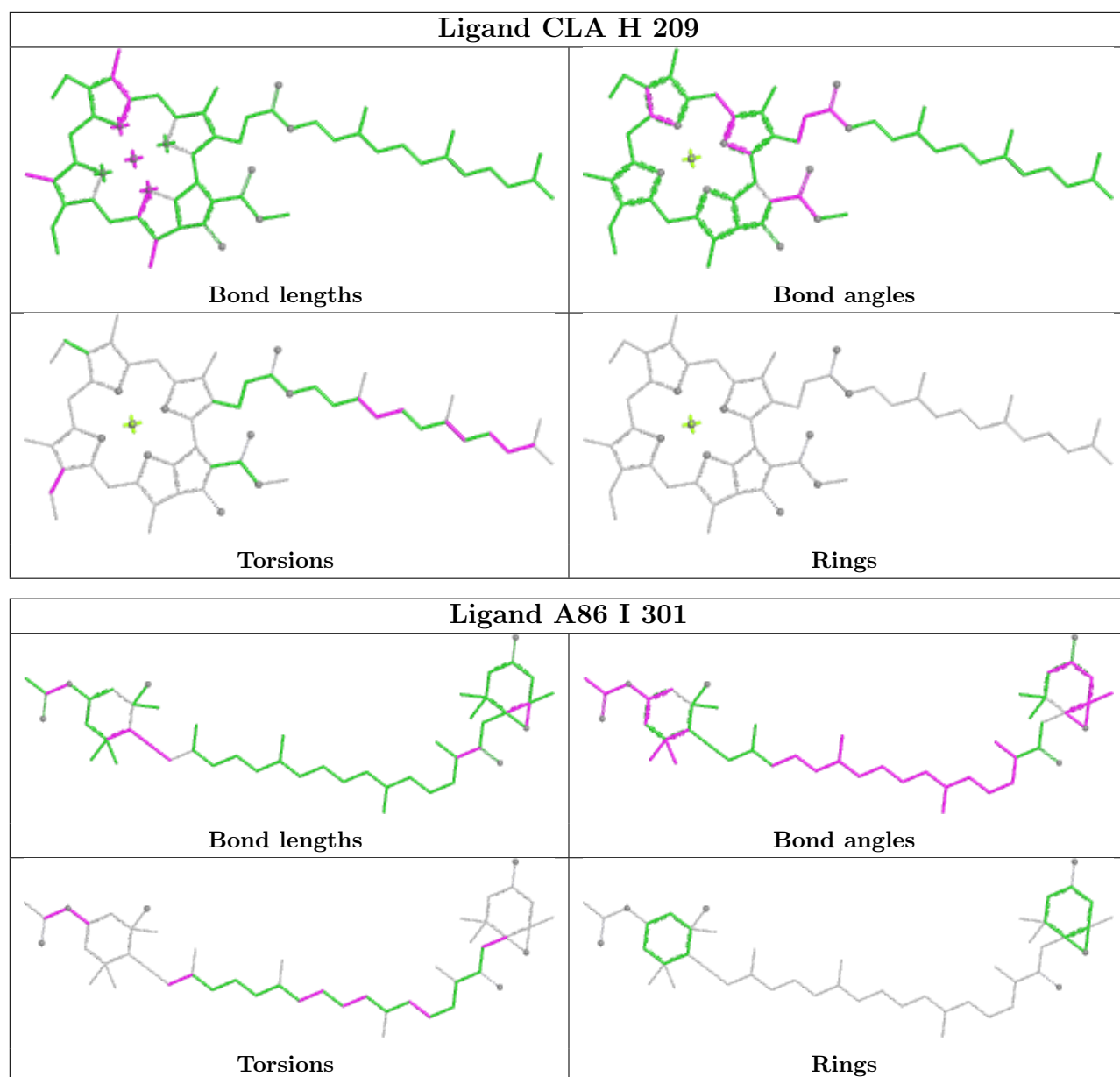


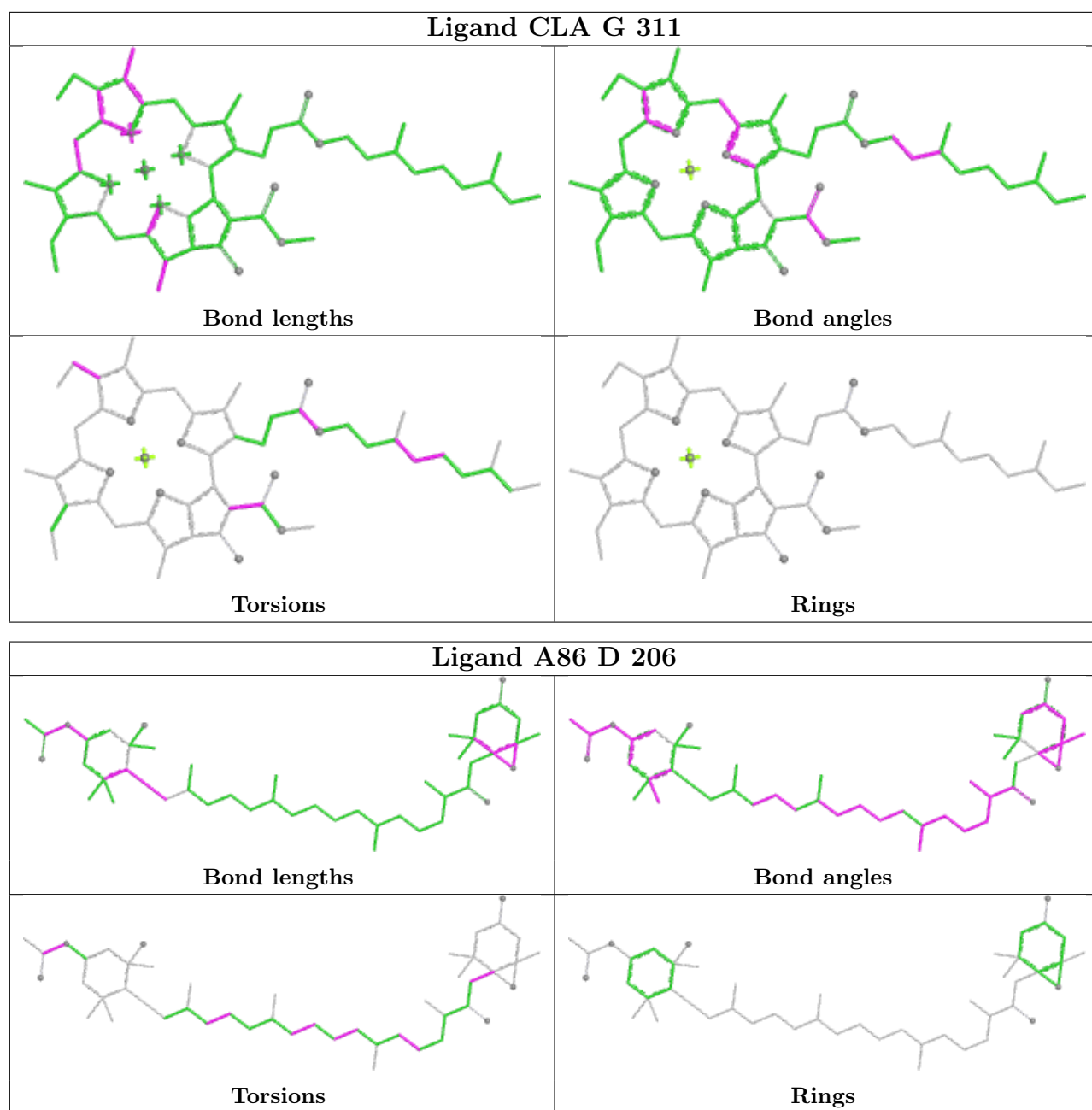
Ligand A86 b 848



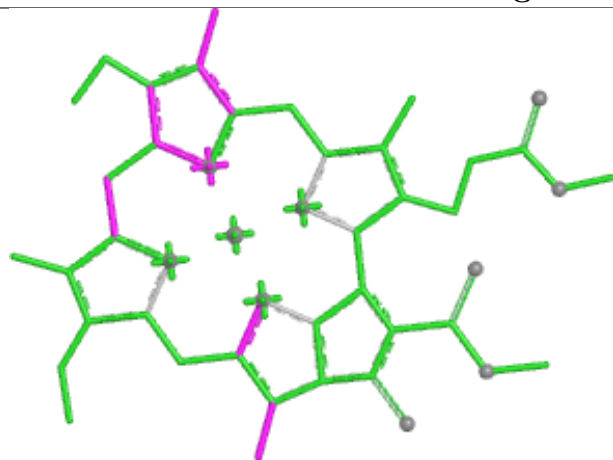
Ligand CLA b 809**Ligand CLA a 838**



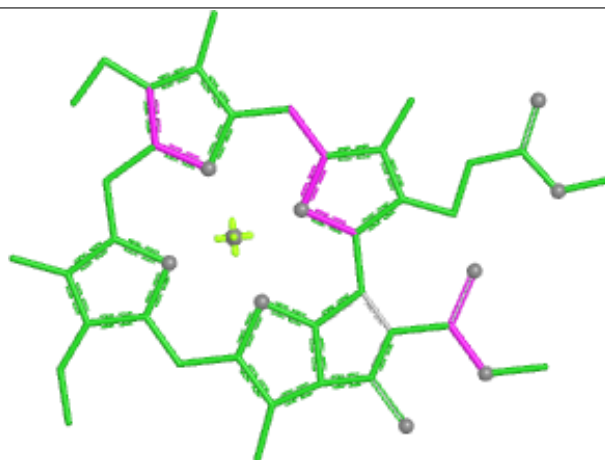




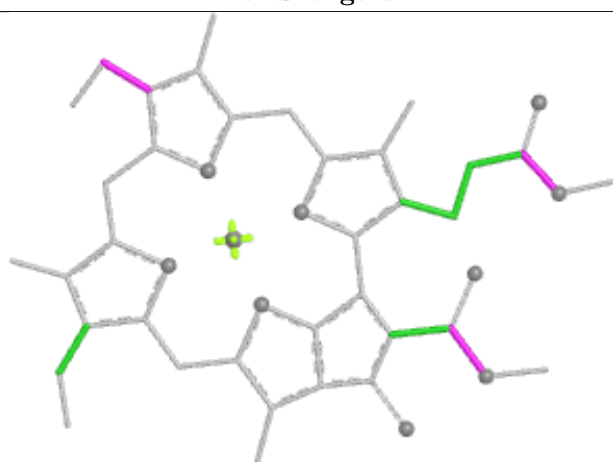
Ligand CLA A 206



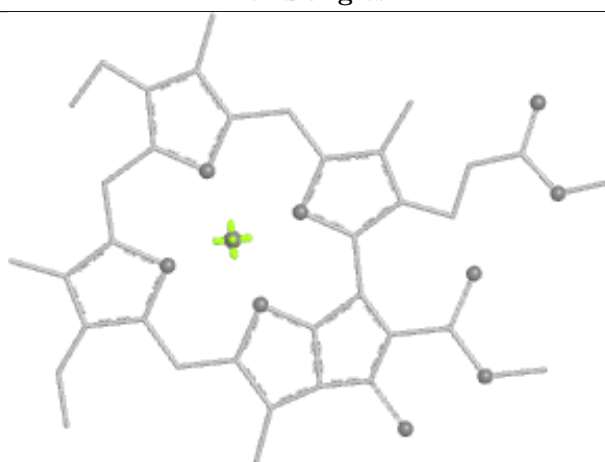
Bond lengths



Bond angles

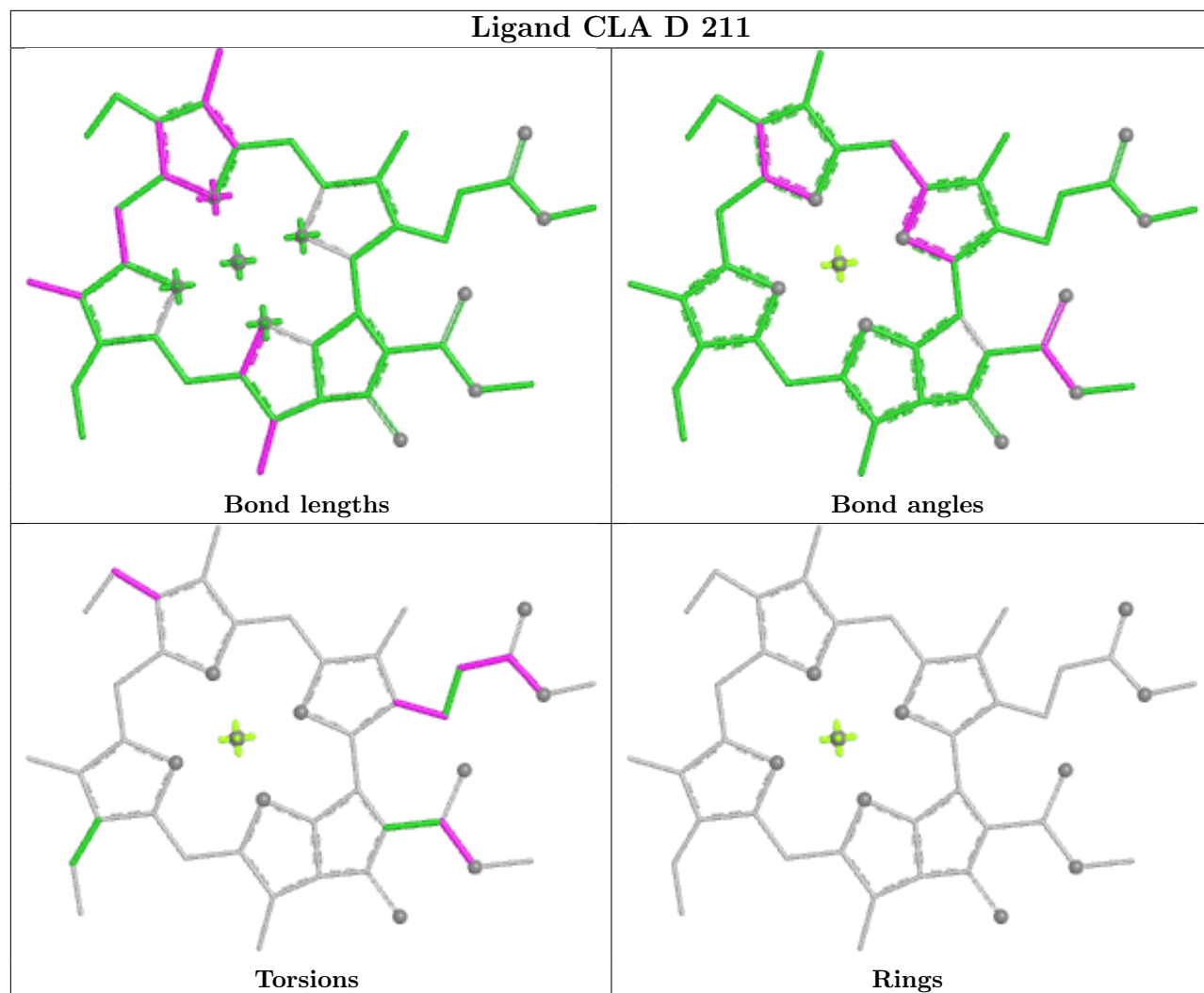


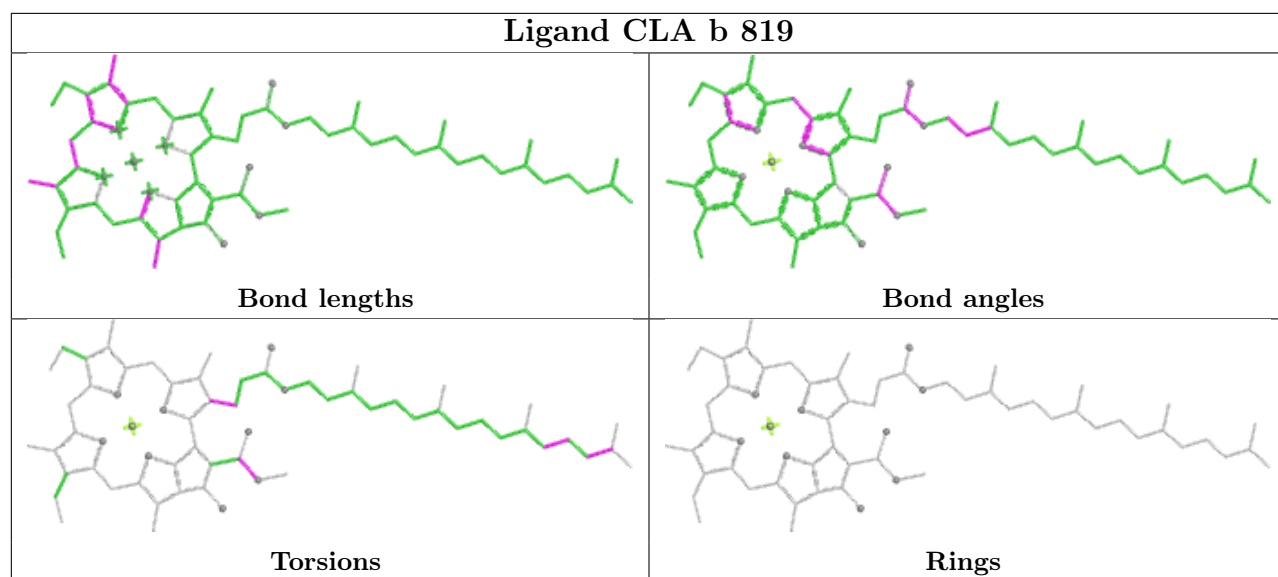
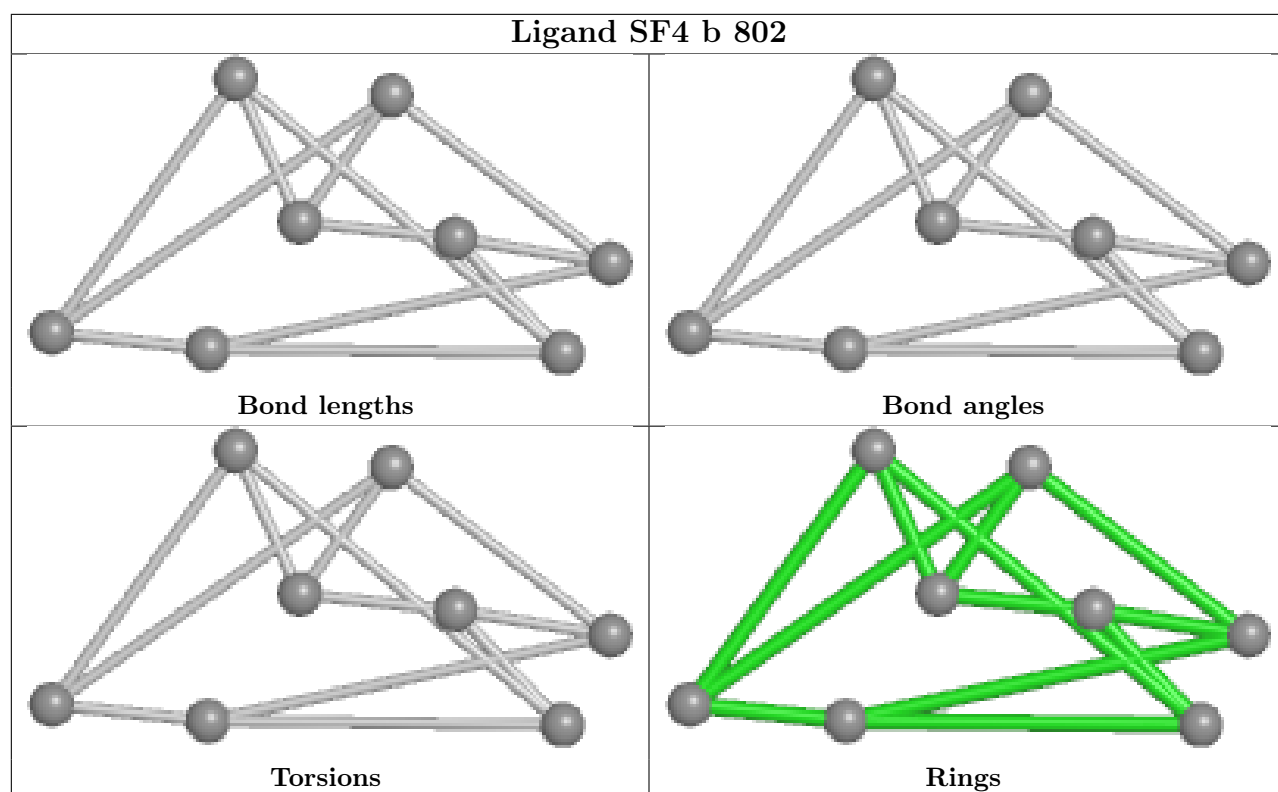
Torsions



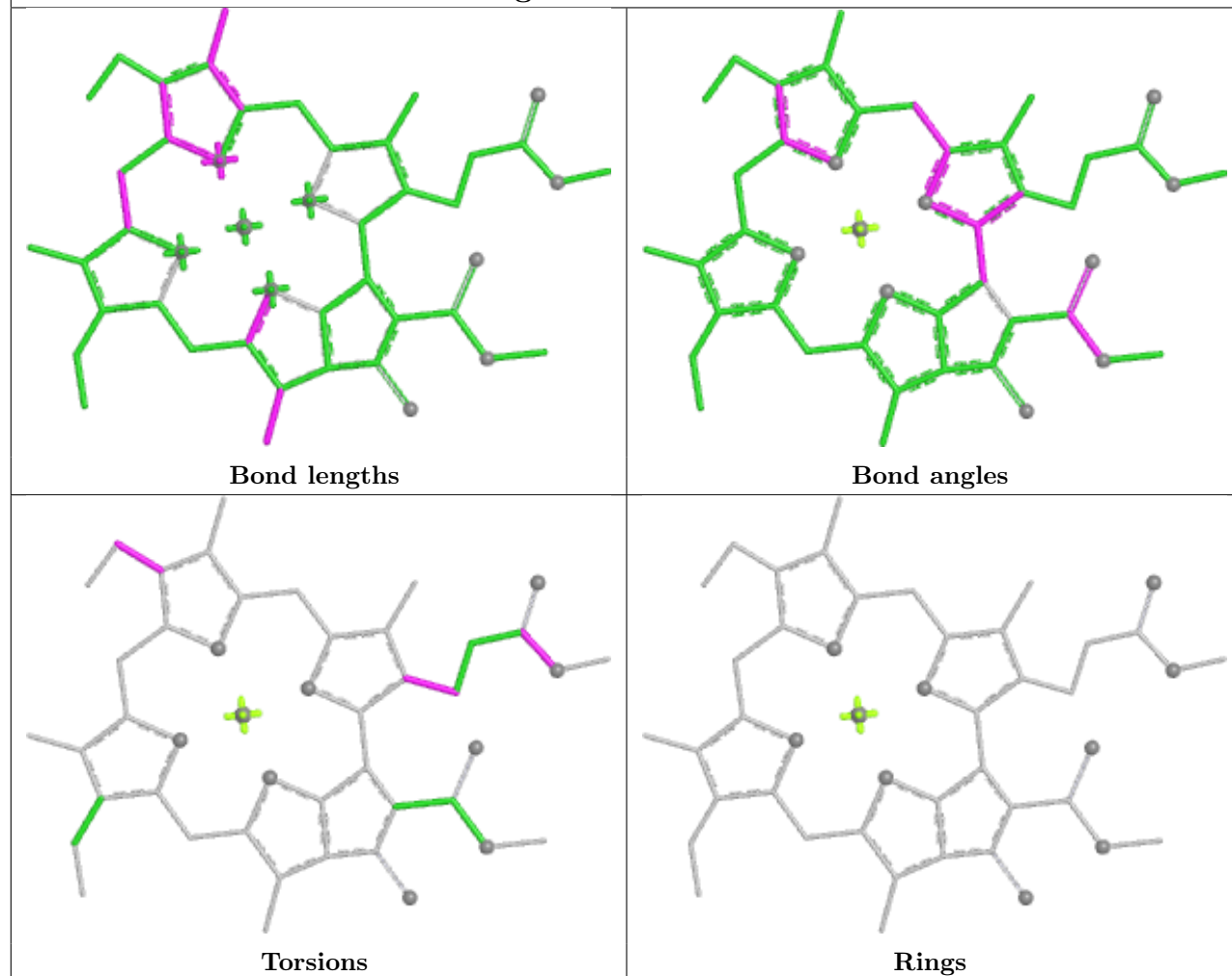
Rings

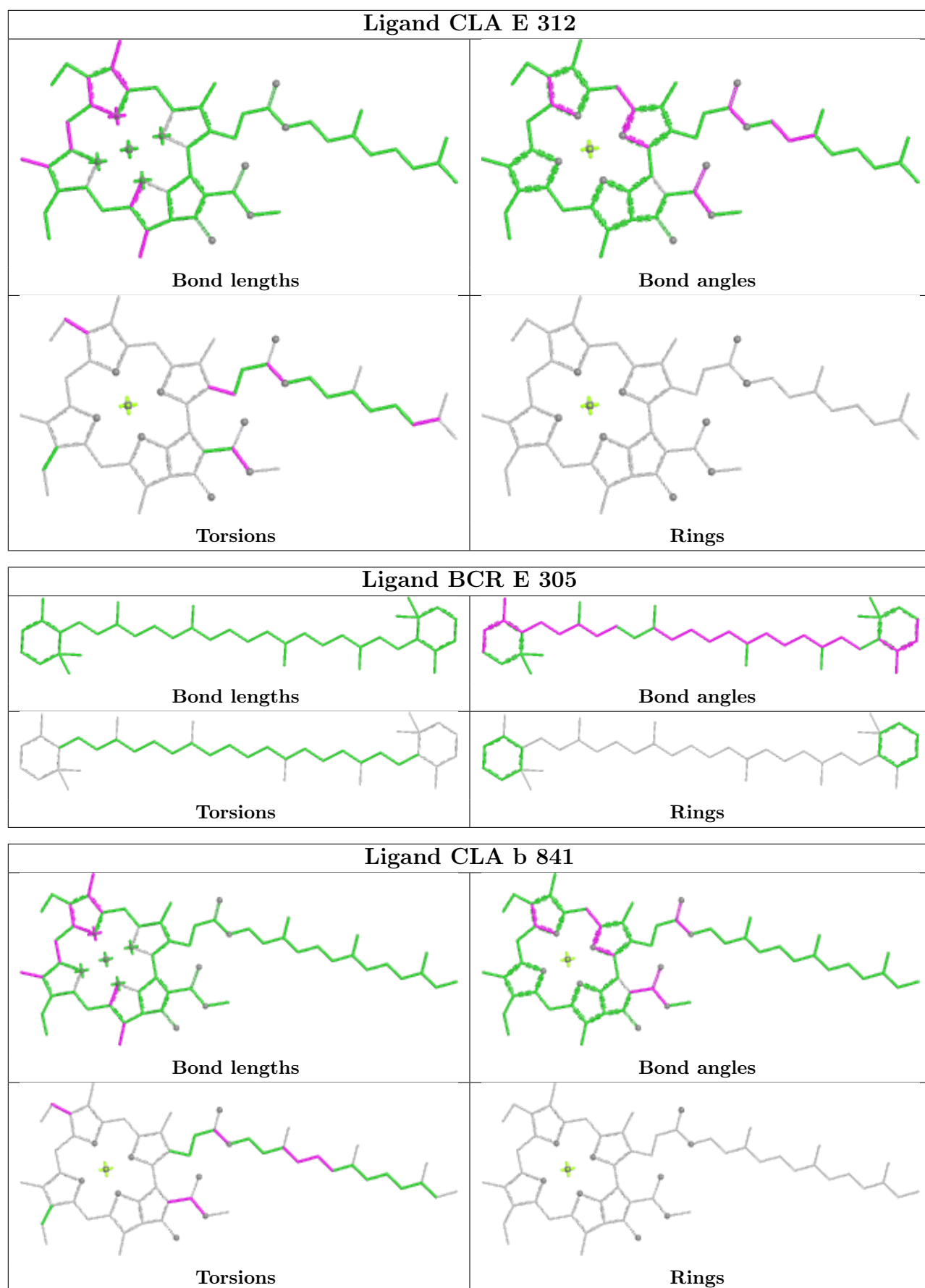
Ligand CLA D 211



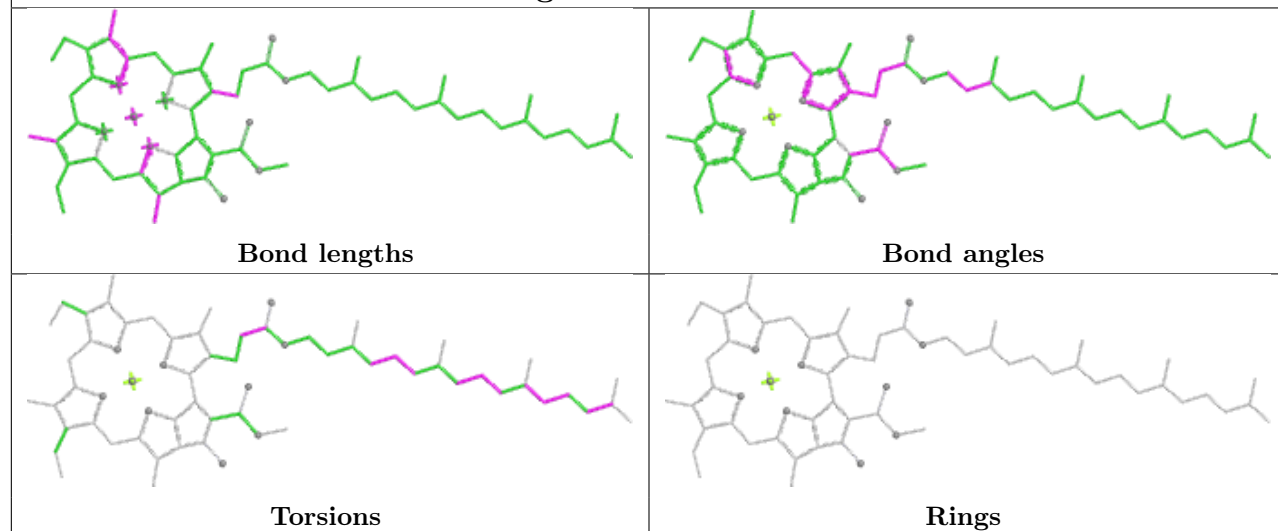


Ligand CLA E 310

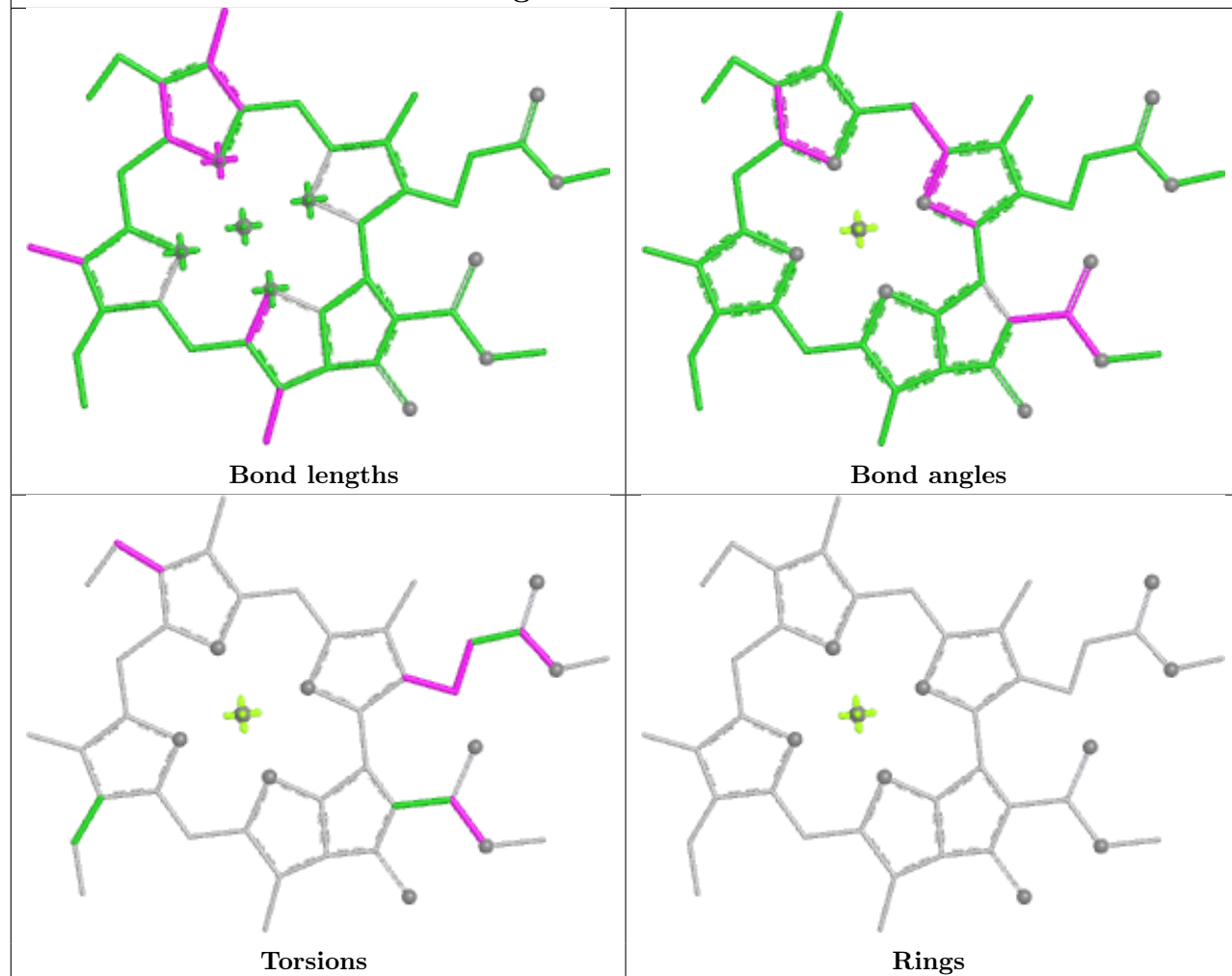


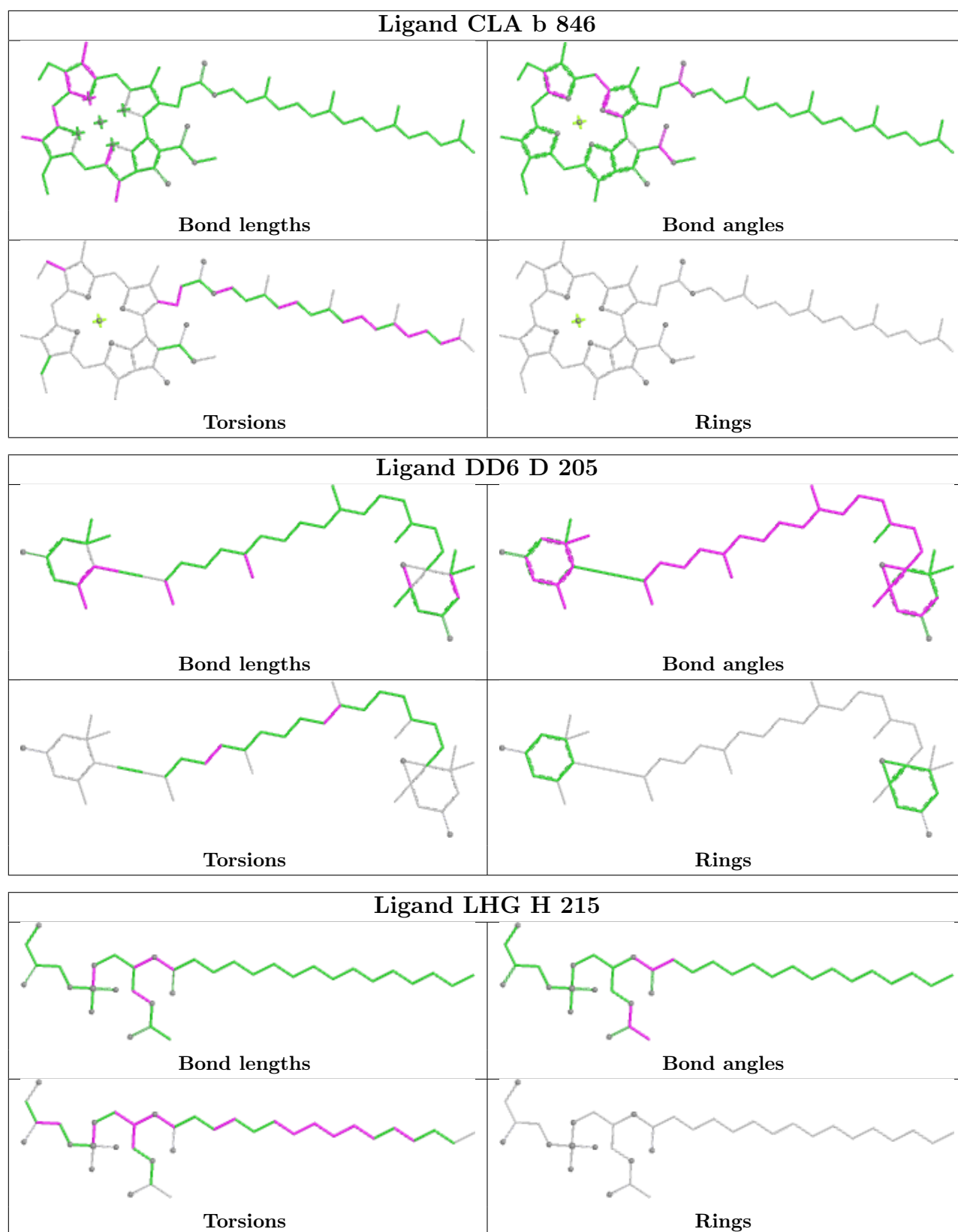


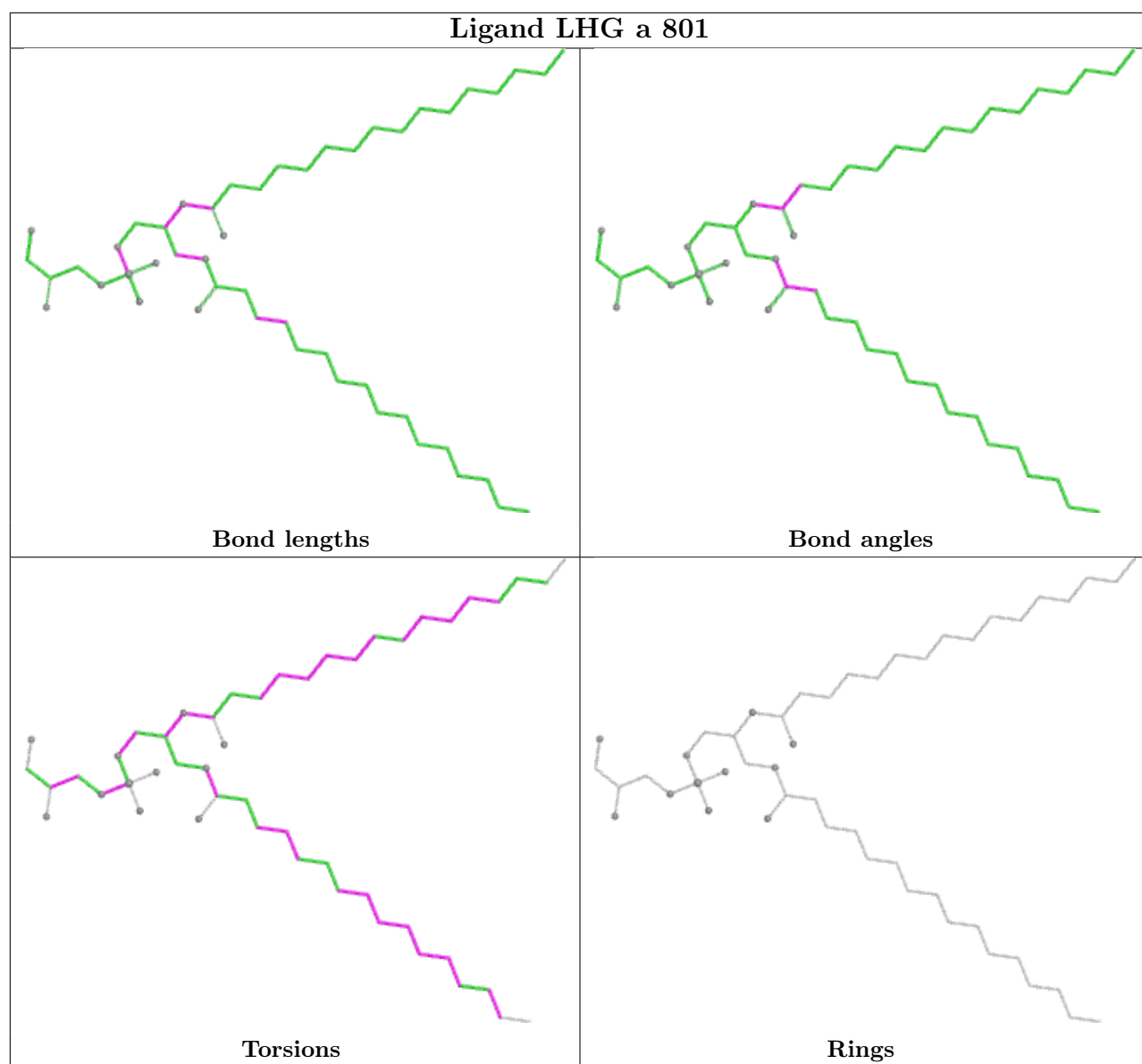
Ligand CLA a 809

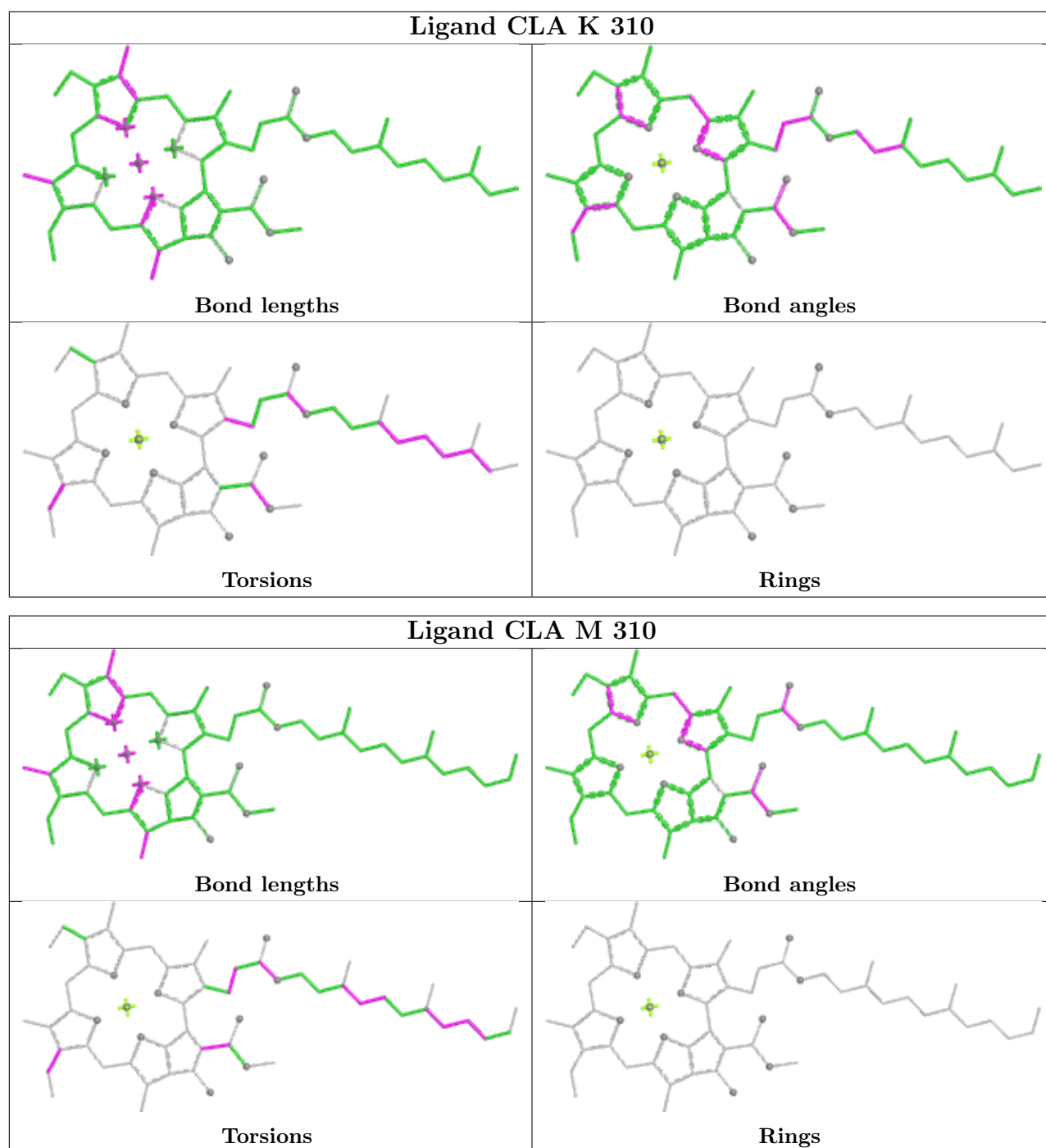


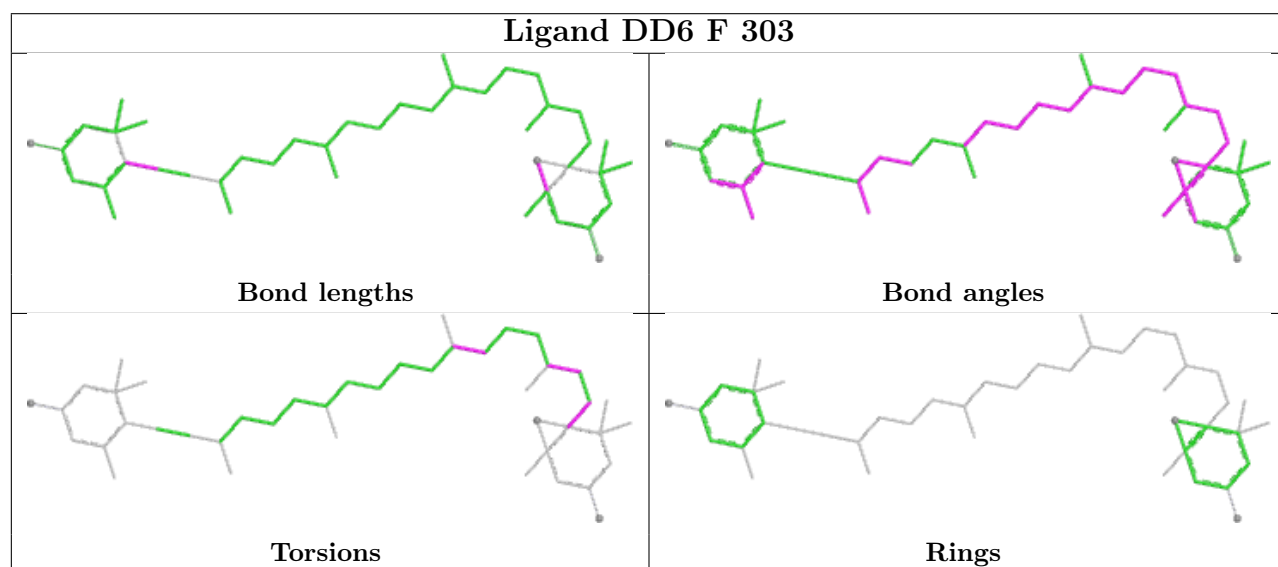
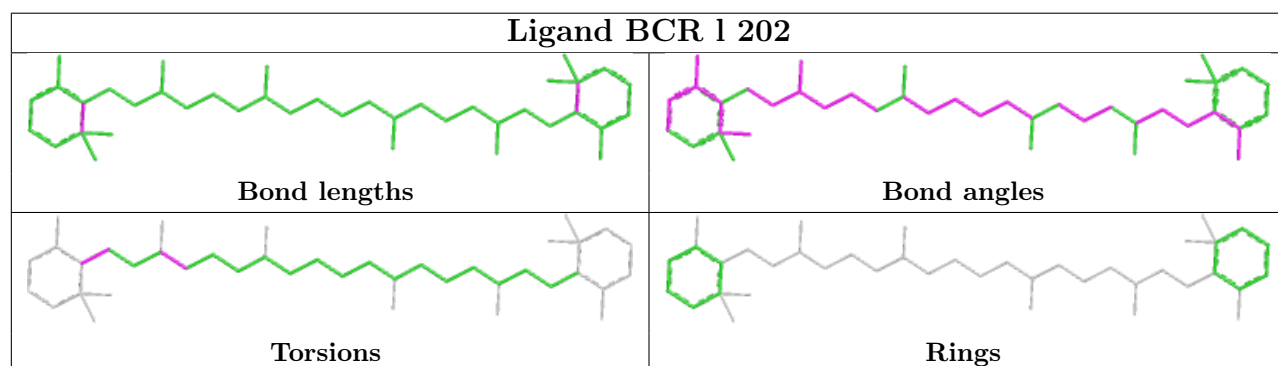
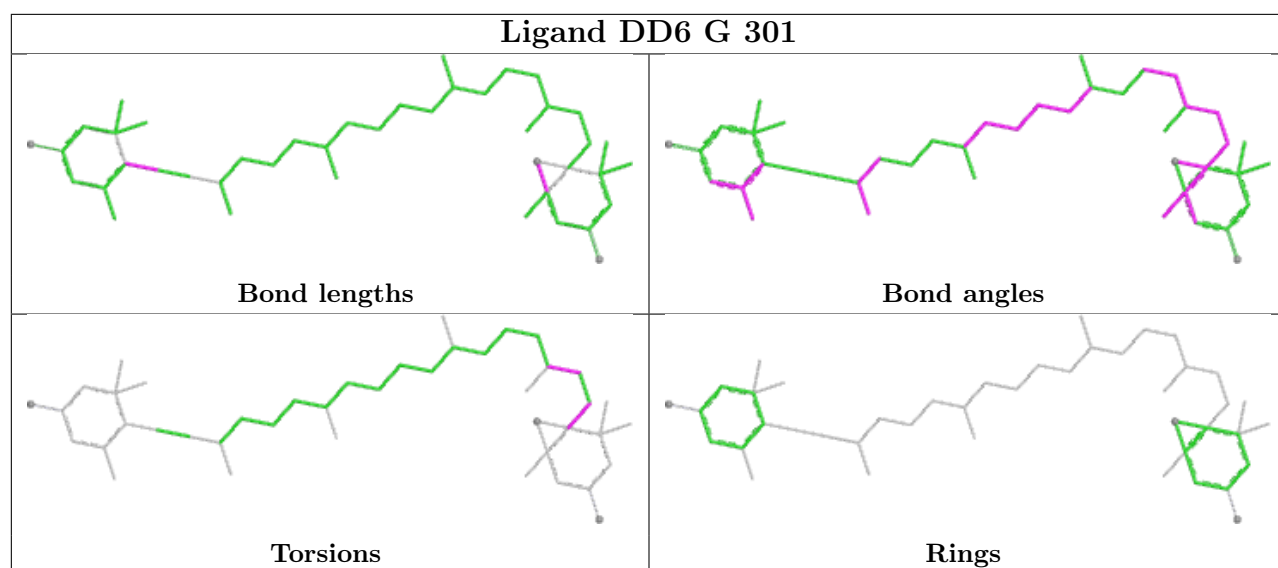
Ligand CLA C 310

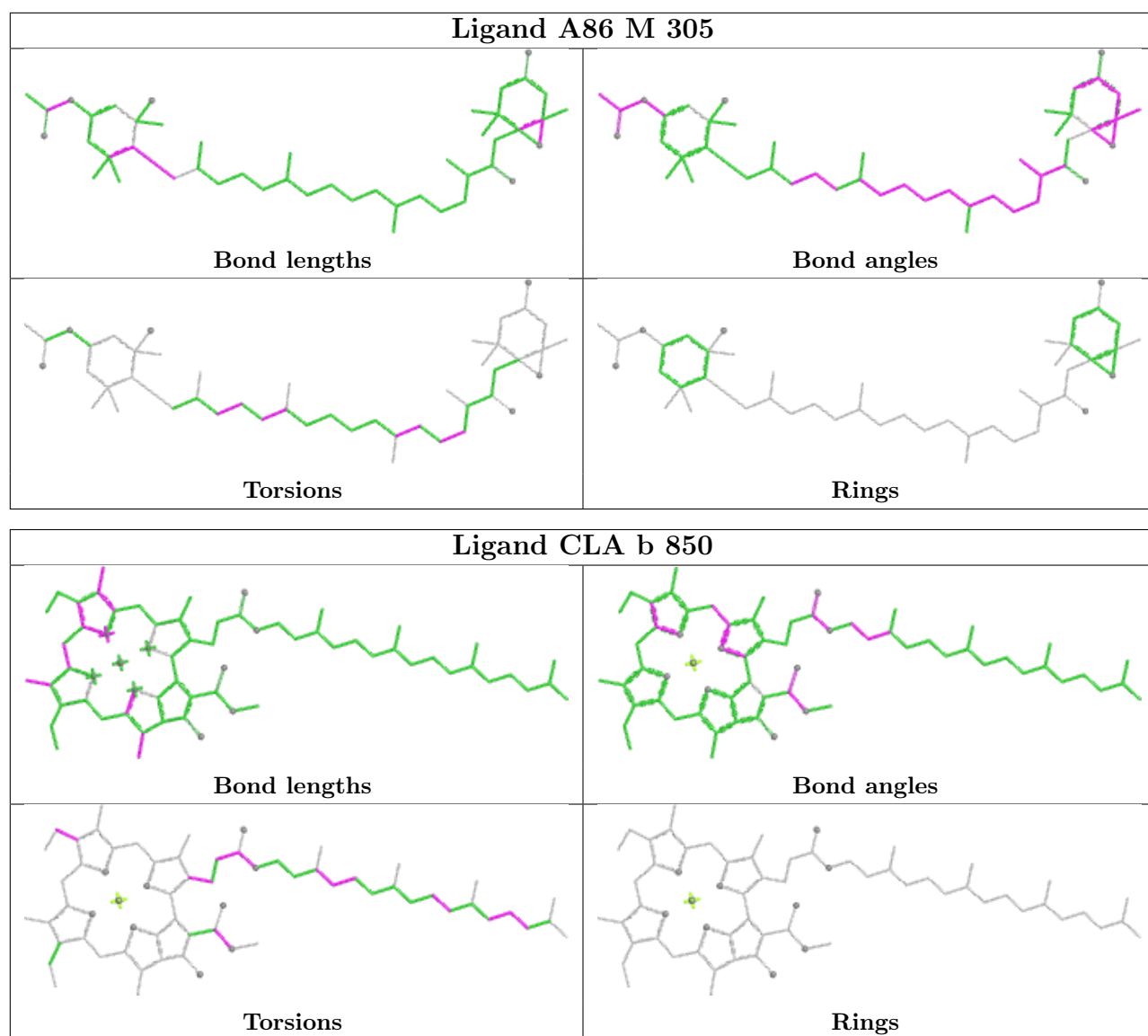




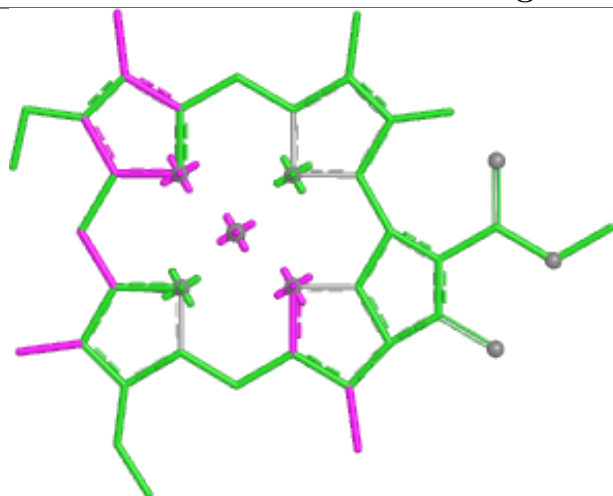




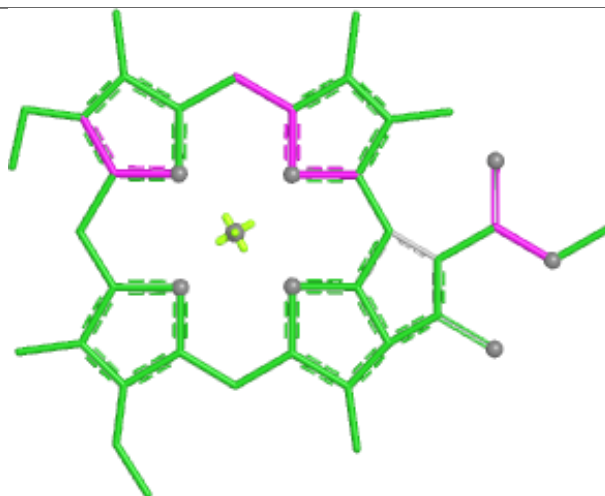




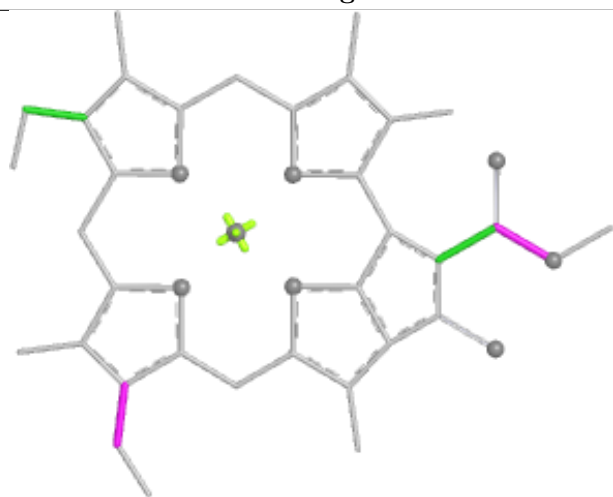
Ligand CLA L 315



Bond lengths



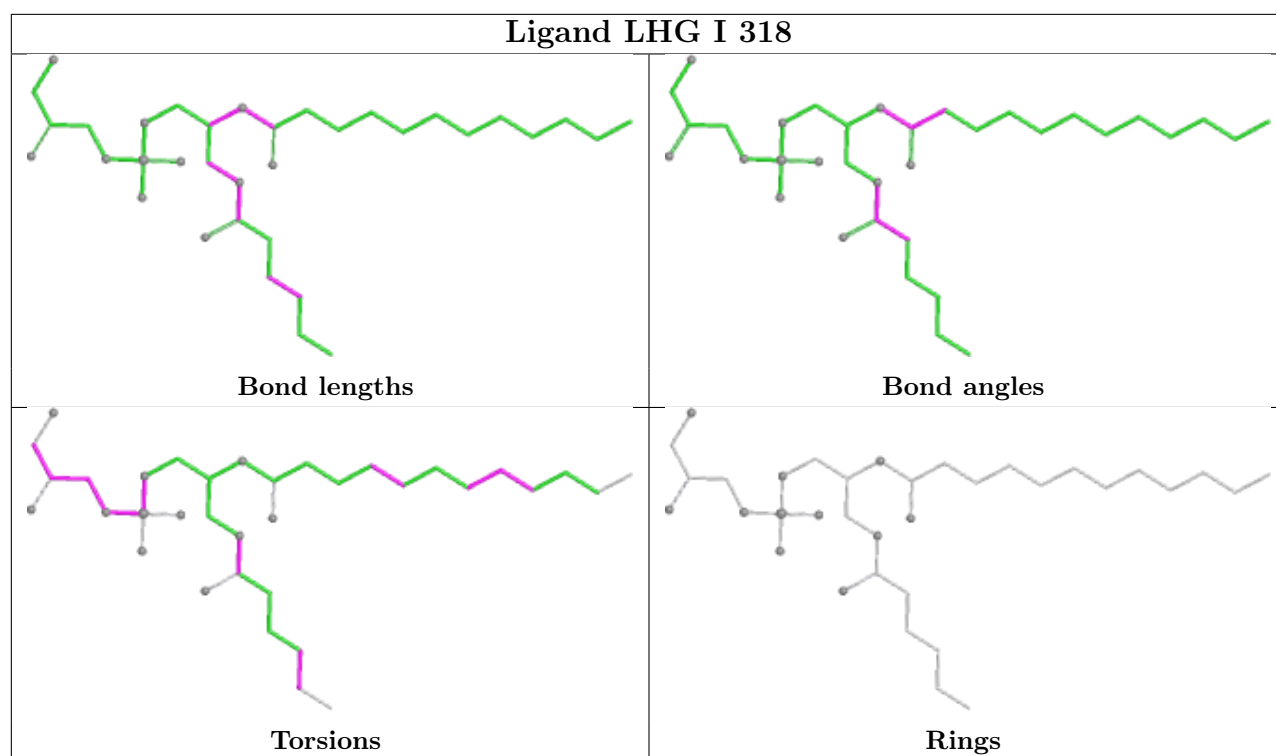
Bond angles

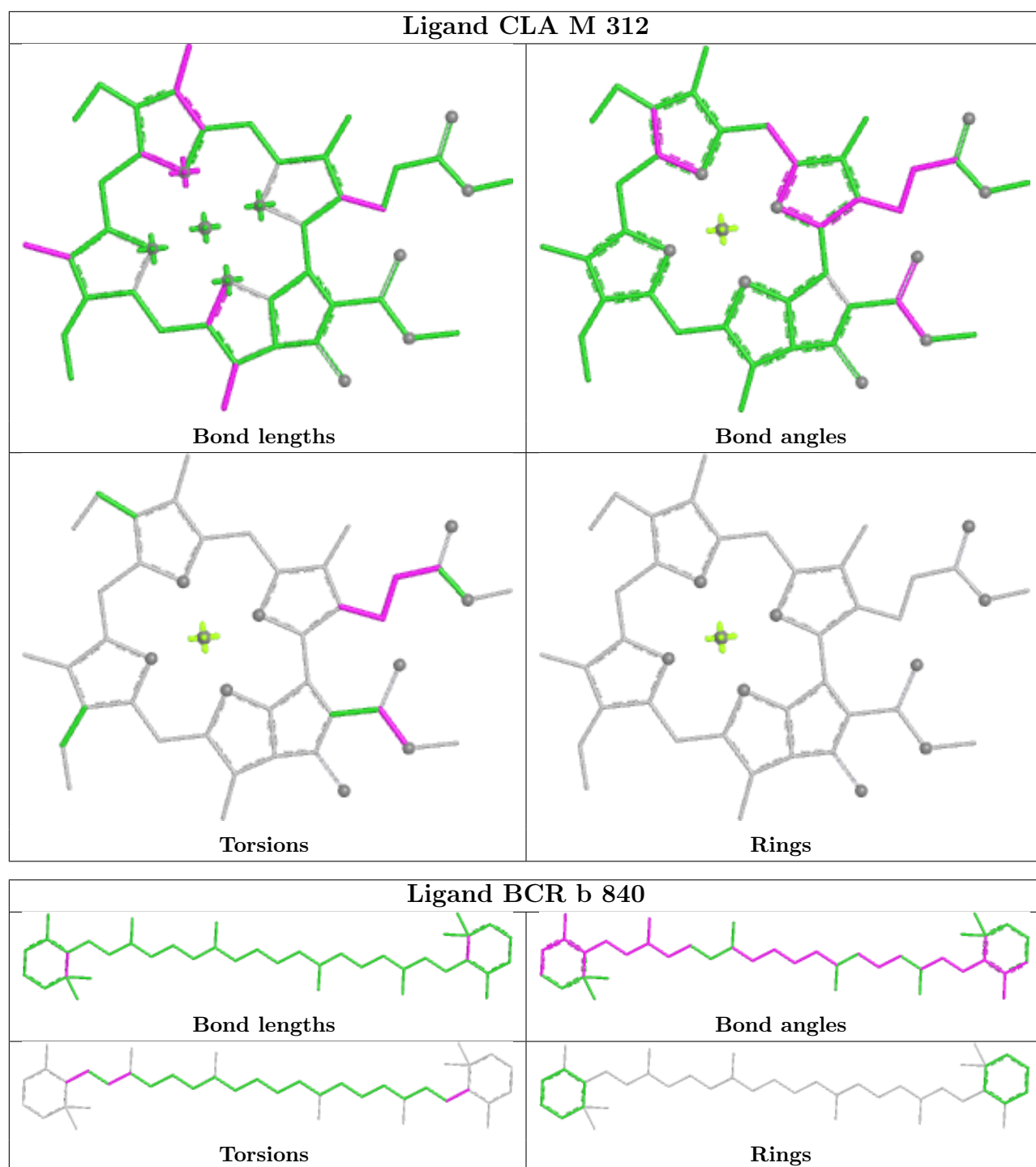


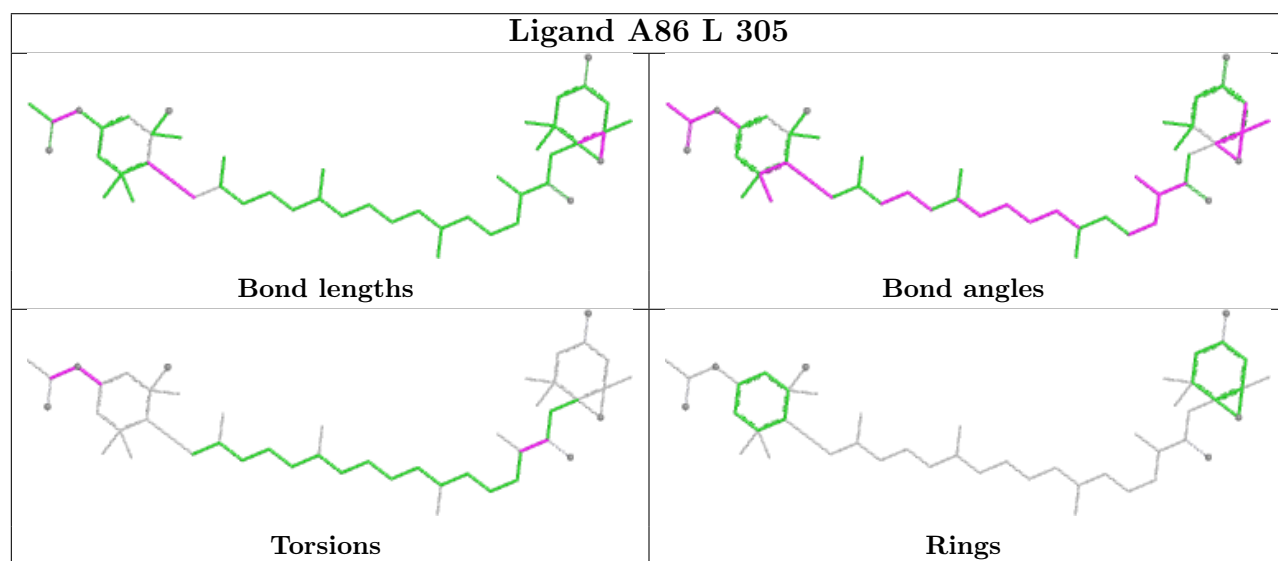
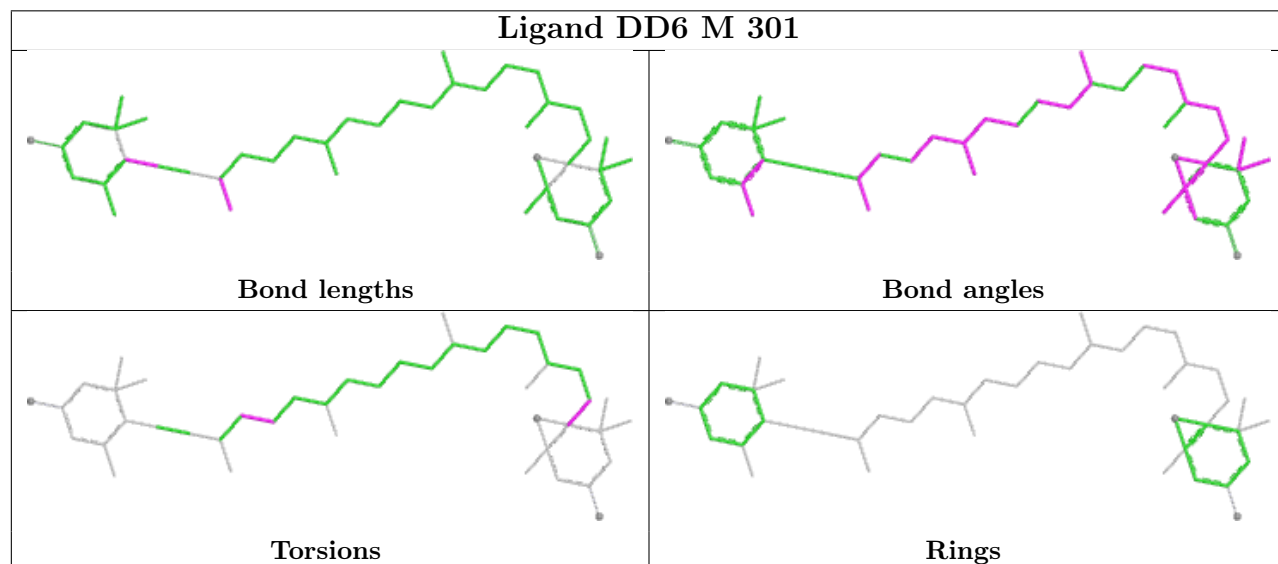
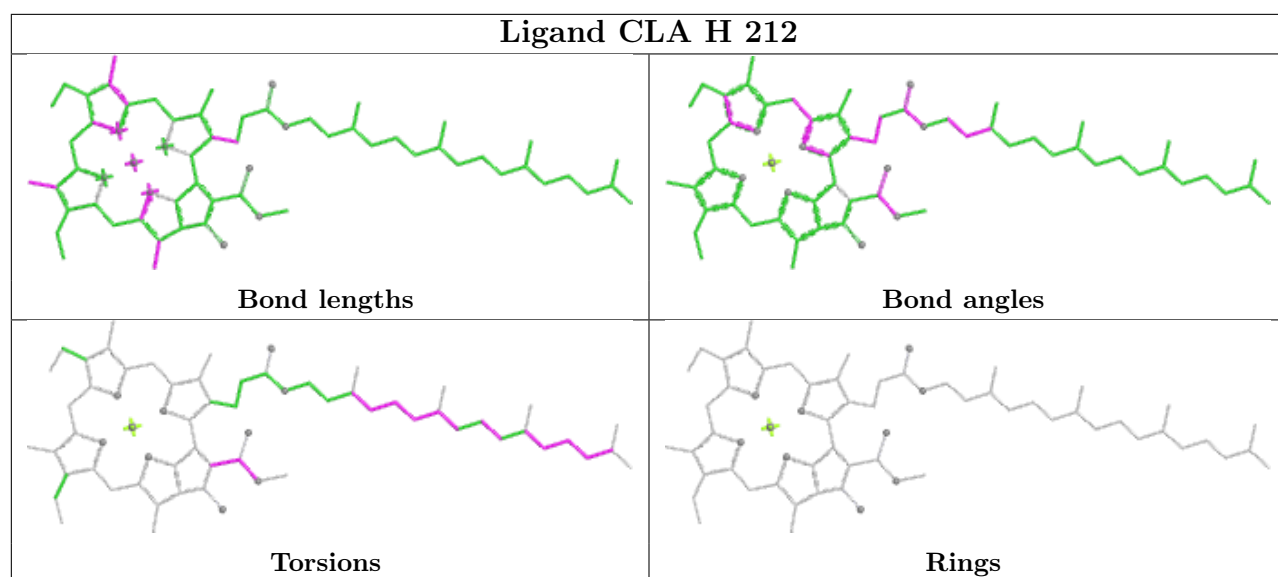
Torsions

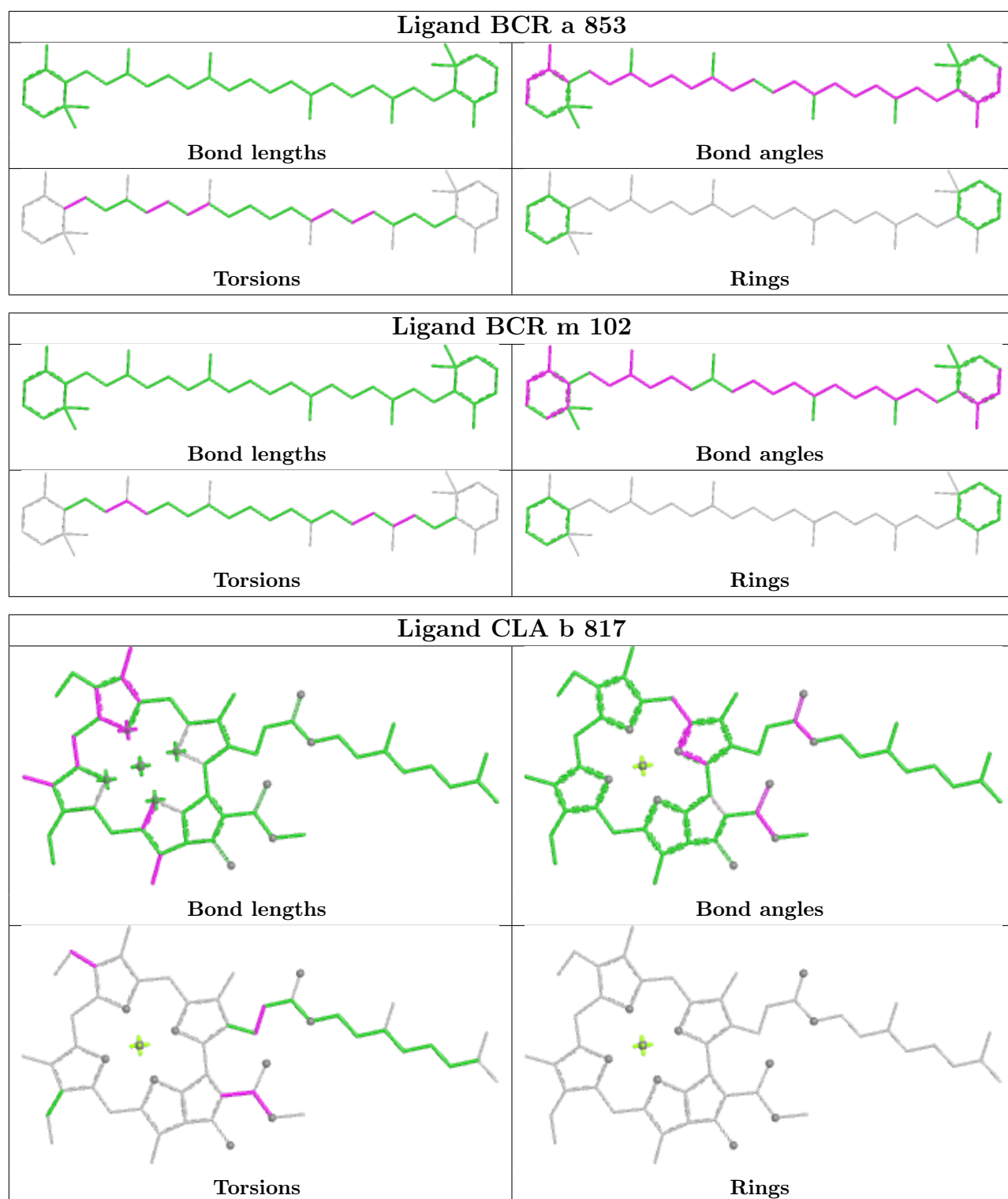


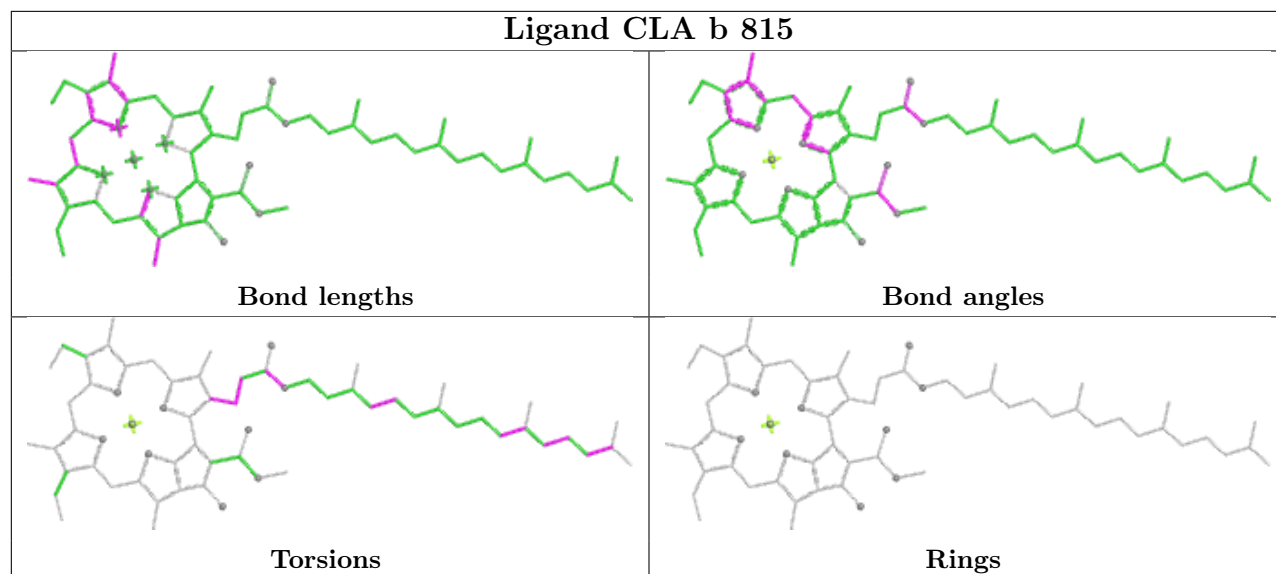
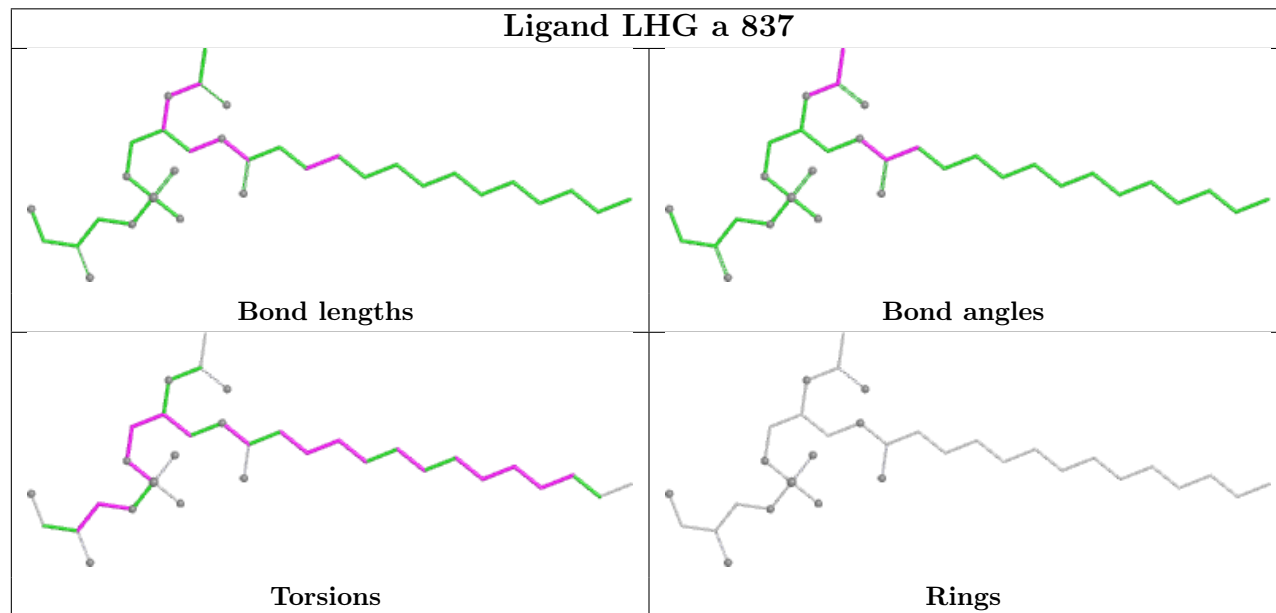
Rings

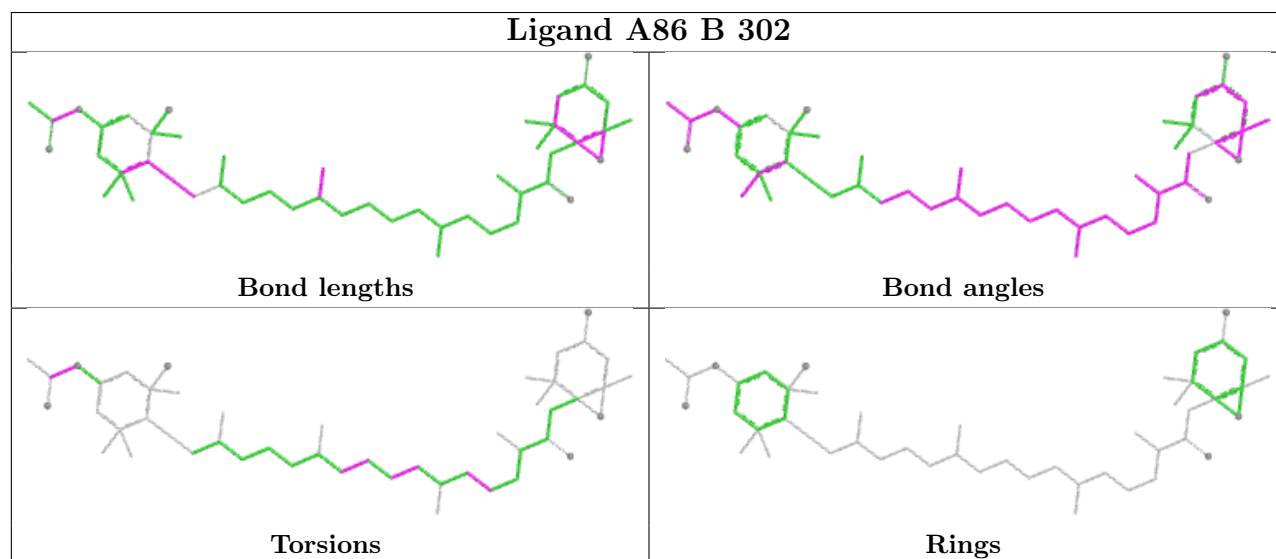
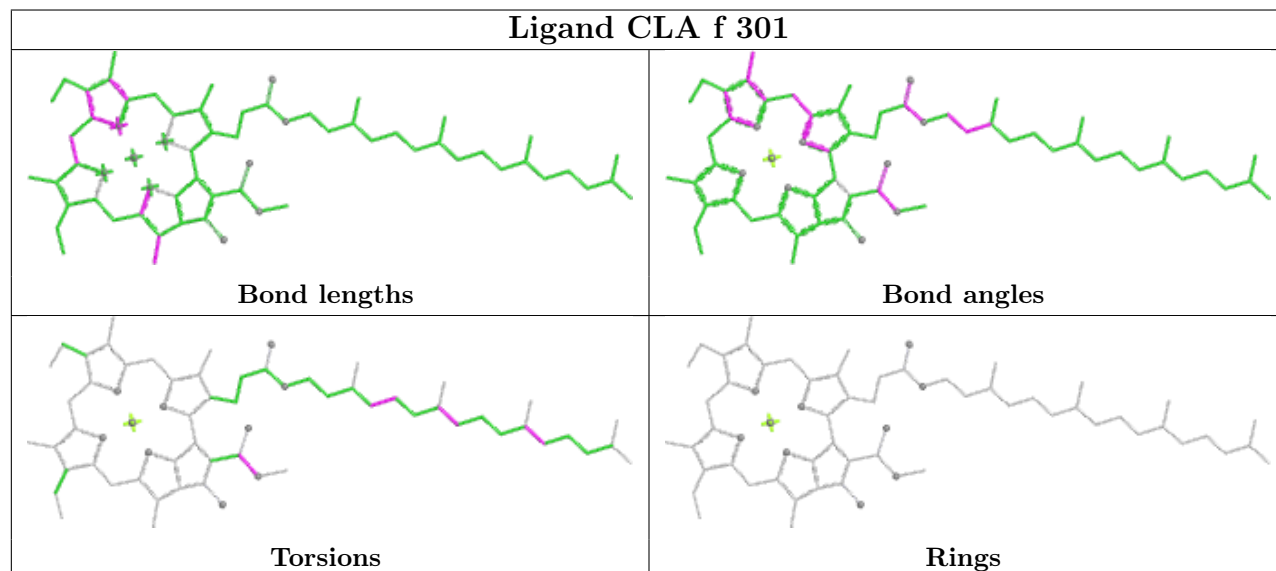
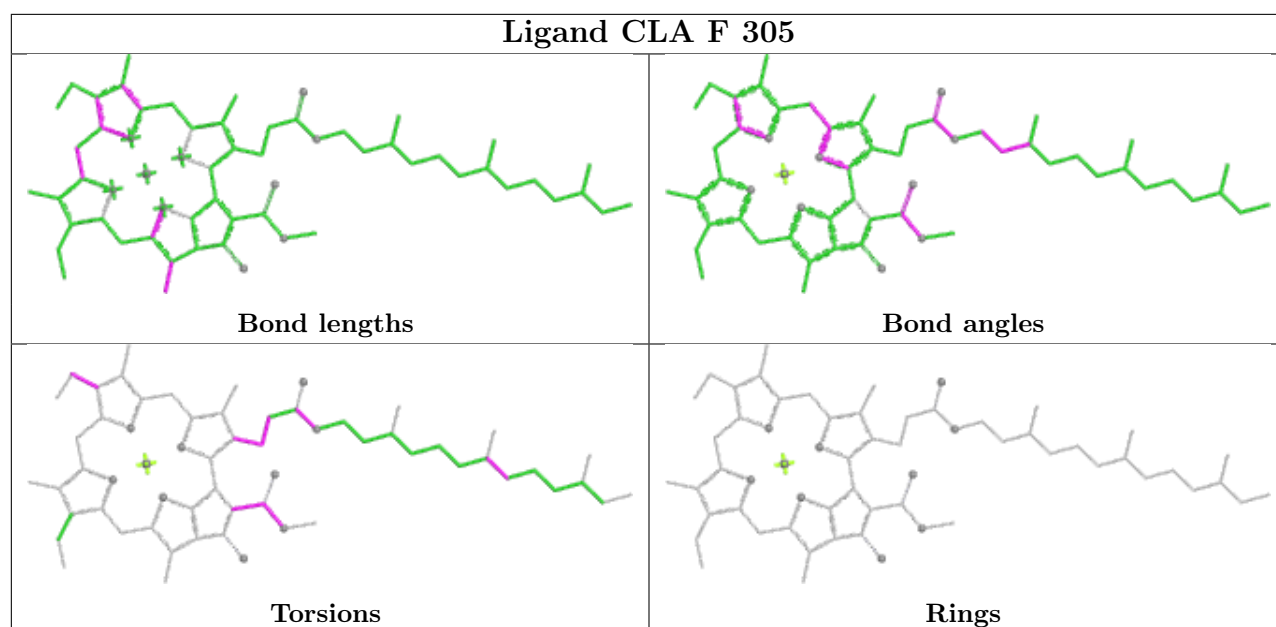


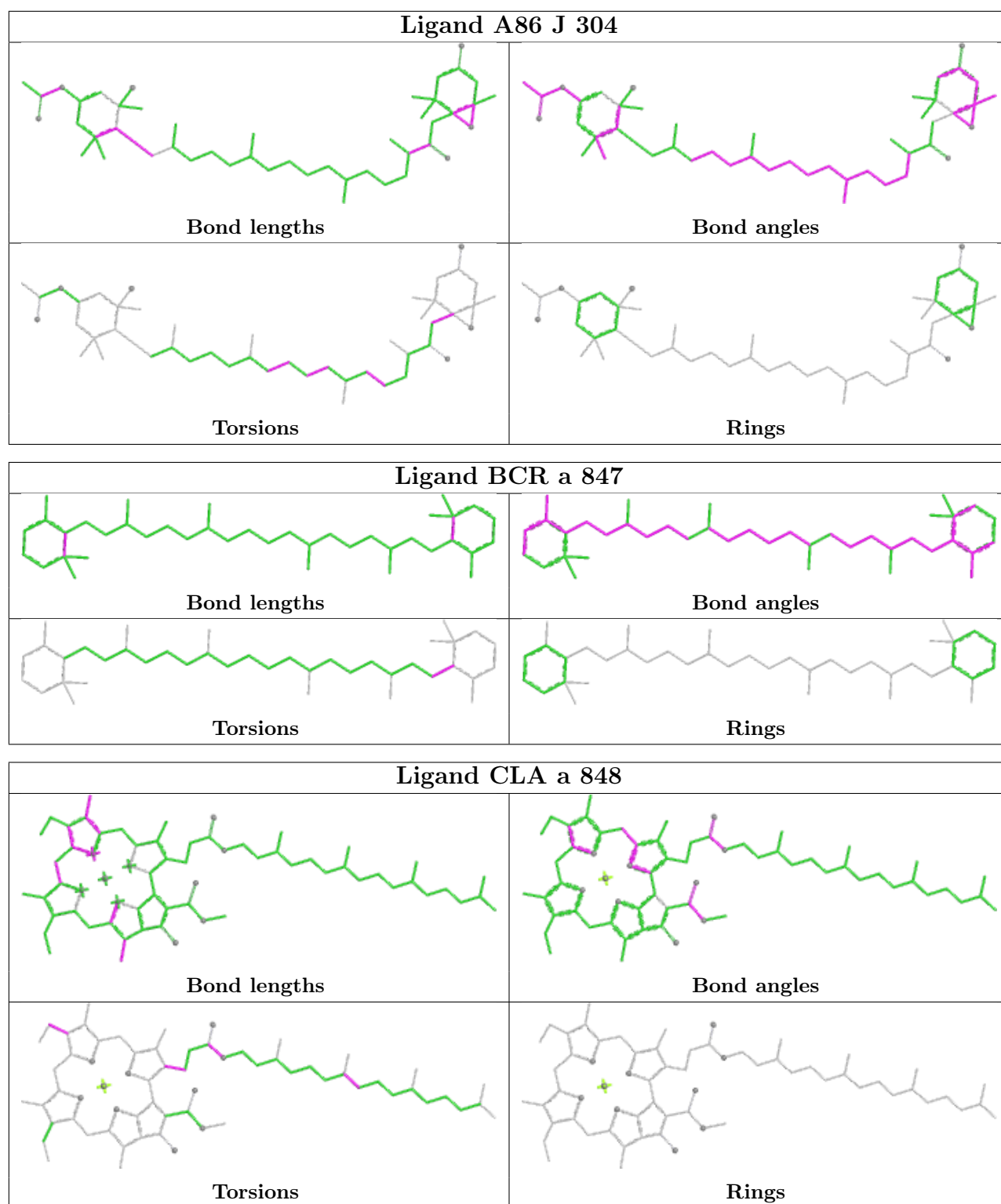




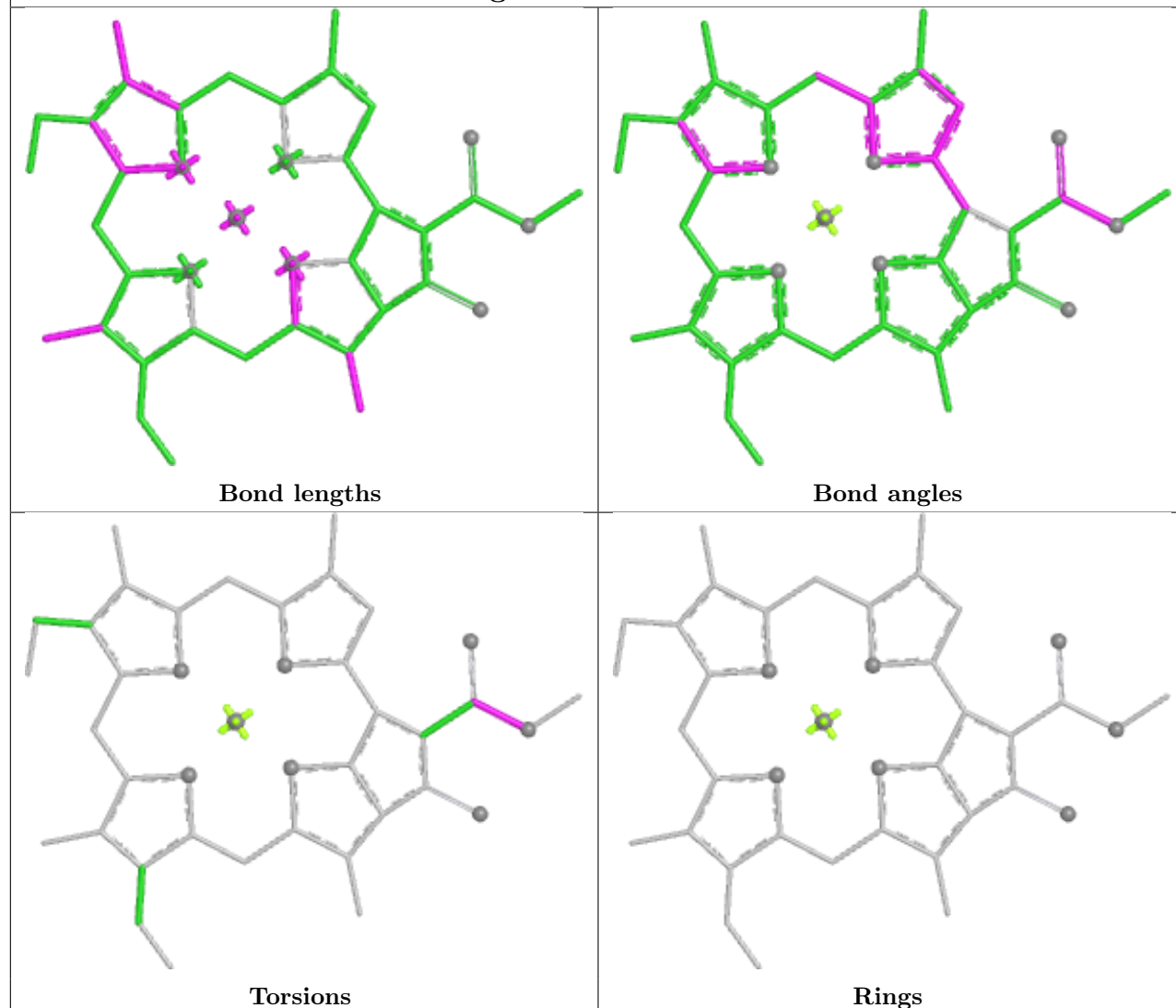


Ligand CLA b 815**Ligand LHG a 837**

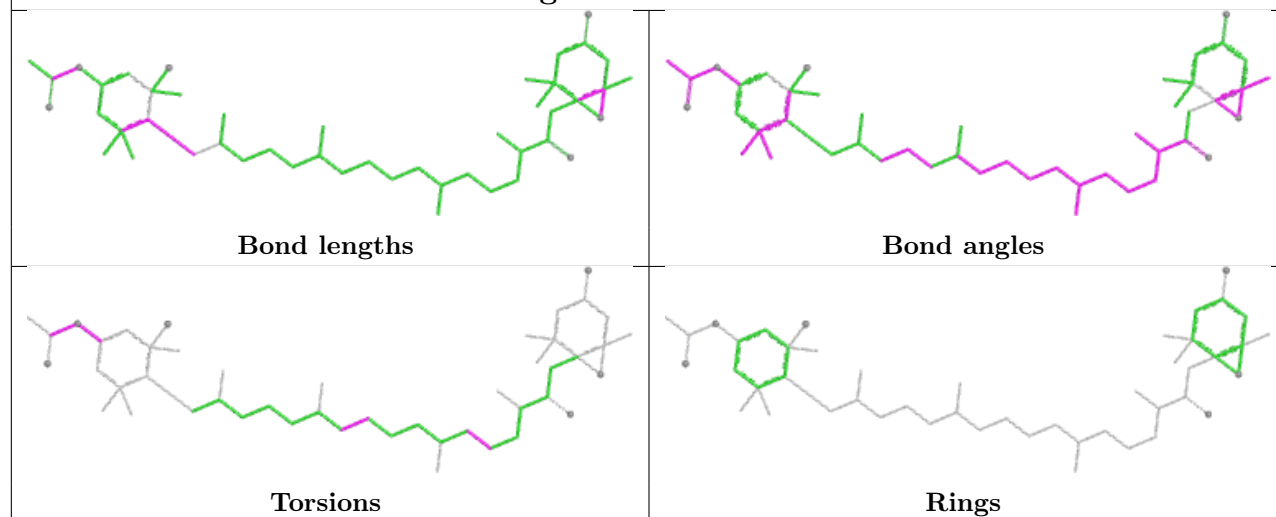




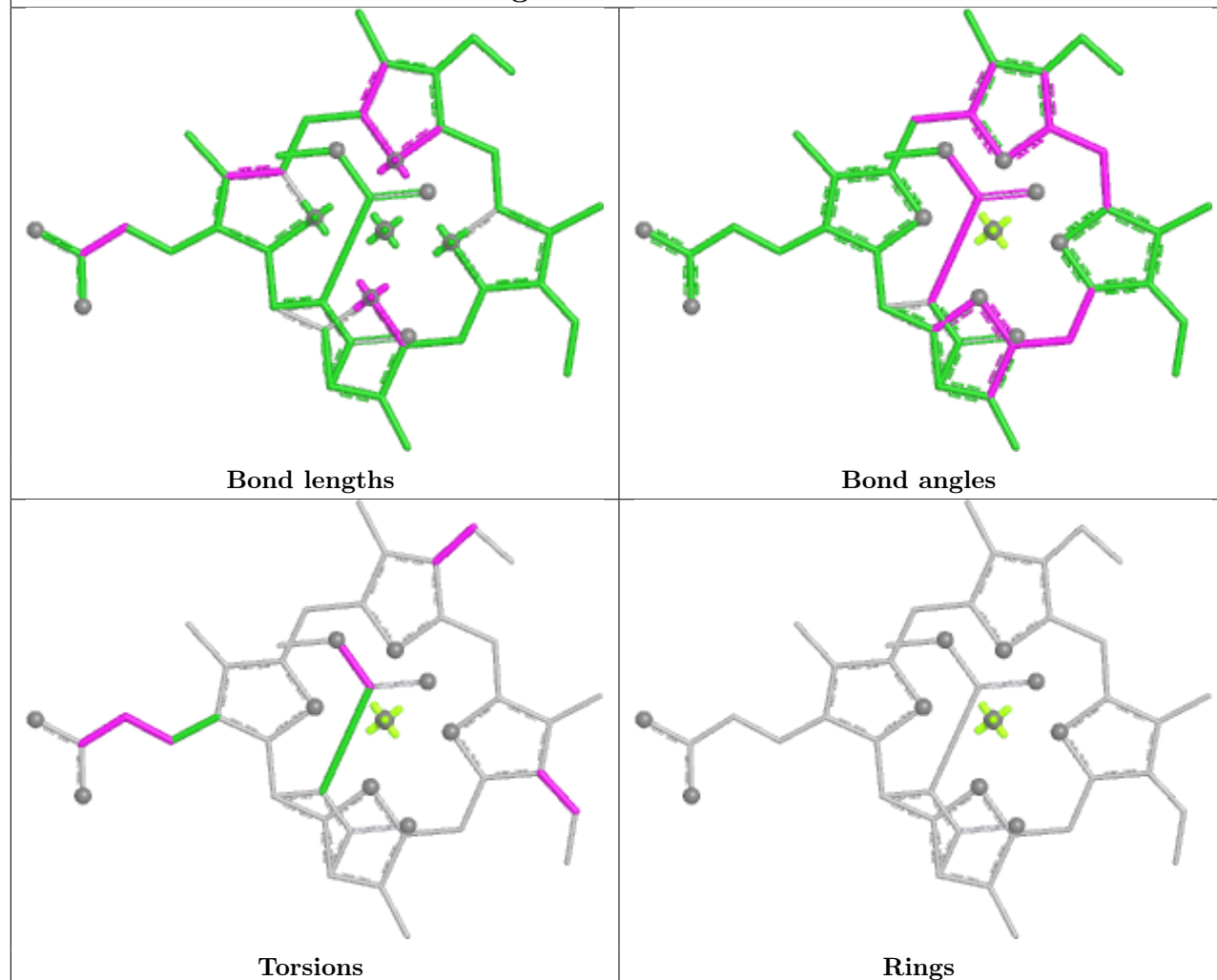
Ligand CLA A 211



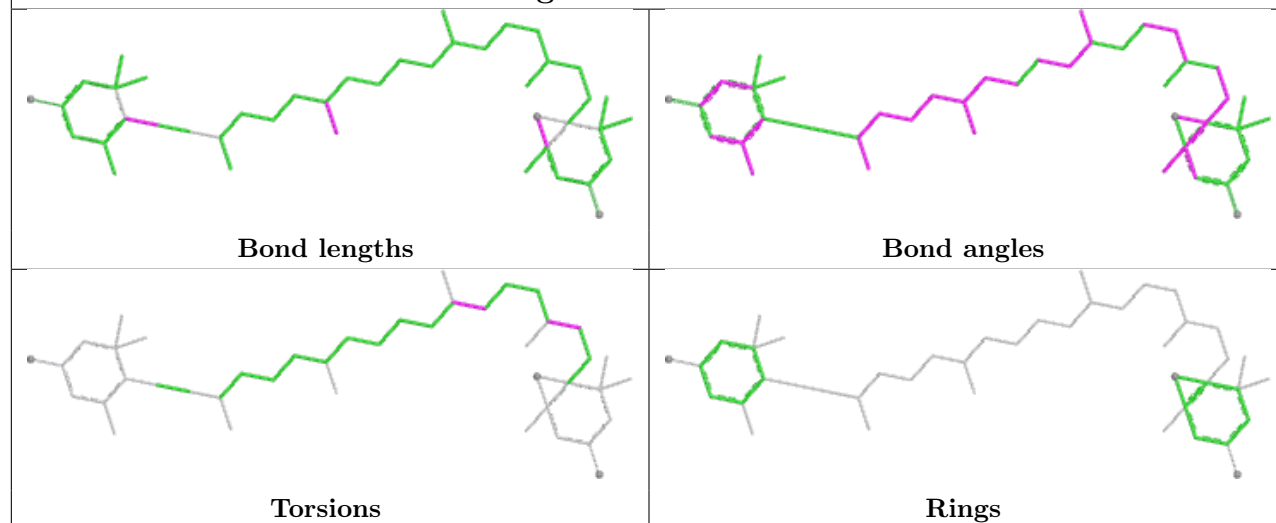
Ligand A86 F 304



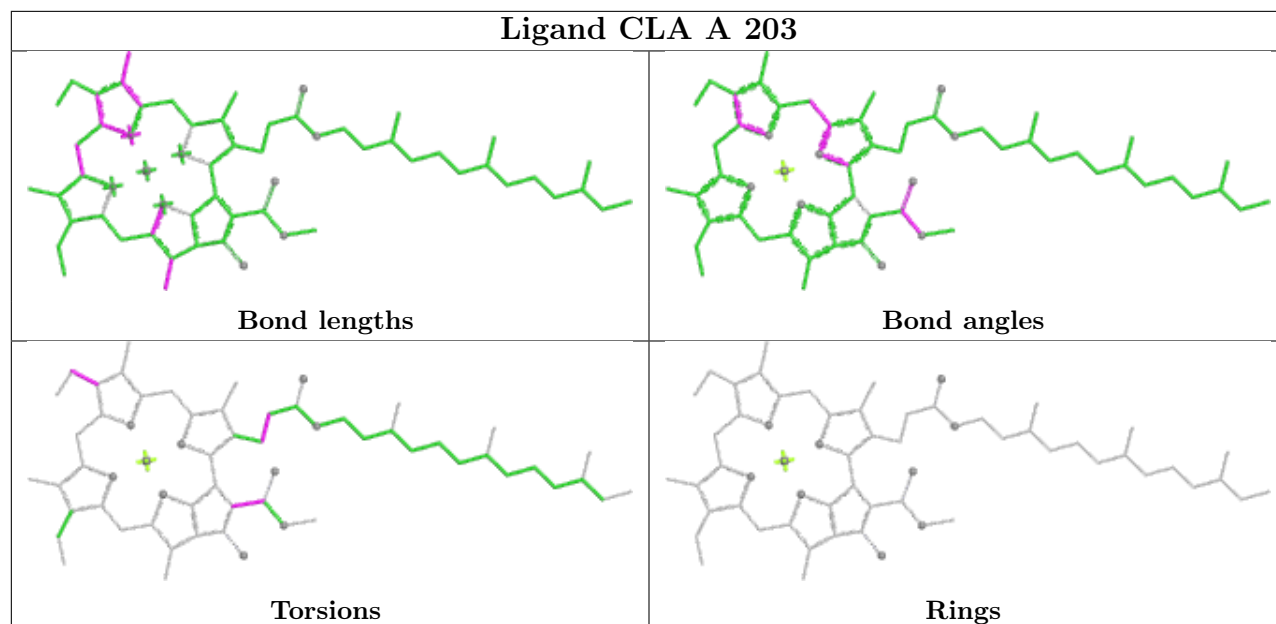
Ligand KC1 L 322



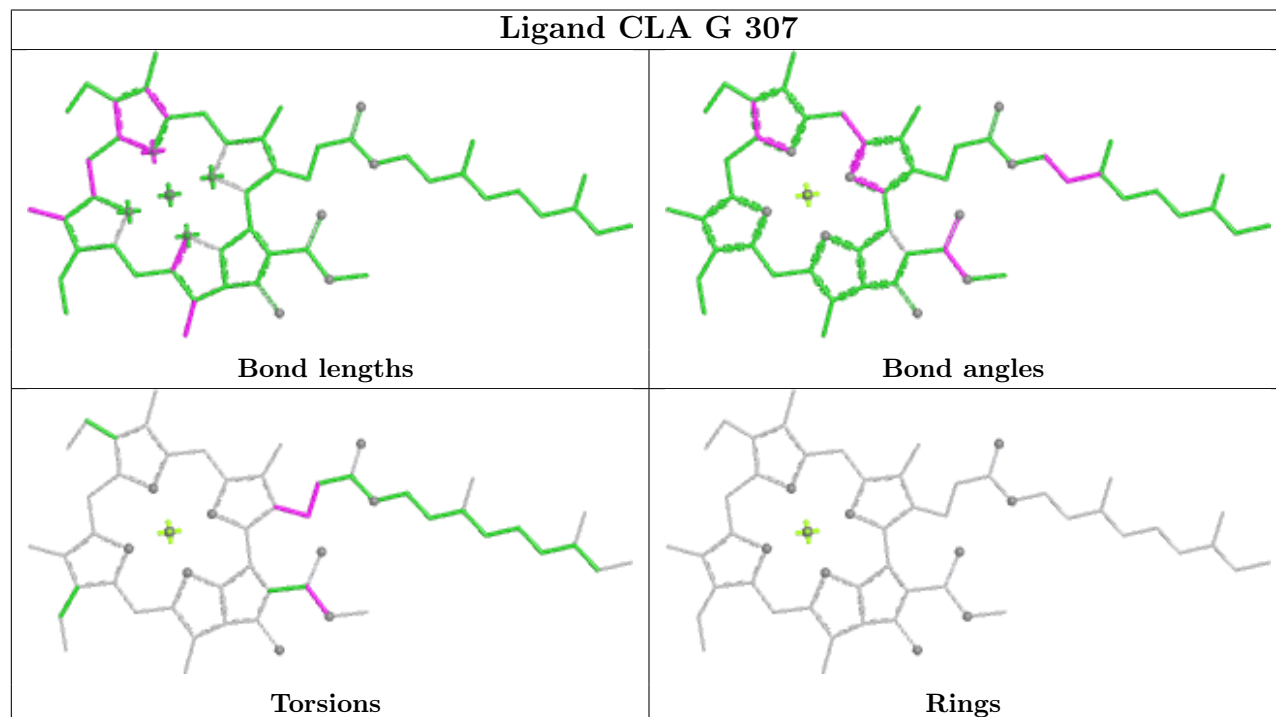
Ligand DD6 J 303

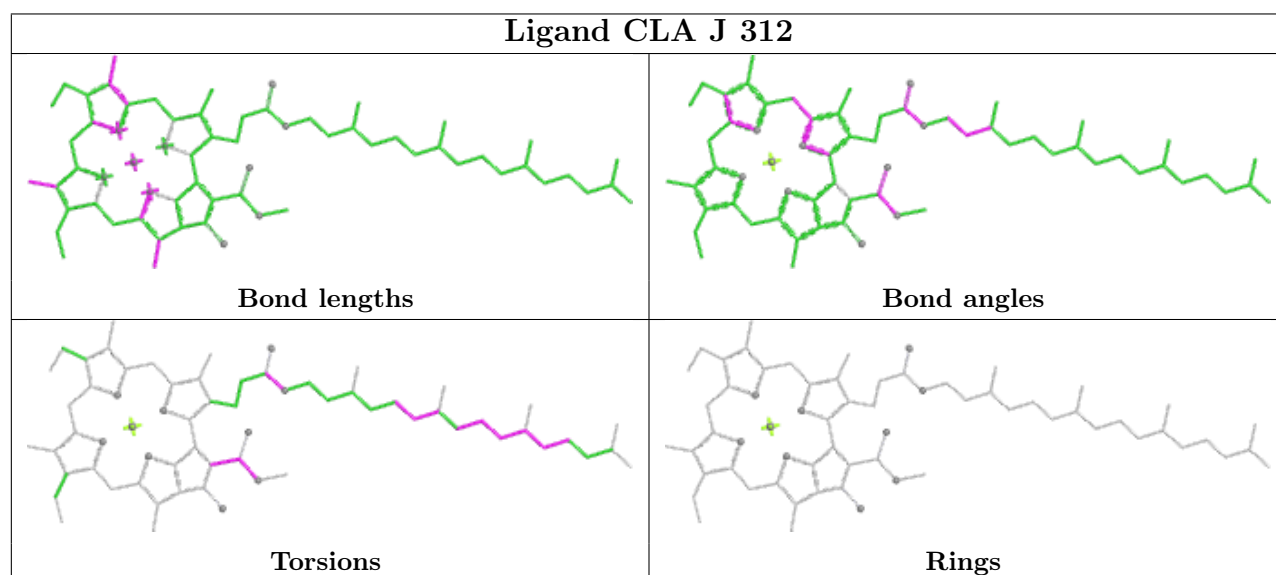
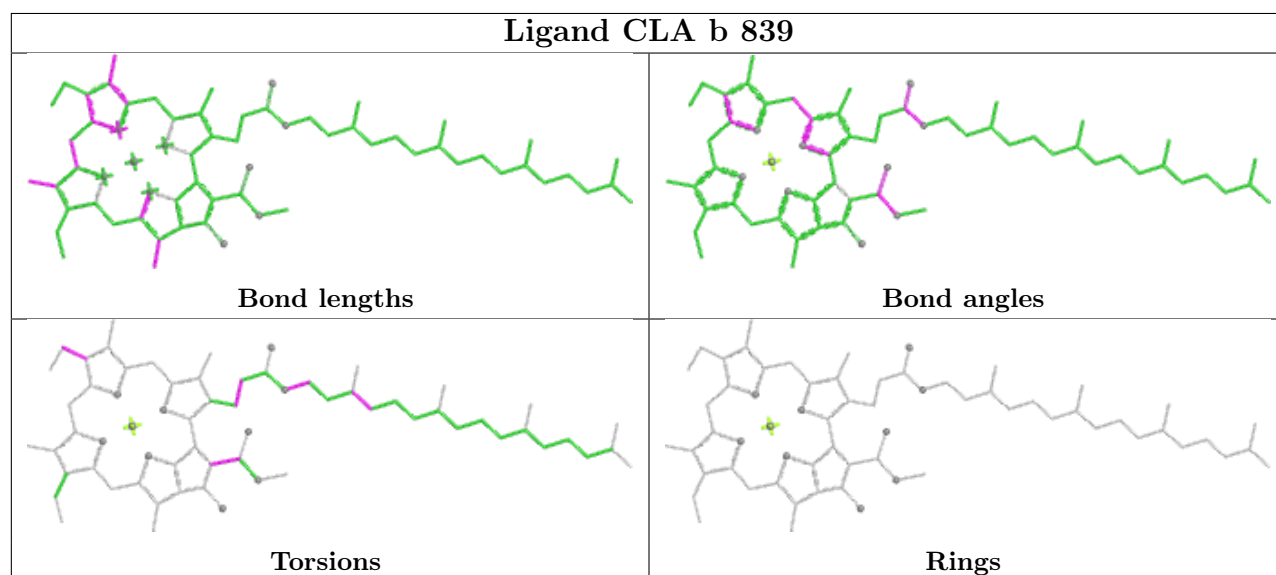
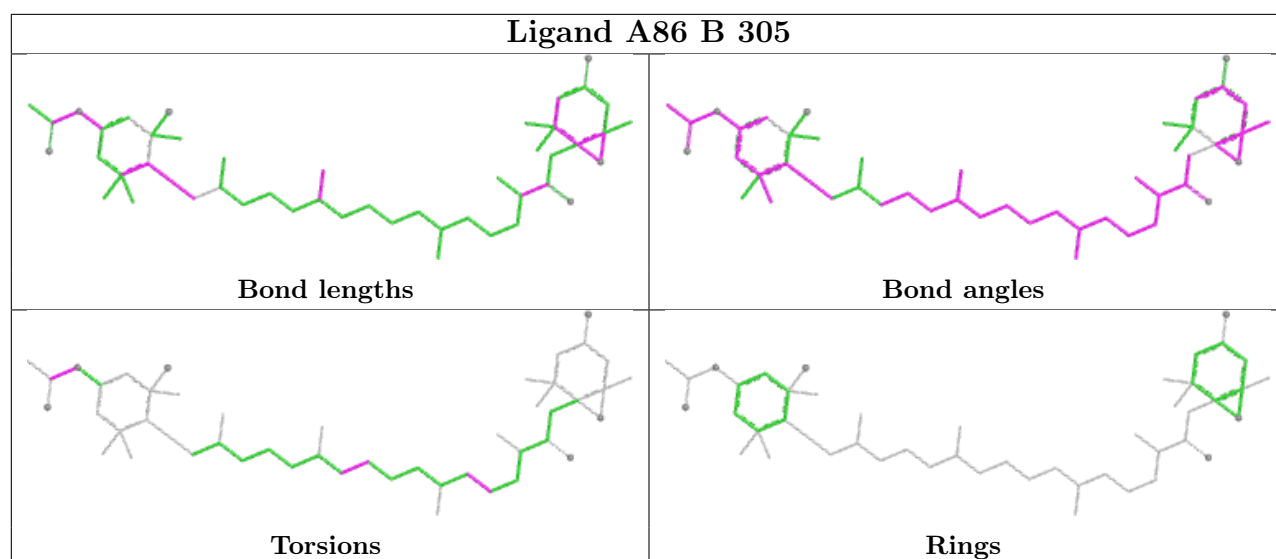


Ligand CLA A 203

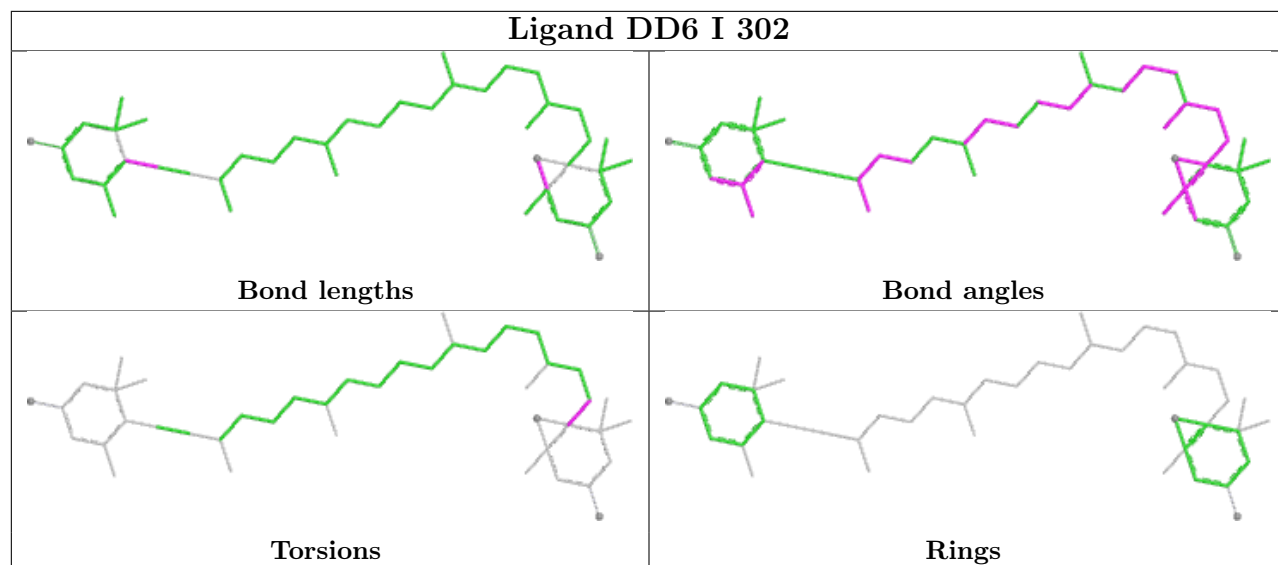


Ligand CLA G 307

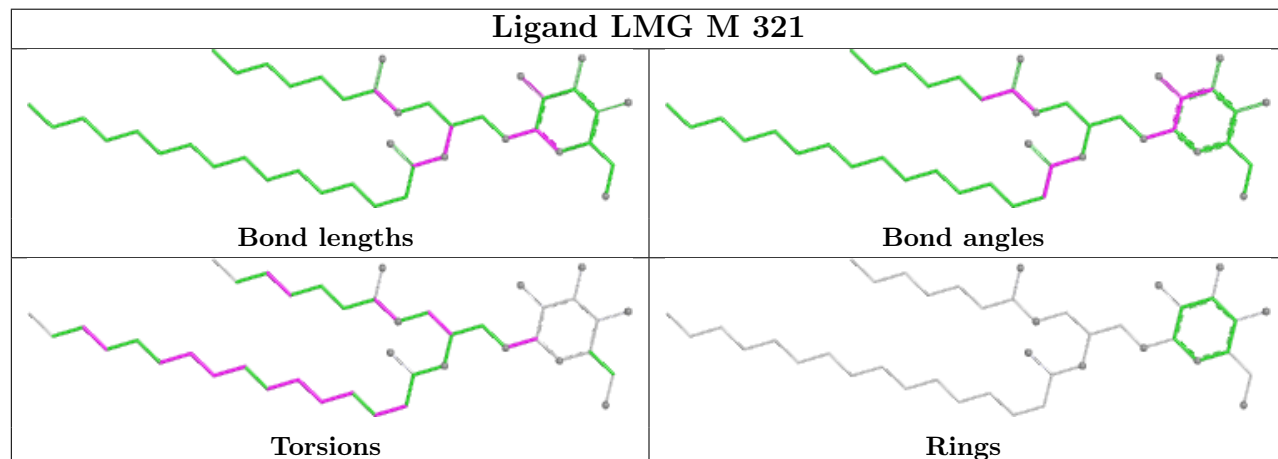




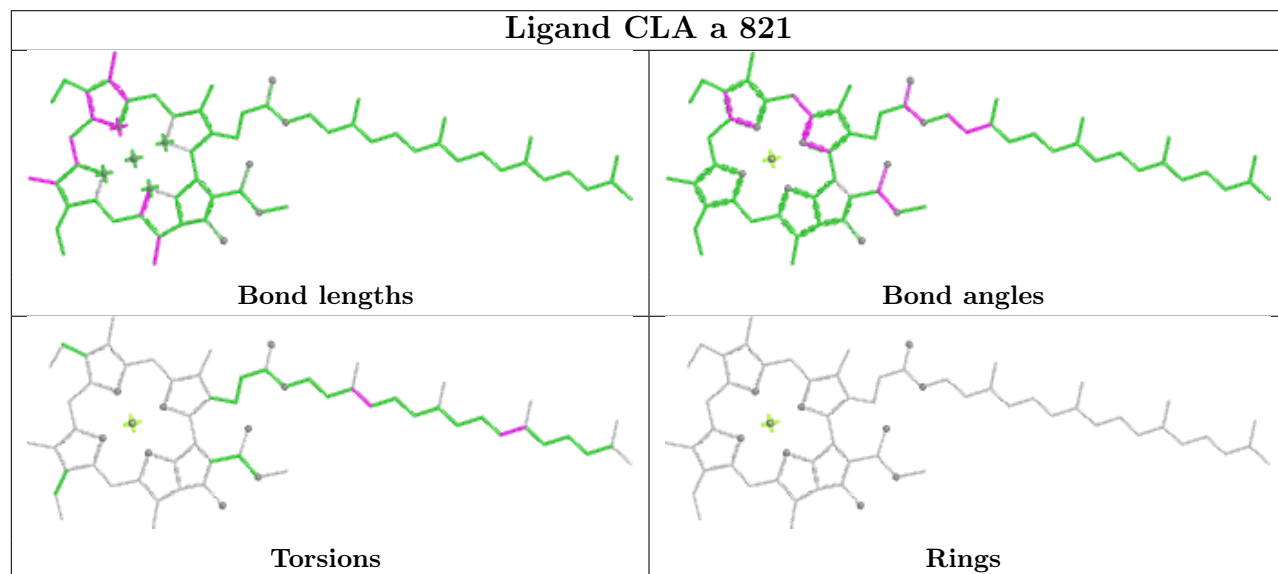
Ligand DD6 I 302



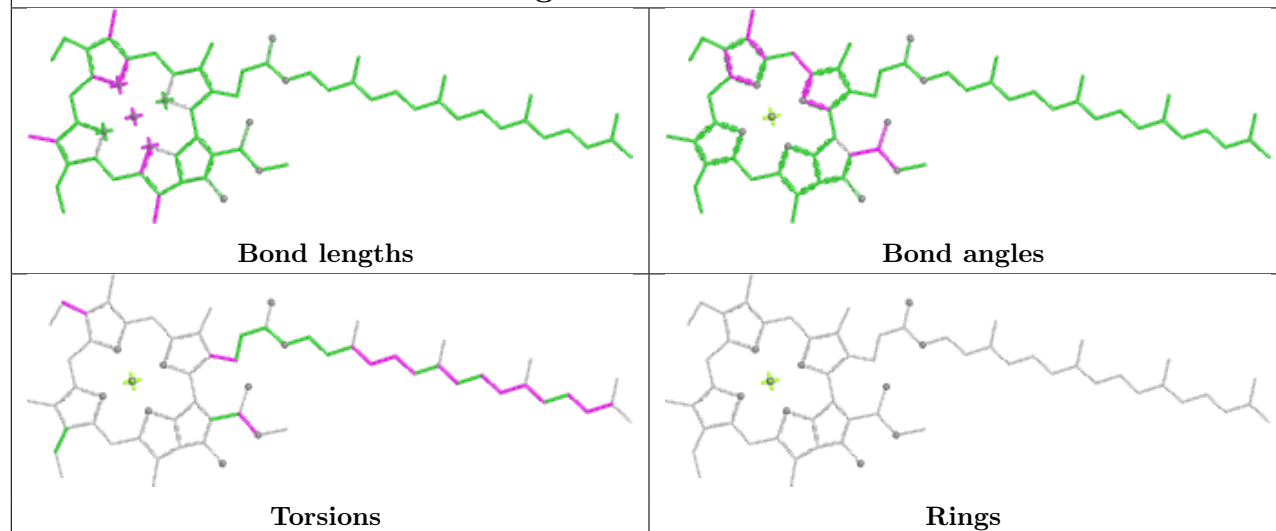
Ligand LMG M 321



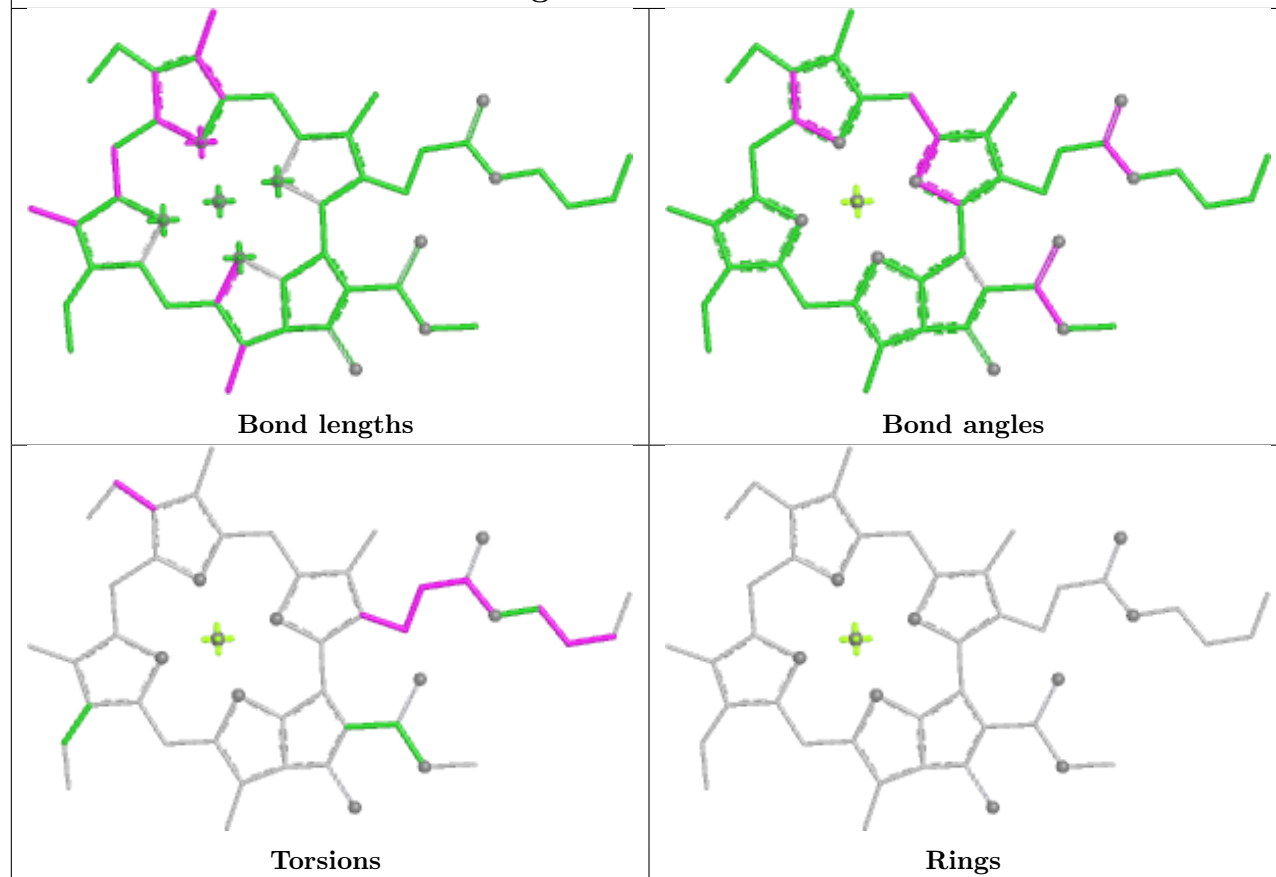
Ligand CLA a 821



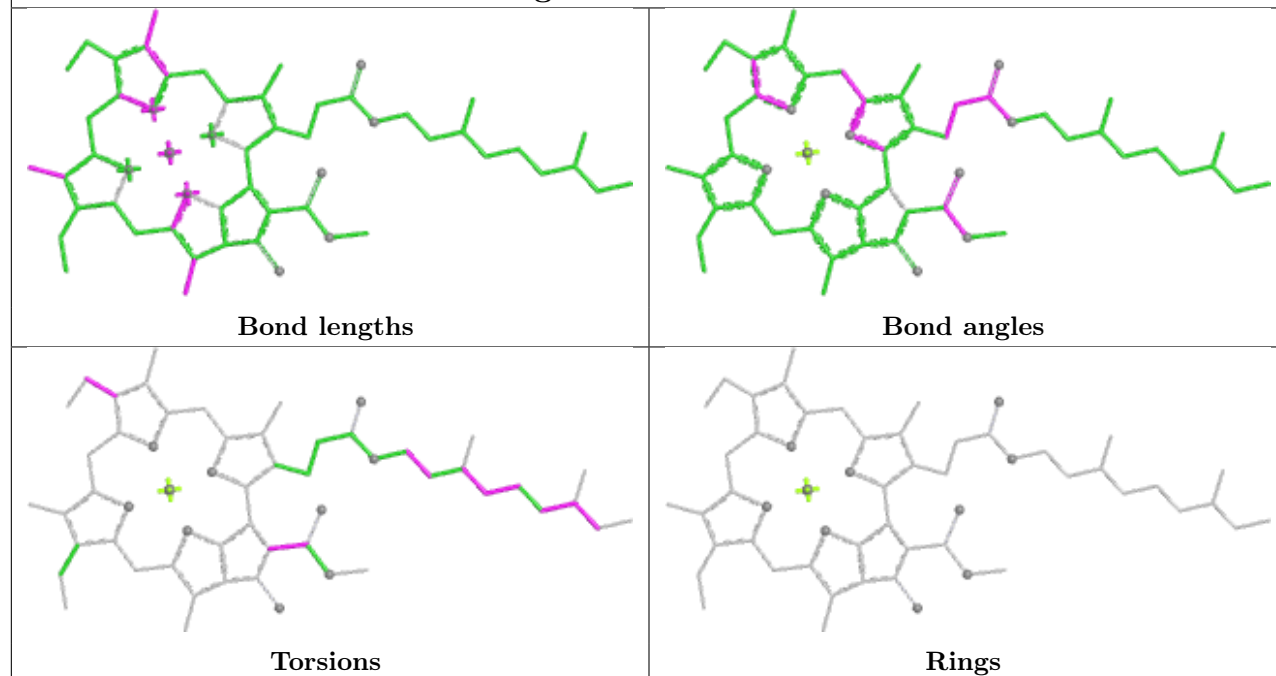
Ligand CLA b 844



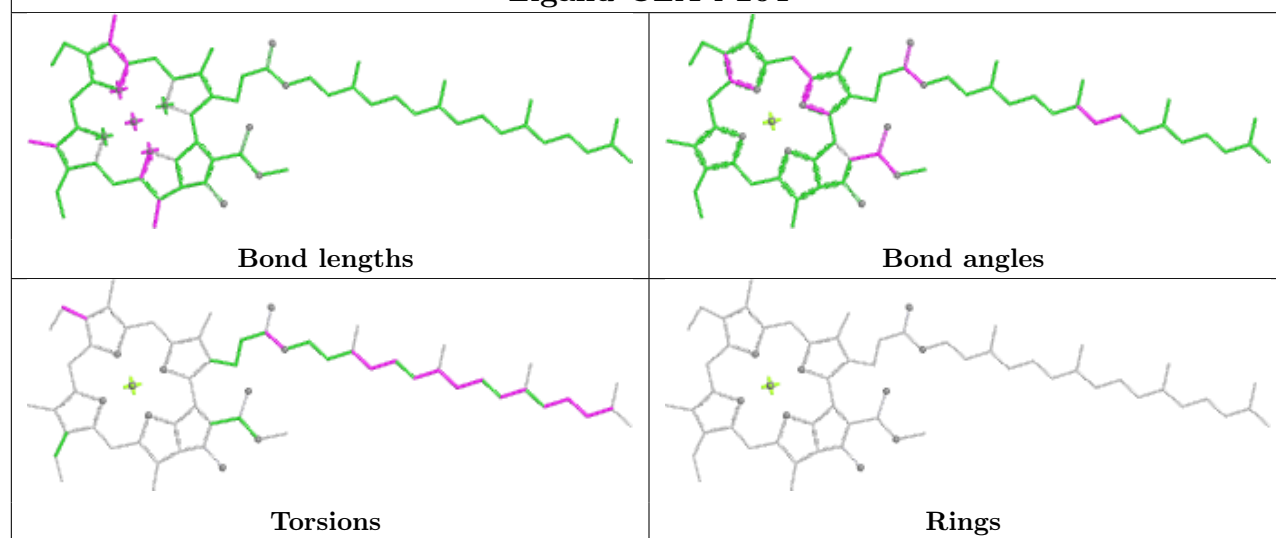
Ligand CLA D 209



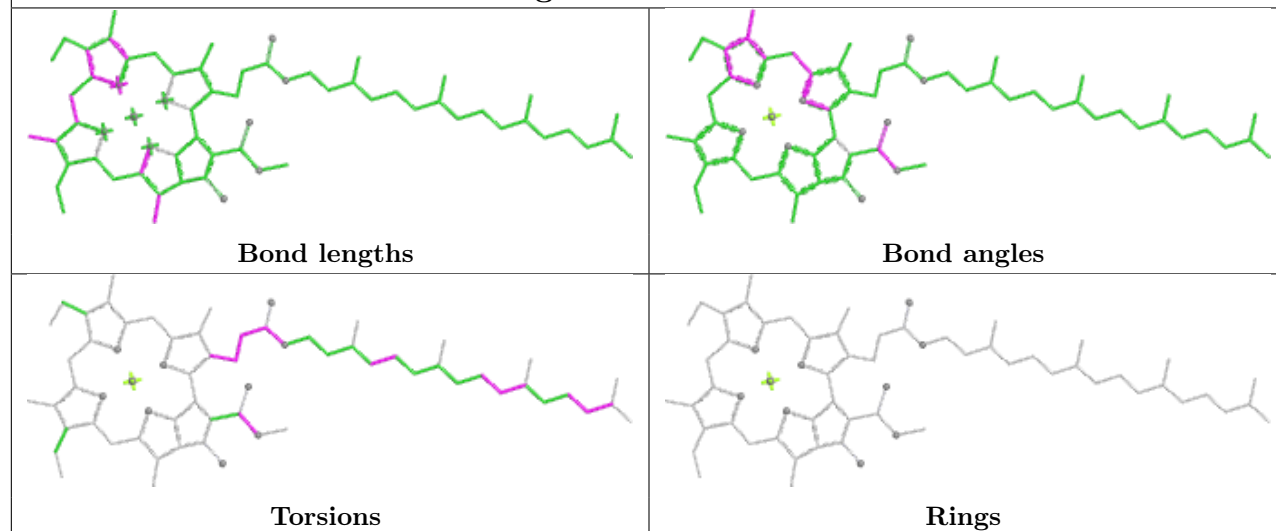
Ligand CLA L 312



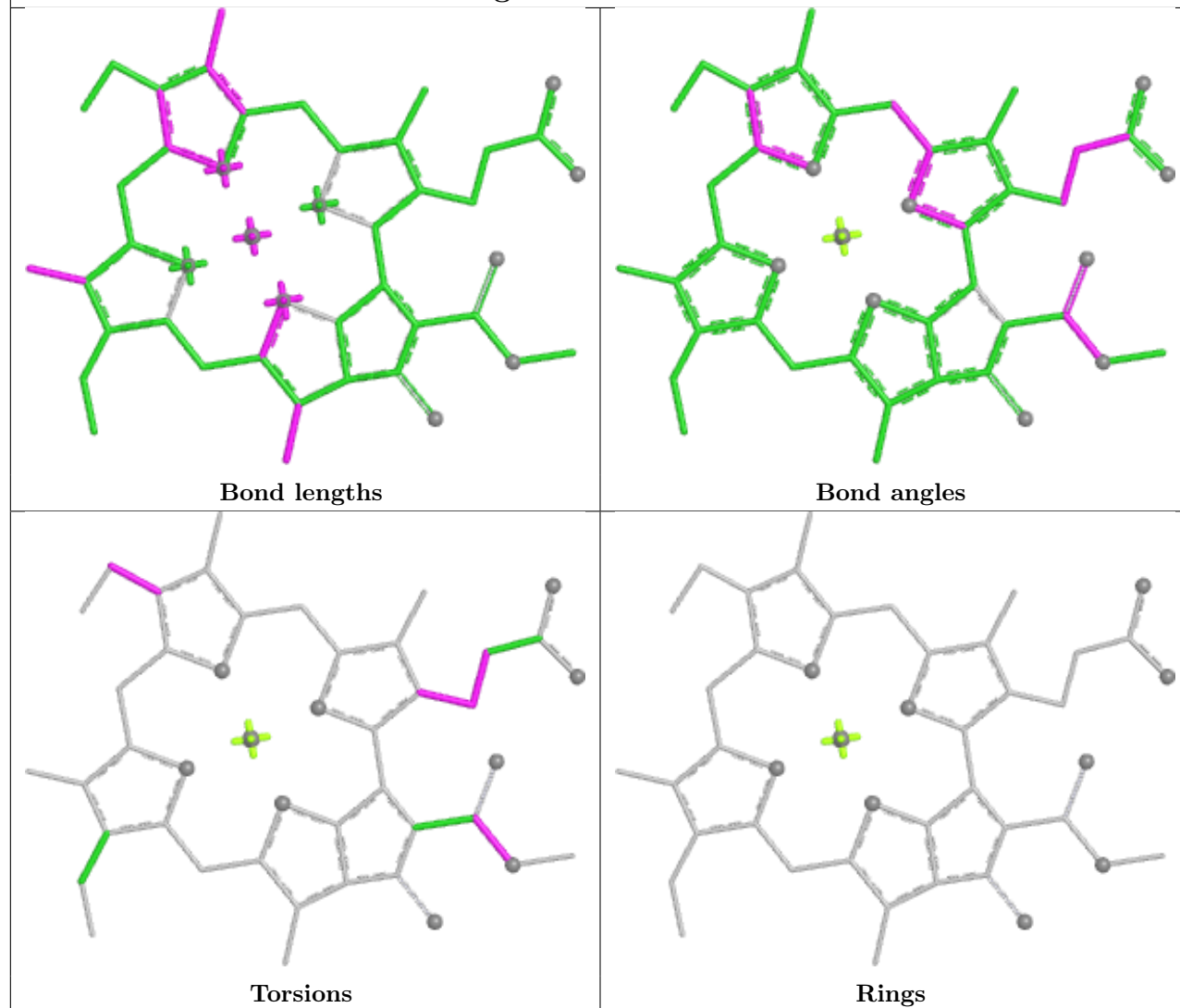
Ligand CLA I 204



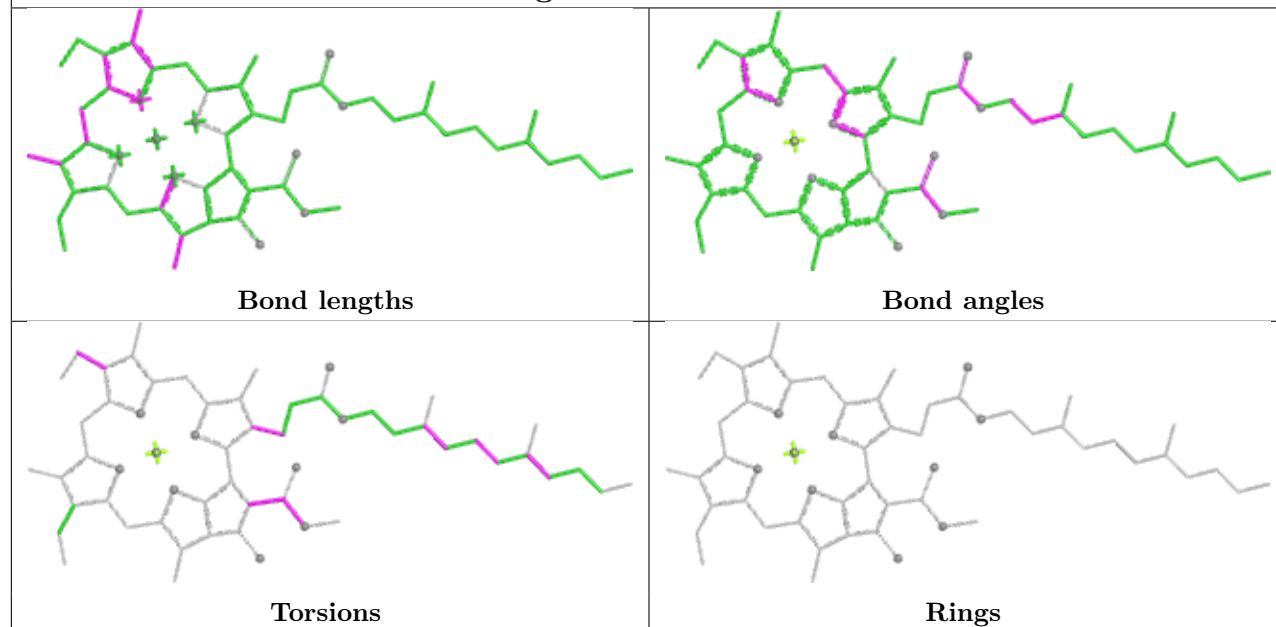
Ligand CLA b 823



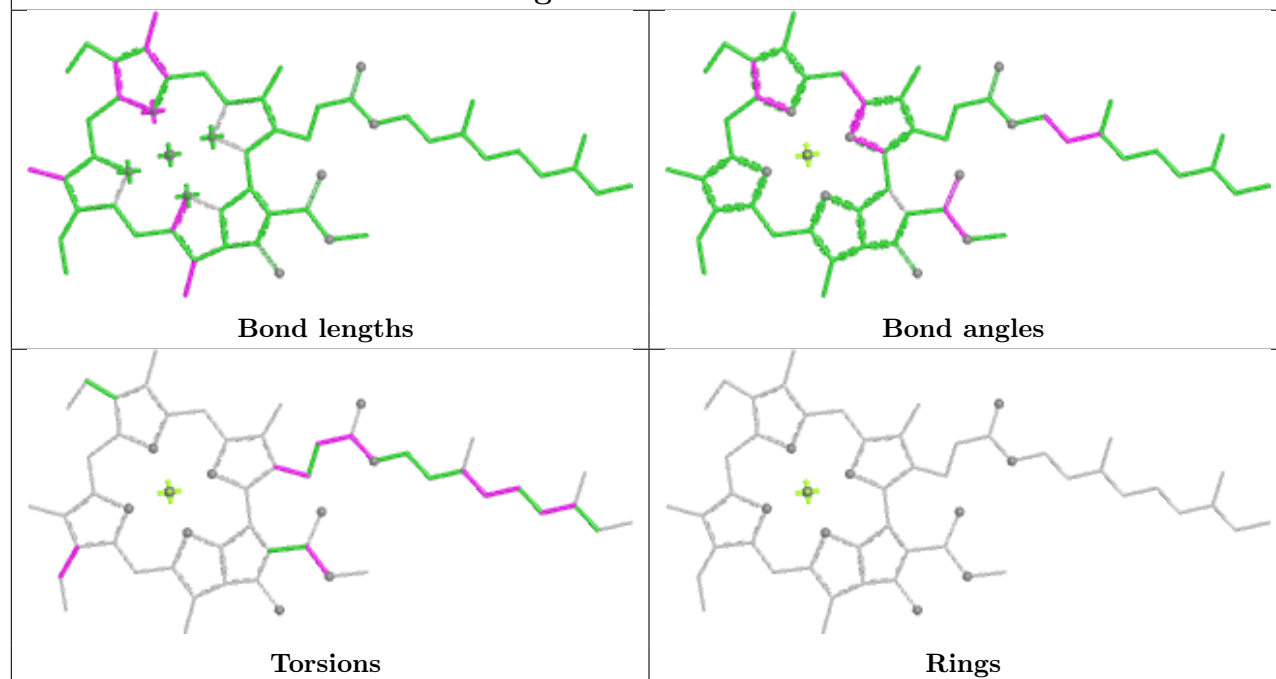
Ligand CLA L 321



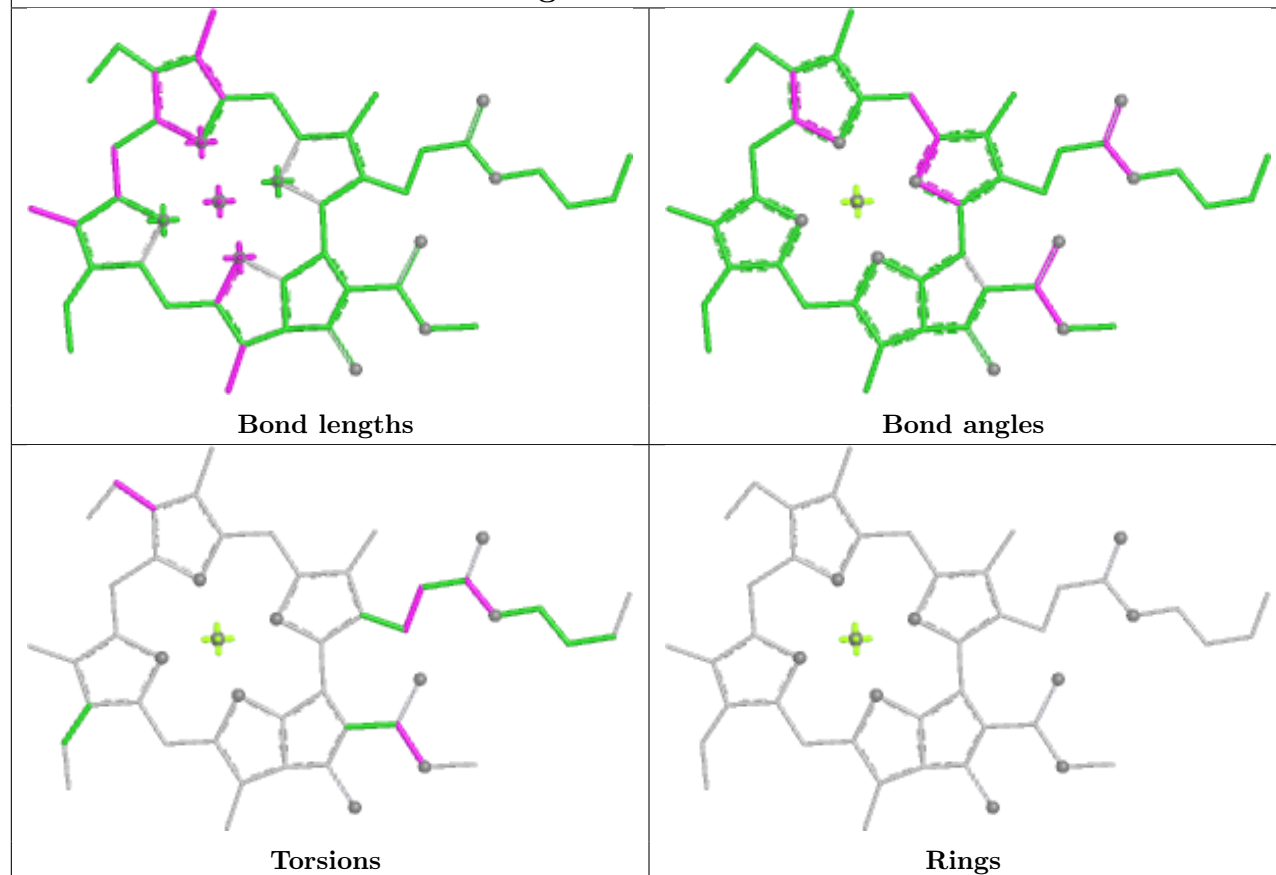
Ligand CLA b 824



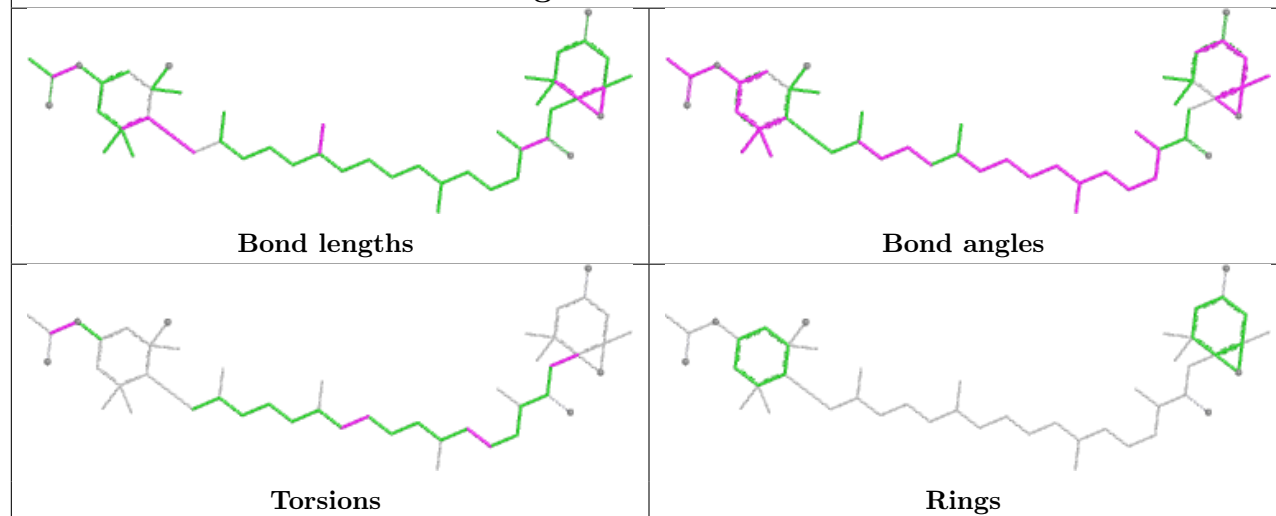
Ligand CLA L 316

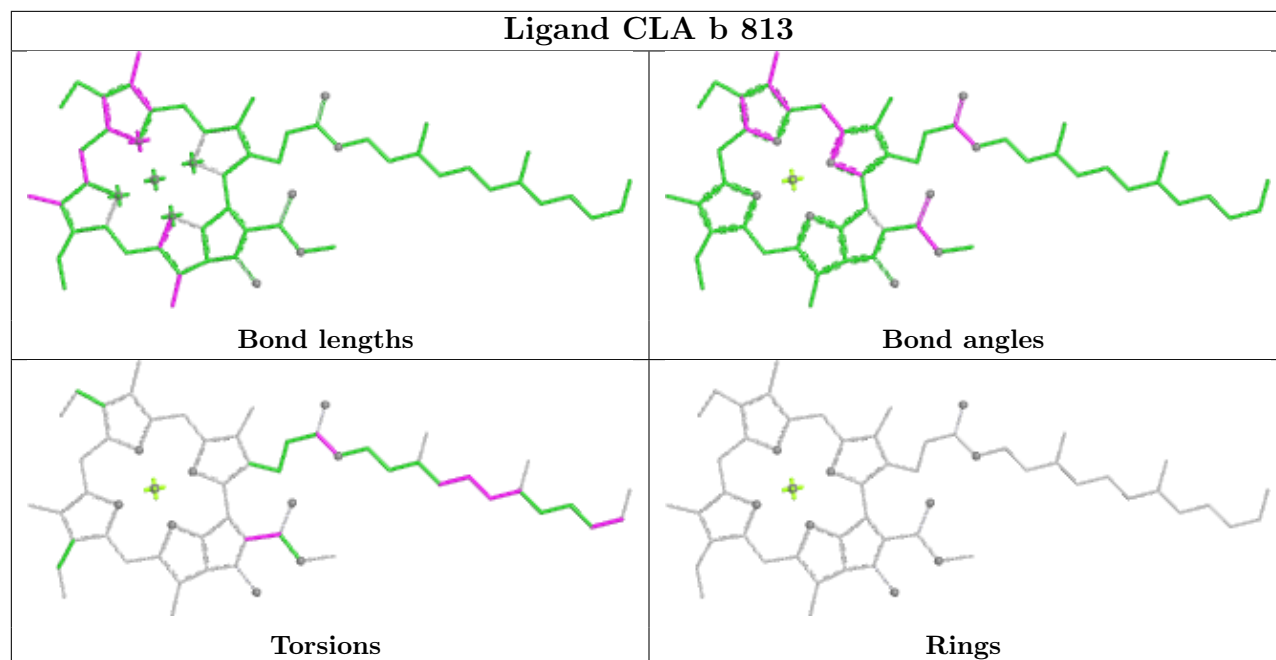
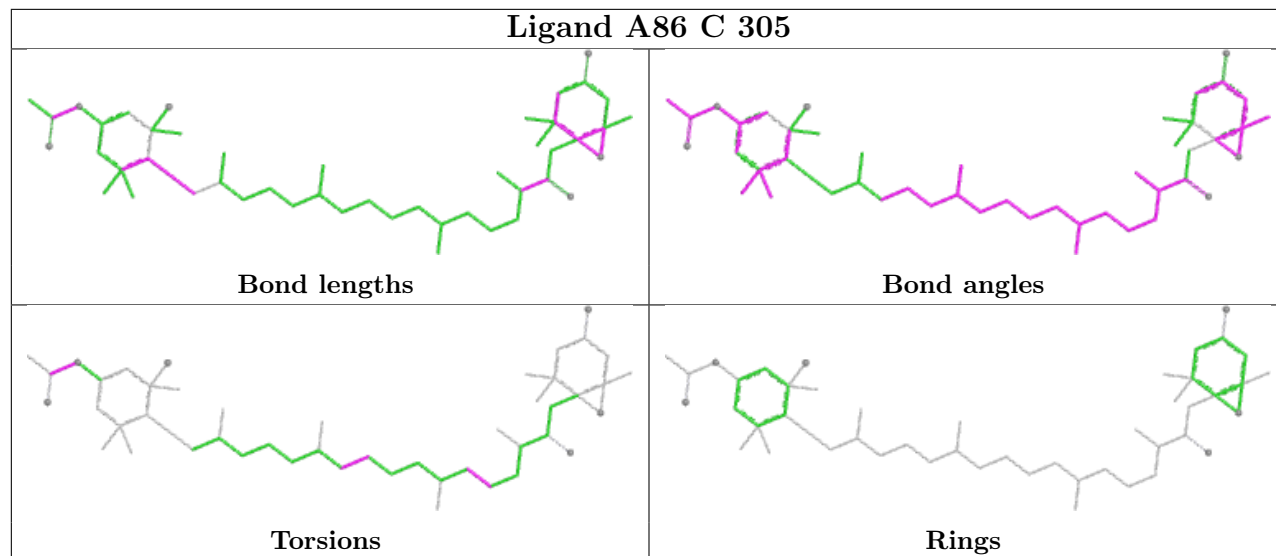


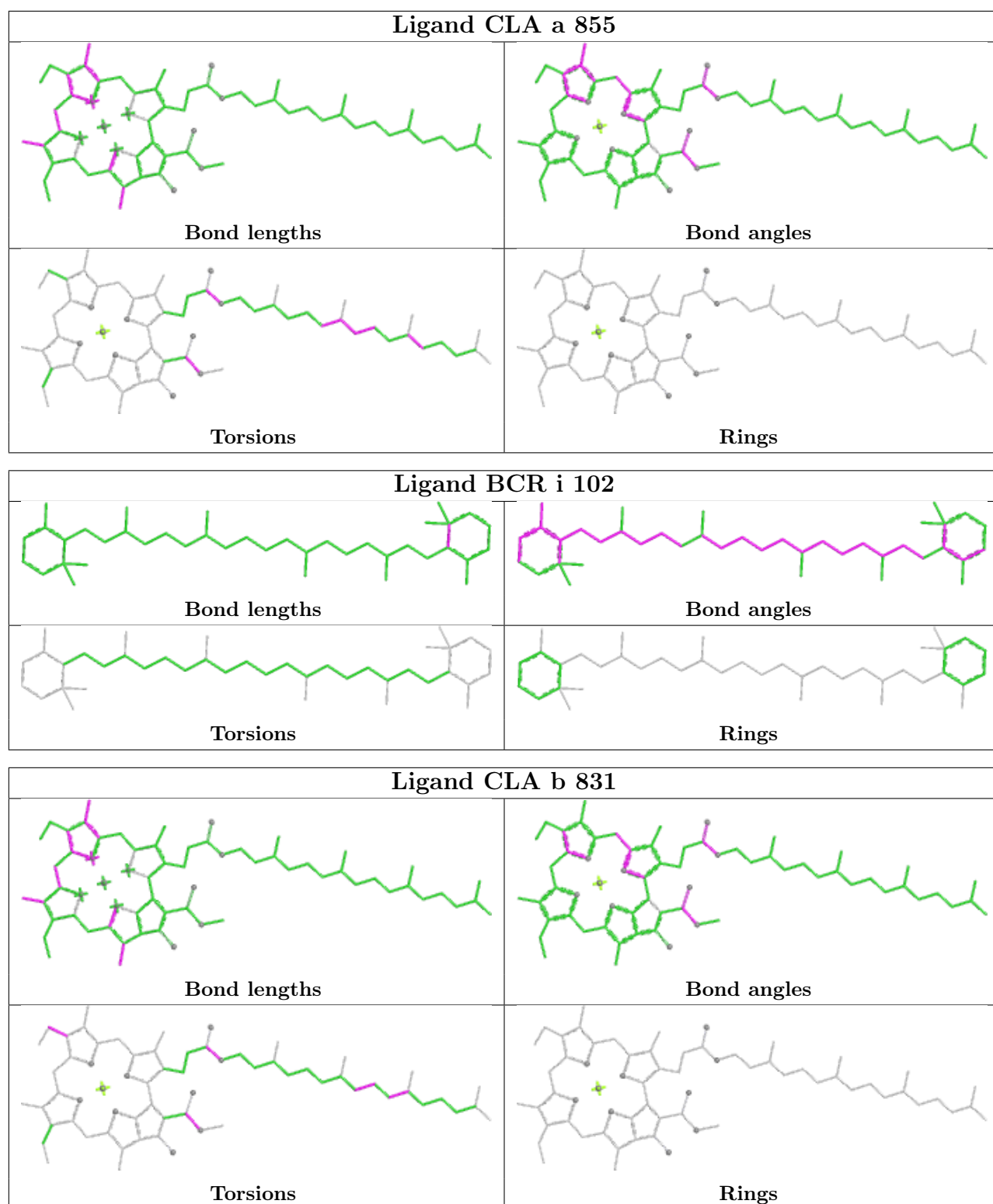
Ligand CLA I 314

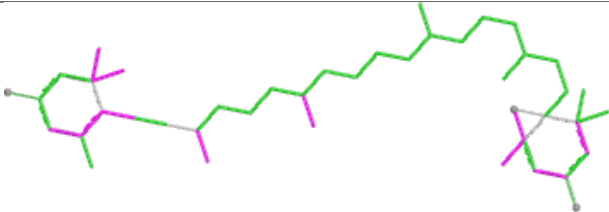
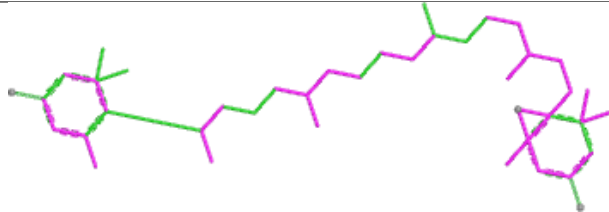
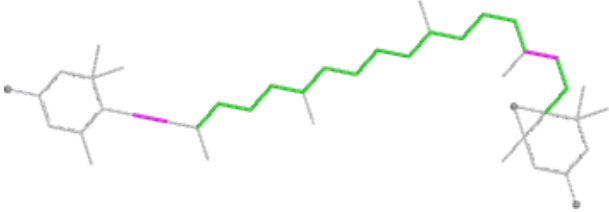
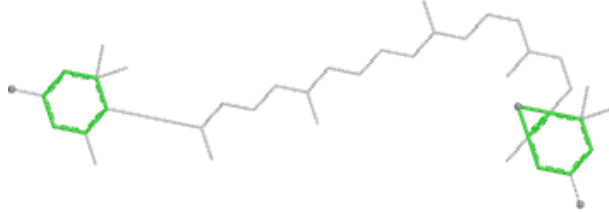


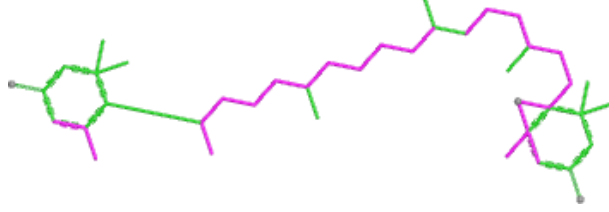
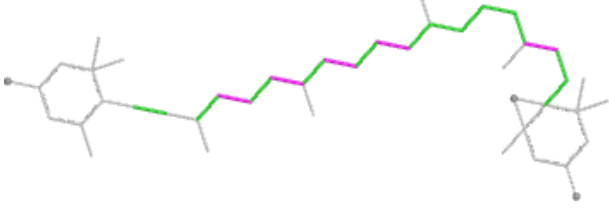
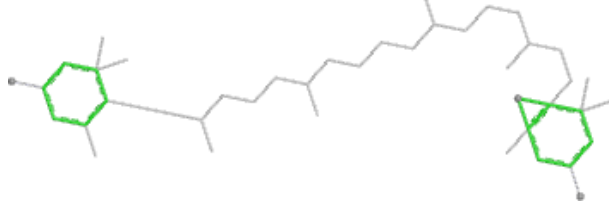
Ligand A86 M 302

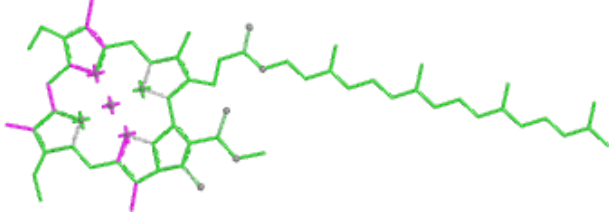
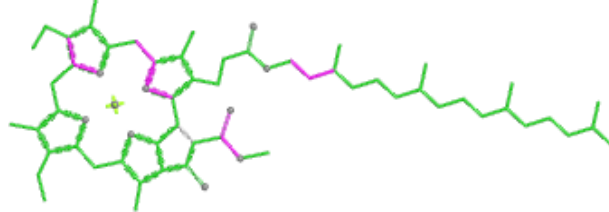
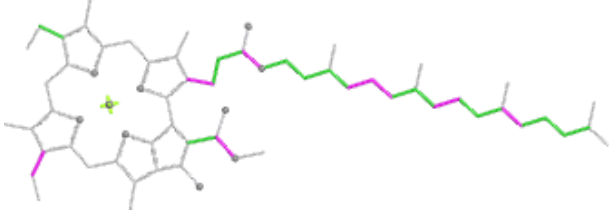
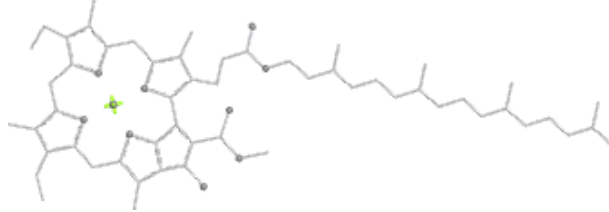


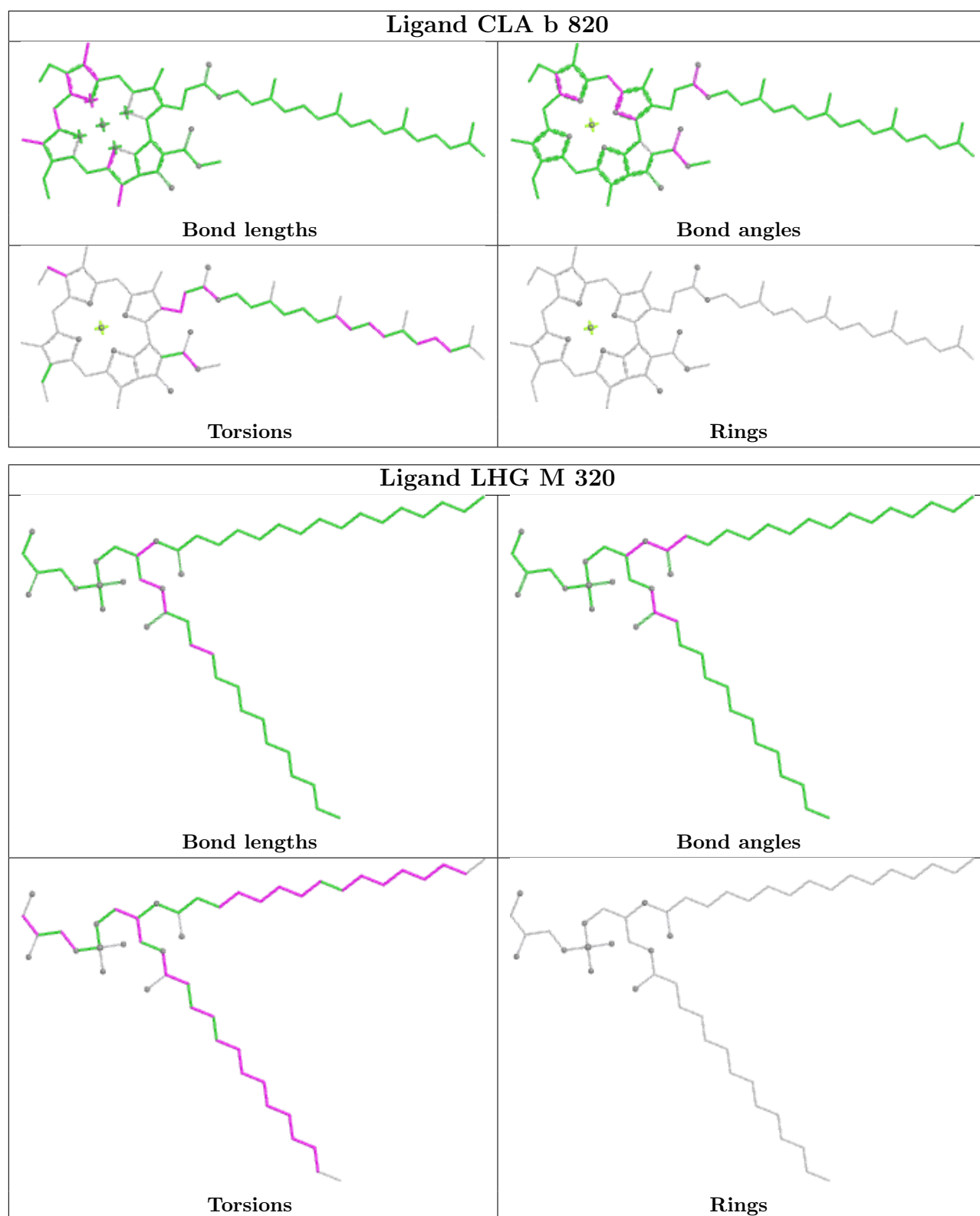
Ligand CLA b 813**Ligand A86 C 305**



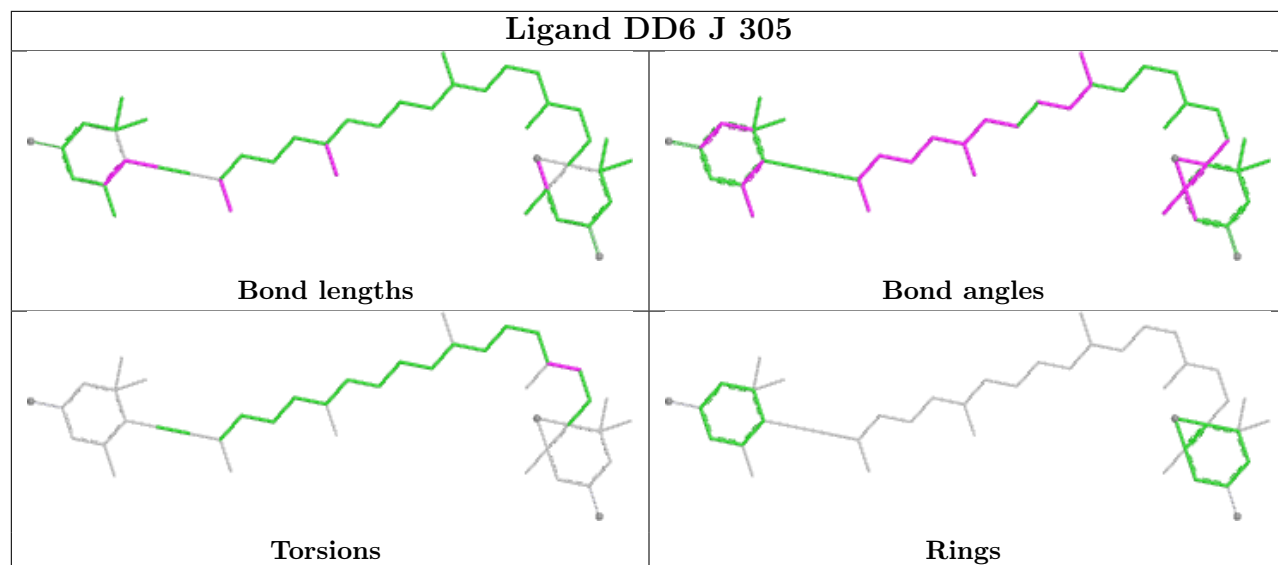
Ligand DD6 H 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DD6 A 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

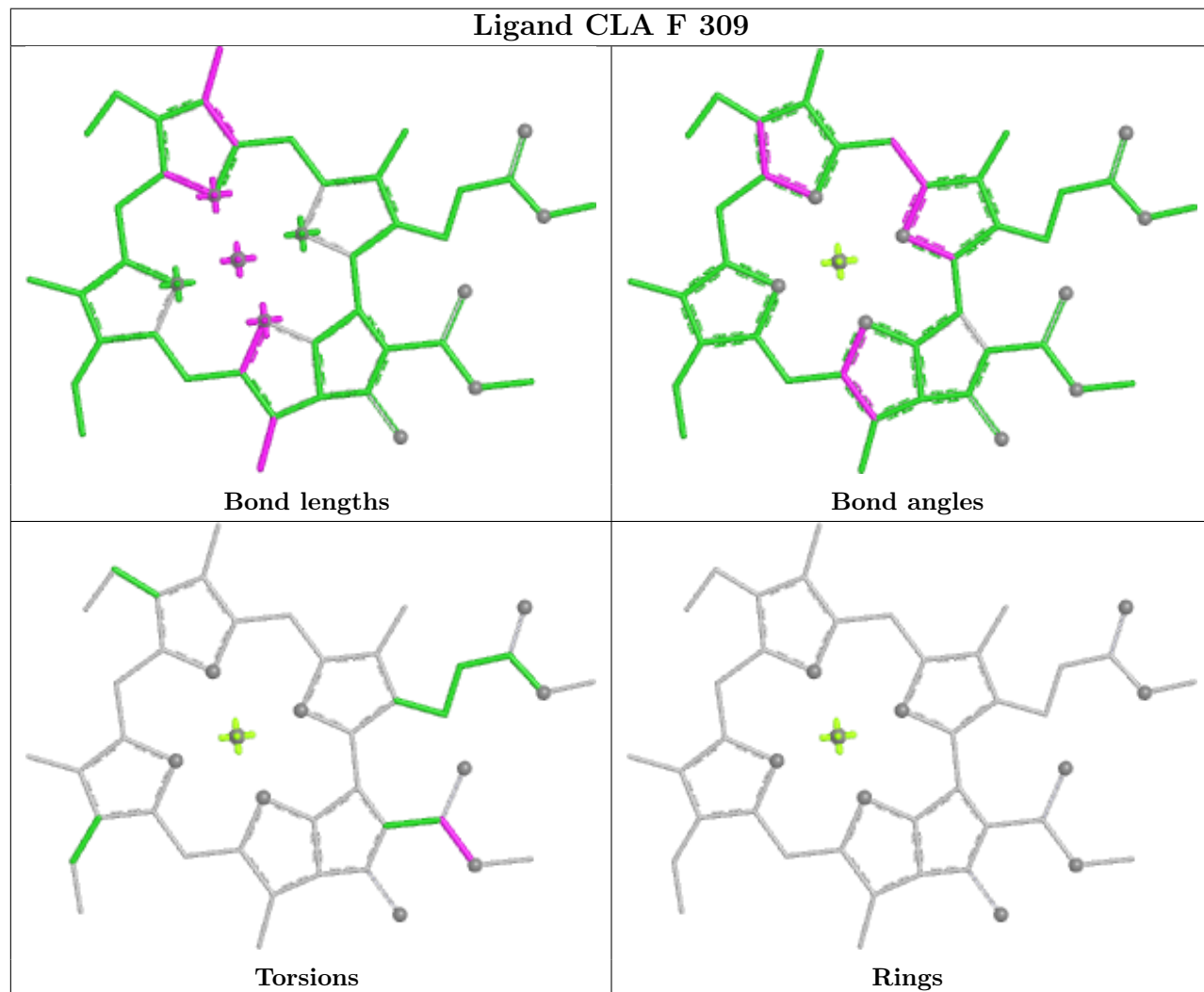
Ligand CLA L 313	
	
Bond lengths	Bond angles
	
Torsions	Rings



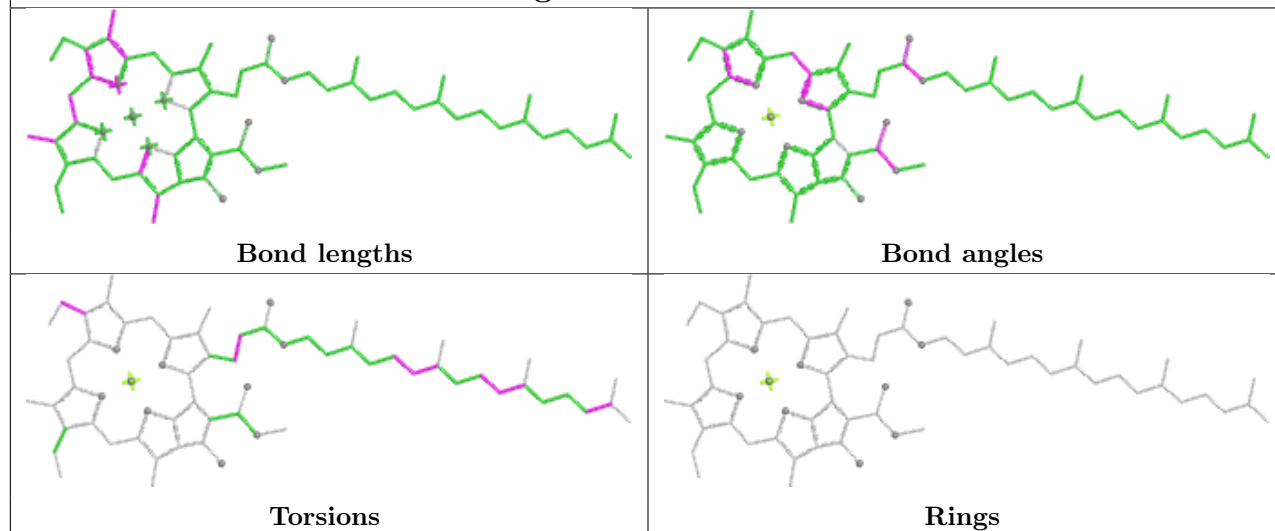
Ligand DD6 J 305



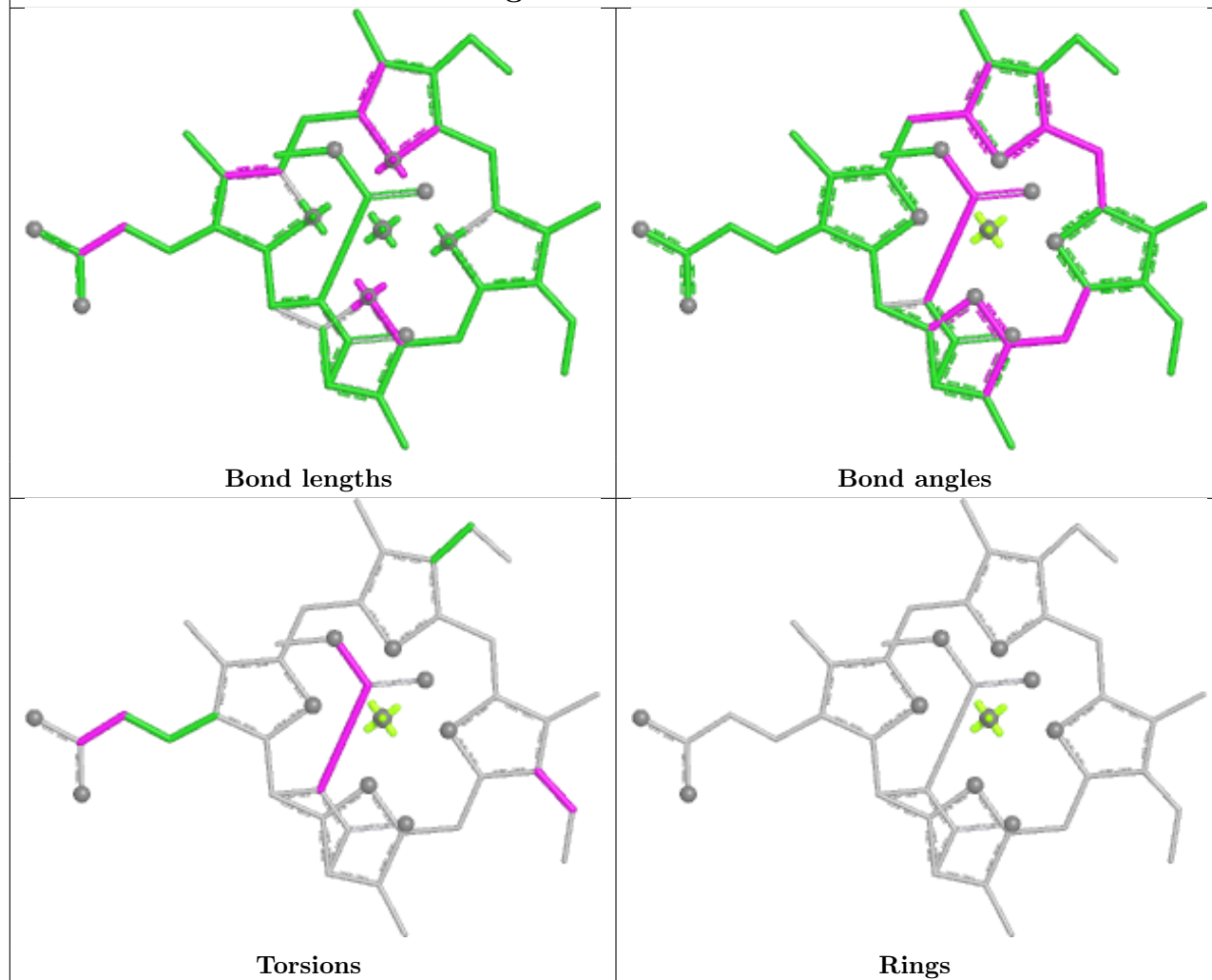
Ligand CLA F 309



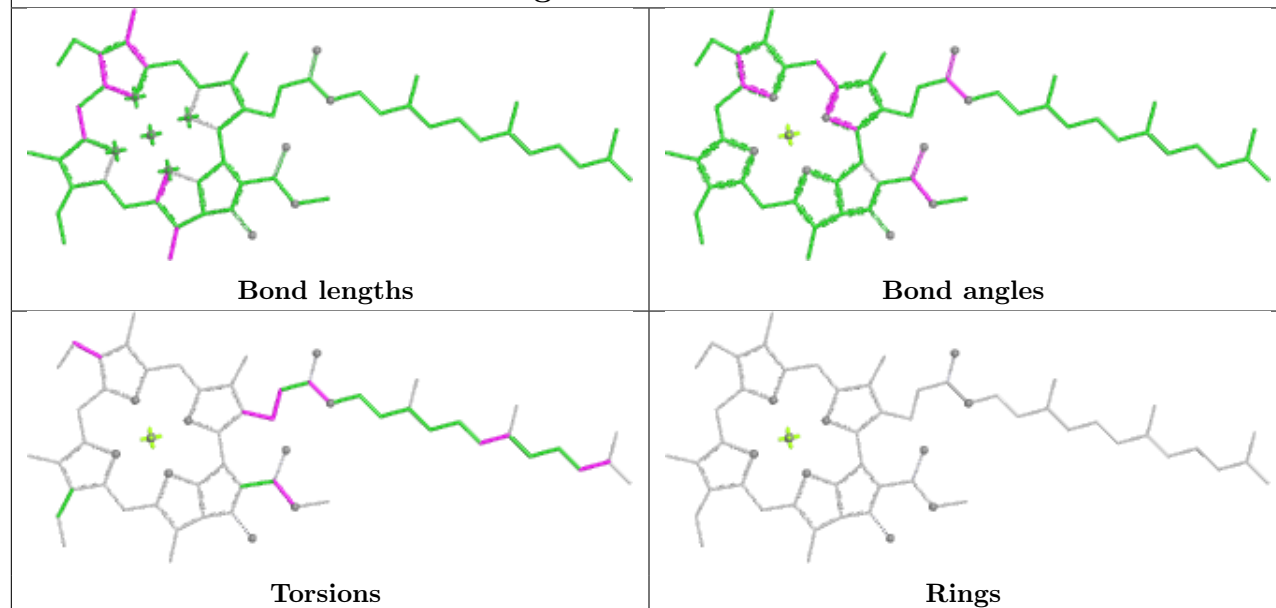
Ligand CLA b 808



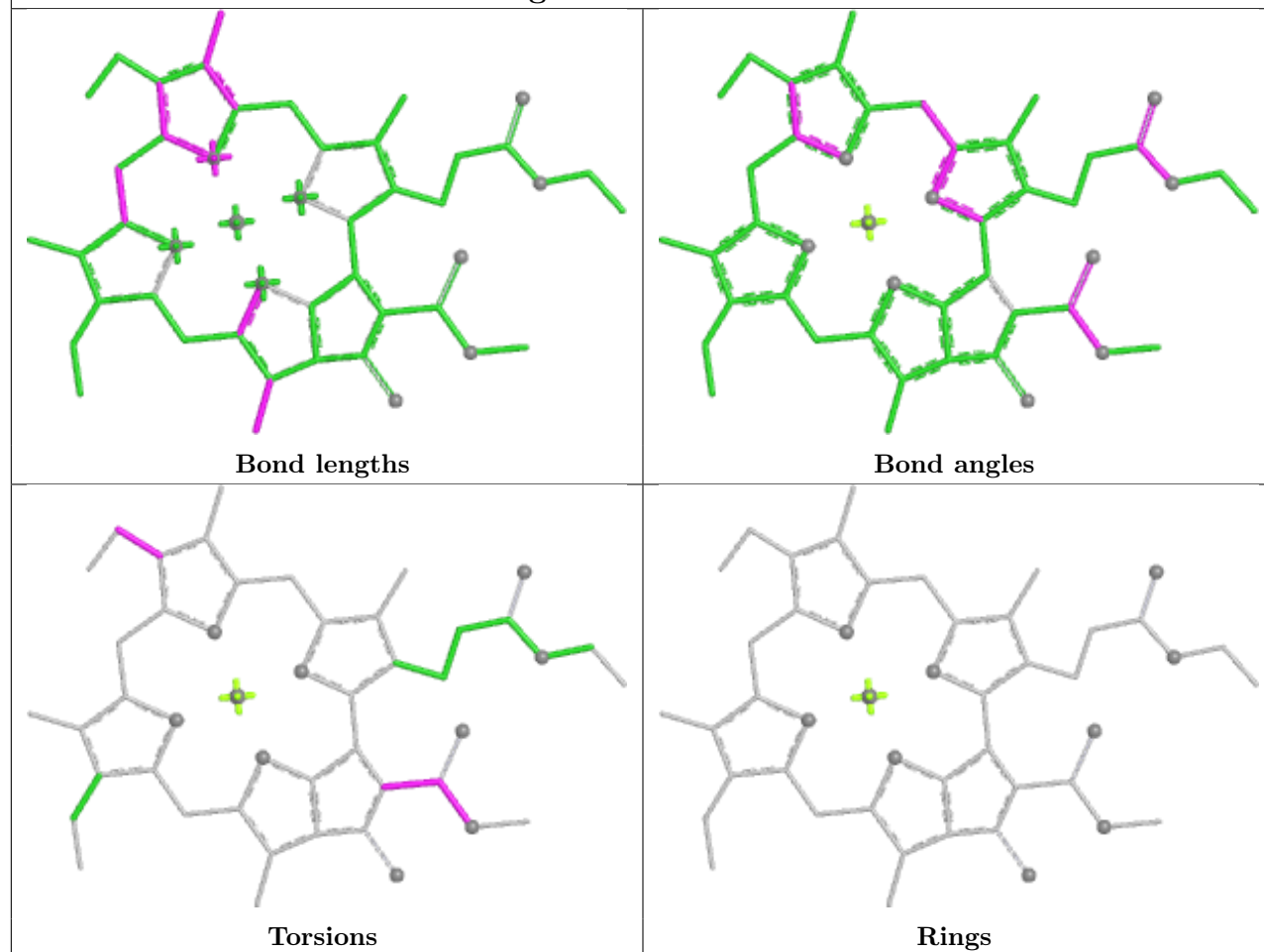
Ligand KC1 K 315

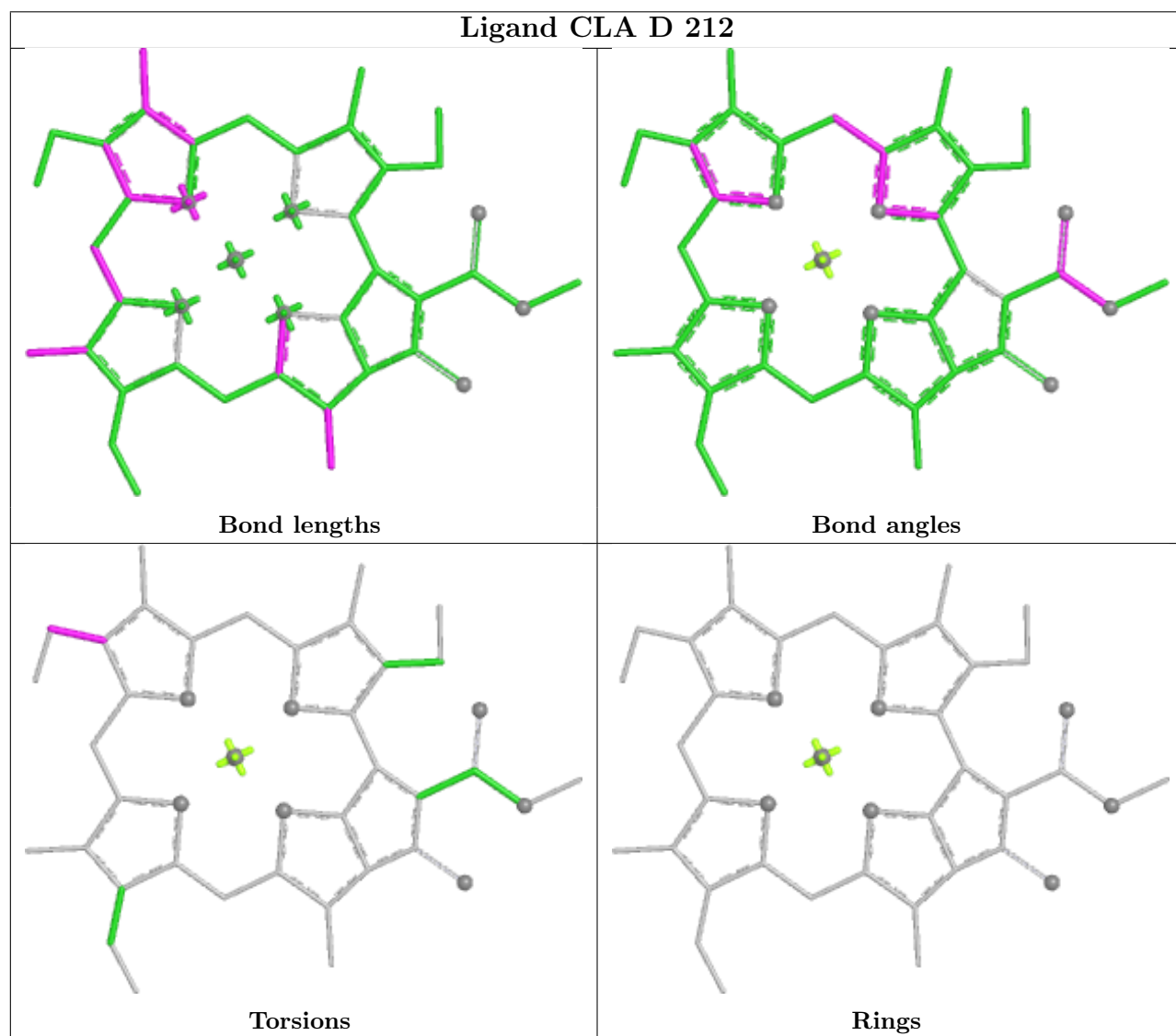
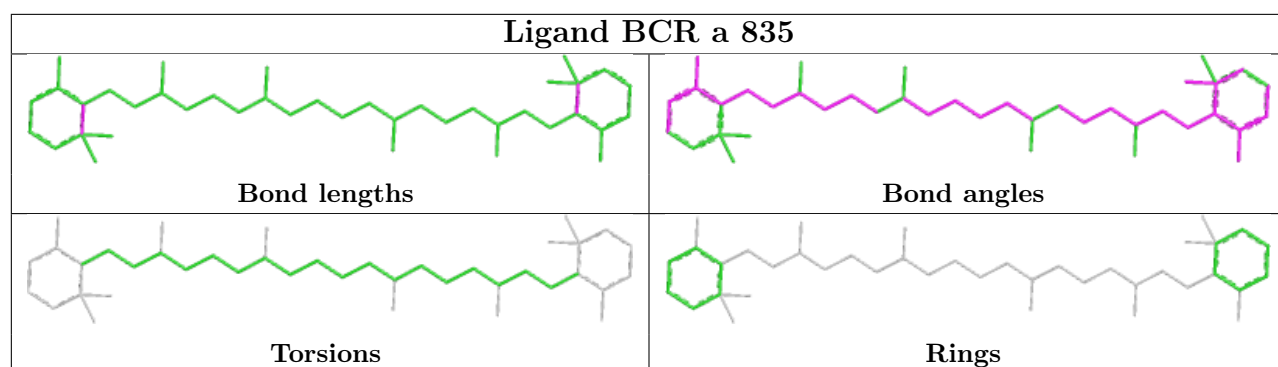


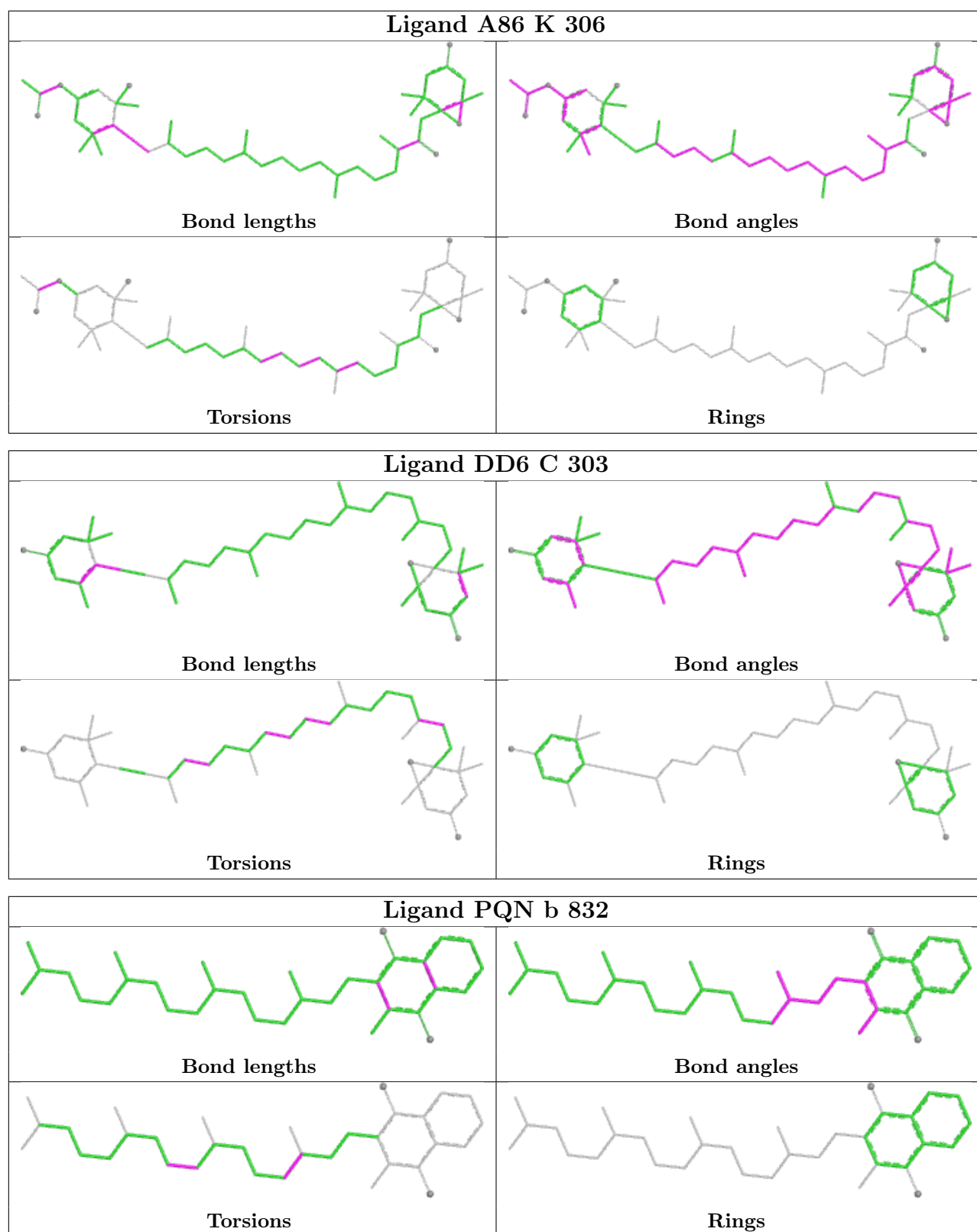
Ligand CLA F 310



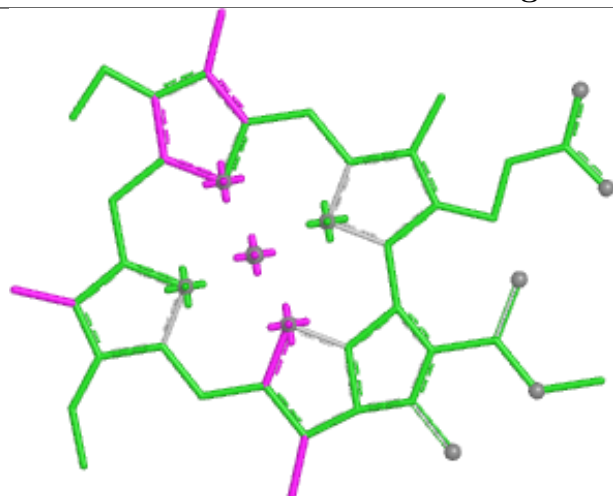
Ligand CLA F 314



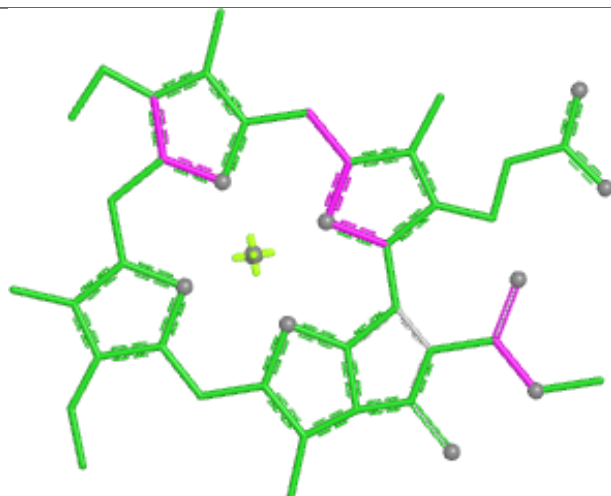




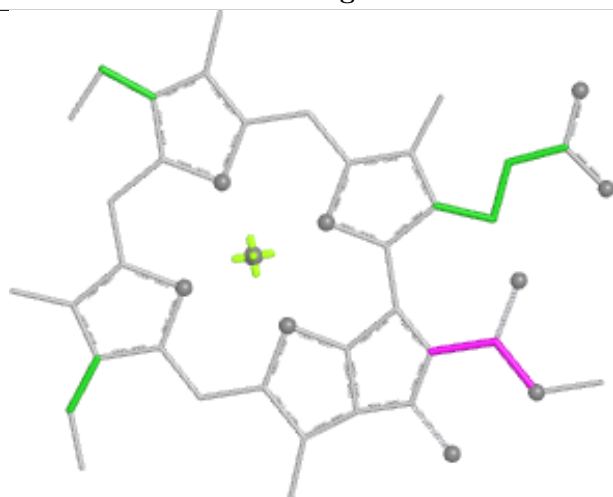
Ligand CLA I 316



Bond lengths



Bond angles

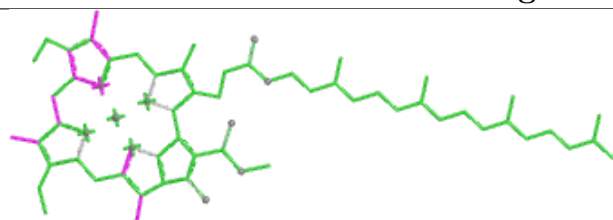


Torsions

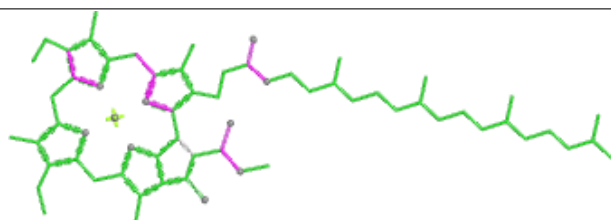


Rings

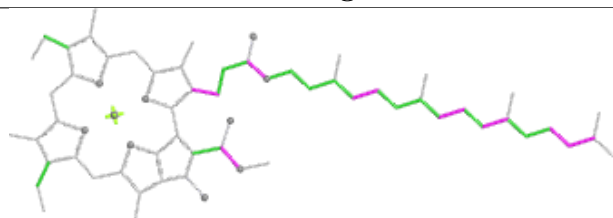
Ligand CLA a 808



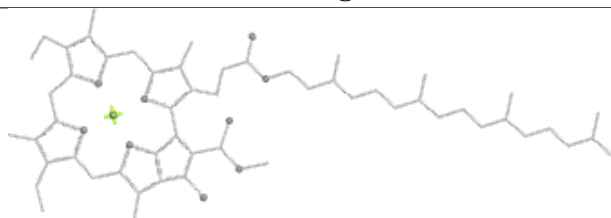
Bond lengths



Bond angles

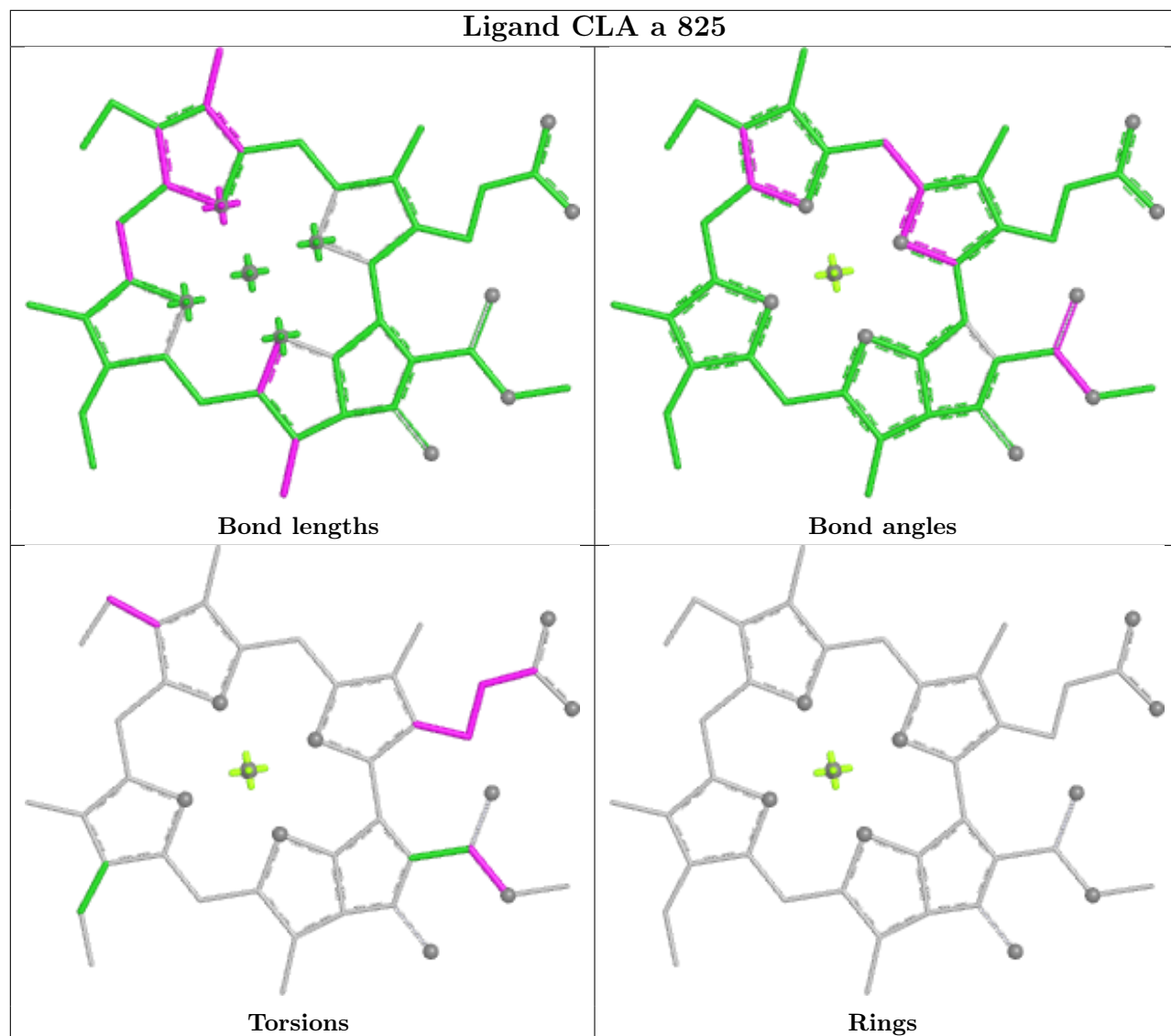


Torsions

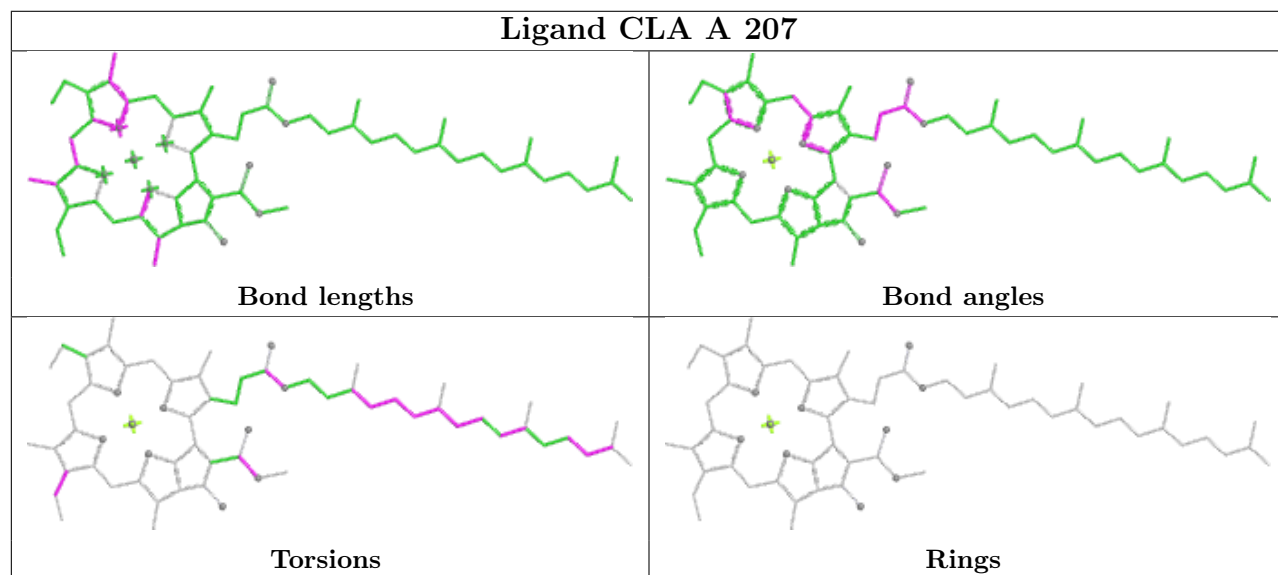


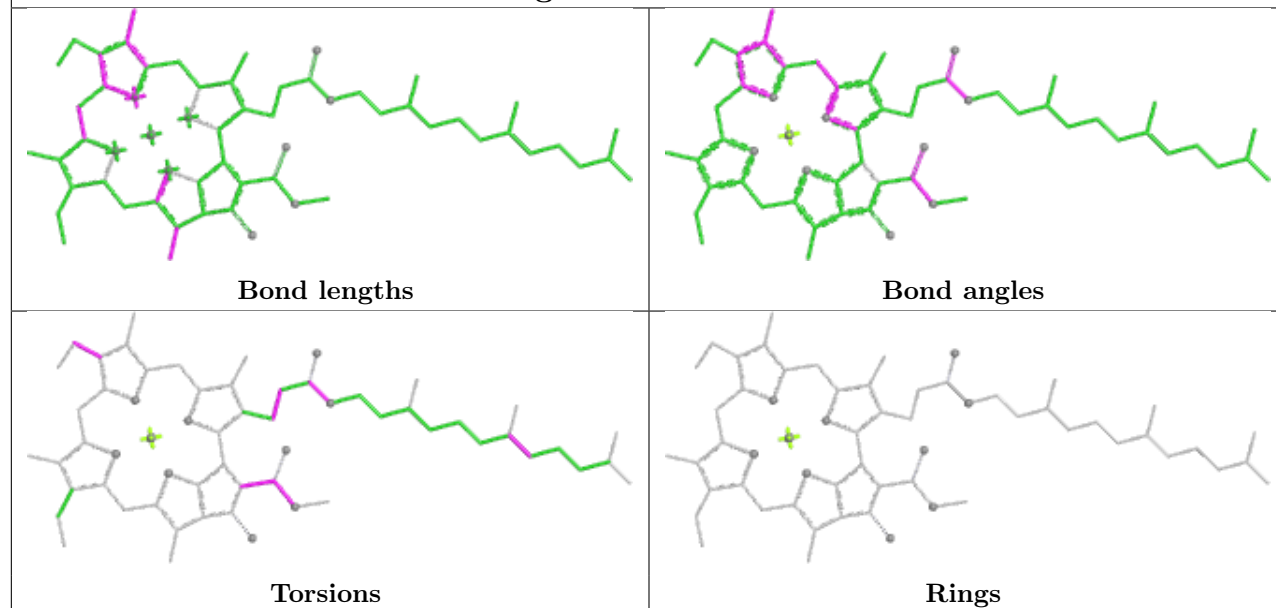
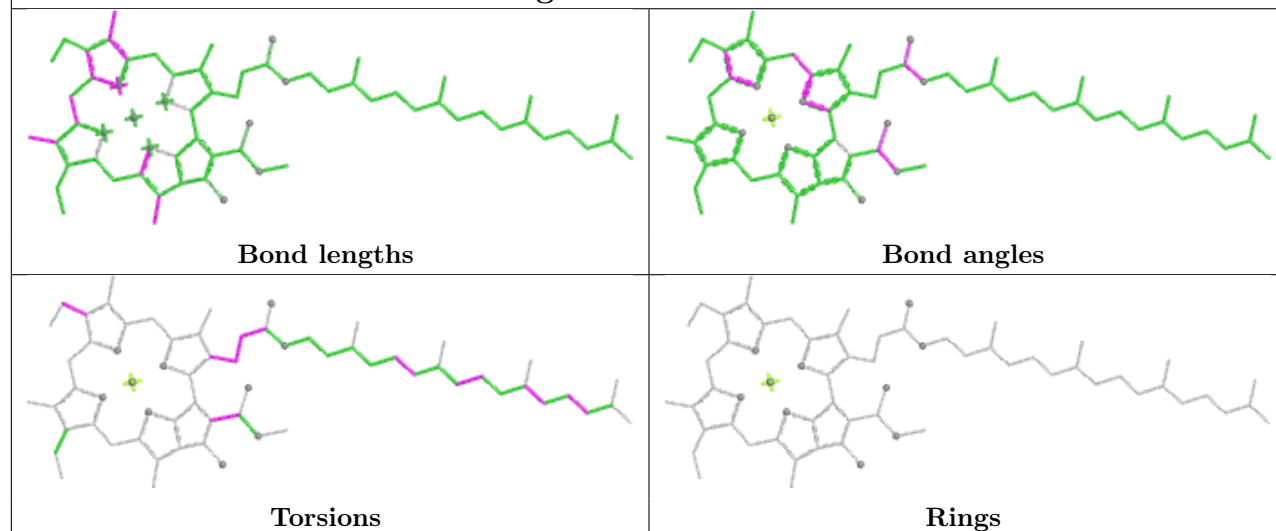
Rings

Ligand CLA a 825

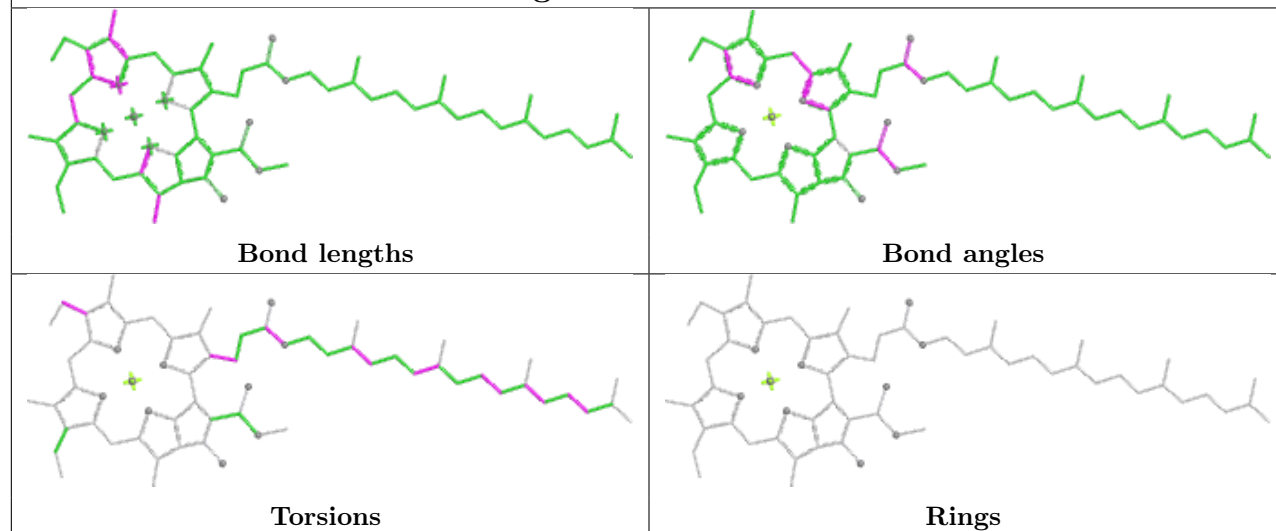


Ligand CLA A 207

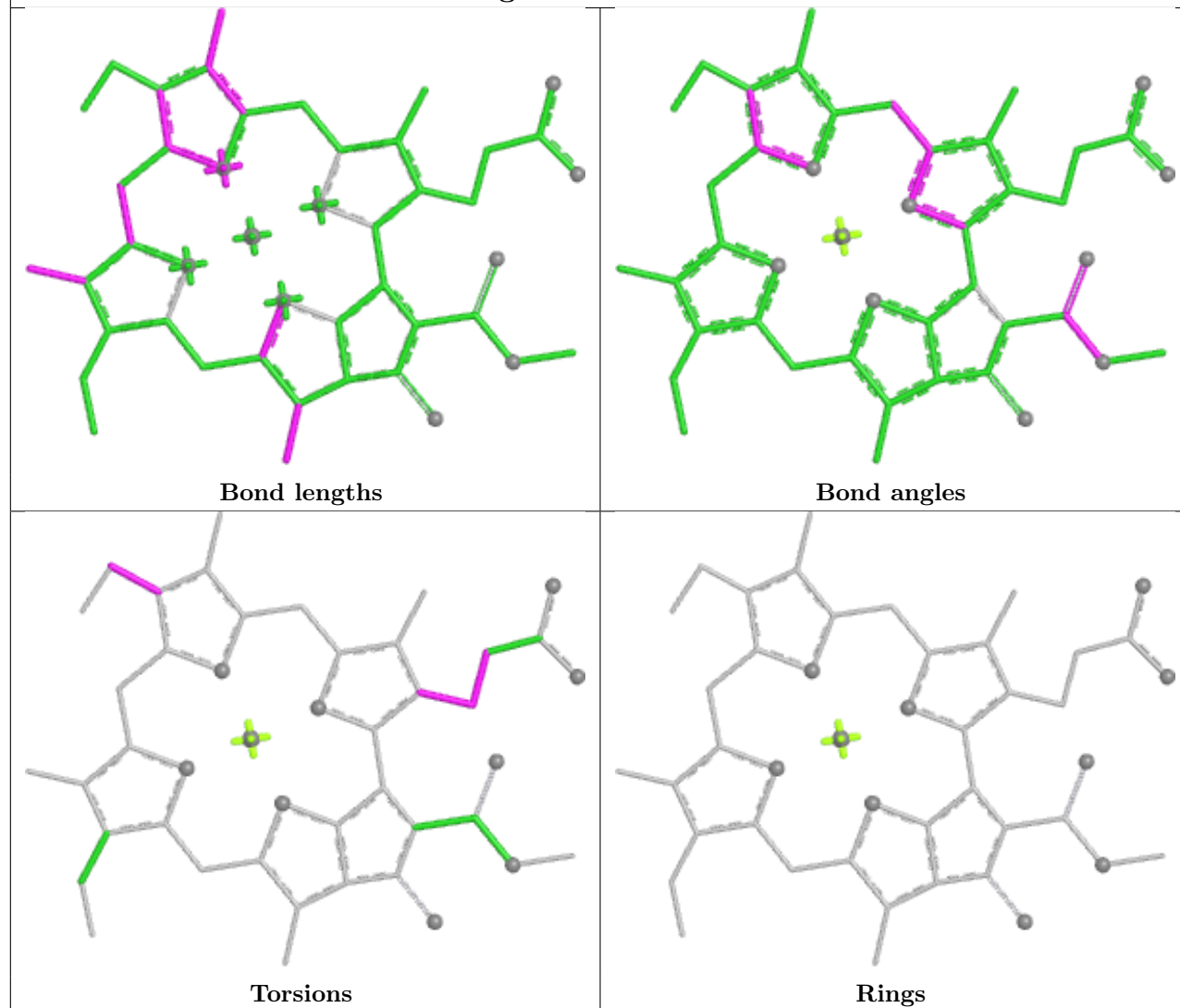


Ligand CLA b 827**Ligand CLA a 810**

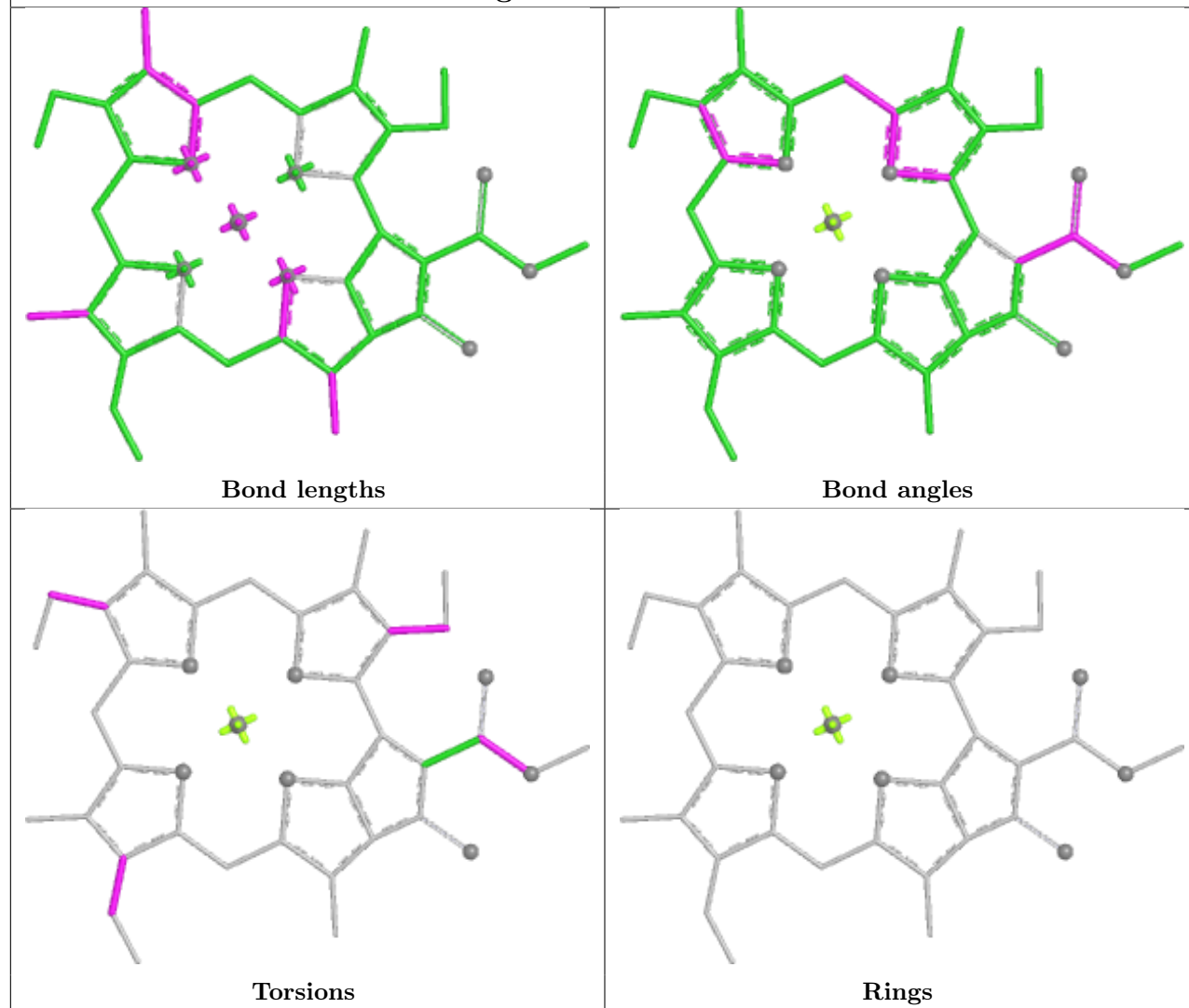
Ligand CLA E 309



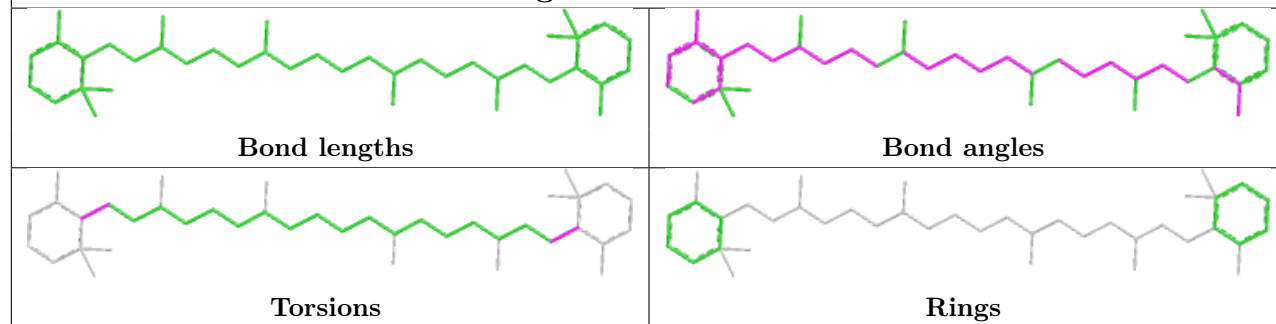
Ligand CLA f 303

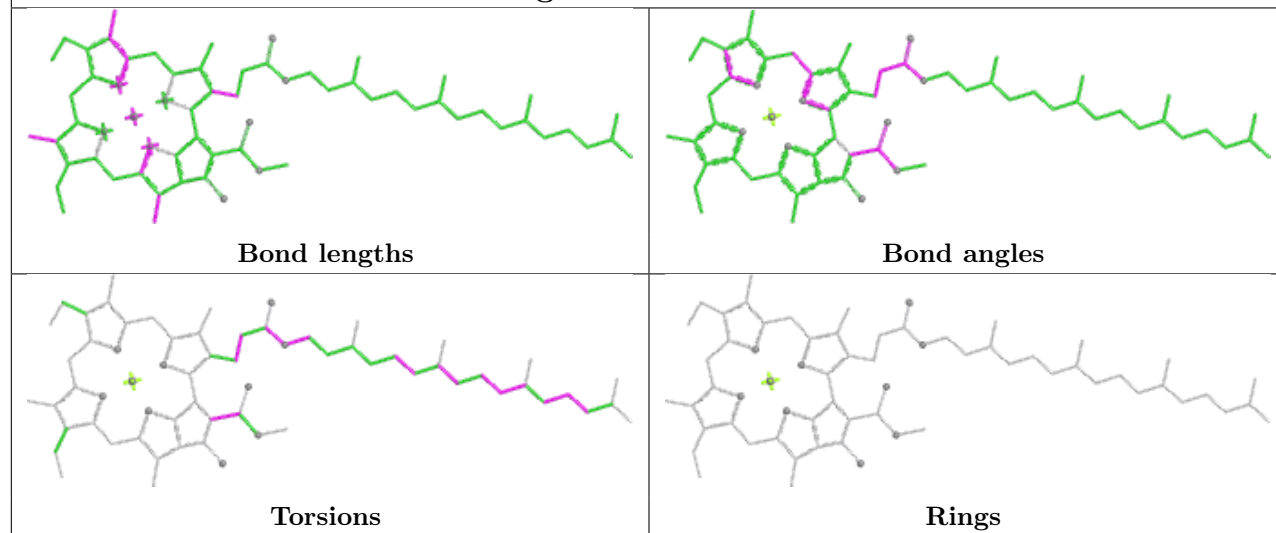
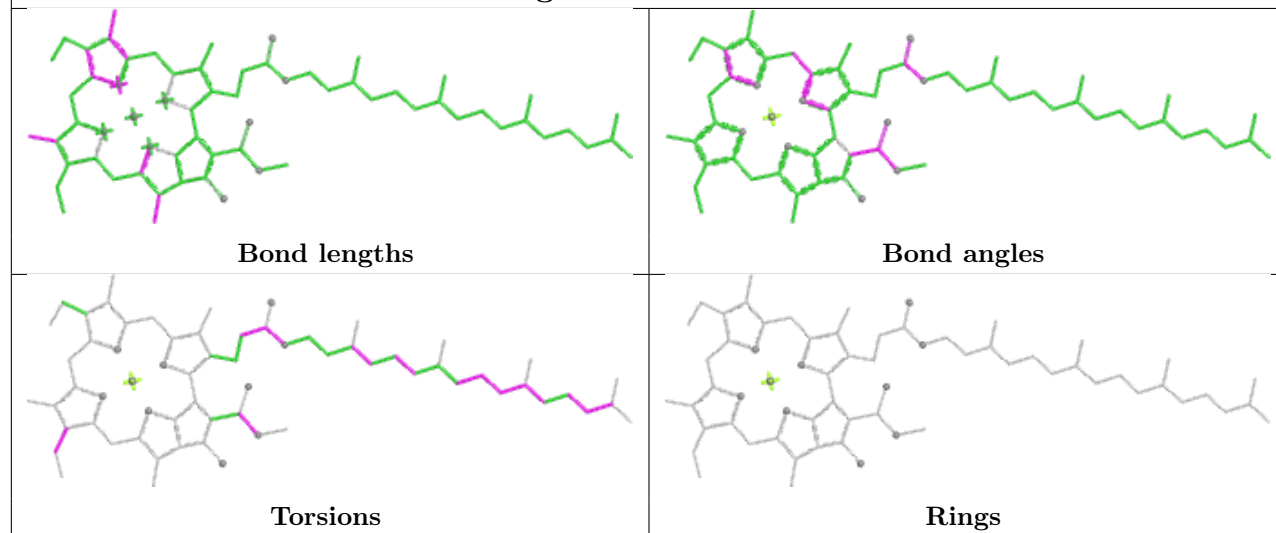


Ligand CLA C 317

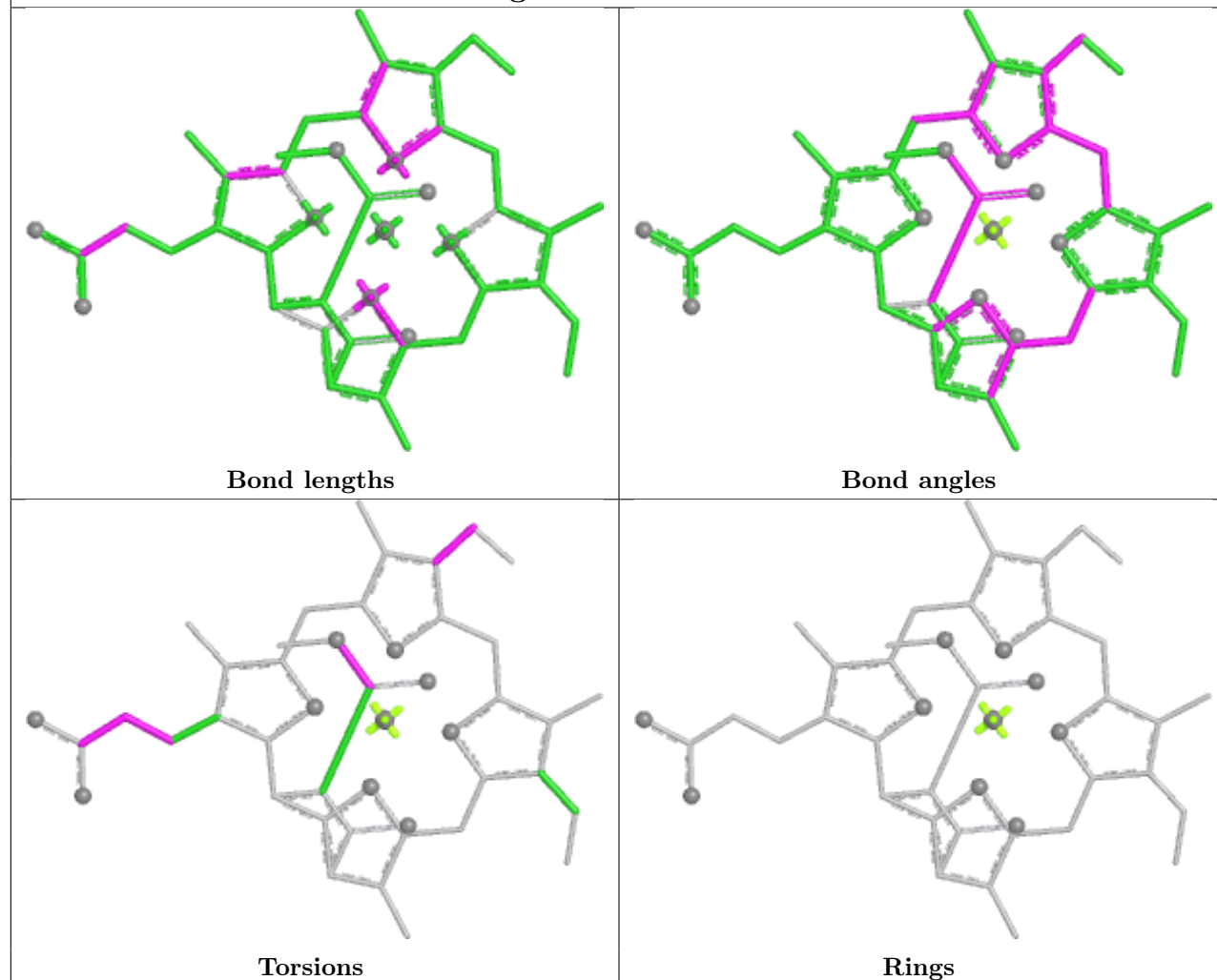


Ligand BCR r 203

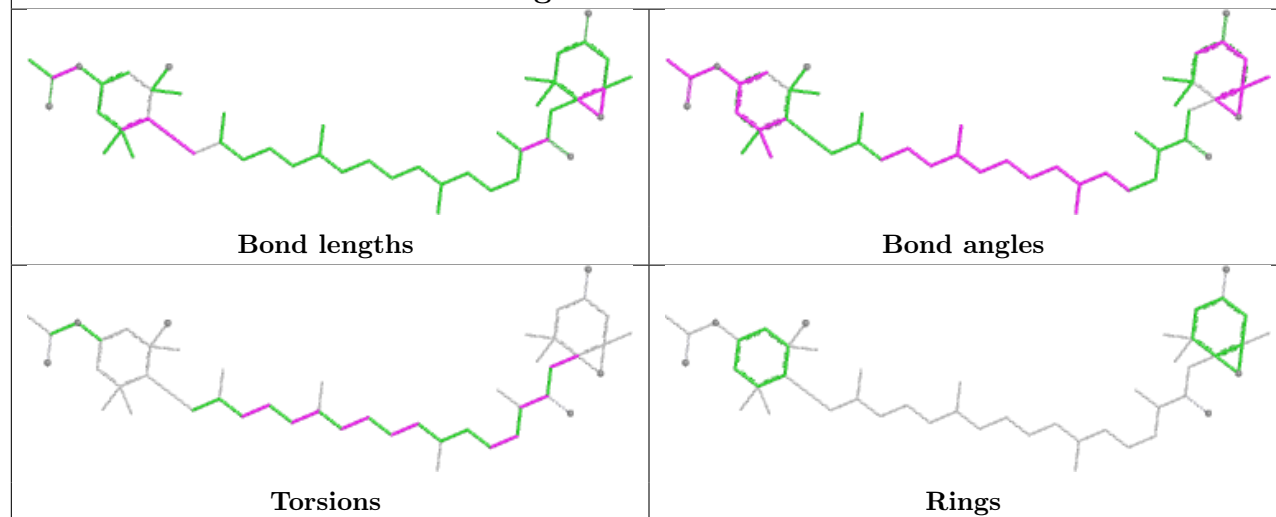


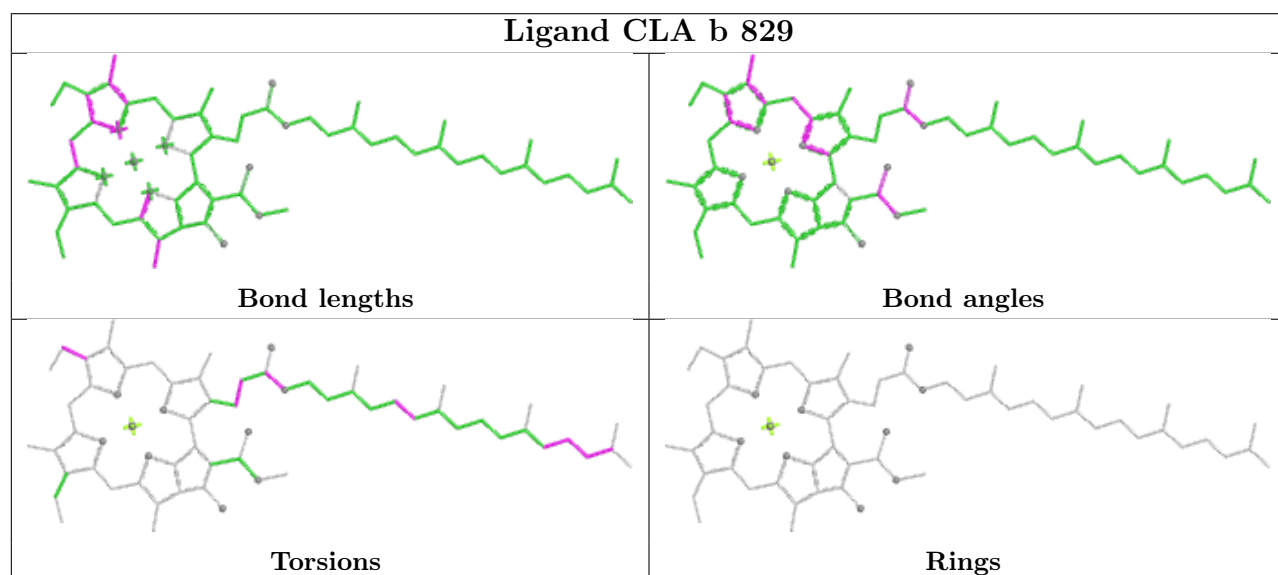
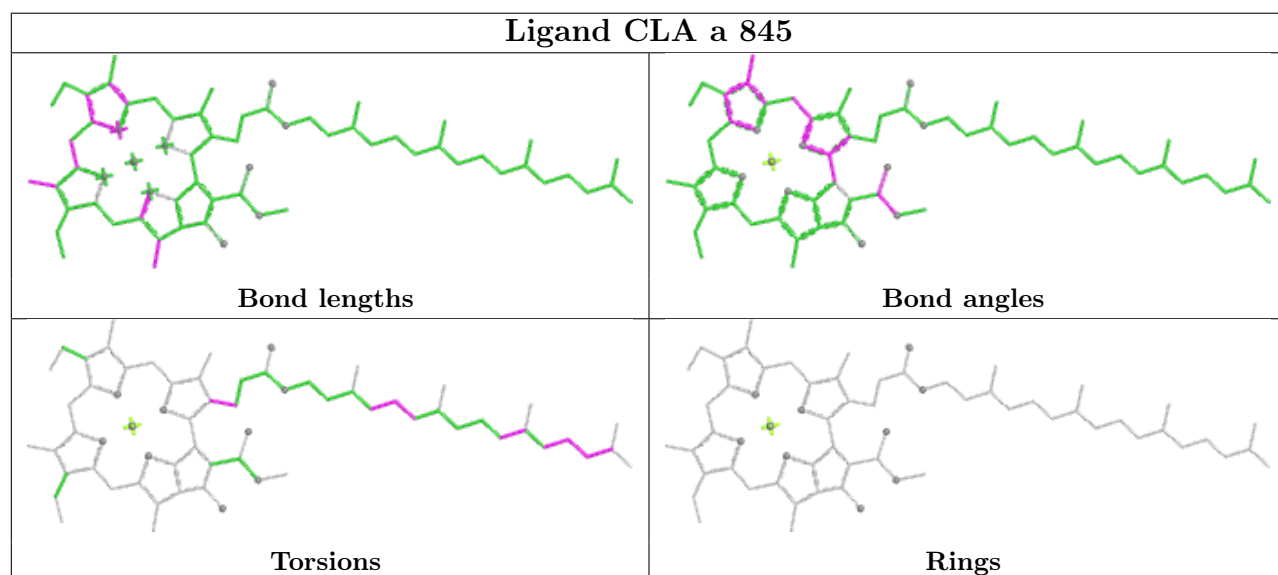
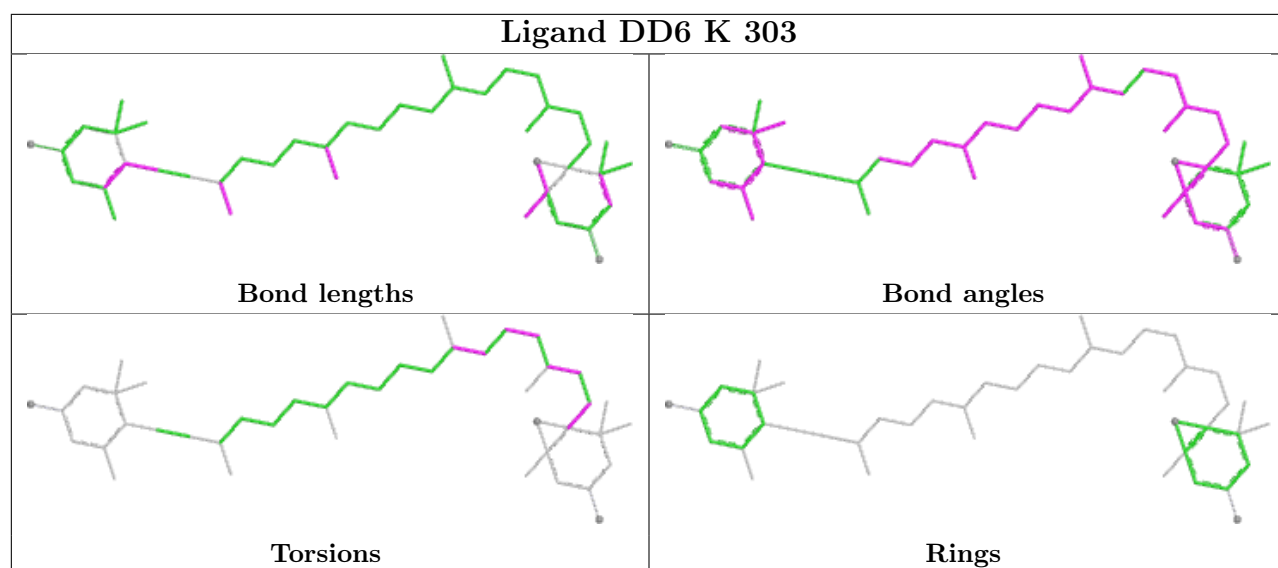
Ligand CLA a 805**Ligand CLA J 314**

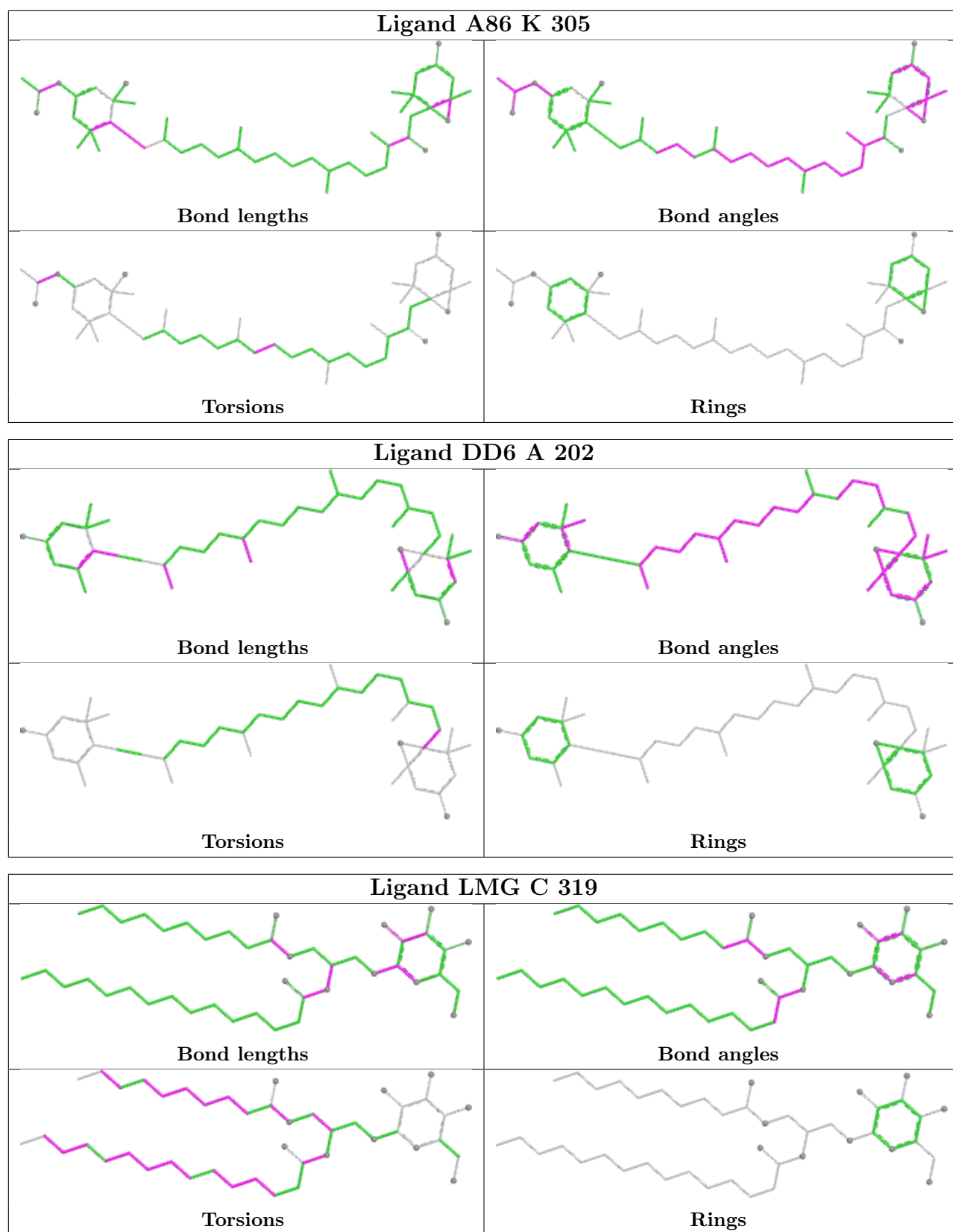
Ligand KC1 B 313

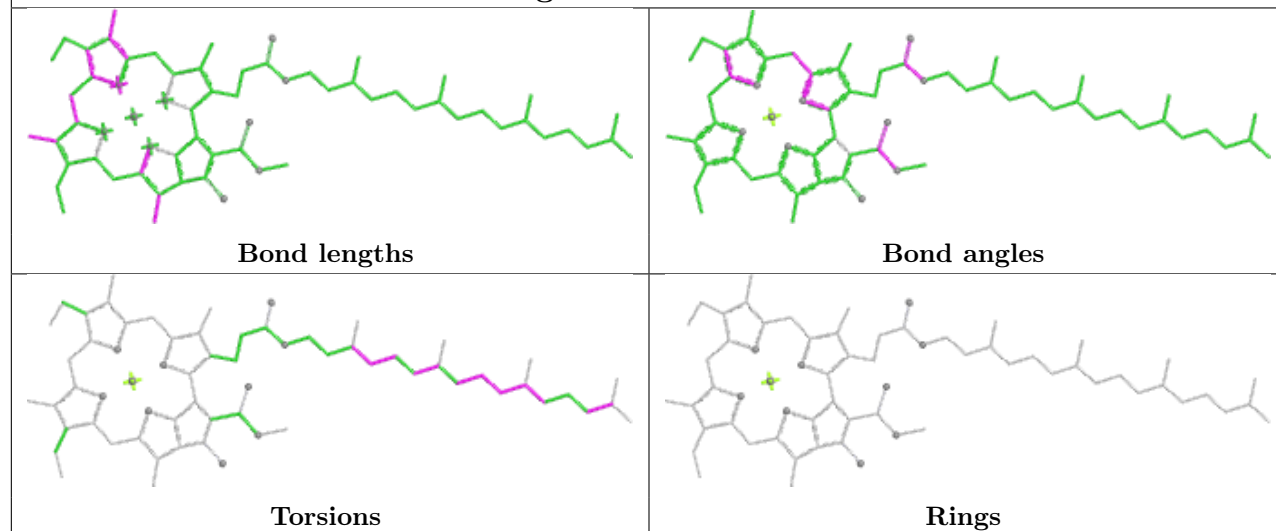
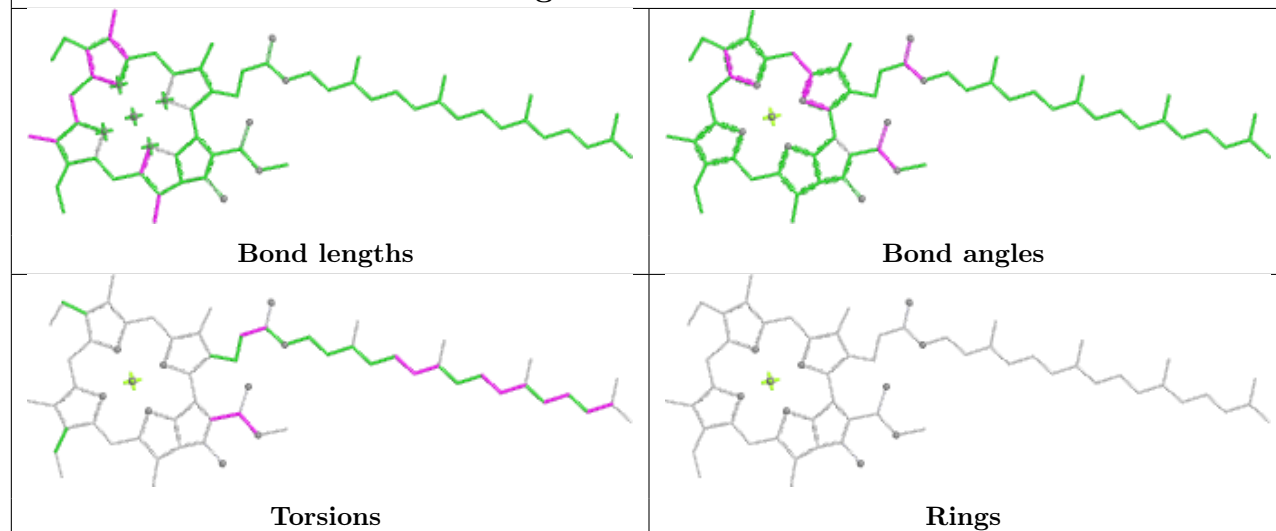
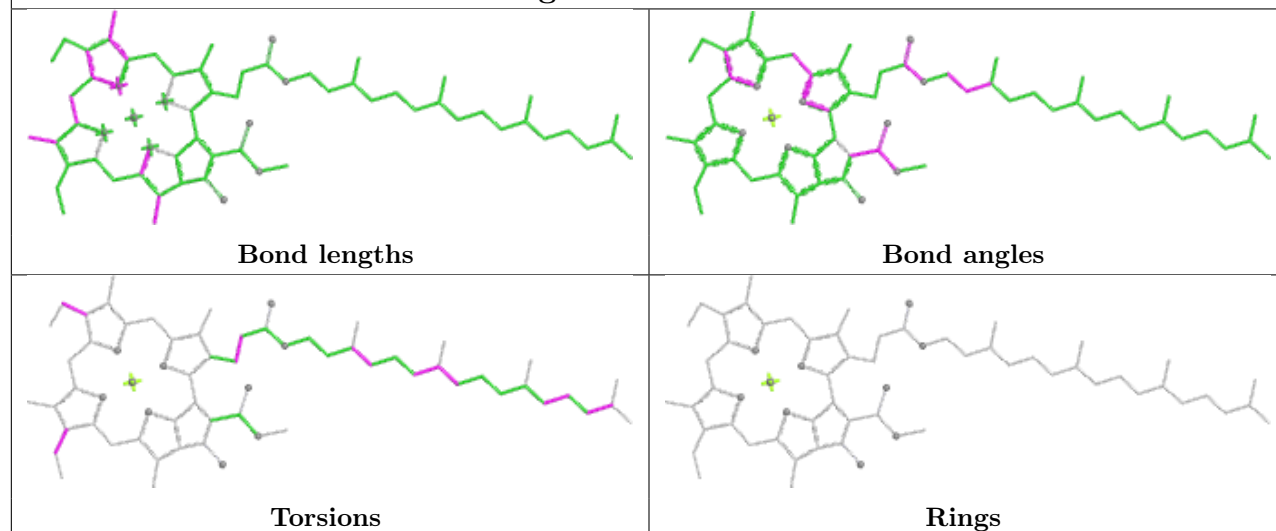


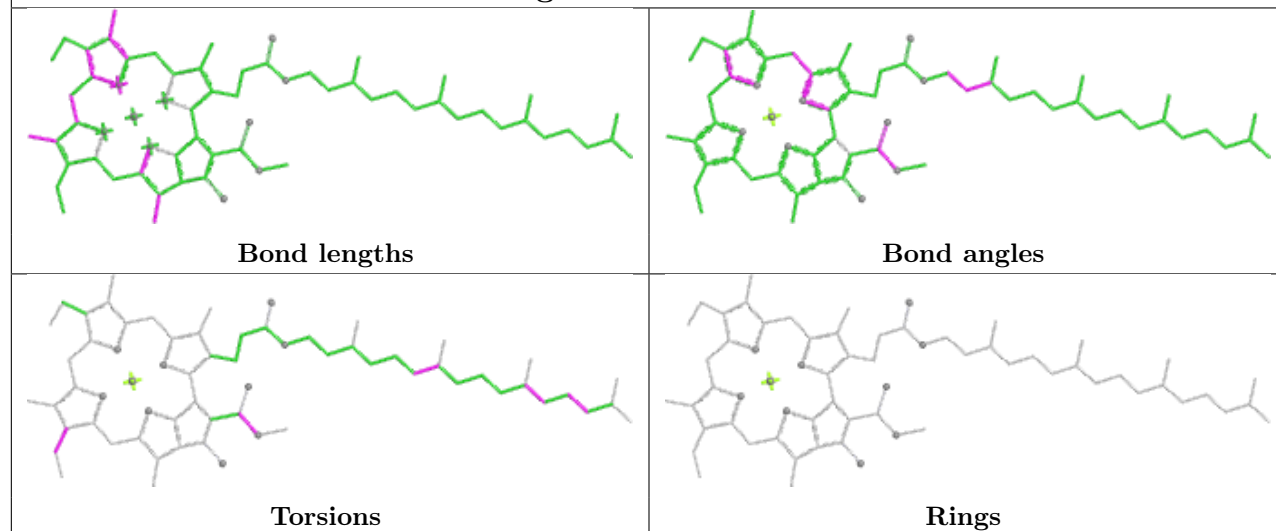
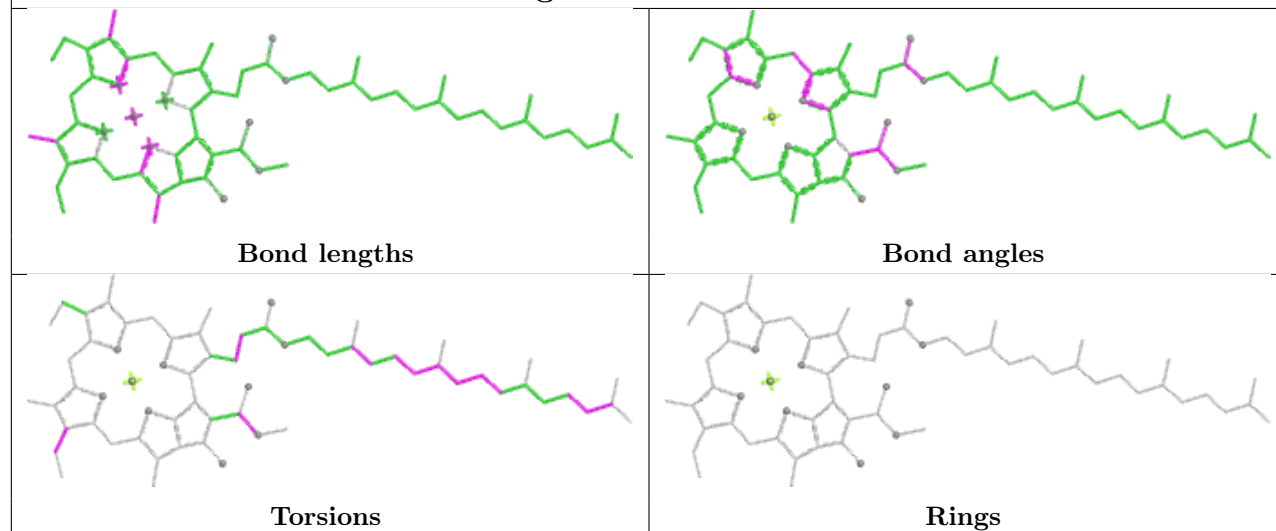
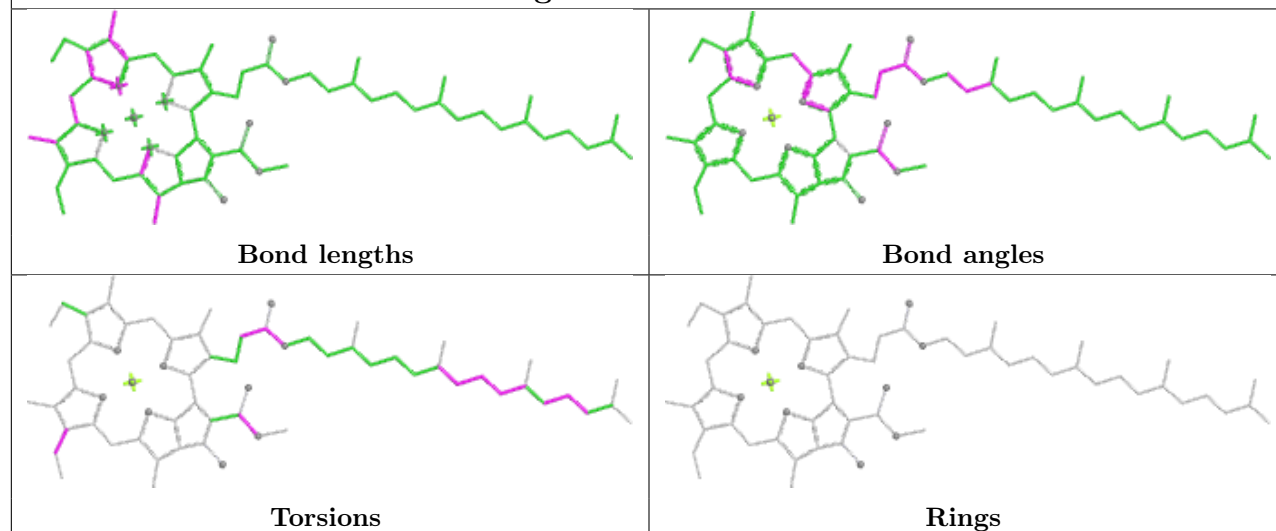
Ligand A86 M 303



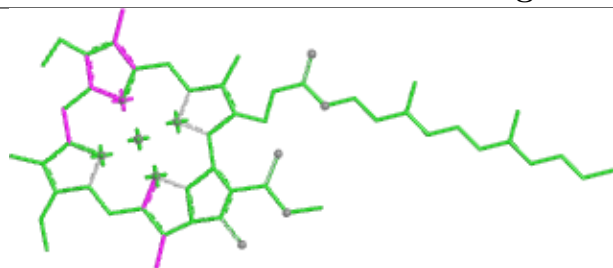




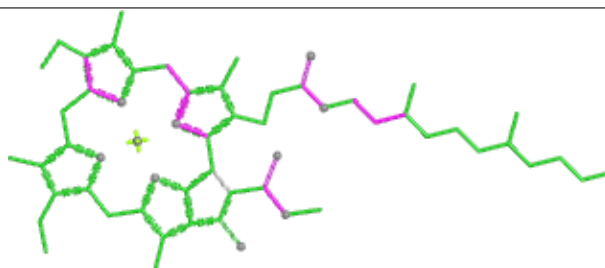
Ligand CLA J 311**Ligand CLA b 803****Ligand CLA I 308**

Ligand CLA a 804**Ligand CLA a 856****Ligand CLA L 309**

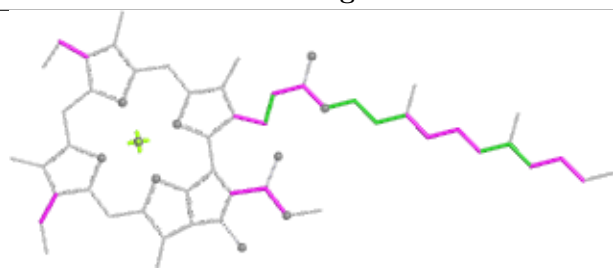
Ligand CLA F 315



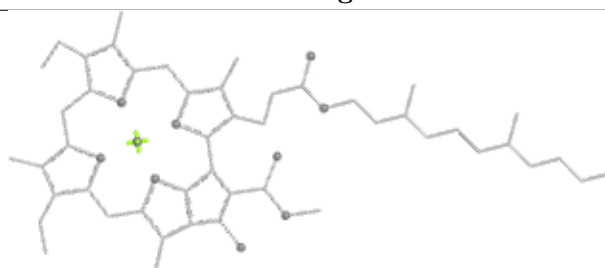
Bond lengths



Bond angles

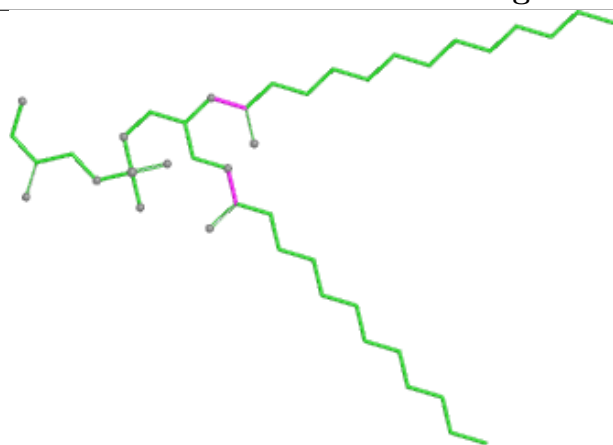


Torsions

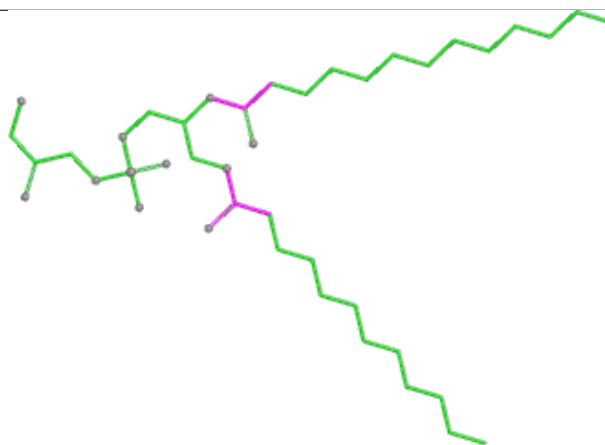


Rings

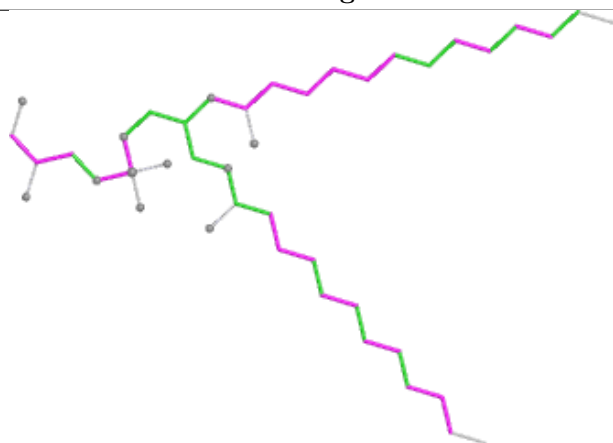
Ligand LHG B 315



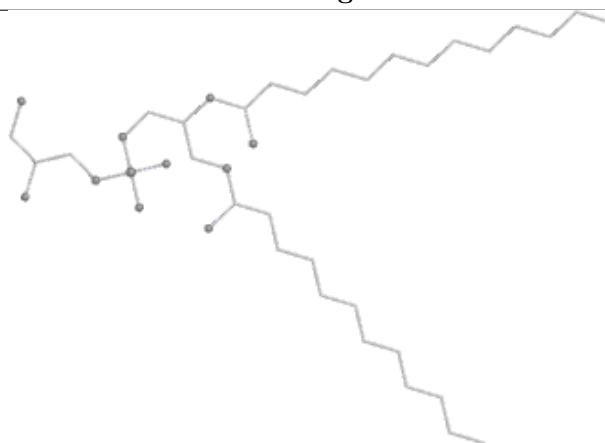
Bond lengths



Bond angles

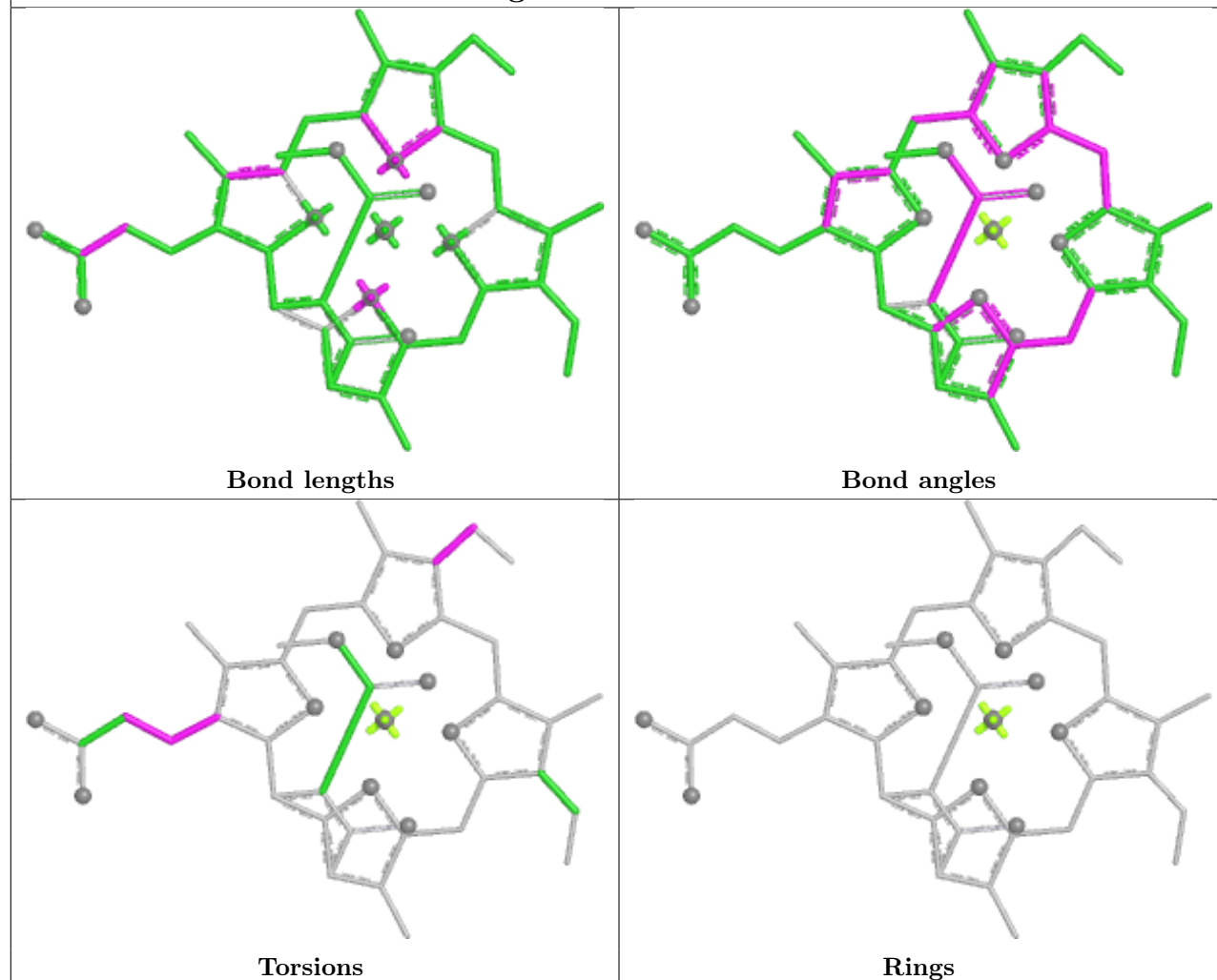


Torsions

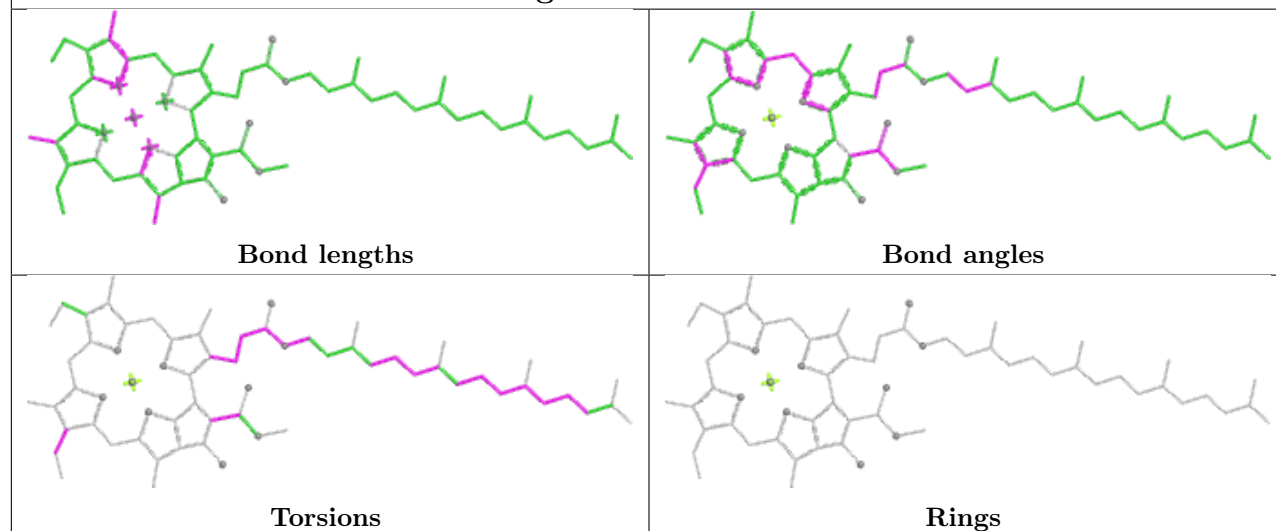


Rings

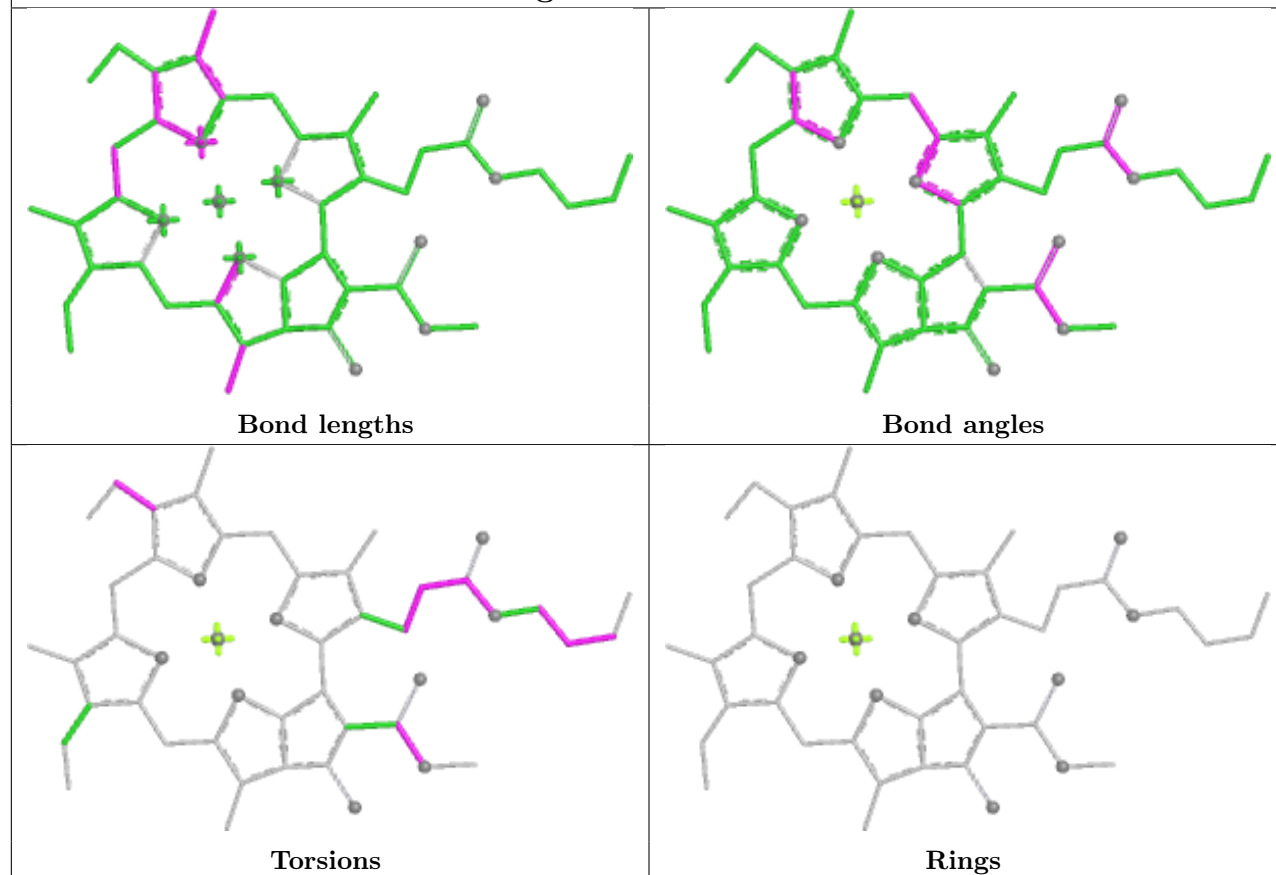
Ligand KC1 G 313



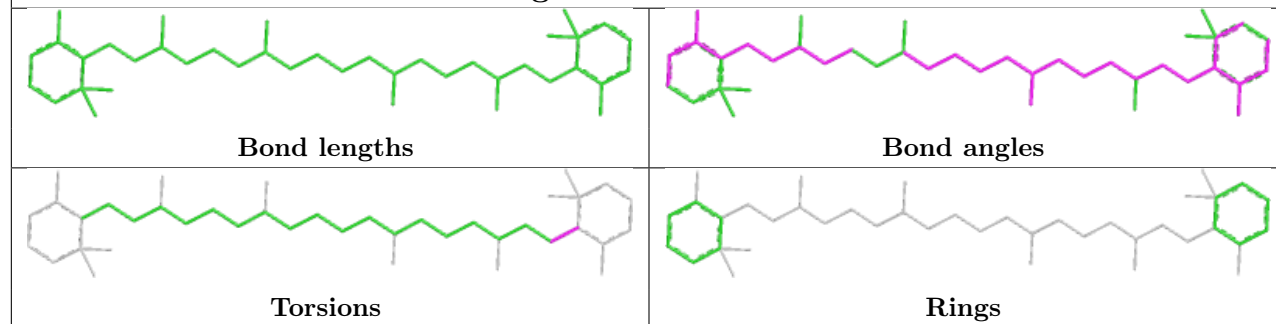
Ligand CLA a 815

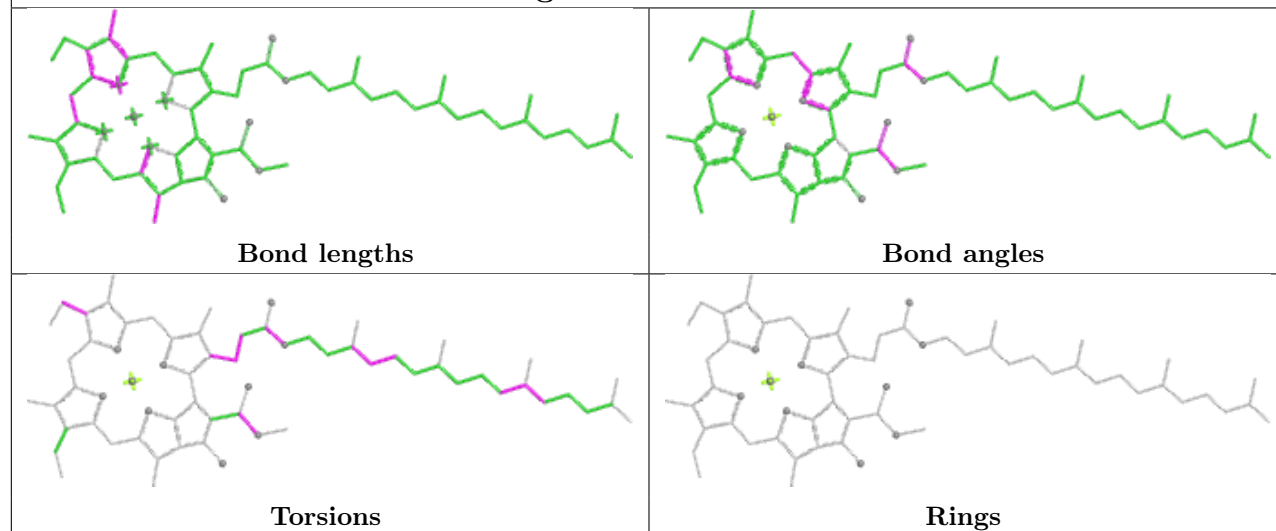
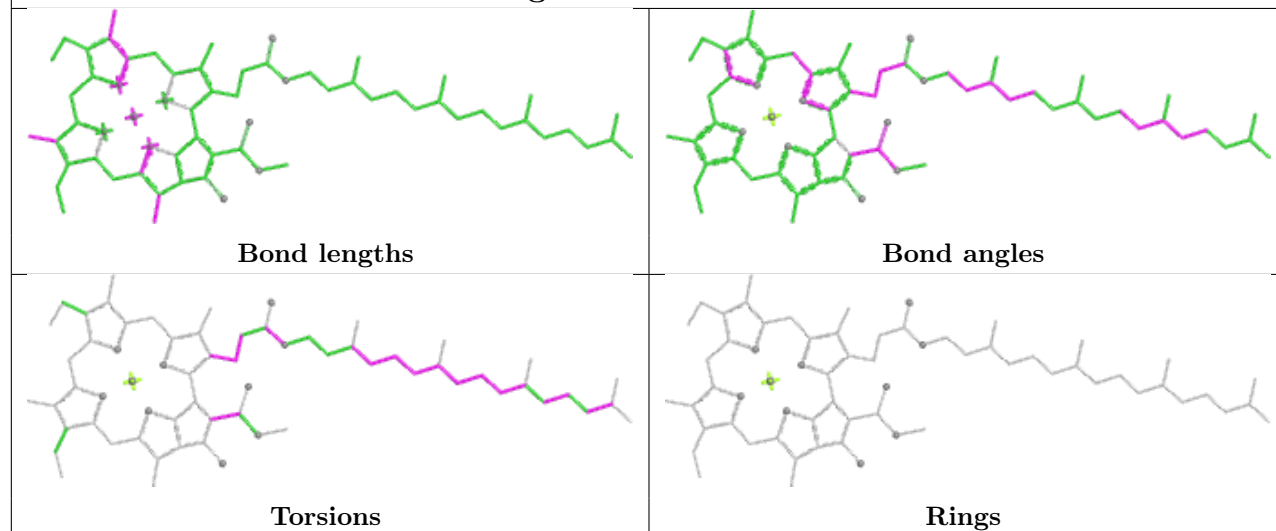


Ligand CLA a 819

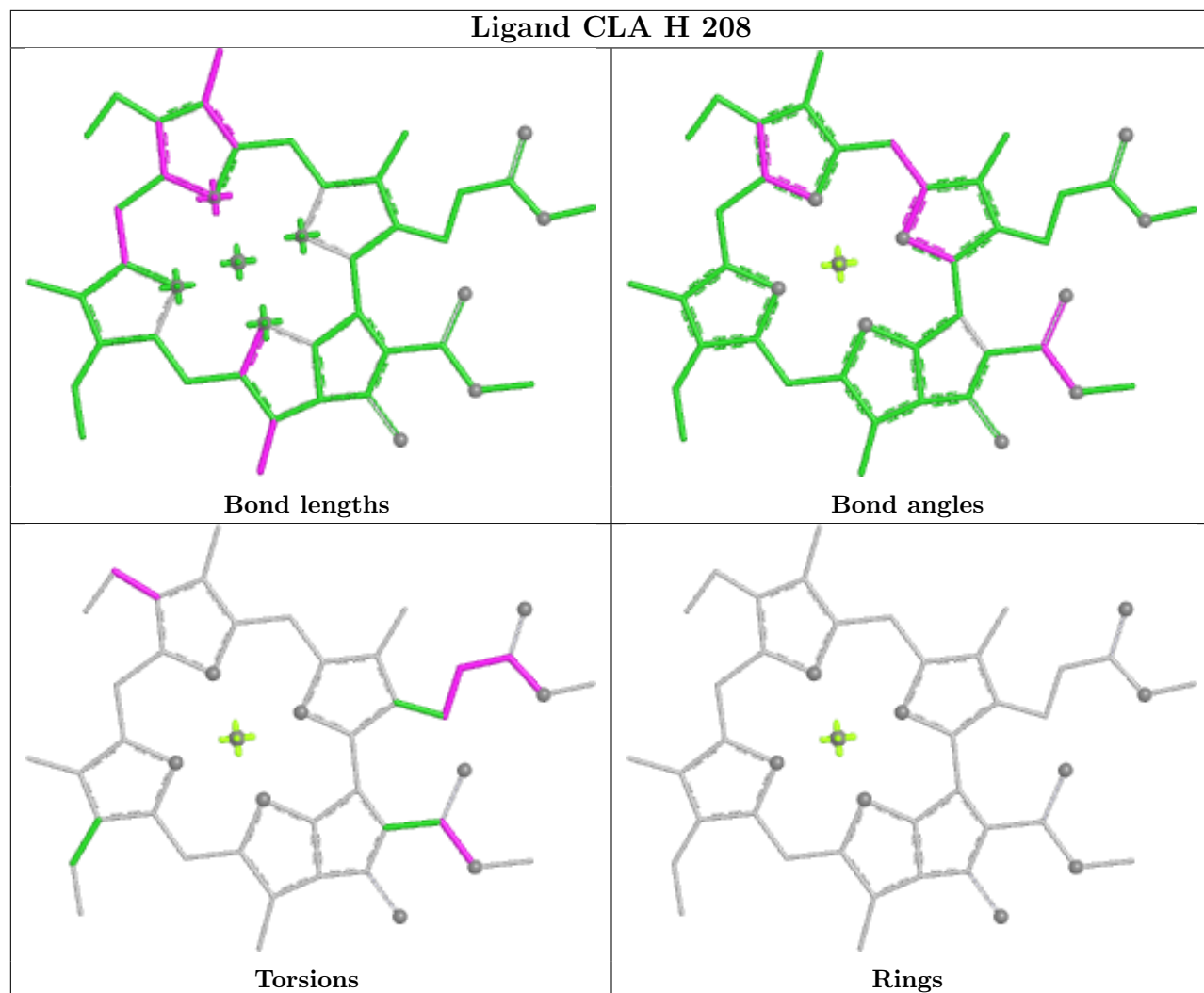


Ligand BCR E 304

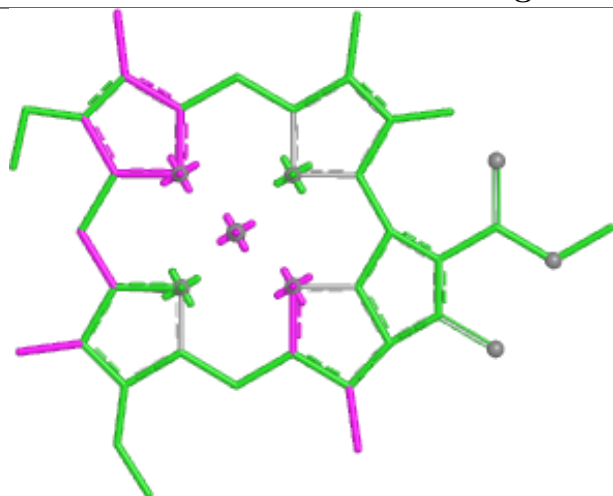


Ligand CLA a 846**Ligand CLA M 313**

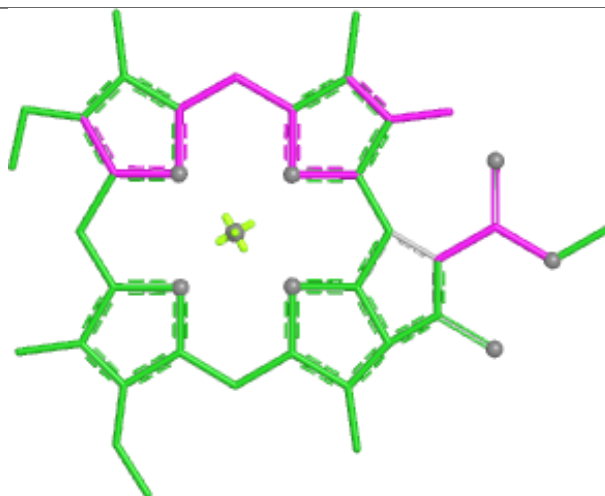
Ligand CLA H 208



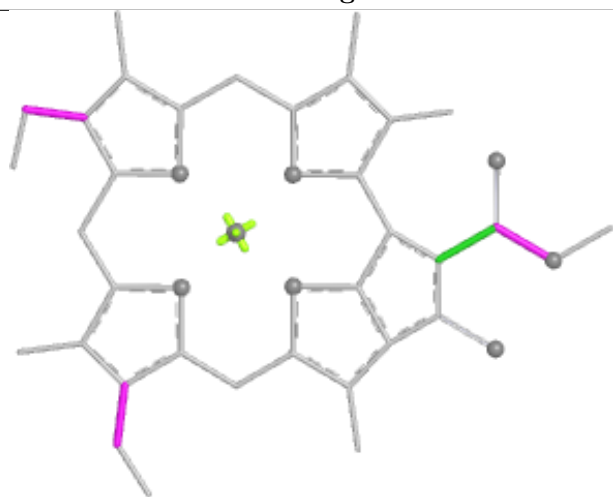
Ligand CLA C 314



Bond lengths



Bond angles

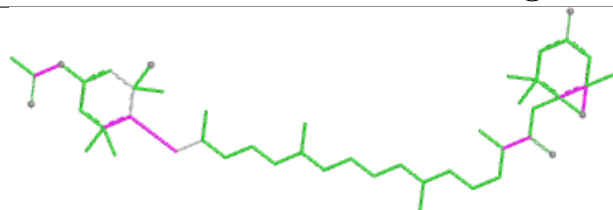


Torsions

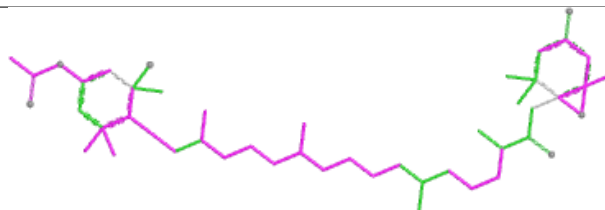


Rings

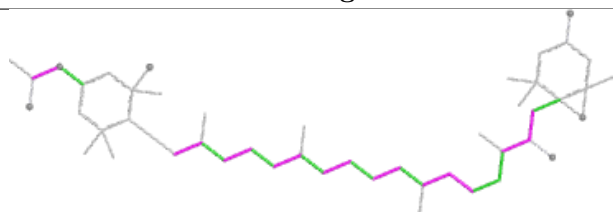
Ligand A86 J 316



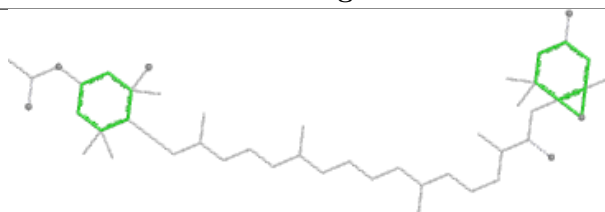
Bond lengths



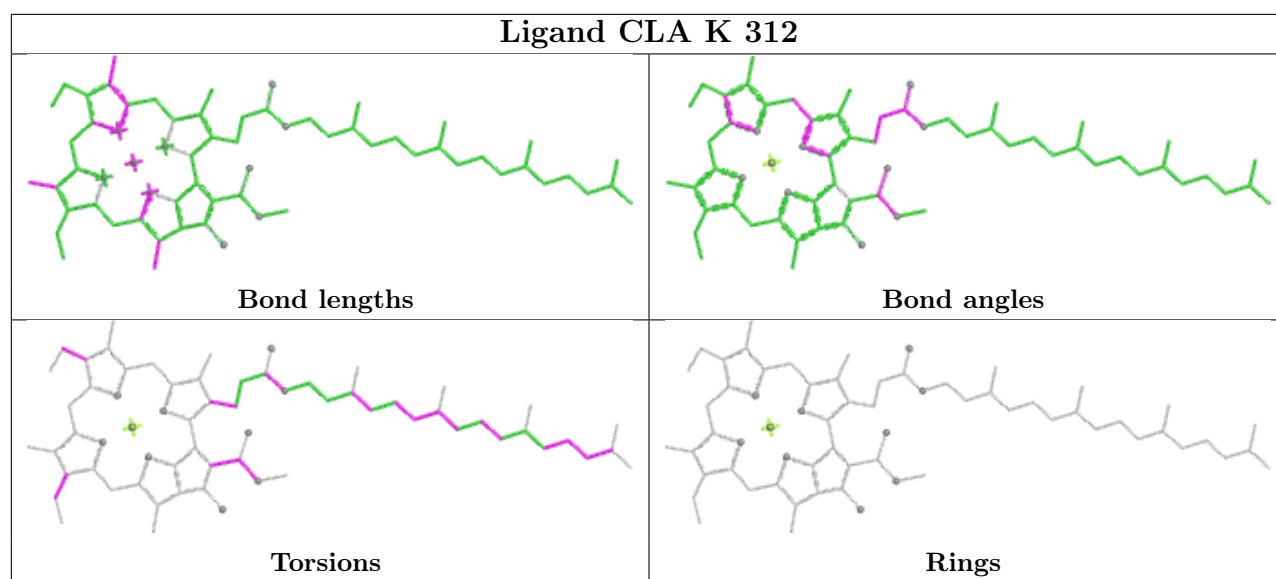
Bond angles



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.

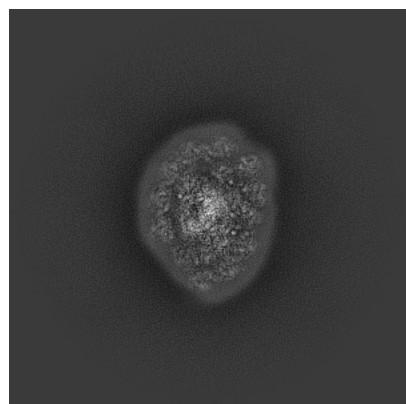
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60032. These allow visual inspection of the internal detail of the map and identification of artifacts.

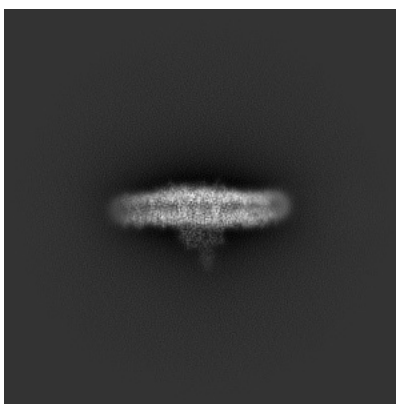
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

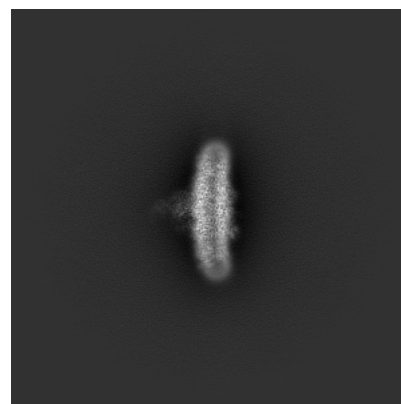
6.1.1 Primary map



X

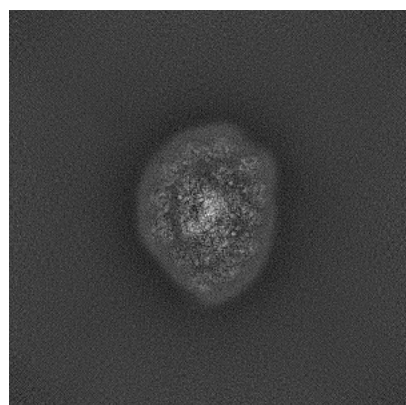


Y

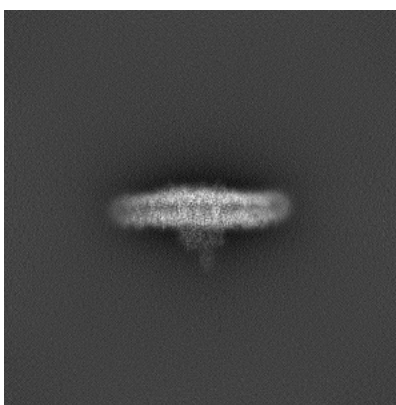


Z

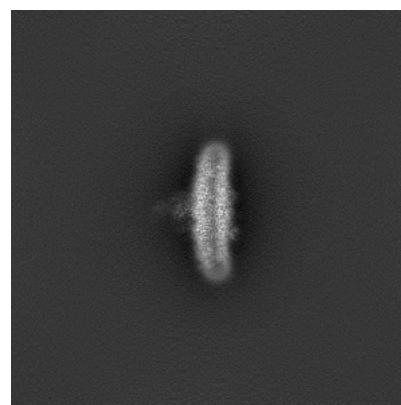
6.1.2 Raw map



X



Y

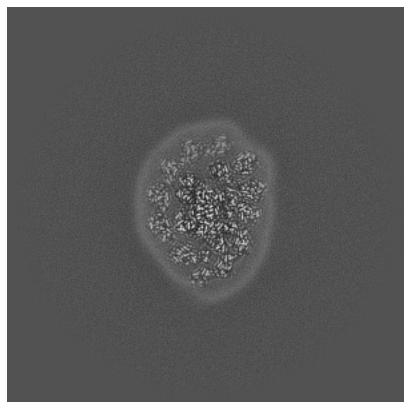


Z

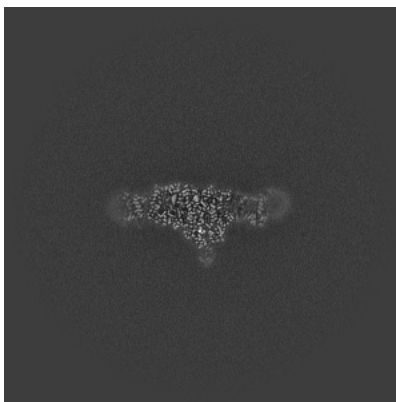
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

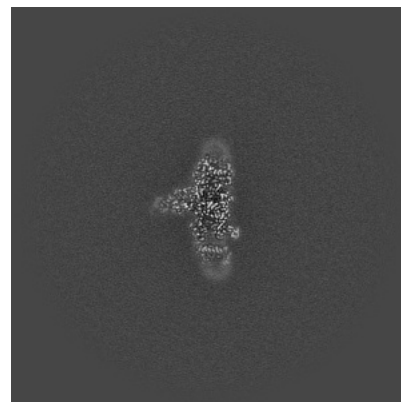
6.2.1 Primary map



X Index: 256

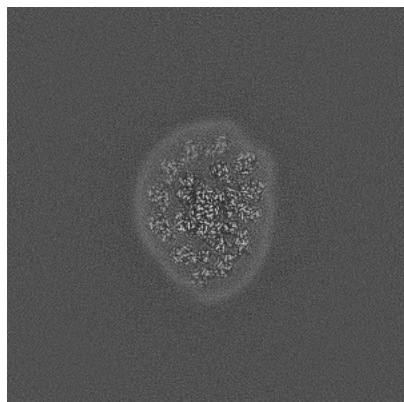


Y Index: 256

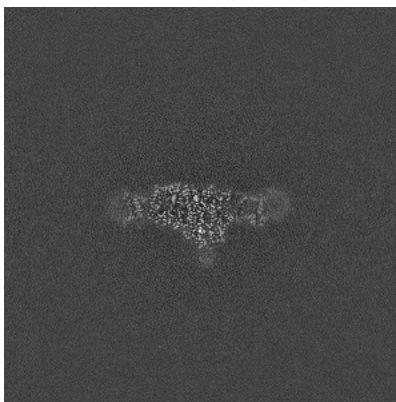


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

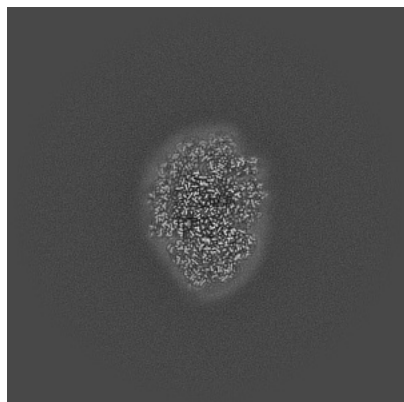


Z Index: 256

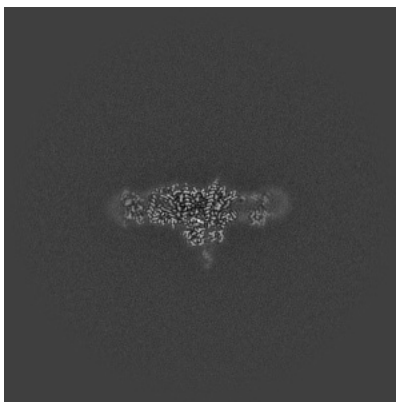
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

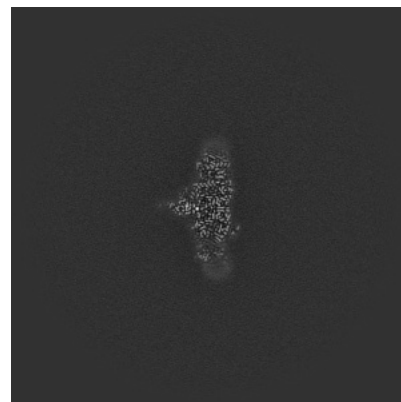
6.3.1 Primary map



X Index: 245

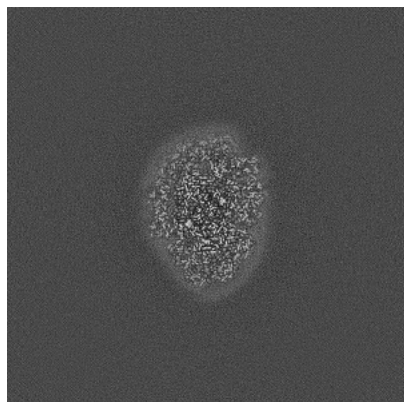


Y Index: 252

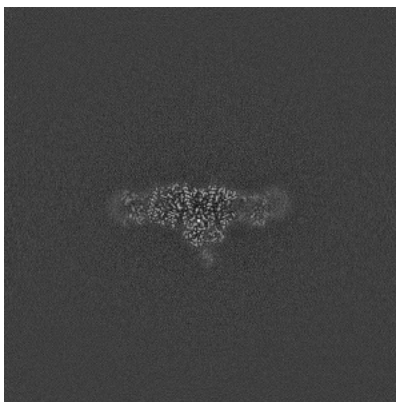


Z Index: 249

6.3.2 Raw map



X Index: 246



Y Index: 253

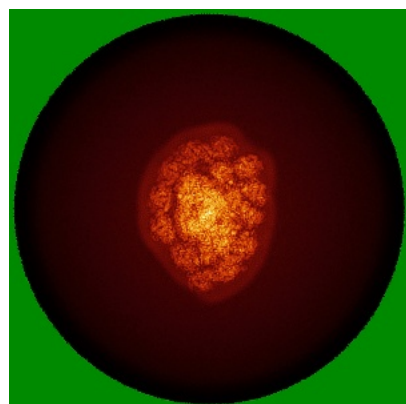


Z Index: 249

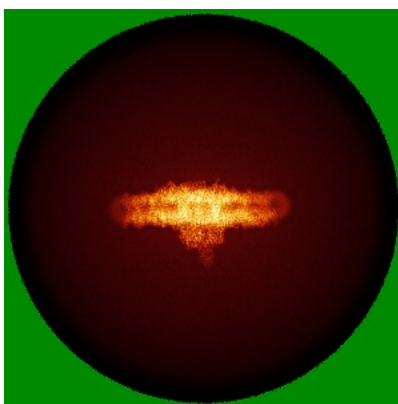
The images above show the largest variance slices of the map in three orthogonal directions.

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

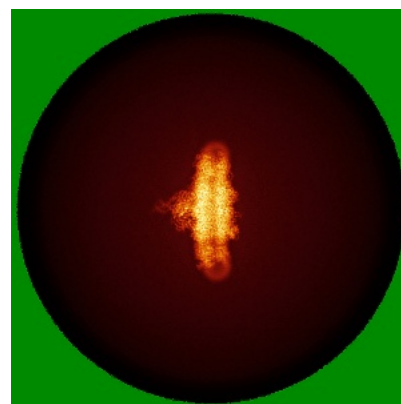
6.4.1 Primary map



X

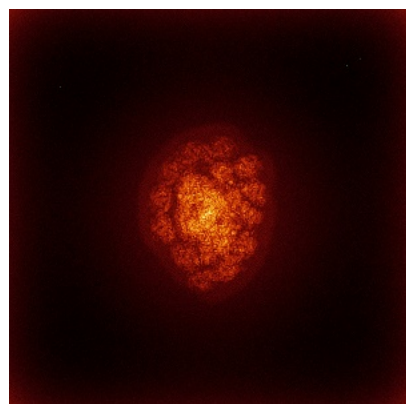


Y

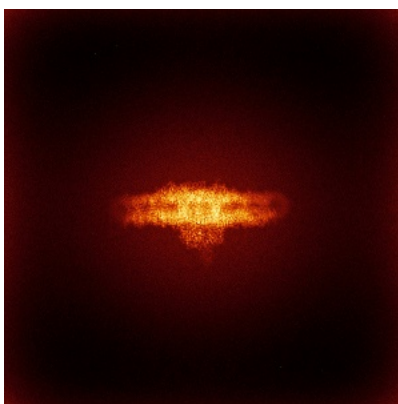


Z

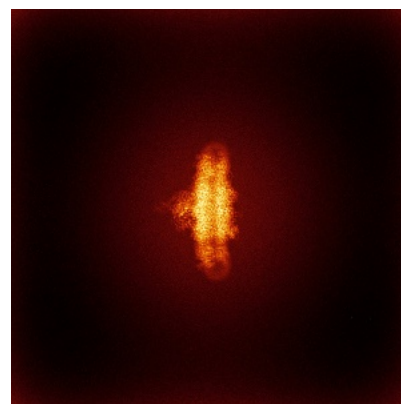
6.4.2 Raw map



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



X



Y



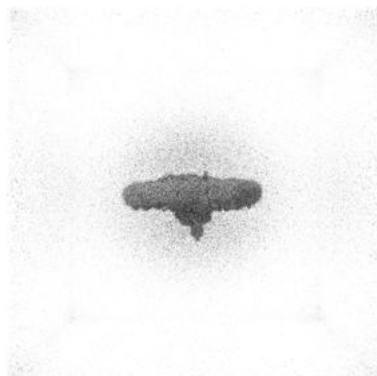
Z

The images above show the 3D surface view of the map at the recommended contour level 0.088. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

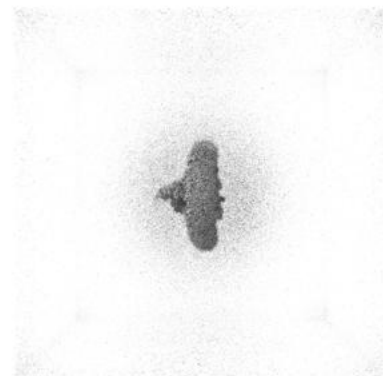
6.5.2 Raw map



X



Y



Z

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.

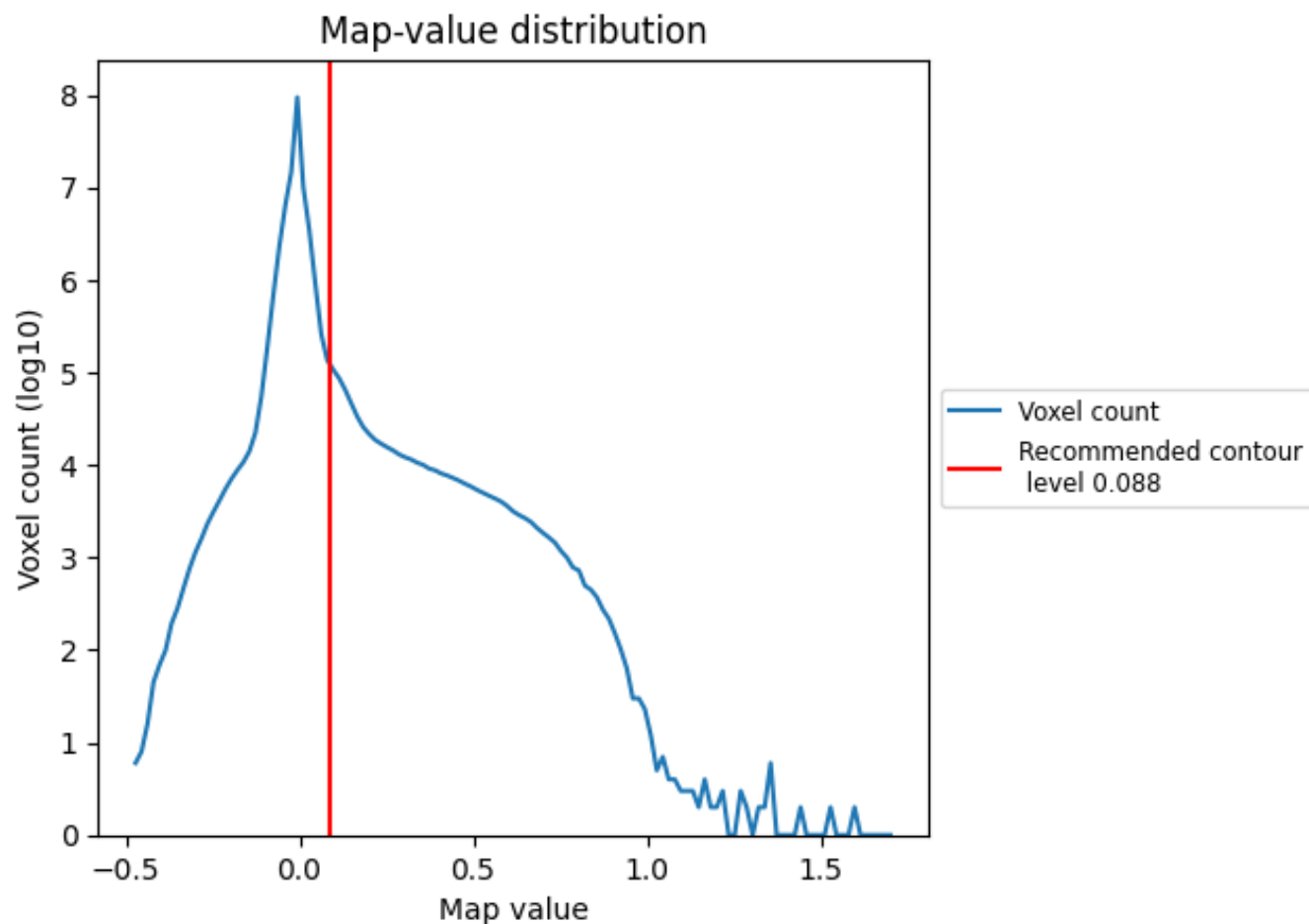
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

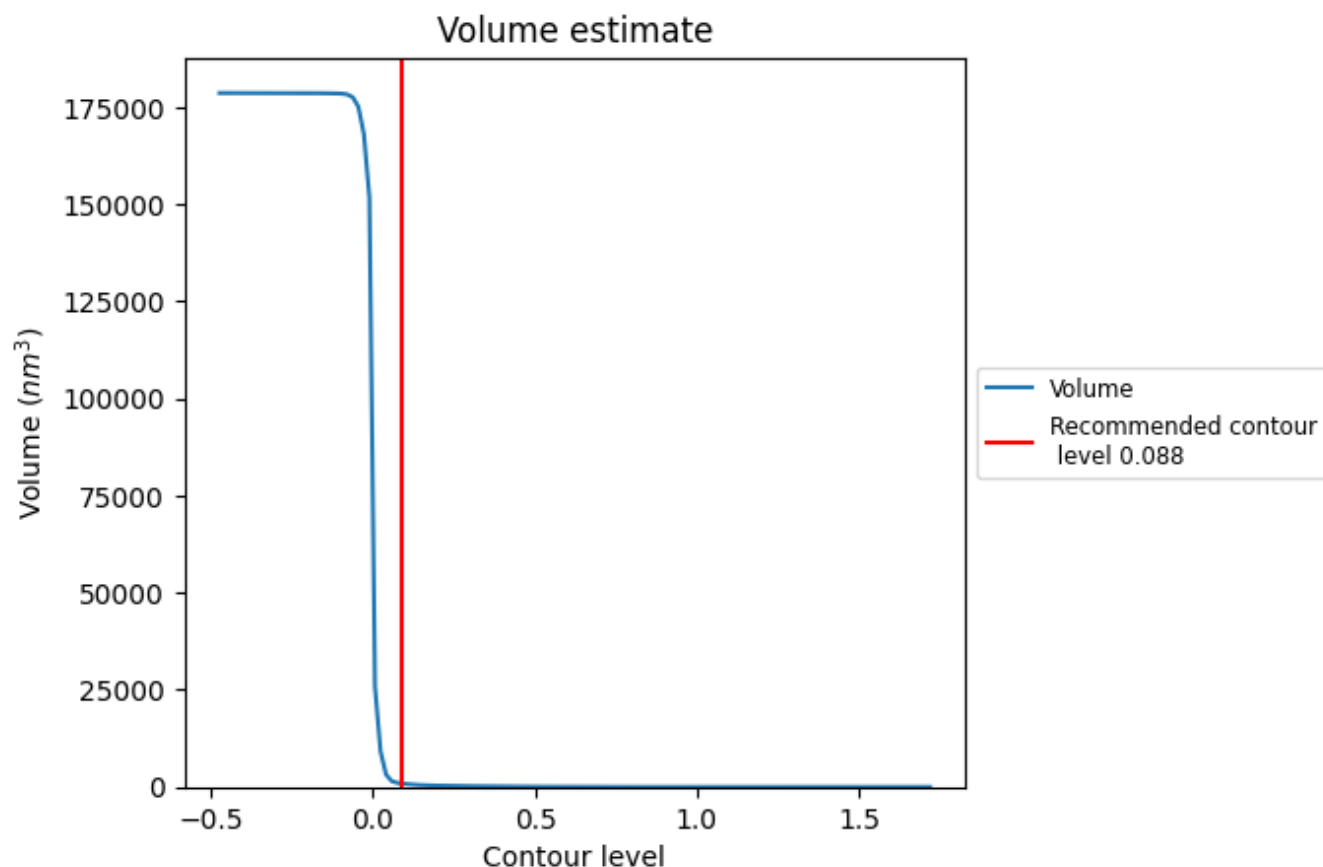
This section contains the results of statistical analysis of the map.

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.

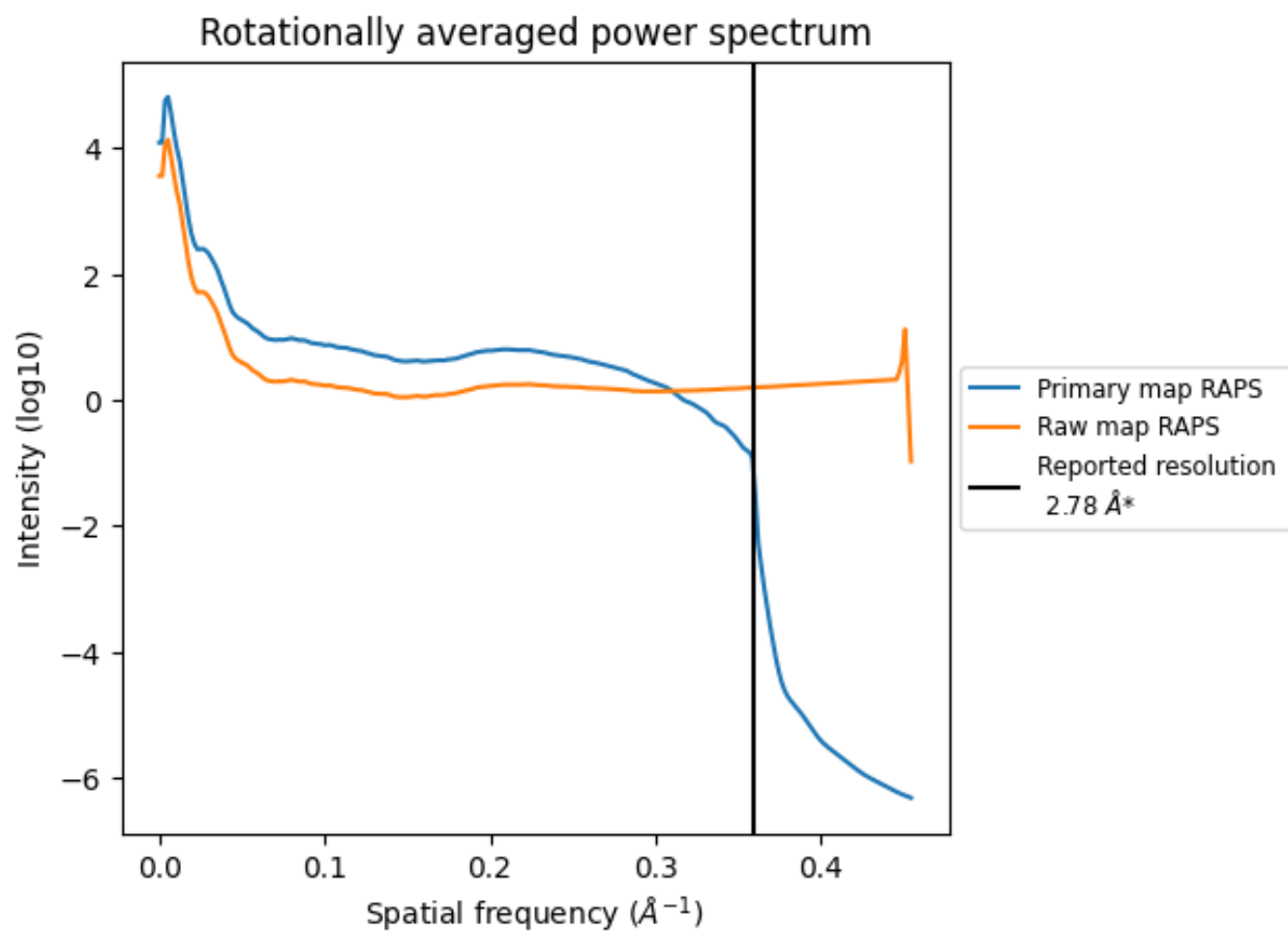
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 920 nm³; this corresponds to an approximate mass of 831 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 ⓘ

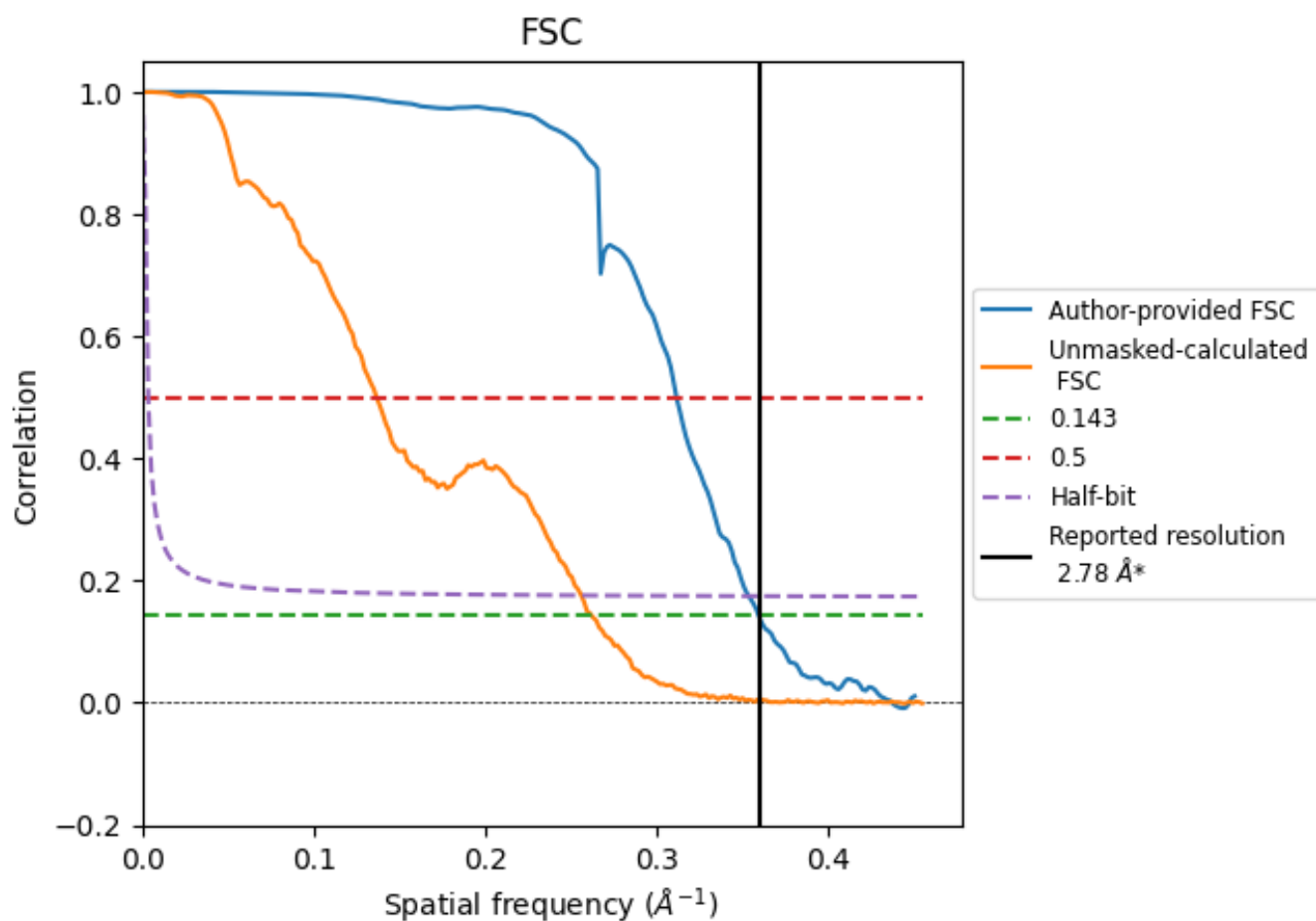


*Reported resolution corresponds to spatial frequency of 0.360 Å⁻¹

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 0.360 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

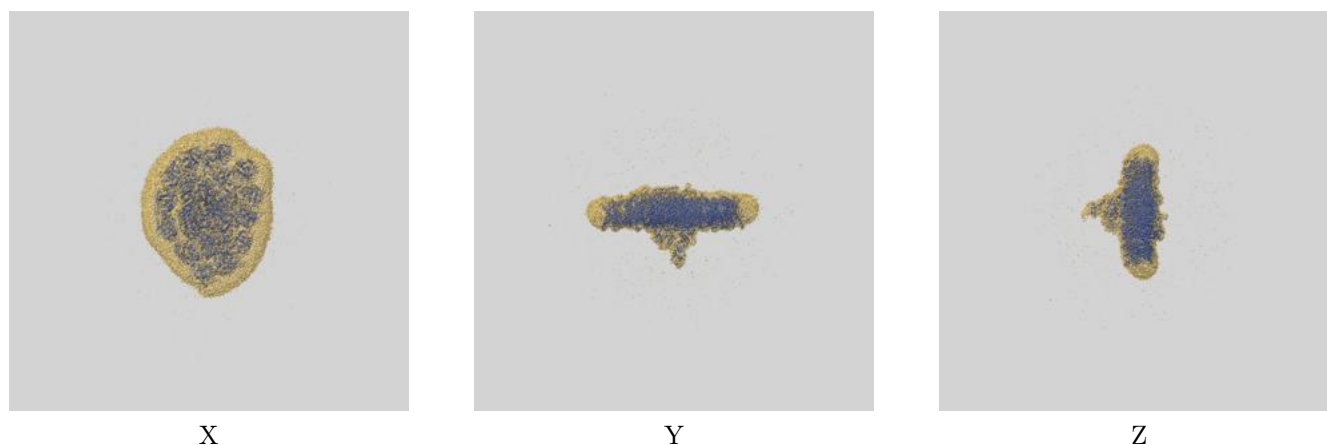
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.78	3.21	2.83
Unmasked-calculated*	3.82	7.32	3.91

*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 3.82 differs from the reported value 2.78 by more than 10 %

9 Map-model fit [i](#)

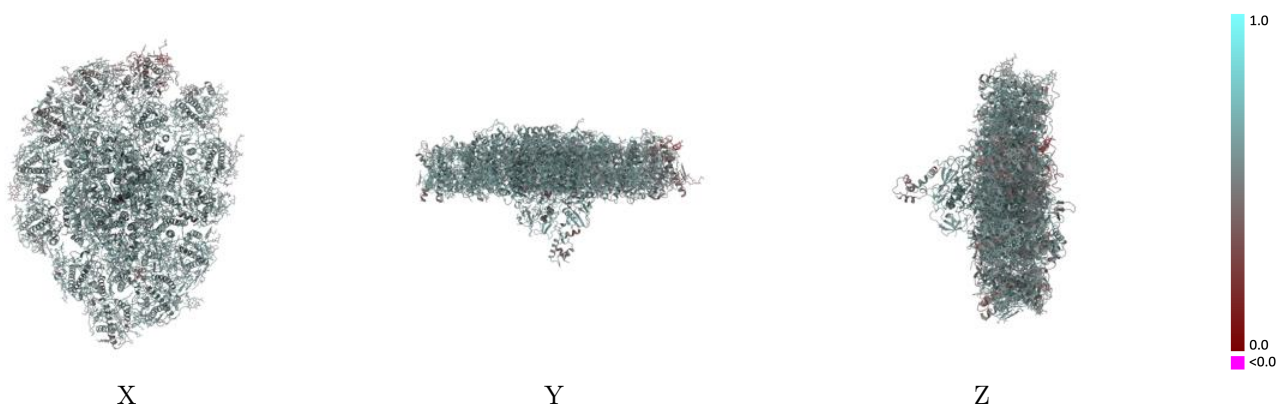
This section contains information regarding the fit between EMDB map EMD-60032 and PDB model 8ZEH. Per-residue inclusion information can be found in section 3 on page 38.

9.1 Map-model overlay [i](#)



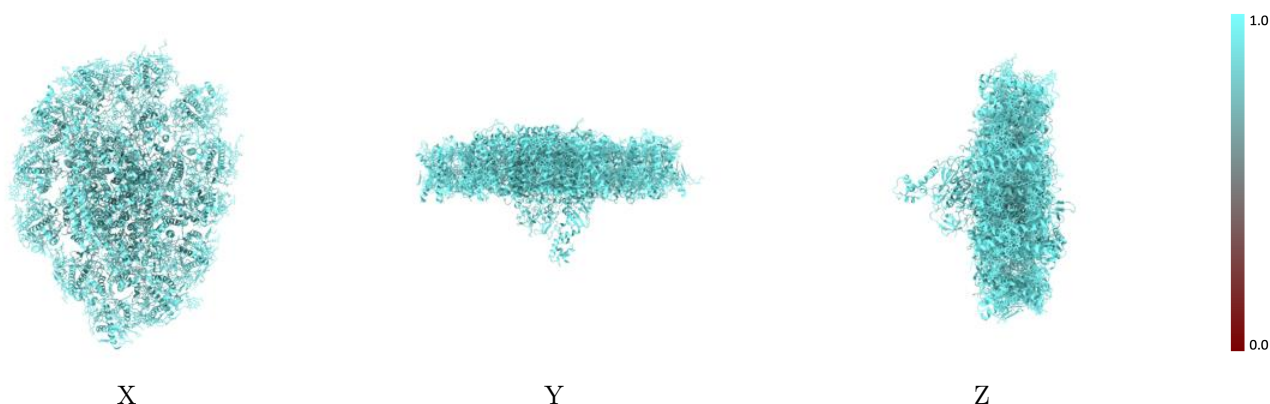
The images above show the 3D surface view of the map at the recommended contour level 0.088 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



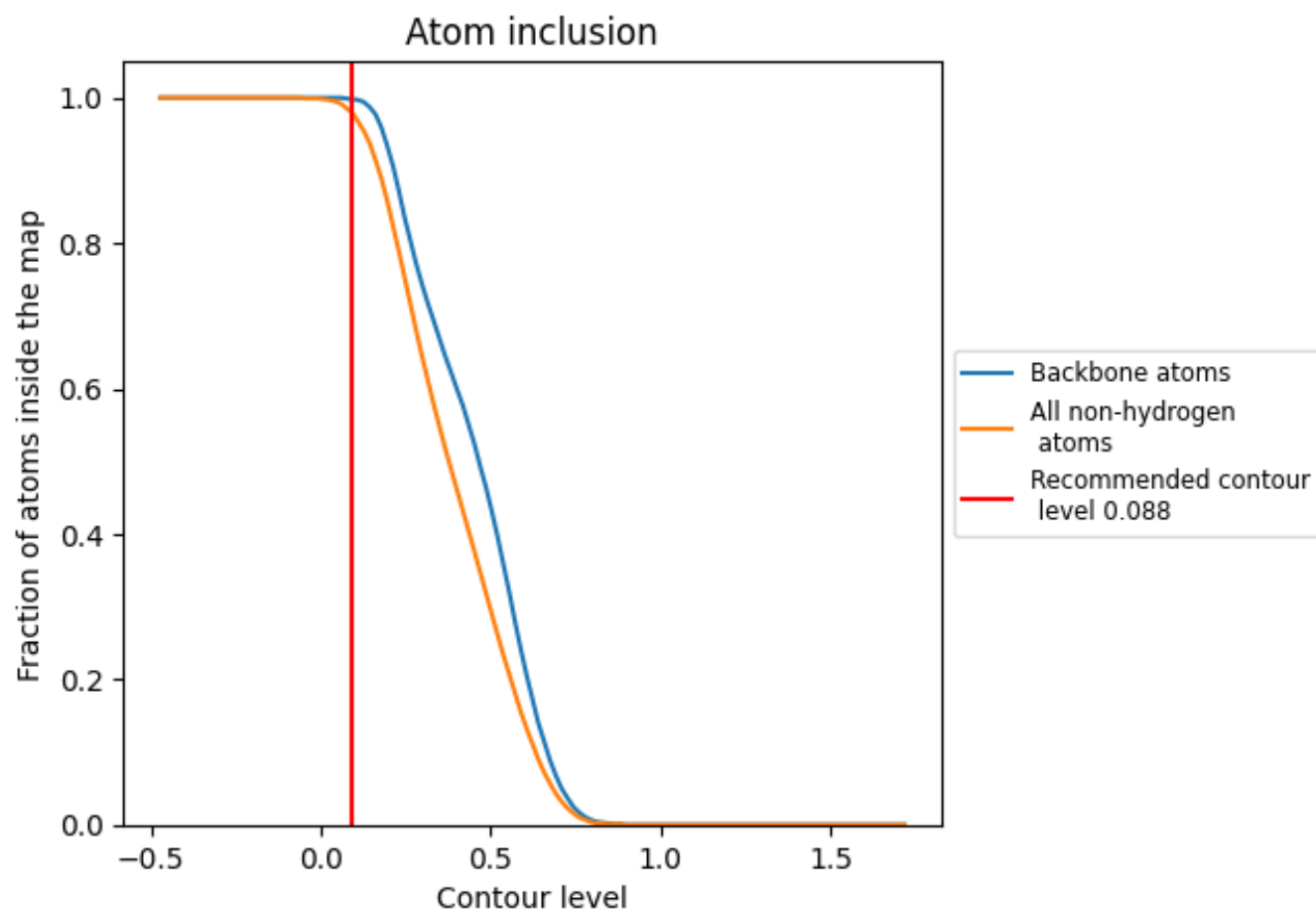
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.088).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.088) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9810	 0.5660
A	 0.9750	 0.5410
B	 0.9790	 0.5580
C	 0.9820	 0.5480
D	 0.9770	 0.5730
E	 0.9840	 0.5710
F	 0.9540	 0.4550
G	 0.9760	 0.5470
H	 0.9870	 0.5760
I	 0.9800	 0.5430
J	 0.9780	 0.5160
K	 0.9810	 0.5730
L	 0.9710	 0.5180
M	 0.9850	 0.5780
a	 0.9890	 0.5990
b	 0.9860	 0.5970
c	 0.9900	 0.5880
d	 0.9940	 0.5920
e	 0.9710	 0.5630
f	 0.9800	 0.5790
g	 0.9490	 0.5090
i	 0.9900	 0.5990
j	 0.9680	 0.5650
l	 0.9940	 0.5920
m	 0.9770	 0.5700
r	 0.9820	 0.5740

