



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 12:38 PM JST

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:

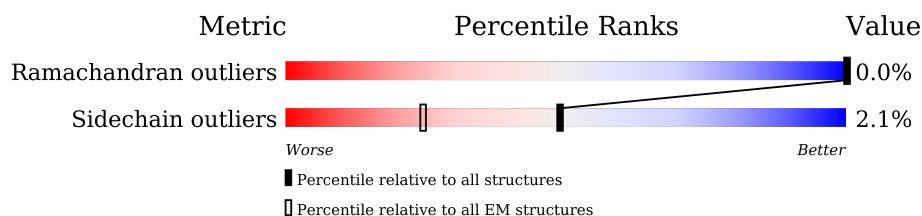
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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.



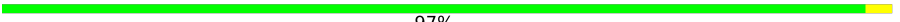
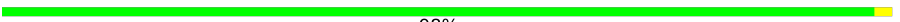






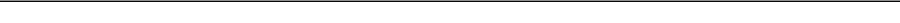

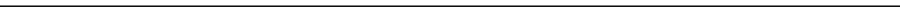


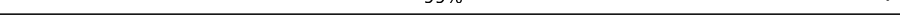
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	
5	F	170	
6	G	174	
7	H	168	
8	I	172	
9	J	183	

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Mol	Chain	Length	Quality of chain
10	K	176	 97%
11	L	217	 98%
12	M	171	 98%
13	a	743	 99%
14	d	132	 98%
15	e	62	 95% 5%
16	f	160	 99%
17	g	131	 97%
18	i	33	 100%
19	j	40	 92% 8%
20	l	146	 99%
21	m	29	 100%
22	r	89	 99%
23	D	164	 98%
24	b	732	 99%
25	c	80	 100%

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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
27	CLA	E	314	X	-	-	-
27	CLA	E	315	X	-	-	-
27	CLA	F	305	X	-	-	-
27	CLA	F	306	X	-	-	-
27	CLA	F	307	X	-	-	-
27	CLA	F	308	X	-	-	-
27	CLA	F	309	X	-	-	-
27	CLA	F	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-

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		

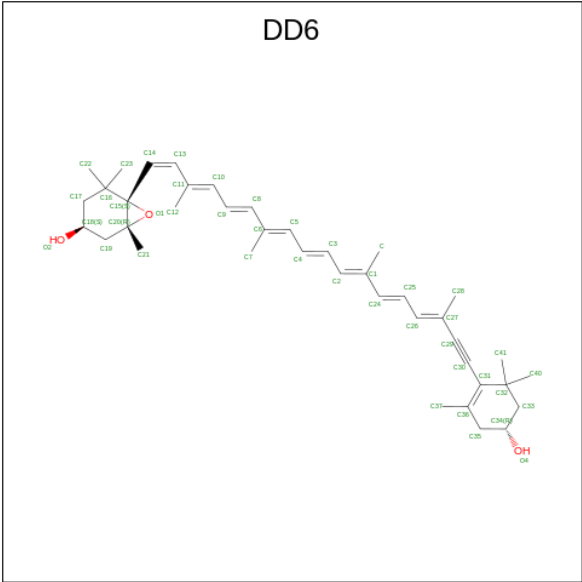
- Molecule 24 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

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).



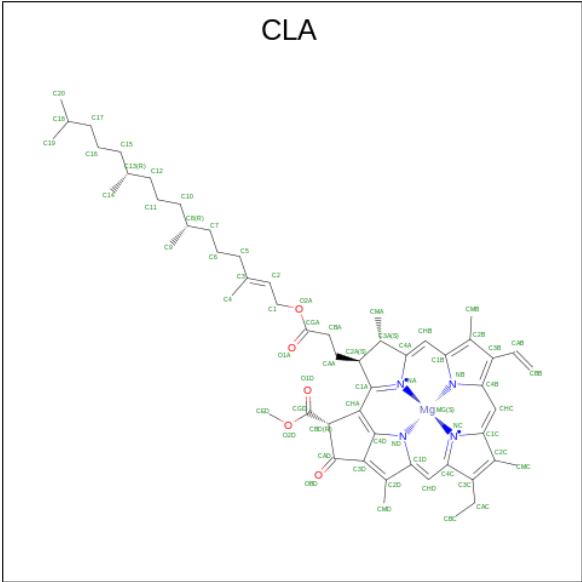
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			43	40	3	
26	A	1	Total	C	O	0
			43	40	3	
26	B	1	Total	C	O	0
			43	40	3	
26	C	1	Total	C	O	0
			43	40	3	
26	E	1	Total	C	O	0
			43	40	3	
26	E	1	Total	C	O	0
			43	40	3	
26	E	1	Total	C	O	0
			43	40	3	
26	E	1	Total	C	O	0
			43	40	3	
26	F	1	Total	C	O	0
			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	C	Mg	N	O	0
			55	45	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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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 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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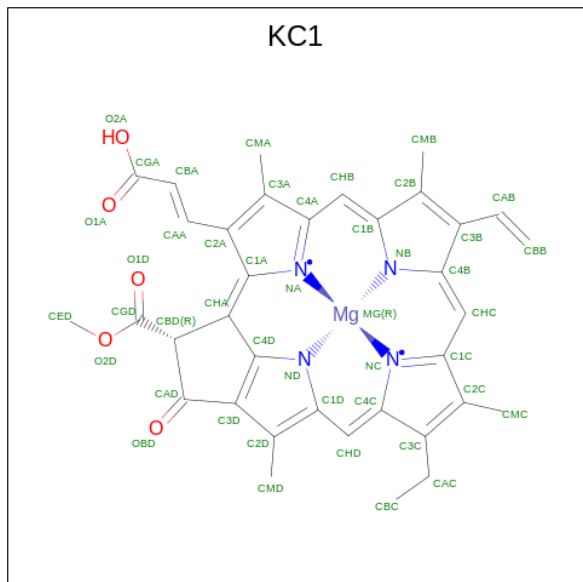
Mol	Chain	Residues	Atoms					AltConf
27	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 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).



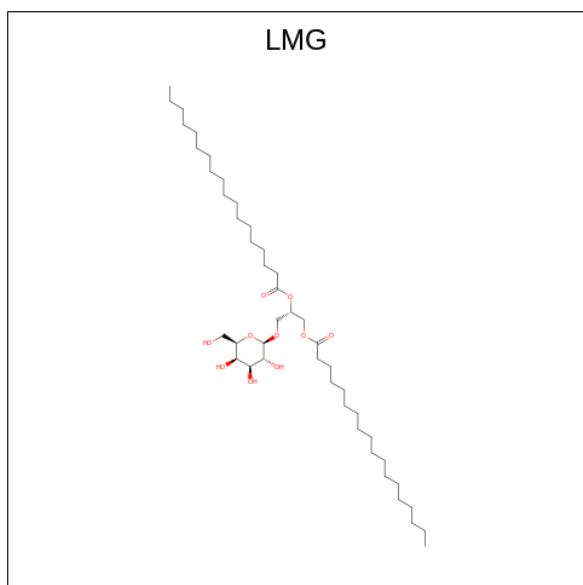
Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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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).



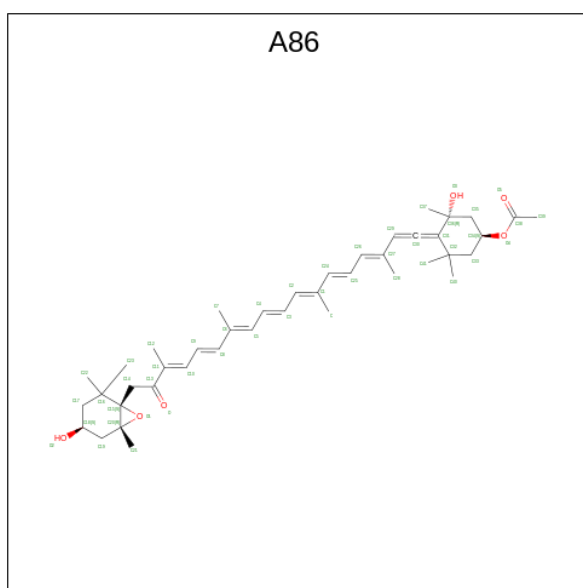
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			51	41	10	
29	A	1	Total	C	O	0
			41	31	10	

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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).



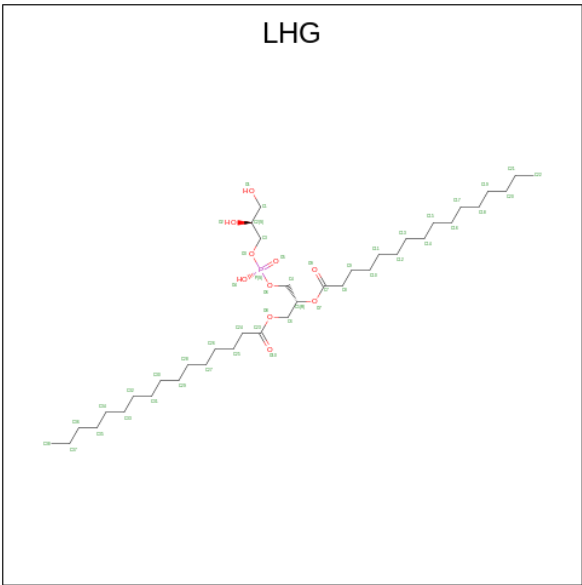
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			48	42	6	
30	B	1	Total	C	O	0
			48	42	6	
30	B	1	Total	C	O	0
			48	42	6	
30	B	1	Total	C	O	0
			48	42	6	
30	B	1	Total	C	O	0
			48	42	6	
30	C	1	Total	C	O	0
			48	42	6	
30	C	1	Total	C	O	0
			48	42	6	
30	C	1	Total	C	O	0
			48	42	6	
30	E	1	Total	C	O	0
			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).



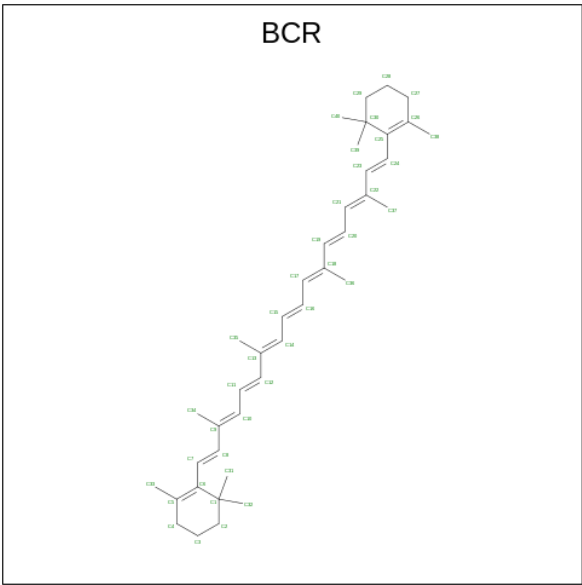
Mol	Chain	Residues	Atoms				AltConf
31	B	1	Total	C	O	P	0
			42	31	10	1	
31	E	1	Total	C	O	P	0
			42	31	10	1	
31	E	1	Total	C	O	P	0
			49	38	10	1	
31	H	1	Total	C	O	P	0
			35	24	10	1	
31	I	1	Total	C	O	P	0
			35	24	10	1	
31	K	1	Total	C	O	P	0
			33	24	8	1	
31	M	1	Total	C	O	P	0
			47	36	10	1	
31	a	1	Total	C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



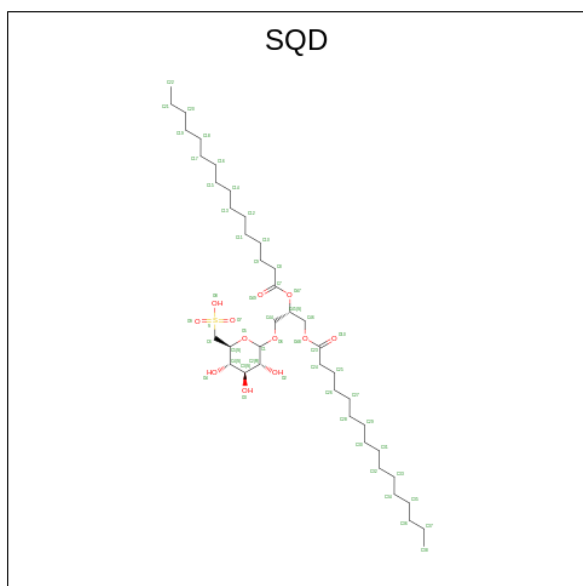
Mol	Chain	Residues	Atoms		AltConf
32	E	1	Total	C	0
			40	40	
32	E	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	f	1	Total	C	0
			40	40	
32	f	1	Total	C	0
			40	40	
32	i	1	Total	C	0
			40	40	

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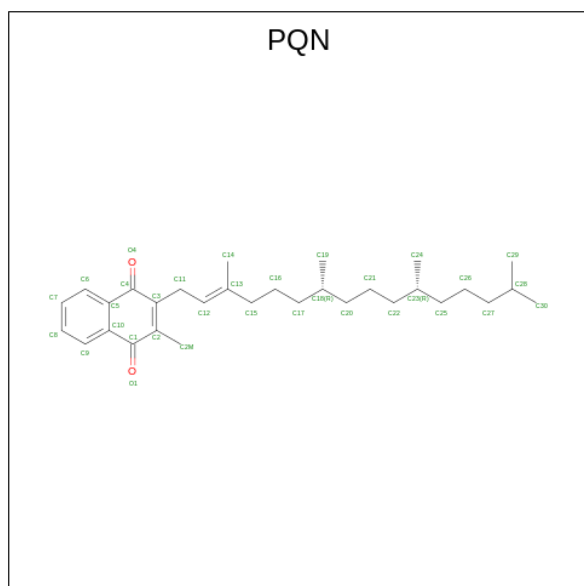
Mol	Chain	Residues	Atoms	AltConf
32	i	1	Total C 40 40	0
32	j	1	Total C 40 40	0
32	j	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	m	1	Total C 40 40	0
32	r	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0

- 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).



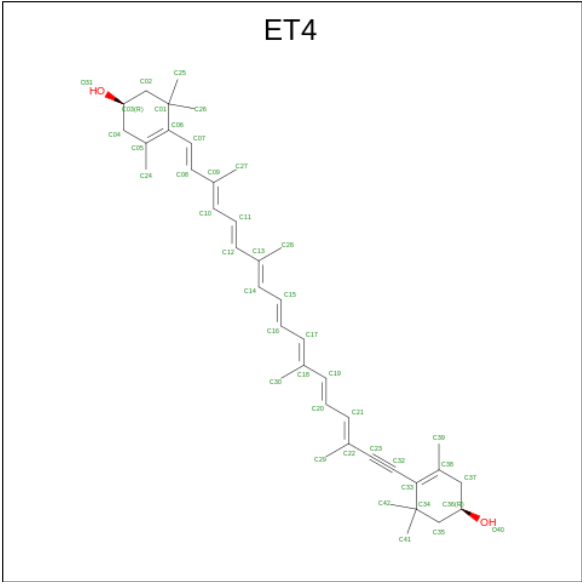
Mol	Chain	Residues	Atoms				AltConf
33	J	1	Total	C	O	S	0
			33	23	9	1	

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



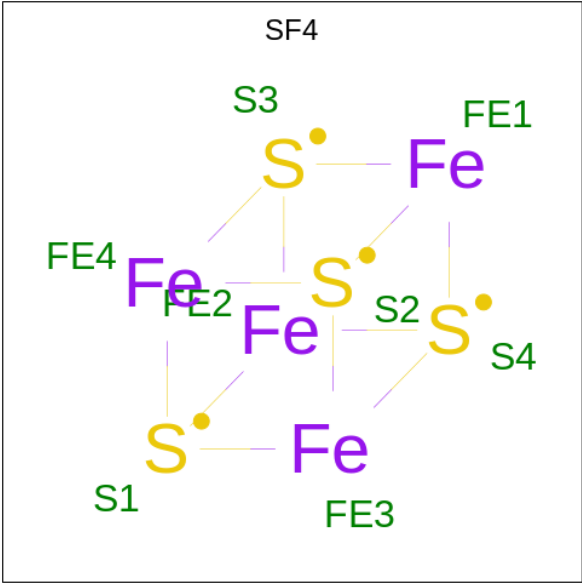
Mol	Chain	Residues	Atoms				AltConf
34	a	1	Total	C	O		0
			33	31	2		
34	b	1	Total	C	O		0
			33	31	2		

- 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).



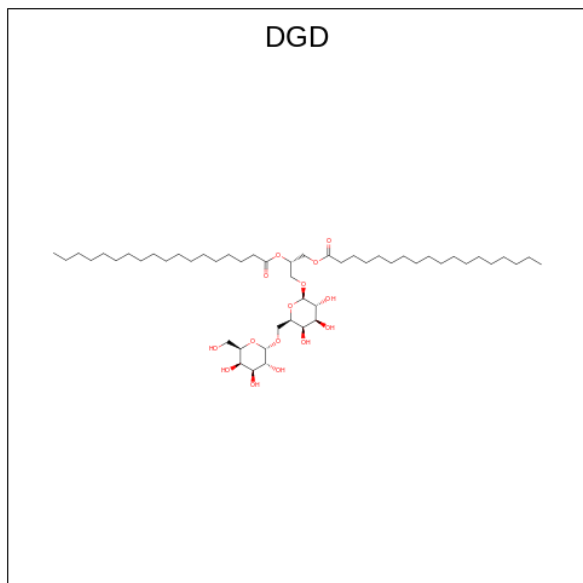
Mol	Chain	Residues	Atoms			AltConf
36	b	1	Total	Fe	S	0
			8	4	4	
36	c	1	Total	Fe	S	0
			8	4	4	

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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

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.

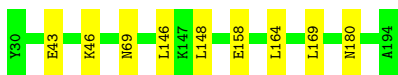
- Molecule 1: Tp-Lhcr18

Chain A:  99%



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

Chain B:  95% 5%



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

Chain C:  98%



- Molecule 4: Tp-RedCAP

Chain E:  100%

There are no outlier residues recorded for this chain.

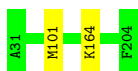
- Molecule 5: Tp-Lhcr20

Chain F:  96%



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

Chain G:  99%



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

Chain H: 100%

There are no outlier residues recorded for this chain.

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

Chain I: 98%



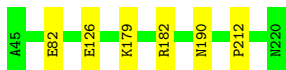
- Molecule 9: Fucoxanthin chl a/c light-harvesting protein

Chain J: 96%



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

Chain K: 97%



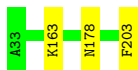
- Molecule 11: Fucoxanthin chlorophyll a/c light-harvesting protein

Chain L: 98%



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

Chain M: 98%



- Molecule 13: Photosystem I P700 chlorophyll a apoprotein A1

Chain a: 99%



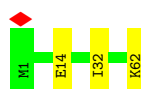
- Molecule 14: Photosystem I reaction center subunit II

Chain d: 98%



- Molecule 15: Photosystem I reaction center subunit IV

Chain e: 95%



- Molecule 16: Photosystem I reaction center subunit III

Chain f: 99%



- Molecule 17: Photosystem I reaction center subunit Psa29

Chain g: 97%



- Molecule 18: Photosystem I reaction center subunit VIII

Chain i: 100%

There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem I reaction center subunit IX

Chain j: 92%



- Molecule 20: Photosystem I reaction center subunit XI

Chain l: 99%



- Molecule 21: Photosystem I reaction center subunit XII

Chain m: 100%

There are no outlier residues recorded for this chain.

- Molecule 22: Tp-PsaR

Chain r: 99%



- Molecule 23: Pt17531-like protein

Chain D: 98%



- Molecule 24: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 99%



- Molecule 25: Photosystem I iron-sulfur center

Chain c: 100%

There are no outlier residues recorded for this chain.

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 (Å)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.30	0/1206	0.42	0/1637
2	B	0.34	0/1324	0.39	0/1804
3	C	0.33	0/1339	0.40	0/1813
4	E	0.33	0/1450	0.40	0/1974
5	F	0.33	0/1330	0.42	0/1794
6	G	0.32	0/1348	0.41	0/1815
7	H	0.33	0/1334	0.41	0/1809
8	I	0.35	0/1348	0.43	0/1820
9	J	0.33	0/1426	0.39	0/1931
10	K	0.34	0/1368	0.39	0/1845
11	L	0.29	0/1716	0.39	0/2327
12	M	0.33	0/1345	0.41	0/1823
13	a	0.34	0/6049	0.41	0/8234
14	d	0.32	0/1067	0.41	0/1441
15	e	0.31	0/511	0.40	0/690
16	f	0.33	0/1271	0.42	0/1727
17	g	0.29	0/1003	0.41	0/1354
18	i	0.32	0/264	0.40	0/360
19	j	0.34	0/342	0.50	0/463
20	l	0.35	0/1123	0.44	0/1523
21	m	0.35	0/222	0.38	0/300
22	r	0.31	0/704	0.37	0/957
23	D	0.32	0/1304	0.39	0/1771
24	b	0.33	0/6034	0.41	0/8236
25	c	0.33	0/609	0.44	0/826
All	All	0.33	0/37037	0.41	0/50274

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.

There are no bond angle outliers.

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	22	48
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%)	22	48
11	L	215/217 (99%)	211 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	121 (99%)	1 (1%)	79	92
2	B	133/133 (100%)	124 (93%)	9 (7%)	13	34
3	C	129/130 (99%)	126 (98%)	3 (2%)	45	75
4	E	144/144 (100%)	144 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	133/133 (100%)	127 (96%)	6 (4%)	23	52
6	G	139/139 (100%)	137 (99%)	2 (1%)	62	85
7	H	136/136 (100%)	136 (100%)	0	100	100
8	I	136/136 (100%)	133 (98%)	3 (2%)	47	76
9	J	139/139 (100%)	131 (94%)	8 (6%)	17	42
10	K	134/134 (100%)	129 (96%)	5 (4%)	29	60
11	L	173/173 (100%)	168 (97%)	5 (3%)	37	68
12	M	133/133 (100%)	130 (98%)	3 (2%)	45	75
13	a	603/603 (100%)	597 (99%)	6 (1%)	73	89
14	d	111/111 (100%)	110 (99%)	1 (1%)	75	91
15	e	55/55 (100%)	52 (94%)	3 (6%)	18	44
16	f	132/132 (100%)	130 (98%)	2 (2%)	60	84
17	g	98/98 (100%)	94 (96%)	4 (4%)	26	56
18	i	28/28 (100%)	28 (100%)	0	100	100
19	j	36/36 (100%)	33 (92%)	3 (8%)	9	26
20	l	113/113 (100%)	112 (99%)	1 (1%)	75	91
21	m	22/22 (100%)	22 (100%)	0	100	100
22	r	72/72 (100%)	71 (99%)	1 (1%)	62	85
23	D	128/128 (100%)	124 (97%)	4 (3%)	35	66
24	b	597/597 (100%)	589 (99%)	8 (1%)	65	86
25	c	69/69 (100%)	69 (100%)	0	100	100
All	All	3715/3716 (100%)	3637 (98%)	78 (2%)	49	77

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

Mol	Chain	Res	Type
17	g	91	TYR
24	b	112	VAL
17	g	158	LEU
22	r	113	TYR
24	b	256	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
10	K	220	ASN
24	b	89	HIS
13	a	12	ASN
24	b	34	HIS
24	b	472	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	F	311	5	60,68,73	1.55	7 (11%)	70,107,113	1.40	7 (10%)
32	BCR	b	837	-	41,41,41	0.74	0	56,56,56	2.00	18 (32%)
27	CLA	a	811	13,27	62,70,73	1.51	6 (9%)	72,109,113	1.39	6 (8%)
27	CLA	E	309	4	65,73,73	1.49	6 (9%)	76,113,113	1.35	7 (9%)
30	A86	K	307	-	44,50,50	1.33	5 (11%)	51,76,76	2.31	15 (29%)
31	LHG	K	320	-	32,32,48	1.27	7 (21%)	36,37,54	1.15	2 (5%)
26	DD6	G	301	-	39,45,45	2.01	3 (7%)	52,67,67	1.84	12 (23%)
27	CLA	a	855	13	65,73,73	1.45	6 (9%)	76,113,113	1.45	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	M	304	-	39,45,45	2.27	6 (15%)	52,67,67	2.72	12 (23%)
30	A86	M	305	-	44,50,50	1.29	4 (9%)	51,76,76	2.14	14 (27%)
27	CLA	D	214	23	56,64,73	1.59	7 (12%)	65,102,113	1.52	7 (10%)
27	CLA	M	319	12	46,54,73	1.72	9 (19%)	53,90,113	1.50	7 (13%)
31	LHG	a	834	27	26,26,48	1.28	5 (19%)	29,32,54	1.20	2 (6%)
26	DD6	K	303	-	39,45,45	2.31	7 (17%)	52,67,67	2.80	20 (38%)
27	CLA	B	310	2	46,54,73	1.77	6 (13%)	53,90,113	1.54	6 (11%)
27	CLA	b	812	24	60,68,73	1.49	10 (16%)	70,107,113	1.51	8 (11%)
27	CLA	b	824	24	58,66,73	1.56	6 (10%)	67,104,113	1.48	8 (11%)
27	CLA	D	209	23	49,57,73	1.71	7 (14%)	55,93,113	1.56	7 (12%)
30	A86	J	316	-	44,50,50	1.35	5 (11%)	51,76,76	3.63	25 (49%)
27	CLA	L	318	11	41,50,73	1.77	8 (19%)	46,85,113	1.63	6 (13%)
30	A86	K	301	-	44,50,50	1.26	3 (6%)	51,76,76	2.19	17 (33%)
28	KC1	F	312	5	48,53,53	1.51	7 (14%)	55,89,89	1.87	8 (14%)
27	CLA	L	319	-	45,53,73	1.76	9 (20%)	52,89,113	1.68	8 (15%)
27	CLA	M	318	12	46,54,73	1.73	10 (21%)	53,90,113	1.58	7 (13%)
31	LHG	E	318	-	48,48,48	1.11	6 (12%)	51,54,54	1.03	3 (5%)
27	CLA	J	307	9	65,73,73	1.46	9 (13%)	76,113,113	1.42	8 (10%)
30	A86	M	302	-	44,50,50	1.51	8 (18%)	51,76,76	3.16	24 (47%)
27	CLA	a	821	13	65,73,73	1.47	7 (10%)	76,113,113	1.42	7 (9%)
27	CLA	b	845	24	62,70,73	1.50	6 (9%)	72,109,113	1.44	6 (8%)
27	CLA	C	318	3	42,50,73	1.78	10 (23%)	48,85,113	1.60	6 (12%)
32	BCR	l	202	-	41,41,41	0.99	2 (4%)	56,56,56	2.04	16 (28%)
26	DD6	F	303	-	39,45,45	2.04	3 (7%)	52,67,67	2.00	14 (26%)
27	CLA	M	311	-	46,54,73	1.72	10 (21%)	53,90,113	1.63	8 (15%)
29	LMG	L	323	-	46,46,55	1.98	6 (13%)	54,54,63	2.19	8 (14%)
30	A86	K	306	-	44,50,50	1.34	5 (11%)	51,76,76	2.31	19 (37%)
27	CLA	a	828	13	65,73,73	1.52	7 (10%)	76,113,113	1.39	7 (9%)
32	BCR	f	305	-	41,41,41	0.94	1 (2%)	56,56,56	1.94	18 (32%)
30	A86	M	303	-	44,50,50	1.43	5 (11%)	51,76,76	3.79	23 (45%)
27	CLA	b	805	24	45,53,73	1.74	12 (26%)	52,89,113	1.69	8 (15%)
28	KC1	I	312	8	48,53,53	1.78	7 (14%)	55,89,89	1.87	10 (18%)
30	A86	r	202	-	44,50,50	1.51	8 (18%)	51,76,76	3.78	27 (52%)
27	CLA	L	315	11	41,49,73	1.81	10 (24%)	47,84,113	1.56	6 (12%)
27	CLA	D	212	23	42,50,73	1.80	6 (14%)	48,85,113	1.58	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	a	820	13	51,59,73	1.64	11 (21%)	59,96,113	1.69	7 (11%)
30	A86	B	302	-	44,50,50	1.61	9 (20%)	51,76,76	3.40	23 (45%)
27	CLA	F	308	-	62,70,73	1.52	6 (9%)	72,109,113	1.42	8 (11%)
27	CLA	D	217	-	41,49,73	1.80	6 (14%)	47,84,113	1.65	8 (17%)
27	CLA	M	315	12	41,49,73	1.83	6 (14%)	47,84,113	1.71	7 (14%)
27	CLA	K	313	10	52,60,73	1.60	9 (17%)	60,97,113	1.63	9 (15%)
27	CLA	D	211	23	46,54,73	1.75	7 (15%)	53,90,113	1.54	6 (11%)
30	A86	m	101	-	44,50,50	1.35	4 (9%)	51,76,76	3.28	25 (49%)
27	CLA	B	312	2	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
30	A86	D	203	-	44,50,50	1.34	4 (9%)	51,76,76	3.59	21 (41%)
27	CLA	b	826	-	45,53,73	1.80	6 (13%)	52,89,113	1.58	7 (13%)
31	LHG	E	316	-	41,41,48	1.00	2 (4%)	44,47,54	1.21	4 (9%)
27	CLA	a	817	13	65,73,73	1.48	6 (9%)	76,113,113	1.40	9 (11%)
27	CLA	G	311	6	56,64,73	1.57	6 (10%)	65,102,113	1.44	7 (10%)
27	CLA	H	212	7	65,73,73	1.45	11 (16%)	76,113,113	1.53	9 (11%)
27	CLA	K	318	10	46,54,73	1.70	9 (19%)	53,90,113	1.60	8 (15%)
31	LHG	a	801	-	48,48,48	1.10	5 (10%)	51,54,54	0.97	2 (3%)
27	CLA	G	306	-	46,54,73	1.75	6 (13%)	53,90,113	1.57	6 (11%)
27	CLA	F	313	-	41,49,73	1.80	6 (14%)	47,84,113	1.72	8 (17%)
36	SF4	b	802	24	0,12,12	-	-	-	-	-
27	CLA	B	309	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
27	CLA	D	216	23	46,54,73	1.70	10 (21%)	53,90,113	1.55	7 (13%)
27	CLA	b	839	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	7 (9%)
27	CLA	b	813	24	59,67,73	1.53	6 (10%)	68,105,113	1.47	7 (10%)
26	DD6	E	307	-	39,45,45	1.99	3 (7%)	52,67,67	1.79	13 (25%)
27	CLA	b	850	-	65,73,73	1.49	6 (9%)	76,113,113	1.39	7 (9%)
27	CLA	B	311	2	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
27	CLA	b	829	-	65,73,73	1.48	6 (9%)	76,113,113	1.42	8 (10%)
27	CLA	H	205	7	65,73,73	1.44	10 (15%)	76,113,113	1.40	9 (11%)
27	CLA	D	208	23	65,73,73	1.48	10 (15%)	76,113,113	1.52	11 (14%)
27	CLA	b	803	24	65,73,73	1.47	6 (9%)	76,113,113	1.39	6 (7%)
27	CLA	E	314	4	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
27	CLA	J	308	9	56,64,73	1.61	6 (10%)	65,102,113	1.45	7 (10%)
27	CLA	L	321	11	45,53,73	1.78	10 (22%)	52,89,113	1.59	8 (15%)
31	LHG	a	802	-	48,48,48	1.07	5 (10%)	51,54,54	0.93	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	J	302	-	39,45,45	2.07	2 (5%)	52,67,67	2.34	17 (32%)
32	BCR	m	102	-	41,41,41	0.67	0	56,56,56	2.14	16 (28%)
27	CLA	M	310	-	59,67,73	1.51	10 (16%)	68,105,113	1.44	7 (10%)
27	CLA	A	207	1	65,73,73	1.42	9 (13%)	76,113,113	1.41	8 (10%)
27	CLA	a	809	13	65,73,73	1.47	11 (16%)	76,113,113	1.56	11 (14%)
27	CLA	G	309	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
27	CLA	b	838	24	60,68,73	1.52	10 (16%)	70,107,113	1.55	8 (11%)
36	SF4	c	102	25	0,12,12	-	-	-		
27	CLA	a	812	13	65,73,73	1.47	7 (10%)	76,113,113	1.40	7 (9%)
26	DD6	G	303	-	39,45,45	2.01	3 (7%)	52,67,67	1.82	14 (26%)
27	CLA	f	302	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
27	CLA	H	204	-	54,62,73	1.61	10 (18%)	62,99,113	1.61	6 (9%)
32	BCR	a	835	-	41,41,41	0.93	1 (2%)	56,56,56	1.93	20 (35%)
27	CLA	b	815	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
27	CLA	J	312	9	65,73,73	1.46	10 (15%)	76,113,113	1.41	7 (9%)
27	CLA	a	841	13	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
28	KC1	H	211	7	48,53,53	1.82	8 (16%)	55,89,89	1.95	11 (20%)
27	CLA	b	830	24	65,73,73	1.47	10 (15%)	76,113,113	1.52	10 (13%)
28	KC1	G	313	6	48,53,53	1.52	7 (14%)	55,89,89	1.86	10 (18%)
27	CLA	J	315	9	49,57,73	1.63	10 (20%)	55,93,113	1.52	7 (12%)
27	CLA	b	842	24	65,73,73	1.49	6 (9%)	76,113,113	1.41	7 (9%)
30	A86	B	305	-	44,50,50	1.50	6 (13%)	51,76,76	3.14	26 (50%)
27	CLA	B	307	2	65,73,73	1.49	7 (10%)	76,113,113	1.37	7 (9%)
30	A86	C	304	-	44,50,50	1.44	5 (11%)	51,76,76	2.68	16 (31%)
27	CLA	a	818	13	45,53,73	1.80	6 (13%)	52,89,113	1.58	6 (11%)
30	A86	K	302	-	44,50,50	1.28	4 (9%)	51,76,76	2.59	19 (37%)
28	KC1	C	308	3	48,53,53	1.51	7 (14%)	55,89,89	1.92	10 (18%)
27	CLA	H	209	-	60,68,73	1.46	10 (16%)	70,107,113	1.59	9 (12%)
30	A86	H	201	-	44,50,50	1.61	9 (20%)	51,76,76	3.40	23 (45%)
32	BCR	a	853	-	41,41,41	0.71	0	56,56,56	2.15	18 (32%)
30	A86	A	213	-	44,50,50	1.31	5 (11%)	51,76,76	2.26	18 (35%)
27	CLA	H	208	7	46,54,73	1.76	6 (13%)	53,90,113	1.57	6 (11%)
27	CLA	E	312	4	55,63,73	1.60	6 (10%)	64,101,113	1.51	7 (10%)
30	A86	L	306	-	44,50,50	1.26	3 (6%)	51,76,76	2.15	14 (27%)
27	CLA	I	317	-	46,54,73	1.72	7 (15%)	53,90,113	1.58	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	D	210	-	56,64,73	1.57	10 (17%)	65,102,113	1.54	9 (13%)
27	CLA	C	311	3	60,68,73	1.55	9 (15%)	70,107,113	1.45	9 (12%)
29	LMG	J	317	-	51,51,55	1.41	6 (11%)	59,59,63	1.27	7 (11%)
27	CLA	H	213	7	65,73,73	1.44	11 (16%)	76,113,113	1.50	10 (13%)
30	A86	K	305	-	44,50,50	1.28	5 (11%)	51,76,76	2.17	16 (31%)
27	CLA	C	317	-	42,50,73	1.81	10 (23%)	48,85,113	1.69	8 (16%)
30	A86	B	301	-	44,50,50	1.30	4 (9%)	51,76,76	2.80	18 (35%)
27	CLA	a	830	13	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
27	CLA	a	825	13	45,53,73	1.79	6 (13%)	52,89,113	1.59	6 (11%)
36	SF4	c	101	25	0,12,12	-	-	-	-	-
32	BCR	E	305	-	41,41,41	0.72	0	56,56,56	2.02	16 (28%)
27	CLA	I	316	8	45,53,73	1.71	9 (20%)	52,89,113	1.56	6 (11%)
27	CLA	F	315	5	58,66,73	1.59	6 (10%)	67,104,113	1.41	9 (13%)
29	LMG	M	321	-	42,42,55	1.57	6 (14%)	50,50,63	1.38	5 (10%)
27	CLA	F	309	5	46,54,73	1.68	10 (21%)	53,90,113	1.58	6 (11%)
27	CLA	b	810	24	55,63,73	1.62	7 (12%)	64,101,113	1.47	6 (9%)
27	CLA	A	210	1	46,54,73	1.73	9 (19%)	53,90,113	1.58	7 (13%)
27	CLA	a	813	13	50,58,73	1.65	6 (12%)	58,95,113	1.62	7 (12%)
27	CLA	a	805	13	65,73,73	1.44	11 (16%)	76,113,113	1.59	10 (13%)
27	CLA	K	311	-	52,60,73	1.61	10 (19%)	60,97,113	1.58	9 (15%)
27	CLA	J	309	-	65,73,73	1.45	11 (16%)	76,113,113	1.43	8 (10%)
27	CLA	b	816	24	46,54,73	1.73	6 (13%)	53,90,113	1.62	6 (11%)
27	CLA	b	827	24	60,68,73	1.51	6 (10%)	70,107,113	1.53	7 (10%)
27	CLA	a	838	13	65,73,73	1.46	6 (9%)	76,113,113	1.38	7 (9%)
27	CLA	b	820	24	65,73,73	1.47	7 (10%)	76,113,113	1.37	7 (9%)
27	CLA	l	204	20	65,73,73	1.45	11 (16%)	76,113,113	1.56	9 (11%)
27	CLA	C	310	3	46,54,73	1.66	7 (15%)	53,90,113	1.55	7 (13%)
27	CLA	G	314	-	41,49,73	1.83	5 (12%)	47,84,113	1.70	7 (14%)
32	BCR	b	840	-	41,41,41	1.02	2 (4%)	56,56,56	2.04	21 (37%)
27	CLA	J	314	-	65,73,73	1.46	9 (13%)	76,113,113	1.38	7 (9%)
27	CLA	b	822	24	50,58,73	1.69	6 (12%)	58,95,113	1.50	8 (13%)
27	CLA	K	316	10	65,73,73	1.45	11 (16%)	76,113,113	1.50	10 (13%)
29	LMG	D	202	-	46,46,55	1.83	5 (10%)	54,54,63	1.36	5 (9%)
27	CLA	G	312	6	61,69,73	1.52	6 (9%)	71,108,113	1.43	7 (9%)
31	LHG	B	315	-	41,41,48	0.98	2 (4%)	44,47,54	1.08	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	f	303	16	45,53,73	1.77	6 (13%)	52,89,113	1.60	6 (11%)
27	CLA	I	310	8	47,55,73	1.73	5 (10%)	54,91,113	1.53	7 (12%)
27	CLA	A	205	1	65,73,73	1.43	9 (13%)	76,113,113	1.42	9 (11%)
27	CLA	B	306	2	58,65,73	1.53	9 (15%)	67,102,113	1.38	5 (7%)
27	CLA	I	306	8	65,73,73	1.47	7 (10%)	76,113,113	1.36	7 (9%)
34	PQN	a	831	-	34,34,34	1.59	2 (5%)	42,45,45	1.06	2 (4%)
27	CLA	b	849	24	54,62,73	1.61	6 (11%)	62,99,113	1.44	6 (9%)
27	CLA	a	824	13	50,58,73	1.68	6 (12%)	58,95,113	1.56	8 (13%)
27	CLA	B	308	2	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
27	CLA	a	804	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	8 (10%)
27	CLA	b	819	24	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
27	CLA	I	315	-	55,63,73	1.56	10 (18%)	64,101,113	1.52	8 (12%)
27	CLA	C	307	3	65,73,73	1.44	10 (15%)	76,113,113	1.45	9 (11%)
26	DD6	A	201	-	39,45,45	2.18	4 (10%)	52,67,67	2.03	15 (28%)
32	BCR	i	103	-	41,41,41	0.70	0	56,56,56	2.04	13 (23%)
27	CLA	F	306	5	55,63,73	1.62	6 (10%)	64,101,113	1.43	9 (14%)
27	CLA	F	314	5	47,55,73	1.75	6 (12%)	54,91,113	1.55	7 (12%)
32	BCR	l	205	-	41,41,41	0.86	0	56,56,56	2.07	15 (26%)
27	CLA	I	309	8	46,54,73	1.74	9 (19%)	53,90,113	1.61	7 (13%)
27	CLA	a	844	-	65,73,73	1.43	11 (16%)	76,113,113	1.50	9 (11%)
28	KC1	L	314	-	48,53,53	1.71	7 (14%)	55,89,89	1.92	12 (21%)
27	CLA	l	203	20	49,57,73	1.66	9 (18%)	55,93,113	1.62	8 (14%)
30	A86	E	301	-	44,50,50	1.45	6 (13%)	51,76,76	2.82	22 (43%)
27	CLA	l	206	-	45,53,73	1.75	6 (13%)	52,89,113	1.63	6 (11%)
27	CLA	b	801	-	65,73,73	1.48	12 (18%)	76,113,113	1.57	8 (10%)
27	CLA	I	305	-	45,53,73	1.74	9 (20%)	52,89,113	1.58	8 (15%)
27	CLA	b	828	24	47,55,73	1.76	7 (14%)	54,91,113	1.55	7 (12%)
32	BCR	b	833	-	41,41,41	0.71	0	56,56,56	1.92	14 (25%)
27	CLA	b	846	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	8 (10%)
27	CLA	a	803	13	65,73,73	1.53	11 (16%)	76,113,113	1.44	10 (13%)
27	CLA	a	823	13	65,73,73	1.50	6 (9%)	76,113,113	1.38	7 (9%)
30	A86	D	204	-	44,50,50	1.54	8 (18%)	51,76,76	3.73	22 (43%)
26	DD6	D	205	-	39,45,45	2.22	7 (17%)	52,67,67	3.22	26 (50%)
27	CLA	a	814	-	45,53,73	1.79	6 (13%)	52,89,113	1.59	6 (11%)
31	LHG	a	837	-	32,32,48	1.28	5 (15%)	35,38,54	1.17	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	A86	K	304	27	44,50,50	1.26	3 (6%)	51,76,76	2.32	14 (27%)
37	DGD	b	835	-	61,61,67	0.85	2 (3%)	75,75,81	1.10	4 (5%)
29	LMG	j	103	-	37,37,55	1.58	5 (13%)	45,45,63	3.61	8 (17%)
32	BCR	f	304	-	41,41,41	0.73	0	56,56,56	1.96	16 (28%)
26	DD6	C	303	-	39,45,45	2.20	5 (12%)	52,67,67	2.32	18 (34%)
27	CLA	E	313	4	45,53,73	1.76	11 (24%)	52,89,113	1.62	9 (17%)
27	CLA	L	316	11	56,64,73	1.55	9 (16%)	65,102,113	1.54	8 (12%)
26	DD6	G	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.86	14 (26%)
27	CLA	H	207	7	65,73,73	1.45	10 (15%)	76,113,113	1.51	9 (11%)
27	CLA	a	822	13	65,73,73	1.48	6 (9%)	76,113,113	1.42	8 (10%)
28	KC1	L	322	28	48,53,53	1.82	8 (16%)	55,89,89	1.98	11 (20%)
27	CLA	J	313	-	46,54,73	1.71	10 (21%)	53,90,113	1.58	6 (11%)
29	LMG	a	852	-	33,33,55	1.62	5 (15%)	41,41,63	3.62	8 (19%)
32	BCR	r	203	-	41,41,41	0.70	0	56,56,56	1.76	15 (26%)
27	CLA	a	849	13	65,73,73	1.48	6 (9%)	76,113,113	1.40	6 (7%)
26	DD6	L	303	-	39,45,45	2.24	6 (15%)	52,67,67	2.12	17 (32%)
27	CLA	a	816	13	65,73,73	1.49	7 (10%)	76,113,113	1.37	8 (10%)
26	DD6	I	304	-	39,45,45	2.34	7 (17%)	52,67,67	2.48	18 (34%)
27	CLA	b	843	24	65,73,73	1.48	6 (9%)	76,113,113	1.40	8 (10%)
30	A86	I	303	-	44,50,50	1.44	5 (11%)	51,76,76	3.08	24 (47%)
27	CLA	D	213	23	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
27	CLA	a	810	13	65,73,73	1.49	8 (12%)	76,113,113	1.38	7 (9%)
26	DD6	A	202	-	39,45,45	2.33	6 (15%)	52,67,67	2.70	17 (32%)
31	LHG	b	836	27	48,48,48	1.10	3 (6%)	51,54,54	1.03	3 (5%)
28	KC1	C	313	-	48,53,53	1.53	7 (14%)	55,89,89	1.87	11 (20%)
27	CLA	a	845	-	65,73,73	1.45	6 (9%)	76,113,113	1.46	7 (9%)
27	CLA	G	317	6	49,57,73	1.71	5 (10%)	55,93,113	1.56	7 (12%)
26	DD6	L	301	-	39,45,45	2.04	2 (5%)	52,67,67	2.17	18 (34%)
27	CLA	a	854	13	55,63,73	1.60	6 (10%)	64,101,113	1.50	7 (10%)
26	DD6	E	302	-	39,45,45	2.00	3 (7%)	52,67,67	1.91	10 (19%)
27	CLA	C	314	3	41,49,73	1.79	10 (24%)	47,84,113	1.64	8 (17%)
26	DD6	M	301	-	39,45,45	2.11	2 (5%)	52,67,67	2.00	15 (28%)
27	CLA	M	313	12	65,73,73	1.45	10 (15%)	76,113,113	1.61	13 (17%)
30	A86	D	206	-	44,50,50	1.46	6 (13%)	51,76,76	3.10	21 (41%)
33	SQD	J	318	-	31,32,54	3.14	8 (25%)	34,36,65	2.92	9 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	I	314	8	49,57,73	1.68	10 (20%)	55,93,113	1.47	7 (12%)
27	CLA	a	848	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	8 (10%)
27	CLA	L	313	11	65,73,73	1.43	10 (15%)	76,113,113	1.45	8 (10%)
29	LMG	C	301	-	31,31,55	1.61	6 (19%)	39,39,63	3.02	7 (17%)
28	KC1	A	209	-	48,53,53	1.60	7 (14%)	55,89,89	1.85	11 (20%)
27	CLA	K	310	10	56,64,73	1.57	10 (17%)	65,102,113	1.61	10 (15%)
27	CLA	b	804	24	65,73,73	1.46	12 (18%)	76,113,113	1.41	9 (11%)
27	CLA	F	317	-	47,55,73	1.64	6 (12%)	54,91,113	1.56	6 (11%)
31	LHG	I	318	-	34,34,48	1.29	5 (14%)	37,40,54	1.13	2 (5%)
30	A86	C	302	-	44,50,50	1.50	6 (13%)	51,76,76	2.99	22 (43%)
27	CLA	K	314	30,10	65,73,73	1.56	8 (12%)	76,113,113	1.82	16 (21%)
27	CLA	A	203	1	61,69,73	1.52	6 (9%)	71,108,113	1.43	6 (8%)
27	CLA	C	312	3	61,69,73	1.52	10 (16%)	71,108,113	1.47	7 (9%)
30	A86	b	848	-	44,50,50	1.42	6 (13%)	51,76,76	2.22	13 (25%)
28	KC1	K	315	10	48,53,53	1.78	8 (16%)	55,89,89	1.87	10 (18%)
26	DD6	B	303	-	39,45,45	2.32	6 (15%)	52,67,67	2.91	20 (38%)
27	CLA	a	839	13	60,68,73	1.53	12 (20%)	70,107,113	1.62	10 (14%)
28	KC1	M	314	-	48,53,53	1.79	8 (16%)	55,89,89	2.03	13 (23%)
27	CLA	A	211	-	39,48,73	1.78	10 (25%)	45,82,113	1.73	8 (17%)
27	CLA	C	315	3	42,50,73	1.84	5 (11%)	48,85,113	1.59	6 (12%)
27	CLA	H	214	7	45,53,73	1.77	5 (11%)	52,89,113	1.61	6 (11%)
27	CLA	a	850	13	56,64,73	1.59	6 (10%)	65,102,113	1.46	6 (9%)
28	KC1	L	320	28	48,53,53	1.51	7 (14%)	55,89,89	1.87	11 (20%)
26	DD6	E	306	-	39,45,45	2.13	3 (7%)	52,67,67	3.02	23 (44%)
27	CLA	F	316	-	41,49,73	1.87	5 (12%)	47,84,113	1.58	9 (19%)
27	CLA	G	307	6	56,64,73	1.59	7 (12%)	65,102,113	1.50	8 (12%)
27	CLA	i	101	-	60,68,73	1.54	6 (10%)	70,107,113	1.42	9 (12%)
32	BCR	b	834	-	41,41,41	0.71	0	56,56,56	3.24	21 (37%)
27	CLA	A	206	1	46,54,73	1.74	5 (10%)	53,90,113	1.54	6 (11%)
31	LHG	a	833	-	48,48,48	1.11	3 (6%)	51,54,54	1.00	3 (5%)
27	CLA	b	831	31	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
27	CLA	b	823	24	65,73,73	1.48	6 (9%)	76,113,113	1.44	6 (7%)
31	LHG	H	215	-	34,34,48	1.12	3 (8%)	37,40,54	0.97	2 (5%)
28	KC1	K	308	-	48,53,53	1.70	7 (14%)	55,89,89	1.99	13 (23%)
30	A86	L	304	-	44,50,50	1.23	4 (9%)	51,76,76	2.46	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	b	817	24	55,63,73	1.61	6 (10%)	64,101,113	1.46	7 (10%)
26	DD6	M	306	-	39,45,45	2.36	7 (17%)	52,67,67	2.84	15 (28%)
32	BCR	a	851	-	41,41,41	1.03	2 (4%)	56,56,56	1.82	13 (23%)
27	CLA	I	313	8	41,49,73	1.77	10 (24%)	47,84,113	1.71	9 (19%)
29	LMG	l	201	-	40,40,55	1.23	4 (10%)	48,48,63	1.76	4 (8%)
29	LMG	C	319	27	44,44,55	1.31	7 (15%)	52,52,63	1.86	4 (7%)
27	CLA	b	806	24	65,73,73	1.48	6 (9%)	76,113,113	1.45	6 (7%)
27	CLA	K	317	10	41,49,73	1.81	10 (24%)	47,84,113	1.77	8 (17%)
27	CLA	a	856	-	65,73,73	1.45	11 (16%)	76,113,113	1.54	10 (13%)
27	CLA	F	305	5	61,69,73	1.56	6 (9%)	71,108,113	1.39	7 (9%)
34	PQN	b	832	-	34,34,34	1.58	2 (5%)	42,45,45	1.18	3 (7%)
30	A86	I	301	-	44,50,50	1.44	6 (13%)	51,76,76	2.96	22 (43%)
27	CLA	b	818	24	60,68,73	1.54	7 (11%)	70,107,113	1.41	7 (10%)
32	BCR	E	304	-	41,41,41	0.68	0	56,56,56	1.87	17 (30%)
27	CLA	L	307	-	54,62,73	1.58	10 (18%)	62,99,113	1.49	6 (9%)
29	LMG	I	319	-	37,37,55	2.10	6 (16%)	45,45,63	2.70	4 (8%)
27	CLA	F	310	5	60,68,73	1.55	6 (10%)	70,107,113	1.41	7 (10%)
27	CLA	D	215	-	41,49,73	1.84	6 (14%)	47,84,113	1.67	7 (14%)
26	DD6	H	202	-	39,45,45	2.47	11 (28%)	52,67,67	2.56	20 (38%)
27	CLA	b	807	24	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
27	CLA	a	832	31	52,60,73	1.66	7 (13%)	60,97,113	1.53	7 (11%)
27	CLA	M	307	29	61,69,73	1.47	10 (16%)	71,108,113	1.51	8 (11%)
32	BCR	a	836	-	41,41,41	0.73	0	56,56,56	1.96	14 (25%)
30	A86	B	304	-	44,50,50	1.53	7 (15%)	51,76,76	2.80	18 (35%)
26	DD6	E	303	-	39,45,45	2.53	8 (20%)	52,67,67	3.41	16 (30%)
26	DD6	G	305	-	39,45,45	1.95	3 (7%)	52,67,67	1.92	14 (26%)
27	CLA	B	314	2	41,49,73	1.84	10 (24%)	47,84,113	1.62	8 (17%)
27	CLA	D	207	-	61,69,73	1.52	10 (16%)	71,108,113	1.48	8 (11%)
27	CLA	C	309	-	62,70,73	1.48	10 (16%)	72,109,113	1.59	10 (13%)
30	A86	L	305	-	44,50,50	1.26	3 (6%)	51,76,76	2.01	12 (23%)
26	DD6	J	305	-	39,45,45	2.21	5 (12%)	52,67,67	2.78	15 (28%)
27	CLA	J	311	9	65,73,73	1.46	9 (13%)	76,113,113	1.37	7 (9%)
27	CLA	a	840	13	65,73,73	1.49	6 (9%)	76,113,113	1.44	7 (9%)
30	A86	L	302	-	44,50,50	1.26	3 (6%)	51,76,76	2.67	16 (31%)
27	CLA	K	312	-	65,73,73	1.46	10 (15%)	76,113,113	1.42	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	b	825	-	65,73,73	1.48	10 (15%)	76,113,113	1.57	8 (10%)
27	CLA	I	308	-	65,73,73	1.42	9 (13%)	76,113,113	1.40	8 (10%)
27	CLA	b	808	24	65,73,73	1.47	6 (9%)	76,113,113	1.36	7 (9%)
27	CLA	A	208	1	54,62,73	1.62	10 (18%)	62,99,113	1.51	7 (11%)
29	LMG	E	317	-	43,43,55	2.06	7 (16%)	51,51,63	1.98	7 (13%)
27	CLA	J	310	9	46,54,73	1.69	8 (17%)	53,90,113	1.53	8 (15%)
32	BCR	j	101	-	41,41,41	0.70	0	56,56,56	2.06	14 (25%)
30	A86	J	301	-	44,50,50	1.36	5 (11%)	51,76,76	2.94	21 (41%)
28	KC1	B	313	-	48,53,53	1.72	8 (16%)	55,89,89	1.98	10 (18%)
27	CLA	a	829	13	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
27	CLA	f	301	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	8 (10%)
31	LHG	D	201	-	48,48,48	1.07	4 (8%)	51,54,54	1.03	2 (3%)
27	CLA	L	317	11	45,53,73	1.76	6 (13%)	52,89,113	1.58	6 (11%)
27	CLA	L	311	11	39,48,73	1.83	8 (20%)	45,82,113	1.67	8 (17%)
27	CLA	r	201	22	45,53,73	1.77	6 (13%)	52,89,113	1.58	7 (13%)
26	DD6	J	303	-	39,45,45	2.10	3 (7%)	52,67,67	2.19	14 (26%)
27	CLA	M	317	-	45,53,73	1.72	9 (20%)	52,89,113	1.64	10 (19%)
26	DD6	I	302	-	39,45,45	1.99	3 (7%)	52,67,67	1.75	13 (25%)
27	CLA	M	308	12	60,68,73	1.51	10 (16%)	70,107,113	1.45	9 (12%)
27	CLA	a	806	13,27	55,63,73	1.65	6 (10%)	64,101,113	1.49	8 (12%)
27	CLA	G	316	6	55,63,73	1.63	6 (10%)	64,101,113	1.44	8 (12%)
27	CLA	G	315	6	42,50,73	1.82	6 (14%)	48,85,113	1.61	6 (12%)
27	CLA	a	815	13	65,73,73	1.44	10 (15%)	76,113,113	1.57	12 (15%)
27	CLA	E	311	4	65,73,73	1.47	11 (16%)	76,113,113	1.44	9 (11%)
27	CLA	K	309	10	65,73,73	1.43	10 (15%)	76,113,113	1.47	7 (9%)
27	CLA	M	316	12	54,62,73	1.65	11 (20%)	62,99,113	1.69	11 (17%)
32	BCR	a	847	-	41,41,41	0.97	2 (4%)	56,56,56	1.95	19 (33%)
30	A86	H	203	-	44,50,50	1.46	5 (11%)	51,76,76	2.90	24 (47%)
27	CLA	a	808	13	65,73,73	1.46	6 (9%)	76,113,113	1.39	6 (7%)
30	A86	F	301	-	44,50,50	1.26	4 (9%)	51,76,76	2.69	16 (31%)
31	LHG	j	102	-	48,48,48	1.10	6 (12%)	51,54,54	0.92	2 (3%)
27	CLA	E	315	-	56,64,73	1.56	6 (10%)	65,102,113	1.52	6 (9%)
30	A86	G	302	-	44,50,50	1.54	6 (13%)	51,76,76	3.69	28 (54%)
32	BCR	i	102	-	41,41,41	0.76	0	56,56,56	1.94	17 (30%)
27	CLA	K	319	10	46,54,73	1.67	10 (21%)	53,90,113	1.52	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	b	847	24	65,73,73	1.49	6 (9%)	76,113,113	1.35	7 (9%)
27	CLA	L	308	11	65,73,73	1.44	10 (15%)	76,113,113	1.40	11 (14%)
35	ET4	l	207	-	41,43,43	1.46	6 (14%)	54,60,60	2.27	19 (35%)
27	CLA	H	206	7	65,73,73	1.43	11 (16%)	76,113,113	1.62	13 (17%)
27	CLA	j	104	19	41,49,73	1.84	6 (14%)	47,84,113	1.67	7 (14%)
31	LHG	M	320	-	46,46,48	1.10	4 (8%)	49,52,54	1.05	3 (6%)
30	A86	F	304	-	44,50,50	1.26	4 (9%)	51,76,76	2.70	20 (39%)
27	CLA	I	307	8	55,63,73	1.56	10 (18%)	64,101,113	1.54	7 (10%)
27	CLA	C	306	29	45,53,73	1.78	6 (13%)	52,89,113	1.59	6 (11%)
27	CLA	H	210	7	57,65,73	1.53	10 (17%)	66,103,113	1.50	7 (10%)
30	A86	J	304	-	44,50,50	1.34	5 (11%)	51,76,76	2.88	21 (41%)
30	A86	C	305	-	44,50,50	1.52	6 (13%)	51,76,76	3.11	24 (47%)
27	CLA	a	819	13	49,57,73	1.70	6 (12%)	55,93,113	1.58	7 (12%)
27	CLA	a	846	13	65,73,73	1.48	6 (9%)	76,113,113	1.39	8 (10%)
27	CLA	L	310	-	65,73,73	1.45	9 (13%)	76,113,113	1.38	8 (10%)
27	CLA	E	308	4	65,73,73	1.47	7 (10%)	76,113,113	1.42	7 (9%)
27	CLA	G	310	6	46,54,73	1.76	5 (10%)	53,90,113	1.54	6 (11%)
26	DD6	F	302	-	39,45,45	2.03	2 (5%)	52,67,67	1.99	11 (21%)
27	CLA	b	841	24	61,69,73	1.52	7 (11%)	71,108,113	1.46	8 (11%)
27	CLA	M	309	12	65,73,73	1.44	10 (15%)	76,113,113	1.48	9 (11%)
27	CLA	C	316	3	41,49,73	1.81	10 (24%)	47,84,113	1.68	9 (19%)
27	CLA	b	811	24	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
29	LMG	A	214	27	41,41,55	1.76	7 (17%)	49,49,63	1.59	5 (10%)
27	CLA	a	842	-	65,73,73	1.49	10 (15%)	76,113,113	1.46	9 (11%)
27	CLA	L	312	11	56,64,73	1.54	9 (16%)	65,102,113	1.47	8 (12%)
27	CLA	F	307	5	59,67,73	1.57	6 (10%)	68,105,113	1.44	6 (8%)
27	CLA	b	814	24	55,63,73	1.61	7 (12%)	64,101,113	1.49	6 (9%)
29	LMG	A	212	-	51,51,55	1.14	5 (9%)	59,59,63	1.58	5 (8%)
27	CLA	b	821	24	65,73,73	1.44	11 (16%)	76,113,113	1.59	9 (11%)
27	CLA	a	826	13	51,59,73	1.64	7 (13%)	59,96,113	1.56	7 (11%)
27	CLA	M	312	12	46,54,73	1.70	10 (21%)	53,90,113	1.65	10 (18%)
32	BCR	j	105	-	41,41,41	0.73	0	56,56,56	2.09	13 (23%)
27	CLA	a	827	13	60,68,73	1.56	11 (18%)	70,107,113	1.55	9 (12%)
27	CLA	G	308	6	54,62,73	1.63	6 (11%)	62,99,113	1.49	7 (11%)
27	CLA	I	311	8	65,73,73	1.39	11 (16%)	76,113,113	1.57	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	a	843	-	65,73,73	1.47	10 (15%)	76,113,113	1.47	8 (10%)
27	CLA	E	310	4	46,54,73	1.75	6 (13%)	53,90,113	1.53	7 (13%)
27	CLA	L	309	11	65,73,73	1.48	8 (12%)	76,113,113	1.42	9 (11%)
27	CLA	A	204	1	65,73,73	1.45	10 (15%)	76,113,113	1.50	8 (10%)
28	KC1	J	306	-	48,53,53	1.71	7 (14%)	55,89,89	1.95	12 (21%)
27	CLA	b	809	24	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
27	CLA	b	844	24	65,73,73	1.45	10 (15%)	76,113,113	1.46	7 (9%)
27	CLA	a	807	13	65,73,73	1.45	7 (10%)	76,113,113	1.47	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	F	311	5	1/1/14/20	13/31/109/115	-
32	BCR	b	837	-	-	5/29/63/63	0/2/2/2
27	CLA	a	811	13,27	1/1/14/20	12/34/112/115	-
27	CLA	E	309	4	1/1/15/20	12/37/115/115	-
30	A86	K	307	-	-	3/34/90/90	1/3/3/3
31	LHG	K	320	-	-	24/34/34/53	-
26	DD6	G	301	-	-	3/26/80/80	0/3/3/3
27	CLA	a	855	13	1/1/15/20	13/37/115/115	-
26	DD6	M	304	-	-	0/26/80/80	0/3/3/3
30	A86	M	305	-	-	6/34/90/90	0/3/3/3
27	CLA	D	214	23	1/1/13/20	9/27/105/115	-
27	CLA	M	319	12	1/1/11/20	7/15/93/115	-
31	LHG	a	834	27	-	12/31/31/53	-
26	DD6	K	303	-	-	6/26/80/80	0/3/3/3
27	CLA	B	310	2	1/1/11/20	4/15/93/115	-
27	CLA	b	812	24	1/1/14/20	10/31/109/115	-
27	CLA	b	824	24	1/1/13/20	11/29/107/115	-
27	CLA	D	209	23	1/1/11/20	9/18/96/115	-
30	A86	J	316	-	-	15/34/90/90	0/3/3/3
27	CLA	L	318	11	1/1/10/20	1/9/87/115	-
30	A86	K	301	-	-	9/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	KC1	F	312	5	-	5/15/71/71	-
27	CLA	L	319	-	1/1/11/20	4/13/91/115	-
27	CLA	M	318	12	1/1/11/20	11/15/93/115	-
31	LHG	E	318	-	-	35/53/53/53	-
27	CLA	J	307	9	1/1/15/20	10/37/115/115	-
30	A86	M	302	-	-	5/34/90/90	0/3/3/3
27	CLA	a	821	13	1/1/15/20	4/37/115/115	-
27	CLA	b	845	24	1/1/14/20	10/34/112/115	-
27	CLA	C	318	3	1/1/10/20	5/10/88/115	-
32	BCR	l	202	-	-	6/29/63/63	0/2/2/2
26	DD6	F	303	-	-	5/26/80/80	0/3/3/3
27	CLA	M	311	-	1/1/11/20	7/15/93/115	-
29	LMG	L	323	-	-	23/41/61/70	0/1/1/1
30	A86	K	306	-	-	5/34/90/90	0/3/3/3
27	CLA	a	828	13	1/1/15/20	12/37/115/115	-
32	BCR	f	305	-	-	9/29/63/63	0/2/2/2
30	A86	M	303	-	-	11/34/90/90	0/3/3/3
27	CLA	b	805	24	1/1/11/20	3/13/91/115	-
28	KC1	I	312	8	-	6/15/71/71	-
30	A86	r	202	-	-	5/34/90/90	0/3/3/3
27	CLA	L	315	11	1/1/10/20	6/8/86/115	-
27	CLA	D	212	23	1/1/10/20	1/10/88/115	-
27	CLA	a	820	13	1/1/12/20	5/21/99/115	-
30	A86	B	302	-	-	5/34/90/90	0/3/3/3
27	CLA	F	308	-	1/1/14/20	9/34/112/115	-
27	CLA	D	217	-	1/1/10/20	5/8/86/115	-
27	CLA	M	315	12	1/1/10/20	2/8/86/115	-
27	CLA	K	313	10	1/1/12/20	9/22/100/115	-
27	CLA	D	211	23	1/1/11/20	9/15/93/115	-
30	A86	m	101	-	-	7/34/90/90	0/3/3/3
27	CLA	B	312	2	1/1/15/20	11/37/115/115	-
30	A86	D	203	-	-	10/34/90/90	0/3/3/3
27	CLA	b	826	-	1/1/11/20	4/13/91/115	-
31	LHG	E	316	-	-	6/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	817	13	1/1/15/20	15/37/115/115	-
27	CLA	G	311	6	1/1/13/20	8/27/105/115	-
27	CLA	H	212	7	1/1/15/20	18/37/115/115	-
27	CLA	K	318	10	1/1/11/20	6/15/93/115	-
31	LHG	a	801	-	-	28/53/53/53	-
27	CLA	G	306	-	1/1/11/20	8/15/93/115	-
27	CLA	F	313	-	1/1/10/20	2/8/86/115	-
36	SF4	b	802	24	-	-	0/6/5/5
27	CLA	B	309	-	1/1/15/20	12/37/115/115	-
27	CLA	D	216	23	1/1/11/20	5/15/93/115	-
27	CLA	b	839	-	1/1/15/20	5/37/115/115	-
27	CLA	b	813	24	1/1/13/20	9/30/108/115	-
26	DD6	E	307	-	-	1/26/80/80	0/3/3/3
27	CLA	b	850	-	1/1/15/20	14/37/115/115	-
27	CLA	B	311	2	1/1/15/20	11/37/115/115	-
27	CLA	b	829	-	1/1/15/20	9/37/115/115	-
27	CLA	H	205	7	1/1/15/20	12/37/115/115	-
27	CLA	D	208	23	1/1/15/20	13/37/115/115	-
27	CLA	b	803	24	1/1/15/20	12/37/115/115	-
27	CLA	E	314	4	1/1/15/20	10/37/115/115	-
27	CLA	J	308	9	1/1/13/20	7/27/105/115	-
27	CLA	L	321	11	1/1/11/20	6/13/91/115	-
31	LHG	a	802	-	-	33/53/53/53	-
26	DD6	J	302	-	-	10/26/80/80	0/3/3/3
32	BCR	m	102	-	-	7/29/63/63	0/2/2/2
27	CLA	M	310	-	1/1/13/20	14/30/108/115	-
27	CLA	A	207	1	1/1/15/20	18/37/115/115	-
27	CLA	a	809	13	1/1/15/20	9/37/115/115	-
27	CLA	G	309	-	1/1/15/20	26/37/115/115	-
27	CLA	b	838	24	1/1/14/20	14/31/109/115	-
36	SF4	c	102	25	-	-	0/6/5/5
27	CLA	a	812	13	1/1/15/20	7/37/115/115	-
26	DD6	G	303	-	-	0/26/80/80	0/3/3/3
27	CLA	f	302	-	1/1/15/20	10/37/115/115	-
27	CLA	H	204	-	1/1/12/20	10/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	BCR	a	835	-	-	0/29/63/63	0/2/2/2
27	CLA	b	815	-	1/1/15/20	11/37/115/115	-
27	CLA	J	312	9	1/1/15/20	17/37/115/115	-
27	CLA	a	841	13	1/1/15/20	9/37/115/115	-
28	KC1	H	211	7	-	9/15/71/71	-
27	CLA	b	830	24	1/1/15/20	14/37/115/115	-
28	KC1	G	313	6	-	5/15/71/71	-
27	CLA	J	315	9	1/1/11/20	11/18/96/115	-
27	CLA	b	842	24	1/1/15/20	9/37/115/115	-
30	A86	B	305	-	-	4/34/90/90	0/3/3/3
27	CLA	B	307	2	1/1/15/20	7/37/115/115	-
30	A86	C	304	-	-	3/34/90/90	0/3/3/3
27	CLA	a	818	13	1/1/11/20	7/13/91/115	-
30	A86	K	302	-	-	8/34/90/90	0/3/3/3
28	KC1	C	308	3	-	7/15/71/71	-
27	CLA	H	209	-	1/1/14/20	9/31/109/115	-
30	A86	H	201	-	-	5/34/90/90	0/3/3/3
32	BCR	a	853	-	-	8/29/63/63	0/2/2/2
30	A86	A	213	-	-	4/34/90/90	0/3/3/3
27	CLA	H	208	7	1/1/11/20	8/15/93/115	-
27	CLA	E	312	4	1/1/13/20	9/25/103/115	-
30	A86	L	306	-	-	6/34/90/90	0/3/3/3
27	CLA	I	317	-	1/1/11/20	7/15/93/115	-
27	CLA	D	210	-	1/1/13/20	6/27/105/115	-
27	CLA	C	311	3	1/1/14/20	12/31/109/115	-
29	LMG	J	317	-	-	26/46/66/70	0/1/1/1
27	CLA	H	213	7	1/1/15/20	15/37/115/115	-
30	A86	K	305	-	-	3/34/90/90	0/3/3/3
27	CLA	C	317	-	1/1/10/20	8/10/88/115	-
30	A86	B	301	-	-	12/34/90/90	0/3/3/3
27	CLA	a	830	13	1/1/15/20	11/37/115/115	-
27	CLA	a	825	13	1/1/11/20	9/13/91/115	-
36	SF4	c	101	25	-	-	0/6/5/5
32	BCR	E	305	-	-	0/29/63/63	0/2/2/2
27	CLA	I	316	8	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	F	315	5	1/1/13/20	16/29/107/115	-
29	LMG	M	321	-	-	15/37/57/70	0/1/1/1
27	CLA	F	309	5	1/1/11/20	2/15/93/115	-
27	CLA	b	810	24	1/1/13/20	3/25/103/115	-
27	CLA	A	210	1	1/1/11/20	4/15/93/115	-
27	CLA	a	813	13	1/1/12/20	8/19/97/115	-
27	CLA	a	805	13	1/1/15/20	13/37/115/115	-
27	CLA	K	311	-	1/1/12/20	13/22/100/115	-
27	CLA	J	309	-	1/1/15/20	21/37/115/115	-
27	CLA	b	816	24	1/1/11/20	5/15/93/115	-
27	CLA	b	827	24	1/1/14/20	8/31/109/115	-
27	CLA	a	838	13	1/1/15/20	13/37/115/115	-
27	CLA	b	820	24	1/1/15/20	14/37/115/115	-
27	CLA	l	204	20	1/1/15/20	16/37/115/115	-
27	CLA	C	310	3	1/1/11/20	6/15/93/115	-
27	CLA	G	314	-	1/1/10/20	3/8/86/115	-
32	BCR	b	840	-	-	6/29/63/63	0/2/2/2
27	CLA	J	314	-	1/1/15/20	15/37/115/115	-
27	CLA	b	822	24	1/1/12/20	8/19/97/115	-
27	CLA	K	316	10	1/1/15/20	18/37/115/115	-
29	LMG	D	202	-	-	17/41/61/70	0/1/1/1
27	CLA	G	312	6	1/1/14/20	12/33/111/115	-
31	LHG	B	315	-	-	25/46/46/53	-
27	CLA	f	303	16	1/1/11/20	3/13/91/115	-
27	CLA	I	310	8	1/1/11/20	7/16/94/115	-
27	CLA	A	205	1	1/1/15/20	21/37/115/115	-
27	CLA	B	306	2	1/1/12/20	17/27/101/115	-
27	CLA	I	306	8	1/1/15/20	11/37/115/115	-
34	PQN	a	831	-	-	2/23/43/43	0/2/2/2
27	CLA	b	849	24	1/1/12/20	8/24/102/115	-
27	CLA	a	824	13	1/1/12/20	5/19/97/115	-
27	CLA	B	308	2	1/1/15/20	11/37/115/115	-
27	CLA	a	804	-	1/1/15/20	10/37/115/115	-
27	CLA	b	819	24	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	I	315	-	1/1/13/20	11/25/103/115	-
27	CLA	C	307	3	1/1/15/20	7/37/115/115	-
26	DD6	A	201	-	-	7/26/80/80	0/3/3/3
32	BCR	i	103	-	-	4/29/63/63	0/2/2/2
27	CLA	F	306	5	1/1/13/20	10/25/103/115	-
27	CLA	F	314	5	1/1/11/20	3/16/94/115	-
32	BCR	l	205	-	-	8/29/63/63	0/2/2/2
27	CLA	I	309	8	1/1/11/20	8/15/93/115	-
27	CLA	a	844	-	1/1/15/20	10/37/115/115	-
28	KC1	L	314	-	-	11/15/71/71	-
27	CLA	l	203	20	1/1/11/20	8/18/96/115	-
30	A86	E	301	-	-	5/34/90/90	0/3/3/3
27	CLA	l	206	-	1/1/11/20	4/13/91/115	-
27	CLA	b	801	-	1/1/15/20	9/37/115/115	-
27	CLA	I	305	-	1/1/11/20	5/13/91/115	-
27	CLA	b	828	24	1/1/11/20	5/16/94/115	-
32	BCR	b	833	-	-	0/29/63/63	0/2/2/2
27	CLA	b	846	-	1/1/15/20	12/37/115/115	-
27	CLA	a	803	13	1/1/15/20	15/37/115/115	-
27	CLA	a	823	13	1/1/15/20	10/37/115/115	-
30	A86	D	204	-	-	4/34/90/90	0/3/3/3
26	DD6	D	205	-	-	3/26/80/80	0/3/3/3
27	CLA	a	814	-	1/1/11/20	4/13/91/115	-
31	LHG	a	837	-	-	20/36/36/53	-
30	A86	K	304	27	-	3/34/90/90	0/3/3/3
37	DGD	b	835	-	-	27/49/89/95	0/2/2/2
29	LMG	j	103	-	-	16/32/52/70	0/1/1/1
32	BCR	f	304	-	-	2/29/63/63	0/2/2/2
26	DD6	C	303	-	-	5/26/80/80	0/3/3/3
27	CLA	E	313	4	1/1/11/20	3/13/91/115	-
27	CLA	L	316	11	1/1/13/20	17/27/105/115	-
26	DD6	G	304	-	-	0/26/80/80	0/3/3/3
27	CLA	H	207	7	1/1/15/20	10/37/115/115	-
27	CLA	a	822	13	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	KC1	L	322	28	-	8/15/71/71	-
27	CLA	J	313	-	1/1/11/20	10/15/93/115	-
29	LMG	a	852	-	-	16/28/48/70	0/1/1/1
32	BCR	r	203	-	-	4/29/63/63	0/2/2/2
27	CLA	a	849	13	1/1/15/20	13/37/115/115	-
26	DD6	L	303	-	-	0/26/80/80	0/3/3/3
27	CLA	a	816	13	1/1/15/20	7/37/115/115	-
26	DD6	I	304	-	-	3/26/80/80	0/3/3/3
27	CLA	b	843	24	1/1/15/20	14/37/115/115	-
30	A86	I	303	-	-	5/34/90/90	0/3/3/3
27	CLA	D	213	23	1/1/15/20	8/37/115/115	-
27	CLA	a	810	13	1/1/15/20	10/37/115/115	-
26	DD6	A	202	-	-	3/26/80/80	0/3/3/3
31	LHG	b	836	27	-	32/53/53/53	-
28	KC1	C	313	-	-	7/15/71/71	-
27	CLA	a	845	-	1/1/15/20	12/37/115/115	-
27	CLA	G	317	6	1/1/11/20	7/18/96/115	-
26	DD6	L	301	-	-	8/26/80/80	0/3/3/3
27	CLA	a	854	13	1/1/13/20	10/25/103/115	-
26	DD6	E	302	-	-	3/26/80/80	0/3/3/3
27	CLA	C	314	3	1/1/10/20	4/8/86/115	-
26	DD6	M	301	-	-	2/26/80/80	0/3/3/3
27	CLA	M	313	12	1/1/15/20	21/37/115/115	-
30	A86	D	206	-	-	6/34/90/90	0/3/3/3
33	SQD	J	318	-	-	18/33/33/69	-
27	CLA	I	314	8	1/1/11/20	7/18/96/115	-
27	CLA	a	848	-	1/1/15/20	8/37/115/115	-
27	CLA	L	313	11	1/1/15/20	14/37/115/115	-
29	LMG	C	301	-	-	14/26/46/70	0/1/1/1
28	KC1	A	209	-	-	9/15/71/71	-
27	CLA	K	310	10	1/1/13/20	16/27/105/115	-
27	CLA	b	804	24	1/1/15/20	16/37/115/115	-
27	CLA	F	317	-	1/1/11/20	8/16/94/115	-
31	LHG	I	318	-	-	15/39/39/53	-

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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	30,10	1/1/15/20	20/37/115/115	-
27	CLA	A	203	1	1/1/14/20	3/33/111/115	-
27	CLA	C	312	3	1/1/14/20	10/33/111/115	-
30	A86	b	848	-	-	16/34/90/90	0/3/3/3
28	KC1	K	315	10	-	5/15/71/71	-
26	DD6	B	303	-	-	0/26/80/80	0/3/3/3
27	CLA	a	839	13	1/1/14/20	14/31/109/115	-
28	KC1	M	314	-	-	7/15/71/71	-
27	CLA	A	211	-	1/1/9/20	4/8/82/115	-
27	CLA	C	315	3	1/1/10/20	4/10/88/115	-
27	CLA	H	214	7	1/1/11/20	4/13/91/115	-
27	CLA	a	850	13	1/1/13/20	9/27/105/115	-
28	KC1	L	320	28	-	6/15/71/71	-
27	CLA	F	316	-	1/1/10/20	4/8/86/115	-
26	DD6	E	306	-	-	10/26/80/80	0/3/3/3
27	CLA	G	307	6	1/1/13/20	6/27/105/115	-
27	CLA	i	101	-	1/1/14/20	11/31/109/115	-
32	BCR	b	834	-	-	6/29/63/63	0/2/2/2
27	CLA	A	206	1	1/1/11/20	4/15/93/115	-
31	LHG	a	833	-	-	26/53/53/53	-
27	CLA	b	831	31	1/1/15/20	7/37/115/115	-
27	CLA	b	823	24	1/1/15/20	18/37/115/115	-
31	LHG	H	215	-	-	19/38/38/53	-
28	KC1	K	308	-	-	8/15/71/71	-
30	A86	L	304	-	-	6/34/90/90	0/3/3/3
27	CLA	b	817	24	1/1/13/20	3/25/103/115	-
26	DD6	M	306	-	-	2/26/80/80	0/3/3/3
32	BCR	a	851	-	-	4/29/63/63	0/2/2/2
27	CLA	I	313	8	1/1/10/20	8/8/86/115	-
29	LMG	l	201	-	-	16/35/55/70	0/1/1/1
29	LMG	C	319	27	-	19/39/59/70	0/1/1/1
27	CLA	b	806	24	1/1/15/20	13/37/115/115	-
27	CLA	K	317	10	1/1/10/20	5/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	856	-	1/1/15/20	16/37/115/115	-
27	CLA	F	305	5	1/1/14/20	12/33/111/115	-
34	PQN	b	832	-	-	3/23/43/43	0/2/2/2
30	A86	I	301	-	-	10/34/90/90	0/3/3/3
27	CLA	b	818	24	1/1/14/20	17/31/109/115	-
32	BCR	E	304	-	-	2/29/63/63	0/2/2/2
27	CLA	L	307	-	1/1/12/20	14/24/102/115	-
29	LMG	I	319	-	-	13/32/52/70	0/1/1/1
27	CLA	F	310	5	1/1/14/20	12/31/109/115	-
27	CLA	D	215	-	1/1/10/20	2/8/86/115	-
26	DD6	H	202	-	-	3/26/80/80	0/3/3/3
27	CLA	b	807	24	1/1/15/20	17/37/115/115	-
27	CLA	a	832	31	1/1/12/20	6/22/100/115	-
27	CLA	M	307	29	1/1/14/20	11/33/111/115	-
32	BCR	a	836	-	-	4/29/63/63	0/2/2/2
30	A86	B	304	-	-	3/34/90/90	0/3/3/3
26	DD6	E	303	-	-	6/26/80/80	0/3/3/3
26	DD6	G	305	-	-	2/26/80/80	0/3/3/3
27	CLA	B	314	2	1/1/10/20	2/8/86/115	-
27	CLA	D	207	-	1/1/14/20	10/33/111/115	-
27	CLA	C	309	-	1/1/14/20	12/34/112/115	-
30	A86	L	305	-	-	7/34/90/90	0/3/3/3
26	DD6	J	305	-	-	2/26/80/80	0/3/3/3
27	CLA	J	311	9	1/1/15/20	14/37/115/115	-
27	CLA	a	840	13	1/1/15/20	12/37/115/115	-
30	A86	L	302	-	-	8/34/90/90	0/3/3/3
27	CLA	K	312	-	1/1/15/20	23/37/115/115	-
27	CLA	b	825	-	1/1/15/20	17/37/115/115	-
27	CLA	I	308	-	1/1/15/20	13/37/115/115	-
27	CLA	b	808	24	1/1/15/20	10/37/115/115	-
27	CLA	A	208	1	1/1/12/20	10/24/102/115	-
29	LMG	E	317	-	-	21/38/58/70	0/1/1/1
27	CLA	J	310	9	1/1/11/20	9/15/93/115	-
32	BCR	j	101	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	A86	J	301	-	-	7/34/90/90	0/3/3/3
28	KC1	B	313	-	-	8/15/71/71	-
27	CLA	a	829	13	1/1/15/20	10/37/115/115	-
27	CLA	f	301	-	1/1/15/20	10/37/115/115	-
31	LHG	D	201	-	-	32/53/53/53	-
27	CLA	L	317	11	1/1/11/20	5/13/91/115	-
27	CLA	L	311	11	1/1/9/20	6/8/82/115	-
27	CLA	r	201	22	1/1/11/20	12/13/91/115	-
26	DD6	J	303	-	-	4/26/80/80	0/3/3/3
27	CLA	M	317	-	-	7/13/91/115	-
26	DD6	I	302	-	-	1/26/80/80	0/3/3/3
27	CLA	M	308	12	1/1/14/20	13/31/109/115	-
27	CLA	a	806	13,27	1/1/13/20	6/25/103/115	-
27	CLA	G	316	6	1/1/13/20	7/25/103/115	-
27	CLA	G	315	6	1/1/10/20	4/10/88/115	-
27	CLA	a	815	13	1/1/15/20	24/37/115/115	-
27	CLA	E	311	4	1/1/15/20	11/37/115/115	-
27	CLA	K	309	10	1/1/15/20	17/37/115/115	-
27	CLA	M	316	12	1/1/12/20	8/24/102/115	-
32	BCR	a	847	-	-	2/29/63/63	0/2/2/2
30	A86	H	203	-	-	4/34/90/90	0/3/3/3
27	CLA	a	808	13	1/1/15/20	13/37/115/115	-
30	A86	F	301	-	-	9/34/90/90	0/3/3/3
31	LHG	j	102	-	-	20/53/53/53	-
27	CLA	E	315	-	1/1/13/20	7/27/105/115	-
30	A86	G	302	-	-	14/34/90/90	0/3/3/3
32	BCR	i	102	-	-	0/29/63/63	0/2/2/2
27	CLA	K	319	10	1/1/11/20	7/15/93/115	-
27	CLA	b	847	24	1/1/15/20	12/37/115/115	-
27	CLA	L	308	11	1/1/15/20	10/37/115/115	-
35	ET4	l	207	-	-	3/25/67/67	0/2/2/2
27	CLA	H	206	7	1/1/15/20	15/37/115/115	-
27	CLA	j	104	19	1/1/10/20	2/8/86/115	-
31	LHG	M	320	-	-	30/51/51/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	A86	F	304	-	-	5/34/90/90	0/3/3/3
27	CLA	I	307	8	1/1/13/20	8/25/103/115	-
27	CLA	C	306	29	1/1/11/20	4/13/91/115	-
27	CLA	H	210	7	1/1/13/20	8/28/106/115	-
30	A86	J	304	-	-	4/34/90/90	0/3/3/3
30	A86	C	305	-	-	4/34/90/90	0/3/3/3
27	CLA	a	819	13	1/1/11/20	10/18/96/115	-
27	CLA	a	846	13	1/1/15/20	17/37/115/115	-
27	CLA	L	310	-	1/1/15/20	15/37/115/115	-
27	CLA	E	308	4	1/1/15/20	14/37/115/115	-
27	CLA	G	310	6	1/1/11/20	6/15/93/115	-
26	DD6	F	302	-	-	1/26/80/80	0/3/3/3
27	CLA	b	841	24	1/1/14/20	10/33/111/115	-
27	CLA	M	309	12	1/1/15/20	13/37/115/115	-
27	CLA	C	316	3	1/1/10/20	3/8/86/115	-
27	CLA	b	811	24	1/1/15/20	10/37/115/115	-
29	LMG	A	214	27	-	28/36/56/70	0/1/1/1
27	CLA	a	842	-	1/1/15/20	13/37/115/115	-
27	CLA	L	312	11	1/1/13/20	8/27/105/115	-
27	CLA	F	307	5	1/1/13/20	9/30/108/115	-
27	CLA	b	814	24	1/1/13/20	12/25/103/115	-
29	LMG	A	212	-	-	24/46/66/70	0/1/1/1
27	CLA	b	821	24	1/1/15/20	17/37/115/115	-
27	CLA	a	826	13	1/1/12/20	10/21/99/115	-
27	CLA	M	312	12	1/1/11/20	7/15/93/115	-
32	BCR	j	105	-	-	5/29/63/63	0/2/2/2
27	CLA	a	827	13	1/1/14/20	14/31/109/115	-
27	CLA	G	308	6	1/1/12/20	9/24/102/115	-
27	CLA	I	311	8	1/1/15/20	21/37/115/115	-
27	CLA	a	843	-	1/1/15/20	21/37/115/115	-
27	CLA	E	310	4	1/1/11/20	6/15/93/115	-
27	CLA	L	309	11	1/1/15/20	17/37/115/115	-
27	CLA	A	204	1	1/1/15/20	17/37/115/115	-
28	KC1	J	306	-	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	b	809	24	1/1/15/20	10/37/115/115	-
27	CLA	b	844	24	1/1/15/20	17/37/115/115	-
27	CLA	a	807	13	1/1/15/20	15/37/115/115	-

The worst 5 of 2405 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	318	SQD	C6-S	-12.45	1.59	1.77
29	L	323	LMG	O6-C1	10.89	1.69	1.41
29	E	317	LMG	O2-C2	-10.76	1.17	1.43
29	I	319	LMG	O2-C2	-10.03	1.19	1.43
29	D	202	LMG	O2-C2	-9.32	1.21	1.43

The worst 5 of 3596 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j	103	LMG	O2-C2-C1	-21.31	58.28	110.05
29	a	852	LMG	O2-C2-C1	-18.82	64.32	110.05
26	E	303	DD6	C21-C20-C15	-16.15	95.19	122.26
30	r	202	A86	O1-C20-C19	-15.67	101.61	113.38
29	C	301	LMG	O2-C2-C1	15.26	147.12	110.05

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 3471 torsion outliers are listed below:

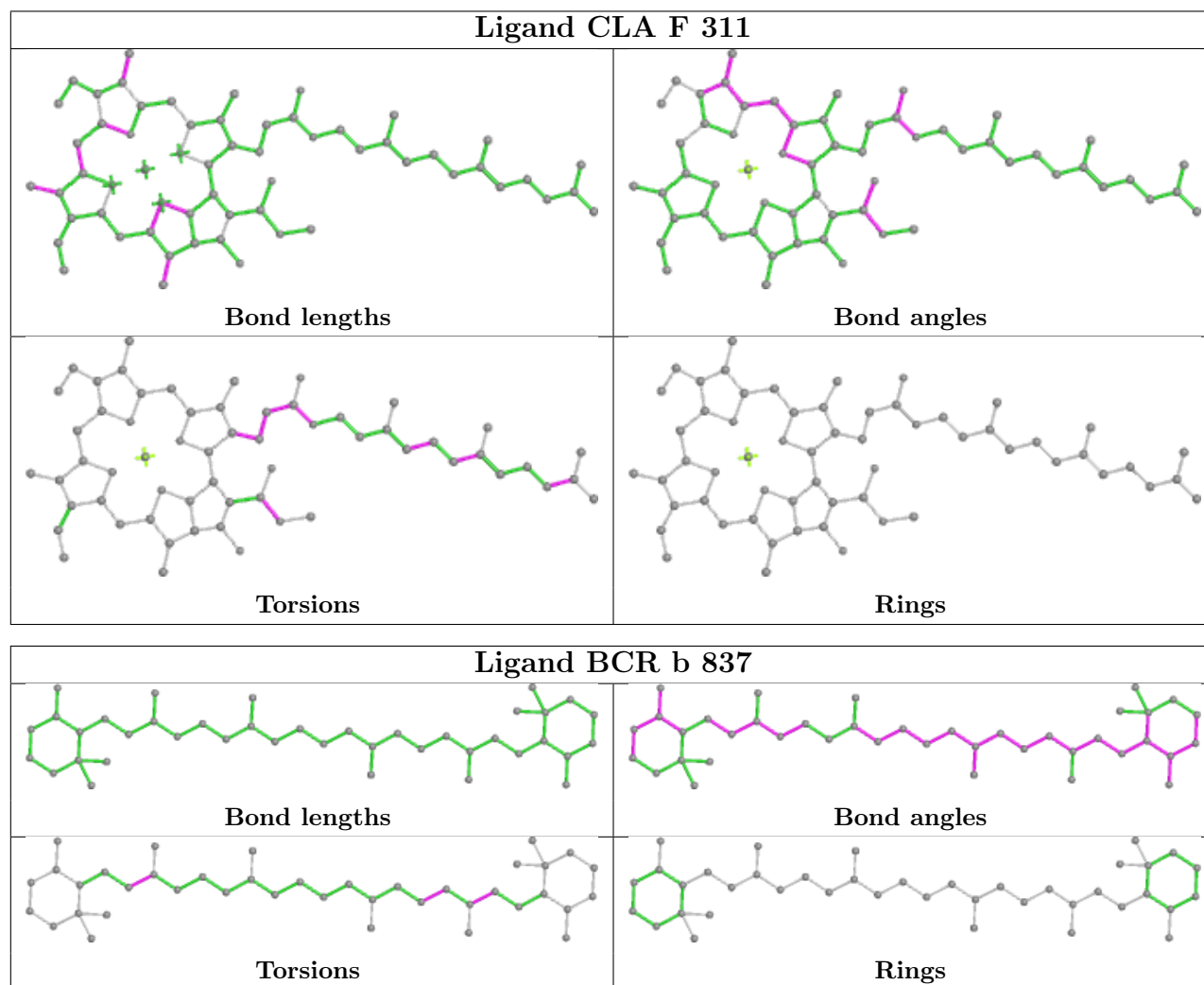
Mol	Chain	Res	Type	Atoms
26	A	201	DD6	C12-C11-C13-C14
26	A	201	DD6	C1-C2-C3-C4
26	A	202	DD6	C13-C14-C15-C16
26	A	202	DD6	C13-C14-C15-C20
26	E	302	DD6	C10-C11-C13-C14

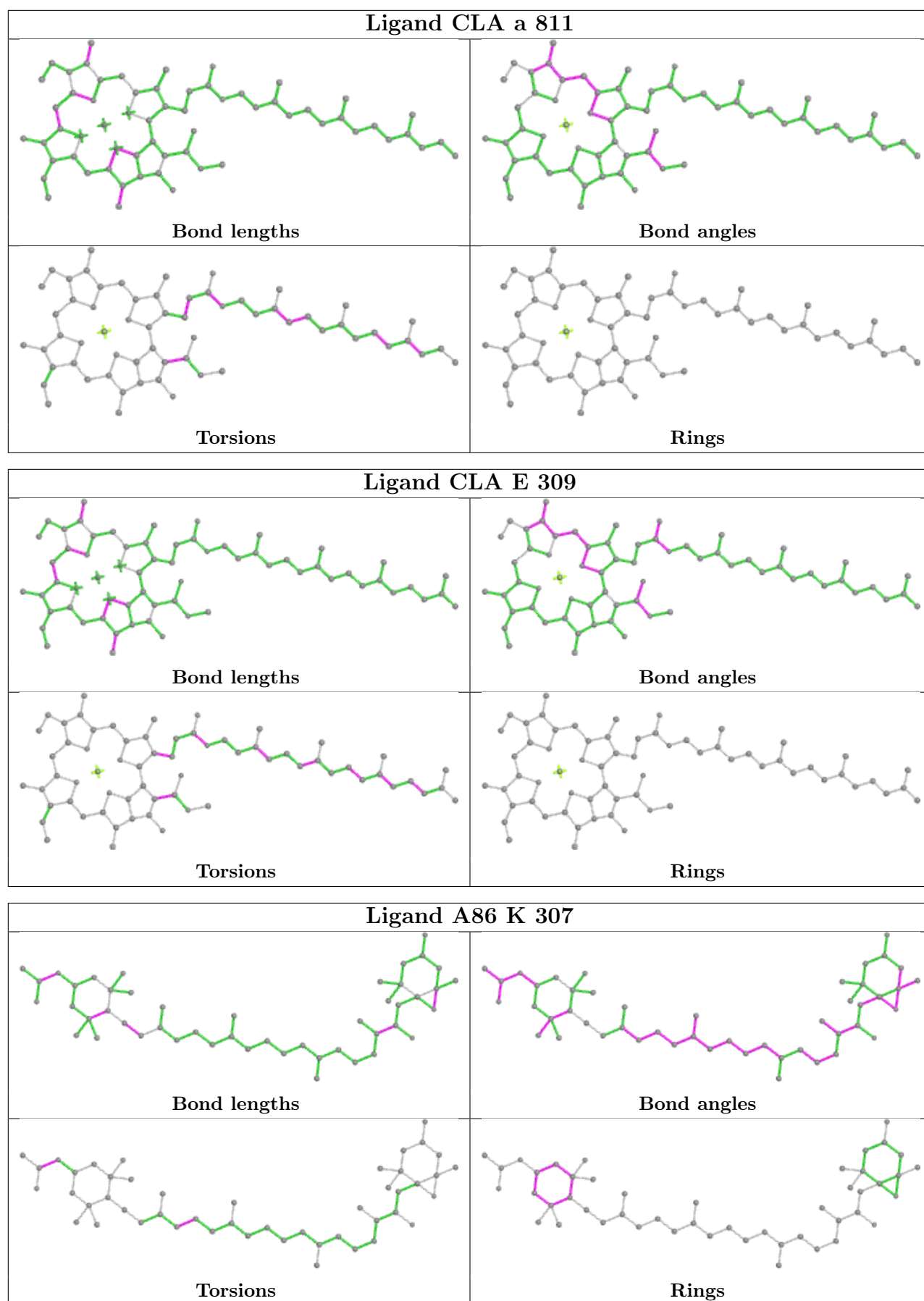
All (1) ring outliers are listed below:

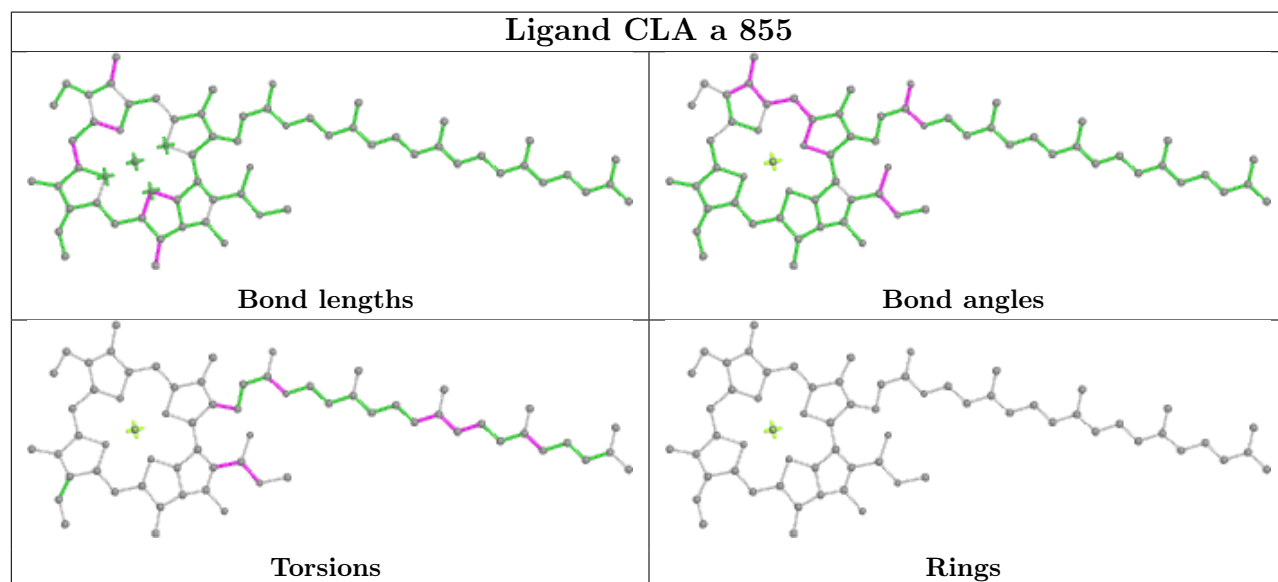
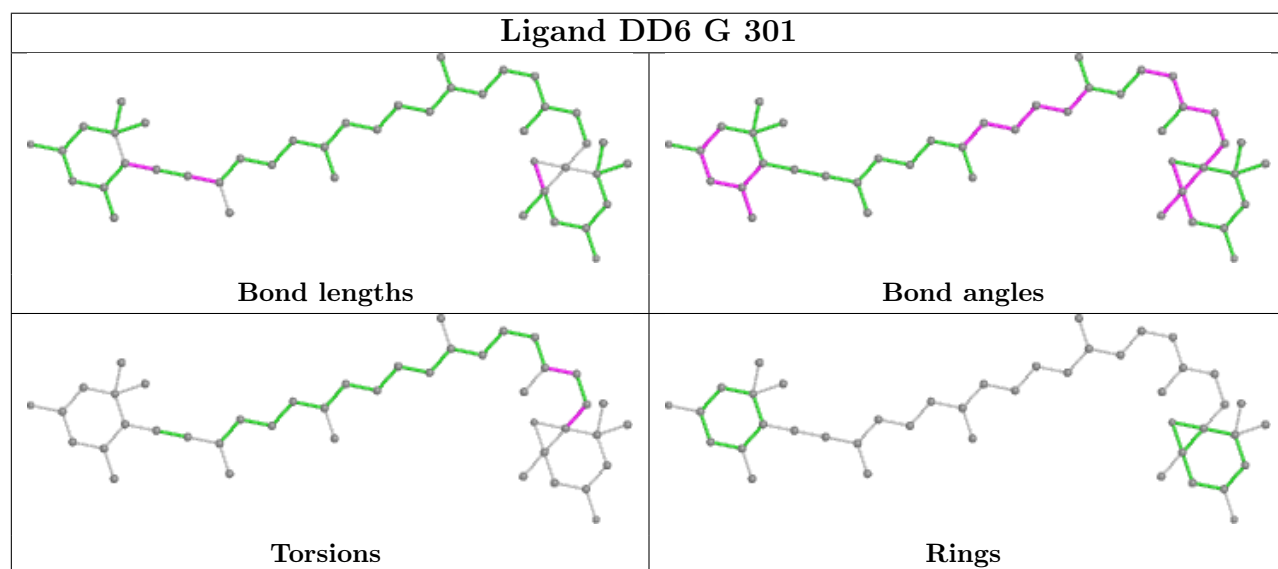
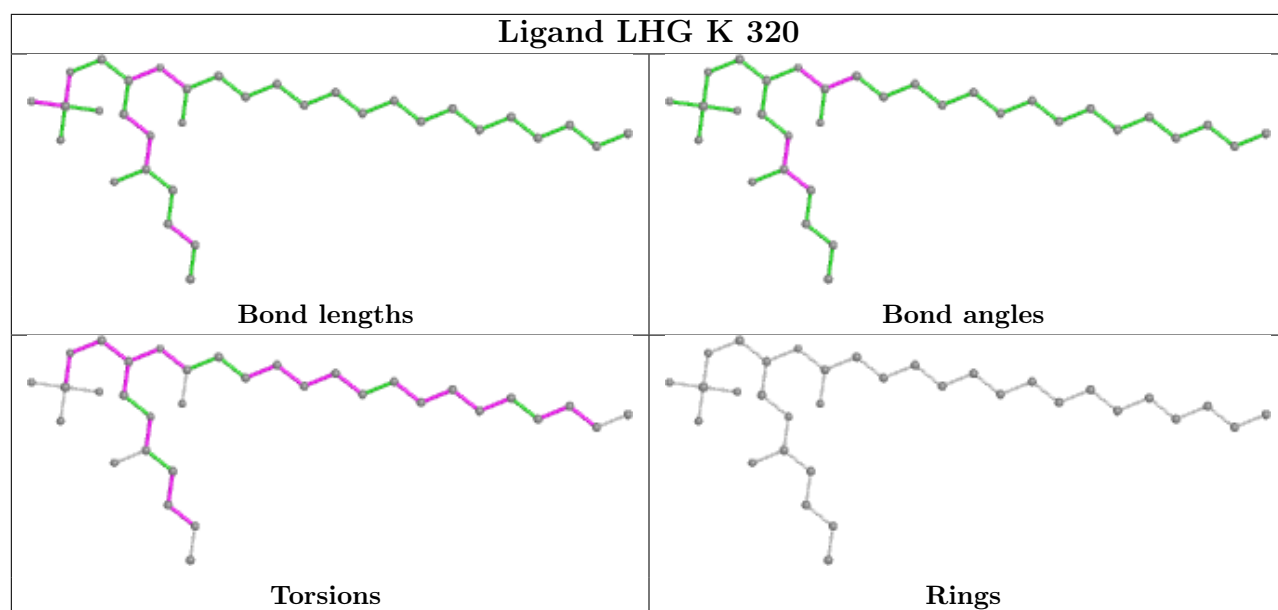
Mol	Chain	Res	Type	Atoms
30	K	307	A86	C31-C32-C33-C34-C35-C36

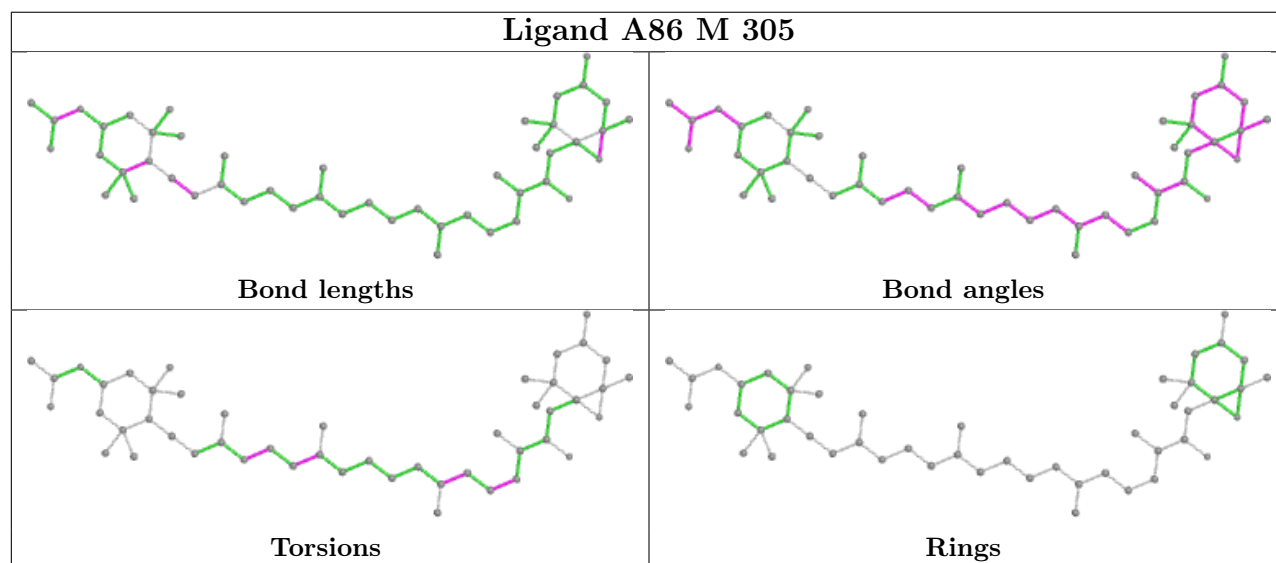
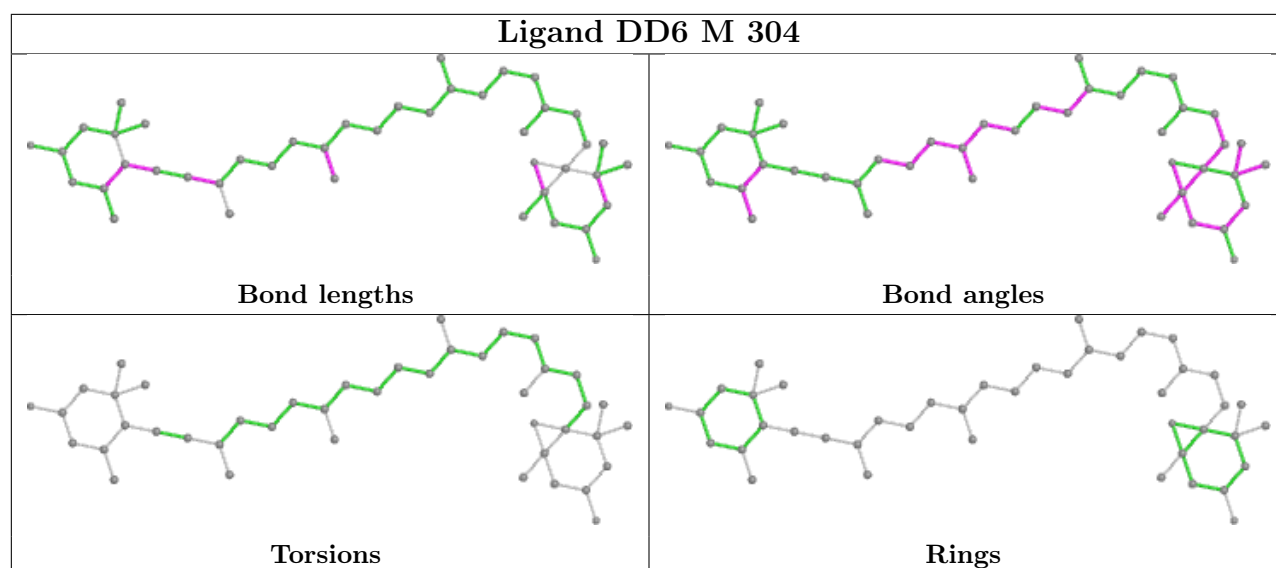
No monomer is involved in short contacts.

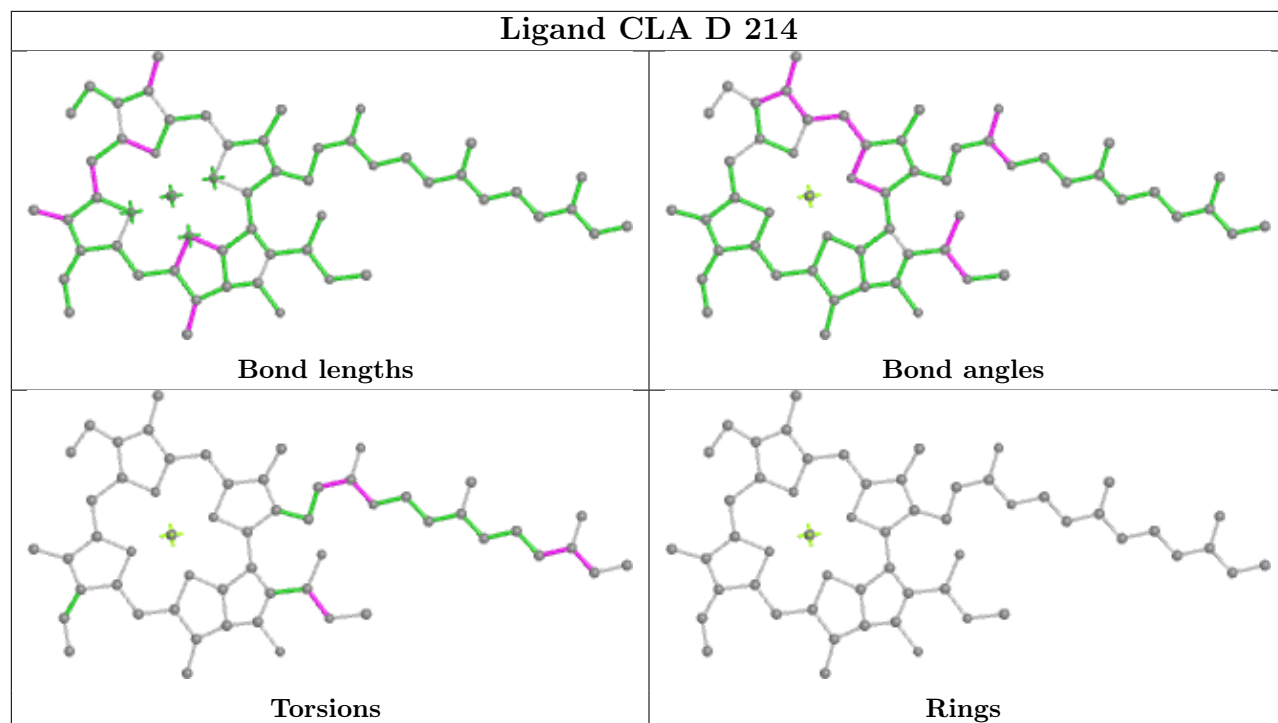
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

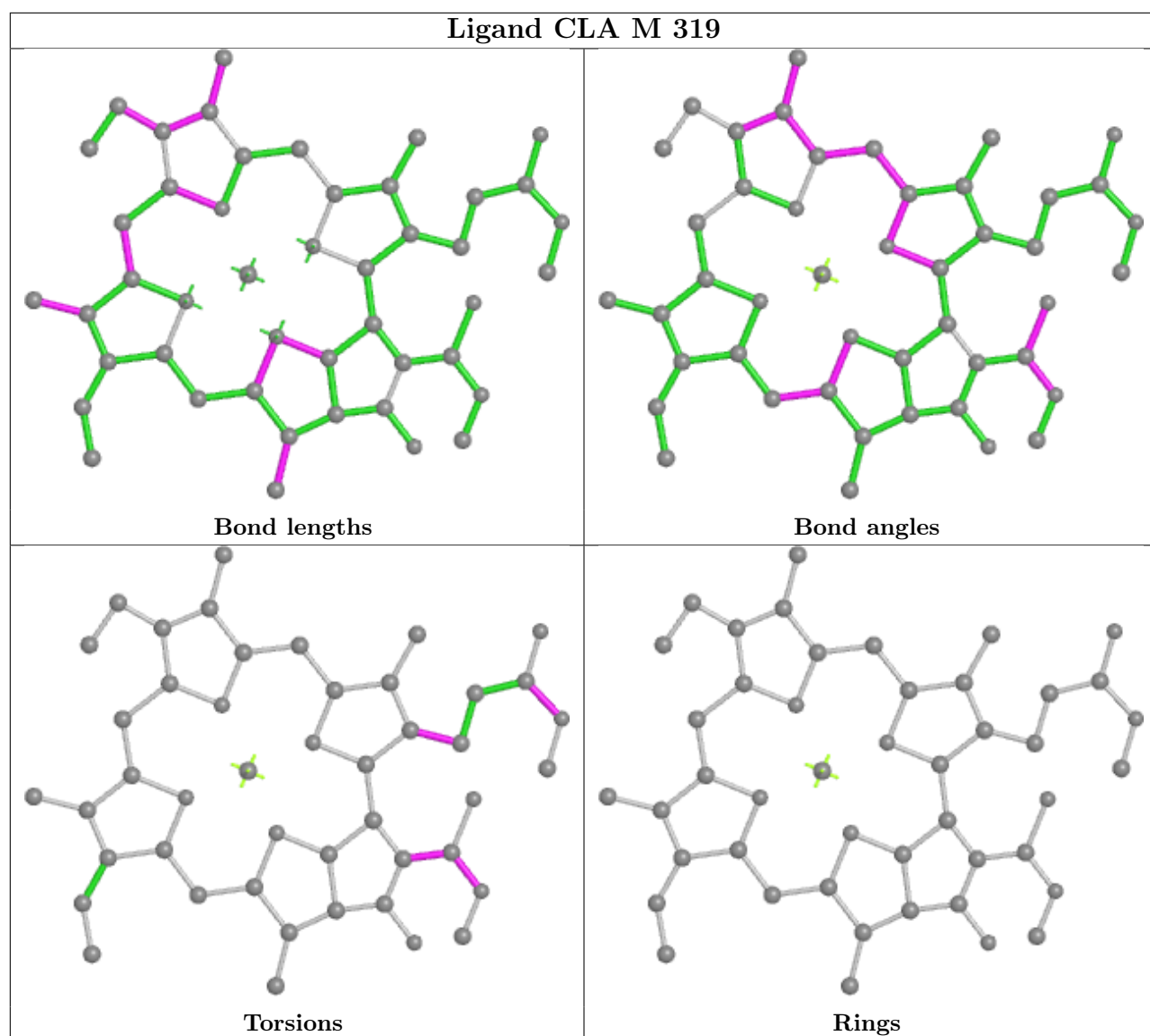


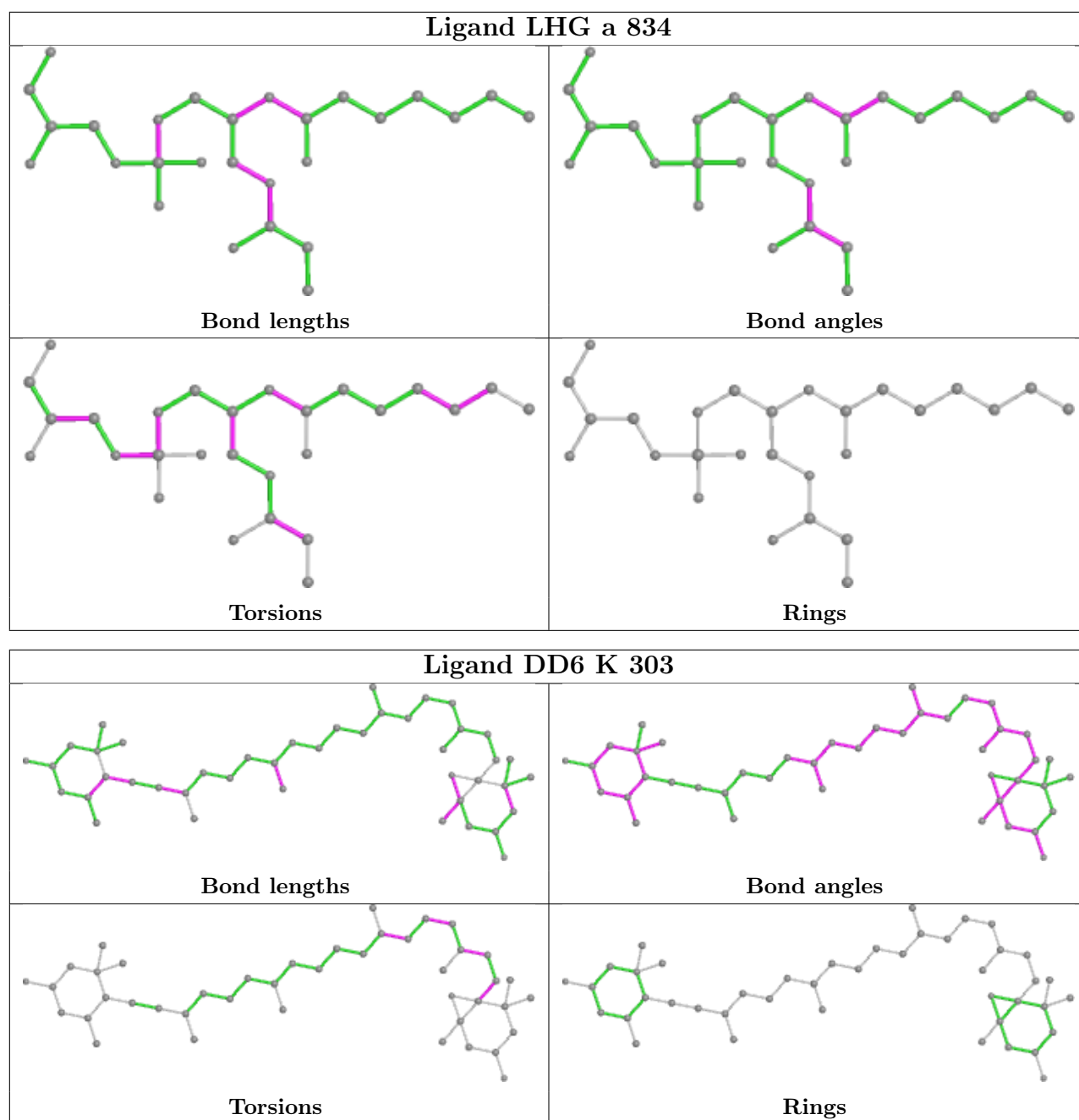




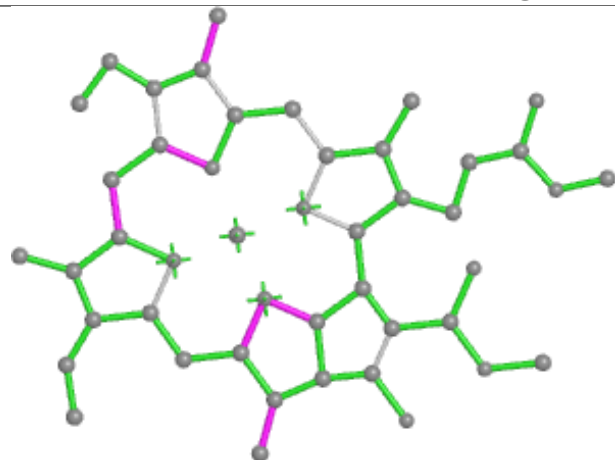




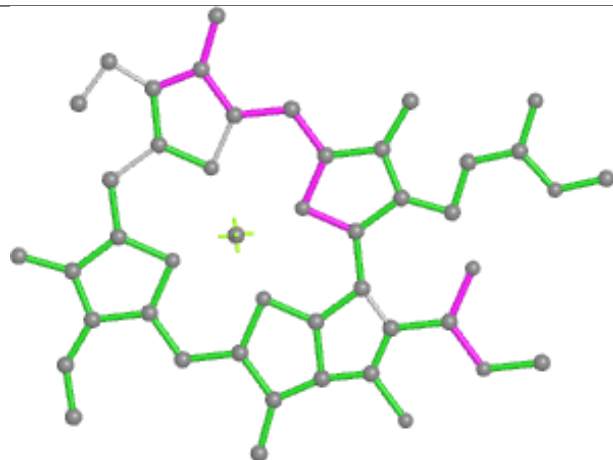




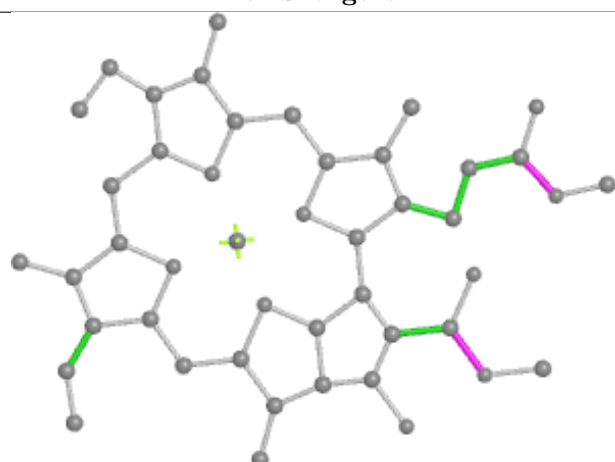
Ligand CLA B 310



Bond lengths



Bond angles

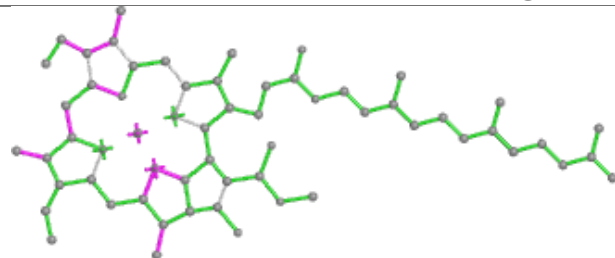


Torsions

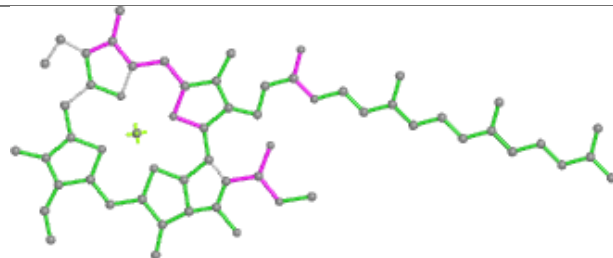


Rings

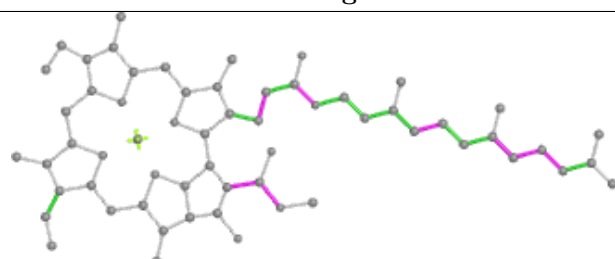
Ligand CLA b 812



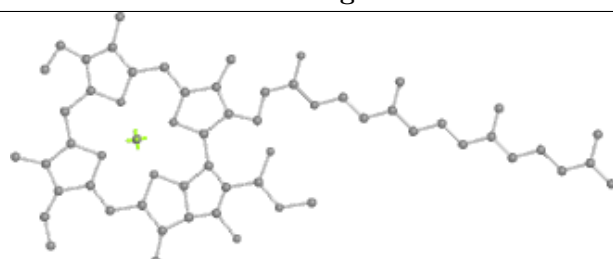
Bond lengths



Bond angles

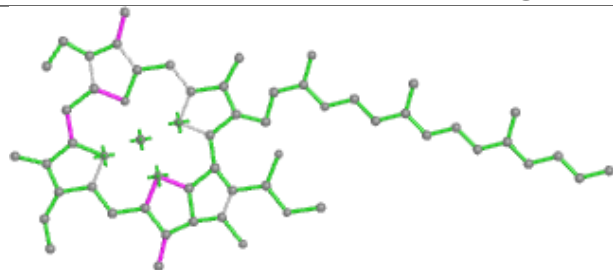


Torsions

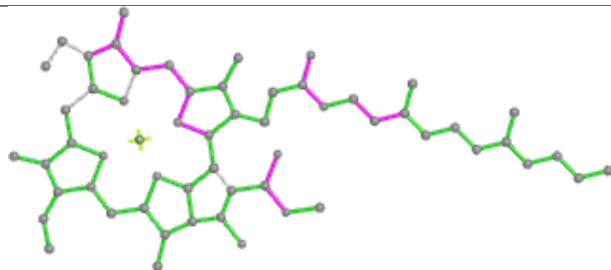


Rings

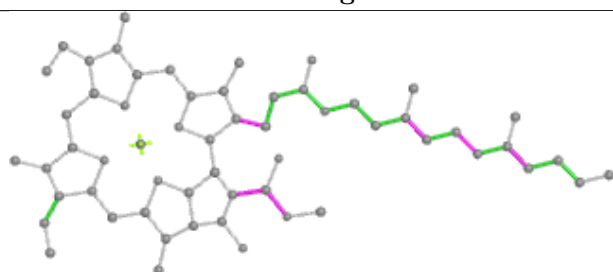
Ligand CLA b 824



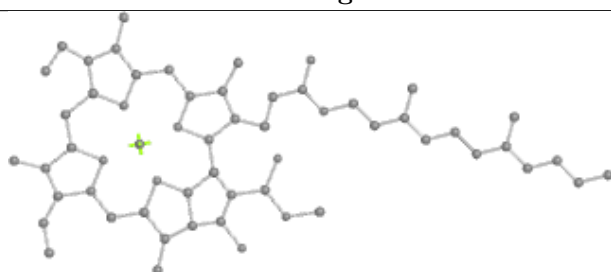
Bond lengths



Bond angles

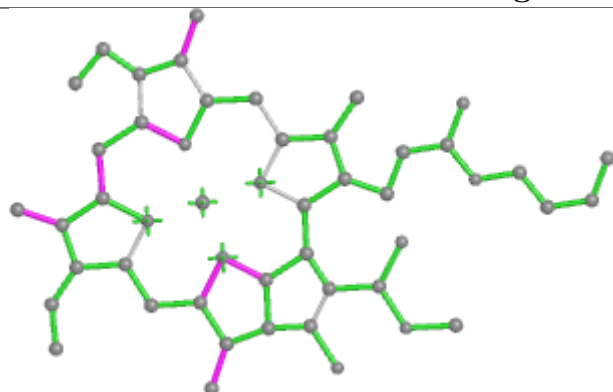


Torsions

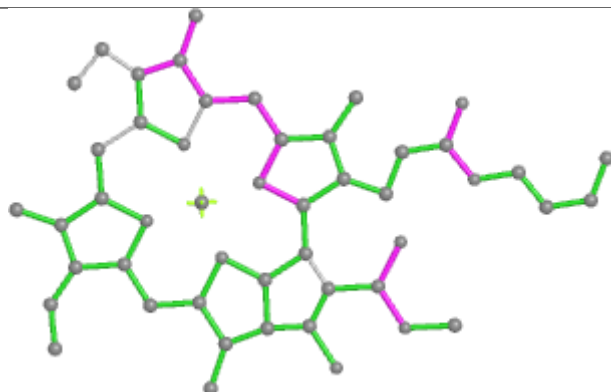


Rings

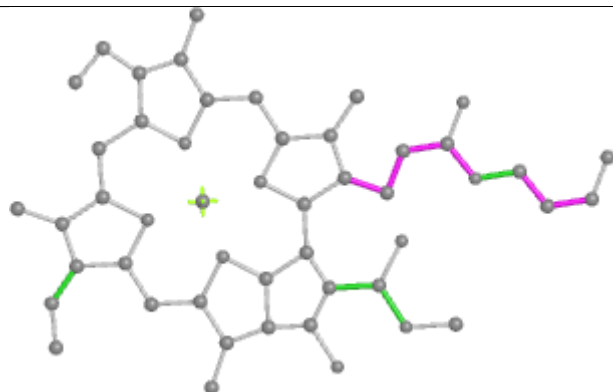
Ligand CLA D 209



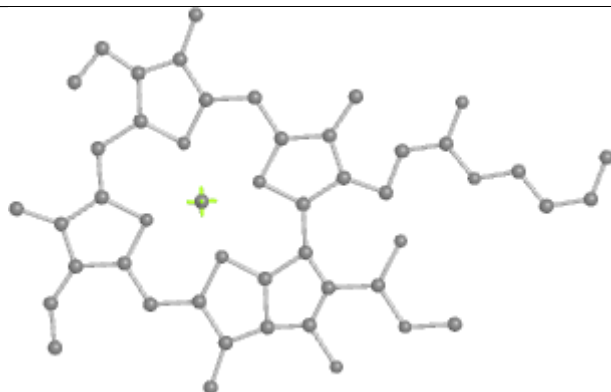
Bond lengths



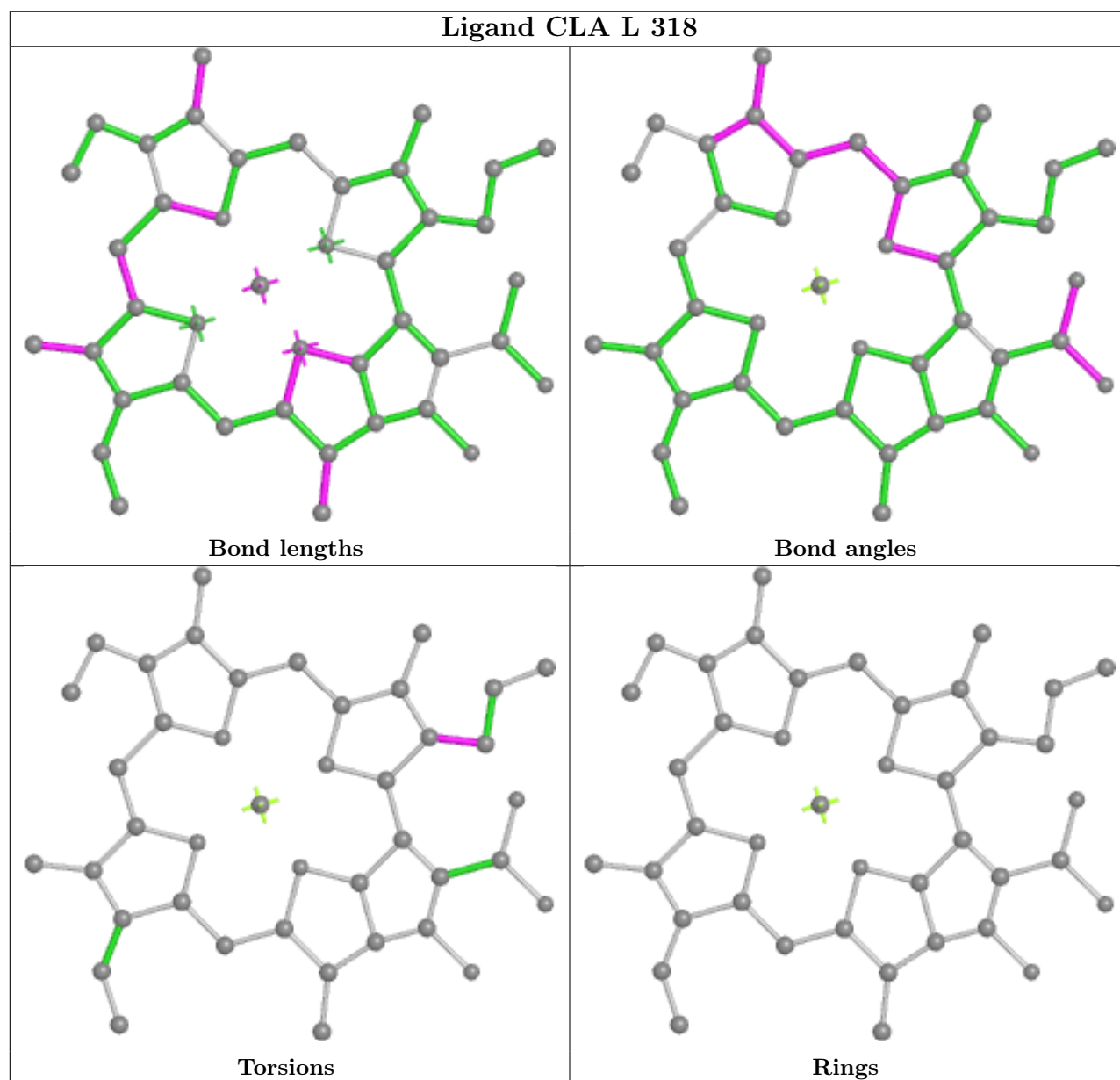
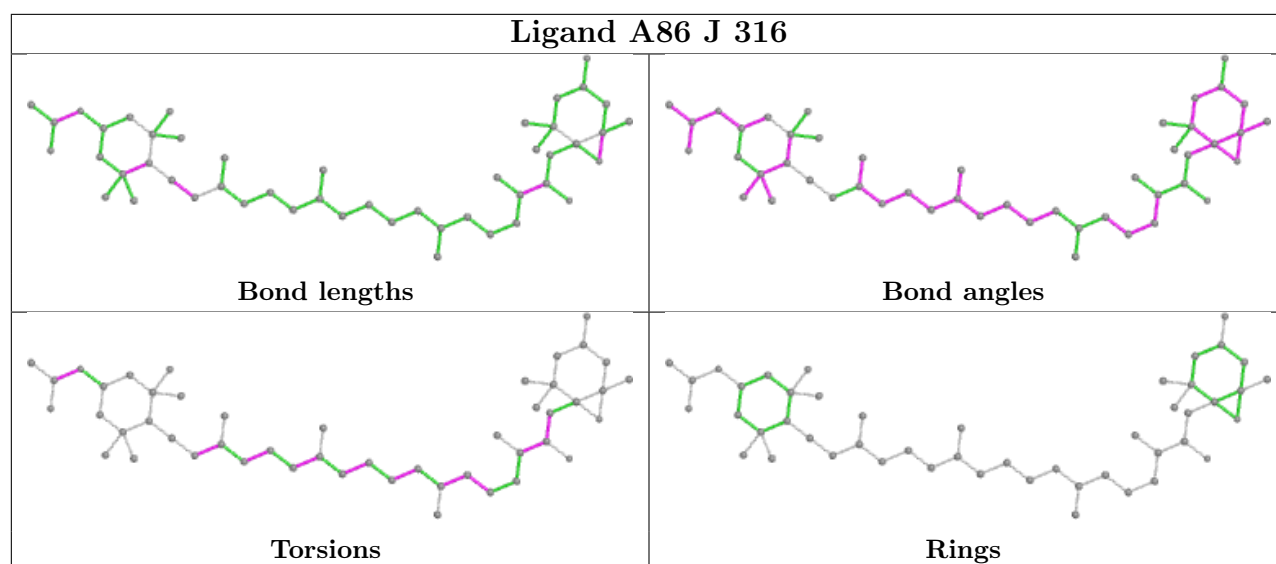
Bond angles

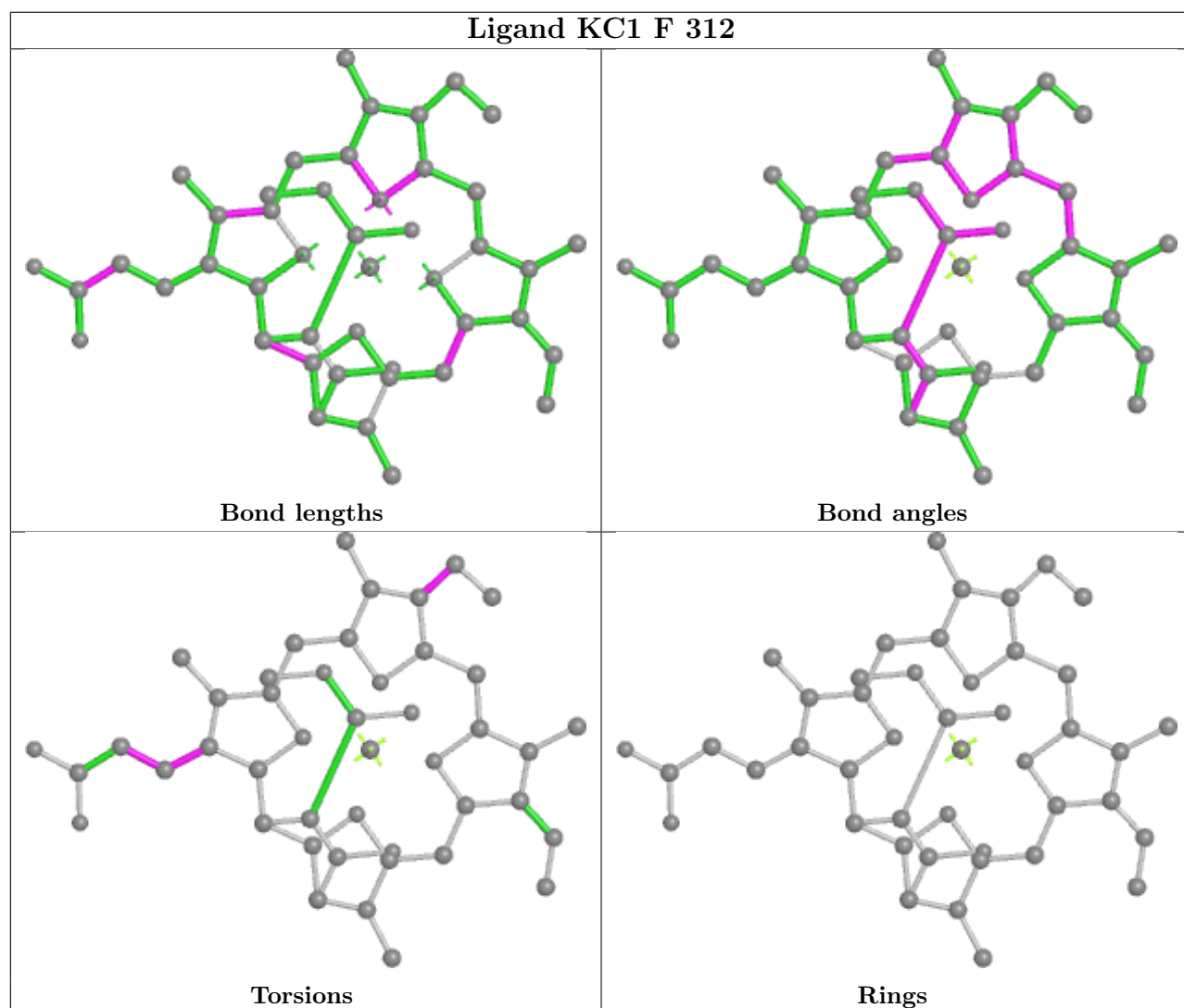
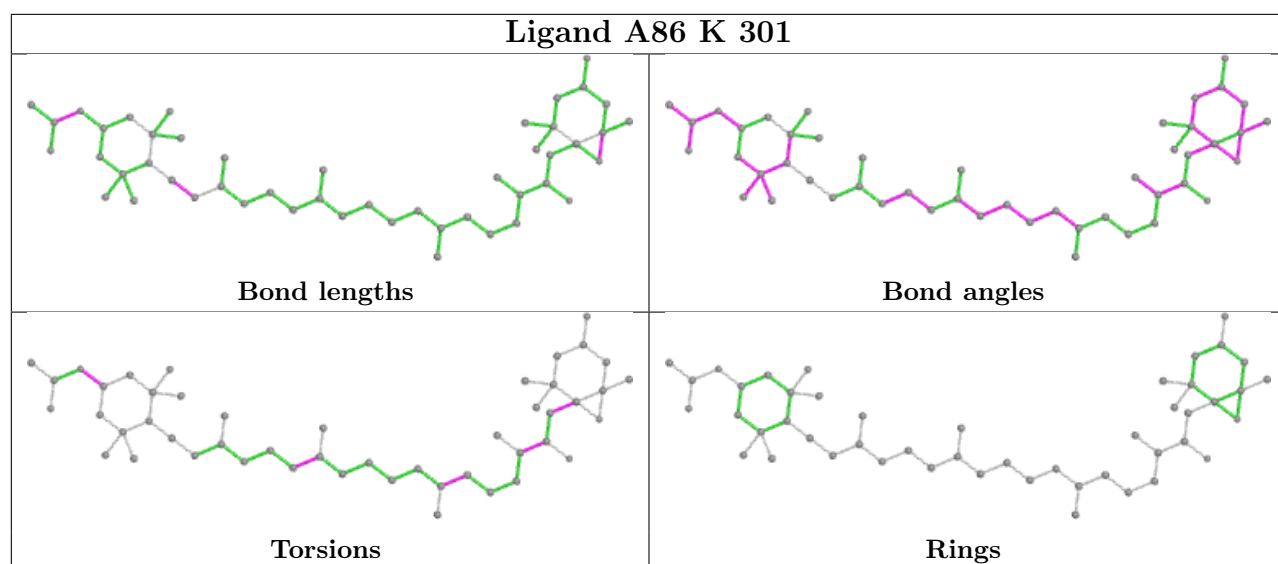


Torsions

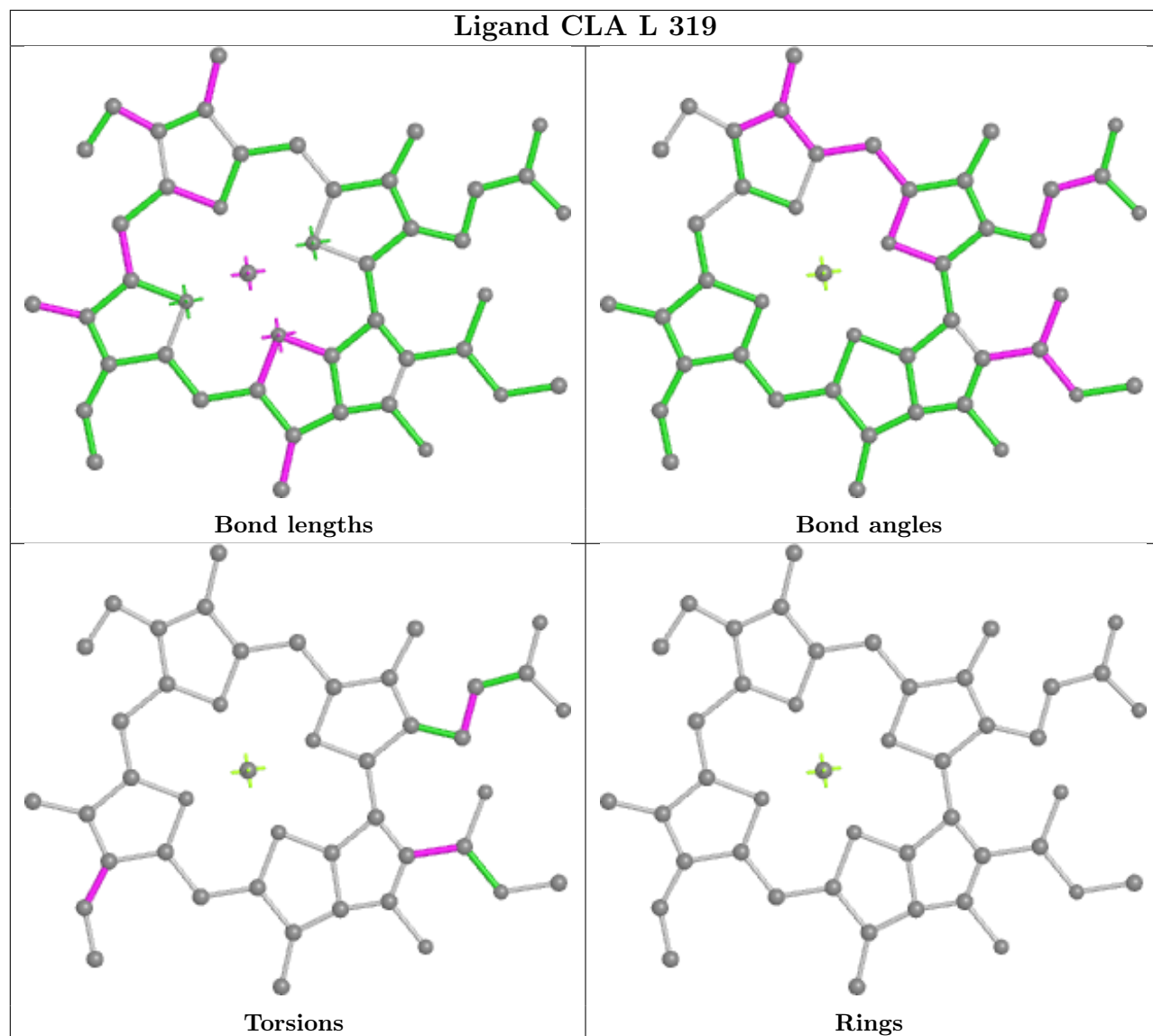


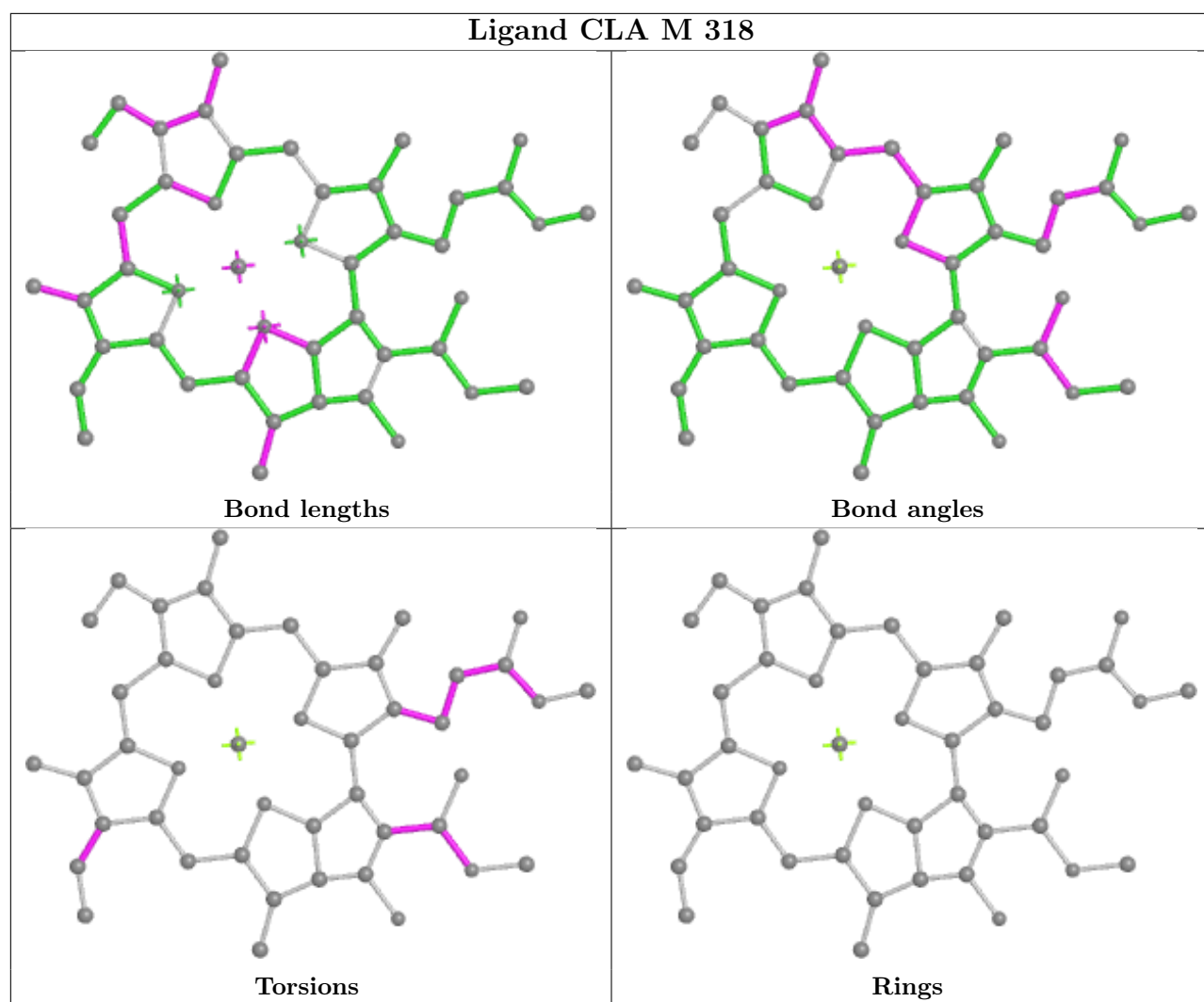
Rings

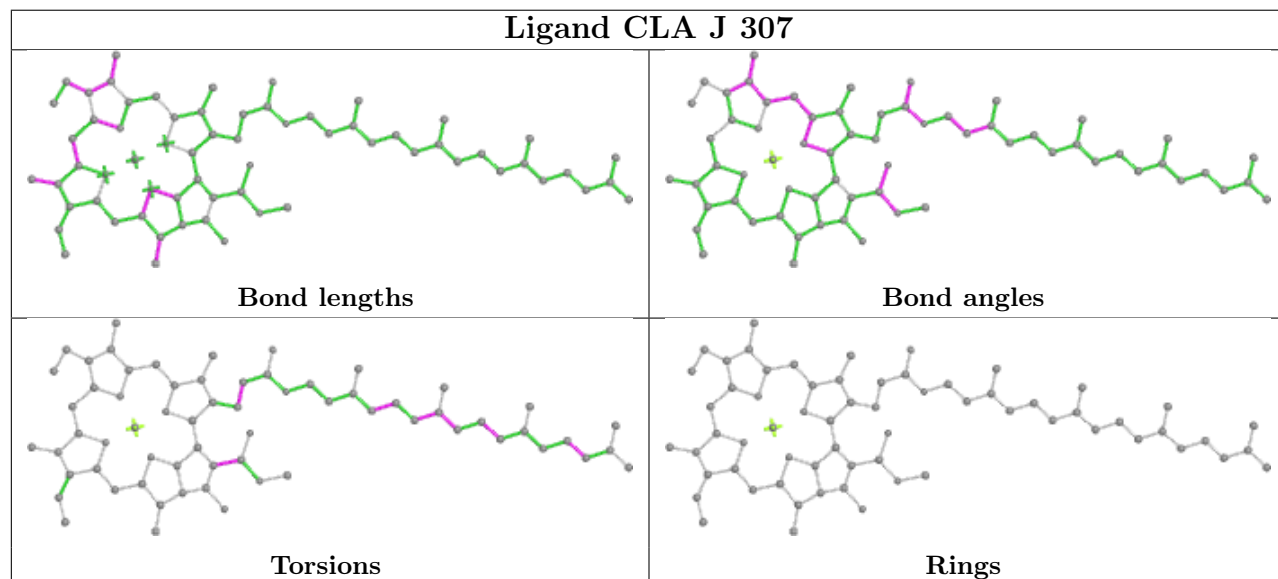
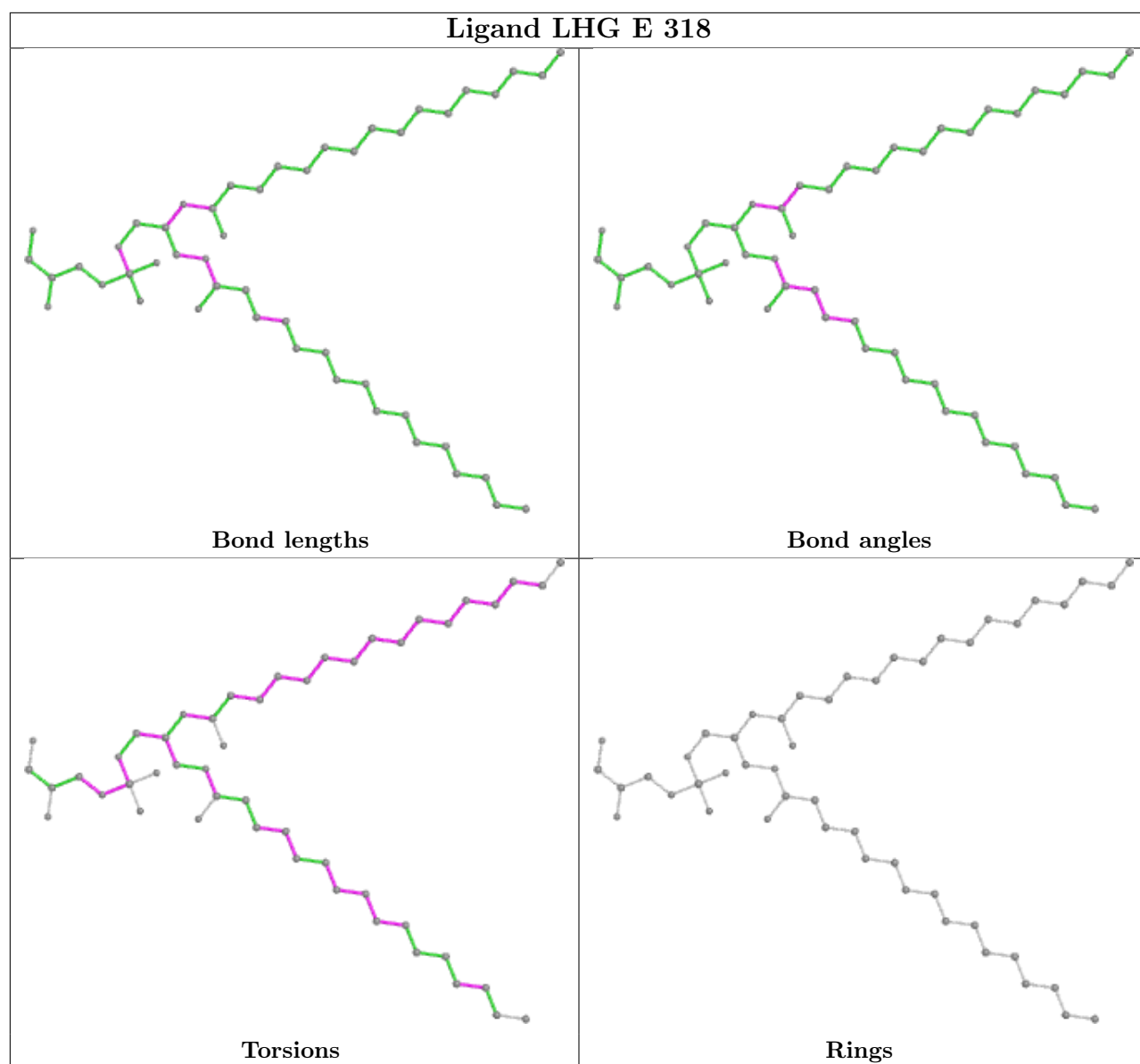


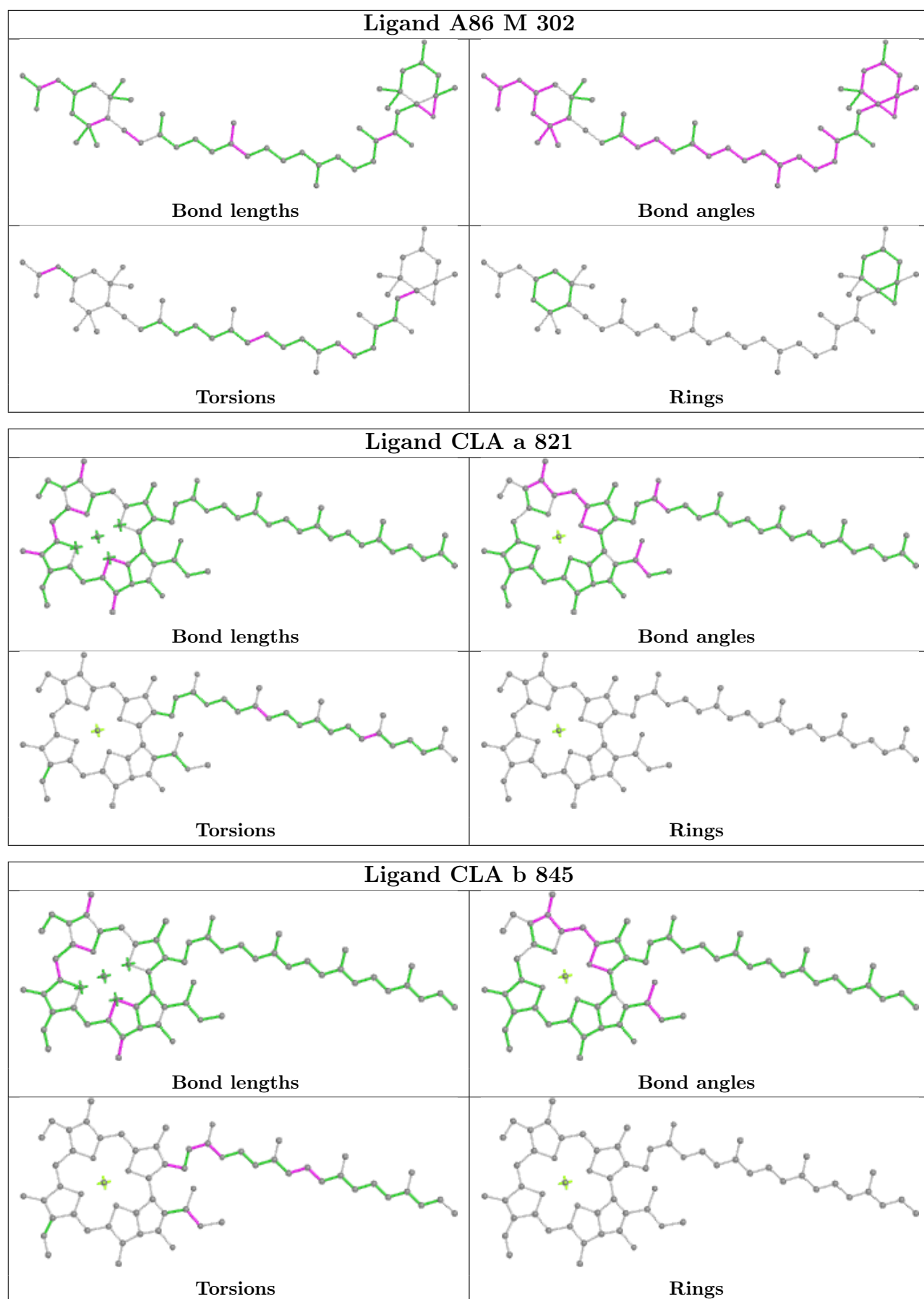


Ligand CLA L 319

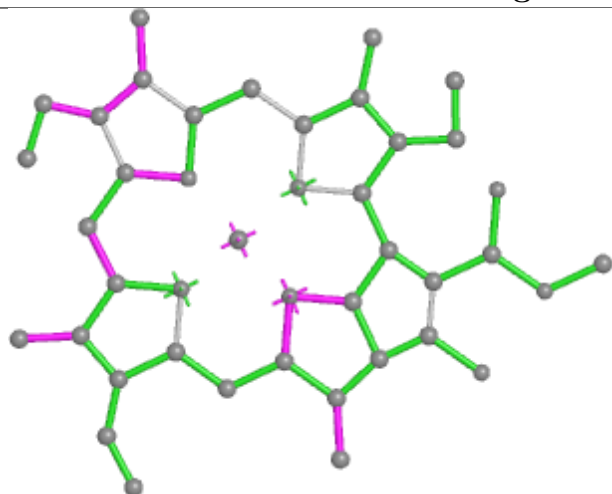




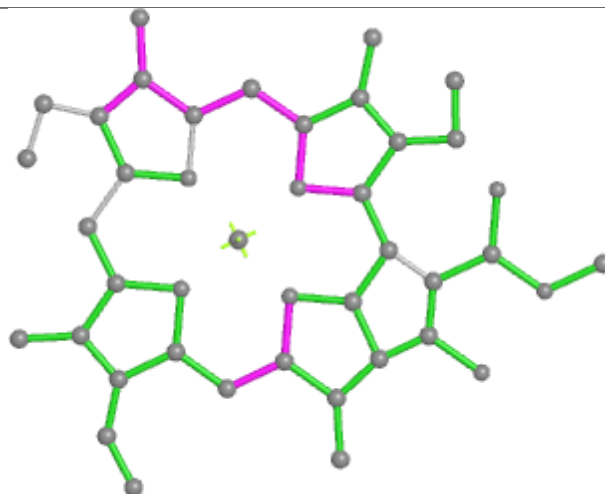




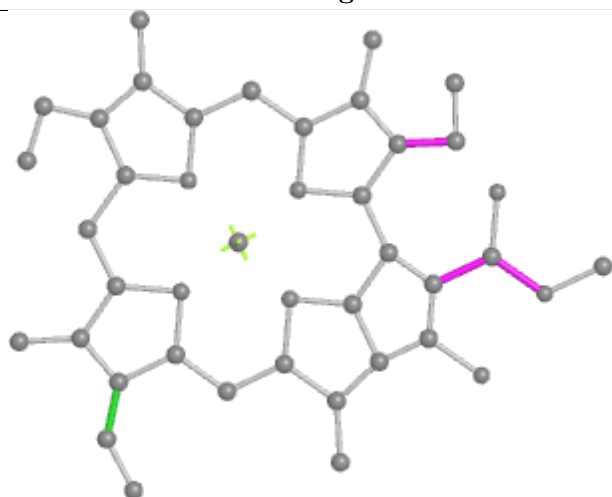
Ligand CLA C 318



Bond lengths



Bond angles

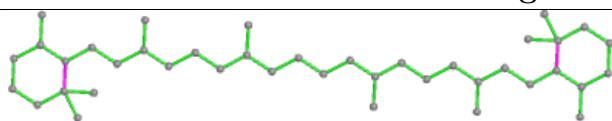


Torsions

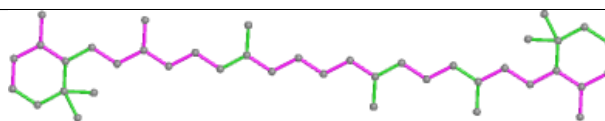


Rings

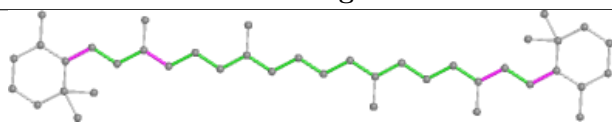
Ligand BCR 1 202



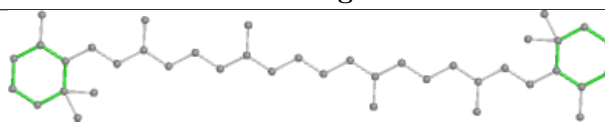
Bond lengths



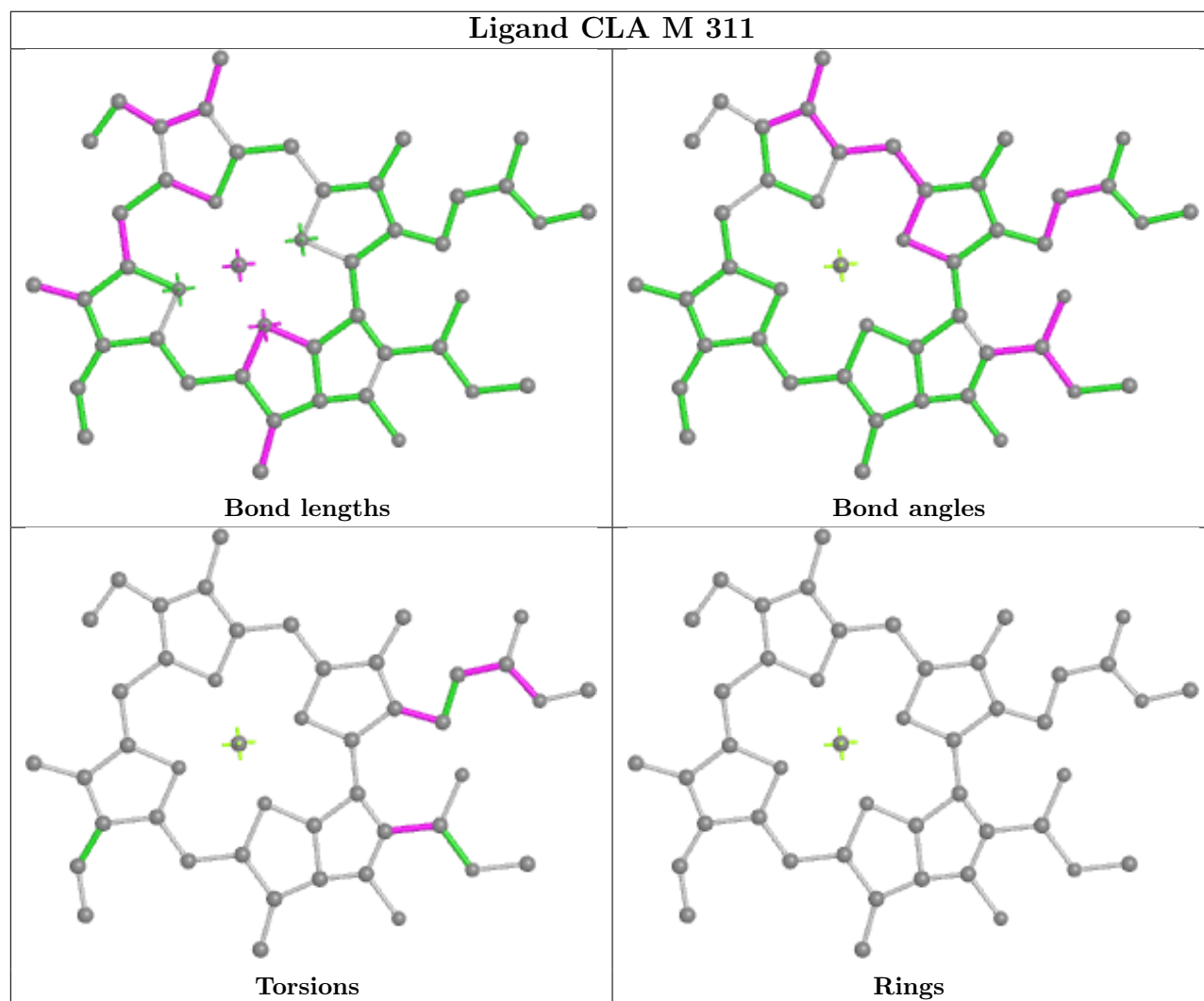
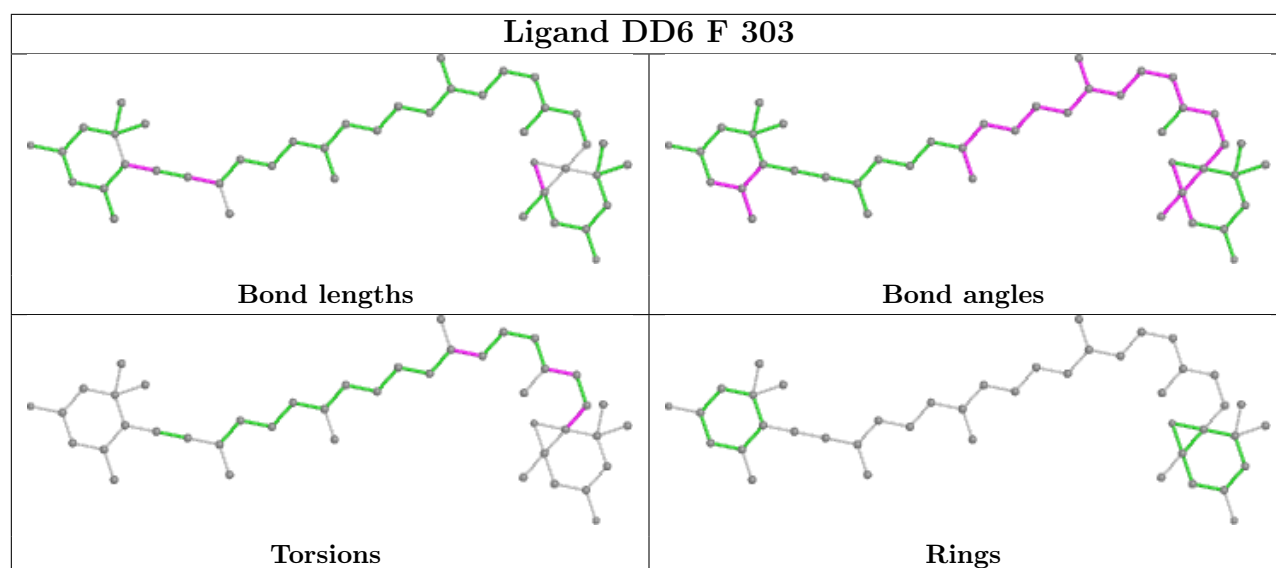
Bond angles

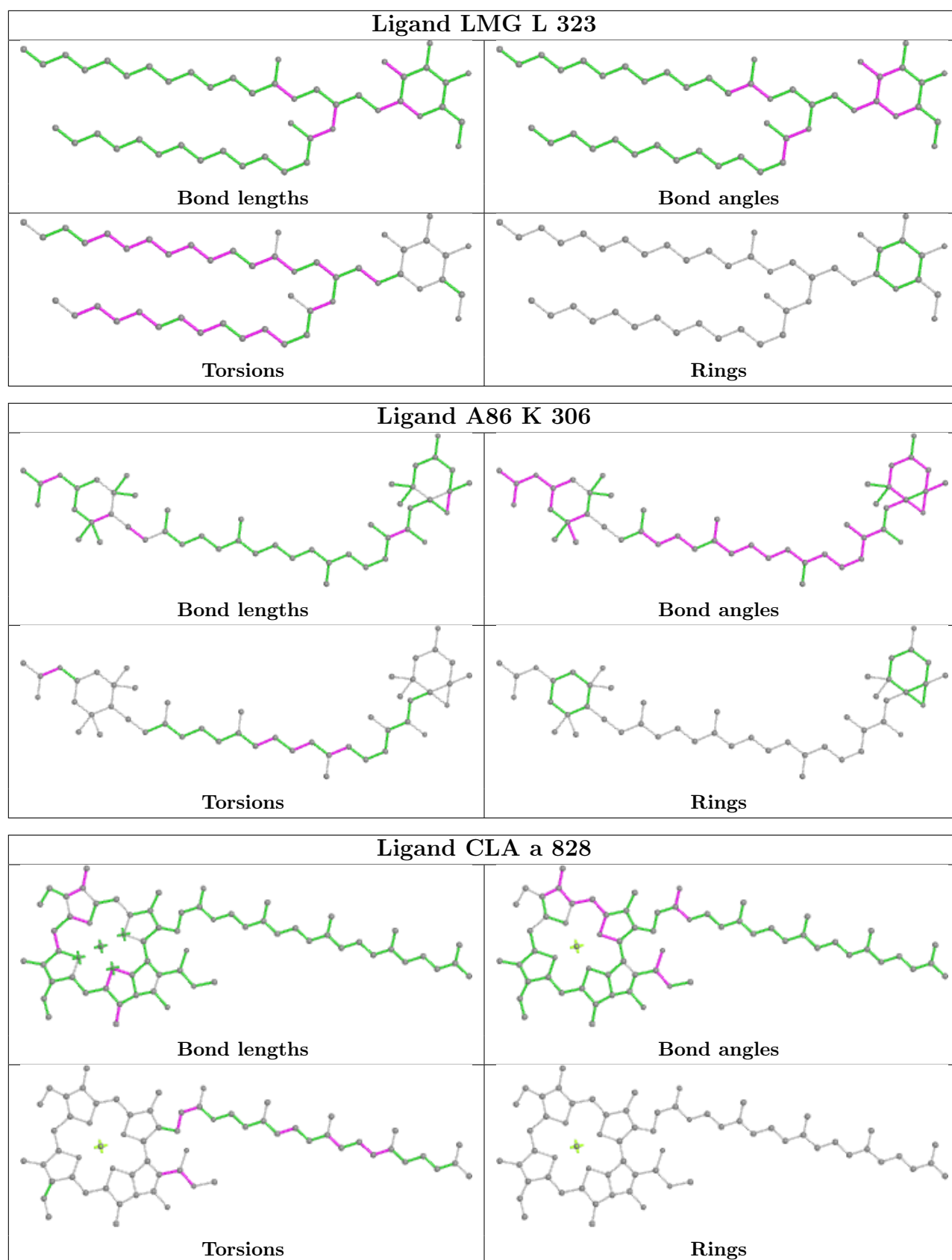


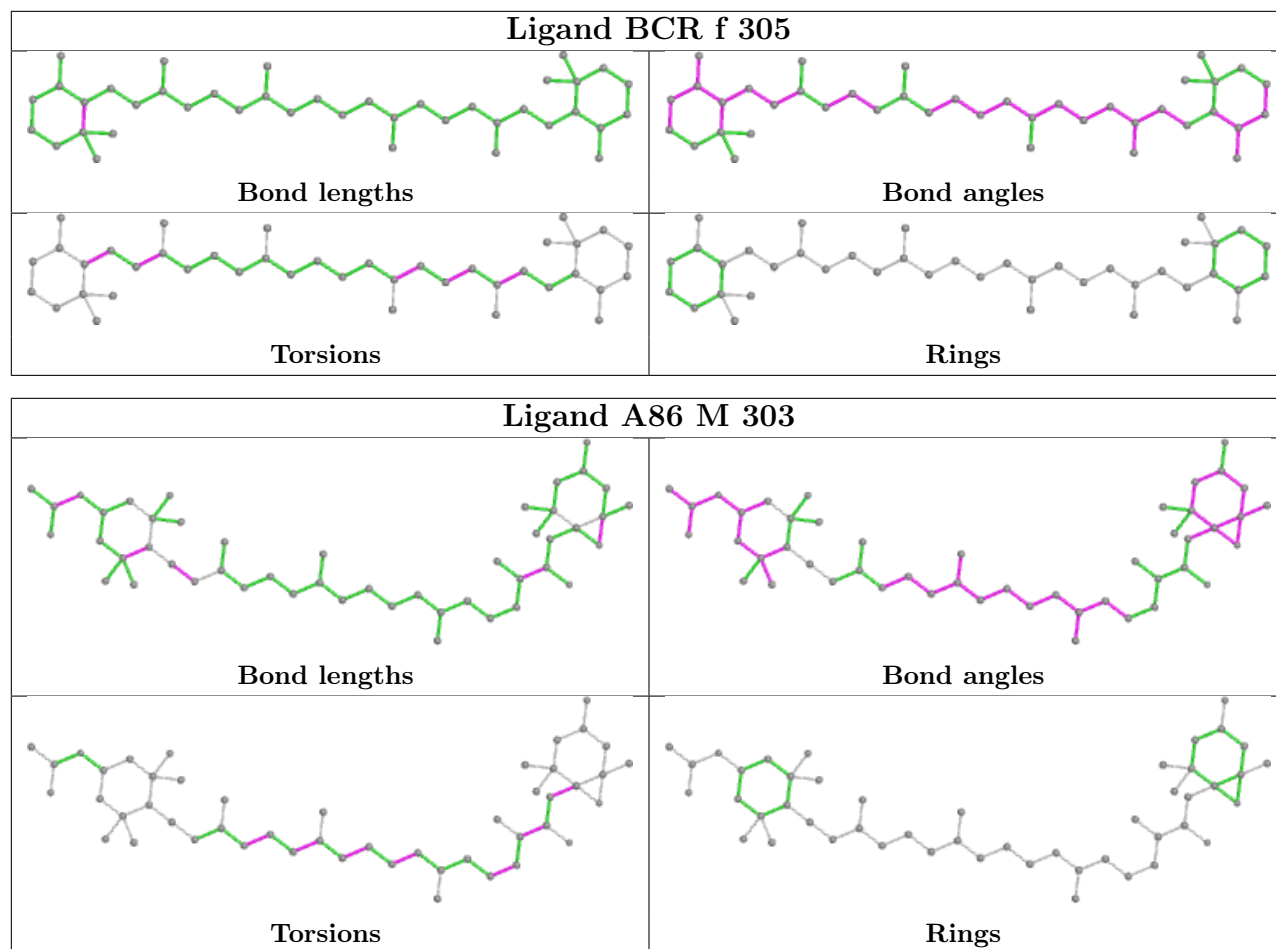
Torsions



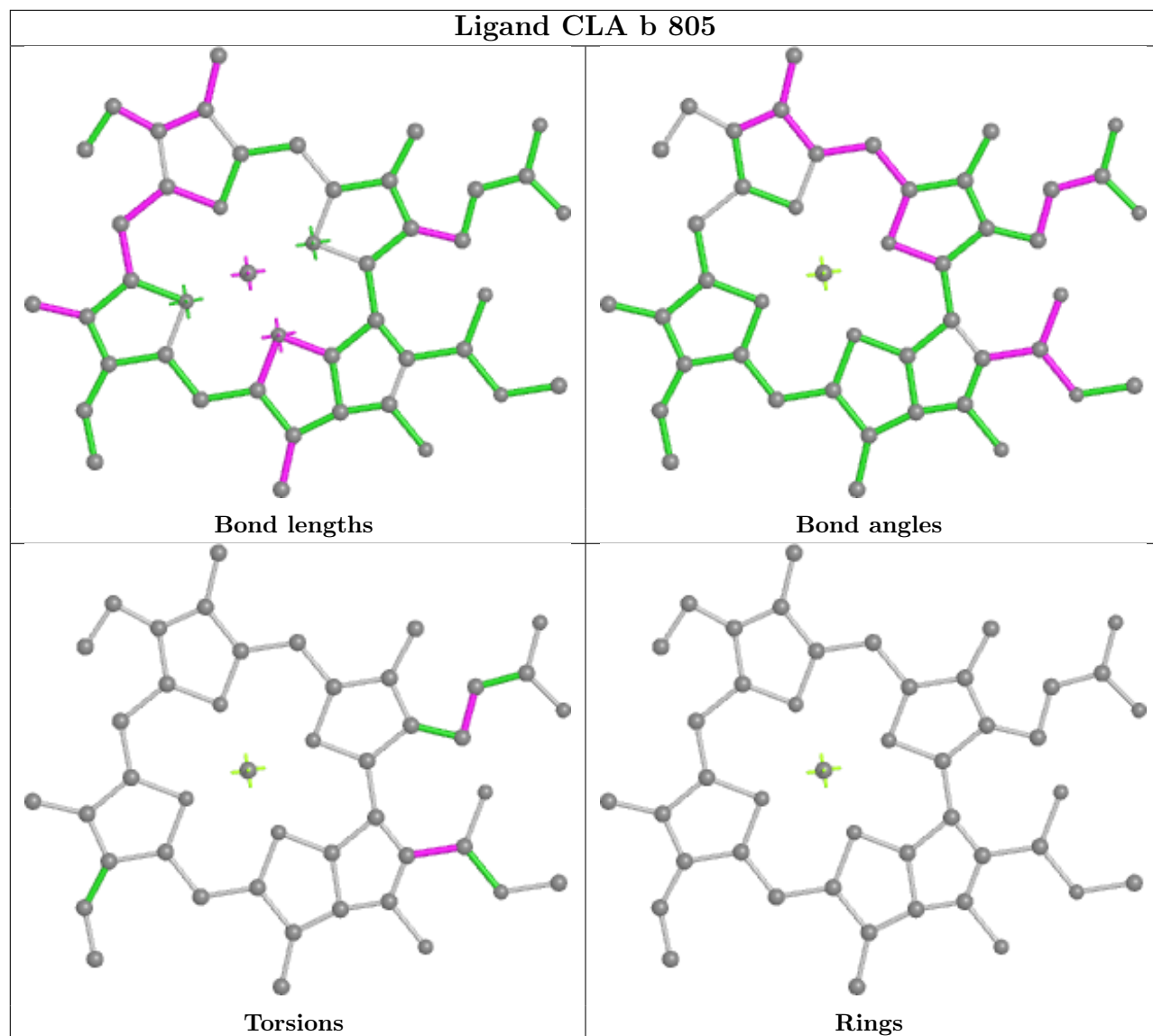
Rings



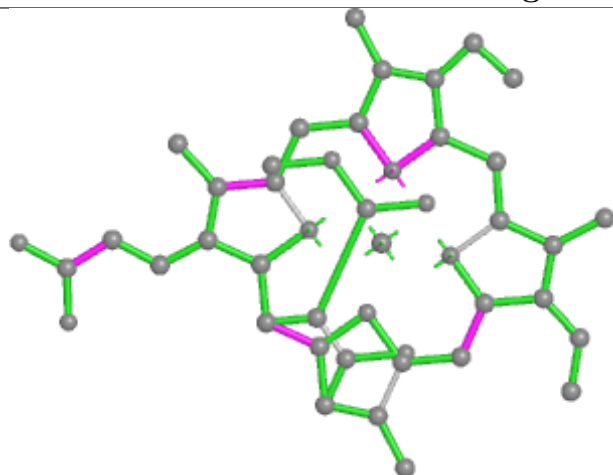




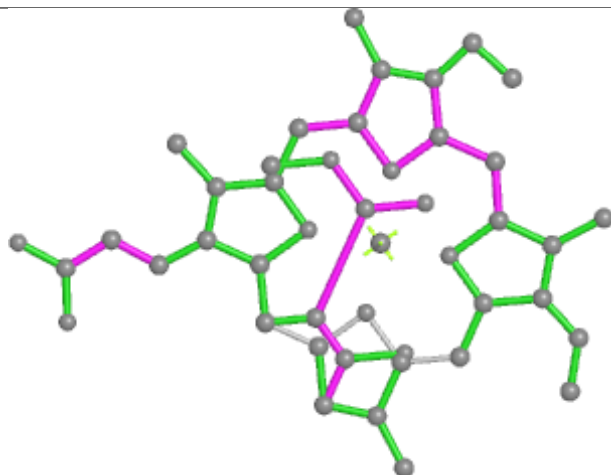
Ligand CLA b 805



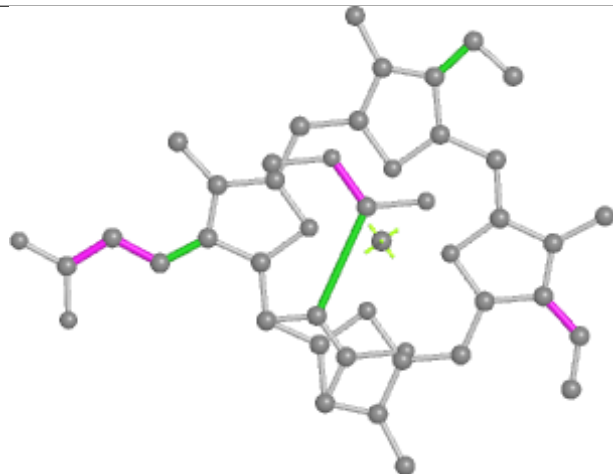
Ligand KC1 I 312



Bond lengths



Bond angles

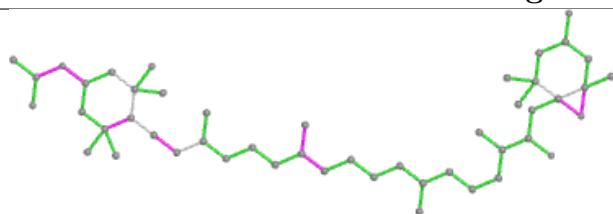


Torsions

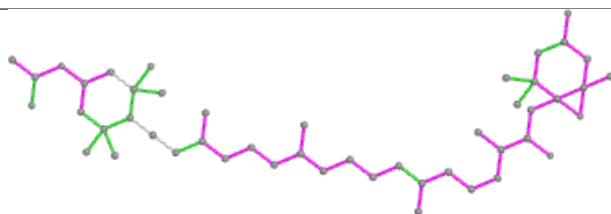


Rings

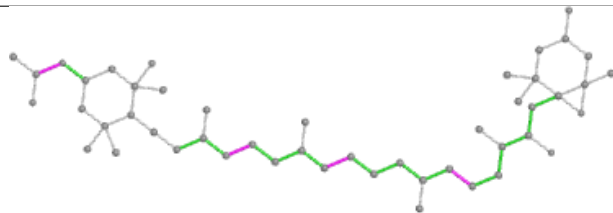
Ligand A86 r 202



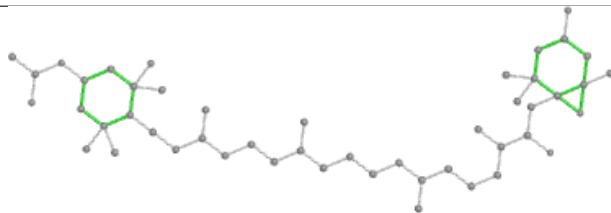
Bond lengths



Bond angles

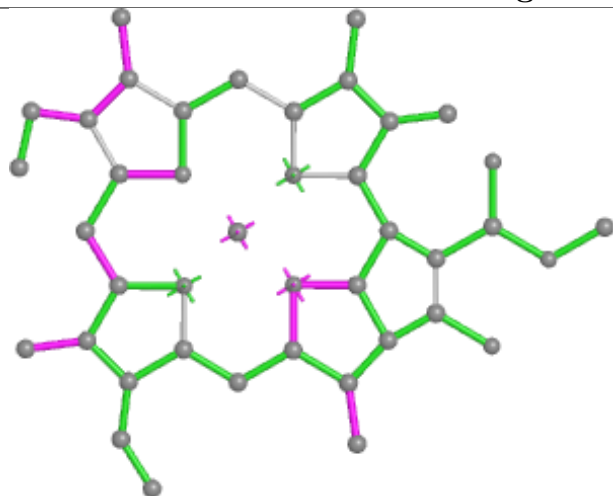


Torsions

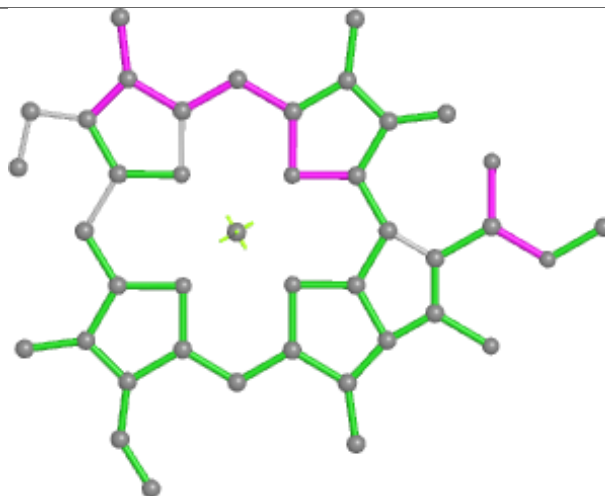


Rings

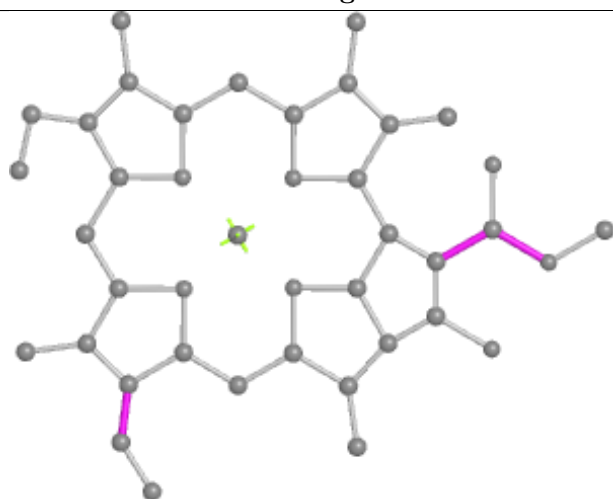
Ligand CLA L 315



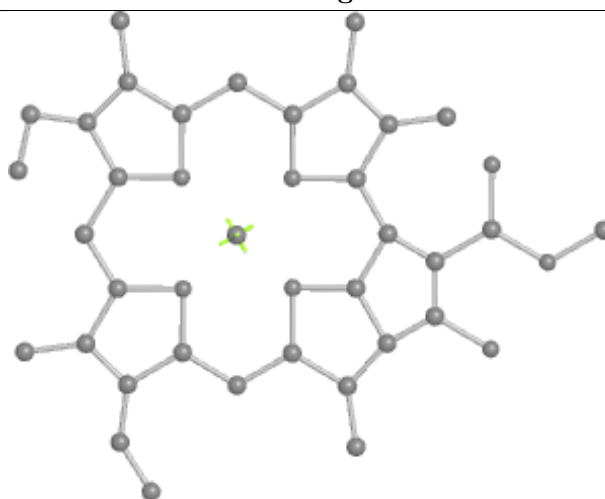
Bond lengths



Bond angles

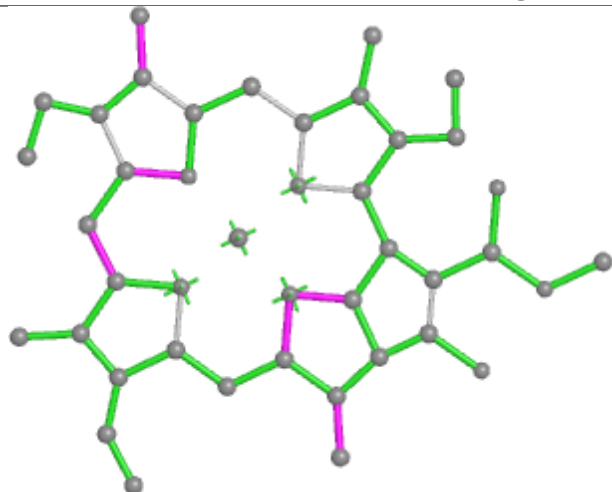


Torsions

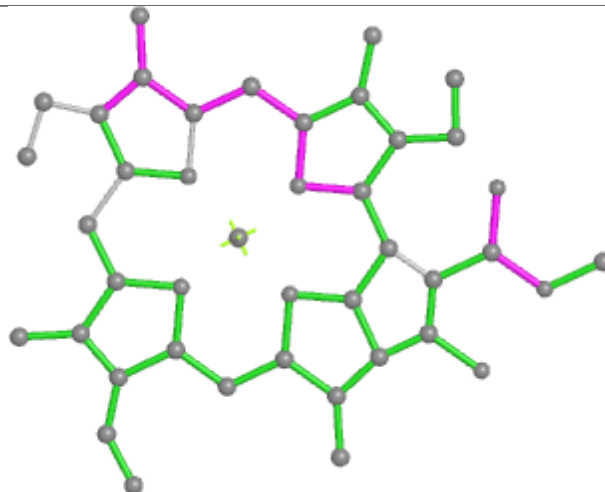


Rings

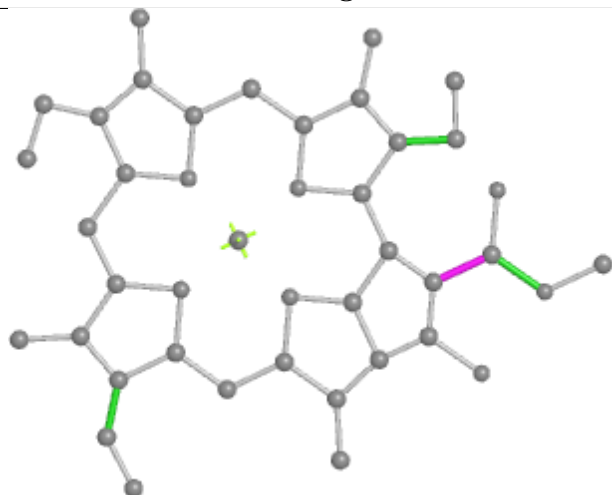
Ligand CLA D 212



Bond lengths



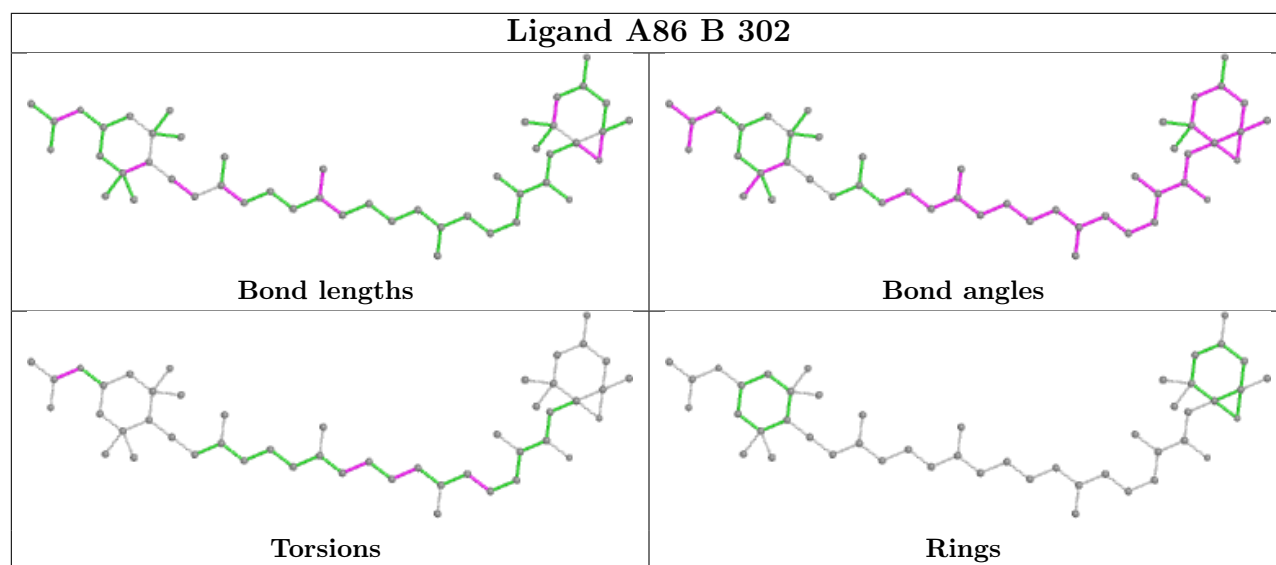
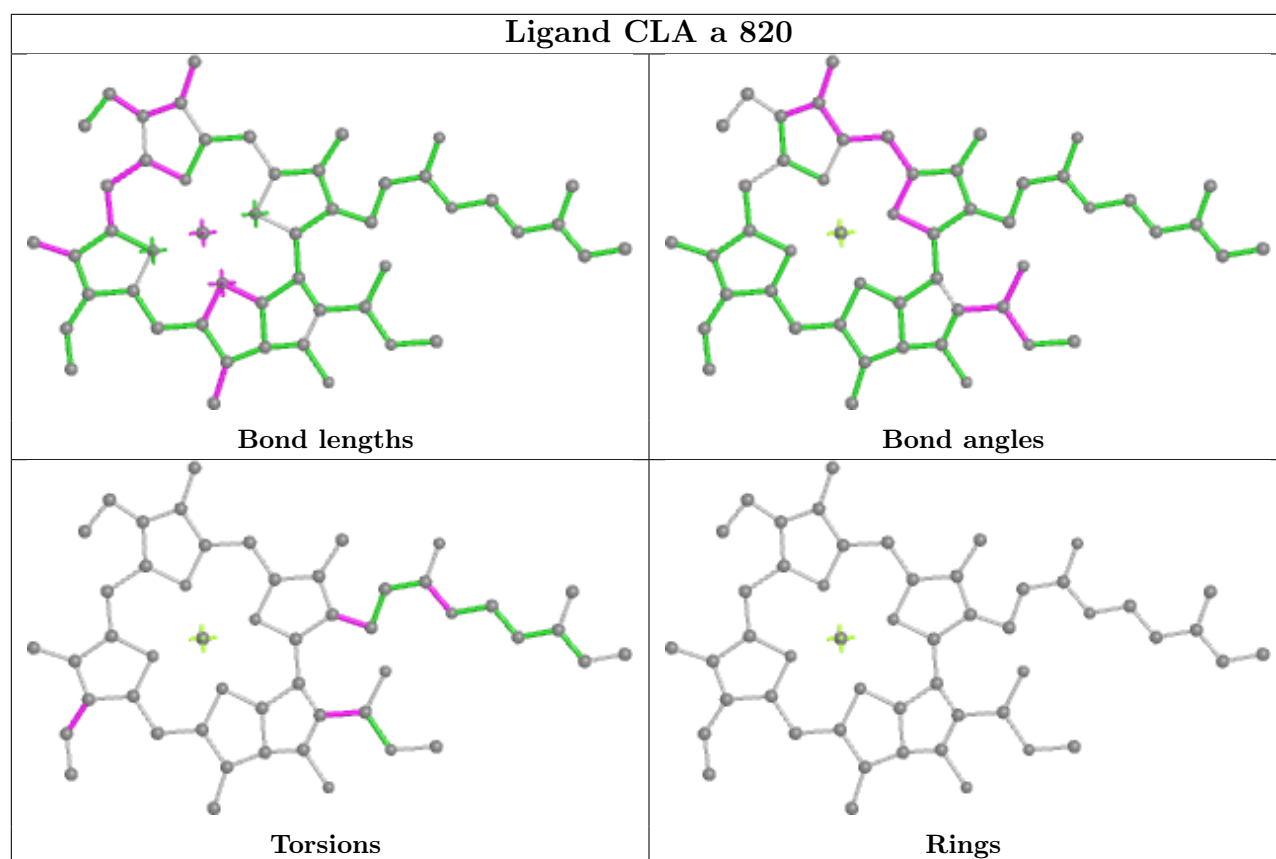
Bond angles



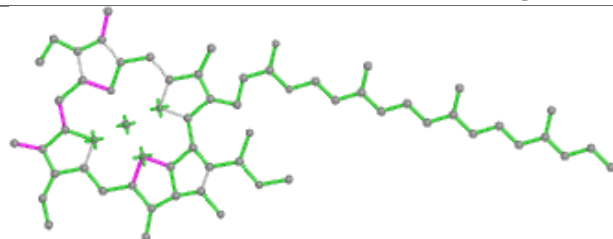
Torsions



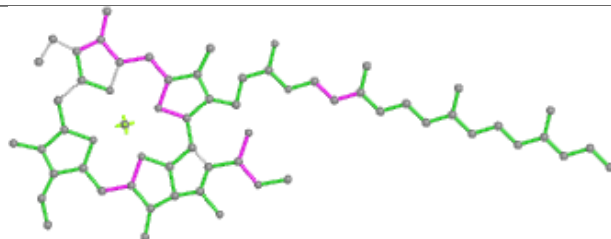
Rings



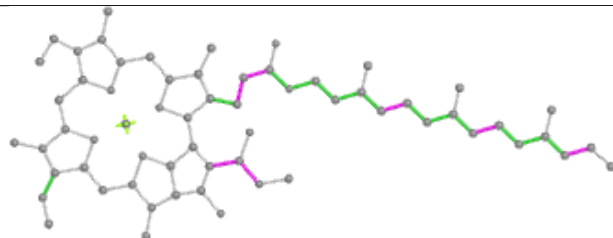
Ligand CLA F 308



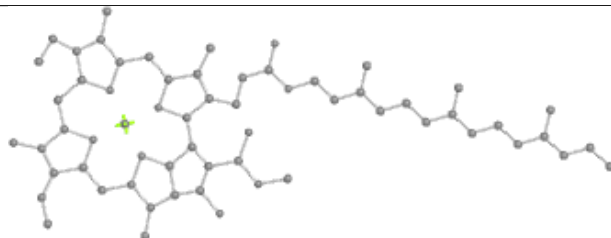
Bond lengths



Bond angles

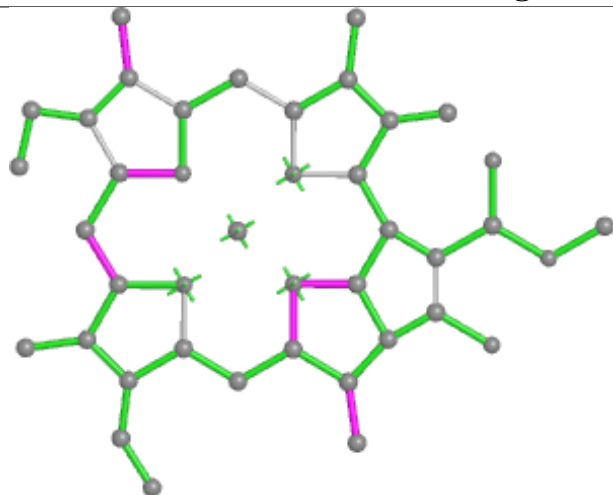


Torsions

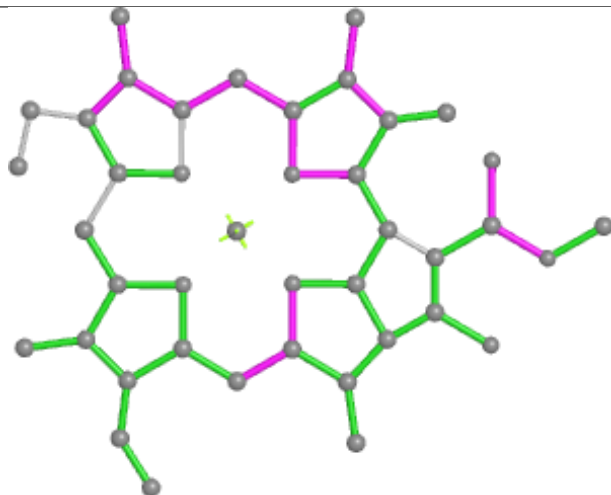


Rings

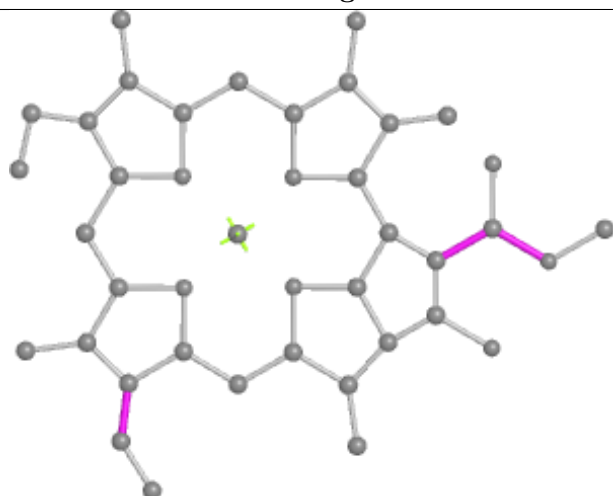
Ligand CLA D 217



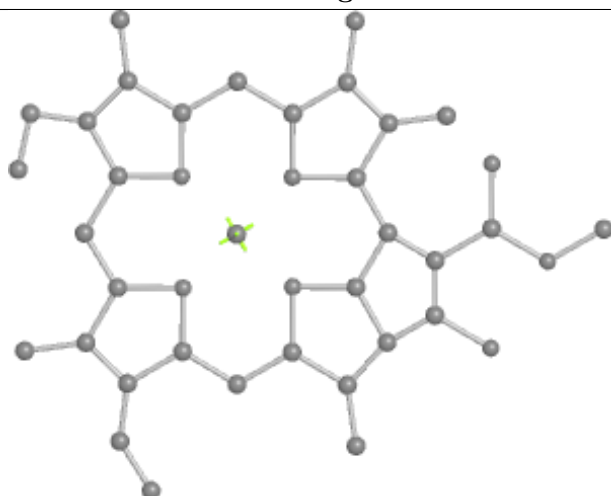
Bond lengths



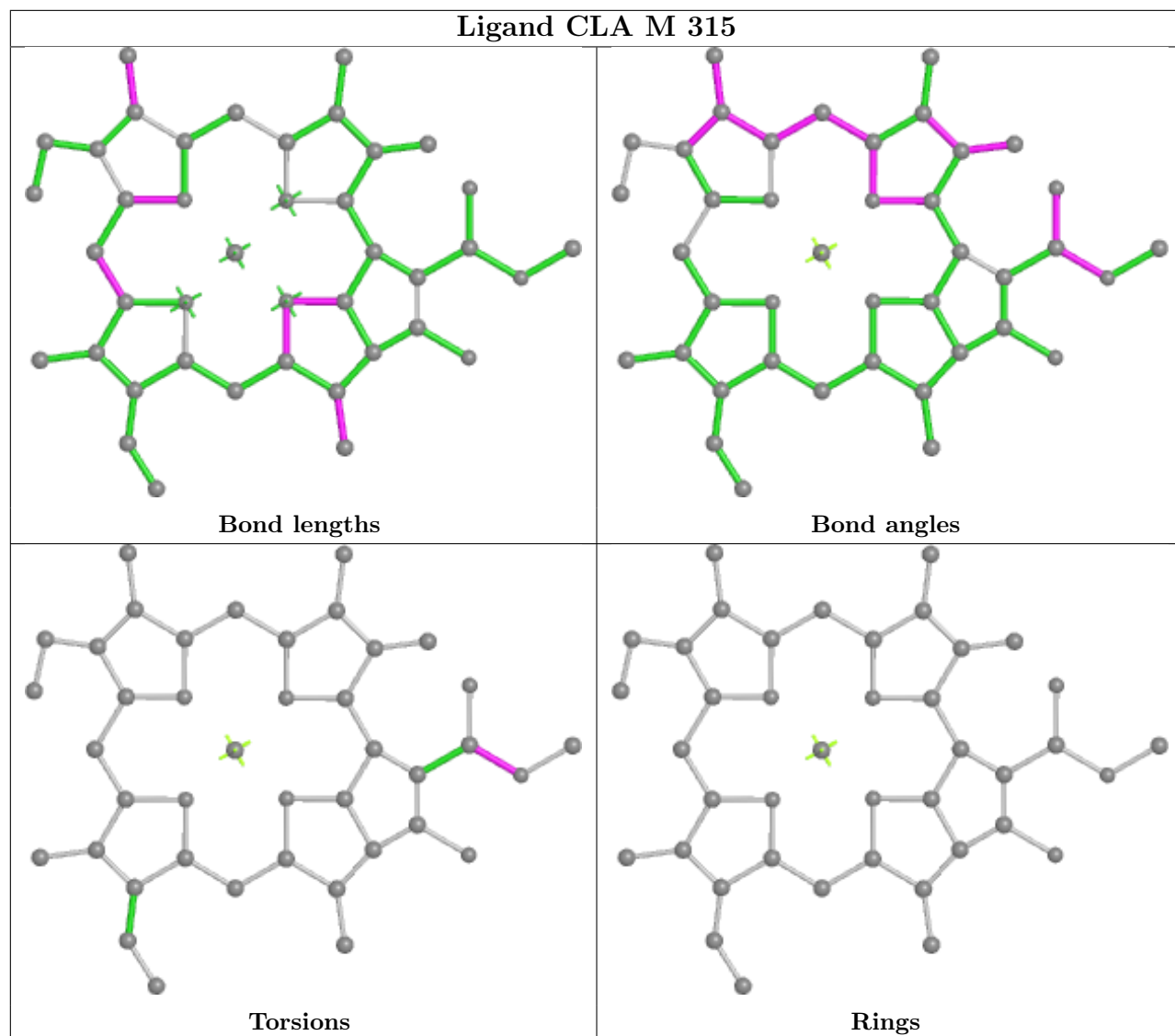
Bond angles

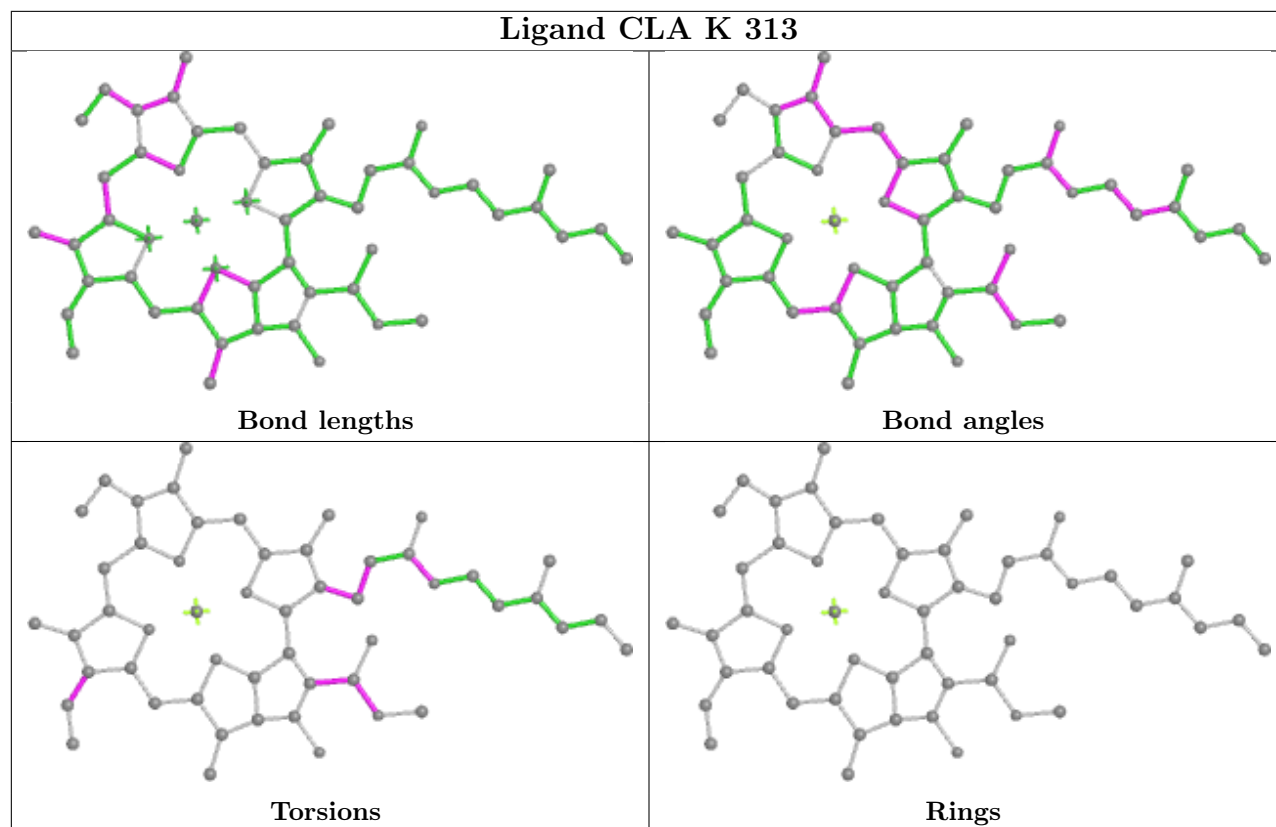


Torsions

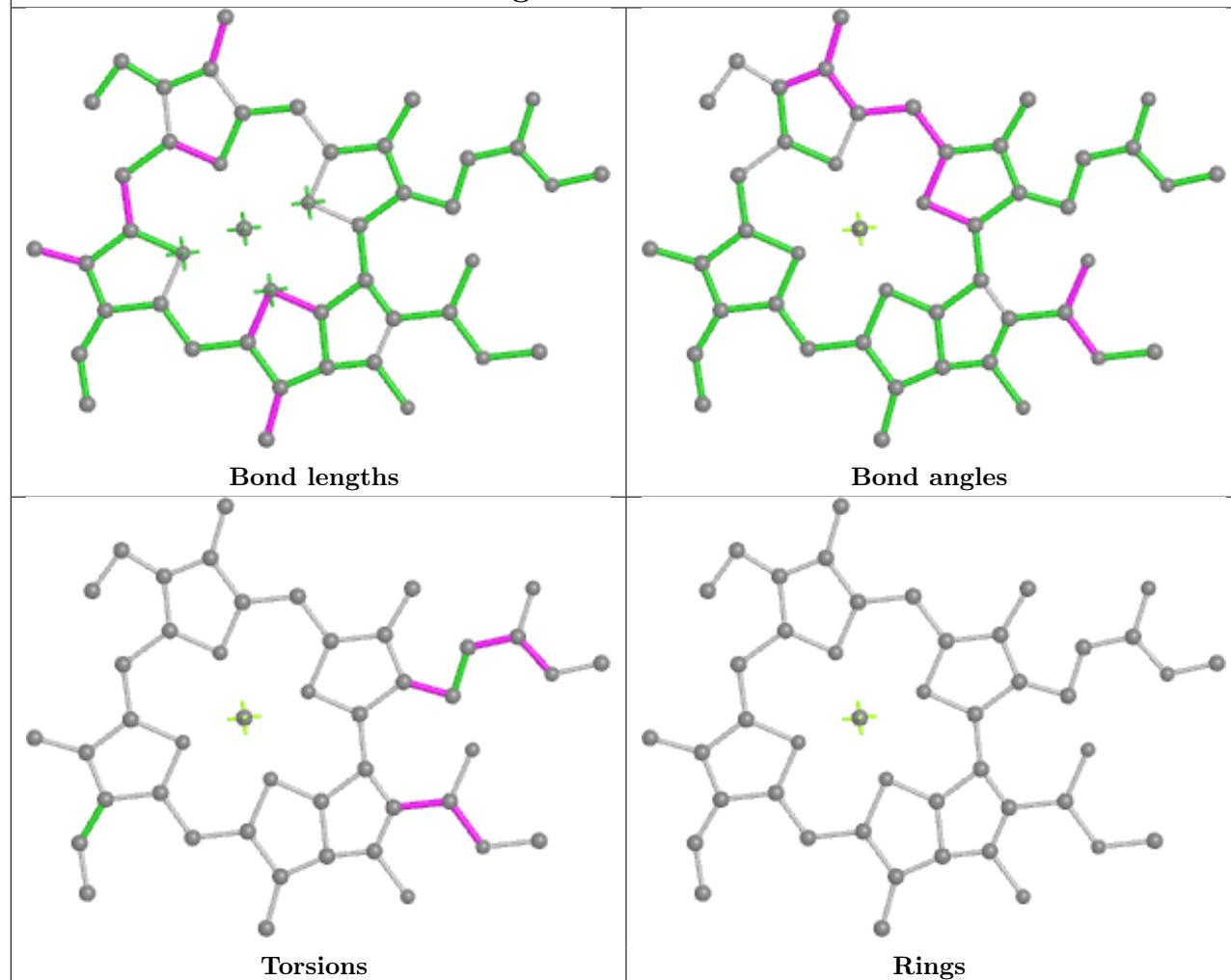


Rings

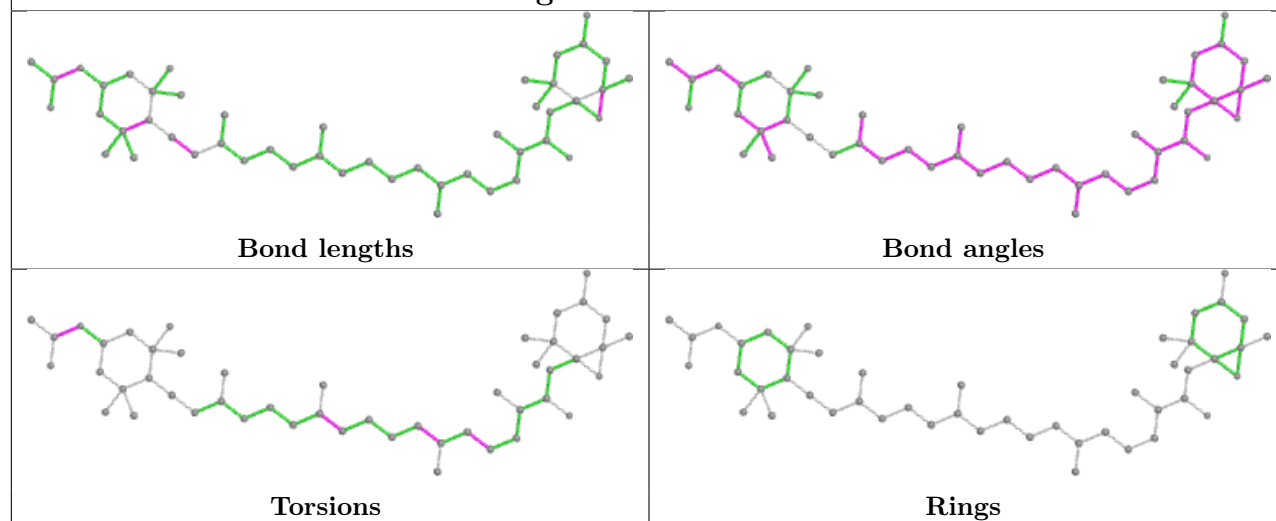


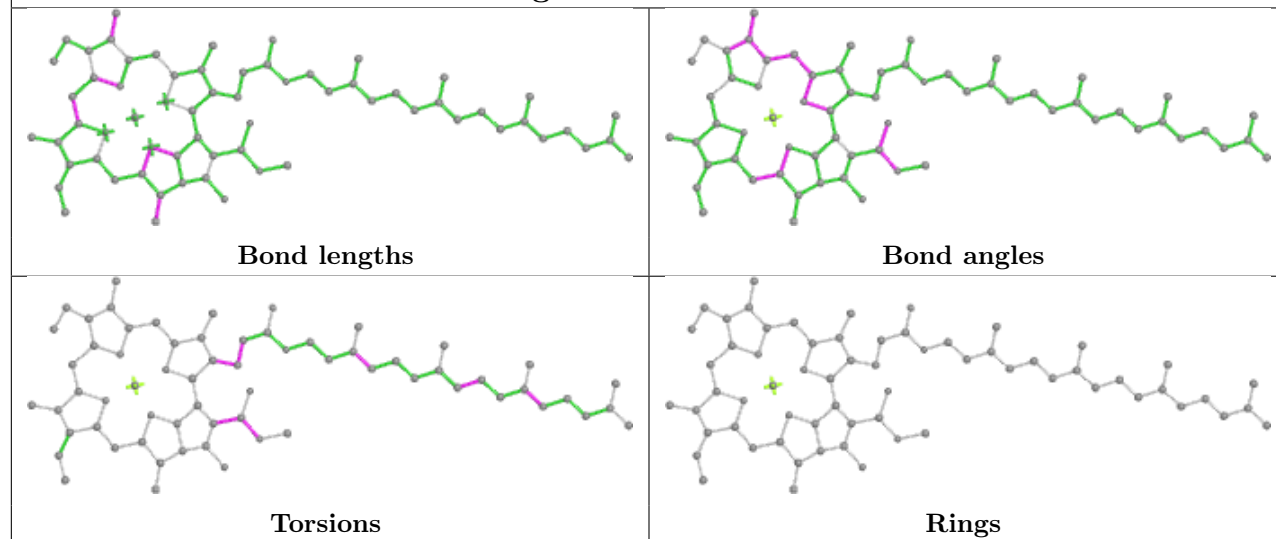
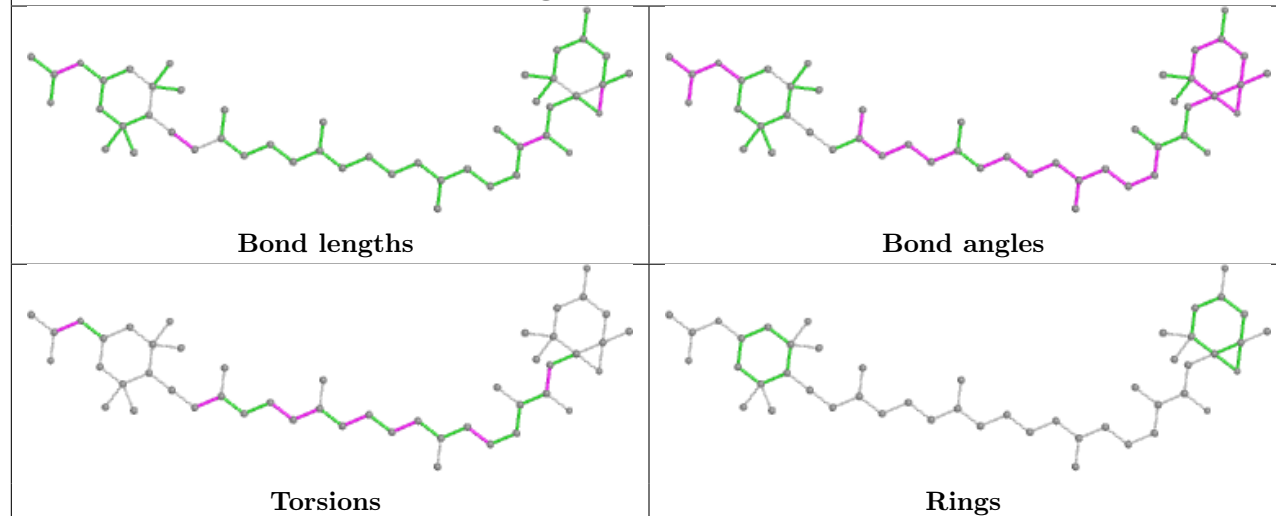


Ligand CLA D 211

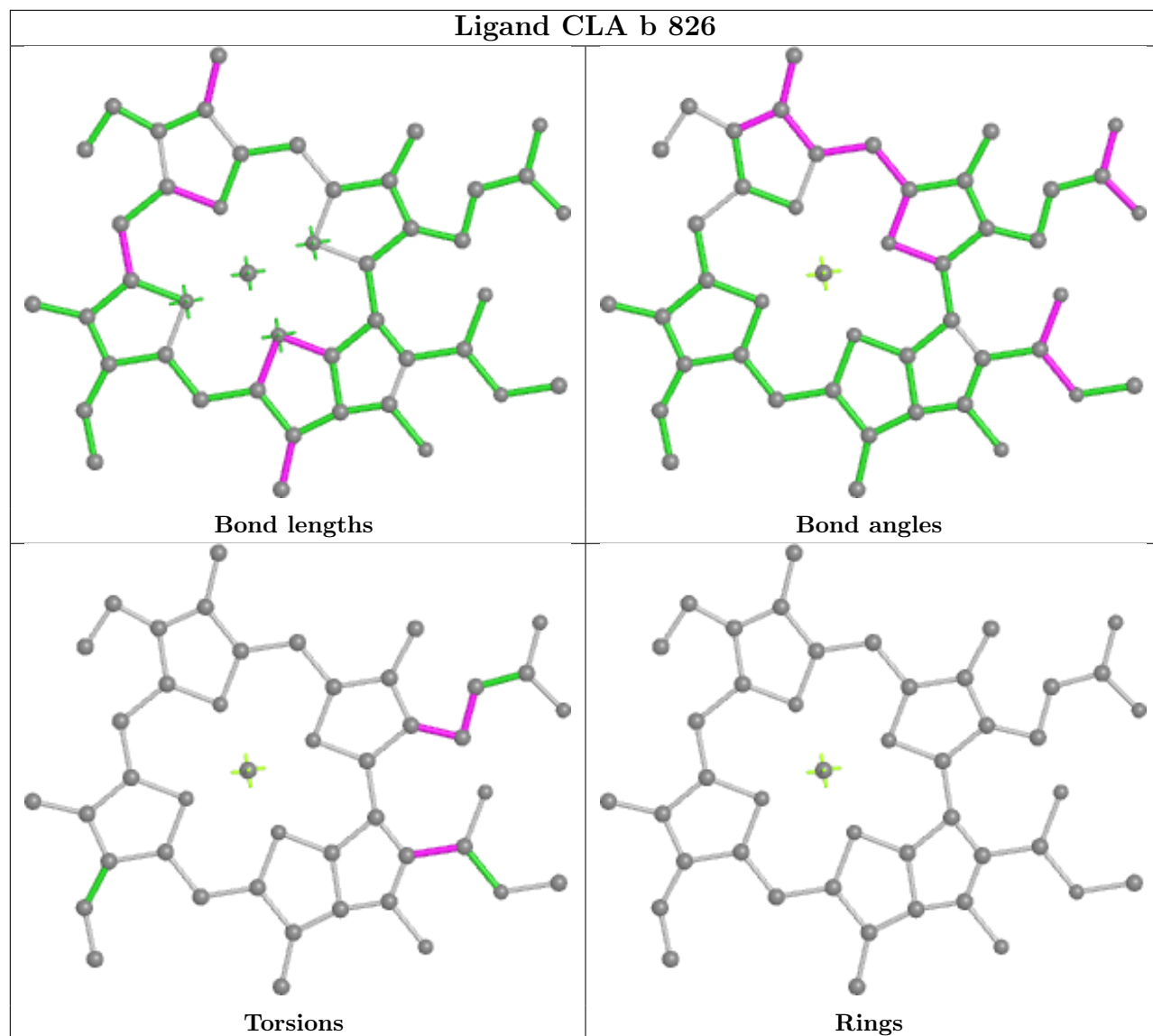


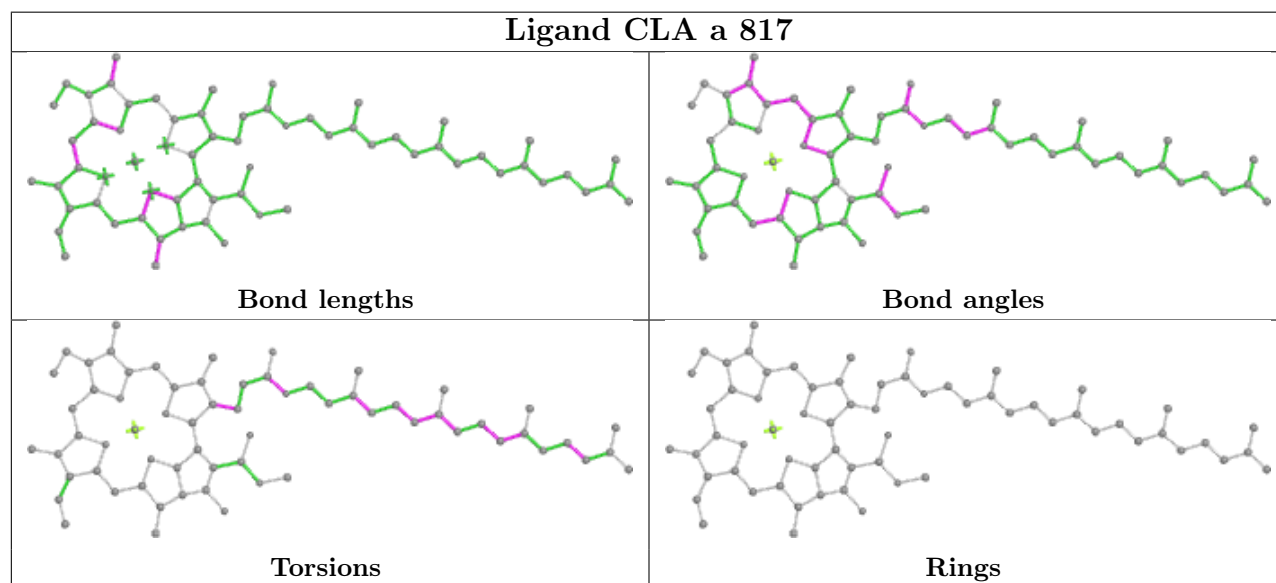
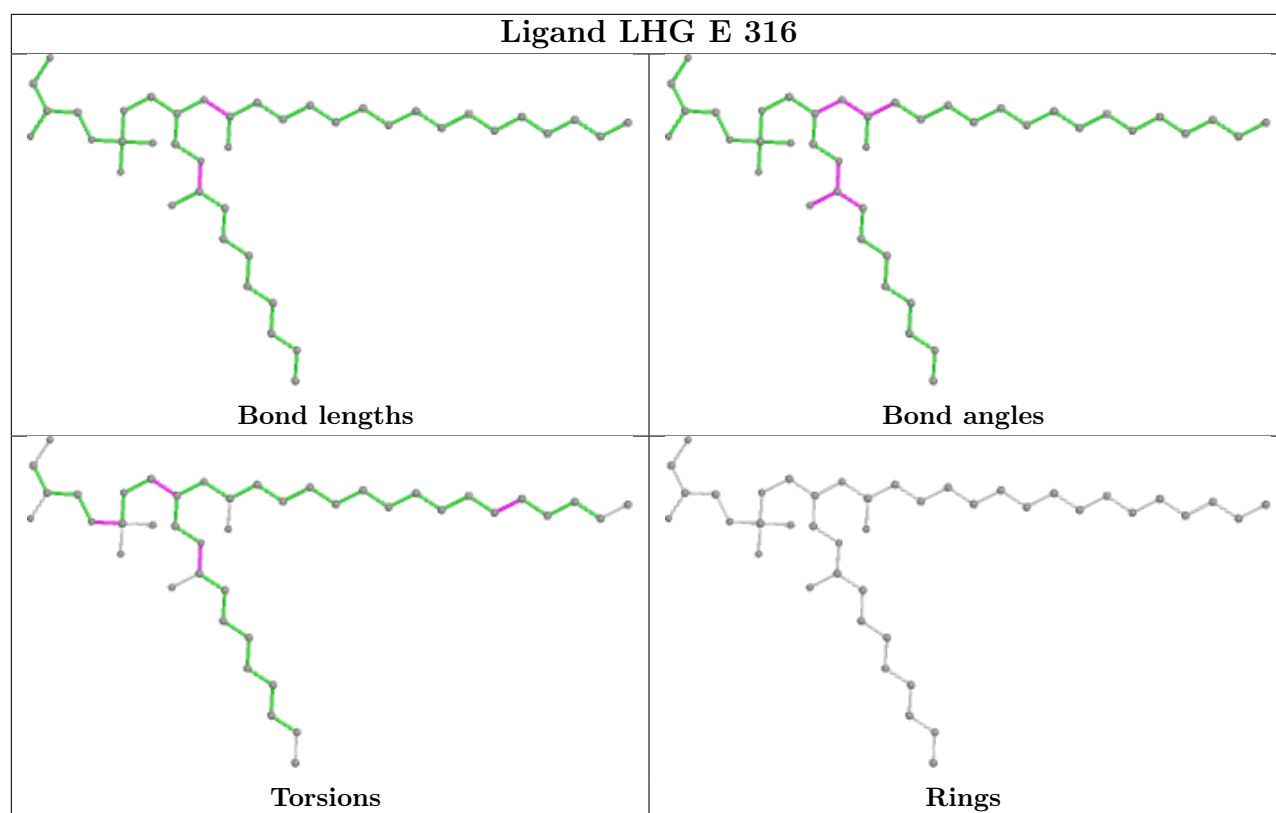
Ligand A86 m 101

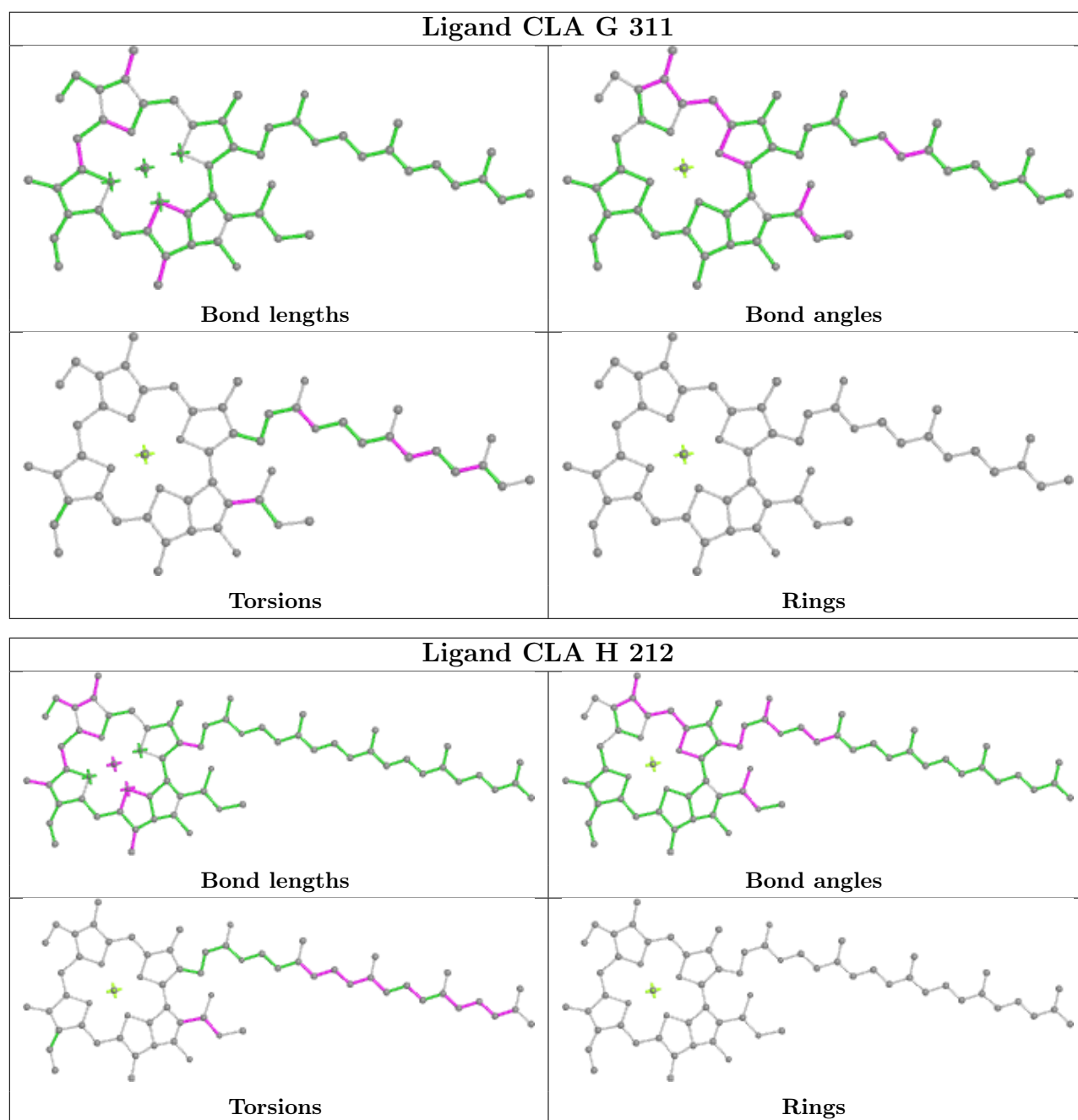


Ligand CLA B 312**Ligand A86 D 203**

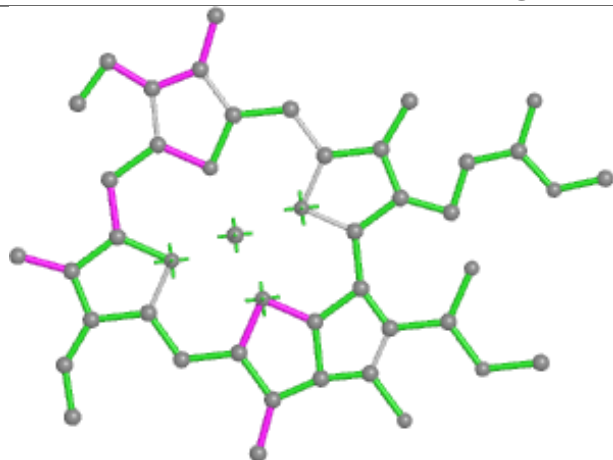
Ligand CLA b 826



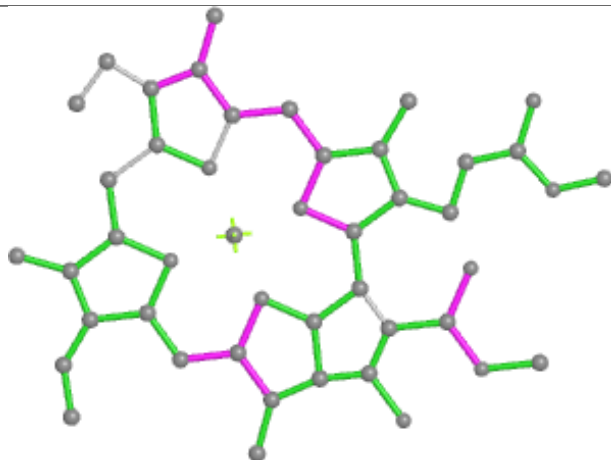




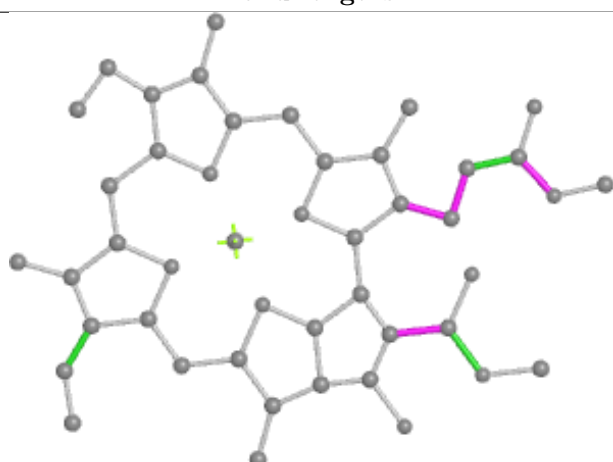
Ligand CLA K 318



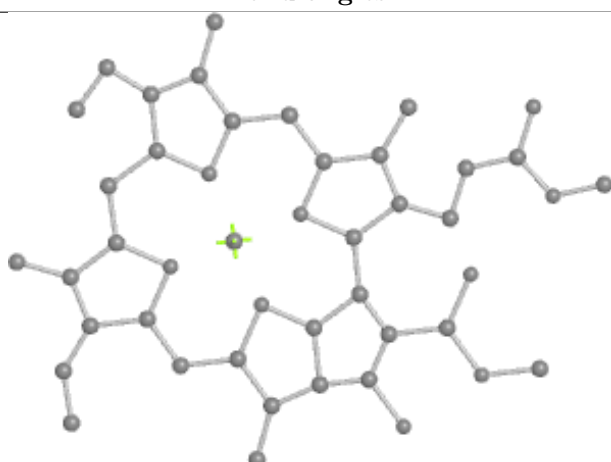
Bond lengths



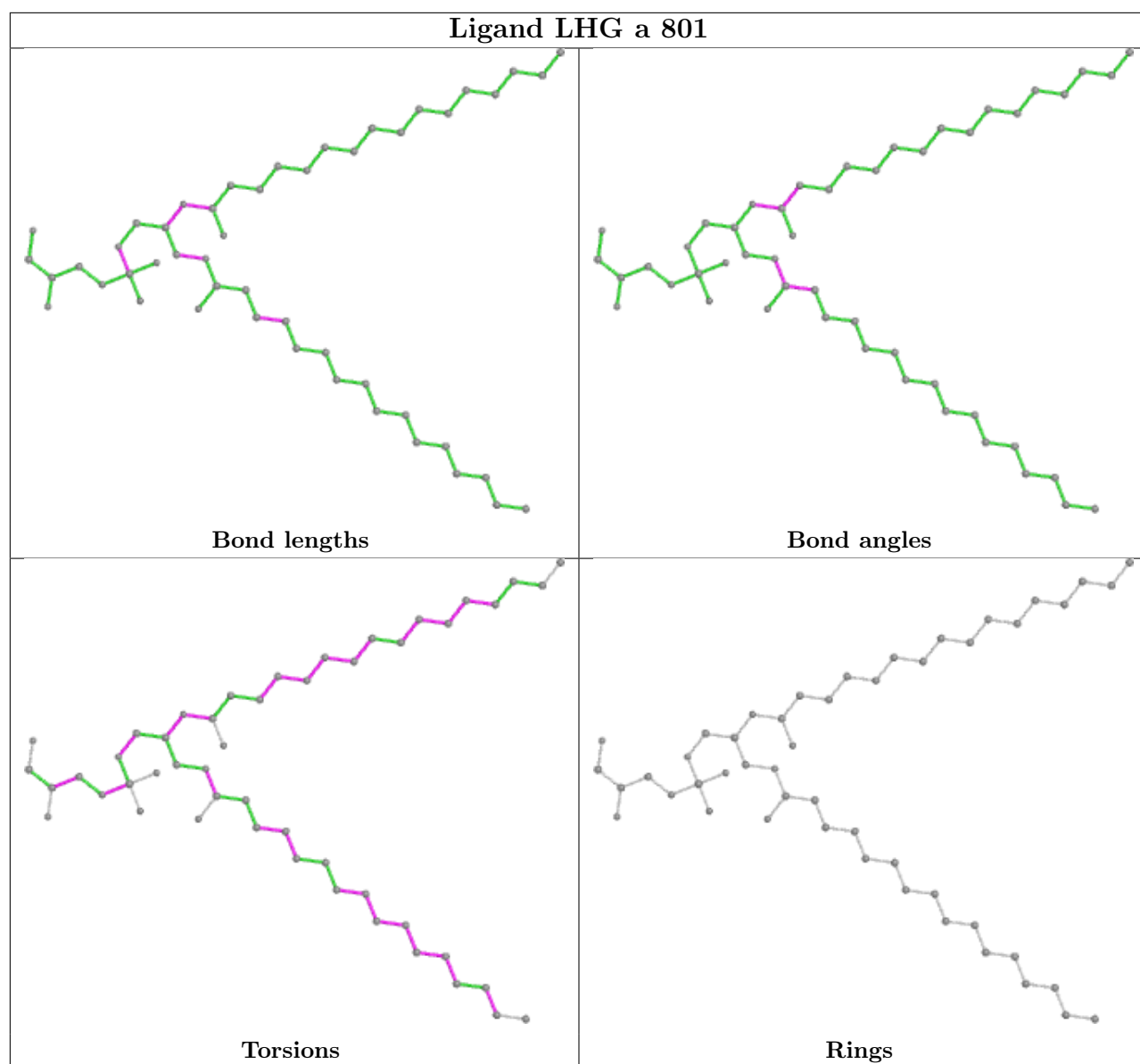
Bond angles

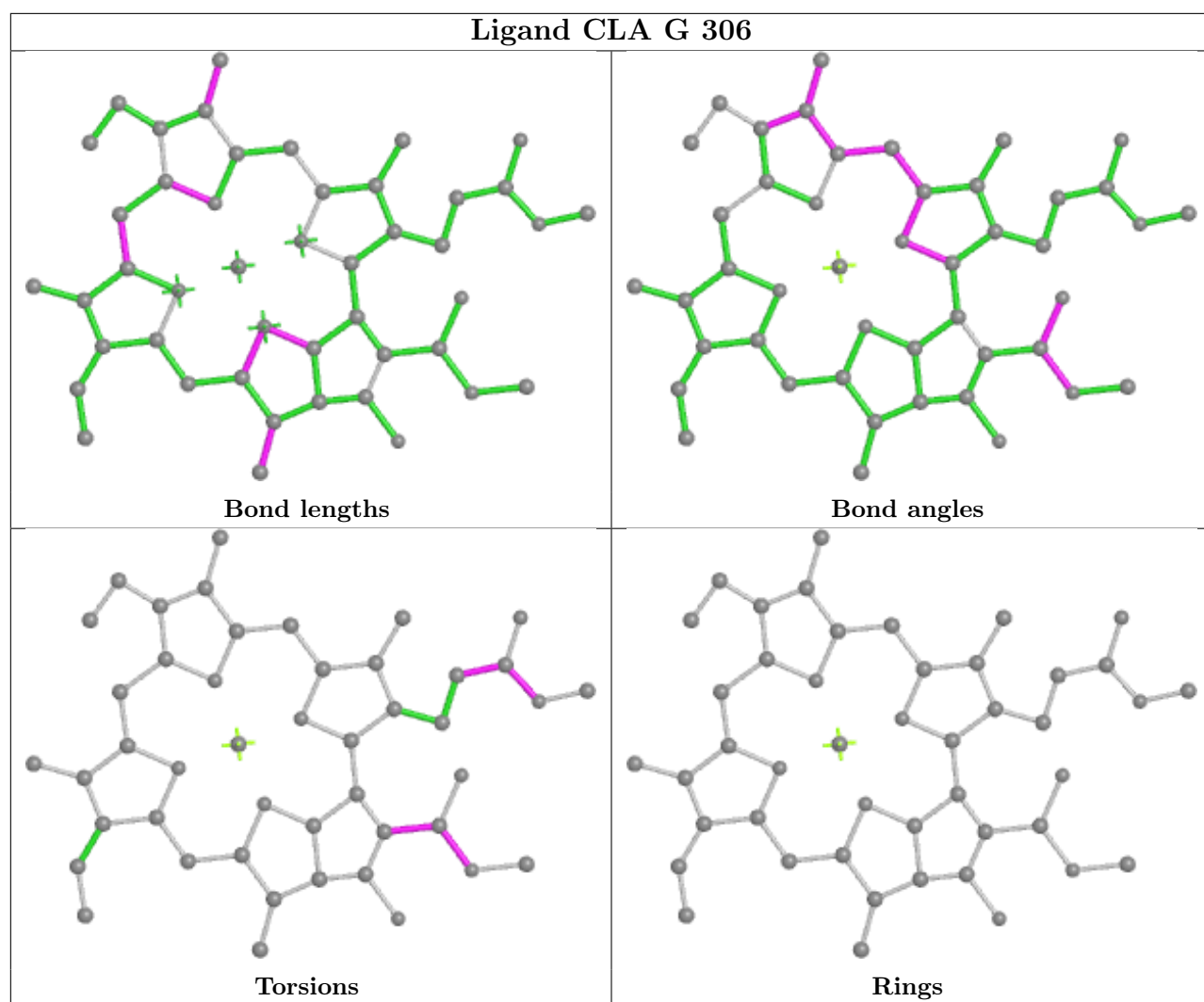


Torsions

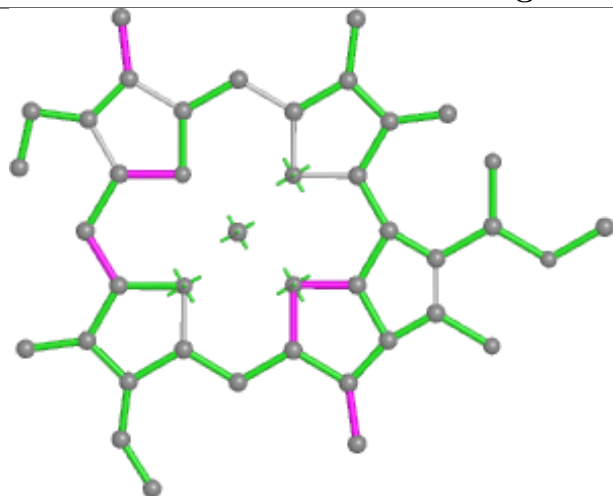


Rings

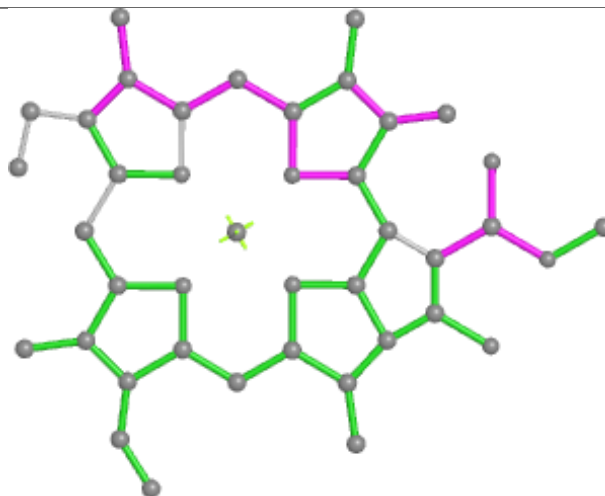




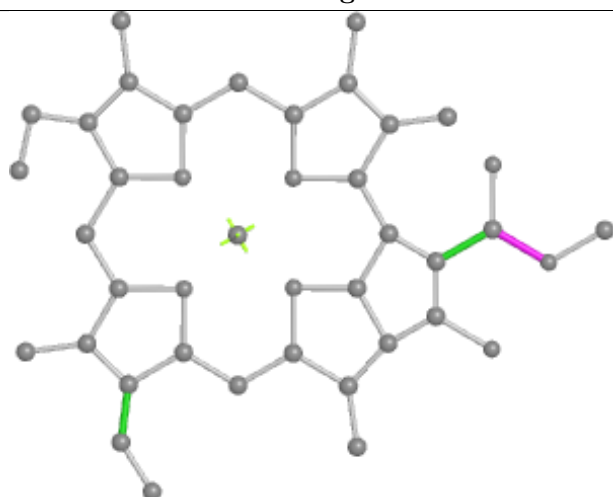
Ligand CLA F 313



Bond lengths



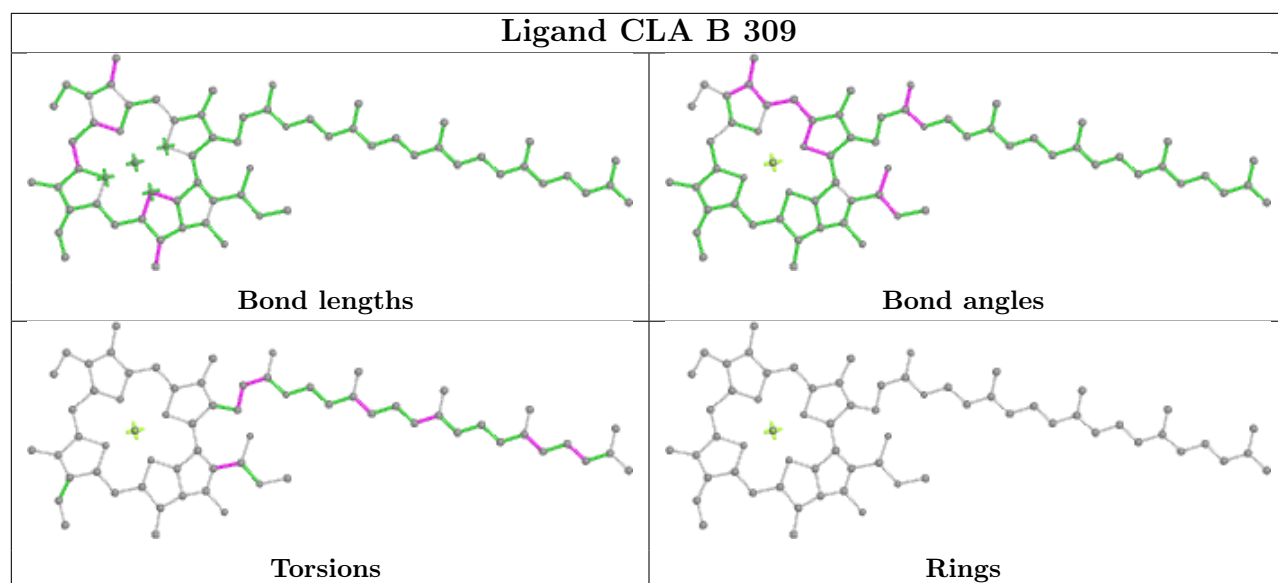
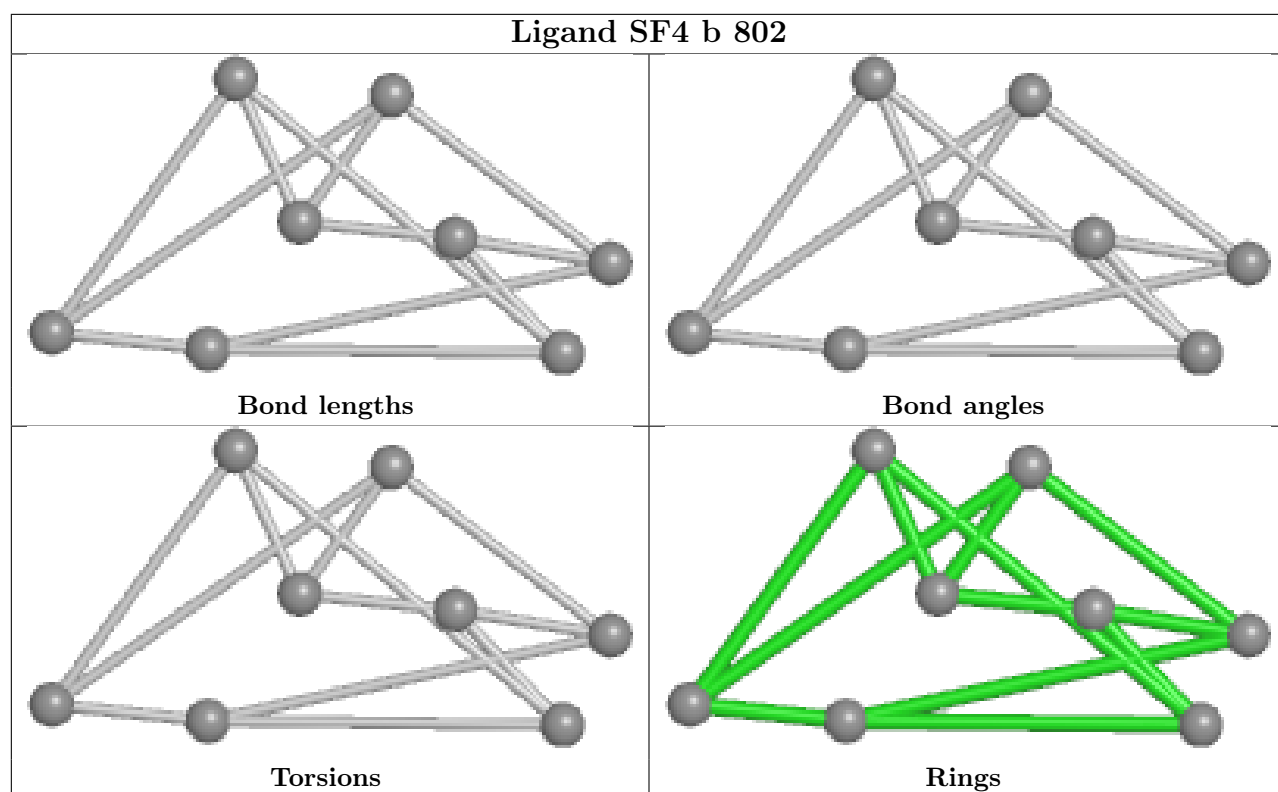
Bond angles



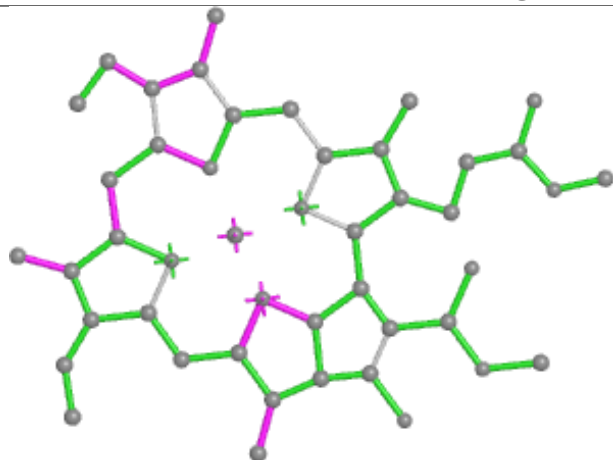
Torsions



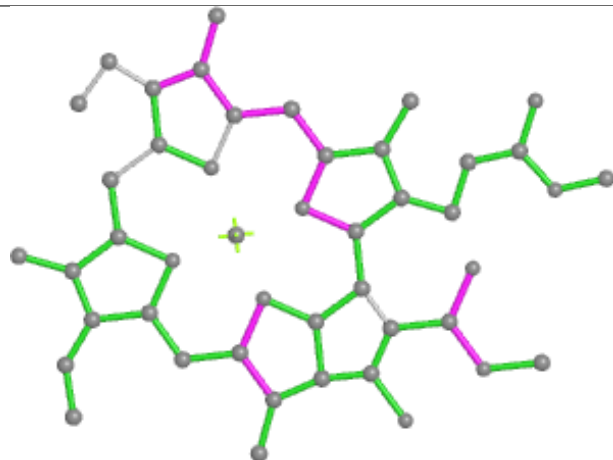
Rings



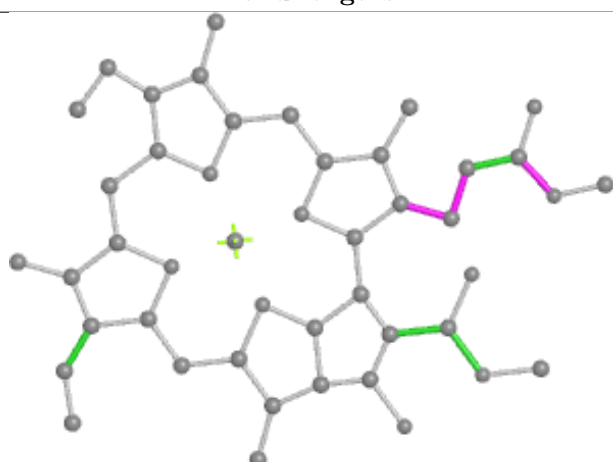
Ligand CLA D 216



Bond lengths



Bond angles

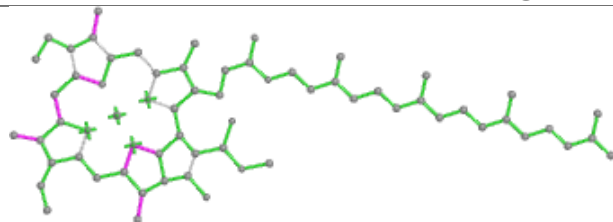


Torsions

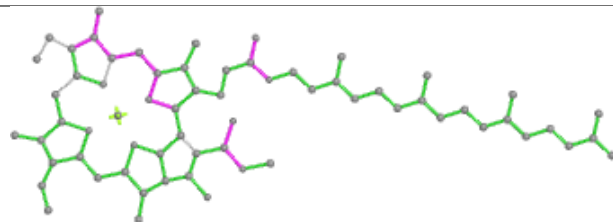


Rings

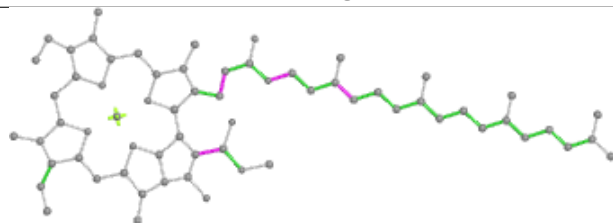
Ligand CLA b 839



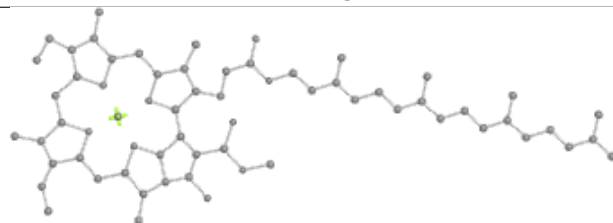
Bond lengths



Bond angles

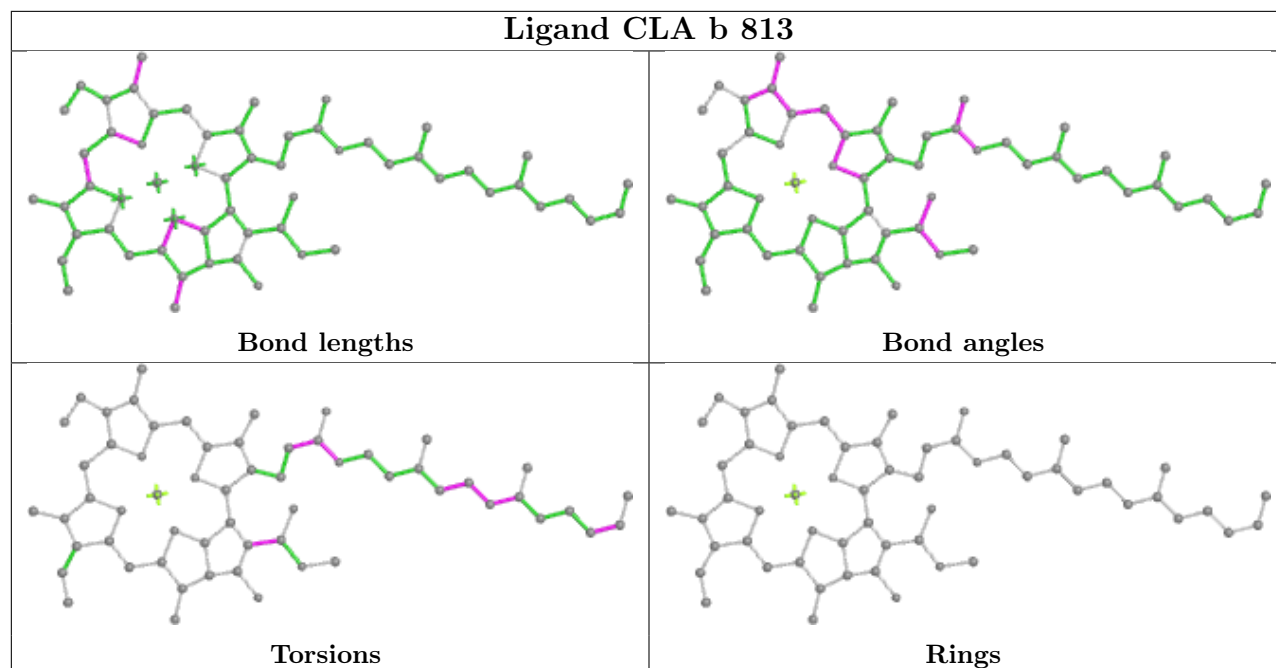


Torsions

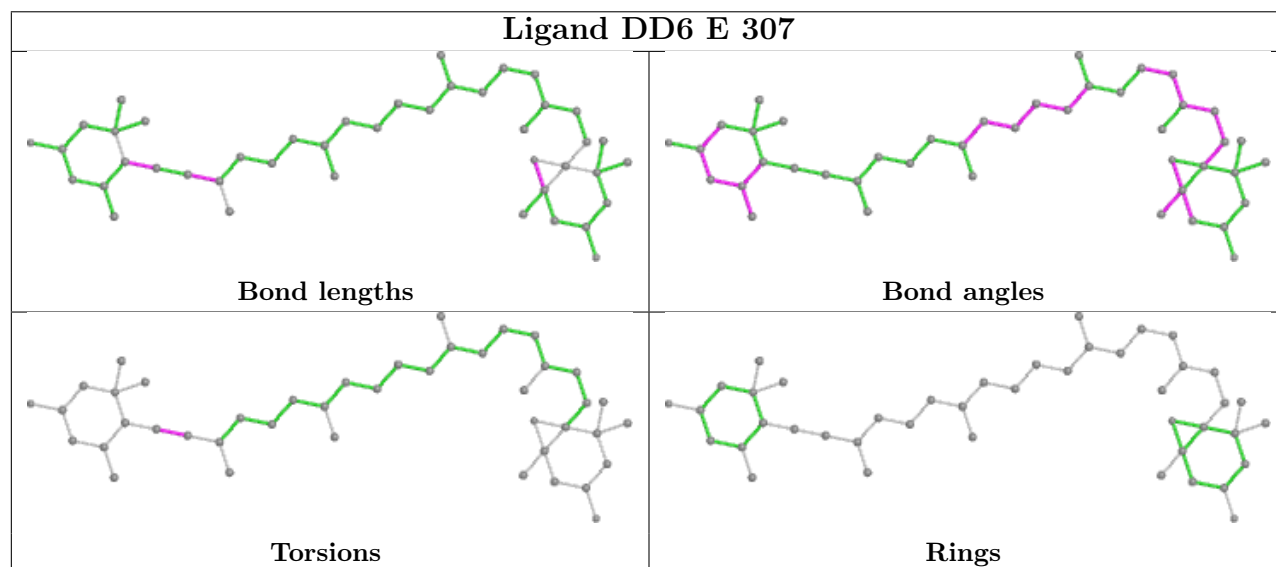


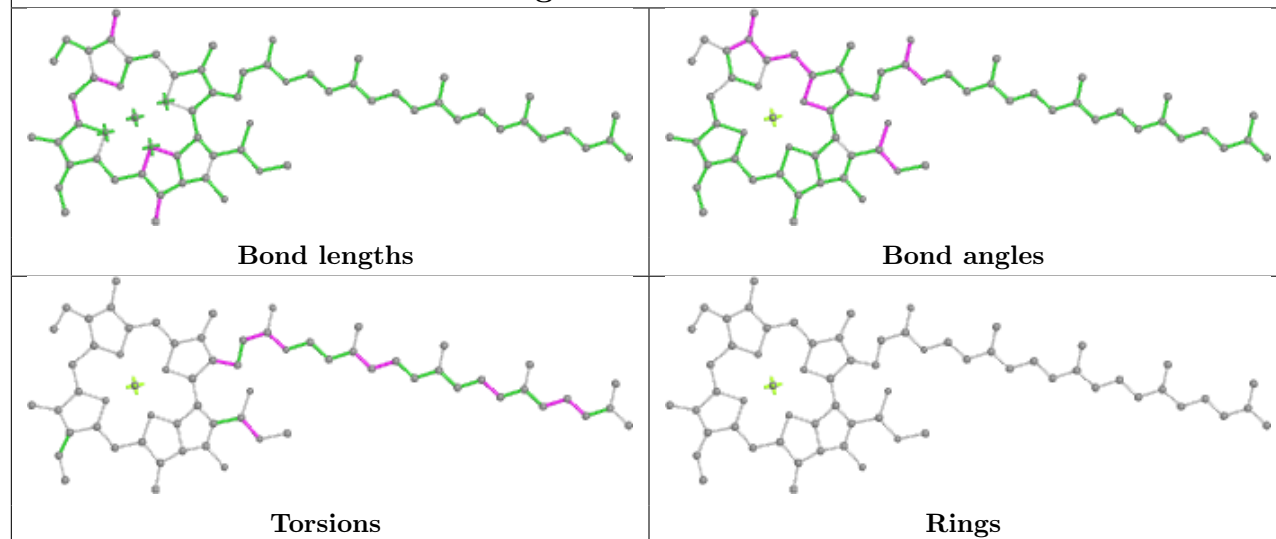
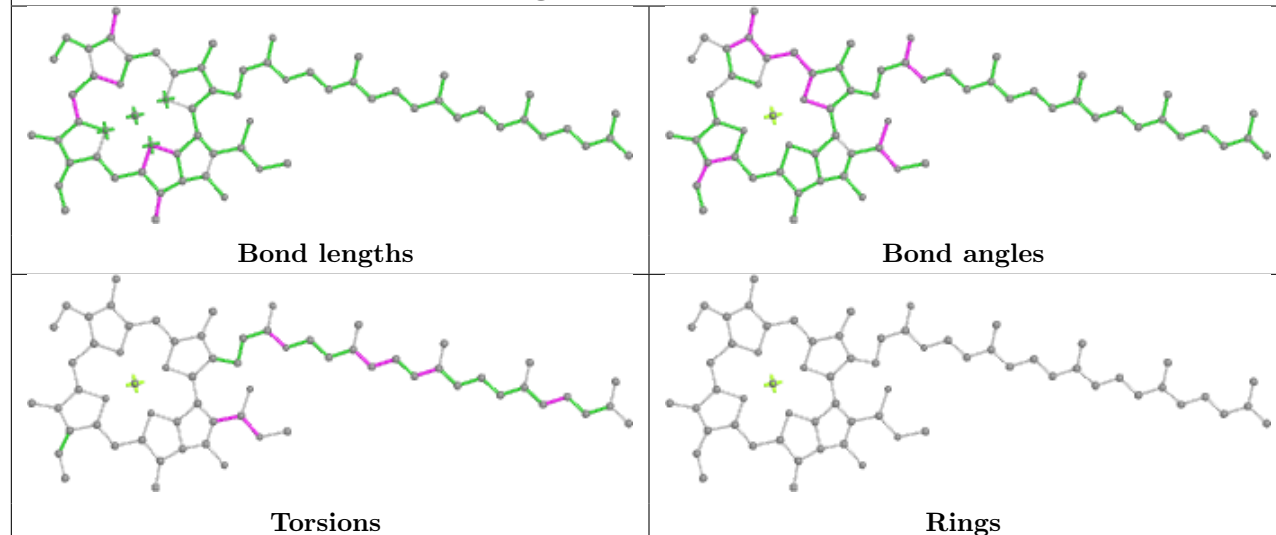
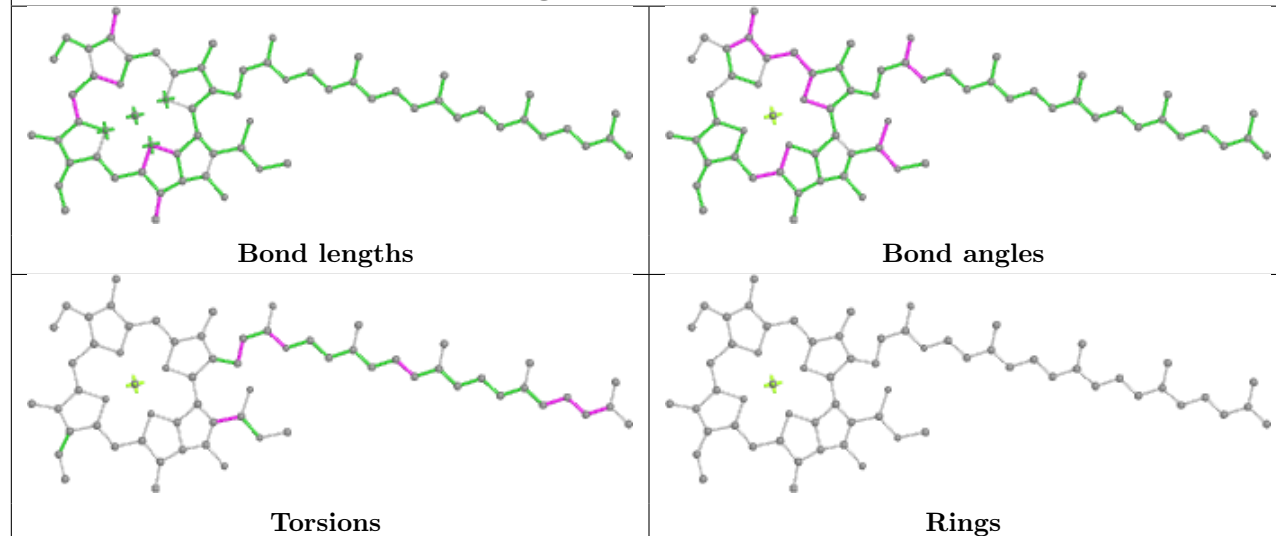
Rings

Ligand CLA b 813

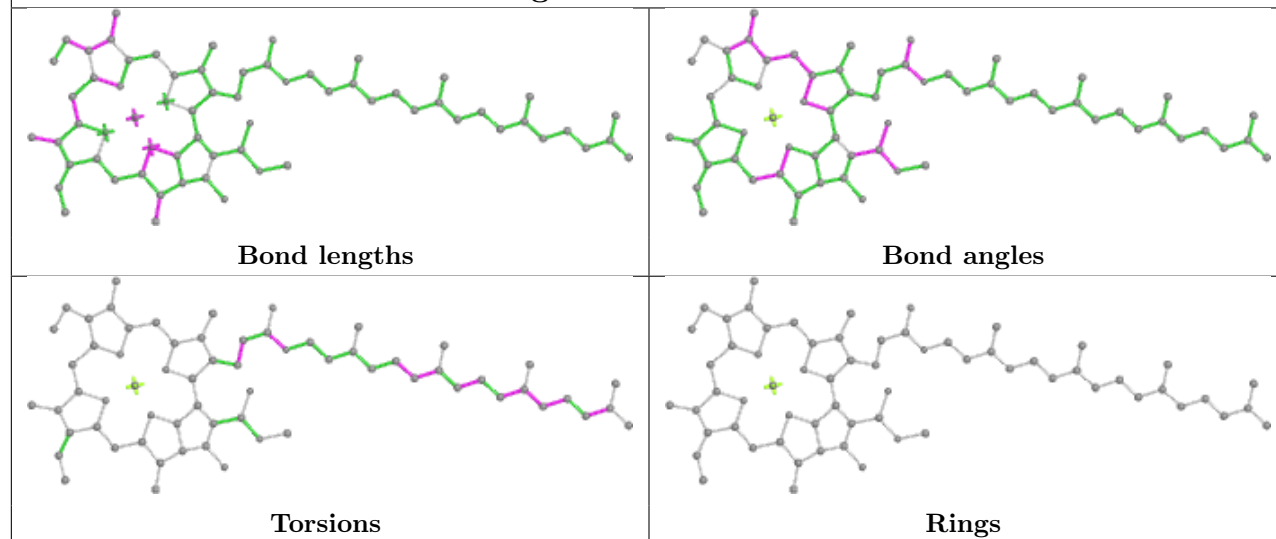


Ligand DD6 E 307

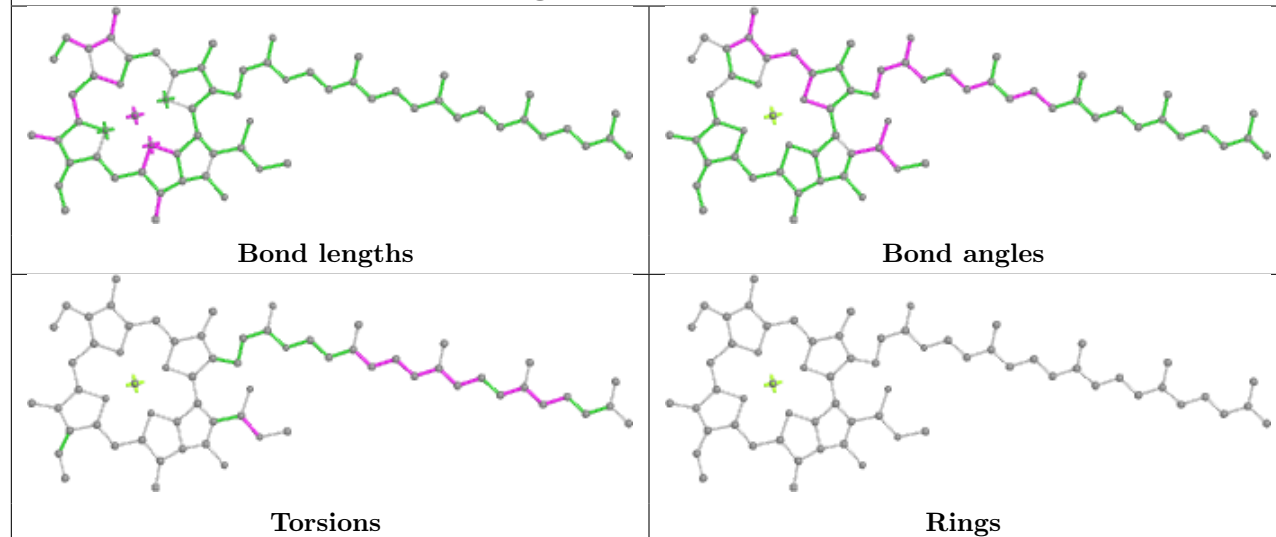


Ligand CLA b 850**Ligand CLA B 311****Ligand CLA b 829**

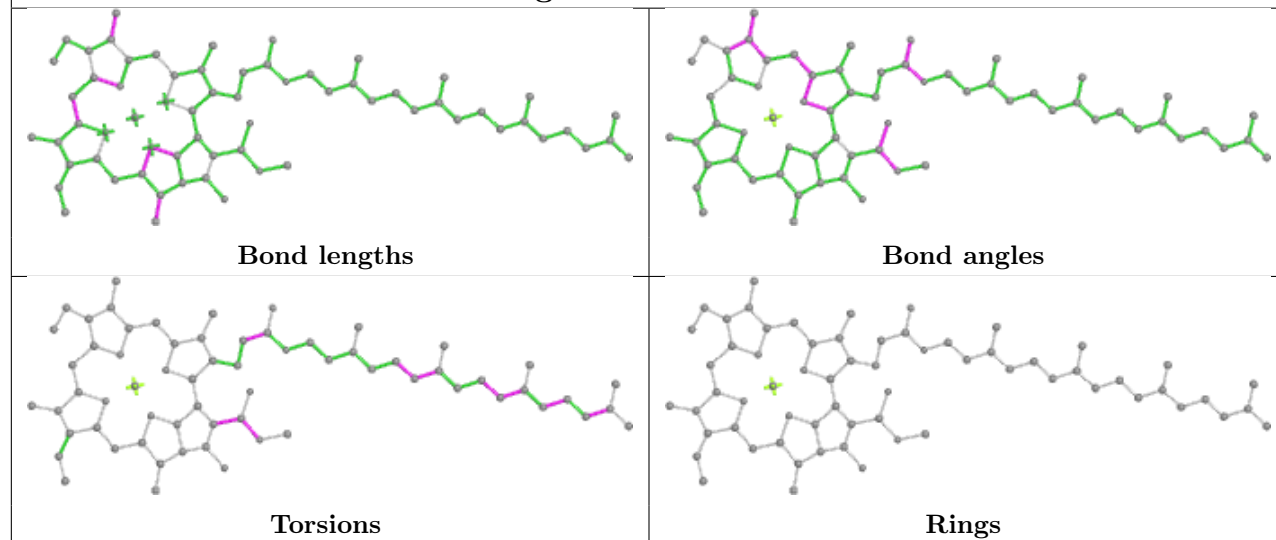
Ligand CLA H 205



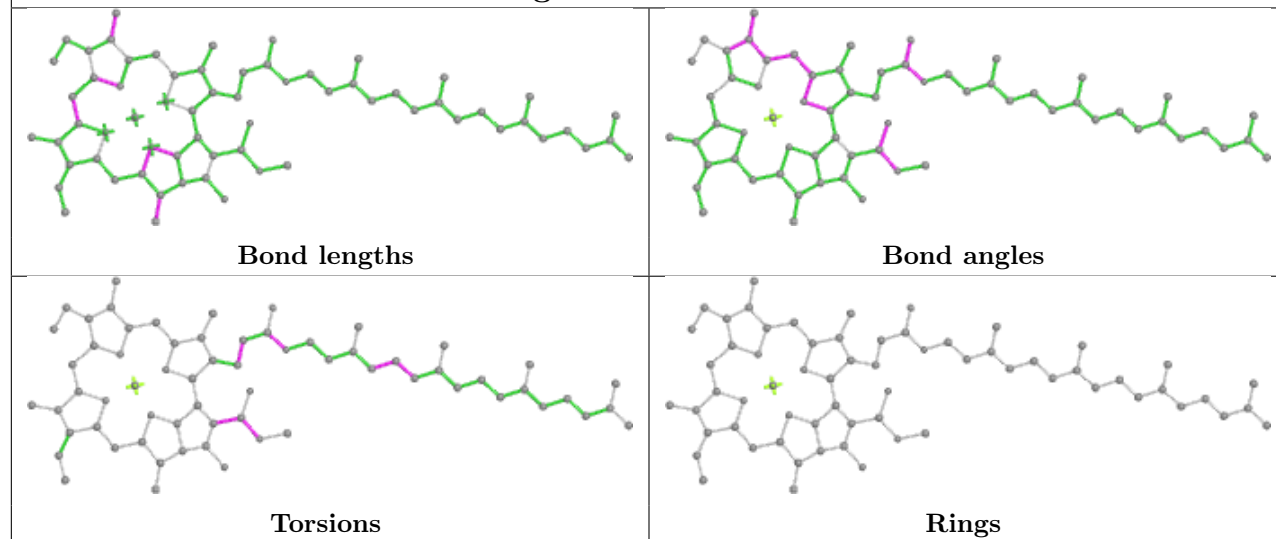
Ligand CLA D 208



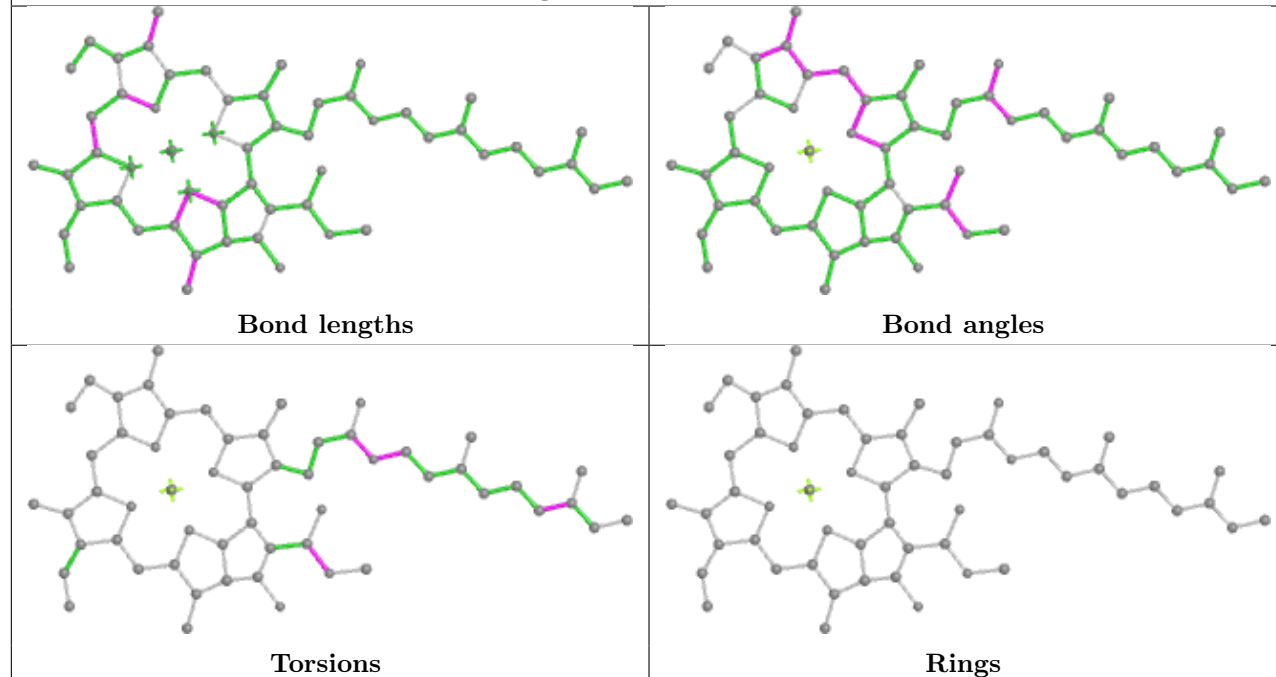
Ligand CLA b 803



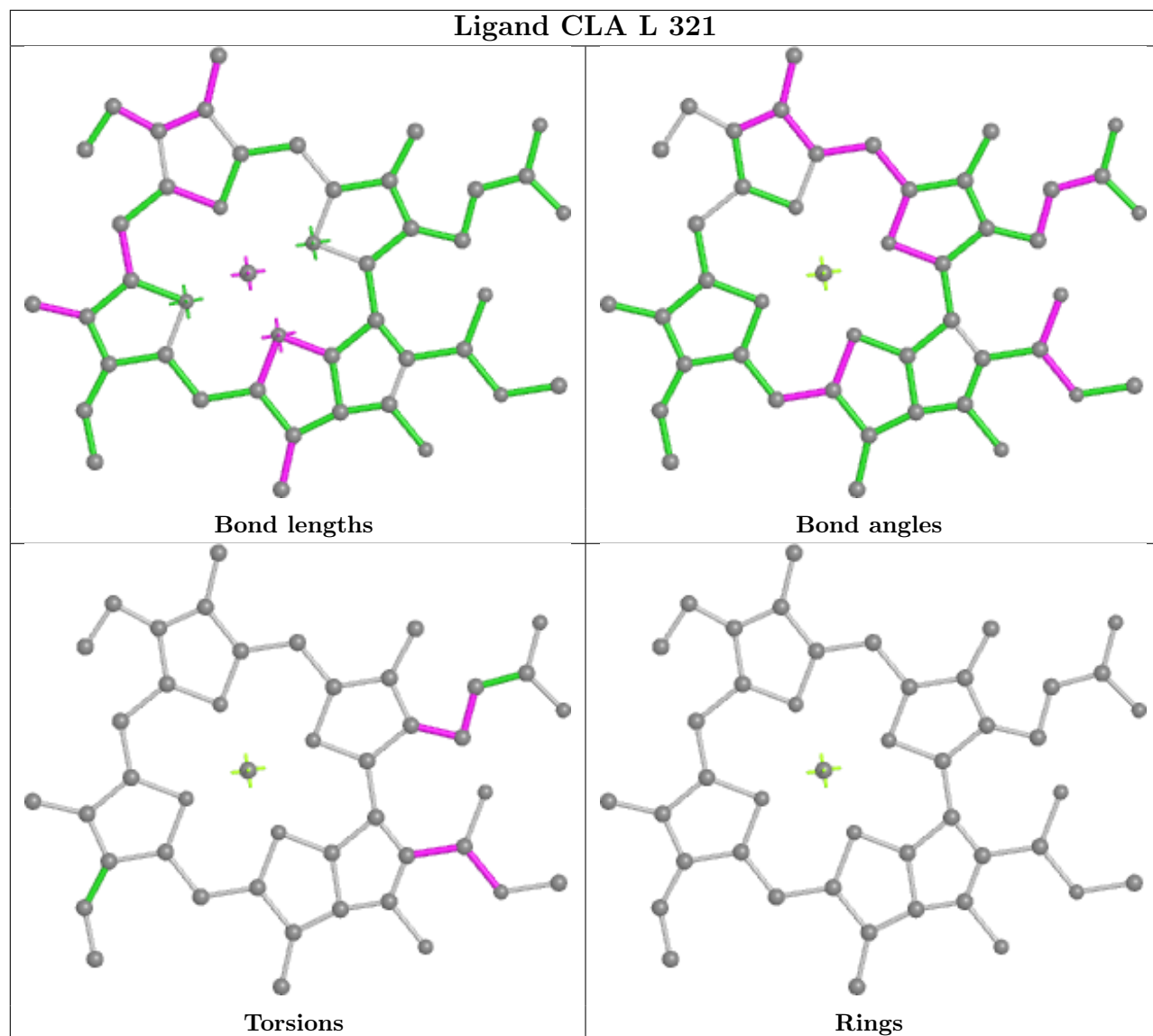
Ligand CLA E 314

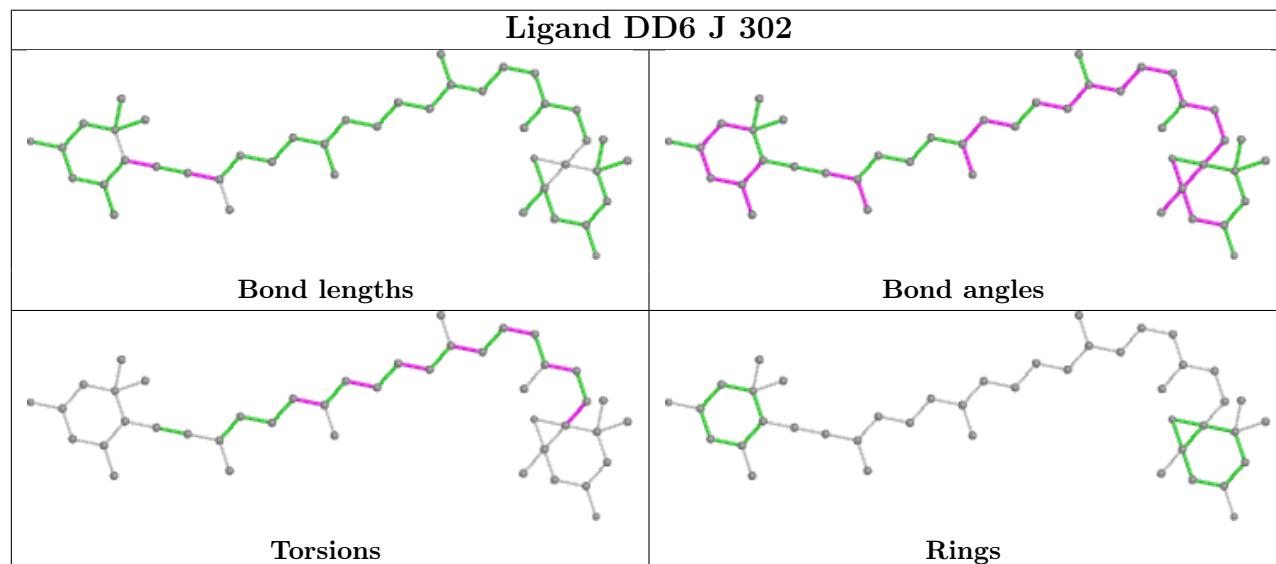
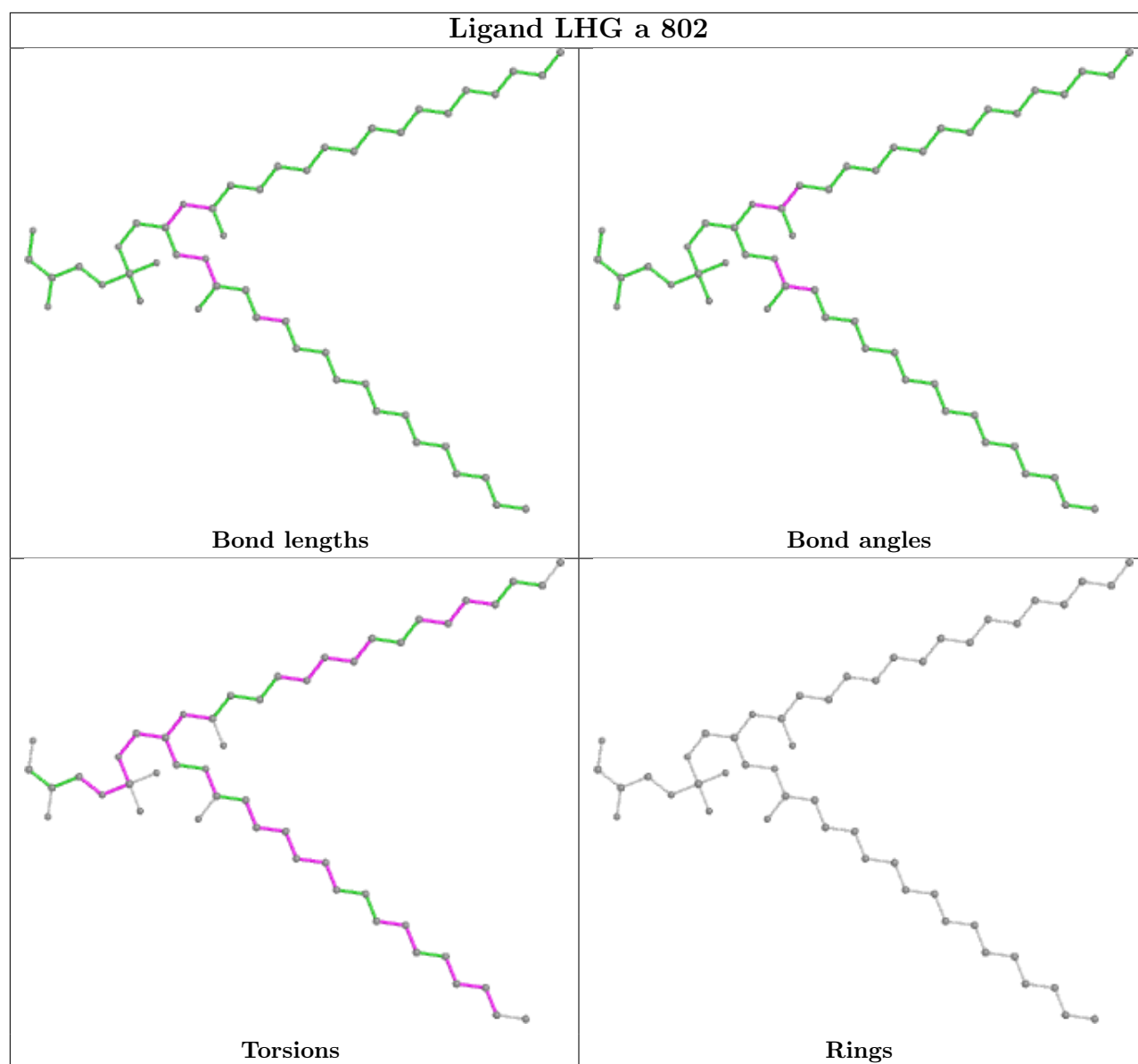


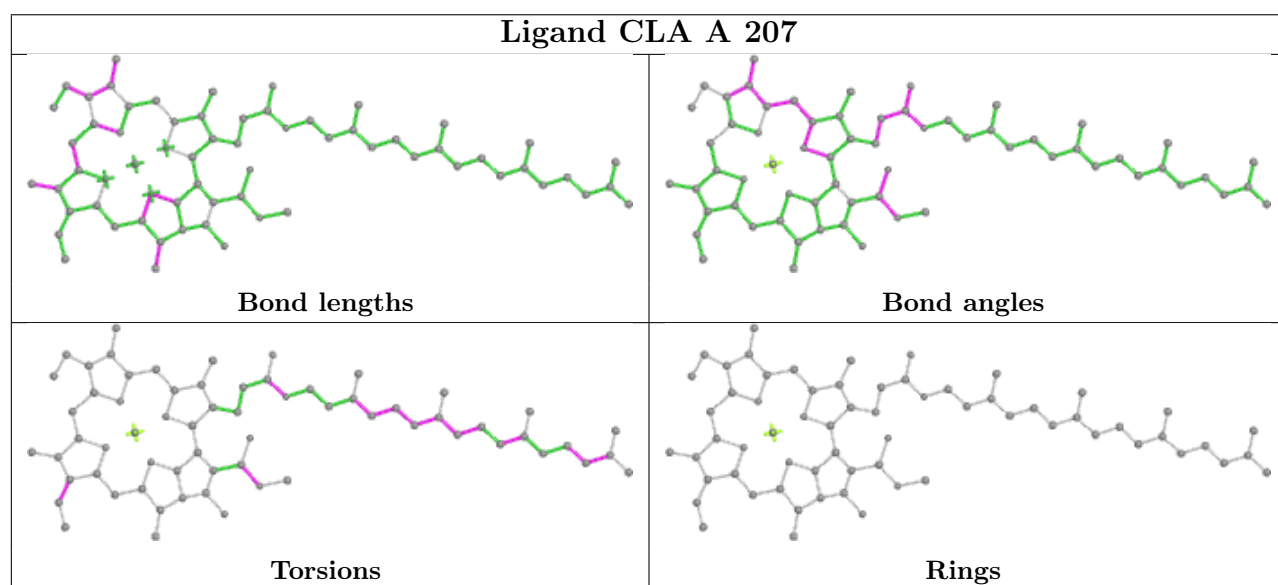
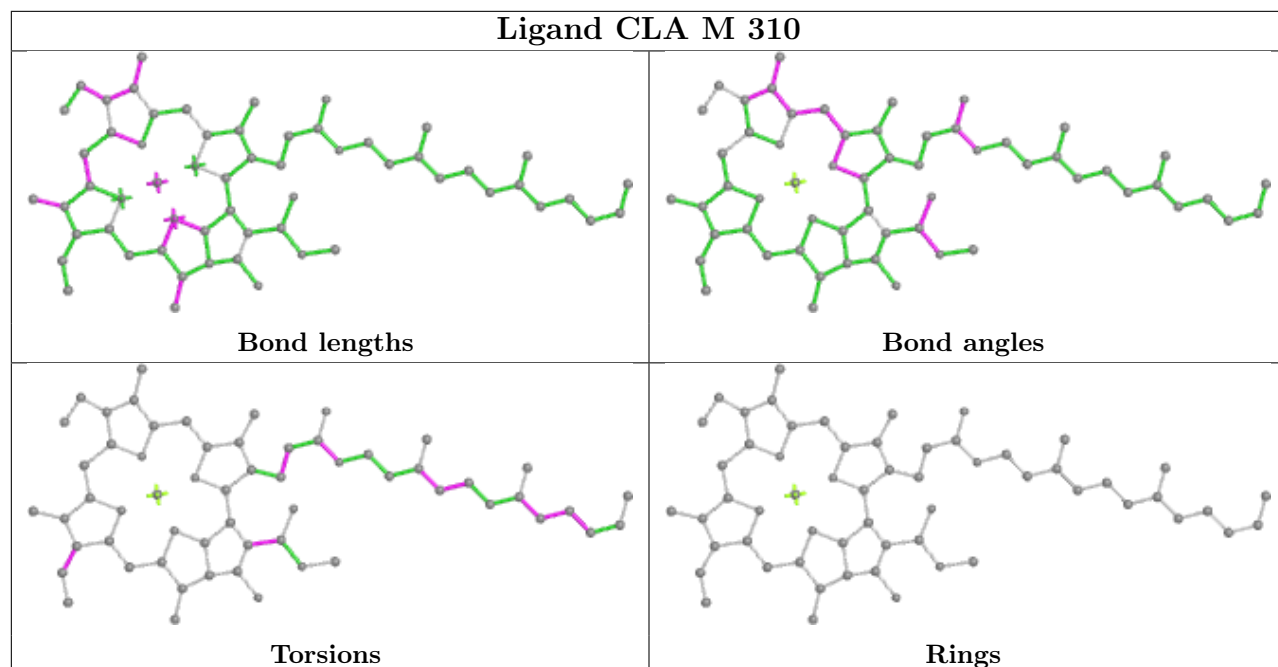
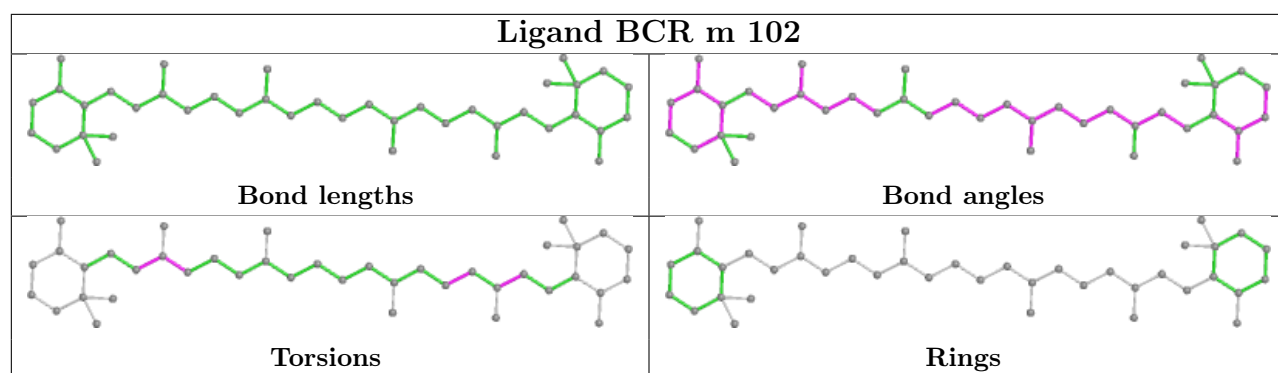
Ligand CLA J 308

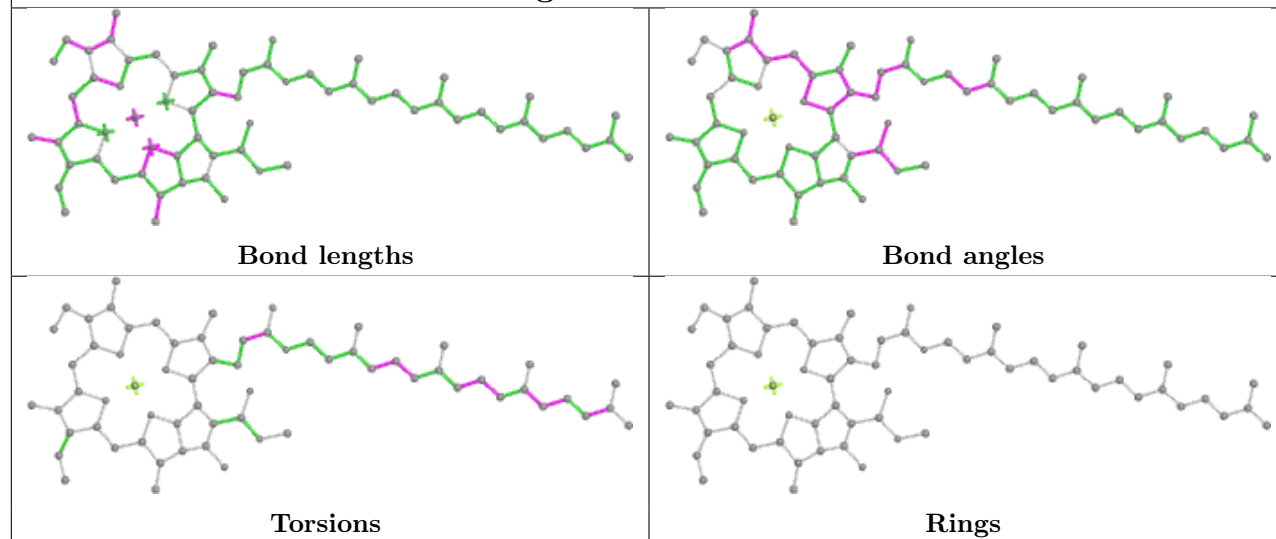
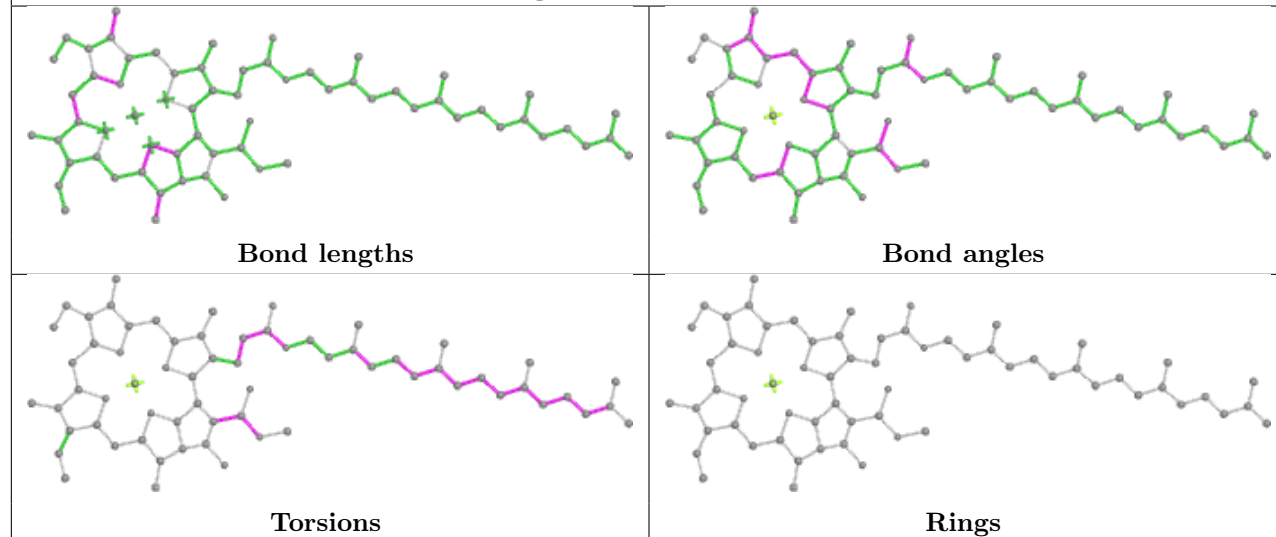


Ligand CLA L 321

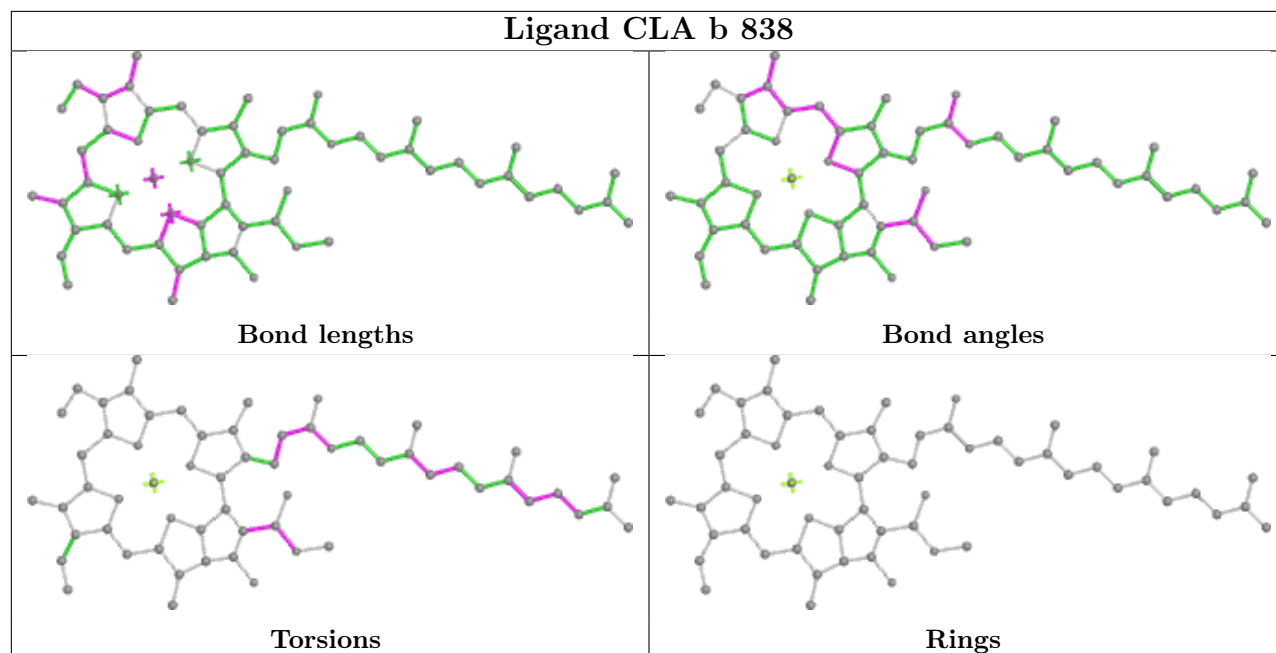




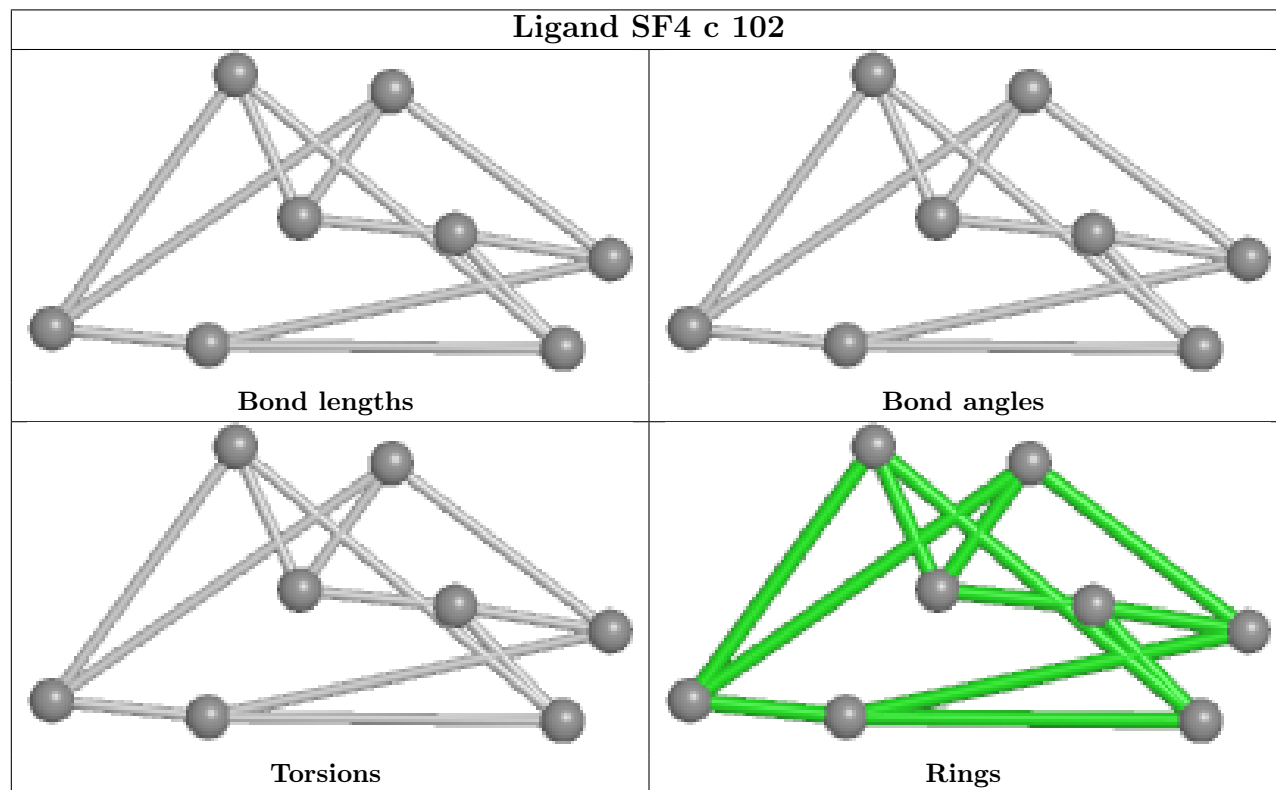


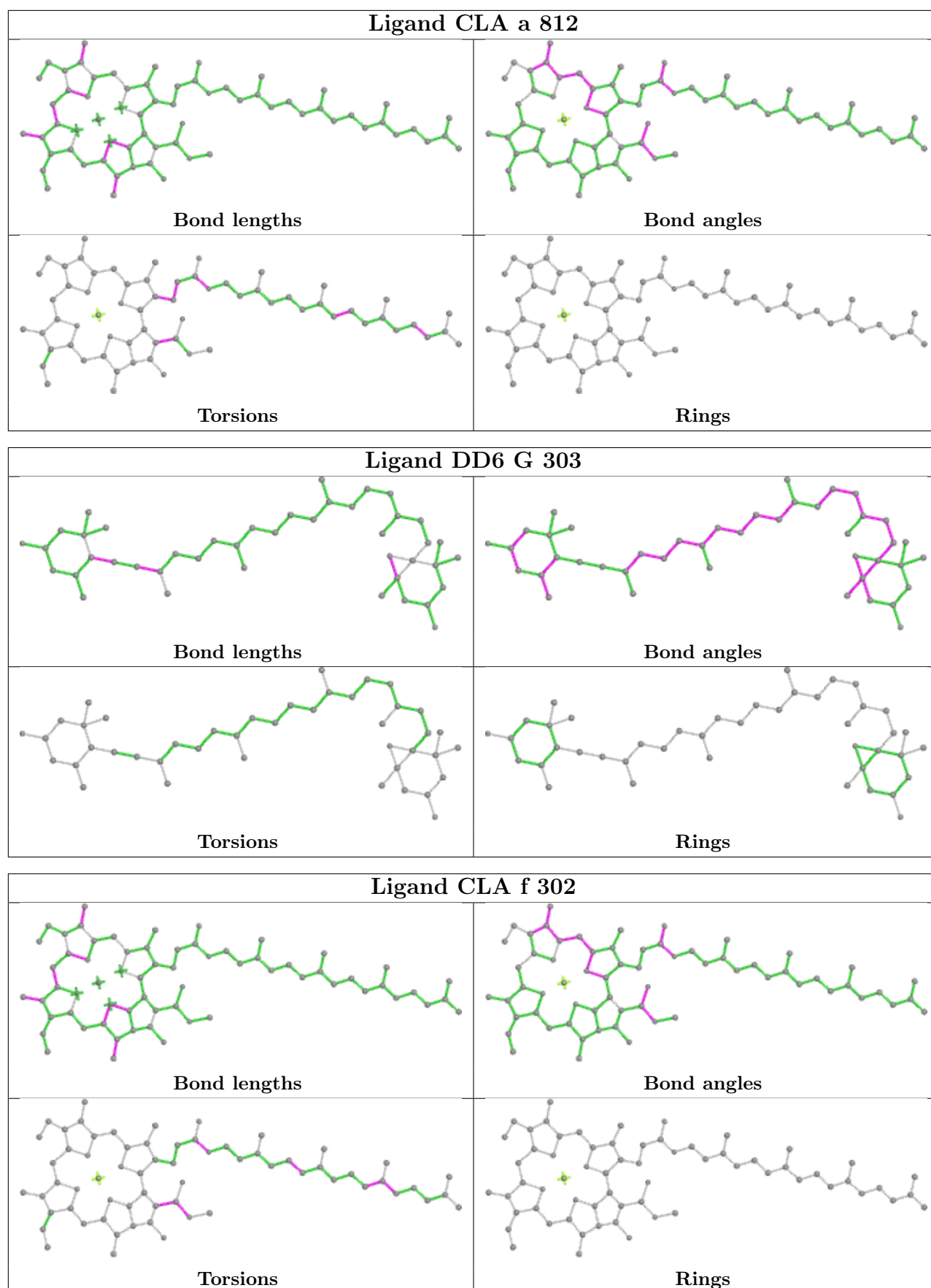
Ligand CLA a 809**Ligand CLA G 309**

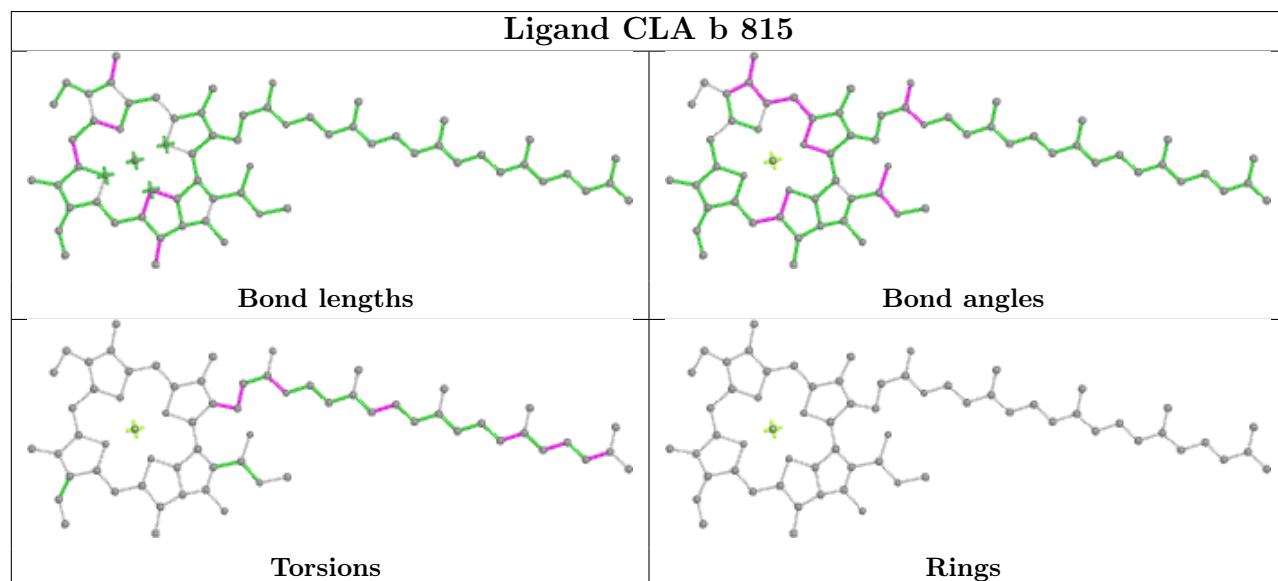
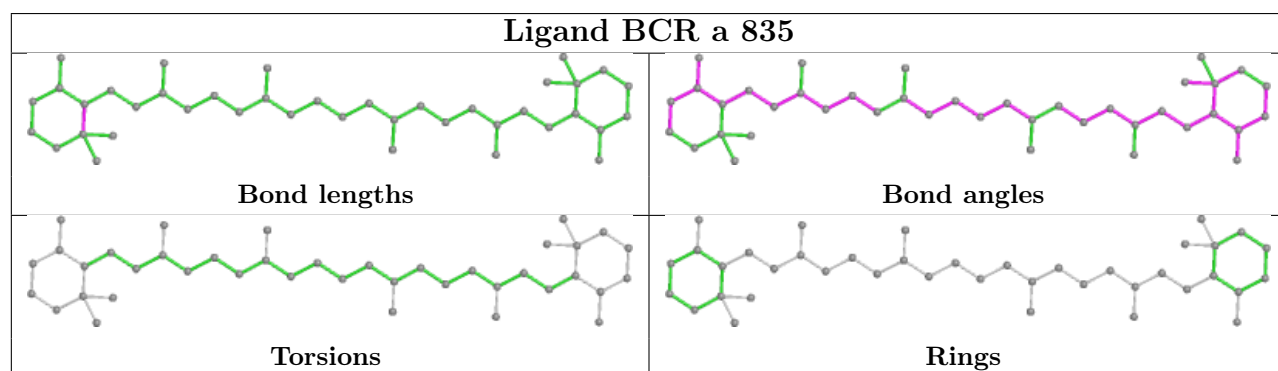
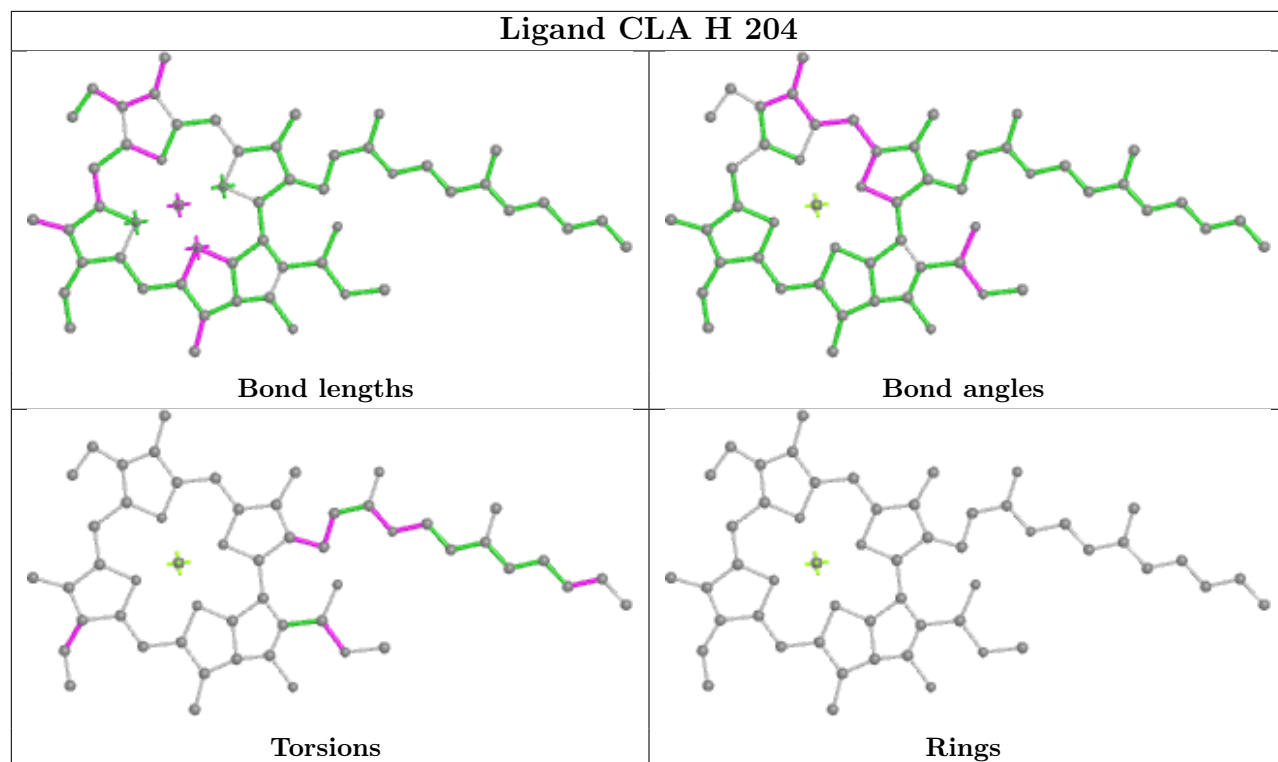
Ligand CLA b 838

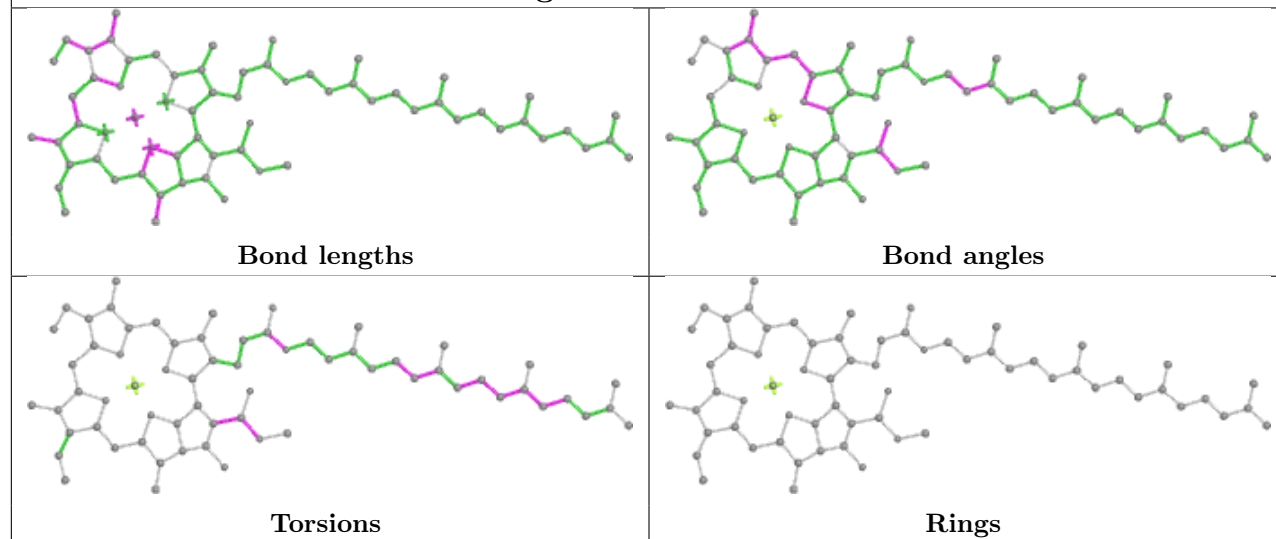
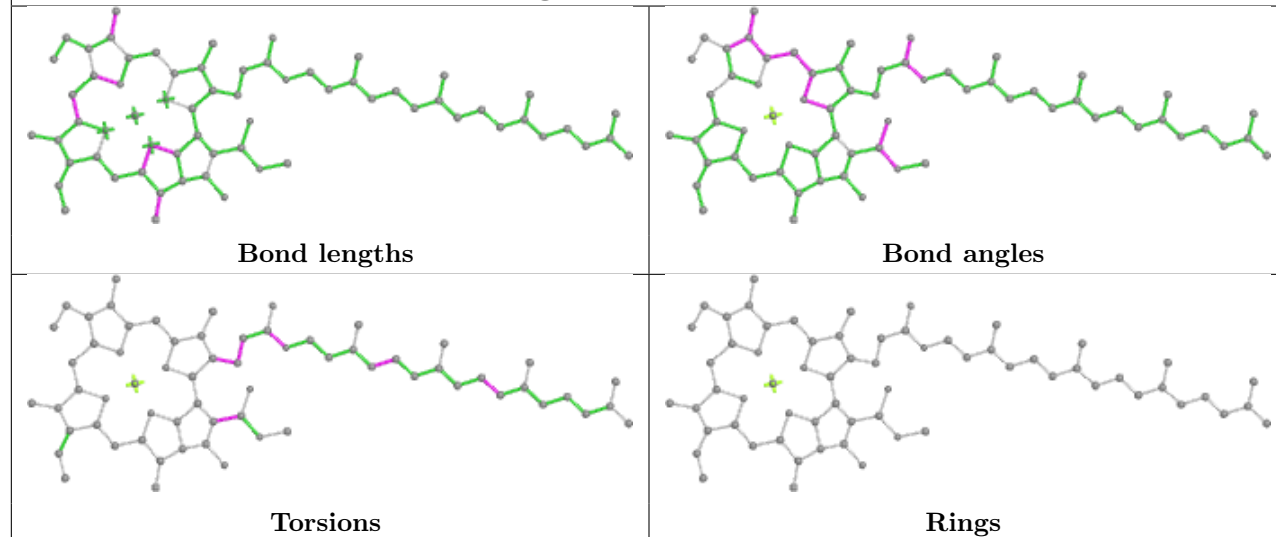


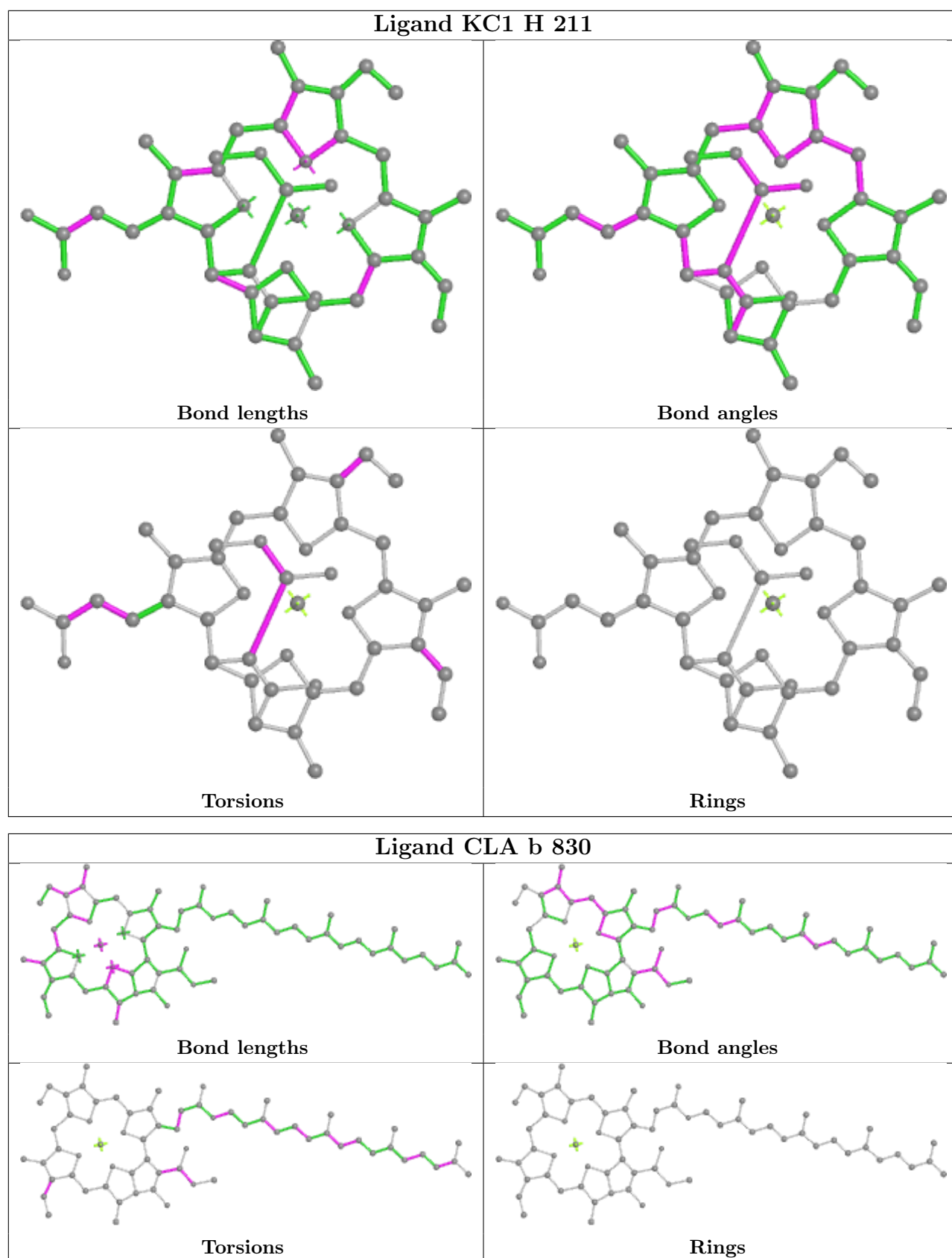
Ligand SF4 c 102



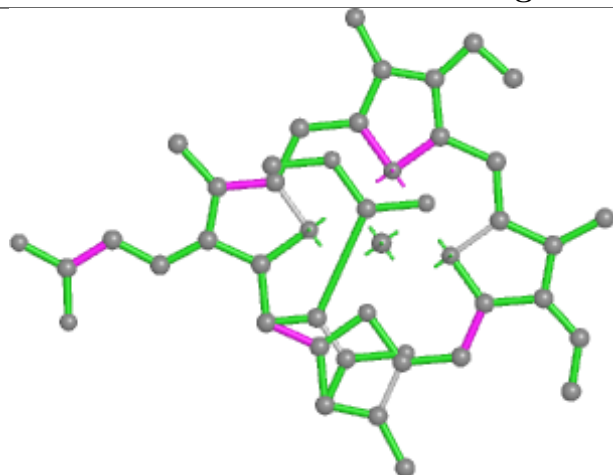




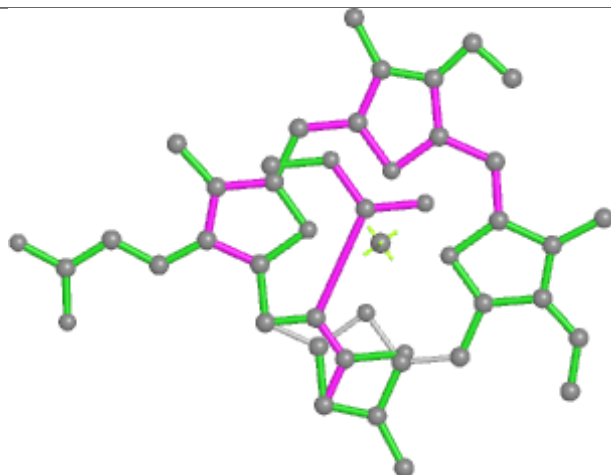
Ligand CLA J 312**Ligand CLA a 841**



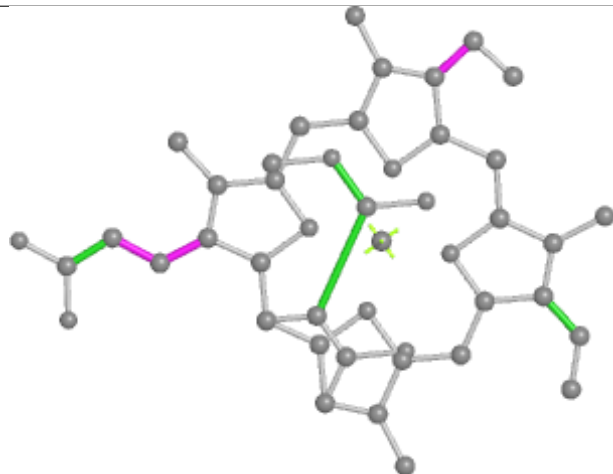
Ligand KC1 G 313



Bond lengths



Bond angles

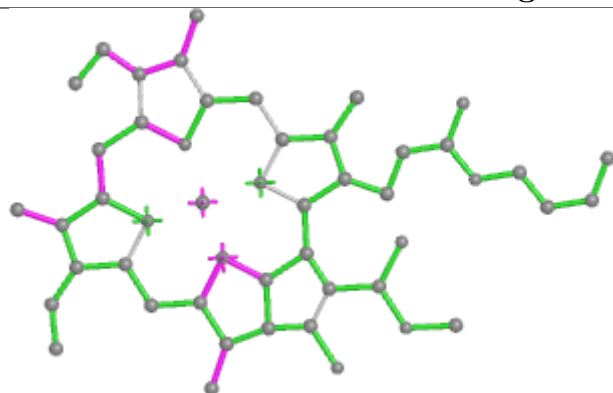


Torsions

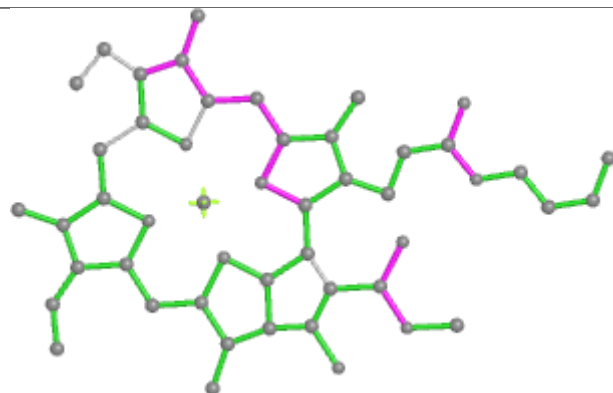


Rings

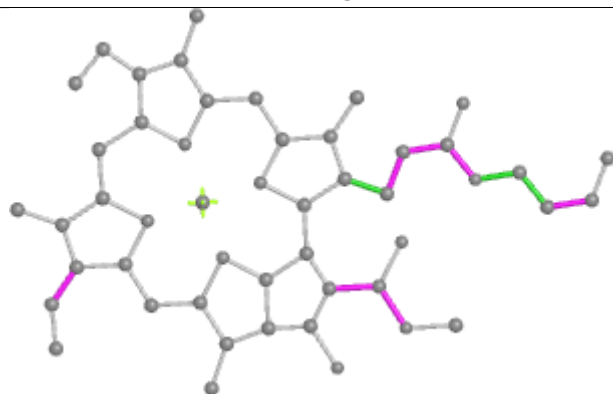
Ligand CLA J 315



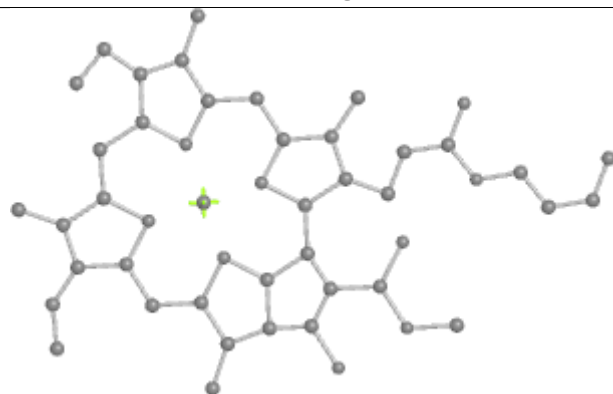
Bond lengths



Bond angles

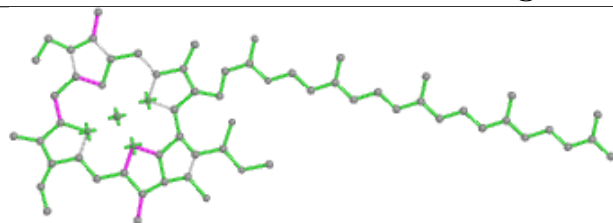


Torsions

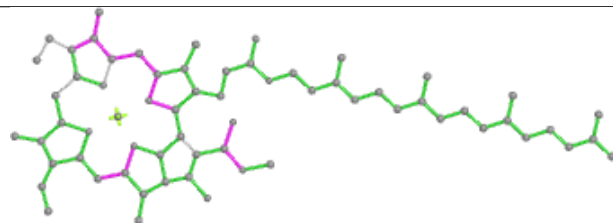


Rings

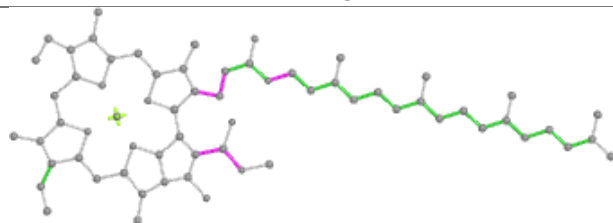
Ligand CLA b 842



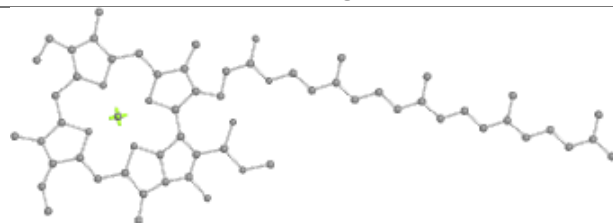
Bond lengths



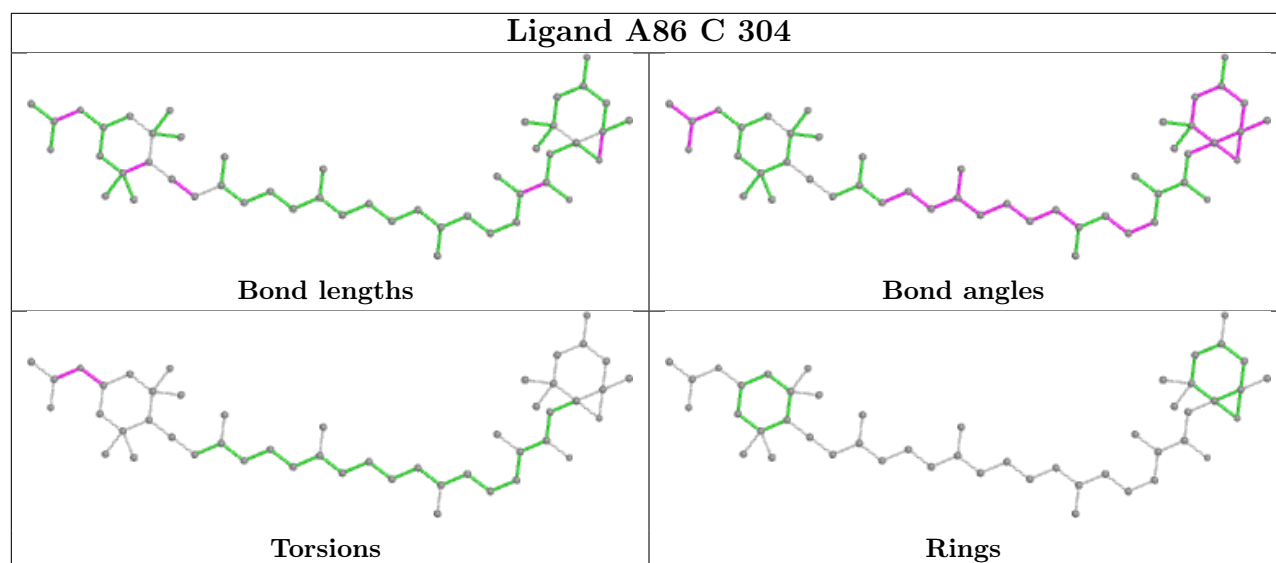
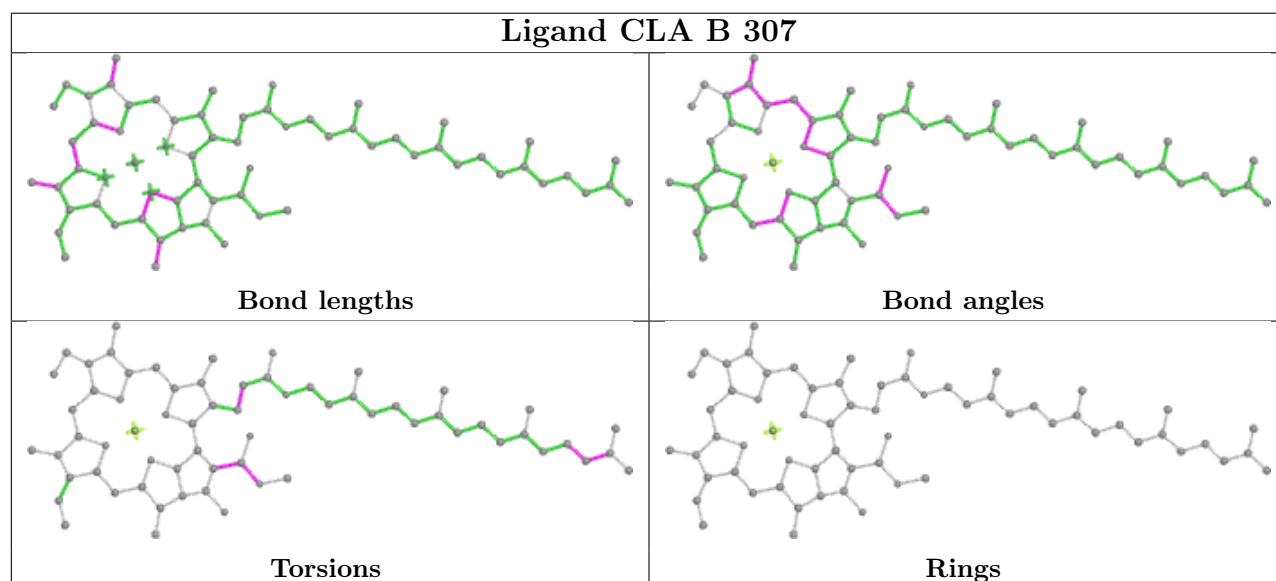
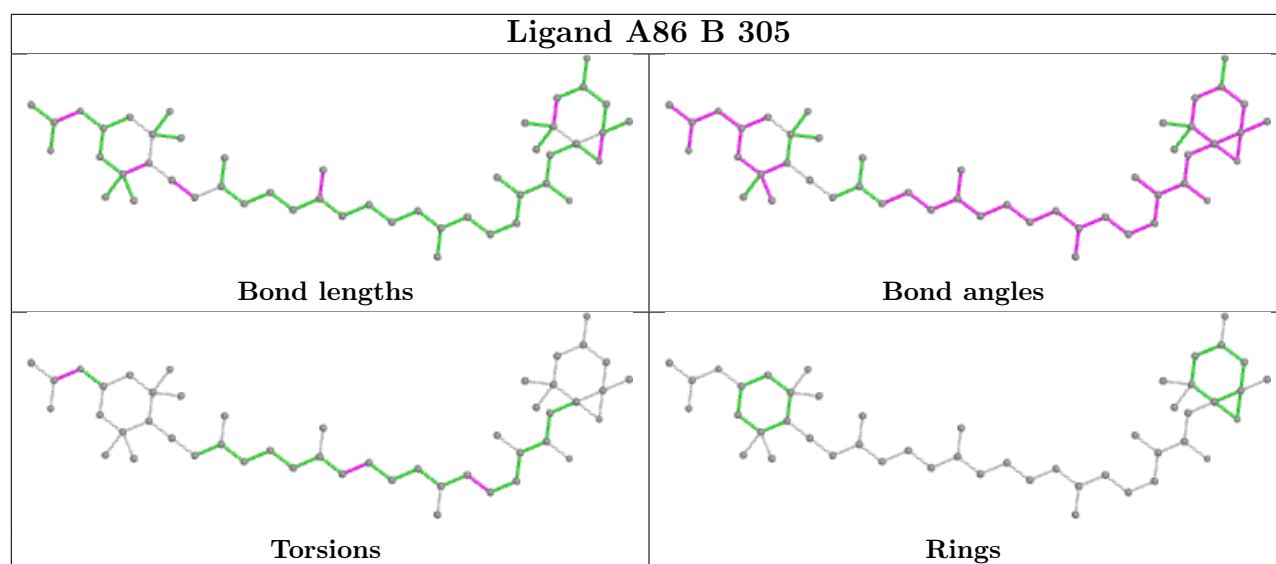
Bond angles



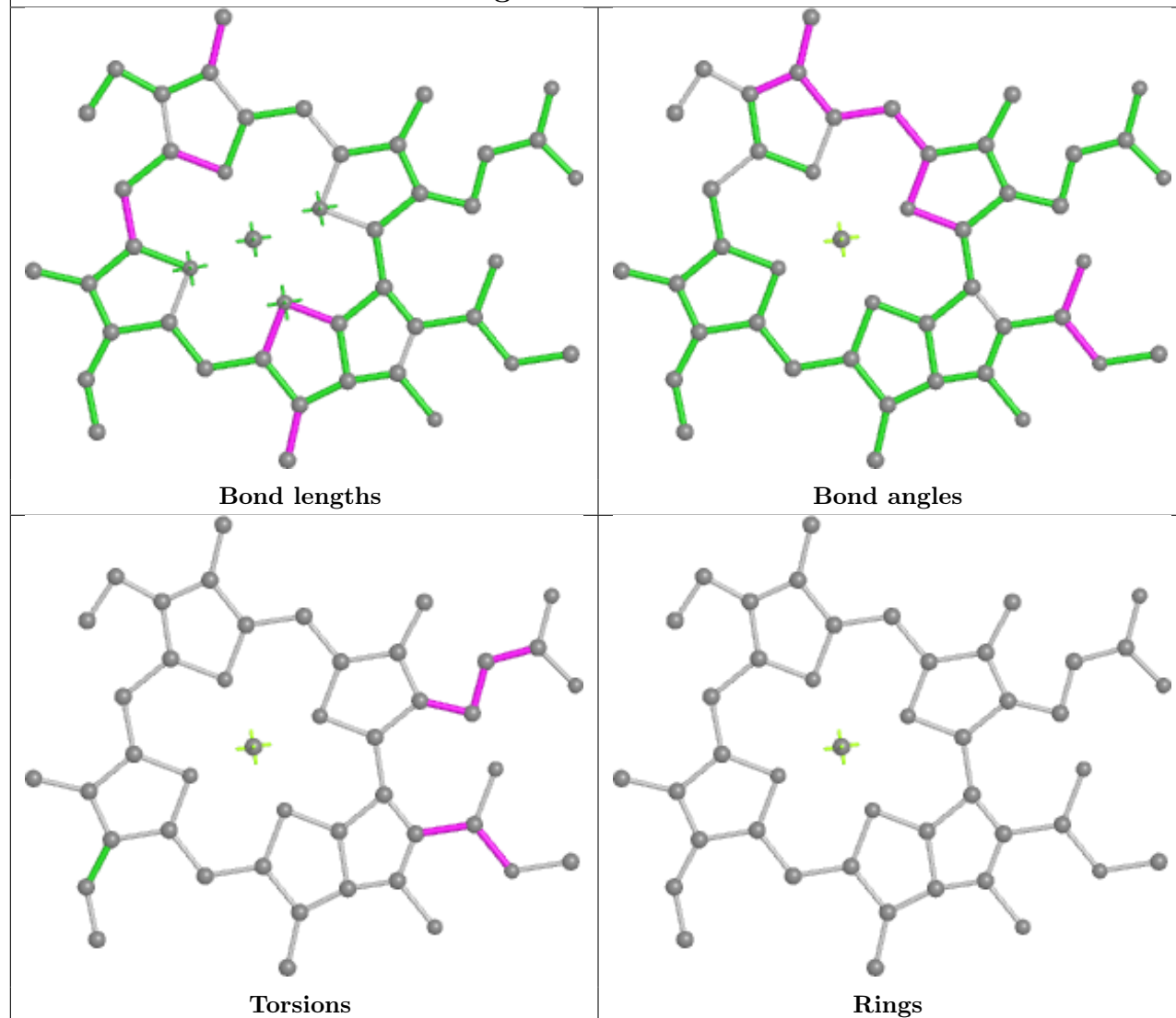
Torsions



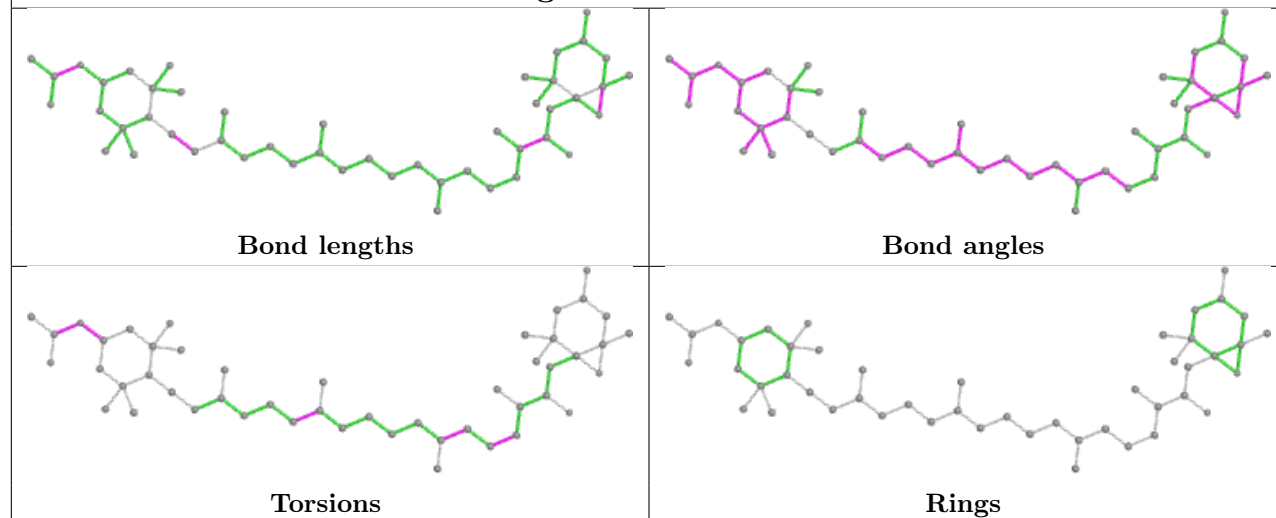
Rings



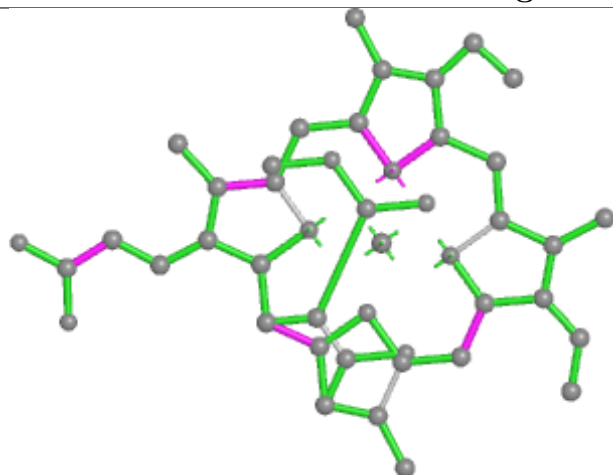
Ligand CLA a 818



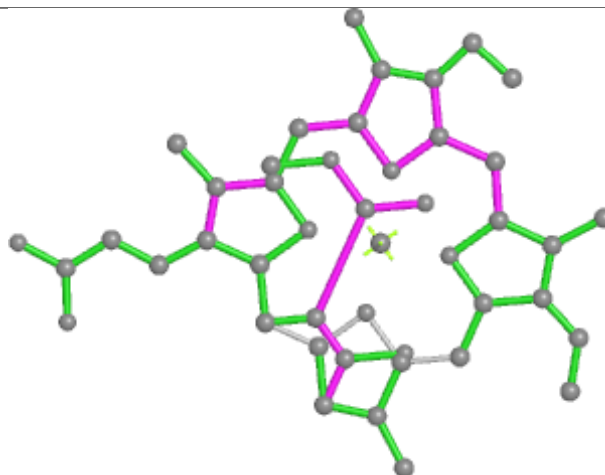
Ligand A86 K 302



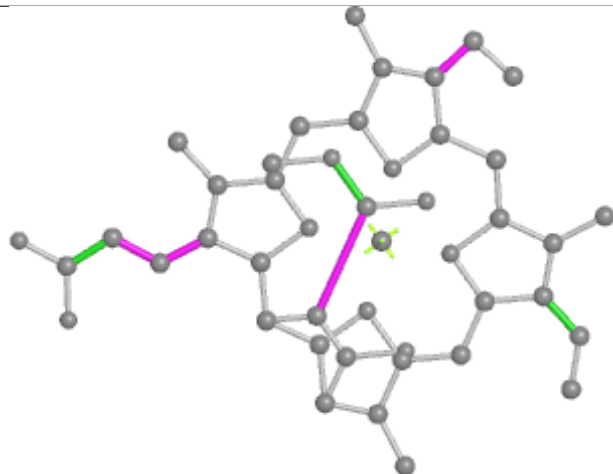
Ligand KC1 C 308



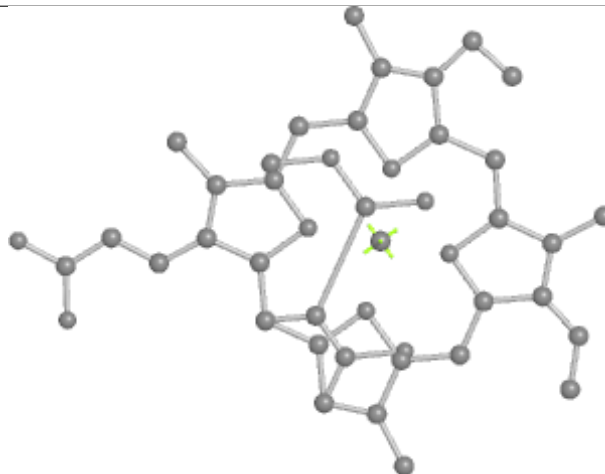
Bond lengths



Bond angles

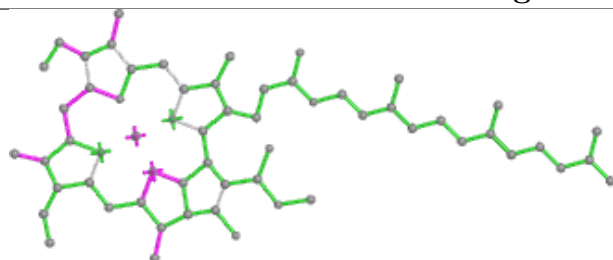


Torsions

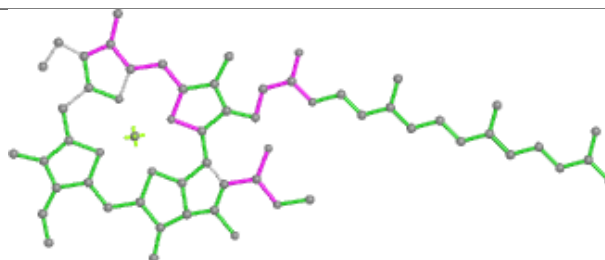


Rings

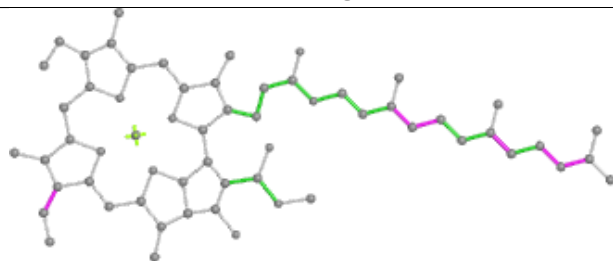
Ligand CLA H 209



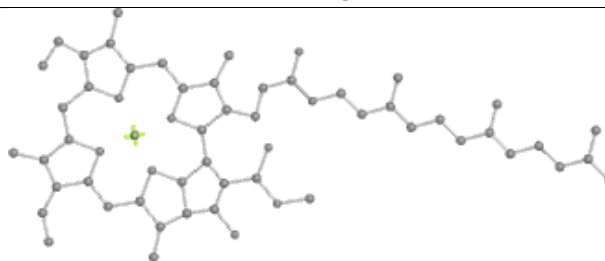
Bond lengths



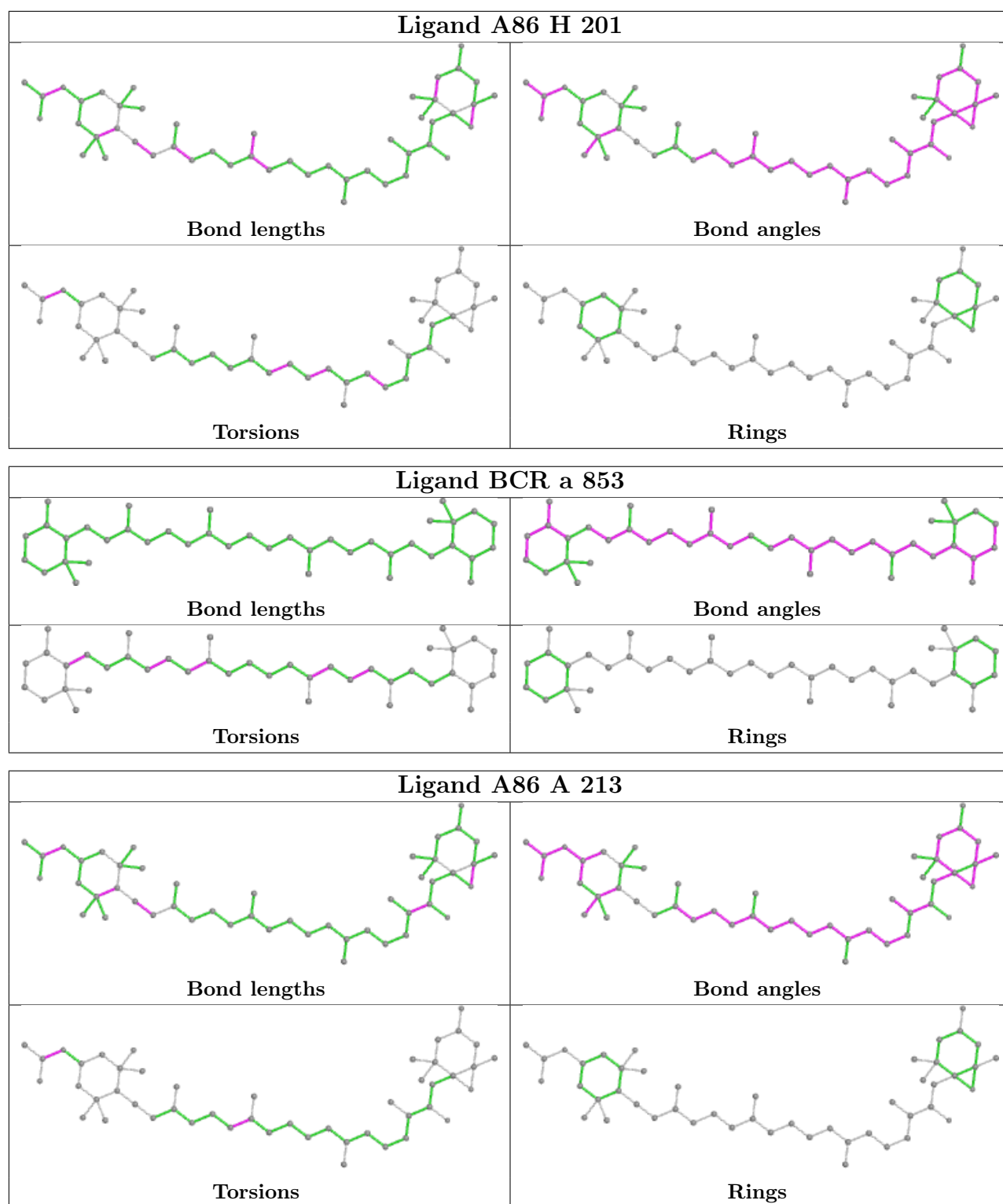
Bond angles



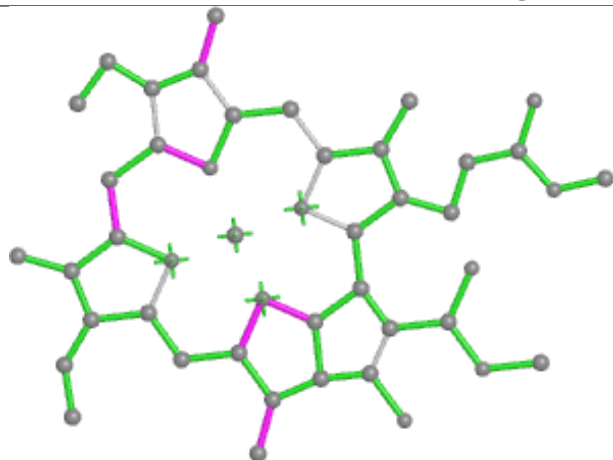
Torsions



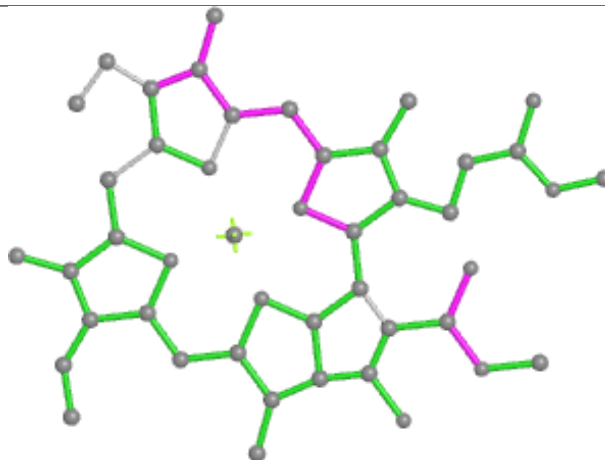
Rings



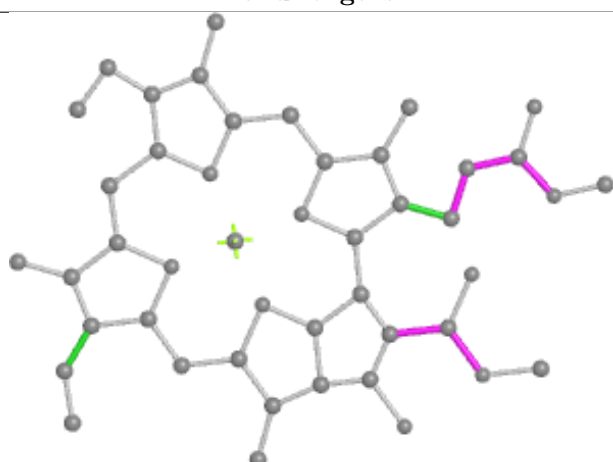
Ligand CLA H 208



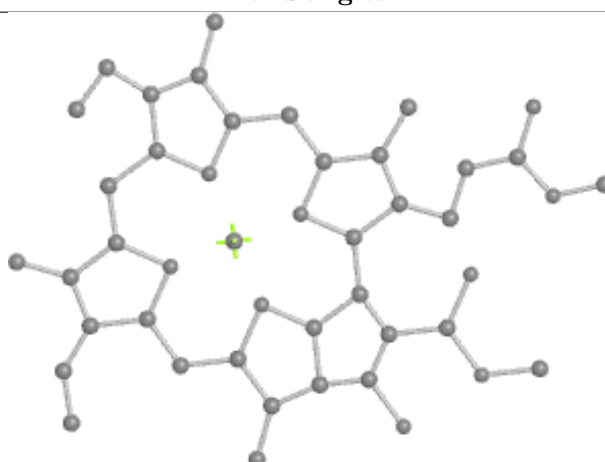
Bond lengths



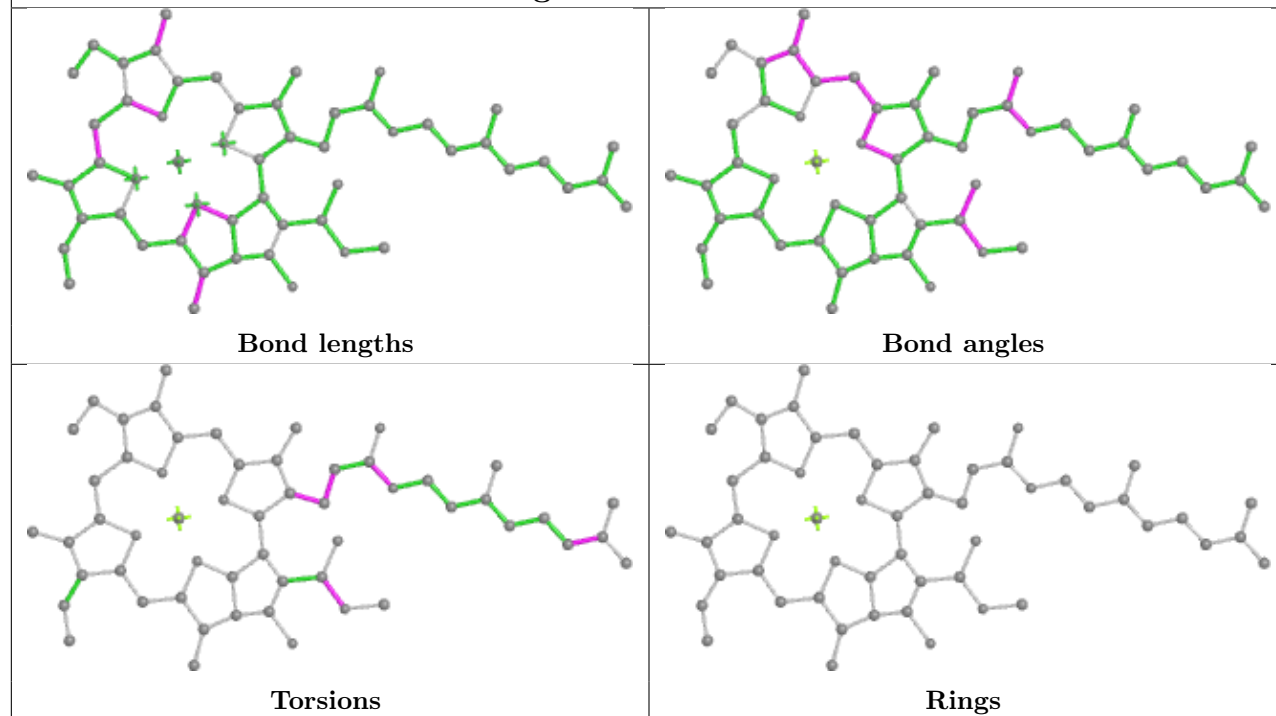
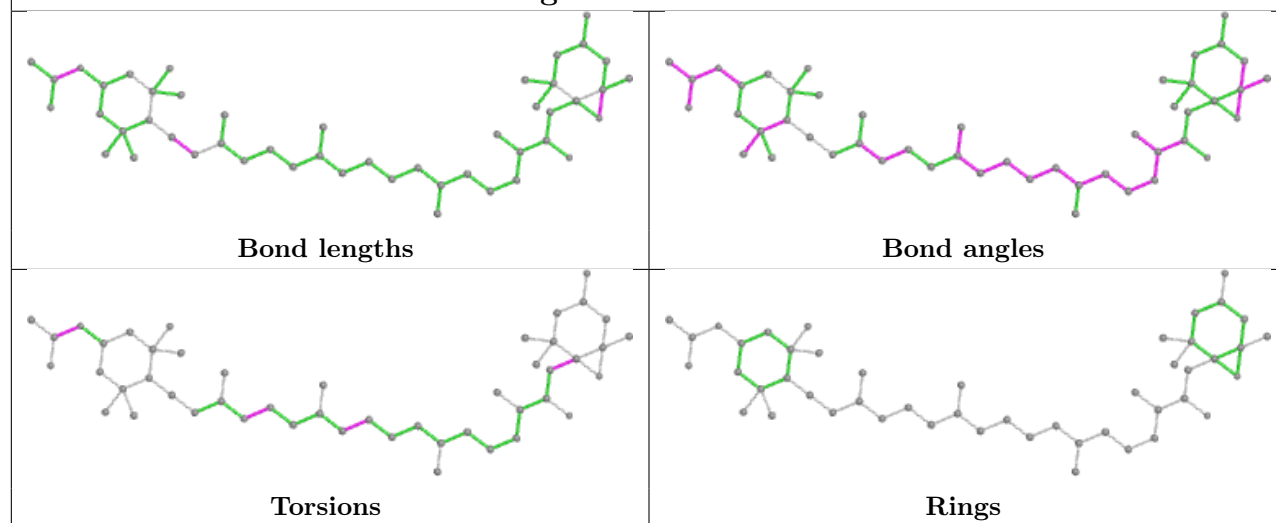
Bond angles



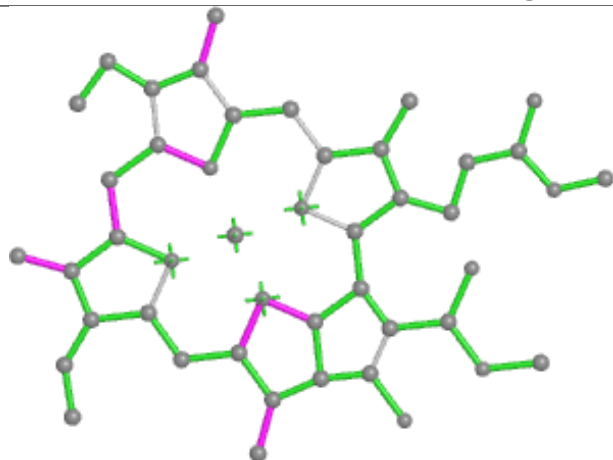
Torsions



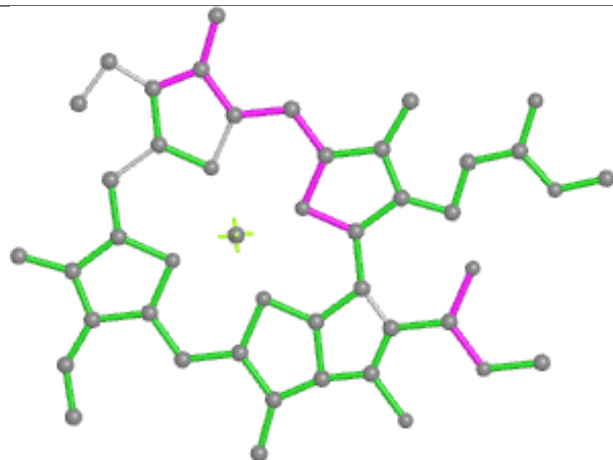
Rings

Ligand CLA E 312**Ligand A86 L 306**

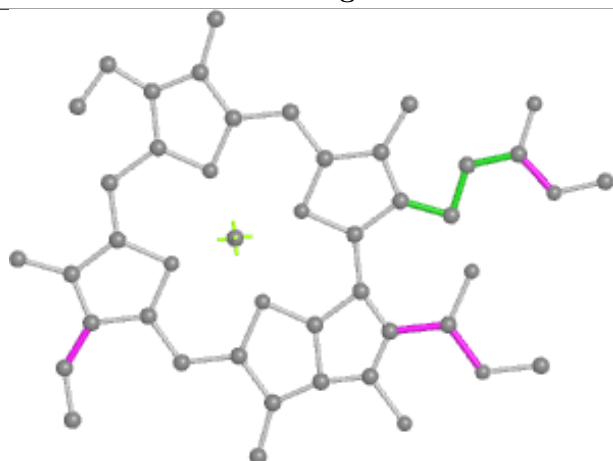
Ligand CLA I 317



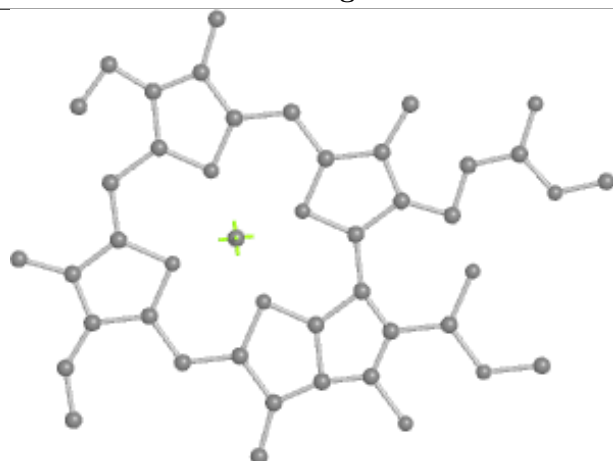
Bond lengths



Bond angles

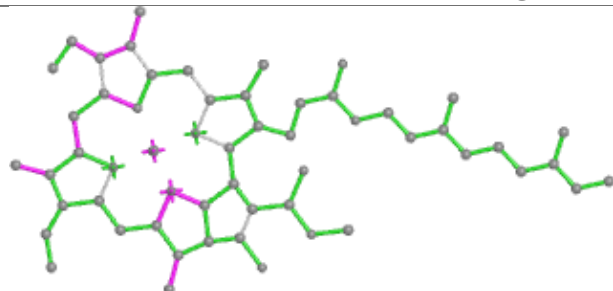


Torsions

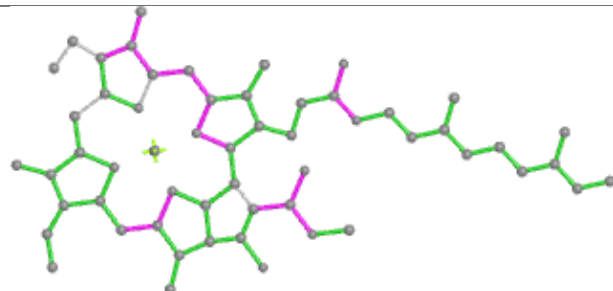


Rings

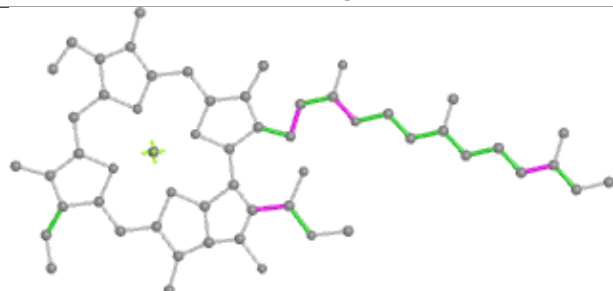
Ligand CLA D 210



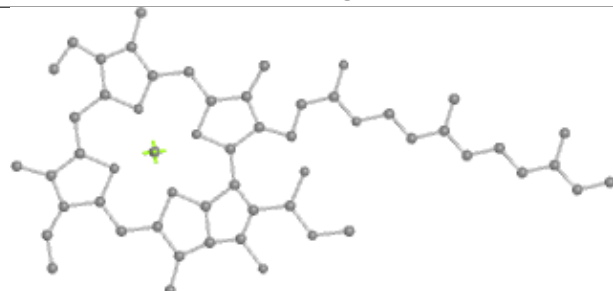
Bond lengths



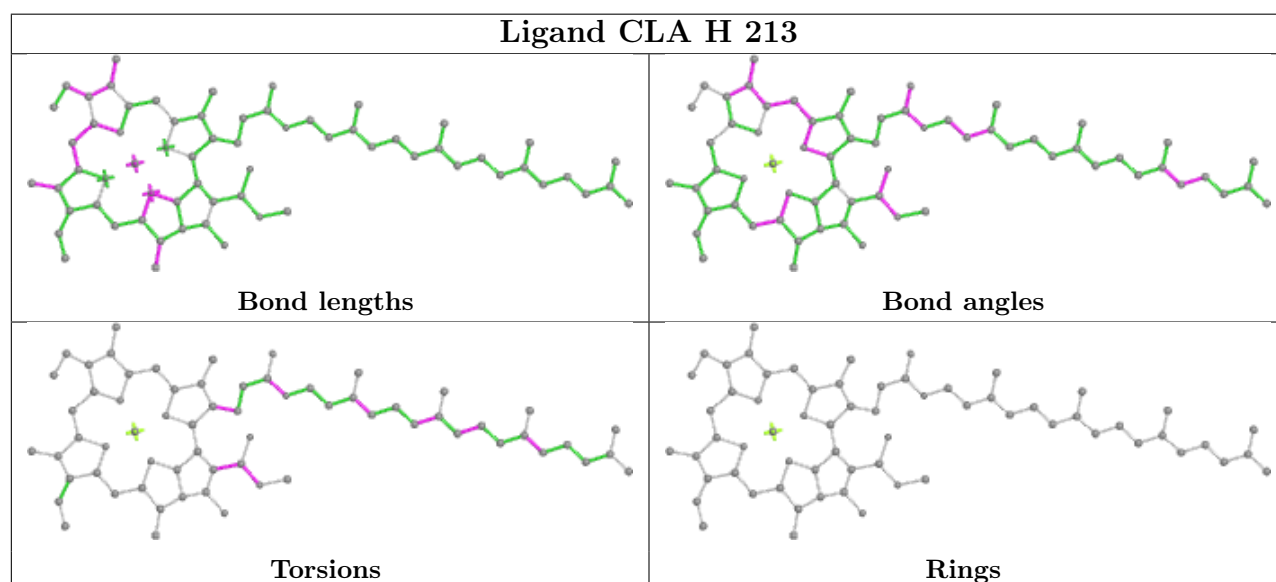
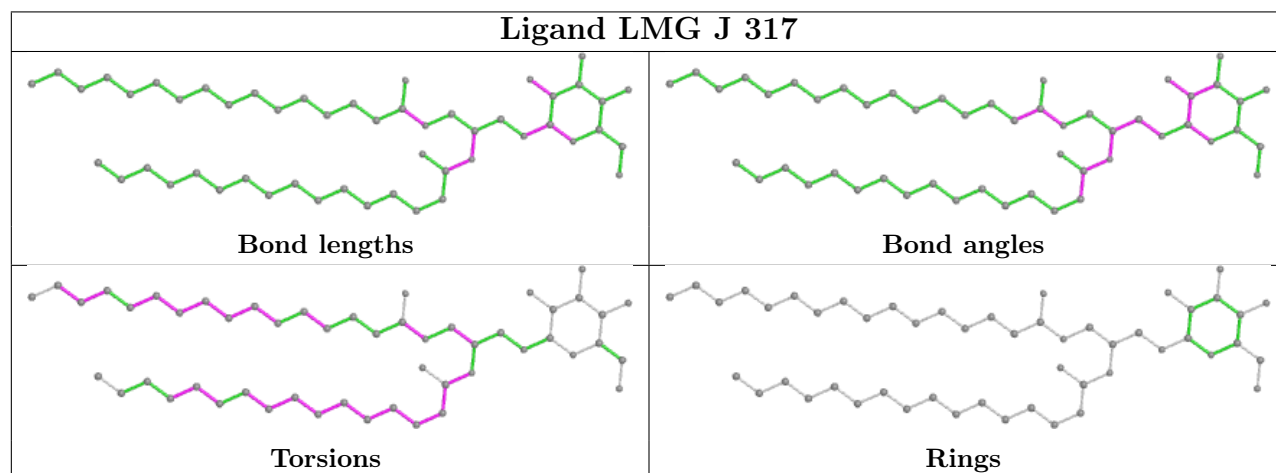
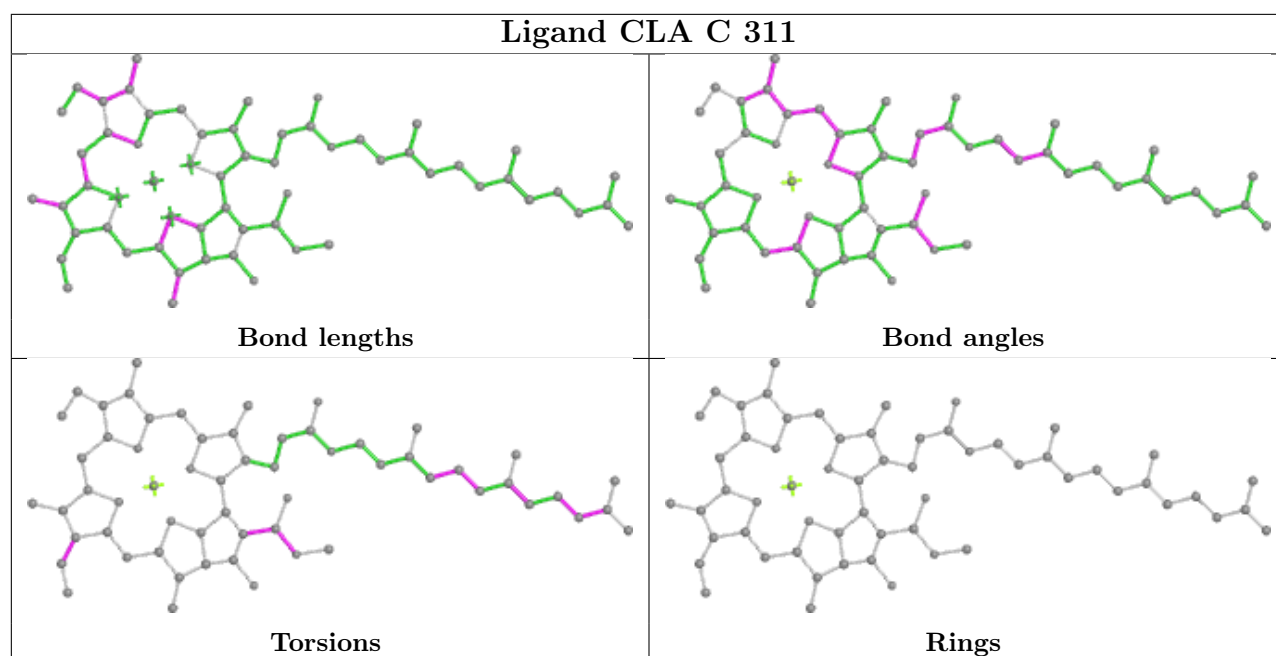
Bond angles



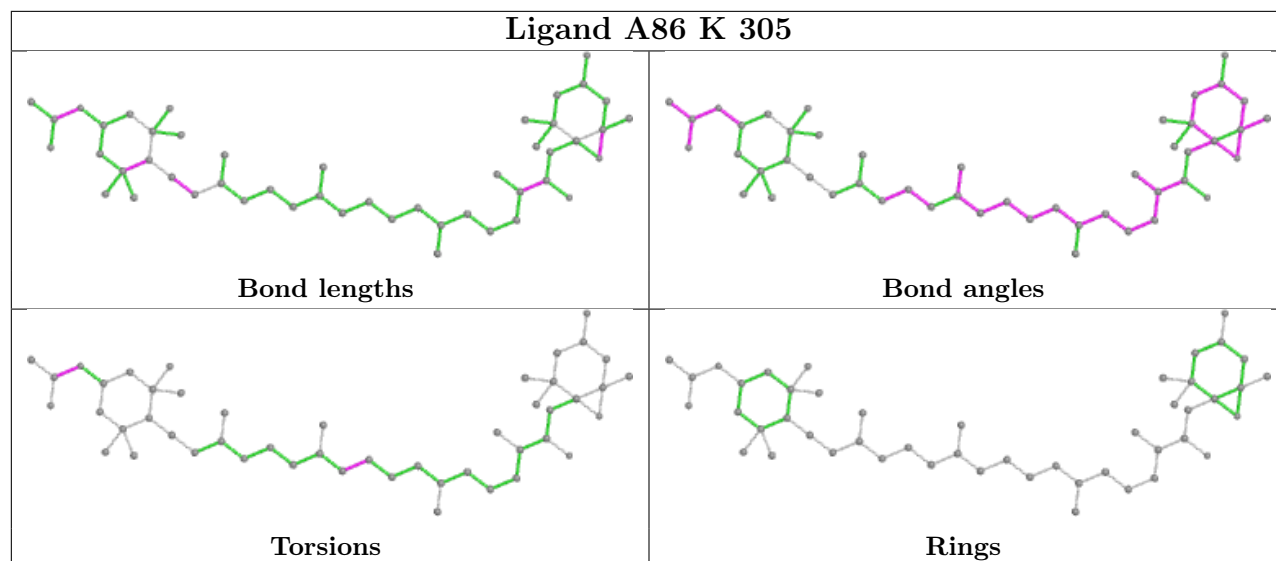
Torsions



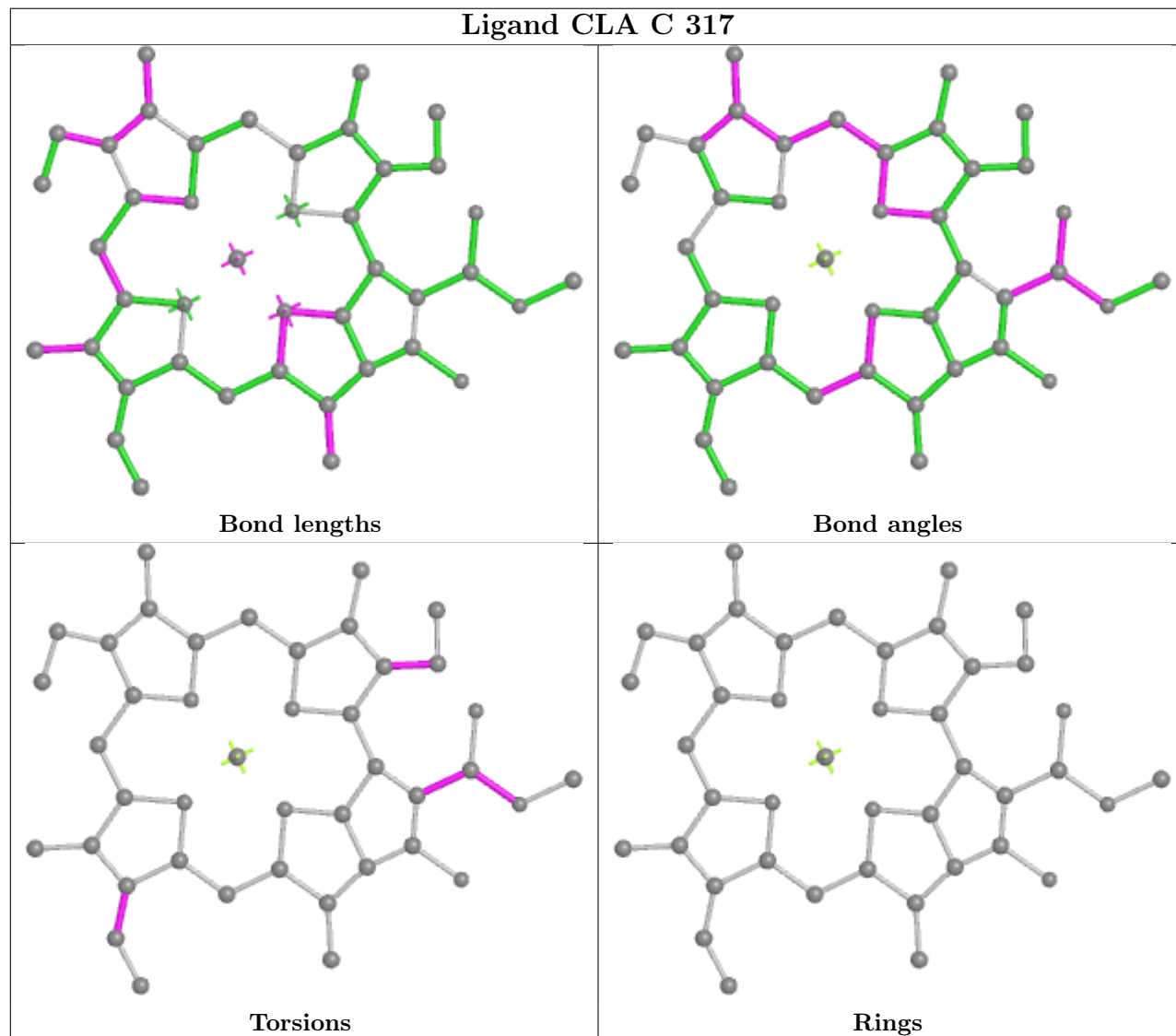
Rings

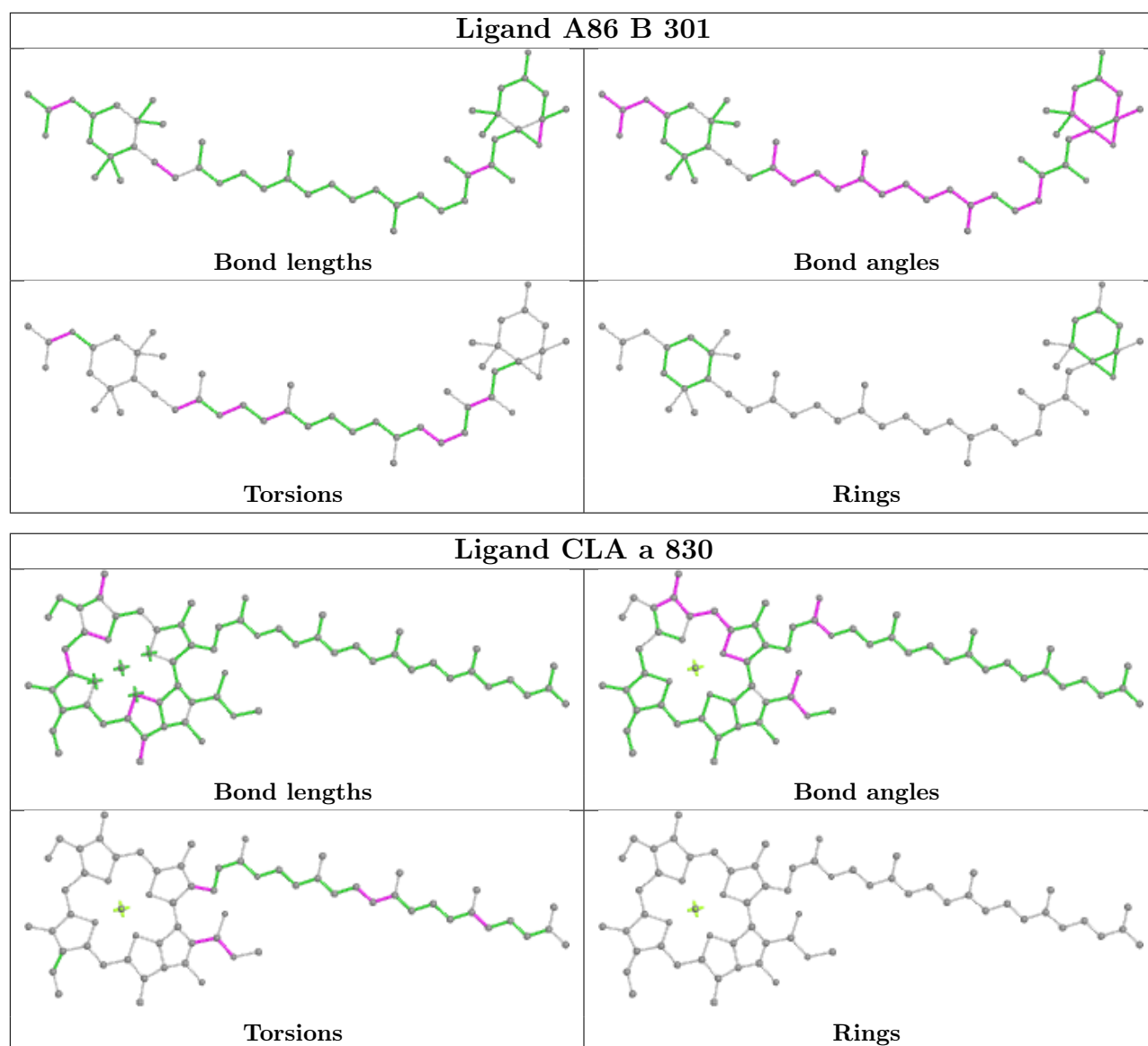


Ligand A86 K 305

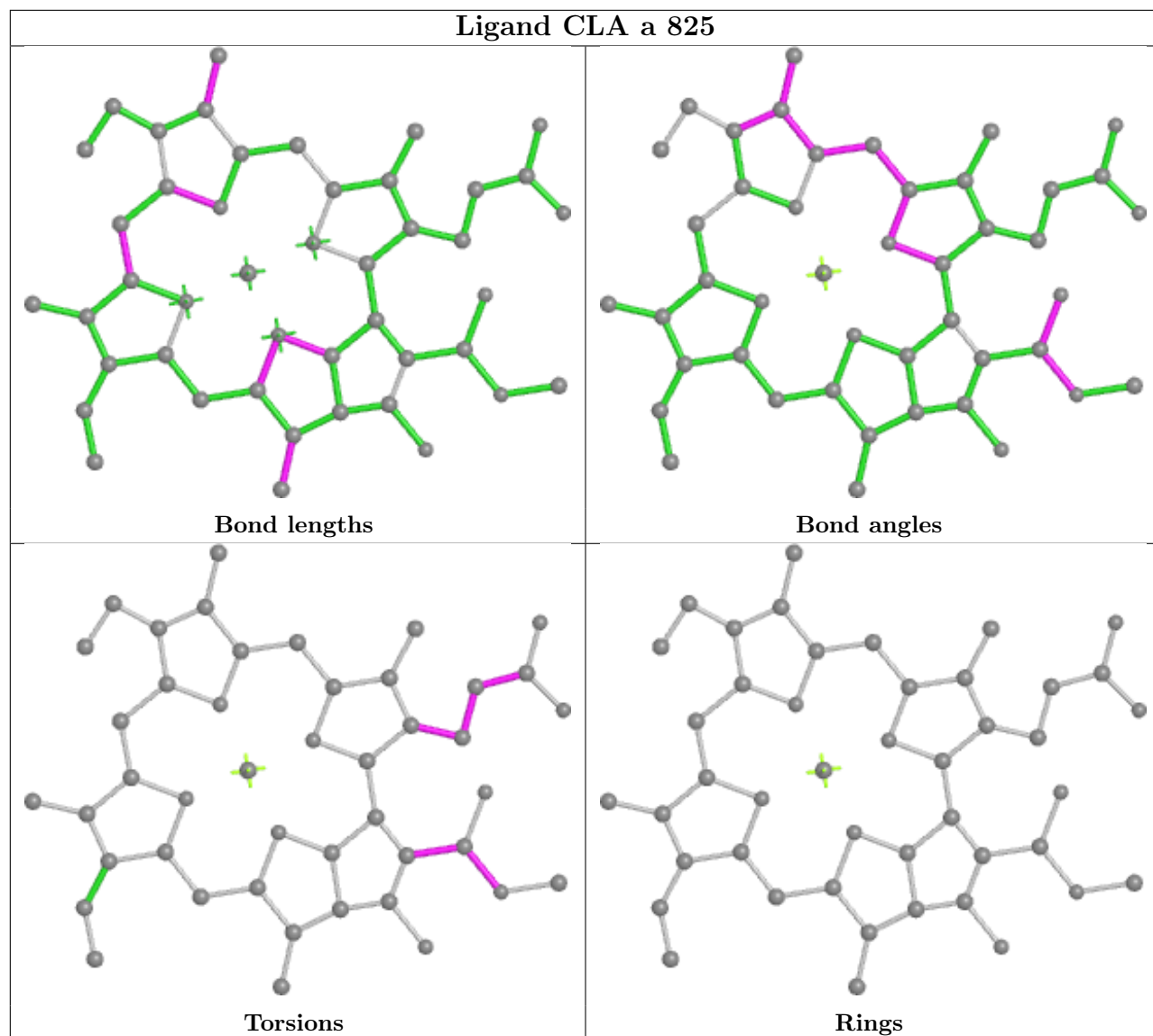


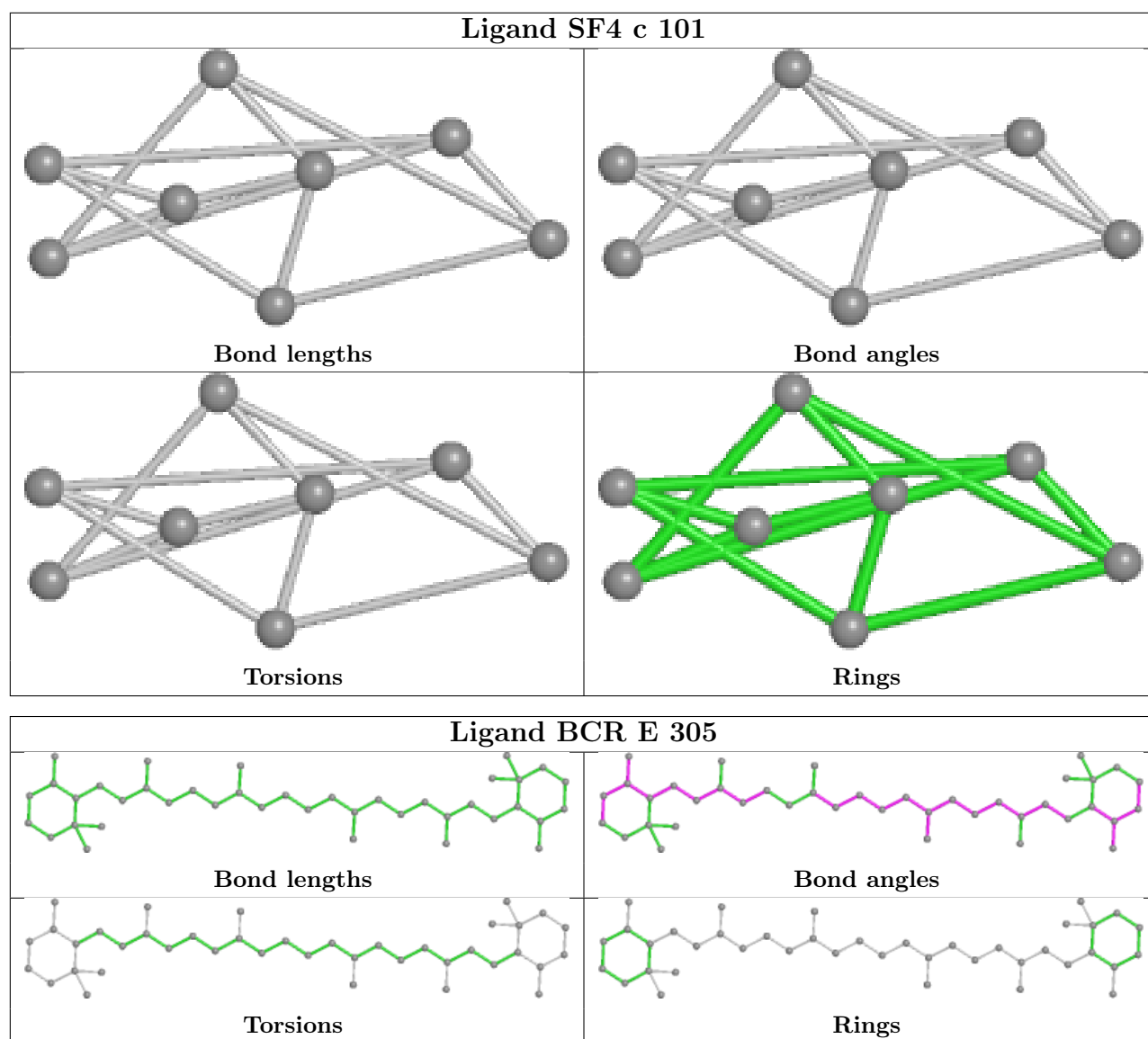
Ligand CLA C 317



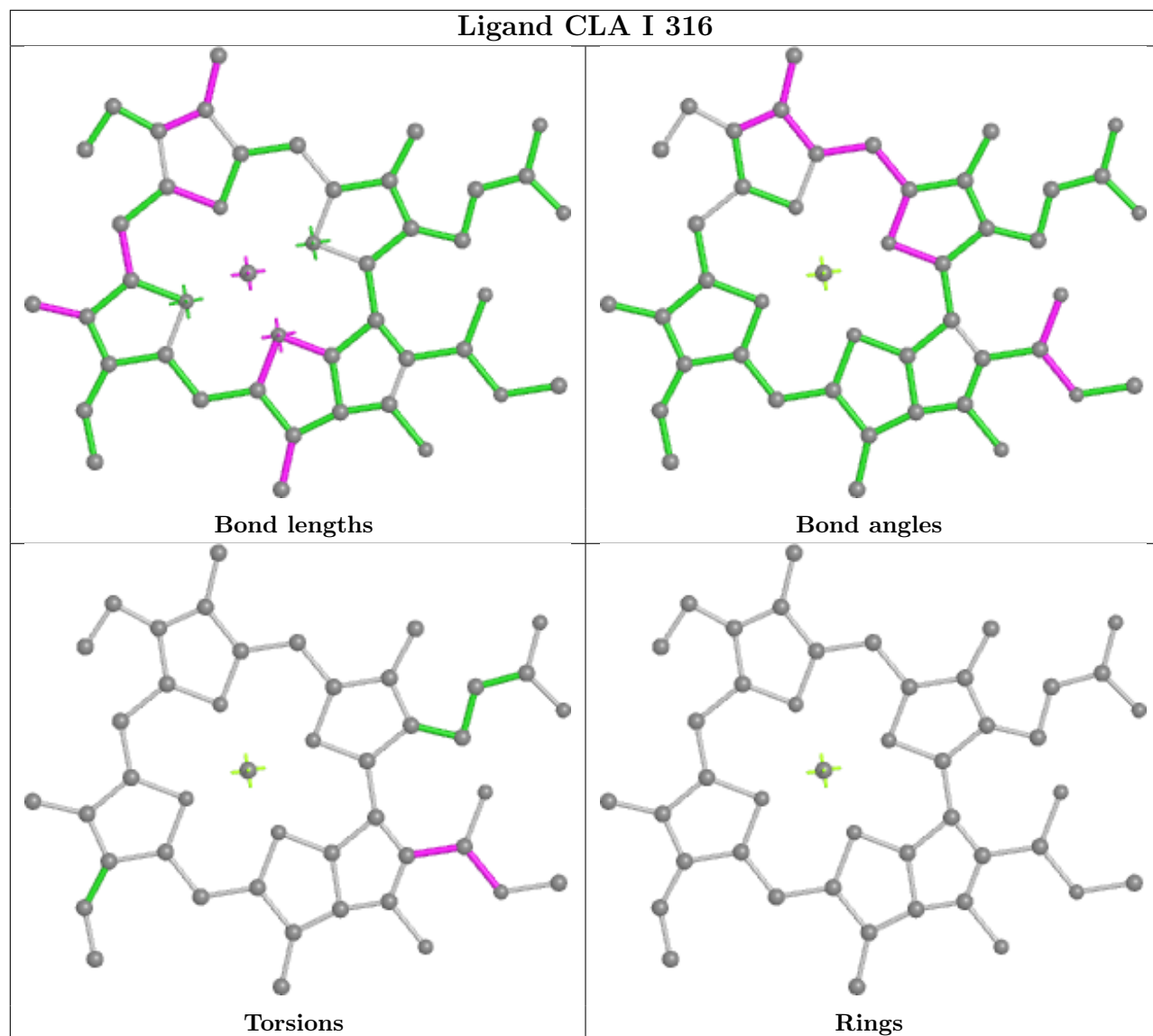


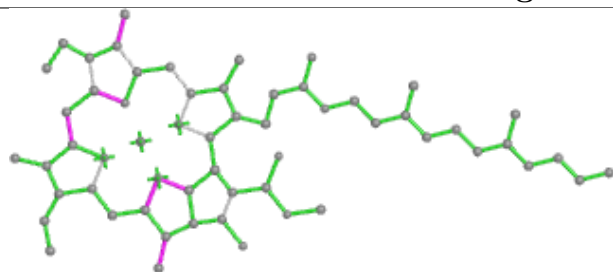
Ligand CLA a 825



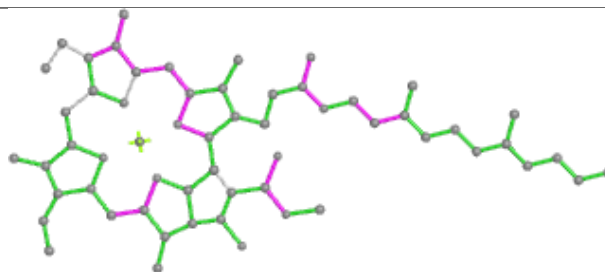


Ligand CLA I 316

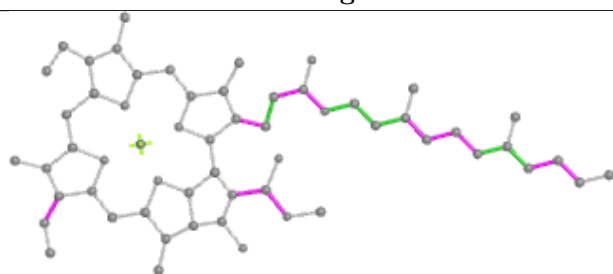


Ligand CLA F 315

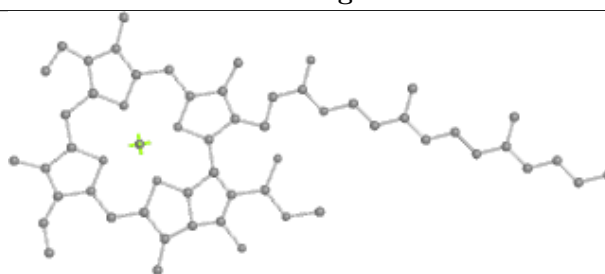
Bond lengths



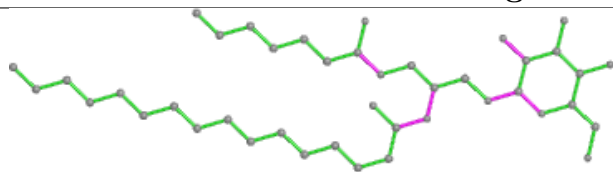
Bond angles



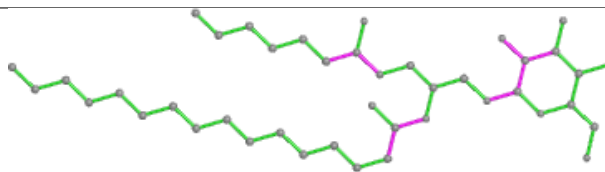
Torsions



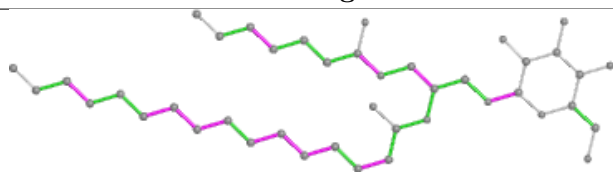
Rings

Ligand LMG M 321

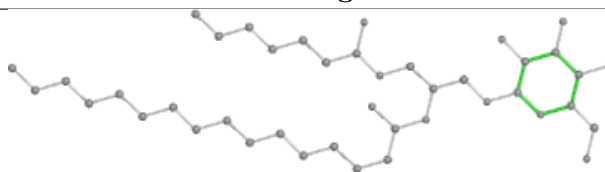
Bond lengths



Bond angles

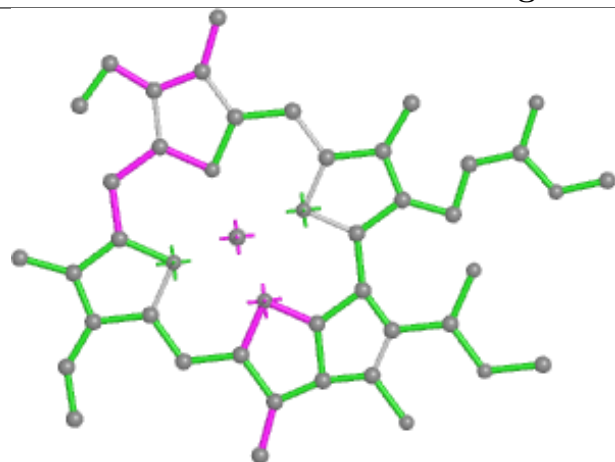


Torsions

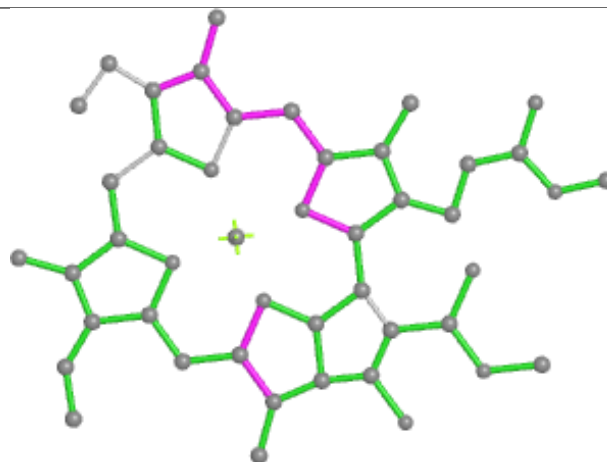


Rings

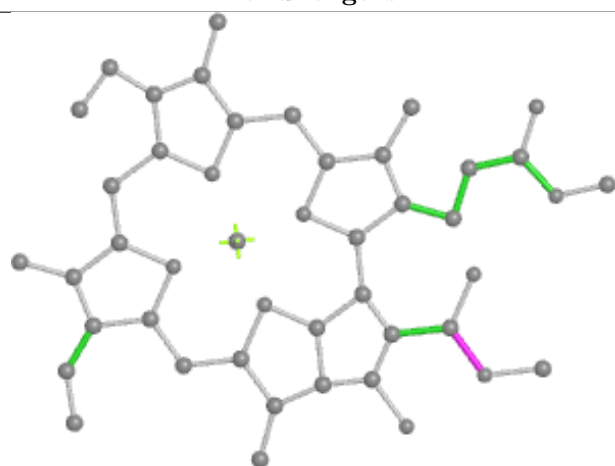
Ligand CLA F 309



Bond lengths



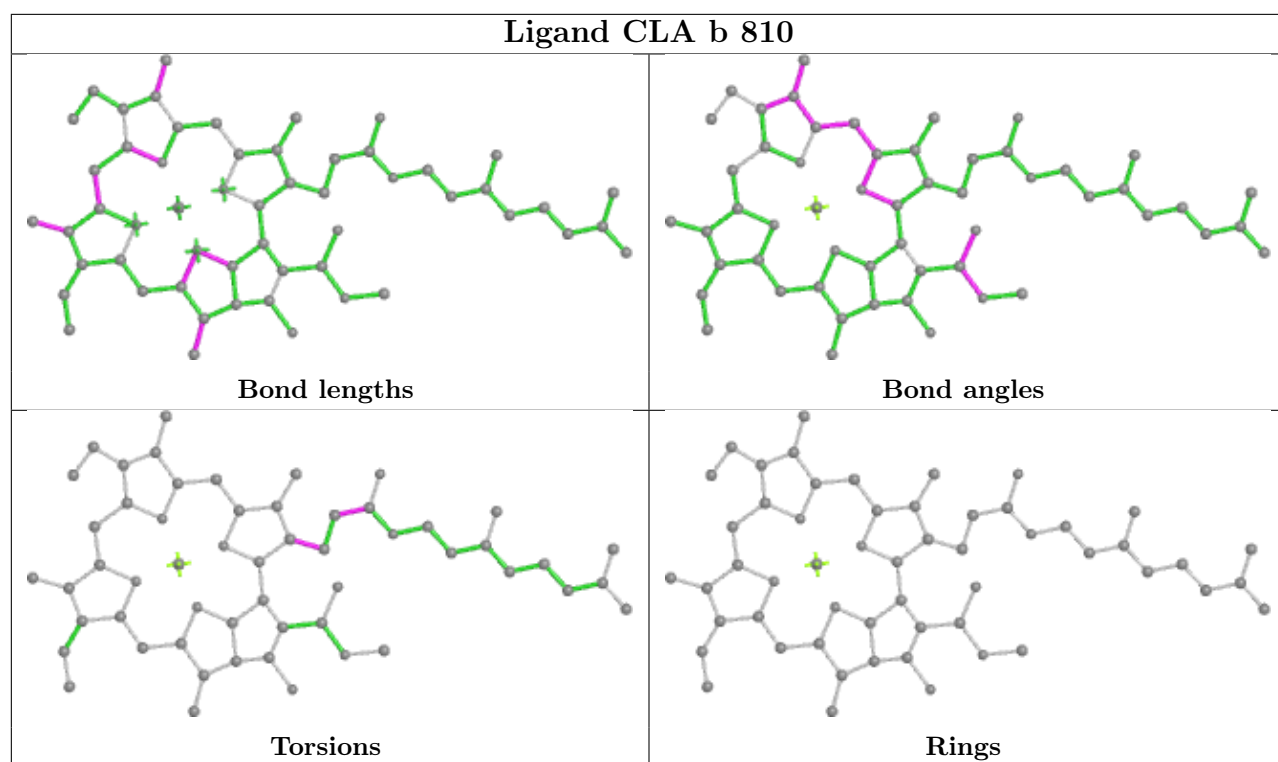
Bond angles



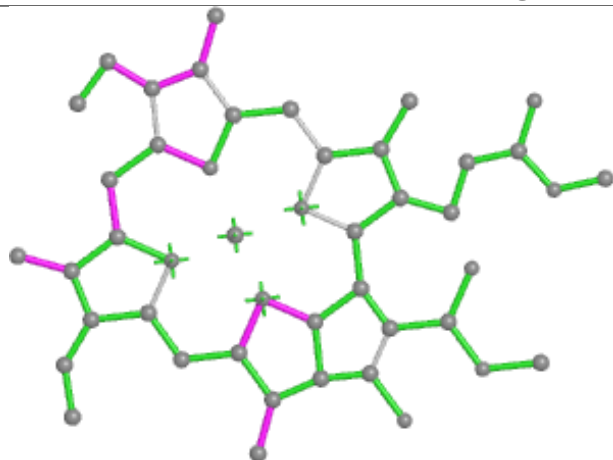
Torsions



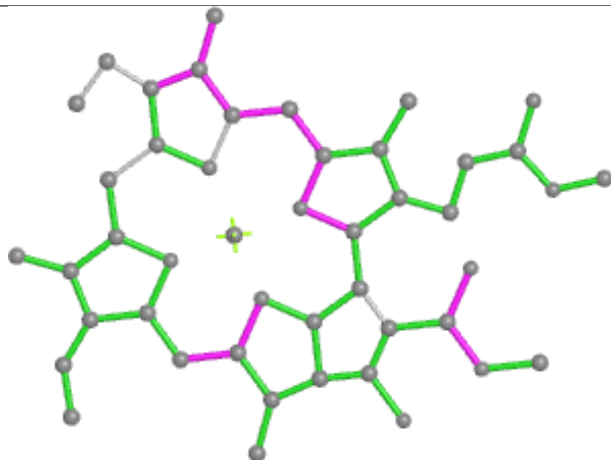
Rings



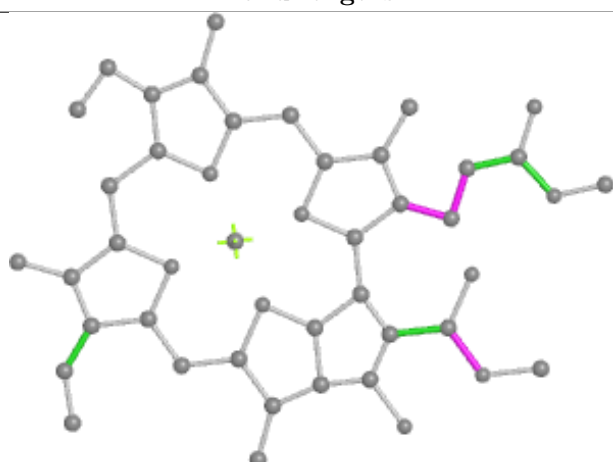
Ligand CLA A 210



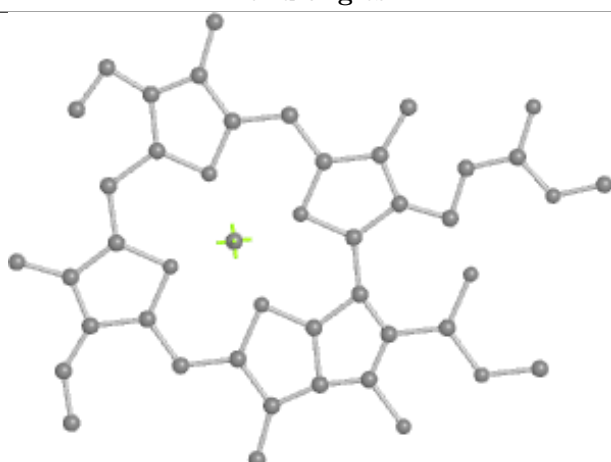
Bond lengths



Bond angles

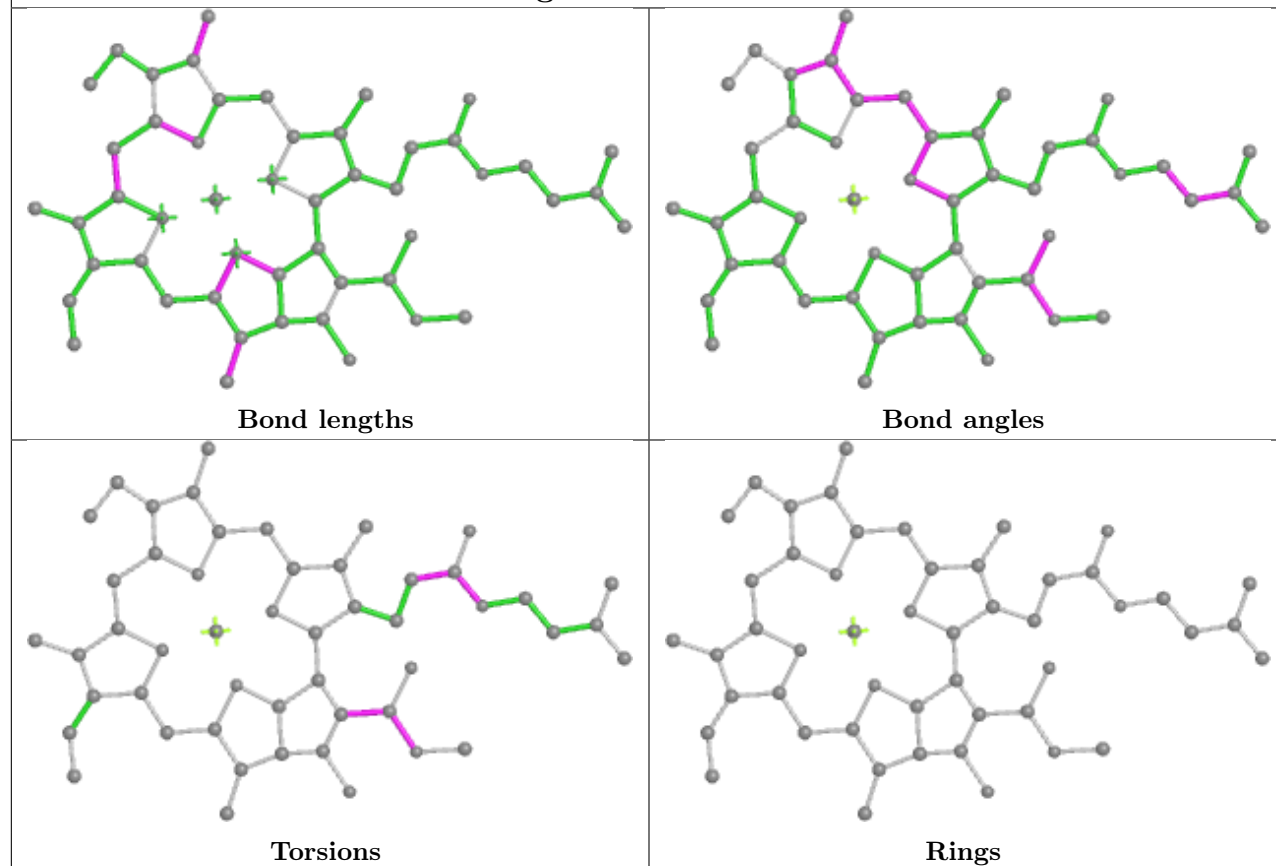


Torsions

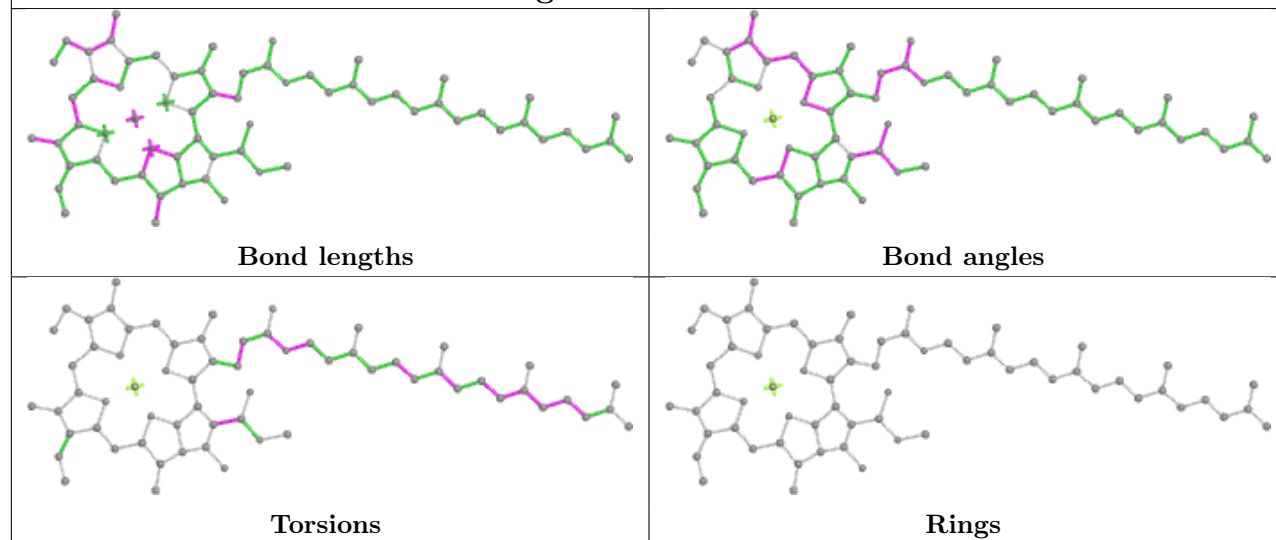


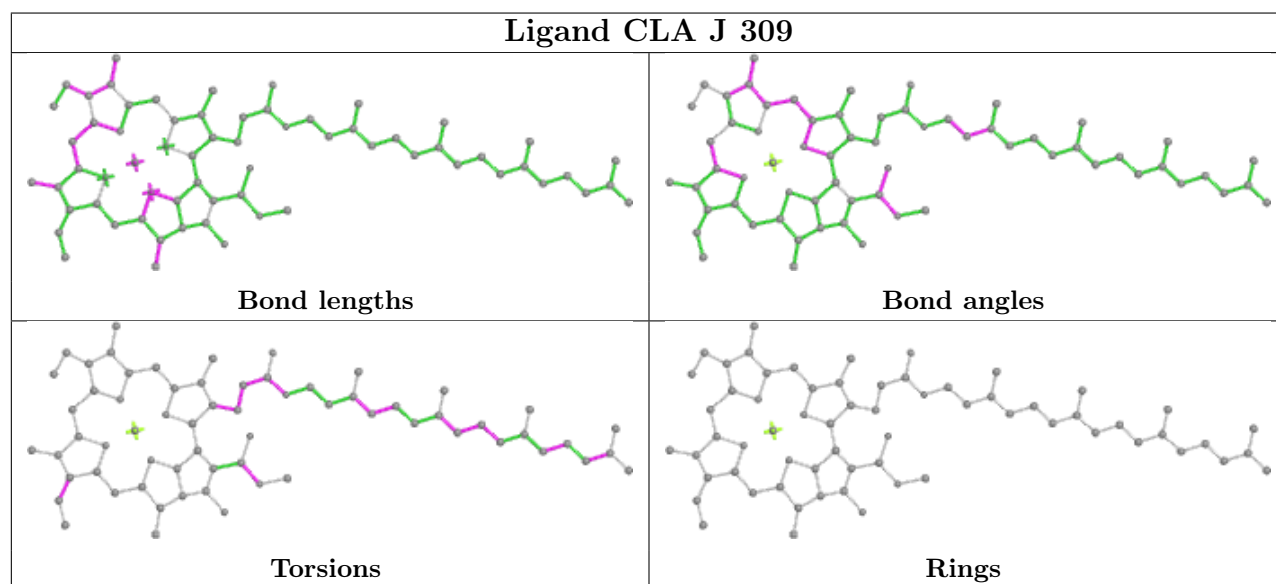
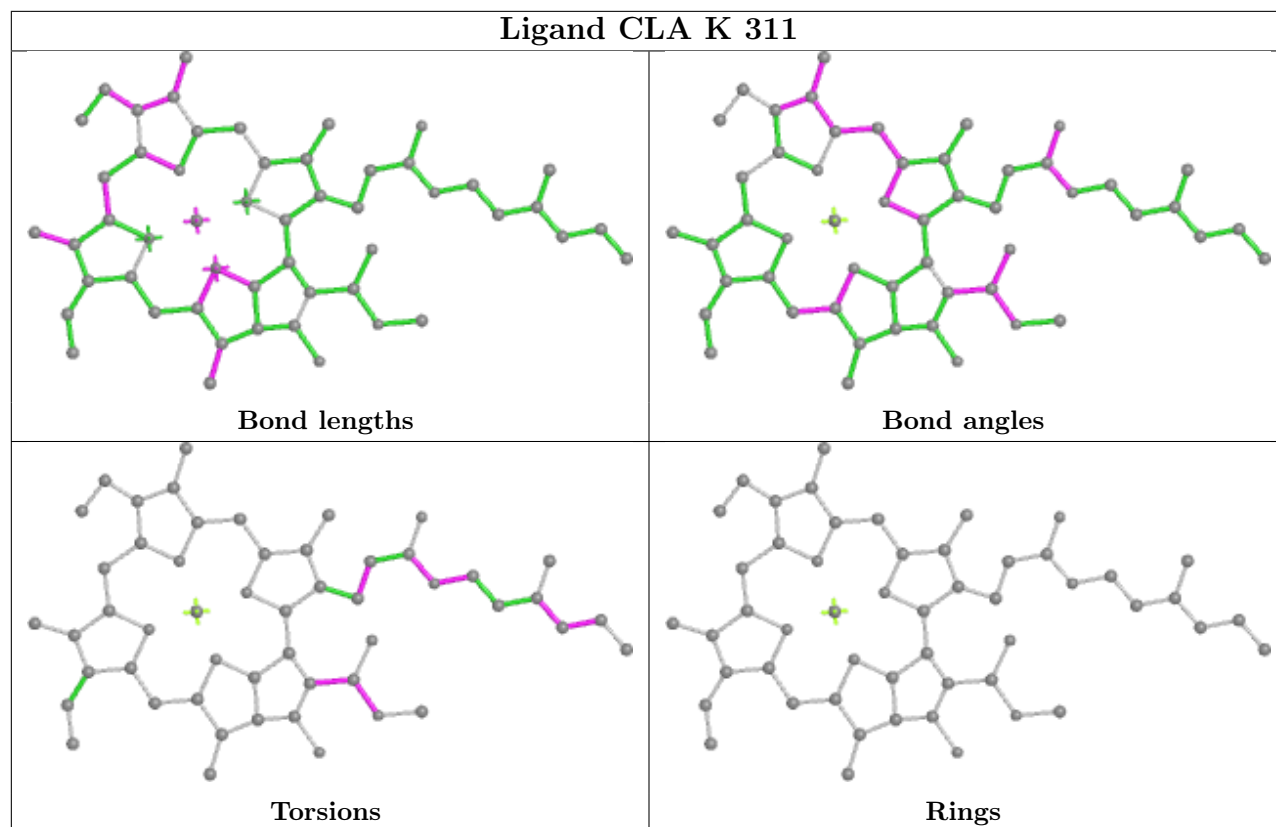
Rings

Ligand CLA a 813

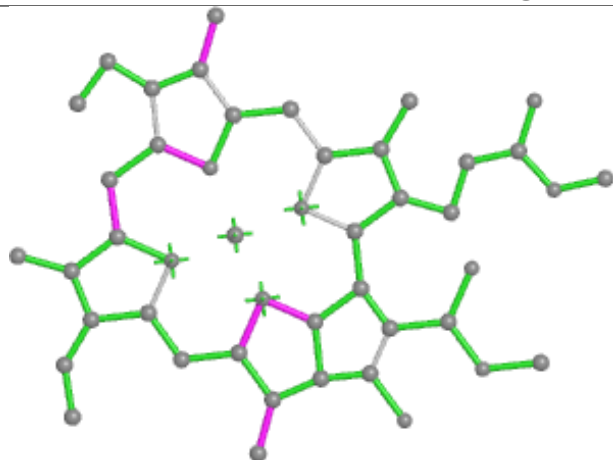


Ligand CLA a 805

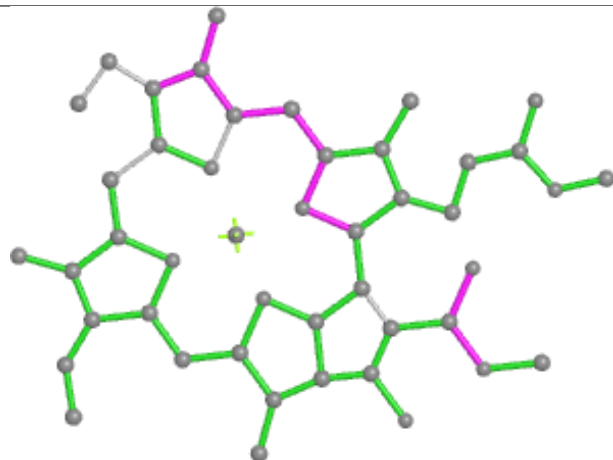




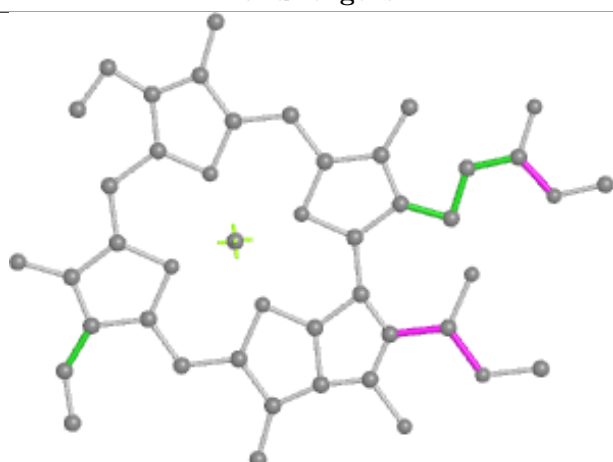
Ligand CLA b 816



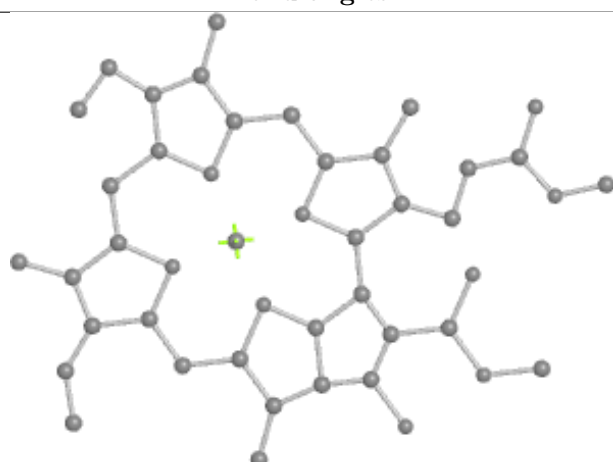
Bond lengths



Bond angles

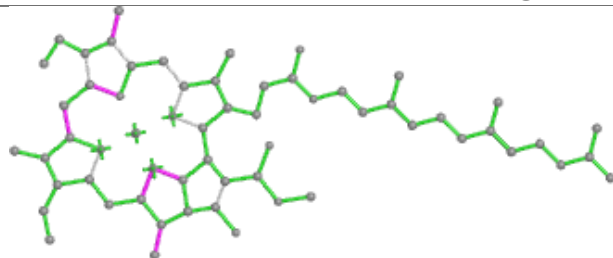


Torsions

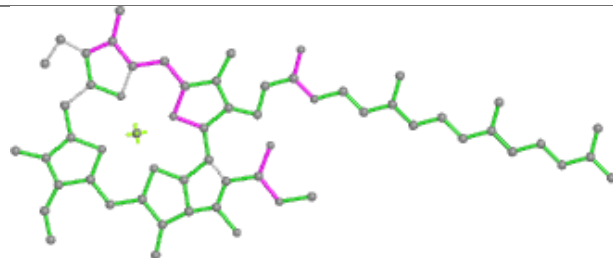


Rings

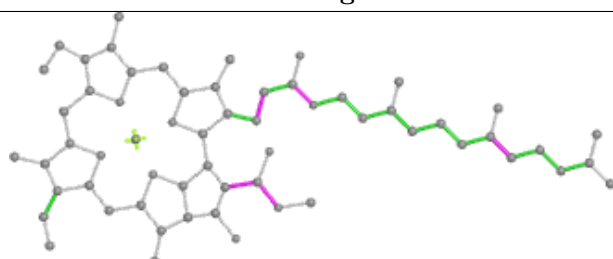
Ligand CLA b 827



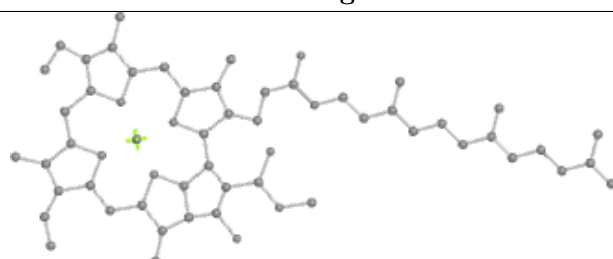
Bond lengths



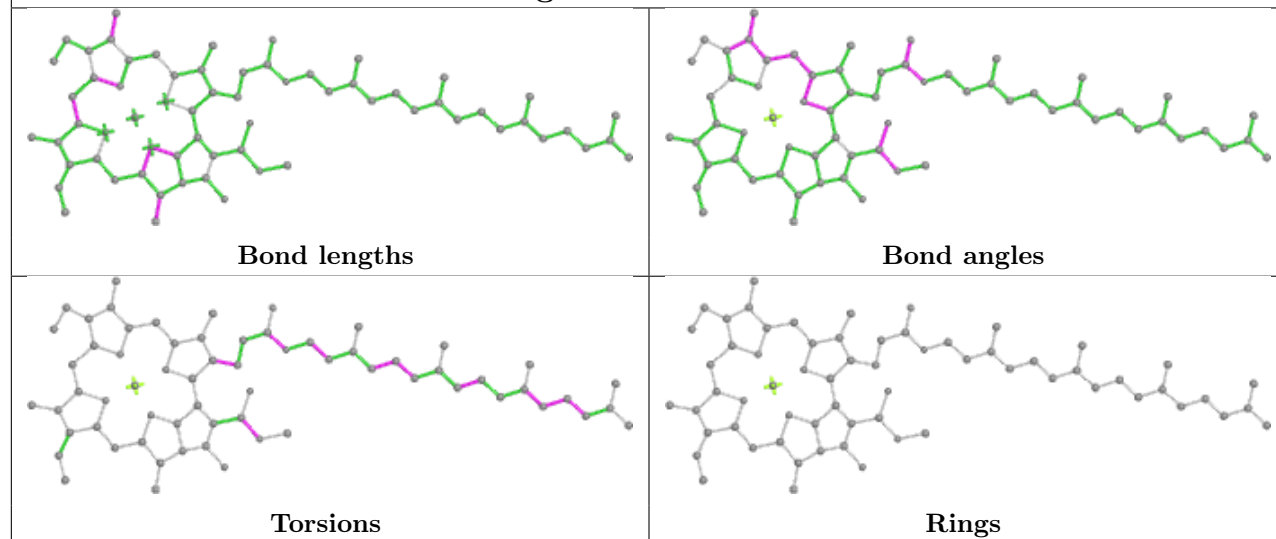
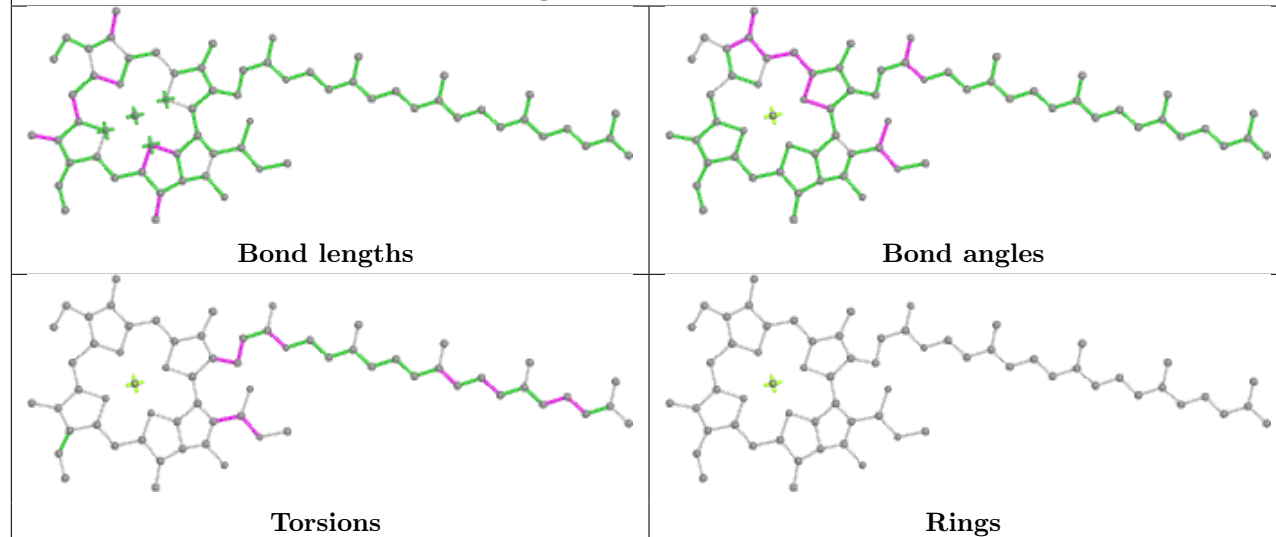
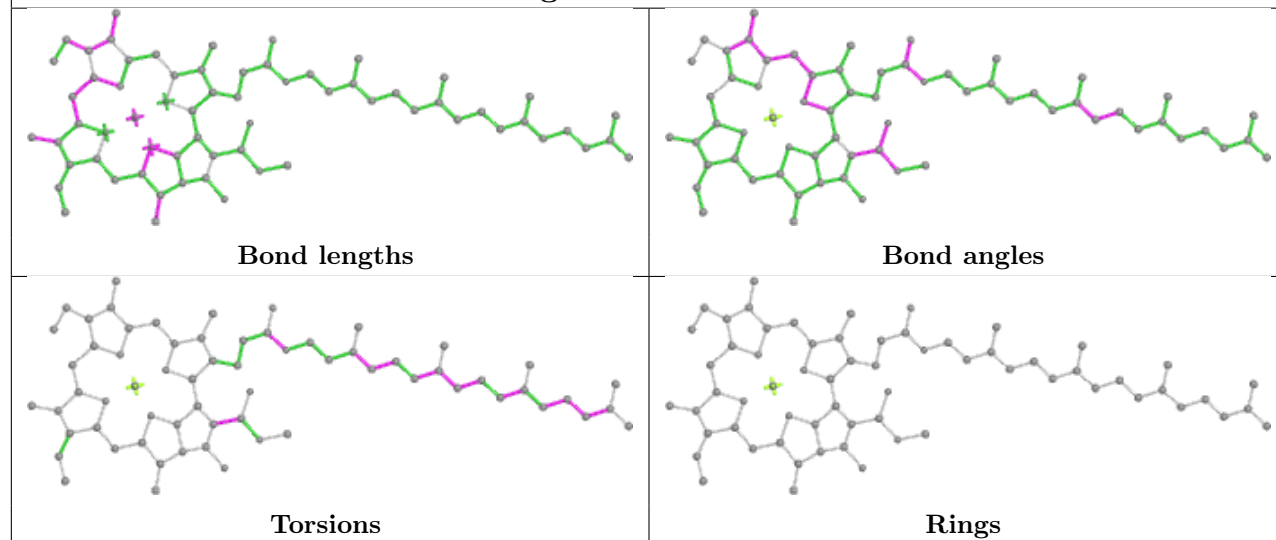
Bond angles



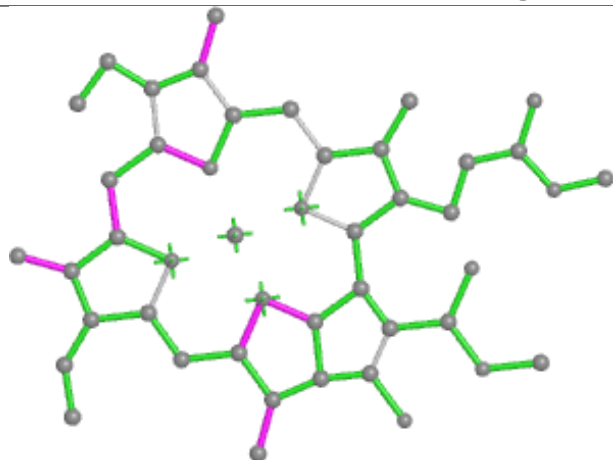
Torsions



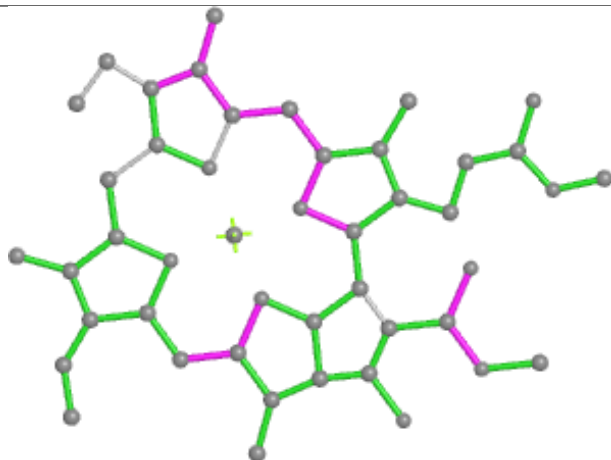
Rings

Ligand CLA a 838**Ligand CLA b 820****Ligand CLA l 204**

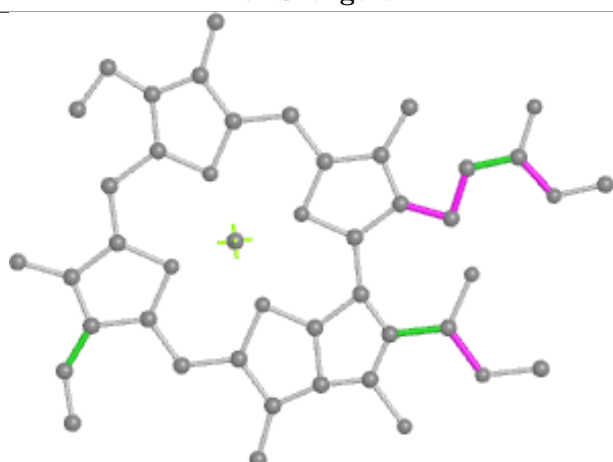
Ligand CLA C 310



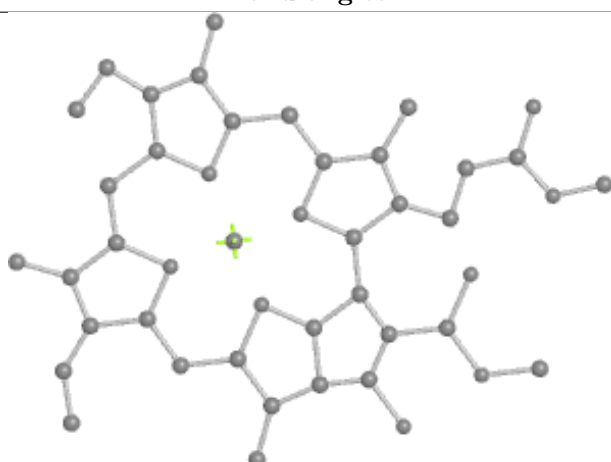
Bond lengths



Bond angles

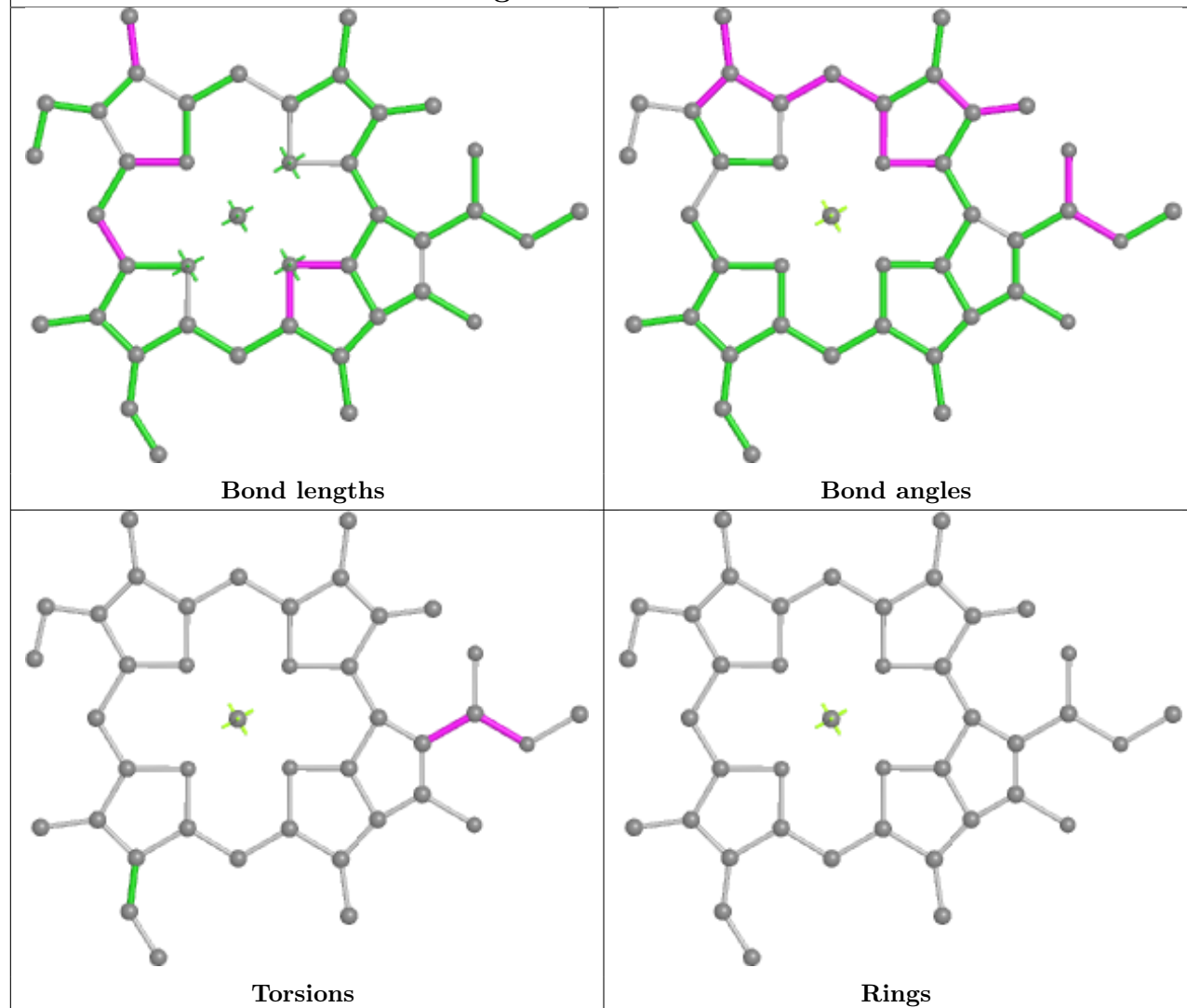


Torsions

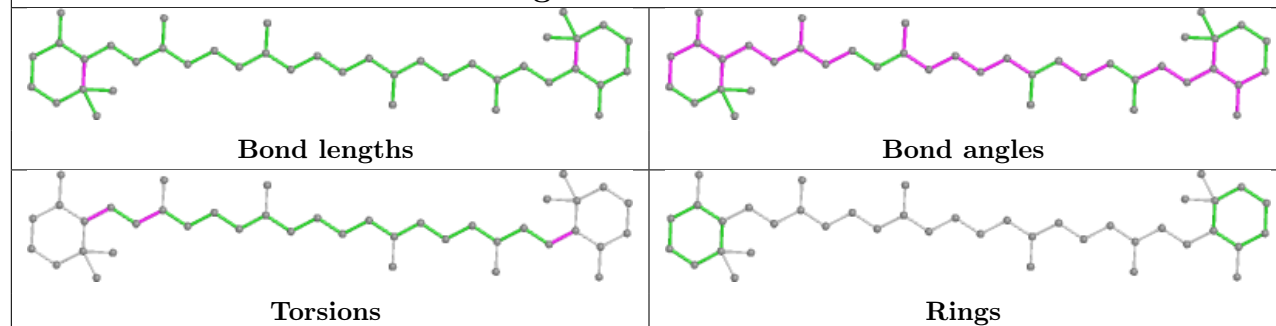


Rings

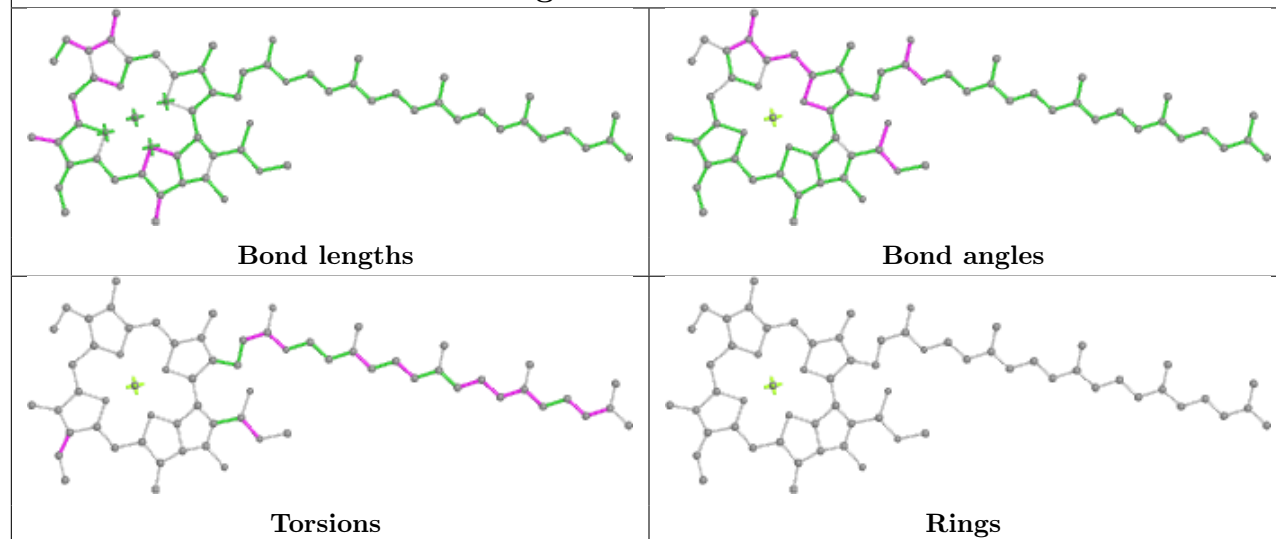
Ligand CLA G 314



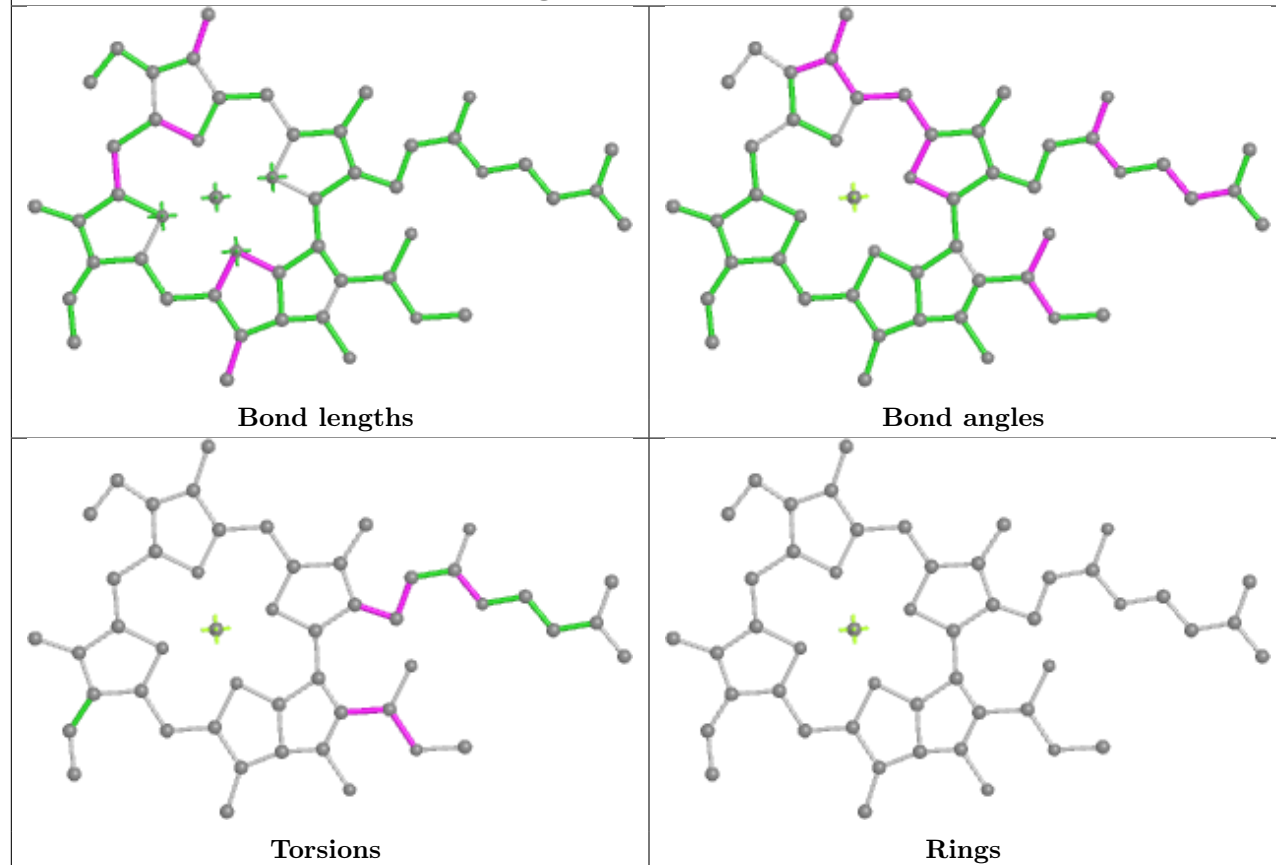
Ligand BCR b 840

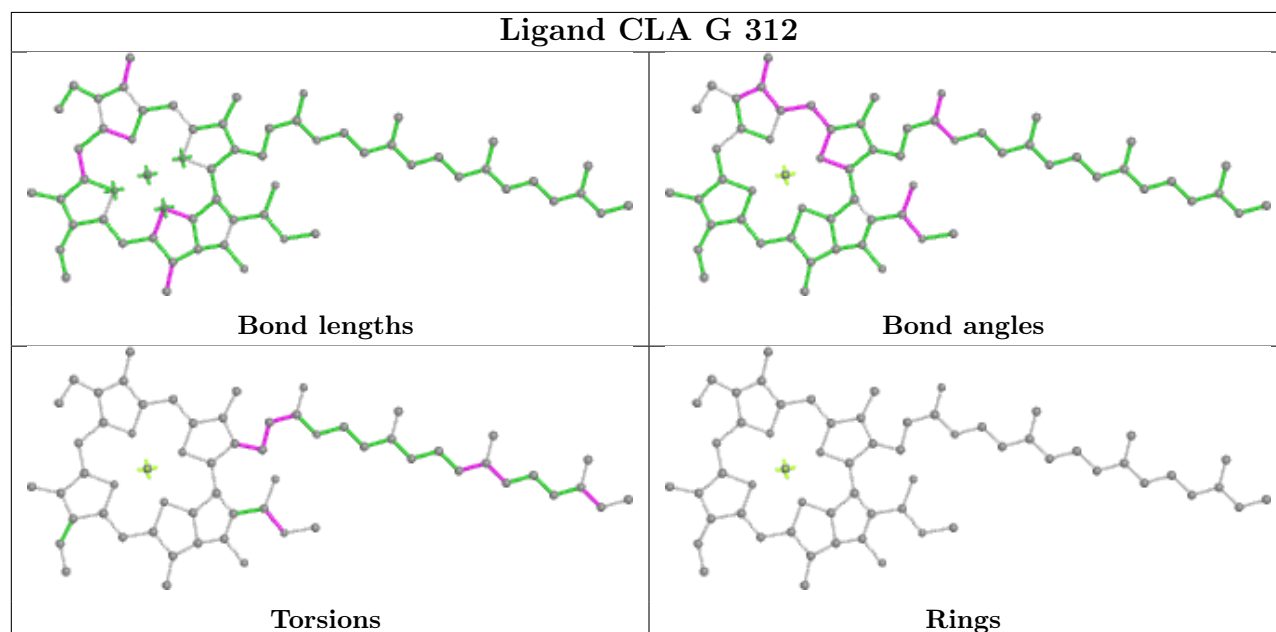
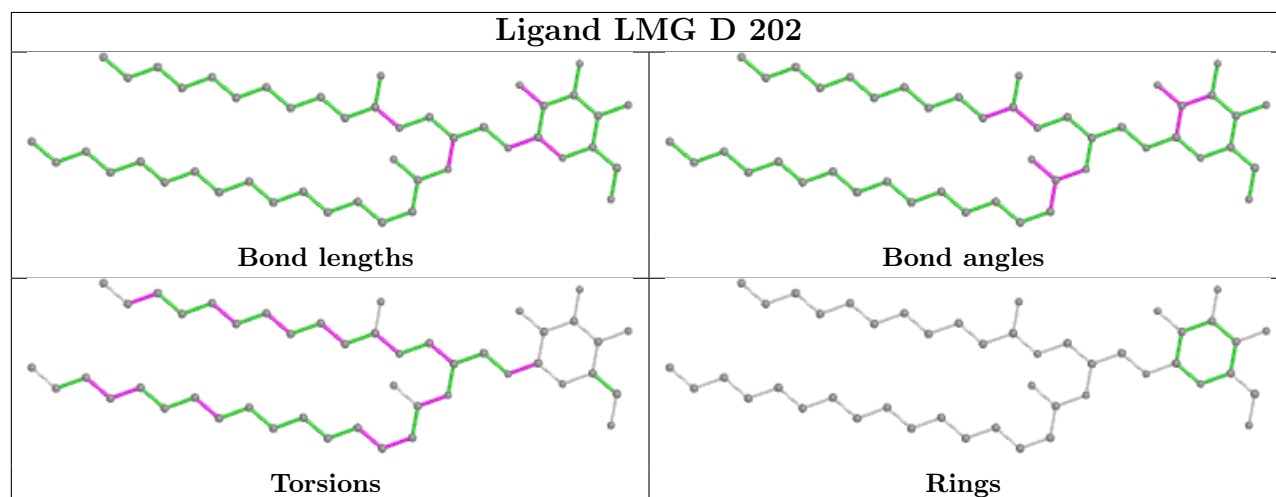
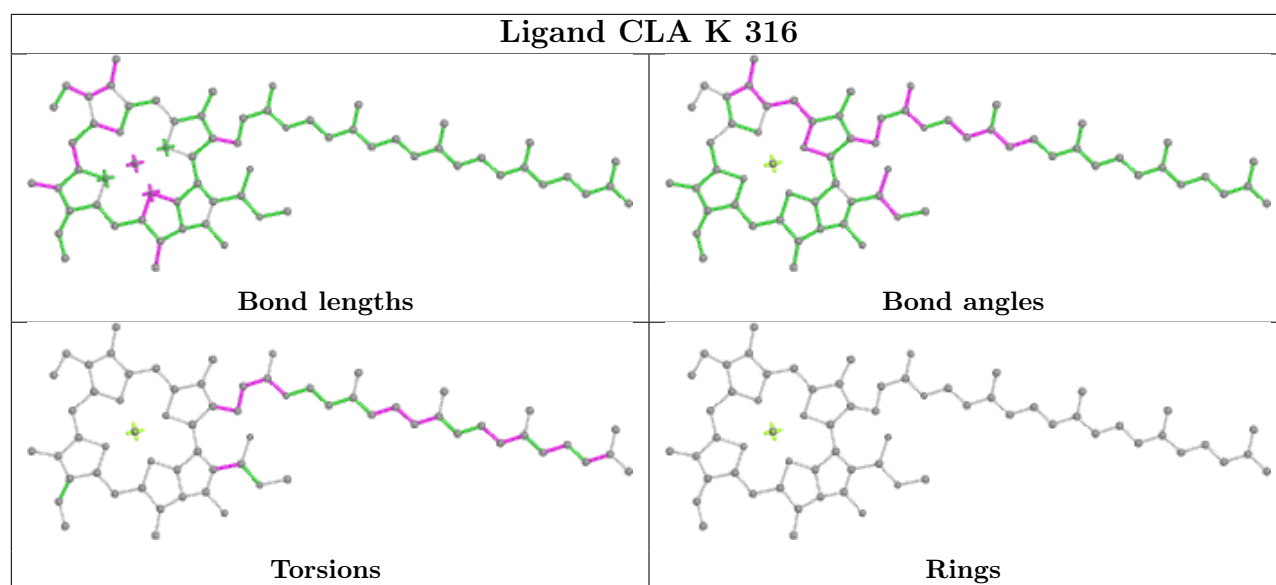


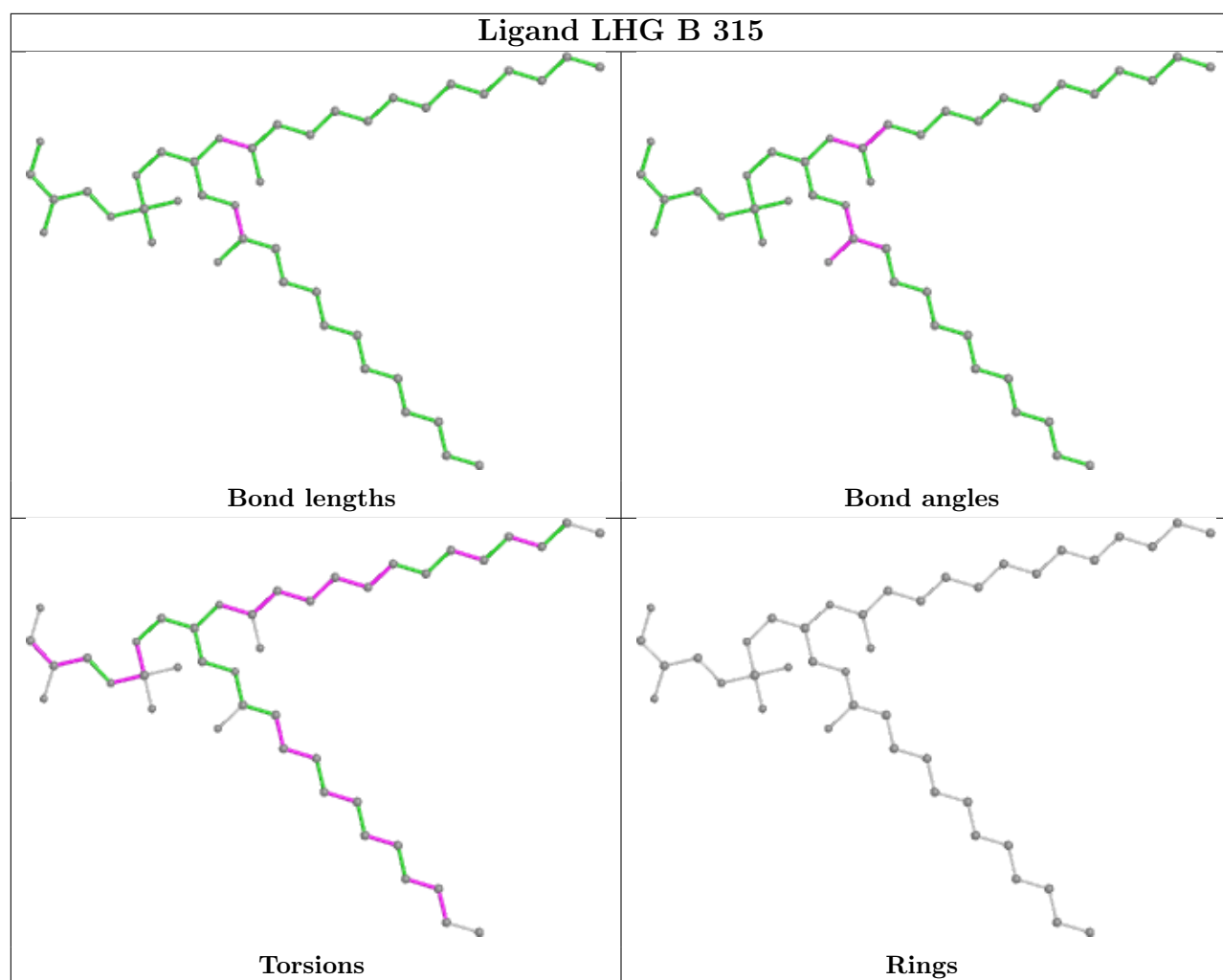
Ligand CLA J 314



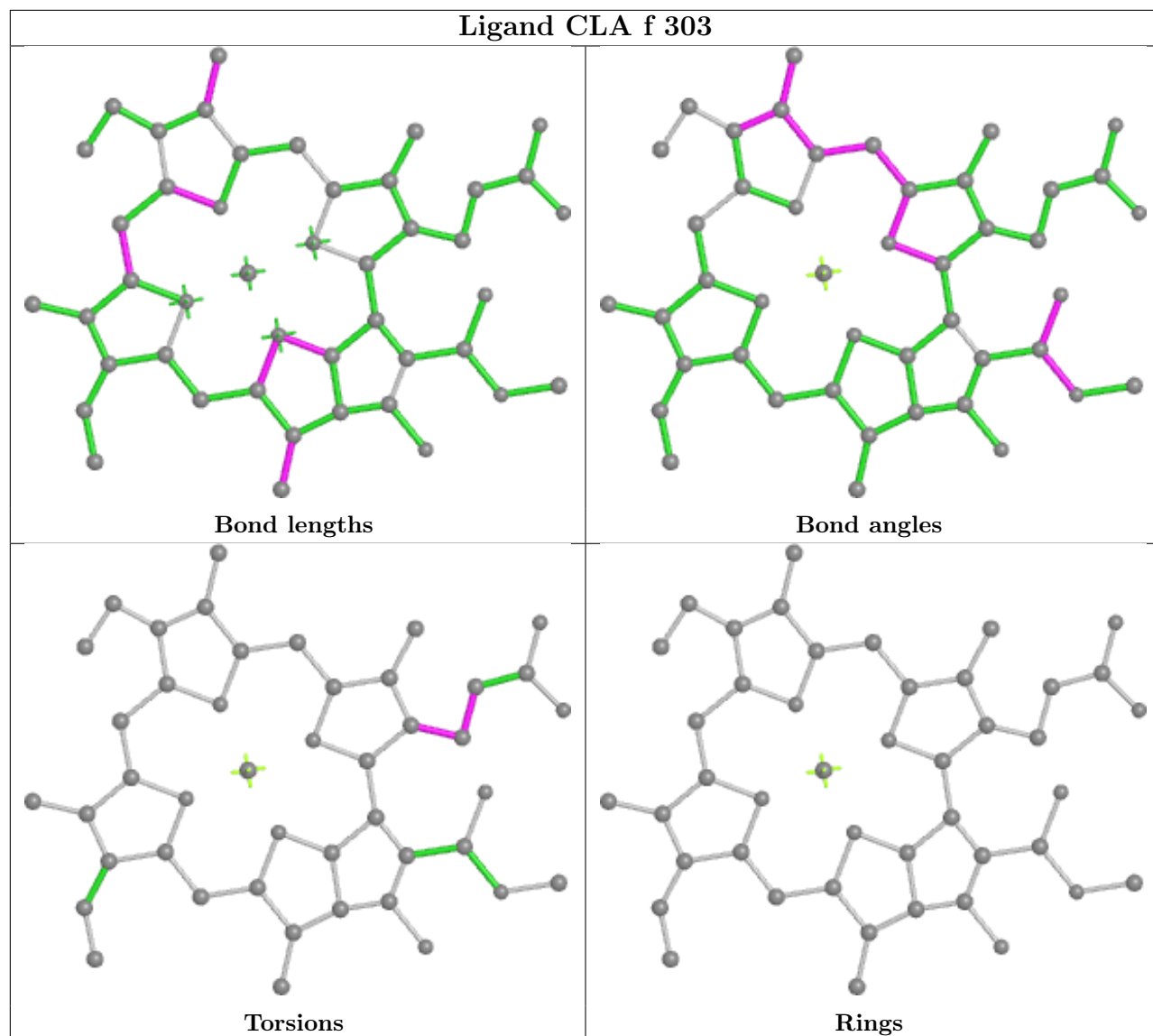
Ligand CLA b 822



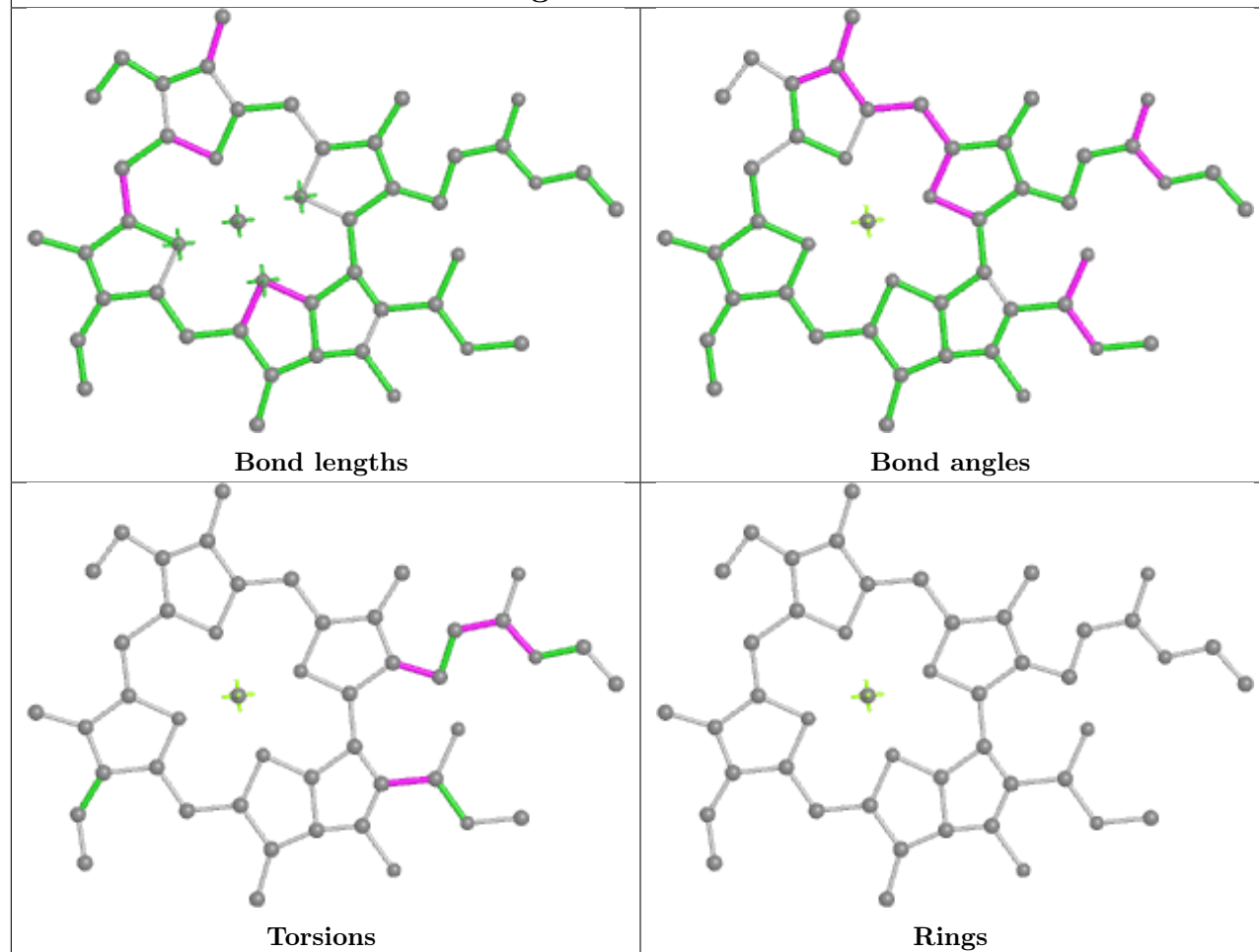




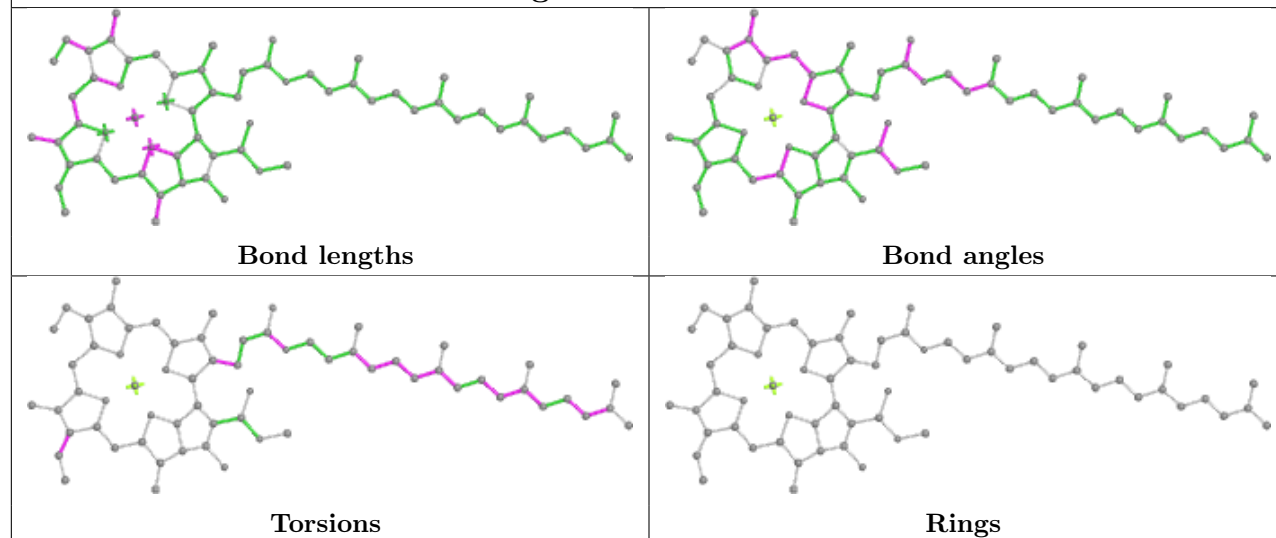
Ligand CLA f 303

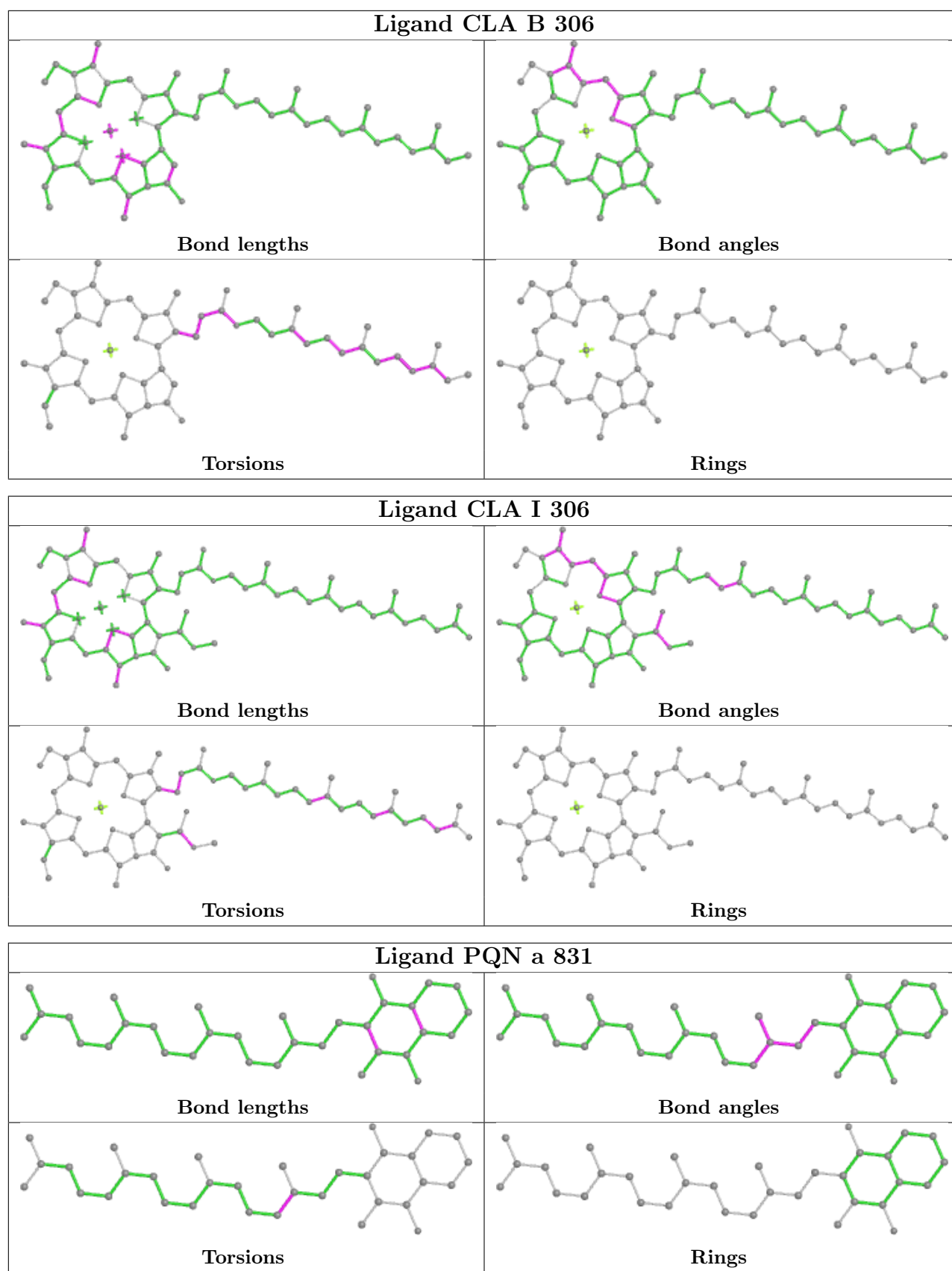


Ligand CLA I 310

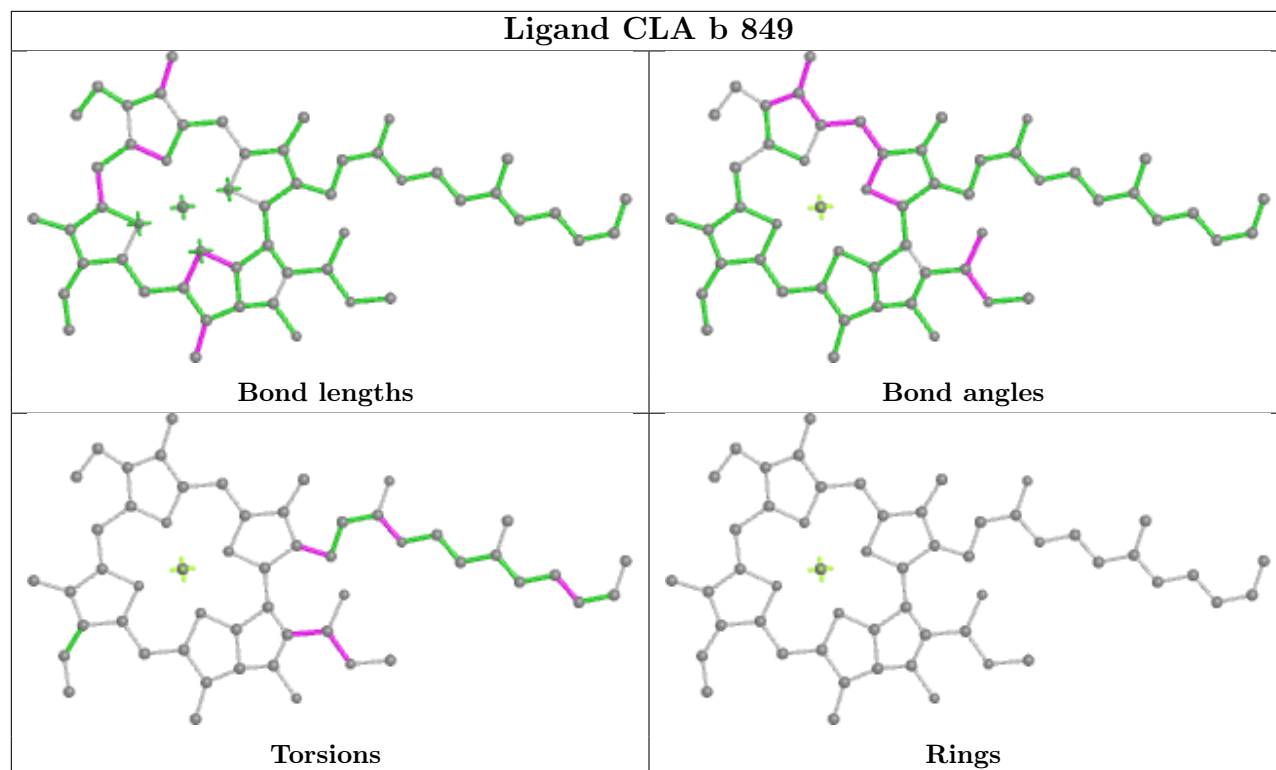


Ligand CLA A 205

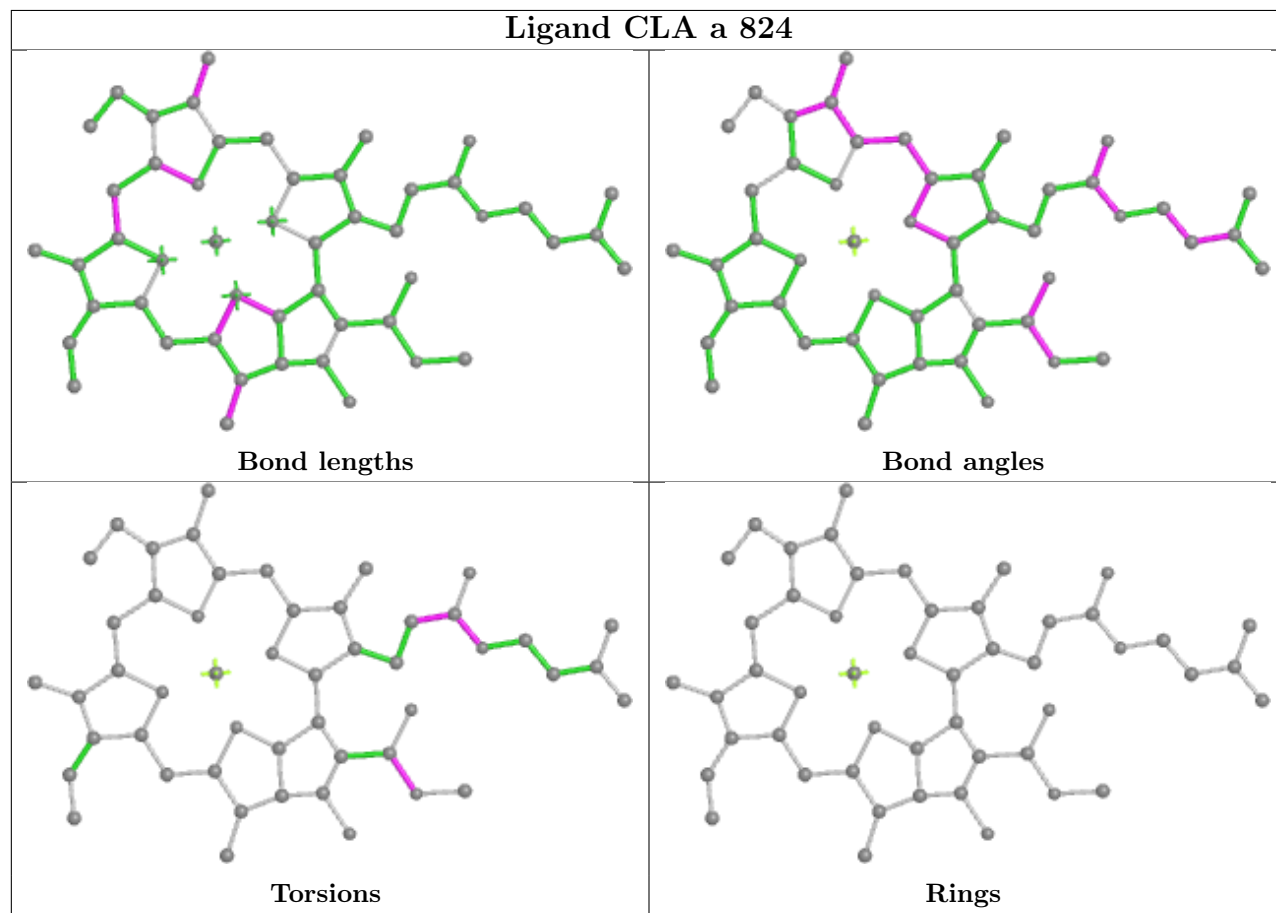


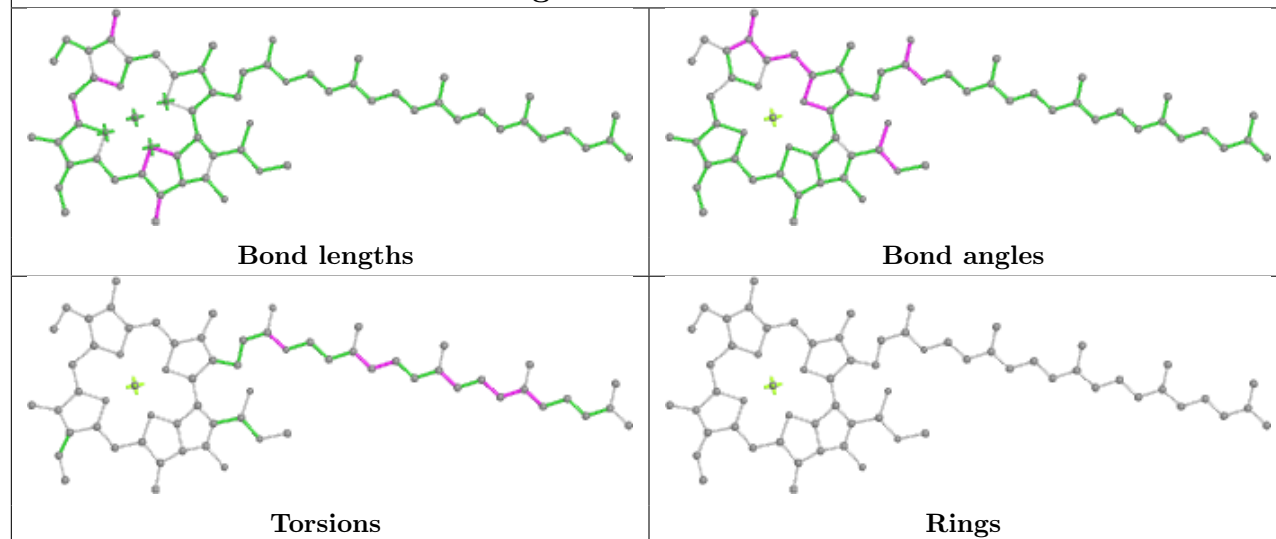
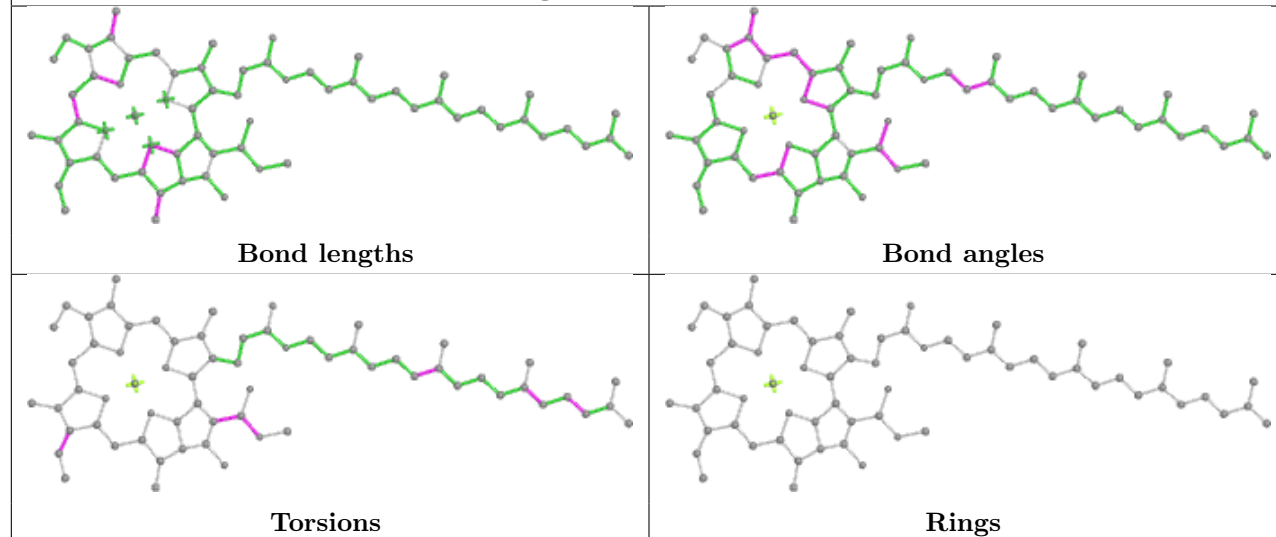
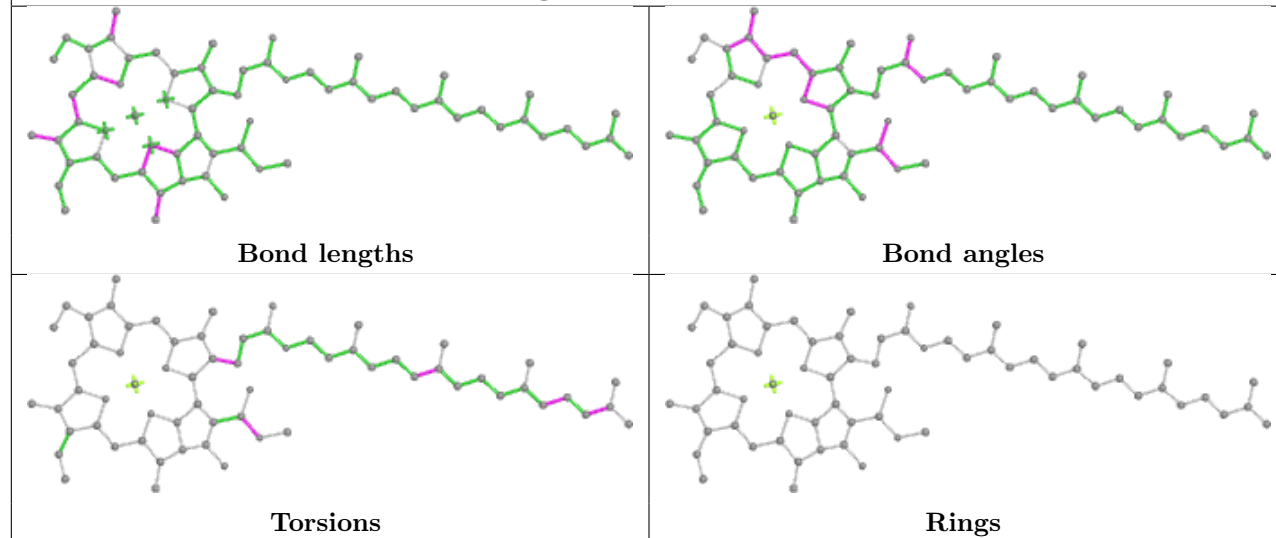


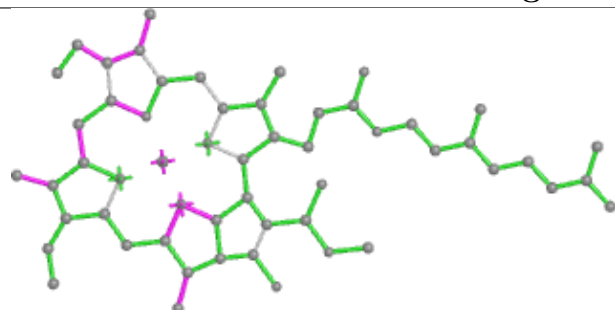
Ligand CLA b 849



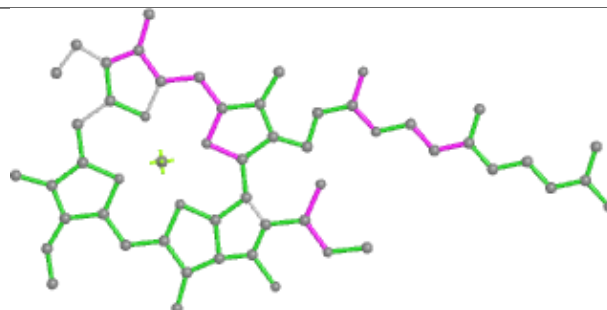
Ligand CLA a 824



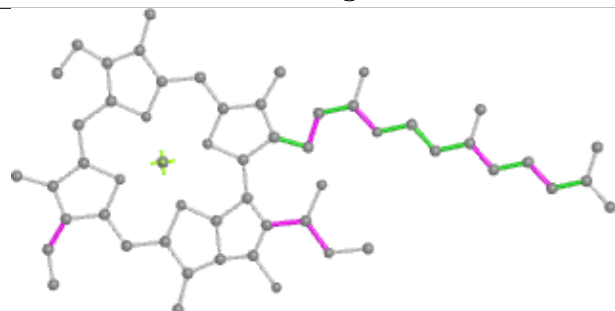
Ligand CLA B 308**Ligand CLA a 804****Ligand CLA b 819**

Ligand CLA I 315

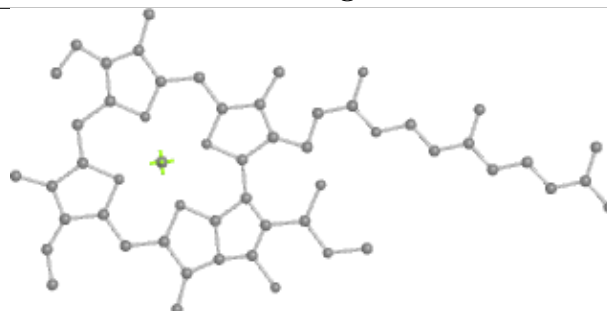
Bond lengths



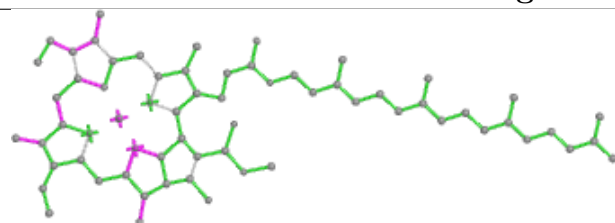
Bond angles



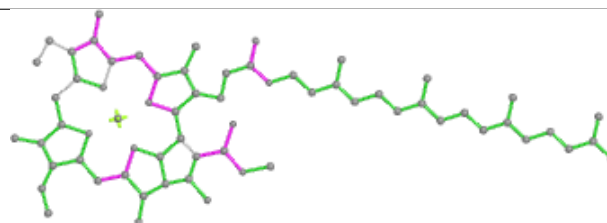
Torsions



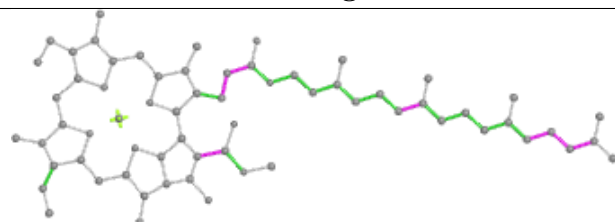
Rings

Ligand CLA C 307

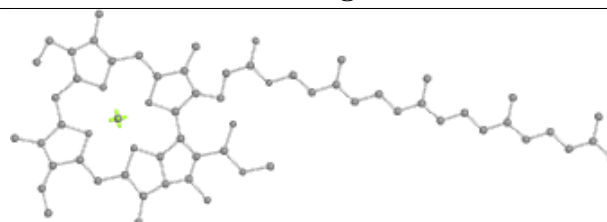
Bond lengths



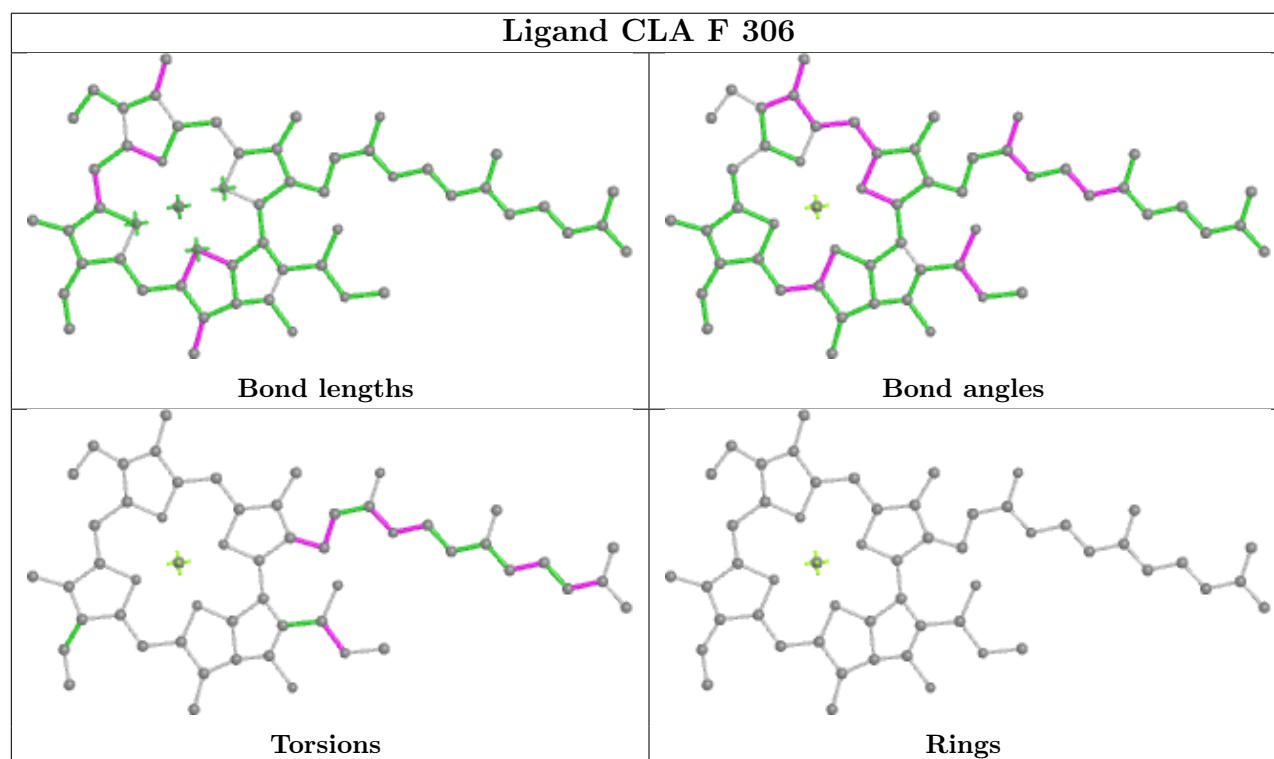
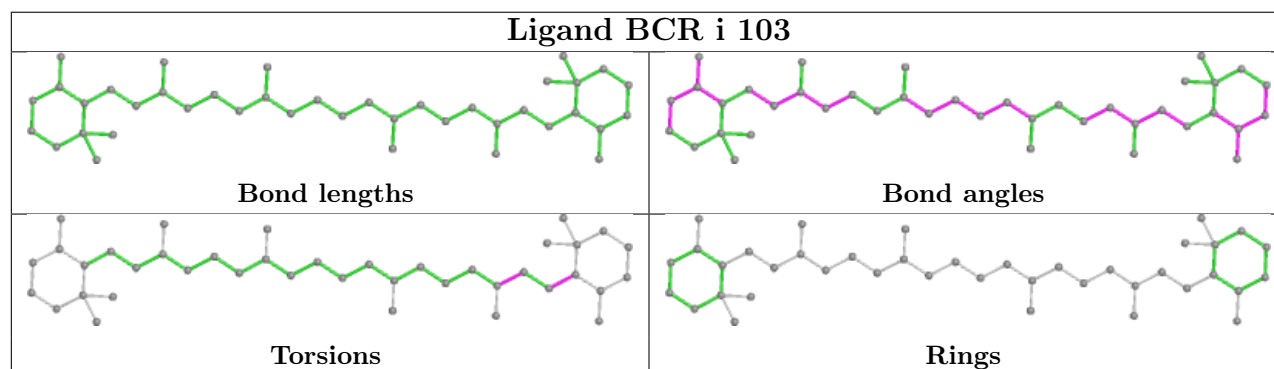
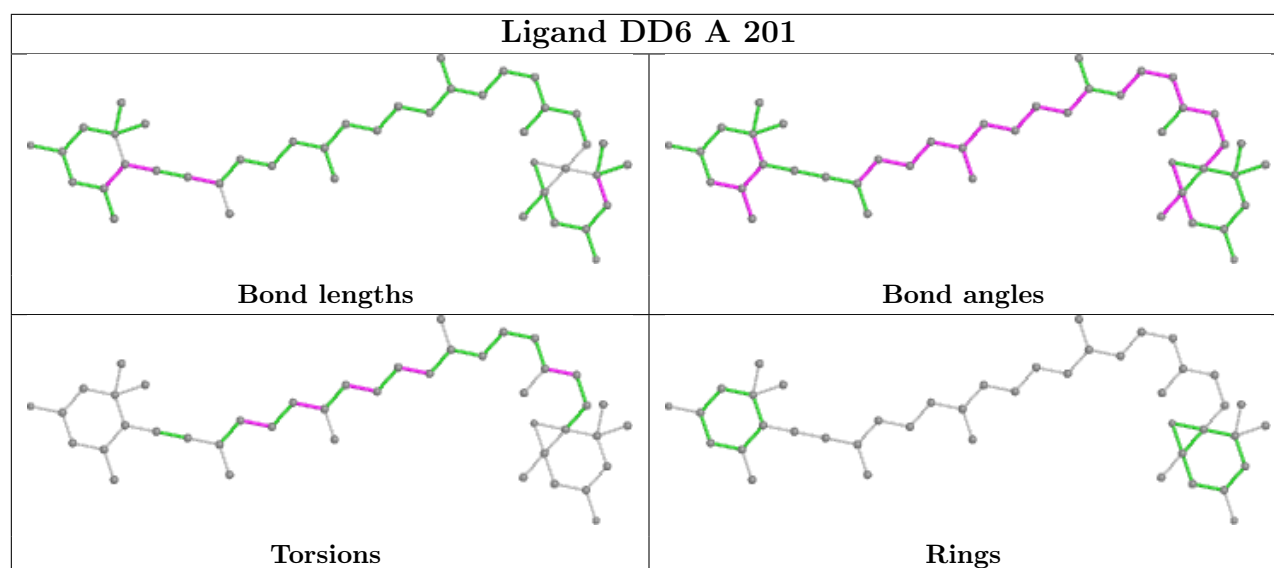
Bond angles



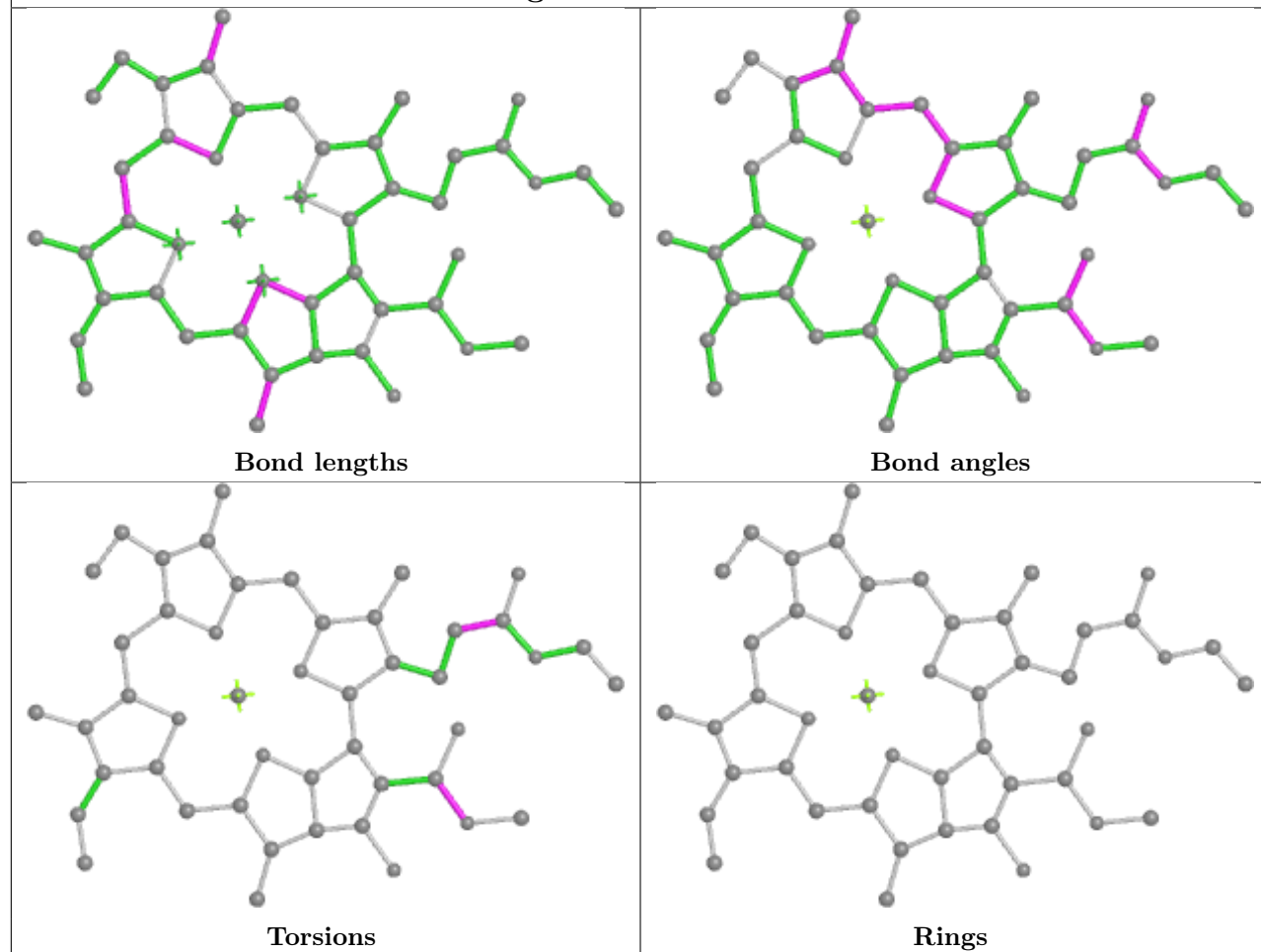
Torsions



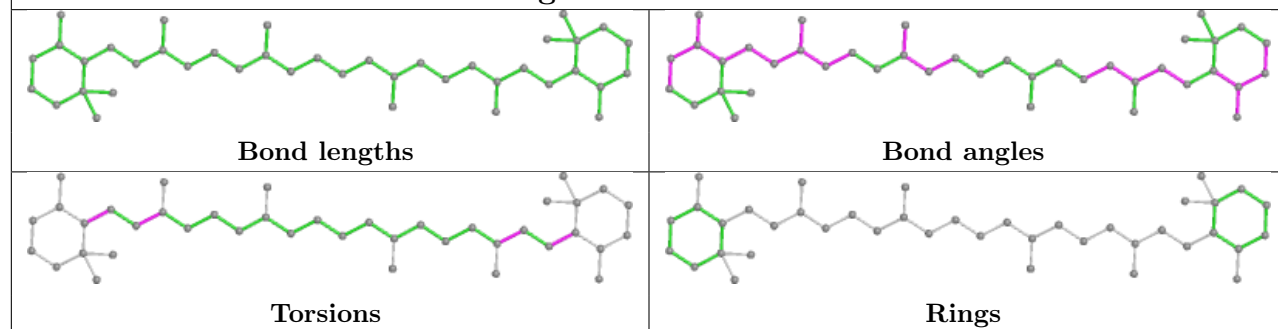
Rings



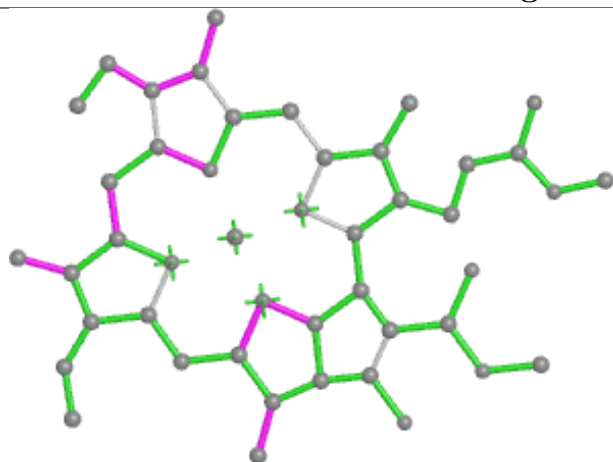
Ligand CLA F 314



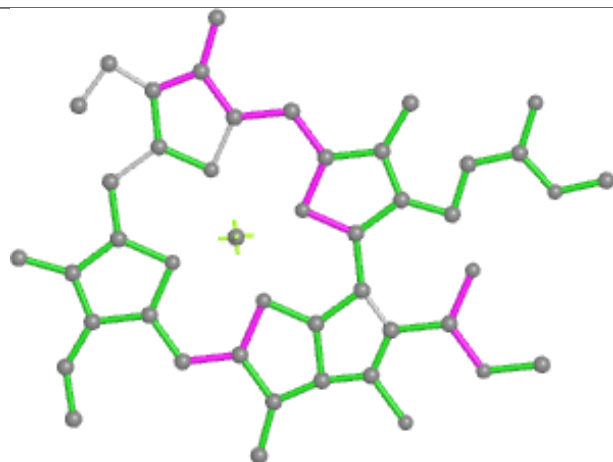
Ligand BCR 1 205



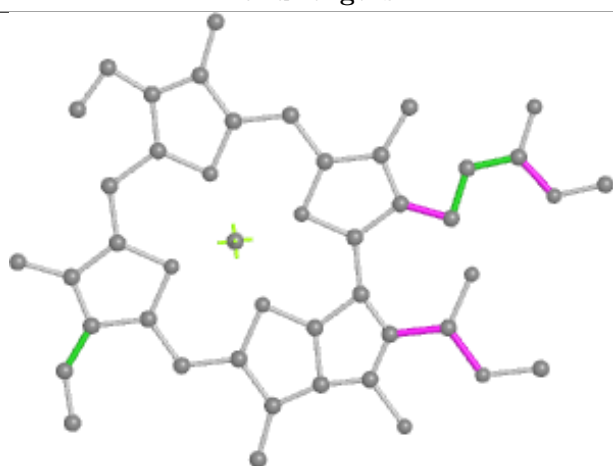
Ligand CLA I 309



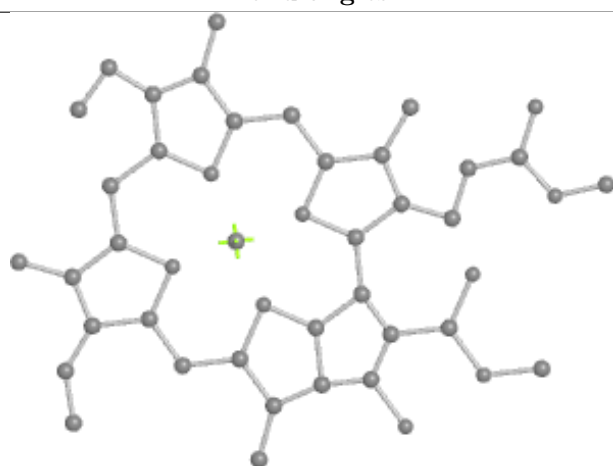
Bond lengths



Bond angles

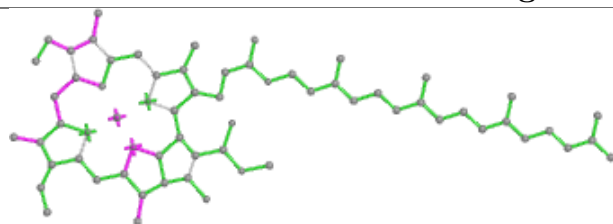


Torsions

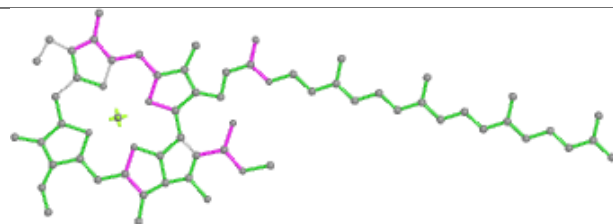


Rings

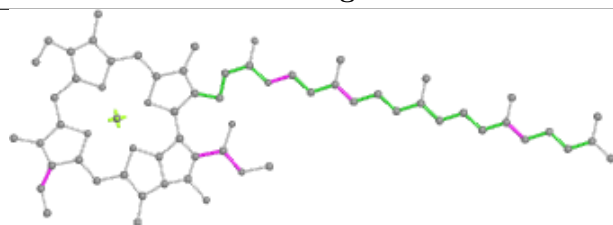
Ligand CLA a 844



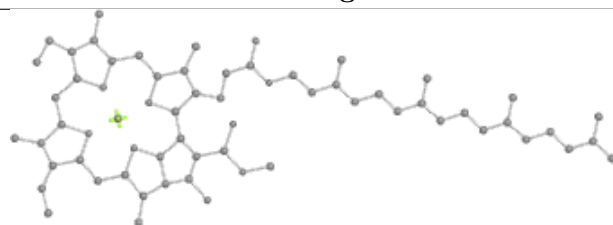
Bond lengths



Bond angles

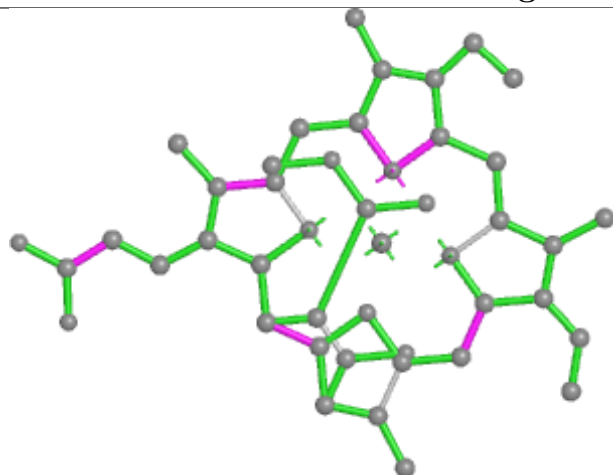


Torsions

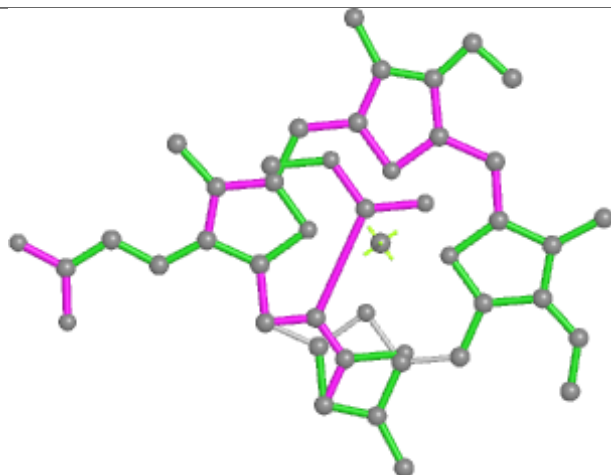


Rings

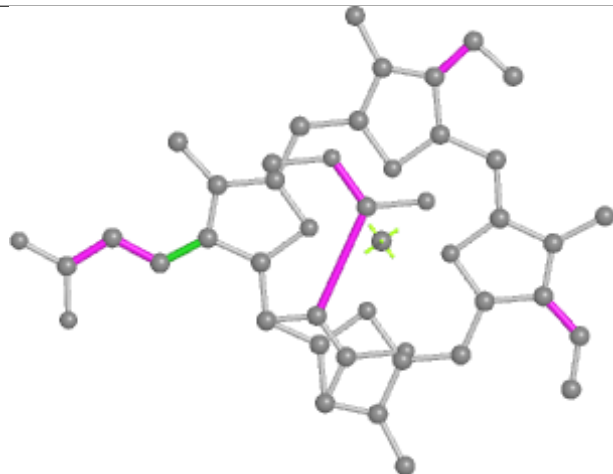
Ligand KC1 L 314



Bond lengths



Bond angles

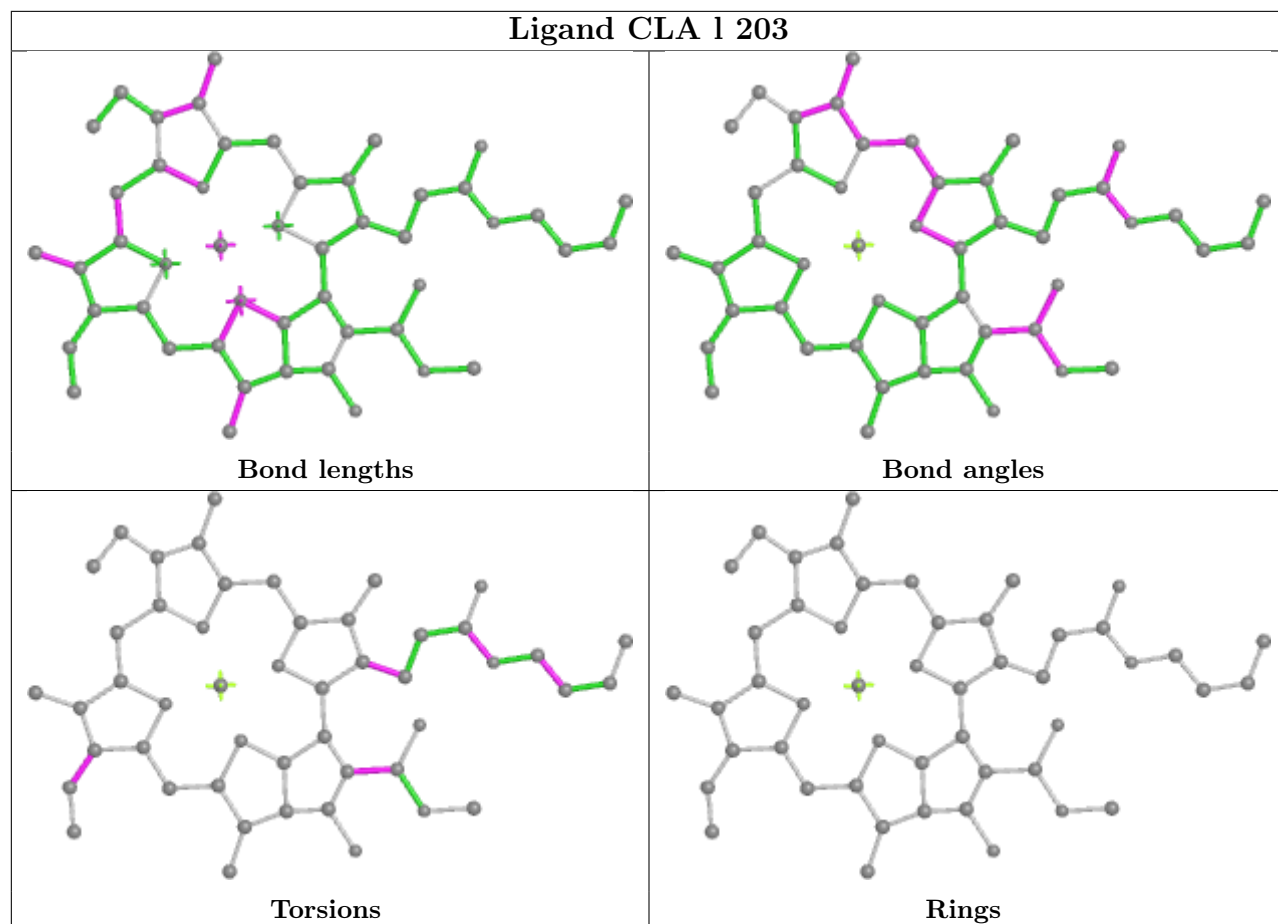


Torsions

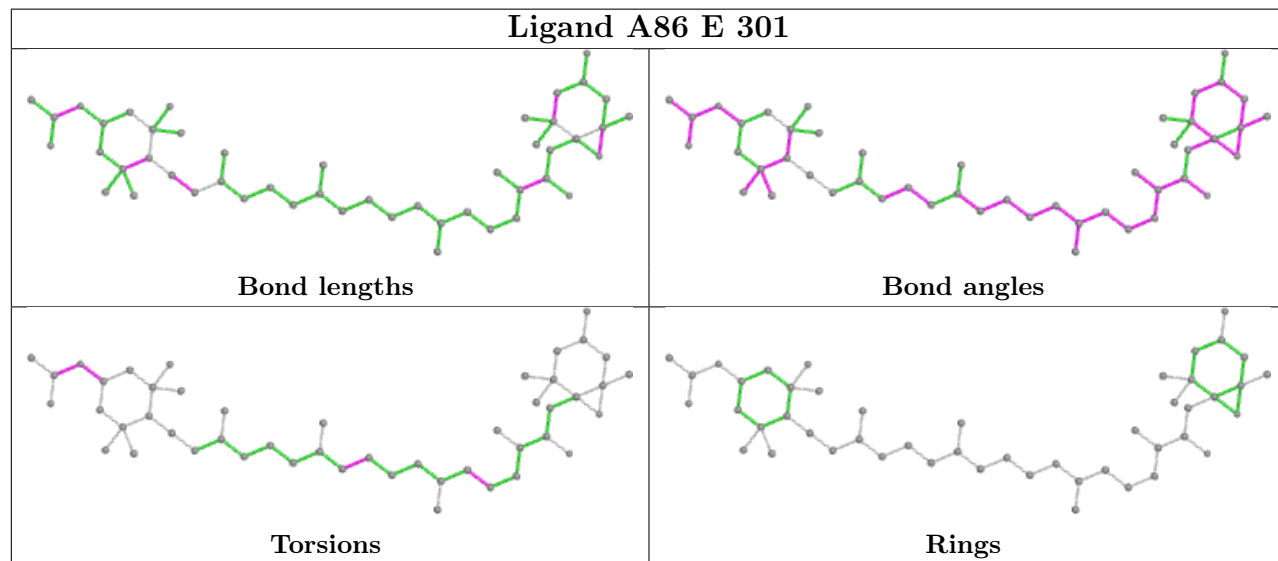


Rings

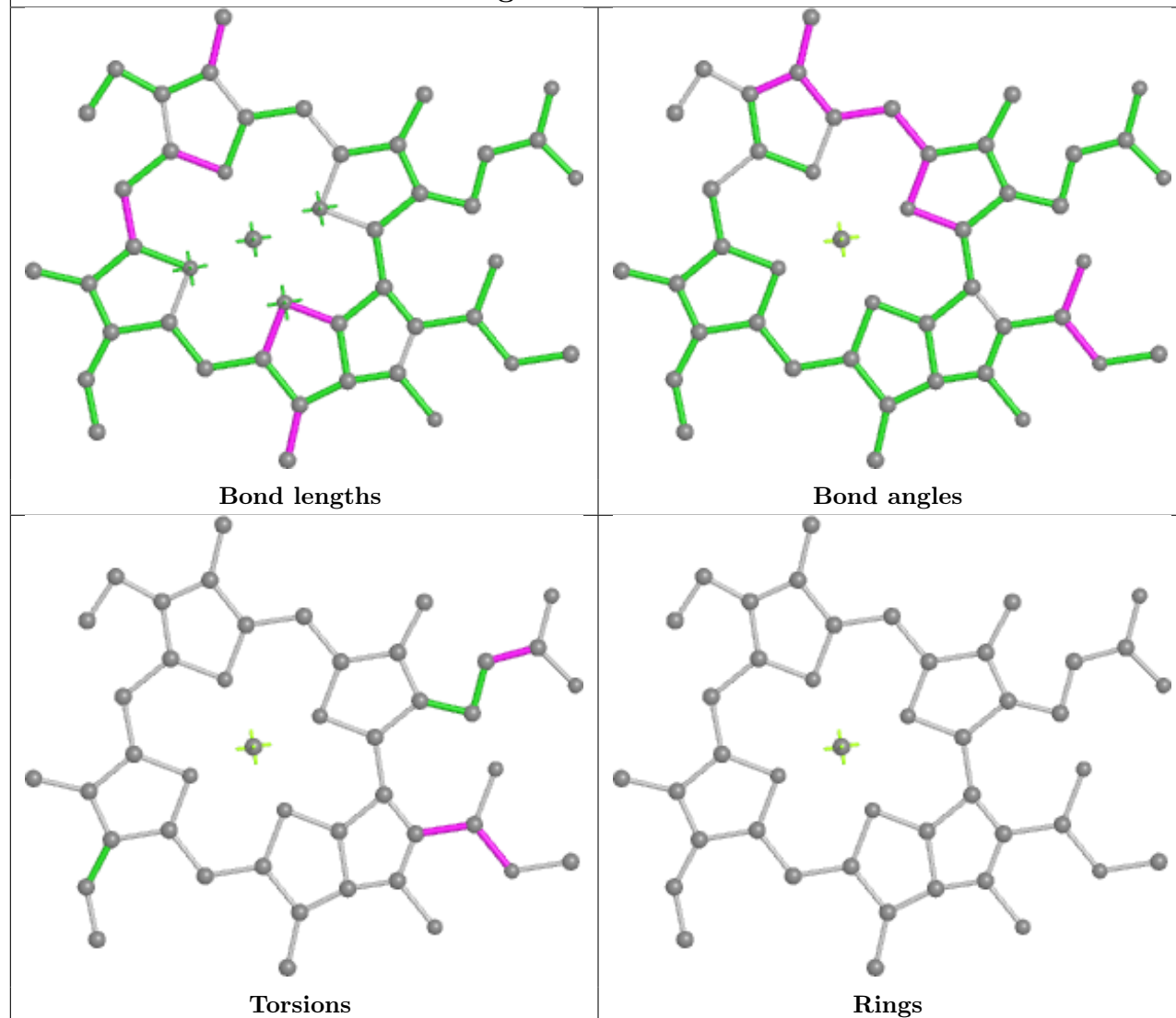
Ligand CLA 1 203



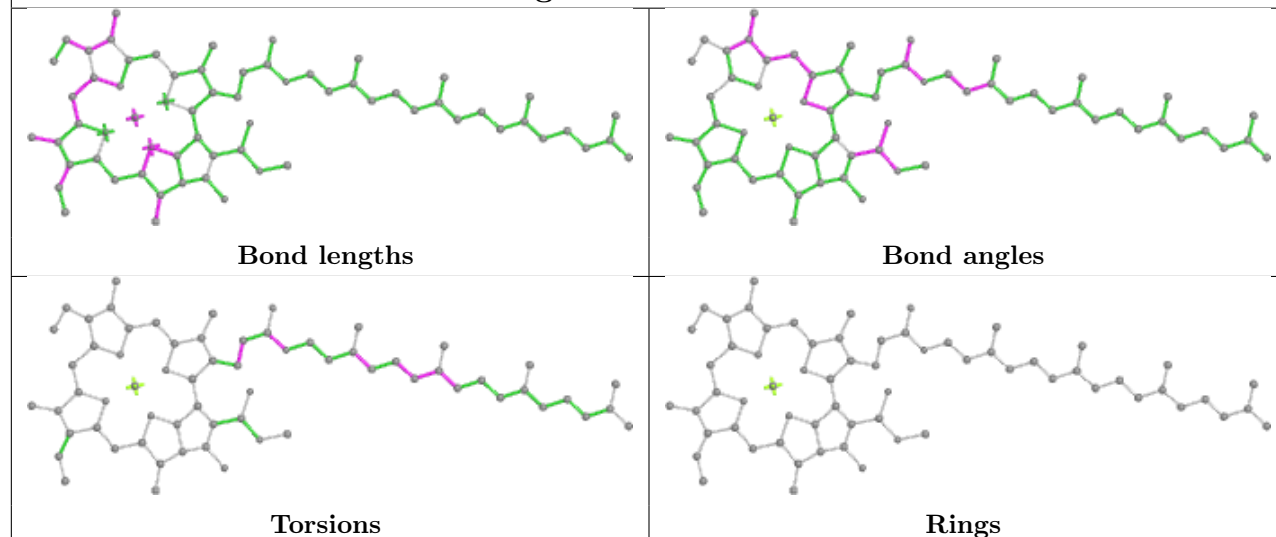
Ligand A86 E 301



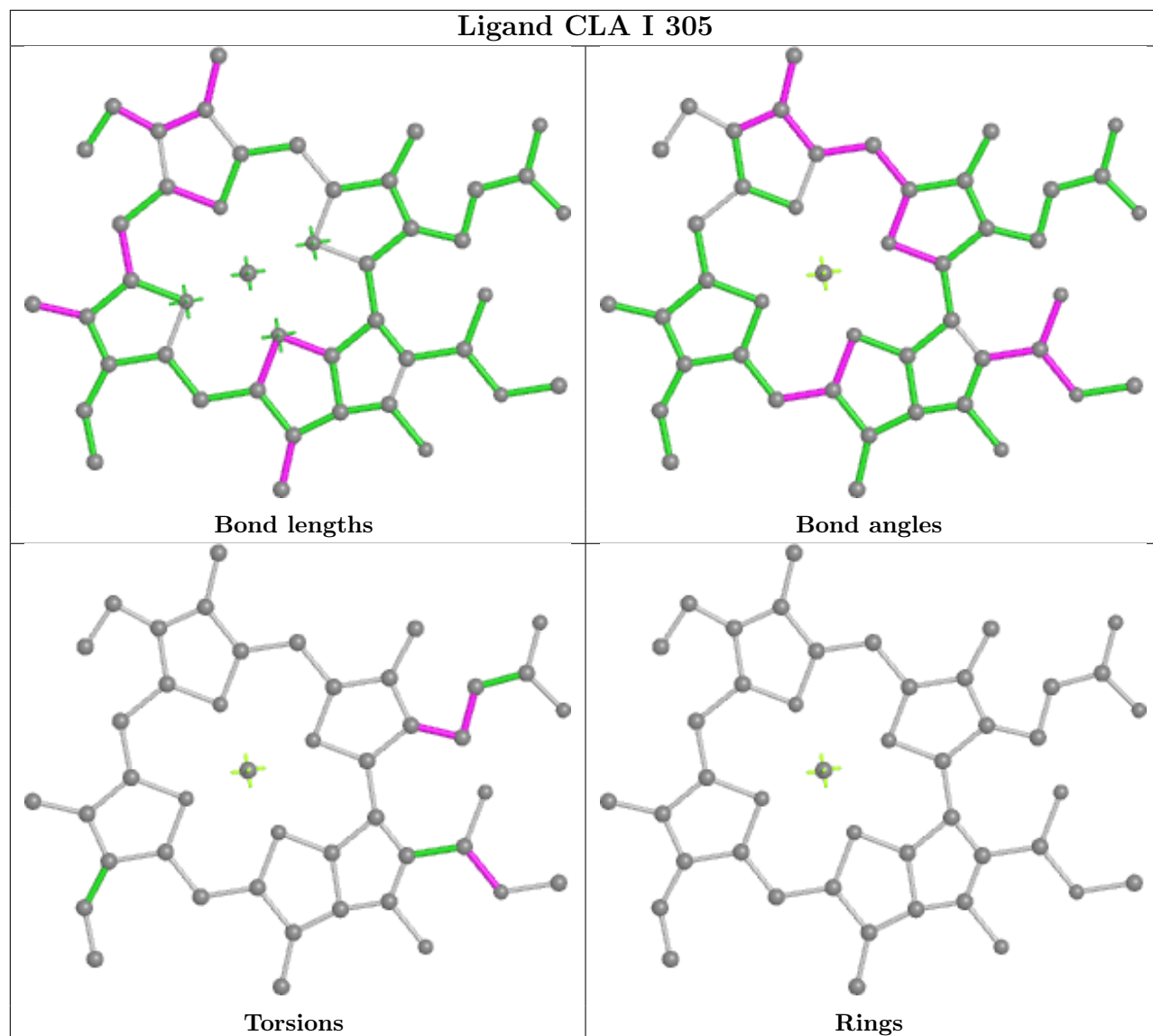
Ligand CLA l 206



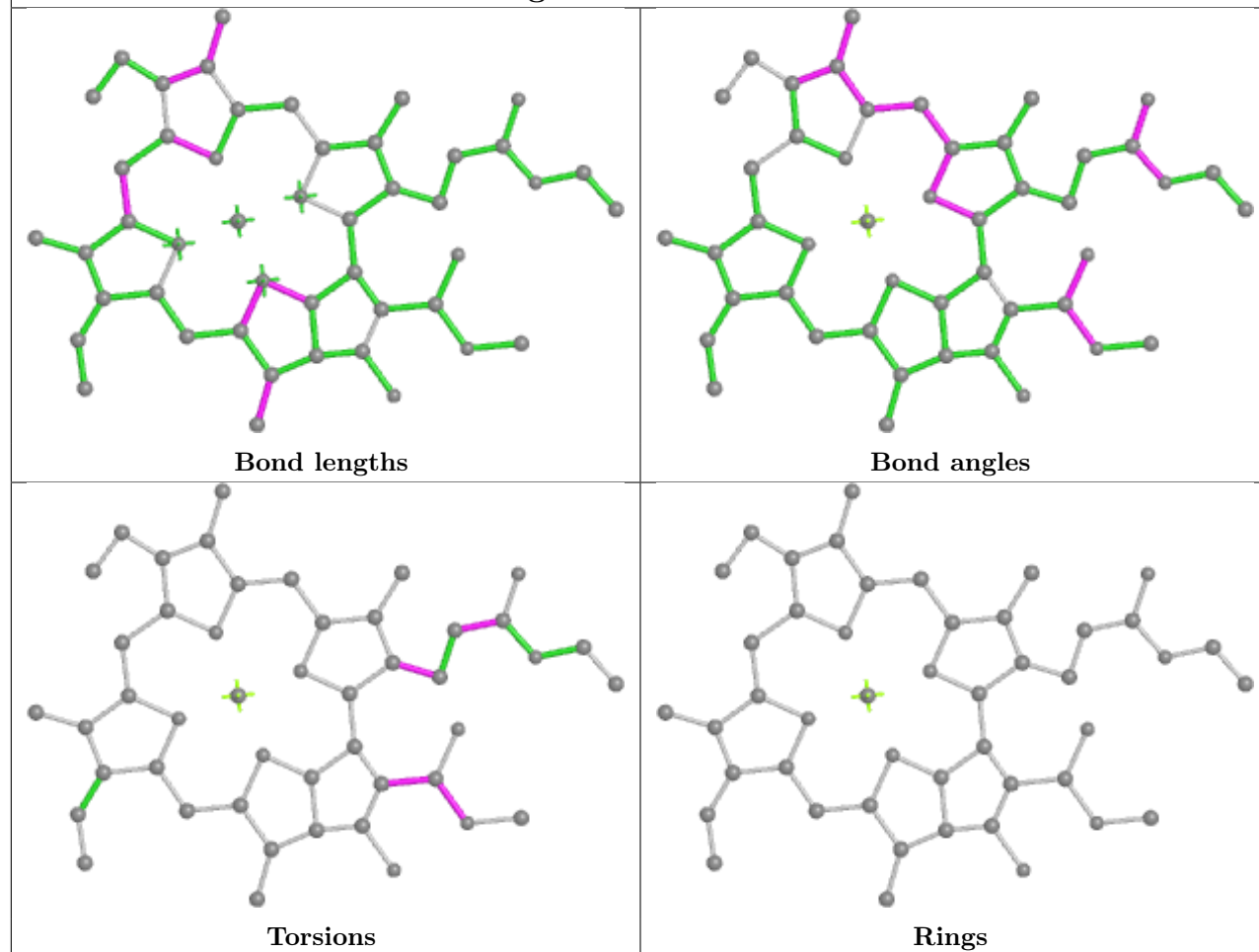
Ligand CLA b 801



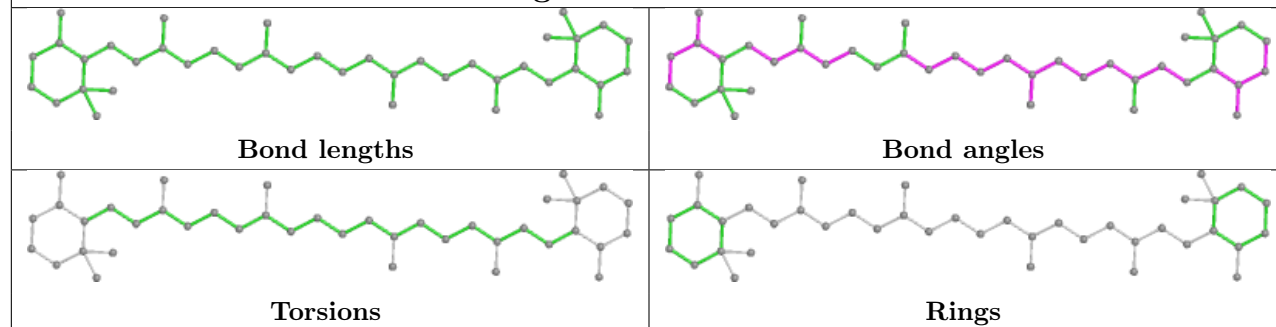
Ligand CLA I 305



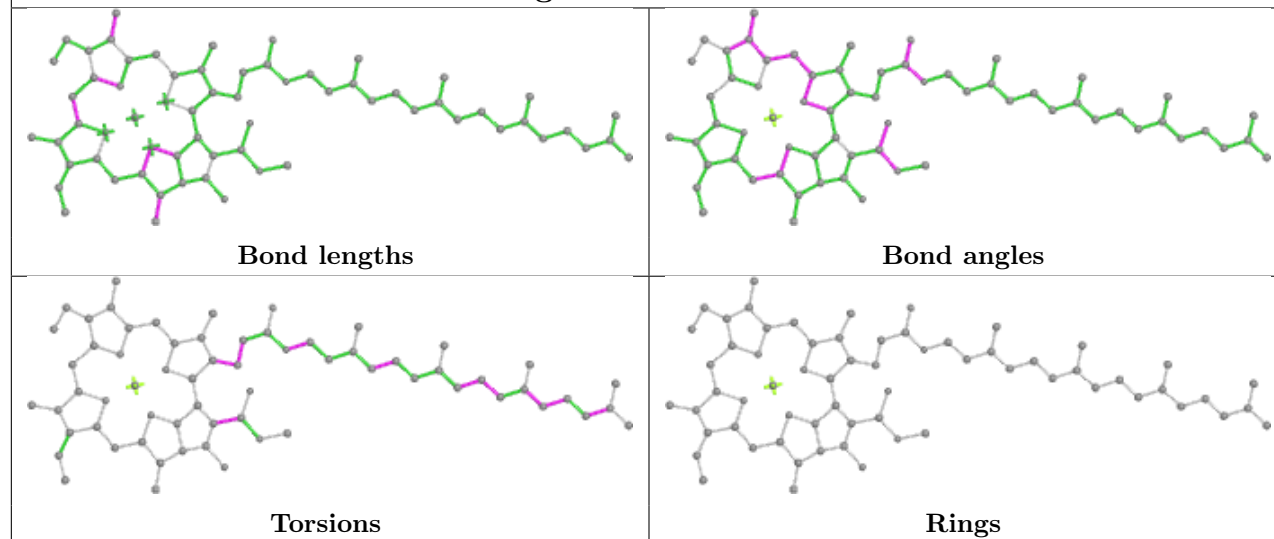
Ligand CLA b 828



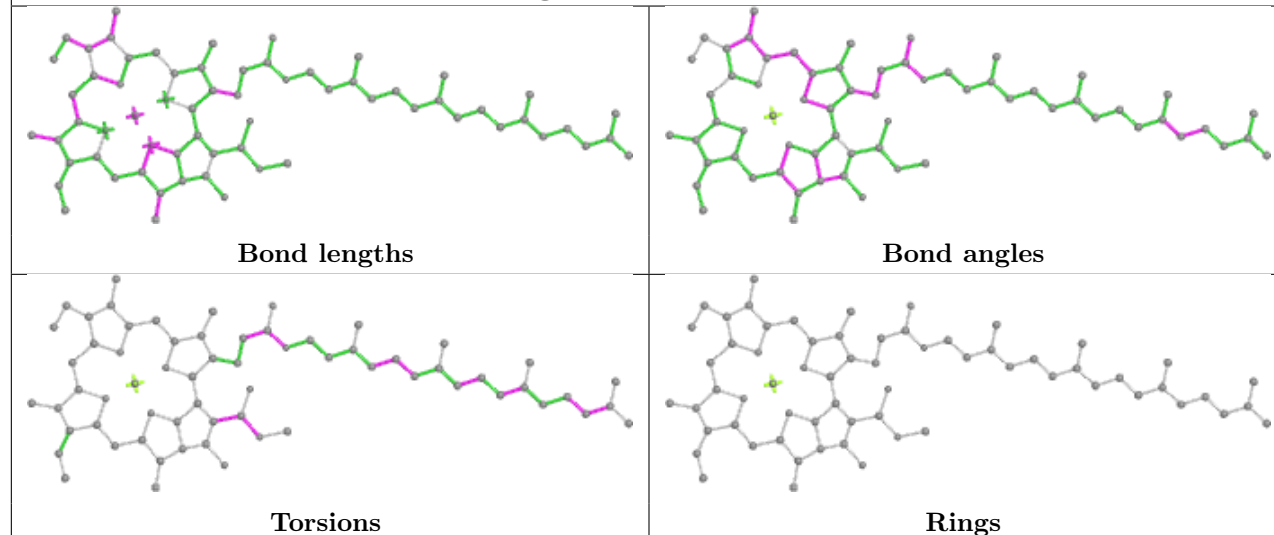
Ligand BCR b 833



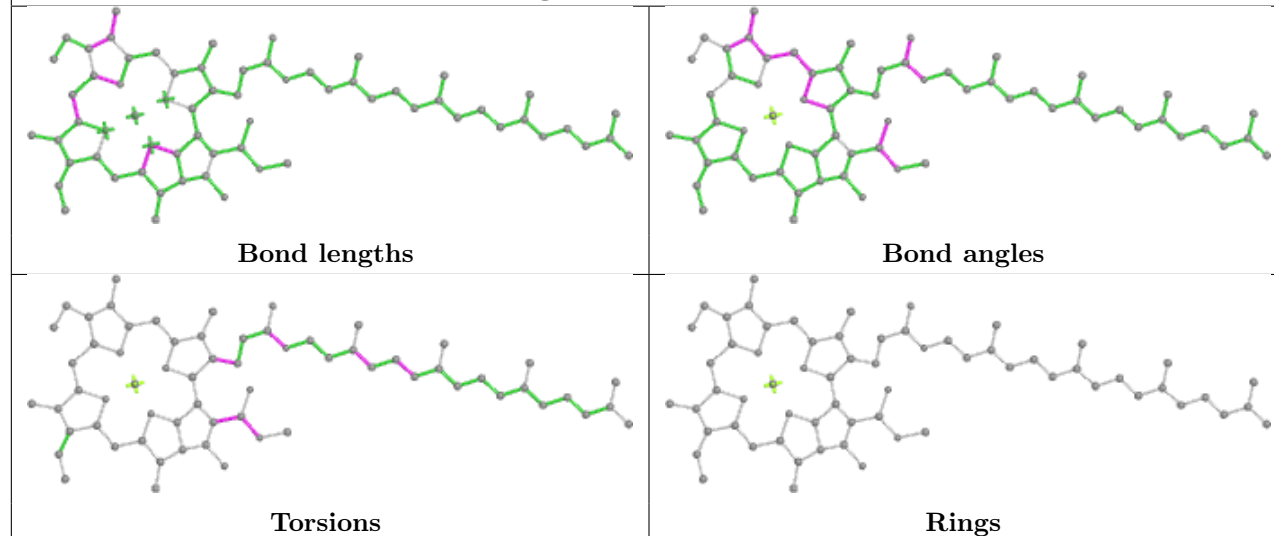
Ligand CLA b 846

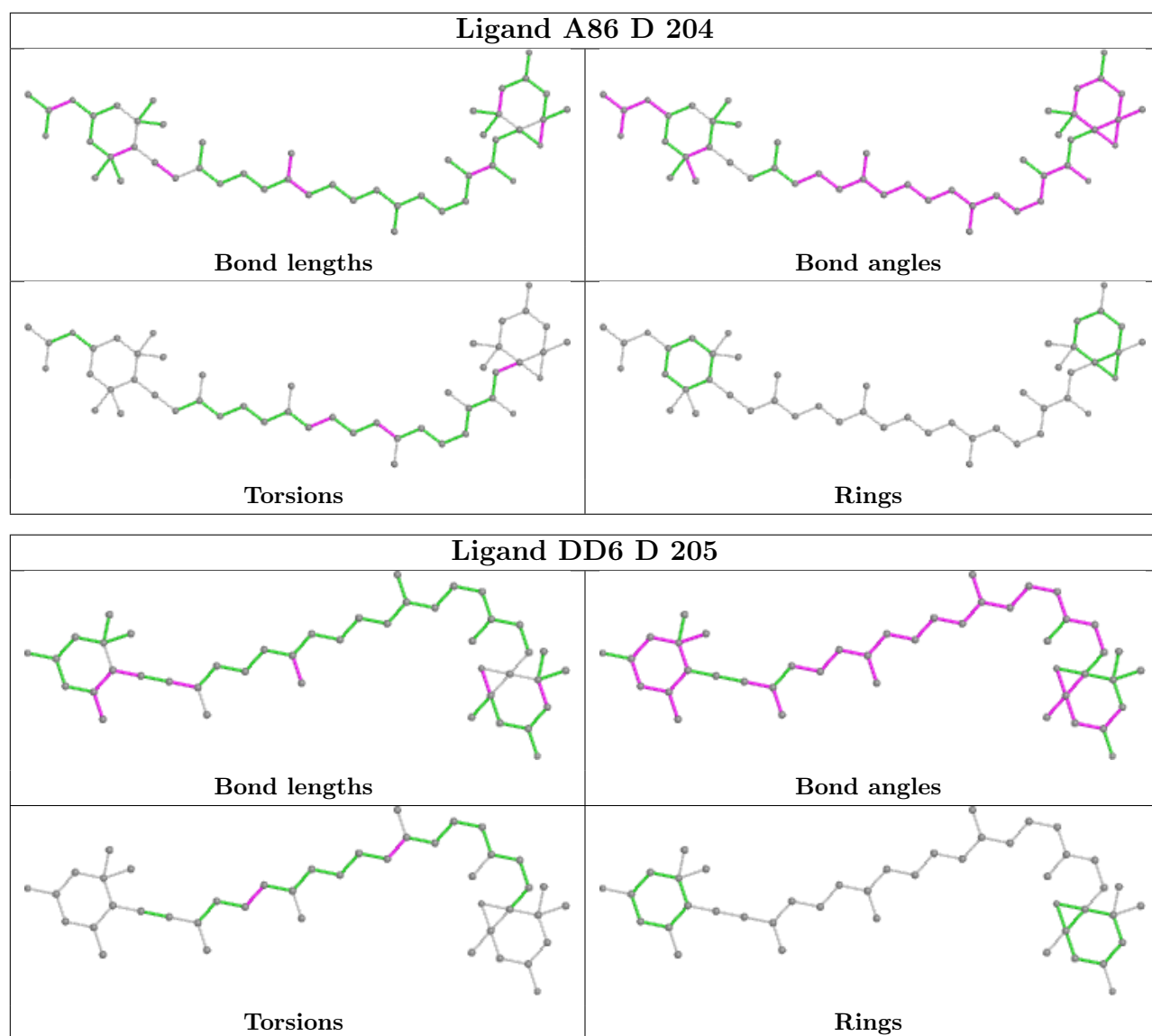


Ligand CLA a 803

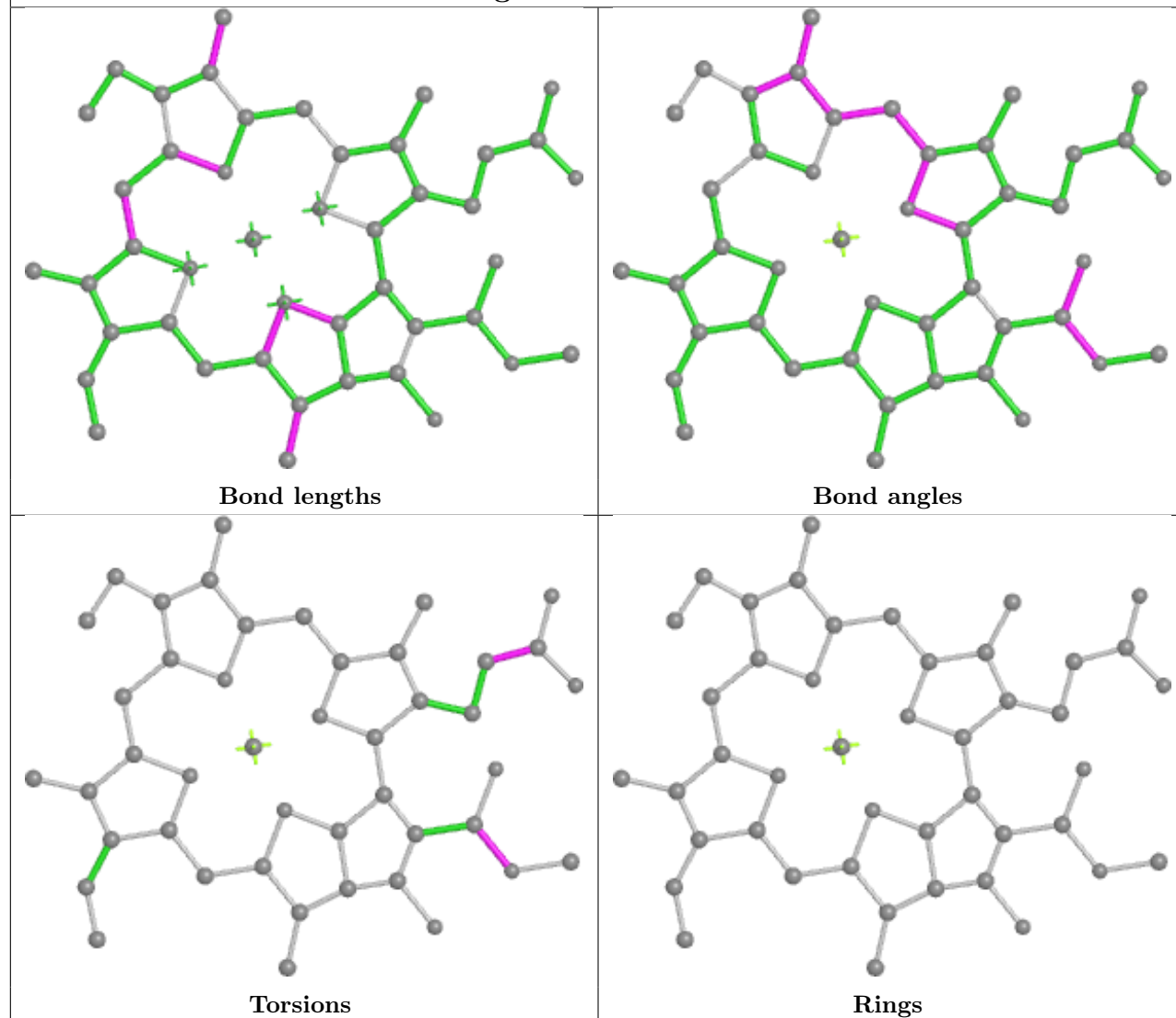


Ligand CLA a 823

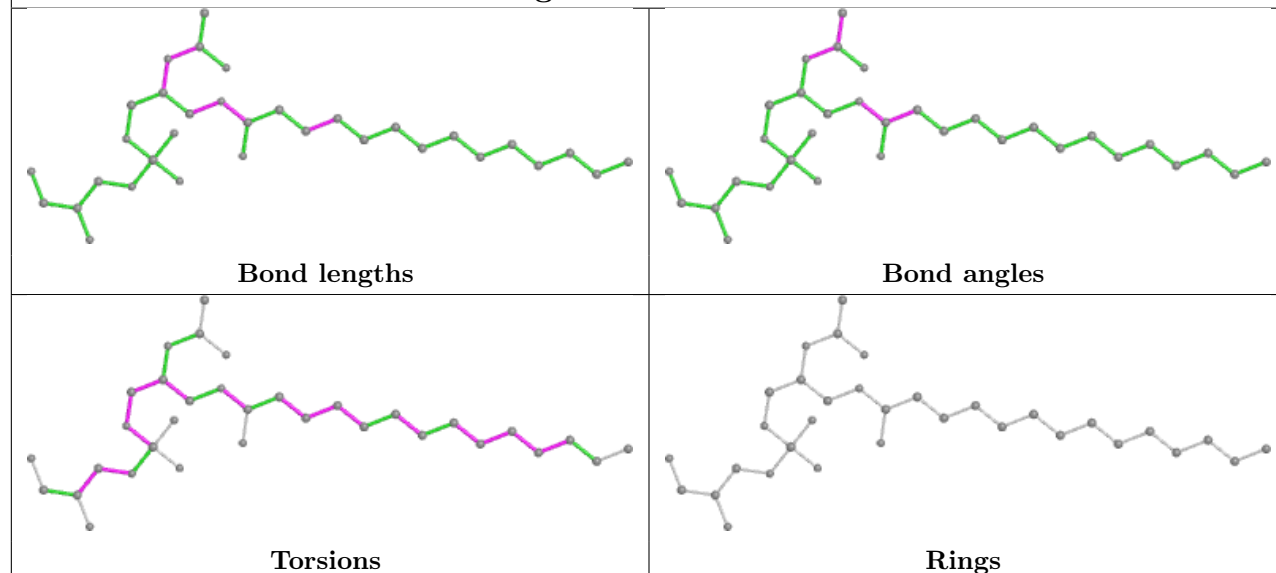


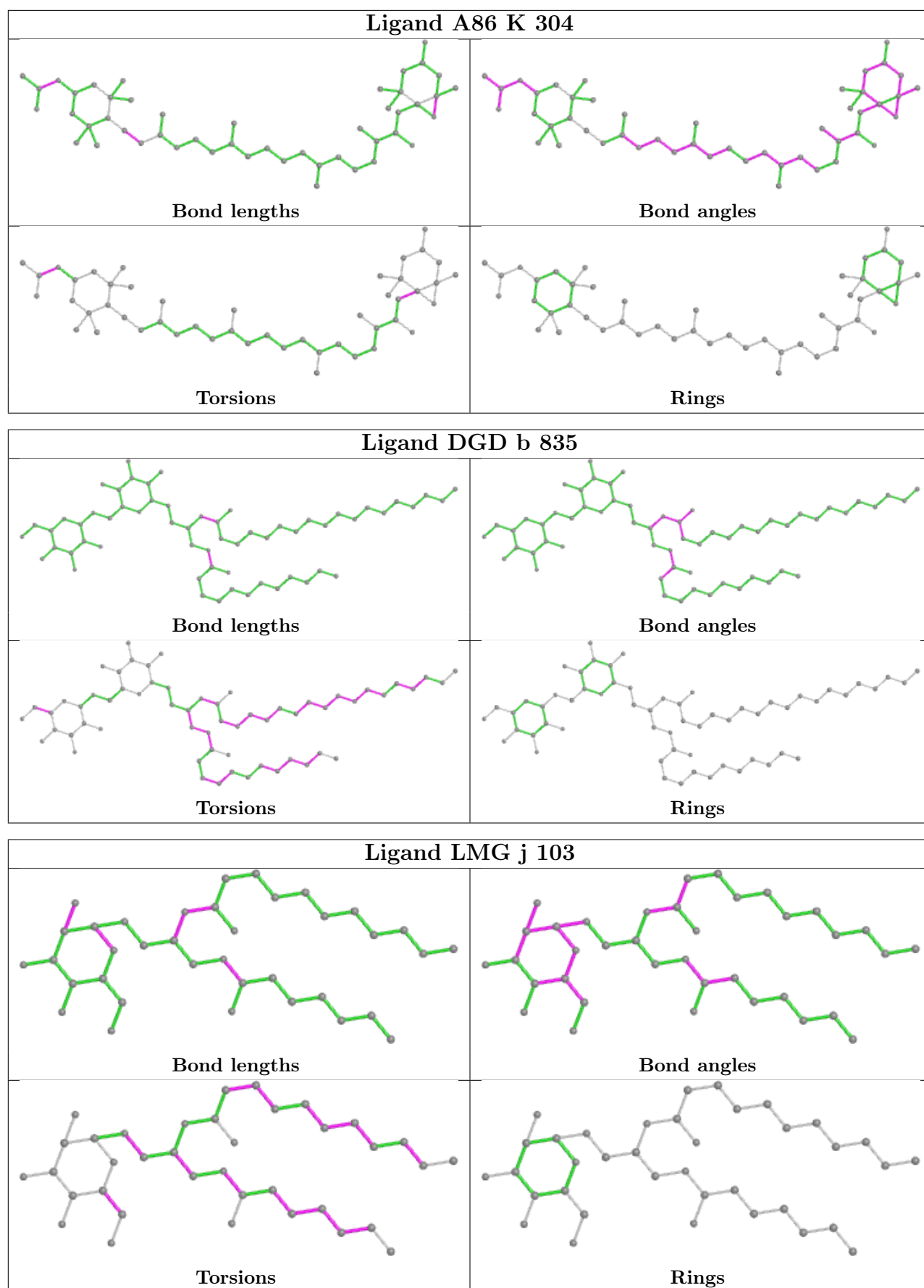


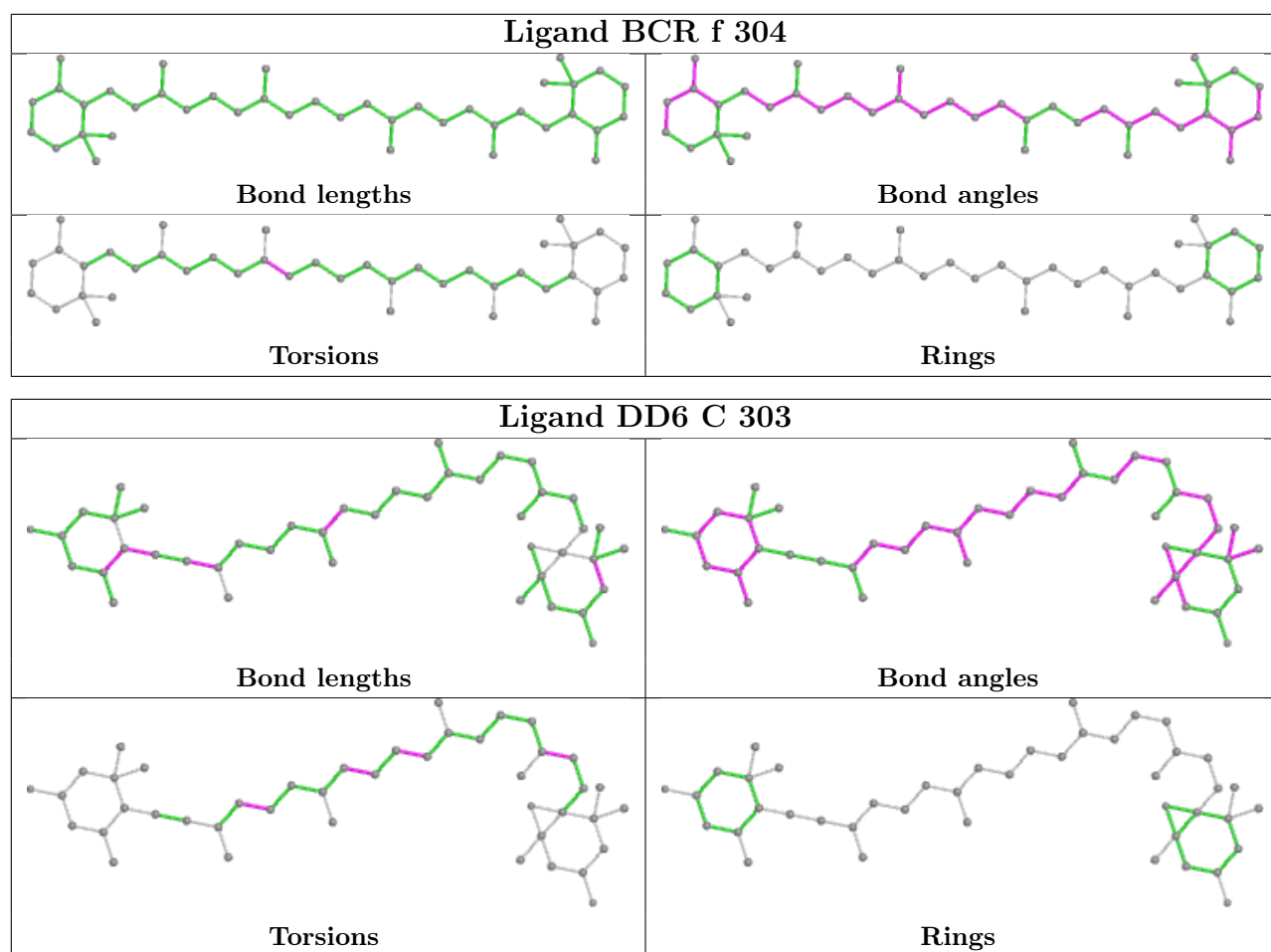
Ligand CLA a 814



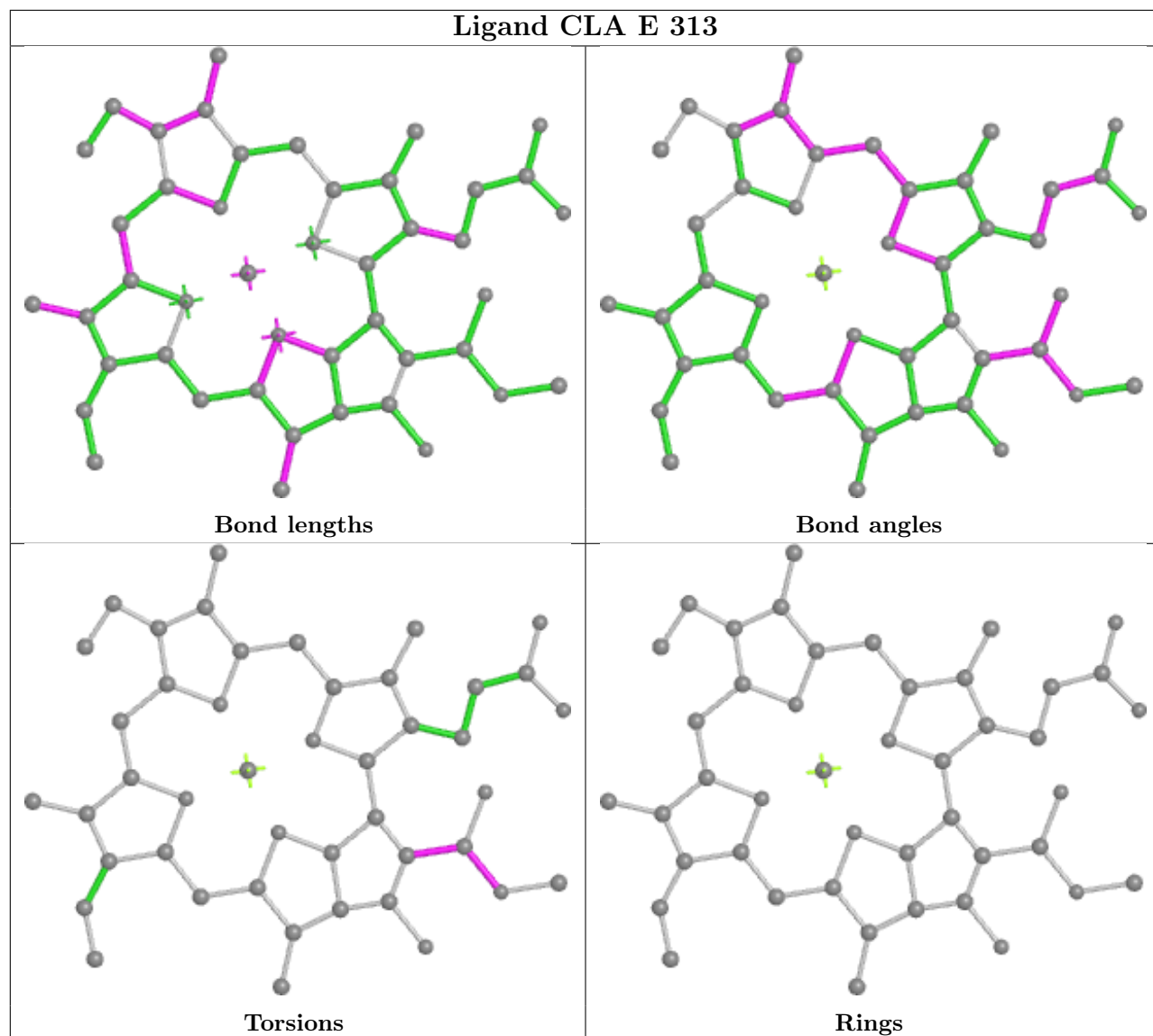
Ligand LHG a 837

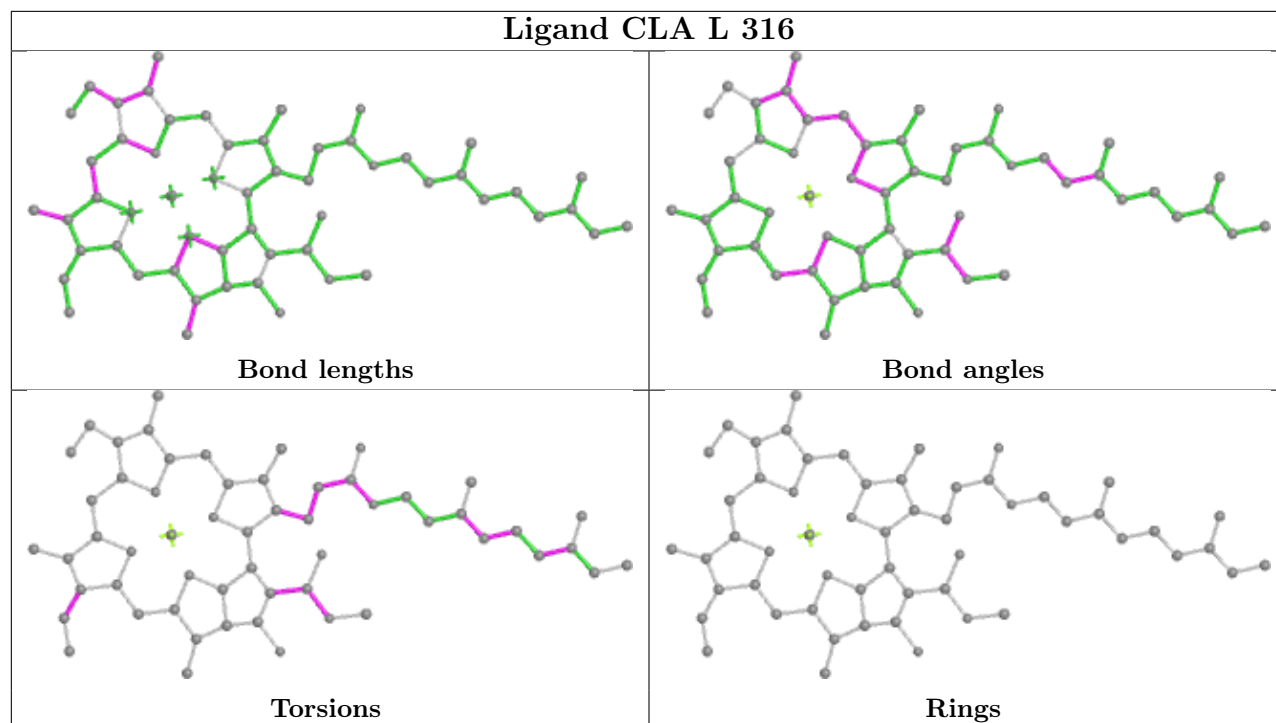
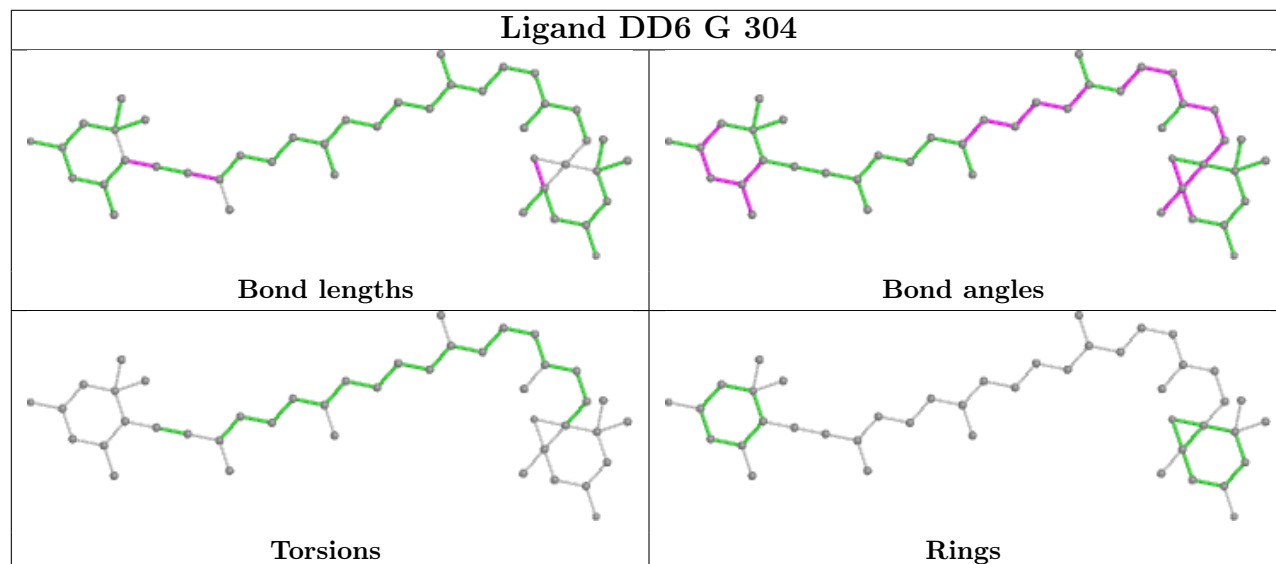




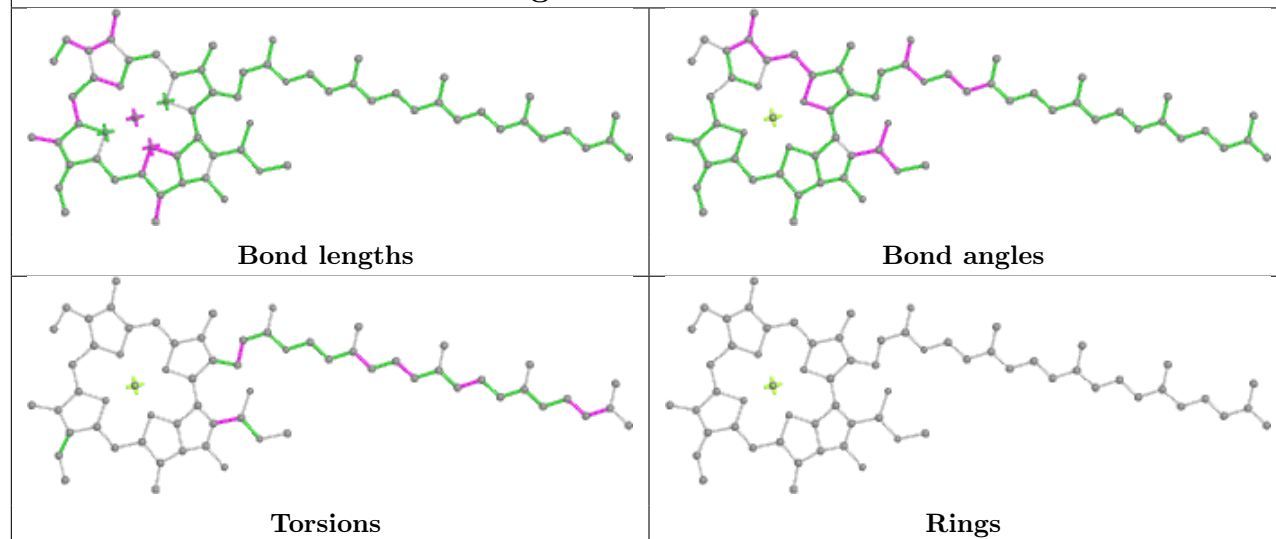


Ligand CLA E 313

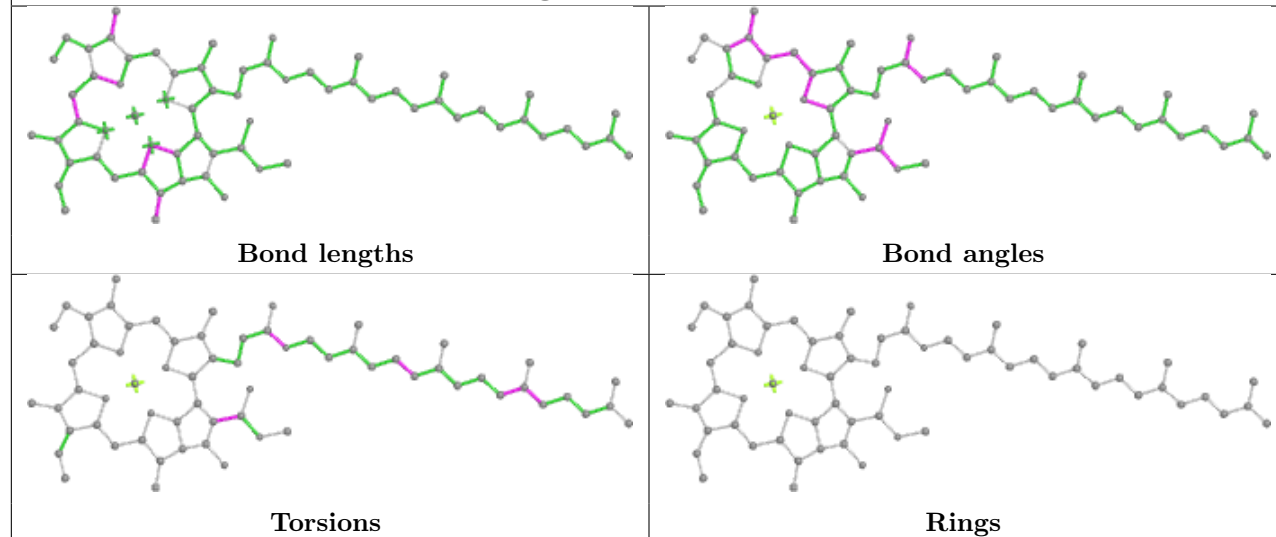


Ligand CLA L 316**Ligand DD6 G 304**

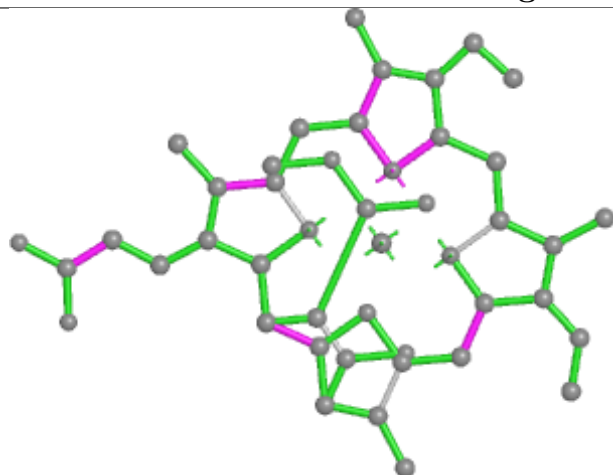
Ligand CLA H 207



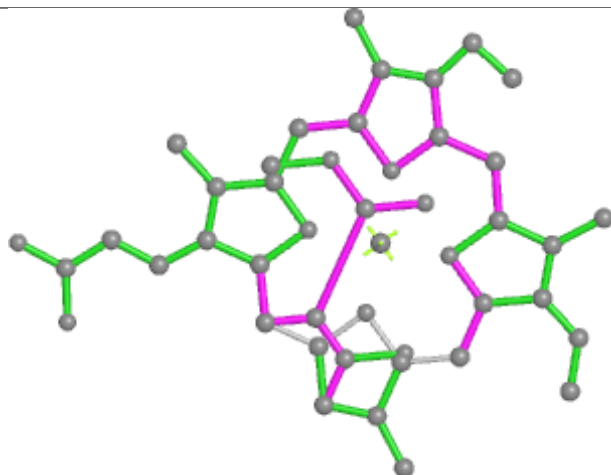
Ligand CLA a 822



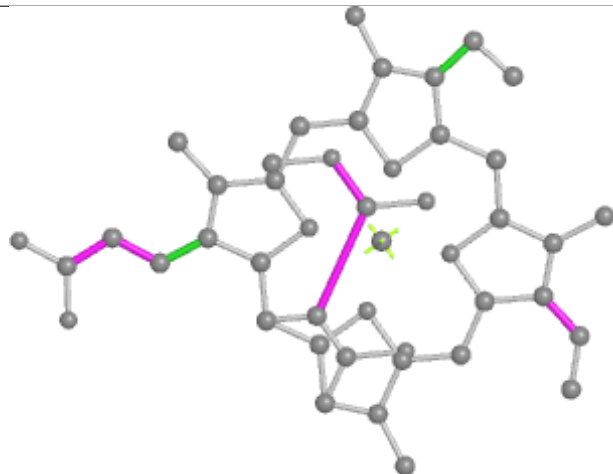
Ligand KC1 L 322



Bond lengths



Bond angles

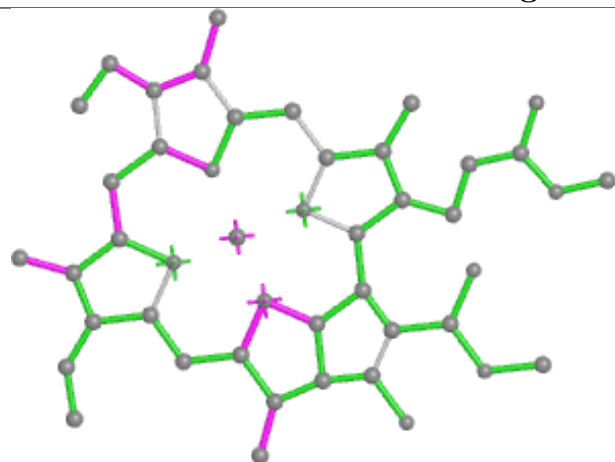


Torsions

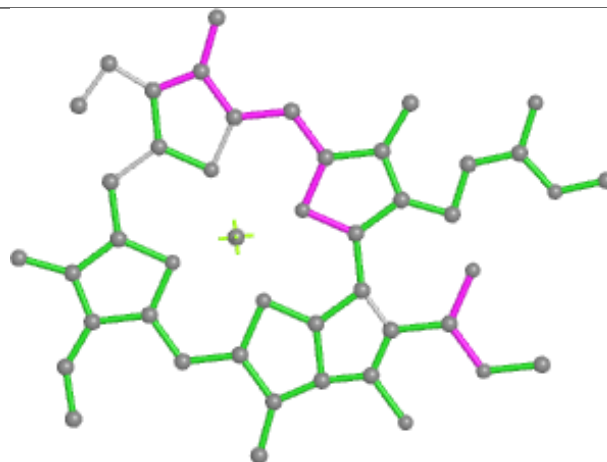


Rings

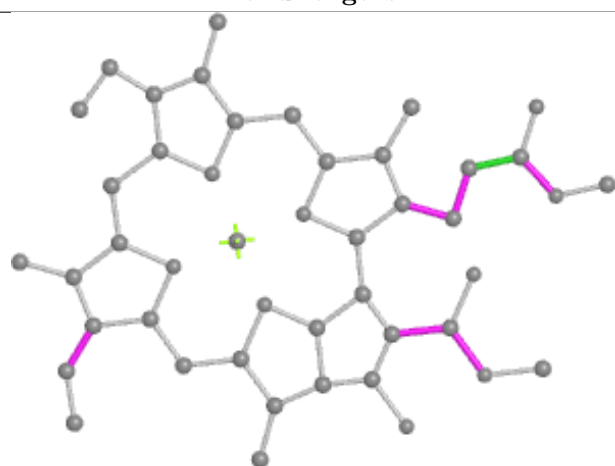
Ligand CLA J 313



Bond lengths



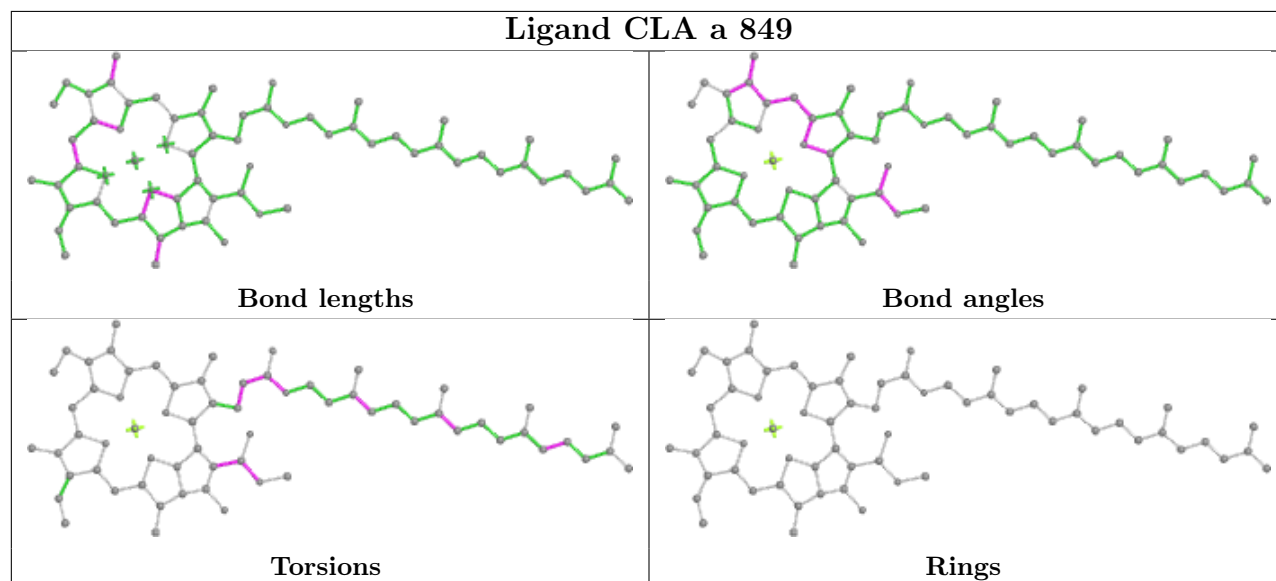
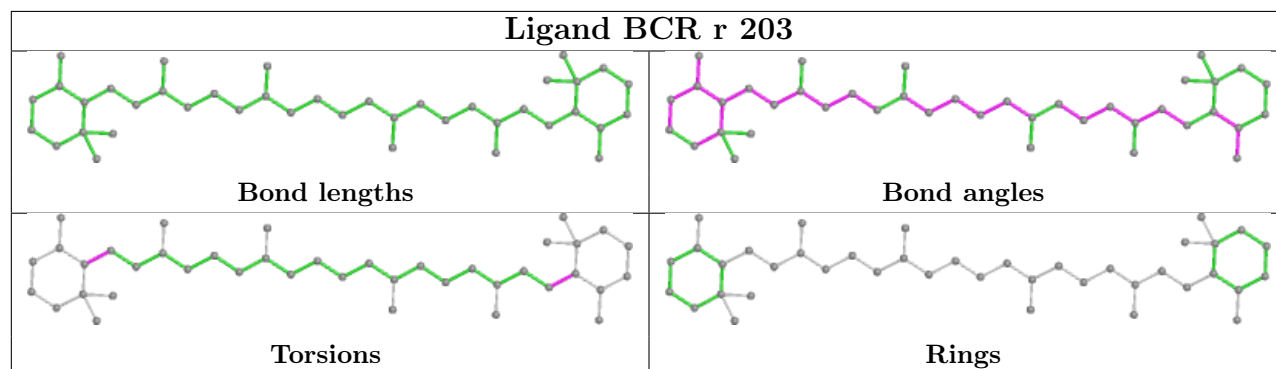
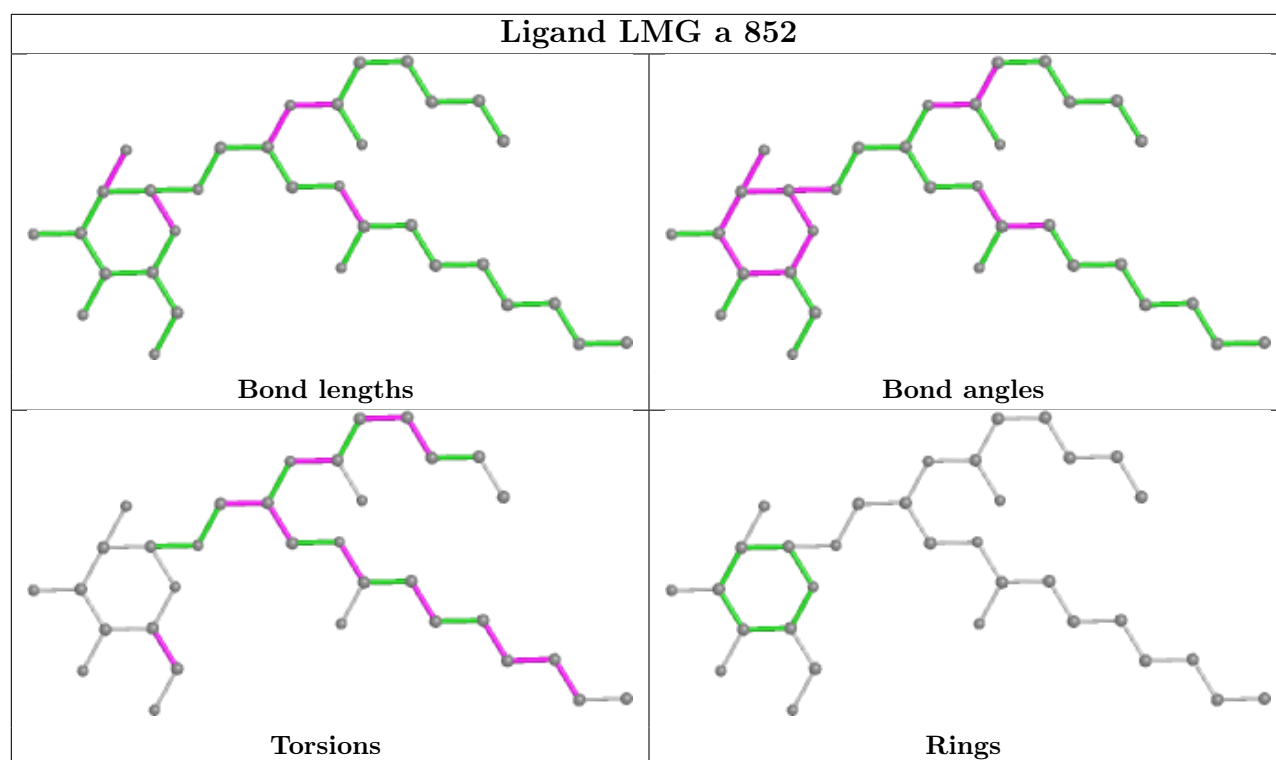
Bond angles

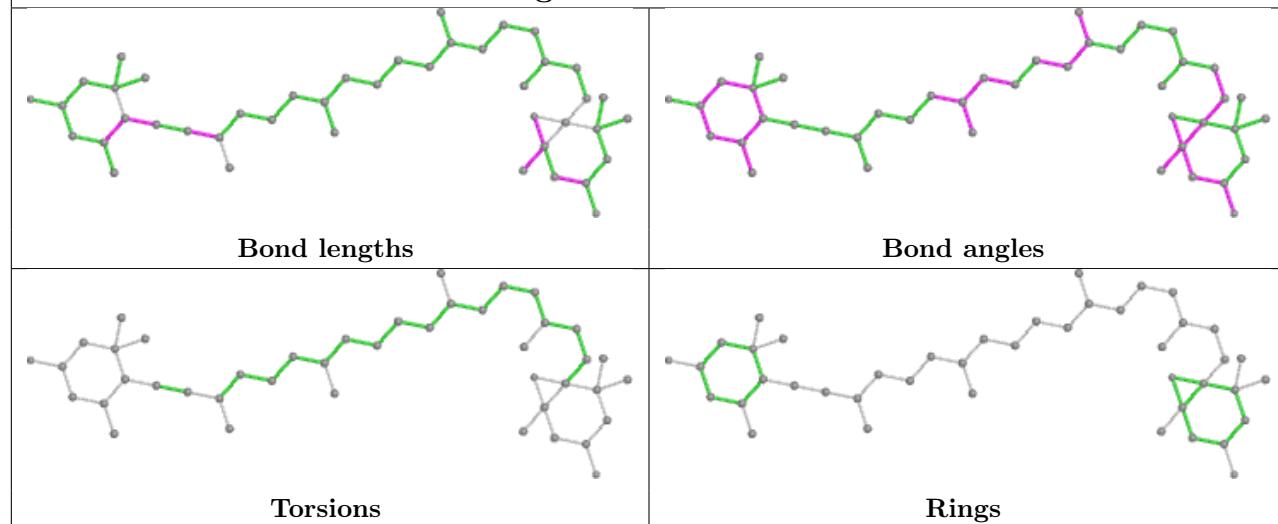
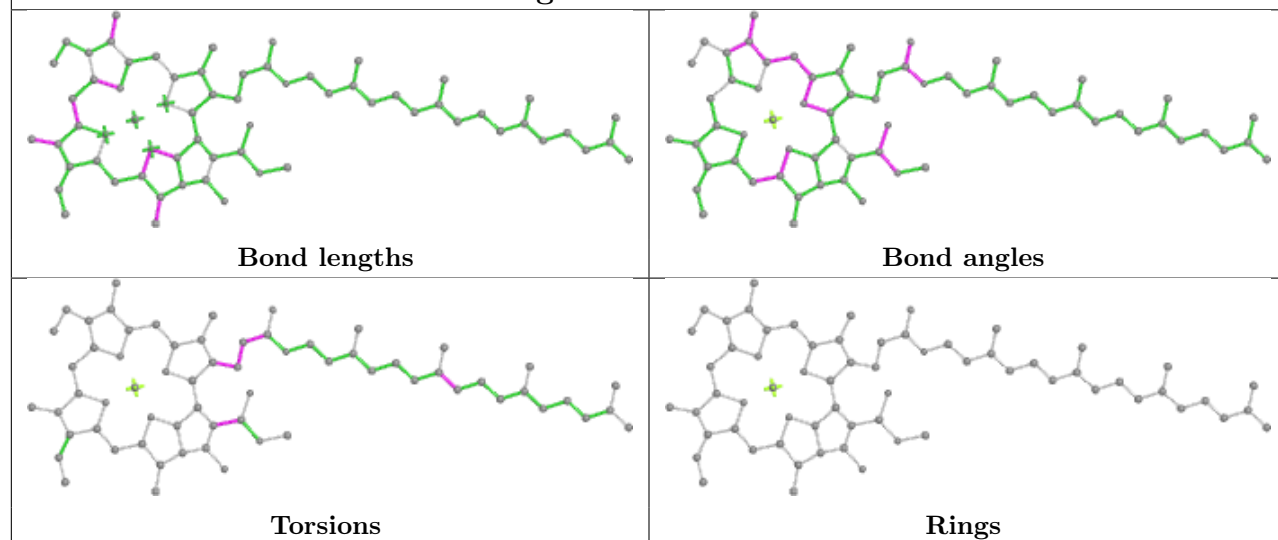
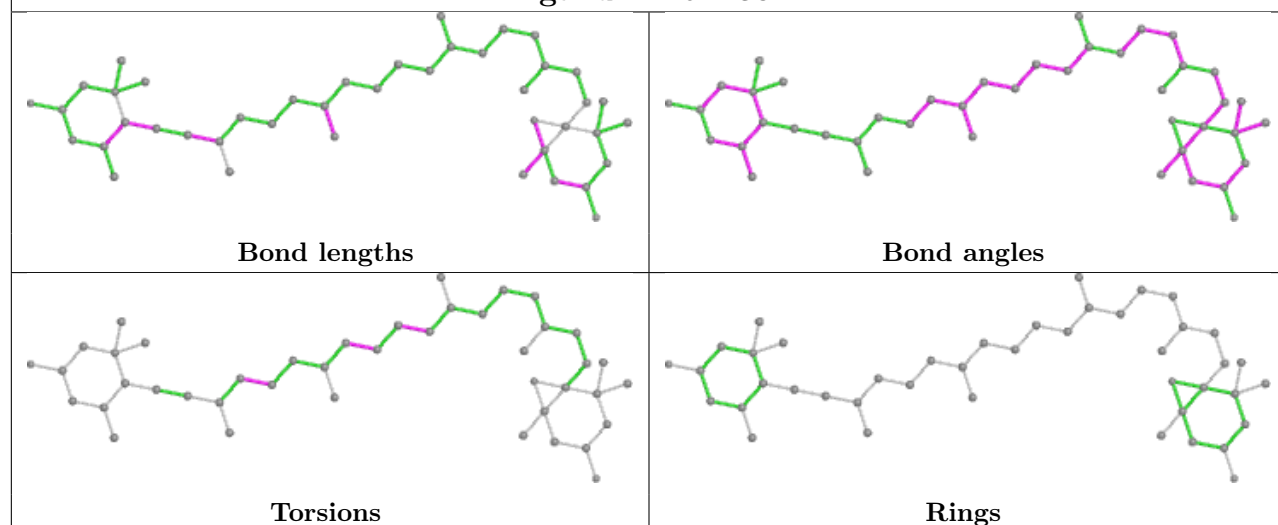


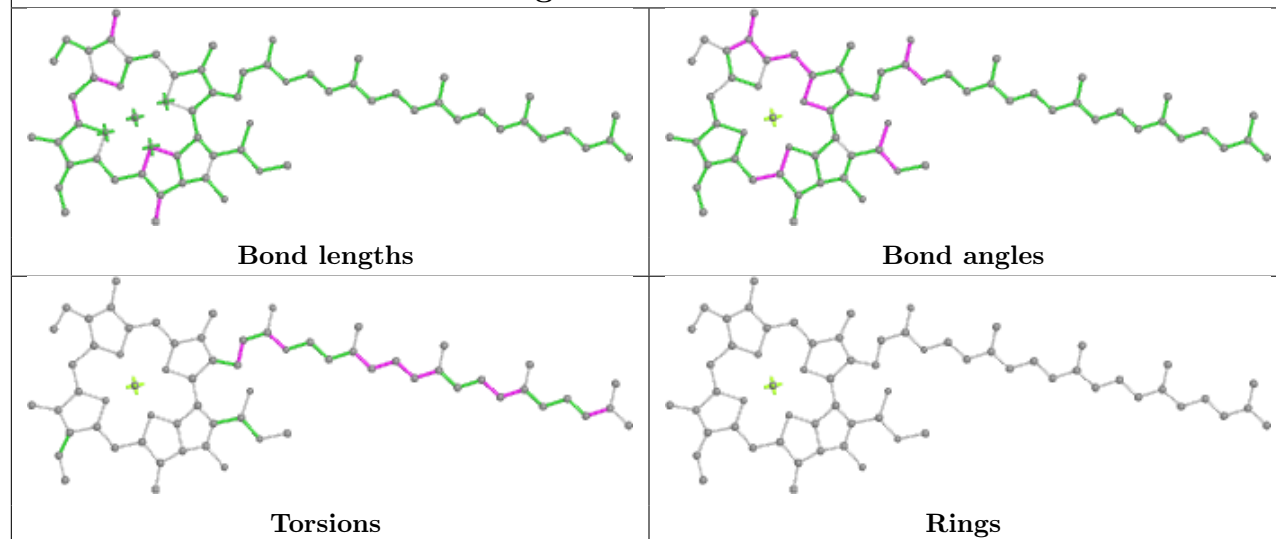
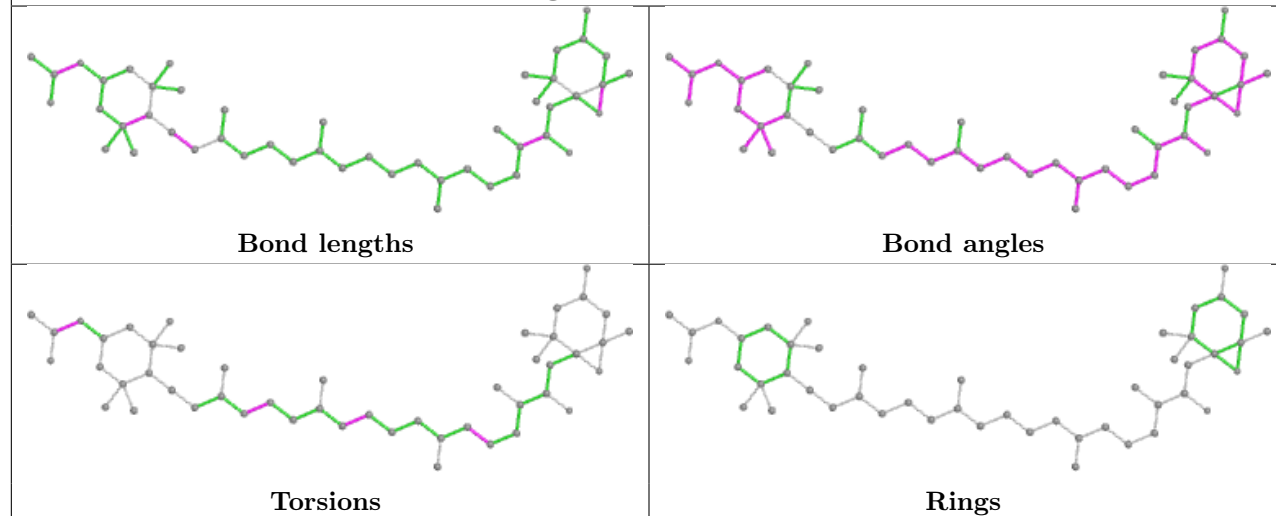
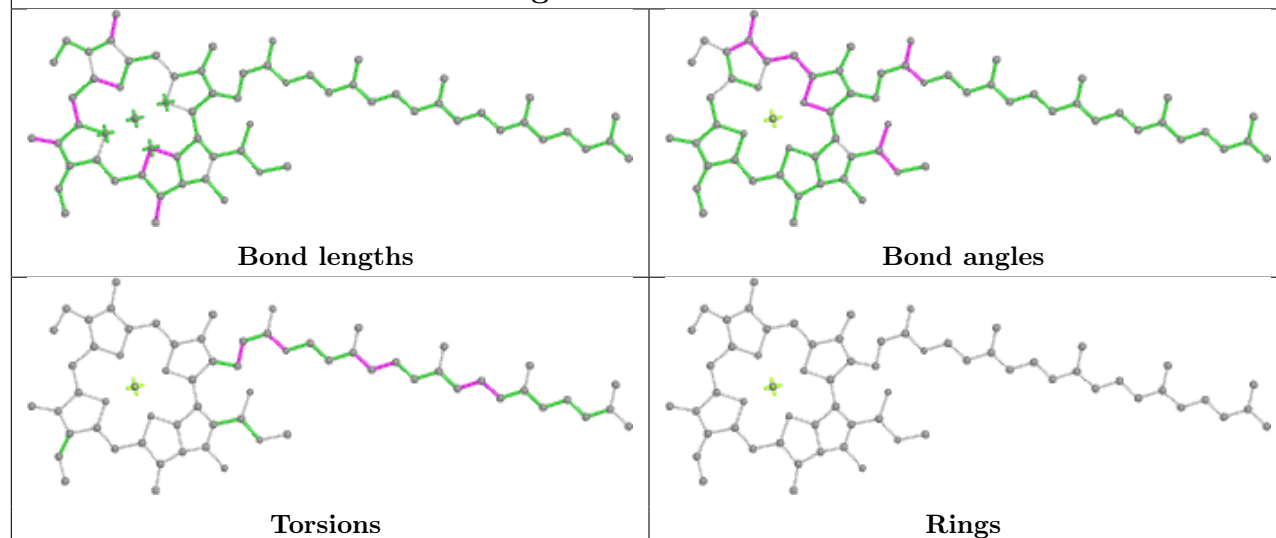
Torsions

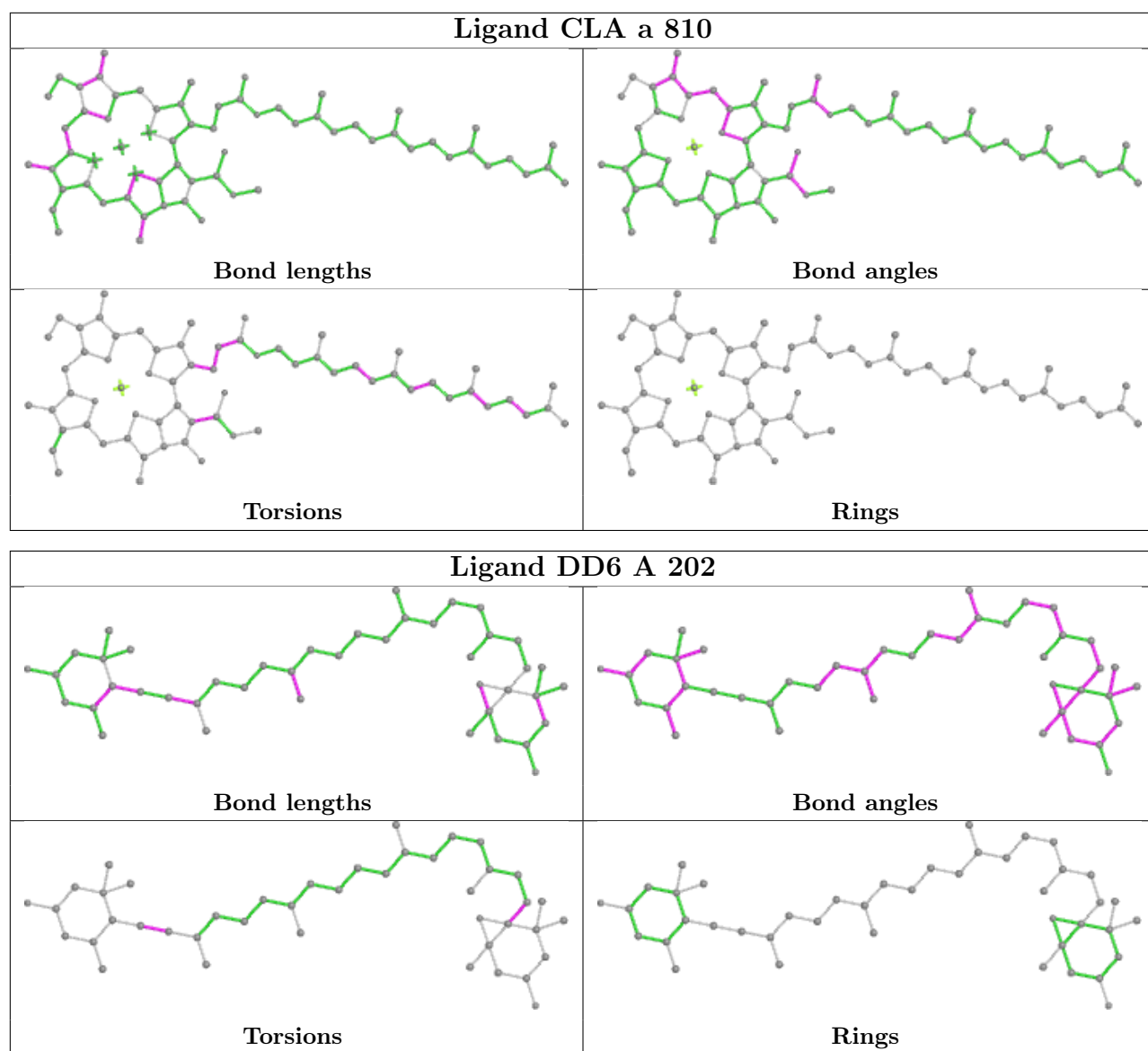


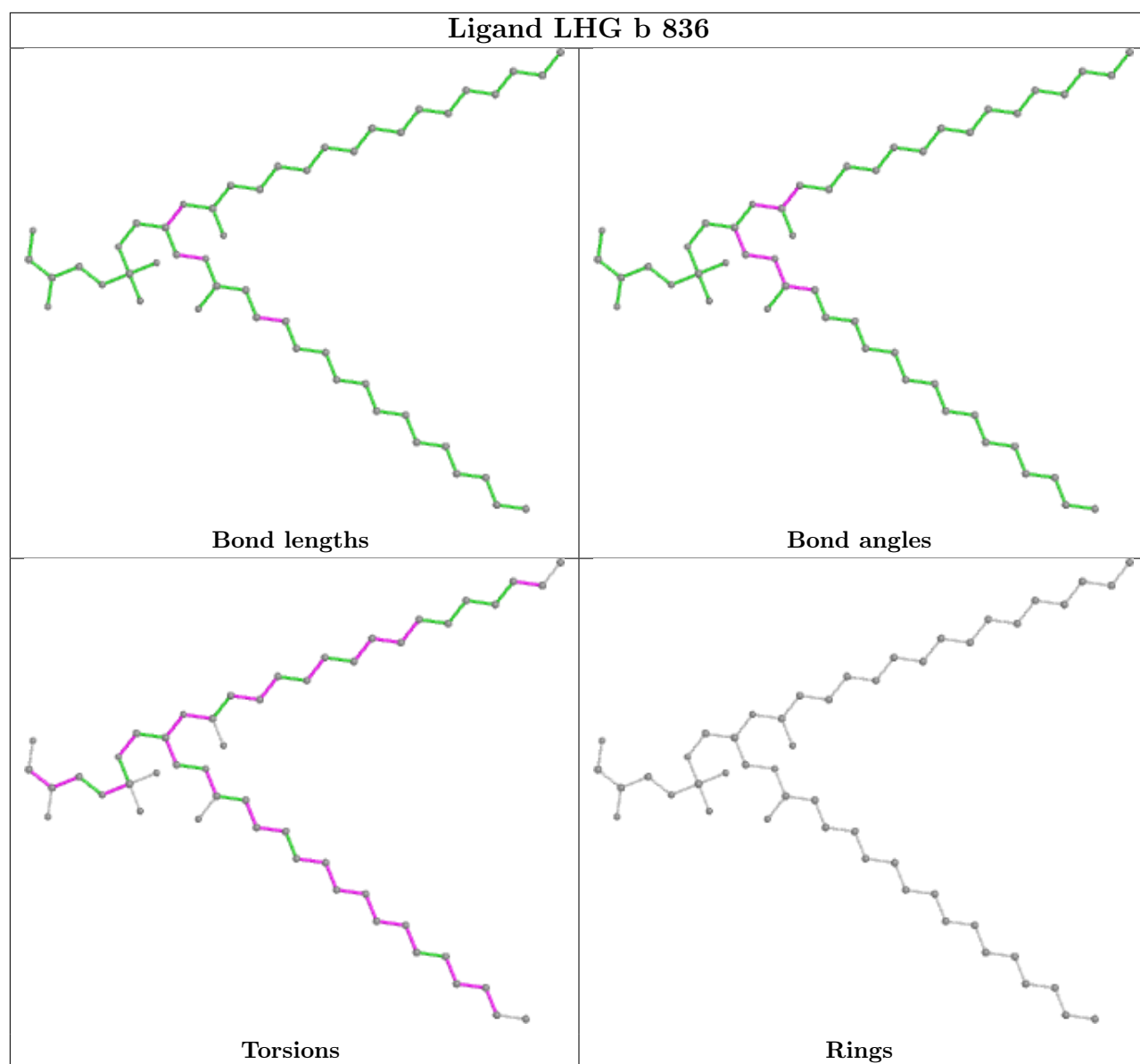
Rings



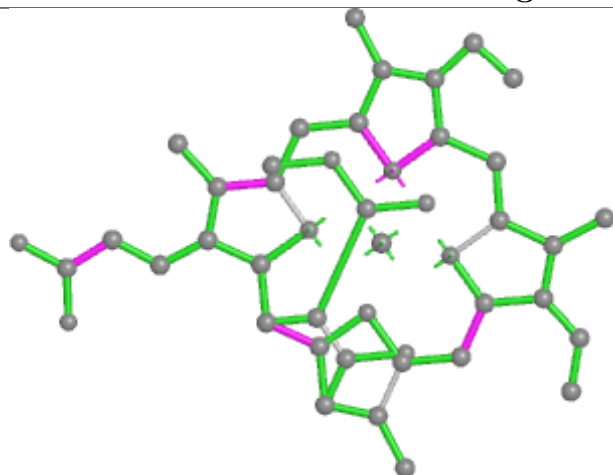
Ligand DD6 L 303**Ligand CLA a 816****Ligand DD6 I 304**

Ligand CLA b 843**Ligand A86 I 303****Ligand CLA D 213**

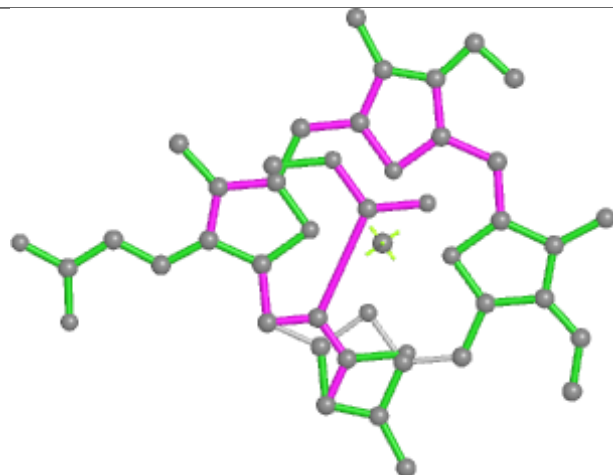




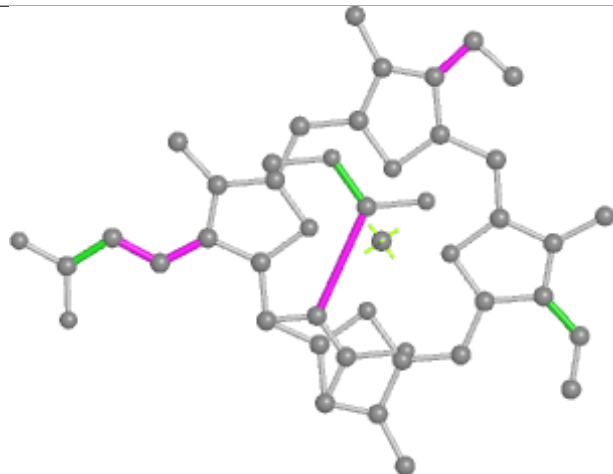
Ligand KC1 C 313



Bond lengths



Bond angles

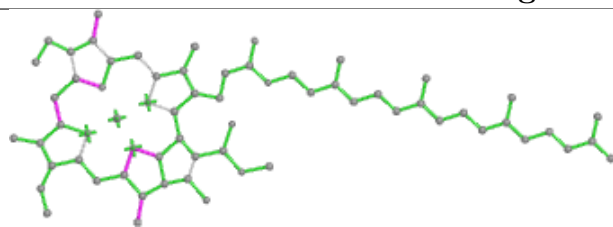


Torsions

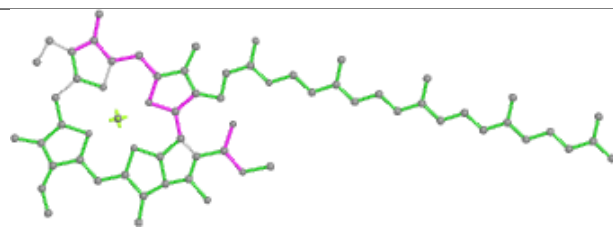


Rings

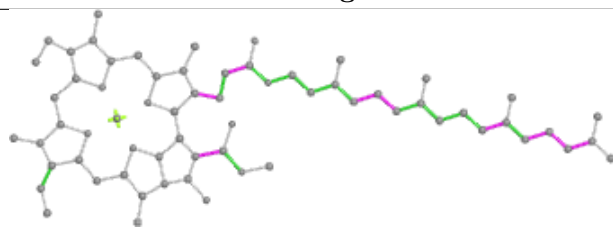
Ligand CLA a 845



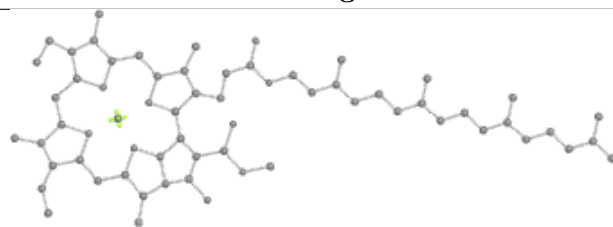
Bond lengths



Bond angles

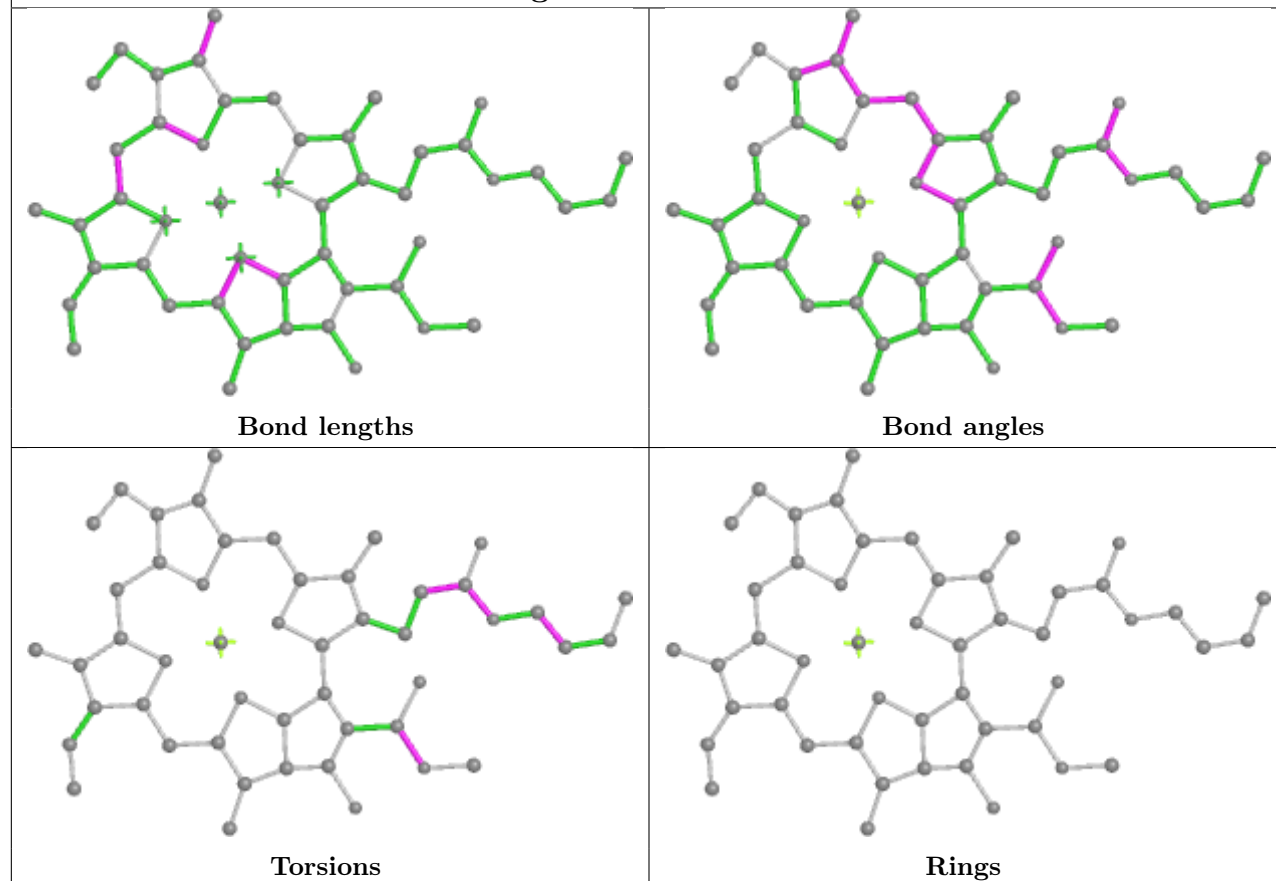


Torsions

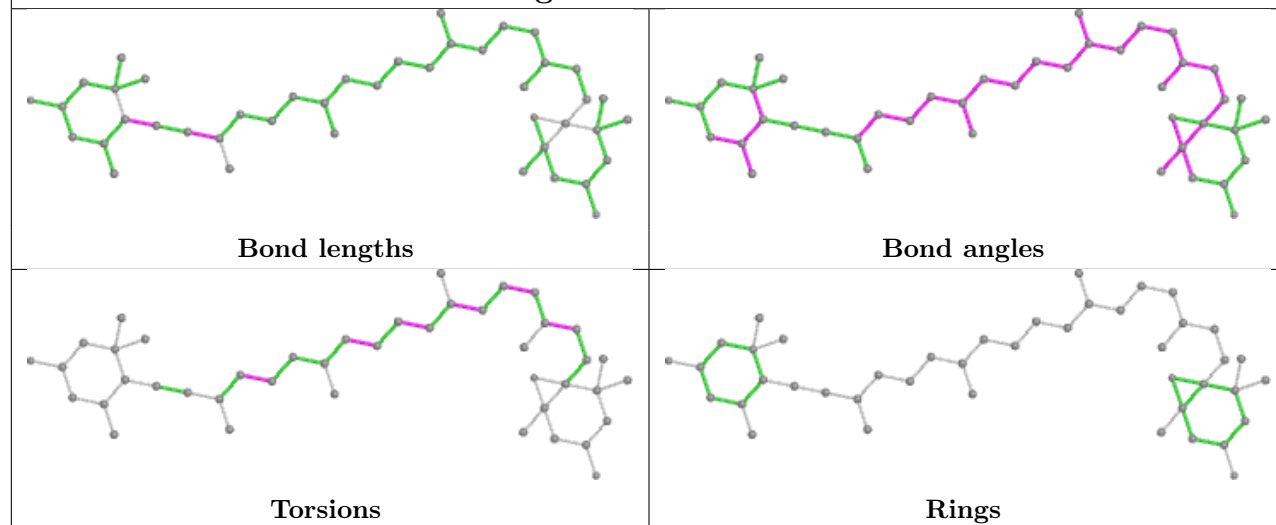


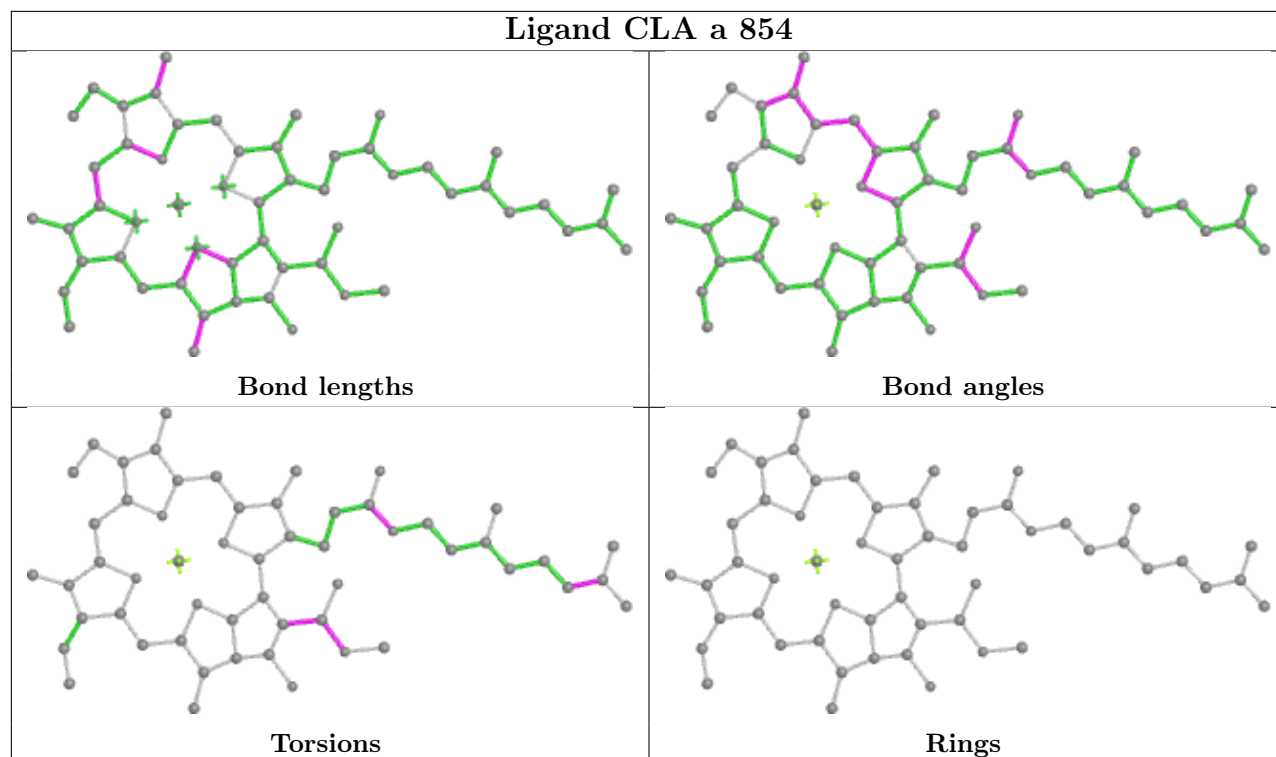
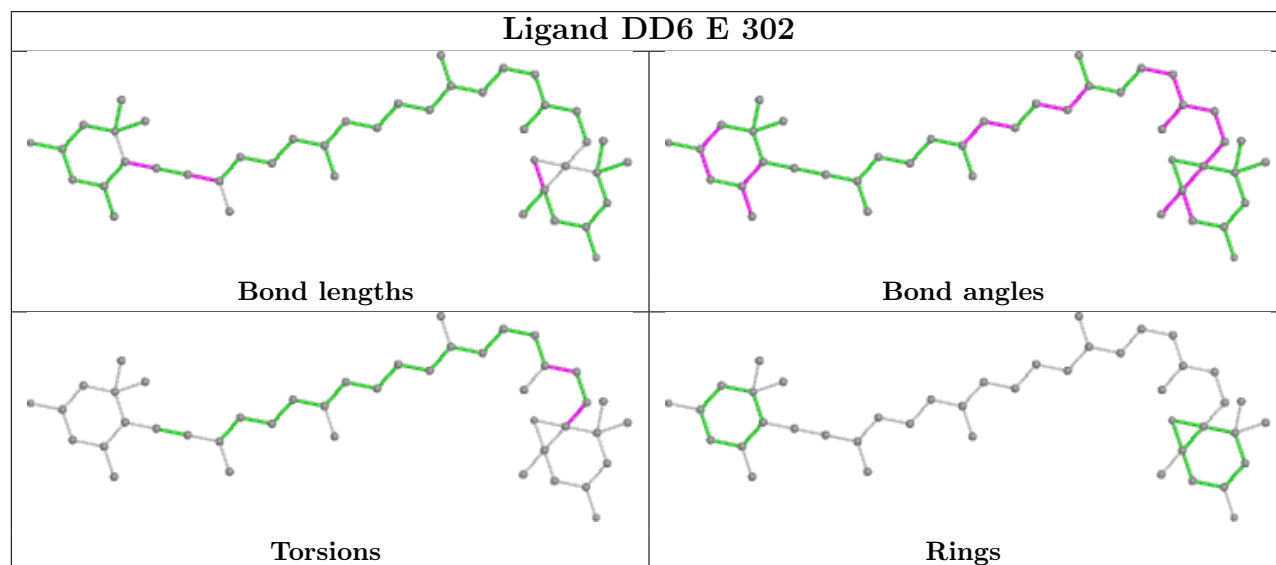
Rings

Ligand CLA G 317

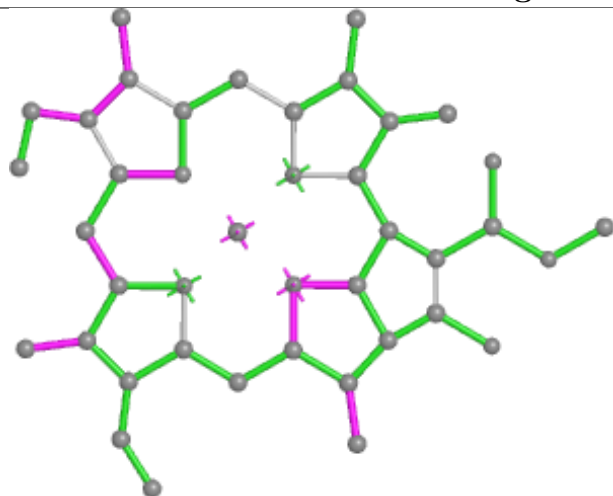


Ligand DD6 L 301

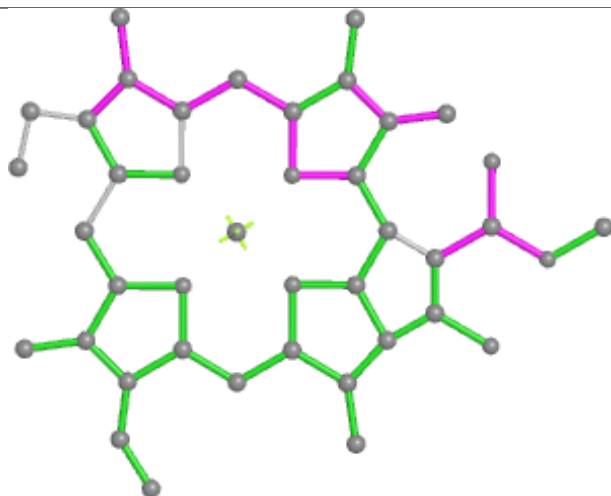


Ligand CLA a 854**Ligand DD6 E 302**

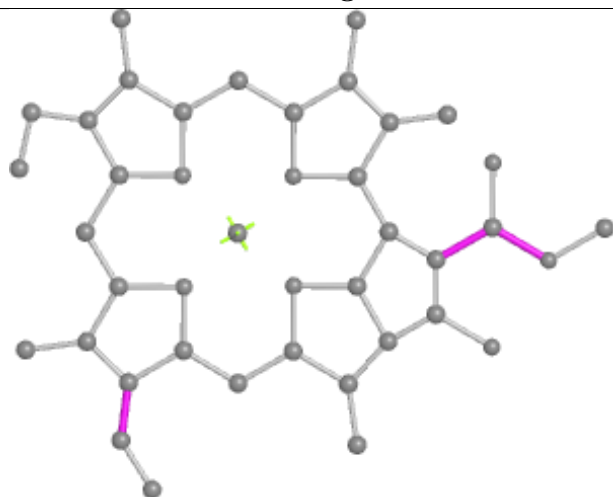
Ligand CLA C 314



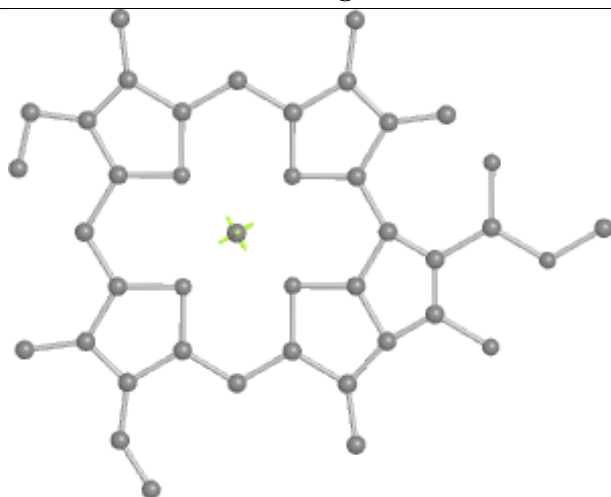
Bond lengths



Bond angles

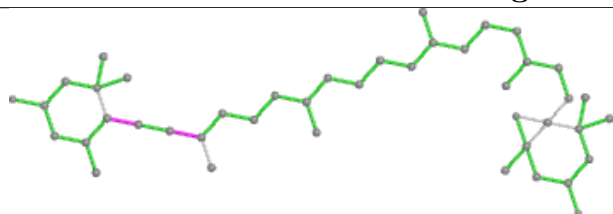


Torsions

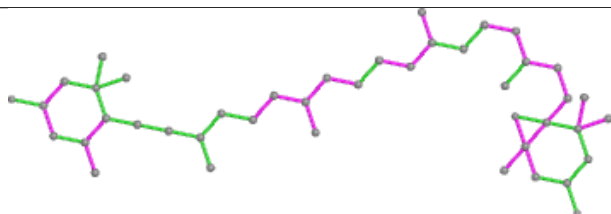


Rings

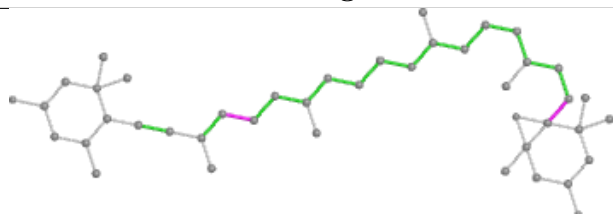
Ligand DD6 M 301



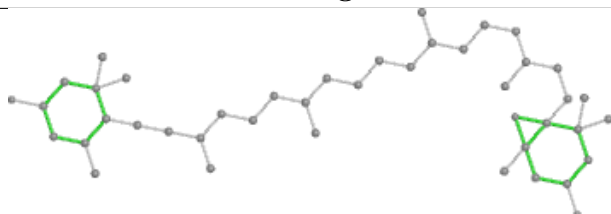
Bond lengths



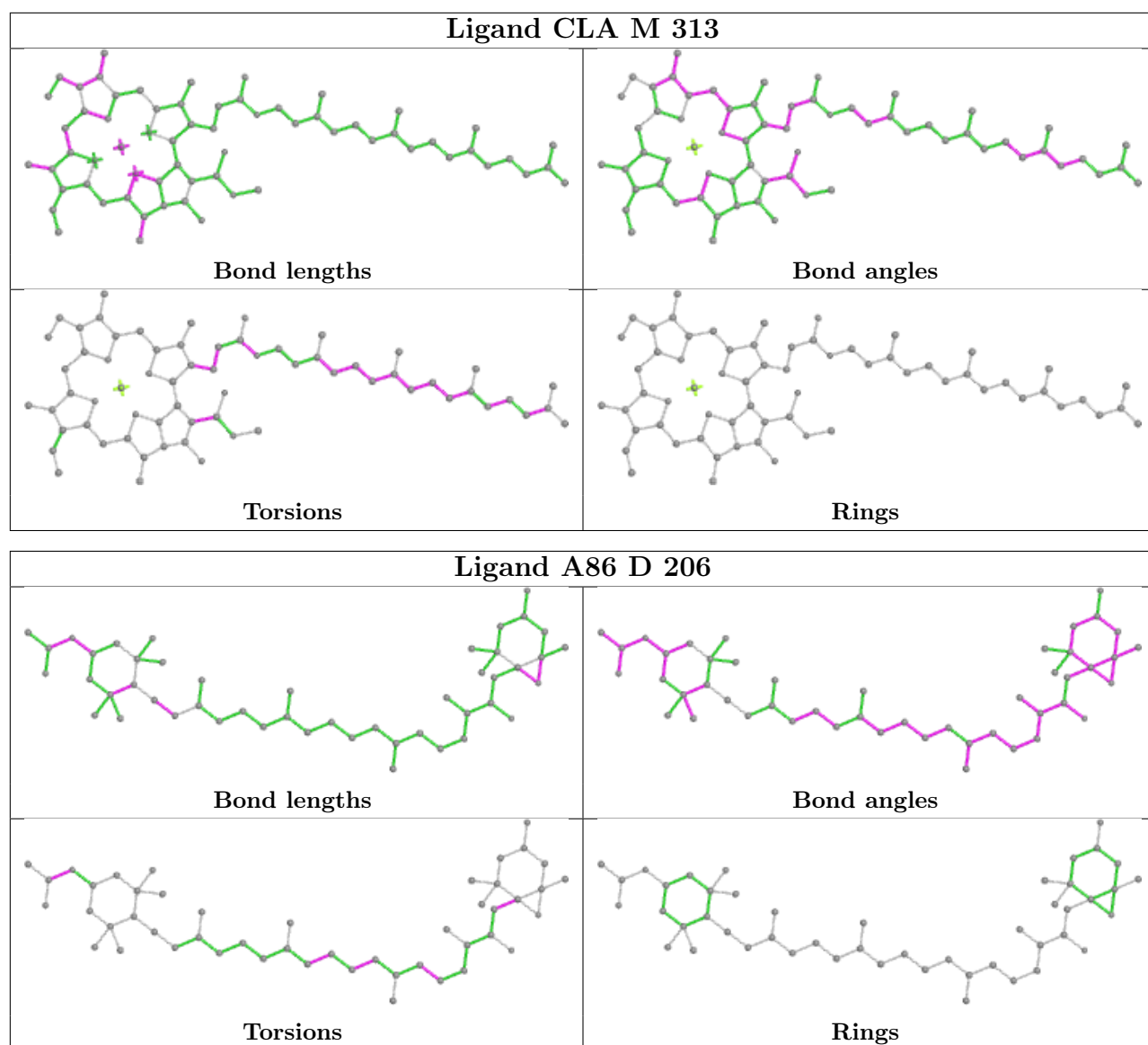
Bond angles

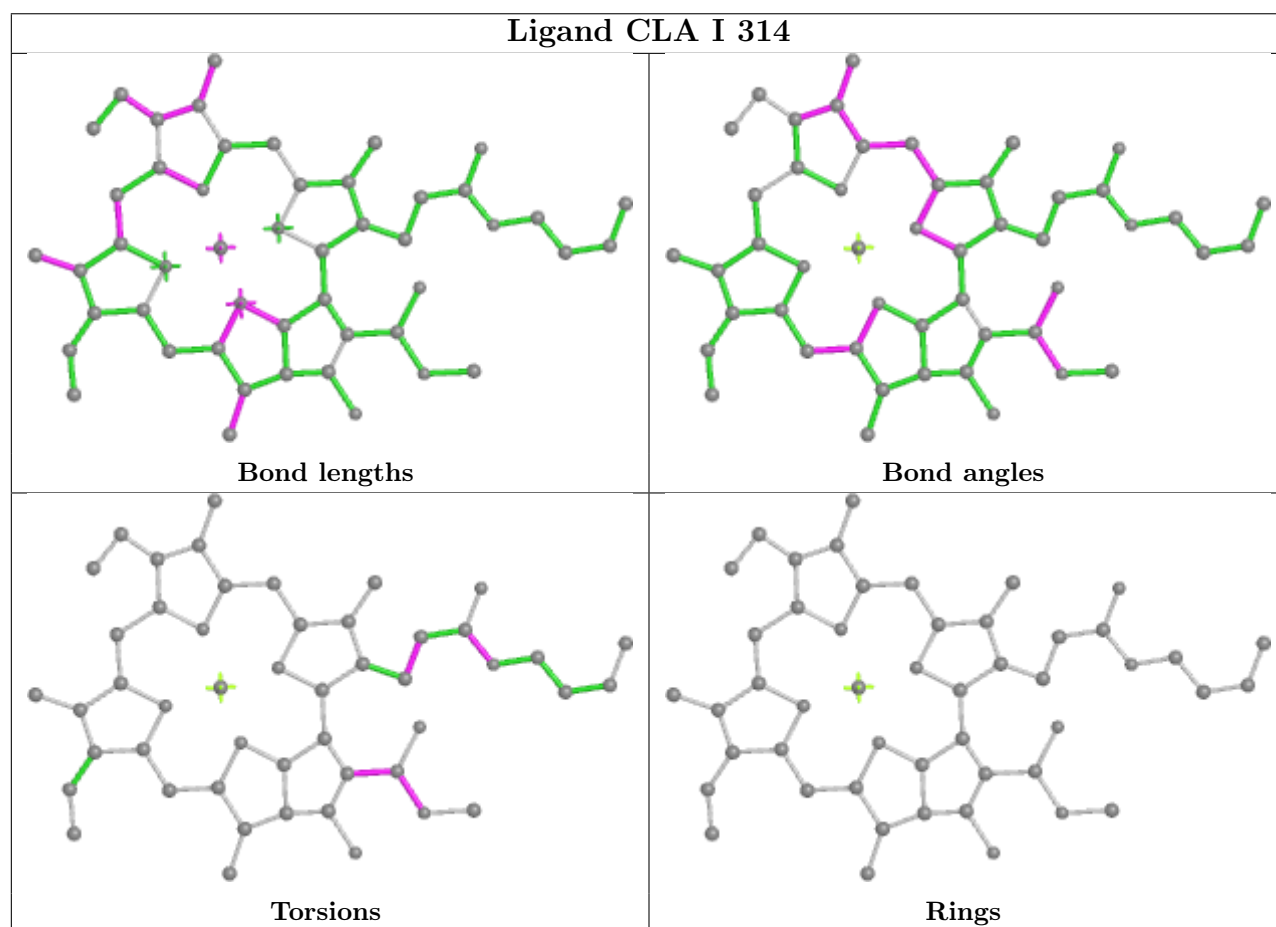
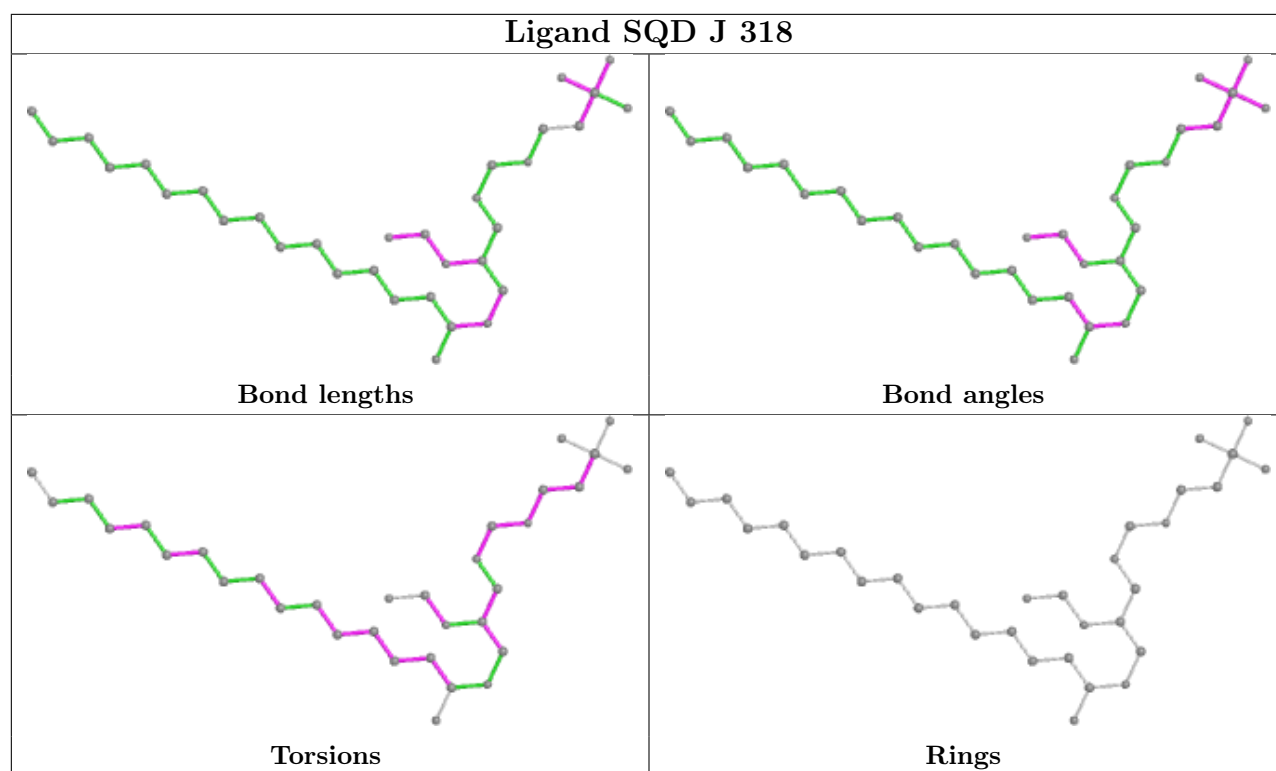


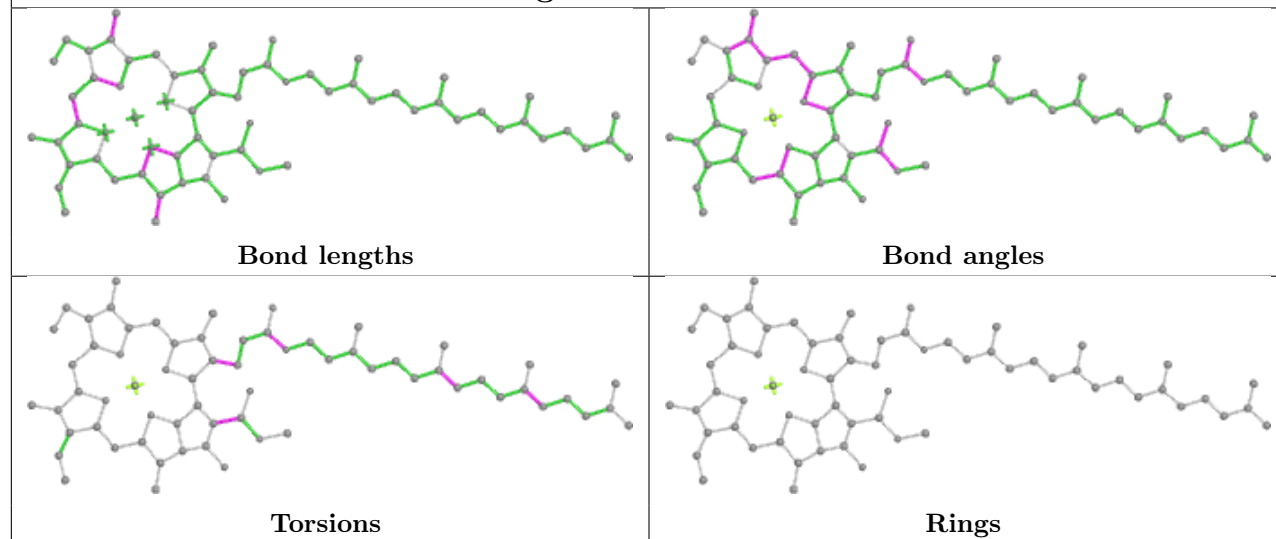
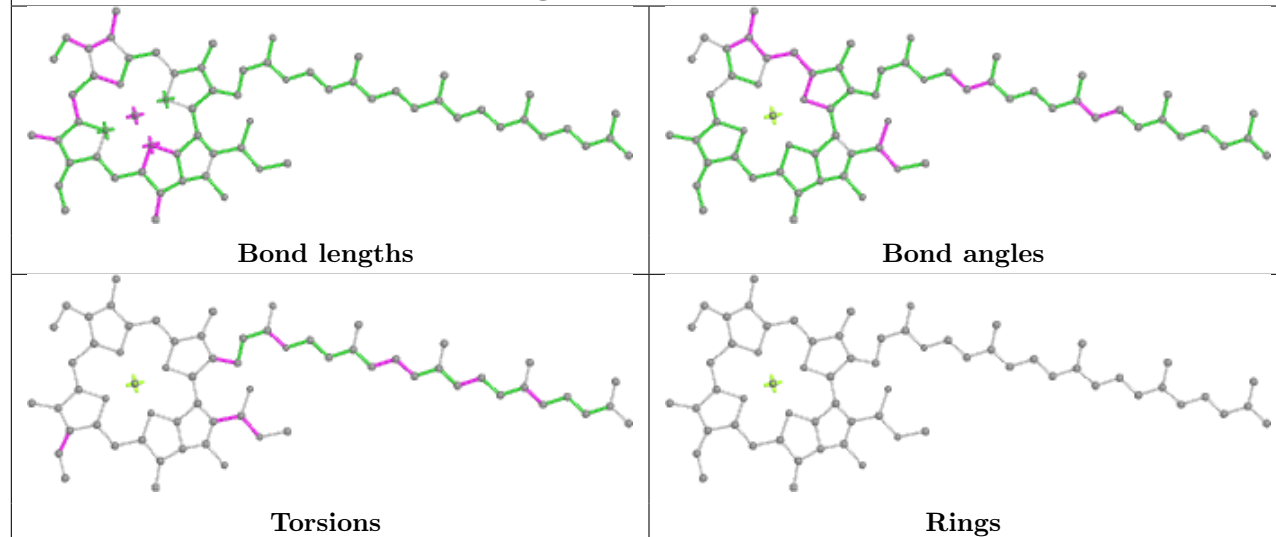
Torsions

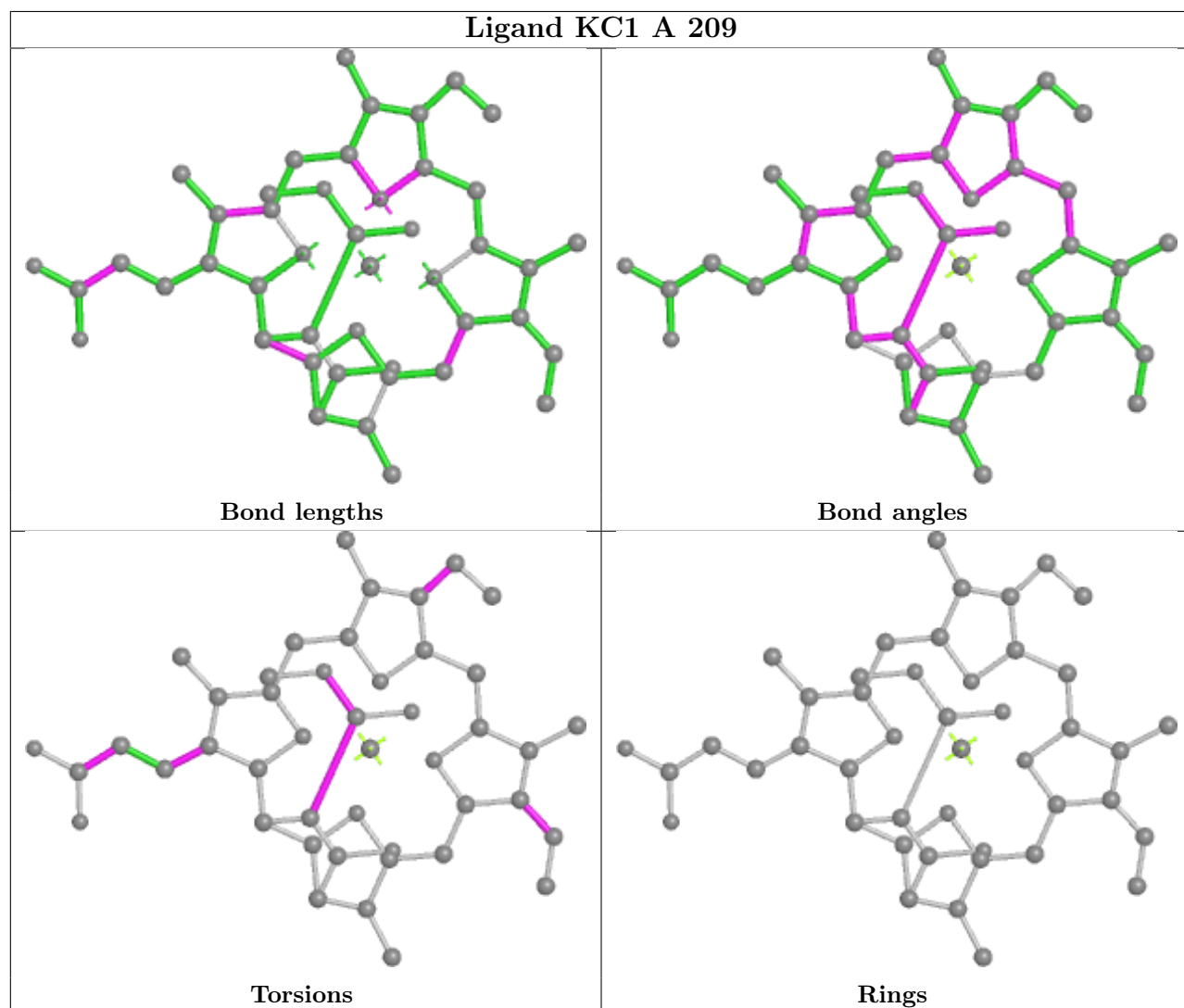
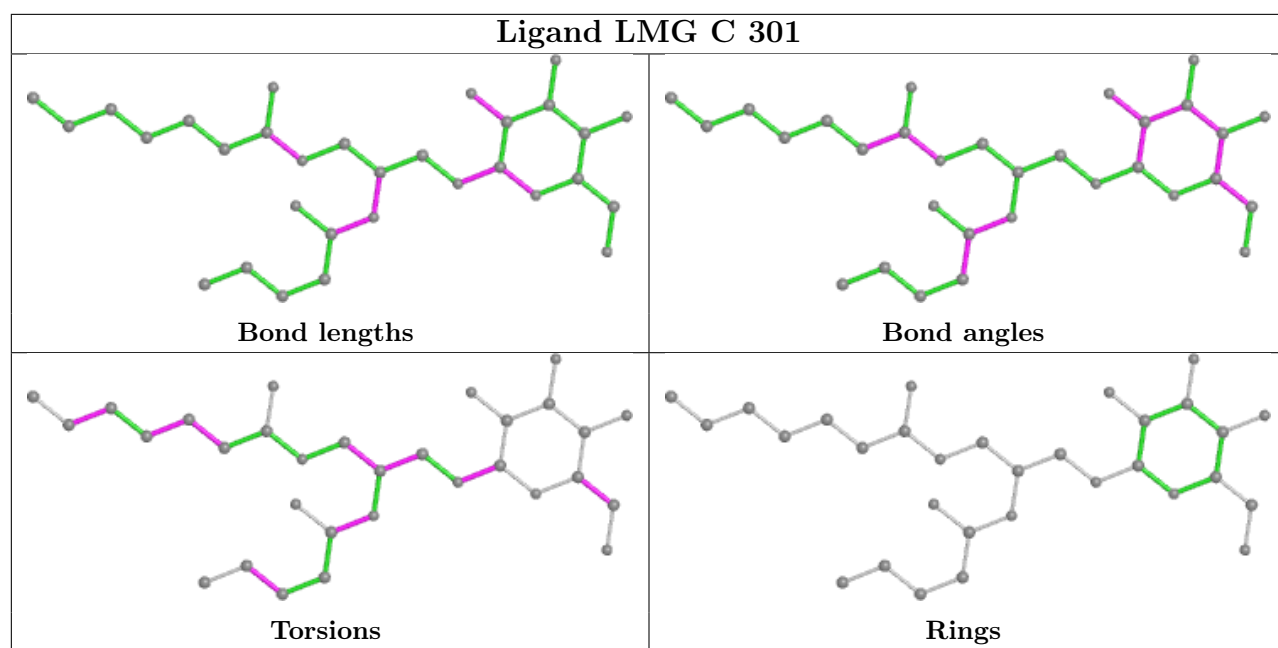


Rings

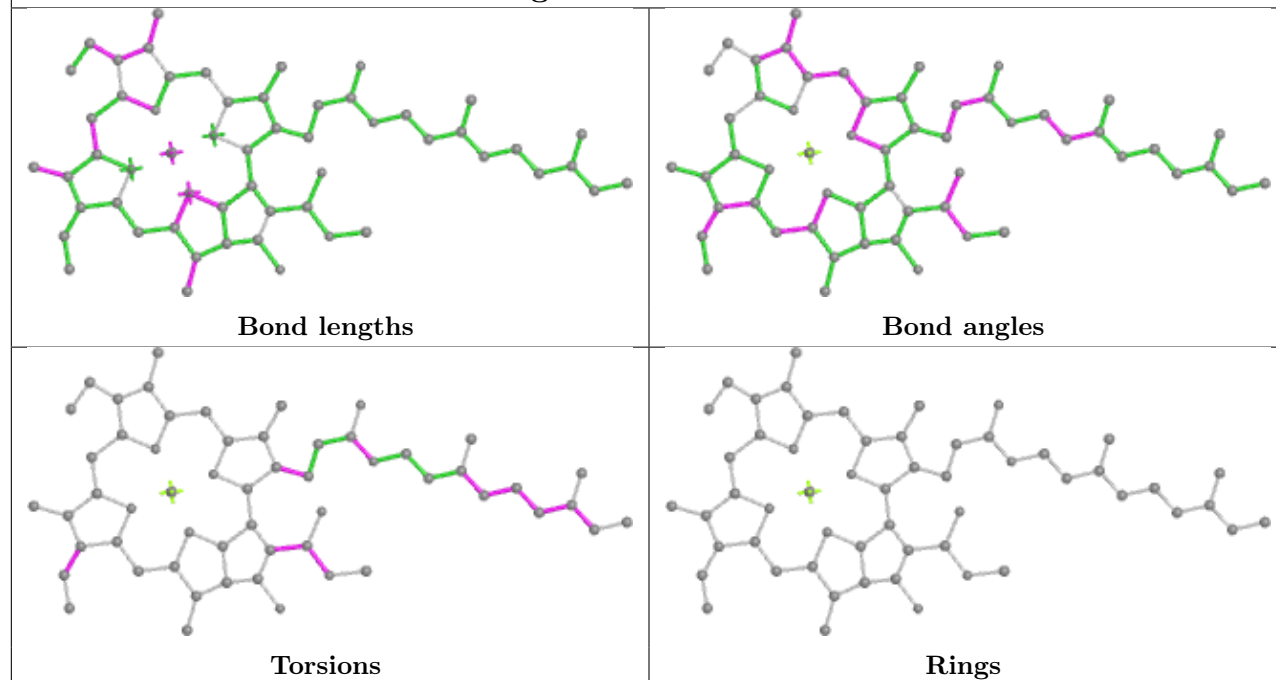




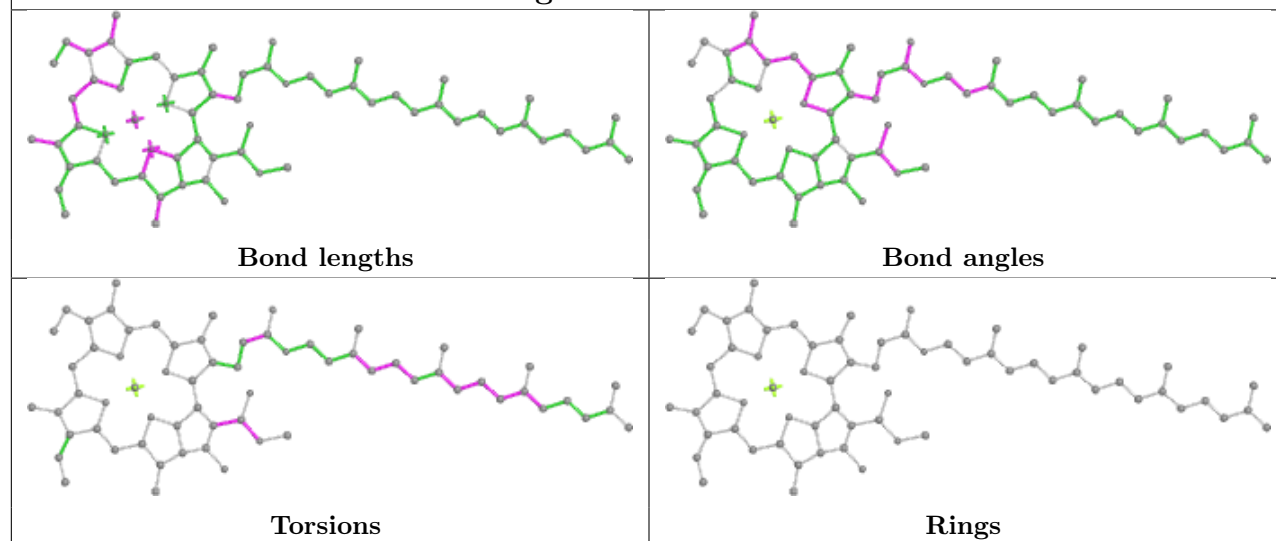
Ligand CLA a 848**Ligand CLA L 313**



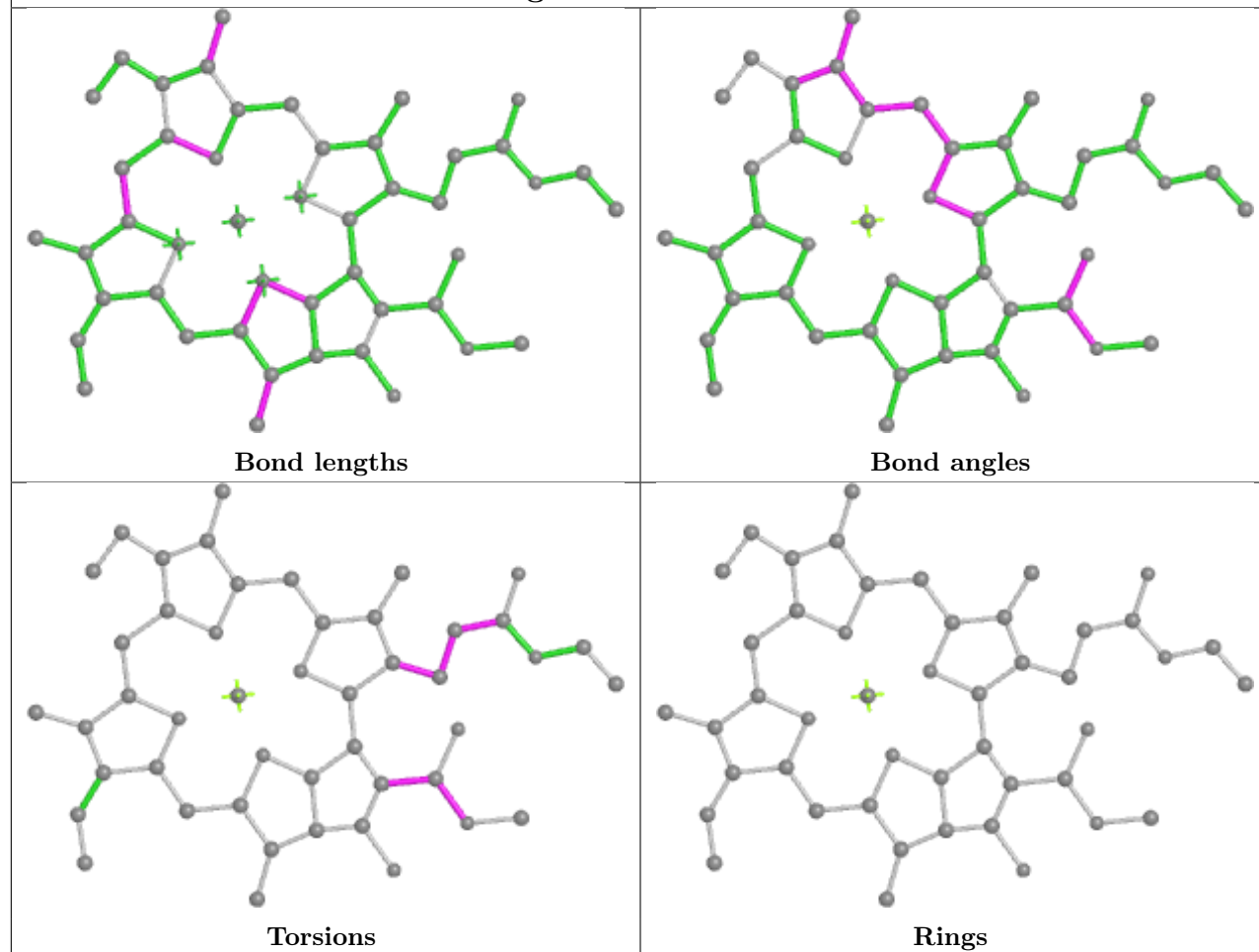
Ligand CLA K 310



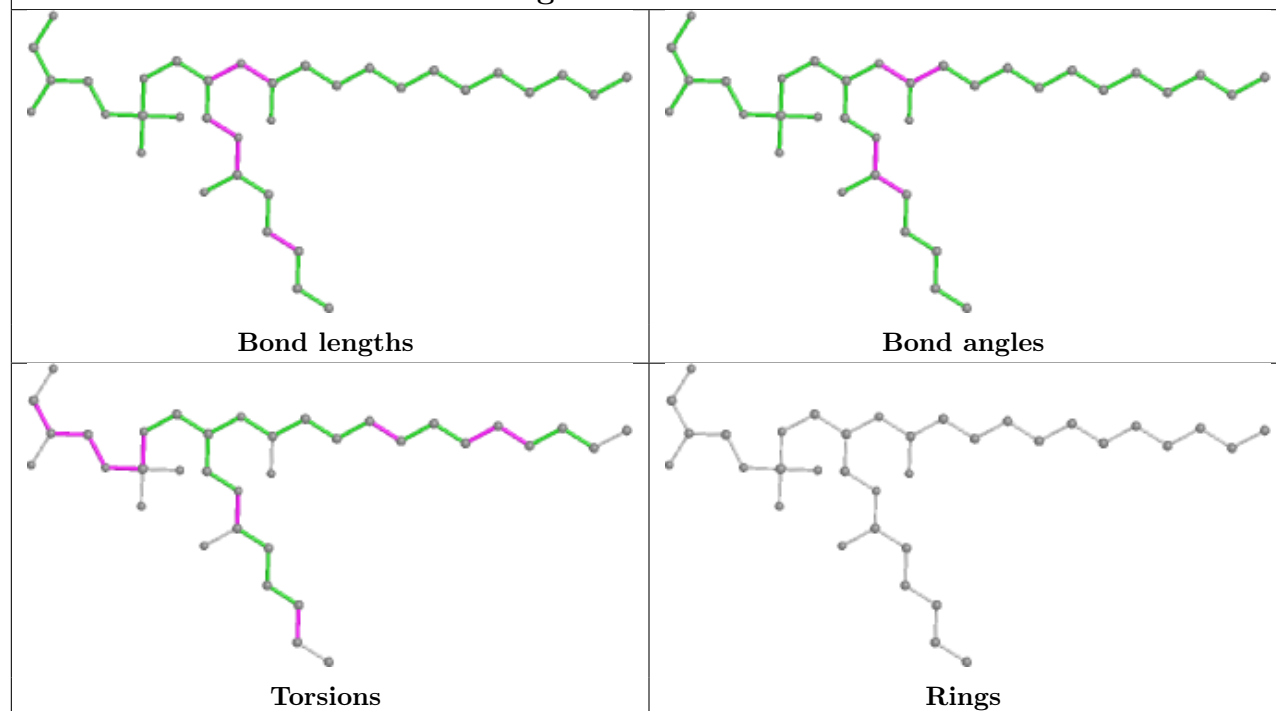
Ligand CLA b 804

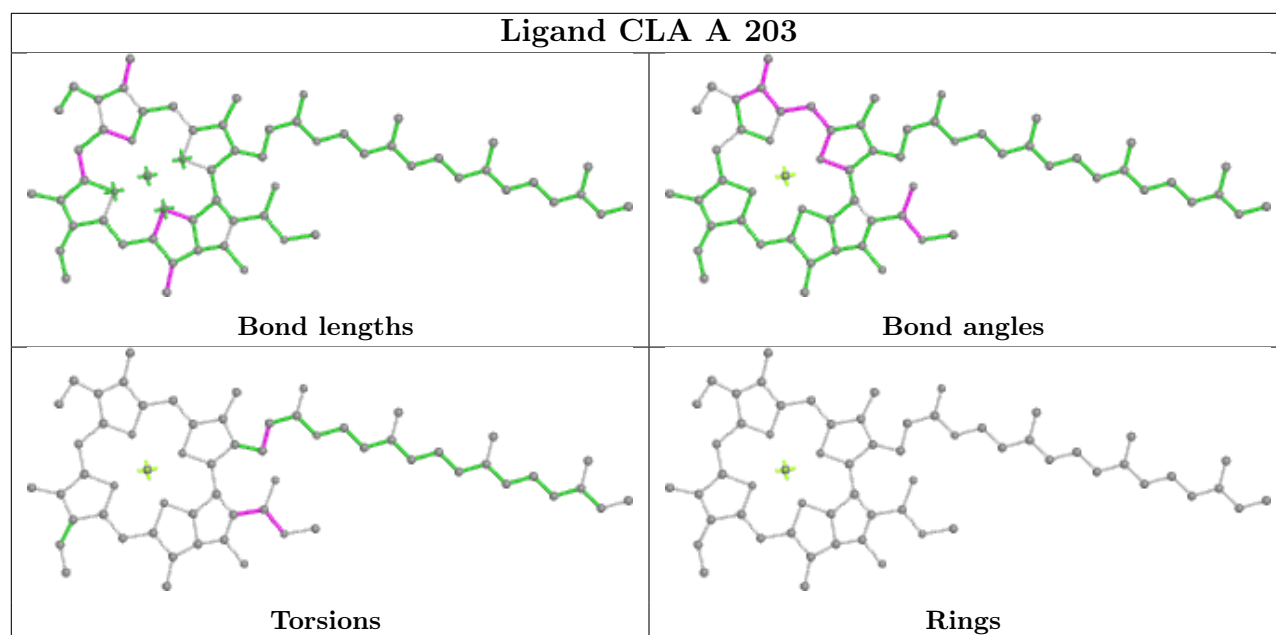
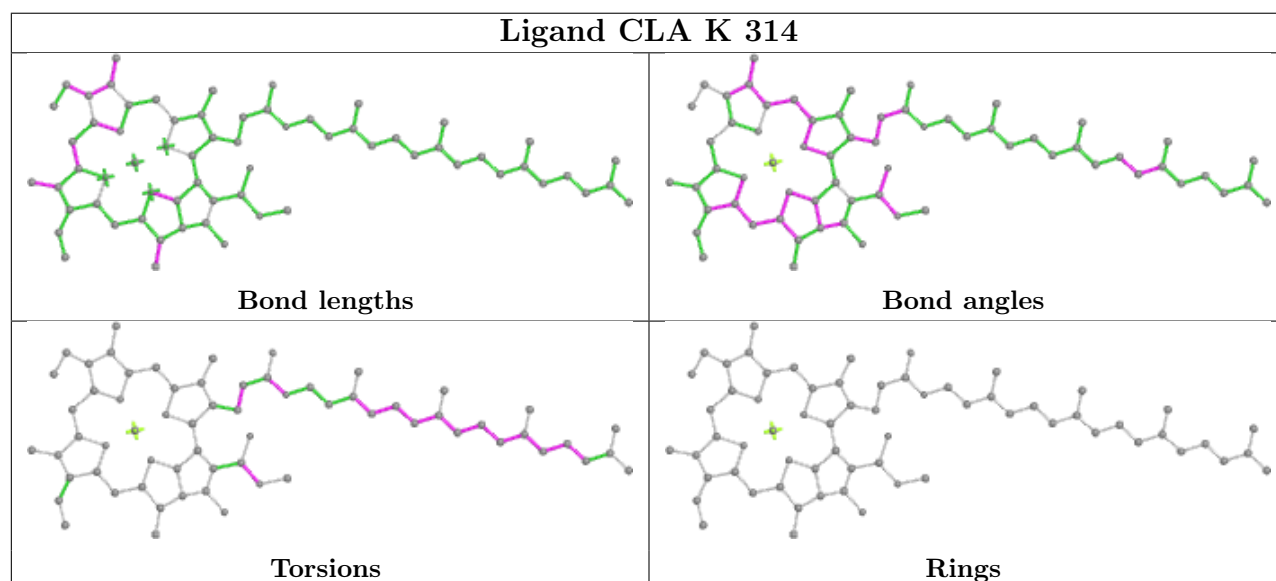
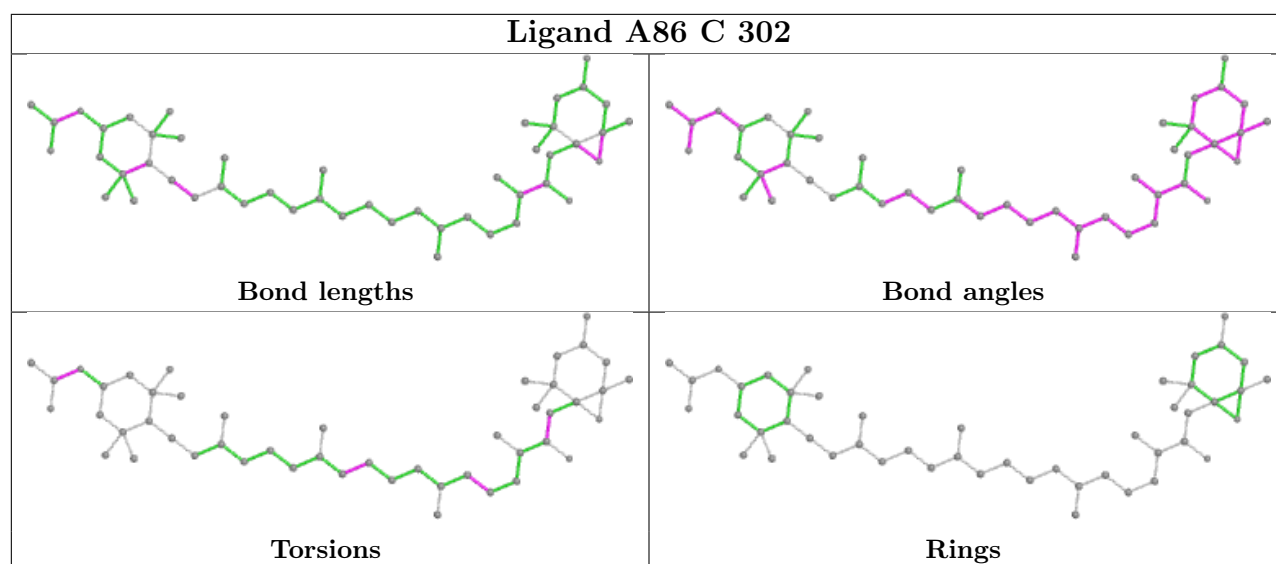


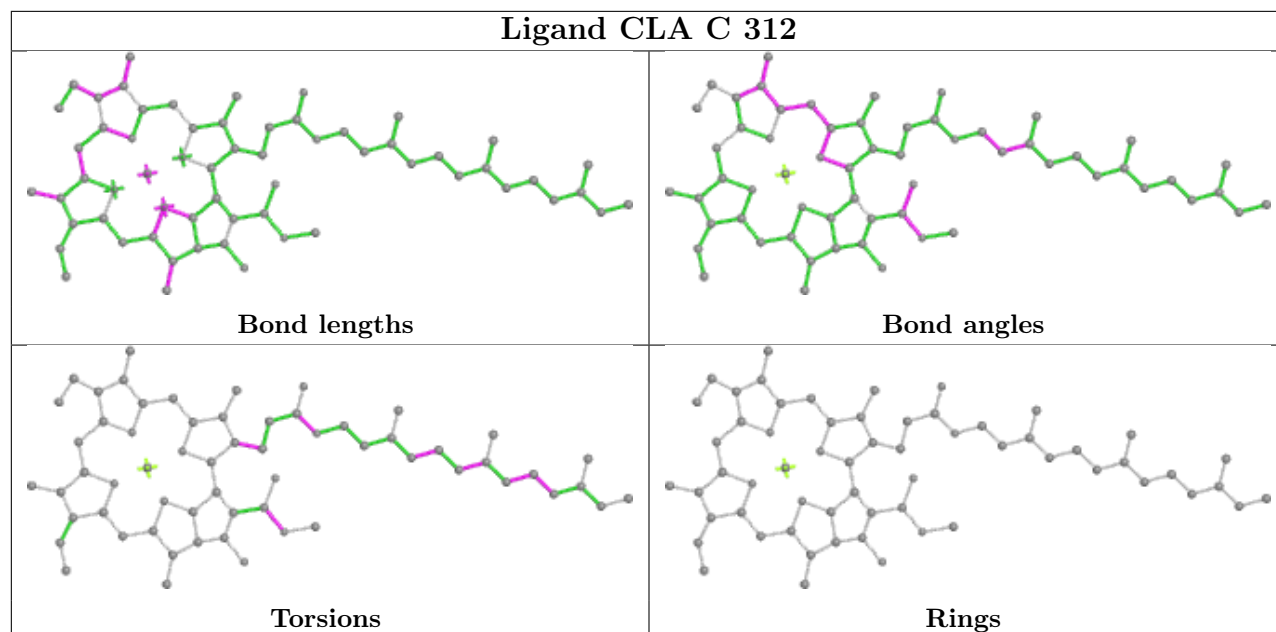
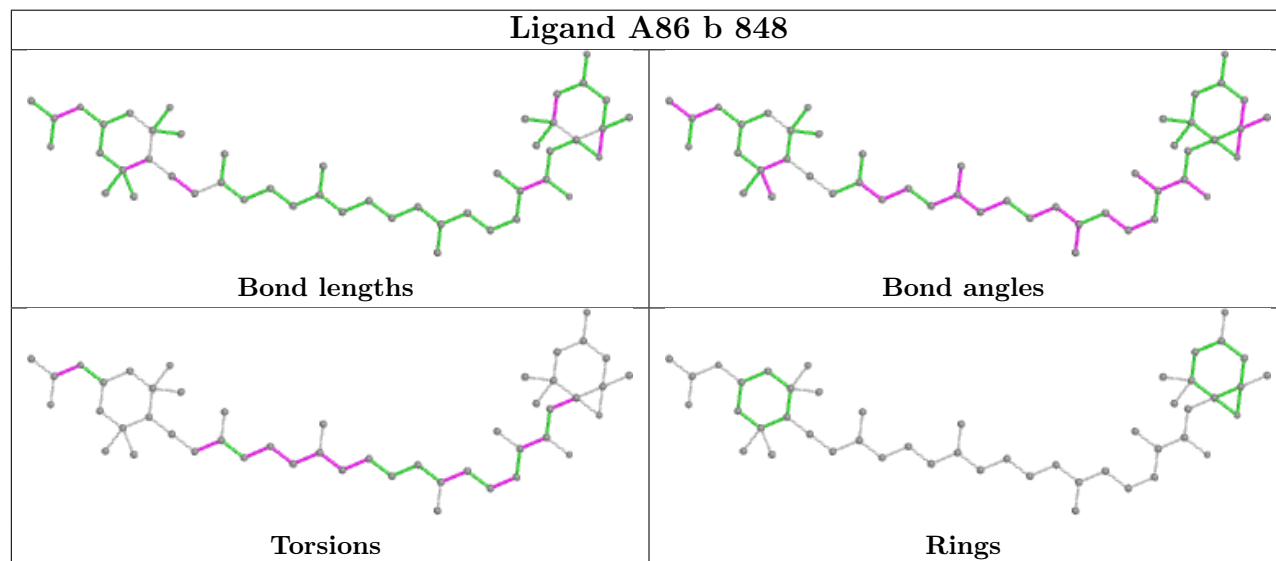
Ligand CLA F 317

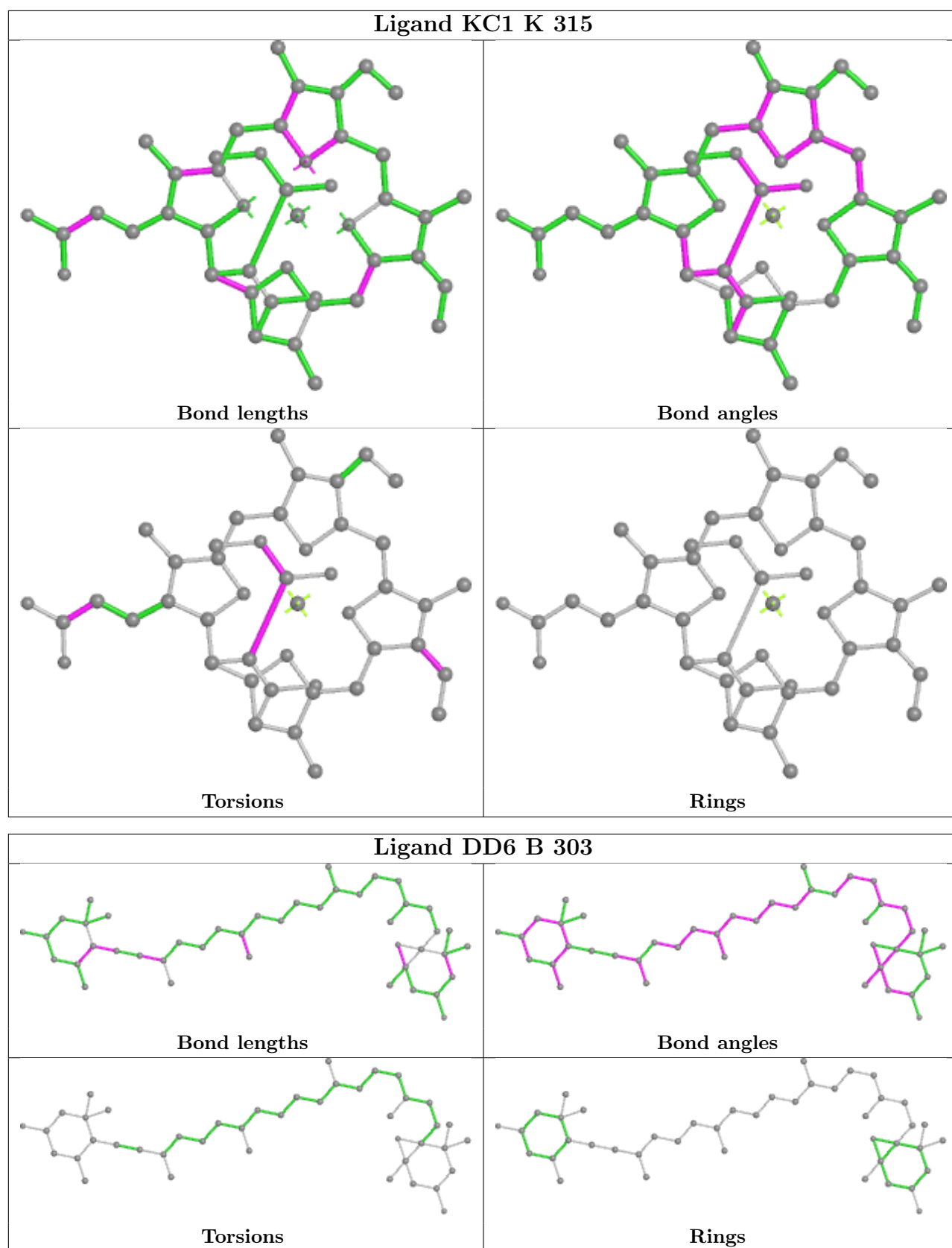


Ligand LHG I 318

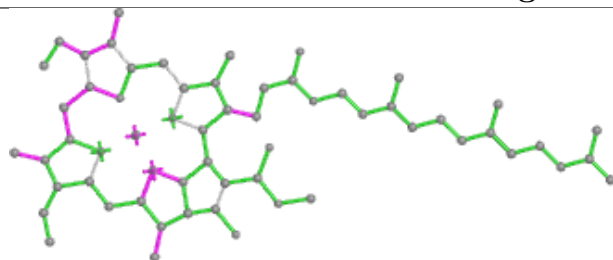




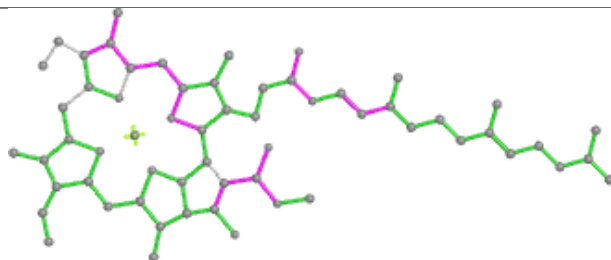
Ligand CLA C 312**Ligand A86 b 848**



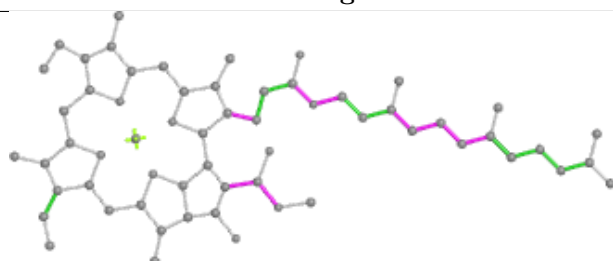
Ligand CLA a 839



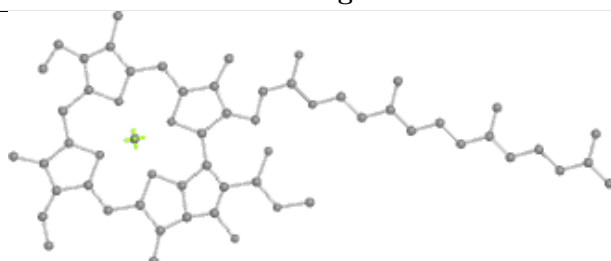
Bond lengths



Bond angles

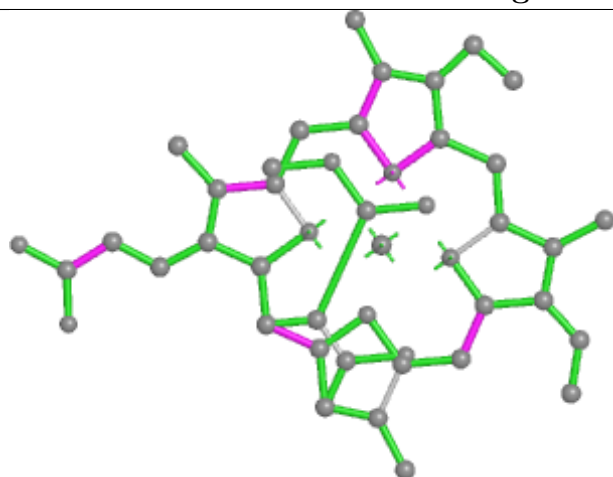


Torsions

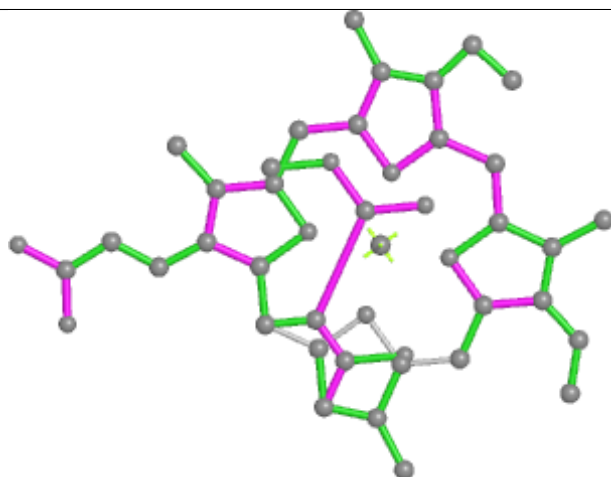


Rings

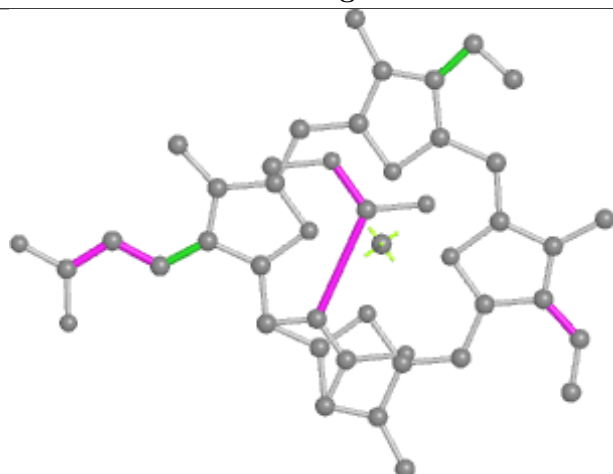
Ligand KC1 M 314



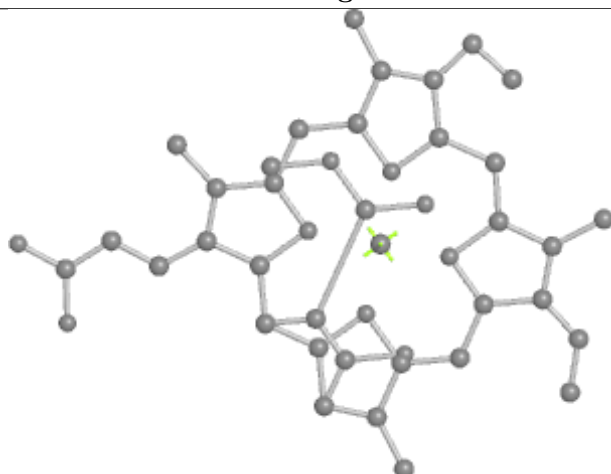
Bond lengths



Bond angles

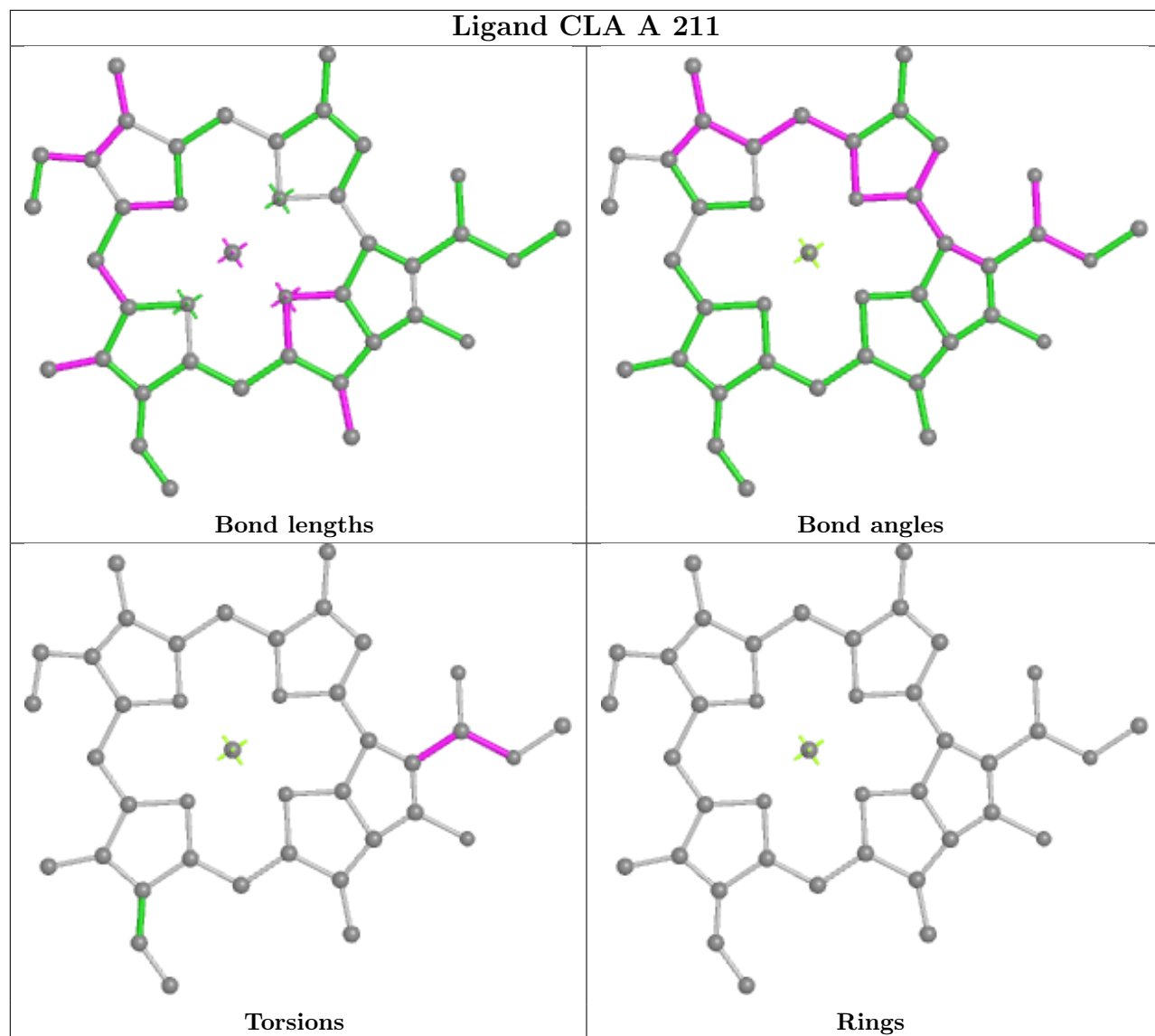


Torsions

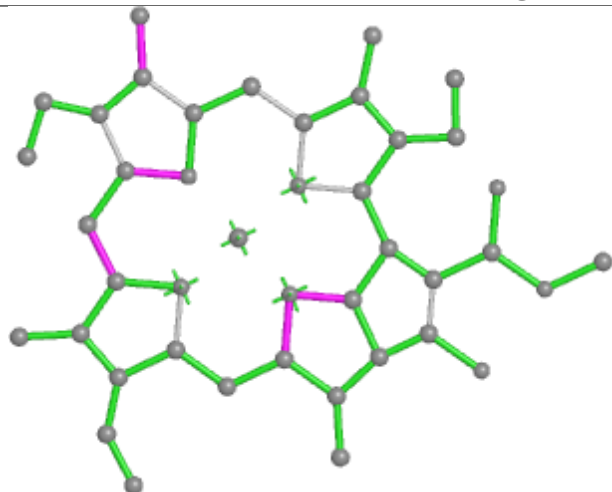


Rings

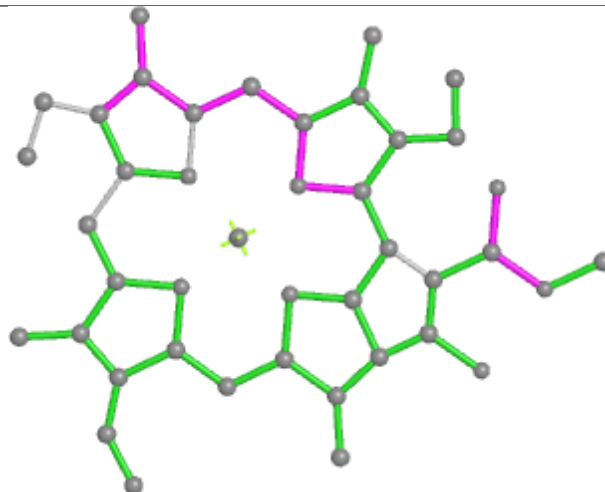
Ligand CLA A 211



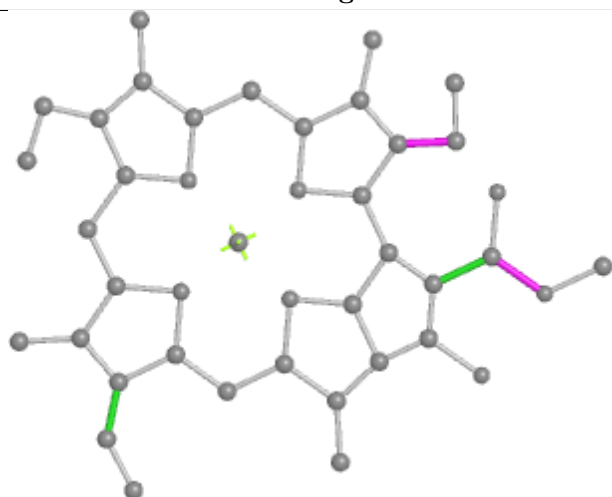
Ligand CLA C 315



Bond lengths



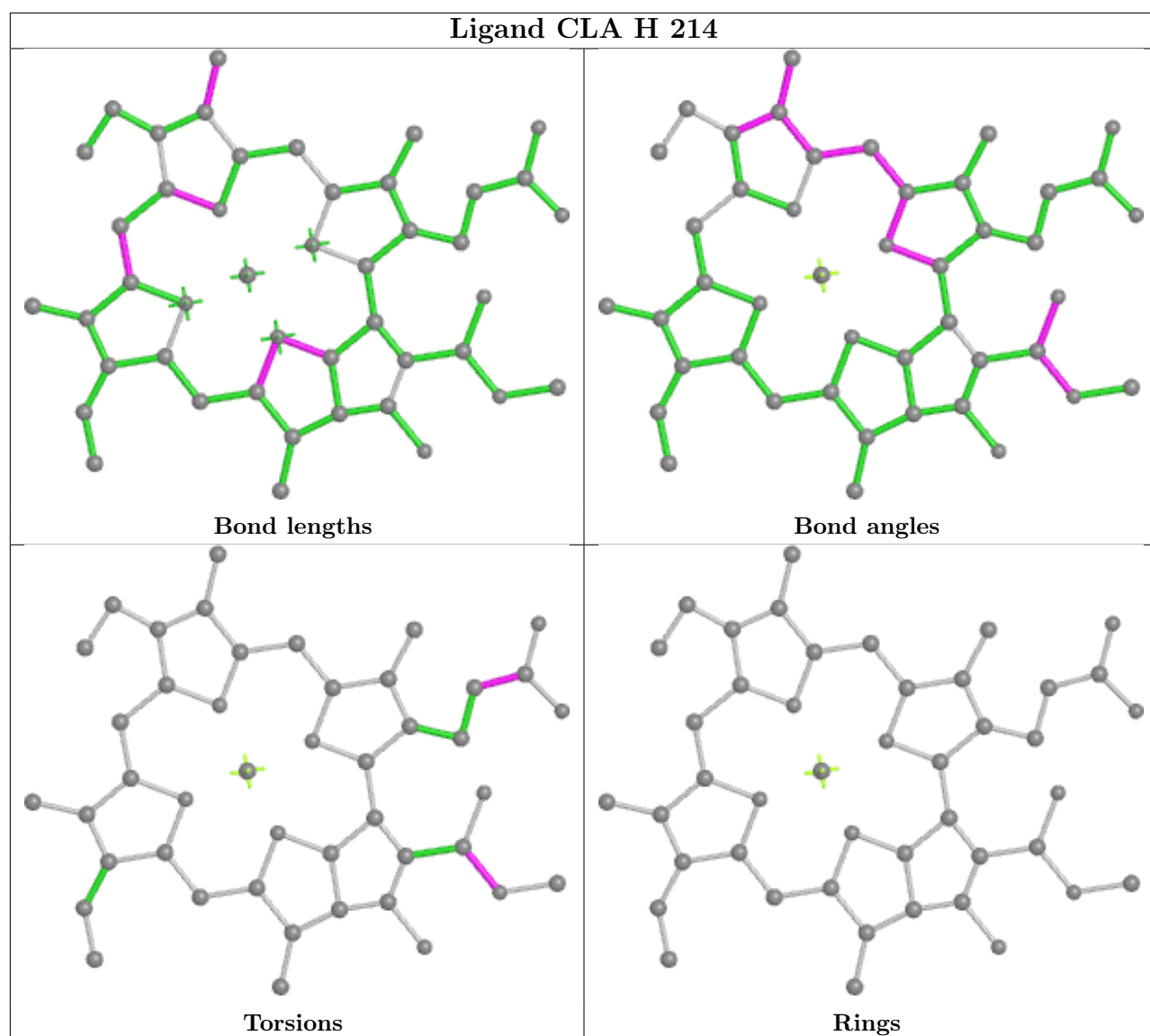
Bond angles

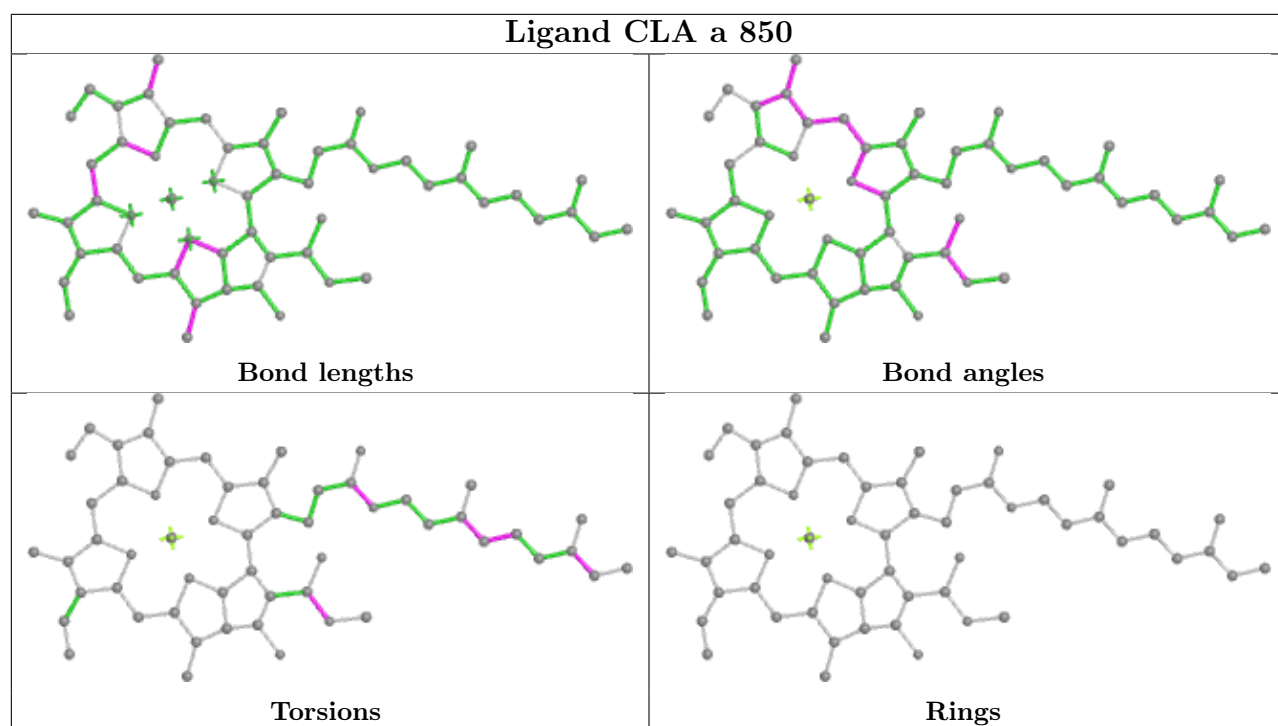


Torsions

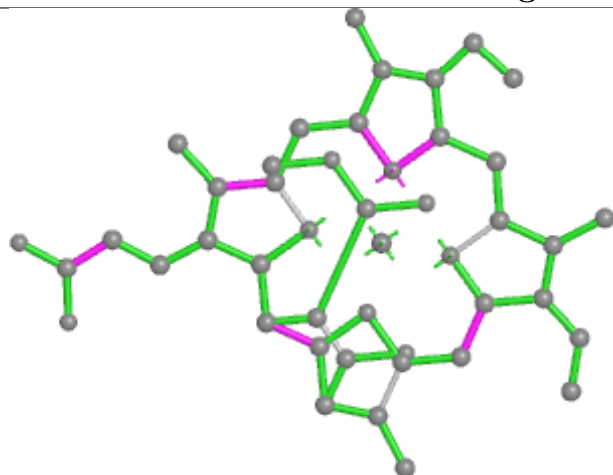


Rings

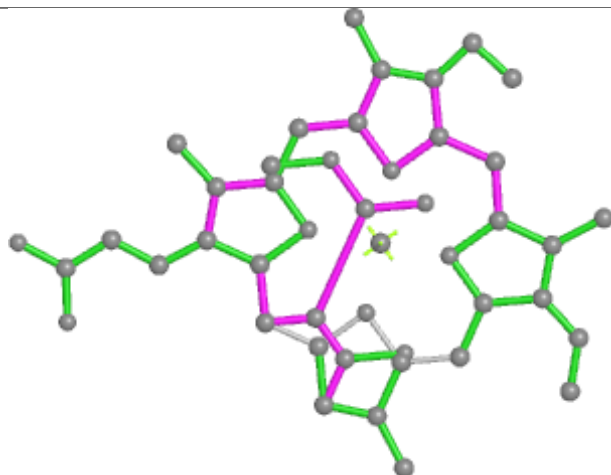




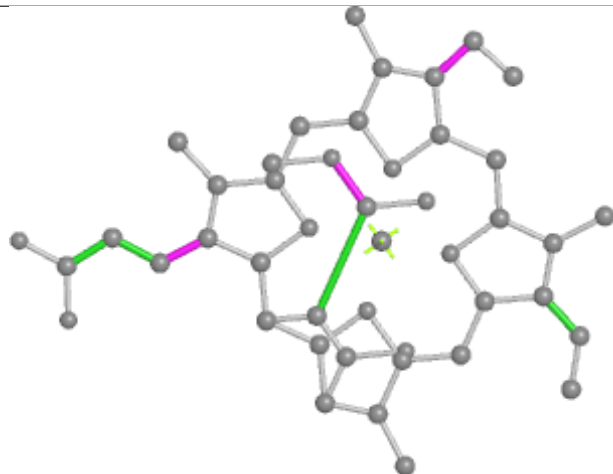
Ligand KC1 L 320



Bond lengths



Bond angles

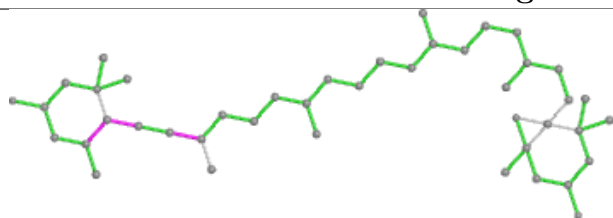


Torsions

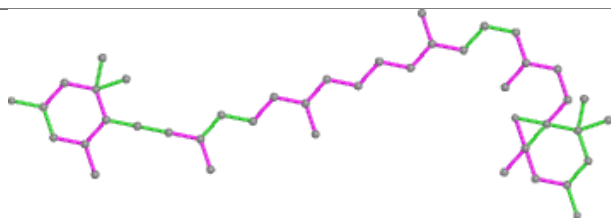


Rings

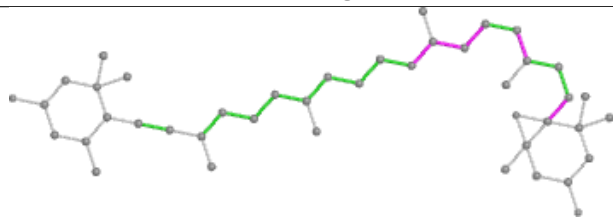
Ligand DD6 E 306



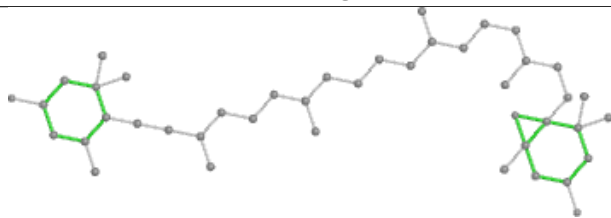
Bond lengths



Bond angles

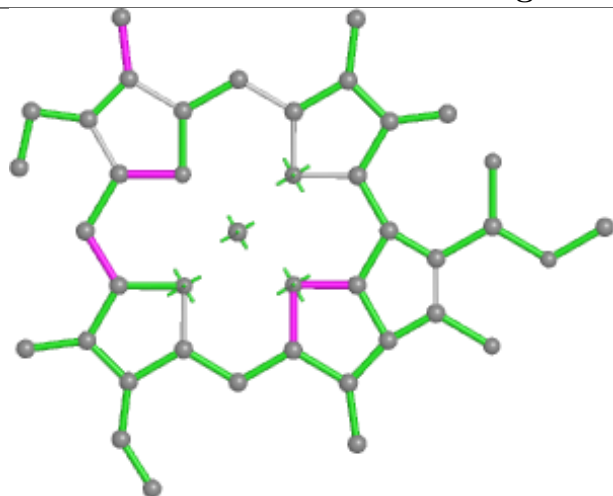


Torsions

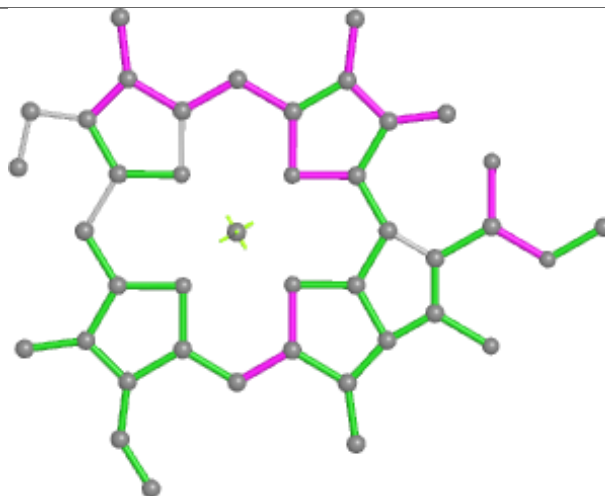


Rings

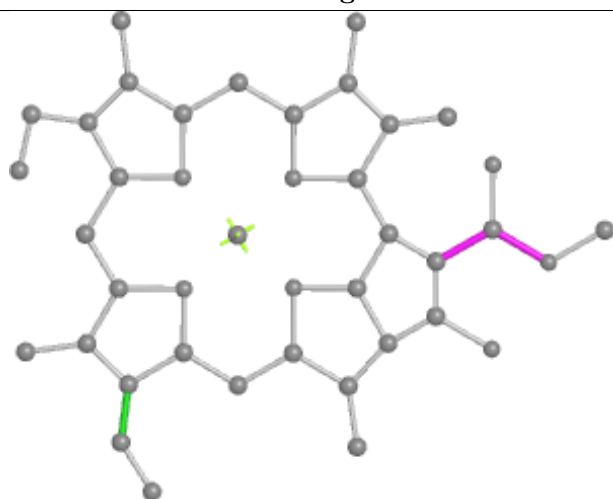
Ligand CLA F 316



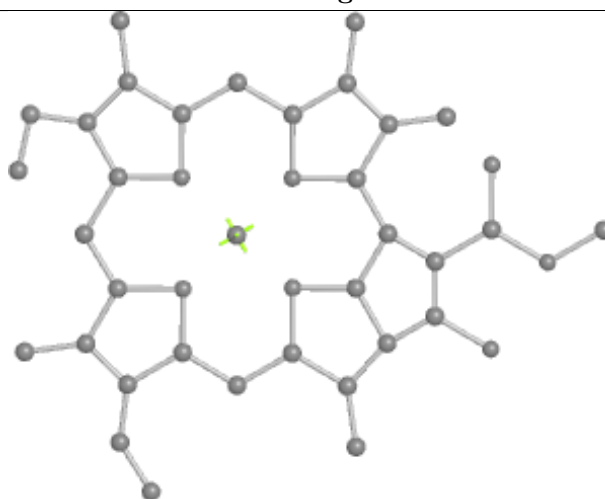
Bond lengths



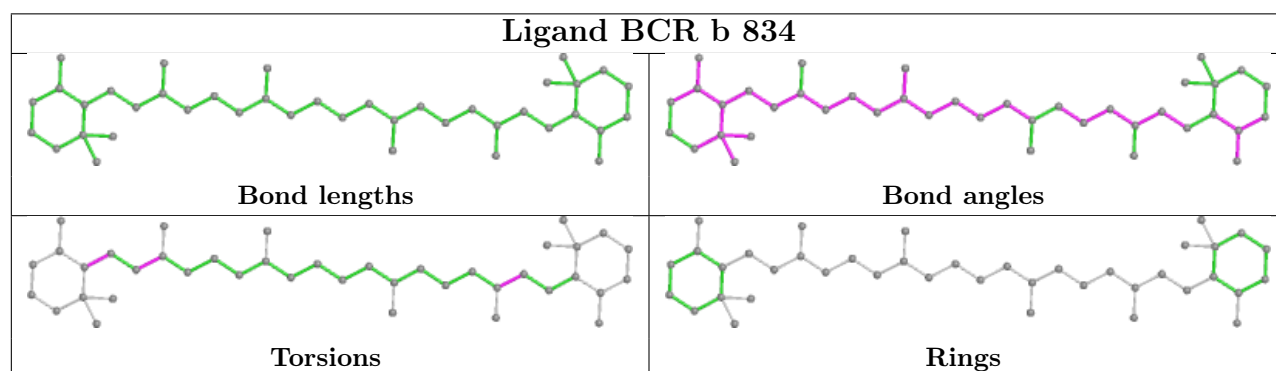
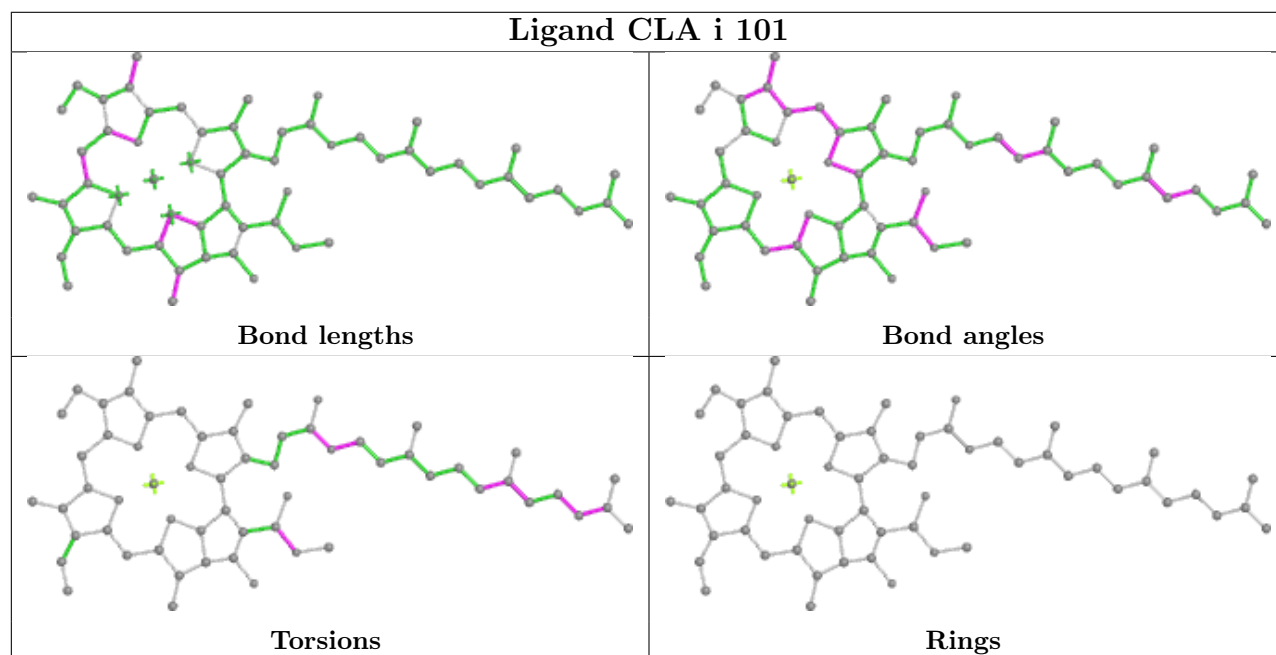
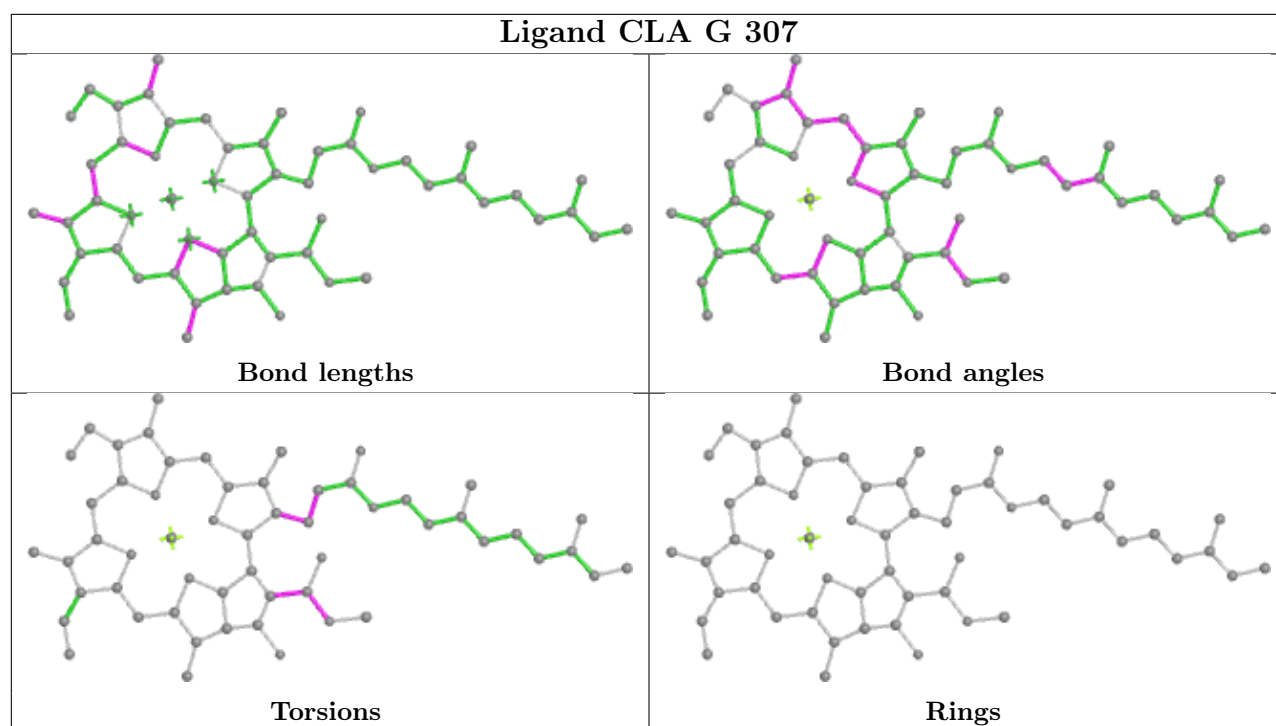
Bond angles



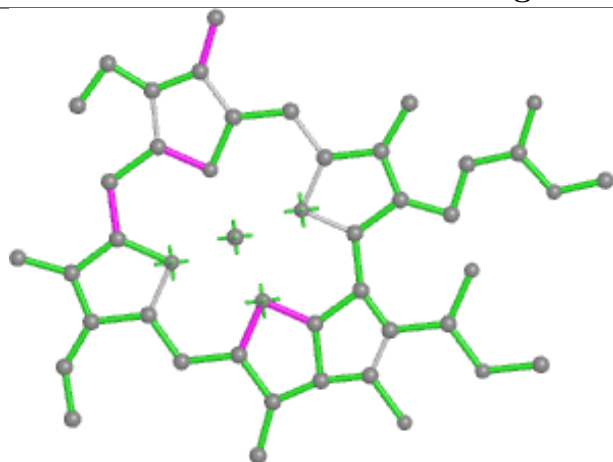
Torsions



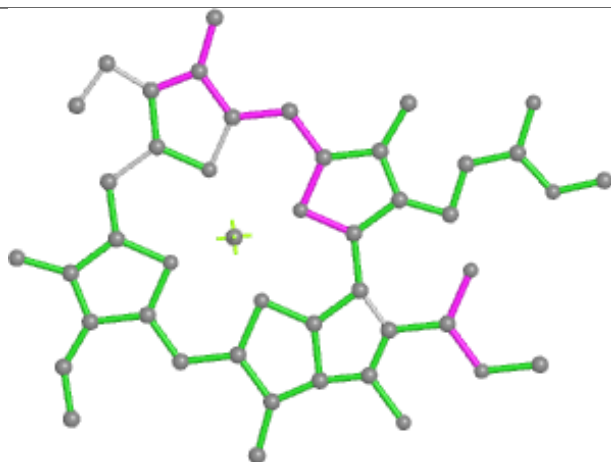
Rings



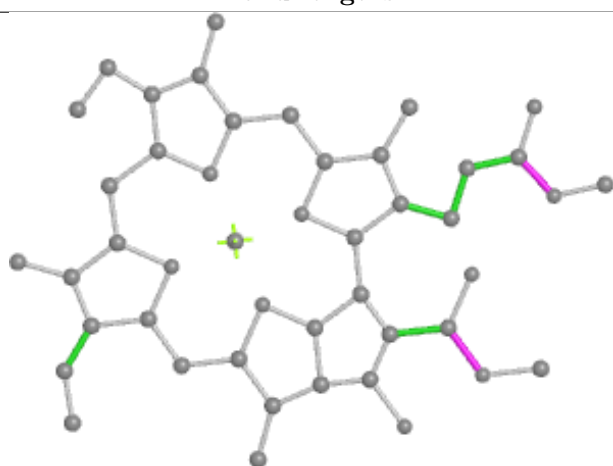
Ligand CLA A 206



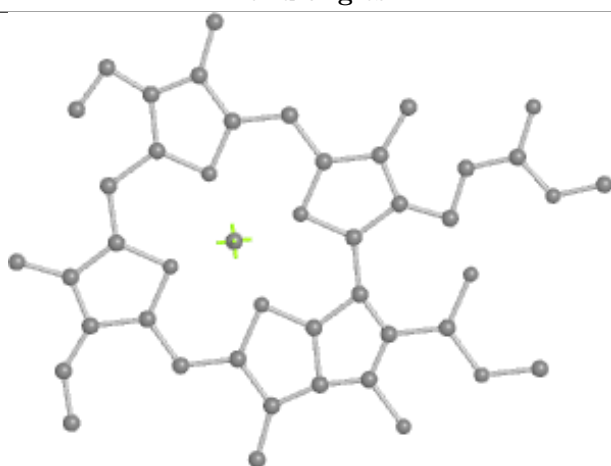
Bond lengths



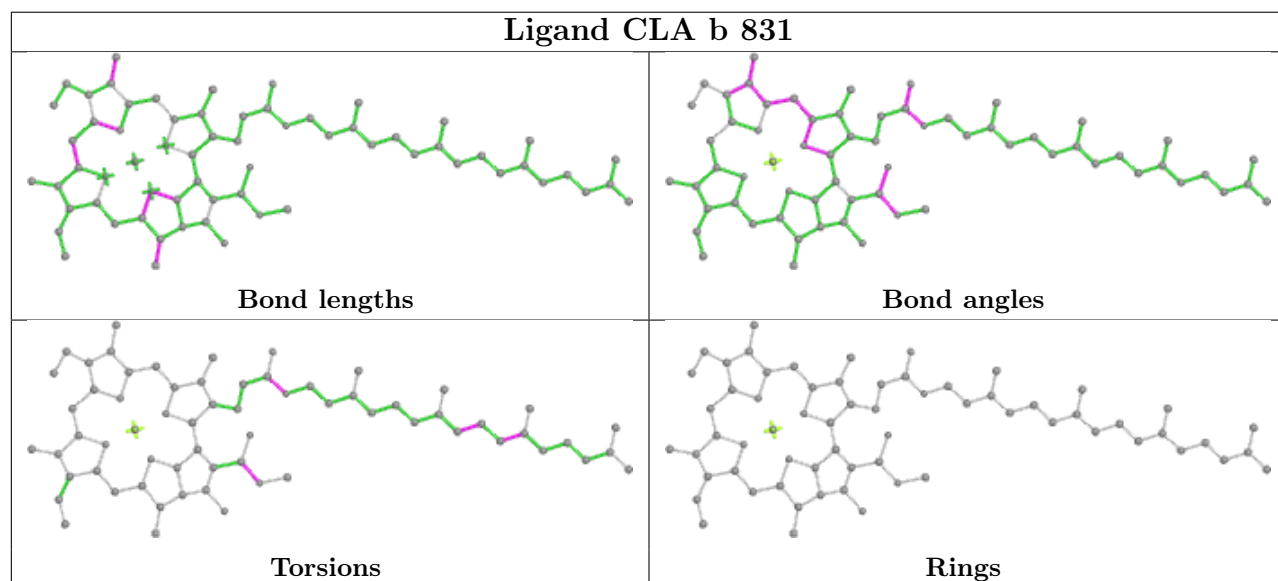
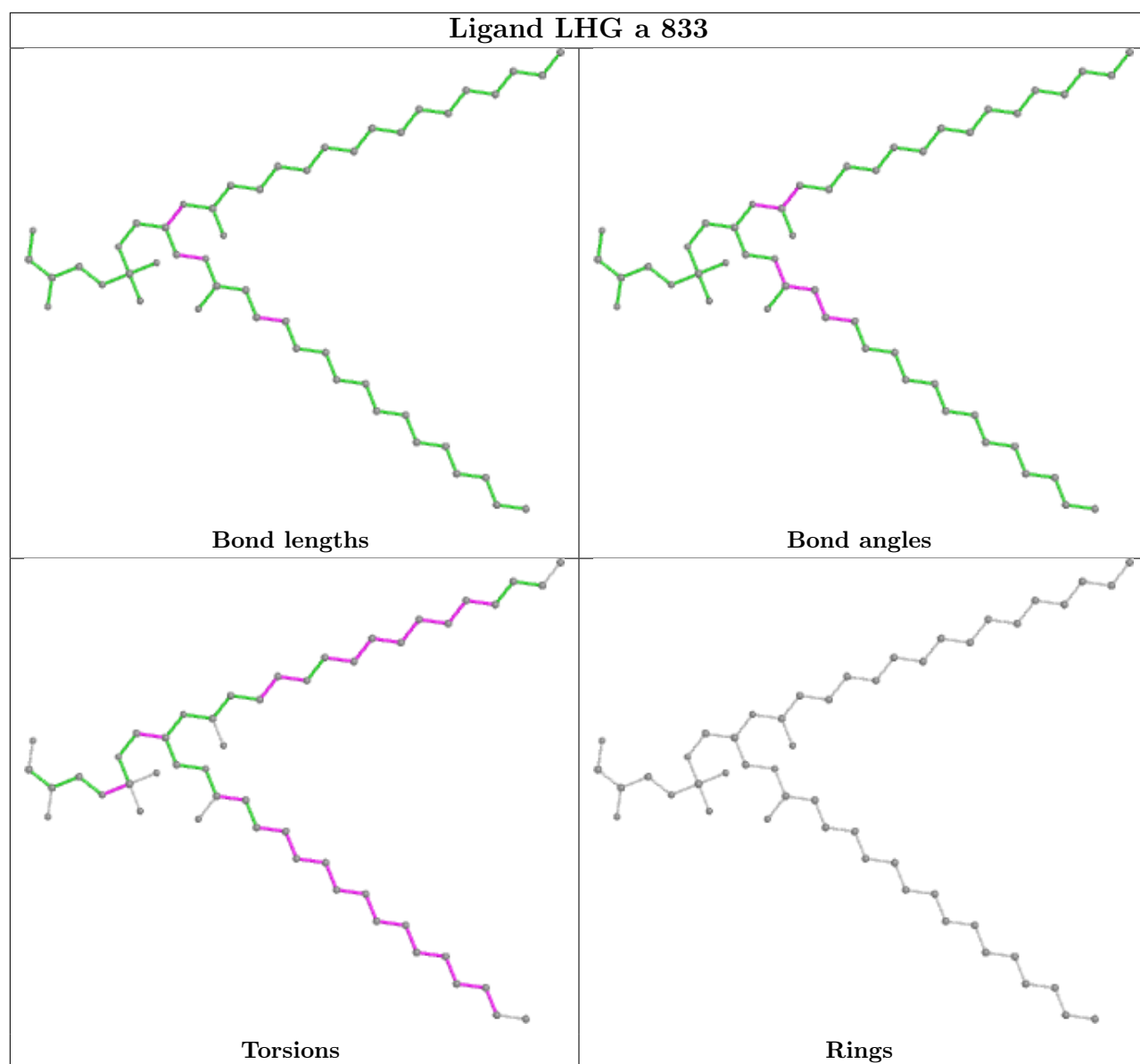
Bond angles

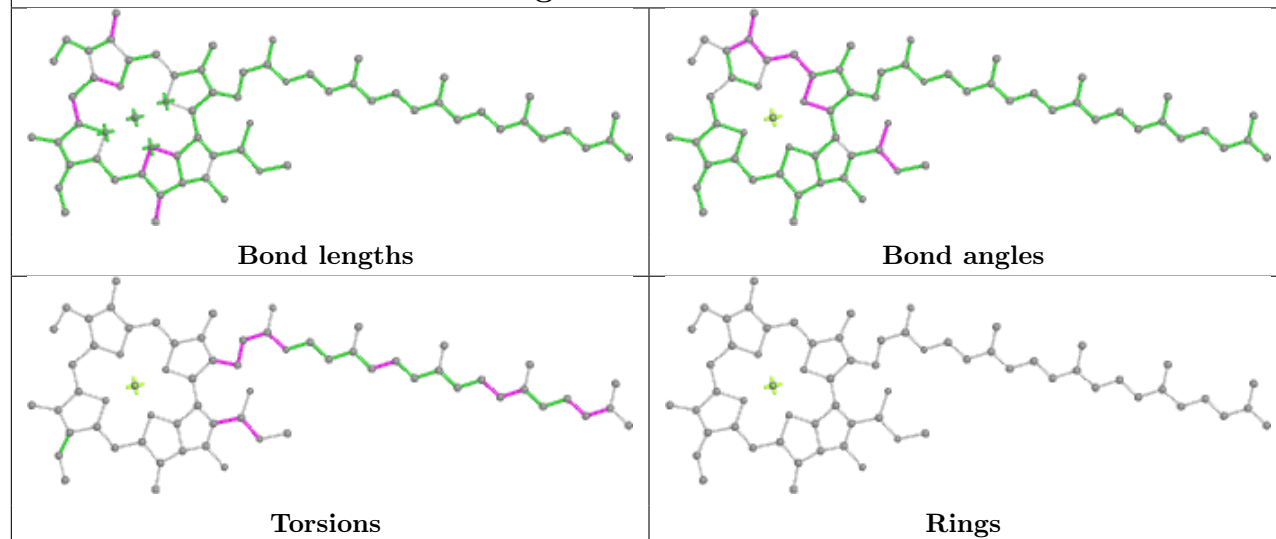
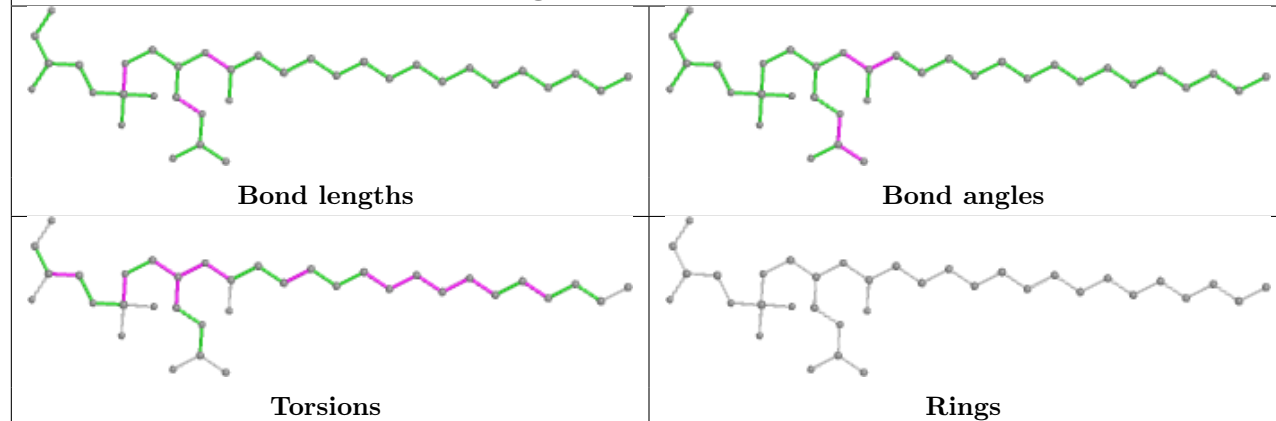


Torsions

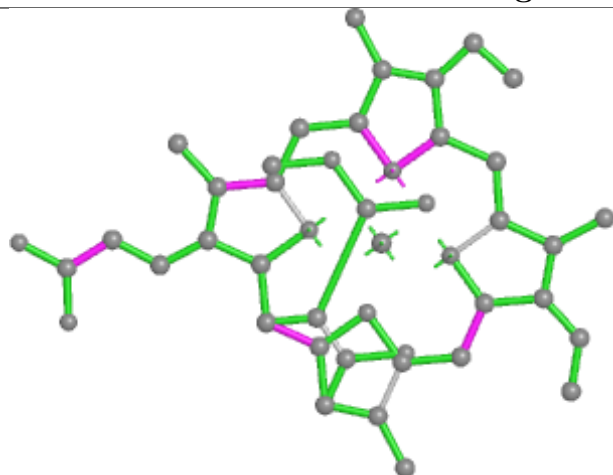


Rings

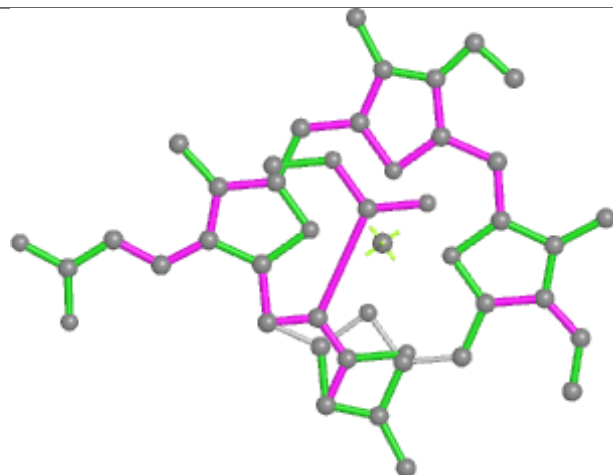


Ligand CLA b 823**Ligand LHG H 215**

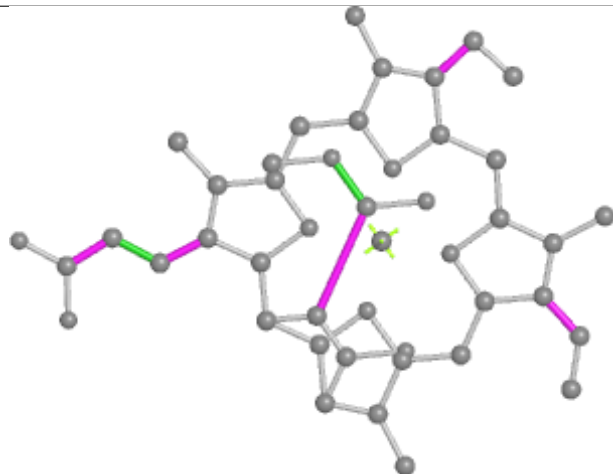
Ligand KC1 K 308



Bond lengths



Bond angles

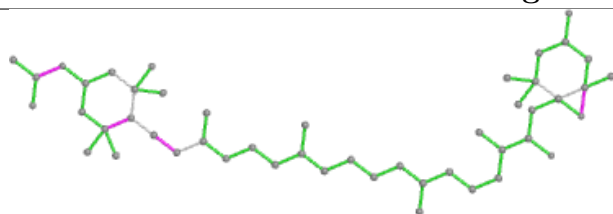


Torsions

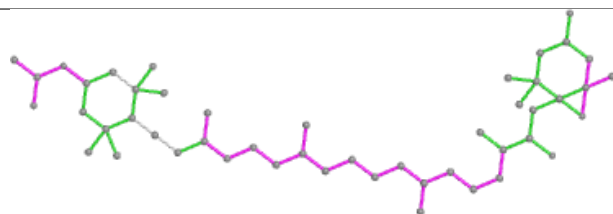


Rings

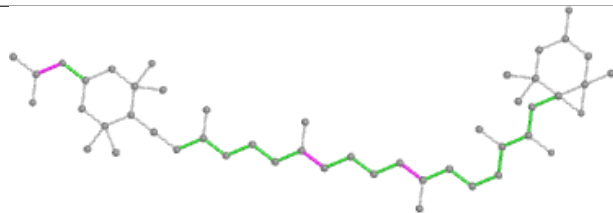
Ligand A86 L 304



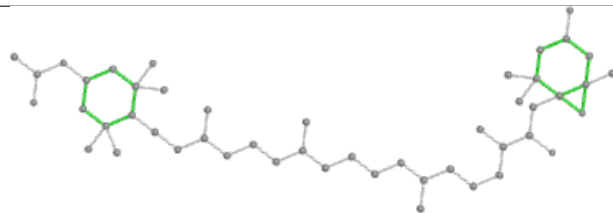
Bond lengths



Bond angles

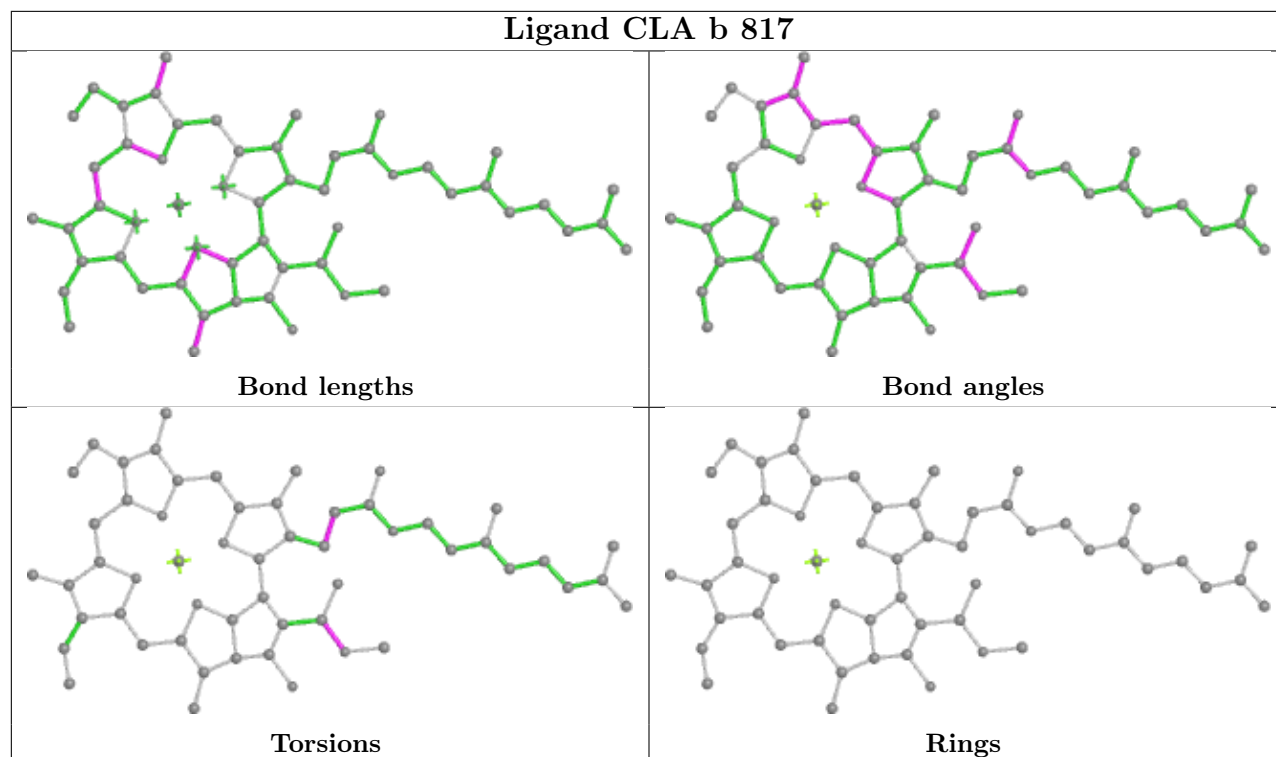


Torsions

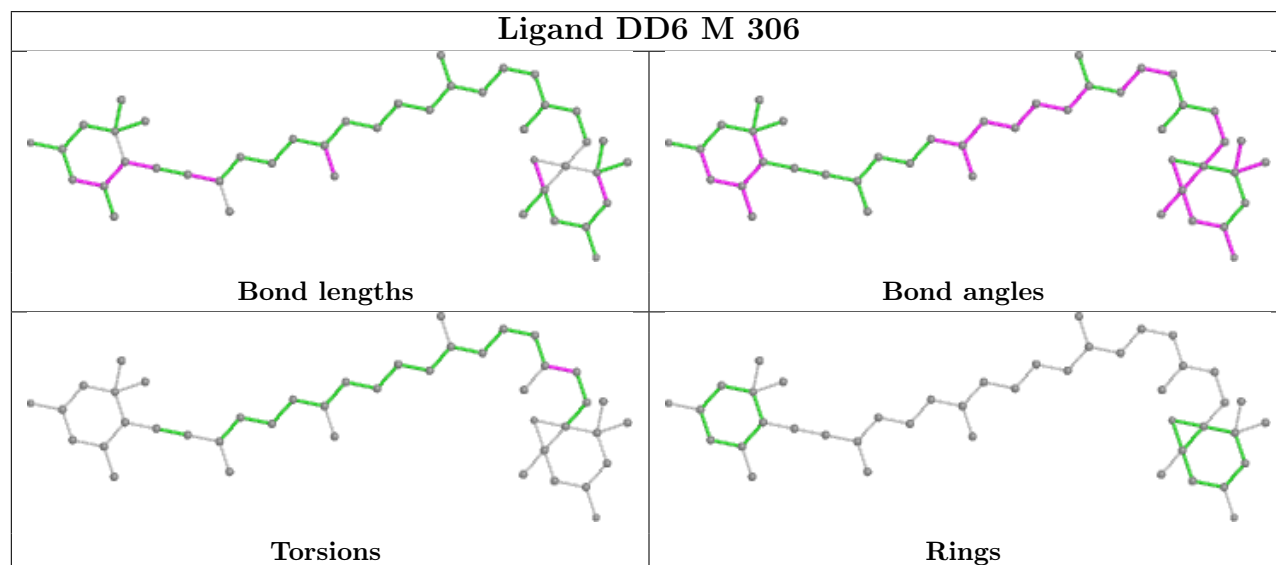


Rings

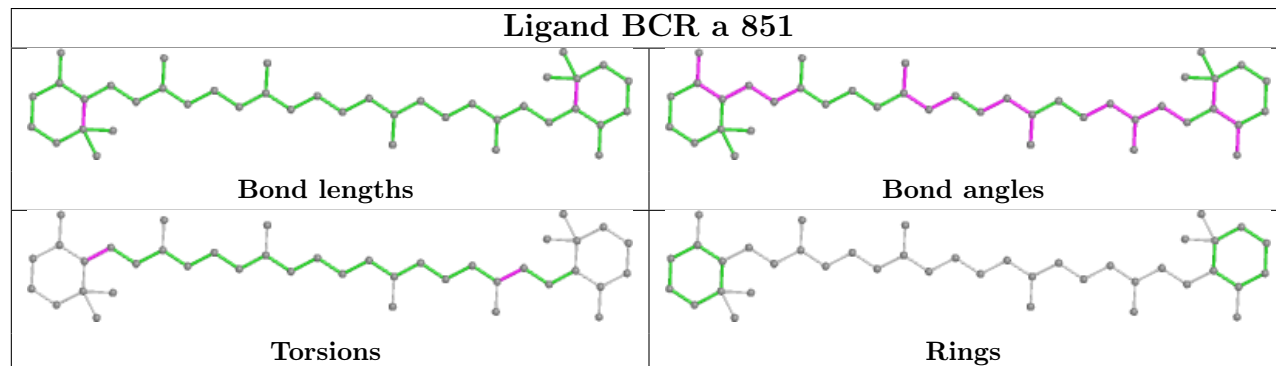
Ligand CLA b 817



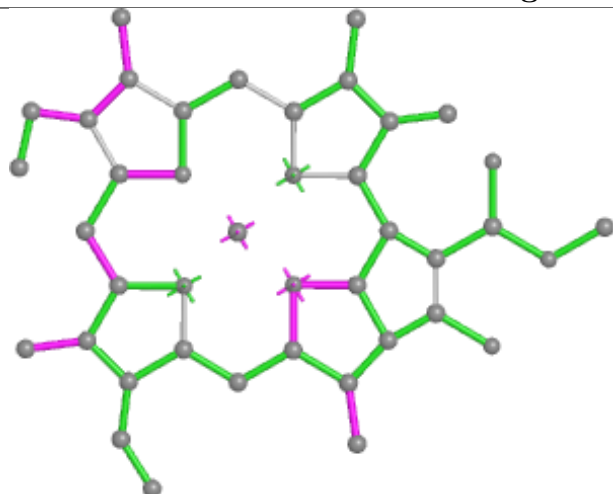
Ligand DD6 M 306



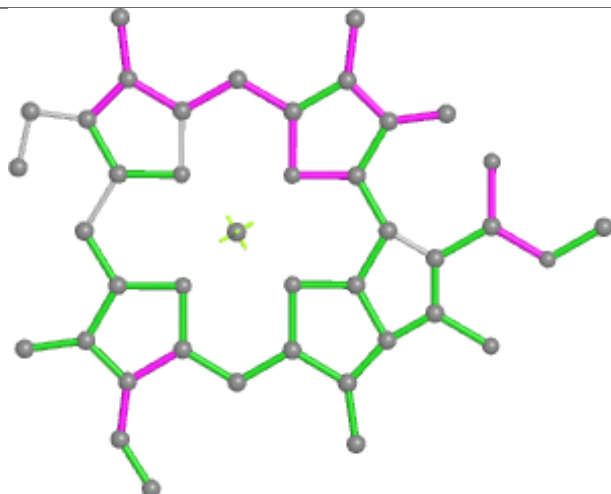
Ligand BCR a 851



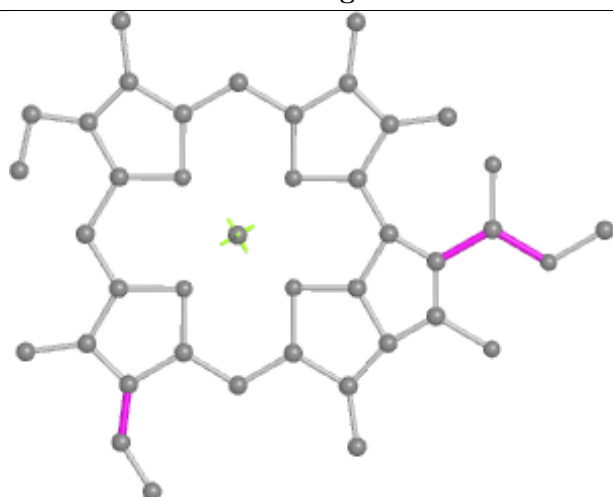
Ligand CLA I 313



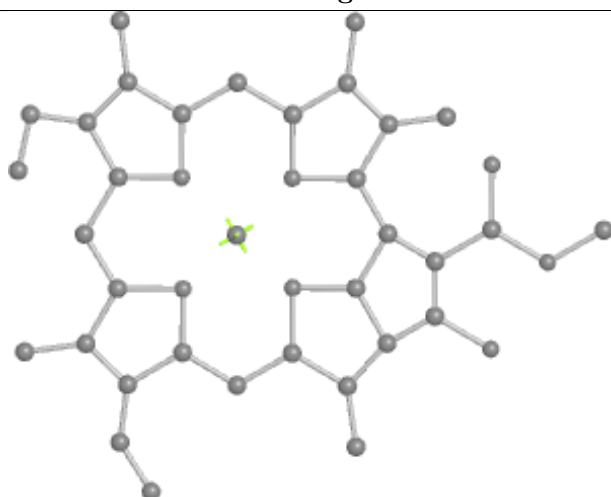
Bond lengths



Bond angles

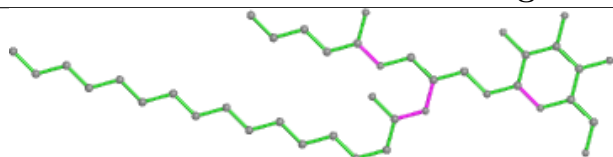


Torsions

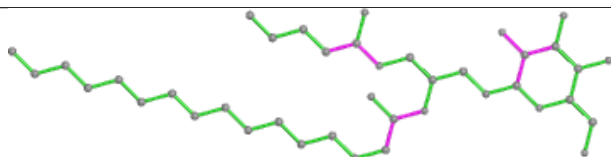


Rings

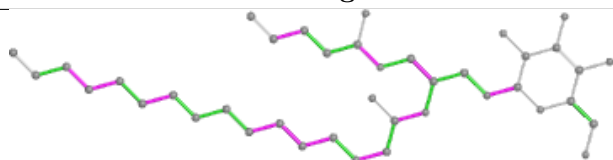
Ligand LMG I 201



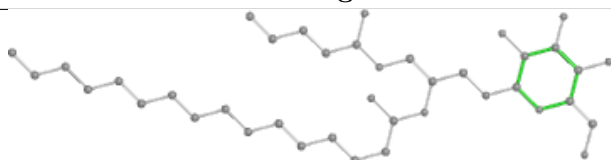
Bond lengths



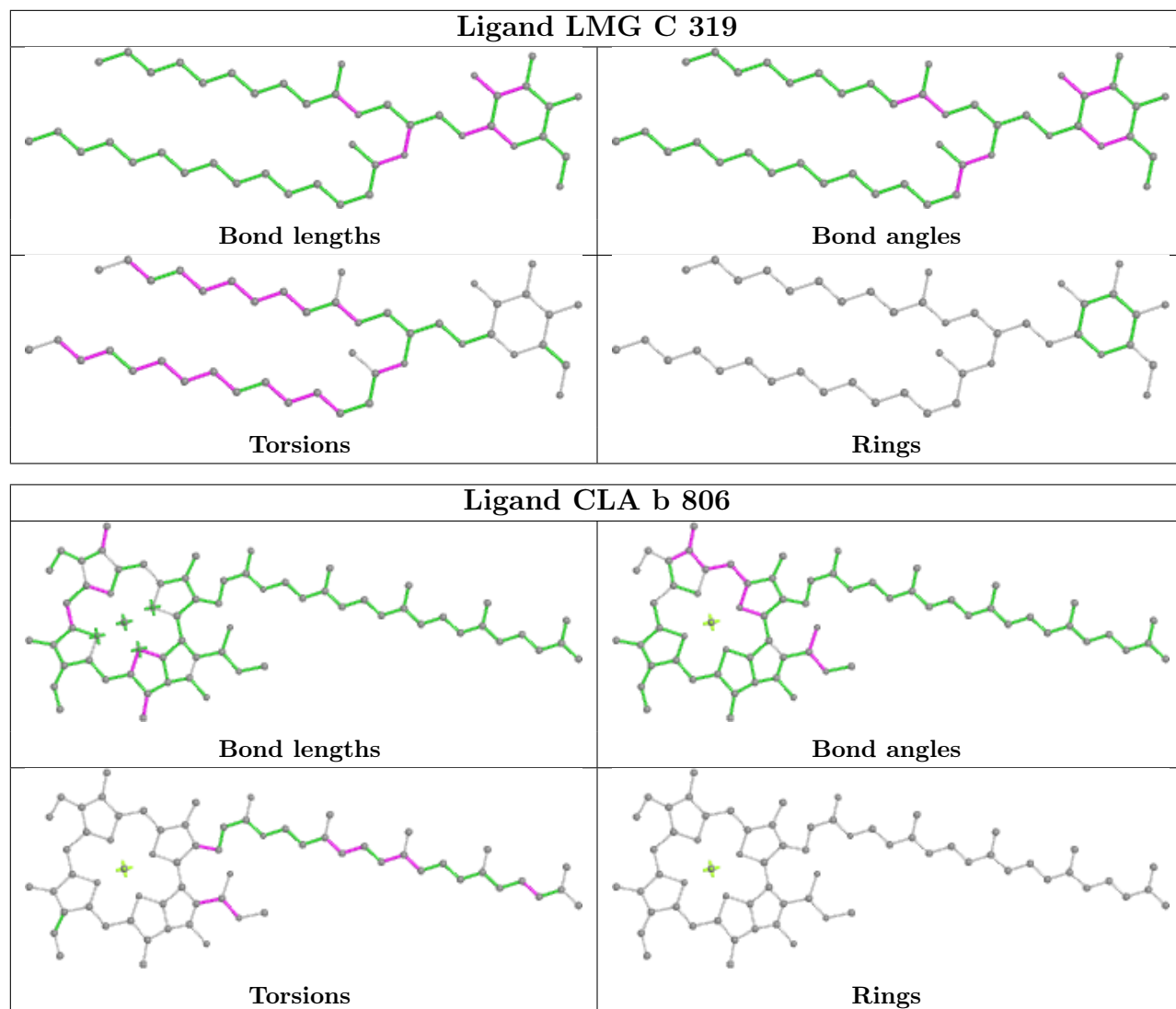
Bond angles



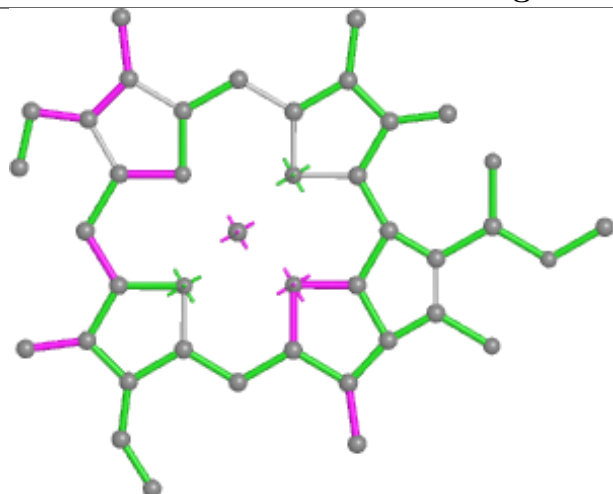
Torsions



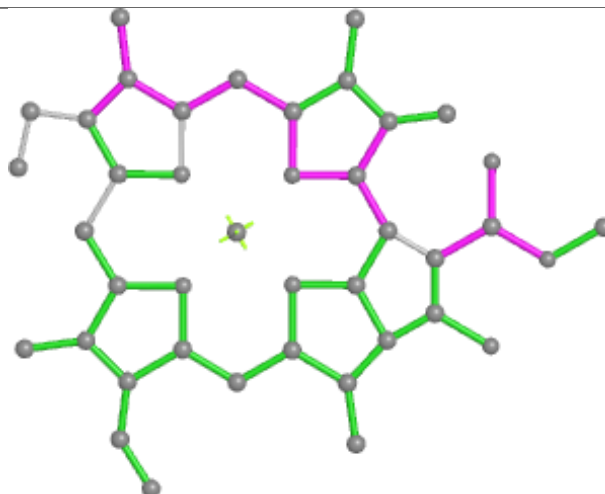
Rings



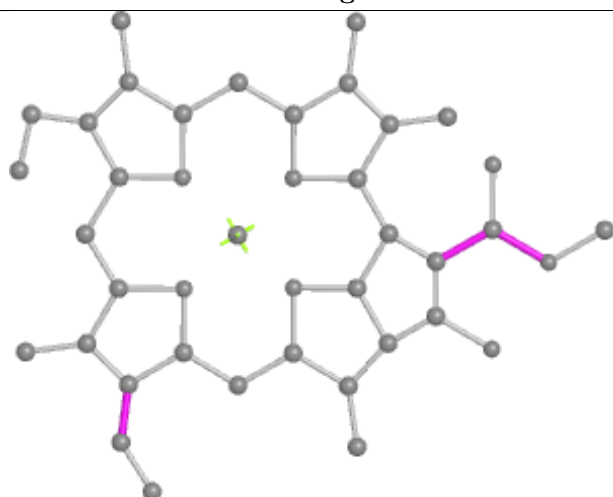
Ligand CLA K 317



Bond lengths



Bond angles

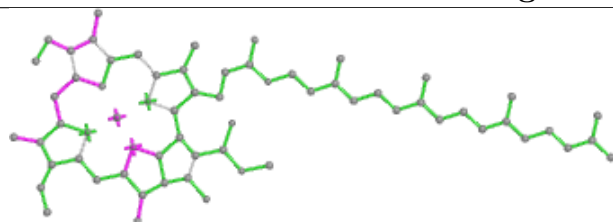


Torsions

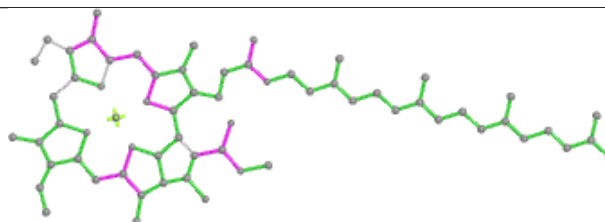


Rings

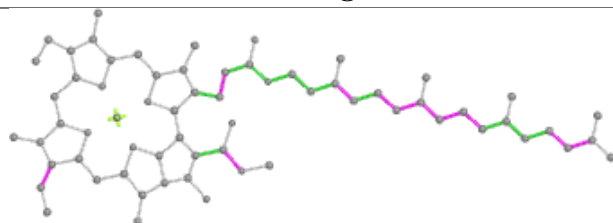
Ligand CLA a 856



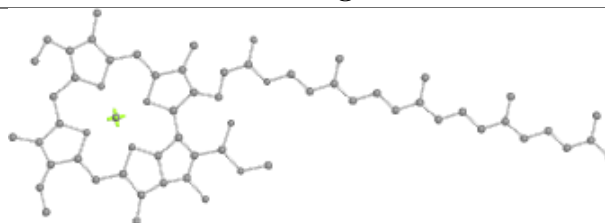
Bond lengths



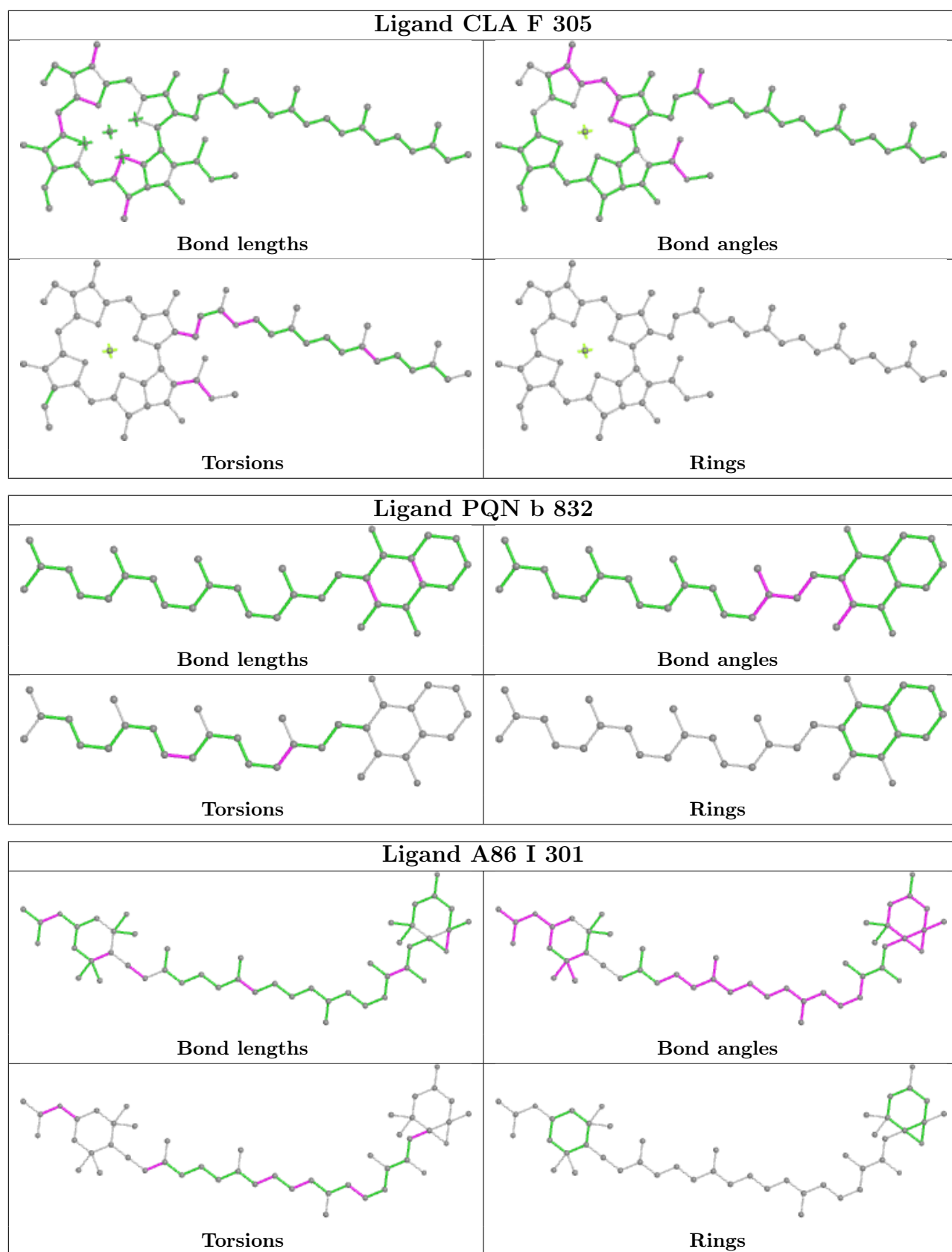
Bond angles

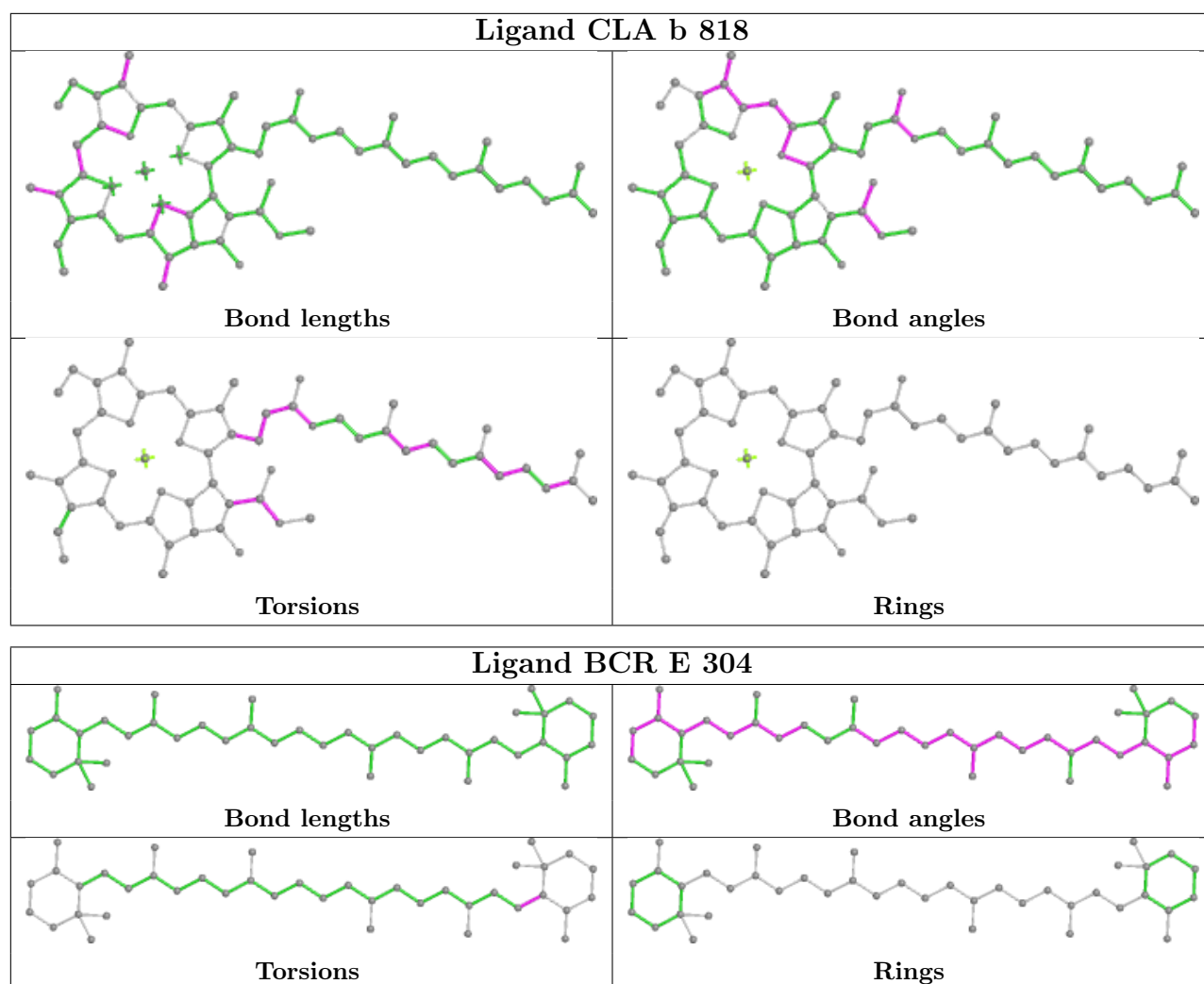


Torsions

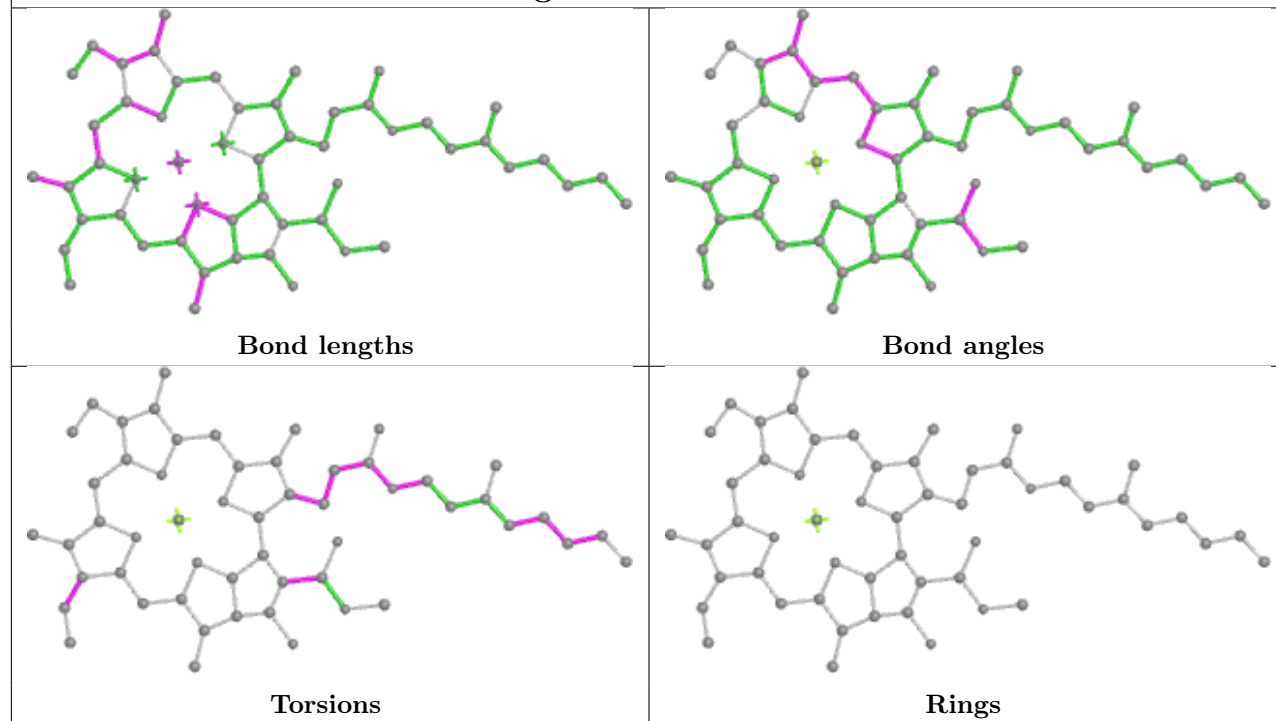


Rings

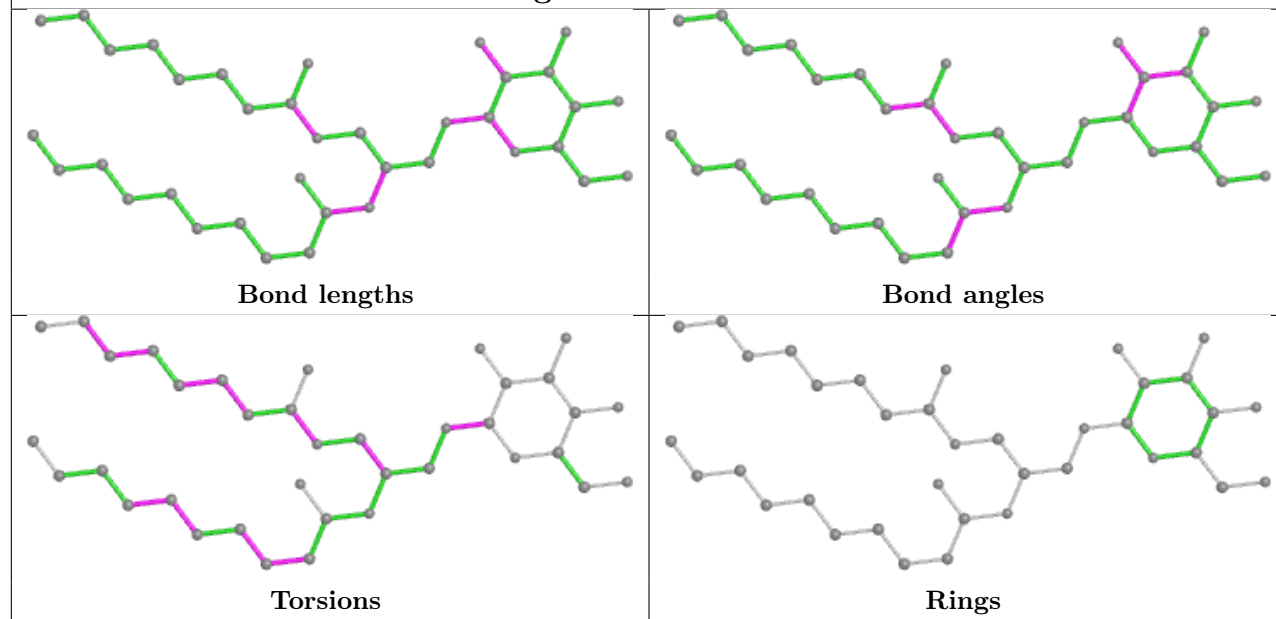




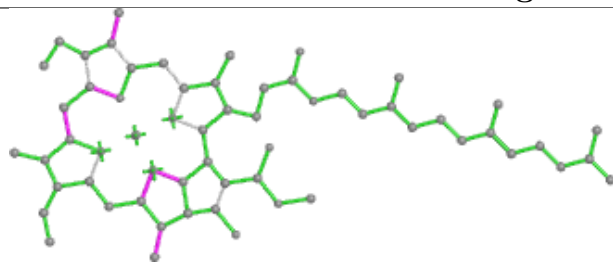
Ligand CLA L 307



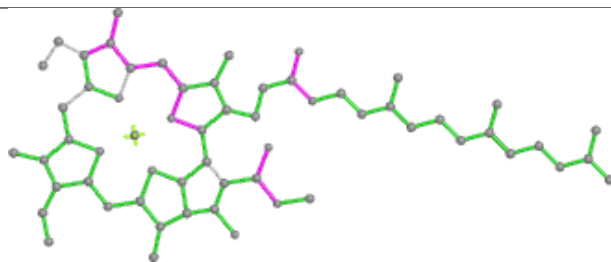
Ligand LMG I 319



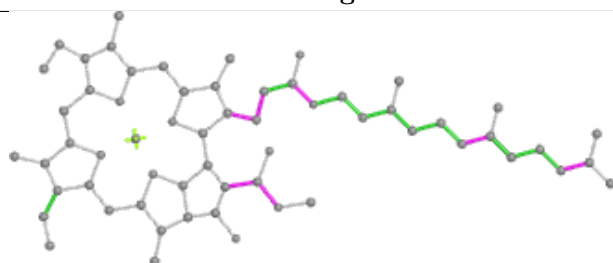
Ligand CLA F 310



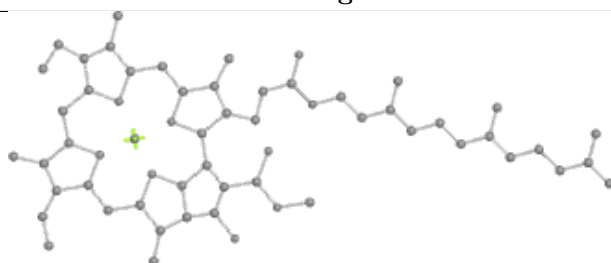
Bond lengths



Bond angles

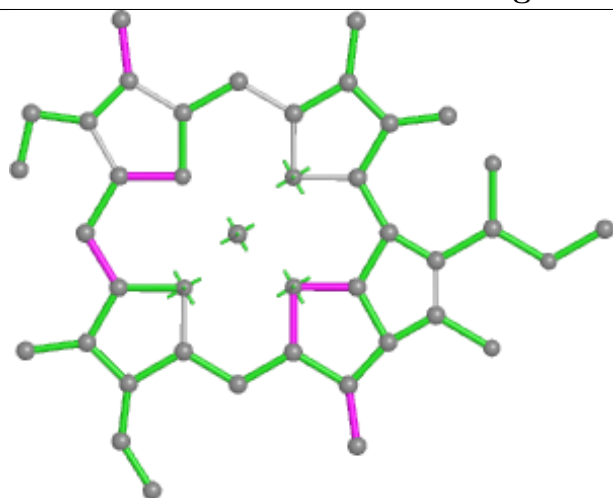


Torsions

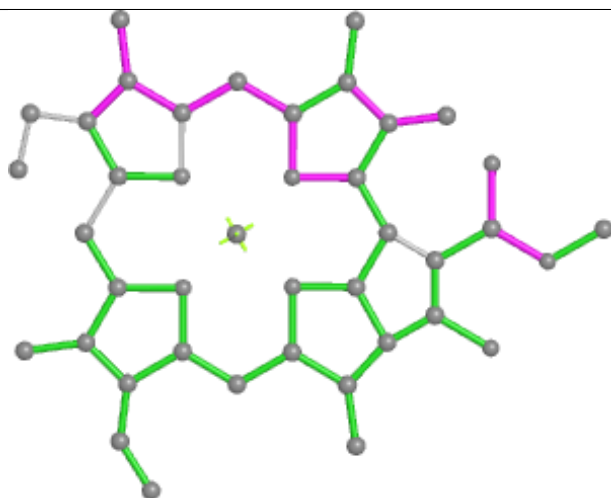


Rings

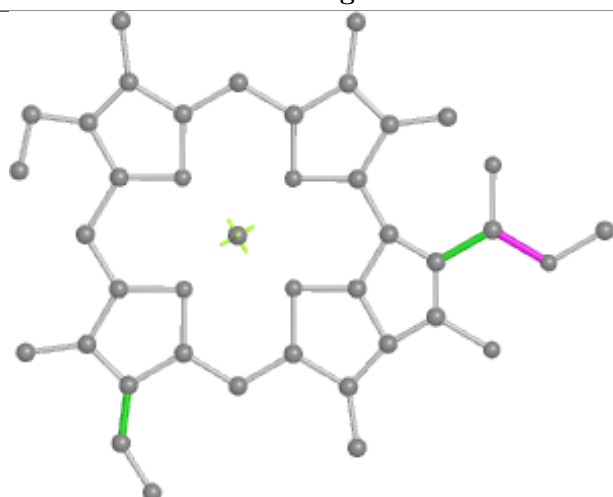
Ligand CLA D 215



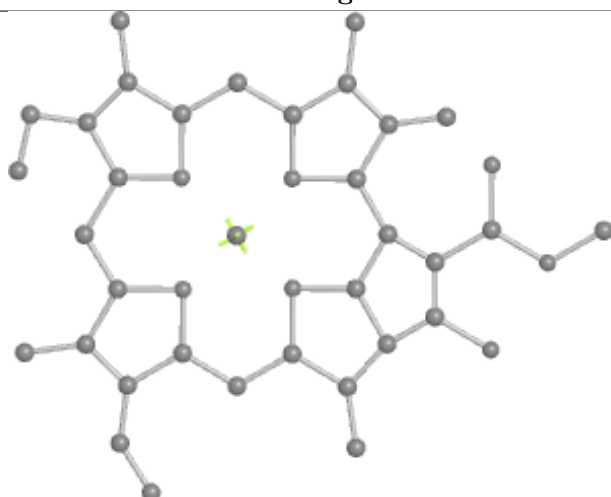
Bond lengths



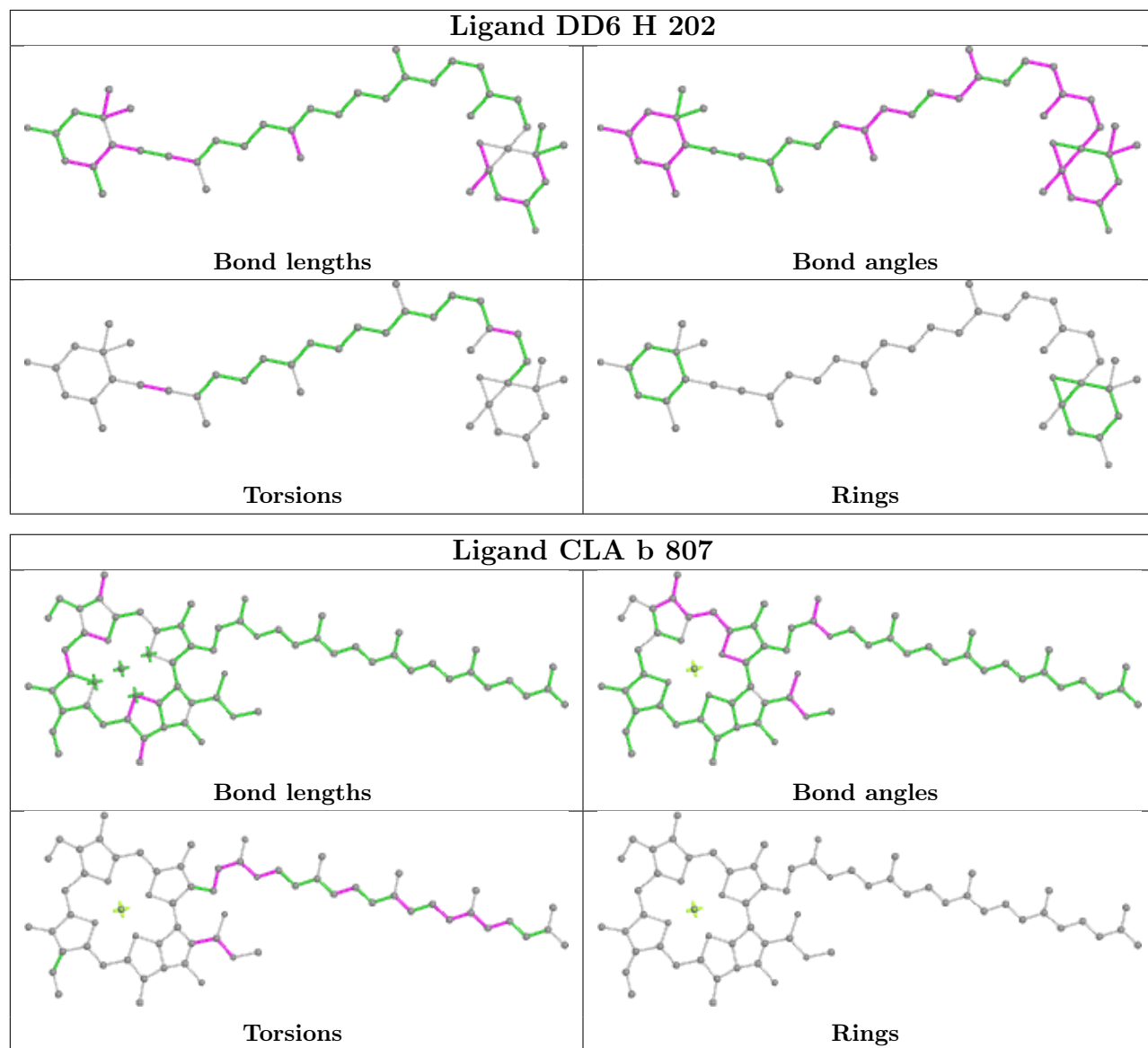
Bond angles

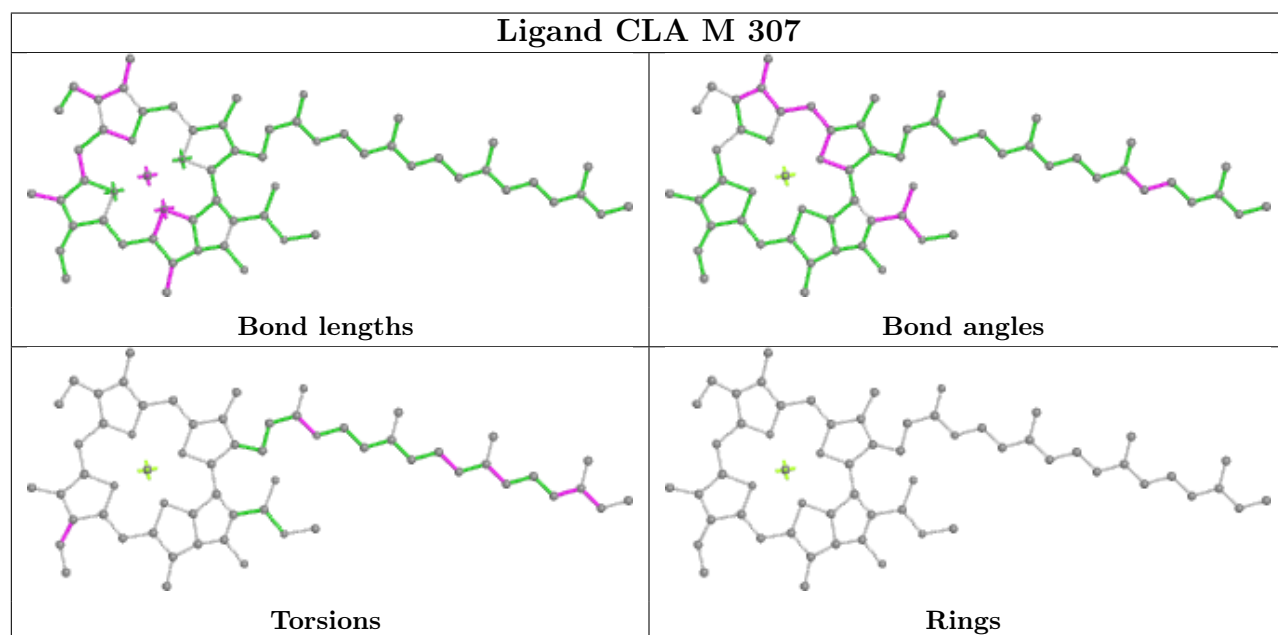
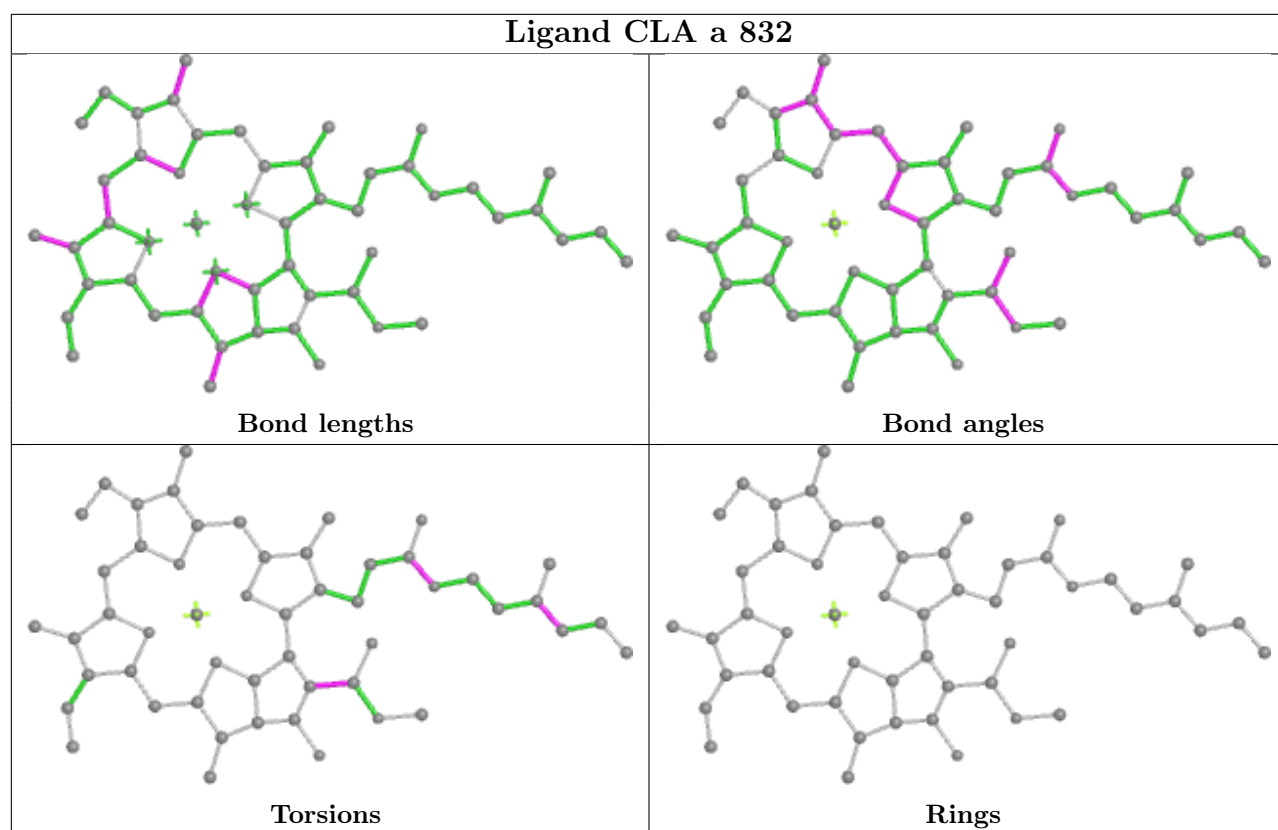


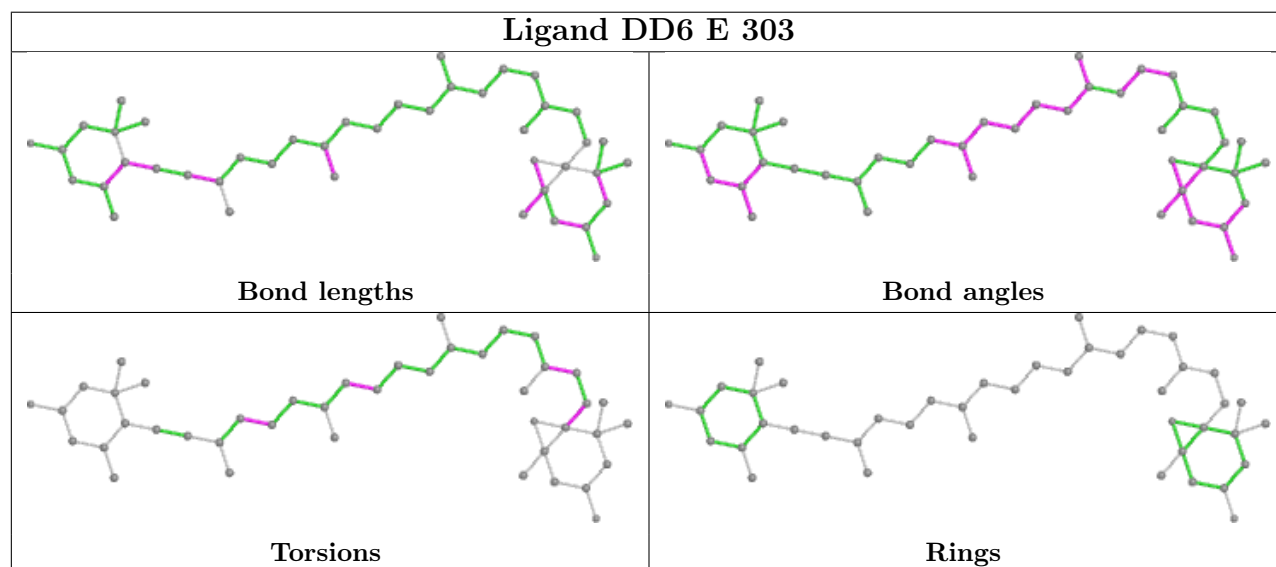
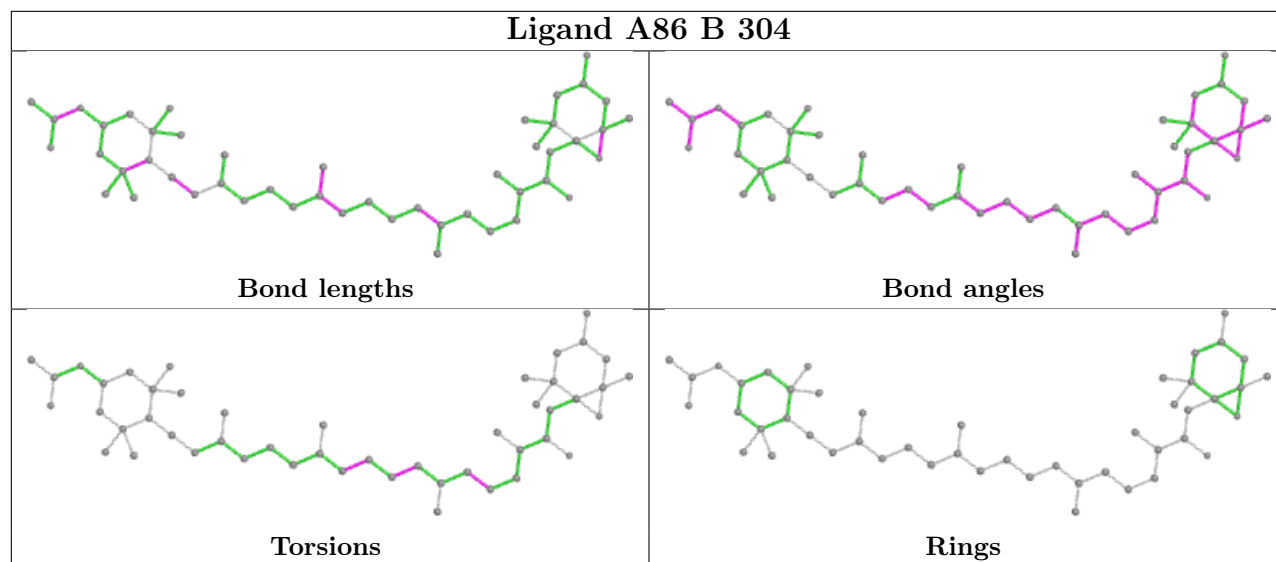
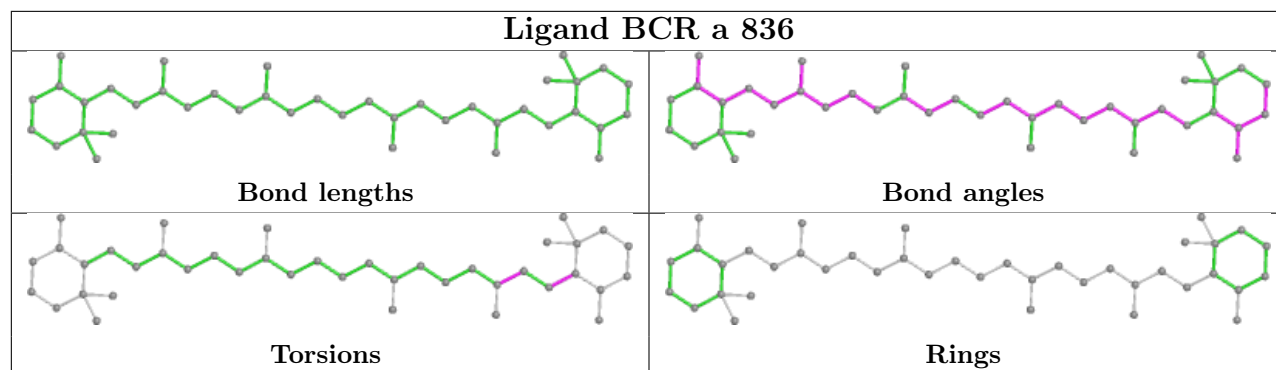
Torsions

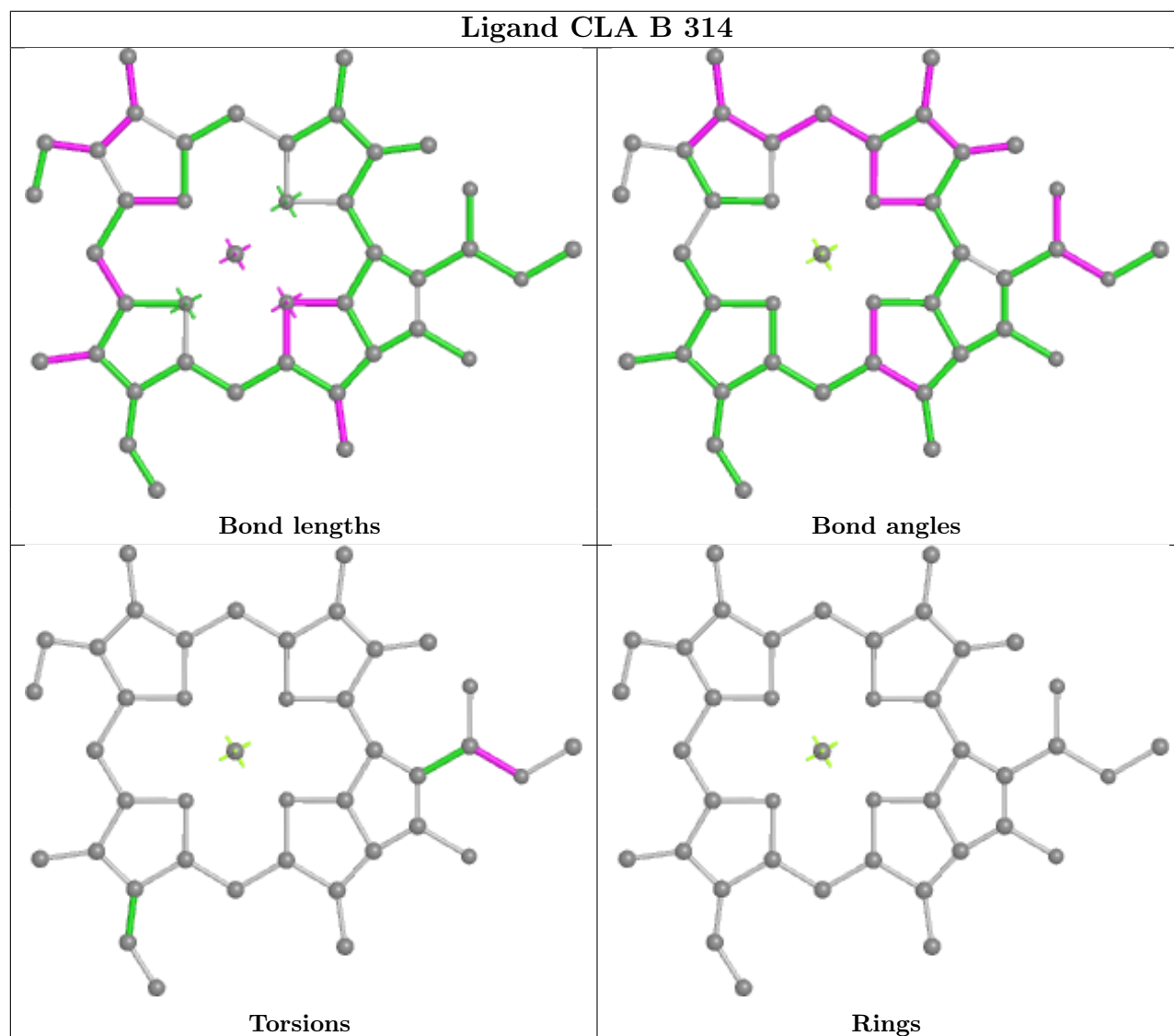
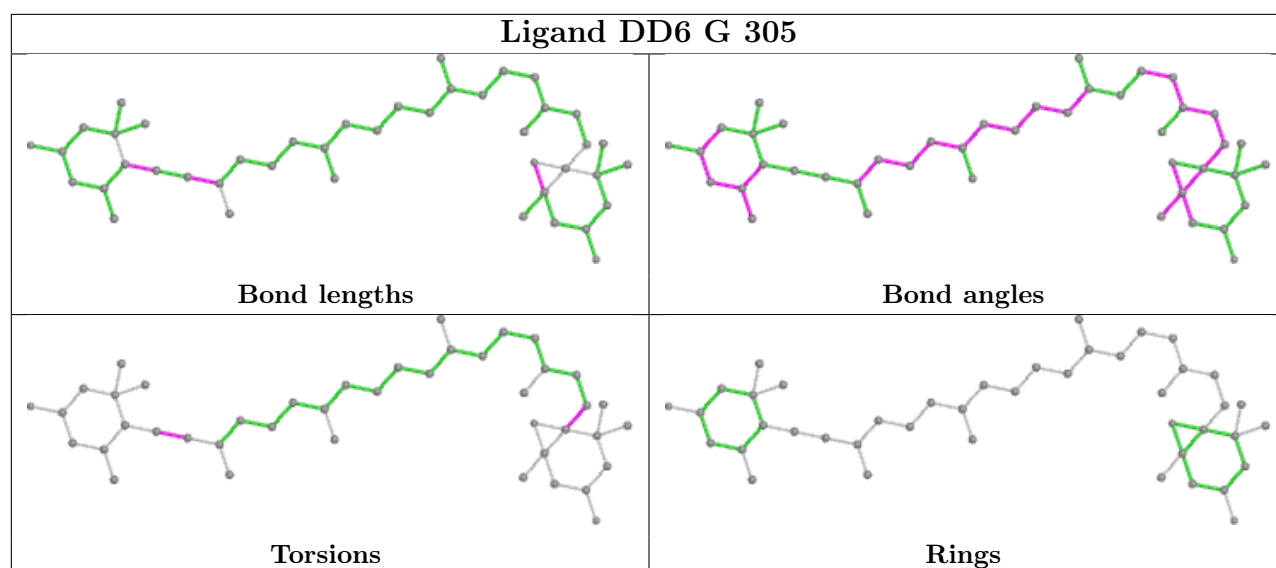


Rings

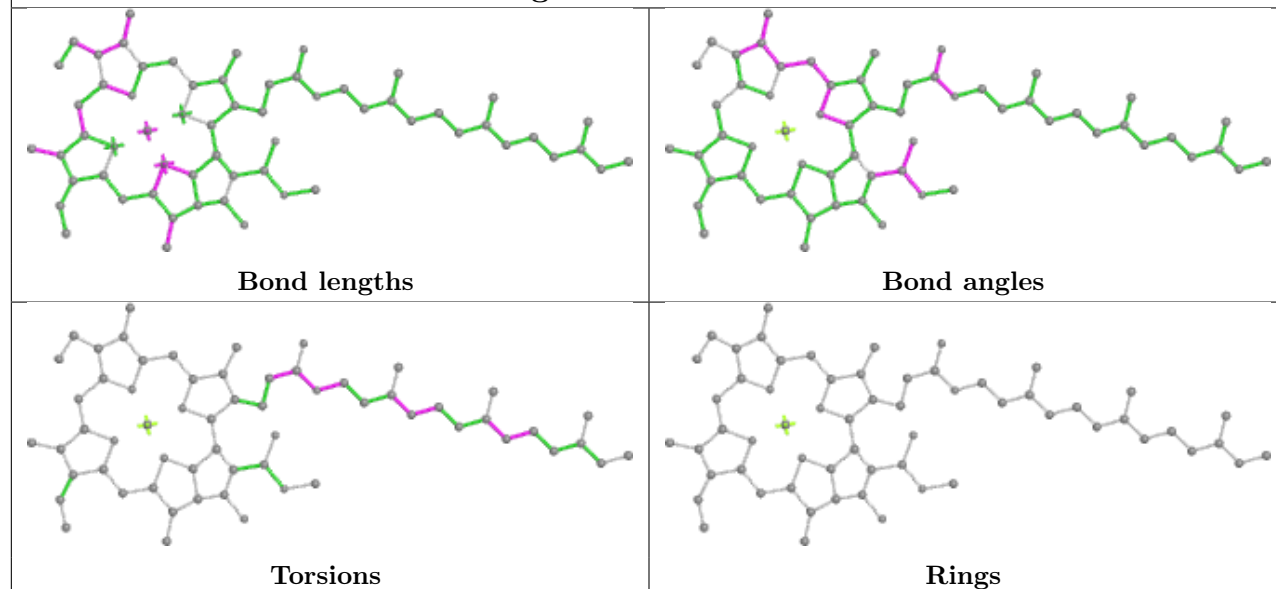




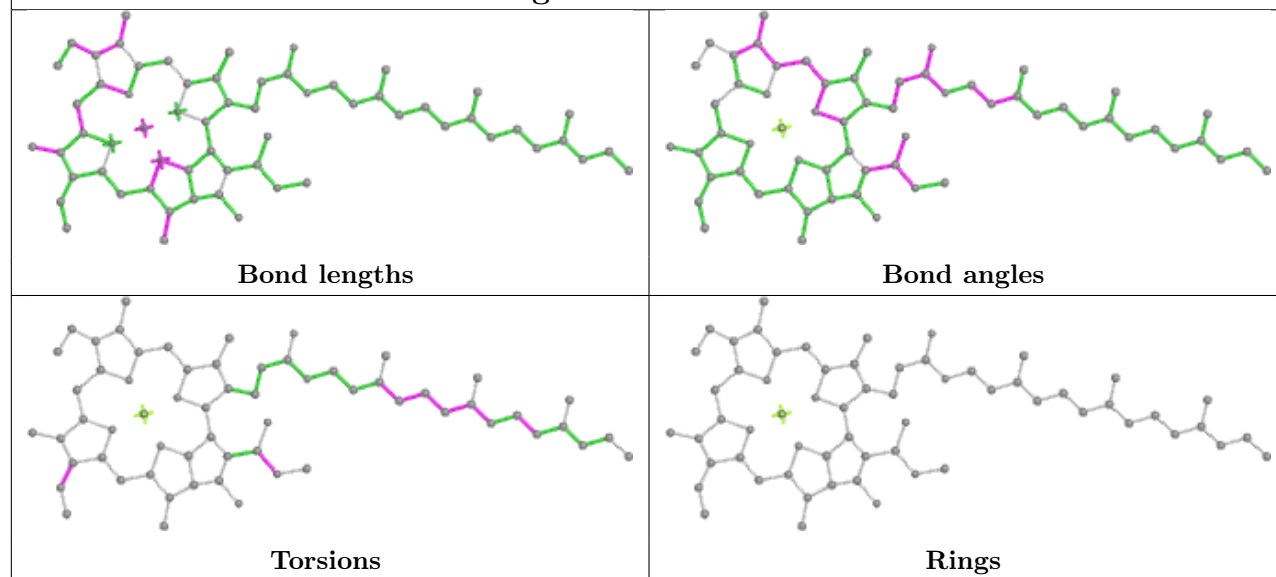


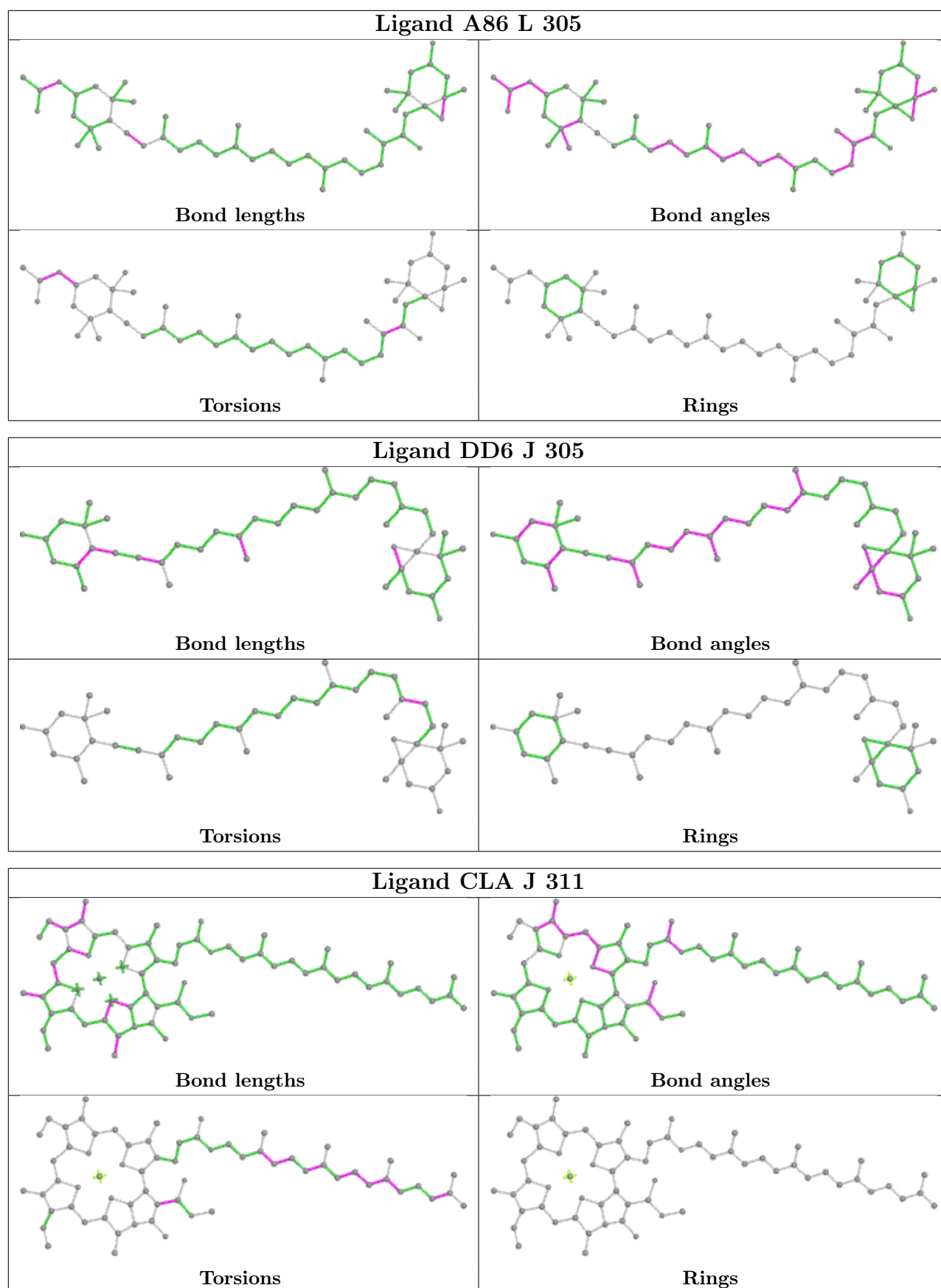


Ligand CLA D 207

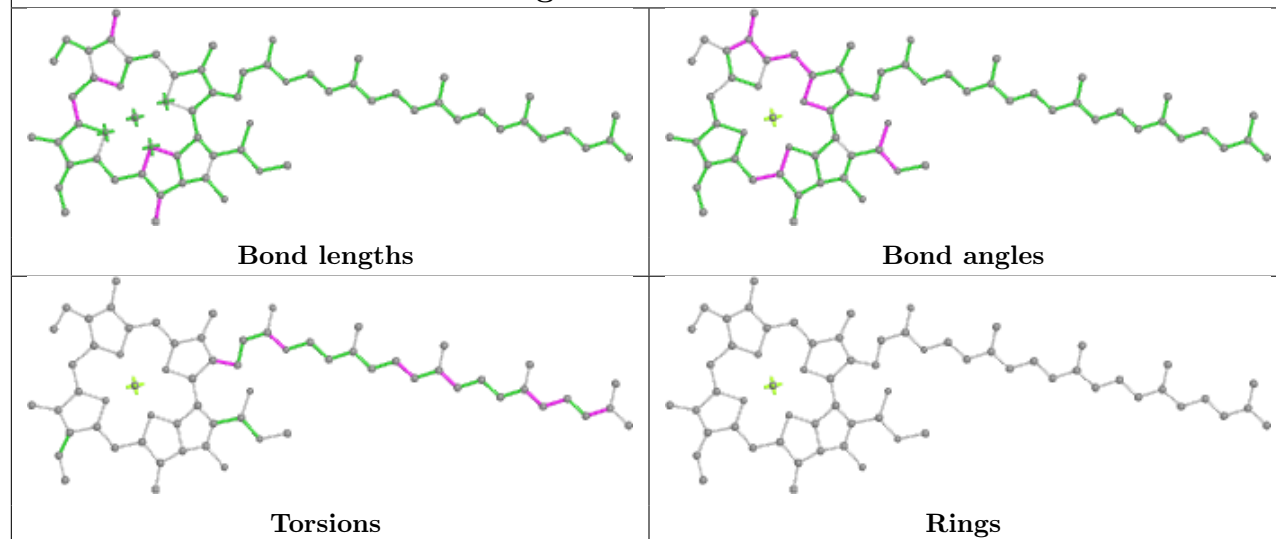


Ligand CLA C 309

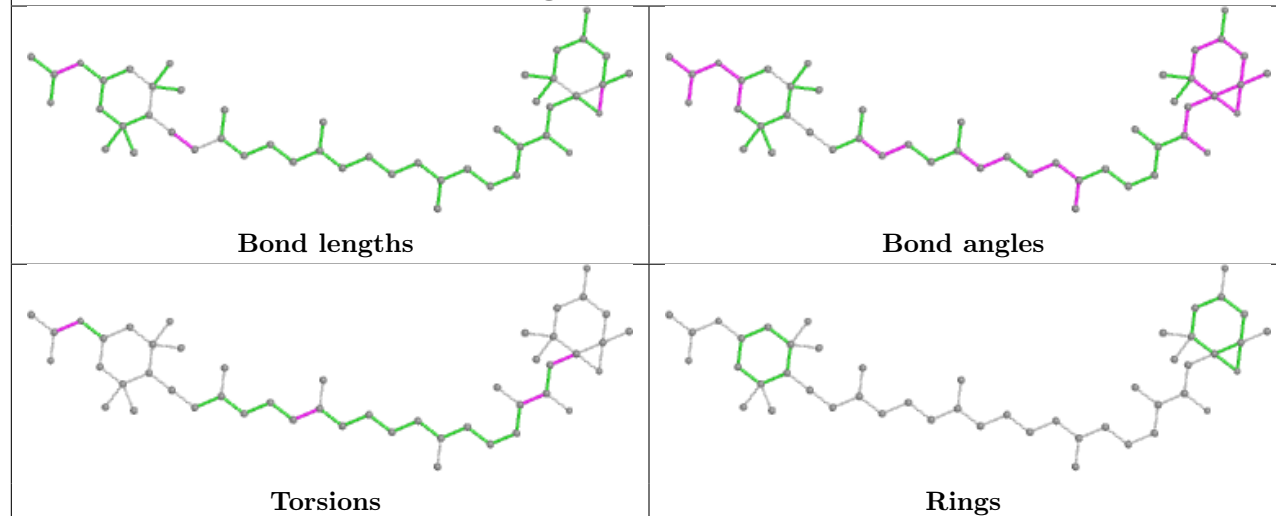




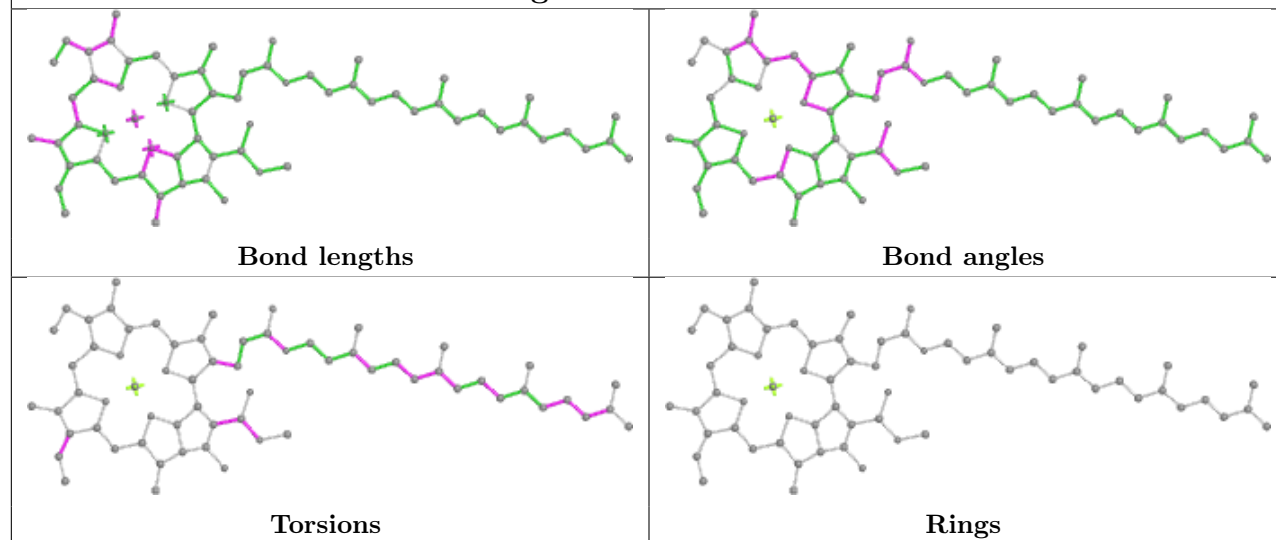
Ligand CLA a 840

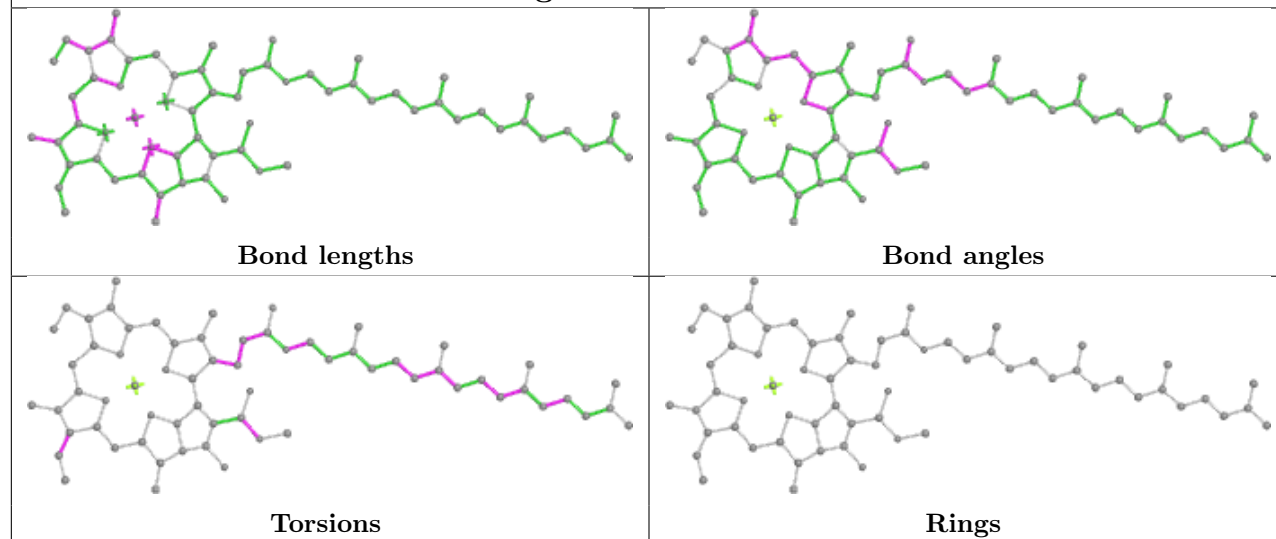
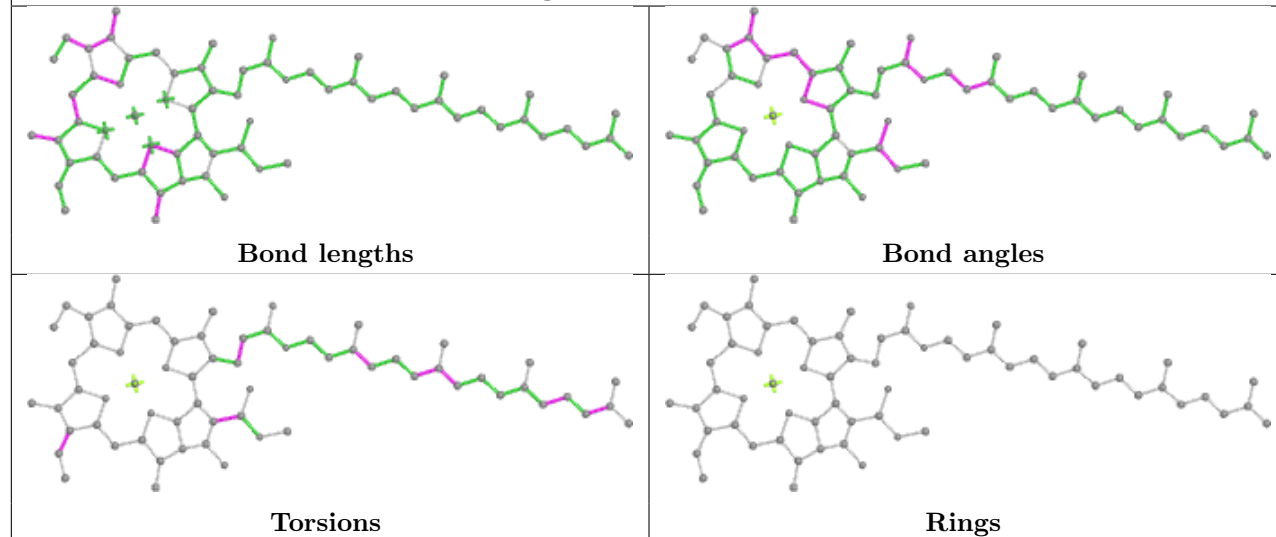
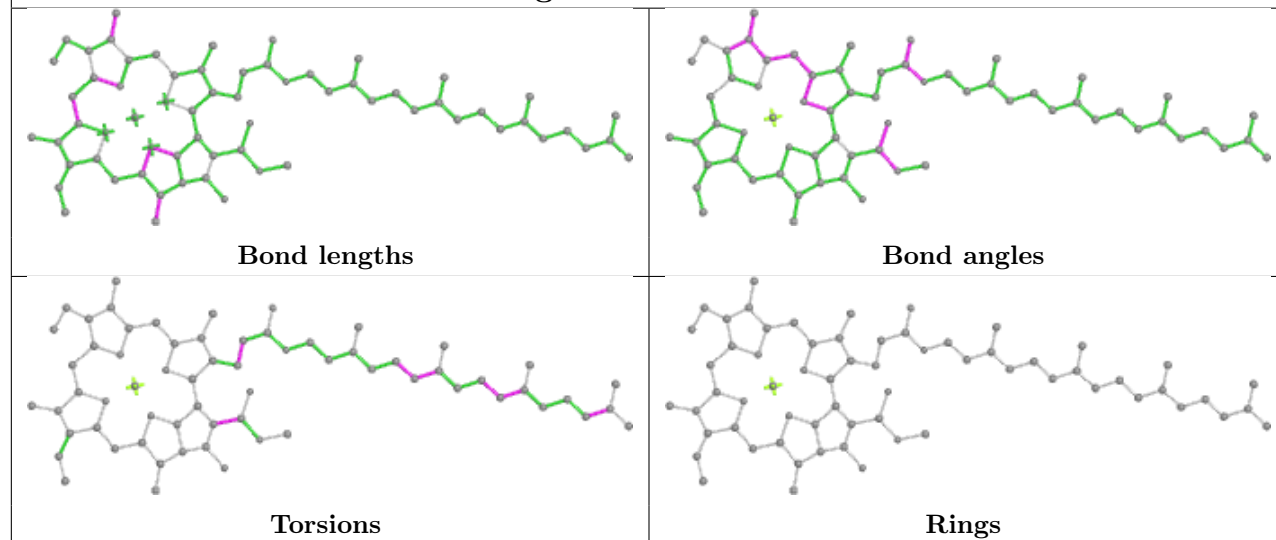


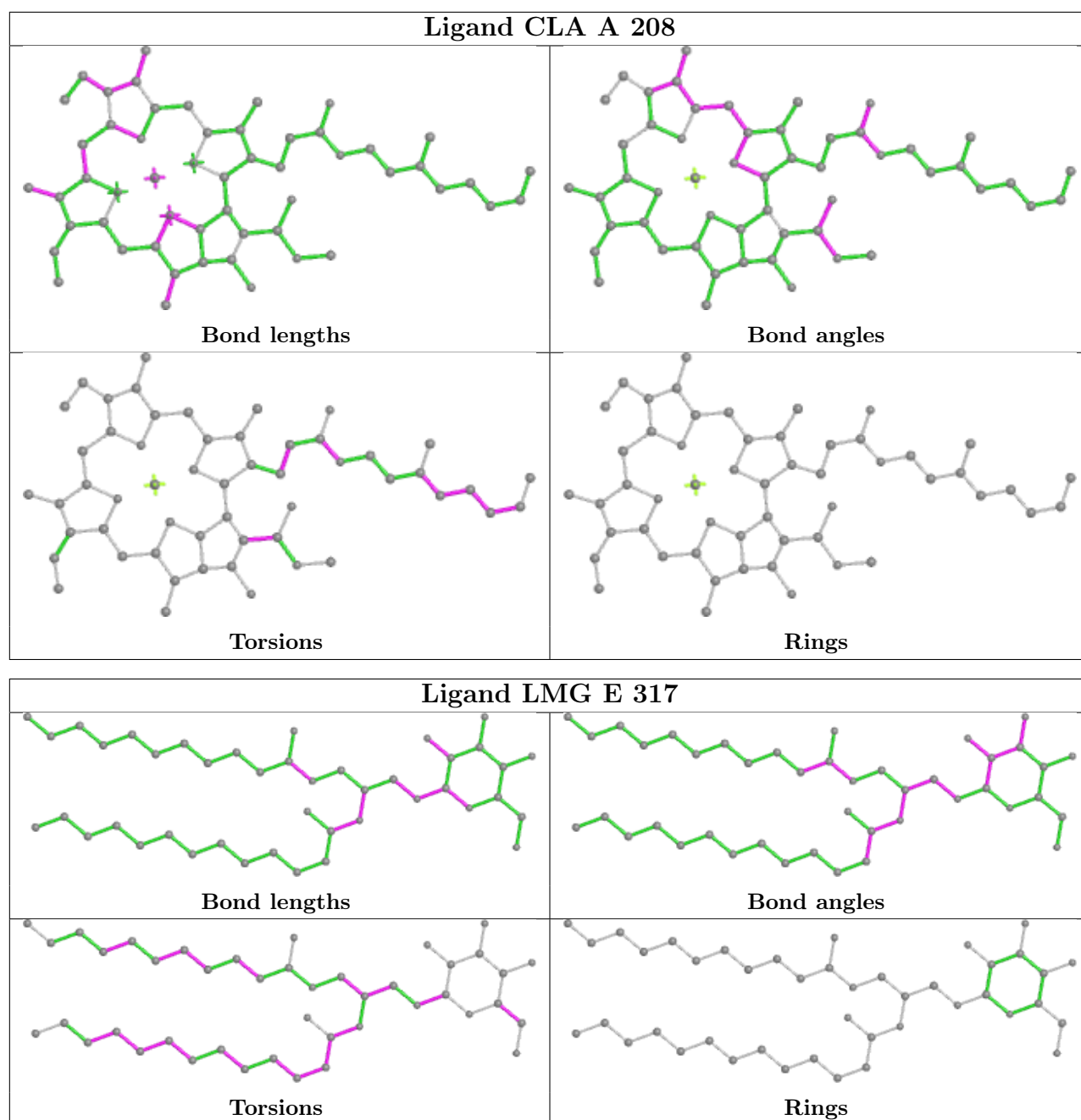
Ligand A86 L 302



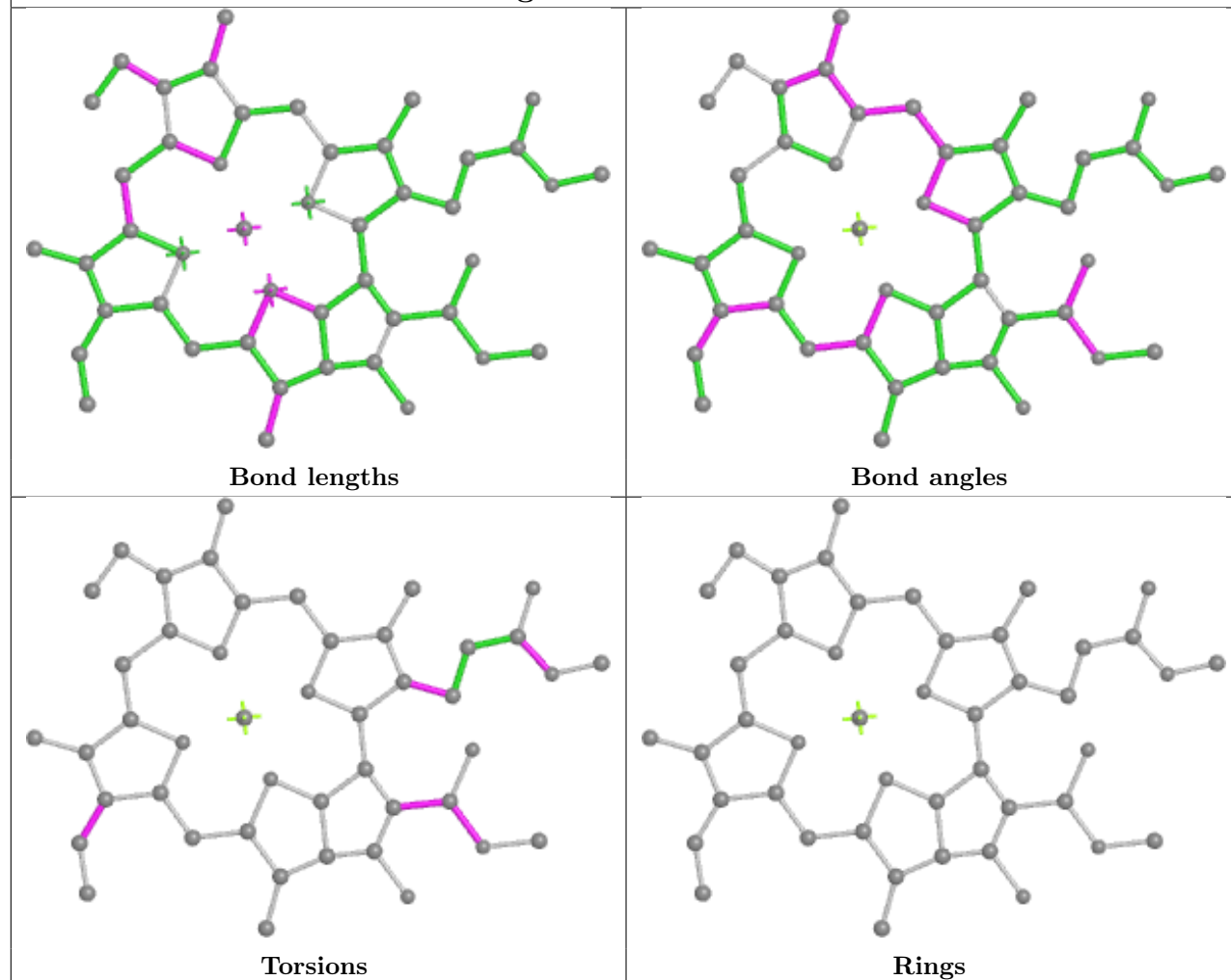
Ligand CLA K 312



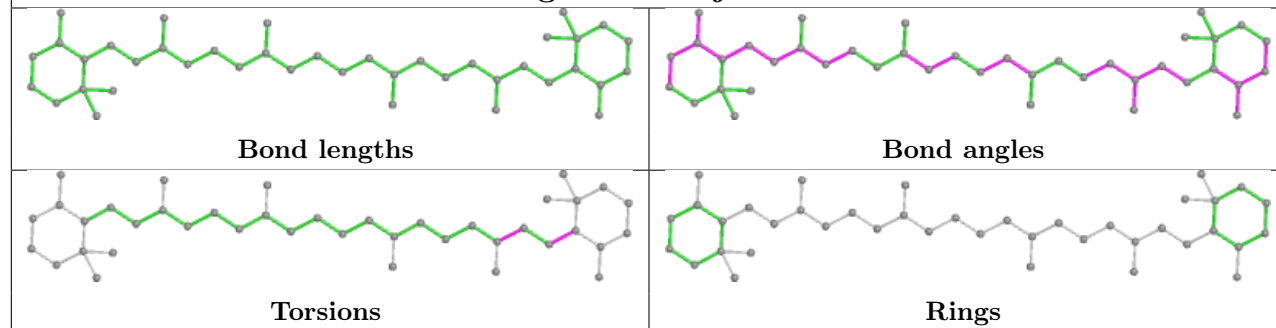
Ligand CLA b 825**Ligand CLA I 308****Ligand CLA b 808**



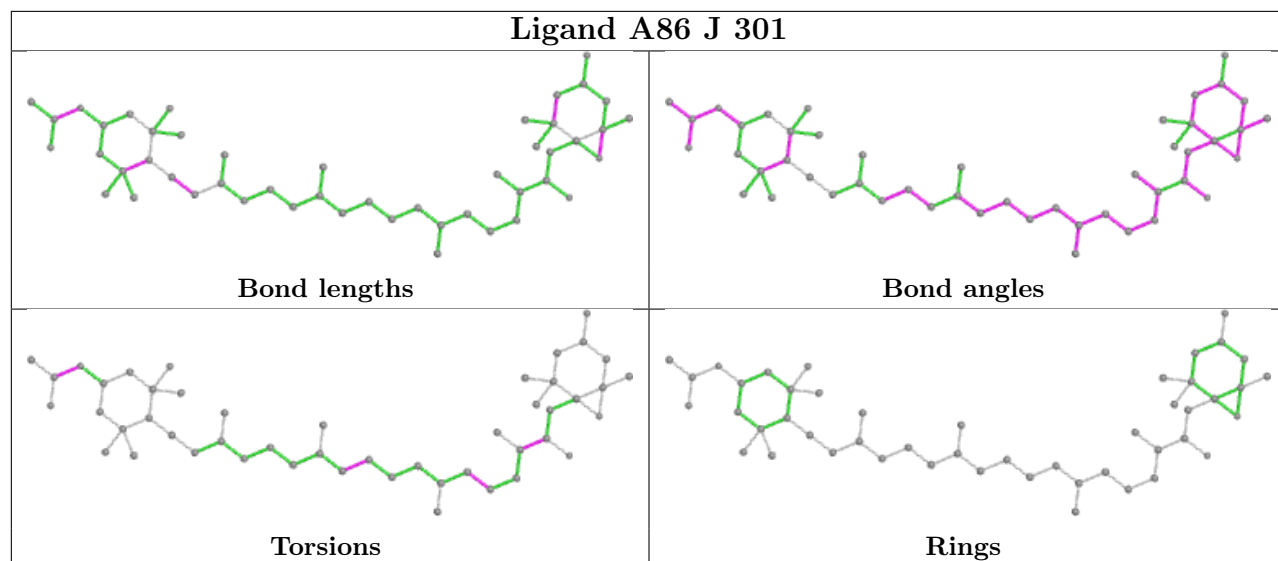
Ligand CLA J 310



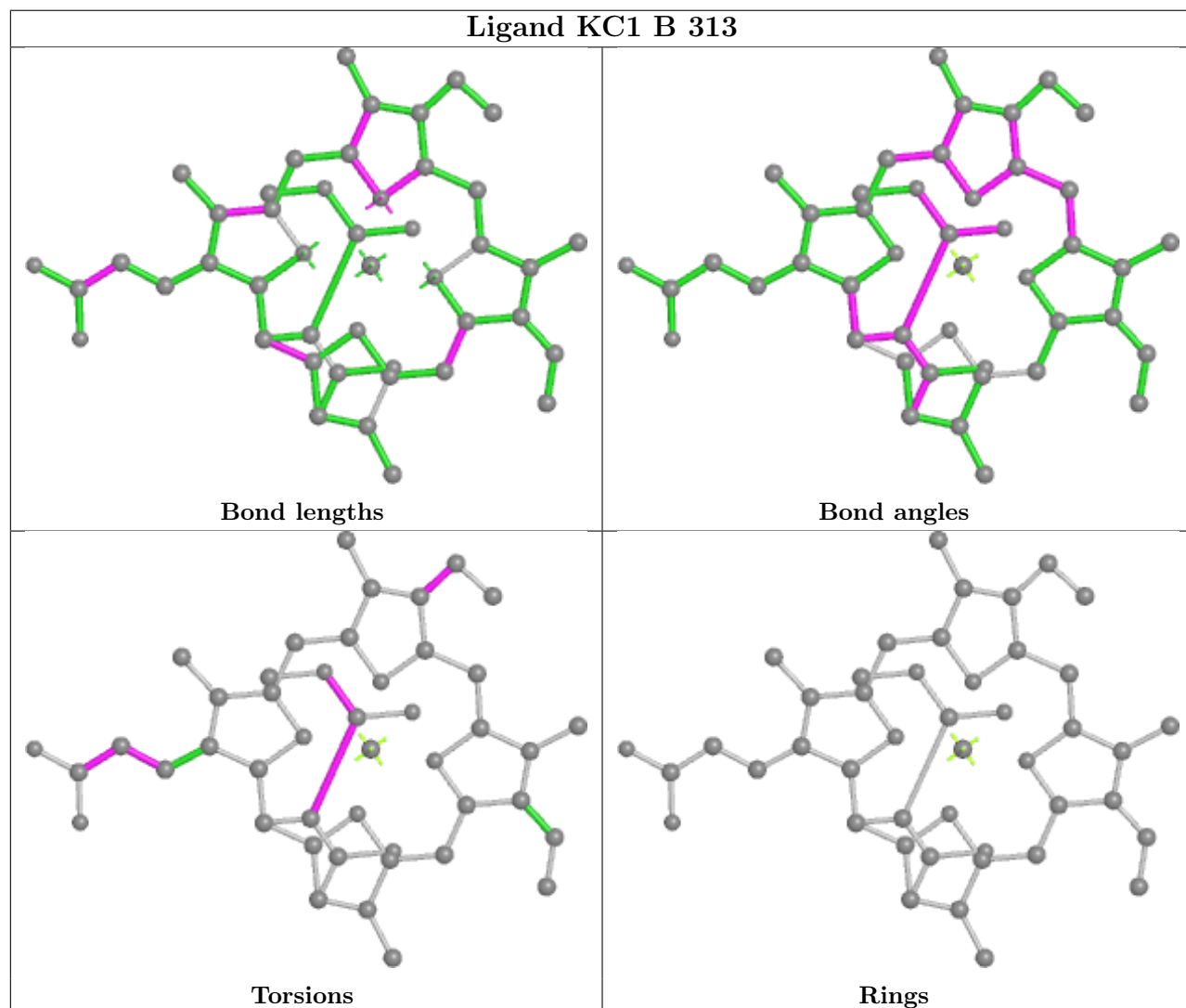
Ligand BCR j 101

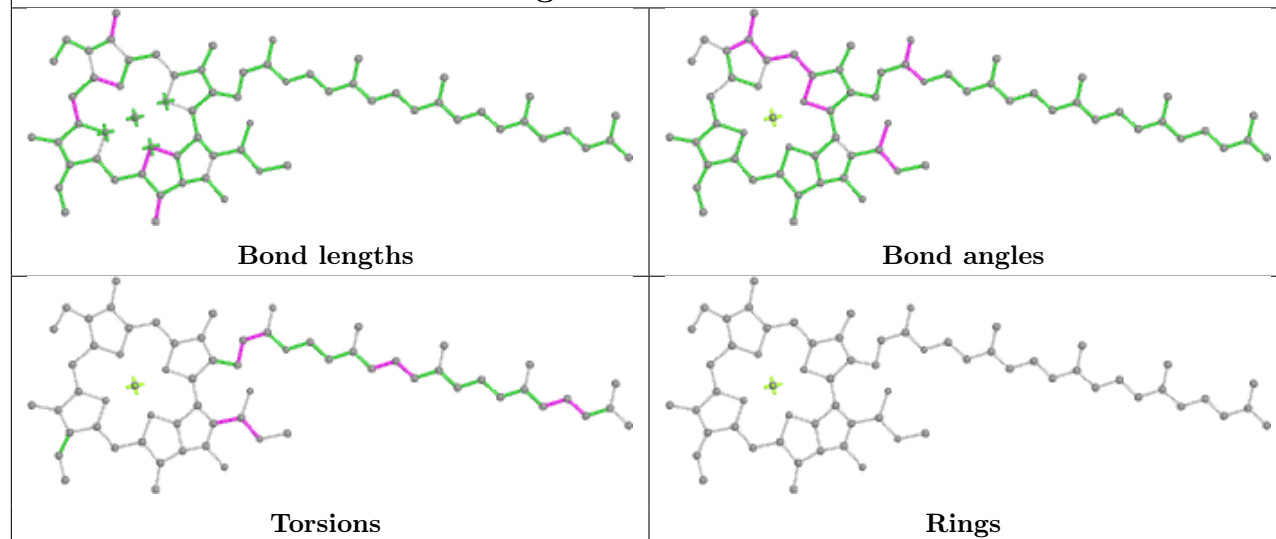
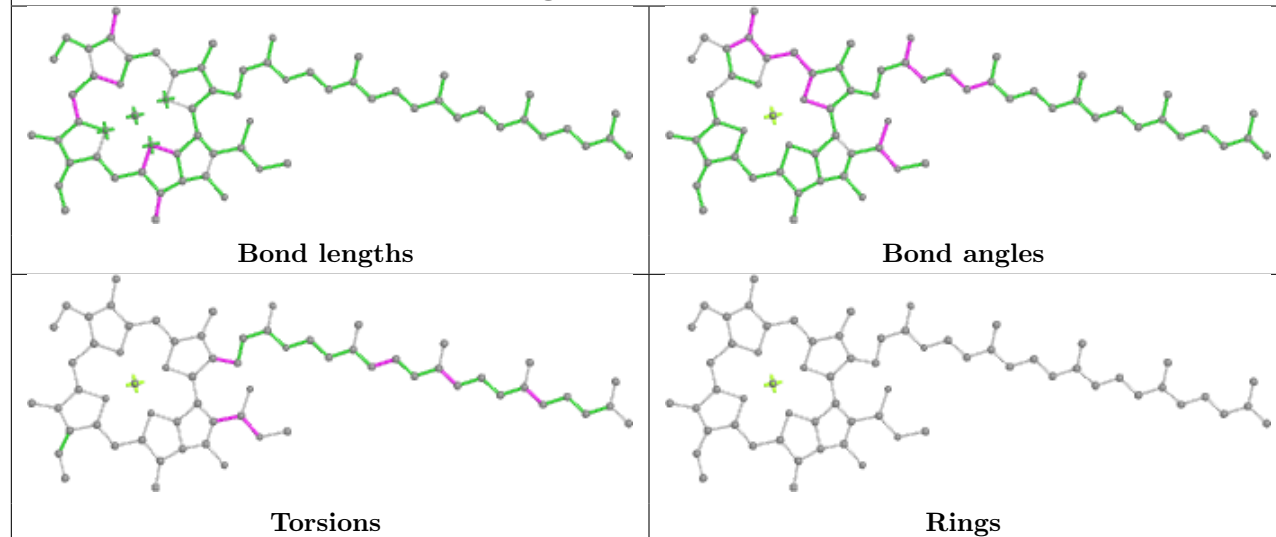


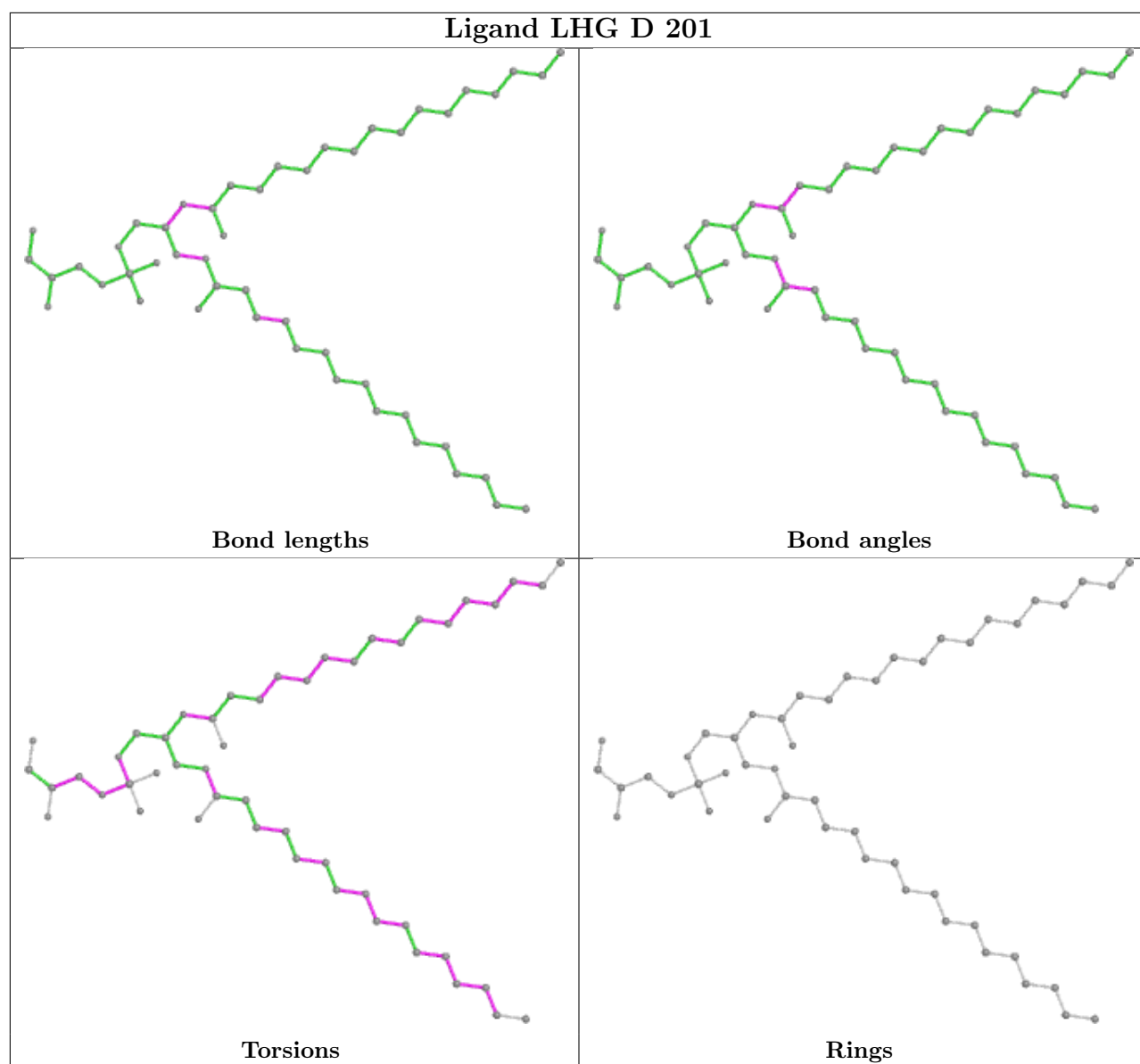
Ligand A86 J 301



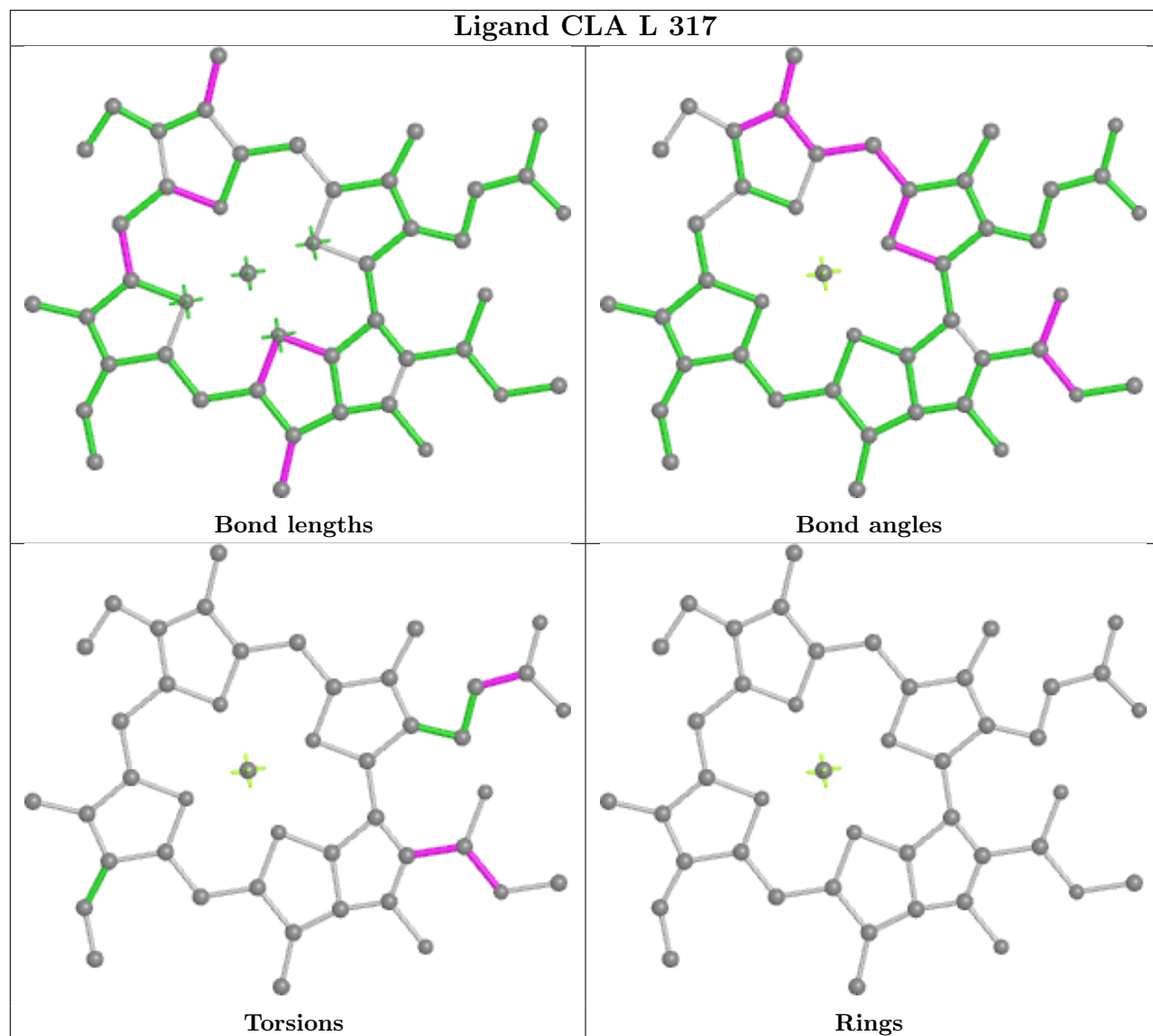
Ligand KC1 B 313



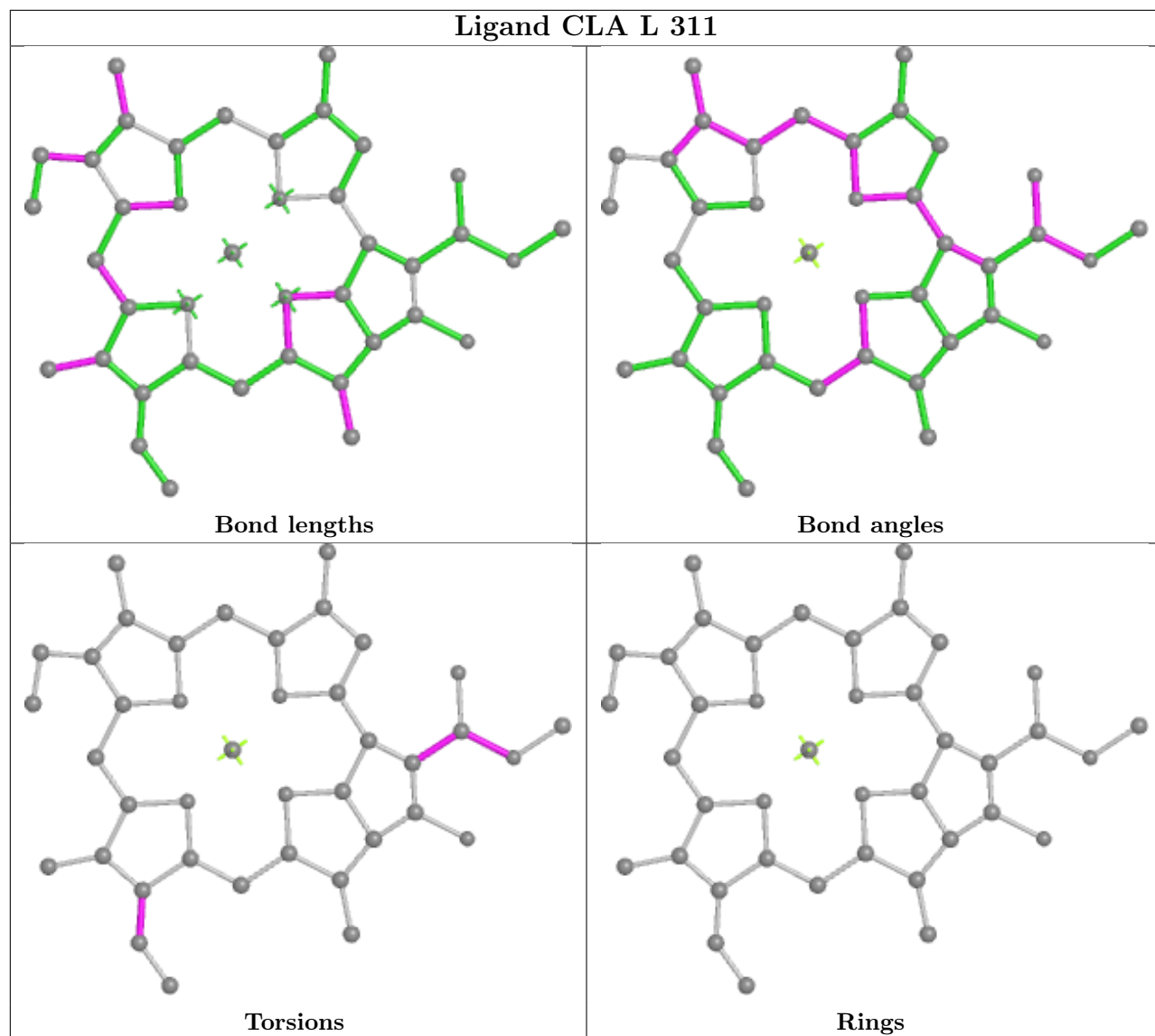
Ligand CLA a 829**Ligand CLA f 301**



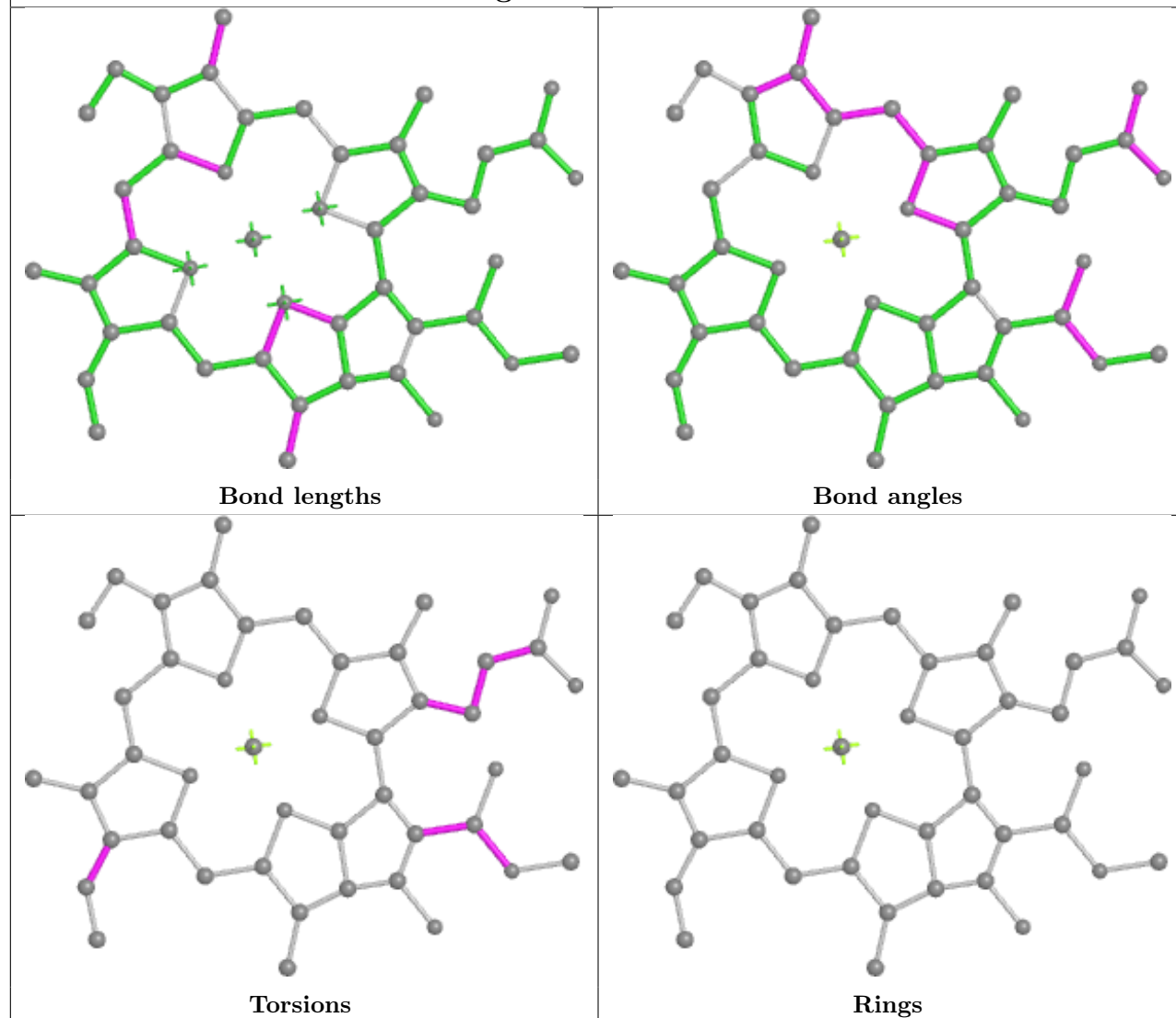
Ligand CLA L 317



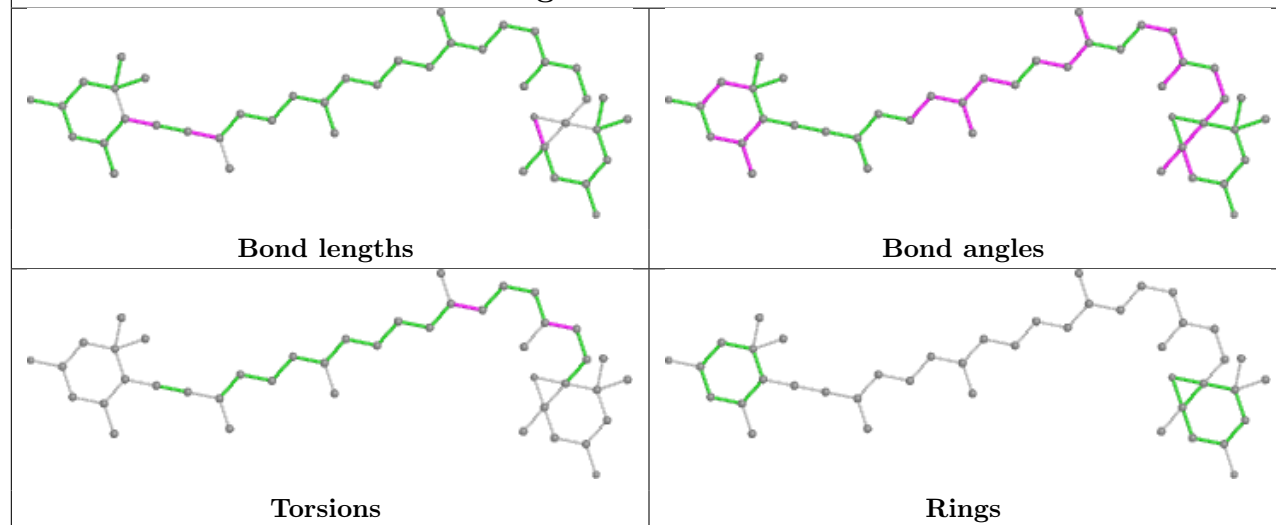
Ligand CLA L 311

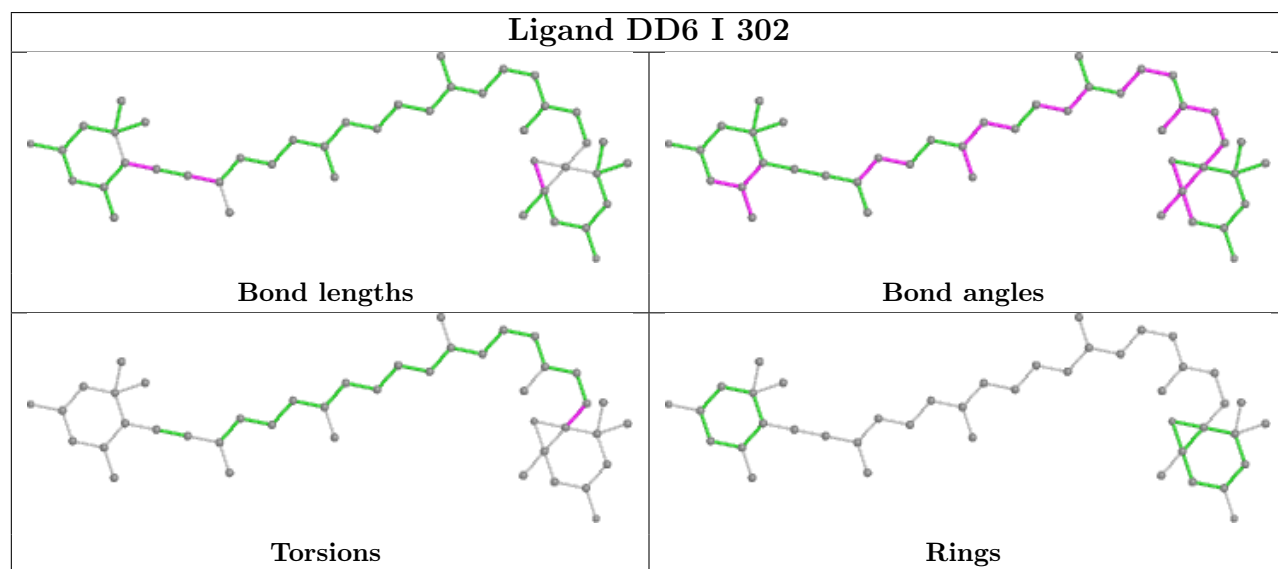
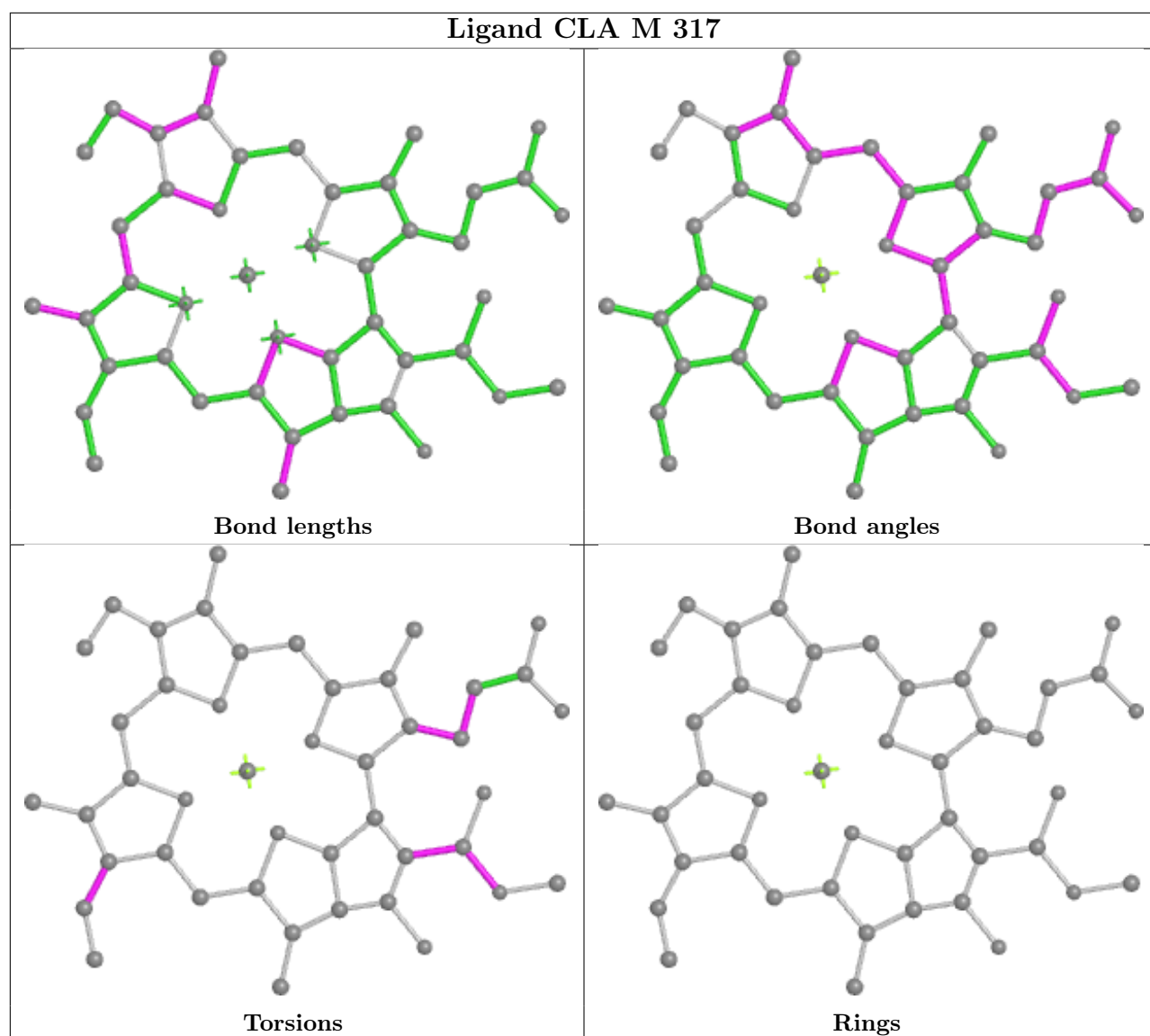


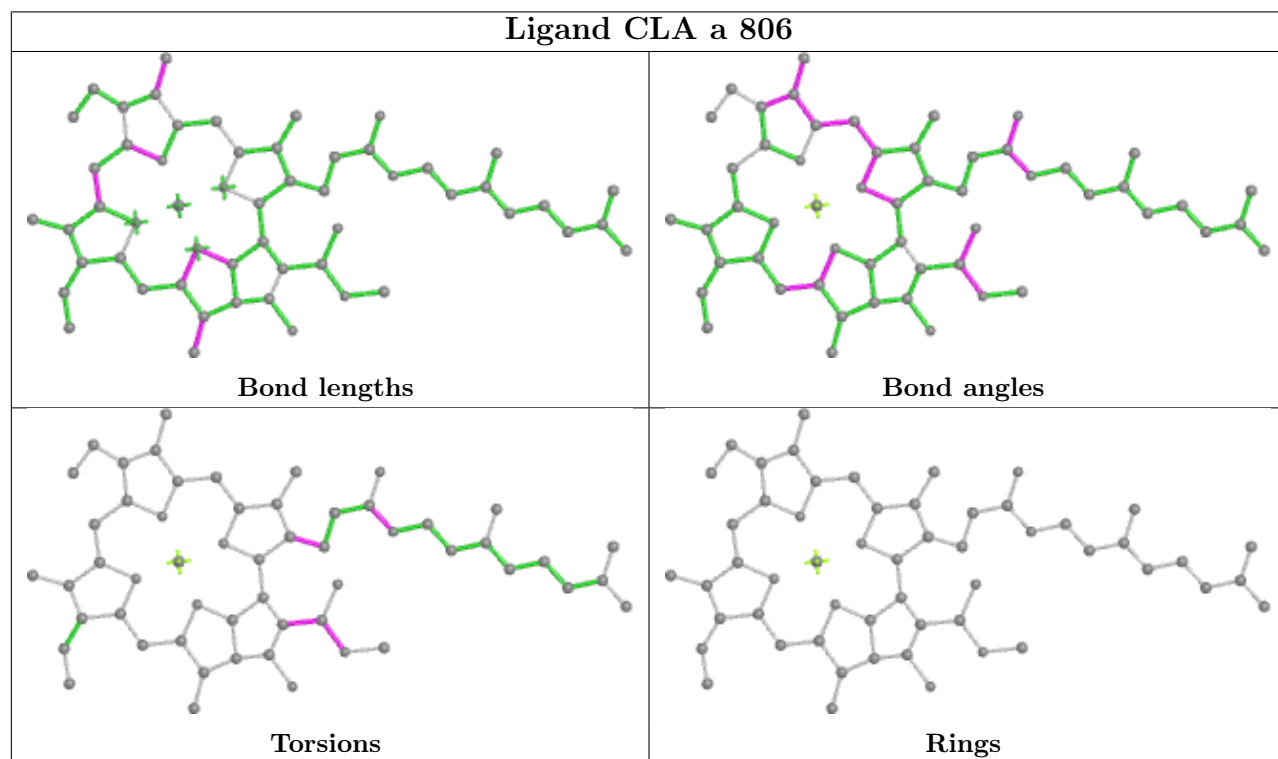
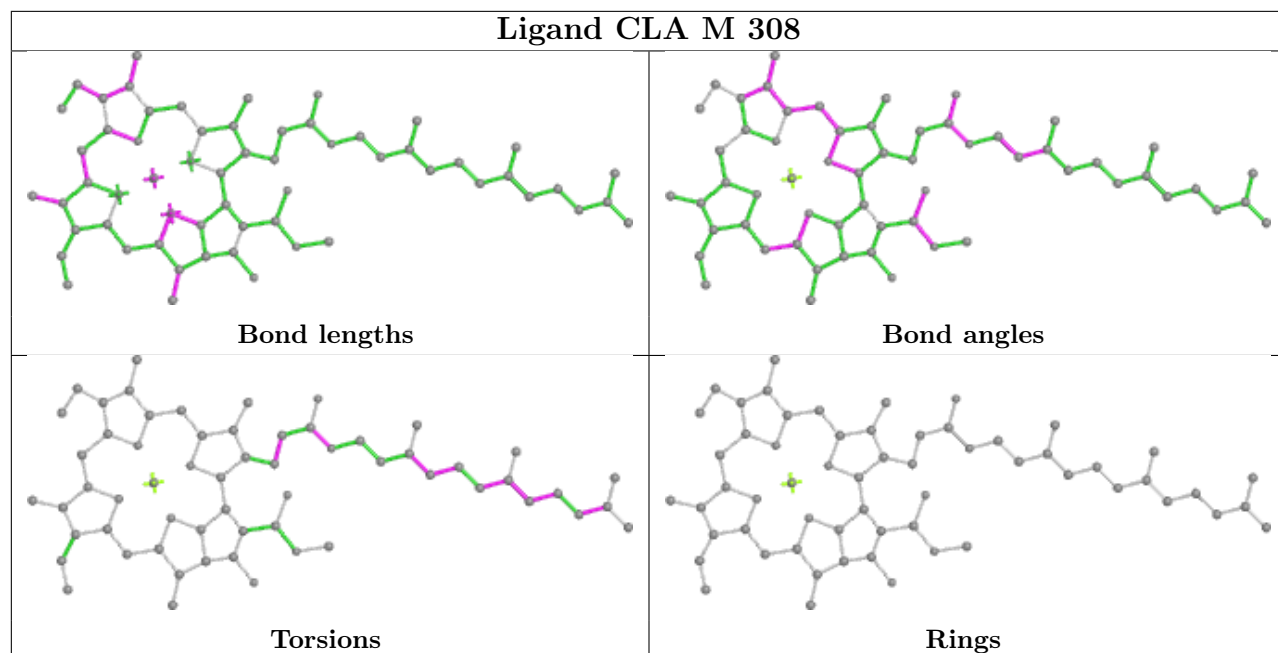
Ligand CLA r 201

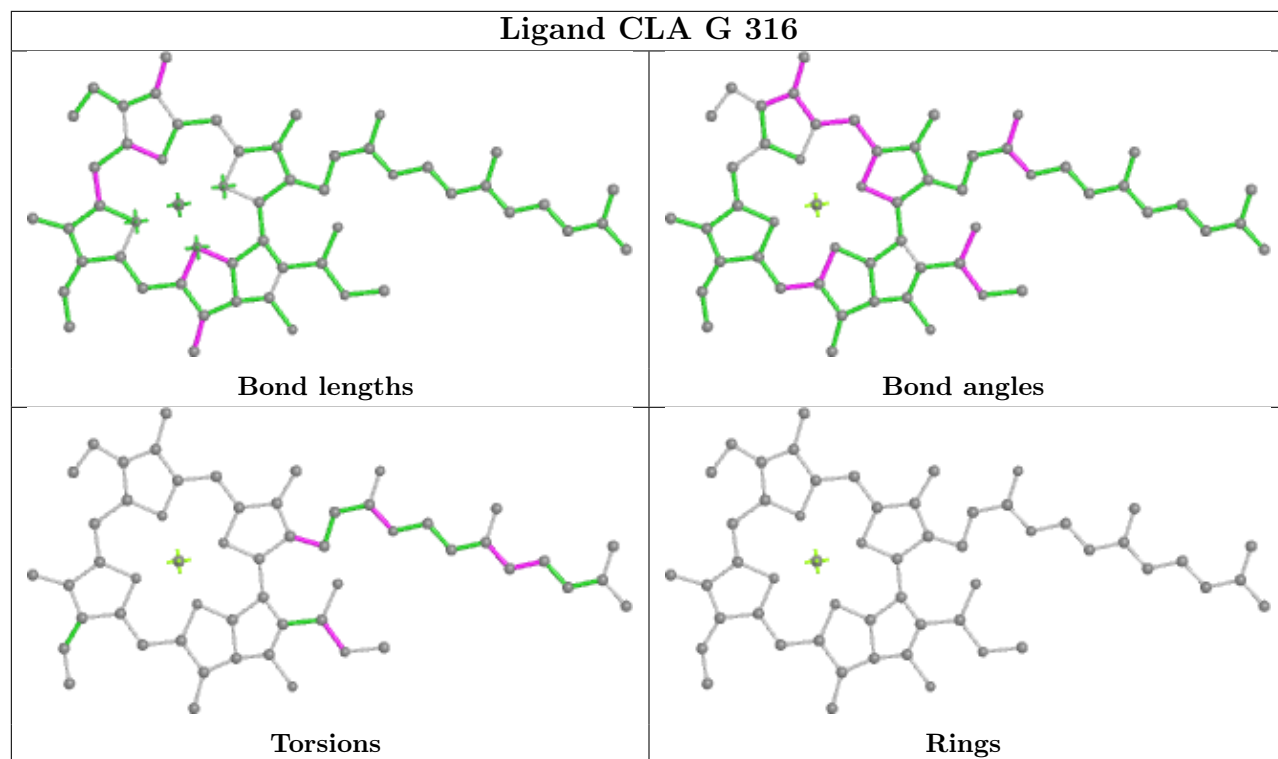


Ligand DD6 J 303

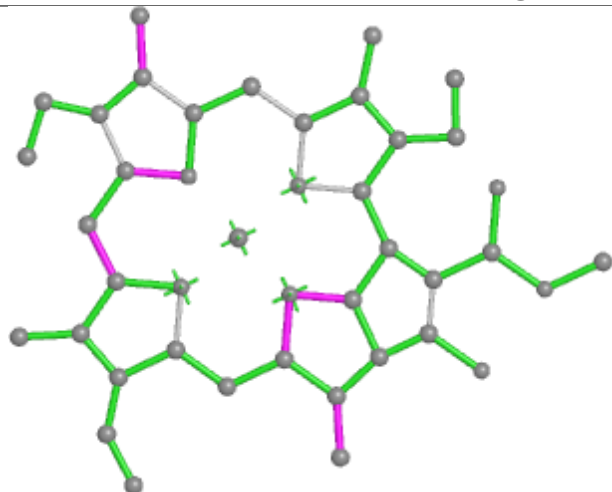




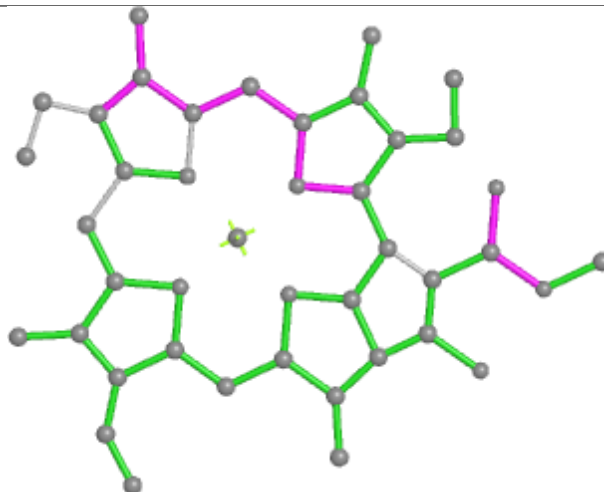




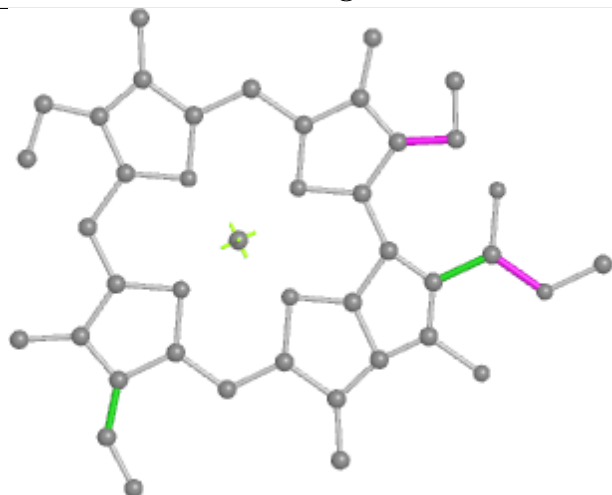
Ligand CLA G 315



Bond lengths



Bond angles

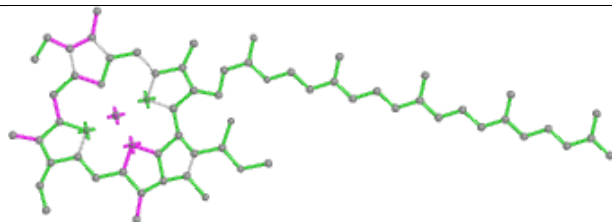


Torsions

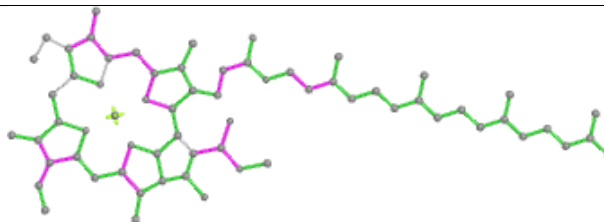


Rings

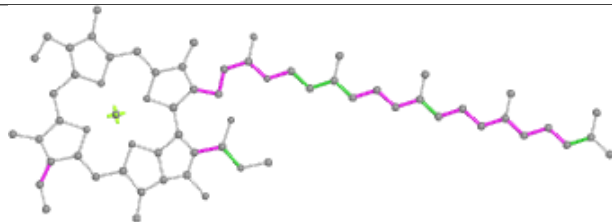
Ligand CLA a 815



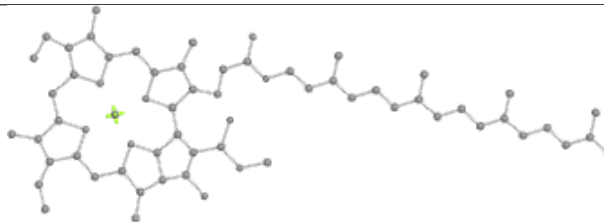
Bond lengths



Bond angles

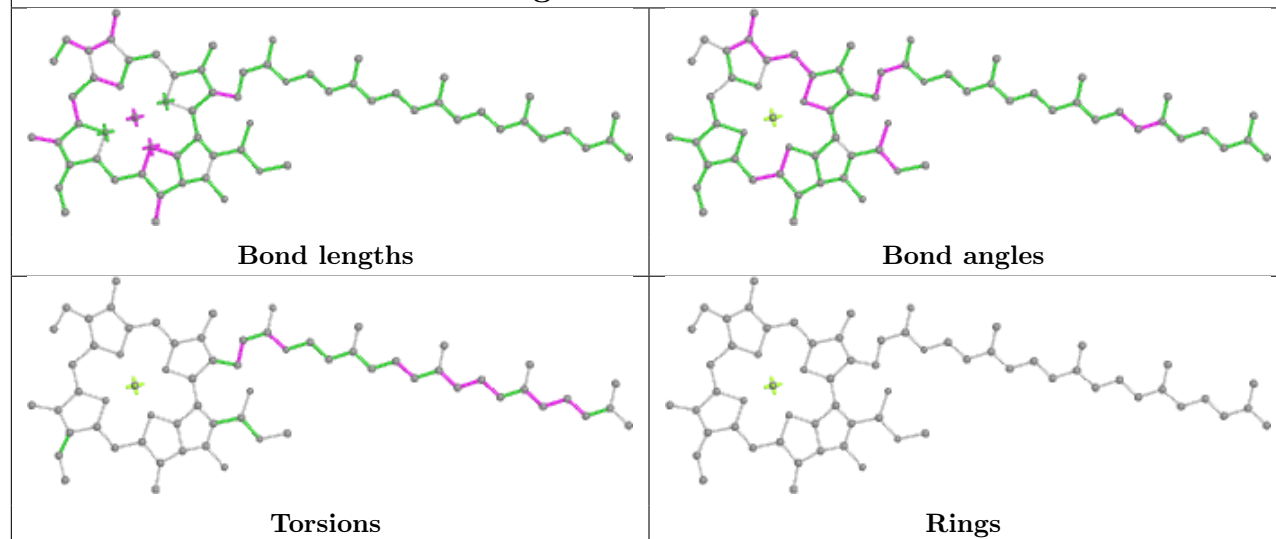


Torsions

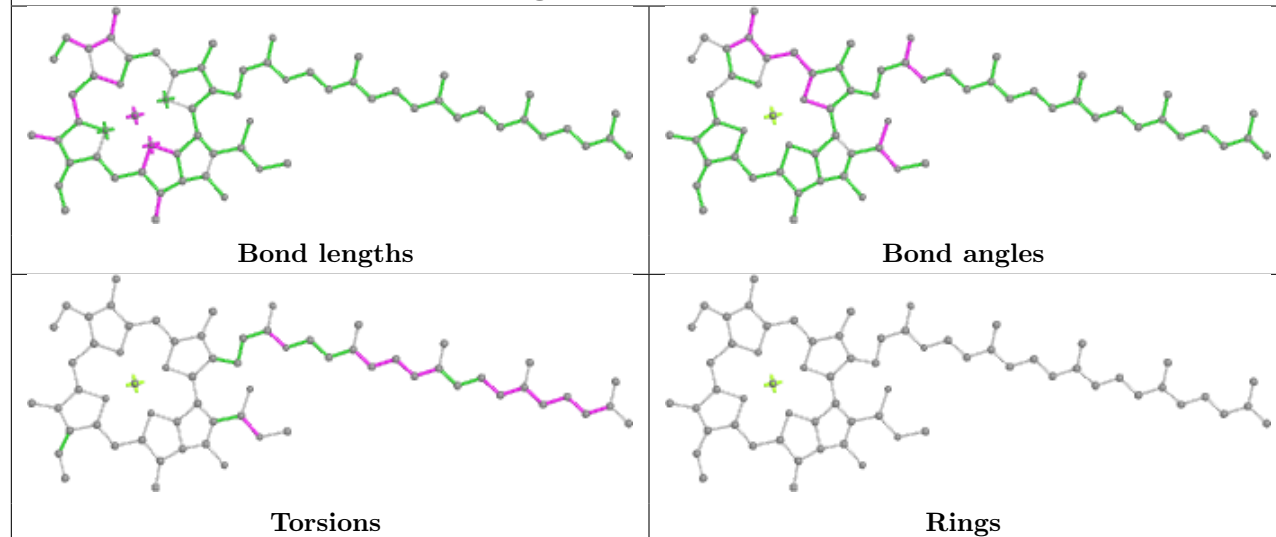


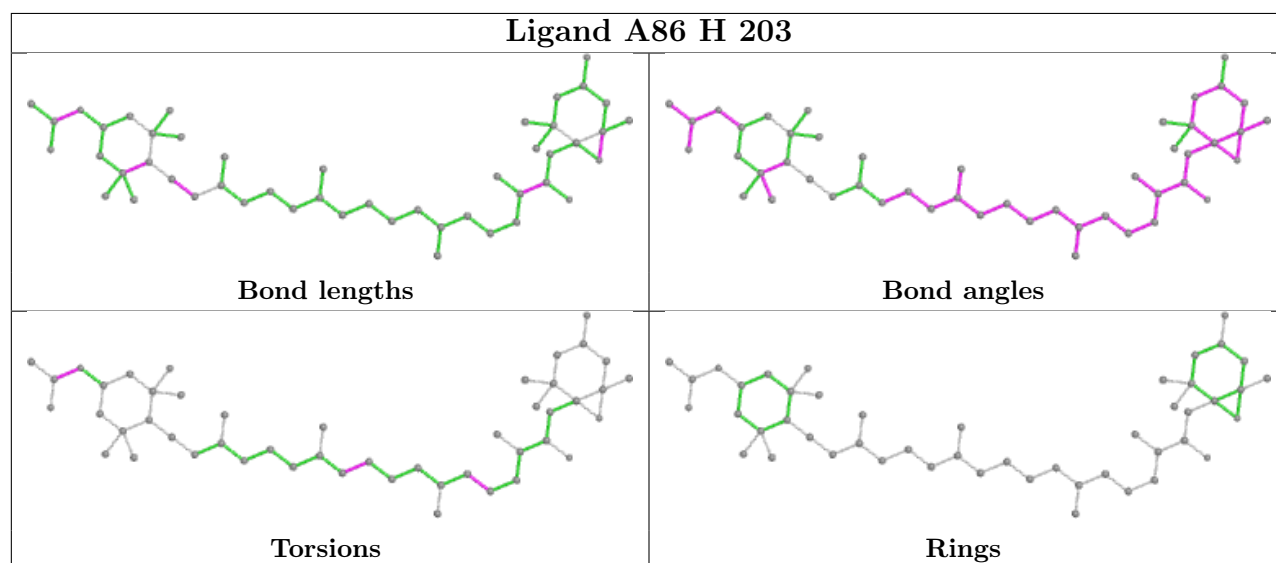
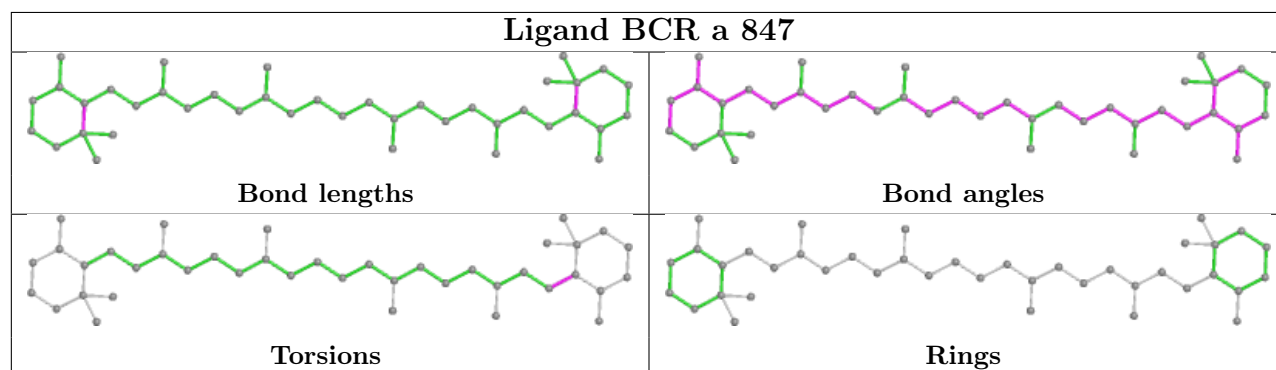
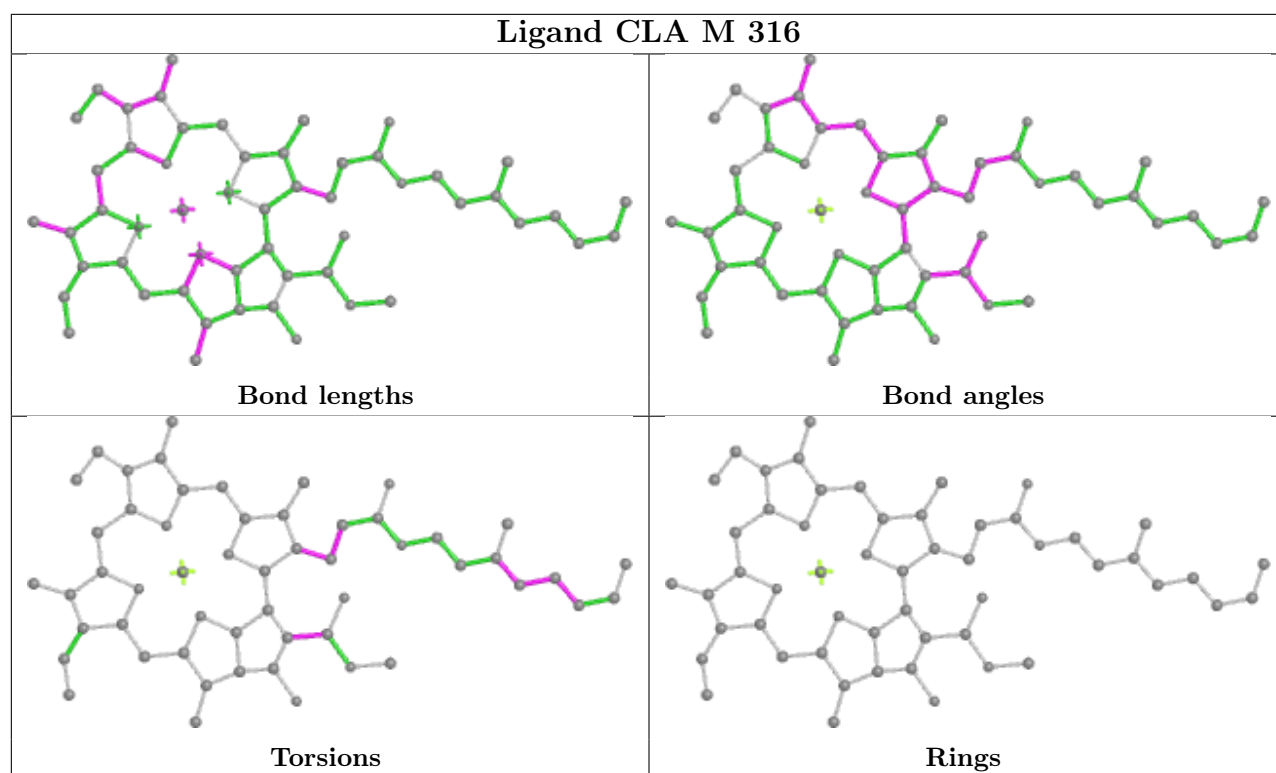
Rings

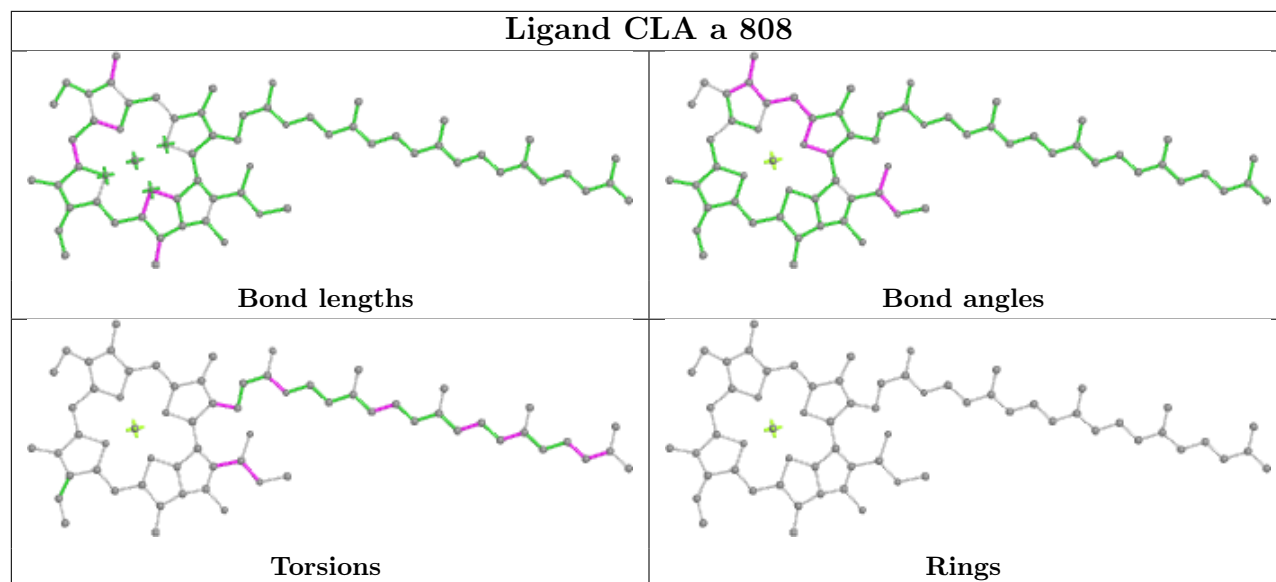
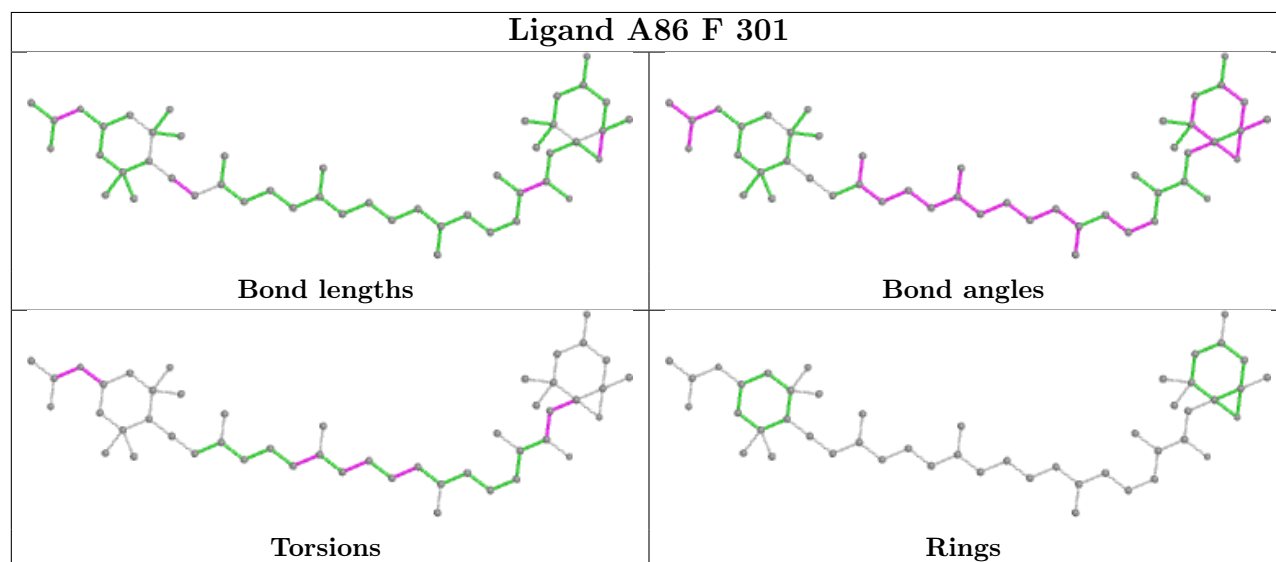
Ligand CLA E 311

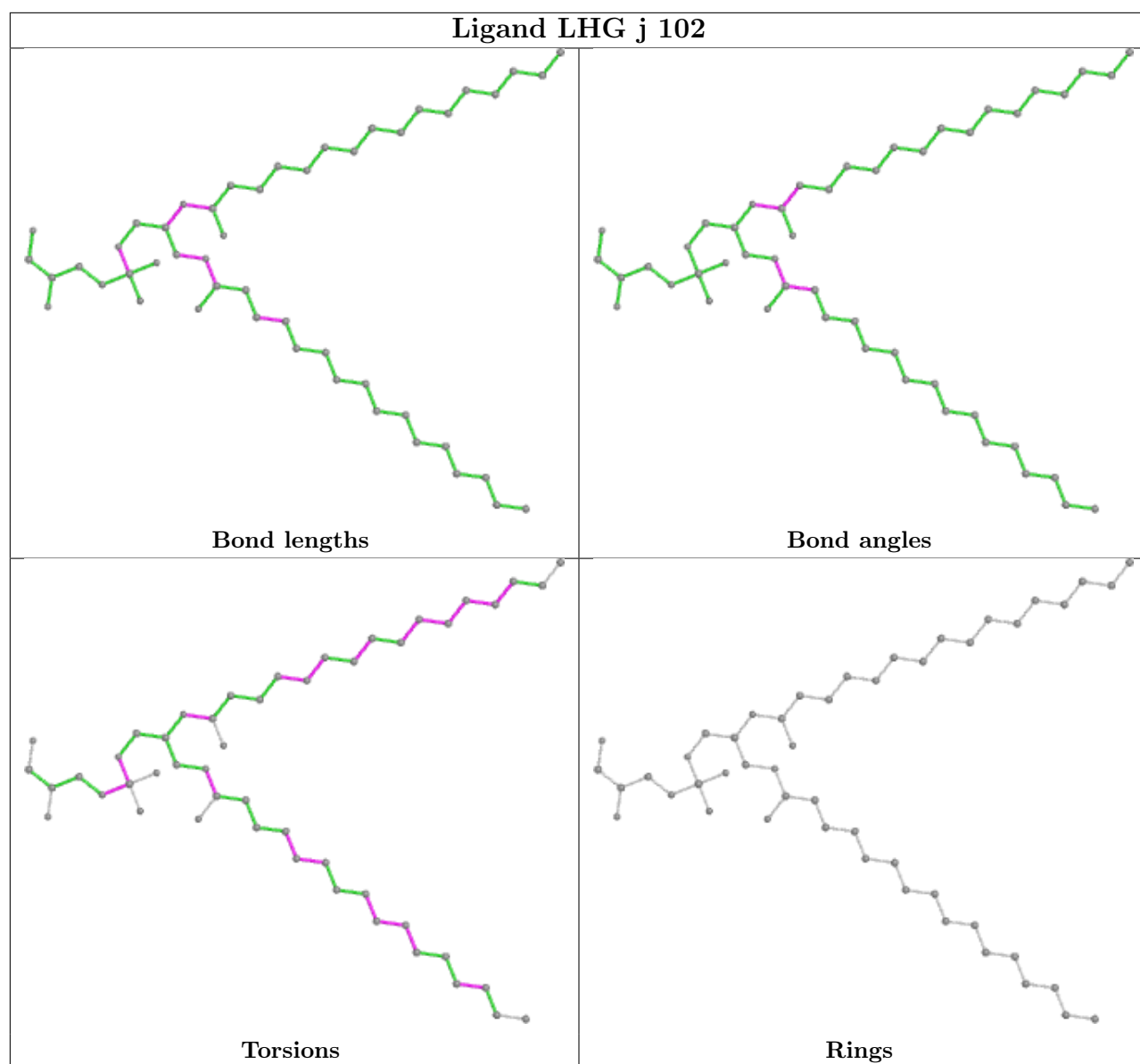


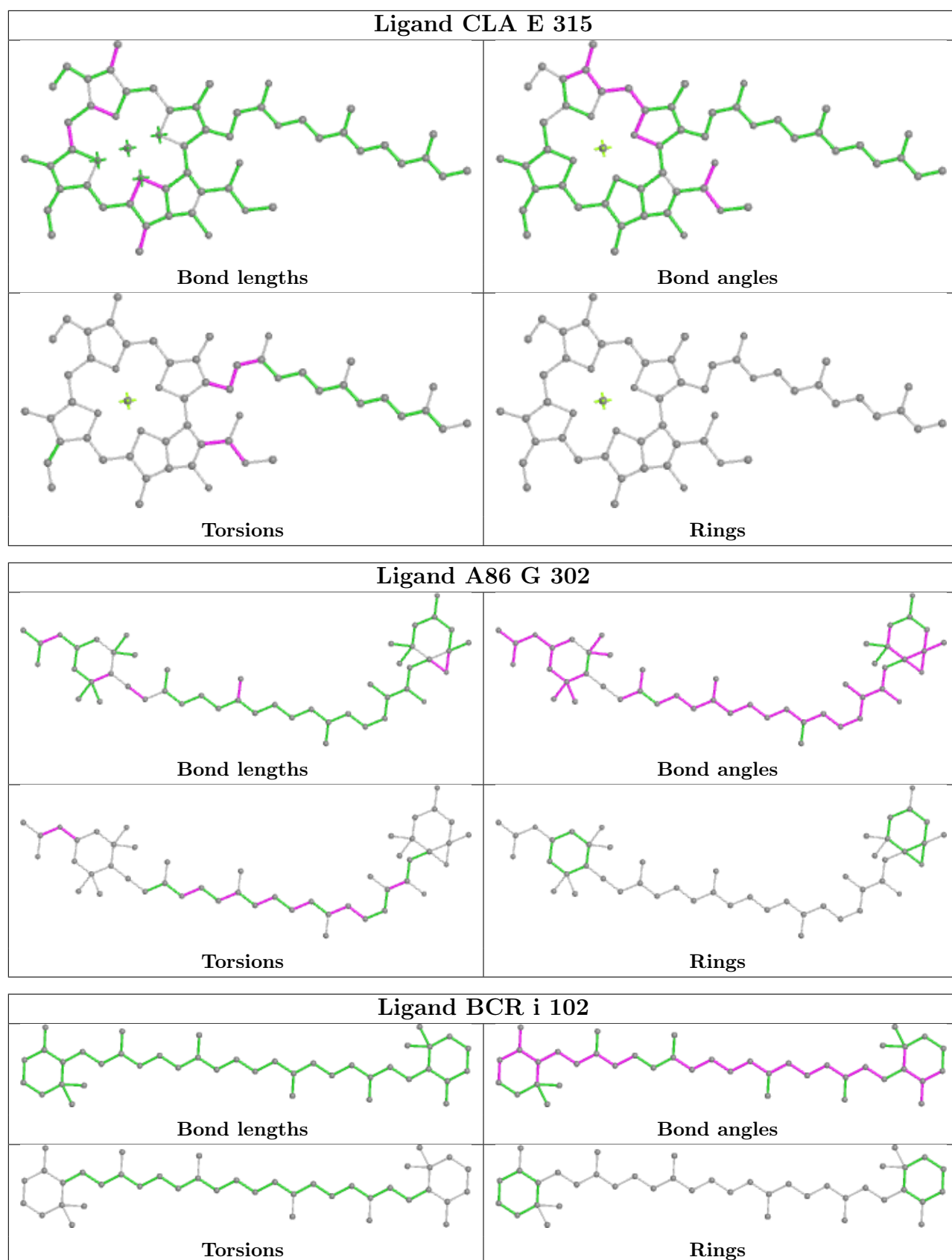
Ligand CLA K 309



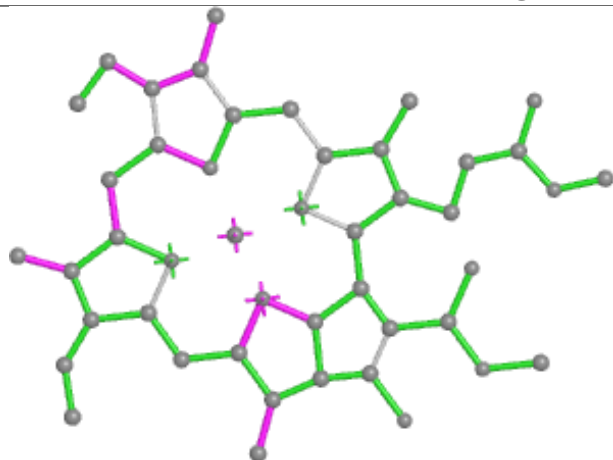


Ligand CLA a 808**Ligand A86 F 301**

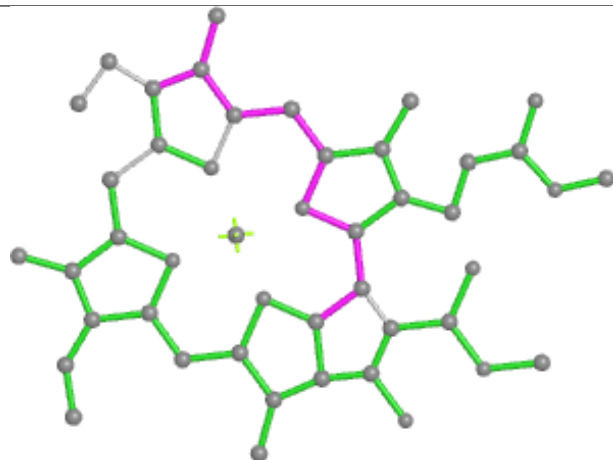




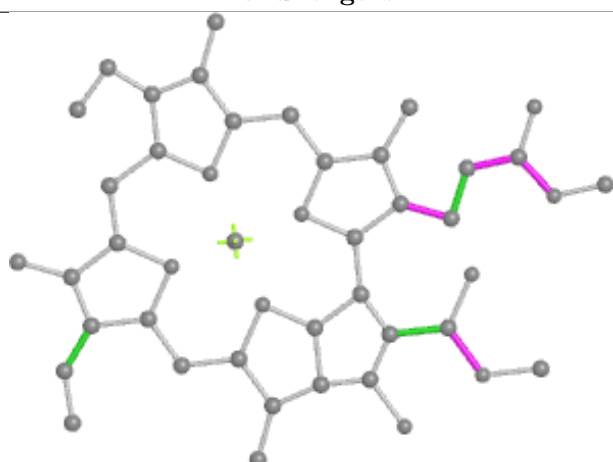
Ligand CLA K 319



Bond lengths



Bond angles

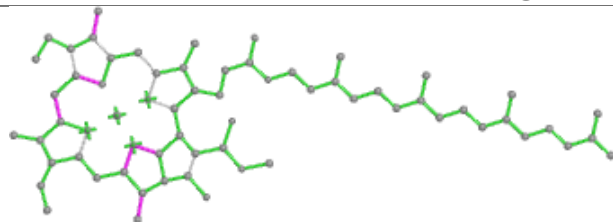


Torsions

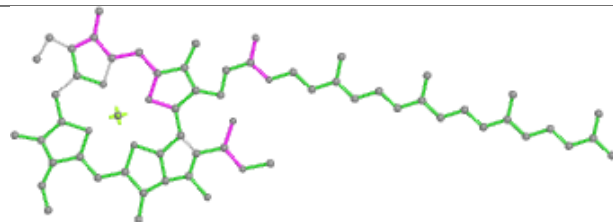


Rings

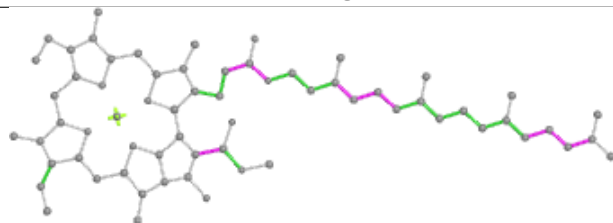
Ligand CLA b 847



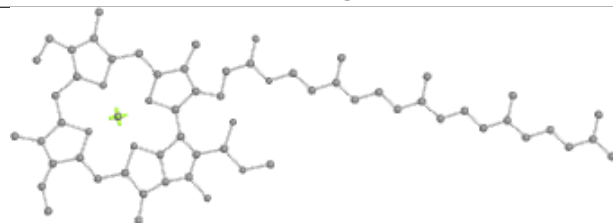
Bond lengths



Bond angles

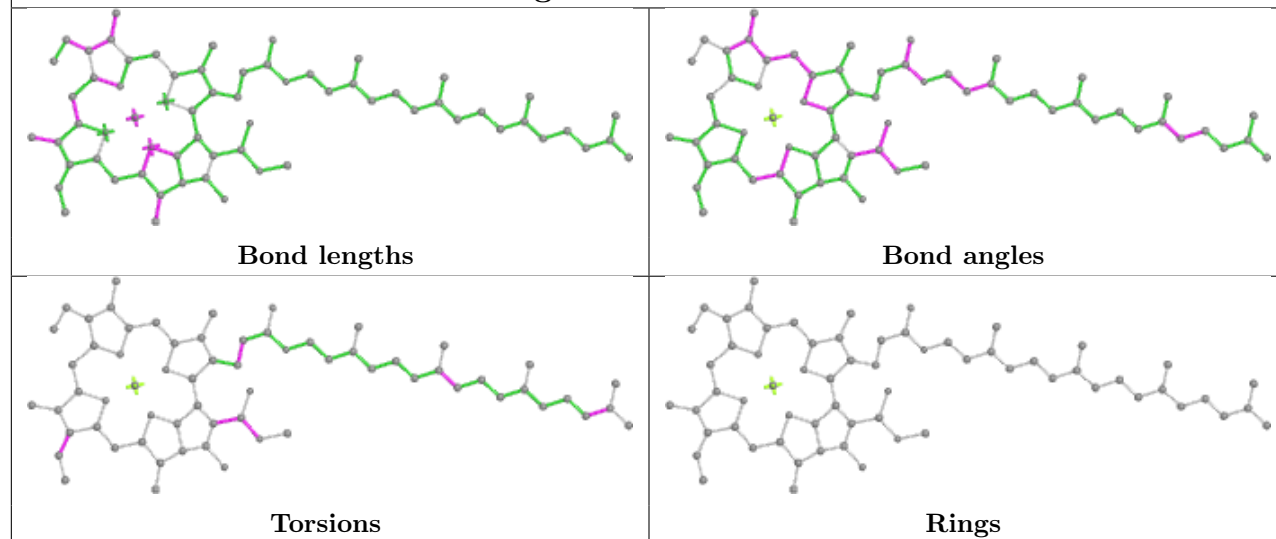


Torsions

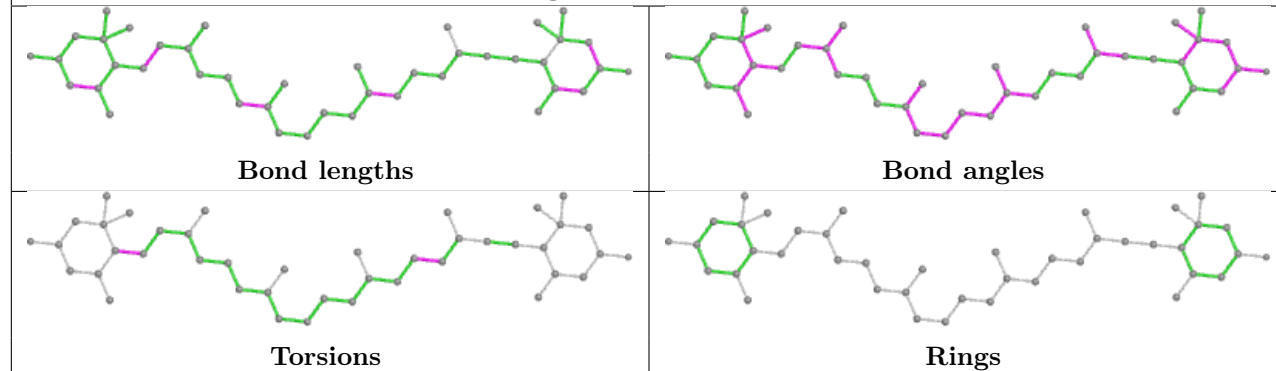


Rings

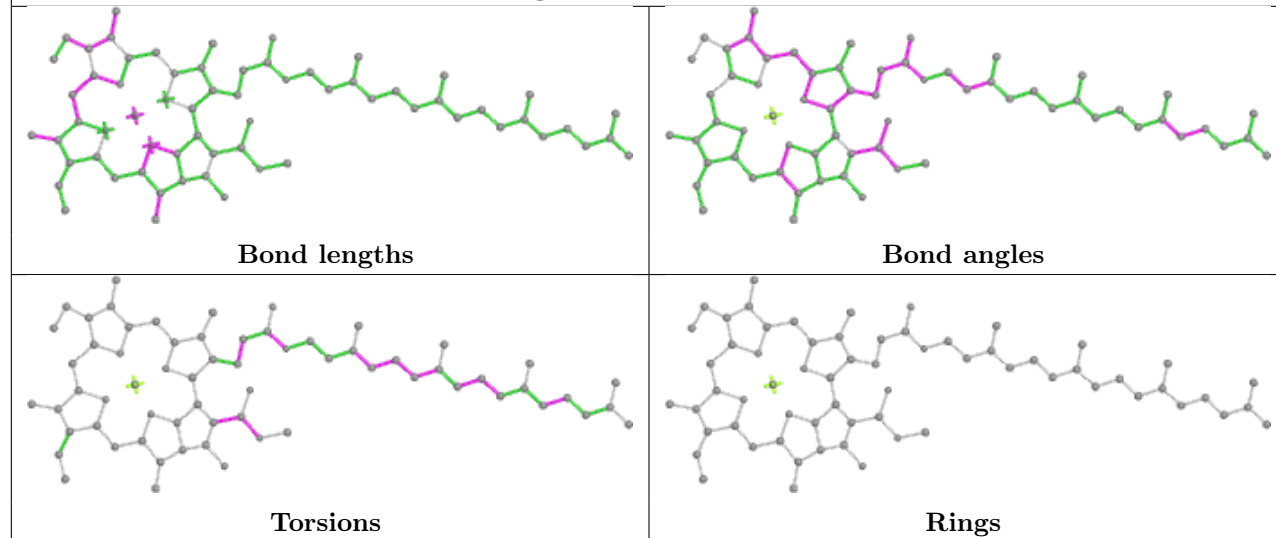
Ligand CLA L 308



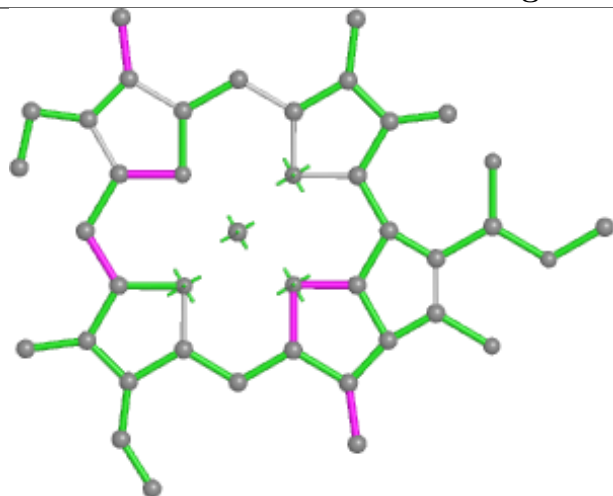
Ligand ET4 l 207



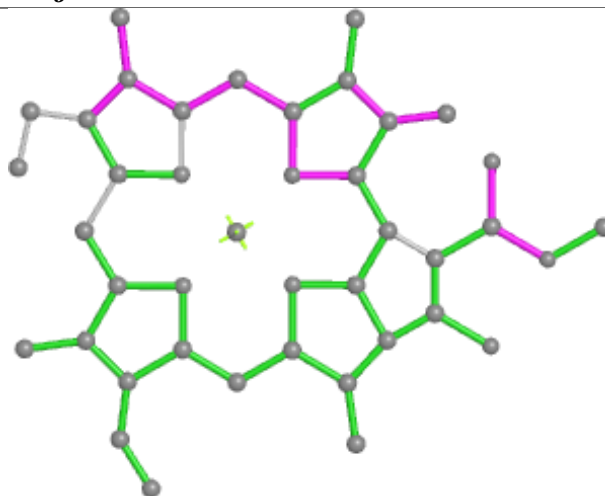
Ligand CLA H 206



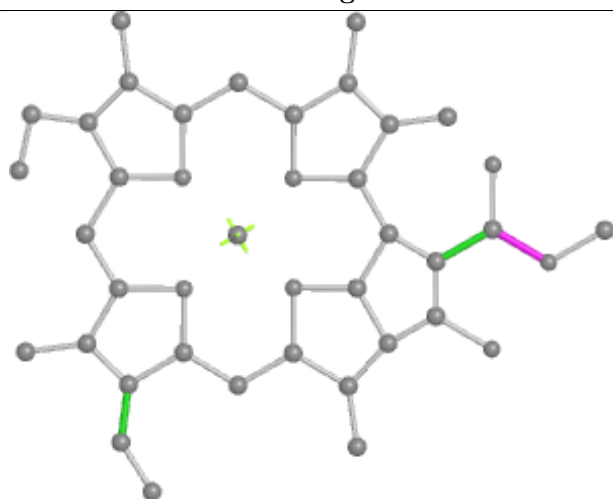
Ligand CLA j 104



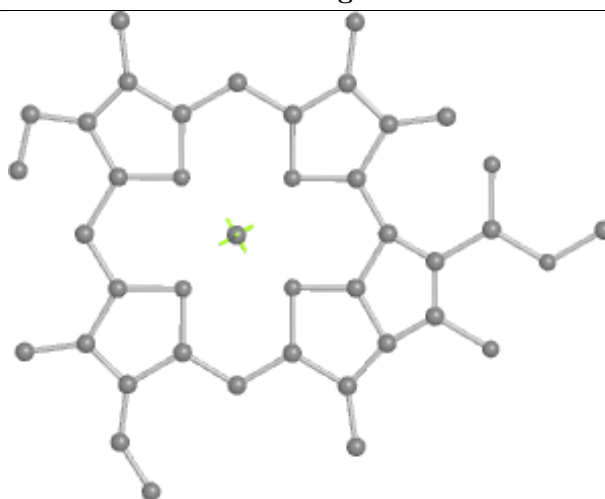
Bond lengths



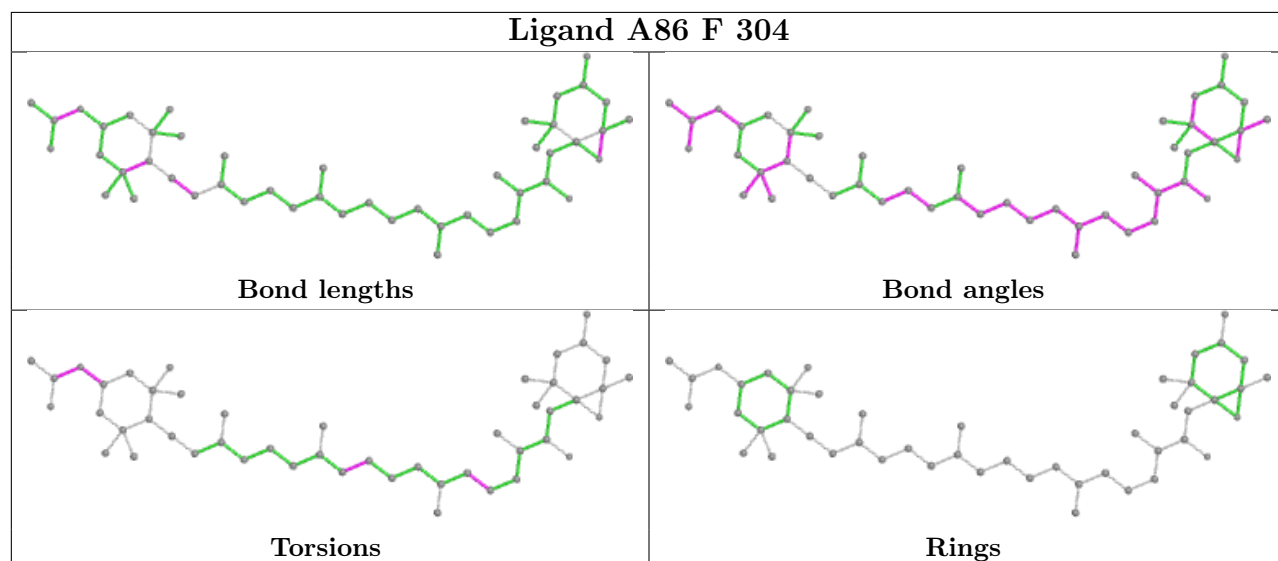
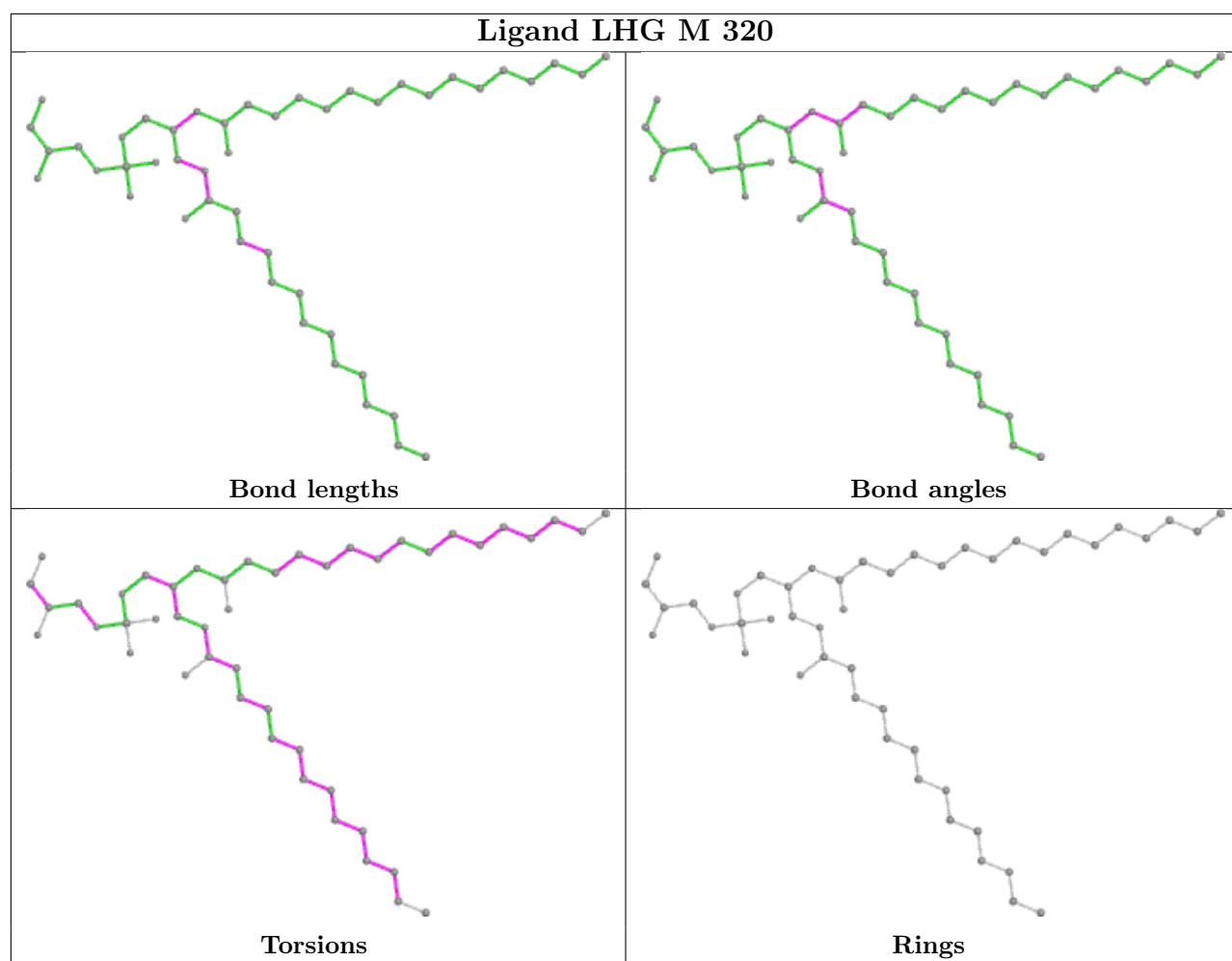
Bond angles

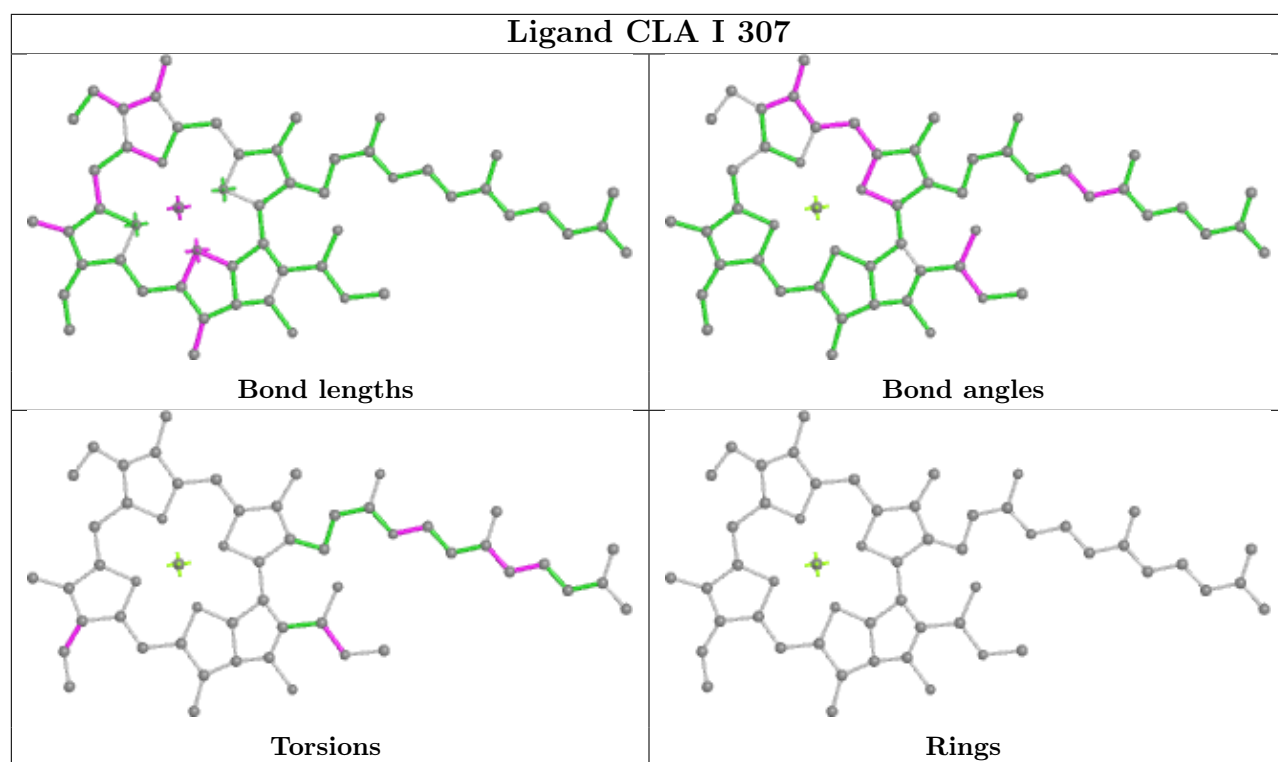


Torsions

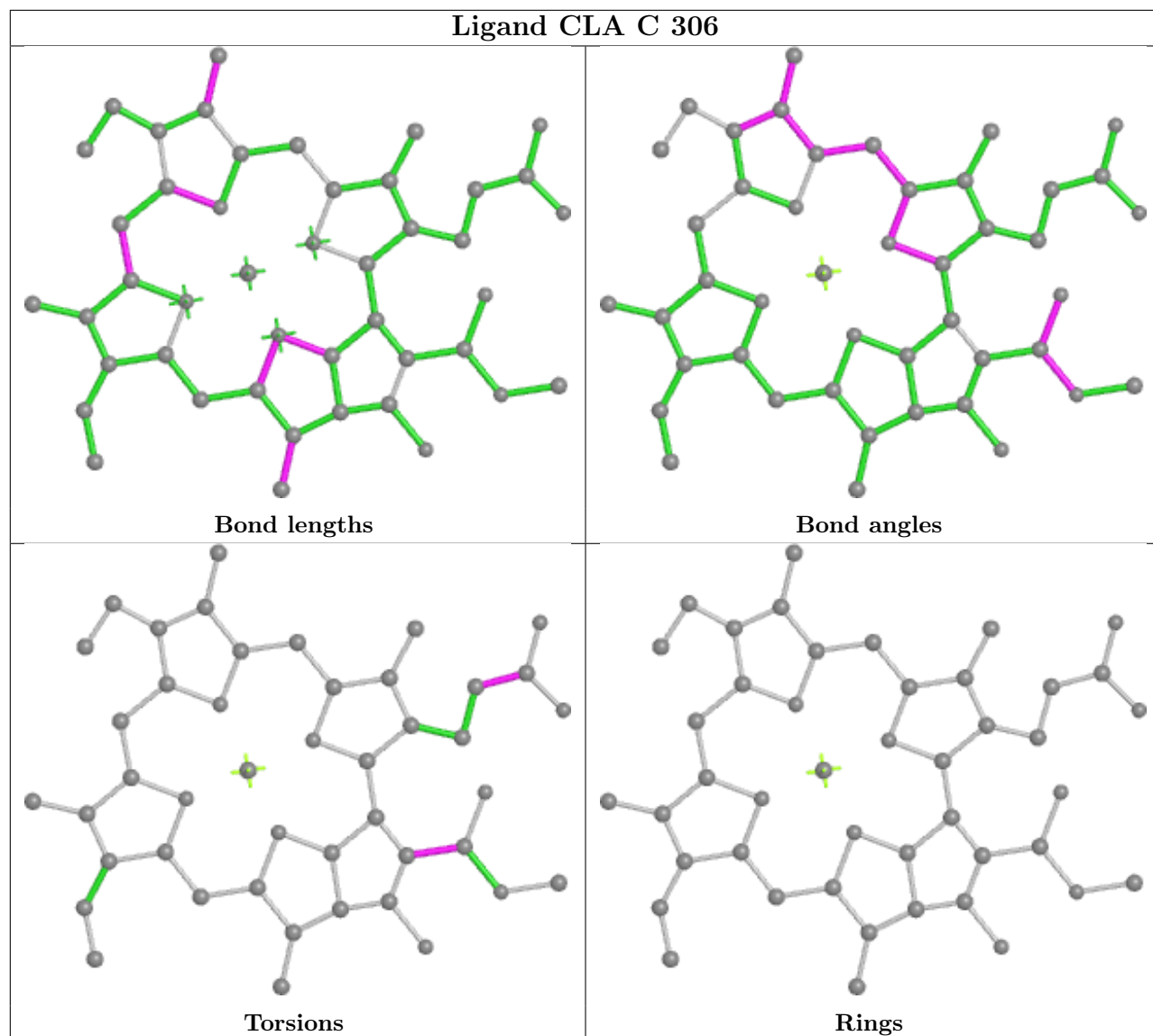


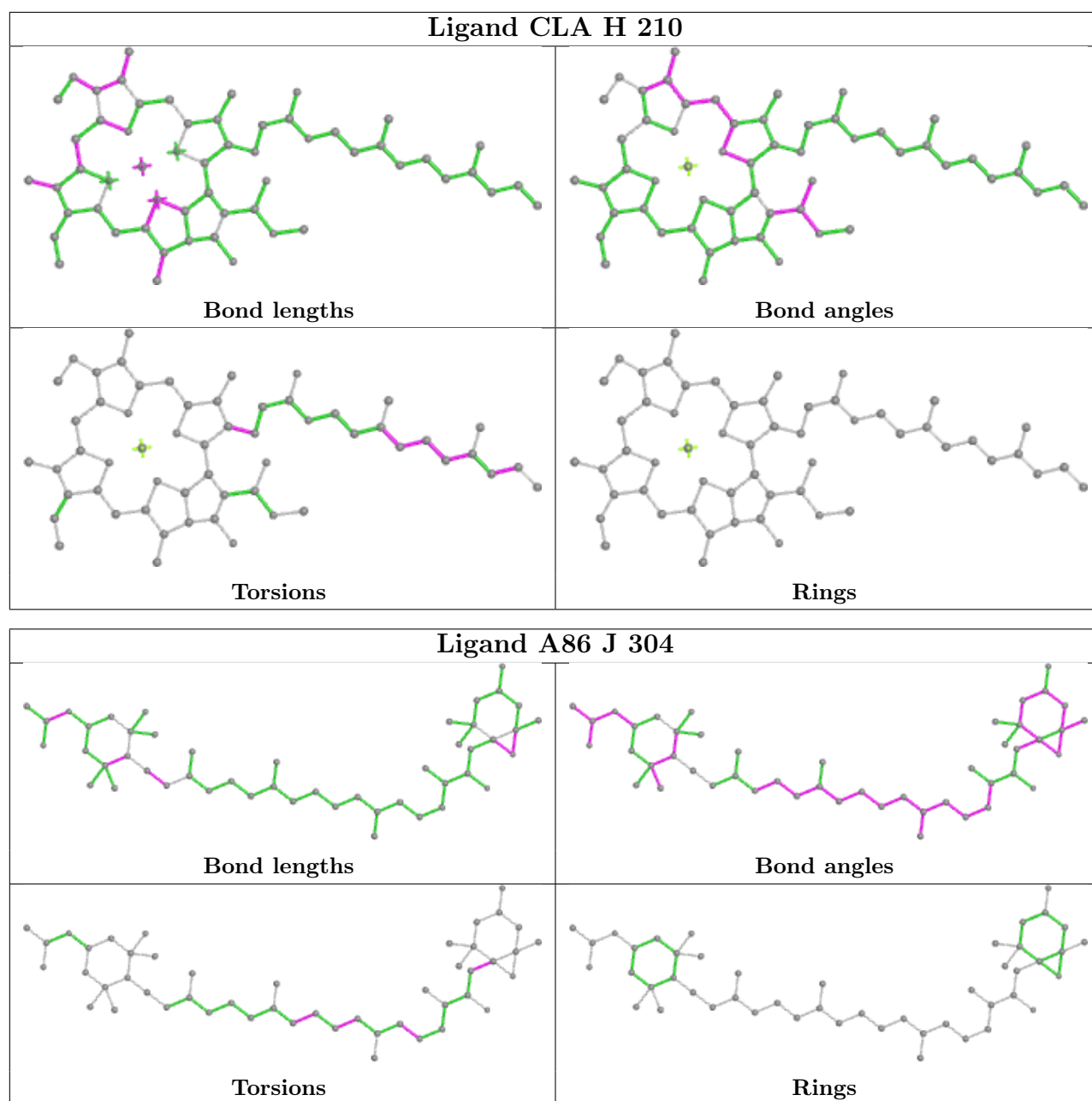
Rings

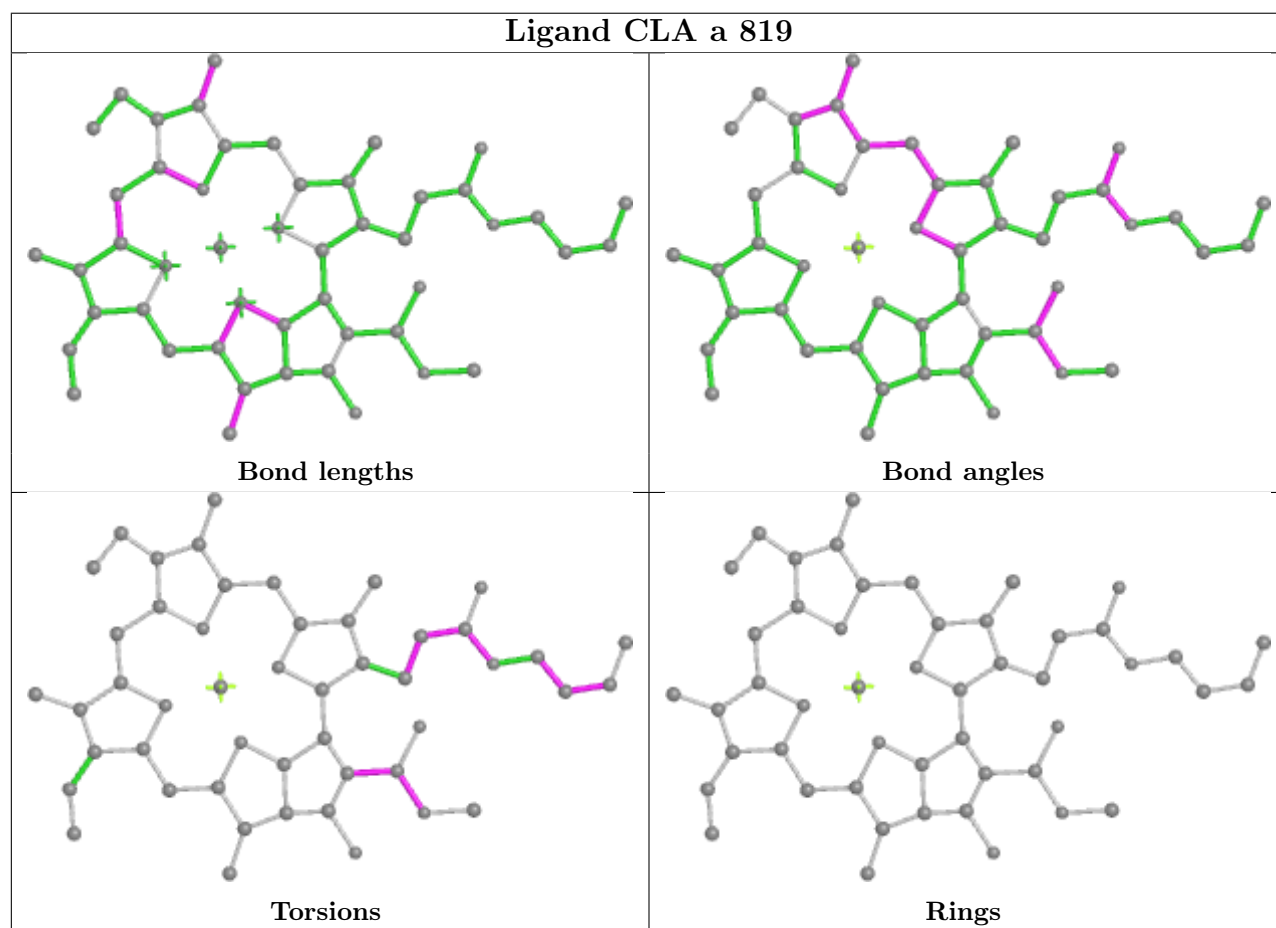
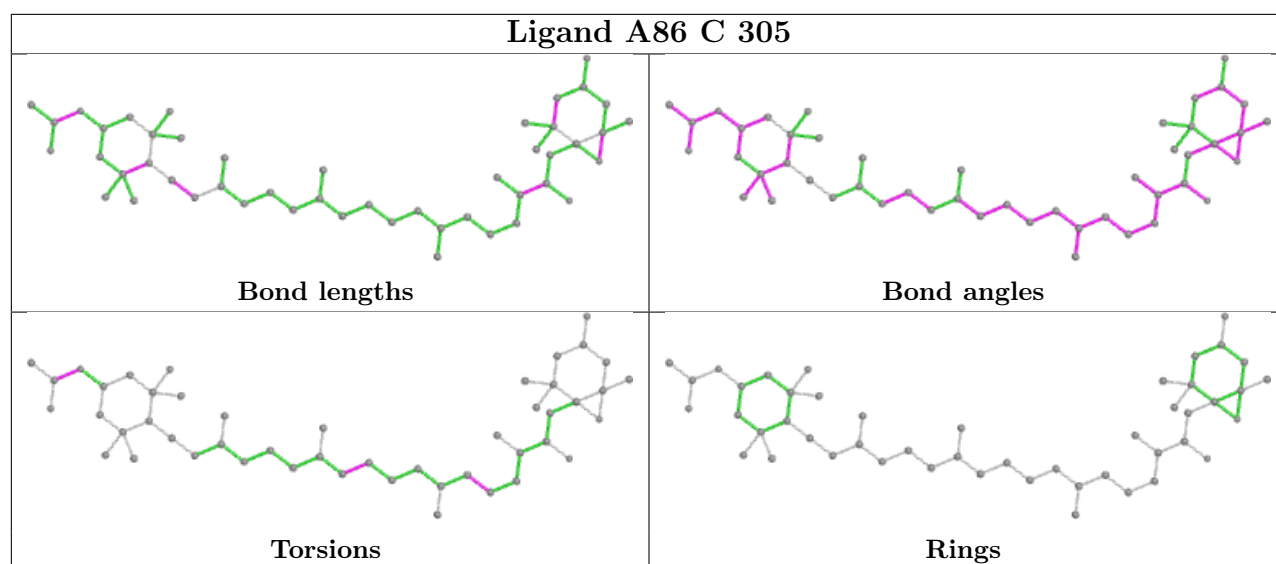


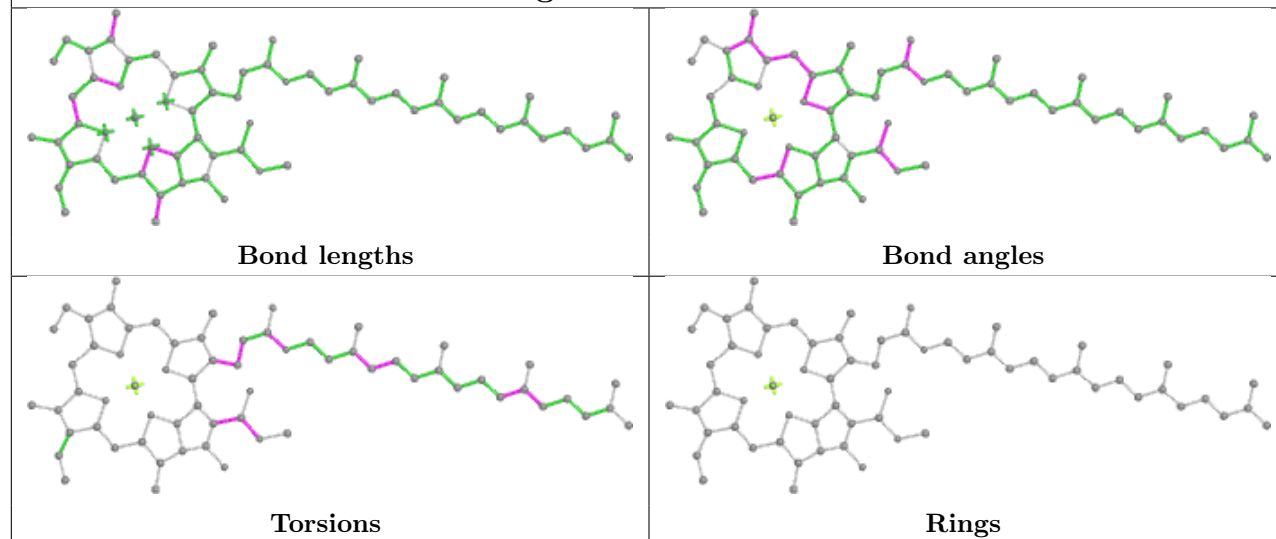
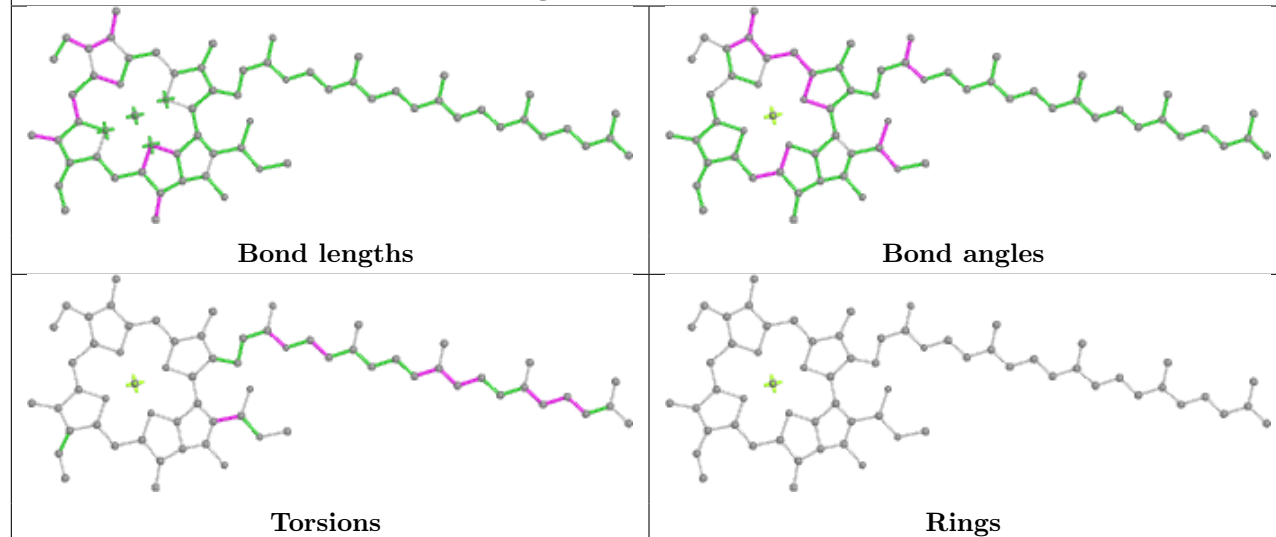
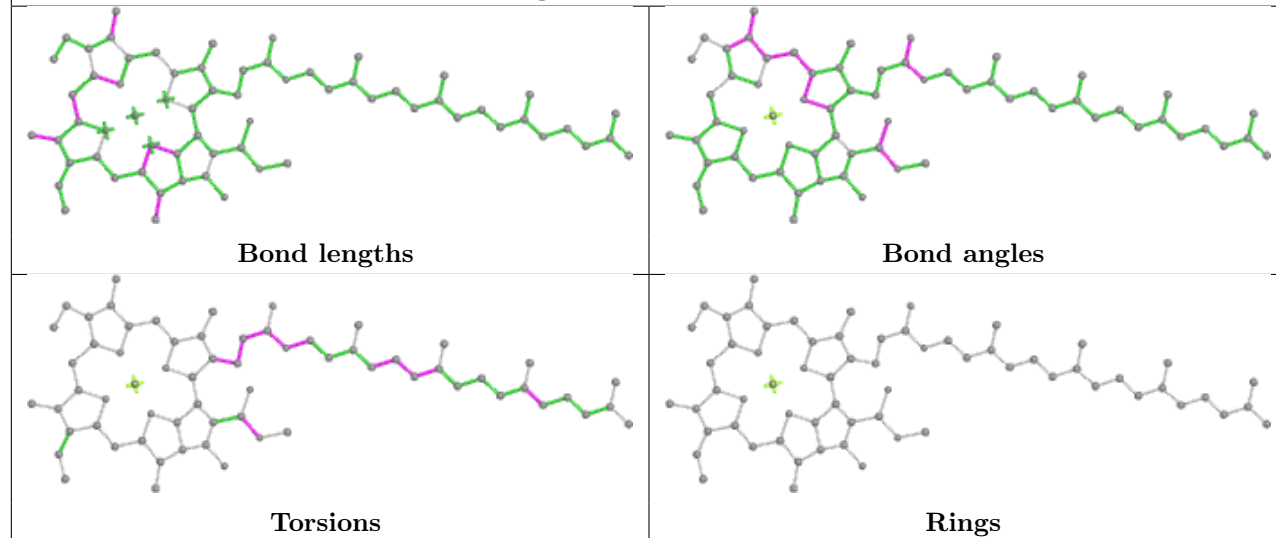


Ligand CLA C 306

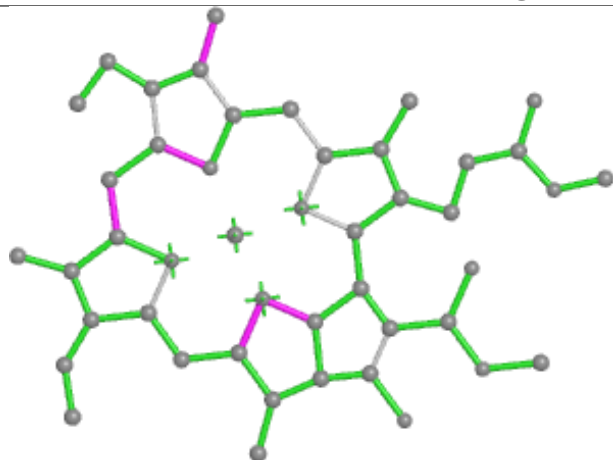




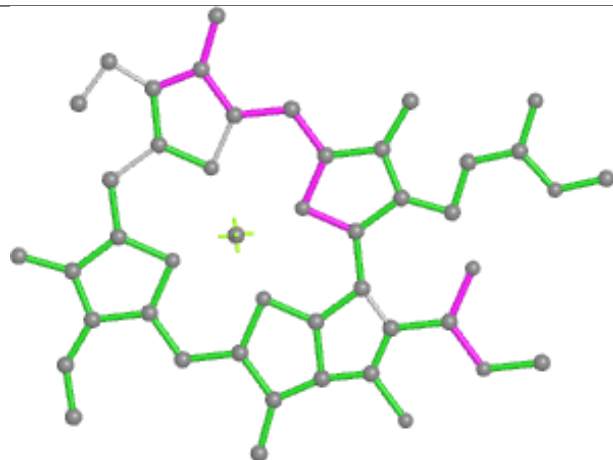


Ligand CLA a 846**Ligand CLA L 310****Ligand CLA E 308**

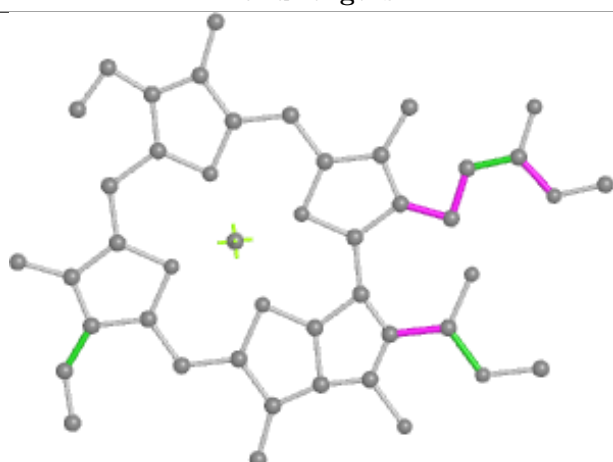
Ligand CLA G 310



Bond lengths



Bond angles

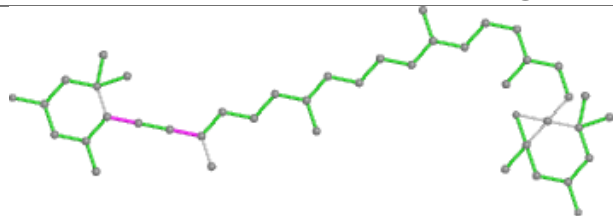


Torsions

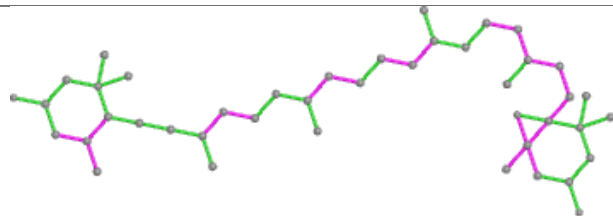


Rings

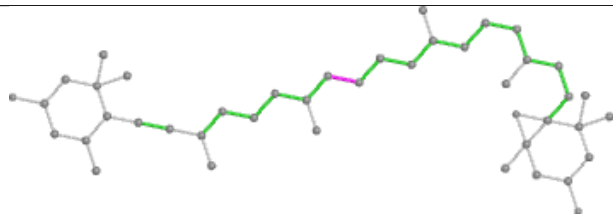
Ligand DD6 F 302



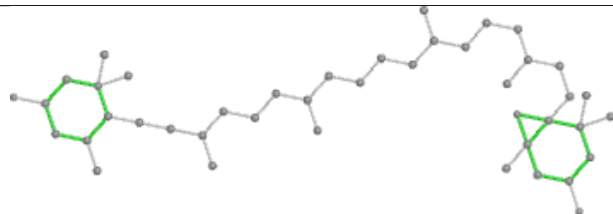
Bond lengths



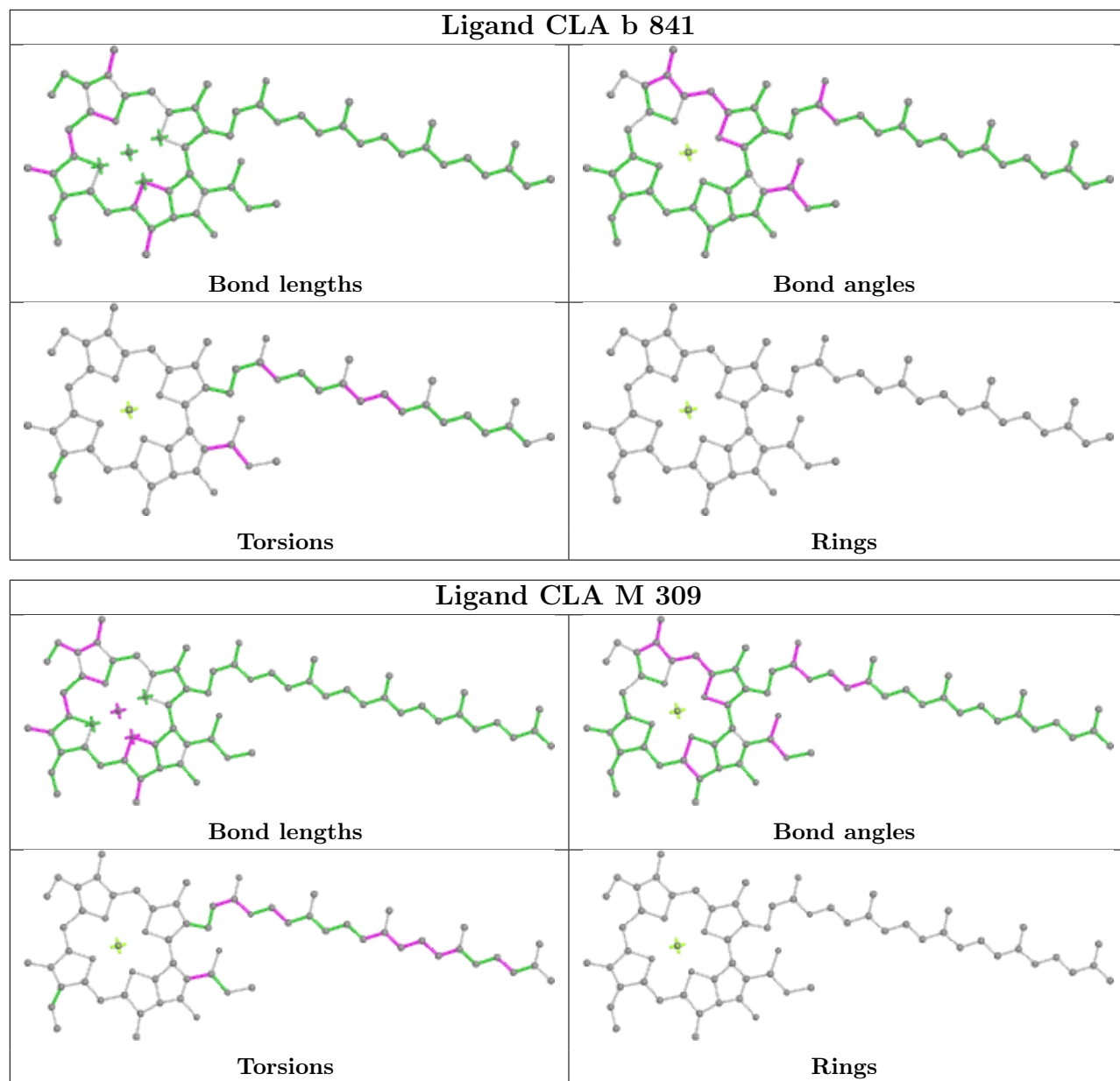
Bond angles



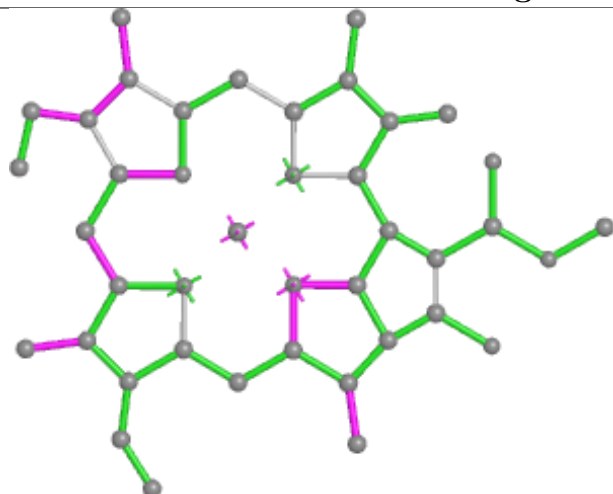
Torsions



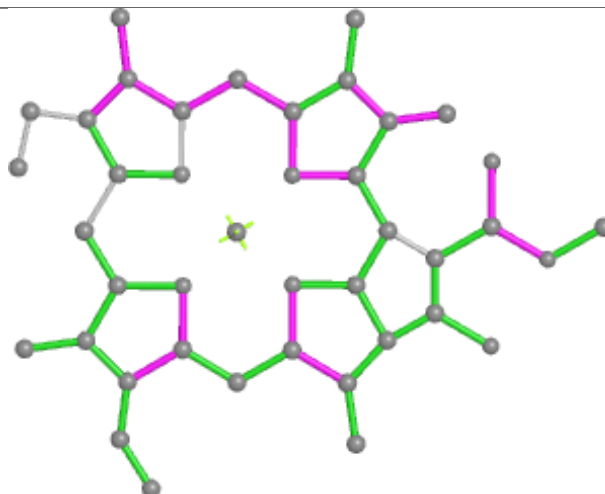
Rings



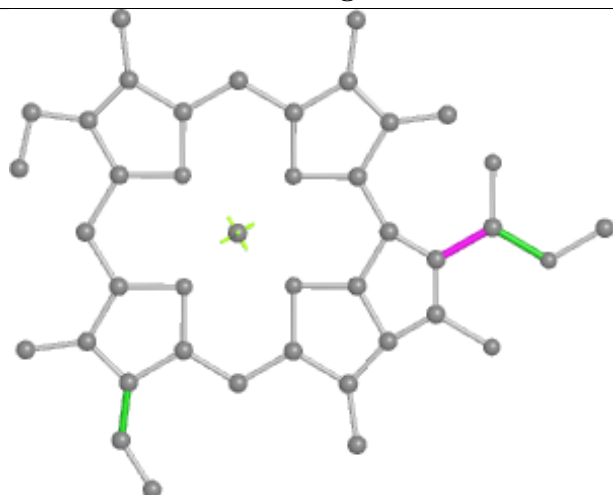
Ligand CLA C 316



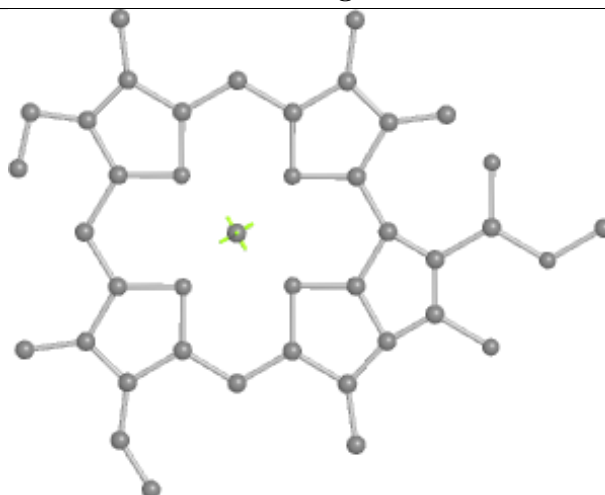
Bond lengths



Bond angles

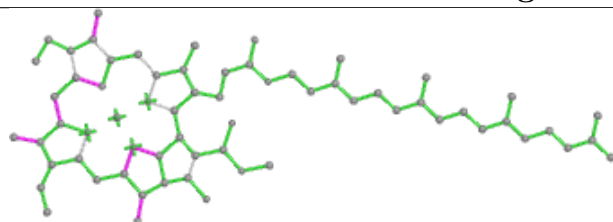


Torsions

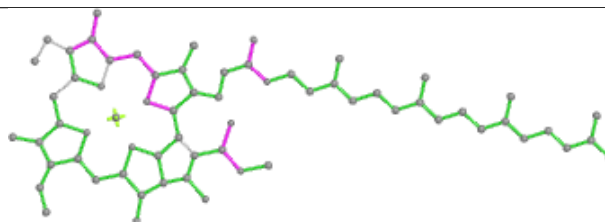


Rings

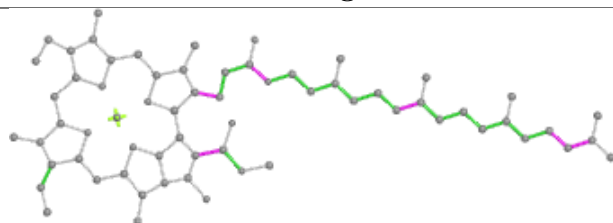
Ligand CLA b 811



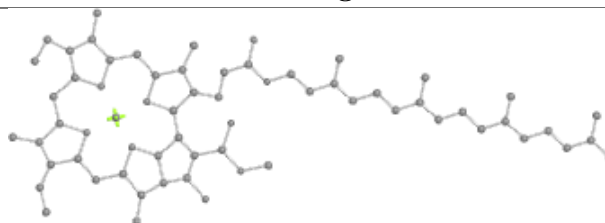
Bond lengths



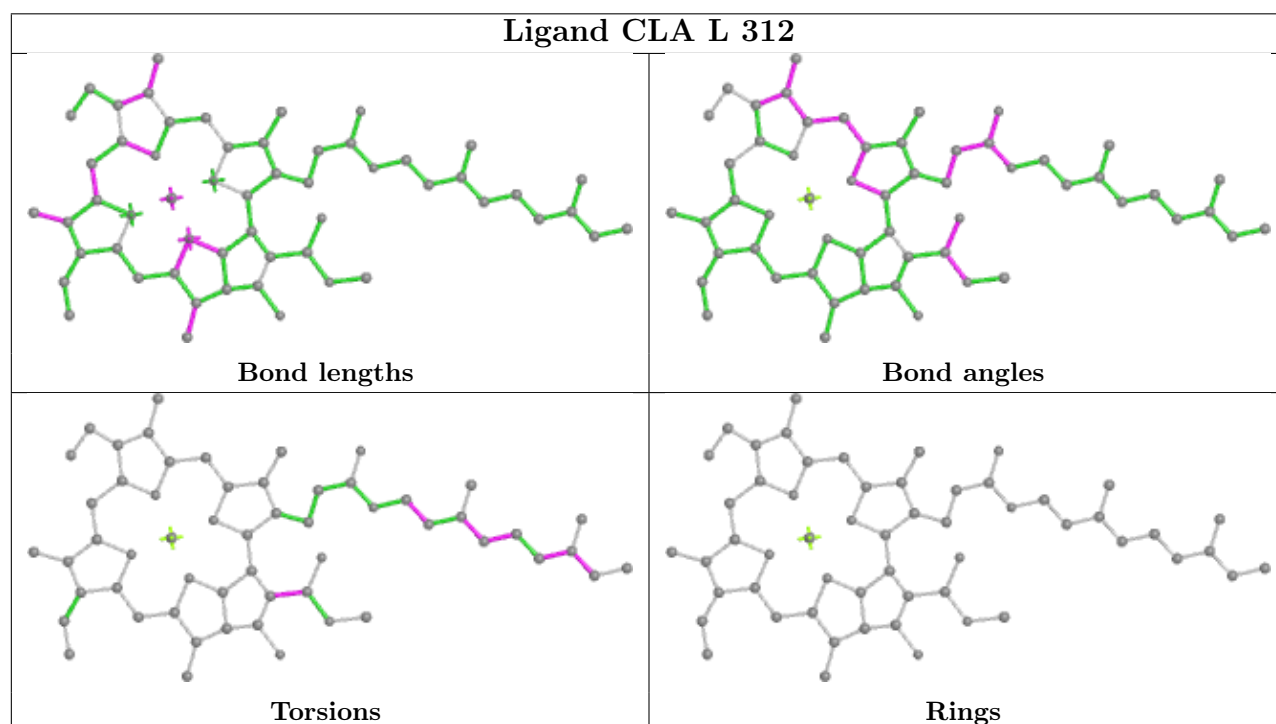
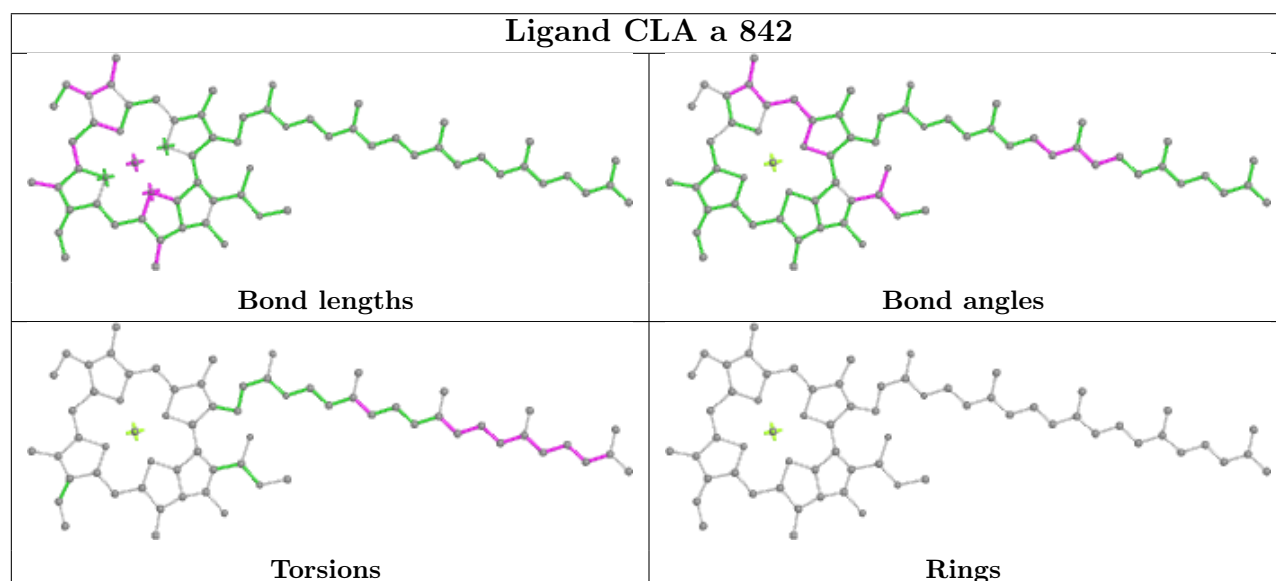
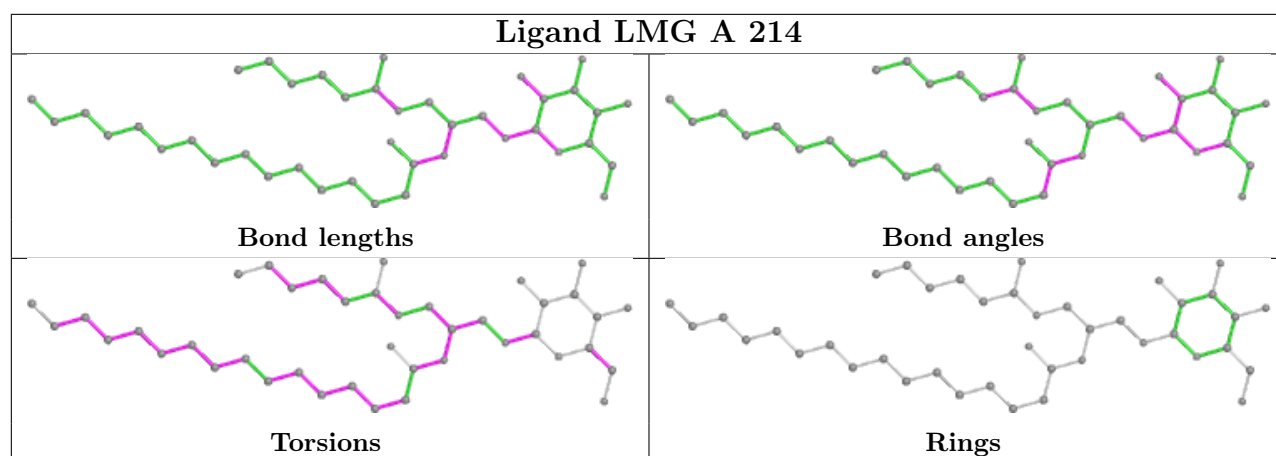
Bond angles



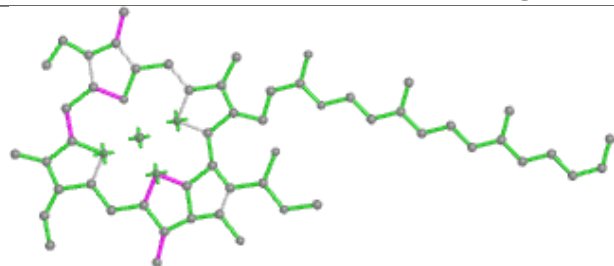
Torsions



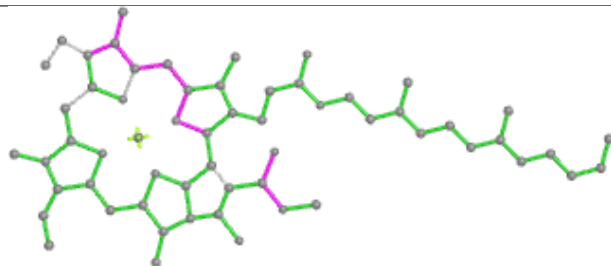
Rings



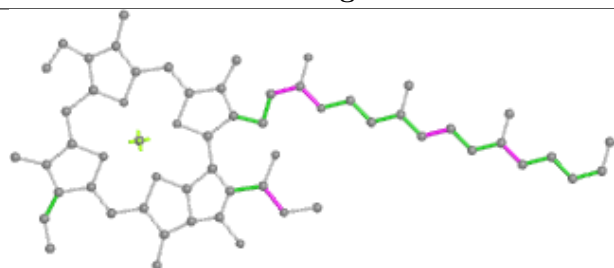
Ligand CLA F 307



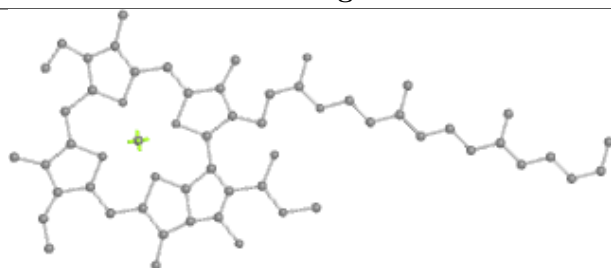
Bond lengths



Bond angles

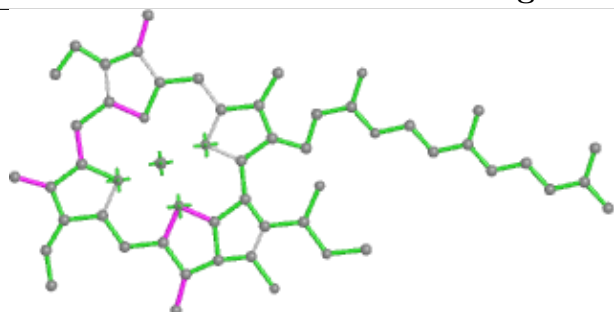


Torsions

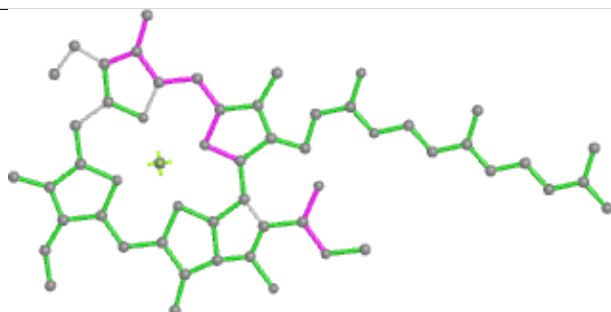


Rings

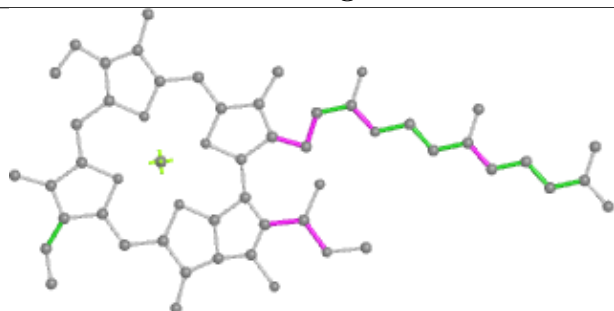
Ligand CLA b 814



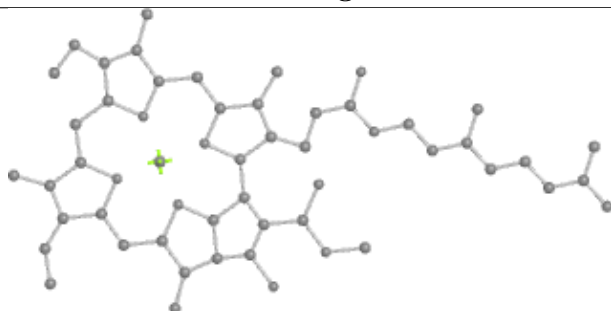
Bond lengths



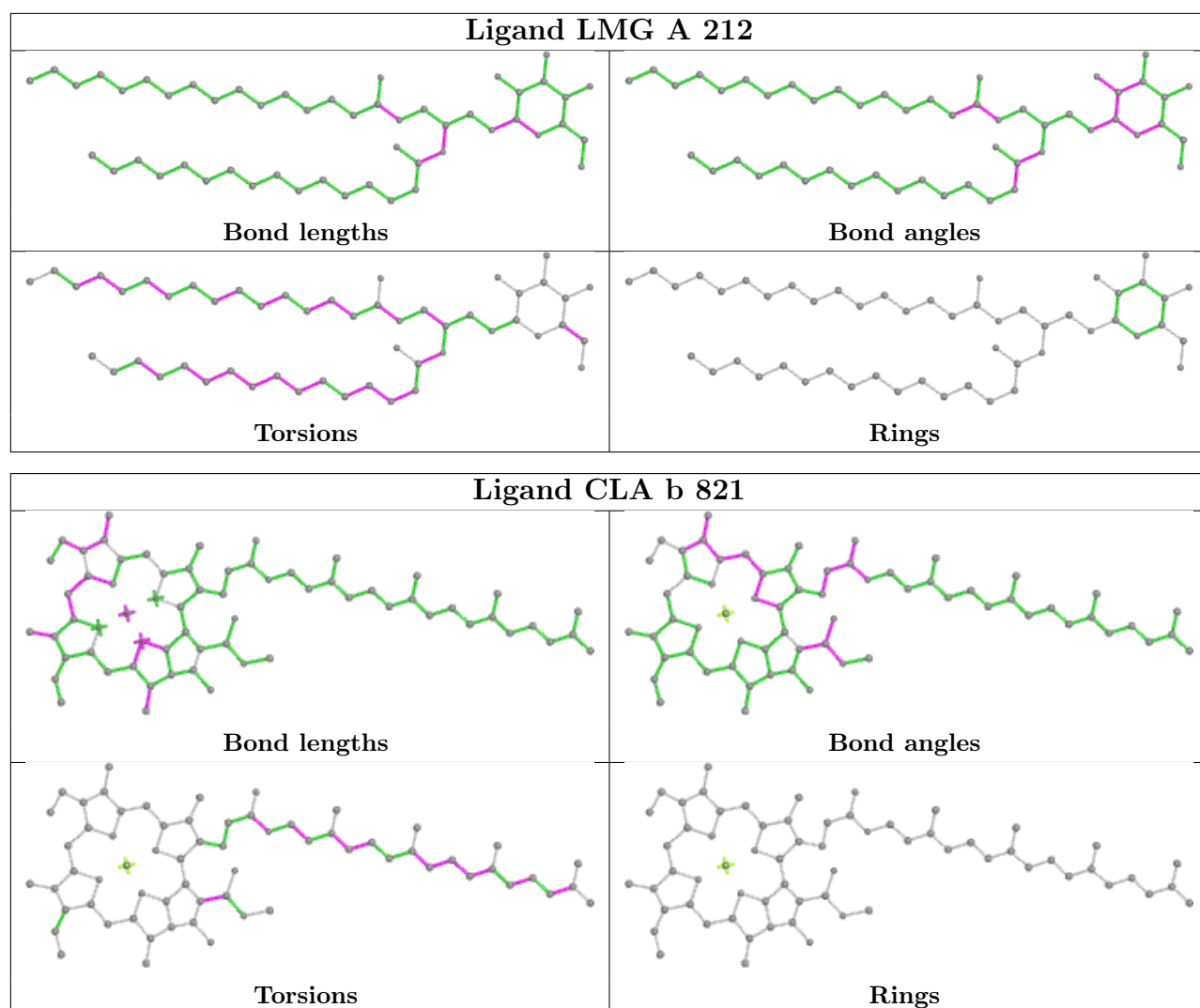
Bond angles



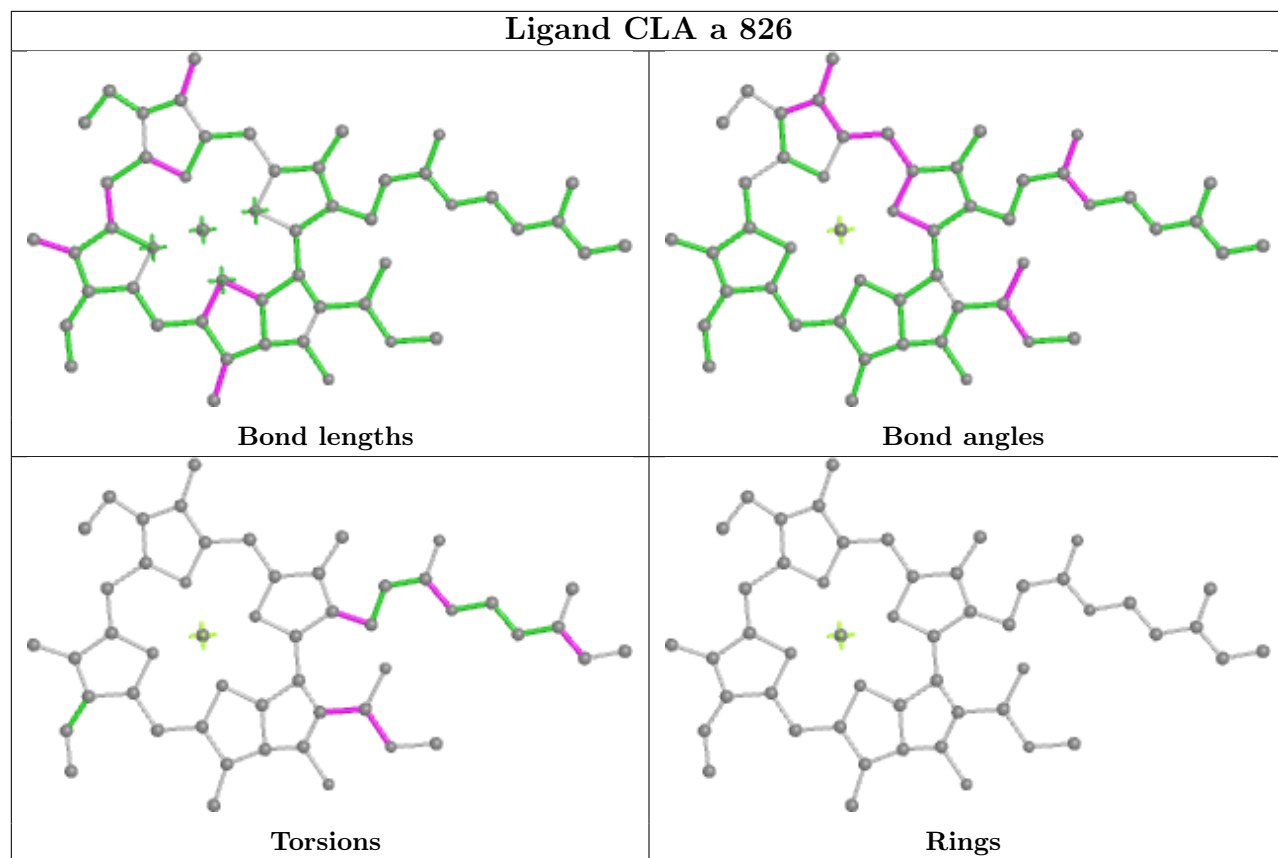
Torsions

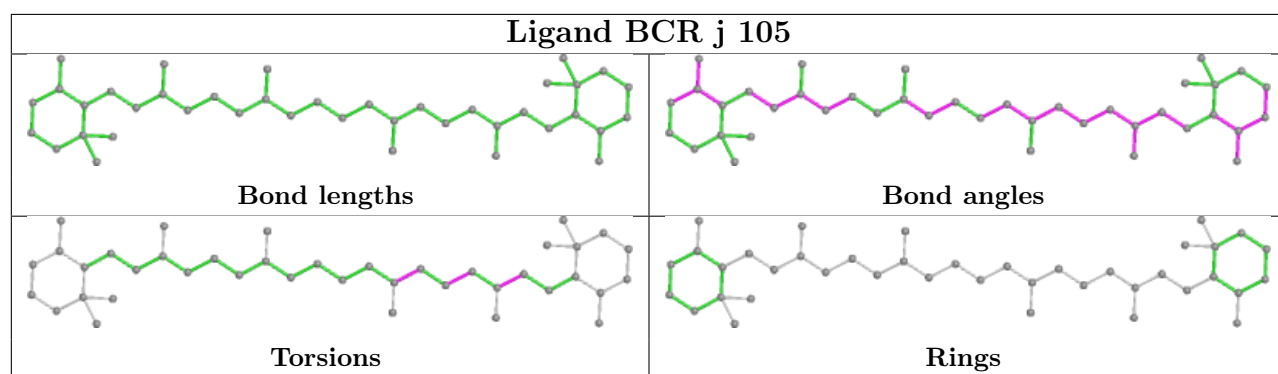
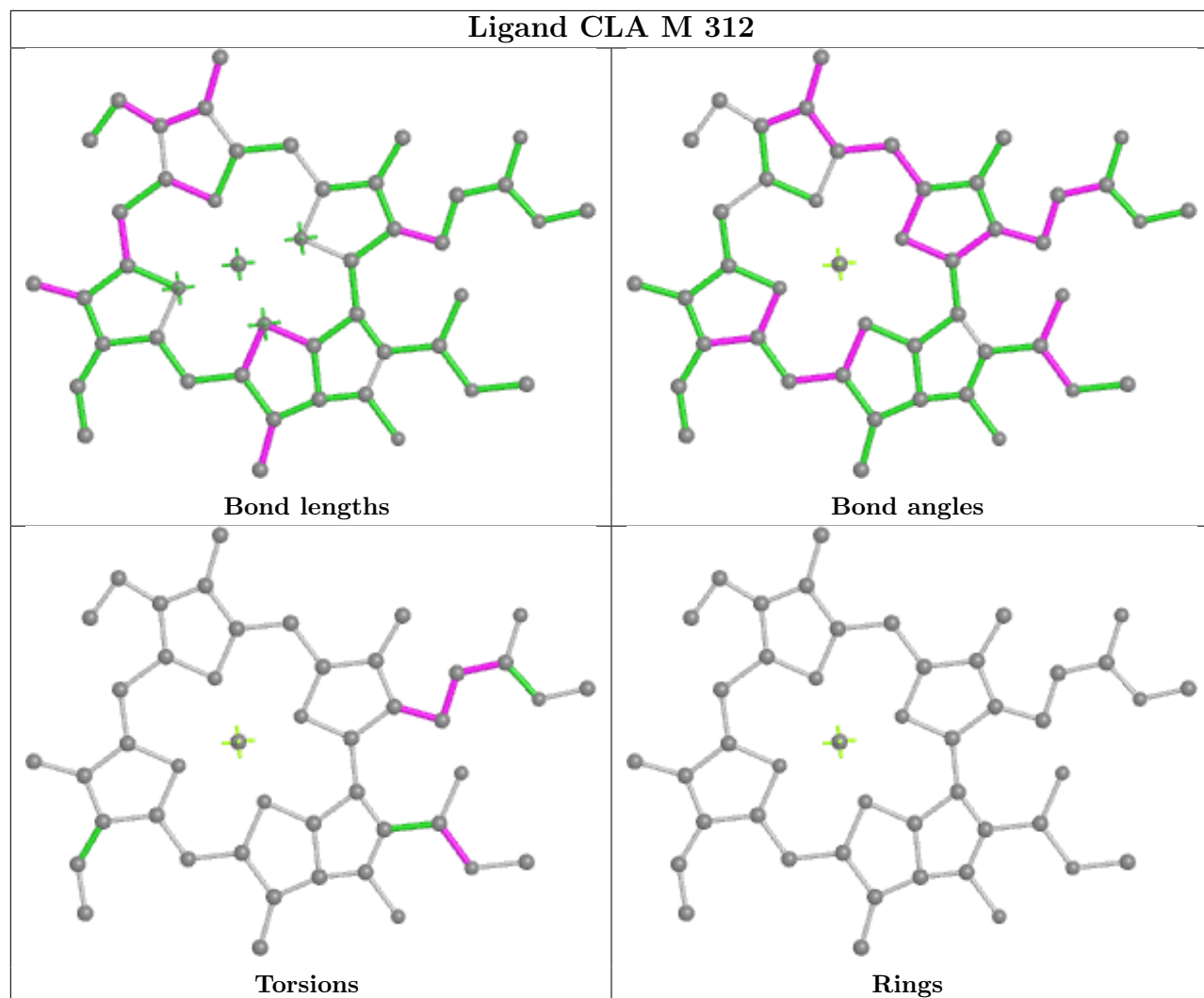


Rings

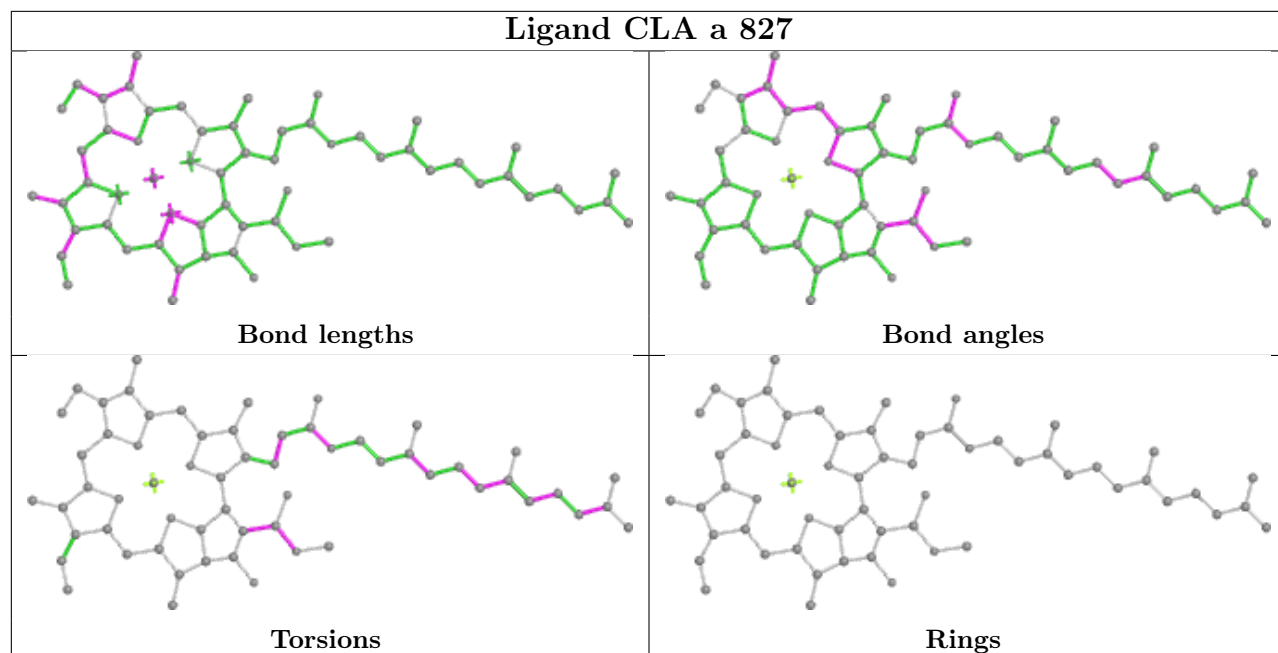


Ligand CLA a 826

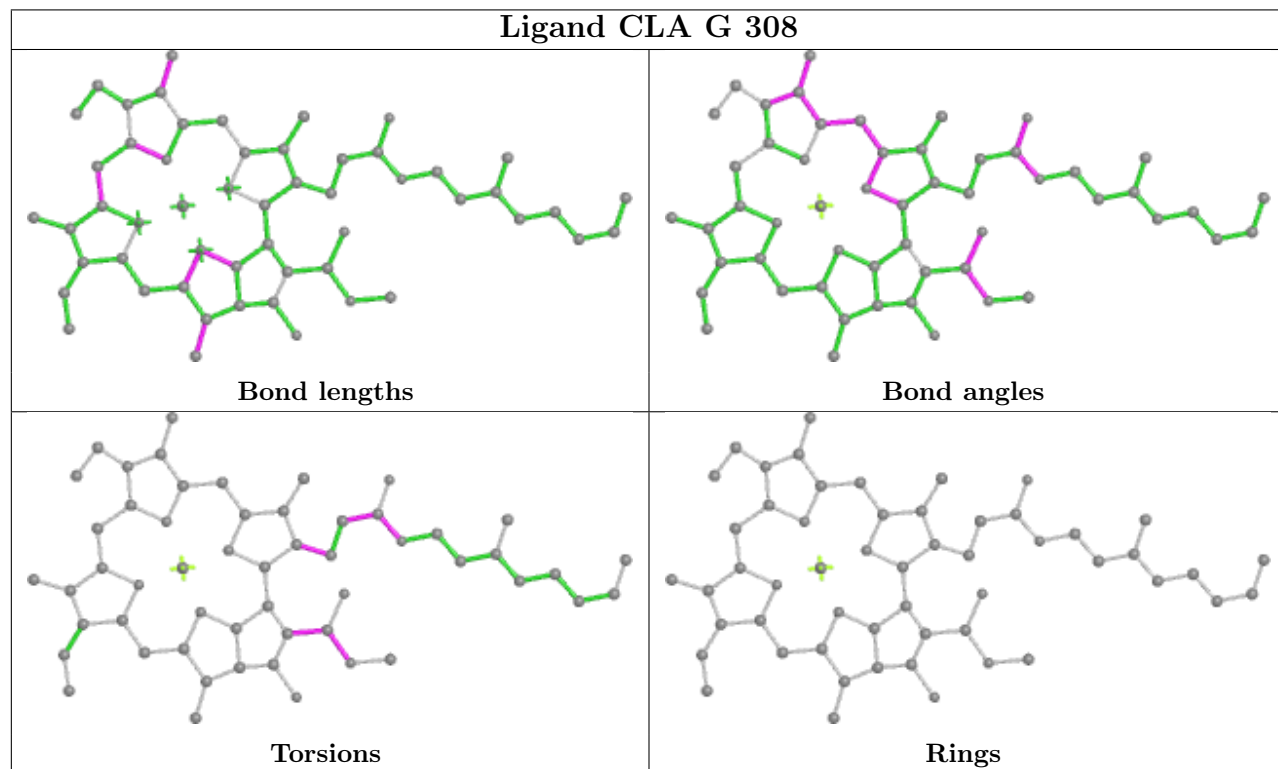


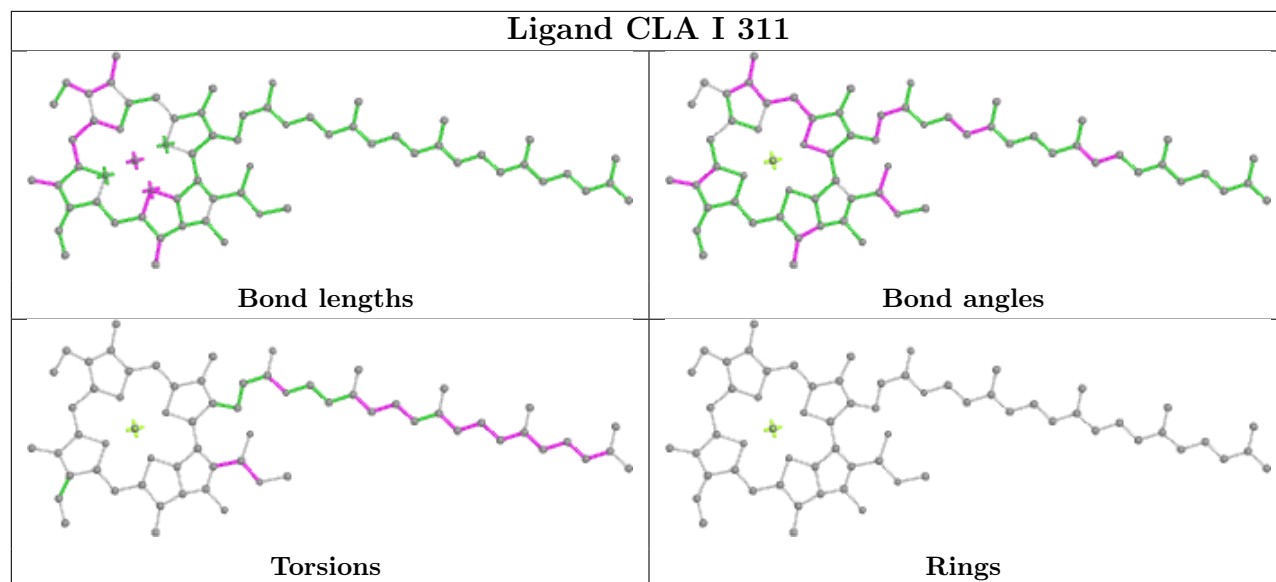
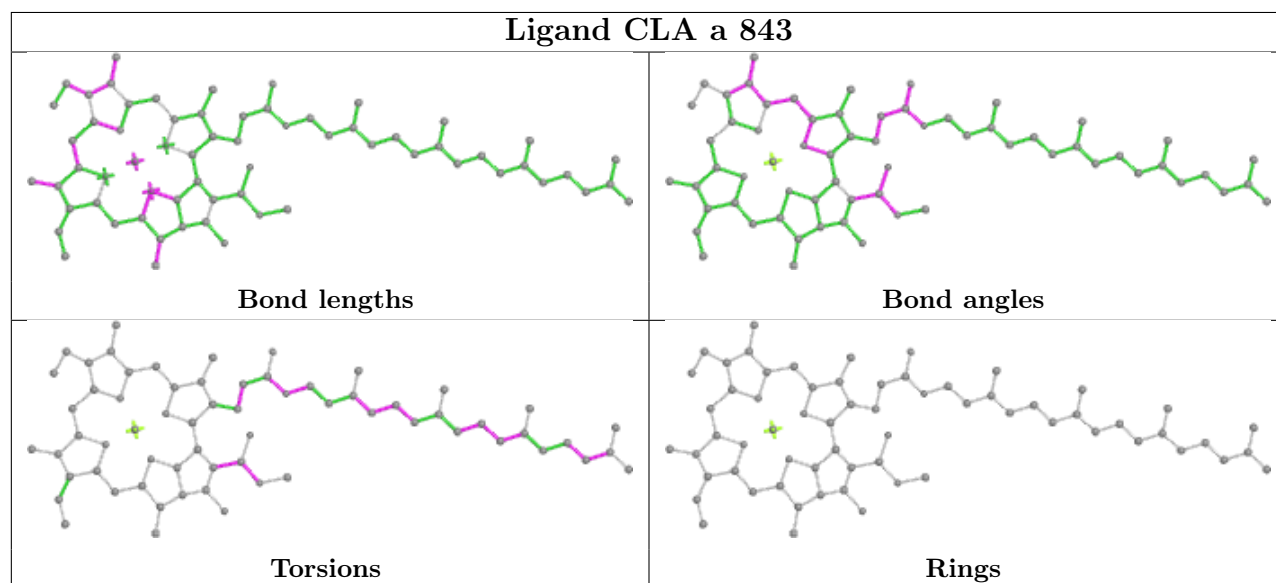


Ligand CLA a 827

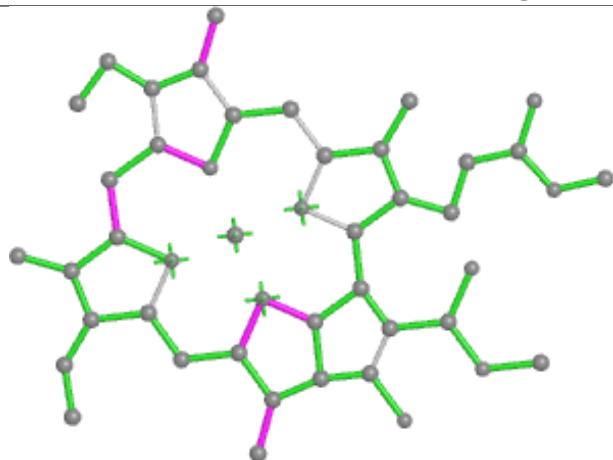


Ligand CLA G 308

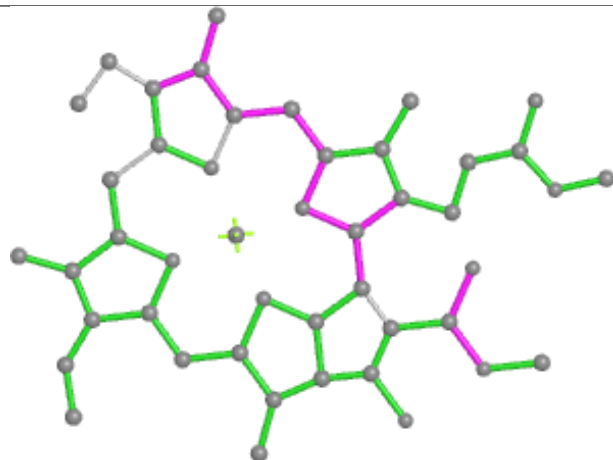


Ligand CLA I 311**Ligand CLA a 843**

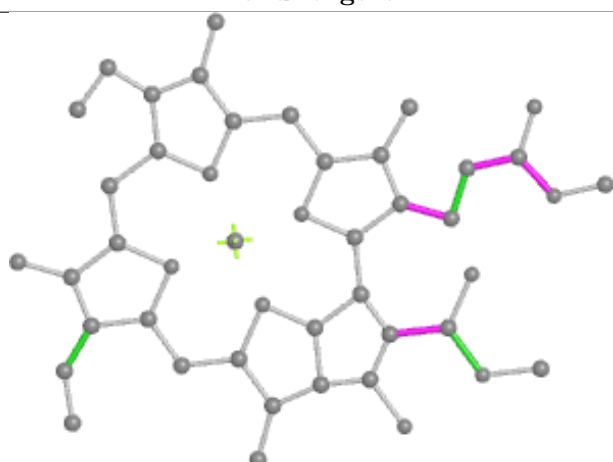
Ligand CLA E 310



Bond lengths



Bond angles

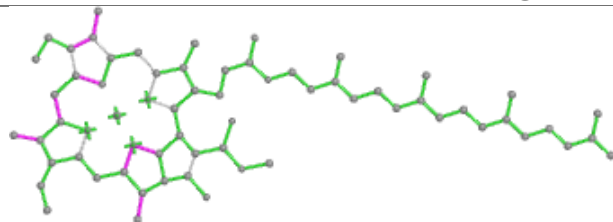


Torsions

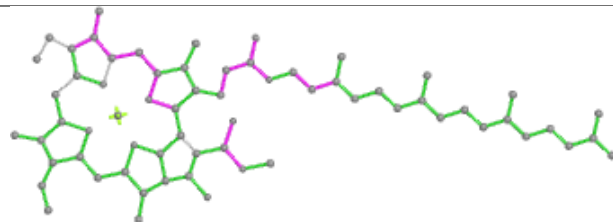


Rings

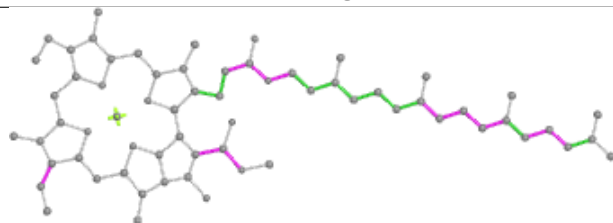
Ligand CLA L 309



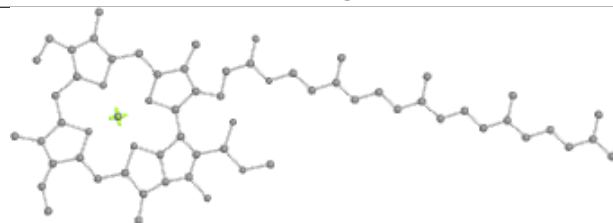
Bond lengths



Bond angles

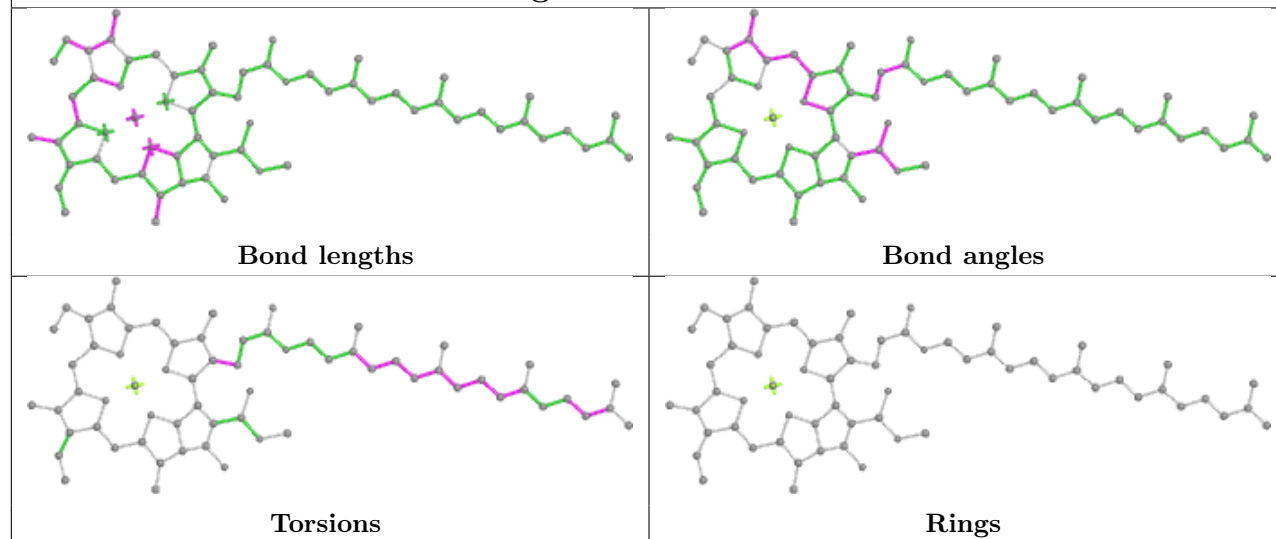


Torsions

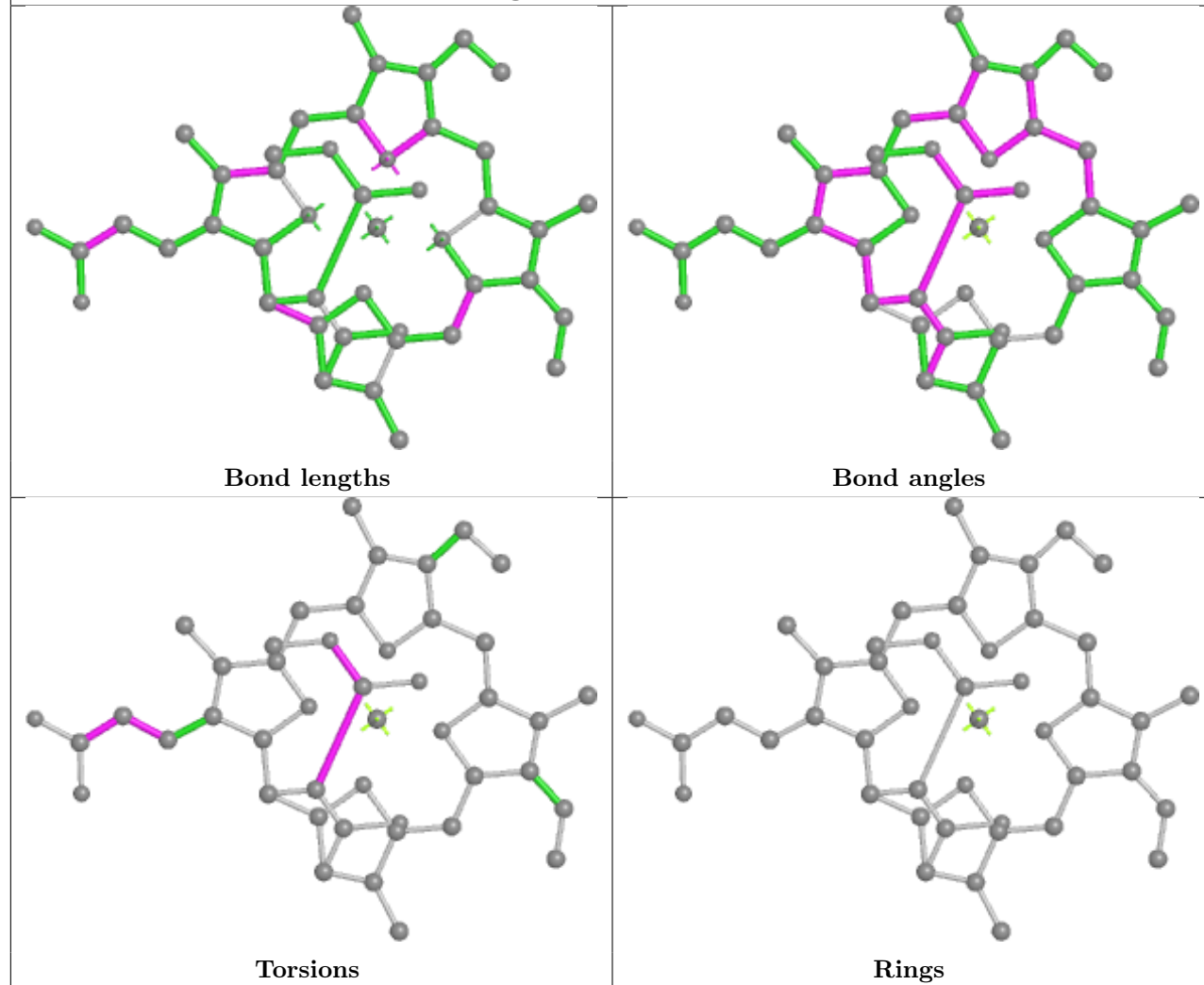


Rings

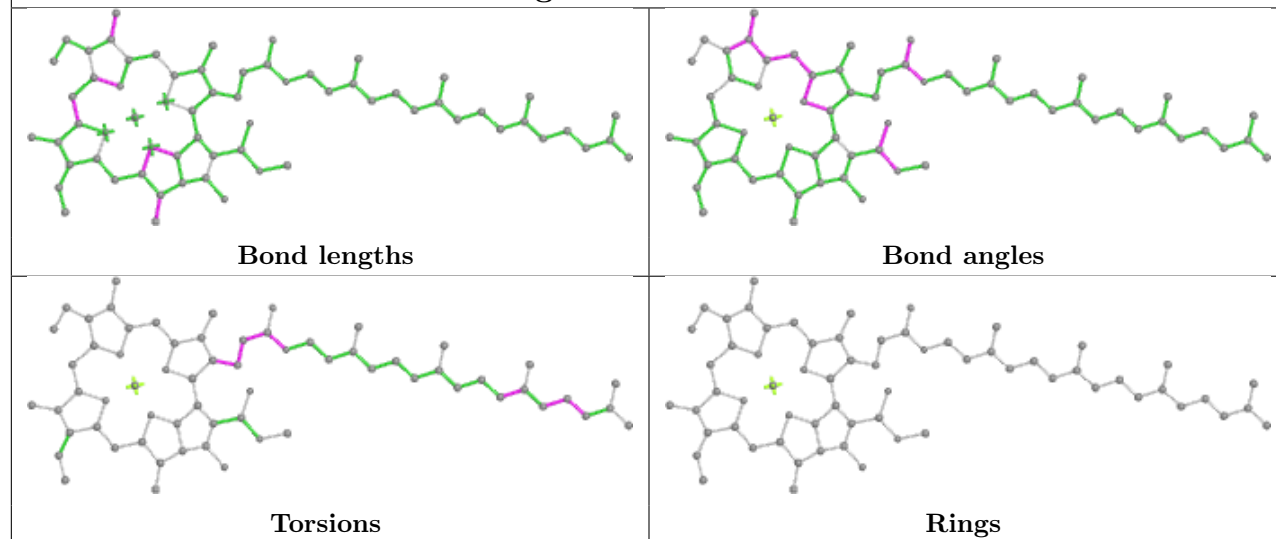
Ligand CLA A 204



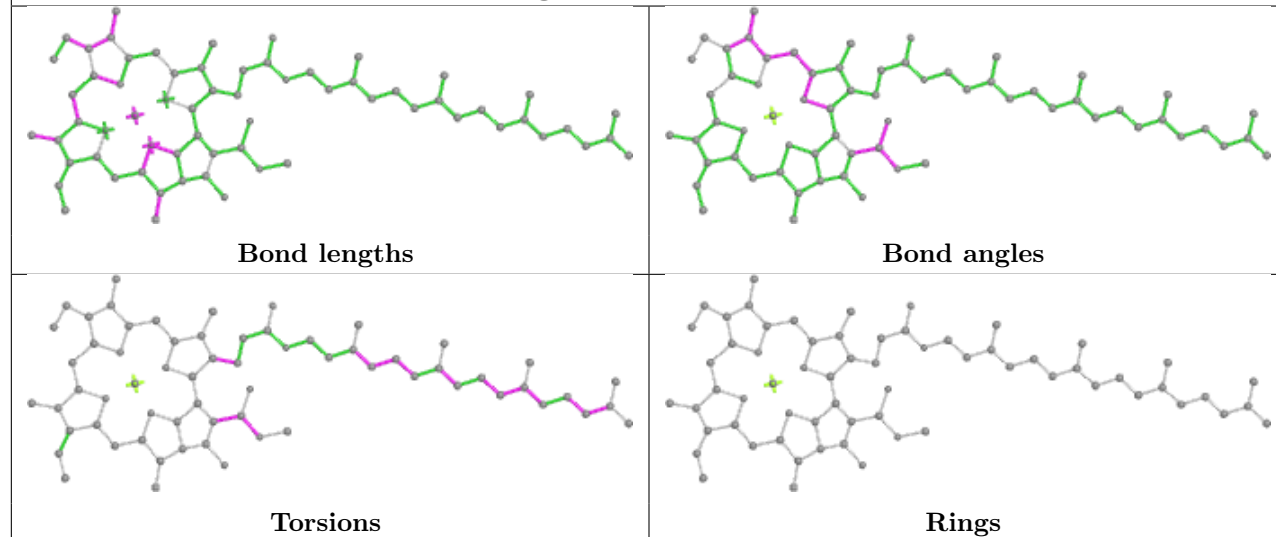
Ligand KC1 J 306



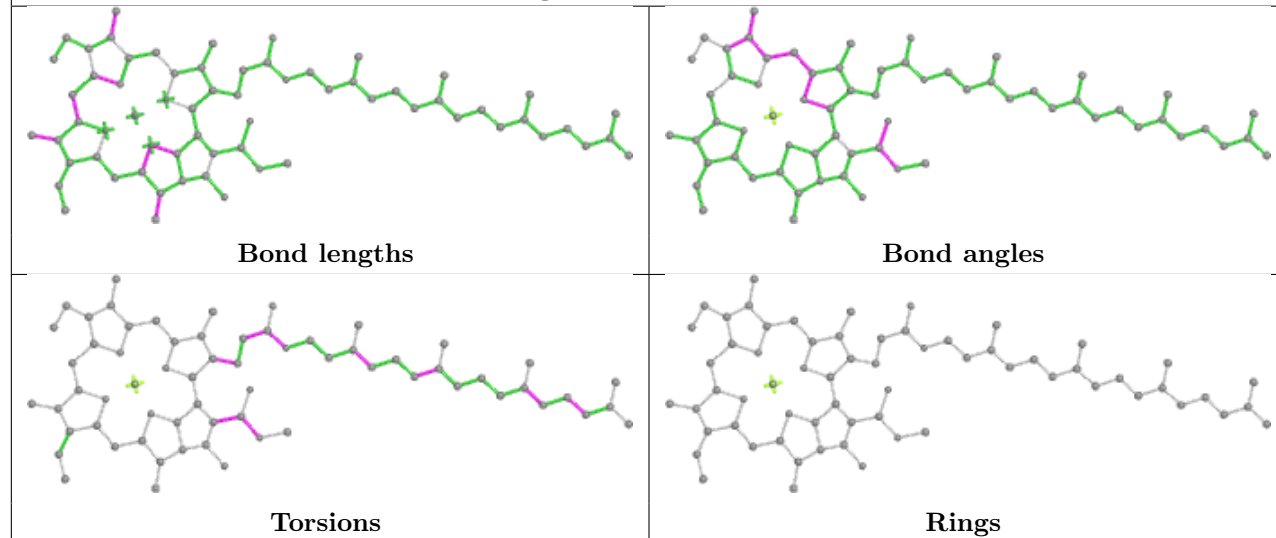
Ligand CLA b 809



Ligand CLA b 844



Ligand CLA a 807



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.

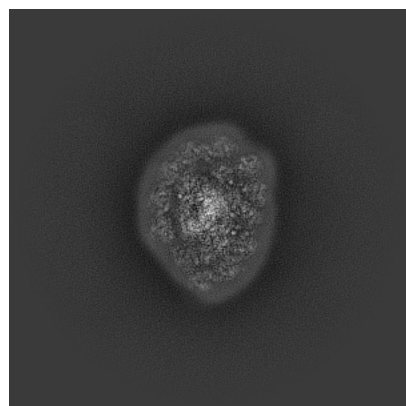
6 Map visualisation [i](#)

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.

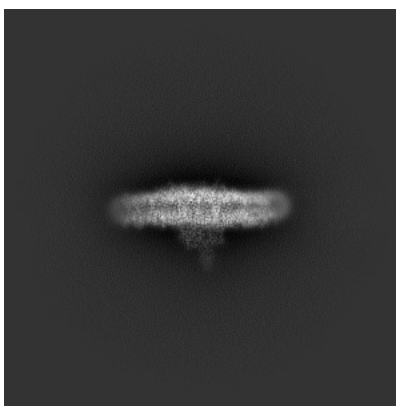
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

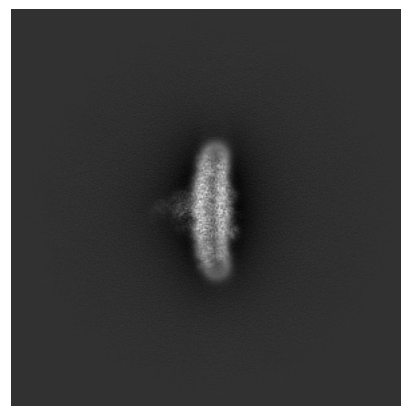
6.1.1 Primary map



X

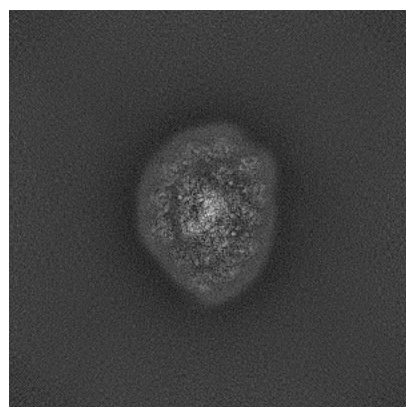


Y

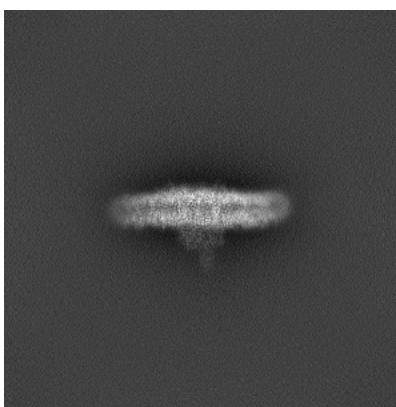


Z

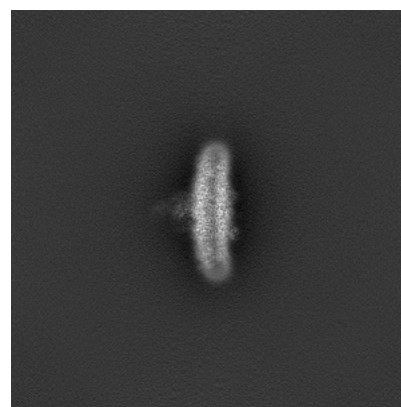
6.1.2 Raw map



X



Y

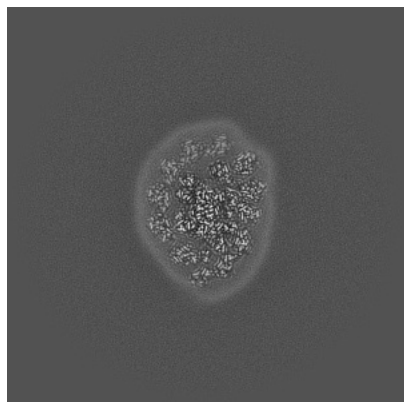


Z

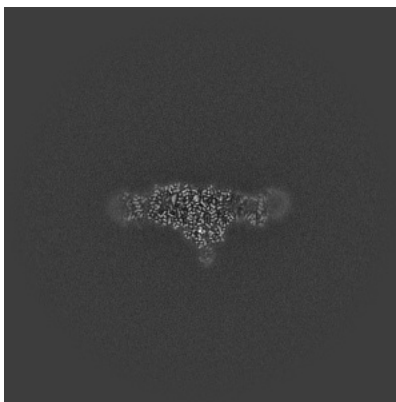
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

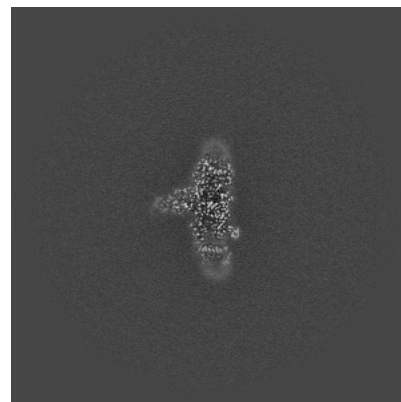
6.2.1 Primary map



X Index: 256

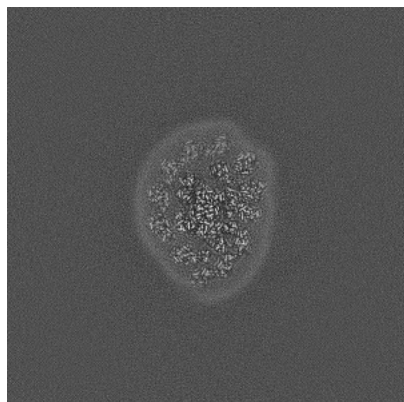


Y Index: 256

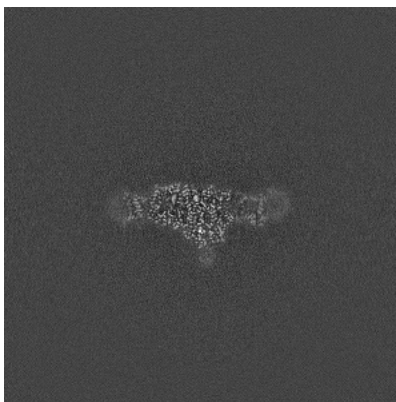


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

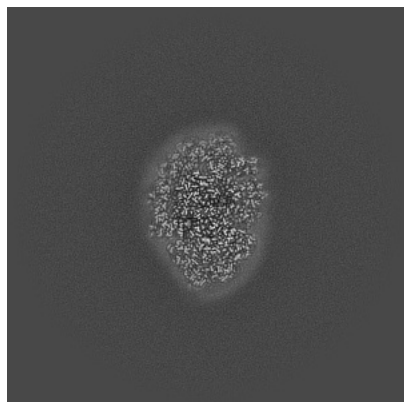


Z Index: 256

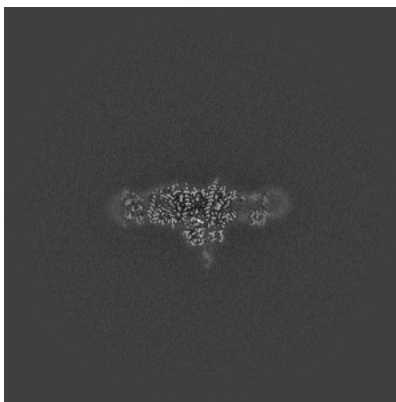
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

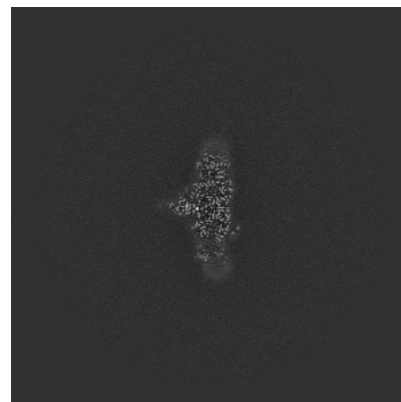
6.3.1 Primary map



X Index: 245

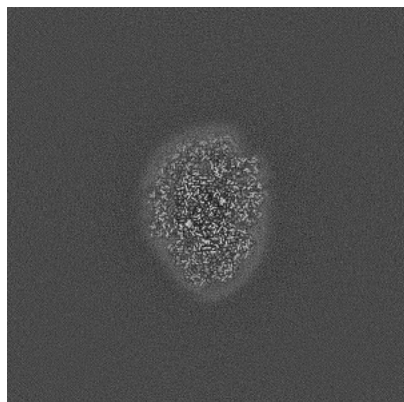


Y Index: 252

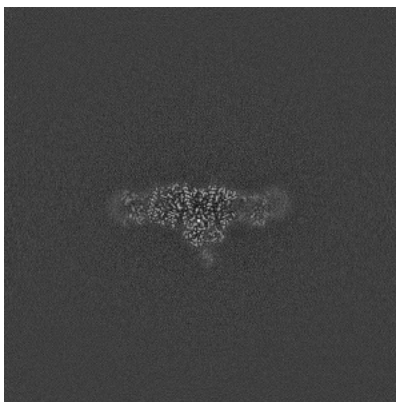


Z Index: 249

6.3.2 Raw map



X Index: 246



Y Index: 253

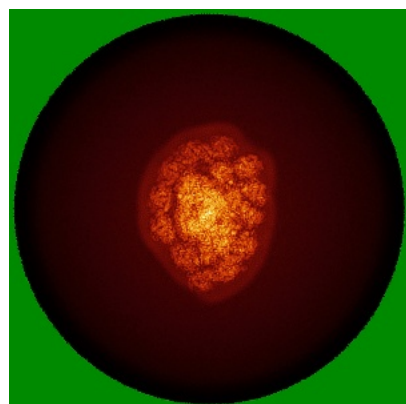


Z Index: 249

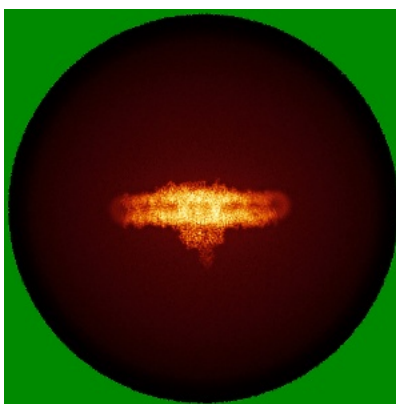
The images above show the largest variance slices of the map in three orthogonal directions.

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

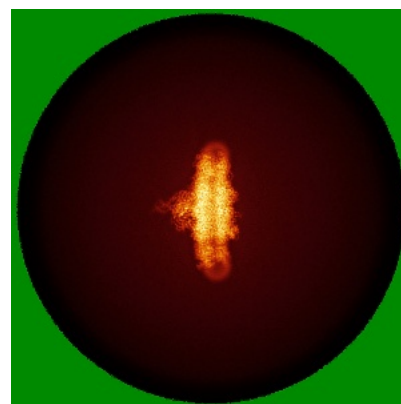
6.4.1 Primary map



X

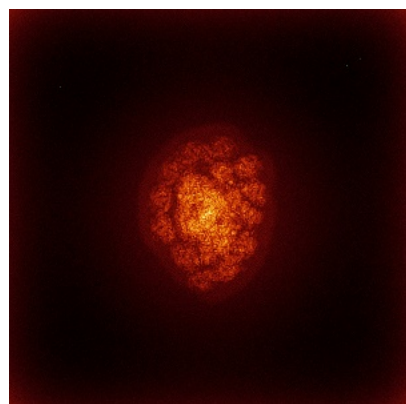


Y

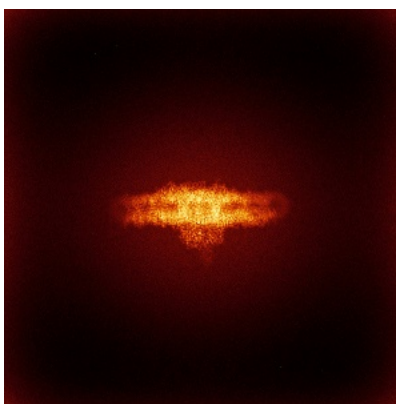


Z

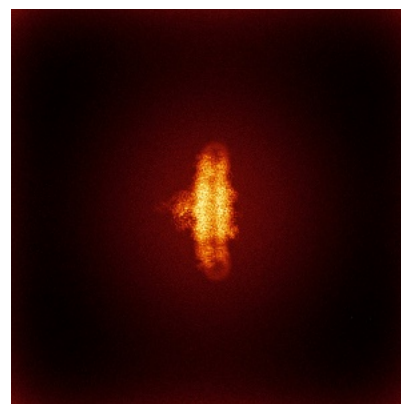
6.4.2 Raw map



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



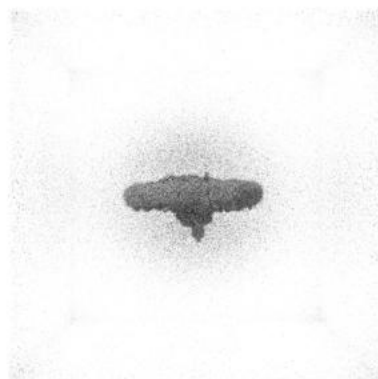
Z

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.

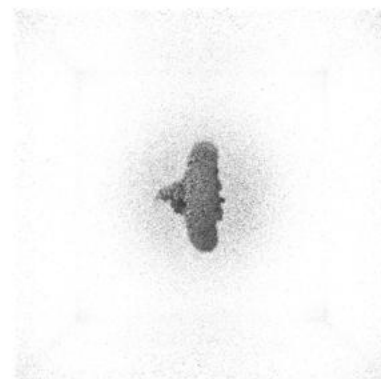
6.5.2 Raw map



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.

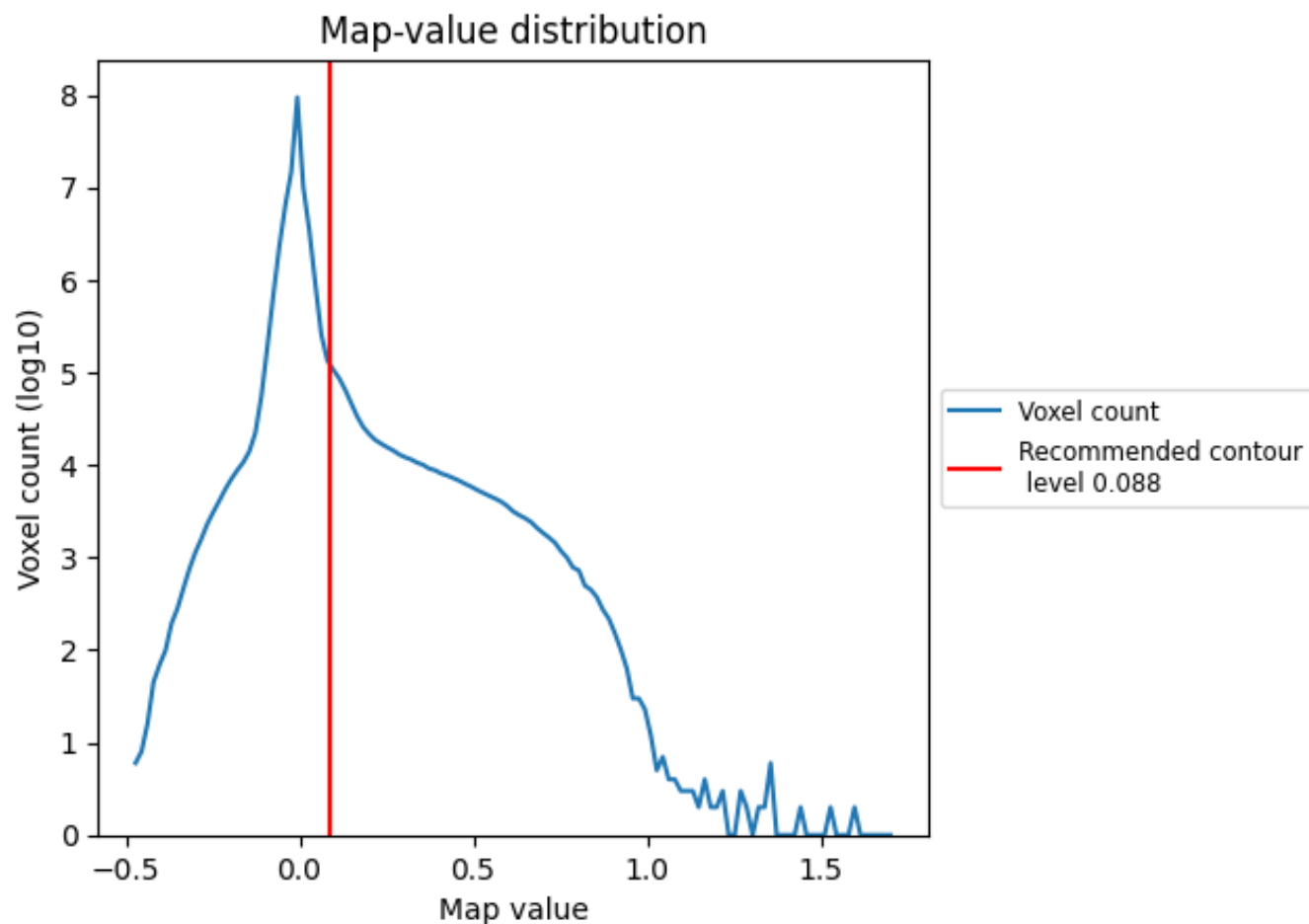
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

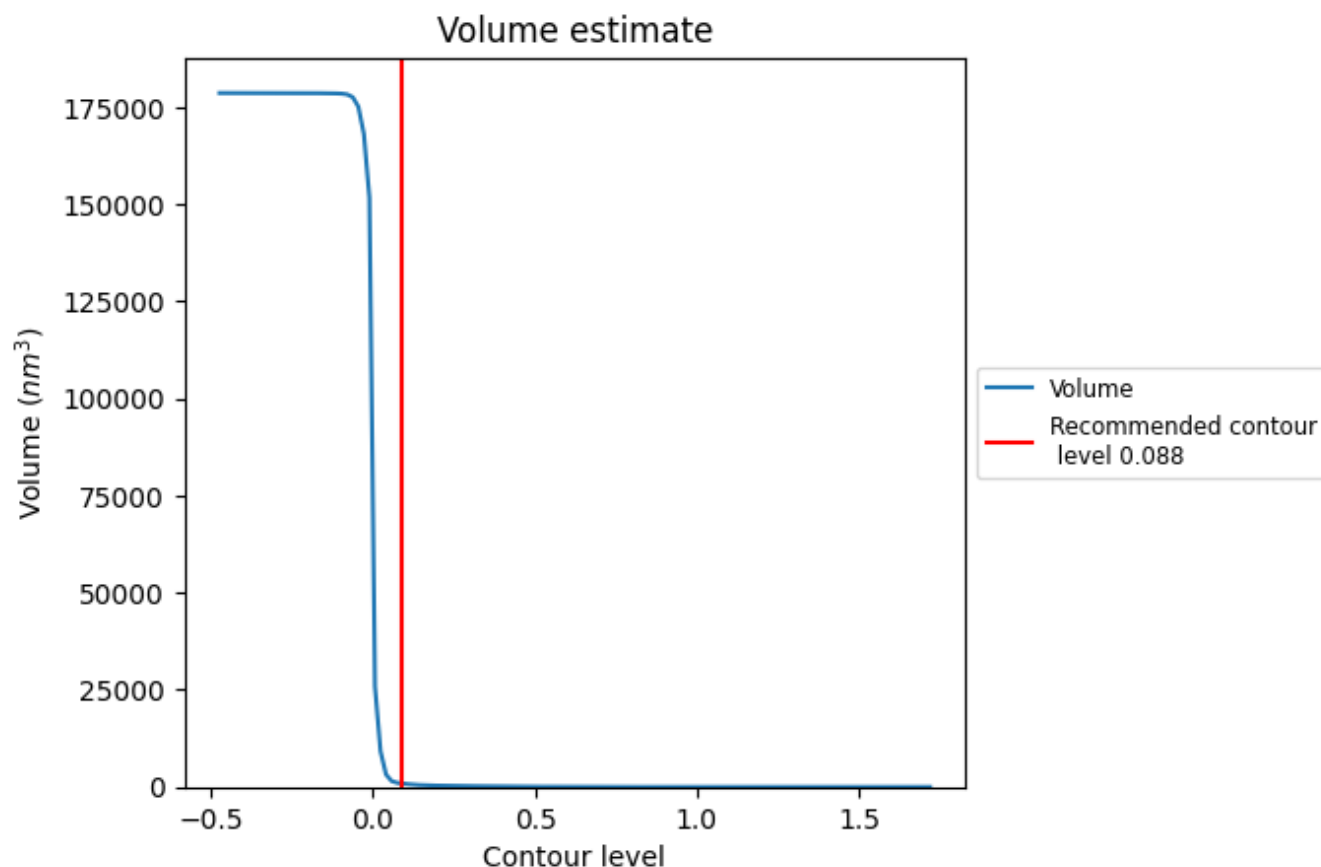
This section contains the results of statistical analysis of the map.

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.

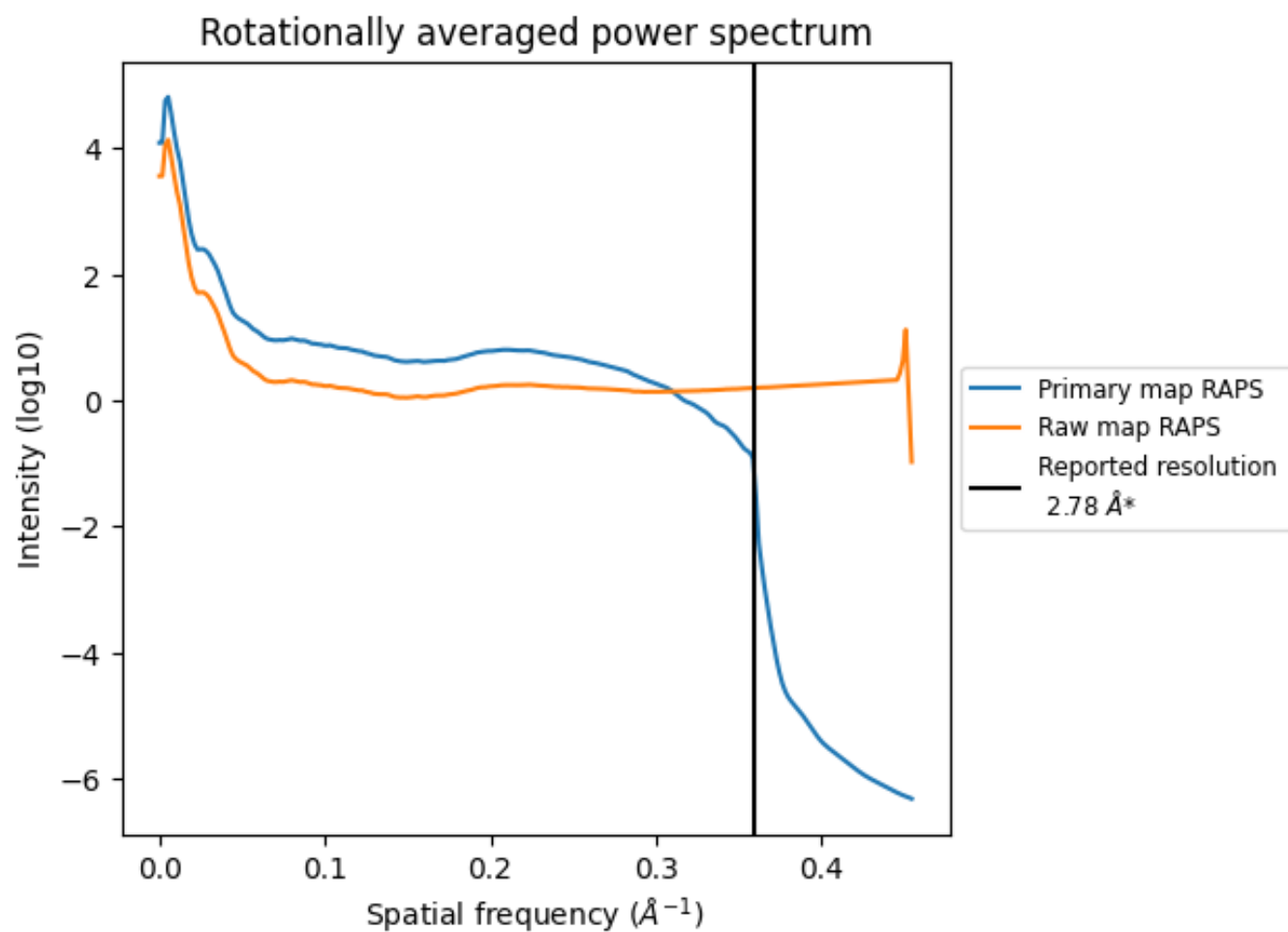
7.2 Volume estimate [i](#)



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 ⓘ

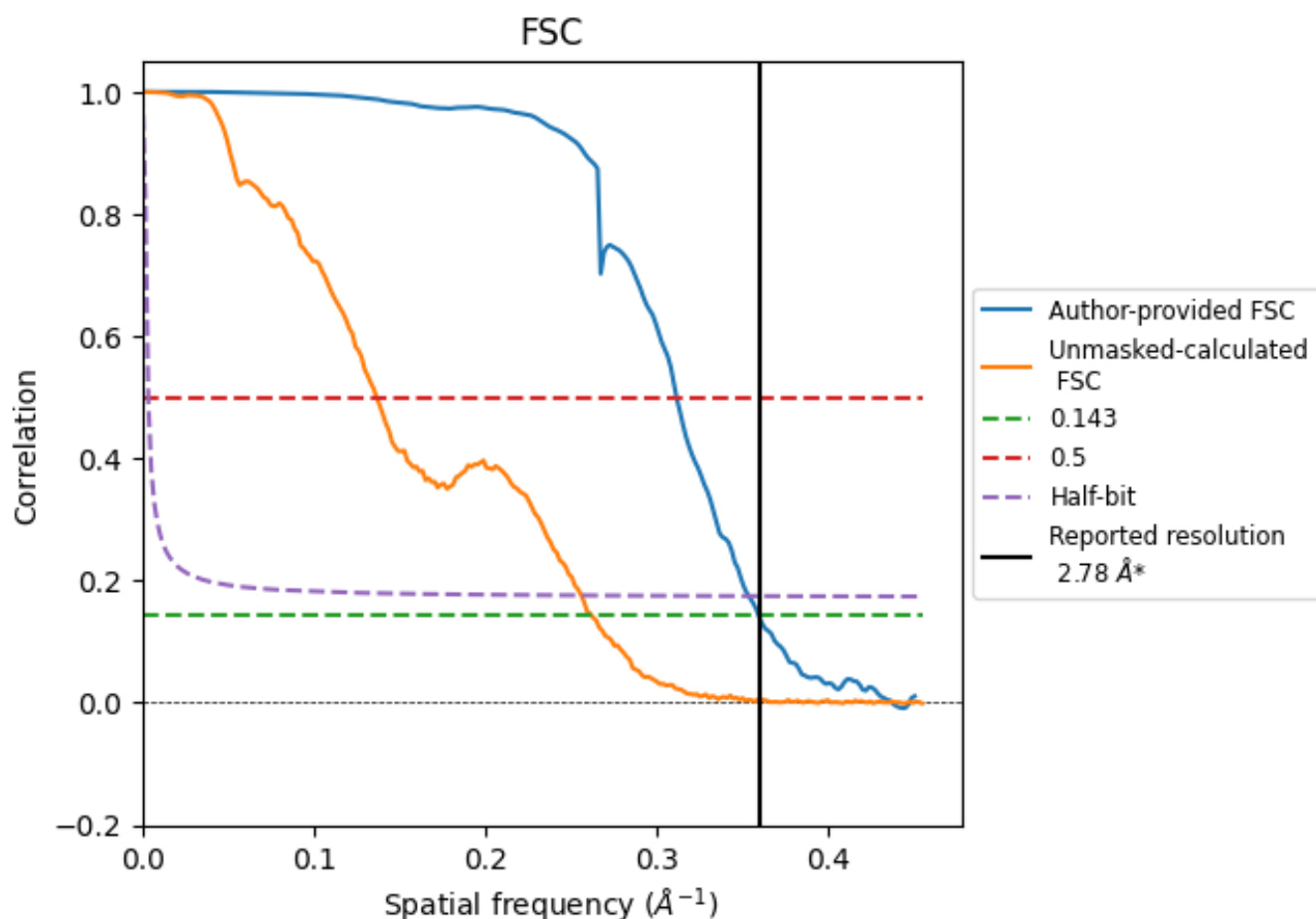


*Reported resolution corresponds to spatial frequency of 0.360 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

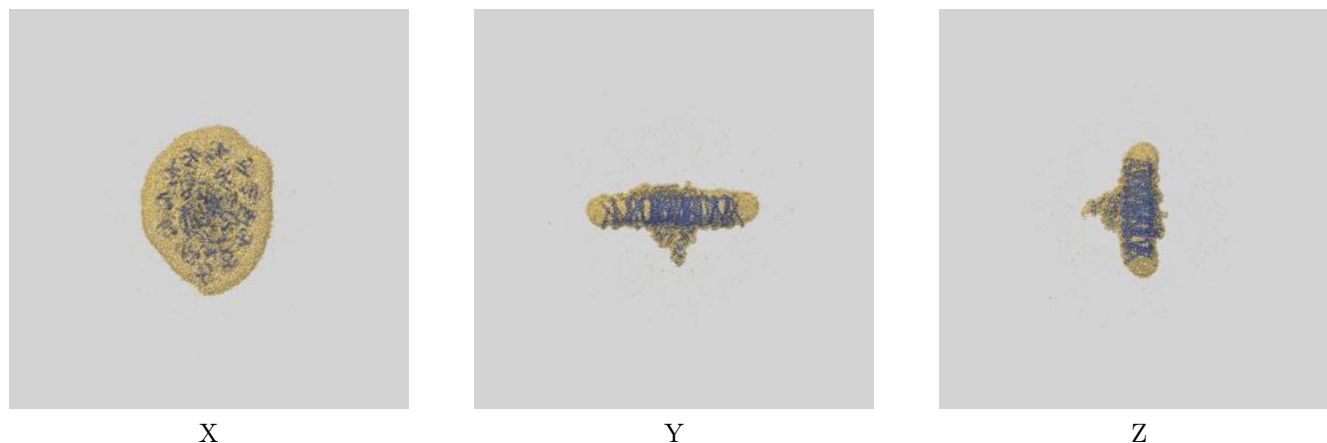
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.78	3.21	2.83
Unmasked-calculated*	3.82	7.32	3.91

*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](#)



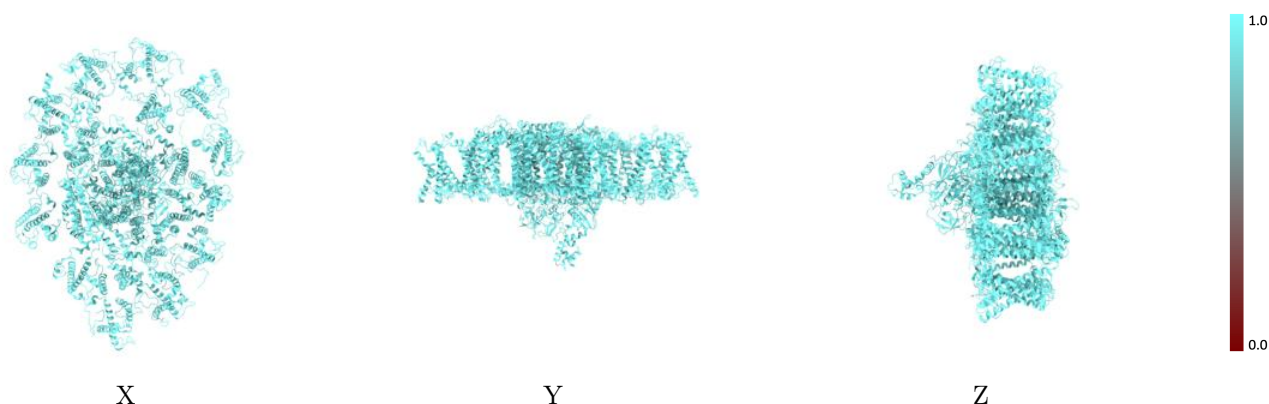
The images above show the 3D surface view of the map at the recommended contour level 0.088 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



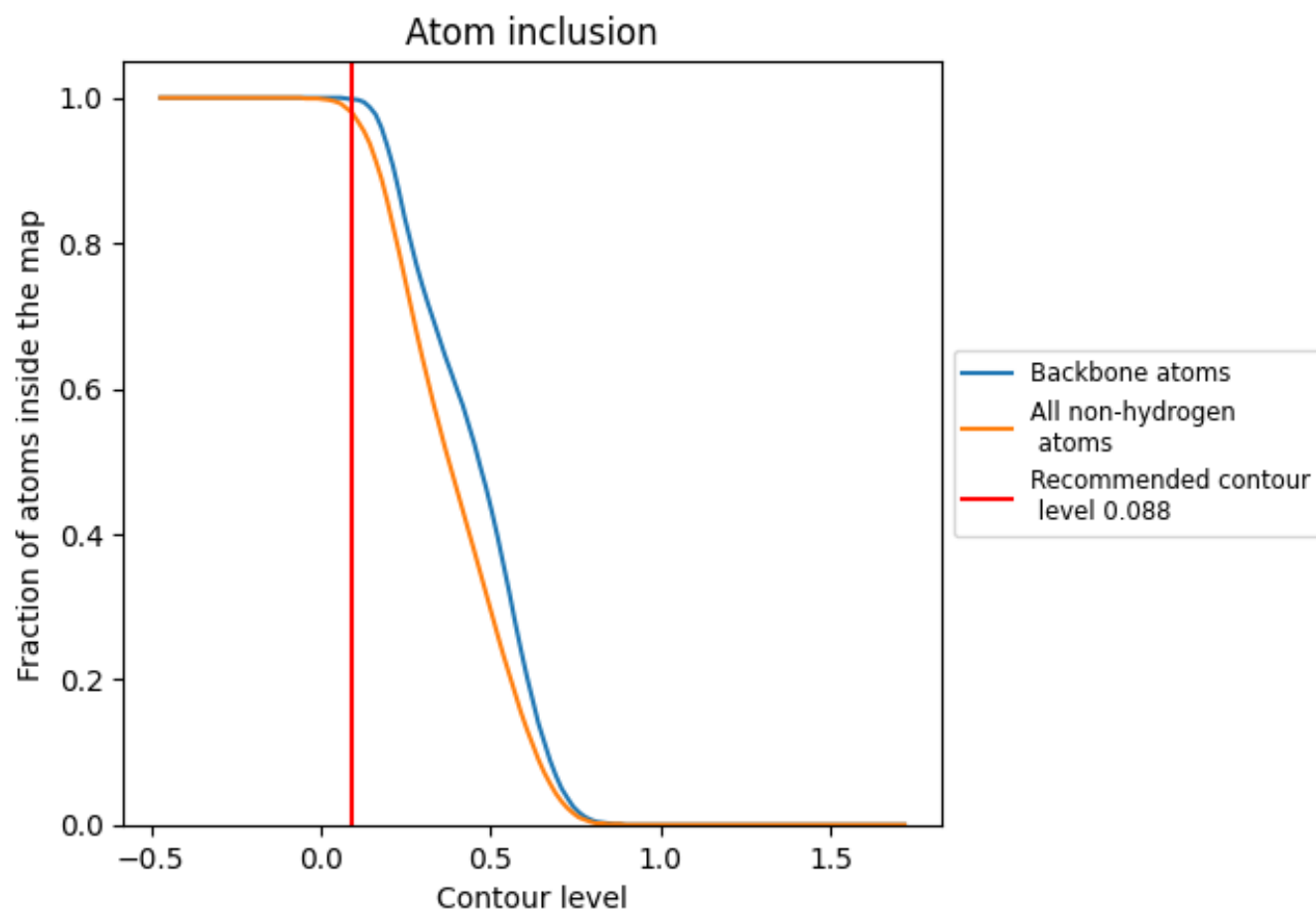
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div><div></div></div> 0.9810	<div><div></div></div> 0.5660
A	<div><div></div></div> 0.9750	<div><div></div></div> 0.5410
B	<div><div></div></div> 0.9790	<div><div></div></div> 0.5580
C	<div><div></div></div> 0.9820	<div><div></div></div> 0.5480
D	<div><div></div></div> 0.9770	<div><div></div></div> 0.5730
E	<div><div></div></div> 0.9840	<div><div></div></div> 0.5710
F	<div><div></div></div> 0.9540	<div><div></div></div> 0.4550
G	<div><div></div></div> 0.9760	<div><div></div></div> 0.5470
H	<div><div></div></div> 0.9870	<div><div></div></div> 0.5760
I	<div><div></div></div> 0.9800	<div><div></div></div> 0.5430
J	<div><div></div></div> 0.9780	<div><div></div></div> 0.5160
K	<div><div></div></div> 0.9810	<div><div></div></div> 0.5730
L	<div><div></div></div> 0.9710	<div><div></div></div> 0.5180
M	<div><div></div></div> 0.9850	<div><div></div></div> 0.5780
a	<div><div></div></div> 0.9890	<div><div></div></div> 0.5990
b	<div><div></div></div> 0.9860	<div><div></div></div> 0.5970
c	<div><div></div></div> 0.9900	<div><div></div></div> 0.5880
d	<div><div></div></div> 0.9940	<div><div></div></div> 0.5920
e	<div><div></div></div> 0.9710	<div><div></div></div> 0.5630
f	<div><div></div></div> 0.9800	<div><div></div></div> 0.5790
g	<div><div></div></div> 0.9490	<div><div></div></div> 0.5090
i	<div><div></div></div> 0.9900	<div><div></div></div> 0.5990
j	<div><div></div></div> 0.9680	<div><div></div></div> 0.5650
l	<div><div></div></div> 0.9940	<div><div></div></div> 0.5920
m	<div><div></div></div> 0.9770	<div><div></div></div> 0.5700
r	<div><div></div></div> 0.9820	<div><div></div></div> 0.5740

