



## wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 09:30 PM UTC

PDB ID : 9V7U / pdb\_00009v7u  
EMDB ID : EMD-64824  
Title : PSI-LHCE supercomplex from Euglena gracilis.  
Authors : Bai, T.Y.; Mao, Z.Y.; Tian, L.R.  
Deposited on : 2025-05-28  
Resolution : 2.63 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](mailto: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>.

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

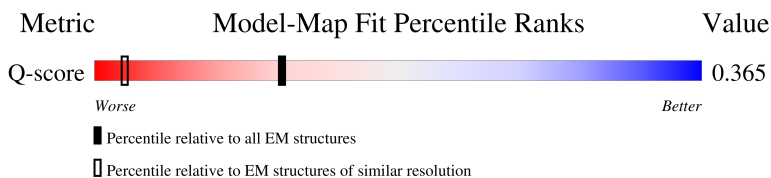
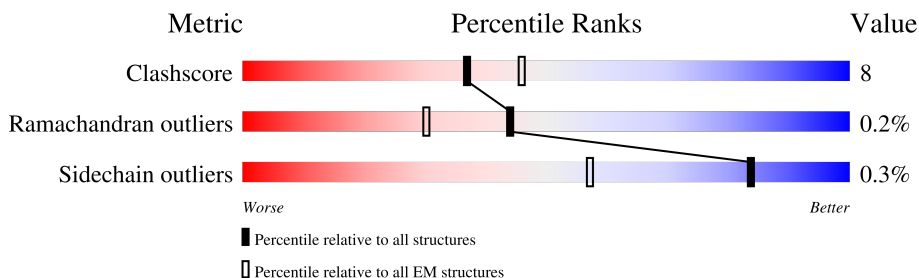
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.63 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





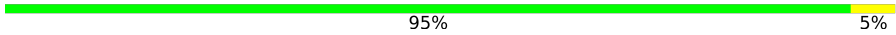

















Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8888 ( 2.13 - 3.13 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	
2	B	734	
3	C	81	
4	D	186	

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Mol	Chain	Length	Quality of chain
5	E	63	 84% 16%
6	F	168	 91% 9%
7	J	37	 95% 5%
8	M	31	 84% 16%
9	a	166	 90% 10%
10	b	169	 83% 17%
11	c	221	 90% 10%
12	d	220	 92% 8%
13	e	199	 87% 13%
14	h	174	 87% 12%
15	i	177	 84% 16%
16	j	183	 86% 14%
17	k	172	 89% 11%
18	l	167	 85% 15%
19	m	168	 85% 15%
20	f	174	 84% 16%
21	g	178	 90% 10%
22	n	184	 81% 18%
23	o	164	 83% 17%
24	p	148	 85% 15%

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
25	CLA	A	801	X	-	-	-
25	CLA	A	802	X	-	-	-
25	CLA	A	804	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	806	X	-	-	-
25	CLA	A	807	X	-	-	-
25	CLA	A	808	X	-	-	-
25	CLA	A	809	X	-	-	-
25	CLA	A	810	X	-	-	-
25	CLA	A	811	X	-	-	-
25	CLA	A	812	X	-	-	-
25	CLA	A	813	X	-	-	-
25	CLA	A	814	X	-	-	-
25	CLA	A	815	X	-	-	-
25	CLA	A	816	X	-	-	-
25	CLA	A	817	X	-	-	-
25	CLA	A	818	X	-	-	-
25	CLA	A	819	X	-	-	-
25	CLA	A	820	X	-	-	-
25	CLA	A	821	X	-	-	-
25	CLA	A	822	X	-	-	-
25	CLA	A	823	X	-	-	-
25	CLA	A	824	X	-	-	-
25	CLA	A	825	X	-	-	-
25	CLA	A	826	X	-	-	-
25	CLA	A	827	X	-	-	-
25	CLA	A	828	X	-	-	-
25	CLA	A	829	X	-	-	-
25	CLA	A	830	X	-	-	-
25	CLA	A	831	X	-	-	-
25	CLA	A	832	X	-	-	-
25	CLA	A	833	X	-	-	-
25	CLA	A	840	X	-	-	-
25	CLA	A	841	X	-	-	-
25	CLA	A	842	X	-	-	-
25	CLA	A	843	X	-	-	-
25	CLA	A	844	X	-	-	-
25	CLA	A	845	X	-	-	-
25	CLA	A	846	X	-	-	-
25	CLA	A	847	X	-	-	-
25	CLA	A	848	X	-	-	-
25	CLA	A	849	X	-	-	-
25	CLA	A	850	X	-	-	-
25	CLA	A	851	X	-	-	-
25	CLA	A	852	X	-	-	-
25	CLA	A	853	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	857	X	-	-	-
25	CLA	B	802	X	-	-	-
25	CLA	B	803	X	-	-	-
25	CLA	B	804	X	-	-	-
25	CLA	B	805	X	-	-	-
25	CLA	B	806	X	-	-	-
25	CLA	B	807	X	-	-	-
25	CLA	B	808	X	-	-	-
25	CLA	B	809	X	-	-	-
25	CLA	B	810	X	-	-	-
25	CLA	B	811	X	-	-	-
25	CLA	B	812	X	-	-	-
25	CLA	B	813	X	-	-	-
25	CLA	B	814	X	-	-	-
25	CLA	B	815	X	-	-	-
25	CLA	B	816	X	-	-	-
25	CLA	B	817	X	-	-	-
25	CLA	B	818	X	-	-	-
25	CLA	B	819	X	-	-	-
25	CLA	B	820	X	-	-	-
25	CLA	B	821	X	-	-	-
25	CLA	B	822	X	-	-	-
25	CLA	B	823	X	-	-	-
25	CLA	B	824	X	-	-	-
25	CLA	B	825	X	-	-	-
25	CLA	B	826	X	-	-	-
25	CLA	B	834	X	-	-	-
25	CLA	B	836	X	-	-	-
25	CLA	B	837	X	-	-	-
25	CLA	B	838	X	-	-	-
25	CLA	B	839	X	-	-	-
25	CLA	B	840	X	-	-	-
25	CLA	B	841	X	-	-	-
25	CLA	B	842	X	-	-	-
25	CLA	B	843	X	-	-	-
25	CLA	B	844	X	-	-	-
25	CLA	B	845	X	-	-	-
25	CLA	B	846	X	-	-	-
25	CLA	B	847	X	-	-	-
25	CLA	B	848	X	-	-	-
25	CLA	F	201	X	-	-	-
25	CLA	F	202	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	J	103	X	-	-	-
25	CLA	a	203	X	-	-	-
25	CLA	a	204	X	-	-	-
25	CLA	a	205	X	-	-	-
25	CLA	a	206	X	-	-	-
25	CLA	a	207	X	-	-	-
25	CLA	a	208	X	-	-	-
25	CLA	a	209	X	-	-	-
25	CLA	a	210	X	-	-	-
25	CLA	a	211	X	-	-	-
25	CLA	a	212	X	-	-	-
25	CLA	a	213	X	-	-	-
25	CLA	b	203	X	-	-	-
25	CLA	b	204	X	-	-	-
25	CLA	b	205	X	-	-	-
25	CLA	b	206	X	-	-	-
25	CLA	b	207	X	-	-	-
25	CLA	b	208	X	-	-	-
25	CLA	b	209	X	-	-	-
25	CLA	b	210	X	-	-	-
25	CLA	b	211	X	-	-	-
25	CLA	b	212	X	-	-	-
25	CLA	b	213	X	-	-	-
25	CLA	c	302	X	-	-	-
25	CLA	c	303	X	-	-	-
25	CLA	c	304	X	-	-	-
25	CLA	c	305	X	-	-	-
25	CLA	c	306	X	-	-	-
25	CLA	c	308	X	-	-	-
25	CLA	c	309	X	-	-	-
25	CLA	c	310	X	-	-	-
25	CLA	c	311	X	-	-	-
25	CLA	c	312	X	-	-	-
25	CLA	c	313	X	-	-	-
25	CLA	c	314	X	-	-	-
25	CLA	c	315	X	-	-	-
25	CLA	d	301	X	-	-	-
25	CLA	d	303	X	-	-	-
25	CLA	d	304	X	-	-	-
25	CLA	d	305	X	-	-	-
25	CLA	d	306	X	-	-	-
25	CLA	d	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	d	312	X	-	-	-
25	CLA	d	313	X	-	-	-
25	CLA	d	314	X	-	-	-
25	CLA	d	315	X	-	-	-
25	CLA	d	316	X	-	-	-
25	CLA	e	201	X	-	-	-
25	CLA	e	204	X	-	-	-
25	CLA	e	205	X	-	-	-
25	CLA	e	206	X	-	-	-
25	CLA	e	207	X	-	-	-
25	CLA	e	208	X	-	-	-
25	CLA	e	210	X	-	-	-
25	CLA	e	211	X	-	-	-
25	CLA	e	212	X	-	-	-
25	CLA	e	213	X	-	-	-
25	CLA	e	214	X	-	-	-
25	CLA	e	215	X	-	-	-
25	CLA	e	216	X	-	-	-
25	CLA	e	217	X	-	-	-
25	CLA	f	601	X	-	-	-
25	CLA	f	602	X	-	-	-
25	CLA	f	603	X	-	-	-
25	CLA	f	604	X	-	-	-
25	CLA	f	605	X	-	-	-
25	CLA	f	606	X	-	-	-
25	CLA	f	607	X	-	-	-
25	CLA	f	608	X	-	-	-
25	CLA	f	609	X	-	-	-
25	CLA	f	610	X	-	-	-
25	CLA	f	611	X	-	-	-
25	CLA	f	612	X	-	-	-
25	CLA	g	203	X	-	-	-
25	CLA	g	204	X	-	-	-
25	CLA	g	205	X	-	-	-
25	CLA	g	206	X	-	-	-
25	CLA	g	207	X	-	-	-
25	CLA	g	208	X	-	-	-
25	CLA	g	209	X	-	-	-
25	CLA	g	210	X	-	-	-
25	CLA	g	211	X	-	-	-
25	CLA	g	212	X	-	-	-
25	CLA	g	213	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	g	214	X	-	-	-
25	CLA	g	215	X	-	-	-
25	CLA	h	203	X	-	-	-
25	CLA	h	204	X	-	-	-
25	CLA	h	205	X	-	-	-
25	CLA	h	206	X	-	-	-
25	CLA	h	207	X	-	-	-
25	CLA	h	208	X	-	-	-
25	CLA	h	209	X	-	-	-
25	CLA	h	210	X	-	-	-
25	CLA	h	211	X	-	-	-
25	CLA	h	212	X	-	-	-
25	CLA	h	213	X	-	-	-
25	CLA	h	214	X	-	-	-
25	CLA	h	215	X	-	-	-
25	CLA	i	202	X	-	-	-
25	CLA	i	203	X	-	-	-
25	CLA	i	204	X	-	-	-
25	CLA	i	205	X	-	-	-
25	CLA	i	206	X	-	-	-
25	CLA	i	207	X	-	-	-
25	CLA	i	208	X	-	-	-
25	CLA	i	209	X	-	-	-
25	CLA	i	210	X	-	-	-
25	CLA	i	211	X	-	-	-
25	CLA	i	212	X	-	-	-
25	CLA	i	213	X	-	-	-
25	CLA	j	203	X	-	-	-
25	CLA	j	204	X	-	-	-
25	CLA	j	205	X	-	-	-
25	CLA	j	206	X	-	-	-
25	CLA	j	207	X	-	-	-
25	CLA	j	208	X	-	-	-
25	CLA	j	209	X	-	-	-
25	CLA	j	210	X	-	-	-
25	CLA	j	211	X	-	-	-
25	CLA	j	212	X	-	-	-
25	CLA	j	213	X	-	-	-
25	CLA	j	214	X	-	-	-
25	CLA	j	215	X	-	-	-
25	CLA	k	202	X	-	-	-
25	CLA	k	203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	k	204	X	-	-	-
25	CLA	k	205	X	-	-	-
25	CLA	k	206	X	-	-	-
25	CLA	k	207	X	-	-	-
25	CLA	k	208	X	-	-	-
25	CLA	k	209	X	-	-	-
25	CLA	k	210	X	-	-	-
25	CLA	k	211	X	-	-	-
25	CLA	k	212	X	-	-	-
25	CLA	k	213	X	-	-	-
25	CLA	k	214	X	-	-	-
25	CLA	l	601	X	-	-	-
25	CLA	l	602	X	-	-	-
25	CLA	l	603	X	-	-	-
25	CLA	l	604	X	-	-	-
25	CLA	l	605	X	-	-	-
25	CLA	l	606	X	-	-	-
25	CLA	l	607	X	-	-	-
25	CLA	l	608	X	-	-	-
25	CLA	l	609	X	-	-	-
25	CLA	l	610	X	-	-	-
25	CLA	l	611	X	-	-	-
25	CLA	l	612	X	-	-	-
25	CLA	m	202	X	-	-	-
25	CLA	m	203	X	-	-	-
25	CLA	m	204	X	-	-	-
25	CLA	m	205	X	-	-	-
25	CLA	m	206	X	-	-	-
25	CLA	m	207	X	-	-	-
25	CLA	m	208	X	-	-	-
25	CLA	m	209	X	-	-	-
25	CLA	m	210	X	-	-	-
25	CLA	m	211	X	-	-	-
25	CLA	n	201	X	-	-	-
25	CLA	n	202	X	-	-	-
25	CLA	n	203	X	-	-	-
25	CLA	n	204	X	-	-	-
25	CLA	n	205	X	-	-	-
25	CLA	n	206	X	-	-	-
25	CLA	n	207	X	-	-	-
25	CLA	n	208	X	-	-	-
25	CLA	n	209	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	n	210	X	-	-	-
25	CLA	n	211	X	-	-	-
25	CLA	o	601	X	-	-	-
25	CLA	o	602	X	-	-	-
25	CLA	o	603	X	-	-	-
25	CLA	o	604	X	-	-	-
25	CLA	o	605	X	-	-	-
25	CLA	o	606	X	-	-	-
25	CLA	o	607	X	-	-	-
25	CLA	o	608	X	-	-	-
25	CLA	o	609	X	-	-	-
25	CLA	o	610	X	-	-	-
25	CLA	p	601	X	-	-	-
25	CLA	p	602	X	-	-	-
25	CLA	p	603	X	-	-	-
25	CLA	p	604	X	-	-	-
25	CLA	p	605	X	-	-	-
25	CLA	p	606	X	-	-	-
25	CLA	p	607	X	-	-	-
25	CLA	p	608	X	-	-	-
25	CLA	p	609	X	-	-	-
35	CHL	c	307	X	-	-	-
35	CHL	d	307	X	-	-	-
35	CHL	d	308	X	-	-	-
35	CHL	d	309	X	-	-	-
35	CHL	d	310	X	-	-	-
35	CHL	e	209	X	-	-	-

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 55406 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5878	3860	994	1003	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5861	3855	984	1007	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			596	363	104	118	11		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	186	Total	C	N	O	S	0	0
			1393	892	235	262	4		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	63	Total	C	N	O	0	0
			481	311	81	89		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	168	Total	C	N	O	S	0	0
			1250	801	206	239	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	37	Total	C	N	O	S	0	0
			305	209	43	52	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	31	Total	C	N	O	S	0	0
			243	162	37	43	1		

- Molecule 9 is a protein called Chloroplast light-harvesting complex I protein.

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

- Molecule 10 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	169	Total	C	N	O	S	0	0
			1302	842	213	243	4		

- Molecule 11 is a protein called LHCE 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	221	Total	C	N	O	S	0	0
			1676	1087	282	302	5		

- Molecule 12 is a protein called Light harvesting chlorophyll a /b binding protein of PSII.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	220	Total	C	N	O	S	0	0
			1669	1088	275	302	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	199	Total	C	N	O	S	0	0
			1517	981	256	275	5		

- Molecule 14 is a protein called LHCE 8.



Mol	Chain	Residues	Atoms					AltConf	Trace
14	h	174	Total	C	N	O	S	0	0
			1350	865	233	247	5		

- Molecule 15 is a protein called LHCE 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	i	177	Total	C	N	O	S	0	0
			1355	865	242	244	4		

- Molecule 16 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	j	183	Total	C	N	O	S	0	0
			1450	944	246	254	6		

- Molecule 17 is a protein called Chloroplast light-harvesting complex I protein.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	l	167	Total	C	N	O	S	0	0
			1256	811	214	227	4		

- Molecule 19 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	m	168	Total	C	N	O	S	0	0
			1260	813	215	228	4		

- Molecule 20 is a protein called Chloroplast light-harvesting complex I protein, Lhca7\_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	174	Total	C	N	O	S	0	0
			1332	851	236	241	4		

- Molecule 21 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	178	Total	C	N	O	S	0	0
			1406	914	240	246	6		

- Molecule 22 is a protein called Chloroplast light-harvesting complex II protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	184	Total	C	N	O	S	0	0
			1411	921	232	254	4		

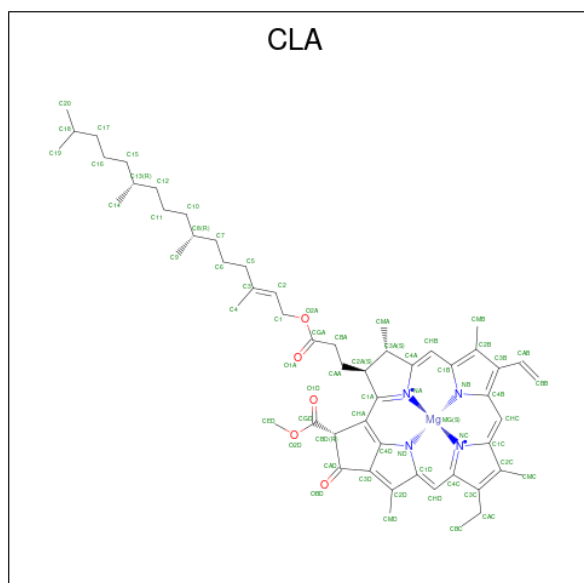
- Molecule 23 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	164	Total	C	N	O	S	0	0
			1230	794	208	224	4		

- Molecule 24 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	148	Total	C	N	O	S	0	0
			1126	727	188	207	4		

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



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

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	A	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	A	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	A	1	Total 64	C 55	Mg 1	N 4	O 4	0
25	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	A	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	A	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	B	1	Total 49	C 40	Mg 1	N 4	O 4	0
25	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	B	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	F	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	J	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	a	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	a	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	a	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	a	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	b	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	b	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	b	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	b	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	c	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	c	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	c	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	c	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	c	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	c	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	c	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	c	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	c	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	c	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	d	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	d	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
25	d	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	d	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	d	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	h	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	h	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	h	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	h	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	h	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	h	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	h	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	h	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	h	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	h	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	i	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	i	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	i	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	i	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	i	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	i	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	i	1	Total 43	C 35	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
25	i	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	i	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	i	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	i	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	j	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	j	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	j	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	j	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	j	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	j	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	j	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	j	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	j	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	j	1	Total 62	C 52	Mg 1	N 4	O 5	0
25	j	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	j	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	j	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	k	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	k	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	k	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	k	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	k	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	m	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	m	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	m	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	m	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	m	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	f	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
25	f	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	g	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	n	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	n	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	n	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	n	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	n	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	n	1	Total 41	C 33	Mg 1	N 4	O 3	0

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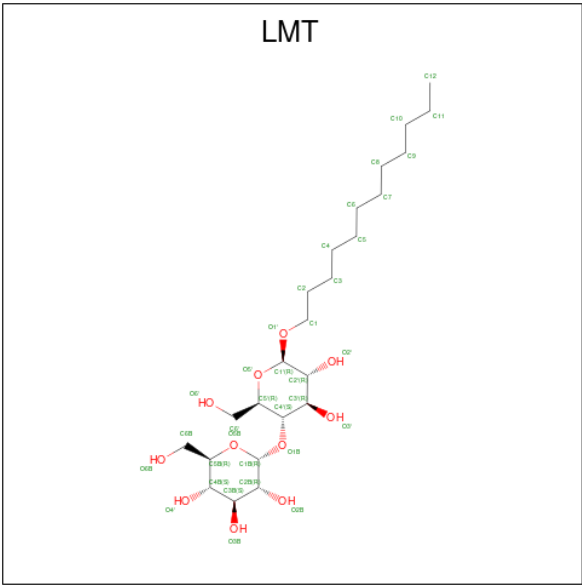
Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	n	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	n	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	n	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	o	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	o	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	o	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	o	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	o	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	o	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	o	1	Total 42	C 35	Mg 1	N 4	O 2	0
25	o	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	o	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	p	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	p	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	p	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	p	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	p	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	p	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

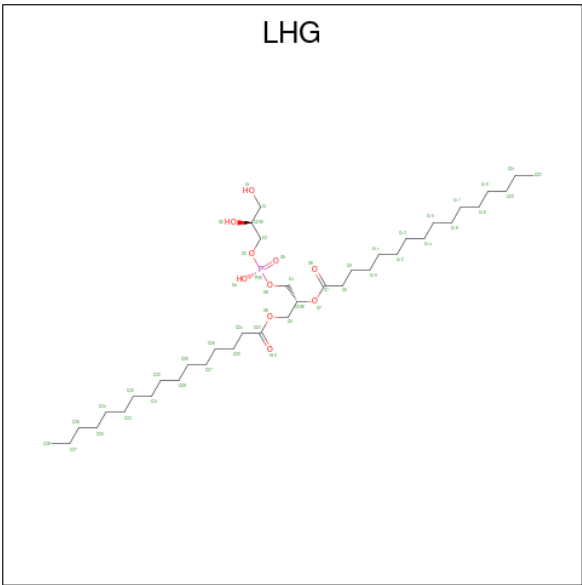
- Molecule 26 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			35	24	11	

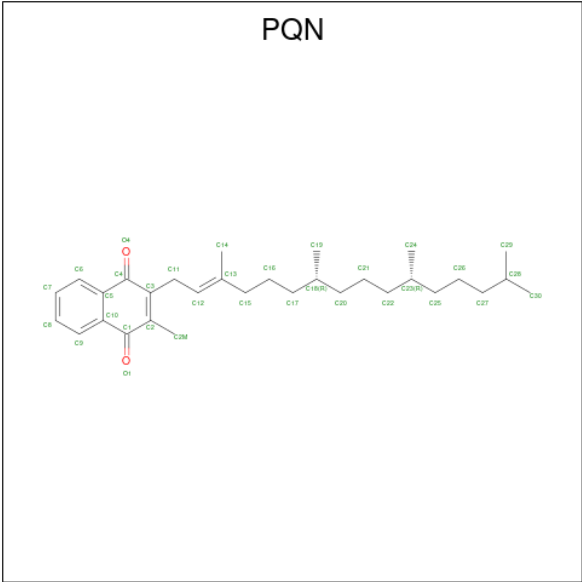
- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).





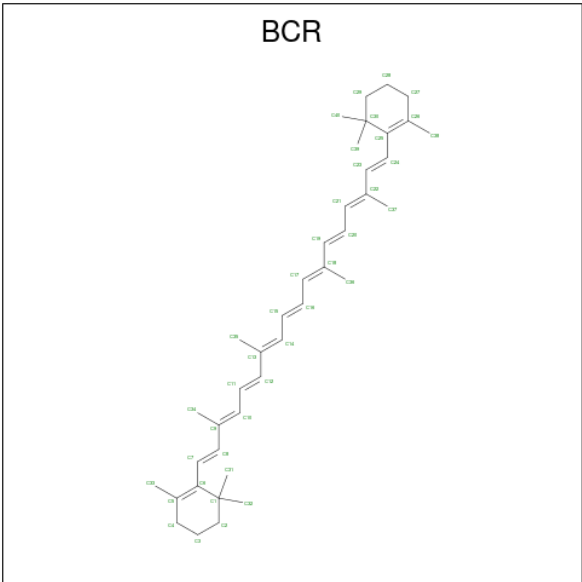
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	P	0
			38	27	10	1	
27	A	1	Total	C	O	P	0
			49	38	10	1	
27	a	1	Total	C	O	P	0
			26	15	10	1	
27	b	1	Total	C	O	P	0
			31	20	10	1	
27	c	1	Total	C	O	P	0
			30	19	10	1	
27	d	1	Total	C	O	P	0
			29	18	10	1	
27	h	1	Total	C	O	P	0
			30	19	10	1	
27	h	1	Total	C	O	P	0
			31	20	10	1	
27	i	1	Total	C	O	P	0
			36	25	10	1	
27	j	1	Total	C	O	P	0
			37	26	10	1	
27	m	1	Total	C	O	P	0
			32	21	10	1	
27	g	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



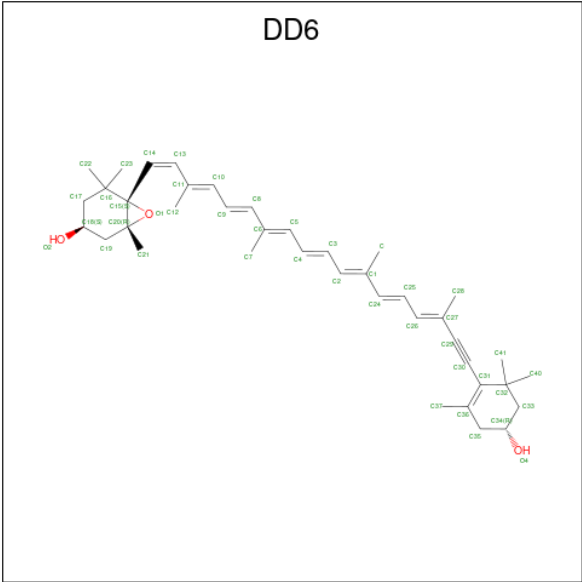
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			33	31	2	
28	B	1	Total	C	O	0
			33	31	2	
28	B	1	Total	C	O	0
			27	25	2	
28	F	1	Total	C	O	0
			26	24	2	

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



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

- Molecule 30 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: C<sub>40</sub>H<sub>54</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			43	40	3	
30	A	1	Total	C	O	0
			43	40	3	
30	F	1	Total	C	O	0
			43	40	3	
30	J	1	Total	C	O	0
			43	40	3	
30	J	1	Total	C	O	0
			43	40	3	
30	a	1	Total	C	O	0
			43	40	3	
30	a	1	Total	C	O	0
			43	40	3	
30	b	1	Total	C	O	0
			43	40	3	
30	b	1	Total	C	O	0
			43	40	3	
30	c	1	Total	C	O	0
			43	40	3	
30	c	1	Total	C	O	0
			43	40	3	
30	c	1	Total	C	O	0
			43	40	3	
30	d	1	Total	C	O	0
			43	40	3	
30	d	1	Total	C	O	0
			43	40	3	

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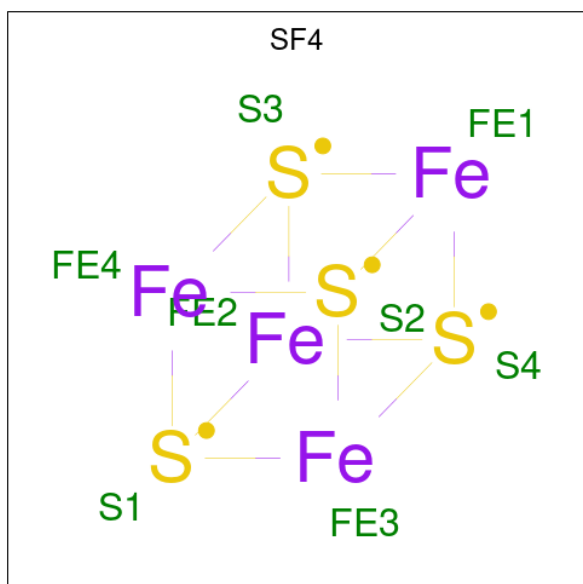
Mol	Chain	Residues	Atoms			AltConf
30	d	1	Total 43	C 40	O 3	0
30	e	1	Total 43	C 40	O 3	0
30	e	1	Total 43	C 40	O 3	0
30	e	1	Total 43	C 40	O 3	0
30	h	1	Total 43	C 40	O 3	0
30	h	1	Total 43	C 40	O 3	0
30	i	1	Total 43	C 40	O 3	0
30	i	1	Total 43	C 40	O 3	0
30	i	1	Total 43	C 40	O 3	0
30	j	1	Total 43	C 40	O 3	0
30	j	1	Total 43	C 40	O 3	0
30	k	1	Total 43	C 40	O 3	0
30	k	1	Total 43	C 40	O 3	0
30	l	1	Total 43	C 40	O 3	0
30	l	1	Total 43	C 40	O 3	0
30	m	1	Total 43	C 40	O 3	0
30	m	1	Total 43	C 40	O 3	0
30	f	1	Total 43	C 40	O 3	0
30	f	1	Total 43	C 40	O 3	0
30	g	1	Total 43	C 40	O 3	0
30	g	1	Total 43	C 40	O 3	0

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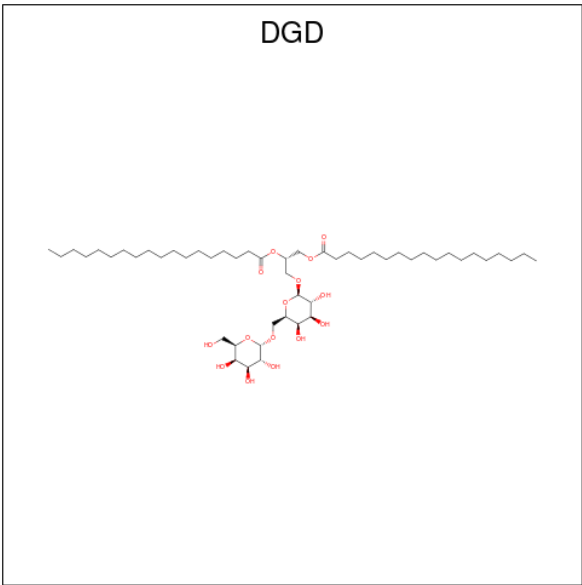
Mol	Chain	Residues	Atoms			AltConf
30	n	1	Total	C	O	0
			43	40	3	
30	n	1	Total	C	O	0
			43	40	3	
30	n	1	Total	C	O	0
			43	40	3	
30	o	1	Total	C	O	0
			43	40	3	
30	o	1	Total	C	O	0
			43	40	3	
30	p	1	Total	C	O	0
			43	40	3	

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



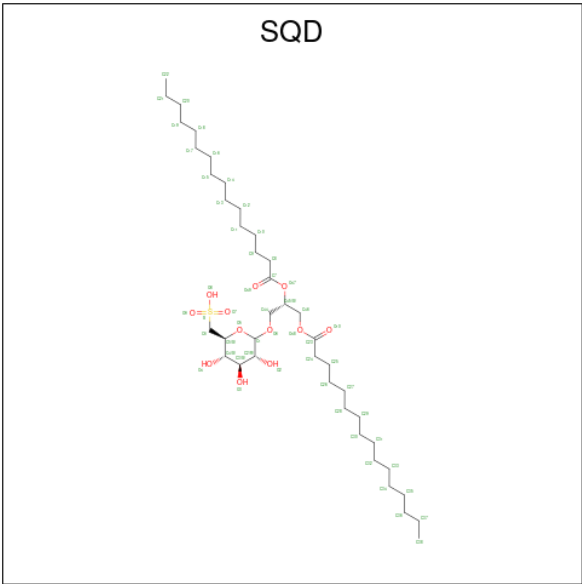
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	Fe	S	0
			8	4	4	
31	C	1	Total	Fe	S	0
			8	4	4	
31	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $\text{C}_{51}\text{H}_{96}\text{O}_{15}$ ).



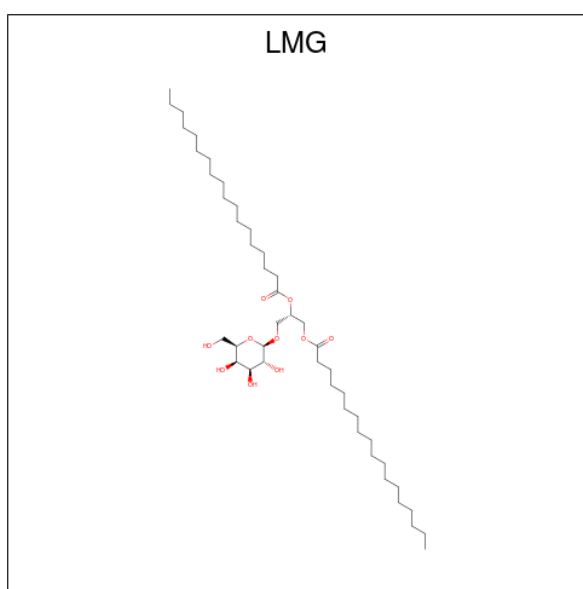
Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			54	39	15	
32	b	1	Total	C	O	0
			48	33	15	
32	e	1	Total	C	O	0
			36	21	15	

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms				AltConf
33	D	1	Total	C	O	S	0
			36	23	12	1	
33	F	1	Total	C	O	S	0
			39	26	12	1	
33	J	1	Total	C	O	S	0
			27	14	12	1	
33	g	1	Total	C	O	S	0
			32	19	12	1	

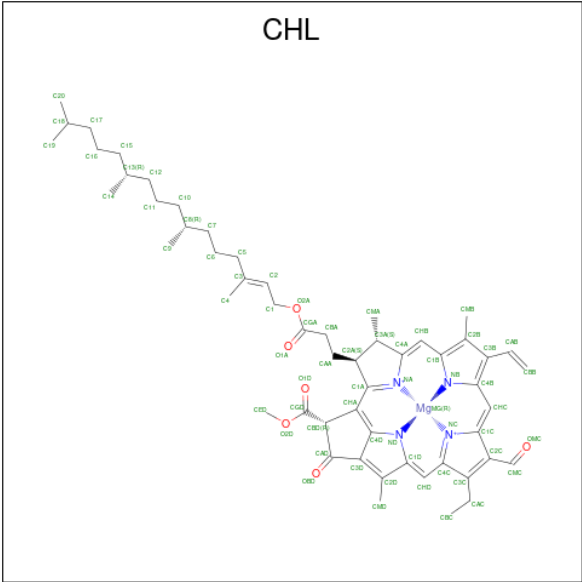
- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			AltConf
34	a	1	Total	C	O	0
			43	33	10	
34	e	1	Total	C	O	0
			52	42	10	
34	j	1	Total	C	O	0
			44	34	10	
34	k	1	Total	C	O	0
			36	26	10	

- Molecule 35 is CHLOROPHYLL B (CCD ID: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).



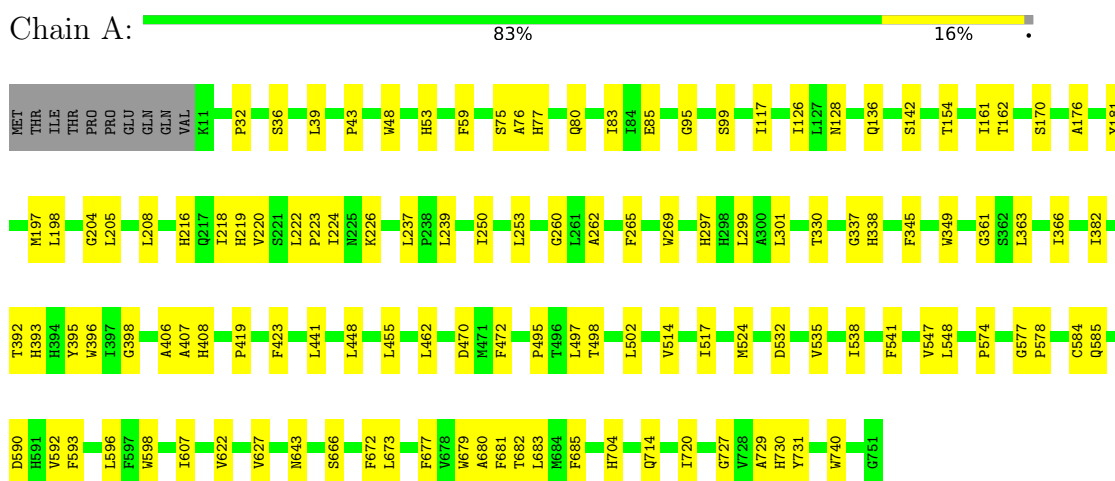


Mol	Chain	Residues	Atoms					AltConf
35	c	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
35	d	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	e	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

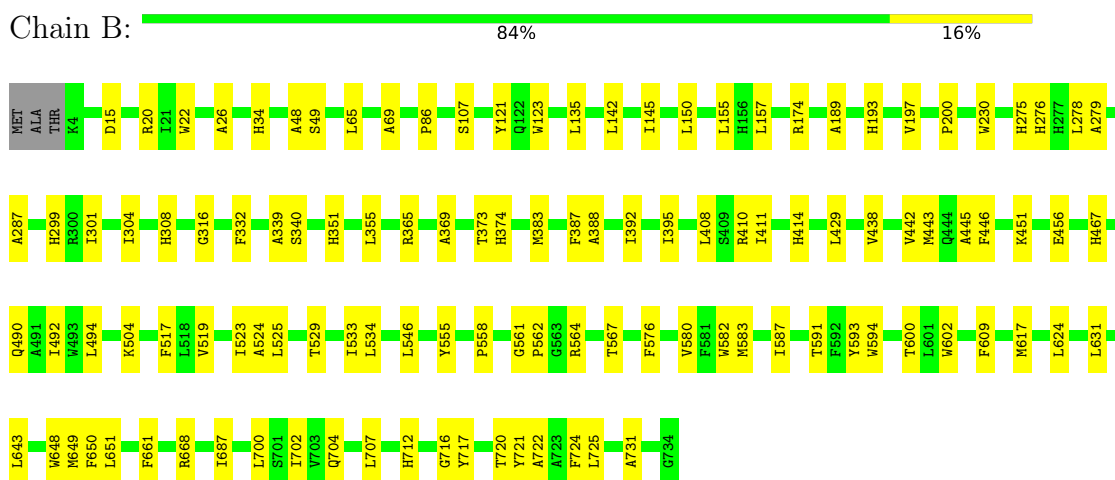
### 3 Residue-property plots

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

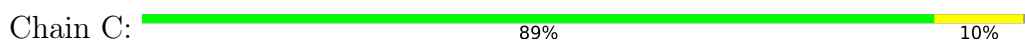
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



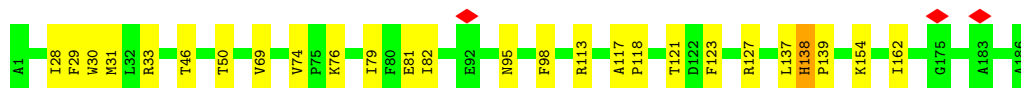
- Molecule 3: Photosystem I iron-sulfur center





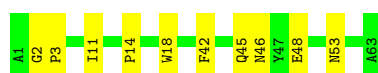
- Molecule 4: PsaD

Chain D: 86% 13%



- Molecule 5: PsaE

Chain E: 84% 16%



- Molecule 6: PsaF

Chain F: 91% 9%



- Molecule 7: Photosystem I reaction center subunit IX

Chain J: 95% 5%



- Molecule 8: Photosystem I reaction center subunit XII

Chain M: 84% 16%



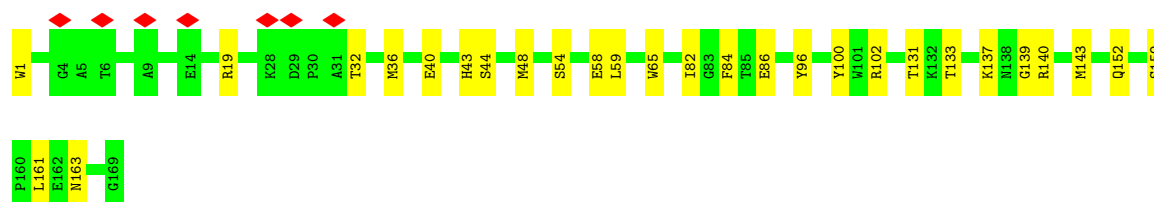
- Molecule 9: Chloroplast light-harvesting complex I protein

Chain a: 90% 10%



- Molecule 10: Chloroplast light-harvesting complex I protein

Chain b: 83% 17%



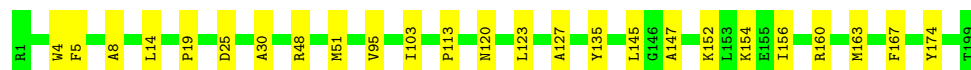
- Molecule 11: LHCE 3



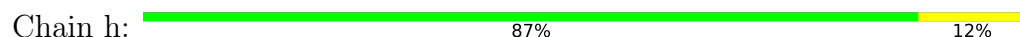
- Molecule 12: Light harvesting chlorophyll a /b binding protein of PSII



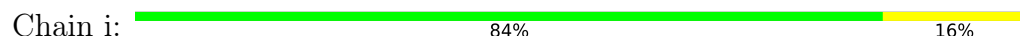
- Molecule 13: Chloroplast light-harvesting complex II protein



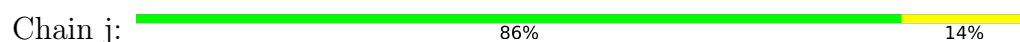
- Molecule 14: LHCE 8




- Molecule 15: LHCE 9



- Molecule 16: Chloroplast light-harvesting complex I protein




- Molecule 17: Chloroplast light-harvesting complex I protein

Chain k:  89% 11%




- Molecule 18: Chloroplast light-harvesting complex I protein

Chain l:  85% 15%




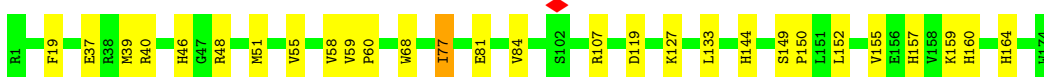
- Molecule 19: Chloroplast light-harvesting complex I protein

Chain m:  85% 15%




- Molecule 20: Chloroplast light-harvesting complex I protein, Lhca7\_2

Chain f:  84% 16%




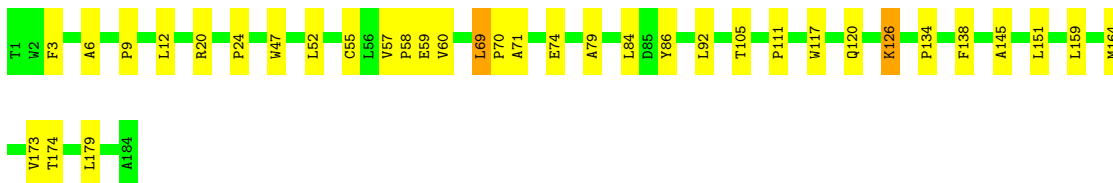
- Molecule 21: Chloroplast light-harvesting complex I protein

Chain g:  90% 10%




- Molecule 22: Chloroplast light-harvesting complex II protein

Chain n:  81% 18%

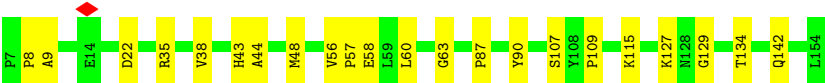
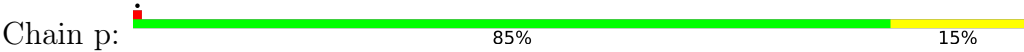


- Molecule 23: Chloroplast light-harvesting complex I protein

Chain o:  83% 17%



● Molecule 24: Chloroplast light-harvesting complex I protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	562173	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	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 (6k x 4k)	Depositor
Maximum map value	1.404	Depositor
Minimum map value	-0.611	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size ( $\text{\AA}$ )	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.04, 1.04, 1.04	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: SF4, LHG, CLA, DD6, SQD, DGD, CHL, LMT, PQN, LMG, BCR

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	0.17	0/6079	0.28	0/8287
2	B	0.17	0/6071	0.28	0/8277
3	C	0.16	0/606	0.30	0/819
4	D	0.13	0/1426	0.27	0/1941
5	E	0.13	0/491	0.25	0/669
6	F	0.14	0/1275	0.26	0/1739
7	J	0.14	0/314	0.24	0/429
8	M	0.16	0/247	0.24	0/332
9	a	0.14	0/1311	0.25	0/1772
10	b	0.13	0/1344	0.28	0/1829
11	c	0.14	0/1719	0.25	0/2336
12	d	0.15	0/1719	0.27	0/2343
13	e	0.13	0/1566	0.25	0/2141
14	h	0.14	0/1388	0.28	0/1886
15	i	0.16	0/1391	0.30	0/1894
16	j	0.16	0/1499	0.27	0/2045
17	k	0.14	0/1377	0.26	0/1871
18	l	0.13	0/1293	0.26	0/1763
19	m	0.14	0/1297	0.30	0/1768
20	f	0.10	0/1367	0.26	0/1861
21	g	0.12	0/1452	0.25	0/1980
22	n	0.11	0/1458	0.26	0/1993
23	o	0.12	0/1266	0.28	0/1727
24	p	0.11	0/1156	0.26	0/1572
All	All	0.15	0/39112	0.27	0/53274

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
4	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
4	D	138	HIS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5878	0	5745	99	0
2	B	5861	0	5659	102	0
3	C	596	0	571	6	0
4	D	1393	0	1371	17	0
5	E	481	0	479	9	0
6	F	1250	0	1259	13	0
7	J	305	0	317	2	0
8	M	243	0	258	4	0
9	a	1274	0	1235	13	0
10	b	1302	0	1244	19	0
11	c	1676	0	1689	16	0
12	d	1669	0	1650	16	0
13	e	1517	0	1468	19	0
14	h	1350	0	1324	18	0
15	i	1355	0	1336	24	0
16	j	1450	0	1401	20	0
17	k	1338	0	1314	13	0
18	l	1256	0	1234	20	0
19	m	1260	0	1236	24	0
20	f	1332	0	1312	16	0
21	g	1406	0	1358	15	0
22	n	1411	0	1372	24	0
23	o	1230	0	1205	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	p	1126	0	1115	13	0
25	A	2599	0	2480	118	0
25	B	2182	0	2078	111	0
25	F	87	0	64	6	0
25	J	50	0	39	2	0
25	a	571	0	488	24	0
25	b	492	0	373	14	0
25	c	638	0	527	22	0
25	d	521	0	418	11	0
25	e	676	0	551	18	0
25	f	553	0	448	10	0
25	g	598	0	467	22	0
25	h	642	0	533	27	0
25	i	603	0	527	15	0
25	j	667	0	568	19	0
25	k	631	0	520	14	0
25	l	562	0	459	17	0
25	m	461	0	369	15	0
25	n	499	0	389	14	0
25	o	429	0	320	12	0
25	p	393	0	297	9	0
26	A	35	0	46	0	0
27	A	87	0	123	7	0
27	a	26	0	22	1	0
27	b	31	0	32	3	0
27	c	30	0	29	3	0
27	d	29	0	28	3	0
27	g	35	0	40	0	0
27	h	61	0	62	3	0
27	i	36	0	42	2	0
27	j	37	0	44	4	0
27	m	32	0	34	2	0
28	A	33	0	46	5	0
28	B	60	0	78	2	0
28	F	26	0	29	0	0
29	A	160	0	224	9	0
29	B	280	0	392	26	0
29	J	40	0	56	3	0
29	M	40	0	56	2	0
30	A	86	0	0	0	0
30	F	43	0	0	0	0
30	J	86	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	86	0	0	1	0
30	b	86	0	0	0	0
30	c	129	0	0	0	0
30	d	129	0	0	1	0
30	e	129	0	0	0	0
30	f	86	0	0	0	0
30	g	86	0	0	0	0
30	h	86	0	0	0	0
30	i	129	0	0	1	0
30	j	86	0	0	0	0
30	k	86	0	0	0	0
30	l	86	0	0	0	0
30	m	86	0	0	2	0
30	n	129	0	0	1	0
30	o	86	0	0	0	0
30	p	43	0	0	0	0
31	A	8	0	0	0	0
31	C	16	0	0	0	0
32	B	54	0	66	2	0
32	b	48	0	54	3	0
32	e	36	0	30	2	0
33	D	36	0	36	0	0
33	F	39	0	42	0	0
33	J	27	0	18	0	0
33	g	32	0	28	2	0
34	a	43	0	56	0	0
34	e	52	0	77	5	0
34	j	44	0	61	0	0
34	k	36	0	42	3	0
35	c	49	0	34	3	0
35	d	186	0	128	7	0
35	e	46	0	31	0	0
All	All	55406	0	51153	806	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 806 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:m:7:PHE:HA	25:m:202:CLA:NB	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:30:ALA:HB2	25:e:205:CLA:HBA1	1.63	0.81
23:o:47:ALA:HB1	23:o:132:GLY:HA3	1.64	0.78
25:A:824:CLA:HBD	25:A:824:CLA:HBA1	1.67	0.76
1:A:740:TRP:HB2	25:A:824:CLA:HBB1	1.69	0.74

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	713 (96%)	24 (3%)	2 (0%)	36	50
2	B	729/734 (99%)	705 (97%)	23 (3%)	1 (0%)	48	64
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	184/186 (99%)	173 (94%)	10 (5%)	1 (0%)	24	36
5	E	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
6	F	166/168 (99%)	163 (98%)	3 (2%)	0	100	100
7	J	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
8	M	29/31 (94%)	29 (100%)	0	0	100	100
9	a	164/166 (99%)	158 (96%)	6 (4%)	0	100	100
10	b	167/169 (99%)	158 (95%)	9 (5%)	0	100	100
11	c	219/221 (99%)	208 (95%)	11 (5%)	0	100	100
12	d	218/220 (99%)	207 (95%)	10 (5%)	1 (0%)	24	36
13	e	197/199 (99%)	190 (96%)	6 (3%)	1 (0%)	24	36
14	h	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
15	i	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
16	j	181/183 (99%)	179 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	k	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
18	l	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
19	m	166/168 (99%)	155 (93%)	11 (7%)	0	100	100
20	f	172/174 (99%)	151 (88%)	20 (12%)	1 (1%)	21	31
21	g	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
22	n	182/184 (99%)	155 (85%)	25 (14%)	2 (1%)	11	16
23	o	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	21	31
24	p	146/148 (99%)	131 (90%)	14 (10%)	1 (1%)	18	27
All	All	4853/4915 (99%)	4619 (95%)	223 (5%)	11 (0%)	44	58

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	f	77	ILE
1	A	205	LEU
1	A	497	LEU
2	B	107	SER
13	e	95	VAL

### 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	621/632 (98%)	619 (100%)	2 (0%)	86	93
2	B	607/609 (100%)	607 (100%)	0	100	100
3	C	69/70 (99%)	68 (99%)	1 (1%)	59	75
4	D	140/140 (100%)	139 (99%)	1 (1%)	76	86
5	E	49/49 (100%)	49 (100%)	0	100	100
6	F	127/127 (100%)	127 (100%)	0	100	100
7	J	34/34 (100%)	34 (100%)	0	100	100
8	M	26/26 (100%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	a	125/125 (100%)	125 (100%)	0	100	100
10	b	130/130 (100%)	129 (99%)	1 (1%)	73	84
11	c	172/172 (100%)	172 (100%)	0	100	100
12	d	167/167 (100%)	167 (100%)	0	100	100
13	e	152/152 (100%)	152 (100%)	0	100	100
14	h	142/142 (100%)	140 (99%)	2 (1%)	59	75
15	i	137/137 (100%)	137 (100%)	0	100	100
16	j	145/145 (100%)	145 (100%)	0	100	100
17	k	141/141 (100%)	140 (99%)	1 (1%)	76	86
18	l	122/122 (100%)	122 (100%)	0	100	100
19	m	122/122 (100%)	122 (100%)	0	100	100
20	f	135/135 (100%)	134 (99%)	1 (1%)	76	86
21	g	140/140 (100%)	140 (100%)	0	100	100
22	n	140/140 (100%)	140 (100%)	0	100	100
23	o	119/119 (100%)	118 (99%)	1 (1%)	73	84
24	p	114/114 (100%)	111 (97%)	3 (3%)	40	61
All	All	3876/3890 (100%)	3863 (100%)	13 (0%)	84	93

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	k	31	LYS
20	f	127	LYS
24	p	134	THR
24	p	115	LYS
24	p	127	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
16	j	89	GLN
22	n	63	ASN
16	j	179	HIS
20	f	164	HIS
5	E	21	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

367 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	$\# Z  > 2$
30	DD6	i	216	-	40,45,45	1.35	4 (10%)	51,67,67	2.04	13 (25%)
25	CLA	c	315	11	51,55,73	1.36	6 (11%)	60,91,113	1.73	6 (10%)
25	CLA	B	815	2	53,57,73	1.36	6 (11%)	61,93,113	1.71	7 (11%)
25	CLA	A	818	1	69,73,73	1.22	7 (10%)	82,113,113	1.56	11 (13%)
25	CLA	k	214	17	54,58,73	1.36	6 (11%)	64,95,113	1.77	7 (10%)
25	CLA	n	207	-	45,49,73	1.44	8 (17%)	54,84,113	1.85	9 (16%)
25	CLA	g	208	21	54,58,73	1.38	7 (12%)	64,95,113	1.74	6 (9%)
32	DGD	e	203	-	37,37,67	1.22	1 (2%)	51,51,81	1.09	1 (1%)
29	BCR	B	833	-	41,41,41	0.81	1 (2%)	56,56,56	1.13	4 (7%)
29	BCR	B	828	-	41,41,41	0.80	2 (4%)	56,56,56	1.19	5 (8%)
33	SQD	J	102	-	25,27,54	1.83	7 (28%)	35,38,65	1.56	7 (20%)
34	LMG	a	202	-	43,43,55	0.88	2 (4%)	51,51,63	1.17	2 (3%)
25	CLA	j	215	16	54,58,73	1.37	7 (12%)	64,95,113	1.81	6 (9%)
30	DD6	f	613	-	40,45,45	1.30	4 (10%)	51,67,67	2.15	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	e	215	13	47,51,73	1.39	7 (14%)	55,86,113	1.86	5 (9%)
35	CHL	d	309	-	37,51,74	2.21	10 (27%)	30,86,114	3.23	14 (46%)
25	CLA	A	829	1	62,66,73	1.29	6 (9%)	73,104,113	1.66	6 (8%)
30	DD6	c	317	-	40,45,45	1.51	6 (15%)	51,67,67	2.02	16 (31%)
28	PQN	B	835	-	28,28,34	1.06	2 (7%)	35,37,45	1.94	10 (28%)
35	CHL	d	308	-	40,54,74	2.23	12 (30%)	34,90,114	3.26	17 (50%)
30	DD6	g	217	-	40,45,45	1.43	5 (12%)	51,67,67	2.10	12 (23%)
25	CLA	J	103	7	54,58,73	1.38	7 (12%)	64,95,113	1.78	9 (14%)
30	DD6	a	215	-	40,45,45	1.51	6 (15%)	51,67,67	1.99	12 (23%)
25	CLA	B	823	2	64,68,73	1.26	5 (7%)	76,107,113	1.57	12 (15%)
25	CLA	j	213	16	46,50,73	1.39	6 (13%)	53,85,113	1.83	6 (11%)
25	CLA	n	209	22	45,49,73	1.45	7 (15%)	54,84,113	1.74	7 (12%)
25	CLA	A	804	1	64,68,73	1.28	8 (12%)	76,107,113	1.73	10 (13%)
25	CLA	A	821	-	68,72,73	1.23	7 (10%)	80,111,113	1.62	10 (12%)
30	DD6	m	212	-	40,45,45	1.36	4 (10%)	51,67,67	2.02	12 (23%)
25	CLA	B	824	2	69,73,73	1.21	7 (10%)	82,113,113	1.59	10 (12%)
25	CLA	B	838	2	65,69,73	1.26	8 (12%)	77,108,113	1.72	8 (10%)
25	CLA	d	311	12	53,57,73	1.36	7 (13%)	61,93,113	1.85	5 (8%)
25	CLA	B	813	2	53,57,73	1.41	7 (13%)	62,93,113	1.71	7 (11%)
25	CLA	c	311	27	47,51,73	1.39	6 (12%)	55,86,113	1.76	5 (9%)
25	CLA	a	212	9	59,63,73	1.32	6 (10%)	70,101,113	1.73	8 (11%)
28	PQN	B	827	-	34,34,34	1.13	3 (8%)	43,45,45	1.81	10 (23%)
25	CLA	A	831	1	52,56,73	1.38	7 (13%)	61,92,113	1.78	7 (11%)
30	DD6	l	614	-	40,45,45	1.48	6 (15%)	51,67,67	2.01	14 (27%)
25	CLA	B	817	-	54,58,73	1.38	7 (12%)	64,95,113	1.70	7 (10%)
25	CLA	e	216	13	59,63,73	1.32	7 (11%)	70,101,113	1.69	7 (10%)
25	CLA	f	603	20	47,51,73	1.42	6 (12%)	55,86,113	1.81	6 (10%)
25	CLA	e	214	-	46,50,73	1.40	6 (13%)	53,85,113	1.71	6 (11%)
25	CLA	o	604	-	46,50,73	1.41	7 (15%)	53,85,113	1.81	6 (11%)
30	DD6	p	610	-	40,45,45	1.29	4 (10%)	51,67,67	2.16	14 (27%)
25	CLA	o	601	23	45,49,73	1.47	10 (22%)	54,84,113	1.71	9 (16%)
25	CLA	p	608	24	47,51,73	1.39	6 (12%)	55,86,113	1.66	5 (9%)
25	CLA	l	605	-	47,51,73	1.38	7 (14%)	55,86,113	1.79	6 (10%)
32	DGD	B	849	-	55,55,67	1.09	1 (1%)	69,69,81	1.03	1 (1%)
25	CLA	c	306	-	47,51,73	1.39	6 (12%)	55,86,113	1.78	6 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	g	211	21	46,50,73	1.41	7 (15%)	53,85,113	1.87	3 (5%)
25	CLA	n	202	22	59,63,73	1.34	7 (11%)	70,101,113	1.73	6 (8%)
25	CLA	f	605	20	46,50,73	1.40	7 (15%)	53,85,113	1.91	5 (9%)
25	CLA	B	844	2	69,73,73	1.24	8 (11%)	82,113,113	1.70	12 (14%)
25	CLA	A	833	1	69,73,73	1.20	6 (8%)	82,113,113	1.51	10 (12%)
25	CLA	e	211	-	52,56,73	1.36	7 (13%)	61,92,113	1.72	6 (9%)
25	CLA	m	210	19	47,51,73	1.39	6 (12%)	55,86,113	1.81	5 (9%)
30	DD6	n	213	-	40,45,45	1.34	5 (12%)	51,67,67	1.38	9 (17%)
27	LHG	j	202	25	36,36,48	1.58	2 (5%)	39,42,54	1.29	5 (12%)
25	CLA	l	610	18	52,56,73	1.37	6 (11%)	61,92,113	1.73	7 (11%)
25	CLA	g	207	-	49,53,73	1.43	7 (14%)	58,89,113	1.83	4 (6%)
25	CLA	A	842	1	53,57,73	1.35	6 (11%)	61,93,113	1.80	6 (9%)
25	CLA	f	608	-	46,50,73	1.41	7 (15%)	53,85,113	1.91	6 (11%)
27	LHG	b	201	-	30,30,48	1.81	2 (6%)	33,36,54	1.33	4 (12%)
25	CLA	h	211	14	62,66,73	1.29	7 (11%)	73,104,113	1.69	8 (10%)
25	CLA	b	207	-	49,53,73	1.40	7 (14%)	58,89,113	1.81	5 (8%)
25	CLA	e	210	-	47,51,73	1.38	6 (12%)	55,86,113	1.85	5 (9%)
25	CLA	b	209	10	49,53,73	1.39	7 (14%)	58,89,113	1.79	7 (12%)
30	DD6	e	218	-	40,45,45	1.40	6 (15%)	51,67,67	1.43	9 (17%)
25	CLA	p	606	24	54,58,73	1.41	8 (14%)	64,95,113	1.77	7 (10%)
25	CLA	A	817	1	60,64,73	1.30	8 (13%)	71,102,113	1.68	6 (8%)
25	CLA	o	605	-	47,51,73	1.38	7 (14%)	55,86,113	1.78	4 (7%)
25	CLA	A	816	1	47,51,73	1.38	7 (14%)	55,86,113	1.77	4 (7%)
29	BCR	B	801	-	41,41,41	0.73	0	56,56,56	1.24	6 (10%)
32	DGD	b	202	-	49,49,67	1.22	6 (12%)	63,63,81	1.07	3 (4%)
31	SF4	C	102	3	0,12,12	-	-	-	-	-
25	CLA	d	316	12	46,50,73	1.37	6 (13%)	53,85,113	1.76	5 (9%)
25	CLA	o	603	23	47,51,73	1.44	7 (14%)	55,86,113	1.78	5 (9%)
30	DD6	f	614	-	40,45,45	1.29	4 (10%)	51,67,67	2.29	17 (33%)
25	CLA	o	606	23	49,53,73	1.40	6 (12%)	58,89,113	1.83	7 (12%)
25	CLA	p	602	24	47,51,73	1.42	9 (19%)	55,86,113	1.93	8 (14%)
30	DD6	J	105	-	40,45,45	1.36	6 (15%)	51,67,67	1.43	8 (15%)
25	CLA	o	602	23	51,55,73	1.38	6 (11%)	60,91,113	1.80	7 (11%)
25	CLA	a	204	9	64,68,73	1.26	5 (7%)	76,107,113	1.58	13 (17%)
25	CLA	i	203	15	68,72,73	1.24	7 (10%)	80,111,113	1.64	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	l	611	18	46,50,73	1.42	6 (13%)	53,85,113	1.88	6 (11%)
25	CLA	a	210	27	49,53,73	1.41	6 (12%)	58,89,113	1.80	7 (12%)
25	CLA	c	305	-	52,56,73	1.37	6 (11%)	61,92,113	1.77	7 (11%)
25	CLA	d	313	27	49,53,73	1.41	7 (14%)	58,89,113	1.79	6 (10%)
25	CLA	g	205	21	46,50,73	1.43	7 (15%)	53,85,113	1.73	5 (9%)
25	CLA	p	603	24	46,50,73	1.45	7 (15%)	53,85,113	1.61	4 (7%)
25	CLA	l	609	18	47,51,73	1.39	6 (12%)	55,86,113	1.81	4 (7%)
25	CLA	B	839	-	64,68,73	1.28	7 (10%)	76,107,113	1.74	9 (11%)
25	CLA	B	811	2	67,71,73	1.22	7 (10%)	79,110,113	1.71	9 (11%)
25	CLA	f	610	20	63,67,73	1.28	6 (9%)	74,105,113	1.67	8 (10%)
30	DD6	g	216	-	40,45,45	1.35	4 (10%)	51,67,67	2.15	14 (27%)
25	CLA	o	608	23	46,50,73	1.57	9 (19%)	55,84,113	1.91	5 (9%)
25	CLA	e	217	13	46,50,73	1.38	6 (13%)	53,85,113	1.81	3 (5%)
25	CLA	e	204	13	45,49,73	1.41	6 (13%)	52,84,113	1.84	7 (13%)
25	CLA	c	312	11	47,51,73	1.39	7 (14%)	55,86,113	1.82	5 (9%)
30	DD6	n	212	-	40,45,45	1.30	4 (10%)	51,67,67	2.37	13 (25%)
25	CLA	b	203	-	46,50,73	1.41	7 (15%)	53,85,113	1.84	6 (11%)
25	CLA	B	843	2	67,71,73	1.22	6 (8%)	79,110,113	1.58	9 (11%)
25	CLA	j	211	16	59,63,73	1.32	7 (11%)	70,101,113	1.71	8 (11%)
27	LHG	A	805	25	37,37,48	1.52	2 (5%)	40,43,54	1.25	5 (12%)
25	CLA	A	820	1	61,65,73	1.29	7 (11%)	72,103,113	1.76	11 (15%)
25	CLA	B	819	2	69,73,73	1.22	7 (10%)	82,113,113	1.51	7 (8%)
25	CLA	B	805	2	69,73,73	1.20	6 (8%)	82,113,113	1.67	10 (12%)
29	BCR	A	838	-	41,41,41	0.79	1 (2%)	56,56,56	1.07	5 (8%)
30	DD6	o	611	-	40,45,45	1.32	4 (10%)	51,67,67	2.02	11 (21%)
29	BCR	B	829	-	41,41,41	0.76	1 (2%)	56,56,56	1.09	4 (7%)
25	CLA	k	207	17	54,58,73	1.37	7 (12%)	64,95,113	1.74	8 (12%)
25	CLA	b	205	10	47,51,73	1.38	7 (14%)	55,86,113	1.83	4 (7%)
30	DD6	d	318	-	40,45,45	1.54	5 (12%)	51,67,67	2.05	13 (25%)
25	CLA	n	205	-	46,50,73	1.39	6 (13%)	53,85,113	1.81	3 (5%)
25	CLA	A	841	-	61,65,73	1.28	7 (11%)	72,103,113	1.68	7 (9%)
25	CLA	A	847	1	47,51,73	1.38	5 (10%)	55,86,113	1.67	4 (7%)
30	DD6	l	613	-	40,45,45	1.44	5 (12%)	51,67,67	2.03	14 (27%)
29	BCR	B	832	-	41,41,41	1.49	4 (9%)	56,56,56	1.32	9 (16%)
25	CLA	l	602	18	63,67,73	1.28	8 (12%)	74,105,113	1.66	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	a	205	9	57,61,73	1.34	7 (12%)	67,98,113	1.74	8 (11%)
27	LHG	c	301	25	29,29,48	1.80	2 (6%)	32,35,54	1.38	5 (15%)
30	DD6	o	612	-	40,45,45	1.38	4 (10%)	51,67,67	2.03	13 (25%)
30	DD6	e	220	-	40,45,45	1.37	8 (20%)	51,67,67	1.59	8 (15%)
25	CLA	i	210	15	47,51,73	1.38	7 (14%)	55,86,113	1.82	5 (9%)
30	DD6	A	854	-	40,45,45	1.54	4 (10%)	51,67,67	2.14	15 (29%)
25	CLA	A	812	1	69,73,73	1.21	6 (8%)	82,113,113	1.60	8 (9%)
30	DD6	k	215	-	40,45,45	1.46	5 (12%)	51,67,67	2.04	12 (23%)
25	CLA	k	203	17	57,61,73	1.34	7 (12%)	67,98,113	1.71	9 (13%)
25	CLA	e	207	-	54,58,73	1.37	7 (12%)	64,95,113	1.75	10 (15%)
25	CLA	f	601	20	46,50,73	1.41	6 (13%)	53,85,113	1.74	5 (9%)
25	CLA	n	204	22	46,50,73	1.40	6 (13%)	53,85,113	1.81	6 (11%)
25	CLA	B	845	2	69,73,73	1.22	6 (8%)	82,113,113	1.69	6 (7%)
30	DD6	i	215	-	40,45,45	1.51	7 (17%)	51,67,67	2.01	13 (25%)
25	CLA	a	206	-	49,53,73	1.41	7 (14%)	58,89,113	1.74	7 (12%)
25	CLA	f	609	20	46,50,73	1.44	6 (13%)	53,85,113	1.60	4 (7%)
25	CLA	l	603	18	47,51,73	1.39	7 (14%)	55,86,113	1.86	5 (9%)
25	CLA	A	824	1	62,66,73	1.28	6 (9%)	73,104,113	1.69	9 (12%)
25	CLA	d	305	12	46,50,73	1.38	7 (15%)	53,85,113	1.90	4 (7%)
25	CLA	A	846	1	69,73,73	1.21	7 (10%)	82,113,113	1.67	11 (13%)
25	CLA	B	848	-	69,73,73	1.20	7 (10%)	82,113,113	1.68	8 (9%)
30	DD6	h	216	-	40,45,45	1.47	5 (12%)	51,67,67	2.03	12 (23%)
25	CLA	k	212	17	46,50,73	1.39	6 (13%)	53,85,113	1.79	5 (9%)
27	LHG	i	201	25	35,35,48	1.58	2 (5%)	38,41,54	1.30	5 (13%)
25	CLA	i	206	-	69,73,73	1.22	7 (10%)	82,113,113	1.66	8 (9%)
25	CLA	j	212	16	66,70,73	1.23	5 (7%)	78,109,113	1.67	9 (11%)
27	LHG	h	202	25	30,30,48	1.73	2 (6%)	33,36,54	1.39	5 (15%)
25	CLA	A	857	-	57,61,73	1.34	7 (12%)	67,98,113	1.69	7 (10%)
25	CLA	i	207	15	47,51,73	1.37	6 (12%)	55,86,113	1.84	5 (9%)
25	CLA	l	604	-	47,51,73	1.39	6 (12%)	55,86,113	1.71	5 (9%)
25	CLA	c	310	11	59,63,73	1.31	8 (13%)	70,101,113	1.72	9 (12%)
25	CLA	d	303	-	54,58,73	1.36	7 (12%)	64,95,113	1.87	9 (14%)
25	CLA	l	608	-	47,51,73	1.39	6 (12%)	55,86,113	1.82	6 (10%)
30	DD6	F	203	-	40,45,45	1.36	4 (10%)	51,67,67	1.37	8 (15%)
25	CLA	B	814	2	63,67,73	1.28	7 (11%)	74,105,113	1.71	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	g	215	21	49,53,73	1.40	7 (14%)	58,89,113	1.76	6 (10%)
25	CLA	a	207	-	57,61,73	1.33	6 (10%)	67,98,113	1.72	8 (11%)
25	CLA	k	209	-	46,50,73	1.40	6 (13%)	53,85,113	1.80	4 (7%)
25	CLA	d	312	12	63,67,73	1.28	6 (9%)	74,105,113	1.74	8 (10%)
25	CLA	e	208	13	46,50,73	1.40	6 (13%)	53,85,113	1.88	5 (9%)
25	CLA	h	214	14	46,50,73	1.39	7 (15%)	53,85,113	1.89	4 (7%)
25	CLA	F	201	-	46,50,73	1.40	6 (13%)	53,85,113	1.87	5 (9%)
30	DD6	c	316	-	40,45,45	1.54	7 (17%)	51,67,67	2.05	14 (27%)
30	DD6	e	219	-	40,45,45	1.49	5 (12%)	51,67,67	2.04	13 (25%)
25	CLA	n	206	-	46,50,73	1.41	7 (15%)	53,85,113	1.80	5 (9%)
25	CLA	l	612	-	46,50,73	1.41	7 (15%)	53,85,113	1.97	5 (9%)
25	CLA	A	850	1	59,63,73	1.30	6 (10%)	70,101,113	1.64	9 (12%)
25	CLA	i	205	-	47,51,73	1.38	7 (14%)	55,86,113	1.75	5 (9%)
29	BCR	J	101	-	41,41,41	1.42	7 (17%)	56,56,56	1.49	11 (19%)
26	LMT	A	803	-	36,36,36	0.55	0	47,47,47	0.66	0
25	CLA	b	204	10	57,61,73	1.35	7 (12%)	67,98,113	1.74	9 (13%)
25	CLA	g	209	21	59,63,73	1.30	6 (10%)	70,101,113	1.68	8 (11%)
25	CLA	b	212	10	56,60,73	1.35	8 (14%)	65,97,113	1.80	8 (12%)
25	CLA	a	203	9	54,58,73	1.38	6 (11%)	64,95,113	1.67	8 (12%)
27	LHG	g	201	25	34,34,48	1.63	2 (5%)	37,40,54	1.32	5 (13%)
25	CLA	n	208	22	49,53,73	1.41	7 (14%)	58,89,113	1.85	4 (6%)
35	CHL	e	209	-	40,54,74	2.22	12 (30%)	34,90,114	3.24	17 (50%)
25	CLA	B	822	2	64,68,73	1.26	7 (10%)	76,107,113	1.70	10 (13%)
27	LHG	a	201	25	25,25,48	1.91	2 (8%)	28,31,54	1.43	5 (17%)
30	DD6	b	215	-	40,45,45	1.44	5 (12%)	51,67,67	2.03	14 (27%)
25	CLA	A	828	1	47,51,73	1.39	6 (12%)	55,86,113	1.82	7 (12%)
25	CLA	A	852	1	52,56,73	1.37	6 (11%)	61,92,113	1.91	7 (11%)
25	CLA	A	815	1	62,66,73	1.27	6 (9%)	73,104,113	1.84	8 (10%)
30	DD6	d	317	-	40,45,45	1.48	5 (12%)	51,67,67	2.03	13 (25%)
25	CLA	a	209	9	58,62,73	1.31	5 (8%)	68,99,113	1.79	8 (11%)
30	DD6	A	855	-	40,45,45	1.42	4 (10%)	51,67,67	2.25	19 (37%)
25	CLA	a	208	9	54,58,73	1.38	7 (12%)	64,95,113	1.78	7 (10%)
25	CLA	A	851	1	49,53,73	1.39	7 (14%)	58,89,113	1.80	8 (13%)
30	DD6	c	318	-	40,45,45	1.36	4 (10%)	51,67,67	2.20	16 (31%)
25	CLA	B	834	2	59,63,73	1.32	6 (10%)	70,101,113	1.73	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	A	819	-	69,73,73	1.21	7 (10%)	82,113,113	1.56	11 (13%)
25	CLA	d	306	-	56,60,73	1.36	7 (12%)	65,97,113	1.74	8 (12%)
25	CLA	p	601	-	46,50,73	1.39	7 (15%)	53,85,113	1.68	6 (11%)
25	CLA	i	209	27	47,51,73	1.38	6 (12%)	55,86,113	1.84	6 (10%)
25	CLA	j	214	16	47,51,73	1.37	7 (14%)	55,86,113	1.83	5 (9%)
25	CLA	o	610	23	47,51,73	1.41	7 (14%)	55,86,113	1.78	6 (10%)
25	CLA	A	814	1	63,67,73	1.28	7 (11%)	74,105,113	1.73	10 (13%)
25	CLA	p	609	24	47,51,73	1.41	7 (14%)	55,86,113	1.86	8 (14%)
25	CLA	A	830	1	56,60,73	1.35	6 (10%)	65,97,113	1.71	10 (15%)
25	CLA	d	304	12	61,65,73	1.29	6 (9%)	72,103,113	1.72	9 (12%)
25	CLA	l	607	18	58,62,73	1.32	5 (8%)	68,99,113	1.69	7 (10%)
25	CLA	k	213	17	46,50,73	1.40	7 (15%)	53,85,113	1.88	6 (11%)
25	CLA	B	836	2	57,61,73	1.35	7 (12%)	67,98,113	1.73	8 (11%)
30	DD6	b	214	-	40,45,45	1.39	4 (10%)	51,67,67	2.13	12 (23%)
30	DD6	h	217	-	40,45,45	1.46	4 (10%)	51,67,67	2.01	13 (25%)
25	CLA	f	606	20	46,50,73	1.41	7 (15%)	53,85,113	1.79	6 (11%)
25	CLA	k	208	17	61,65,73	1.28	6 (9%)	72,103,113	1.68	9 (12%)
25	CLA	B	821	2	64,68,73	1.27	7 (10%)	76,107,113	1.70	9 (11%)
25	CLA	k	202	17	47,51,73	1.39	7 (14%)	55,86,113	1.75	6 (10%)
25	CLA	h	213	14	47,51,73	1.38	6 (12%)	55,86,113	1.71	5 (9%)
25	CLA	A	809	1	69,73,73	1.21	6 (8%)	82,113,113	1.65	7 (8%)
25	CLA	c	308	-	54,58,73	1.37	7 (12%)	64,95,113	1.70	9 (14%)
25	CLA	i	202	15	57,61,73	1.34	7 (12%)	67,98,113	1.73	8 (11%)
25	CLA	b	208	-	45,49,73	1.44	8 (17%)	54,84,113	1.85	7 (12%)
25	CLA	A	813	1	62,66,73	1.28	6 (9%)	73,104,113	1.67	8 (10%)
25	CLA	e	213	13	59,63,73	1.29	6 (10%)	70,101,113	1.70	9 (12%)
25	CLA	A	827	1	47,51,73	1.38	7 (14%)	55,86,113	1.82	6 (10%)
25	CLA	k	206	-	54,58,73	1.37	7 (12%)	64,95,113	1.82	8 (12%)
33	SQD	g	202	-	30,32,54	1.87	7 (23%)	40,43,65	1.51	6 (15%)
30	DD6	J	104	-	40,45,45	1.54	6 (15%)	51,67,67	2.10	14 (27%)
25	CLA	f	612	20	47,51,73	1.40	7 (14%)	55,86,113	1.81	5 (9%)
25	CLA	m	211	19	46,50,73	1.40	6 (13%)	53,85,113	1.79	7 (13%)
35	CHL	c	307	-	43,57,74	2.16	11 (25%)	37,93,114	3.07	17 (45%)
25	CLA	A	811	1	54,58,73	1.39	7 (12%)	64,95,113	1.81	10 (15%)
25	CLA	A	845	-	52,56,73	1.36	7 (13%)	61,92,113	1.74	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	B	803	-	59,63,73	1.30	5 (8%)	70,101,113	1.89	11 (15%)
34	LMG	k	201	-	36,36,55	0.96	2 (5%)	44,44,63	1.12	3 (6%)
25	CLA	A	808	1	64,68,73	1.25	6 (9%)	76,107,113	1.74	9 (11%)
25	CLA	c	309	11	64,68,73	1.27	6 (9%)	76,107,113	1.72	8 (10%)
25	CLA	c	314	11	46,50,73	1.40	7 (15%)	53,85,113	1.76	6 (11%)
25	CLA	e	206	13	49,53,73	1.40	8 (16%)	58,89,113	1.80	6 (10%)
25	CLA	j	204	16	59,63,73	1.28	5 (8%)	70,101,113	1.75	8 (11%)
29	BCR	A	839	-	41,41,41	0.76	1 (2%)	56,56,56	1.04	5 (8%)
25	CLA	j	210	27	54,58,73	1.37	7 (12%)	64,95,113	1.78	8 (12%)
30	DD6	d	319	-	40,45,45	1.35	4 (10%)	51,67,67	2.21	16 (31%)
31	SF4	C	101	3	0,12,12	-	-	-	-	-
29	BCR	B	831	-	41,41,41	1.45	4 (9%)	56,56,56	1.32	10 (17%)
25	CLA	a	213	-	67,71,73	1.24	6 (8%)	79,110,113	1.69	10 (12%)
25	CLA	B	837	2	54,58,73	1.38	7 (12%)	64,95,113	1.78	6 (9%)
25	CLA	B	809	2	46,50,73	1.39	6 (13%)	53,85,113	1.84	4 (7%)
25	CLA	p	605	-	46,50,73	1.40	6 (13%)	53,85,113	1.83	5 (9%)
30	DD6	n	214	-	40,45,45	1.35	7 (17%)	51,67,67	1.64	10 (19%)
25	CLA	h	204	14	59,63,73	1.34	7 (11%)	70,101,113	1.73	9 (12%)
25	CLA	k	210	17	47,51,73	1.39	7 (14%)	55,86,113	1.80	6 (10%)
25	CLA	A	825	1	69,73,73	1.23	7 (10%)	82,113,113	1.59	10 (12%)
25	CLA	b	210	10	46,50,73	1.39	6 (13%)	53,85,113	1.82	6 (11%)
25	CLA	k	204	17	46,50,73	1.39	7 (15%)	53,85,113	2.00	4 (7%)
25	CLA	f	607	20	59,63,73	1.34	7 (11%)	70,101,113	1.72	10 (14%)
28	PQN	A	834	-	34,34,34	1.03	2 (5%)	43,45,45	1.75	10 (23%)
25	CLA	h	210	27	47,51,73	1.38	6 (12%)	55,86,113	1.78	6 (10%)
30	DD6	a	214	-	40,45,45	1.41	4 (10%)	51,67,67	2.10	13 (25%)
25	CLA	c	302	11	46,50,73	1.38	7 (15%)	53,85,113	1.73	5 (9%)
25	CLA	m	204	19	58,62,73	1.33	7 (12%)	68,99,113	1.71	9 (13%)
30	DD6	m	213	-	40,45,45	1.43	5 (12%)	51,67,67	2.03	13 (25%)
25	CLA	B	842	2	57,61,73	1.34	7 (12%)	67,98,113	1.64	8 (11%)
25	CLA	A	840	-	67,71,73	1.23	7 (10%)	79,110,113	1.60	9 (11%)
29	BCR	A	836	-	41,41,41	0.82	1 (2%)	56,56,56	1.10	4 (7%)
25	CLA	A	801	1	69,73,73	1.20	7 (10%)	82,113,113	1.73	12 (14%)
27	LHG	A	835	-	48,48,48	1.38	2 (4%)	51,54,54	1.19	5 (9%)
30	DD6	i	214	-	40,45,45	1.50	6 (15%)	51,67,67	2.05	12 (23%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	F	202	6	49,53,73	1.39	6 (12%)	58,89,113	1.75	7 (12%)
25	CLA	m	207	19	54,58,73	1.37	7 (12%)	64,95,113	1.78	7 (10%)
25	CLA	c	304	11	57,61,73	1.33	7 (12%)	67,98,113	1.74	9 (13%)
25	CLA	A	807	-	69,73,73	1.20	7 (10%)	82,113,113	1.64	8 (9%)
33	SQD	D	200	-	34,36,54	1.77	7 (20%)	44,47,65	1.69	10 (22%)
25	CLA	a	211	9	47,51,73	1.39	7 (14%)	55,86,113	1.84	4 (7%)
25	CLA	B	816	-	64,68,73	1.25	6 (9%)	76,107,113	1.72	11 (14%)
25	CLA	b	213	10	46,50,73	1.40	6 (13%)	53,85,113	1.82	6 (11%)
25	CLA	h	207	-	52,56,73	1.37	7 (13%)	61,92,113	1.81	5 (8%)
25	CLA	g	212	21	59,63,73	1.32	7 (11%)	70,101,113	1.75	8 (11%)
25	CLA	e	212	13	56,60,73	1.35	6 (10%)	65,97,113	1.77	7 (10%)
34	LMG	e	202	-	52,52,55	0.81	2 (3%)	60,60,63	1.07	2 (3%)
25	CLA	k	205	17	69,73,73	1.22	6 (8%)	82,113,113	1.61	8 (9%)
25	CLA	g	204	21	57,61,73	1.33	7 (12%)	67,98,113	1.67	8 (11%)
25	CLA	m	203	19	64,68,73	1.27	6 (9%)	76,107,113	1.51	9 (11%)
25	CLA	A	832	1	69,73,73	1.22	6 (8%)	82,113,113	1.56	10 (12%)
25	CLA	A	823	1	68,72,73	1.22	6 (8%)	80,111,113	1.79	6 (7%)
29	BCR	B	830	-	41,41,41	0.79	2 (4%)	56,56,56	1.02	4 (7%)
25	CLA	i	213	15	54,58,73	1.37	7 (12%)	64,95,113	1.79	6 (9%)
25	CLA	e	201	-	57,61,73	1.35	7 (12%)	67,98,113	1.80	7 (10%)
25	CLA	h	205	14	47,51,73	1.37	7 (14%)	55,86,113	1.90	6 (10%)
25	CLA	o	607	23	45,49,73	1.44	9 (20%)	54,84,113	1.74	7 (12%)
25	CLA	h	203	14	54,58,73	1.38	6 (11%)	64,95,113	1.78	9 (14%)
34	LMG	j	201	-	44,44,55	0.85	1 (2%)	52,52,63	1.07	2 (3%)
25	CLA	A	826	1	69,73,73	1.23	7 (10%)	82,113,113	1.72	8 (9%)
25	CLA	f	604	-	46,50,73	1.41	7 (15%)	53,85,113	1.80	6 (11%)
25	CLA	B	808	2	47,51,73	1.39	7 (14%)	55,86,113	1.79	4 (7%)
25	CLA	i	204	15	47,51,73	1.39	7 (14%)	55,86,113	1.72	6 (10%)
27	LHG	h	201	-	29,29,48	1.78	2 (6%)	32,35,54	1.12	2 (6%)
25	CLA	h	206	-	64,68,73	1.27	7 (10%)	76,107,113	1.70	8 (10%)
25	CLA	A	843	1	56,60,73	1.36	6 (10%)	65,97,113	1.85	9 (13%)
25	CLA	f	611	20	46,50,73	1.40	6 (13%)	53,85,113	1.75	7 (13%)
25	CLA	i	212	15	46,50,73	1.39	6 (13%)	53,85,113	1.74	6 (11%)
29	BCR	A	837	-	41,41,41	1.46	4 (9%)	56,56,56	1.41	12 (21%)
25	CLA	c	313	11	57,61,73	1.33	7 (12%)	67,98,113	1.72	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	B	807	2	69,73,73	1.21	6 (8%)	82,113,113	1.64	8 (9%)
25	CLA	o	609	23	46,50,73	1.40	6 (13%)	53,85,113	1.84	6 (11%)
27	LHG	d	302	25	28,28,48	1.80	2 (7%)	31,34,54	1.36	5 (16%)
35	CHL	d	307	12	45,59,74	2.16	12 (26%)	40,96,114	3.06	19 (47%)
25	CLA	h	212	14	57,61,73	1.33	6 (10%)	67,98,113	1.76	9 (13%)
25	CLA	n	210	22	46,50,73	1.41	7 (15%)	53,85,113	1.90	3 (5%)
25	CLA	p	607	24	49,53,73	1.44	7 (14%)	58,89,113	1.70	5 (8%)
25	CLA	i	211	15	63,67,73	1.28	7 (11%)	74,105,113	1.72	10 (13%)
25	CLA	j	207	-	51,55,73	1.39	8 (15%)	60,91,113	1.86	5 (8%)
25	CLA	n	201	22	63,67,73	1.26	6 (9%)	74,105,113	1.79	8 (10%)
25	CLA	d	314	12	46,50,73	1.40	7 (15%)	53,85,113	1.88	3 (5%)
25	CLA	A	810	1	69,73,73	1.21	6 (8%)	82,113,113	1.69	8 (9%)
25	CLA	n	211	22	46,50,73	1.41	8 (17%)	53,85,113	1.72	4 (7%)
27	LHG	m	201	-	31,31,48	1.77	2 (6%)	34,37,54	1.35	5 (14%)
25	CLA	m	206	-	46,50,73	1.40	7 (15%)	53,85,113	1.84	4 (7%)
25	CLA	A	822	-	57,61,73	1.34	7 (12%)	67,98,113	1.73	8 (11%)
25	CLA	g	214	21	46,50,73	1.40	6 (13%)	53,85,113	1.85	5 (9%)
25	CLA	h	209	14	58,62,73	1.31	6 (10%)	68,99,113	1.75	9 (13%)
25	CLA	B	818	2	69,73,73	1.22	6 (8%)	82,113,113	1.60	8 (9%)
25	CLA	g	213	21	46,50,73	1.39	6 (13%)	53,85,113	1.86	7 (13%)
25	CLA	B	802	2	69,73,73	1.20	6 (8%)	82,113,113	1.54	10 (12%)
25	CLA	g	203	21	46,50,73	1.39	7 (15%)	53,85,113	1.80	6 (11%)
31	SF4	A	856	2,1	0,12,12	-	-	-	-	-
25	CLA	j	203	16	54,58,73	1.37	7 (12%)	64,95,113	1.70	9 (14%)
25	CLA	d	315	12	46,50,73	1.39	7 (15%)	53,85,113	1.83	5 (9%)
25	CLA	j	206	-	61,65,73	1.31	7 (11%)	72,103,113	1.74	10 (13%)
35	CHL	d	310	-	40,54,74	2.20	12 (30%)	34,90,114	3.02	16 (47%)
25	CLA	B	806	2	46,50,73	1.39	7 (15%)	53,85,113	1.81	7 (13%)
25	CLA	m	205	-	47,51,73	1.39	6 (12%)	55,86,113	1.89	5 (9%)
25	CLA	B	846	2	54,58,73	1.36	6 (11%)	64,95,113	1.89	10 (15%)
25	CLA	B	826	2	47,51,73	1.37	6 (12%)	55,86,113	1.79	4 (7%)
29	BCR	M	201	-	41,41,41	0.77	1 (2%)	56,56,56	1.17	5 (8%)
25	CLA	k	211	17	56,60,73	1.34	7 (12%)	65,97,113	1.79	8 (12%)
25	CLA	A	849	1	54,58,73	1.37	6 (11%)	64,95,113	1.74	9 (14%)
25	CLA	B	820	2	47,51,73	1.38	8 (17%)	55,86,113	1.79	5 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	j	208	16	54,58,73	1.37	7 (12%)	64,95,113	1.80	7 (10%)
25	CLA	g	206	-	47,51,73	1.38	7 (14%)	55,86,113	1.68	4 (7%)
25	CLA	B	812	2	68,72,73	1.25	7 (10%)	80,111,113	1.67	9 (11%)
25	CLA	A	848	1	55,59,73	1.34	6 (10%)	64,96,113	1.83	9 (14%)
25	CLA	g	210	27	46,50,73	1.39	6 (13%)	53,85,113	1.86	6 (11%)
30	DD6	k	216	-	40,45,45	1.41	4 (10%)	51,67,67	2.02	13 (25%)
25	CLA	d	301	12	45,49,73	1.44	8 (17%)	54,84,113	1.98	8 (14%)
25	CLA	l	601	18	46,50,73	1.40	6 (13%)	53,85,113	1.73	6 (11%)
25	CLA	l	606	18	64,68,73	1.26	7 (10%)	76,107,113	1.72	8 (10%)
25	CLA	A	844	1	64,68,73	1.28	7 (10%)	76,107,113	1.74	11 (14%)
25	CLA	j	205	16	46,50,73	1.41	7 (15%)	53,85,113	1.84	5 (9%)
25	CLA	e	205	13	69,73,73	1.22	7 (10%)	82,113,113	1.57	10 (12%)
25	CLA	h	208	14	54,58,73	1.37	7 (12%)	64,95,113	1.75	7 (10%)
25	CLA	A	853	27	57,61,73	1.33	7 (12%)	67,98,113	1.85	10 (14%)
25	CLA	f	602	20	63,67,73	1.28	6 (9%)	74,105,113	1.66	10 (13%)
28	PQN	F	205	-	27,27,34	1.07	2 (7%)	34,36,45	1.92	9 (26%)
25	CLA	i	208	15	59,63,73	1.30	5 (8%)	70,101,113	1.69	9 (12%)
25	CLA	b	206	-	49,53,73	1.40	7 (14%)	58,89,113	1.80	5 (8%)
25	CLA	j	209	16	68,72,73	1.21	5 (7%)	80,111,113	1.56	8 (10%)
25	CLA	h	215	14	47,51,73	1.39	7 (14%)	55,86,113	1.76	5 (9%)
25	CLA	B	840	2	54,58,73	1.38	6 (11%)	64,95,113	1.62	9 (14%)
30	DD6	j	216	-	40,45,45	1.55	6 (15%)	51,67,67	2.06	12 (23%)
25	CLA	p	604	-	47,51,73	1.41	7 (14%)	55,86,113	1.83	6 (10%)
25	CLA	A	802	-	67,71,73	1.23	5 (7%)	79,110,113	1.61	9 (11%)
25	CLA	B	825	-	47,51,73	1.37	7 (14%)	55,86,113	1.63	4 (7%)
25	CLA	c	303	11	63,67,73	1.27	7 (11%)	74,105,113	1.66	11 (14%)
25	CLA	b	211	-	46,50,73	1.40	6 (13%)	53,85,113	1.83	4 (7%)
25	CLA	m	209	-	47,51,73	1.39	7 (14%)	55,86,113	1.73	5 (9%)
25	CLA	B	804	2	69,73,73	1.21	6 (8%)	82,113,113	1.68	6 (7%)
25	CLA	m	208	19	46,50,73	1.38	6 (13%)	53,85,113	1.73	5 (9%)
30	DD6	j	217	-	40,45,45	1.49	5 (12%)	51,67,67	2.04	12 (23%)
25	CLA	m	202	19	46,50,73	1.42	6 (13%)	53,85,113	1.66	8 (15%)
33	SQD	F	204	-	37,39,54	1.76	8 (21%)	47,50,65	1.47	7 (14%)
25	CLA	B	841	2	63,67,73	1.29	7 (11%)	74,105,113	1.73	7 (9%)
25	CLA	B	810	2	47,51,73	1.38	7 (14%)	55,86,113	1.78	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	B	847	2	54,58,73	1.37	7 (12%)	64,95,113	1.79	7 (10%)
25	CLA	A	806	1	49,53,73	1.39	7 (14%)	58,89,113	1.83	7 (12%)
25	CLA	n	203	-	52,56,73	1.38	7 (13%)	61,92,113	1.79	7 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DD6	i	216	-	-	1/26/80/80	0/3/3/3
25	CLA	c	315	11	1/1/11/20	3/18/94/115	-
25	CLA	B	815	2	1/1/11/20	8/20/96/115	-
25	CLA	A	818	1	1/1/15/20	12/39/115/115	-
25	CLA	k	214	17	1/1/12/20	3/21/97/115	-
25	CLA	n	207	-	1/1/10/20	2/10/86/115	-
25	CLA	g	208	21	1/1/12/20	2/21/97/115	-
32	DGD	e	203	-	-	6/24/64/95	0/2/2/2
29	BCR	B	833	-	-	4/29/63/63	0/2/2/2
29	BCR	B	828	-	-	7/29/63/63	0/2/2/2
33	SQD	J	102	-	-	9/21/41/69	0/1/1/1
34	LMG	a	202	-	-	17/38/58/70	0/1/1/1
25	CLA	j	215	16	1/1/12/20	6/21/97/115	-
30	DD6	f	613	-	-	5/26/80/80	0/3/3/3
25	CLA	e	215	13	1/1/10/20	1/13/89/115	-
35	CHL	d	309	-	3/3/15/26	4/12/110/137	-
25	CLA	A	829	1	1/1/13/20	13/31/107/115	-
30	DD6	c	317	-	-	0/26/80/80	0/3/3/3
28	PQN	B	835	-	-	5/16/36/43	0/2/2/2
35	CHL	d	308	-	3/3/16/26	8/15/113/137	-
30	DD6	g	217	-	-	4/26/80/80	0/3/3/3
25	CLA	J	103	7	1/1/12/20	11/21/97/115	-
30	DD6	a	215	-	-	0/26/80/80	0/3/3/3
25	CLA	B	823	2	1/1/14/20	9/33/109/115	-
25	CLA	j	213	16	1/1/10/20	2/12/88/115	-
25	CLA	n	209	22	1/1/10/20	2/10/86/115	-
25	CLA	A	804	1	1/1/14/20	8/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	821	-	1/1/14/20	15/37/113/115	-
30	DD6	m	212	-	-	6/26/80/80	0/3/3/3
25	CLA	B	824	2	1/1/15/20	21/39/115/115	-
25	CLA	B	838	2	1/1/14/20	6/35/111/115	-
25	CLA	d	311	12	1/1/11/20	5/20/96/115	-
25	CLA	B	813	2	1/1/11/20	5/19/95/115	-
25	CLA	c	311	27	1/1/10/20	1/13/89/115	-
25	CLA	a	212	9	1/1/13/20	13/27/103/115	-
28	PQN	B	827	-	-	8/23/43/43	0/2/2/2
25	CLA	A	831	1	1/1/11/20	3/19/95/115	-
30	DD6	l	614	-	-	3/26/80/80	0/3/3/3
25	CLA	B	817	-	1/1/12/20	9/21/97/115	-
25	CLA	e	216	13	1/1/13/20	4/27/103/115	-
25	CLA	f	603	20	1/1/10/20	1/13/89/115	-
25	CLA	e	214	-	1/1/10/20	3/12/88/115	-
25	CLA	o	604	-	1/1/10/20	3/12/88/115	-
30	DD6	p	610	-	-	3/26/80/80	0/3/3/3
25	CLA	o	601	23	1/1/10/20	2/10/86/115	-
25	CLA	p	608	24	1/1/10/20	3/13/89/115	-
25	CLA	l	605	-	1/1/10/20	5/13/89/115	-
32	DGD	B	849	-	-	19/43/83/95	0/2/2/2
25	CLA	c	306	-	1/1/10/20	3/13/89/115	-
25	CLA	g	211	21	1/1/10/20	4/12/88/115	-
25	CLA	n	202	22	1/1/13/20	13/27/103/115	-
25	CLA	f	605	20	1/1/10/20	2/12/88/115	-
25	CLA	B	844	2	1/1/15/20	14/39/115/115	-
25	CLA	A	833	1	1/1/15/20	14/39/115/115	-
25	CLA	e	211	-	1/1/11/20	6/19/95/115	-
25	CLA	m	210	19	1/1/10/20	3/13/89/115	-
30	DD6	n	213	-	-	13/26/80/80	0/3/3/3
27	LHG	j	202	25	-	24/41/41/53	-
25	CLA	l	610	18	1/1/11/20	7/19/95/115	-
25	CLA	g	207	-	1/1/11/20	6/15/91/115	-
25	CLA	A	842	1	1/1/11/20	9/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	f	608	-	1/1/10/20	2/12/88/115	-
27	LHG	b	201	-	-	23/35/35/53	-
25	CLA	h	211	14	1/1/13/20	8/31/107/115	-
25	CLA	b	207	-	1/1/11/20	6/15/91/115	-
25	CLA	e	210	-	1/1/10/20	6/13/89/115	-
25	CLA	b	209	10	1/1/11/20	2/15/91/115	-
30	DD6	e	218	-	-	10/26/80/80	0/3/3/3
25	CLA	p	606	24	1/1/12/20	10/21/97/115	-
25	CLA	A	817	1	1/1/13/20	10/29/105/115	-
25	CLA	o	605	-	1/1/10/20	5/13/89/115	-
25	CLA	A	816	1	1/1/10/20	5/13/89/115	-
29	BCR	B	801	-	-	8/29/63/63	0/2/2/2
32	DGD	b	202	-	-	19/37/77/95	0/2/2/2
31	SF4	C	102	3	-	-	0/6/5/5
25	CLA	d	316	12	1/1/10/20	4/12/88/115	-
25	CLA	o	603	23	1/1/10/20	5/13/89/115	-
30	DD6	f	614	-	-	7/26/80/80	0/3/3/3
25	CLA	o	606	23	1/1/11/20	5/15/91/115	-
25	CLA	p	602	24	1/1/10/20	8/13/89/115	-
30	DD6	J	105	-	-	15/26/80/80	0/3/3/3
25	CLA	o	602	23	1/1/11/20	8/18/94/115	-
25	CLA	a	204	9	1/1/14/20	17/33/109/115	-
25	CLA	i	203	15	1/1/14/20	13/38/114/115	-
25	CLA	l	611	18	1/1/10/20	4/12/88/115	-
25	CLA	a	210	27	1/1/11/20	5/15/91/115	-
25	CLA	c	305	-	1/1/11/20	5/19/95/115	-
25	CLA	d	313	27	1/1/11/20	5/15/91/115	-
25	CLA	g	205	21	1/1/10/20	2/12/88/115	-
25	CLA	p	603	24	1/1/10/20	4/12/88/115	-
25	CLA	l	609	18	1/1/10/20	6/13/89/115	-
25	CLA	B	839	-	1/1/14/20	13/33/109/115	-
25	CLA	B	811	2	1/1/14/20	17/37/113/115	-
25	CLA	f	610	20	1/1/13/20	13/32/108/115	-
30	DD6	g	216	-	-	4/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	o	608	23	1/1/9/20	4/13/85/115	-
25	CLA	e	217	13	1/1/10/20	4/12/88/115	-
25	CLA	e	204	13	1/1/10/20	5/10/86/115	-
25	CLA	c	312	11	1/1/10/20	3/13/89/115	-
30	DD6	n	212	-	-	5/26/80/80	0/3/3/3
25	CLA	b	203	-	1/1/10/20	4/12/88/115	-
25	CLA	B	843	2	1/1/14/20	14/37/113/115	-
25	CLA	j	211	16	1/1/13/20	9/27/103/115	-
27	LHG	A	805	25	-	17/42/42/53	-
25	CLA	A	820	1	1/1/13/20	9/30/106/115	-
25	CLA	B	819	2	1/1/15/20	14/39/115/115	-
25	CLA	B	805	2	1/1/15/20	13/39/115/115	-
29	BCR	A	838	-	-	5/29/63/63	0/2/2/2
30	DD6	o	611	-	-	5/26/80/80	0/3/3/3
29	BCR	B	829	-	-	2/29/63/63	0/2/2/2
25	CLA	k	207	17	1/1/12/20	2/21/97/115	-
25	CLA	b	205	10	1/1/10/20	5/13/89/115	-
30	DD6	d	318	-	-	3/26/80/80	0/3/3/3
25	CLA	n	205	-	1/1/10/20	6/12/88/115	-
25	CLA	A	841	-	1/1/13/20	7/30/106/115	-
25	CLA	A	847	1	1/1/10/20	6/13/89/115	-
30	DD6	l	613	-	-	2/26/80/80	0/3/3/3
29	BCR	B	832	-	-	13/29/63/63	0/2/2/2
25	CLA	l	602	18	1/1/13/20	12/32/108/115	-
25	CLA	a	205	9	1/1/12/20	6/25/101/115	-
27	LHG	c	301	25	-	11/34/34/53	-
30	DD6	o	612	-	-	3/26/80/80	0/3/3/3
30	DD6	e	220	-	-	15/26/80/80	0/3/3/3
25	CLA	i	210	15	1/1/10/20	4/13/89/115	-
30	DD6	A	854	-	-	3/26/80/80	0/3/3/3
25	CLA	A	812	1	1/1/15/20	15/39/115/115	-
30	DD6	k	215	-	-	2/26/80/80	0/3/3/3
25	CLA	k	203	17	1/1/12/20	10/25/101/115	-
25	CLA	e	207	-	1/1/12/20	4/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	f	601	20	1/1/10/20	6/12/88/115	-
25	CLA	n	204	22	1/1/10/20	4/12/88/115	-
25	CLA	B	845	2	1/1/15/20	9/39/115/115	-
30	DD6	i	215	-	-	3/26/80/80	0/3/3/3
25	CLA	a	206	-	1/1/11/20	4/15/91/115	-
25	CLA	f	609	20	1/1/10/20	4/12/88/115	-
25	CLA	l	603	18	1/1/10/20	1/13/89/115	-
25	CLA	A	824	1	1/1/13/20	13/31/107/115	-
25	CLA	d	305	12	1/1/10/20	4/12/88/115	-
25	CLA	A	846	1	1/1/15/20	20/39/115/115	-
25	CLA	B	848	-	1/1/15/20	18/39/115/115	-
30	DD6	h	216	-	-	3/26/80/80	0/3/3/3
25	CLA	k	212	17	1/1/10/20	4/12/88/115	-
27	LHG	i	201	25	-	20/40/40/53	-
25	CLA	i	206	-	1/1/15/20	13/39/115/115	-
25	CLA	j	212	16	1/1/14/20	9/36/112/115	-
27	LHG	h	202	25	-	11/35/35/53	-
25	CLA	A	857	-	1/1/12/20	7/25/101/115	-
25	CLA	i	207	15	1/1/10/20	4/13/89/115	-
25	CLA	l	604	-	1/1/10/20	2/13/89/115	-
25	CLA	c	310	11	1/1/13/20	13/27/103/115	-
25	CLA	d	303	-	1/1/12/20	6/21/97/115	-
25	CLA	l	608	-	1/1/10/20	3/13/89/115	-
30	DD6	F	203	-	-	18/26/80/80	0/3/3/3
25	CLA	B	814	2	1/1/13/20	10/32/108/115	-
25	CLA	g	215	21	1/1/11/20	4/15/91/115	-
25	CLA	a	207	-	1/1/12/20	12/25/101/115	-
25	CLA	k	209	-	1/1/10/20	2/12/88/115	-
25	CLA	d	312	12	1/1/13/20	14/32/108/115	-
25	CLA	e	208	13	1/1/10/20	2/12/88/115	-
25	CLA	h	214	14	1/1/10/20	6/12/88/115	-
25	CLA	F	201	-	1/1/10/20	0/12/88/115	-
30	DD6	c	316	-	-	4/26/80/80	0/3/3/3
30	DD6	e	219	-	-	5/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	n	206	-	1/1/10/20	3/12/88/115	-
25	CLA	l	612	-	1/1/10/20	6/12/88/115	-
25	CLA	A	850	1	1/1/13/20	7/27/103/115	-
25	CLA	i	205	-	1/1/10/20	3/13/89/115	-
29	BCR	J	101	-	-	17/29/63/63	0/2/2/2
26	LMT	A	803	-	-	7/21/61/61	0/2/2/2
25	CLA	b	204	10	1/1/12/20	9/25/101/115	-
25	CLA	g	209	21	1/1/13/20	11/27/103/115	-
25	CLA	b	212	10	1/1/12/20	9/24/100/115	-
25	CLA	a	203	9	1/1/12/20	5/21/97/115	-
27	LHG	g	201	25	-	25/39/39/53	-
25	CLA	n	208	22	1/1/11/20	7/15/91/115	-
35	CHL	e	209	-	3/3/16/26	8/15/113/137	-
25	CLA	B	822	2	1/1/14/20	18/33/109/115	-
27	LHG	a	201	25	-	8/30/30/53	-
30	DD6	b	215	-	-	1/26/80/80	0/3/3/3
25	CLA	A	828	1	1/1/10/20	6/13/89/115	-
25	CLA	A	852	1	1/1/11/20	3/19/95/115	-
25	CLA	A	815	1	1/1/13/20	17/31/107/115	-
30	DD6	d	317	-	-	2/26/80/80	0/3/3/3
25	CLA	a	209	9	1/1/12/20	9/26/102/115	-
30	DD6	A	855	-	-	9/26/80/80	0/3/3/3
25	CLA	a	208	9	1/1/12/20	5/21/97/115	-
25	CLA	A	851	1	1/1/11/20	1/15/91/115	-
30	DD6	c	318	-	-	8/26/80/80	0/3/3/3
25	CLA	B	834	2	1/1/13/20	6/27/103/115	-
25	CLA	A	819	-	1/1/15/20	12/39/115/115	-
25	CLA	d	306	-	1/1/12/20	7/24/100/115	-
25	CLA	p	601	-	1/1/10/20	3/12/88/115	-
25	CLA	i	209	27	1/1/10/20	4/13/89/115	-
25	CLA	j	214	16	1/1/10/20	5/13/89/115	-
25	CLA	o	610	23	1/1/10/20	7/13/89/115	-
25	CLA	A	814	1	1/1/13/20	10/32/108/115	-
25	CLA	p	609	24	1/1/10/20	5/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	830	1	1/1/12/20	8/24/100/115	-
25	CLA	d	304	12	1/1/13/20	5/30/106/115	-
25	CLA	l	607	18	1/1/12/20	14/26/102/115	-
25	CLA	k	213	17	1/1/10/20	5/12/88/115	-
25	CLA	B	836	2	1/1/12/20	10/25/101/115	-
30	DD6	b	214	-	-	5/26/80/80	0/3/3/3
30	DD6	h	217	-	-	0/26/80/80	0/3/3/3
25	CLA	f	606	20	1/1/10/20	4/12/88/115	-
25	CLA	k	208	17	1/1/13/20	15/30/106/115	-
25	CLA	B	821	2	1/1/14/20	17/33/109/115	-
25	CLA	k	202	17	1/1/10/20	3/13/89/115	-
25	CLA	h	213	14	1/1/10/20	5/13/89/115	-
25	CLA	A	809	1	1/1/15/20	22/39/115/115	-
25	CLA	c	308	-	1/1/12/20	10/21/97/115	-
25	CLA	i	202	15	1/1/12/20	13/25/101/115	-
25	CLA	b	208	-	1/1/10/20	2/10/86/115	-
25	CLA	A	813	1	1/1/13/20	11/31/107/115	-
25	CLA	e	213	13	1/1/13/20	8/27/103/115	-
25	CLA	A	827	1	1/1/10/20	3/13/89/115	-
25	CLA	k	206	-	1/1/12/20	2/21/97/115	-
33	SQD	g	202	-	-	13/27/47/69	0/1/1/1
30	DD6	J	104	-	-	2/26/80/80	0/3/3/3
25	CLA	f	612	20	1/1/10/20	8/13/89/115	-
25	CLA	m	211	19	1/1/10/20	5/12/88/115	-
35	CHL	c	307	-	3/3/16/26	7/19/117/137	-
25	CLA	A	811	1	1/1/12/20	2/21/97/115	-
25	CLA	A	845	-	1/1/11/20	5/19/95/115	-
25	CLA	B	803	-	1/1/13/20	10/27/103/115	-
34	LMG	k	201	-	-	16/31/51/70	0/1/1/1
25	CLA	A	808	1	1/1/14/20	11/33/109/115	-
25	CLA	c	309	11	1/1/14/20	13/33/109/115	-
25	CLA	c	314	11	1/1/10/20	6/12/88/115	-
25	CLA	e	206	13	1/1/11/20	5/15/91/115	-
25	CLA	j	204	16	1/1/13/20	4/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	A	839	-	-	10/29/63/63	0/2/2/2
25	CLA	j	210	27	1/1/12/20	8/21/97/115	-
30	DD6	d	319	-	-	4/26/80/80	0/3/3/3
31	SF4	C	101	3	-	-	0/6/5/5
29	BCR	B	831	-	-	12/29/63/63	0/2/2/2
25	CLA	a	213	-	1/1/14/20	9/37/113/115	-
25	CLA	B	837	2	1/1/12/20	11/21/97/115	-
25	CLA	B	809	2	1/1/10/20	4/12/88/115	-
25	CLA	p	605	-	1/1/10/20	6/12/88/115	-
30	DD6	n	214	-	-	8/26/80/80	0/3/3/3
25	CLA	h	204	14	1/1/13/20	16/27/103/115	-
25	CLA	k	210	17	1/1/10/20	1/13/89/115	-
25	CLA	A	825	1	1/1/15/20	8/39/115/115	-
25	CLA	b	210	10	1/1/10/20	4/12/88/115	-
25	CLA	k	204	17	1/1/10/20	4/12/88/115	-
25	CLA	f	607	20	1/1/13/20	15/27/103/115	-
28	PQN	A	834	-	-	7/23/43/43	0/2/2/2
25	CLA	h	210	27	1/1/10/20	4/13/89/115	-
30	DD6	a	214	-	-	5/26/80/80	0/3/3/3
25	CLA	c	302	11	1/1/10/20	5/12/88/115	-
25	CLA	m	204	19	1/1/12/20	9/26/102/115	-
30	DD6	m	213	-	-	6/26/80/80	0/3/3/3
25	CLA	B	842	2	1/1/12/20	12/25/101/115	-
25	CLA	A	840	-	1/1/14/20	12/37/113/115	-
29	BCR	A	836	-	-	5/29/63/63	0/2/2/2
25	CLA	A	801	1	1/1/15/20	16/39/115/115	-
27	LHG	A	835	-	-	22/53/53/53	-
30	DD6	i	214	-	-	2/26/80/80	0/3/3/3
25	CLA	F	202	6	1/1/11/20	7/15/91/115	-
25	CLA	m	207	19	1/1/12/20	3/21/97/115	-
25	CLA	c	304	11	1/1/12/20	6/25/101/115	-
25	CLA	A	807	-	1/1/15/20	10/39/115/115	-
33	SQD	D	200	-	-	12/31/51/69	0/1/1/1
25	CLA	a	211	9	1/1/10/20	4/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	816	-	1/1/14/20	9/33/109/115	-
25	CLA	b	213	10	1/1/10/20	4/12/88/115	-
25	CLA	h	207	-	1/1/11/20	7/19/95/115	-
25	CLA	g	212	21	1/1/13/20	12/27/103/115	-
25	CLA	e	212	13	1/1/12/20	8/24/100/115	-
34	LMG	e	202	-	-	19/47/67/70	0/1/1/1
25	CLA	k	205	17	1/1/15/20	18/39/115/115	-
25	CLA	g	204	21	1/1/12/20	14/25/101/115	-
25	CLA	m	203	19	1/1/14/20	16/33/109/115	-
25	CLA	A	832	1	1/1/15/20	12/39/115/115	-
25	CLA	A	823	1	1/1/14/20	14/38/114/115	-
29	BCR	B	830	-	-	6/29/63/63	0/2/2/2
25	CLA	i	213	15	1/1/12/20	2/21/97/115	-
25	CLA	e	201	-	1/1/12/20	5/25/101/115	-
25	CLA	h	205	14	1/1/10/20	5/13/89/115	-
25	CLA	o	607	23	1/1/10/20	2/10/86/115	-
25	CLA	h	203	14	1/1/12/20	7/21/97/115	-
34	LMG	j	201	-	-	11/39/59/70	0/1/1/1
25	CLA	A	826	1	1/1/15/20	13/39/115/115	-
25	CLA	f	604	-	1/1/10/20	3/12/88/115	-
25	CLA	B	808	2	1/1/10/20	3/13/89/115	-
25	CLA	i	204	15	1/1/10/20	7/13/89/115	-
27	LHG	h	201	-	-	13/33/33/53	-
25	CLA	h	206	-	1/1/14/20	9/33/109/115	-
25	CLA	A	843	1	1/1/12/20	11/24/100/115	-
25	CLA	f	611	20	1/1/10/20	5/12/88/115	-
25	CLA	i	212	15	1/1/10/20	2/12/88/115	-
29	BCR	A	837	-	-	11/29/63/63	0/2/2/2
25	CLA	c	313	11	1/1/12/20	8/25/101/115	-
25	CLA	B	807	2	1/1/15/20	15/39/115/115	-
25	CLA	o	609	23	1/1/10/20	6/12/88/115	-
27	LHG	d	302	25	-	13/33/33/53	-
35	CHL	d	307	12	3/3/17/26	7/21/119/137	-
25	CLA	h	212	14	1/1/12/20	8/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	n	210	22	1/1/10/20	4/12/88/115	-
25	CLA	p	607	24	1/1/11/20	11/15/91/115	-
25	CLA	i	211	15	1/1/13/20	10/32/108/115	-
25	CLA	j	207	-	1/1/11/20	5/18/94/115	-
25	CLA	n	201	22	1/1/13/20	14/32/108/115	-
25	CLA	d	314	12	1/1/10/20	2/12/88/115	-
25	CLA	A	810	1	1/1/15/20	14/39/115/115	-
25	CLA	n	211	22	1/1/10/20	4/12/88/115	-
27	LHG	m	201	-	-	19/36/36/53	-
25	CLA	m	206	-	1/1/10/20	2/12/88/115	-
25	CLA	A	822	-	1/1/12/20	8/25/101/115	-
25	CLA	g	214	21	1/1/10/20	0/12/88/115	-
25	CLA	h	209	14	1/1/12/20	8/26/102/115	-
25	CLA	B	818	2	1/1/15/20	13/39/115/115	-
25	CLA	g	213	21	1/1/10/20	3/12/88/115	-
25	CLA	B	802	2	1/1/15/20	9/39/115/115	-
25	CLA	g	203	21	1/1/10/20	5/12/88/115	-
31	SF4	A	856	2,1	-	-	0/6/5/5
25	CLA	j	203	16	1/1/12/20	7/21/97/115	-
25	CLA	d	315	12	1/1/10/20	4/12/88/115	-
25	CLA	j	206	-	1/1/13/20	10/30/106/115	-
35	CHL	d	310	-	3/3/16/26	5/15/113/137	-
25	CLA	B	806	2	1/1/10/20	2/12/88/115	-
25	CLA	m	205	-	1/1/10/20	3/13/89/115	-
25	CLA	B	846	2	1/1/12/20	5/21/97/115	-
25	CLA	B	826	2	1/1/10/20	4/13/89/115	-
29	BCR	M	201	-	-	6/29/63/63	0/2/2/2
25	CLA	k	211	17	1/1/12/20	8/24/100/115	-
25	CLA	A	849	1	1/1/12/20	8/21/97/115	-
25	CLA	B	820	2	1/1/10/20	6/13/89/115	-
25	CLA	j	208	16	1/1/12/20	5/21/97/115	-
25	CLA	g	206	-	1/1/10/20	3/13/89/115	-
25	CLA	B	812	2	1/1/14/20	12/38/114/115	-
25	CLA	A	848	1	1/1/12/20	8/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	g	210	27	1/1/10/20	3/12/88/115	-
30	DD6	k	216	-	-	3/26/80/80	0/3/3/3
25	CLA	d	301	12	1/1/10/20	4/10/86/115	-
25	CLA	l	601	18	1/1/10/20	3/12/88/115	-
25	CLA	l	606	18	1/1/14/20	12/33/109/115	-
25	CLA	A	844	1	1/1/14/20	16/33/109/115	-
25	CLA	j	205	16	1/1/10/20	1/12/88/115	-
25	CLA	e	205	13	1/1/15/20	20/39/115/115	-
25	CLA	h	208	14	1/1/12/20	7/21/97/115	-
25	CLA	A	853	27	1/1/12/20	12/25/101/115	-
25	CLA	f	602	20	1/1/13/20	14/32/108/115	-
28	PQN	F	205	-	-	6/15/35/43	0/2/2/2
25	CLA	i	208	15	1/1/13/20	11/27/103/115	-
25	CLA	b	206	-	1/1/11/20	5/15/91/115	-
25	CLA	j	209	16	1/1/14/20	20/38/114/115	-
25	CLA	h	215	14	1/1/10/20	2/13/89/115	-
25	CLA	B	840	2	1/1/12/20	8/21/97/115	-
30	DD6	j	216	-	-	4/26/80/80	0/3/3/3
25	CLA	p	604	-	1/1/10/20	5/13/89/115	-
25	CLA	A	802	-	1/1/14/20	10/37/113/115	-
25	CLA	B	825	-	1/1/10/20	4/13/89/115	-
25	CLA	c	303	11	1/1/13/20	14/32/108/115	-
25	CLA	b	211	-	1/1/10/20	4/12/88/115	-
25	CLA	m	209	-	1/1/10/20	2/13/89/115	-
25	CLA	B	804	2	1/1/15/20	17/39/115/115	-
25	CLA	m	208	19	1/1/10/20	6/12/88/115	-
30	DD6	j	217	-	-	3/26/80/80	0/3/3/3
25	CLA	m	202	19	1/1/10/20	4/12/88/115	-
33	SQD	F	204	-	-	21/34/54/69	0/1/1/1
25	CLA	B	841	2	1/1/13/20	9/32/108/115	-
25	CLA	B	810	2	1/1/10/20	3/13/89/115	-
25	CLA	B	847	2	1/1/12/20	3/21/97/115	-
25	CLA	A	806	1	1/1/11/20	6/15/91/115	-
25	CLA	n	203	-	1/1/11/20	7/19/95/115	-

The worst 5 of 2211 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	201	LHG	P-O3	6.57	1.85	1.59
27	m	201	LHG	P-O3	6.52	1.84	1.59
27	c	301	LHG	P-O3	6.46	1.84	1.59
27	d	302	LHG	P-O3	6.40	1.84	1.59
27	h	201	LHG	P-O3	6.38	1.84	1.59

The worst 5 of 2802 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	e	209	CHL	C1B-CHB-C4A	12.30	129.23	121.32
35	d	308	CHL	C1B-CHB-C4A	12.13	129.12	121.32
35	d	307	CHL	C1B-CHB-C4A	11.88	128.96	121.32
25	A	823	CLA	C4A-NA-C1A	11.45	111.90	106.68
25	k	204	CLA	C4A-NA-C1A	11.39	111.88	106.68

5 of 294 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	801	CLA	ND
25	A	802	CLA	ND
25	A	804	CLA	ND
25	A	806	CLA	ND
25	A	807	CLA	ND

5 of 2782 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	801	CLA	CAD-CBD-CGD-O2D
25	A	802	CLA	C1-C2-C3-C4
25	A	802	CLA	C1-C2-C3-C5
25	A	806	CLA	C4B-C3B-CAB-CBB
25	A	808	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

259 monomers are involved in 540 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	815	CLA	1	0
25	A	818	CLA	5	0
25	k	214	CLA	2	0
25	n	207	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	g	208	CLA	3	0
32	e	203	DGD	2	0
29	B	833	BCR	3	0
29	B	828	BCR	2	0
25	j	215	CLA	1	0
25	e	215	CLA	3	0
35	d	309	CHL	2	0
25	A	829	CLA	3	0
35	d	308	CHL	2	0
25	J	103	CLA	2	0
30	a	215	DD6	1	0
25	B	823	CLA	2	0
25	n	209	CLA	1	0
25	A	804	CLA	2	0
25	A	821	CLA	4	0
30	m	212	DD6	1	0
25	B	824	CLA	5	0
25	B	838	CLA	5	0
25	B	813	CLA	4	0
25	c	311	CLA	3	0
25	a	212	CLA	2	0
28	B	827	PQN	2	0
25	A	831	CLA	2	0
25	B	817	CLA	4	0
25	e	216	CLA	1	0
25	e	214	CLA	1	0
25	o	601	CLA	1	0
25	p	608	CLA	1	0
25	l	605	CLA	1	0
32	B	849	DGD	2	0
25	c	306	CLA	1	0
25	g	211	CLA	1	0
25	n	202	CLA	3	0
25	f	605	CLA	1	0
25	B	844	CLA	2	0
25	A	833	CLA	7	0
25	e	211	CLA	3	0
30	n	213	DD6	1	0
27	j	202	LHG	4	0
25	l	610	CLA	1	0
25	g	207	CLA	4	0
25	A	842	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	201	LHG	3	0
25	h	211	CLA	2	0
25	b	207	CLA	1	0
25	b	209	CLA	2	0
25	p	606	CLA	1	0
25	A	817	CLA	3	0
25	o	605	CLA	1	0
25	A	816	CLA	3	0
29	B	801	BCR	2	0
32	b	202	DGD	3	0
25	d	316	CLA	1	0
25	o	606	CLA	1	0
25	p	602	CLA	3	0
25	o	602	CLA	2	0
25	a	204	CLA	7	0
25	i	203	CLA	2	0
25	l	611	CLA	3	0
25	a	210	CLA	1	0
25	d	313	CLA	1	0
25	g	205	CLA	1	0
25	p	603	CLA	4	0
25	B	839	CLA	5	0
25	B	811	CLA	3	0
25	f	610	CLA	3	0
25	o	608	CLA	1	0
25	c	312	CLA	3	0
25	b	203	CLA	1	0
25	B	843	CLA	7	0
27	A	805	LHG	2	0
25	A	820	CLA	2	0
25	B	819	CLA	6	0
25	B	805	CLA	5	0
29	A	838	BCR	1	0
29	B	829	BCR	2	0
25	k	207	CLA	1	0
25	n	205	CLA	2	0
25	A	841	CLA	3	0
29	B	832	BCR	8	0
25	l	602	CLA	4	0
25	a	205	CLA	1	0
27	c	301	LHG	3	0
25	i	210	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	812	CLA	3	0
25	k	203	CLA	1	0
25	e	207	CLA	1	0
25	B	845	CLA	9	0
30	i	215	DD6	1	0
25	a	206	CLA	1	0
25	l	603	CLA	1	0
25	A	824	CLA	7	0
25	d	305	CLA	2	0
25	A	846	CLA	1	0
25	B	848	CLA	2	0
27	i	201	LHG	2	0
25	i	206	CLA	2	0
25	j	212	CLA	4	0
27	h	202	LHG	2	0
25	A	857	CLA	1	0
25	i	207	CLA	1	0
25	l	604	CLA	1	0
25	c	310	CLA	3	0
25	d	303	CLA	1	0
25	B	814	CLA	1	0
25	a	207	CLA	3	0
25	d	312	CLA	4	0
25	e	208	CLA	1	0
25	h	214	CLA	2	0
25	F	201	CLA	3	0
25	n	206	CLA	1	0
25	l	612	CLA	1	0
25	A	850	CLA	2	0
25	i	205	CLA	1	0
29	J	101	BCR	3	0
25	b	204	CLA	1	0
25	g	209	CLA	7	0
25	b	212	CLA	4	0
25	a	203	CLA	1	0
25	n	208	CLA	1	0
25	B	822	CLA	4	0
27	a	201	LHG	1	0
25	A	815	CLA	5	0
25	a	209	CLA	3	0
25	a	208	CLA	1	0
25	A	819	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	d	306	CLA	2	0
25	o	610	CLA	4	0
25	A	814	CLA	3	0
25	p	609	CLA	1	0
25	A	830	CLA	2	0
25	d	304	CLA	1	0
25	l	607	CLA	4	0
25	B	836	CLA	3	0
25	k	208	CLA	4	0
25	B	821	CLA	2	0
25	A	809	CLA	6	0
25	c	308	CLA	3	0
25	i	202	CLA	2	0
25	b	208	CLA	1	0
25	A	813	CLA	1	0
25	e	213	CLA	4	0
25	k	206	CLA	3	0
33	g	202	SQD	2	0
25	f	612	CLA	1	0
25	m	211	CLA	1	0
35	c	307	CHL	3	0
25	A	845	CLA	2	0
25	B	803	CLA	4	0
34	k	201	LMG	3	0
25	c	309	CLA	2	0
25	c	314	CLA	1	0
25	e	206	CLA	1	0
29	A	839	BCR	2	0
25	j	210	CLA	2	0
30	d	319	DD6	1	0
29	B	831	BCR	4	0
25	a	213	CLA	5	0
25	B	837	CLA	3	0
25	p	605	CLA	1	0
25	h	204	CLA	1	0
25	k	210	CLA	1	0
25	A	825	CLA	3	0
25	b	210	CLA	2	0
25	k	204	CLA	1	0
25	f	607	CLA	1	0
28	A	834	PQN	5	0
25	h	210	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	302	CLA	1	0
25	m	204	CLA	1	0
30	m	213	DD6	1	0
25	B	842	CLA	5	0
25	A	840	CLA	6	0
29	A	836	BCR	3	0
25	A	801	CLA	7	0
27	A	835	LHG	5	0
25	F	202	CLA	3	0
25	c	304	CLA	4	0
25	A	807	CLA	6	0
25	B	816	CLA	4	0
25	h	207	CLA	3	0
25	g	212	CLA	3	0
34	e	202	LMG	5	0
25	k	205	CLA	1	0
25	g	204	CLA	3	0
25	m	203	CLA	5	0
25	A	832	CLA	5	0
25	A	823	CLA	3	0
29	B	830	BCR	5	0
25	i	213	CLA	2	0
25	e	201	CLA	2	0
25	h	205	CLA	1	0
25	o	607	CLA	3	0
25	h	203	CLA	3	0
25	A	826	CLA	4	0
25	f	604	CLA	1	0
25	B	808	CLA	1	0
25	i	204	CLA	2	0
27	h	201	LHG	1	0
25	h	206	CLA	2	0
25	A	843	CLA	3	0
25	f	611	CLA	1	0
25	i	212	CLA	1	0
29	A	837	BCR	3	0
25	c	313	CLA	2	0
25	B	807	CLA	3	0
27	d	302	LHG	3	0
35	d	307	CHL	1	0
25	h	212	CLA	3	0
25	n	210	CLA	1	0

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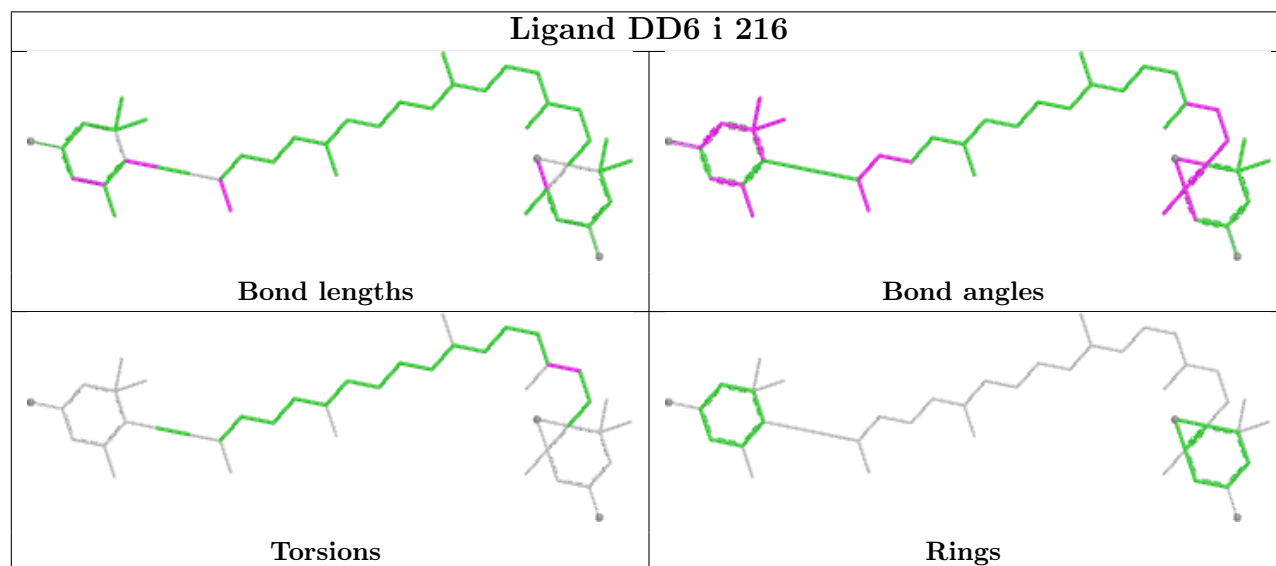
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	p	607	CLA	1	0
25	i	211	CLA	2	0
25	j	207	CLA	1	0
25	n	201	CLA	2	0
25	A	810	CLA	3	0
27	m	201	LHG	2	0
25	m	206	CLA	1	0
25	A	822	CLA	3	0
25	g	214	CLA	1	0
25	h	209	CLA	9	0
25	B	818	CLA	6	0
25	B	802	CLA	9	0
25	g	203	CLA	2	0
25	j	203	CLA	4	0
25	d	315	CLA	1	0
25	j	206	CLA	2	0
35	d	310	CHL	2	0
25	B	846	CLA	4	0
25	B	826	CLA	3	0
29	M	201	BCR	2	0
25	k	211	CLA	2	0
25	A	849	CLA	2	0
25	j	208	CLA	2	0
25	B	812	CLA	3	0
25	l	606	CLA	3	0
25	A	844	CLA	5	0
25	e	205	CLA	4	0
25	h	208	CLA	2	0
25	A	853	CLA	2	0
25	f	602	CLA	2	0
25	i	208	CLA	3	0
25	b	206	CLA	3	0
25	j	209	CLA	3	0
25	B	840	CLA	5	0
25	A	802	CLA	7	0
25	B	825	CLA	1	0
25	c	303	CLA	2	0
25	B	804	CLA	3	0
25	m	208	CLA	3	0
25	m	202	CLA	5	0
25	B	841	CLA	4	0
25	B	810	CLA	1	0

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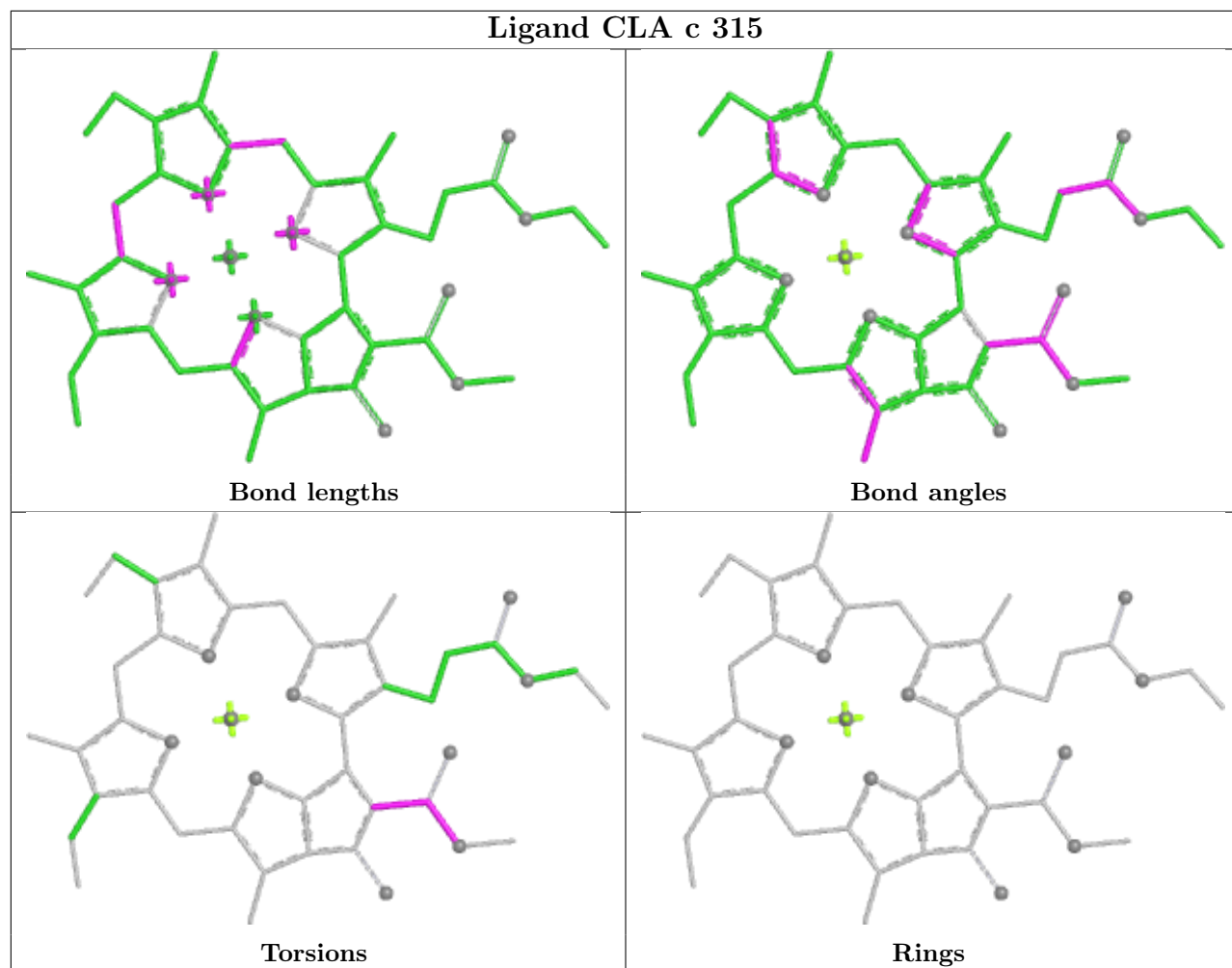
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	847	CLA	3	0
25	A	806	CLA	1	0
25	n	203	CLA	2	0

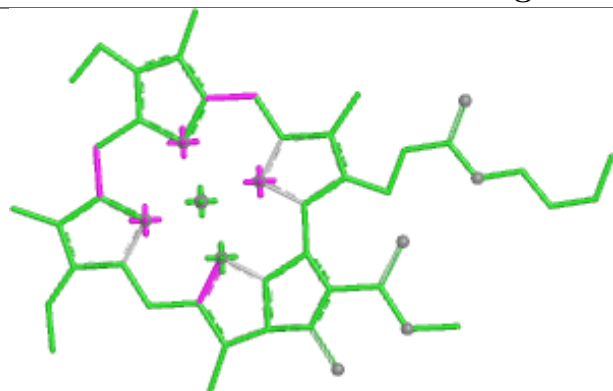
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



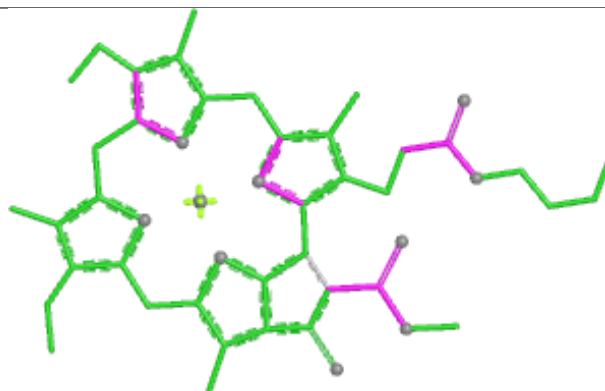
## Ligand CLA c 315



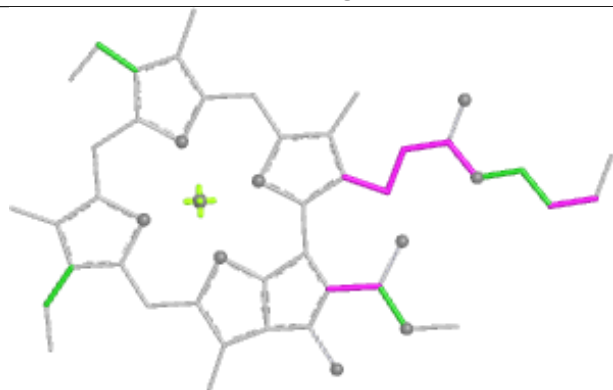
## Ligand CLA B 815



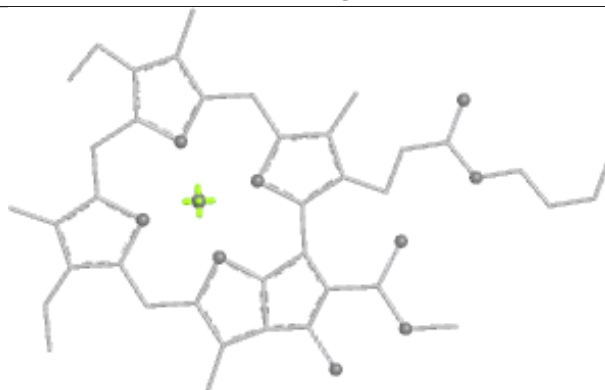
Bond lengths



Bond angles

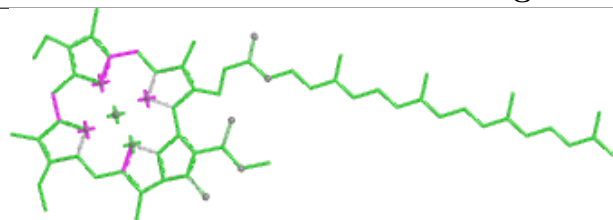


Torsions

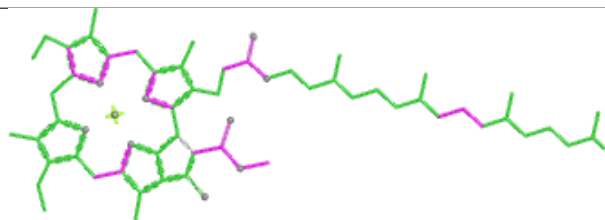


Rings

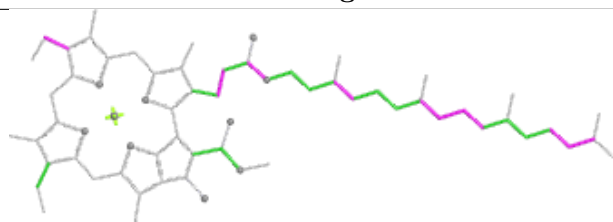
## Ligand CLA A 818



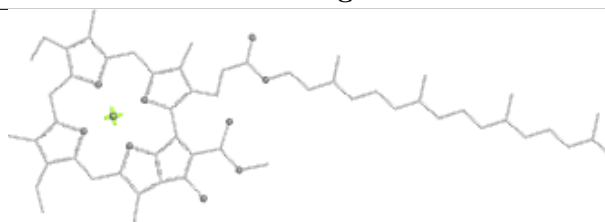
Bond lengths



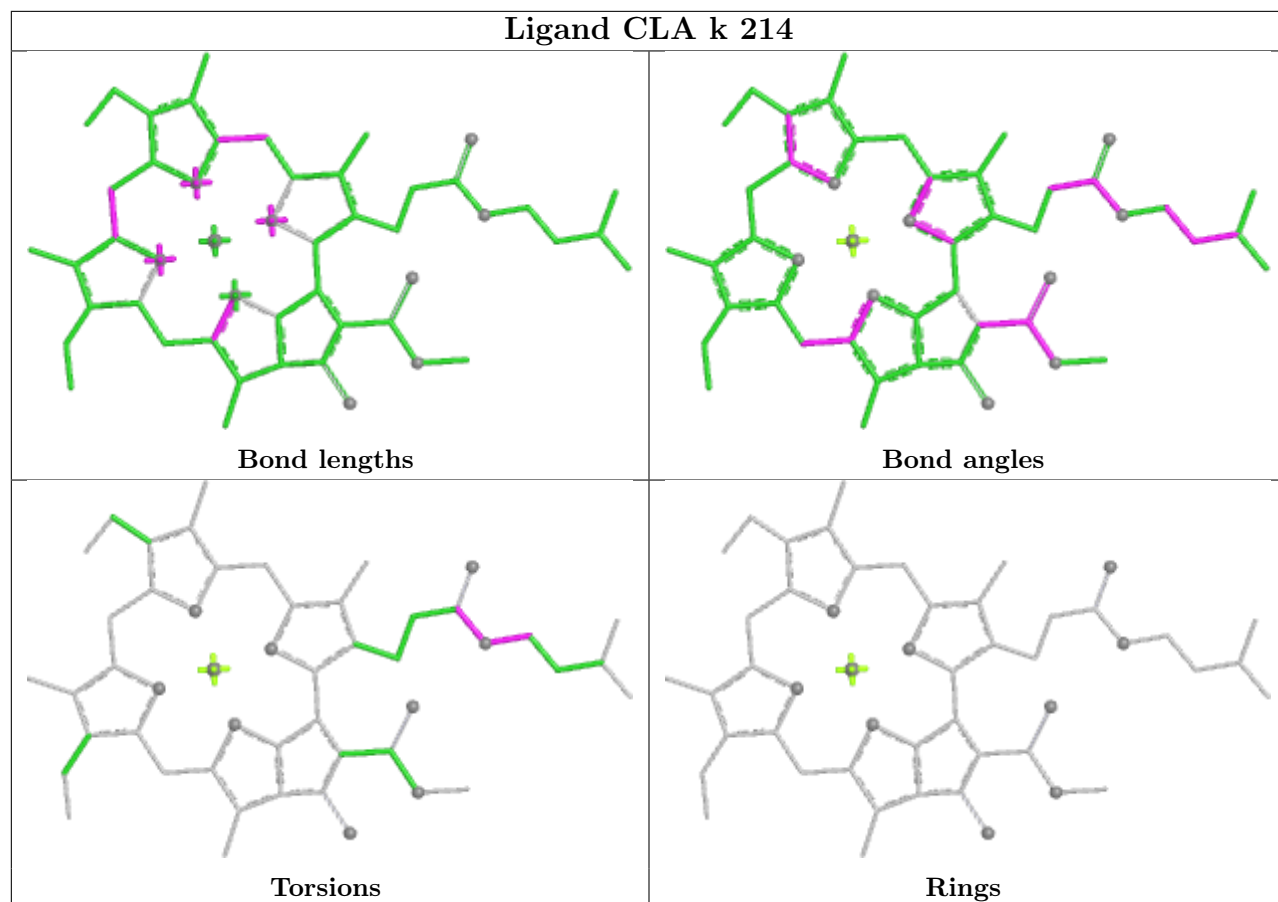
Bond angles



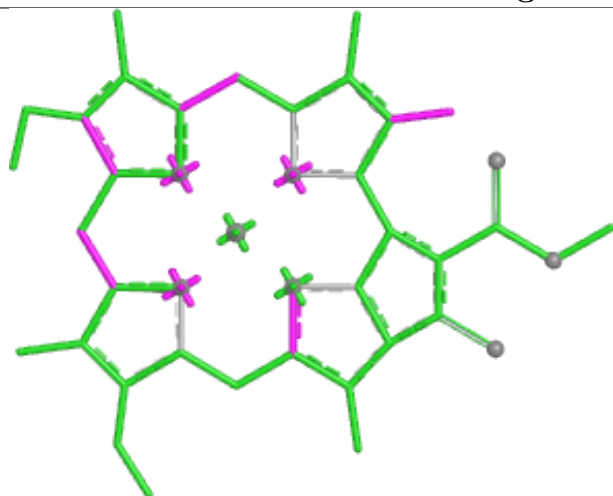
Torsions



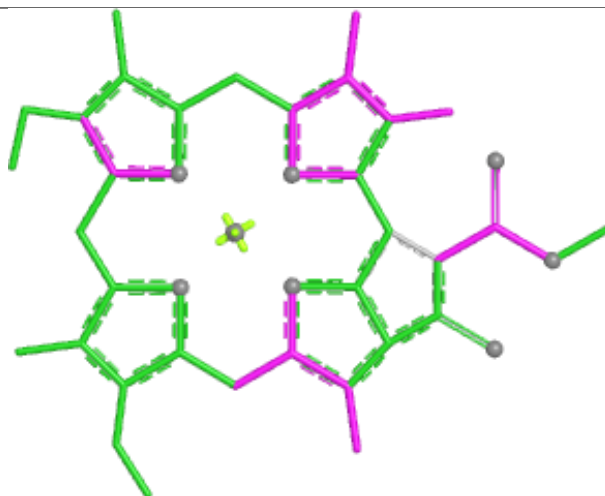
Rings



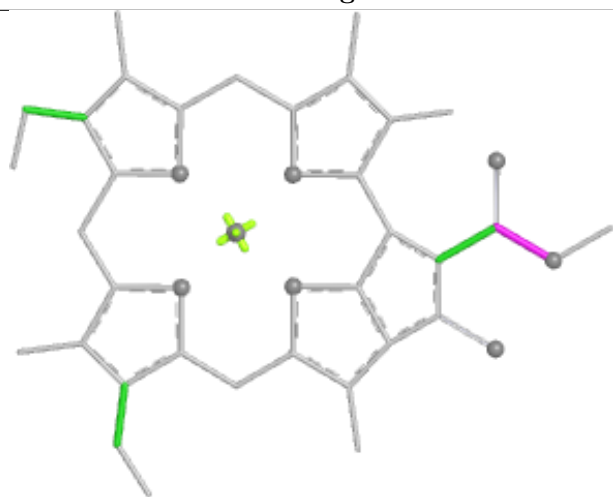
## Ligand CLA n 207



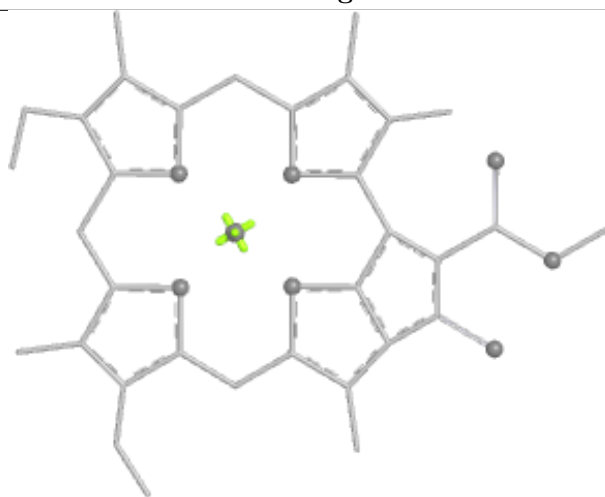
Bond lengths



Bond angles



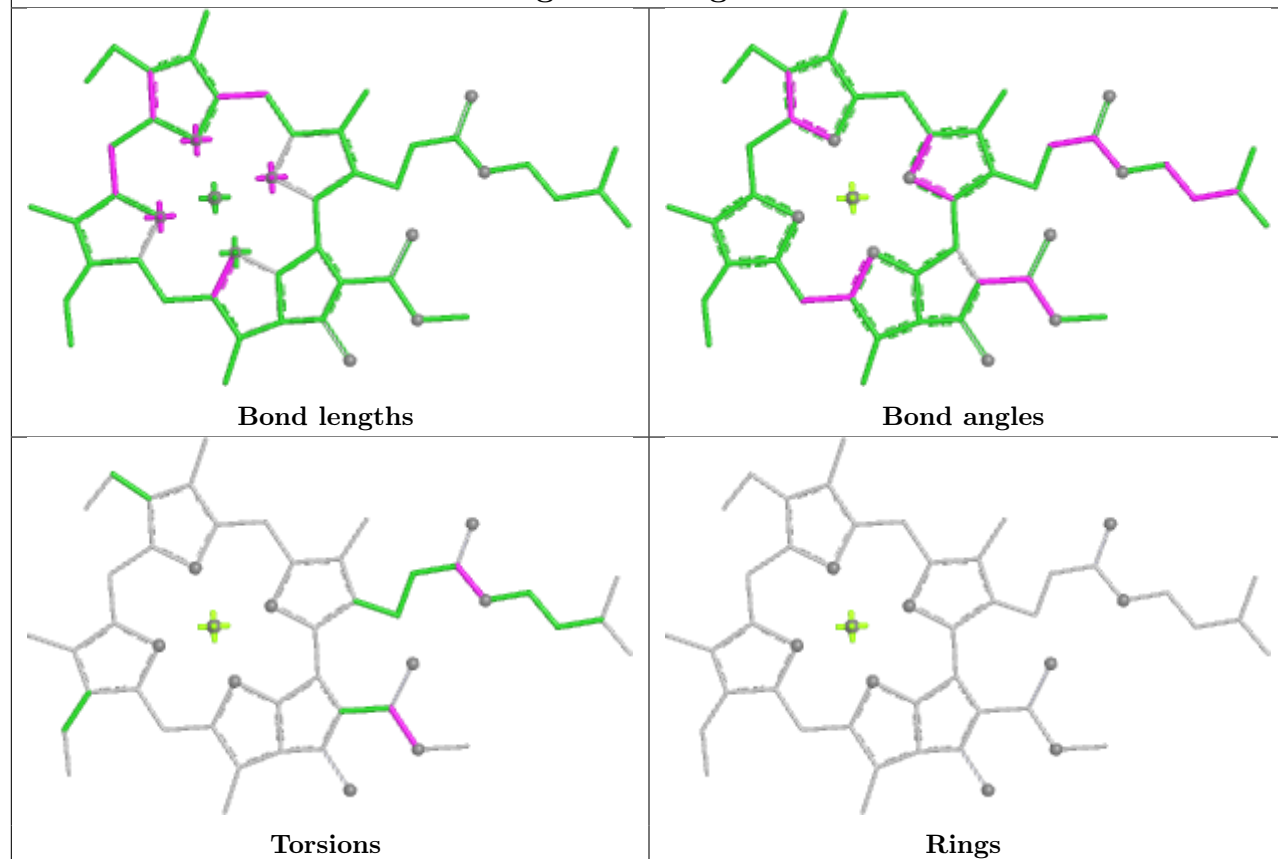
Torsions



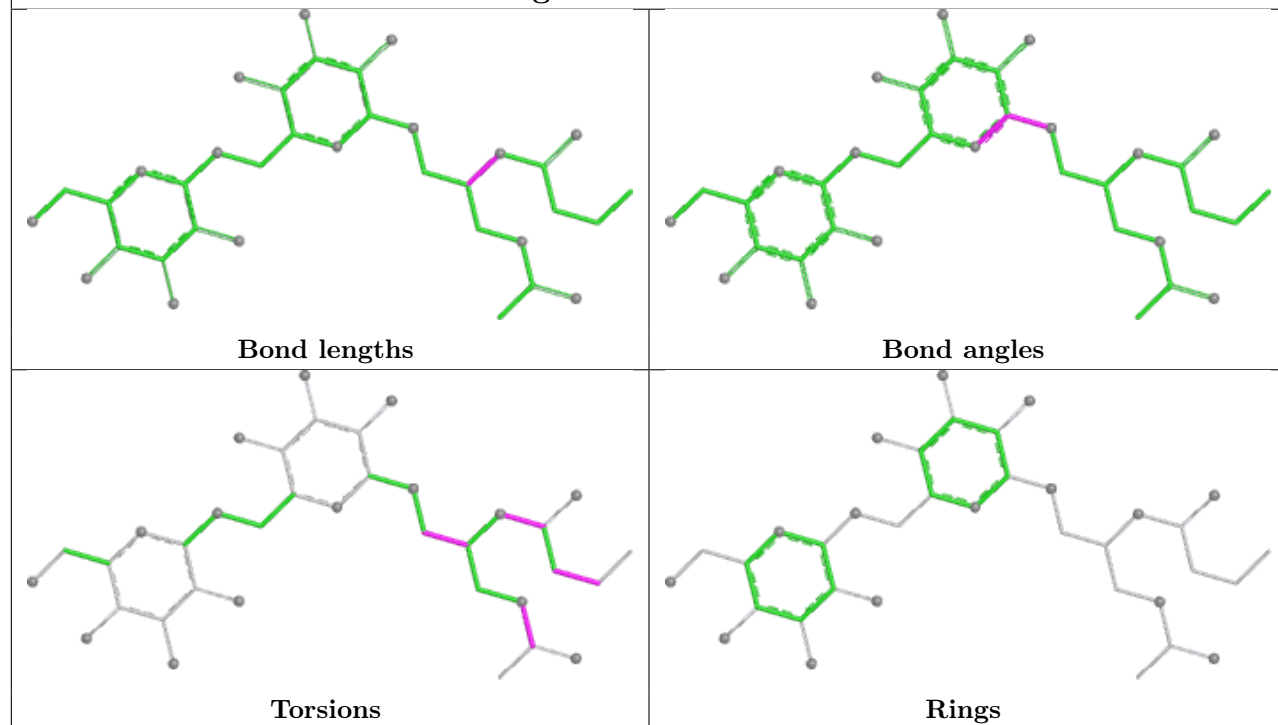
Rings

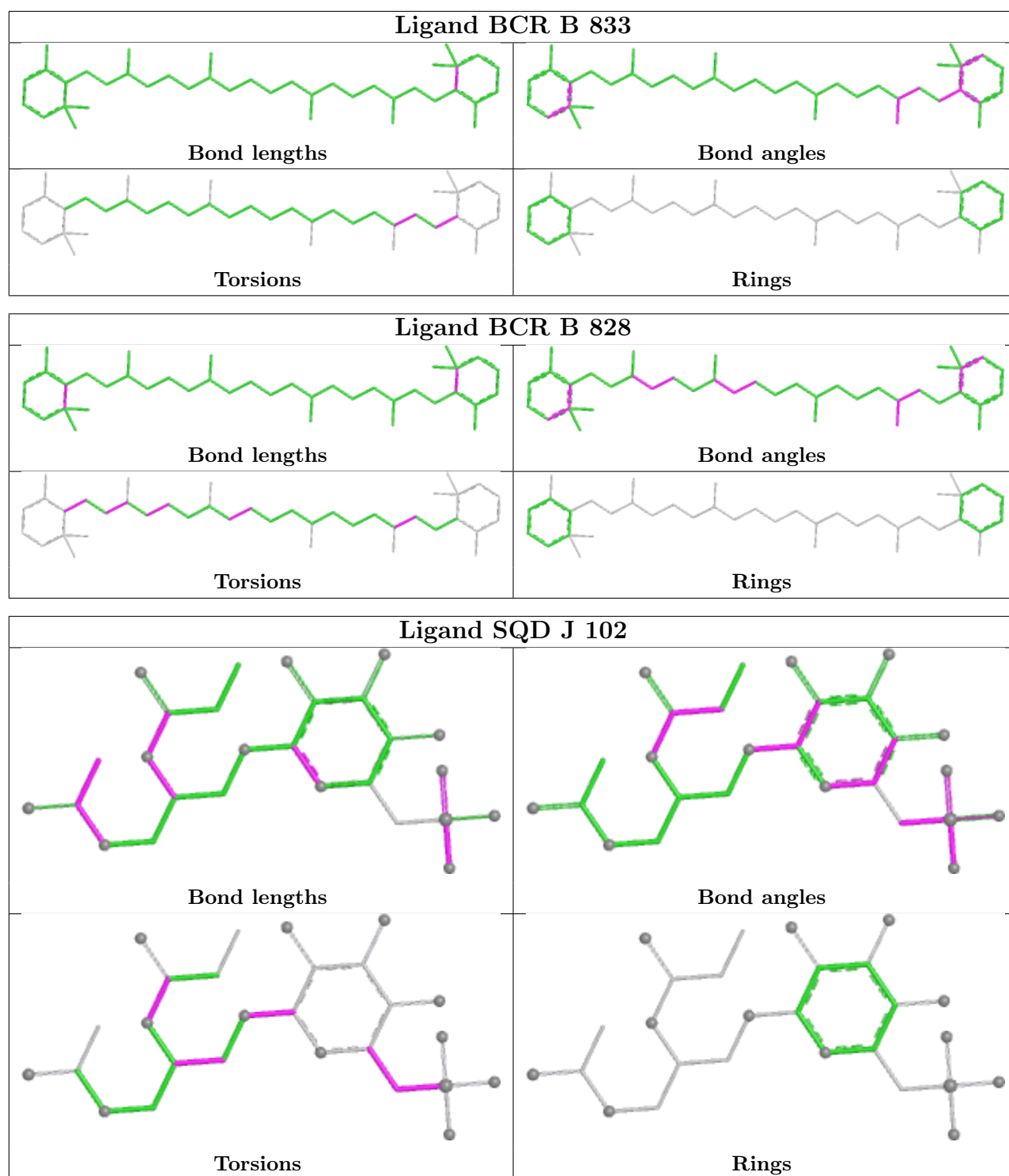


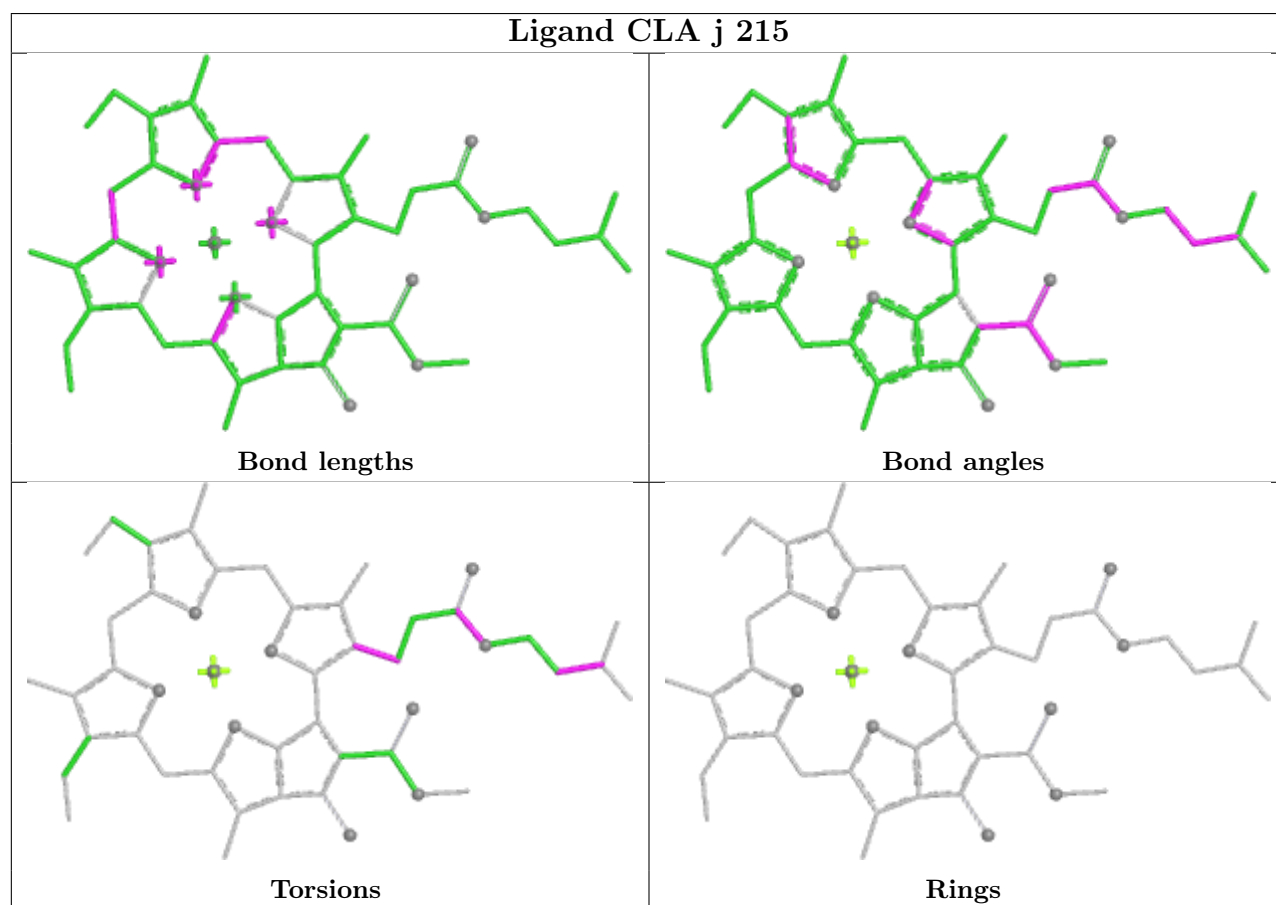
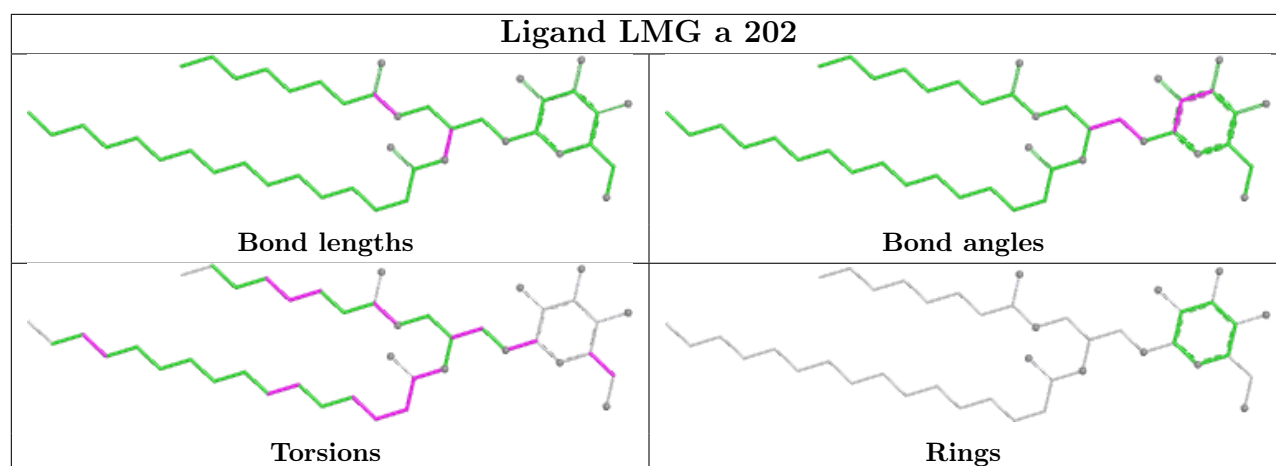
## Ligand CLA g 208

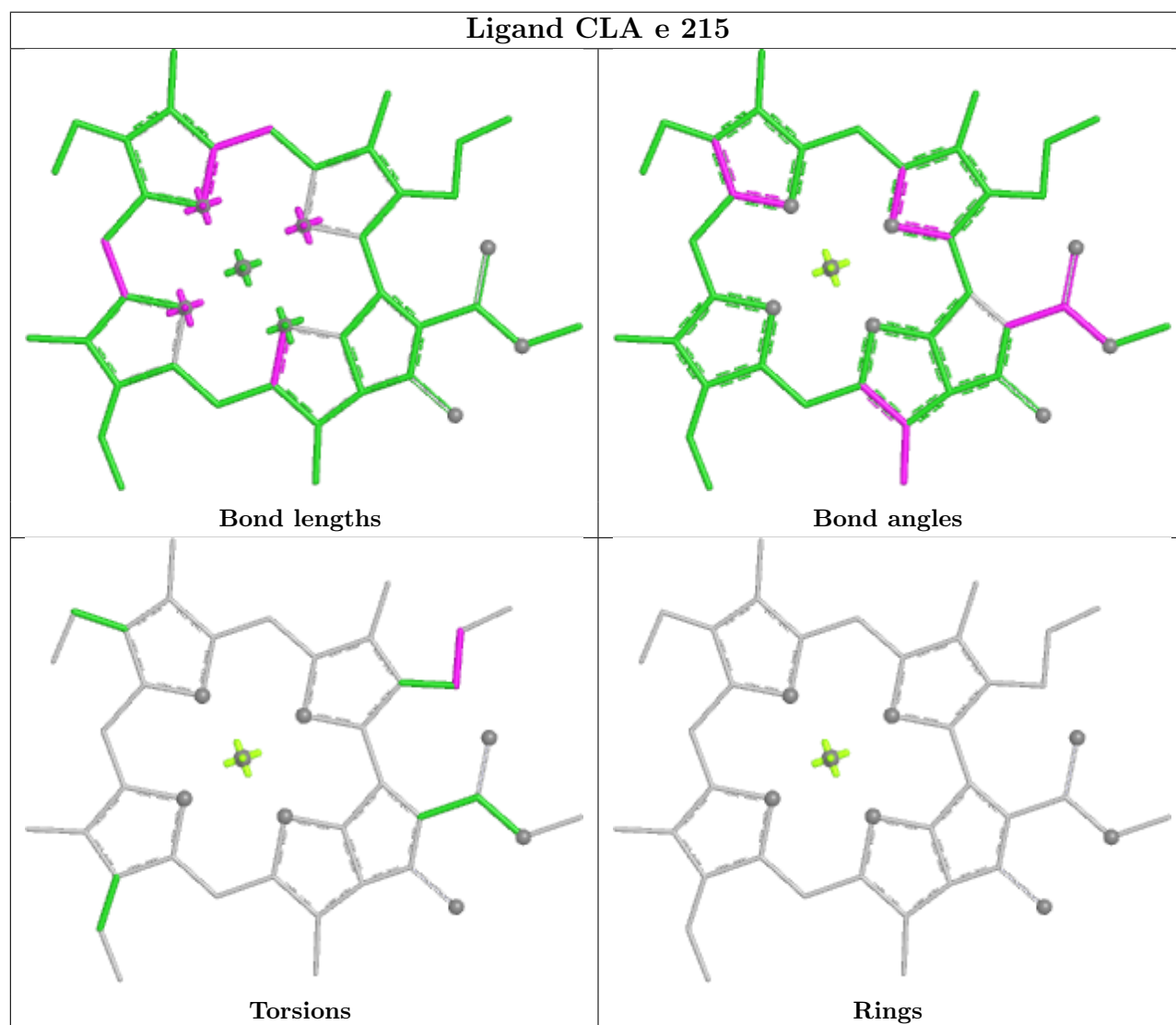
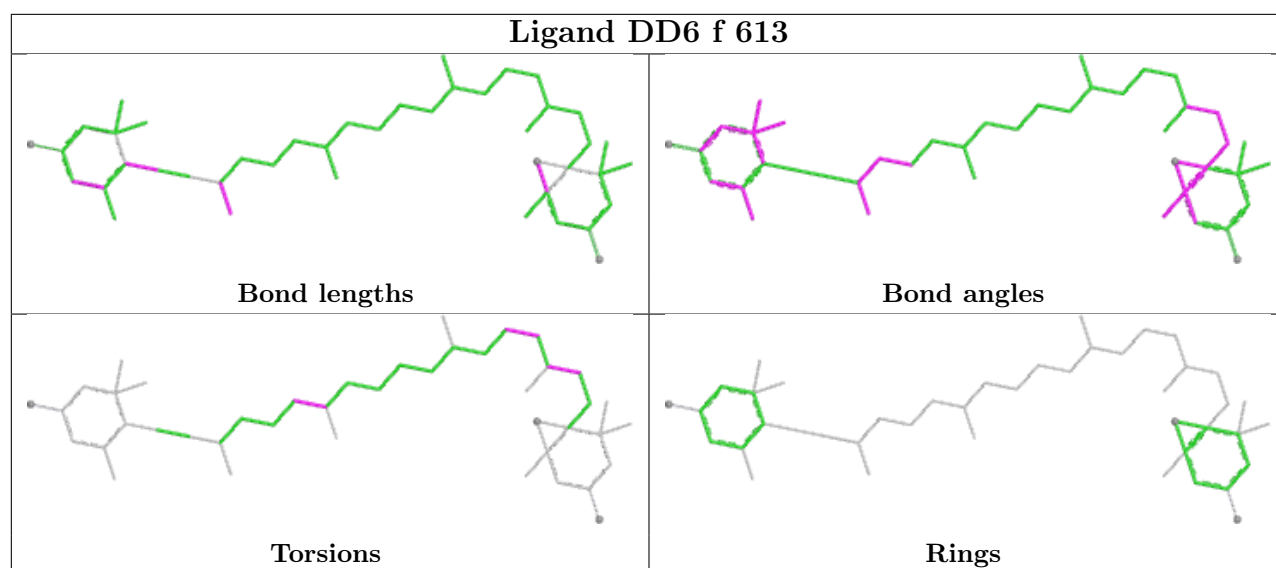


## Ligand DGD e 203

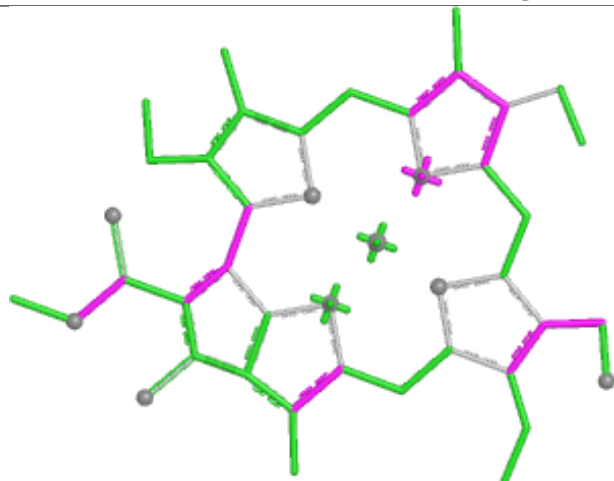




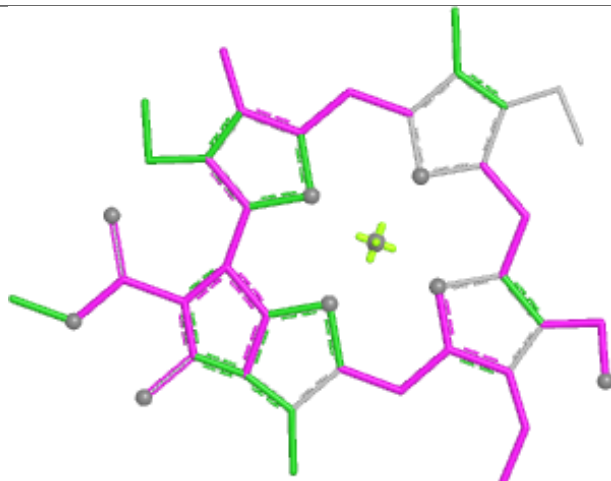




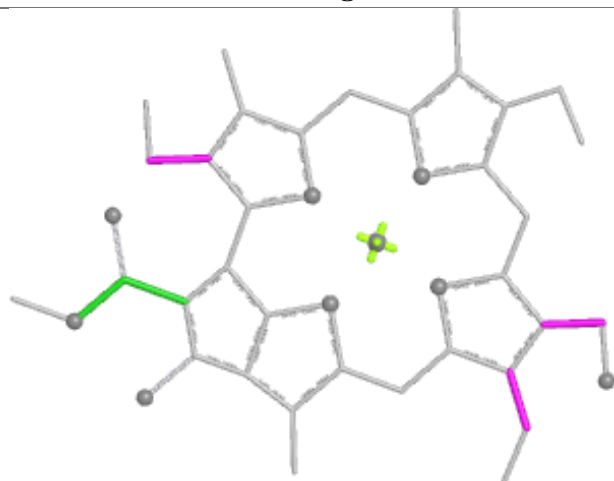
## Ligand CHL d 309



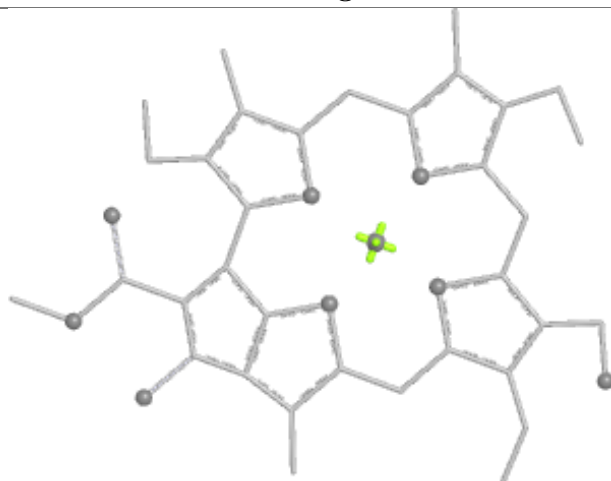
Bond lengths



Bond angles

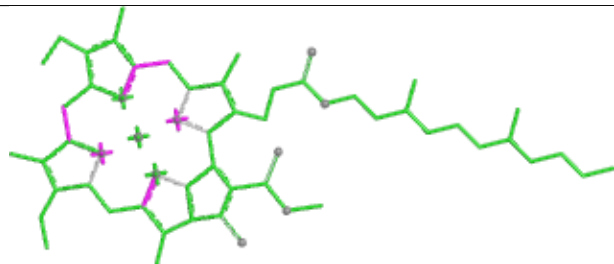


Torsions

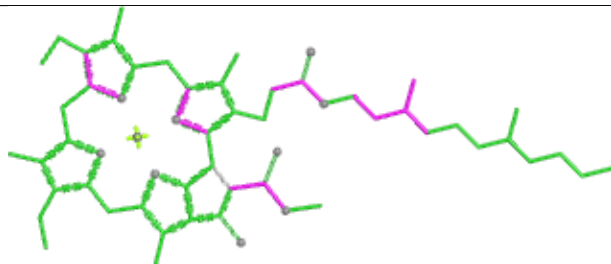


Rings

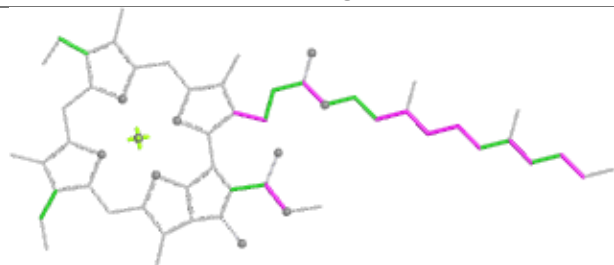
## Ligand CLA A 829



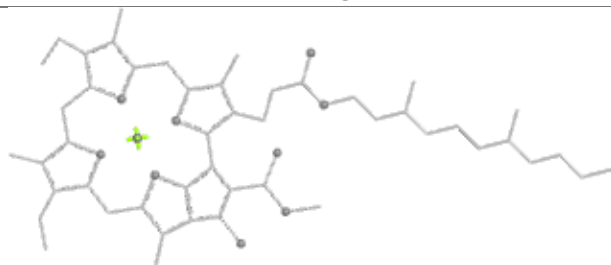
Bond lengths



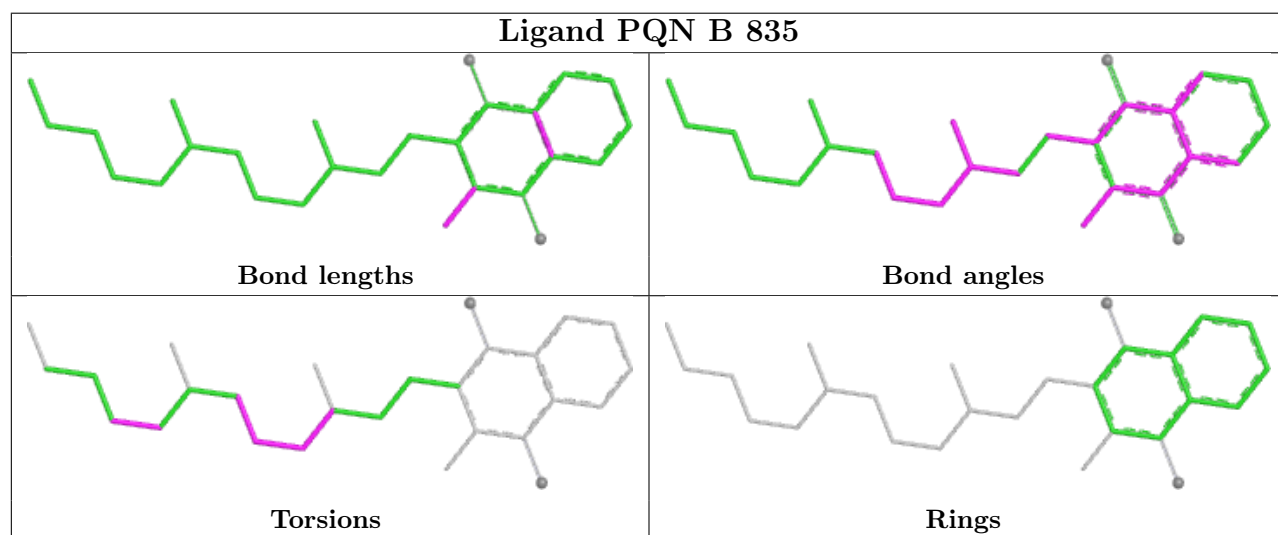
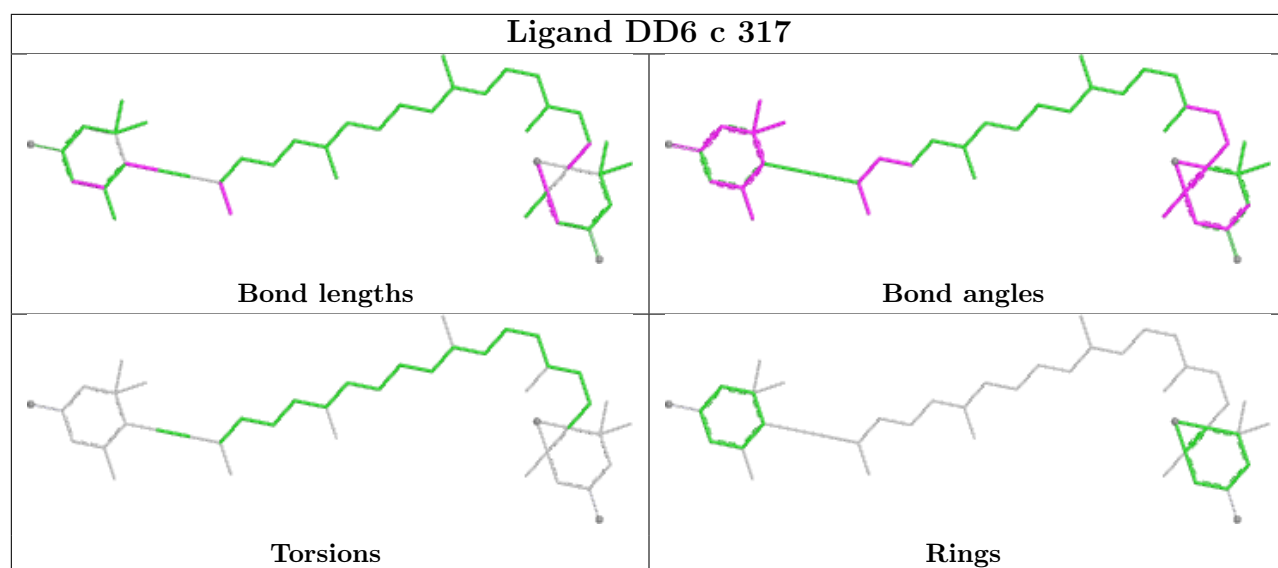
Bond angles



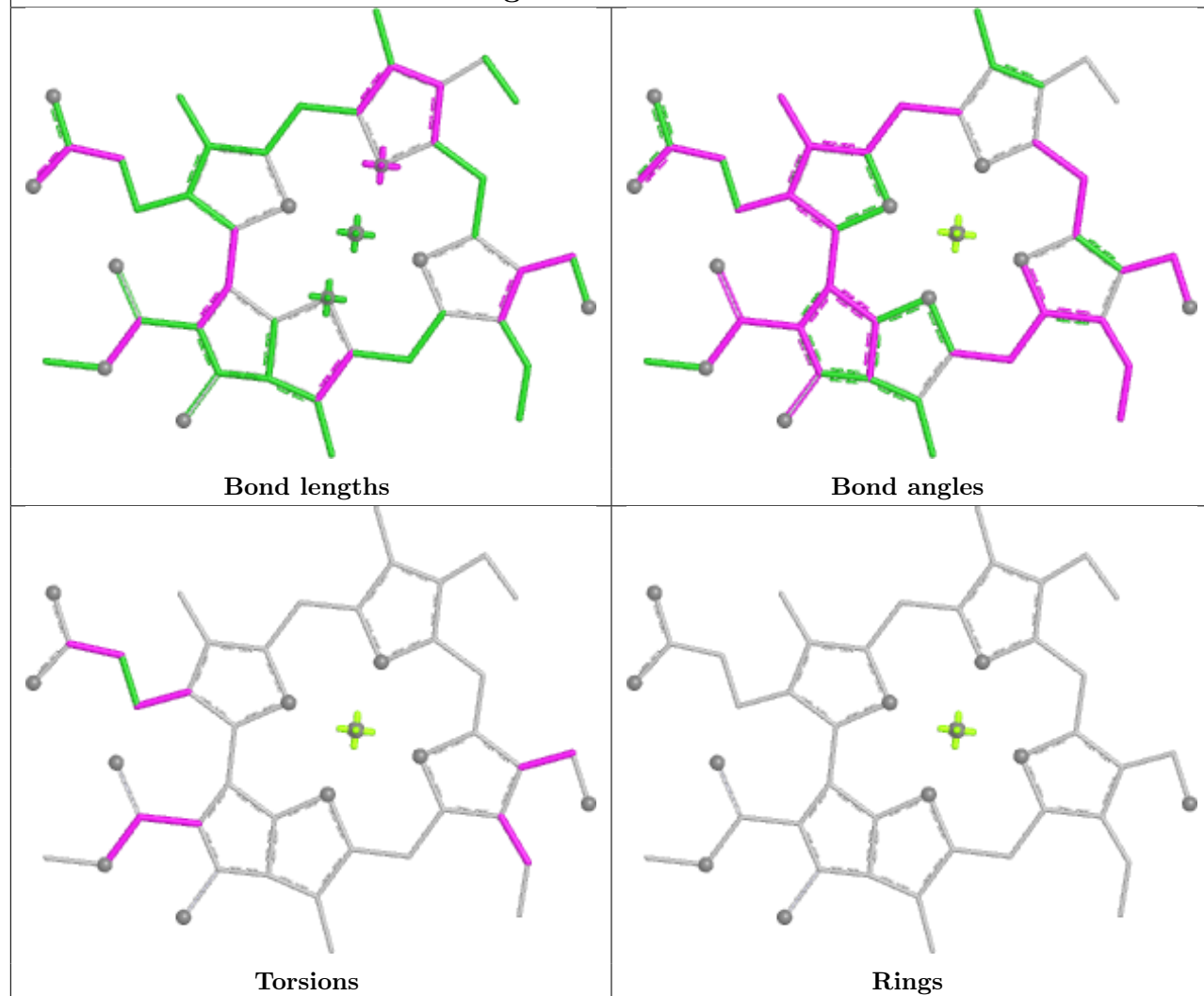
Torsions



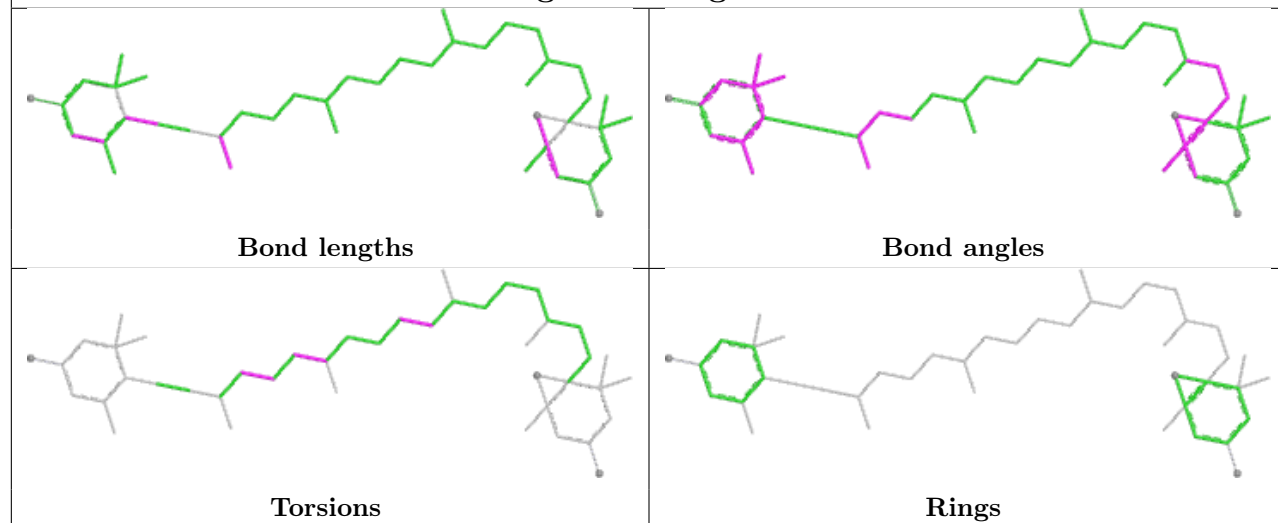
Rings



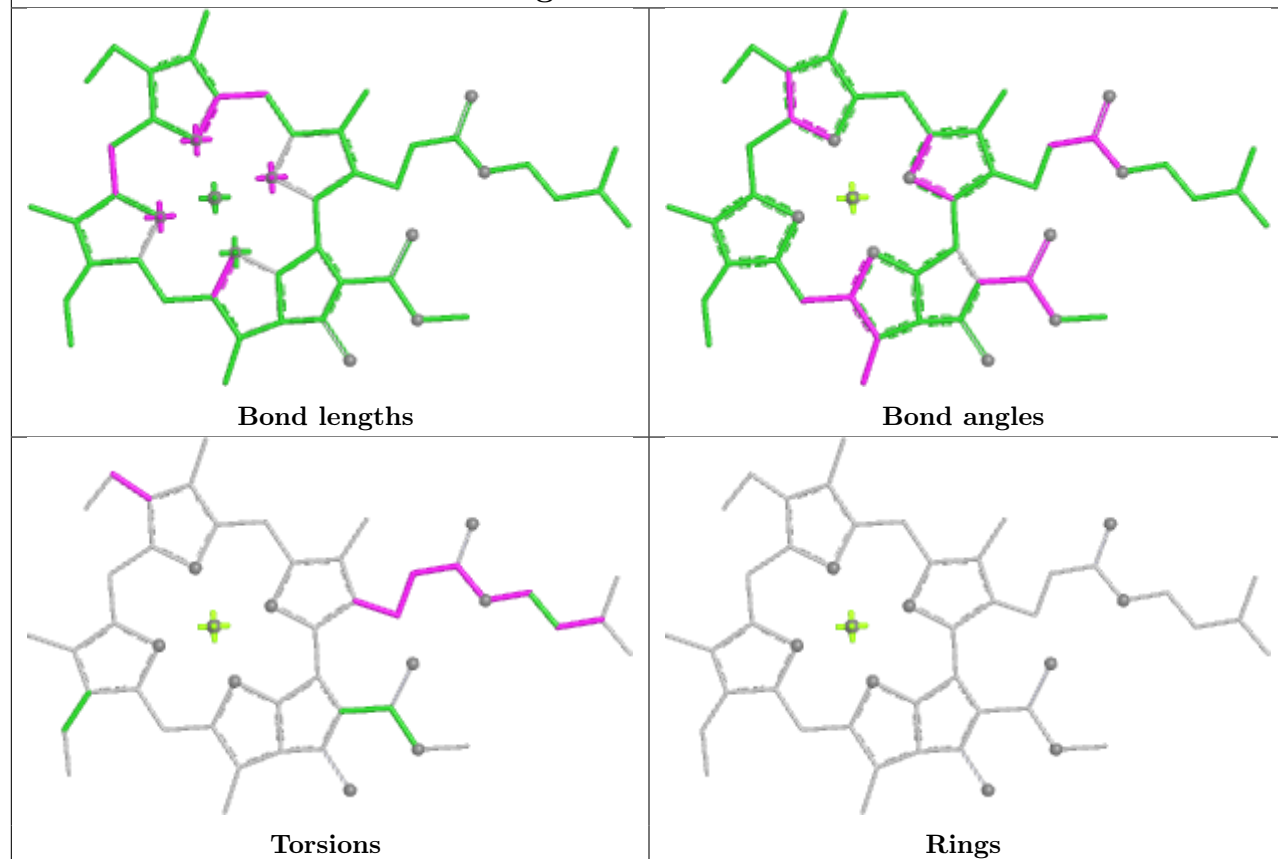
## Ligand CHL d 308



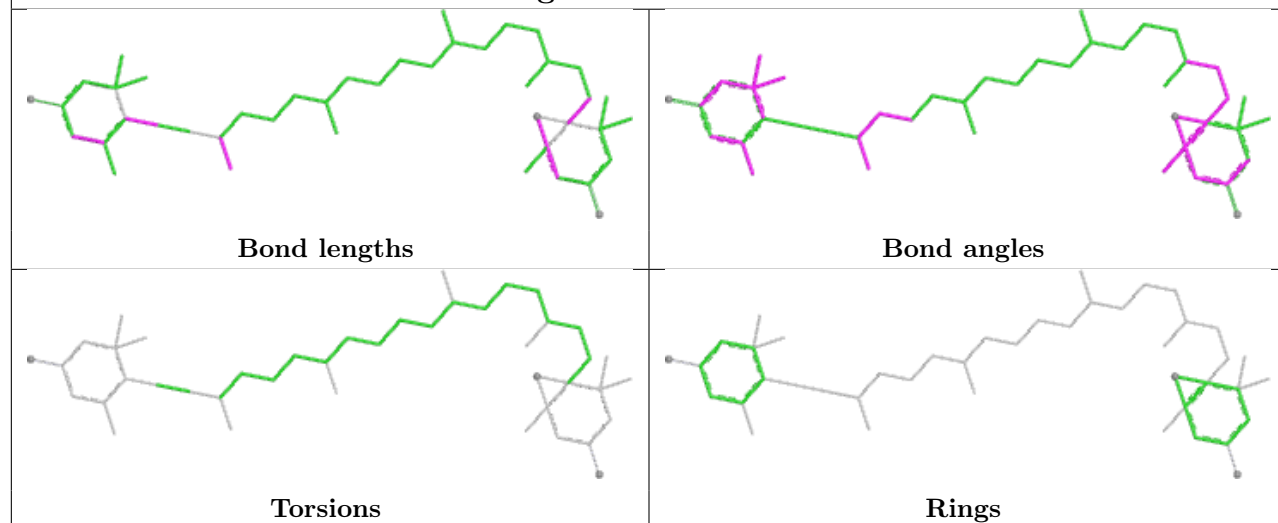
## Ligand DD6 g 217



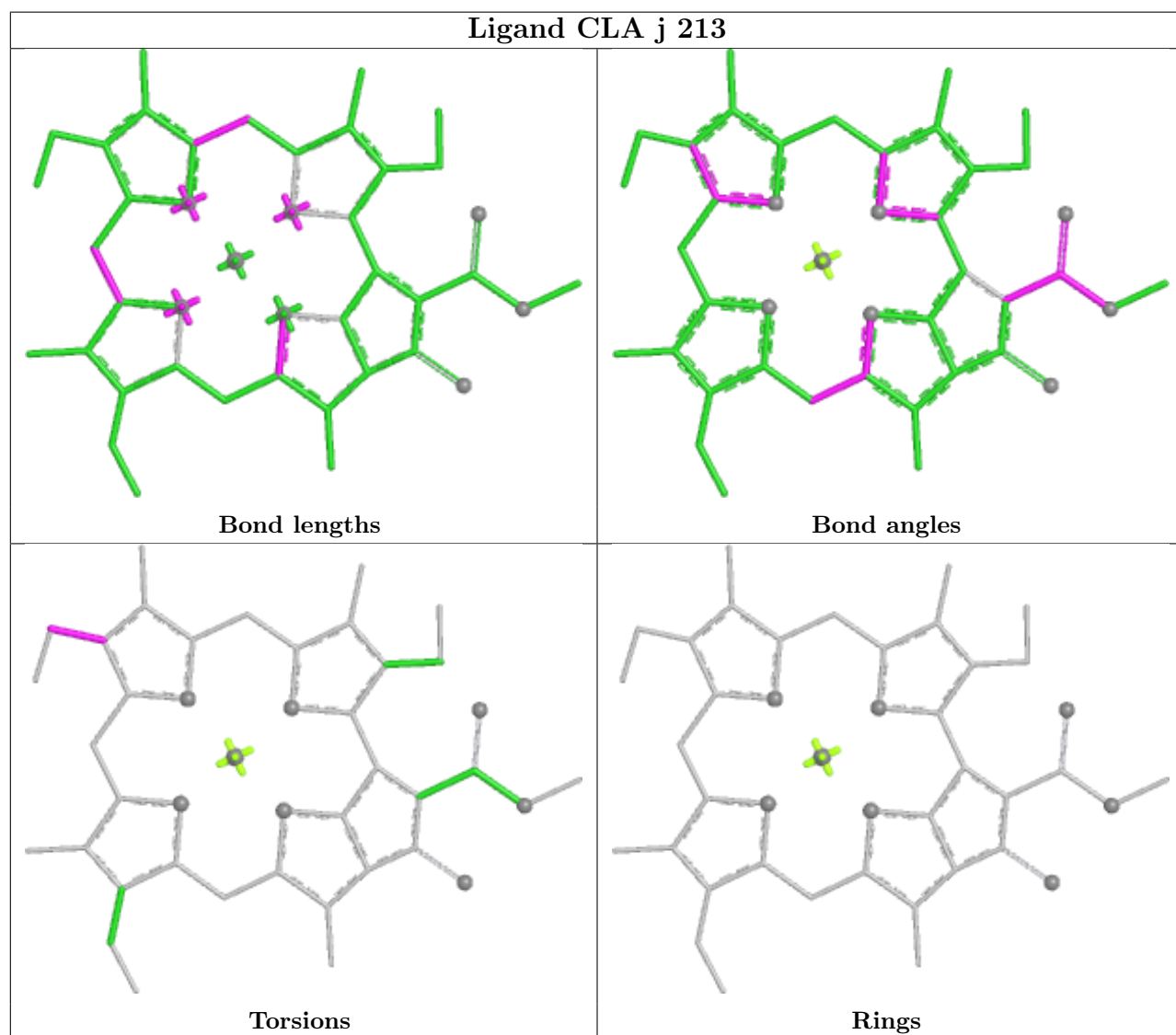
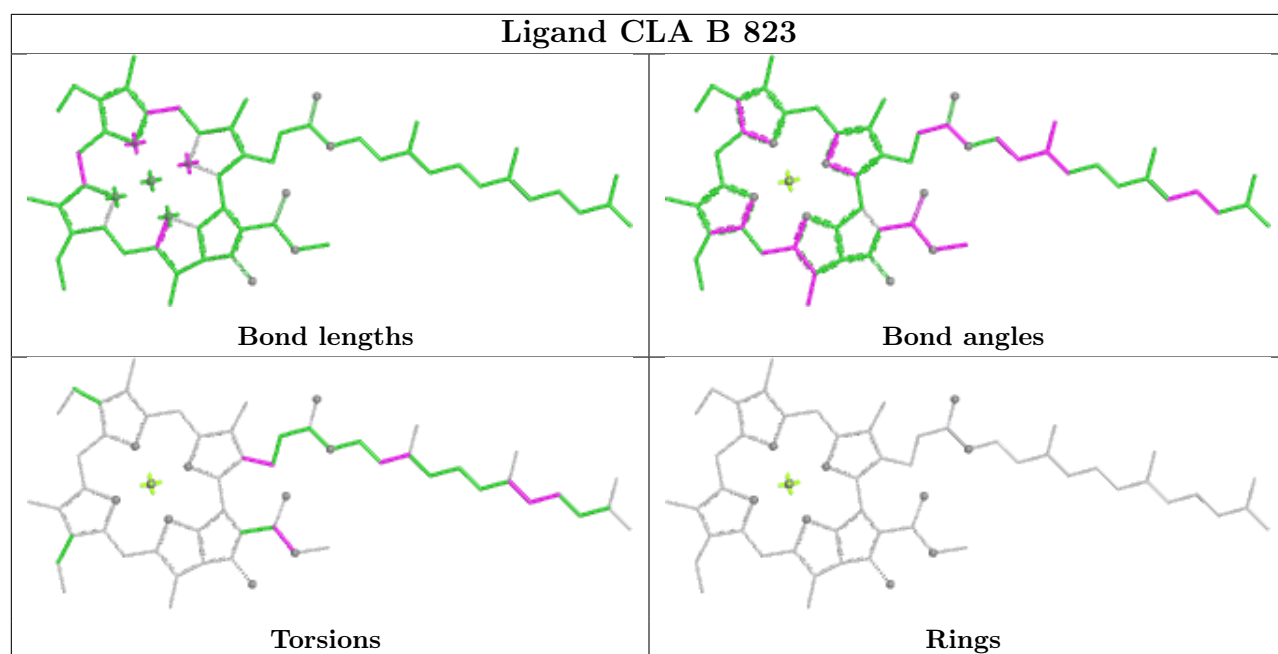
## Ligand CLA J 103



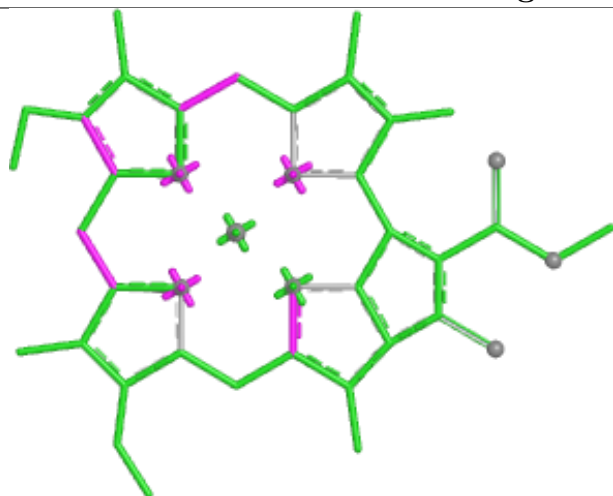
## Ligand DD6 a 215



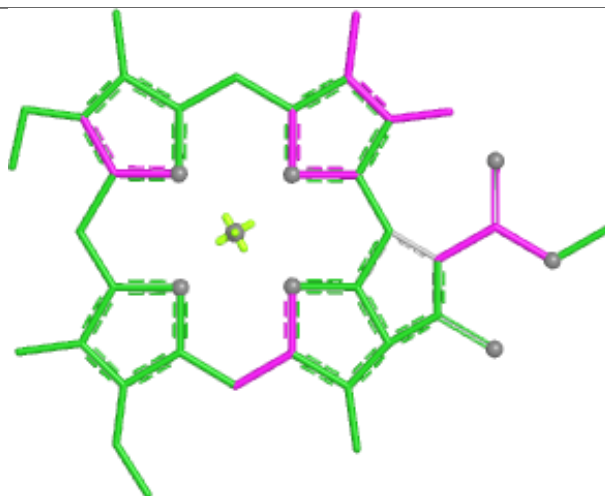




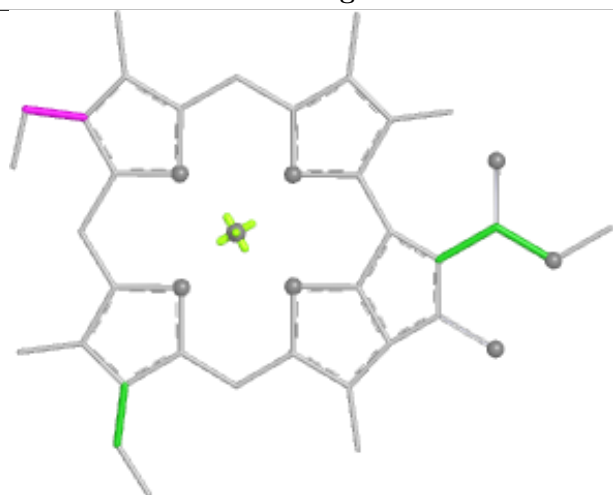
## Ligand CLA n 209



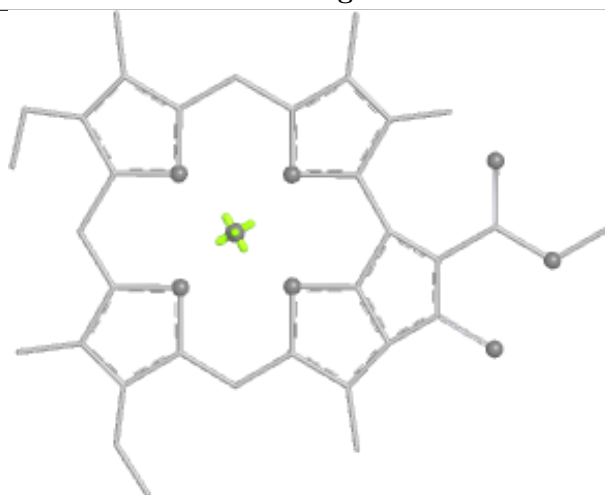
Bond lengths



Bond angles

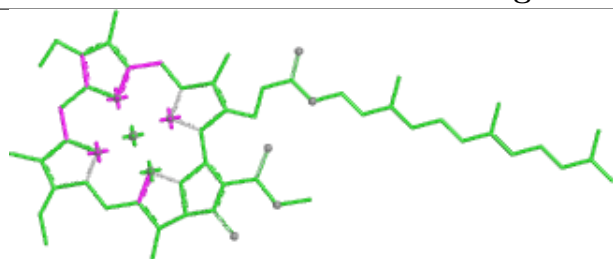


Torsions

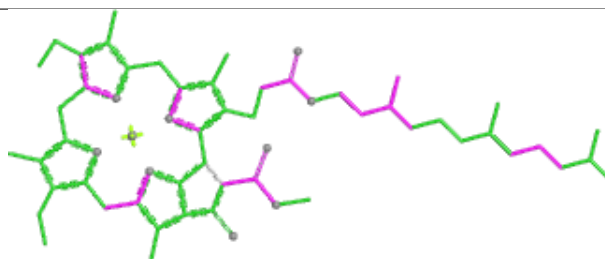


Rings

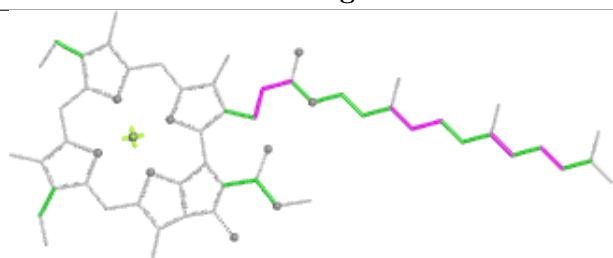
## Ligand CLA A 804



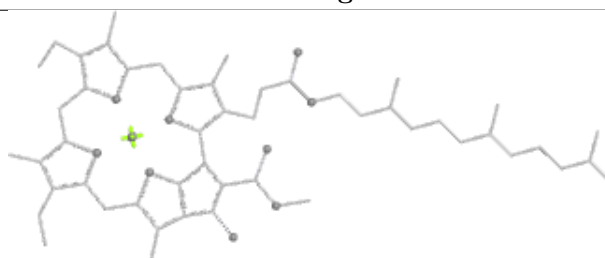
Bond lengths



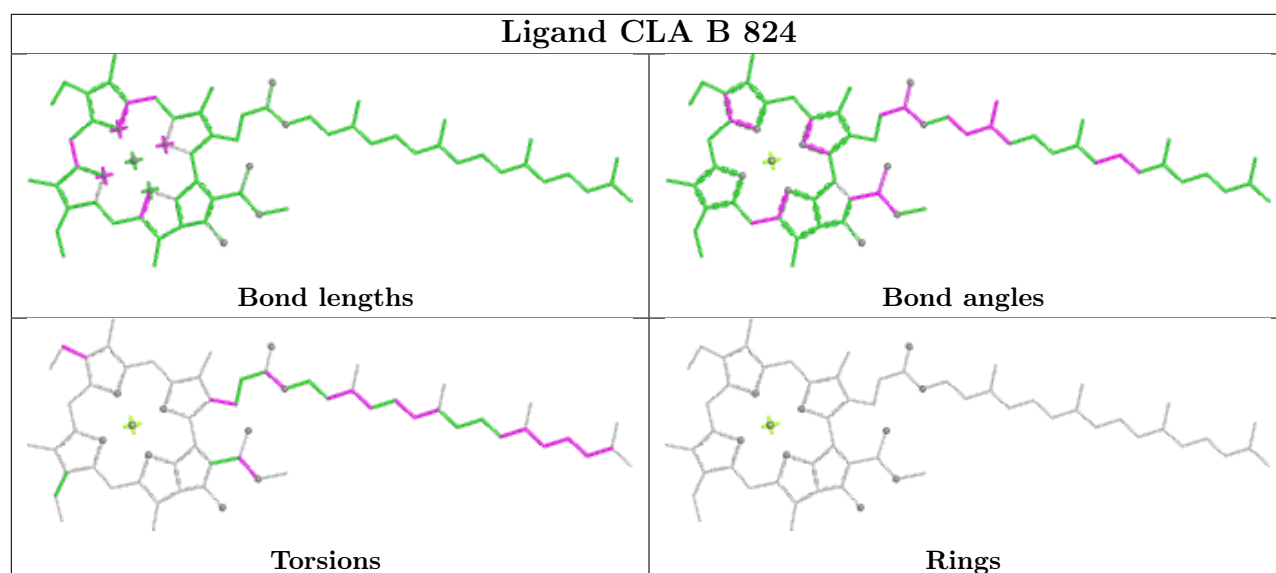
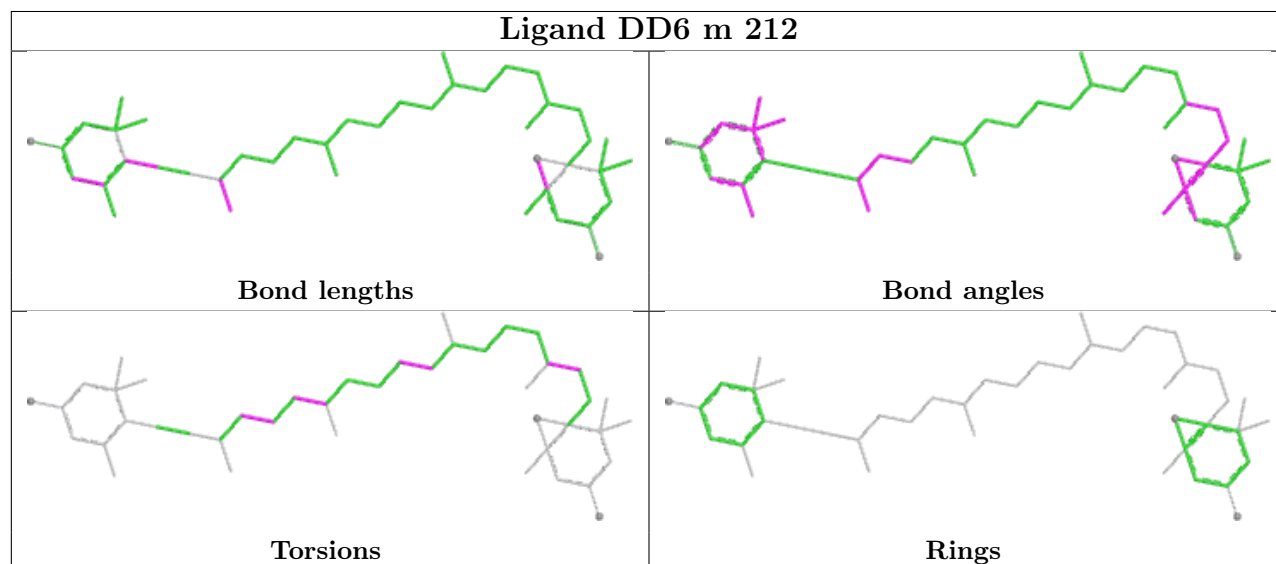
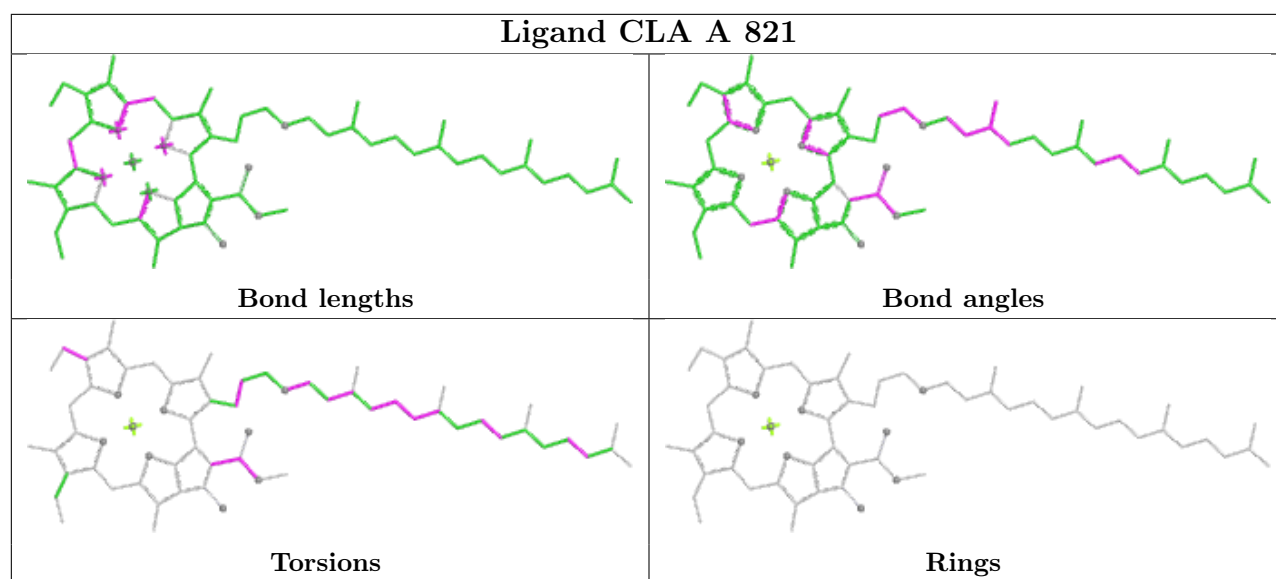
Bond angles



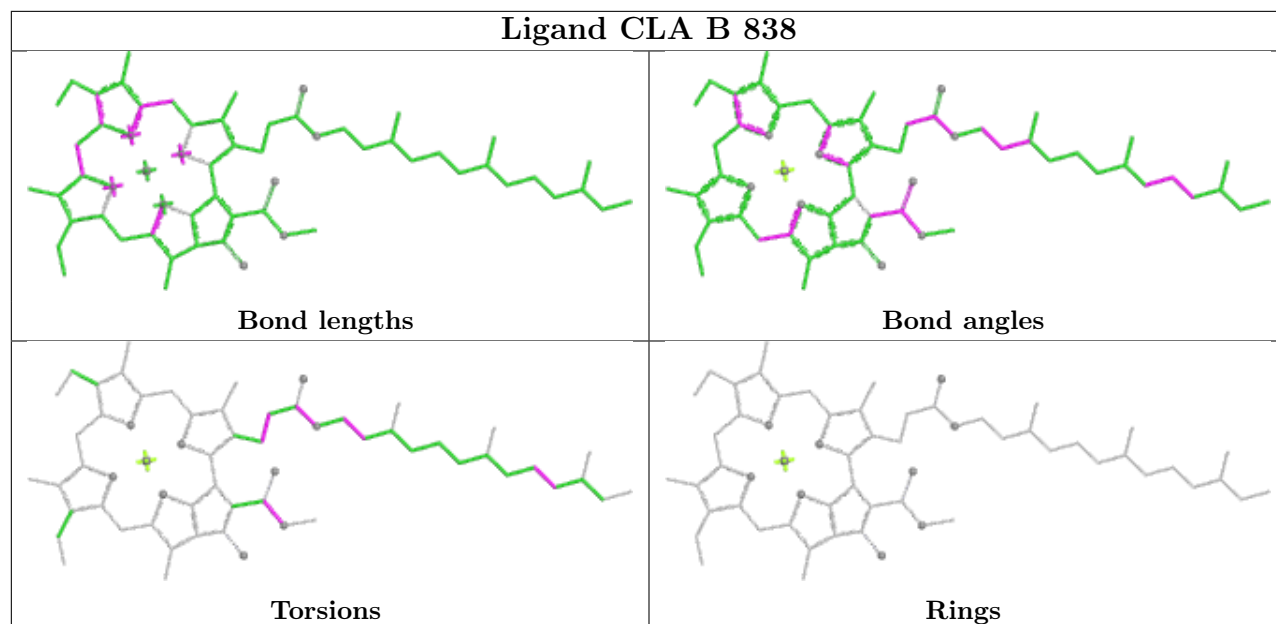
Torsions



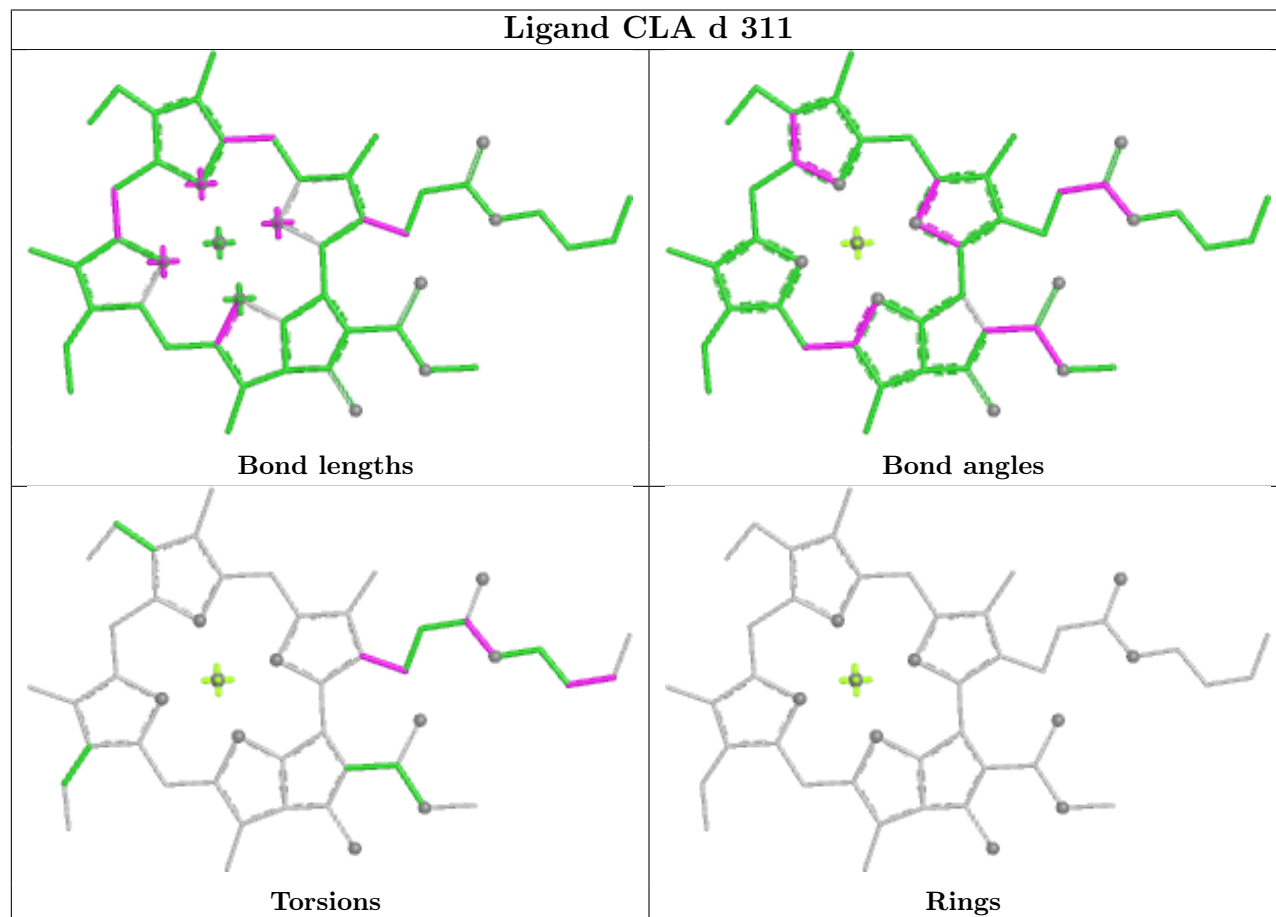
Rings

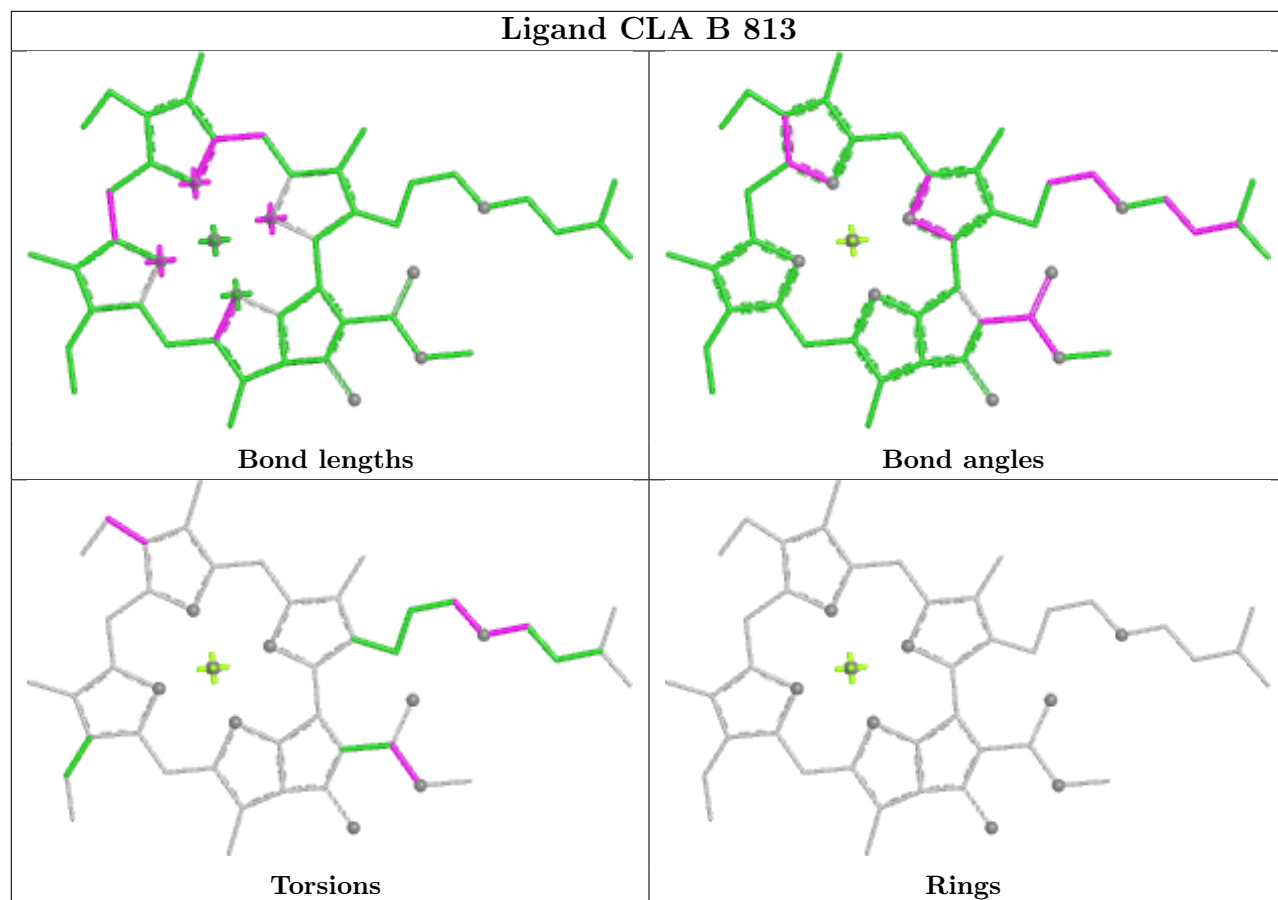


## Ligand CLA B 838

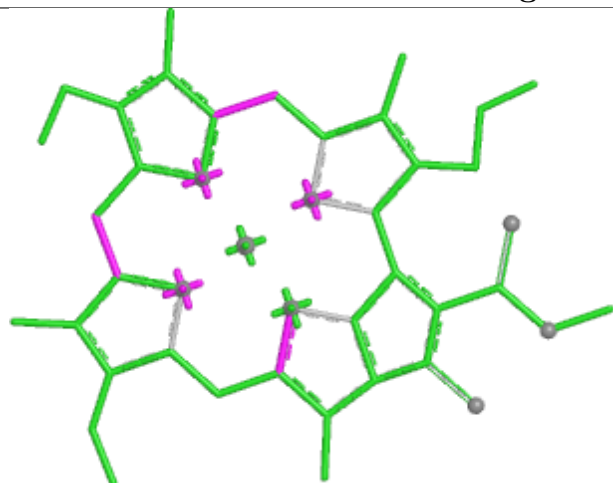


## Ligand CLA d 311

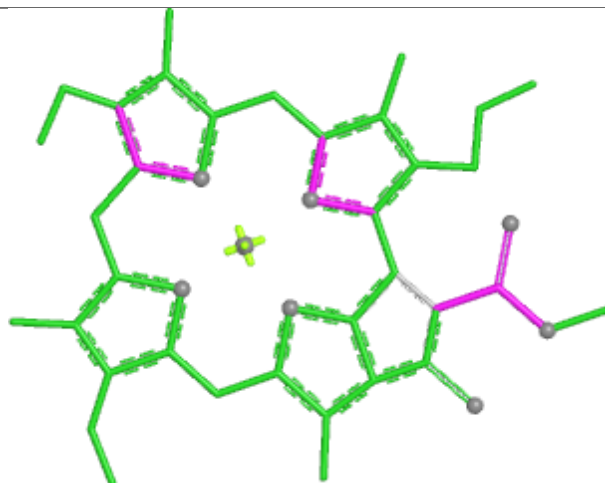




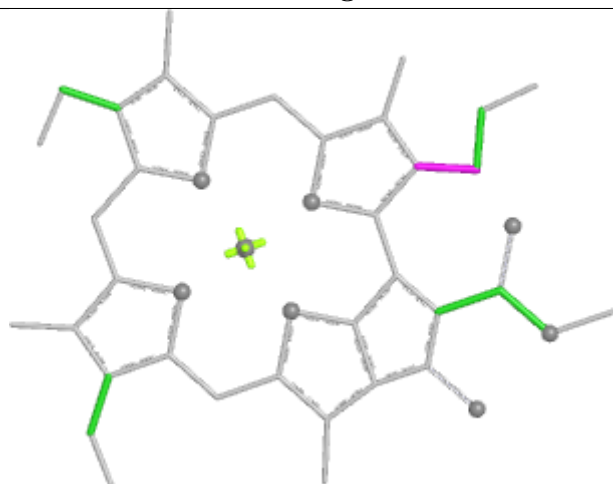
## Ligand CLA c 311



Bond lengths



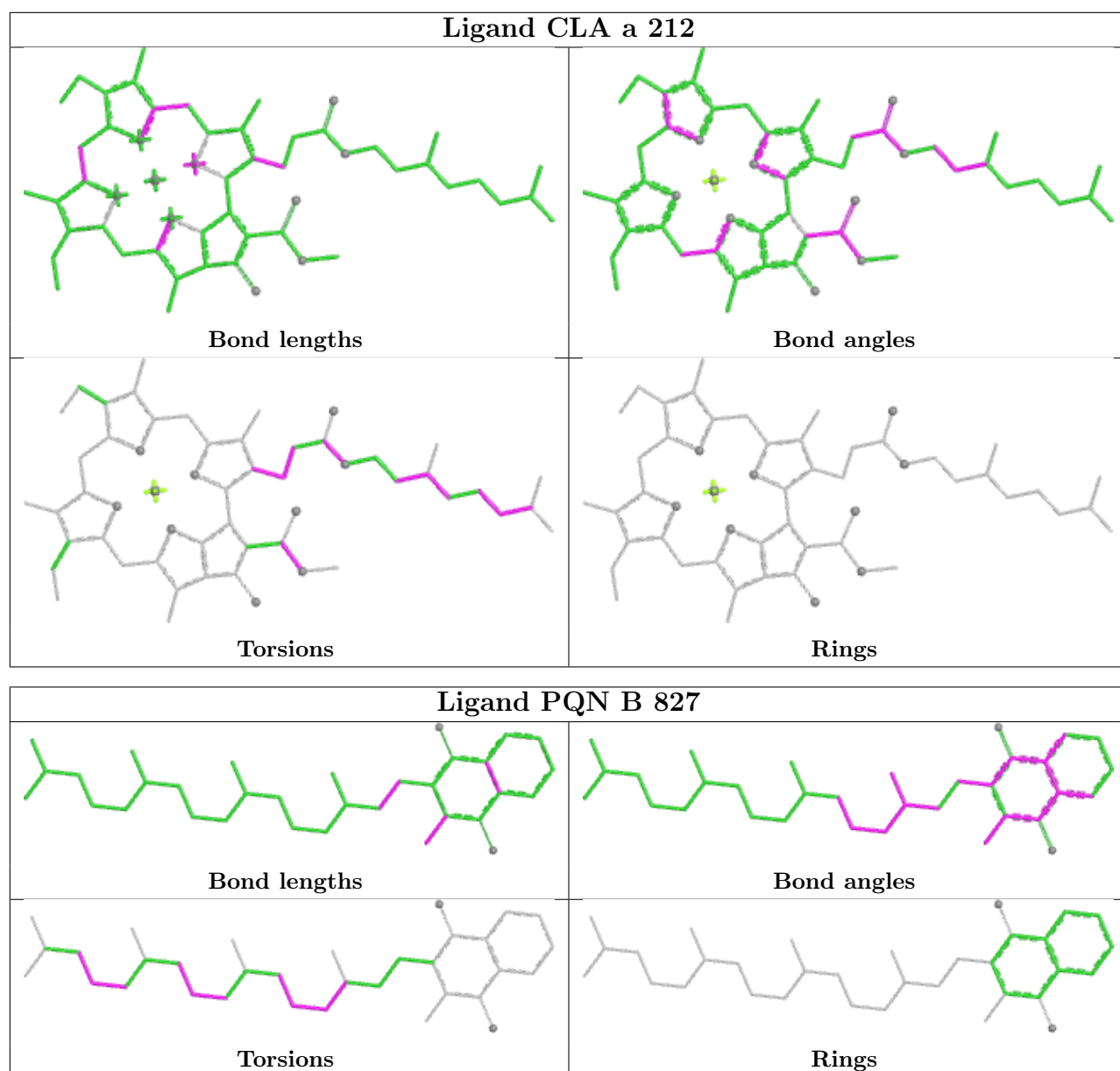
Bond angles



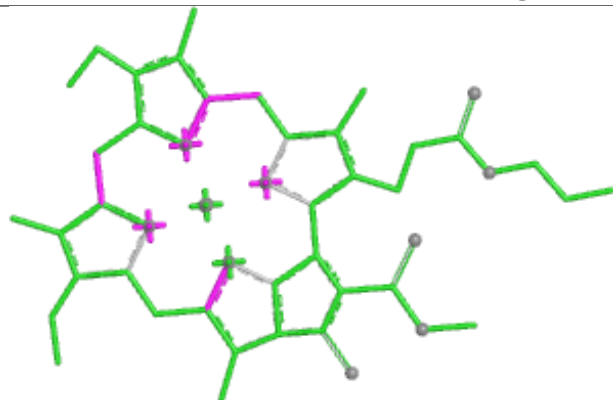
Torsions



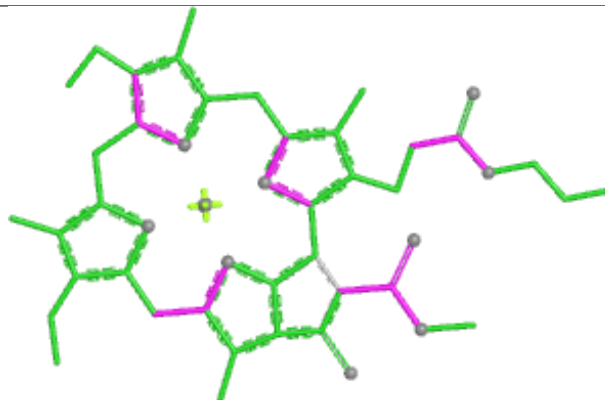
Rings



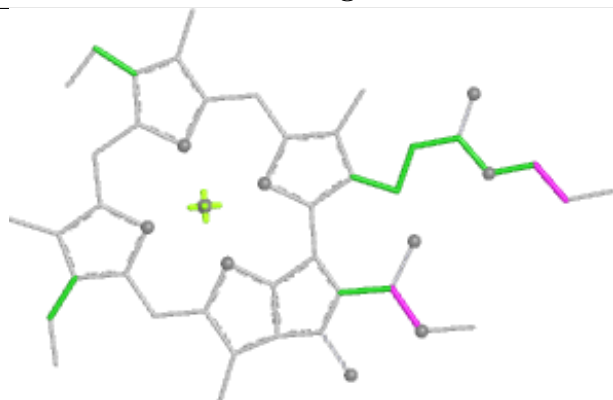
## Ligand CLA A 831



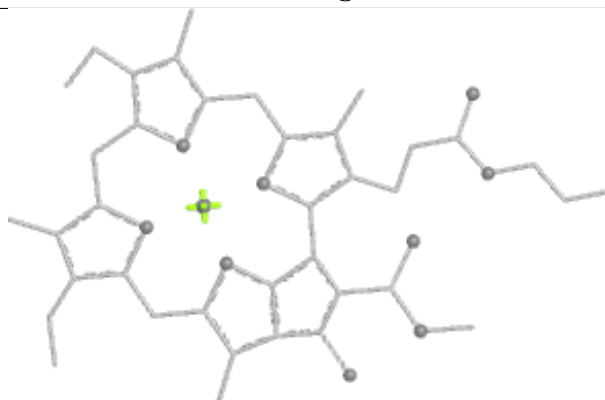
Bond lengths



Bond angles

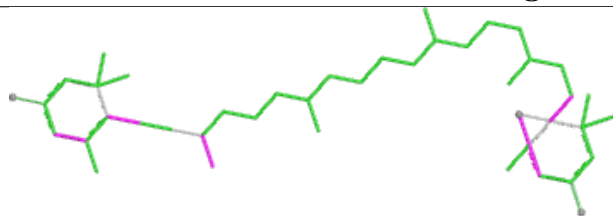


Torsions

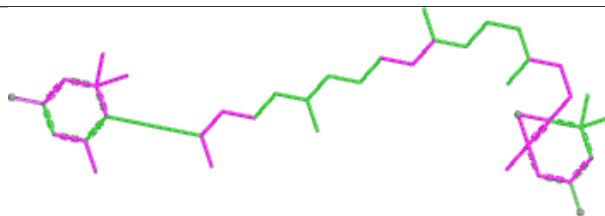


Rings

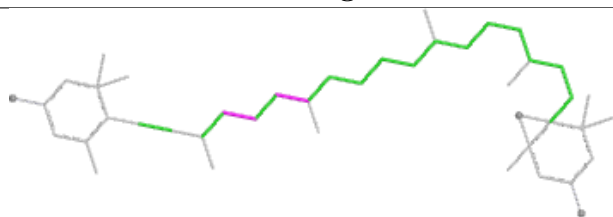
## Ligand DD6 1 614



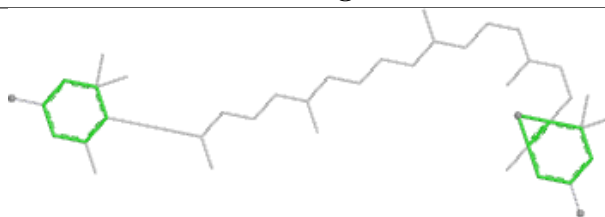
Bond lengths



Bond angles



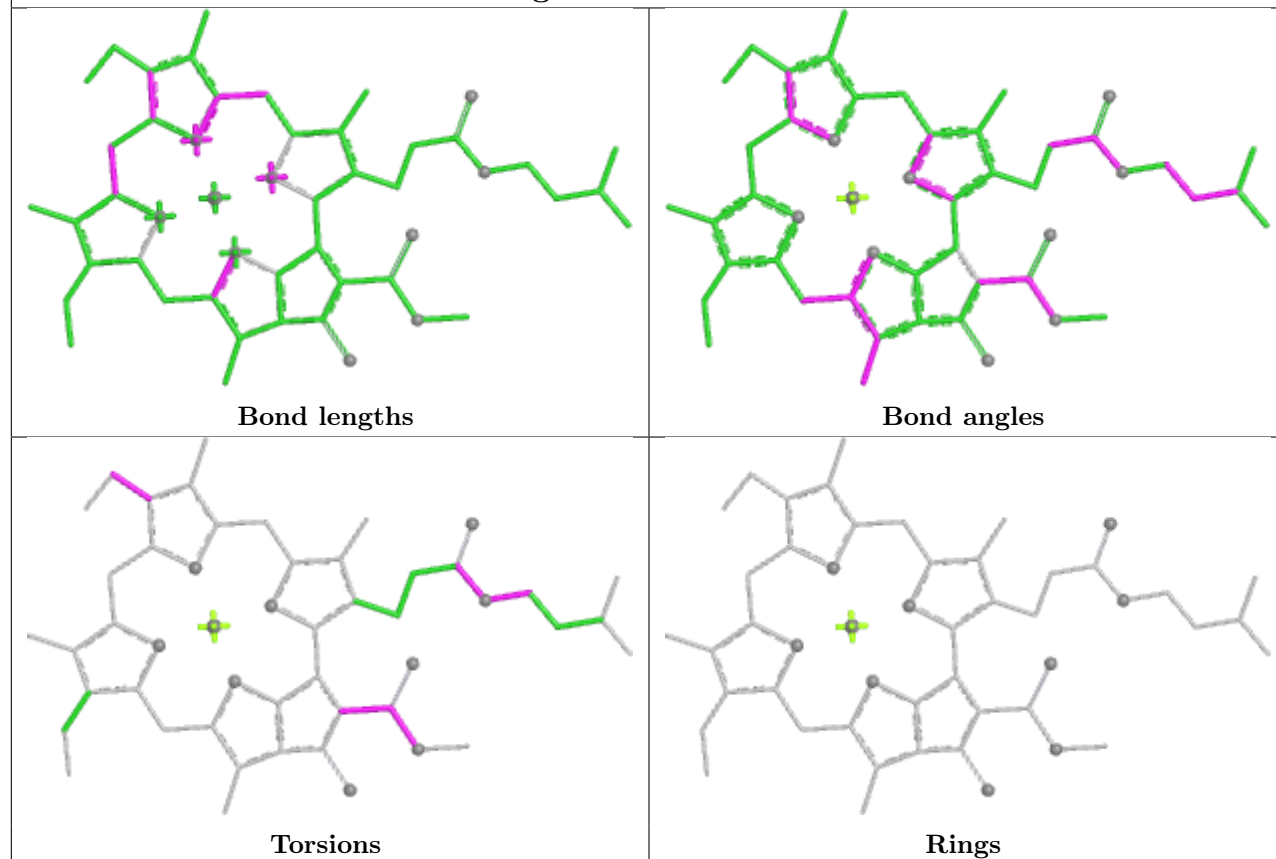
Torsions



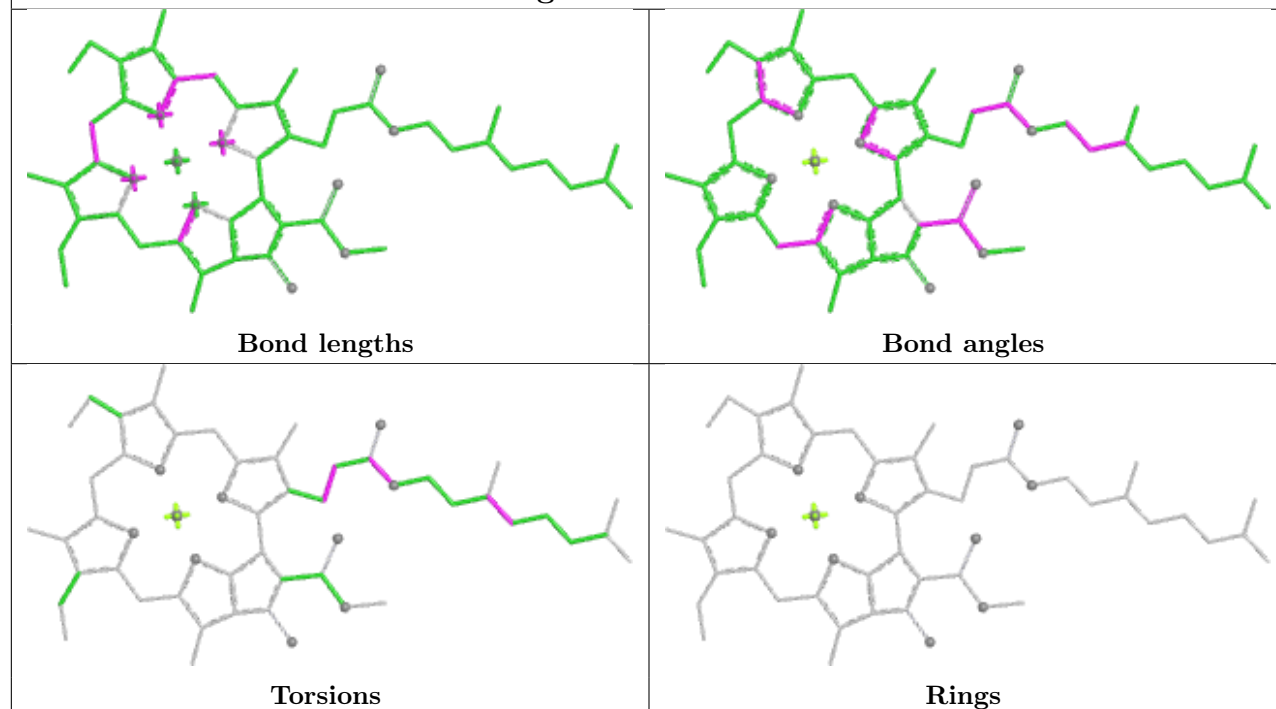
Rings



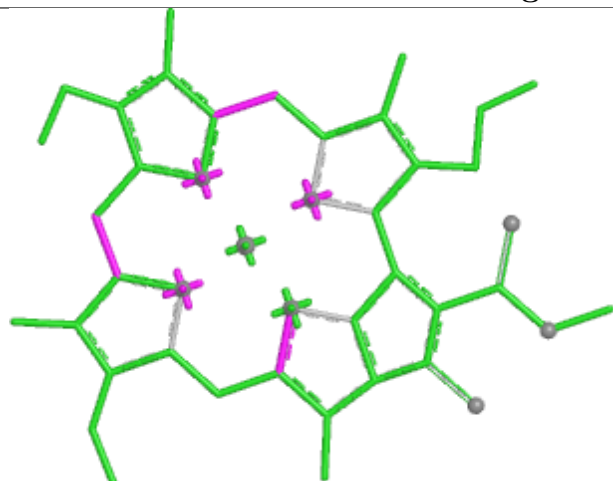
## Ligand CLA B 817



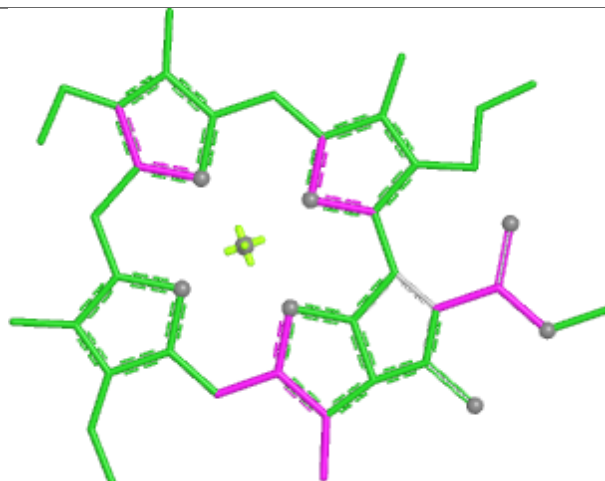
## Ligand CLA e 216



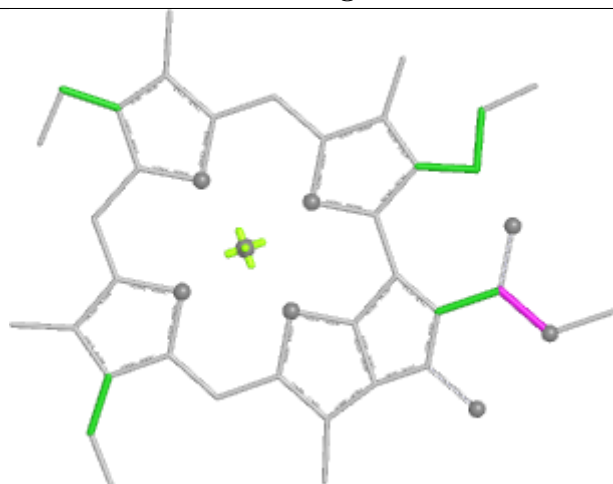
## Ligand CLA f 603



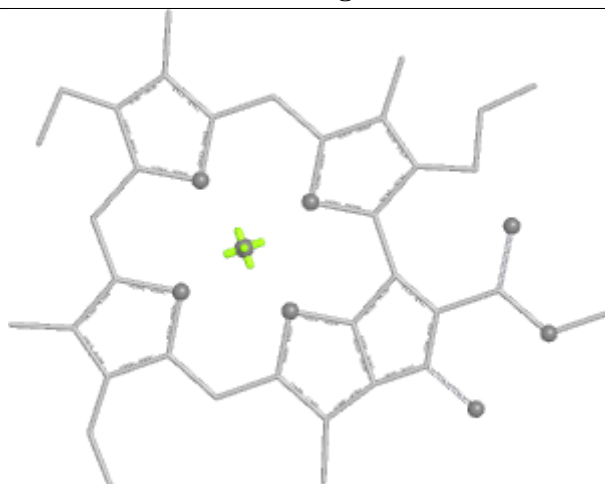
Bond lengths



Bond angles

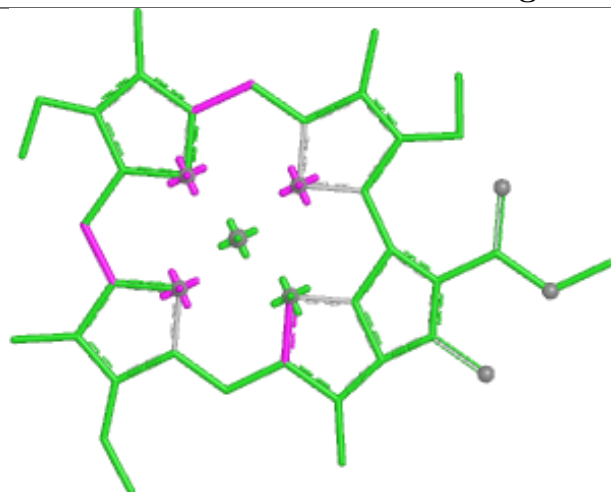


Torsions

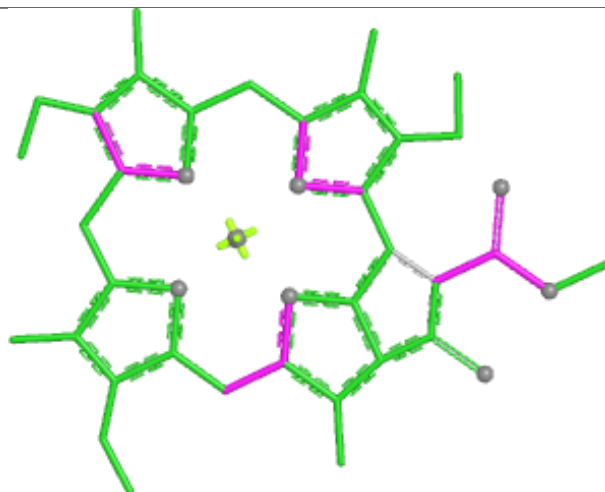


Rings

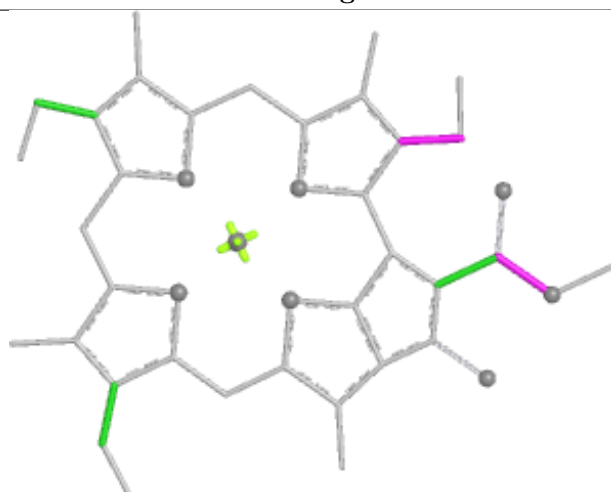
## Ligand CLA e 214



Bond lengths



Bond angles

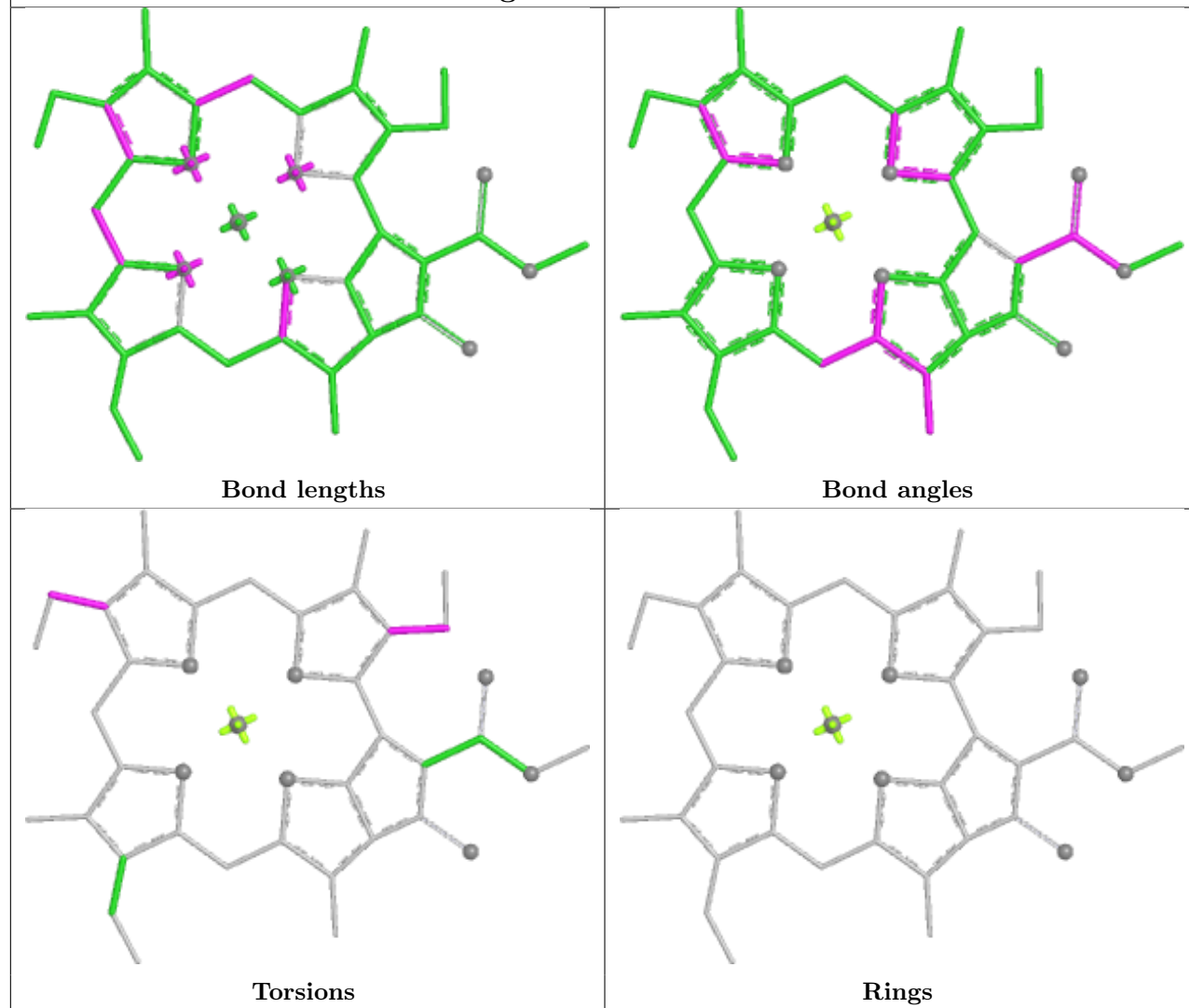


Torsions

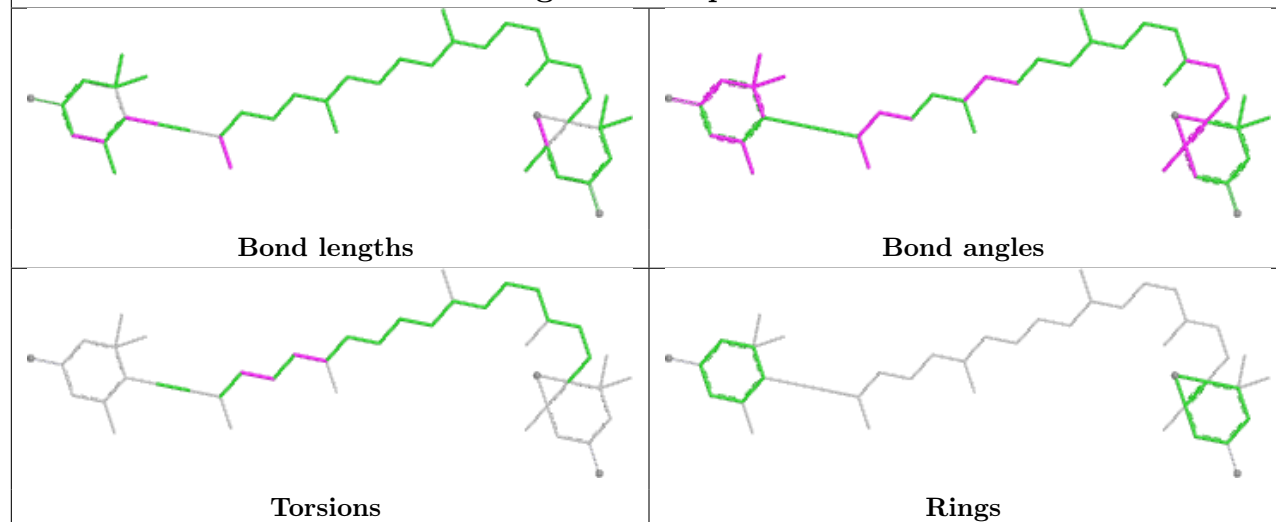


Rings

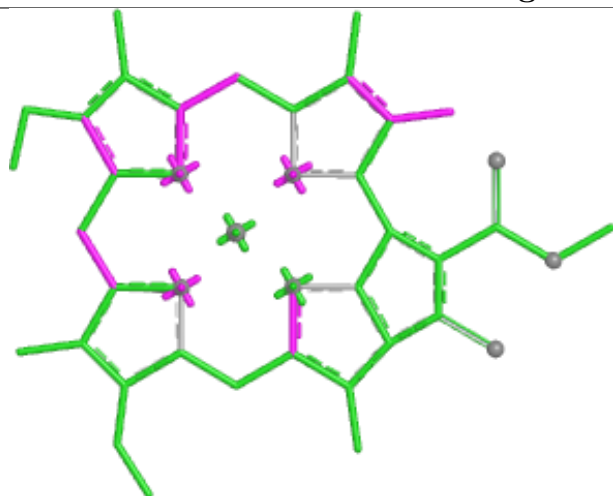
## Ligand CLA o 604



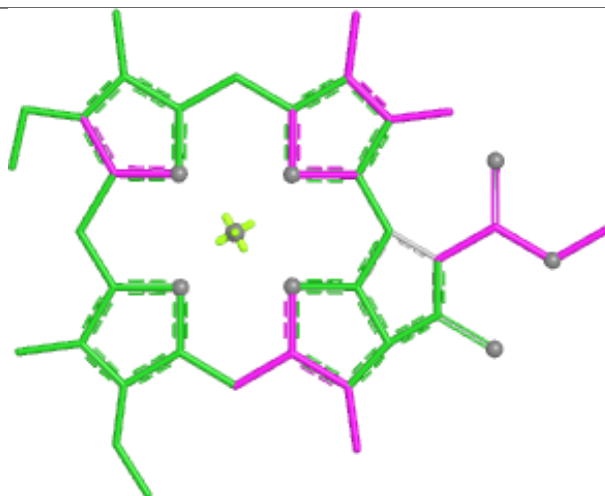
## Ligand DD6 p 610



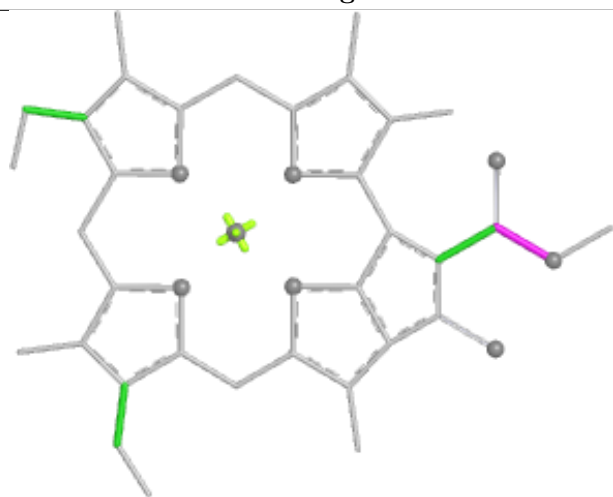
## Ligand CLA o 601



Bond lengths



Bond angles

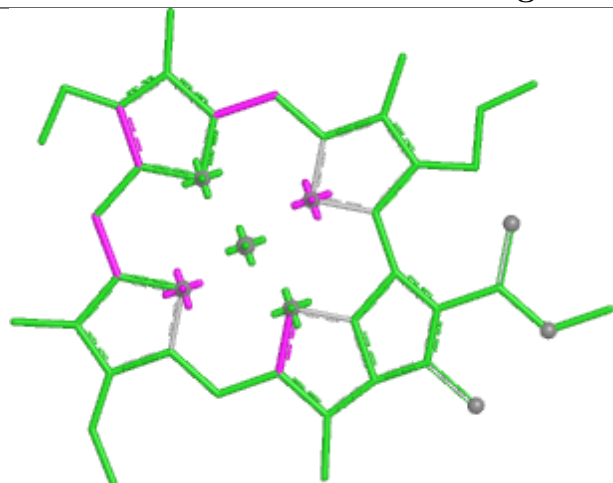


Torsions

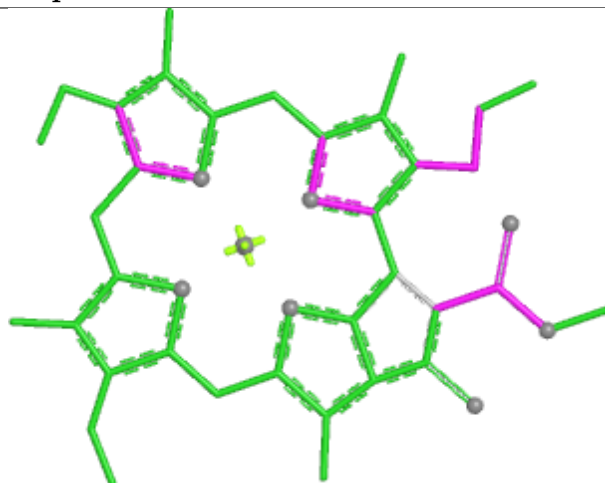


Rings

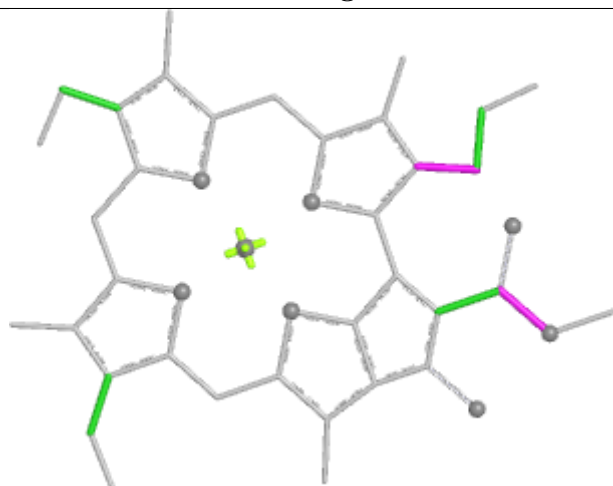
## Ligand CLA p 608



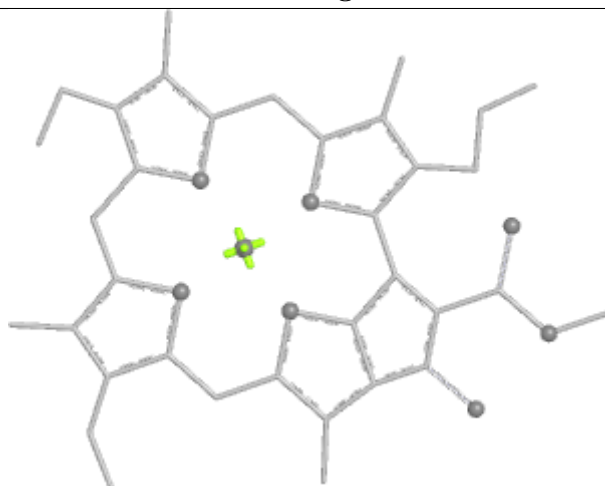
Bond lengths



Bond angles

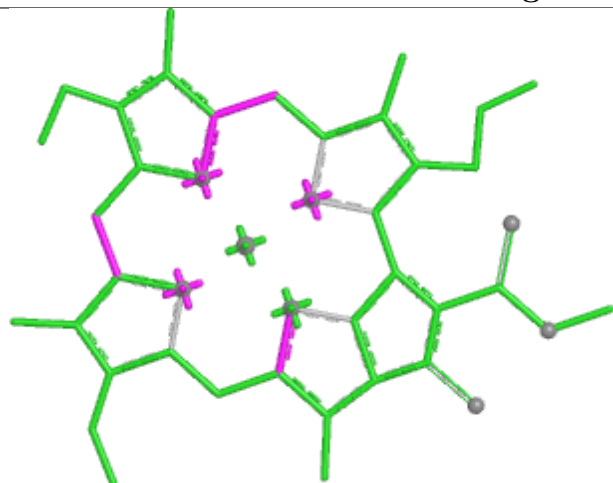


Torsions

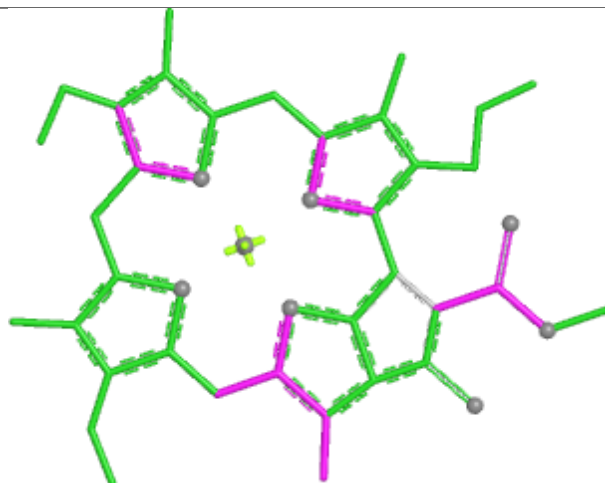


Rings

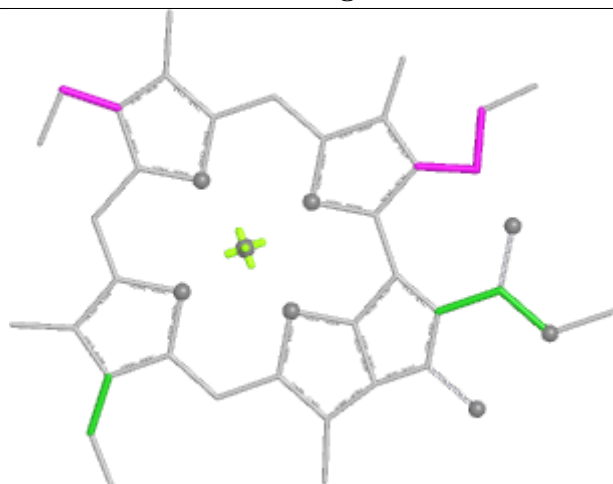
## Ligand CLA 1 605



Bond lengths



Bond angles

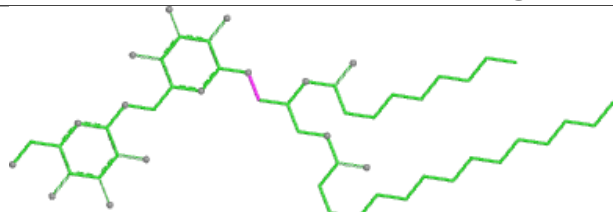


Torsions

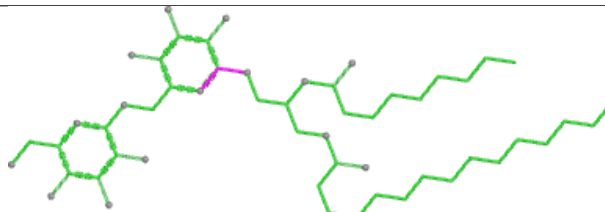


Rings

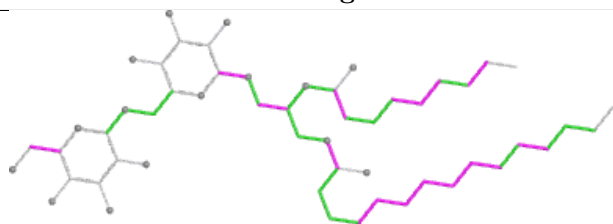
## Ligand DGD B 849



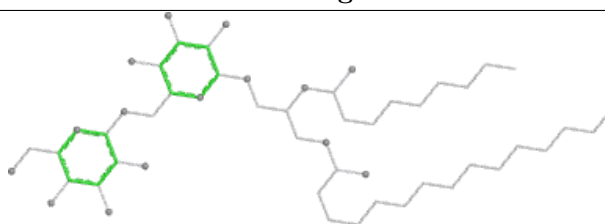
Bond lengths



Bond angles

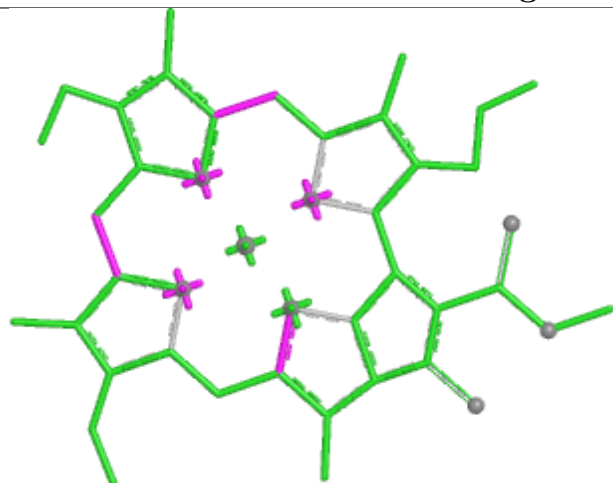


Torsions

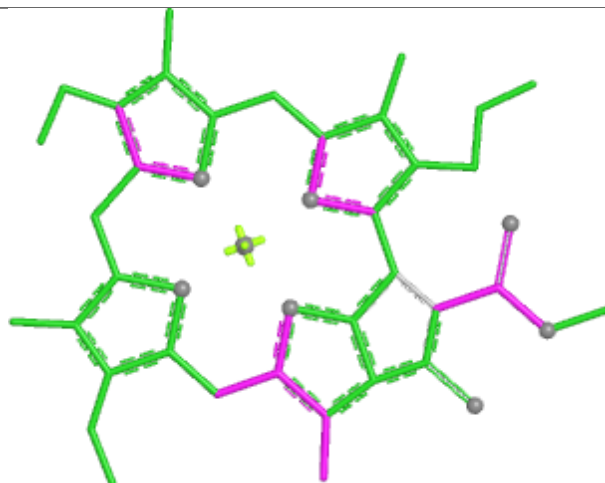


Rings

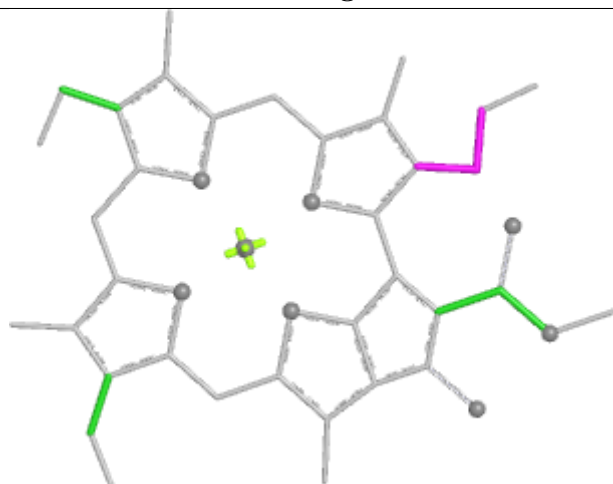
## Ligand CLA c 306



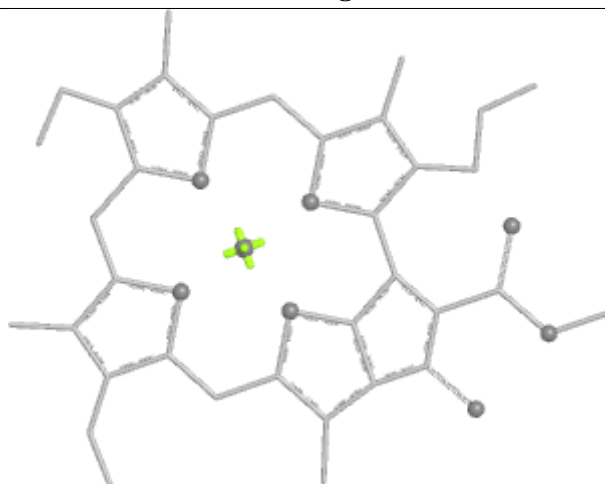
Bond lengths



Bond angles



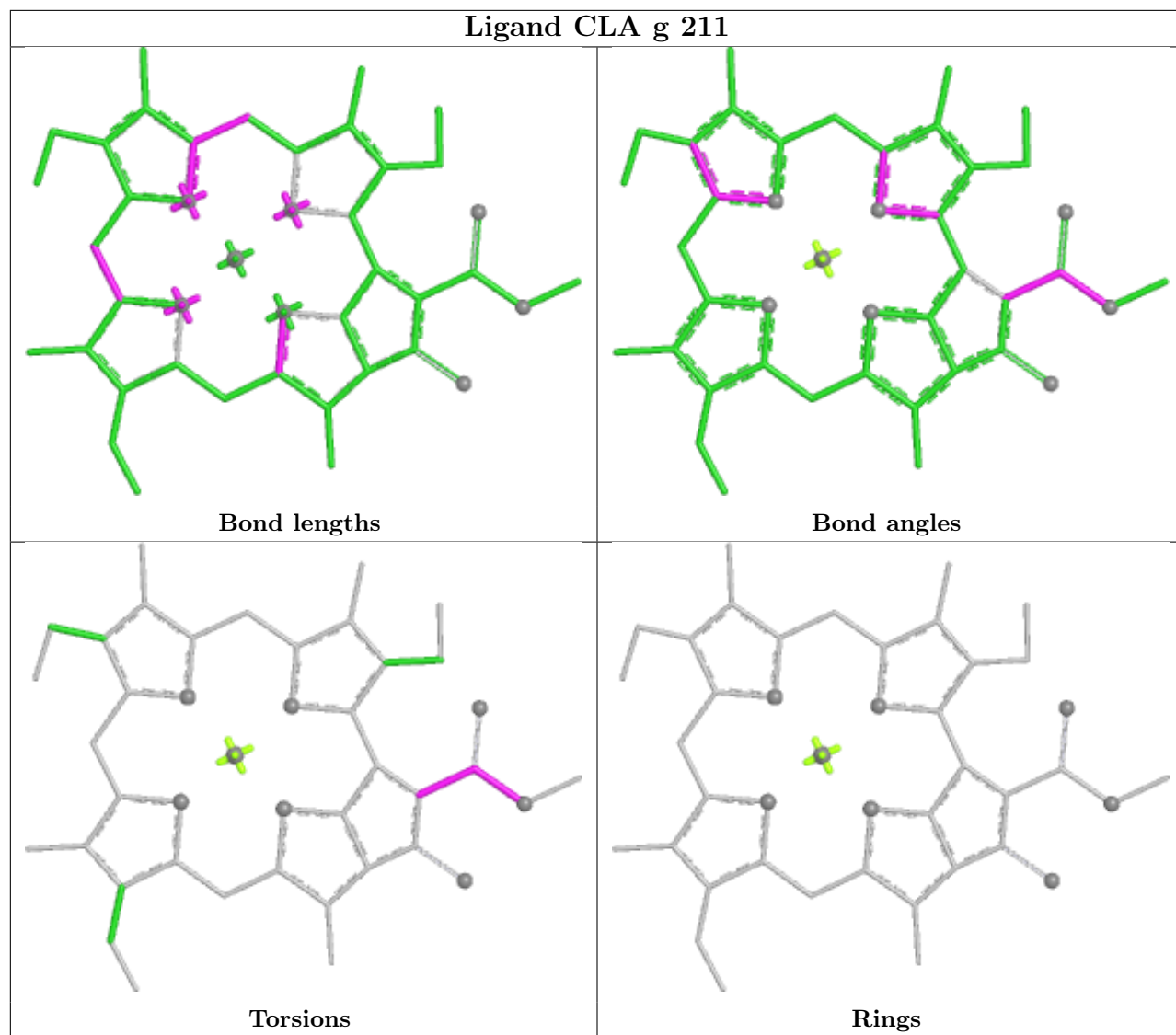
Torsions

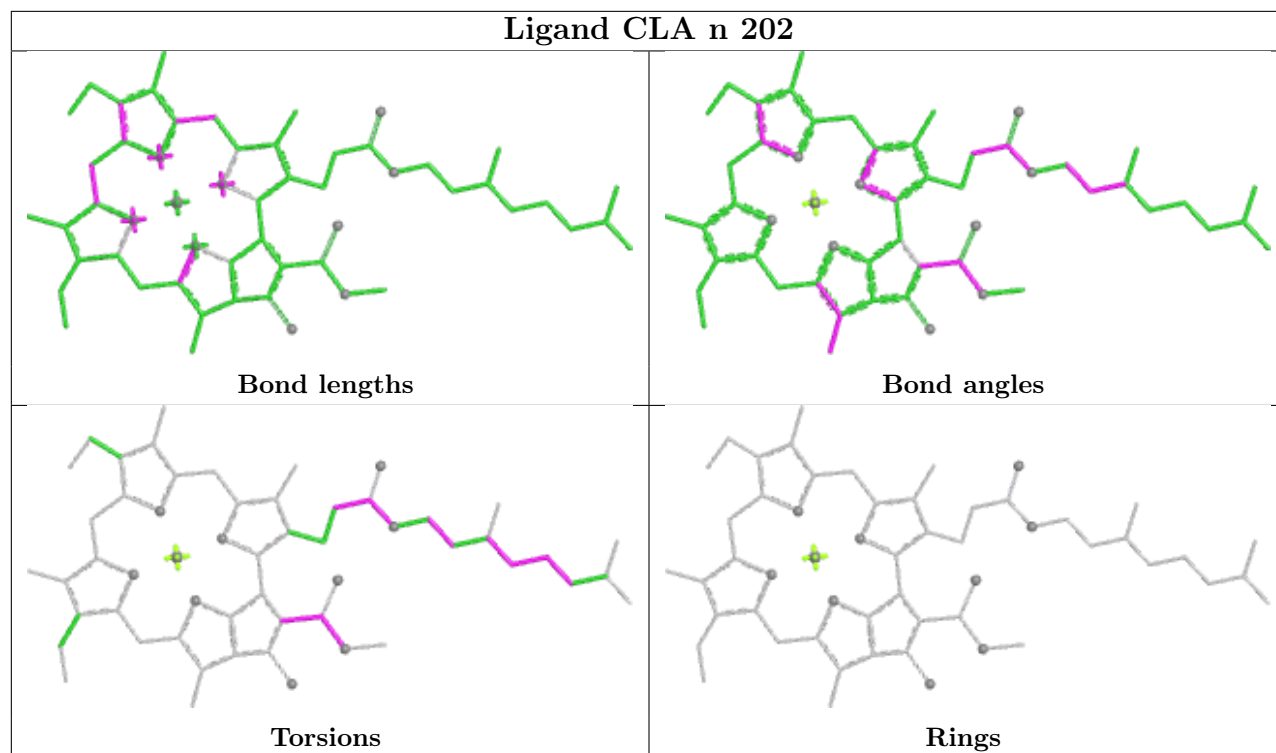


Rings

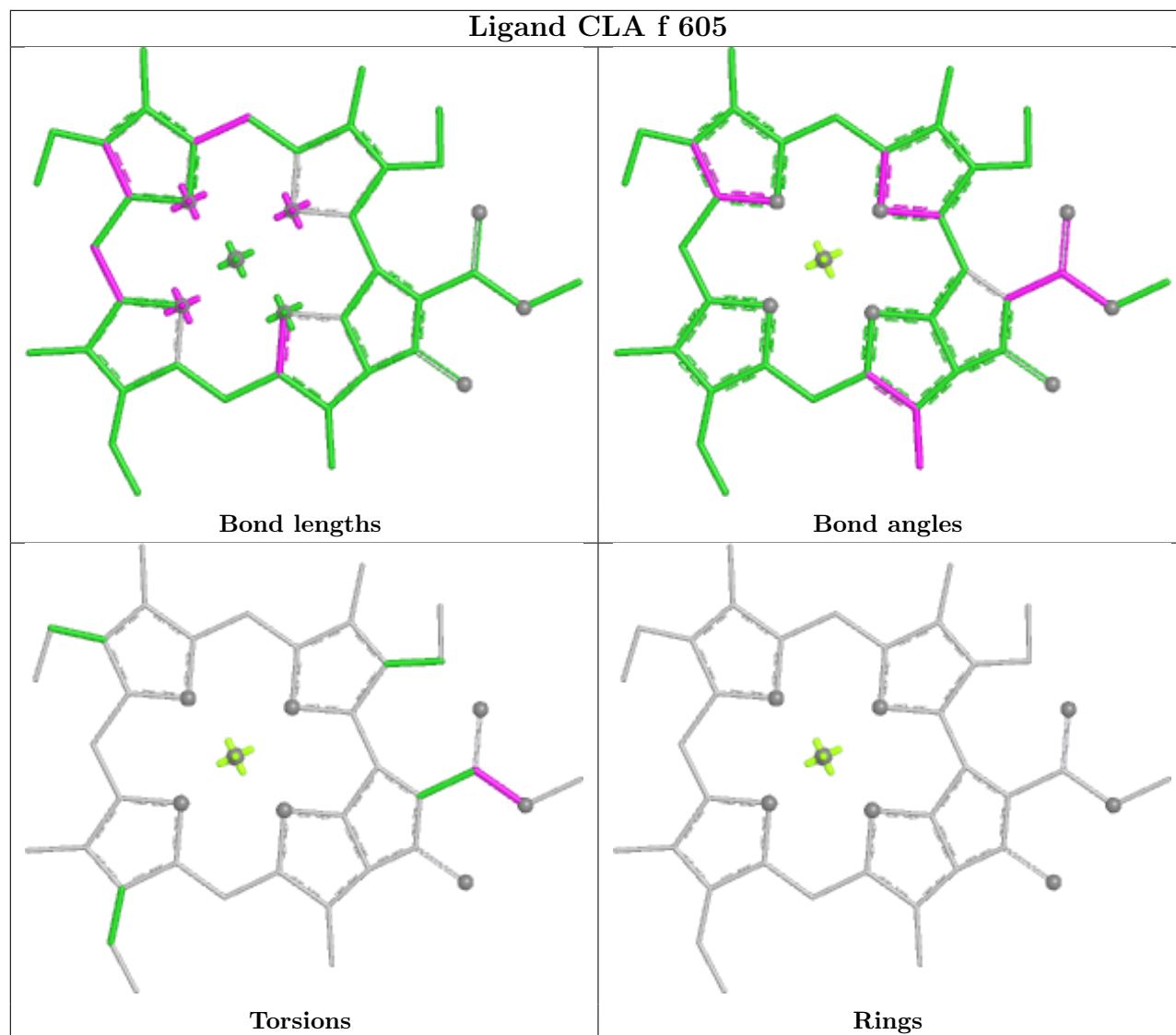


## Ligand CLA g 211

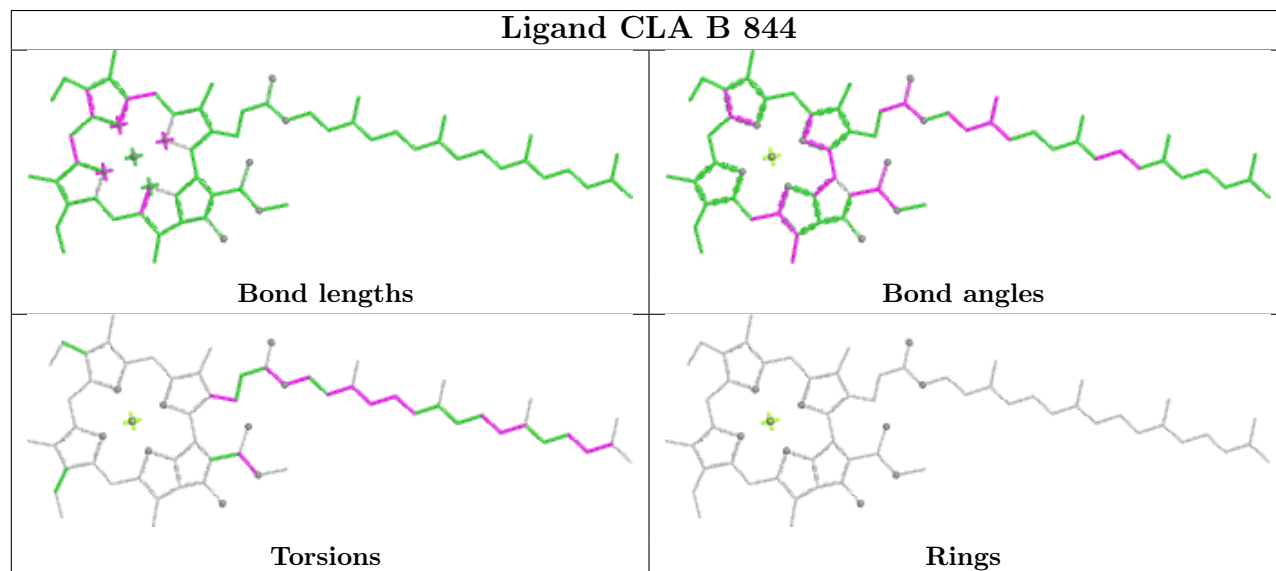


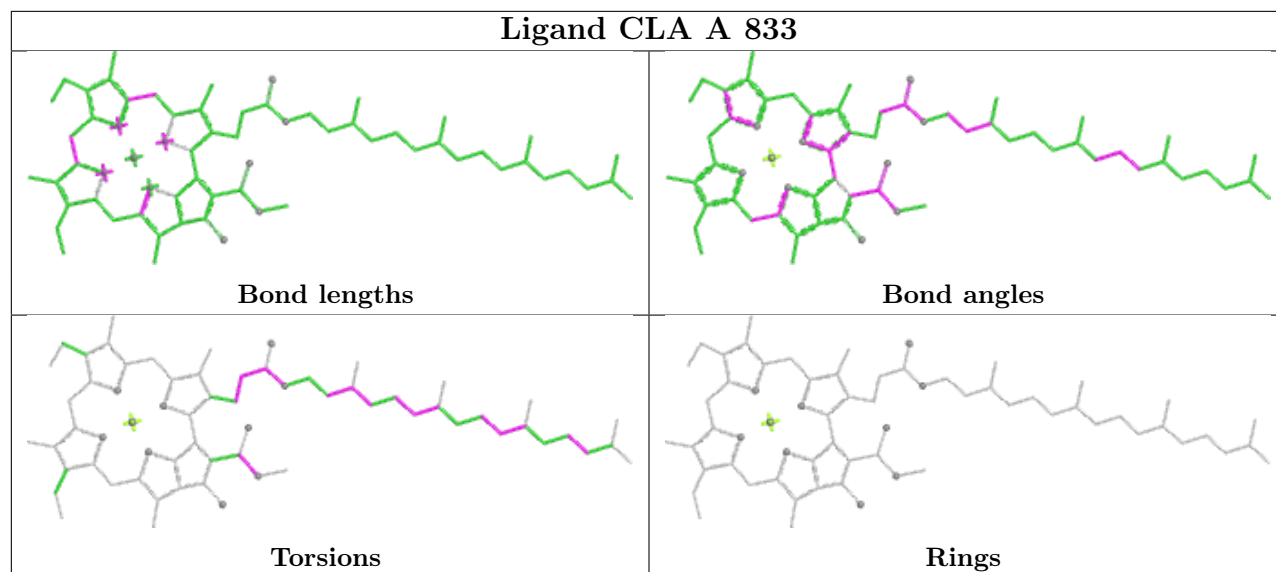
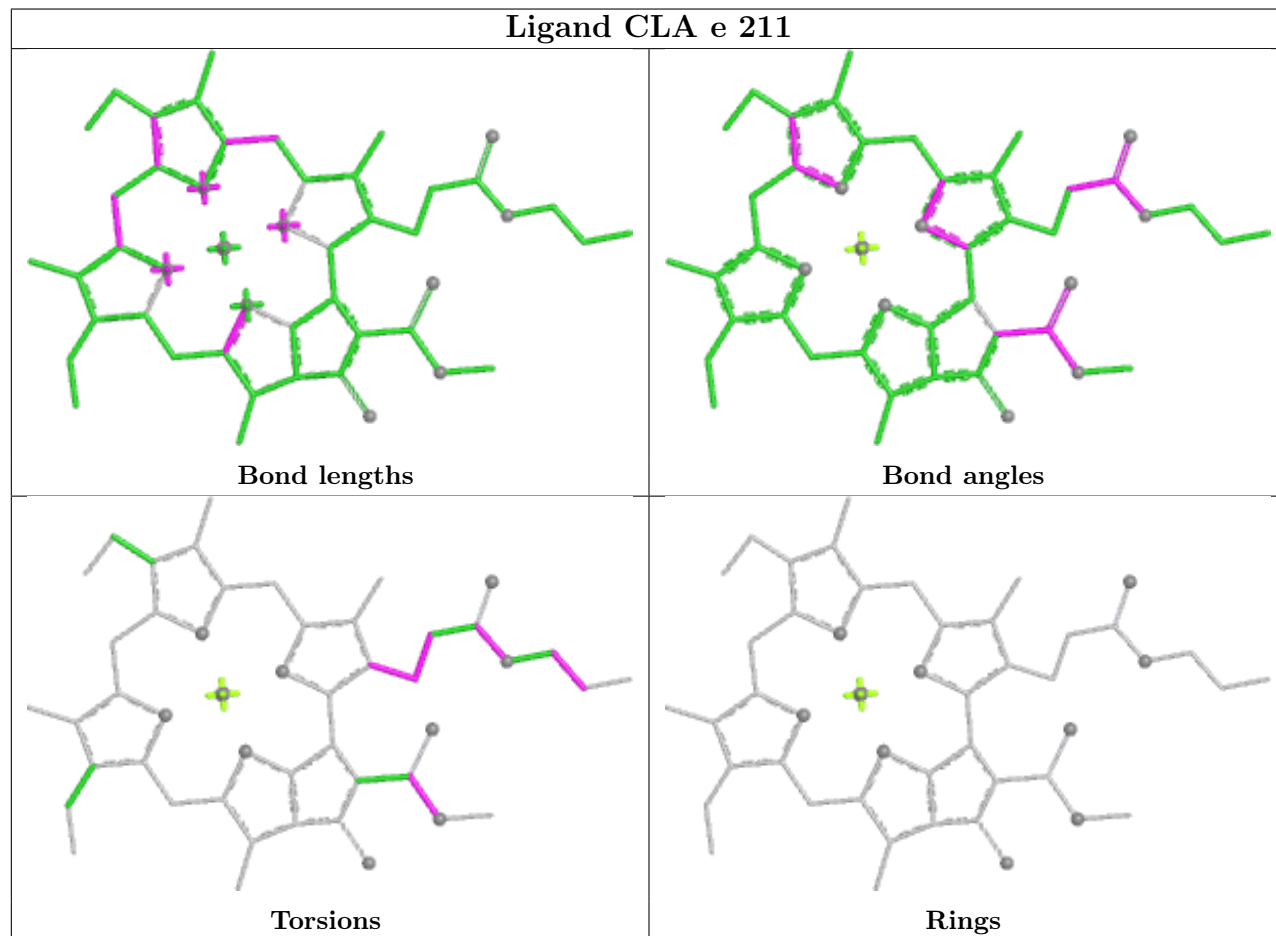


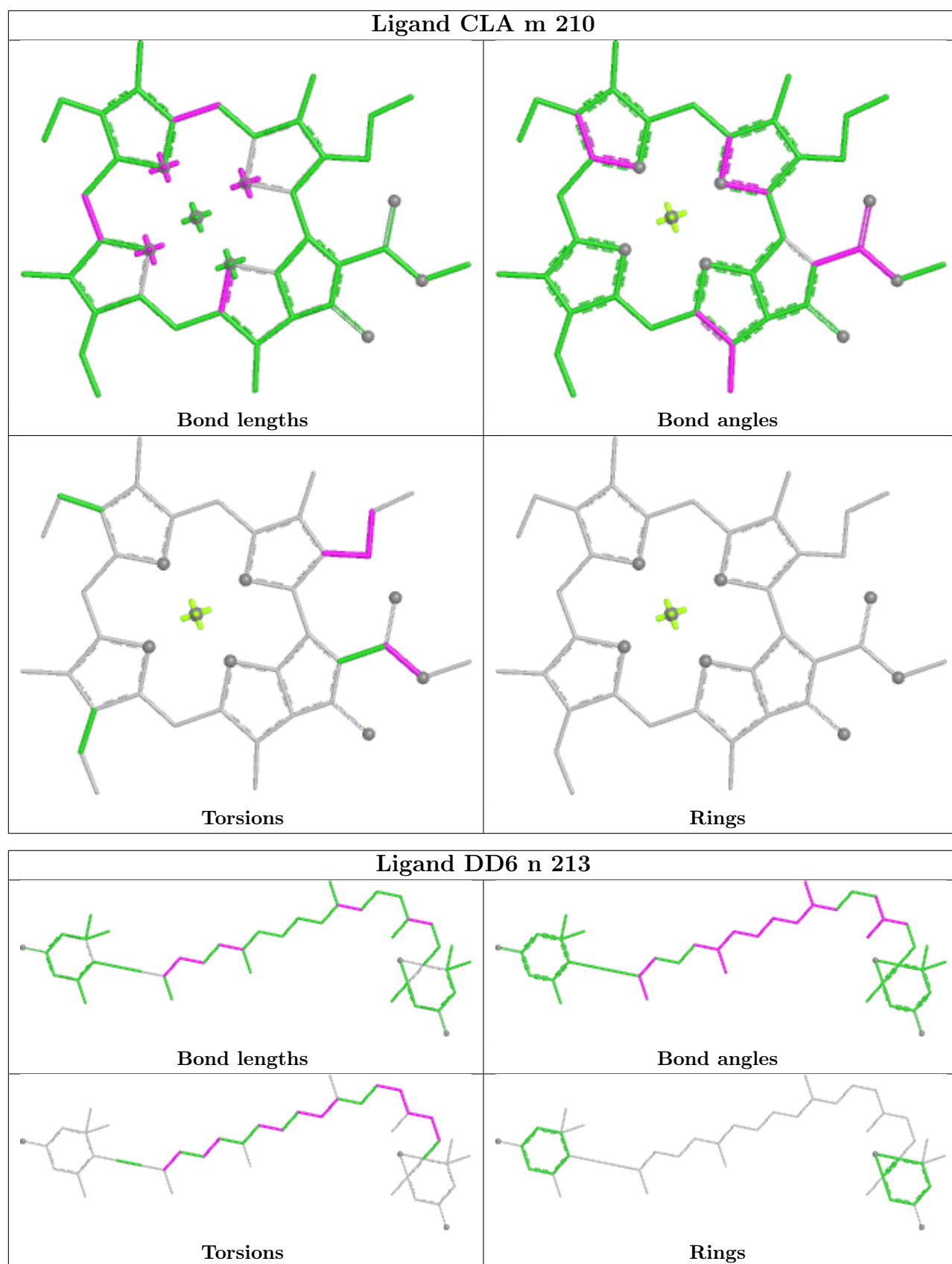
## Ligand CLA f 605

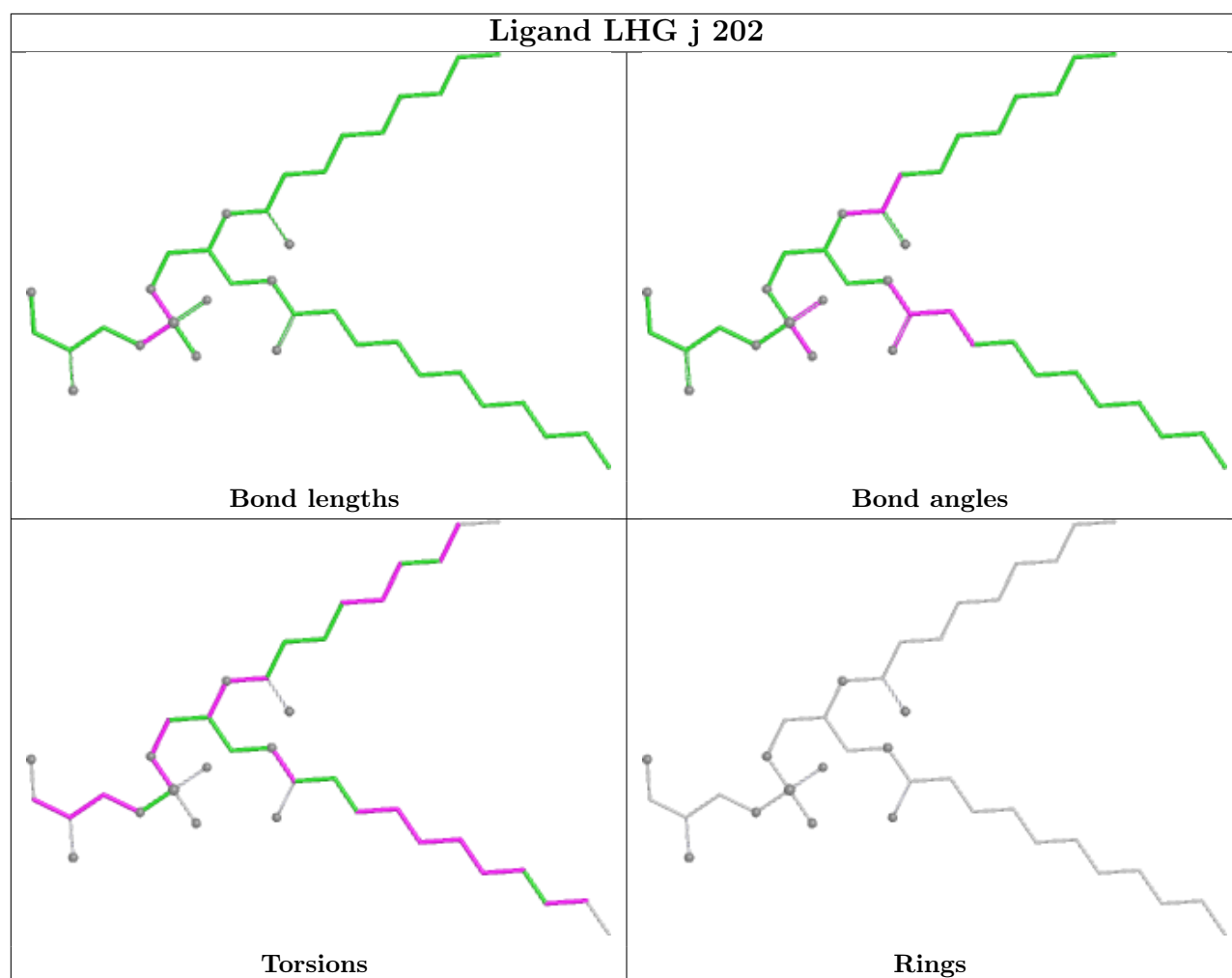


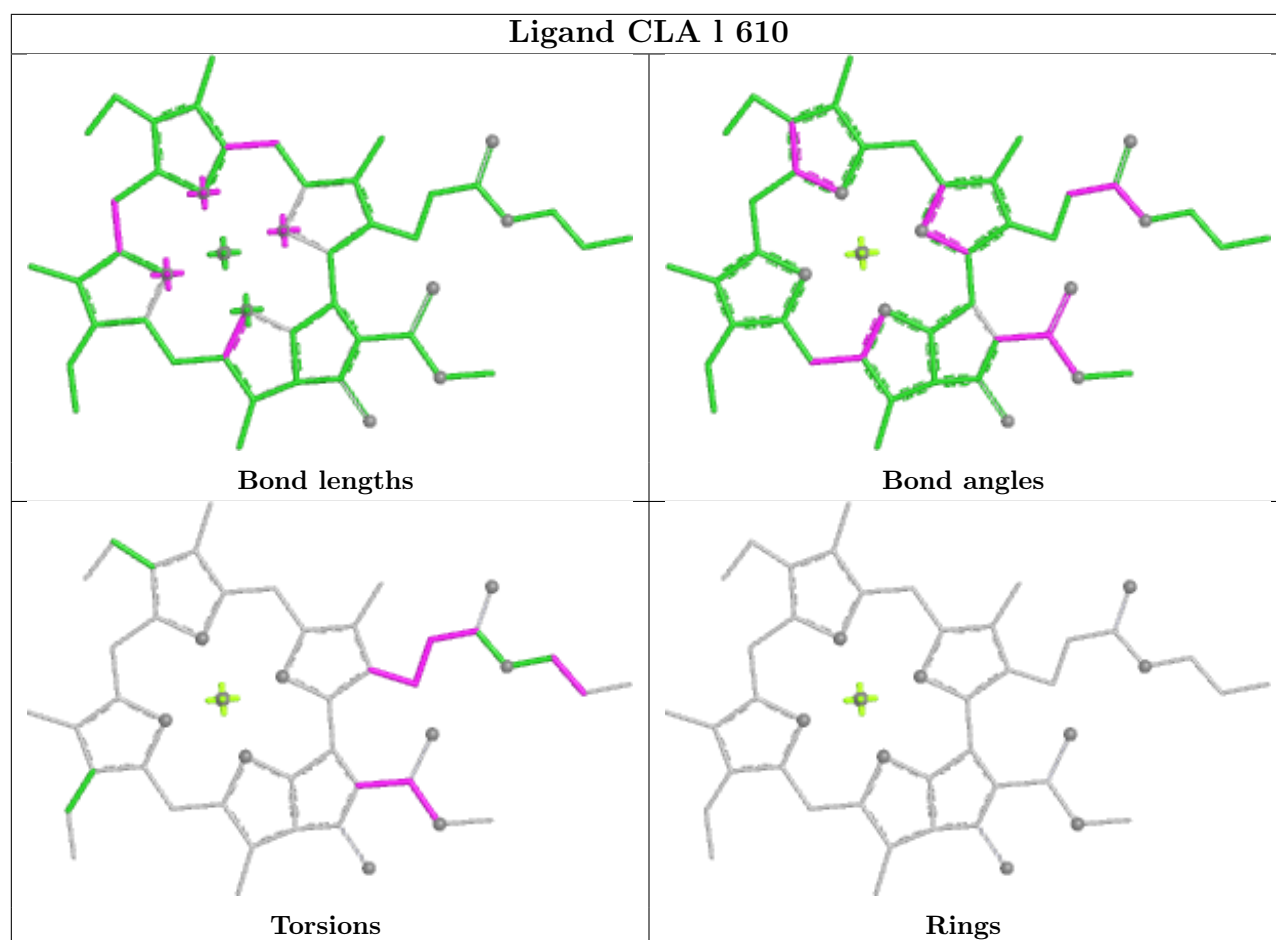
## Ligand CLA B 844



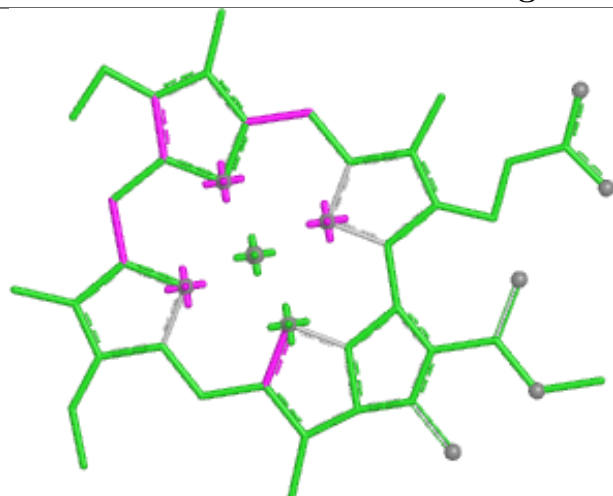
**Ligand CLA A 833****Ligand CLA e 211**



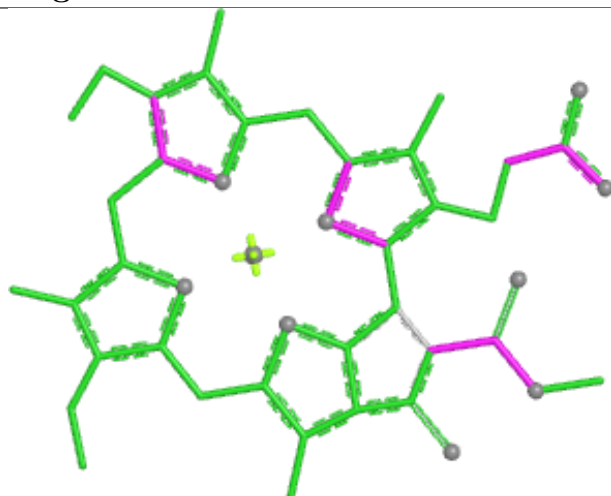




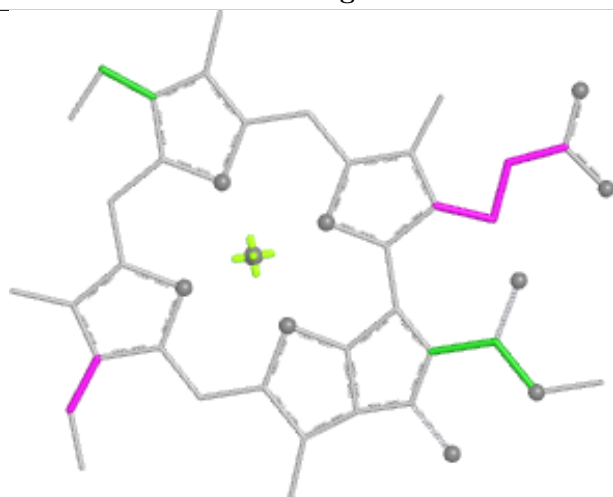
## Ligand CLA g 207



Bond lengths



Bond angles

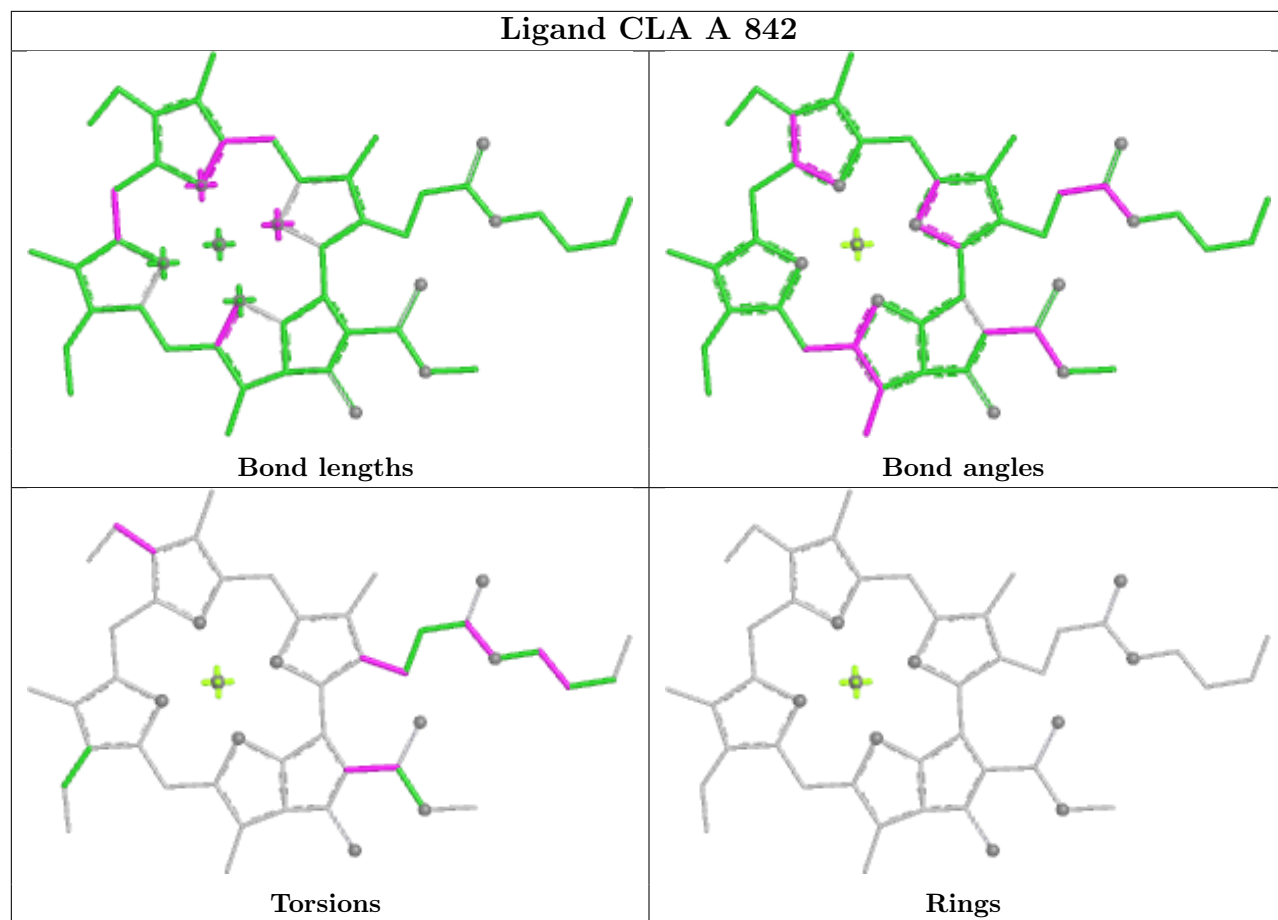


Torsions

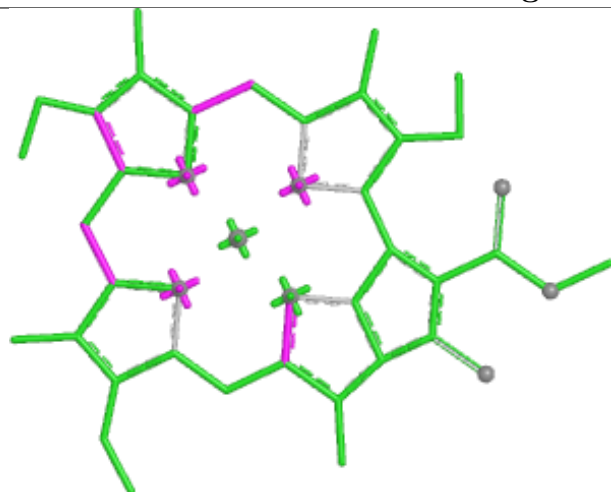


Rings

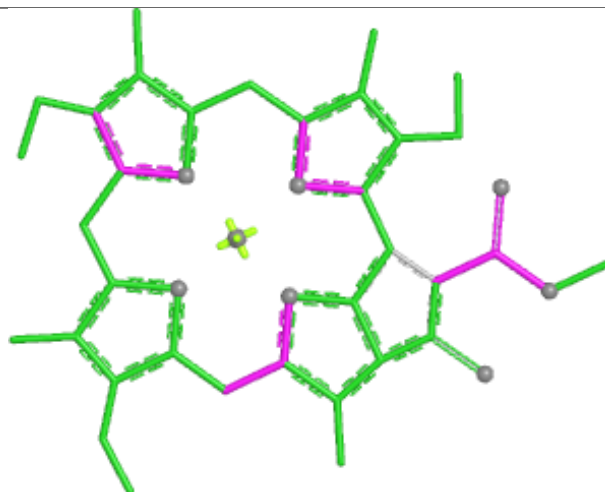




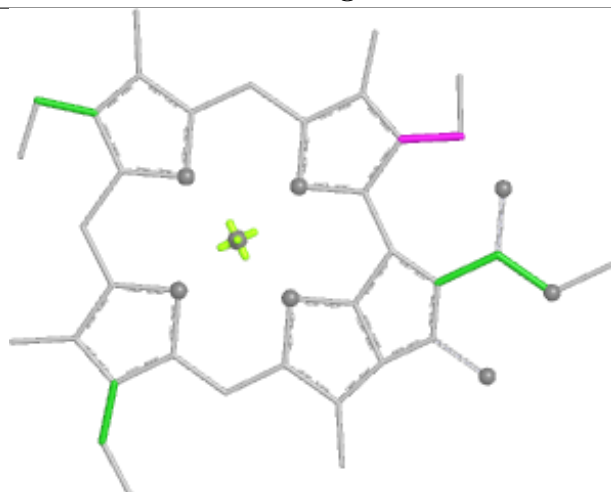
## Ligand CLA f 608



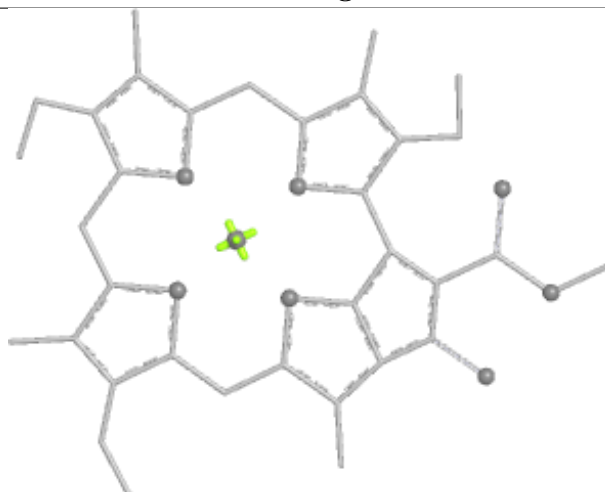
Bond lengths



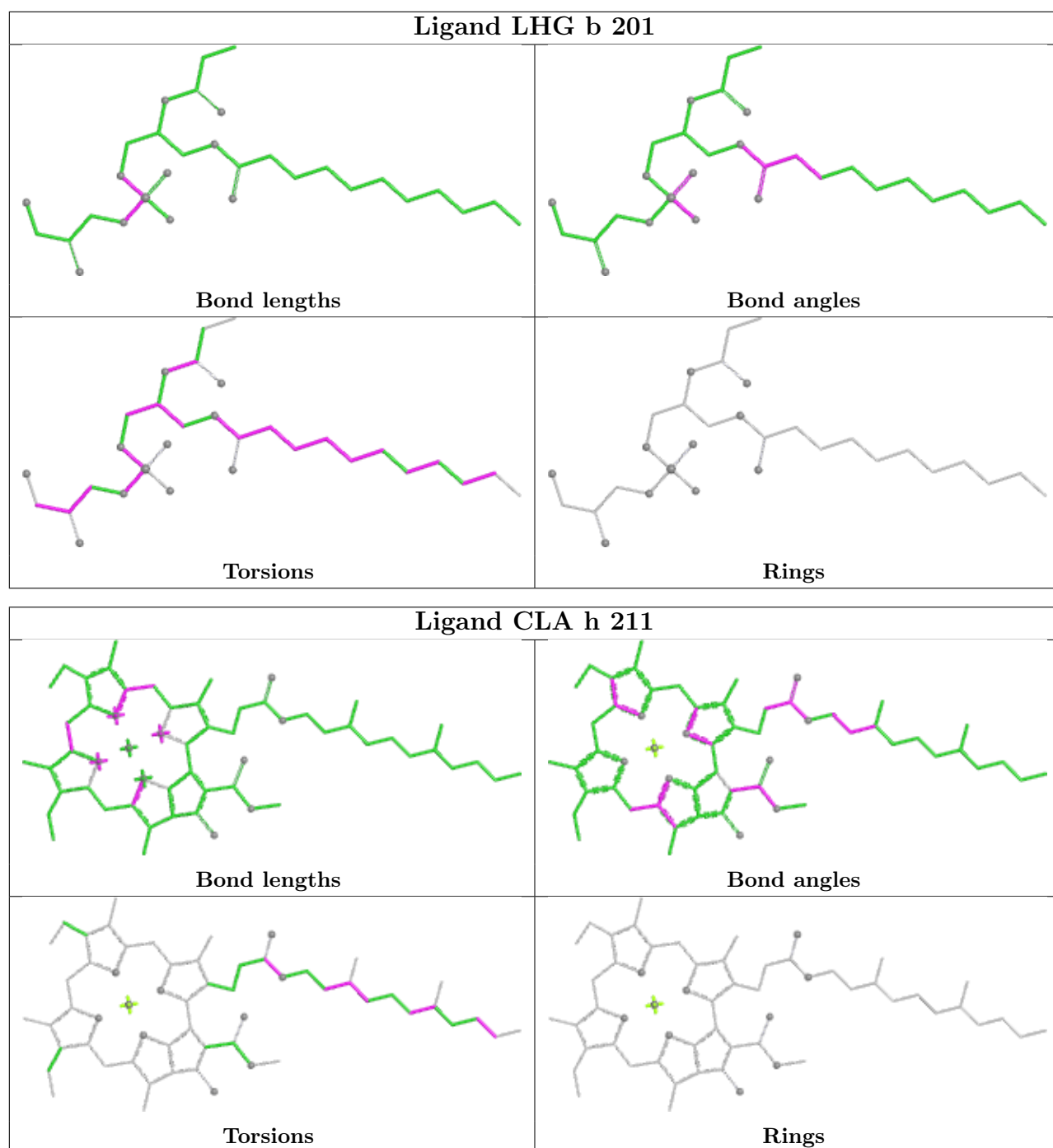
Bond angles



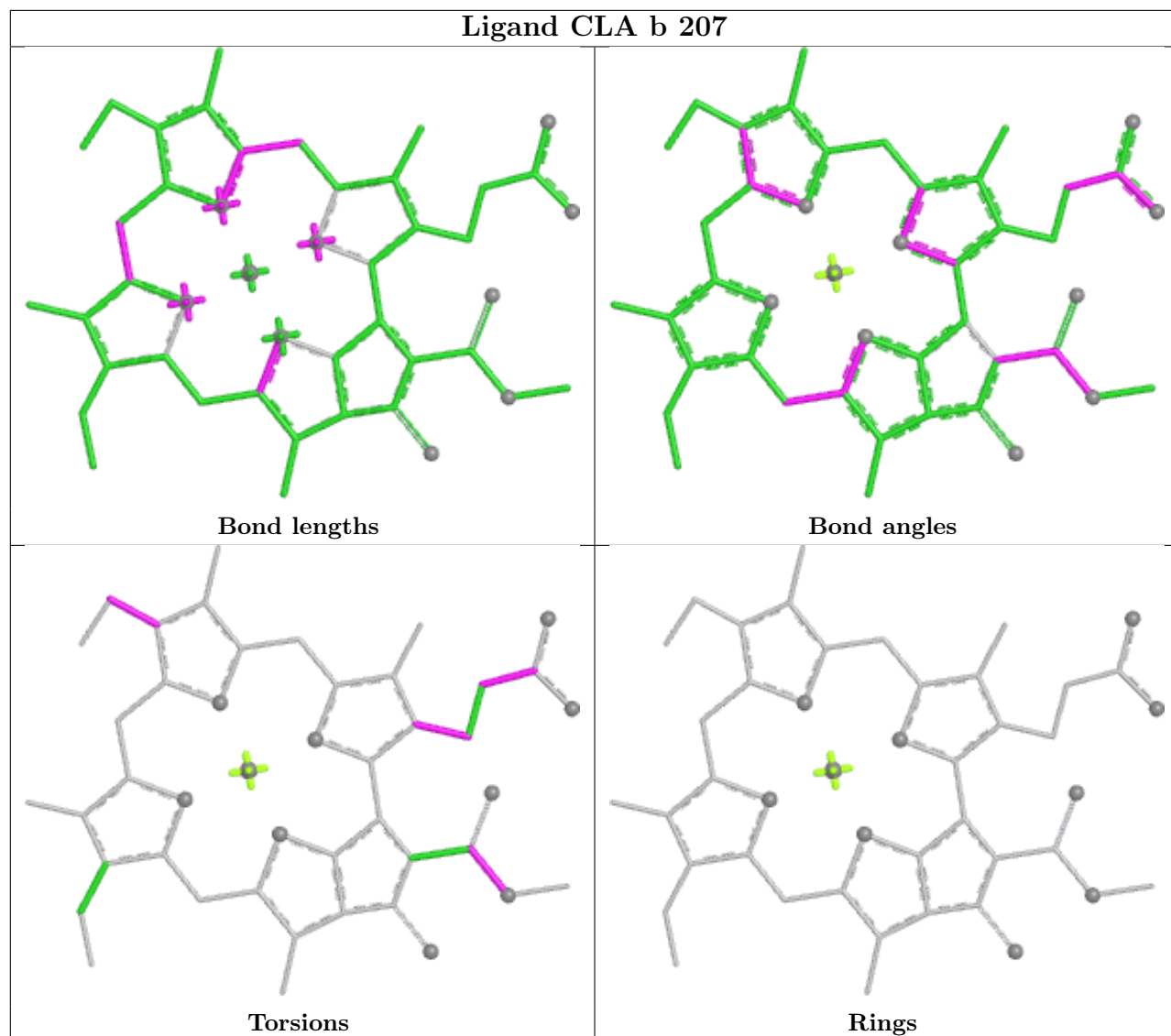
Torsions



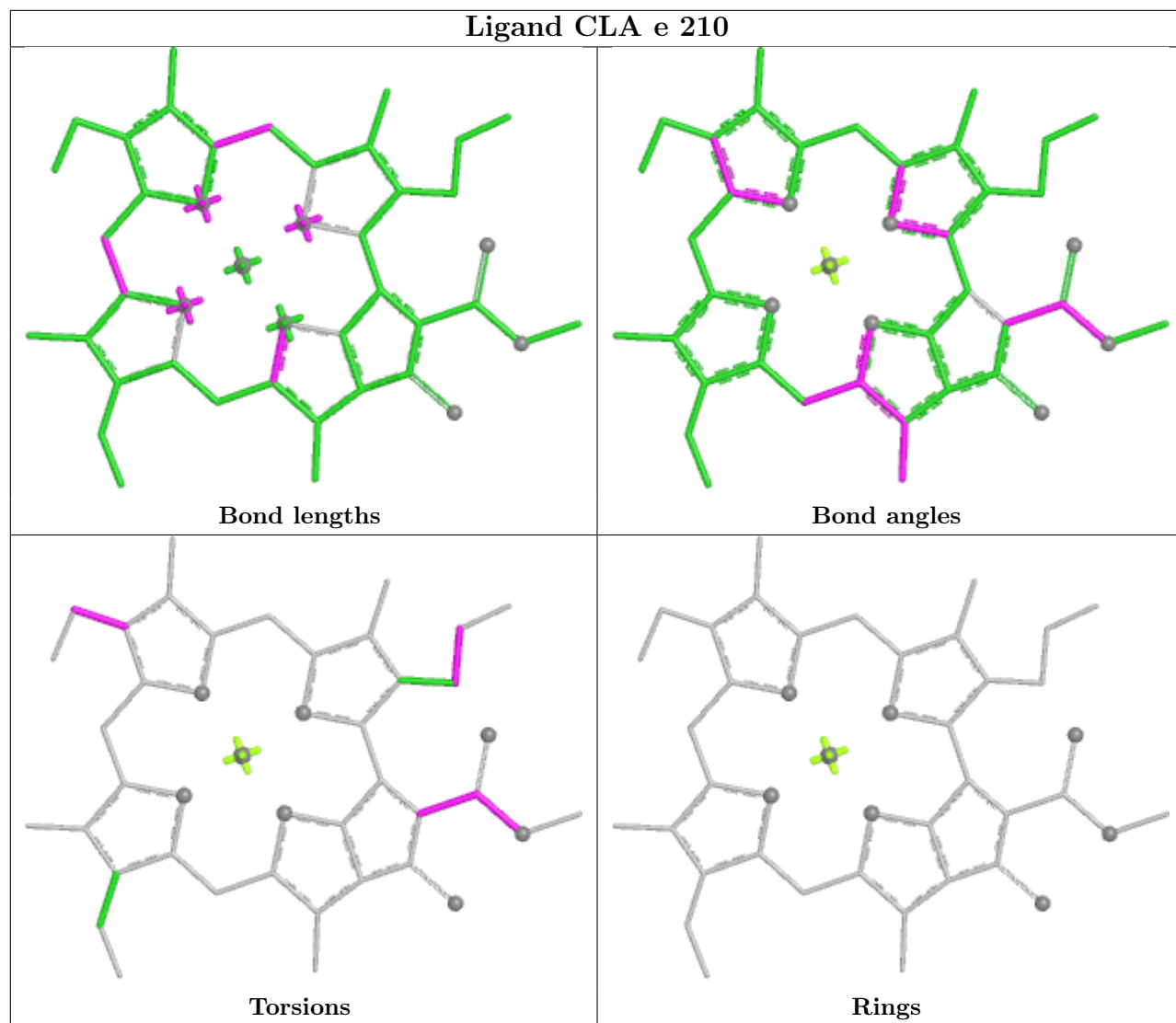
Rings



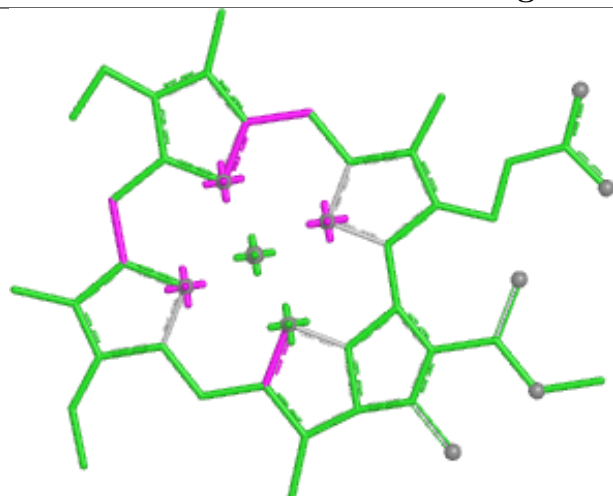
## Ligand CLA b 207



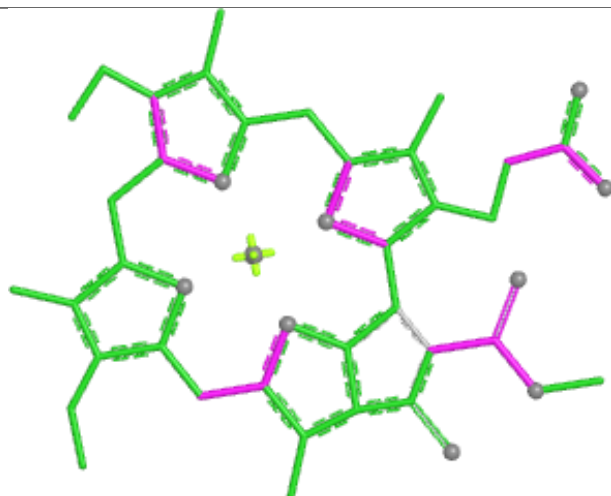
## Ligand CLA e 210



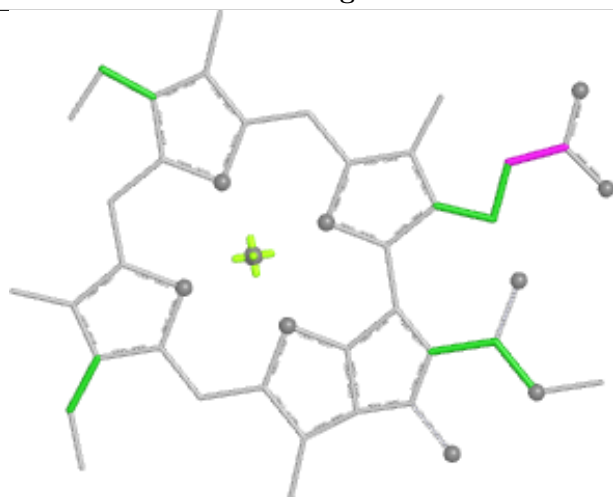
## Ligand CLA b 209



Bond lengths



Bond angles

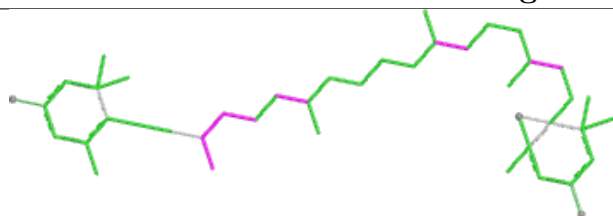


Torsions

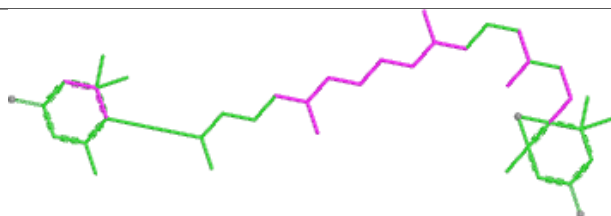


Rings

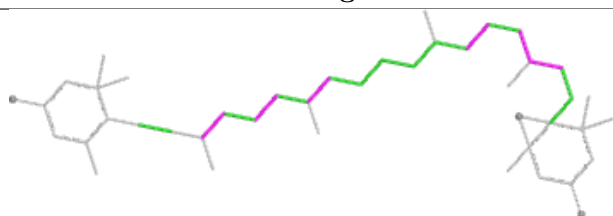
## Ligand DD6 e 218



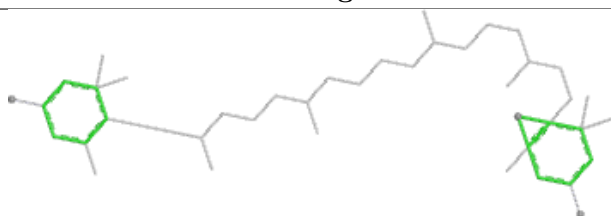
Bond lengths



Bond angles

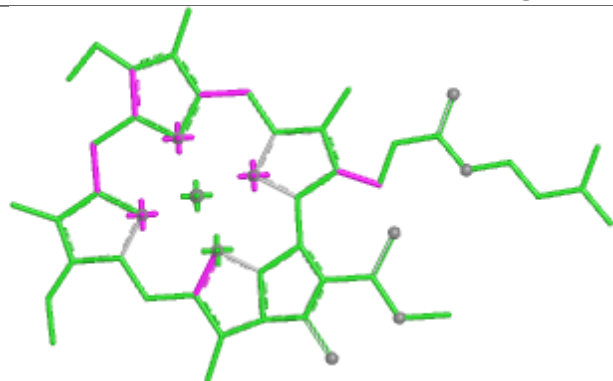


Torsions

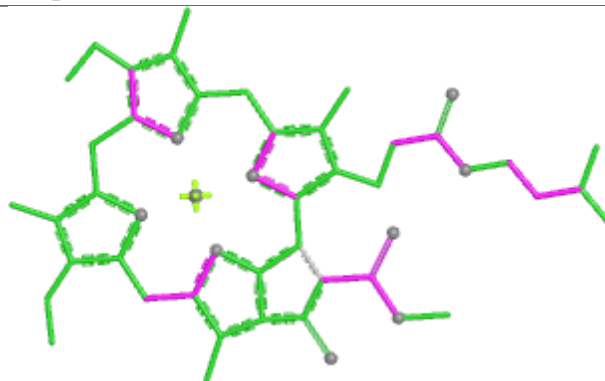


Rings

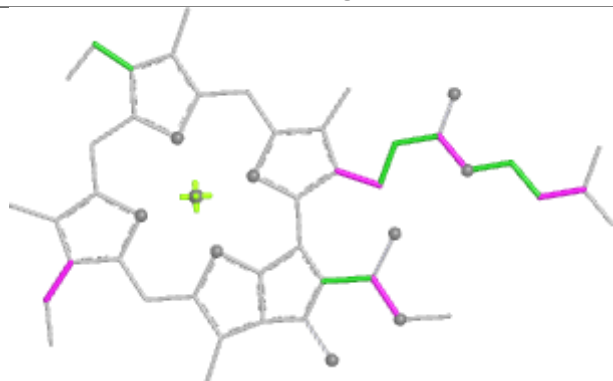
## Ligand CLA p 606



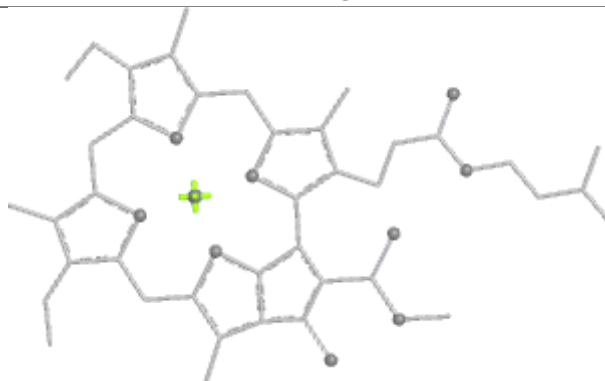
Bond lengths



Bond angles

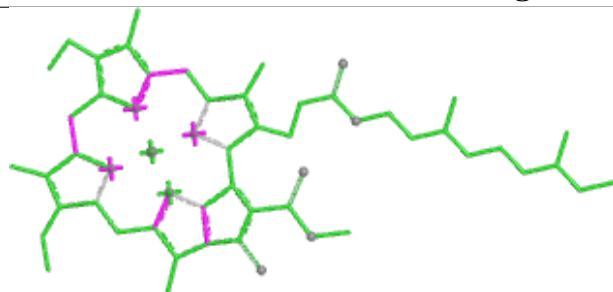


Torsions

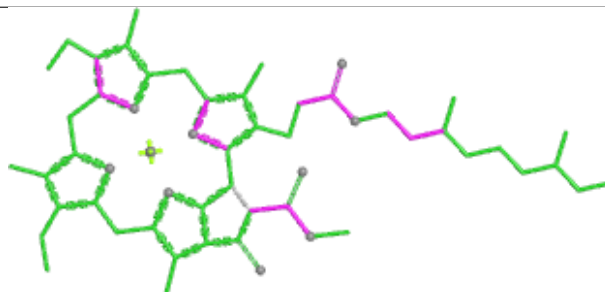


Rings

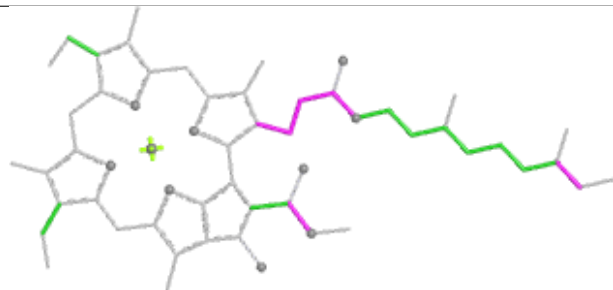
## Ligand CLA A 817



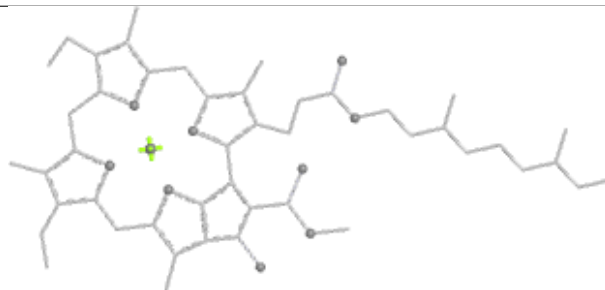
Bond lengths



Bond angles

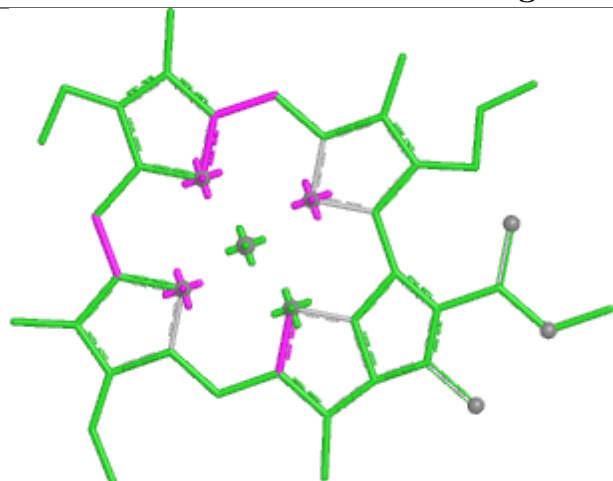


Torsions

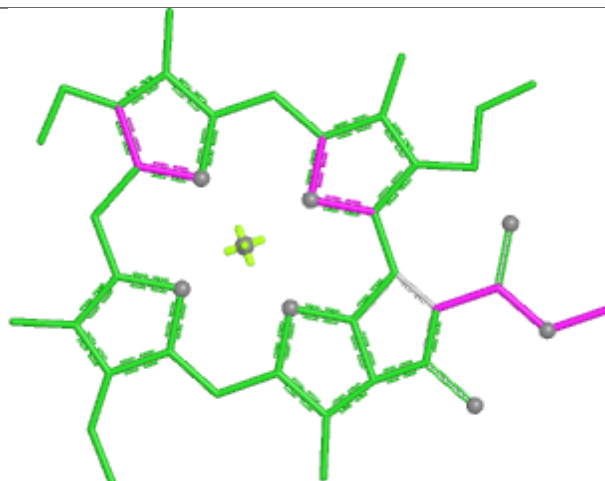


Rings

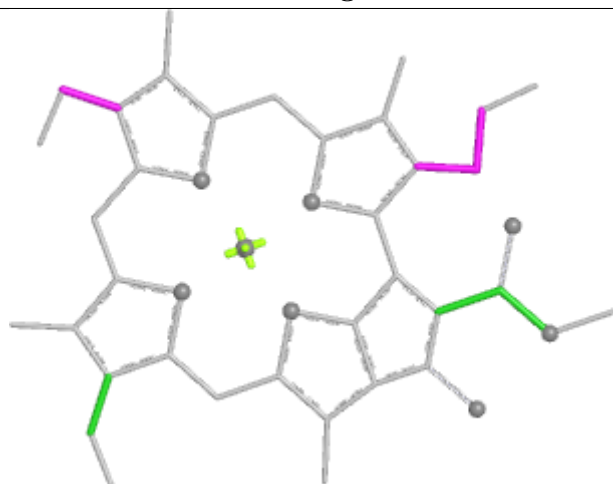
## Ligand CLA o 605



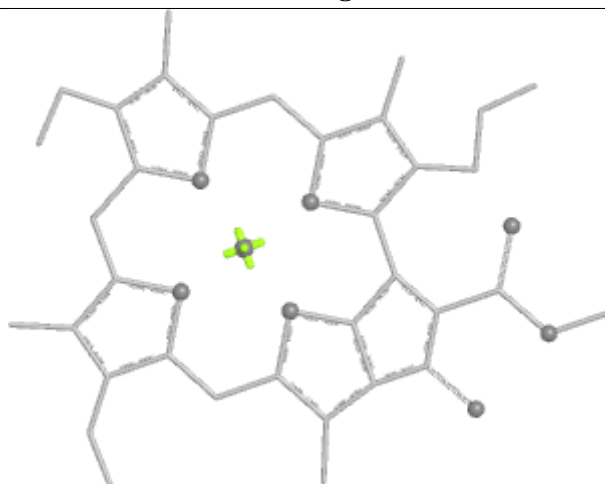
Bond lengths



Bond angles

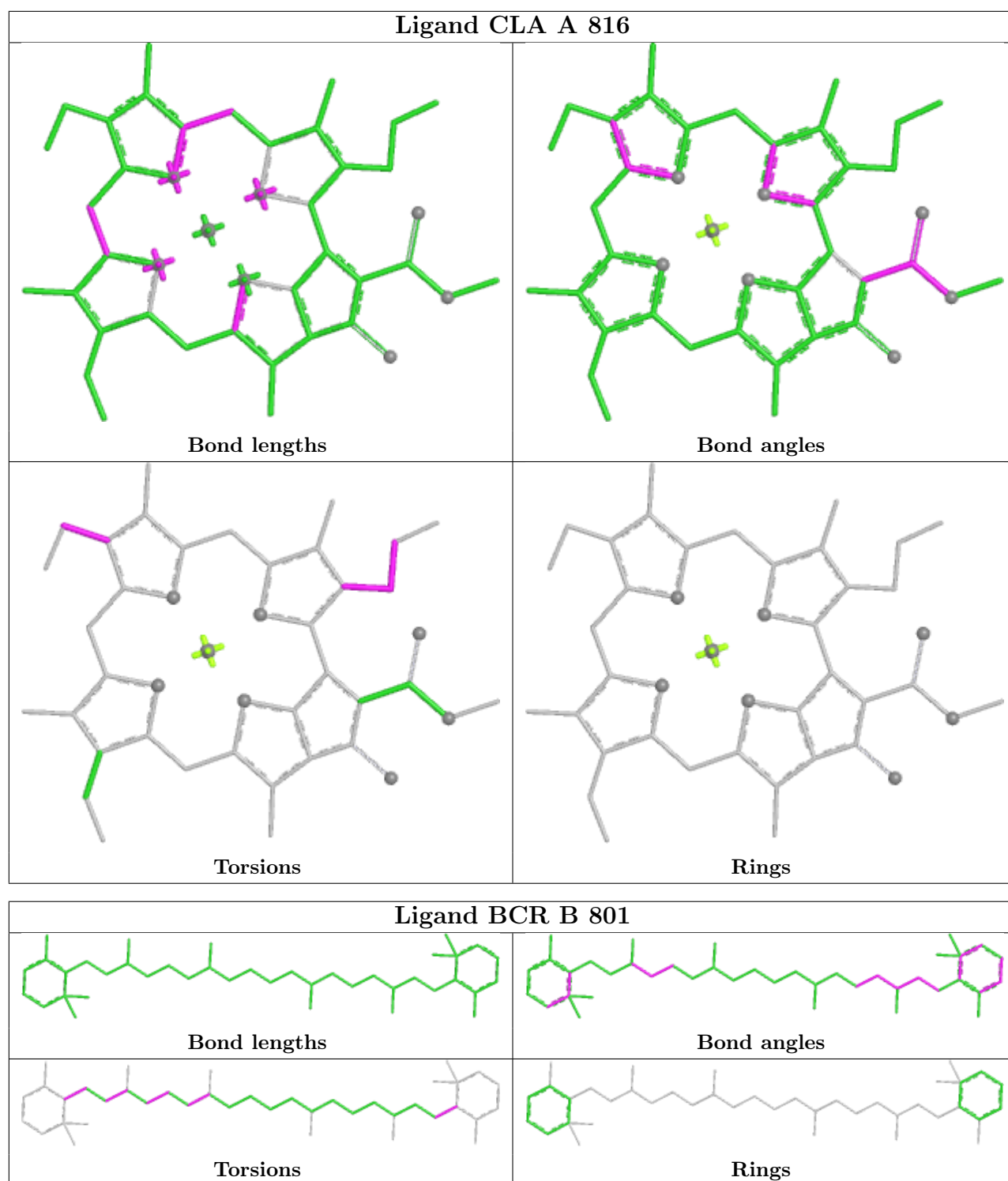


Torsions

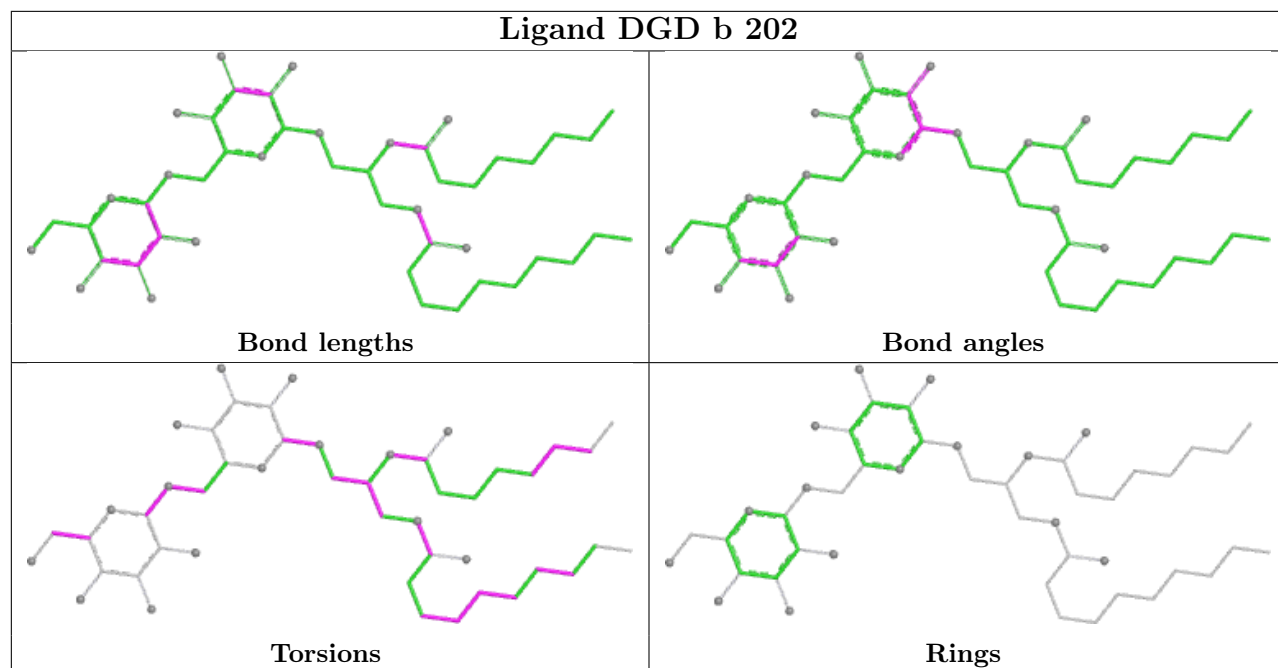


Rings

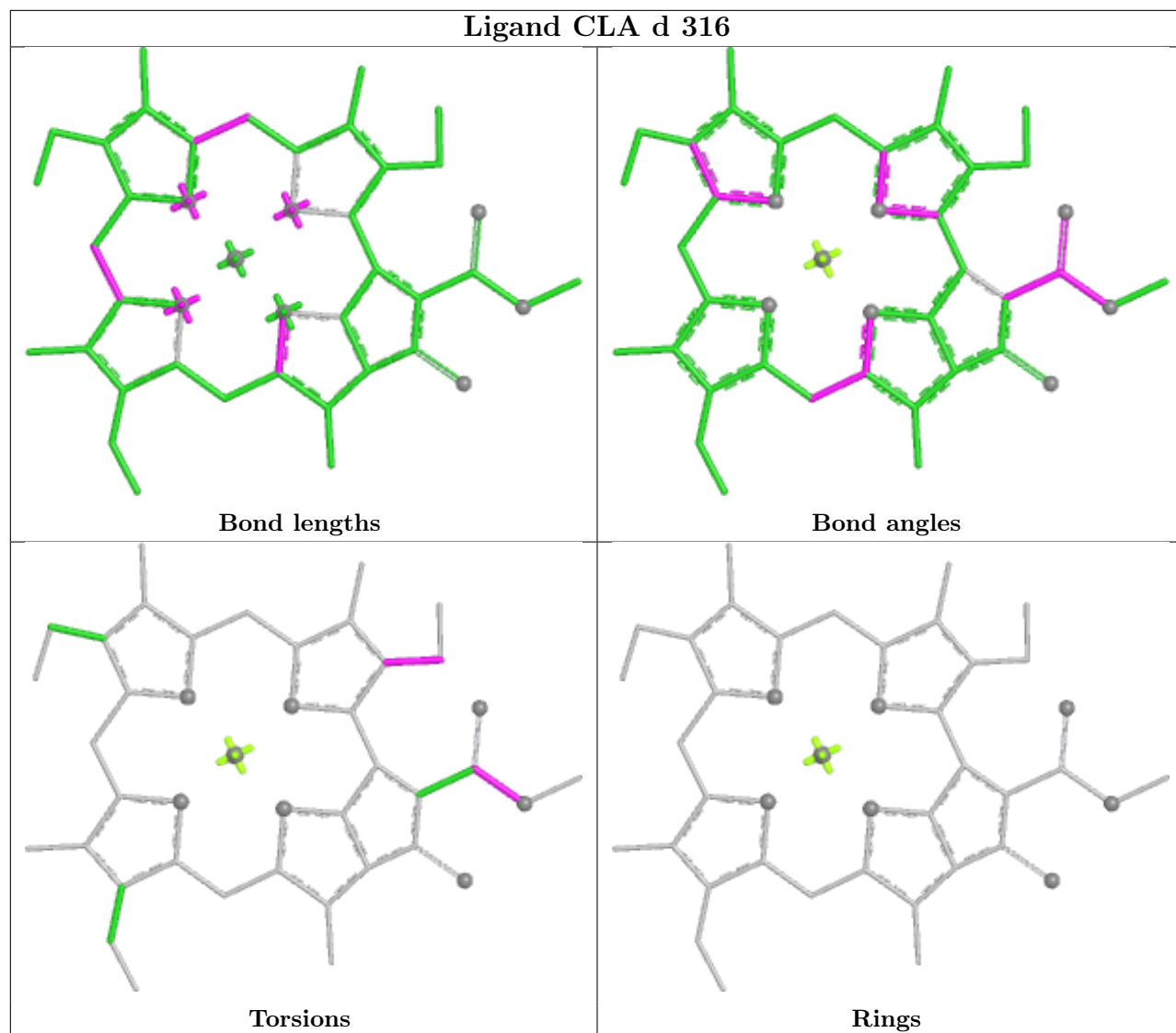




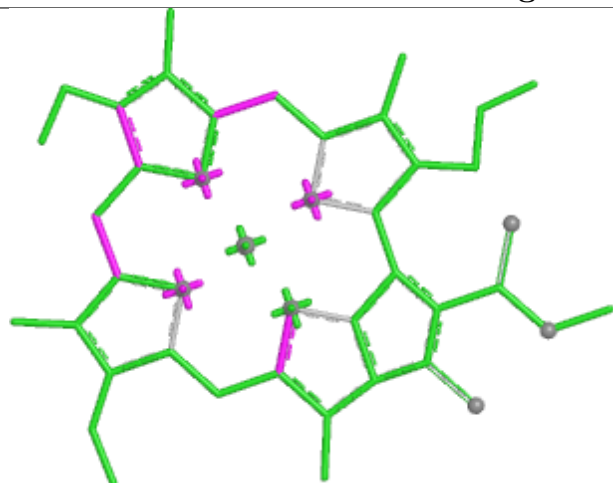
## Ligand DGD b 202



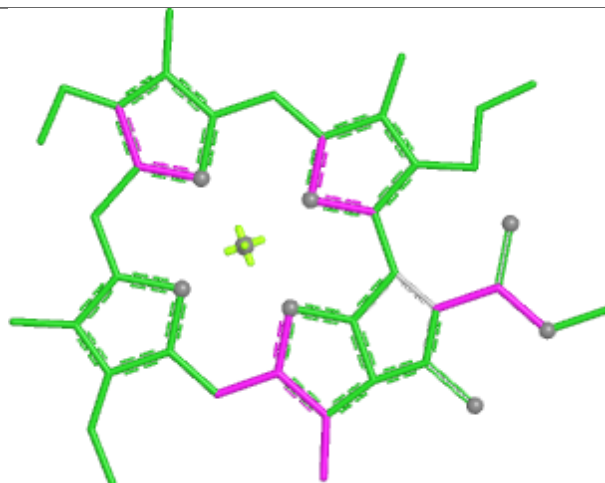
## Ligand CLA d 316



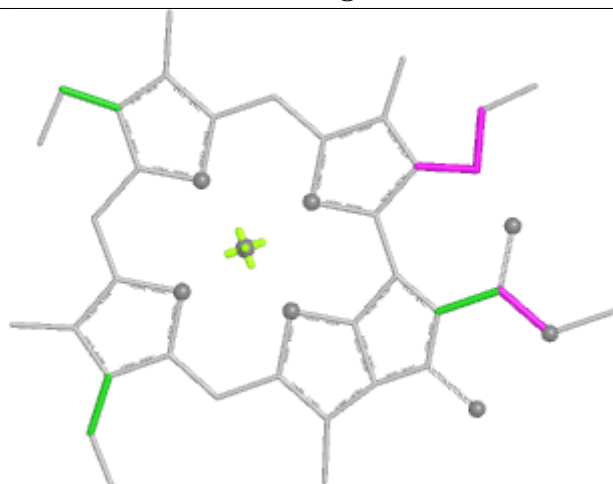
## Ligand CLA o 603



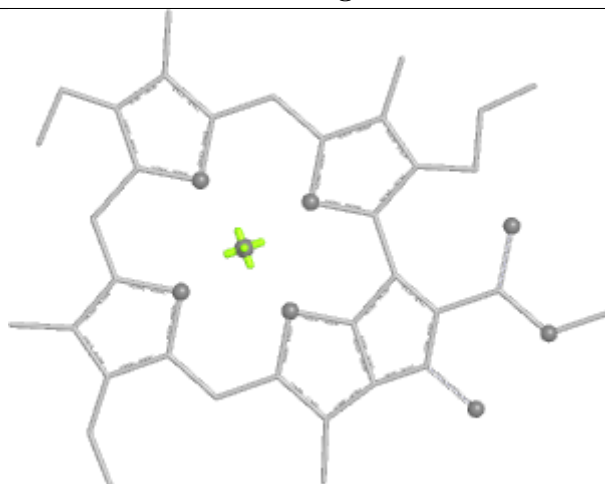
Bond lengths



Bond angles

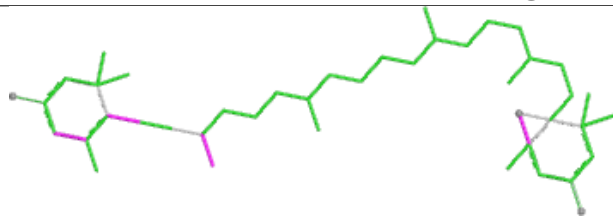


Torsions

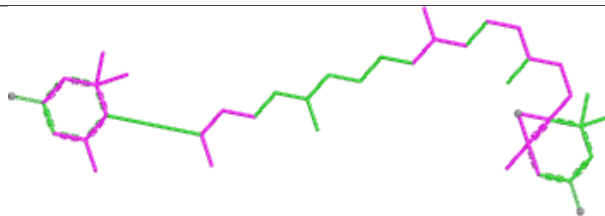


Rings

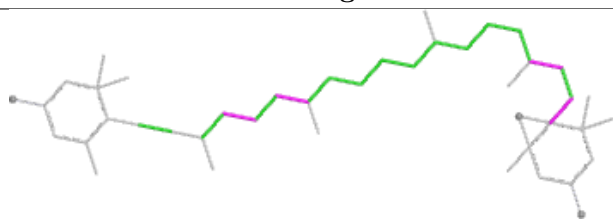
## Ligand DD6 f 614



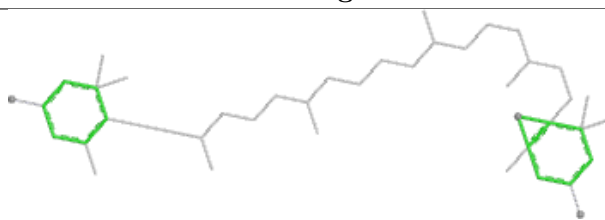
Bond lengths



Bond angles

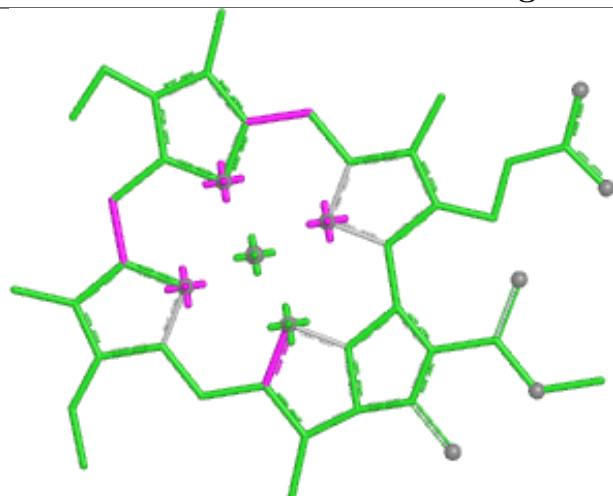


Torsions

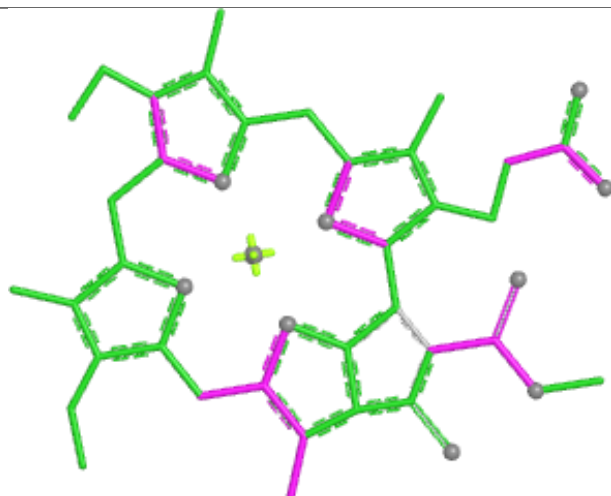


Rings

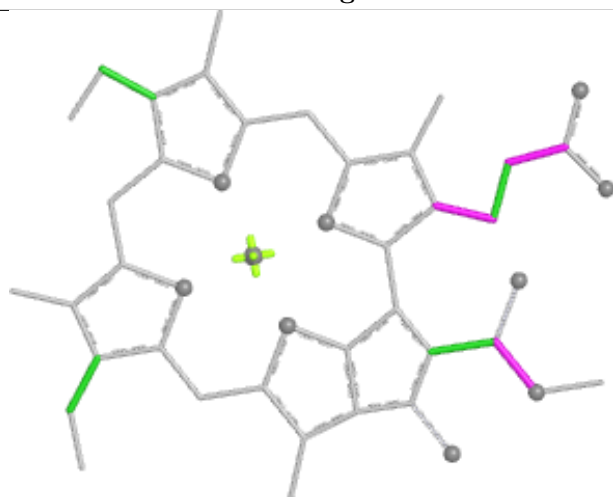
## Ligand CLA o 606



Bond lengths



Bond angles

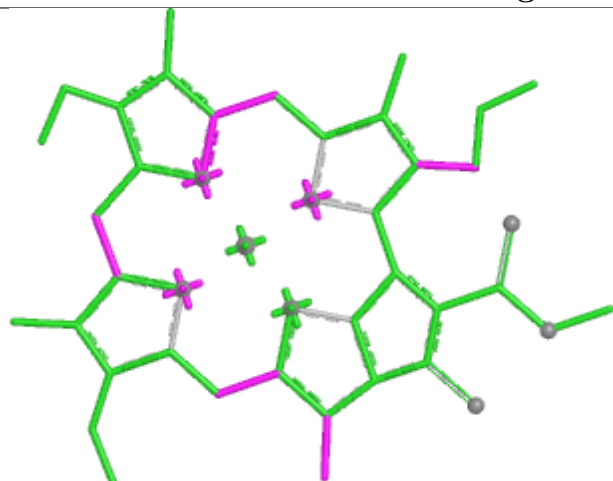


Torsions

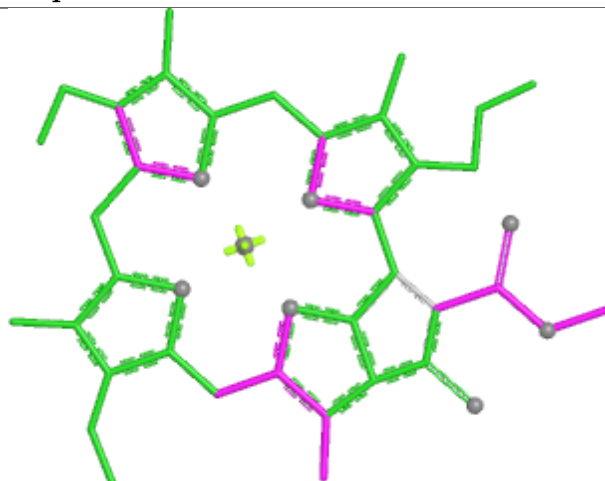


Rings

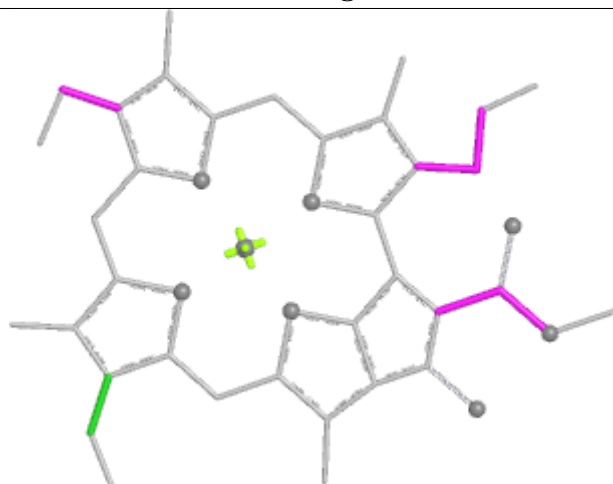
## Ligand CLA p 602



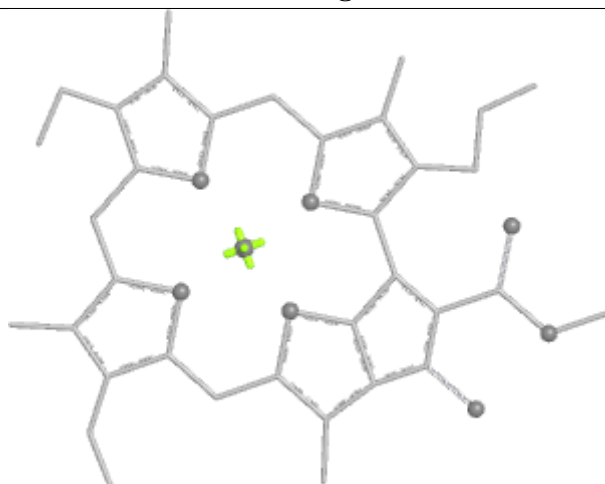
Bond lengths



Bond angles

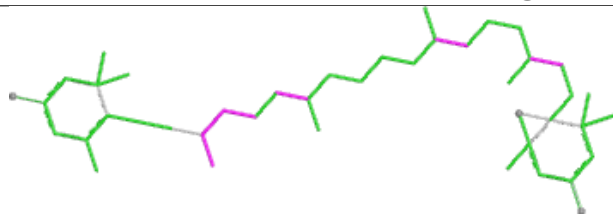


Torsions

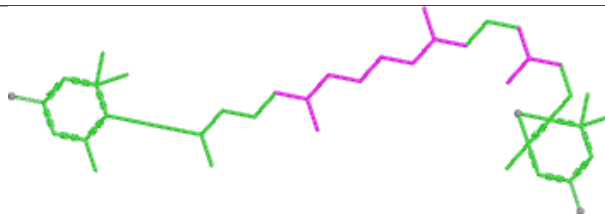


Rings

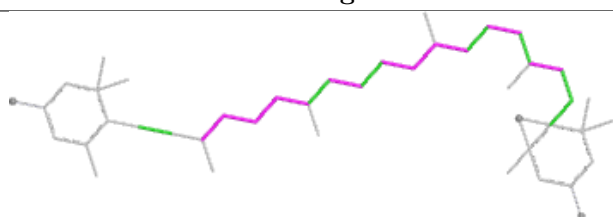
## Ligand DD6 J 105



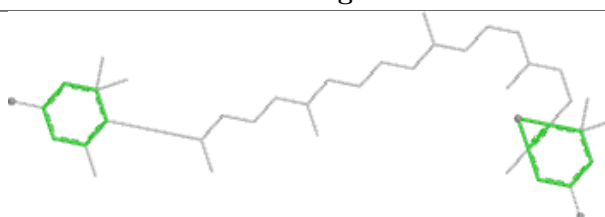
Bond lengths



Bond angles

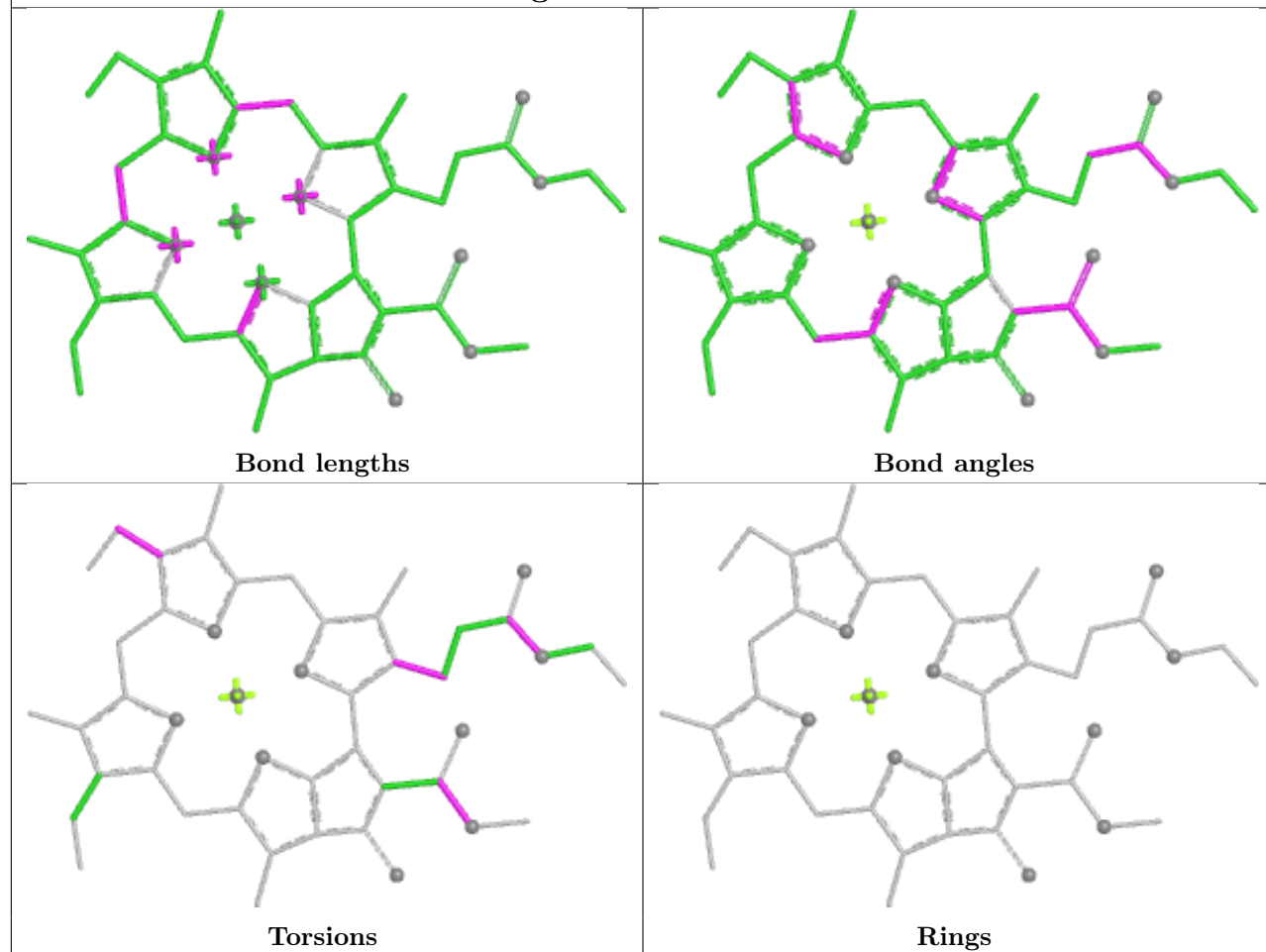


Torsions

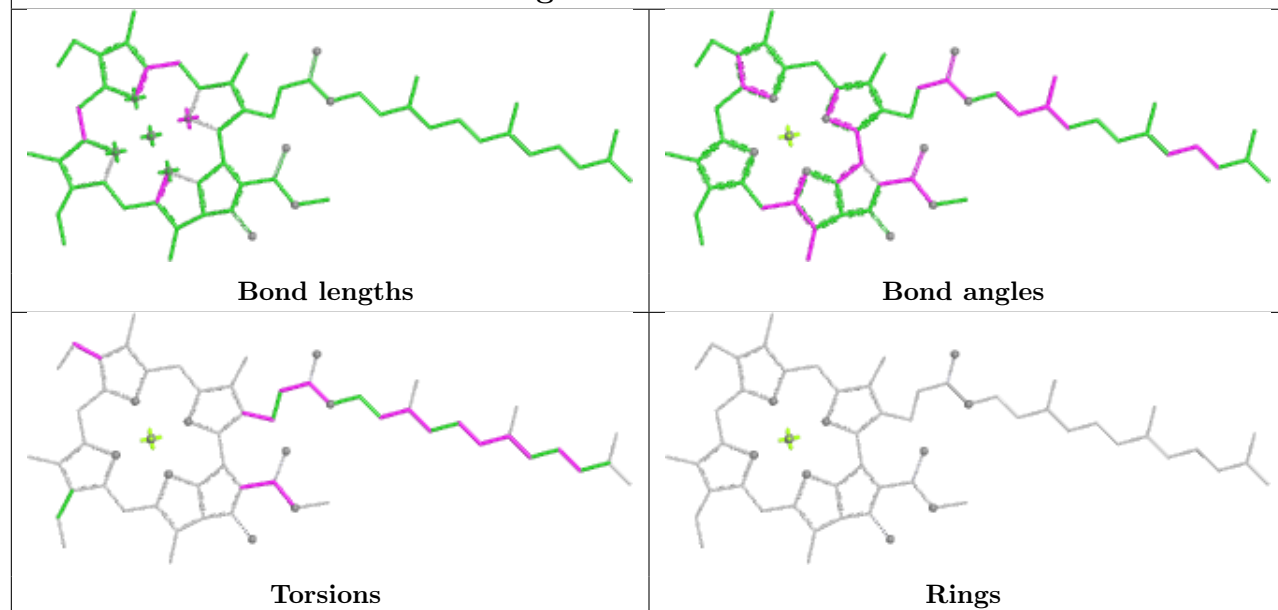


Rings

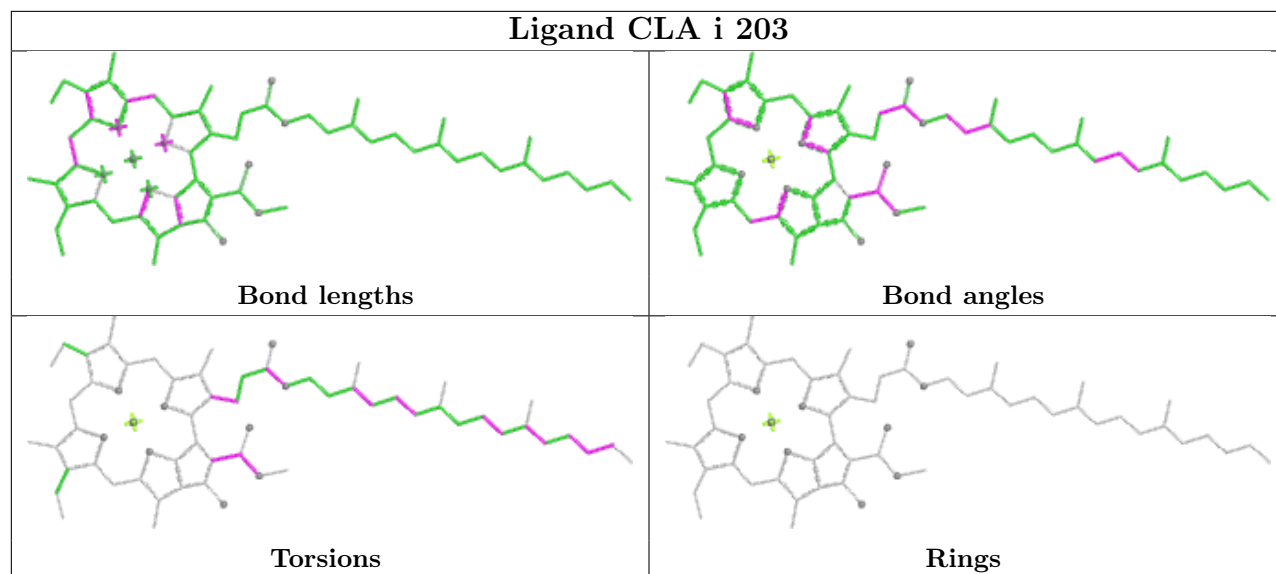
## Ligand CLA o 602



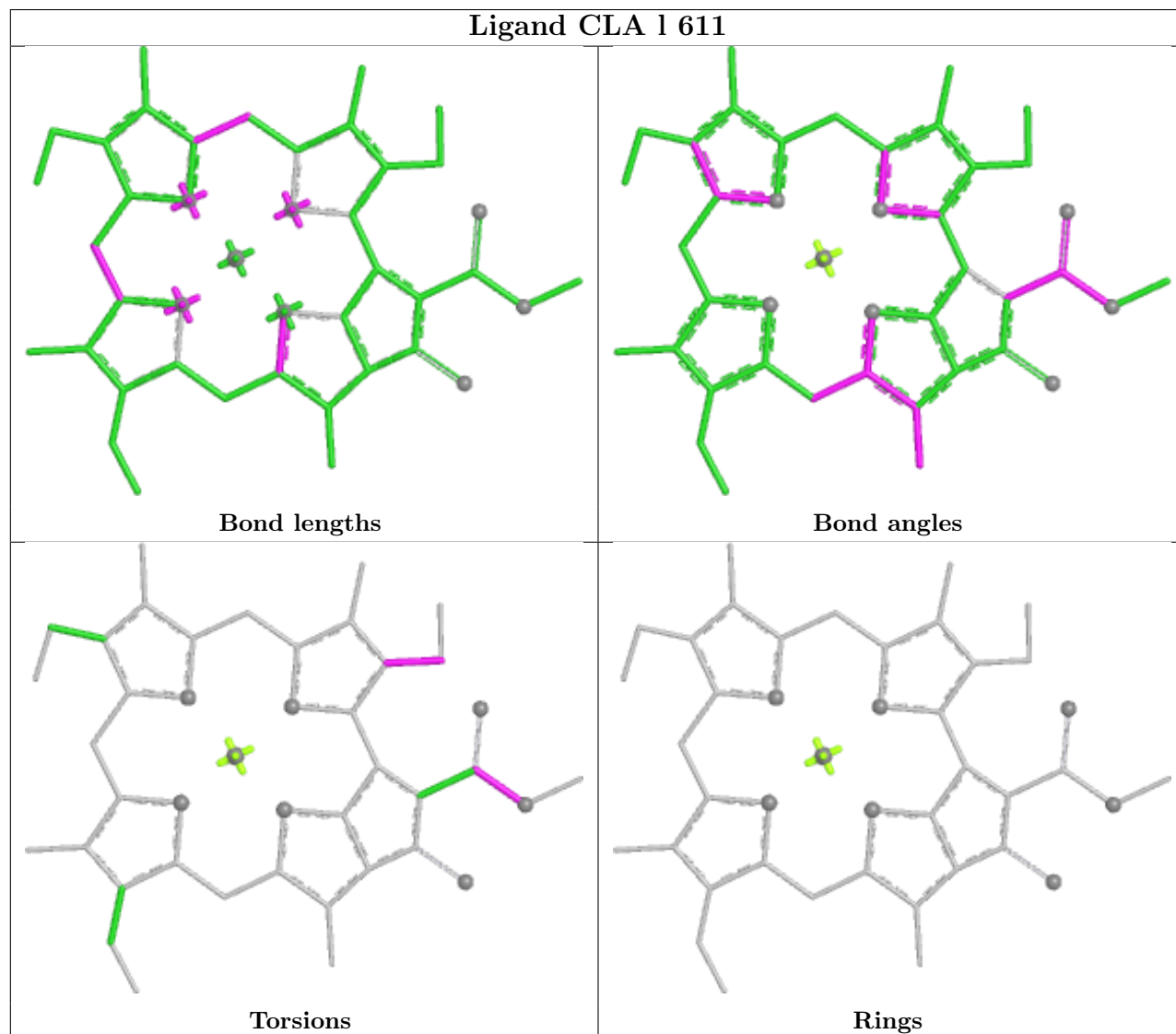
## Ligand CLA a 204



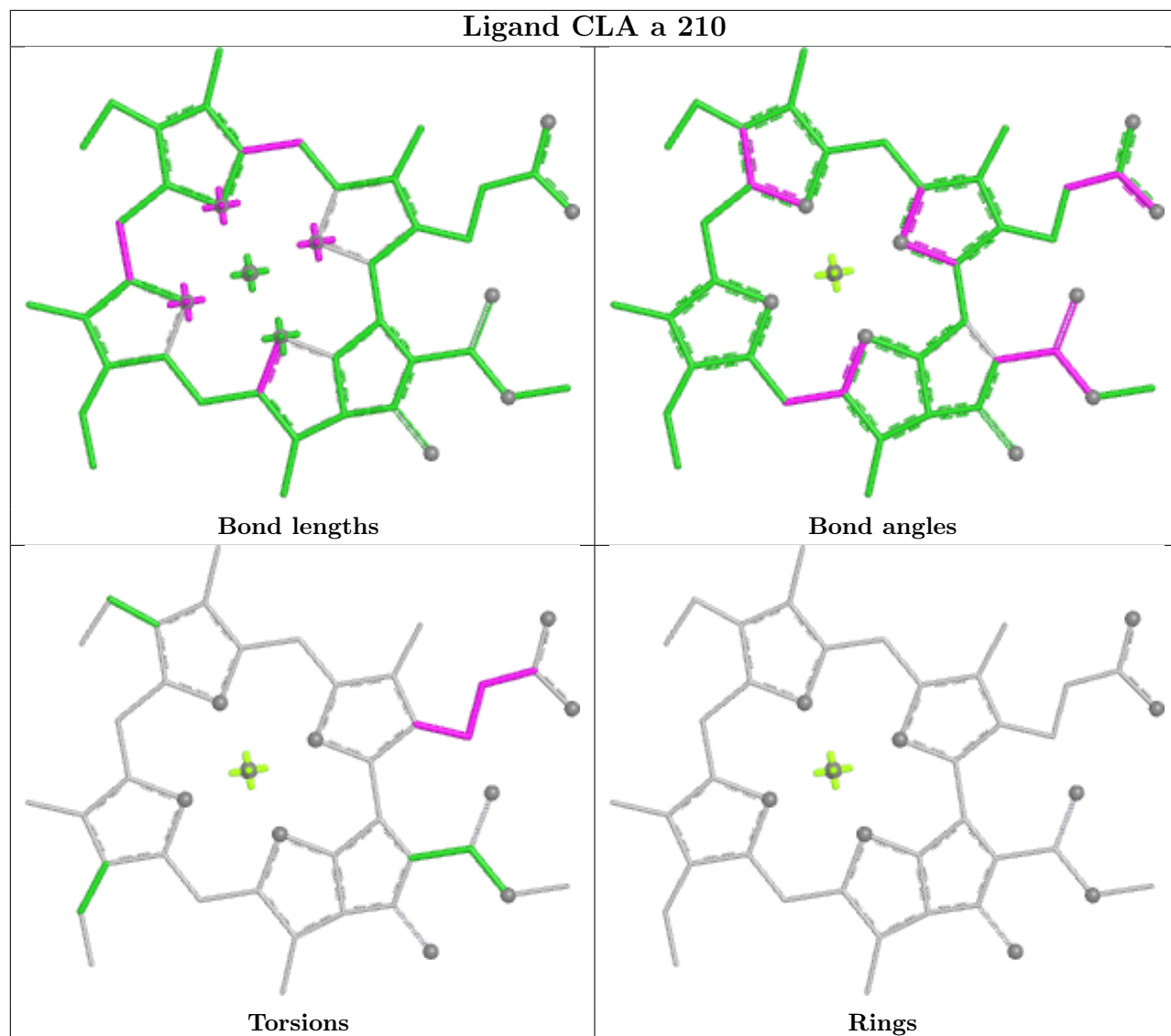
## Ligand CLA i 203



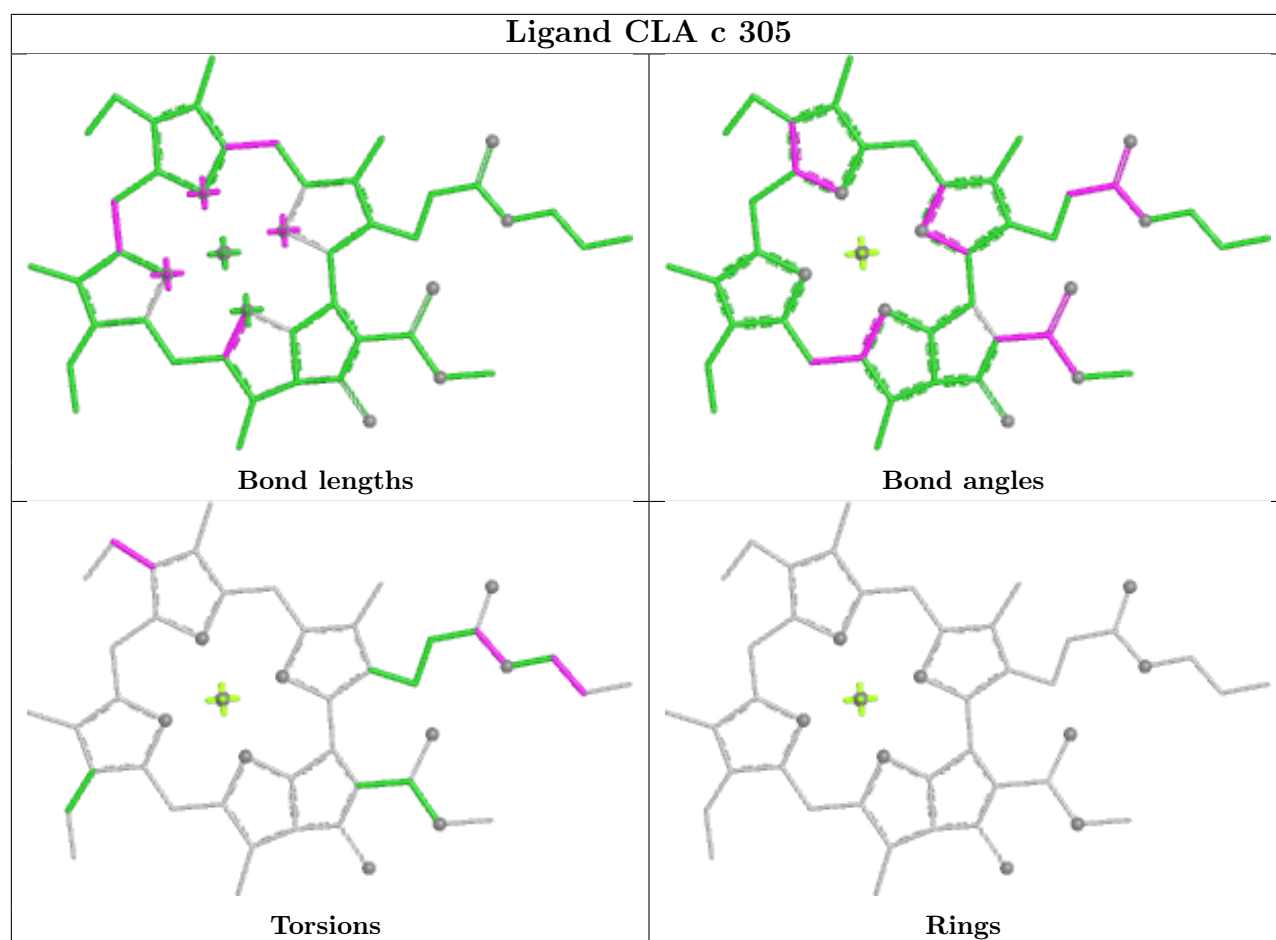
## Ligand CLA l 611



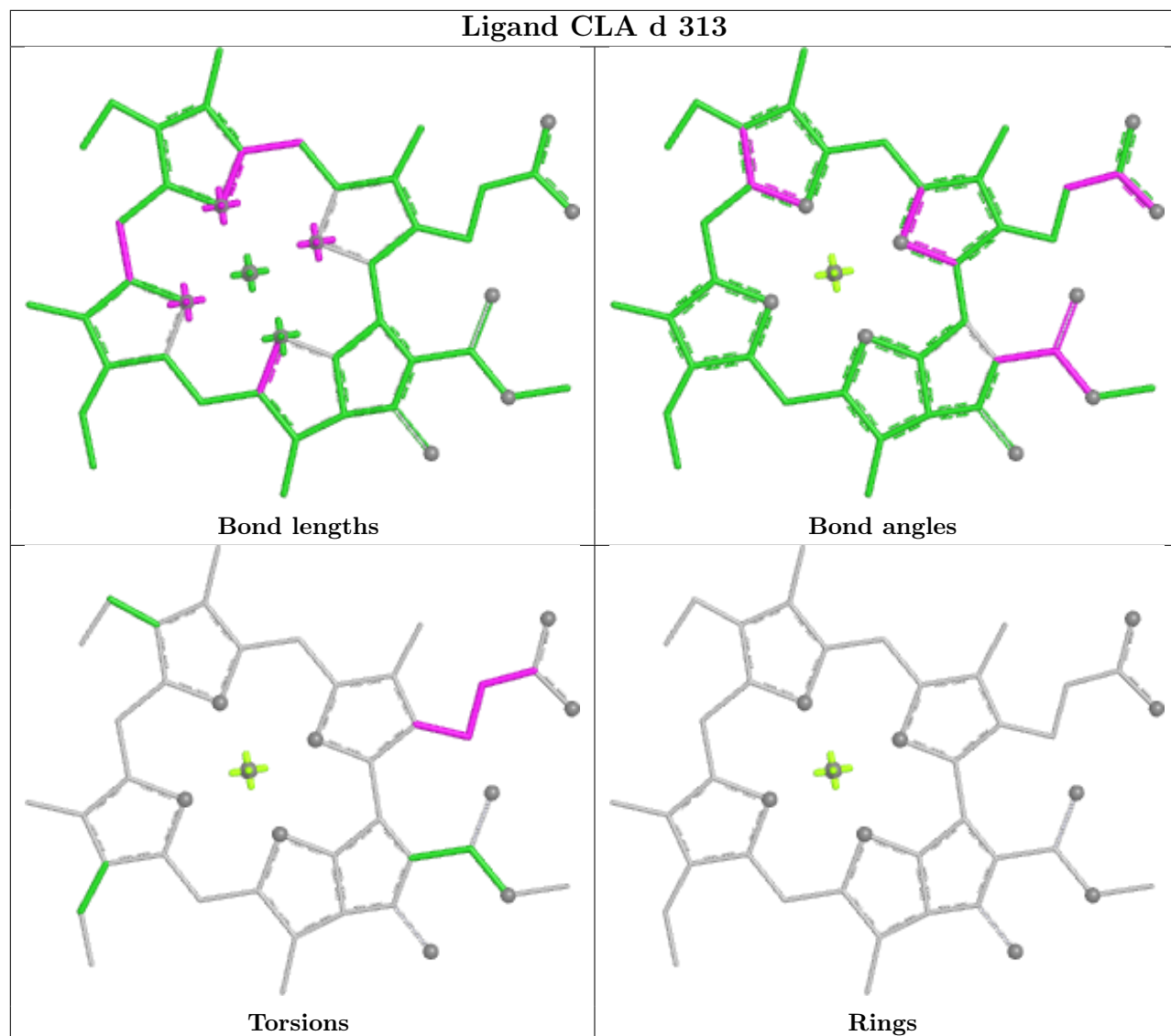
## Ligand CLA a 210



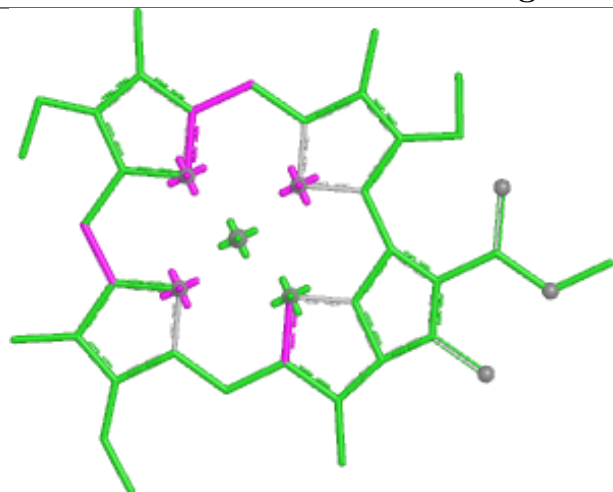




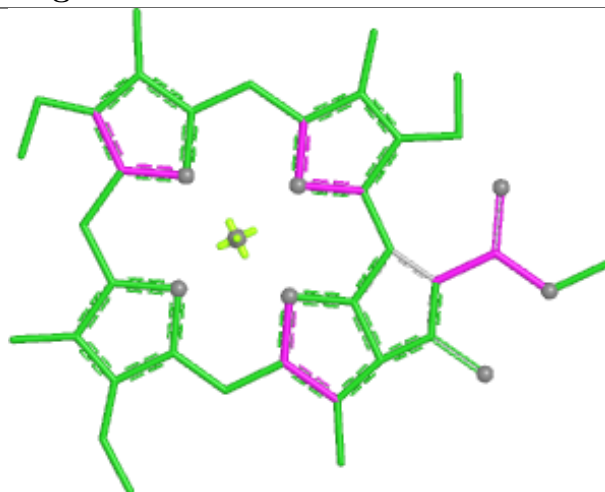
## Ligand CLA d 313



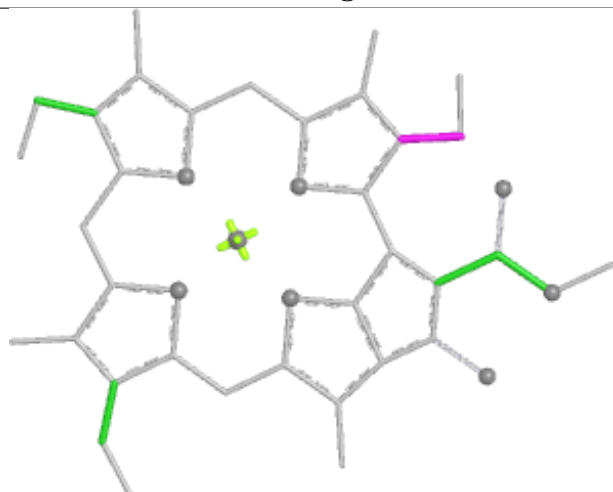
## Ligand CLA g 205



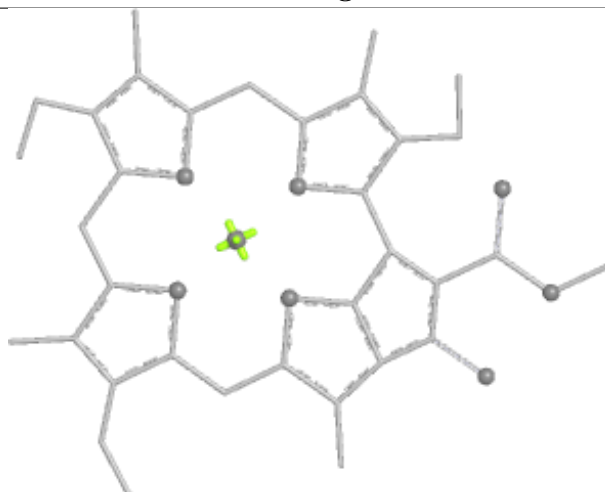
Bond lengths



Bond angles

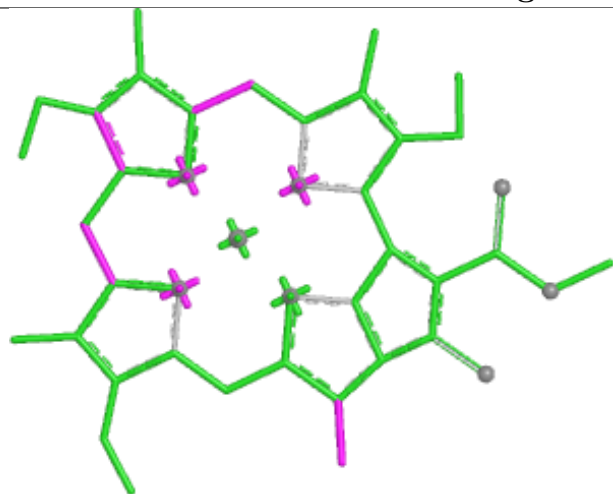


Torsions

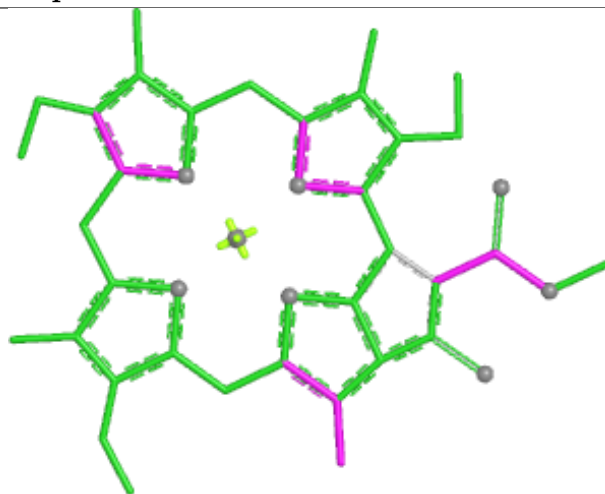


Rings

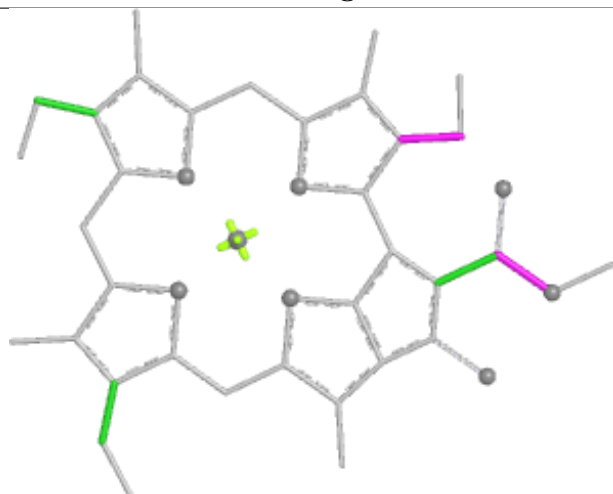
## Ligand CLA p 603



Bond lengths



Bond angles

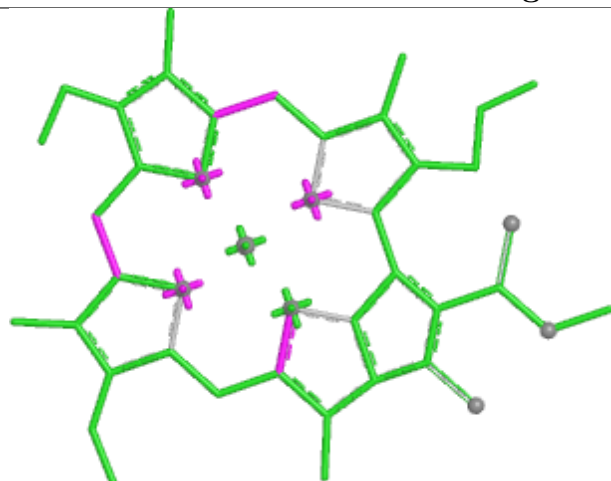


Torsions

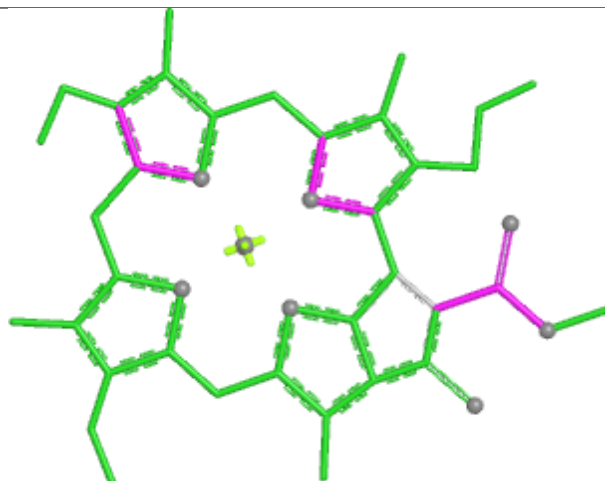


Rings

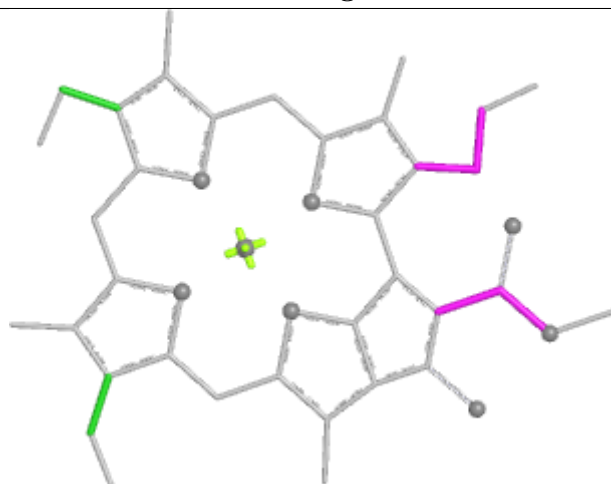
## Ligand CLA 1 609



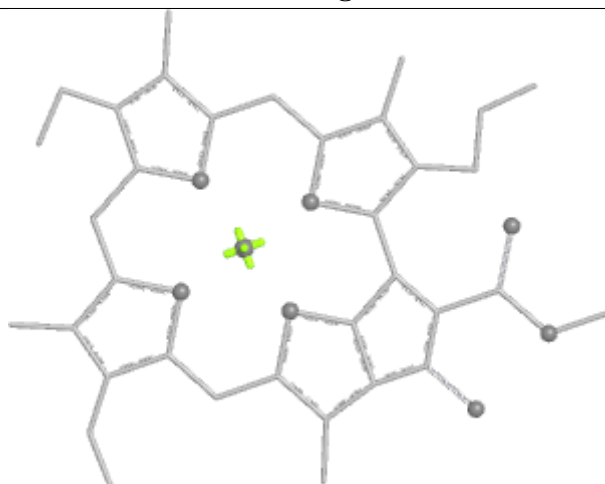
Bond lengths



Bond angles

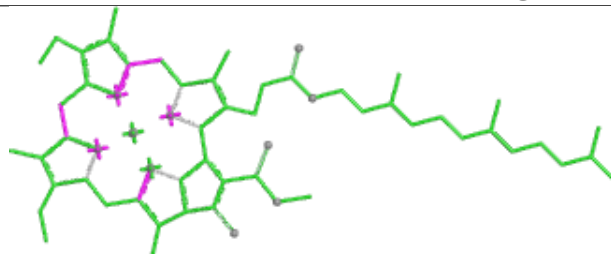


Torsions

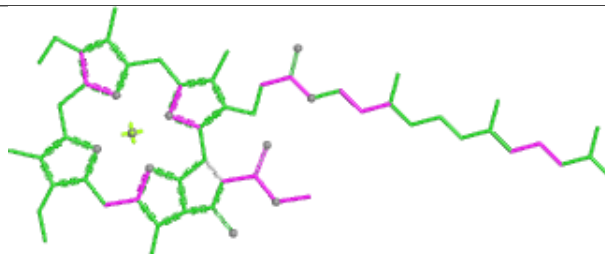


Rings

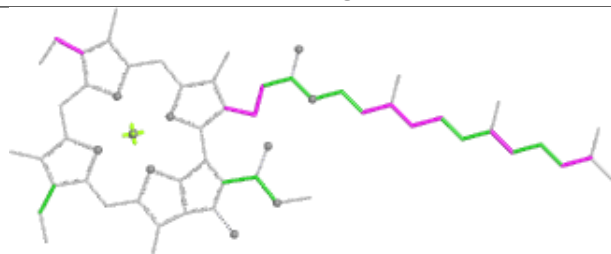
## Ligand CLA B 839



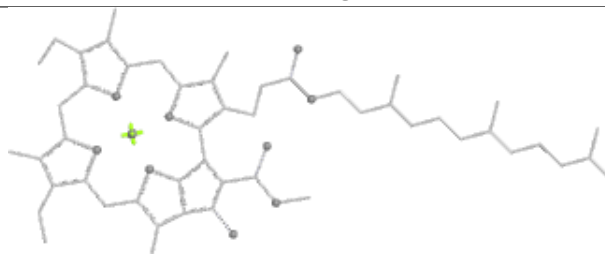
Bond lengths



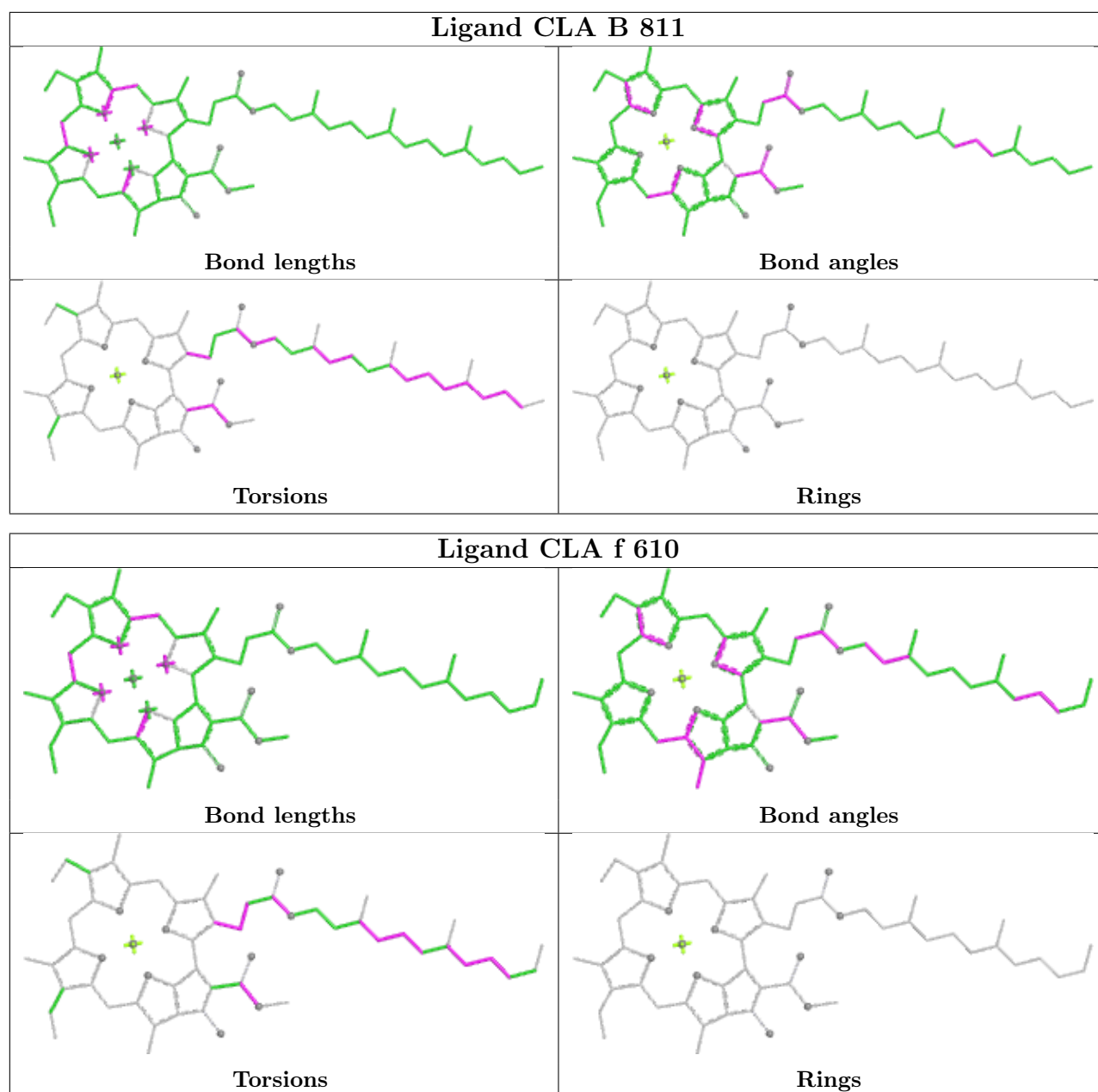
Bond angles

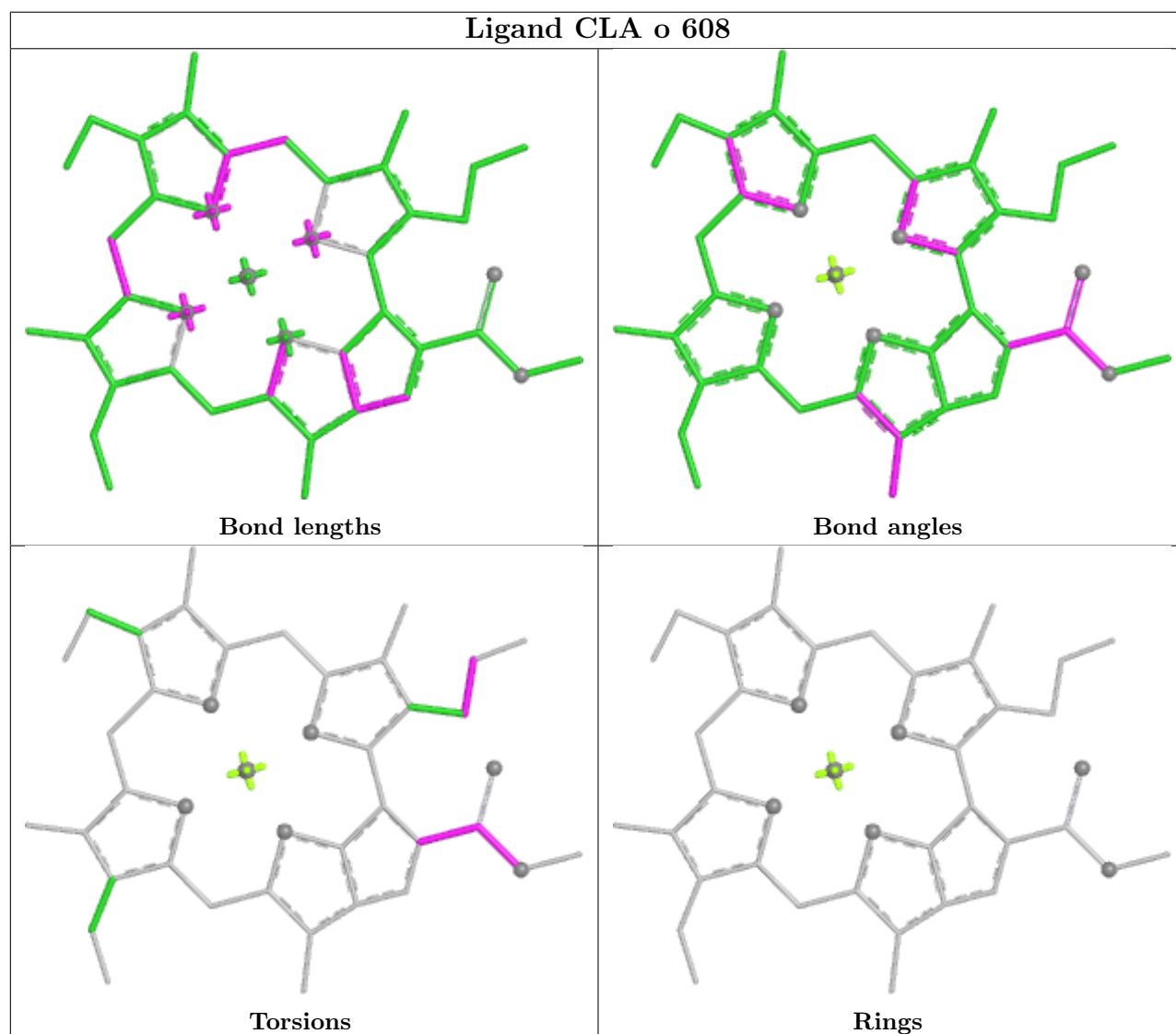
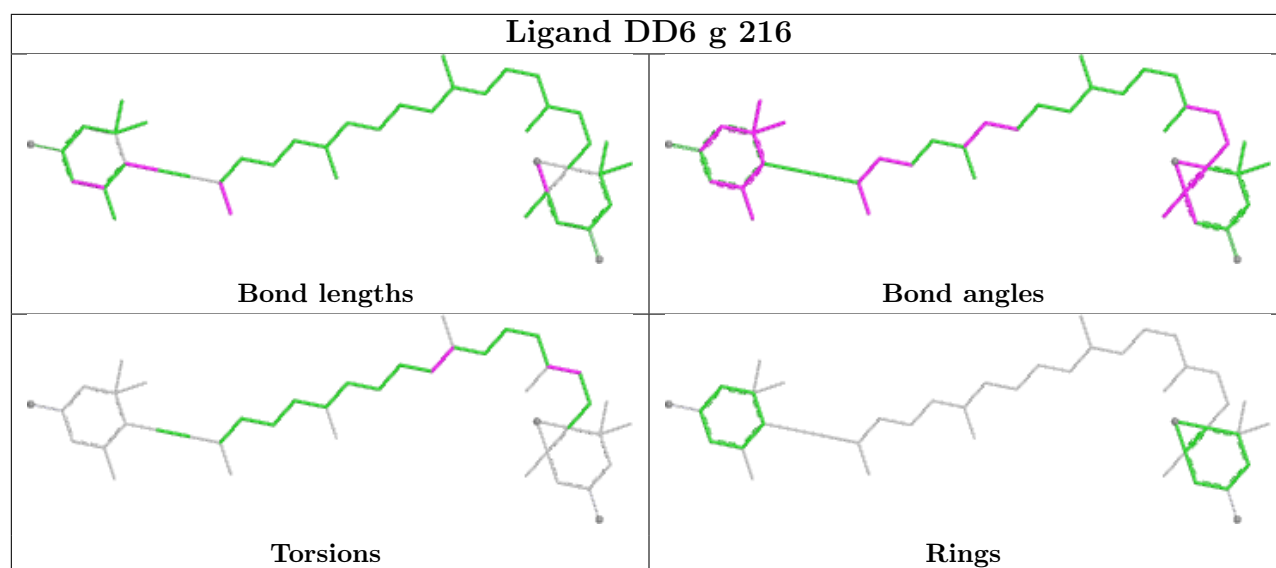


Torsions

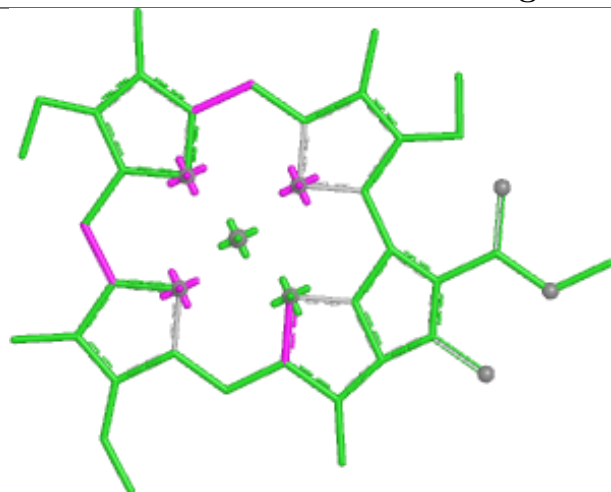


Rings

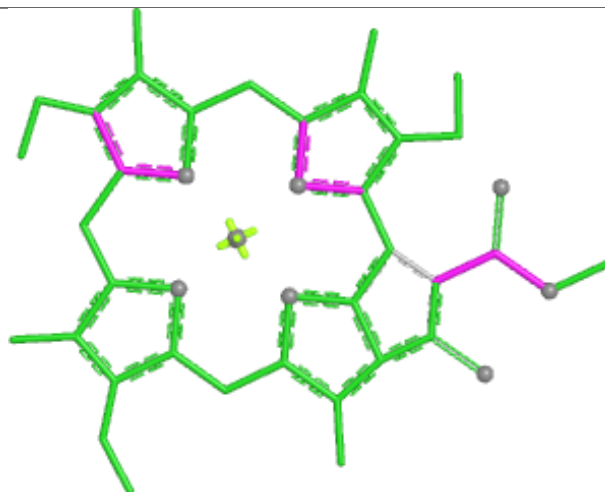




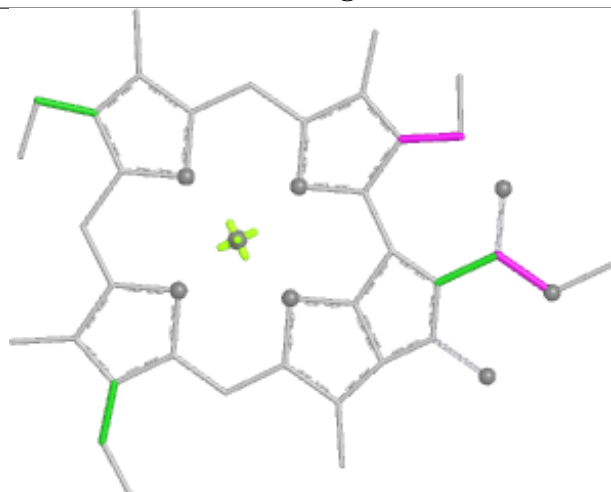
## Ligand CLA e 217



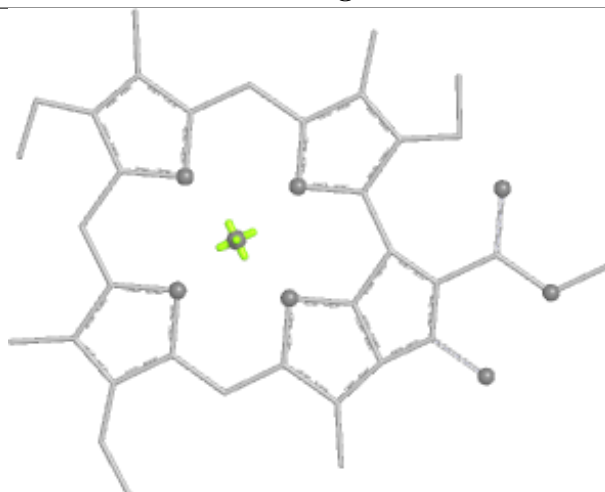
Bond lengths



Bond angles



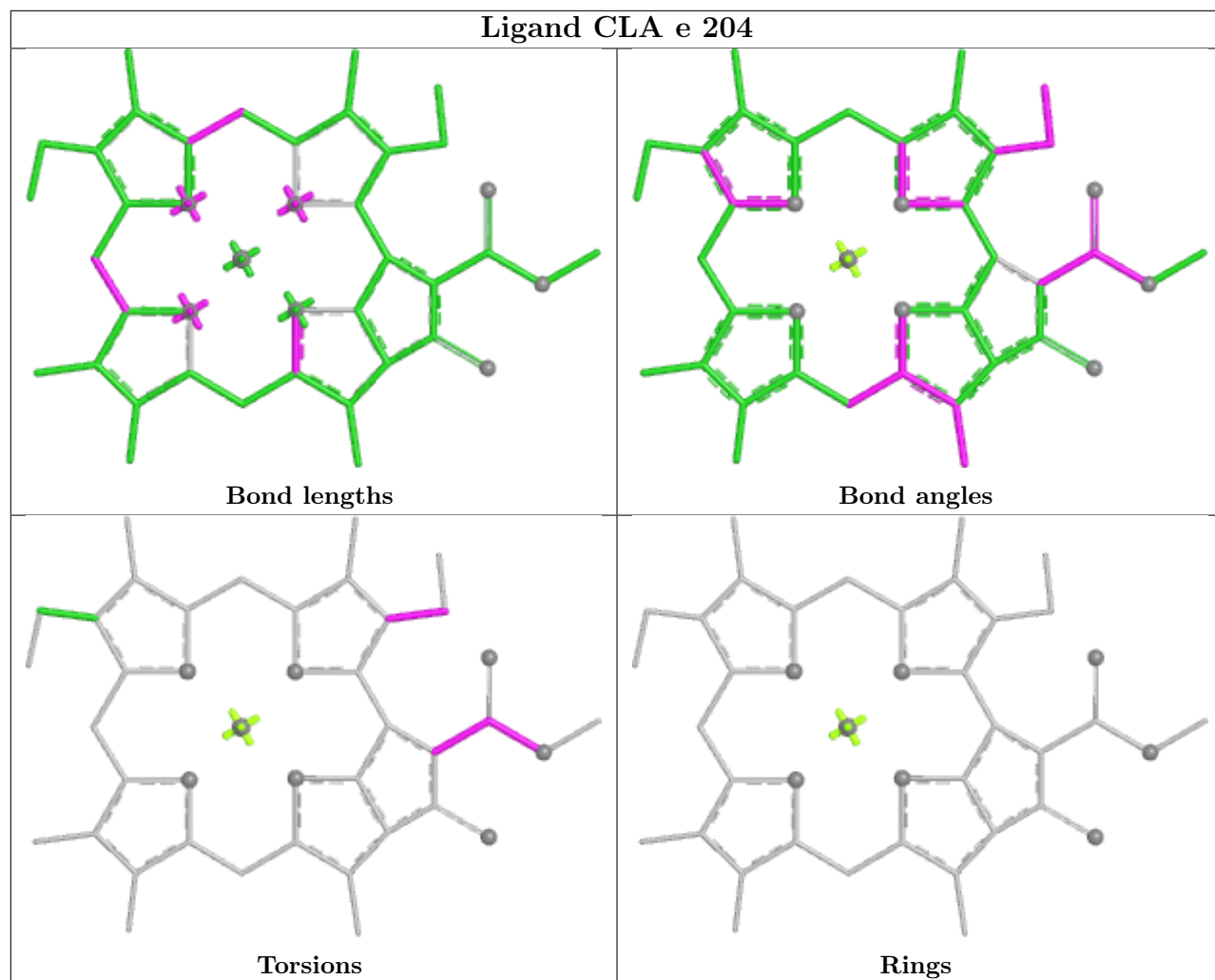
Torsions



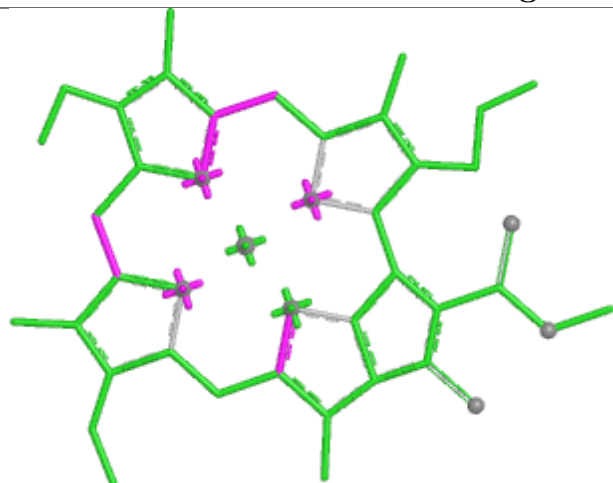
Rings



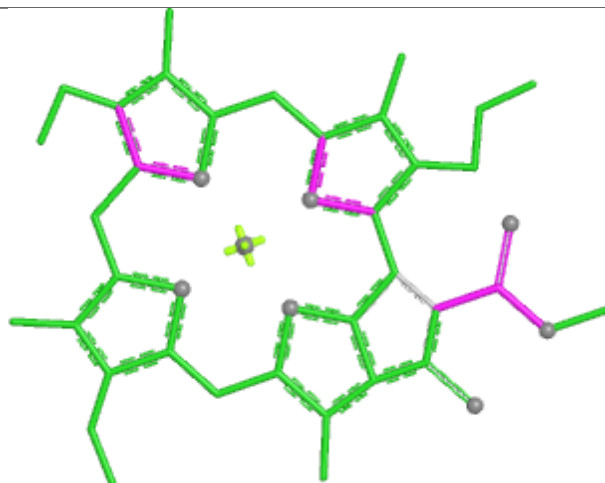
## Ligand CLA e 204



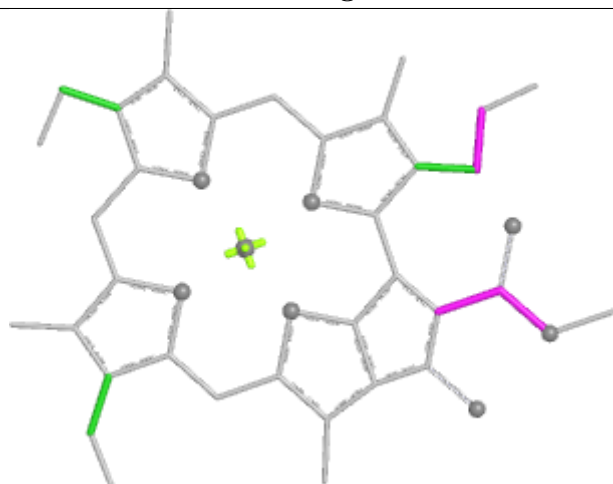
## Ligand CLA c 312



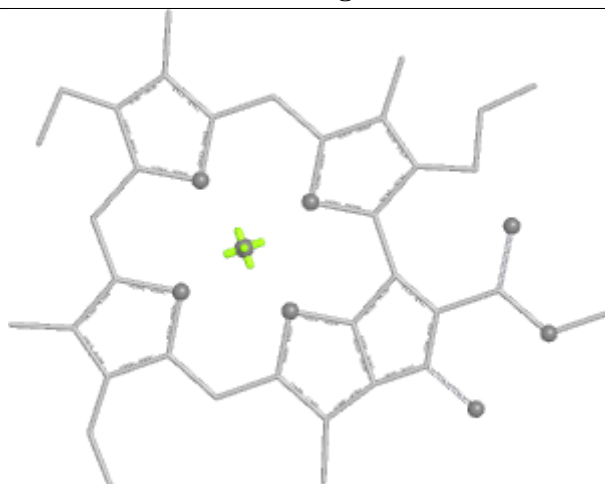
Bond lengths



Bond angles

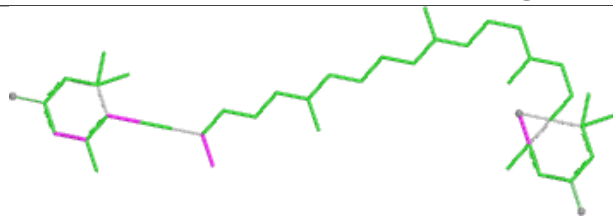


Torsions

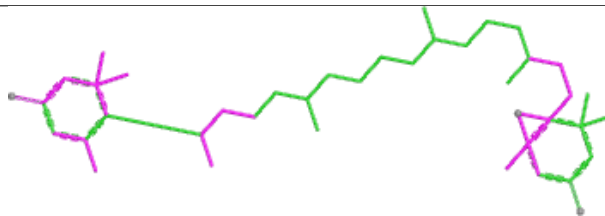


Rings

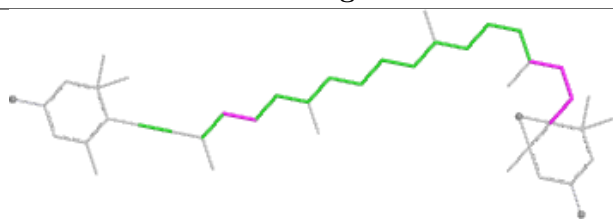
## Ligand DD6 n 212



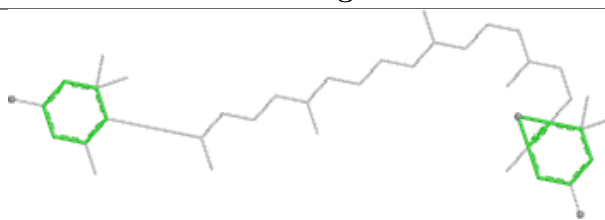
Bond lengths



Bond angles

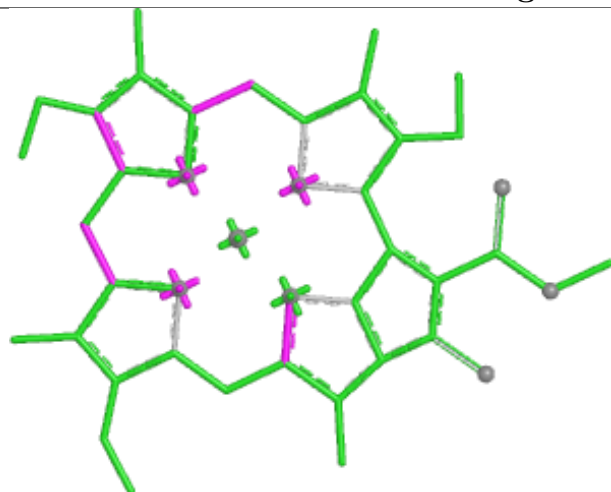


Torsions

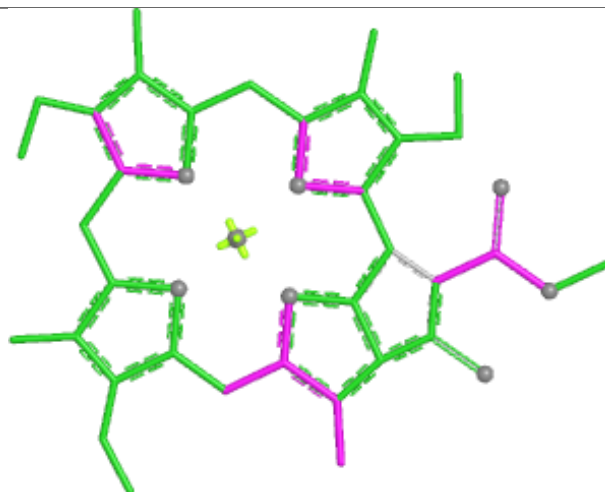


Rings

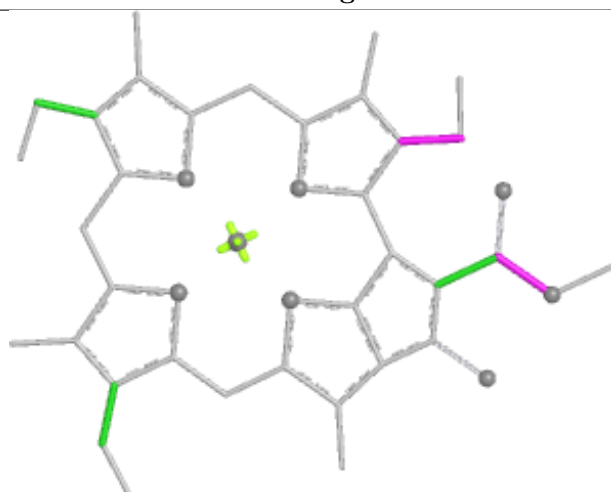
## Ligand CLA b 203



Bond lengths



Bond angles

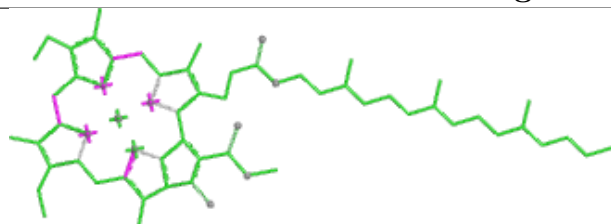


Torsions

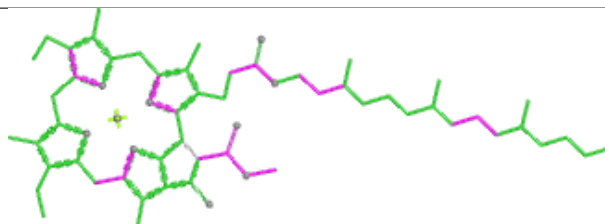


Rings

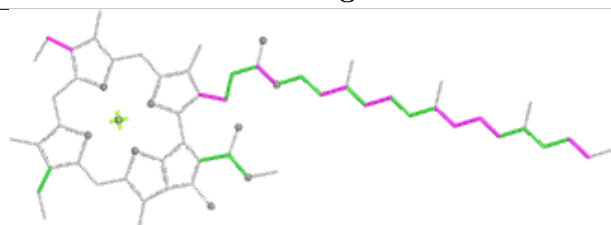
## Ligand CLA B 843



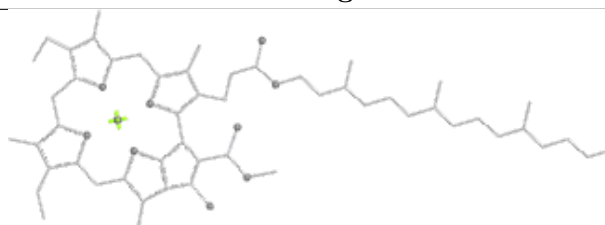
Bond lengths



Bond angles

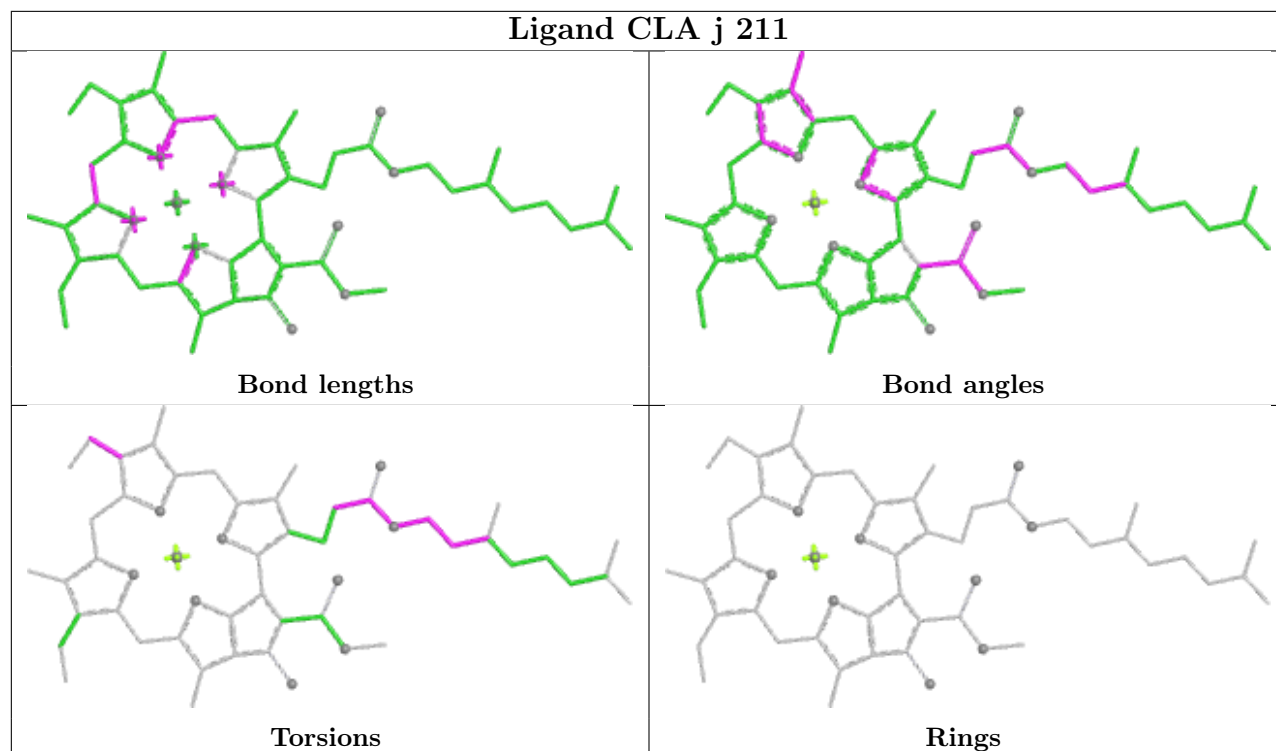


Torsions

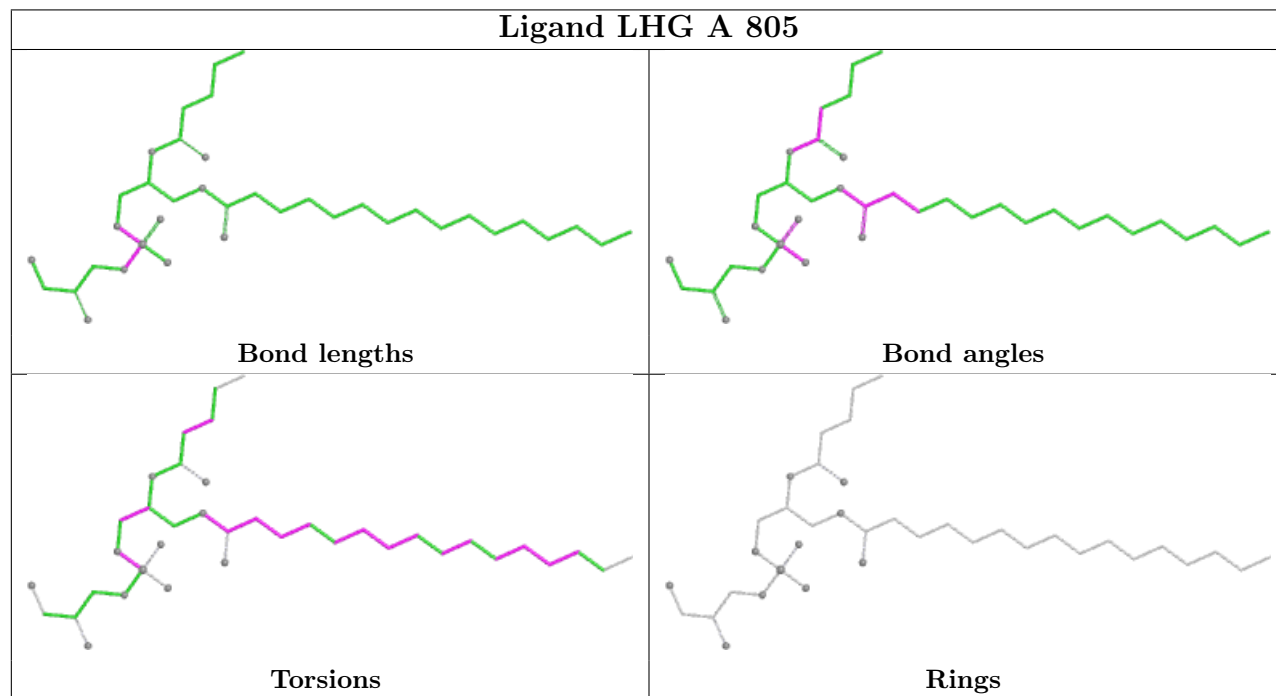


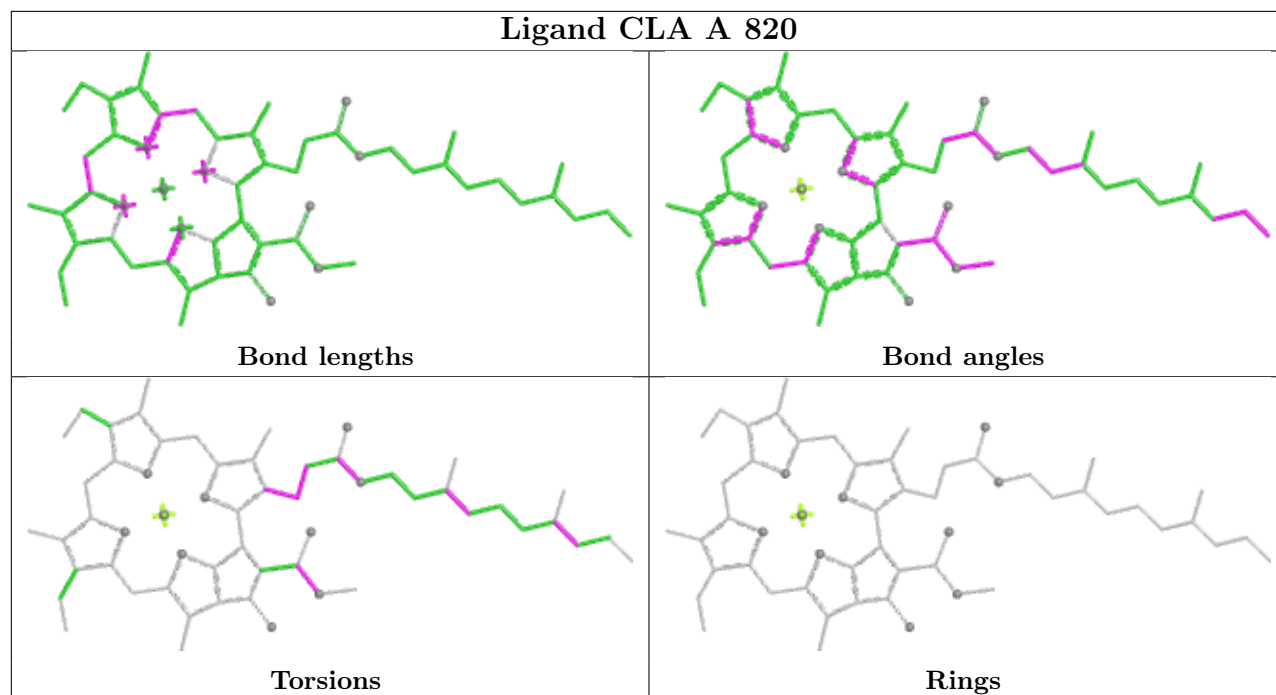
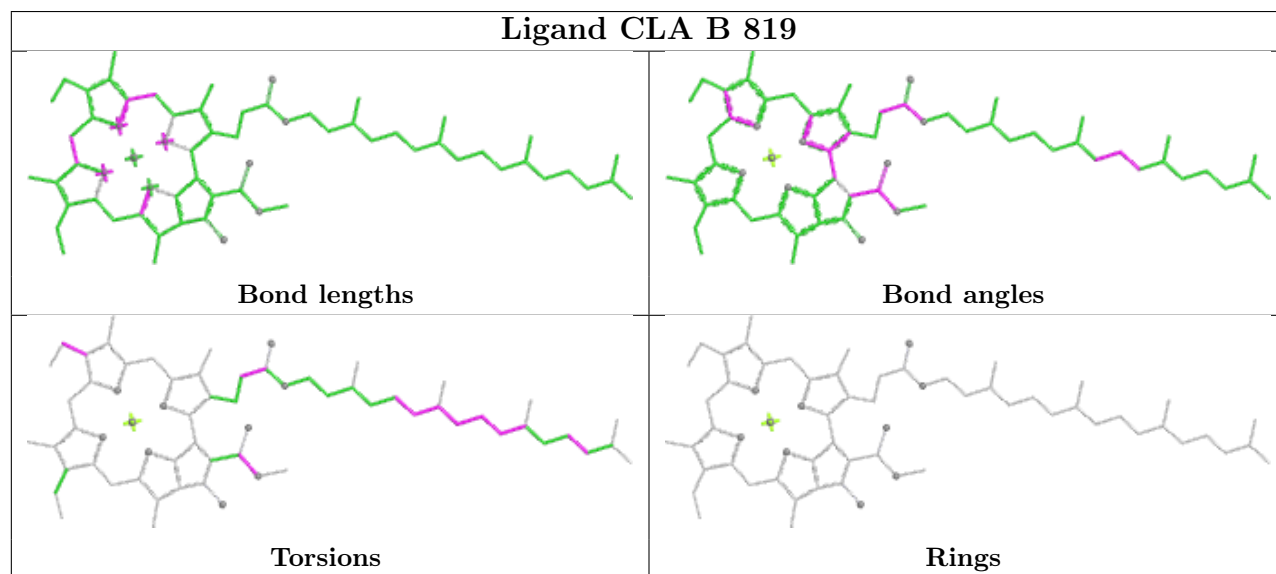
Rings

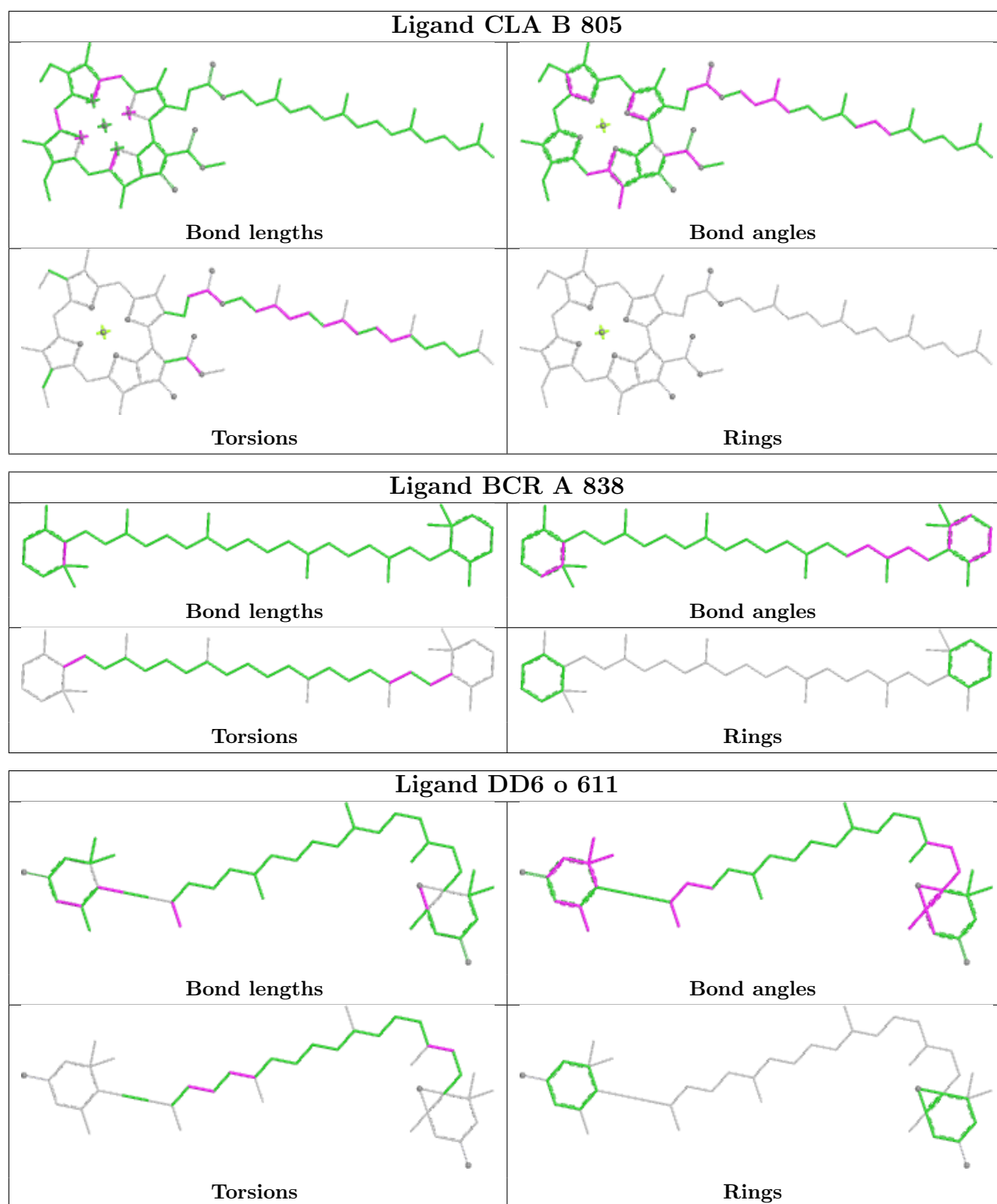
## Ligand CLA j 211

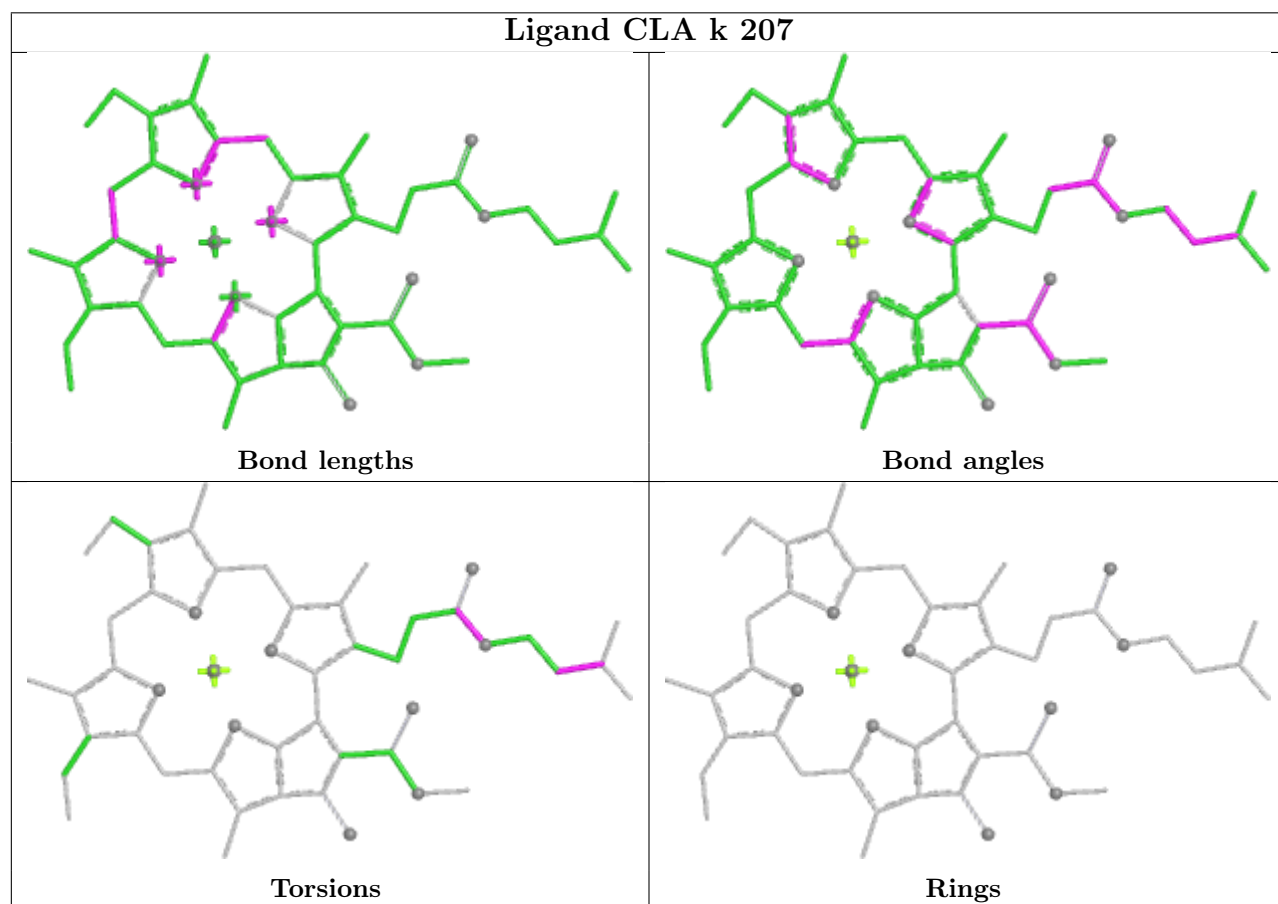
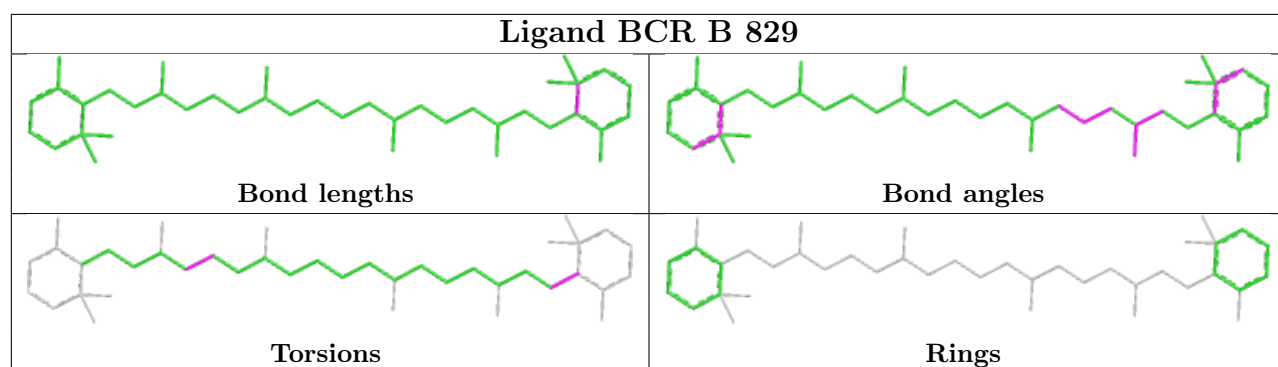


## Ligand LHG A 805

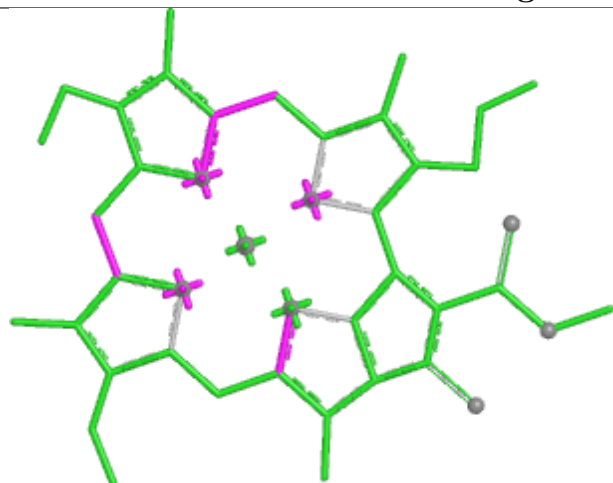


**Ligand CLA A 820****Ligand CLA B 819**

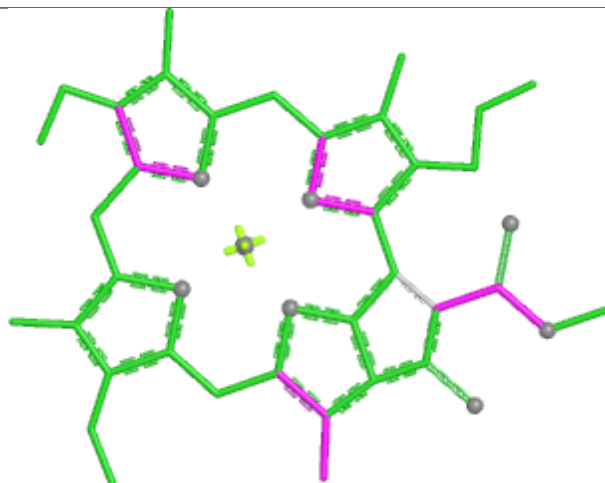




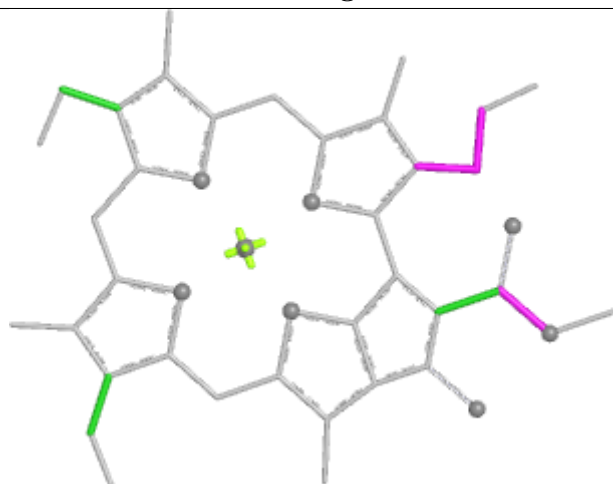
## Ligand CLA b 205



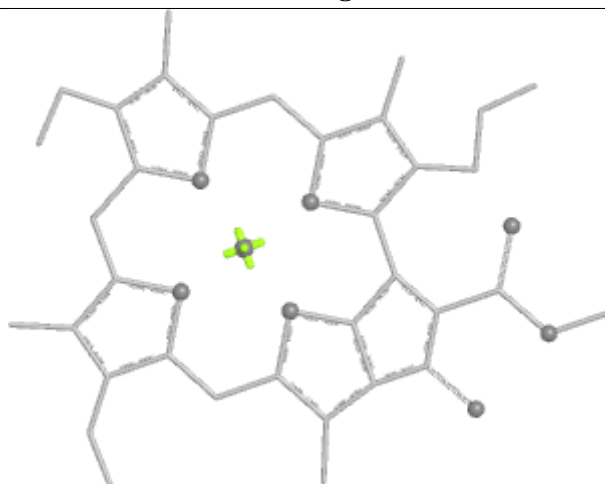
Bond lengths



Bond angles

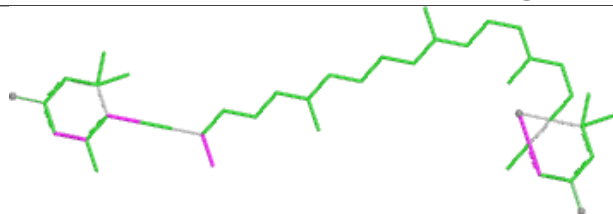


Torsions

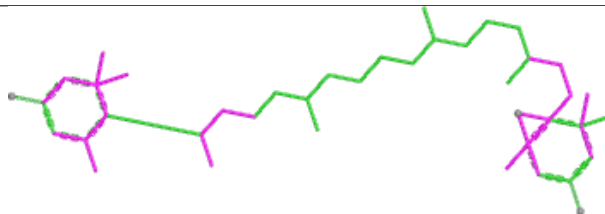


Rings

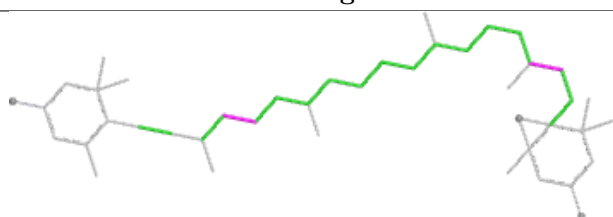
## Ligand DD6 d 318



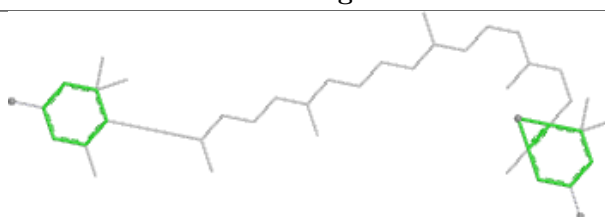
Bond lengths



Bond angles



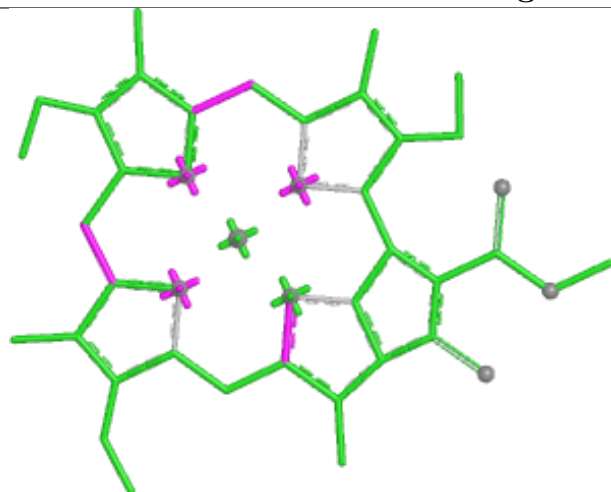
Torsions



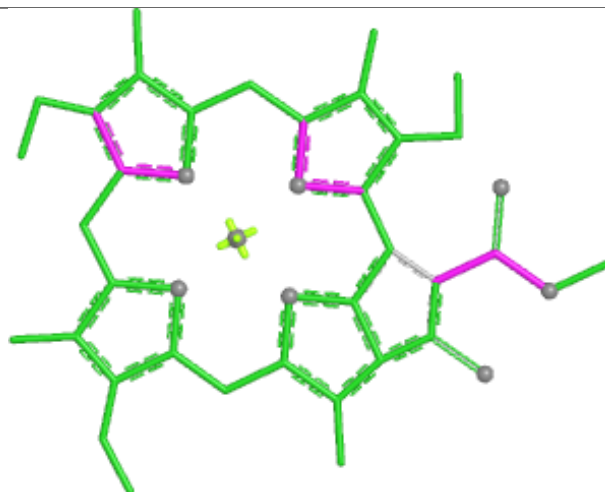
Rings



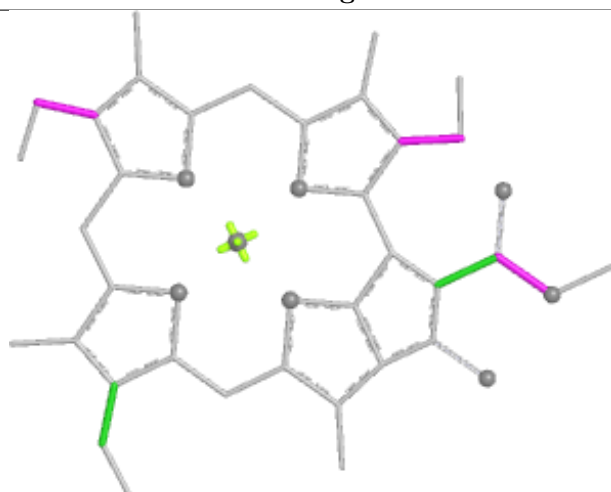
## Ligand CLA n 205



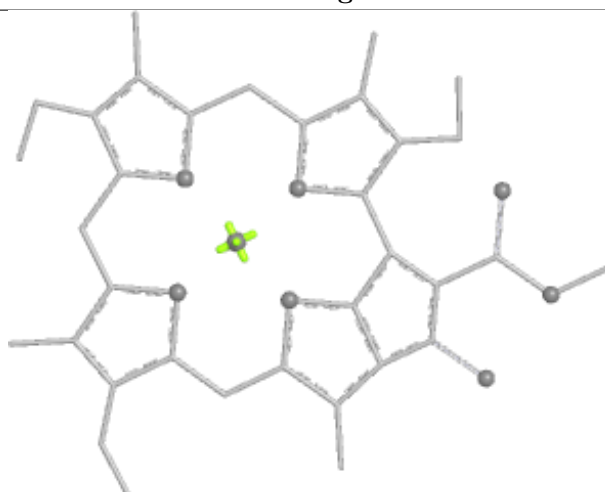
Bond lengths



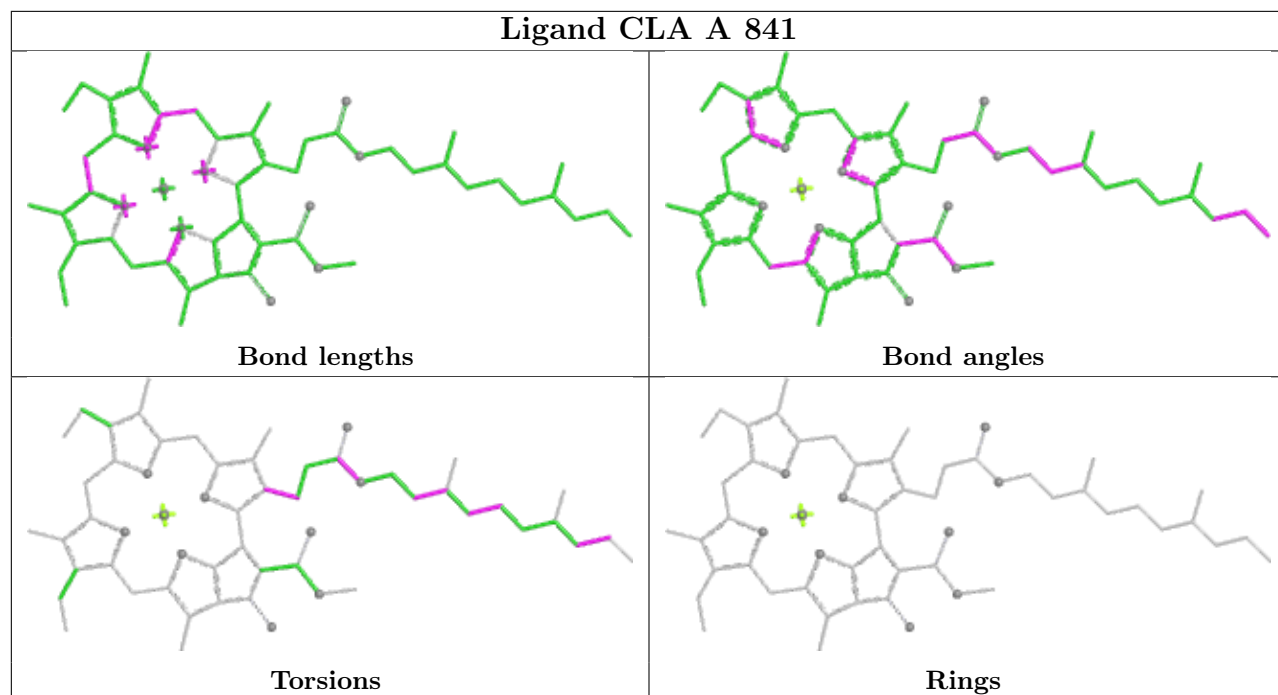
Bond angles



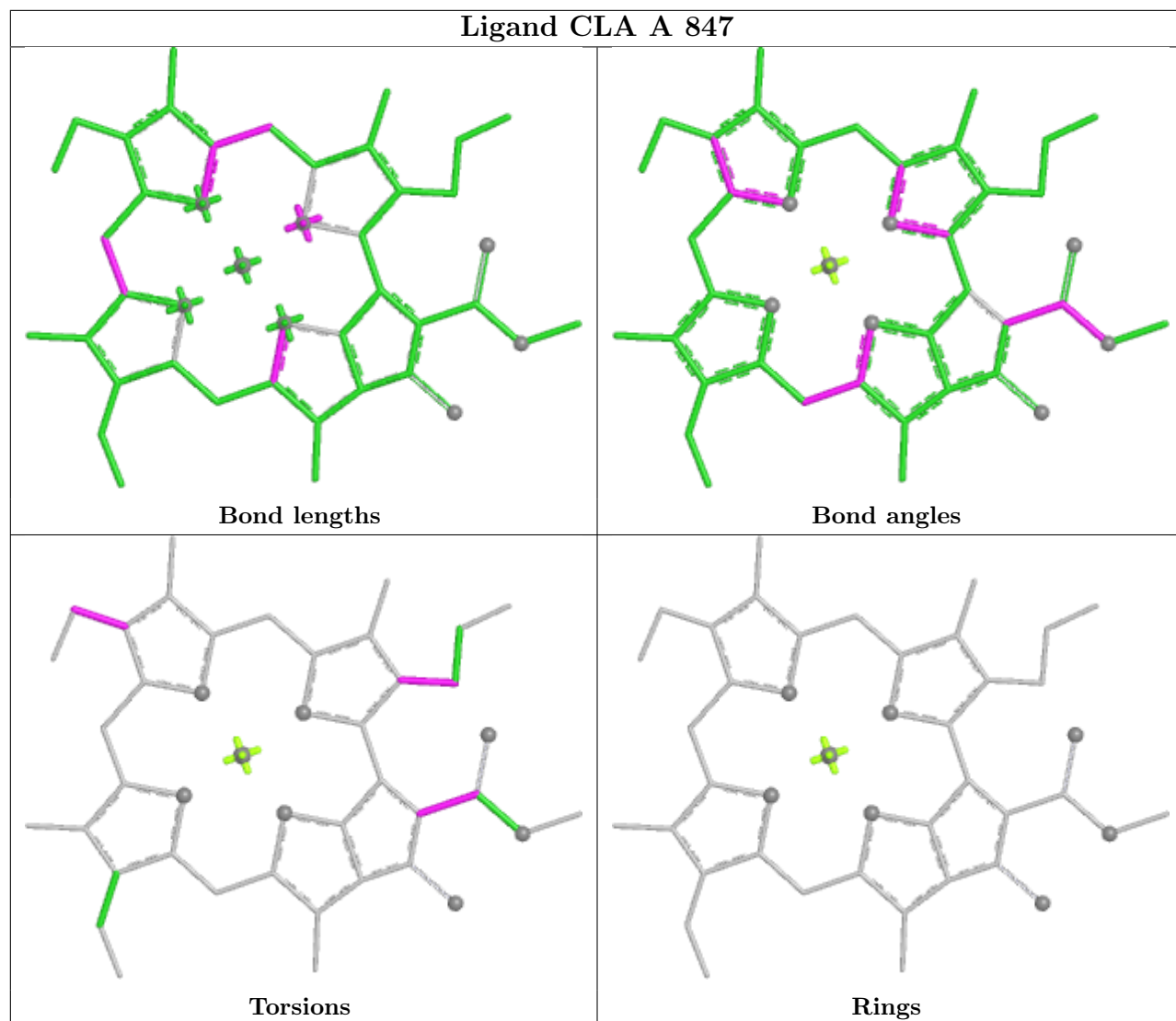
Torsions



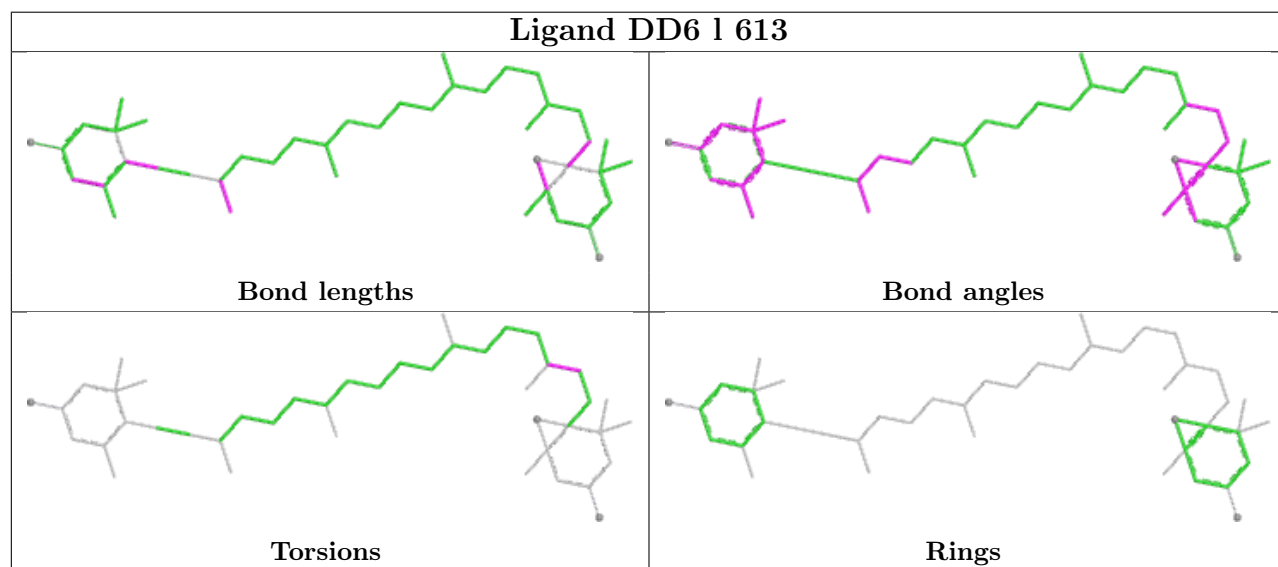
Rings

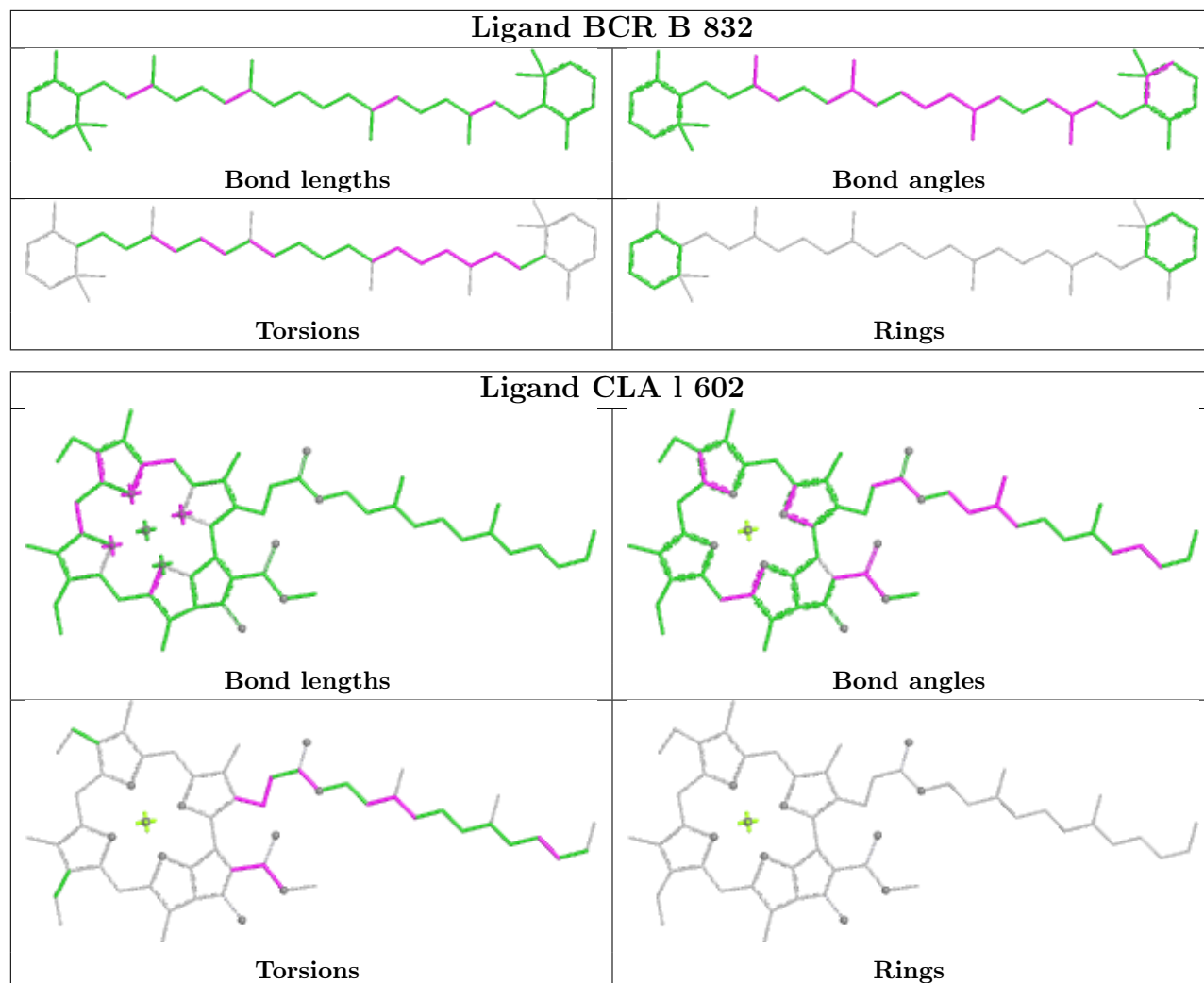


## Ligand CLA A 847

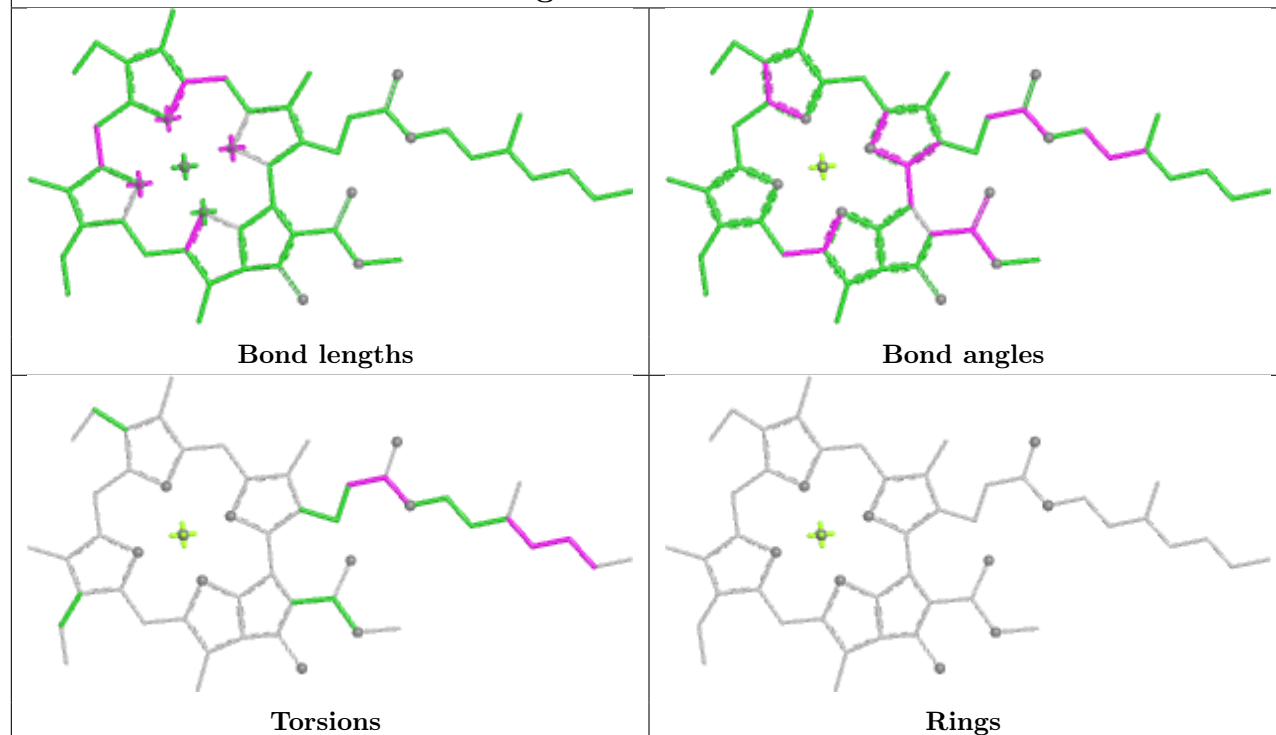


## Ligand DD6 1 613

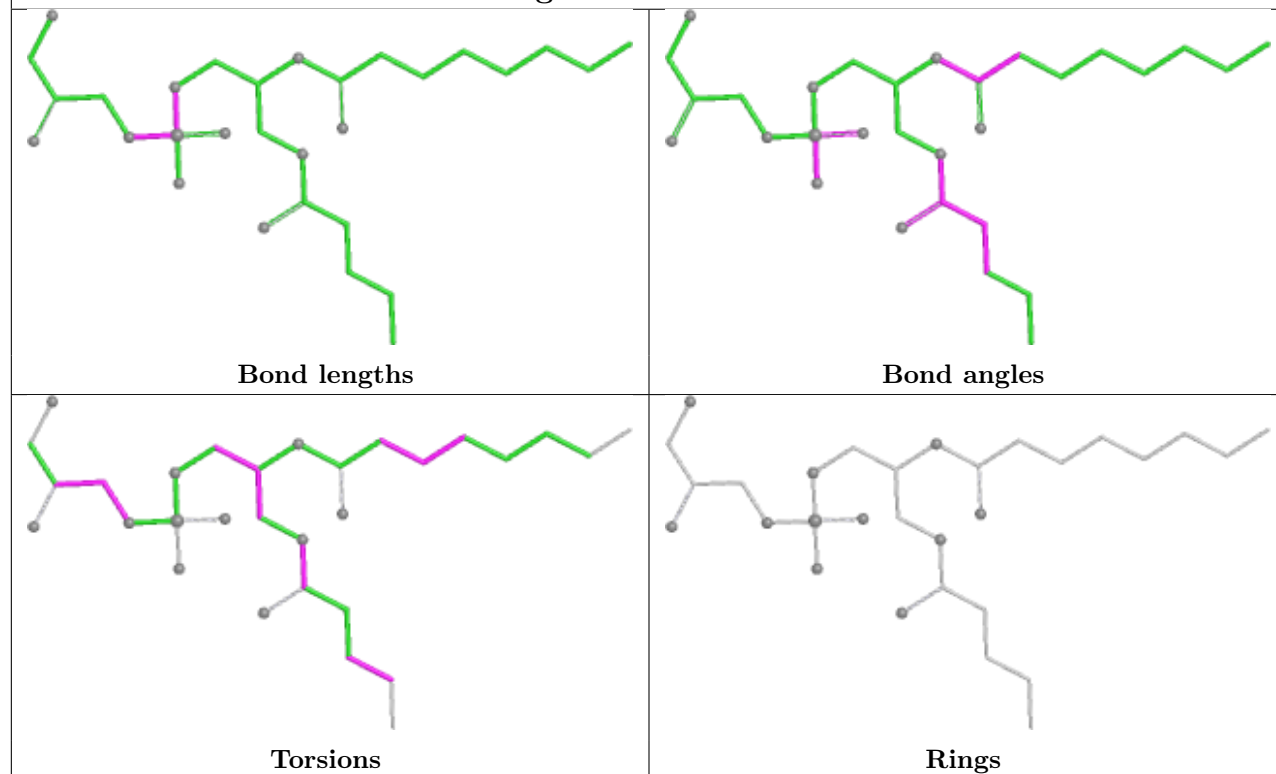


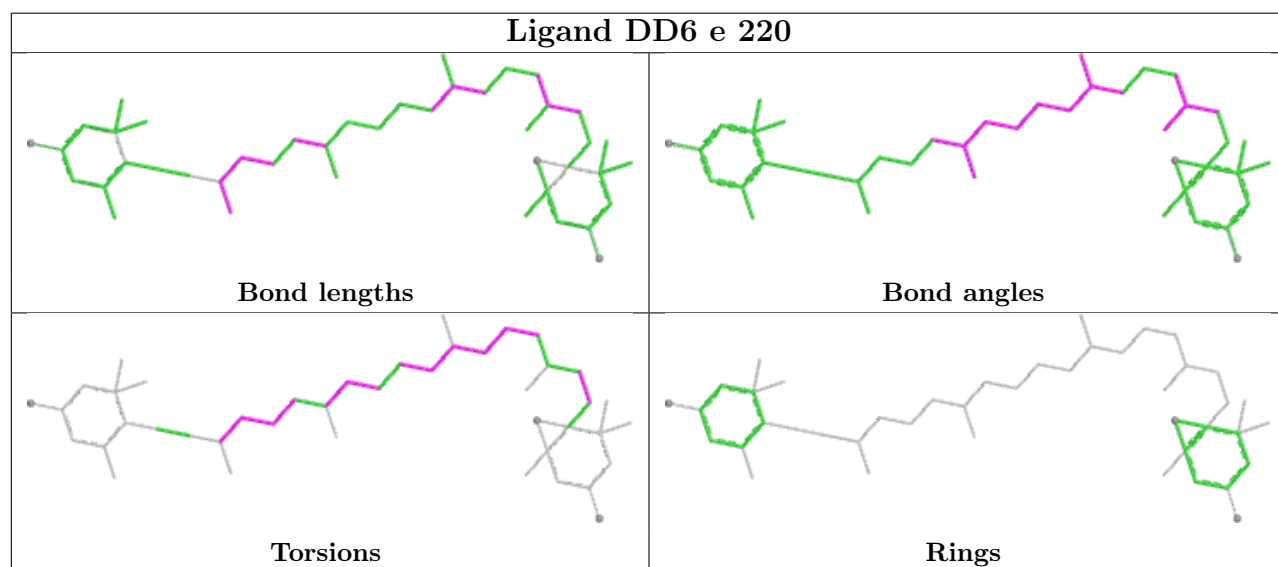
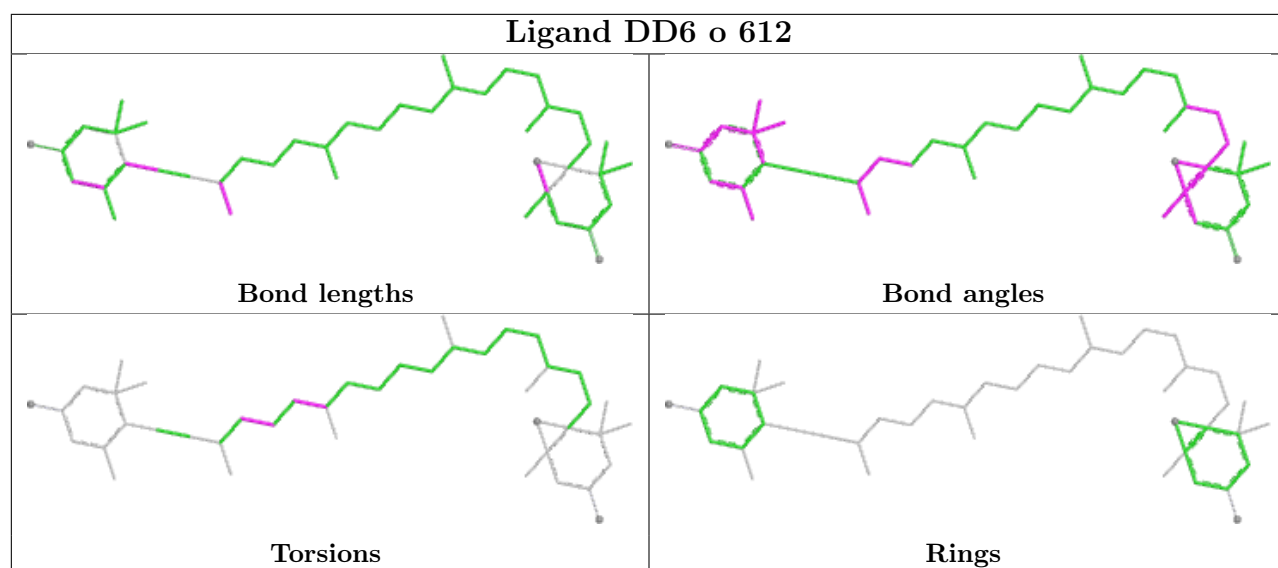


## Ligand CLA a 205

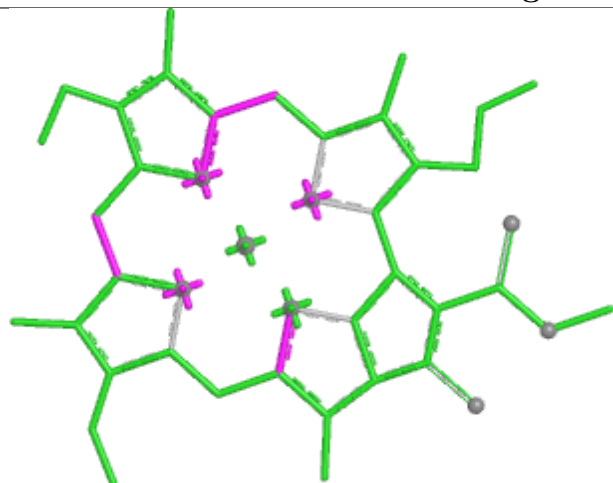


## Ligand LHG c 301

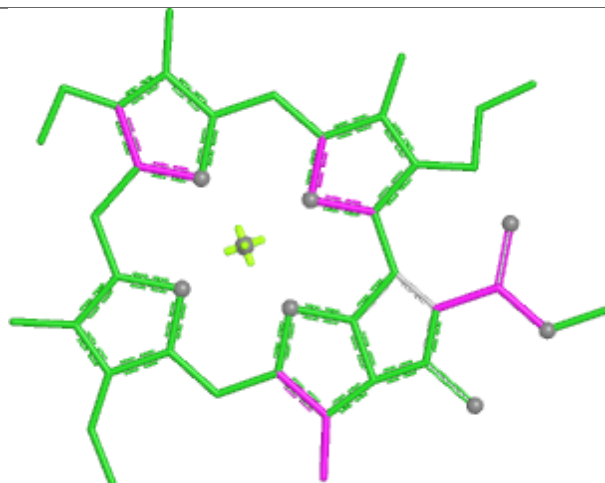




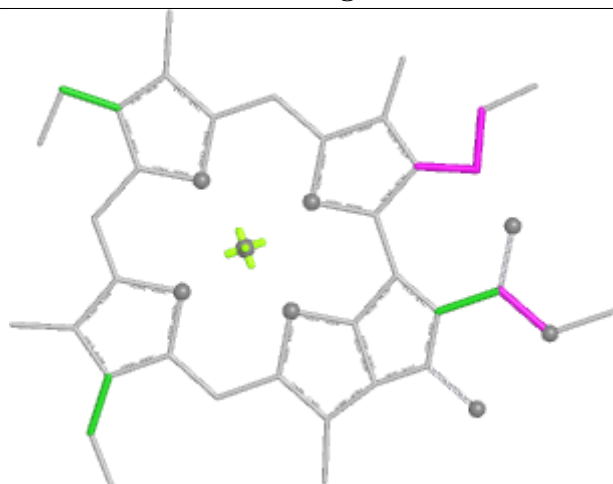
## Ligand CLA i 210



Bond lengths



Bond angles

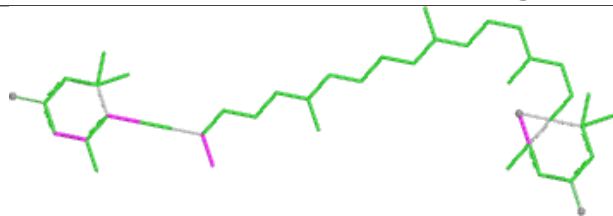


Torsions

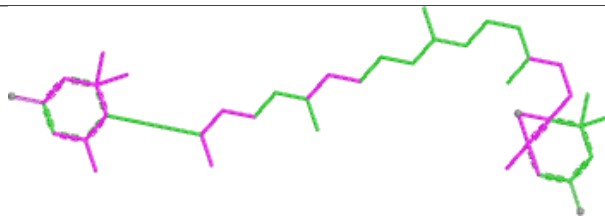


Rings

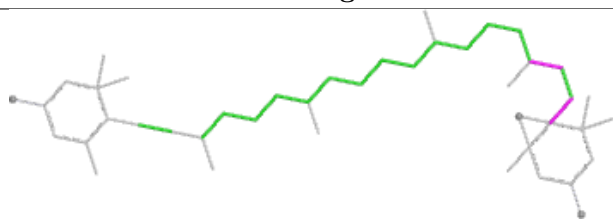
## Ligand DD6 A 854



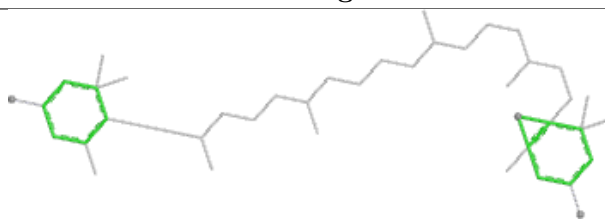
Bond lengths



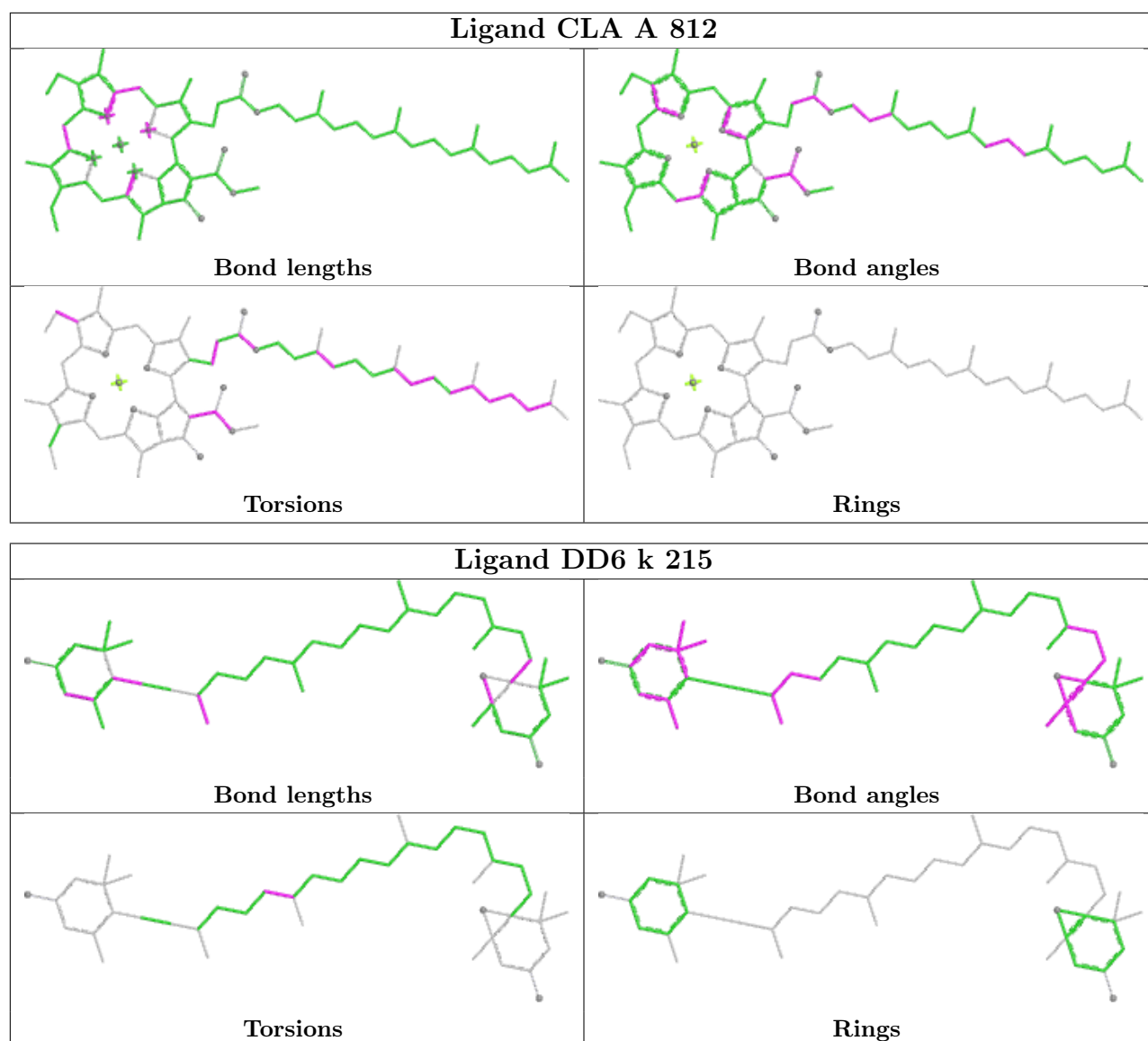
Bond angles



Torsions

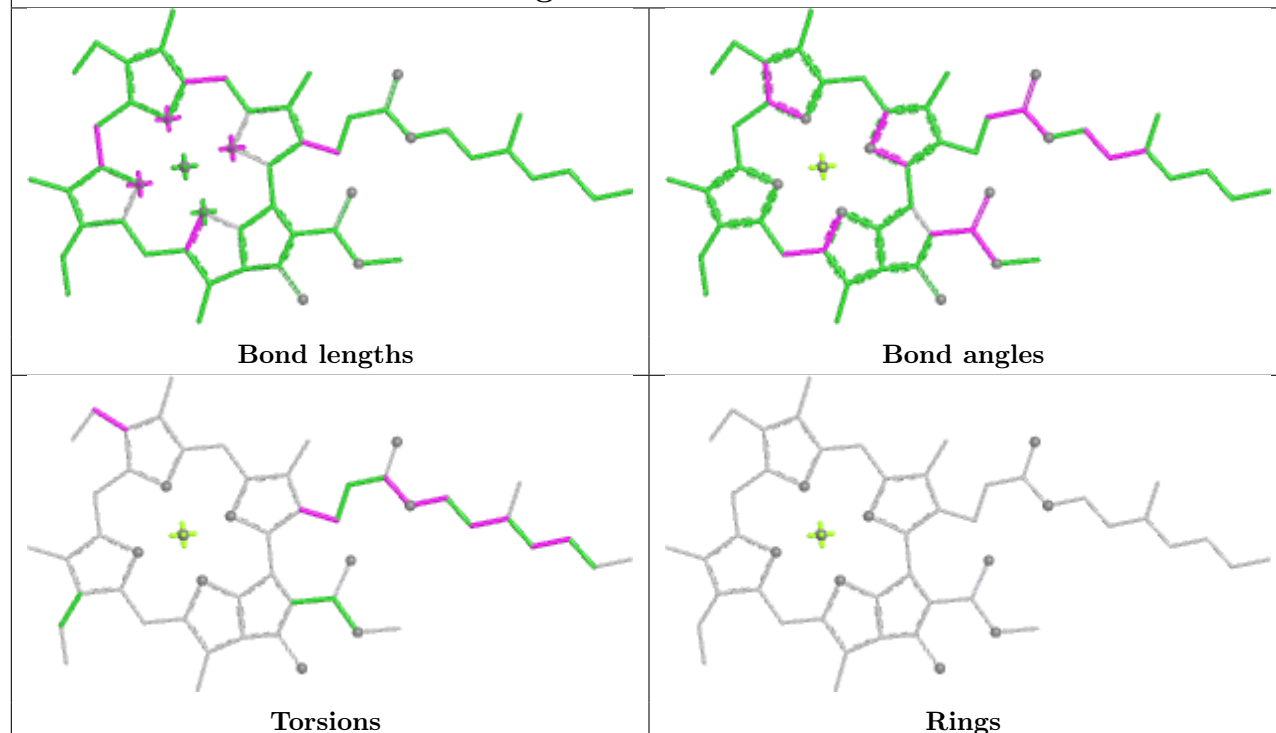


Rings

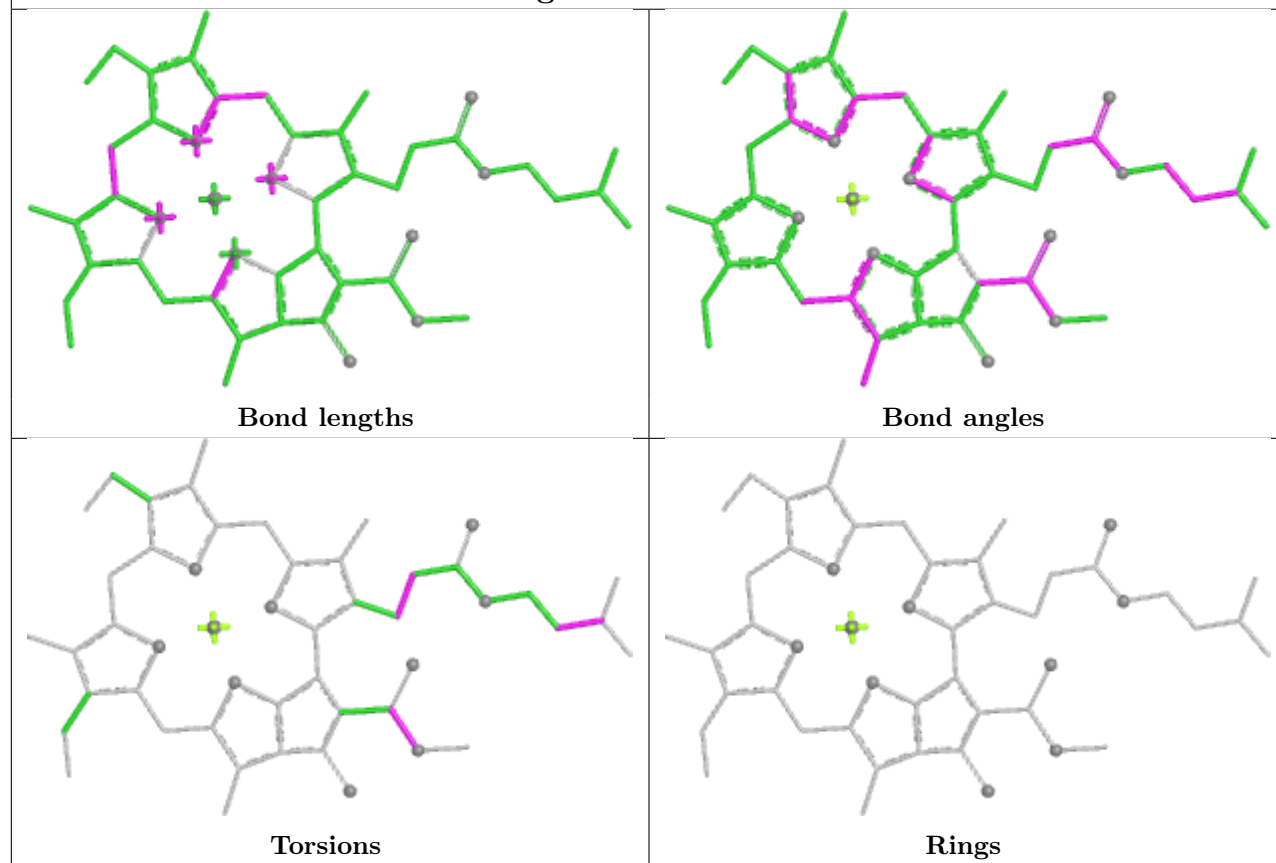




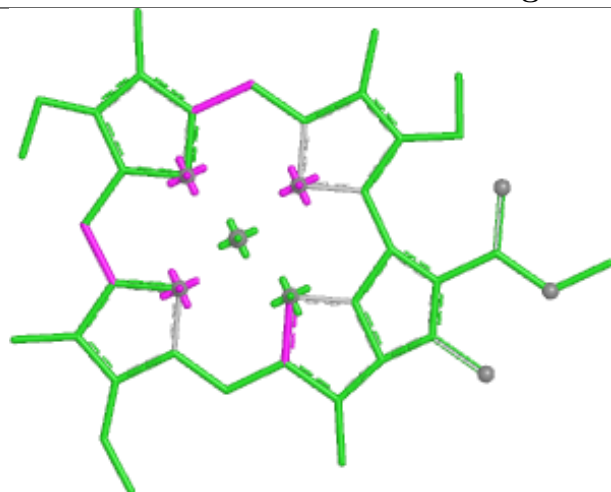
## Ligand CLA k 203



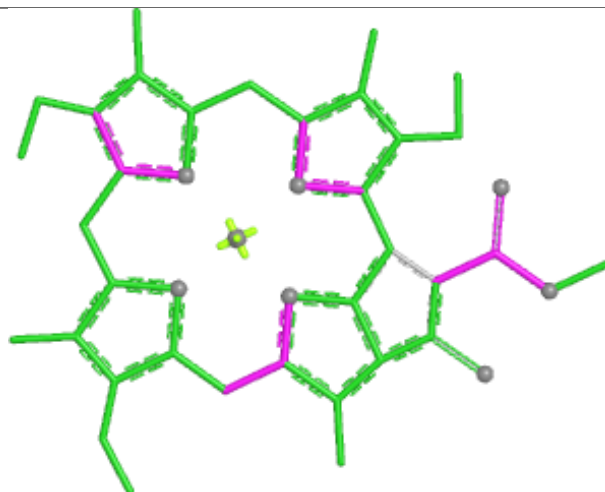
## Ligand CLA e 207



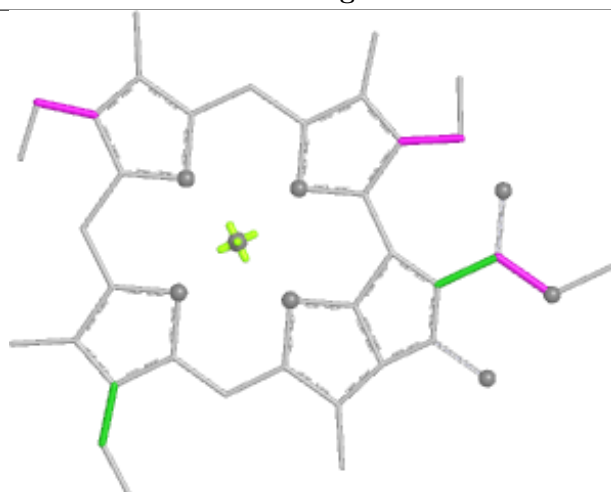
## Ligand CLA f 601



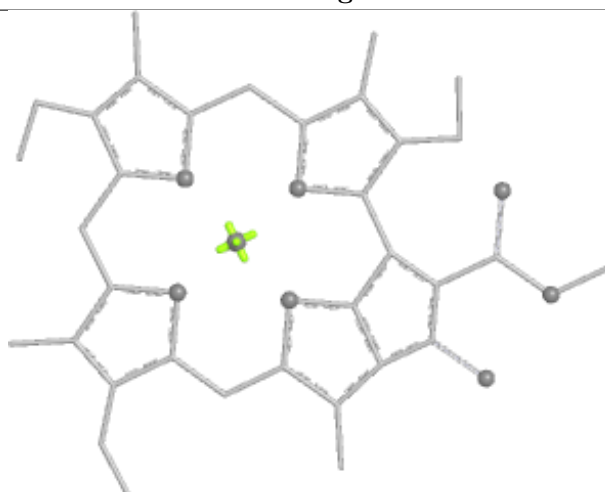
Bond lengths



Bond angles

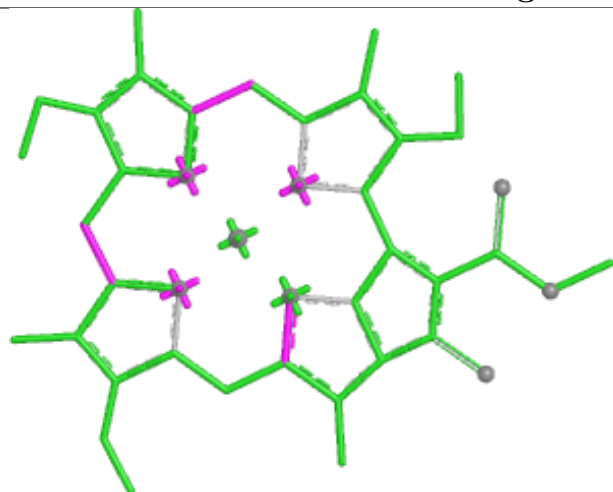


Torsions

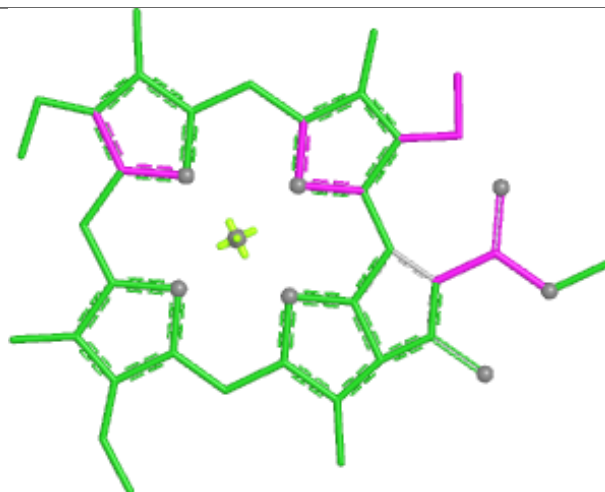


Rings

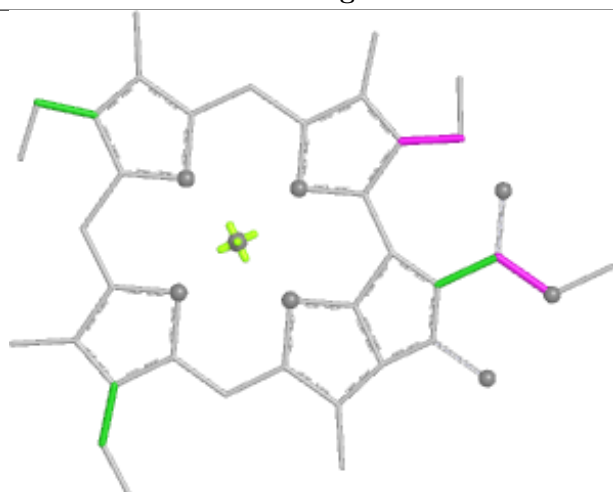
## Ligand CLA n 204



Bond lengths



Bond angles

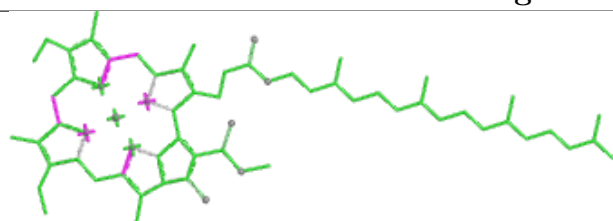


Torsions

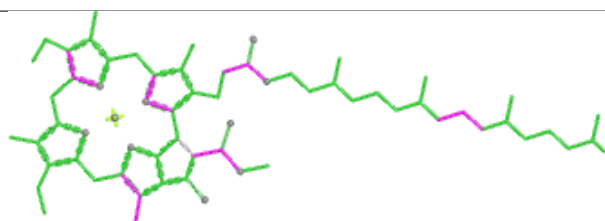


Rings

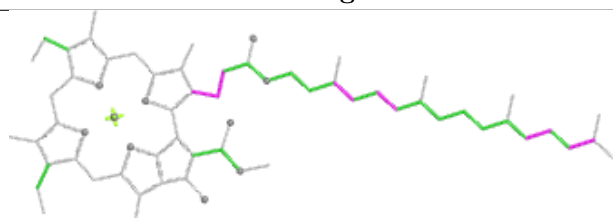
## Ligand CLA B 845



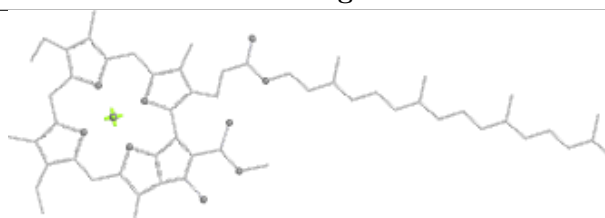
Bond lengths



Bond angles

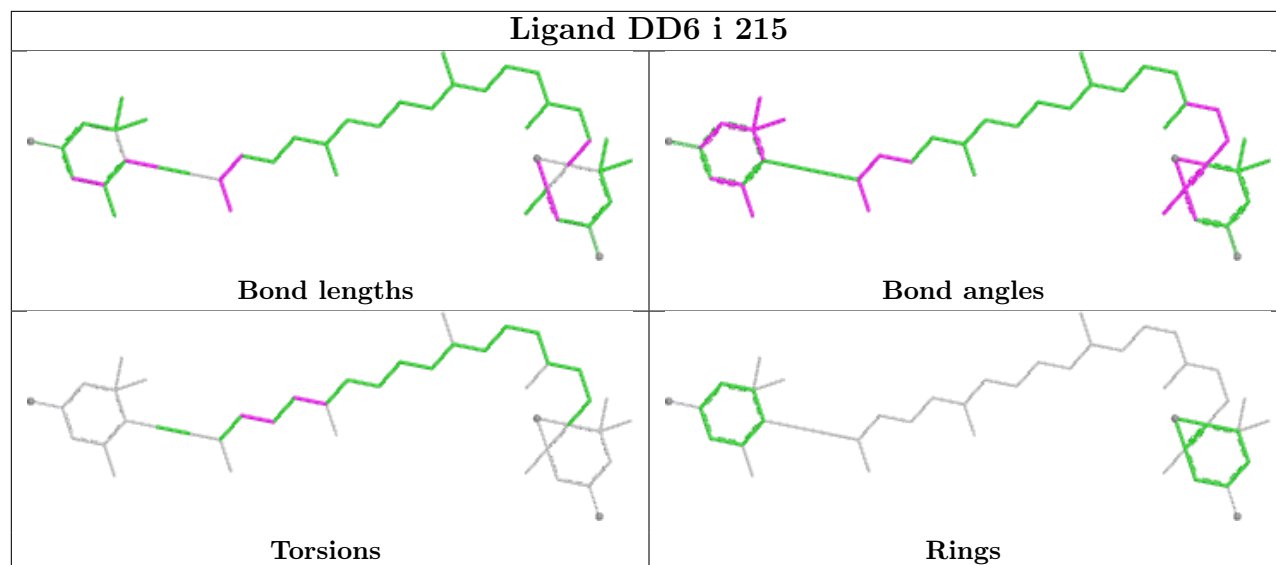


Torsions

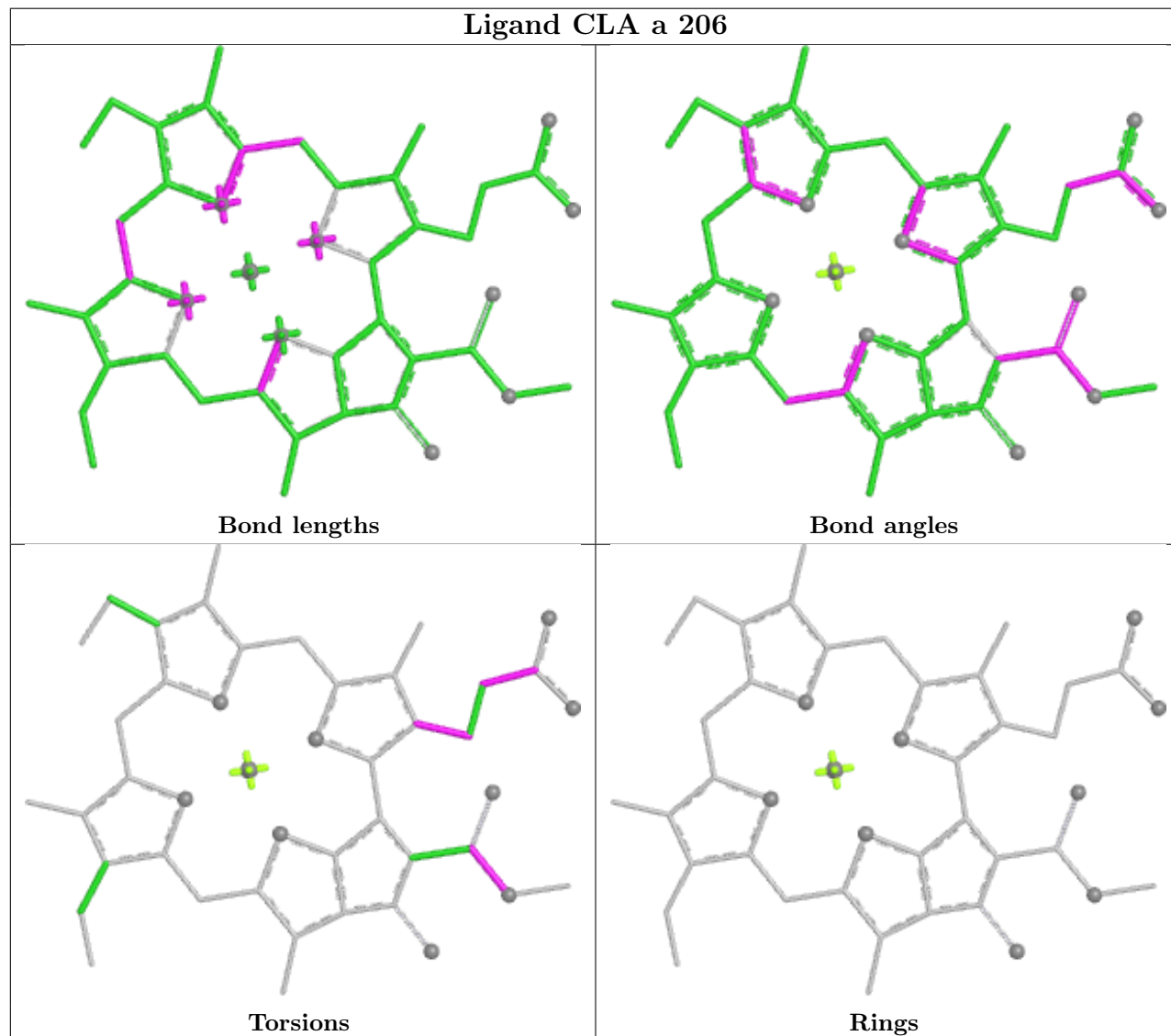


Rings

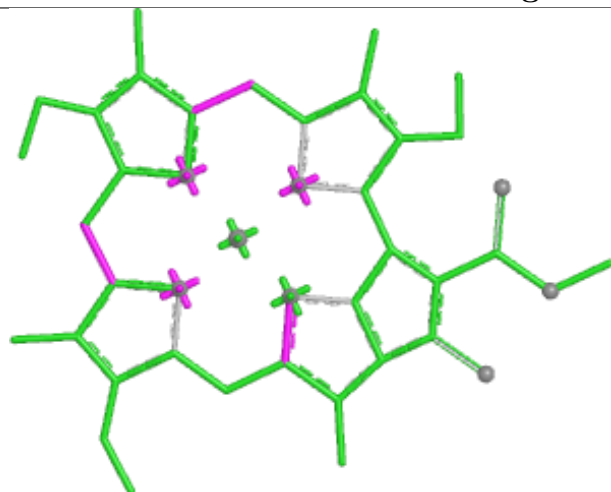
## Ligand DD6 i 215



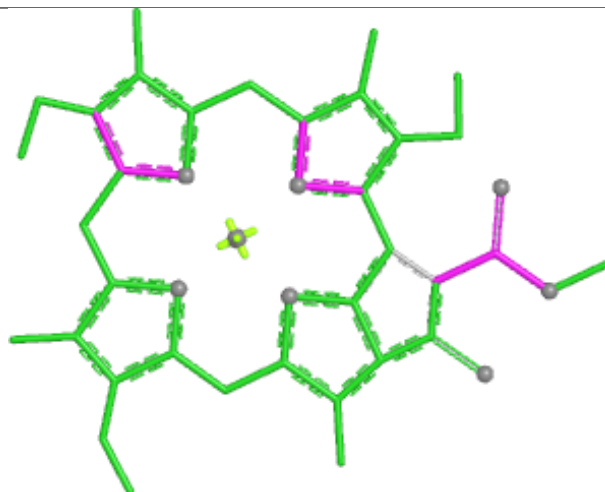
## Ligand CLA a 206



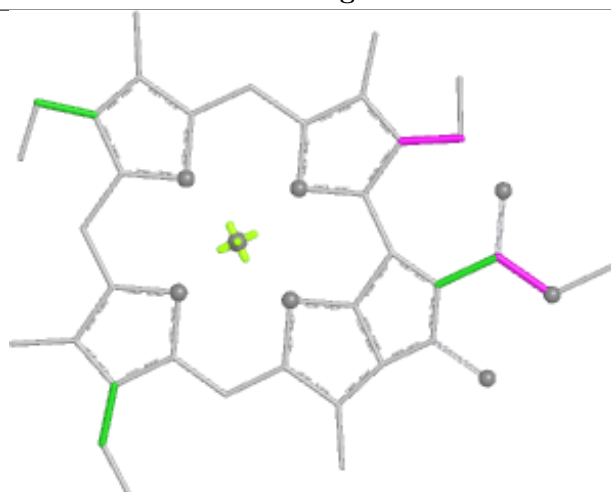
## Ligand CLA f 609



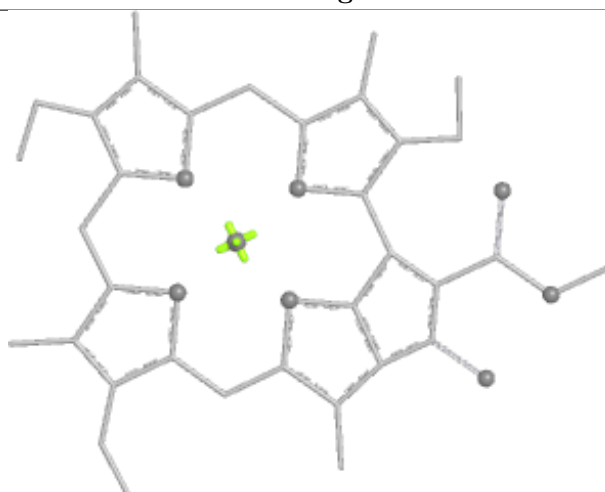
Bond lengths



Bond angles

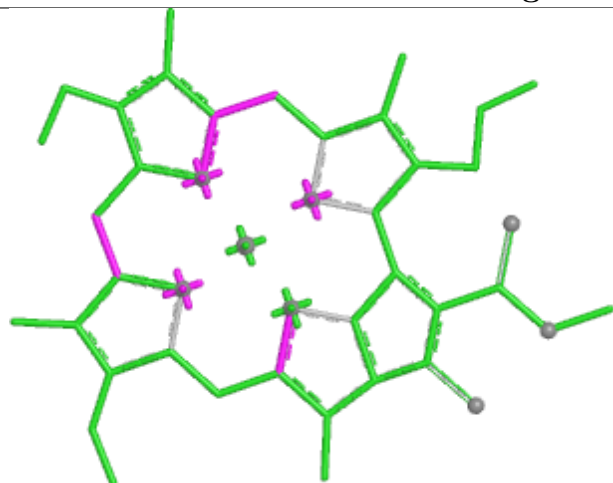


Torsions

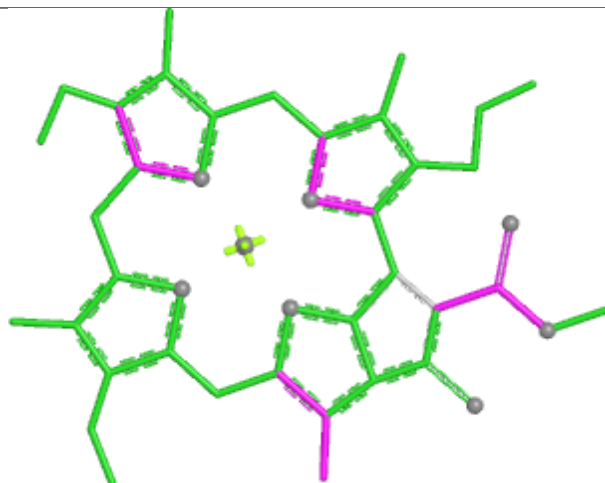


Rings

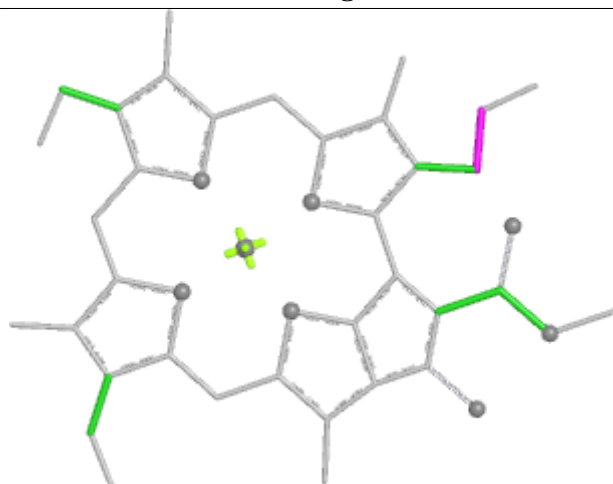
## Ligand CLA 1 603



Bond lengths



Bond angles

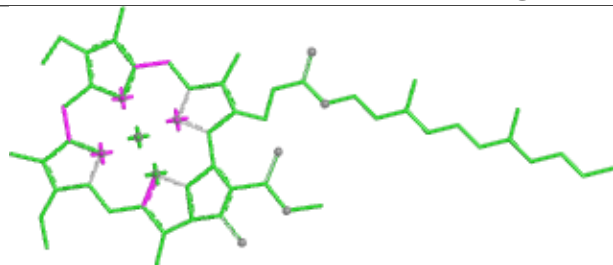


Torsions

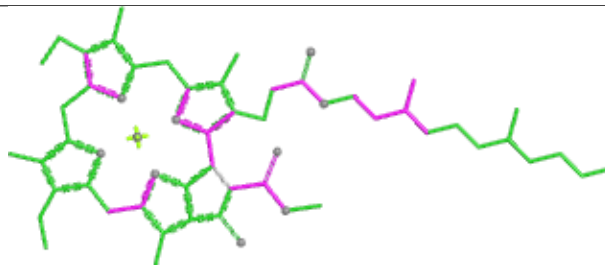


Rings

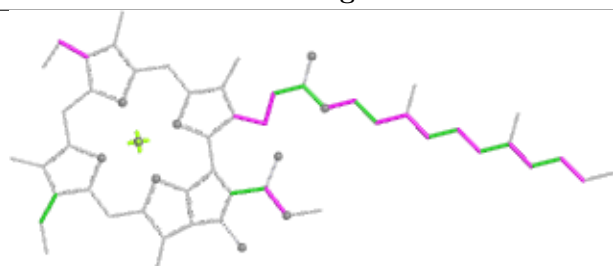
## Ligand CLA A 824



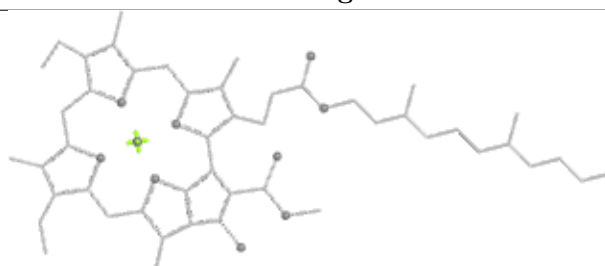
Bond lengths



Bond angles

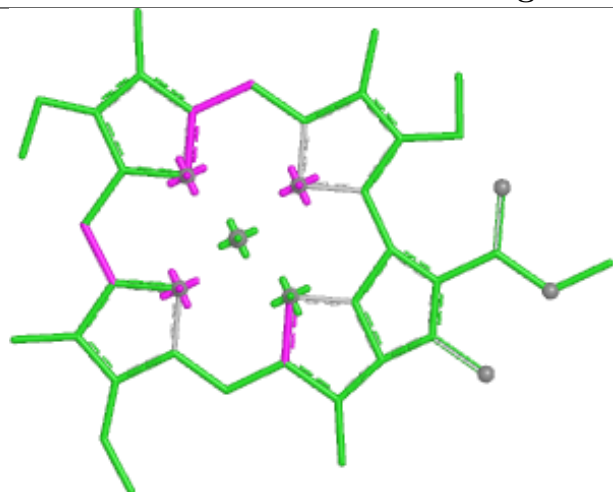


Torsions

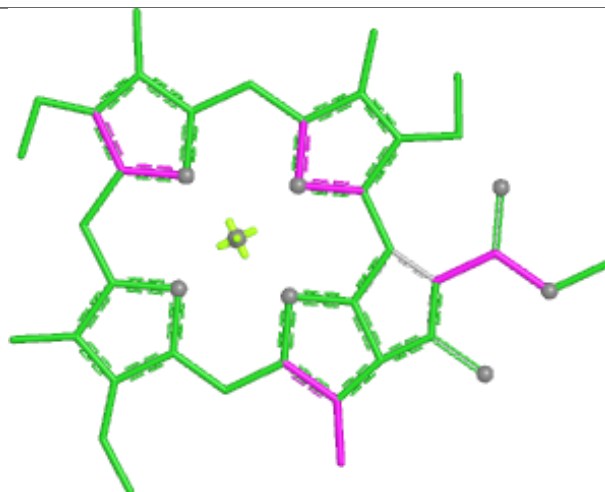


Rings

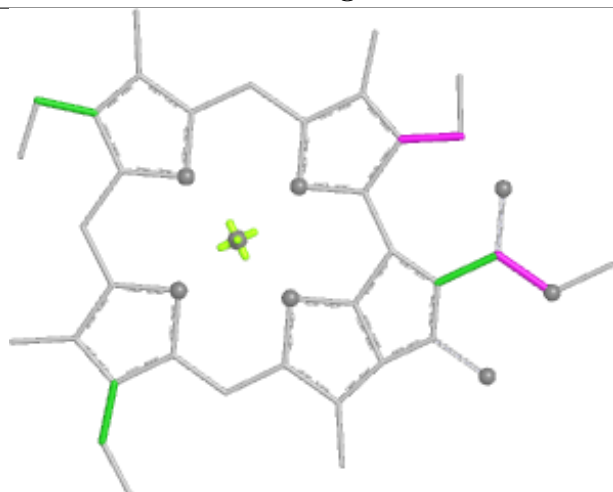
## Ligand CLA d 305



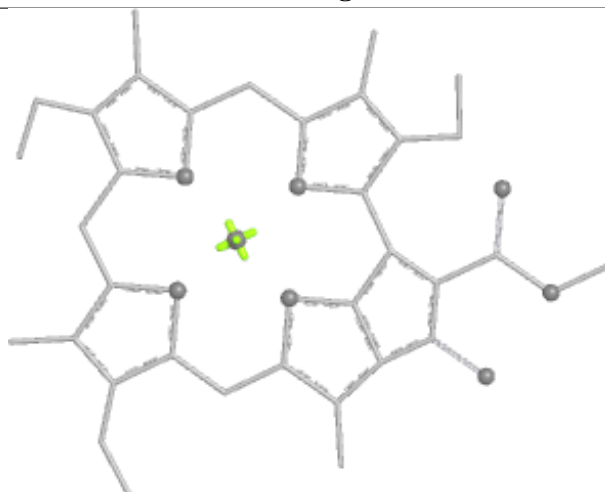
Bond lengths



Bond angles

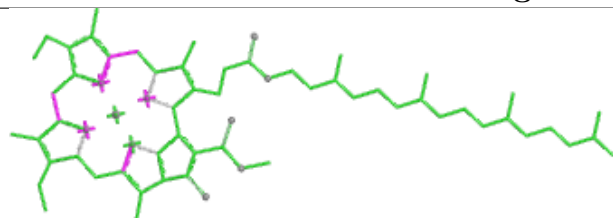


Torsions

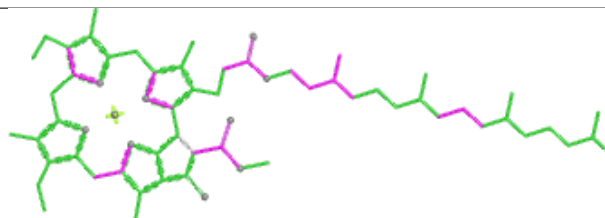


Rings

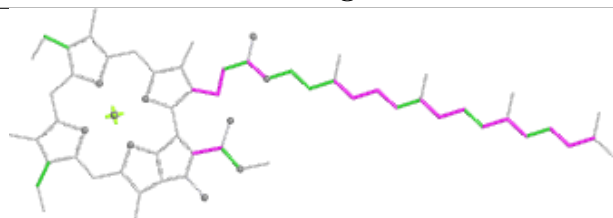
## Ligand CLA A 846



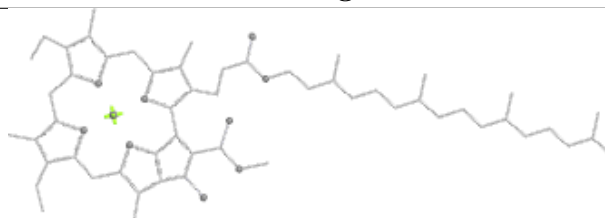
Bond lengths



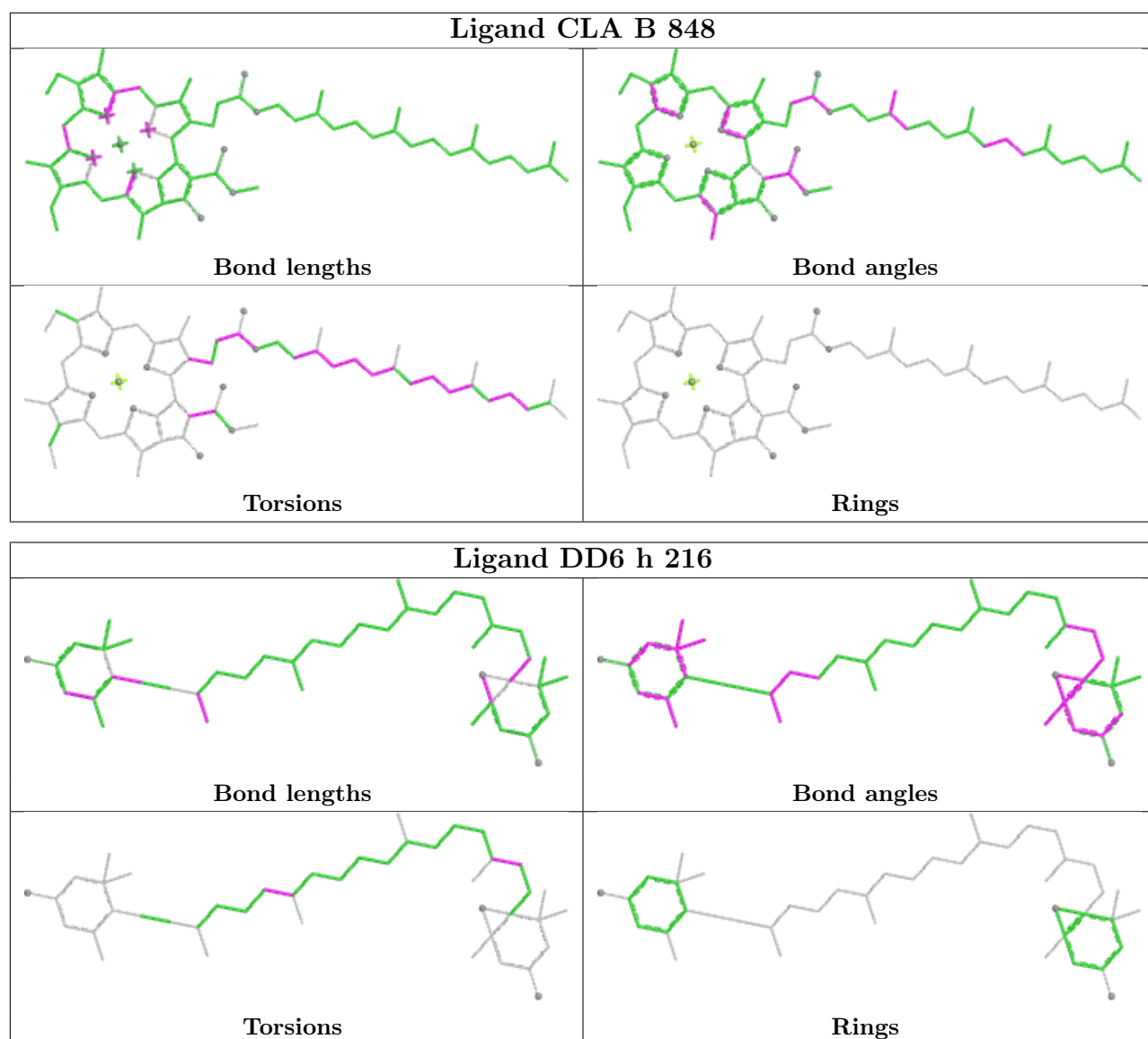
Bond angles



Torsions

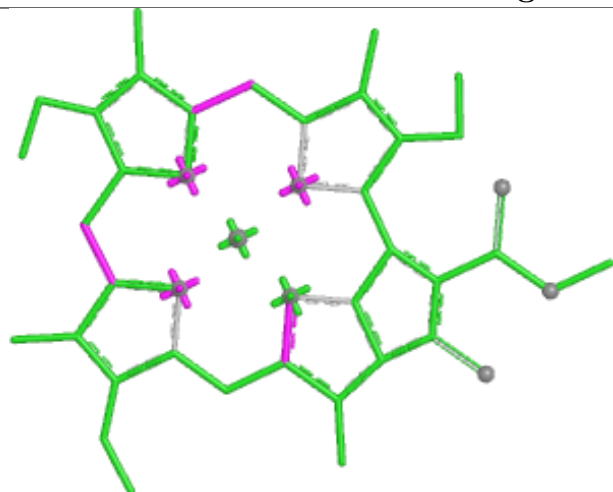


Rings

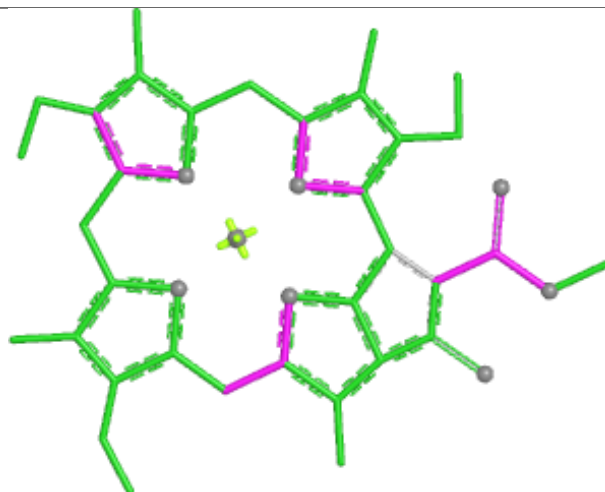




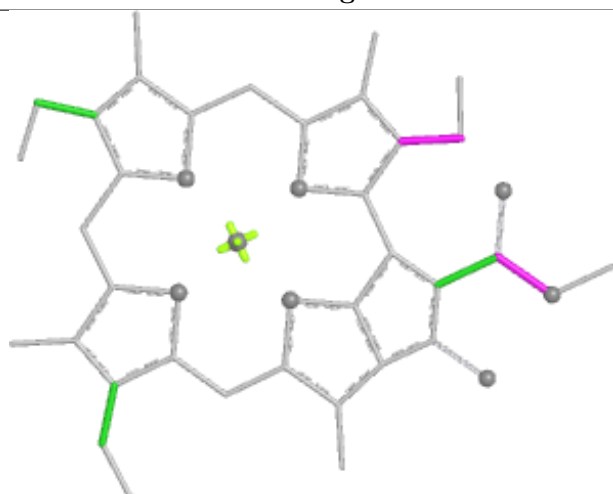
## Ligand CLA k 212



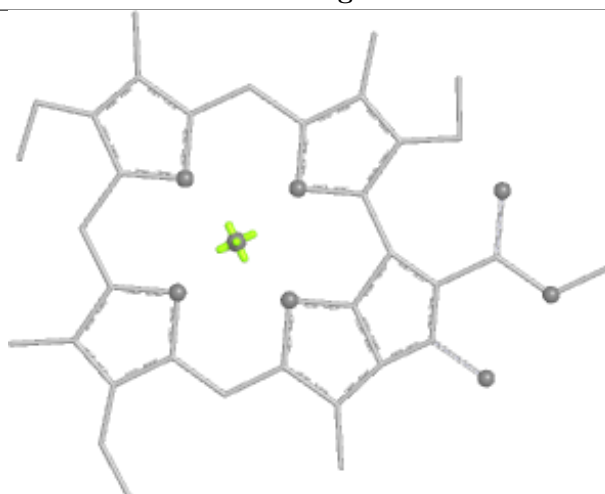
Bond lengths



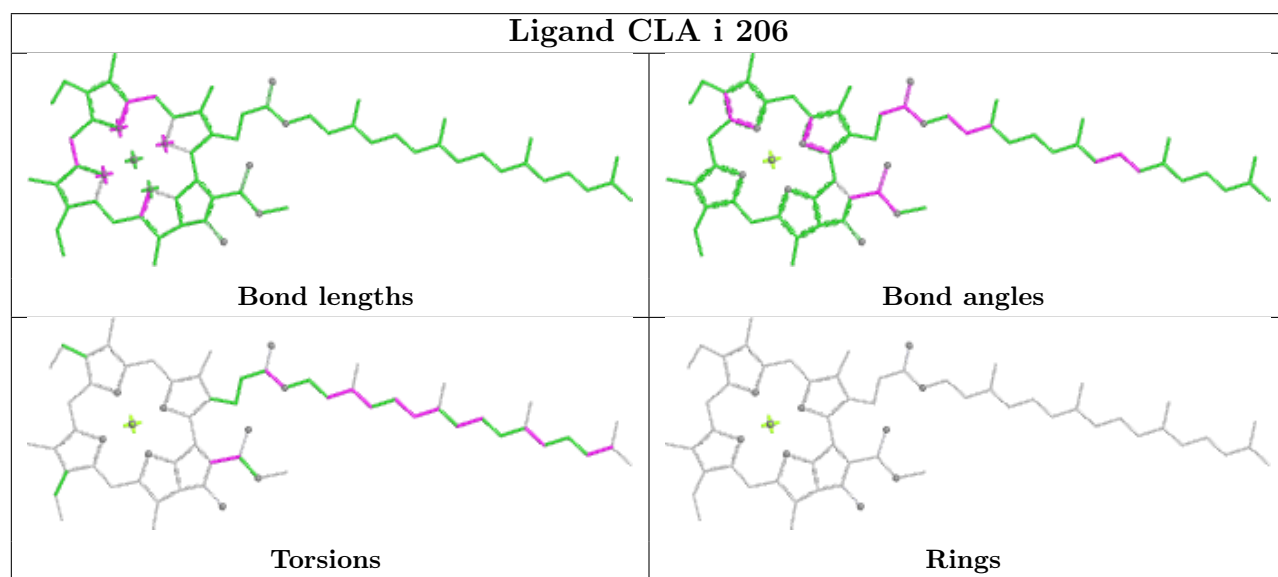
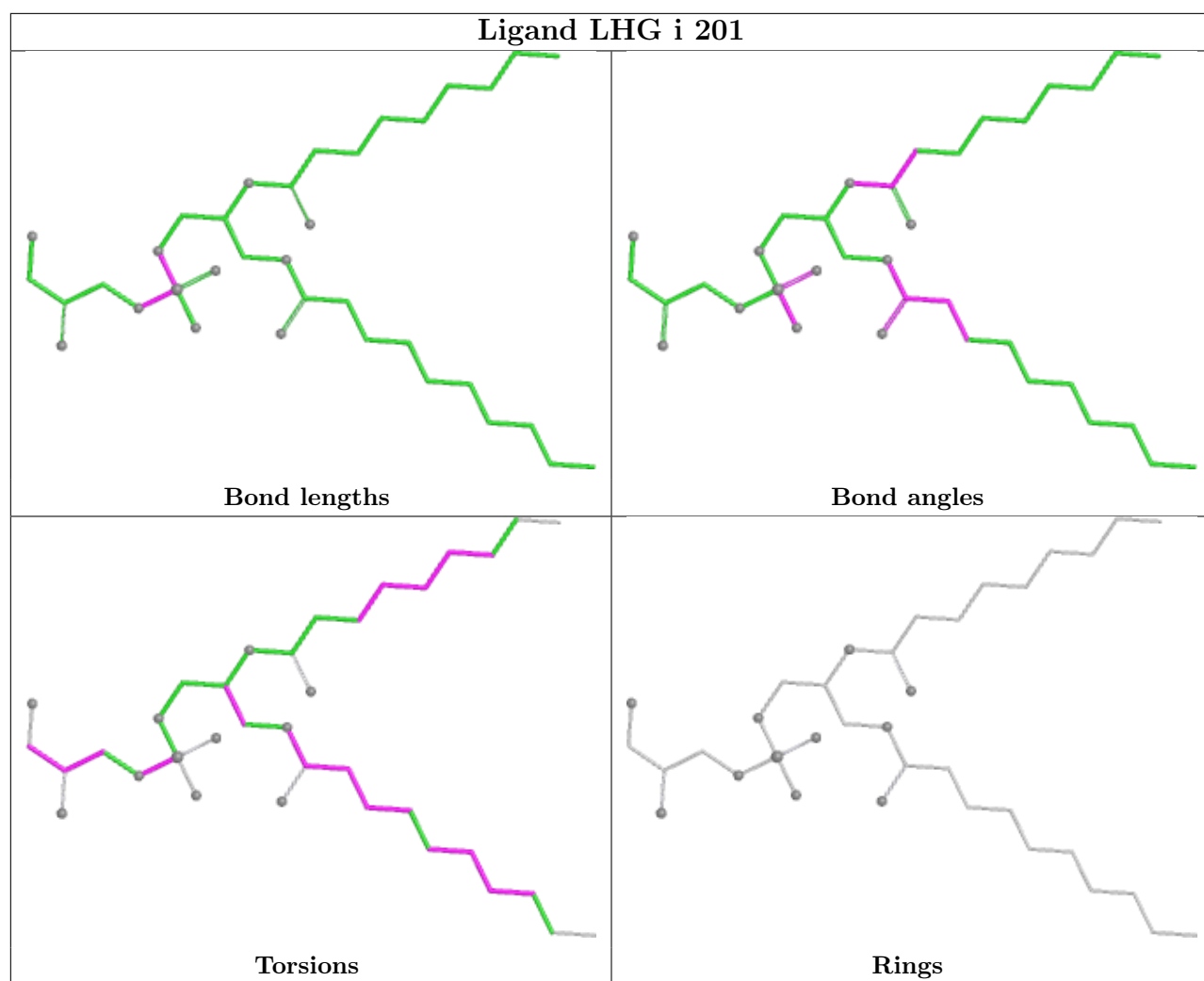
Bond angles



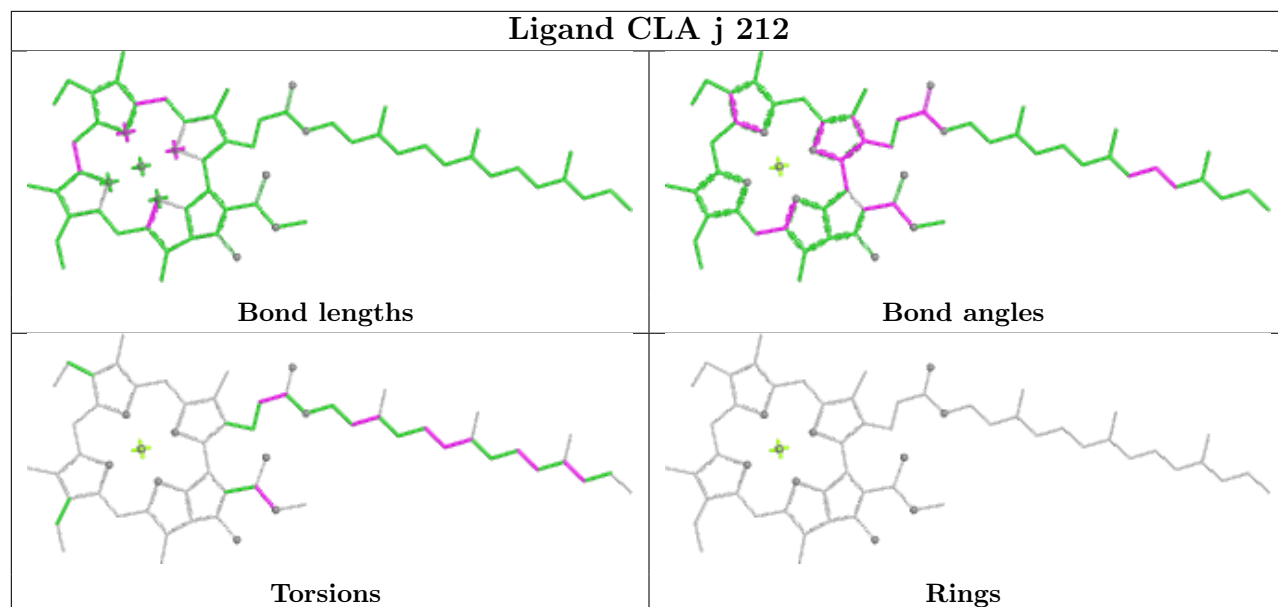
Torsions



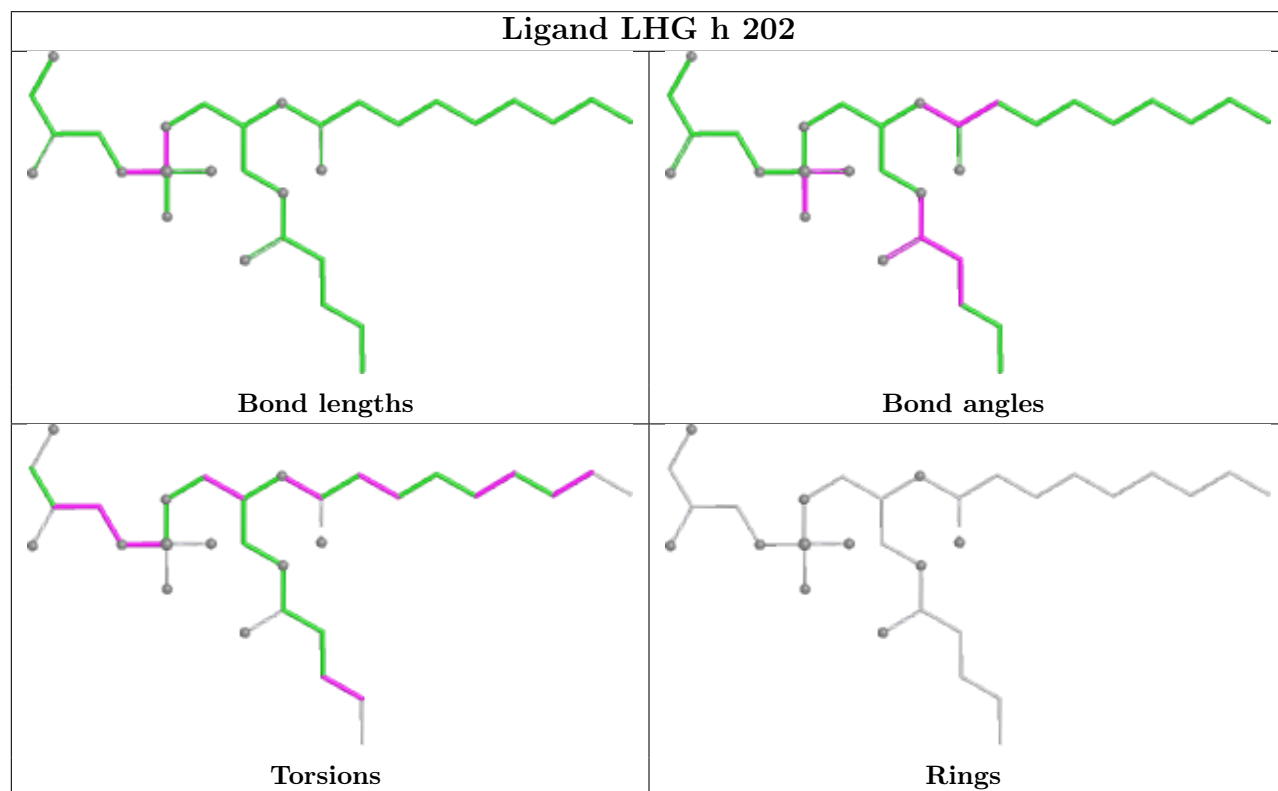
Rings

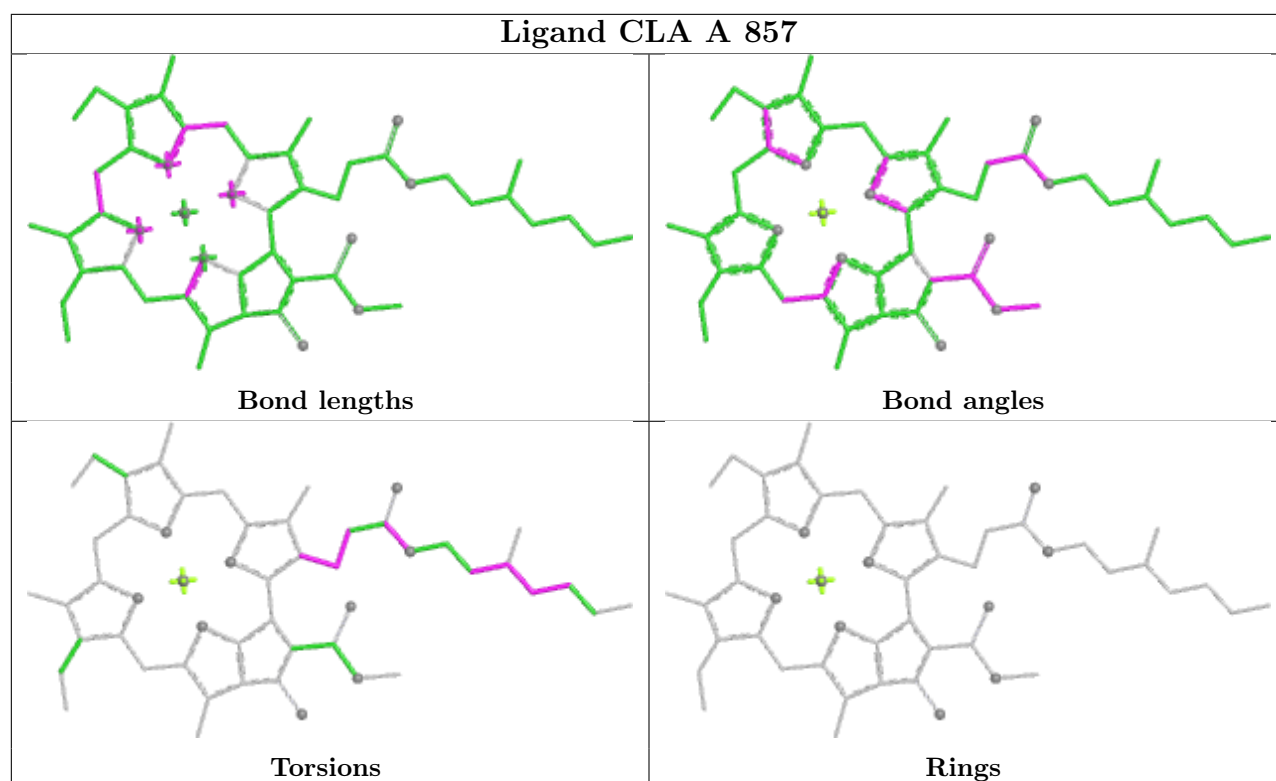


## Ligand CLA j 212

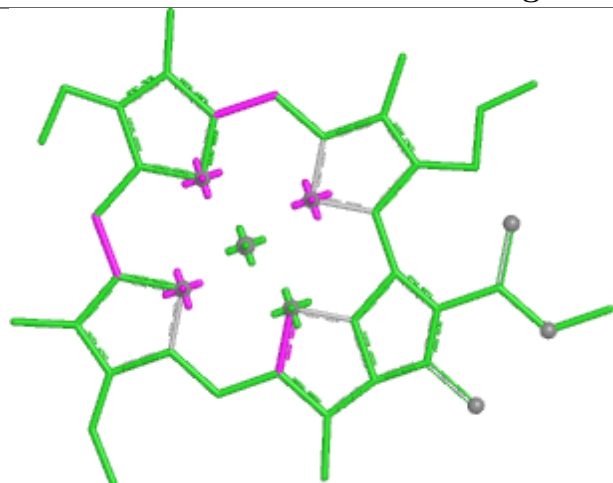


## Ligand LHG h 202

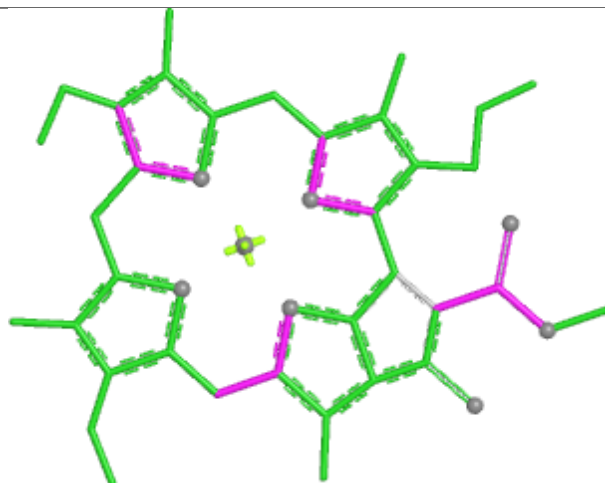




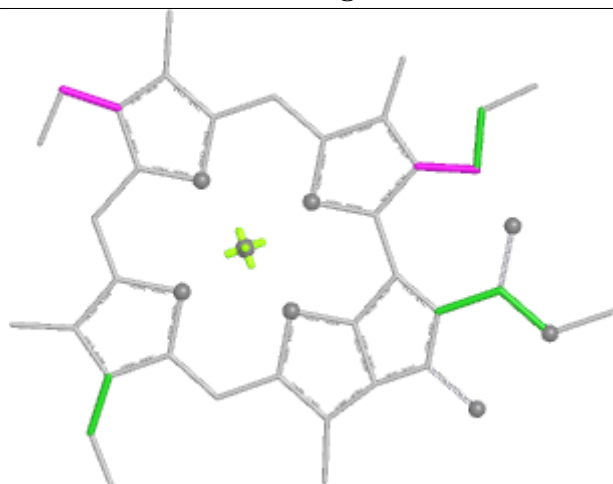
## Ligand CLA i 207



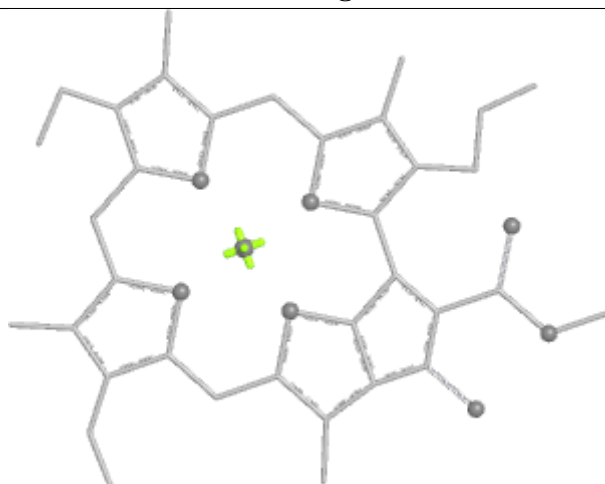
Bond lengths



Bond angles

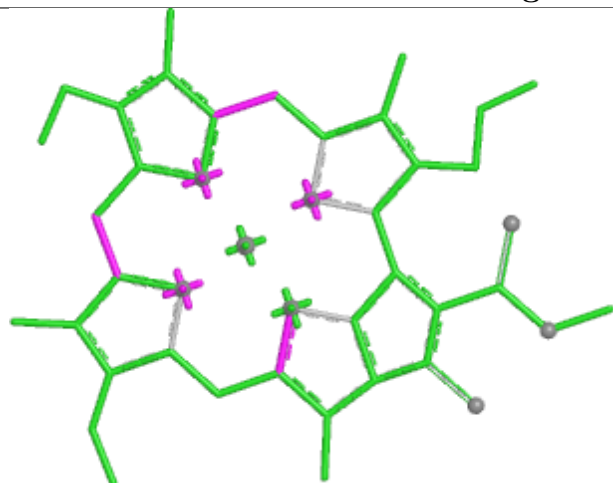


Torsions

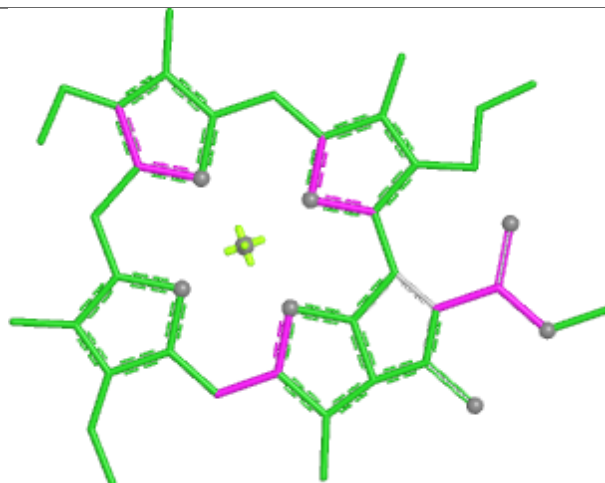


Rings

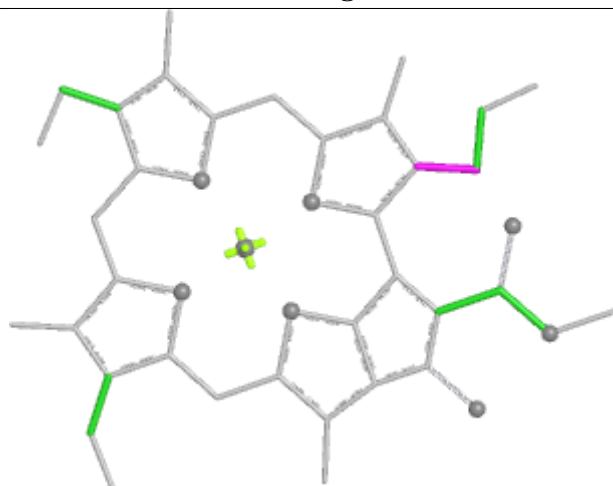
## Ligand CLA 1 604



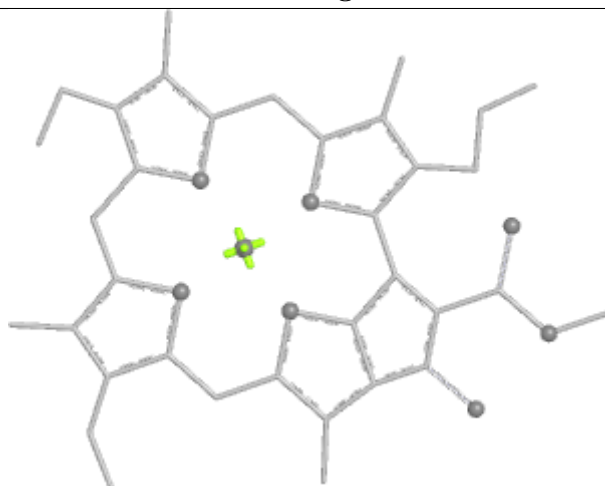
Bond lengths



Bond angles

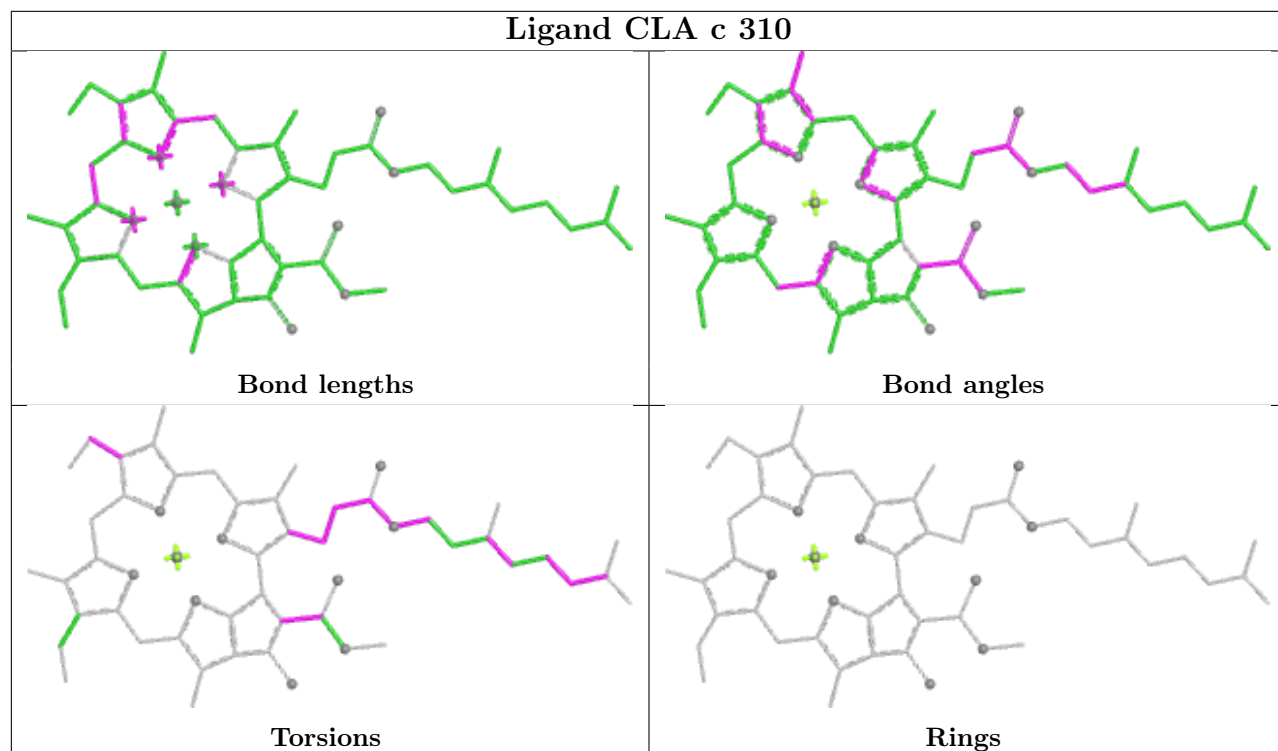


Torsions

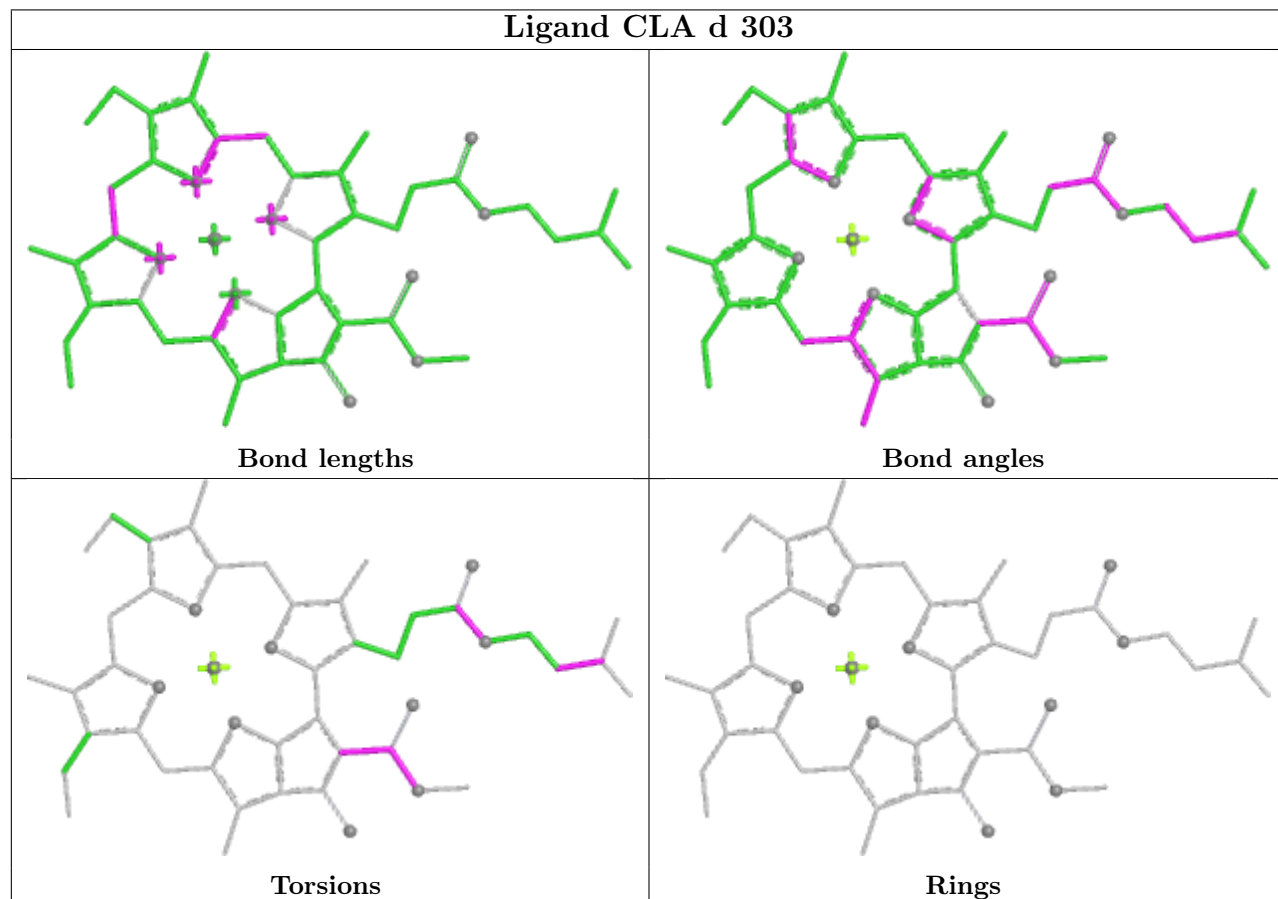


Rings

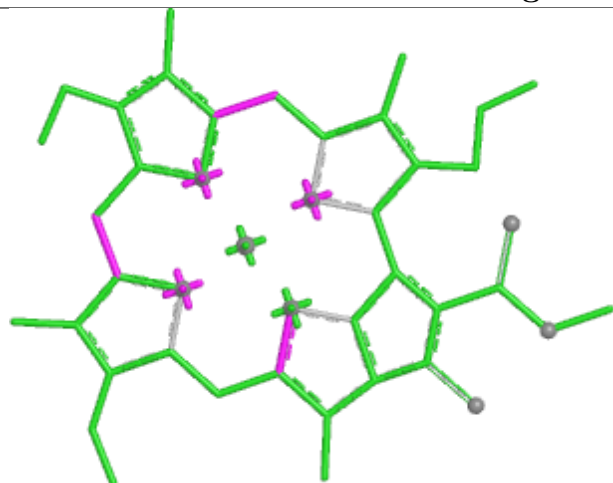
## Ligand CLA c 310



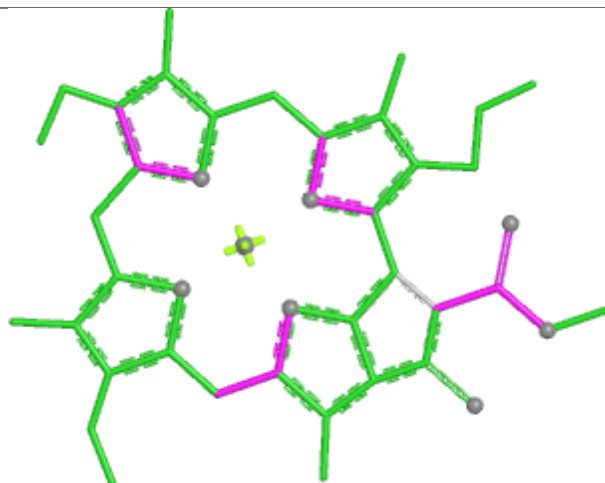
## Ligand CLA d 303



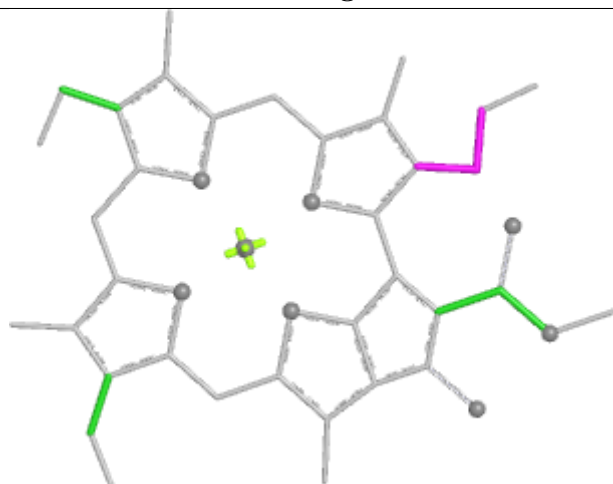
## Ligand CLA 1 608



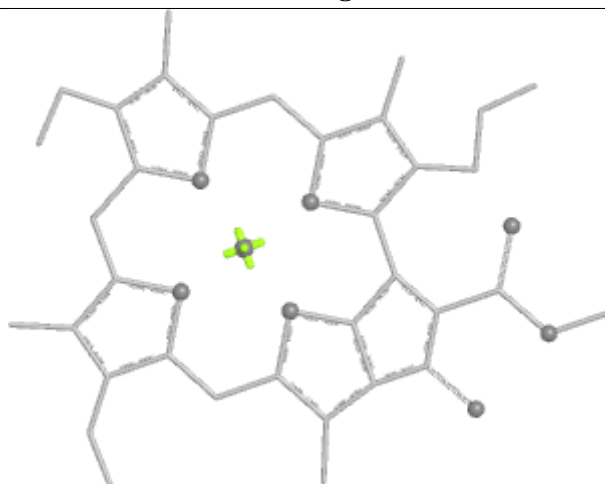
Bond lengths



Bond angles

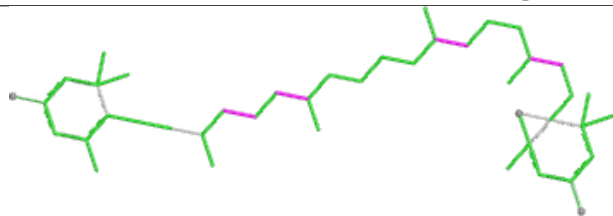


Torsions

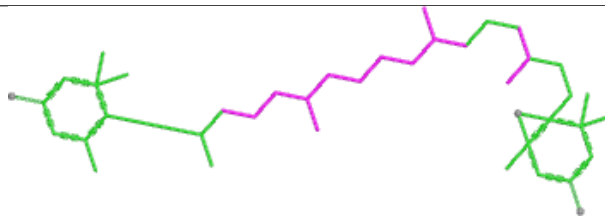


Rings

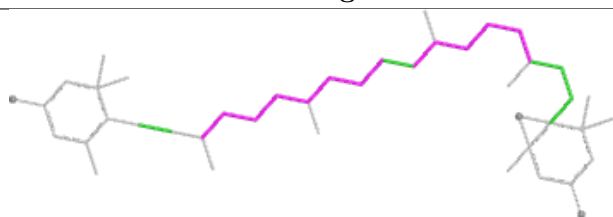
## Ligand DD6 F 203



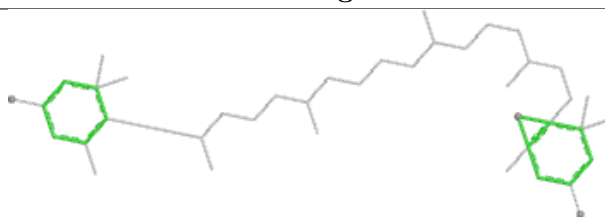
Bond lengths



Bond angles



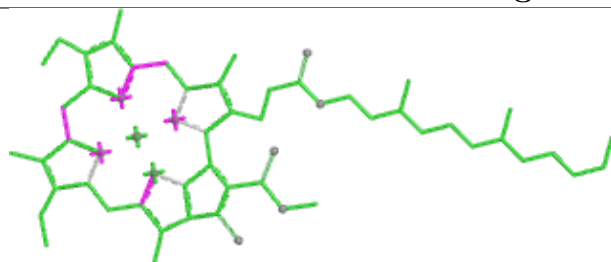
Torsions



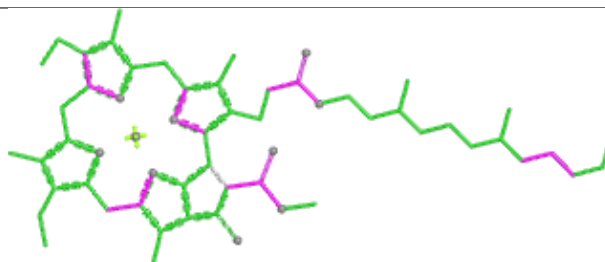
Rings



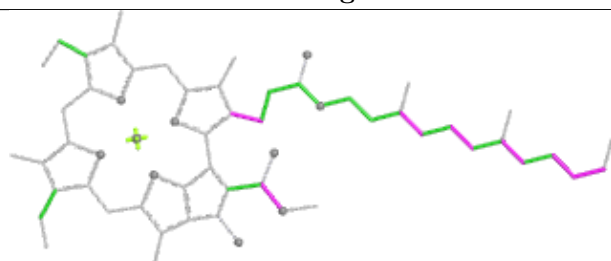
## Ligand CLA B 814



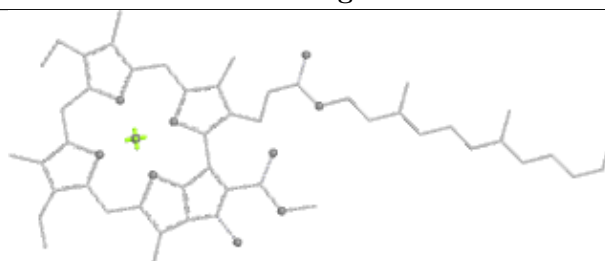
Bond lengths



Bond angles

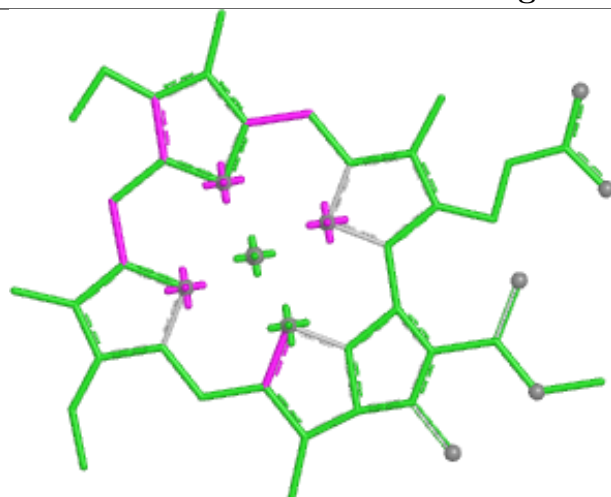


Torsions

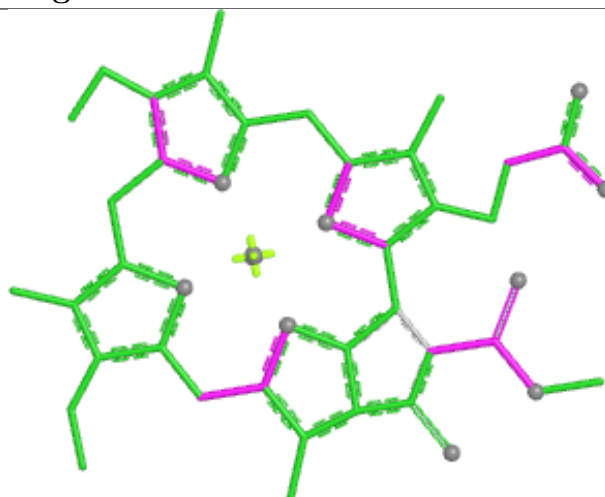


Rings

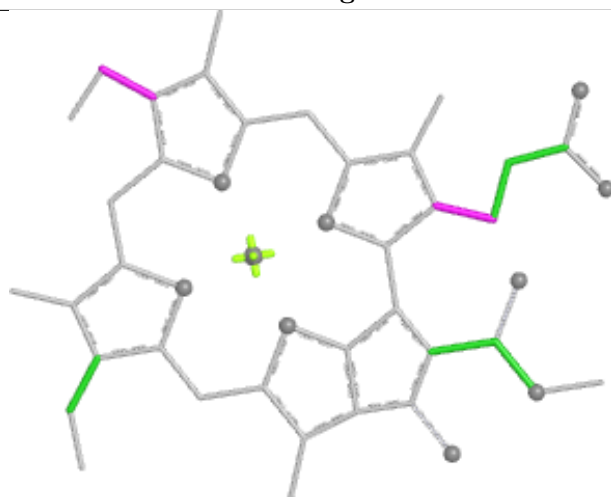
## Ligand CLA g 215



Bond lengths



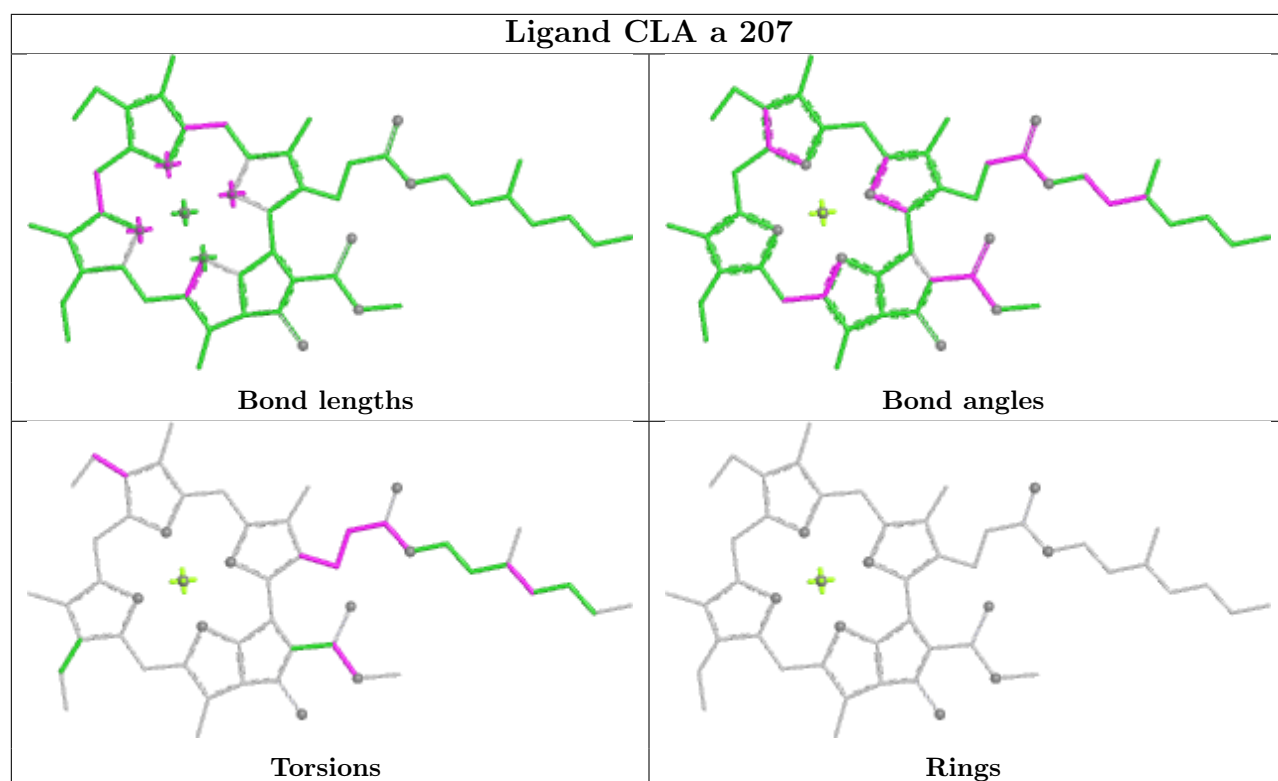
Bond angles



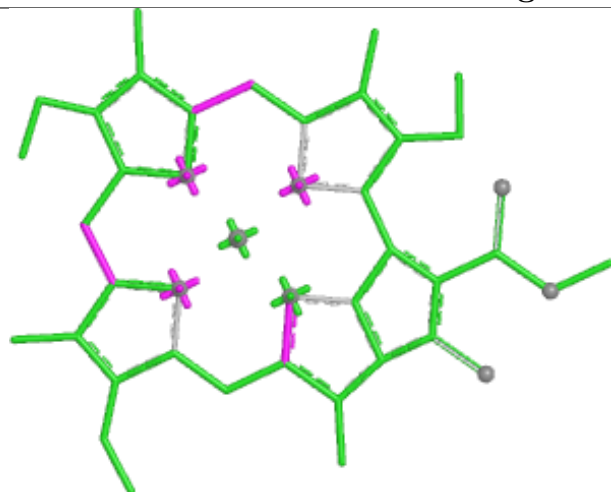
Torsions



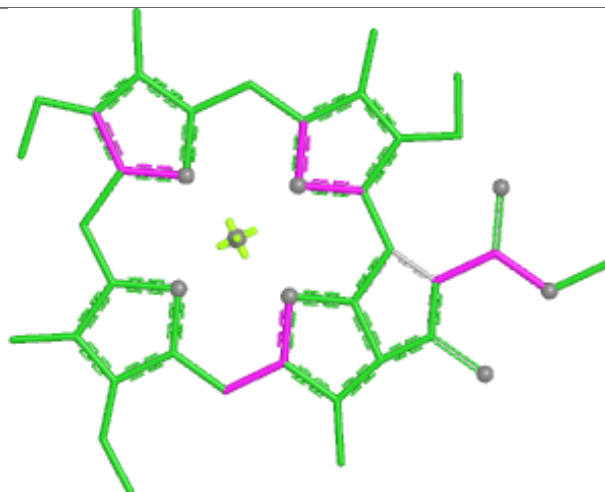
Rings



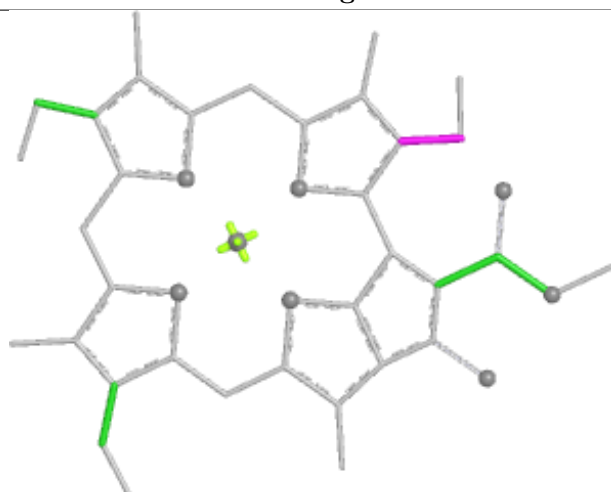
## Ligand CLA k 209



Bond lengths



Bond angles

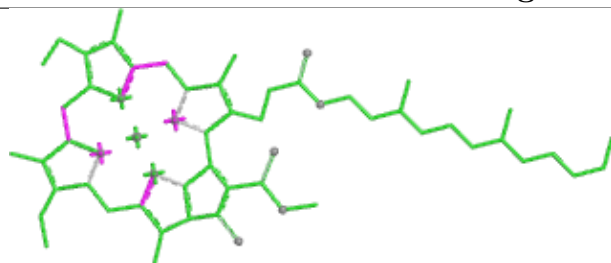


Torsions

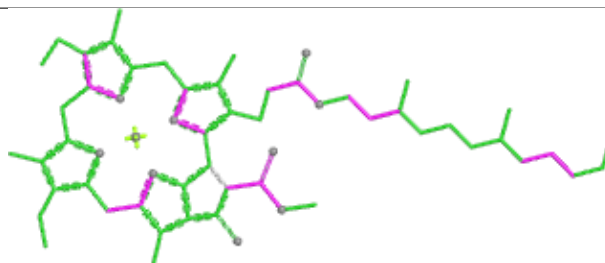


Rings

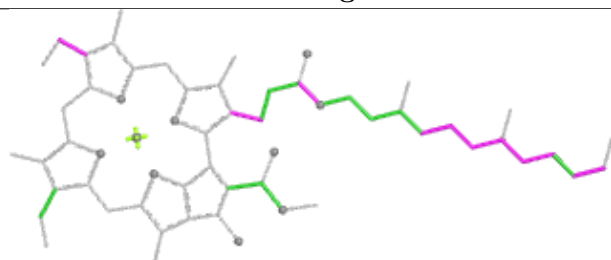
## Ligand CLA d 312



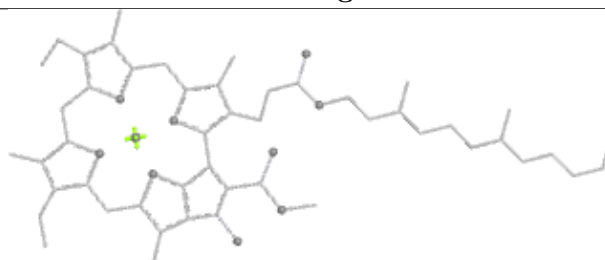
Bond lengths



Bond angles

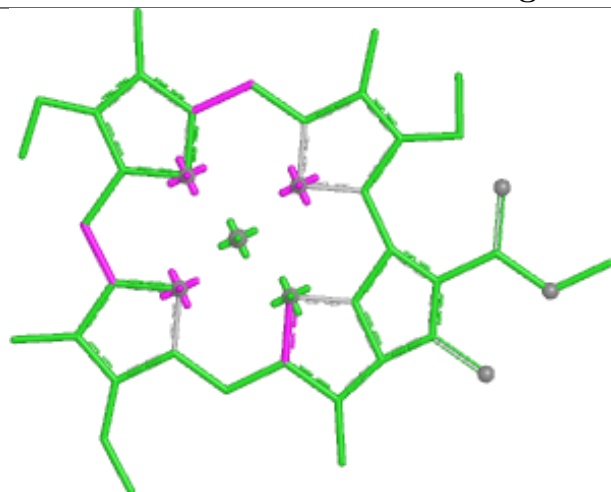


Torsions

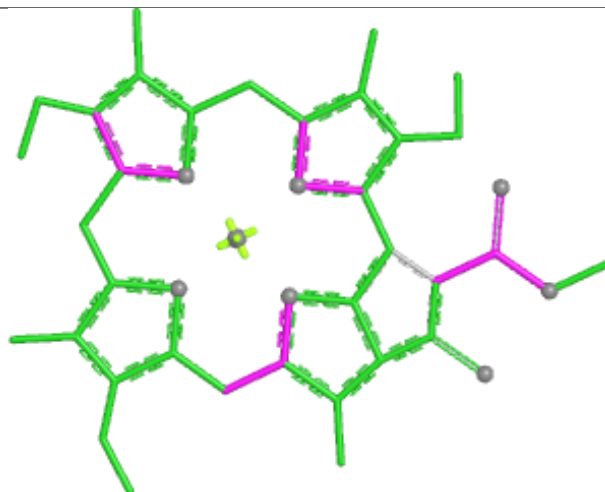


Rings

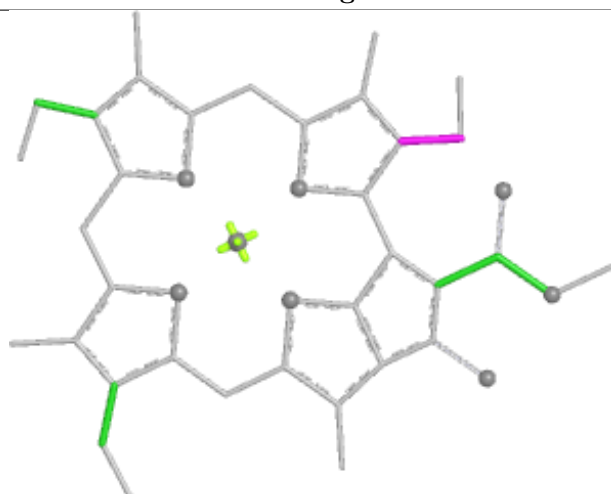
## Ligand CLA e 208



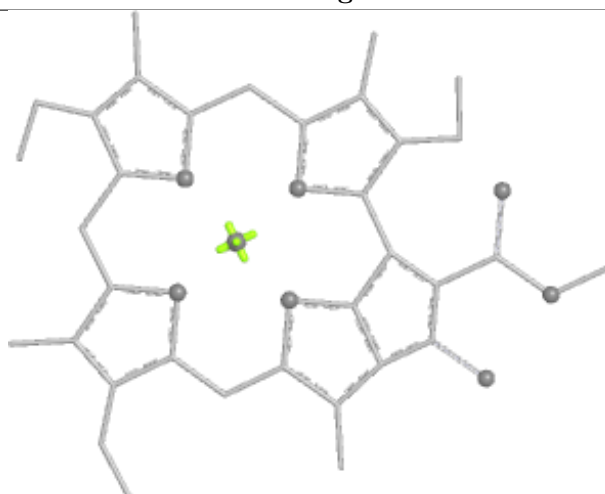
Bond lengths



Bond angles

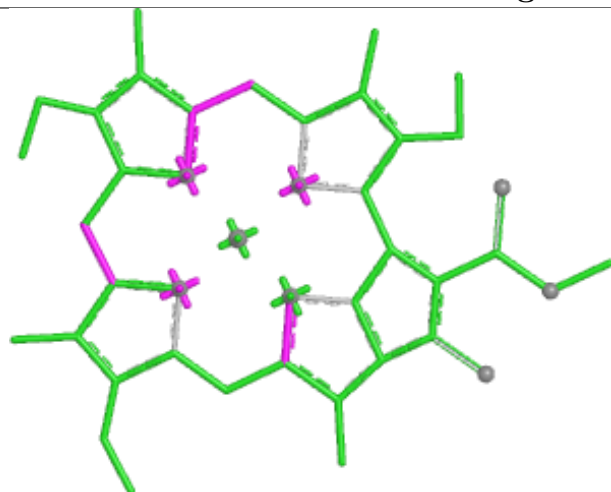


Torsions

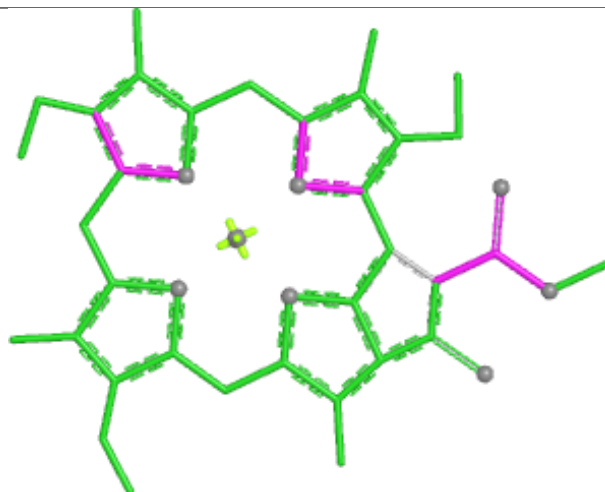


Rings

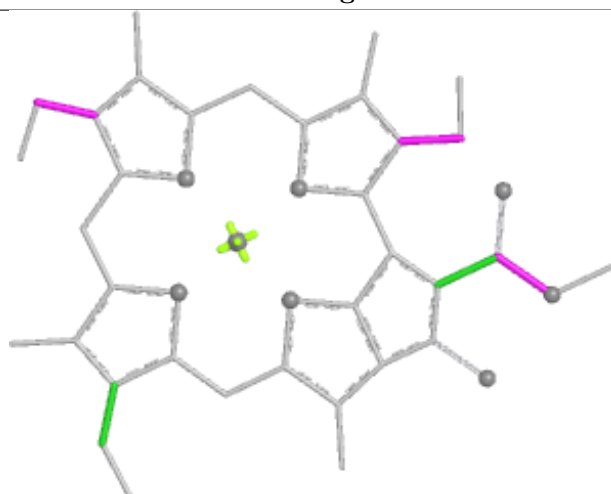
## Ligand CLA h 214



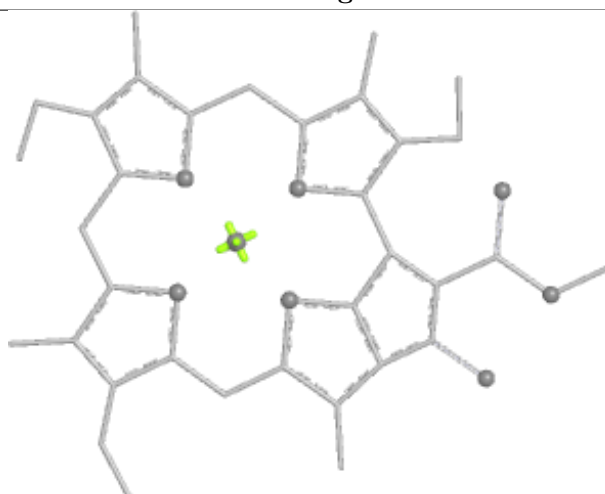
Bond lengths



Bond angles

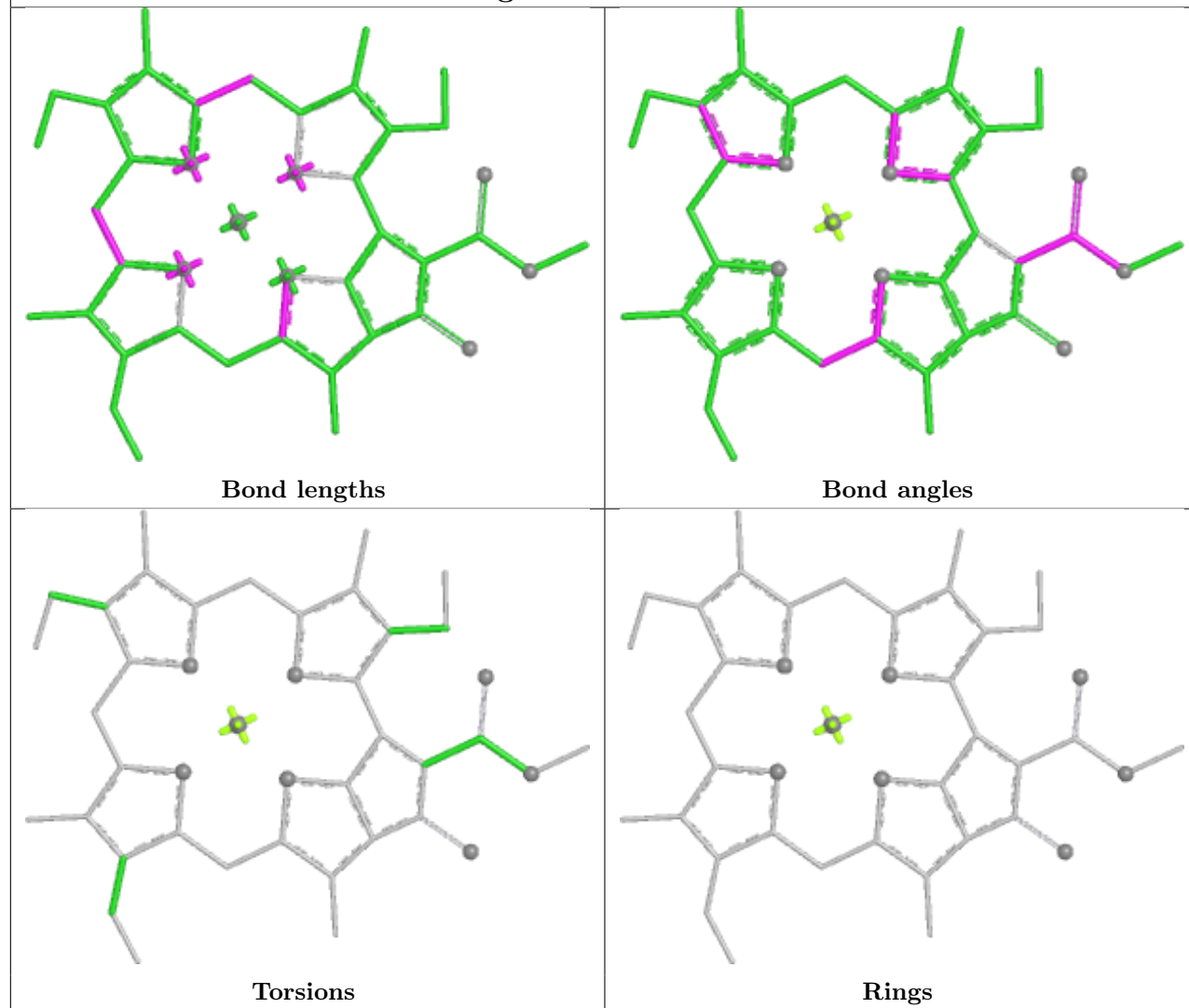


Torsions

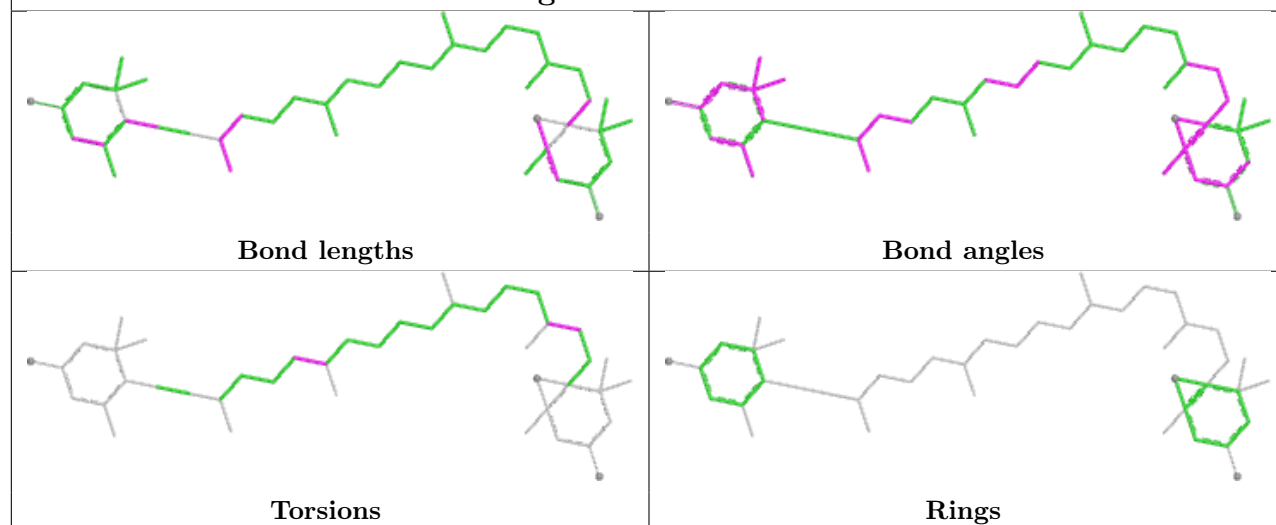


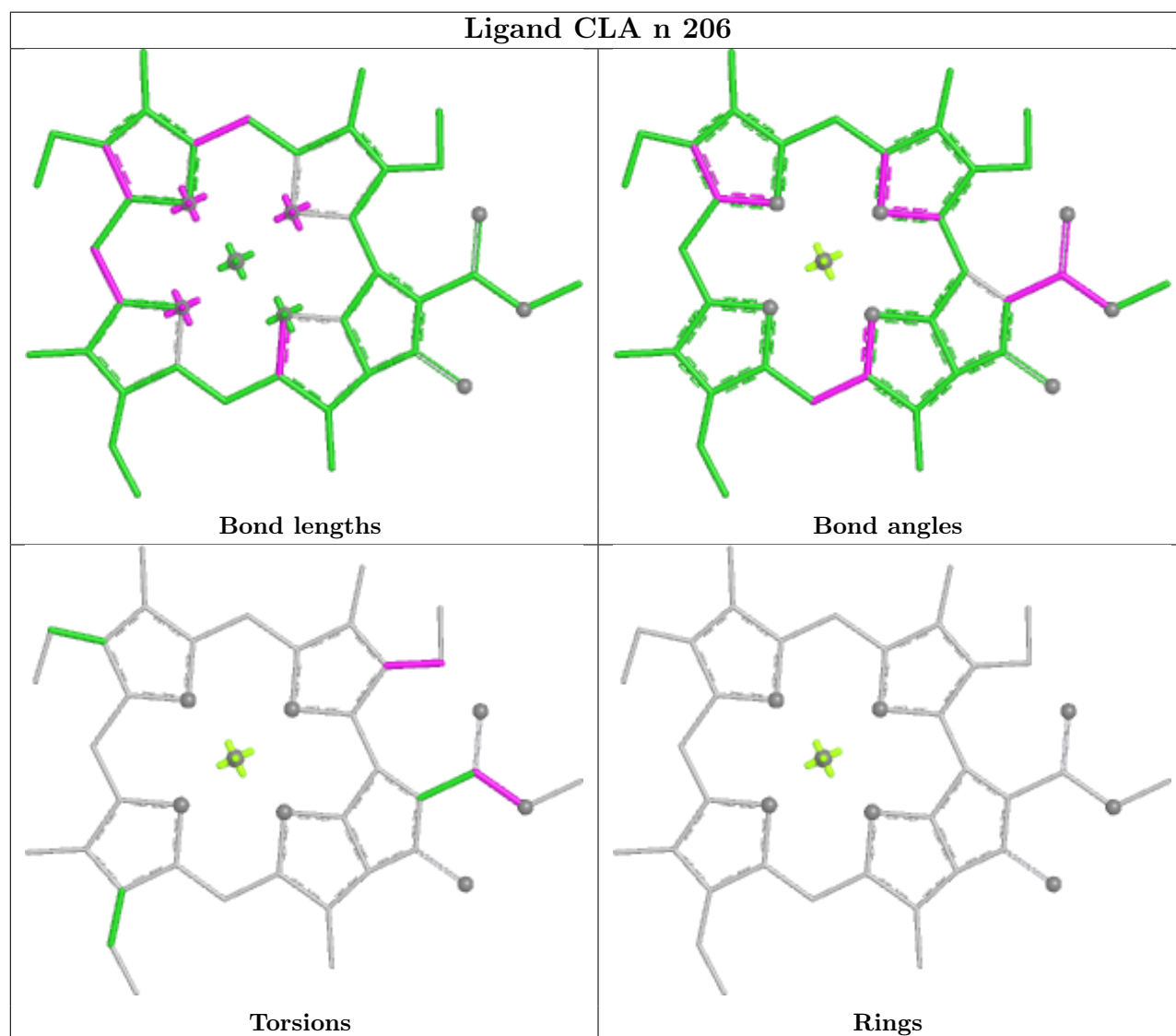
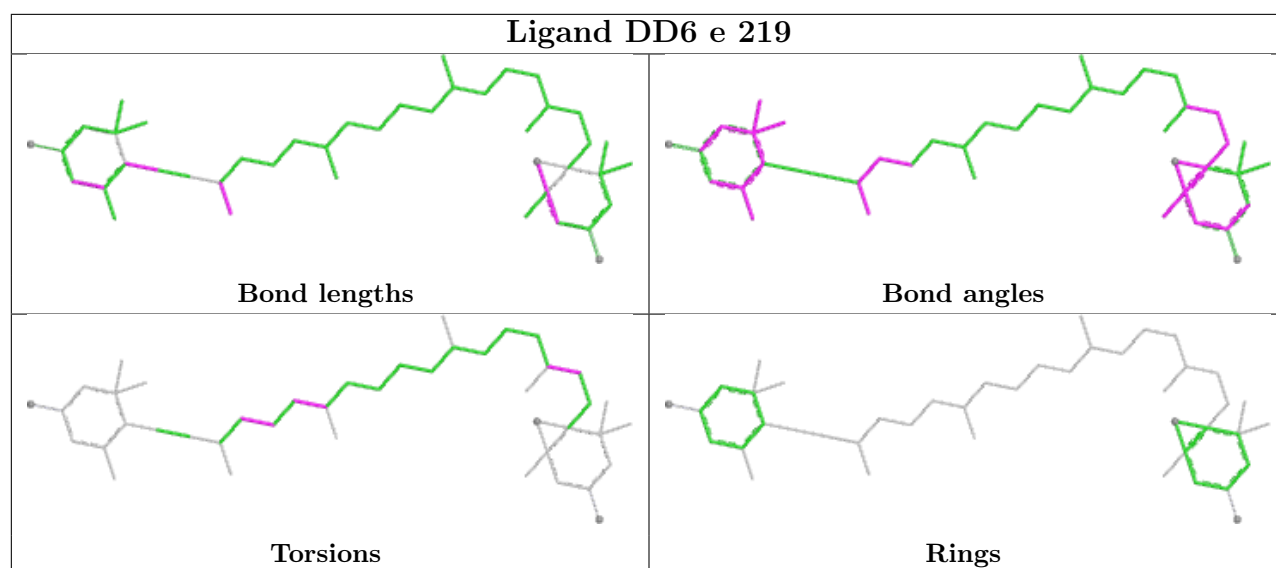
Rings

## Ligand CLA F 201

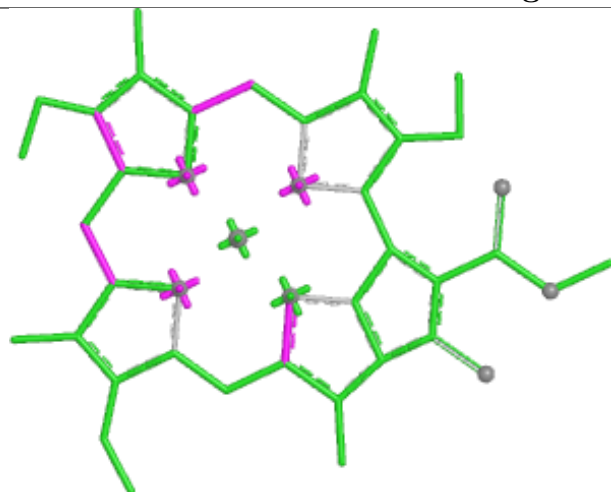


## Ligand DD6 c 316

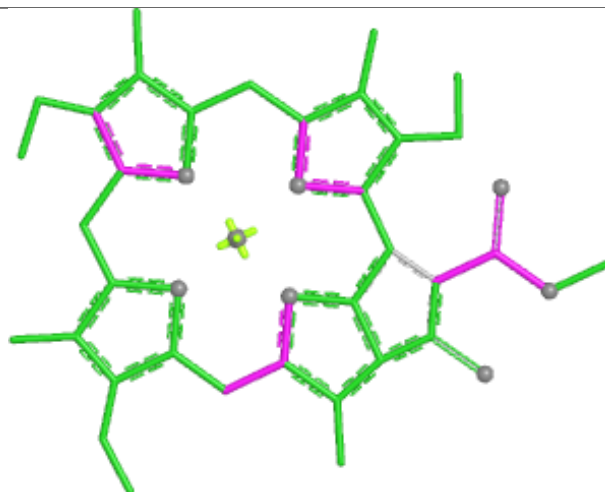




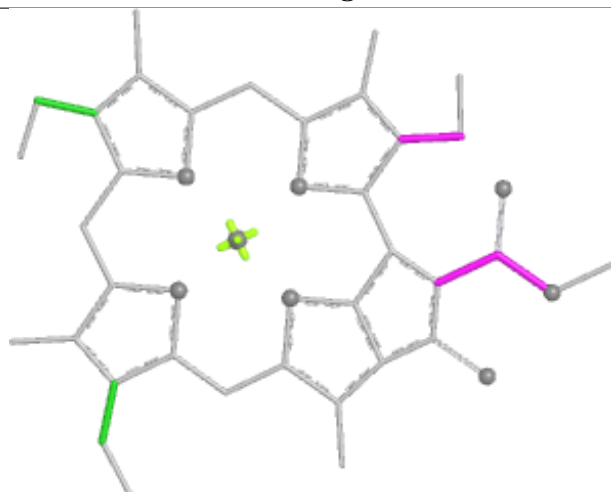
## Ligand CLA 1 612



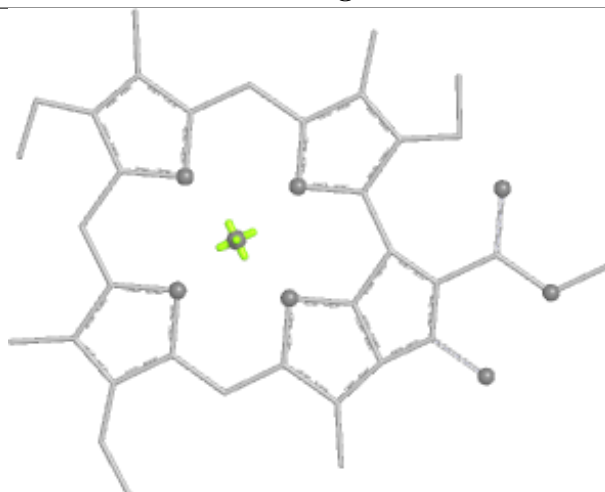
Bond lengths



Bond angles

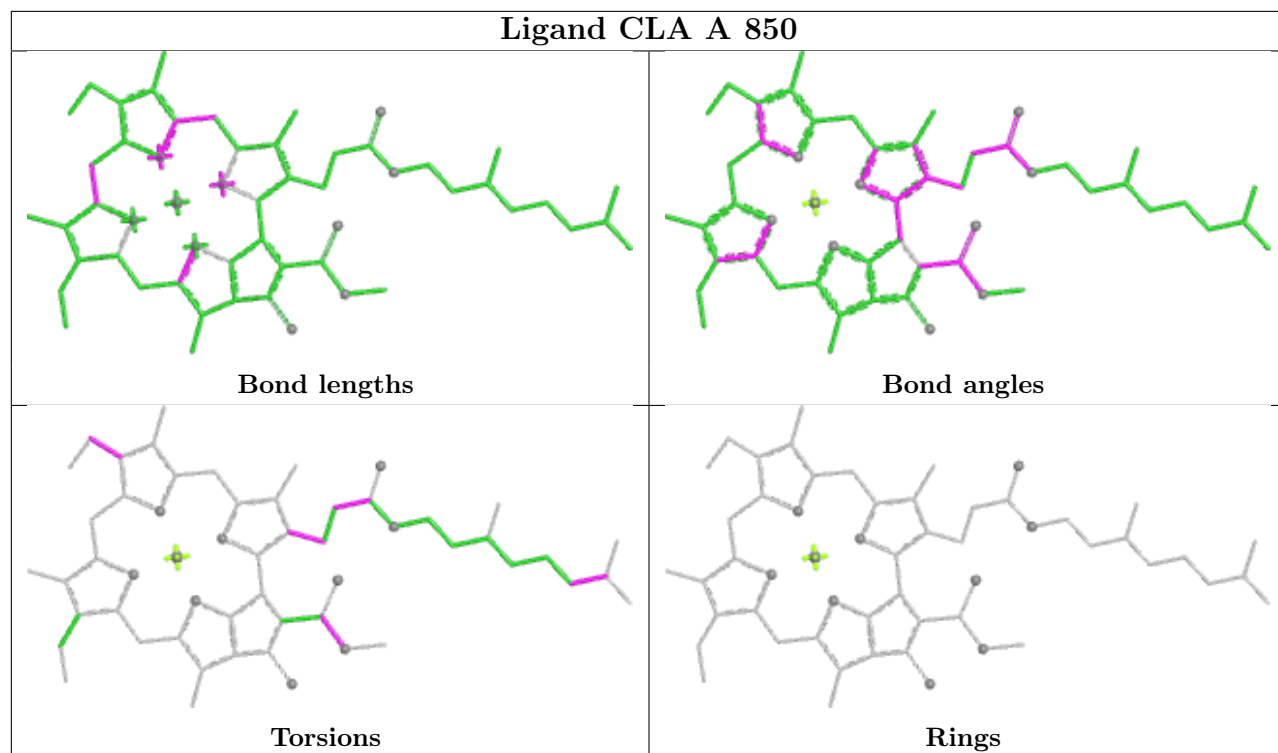


Torsions

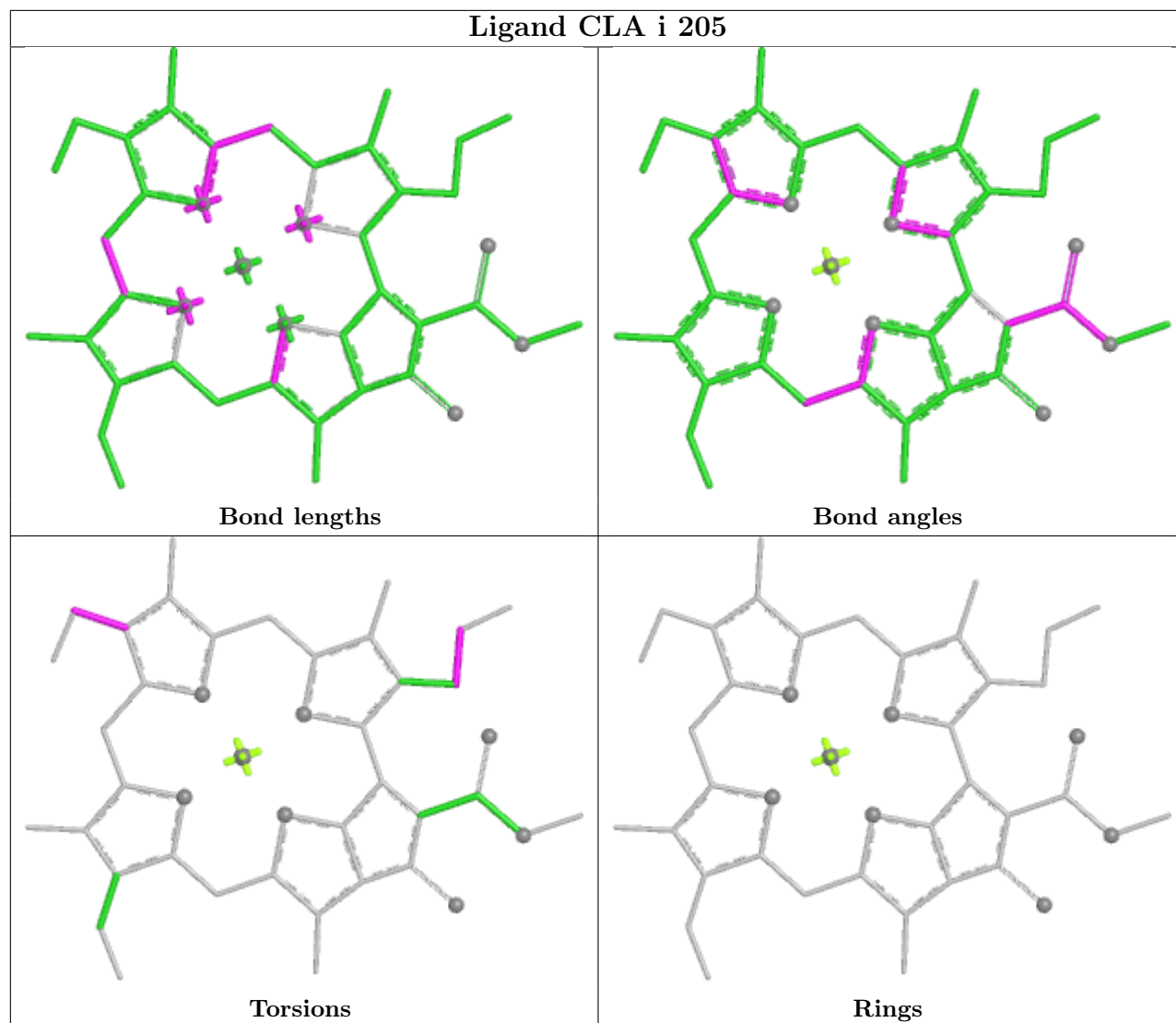


Rings

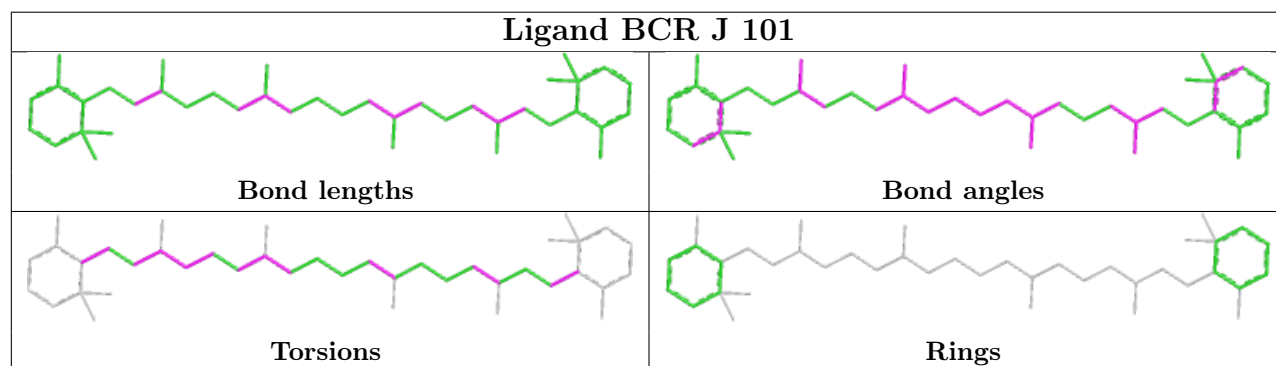


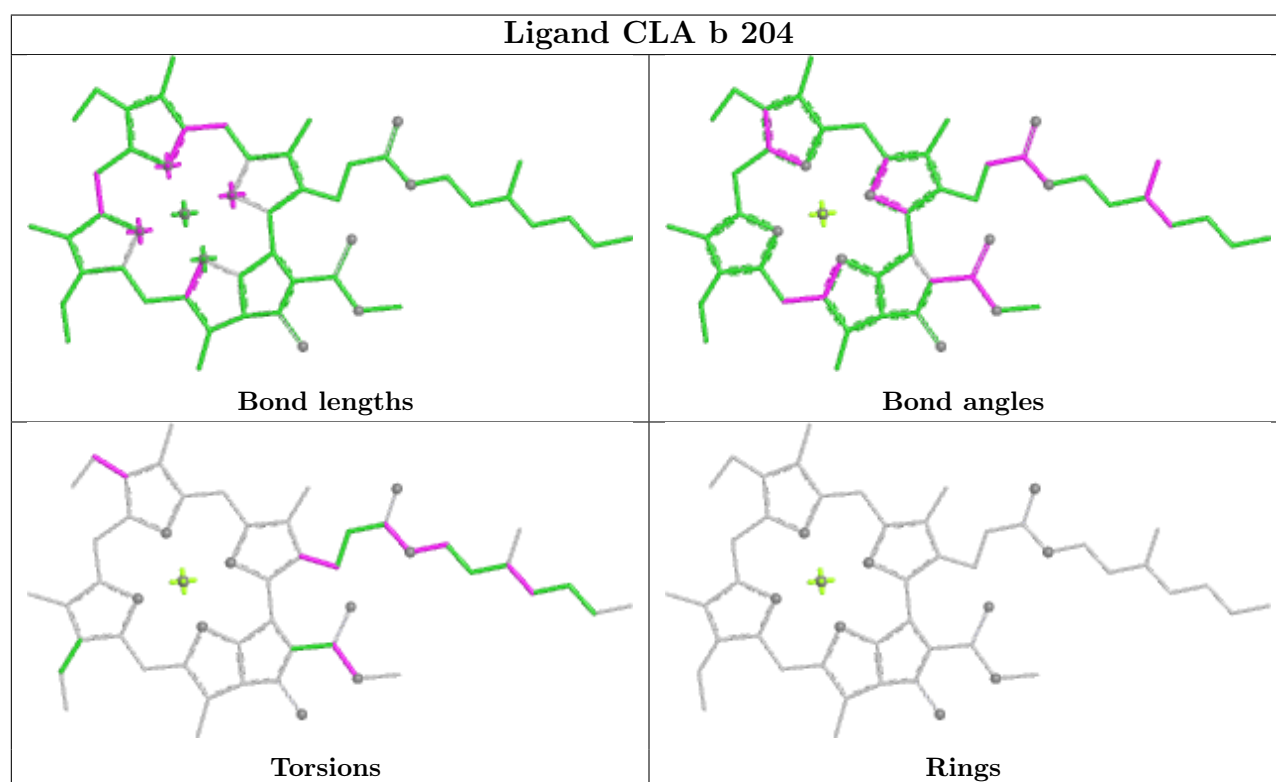
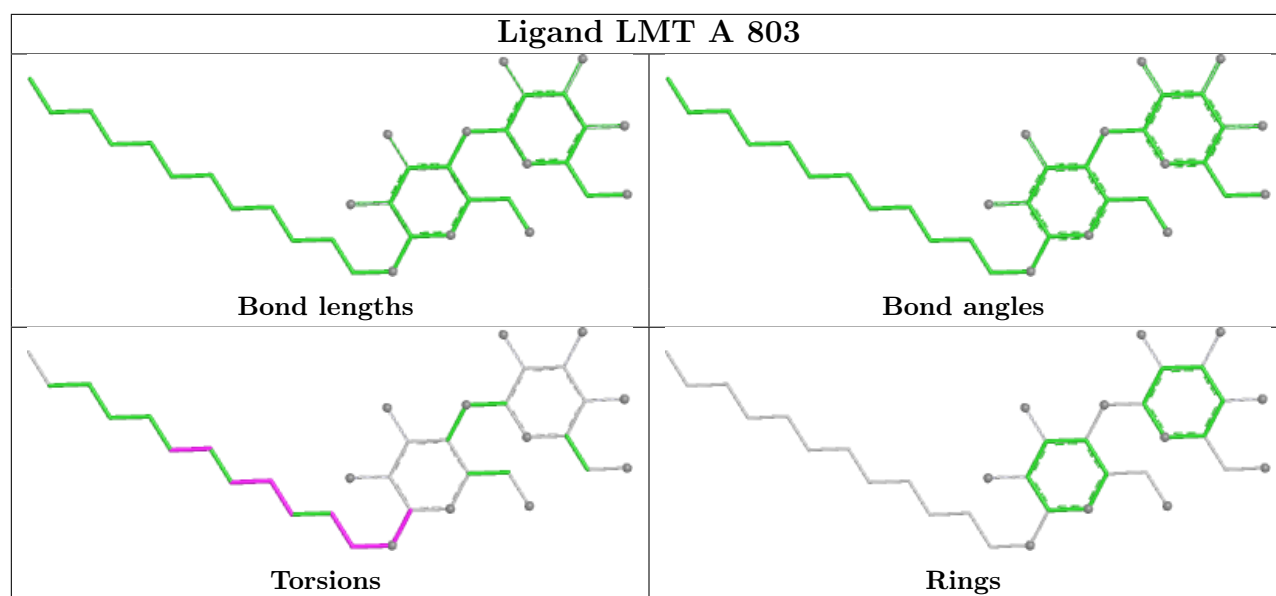


## Ligand CLA i 205

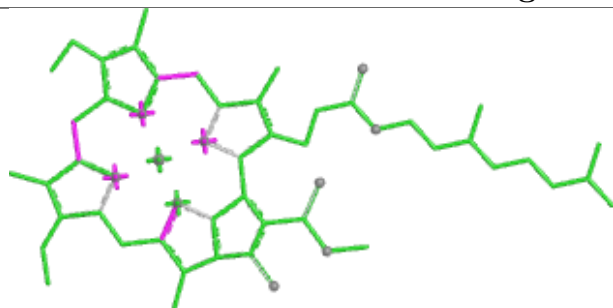


## Ligand BCR J 101

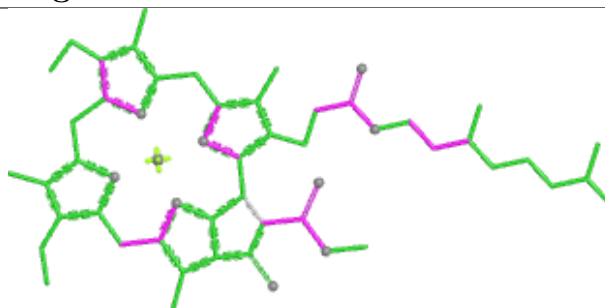




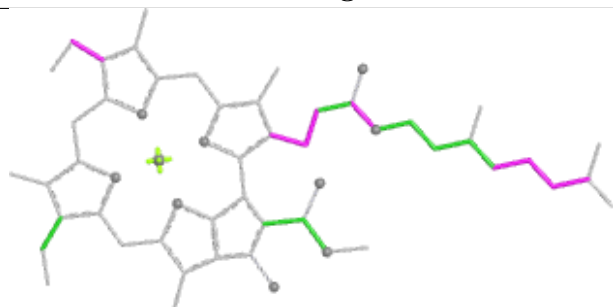
## Ligand CLA g 209



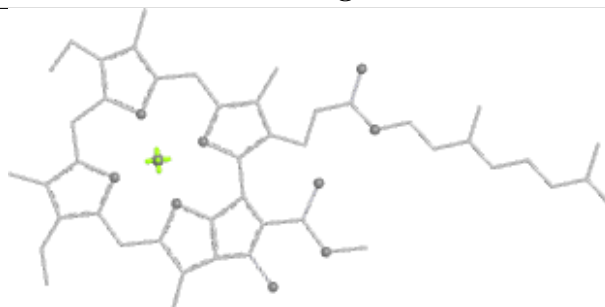
Bond lengths



Bond angles

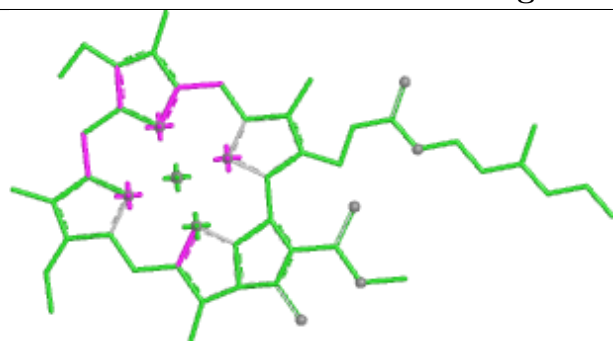


Torsions

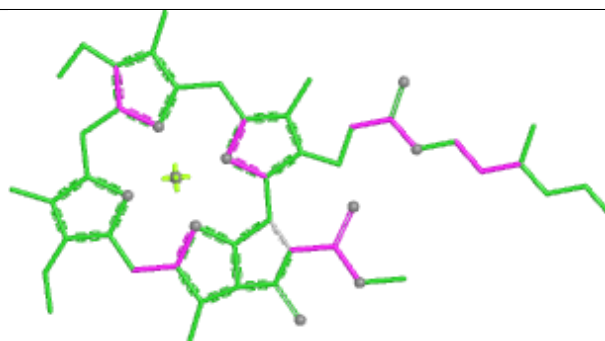


Rings

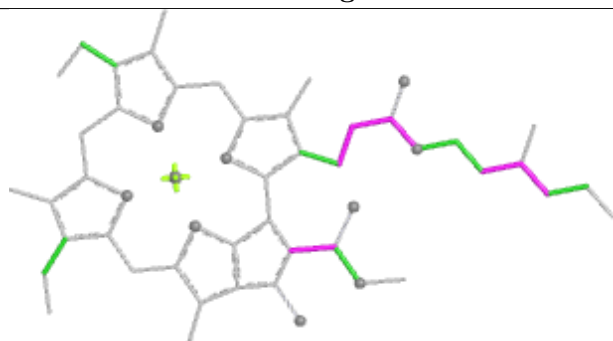
## Ligand CLA b 212



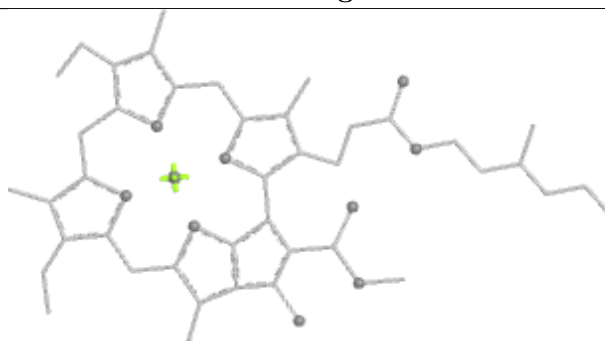
Bond lengths



Bond angles

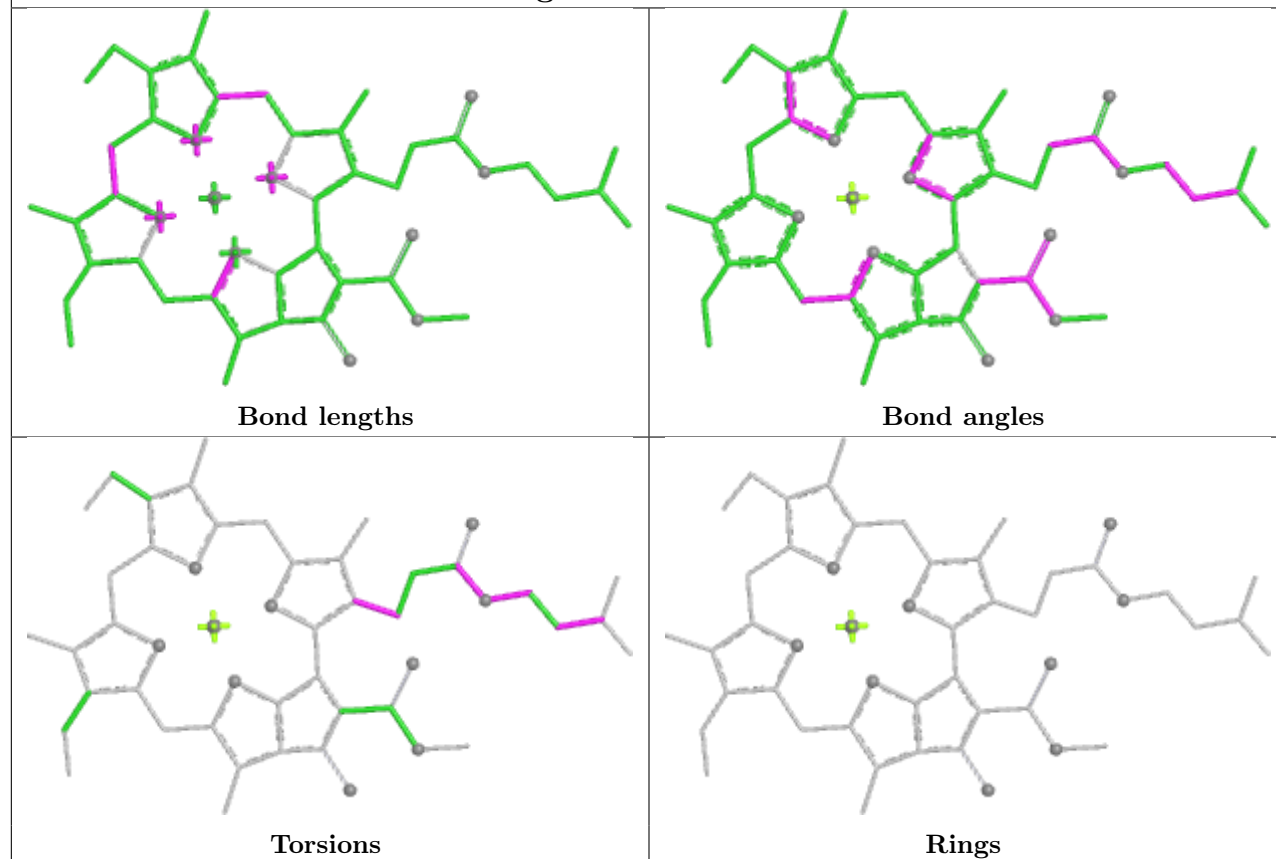


Torsions

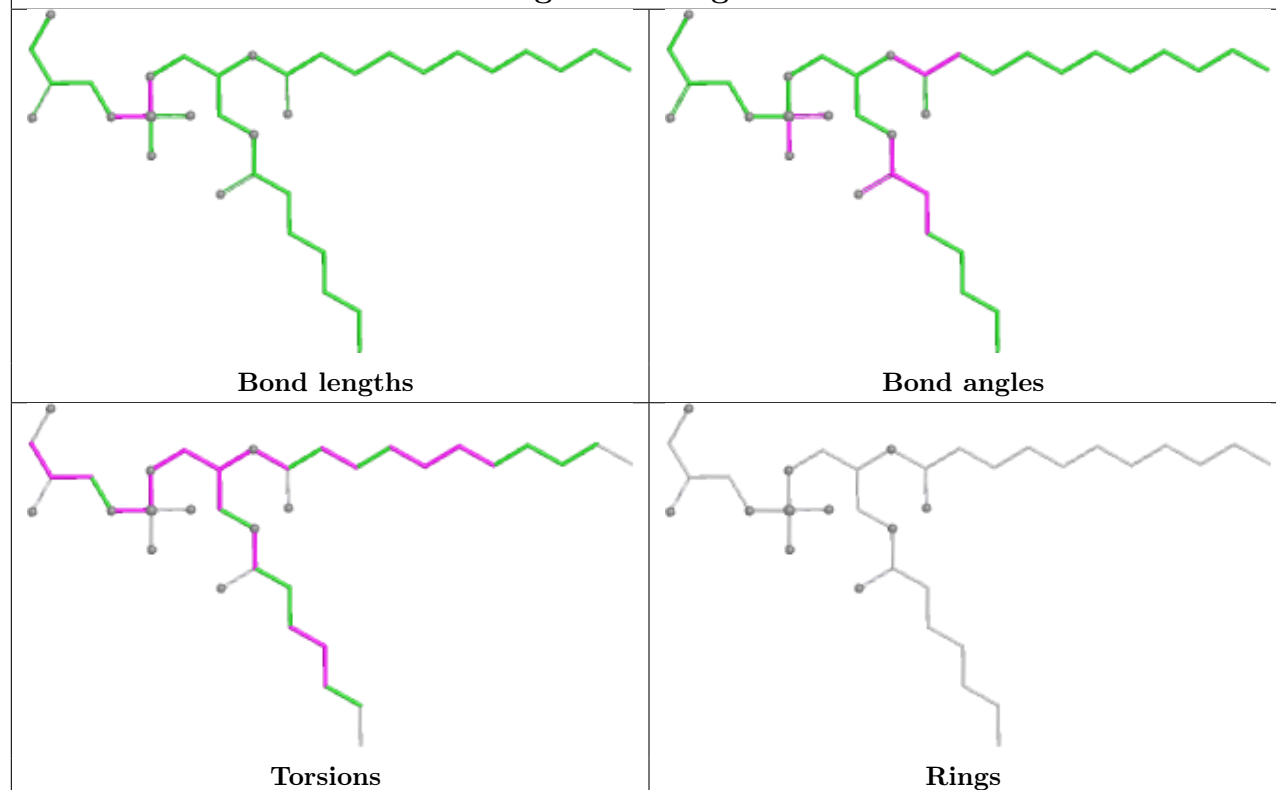


Rings

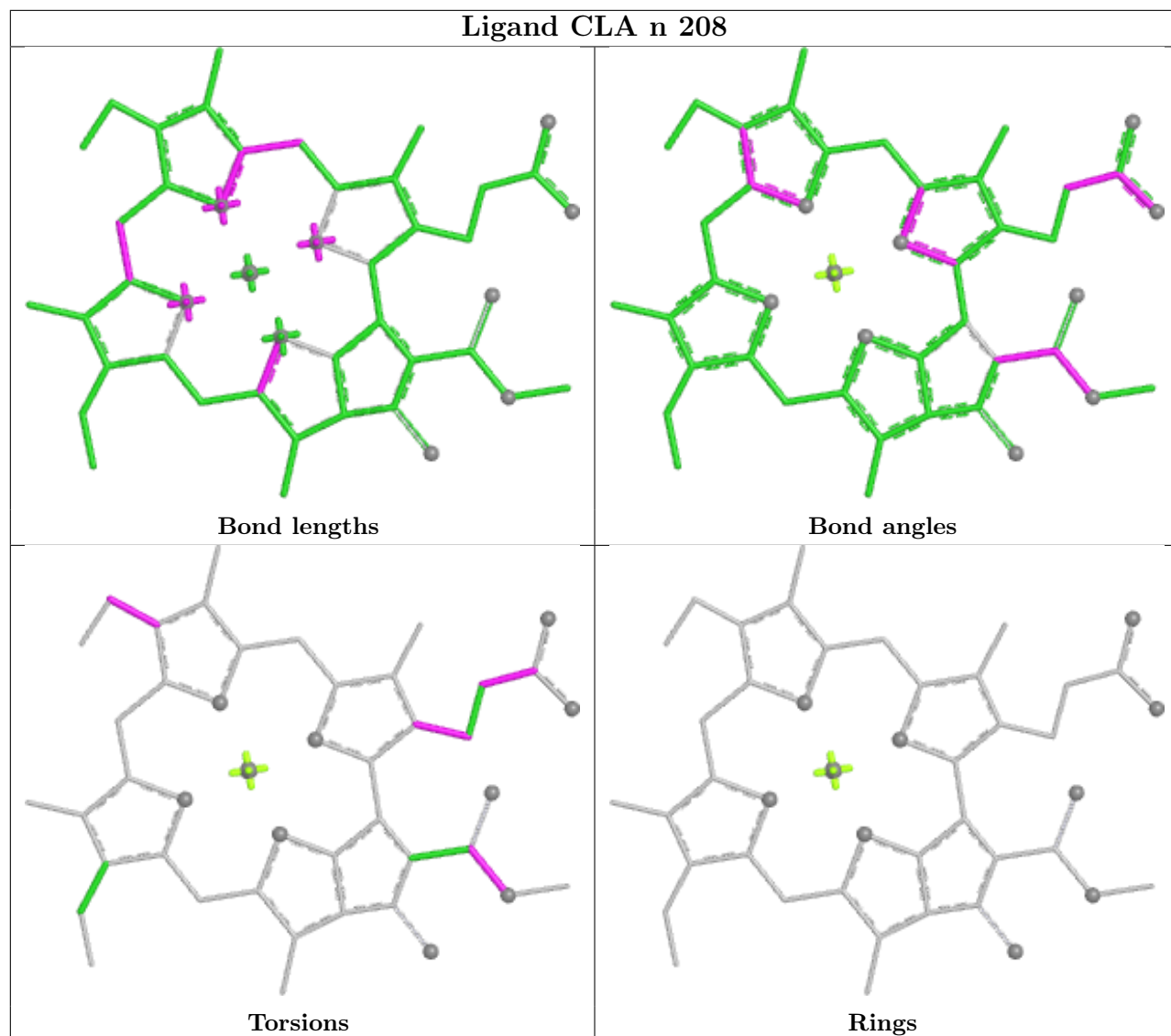
## Ligand CLA a 203



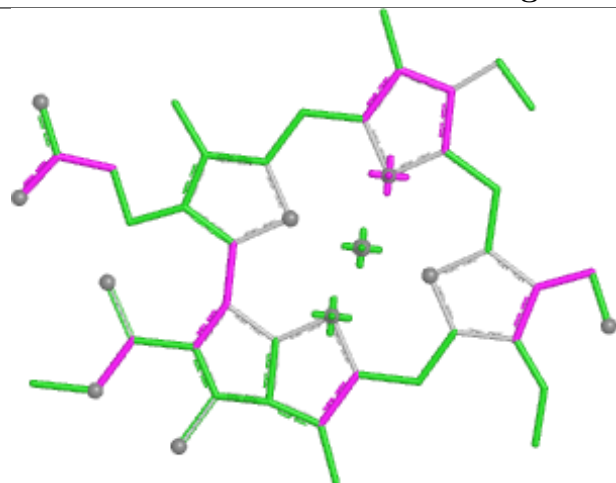
## Ligand LHG g 201



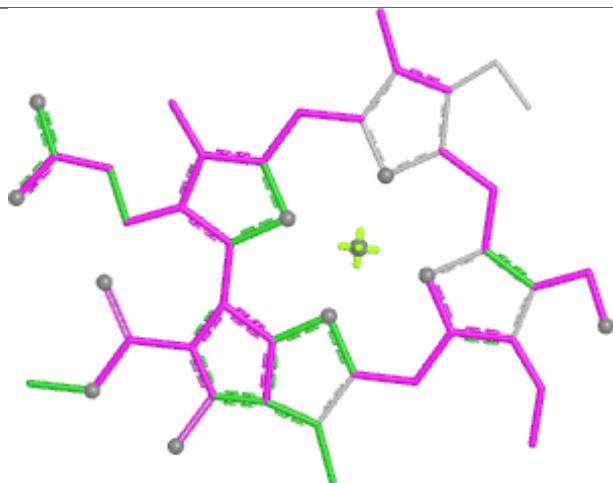
## Ligand CLA n 208



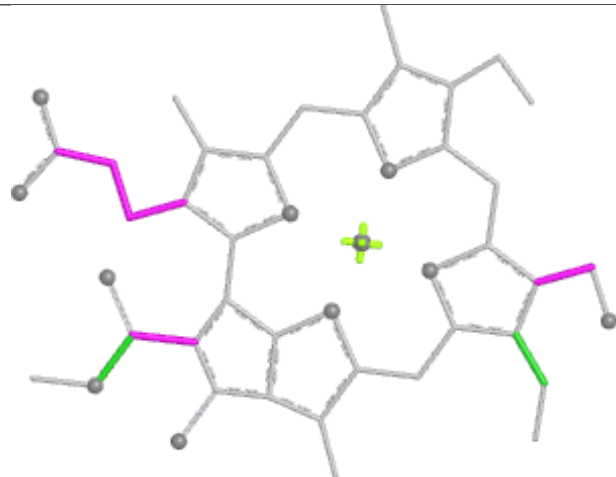
## Ligand CHL e 209



Bond lengths



Bond angles

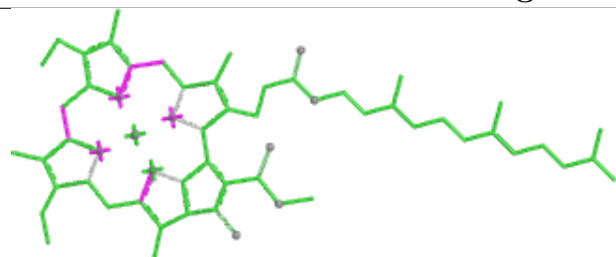


Torsions

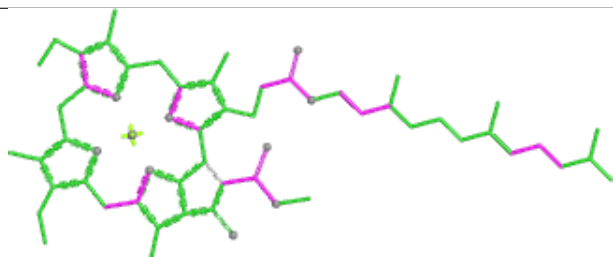


Rings

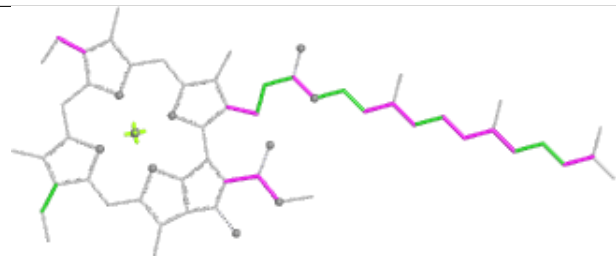
## Ligand CLA B 822



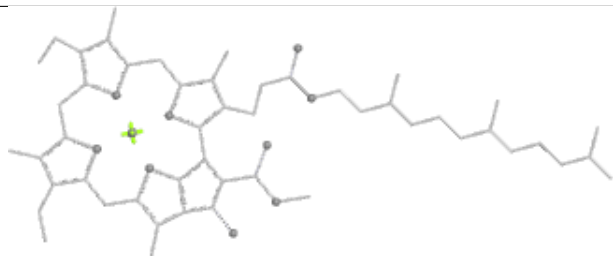
Bond lengths



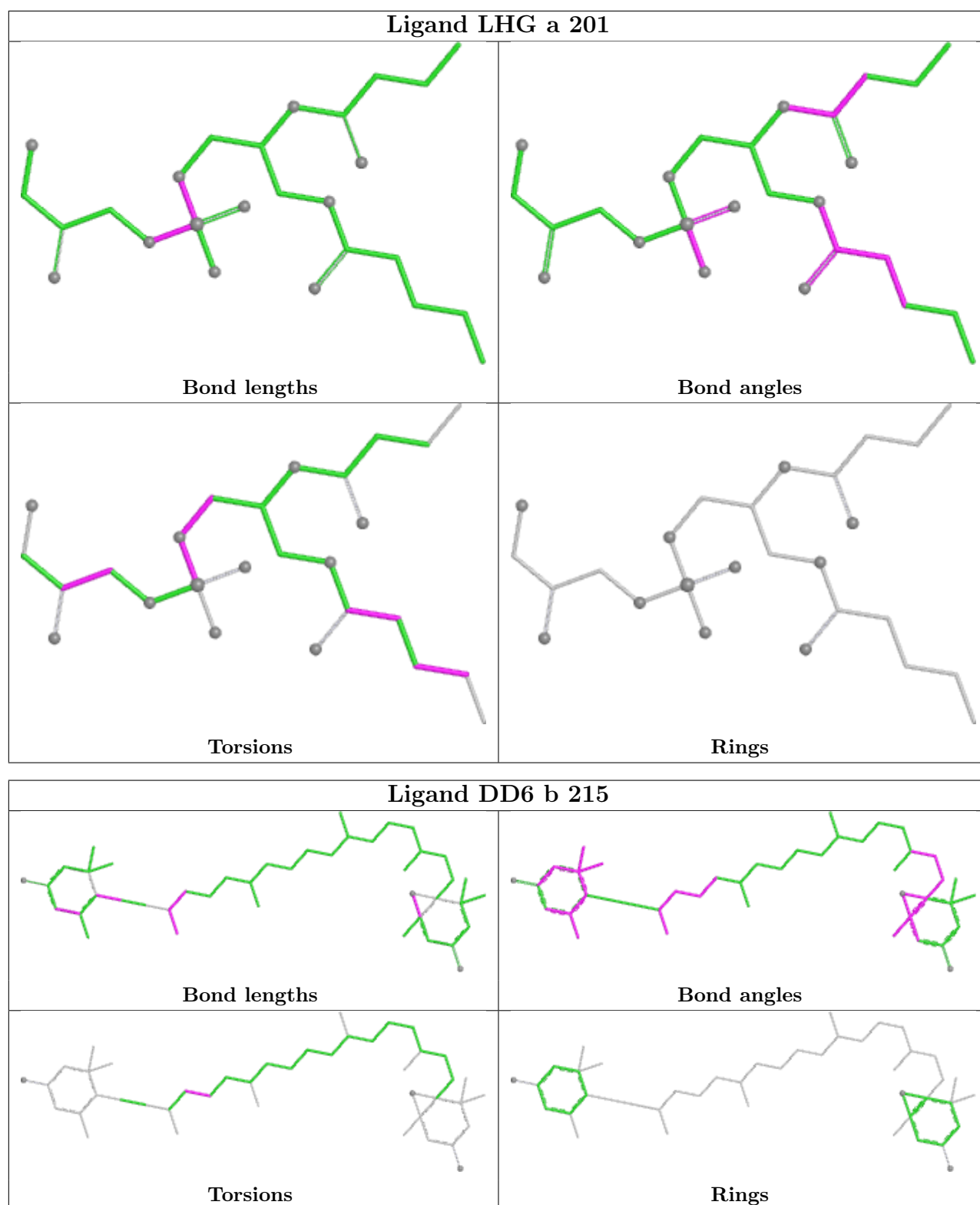
Bond angles



Torsions

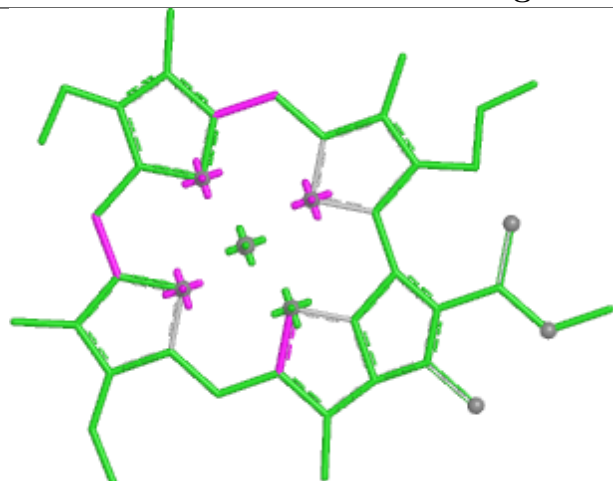


Rings

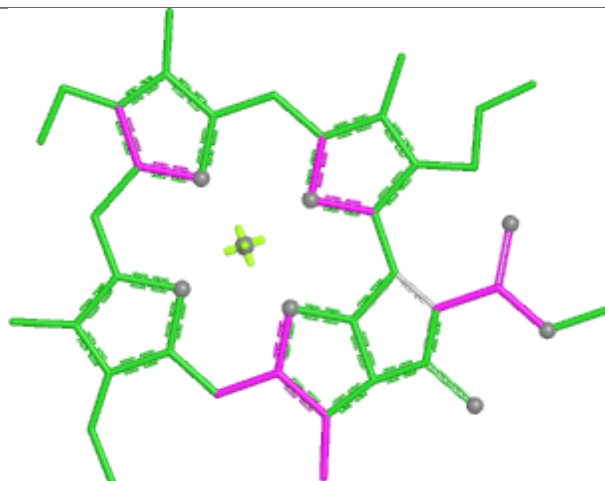




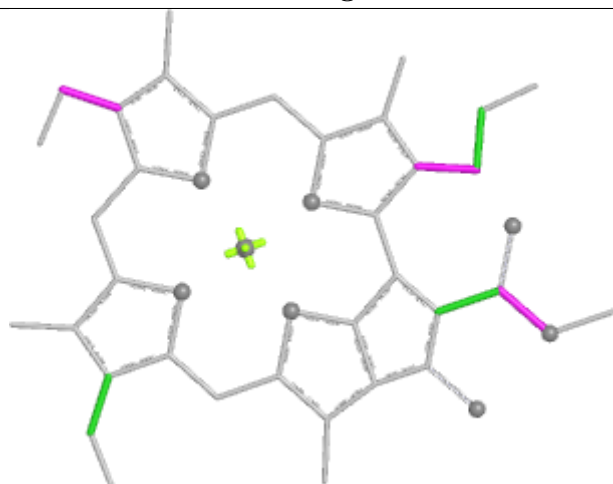
## Ligand CLA A 828



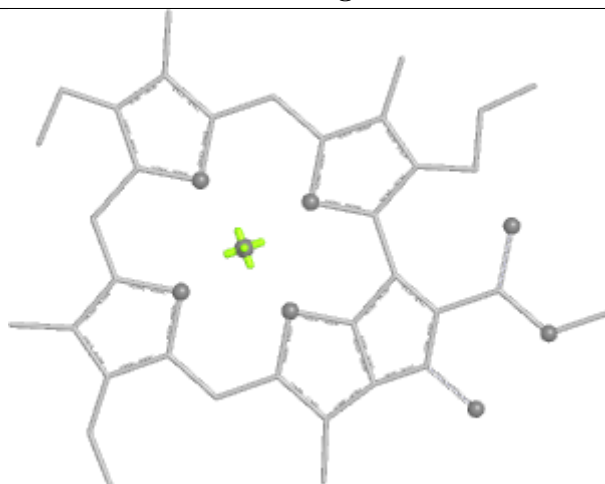
Bond lengths



Bond angles

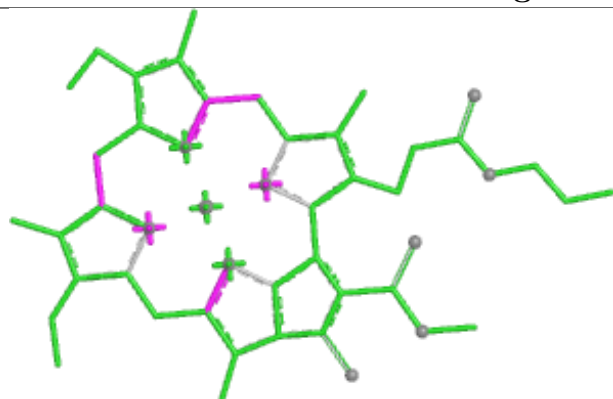


Torsions

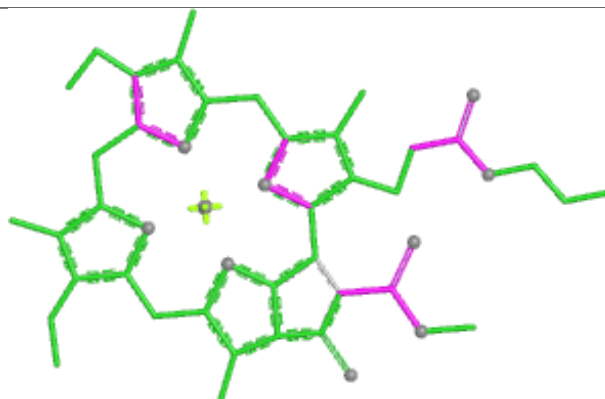


Rings

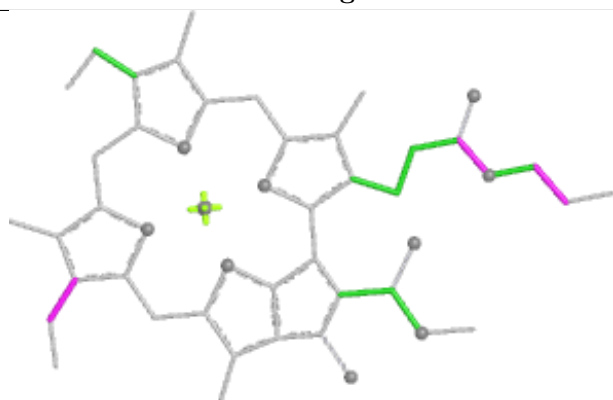
## Ligand CLA A 852



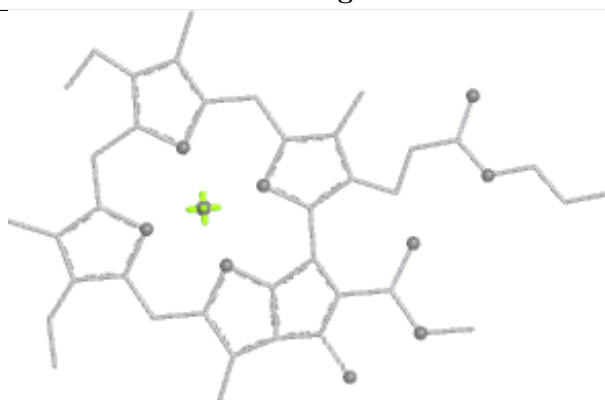
Bond lengths



Bond angles

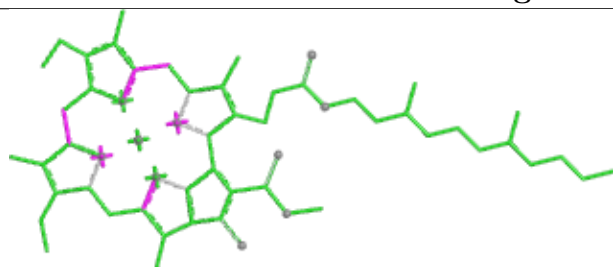


Torsions

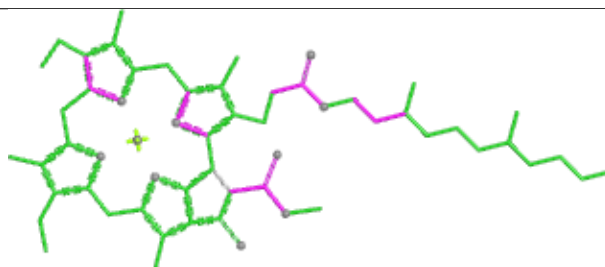


Rings

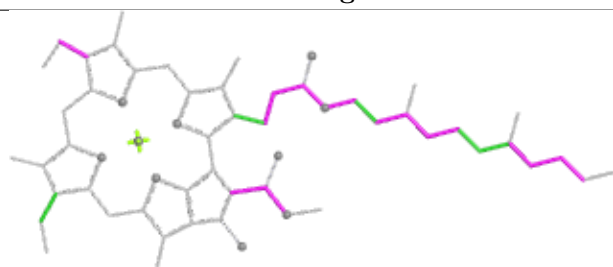
## Ligand CLA A 815



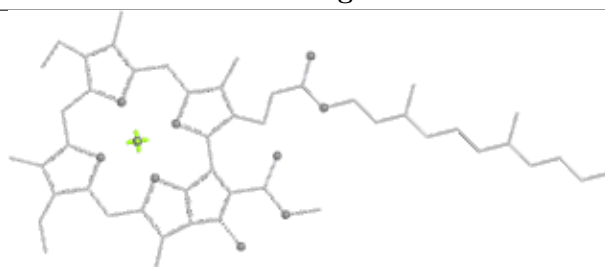
Bond lengths



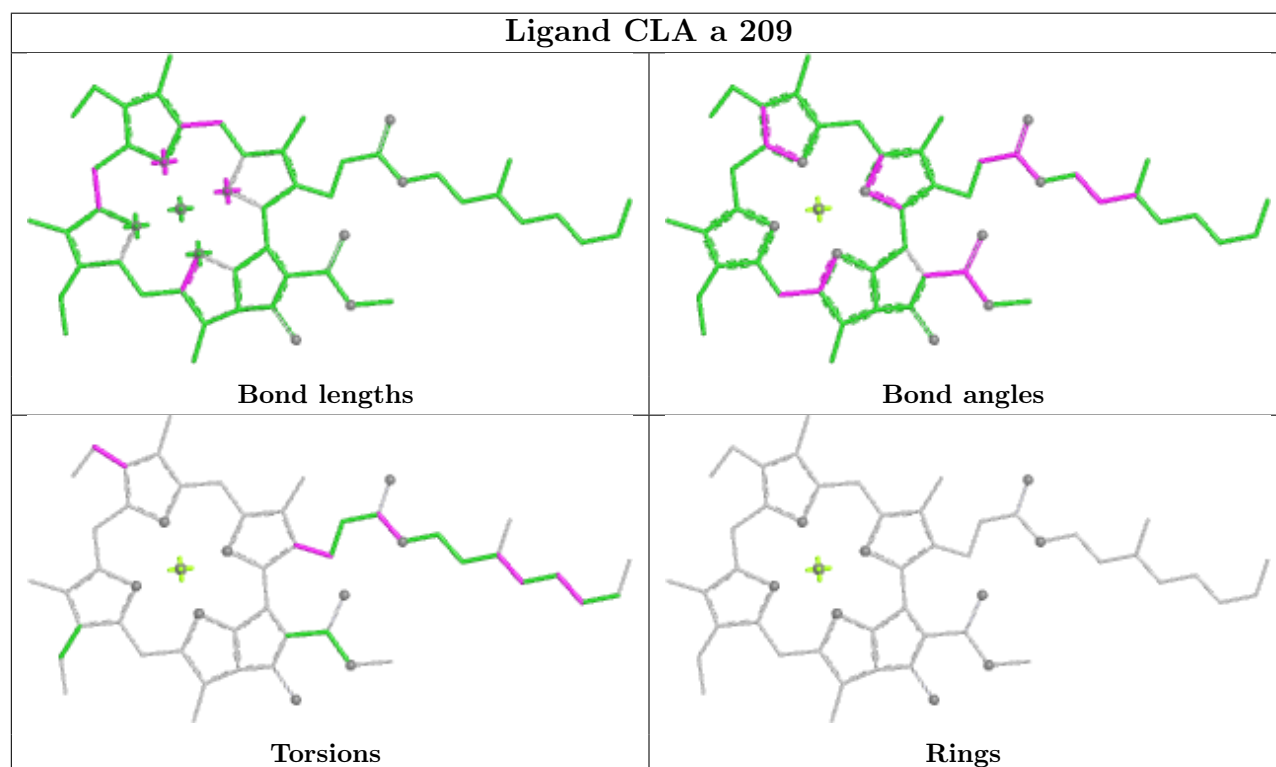
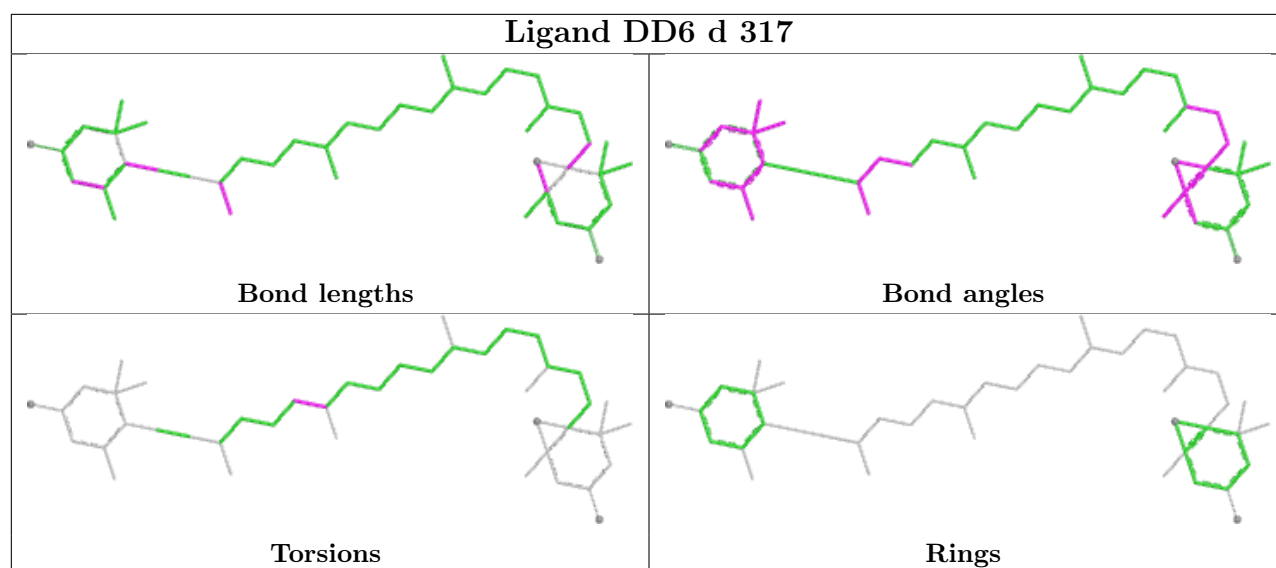
Bond angles

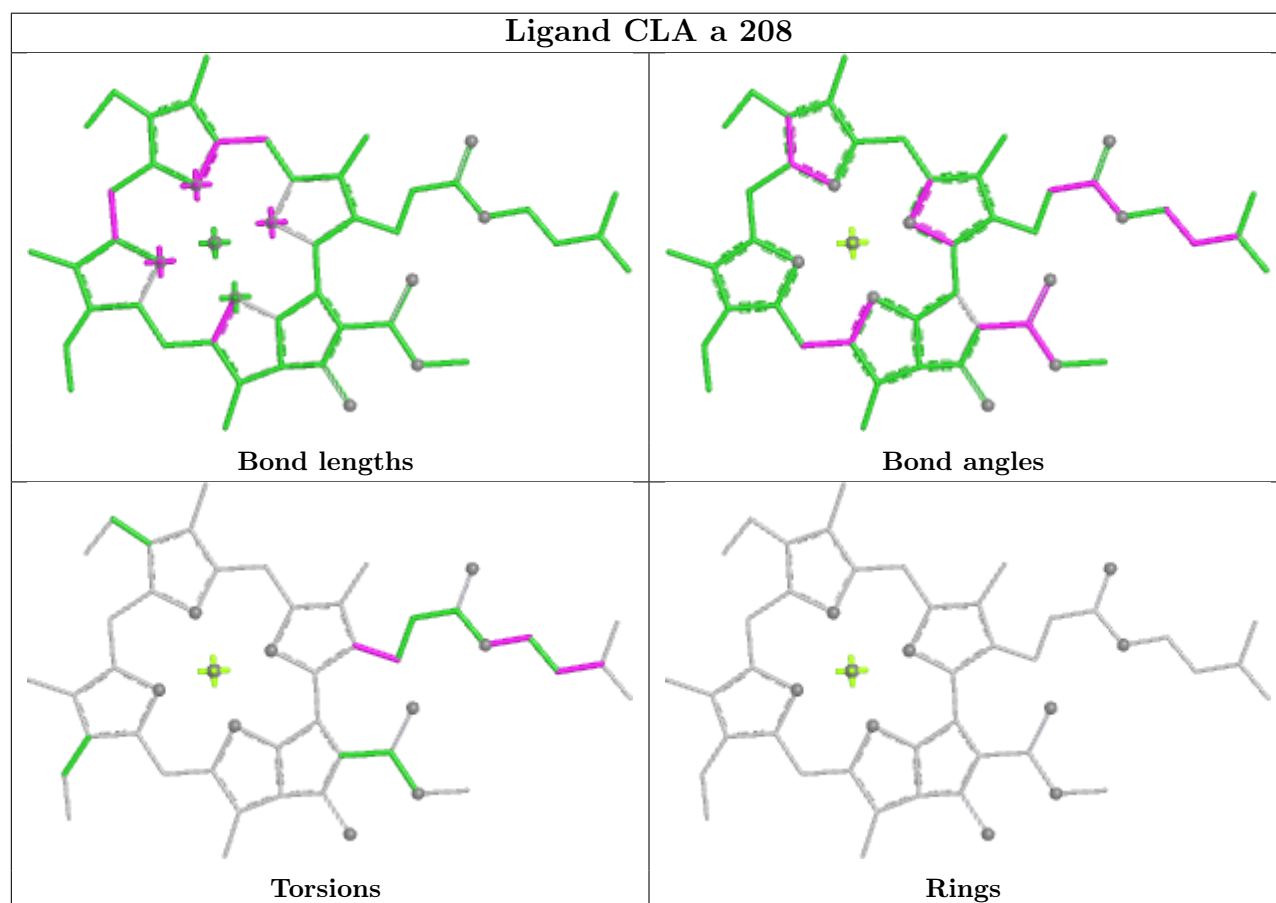
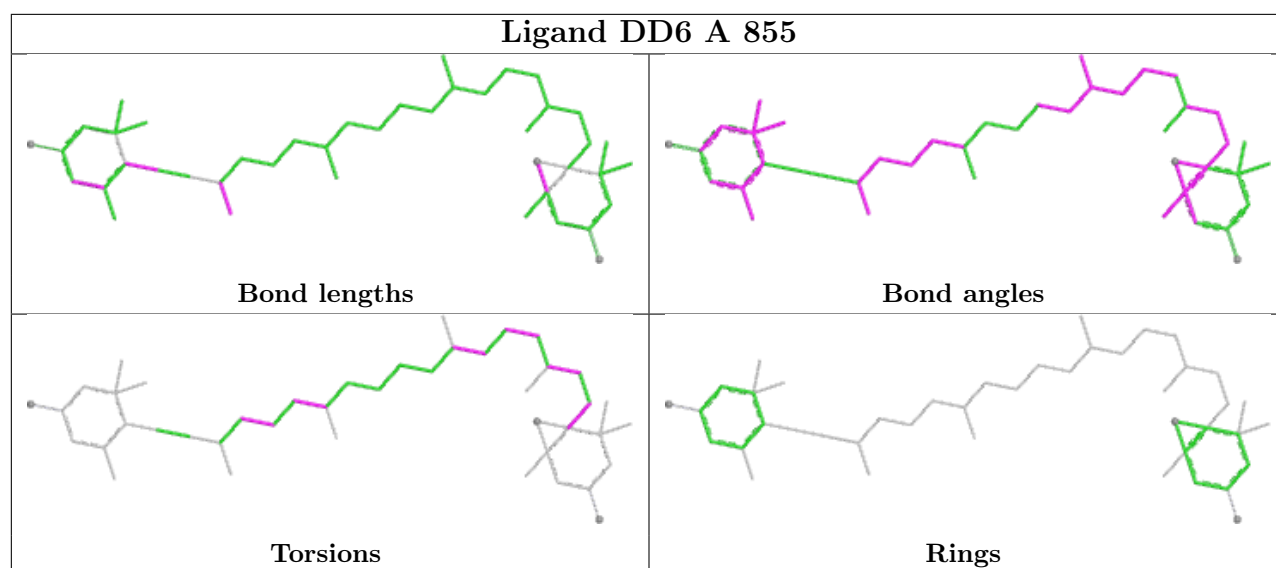


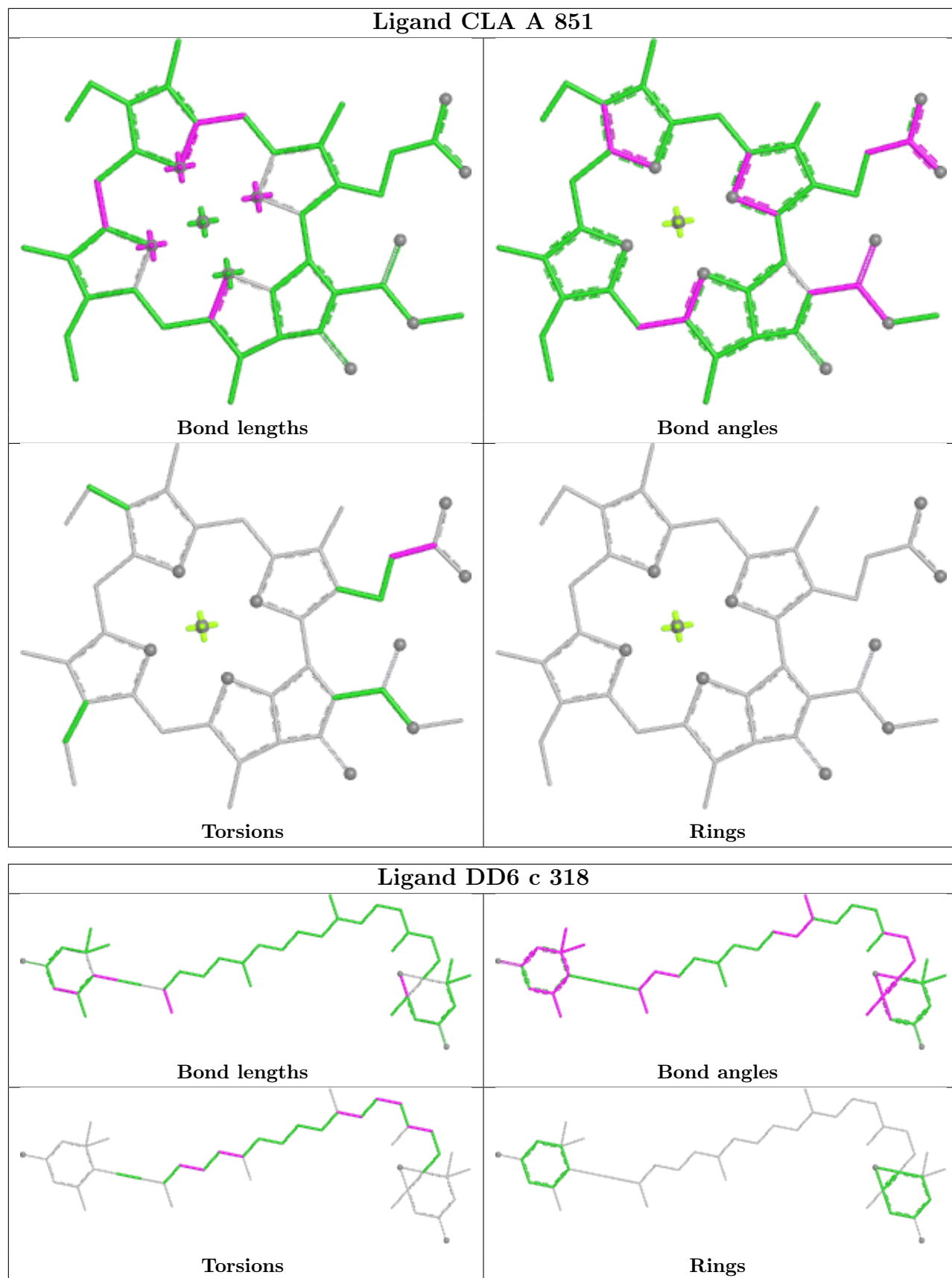
Torsions

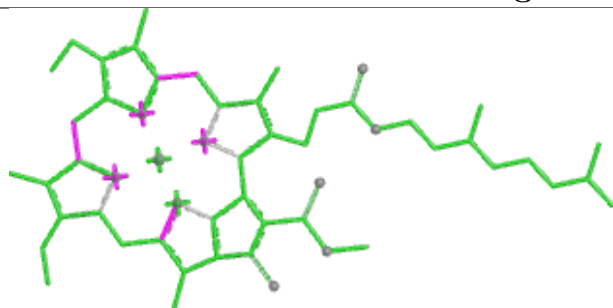


Rings

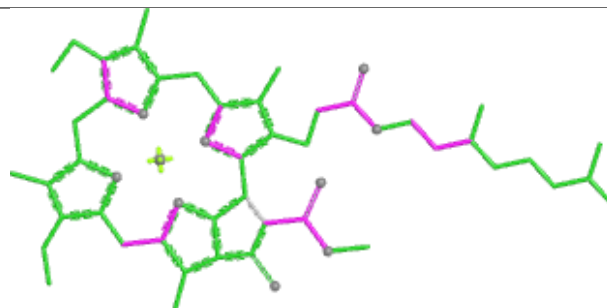




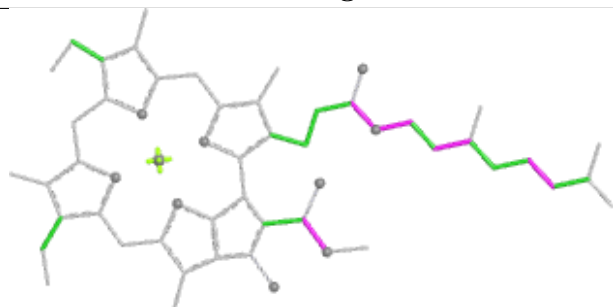


**Ligand CLA B 834**

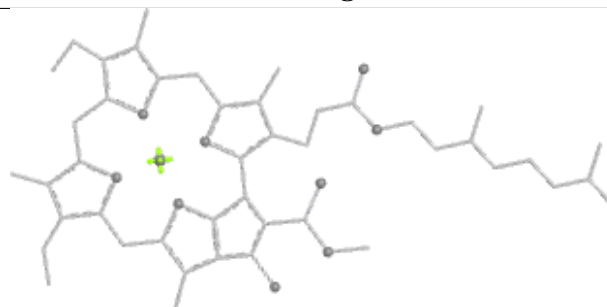
Bond lengths



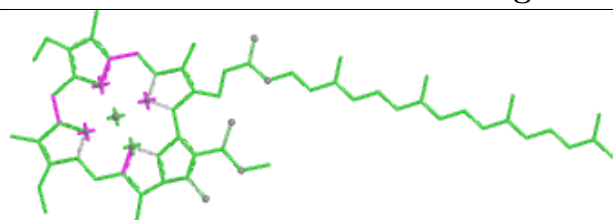
Bond angles



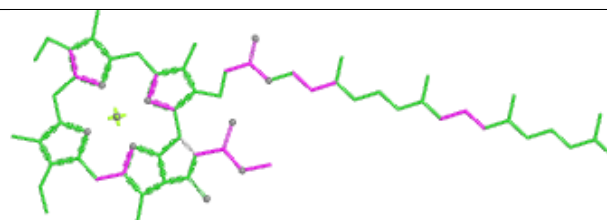
Torsions



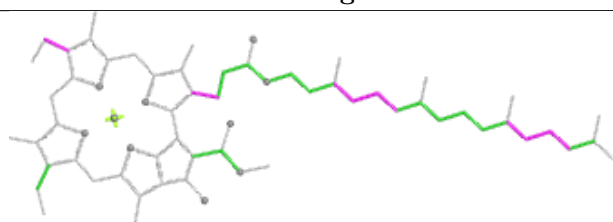
Rings

**Ligand CLA A 819**

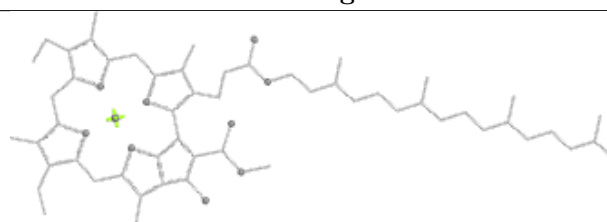
Bond lengths



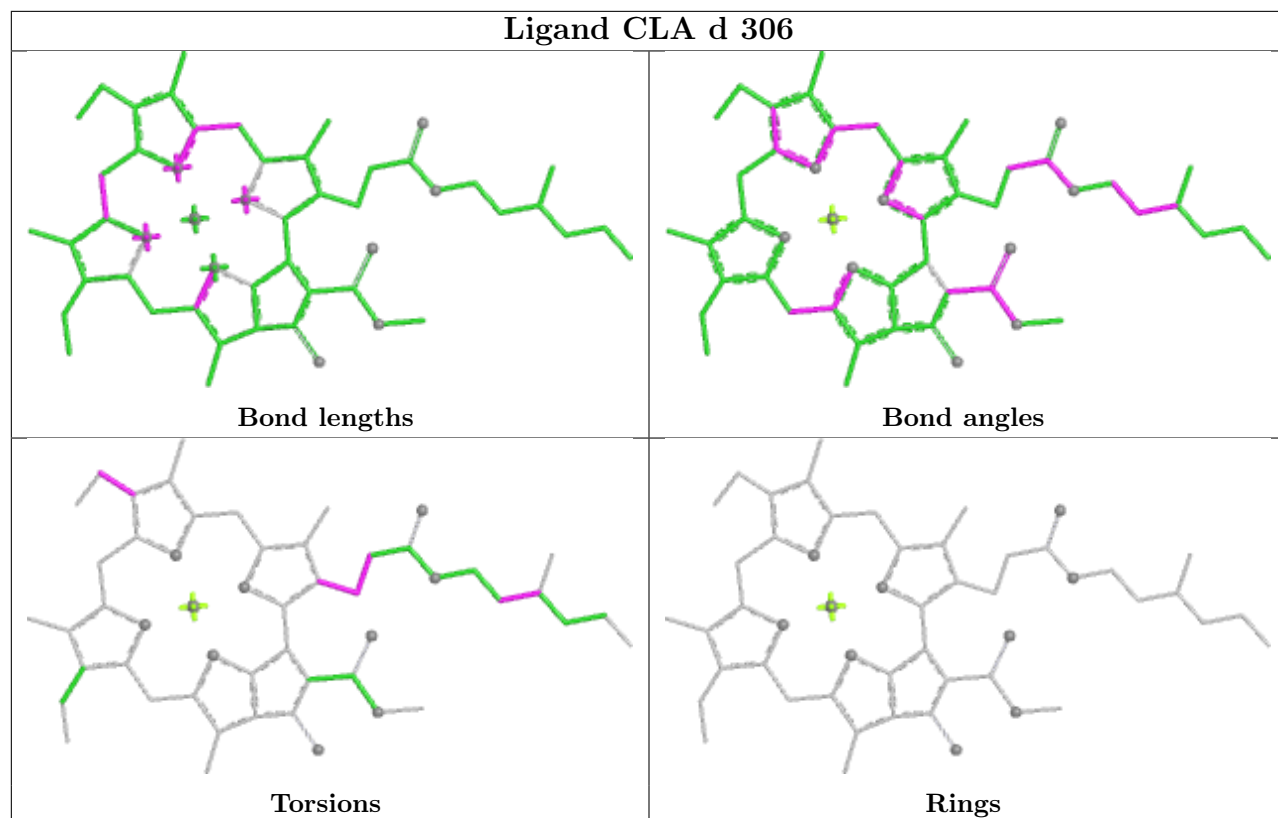
Bond angles



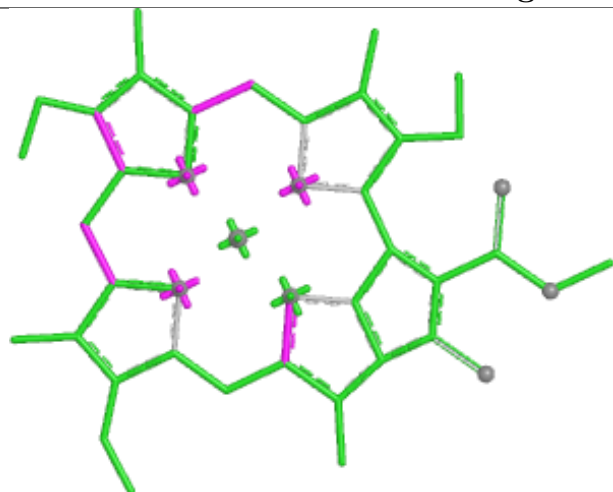
Torsions



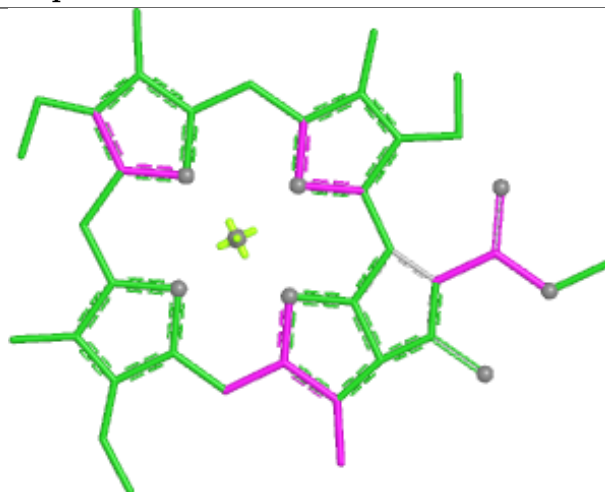
Rings



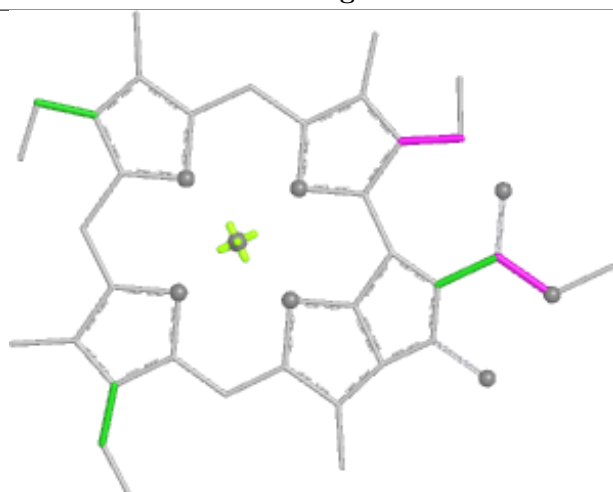
## Ligand CLA p 601



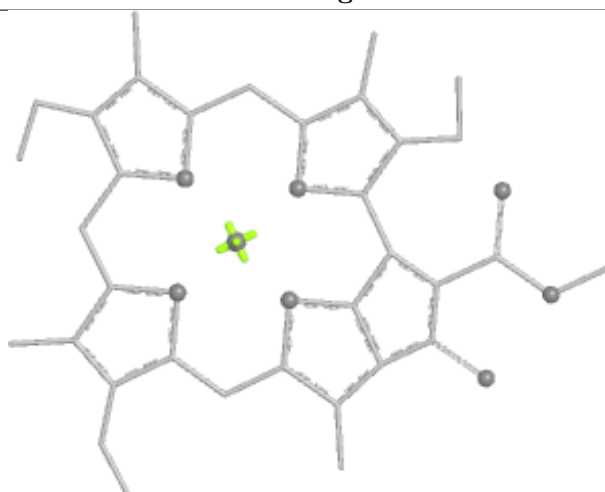
Bond lengths



Bond angles



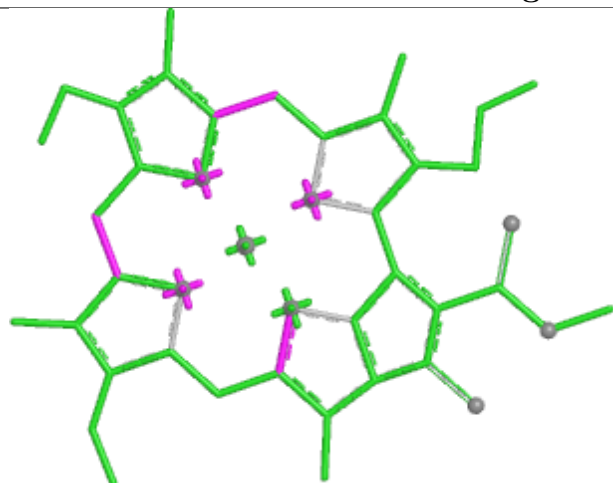
Torsions



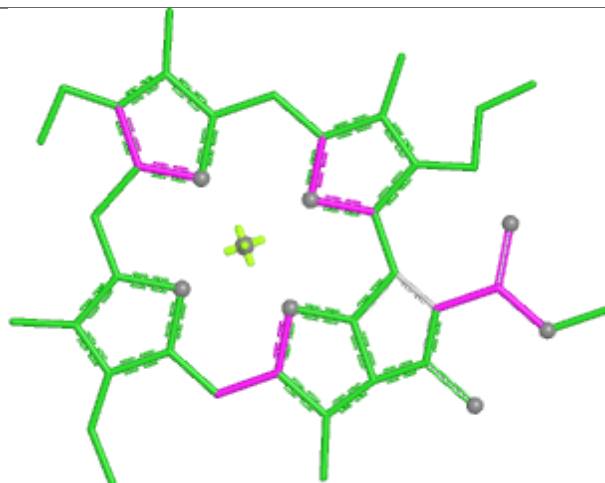
Rings



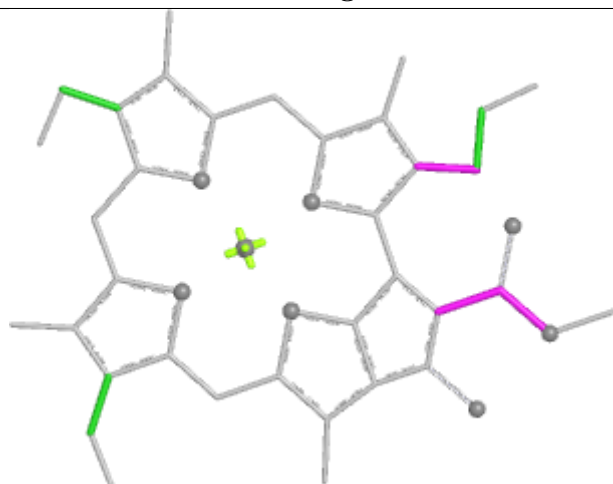
## Ligand CLA i 209



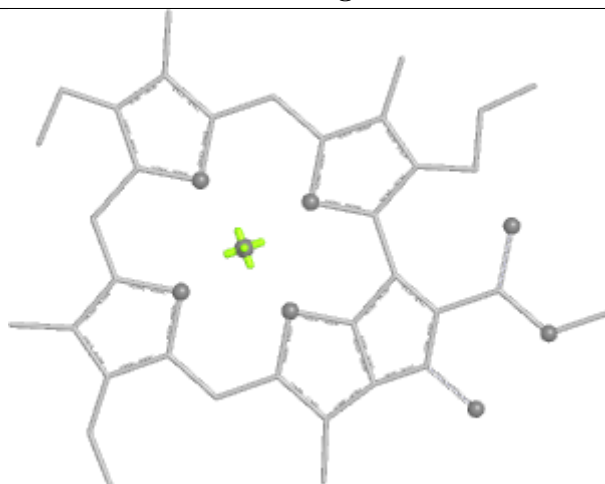
Bond lengths



Bond angles

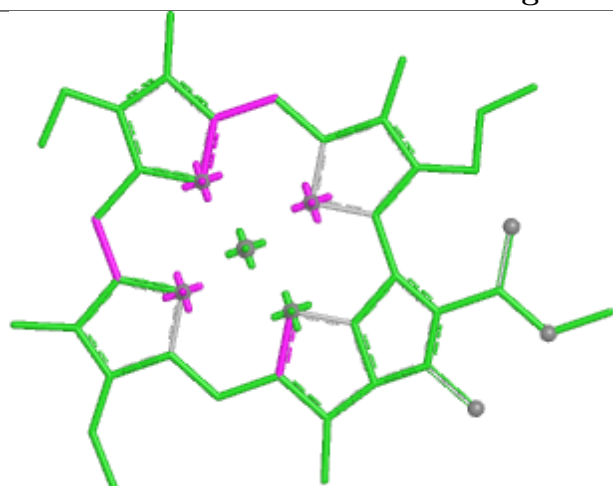


Torsions

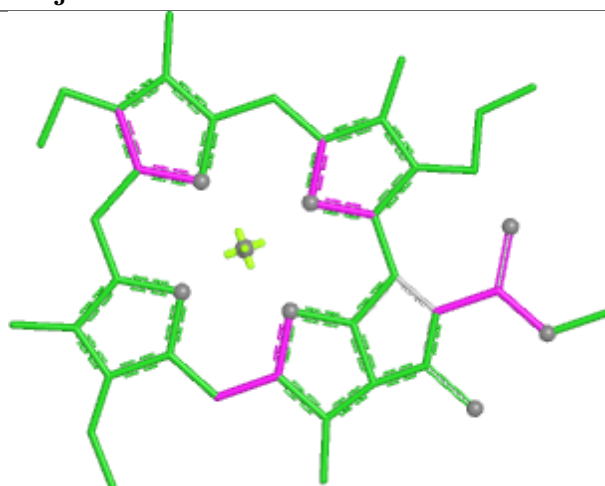


Rings

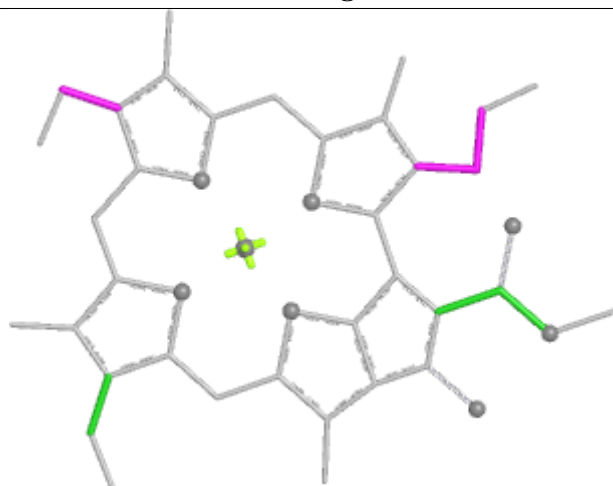
## Ligand CLA j 214



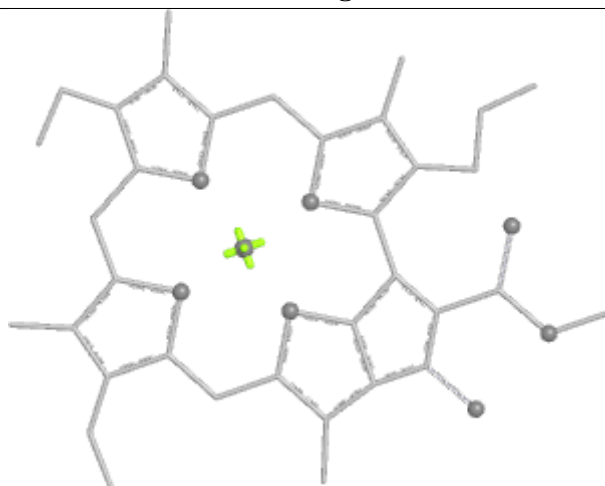
Bond lengths



Bond angles

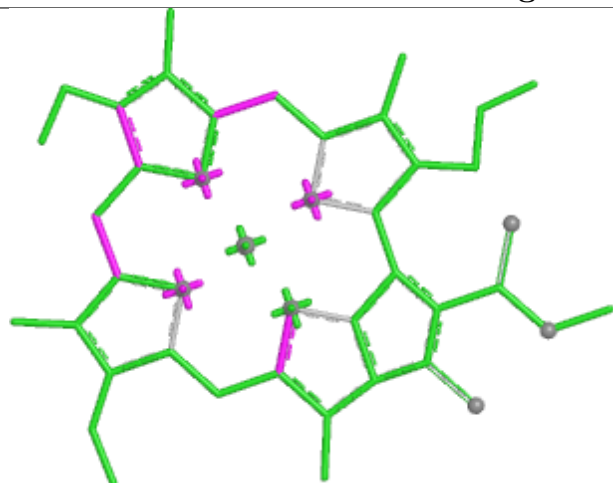


Torsions

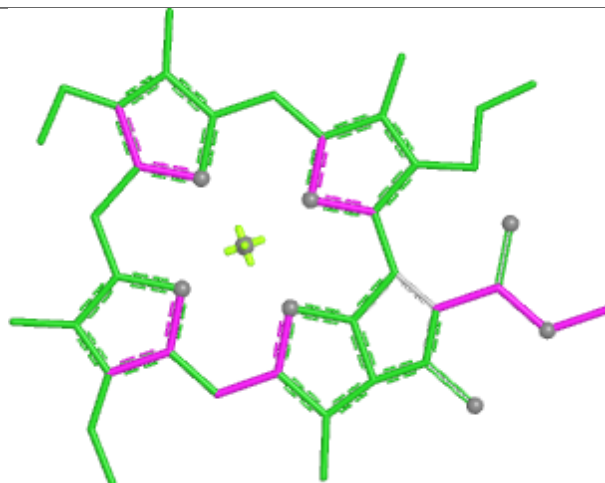


Rings

## Ligand CLA o 610



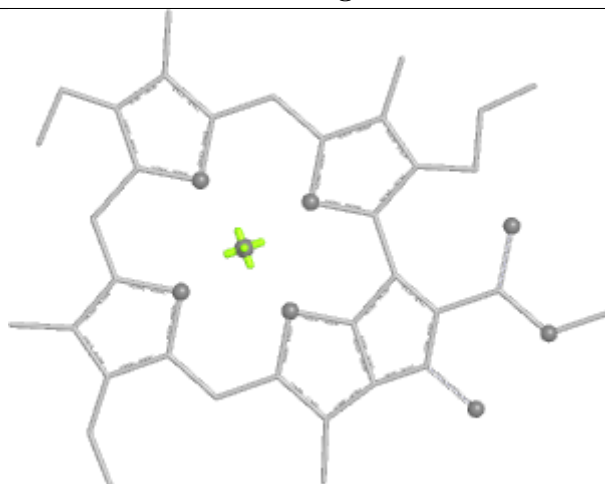
Bond lengths



Bond angles

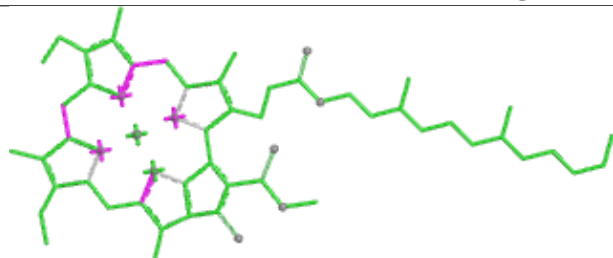


Torsions

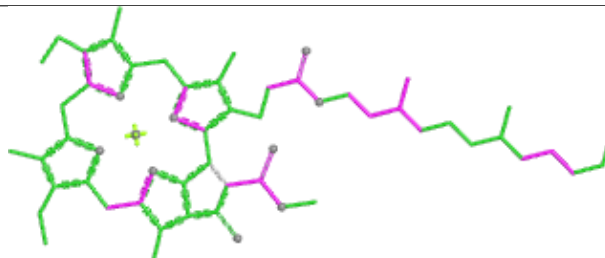


Rings

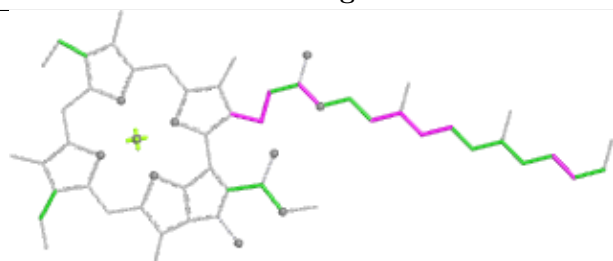
## Ligand CLA A 814



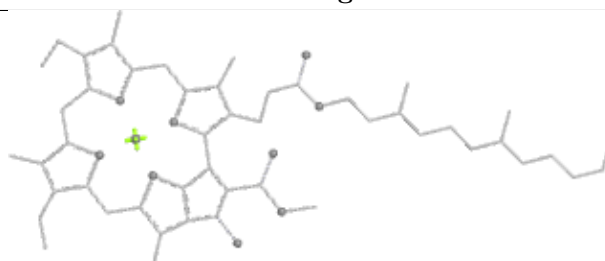
Bond lengths



Bond angles

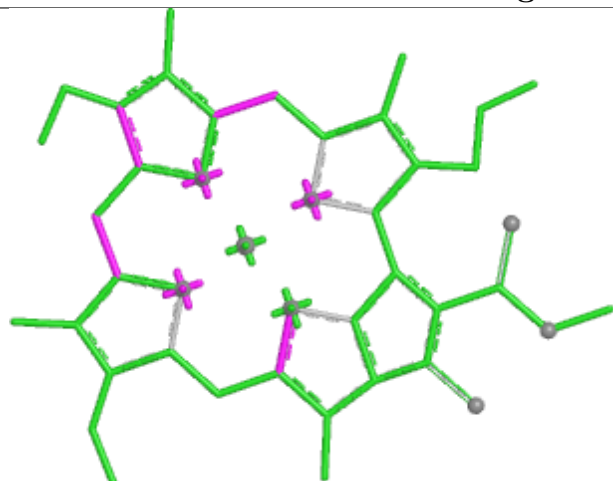


Torsions

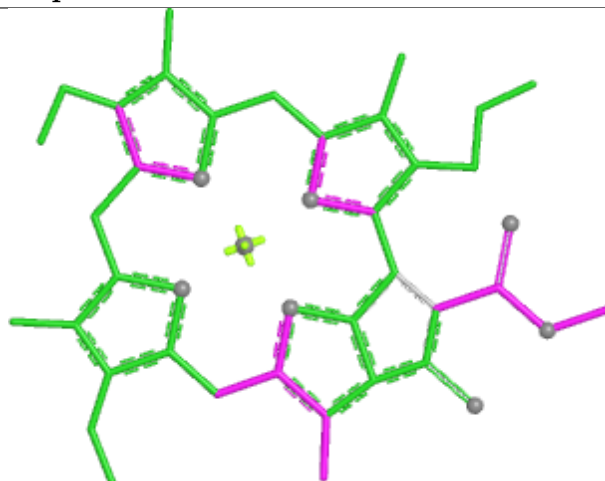


Rings

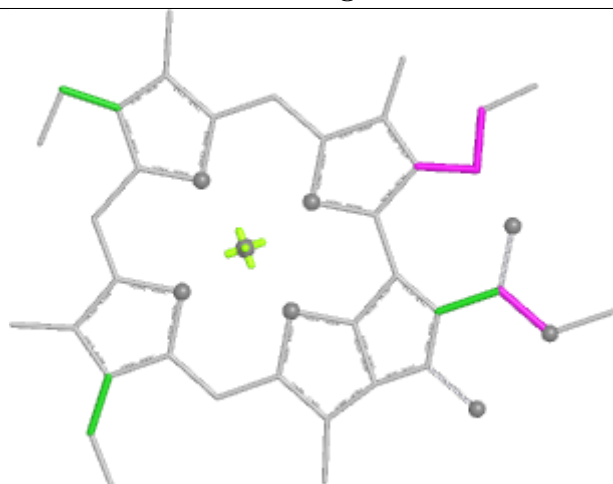
## Ligand CLA p 609



Bond lengths



Bond angles

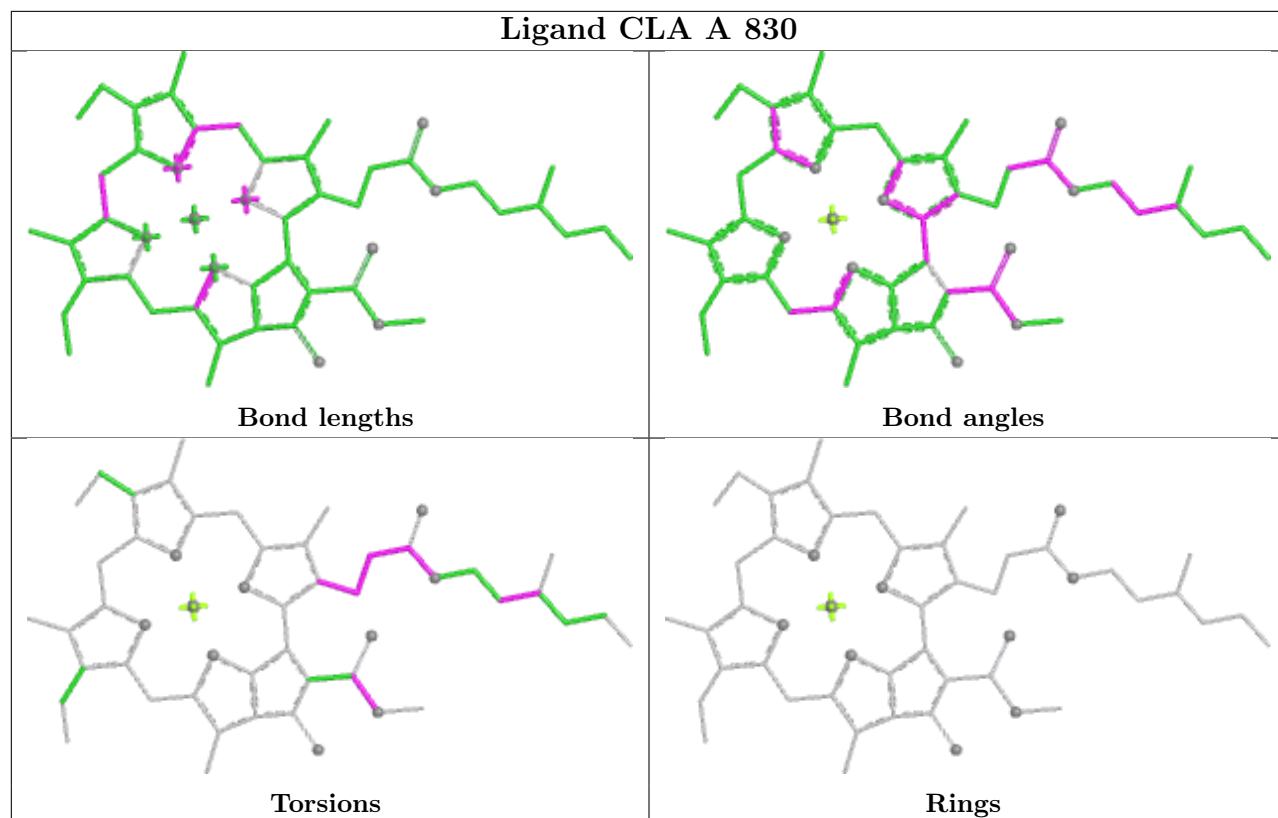


Torsions

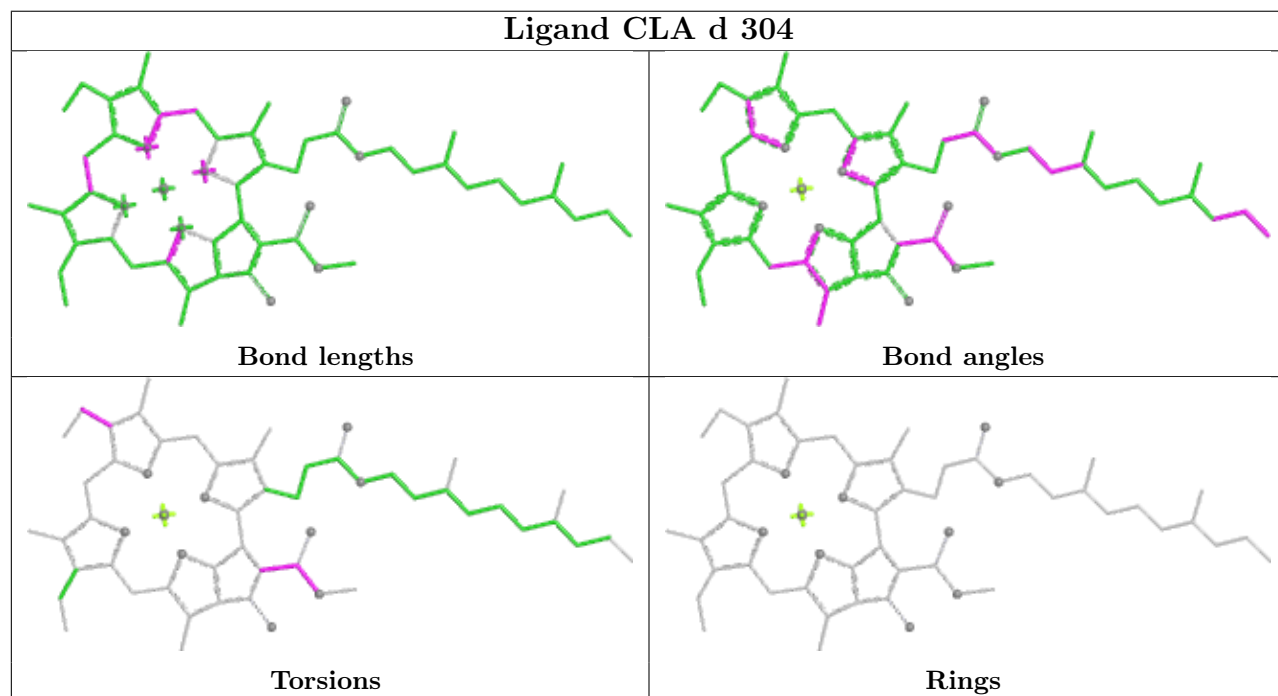


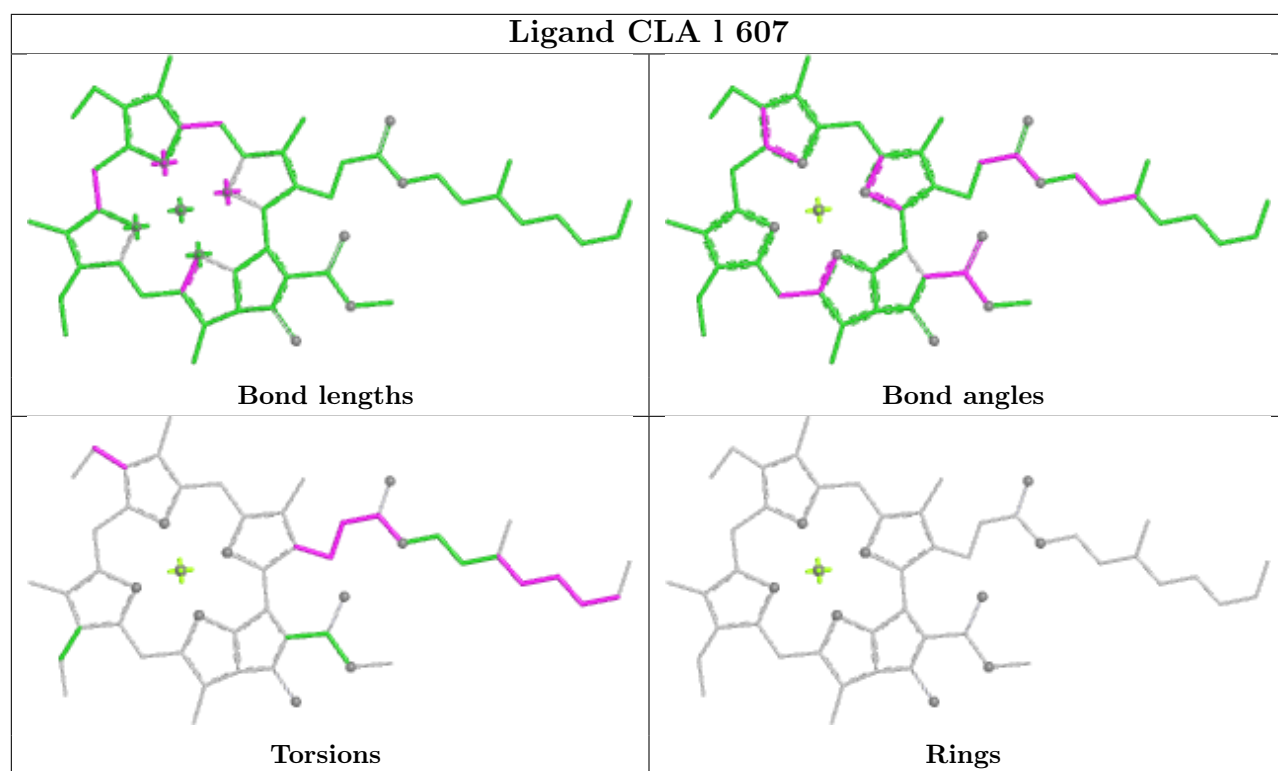
Rings

## Ligand CLA A 830

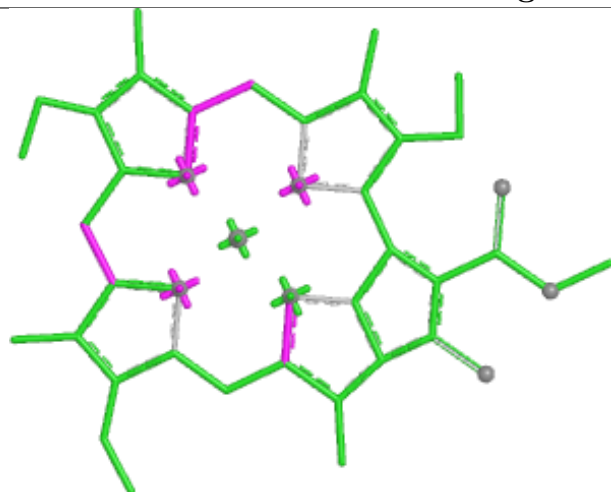


## Ligand CLA d 304

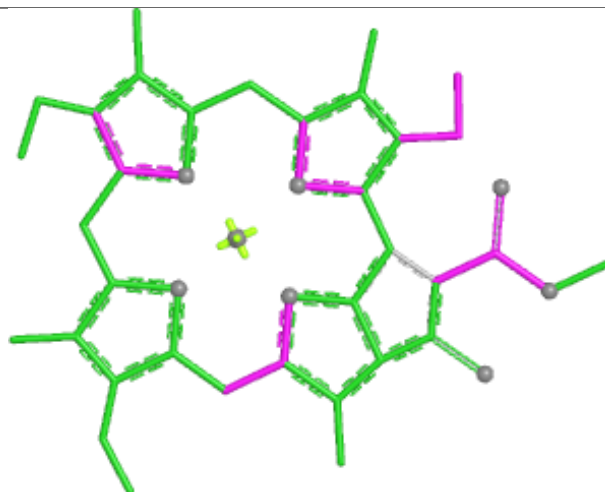




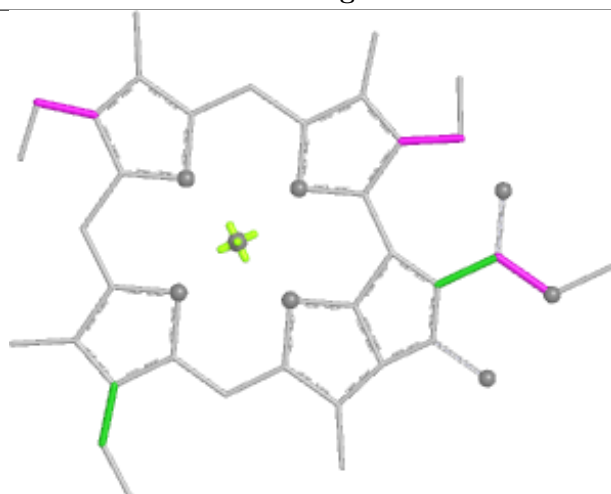
## Ligand CLA k 213



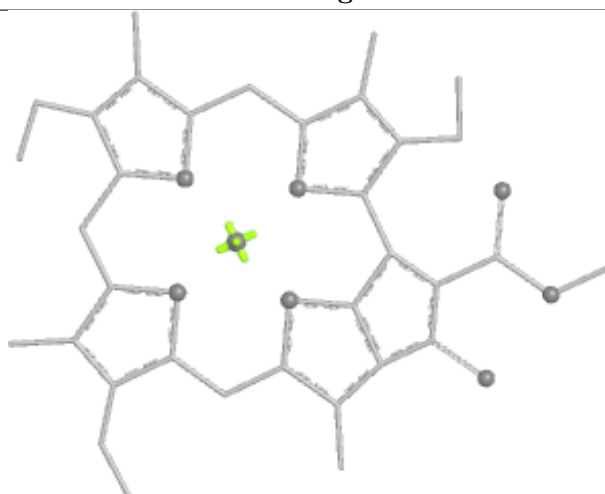
Bond lengths



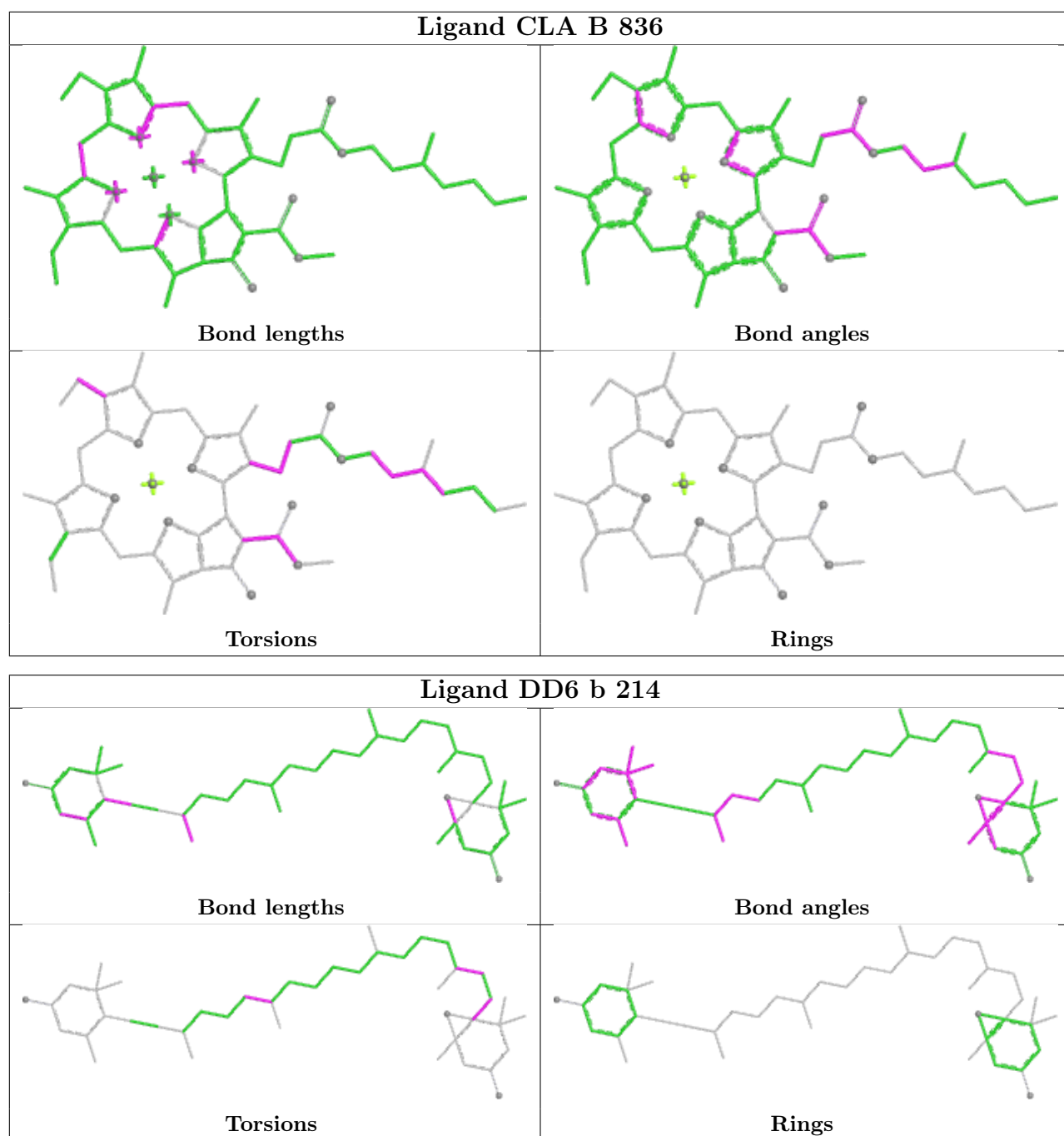
Bond angles



Torsions

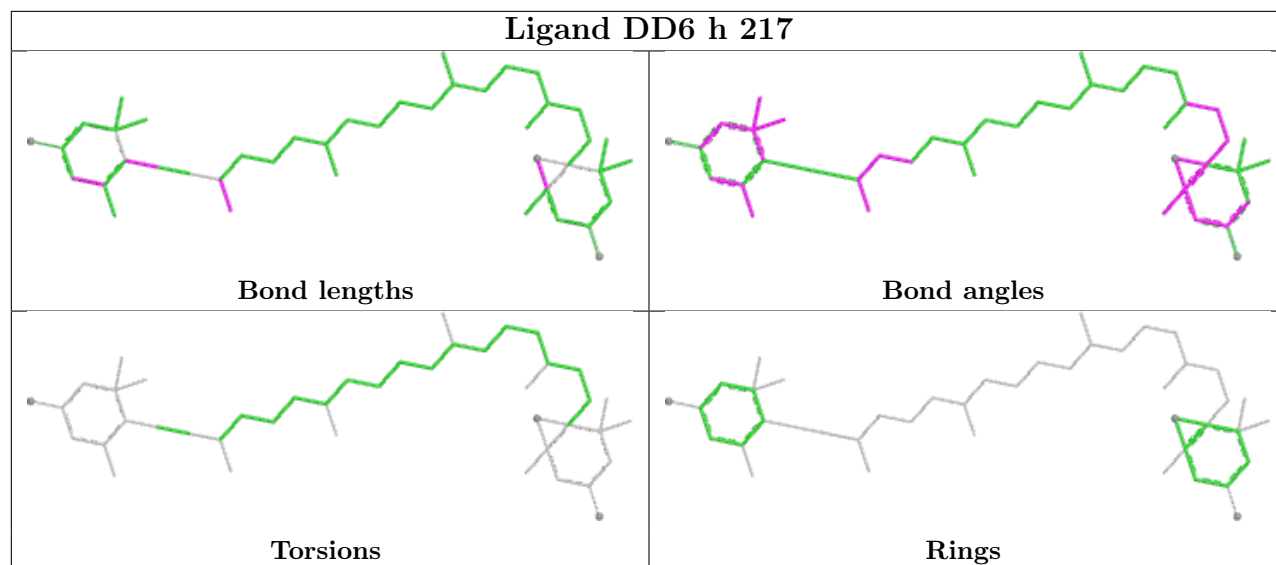


Rings

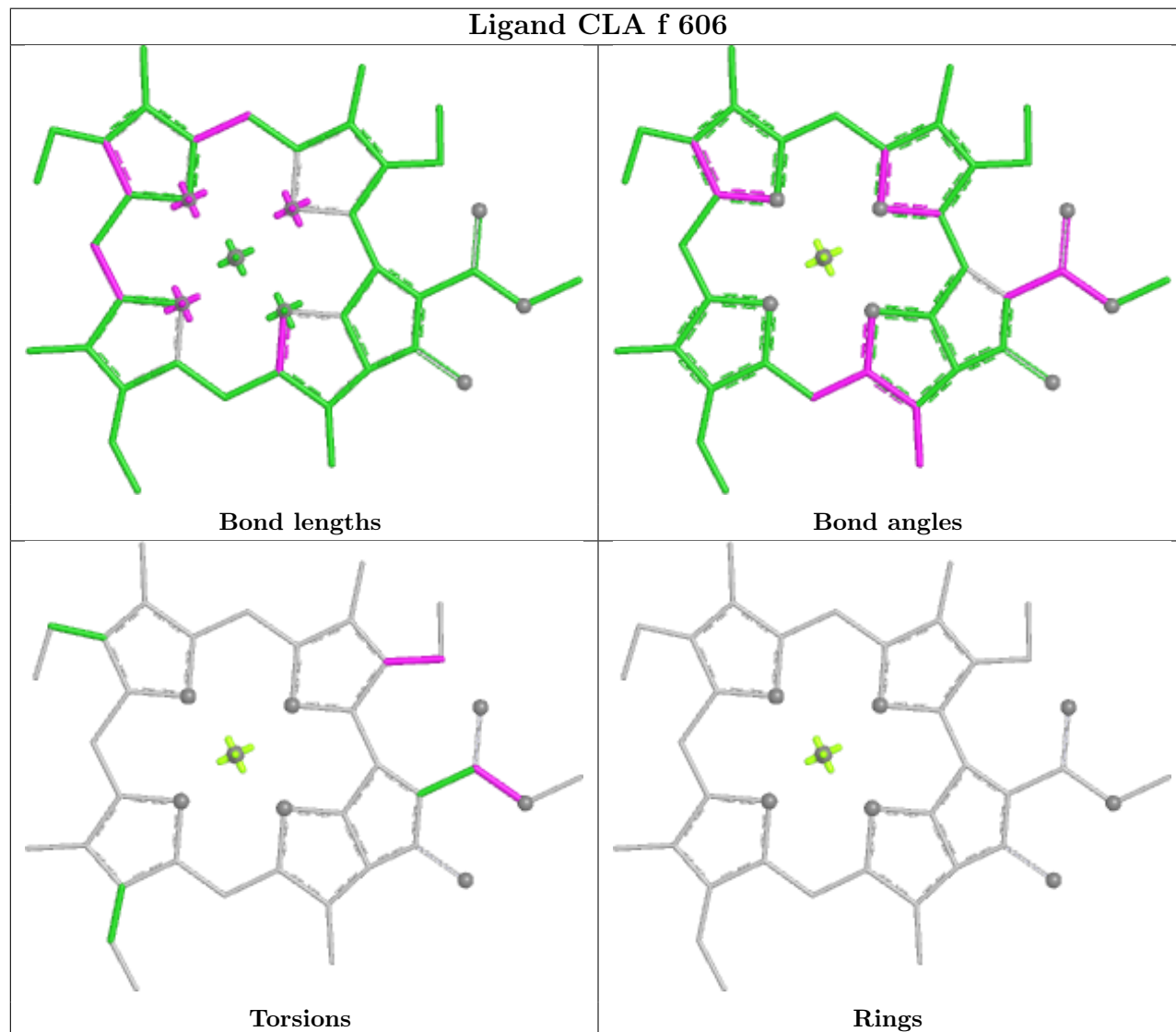




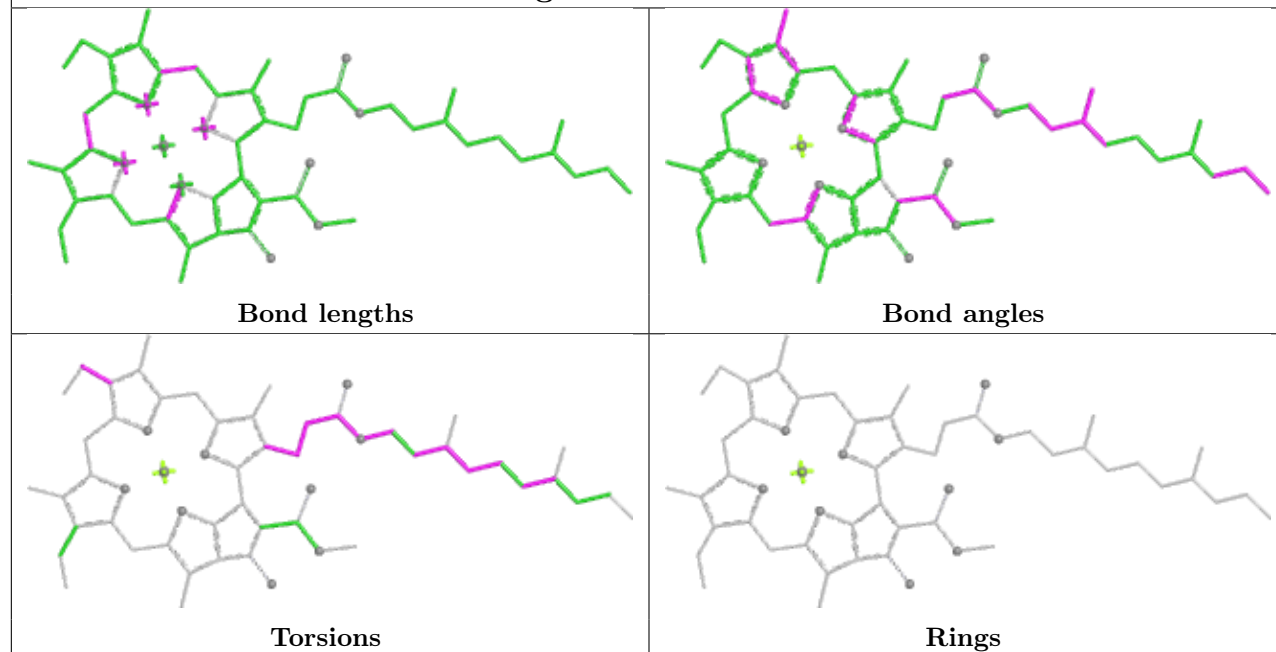
## Ligand DD6 h 217



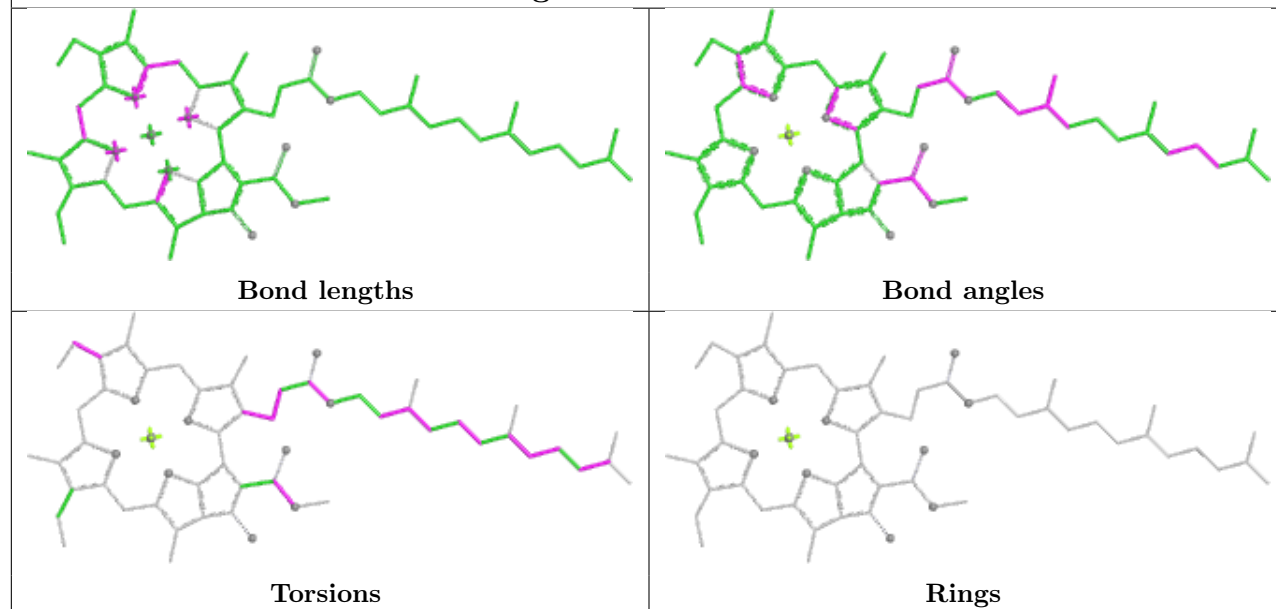
## Ligand CLA f 606



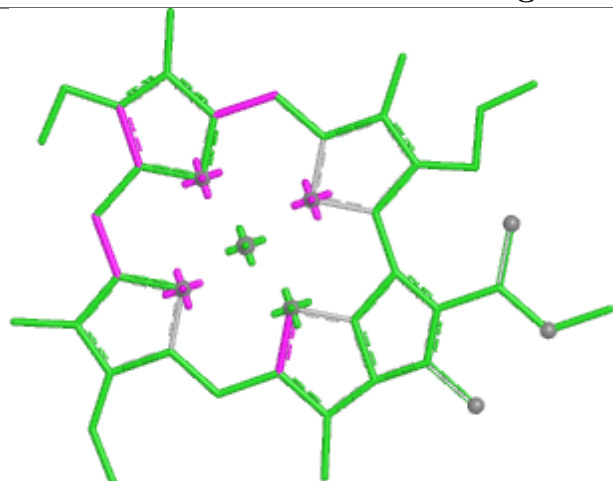
## Ligand CLA k 208



## Ligand CLA B 821



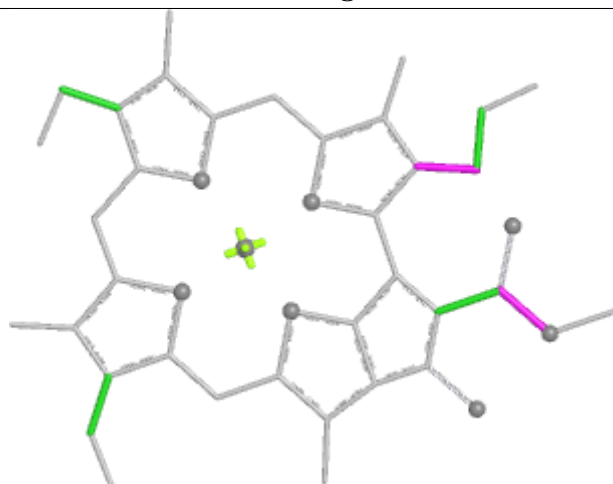
## Ligand CLA k 202



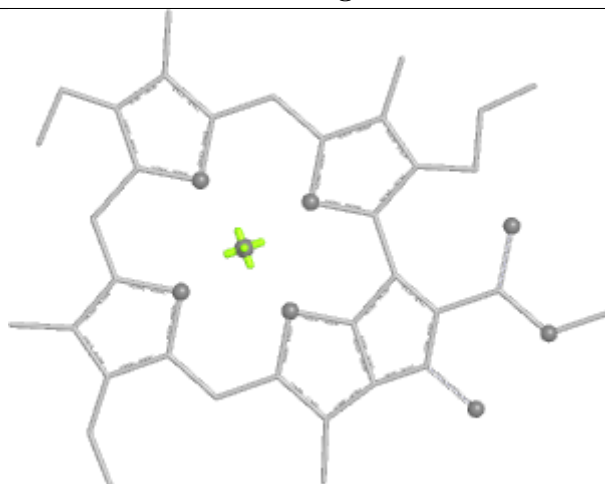
Bond lengths



Bond angles

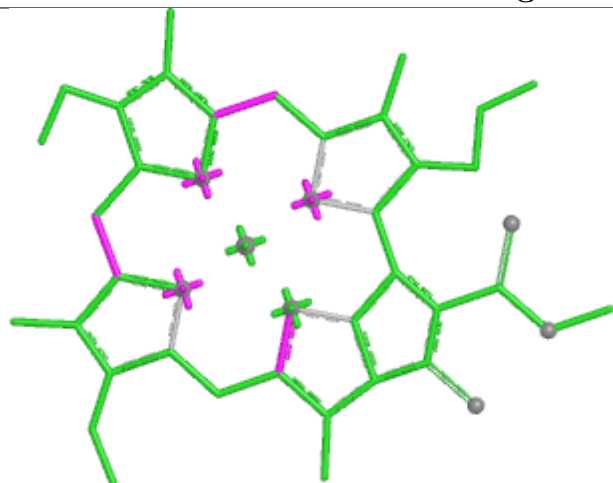


Torsions

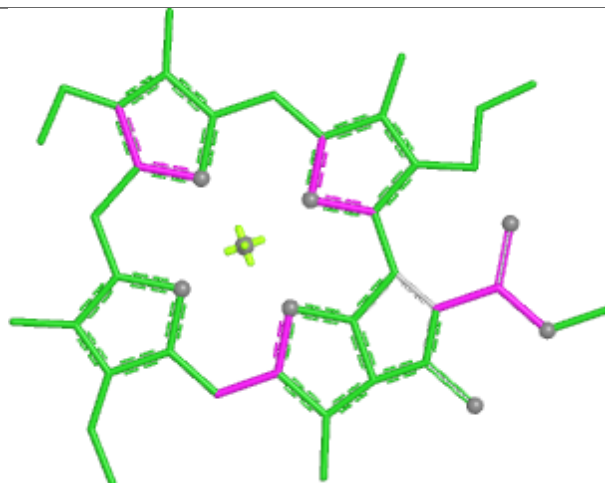


Rings

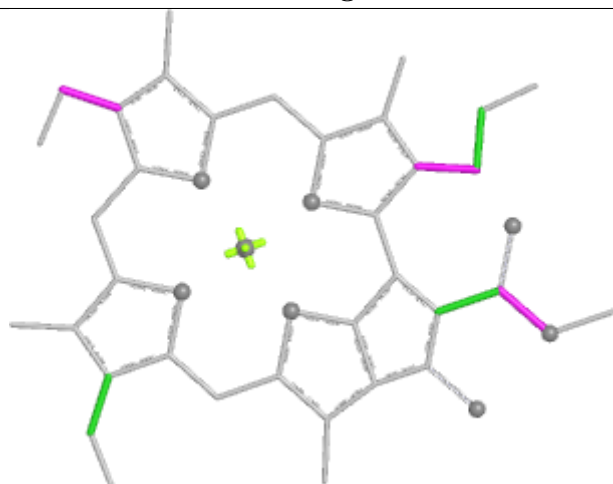
## Ligand CLA h 213



Bond lengths



Bond angles

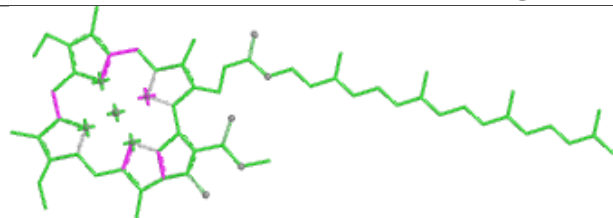


Torsions

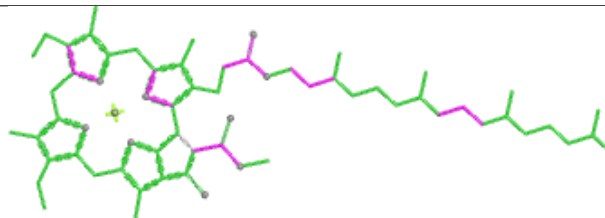


Rings

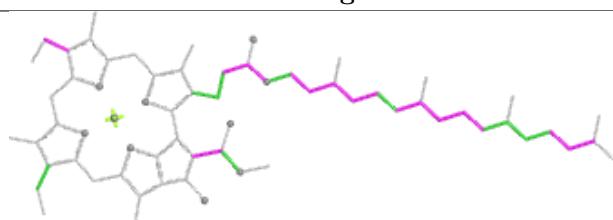
## Ligand CLA A 809



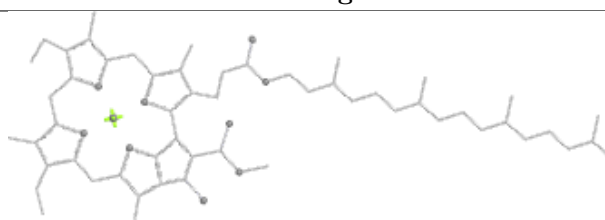
Bond lengths



Bond angles

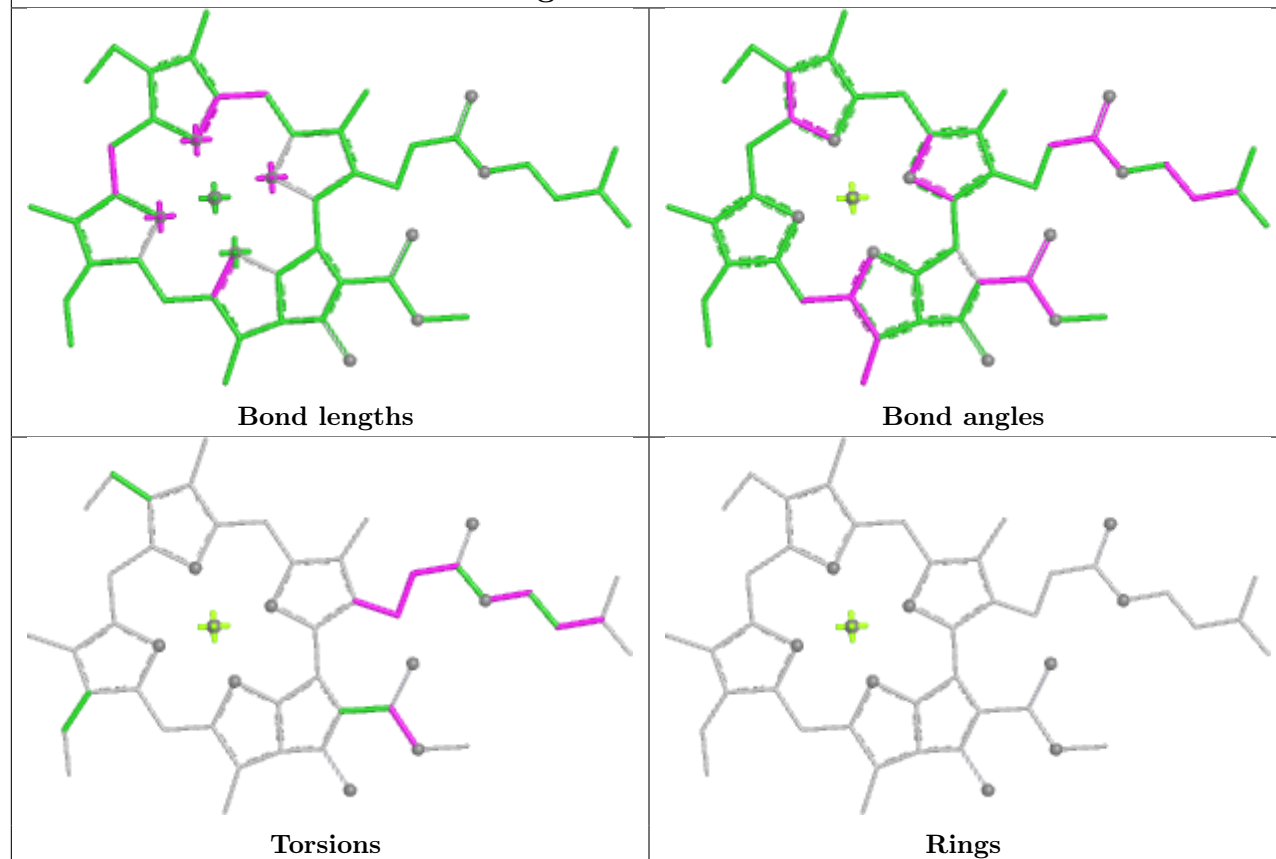


Torsions

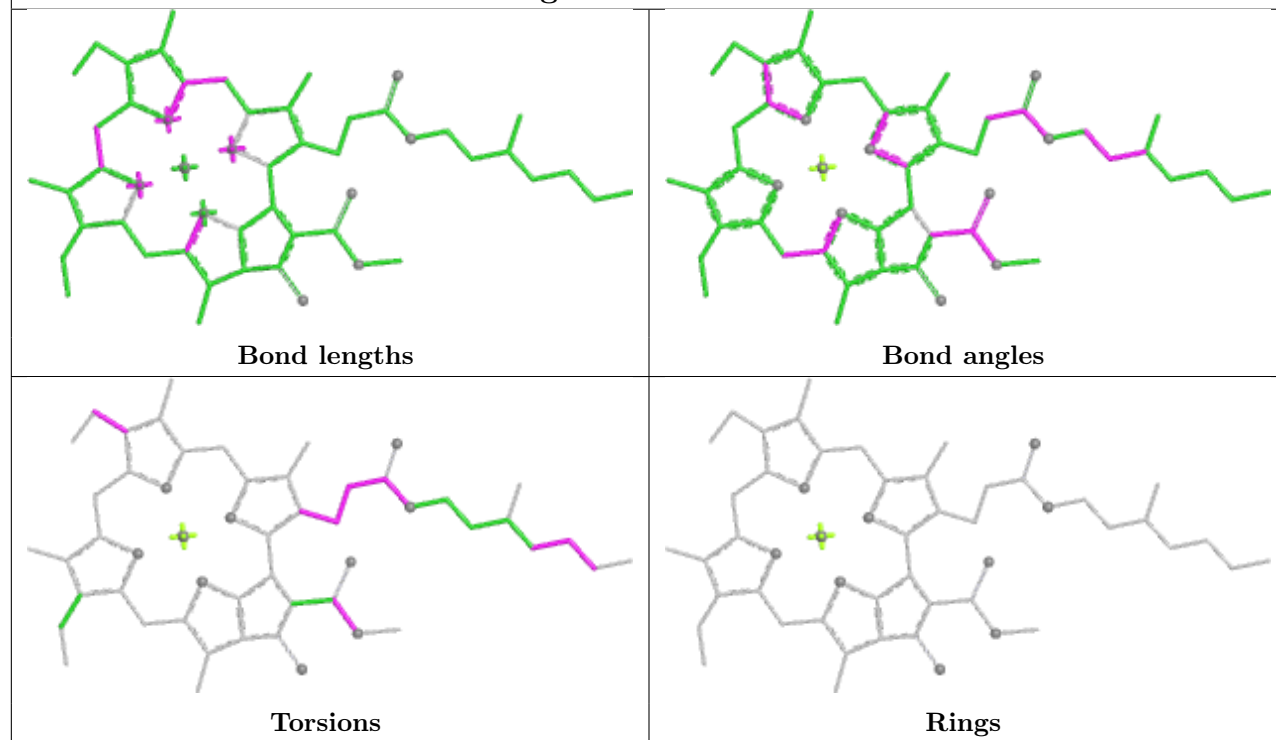


Rings

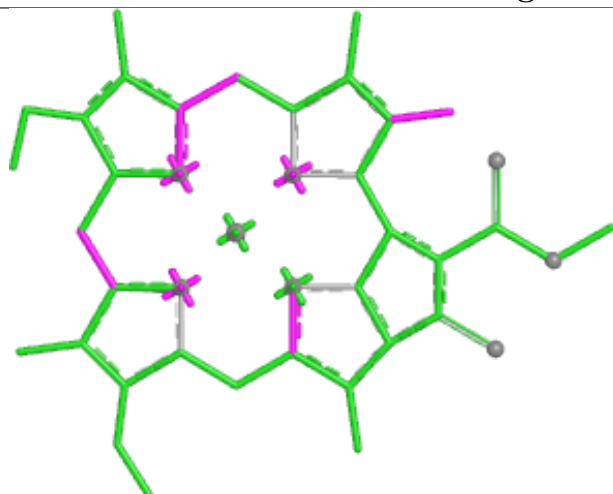
## Ligand CLA c 308



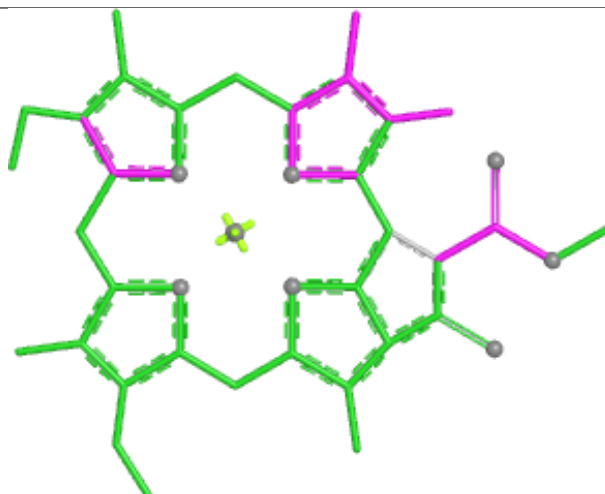
## Ligand CLA i 202



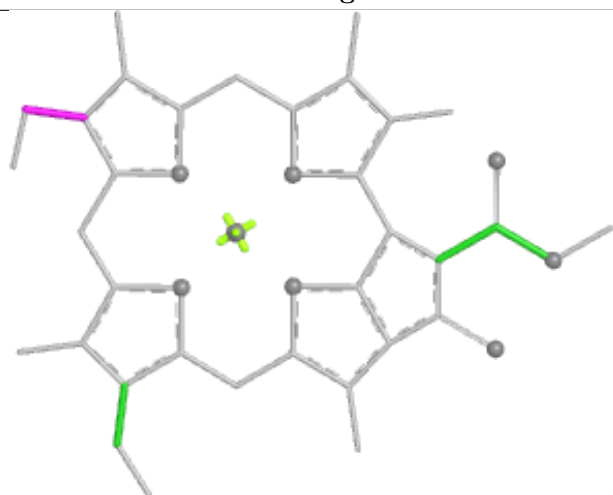
## Ligand CLA b 208



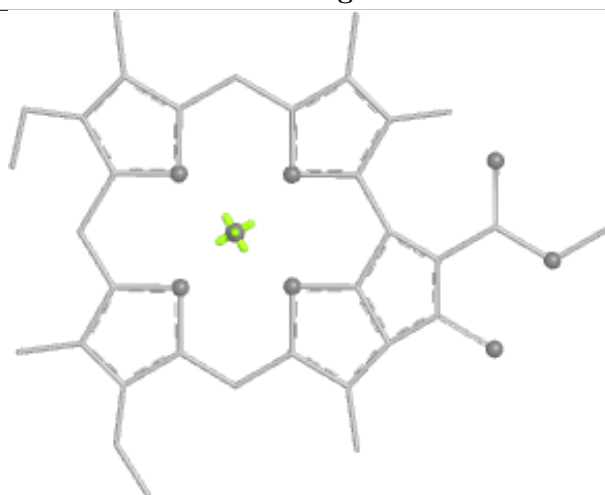
Bond lengths



Bond angles

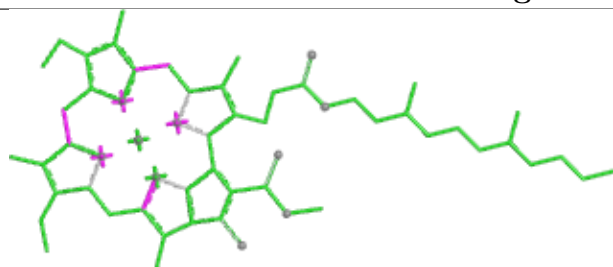


Torsions

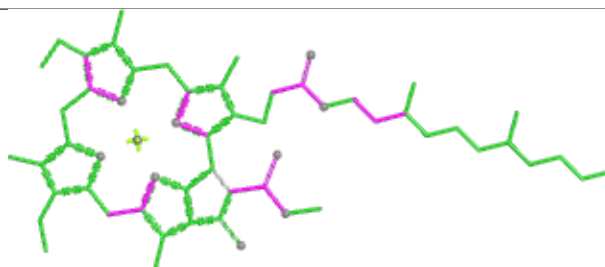


Rings

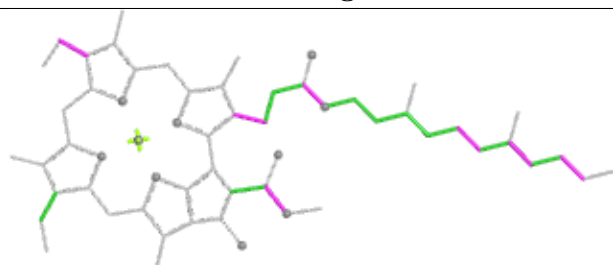
## Ligand CLA A 813



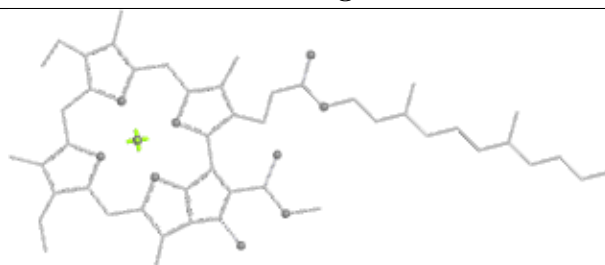
Bond lengths



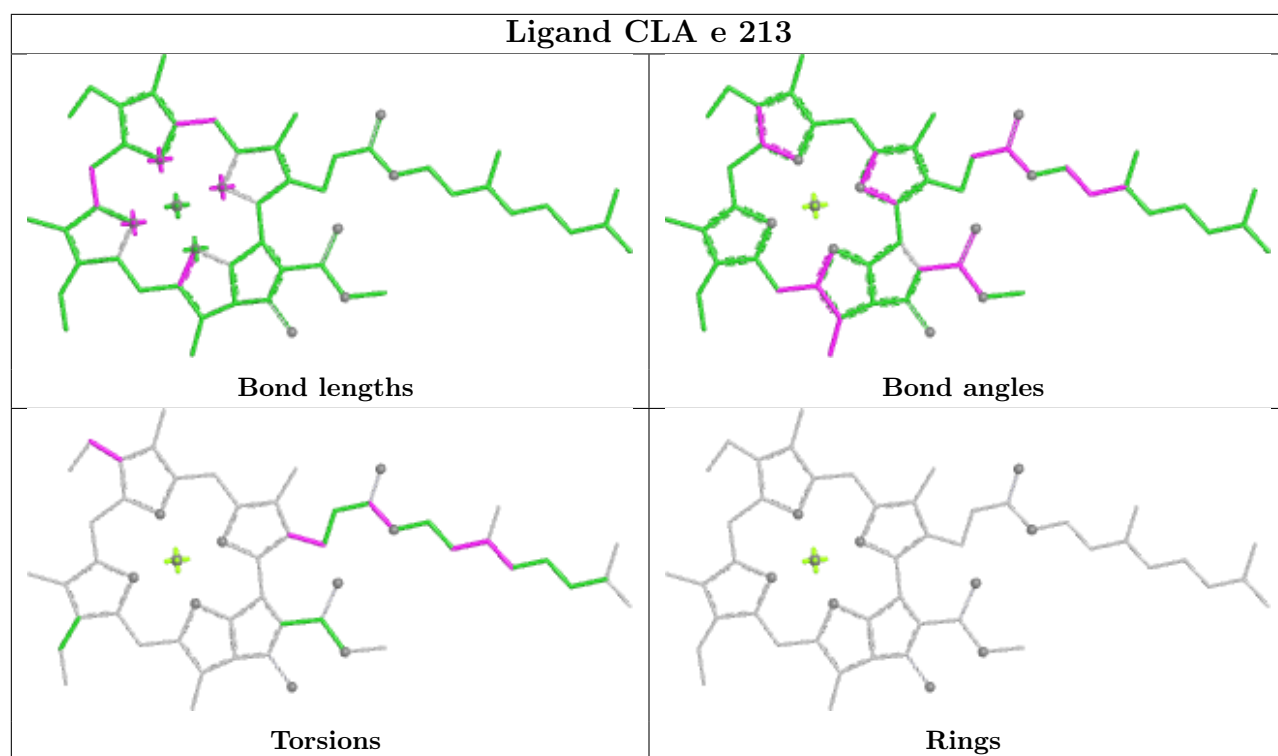
Bond angles



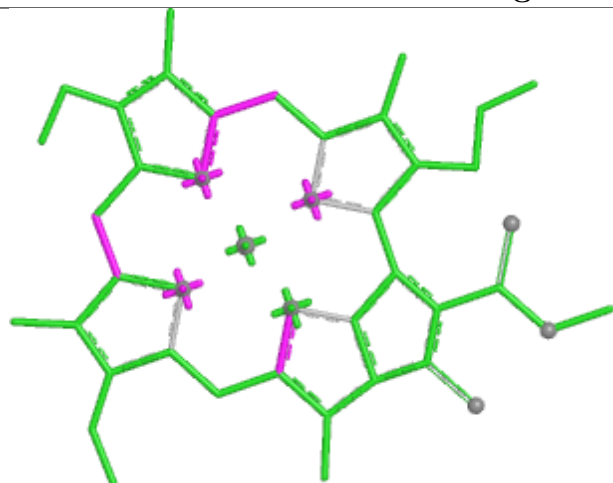
Torsions



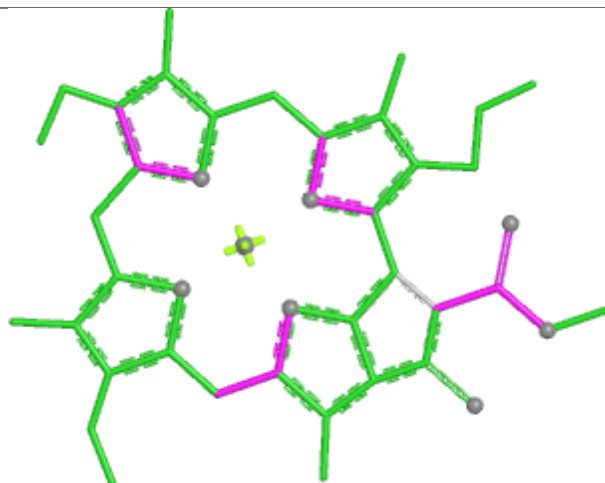
Rings



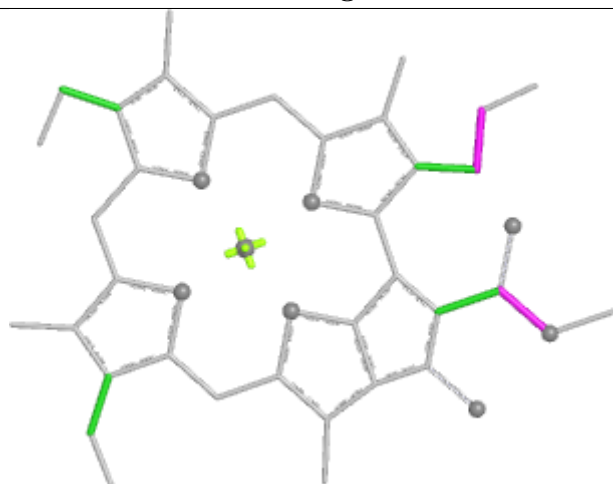
## Ligand CLA A 827



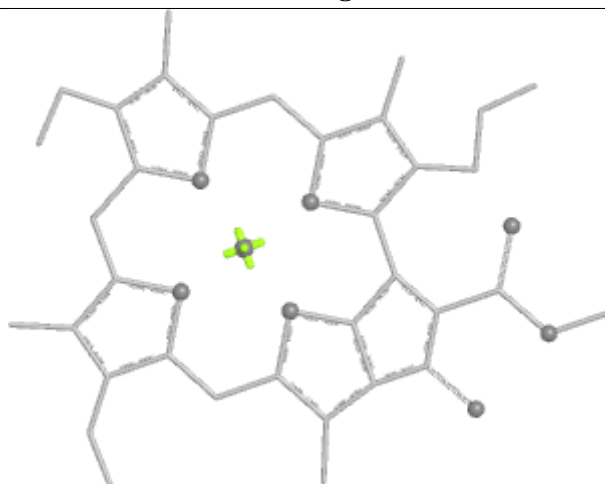
Bond lengths



Bond angles



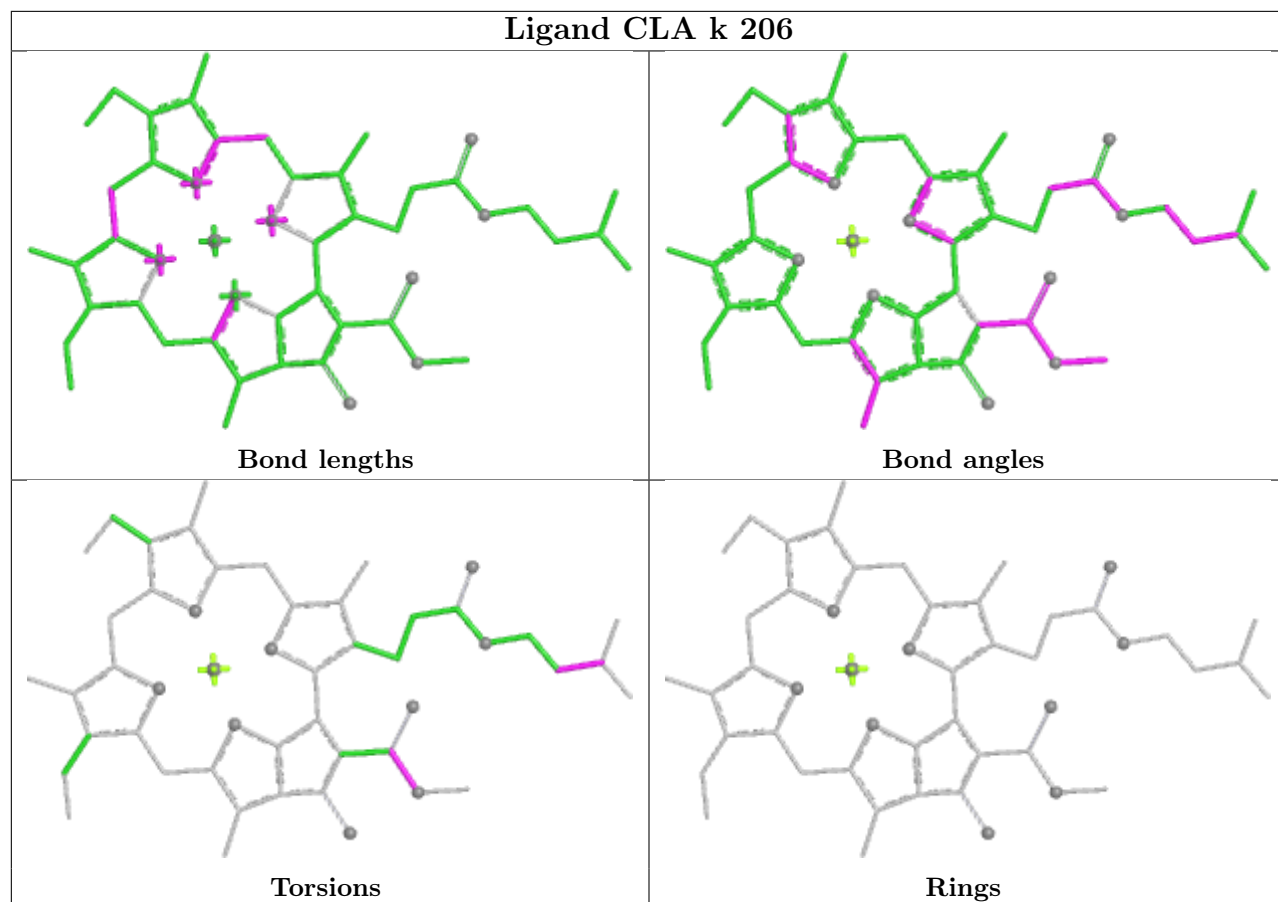
Torsions



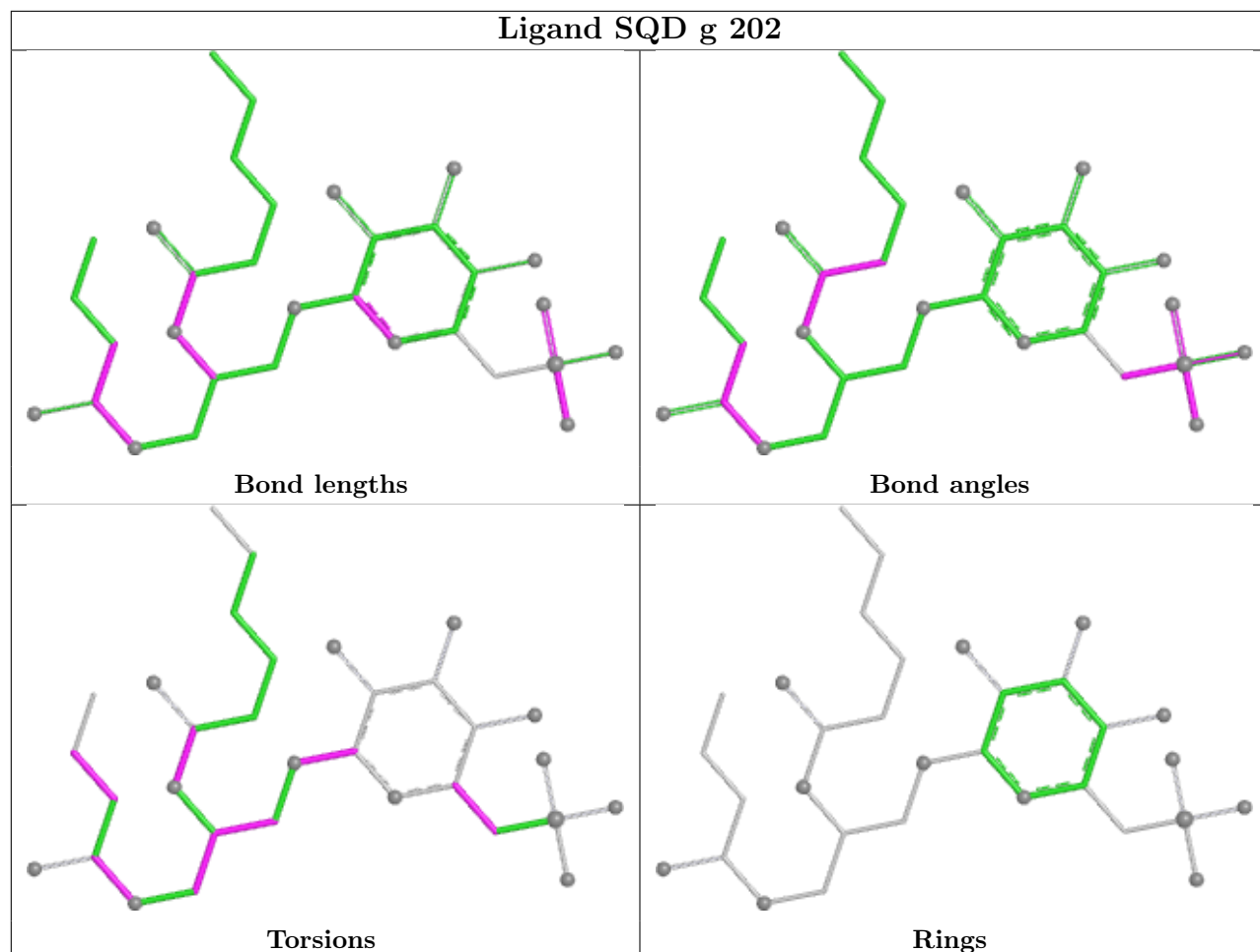
Rings



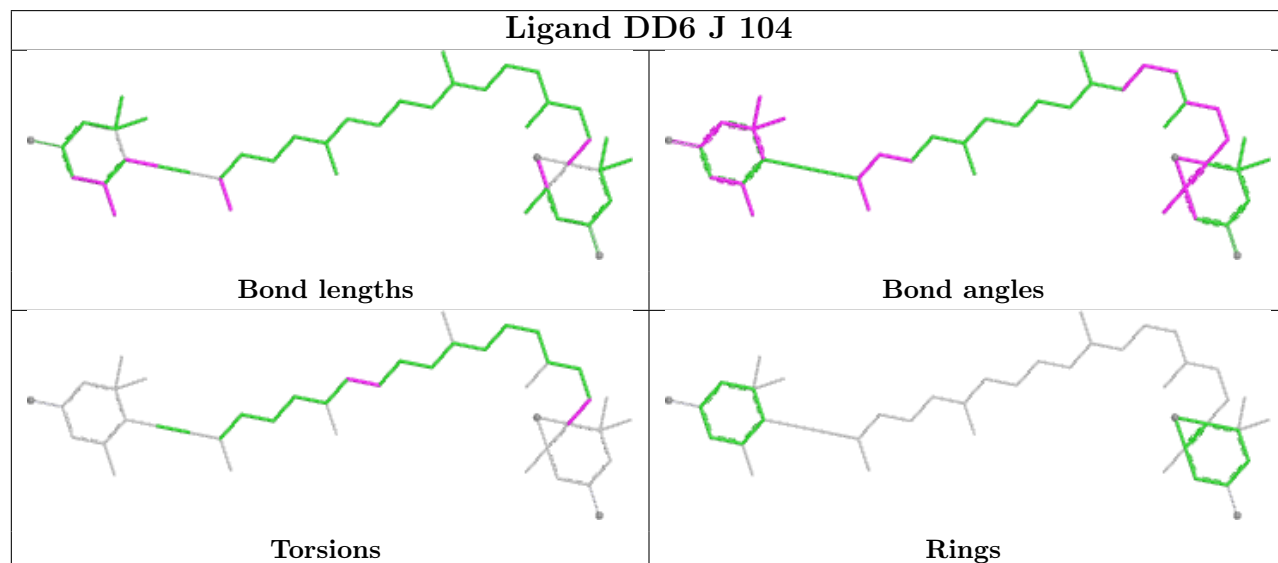
## Ligand CLA k 206



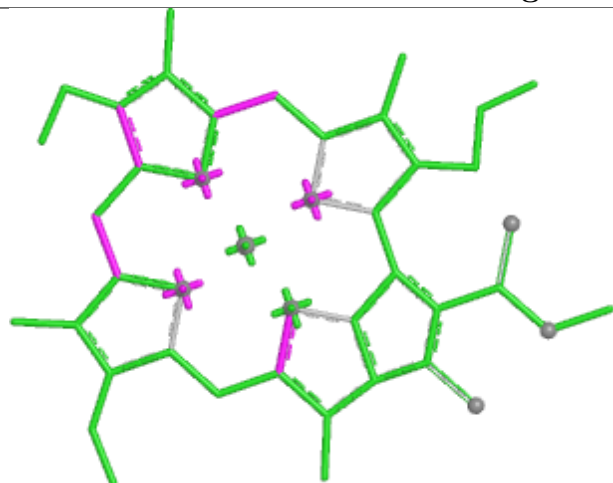
## Ligand SQD g 202



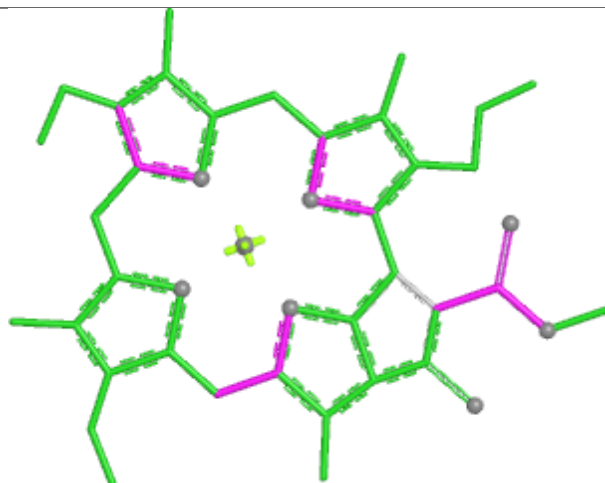
## Ligand DD6 J 104



## Ligand CLA f 612



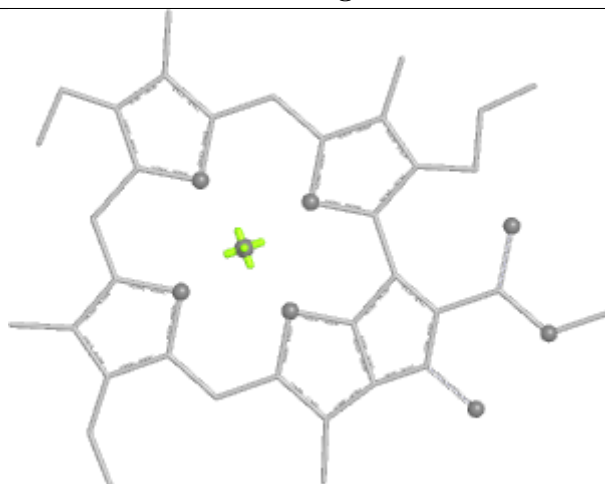
Bond lengths



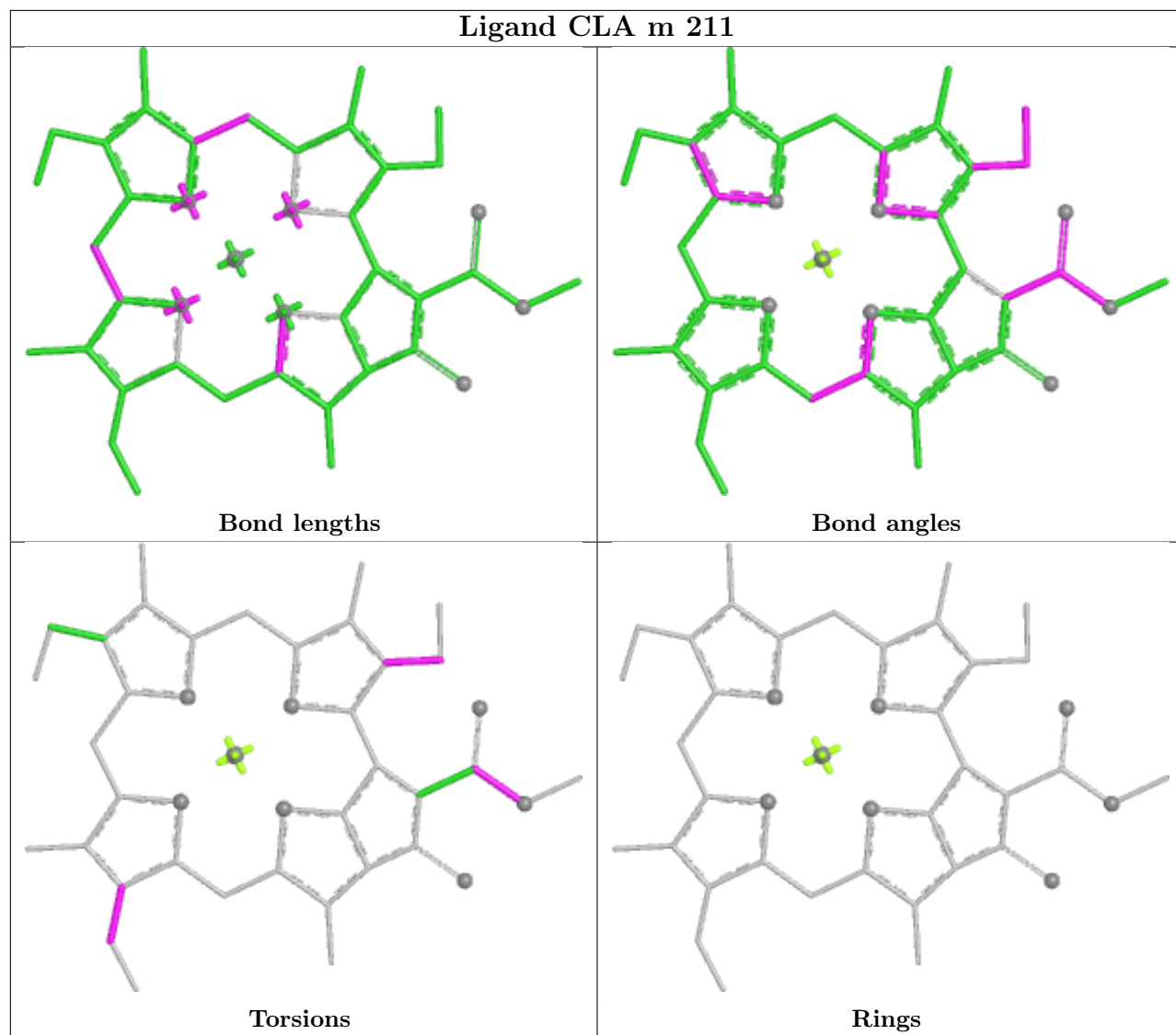
Bond angles



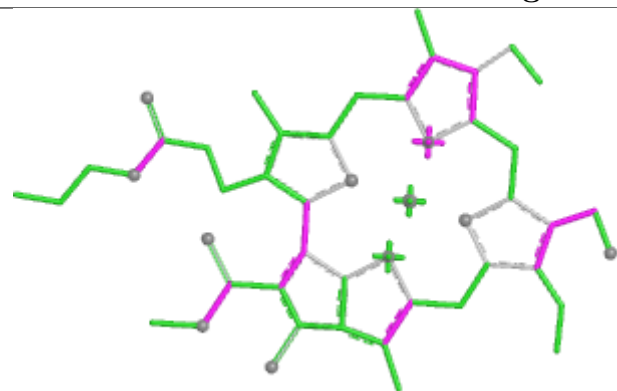
Torsions



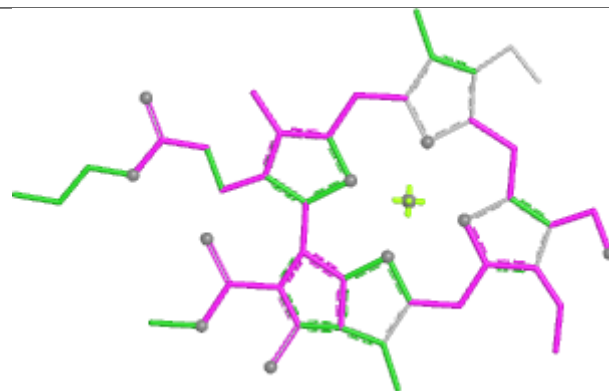
Rings



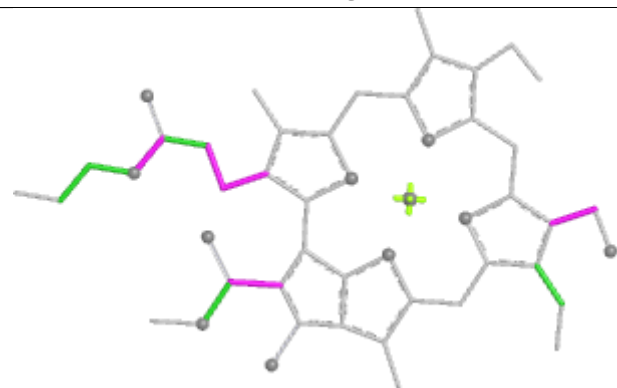
## Ligand CHL c 307



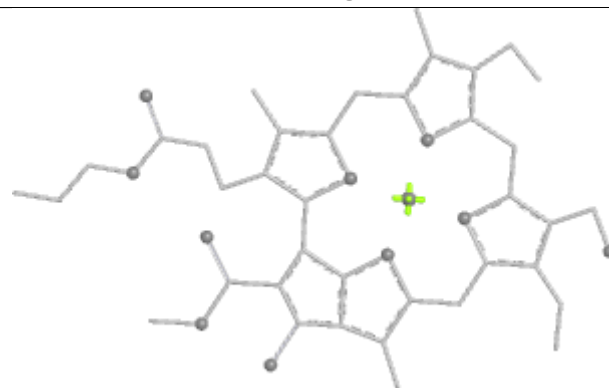
Bond lengths



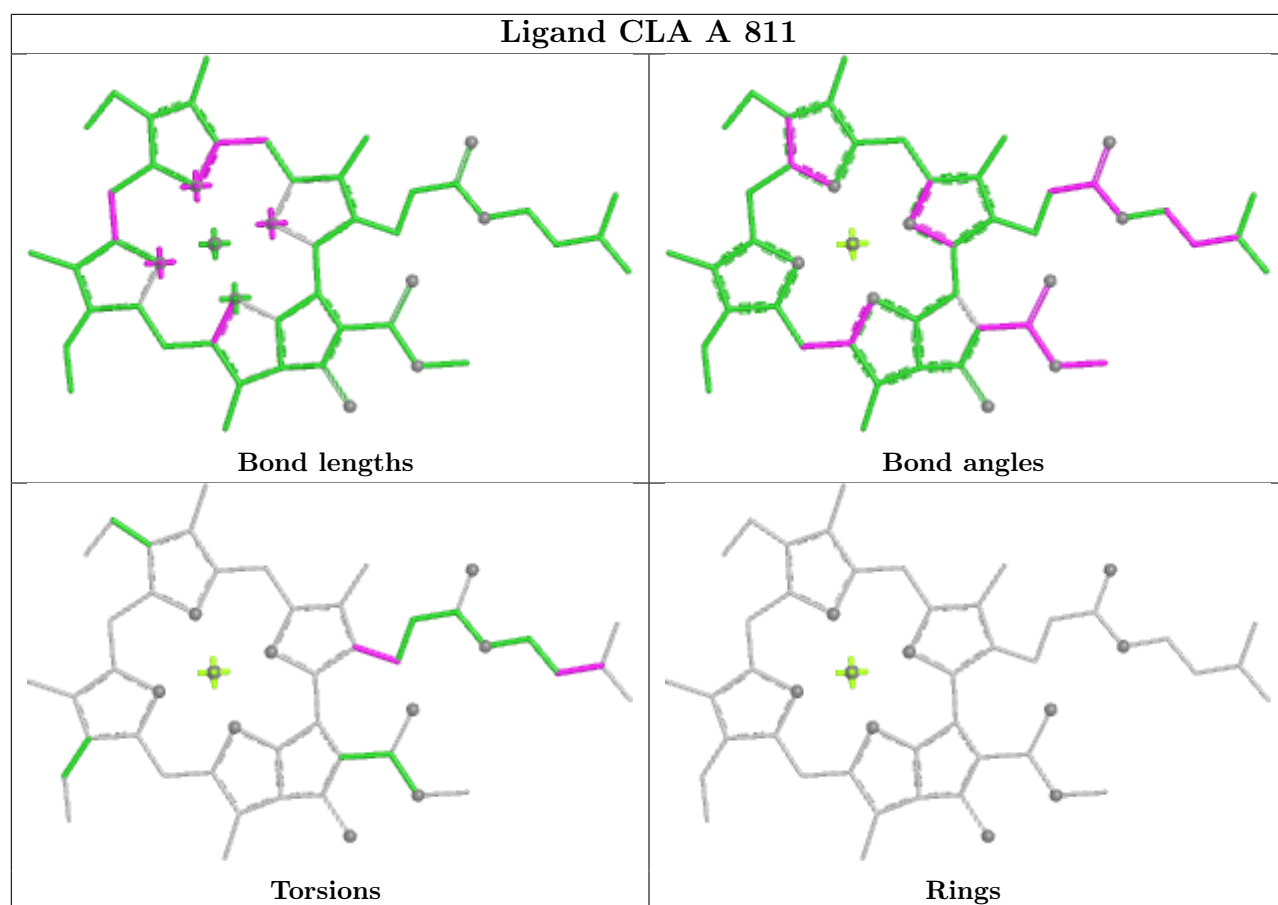
Bond angles



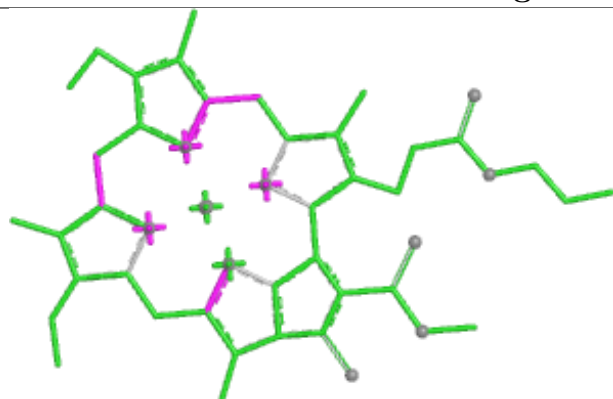
Torsions



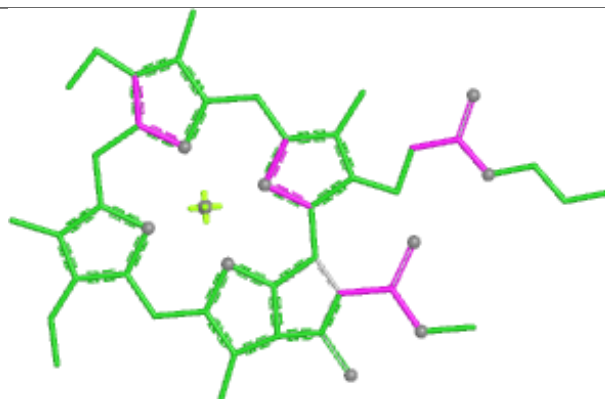
Rings



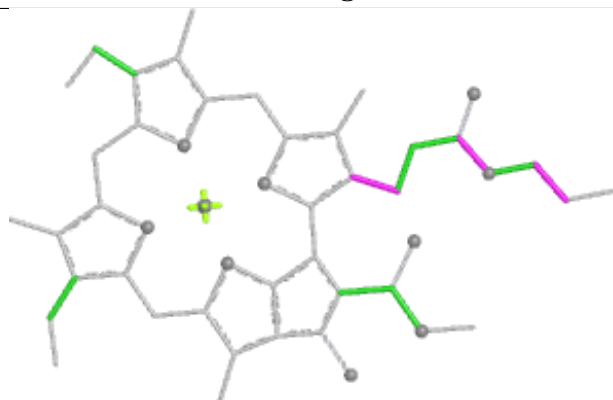
## Ligand CLA A 845



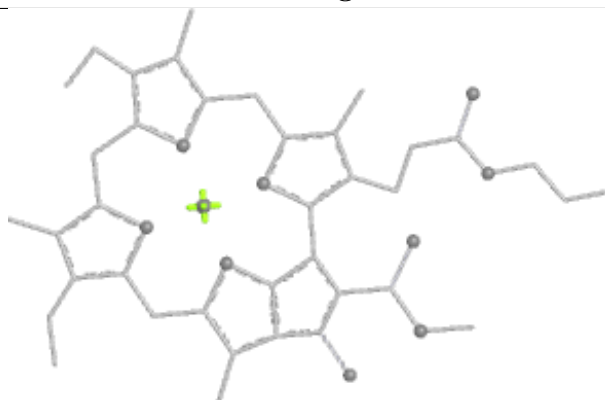
Bond lengths



Bond angles

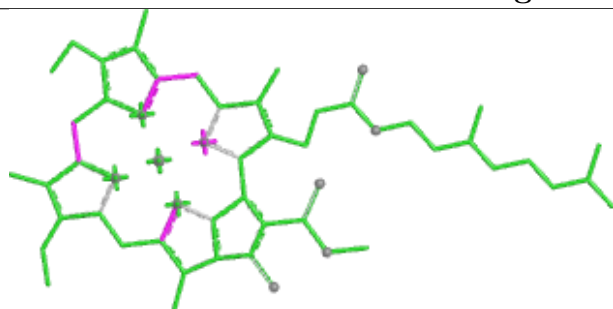


Torsions

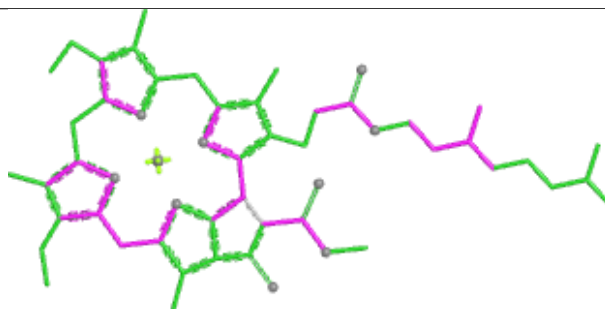


Rings

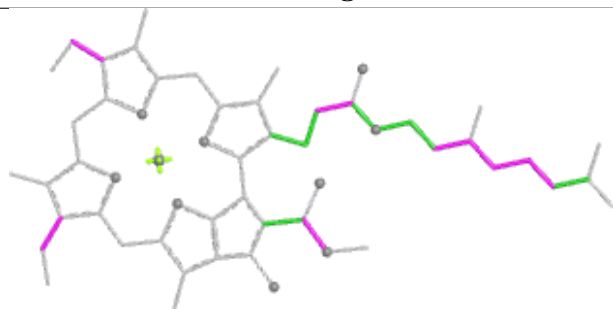
## Ligand CLA B 803



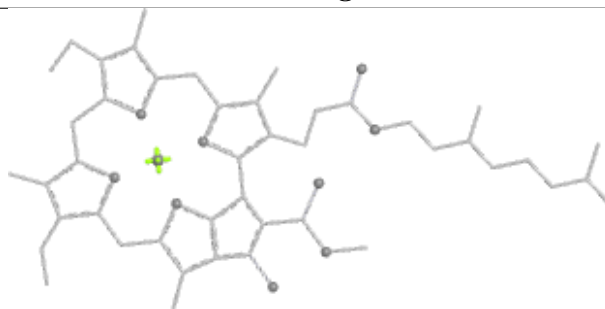
Bond lengths



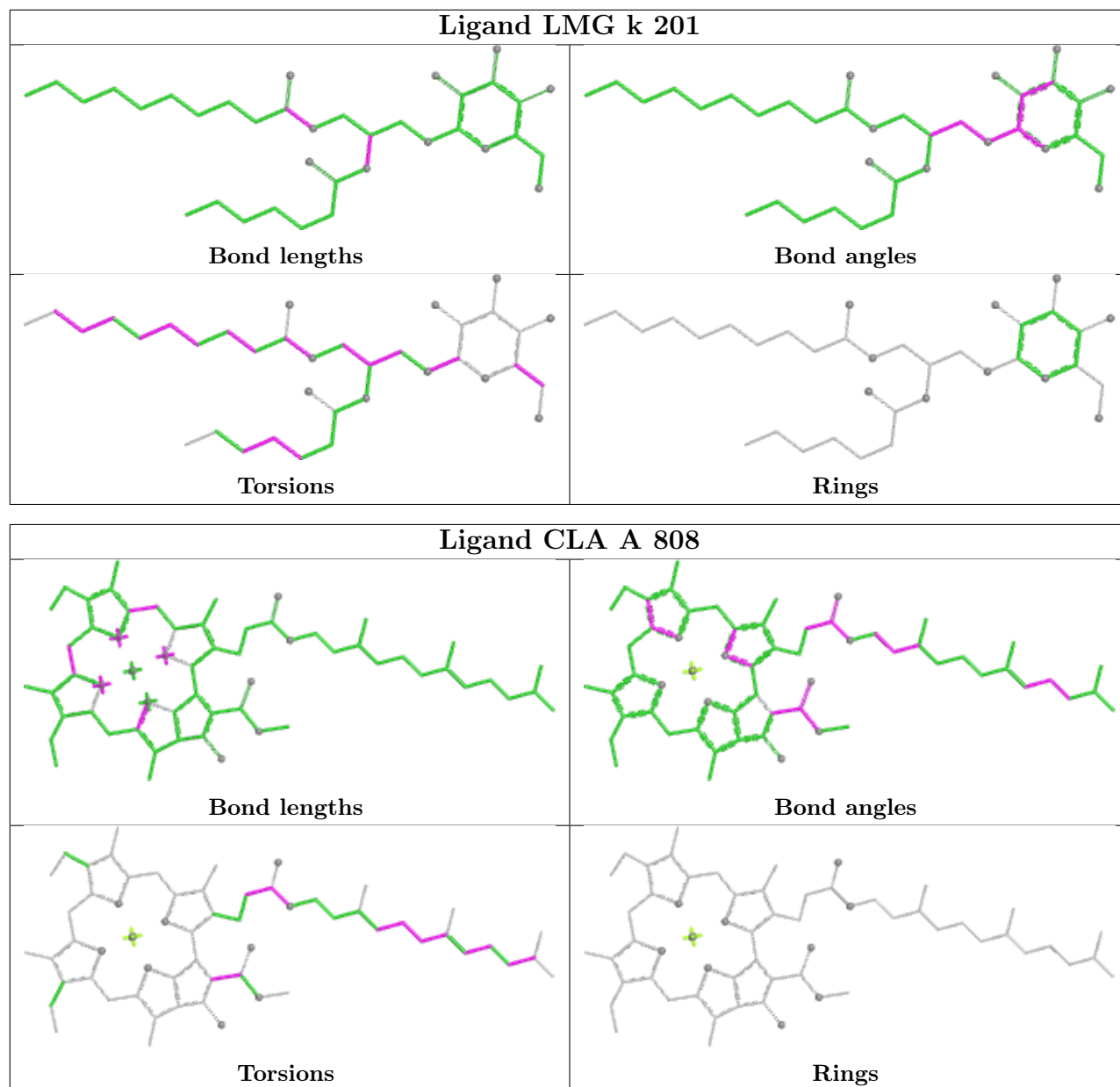
Bond angles



Torsions

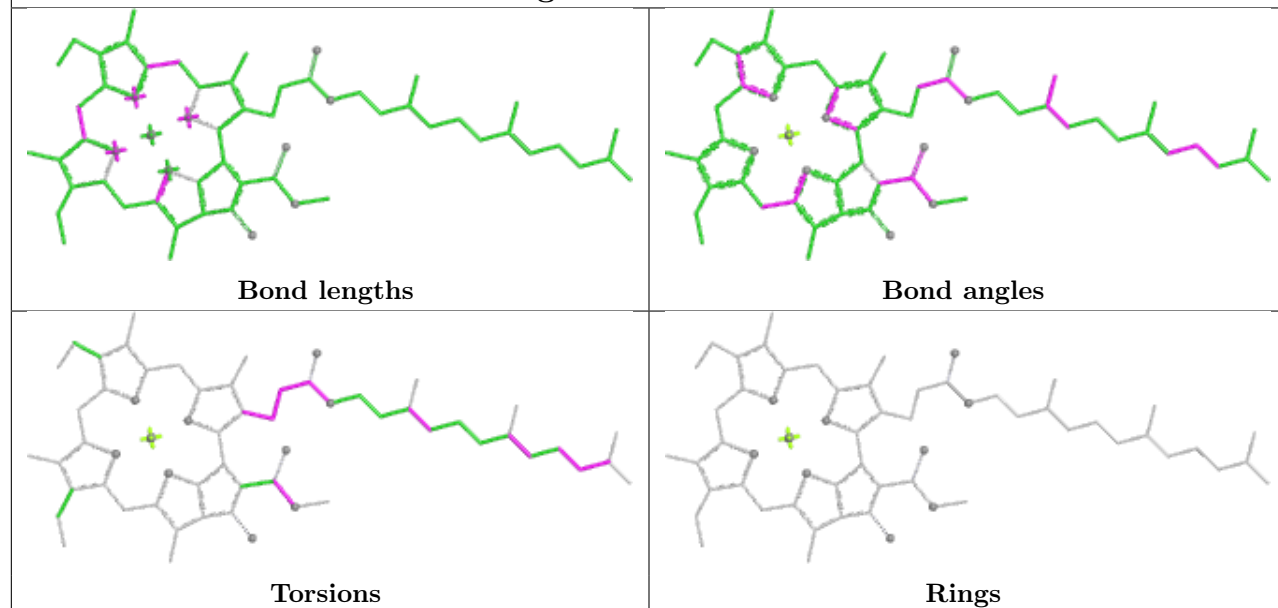


Rings

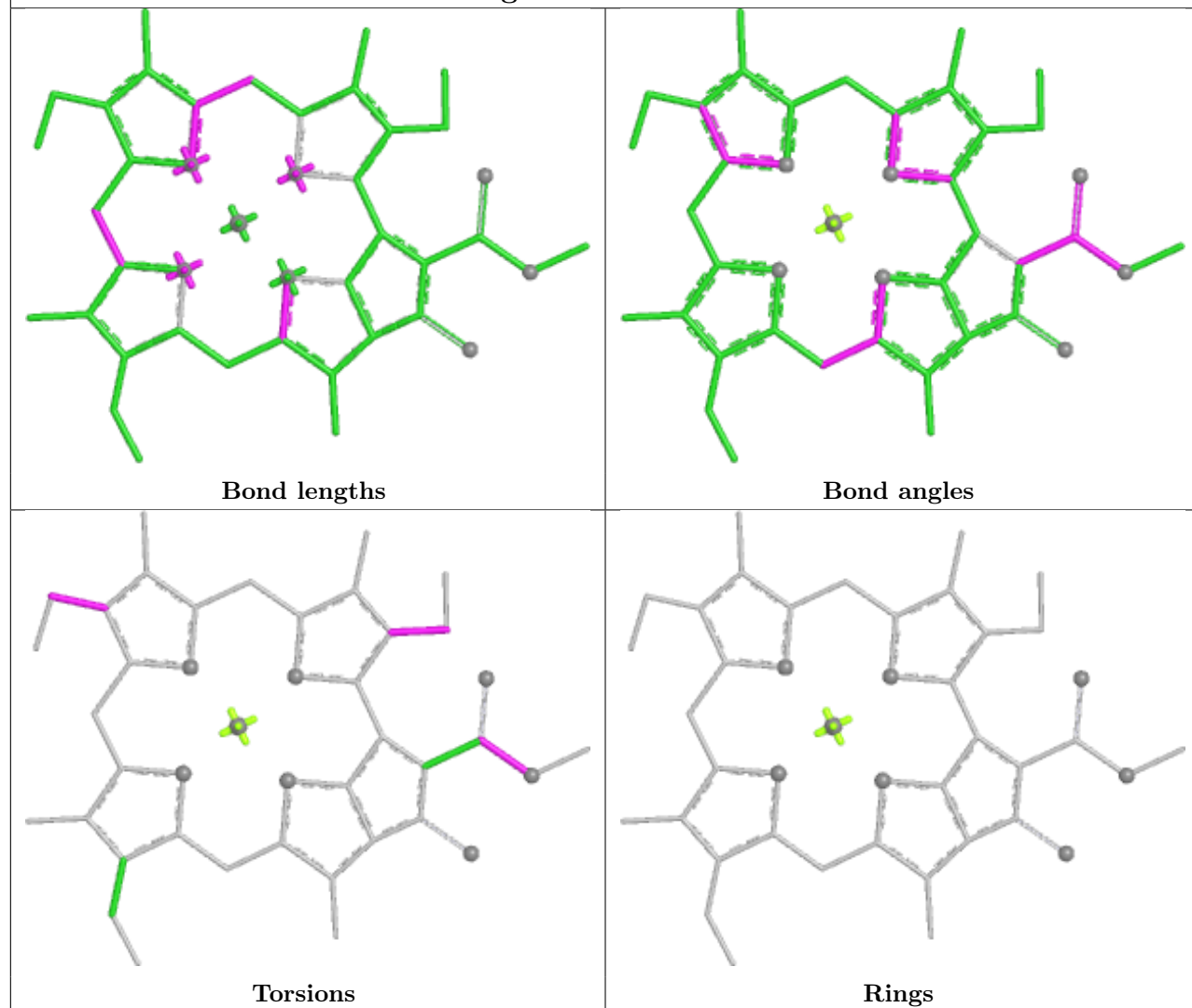




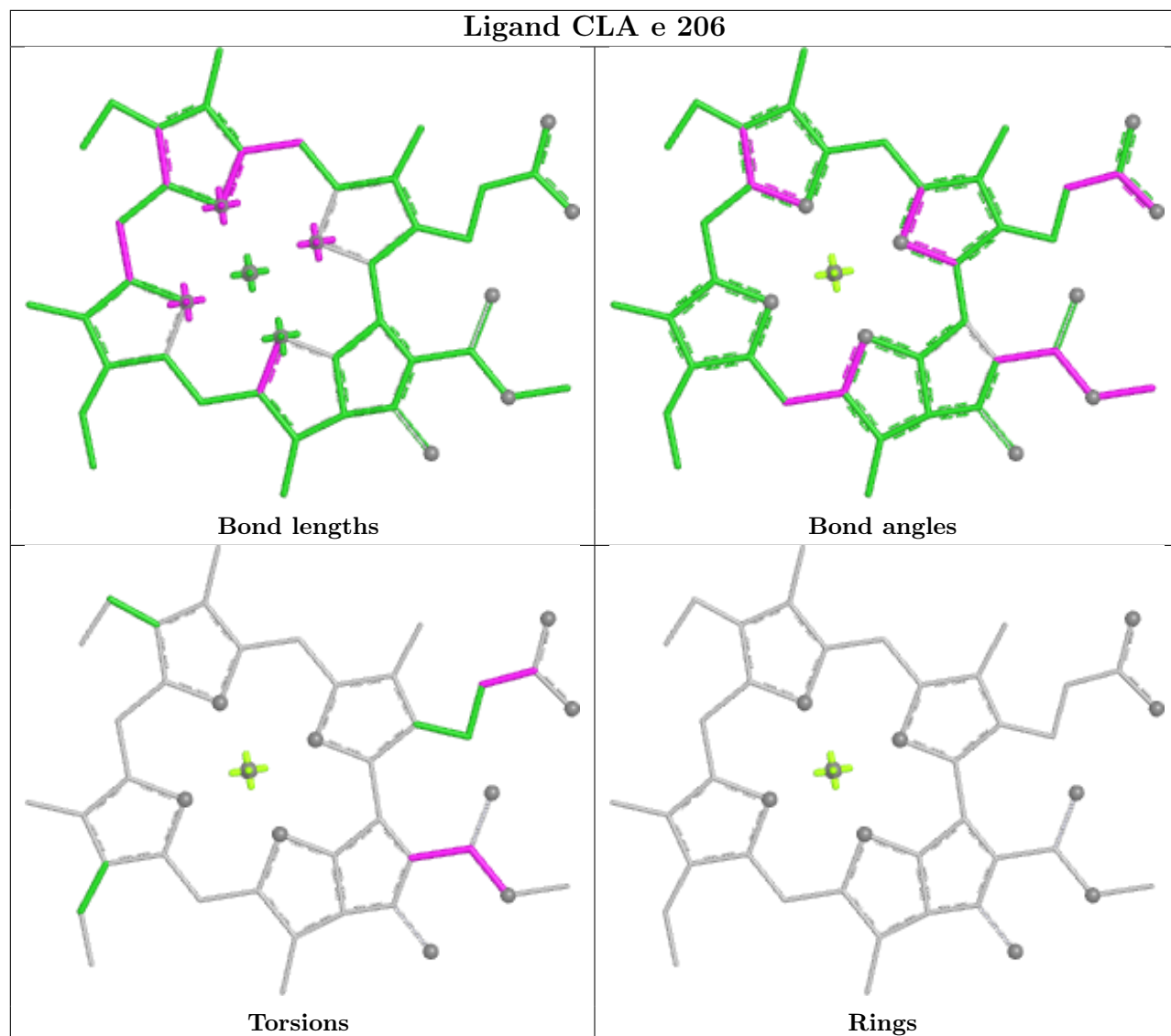
## Ligand CLA c 309

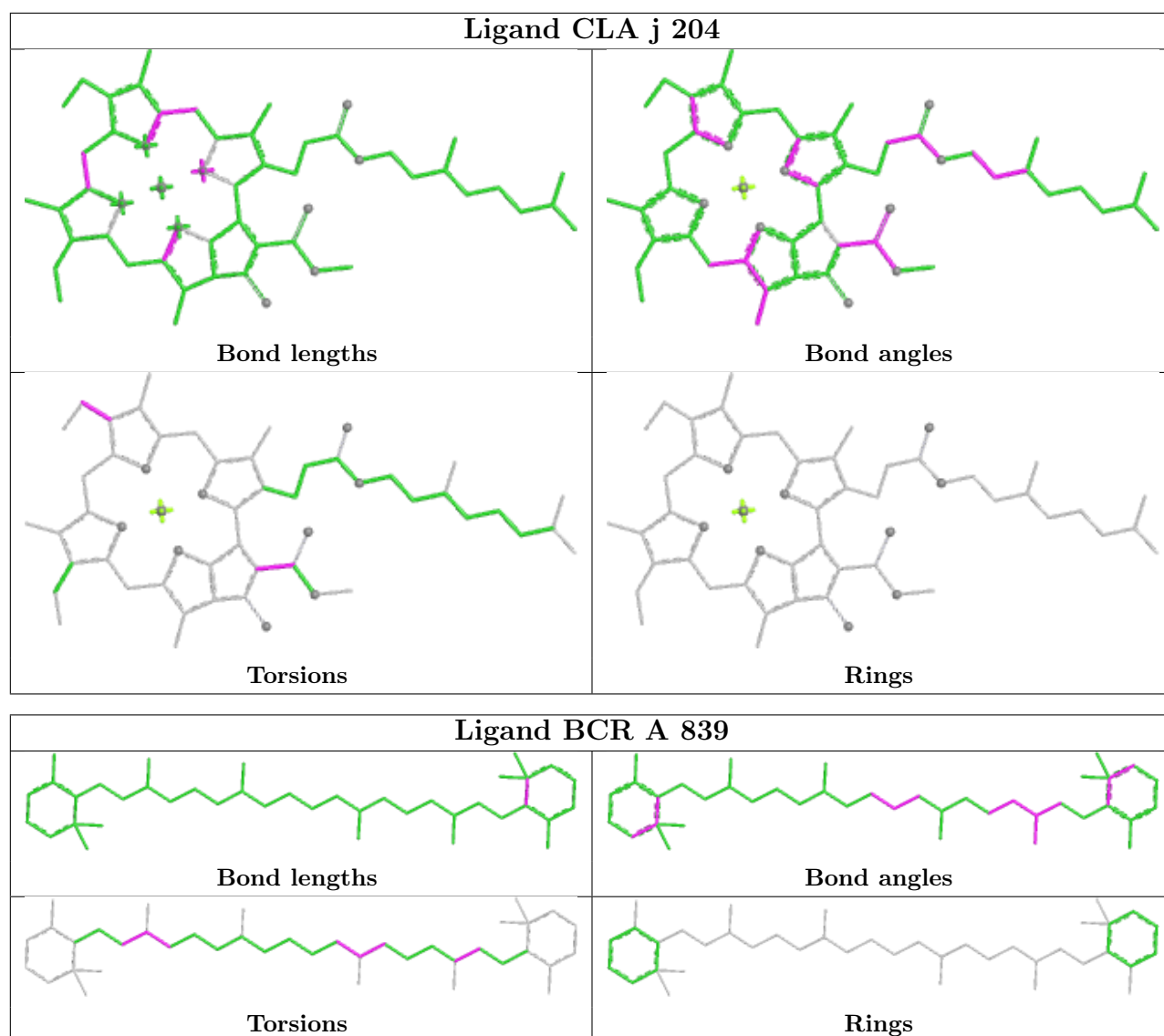


## Ligand CLA c 314

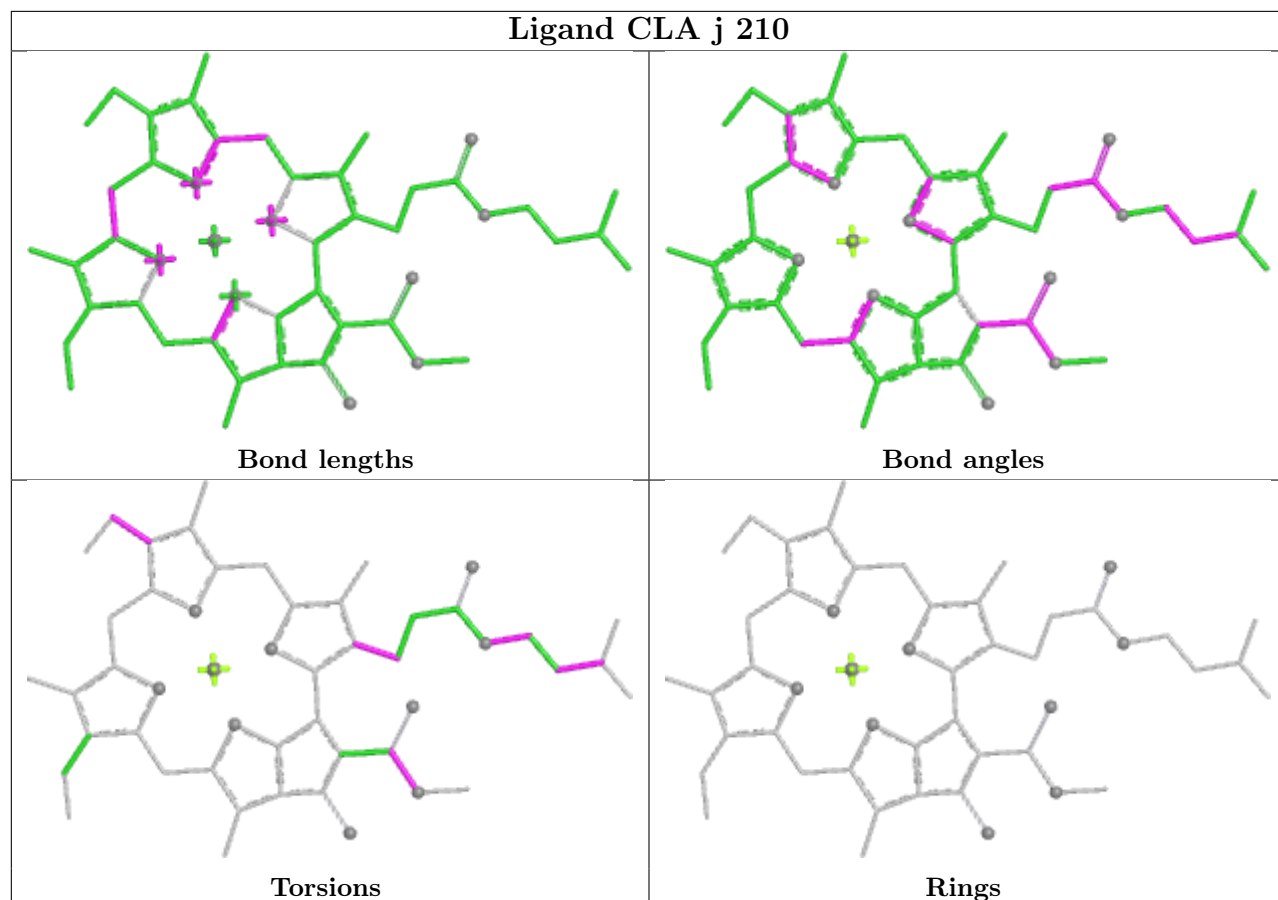


## Ligand CLA e 206

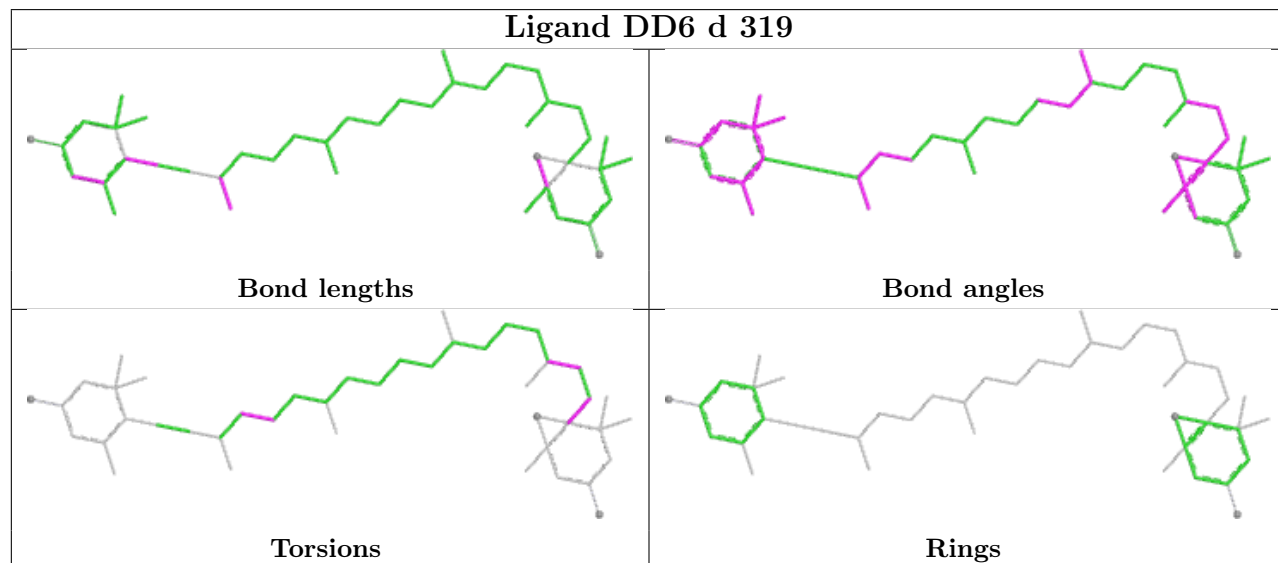


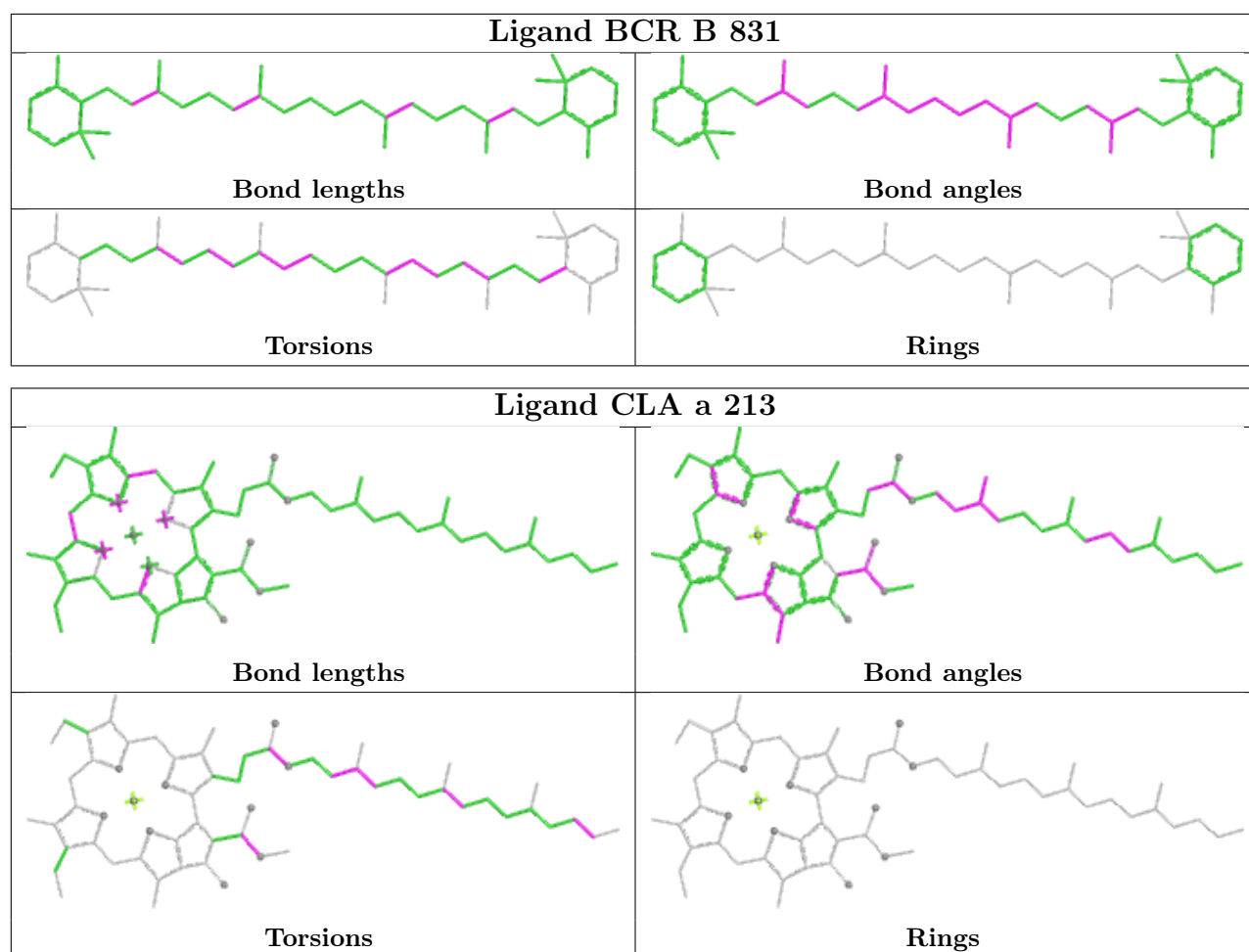


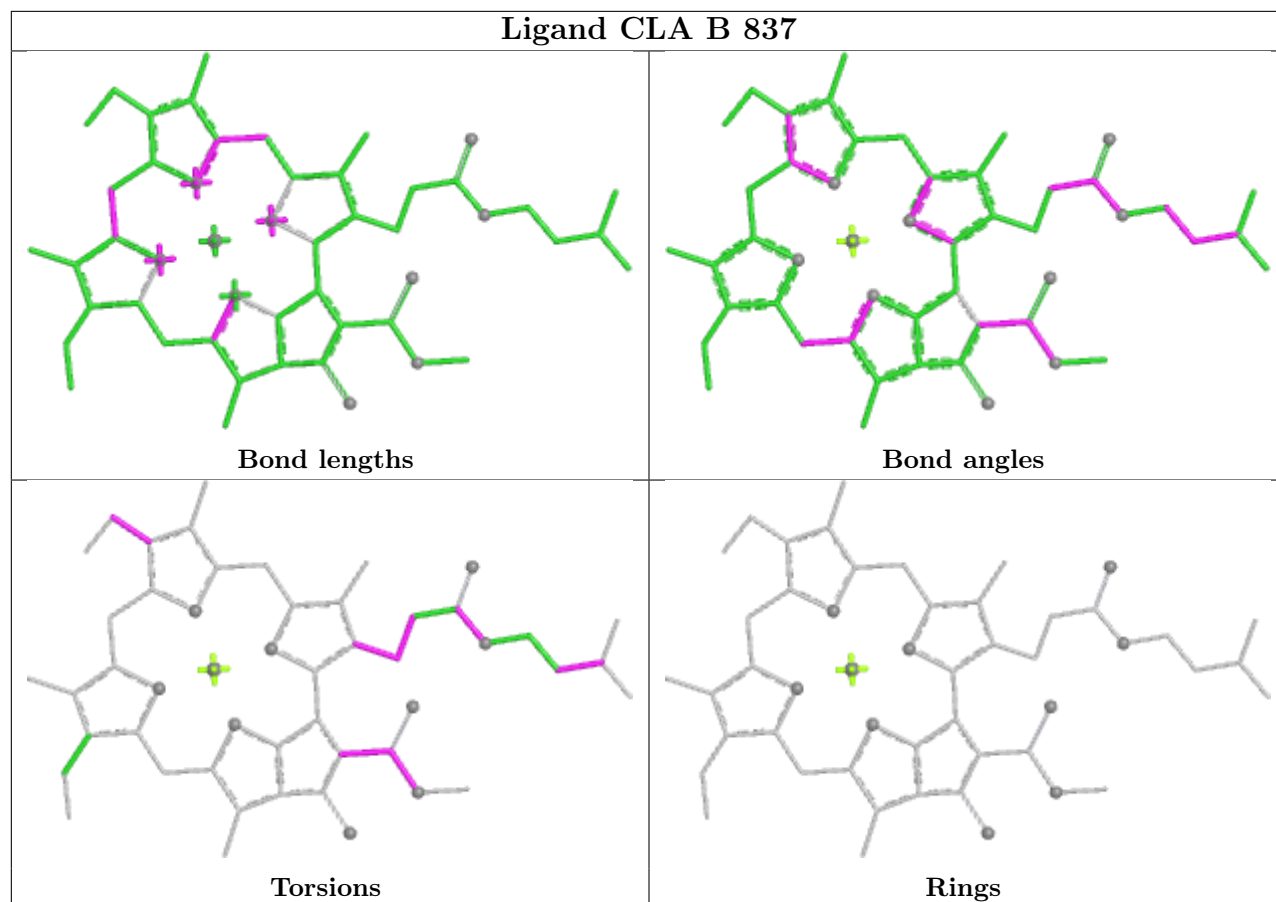
## Ligand CLA j 210



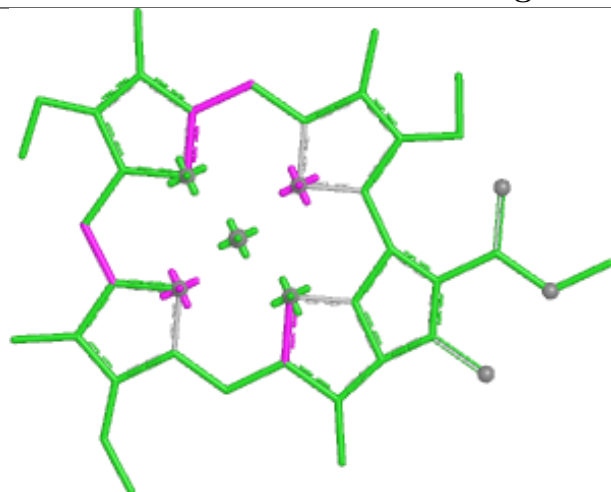
## Ligand DD6 d 319



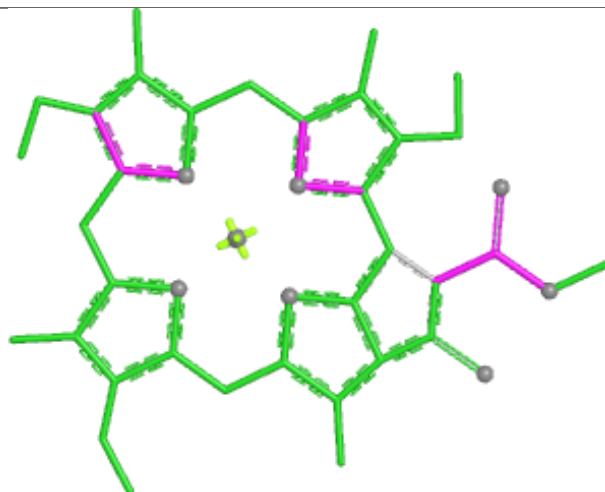




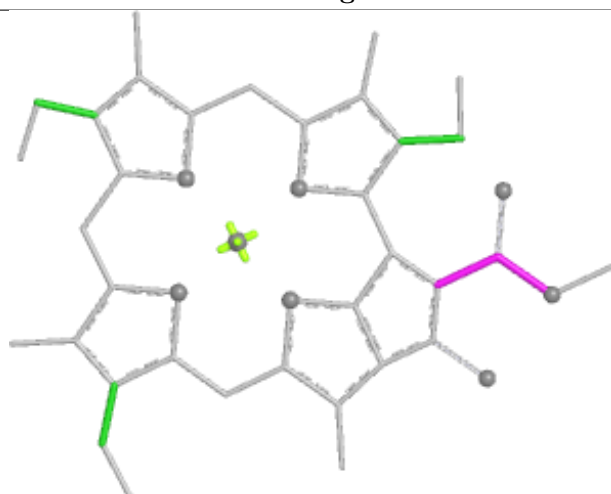
## Ligand CLA B 809



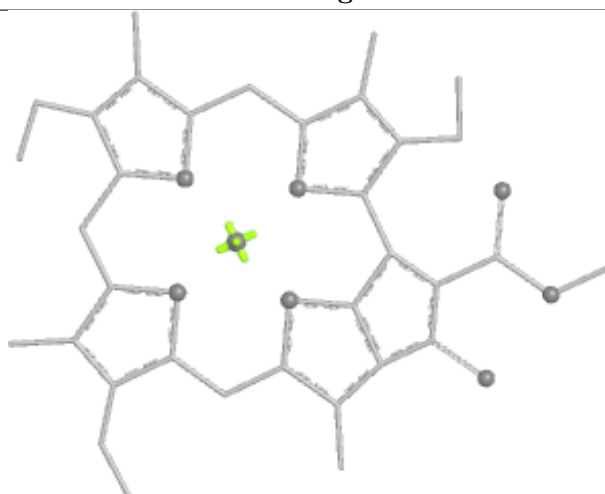
Bond lengths



Bond angles

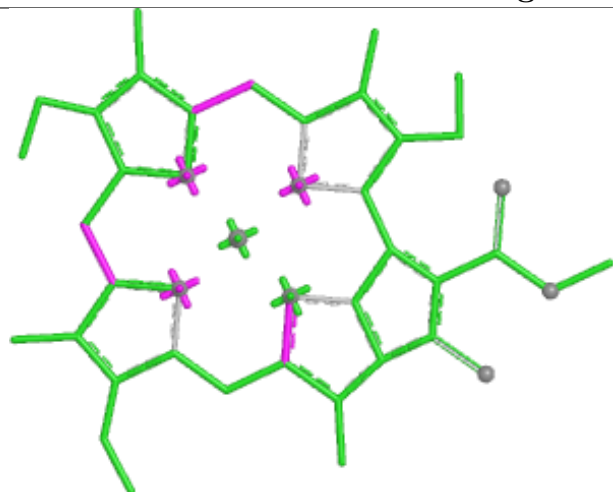


Torsions

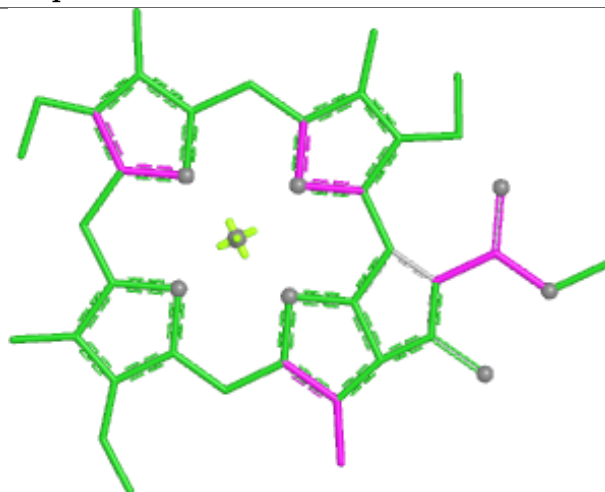


Rings

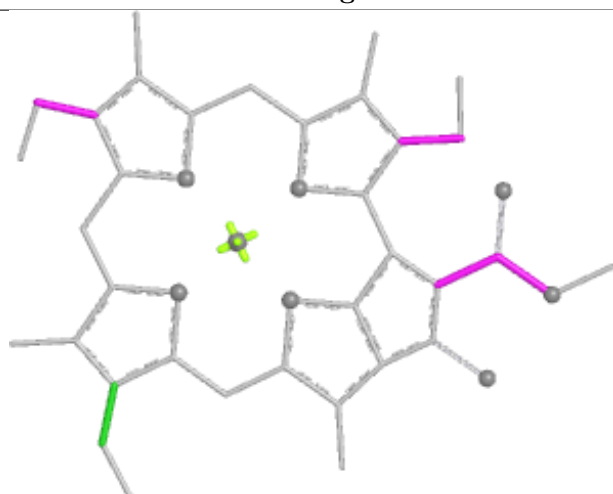
## Ligand CLA p 605



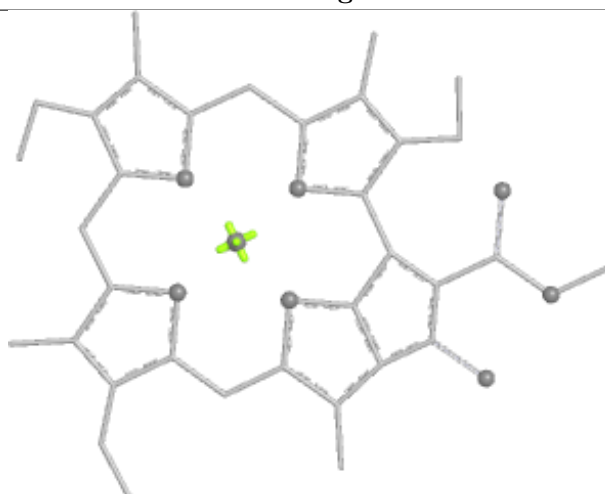
Bond lengths



Bond angles

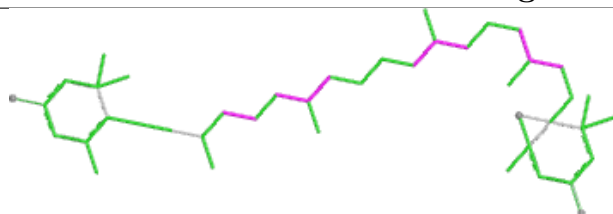


Torsions

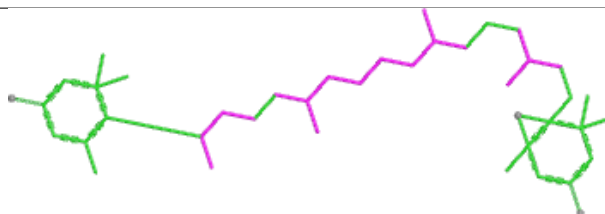


Rings

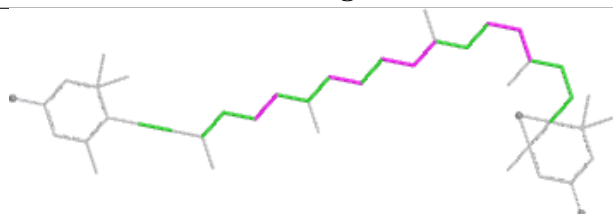
## Ligand DD6 n 214



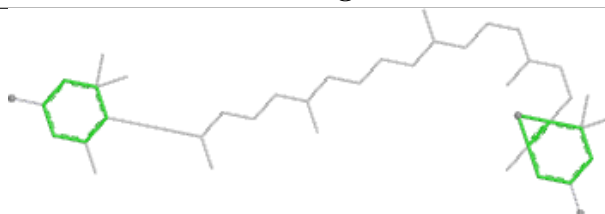
Bond lengths



Bond angles

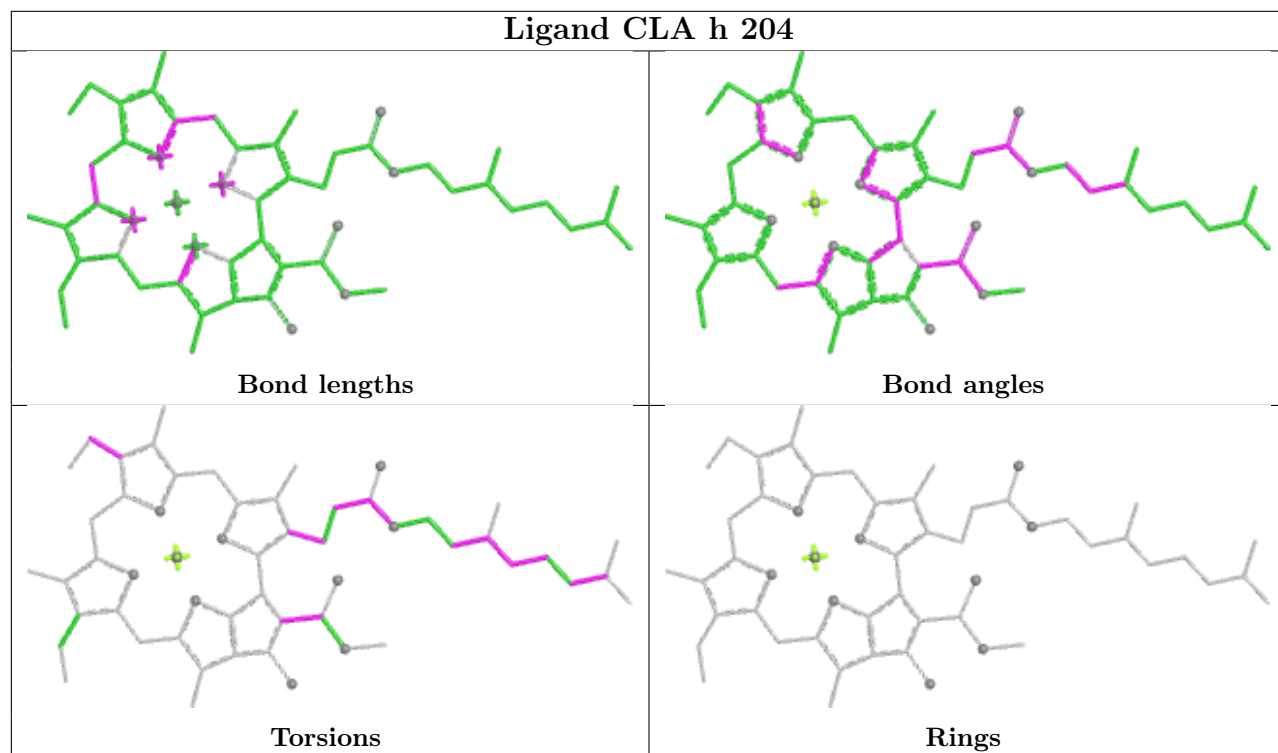


Torsions

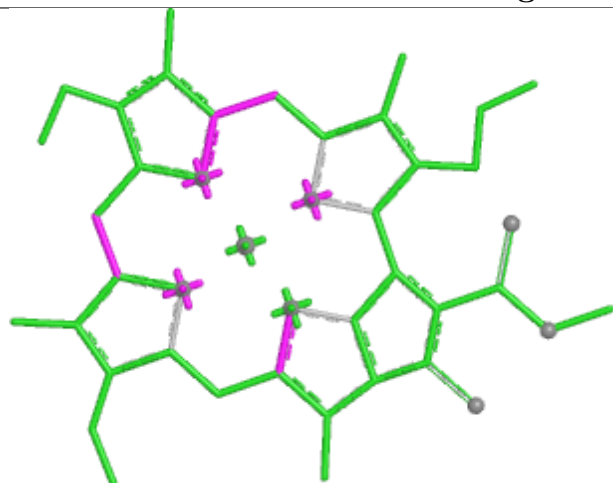


Rings

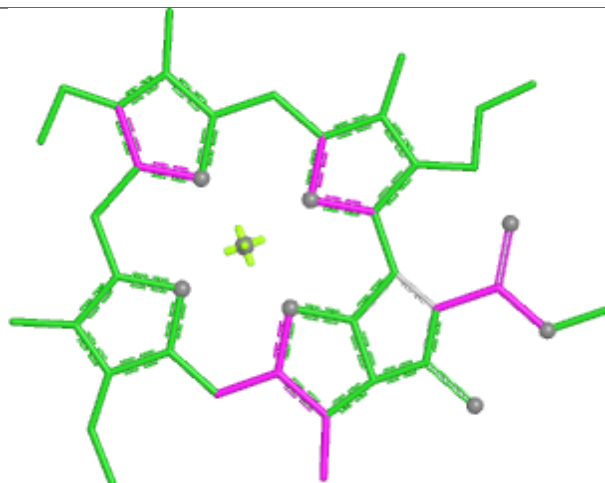




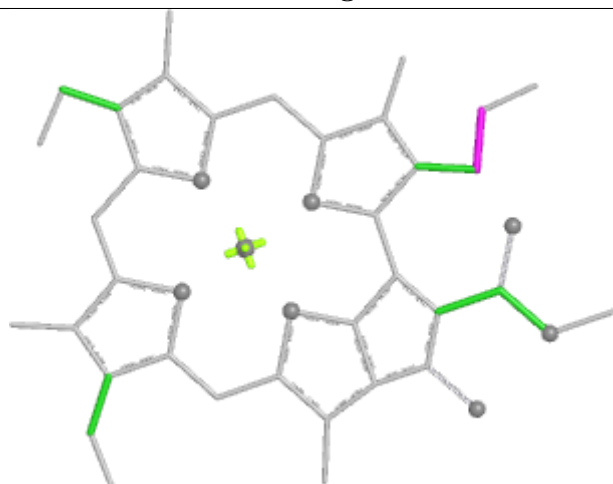
## Ligand CLA k 210



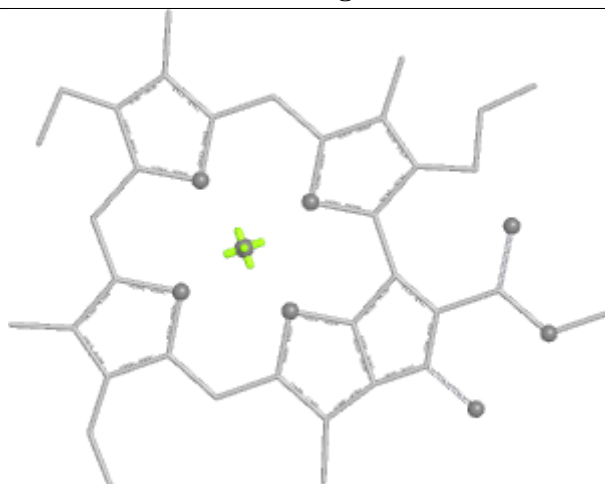
Bond lengths



Bond angles

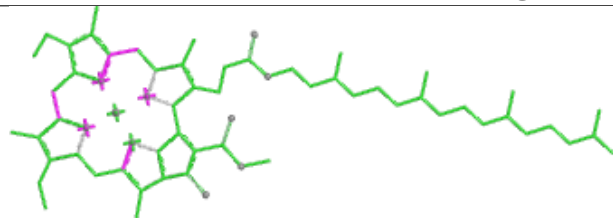


Torsions

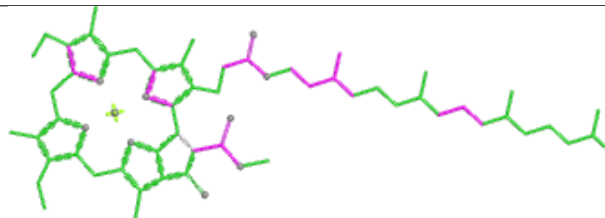


Rings

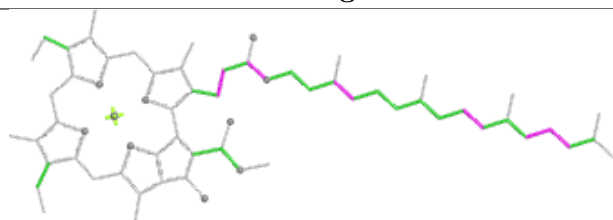
## Ligand CLA A 825



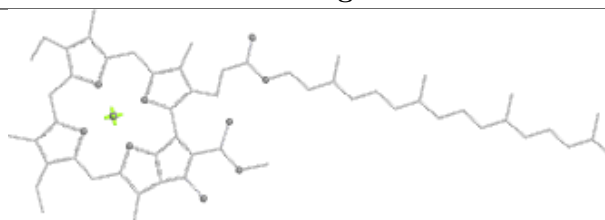
Bond lengths



Bond angles

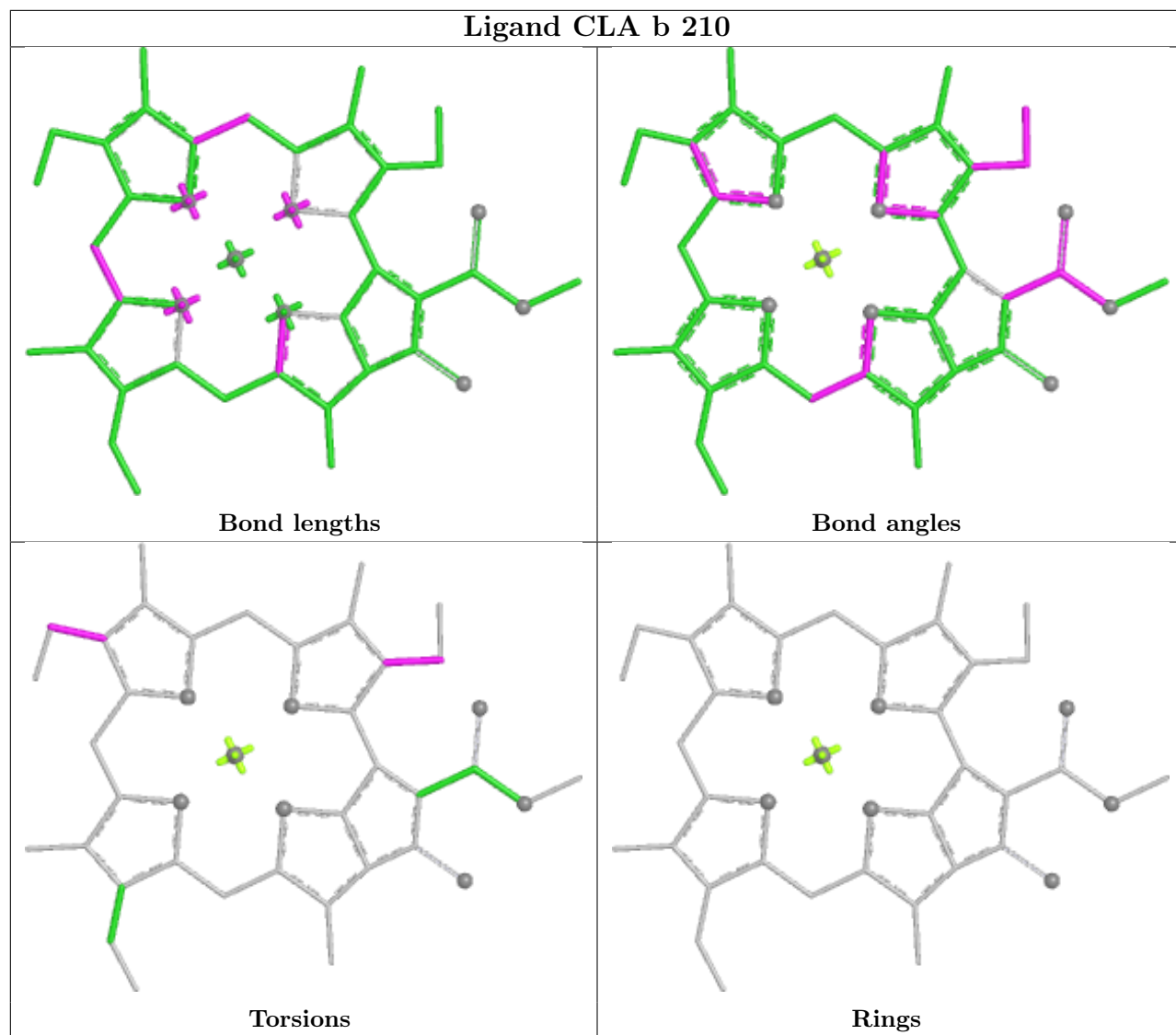


Torsions

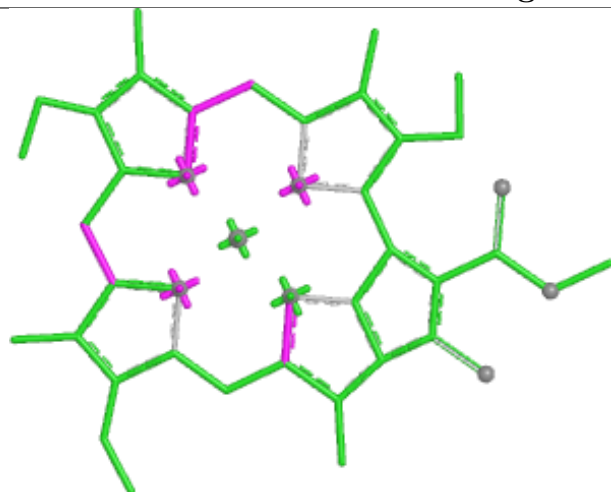


Rings

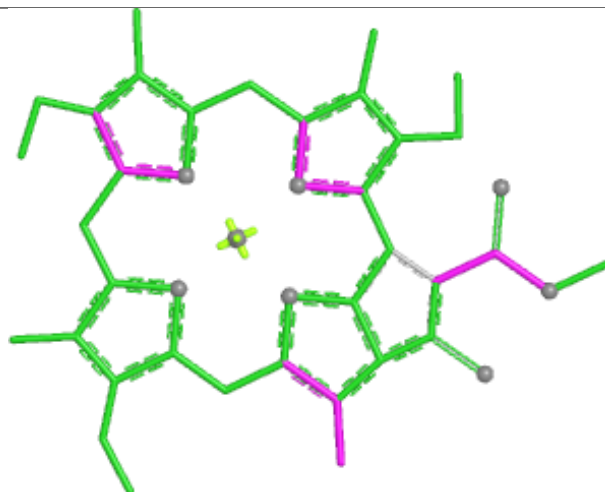
## Ligand CLA b 210



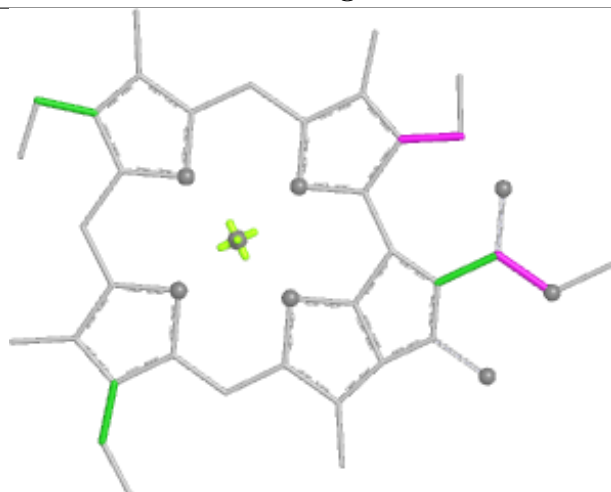
## Ligand CLA k 204



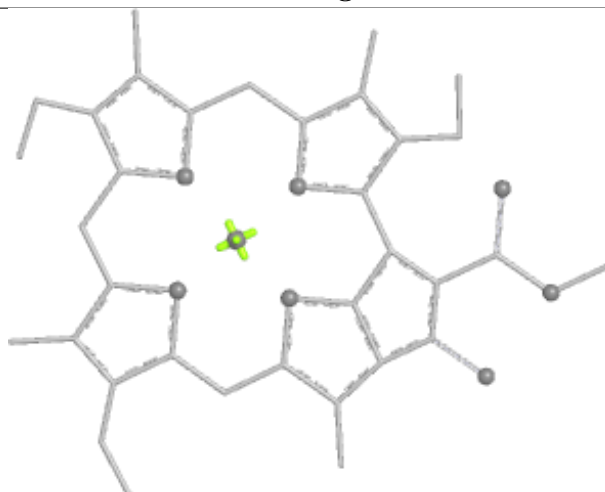
Bond lengths



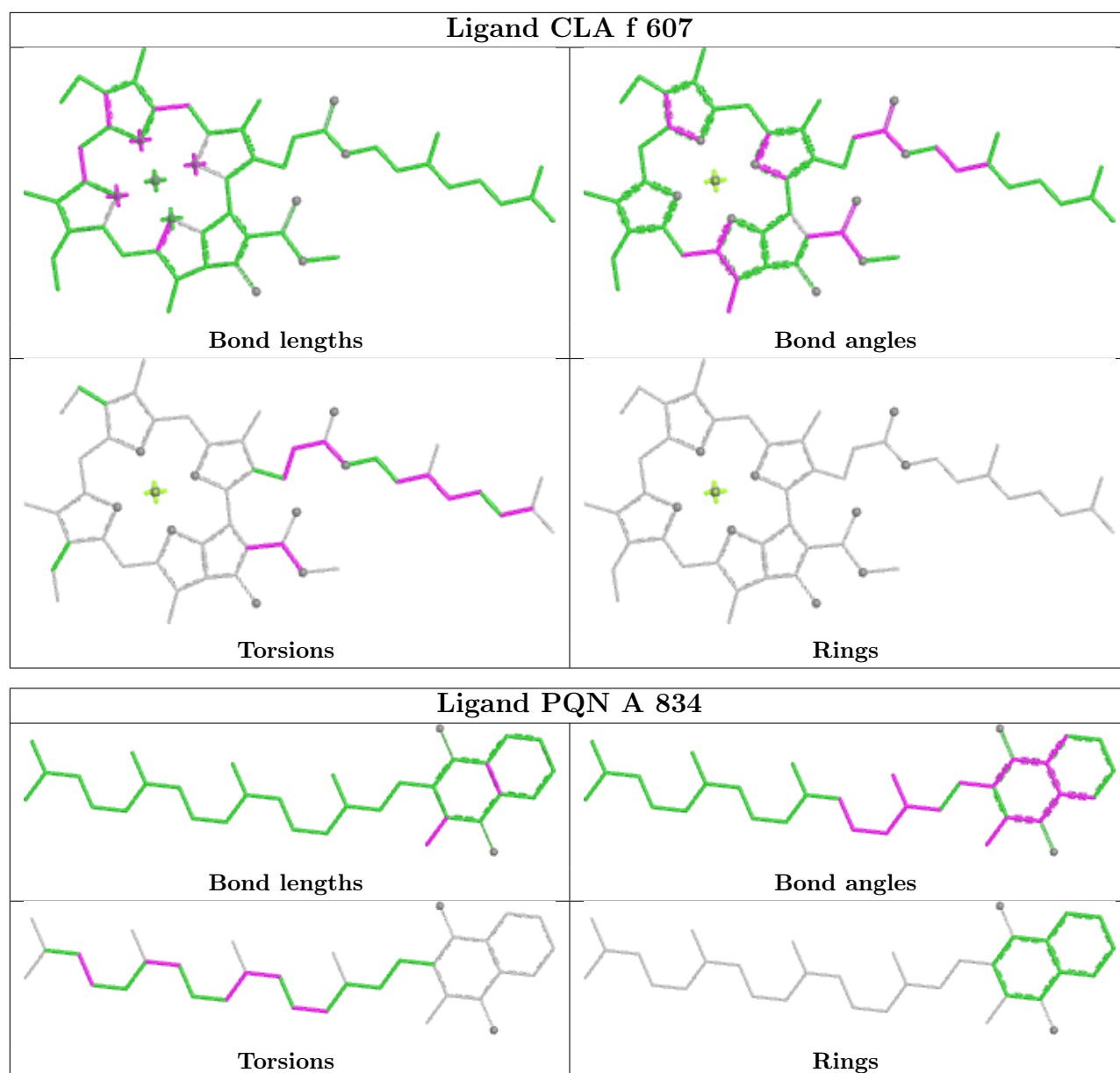
Bond angles

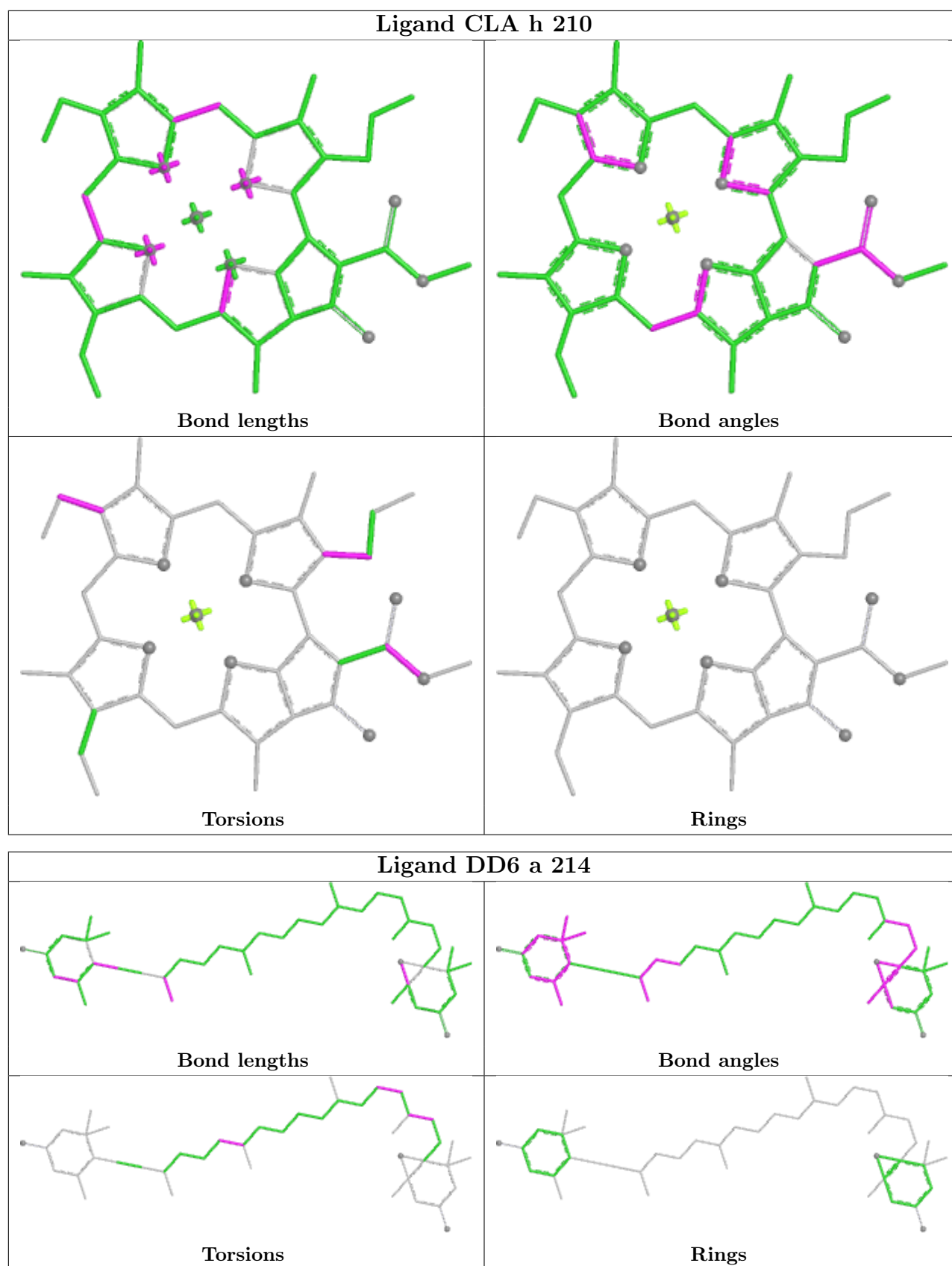


Torsions

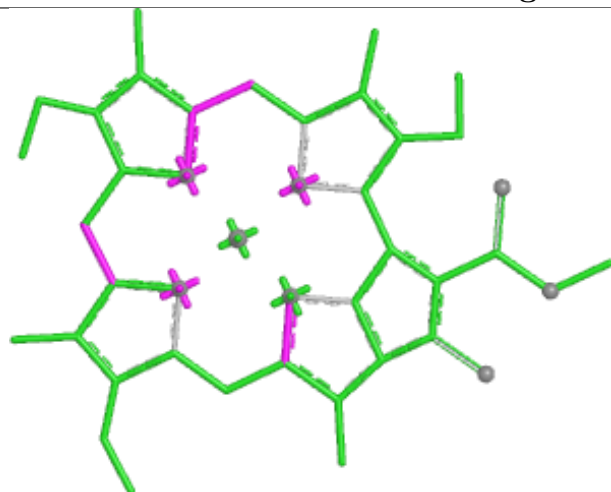


Rings

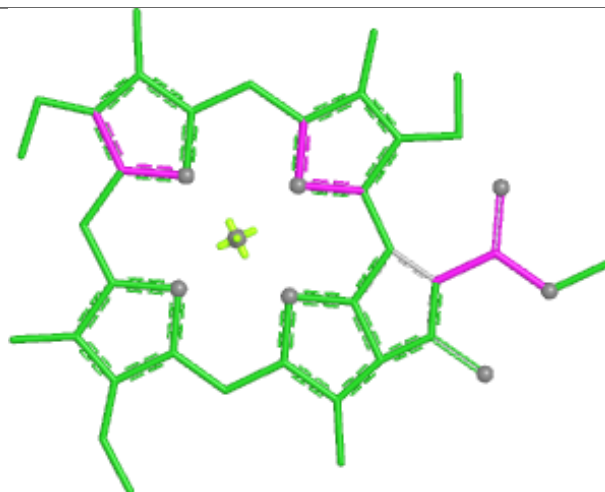




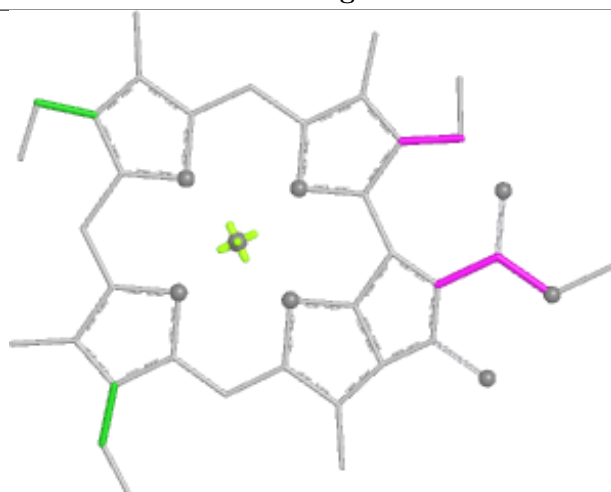
## Ligand CLA c 302



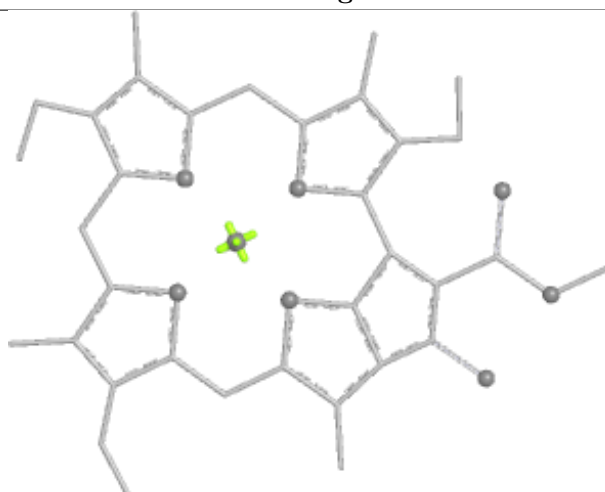
Bond lengths



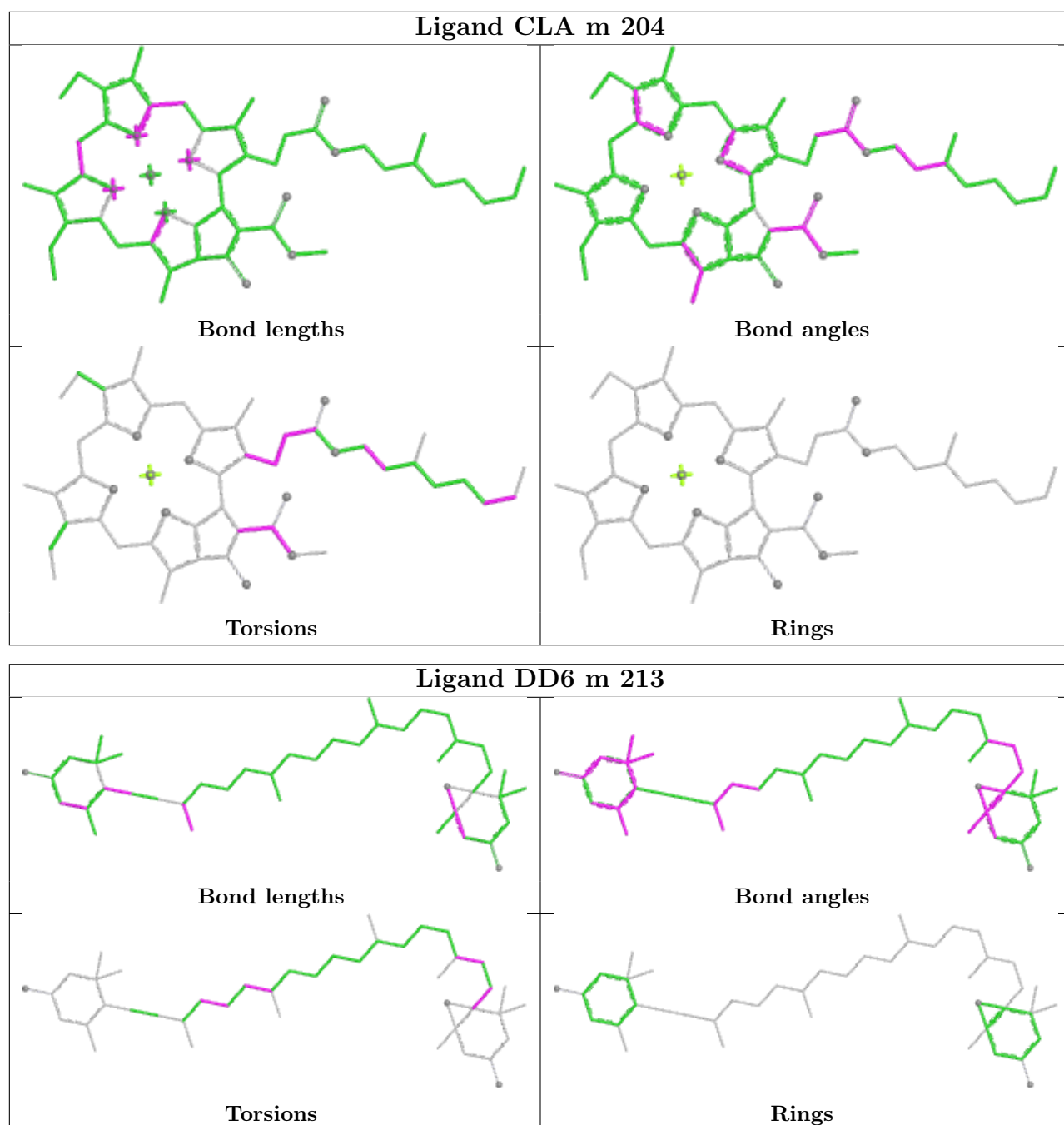
Bond angles



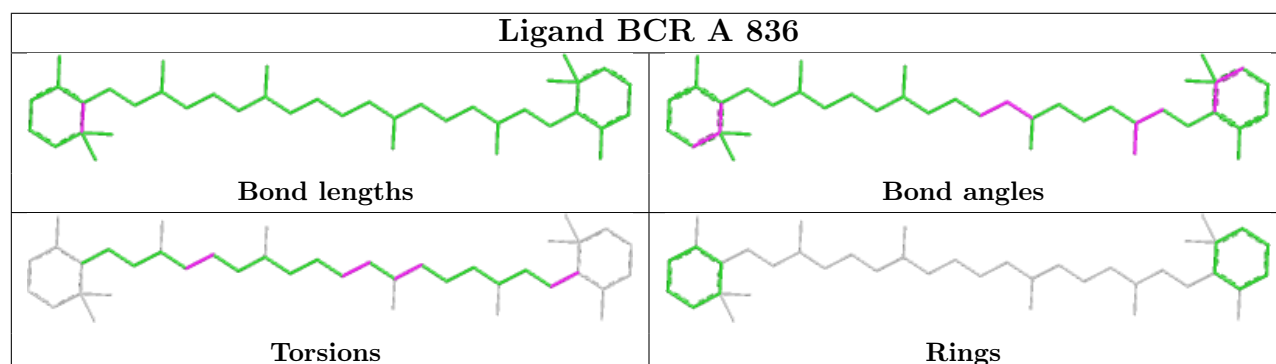
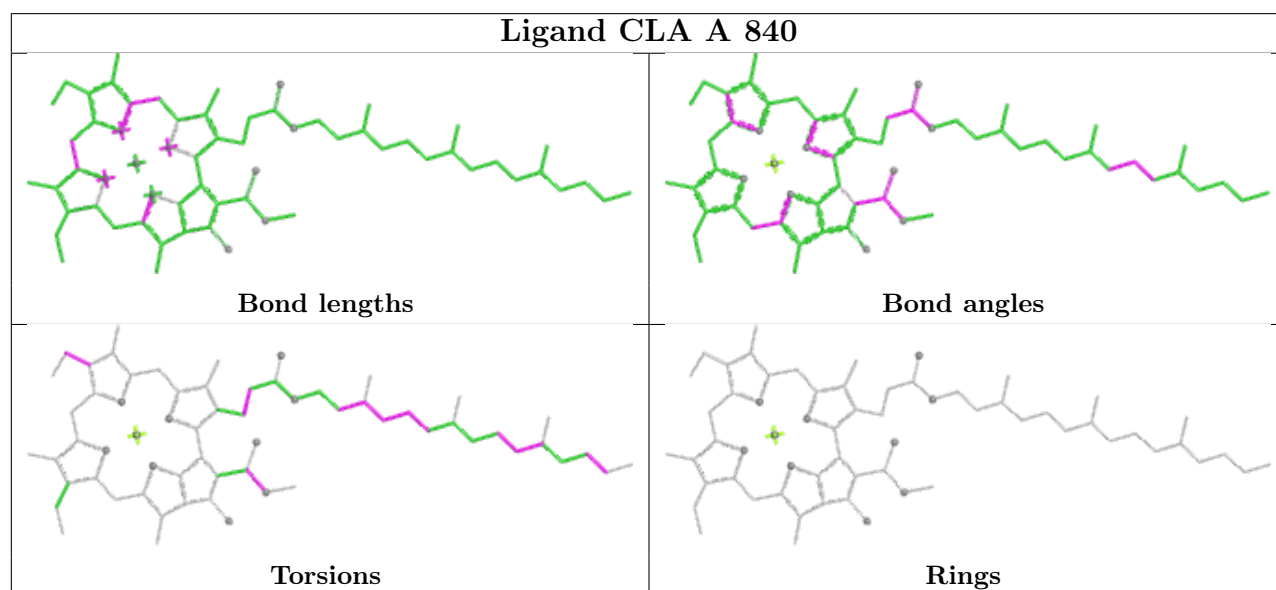
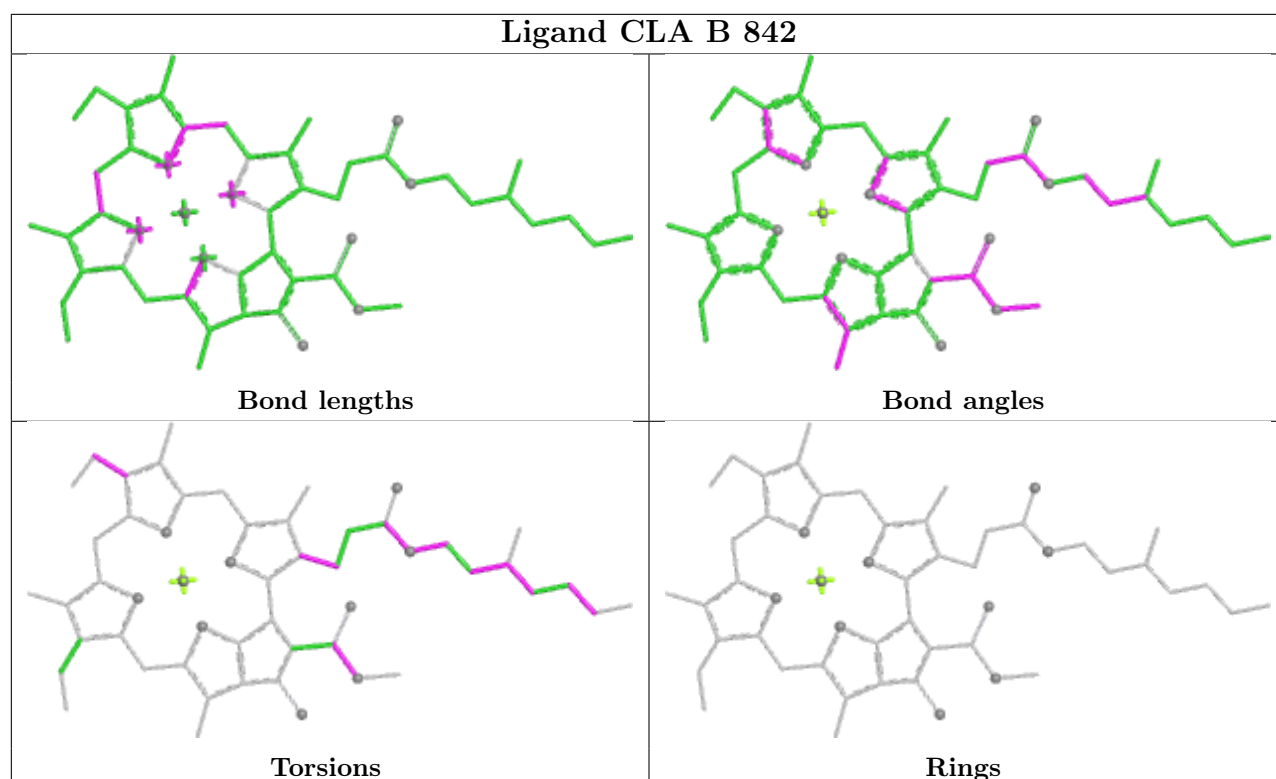
Torsions

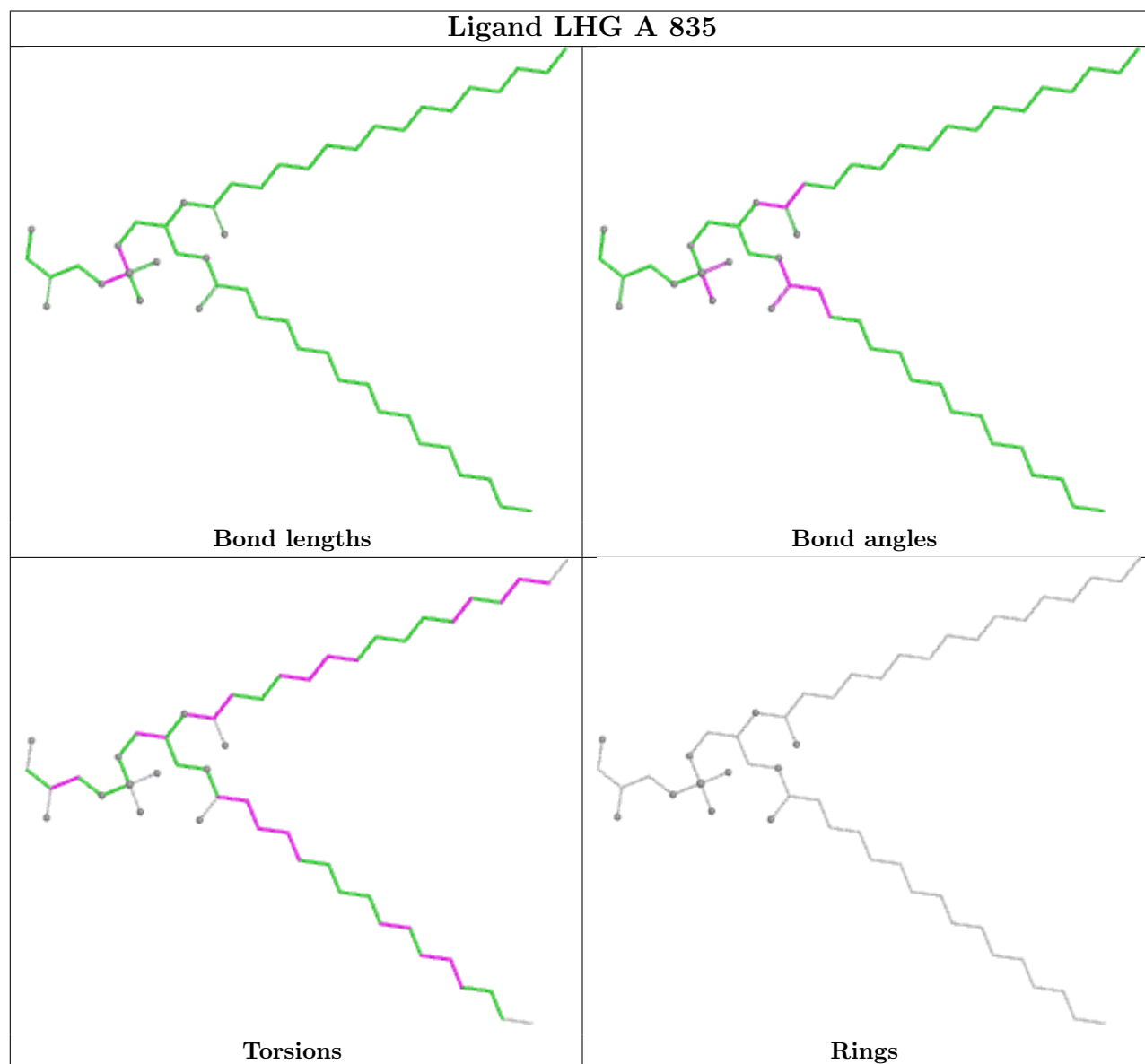
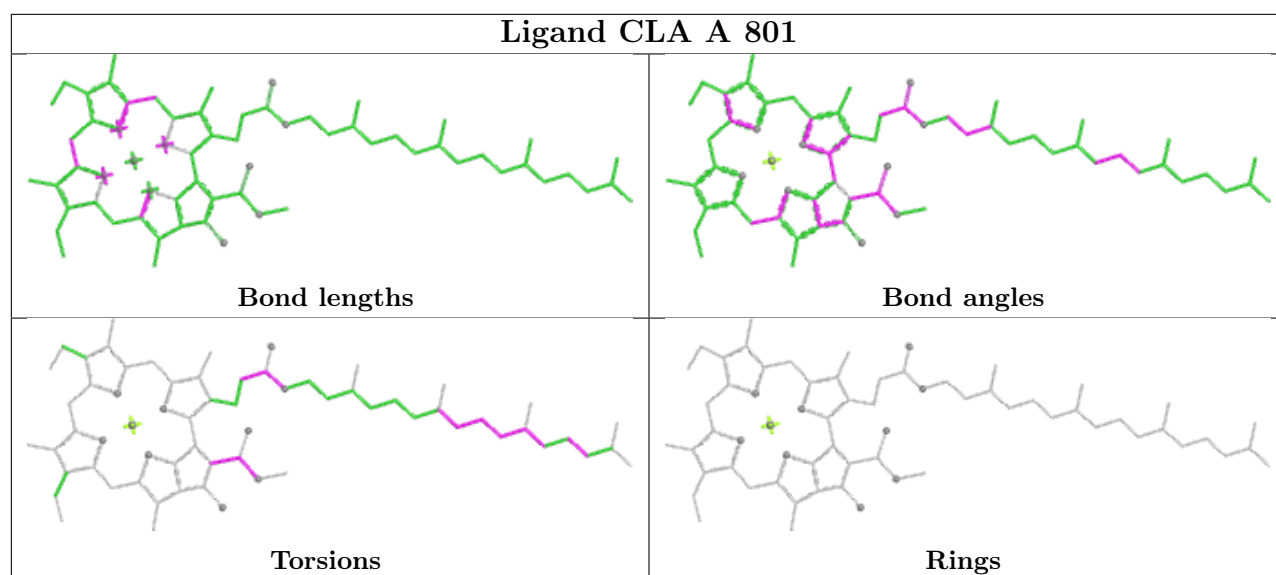


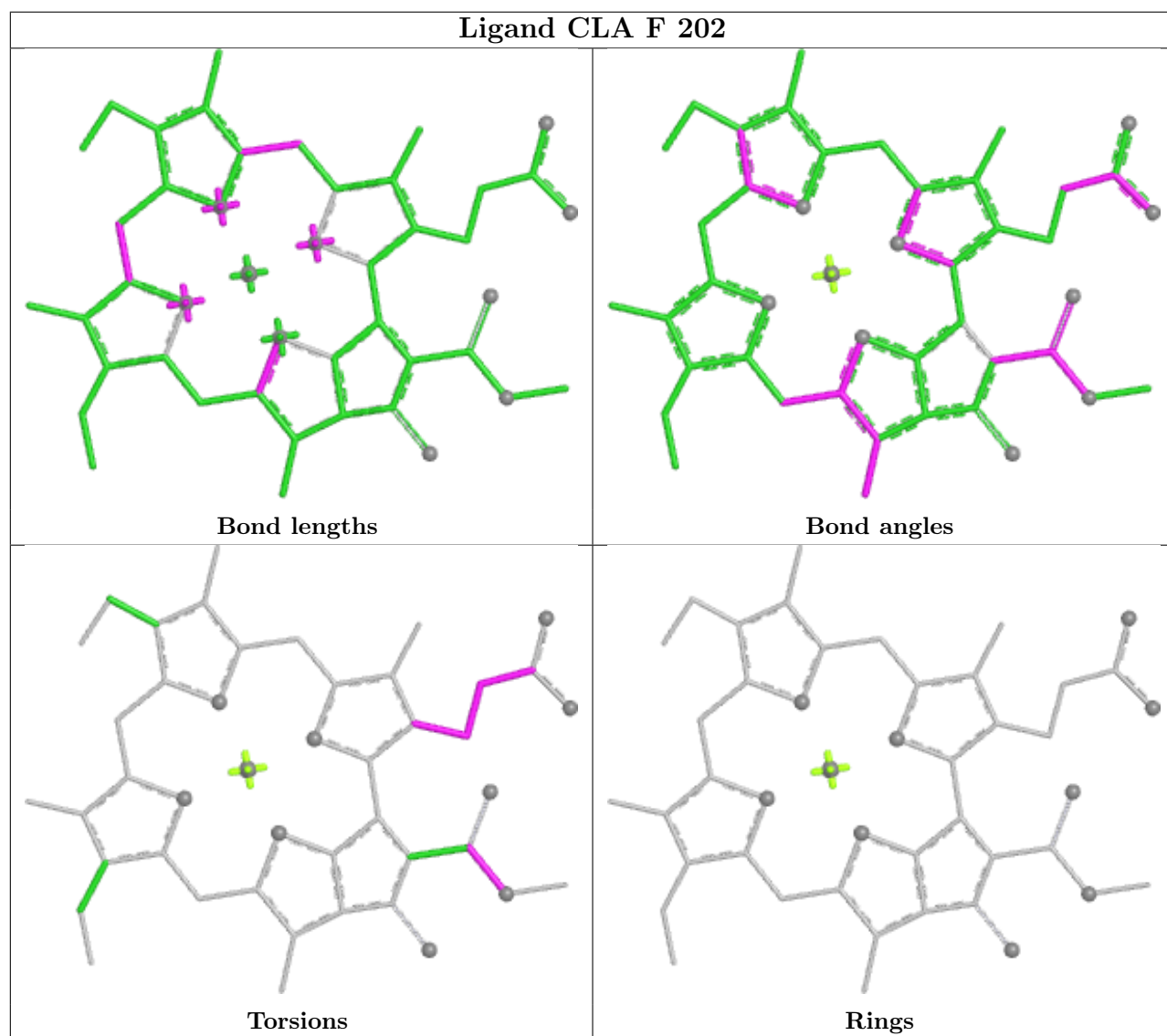
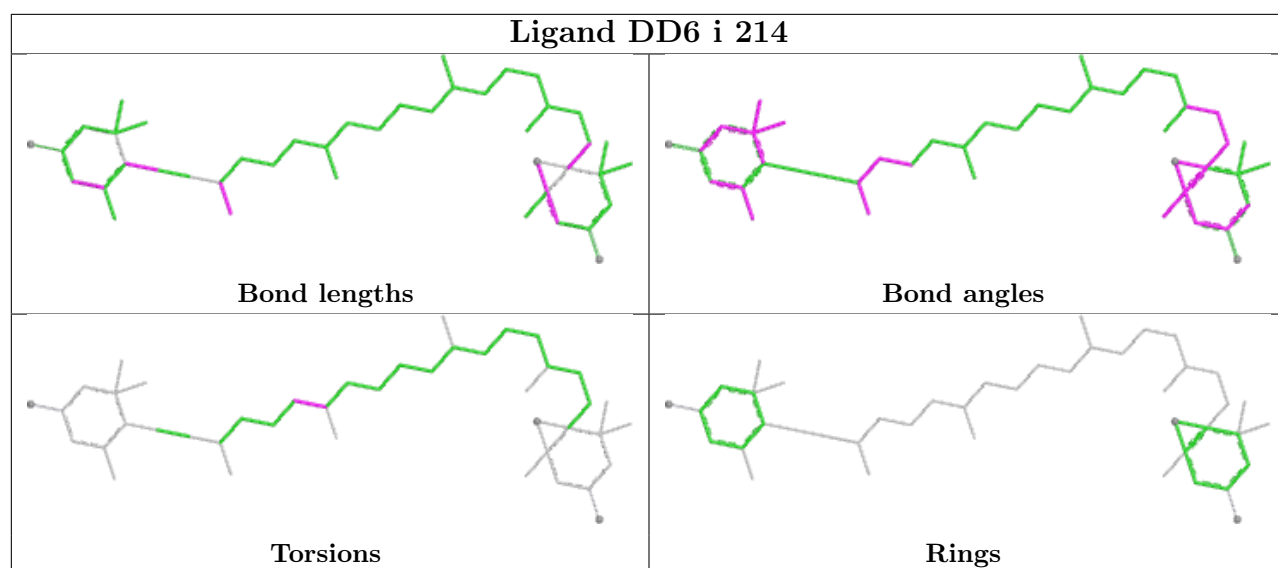
Rings



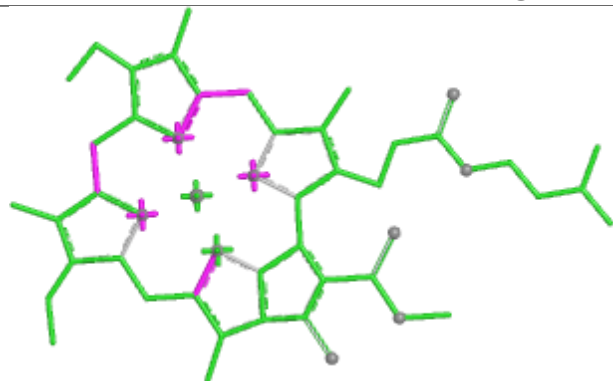




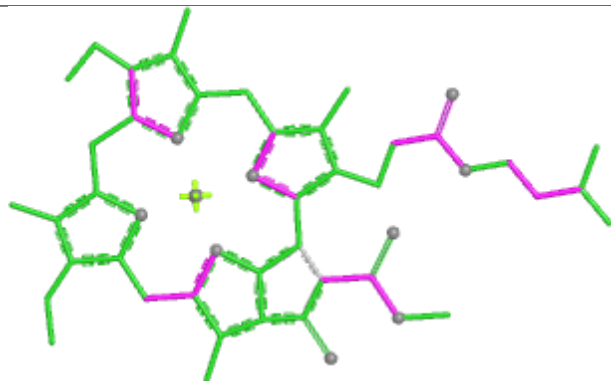




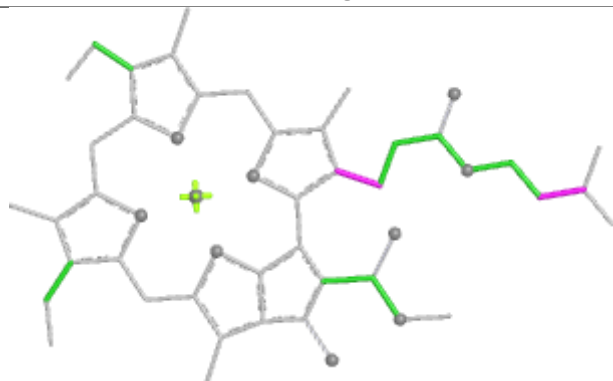
## Ligand CLA m 207



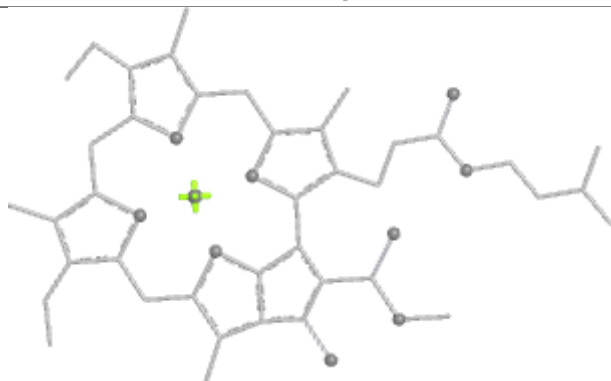
Bond lengths



Bond angles

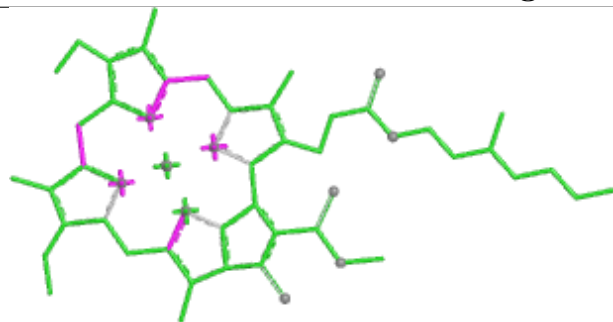


Torsions

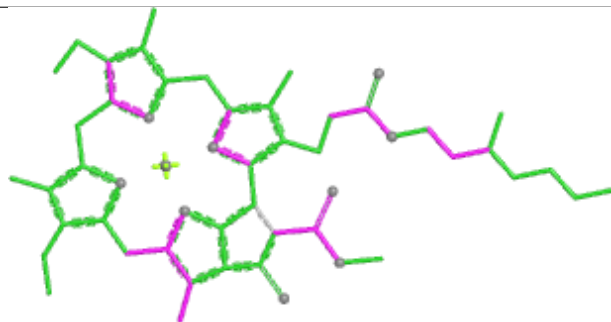


Rings

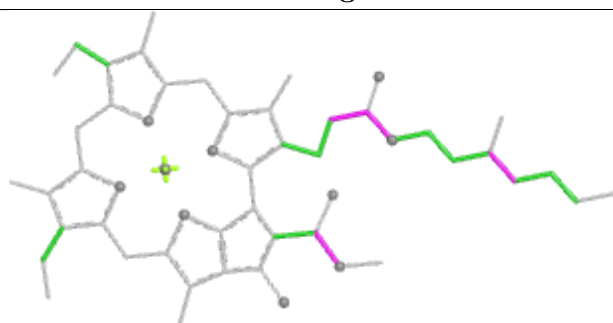
## Ligand CLA c 304



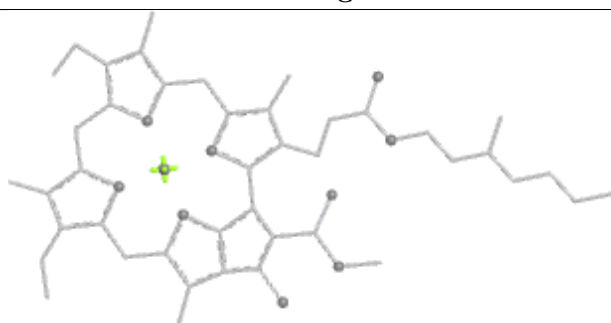
Bond lengths



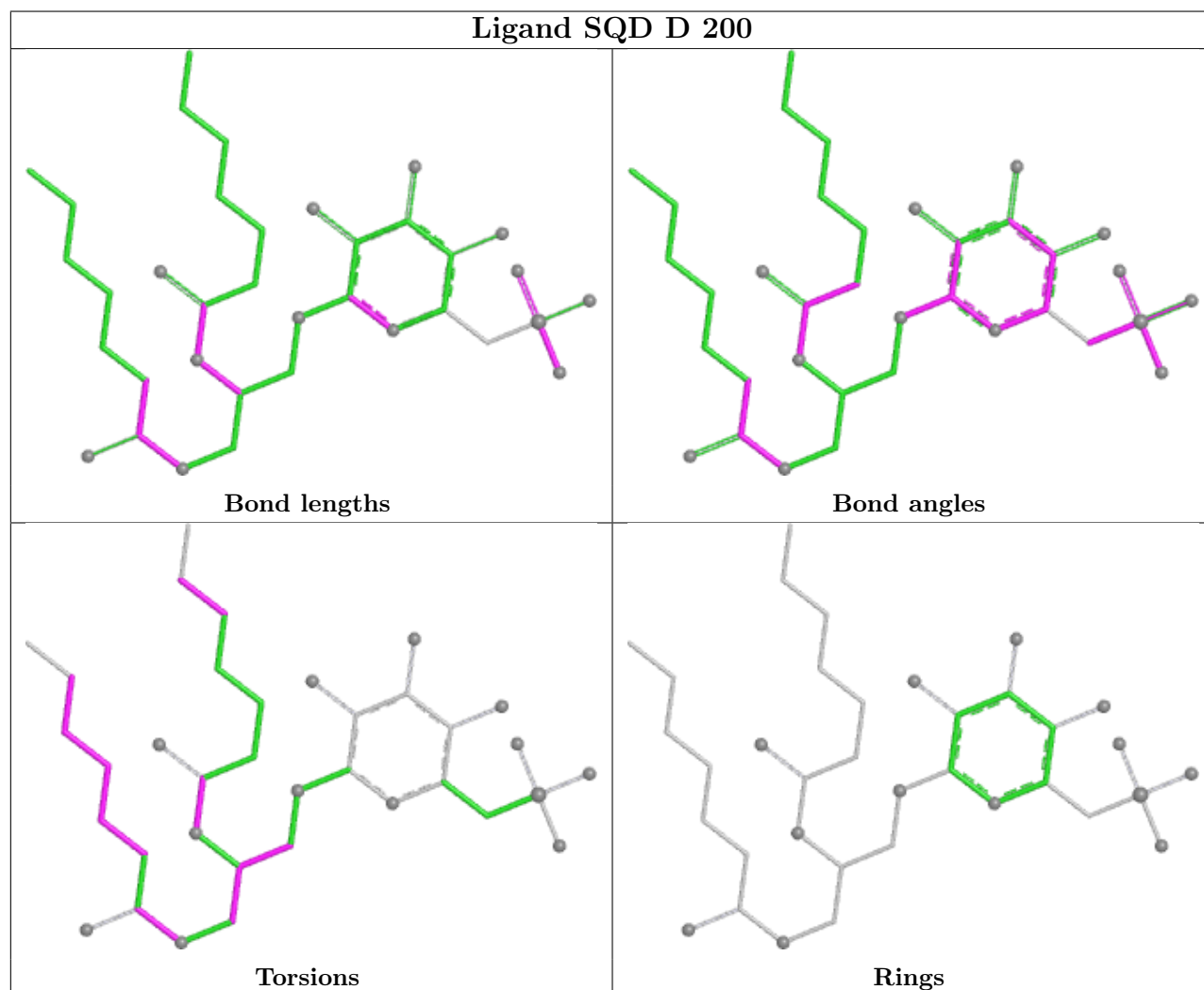
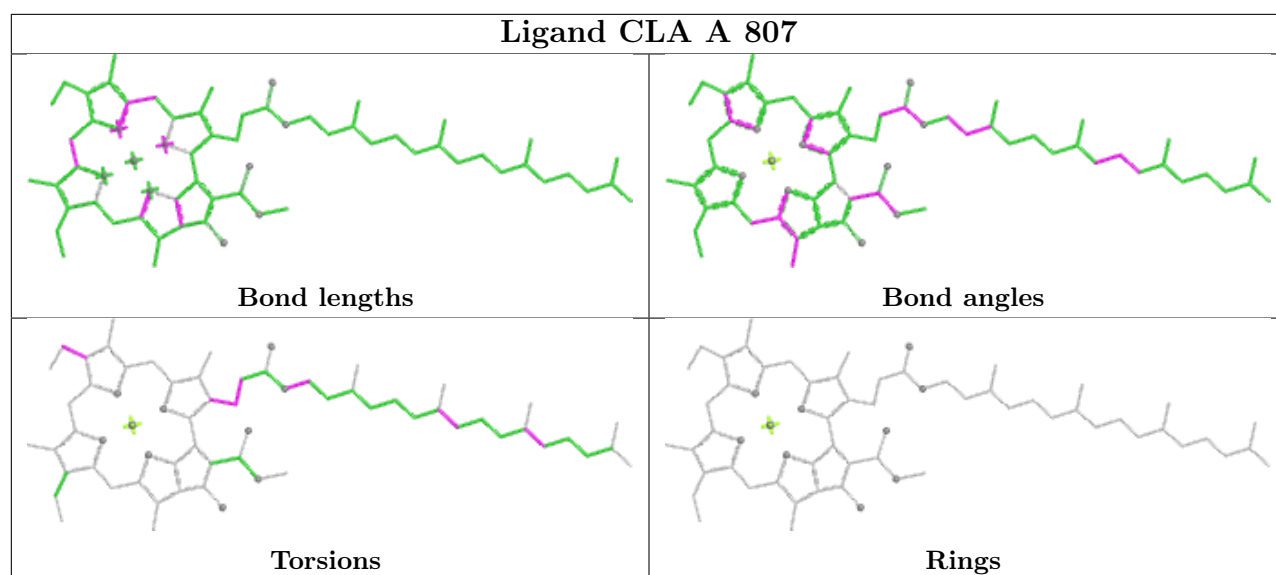
Bond angles



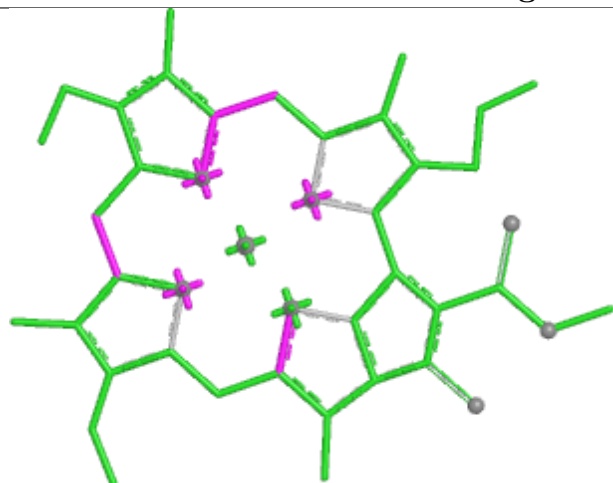
Torsions



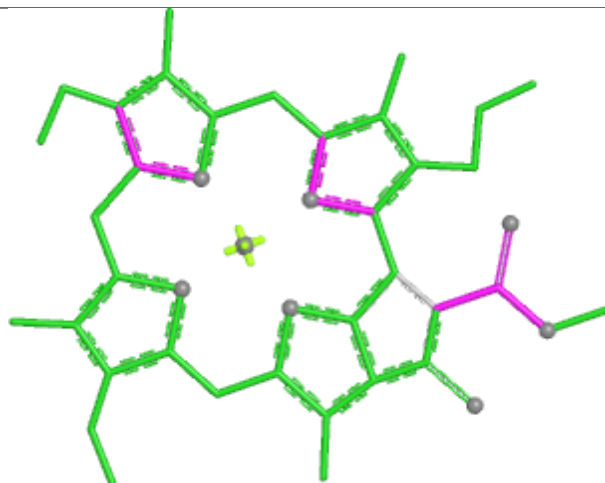
Rings



## Ligand CLA a 211



Bond lengths



Bond angles

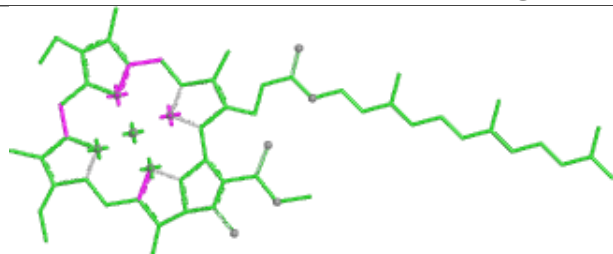


Torsions

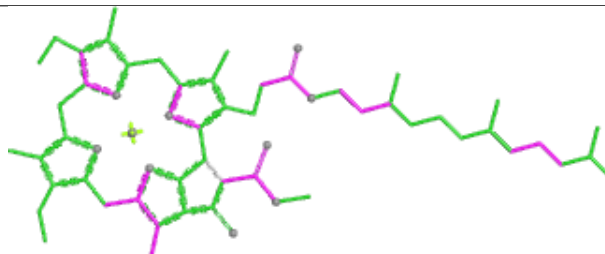


Rings

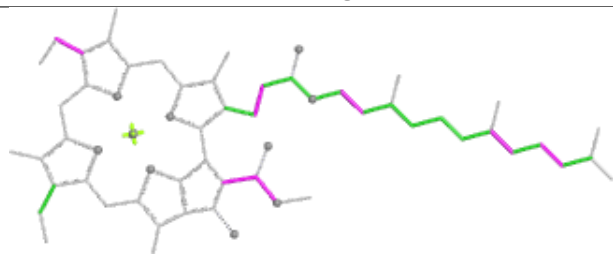
## Ligand CLA B 816



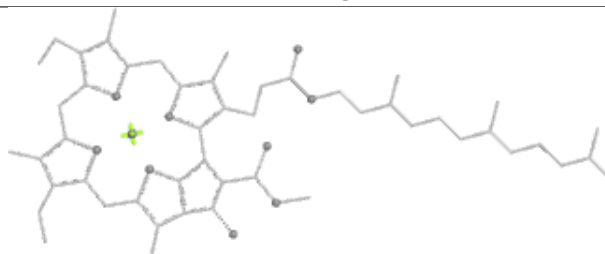
Bond lengths



Bond angles

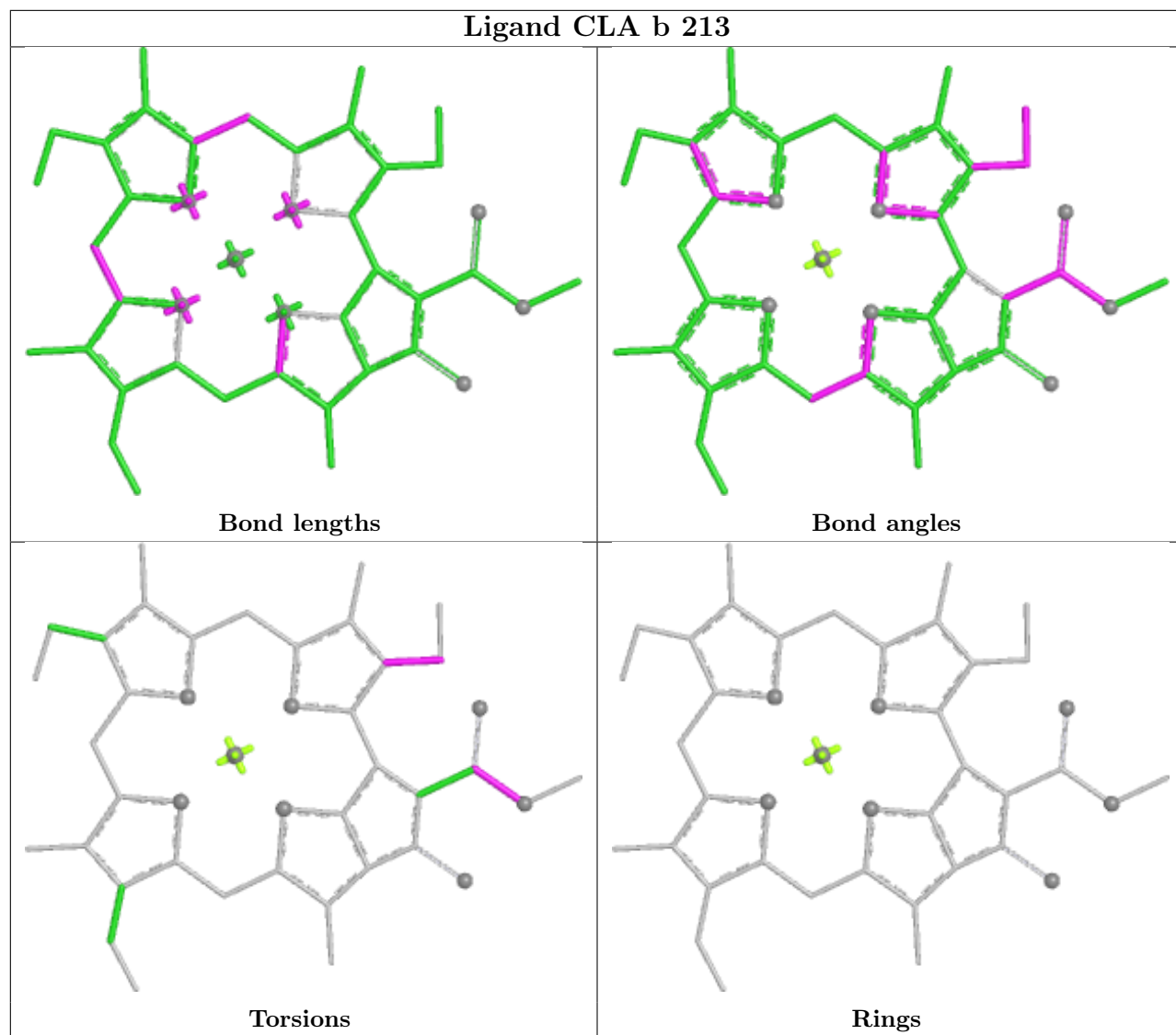


Torsions

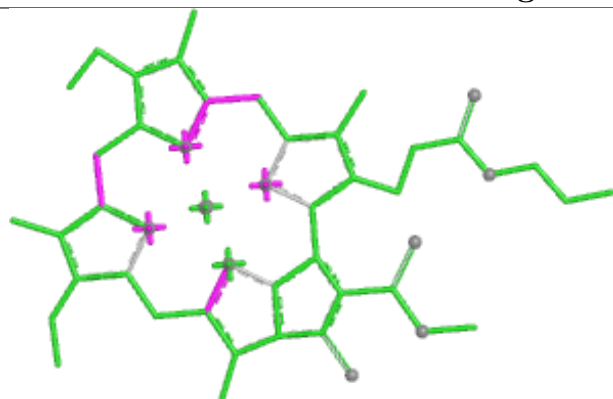


Rings

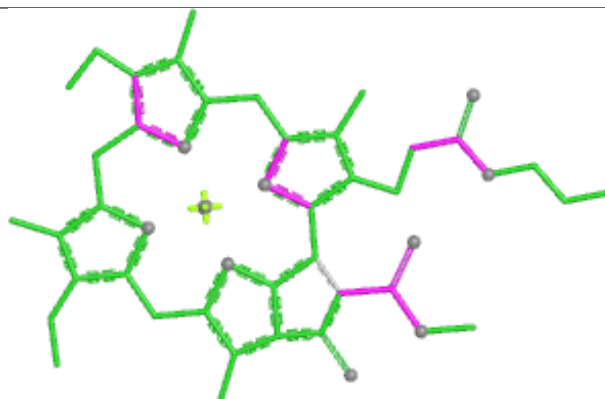
## Ligand CLA b 213



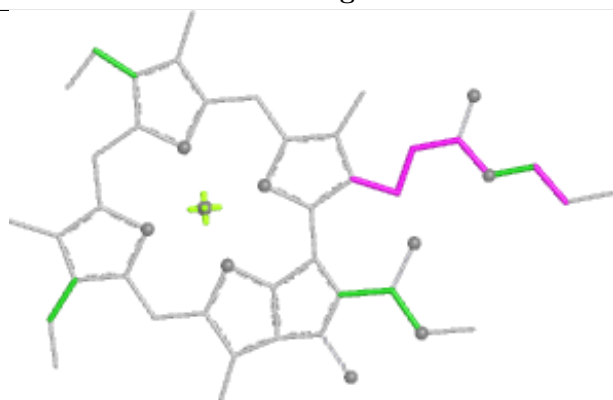
## Ligand CLA h 207



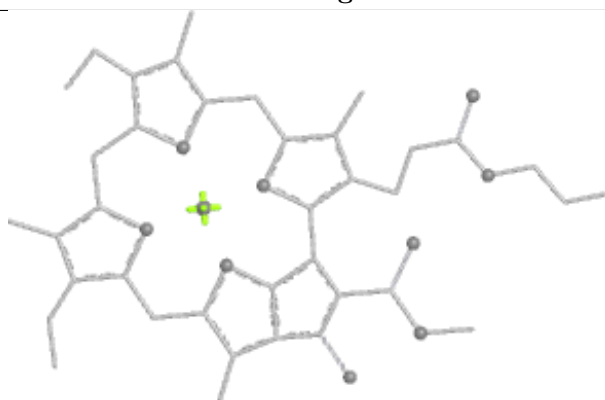
Bond lengths



Bond angles

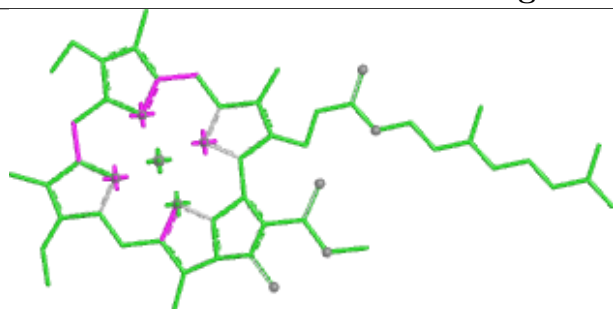


Torsions

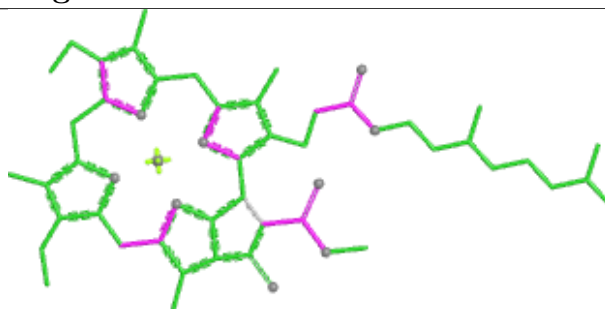


Rings

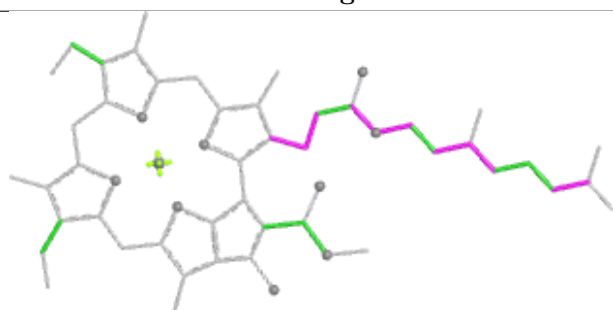
## Ligand CLA g 212



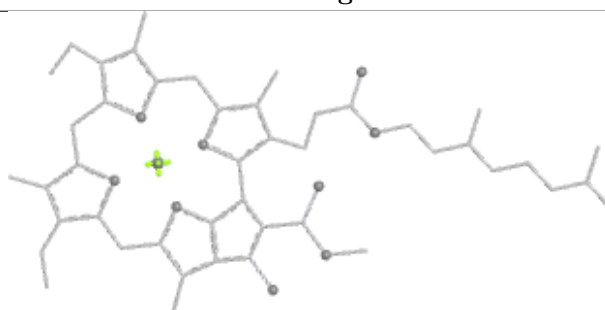
Bond lengths



Bond angles

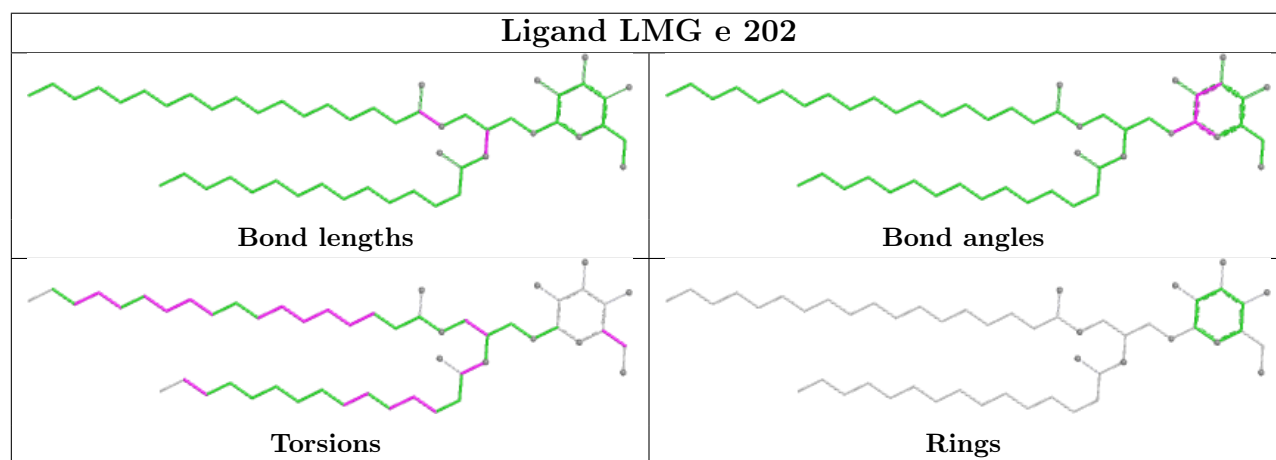
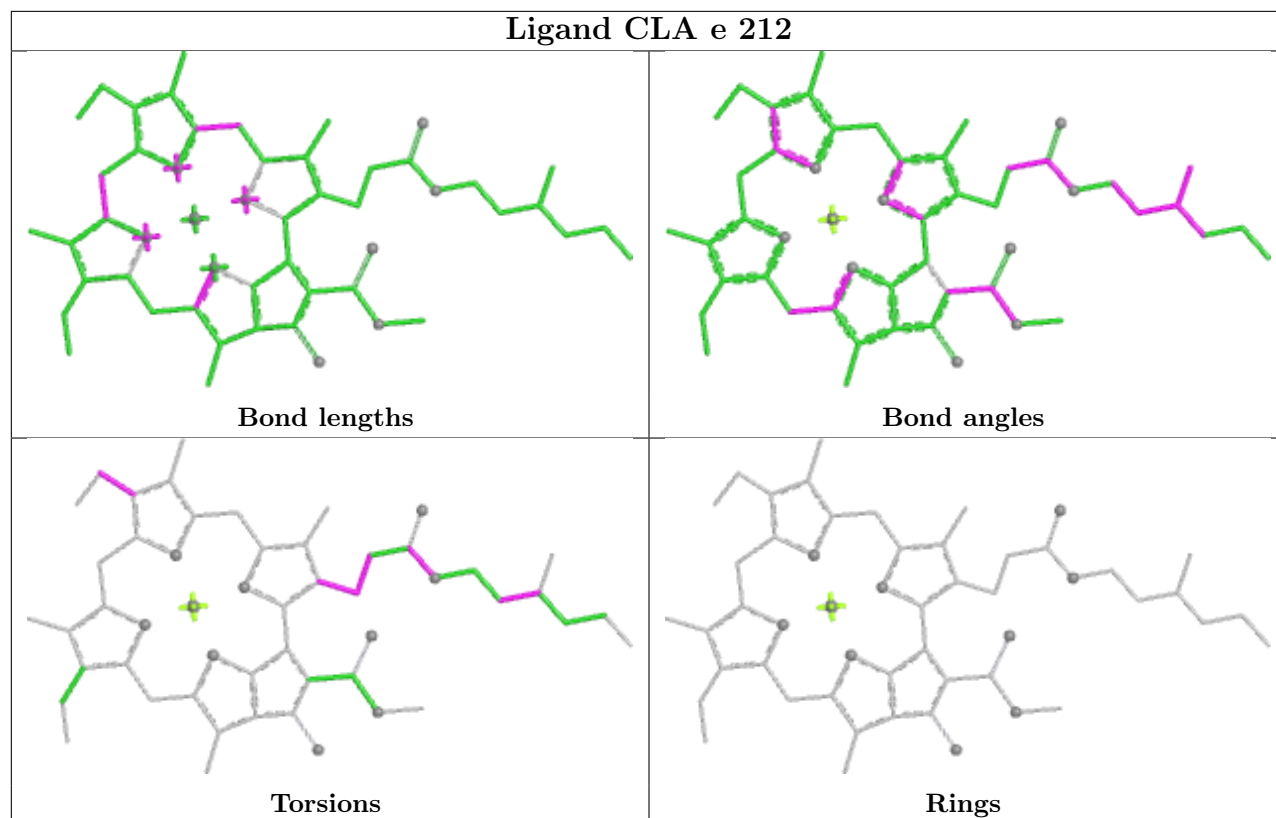


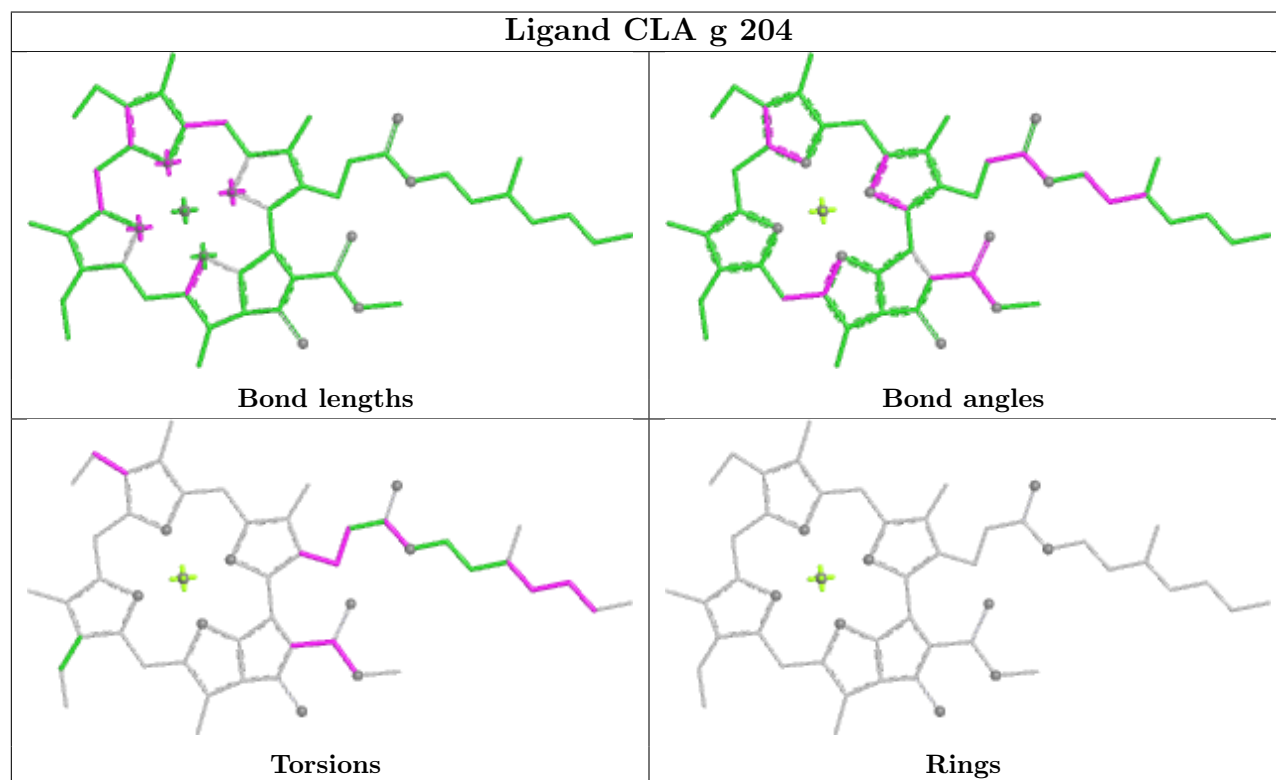
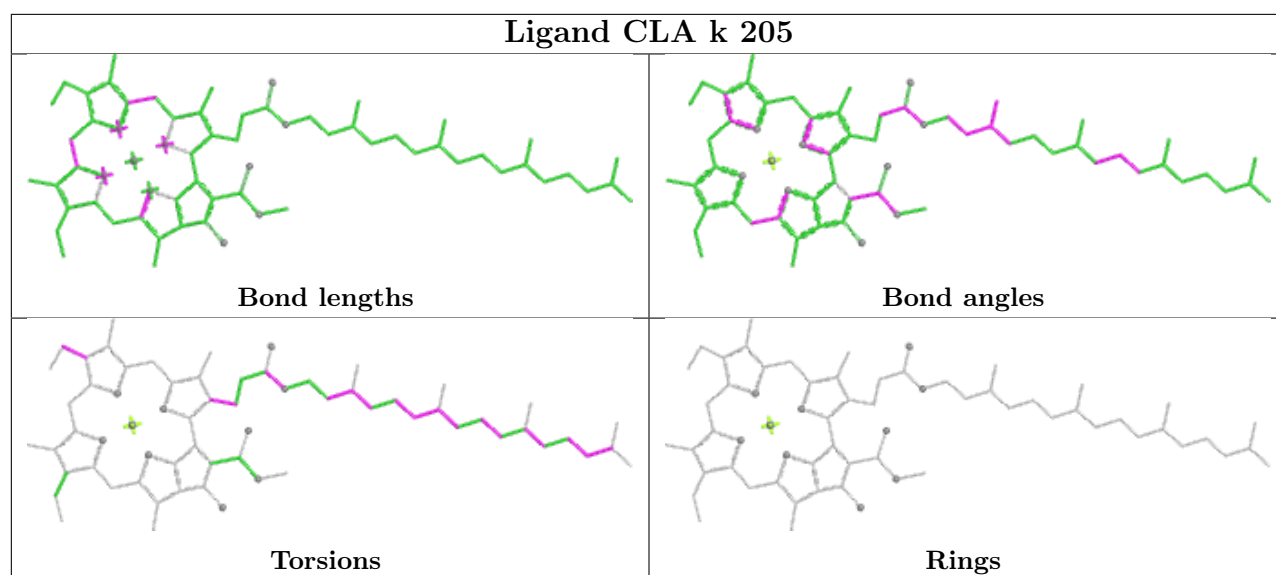
Torsions

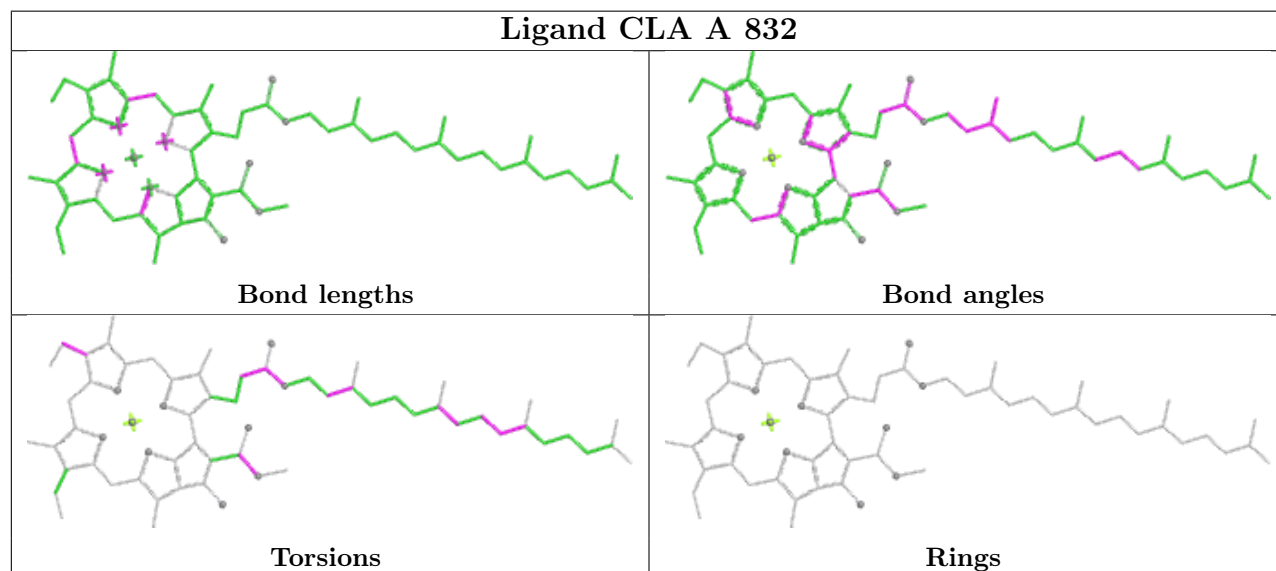
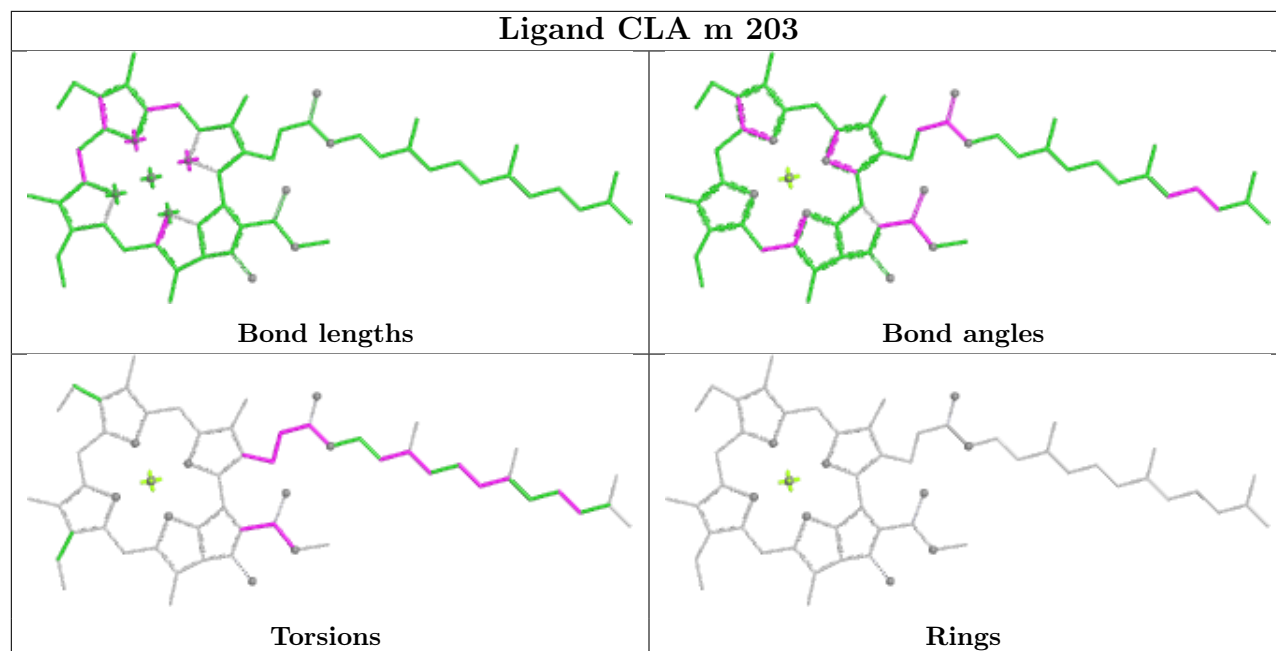


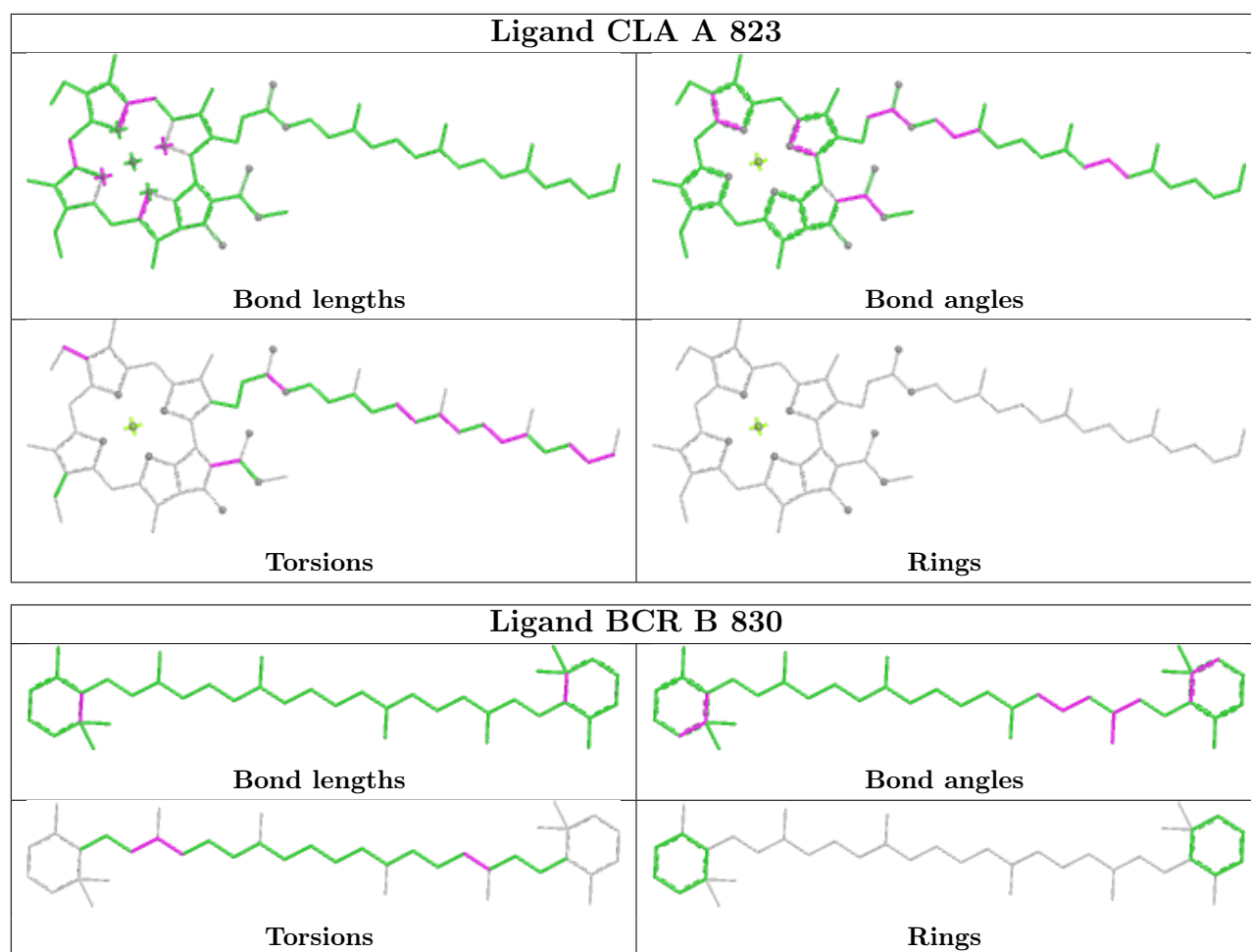
Rings



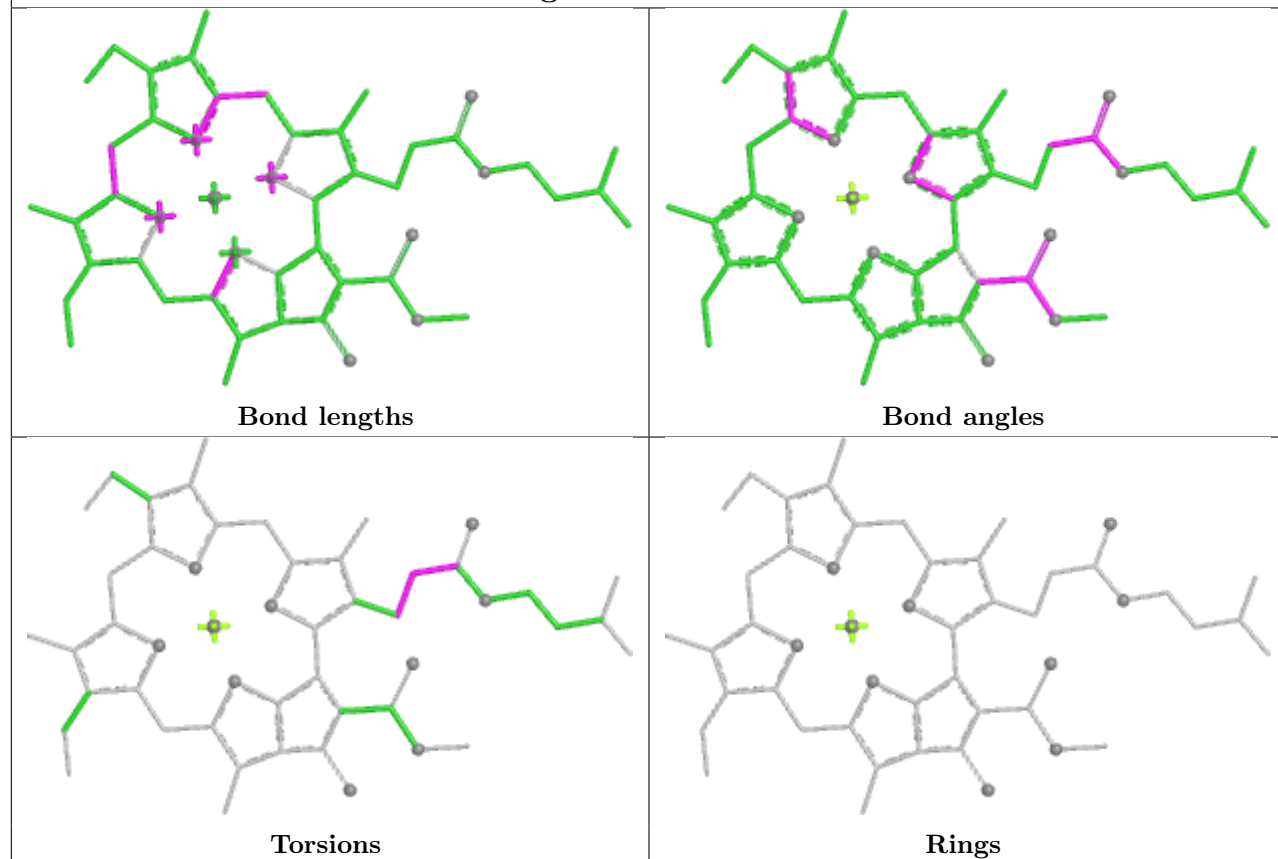




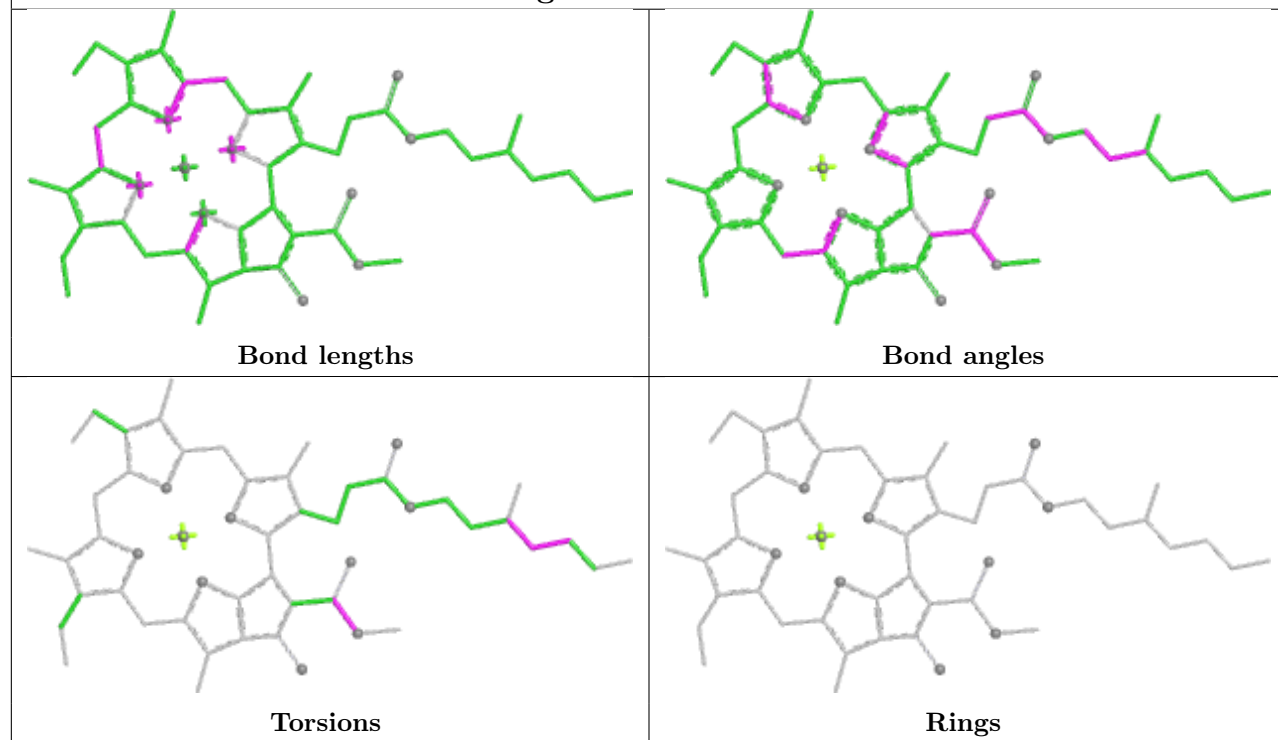




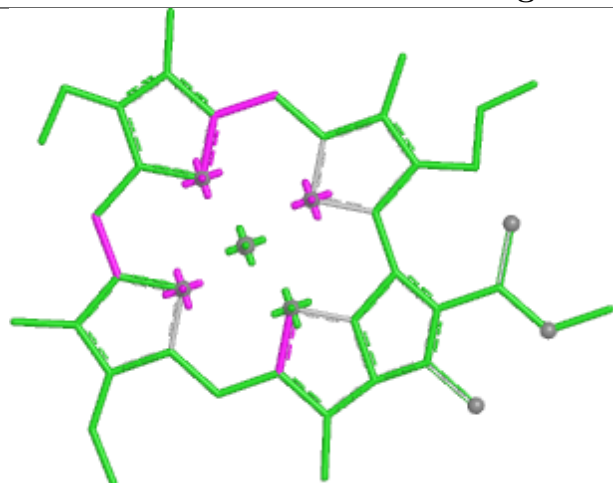
## Ligand CLA i 213



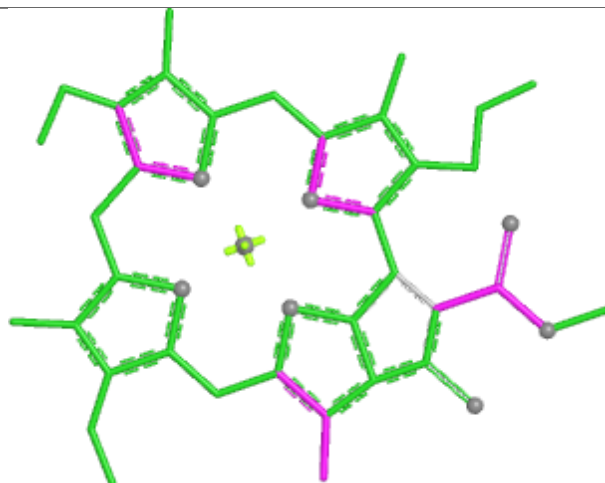
## Ligand CLA e 201



## Ligand CLA h 205



Bond lengths



Bond angles

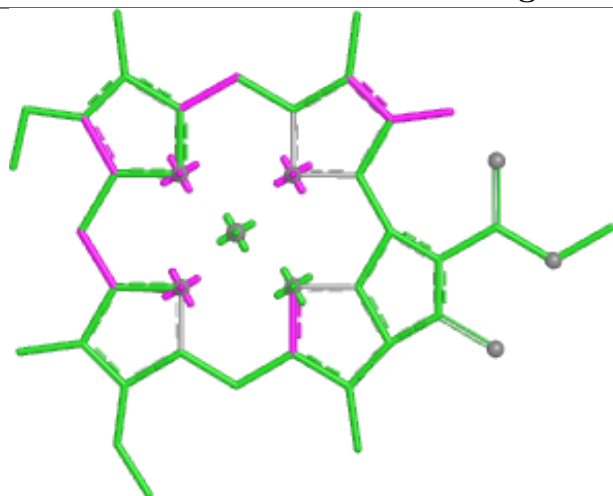


Torsions

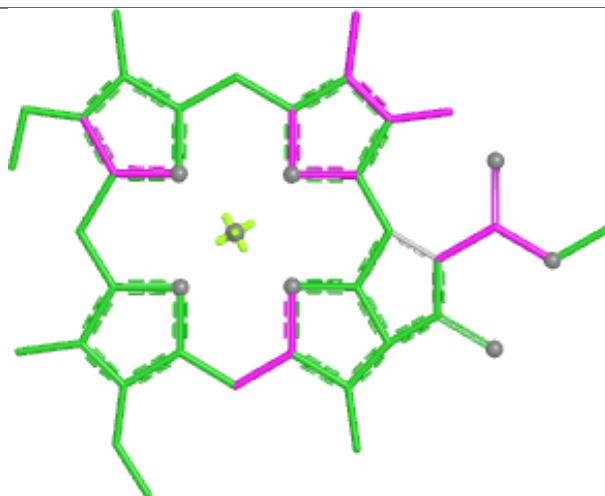


Rings

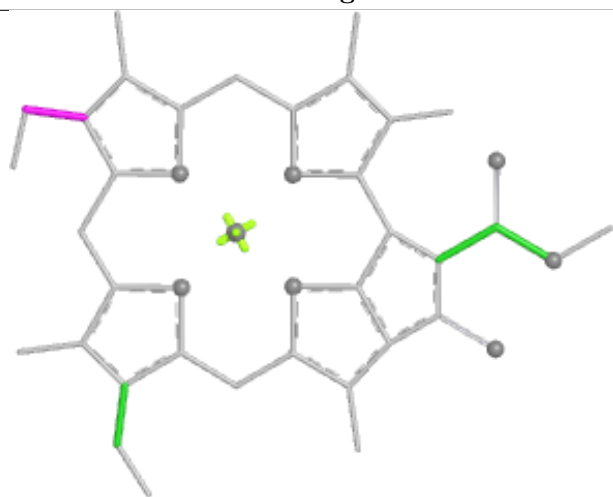
## Ligand CLA o 607



Bond lengths



Bond angles

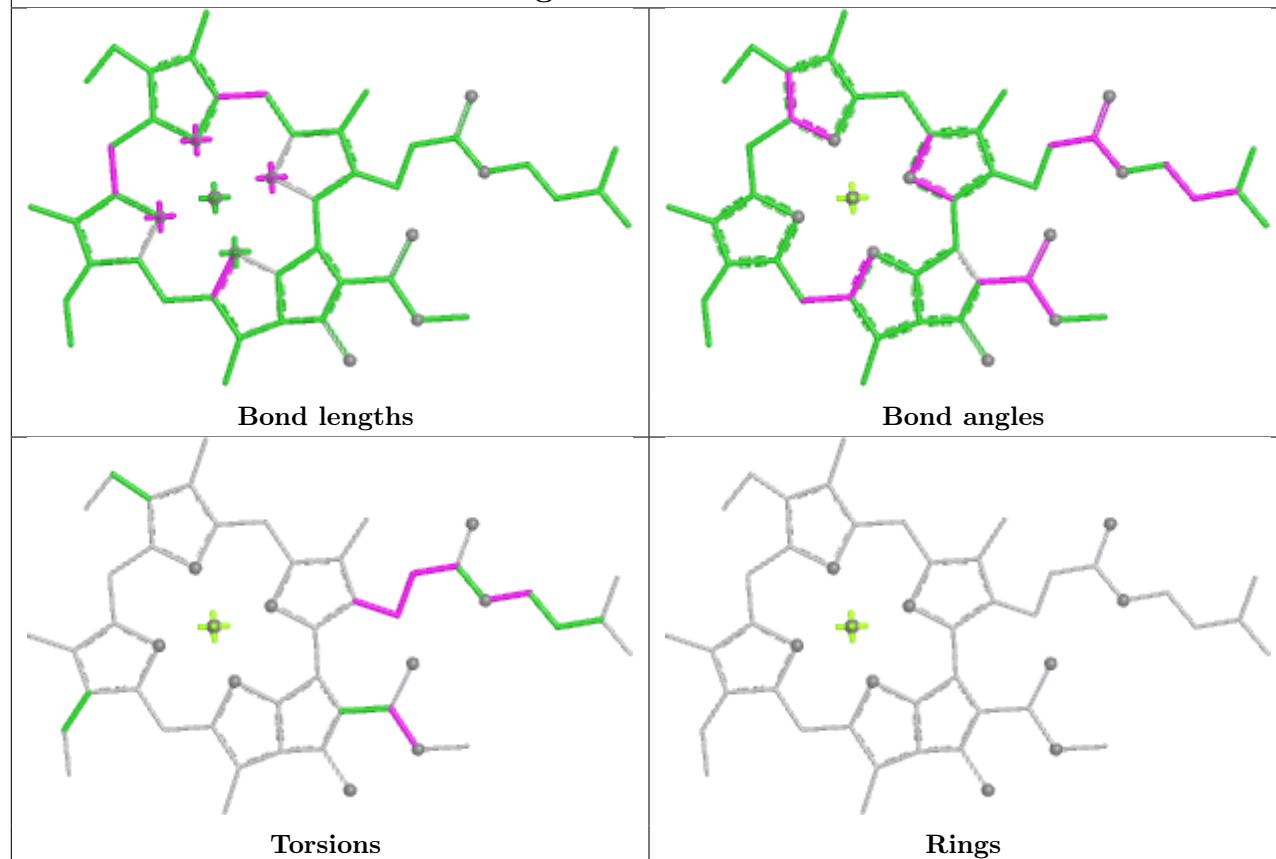


Torsions

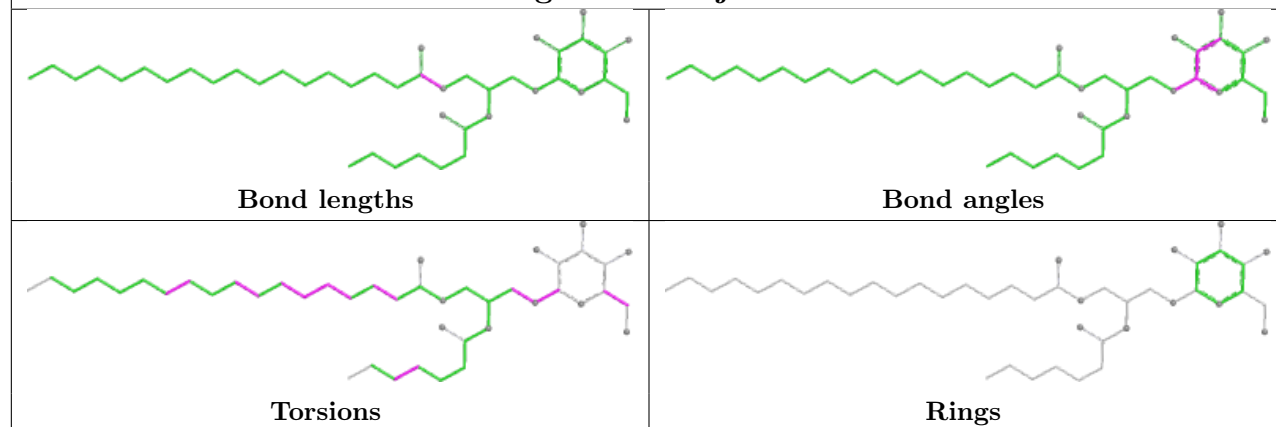


Rings

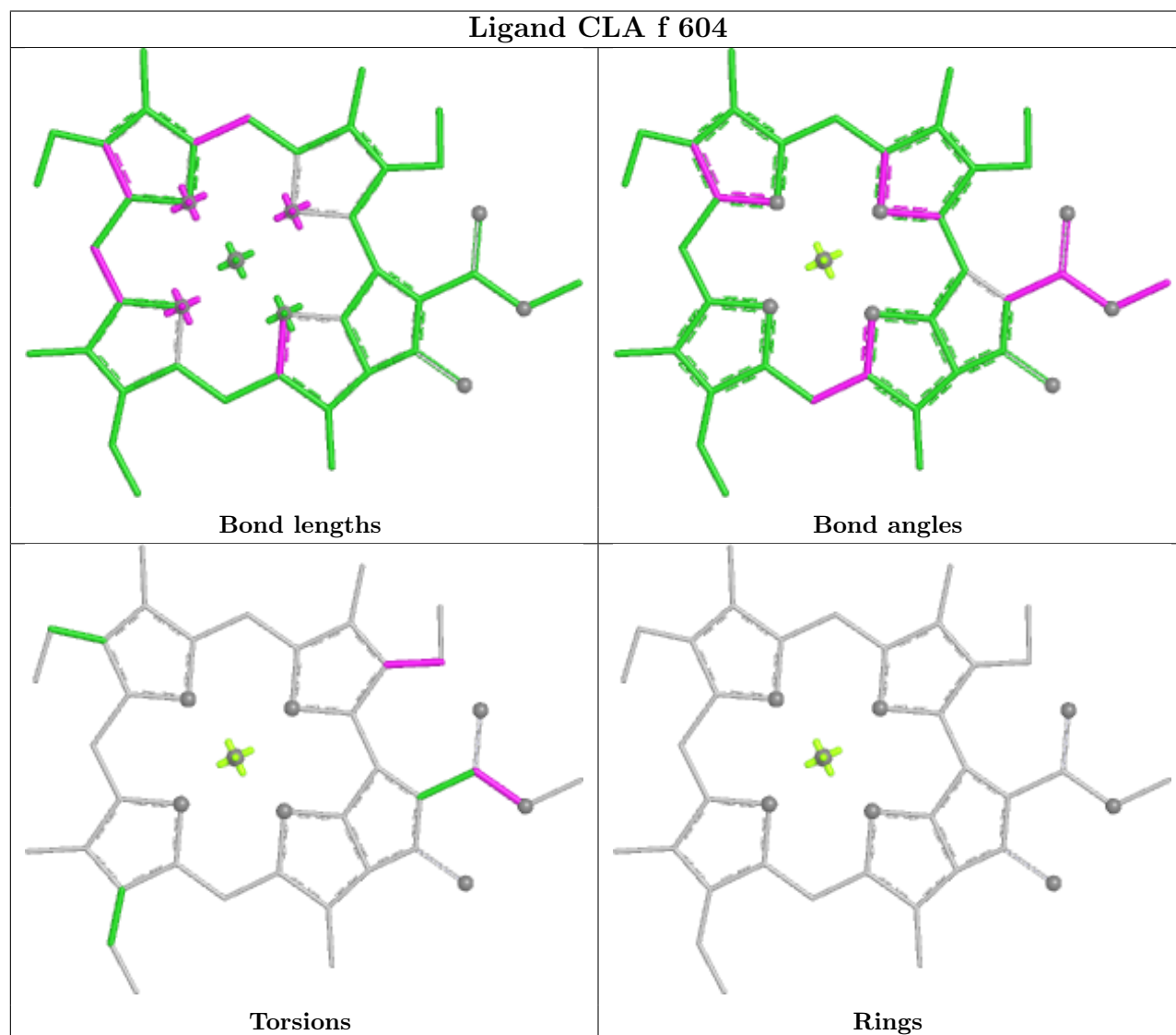
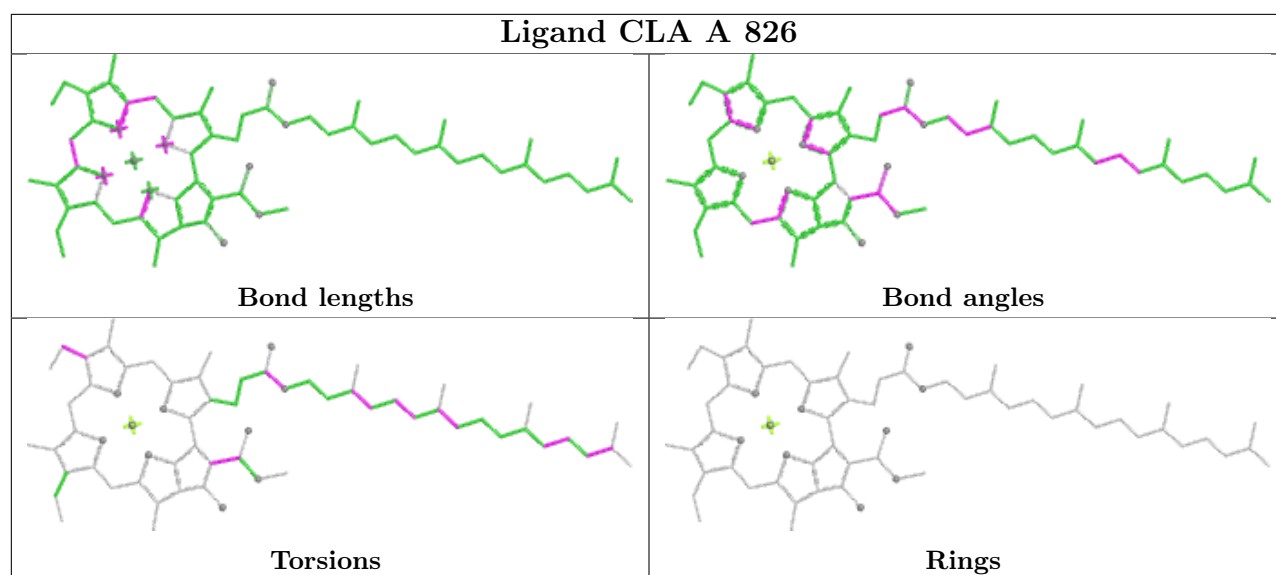
## Ligand CLA h 203



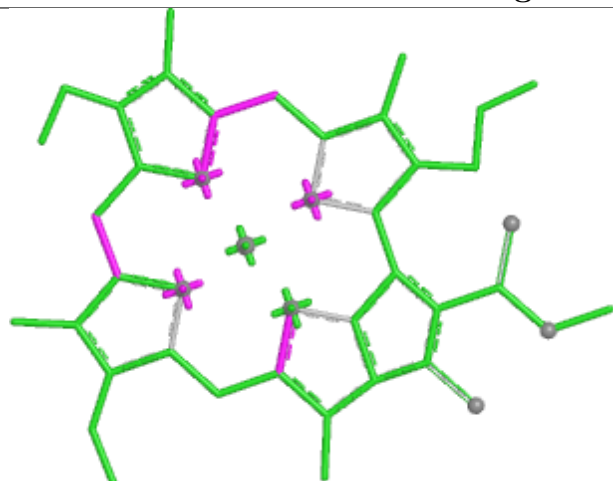
## Ligand LMG j 201



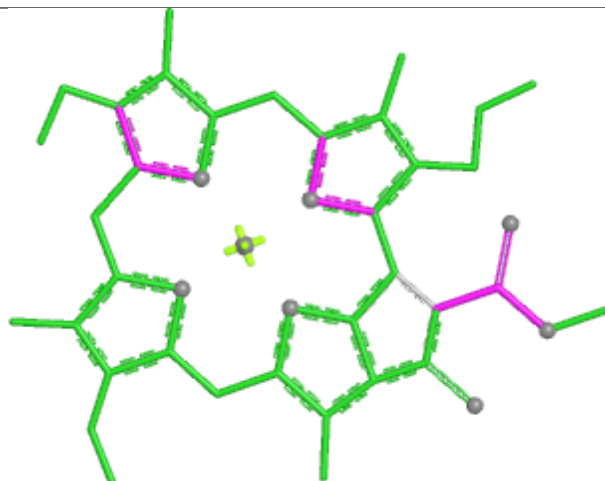




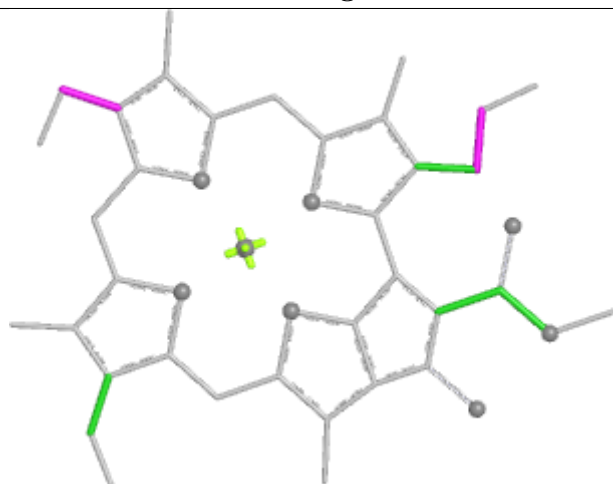
## Ligand CLA B 808



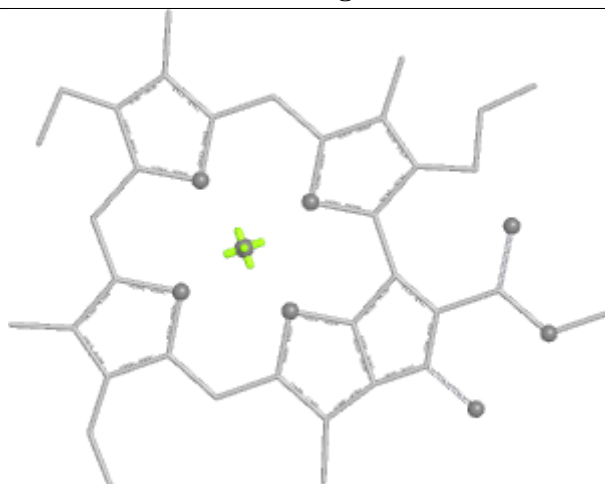
Bond lengths



Bond angles

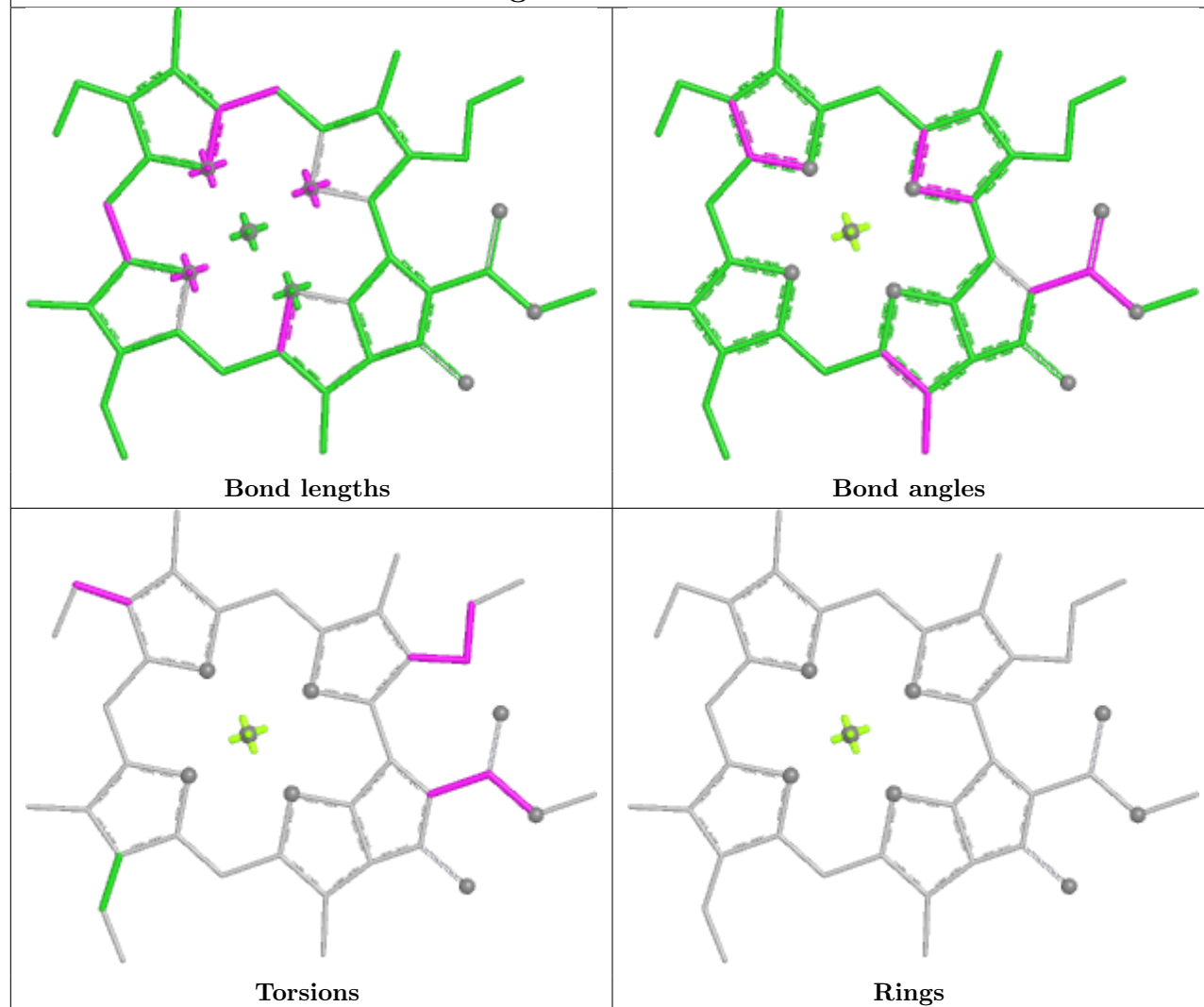


Torsions

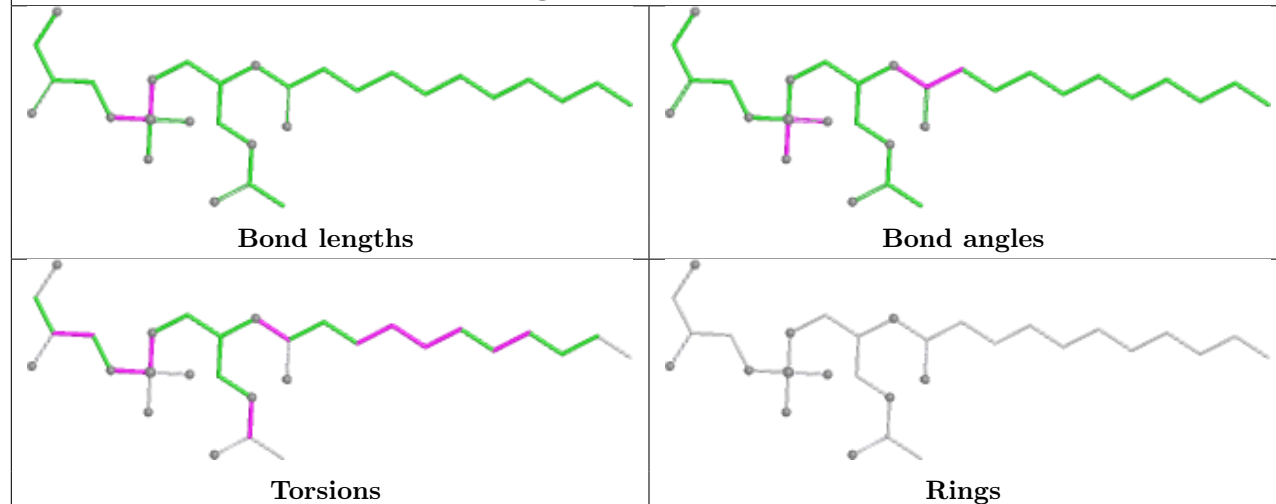


Rings

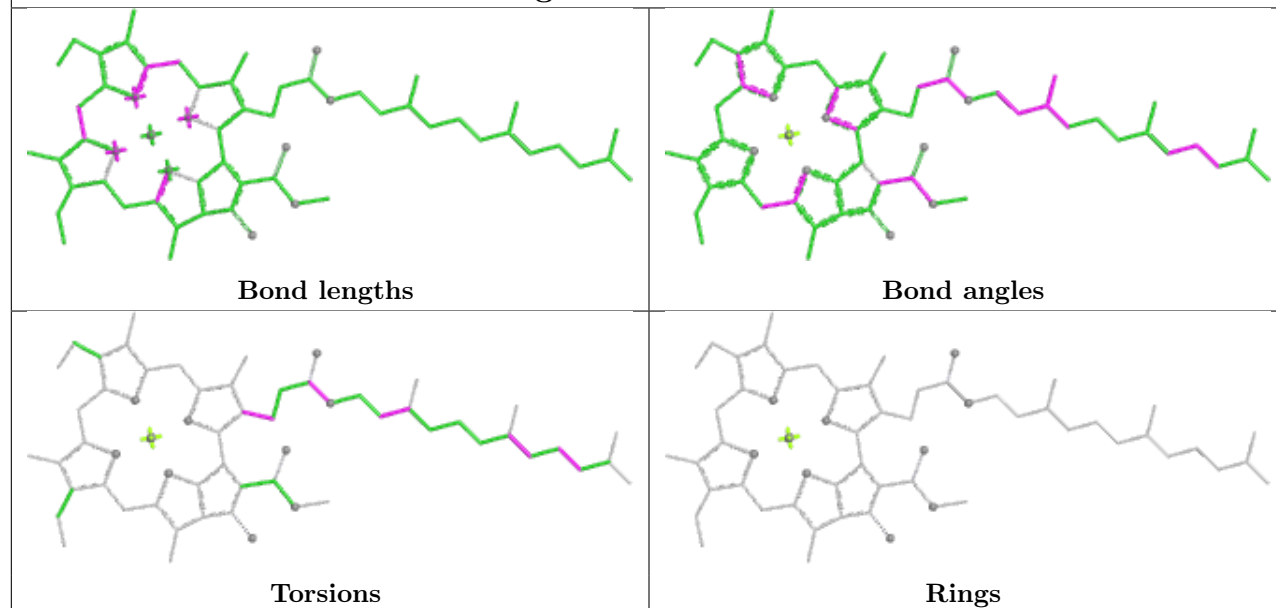
## Ligand CLA i 204



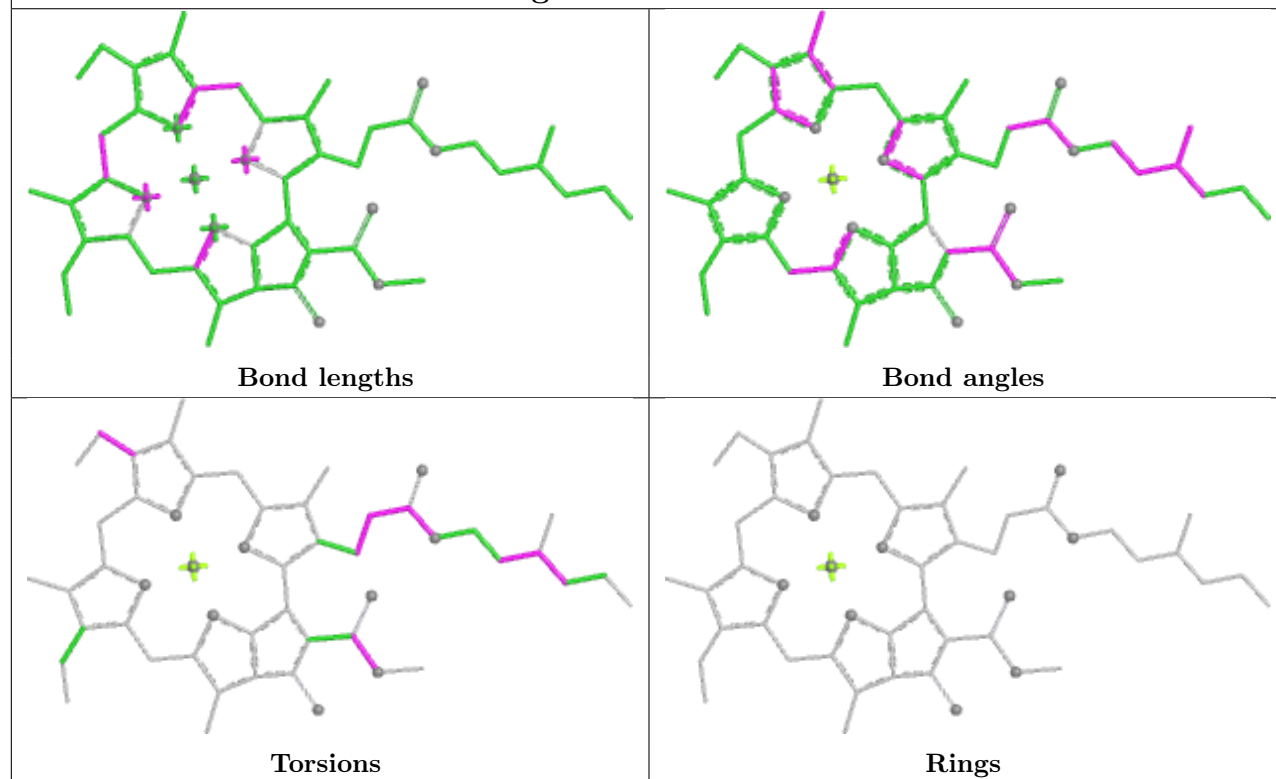
## Ligand LHG h 201



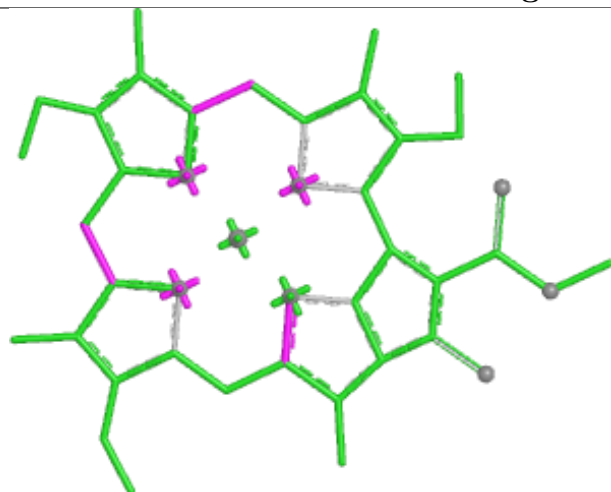
## Ligand CLA h 206



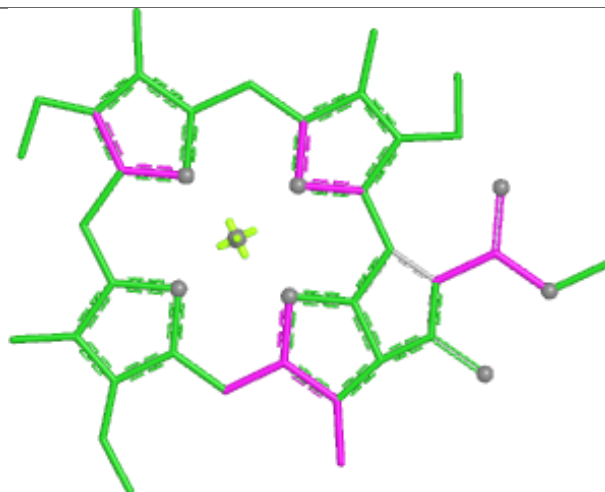
## Ligand CLA A 843



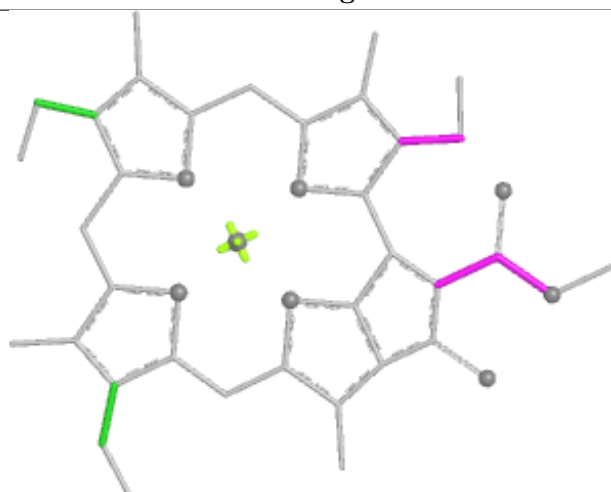
## Ligand CLA f 611



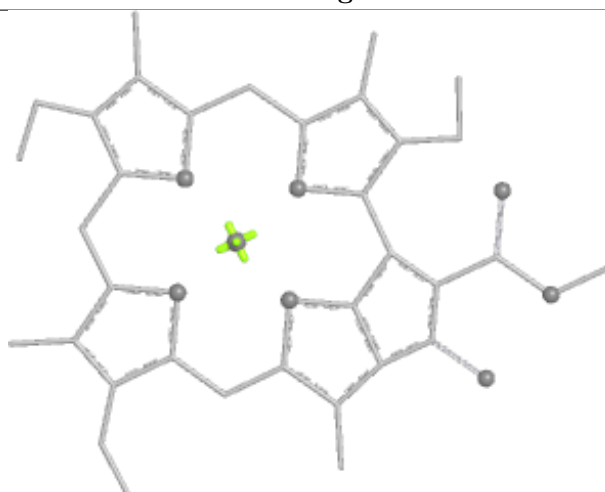
Bond lengths



Bond angles

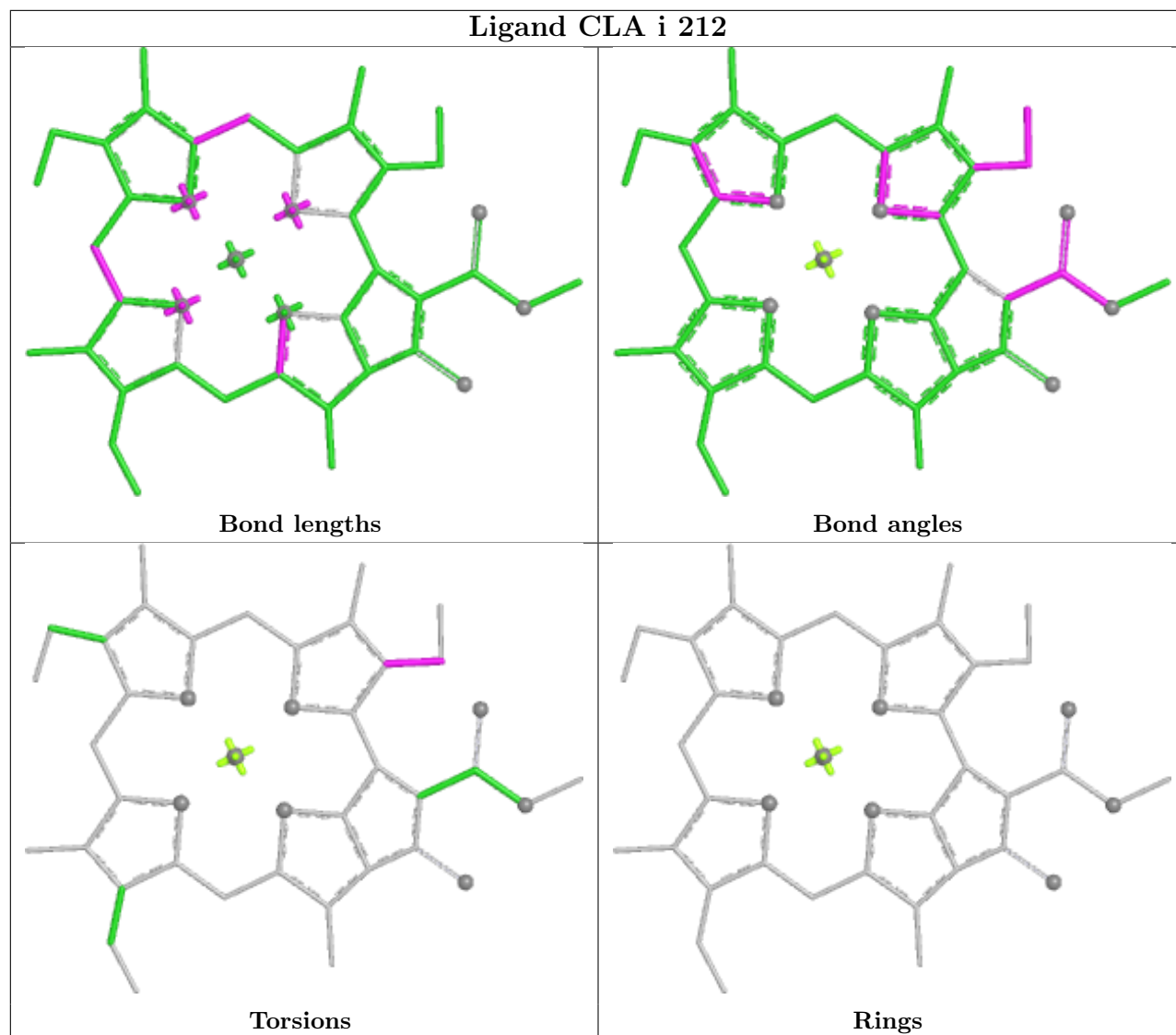


Torsions

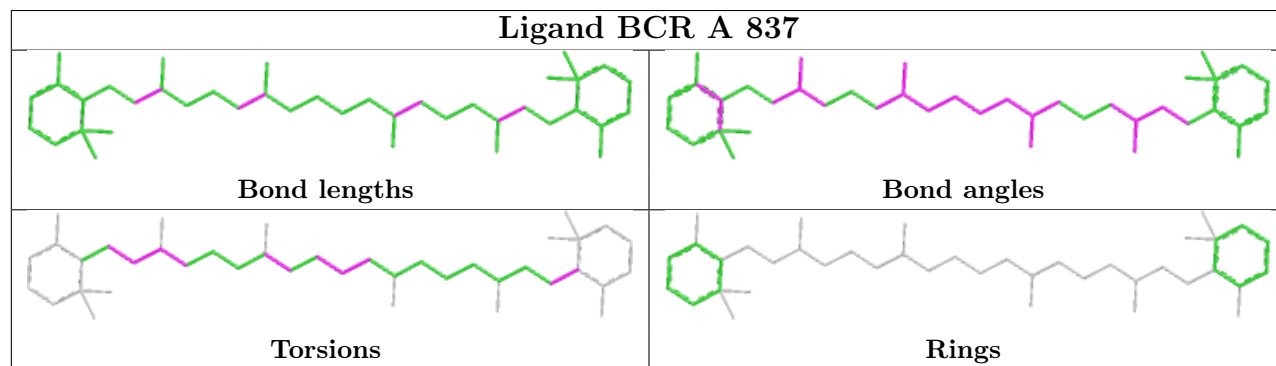


Rings

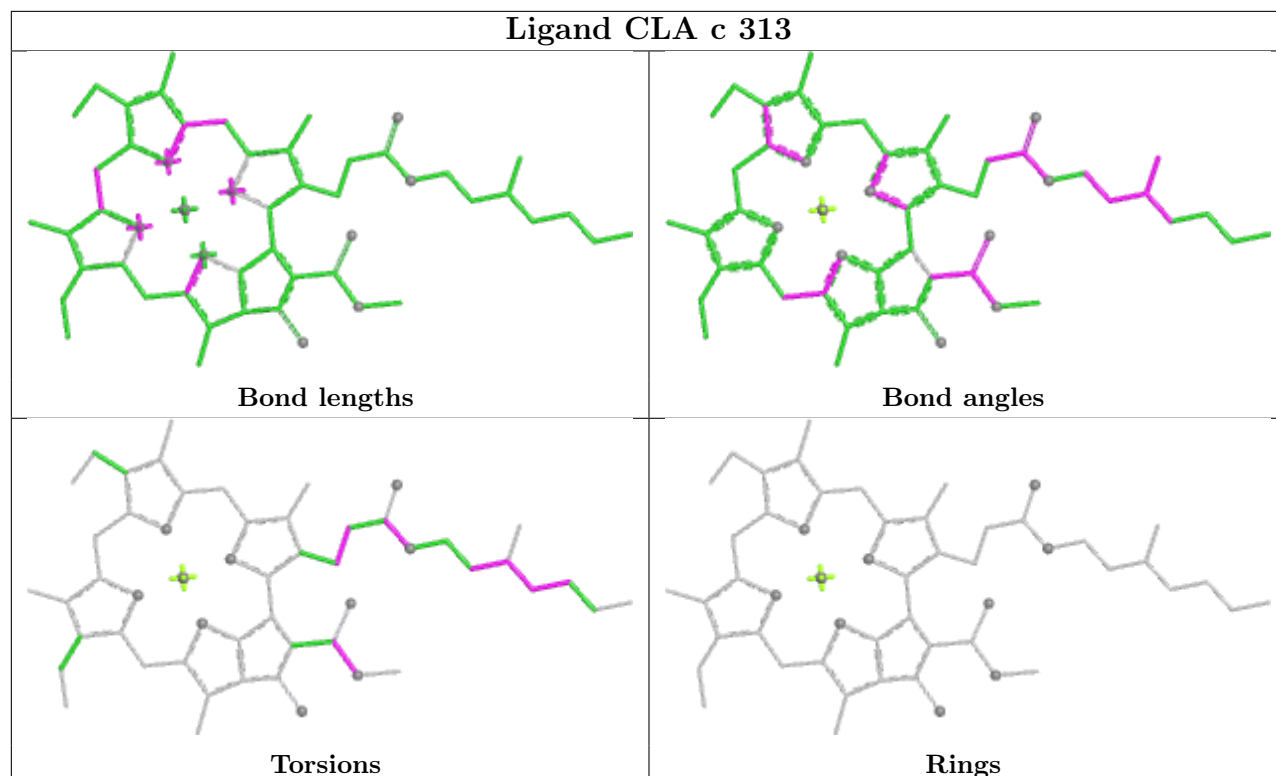
## Ligand CLA i 212



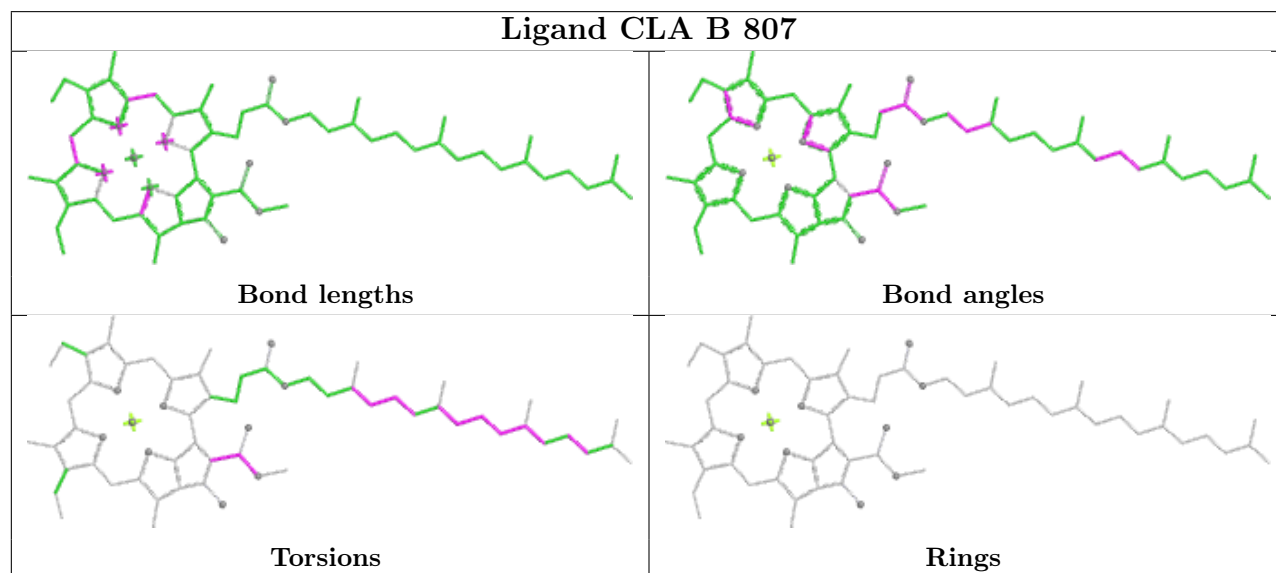
## Ligand BCR A 837



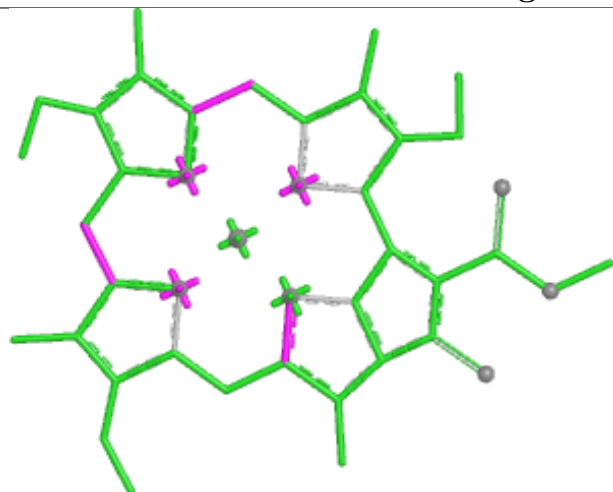
## Ligand CLA c 313



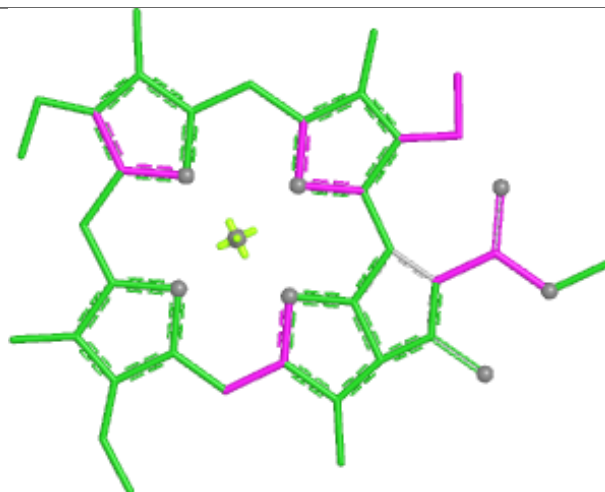
## Ligand CLA B 807



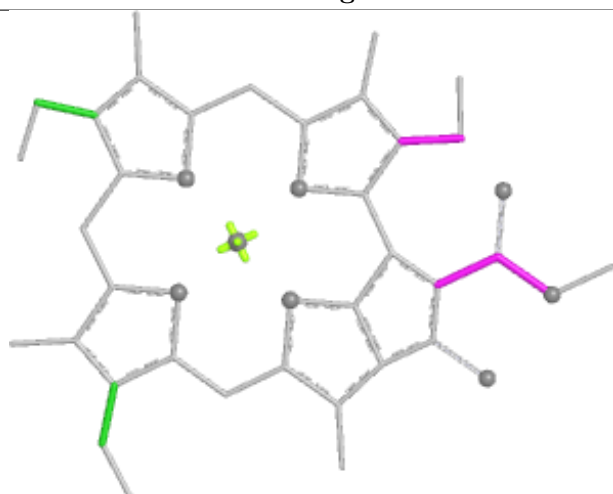
## Ligand CLA o 609



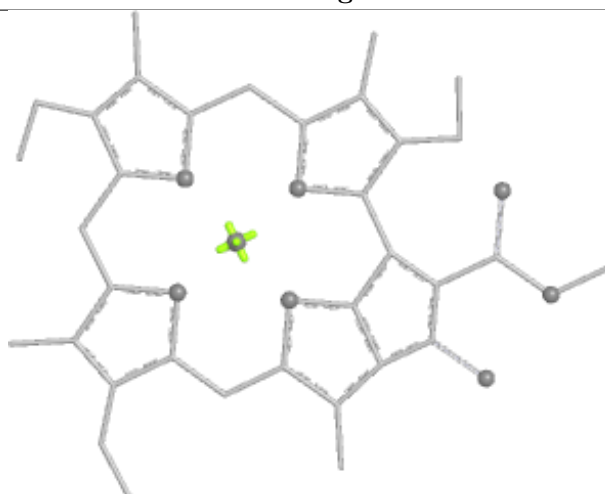
Bond lengths



Bond angles



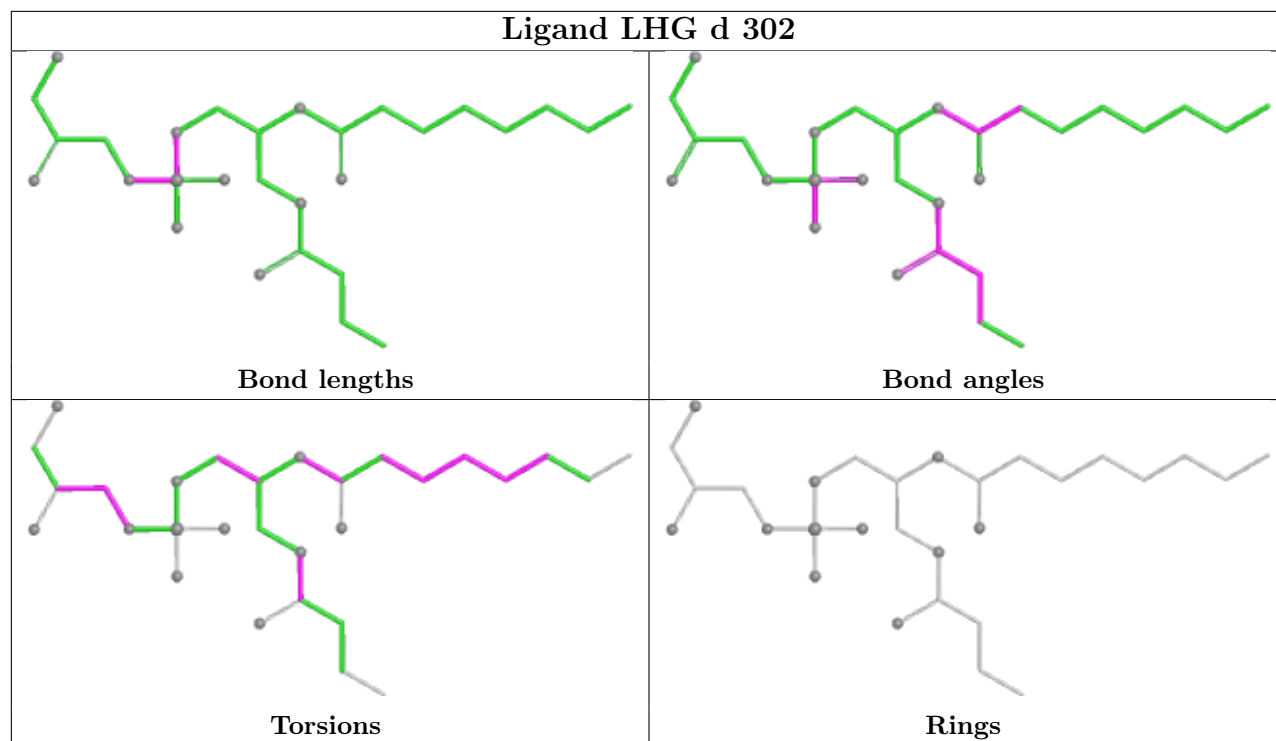
Torsions



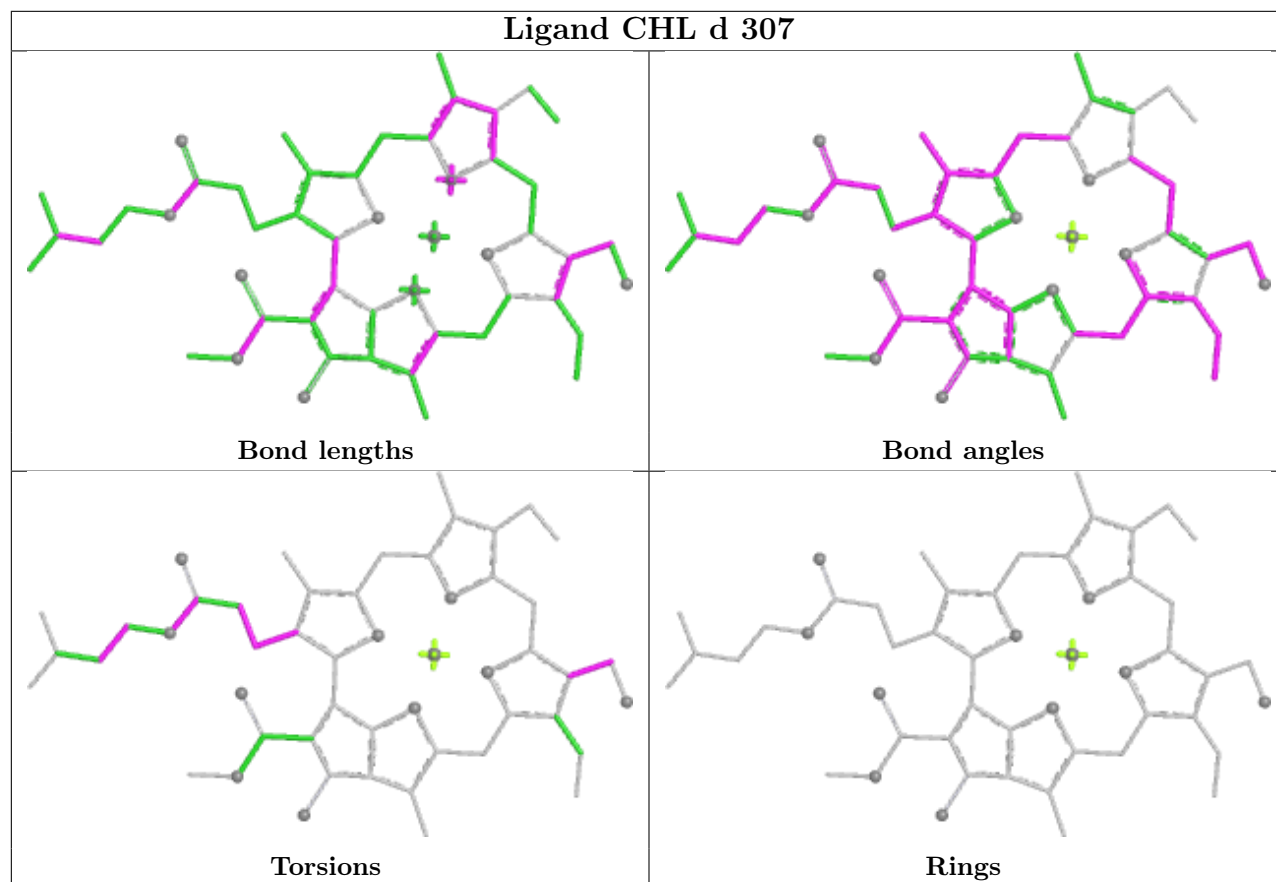
Rings

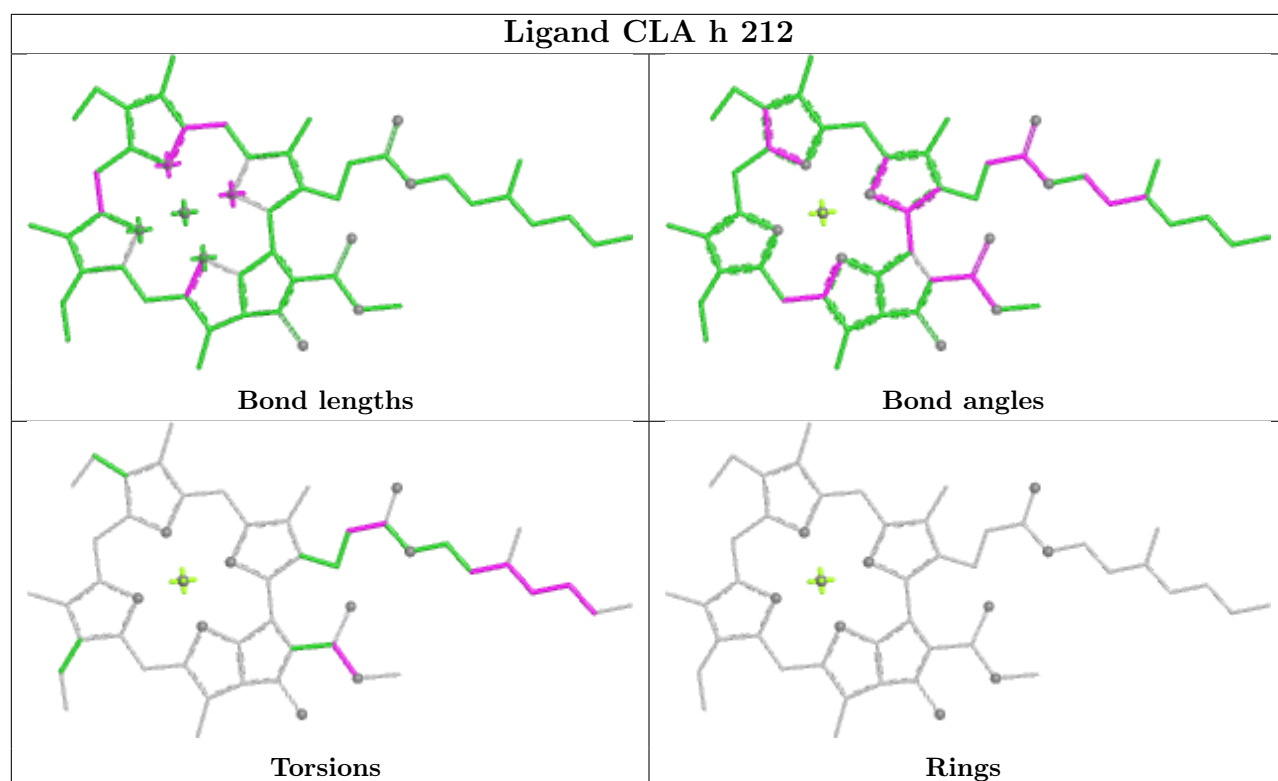


## Ligand LHG d 302

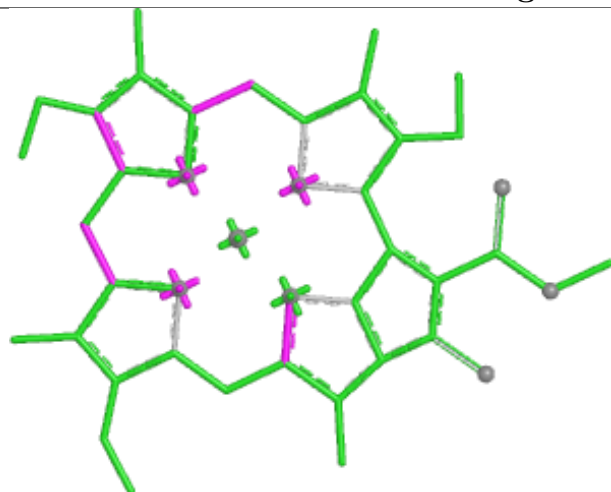


## Ligand CHL d 307

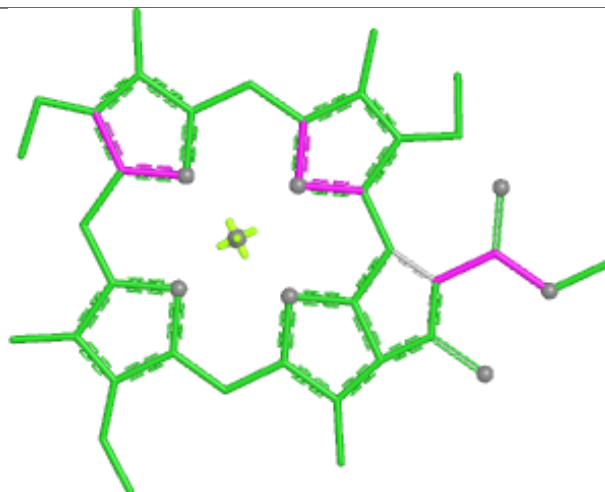




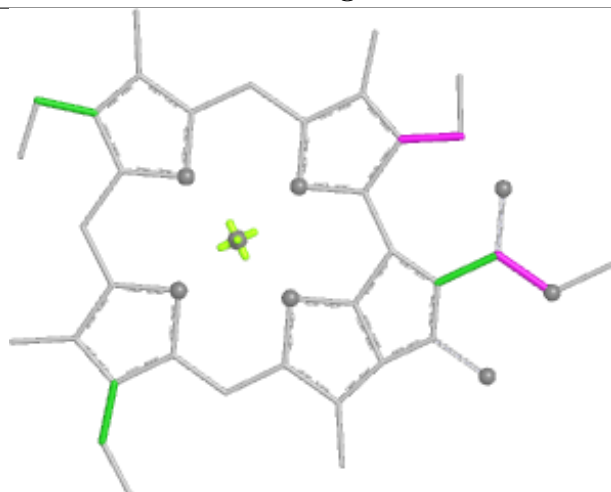
## Ligand CLA n 210



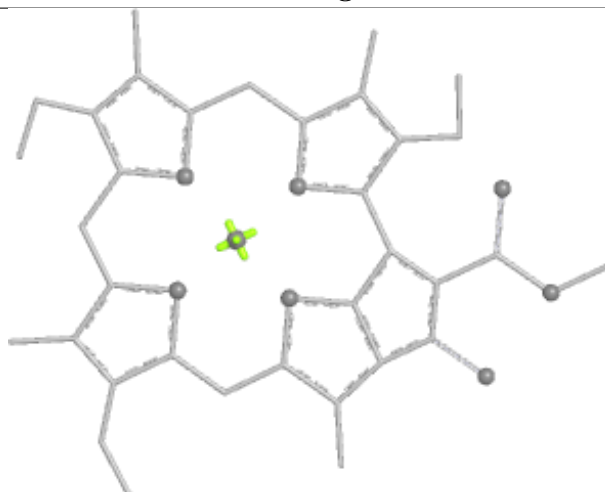
Bond lengths



Bond angles

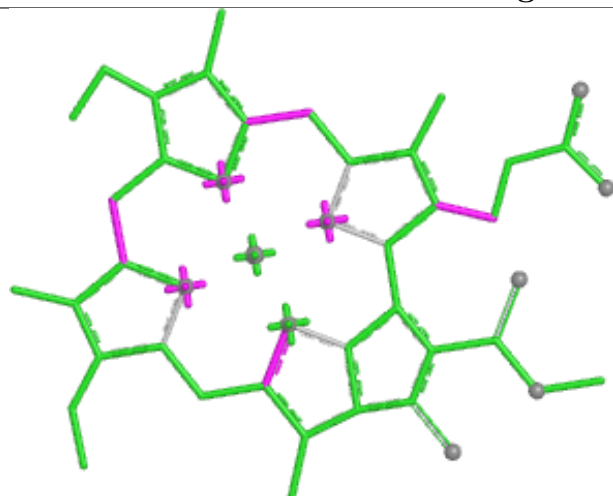


Torsions

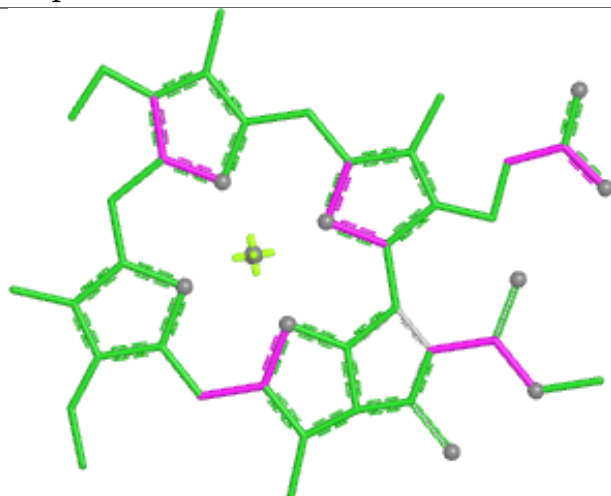


Rings

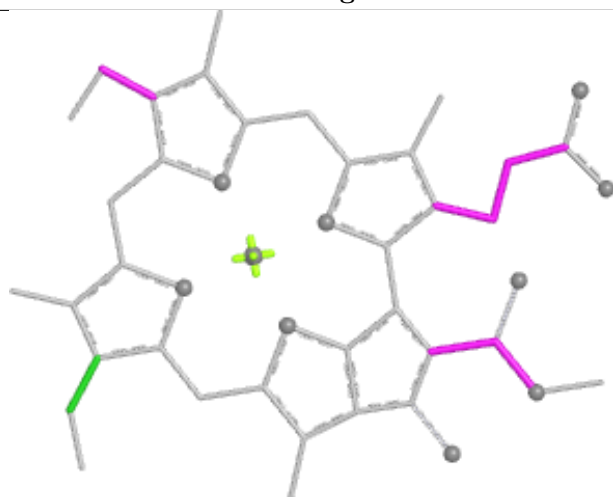
## Ligand CLA p 607



Bond lengths



Bond angles

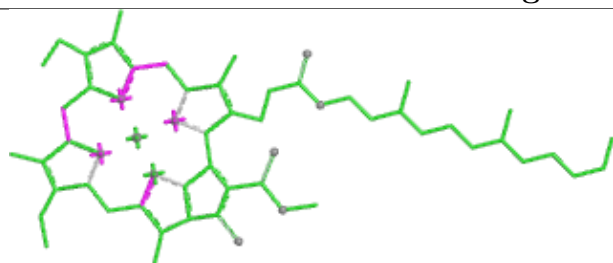


Torsions

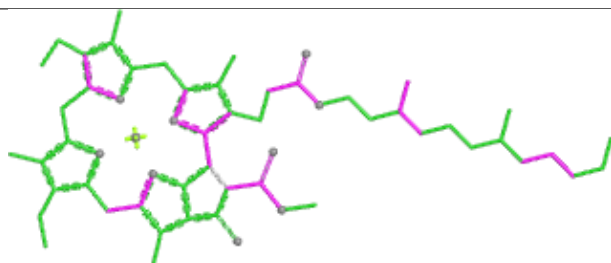


Rings

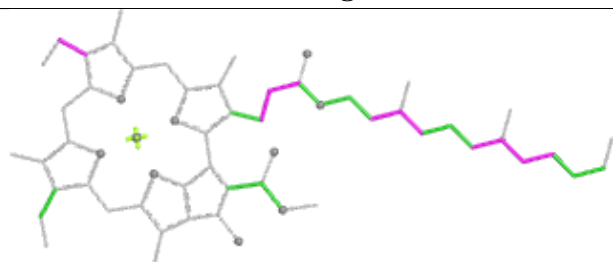
## Ligand CLA i 211



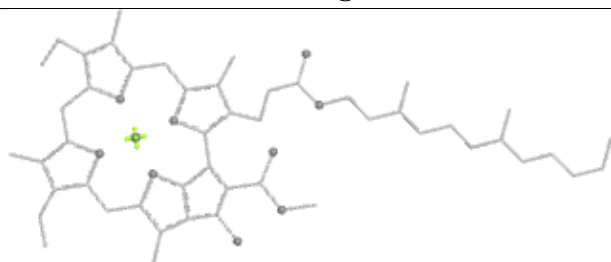
Bond lengths



Bond angles

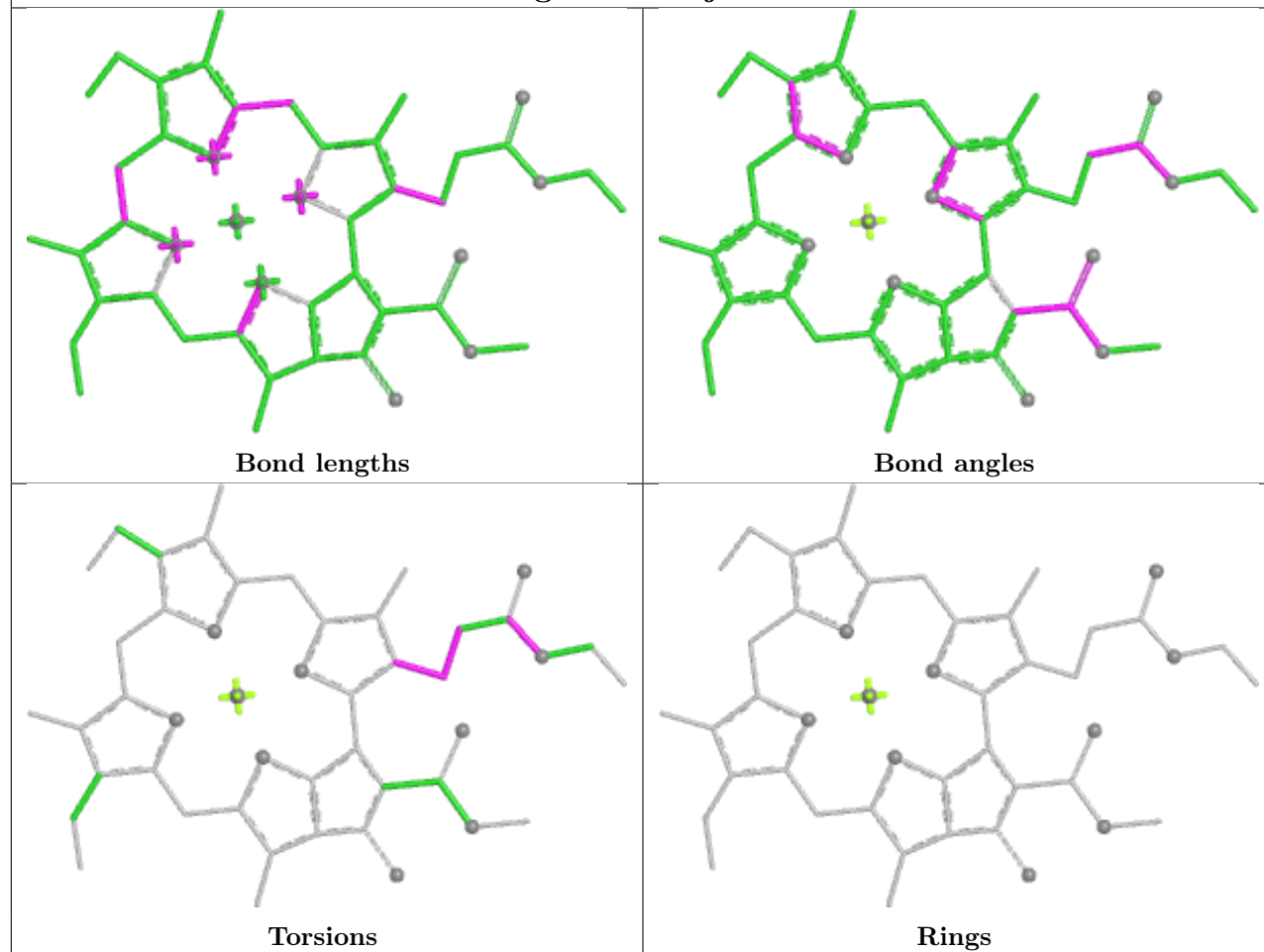


Torsions

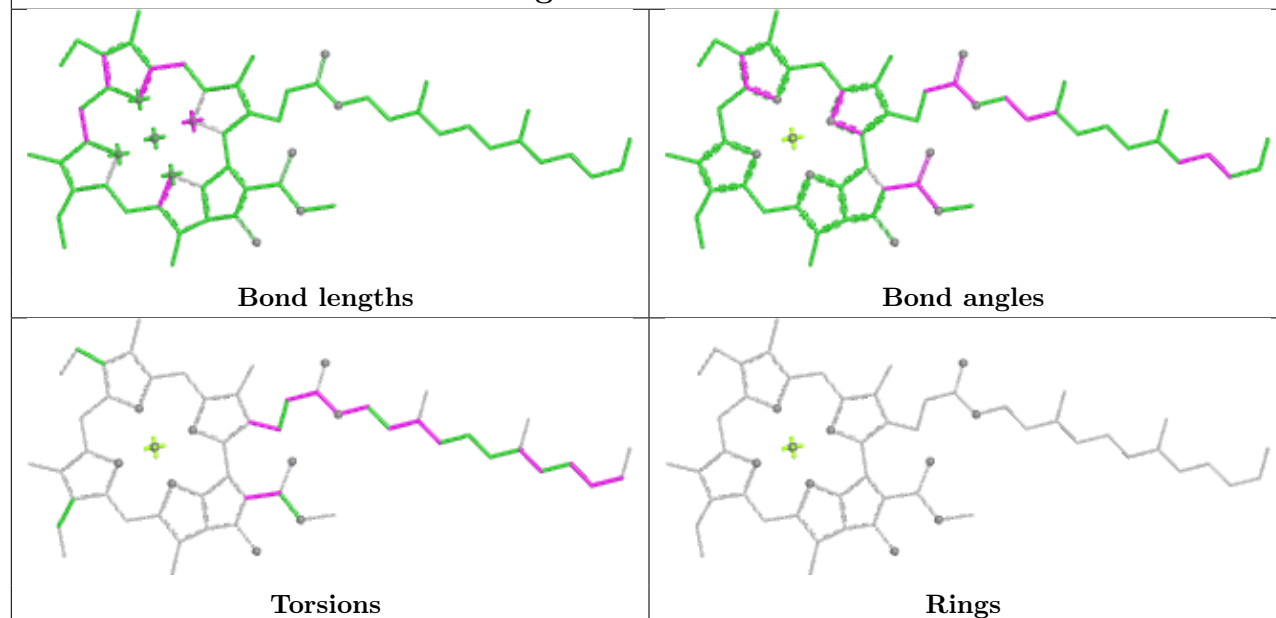


Rings

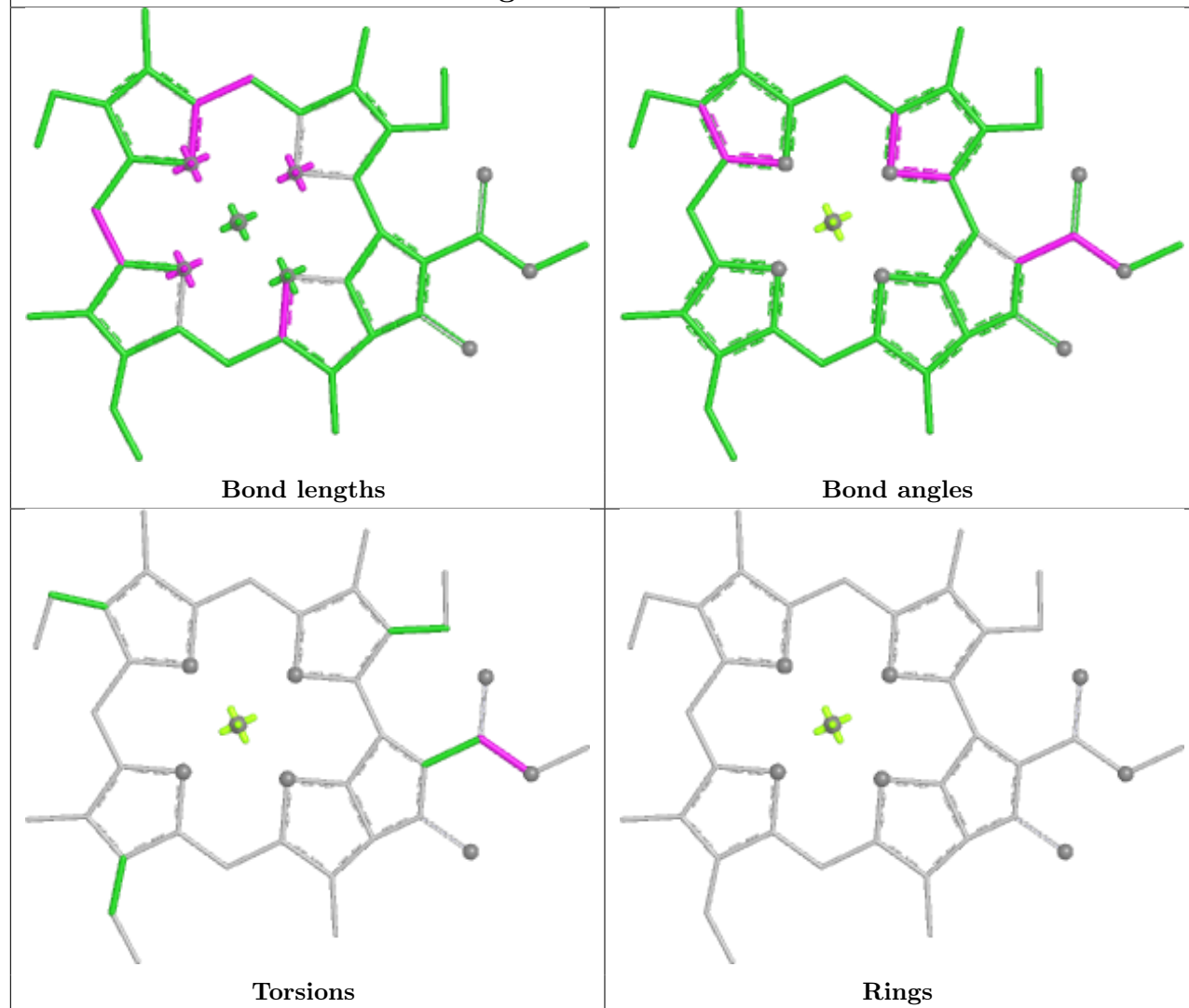
## Ligand CLA j 207



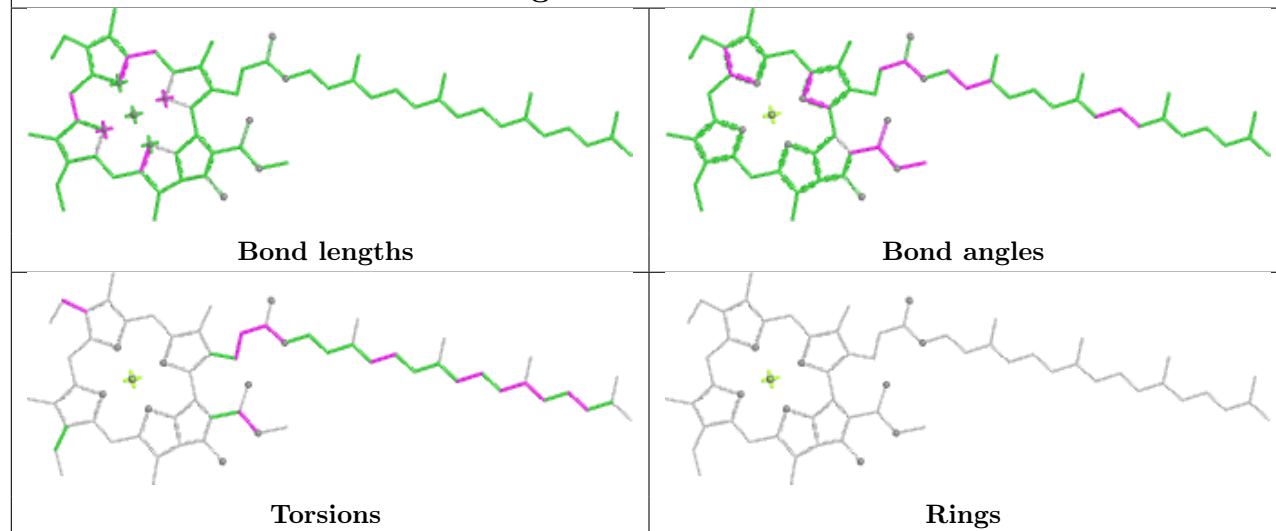
## Ligand CLA n 201



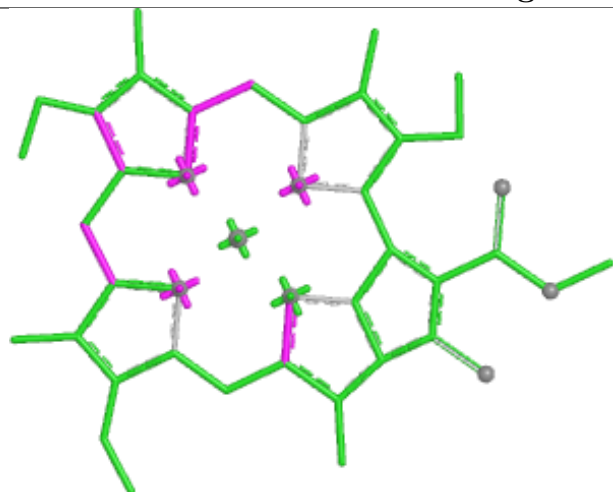
## Ligand CLA d 314



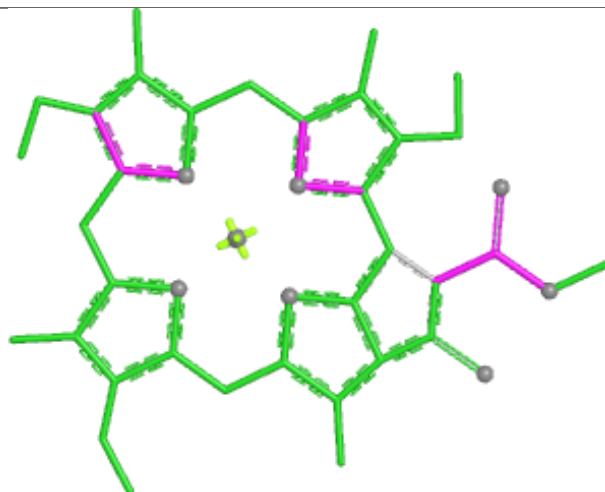
## Ligand CLA A 810



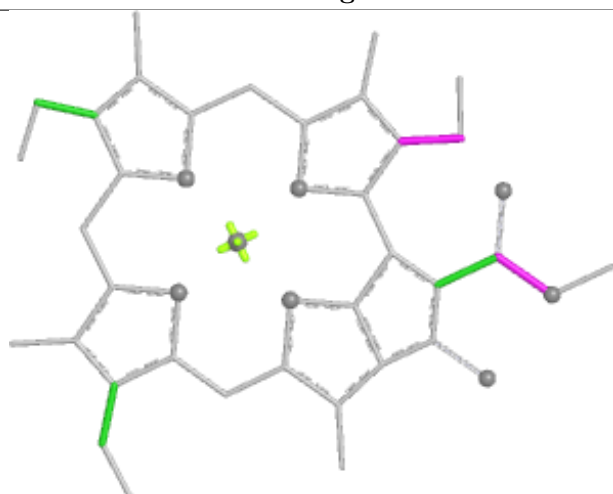
## Ligand CLA n 211



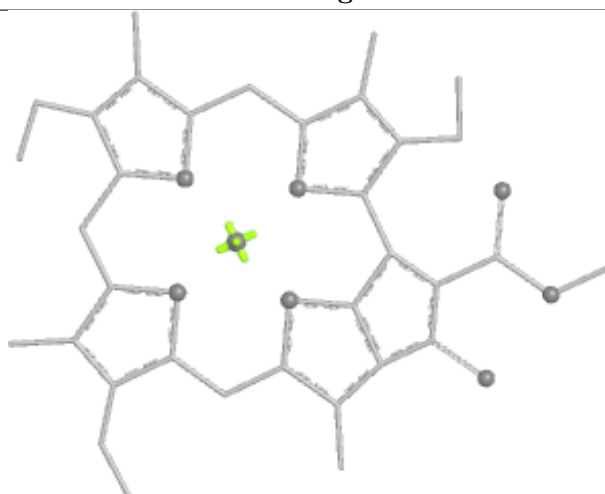
Bond lengths



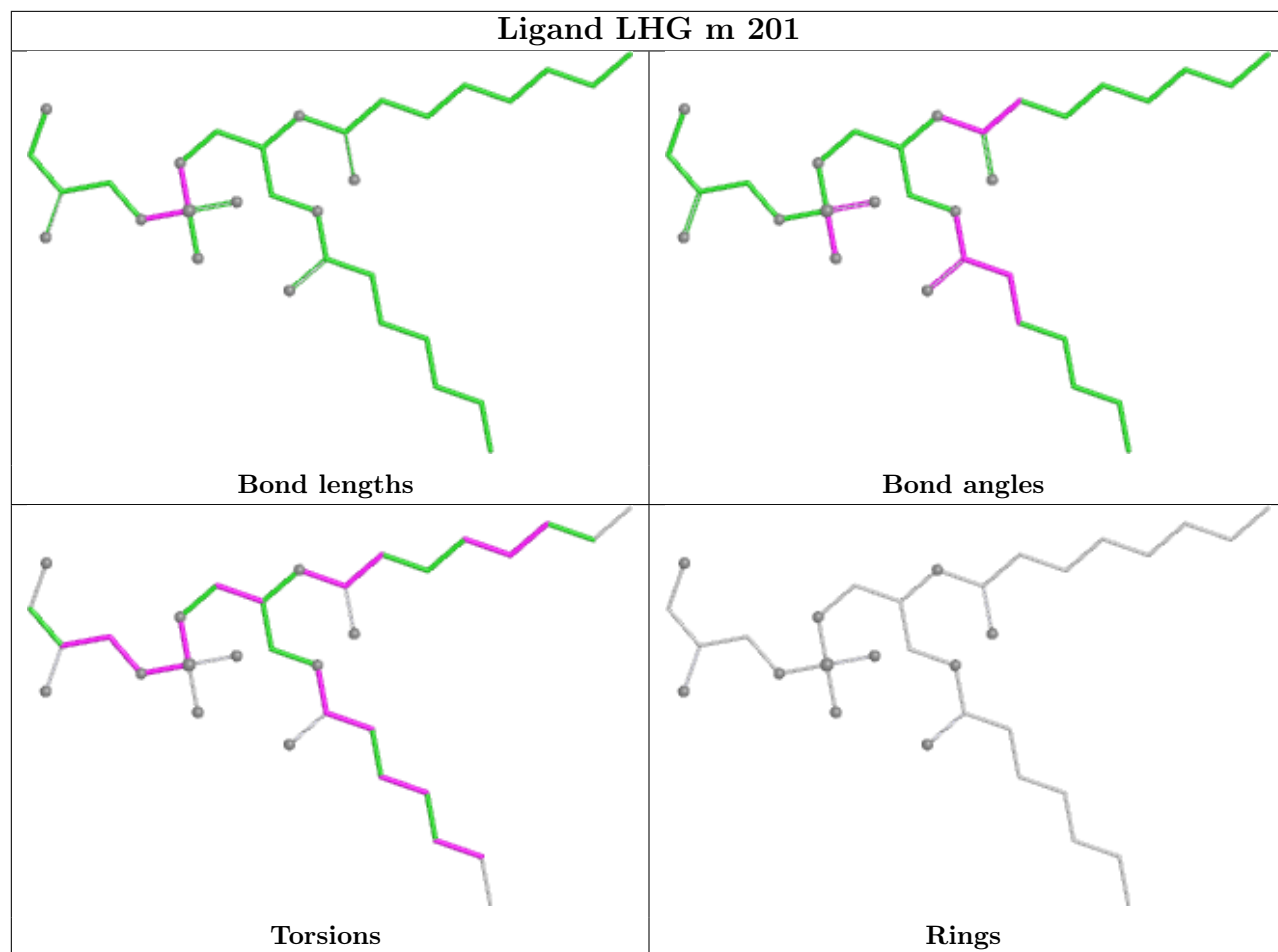
Bond angles



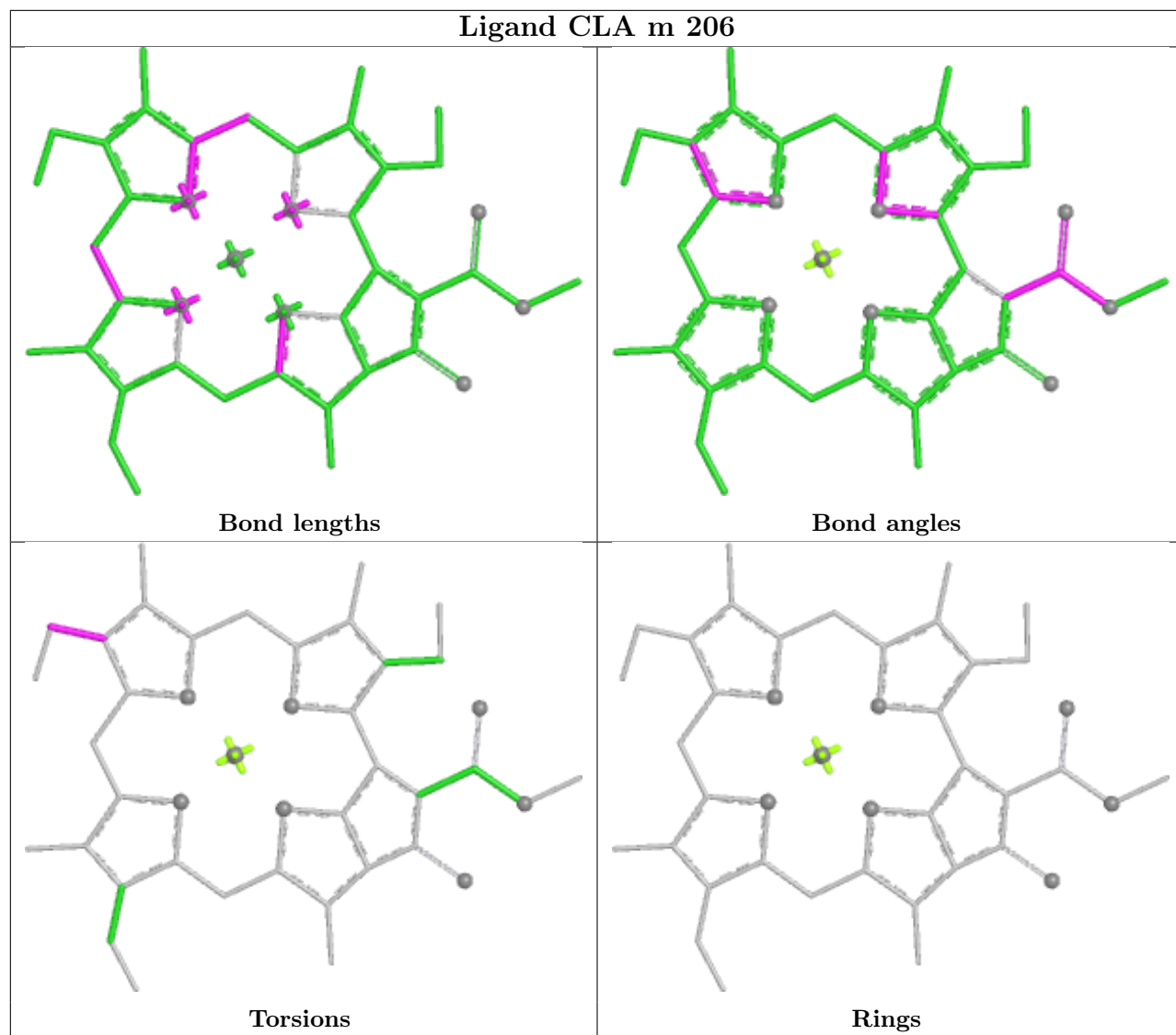
Torsions

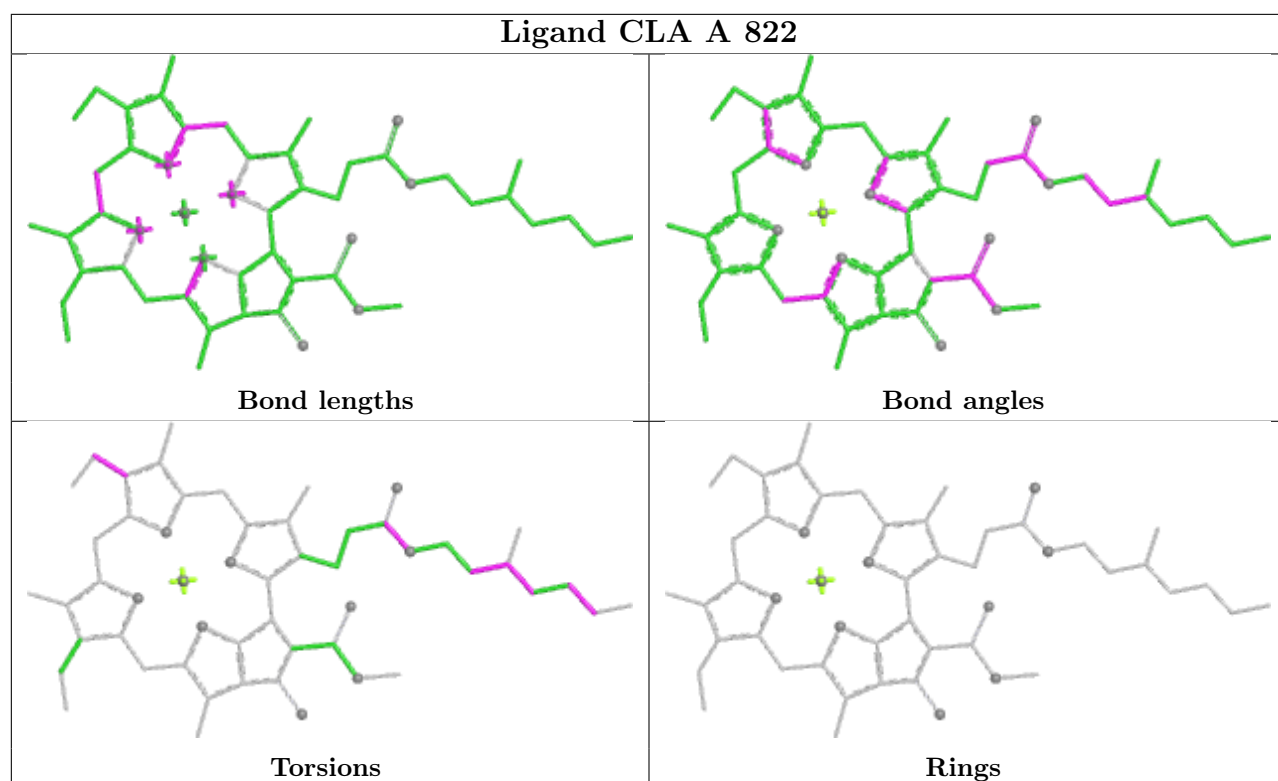


Rings

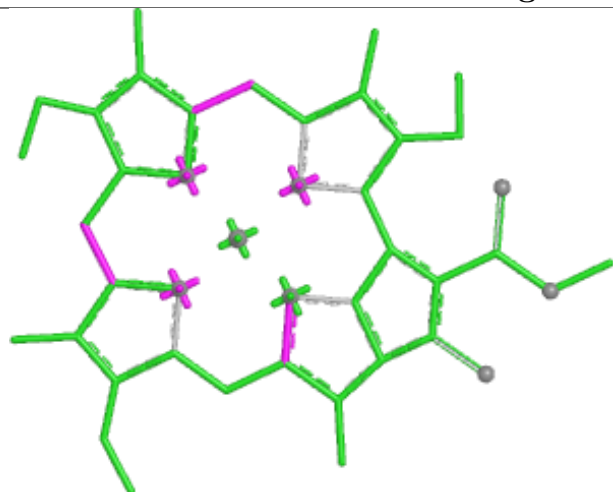




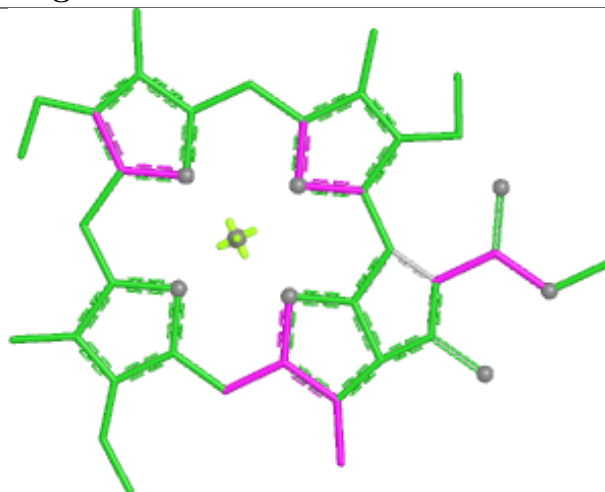




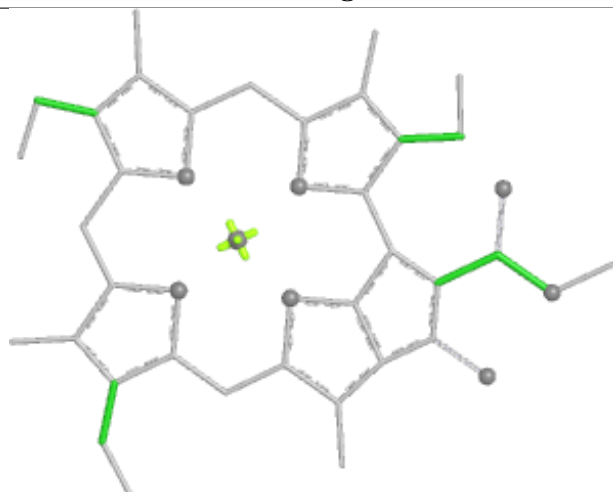
## Ligand CLA g 214



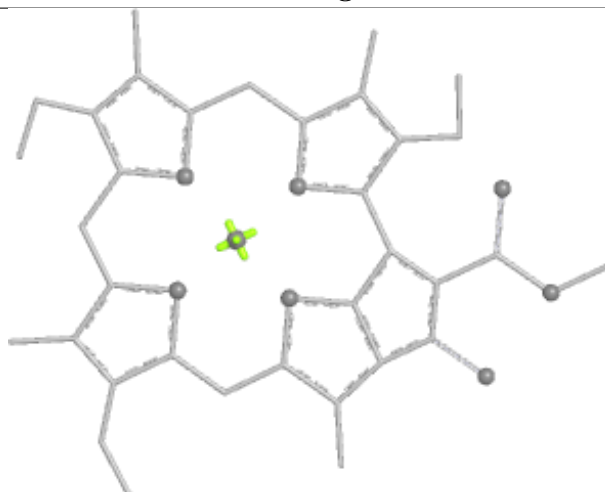
Bond lengths



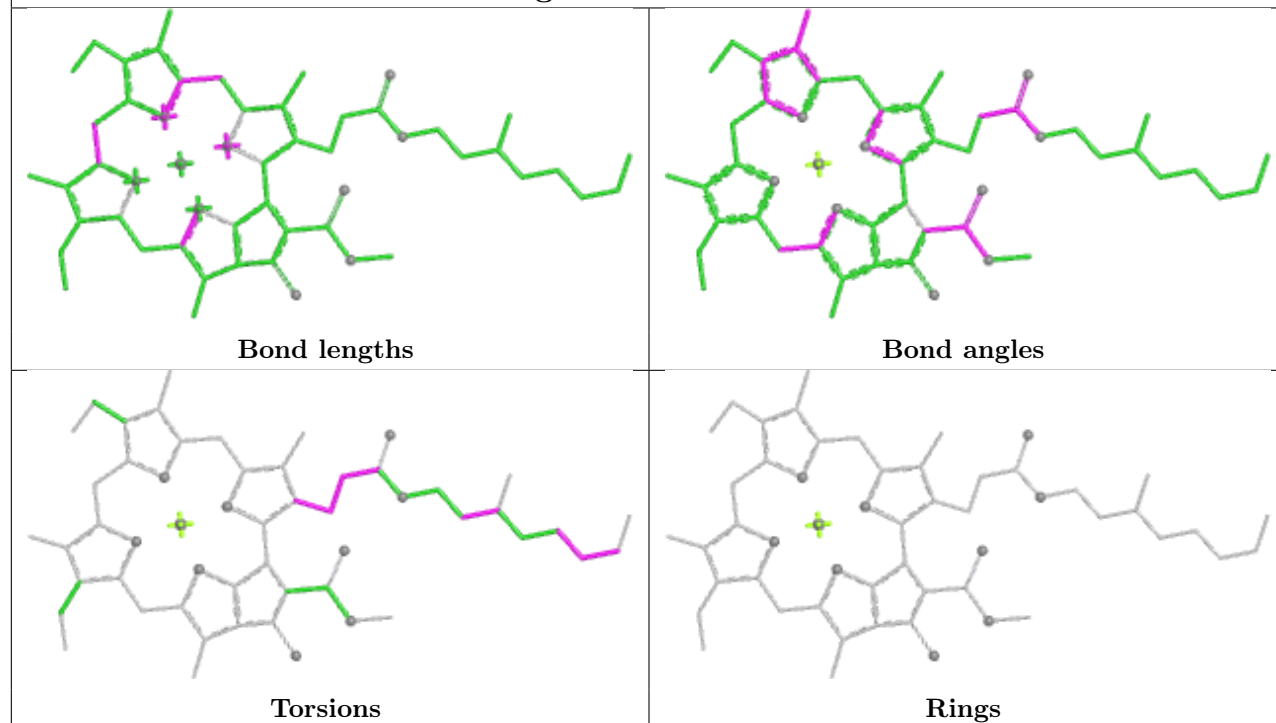
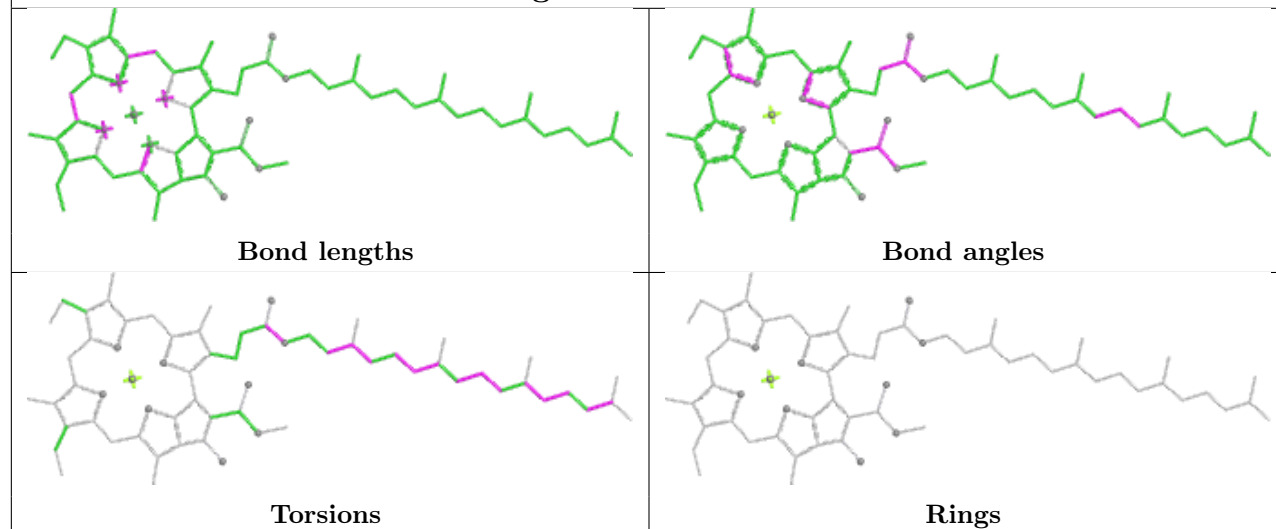
Bond angles



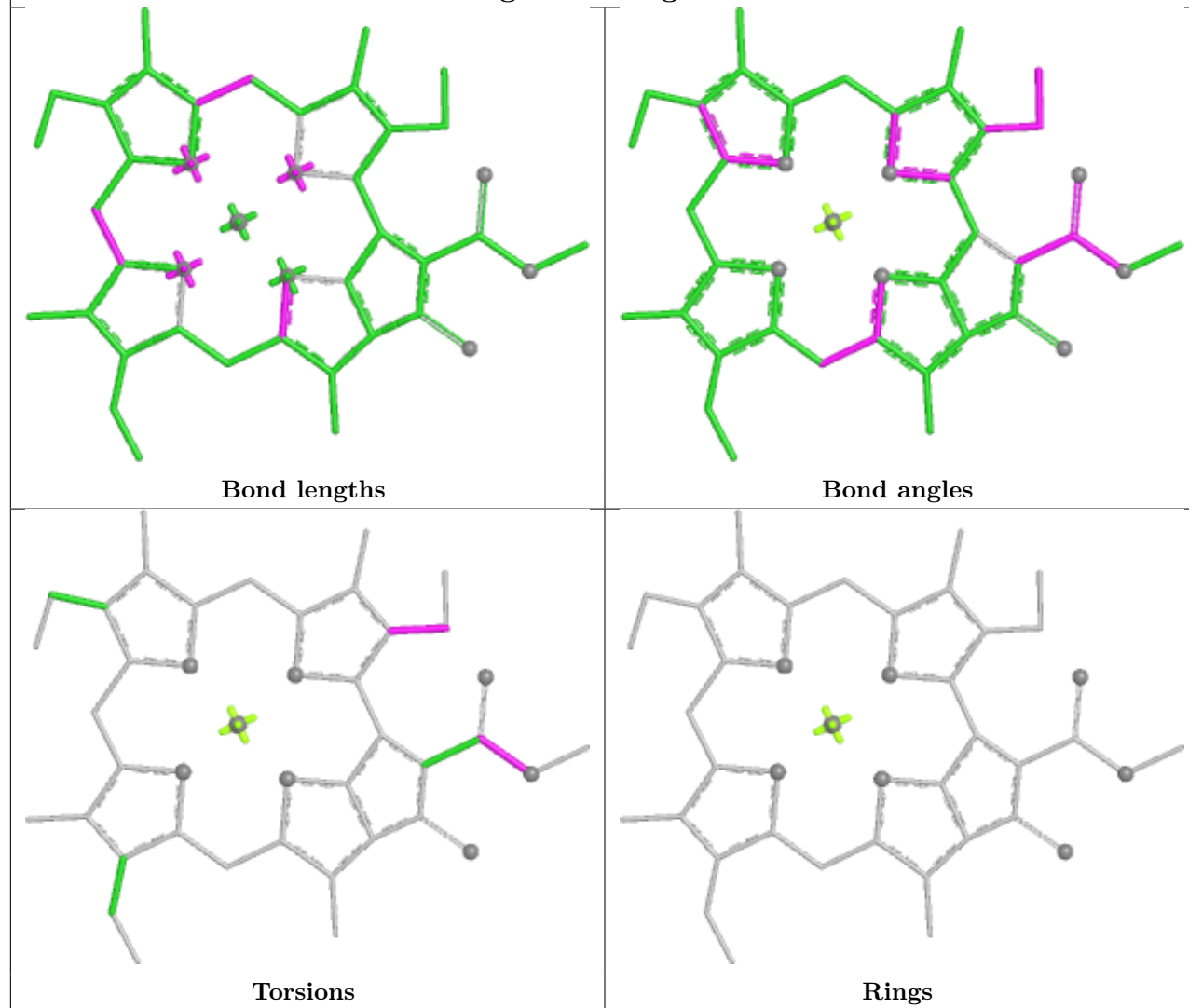
Torsions



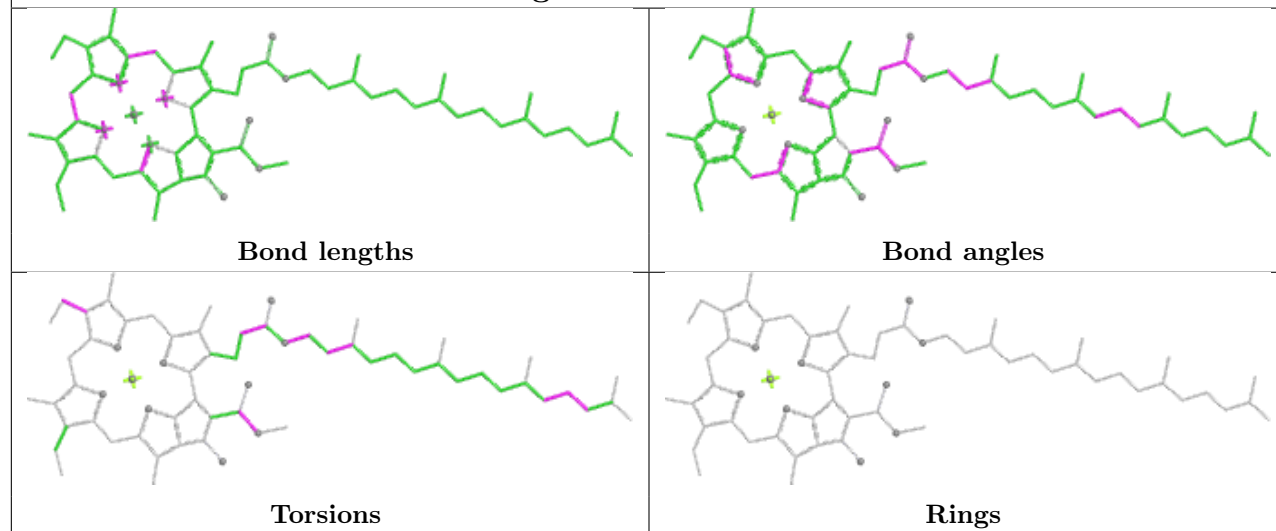
Rings

**Ligand CLA h 209****Ligand CLA B 818**

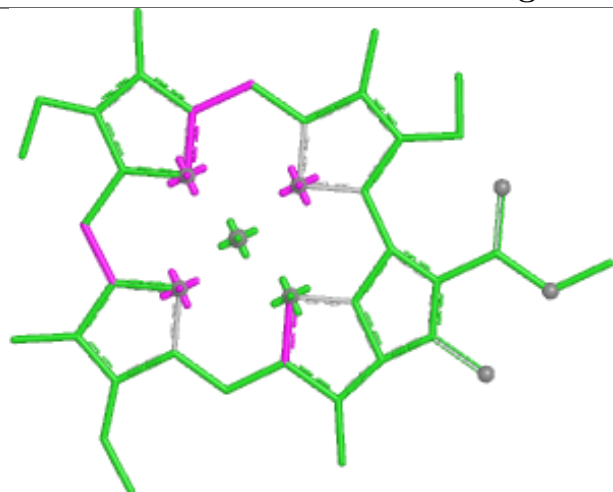
## Ligand CLA g 213



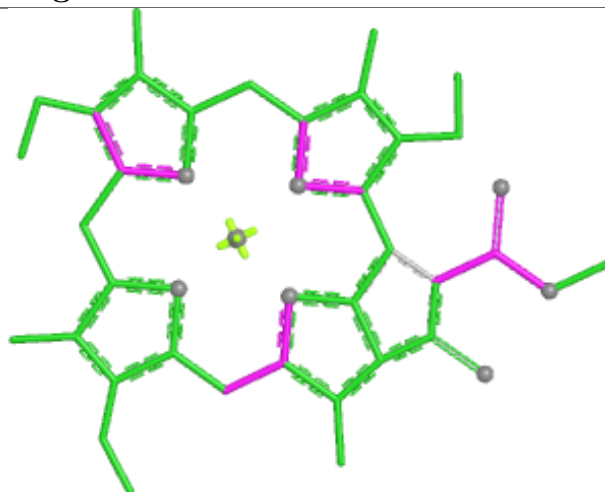
## Ligand CLA B 802



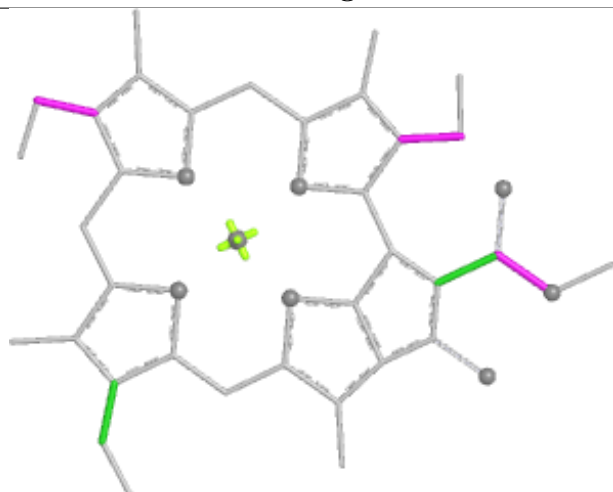
## Ligand CLA g 203



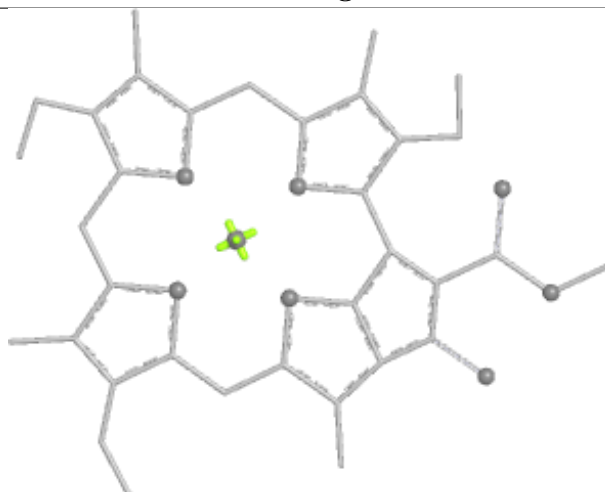
Bond lengths



Bond angles

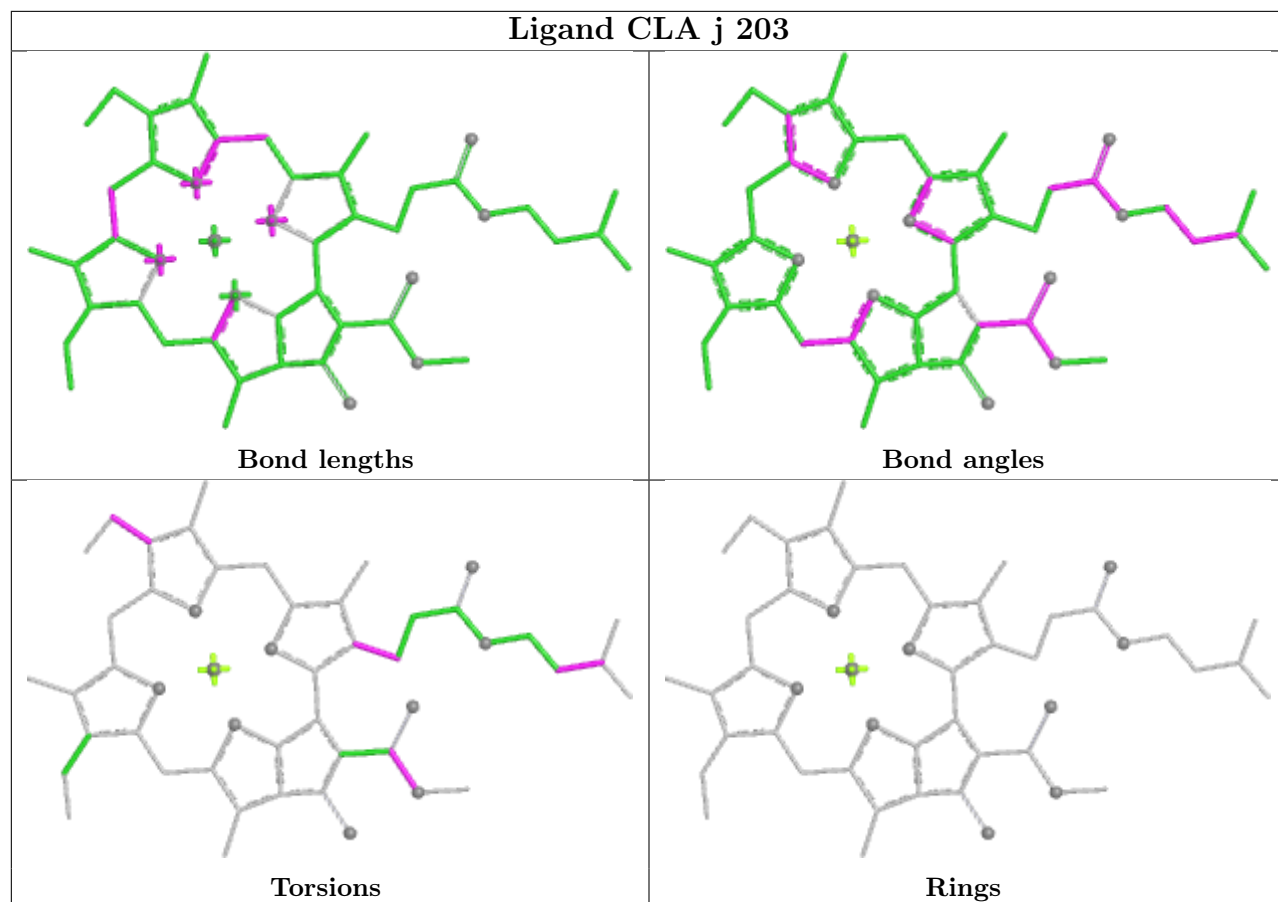


Torsions

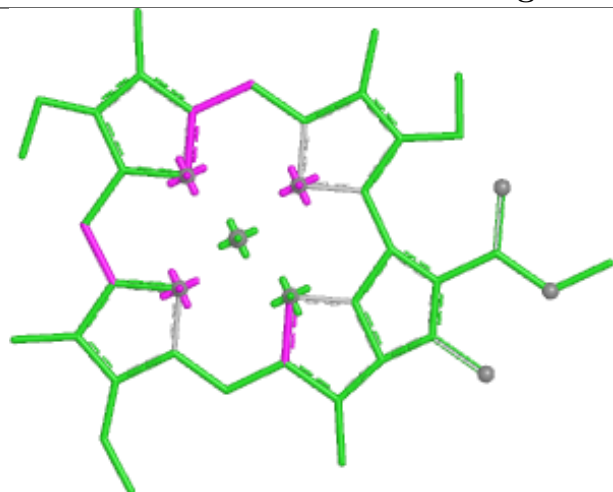


Rings

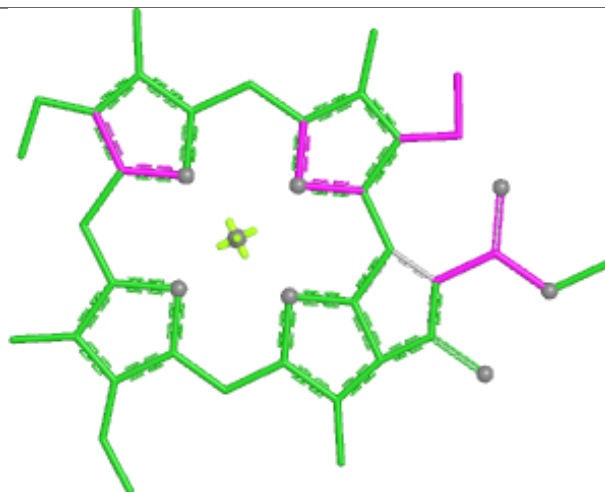
## Ligand CLA j 203



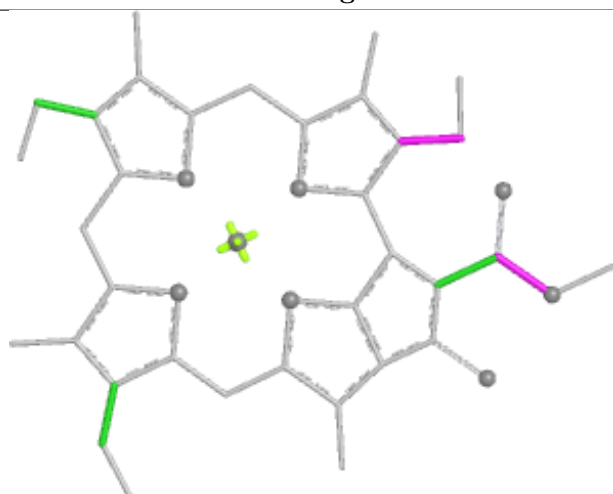
## Ligand CLA d 315



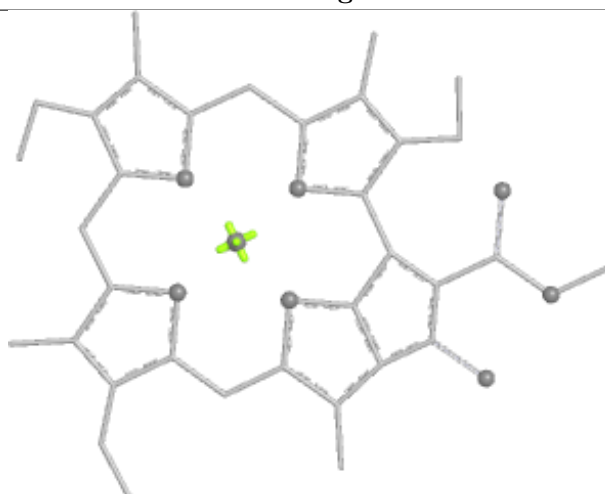
Bond lengths



Bond angles



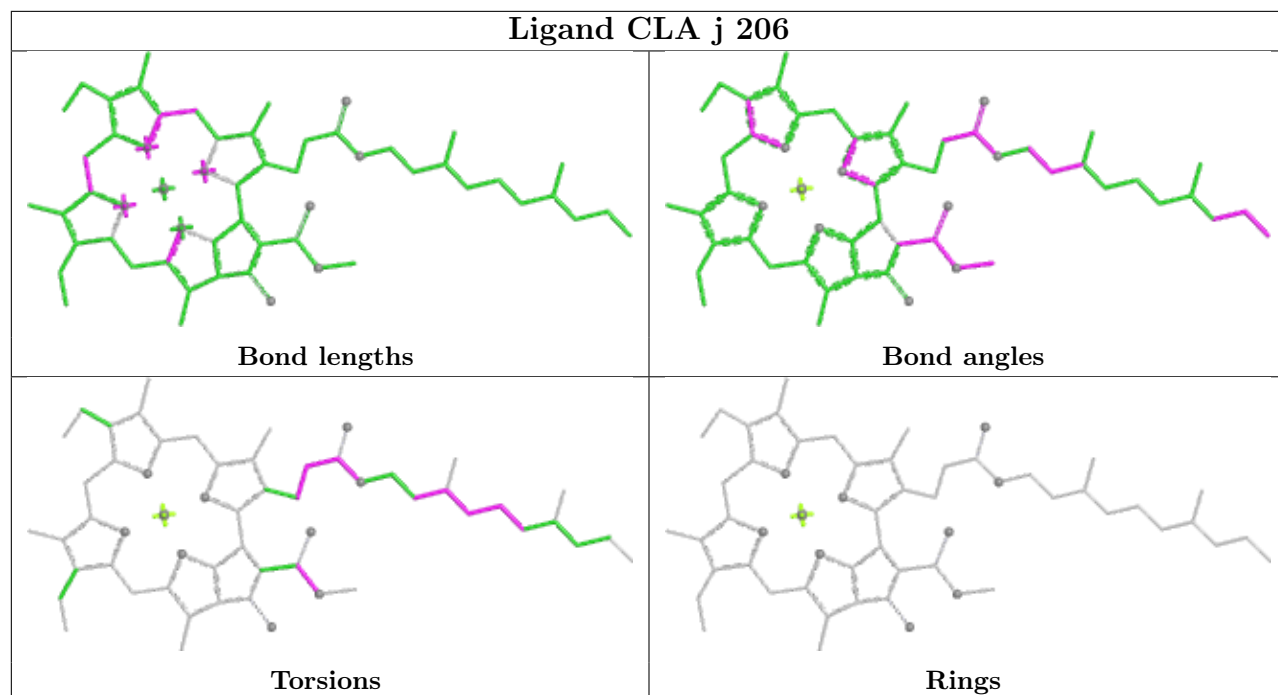
Torsions



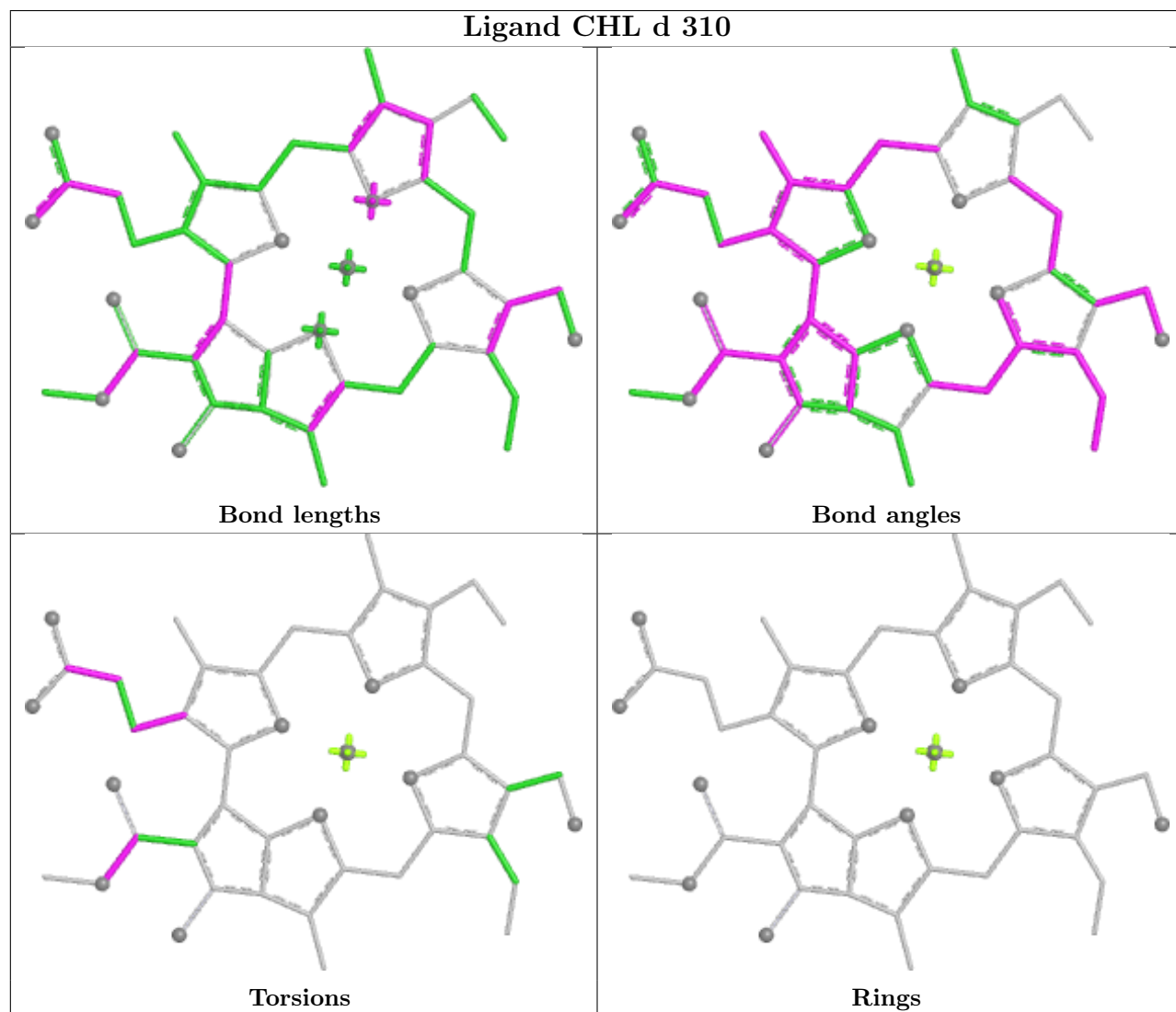
Rings



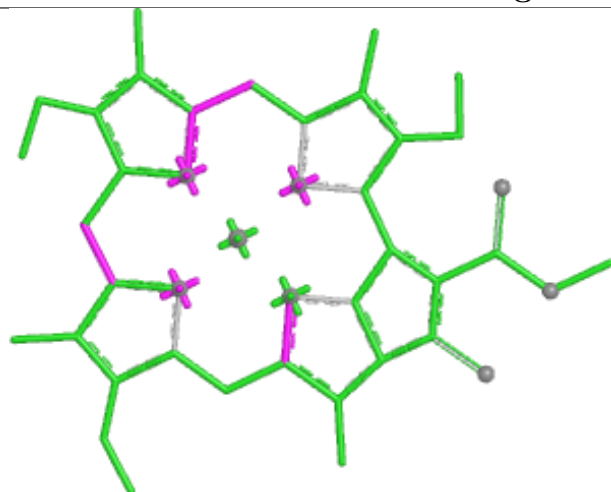
## Ligand CLA j 206



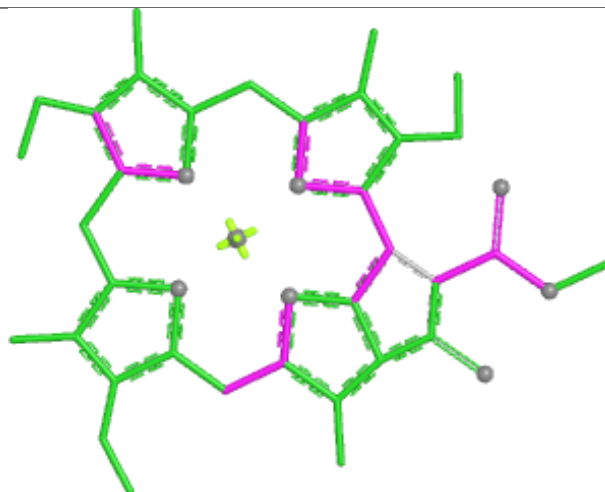
## Ligand CHL d 310



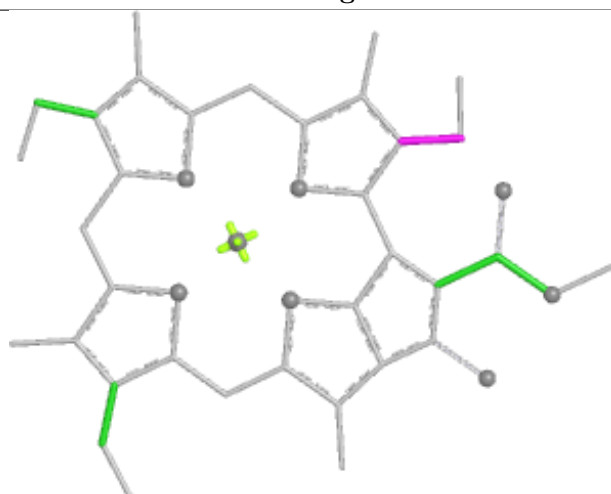
## Ligand CLA B 806



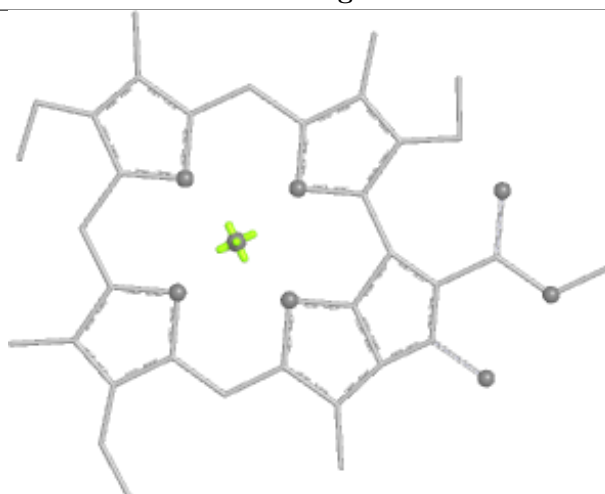
Bond lengths



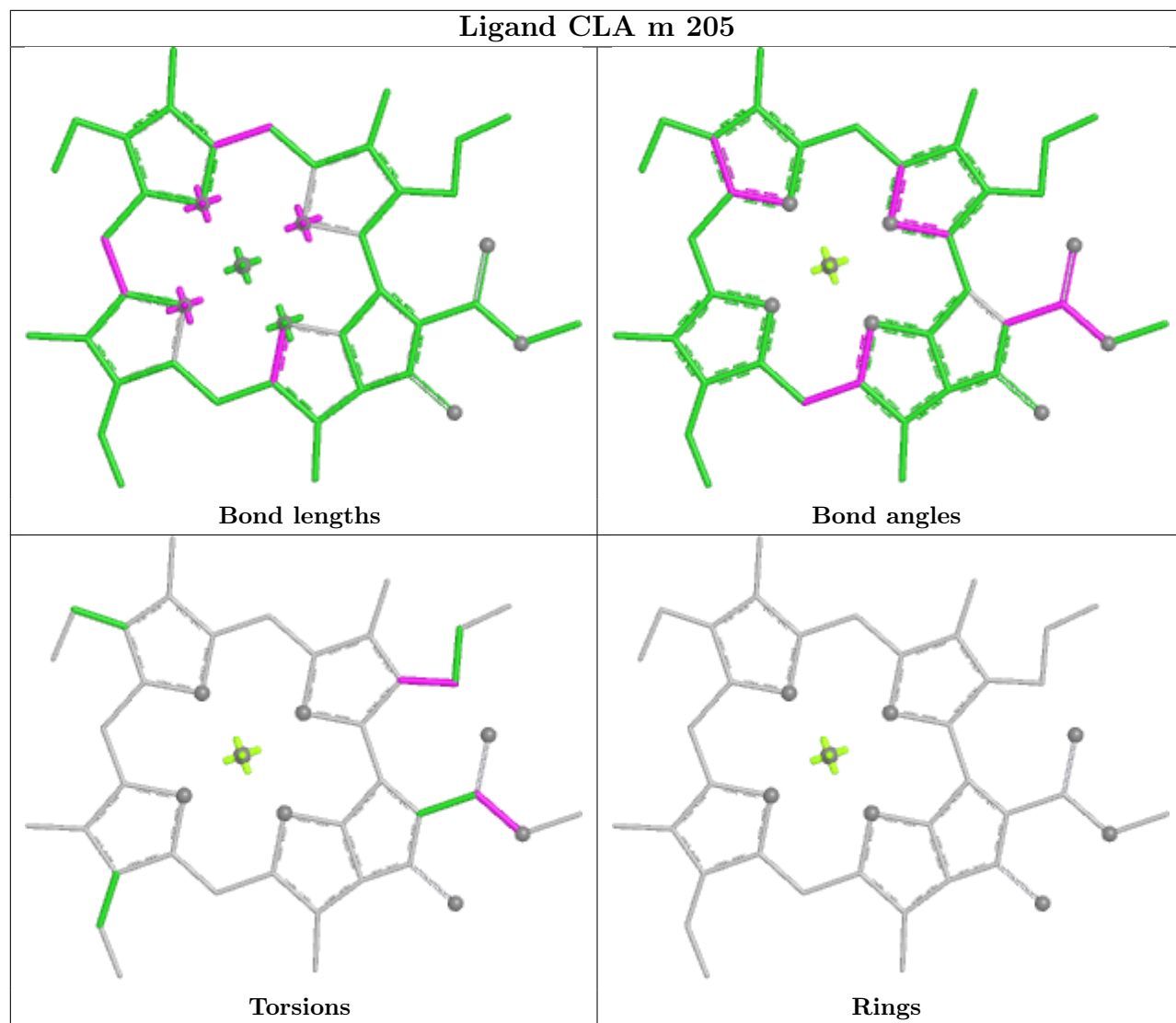
Bond angles

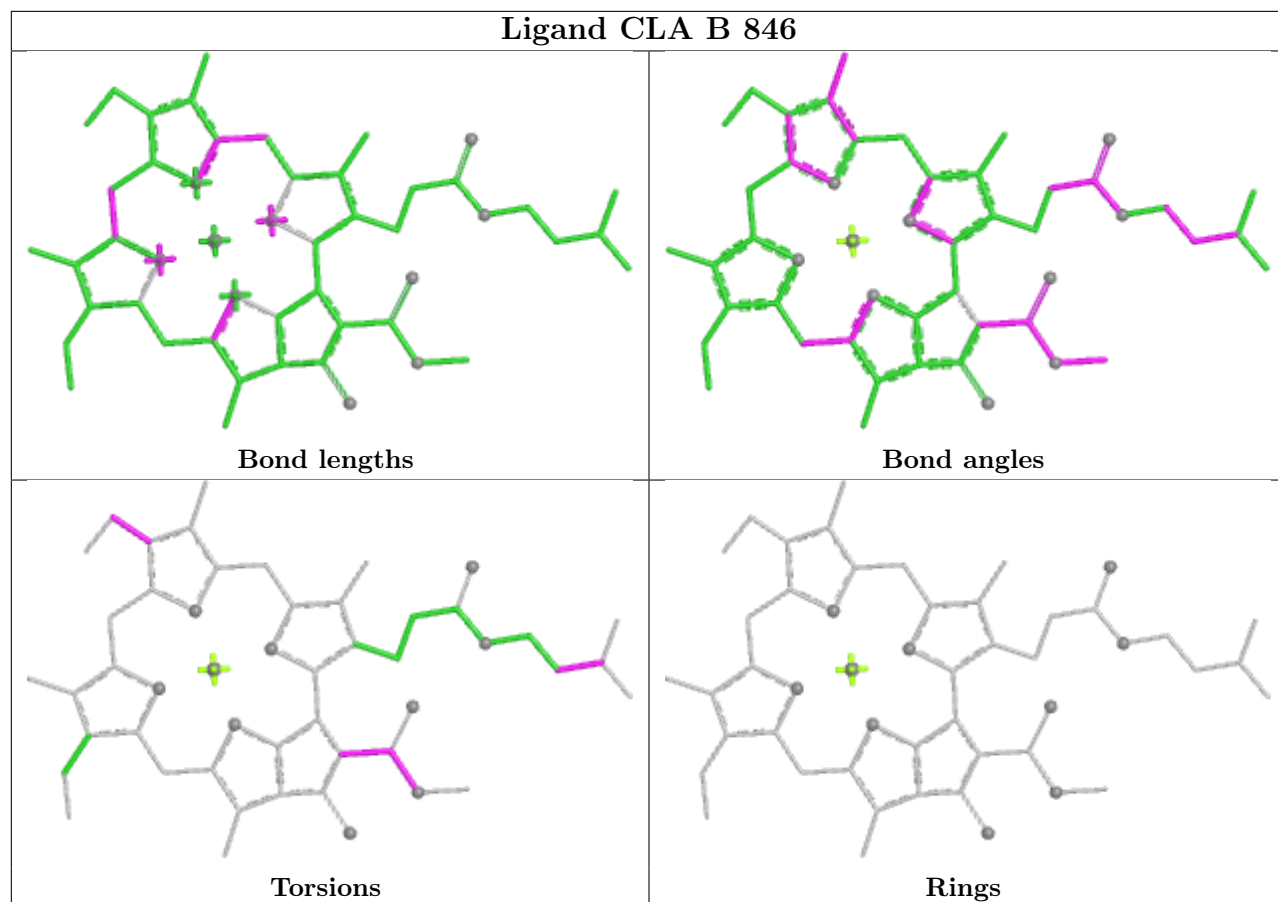


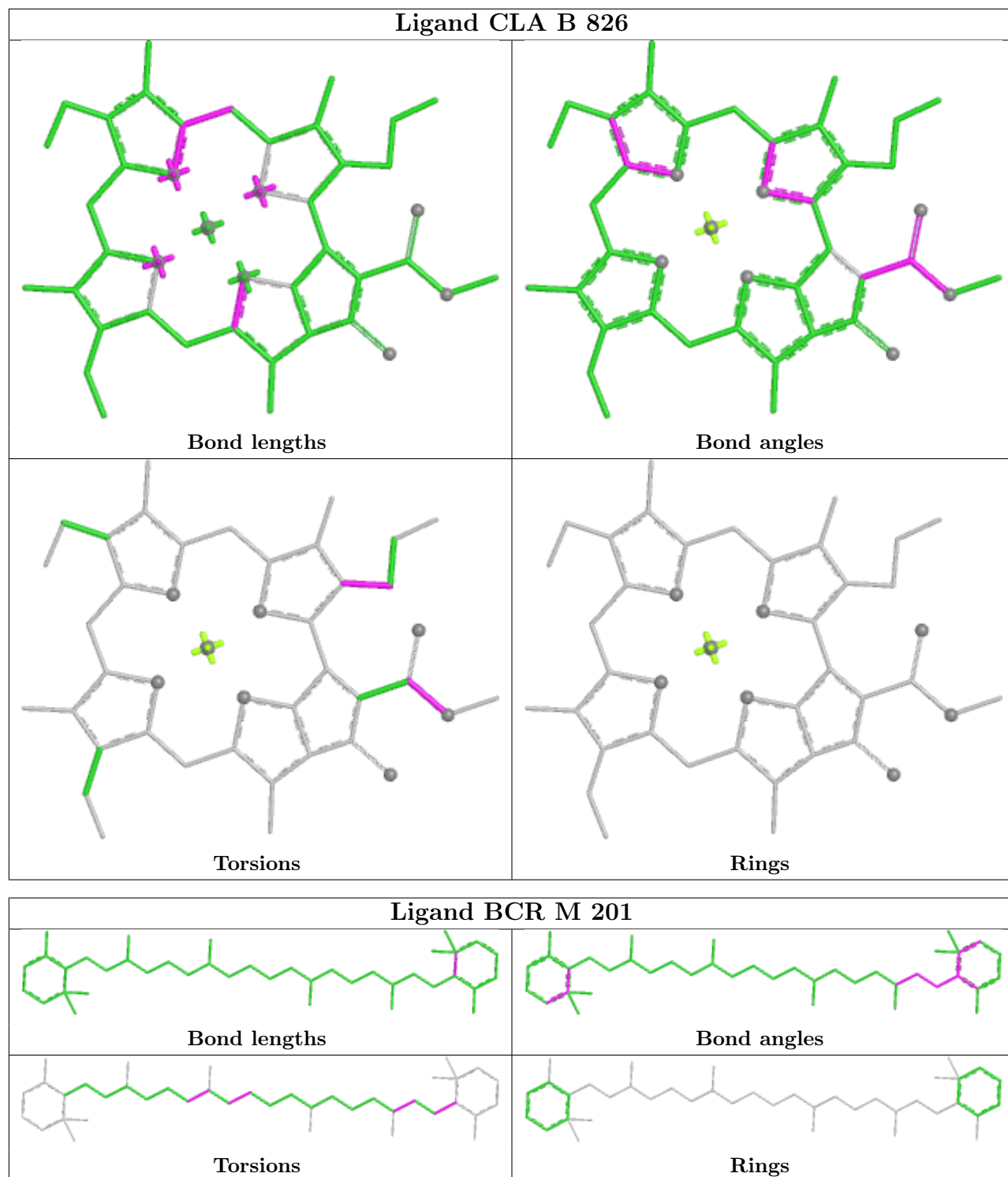
Torsions



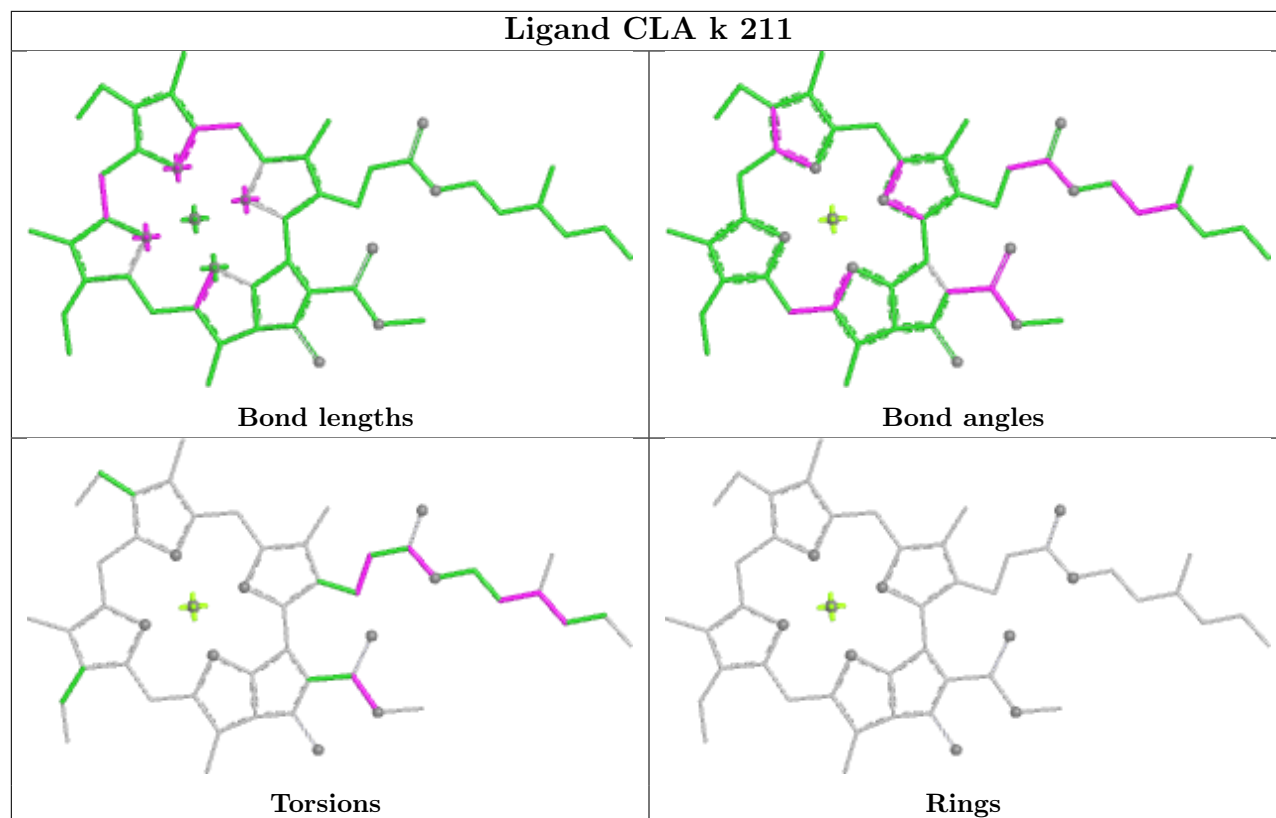
Rings



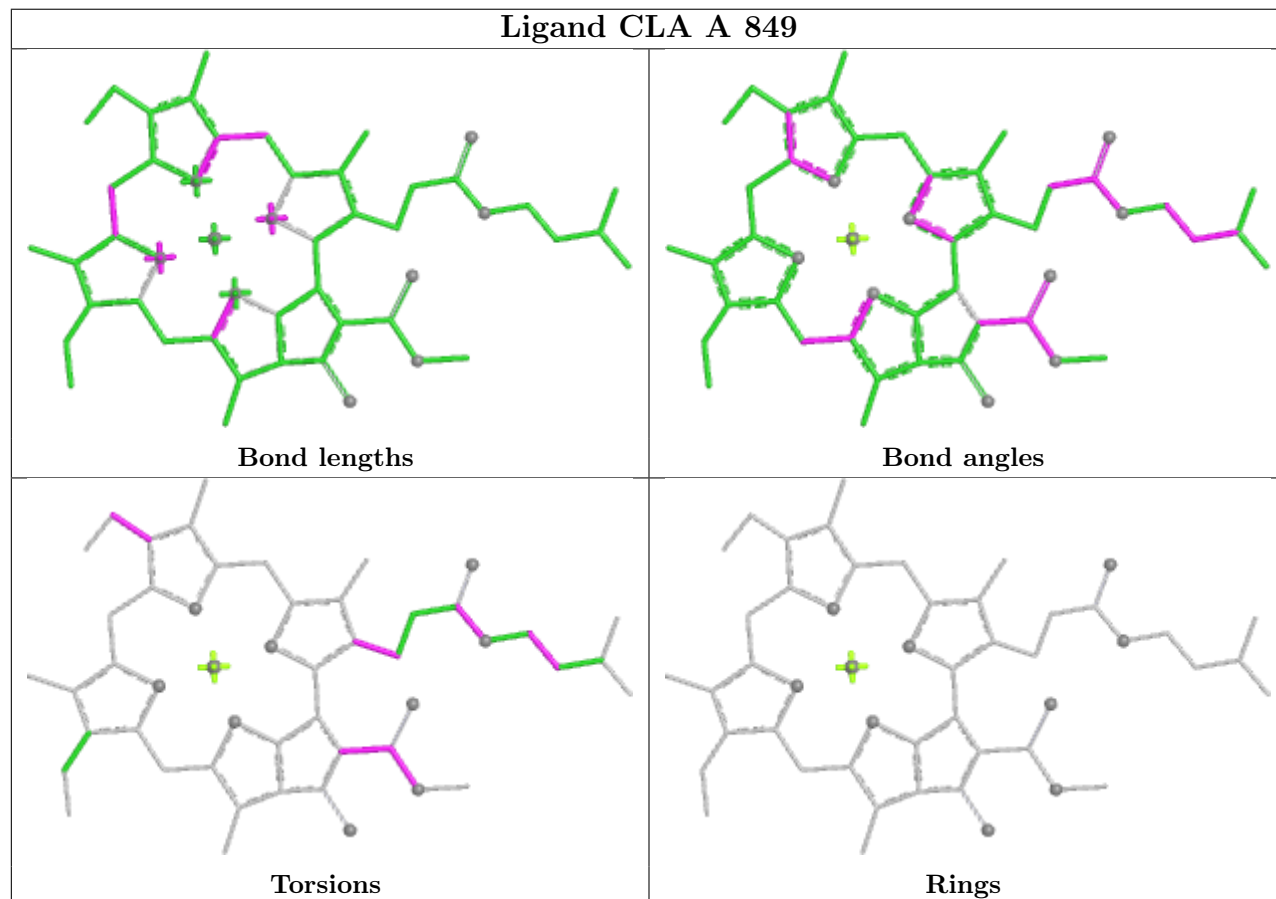




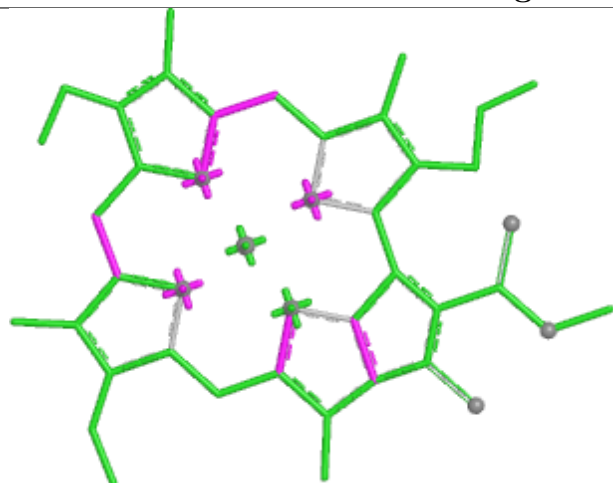
## Ligand CLA k 211



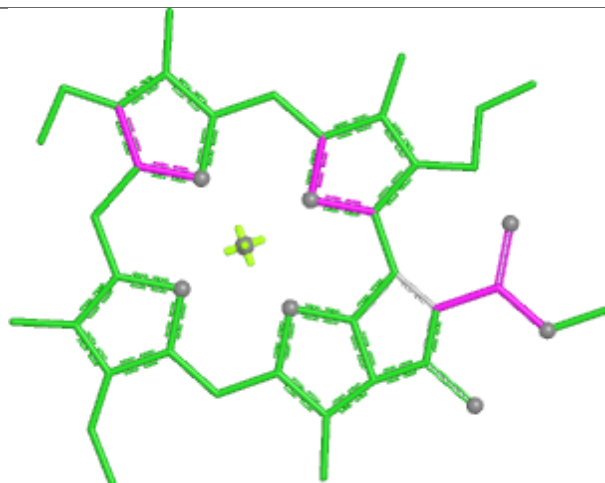
## Ligand CLA A 849



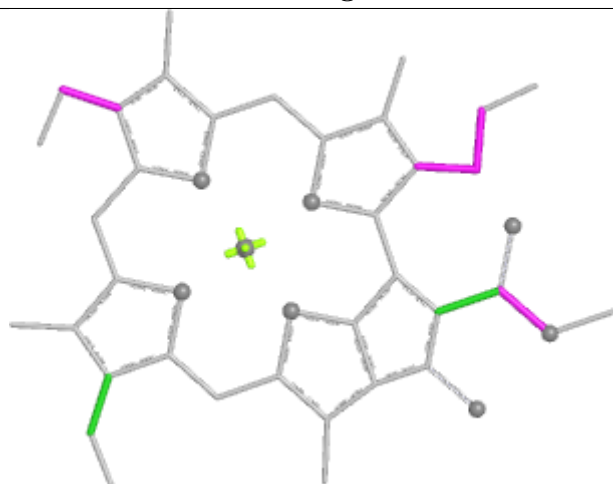
## Ligand CLA B 820



Bond lengths



Bond angles

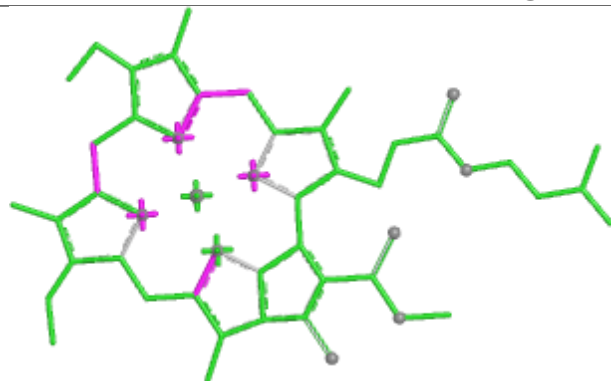


Torsions

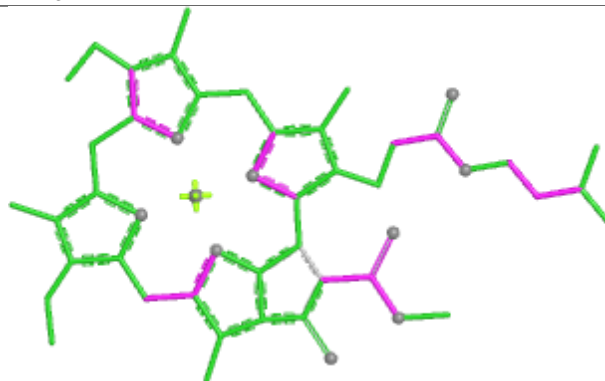


Rings

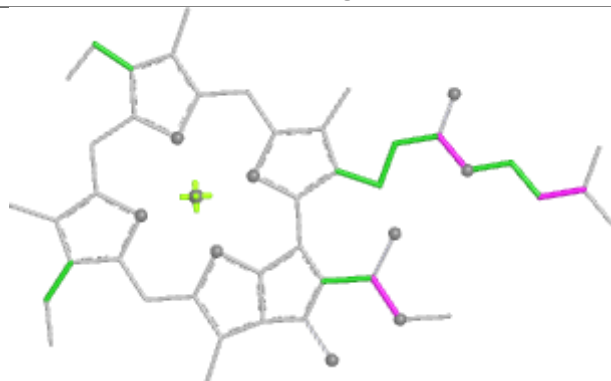
## Ligand CLA j 208



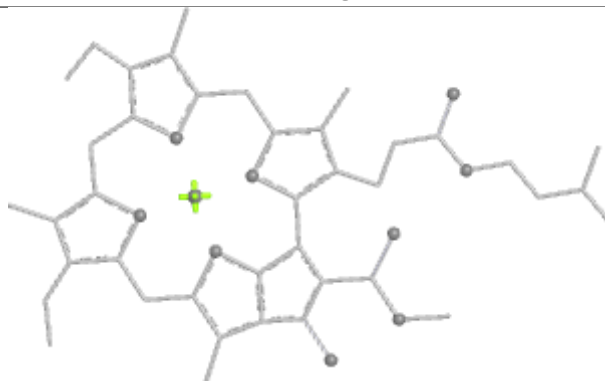
Bond lengths



Bond angles



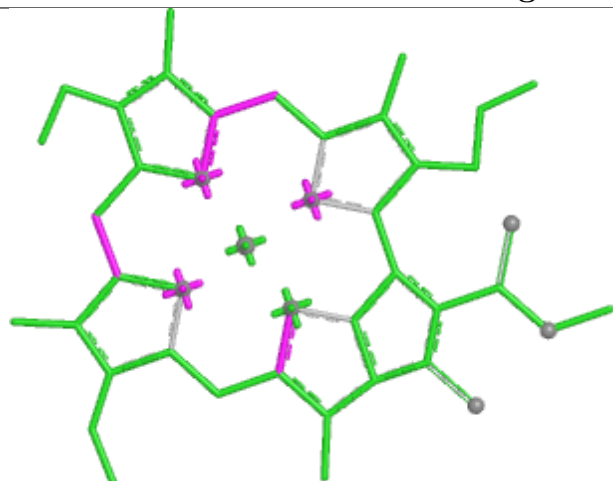
Torsions



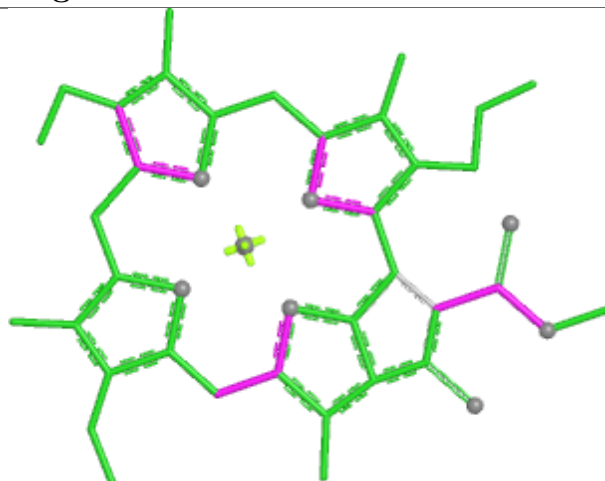
Rings



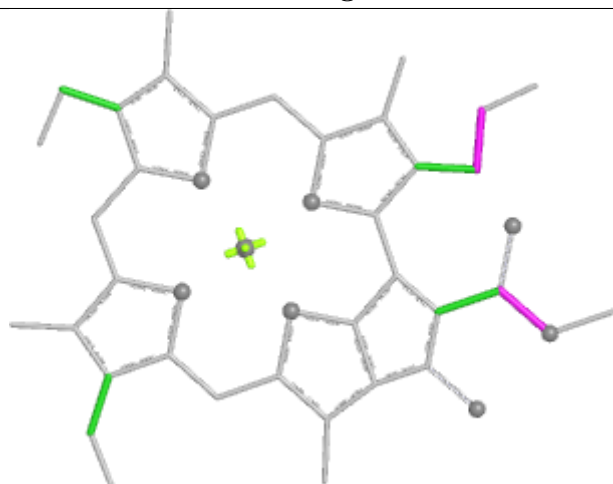
## Ligand CLA g 206



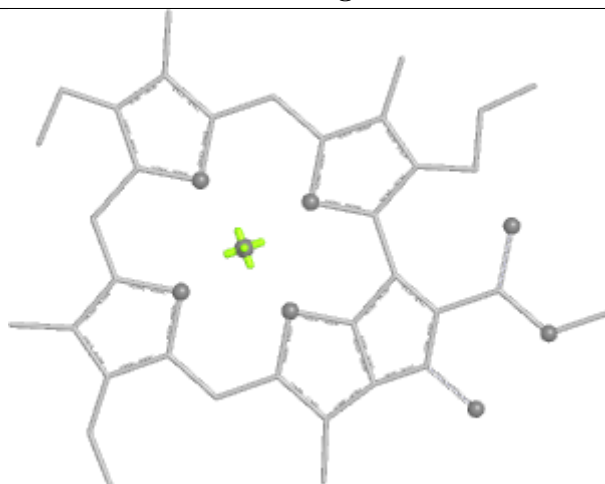
Bond lengths



Bond angles

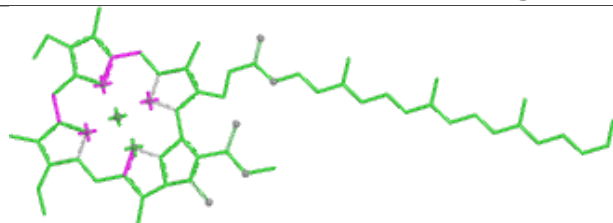


Torsions

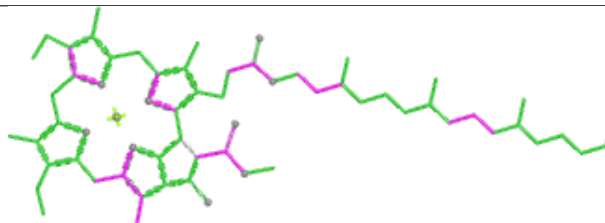


Rings

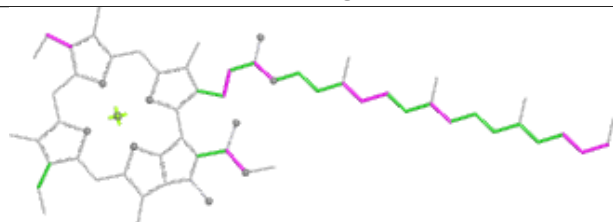
## Ligand CLA B 812



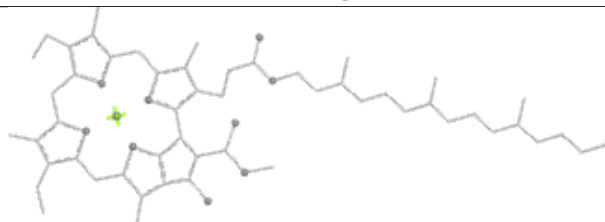
Bond lengths



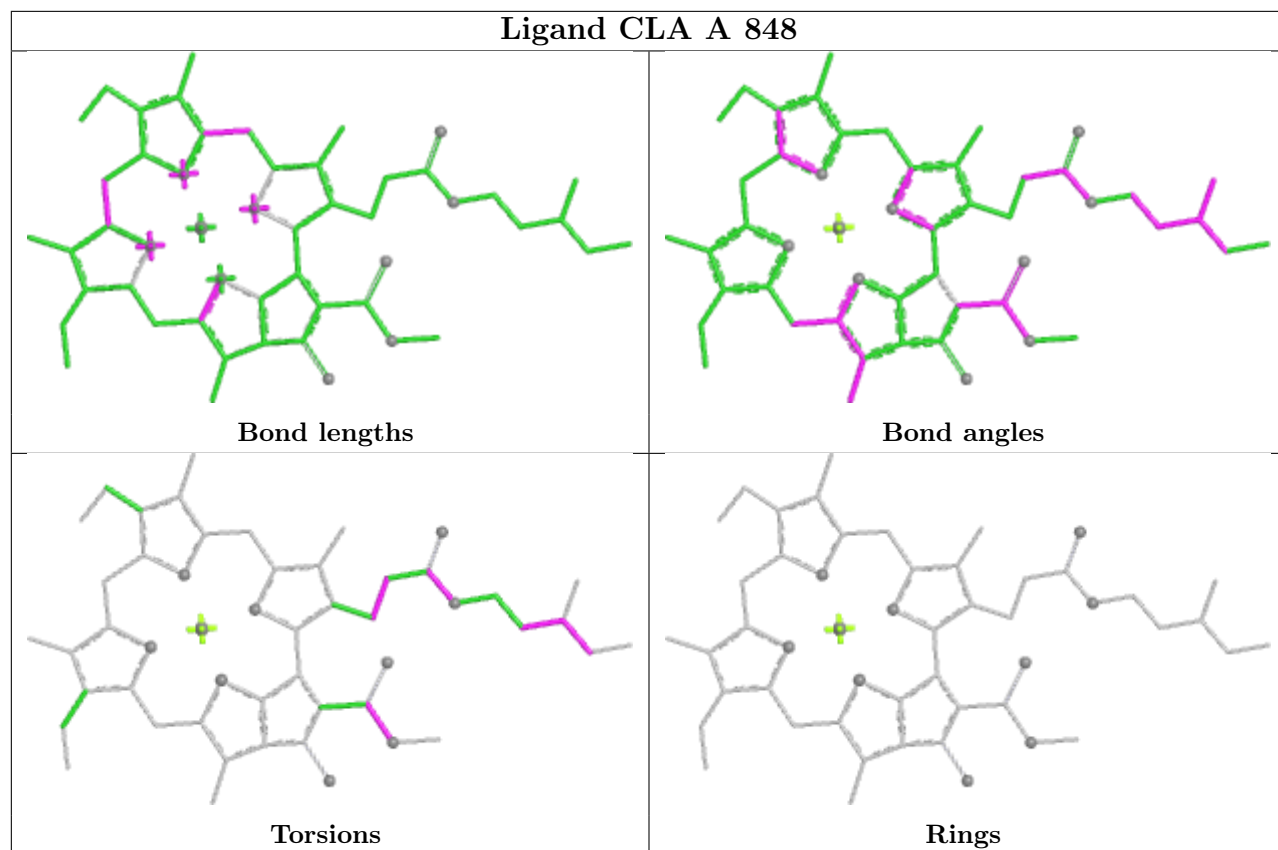
Bond angles



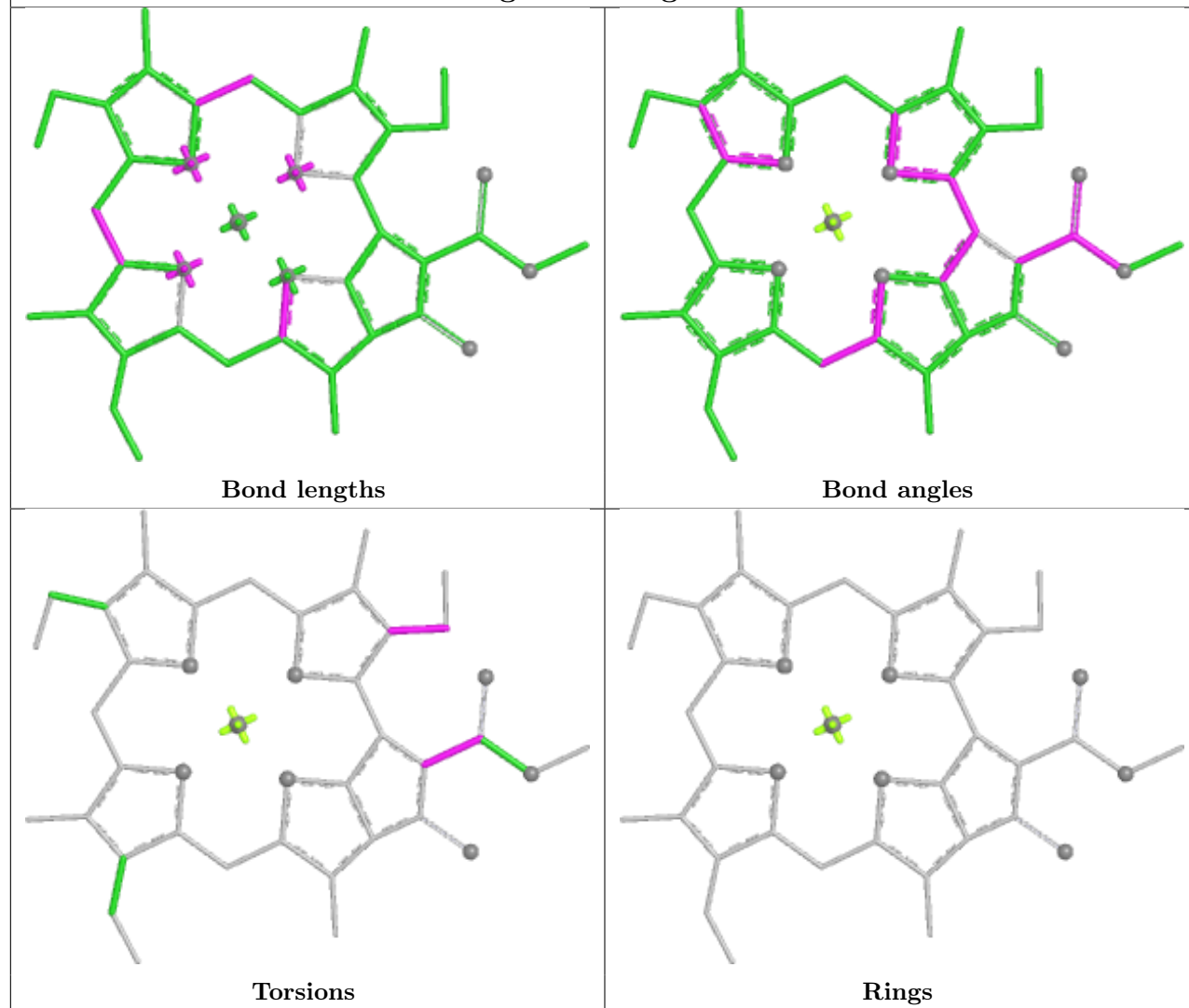
Torsions



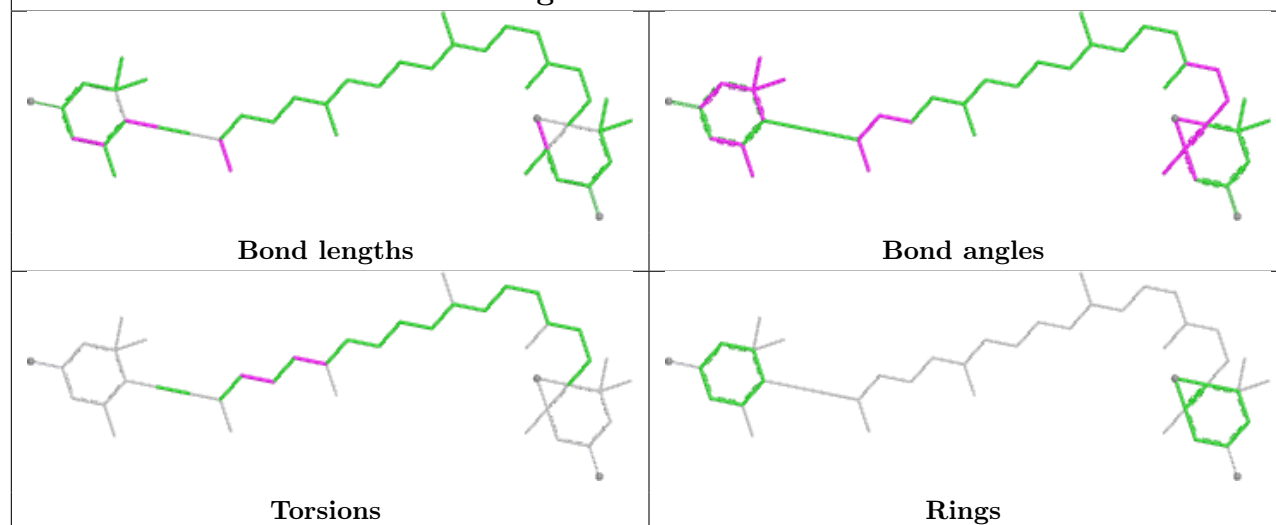
Rings



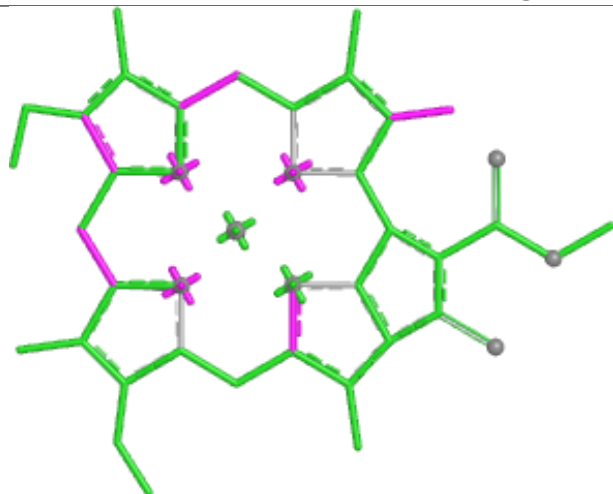
## Ligand CLA g 210



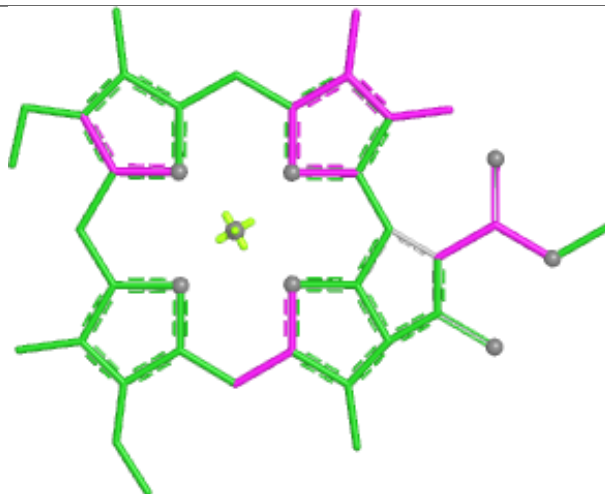
## Ligand DD6 k 216



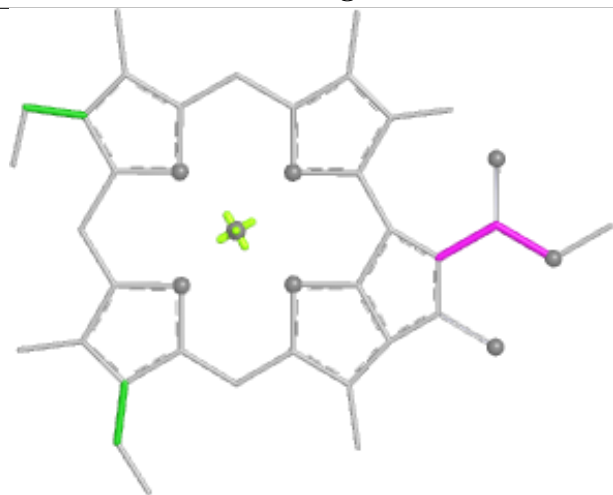
## Ligand CLA d 301



Bond lengths



Bond angles

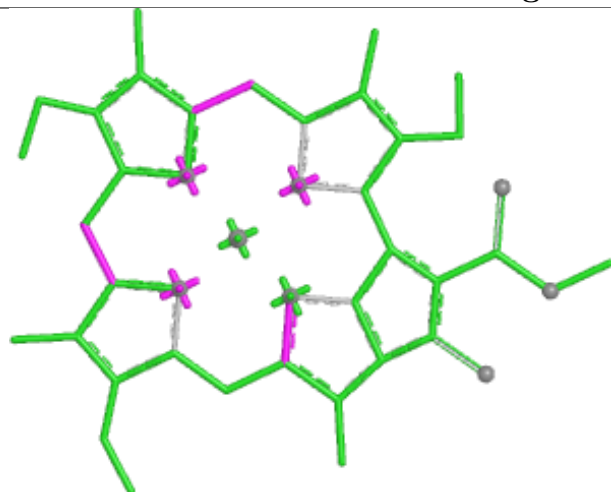


Torsions

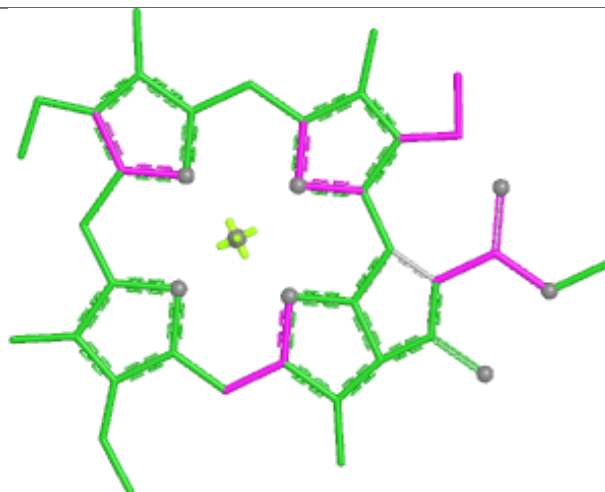


Rings

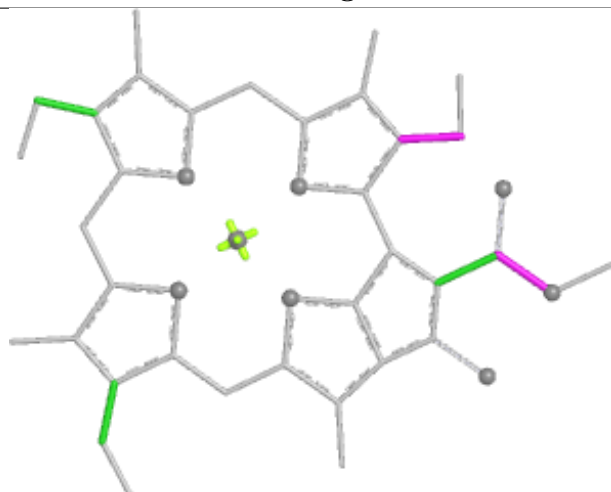
## Ligand CLA 1 601



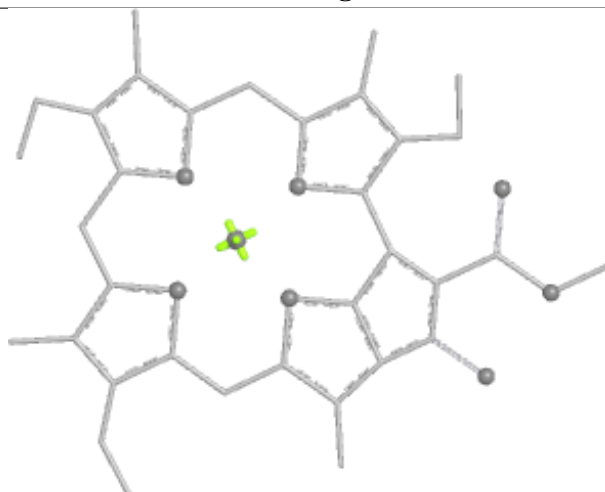
Bond lengths



Bond angles

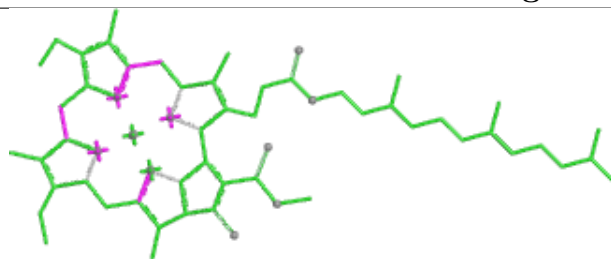


Torsions

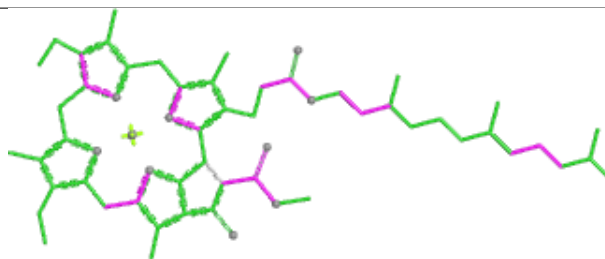


Rings

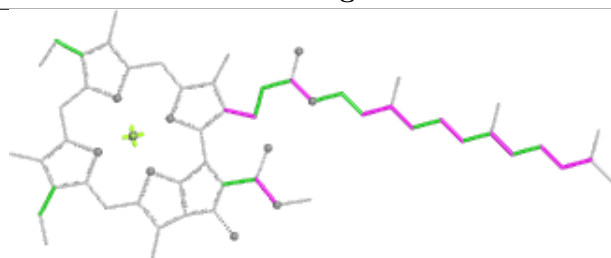
## Ligand CLA 1 606



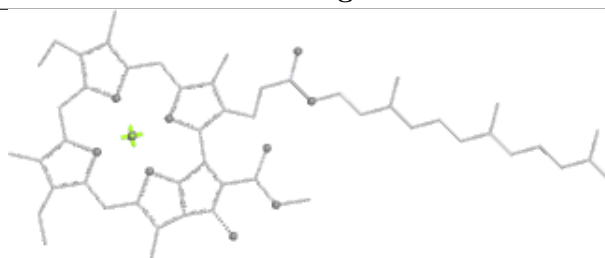
Bond lengths



Bond angles

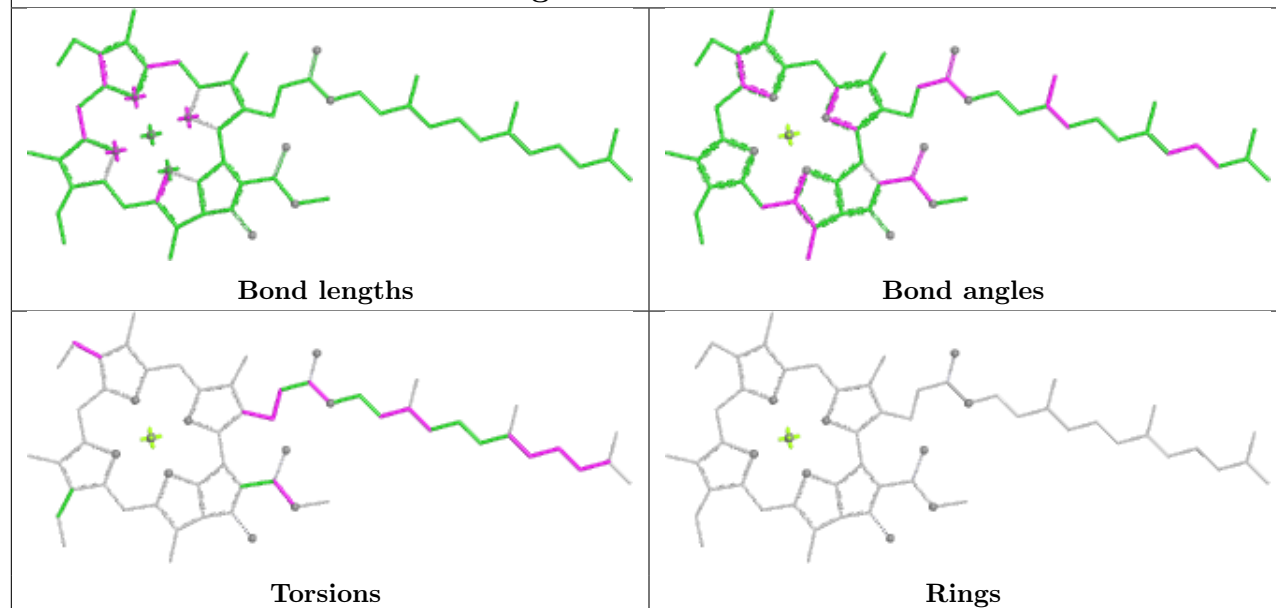


Torsions

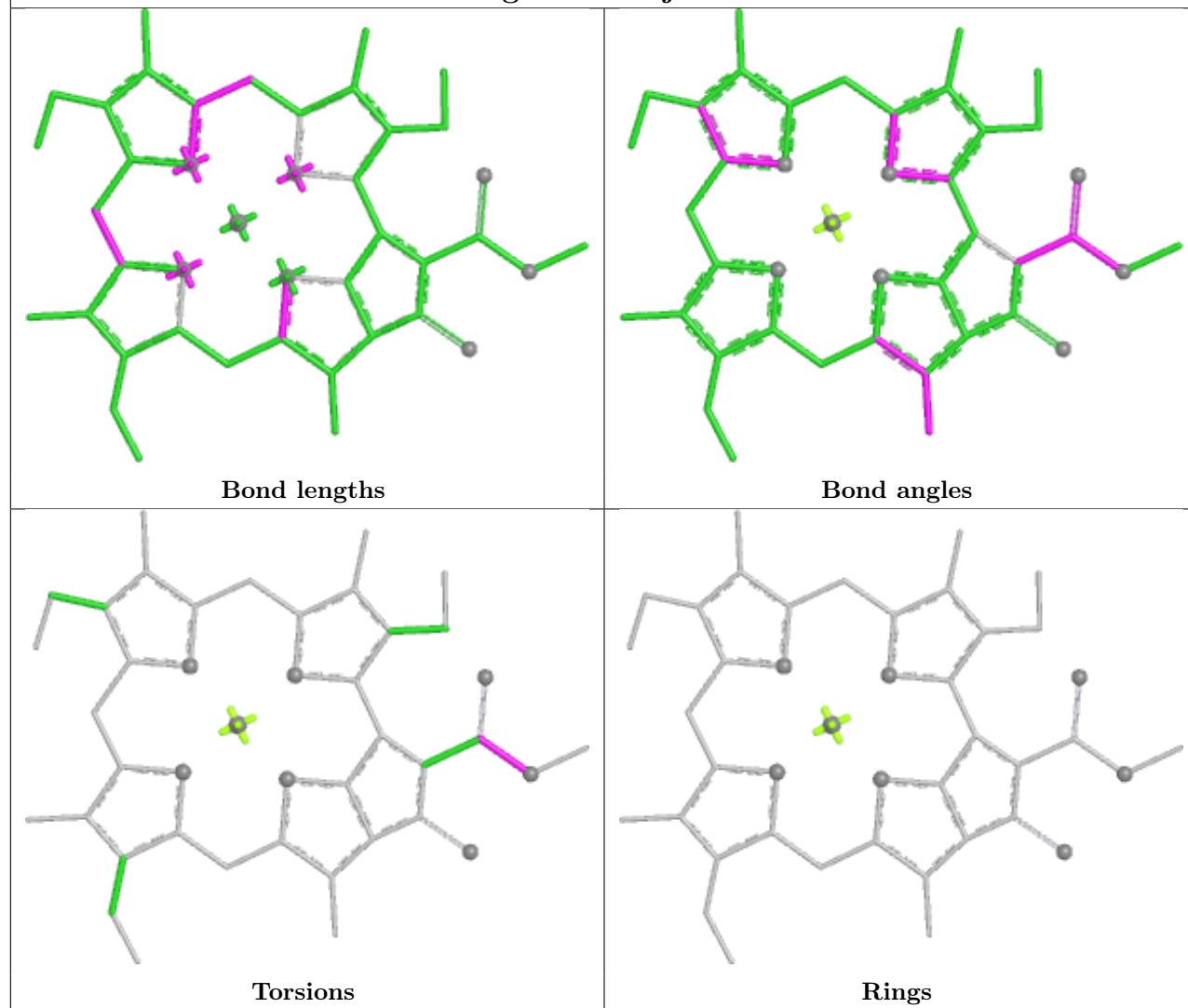


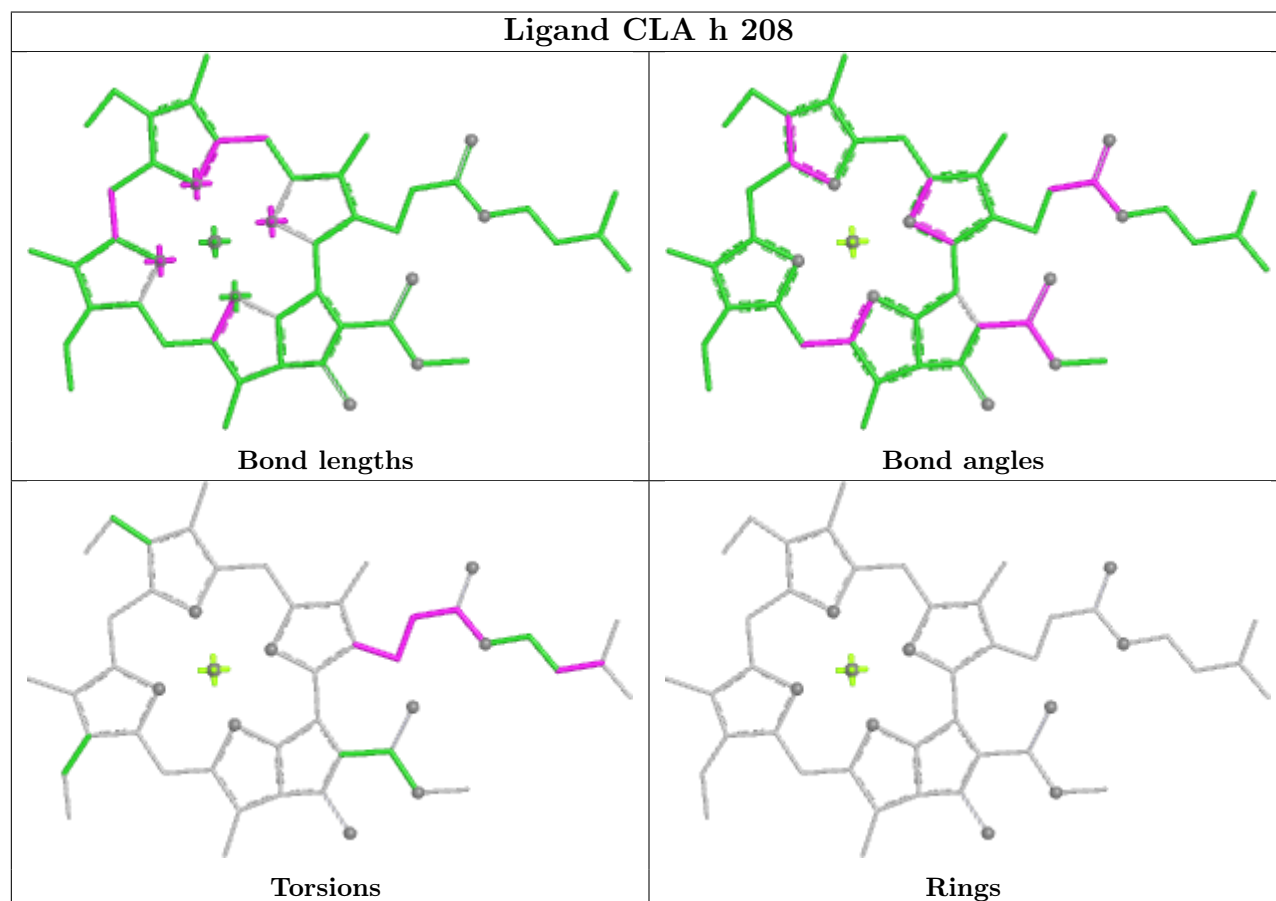
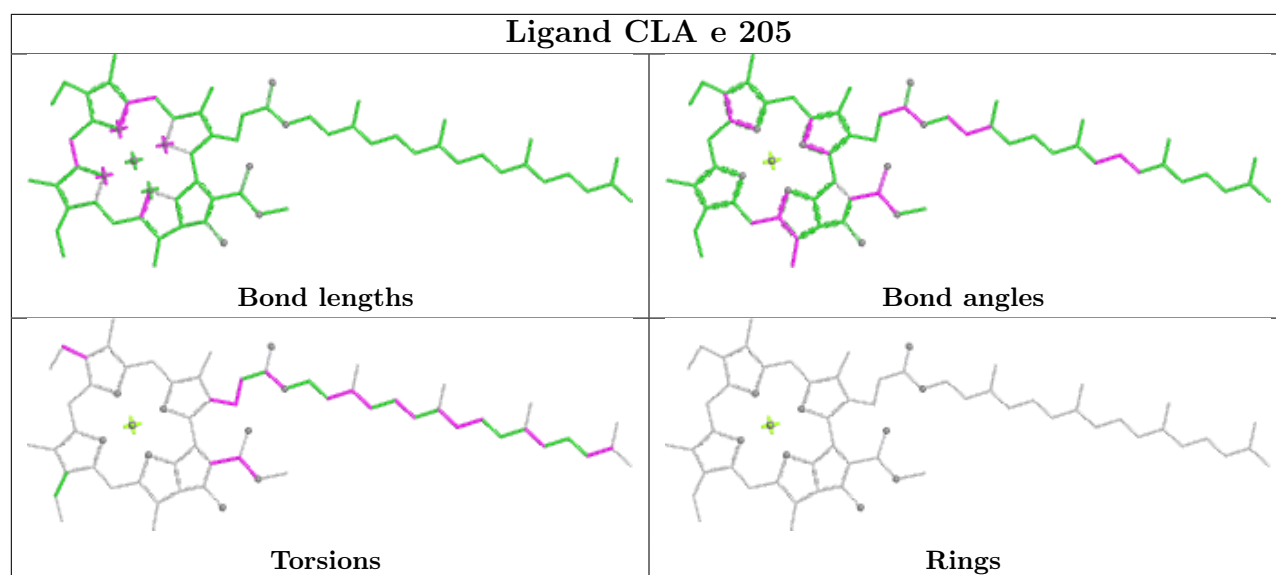
Rings

## Ligand CLA A 844

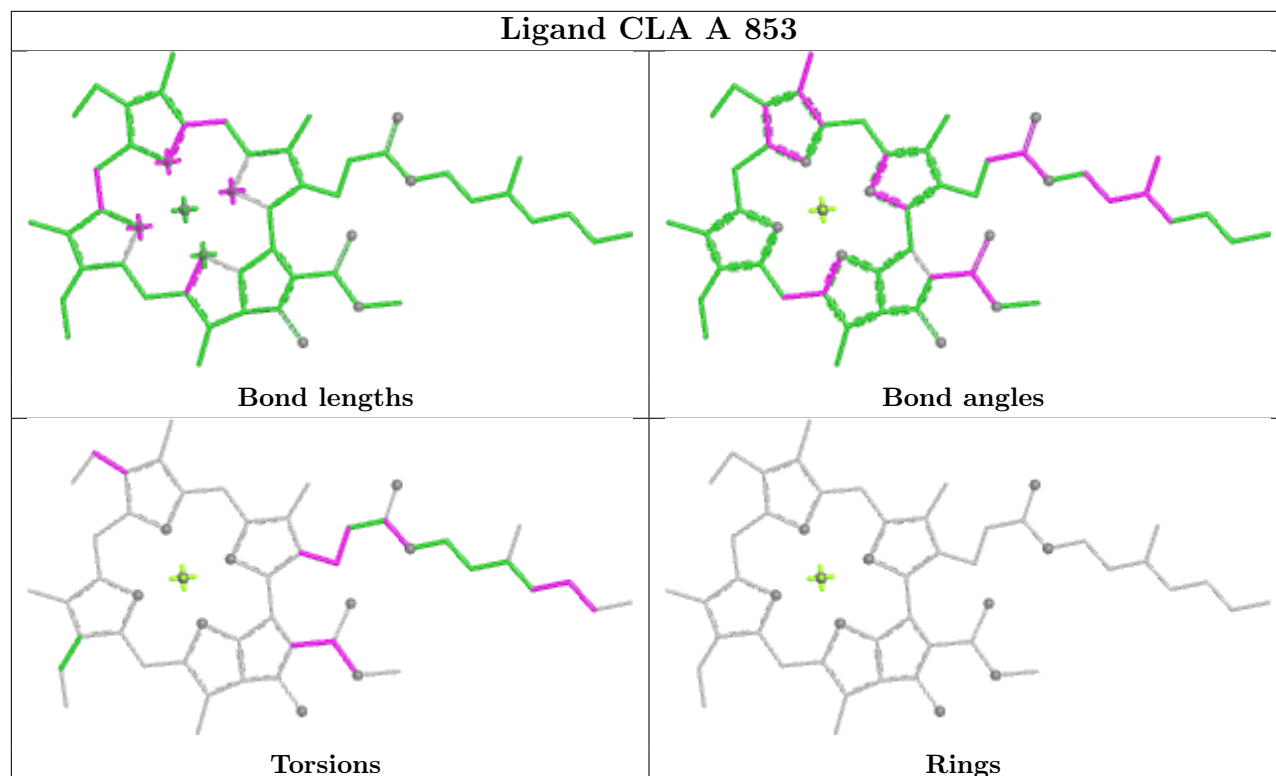


## Ligand CLA j 205

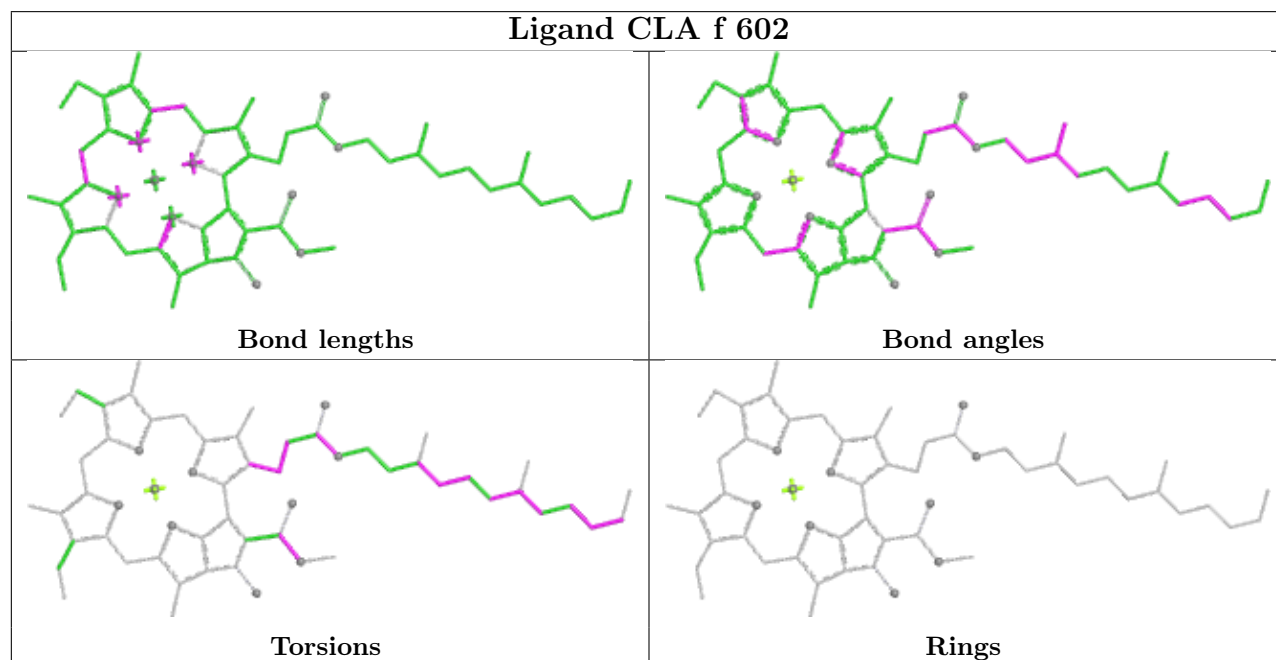




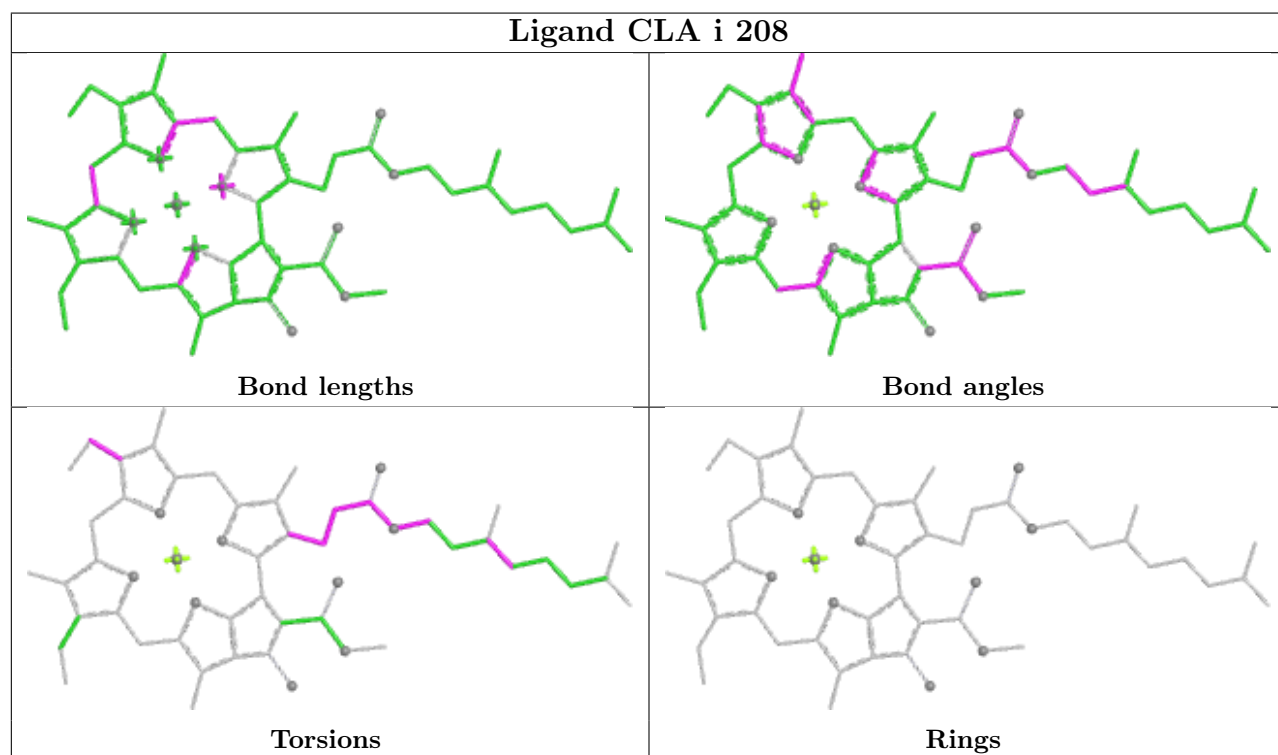
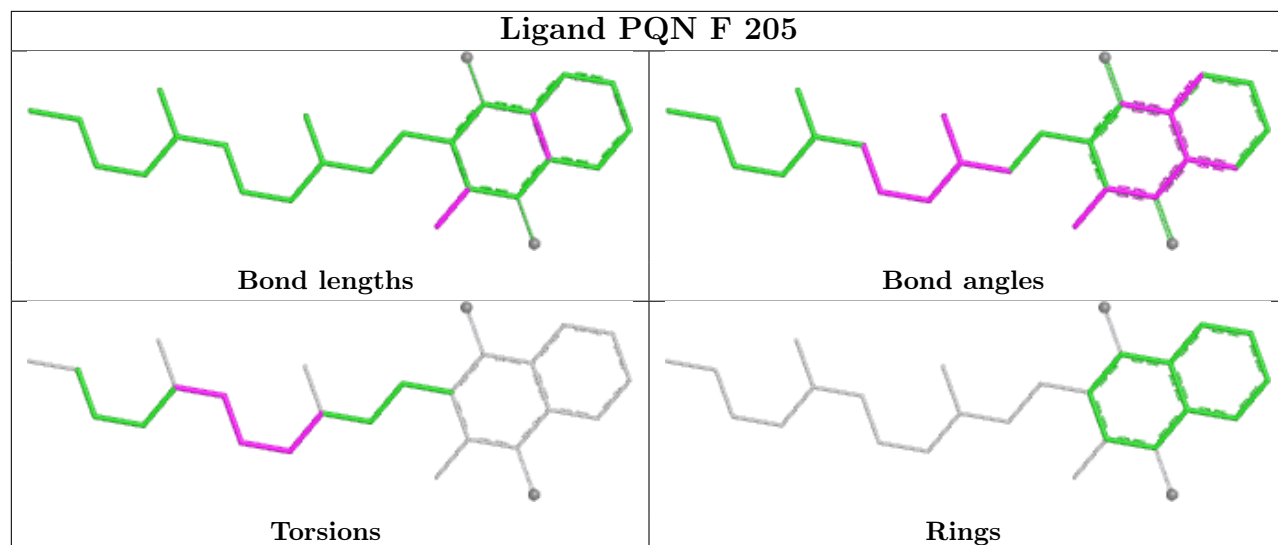
## Ligand CLA A 853



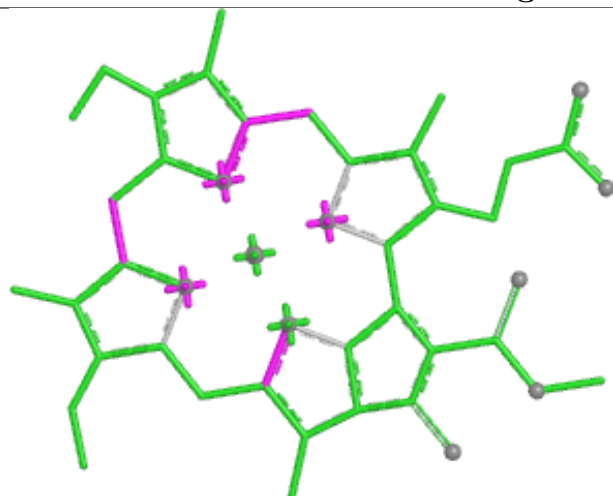
## Ligand CLA f 602



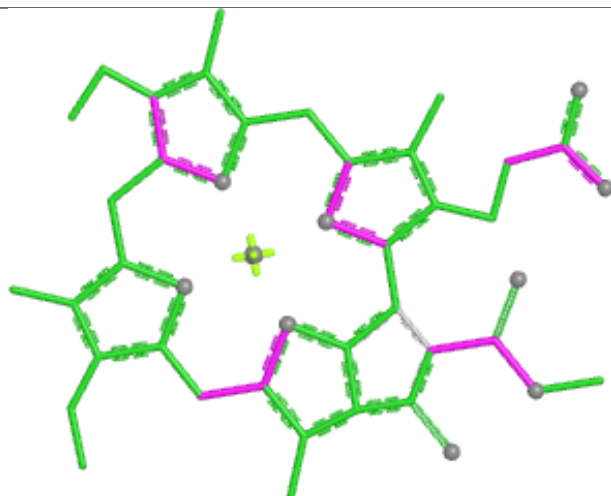




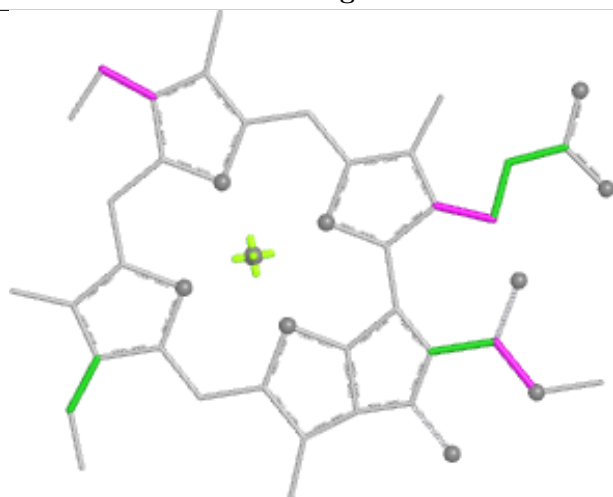
## Ligand CLA b 206



Bond lengths



Bond angles

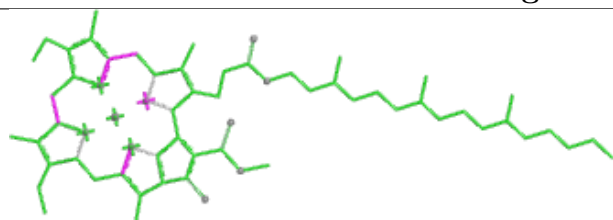


Torsions

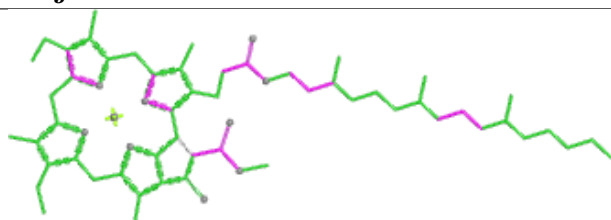


Rings

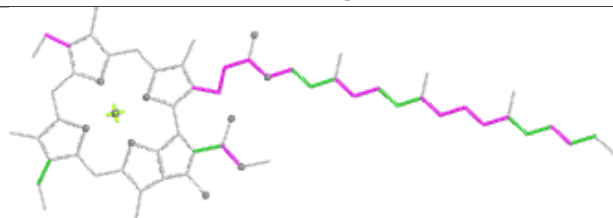
## Ligand CLA j 209



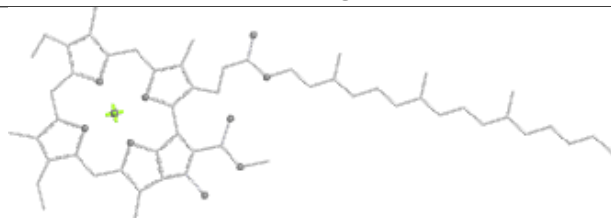
Bond lengths



Bond angles

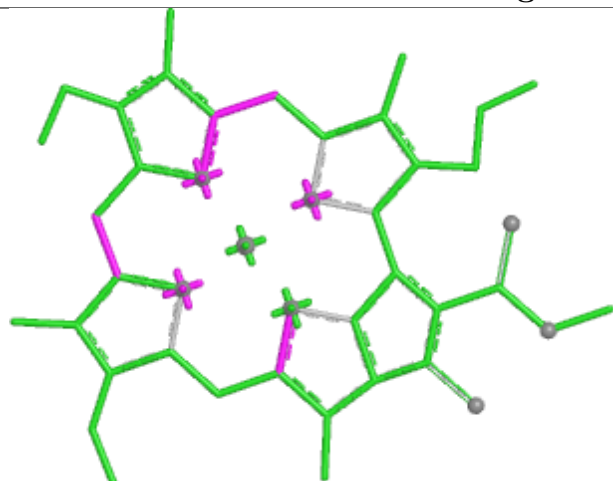


Torsions

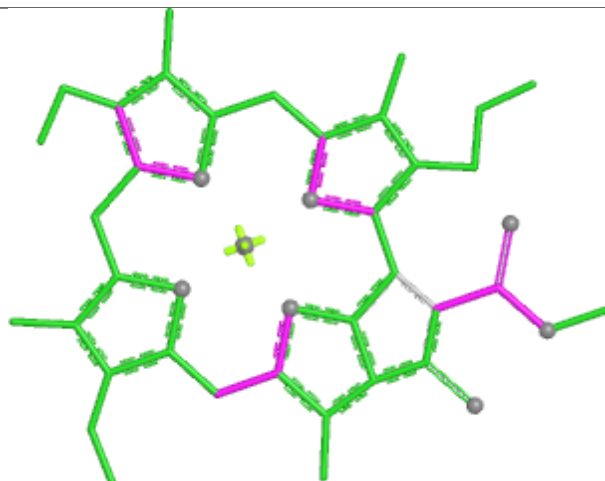


Rings

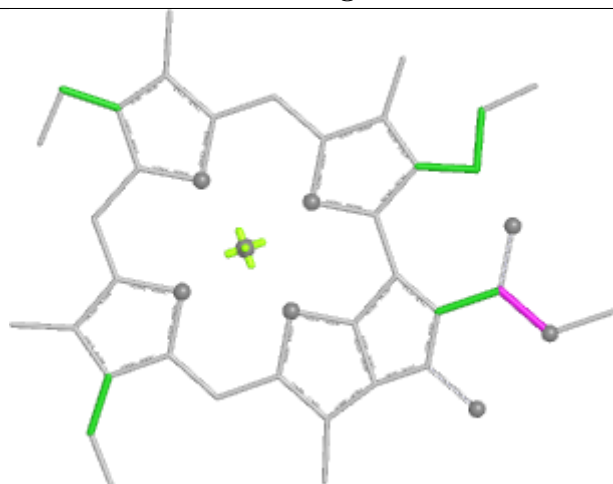
## Ligand CLA h 215



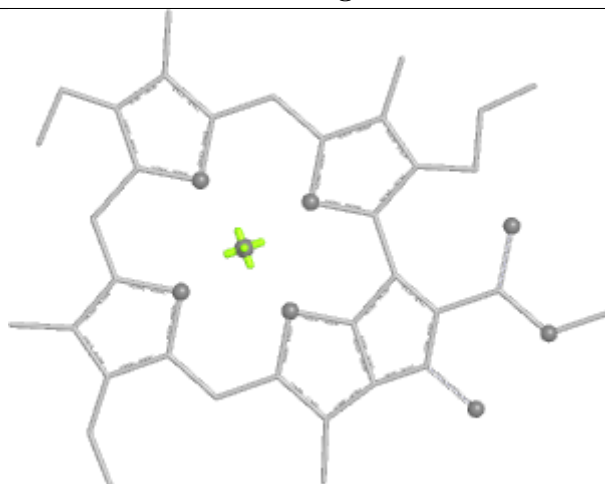
Bond lengths



Bond angles

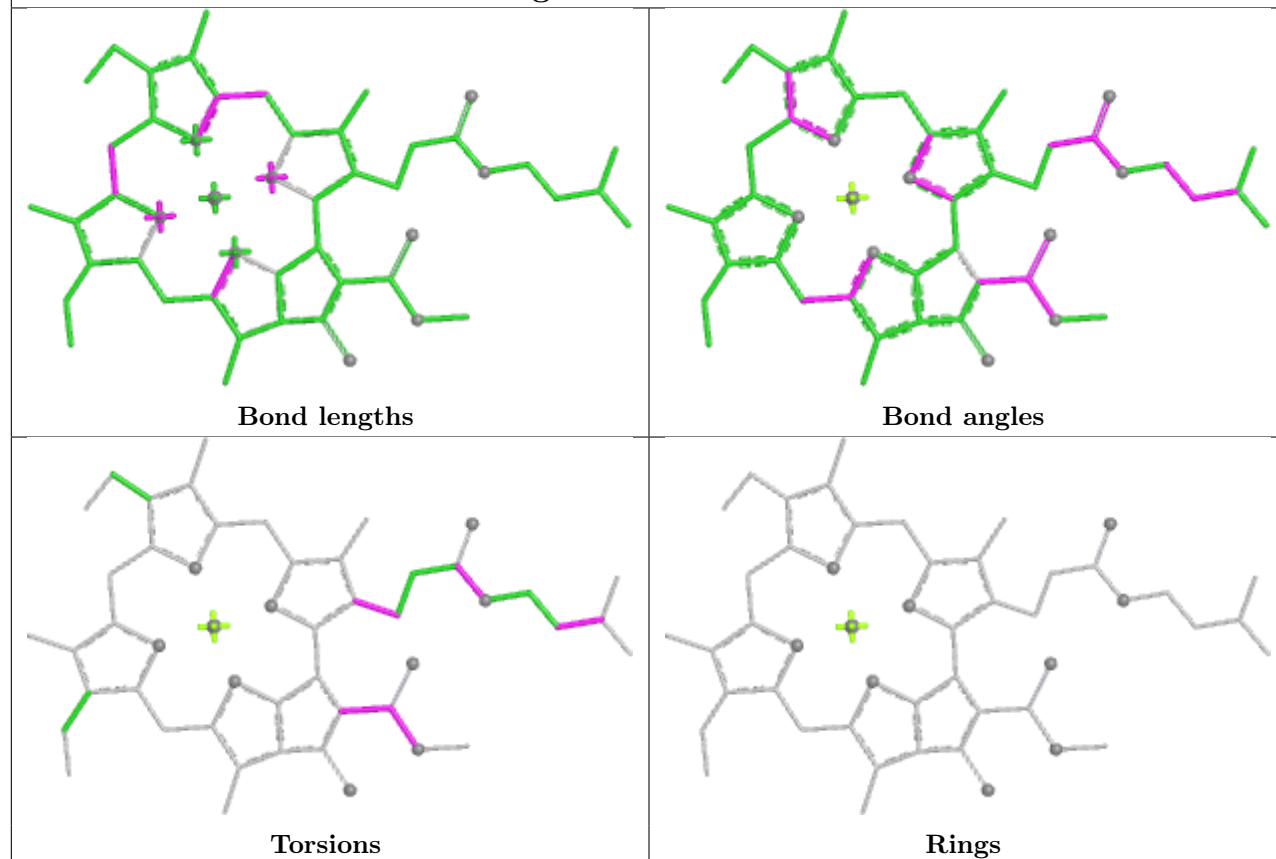


Torsions

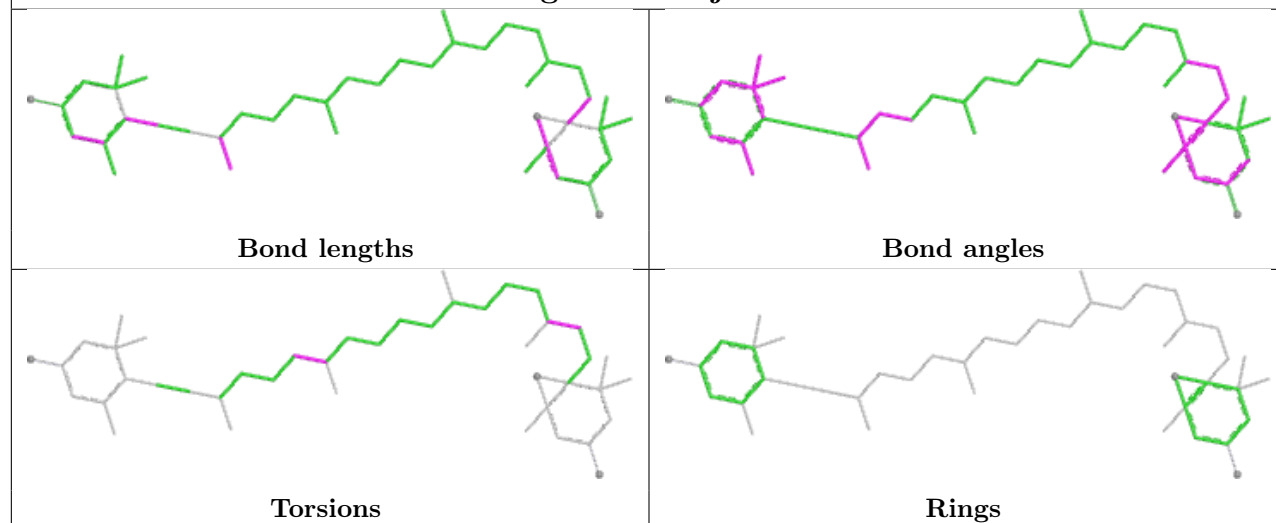


Rings

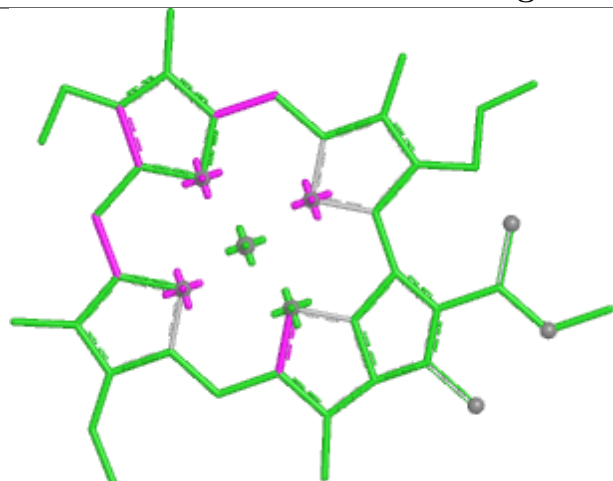
## Ligand CLA B 840



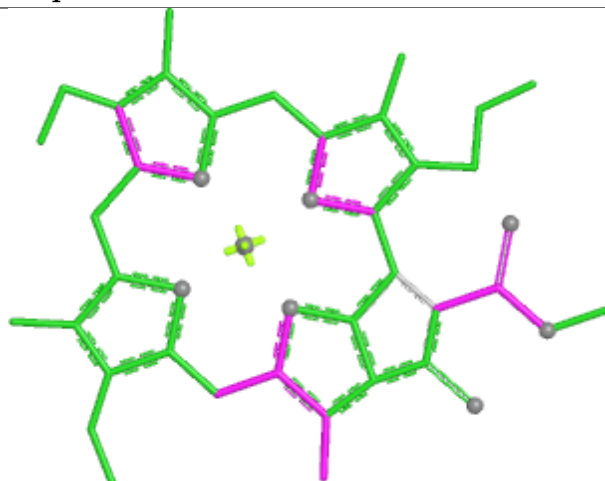
## Ligand DD6 j 216



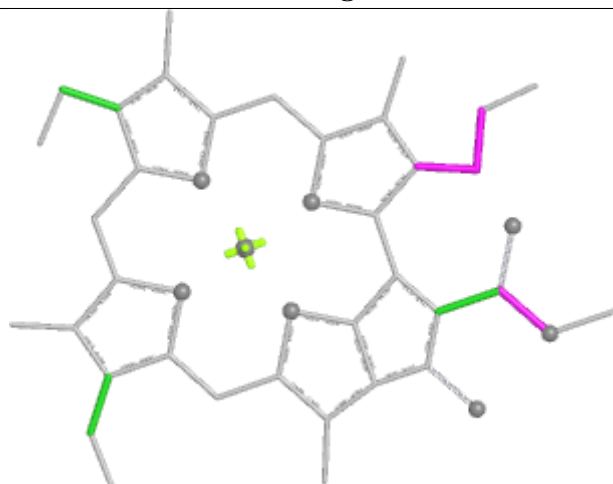
## Ligand CLA p 604



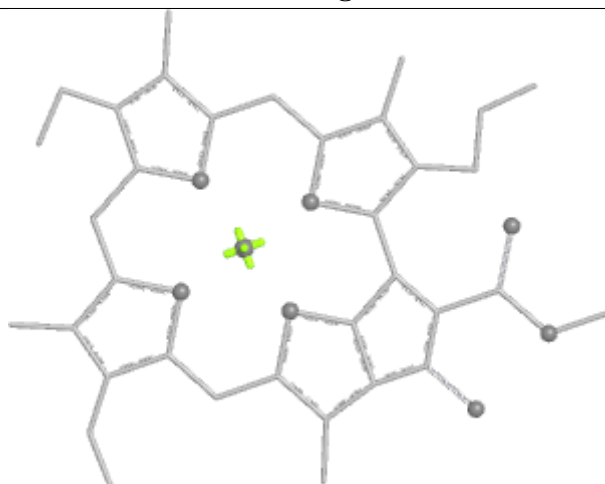
Bond lengths



Bond angles

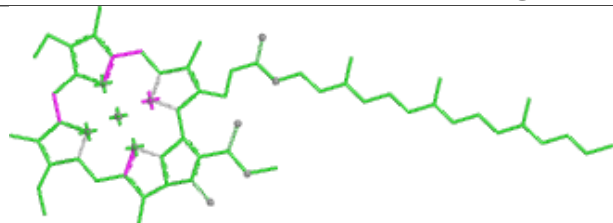


Torsions

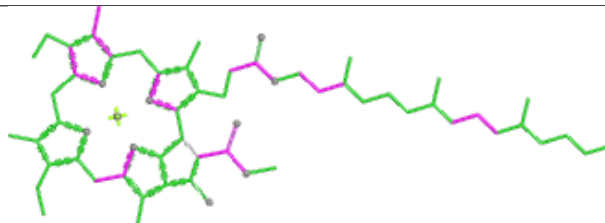


Rings

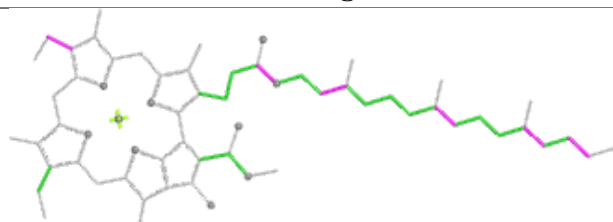
## Ligand CLA A 802



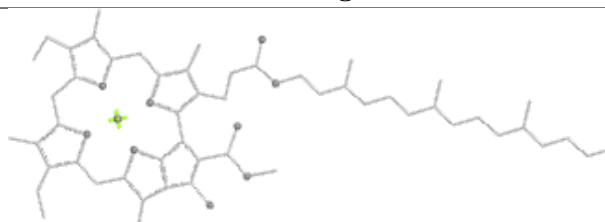
Bond lengths



Bond angles

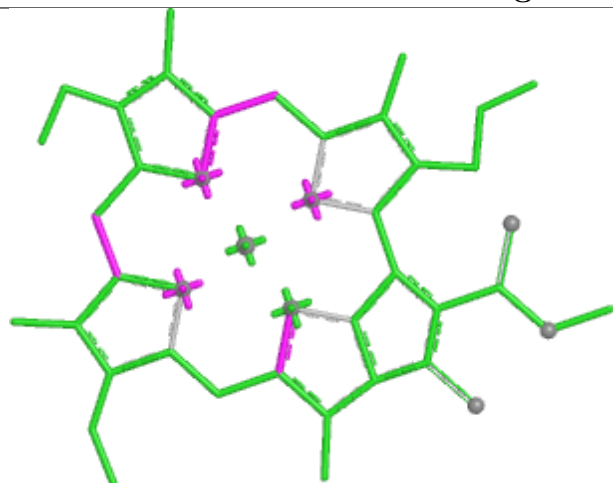


Torsions

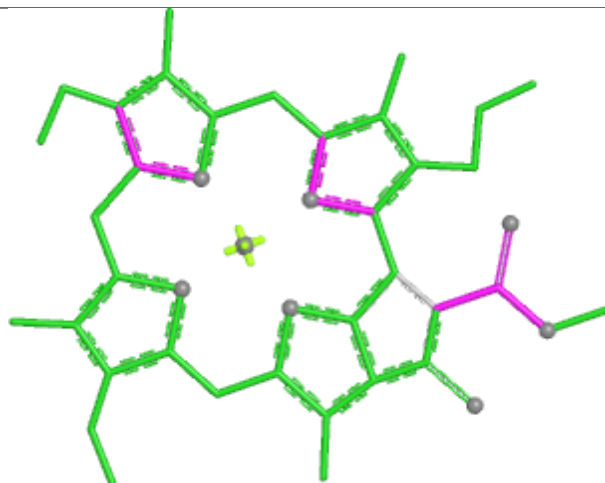


Rings

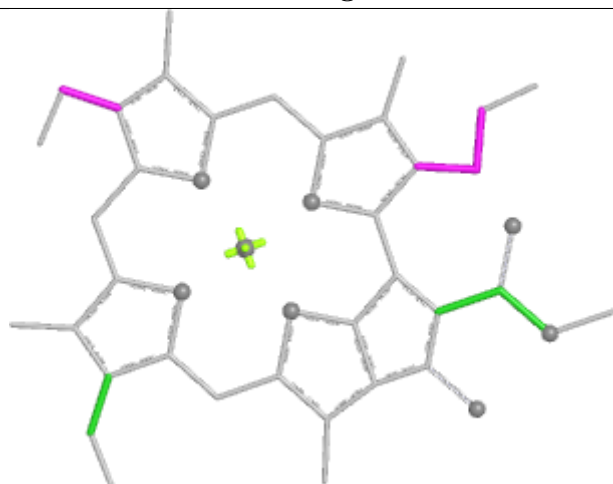
## Ligand CLA B 825



Bond lengths



Bond angles

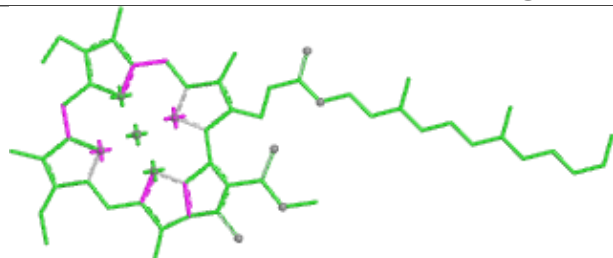


Torsions

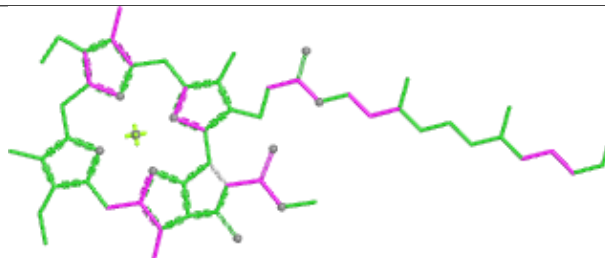


Rings

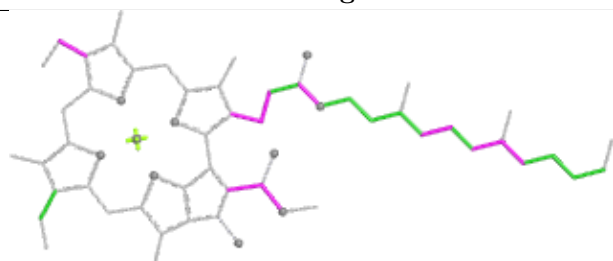
## Ligand CLA c 303



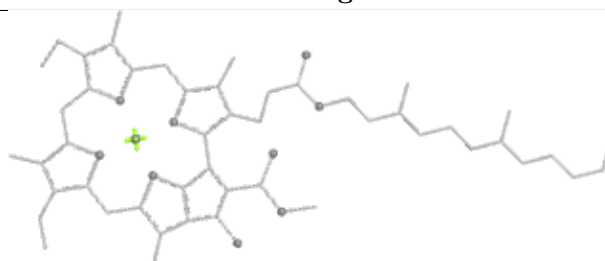
Bond lengths



Bond angles

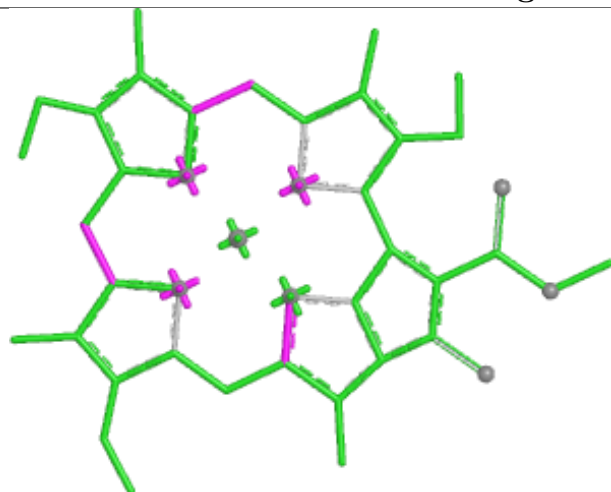


Torsions

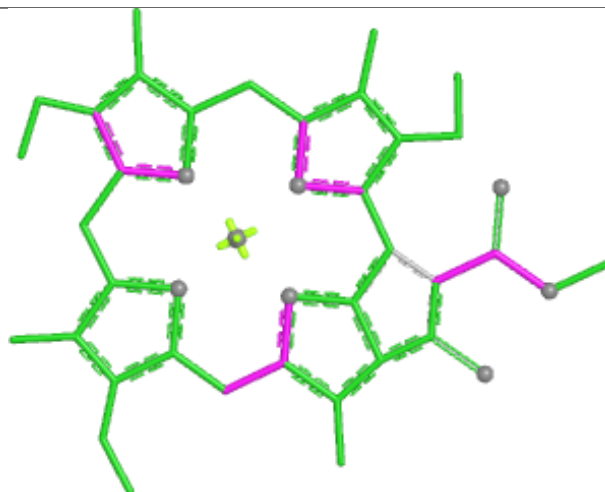


Rings

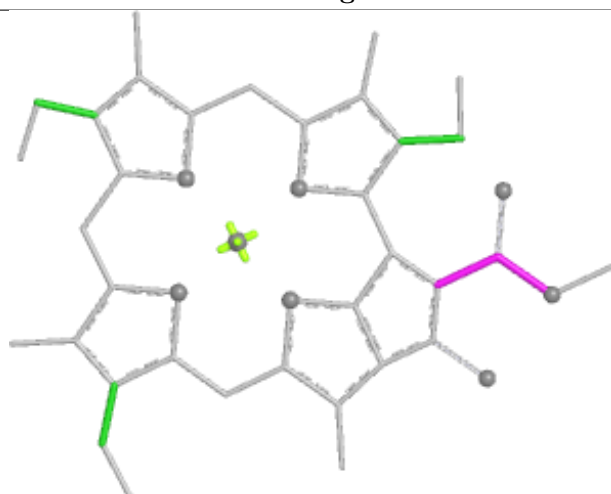
## Ligand CLA b 211



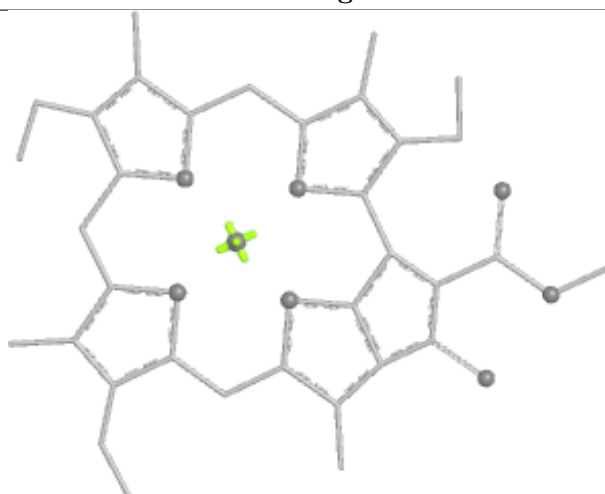
Bond lengths



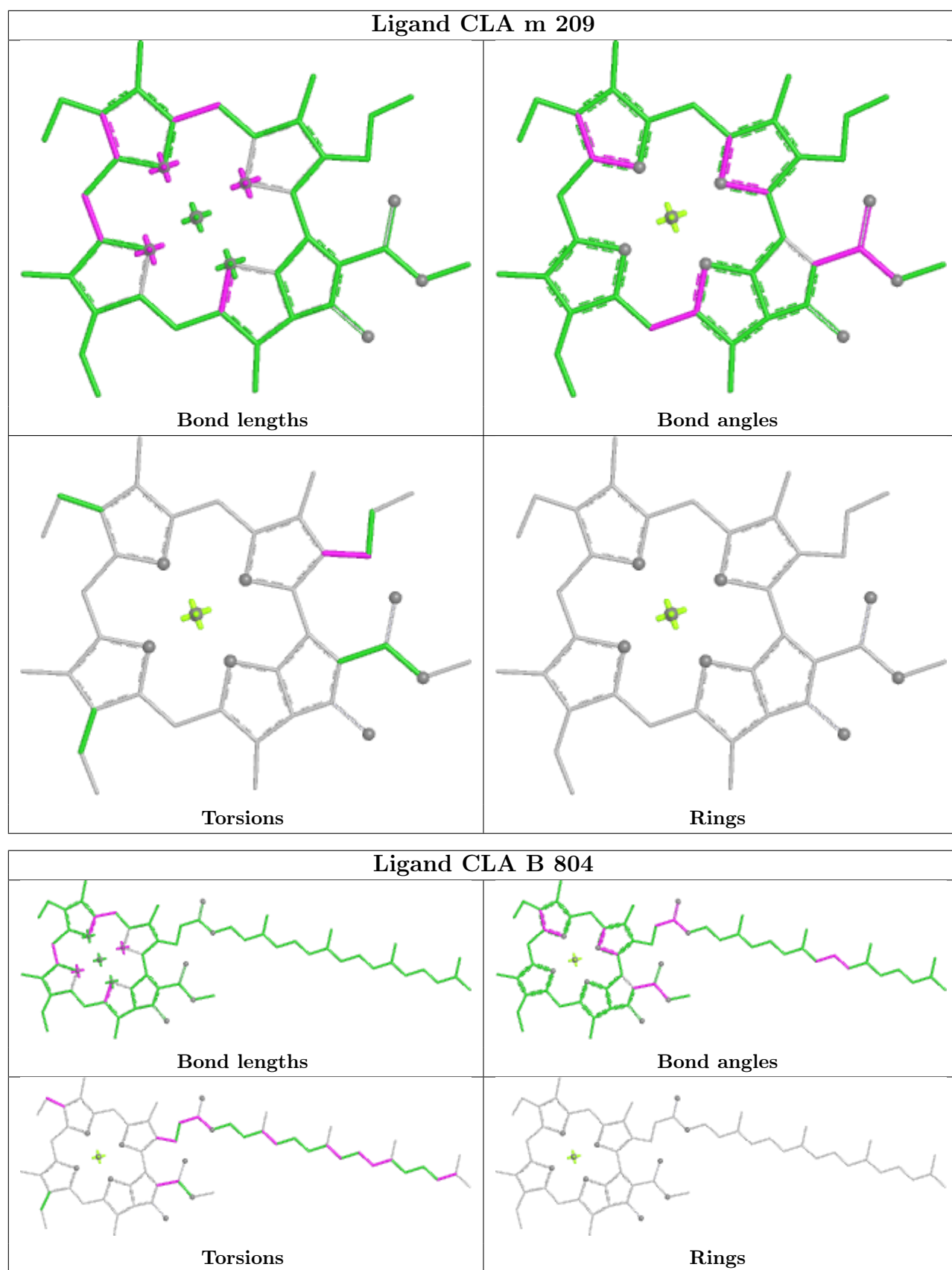
Bond angles



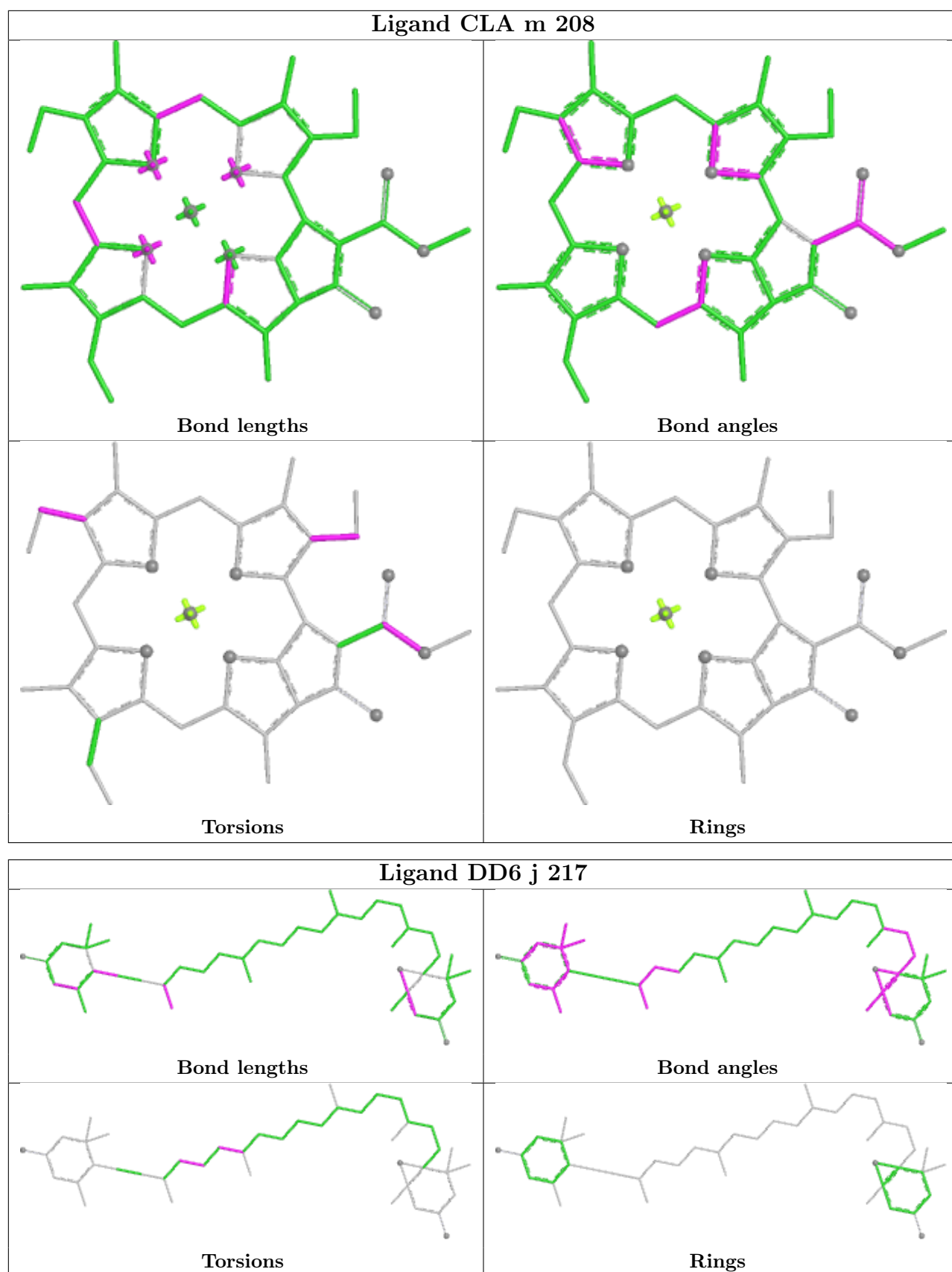
Torsions

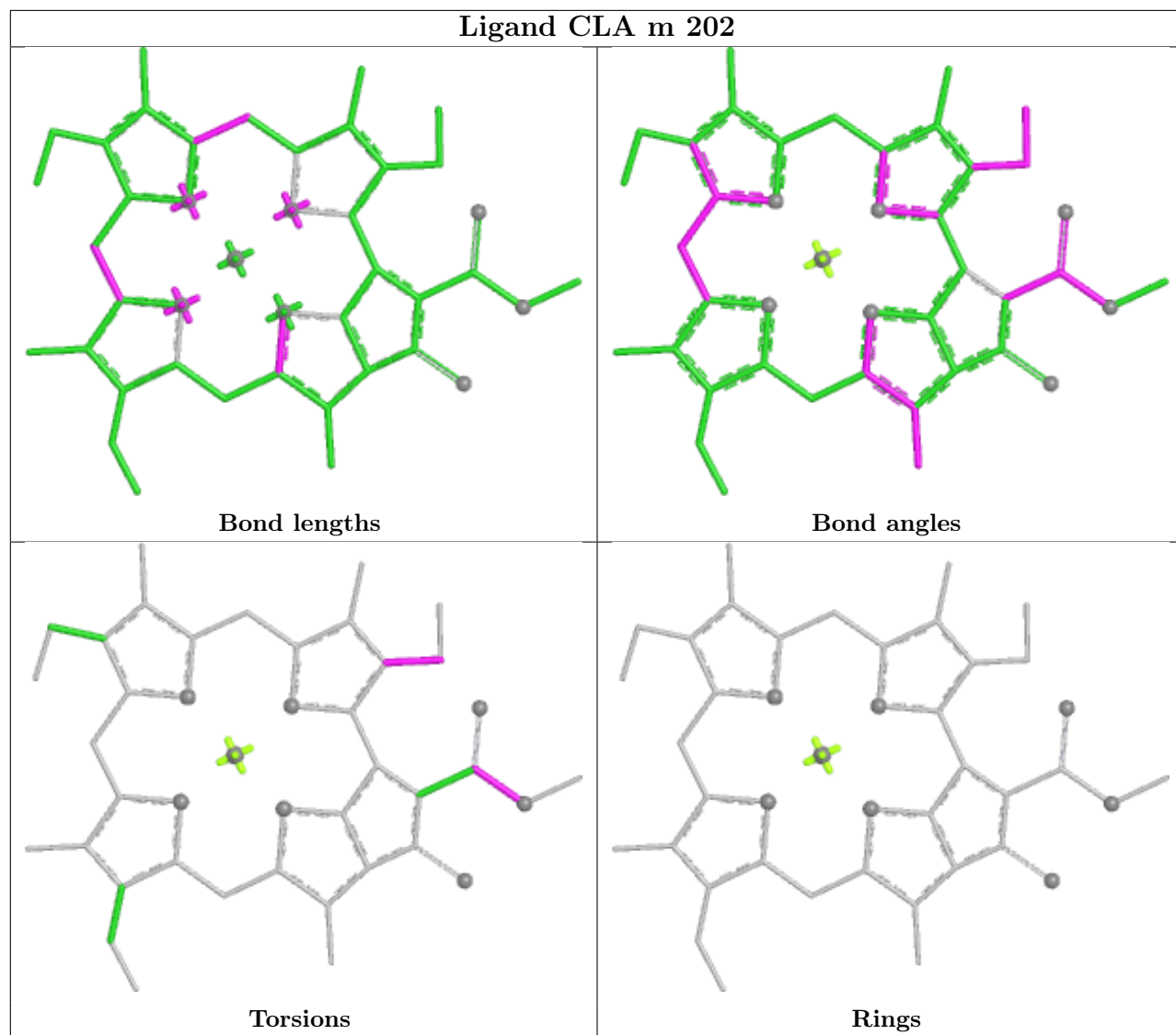


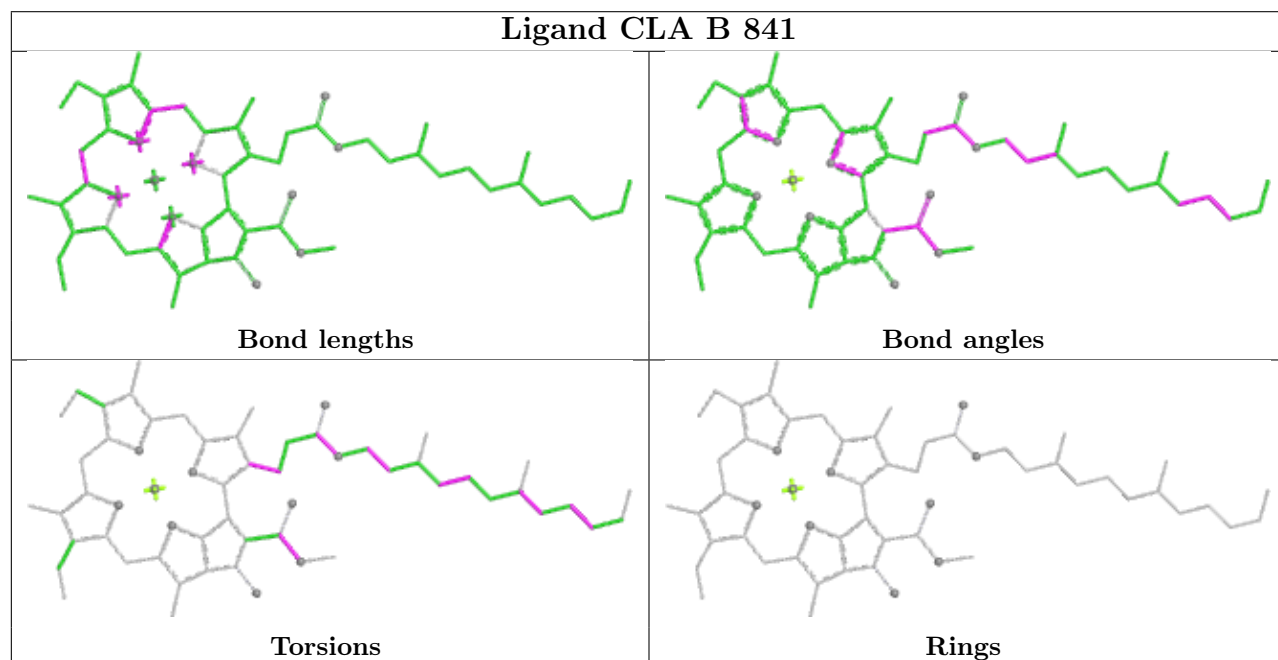
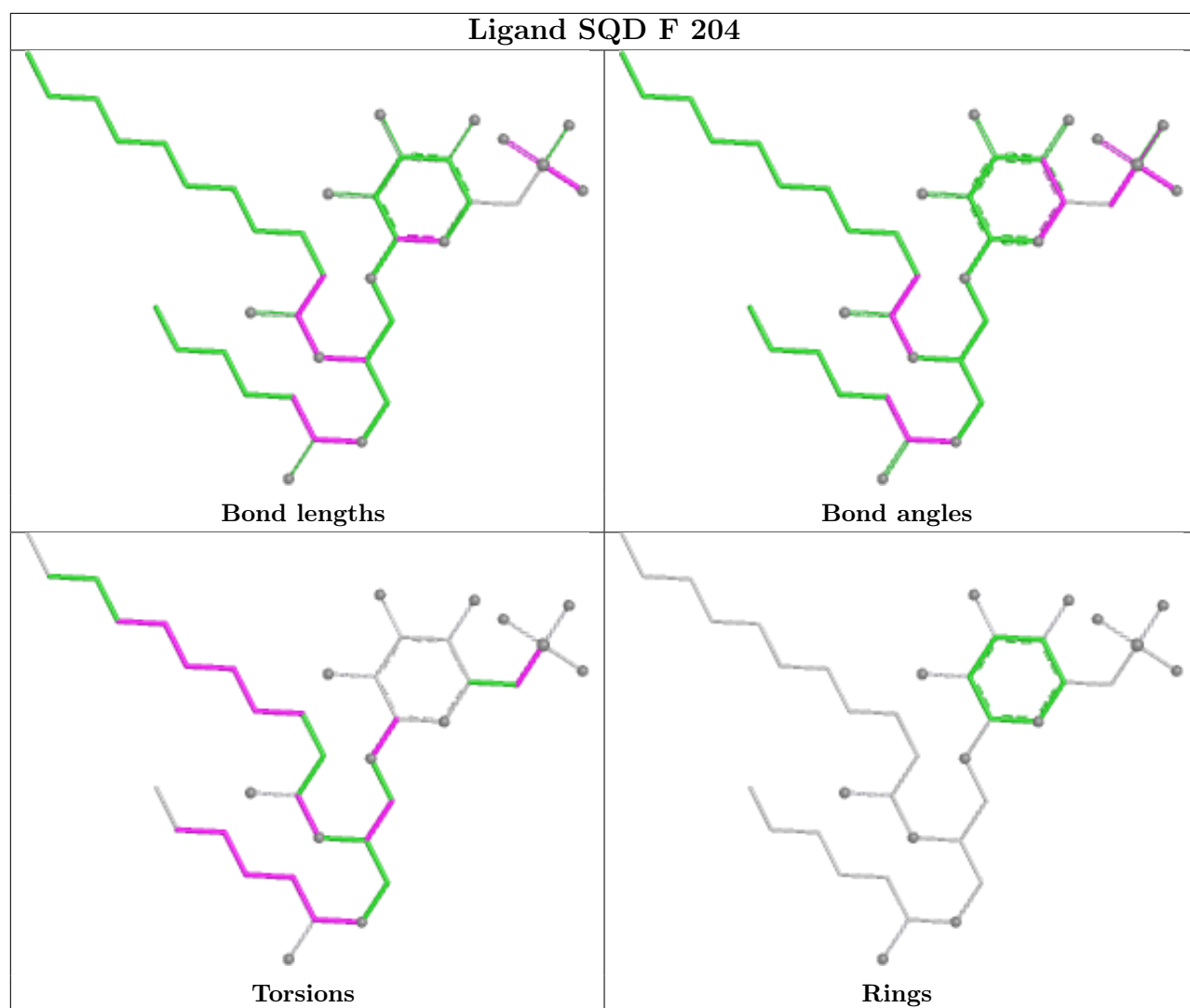
Rings



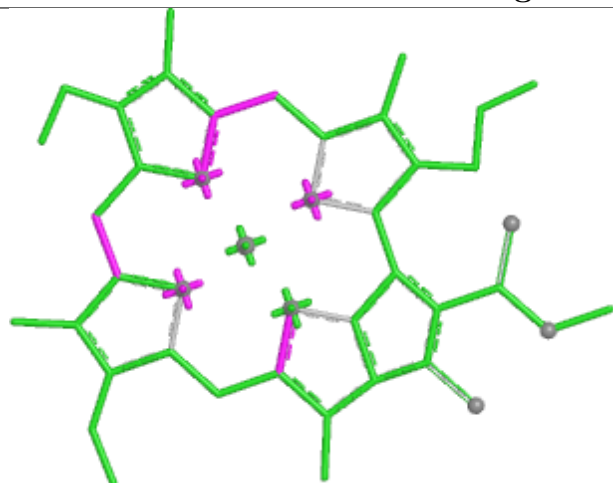




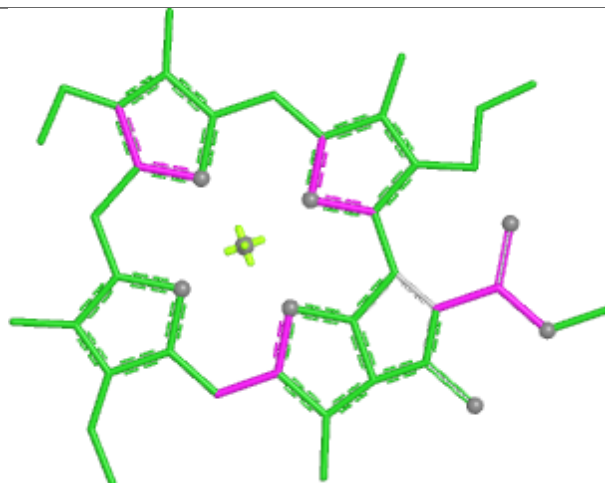




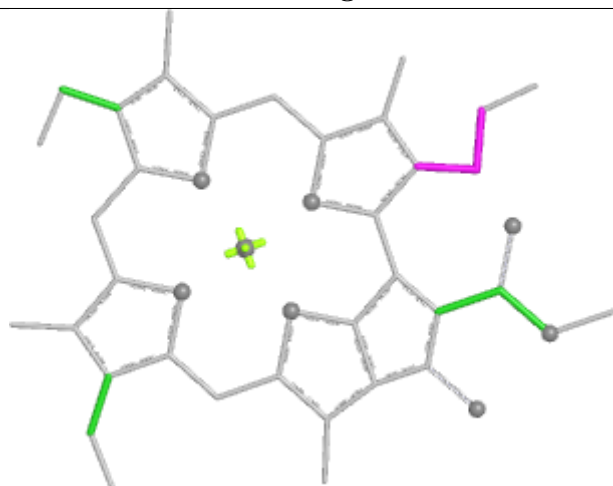
## Ligand CLA B 810



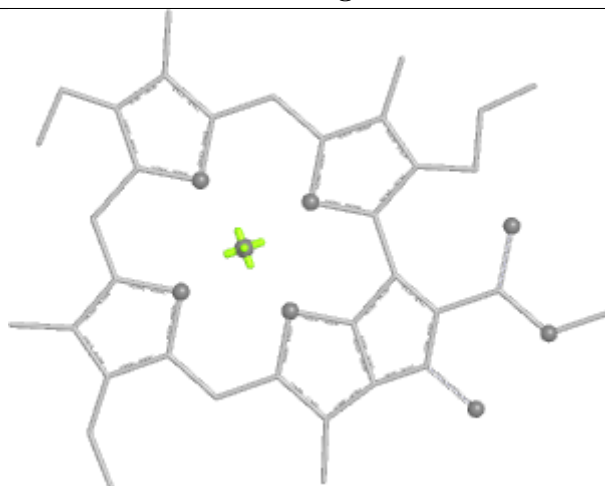
Bond lengths



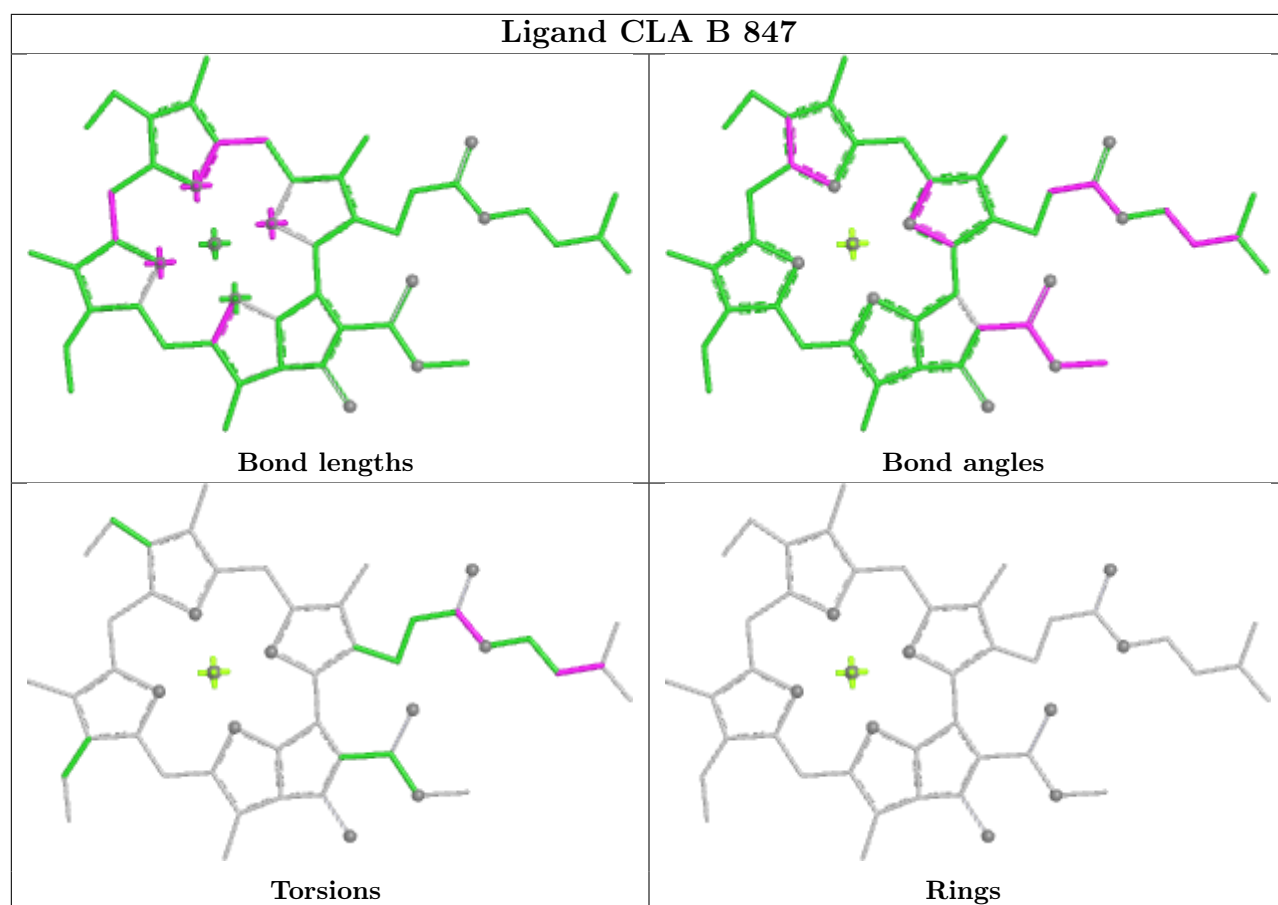
Bond angles



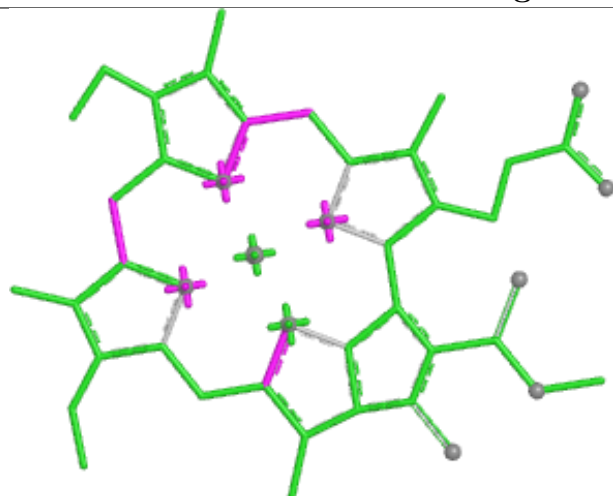
Torsions



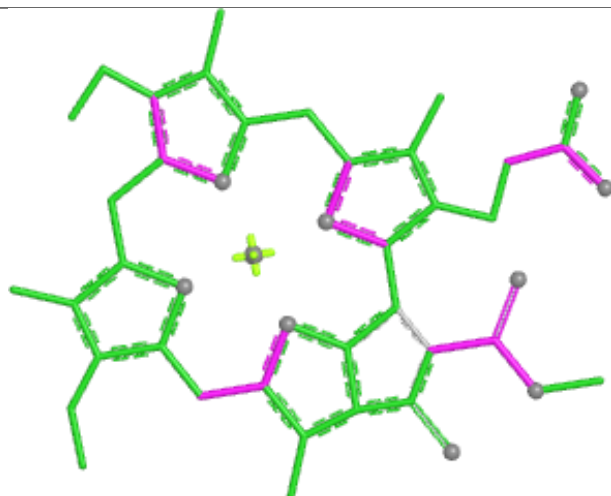
Rings



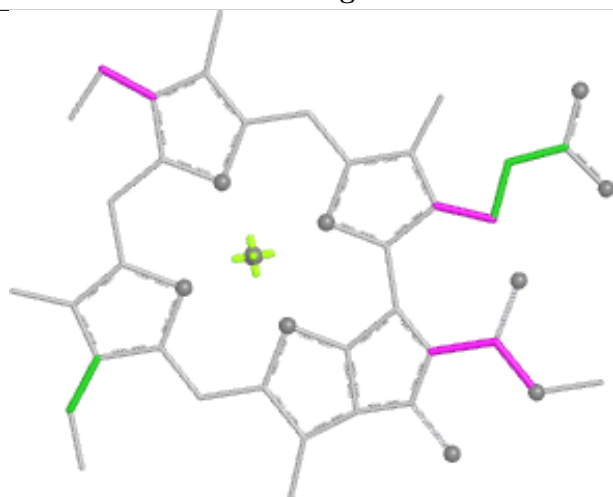
## Ligand CLA A 806



Bond lengths



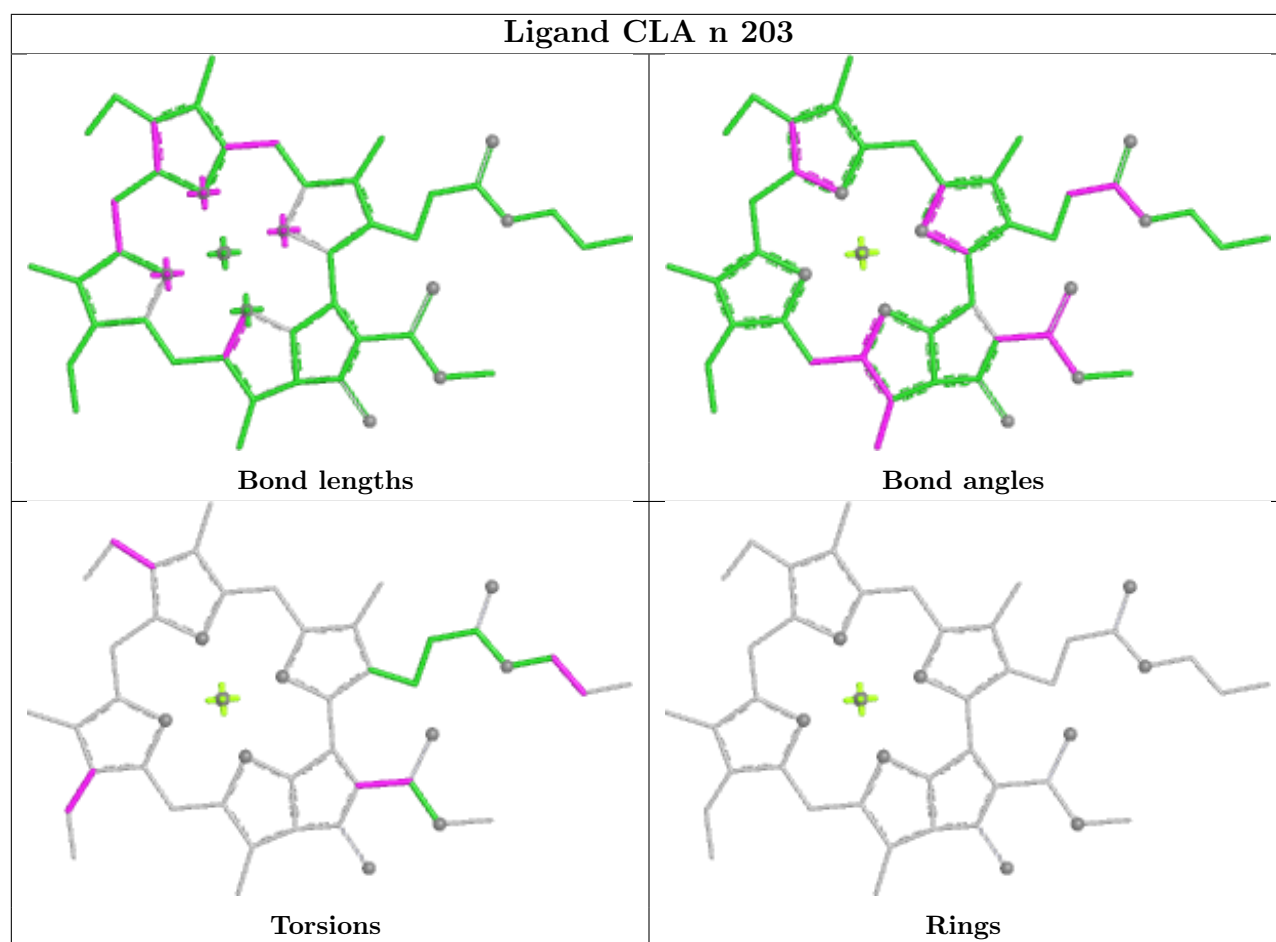
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

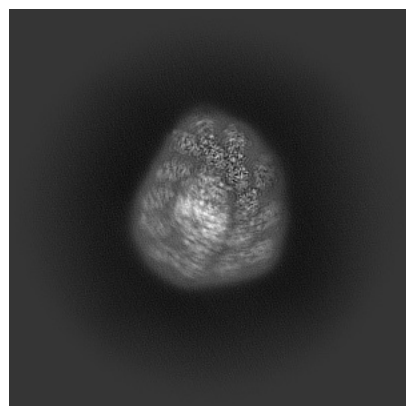
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64824. These allow visual inspection of the internal detail of the map and identification of artifacts.

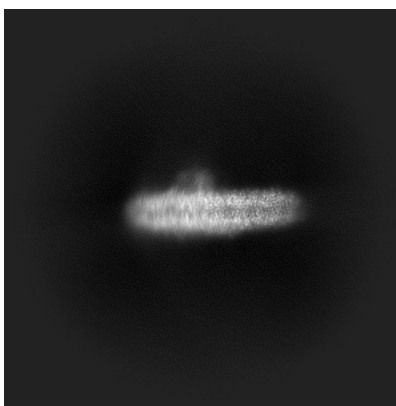
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

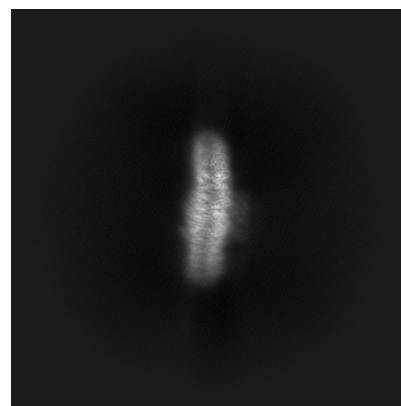
#### 6.1.1 Primary map



X

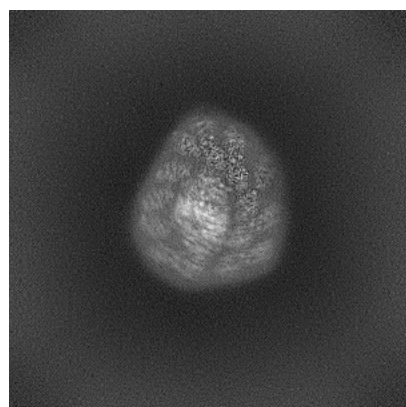


Y

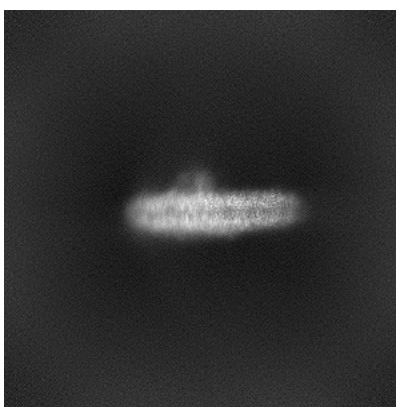


Z

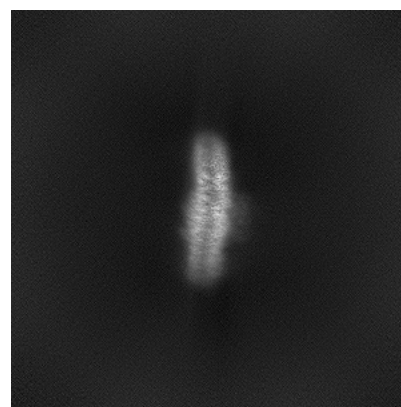
#### 6.1.2 Raw map



X



Y



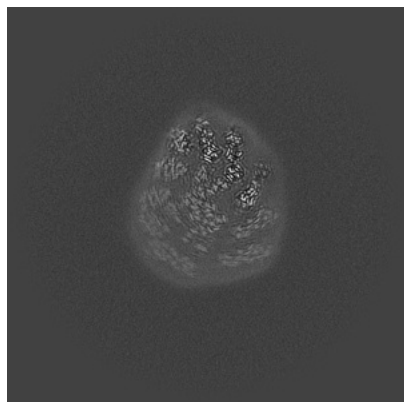
Z

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

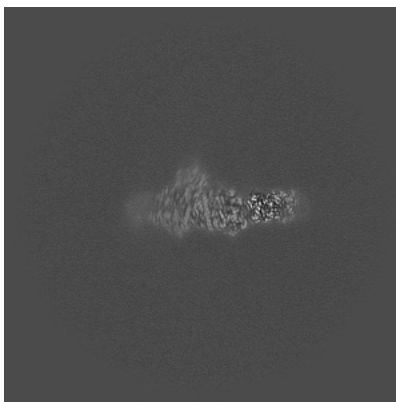


## 6.2 Central slices [i](#)

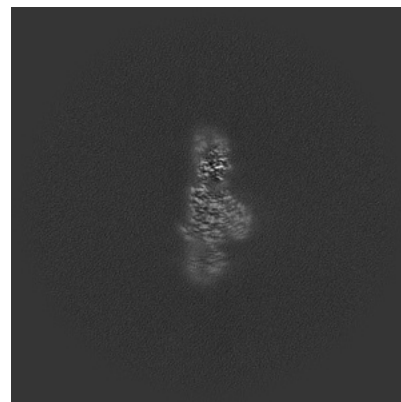
### 6.2.1 Primary map



X Index: 256

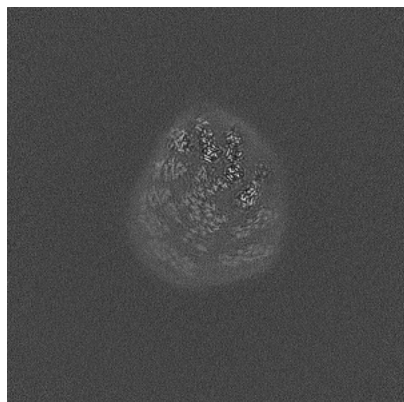


Y Index: 256

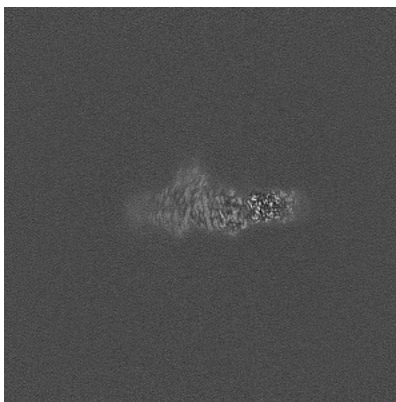


Z Index: 256

### 6.2.2 Raw map



X Index: 256



Y Index: 256

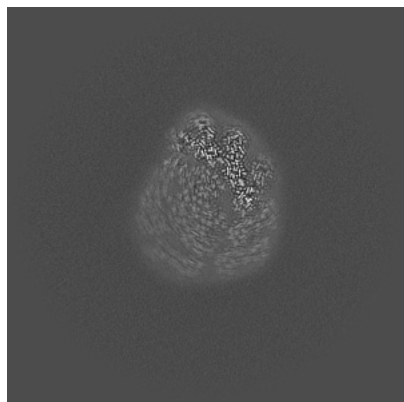


Z Index: 256

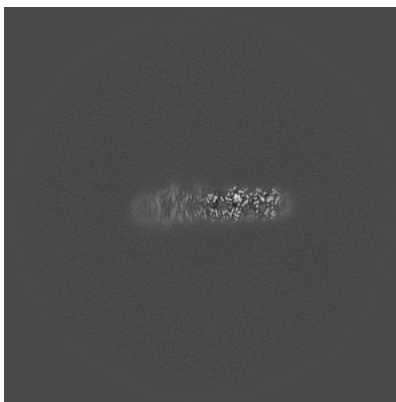
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

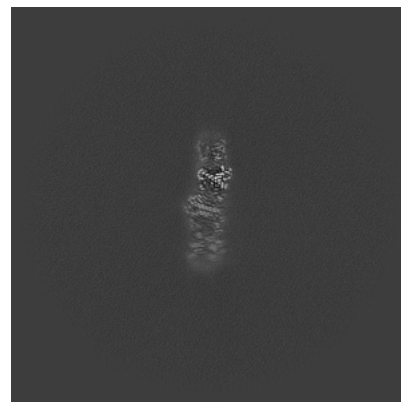
### 6.3.1 Primary map



X Index: 265

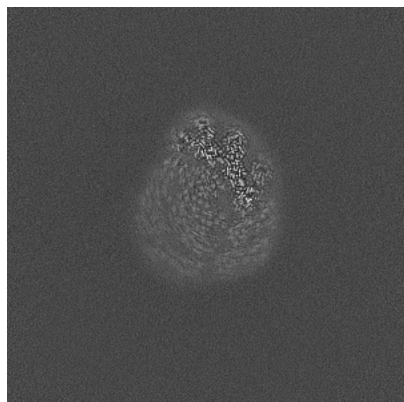


Y Index: 298

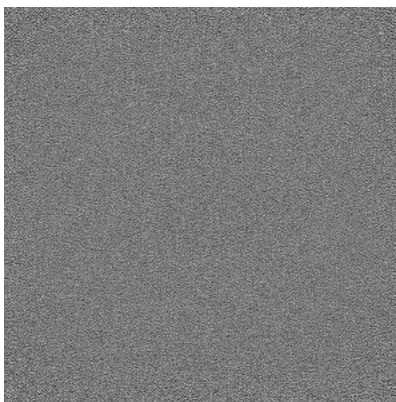


Z Index: 296

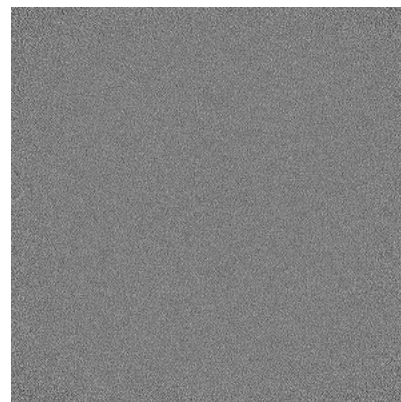
### 6.3.2 Raw map



X Index: 265



Y Index: 0

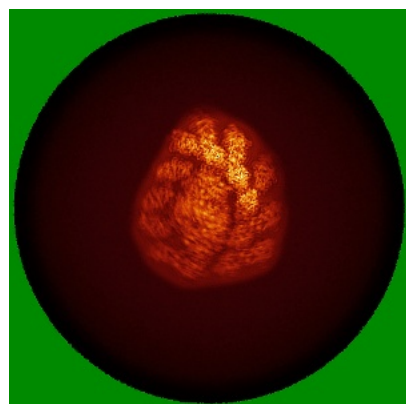


Z Index: 0

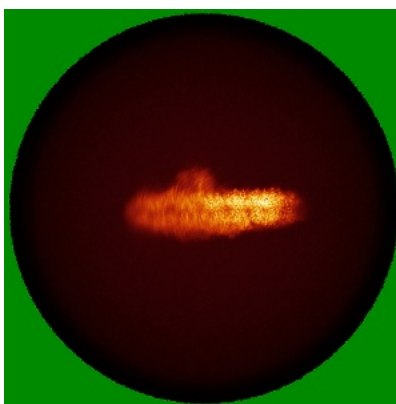
The images above show the largest variance slices of the map in three orthogonal directions.

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

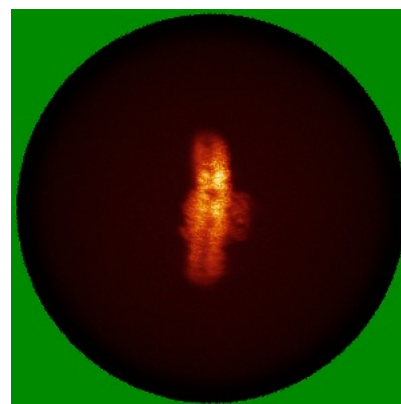
### 6.4.1 Primary map



X

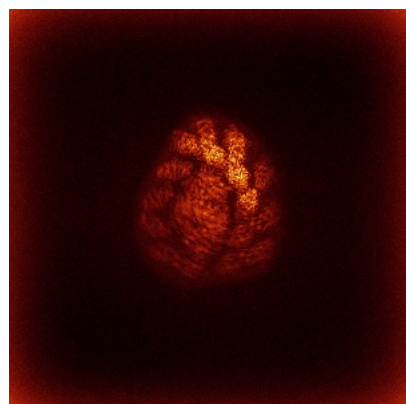


Y

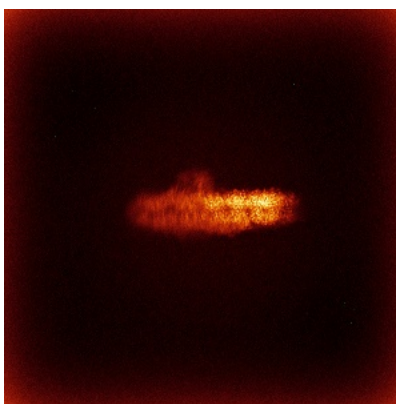


Z

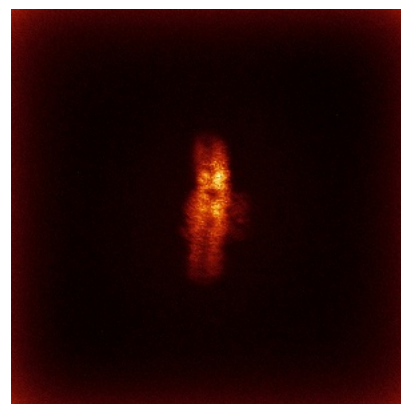
### 6.4.2 Raw map



X



Y

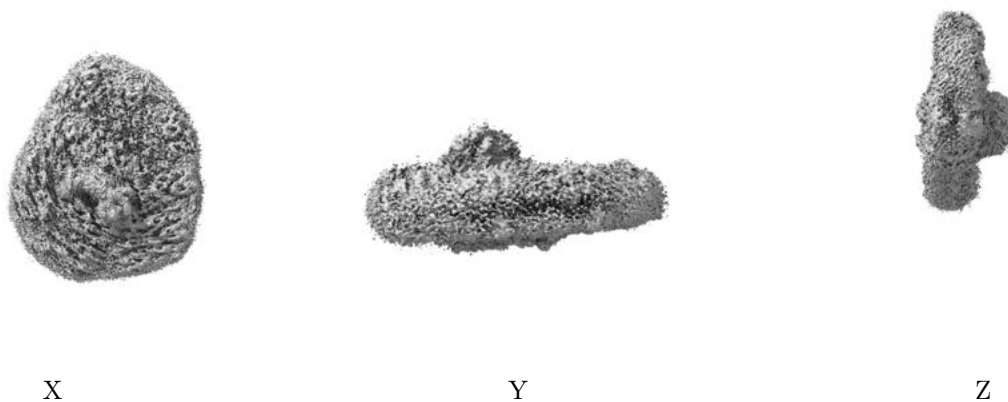


Z

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

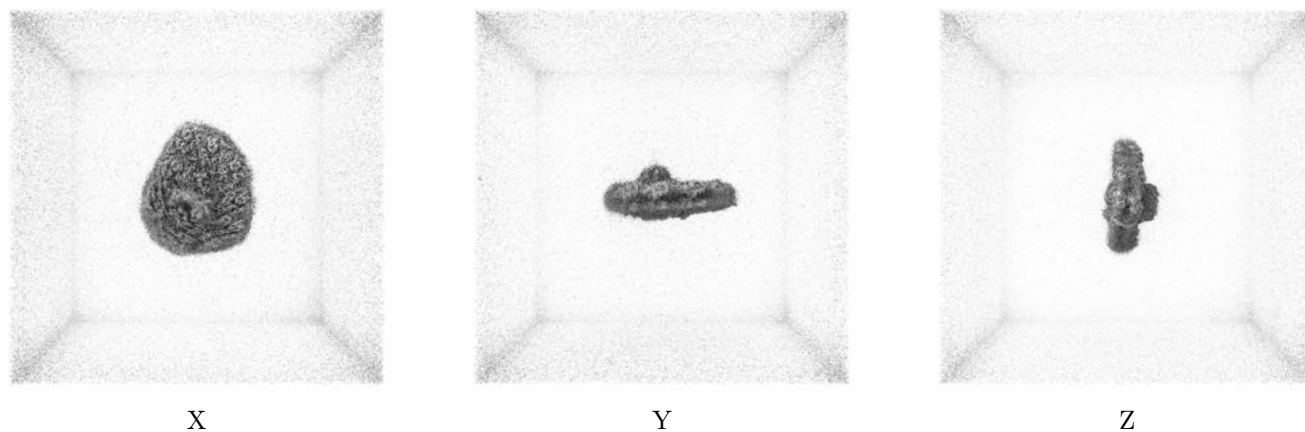
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

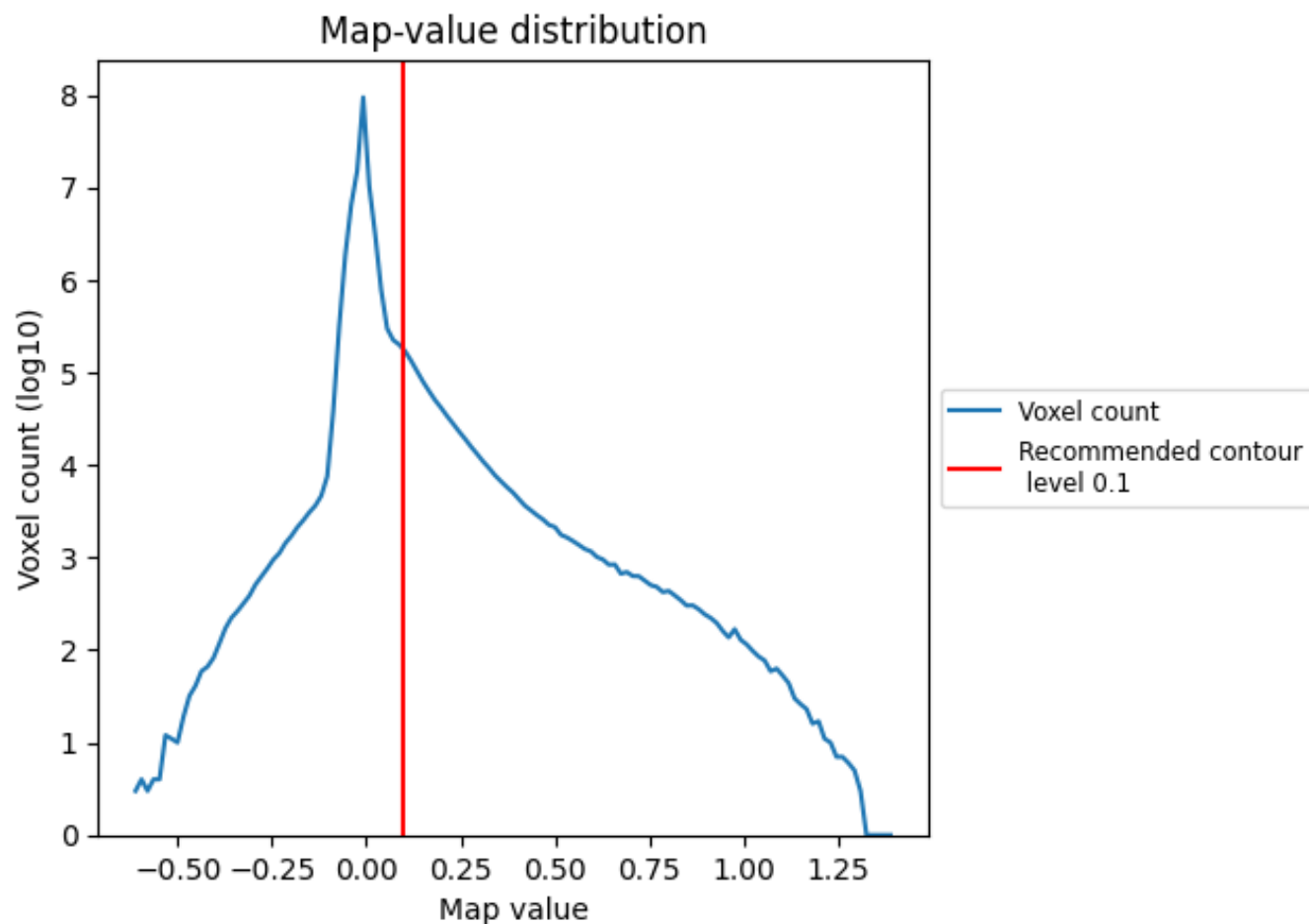
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

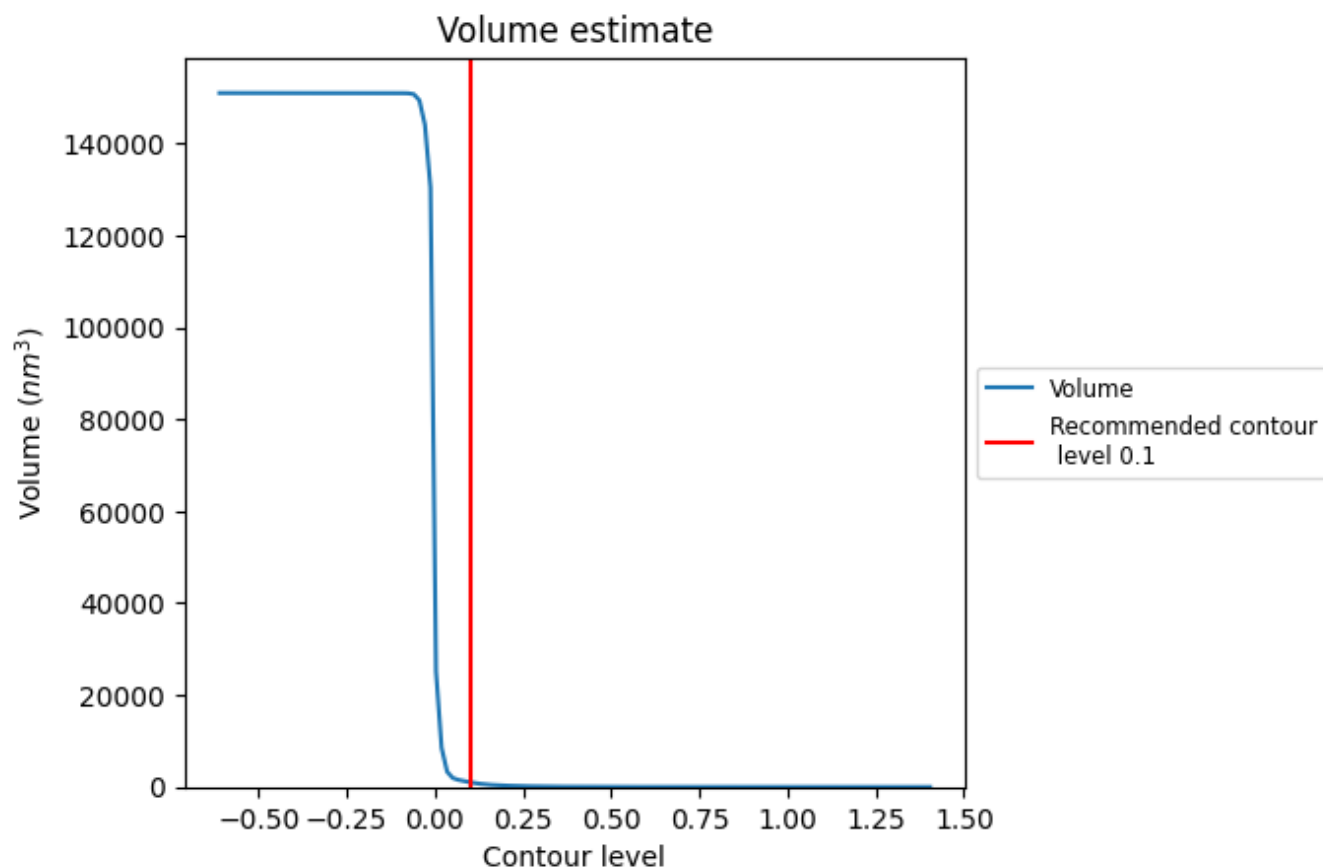
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

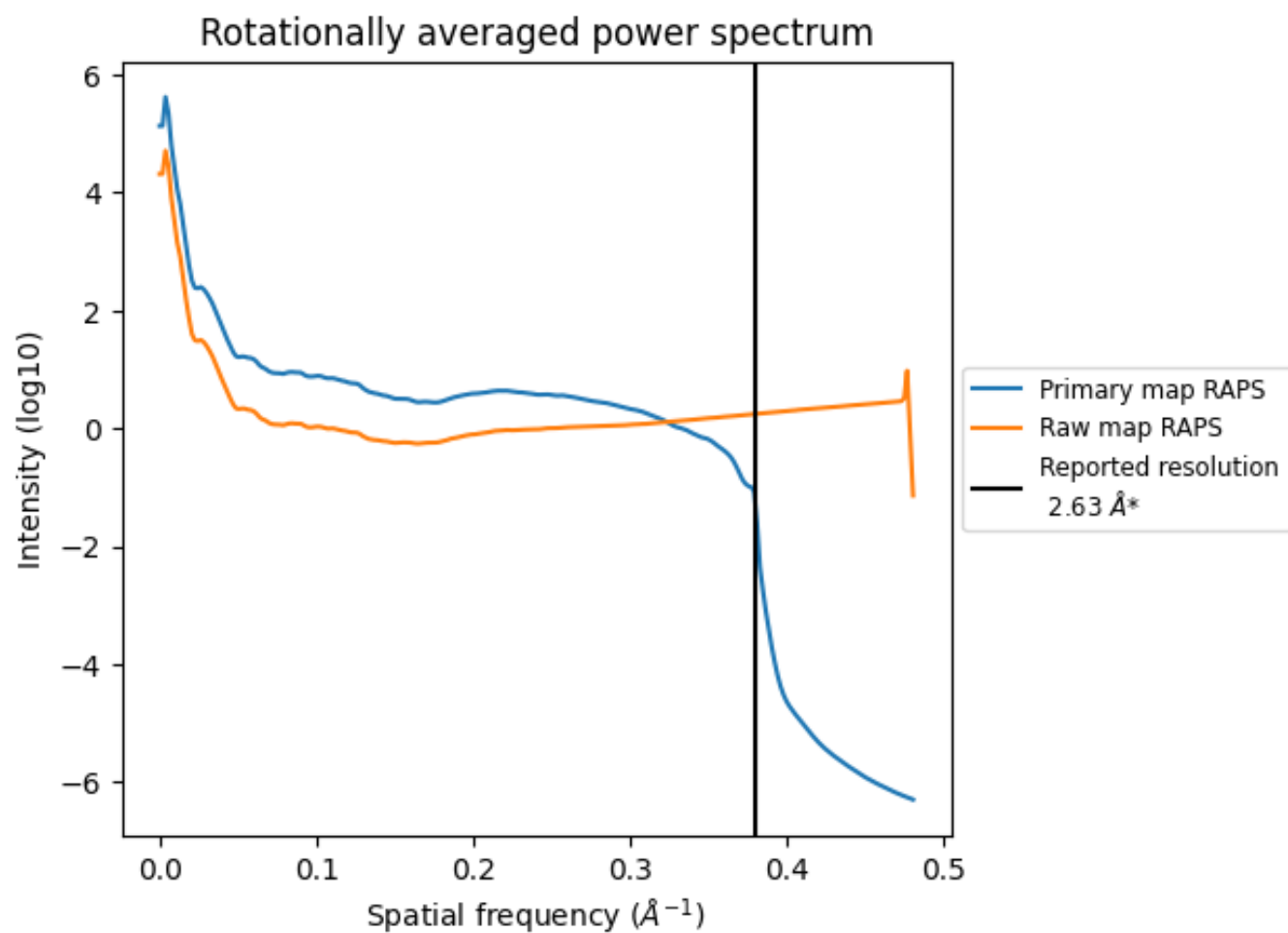


The volume at the recommended contour level is 1012  $\text{nm}^3$ ; this corresponds to an approximate mass of 914 kDa.

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 ⓘ

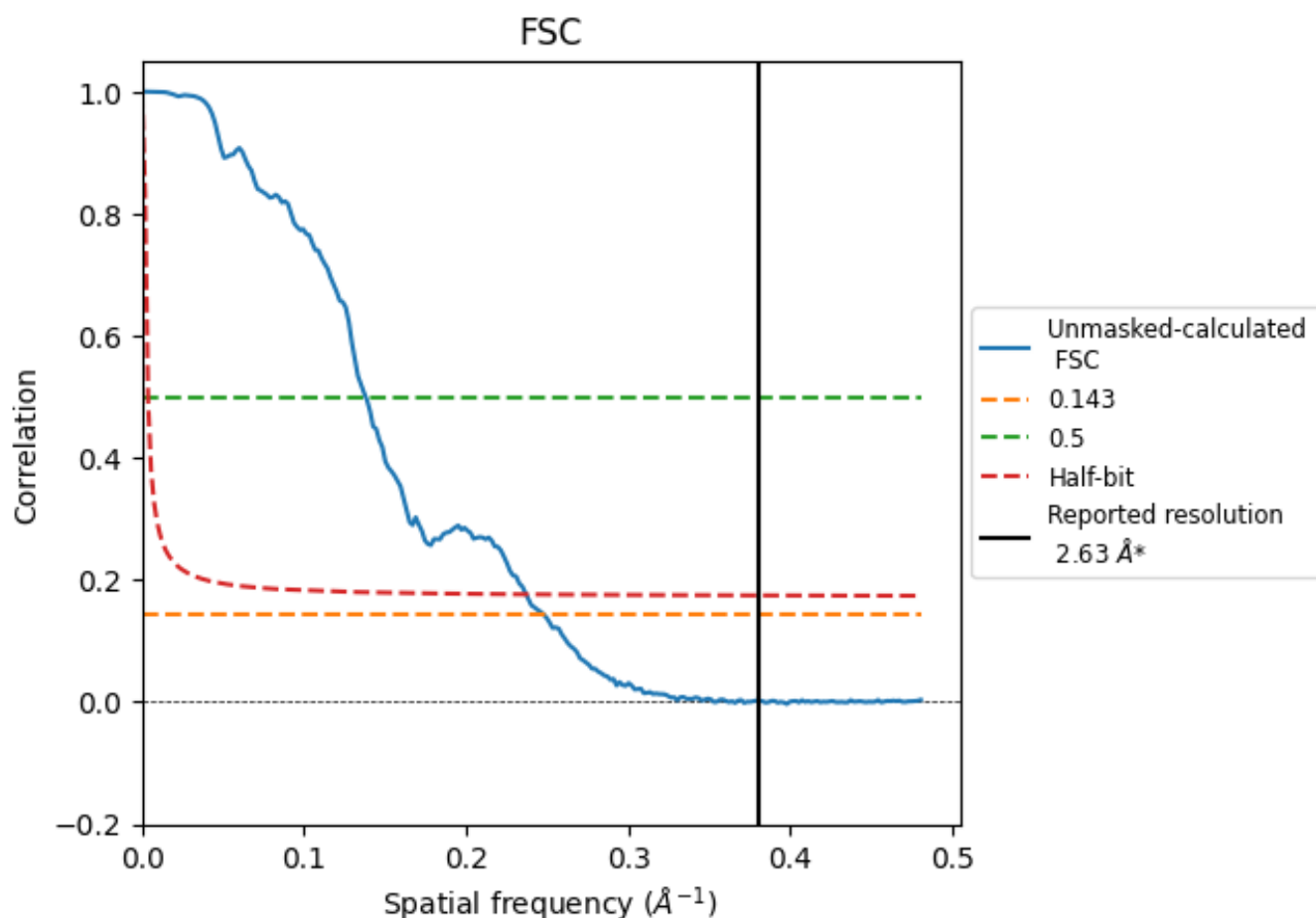


\*Reported resolution corresponds to spatial frequency of 0.380  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.380 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

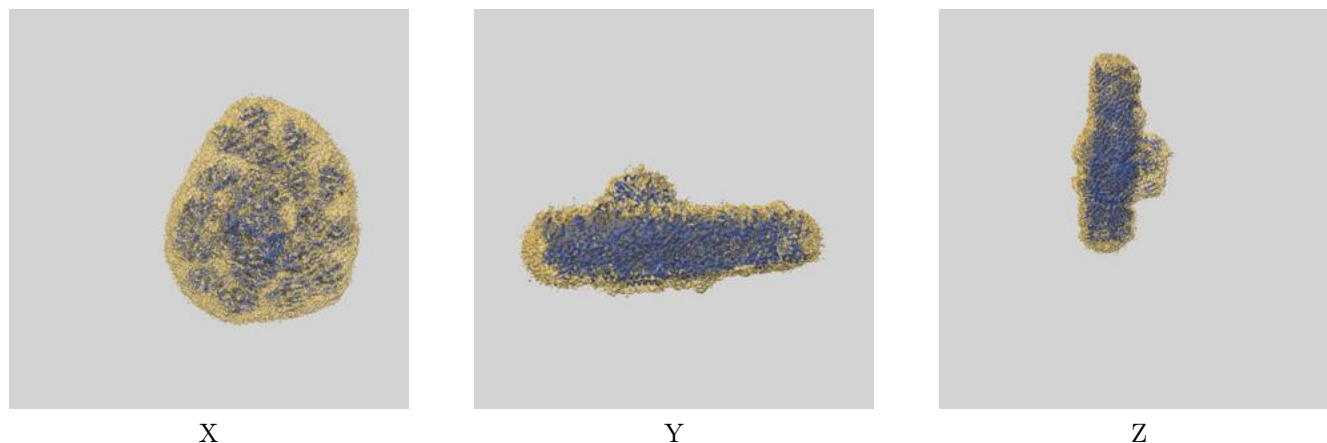
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	7.25	4.22

\*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 4.03 differs from the reported value 2.63 by more than 10 %

## 9 Map-model fit [i](#)

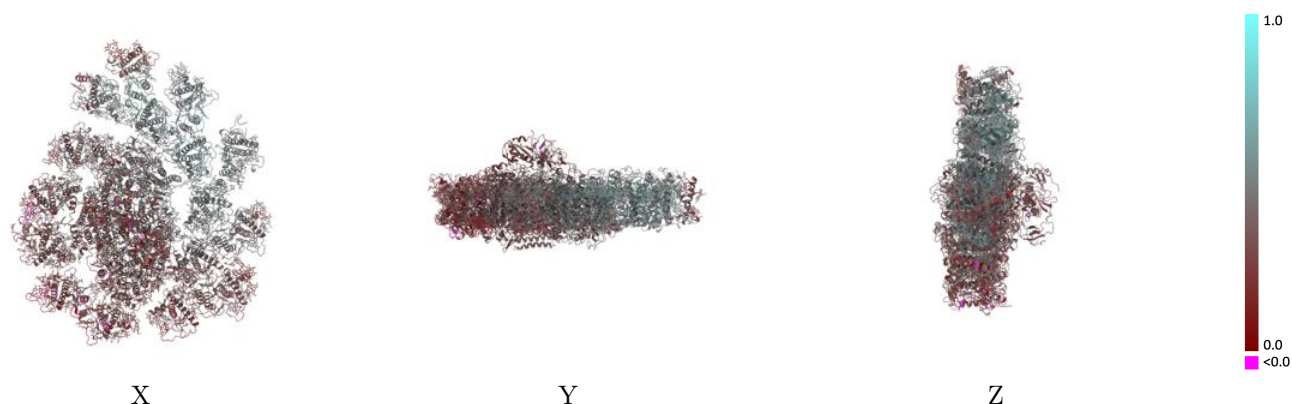
This section contains information regarding the fit between EMDB map EMD-64824 and PDB model 9V7U. Per-residue inclusion information can be found in section [3](#) on page [38](#).

### 9.1 Map-model overlay [i](#)



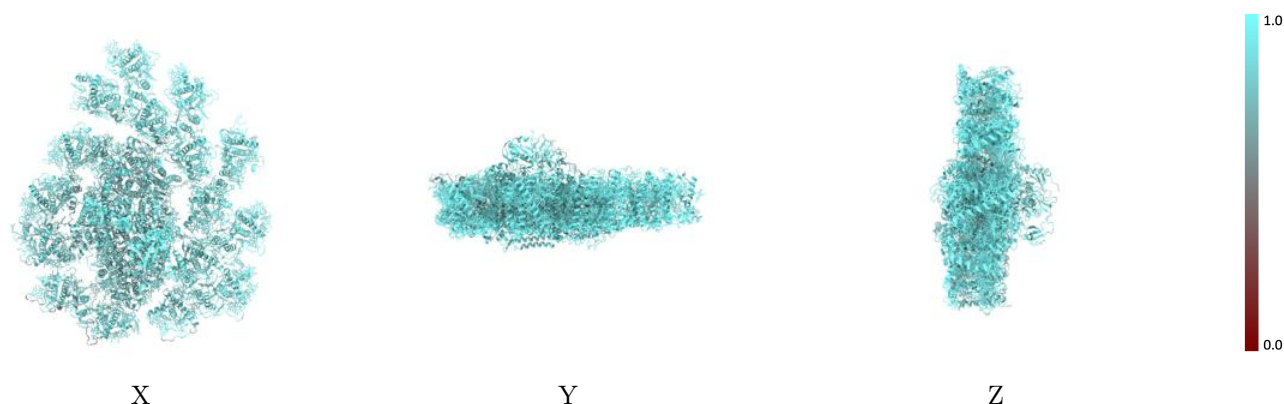
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



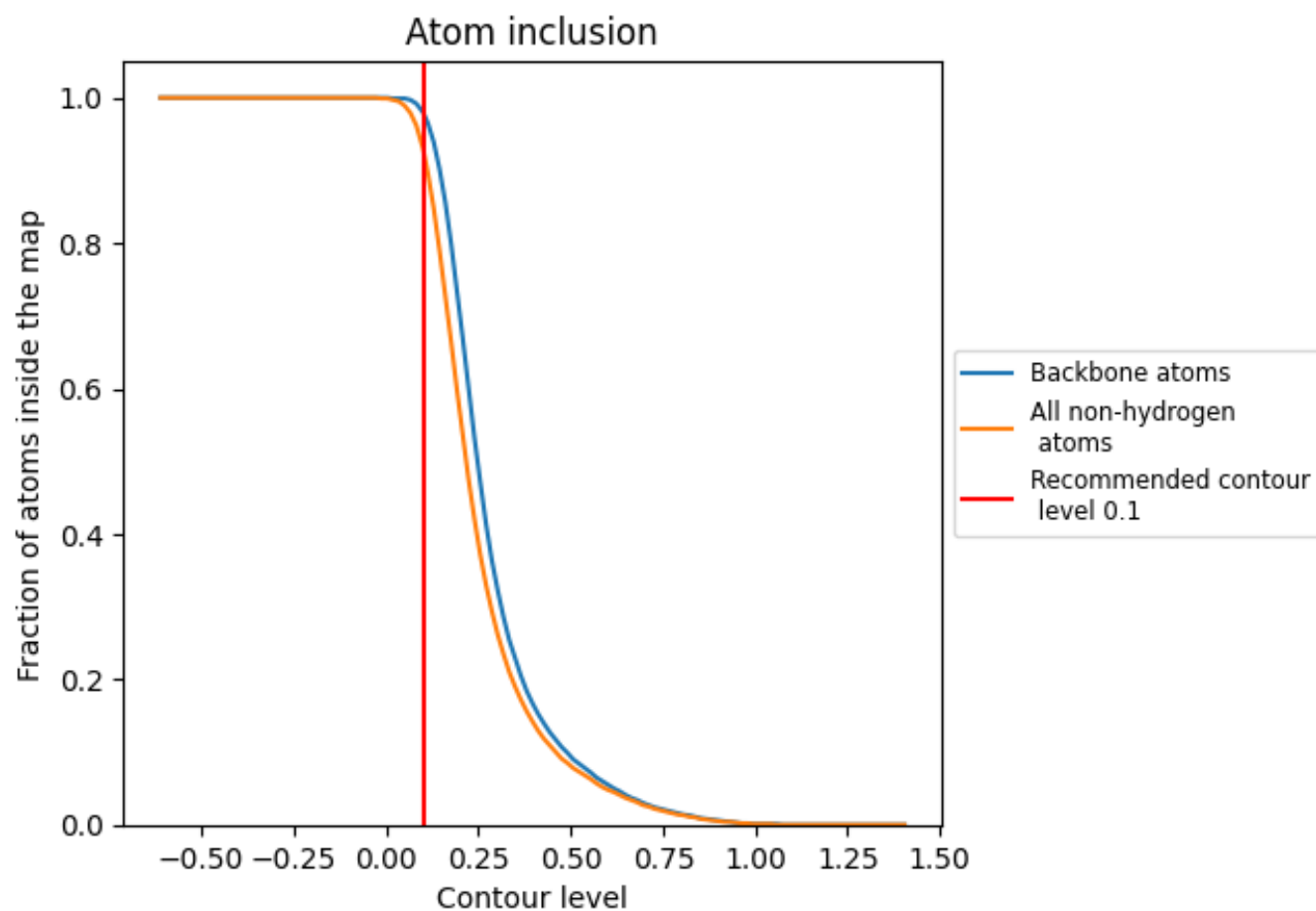
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9300	 0.3650
A	 0.9150	 0.3280
B	 0.9370	 0.3980
C	 0.9800	 0.3050
D	 0.9200	 0.2760
E	 0.9700	 0.3010
F	 0.9170	 0.3260
J	 0.8700	 0.3290
M	 0.9400	 0.4520
a	 0.8740	 0.2280
b	 0.8760	 0.2060
c	 0.8870	 0.2730
d	 0.9070	 0.2940
e	 0.9270	 0.3610
f	 0.9430	 0.4350
g	 0.9730	 0.5340
h	 0.9770	 0.5390
i	 0.9650	 0.4940
j	 0.9360	 0.3740
k	 0.9110	 0.2750
l	 0.9430	 0.2730
m	 0.9470	 0.3760
n	 0.9480	 0.4760
o	 0.9810	 0.5140
p	 0.9400	 0.3720

