



wwPDB EM Validation Summary Report ⓘ

Aug 8, 2026 – 09:32 PM JST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

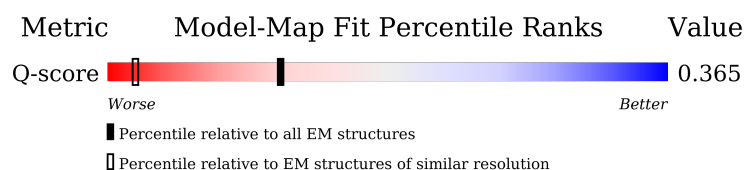
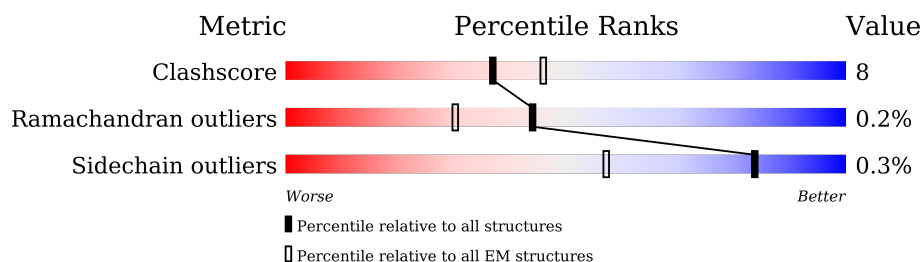
1 Overall quality at a glance

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.



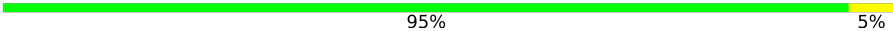
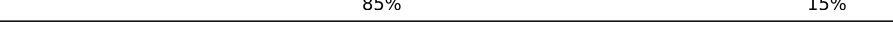
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8888 (2.13 - 3.13)

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 ≥ 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%

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		

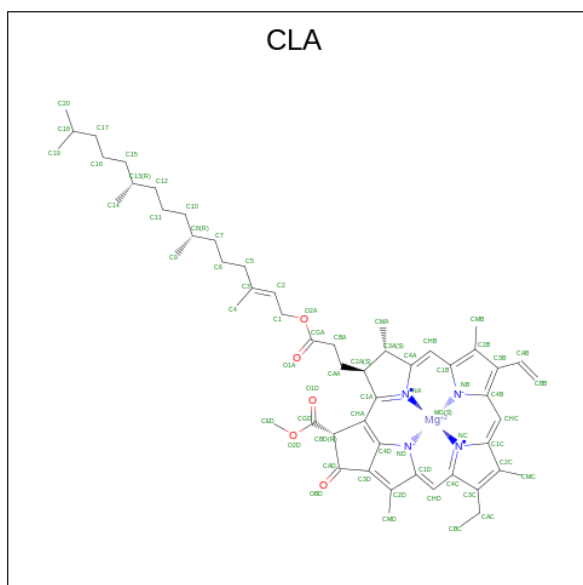
- Molecule 23 is a protein called Chloroplast light-harvesting complex I protein.

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 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 43	C 35	Mg 1	N 4	O 3	0
25	A	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	A	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	A	1	Total 48	C 38	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 63	C 53	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 49	C 39	Mg 1	N 4	O 5	0
25	A	1	Total 52	C 42	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 48	C 38	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 43	C 35	Mg 1	N 4	O 3	0
25	A	1	Total 51	C 41	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 55	C 45	Mg 1	N 4	O 5	0
25	A	1	Total 45	C 35	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
			48	38	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			49	40	1	4	4	
25	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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

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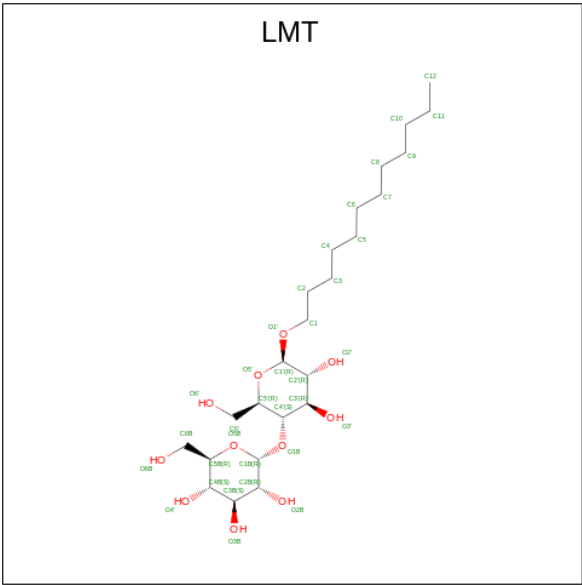
Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	n	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	n	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	n	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	o	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	o	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	o	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	o	1	Total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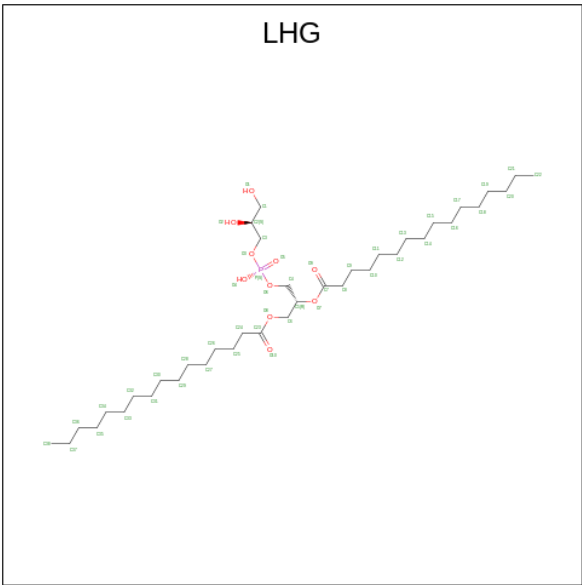
Mol	Chain	Residues	Atoms					AltConf
25	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

- Molecule 26 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



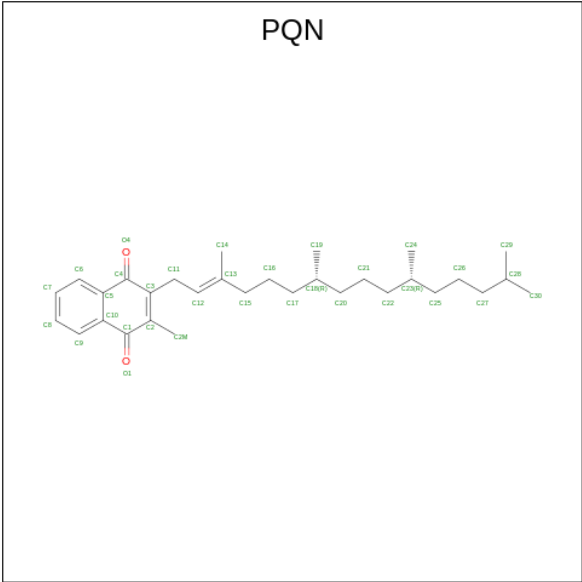
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			35	24	11	

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



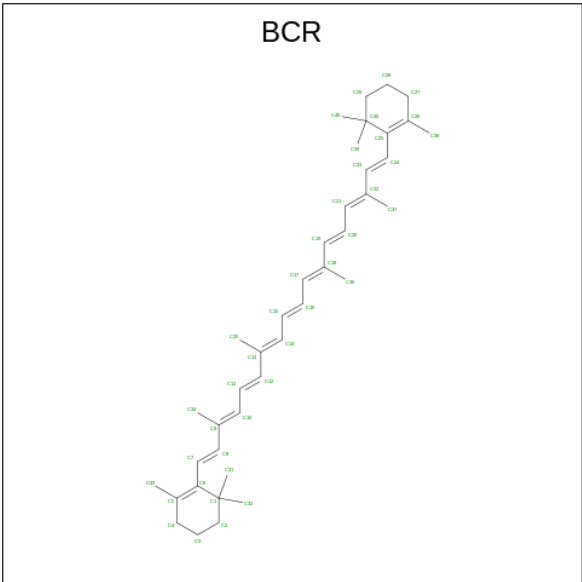
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	P	0
			38	27	10	1	
27	A	1	Total	C	O	P	0
			49	38	10	1	
27	a	1	Total	C	O	P	0
			26	15	10	1	
27	b	1	Total	C	O	P	0
			31	20	10	1	
27	c	1	Total	C	O	P	0
			30	19	10	1	
27	d	1	Total	C	O	P	0
			29	18	10	1	
27	h	1	Total	C	O	P	0
			30	19	10	1	
27	h	1	Total	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: C₃₁H₄₆O₂).



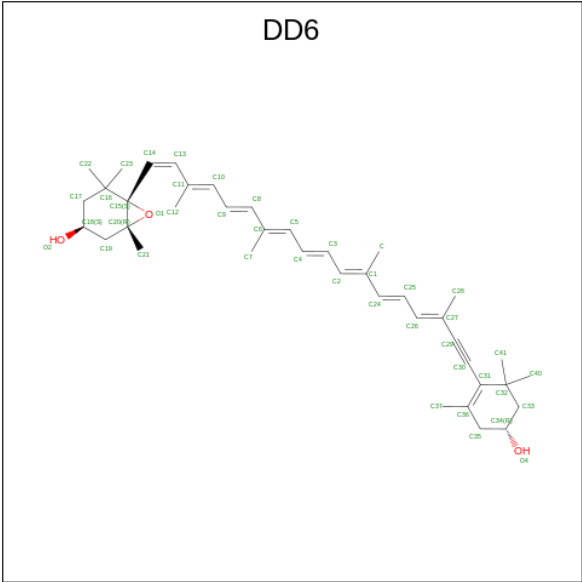
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			33	31	2	
28	B	1	Total	C	O	0
			33	31	2	
28	B	1	Total	C	O	0
			27	25	2	
28	F	1	Total	C	O	0
			26	24	2	

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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: C₄₀H₅₄O₃).



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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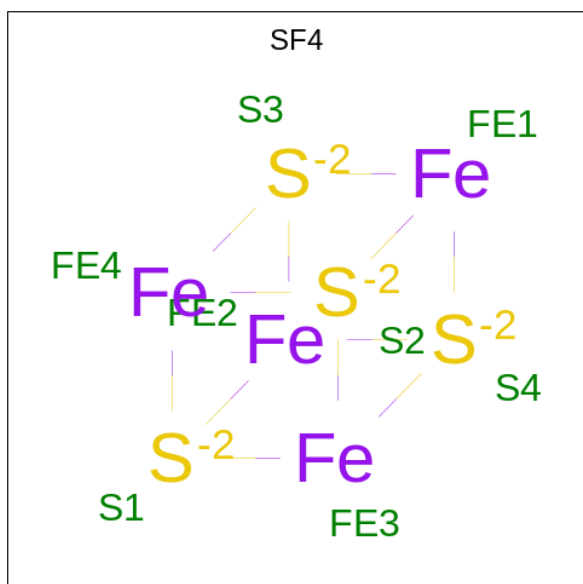
Mol	Chain	Residues	Atoms			AltConf
30	d	1	Total 43	C 40	O 3	0
30	e	1	Total 43	C 40	O 3	0
30	e	1	Total 43	C 40	O 3	0
30	e	1	Total 43	C 40	O 3	0
30	h	1	Total 43	C 40	O 3	0
30	h	1	Total 43	C 40	O 3	0
30	i	1	Total 43	C 40	O 3	0
30	i	1	Total 43	C 40	O 3	0
30	i	1	Total 43	C 40	O 3	0
30	j	1	Total 43	C 40	O 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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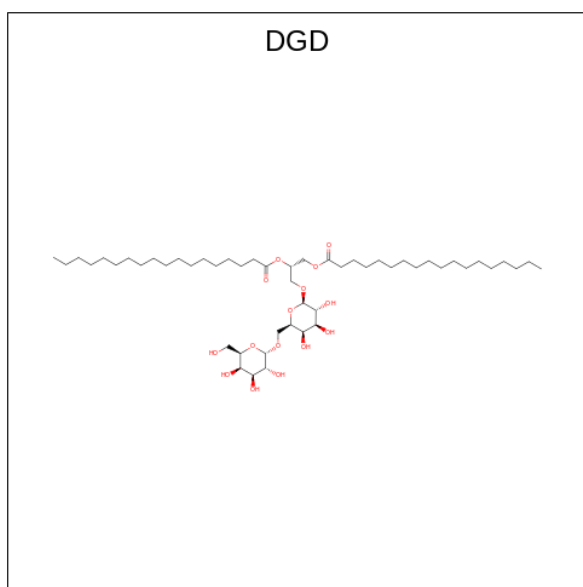
Mol	Chain	Residues	Atoms			AltConf
30	n	1	Total	C	O	0
			43	40	3	
30	n	1	Total	C	O	0
			43	40	3	
30	n	1	Total	C	O	0
			43	40	3	
30	o	1	Total	C	O	0
			43	40	3	
30	o	1	Total	C	O	0
			43	40	3	
30	p	1	Total	C	O	0
			43	40	3	

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



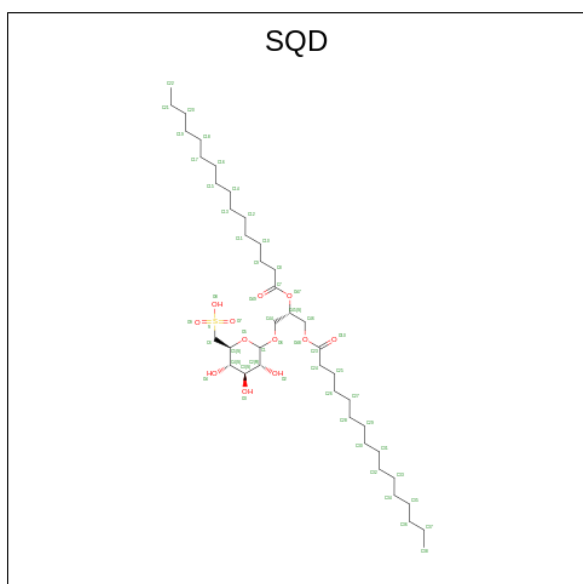
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	Fe	S	0
			8	4	4	
31	C	1	Total	Fe	S	0
			8	4	4	
31	C	1	Total	Fe	S	0
			8	4	4	

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



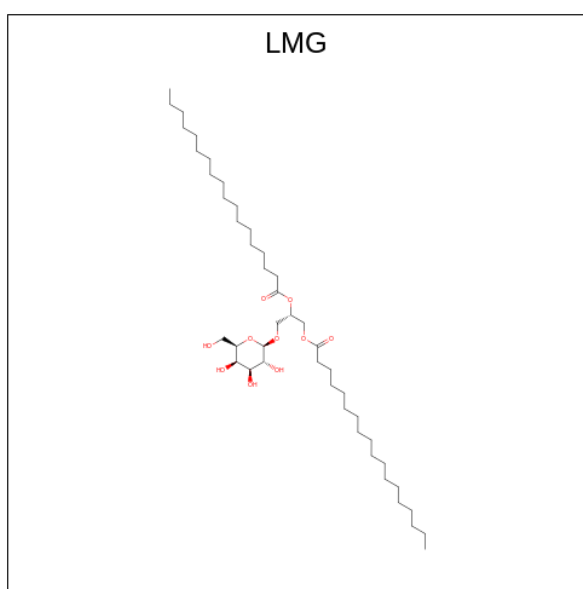
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	B	1	54	39	15	0
32	b	1	48	33	15	0
32	e	1	36	21	15	0

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



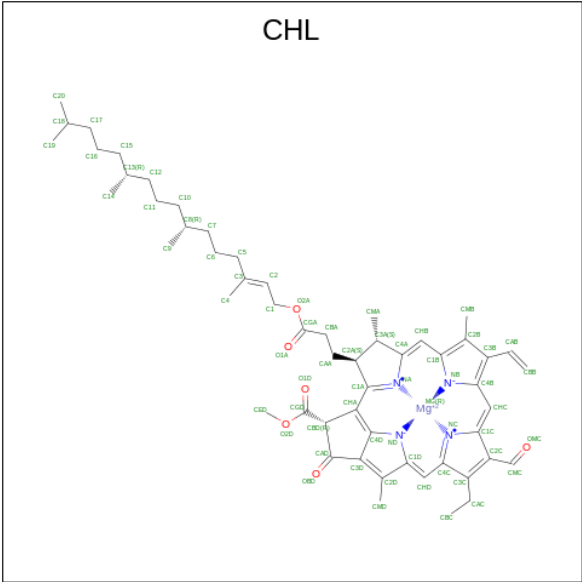
Mol	Chain	Residues	Atoms				AltConf
33	D	1	Total	C	O	S	0
			36	23	12	1	
33	F	1	Total	C	O	S	0
			39	26	12	1	
33	J	1	Total	C	O	S	0
			27	14	12	1	
33	g	1	Total	C	O	S	0
			32	19	12	1	

- 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: $C_{55}H_{70}MgN_4O_6$).

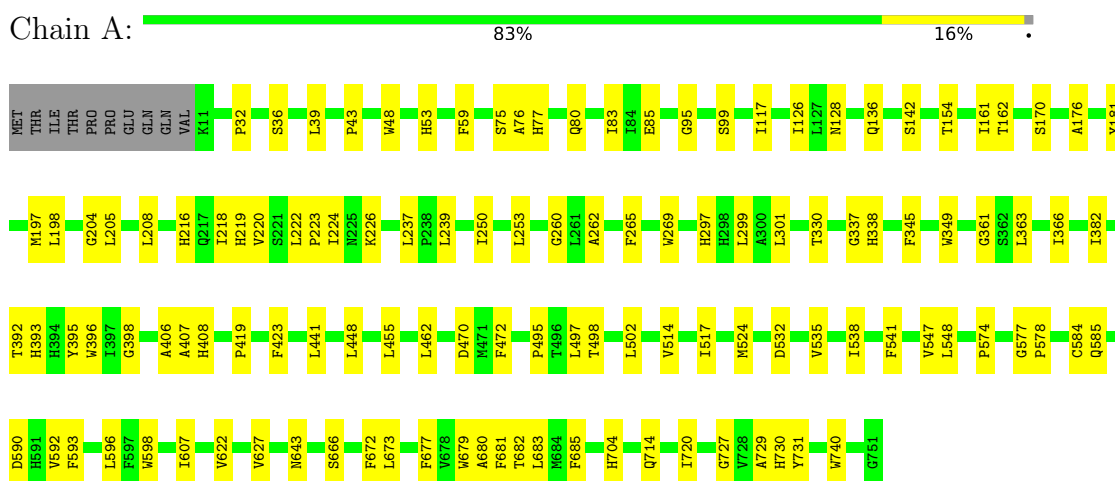


Mol	Chain	Residues	Atoms					AltConf
35	c	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
35	d	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	e	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

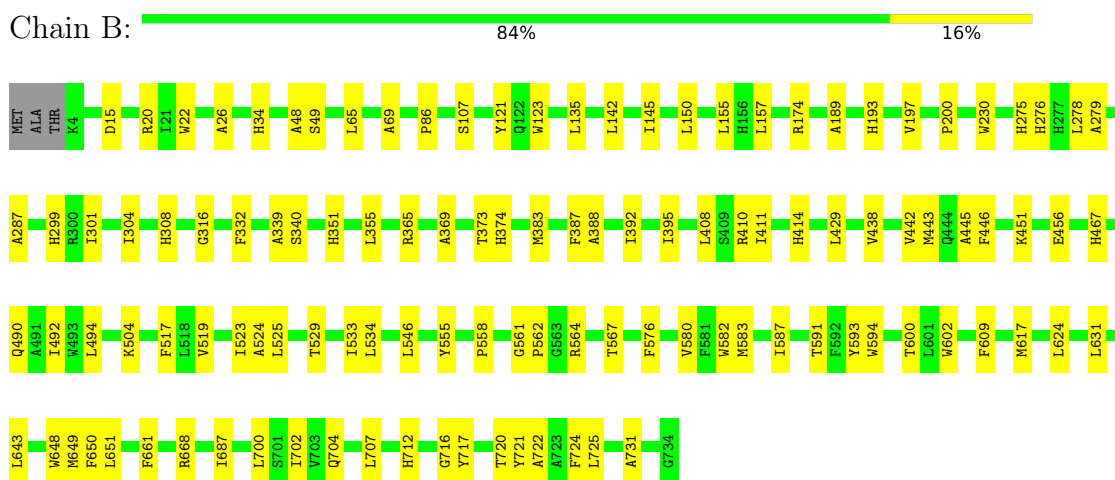
3 Residue-property plots

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.

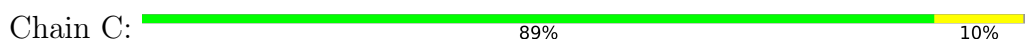
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



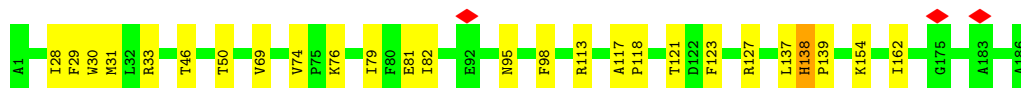
- Molecule 3: Photosystem I iron-sulfur center





- 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%



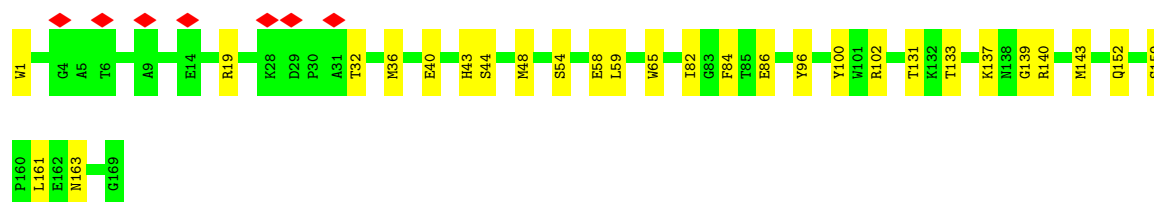
- Molecule 9: Chloroplast light-harvesting complex I protein

Chain a: 90% 10%



- Molecule 10: Chloroplast light-harvesting complex I protein

Chain b: 83% 17%



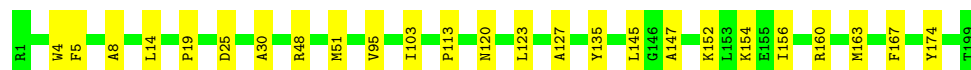
- Molecule 11: LHCE 3



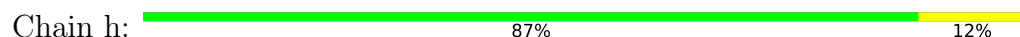
- Molecule 12: Light harvesting chlorophyll a /b binding protein of PSII



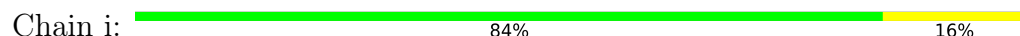
- Molecule 13: Chloroplast light-harvesting complex II protein



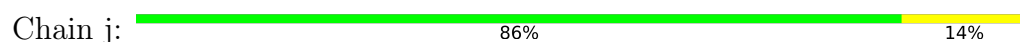
- Molecule 14: LHCE 8



- Molecule 15: LHCE 9



- Molecule 16: Chloroplast light-harvesting complex I protein



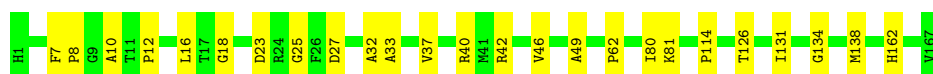
- Molecule 17: Chloroplast light-harvesting complex I protein

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%



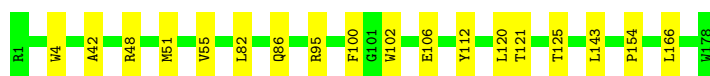
- Molecule 20: Chloroplast light-harvesting complex I protein, Lhca7_2

Chain f:  84% 16%



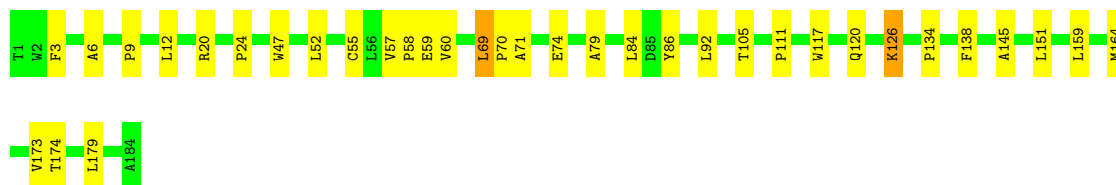
- Molecule 21: Chloroplast light-harvesting complex I protein

Chain g:  90% 10%



- Molecule 22: Chloroplast light-harvesting complex II protein

Chain n:  81% 18%

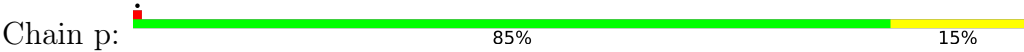


- Molecule 23: Chloroplast light-harvesting complex I protein

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, SQD, LHG, PQN, LMG, DGD, BCR, CHL, CLA, DD6, LMT

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	$\# Z > 2$
34	LMG	k	201	-	36,36,55	0.96	1 (2%)	44,44,63	1.12	3 (6%)
25	CLA	n	211	22	46,50,73	1.43	8 (17%)	55,85,113	1.74	6 (10%)
25	CLA	i	204	15	47,51,73	1.40	8 (17%)	56,86,113	1.75	8 (14%)
30	DD6	n	212	-	39,45,45	1.29	4 (10%)	52,67,67	2.54	16 (30%)
25	CLA	o	601	23	45,49,73	1.48	9 (20%)	54,84,113	1.76	11 (20%)
25	CLA	A	806	1	49,53,73	1.41	8 (16%)	59,89,113	1.85	8 (13%)
25	CLA	b	209	10	49,53,73	1.41	8 (16%)	59,89,113	1.82	10 (16%)
25	CLA	e	213	13	59,63,73	1.30	7 (11%)	71,101,113	1.73	11 (15%)
25	CLA	b	207	-	49,53,73	1.42	8 (16%)	59,89,113	1.85	8 (13%)
25	CLA	b	203	-	46,50,73	1.42	7 (15%)	55,85,113	1.87	7 (12%)
25	CLA	g	215	21	49,53,73	1.42	7 (14%)	59,89,113	1.79	8 (13%)
25	CLA	e	217	13	46,50,73	1.39	7 (15%)	55,85,113	1.84	6 (10%)
25	CLA	B	842	2	57,61,73	1.35	8 (14%)	68,98,113	1.67	11 (16%)
25	CLA	d	315	12	46,50,73	1.41	8 (17%)	55,85,113	1.85	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DD6	b	214	-	39,45,45	1.34	4 (10%)	52,67,67	2.25	16 (30%)
25	CLA	c	309	11	64,68,73	1.28	8 (12%)	77,107,113	1.75	10 (12%)
30	DD6	d	319	-	39,45,45	1.32	4 (10%)	52,67,67	2.40	19 (36%)
30	DD6	l	614	-	39,45,45	1.41	5 (12%)	52,67,67	2.10	18 (34%)
25	CLA	A	802	-	67,71,73	1.25	6 (8%)	80,110,113	1.65	11 (13%)
25	CLA	B	822	2	64,68,73	1.27	8 (12%)	77,107,113	1.73	11 (14%)
25	CLA	j	205	16	46,50,73	1.42	8 (17%)	55,85,113	1.86	8 (14%)
25	CLA	h	209	14	58,62,73	1.32	7 (12%)	69,99,113	1.77	10 (14%)
25	CLA	a	206	-	49,53,73	1.42	8 (16%)	59,89,113	1.77	9 (15%)
33	SQD	g	202	-	31,32,54	1.85	7 (22%)	40,43,65	1.58	6 (15%)
25	CLA	i	206	-	69,73,73	1.23	8 (11%)	83,113,113	1.68	11 (13%)
25	CLA	g	204	21	57,61,73	1.34	7 (12%)	68,98,113	1.71	9 (13%)
25	CLA	A	851	1	49,53,73	1.40	8 (16%)	59,89,113	1.84	9 (15%)
25	CLA	n	205	-	46,50,73	1.41	7 (15%)	55,85,113	1.84	6 (10%)
30	DD6	J	104	-	39,45,45	1.42	4 (10%)	52,67,67	2.22	15 (28%)
25	CLA	c	313	11	57,61,73	1.34	8 (14%)	68,98,113	1.74	10 (14%)
30	DD6	c	316	-	39,45,45	1.46	5 (12%)	52,67,67	2.14	18 (34%)
25	CLA	h	207	-	52,56,73	1.39	8 (15%)	62,92,113	1.84	7 (11%)
25	CLA	n	204	22	46,50,73	1.42	7 (15%)	55,85,113	1.83	9 (16%)
30	DD6	d	318	-	39,45,45	1.47	5 (12%)	52,67,67	2.19	16 (30%)
33	SQD	D	200	-	35,36,54	1.75	7 (20%)	44,47,65	1.75	10 (22%)
25	CLA	A	847	1	47,51,73	1.39	6 (12%)	56,86,113	1.72	6 (10%)
25	CLA	A	829	1	62,66,73	1.30	7 (11%)	74,104,113	1.70	10 (13%)
30	DD6	a	214	-	39,45,45	1.38	4 (10%)	52,67,67	2.22	15 (28%)
25	CLA	B	826	2	47,51,73	1.39	7 (14%)	56,86,113	1.83	7 (12%)
25	CLA	B	838	2	65,69,73	1.28	8 (12%)	78,108,113	1.75	12 (15%)
25	CLA	k	207	17	54,58,73	1.38	8 (14%)	65,95,113	1.77	8 (12%)
25	CLA	e	212	13	56,60,73	1.36	8 (14%)	67,97,113	1.79	9 (13%)
25	CLA	B	808	2	47,51,73	1.40	8 (17%)	56,86,113	1.83	6 (10%)
25	CLA	B	804	2	69,73,73	1.22	7 (10%)	83,113,113	1.70	8 (9%)
25	CLA	a	209	9	58,62,73	1.33	7 (12%)	69,99,113	1.83	10 (14%)
25	CLA	B	820	2	47,51,73	1.40	8 (17%)	56,86,113	1.82	6 (10%)
35	CHL	d	310	-	50,54,74	1.51	7 (14%)	56,90,114	2.03	13 (23%)
31	SF4	C	102	3	0,12,12	-	-	-	-	-
25	CLA	f	611	20	46,50,73	1.41	7 (15%)	55,85,113	1.78	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	o	606	23	49,53,73	1.41	7 (14%)	59,89,113	1.86	9 (15%)
28	PQN	A	834	-	34,34,34	1.02	3 (8%)	42,45,45	1.80	10 (23%)
25	CLA	i	210	15	47,51,73	1.40	8 (17%)	56,86,113	1.85	8 (14%)
25	CLA	b	210	10	46,50,73	1.41	7 (15%)	55,85,113	1.84	8 (14%)
30	DD6	n	214	-	39,45,45	1.63	7 (17%)	52,67,67	1.72	10 (19%)
25	CLA	m	205	-	47,51,73	1.41	8 (17%)	56,86,113	1.93	6 (10%)
25	CLA	o	605	-	47,51,73	1.40	8 (17%)	56,86,113	1.81	8 (14%)
25	CLA	o	603	23	47,51,73	1.46	8 (17%)	56,86,113	1.81	7 (12%)
29	BCR	A	837	-	41,41,41	1.65	10 (24%)	56,56,56	1.50	12 (21%)
25	CLA	g	212	21	59,63,73	1.33	8 (13%)	71,101,113	1.78	11 (15%)
25	CLA	B	845	2	69,73,73	1.23	7 (10%)	83,113,113	1.71	11 (13%)
25	CLA	a	205	9	57,61,73	1.35	8 (14%)	68,98,113	1.77	11 (16%)
27	LHG	m	201	-	31,31,48	1.73	2 (6%)	34,37,54	1.34	5 (14%)
27	LHG	b	201	-	30,30,48	1.77	2 (6%)	33,36,54	1.35	5 (15%)
27	LHG	d	302	25	28,28,48	1.76	2 (7%)	31,34,54	1.33	5 (16%)
25	CLA	o	610	23	47,51,73	1.43	7 (14%)	56,86,113	1.83	8 (14%)
25	CLA	p	607	24	49,53,73	1.45	8 (16%)	59,89,113	1.73	8 (13%)
29	BCR	B	801	-	41,41,41	0.71	0	56,56,56	1.24	7 (12%)
25	CLA	l	610	18	52,56,73	1.38	7 (13%)	62,92,113	1.76	9 (14%)
25	CLA	k	211	17	56,60,73	1.35	8 (14%)	67,97,113	1.82	11 (16%)
25	CLA	h	204	14	59,63,73	1.35	8 (13%)	71,101,113	1.75	11 (15%)
28	PQN	F	205	-	27,27,34	1.04	2 (7%)	33,36,45	1.99	9 (27%)
25	CLA	p	605	-	46,50,73	1.42	8 (17%)	55,85,113	1.84	8 (14%)
34	LMG	e	202	-	52,52,55	0.81	2 (3%)	60,60,63	1.07	3 (5%)
25	CLA	B	841	2	63,67,73	1.30	8 (12%)	75,105,113	1.76	10 (13%)
30	DD6	J	105	-	39,45,45	1.54	8 (20%)	52,67,67	1.53	9 (17%)
25	CLA	n	207	-	45,49,73	1.46	9 (20%)	54,84,113	1.89	11 (20%)
29	BCR	B	831	-	41,41,41	1.66	8 (19%)	56,56,56	1.42	10 (17%)
25	CLA	g	209	21	59,63,73	1.32	7 (11%)	71,101,113	1.71	9 (12%)
25	CLA	g	210	27	46,50,73	1.41	7 (15%)	55,85,113	1.88	8 (14%)
25	CLA	c	304	11	57,61,73	1.34	8 (14%)	68,98,113	1.77	11 (16%)
29	BCR	J	101	-	41,41,41	1.71	8 (19%)	56,56,56	1.58	11 (19%)
25	CLA	A	846	1	69,73,73	1.22	8 (11%)	83,113,113	1.71	13 (15%)
27	LHG	A	835	-	48,48,48	1.35	2 (4%)	51,54,54	1.18	5 (9%)
32	DGD	b	202	-	49,49,67	1.23	6 (12%)	63,63,81	1.08	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	j	213	16	46,50,73	1.41	8 (17%)	55,85,113	1.85	9 (16%)
25	CLA	g	203	21	46,50,73	1.41	8 (17%)	55,85,113	1.82	8 (14%)
25	CLA	c	305	-	52,56,73	1.38	8 (15%)	62,92,113	1.81	10 (16%)
35	CHL	d	309	-	47,51,74	1.41	5 (10%)	52,86,114	2.09	11 (21%)
25	CLA	j	207	-	51,55,73	1.40	8 (15%)	61,91,113	1.89	8 (13%)
25	CLA	d	312	12	63,67,73	1.29	7 (11%)	75,105,113	1.77	9 (12%)
25	CLA	d	303	12	54,58,73	1.38	8 (14%)	65,95,113	1.90	11 (16%)
27	LHG	a	201	25	25,25,48	1.86	2 (8%)	28,31,54	1.42	5 (17%)
25	CLA	j	210	27	54,58,73	1.38	8 (14%)	65,95,113	1.80	8 (12%)
25	CLA	c	308	-	54,58,73	1.38	8 (14%)	65,95,113	1.73	9 (13%)
25	CLA	F	202	6	49,53,73	1.41	7 (14%)	59,89,113	1.78	8 (13%)
25	CLA	m	206	-	46,50,73	1.42	8 (17%)	55,85,113	1.85	4 (7%)
25	CLA	B	814	2	63,67,73	1.30	8 (12%)	75,105,113	1.75	11 (14%)
25	CLA	B	839	-	64,68,73	1.29	8 (12%)	77,107,113	1.77	11 (14%)
25	CLA	i	213	15	54,58,73	1.38	8 (14%)	65,95,113	1.81	9 (13%)
25	CLA	o	602	23	51,55,73	1.39	7 (13%)	61,91,113	1.83	9 (14%)
25	CLA	B	834	2	59,63,73	1.33	7 (11%)	71,101,113	1.75	10 (14%)
25	CLA	i	205	-	47,51,73	1.40	8 (17%)	56,86,113	1.78	5 (8%)
25	CLA	k	205	17	69,73,73	1.23	8 (11%)	83,113,113	1.64	10 (12%)
30	DD6	m	212	-	39,45,45	1.32	4 (10%)	52,67,67	2.14	14 (26%)
25	CLA	c	302	11	46,50,73	1.40	8 (17%)	55,85,113	1.76	8 (14%)
25	CLA	p	604	-	47,51,73	1.43	8 (17%)	56,86,113	1.88	8 (14%)
25	CLA	A	810	1	69,73,73	1.21	7 (10%)	83,113,113	1.72	12 (14%)
25	CLA	h	215	14	47,51,73	1.40	8 (17%)	56,86,113	1.79	7 (12%)
25	CLA	j	206	-	61,65,73	1.32	8 (13%)	73,103,113	1.77	10 (13%)
28	PQN	B	835	-	28,28,34	1.04	2 (7%)	34,37,45	2.00	10 (29%)
25	CLA	B	802	2	69,73,73	1.20	8 (11%)	83,113,113	1.58	12 (14%)
25	CLA	e	206	13	49,53,73	1.42	8 (16%)	59,89,113	1.84	9 (15%)
34	LMG	a	202	-	43,43,55	0.89	1 (2%)	51,51,63	1.18	2 (3%)
25	CLA	j	208	16	54,58,73	1.39	8 (14%)	65,95,113	1.83	9 (13%)
25	CLA	m	211	19	46,50,73	1.42	7 (15%)	55,85,113	1.82	7 (12%)
25	CLA	m	204	19	58,62,73	1.34	8 (13%)	69,99,113	1.73	12 (17%)
25	CLA	e	208	13	46,50,73	1.42	8 (17%)	55,85,113	1.91	7 (12%)
30	DD6	p	610	-	39,45,45	1.29	4 (10%)	52,67,67	2.28	17 (32%)
25	CLA	l	608	-	47,51,73	1.40	7 (14%)	56,86,113	1.86	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	o	608	23	47,50,73	1.55	10 (21%)	51,84,113	2.04	9 (17%)
25	CLA	A	833	1	69,73,73	1.21	7 (10%)	83,113,113	1.54	13 (15%)
30	DD6	n	213	-	39,45,45	1.52	8 (20%)	52,67,67	1.48	9 (17%)
25	CLA	A	848	1	55,59,73	1.35	7 (12%)	66,96,113	1.85	11 (16%)
25	CLA	c	306	-	47,51,73	1.41	8 (17%)	56,86,113	1.82	8 (14%)
25	CLA	l	604	-	47,51,73	1.41	8 (17%)	56,86,113	1.74	7 (12%)
25	CLA	k	206	-	54,58,73	1.38	8 (14%)	65,95,113	1.84	10 (15%)
25	CLA	g	214	21	46,50,73	1.42	8 (17%)	55,85,113	1.88	7 (12%)
25	CLA	i	208	15	59,63,73	1.31	6 (10%)	71,101,113	1.73	10 (14%)
25	CLA	B	843	2	67,71,73	1.23	7 (10%)	80,110,113	1.61	11 (13%)
27	LHG	h	201	-	29,29,48	1.74	2 (6%)	32,35,54	1.10	2 (6%)
25	CLA	A	817	1	60,64,73	1.31	9 (15%)	72,102,113	1.71	9 (12%)
30	DD6	i	214	-	39,45,45	1.42	5 (12%)	52,67,67	2.13	14 (26%)
25	CLA	n	202	22	59,63,73	1.35	8 (13%)	71,101,113	1.76	9 (12%)
25	CLA	k	208	17	61,65,73	1.29	8 (13%)	73,103,113	1.71	11 (15%)
25	CLA	l	602	18	63,67,73	1.30	8 (12%)	75,105,113	1.69	12 (16%)
25	CLA	c	311	27	47,51,73	1.41	7 (14%)	56,86,113	1.79	8 (14%)
35	CHL	c	307	-	53,57,74	1.44	6 (11%)	59,93,114	2.10	14 (23%)
25	CLA	j	211	16	59,63,73	1.33	8 (13%)	71,101,113	1.74	11 (15%)
25	CLA	f	604	-	46,50,73	1.43	7 (15%)	55,85,113	1.83	6 (10%)
25	CLA	k	209	-	46,50,73	1.41	7 (15%)	55,85,113	1.83	7 (12%)
25	CLA	l	612	-	46,50,73	1.43	7 (15%)	55,85,113	2.00	6 (10%)
25	CLA	p	608	24	47,51,73	1.40	7 (14%)	56,86,113	1.70	8 (14%)
25	CLA	h	210	27	47,51,73	1.39	8 (17%)	56,86,113	1.81	8 (14%)
25	CLA	p	601	-	46,50,73	1.41	7 (15%)	55,85,113	1.71	9 (16%)
27	LHG	j	202	25	36,36,48	1.55	2 (5%)	39,42,54	1.28	5 (12%)
25	CLA	A	842	1	53,57,73	1.37	7 (13%)	62,93,113	1.83	8 (12%)
25	CLA	A	830	1	56,60,73	1.36	7 (12%)	67,97,113	1.73	13 (19%)
25	CLA	i	211	15	63,67,73	1.29	8 (12%)	75,105,113	1.75	11 (14%)
25	CLA	J	103	7	54,58,73	1.39	8 (14%)	65,95,113	1.80	11 (16%)
25	CLA	a	207	-	57,61,73	1.34	8 (14%)	68,98,113	1.74	11 (16%)
25	CLA	j	215	16	54,58,73	1.39	8 (14%)	65,95,113	1.84	9 (13%)
25	CLA	A	809	1	69,73,73	1.22	7 (10%)	83,113,113	1.68	10 (12%)
25	CLA	l	605	-	47,51,73	1.40	8 (17%)	56,86,113	1.82	6 (10%)
25	CLA	A	820	1	61,65,73	1.30	8 (13%)	73,103,113	1.79	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DD6	o	612	-	39,45,45	1.34	4 (10%)	52,67,67	2.13	16 (30%)
35	CHL	d	307	12	55,59,74	1.47	7 (12%)	62,96,114	2.07	16 (25%)
25	CLA	f	609	20	46,50,73	1.46	7 (15%)	55,85,113	1.63	7 (12%)
25	CLA	a	208	9	54,58,73	1.39	8 (14%)	65,95,113	1.82	9 (13%)
25	CLA	B	825	-	47,51,73	1.39	8 (17%)	56,86,113	1.66	7 (12%)
27	LHG	g	201	25	34,34,48	1.60	2 (5%)	37,40,54	1.31	5 (13%)
35	CHL	d	308	-	50,54,74	1.51	7 (14%)	56,90,114	2.11	11 (19%)
34	LMG	j	201	-	44,44,55	0.86	1 (2%)	52,52,63	1.08	2 (3%)
25	CLA	A	857	-	57,61,73	1.35	8 (14%)	68,98,113	1.72	9 (13%)
25	CLA	A	852	1	52,56,73	1.38	7 (13%)	62,92,113	1.93	10 (16%)
25	CLA	i	202	15	57,61,73	1.35	8 (14%)	68,98,113	1.76	10 (14%)
25	CLA	m	210	19	47,51,73	1.40	8 (17%)	56,86,113	1.84	8 (14%)
27	LHG	h	202	25	30,30,48	1.69	2 (6%)	33,36,54	1.38	5 (15%)
25	CLA	A	824	1	62,66,73	1.29	7 (11%)	74,104,113	1.72	10 (13%)
25	CLA	o	609	23	46,50,73	1.41	7 (15%)	55,85,113	1.86	6 (10%)
25	CLA	h	212	14	57,61,73	1.34	7 (12%)	68,98,113	1.79	12 (17%)
25	CLA	m	209	-	47,51,73	1.40	7 (14%)	56,86,113	1.77	7 (12%)
25	CLA	e	211	-	52,56,73	1.37	8 (15%)	62,92,113	1.75	8 (12%)
25	CLA	A	850	1	59,63,73	1.31	7 (11%)	71,101,113	1.66	10 (14%)
25	CLA	B	806	2	46,50,73	1.41	8 (17%)	55,85,113	1.84	7 (12%)
25	CLA	e	201	-	57,61,73	1.36	8 (14%)	68,98,113	1.84	9 (13%)
25	CLA	A	843	1	56,60,73	1.37	7 (12%)	67,97,113	1.86	10 (14%)
25	CLA	A	849	1	54,58,73	1.38	7 (12%)	65,95,113	1.76	10 (15%)
25	CLA	o	607	23	45,49,73	1.46	7 (15%)	54,84,113	1.79	10 (18%)
30	DD6	f	614	-	39,45,45	1.28	4 (10%)	52,67,67	2.47	19 (36%)
25	CLA	m	207	19	54,58,73	1.39	8 (14%)	65,95,113	1.82	9 (13%)
25	CLA	n	210	22	46,50,73	1.42	8 (17%)	55,85,113	1.92	7 (12%)
25	CLA	A	827	1	47,51,73	1.40	8 (17%)	56,86,113	1.85	9 (16%)
25	CLA	l	603	18	47,51,73	1.41	8 (17%)	56,86,113	1.89	8 (14%)
25	CLA	b	205	10	47,51,73	1.40	8 (17%)	56,86,113	1.86	8 (14%)
25	CLA	h	203	14	54,58,73	1.39	8 (14%)	65,95,113	1.81	11 (16%)
25	CLA	h	214	14	46,50,73	1.41	8 (17%)	55,85,113	1.91	7 (12%)
33	SQD	J	102	-	26,27,54	1.81	7 (26%)	35,38,65	1.69	8 (22%)
25	CLA	b	211	-	46,50,73	1.41	7 (15%)	55,85,113	1.86	6 (10%)
25	CLA	f	612	20	47,51,73	1.42	7 (14%)	56,86,113	1.84	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LHG	A	805	25	37,37,48	1.49	2 (5%)	40,43,54	1.24	5 (12%)
25	CLA	e	205	13	69,73,73	1.23	8 (11%)	83,113,113	1.60	11 (13%)
25	CLA	l	609	18	47,51,73	1.40	8 (17%)	56,86,113	1.85	8 (14%)
25	CLA	A	845	-	52,56,73	1.38	8 (15%)	62,92,113	1.77	10 (16%)
25	CLA	f	601	20	46,50,73	1.43	7 (15%)	55,85,113	1.77	7 (12%)
25	CLA	h	213	14	47,51,73	1.39	8 (17%)	56,86,113	1.74	7 (12%)
25	CLA	A	807	-	69,73,73	1.21	8 (11%)	83,113,113	1.67	10 (12%)
25	CLA	d	305	12	46,50,73	1.39	8 (17%)	55,85,113	1.92	7 (12%)
25	CLA	d	304	12	61,65,73	1.30	7 (11%)	73,103,113	1.75	11 (15%)
25	CLA	B	811	2	67,71,73	1.23	8 (11%)	80,110,113	1.74	10 (12%)
35	CHL	e	209	-	50,54,74	1.51	7 (14%)	56,90,114	2.13	10 (17%)
25	CLA	a	204	9	64,68,73	1.27	6 (9%)	77,107,113	1.61	15 (19%)
25	CLA	i	207	15	47,51,73	1.39	8 (17%)	56,86,113	1.87	4 (7%)
25	CLA	g	213	21	46,50,73	1.41	7 (15%)	55,85,113	1.89	8 (14%)
25	CLA	b	213	10	46,50,73	1.42	8 (17%)	55,85,113	1.85	8 (14%)
25	CLA	j	204	16	59,63,73	1.29	6 (10%)	71,101,113	1.78	11 (15%)
28	PQN	B	827	-	34,34,34	1.13	4 (11%)	42,45,45	1.87	10 (23%)
25	CLA	m	208	19	46,50,73	1.40	7 (15%)	55,85,113	1.76	7 (12%)
25	CLA	B	821	2	64,68,73	1.28	8 (12%)	77,107,113	1.72	12 (15%)
25	CLA	A	815	1	62,66,73	1.28	7 (11%)	74,104,113	1.86	11 (14%)
25	CLA	p	602	24	47,51,73	1.44	9 (19%)	56,86,113	1.96	9 (16%)
25	CLA	p	609	24	47,51,73	1.43	7 (14%)	56,86,113	1.90	9 (16%)
25	CLA	c	312	11	47,51,73	1.40	8 (17%)	56,86,113	1.84	9 (16%)
25	CLA	B	810	2	47,51,73	1.40	8 (17%)	56,86,113	1.81	7 (12%)
25	CLA	c	303	11	63,67,73	1.28	8 (12%)	75,105,113	1.69	13 (17%)
30	DD6	m	213	-	39,45,45	1.36	5 (12%)	52,67,67	2.12	17 (32%)
25	CLA	c	314	11	46,50,73	1.42	8 (17%)	55,85,113	1.79	8 (14%)
25	CLA	A	813	1	62,66,73	1.29	7 (11%)	74,104,113	1.71	11 (14%)
25	CLA	h	211	14	62,66,73	1.30	8 (12%)	74,104,113	1.73	9 (12%)
25	CLA	A	853	27	57,61,73	1.34	8 (14%)	68,98,113	1.88	13 (19%)
25	CLA	k	210	17	47,51,73	1.40	8 (17%)	56,86,113	1.83	8 (14%)
25	CLA	n	209	22	45,49,73	1.47	7 (15%)	54,84,113	1.79	10 (18%)
30	DD6	h	217	-	39,45,45	1.38	4 (10%)	52,67,67	2.10	14 (26%)
25	CLA	A	832	1	69,73,73	1.22	8 (11%)	83,113,113	1.59	11 (13%)
26	LMT	A	803	-	36,36,36	0.55	0	47,47,47	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	l	606	18	64,68,73	1.27	8 (12%)	77,107,113	1.75	10 (12%)
29	BCR	B	829	-	41,41,41	0.75	0	56,56,56	1.08	4 (7%)
25	CLA	A	844	1	64,68,73	1.29	8 (12%)	77,107,113	1.77	13 (16%)
25	CLA	d	306	-	56,60,73	1.37	8 (14%)	67,97,113	1.76	8 (11%)
30	DD6	j	217	-	39,45,45	1.42	5 (12%)	52,67,67	2.15	15 (28%)
25	CLA	B	844	2	69,73,73	1.25	8 (11%)	83,113,113	1.73	15 (18%)
30	DD6	a	215	-	39,45,45	1.42	5 (12%)	52,67,67	2.10	16 (30%)
25	CLA	A	801	1	69,73,73	1.21	8 (11%)	83,113,113	1.75	15 (18%)
25	CLA	j	209	16	68,72,73	1.22	6 (8%)	81,111,113	1.59	11 (13%)
25	CLA	B	837	2	54,58,73	1.39	8 (14%)	65,95,113	1.81	7 (10%)
32	DGD	e	203	-	37,37,67	1.23	1 (2%)	51,51,81	1.10	1 (1%)
29	BCR	B	832	-	41,41,41	1.67	8 (19%)	56,56,56	1.40	9 (16%)
25	CLA	e	207	-	54,58,73	1.38	8 (14%)	65,95,113	1.78	11 (16%)
30	DD6	i	215	-	39,45,45	1.46	5 (12%)	52,67,67	2.12	15 (28%)
29	BCR	B	833	-	41,41,41	0.80	1 (2%)	56,56,56	1.12	4 (7%)
25	CLA	B	803	-	59,63,73	1.32	6 (10%)	71,101,113	1.93	10 (14%)
25	CLA	l	607	18	58,62,73	1.33	6 (10%)	69,99,113	1.73	9 (13%)
25	CLA	A	818	1	69,73,73	1.23	8 (11%)	83,113,113	1.60	13 (15%)
25	CLA	B	809	2	46,50,73	1.40	7 (15%)	55,85,113	1.87	7 (12%)
25	CLA	B	819	2	69,73,73	1.23	8 (11%)	83,113,113	1.54	9 (10%)
30	DD6	g	216	-	39,45,45	1.31	4 (10%)	52,67,67	2.28	16 (30%)
25	CLA	A	816	1	47,51,73	1.40	8 (17%)	56,86,113	1.80	6 (10%)
25	CLA	A	825	1	69,73,73	1.24	8 (11%)	83,113,113	1.61	11 (13%)
30	DD6	f	613	-	39,45,45	1.27	4 (10%)	52,67,67	2.31	15 (28%)
32	DGD	B	849	-	55,55,67	1.10	0	69,69,81	1.04	2 (2%)
25	CLA	A	840	-	67,71,73	1.24	8 (11%)	80,110,113	1.64	11 (13%)
25	CLA	B	846	2	54,58,73	1.37	7 (12%)	65,95,113	1.91	11 (16%)
25	CLA	B	805	2	69,73,73	1.21	7 (10%)	83,113,113	1.71	13 (15%)
25	CLA	g	205	21	46,50,73	1.44	7 (15%)	55,85,113	1.76	5 (9%)
25	CLA	B	823	2	64,68,73	1.27	6 (9%)	77,107,113	1.60	12 (15%)
25	CLA	A	821	-	68,72,73	1.24	8 (11%)	81,111,113	1.64	12 (14%)
25	CLA	d	301	12	45,49,73	1.45	8 (17%)	54,84,113	2.03	8 (14%)
25	CLA	h	205	14	47,51,73	1.39	8 (17%)	56,86,113	1.94	9 (16%)
25	CLA	d	311	12	53,57,73	1.37	8 (15%)	62,93,113	1.88	8 (12%)
25	CLA	k	212	17	46,50,73	1.41	7 (15%)	55,85,113	1.82	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	818	2	69,73,73	1.23	8 (11%)	83,113,113	1.63	11 (13%)
25	CLA	f	606	20	46,50,73	1.43	7 (15%)	55,85,113	1.82	8 (14%)
25	CLA	A	804	1	64,68,73	1.29	8 (12%)	77,107,113	1.75	10 (12%)
25	CLA	A	814	1	63,67,73	1.29	8 (12%)	75,105,113	1.77	12 (16%)
30	DD6	e	220	-	39,45,45	1.58	8 (20%)	52,67,67	1.69	9 (17%)
25	CLA	e	216	13	59,63,73	1.34	8 (13%)	71,101,113	1.72	9 (12%)
29	BCR	A	838	-	41,41,41	0.78	1 (2%)	56,56,56	1.06	4 (7%)
29	BCR	B	830	-	41,41,41	0.77	2 (4%)	56,56,56	1.01	3 (5%)
25	CLA	i	203	15	68,72,73	1.26	8 (11%)	81,111,113	1.67	12 (14%)
30	DD6	c	318	-	39,45,45	1.32	4 (10%)	52,67,67	2.38	19 (36%)
25	CLA	e	204	13	45,49,73	1.43	7 (15%)	54,84,113	1.86	9 (16%)
25	CLA	l	611	18	46,50,73	1.44	7 (15%)	55,85,113	1.91	8 (14%)
29	BCR	B	828	-	41,41,41	0.78	1 (2%)	56,56,56	1.18	6 (10%)
25	CLA	n	203	-	52,56,73	1.40	7 (13%)	62,92,113	1.81	9 (14%)
25	CLA	B	836	2	57,61,73	1.35	8 (14%)	68,98,113	1.75	10 (14%)
25	CLA	k	202	17	47,51,73	1.40	7 (14%)	56,86,113	1.79	8 (14%)
25	CLA	A	826	1	69,73,73	1.24	8 (11%)	83,113,113	1.74	9 (10%)
29	BCR	M	201	-	41,41,41	0.78	0	56,56,56	1.16	5 (8%)
30	DD6	k	216	-	39,45,45	1.36	4 (10%)	52,67,67	2.10	16 (30%)
30	DD6	h	216	-	39,45,45	1.39	4 (10%)	52,67,67	2.11	16 (30%)
25	CLA	m	202	19	46,50,73	1.43	7 (15%)	55,85,113	1.68	8 (14%)
25	CLA	e	215	13	47,51,73	1.41	8 (17%)	56,86,113	1.89	8 (14%)
25	CLA	k	214	17	54,58,73	1.38	7 (12%)	65,95,113	1.80	9 (13%)
25	CLA	i	212	15	46,50,73	1.41	7 (15%)	55,85,113	1.77	9 (16%)
25	CLA	B	824	2	69,73,73	1.23	8 (11%)	83,113,113	1.62	11 (13%)
30	DD6	c	317	-	39,45,45	1.42	5 (12%)	52,67,67	2.12	16 (30%)
25	CLA	a	203	9	54,58,73	1.39	7 (12%)	65,95,113	1.70	9 (13%)
25	CLA	c	315	11	51,55,73	1.37	8 (15%)	61,91,113	1.76	10 (16%)
25	CLA	h	208	14	54,58,73	1.38	8 (14%)	65,95,113	1.78	9 (13%)
30	DD6	k	215	-	39,45,45	1.37	4 (10%)	52,67,67	2.12	14 (26%)
25	CLA	d	313	27	49,53,73	1.42	8 (16%)	59,89,113	1.82	9 (15%)
25	CLA	B	807	2	69,73,73	1.22	7 (10%)	83,113,113	1.67	10 (12%)
25	CLA	j	212	16	66,70,73	1.24	6 (9%)	79,109,113	1.70	11 (13%)
25	CLA	n	201	22	63,67,73	1.28	6 (9%)	75,105,113	1.83	13 (17%)
25	CLA	A	828	1	47,51,73	1.40	8 (17%)	56,86,113	1.85	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	f	608	-	46,50,73	1.43	7 (15%)	55,85,113	1.93	7 (12%)
30	DD6	l	613	-	39,45,45	1.35	4 (10%)	52,67,67	2.14	16 (30%)
25	CLA	d	316	12	46,50,73	1.39	7 (15%)	55,85,113	1.79	7 (12%)
25	CLA	p	606	24	54,58,73	1.42	7 (12%)	65,95,113	1.79	8 (12%)
30	DD6	b	215	-	39,45,45	1.38	4 (10%)	52,67,67	2.13	16 (30%)
25	CLA	h	206	-	64,68,73	1.28	8 (12%)	77,107,113	1.73	9 (11%)
25	CLA	f	603	20	47,51,73	1.43	8 (17%)	56,86,113	1.84	7 (12%)
25	CLA	A	841	-	61,65,73	1.29	8 (13%)	73,103,113	1.71	10 (13%)
25	CLA	A	823	1	68,72,73	1.22	7 (10%)	81,111,113	1.81	8 (9%)
25	CLA	i	209	27	47,51,73	1.40	8 (17%)	56,86,113	1.88	7 (12%)
25	CLA	A	822	-	57,61,73	1.35	8 (14%)	68,98,113	1.76	10 (14%)
30	DD6	A	854	-	39,45,45	1.36	4 (10%)	52,67,67	2.35	17 (32%)
25	CLA	B	813	2	53,57,73	1.43	8 (15%)	63,93,113	1.74	11 (17%)
27	LHG	c	301	25	29,29,48	1.76	2 (6%)	32,35,54	1.37	5 (15%)
25	CLA	g	207	-	49,53,73	1.45	7 (14%)	59,89,113	1.86	7 (11%)
25	CLA	a	211	9	47,51,73	1.41	8 (17%)	56,86,113	1.87	6 (10%)
25	CLA	B	817	-	54,58,73	1.39	7 (12%)	65,95,113	1.74	9 (13%)
25	CLA	g	206	-	47,51,73	1.40	8 (17%)	56,86,113	1.72	6 (10%)
25	CLA	B	815	2	53,57,73	1.37	8 (15%)	62,93,113	1.74	10 (16%)
25	CLA	g	211	21	46,50,73	1.43	8 (17%)	55,85,113	1.89	6 (10%)
25	CLA	l	601	18	46,50,73	1.42	7 (15%)	55,85,113	1.76	6 (10%)
25	CLA	A	831	1	52,56,73	1.39	8 (15%)	62,92,113	1.81	9 (14%)
31	SF4	A	856	1,2	0,12,12	-	-	-	-	-
25	CLA	e	210	-	47,51,73	1.39	8 (17%)	56,86,113	1.89	7 (12%)
25	CLA	f	605	20	46,50,73	1.42	7 (15%)	55,85,113	1.93	7 (12%)
30	DD6	A	855	-	39,45,45	1.35	4 (10%)	52,67,67	2.35	20 (38%)
25	CLA	a	213	-	67,71,73	1.25	8 (11%)	80,110,113	1.72	11 (13%)
25	CLA	g	208	21	54,58,73	1.39	8 (14%)	65,95,113	1.78	8 (12%)
29	BCR	A	836	-	41,41,41	0.83	1 (2%)	56,56,56	1.10	4 (7%)
25	CLA	A	819	-	69,73,73	1.22	8 (11%)	83,113,113	1.59	13 (15%)
25	CLA	B	840	2	54,58,73	1.39	7 (12%)	65,95,113	1.65	10 (15%)
30	DD6	i	216	-	39,45,45	1.32	4 (10%)	52,67,67	2.17	16 (30%)
25	CLA	B	812	2	68,72,73	1.26	8 (11%)	81,111,113	1.70	10 (12%)
25	CLA	n	206	-	46,50,73	1.43	7 (15%)	55,85,113	1.82	6 (10%)
25	CLA	a	210	27	49,53,73	1.42	8 (16%)	59,89,113	1.84	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	808	1	64,68,73	1.26	8 (12%)	77,107,113	1.77	12 (15%)
25	CLA	b	204	10	57,61,73	1.36	8 (14%)	68,98,113	1.76	9 (13%)
25	CLA	m	203	19	64,68,73	1.28	7 (10%)	77,107,113	1.54	11 (14%)
25	CLA	d	314	12	46,50,73	1.41	8 (17%)	55,85,113	1.90	5 (9%)
25	CLA	f	610	20	63,67,73	1.29	8 (12%)	75,105,113	1.70	11 (14%)
25	CLA	b	212	10	56,60,73	1.36	8 (14%)	67,97,113	1.82	9 (13%)
25	CLA	n	208	22	49,53,73	1.43	8 (16%)	59,89,113	1.87	6 (10%)
25	CLA	B	816	-	64,68,73	1.26	7 (10%)	77,107,113	1.75	14 (18%)
25	CLA	k	203	17	57,61,73	1.35	8 (14%)	68,98,113	1.75	11 (16%)
30	DD6	d	317	-	39,45,45	1.38	4 (10%)	52,67,67	2.14	15 (28%)
25	CLA	F	201	-	46,50,73	1.42	8 (17%)	55,85,113	1.90	5 (9%)
25	CLA	k	204	17	46,50,73	1.41	8 (17%)	55,85,113	2.02	6 (10%)
30	DD6	F	203	-	39,45,45	1.53	7 (17%)	52,67,67	1.51	11 (21%)
25	CLA	b	208	-	45,49,73	1.45	8 (17%)	54,84,113	1.88	9 (16%)
29	BCR	A	839	-	41,41,41	0.74	0	56,56,56	1.03	4 (7%)
25	CLA	p	603	24	46,50,73	1.47	7 (15%)	55,85,113	1.63	6 (10%)
30	DD6	e	218	-	39,45,45	1.52	8 (20%)	52,67,67	1.49	9 (17%)
25	CLA	c	310	11	59,63,73	1.32	8 (13%)	71,101,113	1.75	10 (14%)
27	LHG	i	201	25	35,35,48	1.55	2 (5%)	38,41,54	1.29	5 (13%)
25	CLA	f	602	20	63,67,73	1.29	7 (11%)	75,105,113	1.69	12 (16%)
25	CLA	a	212	9	59,63,73	1.33	6 (10%)	71,101,113	1.77	9 (12%)
31	SF4	C	101	3	0,12,12	-	-	-	-	-
25	CLA	b	206	-	49,53,73	1.42	8 (16%)	59,89,113	1.83	6 (10%)
25	CLA	A	811	1	54,58,73	1.41	8 (14%)	65,95,113	1.84	12 (18%)
25	CLA	o	604	-	46,50,73	1.43	7 (15%)	55,85,113	1.84	8 (14%)
25	CLA	f	607	20	59,63,73	1.35	7 (11%)	71,101,113	1.75	11 (15%)
30	DD6	j	216	-	39,45,45	1.44	5 (12%)	52,67,67	2.13	15 (28%)
25	CLA	j	214	16	47,51,73	1.39	8 (17%)	56,86,113	1.86	6 (10%)
25	CLA	A	812	1	69,73,73	1.22	7 (10%)	83,113,113	1.63	9 (10%)
25	CLA	B	847	2	54,58,73	1.38	8 (14%)	65,95,113	1.81	9 (13%)
33	SQD	F	204	-	38,39,54	1.73	8 (21%)	47,50,65	1.54	7 (14%)
25	CLA	B	848	-	69,73,73	1.21	8 (11%)	83,113,113	1.70	11 (13%)
25	CLA	j	203	16	54,58,73	1.39	8 (14%)	65,95,113	1.73	11 (16%)
25	CLA	e	214	-	46,50,73	1.42	7 (15%)	55,85,113	1.74	8 (14%)
25	CLA	k	213	17	46,50,73	1.42	8 (17%)	55,85,113	1.91	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DD6	e	219	-	39,45,45	1.41	5 (12%)	52,67,67	2.14	14 (26%)
30	DD6	o	611	-	39,45,45	1.30	4 (10%)	52,67,67	2.13	15 (28%)
30	DD6	g	217	-	39,45,45	1.37	5 (12%)	52,67,67	2.21	14 (26%)

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
34	LMG	k	201	-	-	16/31/51/70	0/1/1/1
25	CLA	n	211	22	-	4/12/88/115	-
25	CLA	i	204	15	-	8/13/89/115	-
30	DD6	n	212	-	-	5/26/80/80	0/3/3/3
25	CLA	o	601	23	-	2/10/86/115	-
25	CLA	A	806	1	-	7/15/91/115	-
25	CLA	b	209	10	-	3/15/91/115	-
25	CLA	e	213	13	-	8/27/103/115	-
25	CLA	b	207	-	-	6/15/91/115	-
25	CLA	b	203	-	-	4/12/88/115	-
25	CLA	g	215	21	-	4/15/91/115	-
25	CLA	e	217	13	-	4/12/88/115	-
25	CLA	B	842	2	-	13/25/101/115	-
25	CLA	d	315	12	-	4/12/88/115	-
30	DD6	b	214	-	-	5/26/80/80	0/3/3/3
25	CLA	c	309	11	-	16/33/109/115	-
30	DD6	d	319	-	-	4/26/80/80	0/3/3/3
30	DD6	l	614	-	-	3/26/80/80	0/3/3/3
25	CLA	A	802	-	-	10/37/113/115	-
25	CLA	B	822	2	-	18/33/109/115	-
25	CLA	j	205	16	-	2/12/88/115	-
25	CLA	h	209	14	-	10/26/102/115	-
25	CLA	a	206	-	-	7/15/91/115	-
33	SQD	g	202	-	-	13/27/47/69	0/1/1/1
25	CLA	i	206	-	-	13/39/115/115	-
25	CLA	g	204	21	-	16/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	851	1	-	2/15/91/115	-
25	CLA	n	205	-	-	6/12/88/115	-
30	DD6	J	104	-	-	2/26/80/80	0/3/3/3
25	CLA	c	313	11	-	8/25/101/115	-
30	DD6	c	316	-	-	4/26/80/80	0/3/3/3
25	CLA	h	207	-	-	7/19/95/115	-
25	CLA	n	204	22	-	6/12/88/115	-
30	DD6	d	318	-	-	3/26/80/80	0/3/3/3
33	SQD	D	200	-	-	12/31/51/69	0/1/1/1
25	CLA	A	847	1	-	6/13/89/115	-
25	CLA	A	829	1	-	14/31/107/115	-
30	DD6	a	214	-	-	5/26/80/80	0/3/3/3
25	CLA	B	826	2	-	4/13/89/115	-
25	CLA	B	838	2	-	6/35/111/115	-
25	CLA	k	207	17	-	2/21/97/115	-
25	CLA	e	212	13	-	8/24/100/115	-
25	CLA	B	808	2	-	3/13/89/115	-
25	CLA	B	804	2	-	18/39/115/115	-
25	CLA	a	209	9	-	10/26/102/115	-
25	CLA	B	820	2	-	7/13/89/115	-
35	CHL	d	310	-	-	8/17/93/117	-
31	SF4	C	102	3	-	-	0/6/5/5
25	CLA	f	611	20	-	6/12/88/115	-
25	CLA	o	606	23	-	5/15/91/115	-
28	PQN	A	834	-	-	8/23/43/43	0/2/2/2
25	CLA	i	210	15	-	5/13/89/115	-
25	CLA	b	210	10	-	4/12/88/115	-
30	DD6	n	214	-	-	8/26/80/80	0/3/3/3
25	CLA	m	205	-	-	5/13/89/115	-
25	CLA	o	605	-	-	5/13/89/115	-
25	CLA	o	603	23	-	6/13/89/115	-
29	BCR	A	837	-	-	11/29/63/63	0/2/2/2
25	CLA	g	212	21	-	12/27/103/115	-
25	CLA	B	845	2	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a	205	9	-	8/25/101/115	-
27	LHG	m	201	-	-	20/36/36/53	-
27	LHG	b	201	-	-	24/35/35/53	-
27	LHG	d	302	25	-	14/33/33/53	-
25	CLA	o	610	23	-	5/13/89/115	-
25	CLA	p	607	24	-	11/15/91/115	-
29	BCR	B	801	-	-	9/29/63/63	0/2/2/2
25	CLA	l	610	18	-	7/19/95/115	-
25	CLA	k	211	17	-	10/24/100/115	-
25	CLA	h	204	14	-	15/27/103/115	-
28	PQN	F	205	-	-	5/15/35/43	0/2/2/2
25	CLA	p	605	-	-	6/12/88/115	-
34	LMG	e	202	-	-	19/47/67/70	0/1/1/1
25	CLA	B	841	2	-	10/32/108/115	-
30	DD6	J	105	-	-	15/26/80/80	0/3/3/3
25	CLA	n	207	-	-	2/10/86/115	-
29	BCR	B	831	-	-	11/29/63/63	0/2/2/2
25	CLA	g	209	21	-	10/27/103/115	-
25	CLA	g	210	27	-	3/12/88/115	-
25	CLA	c	304	11	-	6/25/101/115	-
29	BCR	J	101	-	-	17/29/63/63	0/2/2/2
25	CLA	A	846	1	-	18/39/115/115	-
27	LHG	A	835	-	-	22/53/53/53	-
32	DGD	b	202	-	-	18/37/77/95	0/2/2/2
25	CLA	j	213	16	-	3/12/88/115	-
25	CLA	g	203	21	-	6/12/88/115	-
25	CLA	c	305	-	-	6/19/95/115	-
35	CHL	d	309	-	-	4/14/90/117	-
25	CLA	j	207	-	-	5/18/94/115	-
25	CLA	d	312	12	-	14/32/108/115	-
25	CLA	d	303	12	-	6/21/97/115	-
27	LHG	a	201	25	-	9/30/30/53	-
25	CLA	j	210	27	-	8/21/97/115	-
25	CLA	c	308	-	-	11/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	F	202	6	-	9/15/91/115	-
25	CLA	m	206	-	-	2/12/88/115	-
25	CLA	B	814	2	-	12/32/108/115	-
25	CLA	B	839	-	-	15/33/109/115	-
25	CLA	i	213	15	-	4/21/97/115	-
25	CLA	o	602	23	-	10/18/94/115	-
25	CLA	B	834	2	-	6/27/103/115	-
25	CLA	i	205	-	-	3/13/89/115	-
25	CLA	k	205	17	-	20/39/115/115	-
30	DD6	m	212	-	-	5/26/80/80	0/3/3/3
25	CLA	c	302	11	-	6/12/88/115	-
25	CLA	p	604	-	-	5/13/89/115	-
25	CLA	A	810	1	-	14/39/115/115	-
25	CLA	h	215	14	-	2/13/89/115	-
25	CLA	j	206	-	-	11/30/106/115	-
28	PQN	B	835	-	-	5/16/36/43	0/2/2/2
25	CLA	B	802	2	-	10/39/115/115	-
25	CLA	e	206	13	-	5/15/91/115	-
34	LMG	a	202	-	-	18/38/58/70	0/1/1/1
25	CLA	j	208	16	-	5/21/97/115	-
25	CLA	m	211	19	-	5/12/88/115	-
25	CLA	m	204	19	-	10/26/102/115	-
25	CLA	e	208	13	-	3/12/88/115	-
30	DD6	p	610	-	-	3/26/80/80	0/3/3/3
25	CLA	l	608	-	-	3/13/89/115	-
25	CLA	o	608	23	-	4/13/85/115	-
25	CLA	A	833	1	-	15/39/115/115	-
30	DD6	n	213	-	-	13/26/80/80	0/3/3/3
25	CLA	A	848	1	-	8/23/99/115	-
25	CLA	c	306	-	-	4/13/89/115	-
25	CLA	l	604	-	-	4/13/89/115	-
25	CLA	k	206	-	-	2/21/97/115	-
25	CLA	g	214	21	-	0/12/88/115	-
25	CLA	i	208	15	-	12/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	843	2	-	14/37/113/115	-
27	LHG	h	201	-	-	14/33/33/53	-
25	CLA	A	817	1	-	10/29/105/115	-
30	DD6	i	214	-	-	2/26/80/80	0/3/3/3
25	CLA	n	202	22	-	14/27/103/115	-
25	CLA	k	208	17	-	14/30/106/115	-
25	CLA	l	602	18	-	12/32/108/115	-
25	CLA	c	311	27	-	1/13/89/115	-
35	CHL	c	307	-	-	6/21/97/117	-
25	CLA	j	211	16	-	11/27/103/115	-
25	CLA	f	604	-	-	5/12/88/115	-
25	CLA	k	209	-	-	5/12/88/115	-
25	CLA	l	612	-	-	6/12/88/115	-
25	CLA	p	608	24	-	5/13/89/115	-
25	CLA	h	210	27	-	5/13/89/115	-
25	CLA	p	601	-	-	3/12/88/115	-
27	LHG	j	202	25	-	24/41/41/53	-
25	CLA	A	842	1	-	9/20/96/115	-
25	CLA	A	830	1	-	8/24/100/115	-
25	CLA	i	211	15	-	10/32/108/115	-
25	CLA	J	103	7	-	14/21/97/115	-
25	CLA	a	207	-	-	13/25/101/115	-
25	CLA	j	215	16	-	6/21/97/115	-
25	CLA	A	809	1	-	23/39/115/115	-
25	CLA	l	605	-	-	6/13/89/115	-
25	CLA	A	820	1	-	10/30/106/115	-
30	DD6	o	612	-	-	3/26/80/80	0/3/3/3
35	CHL	d	307	12	-	8/23/99/117	-
25	CLA	f	609	20	-	4/12/88/115	-
25	CLA	a	208	9	-	5/21/97/115	-
25	CLA	B	825	-	-	5/13/89/115	-
27	LHG	g	201	25	-	25/39/39/53	-
35	CHL	d	308	-	-	8/17/93/117	-
34	LMG	j	201	-	-	11/39/59/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	857	-	-	8/25/101/115	-
25	CLA	A	852	1	-	5/19/95/115	-
25	CLA	i	202	15	-	14/25/101/115	-
25	CLA	m	210	19	-	3/13/89/115	-
27	LHG	h	202	25	-	11/35/35/53	-
25	CLA	A	824	1	-	16/31/107/115	-
25	CLA	o	609	23	-	8/12/88/115	-
25	CLA	h	212	14	-	10/25/101/115	-
25	CLA	m	209	-	-	3/13/89/115	-
25	CLA	e	211	-	-	6/19/95/115	-
25	CLA	A	850	1	-	8/27/103/115	-
25	CLA	B	806	2	-	2/12/88/115	-
25	CLA	e	201	-	-	7/25/101/115	-
25	CLA	A	843	1	-	12/24/100/115	-
25	CLA	A	849	1	-	10/21/97/115	-
25	CLA	o	607	23	-	2/10/86/115	-
30	DD6	f	614	-	-	7/26/80/80	0/3/3/3
25	CLA	m	207	19	-	4/21/97/115	-
25	CLA	n	210	22	-	4/12/88/115	-
25	CLA	A	827	1	-	3/13/89/115	-
25	CLA	l	603	18	-	2/13/89/115	-
25	CLA	b	205	10	-	6/13/89/115	-
25	CLA	h	203	14	-	9/21/97/115	-
25	CLA	h	214	14	-	6/12/88/115	-
33	SQD	J	102	-	-	10/21/41/69	0/1/1/1
25	CLA	b	211	-	-	4/12/88/115	-
25	CLA	f	612	20	-	9/13/89/115	-
27	LHG	A	805	25	-	19/42/42/53	-
25	CLA	e	205	13	-	20/39/115/115	-
25	CLA	l	609	18	-	6/13/89/115	-
25	CLA	A	845	-	-	5/19/95/115	-
25	CLA	f	601	20	-	7/12/88/115	-
25	CLA	h	213	14	-	4/13/89/115	-
25	CLA	A	807	-	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	d	305	12	-	5/12/88/115	-
25	CLA	d	304	12	-	5/30/106/115	-
25	CLA	B	811	2	-	19/37/113/115	-
35	CHL	e	209	-	-	10/17/93/117	-
25	CLA	a	204	9	-	17/33/109/115	-
25	CLA	i	207	15	-	4/13/89/115	-
25	CLA	g	213	21	-	3/12/88/115	-
25	CLA	b	213	10	-	5/12/88/115	-
25	CLA	j	204	16	-	4/27/103/115	-
28	PQN	B	827	-	-	7/23/43/43	0/2/2/2
25	CLA	m	208	19	-	6/12/88/115	-
25	CLA	B	821	2	-	17/33/109/115	-
25	CLA	A	815	1	-	18/31/107/115	-
25	CLA	p	602	24	-	9/13/89/115	-
25	CLA	p	609	24	-	5/13/89/115	-
25	CLA	c	312	11	-	4/13/89/115	-
25	CLA	B	810	2	-	3/13/89/115	-
25	CLA	c	303	11	-	14/32/108/115	-
30	DD6	m	213	-	-	6/26/80/80	0/3/3/3
25	CLA	c	314	11	-	6/12/88/115	-
25	CLA	A	813	1	-	11/31/107/115	-
25	CLA	h	211	14	-	8/31/107/115	-
25	CLA	A	853	27	-	12/25/101/115	-
25	CLA	k	210	17	-	2/13/89/115	-
25	CLA	n	209	22	-	3/10/86/115	-
30	DD6	h	217	-	-	0/26/80/80	0/3/3/3
25	CLA	A	832	1	-	12/39/115/115	-
26	LMT	A	803	-	-	7/21/61/61	0/2/2/2
25	CLA	l	606	18	-	13/33/109/115	-
29	BCR	B	829	-	-	2/29/63/63	0/2/2/2
25	CLA	A	844	1	-	17/33/109/115	-
25	CLA	d	306	-	-	7/24/100/115	-
30	DD6	j	217	-	-	3/26/80/80	0/3/3/3
25	CLA	B	844	2	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DD6	a	215	-	-	0/26/80/80	0/3/3/3
25	CLA	A	801	1	-	18/39/115/115	-
25	CLA	j	209	16	-	20/38/114/115	-
25	CLA	B	837	2	-	12/21/97/115	-
32	DGD	e	203	-	-	6/24/64/95	0/2/2/2
29	BCR	B	832	-	-	14/29/63/63	0/2/2/2
25	CLA	e	207	-	-	4/21/97/115	-
30	DD6	i	215	-	-	3/26/80/80	0/3/3/3
29	BCR	B	833	-	-	5/29/63/63	0/2/2/2
25	CLA	B	803	-	-	9/27/103/115	-
25	CLA	l	607	18	-	14/26/102/115	-
25	CLA	A	818	1	-	15/39/115/115	-
25	CLA	B	809	2	-	4/12/88/115	-
25	CLA	B	819	2	-	15/39/115/115	-
30	DD6	g	216	-	-	4/26/80/80	0/3/3/3
25	CLA	A	816	1	-	6/13/89/115	-
25	CLA	A	825	1	-	8/39/115/115	-
30	DD6	f	613	-	-	5/26/80/80	0/3/3/3
32	DGD	B	849	-	-	19/43/83/95	0/2/2/2
25	CLA	A	840	-	-	12/37/113/115	-
25	CLA	B	846	2	-	6/21/97/115	-
25	CLA	B	805	2	-	13/39/115/115	-
25	CLA	g	205	21	-	4/12/88/115	-
25	CLA	B	823	2	-	9/33/109/115	-
25	CLA	A	821	-	-	13/37/113/115	-
25	CLA	d	301	12	-	5/10/86/115	-
25	CLA	h	205	14	-	5/13/89/115	-
25	CLA	d	311	12	-	5/20/96/115	-
25	CLA	k	212	17	-	4/12/88/115	-
25	CLA	B	818	2	-	13/39/115/115	-
25	CLA	f	606	20	-	4/12/88/115	-
25	CLA	A	804	1	-	8/33/109/115	-
25	CLA	A	814	1	-	10/32/108/115	-
30	DD6	e	220	-	-	15/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	e	216	13	-	4/27/103/115	-
29	BCR	A	838	-	-	5/29/63/63	0/2/2/2
29	BCR	B	830	-	-	7/29/63/63	0/2/2/2
25	CLA	i	203	15	-	11/38/114/115	-
30	DD6	c	318	-	-	8/26/80/80	0/3/3/3
25	CLA	e	204	13	-	5/10/86/115	-
25	CLA	l	611	18	-	5/12/88/115	-
29	BCR	B	828	-	-	7/29/63/63	0/2/2/2
25	CLA	n	203	-	-	8/19/95/115	-
25	CLA	B	836	2	-	9/25/101/115	-
25	CLA	k	202	17	-	3/13/89/115	-
25	CLA	A	826	1	-	13/39/115/115	-
29	BCR	M	201	-	-	6/29/63/63	0/2/2/2
30	DD6	k	216	-	-	3/26/80/80	0/3/3/3
30	DD6	h	216	-	-	3/26/80/80	0/3/3/3
25	CLA	m	202	19	-	5/12/88/115	-
25	CLA	e	215	13	-	2/13/89/115	-
25	CLA	k	214	17	-	3/21/97/115	-
25	CLA	i	212	15	-	3/12/88/115	-
25	CLA	B	824	2	-	22/39/115/115	-
30	DD6	c	317	-	-	0/26/80/80	0/3/3/3
25	CLA	a	203	9	-	6/21/97/115	-
25	CLA	c	315	11	-	5/18/94/115	-
25	CLA	h	208	14	-	8/21/97/115	-
30	DD6	k	215	-	-	2/26/80/80	0/3/3/3
25	CLA	d	313	27	-	5/15/91/115	-
25	CLA	B	807	2	-	15/39/115/115	-
25	CLA	j	212	16	-	10/36/112/115	-
25	CLA	n	201	22	-	14/32/108/115	-
25	CLA	A	828	1	-	7/13/89/115	-
25	CLA	f	608	-	-	2/12/88/115	-
30	DD6	l	613	-	-	2/26/80/80	0/3/3/3
25	CLA	d	316	12	-	4/12/88/115	-
25	CLA	p	606	24	-	10/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DD6	b	215	-	-	1/26/80/80	0/3/3/3
25	CLA	h	206	-	-	8/33/109/115	-
25	CLA	f	603	20	-	1/13/89/115	-
25	CLA	A	841	-	-	8/30/106/115	-
25	CLA	A	823	1	-	16/38/114/115	-
25	CLA	i	209	27	-	4/13/89/115	-
25	CLA	A	822	-	-	8/25/101/115	-
30	DD6	A	854	-	-	3/26/80/80	0/3/3/3
25	CLA	B	813	2	-	5/19/95/115	-
27	LHG	c	301	25	-	11/34/34/53	-
25	CLA	g	207	-	-	7/15/91/115	-
25	CLA	a	211	9	-	5/13/89/115	-
25	CLA	B	817	-	-	8/21/97/115	-
25	CLA	g	206	-	-	5/13/89/115	-
25	CLA	B	815	2	-	8/20/96/115	-
25	CLA	g	211	21	-	4/12/88/115	-
25	CLA	l	601	18	-	4/12/88/115	-
25	CLA	A	831	1	-	4/19/95/115	-
31	SF4	A	856	1,2	-	-	0/6/5/5
25	CLA	e	210	-	-	7/13/89/115	-
25	CLA	f	605	20	-	2/12/88/115	-
30	DD6	A	855	-	-	9/26/80/80	0/3/3/3
25	CLA	a	213	-	-	12/37/113/115	-
25	CLA	g	208	21	-	5/21/97/115	-
29	BCR	A	836	-	-	5/29/63/63	0/2/2/2
25	CLA	A	819	-	-	12/39/115/115	-
25	CLA	B	840	2	-	8/21/97/115	-
30	DD6	i	216	-	-	1/26/80/80	0/3/3/3
25	CLA	B	812	2	-	13/38/114/115	-
25	CLA	n	206	-	-	3/12/88/115	-
25	CLA	a	210	27	-	6/15/91/115	-
25	CLA	A	808	1	-	11/33/109/115	-
25	CLA	b	204	10	-	11/25/101/115	-
25	CLA	m	203	19	-	16/33/109/115	-
25	CLA	d	314	12	-	3/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	f	610	20	-	14/32/108/115	-
25	CLA	b	212	10	-	11/24/100/115	-
25	CLA	n	208	22	-	7/15/91/115	-
25	CLA	B	816	-	-	10/33/109/115	-
25	CLA	k	203	17	-	10/25/101/115	-
30	DD6	d	317	-	-	2/26/80/80	0/3/3/3
25	CLA	F	201	-	-	0/12/88/115	-
25	CLA	k	204	17	-	5/12/88/115	-
30	DD6	F	203	-	-	18/26/80/80	0/3/3/3
25	CLA	b	208	-	-	2/10/86/115	-
29	BCR	A	839	-	-	12/29/63/63	0/2/2/2
25	CLA	p	603	24	-	4/12/88/115	-
30	DD6	e	218	-	-	9/26/80/80	0/3/3/3
25	CLA	c	310	11	-	13/27/103/115	-
27	LHG	i	201	25	-	19/40/40/53	-
25	CLA	f	602	20	-	14/32/108/115	-
25	CLA	a	212	9	-	14/27/103/115	-
31	SF4	C	101	3	-	-	0/6/5/5
25	CLA	b	206	-	-	5/15/91/115	-
25	CLA	A	811	1	-	2/21/97/115	-
25	CLA	o	604	-	-	3/12/88/115	-
25	CLA	f	607	20	-	15/27/103/115	-
30	DD6	j	216	-	-	4/26/80/80	0/3/3/3
25	CLA	j	214	16	-	5/13/89/115	-
25	CLA	A	812	1	-	16/39/115/115	-
25	CLA	B	847	2	-	3/21/97/115	-
33	SQD	F	204	-	-	21/34/54/69	0/1/1/1
25	CLA	B	848	-	-	18/39/115/115	-
25	CLA	j	203	16	-	8/21/97/115	-
25	CLA	e	214	-	-	3/12/88/115	-
25	CLA	k	213	17	-	5/12/88/115	-
30	DD6	e	219	-	-	5/26/80/80	0/3/3/3
30	DD6	o	611	-	-	5/26/80/80	0/3/3/3
30	DD6	g	217	-	-	4/26/80/80	0/3/3/3

The worst 5 of 2451 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	201	LHG	P-O3	6.37	1.85	1.59
27	m	201	LHG	P-O3	6.32	1.84	1.59
27	c	301	LHG	P-O3	6.28	1.84	1.59
27	d	302	LHG	P-O3	6.22	1.84	1.59
27	h	201	LHG	P-O3	6.19	1.84	1.59

The worst 5 of 3426 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	823	CLA	C4A-NA-C1A	11.56	111.90	106.71
25	k	204	CLA	C4A-NA-C1A	11.50	111.88	106.71
25	B	803	CLA	C4A-NA-C1A	11.20	111.74	106.71
25	o	608	CLA	C4A-NA-C1A	11.17	111.73	106.71
25	A	826	CLA	C4A-NA-C1A	11.10	111.70	106.71

There are no chirality outliers.

5 of 2949 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	801	CLA	CHA-CBD-CGD-O2D
25	A	802	CLA	C1-C2-C3-C4
25	A	802	CLA	C1-C2-C3-C5
25	A	806	CLA	C2B-C3B-CAB-CBB
25	A	806	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

259 monomers are involved in 540 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	k	201	LMG	3	0
25	i	204	CLA	2	0
25	o	601	CLA	1	0
25	A	806	CLA	1	0
25	b	209	CLA	2	0
25	e	213	CLA	4	0
25	b	207	CLA	1	0
25	b	203	CLA	1	0
25	B	842	CLA	5	0
25	d	315	CLA	1	0
25	c	309	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	d	319	DD6	1	0
25	A	802	CLA	7	0
25	B	822	CLA	4	0
25	h	209	CLA	9	0
25	a	206	CLA	1	0
33	g	202	SQD	2	0
25	i	206	CLA	2	0
25	g	204	CLA	3	0
25	n	205	CLA	2	0
25	c	313	CLA	2	0
25	h	207	CLA	3	0
25	A	829	CLA	3	0
25	B	826	CLA	3	0
25	B	838	CLA	5	0
25	k	207	CLA	1	0
25	B	808	CLA	1	0
25	B	804	CLA	3	0
25	a	209	CLA	3	0
35	d	310	CHL	2	0
25	f	611	CLA	1	0
25	o	606	CLA	1	0
28	A	834	PQN	5	0
25	i	210	CLA	1	0
25	b	210	CLA	2	0
25	o	605	CLA	1	0
29	A	837	BCR	3	0
25	g	212	CLA	3	0
25	B	845	CLA	9	0
25	a	205	CLA	1	0
27	m	201	LHG	2	0
27	b	201	LHG	3	0
27	d	302	LHG	3	0
25	o	610	CLA	4	0
25	p	607	CLA	1	0
29	B	801	BCR	2	0
25	l	610	CLA	1	0
25	k	211	CLA	2	0
25	h	204	CLA	1	0
25	p	605	CLA	1	0
34	e	202	LMG	5	0
25	B	841	CLA	4	0
25	n	207	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	831	BCR	4	0
25	g	209	CLA	7	0
25	c	304	CLA	4	0
29	J	101	BCR	3	0
25	A	846	CLA	1	0
27	A	835	LHG	5	0
32	b	202	DGD	3	0
25	g	203	CLA	2	0
35	d	309	CHL	2	0
25	j	207	CLA	1	0
25	d	312	CLA	4	0
25	d	303	CLA	1	0
27	a	201	LHG	1	0
25	j	210	CLA	2	0
25	c	308	CLA	3	0
25	F	202	CLA	3	0
25	m	206	CLA	1	0
25	B	814	CLA	1	0
25	B	839	CLA	5	0
25	i	213	CLA	2	0
25	o	602	CLA	2	0
25	i	205	CLA	1	0
25	k	205	CLA	1	0
30	m	212	DD6	1	0
25	c	302	CLA	1	0
25	A	810	CLA	3	0
25	j	206	CLA	2	0
25	B	802	CLA	9	0
25	e	206	CLA	1	0
25	j	208	CLA	2	0
25	m	211	CLA	1	0
25	m	204	CLA	1	0
25	e	208	CLA	1	0
25	o	608	CLA	1	0
25	A	833	CLA	7	0
30	n	213	DD6	1	0
25	c	306	CLA	1	0
25	l	604	CLA	1	0
25	k	206	CLA	3	0
25	g	214	CLA	1	0
25	i	208	CLA	3	0
25	B	843	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	h	201	LHG	1	0
25	A	817	CLA	3	0
25	n	202	CLA	3	0
25	k	208	CLA	4	0
25	l	602	CLA	4	0
25	c	311	CLA	3	0
35	c	307	CHL	3	0
25	f	604	CLA	1	0
25	l	612	CLA	1	0
25	p	608	CLA	1	0
25	h	210	CLA	1	0
27	j	202	LHG	4	0
25	A	842	CLA	2	0
25	A	830	CLA	2	0
25	i	211	CLA	2	0
25	J	103	CLA	2	0
25	a	207	CLA	3	0
25	j	215	CLA	1	0
25	A	809	CLA	6	0
25	l	605	CLA	1	0
25	A	820	CLA	2	0
35	d	307	CHL	1	0
25	a	208	CLA	1	0
25	B	825	CLA	1	0
35	d	308	CHL	2	0
25	A	857	CLA	1	0
25	i	202	CLA	2	0
27	h	202	LHG	2	0
25	A	824	CLA	7	0
25	h	212	CLA	3	0
25	e	211	CLA	3	0
25	A	850	CLA	2	0
25	e	201	CLA	2	0
25	A	843	CLA	3	0
25	A	849	CLA	2	0
25	o	607	CLA	3	0
25	n	210	CLA	1	0
25	l	603	CLA	1	0
25	h	203	CLA	3	0
25	h	214	CLA	2	0
25	f	612	CLA	1	0
27	A	805	LHG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	e	205	CLA	4	0
25	A	845	CLA	2	0
25	A	807	CLA	6	0
25	d	305	CLA	2	0
25	d	304	CLA	1	0
25	B	811	CLA	3	0
25	a	204	CLA	7	0
25	i	207	CLA	1	0
28	B	827	PQN	2	0
25	m	208	CLA	3	0
25	B	821	CLA	2	0
25	A	815	CLA	5	0
25	p	602	CLA	3	0
25	p	609	CLA	1	0
25	c	312	CLA	3	0
25	B	810	CLA	1	0
25	c	303	CLA	2	0
30	m	213	DD6	1	0
25	c	314	CLA	1	0
25	A	813	CLA	1	0
25	h	211	CLA	2	0
25	A	853	CLA	2	0
25	k	210	CLA	1	0
25	n	209	CLA	1	0
25	A	832	CLA	5	0
25	l	606	CLA	3	0
29	B	829	BCR	2	0
25	A	844	CLA	5	0
25	d	306	CLA	2	0
25	B	844	CLA	2	0
30	a	215	DD6	1	0
25	A	801	CLA	7	0
25	j	209	CLA	3	0
25	B	837	CLA	3	0
32	e	203	DGD	2	0
29	B	832	BCR	8	0
25	e	207	CLA	1	0
30	i	215	DD6	1	0
29	B	833	BCR	3	0
25	B	803	CLA	4	0
25	l	607	CLA	4	0
25	A	818	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	819	CLA	6	0
25	A	816	CLA	3	0
25	A	825	CLA	3	0
32	B	849	DGD	2	0
25	A	840	CLA	6	0
25	B	846	CLA	4	0
25	B	805	CLA	5	0
25	g	205	CLA	1	0
25	B	823	CLA	2	0
25	A	821	CLA	4	0
25	h	205	CLA	1	0
25	B	818	CLA	6	0
25	A	804	CLA	2	0
25	A	814	CLA	3	0
25	e	216	CLA	1	0
29	A	838	BCR	1	0
29	B	830	BCR	5	0
25	i	203	CLA	2	0
25	l	611	CLA	3	0
29	B	828	BCR	2	0
25	n	203	CLA	2	0
25	B	836	CLA	3	0
25	A	826	CLA	4	0
29	M	201	BCR	2	0
25	m	202	CLA	5	0
25	e	215	CLA	3	0
25	k	214	CLA	2	0
25	i	212	CLA	1	0
25	B	824	CLA	5	0
25	a	203	CLA	1	0
25	h	208	CLA	2	0
25	d	313	CLA	1	0
25	B	807	CLA	3	0
25	j	212	CLA	4	0
25	n	201	CLA	2	0
25	d	316	CLA	1	0
25	p	606	CLA	1	0
25	h	206	CLA	2	0
25	A	841	CLA	3	0
25	A	823	CLA	3	0
25	A	822	CLA	3	0
25	B	813	CLA	4	0

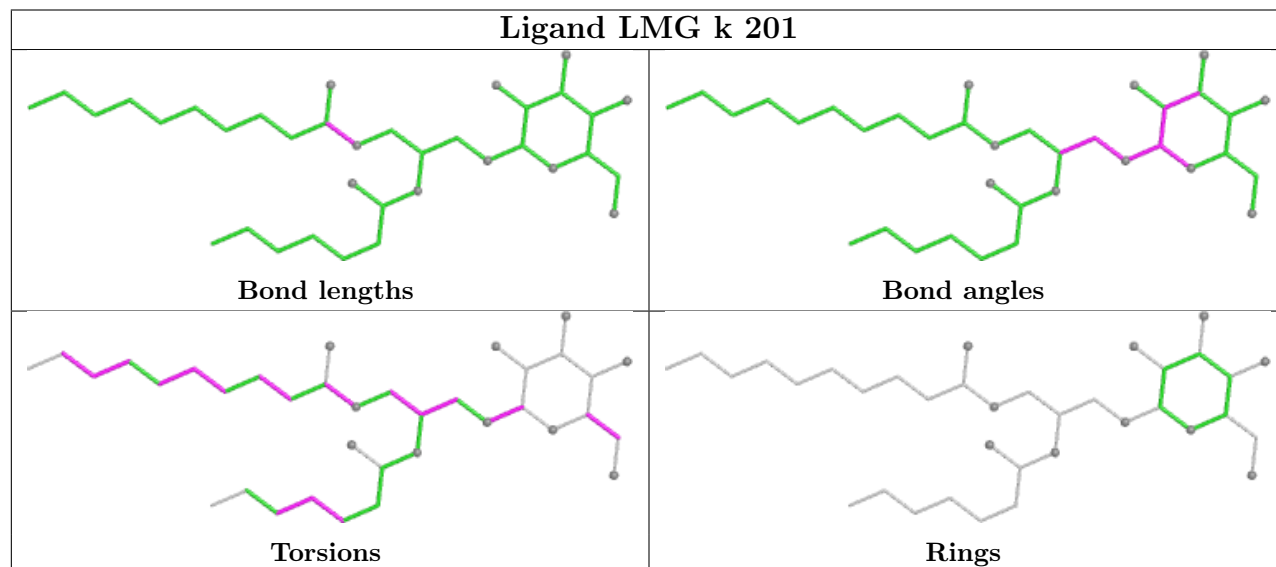
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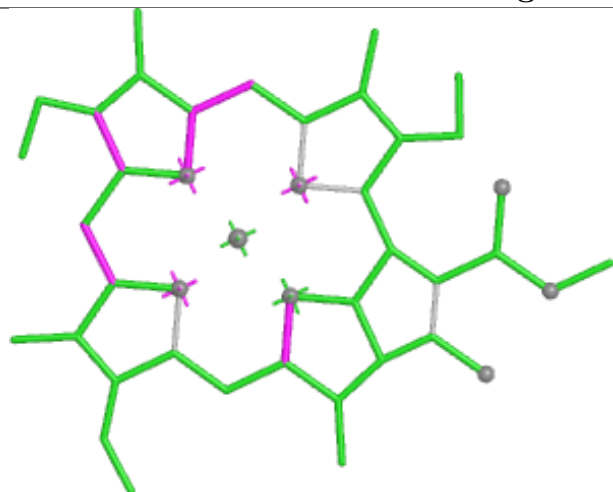
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	c	301	LHG	3	0
25	g	207	CLA	4	0
25	B	817	CLA	4	0
25	B	815	CLA	1	0
25	g	211	CLA	1	0
25	A	831	CLA	2	0
25	f	605	CLA	1	0
25	a	213	CLA	5	0
25	g	208	CLA	3	0
29	A	836	BCR	3	0
25	A	819	CLA	4	0
25	B	840	CLA	5	0
25	B	812	CLA	3	0
25	n	206	CLA	1	0
25	a	210	CLA	1	0
25	b	204	CLA	1	0
25	m	203	CLA	5	0
25	f	610	CLA	3	0
25	b	212	CLA	4	0
25	n	208	CLA	1	0
25	B	816	CLA	4	0
25	k	203	CLA	1	0
25	F	201	CLA	3	0
25	k	204	CLA	1	0
25	b	208	CLA	1	0
29	A	839	BCR	2	0
25	p	603	CLA	4	0
25	c	310	CLA	3	0
27	i	201	LHG	2	0
25	f	602	CLA	2	0
25	a	212	CLA	2	0
25	b	206	CLA	3	0
25	f	607	CLA	1	0
25	A	812	CLA	3	0
25	B	847	CLA	3	0
25	B	848	CLA	2	0
25	j	203	CLA	4	0
25	e	214	CLA	1	0

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

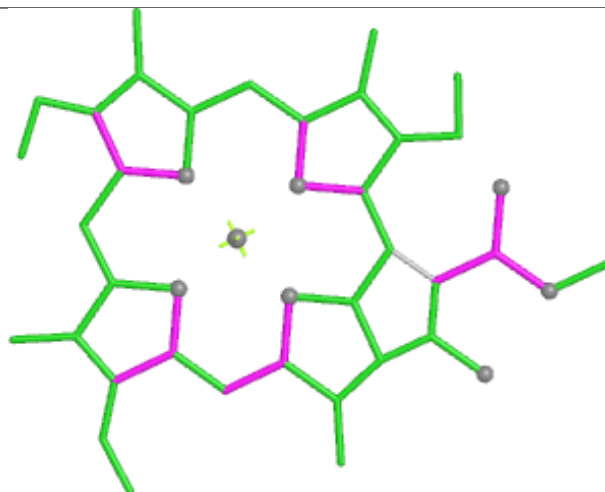
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question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



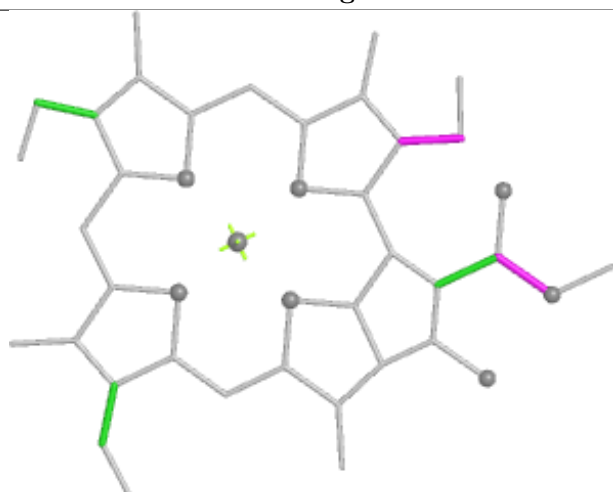
Ligand CLA n 211



Bond lengths



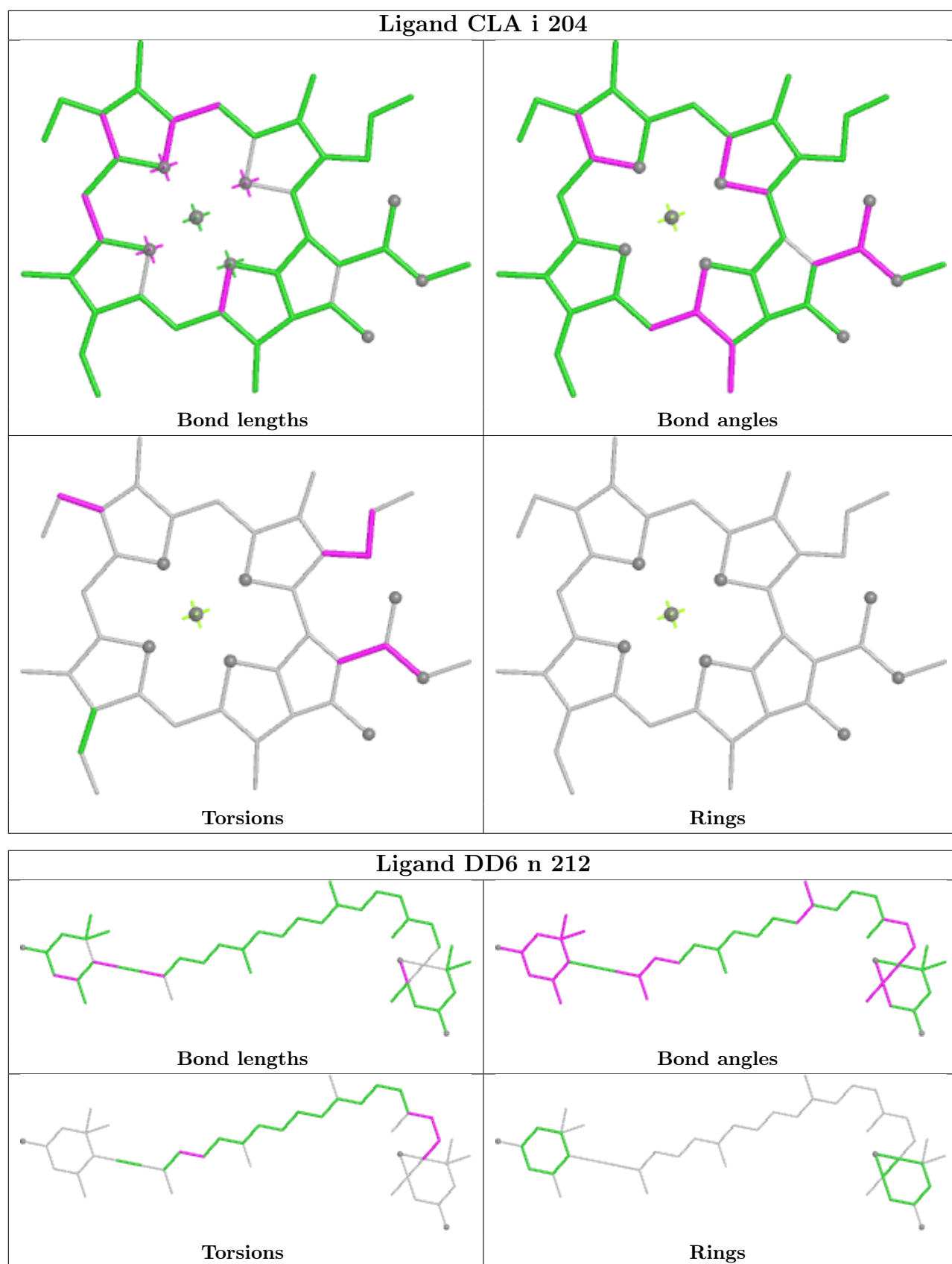
Bond angles

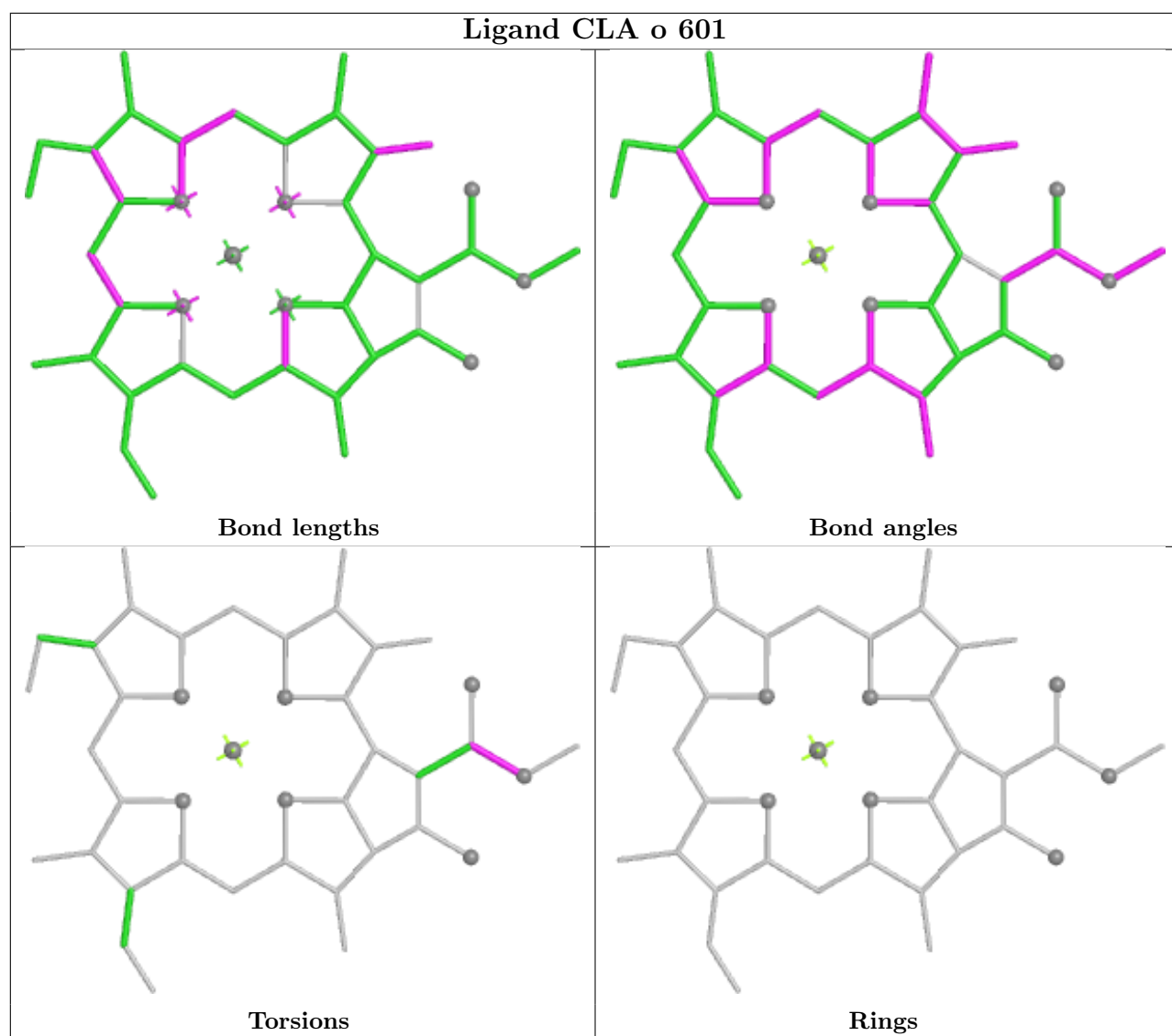


Torsions

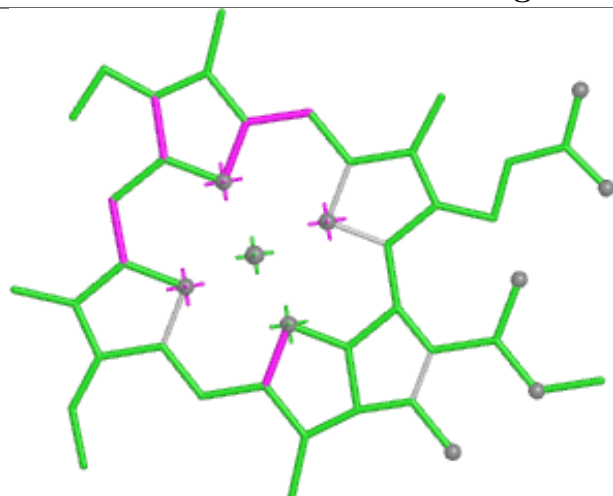


Rings

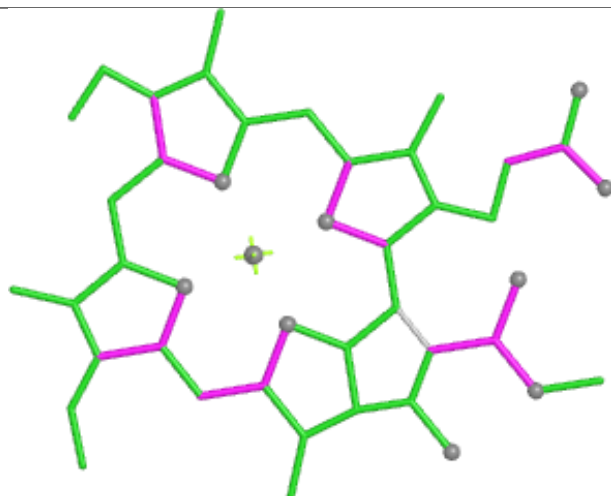




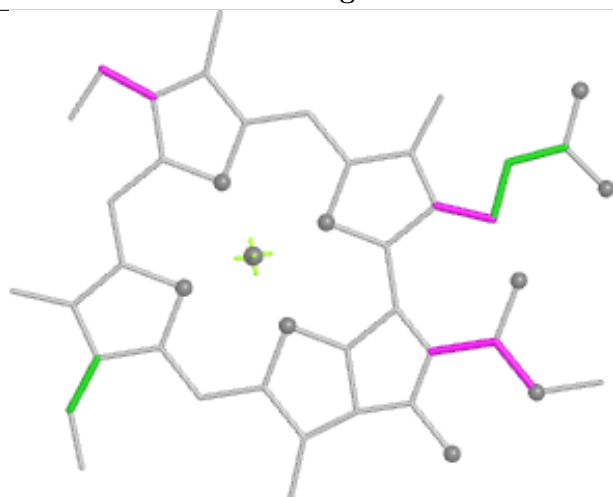
Ligand CLA A 806



Bond lengths



Bond angles

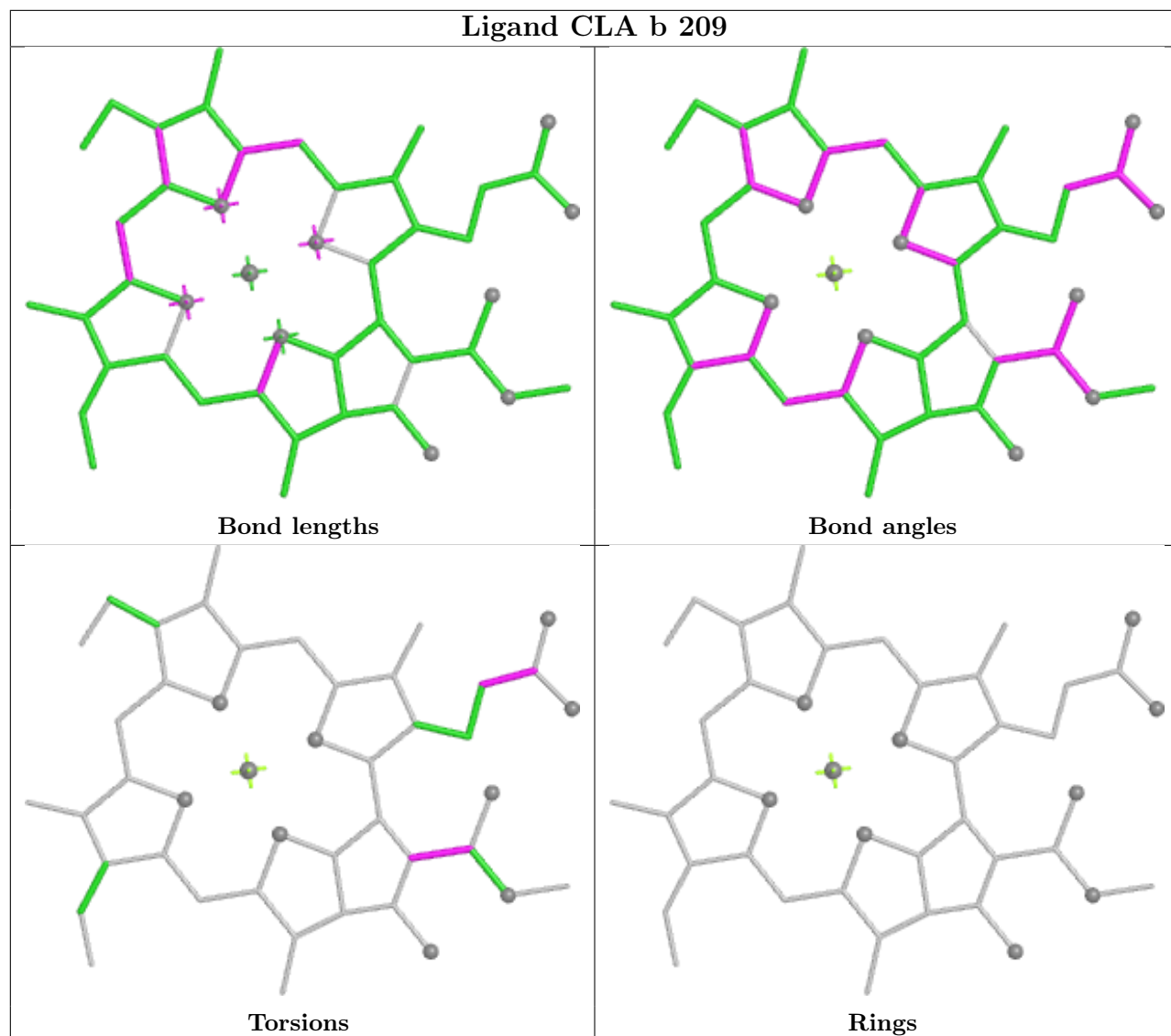


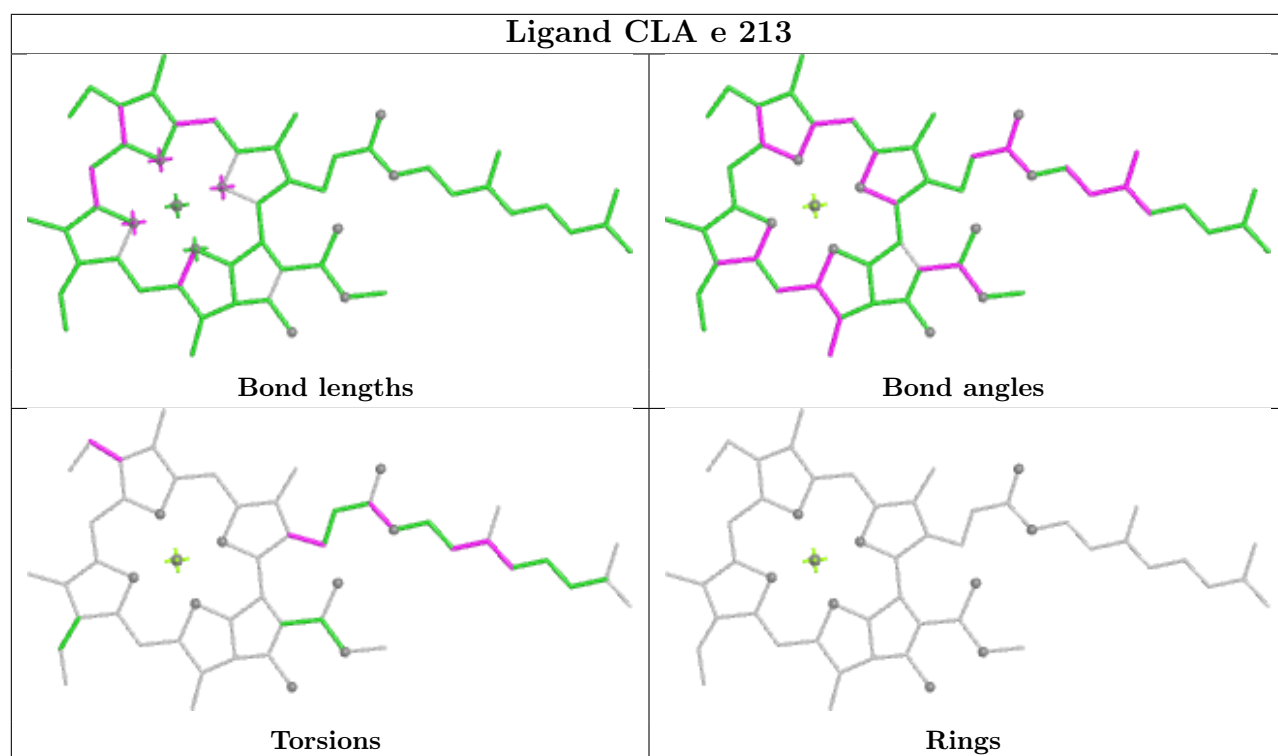
Torsions



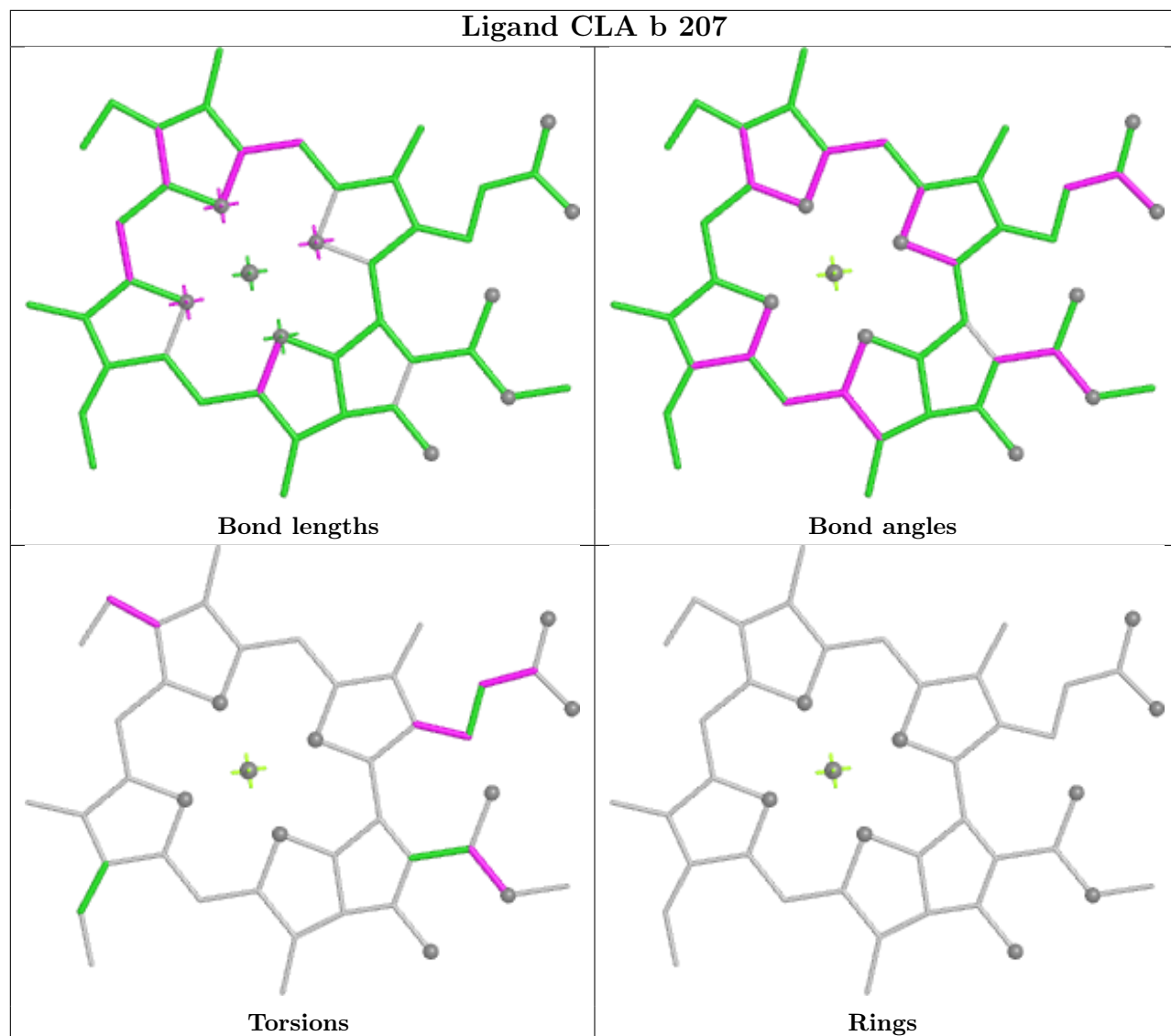
Rings

Ligand CLA b 209

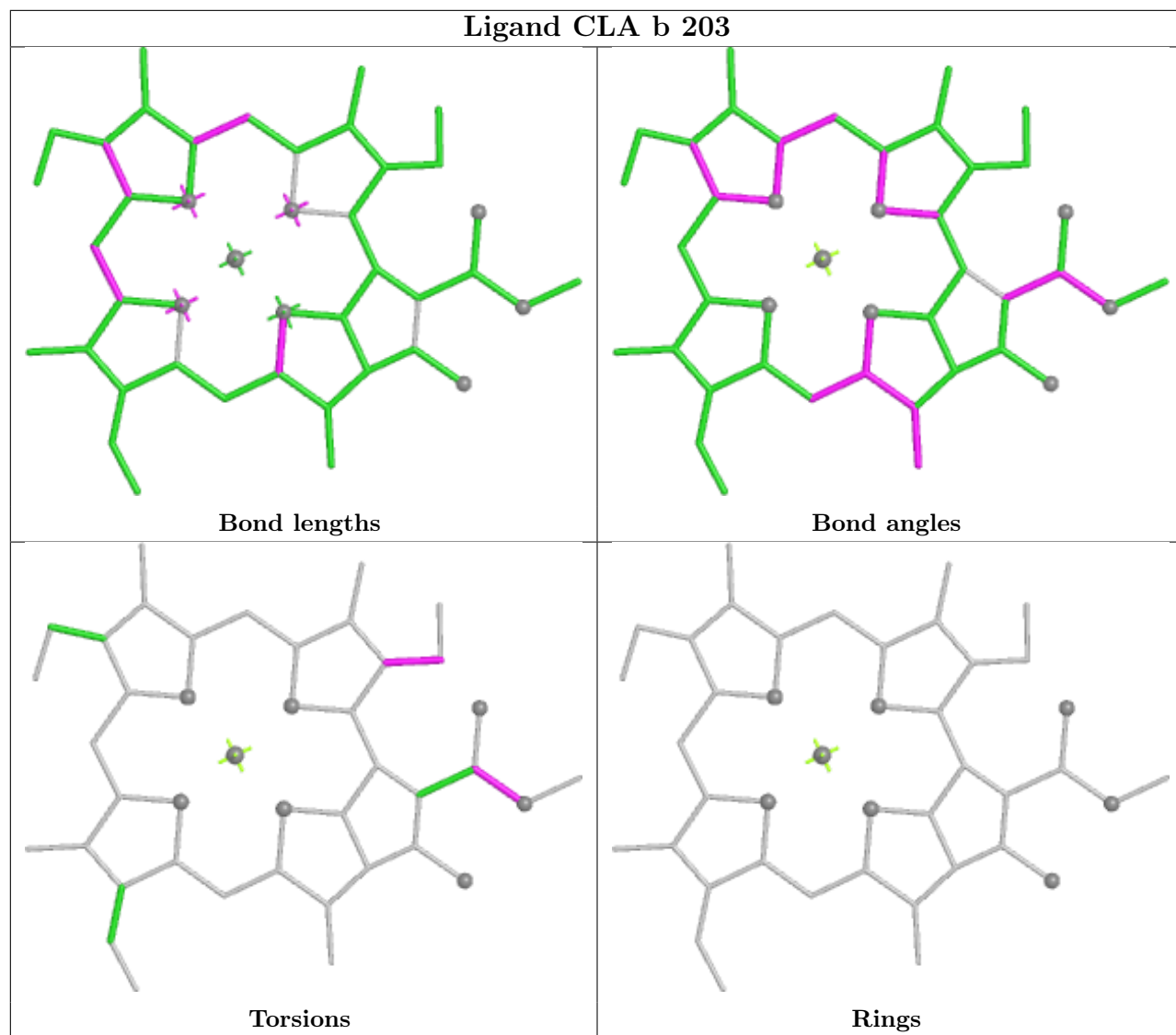




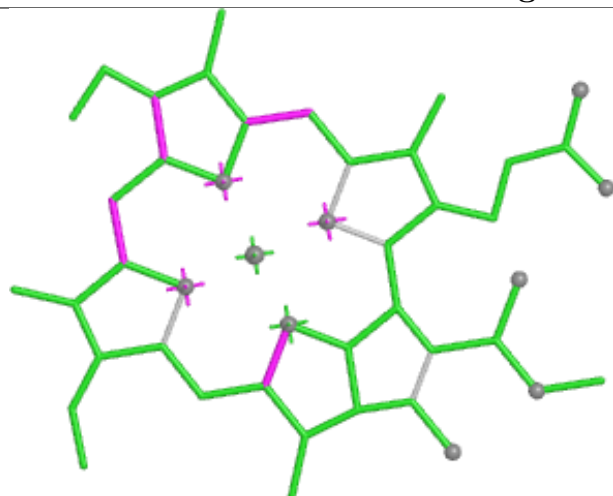
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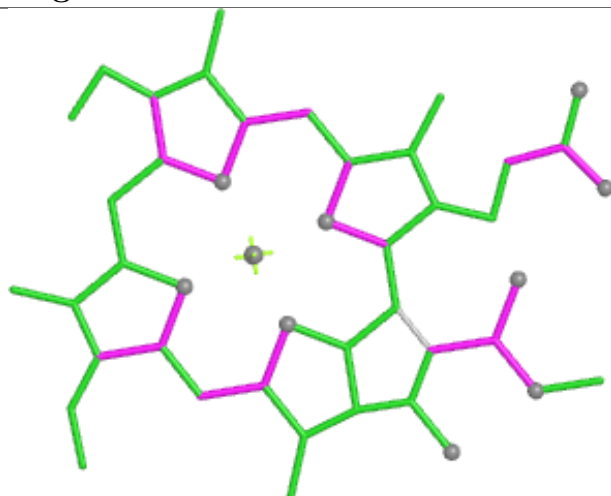
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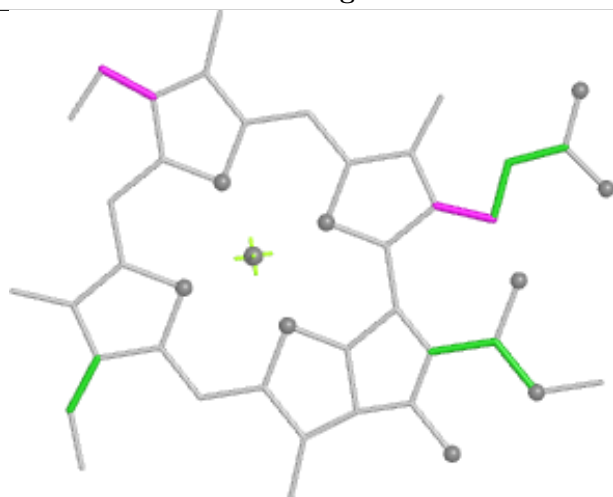
Ligand CLA g 215



Bond lengths



Bond angles

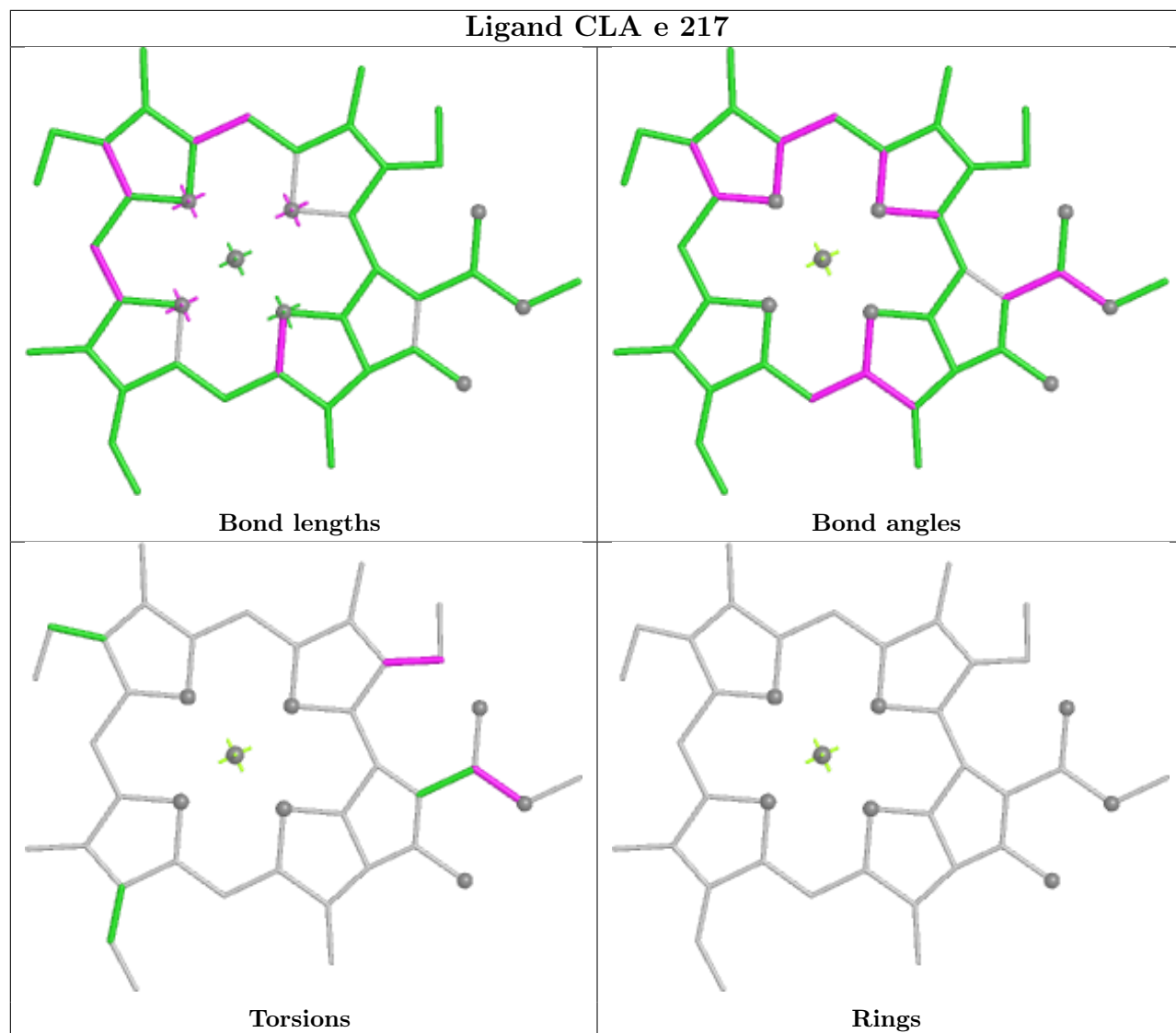


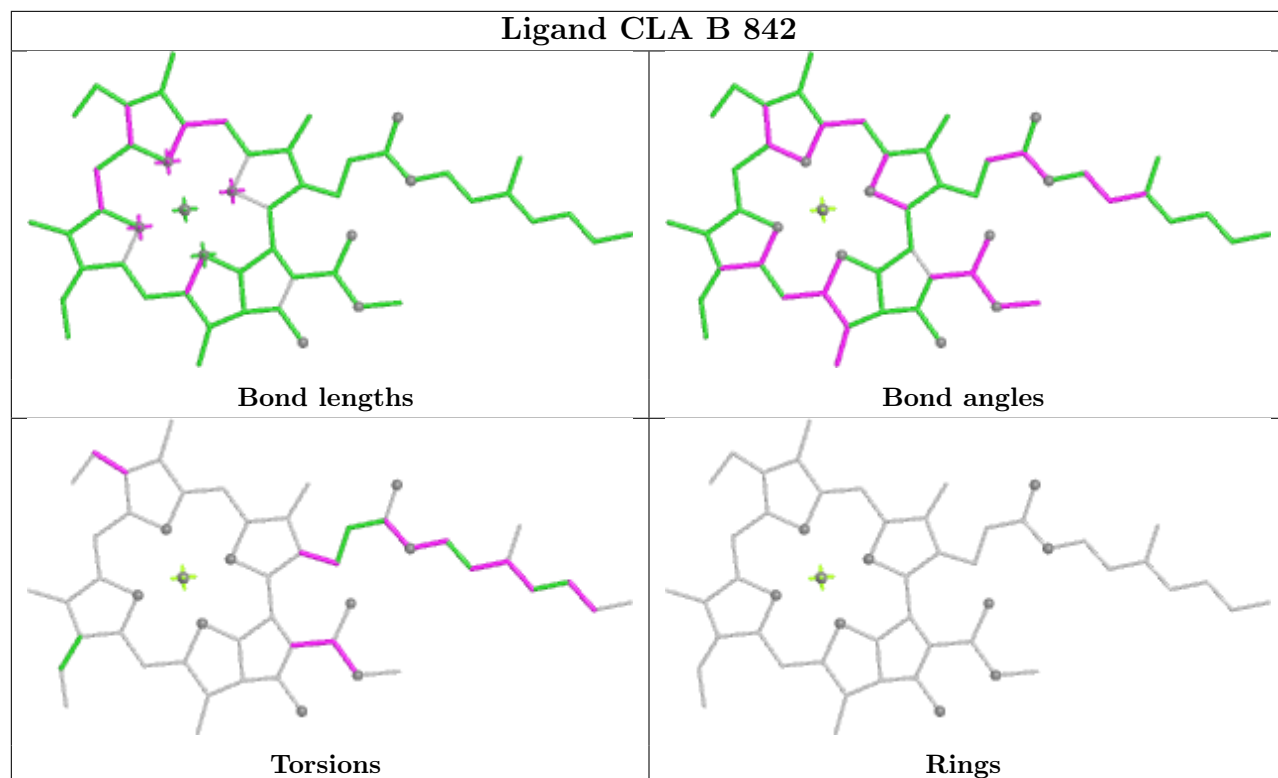
Torsions



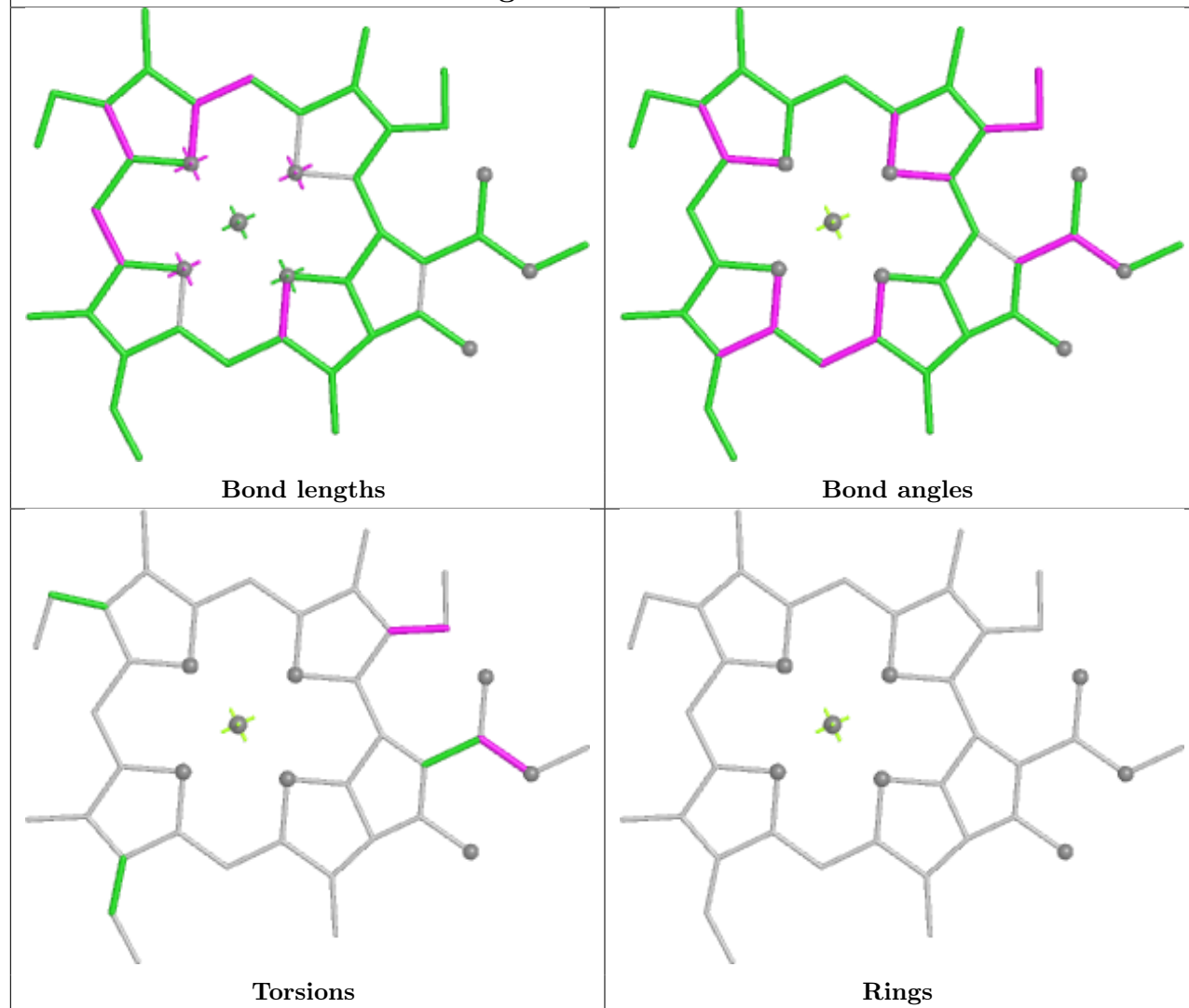
Rings

Ligand CLA e 217

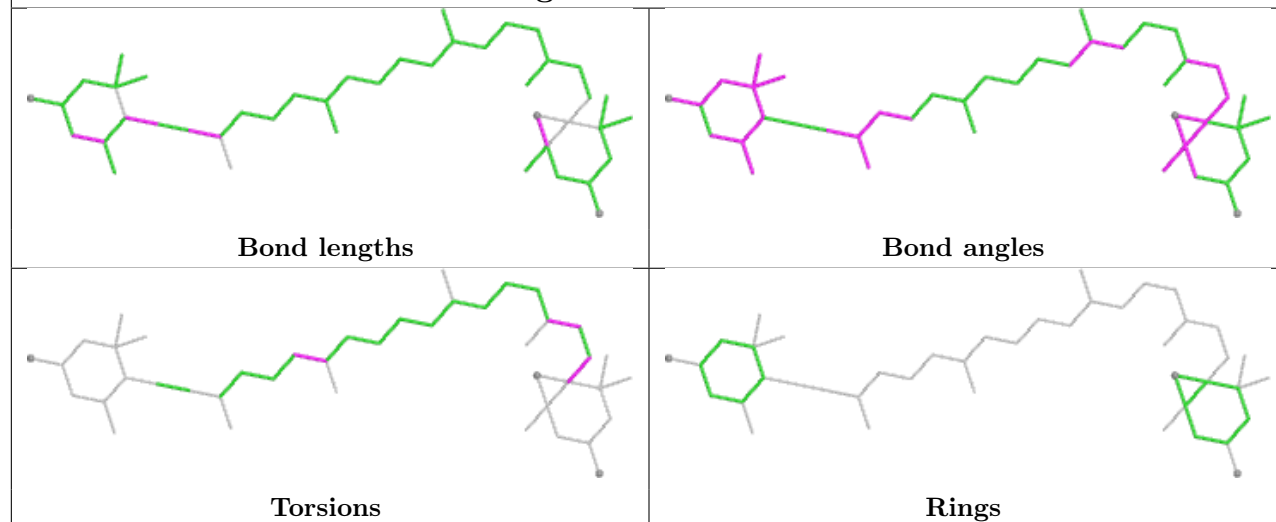


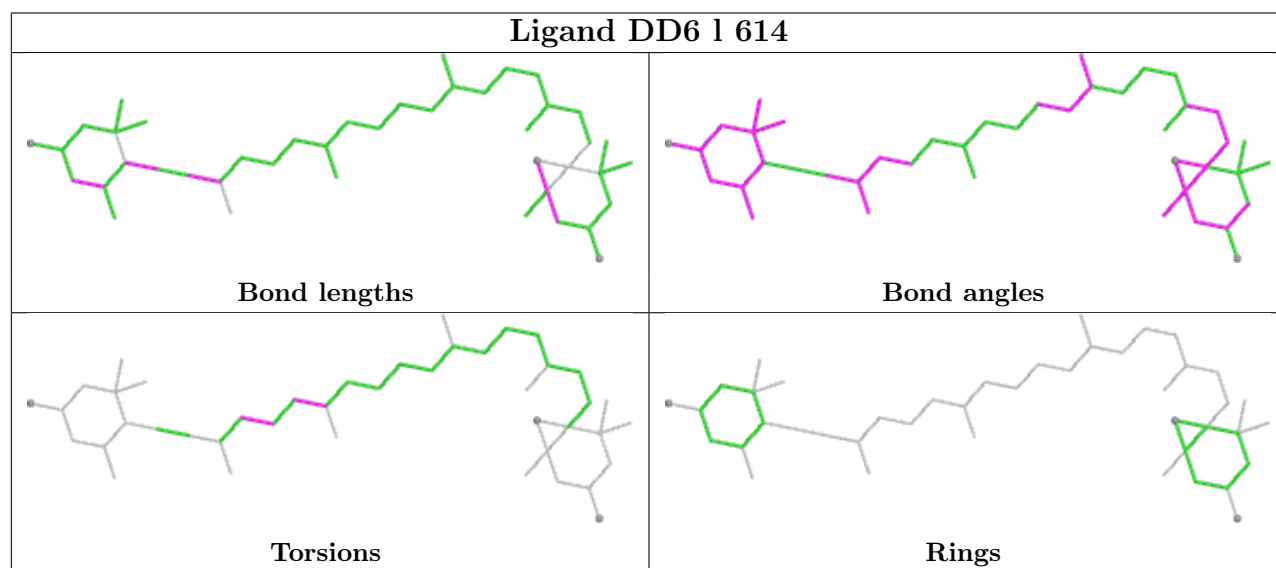
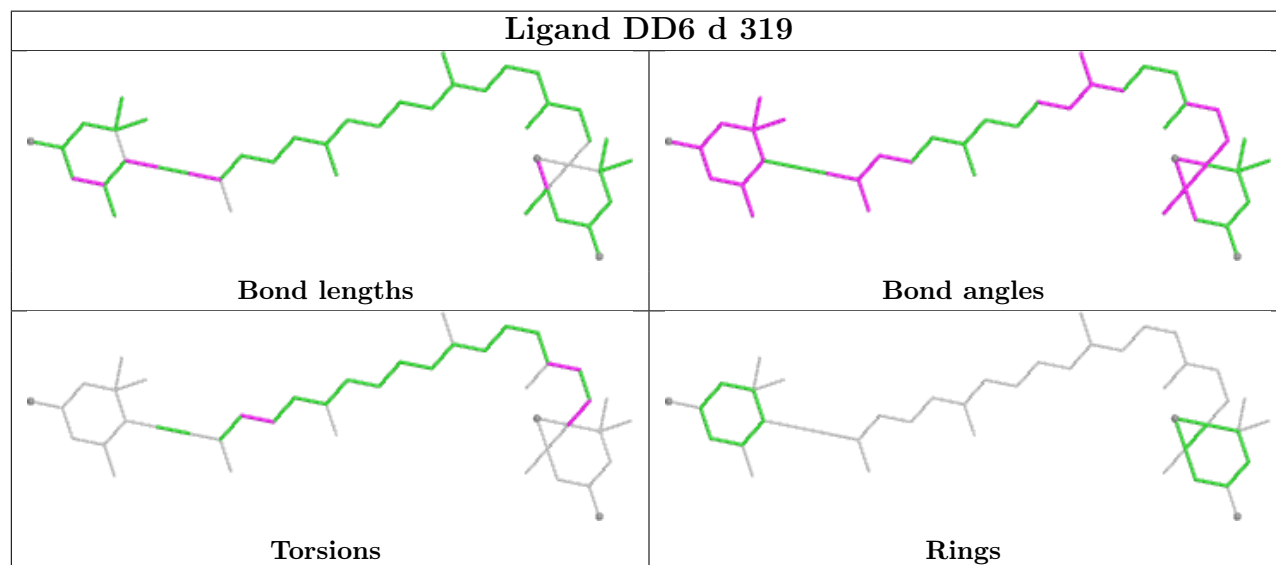
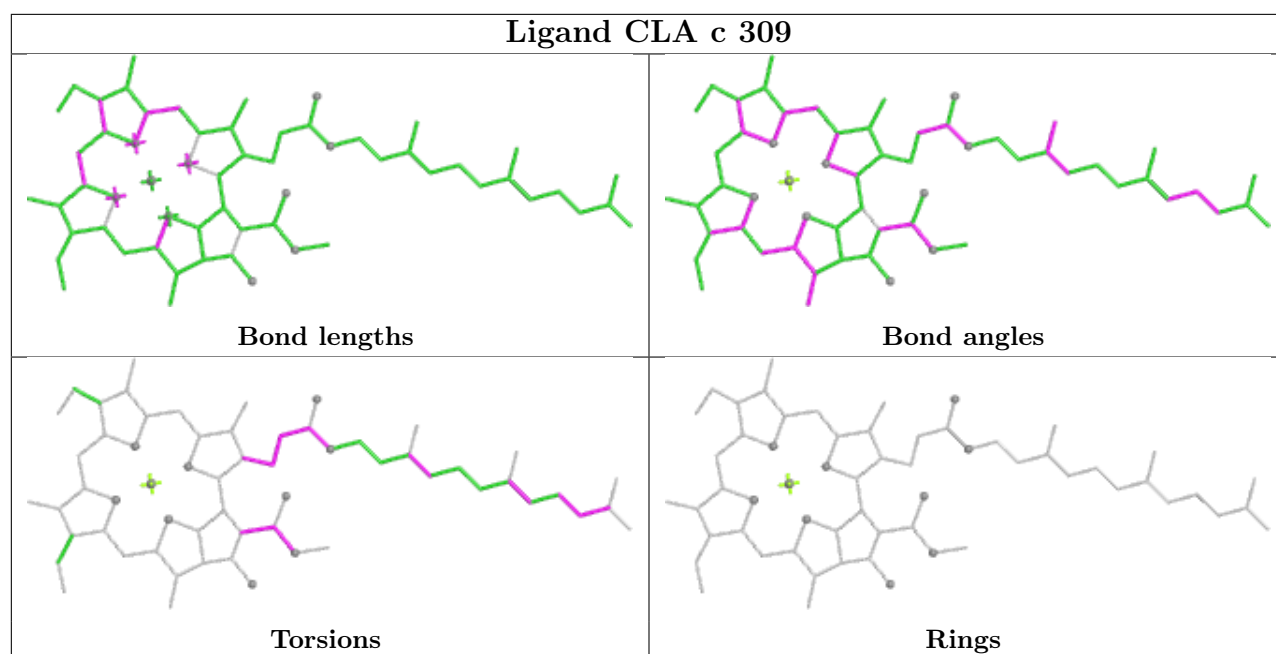


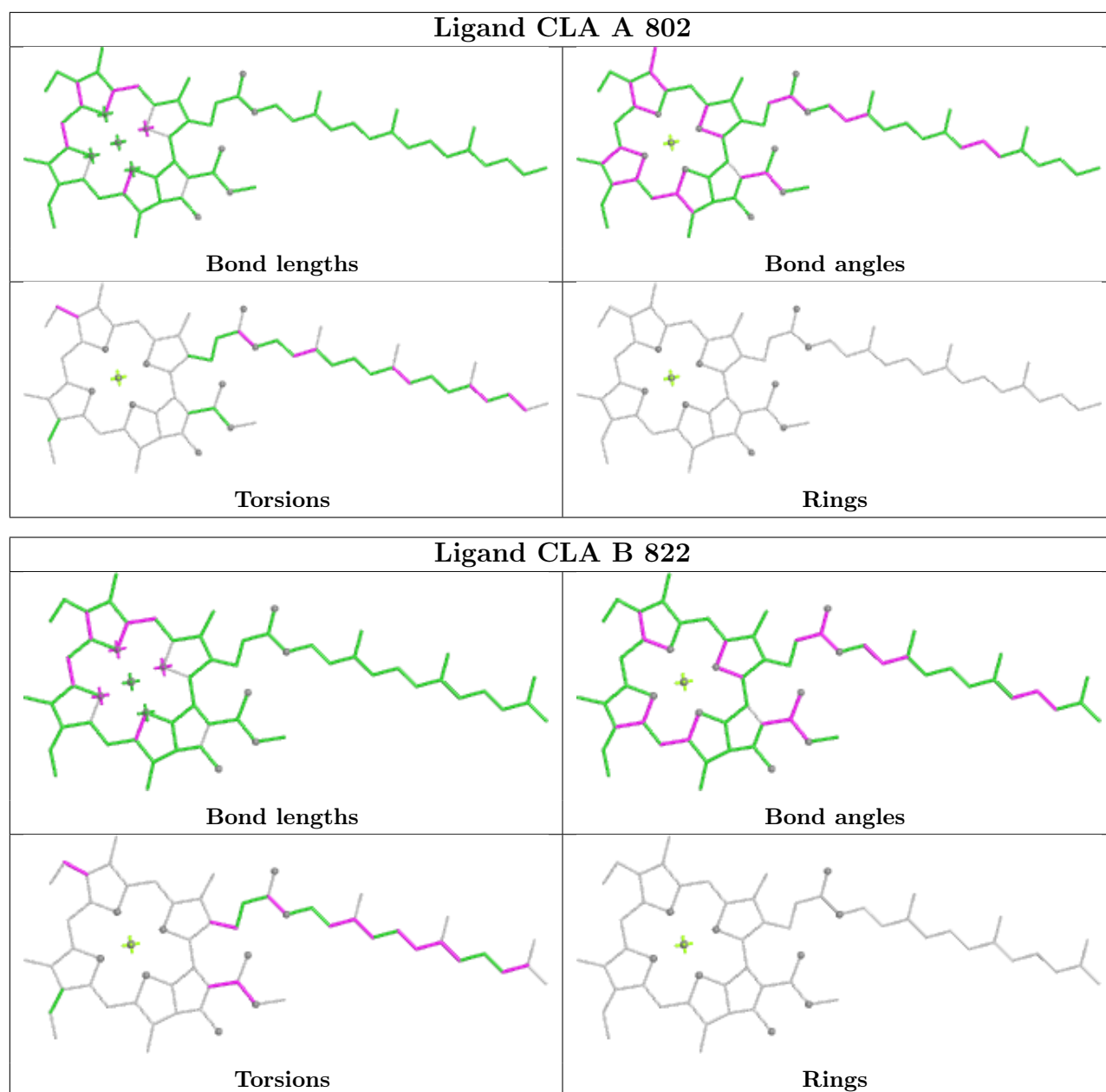
Ligand CLA d 315



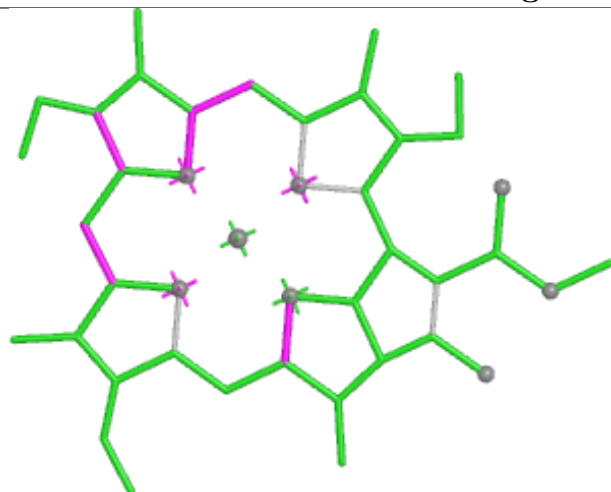
Ligand DD6 b 214



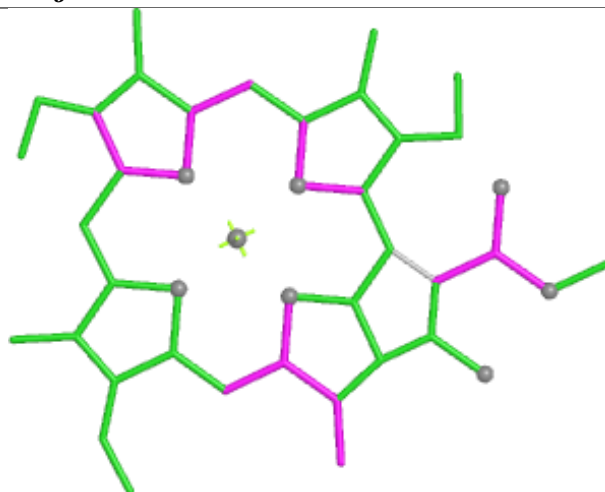




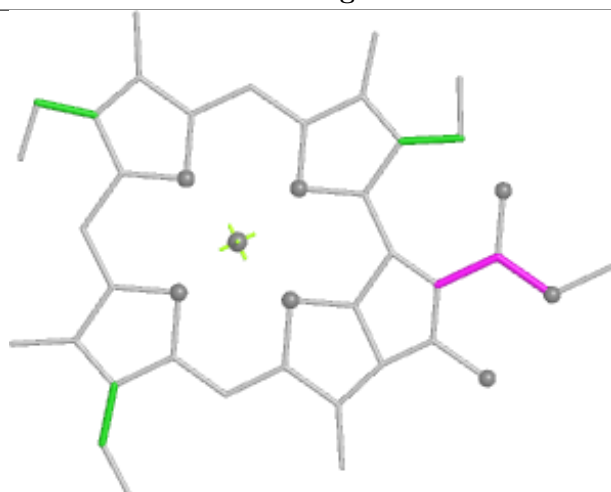
Ligand CLA j 205



Bond lengths



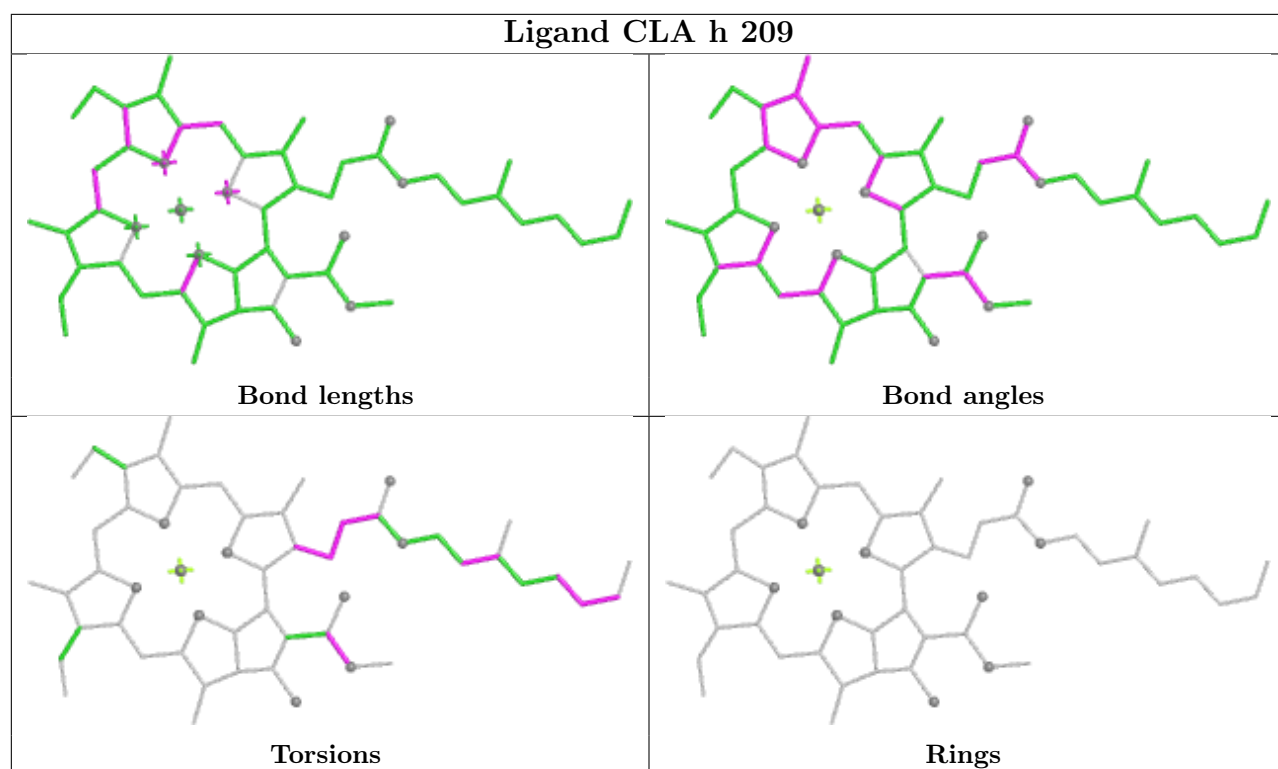
Bond angles



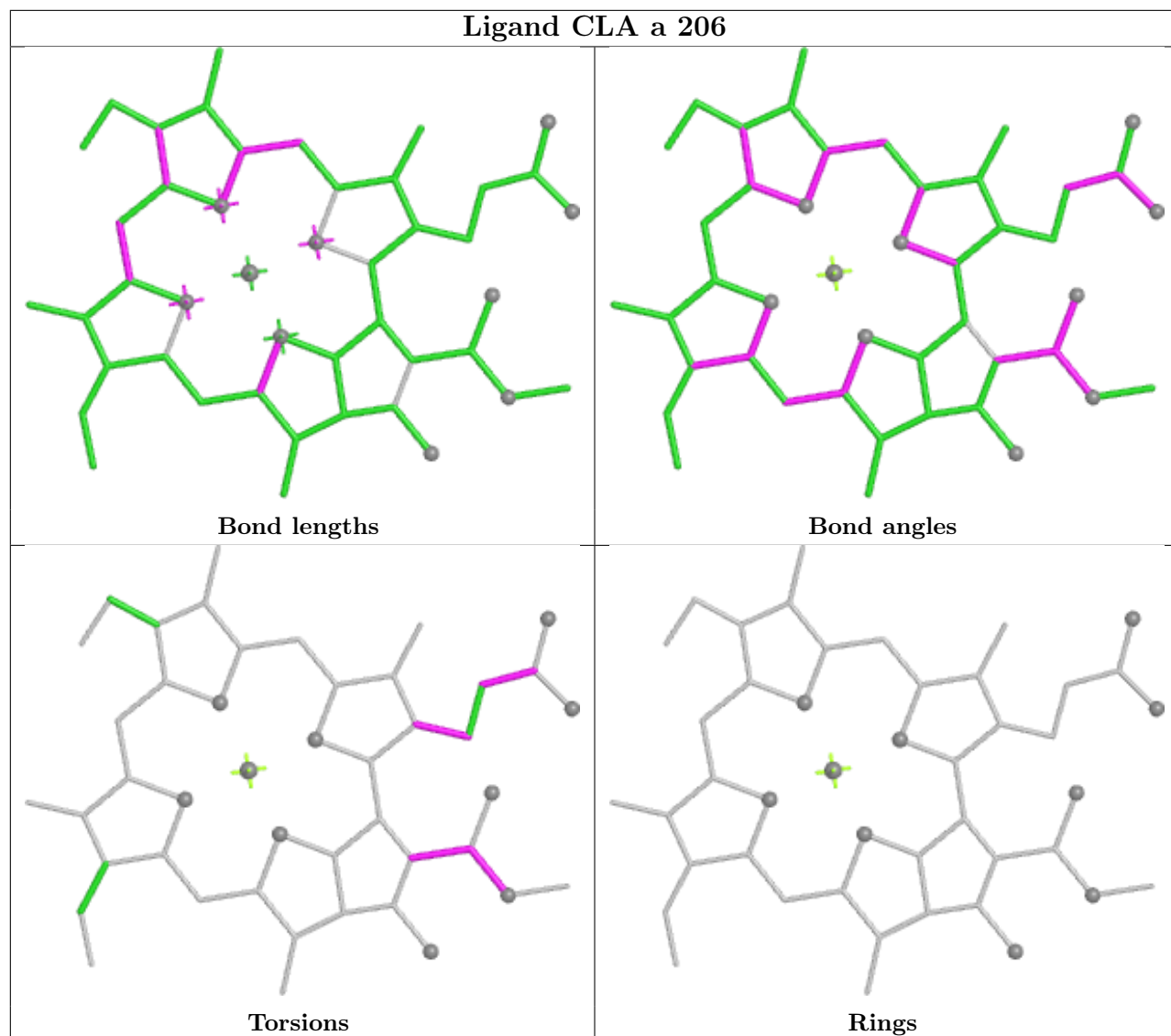
Torsions

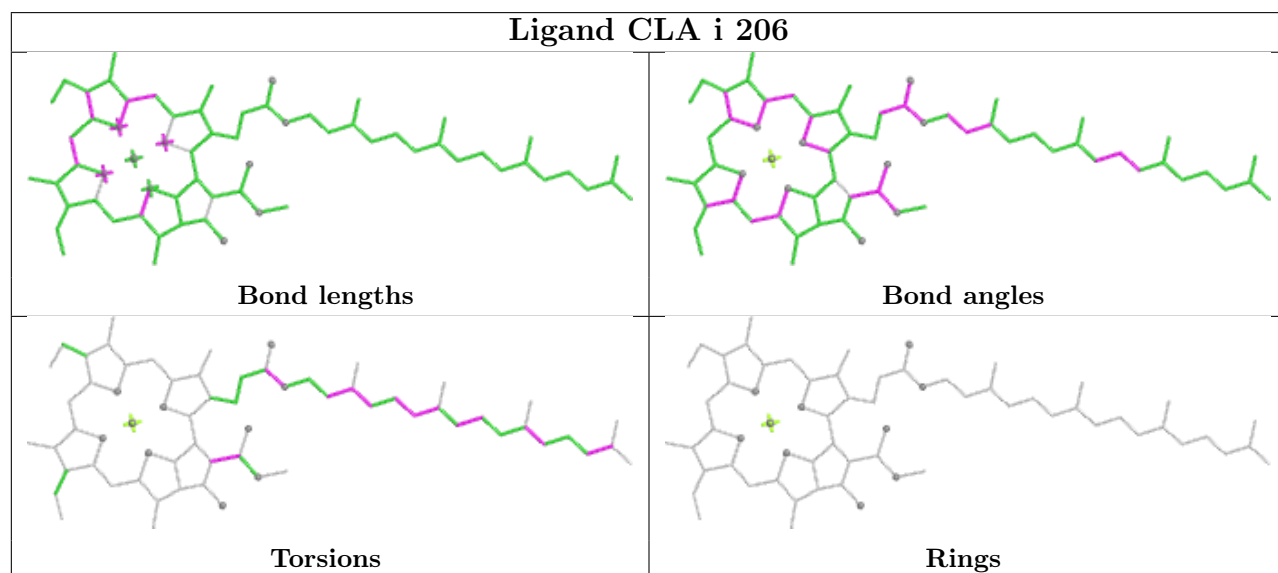
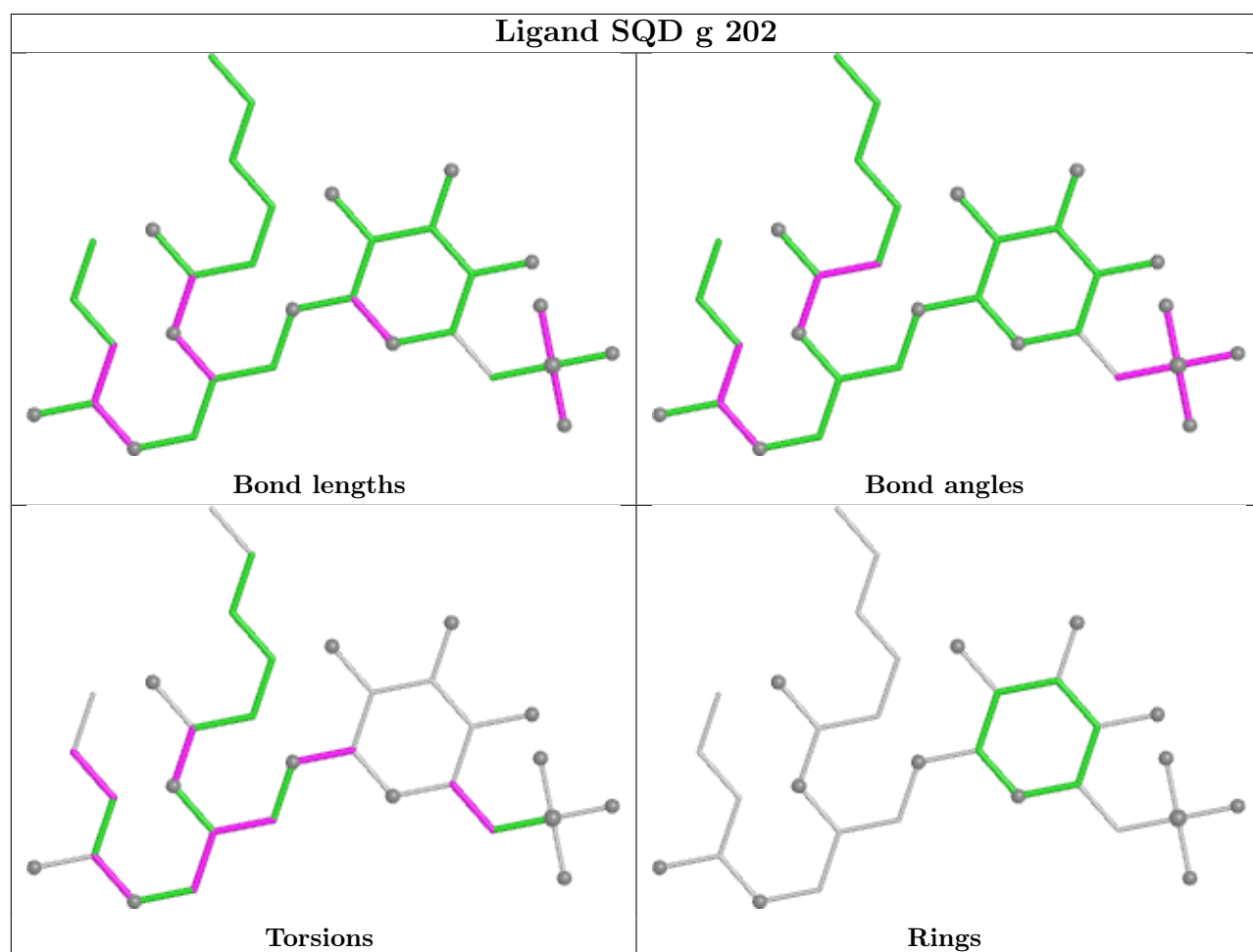


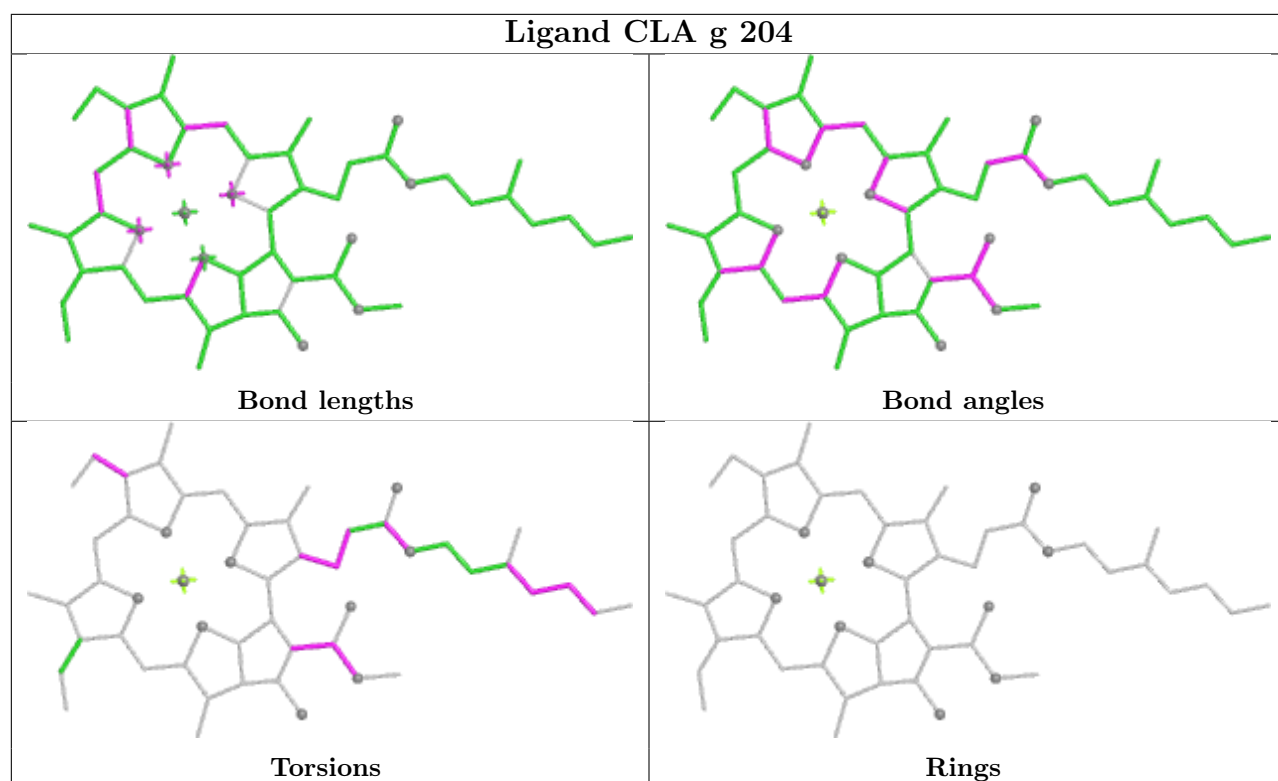
Rings



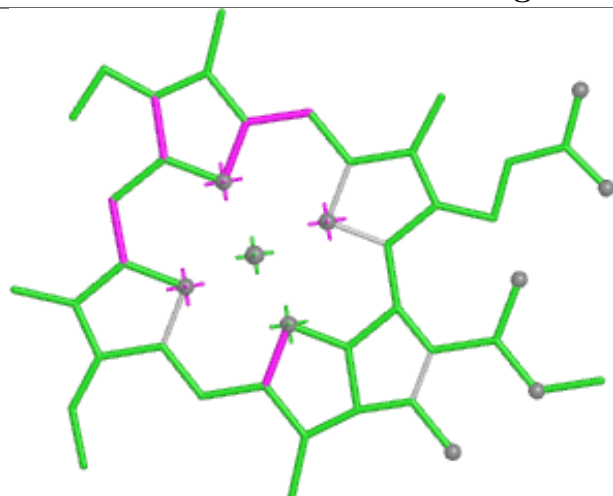
Ligand CLA a 206



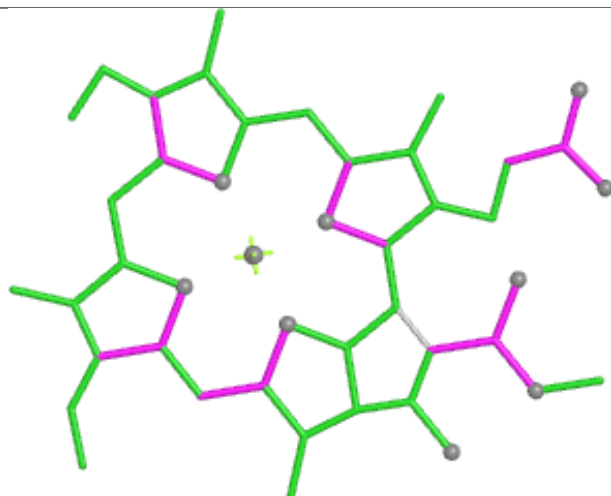




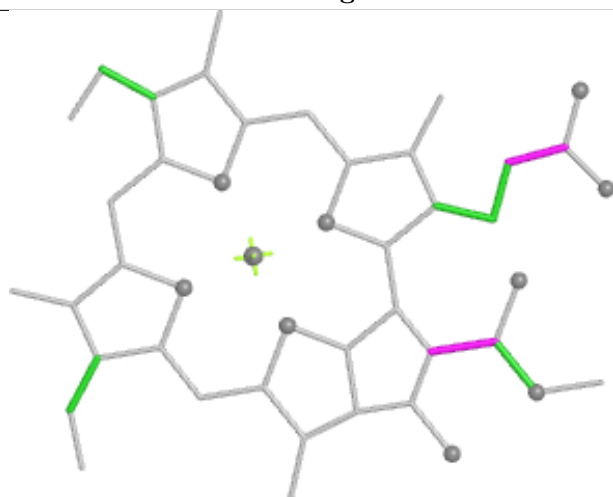
Ligand CLA A 851



Bond lengths



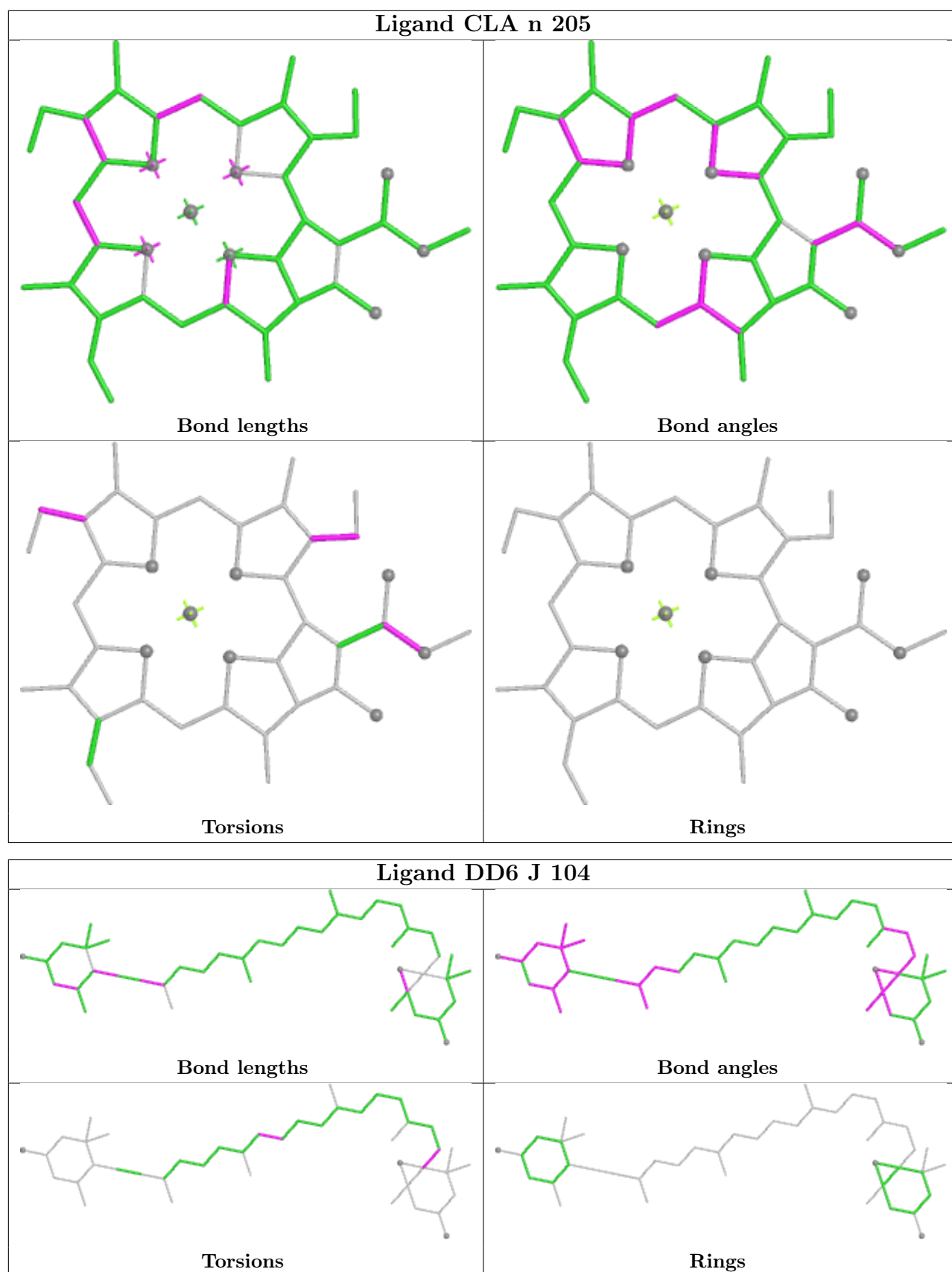
Bond angles

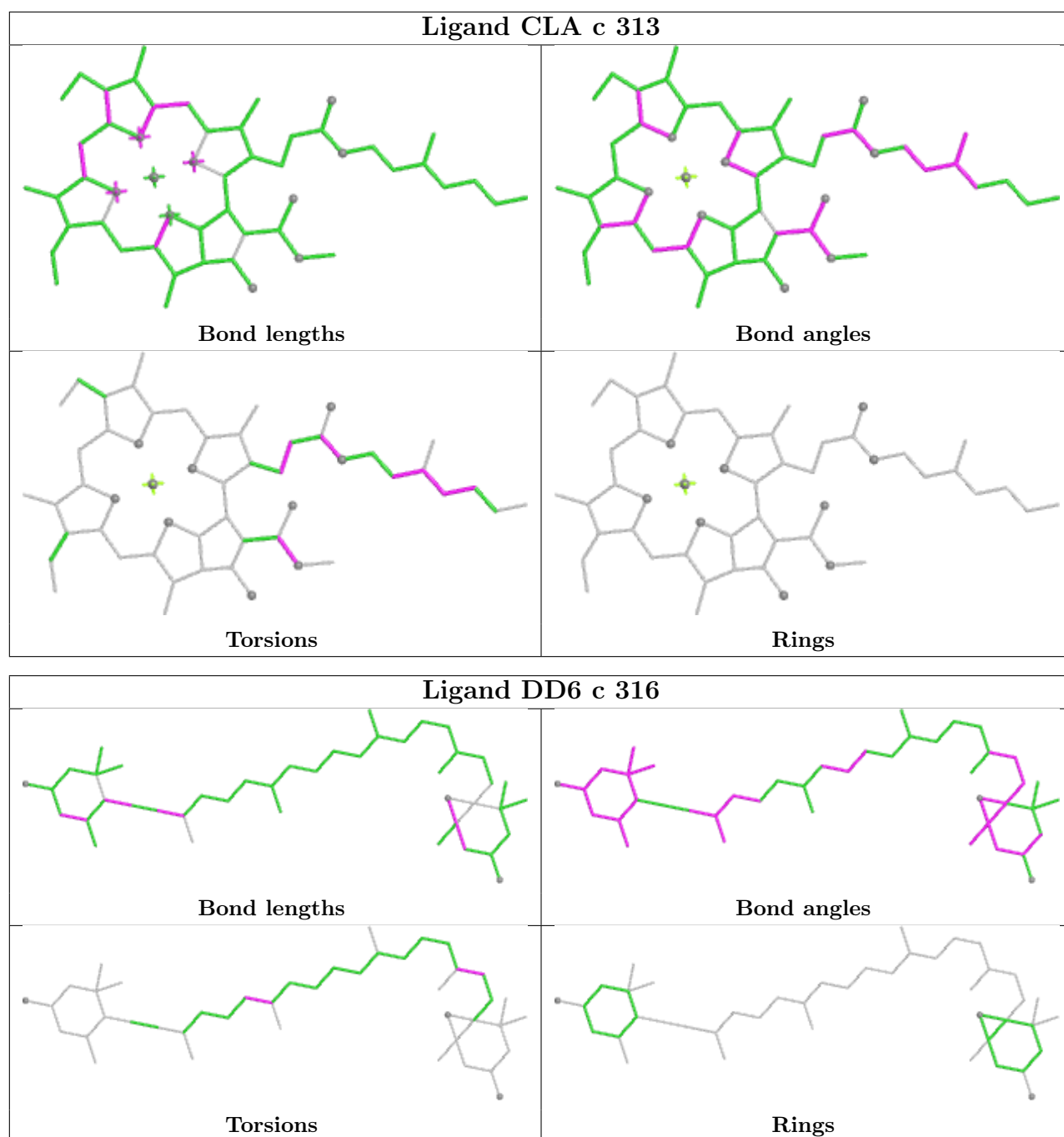


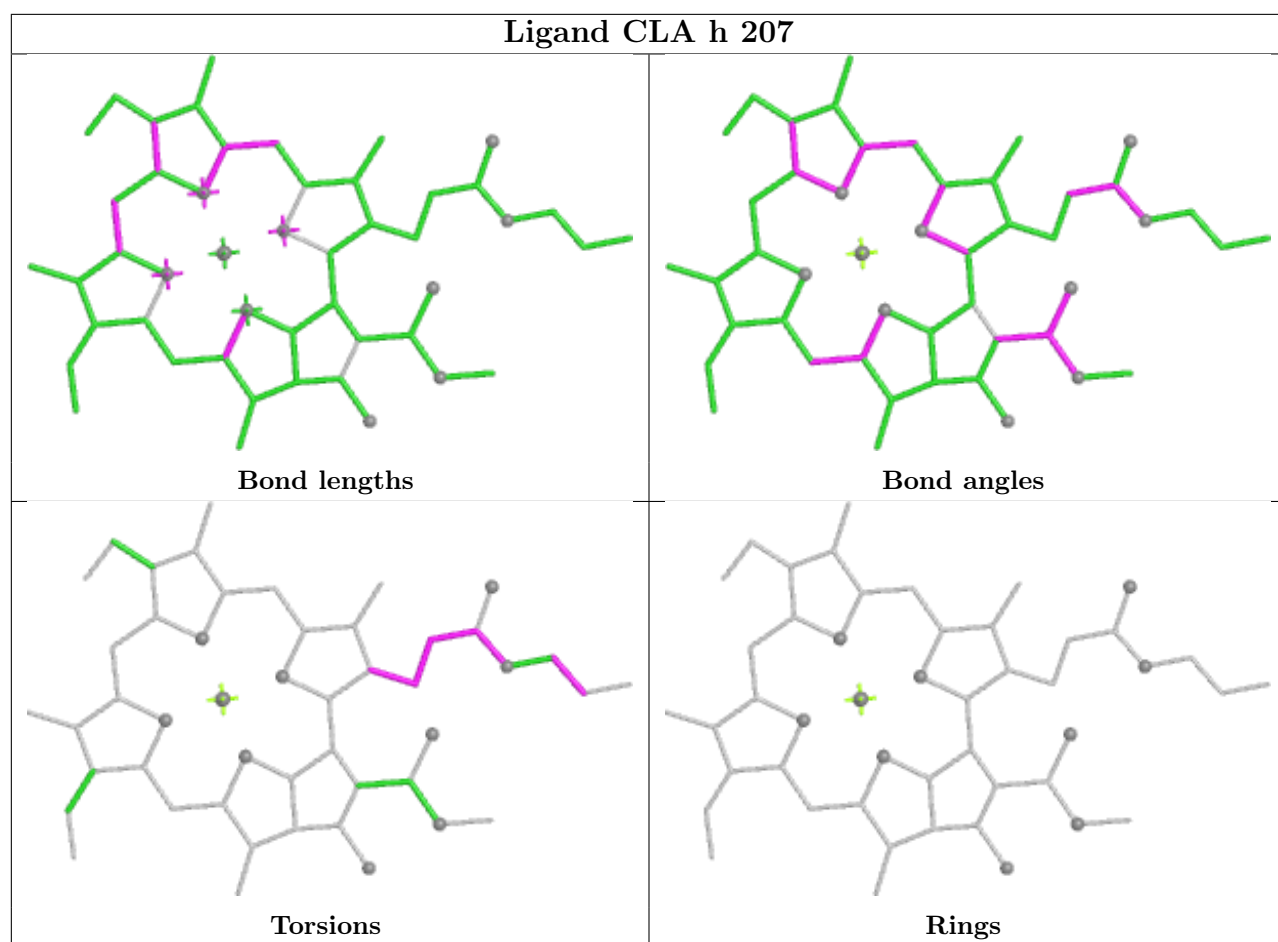
Torsions

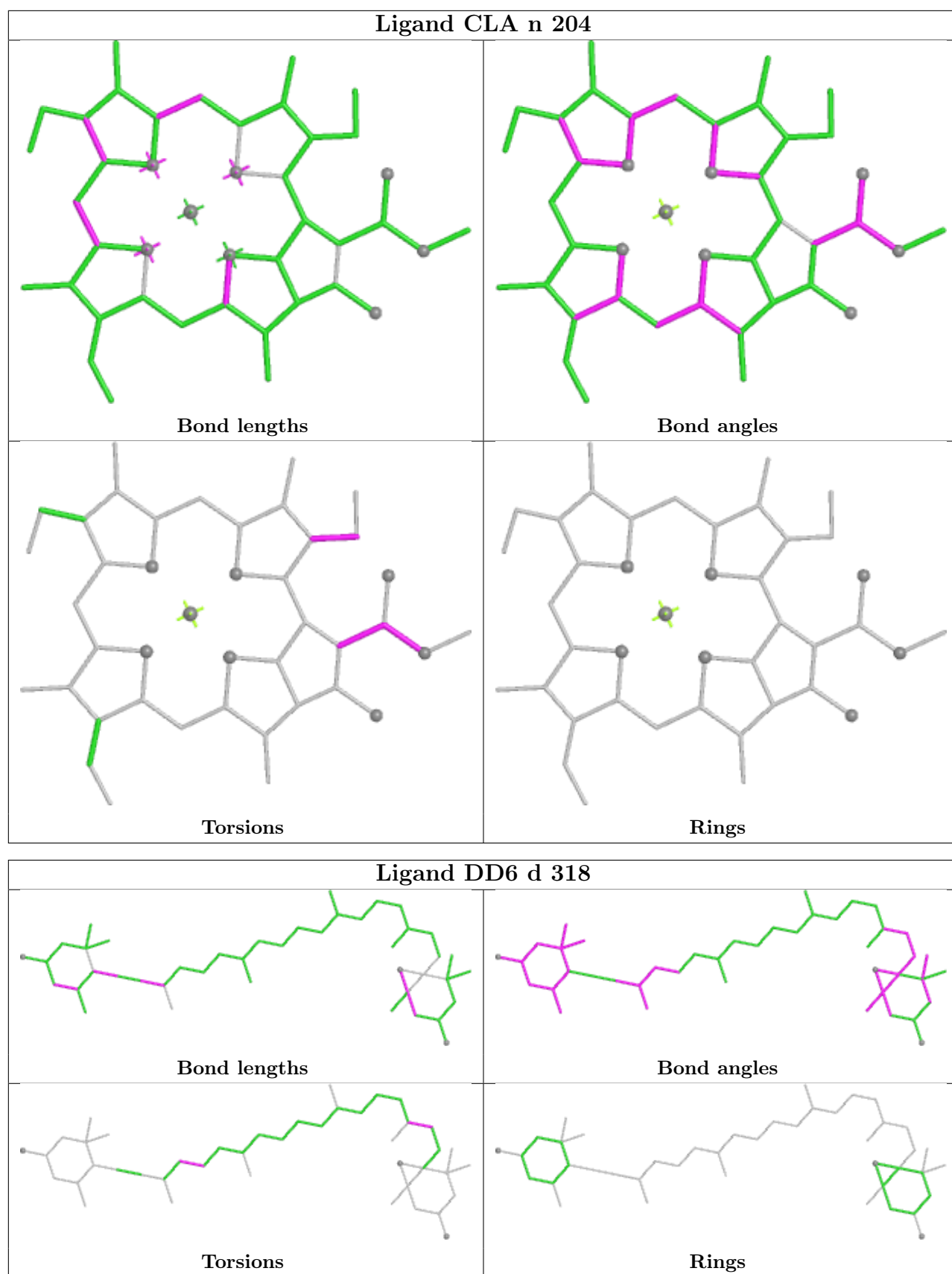


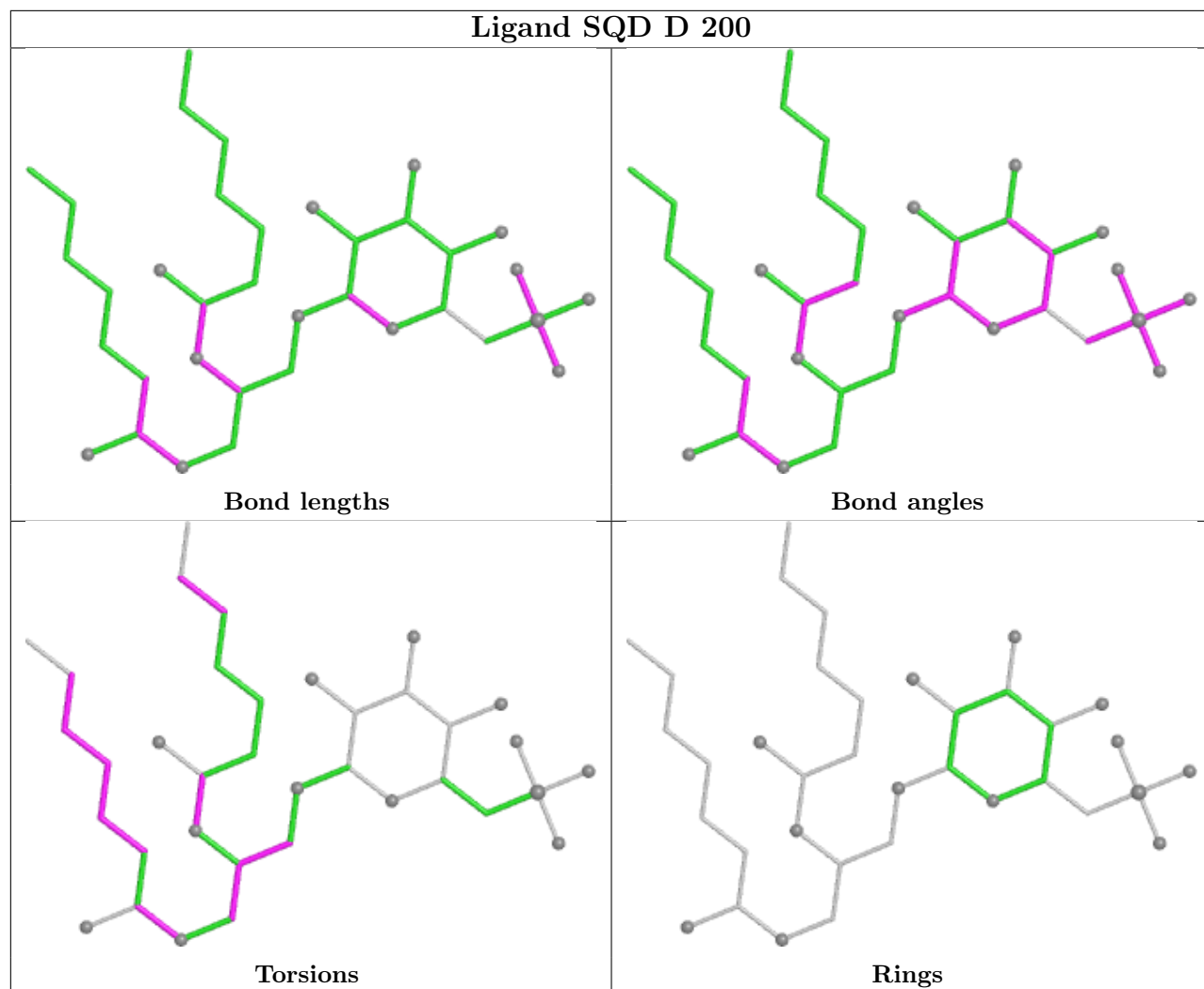
Rings



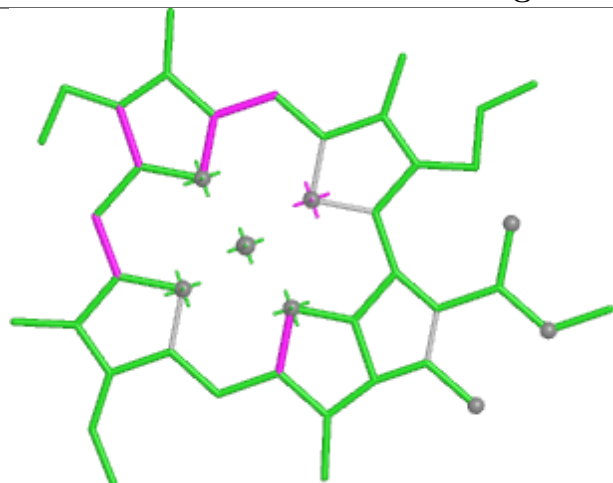




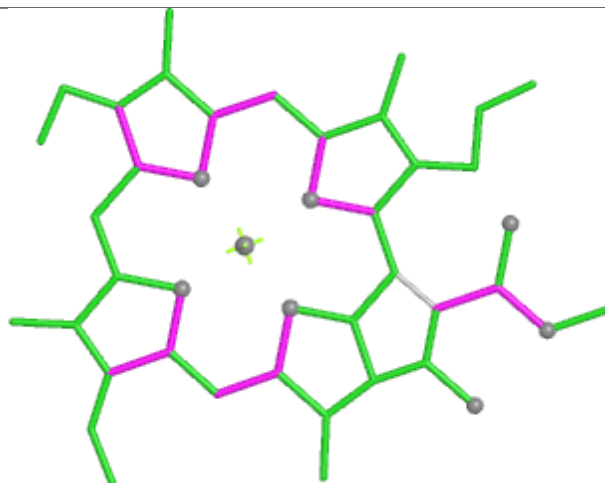




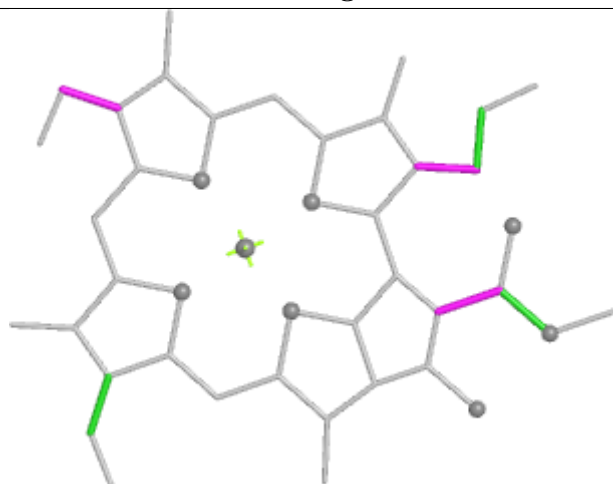
Ligand CLA A 847



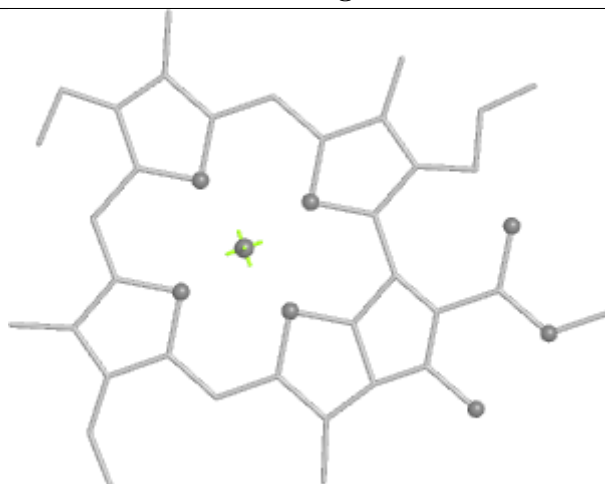
Bond lengths



Bond angles

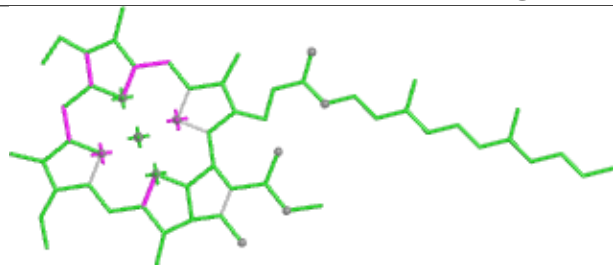


Torsions

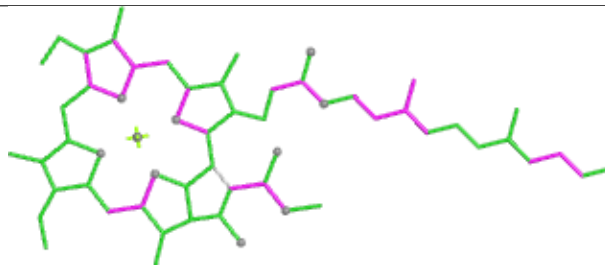


Rings

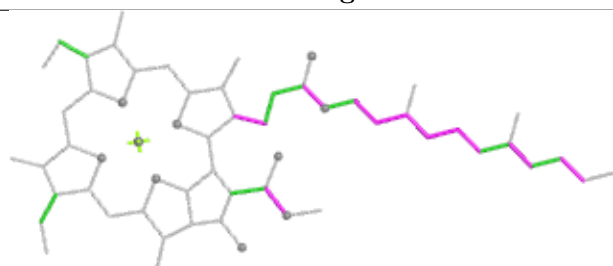
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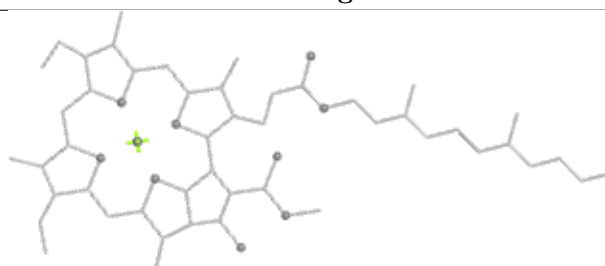
Bond lengths



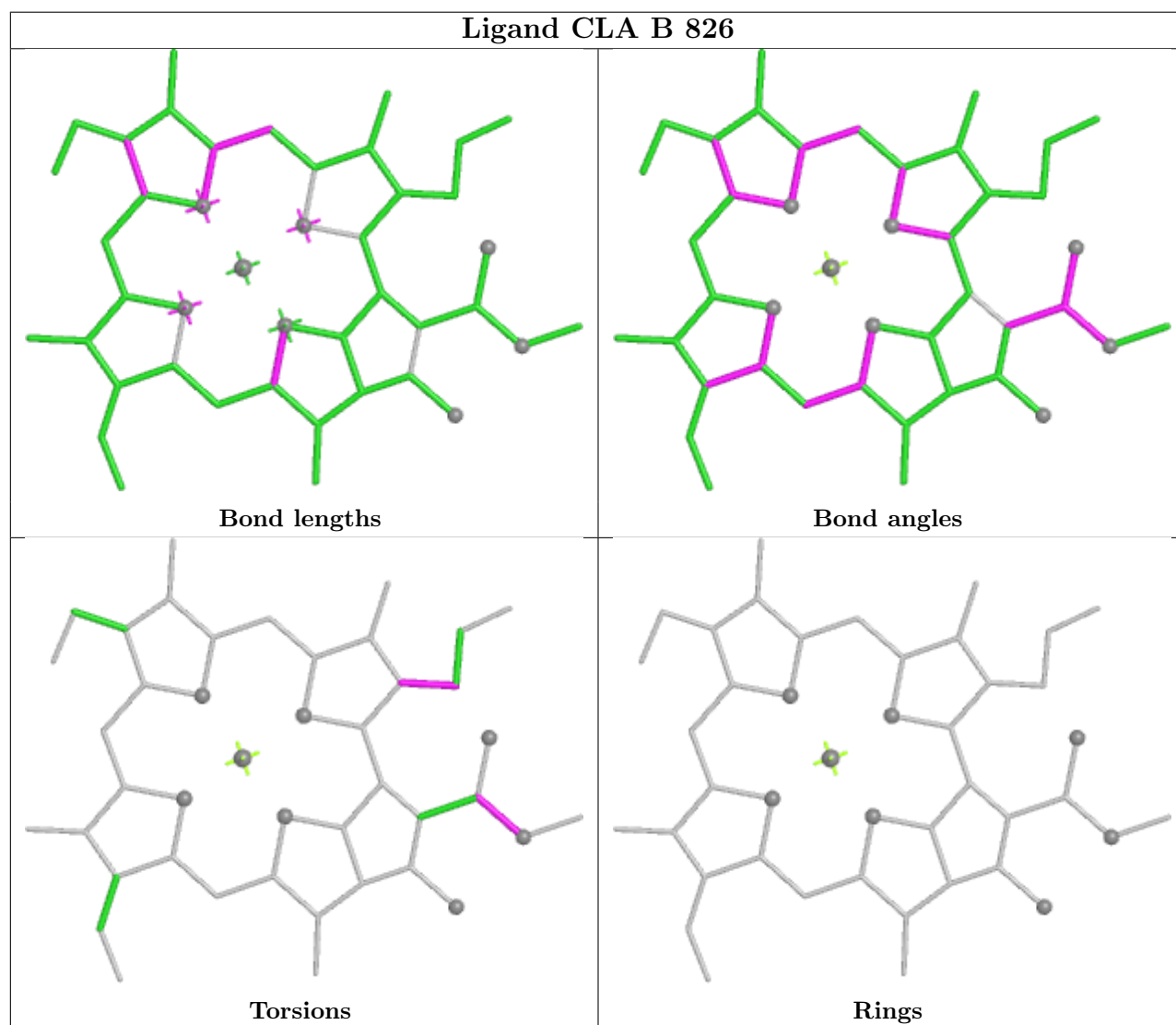
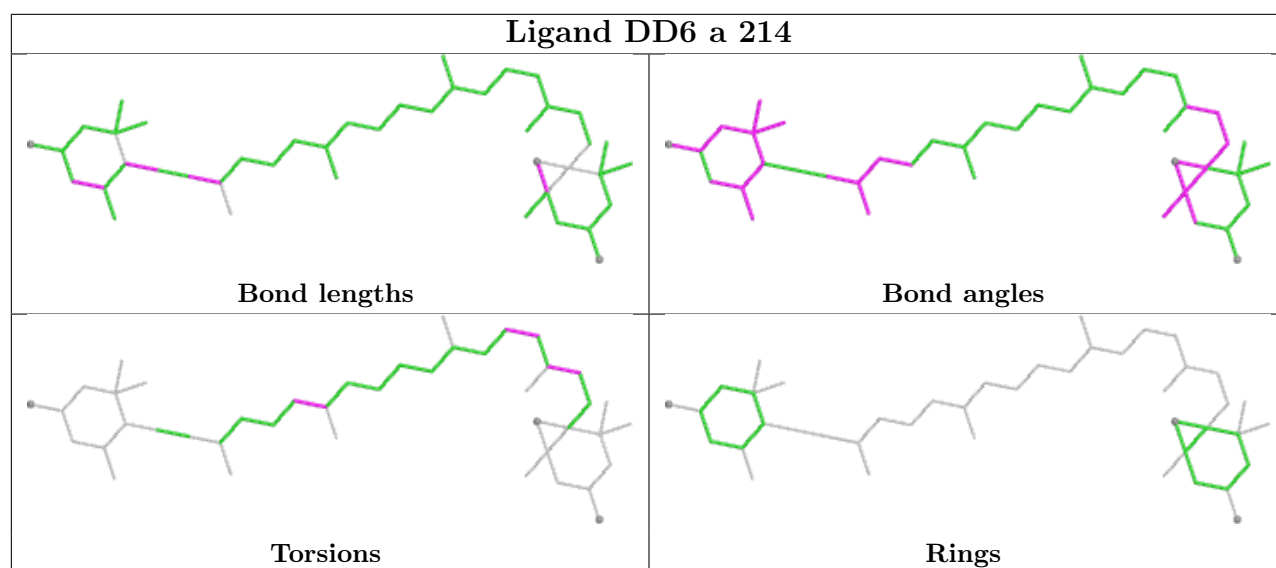
Bond angles

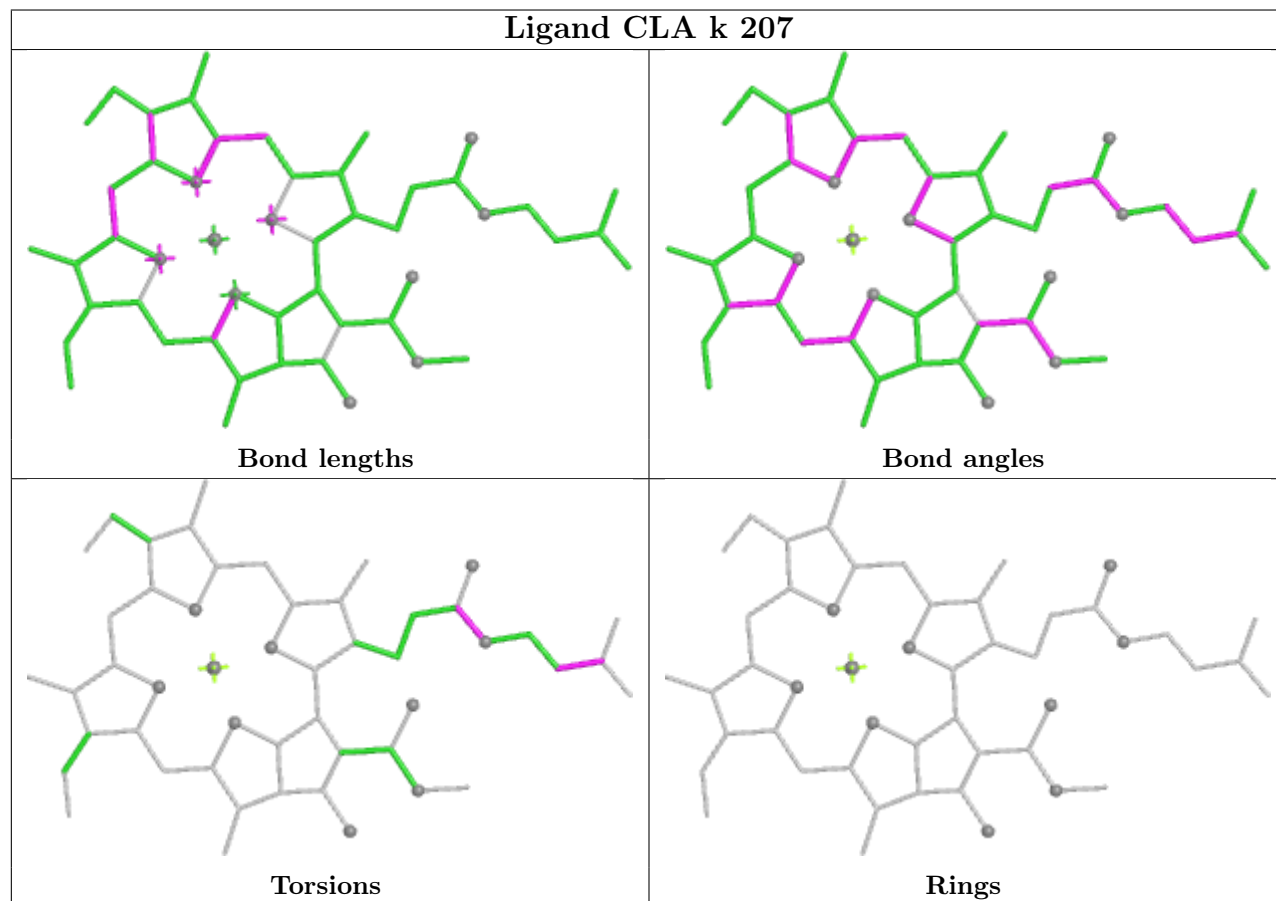
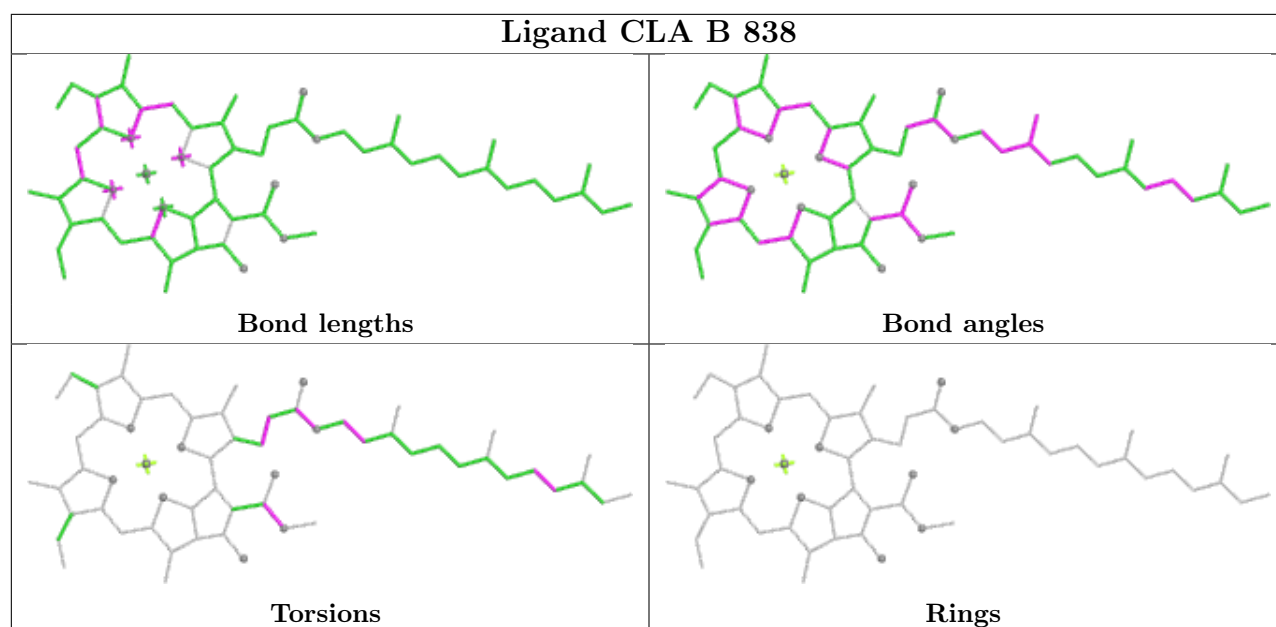


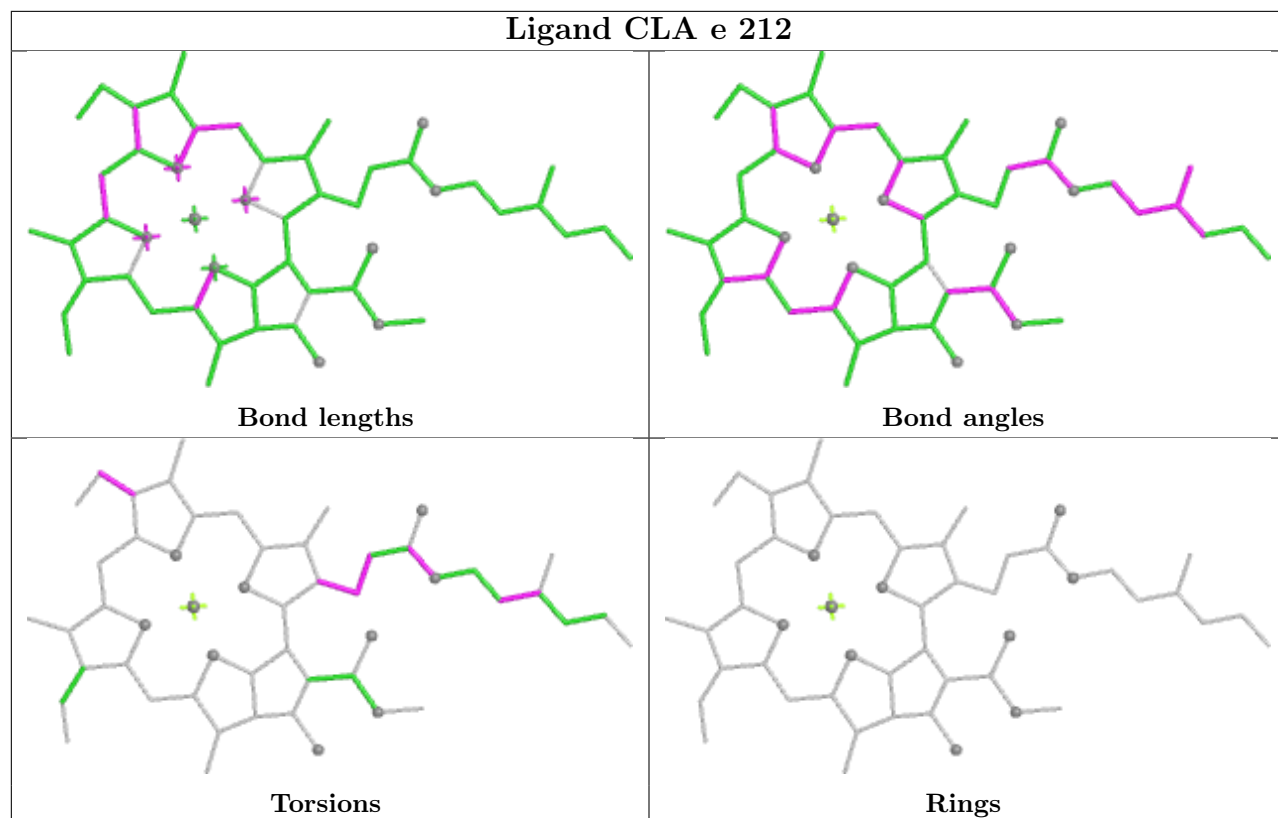
Torsions



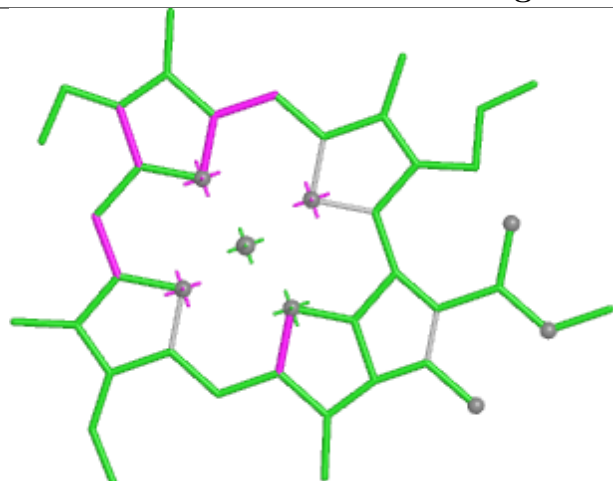
Rings



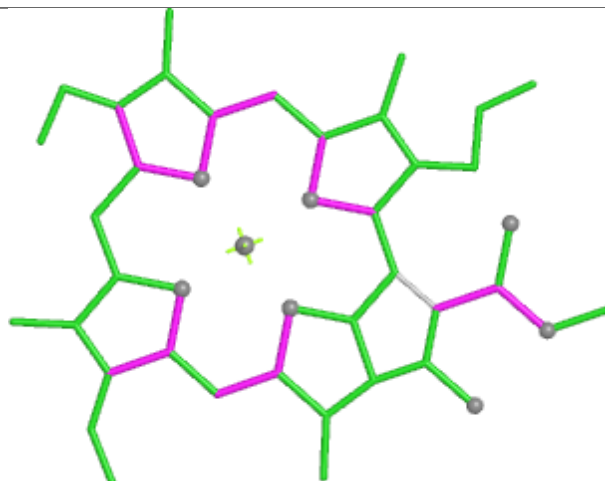




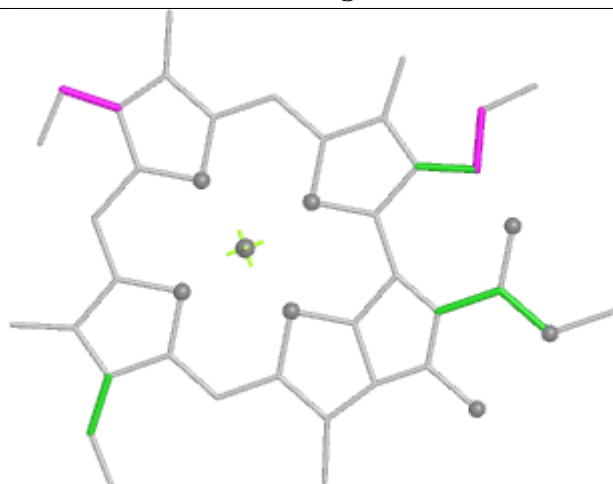
Ligand CLA B 808



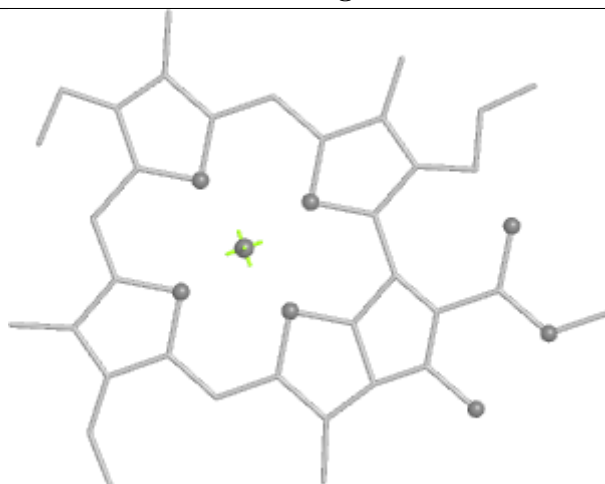
Bond lengths



Bond angles

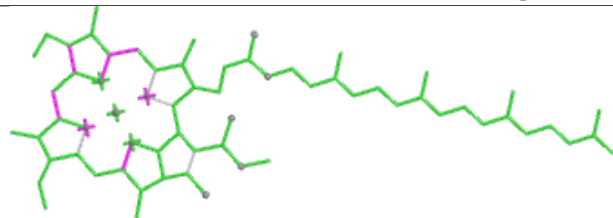


Torsions

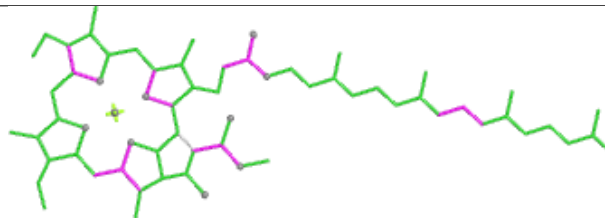


Rings

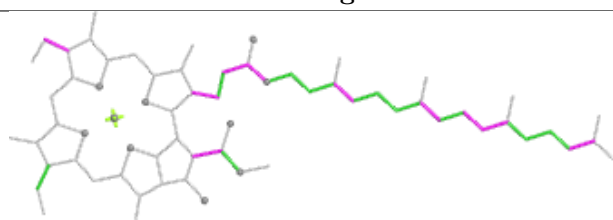
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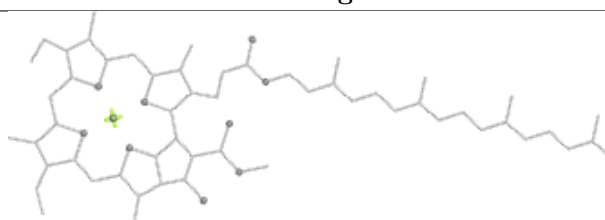
Bond lengths



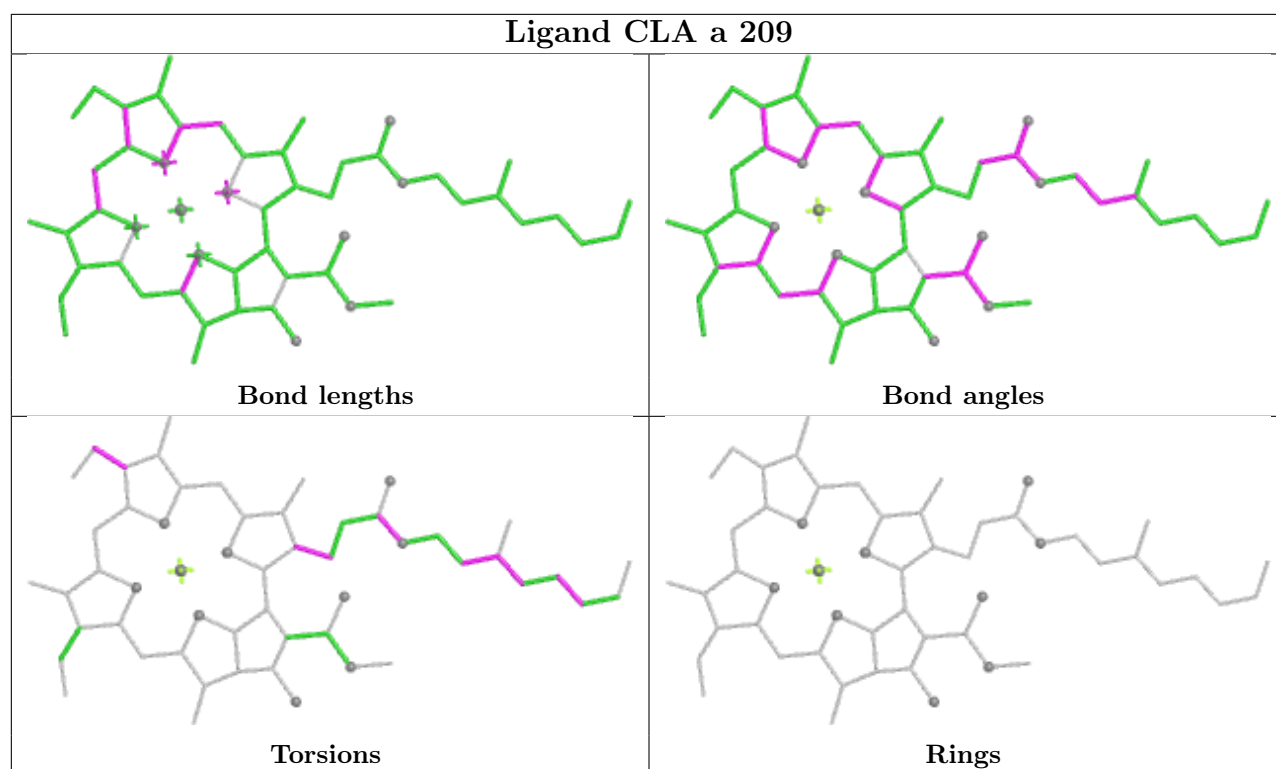
Bond angles



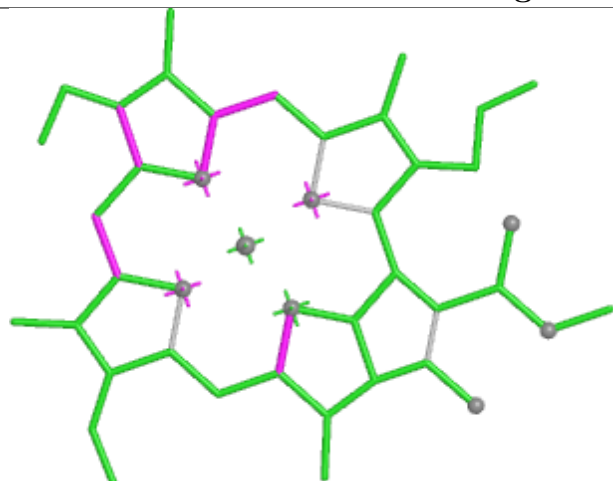
Torsions



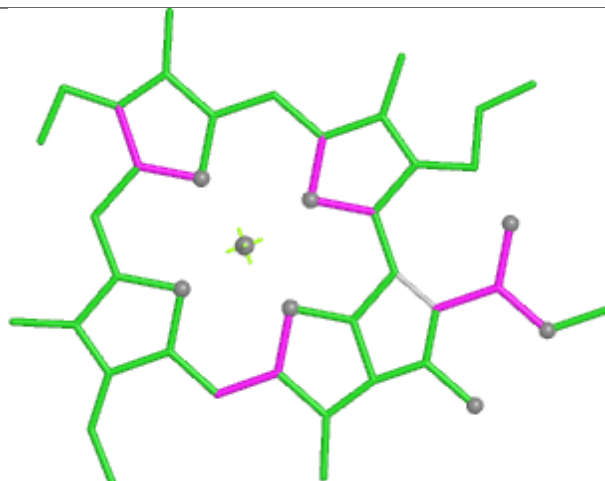
Rings



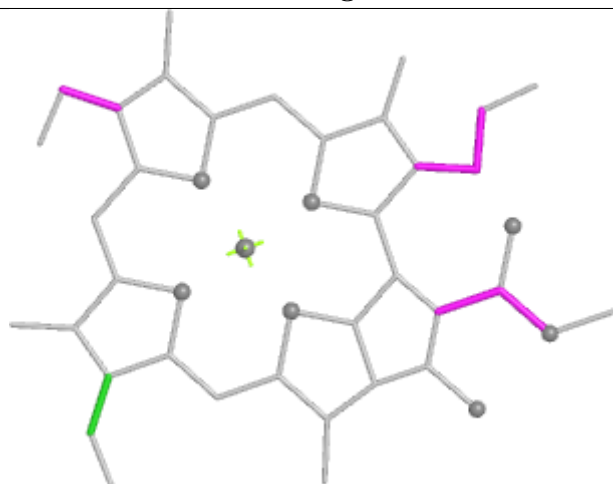
Ligand CLA B 820



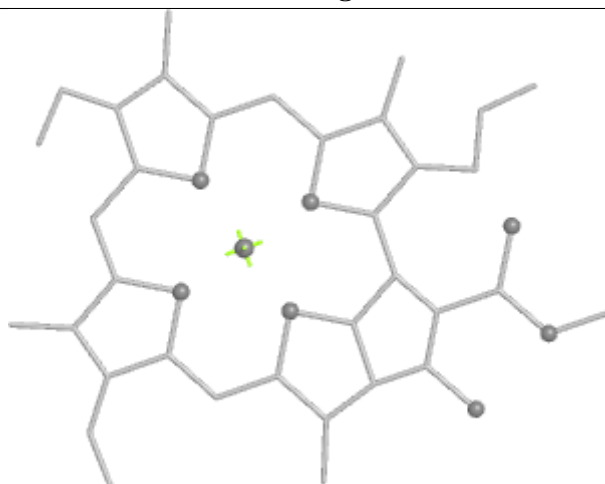
Bond lengths



Bond angles

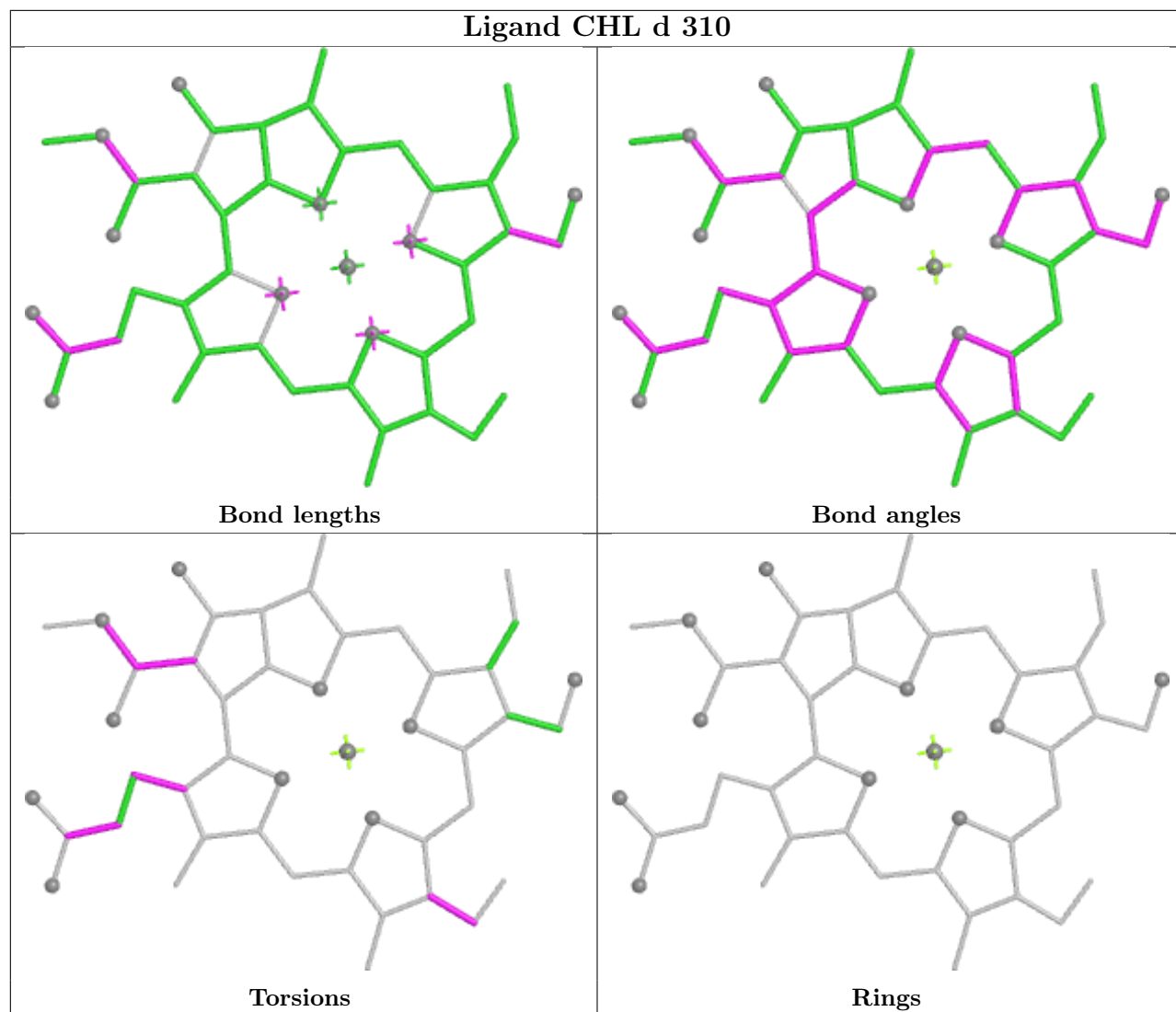


Torsions

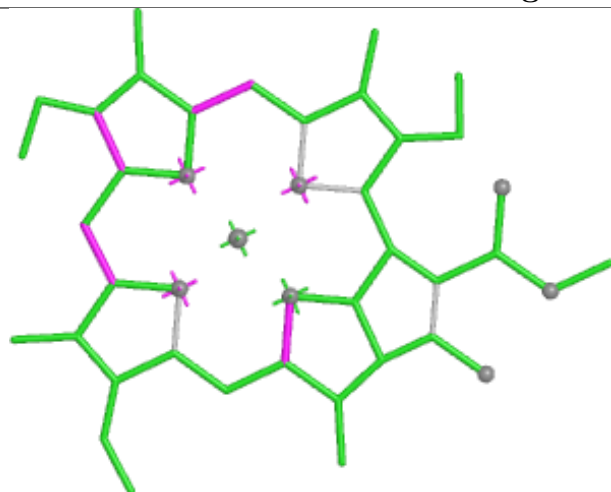


Rings

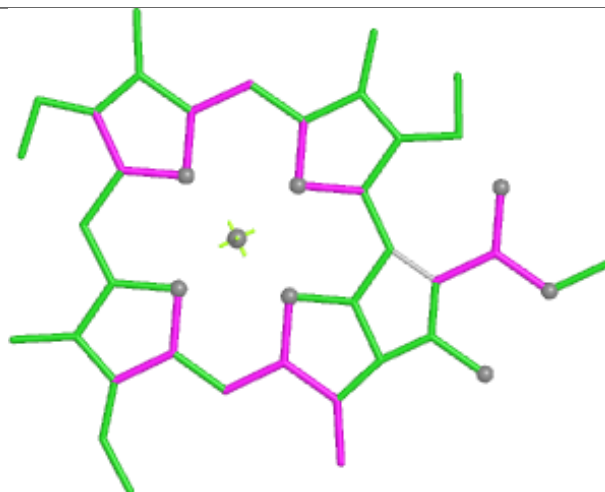
Ligand CHL d 310



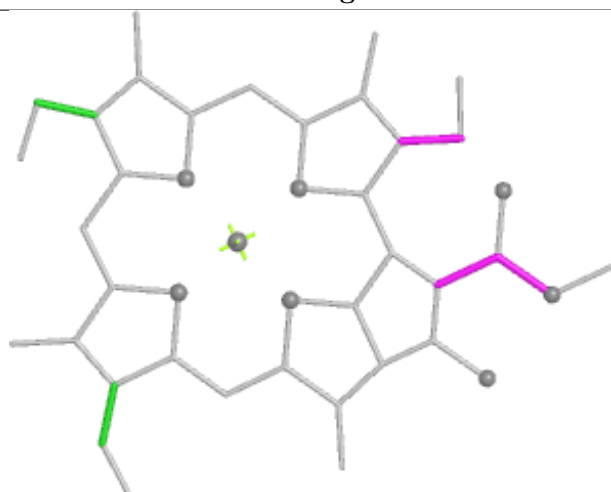
Ligand CLA f 611



Bond lengths



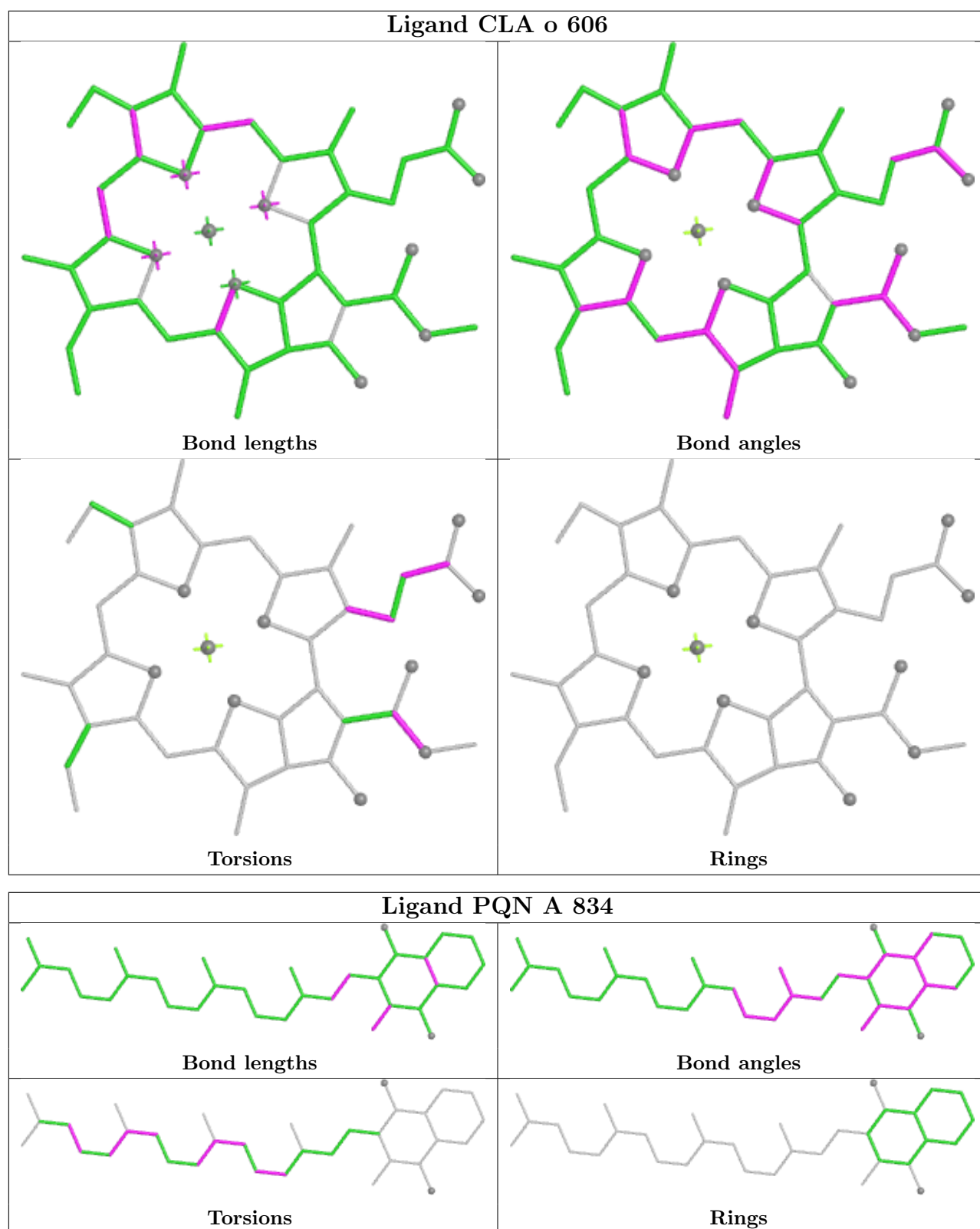
Bond angles



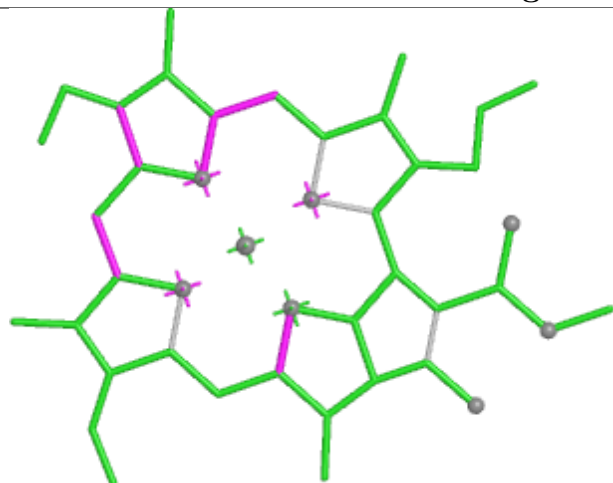
Torsions



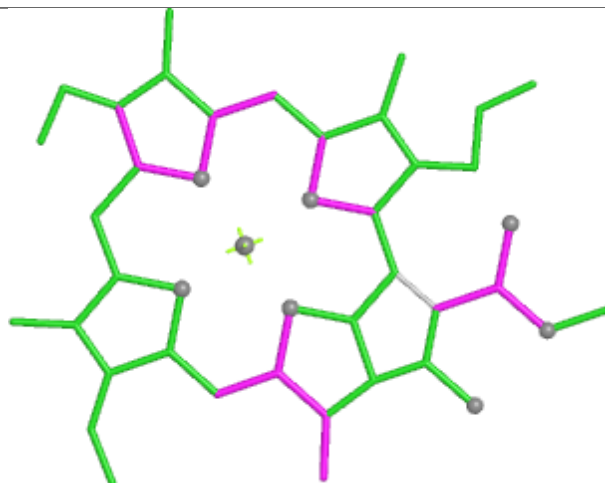
Rings



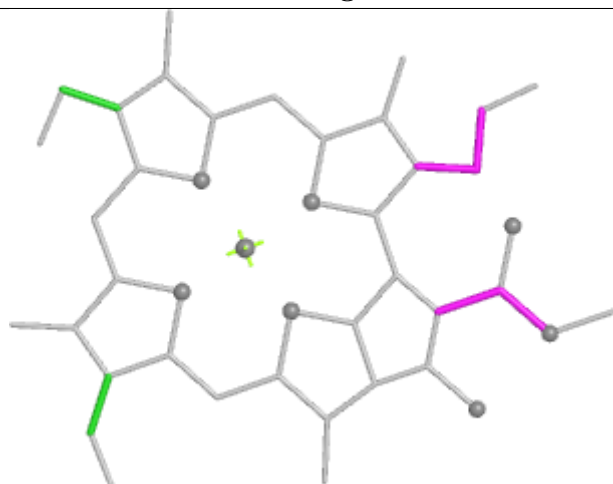
Ligand CLA i 210



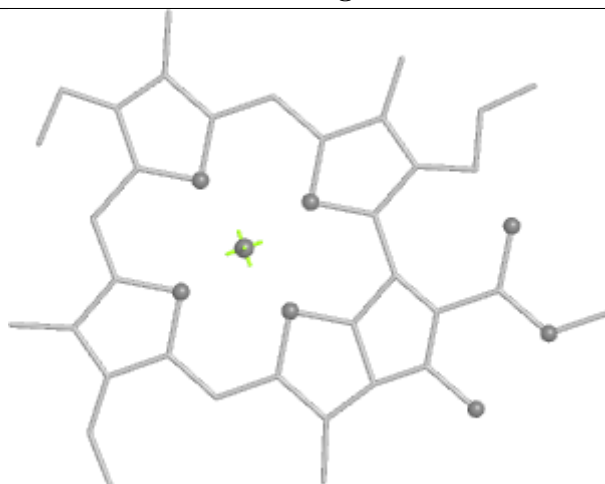
Bond lengths



Bond angles

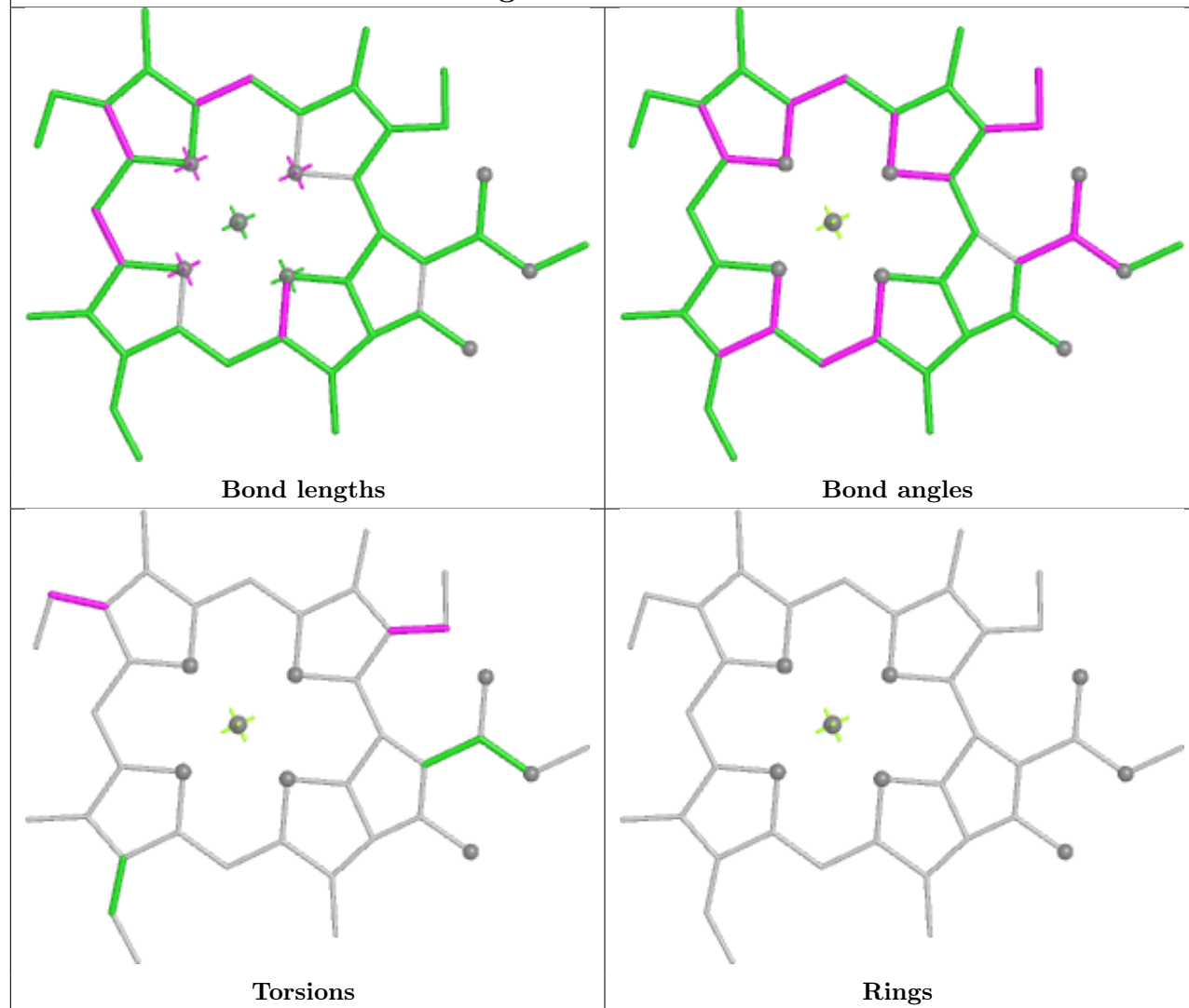


Torsions

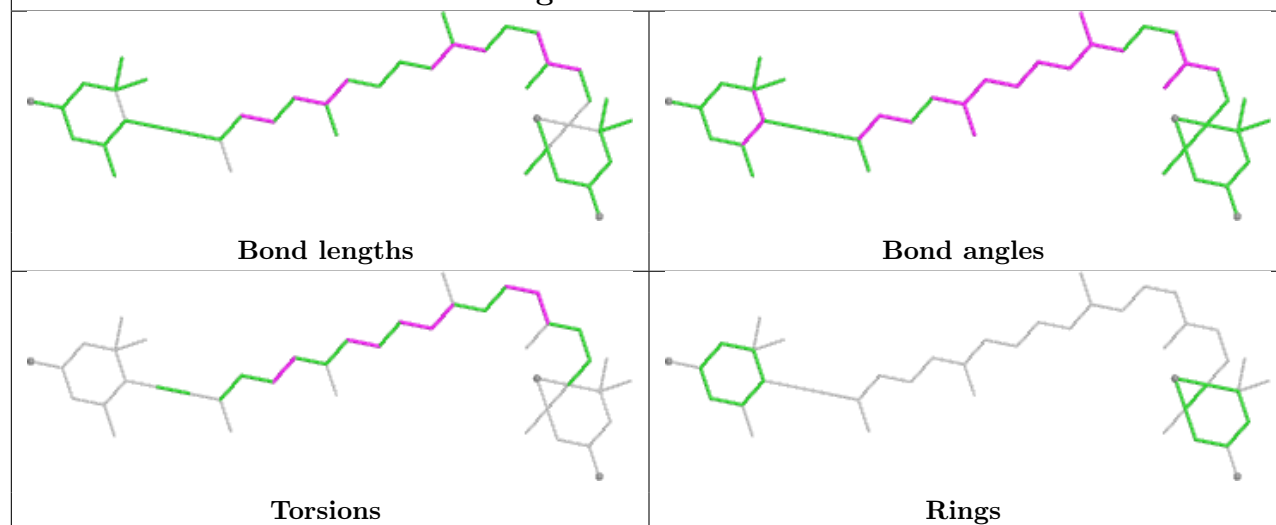


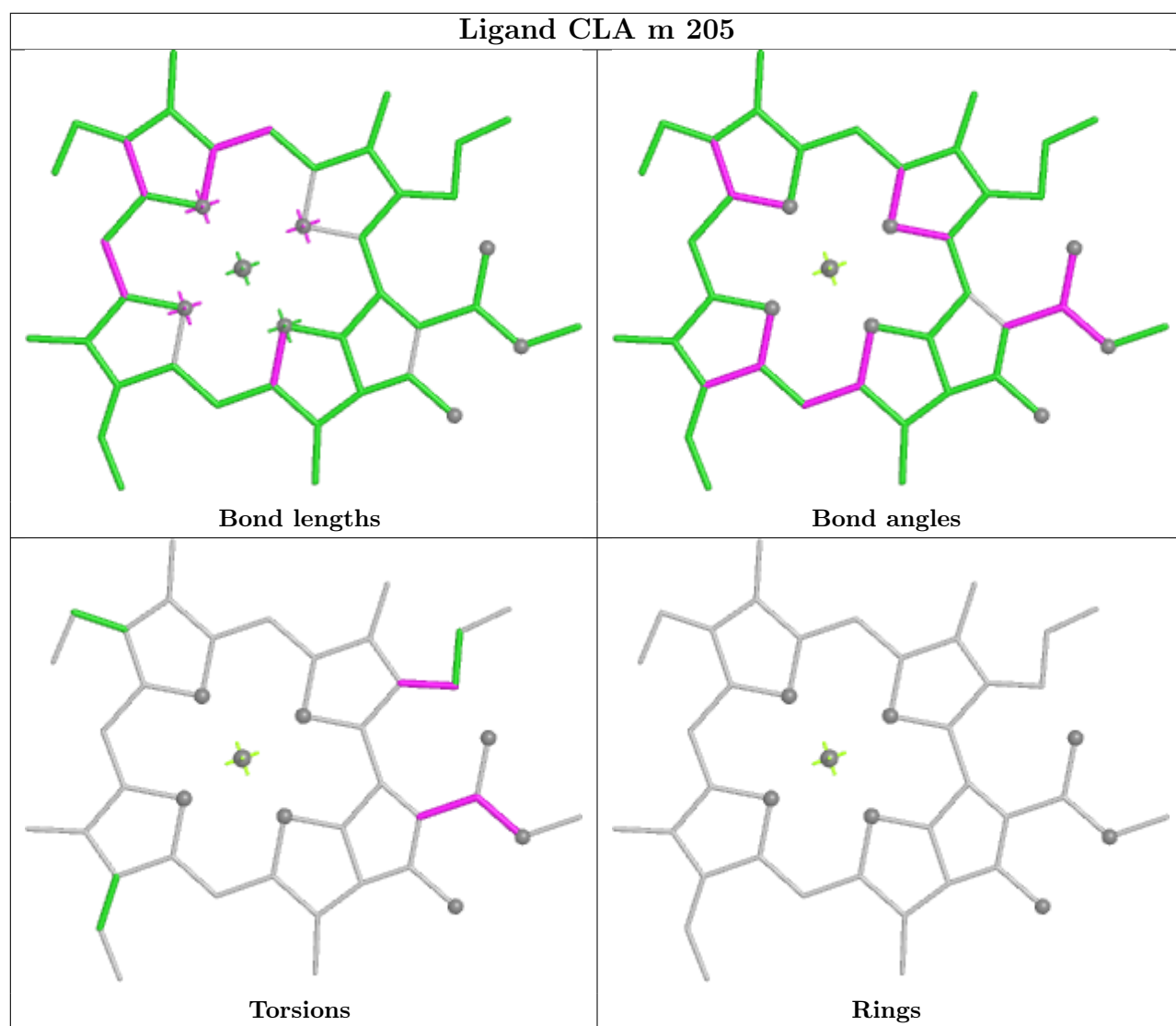
Rings

Ligand CLA b 210

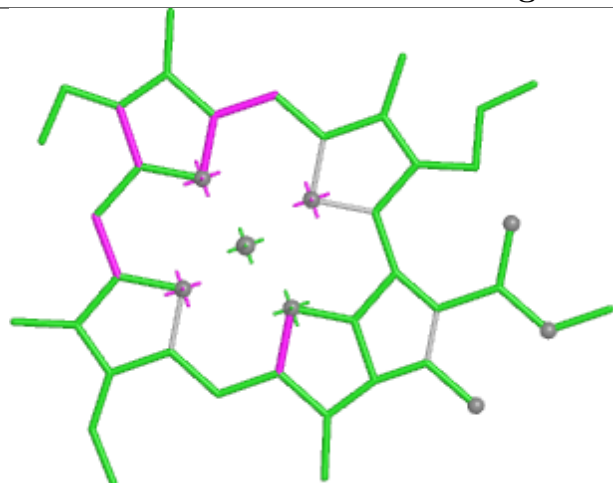


Ligand DD6 n 214

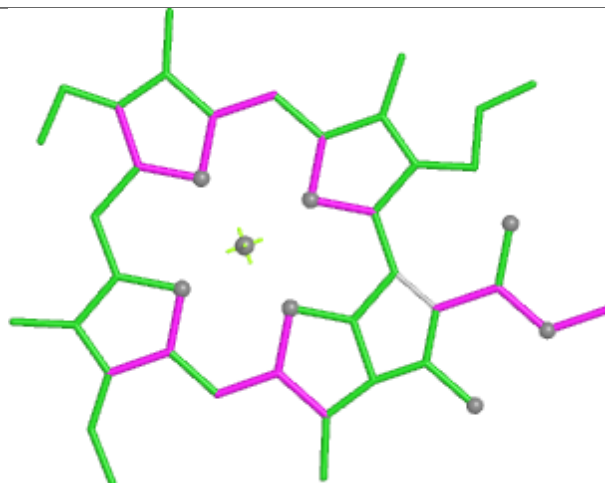




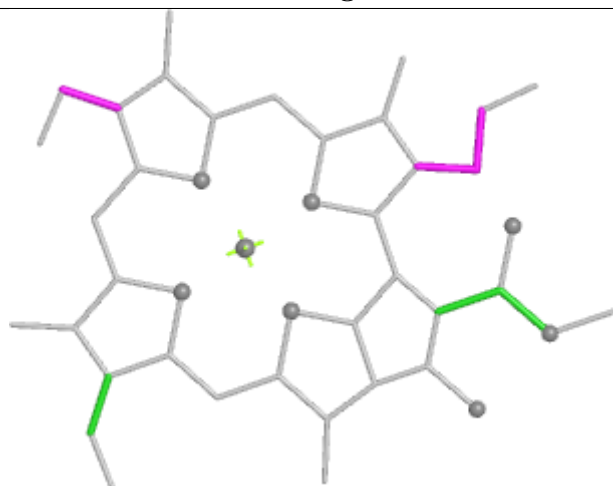
Ligand CLA o 605



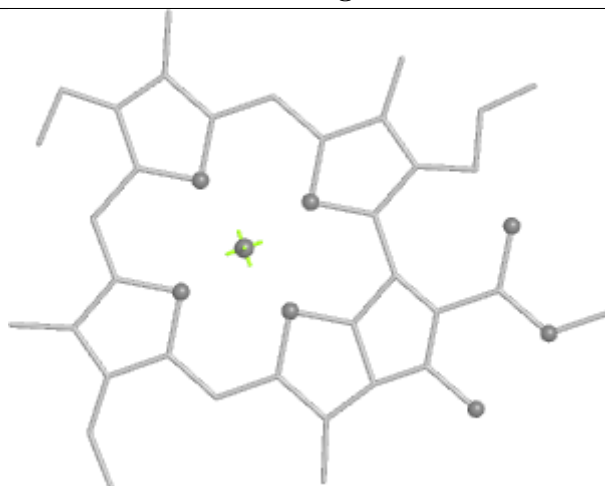
Bond lengths



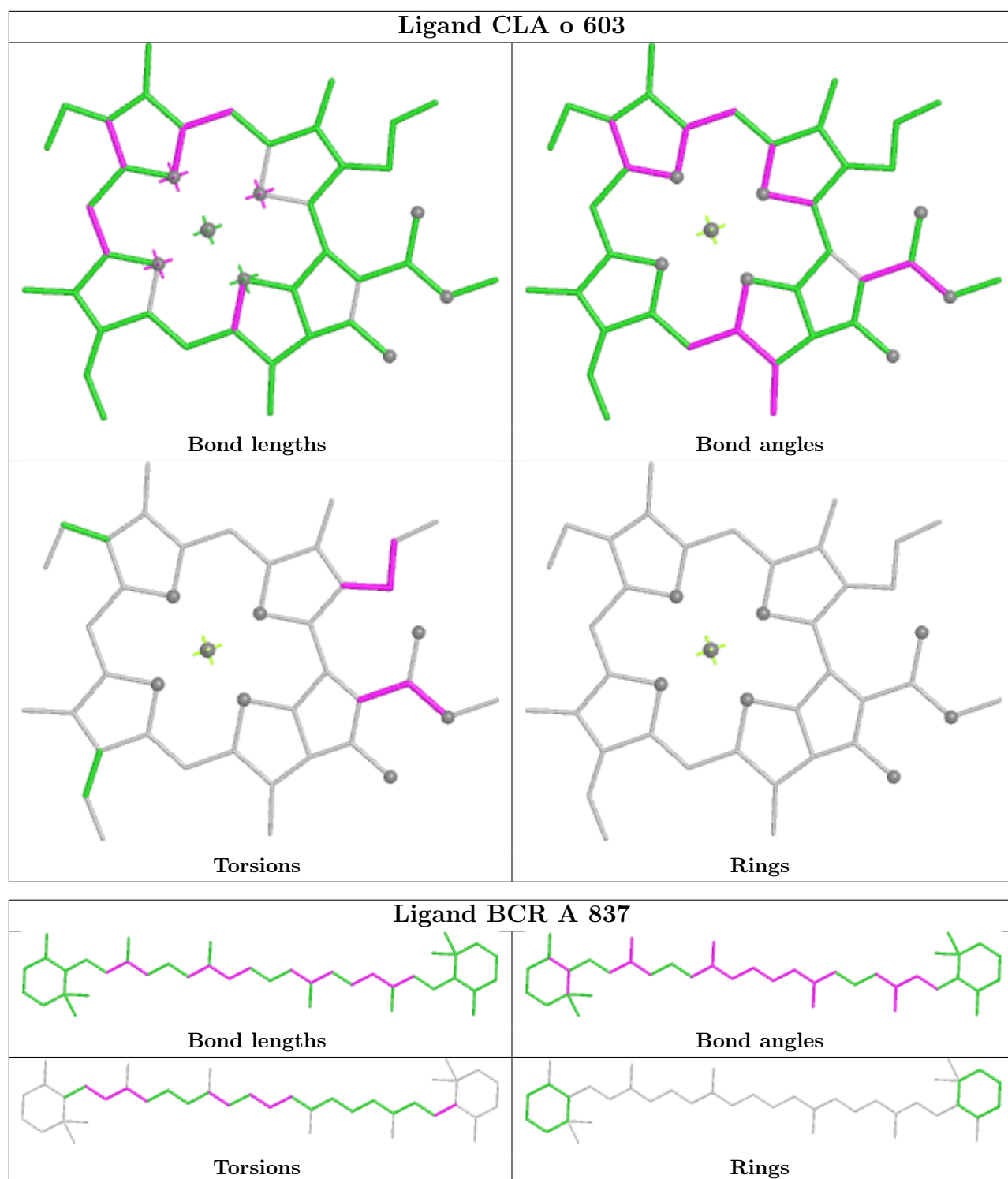
Bond angles

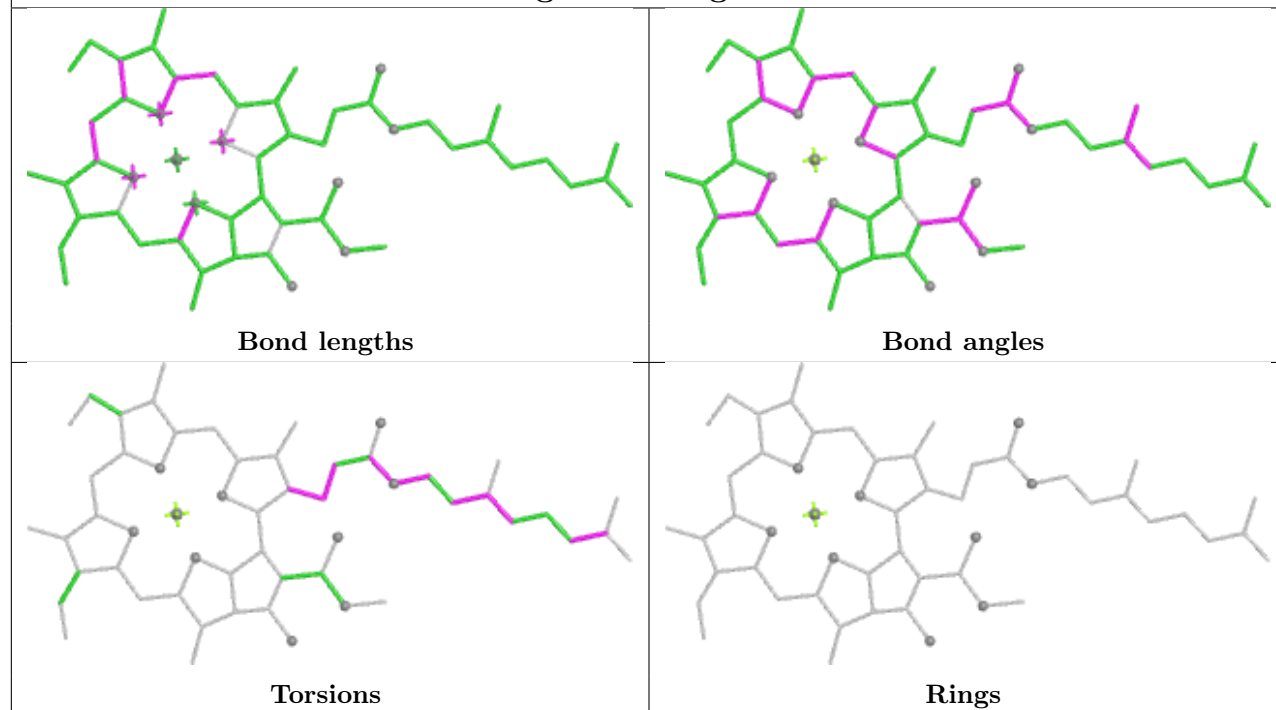
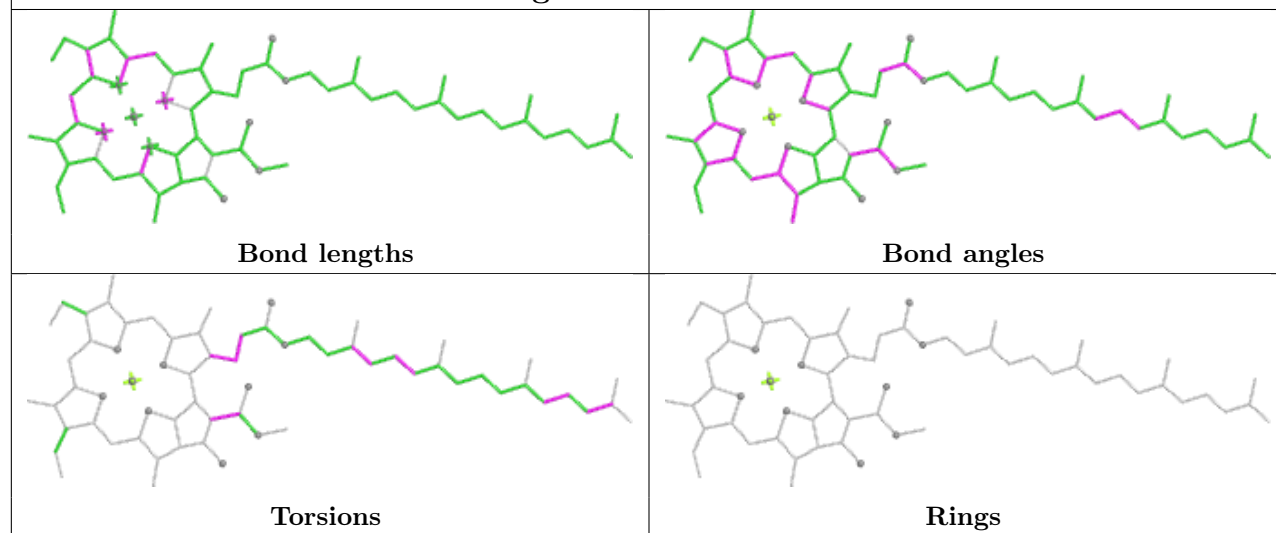


Torsions

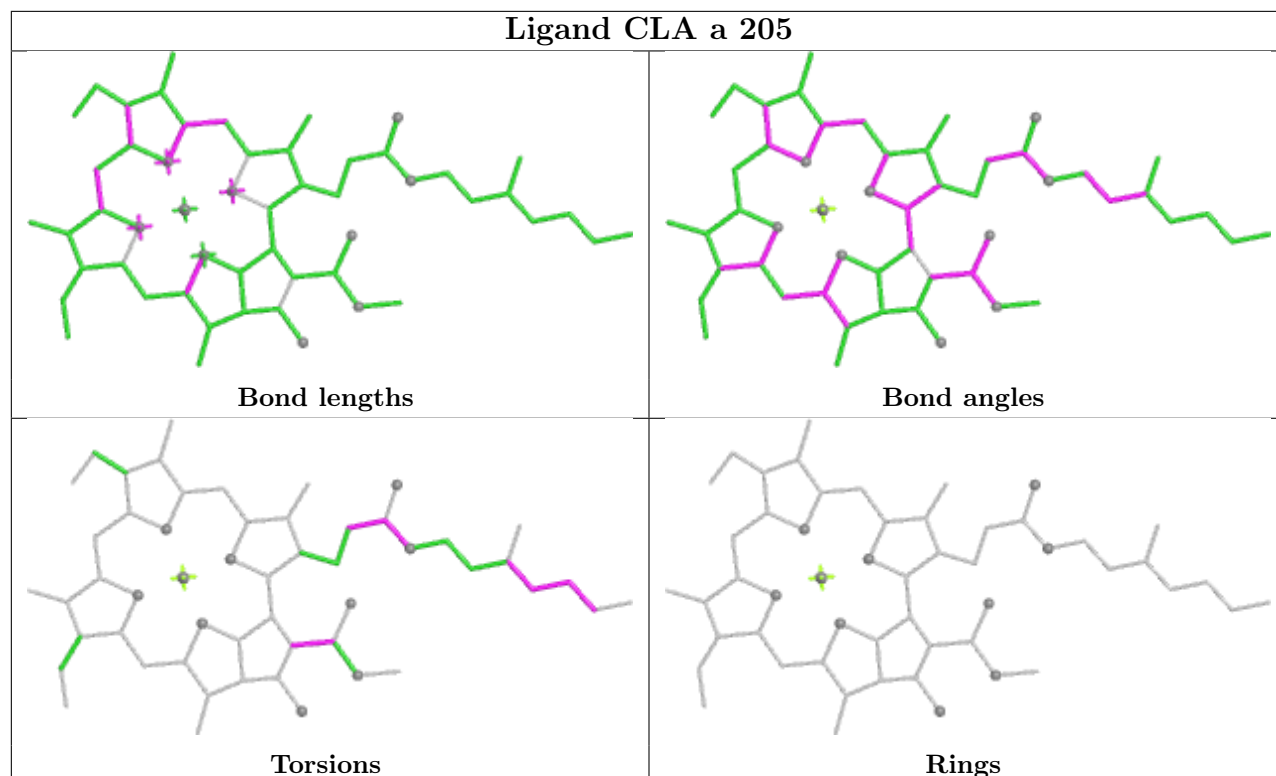


Rings

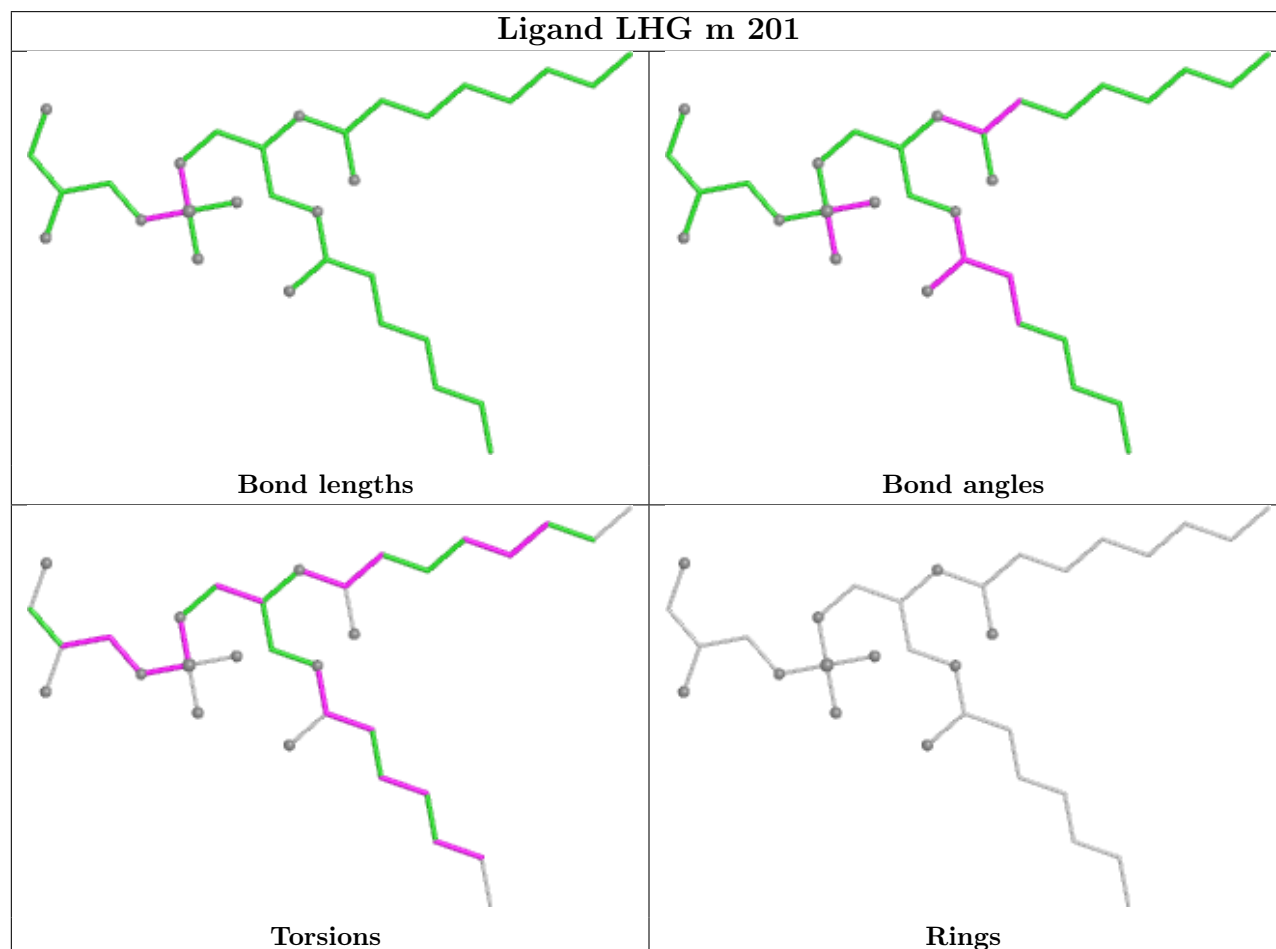


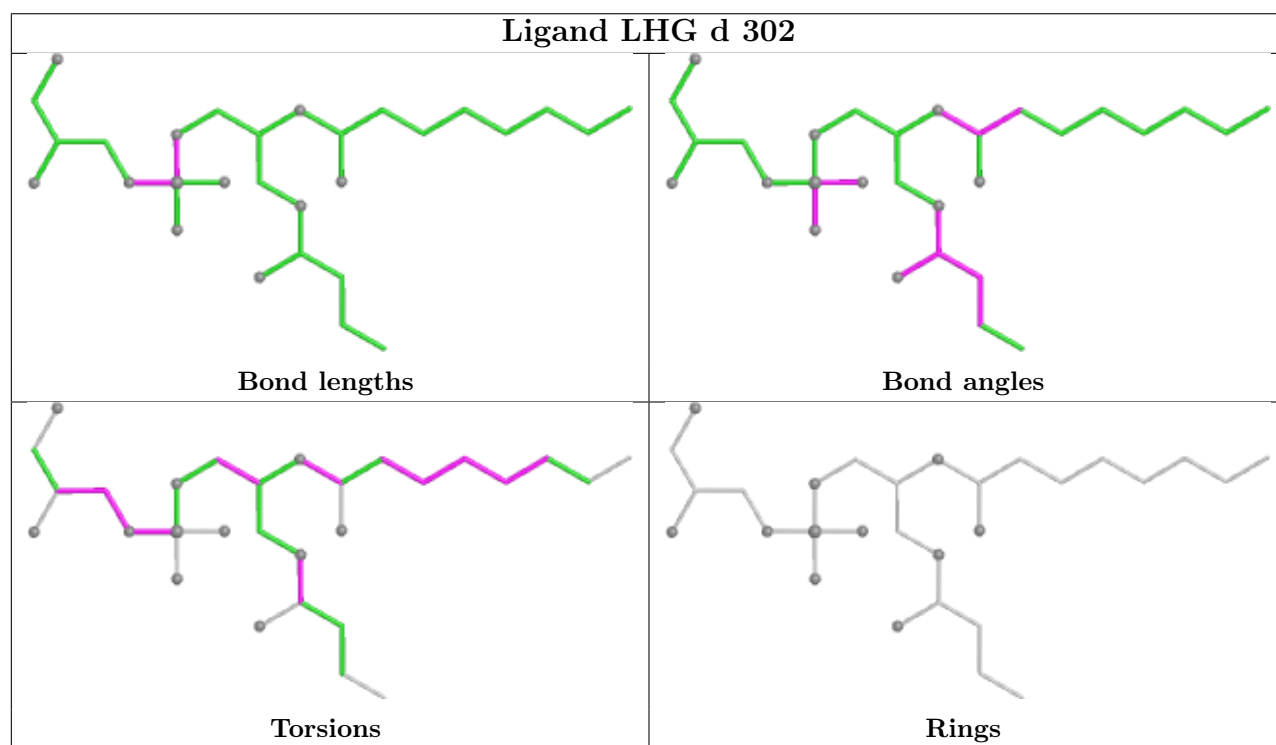
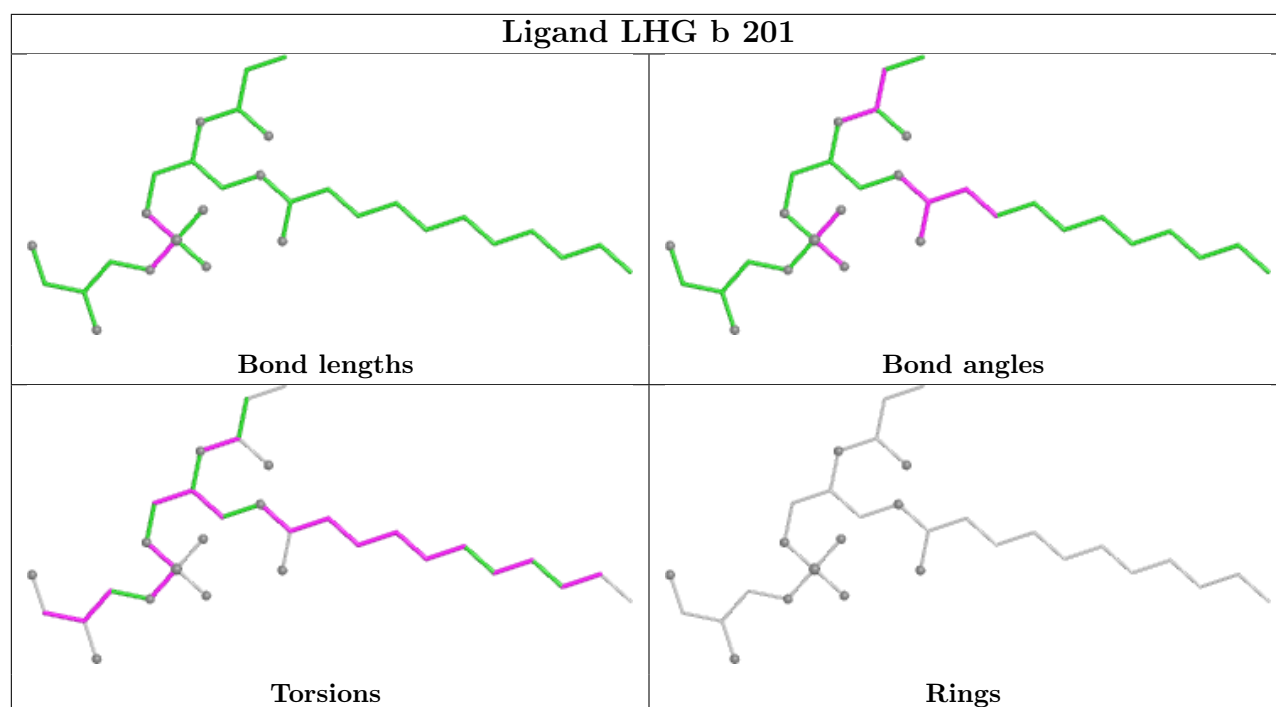
Ligand CLA g 212**Ligand CLA B 845**

Ligand CLA a 205

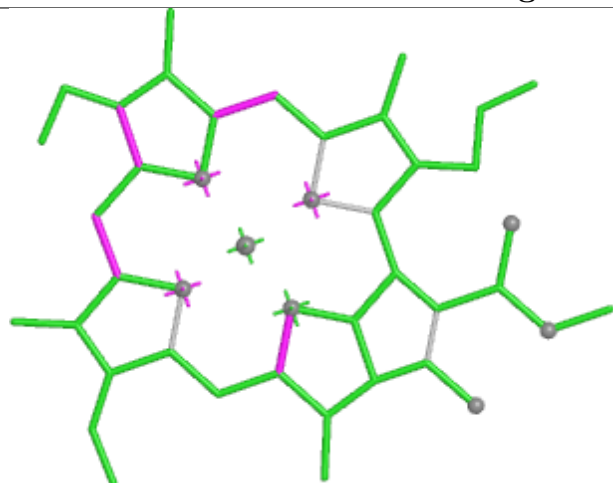


Ligand LHG m 201

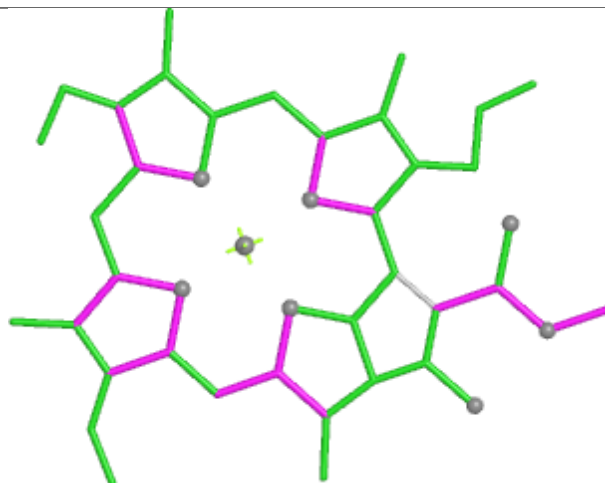




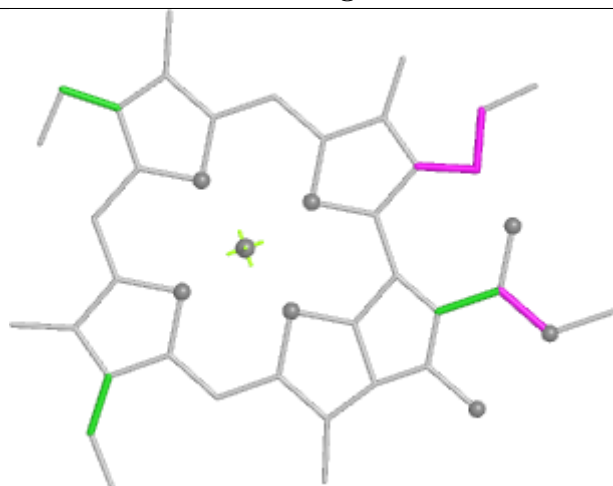
Ligand CLA o 610



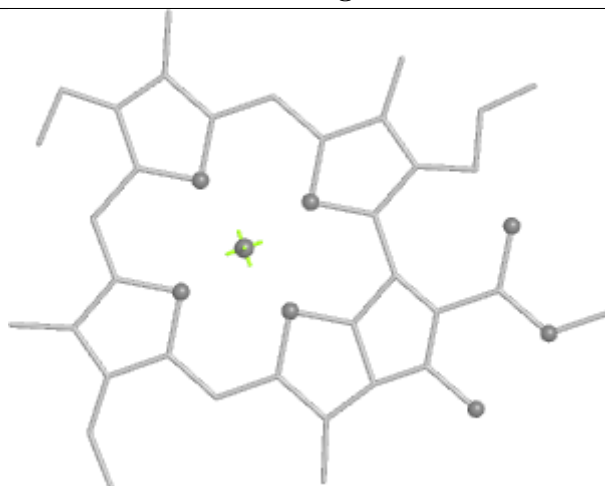
Bond lengths



Bond angles

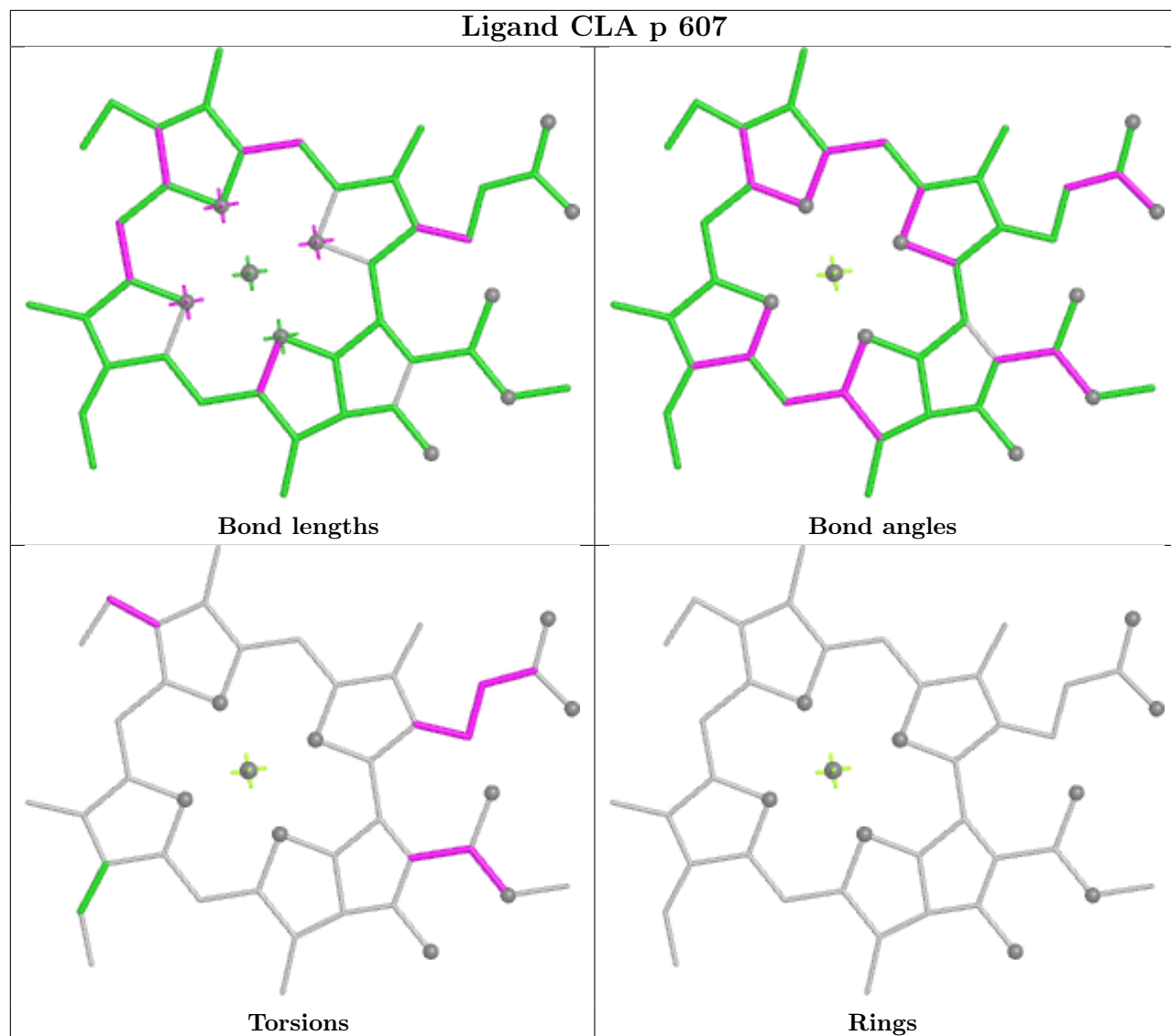


Torsions

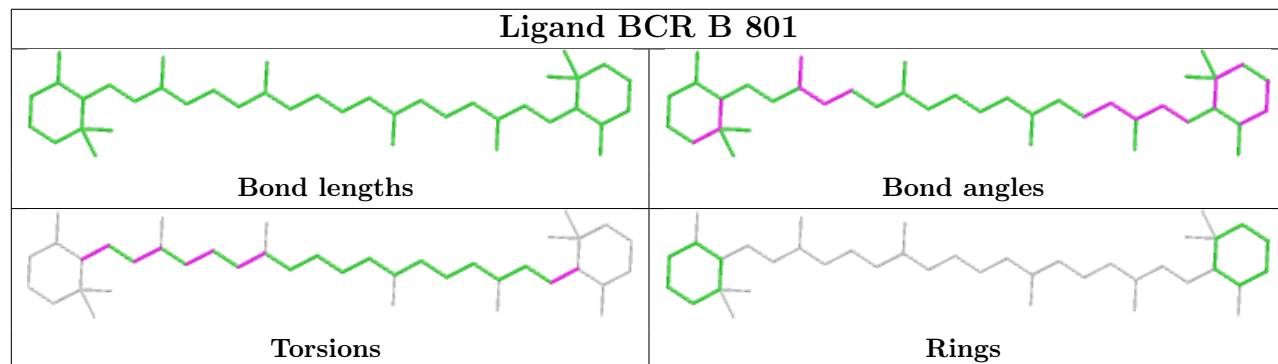


Rings

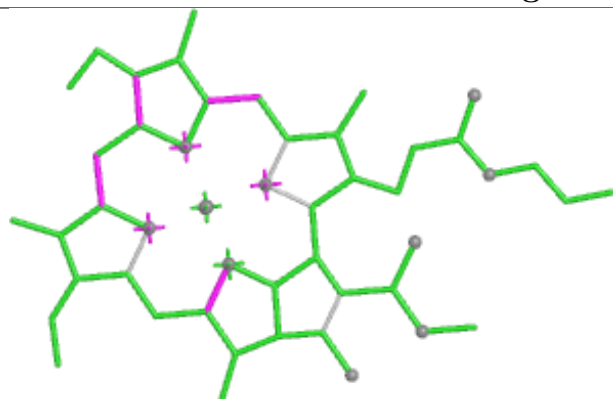
Ligand CLA p 607



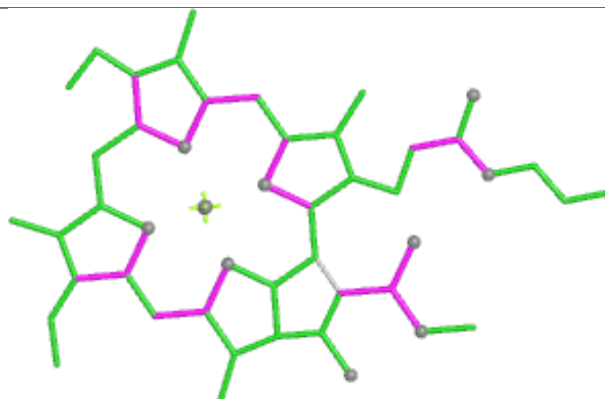
Ligand BCR B 801



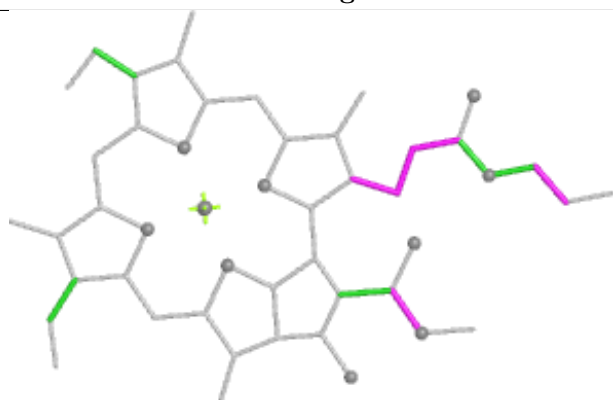
Ligand CLA l 610



Bond lengths



Bond angles

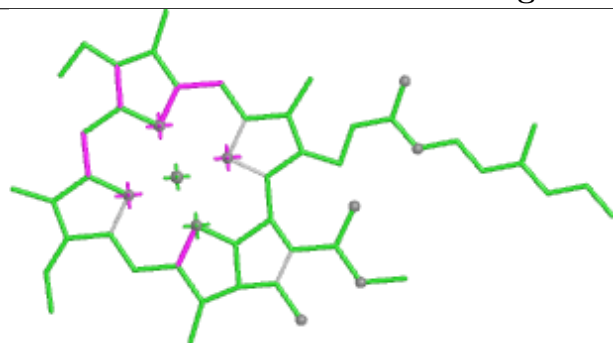


Torsions

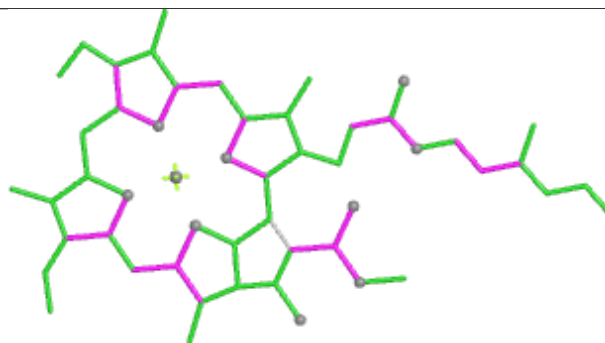


Rings

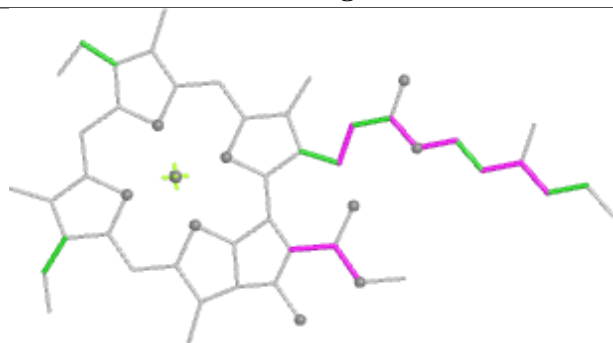
Ligand CLA k 211



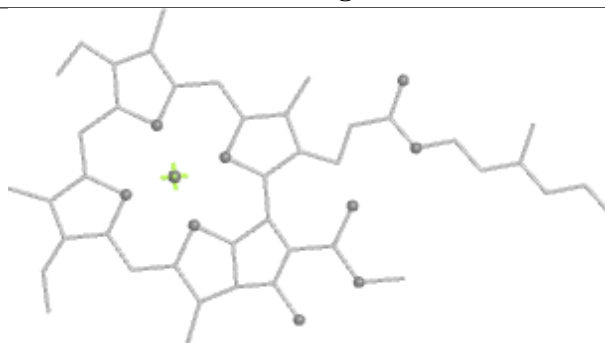
Bond lengths



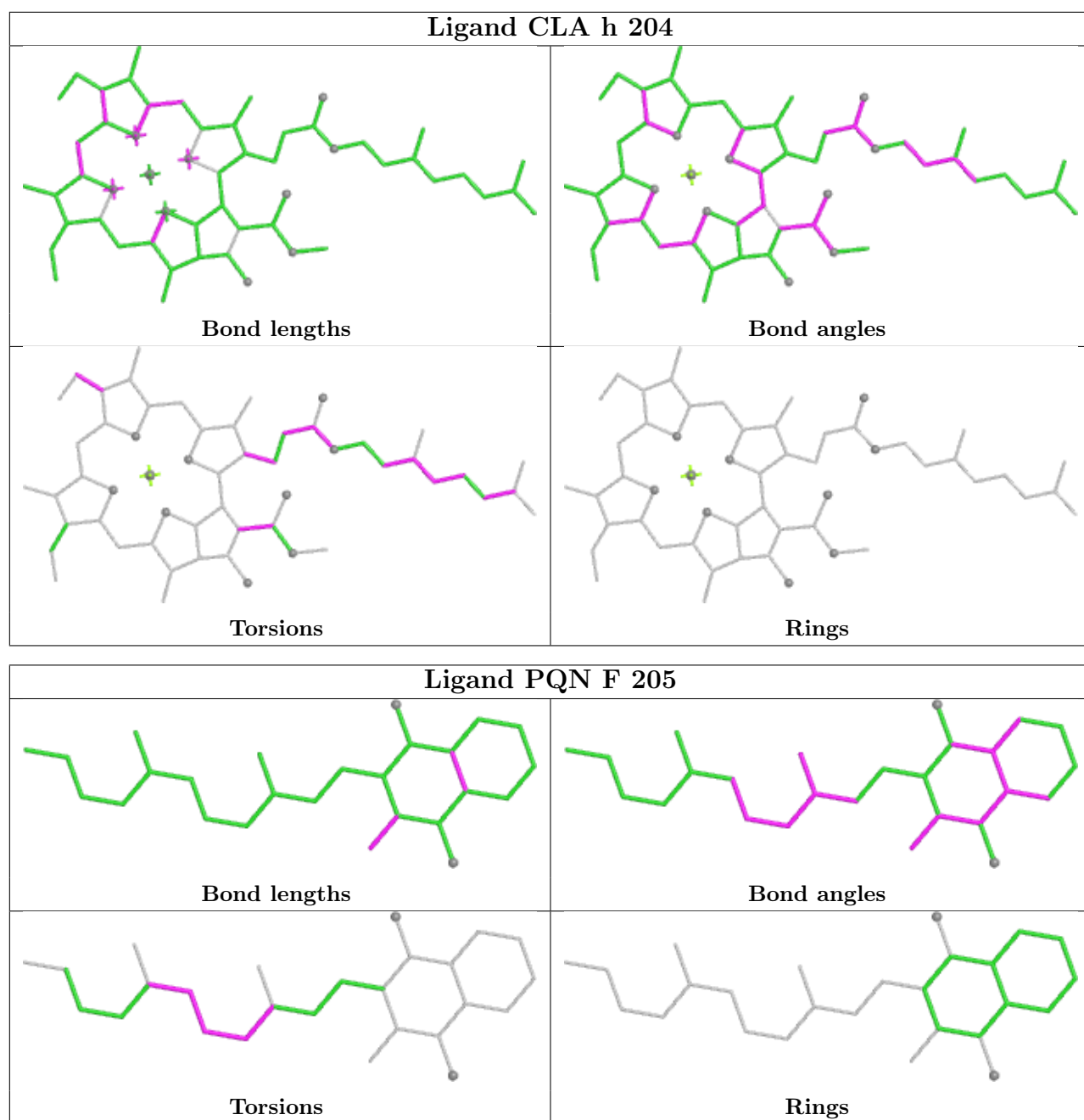
Bond angles



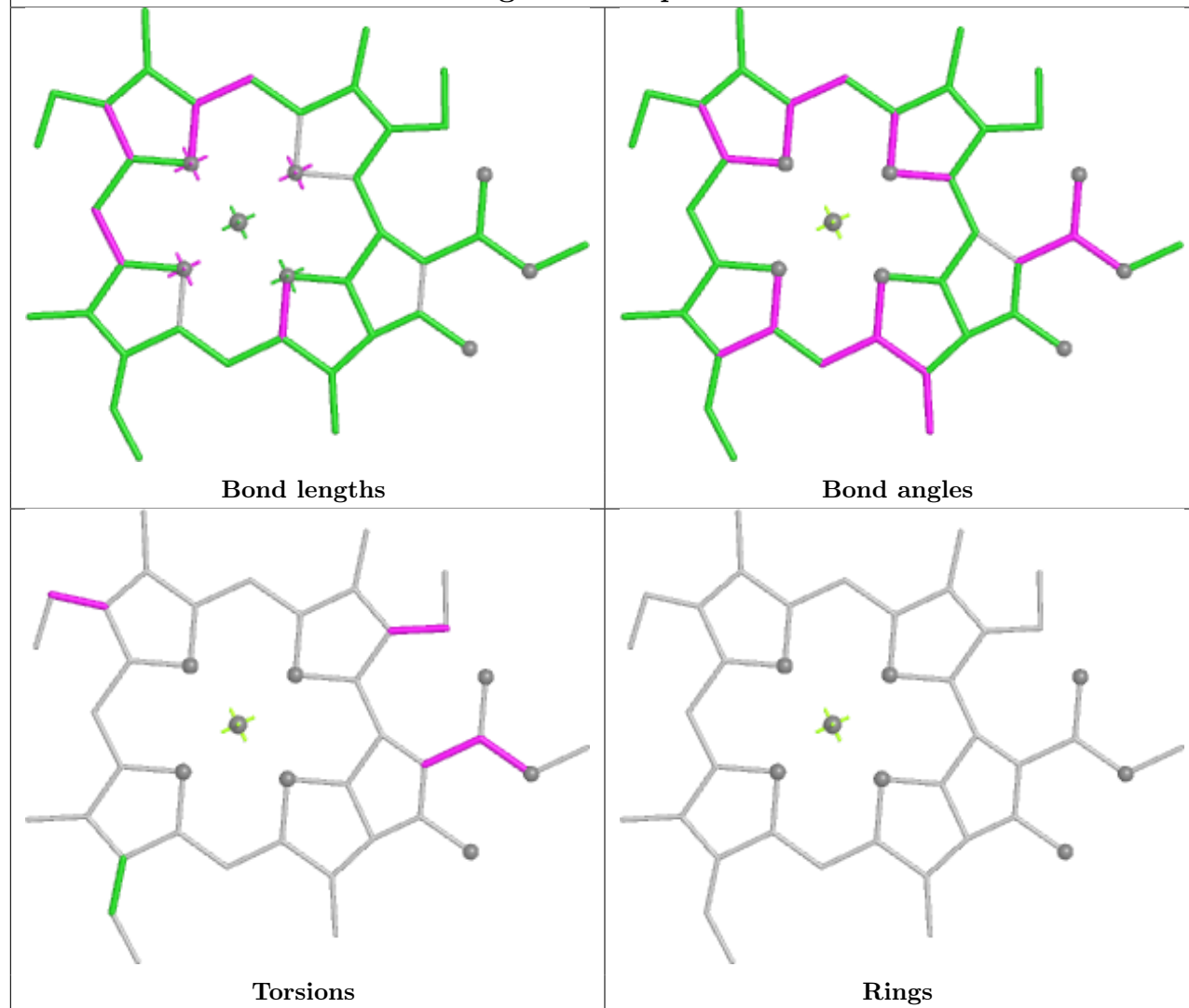
Torsions



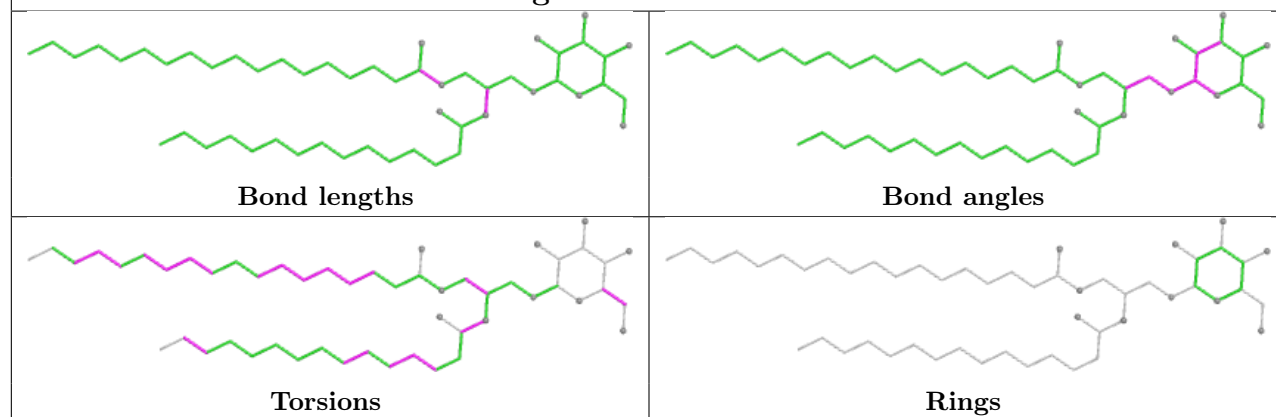
Rings

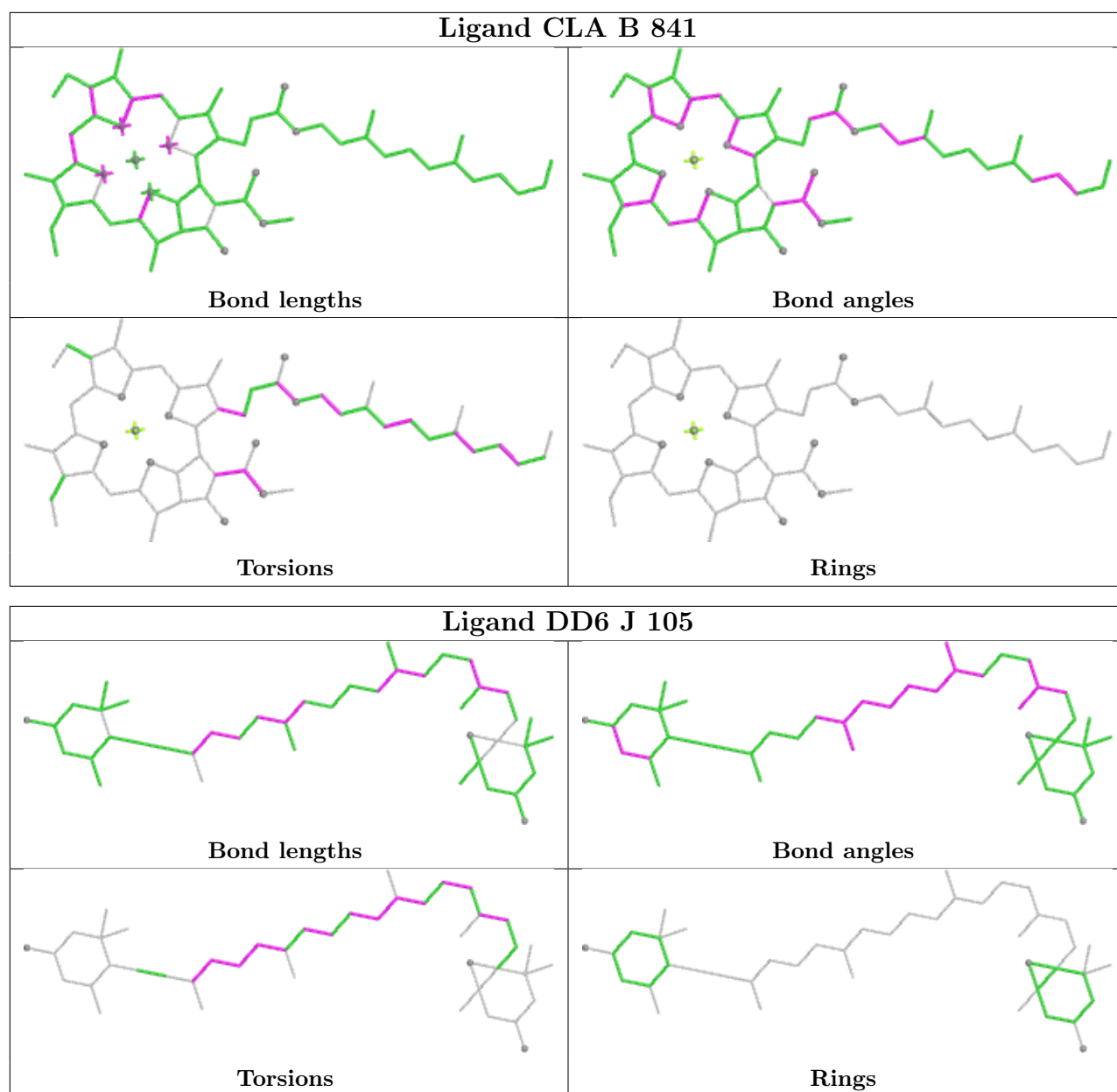


Ligand CLA p 605

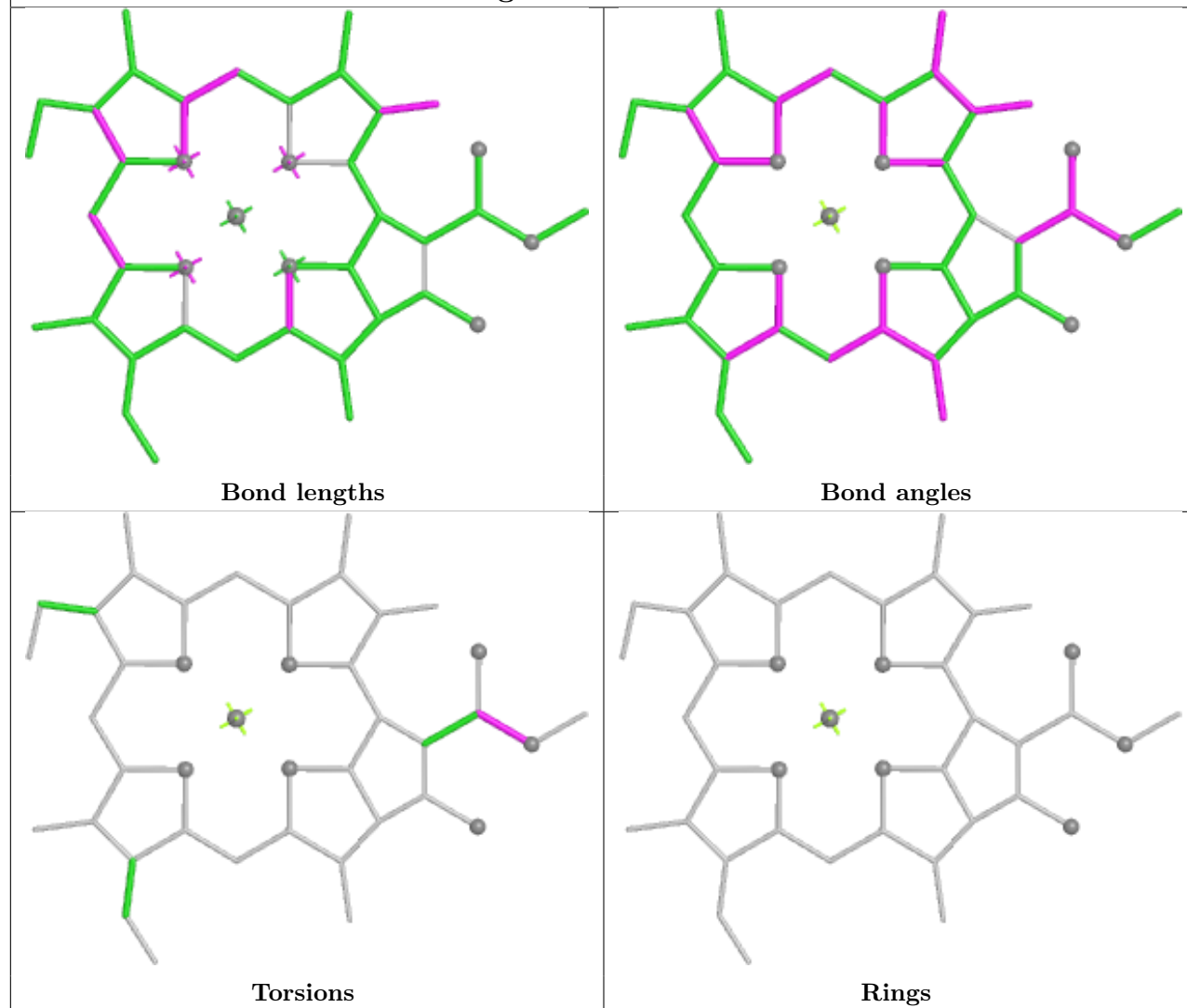


Ligand LMG e 202

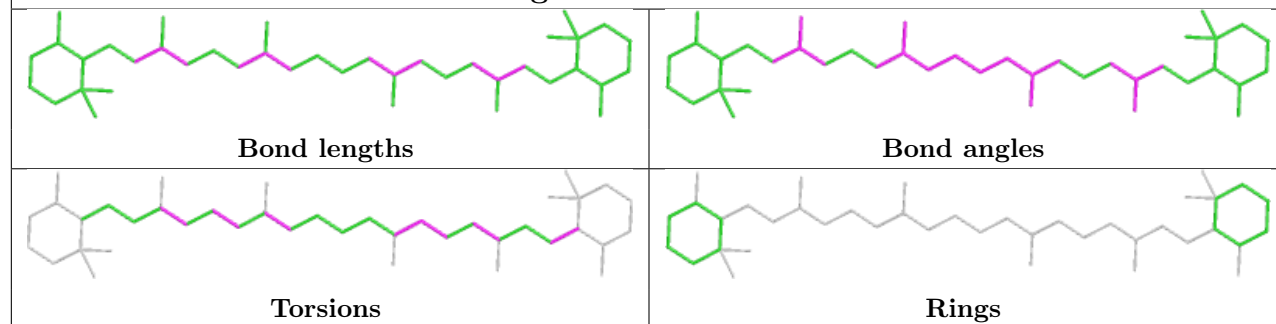


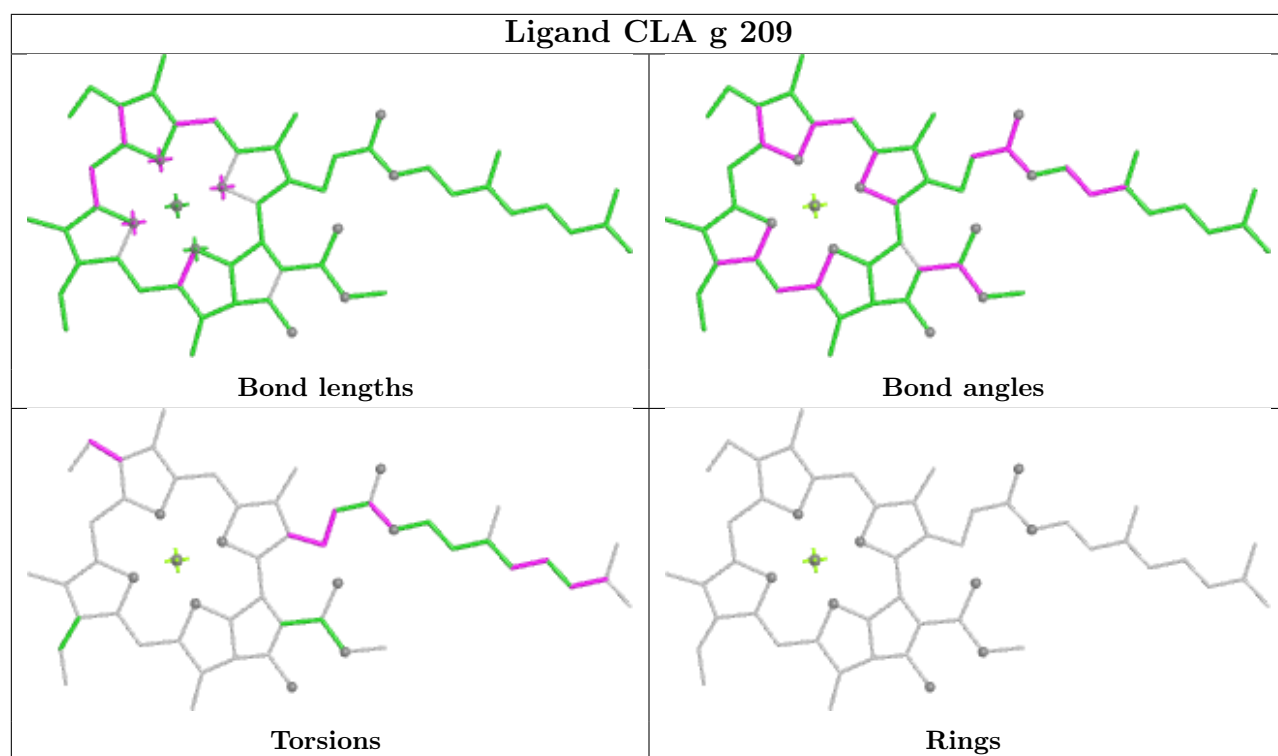


Ligand CLA n 207

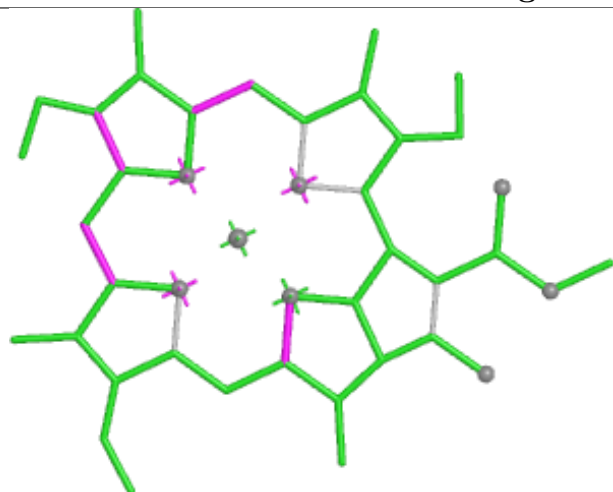


Ligand BCR B 831

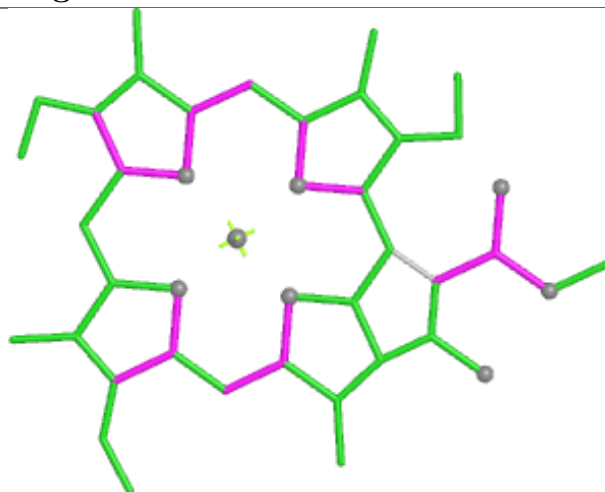




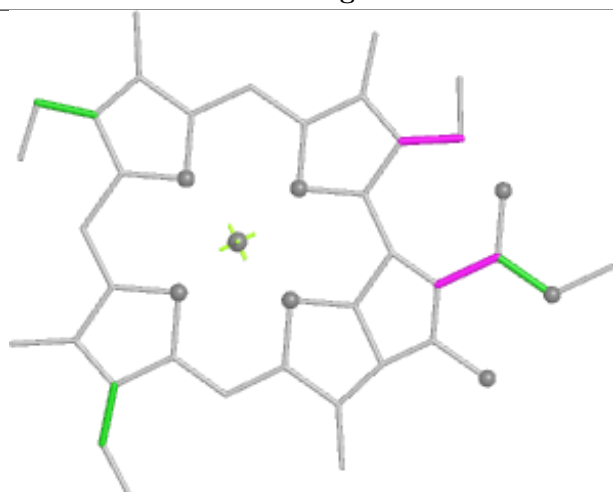
Ligand CLA g 210



Bond lengths



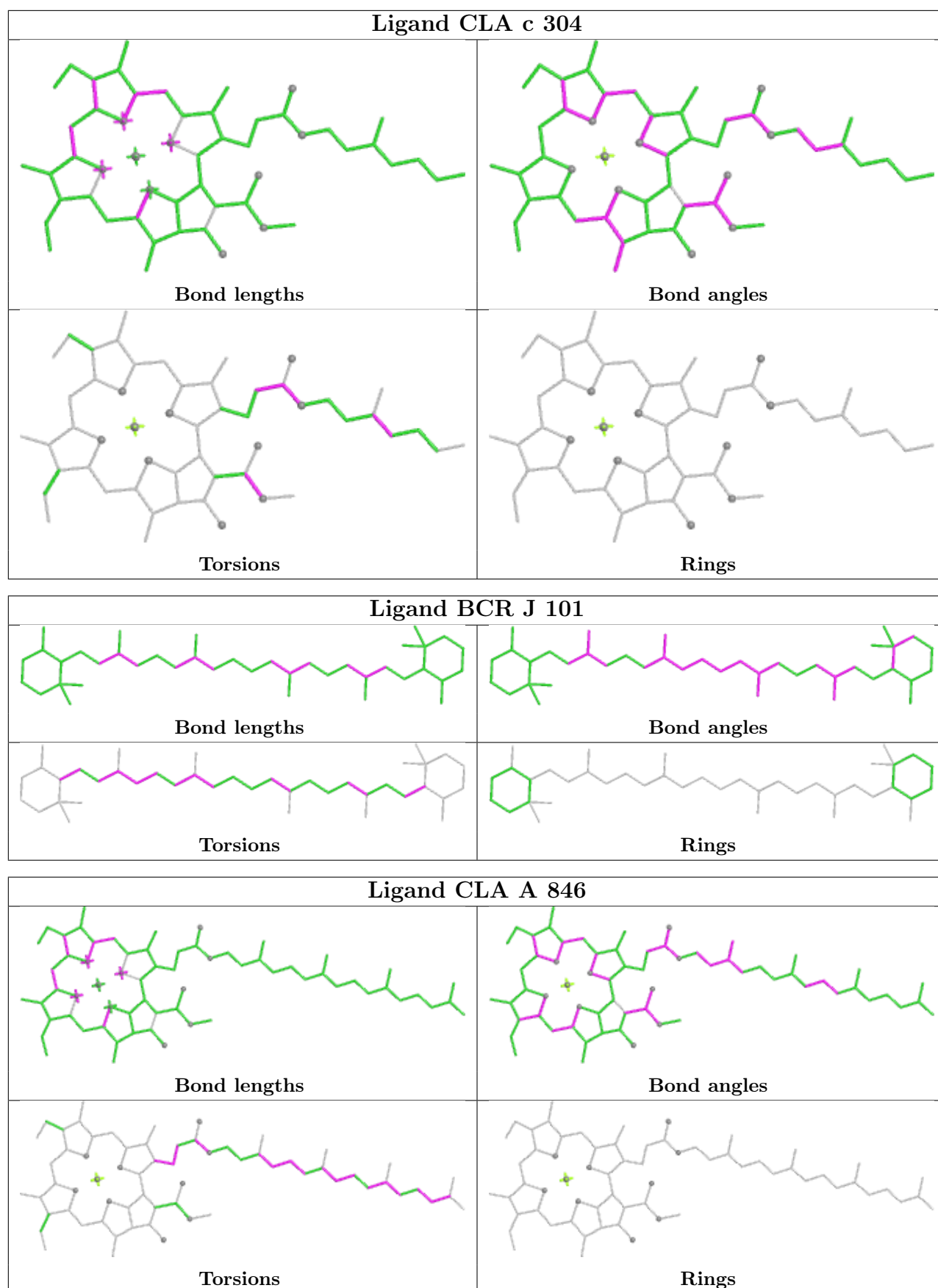
Bond angles

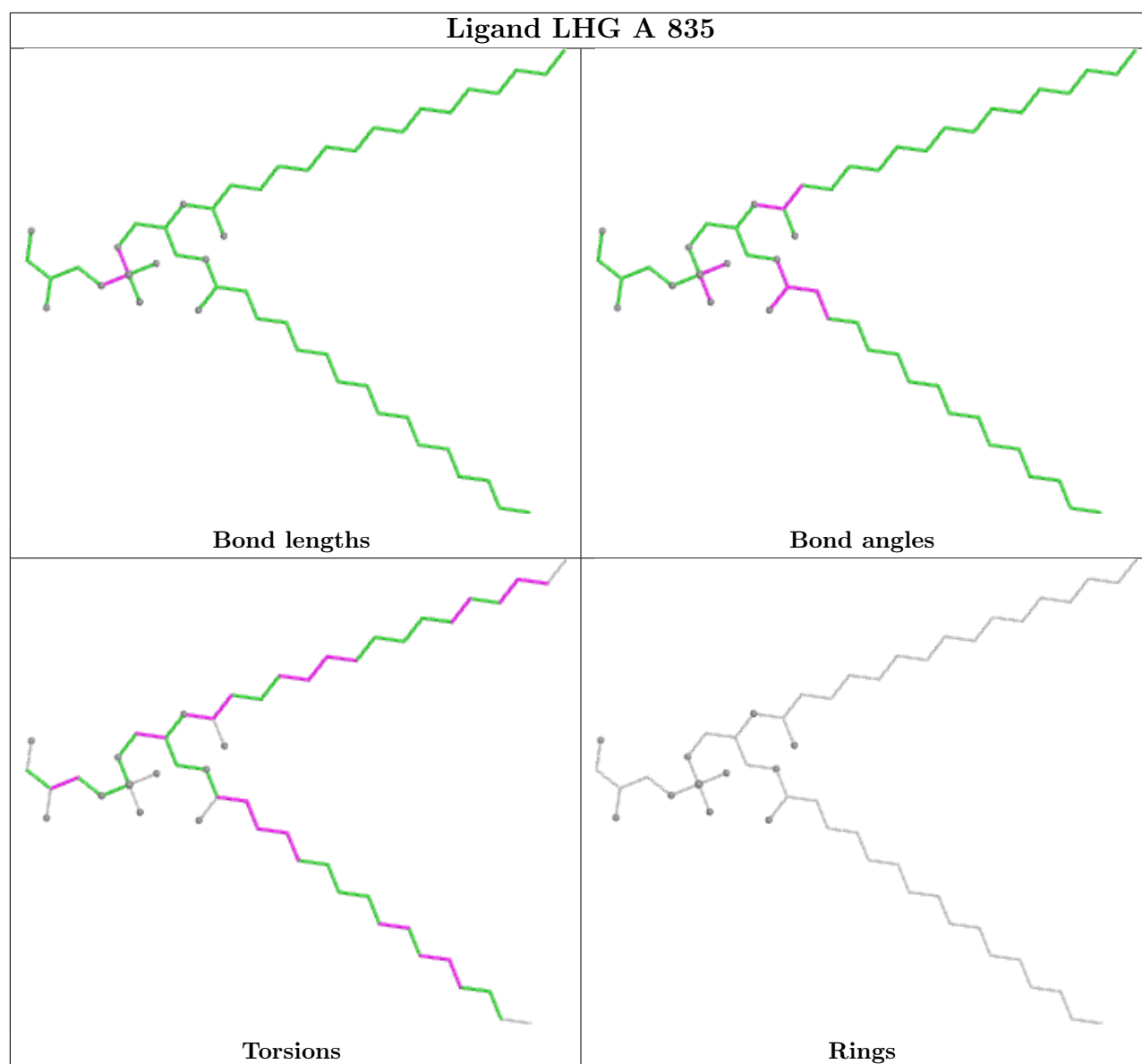


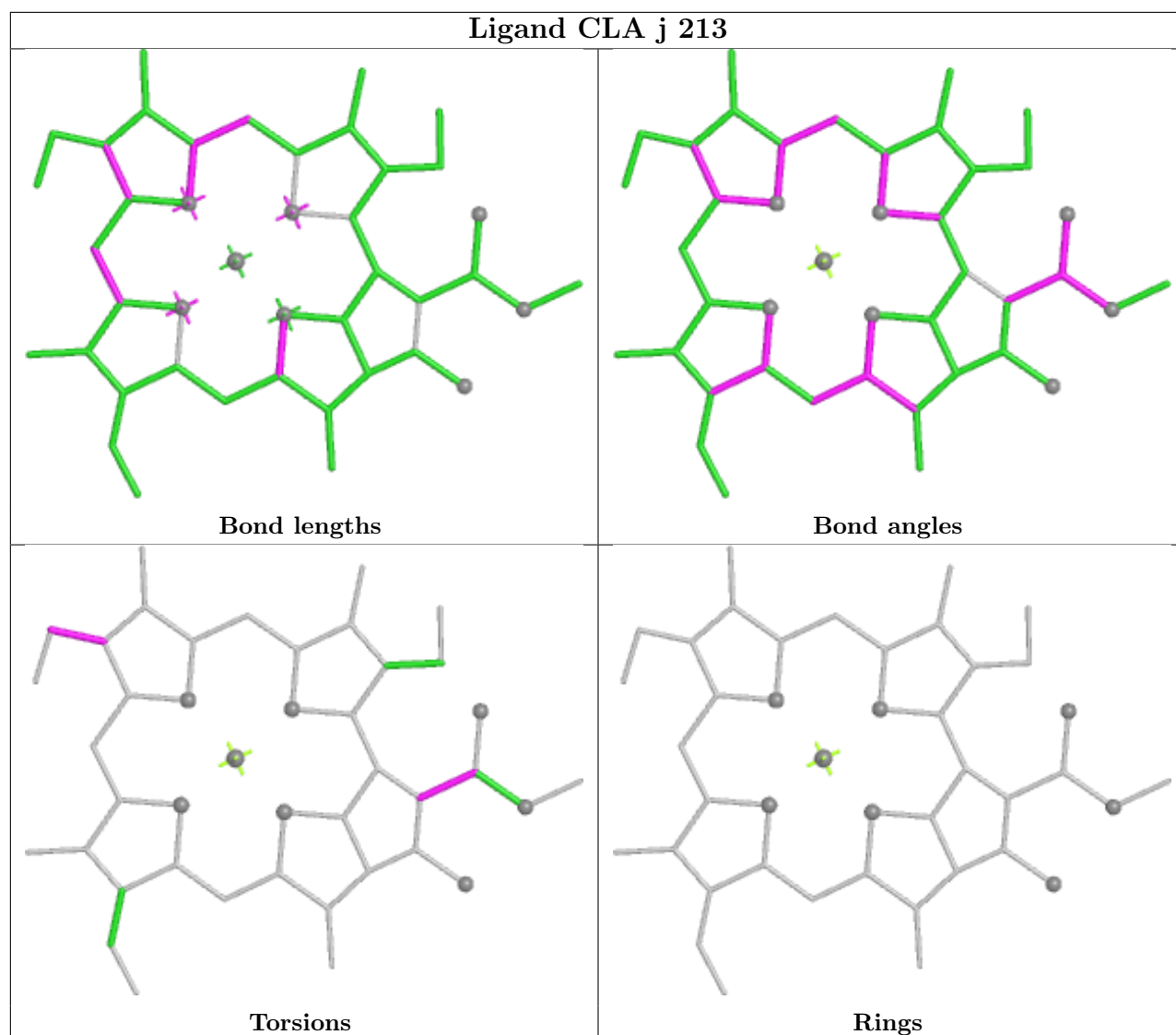
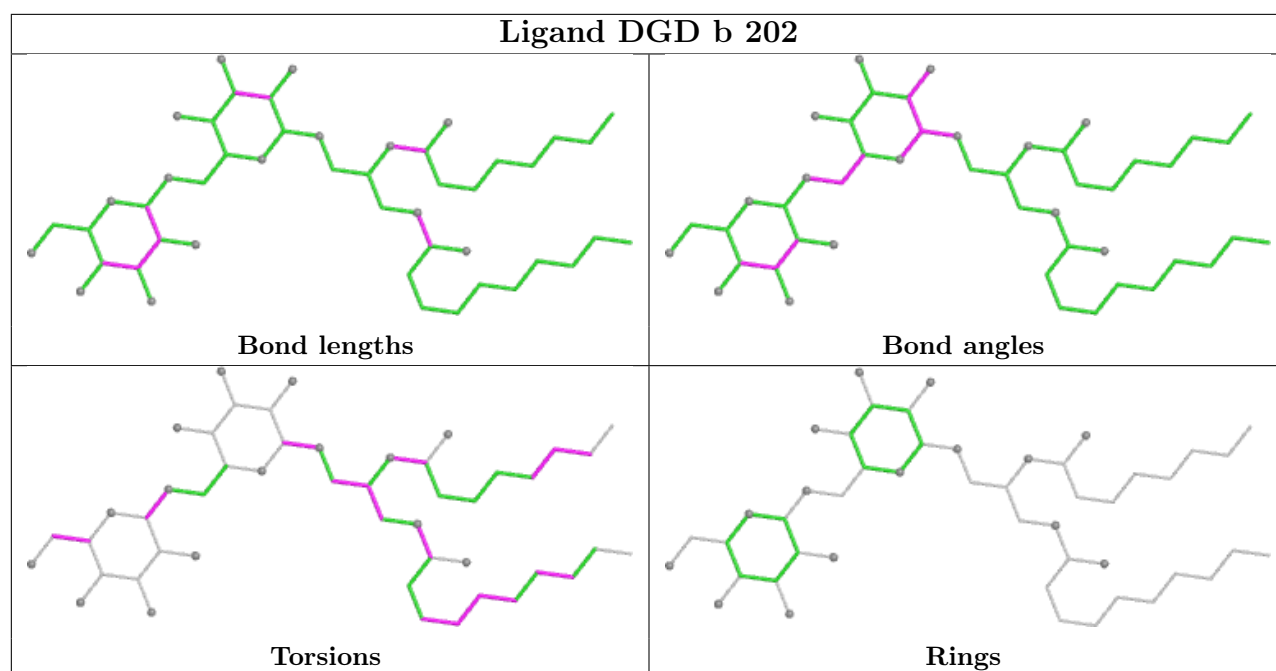
Torsions

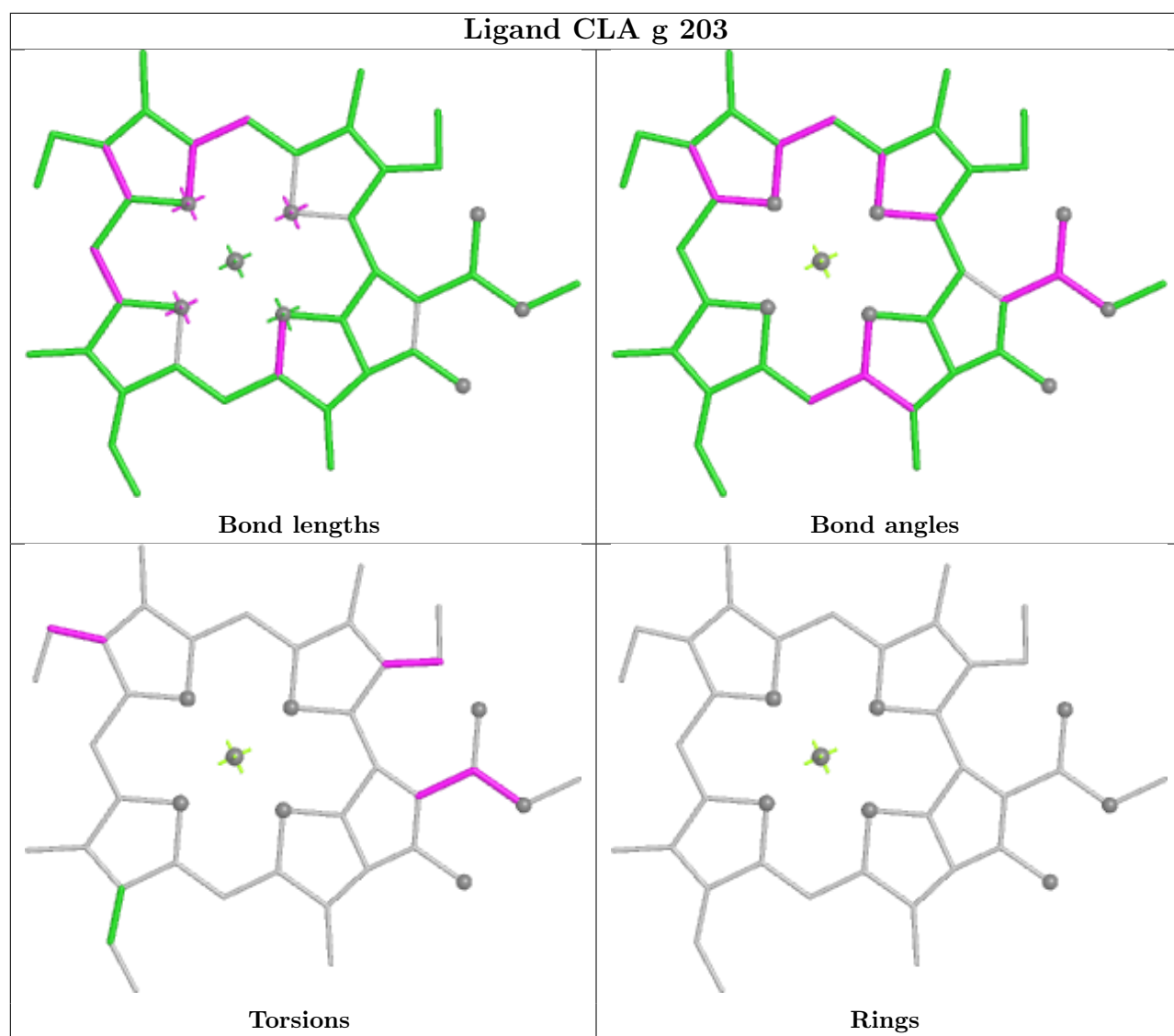


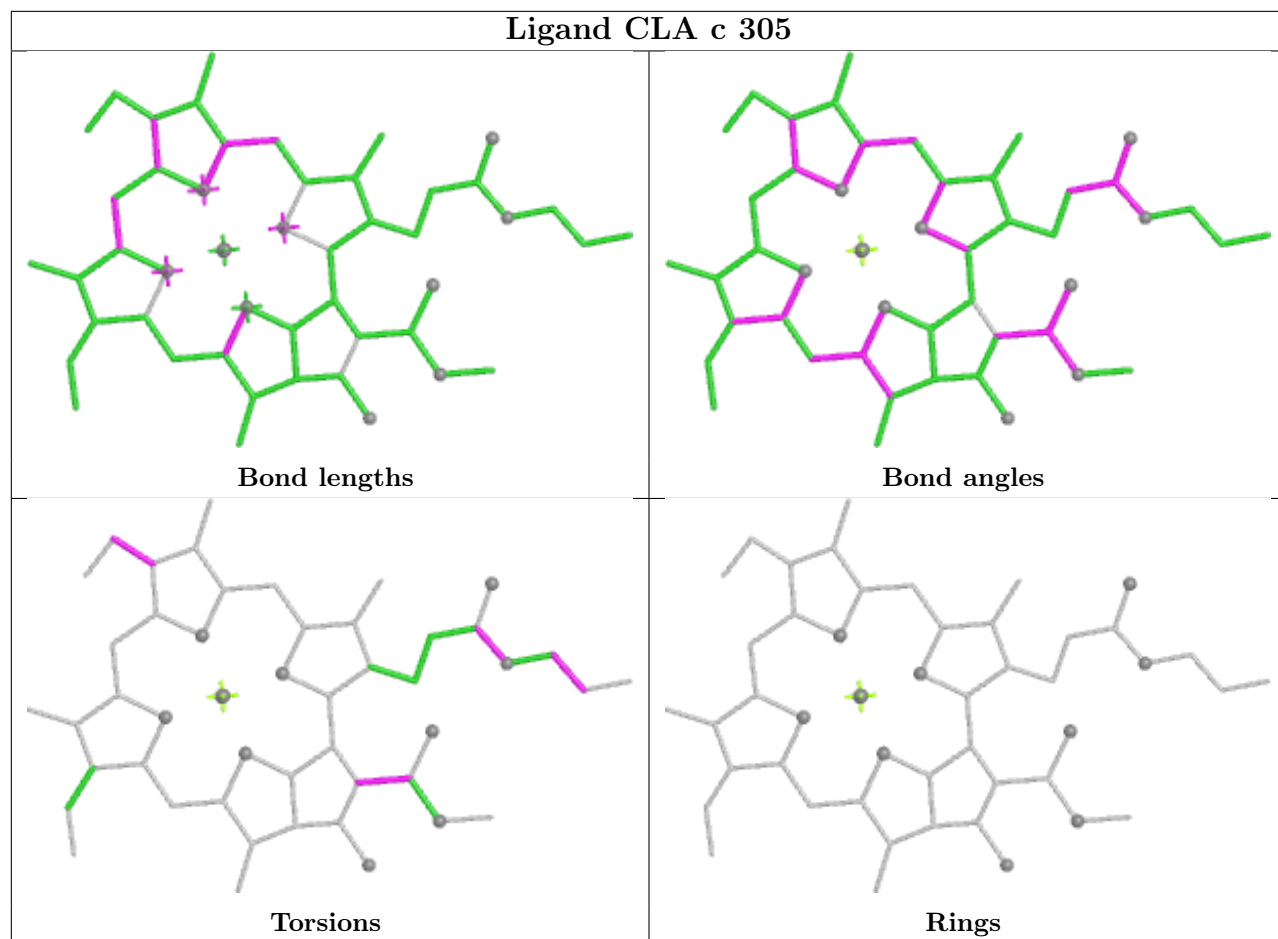
Rings



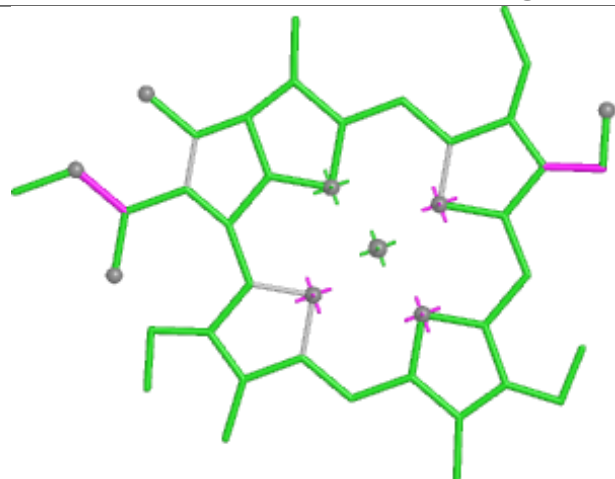




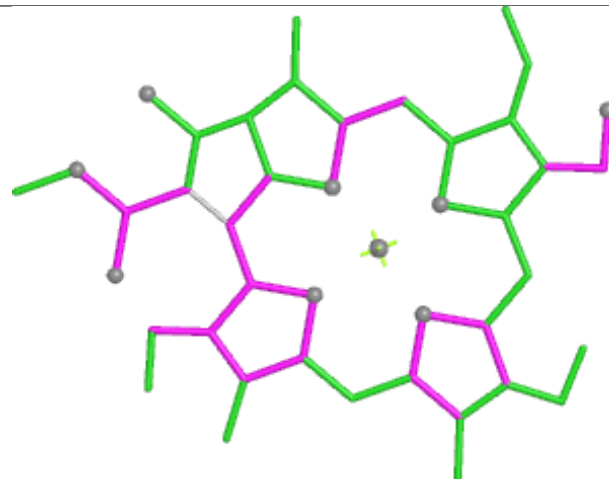




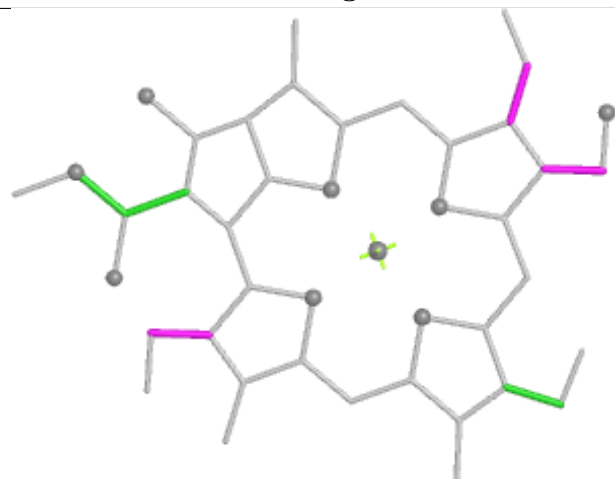
Ligand CHL d 309



Bond lengths



Bond angles

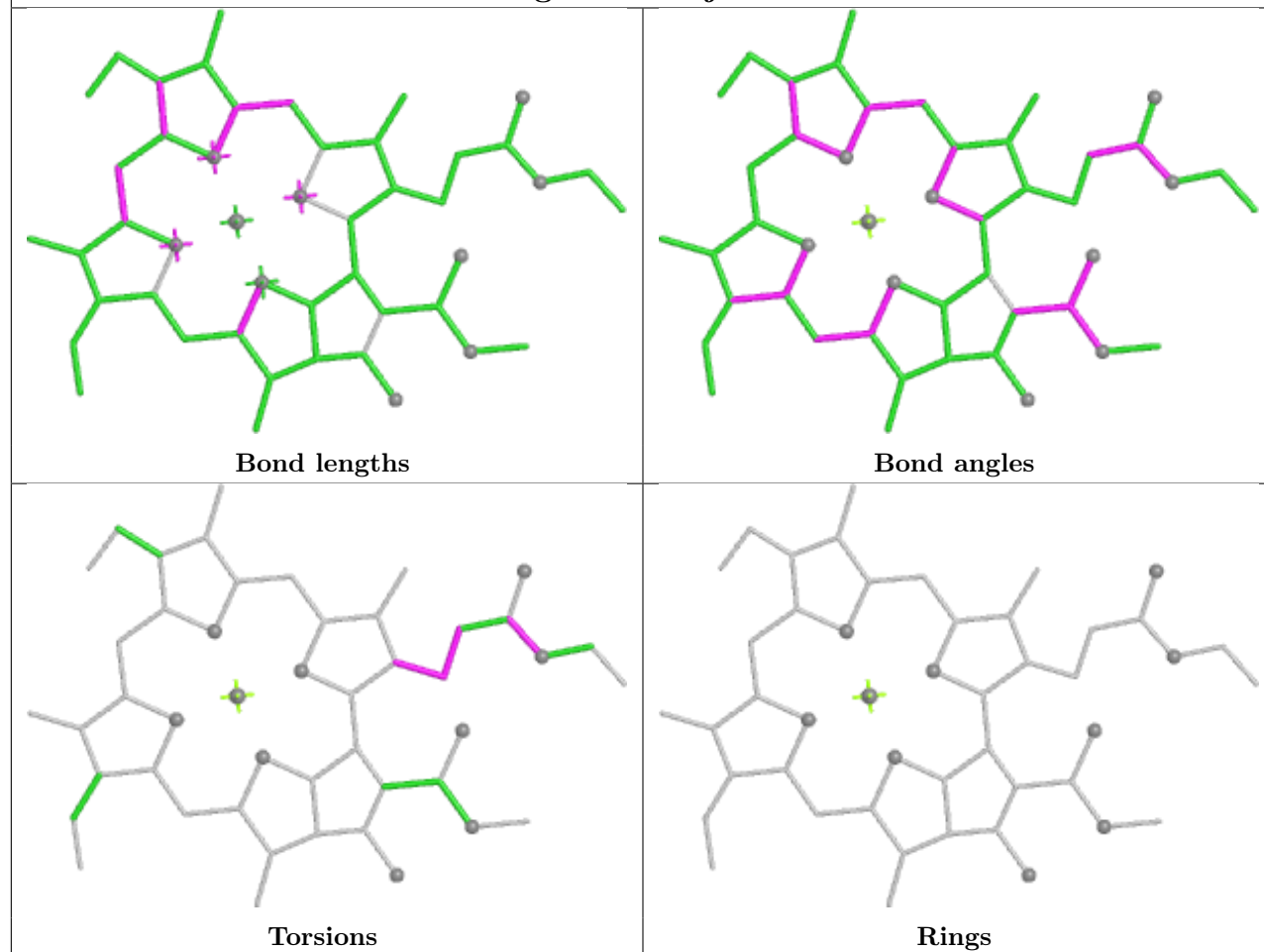


Torsions

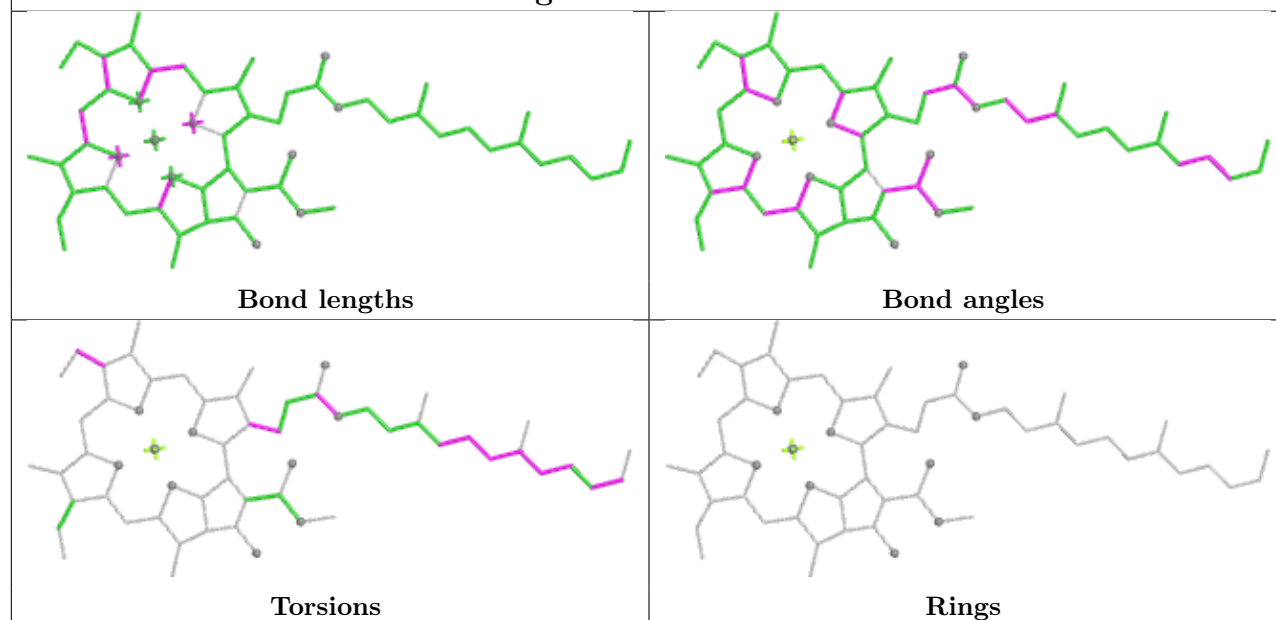


Rings

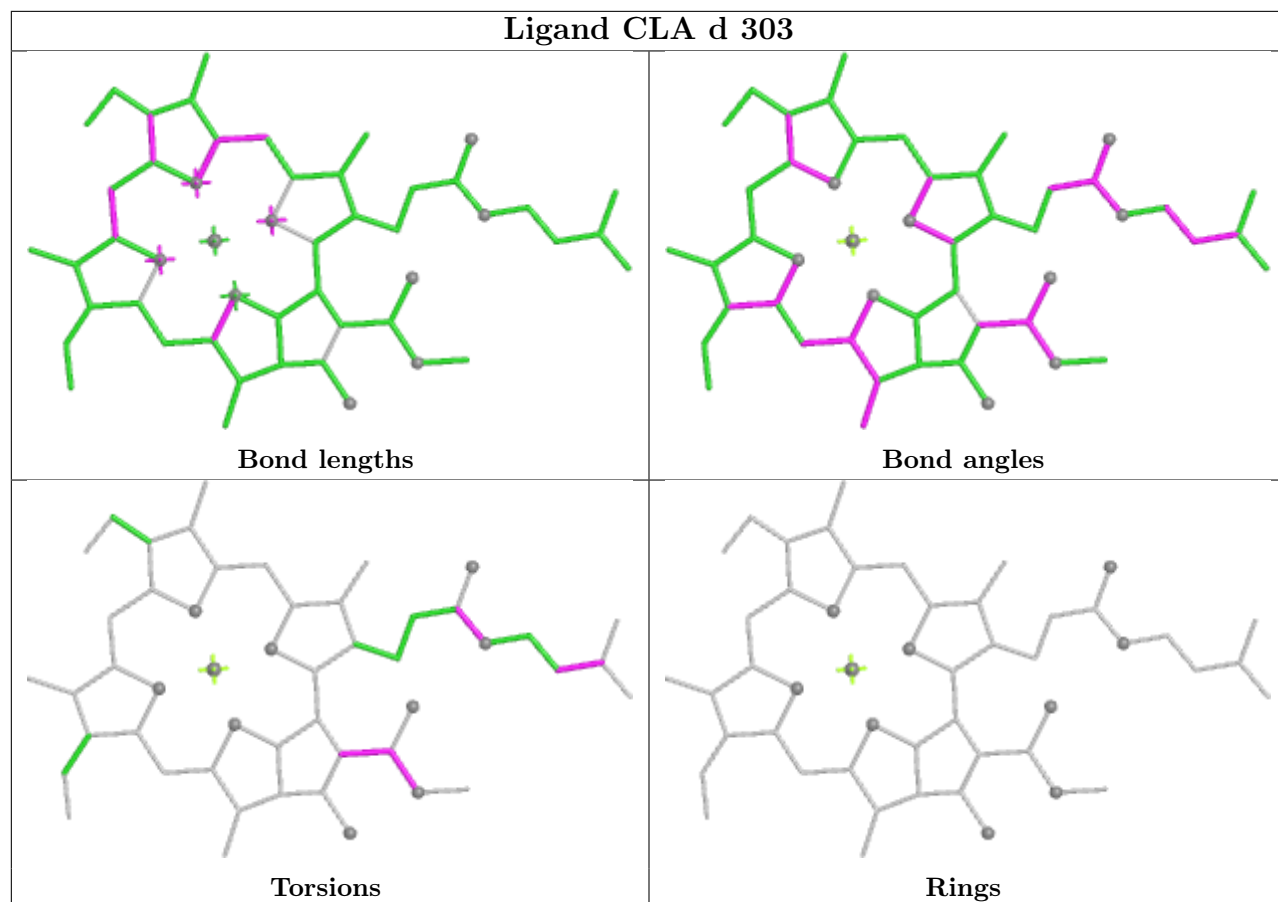
Ligand CLA j 207

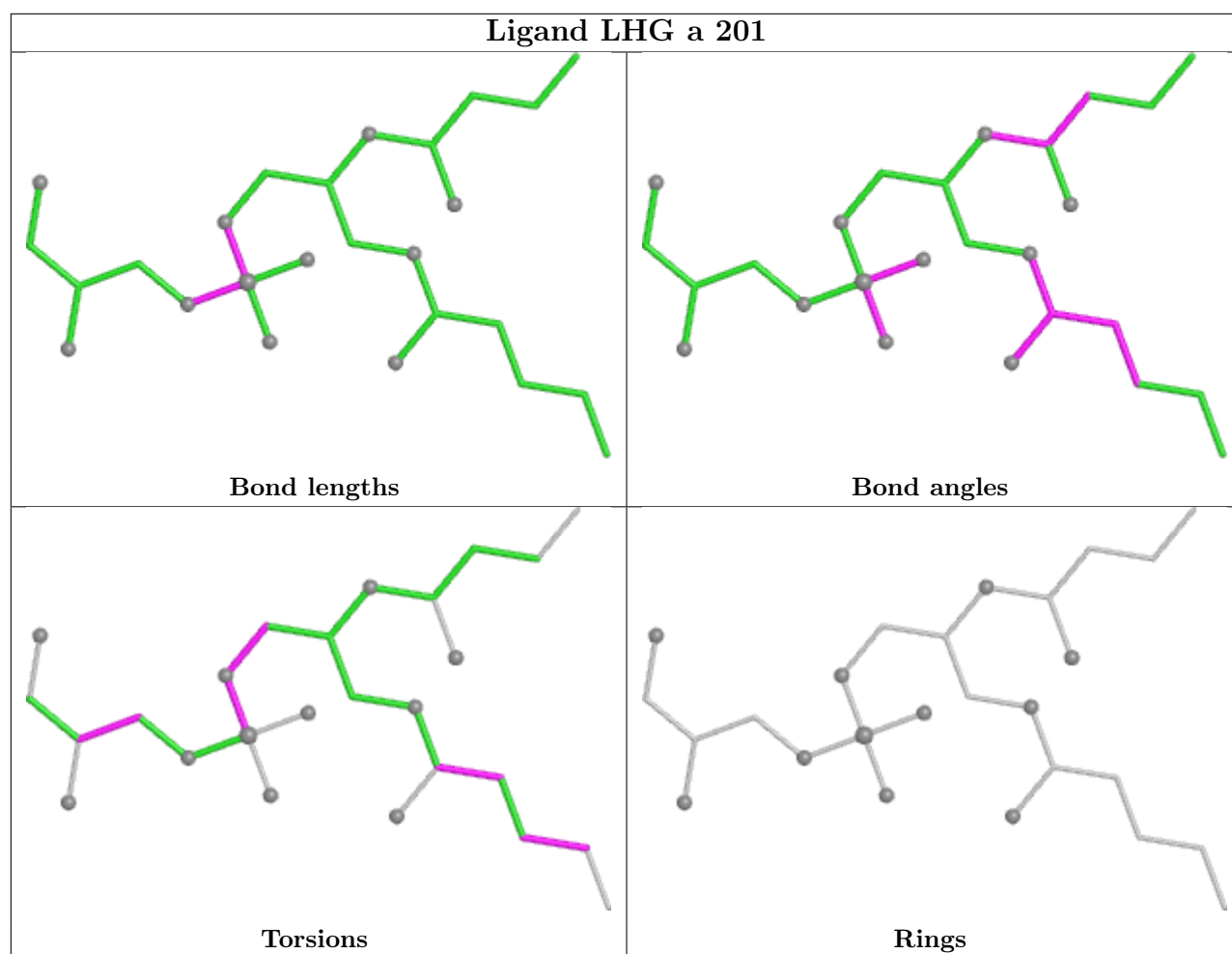


Ligand CLA d 312

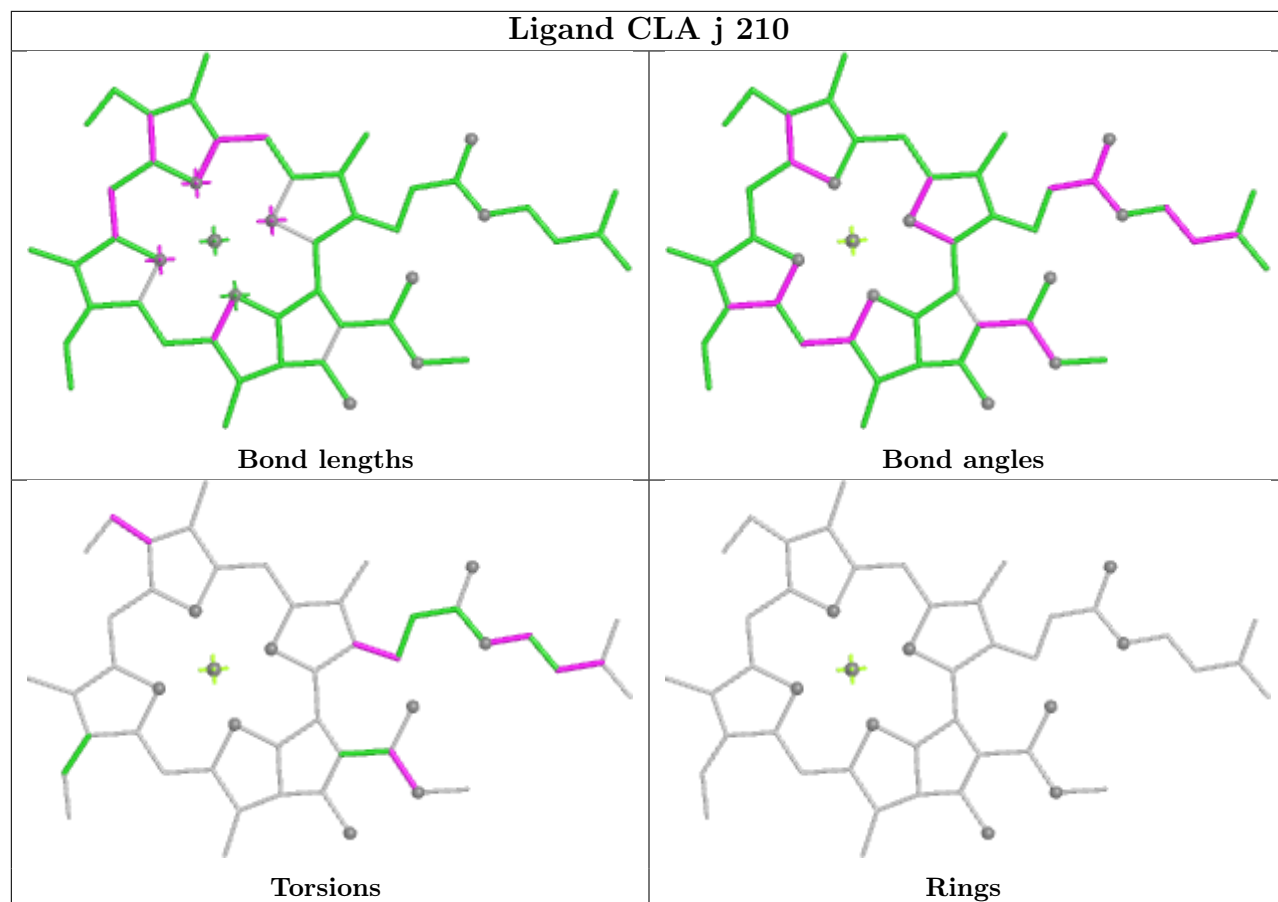


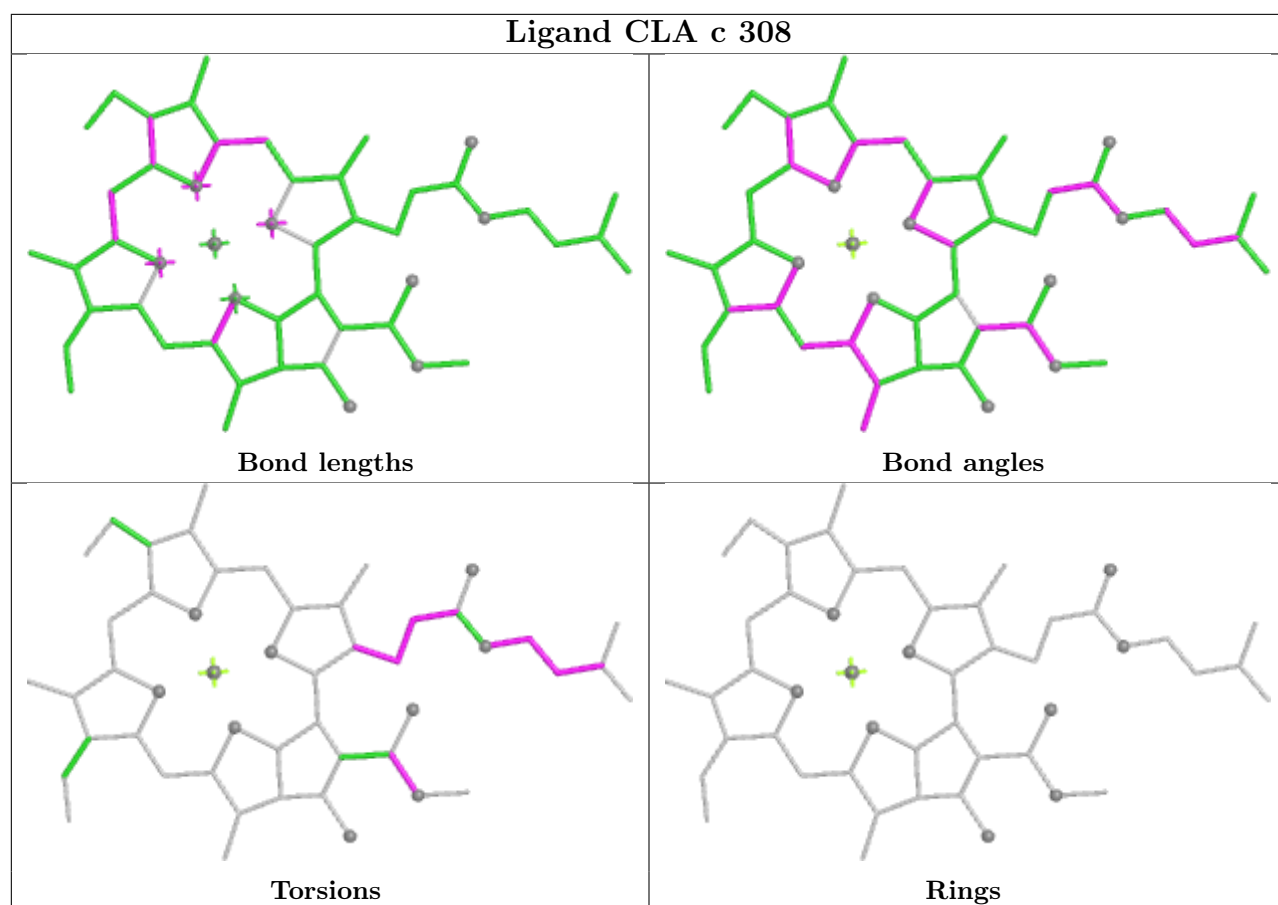
Ligand CLA d 303



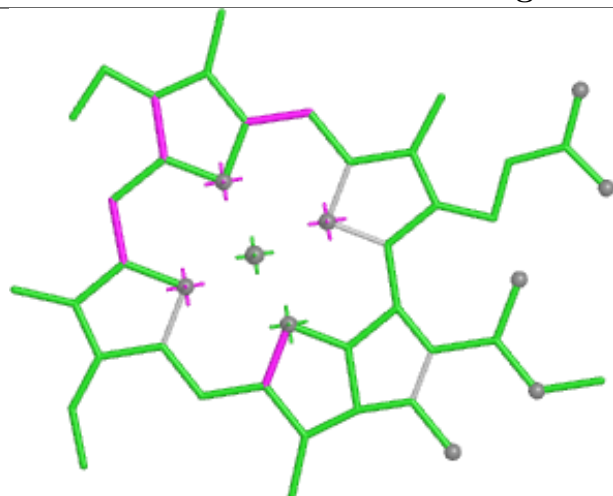


Ligand CLA j 210

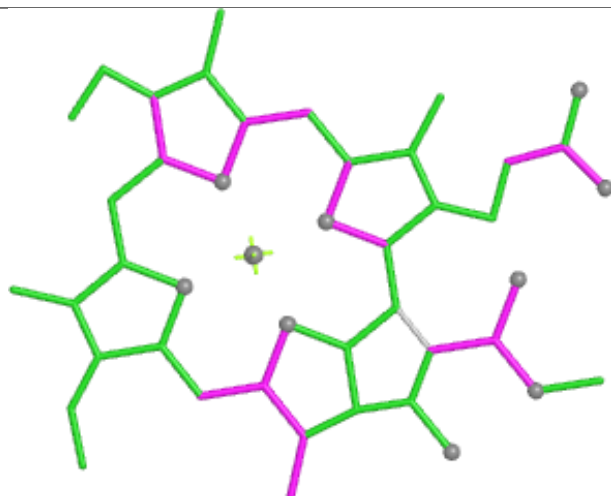




Ligand CLA F 202



Bond lengths



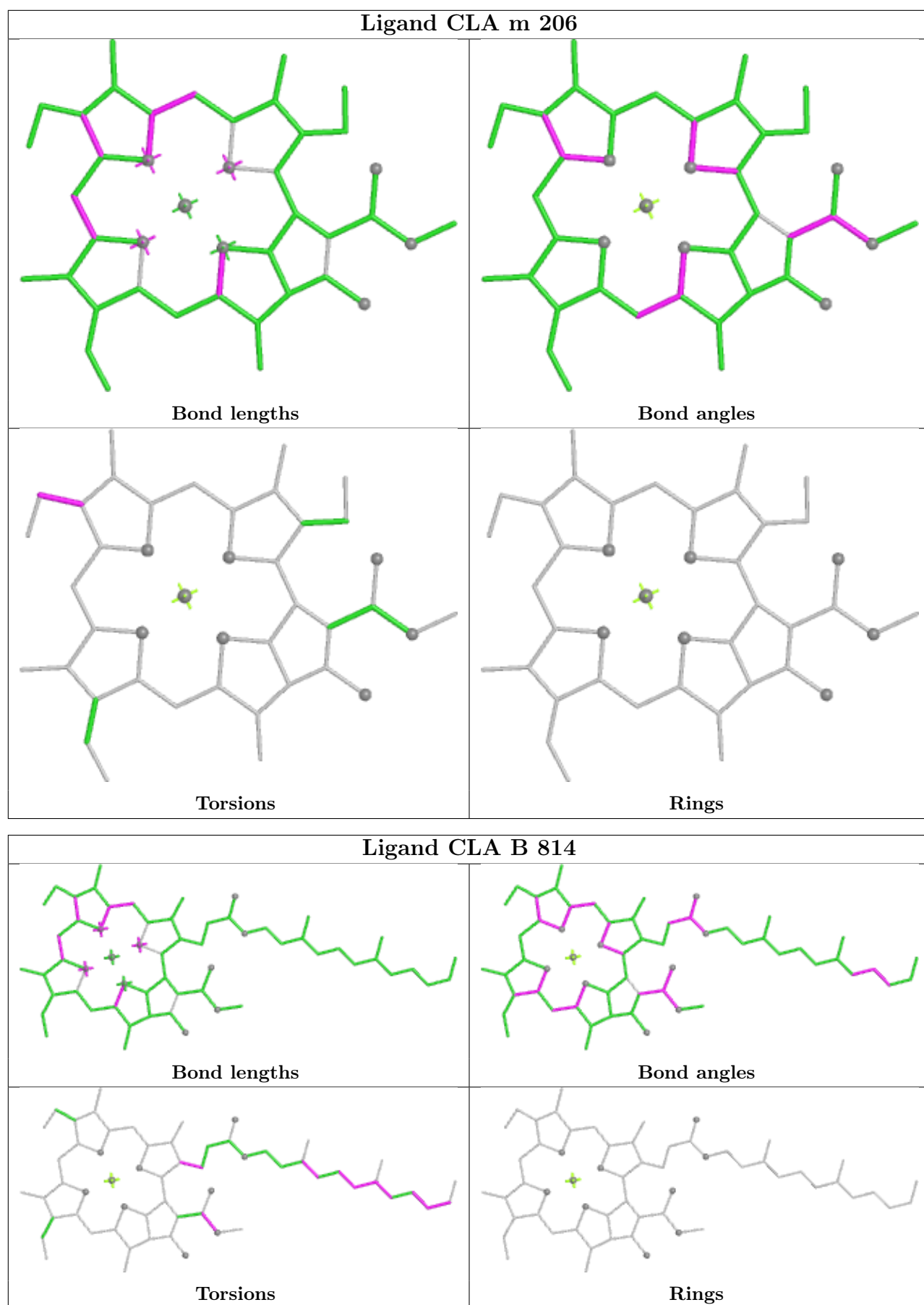
Bond angles



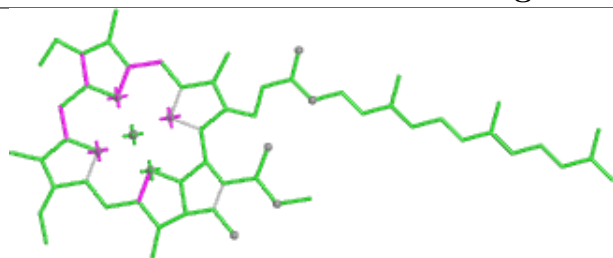
Torsions



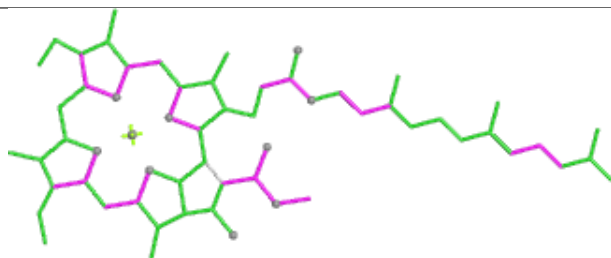
Rings



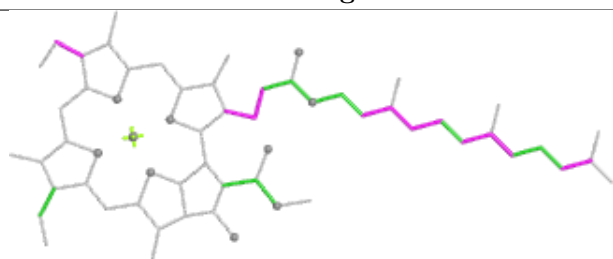
Ligand CLA B 839



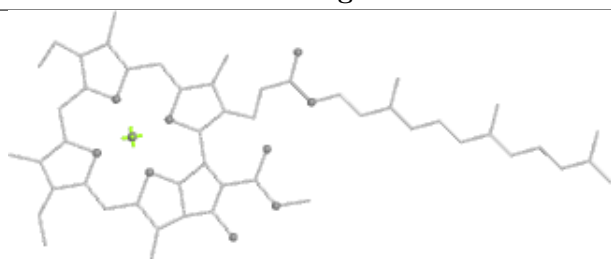
Bond lengths



Bond angles

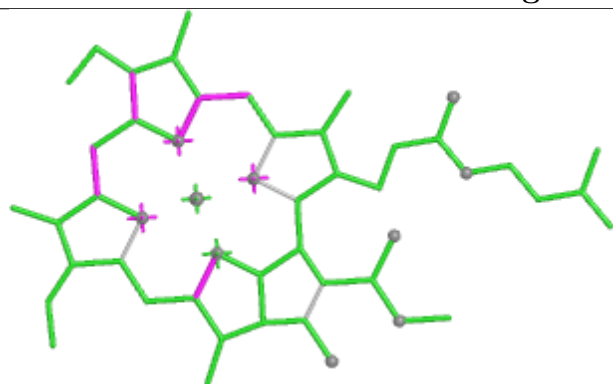


Torsions

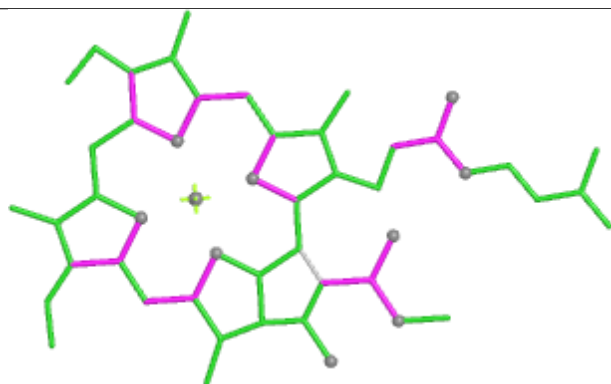


Rings

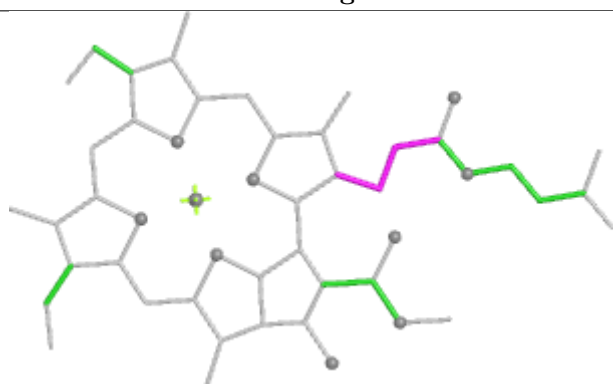
Ligand CLA i 213



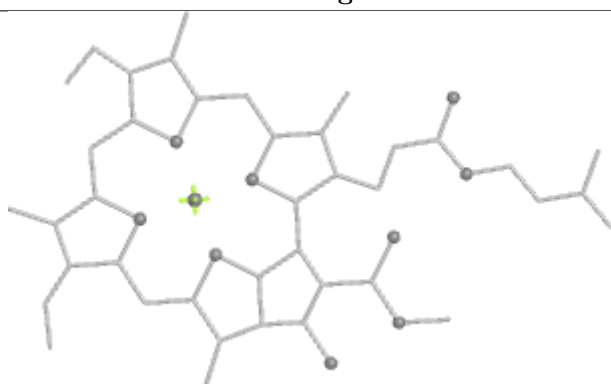
Bond lengths



Bond angles

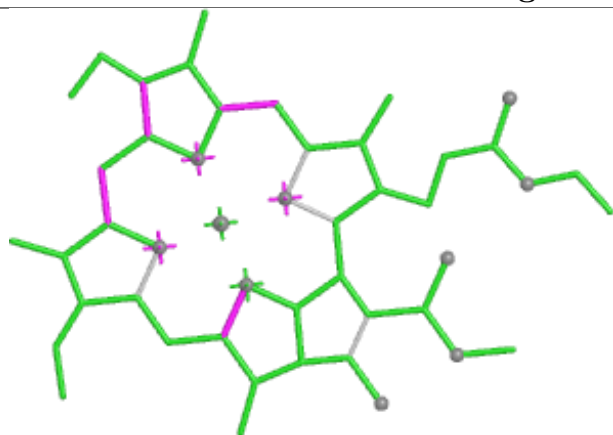


Torsions

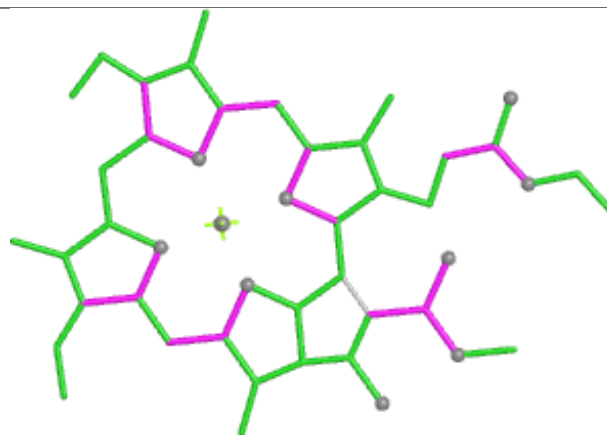


Rings

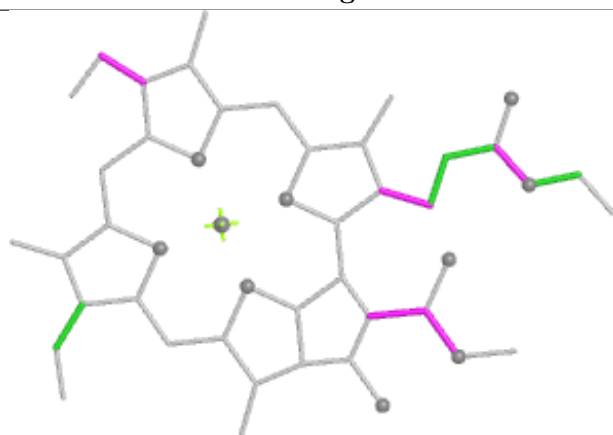
Ligand CLA o 602



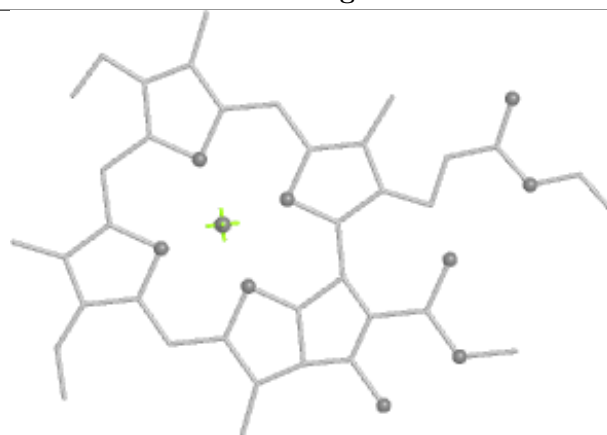
Bond lengths



Bond angles

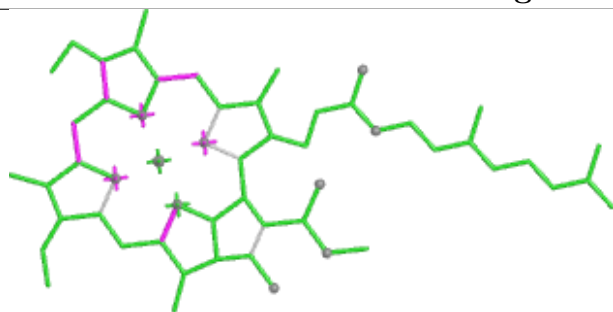


Torsions

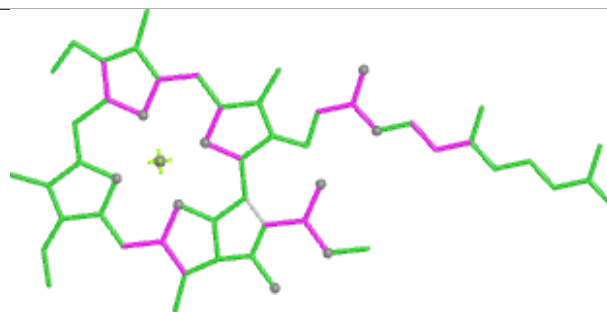


Rings

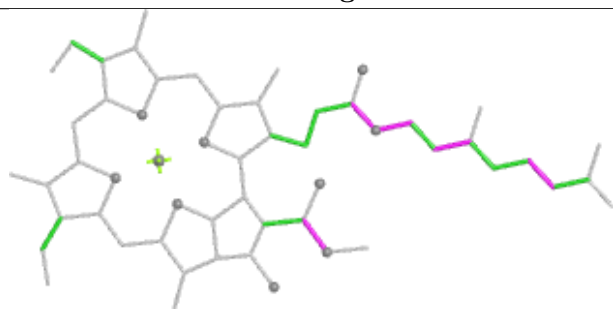
Ligand CLA B 834



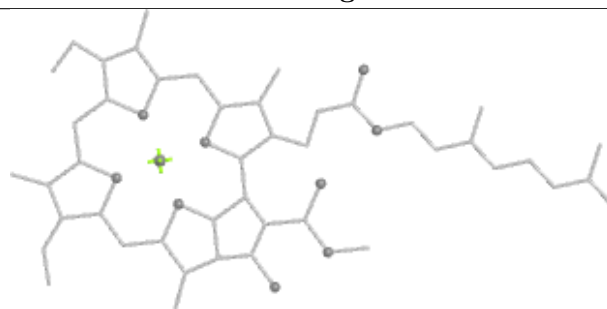
Bond lengths



Bond angles

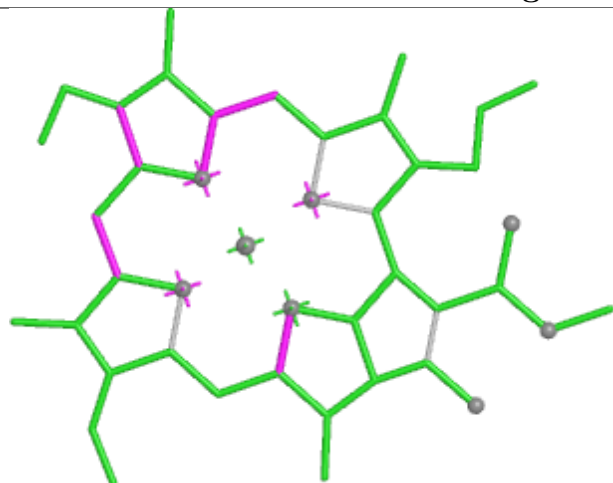


Torsions

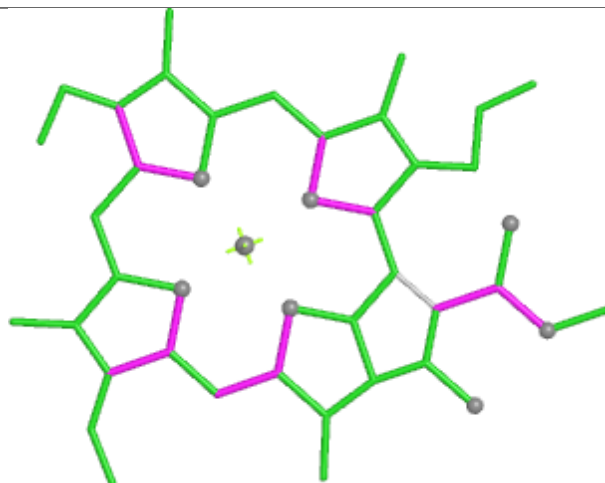


Rings

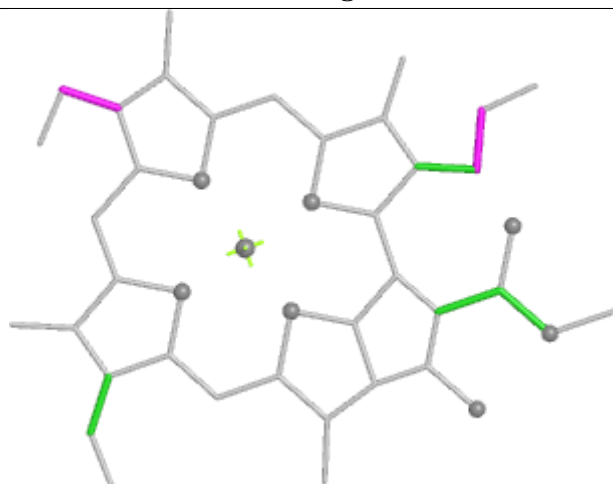
Ligand CLA i 205



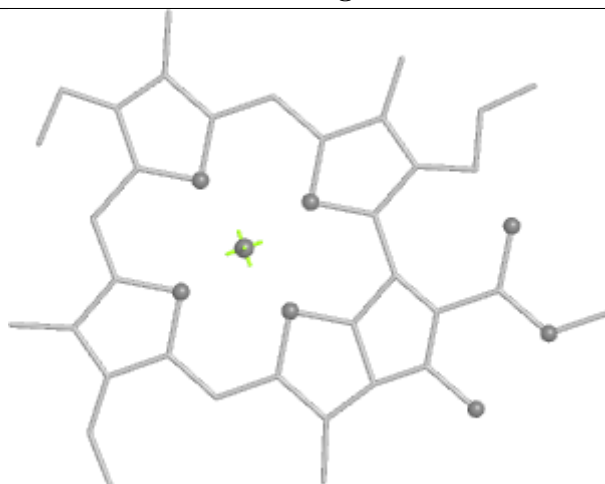
Bond lengths



Bond angles

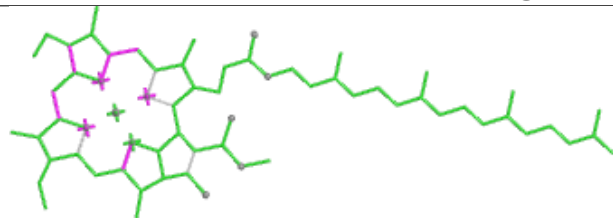


Torsions

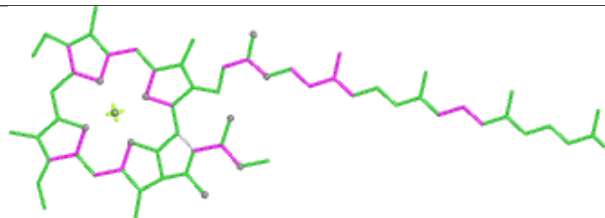


Rings

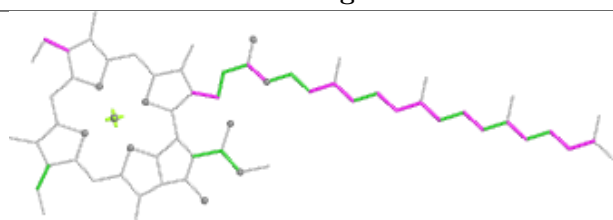
Ligand CLA k 205



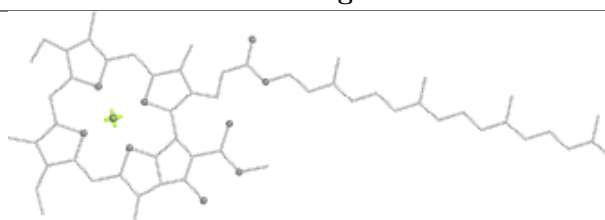
Bond lengths



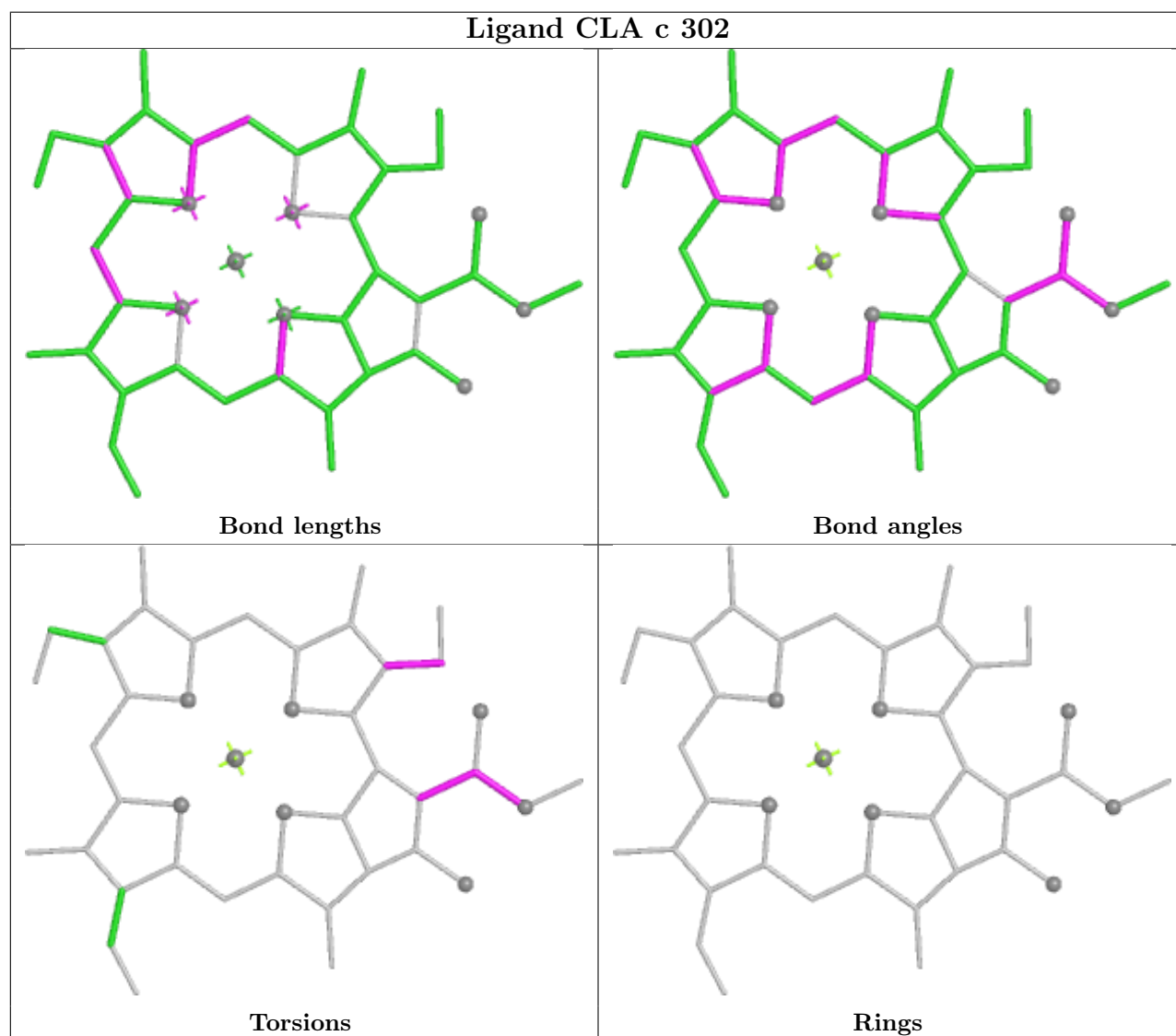
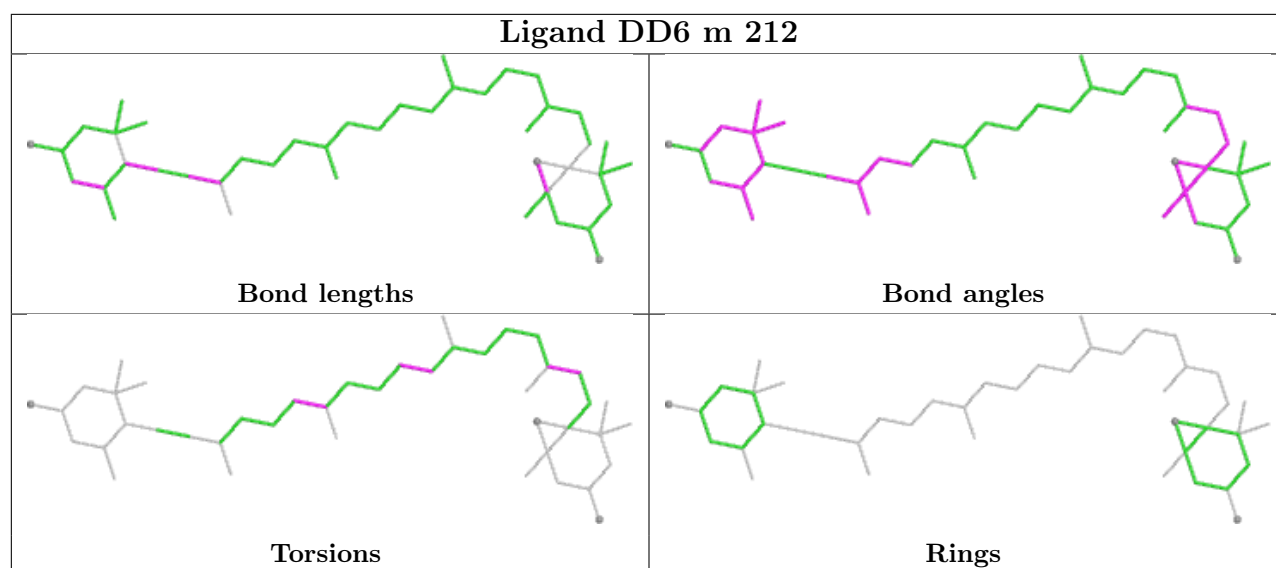
Bond angles



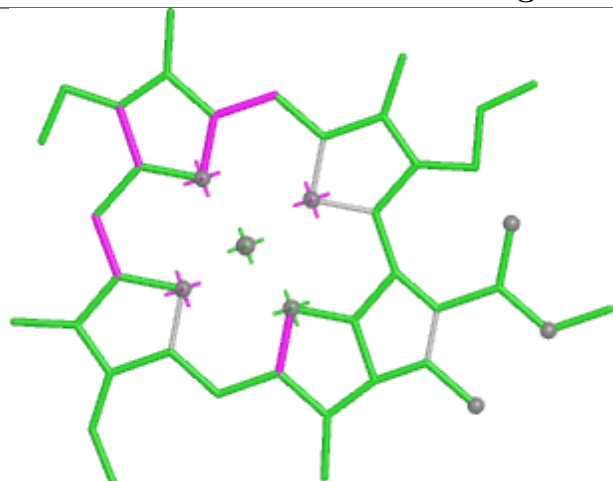
Torsions



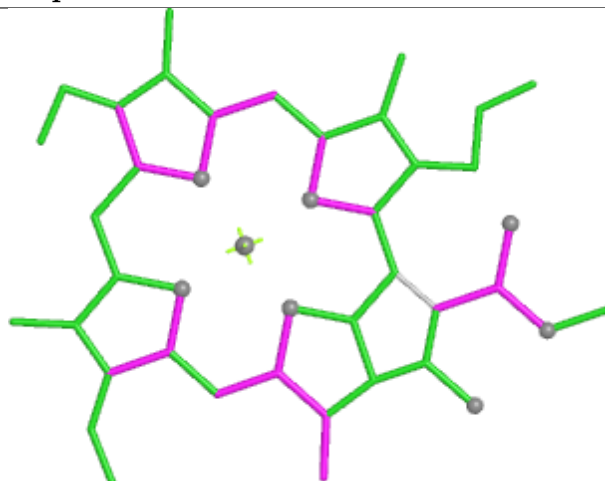
Rings



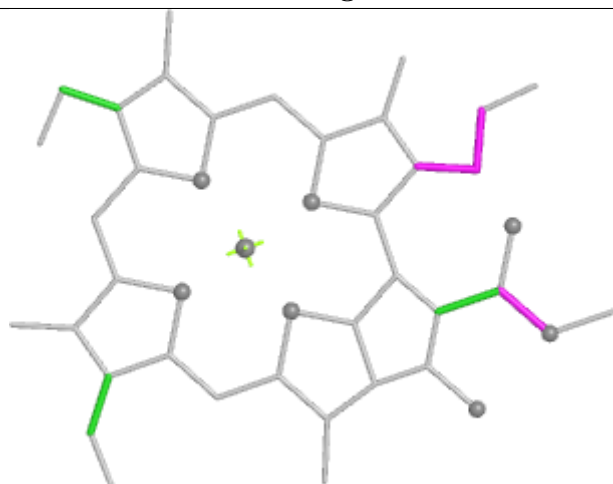
Ligand CLA p 604



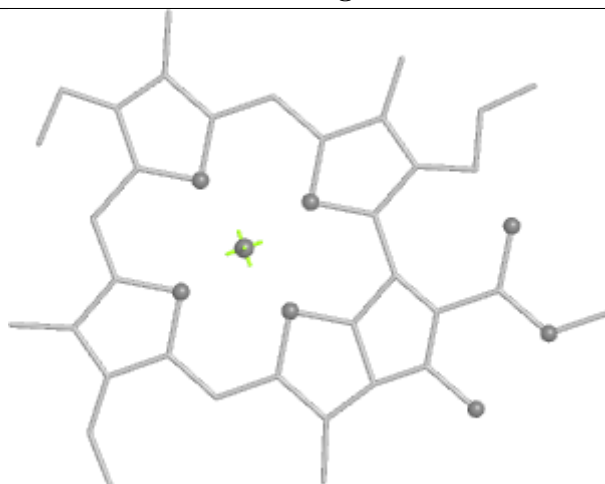
Bond lengths



Bond angles

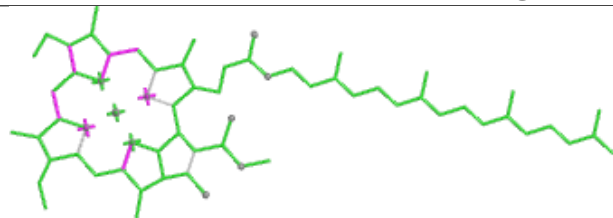


Torsions

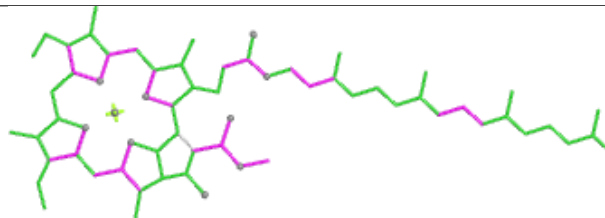


Rings

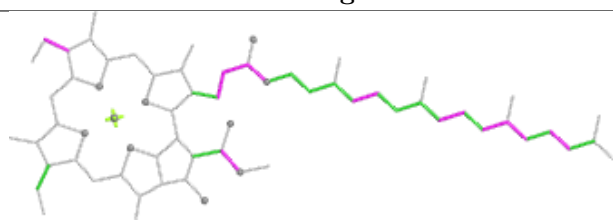
Ligand CLA A 810



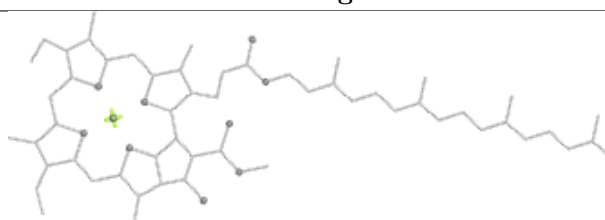
Bond lengths



Bond angles

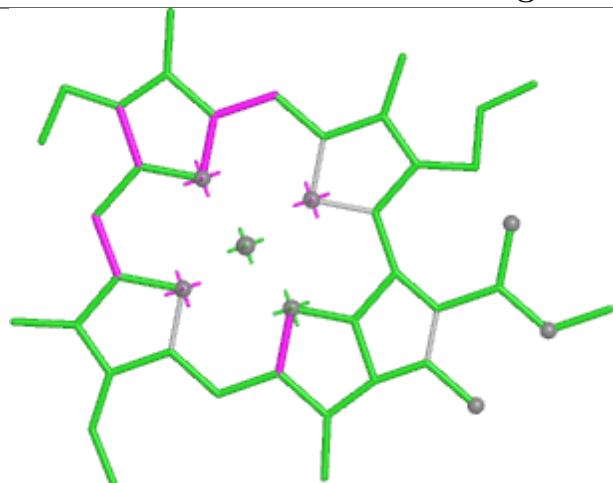


Torsions

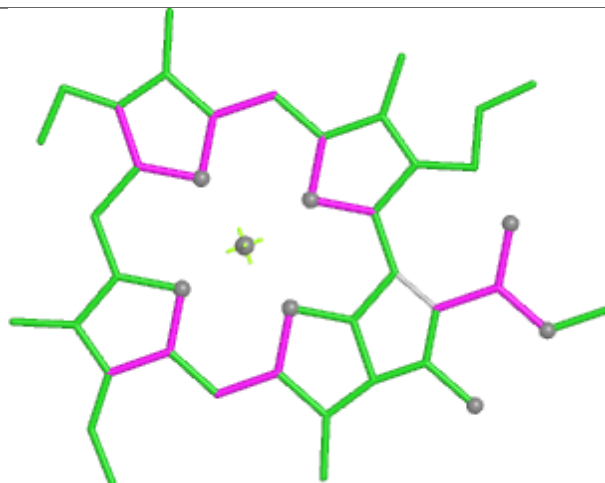


Rings

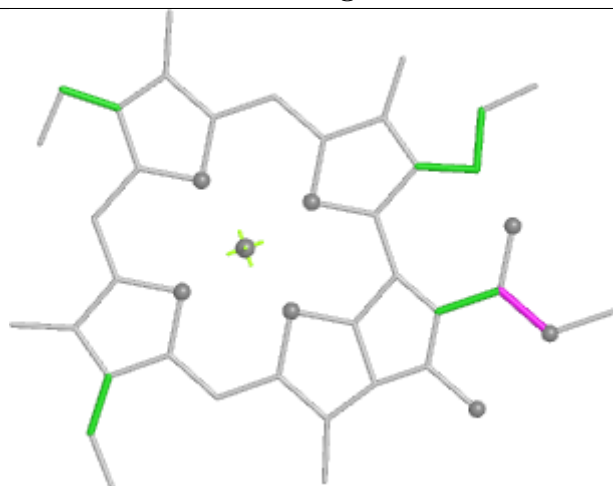
Ligand CLA h 215



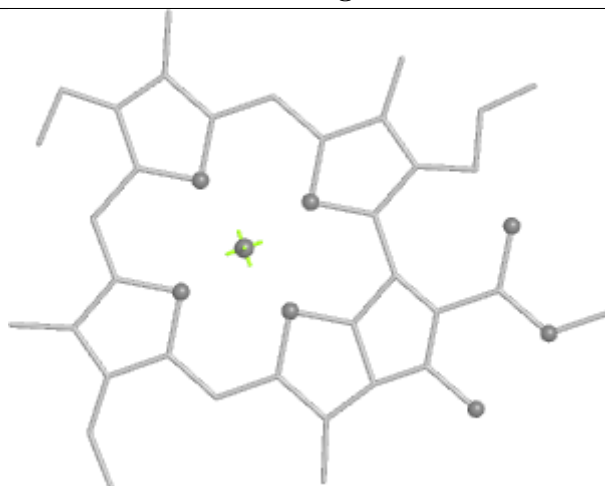
Bond lengths



Bond angles

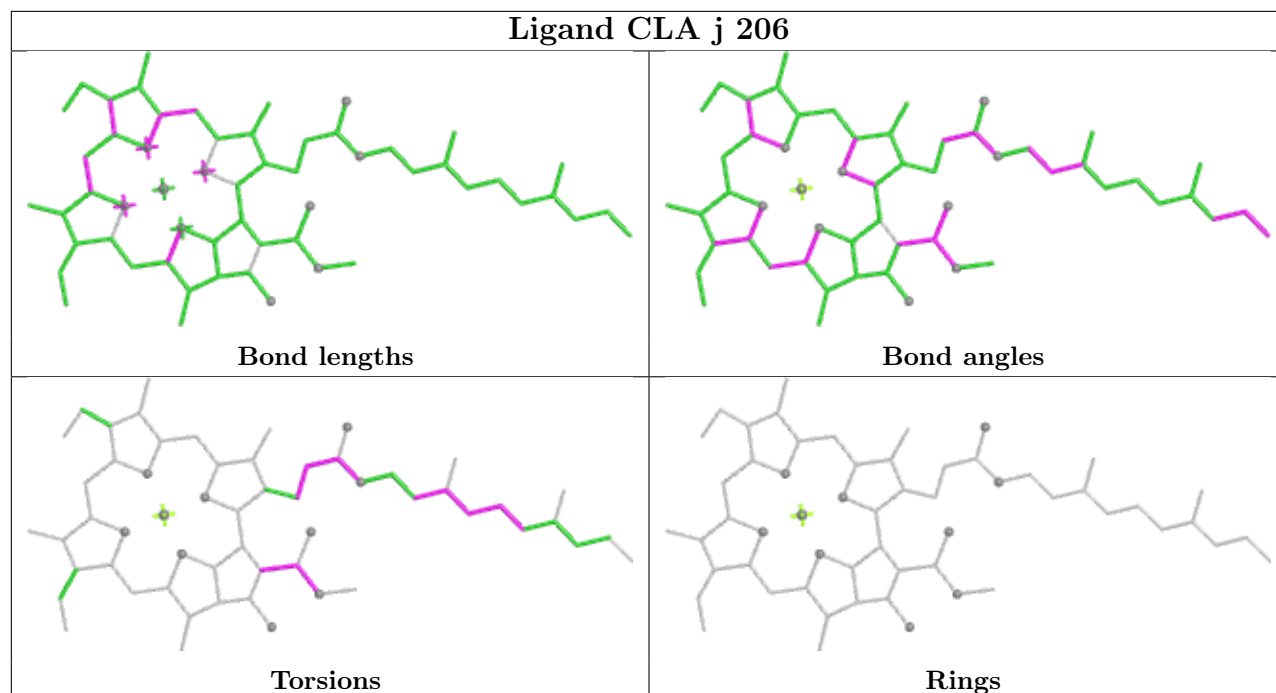


Torsions

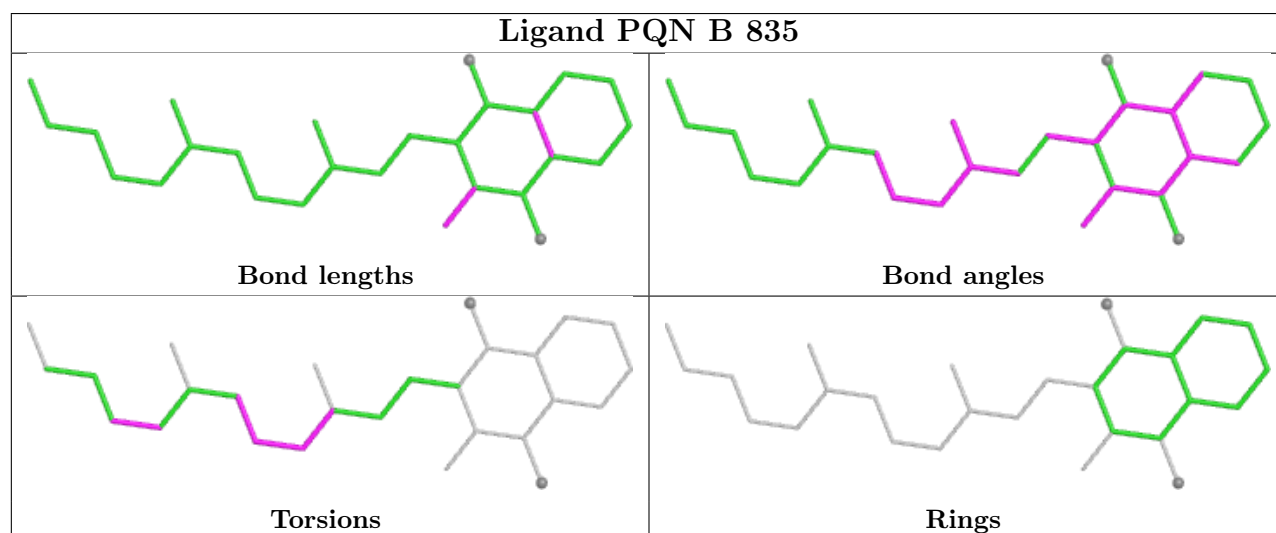


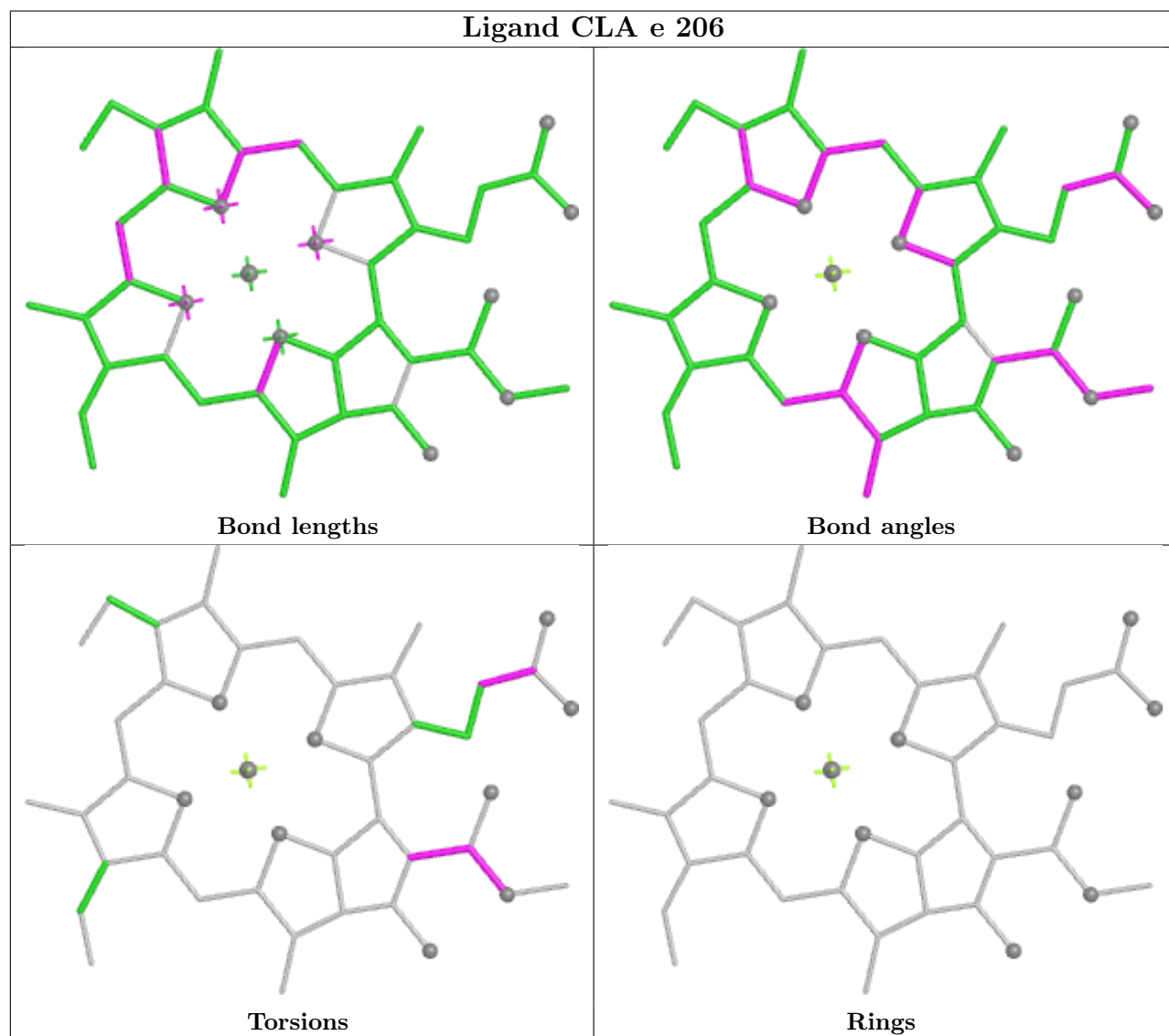
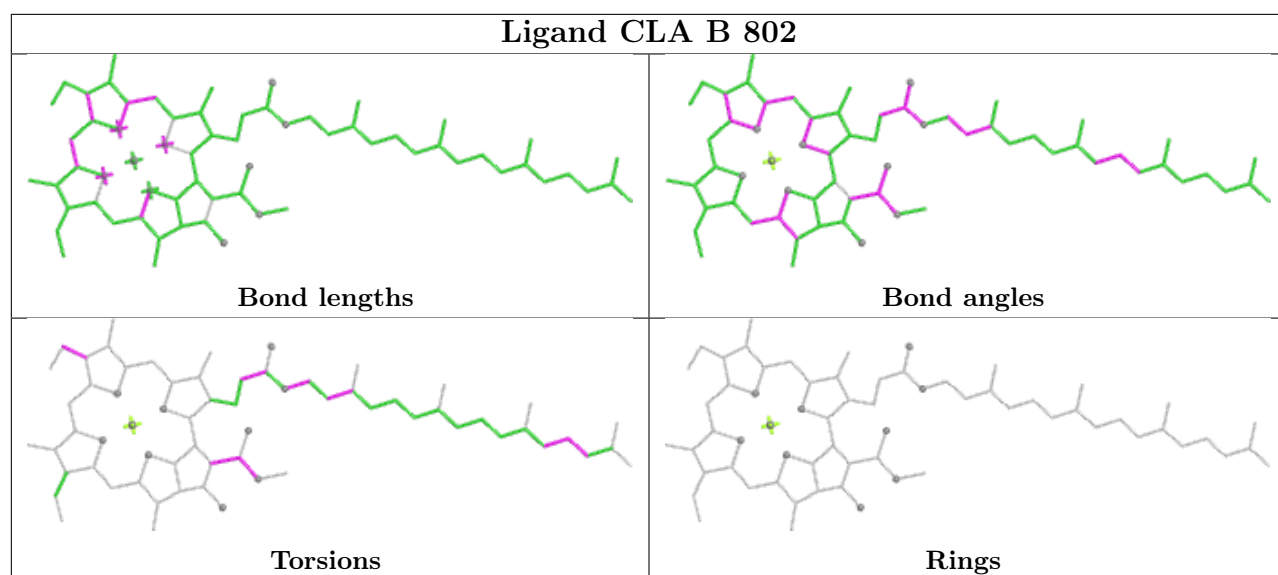
Rings

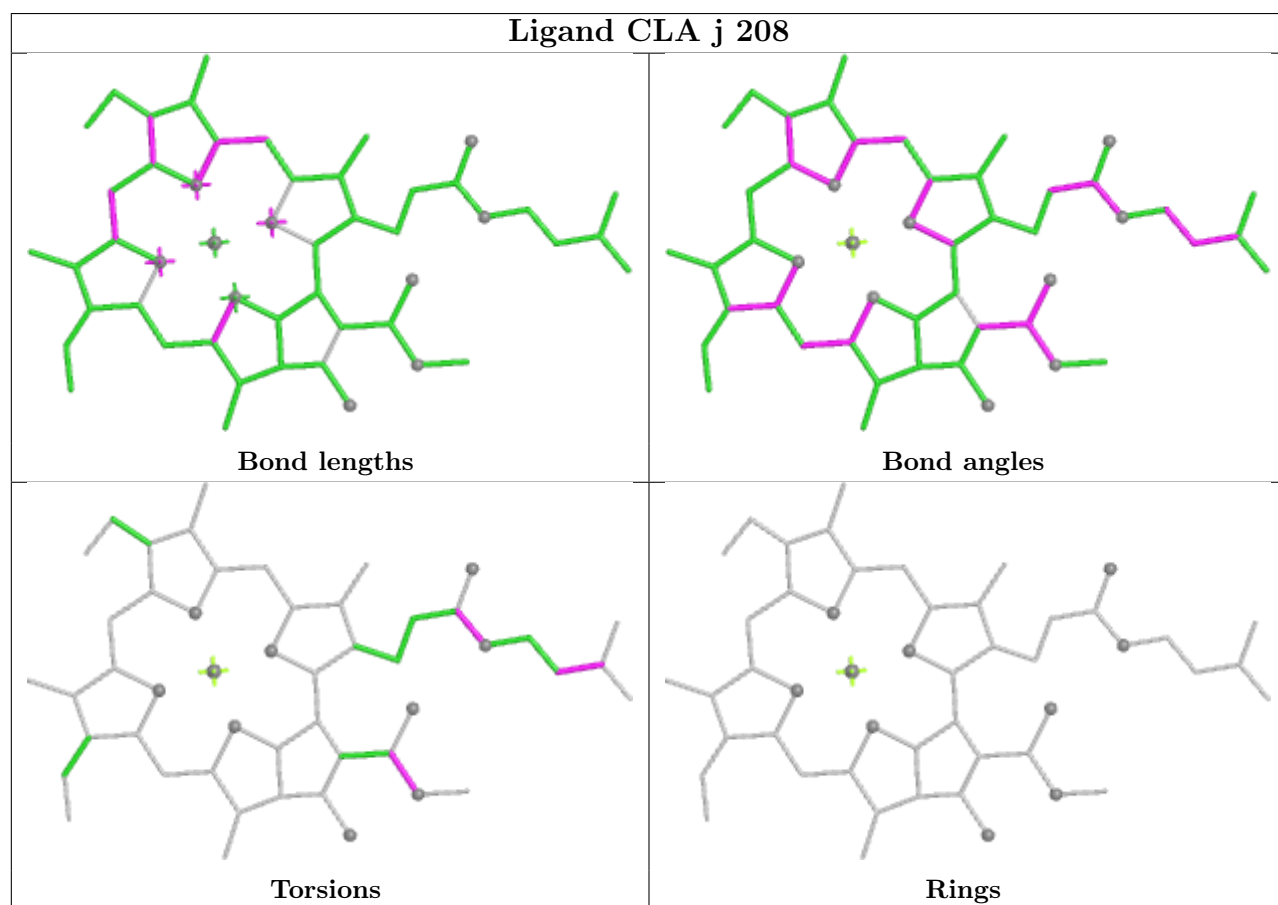
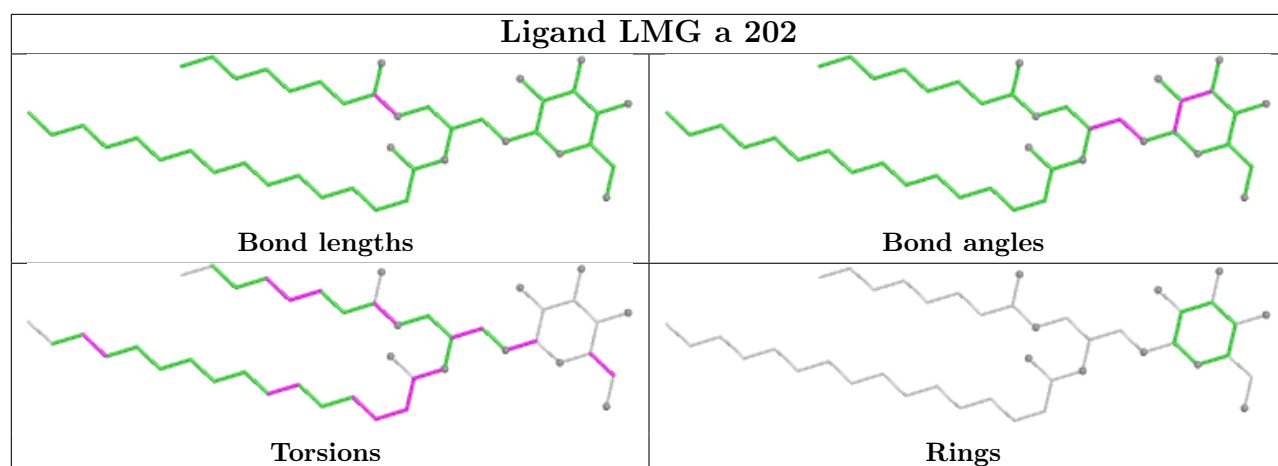
Ligand CLA j 206

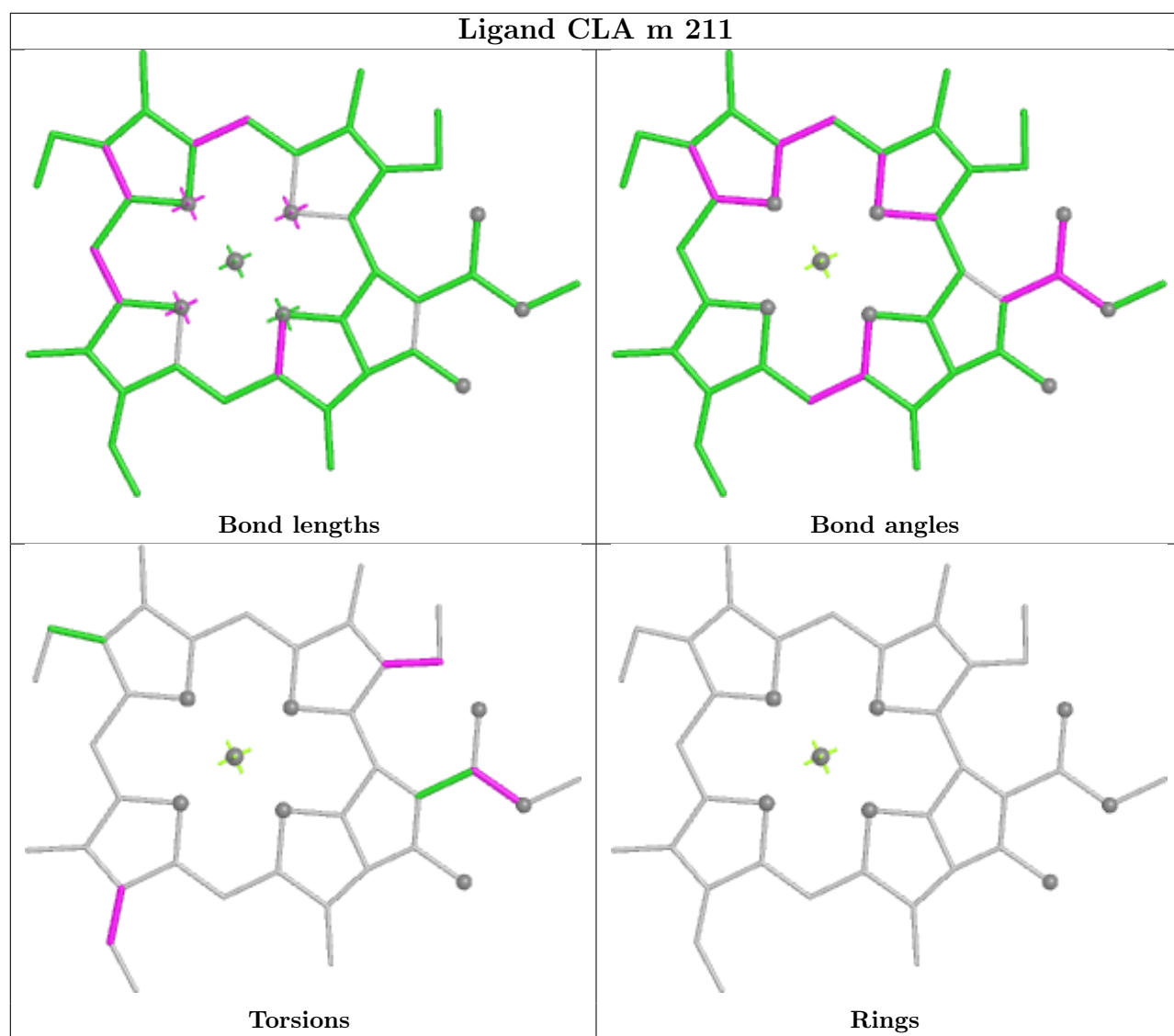


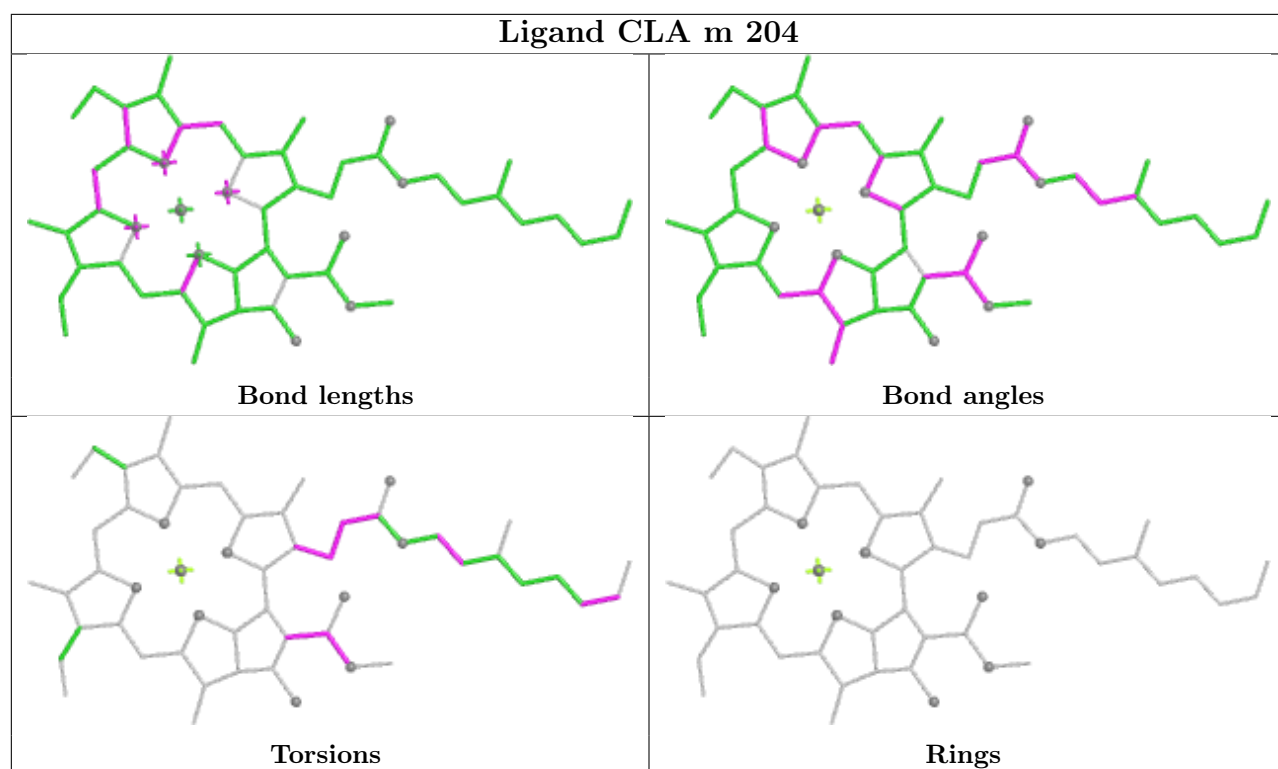
Ligand PQN B 835



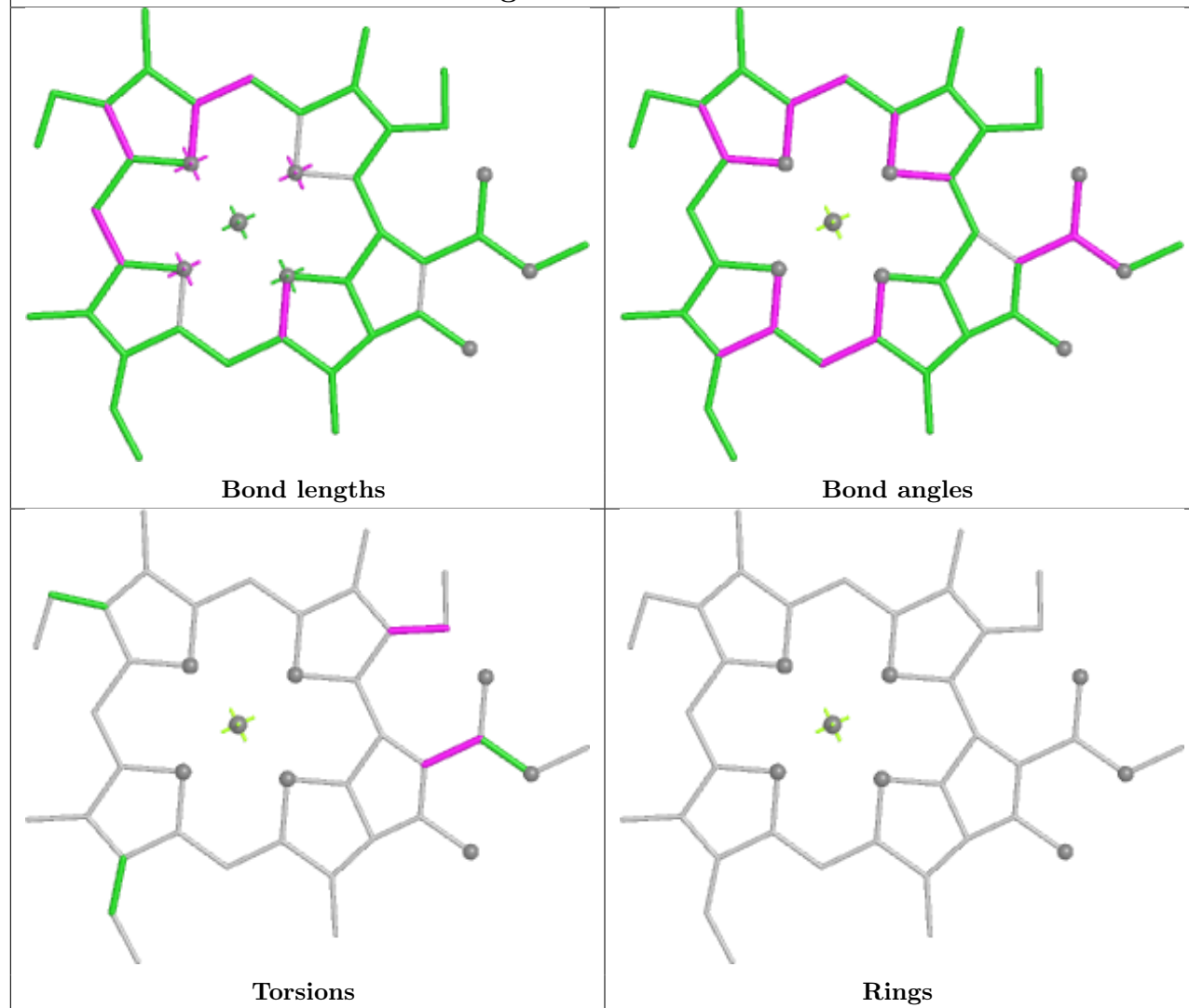




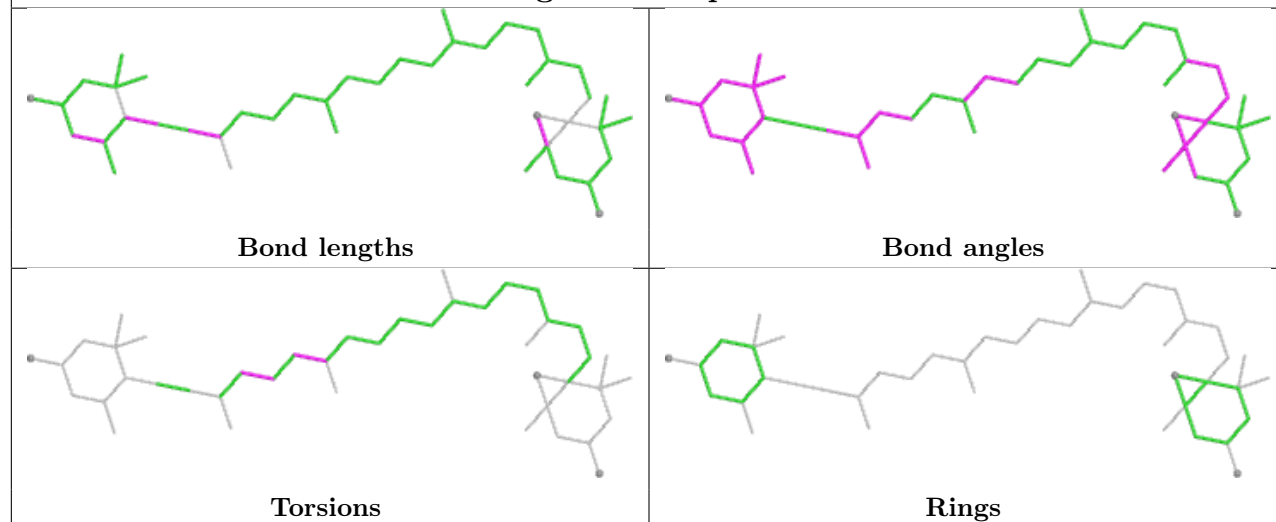




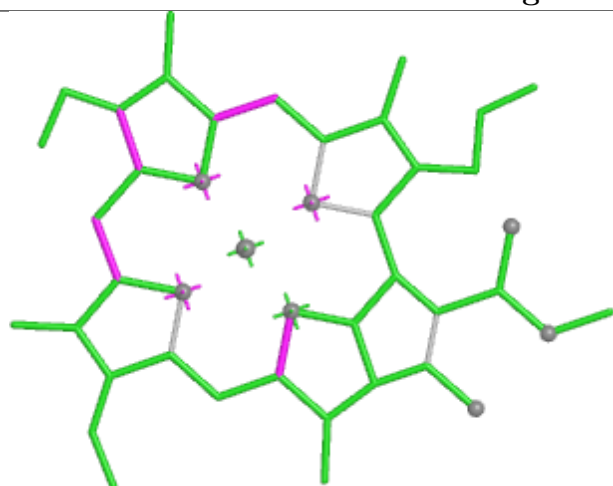
Ligand CLA e 208



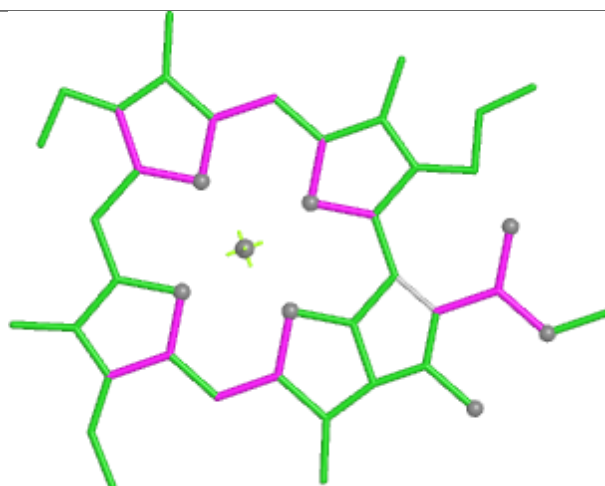
Ligand DD6 p 610



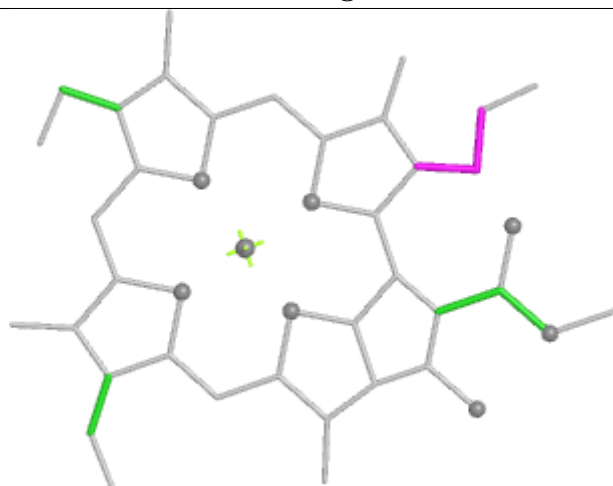
Ligand CLA 1 608



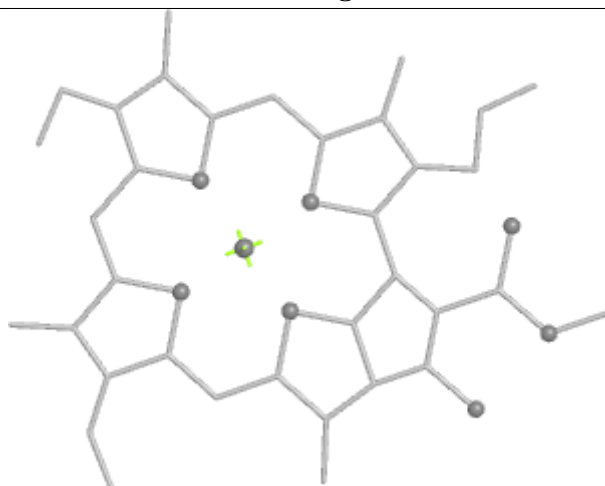
Bond lengths



Bond angles

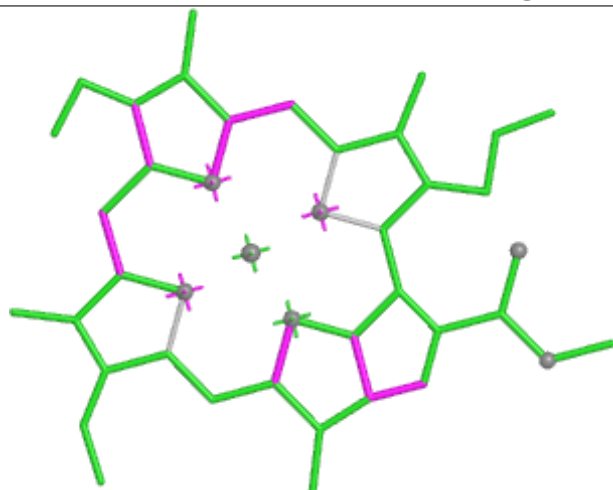


Torsions

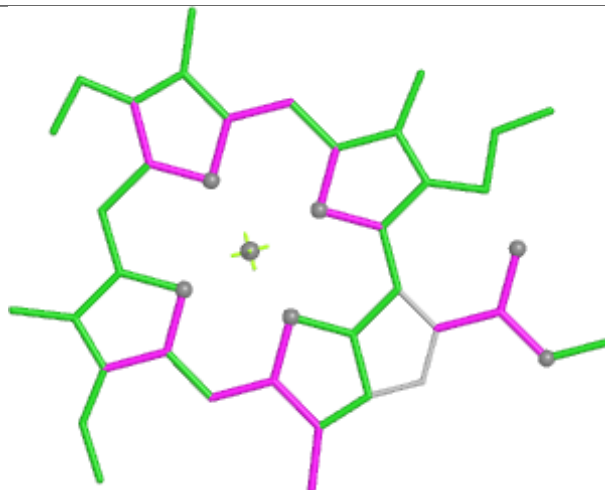


Rings

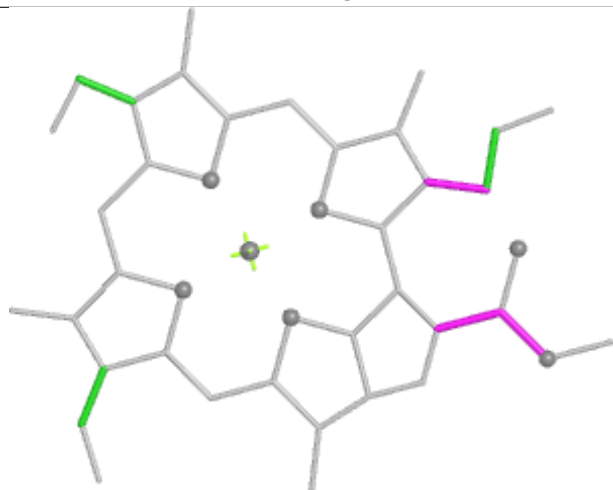
Ligand CLA o 608



Bond lengths



Bond angles

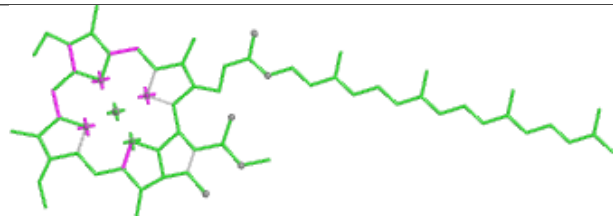


Torsions

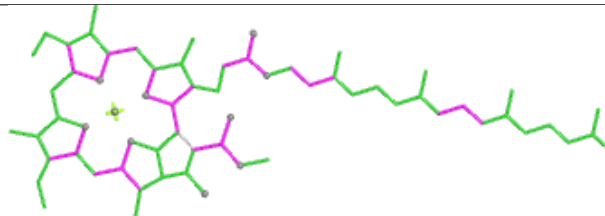


Rings

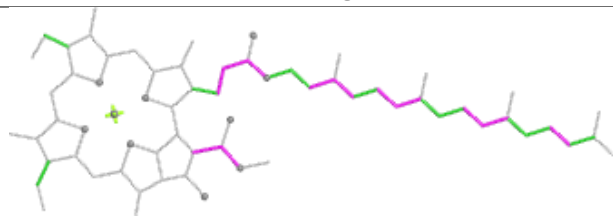
Ligand CLA A 833



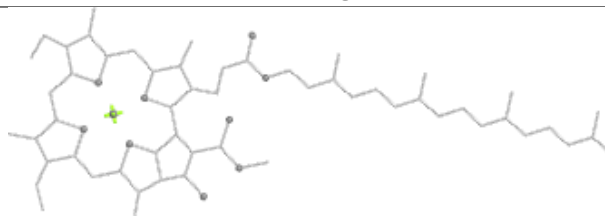
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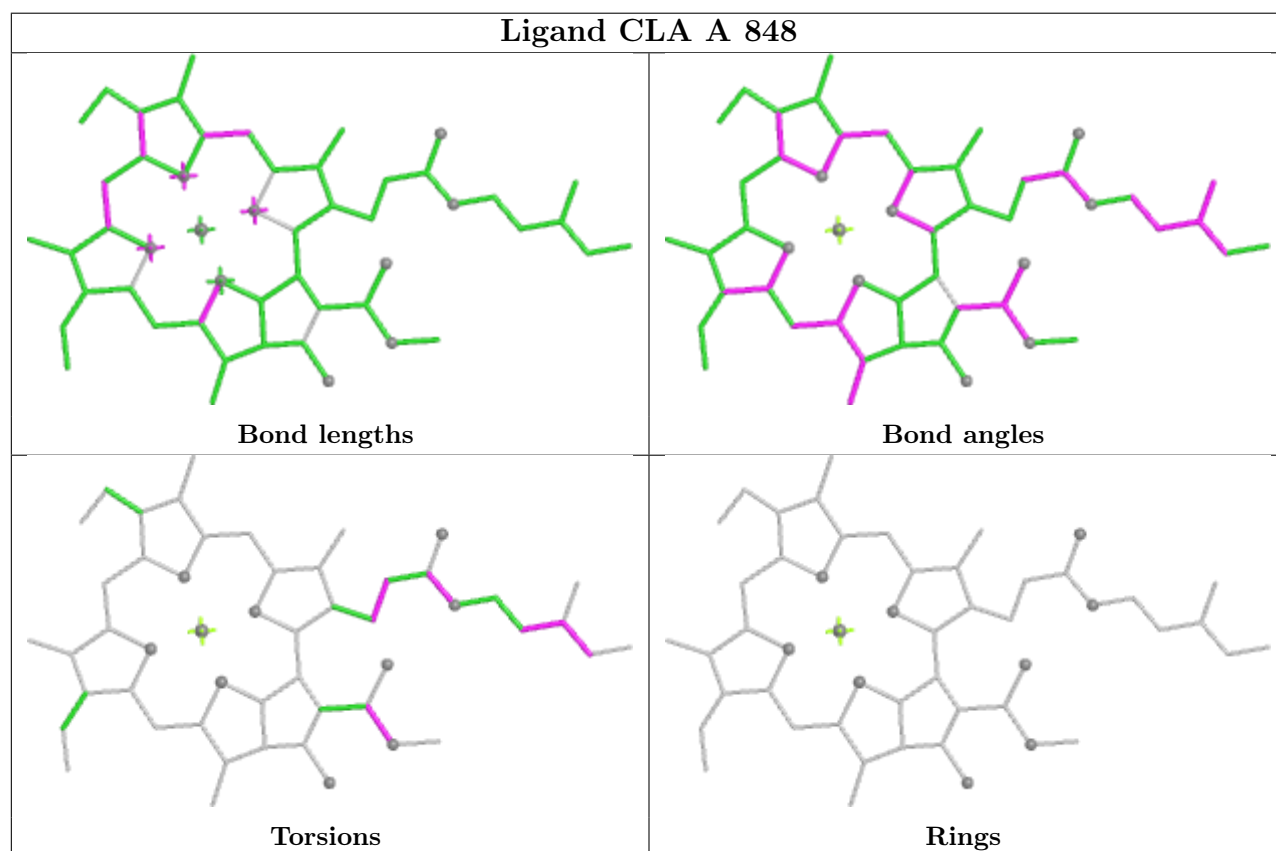
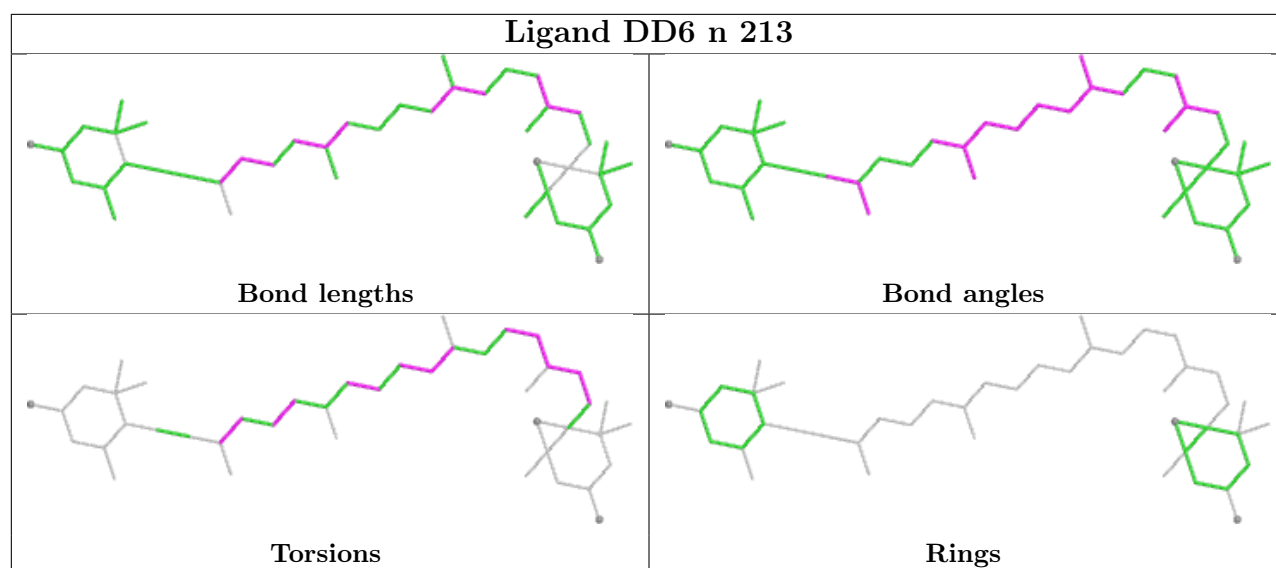
Bond angles



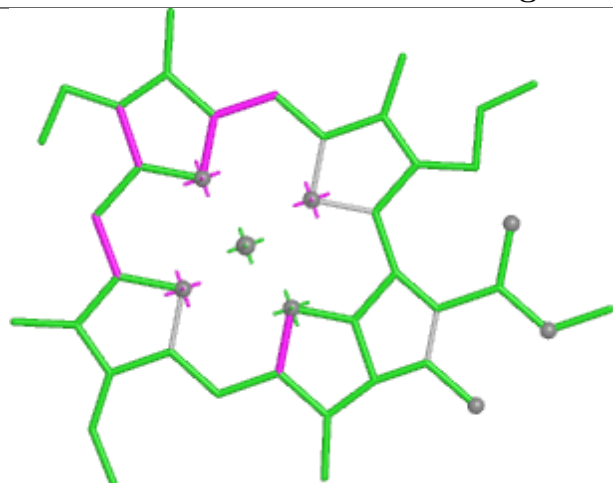
Torsions



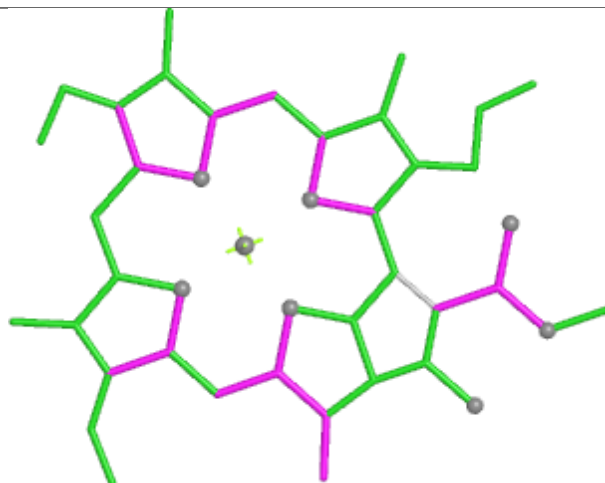
Rings



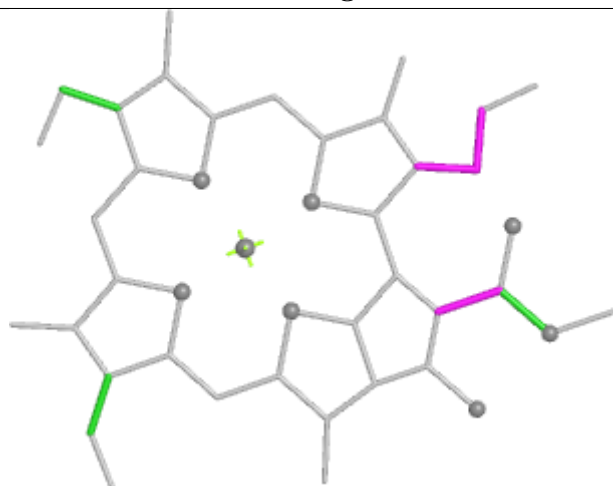
Ligand CLA c 306



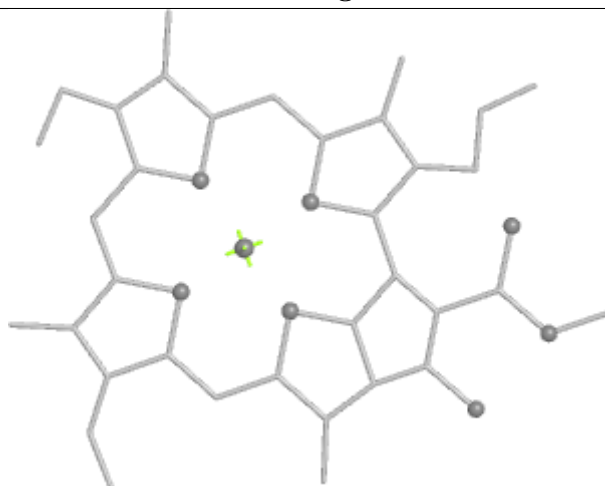
Bond lengths



Bond angles

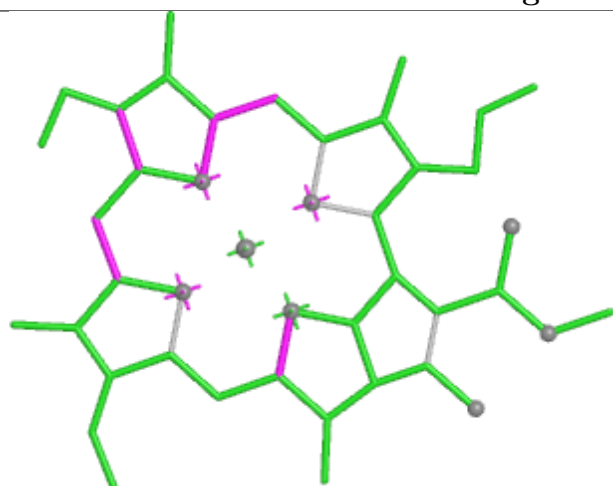


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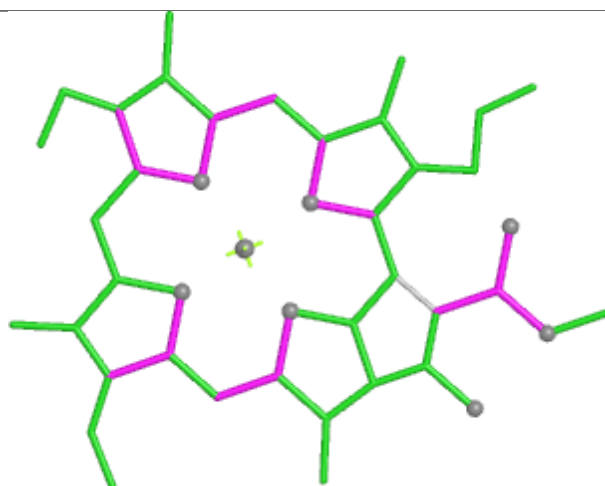


Rings

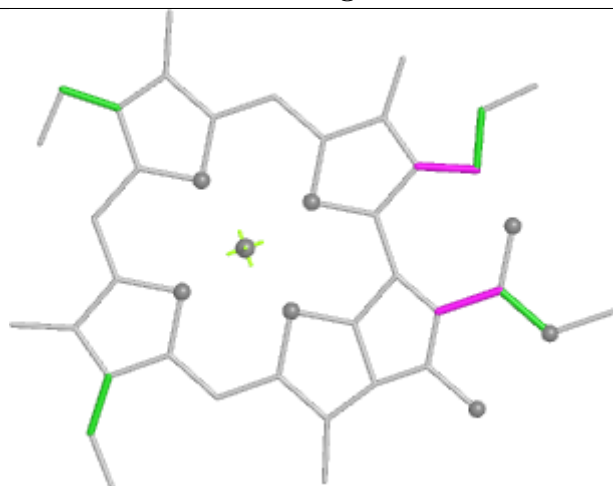
Ligand CLA 1 604



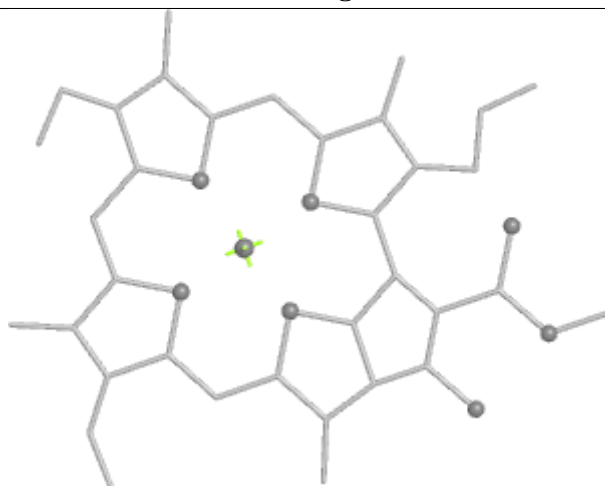
Bond lengths



Bond angles

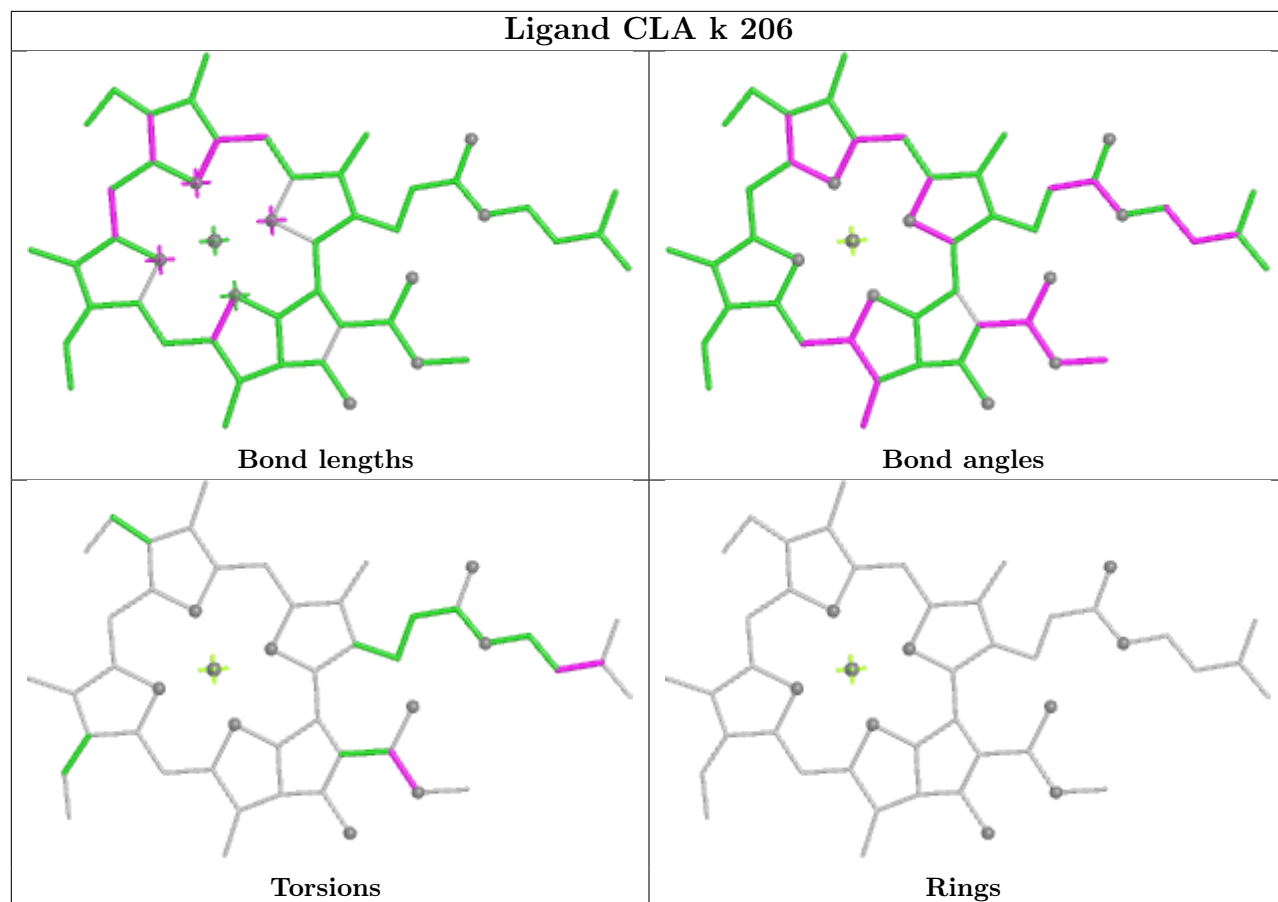


Torsions

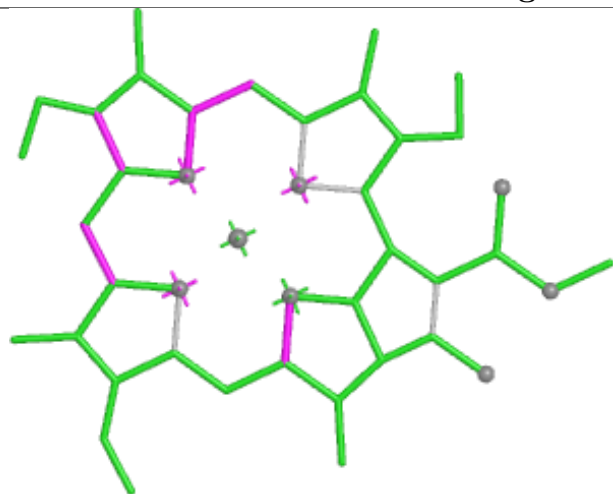


Rings

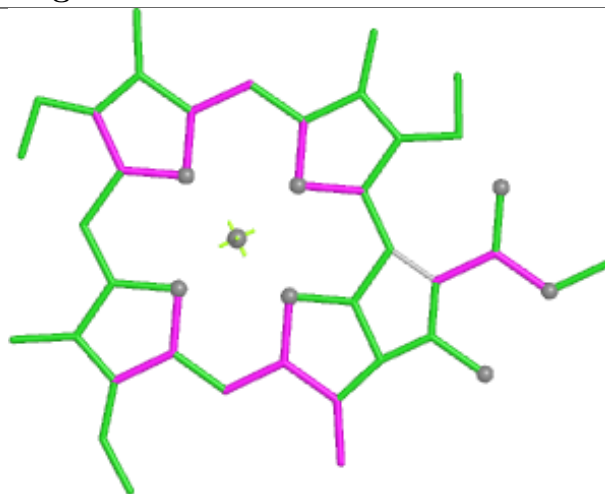
Ligand CLA k 206



Ligand CLA g 214



Bond lengths



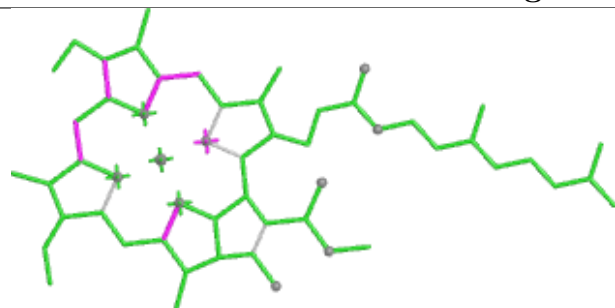
Bond angles



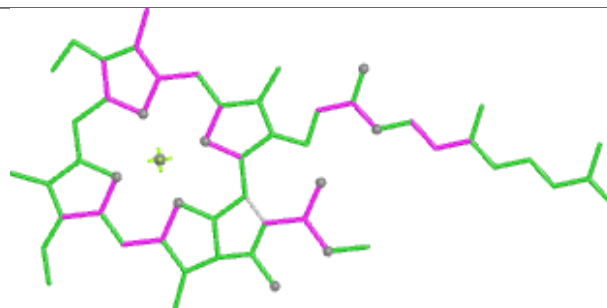
Torsions



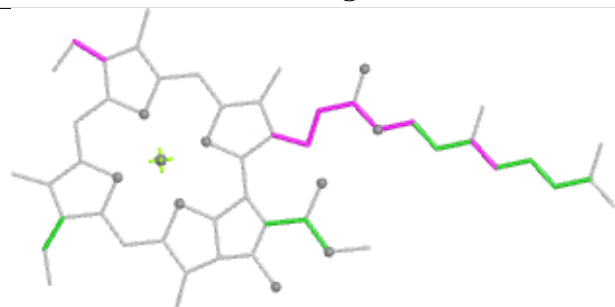
Rings

Ligand CLA i 208

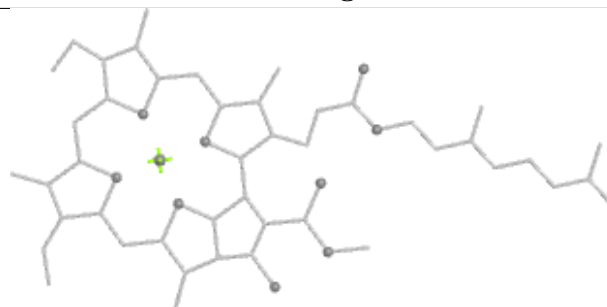
Bond lengths



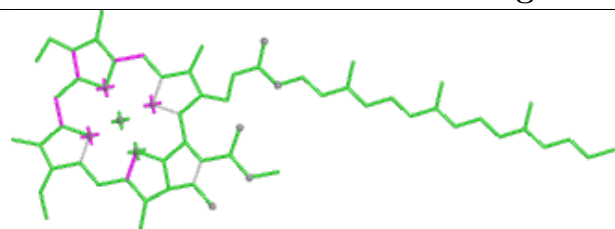
Bond angles



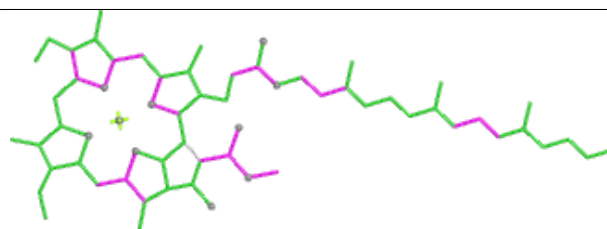
Torsions



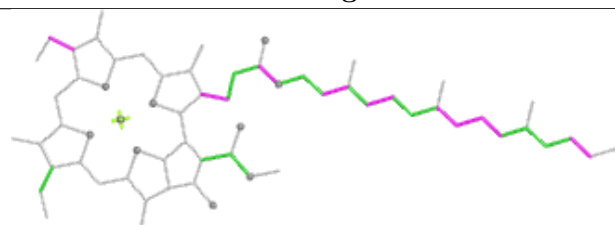
Rings

Ligand CLA B 843

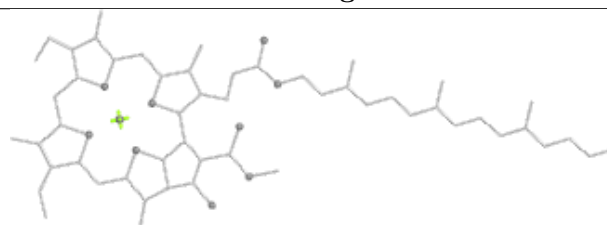
Bond lengths



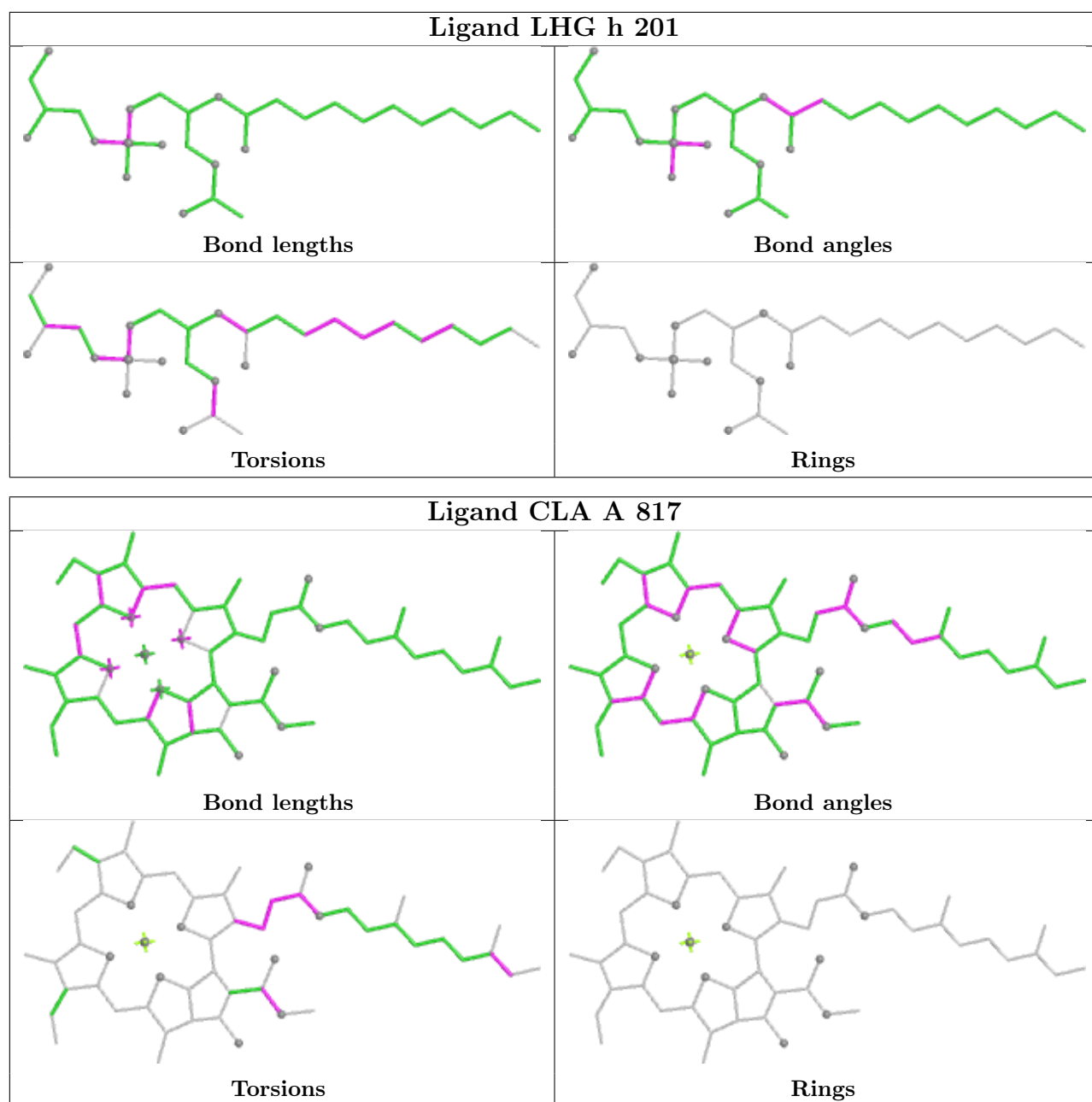
Bond angles

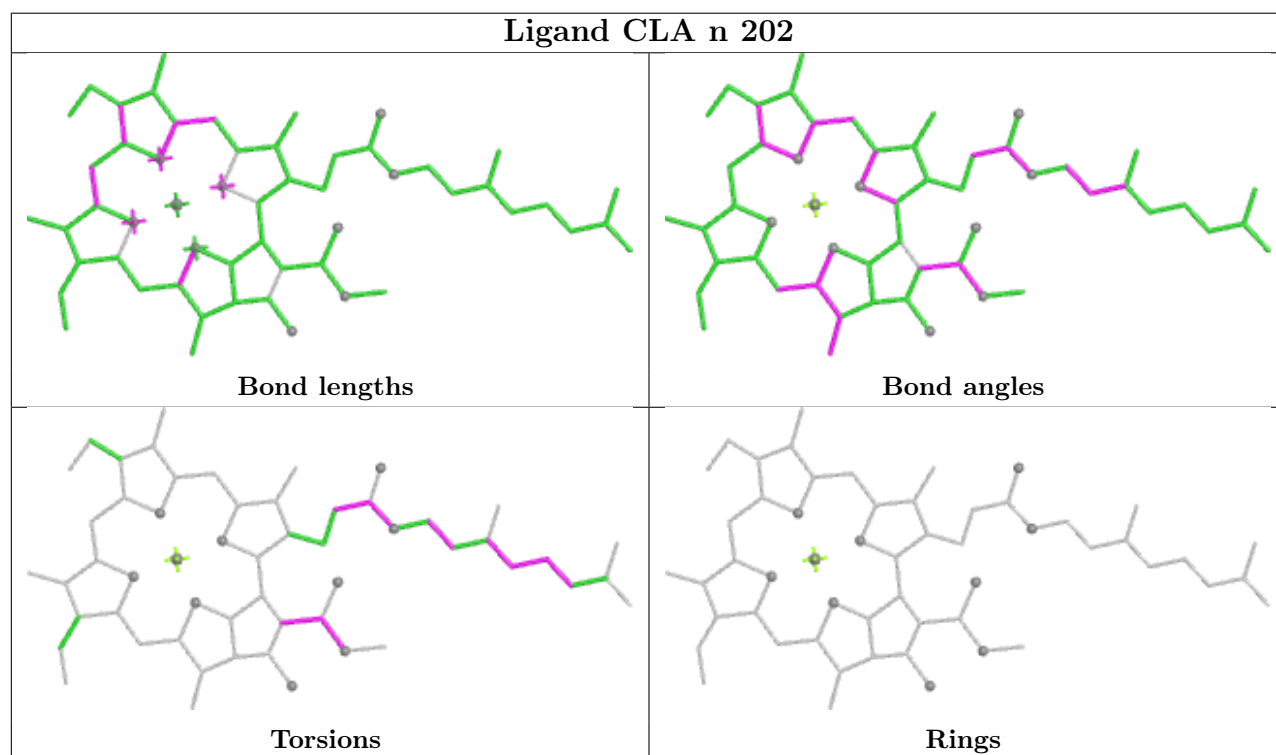
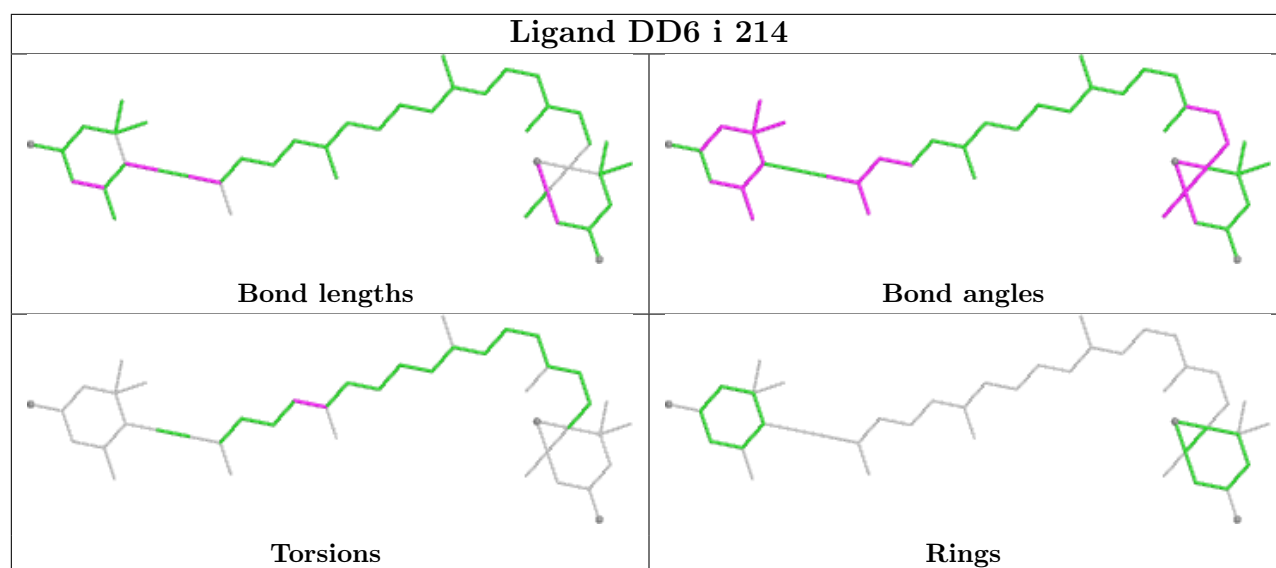


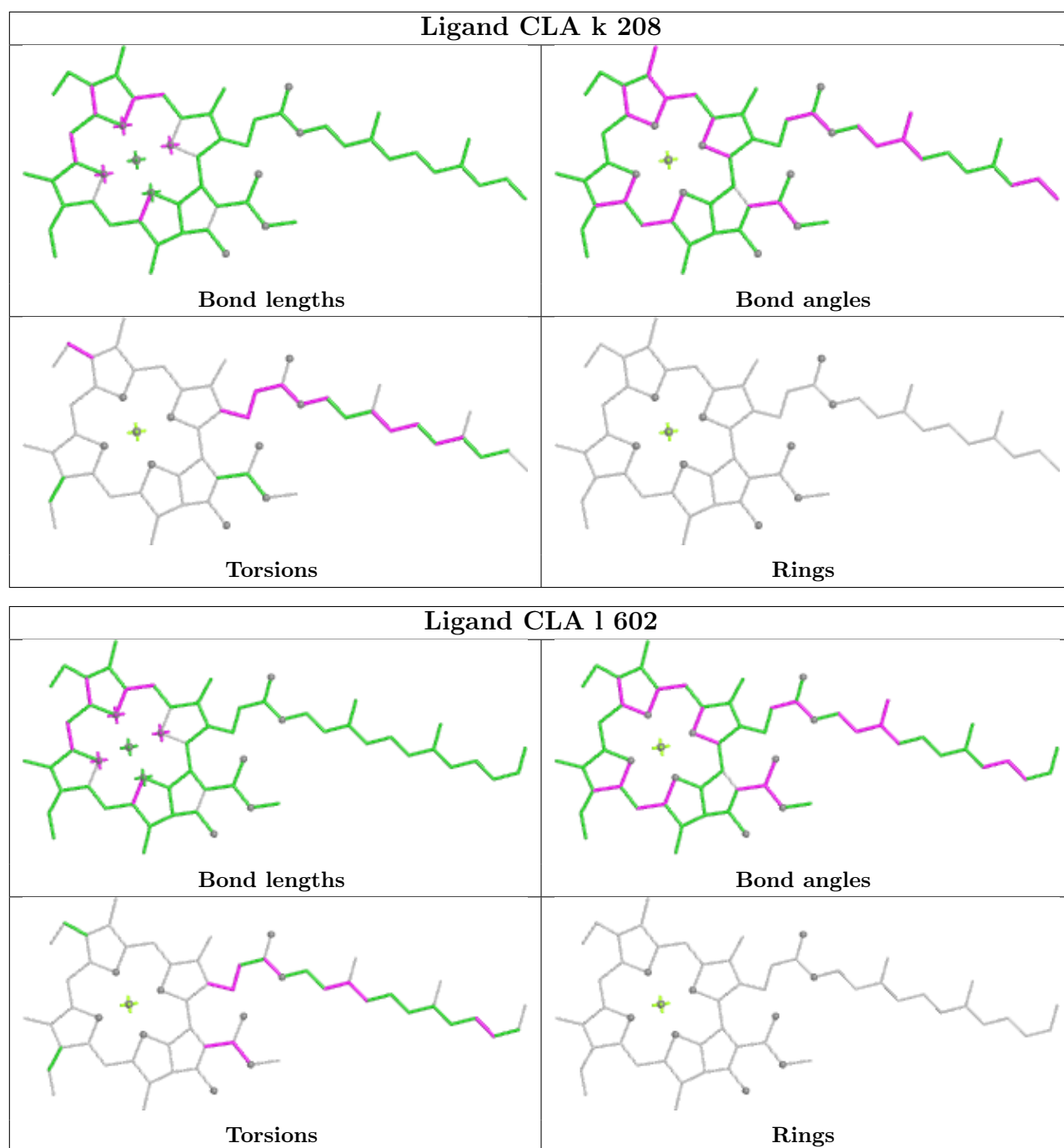
Torsions



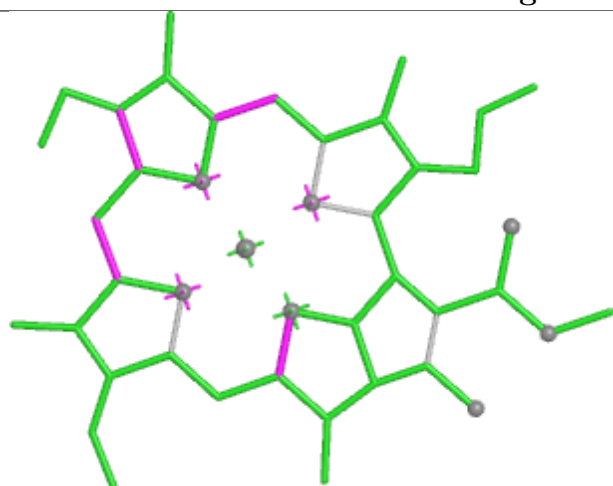
Rings



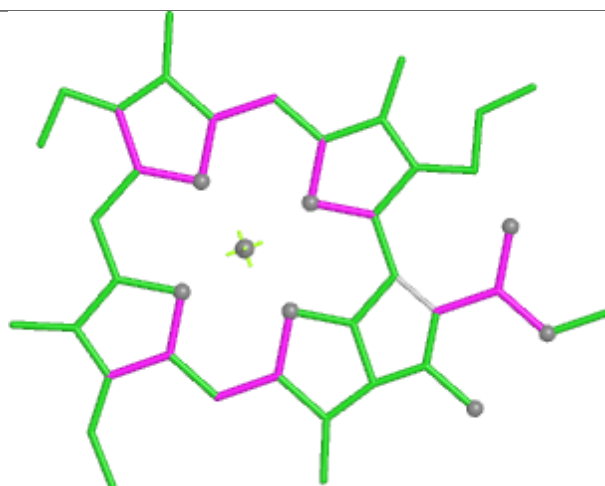




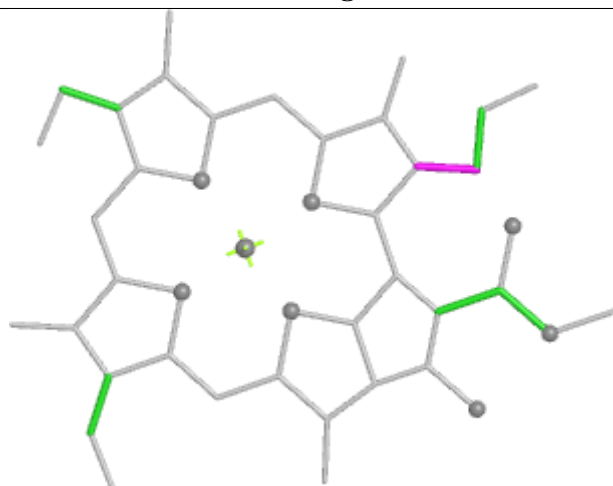
Ligand CLA c 311



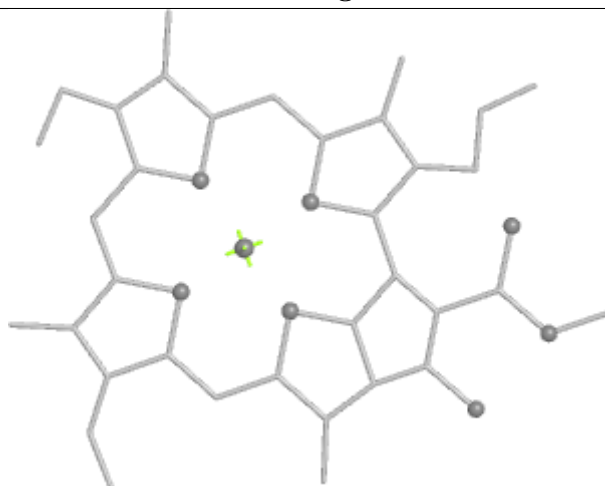
Bond lengths



Bond angles

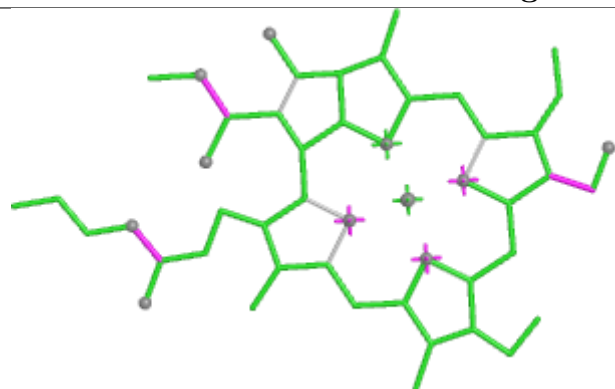


Torsions

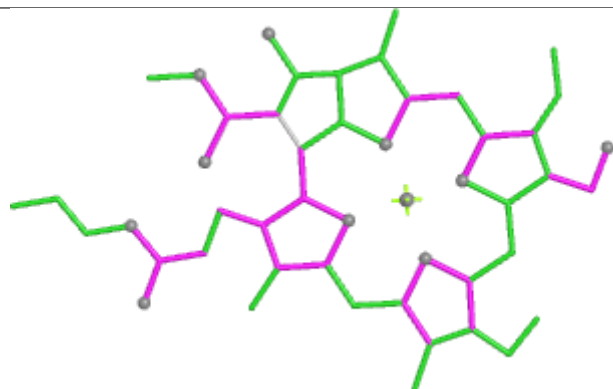


Rings

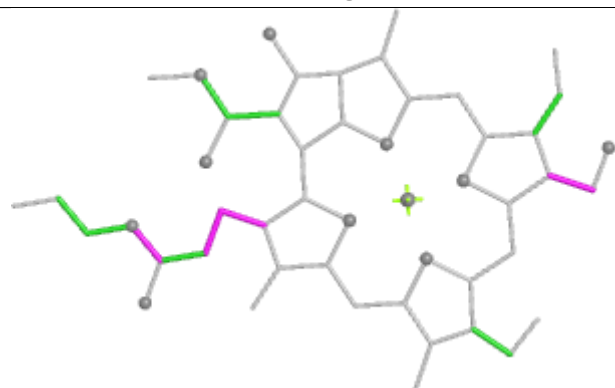
Ligand CHL c 307



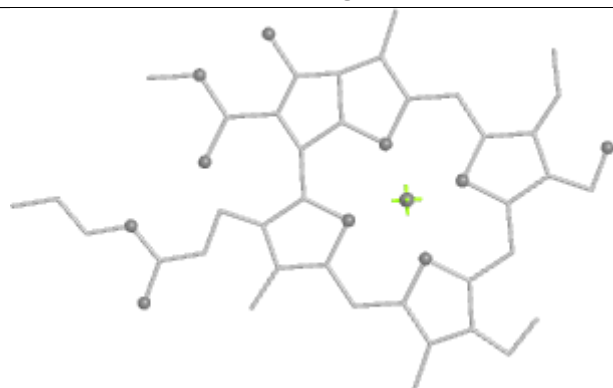
Bond lengths



Bond angles

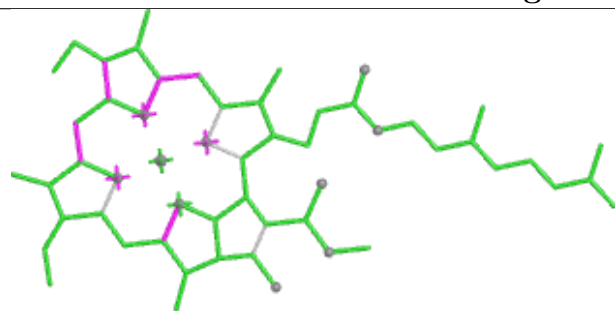


Torsions

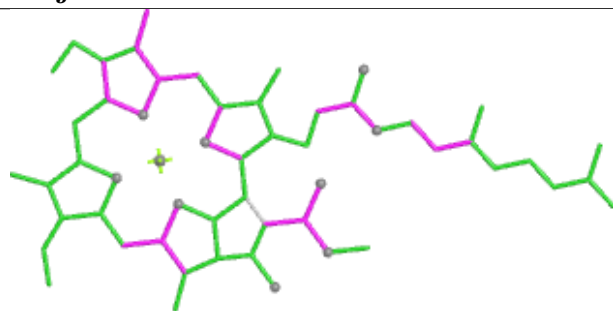


Rings

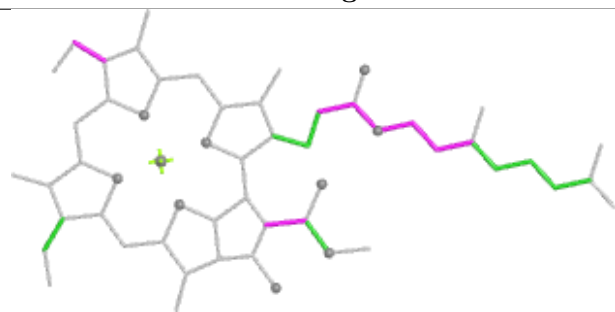
Ligand CLA j 211



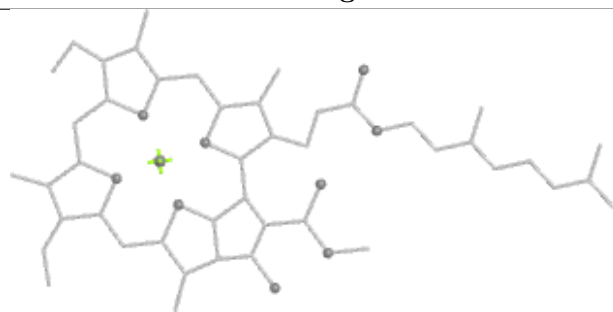
Bond lengths



Bond angles

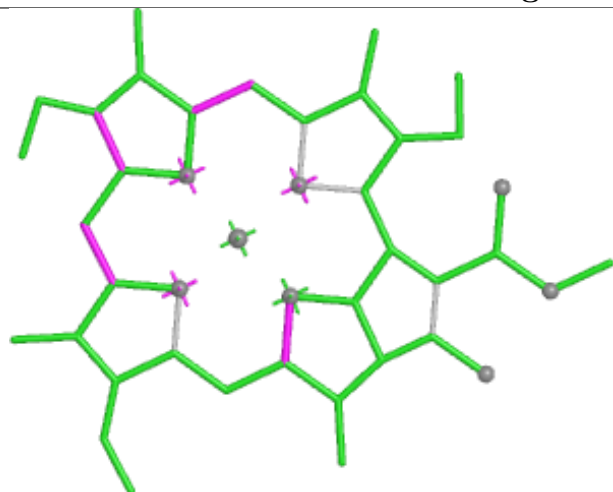


Torsions

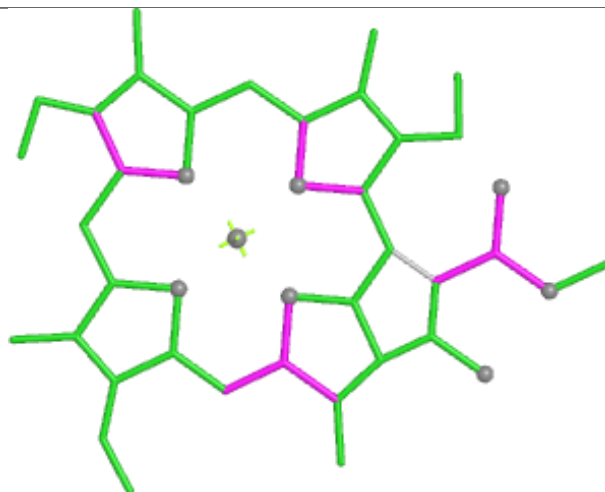


Rings

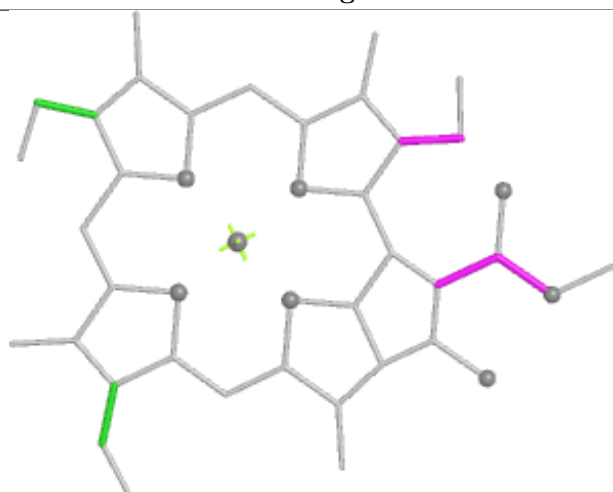
Ligand CLA f 604



Bond lengths



Bond angles

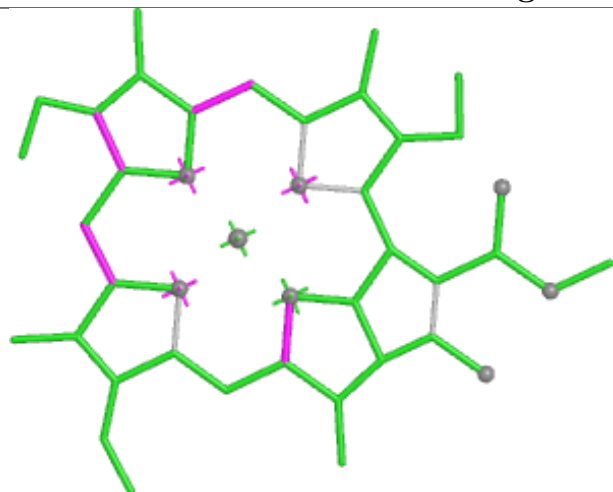


Torsions

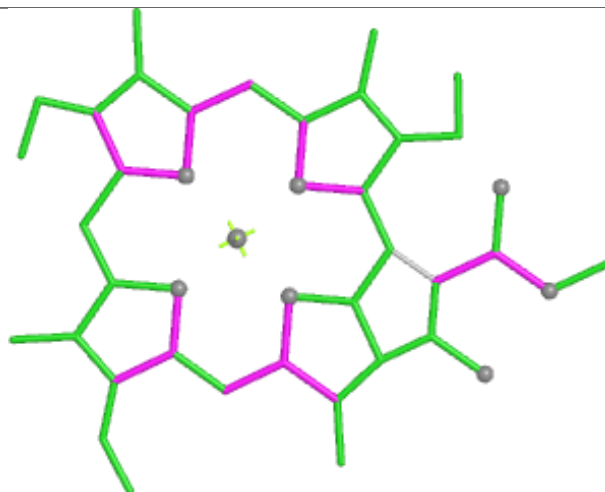


Rings

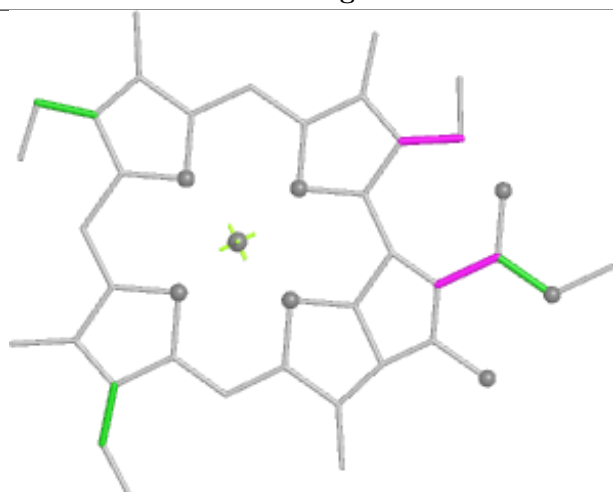
Ligand CLA k 209



Bond lengths



Bond angles

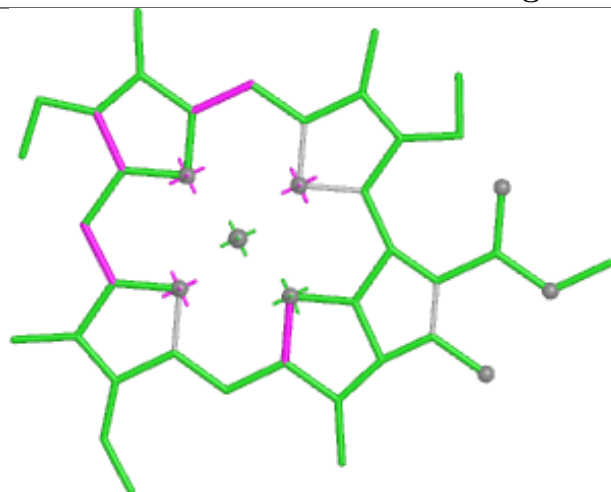


Torsions

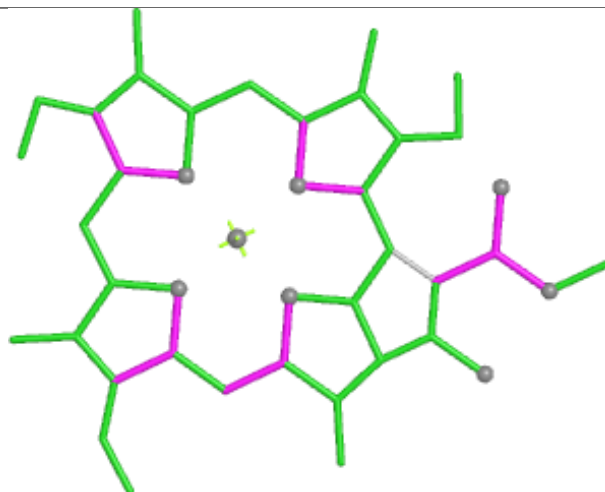


Rings

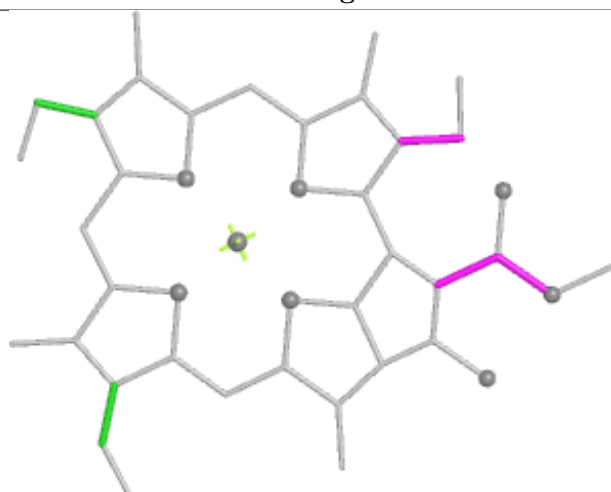
Ligand CLA 1 612



Bond lengths



Bond angles

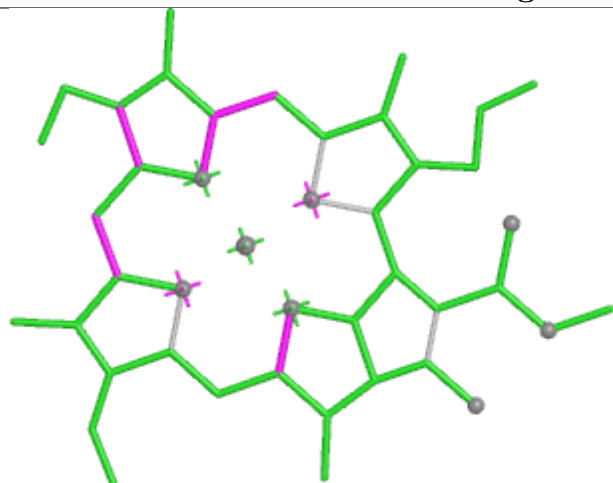


Torsions

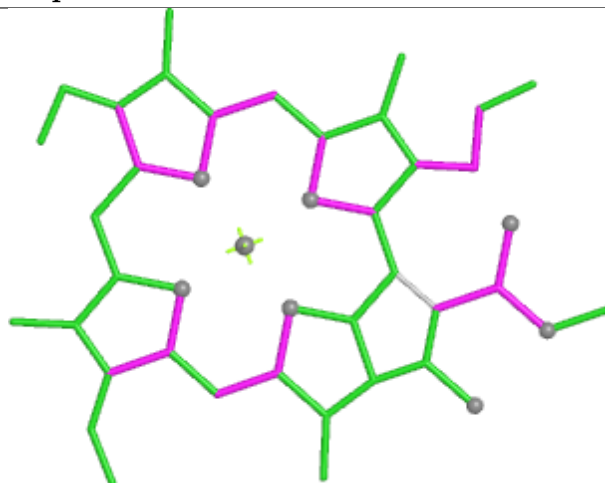


Rings

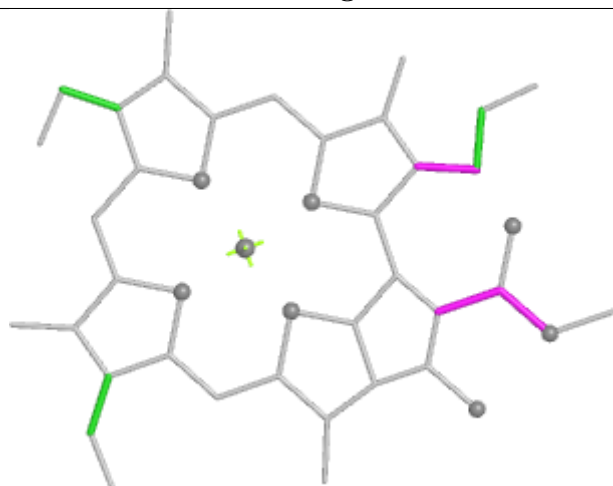
Ligand CLA p 608



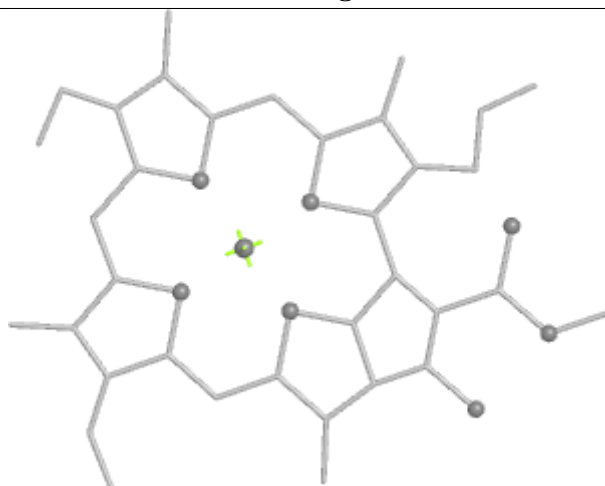
Bond lengths



Bond angles

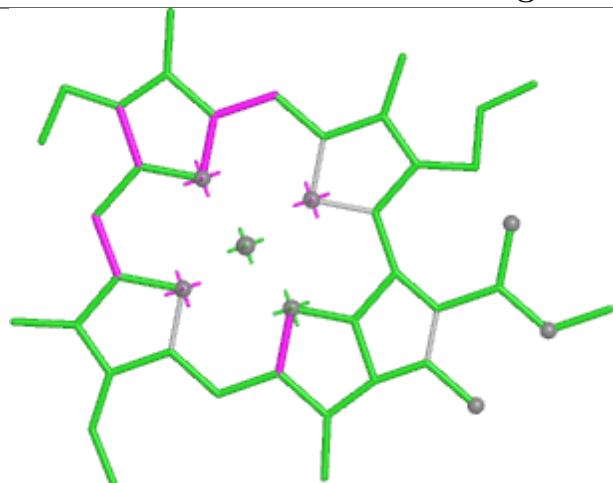


Torsions

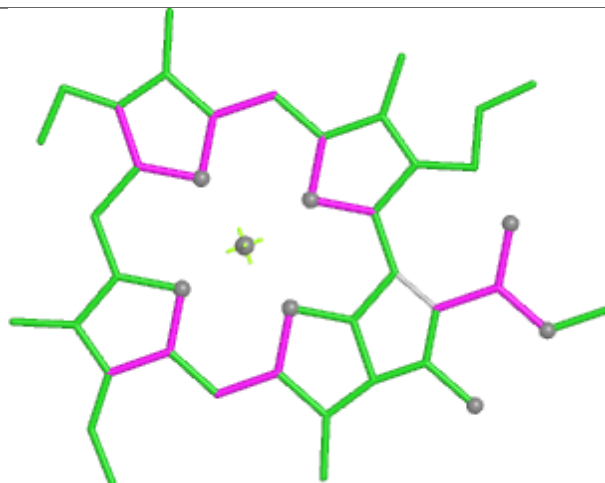


Rings

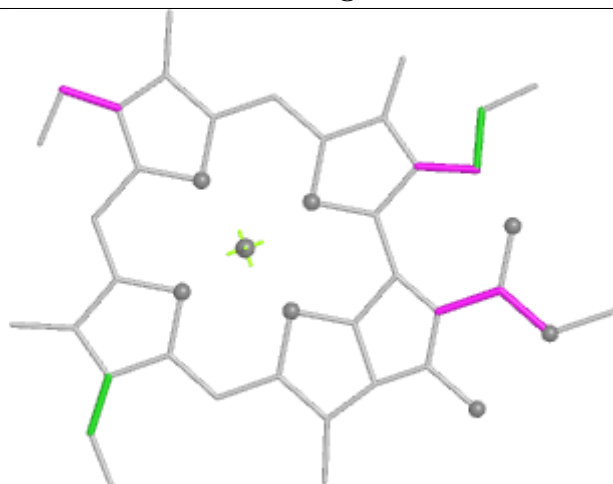
Ligand CLA h 210



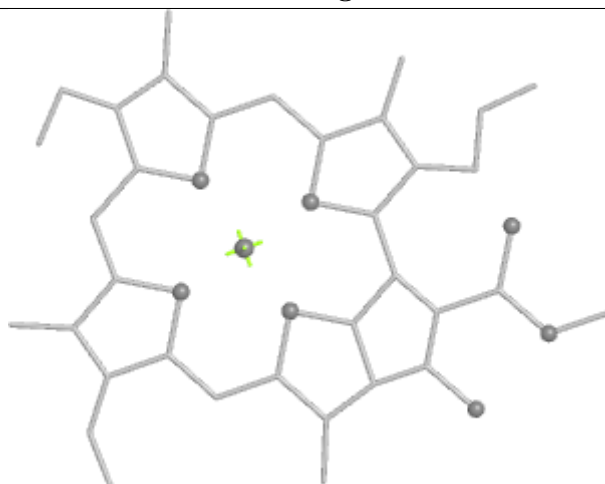
Bond lengths



Bond angles

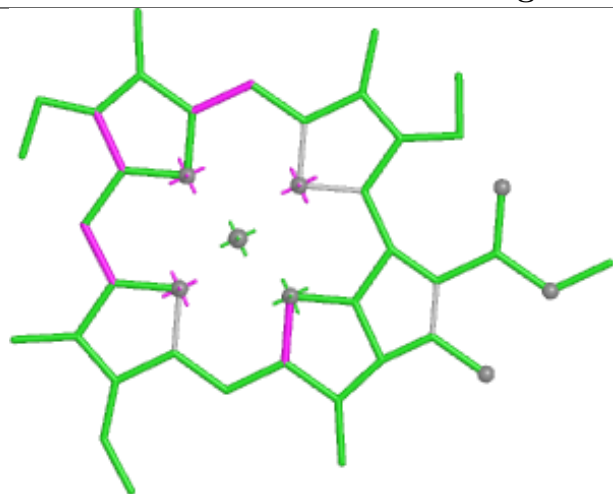


Torsions

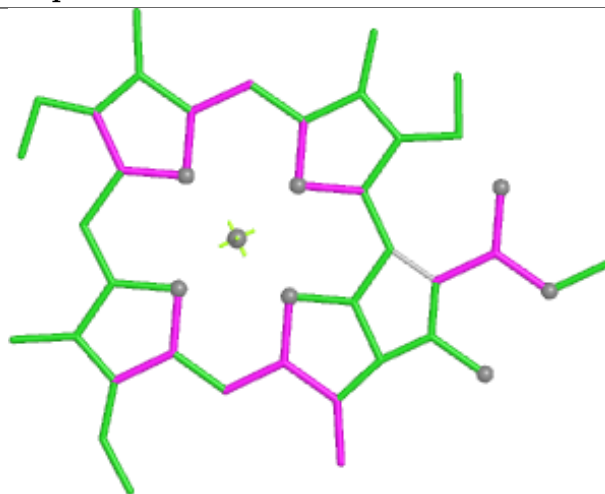


Rings

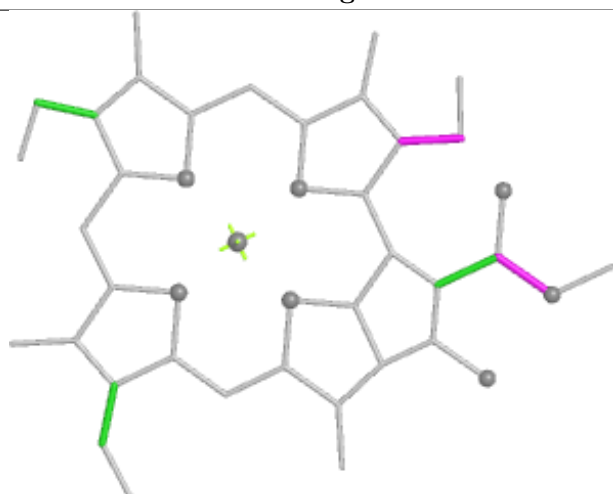
Ligand CLA p 601



Bond lengths



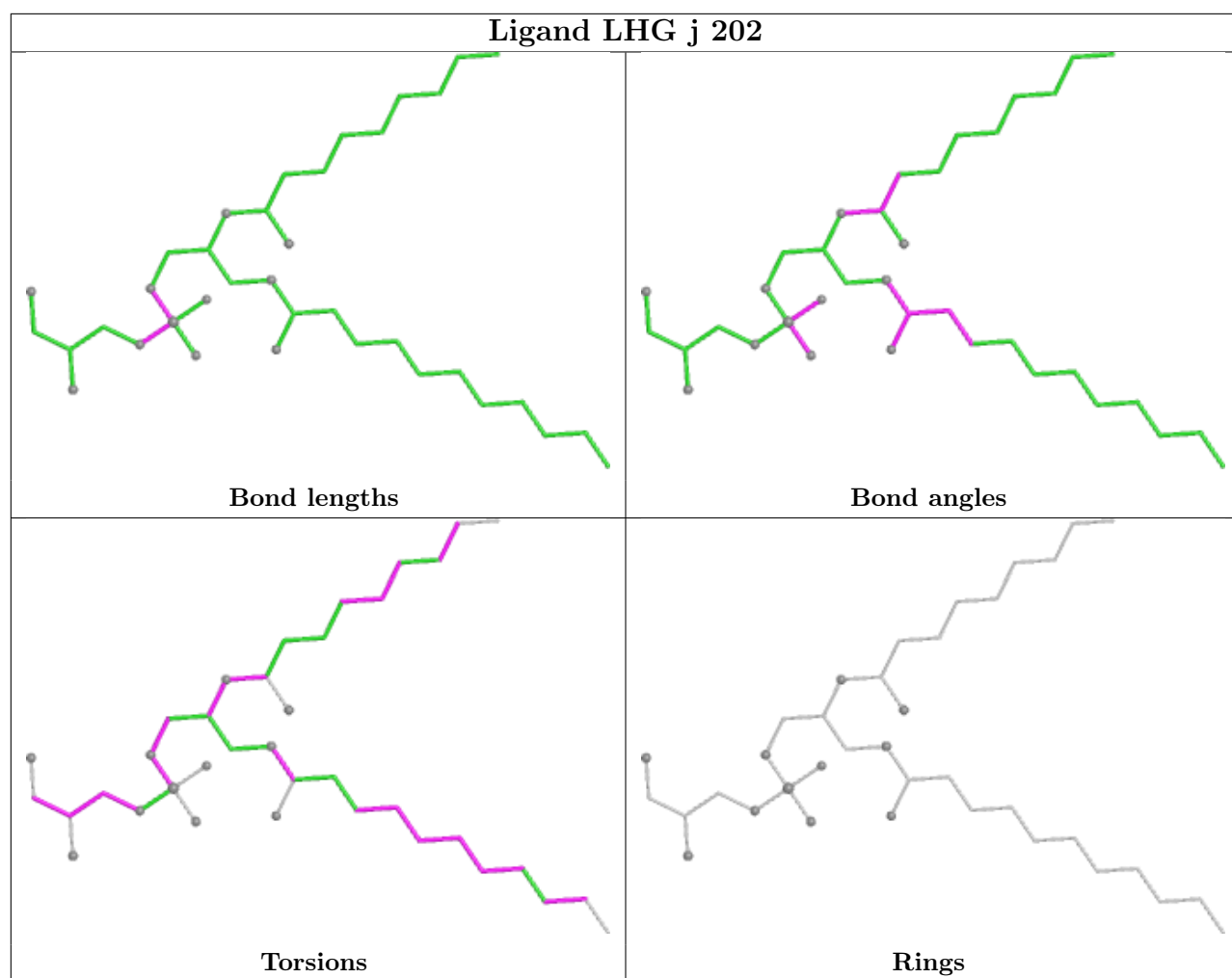
Bond angles



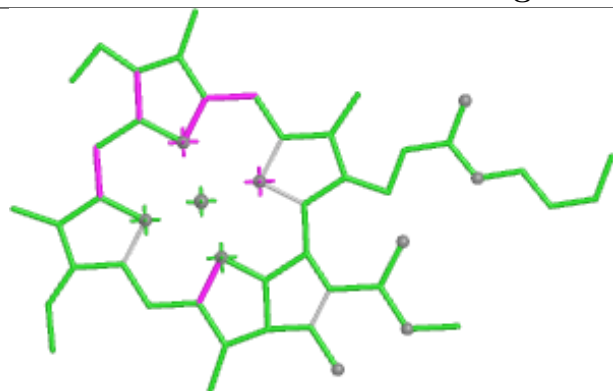
Torsions



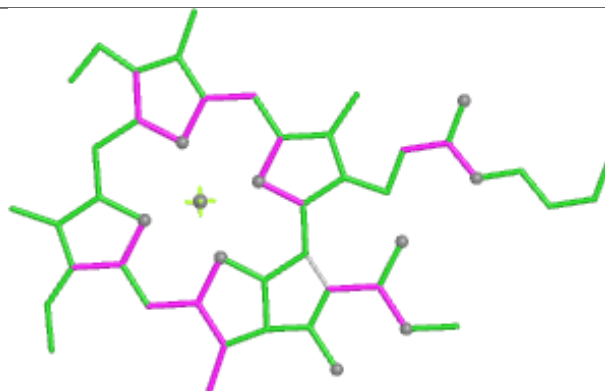
Rings



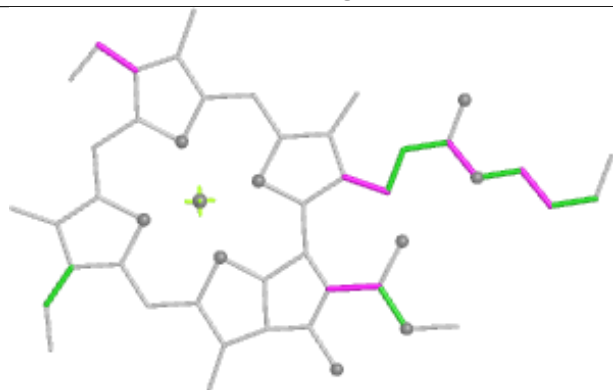
Ligand CLA A 842



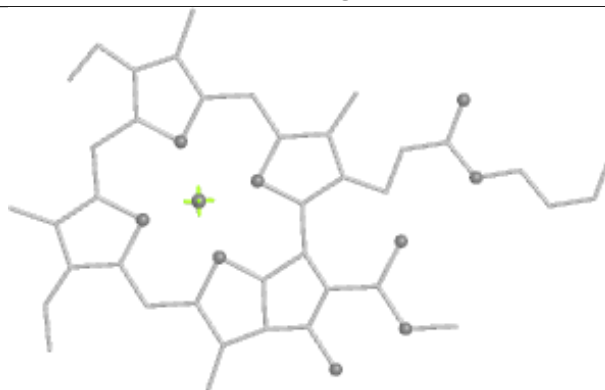
Bond lengths



Bond angles

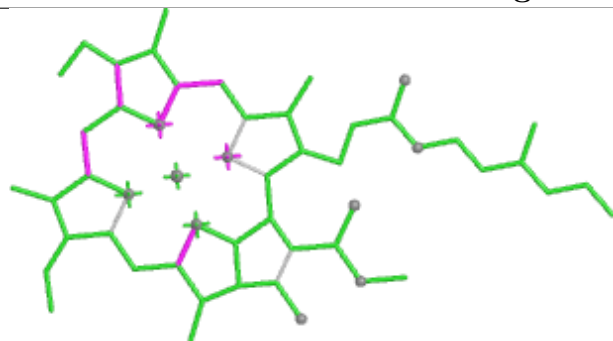


Torsions

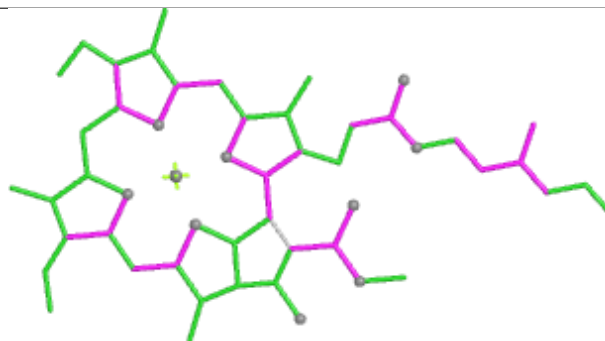


Rings

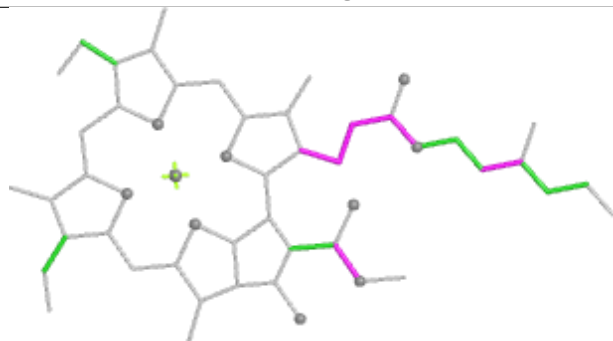
Ligand CLA A 830



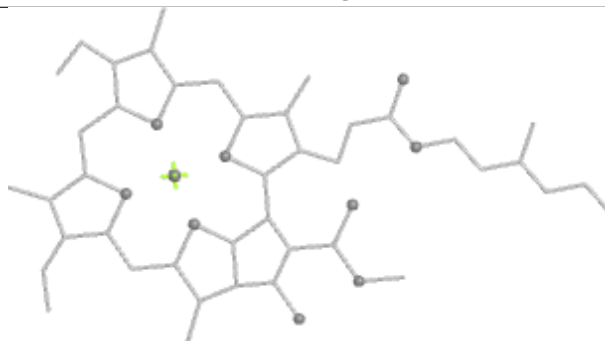
Bond lengths



Bond angles

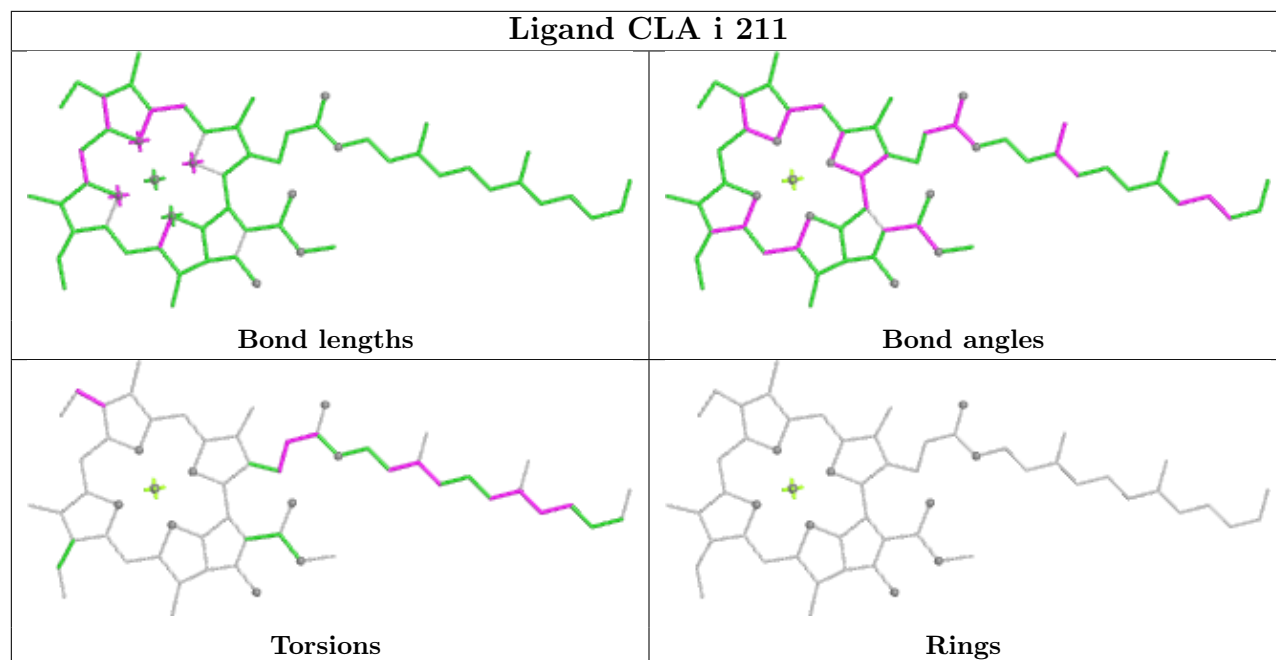


Torsions

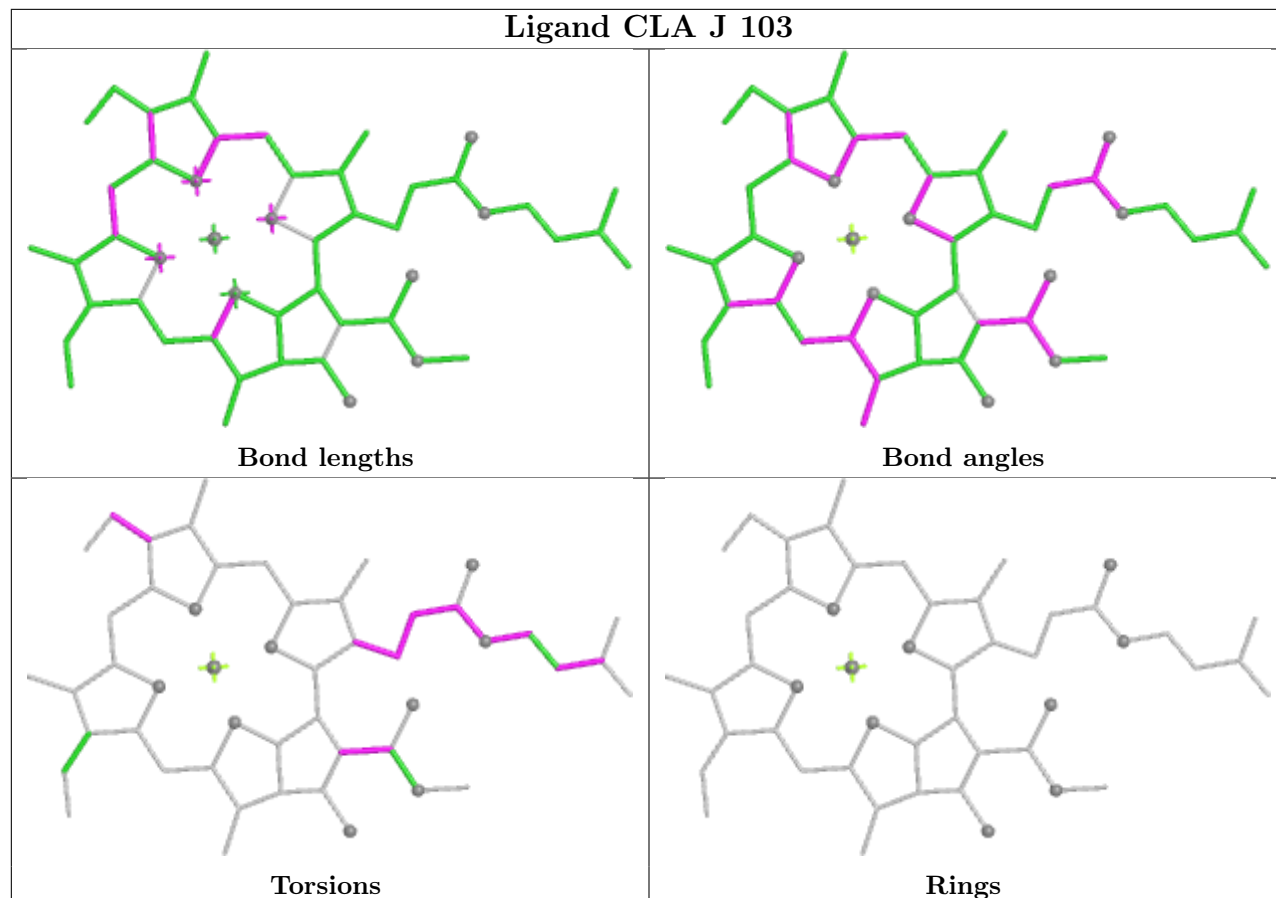


Rings

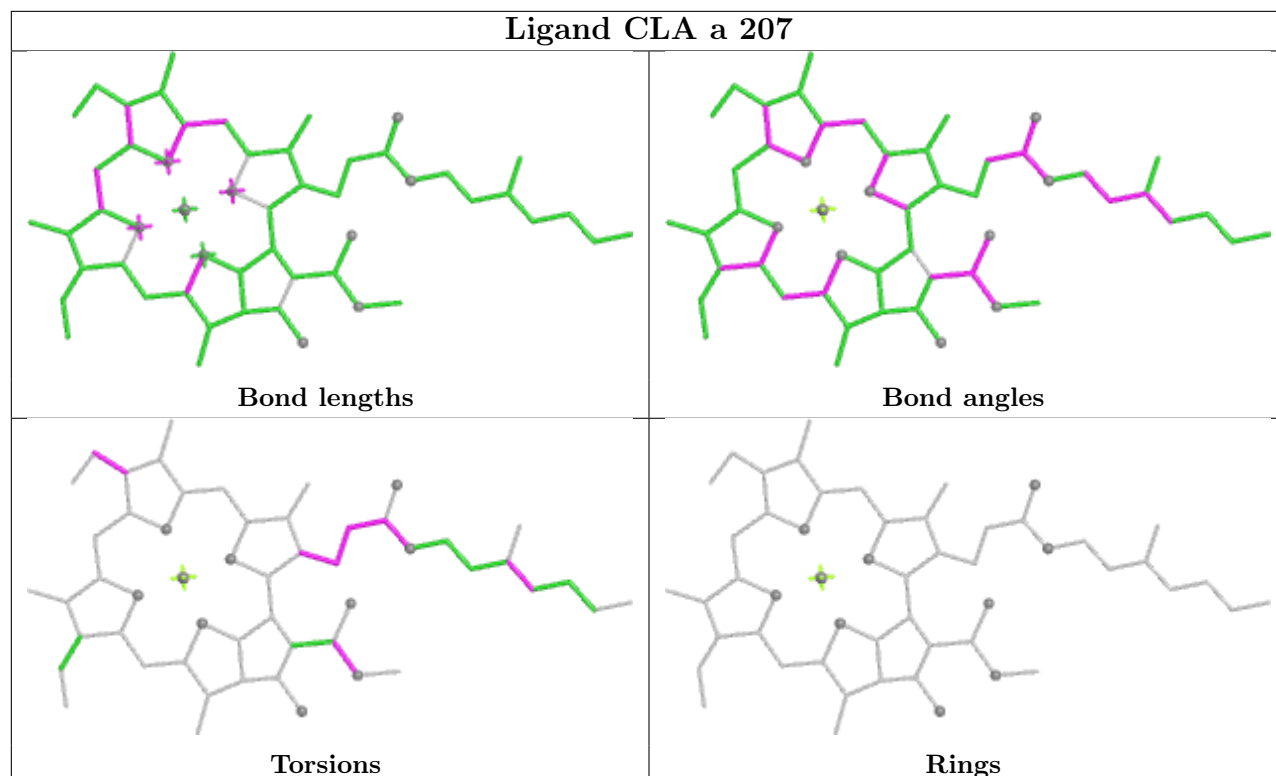
Ligand CLA i 211



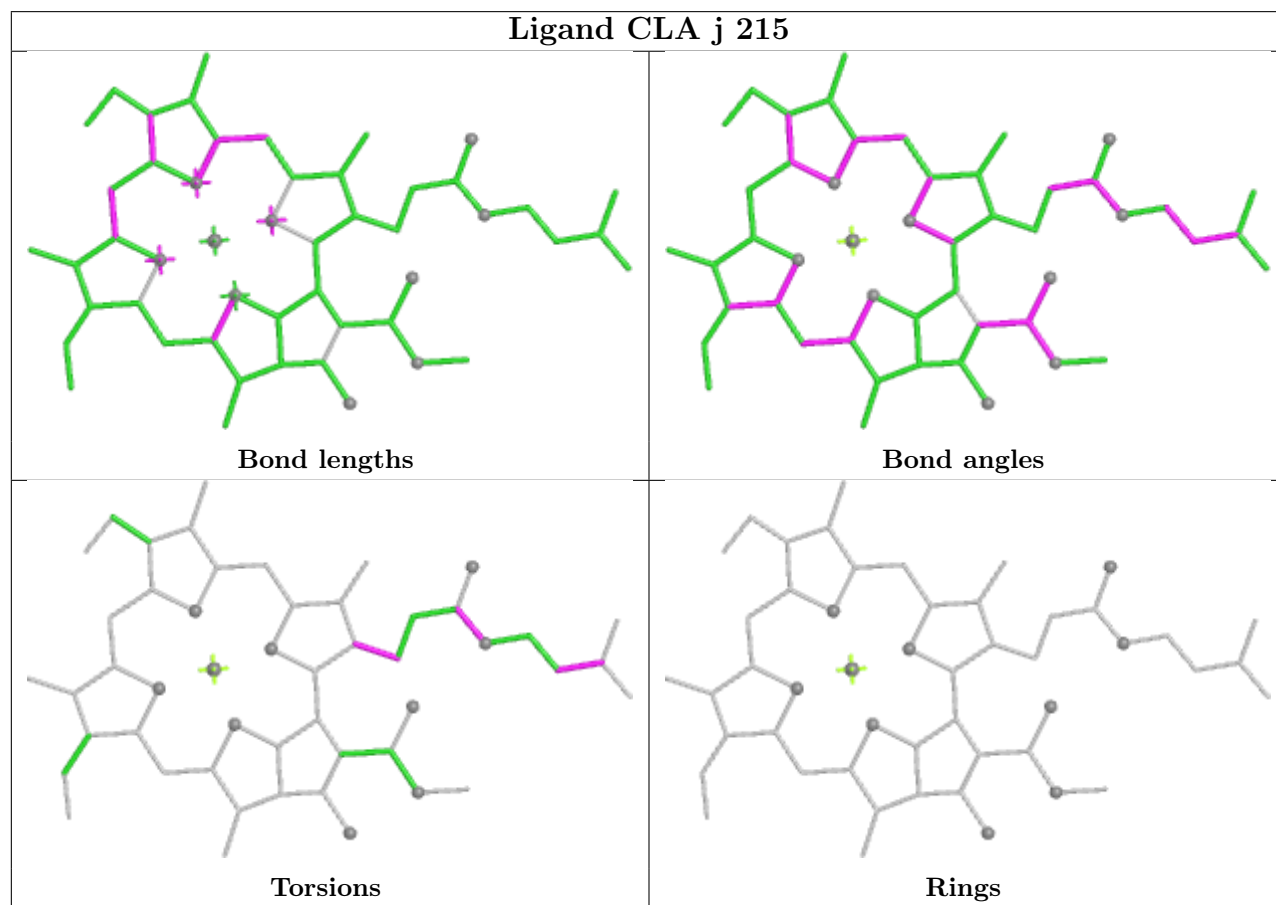
Ligand CLA J 103

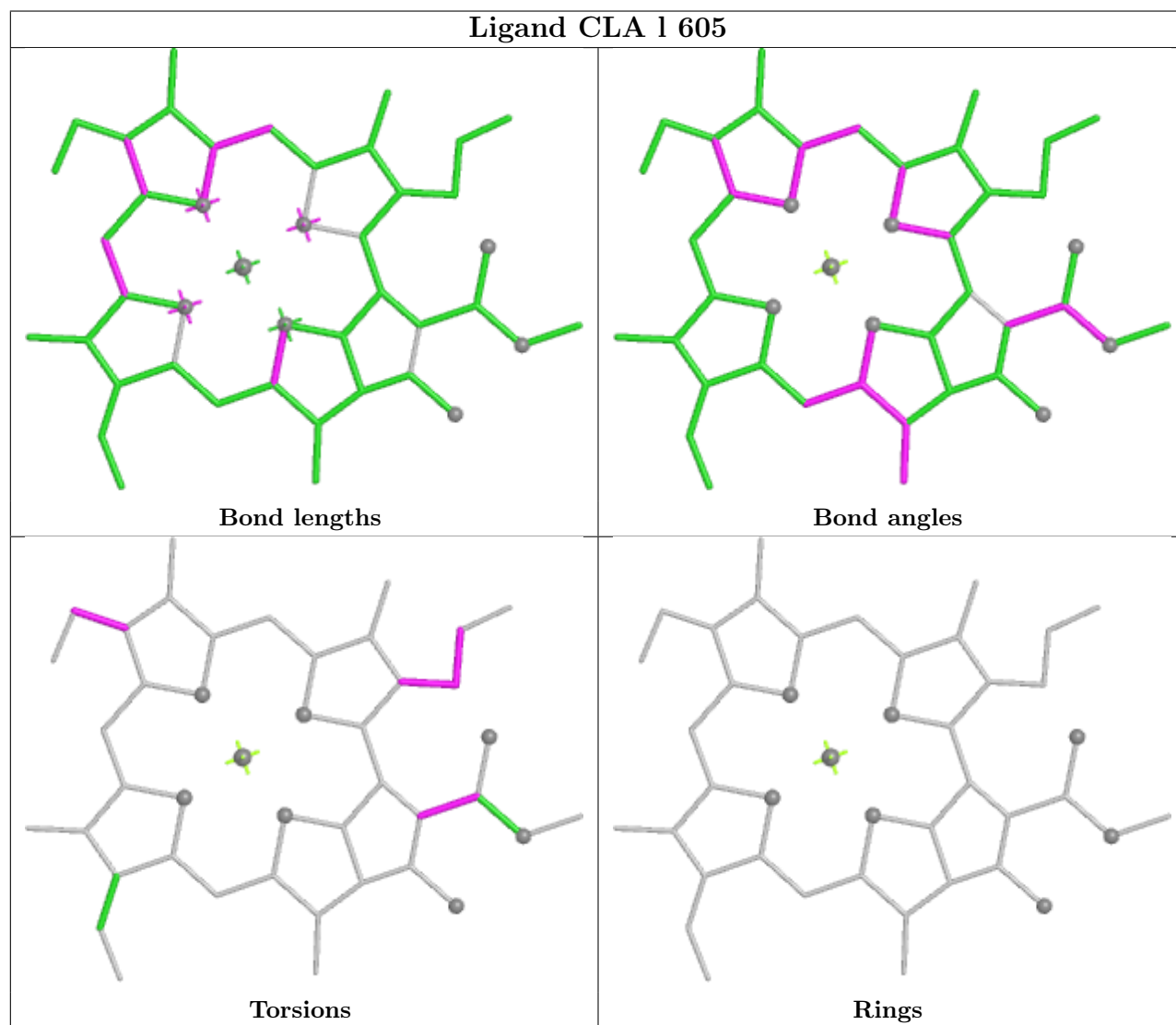
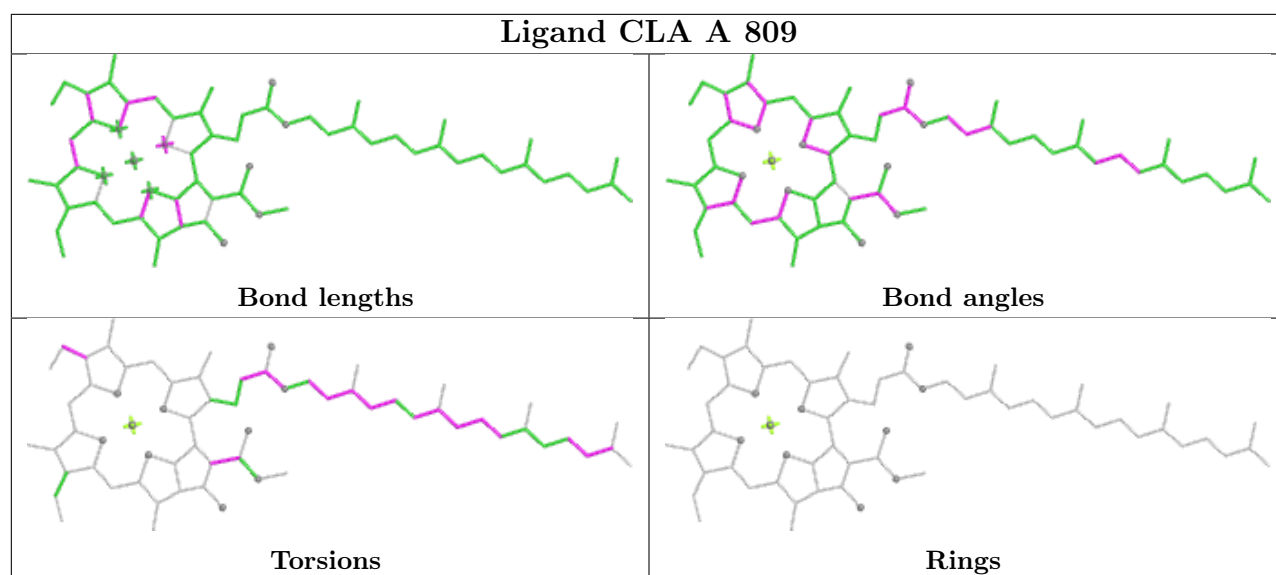


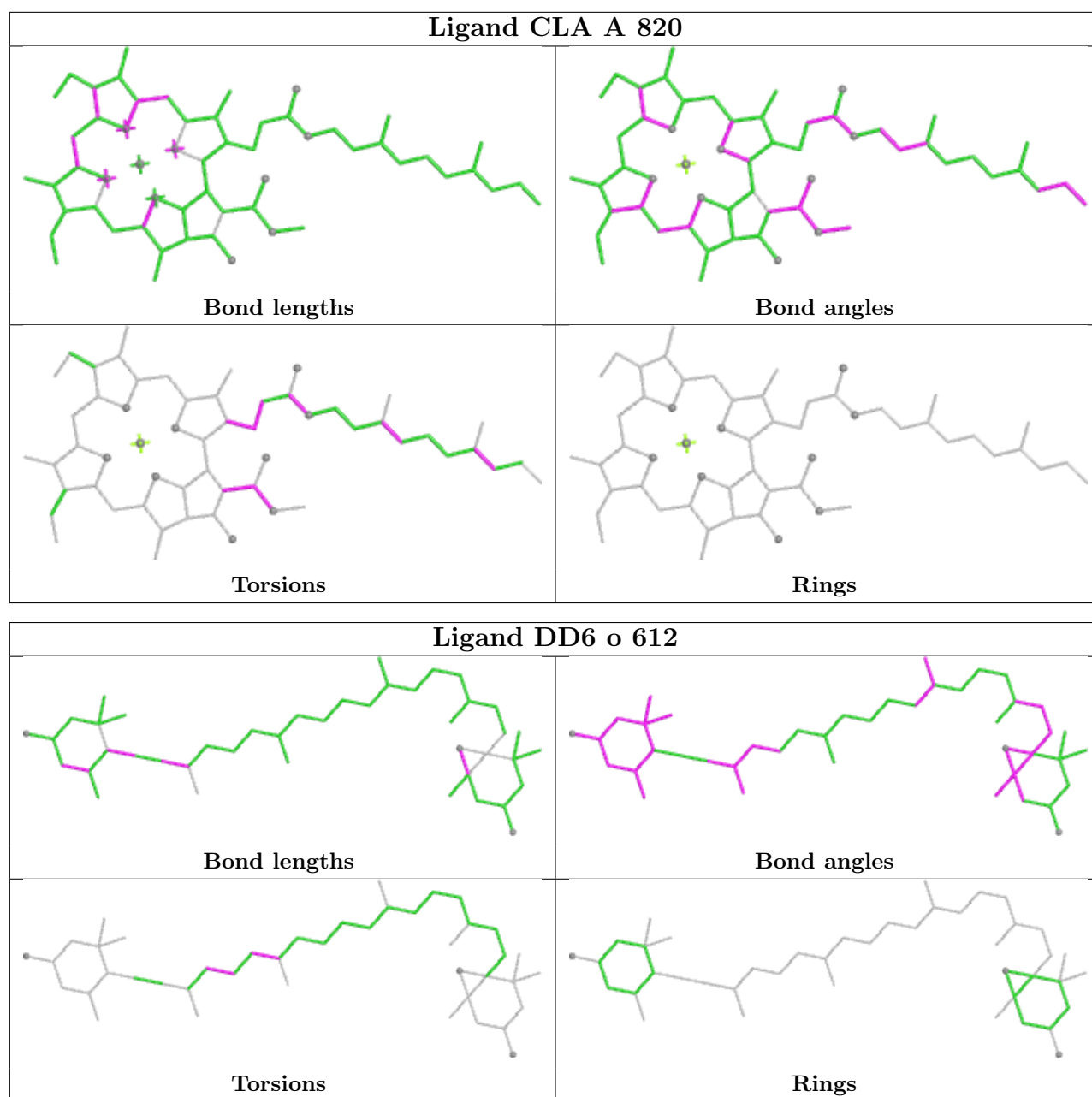
Ligand CLA a 207

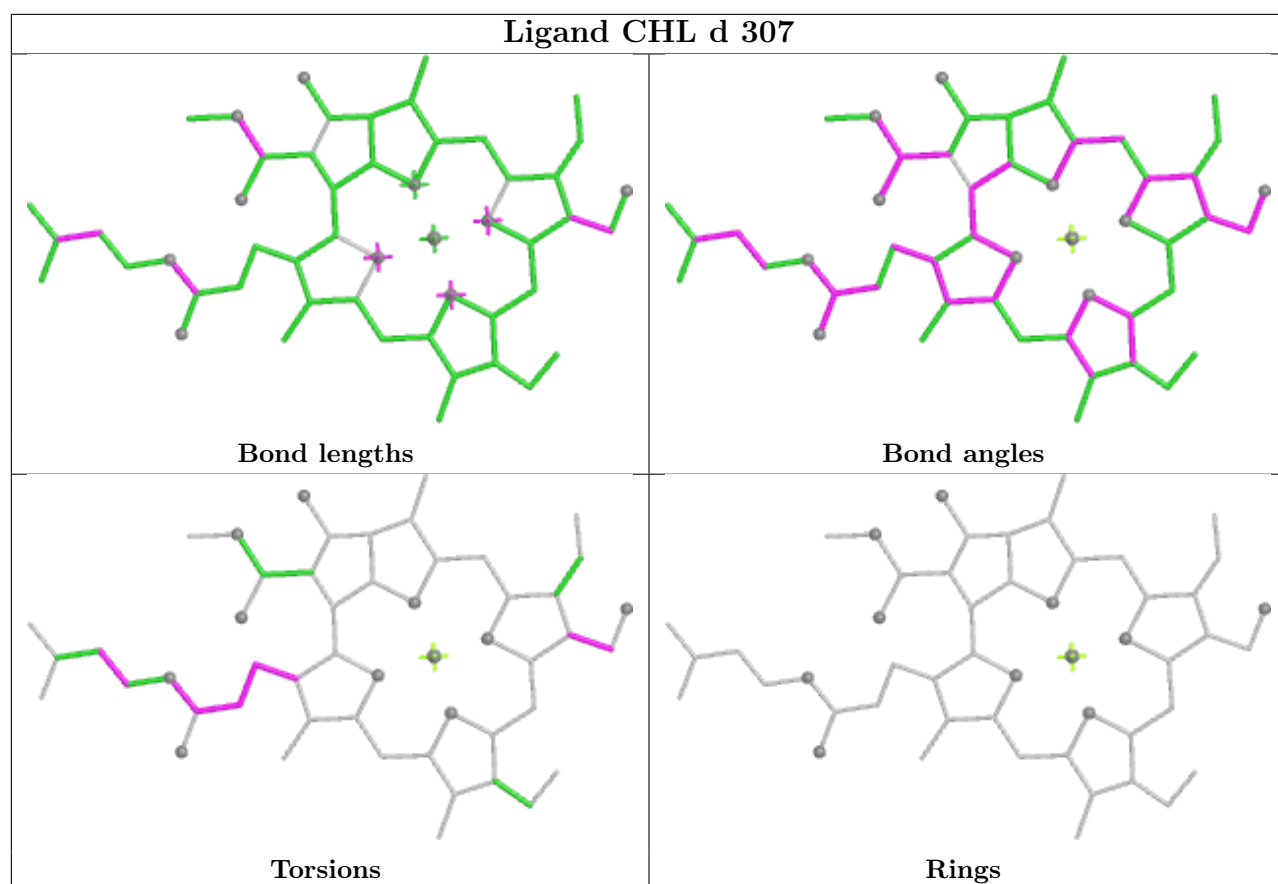


Ligand CLA j 215

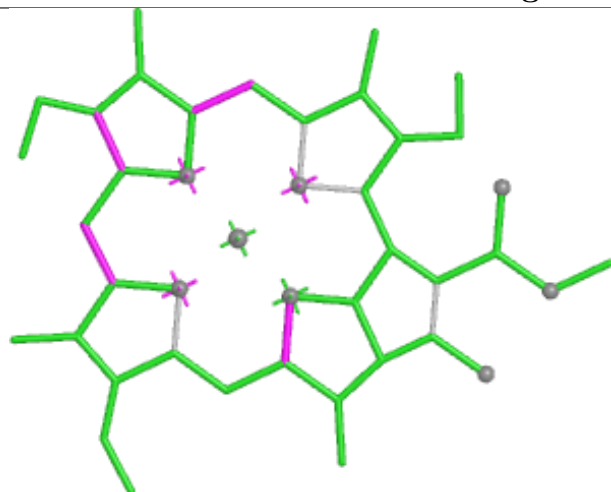




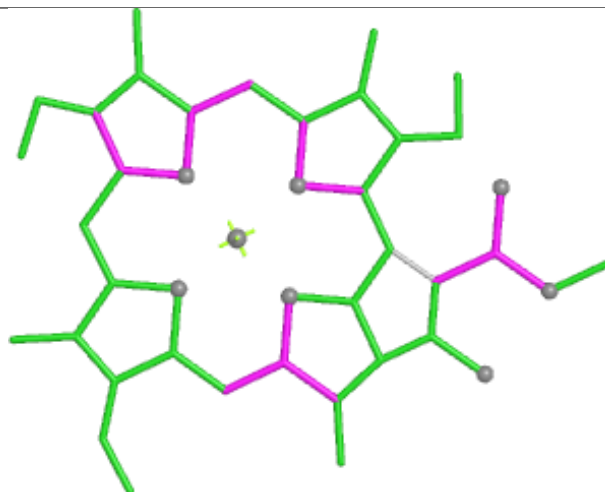




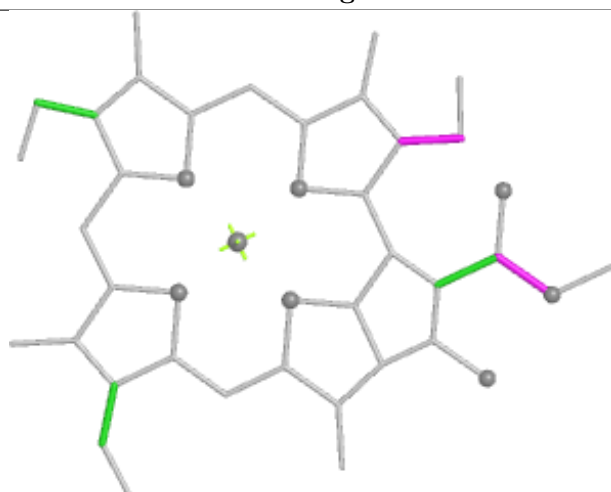
Ligand CLA f 609



Bond lengths



Bond angles

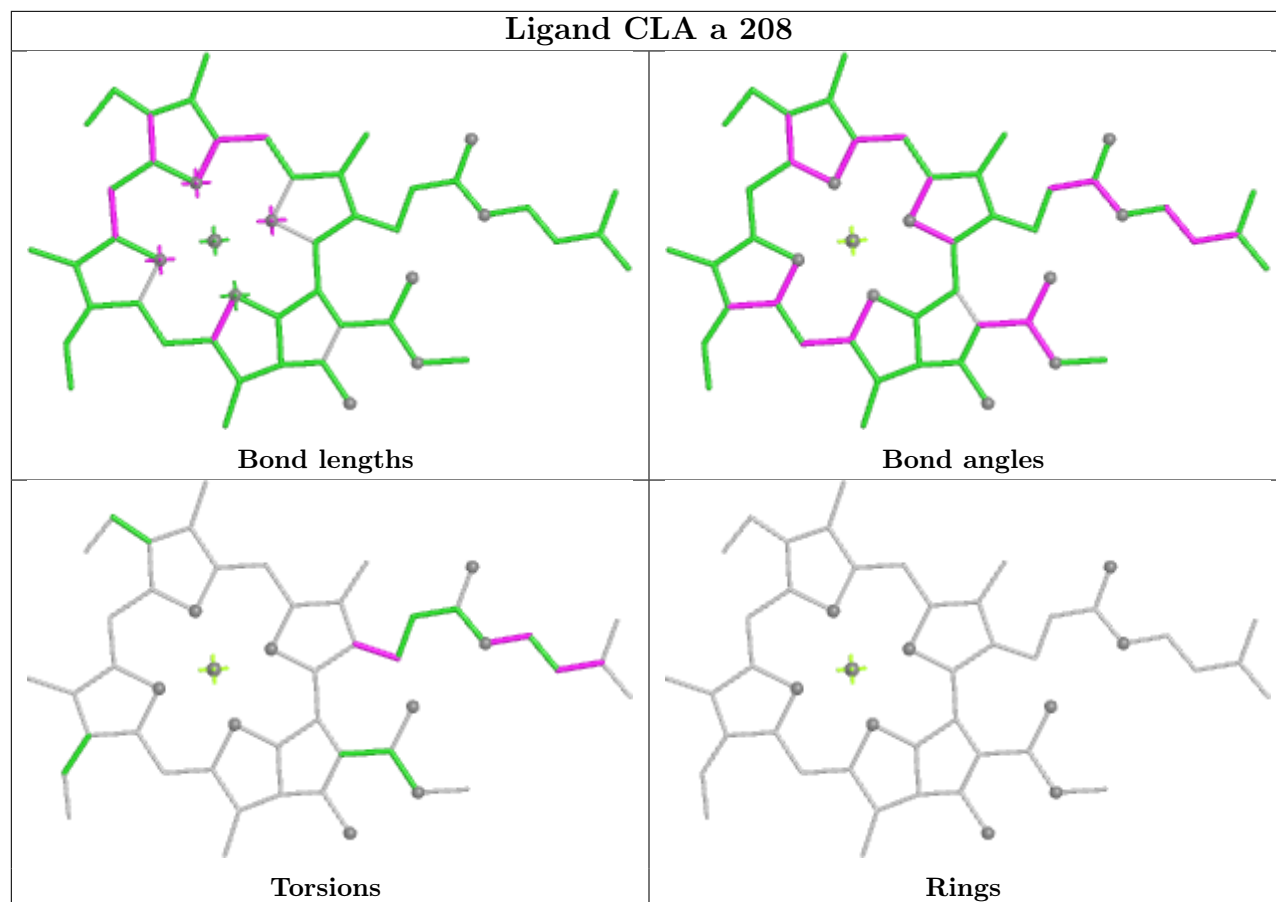


Torsions

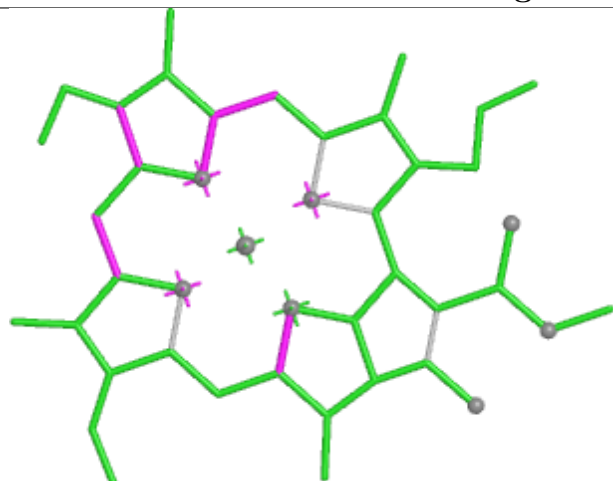


Rings

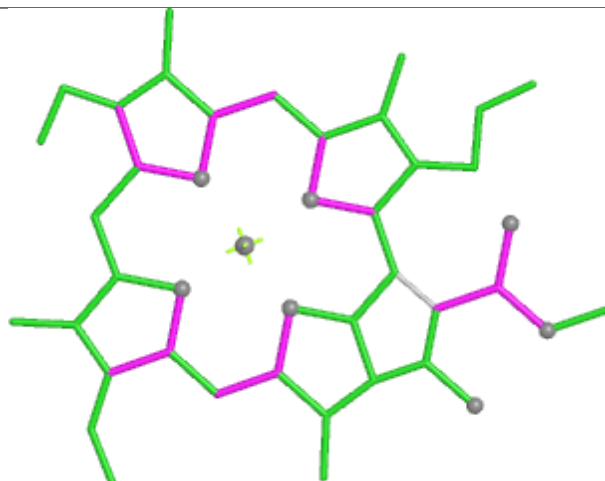
Ligand CLA a 208



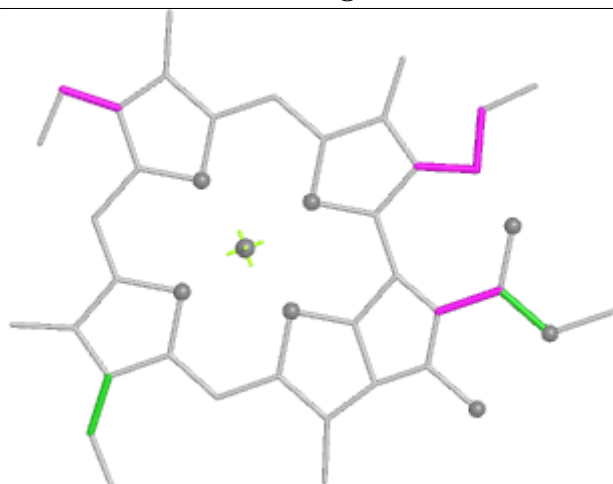
Ligand CLA B 825



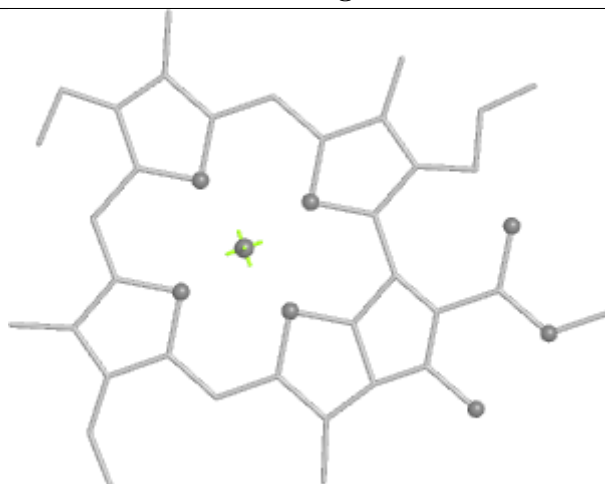
Bond lengths



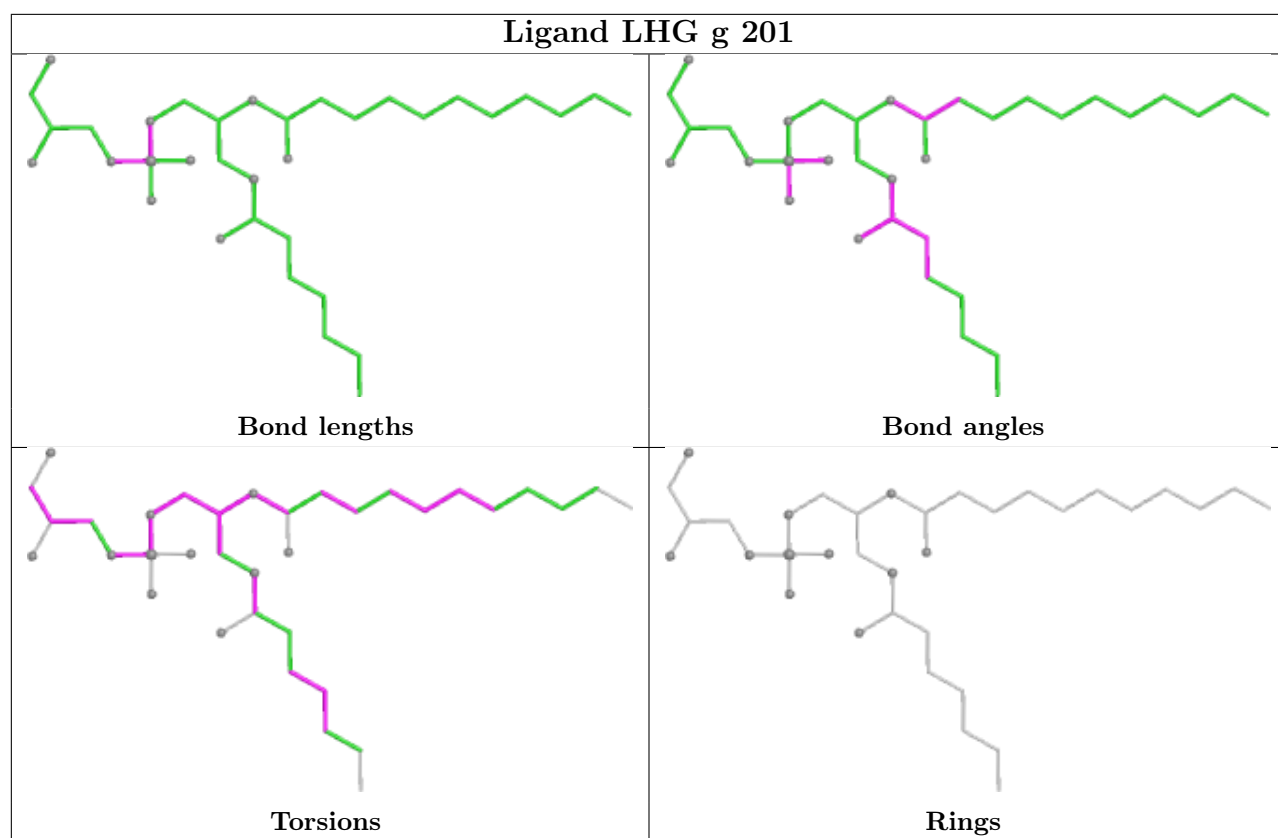
Bond angles



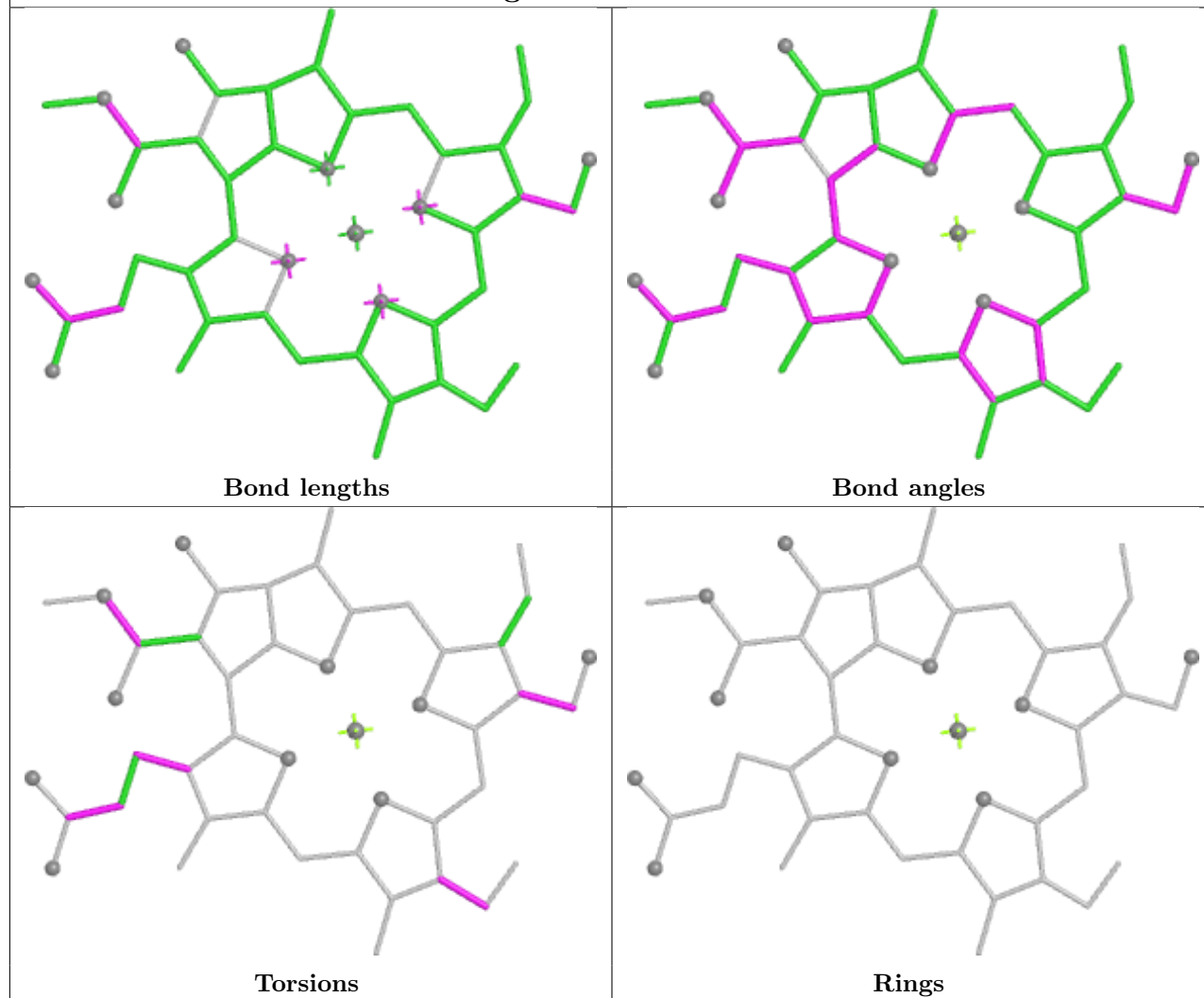
Torsions



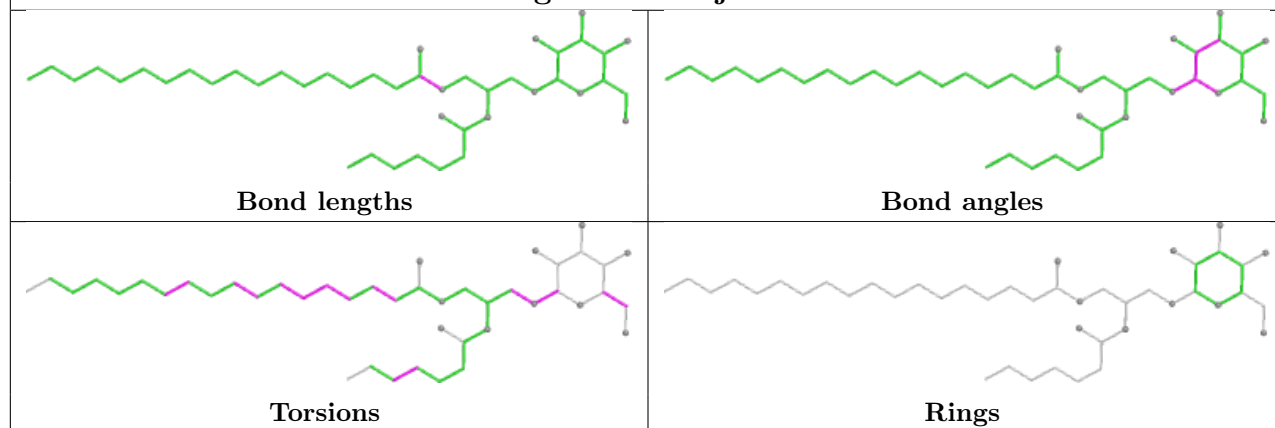
Rings



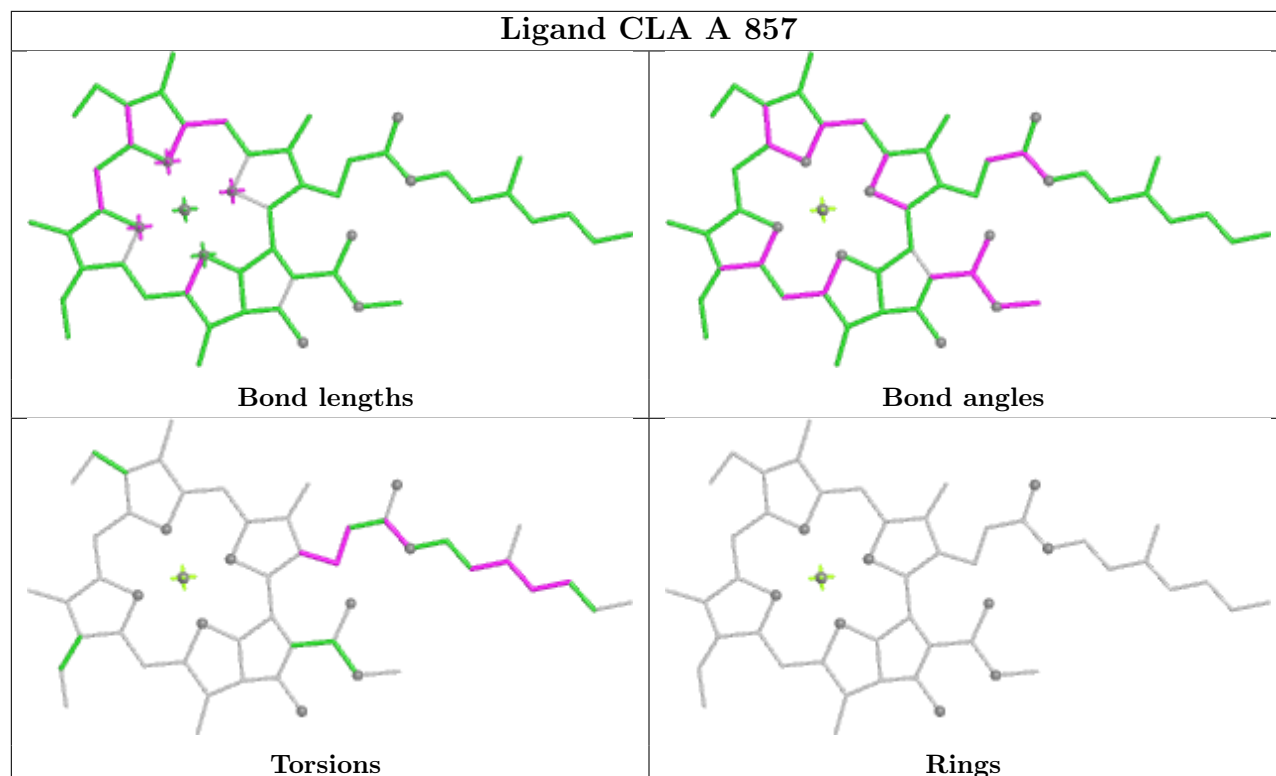
Ligand CHL d 308



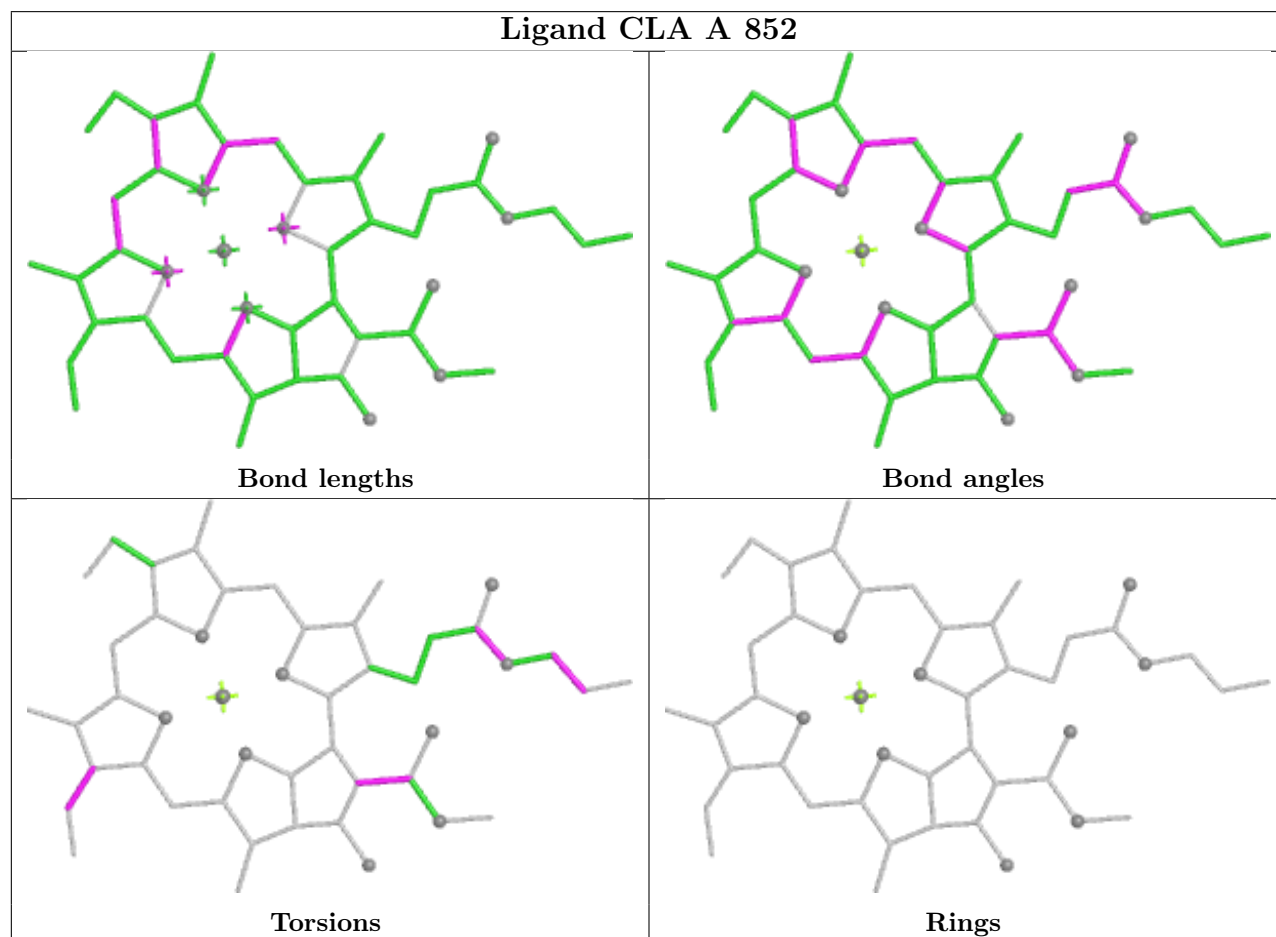
Ligand LMG j 201

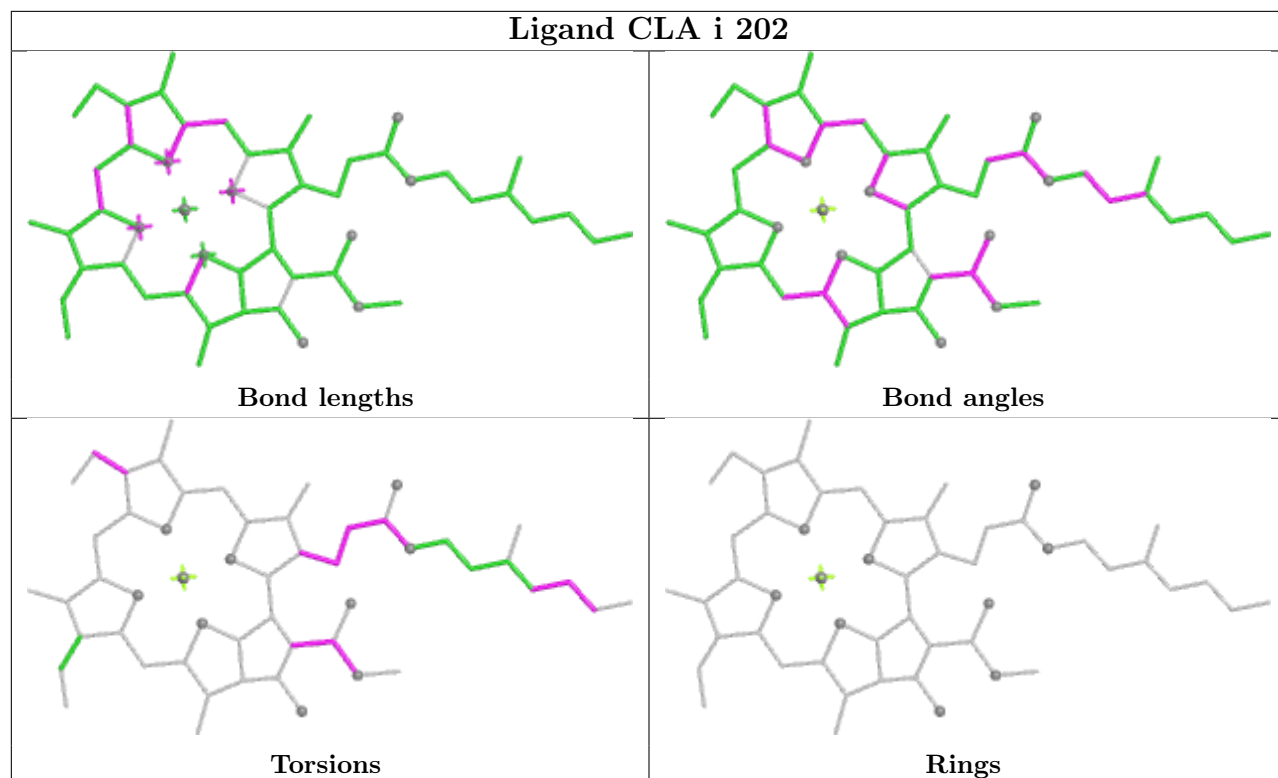


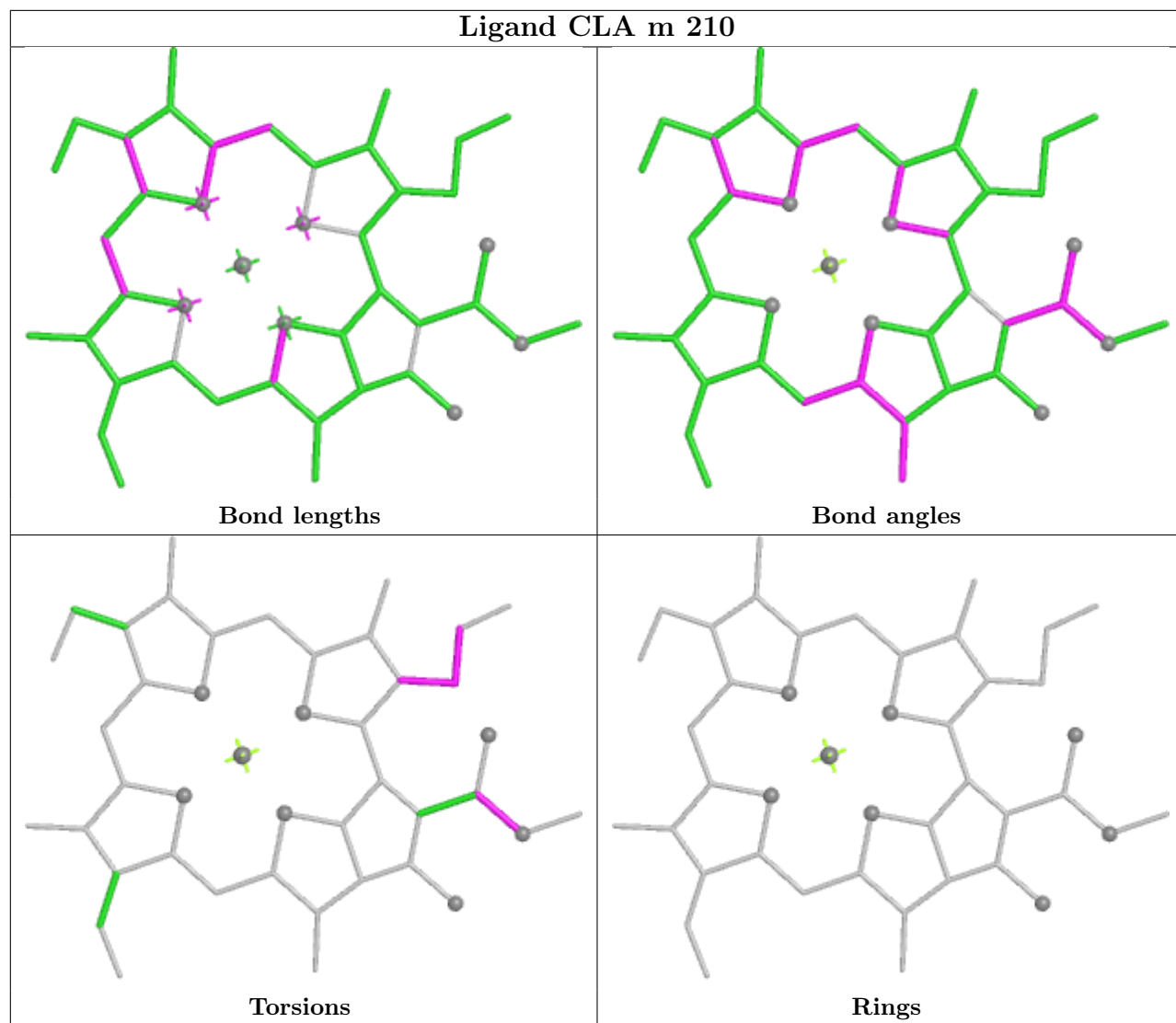
Ligand CLA A 857

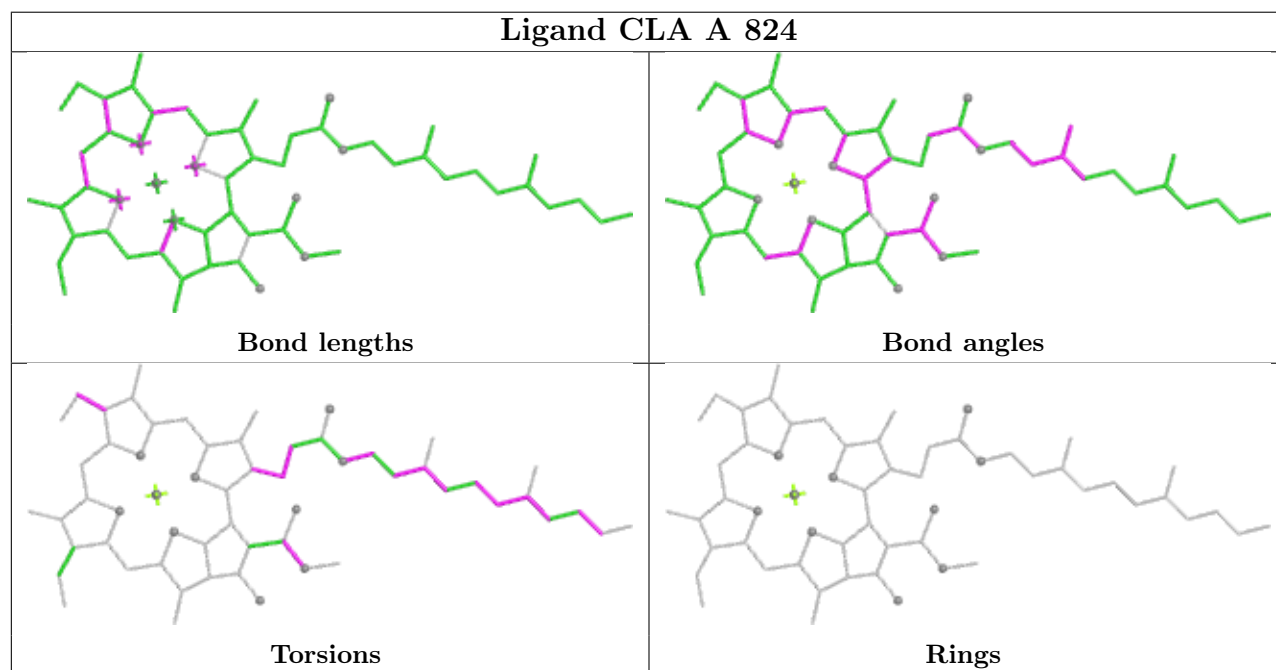
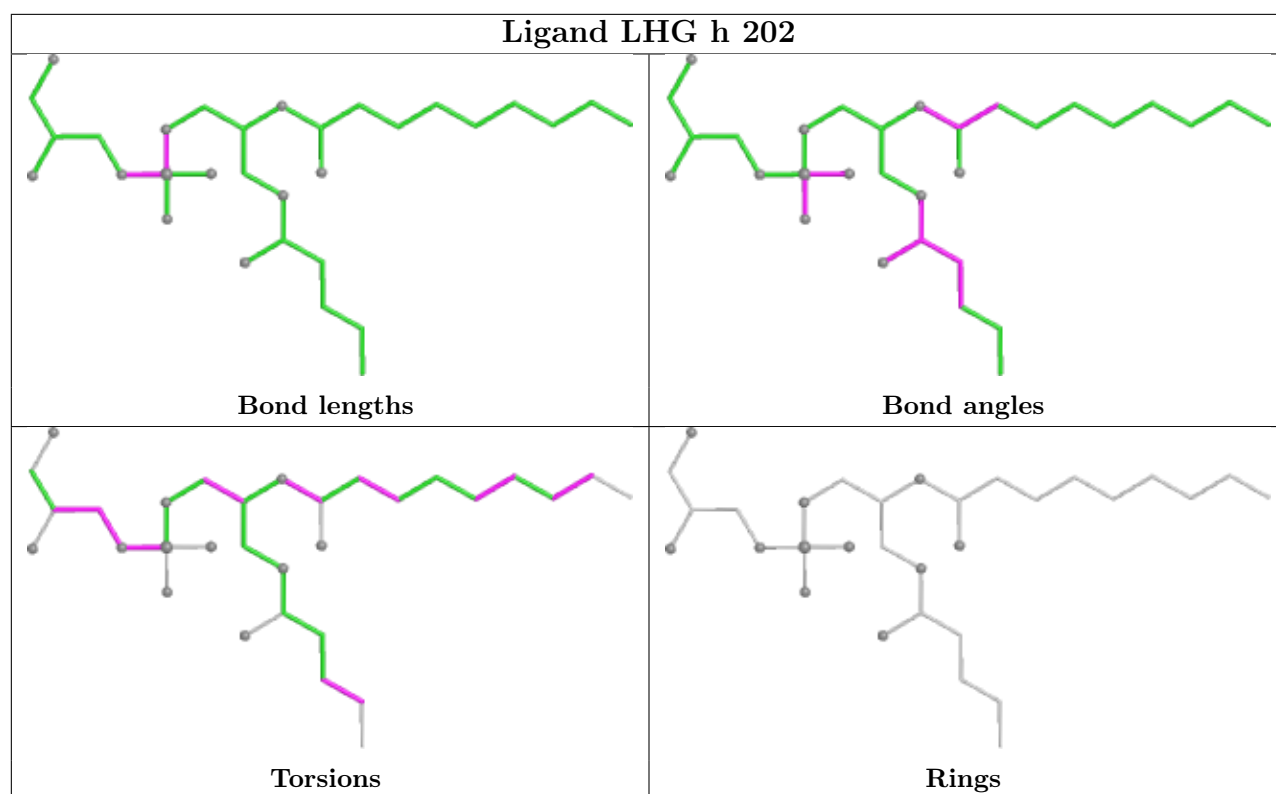


Ligand CLA A 852

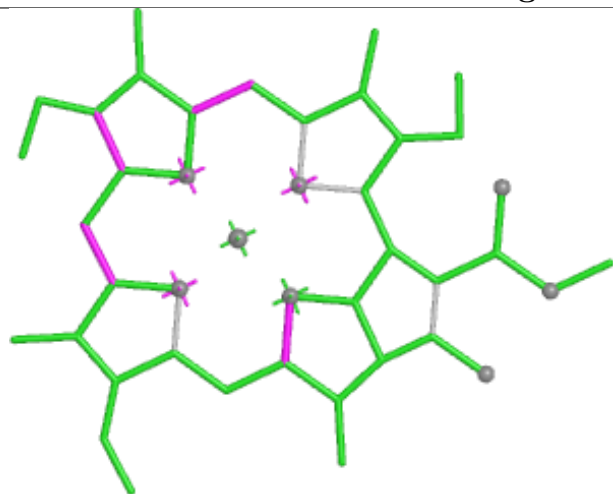




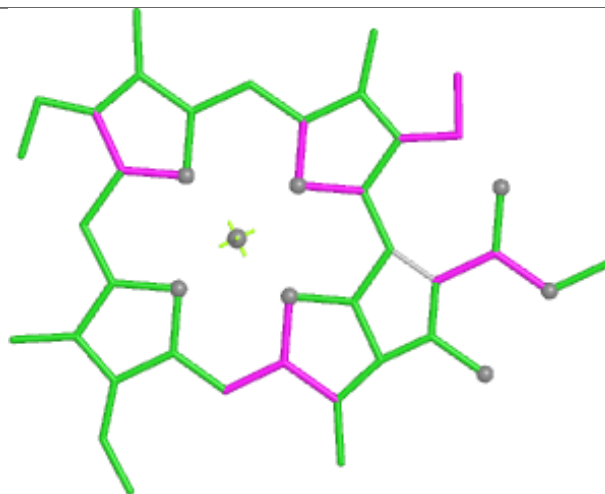




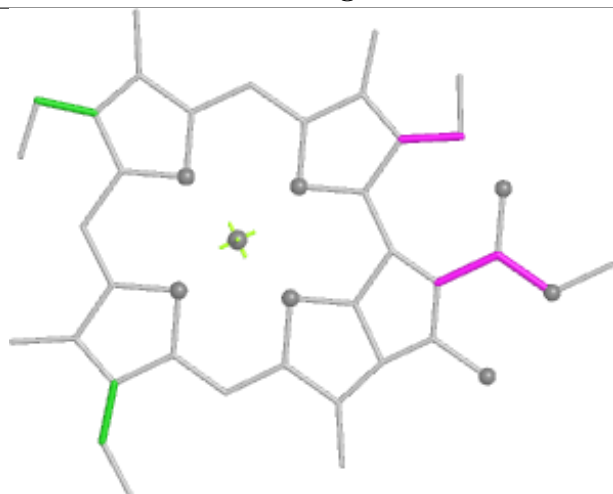
Ligand CLA o 609



Bond lengths



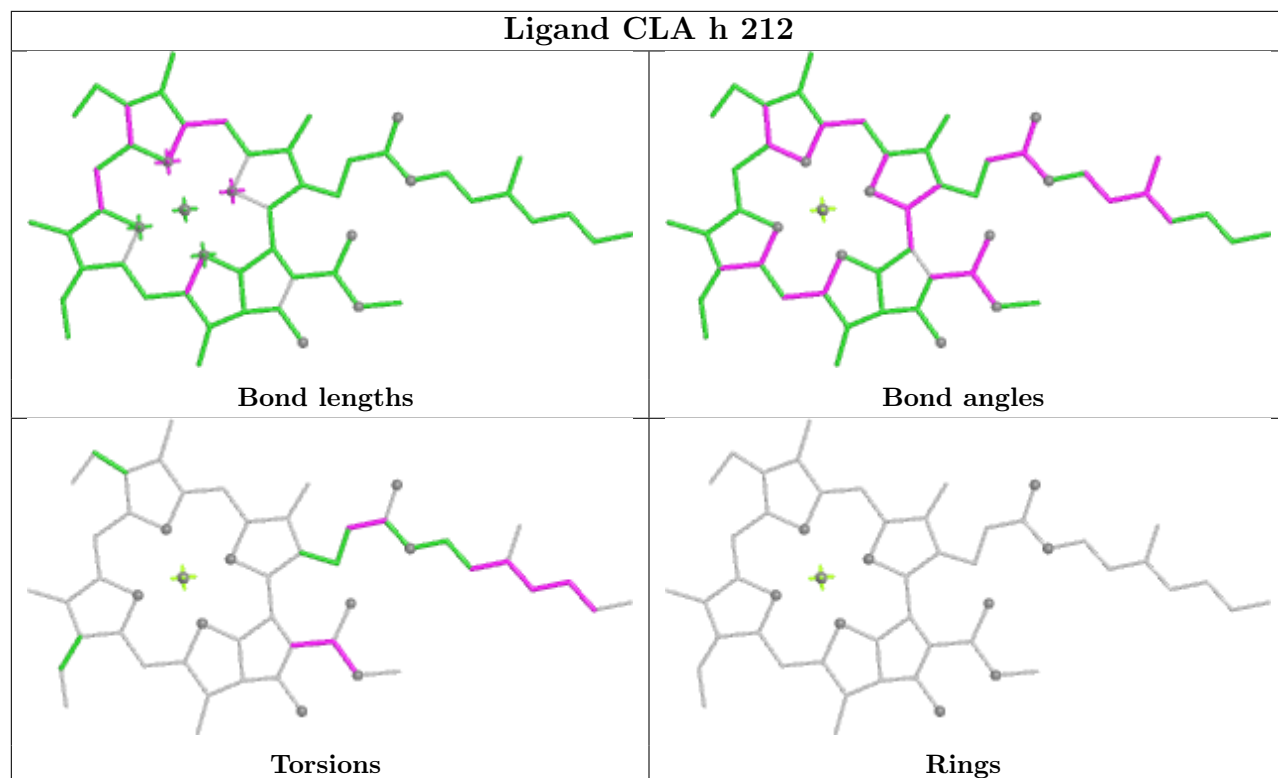
Bond angles

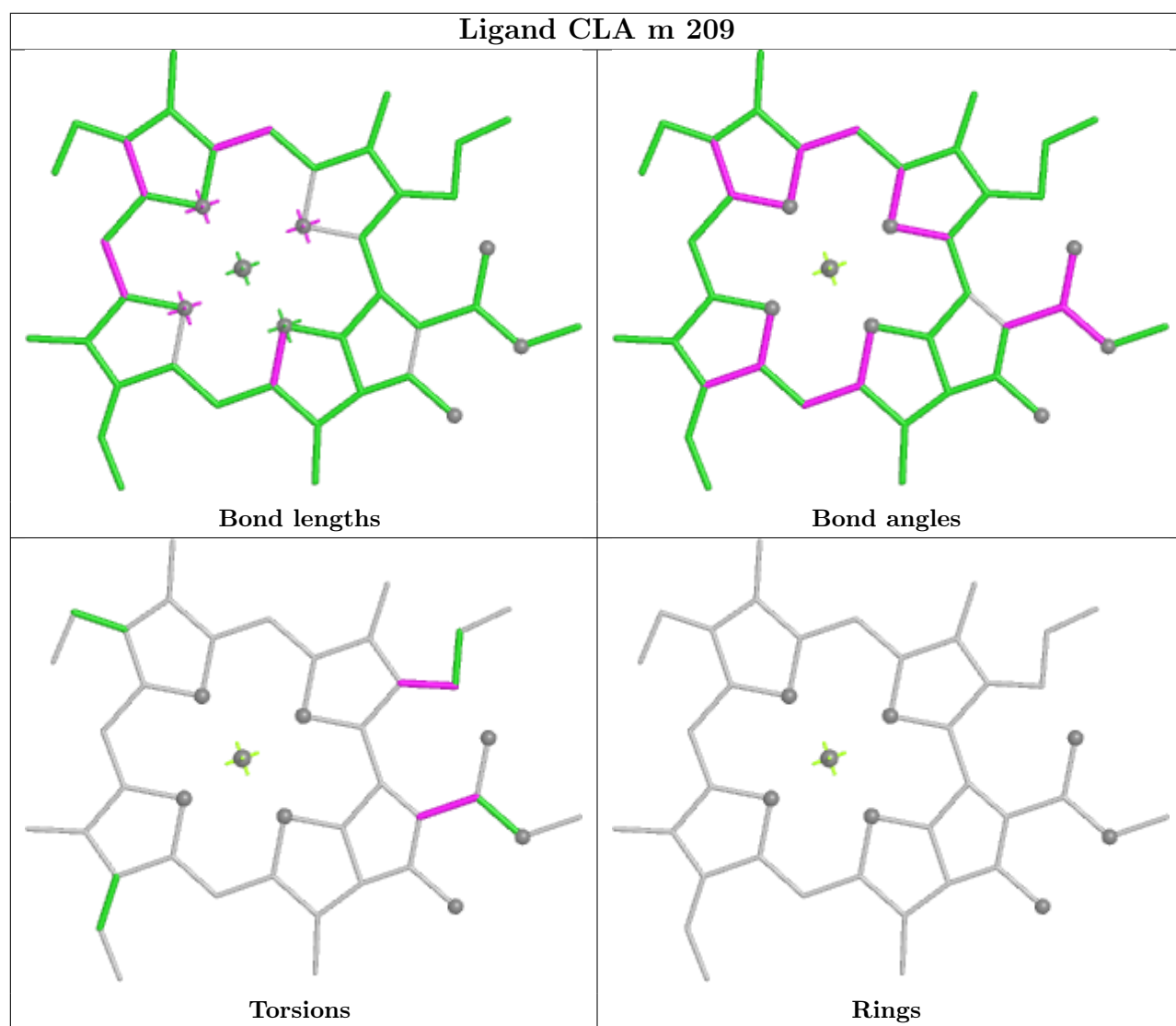


Torsions

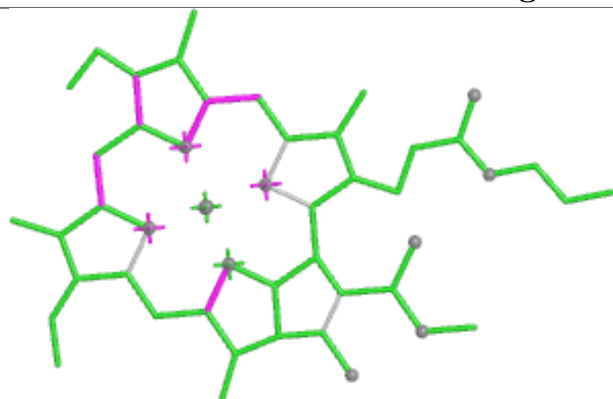


Rings

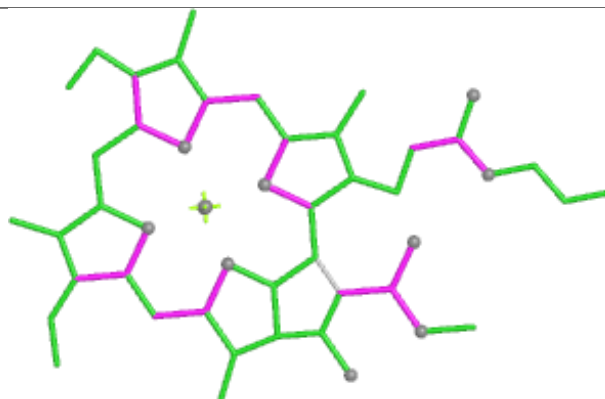




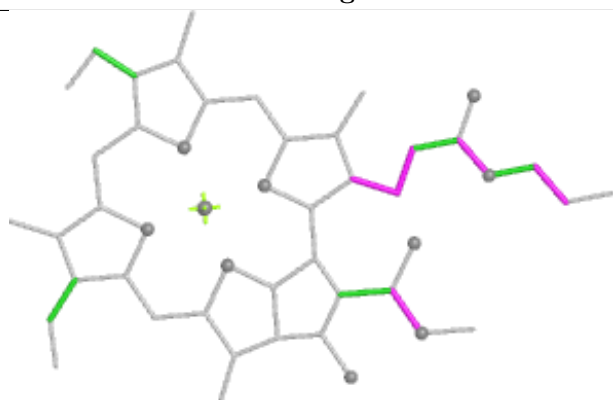
Ligand CLA e 211



Bond lengths



Bond angles

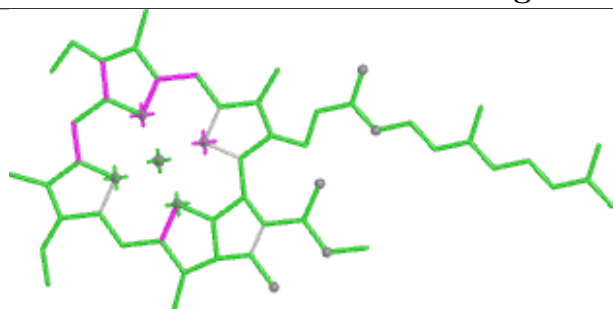


Torsions

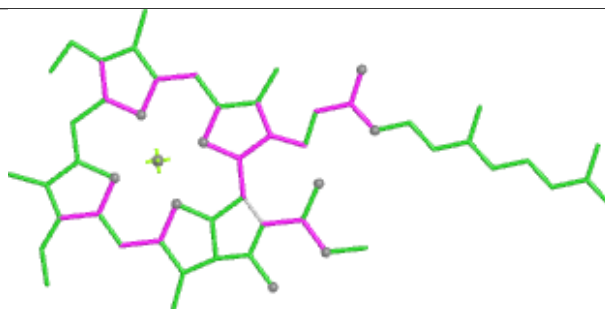


Rings

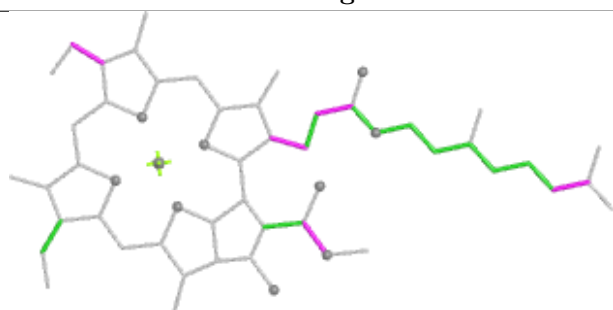
Ligand CLA A 850



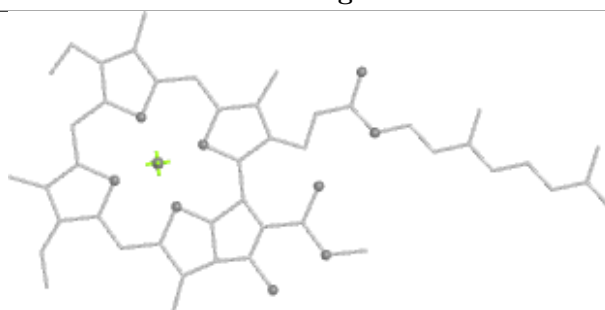
Bond lengths



Bond angles

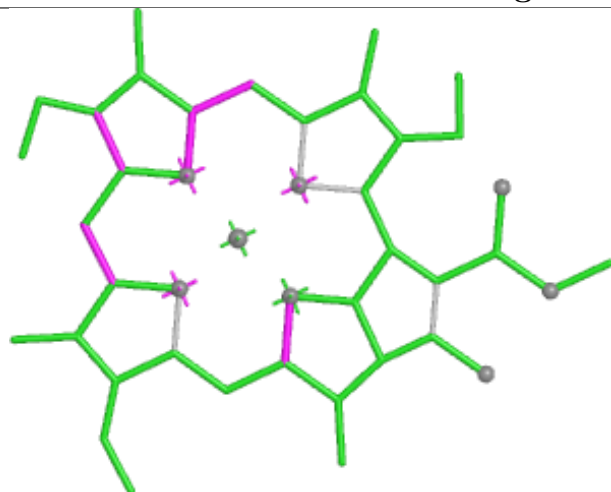


Torsions

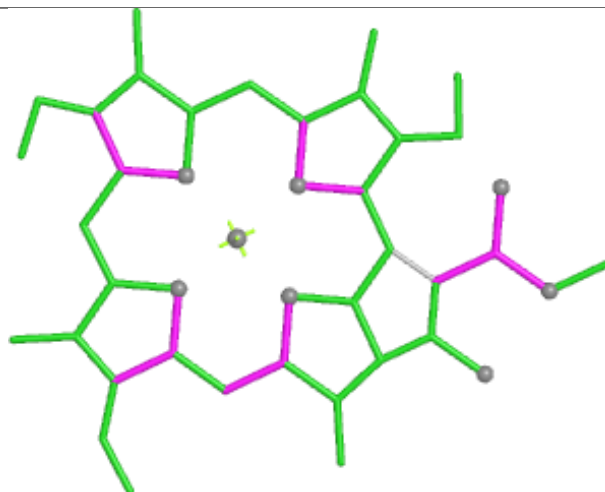


Rings

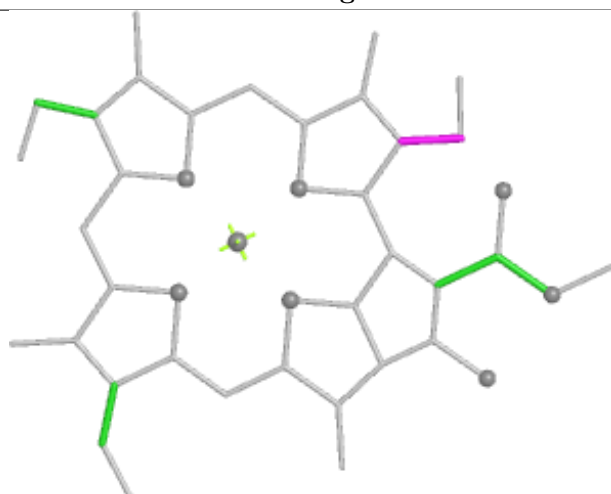
Ligand CLA B 806



Bond lengths



Bond angles

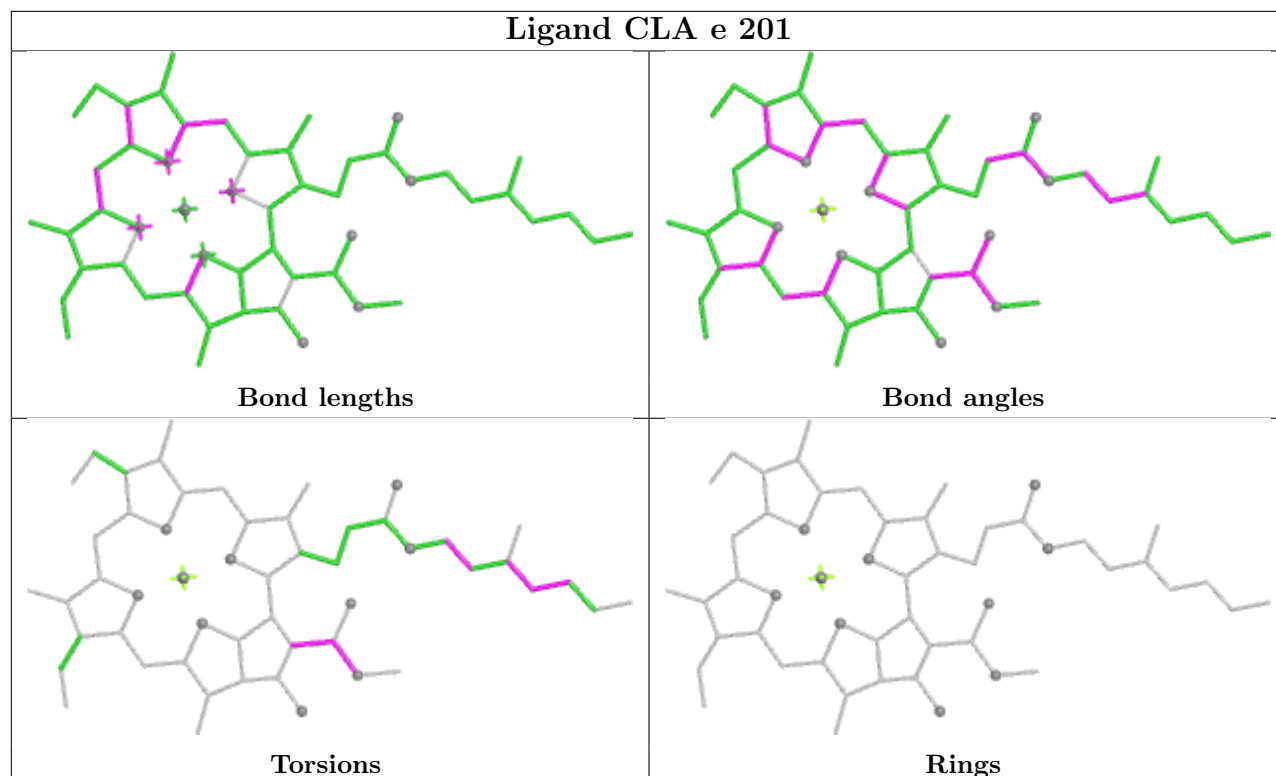


Torsions

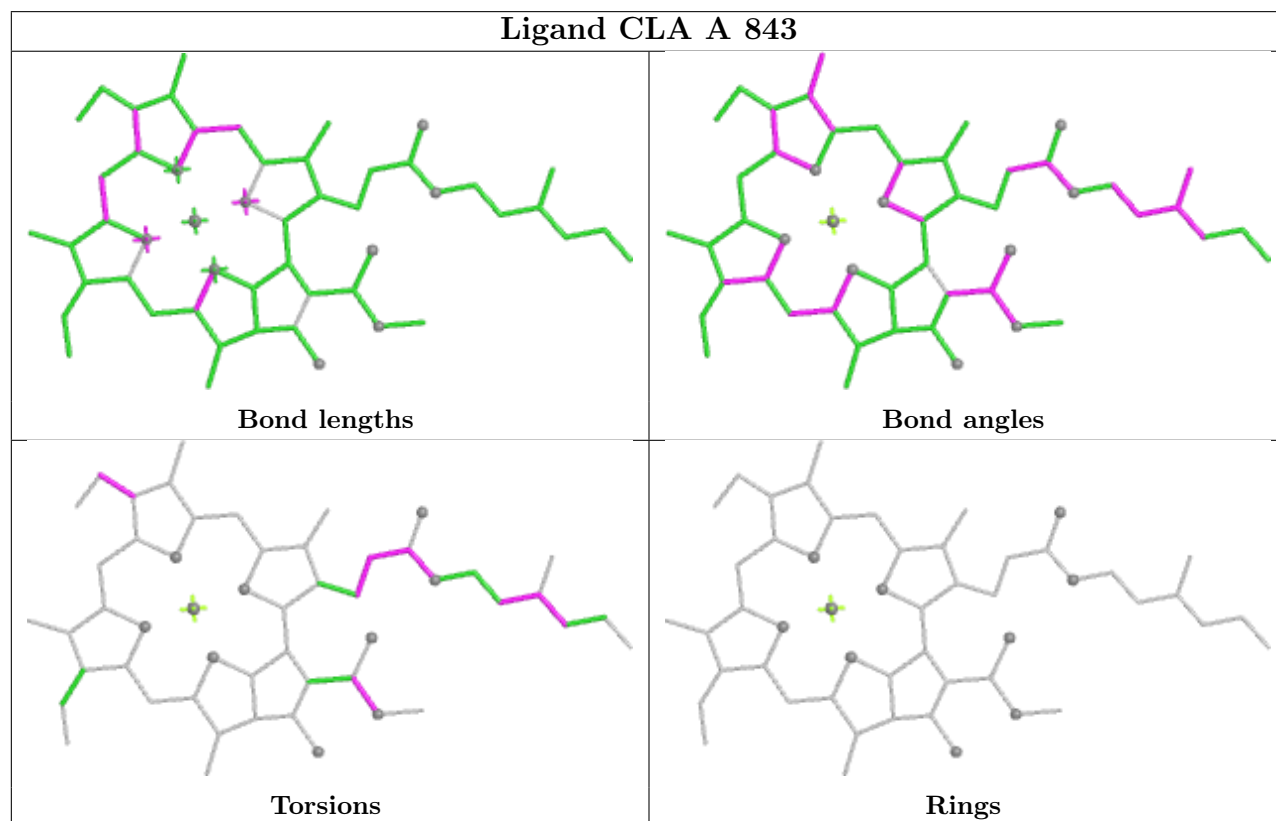


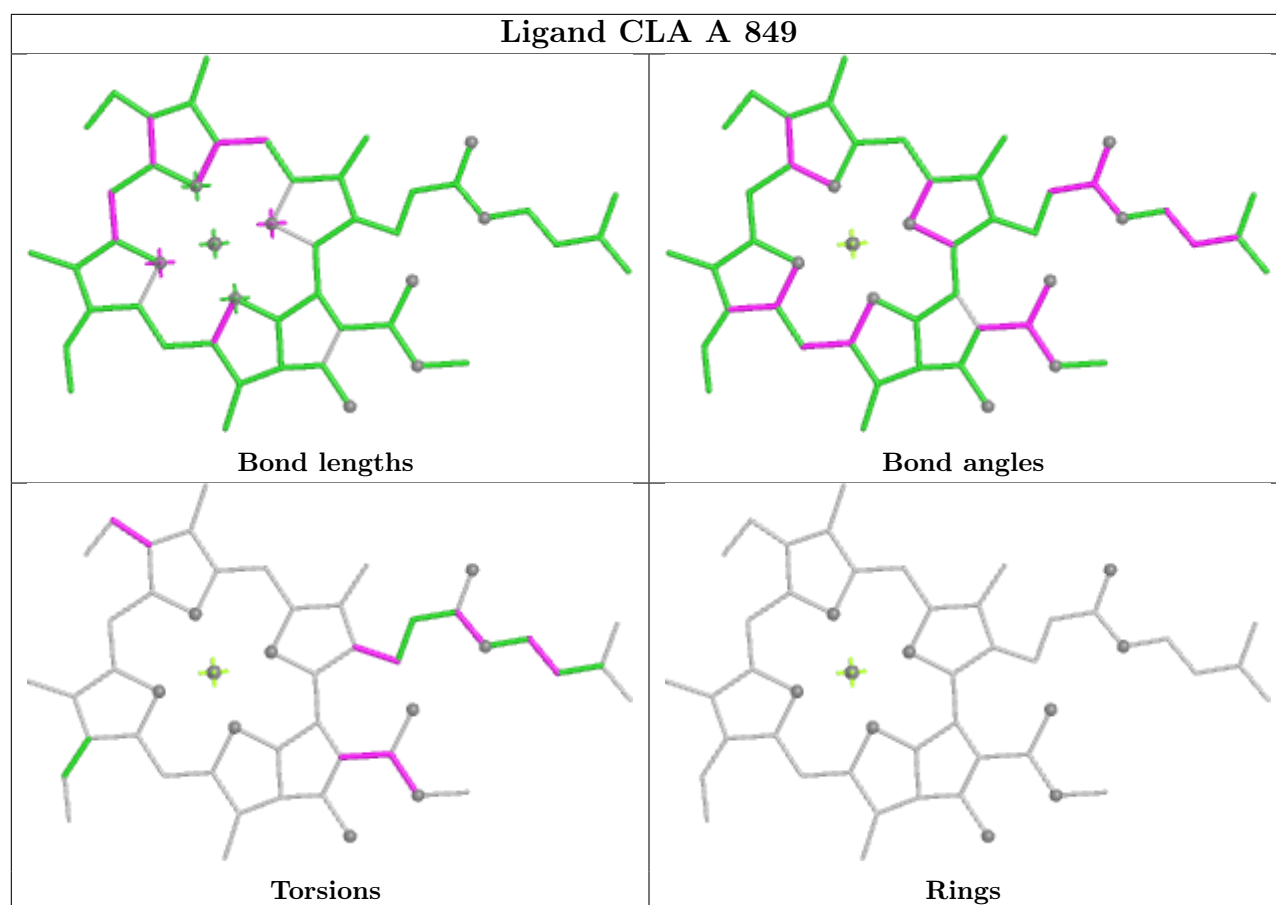
Rings

Ligand CLA e 201

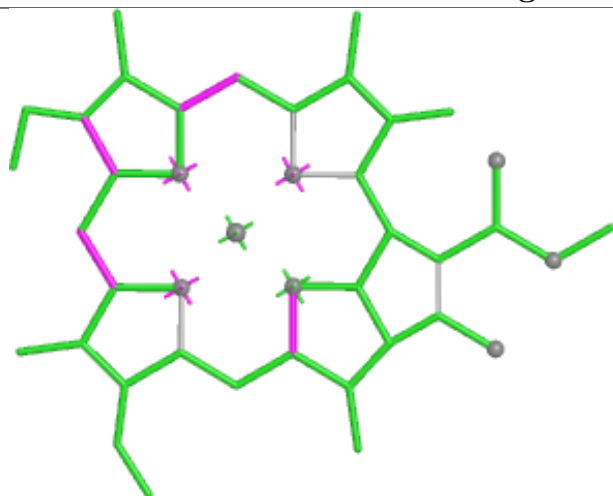


Ligand CLA A 843





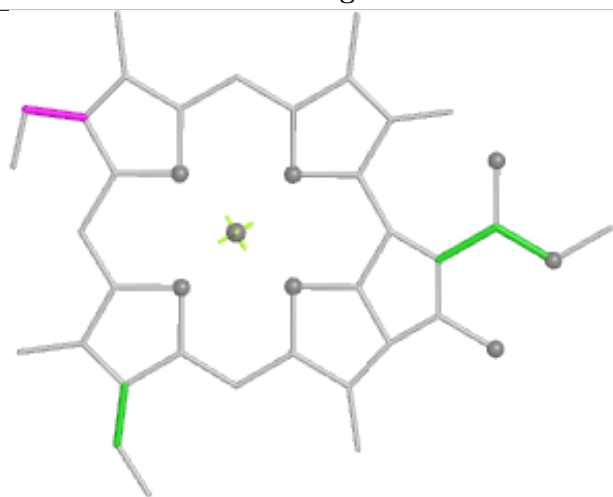
Ligand CLA o 607



Bond lengths



Bond angles

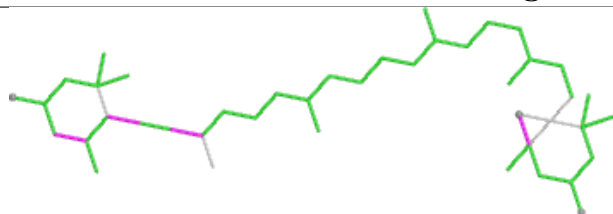


Torsions

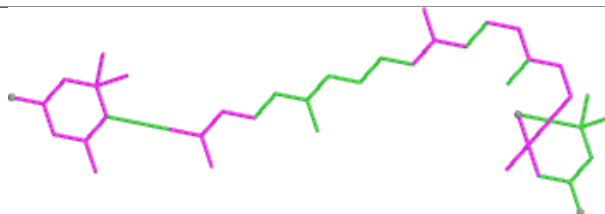


Rings

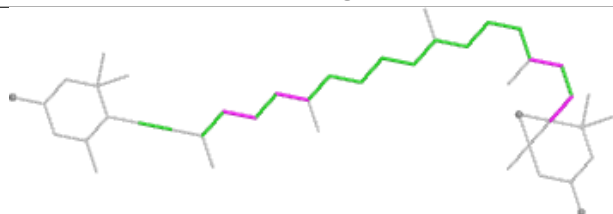
Ligand DD6 f 614



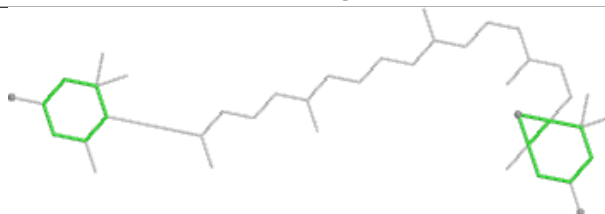
Bond lengths



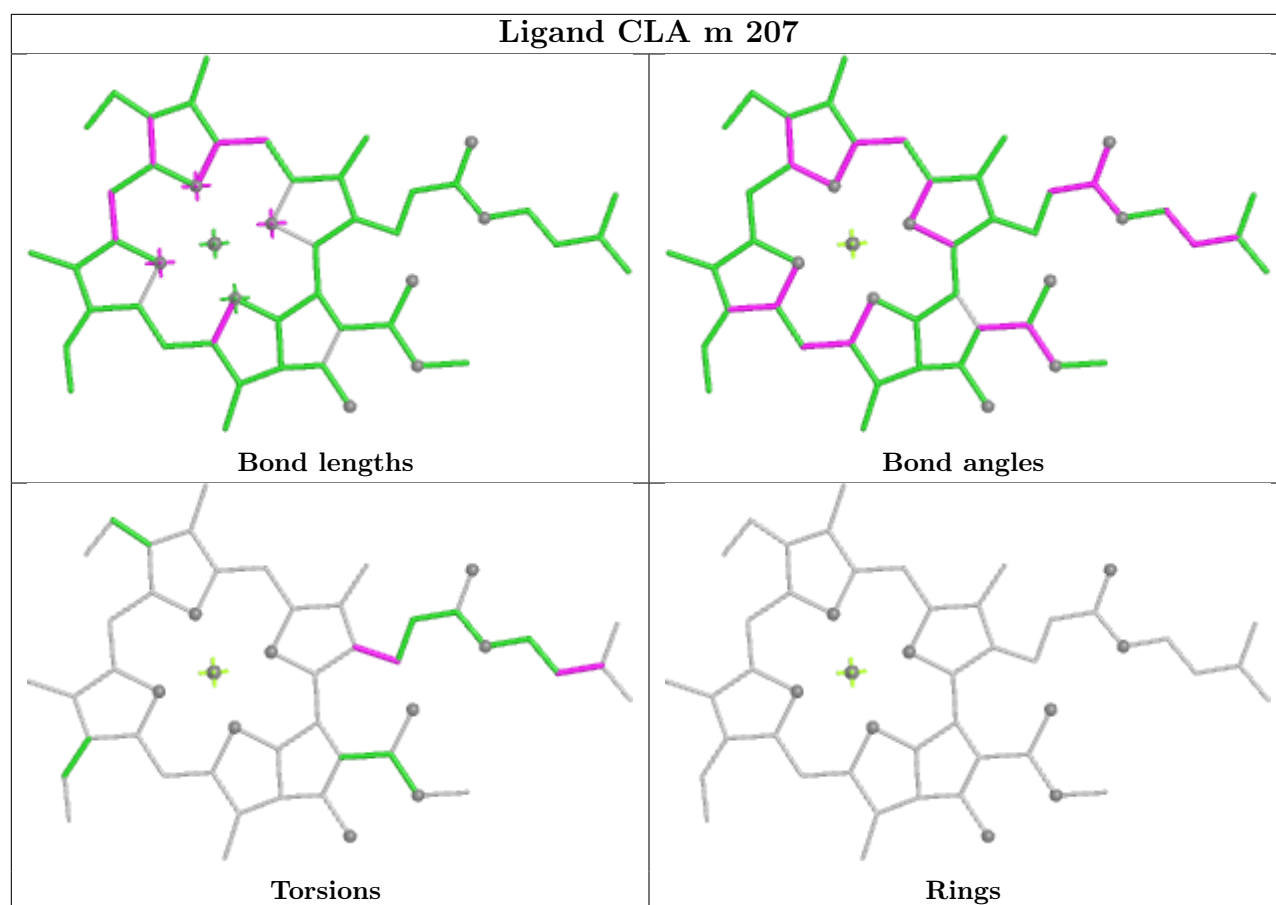
Bond angles



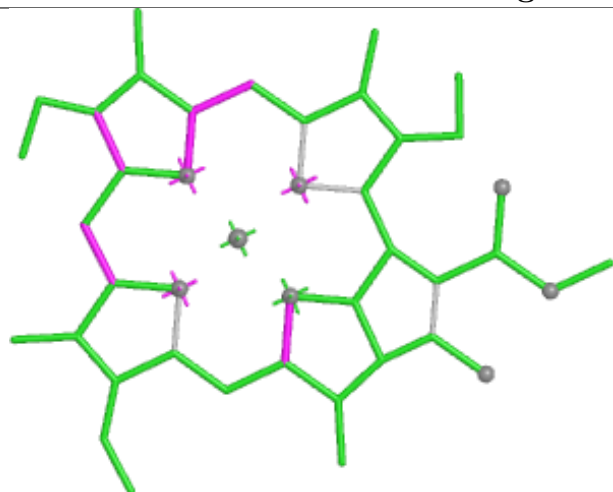
Torsions



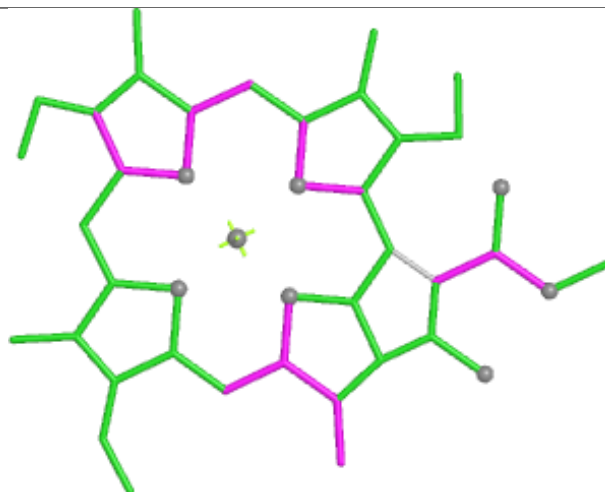
Rings



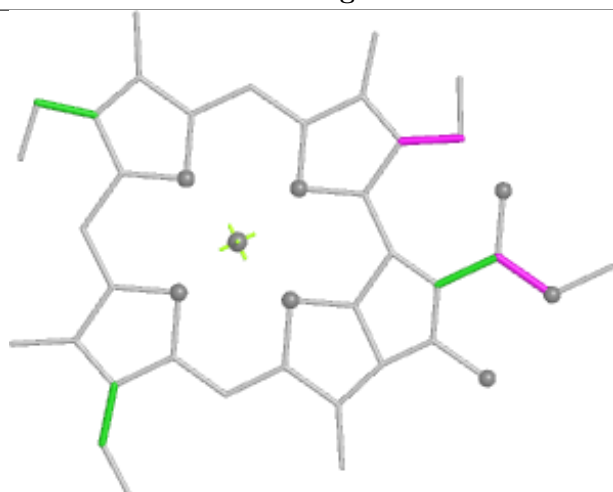
Ligand CLA n 210



Bond lengths



Bond angles

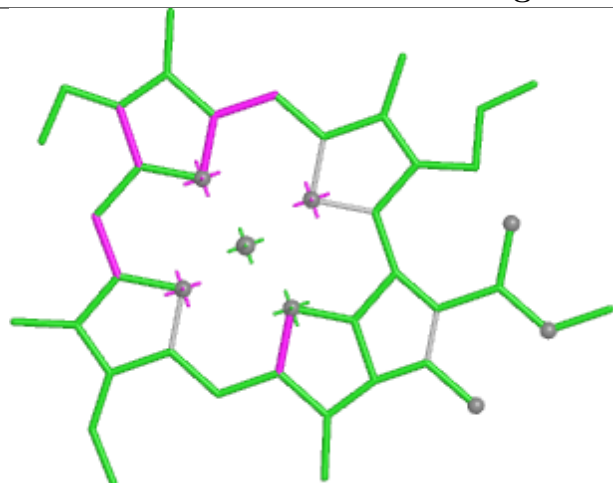


Torsions

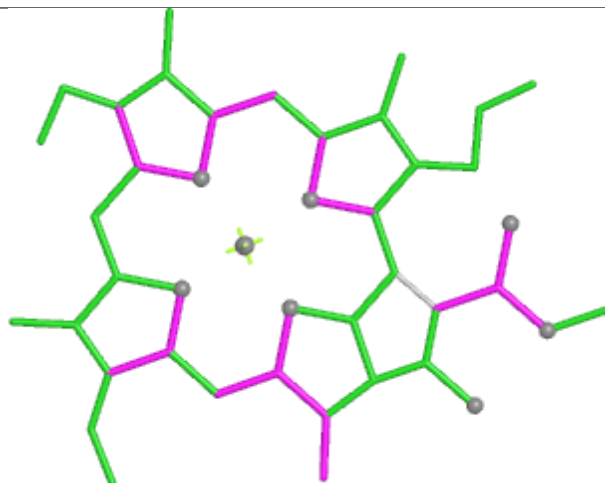


Rings

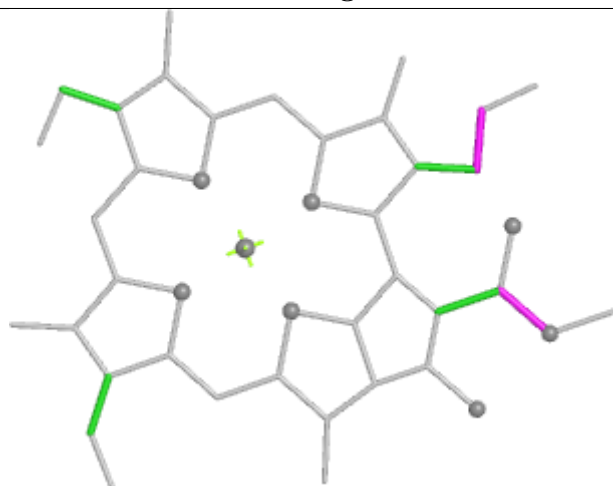
Ligand CLA A 827



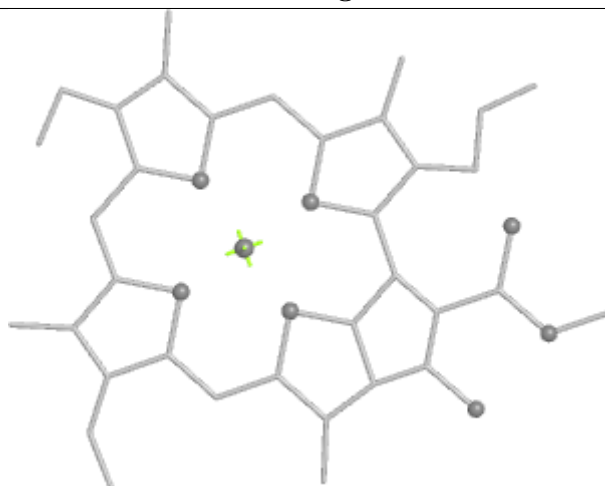
Bond lengths



Bond angles

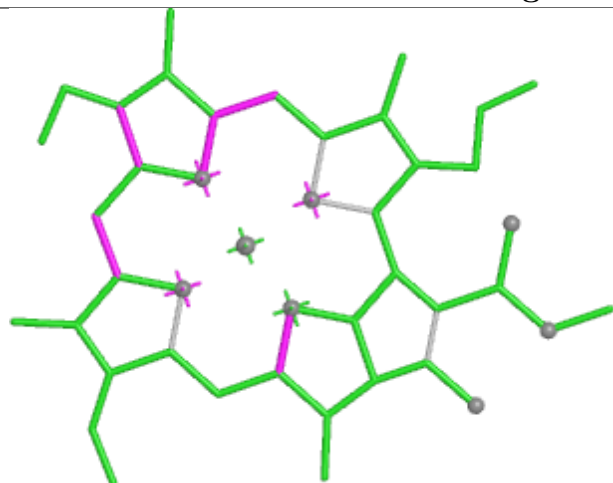


Torsions

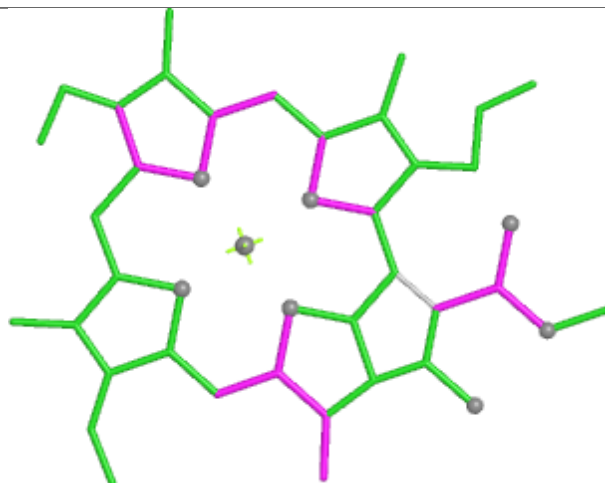


Rings

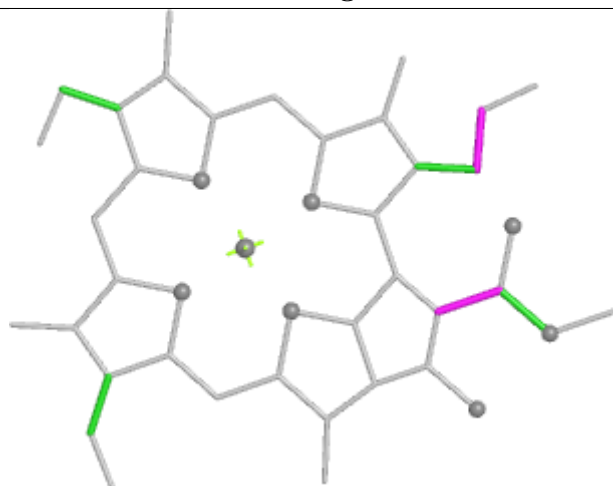
Ligand CLA 1 603



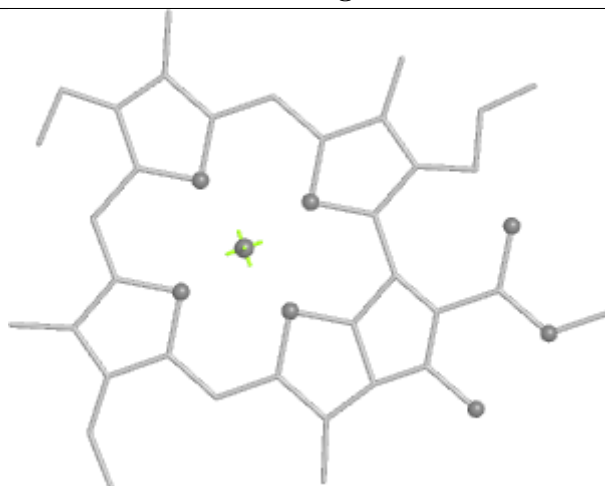
Bond lengths



Bond angles

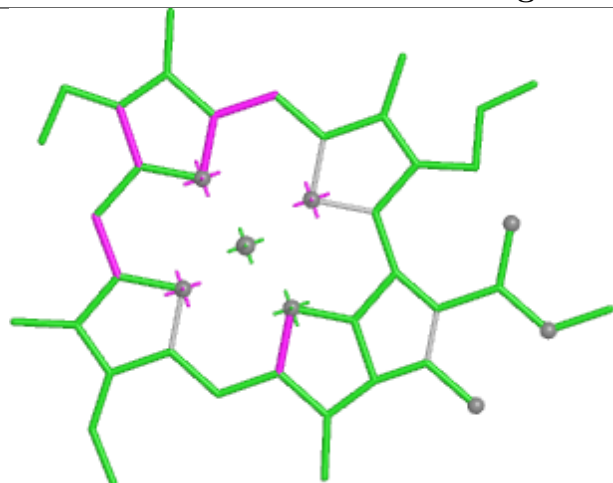


Torsions

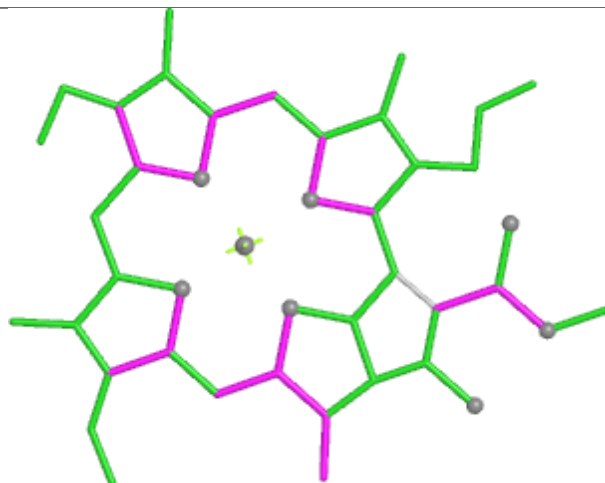


Rings

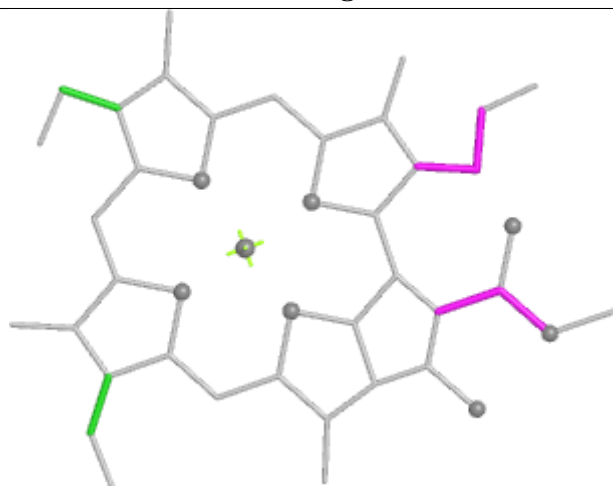
Ligand CLA b 205



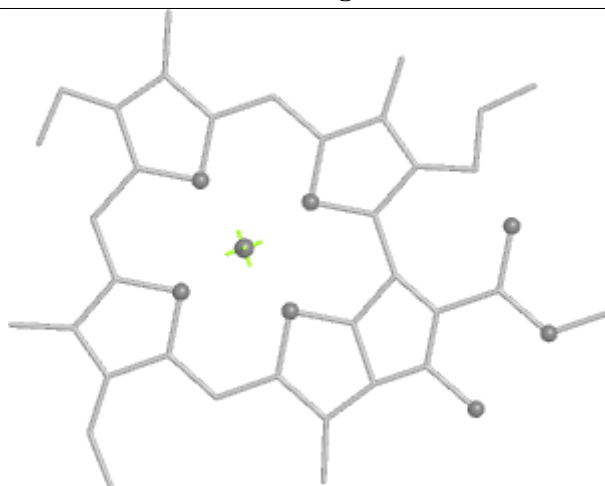
Bond lengths



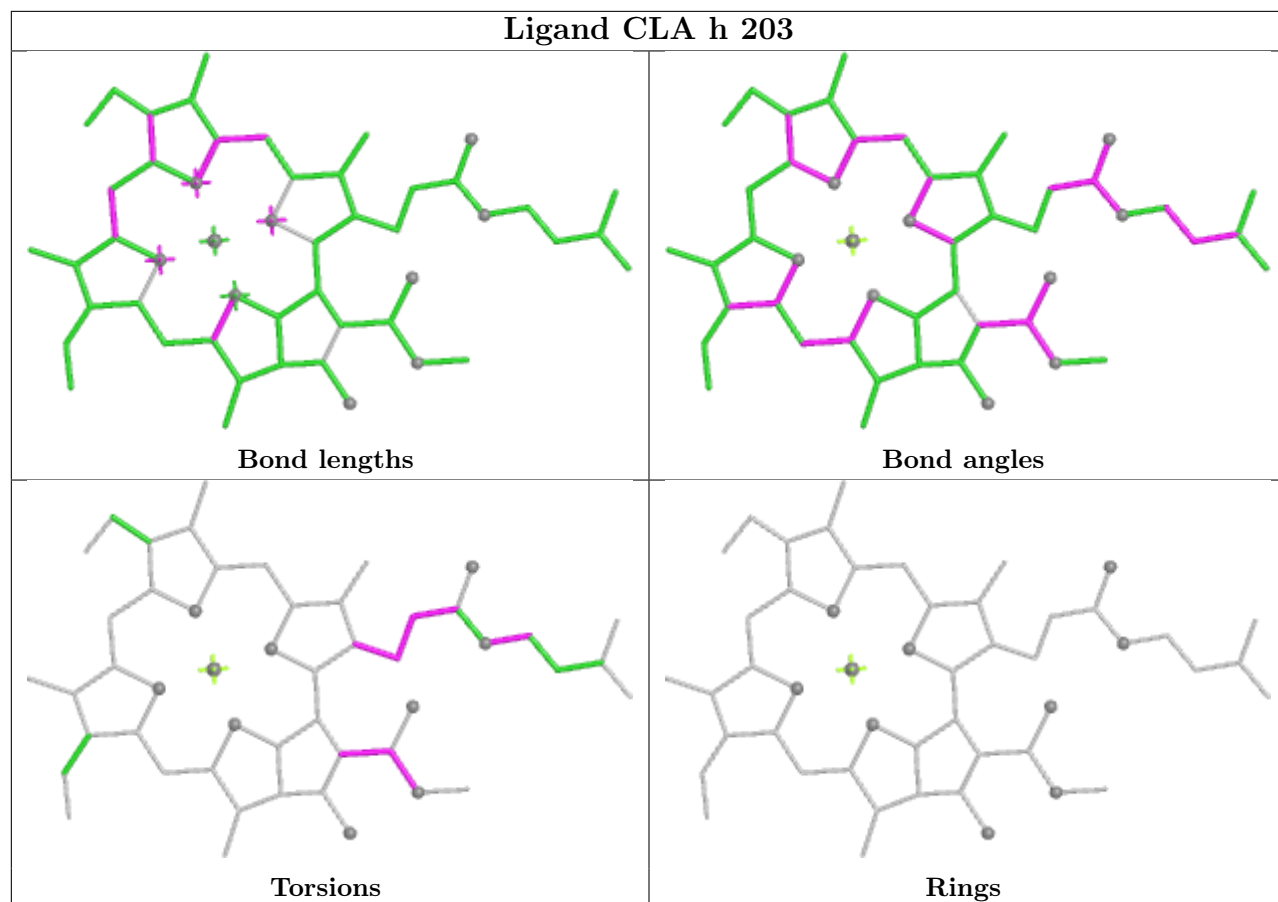
Bond angles



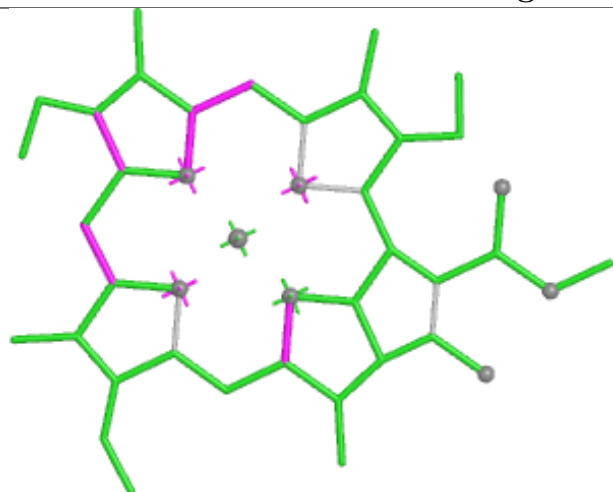
Torsions



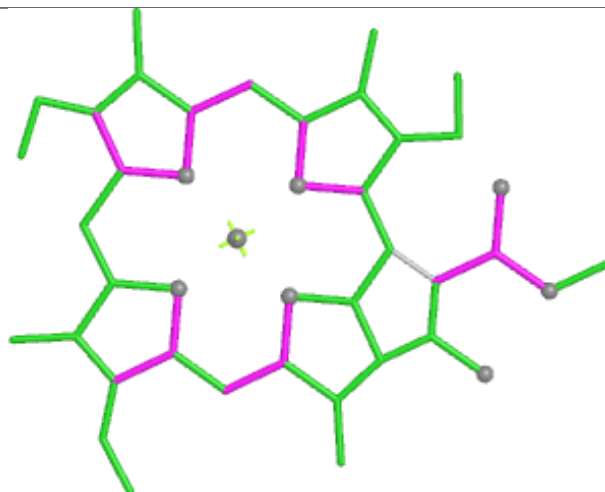
Rings



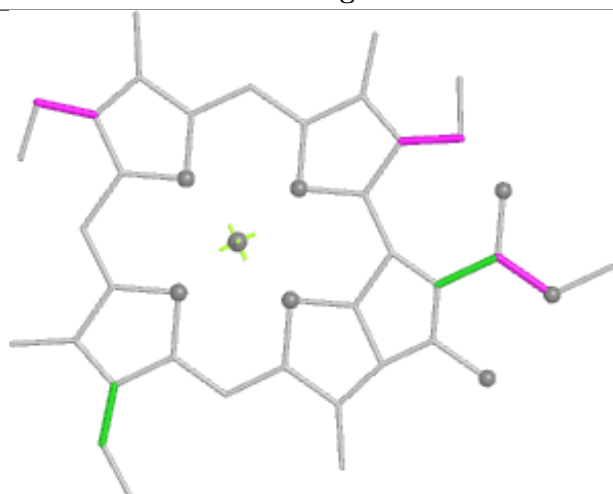
Ligand CLA h 214



Bond lengths



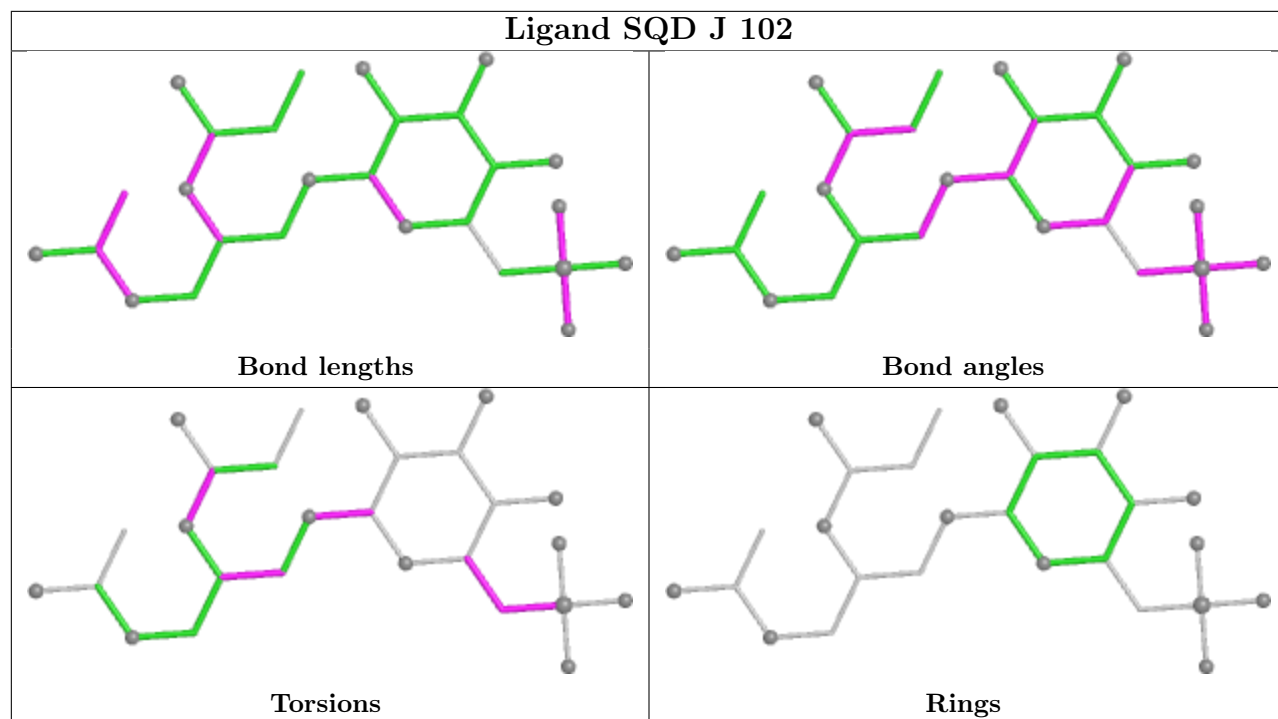
Bond angles



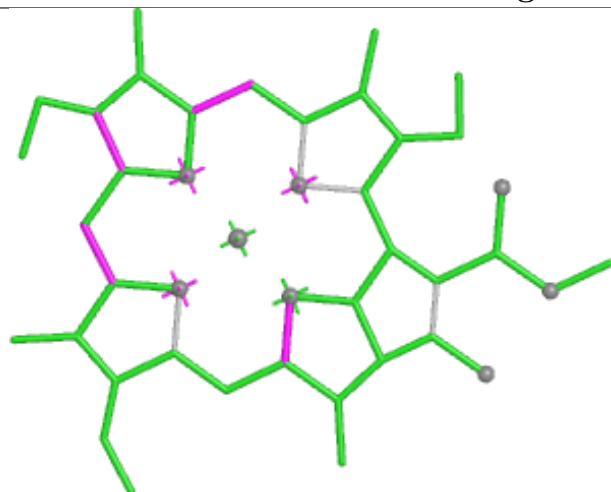
Torsions



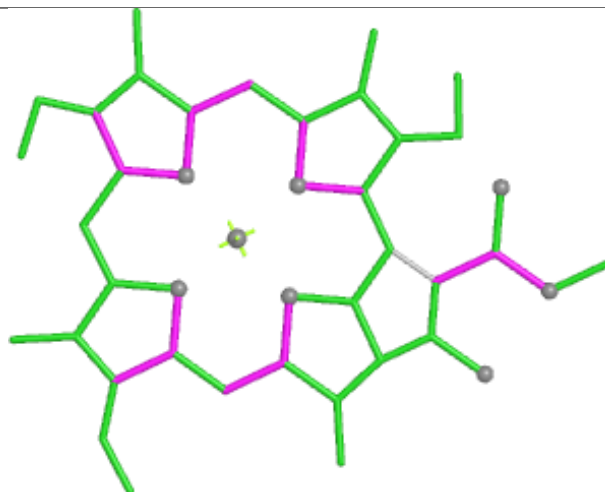
Rings



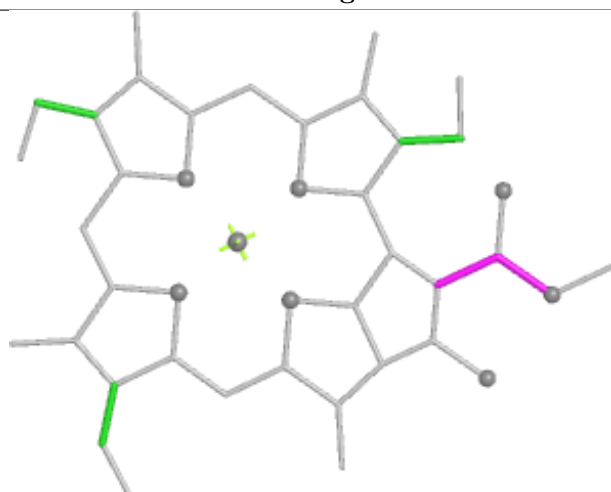
Ligand CLA b 211



Bond lengths



Bond angles

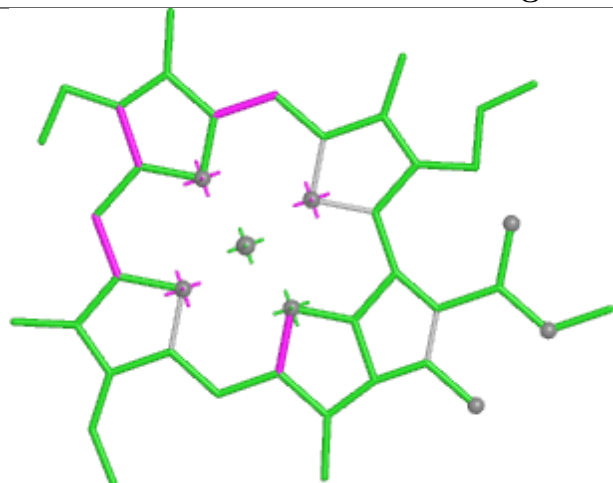


Torsions

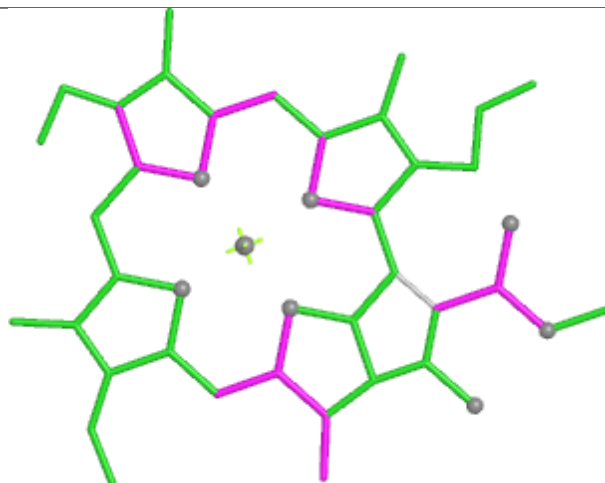


Rings

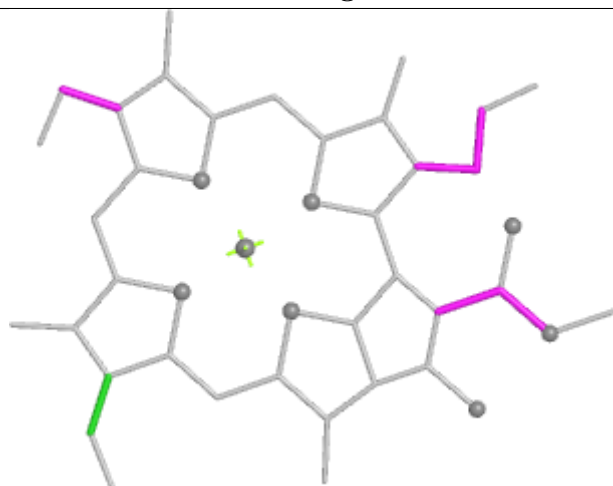
Ligand CLA f 612



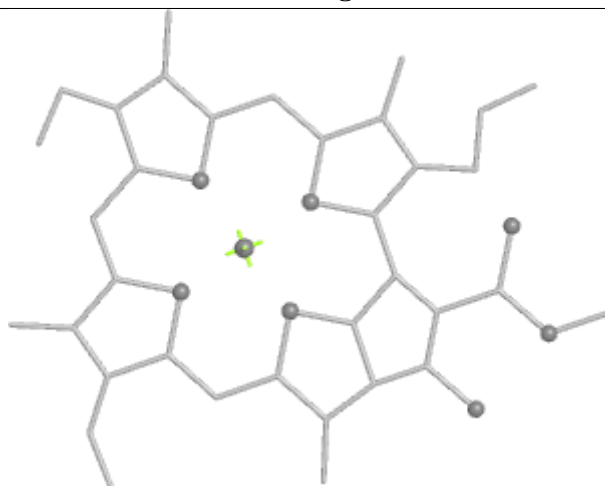
Bond lengths



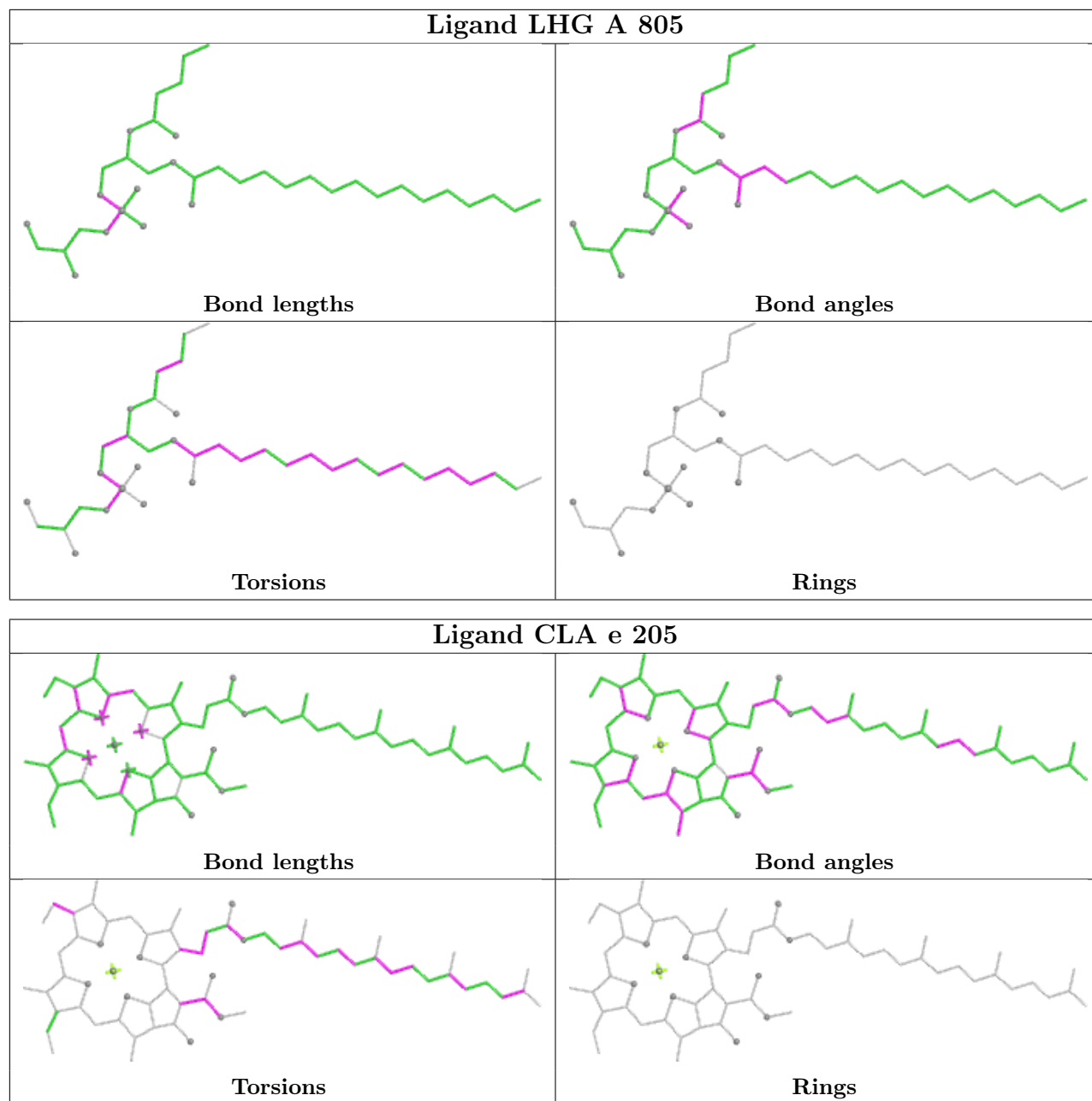
Bond angles



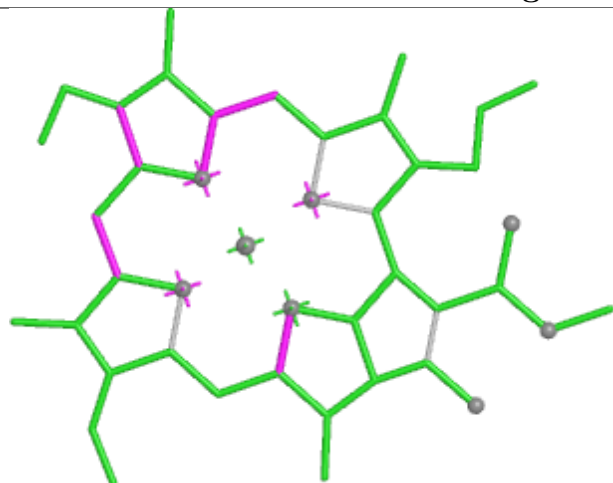
Torsions



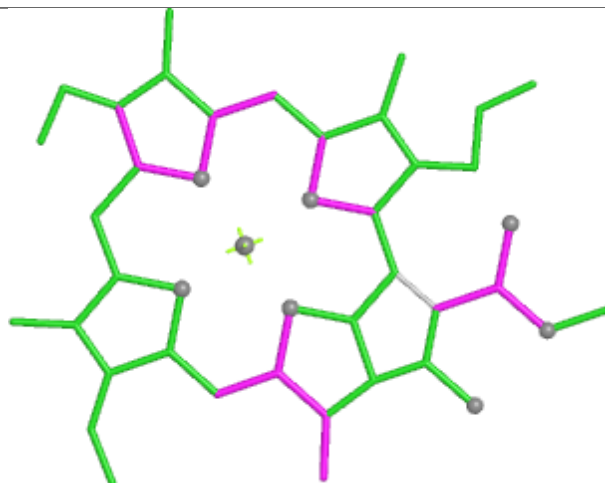
Rings



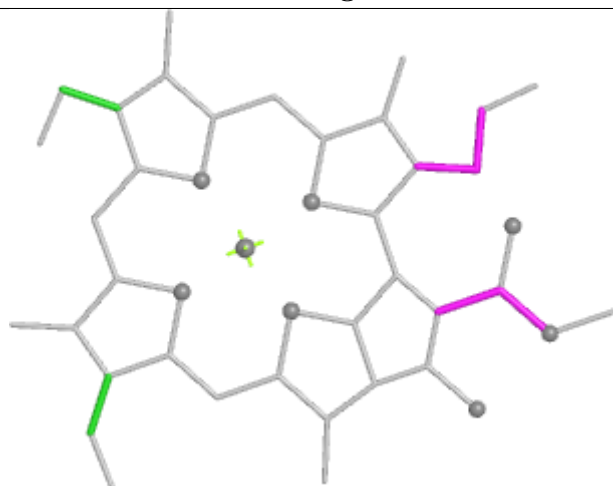
Ligand CLA 1 609



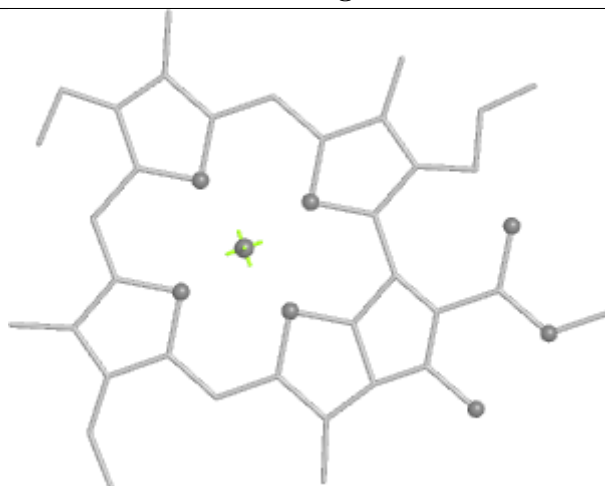
Bond lengths



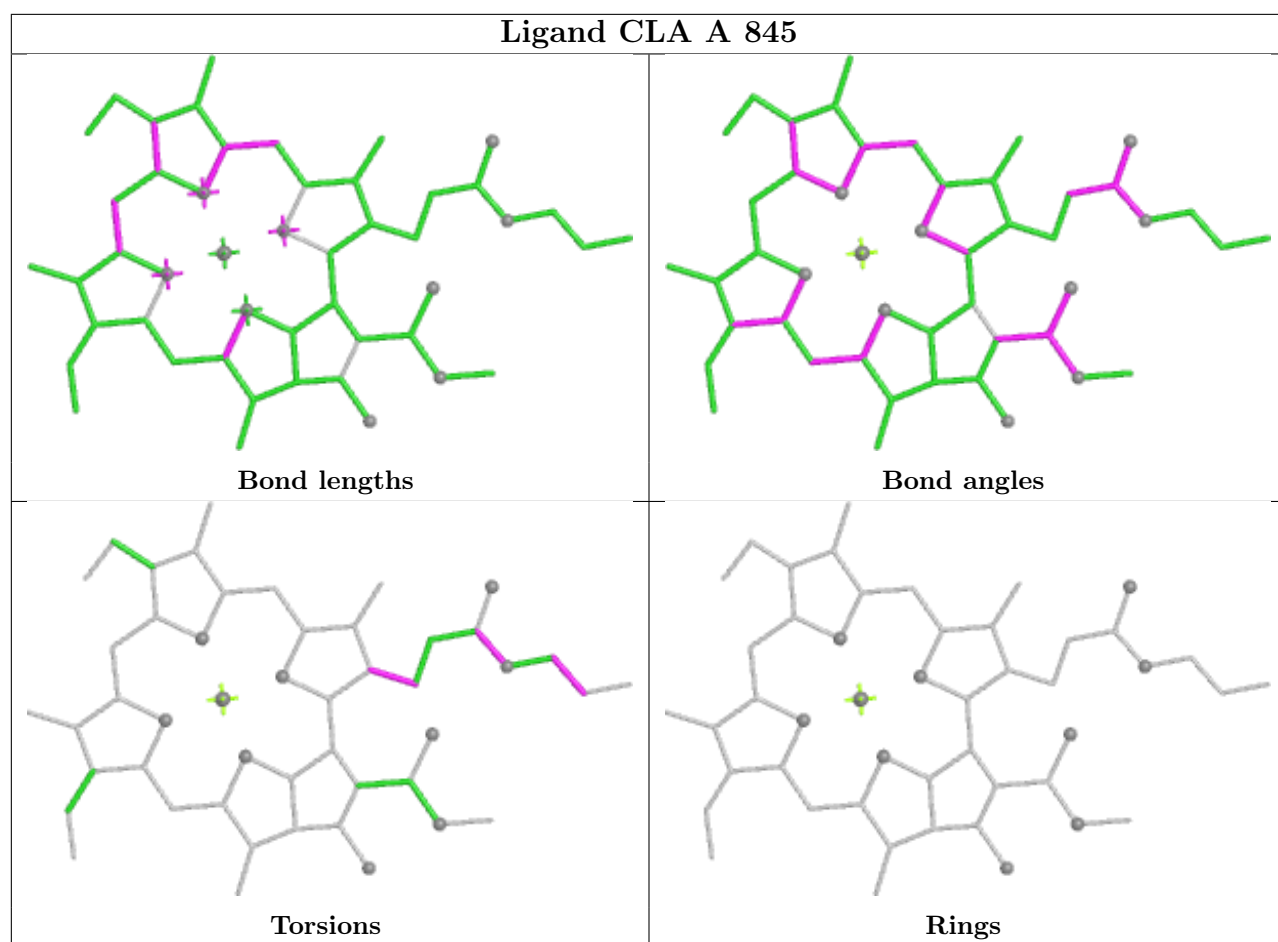
Bond angles



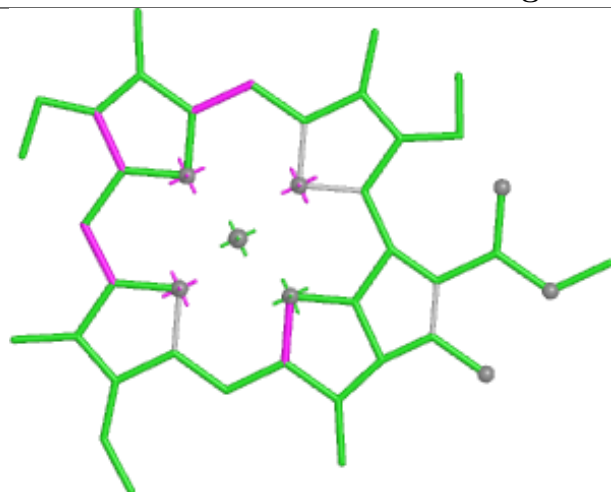
Torsions



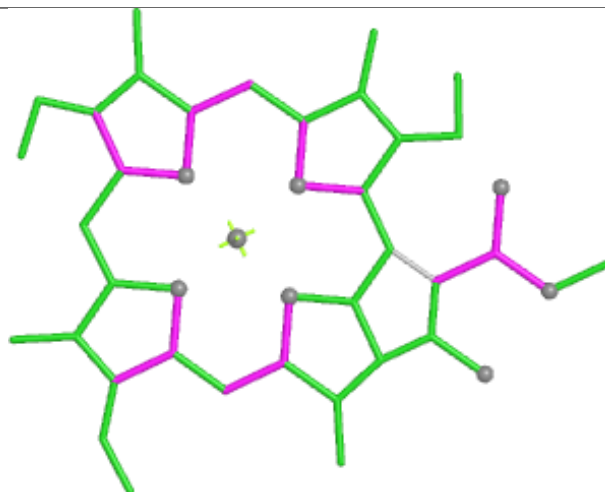
Rings



Ligand CLA f 601



Bond lengths



Bond angles

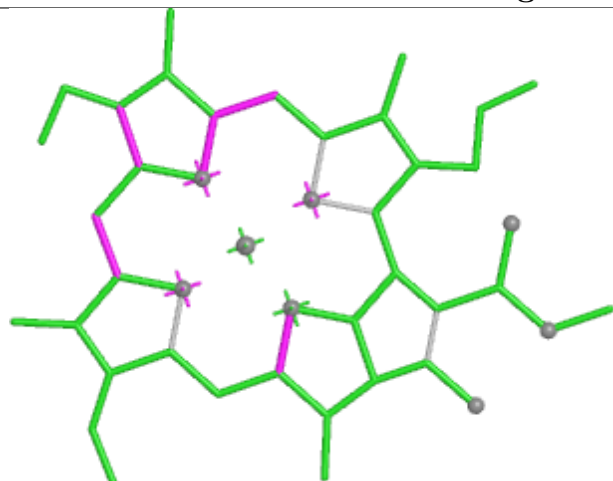


Torsions

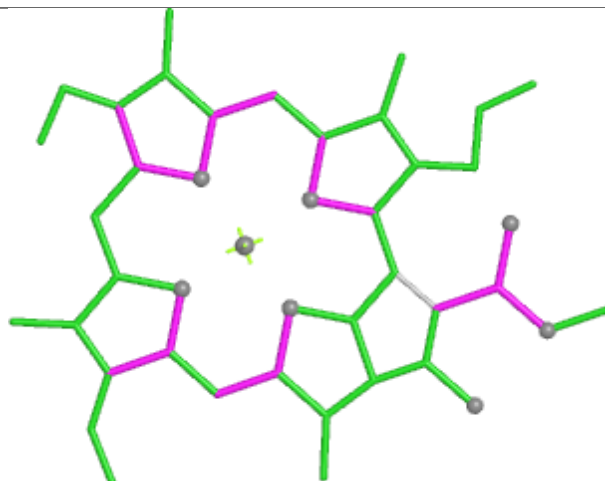


Rings

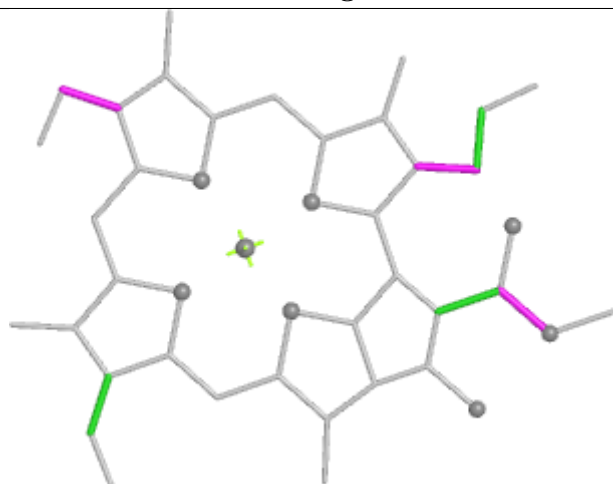
Ligand CLA h 213



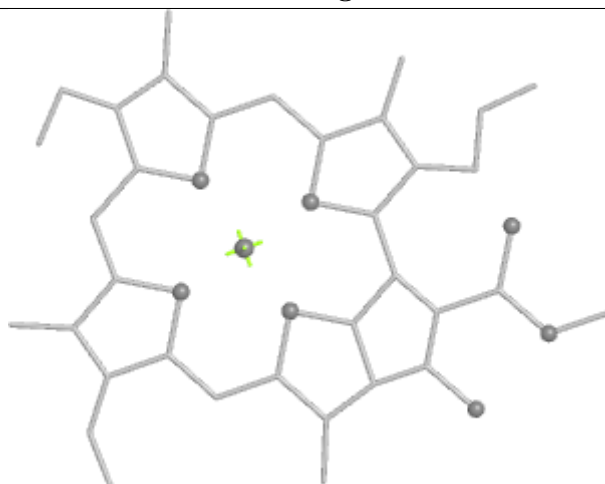
Bond lengths



Bond angles

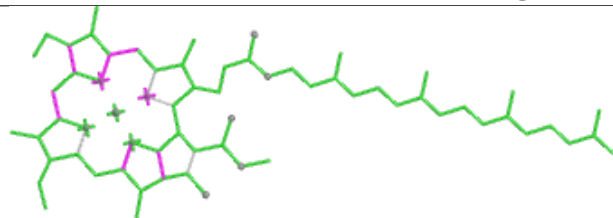


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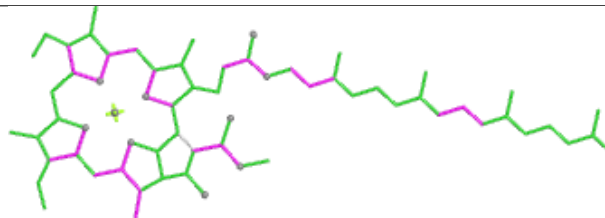


Rings

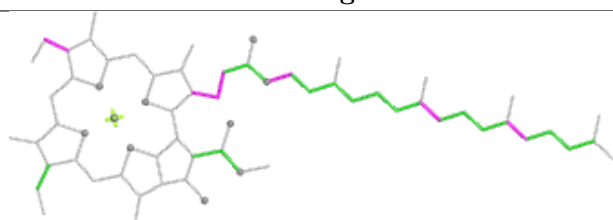
Ligand CLA A 807



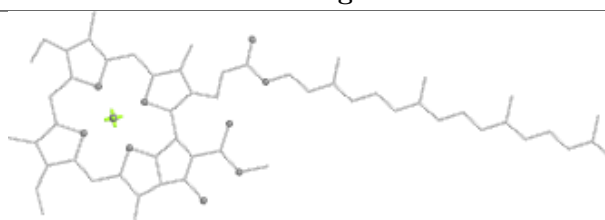
Bond lengths



Bond angles

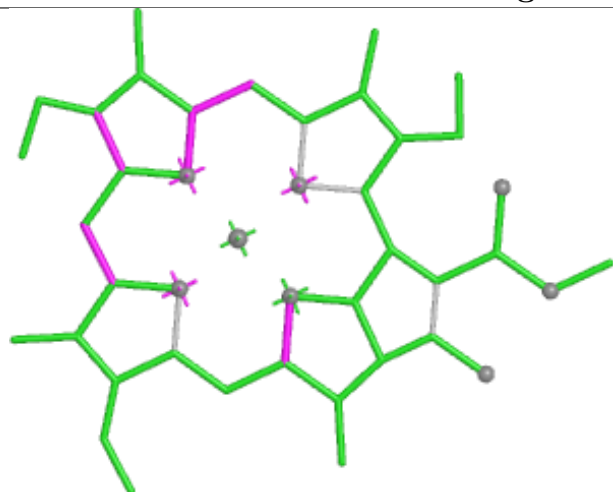


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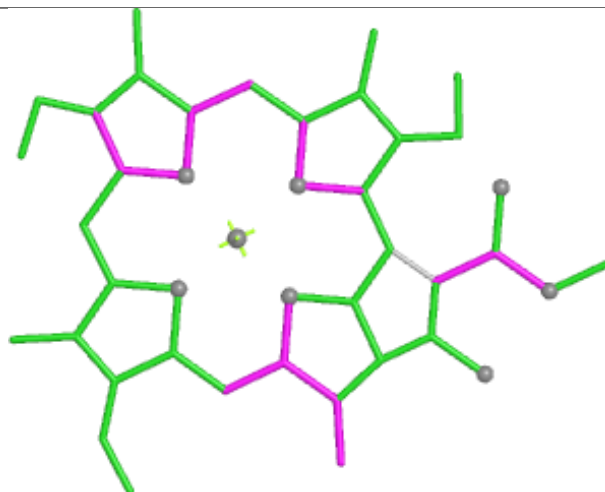


Rings

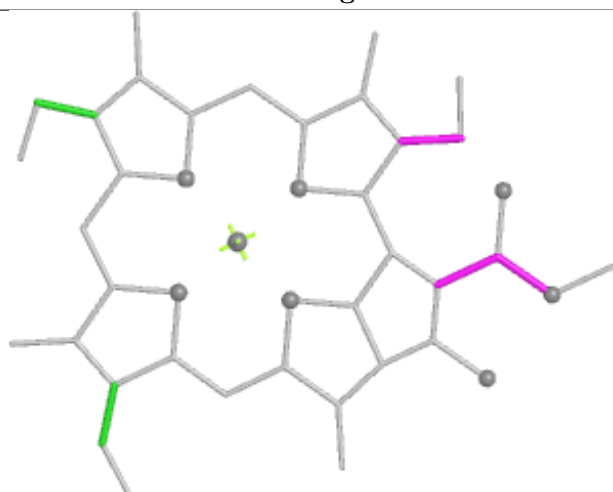
Ligand CLA d 305



Bond lengths



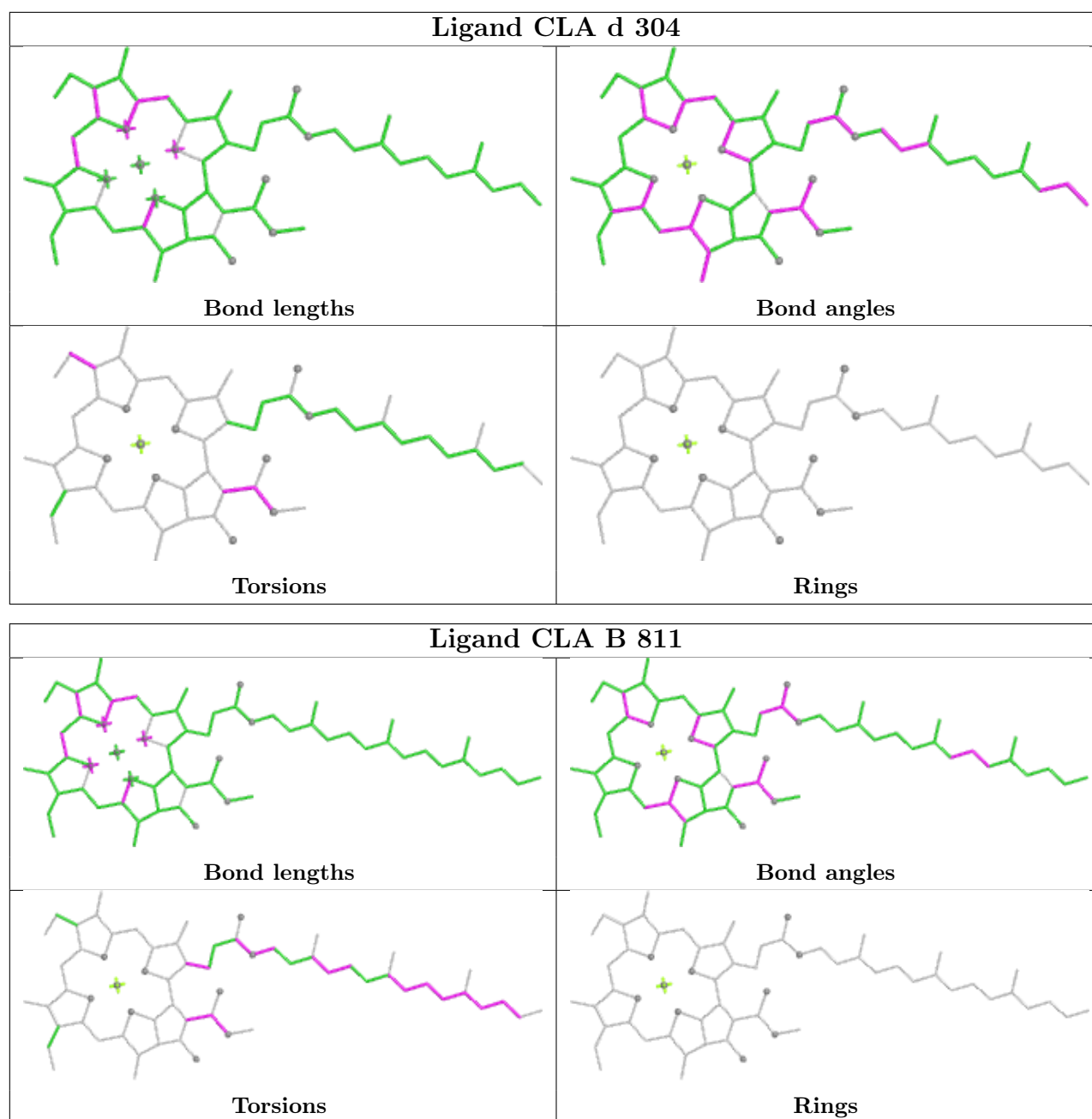
Bond angles



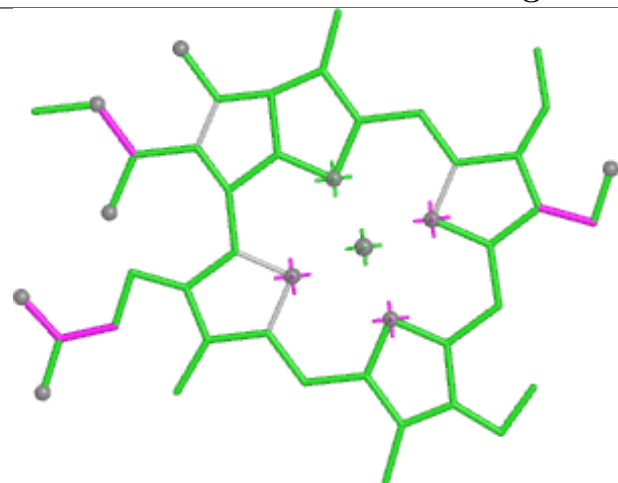
Torsions



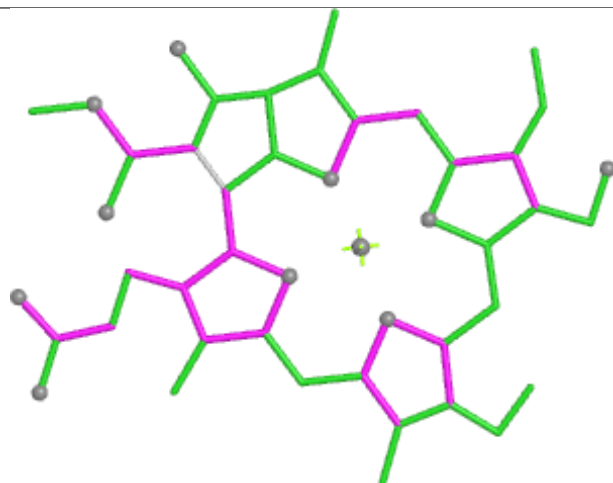
Rings



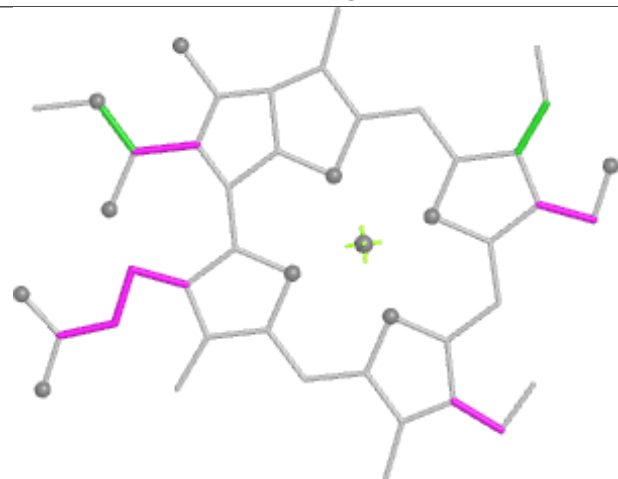
Ligand CHL e 209



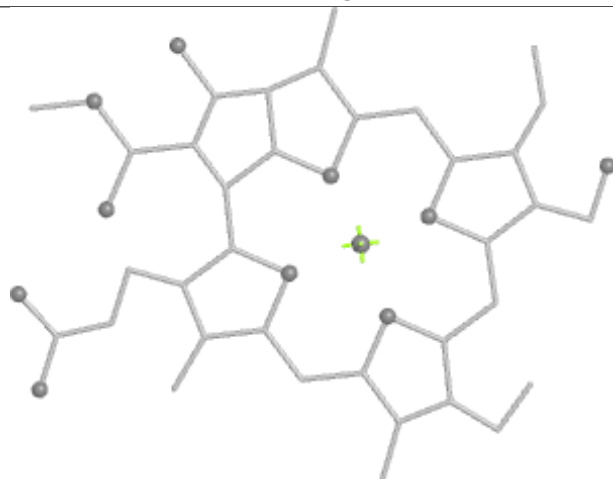
Bond lengths



Bond angles

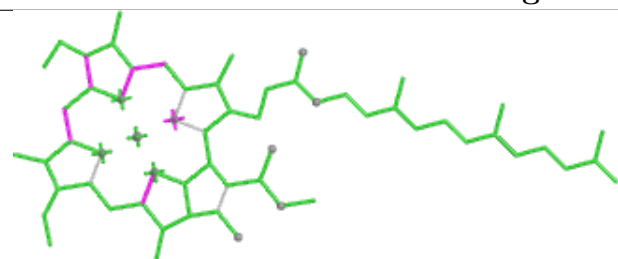


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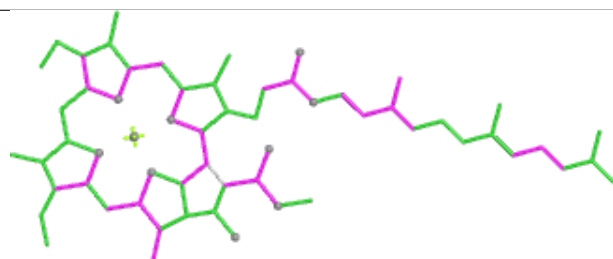


Rings

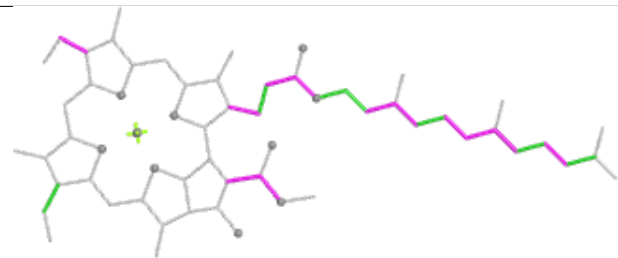
Ligand CLA a 204



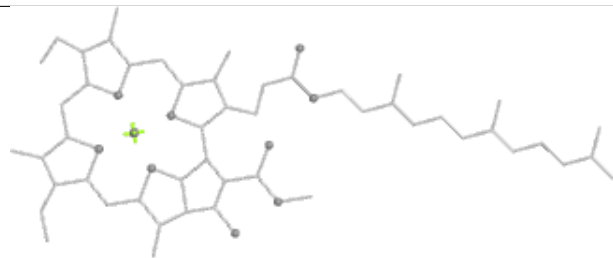
Bond lengths



Bond angles

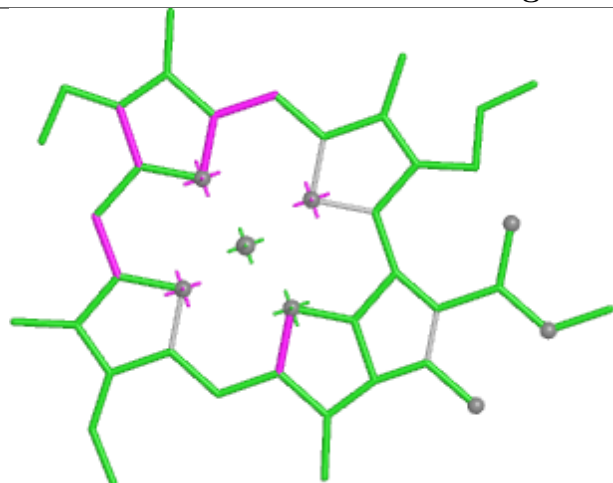


Torsions

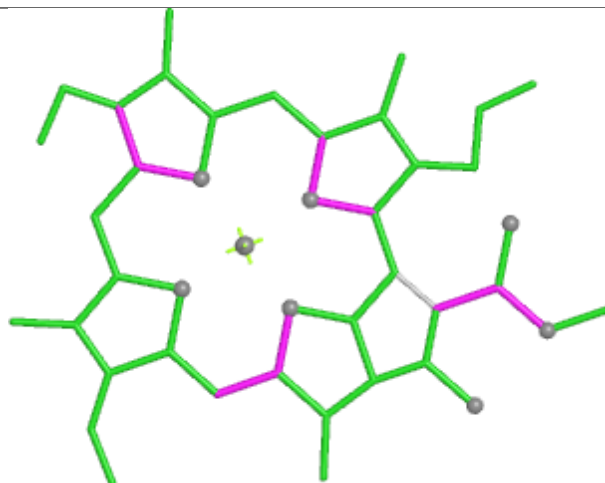


Rings

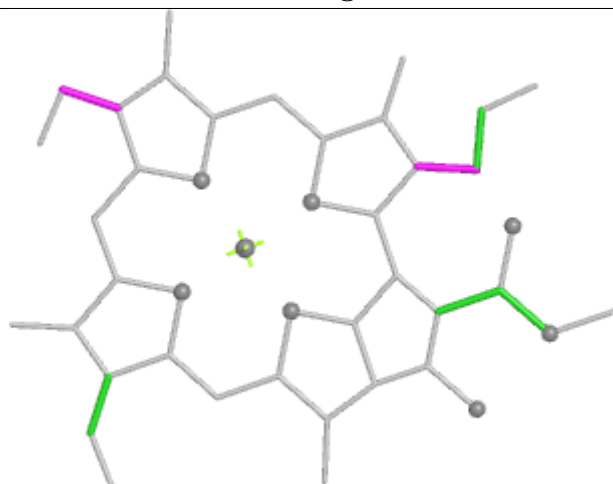
Ligand CLA i 207



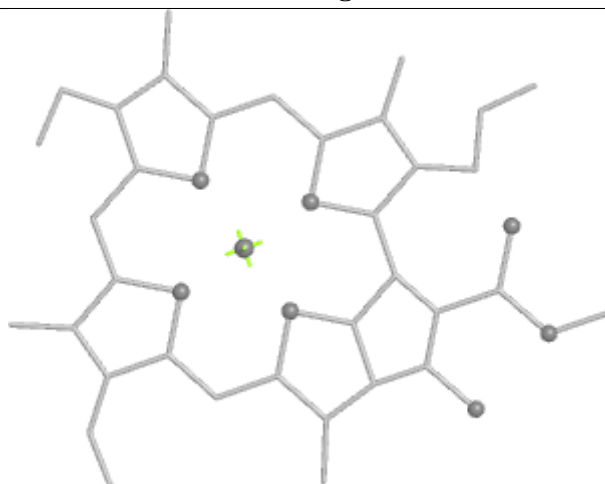
Bond lengths



Bond angles

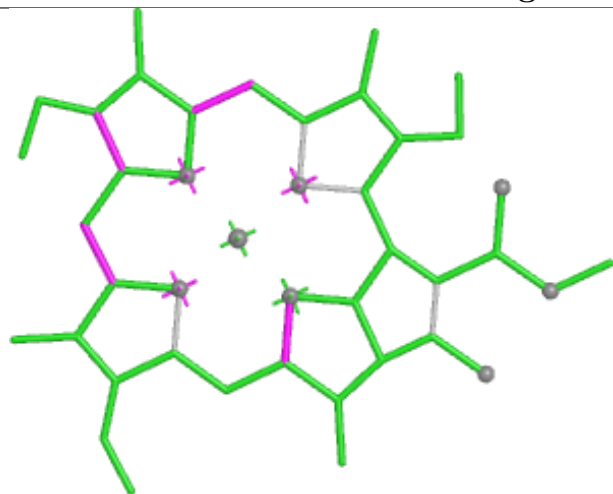


Torsions

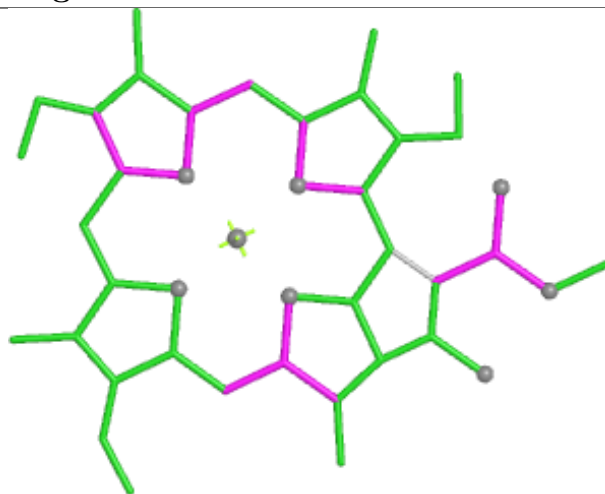


Rings

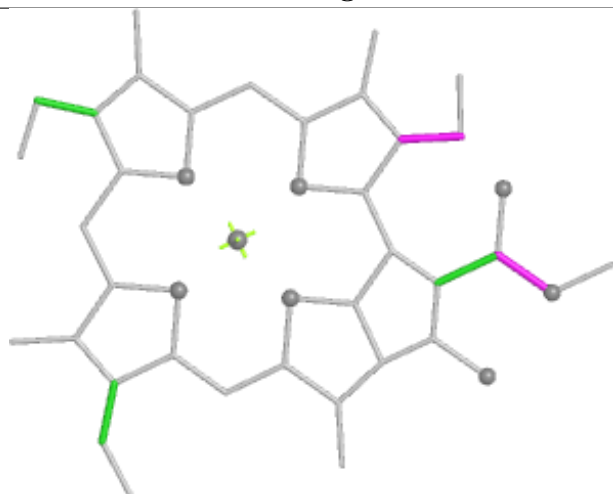
Ligand CLA g 213



Bond lengths



Bond angles

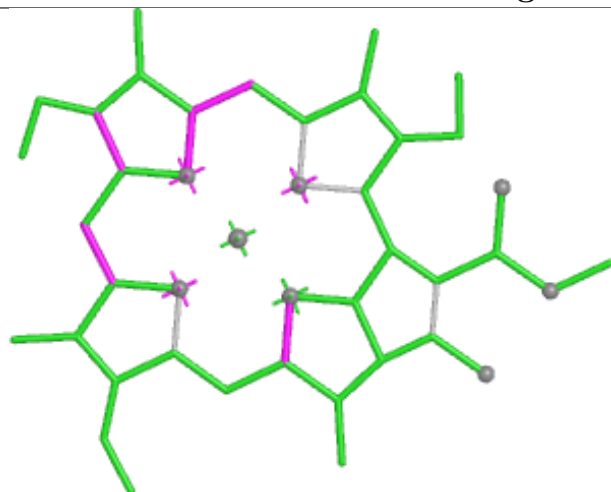


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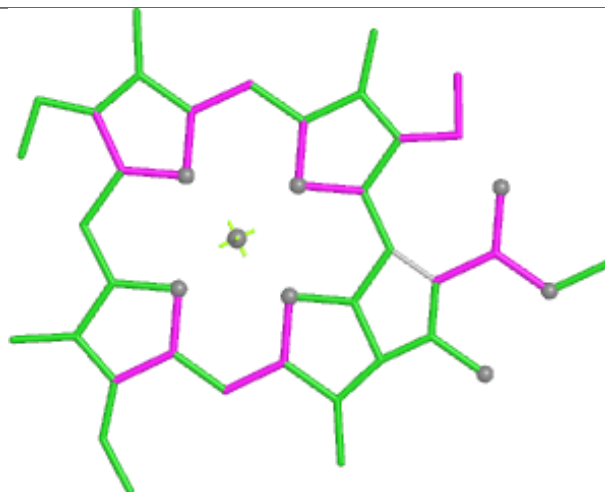


Rings

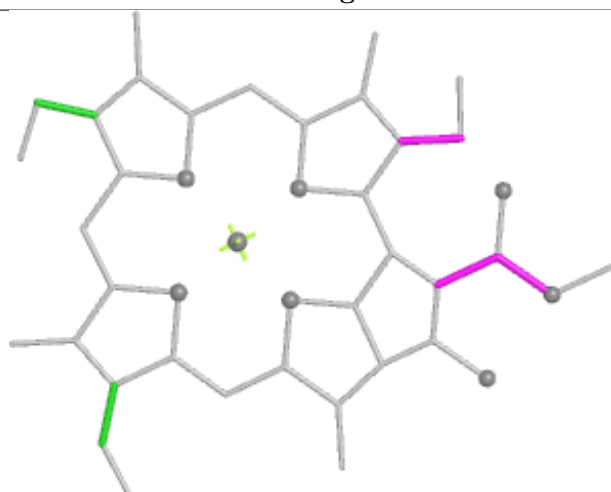
Ligand CLA b 213



Bond lengths



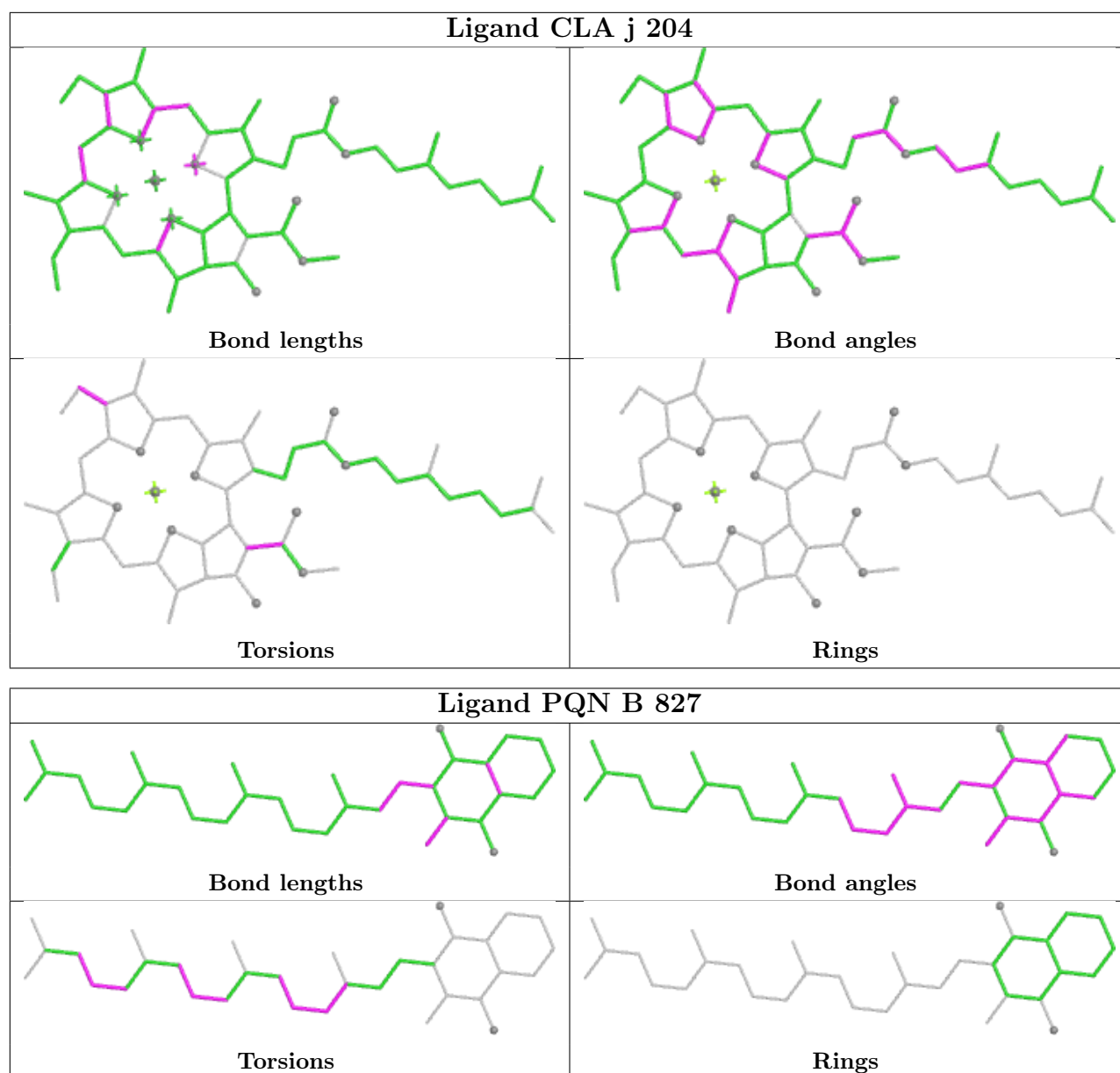
Bond angles

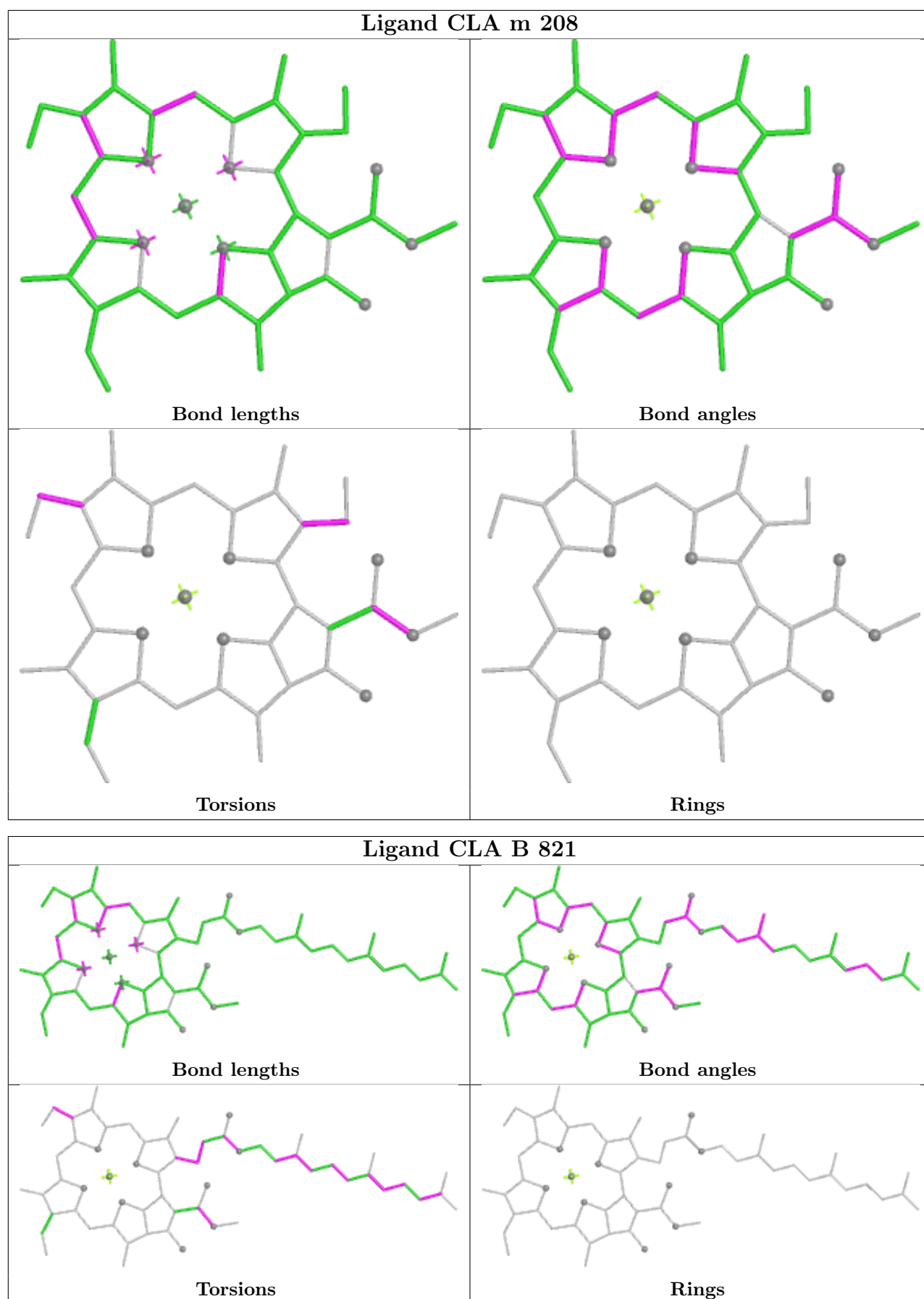


Torsions

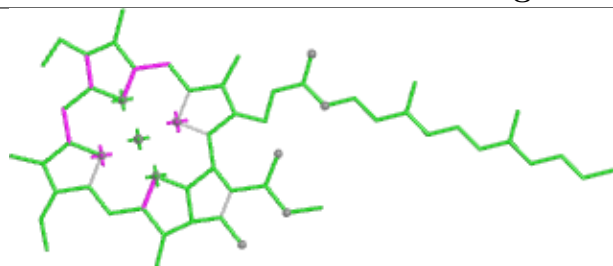


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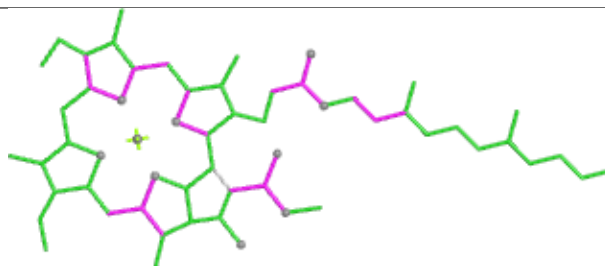




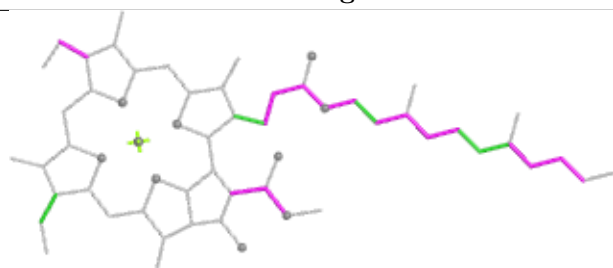
Ligand CLA A 815



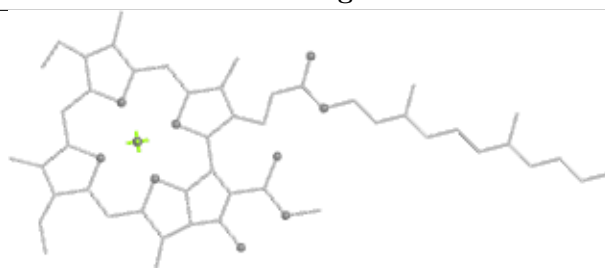
Bond lengths



Bond angles

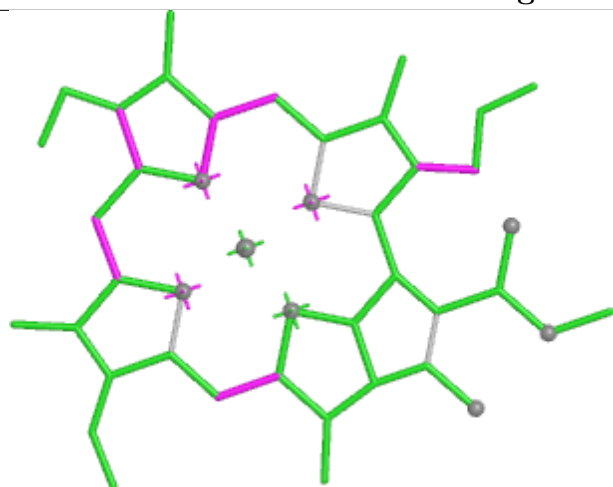


Torsions

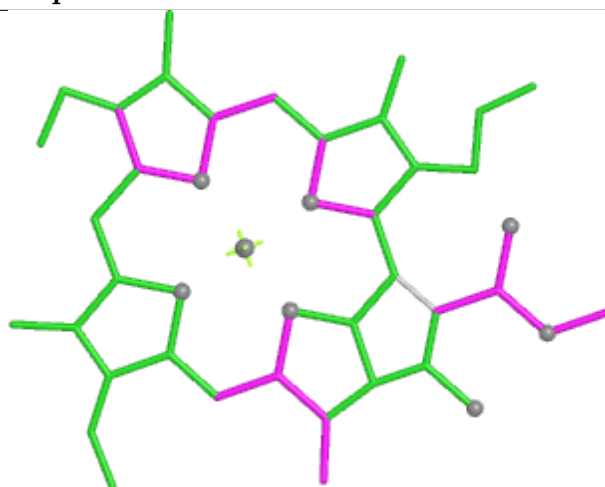


Rings

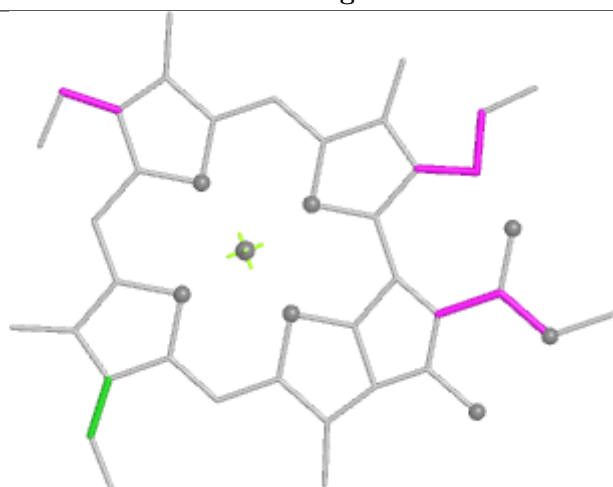
Ligand CLA p 602



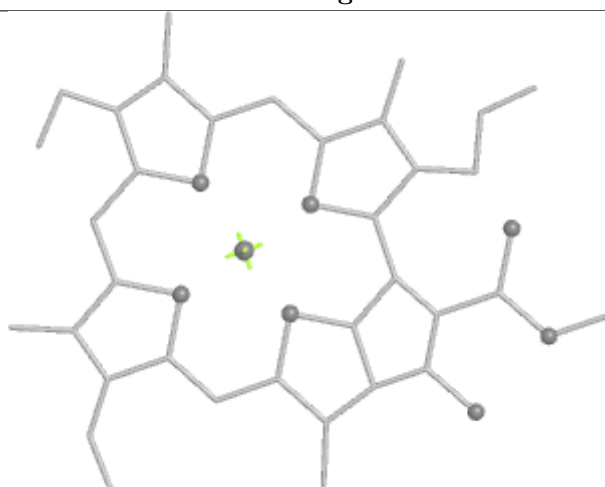
Bond lengths



Bond angles

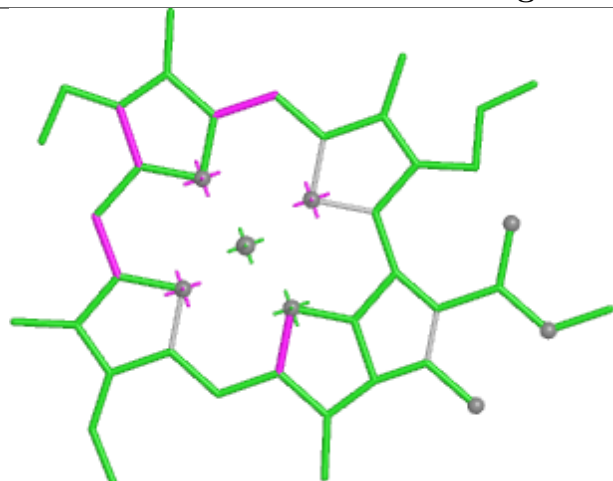


Torsions

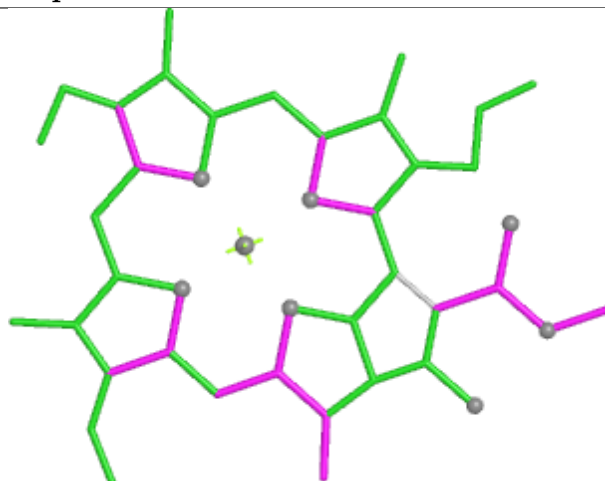


Rings

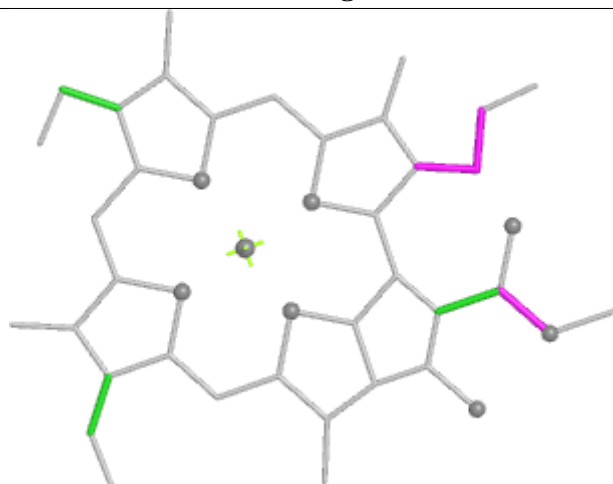
Ligand CLA p 609



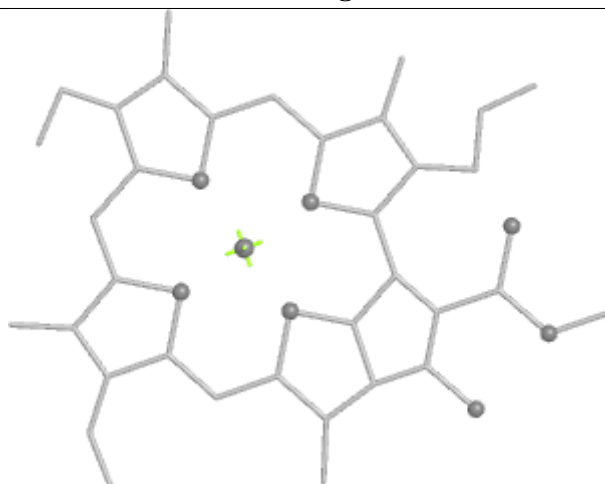
Bond lengths



Bond angles

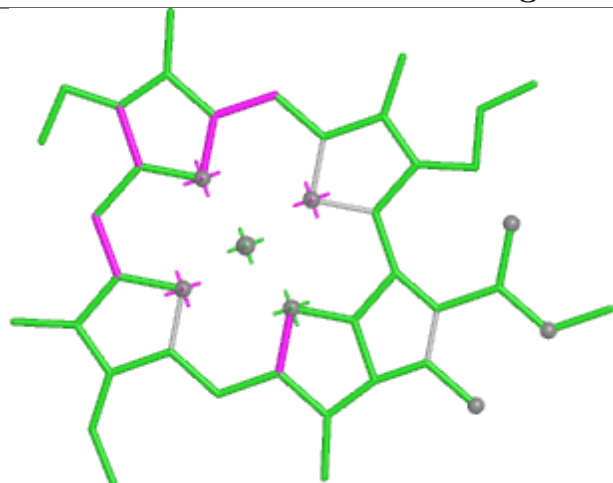


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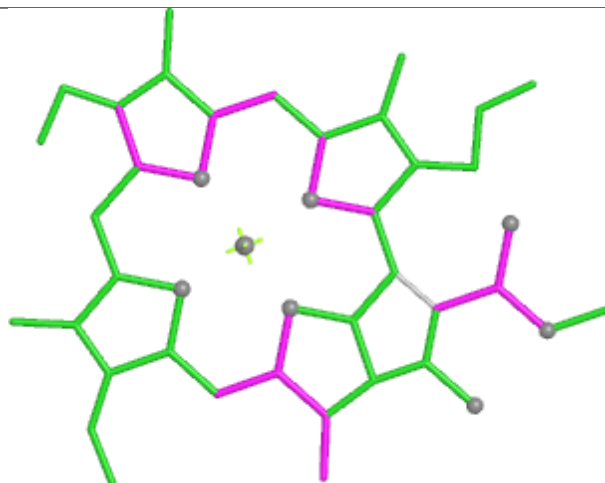


Rings

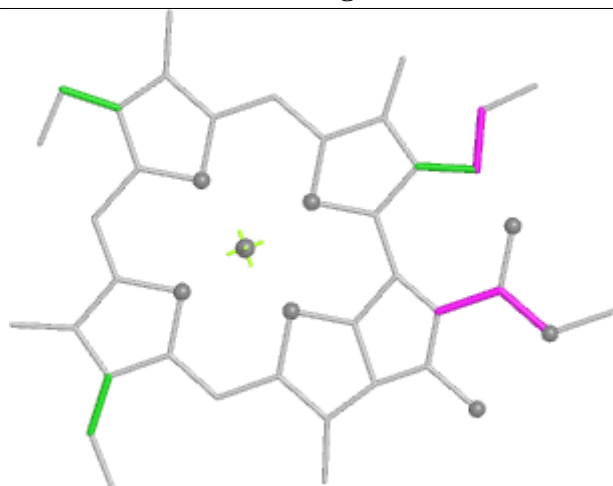
Ligand CLA c 312



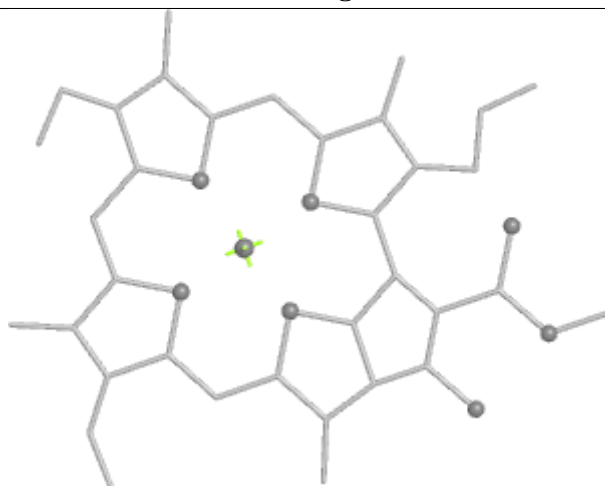
Bond lengths



Bond angles

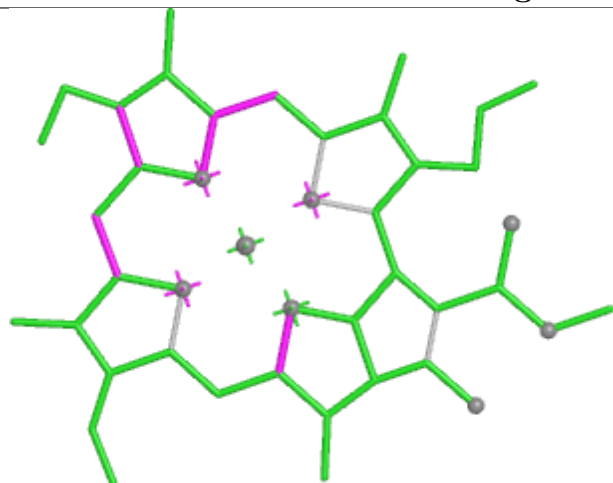


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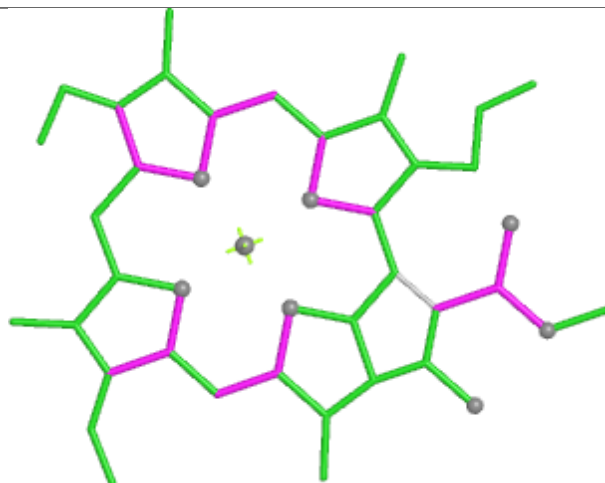


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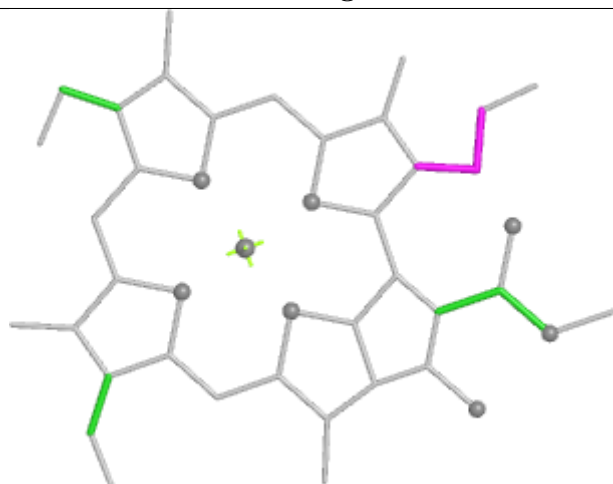
Ligand CLA B 810



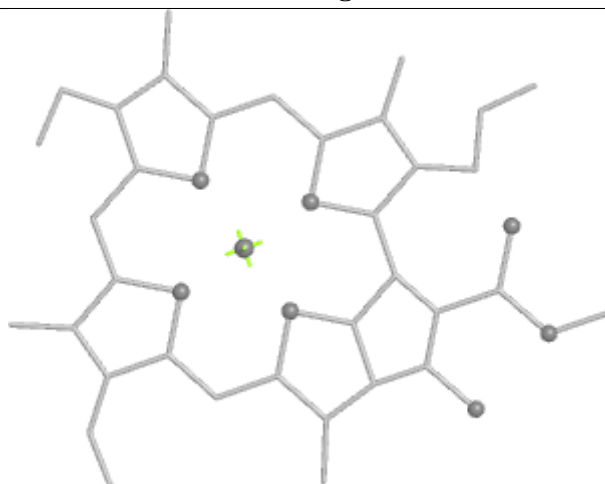
Bond lengths



Bond angles

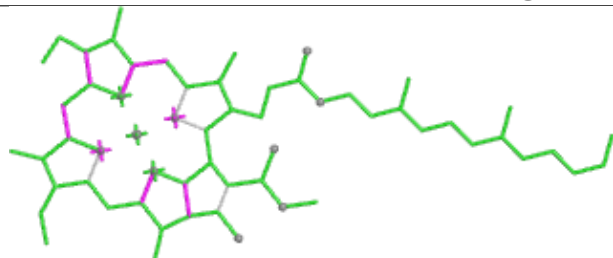


Torsions

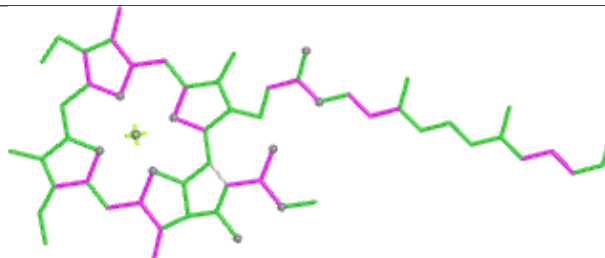


Rings

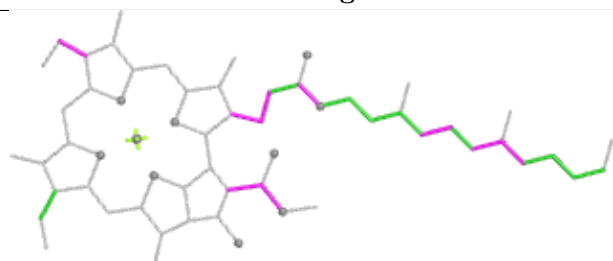
Ligand CLA c 303



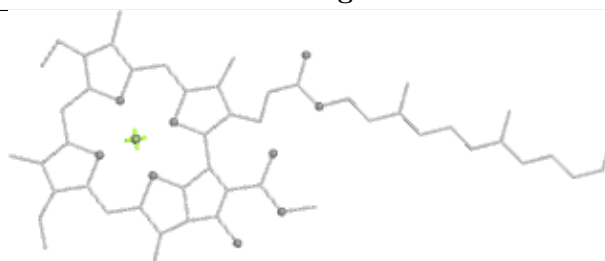
Bond lengths



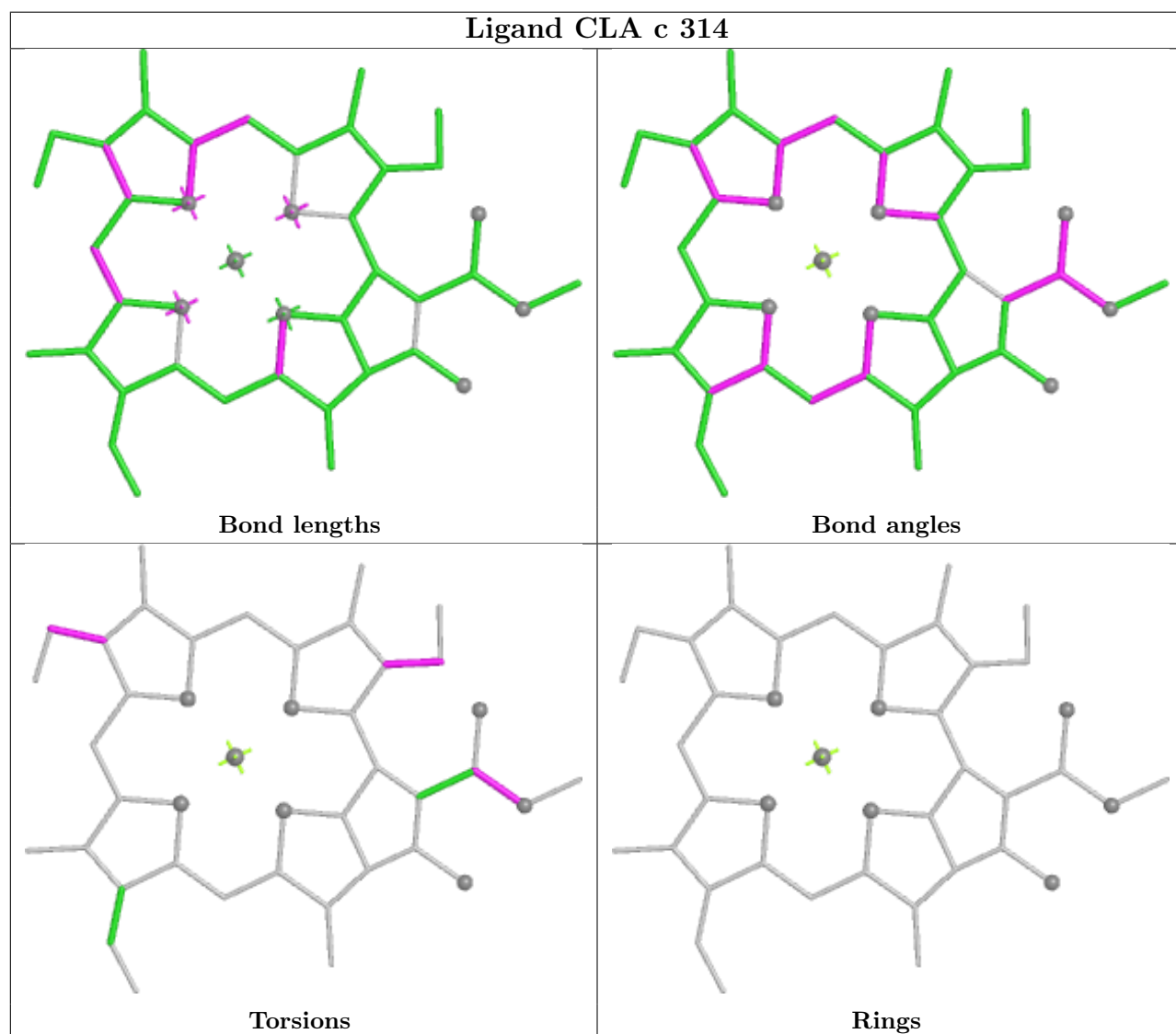
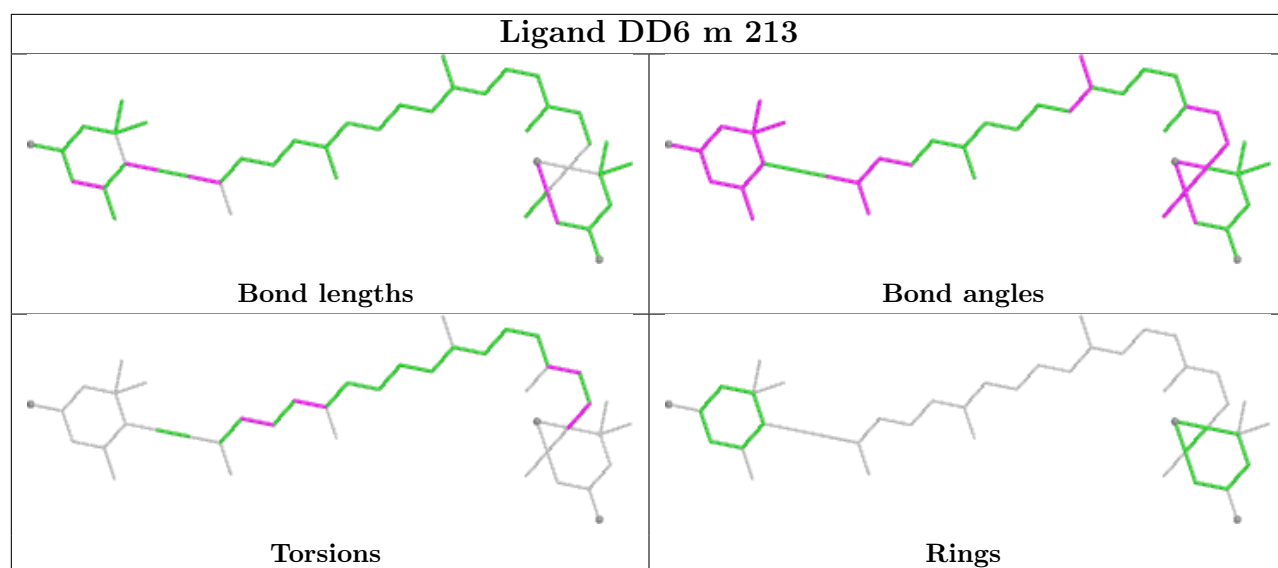
Bond angles



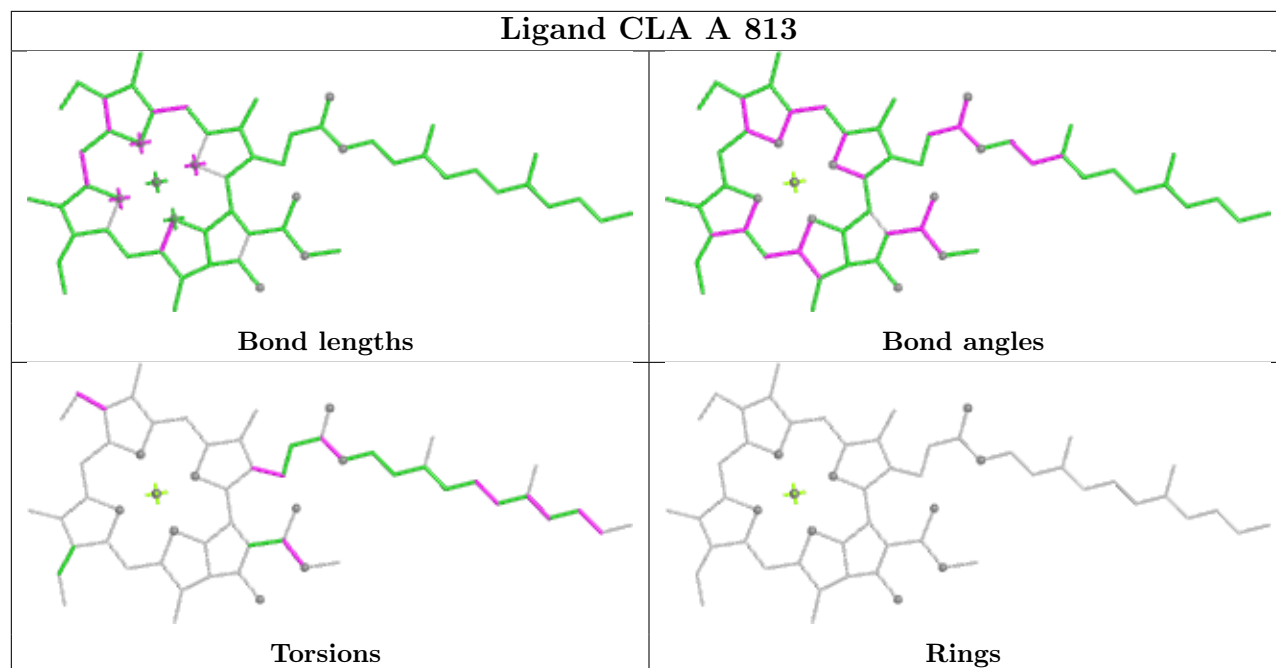
Torsions



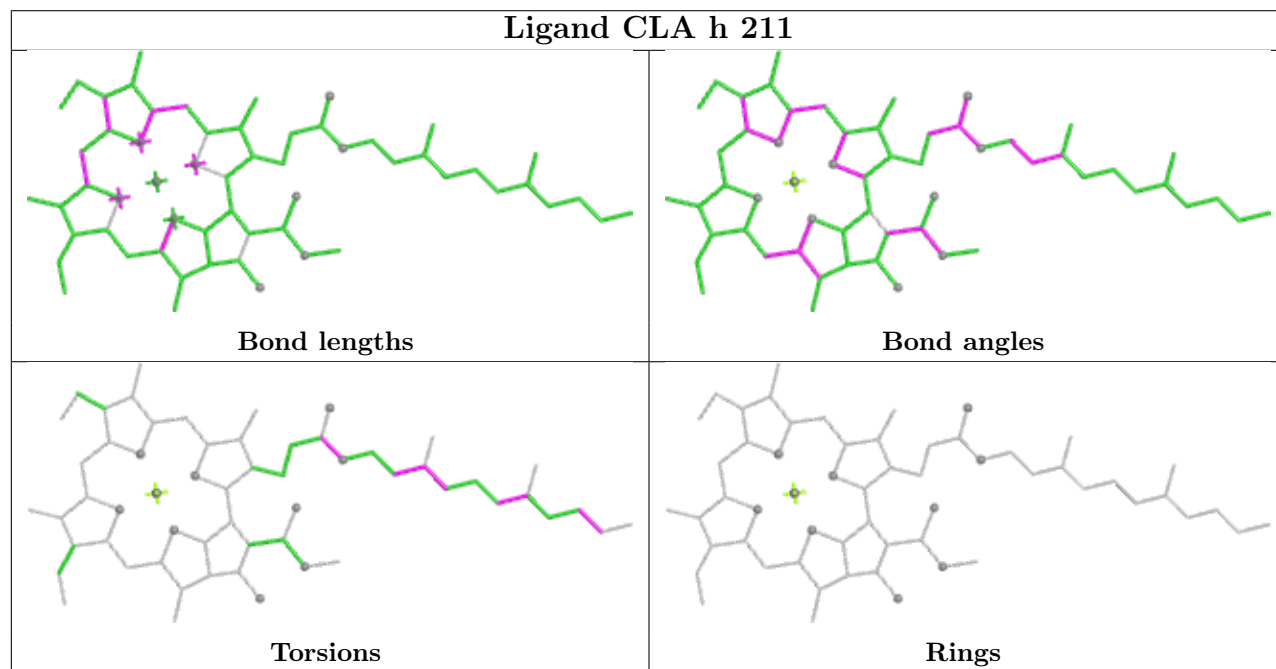
Rings

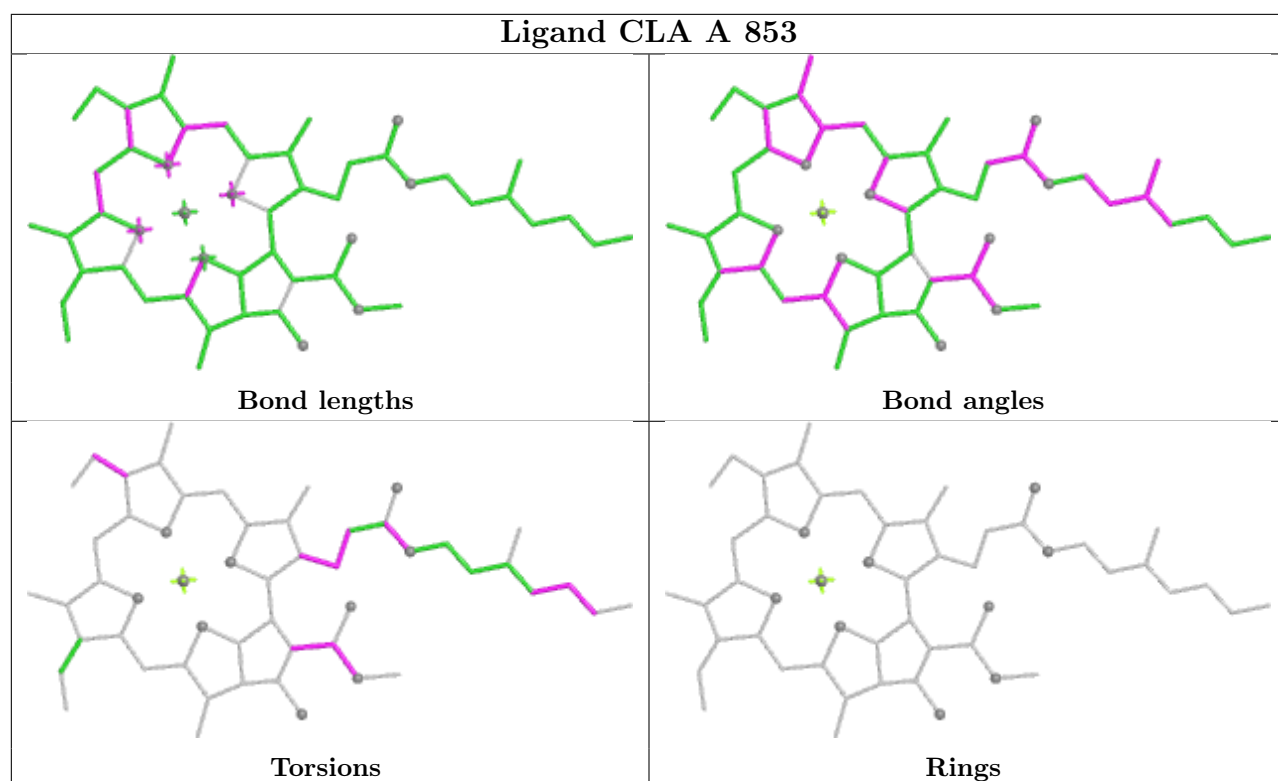


Ligand CLA A 813

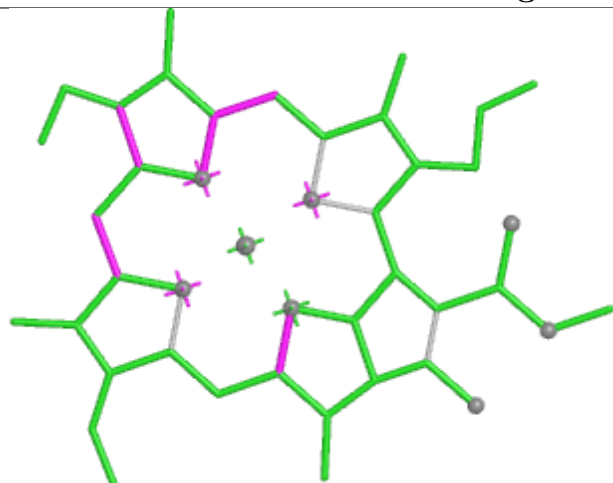


Ligand CLA h 211

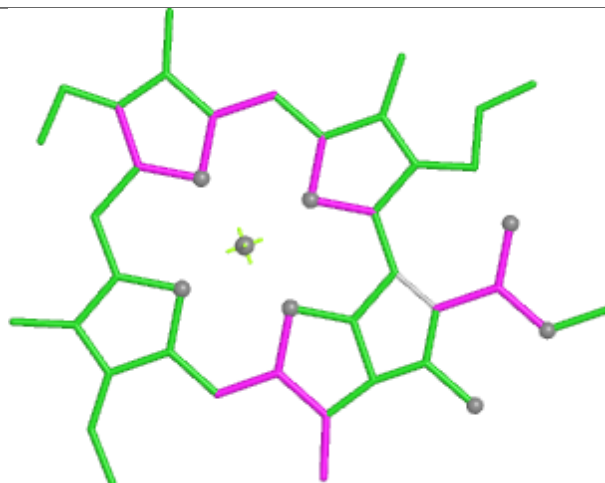




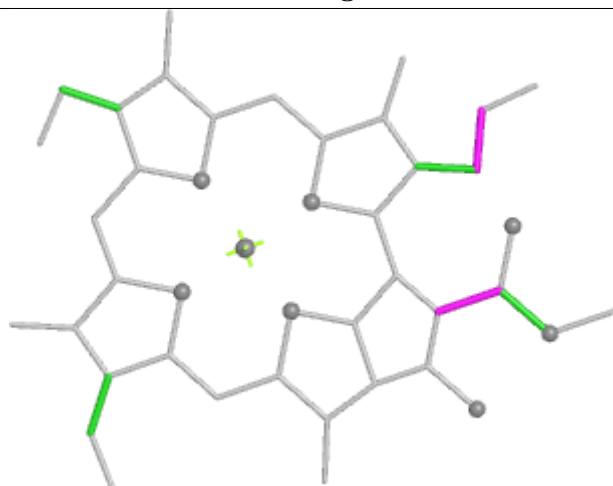
Ligand CLA k 210



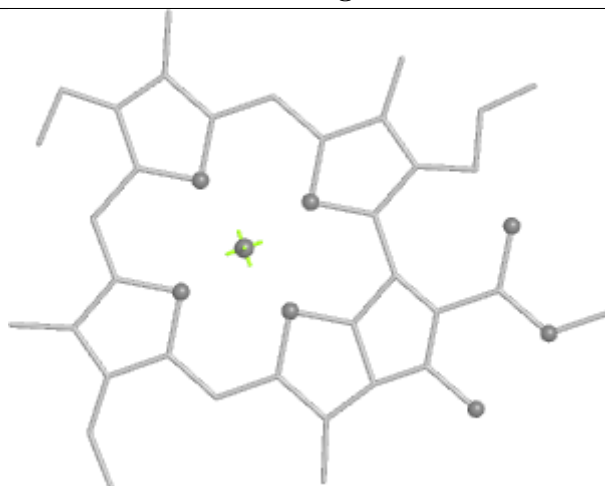
Bond lengths



Bond angles

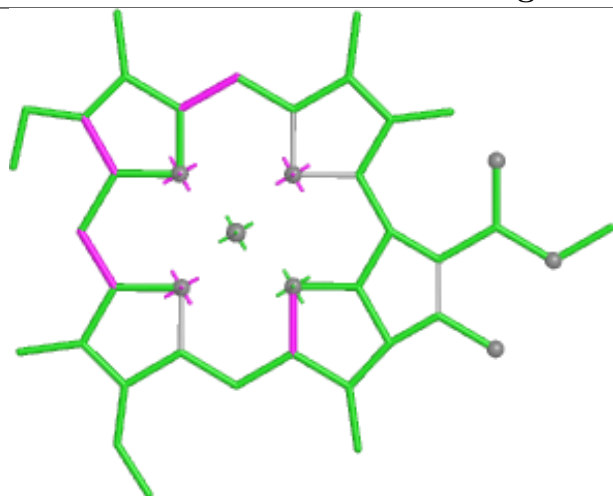


Torsions



Rings

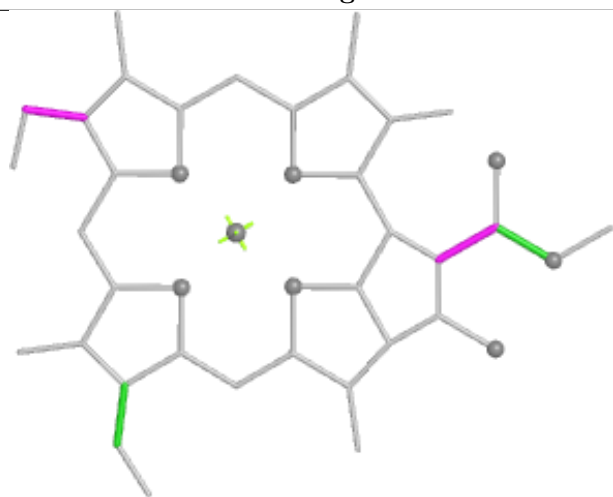
Ligand CLA n 209



Bond lengths



Bond angles

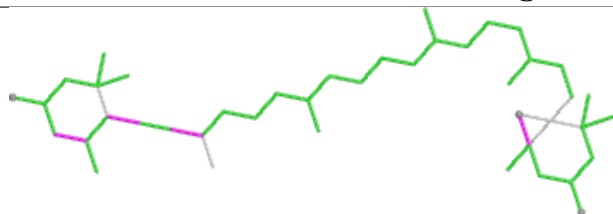


Torsions

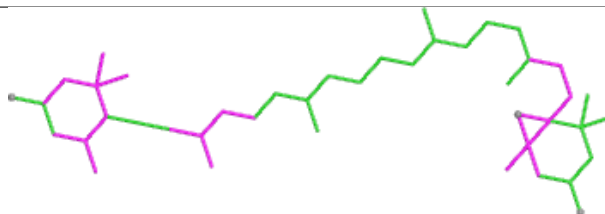


Rings

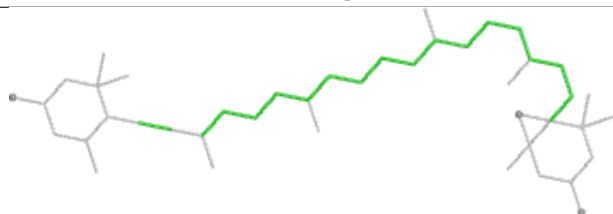
Ligand DD6 h 217



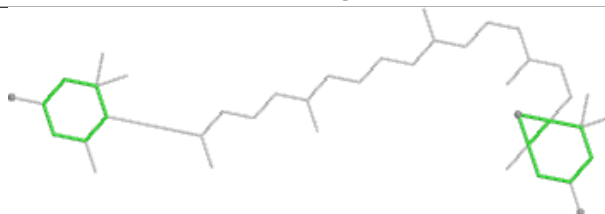
Bond lengths



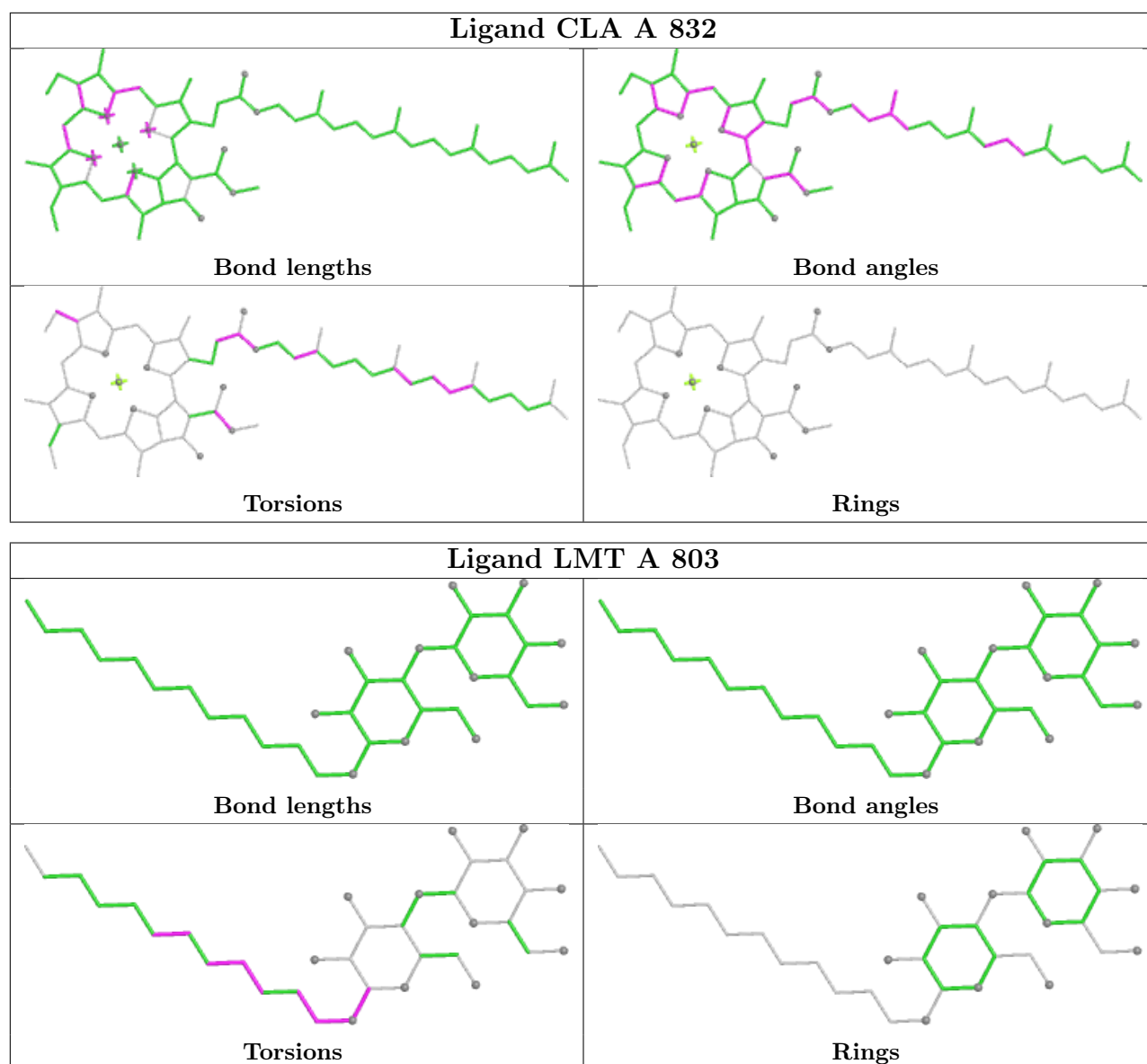
Bond angles

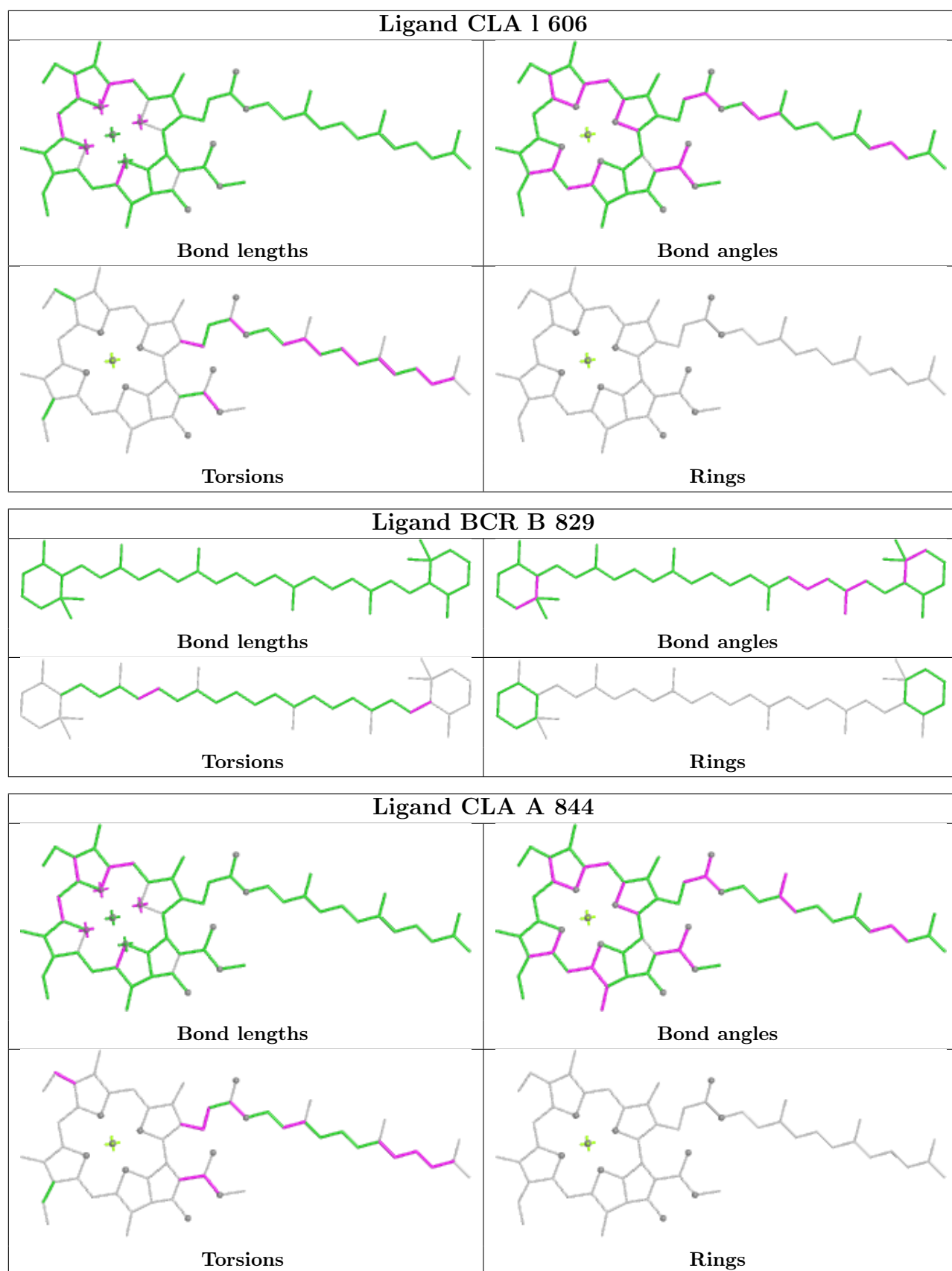


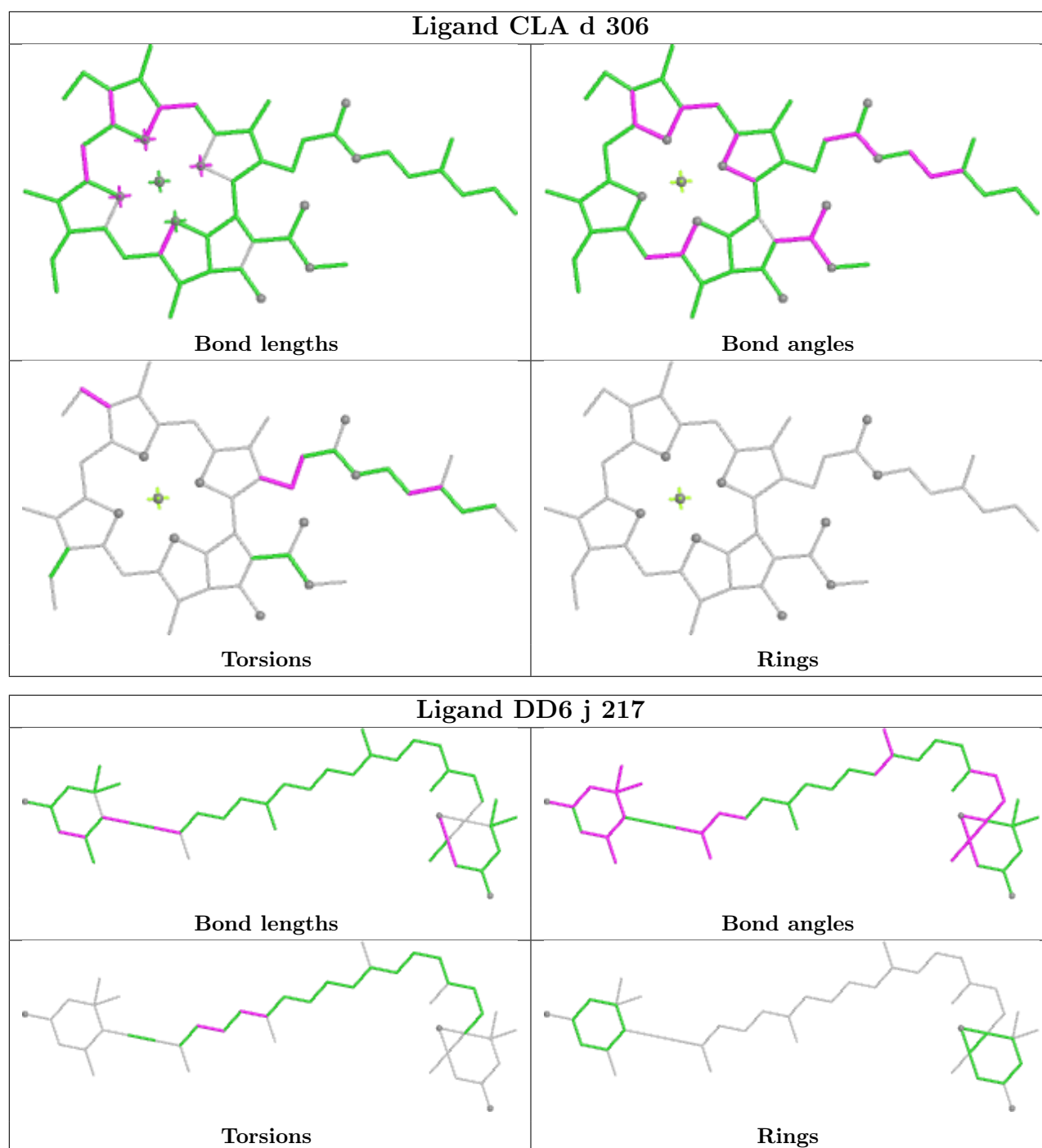
Torsions

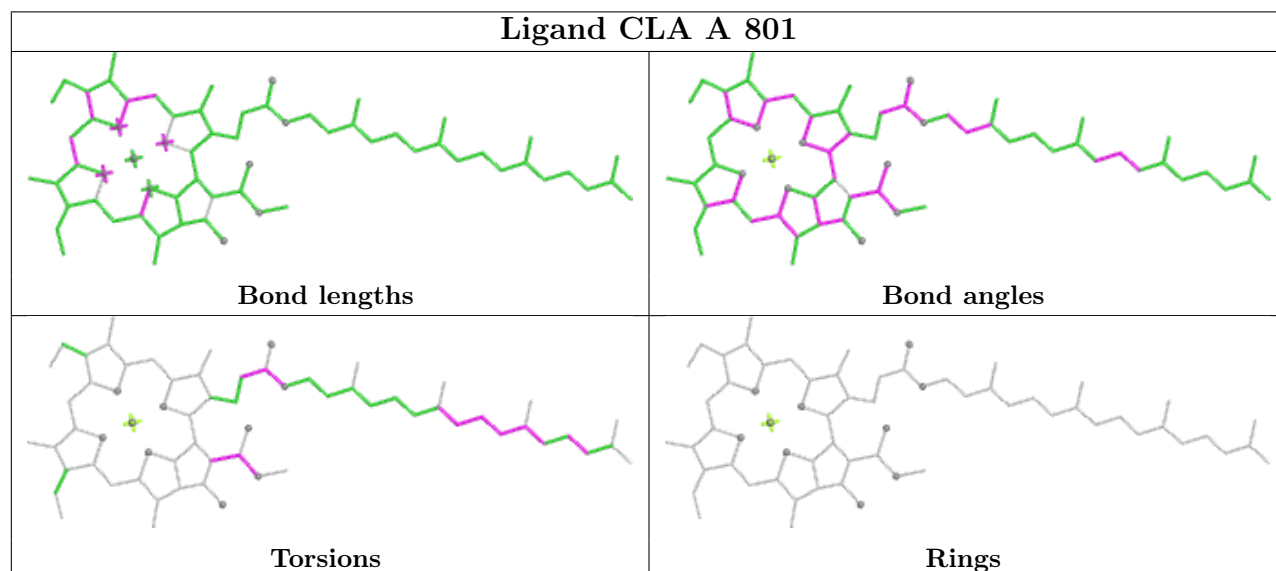
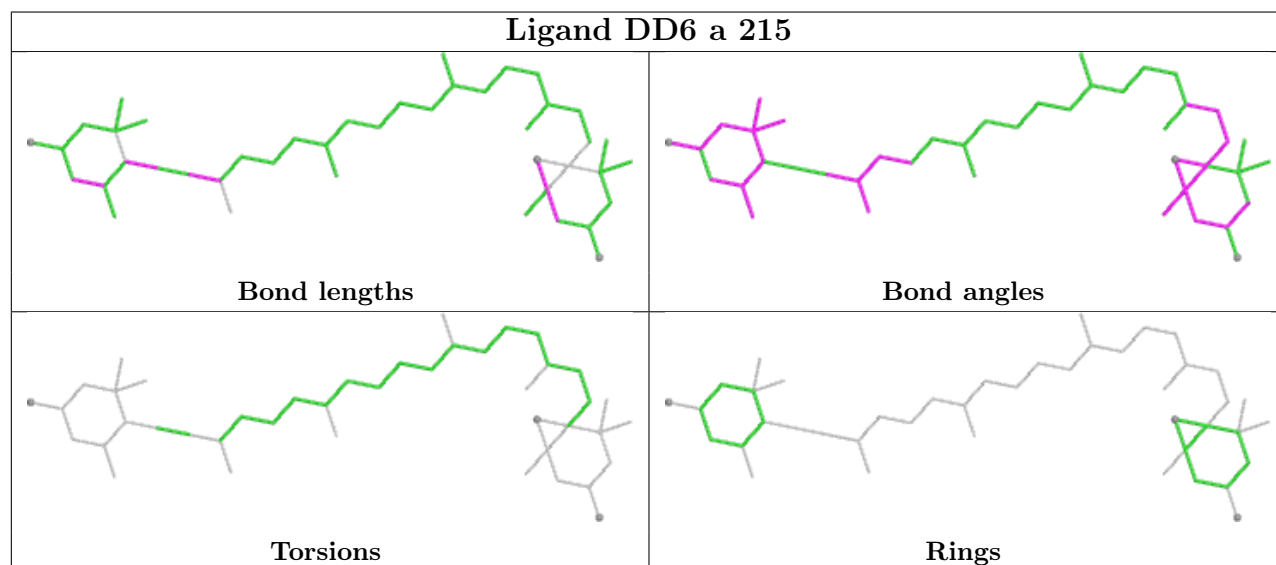
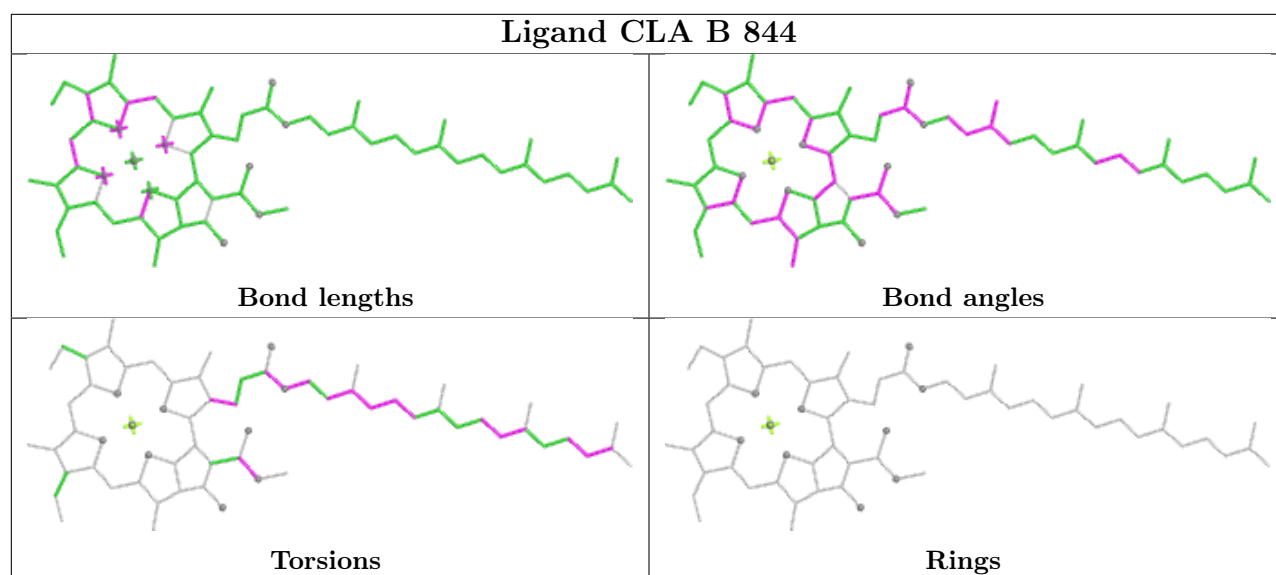


Rings

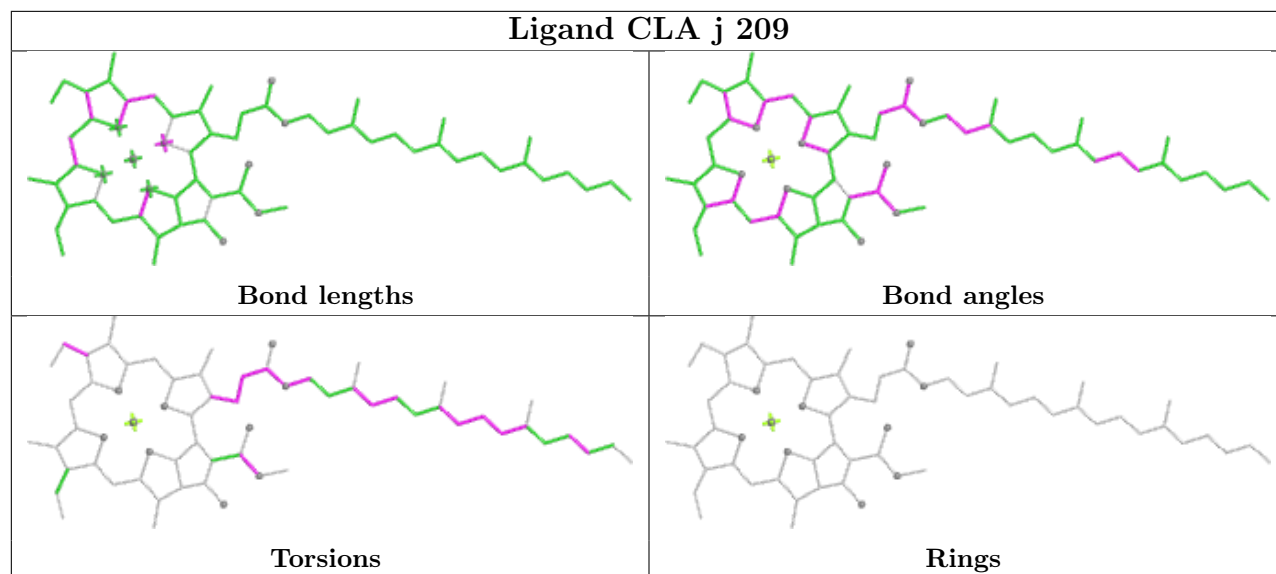




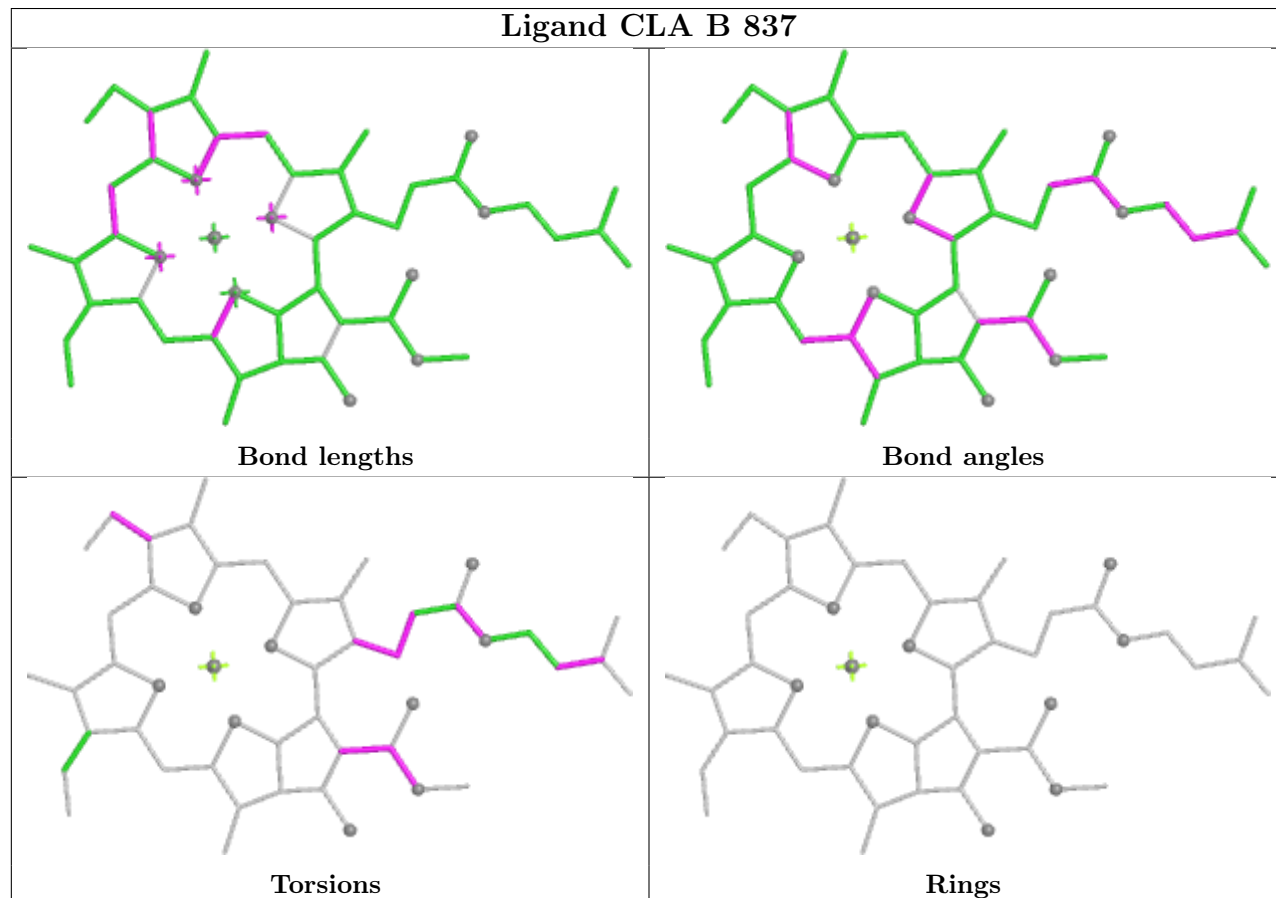


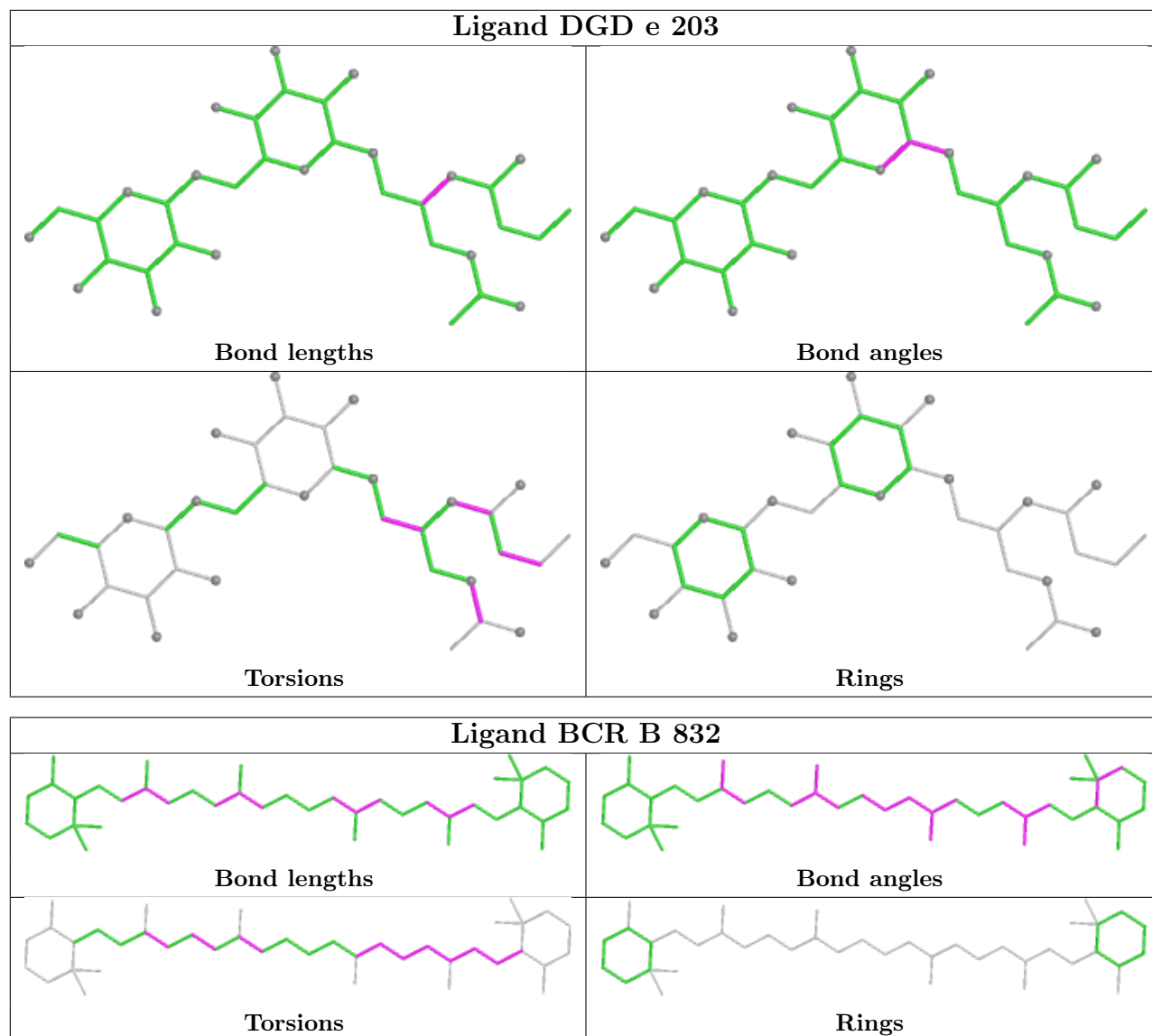


Ligand CLA j 209

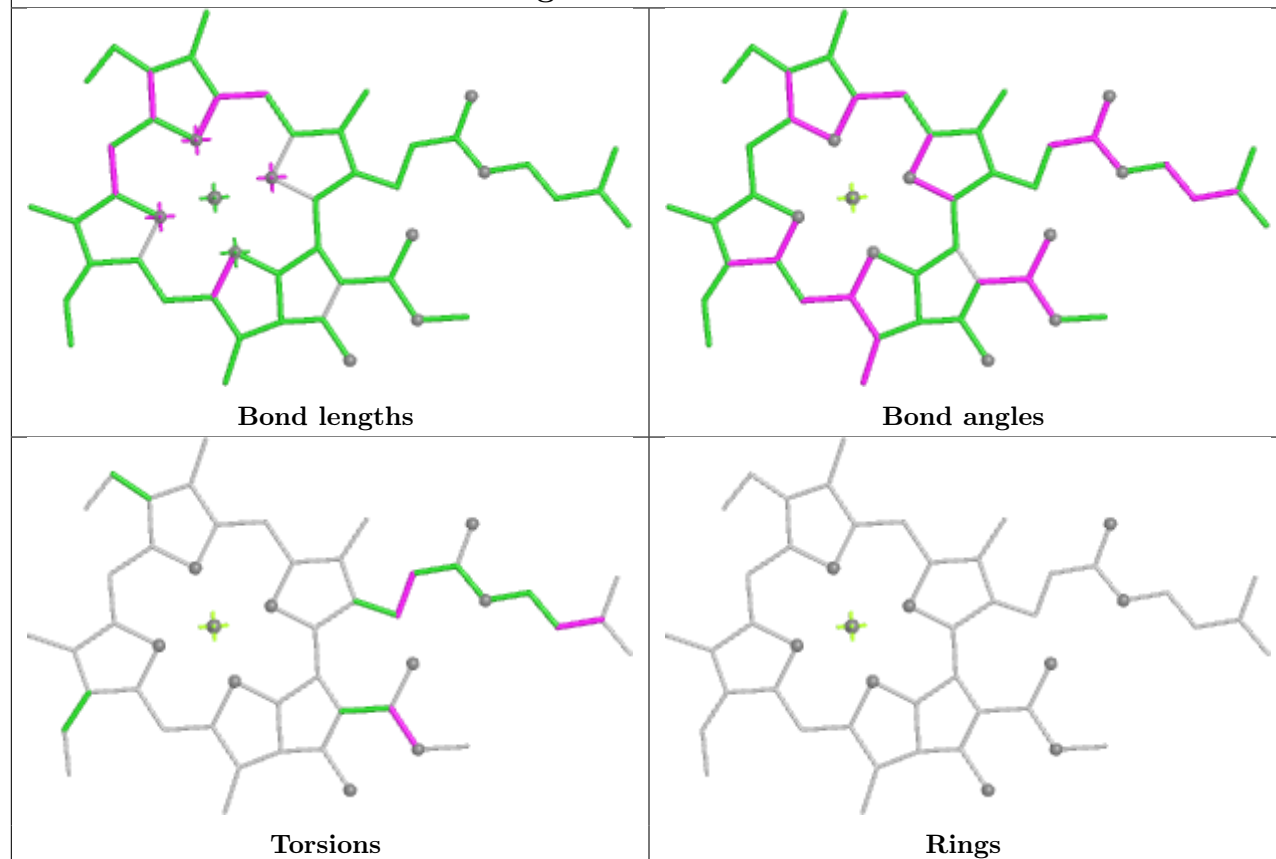


Ligand CLA B 837

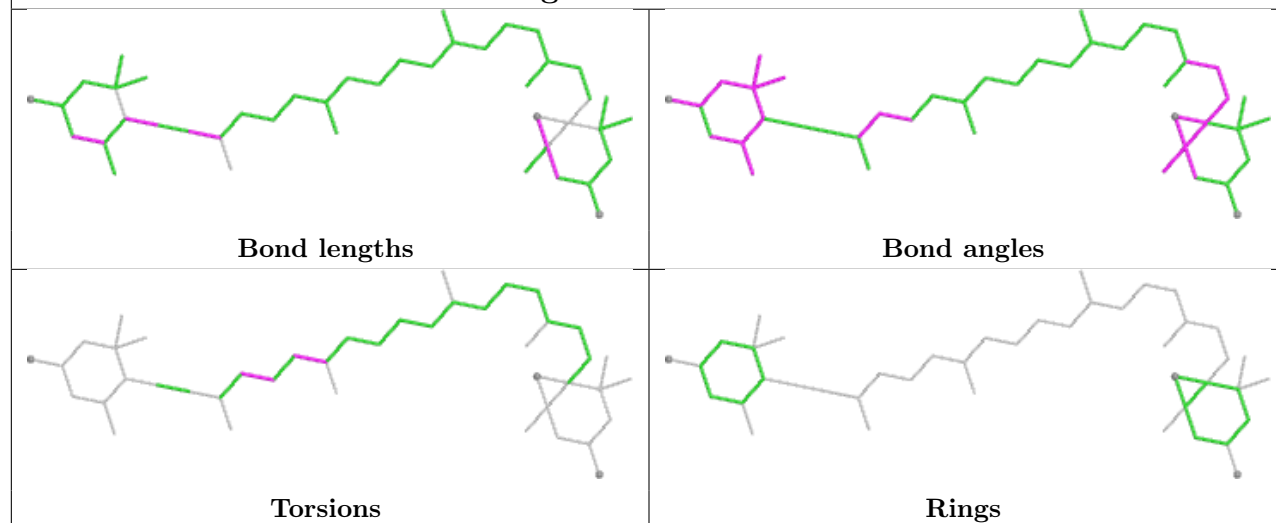


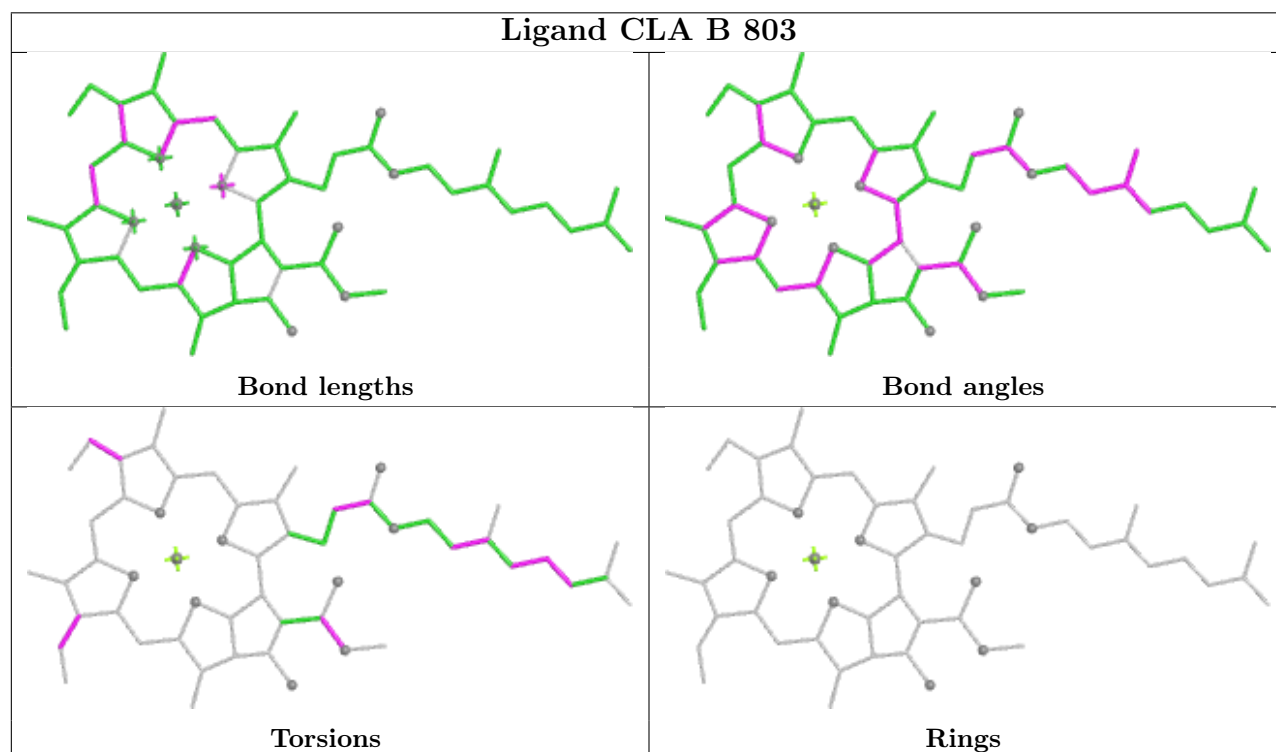
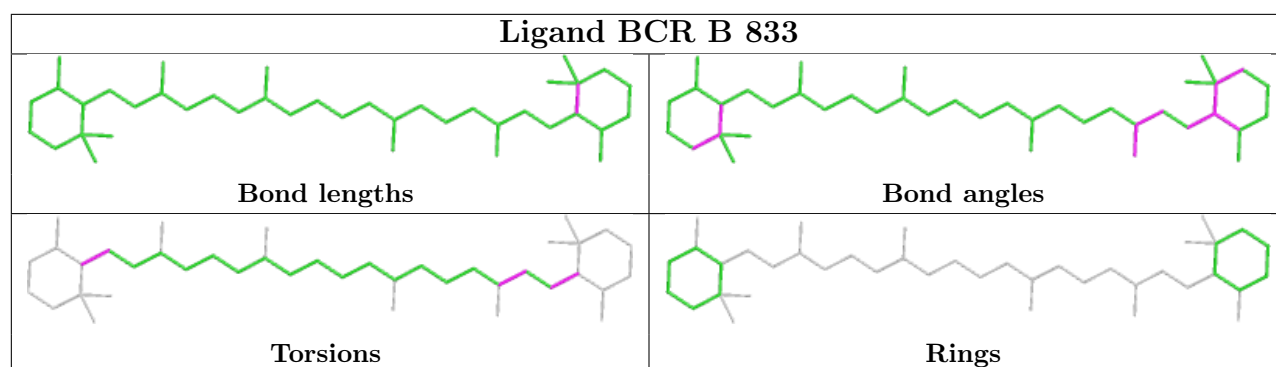


Ligand CLA e 207

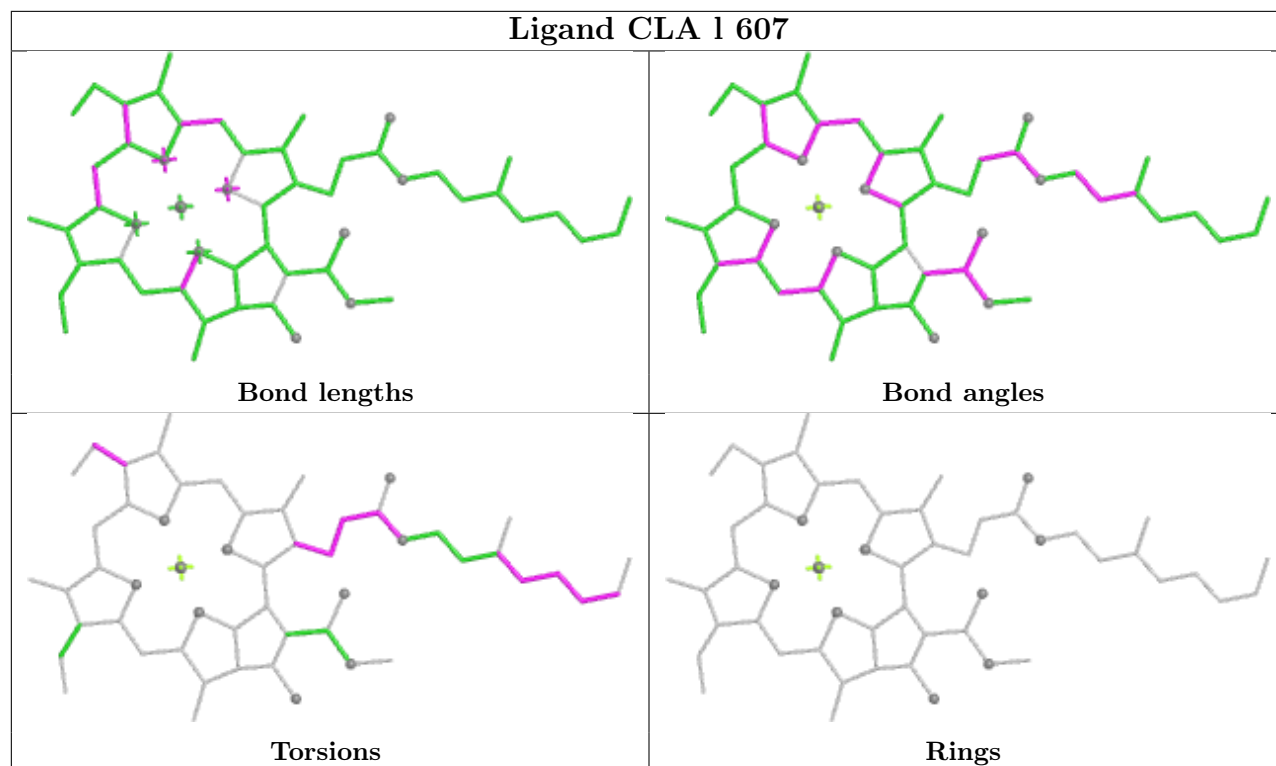


Ligand DD6 i 215

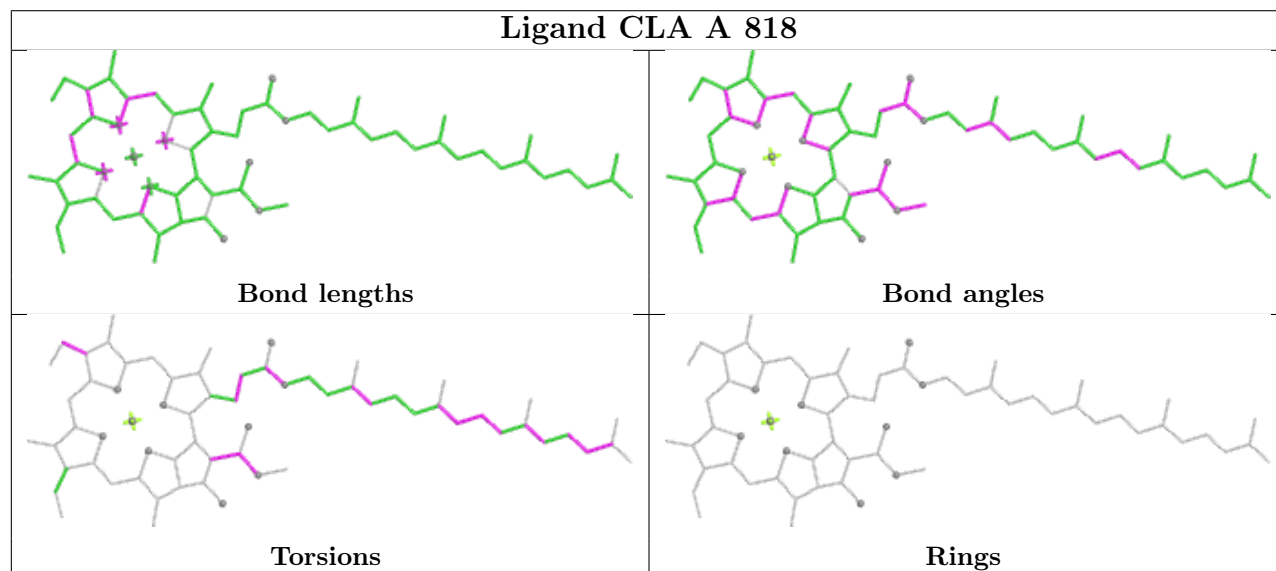




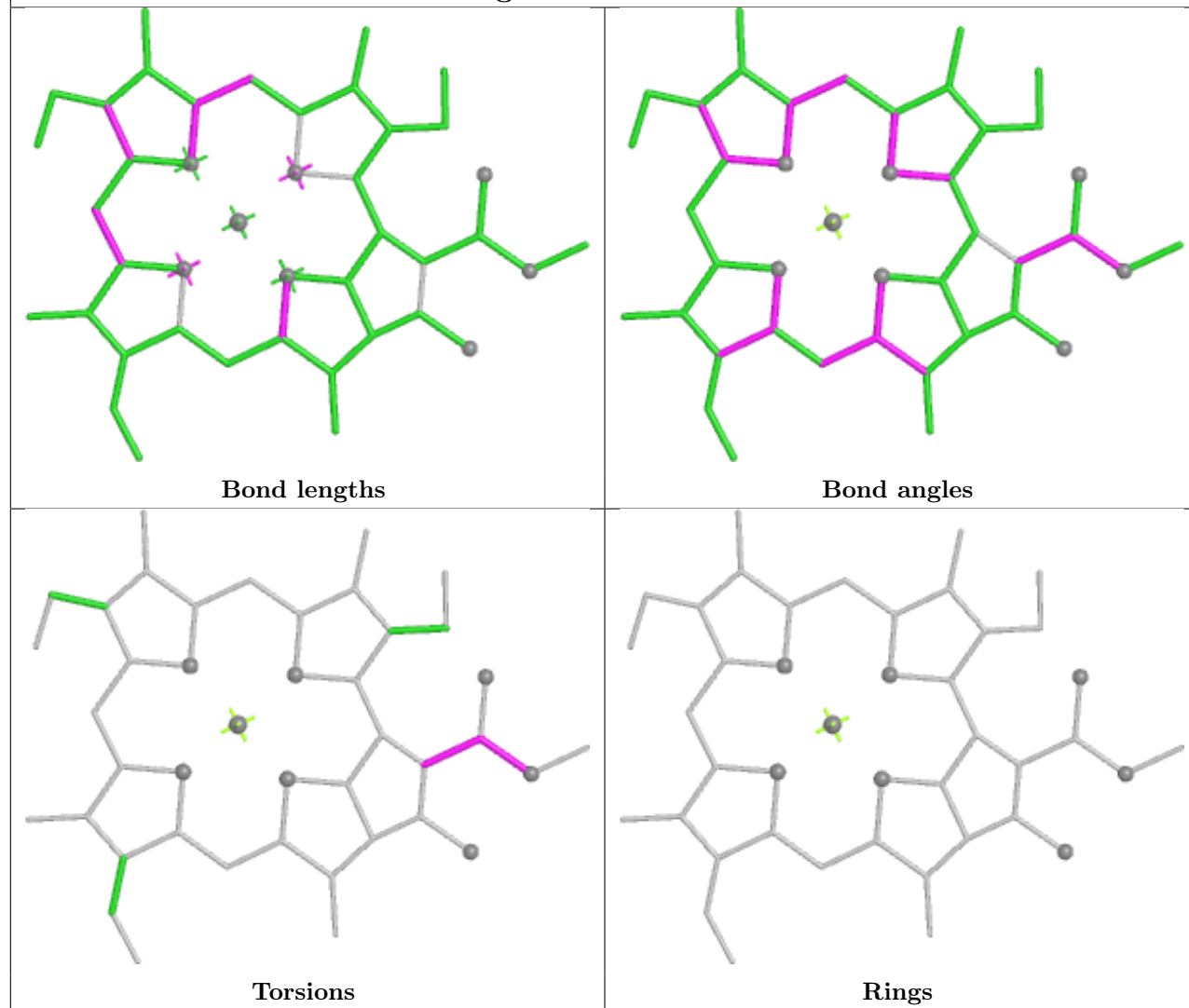
Ligand CLA I 607



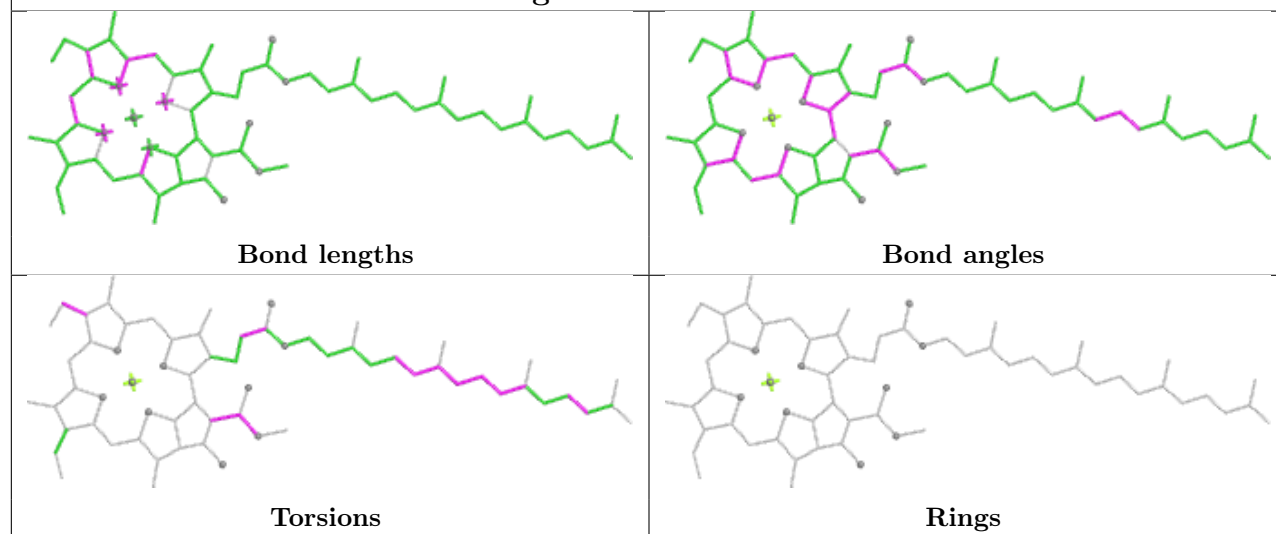
Ligand CLA A 818

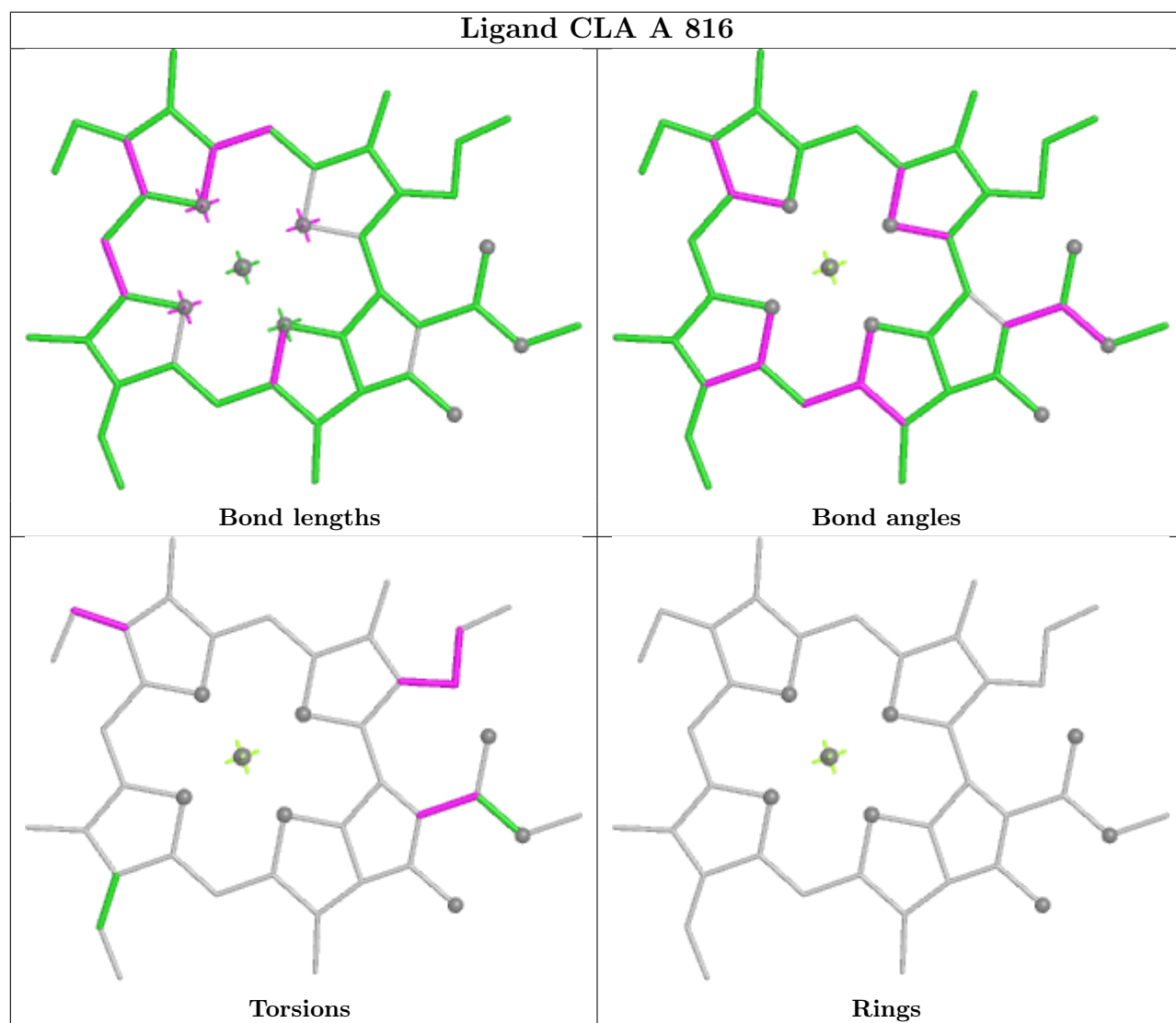
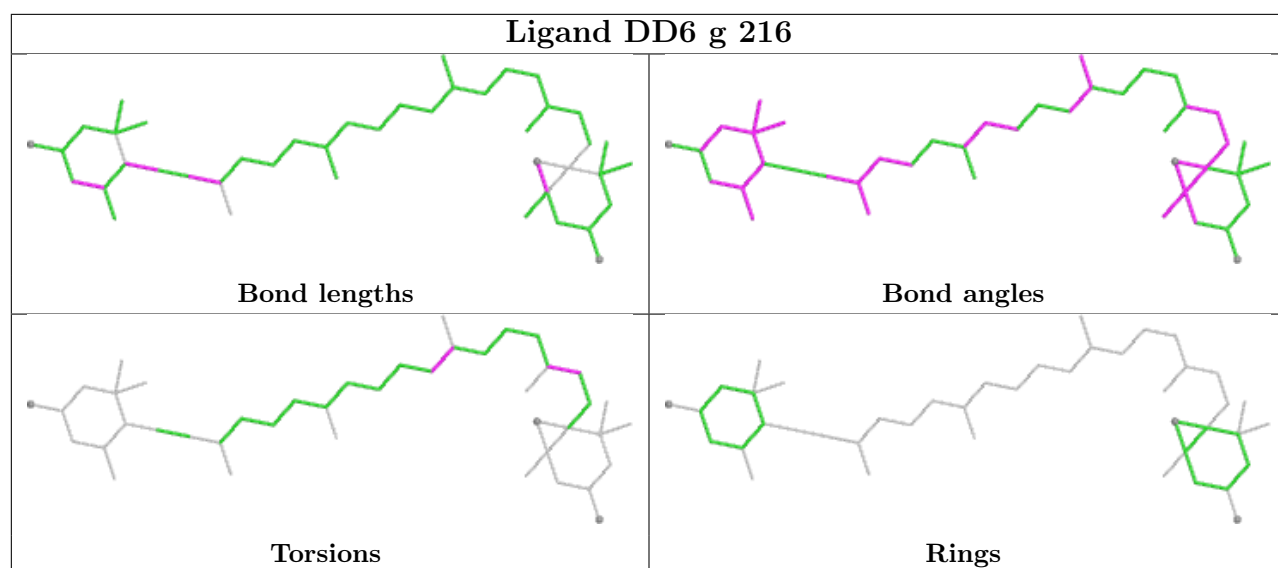


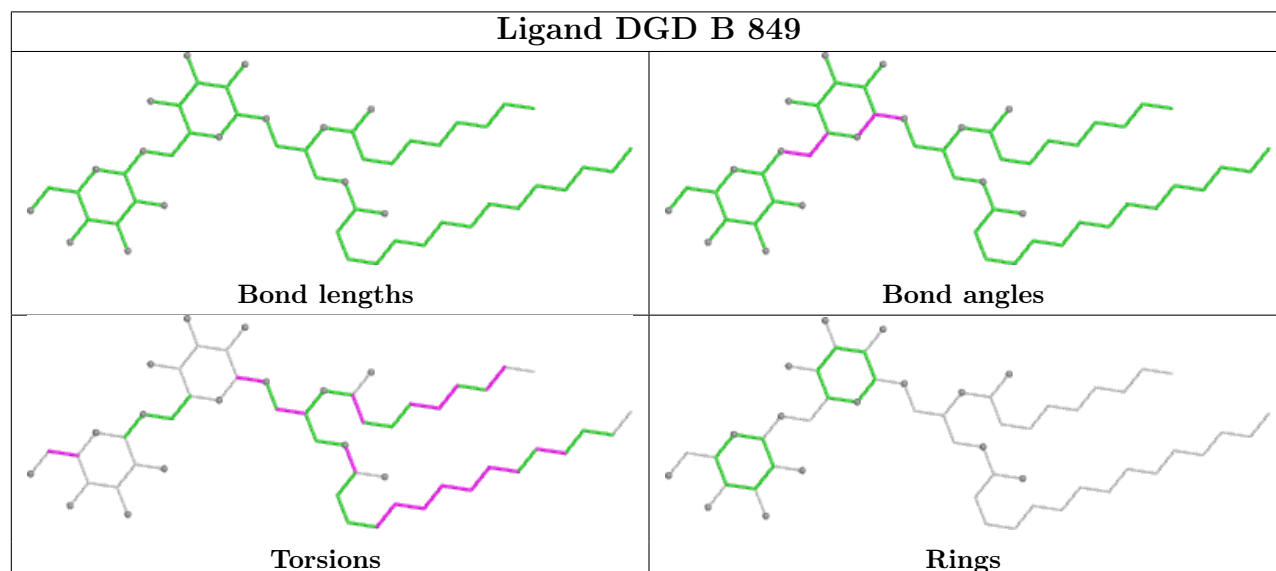
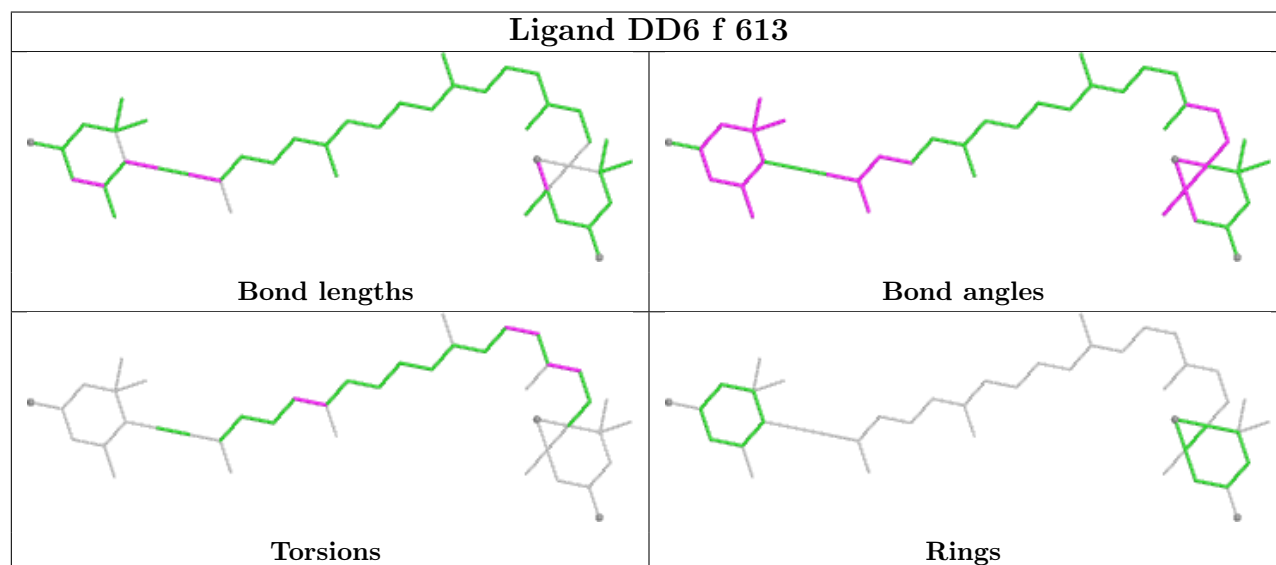
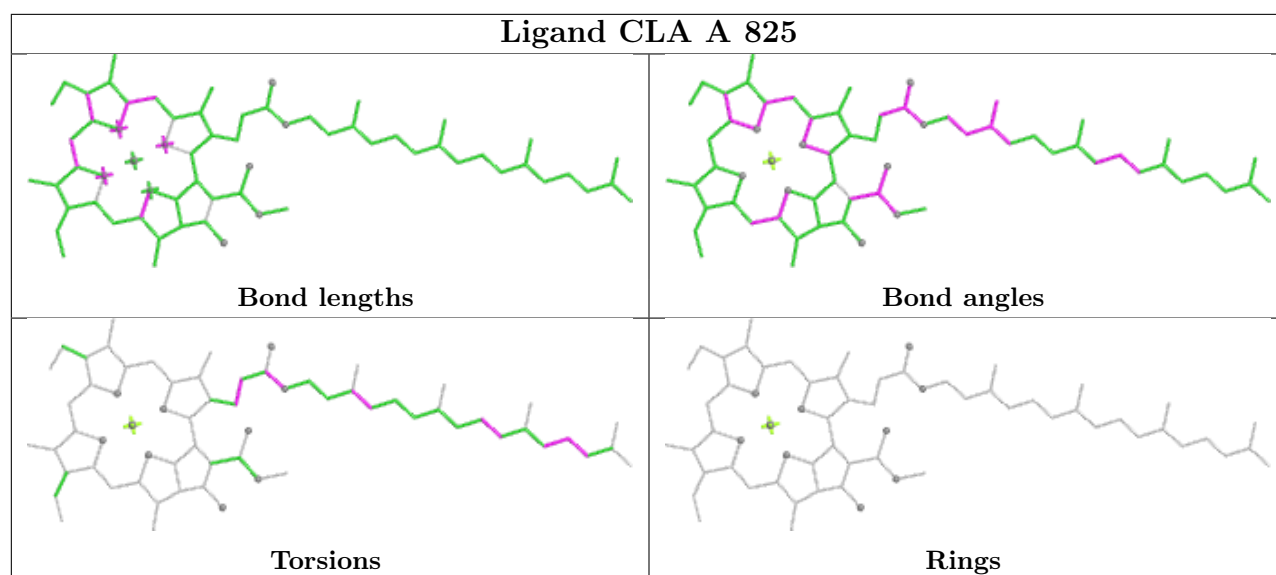
Ligand CLA B 809

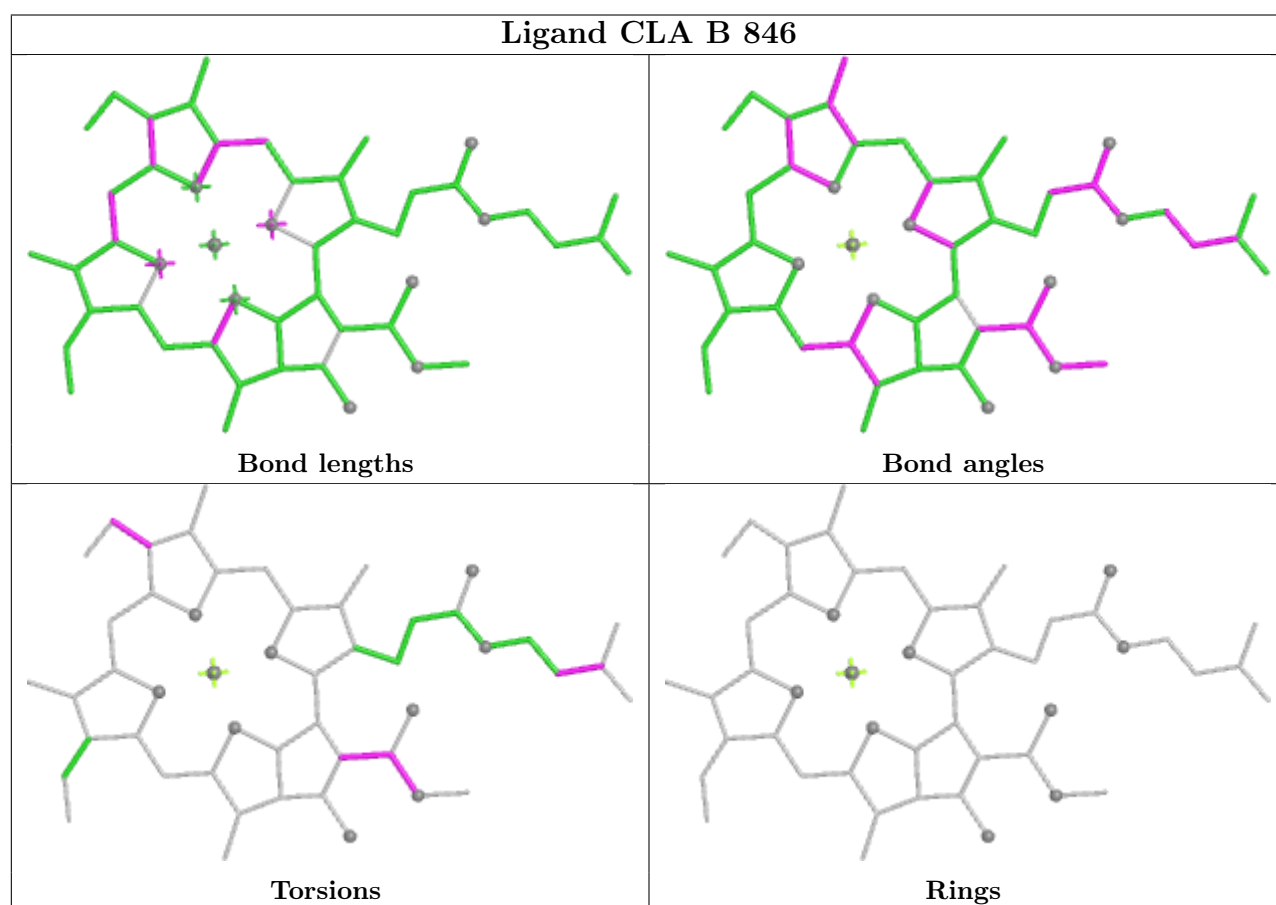
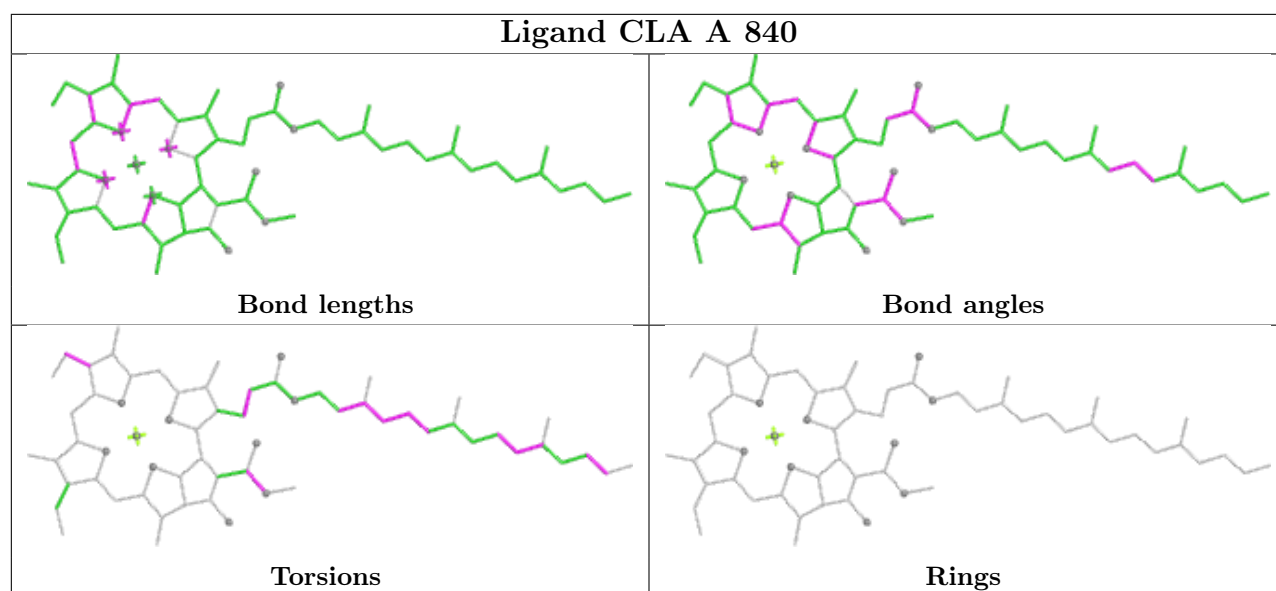


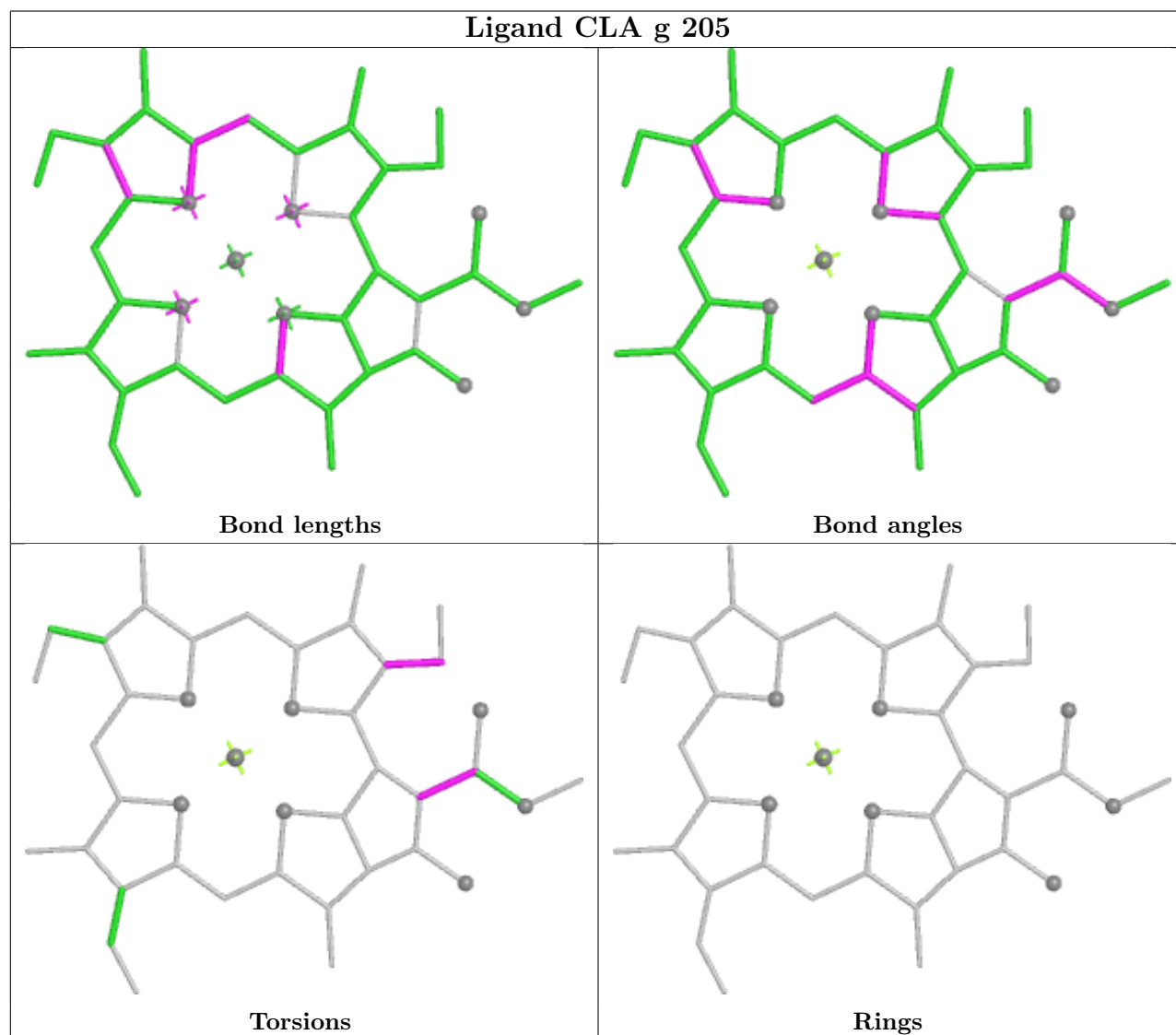
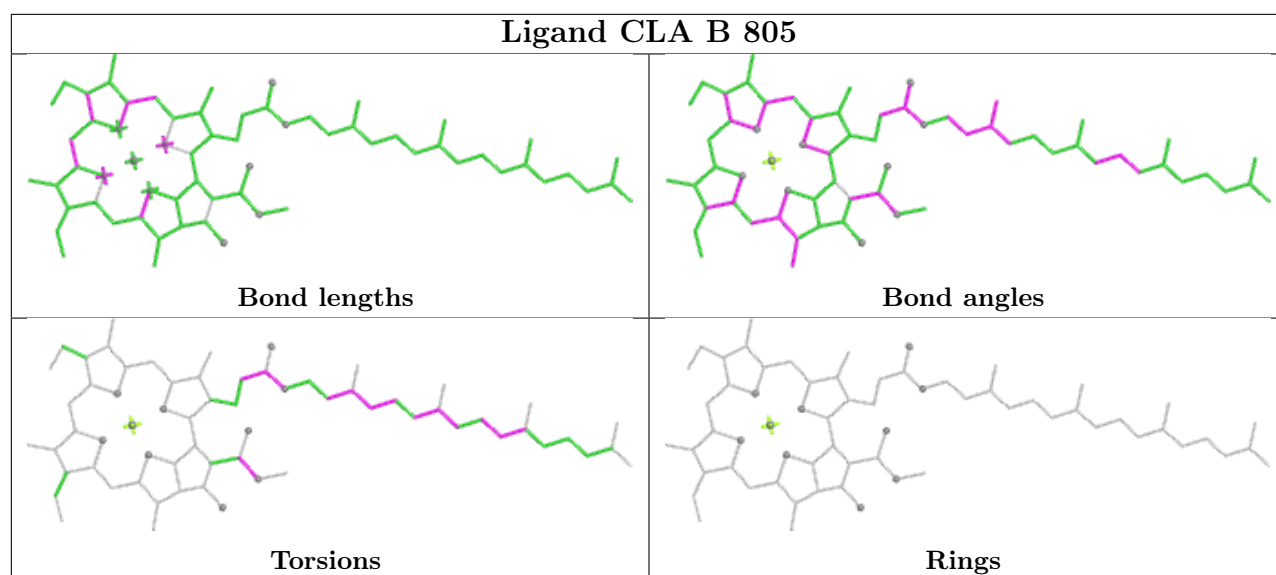
Ligand CLA B 819

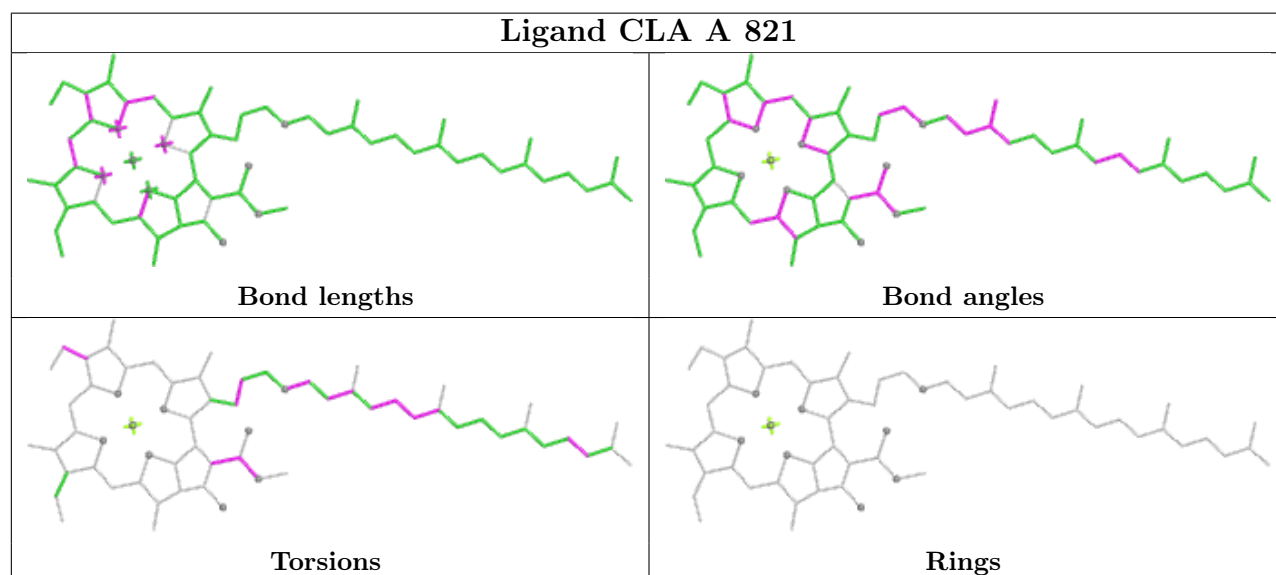
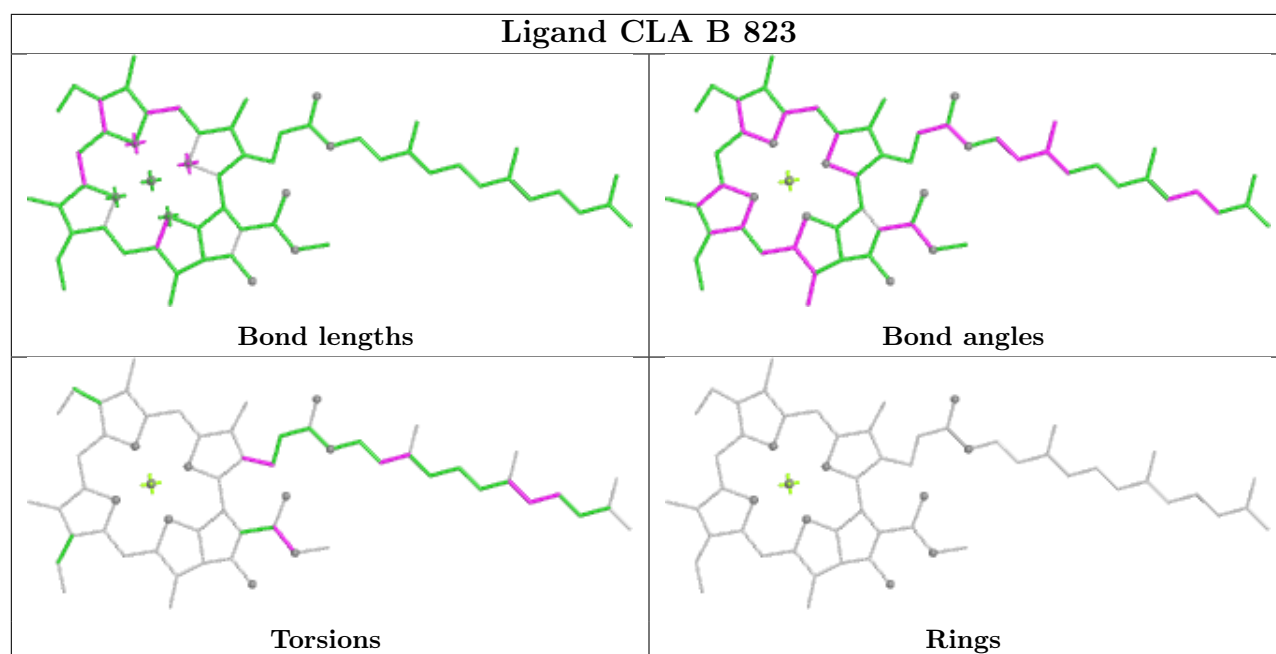




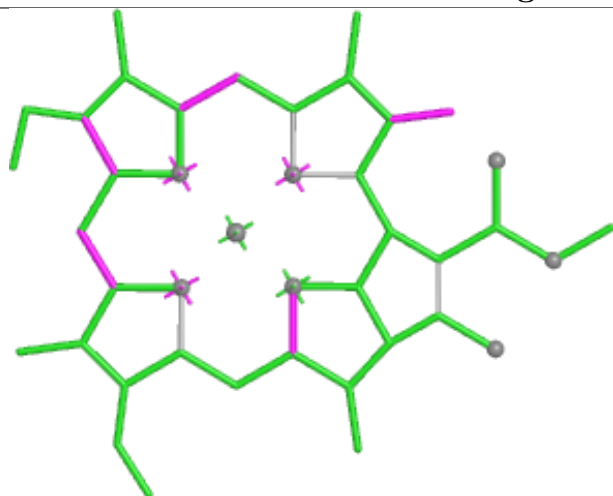








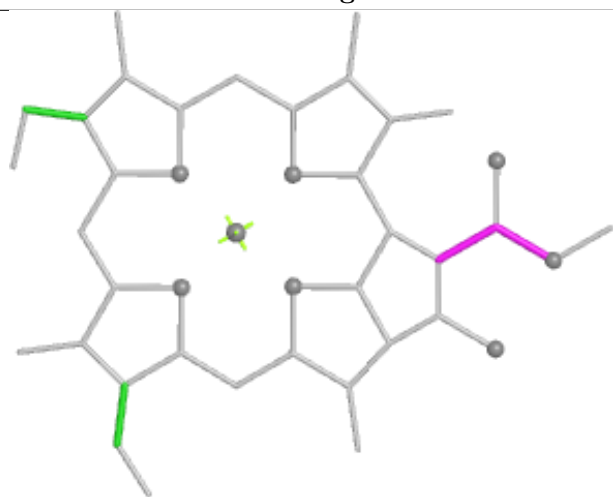
Ligand CLA d 301



Bond lengths



Bond angles

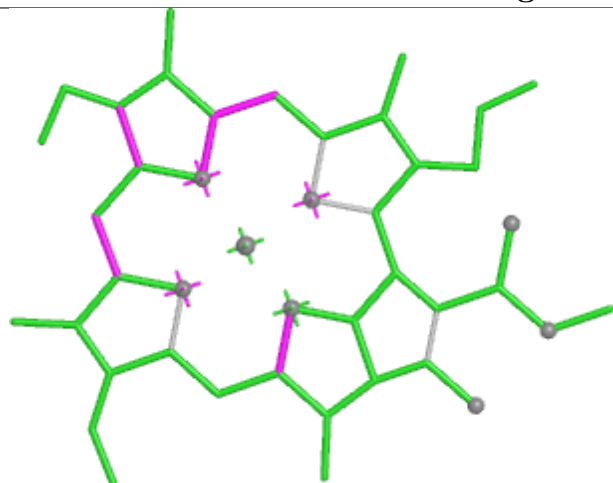


Torsions

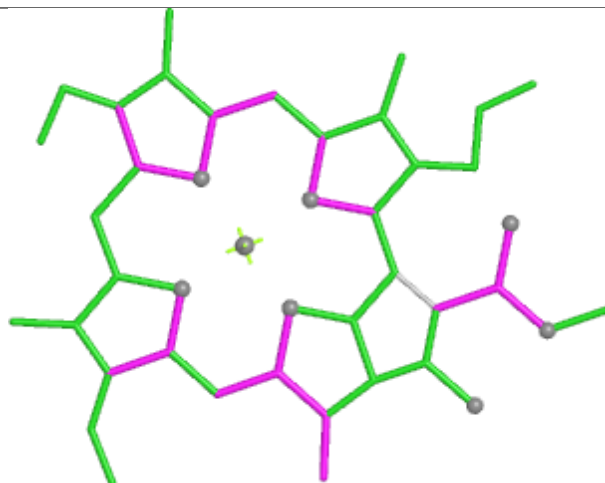


Rings

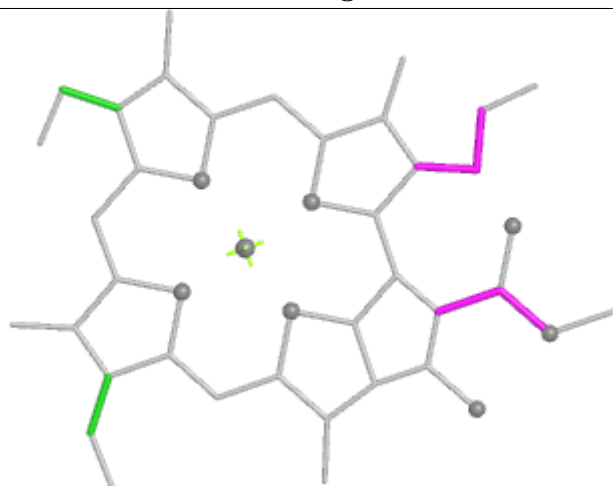
Ligand CLA h 205



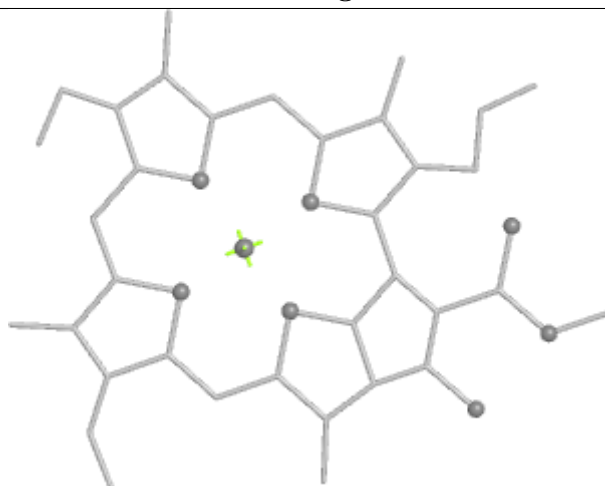
Bond lengths



Bond angles

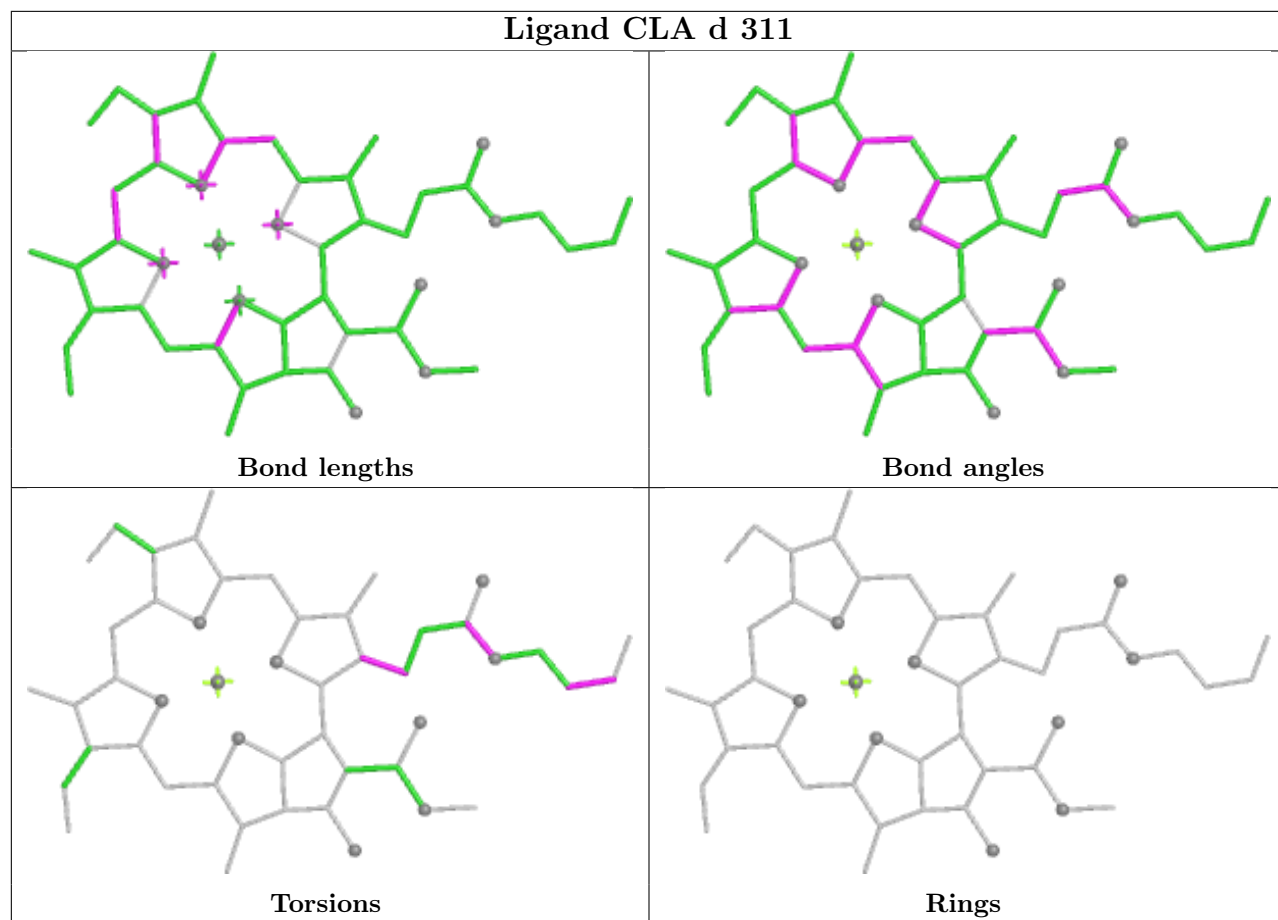


Torsions

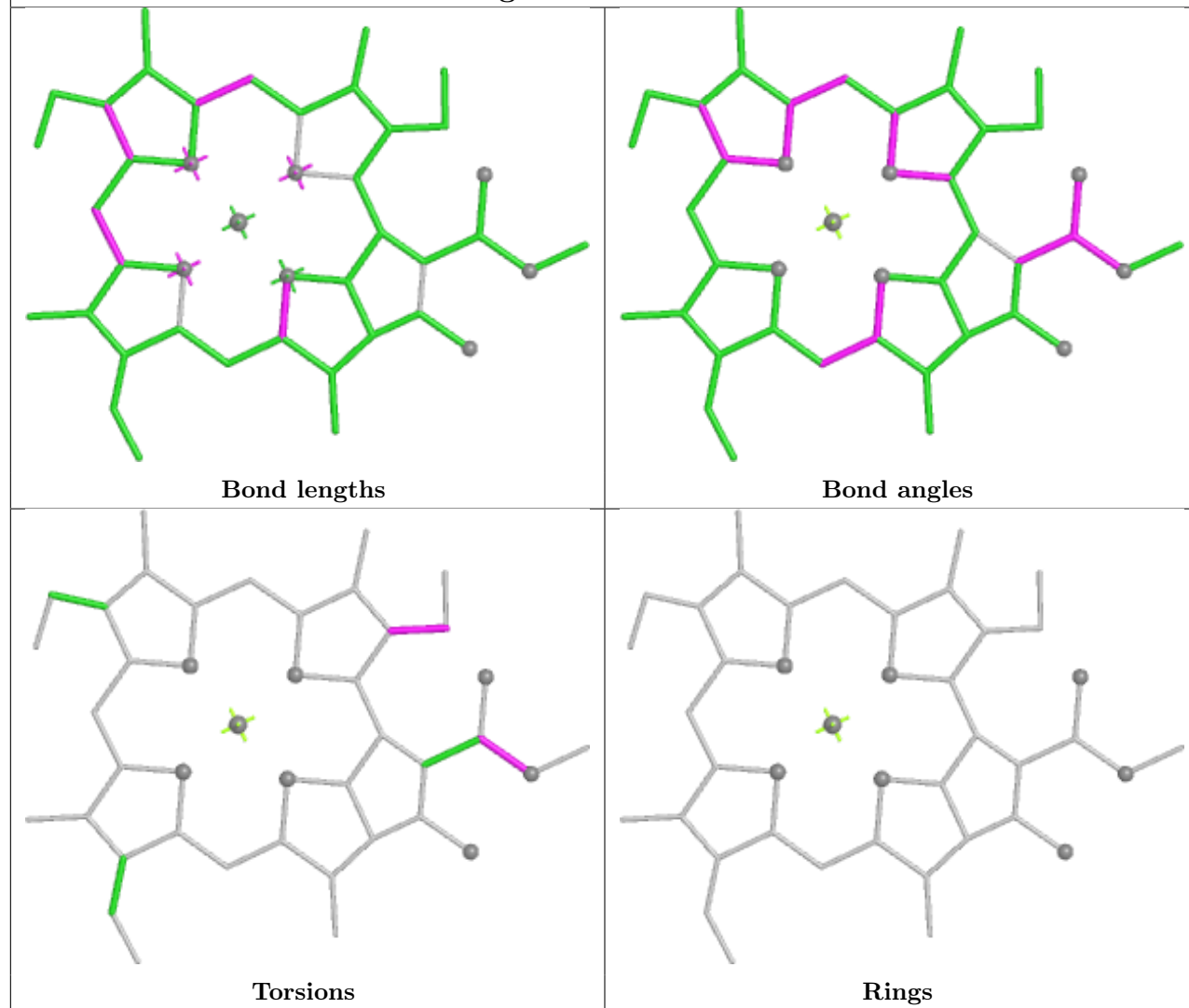


Rings

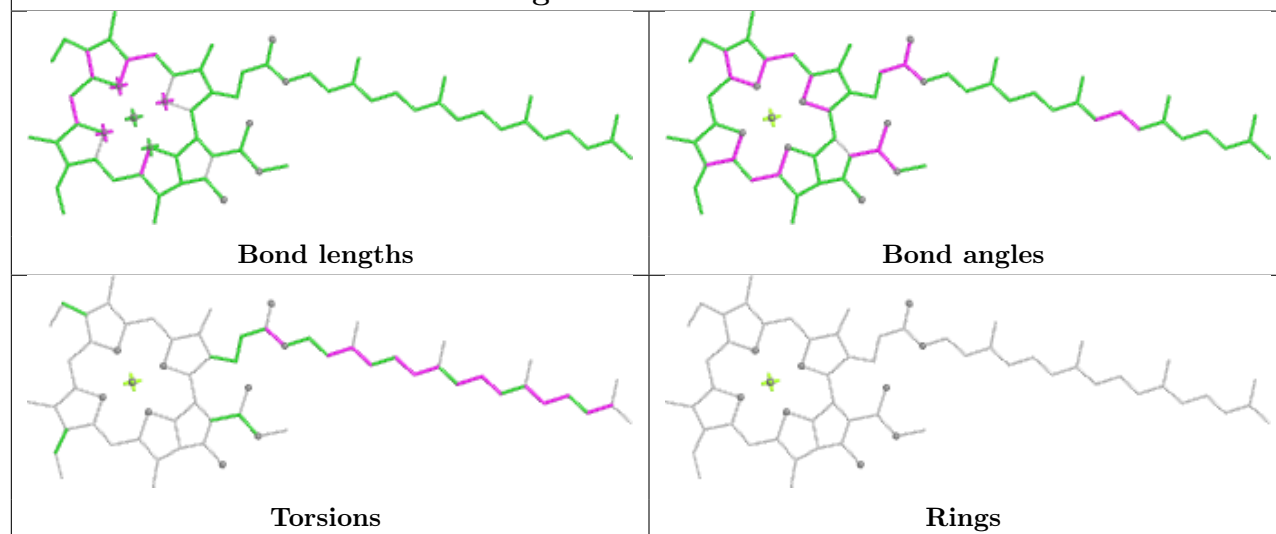
Ligand CLA d 311



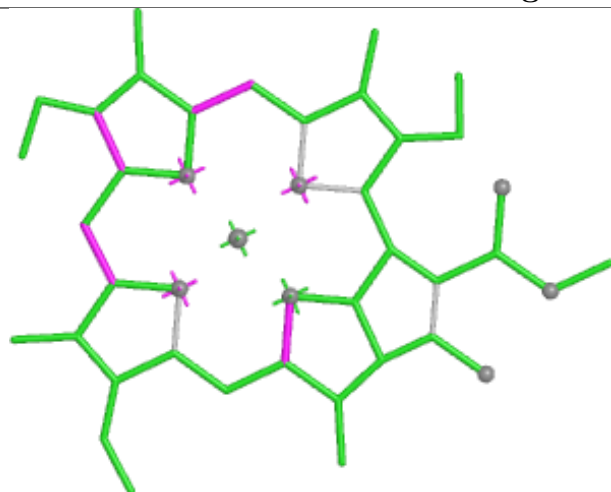
Ligand CLA k 212



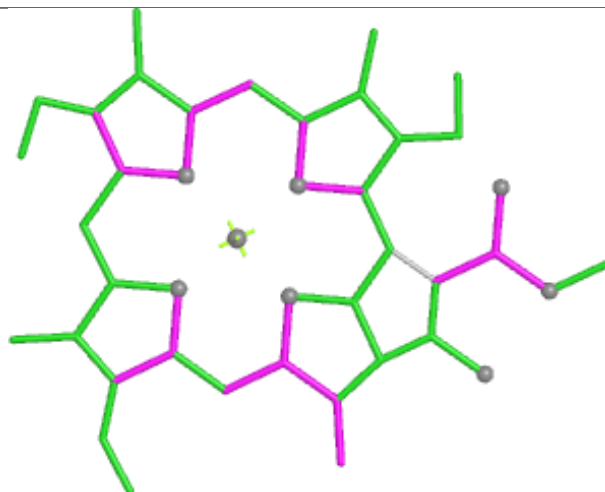
Ligand CLA B 818



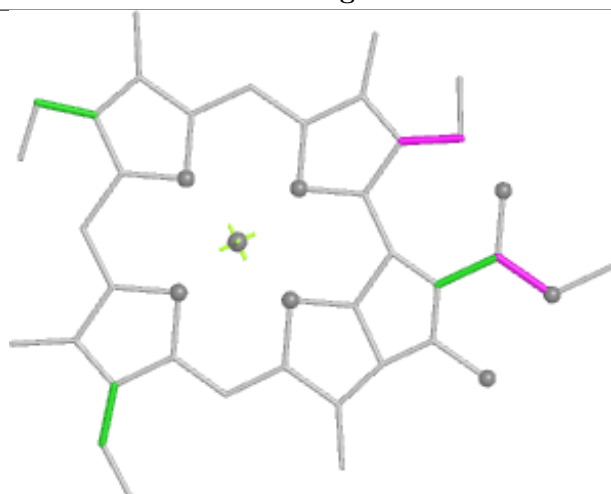
Ligand CLA f 606



Bond lengths



Bond angles

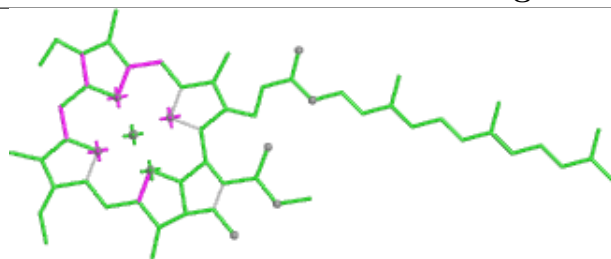


Torsions

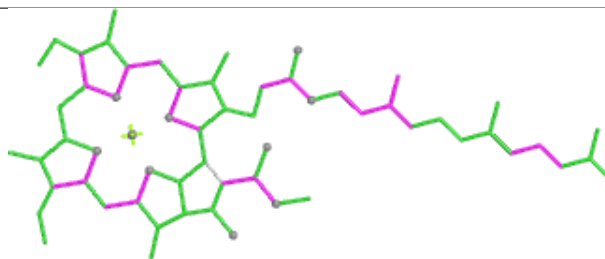


Rings

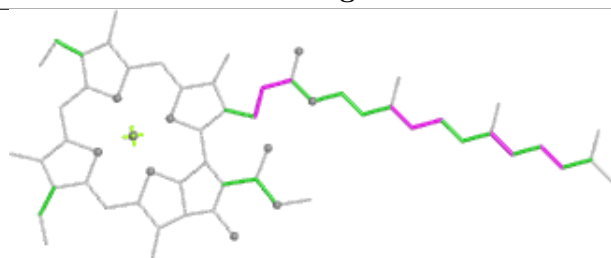
Ligand CLA A 804



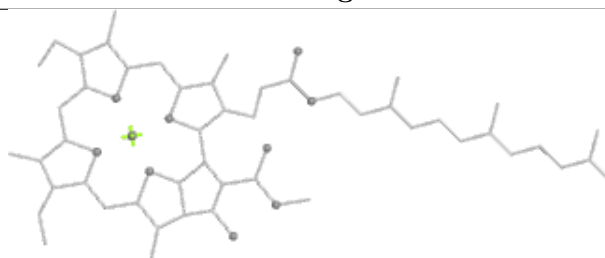
Bond lengths



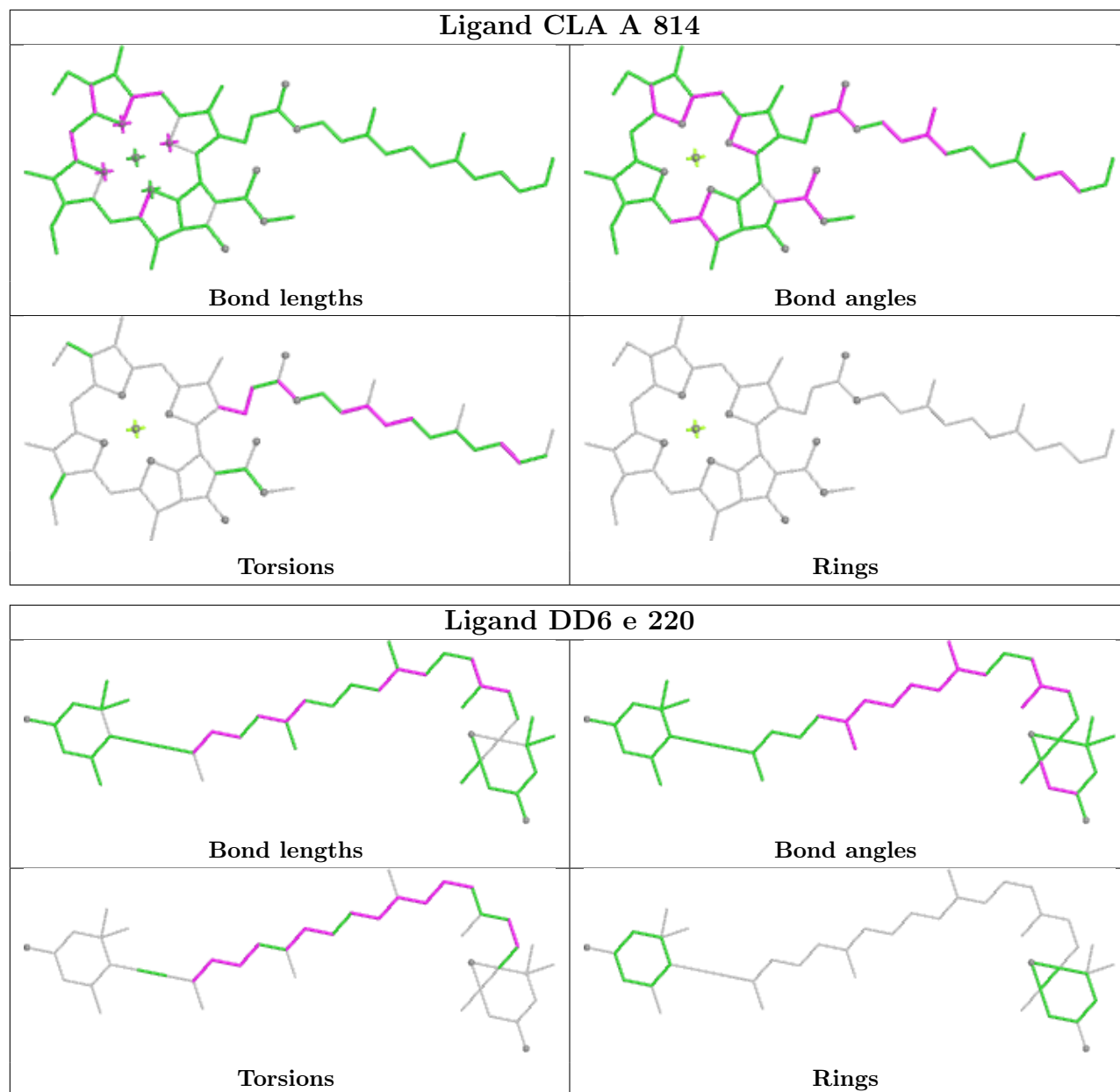
Bond angles

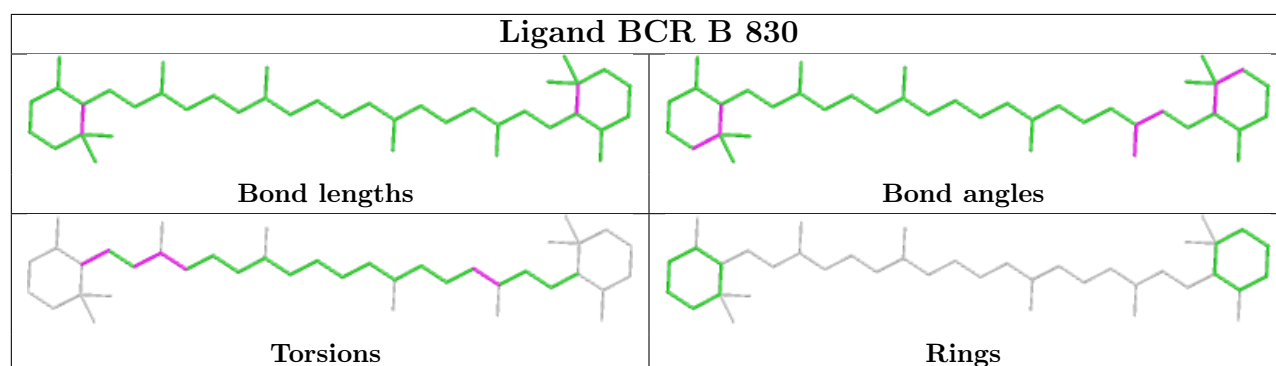
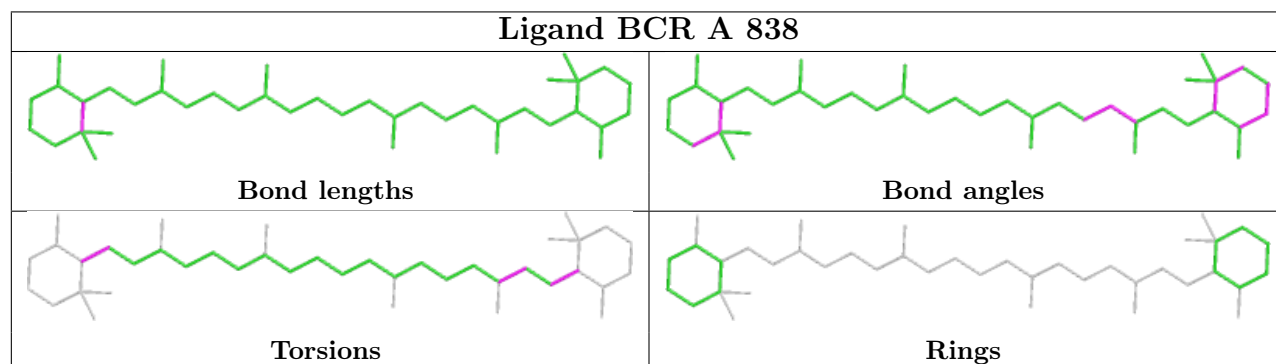
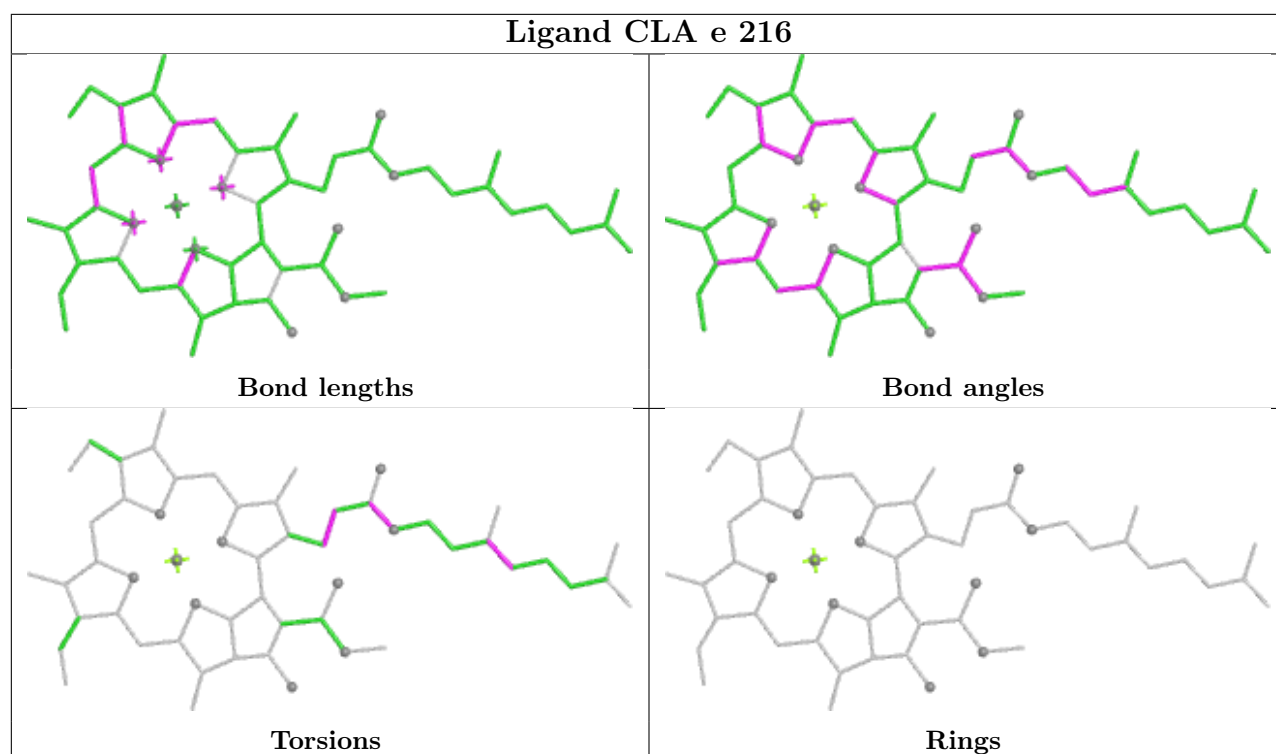


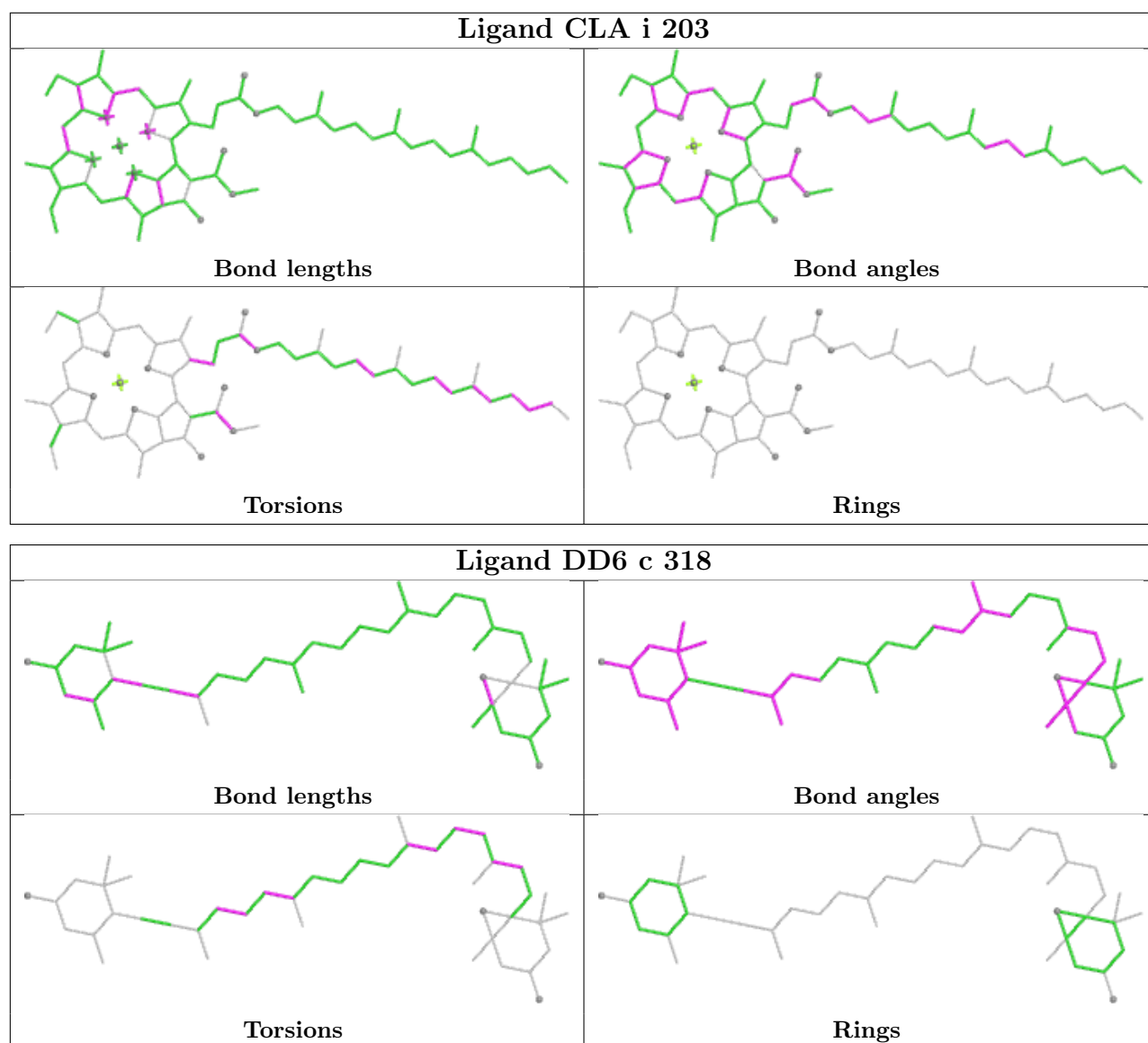
Torsions



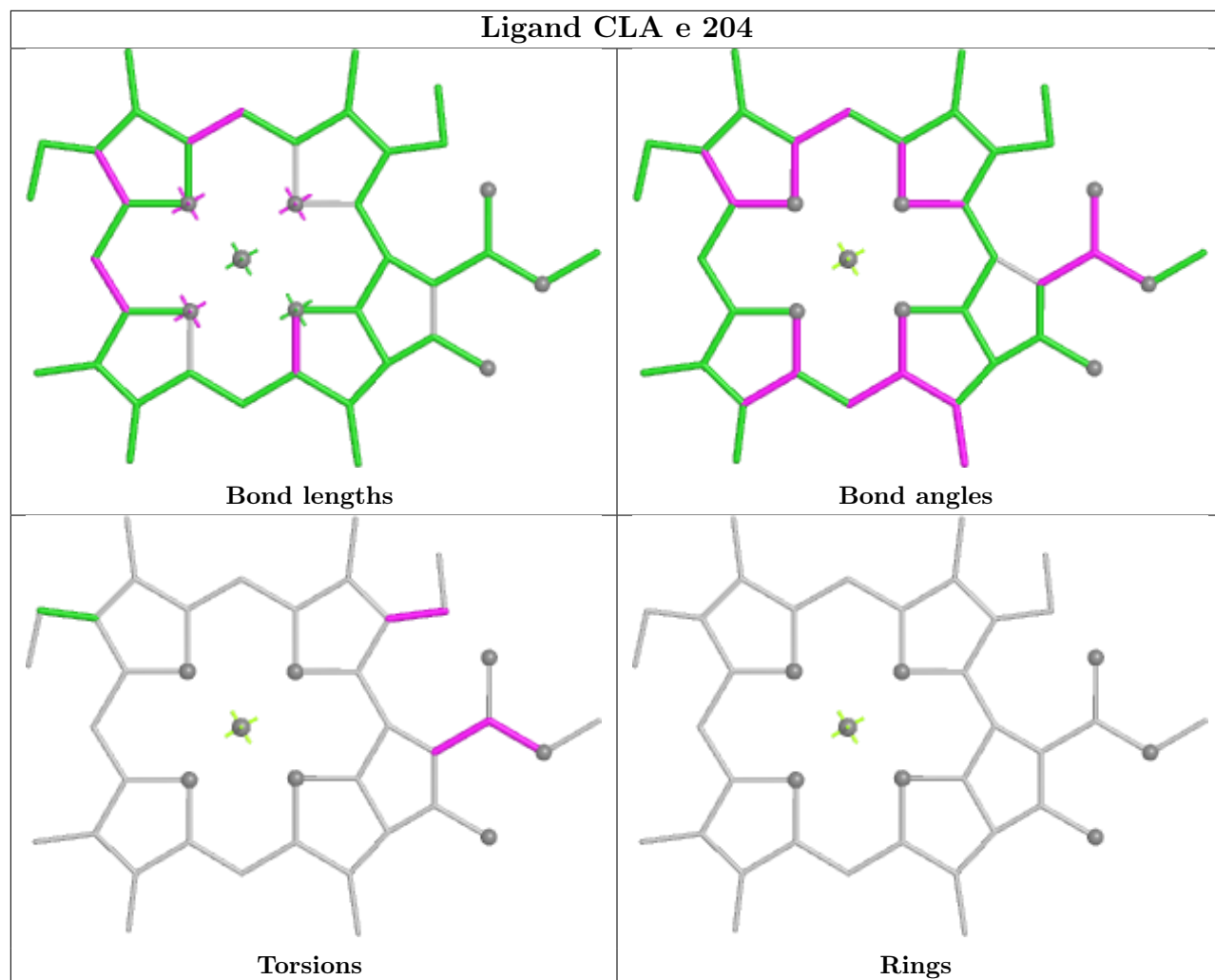
Rings



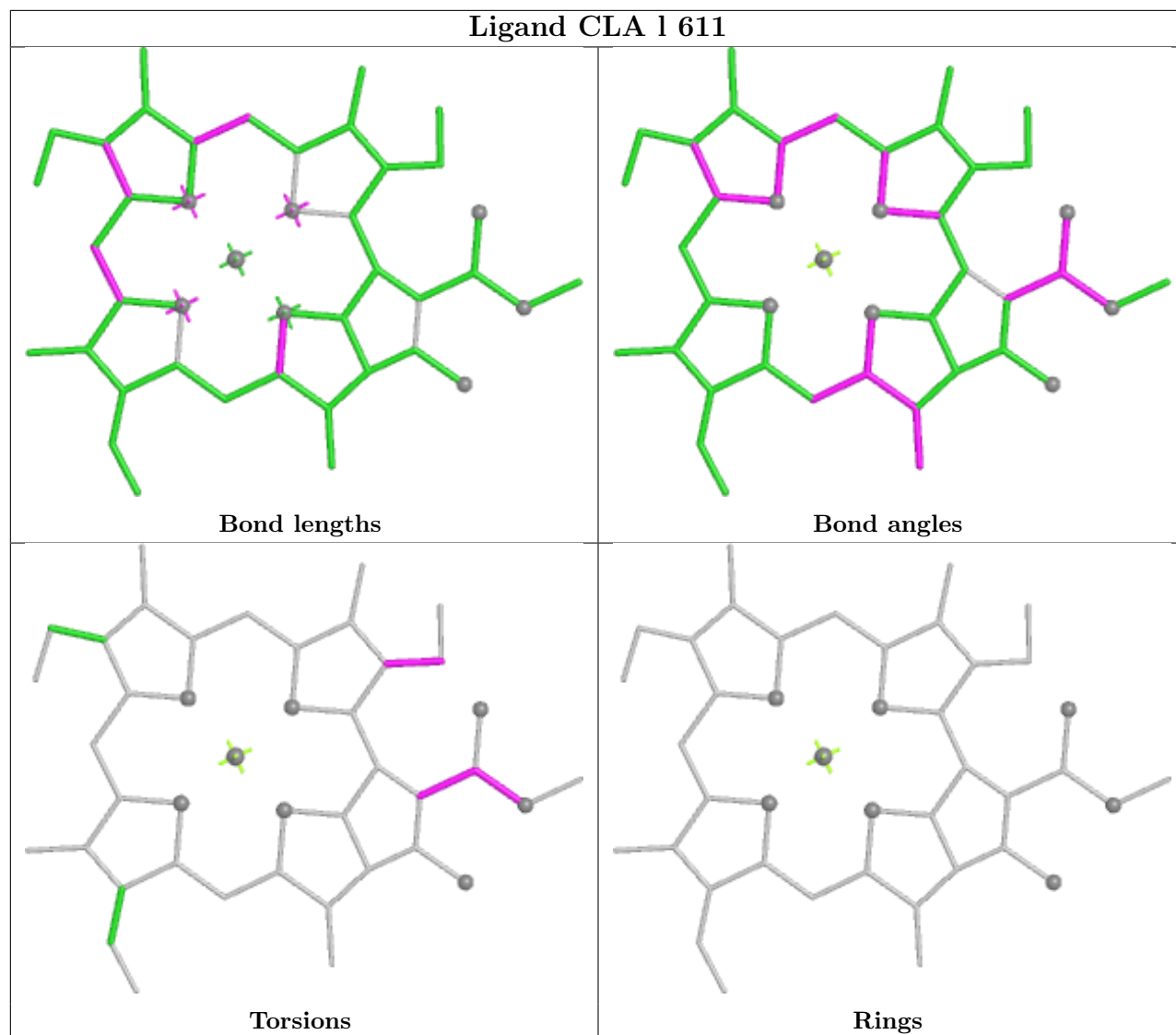




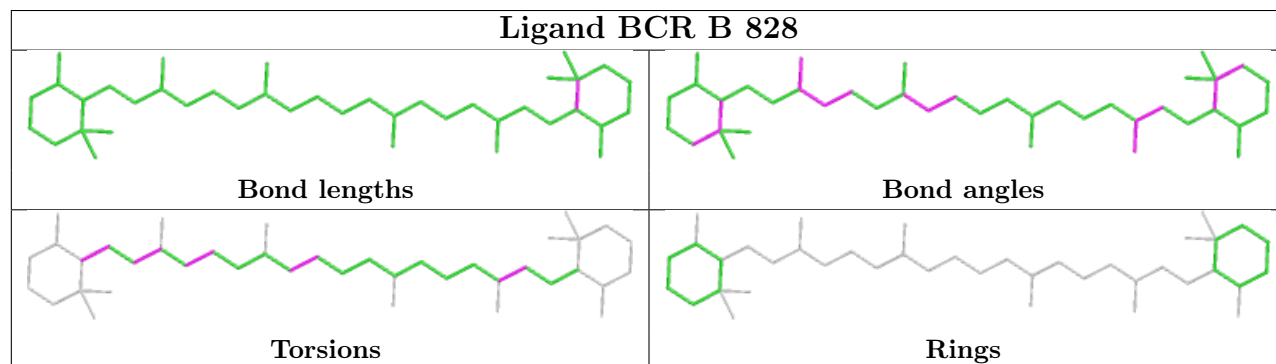
Ligand CLA e 204



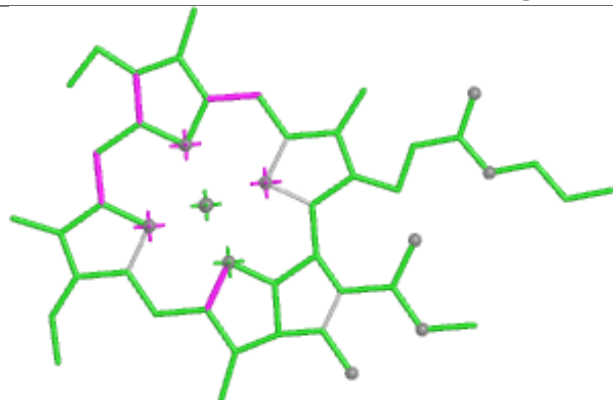
Ligand CLA 1 611



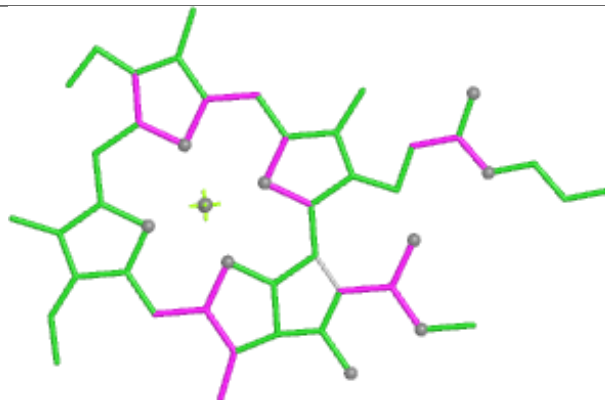
Ligand BCR B 828



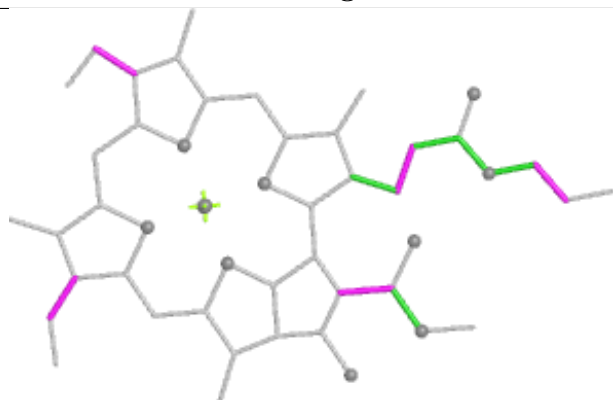
Ligand CLA n 203



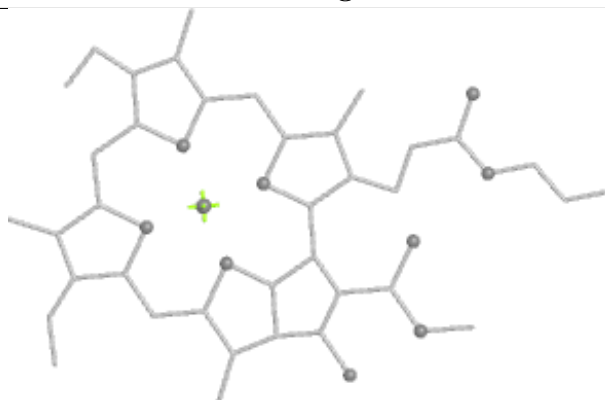
Bond lengths



Bond angles

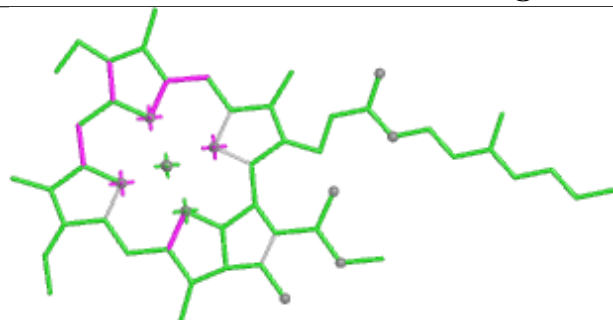


Torsions

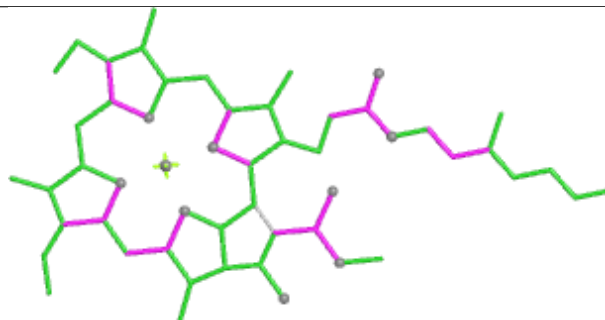


Rings

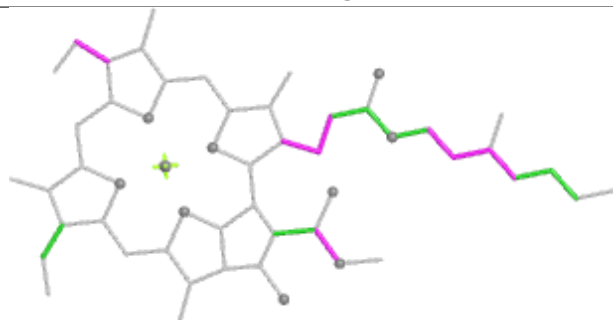
Ligand CLA B 836



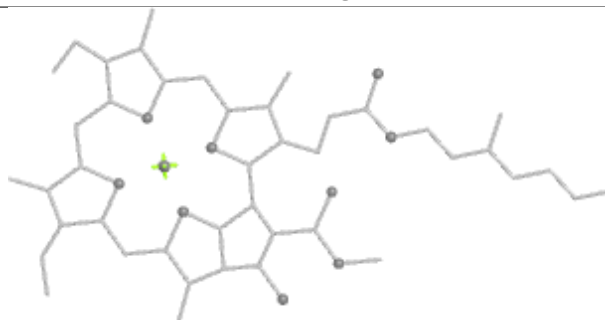
Bond lengths



Bond angles

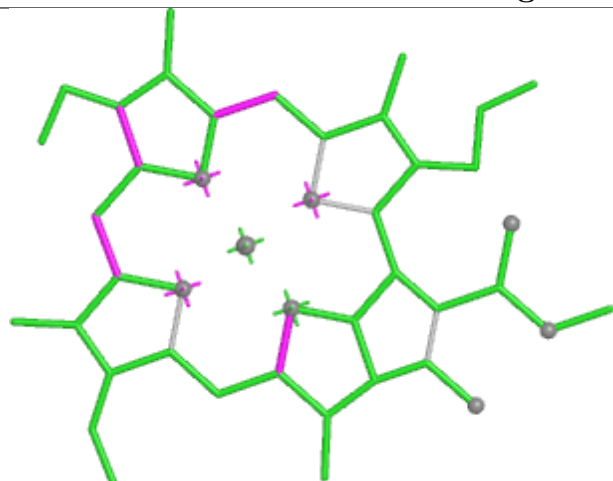


Torsions

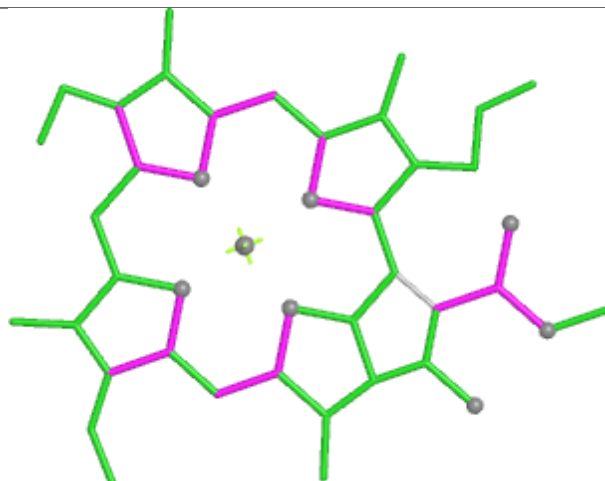


Rings

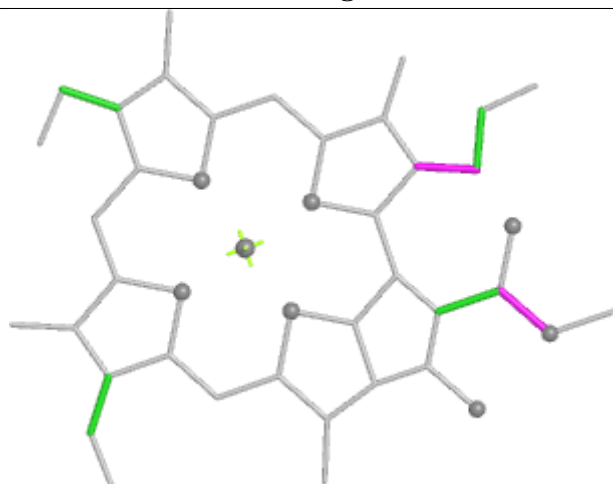
Ligand CLA k 202



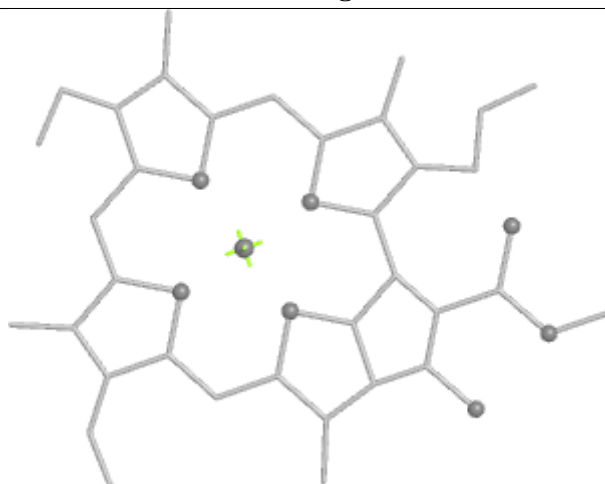
Bond lengths



Bond angles

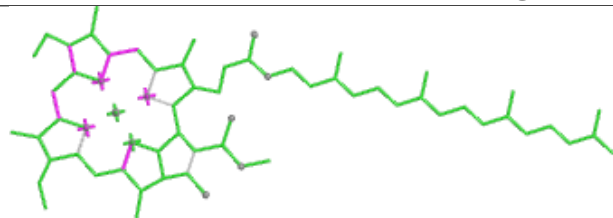


Torsions

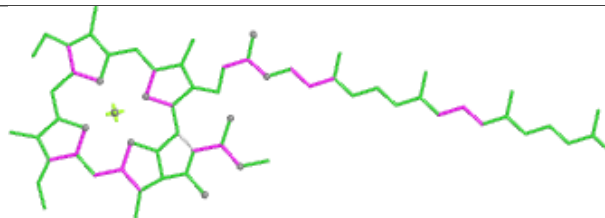


Rings

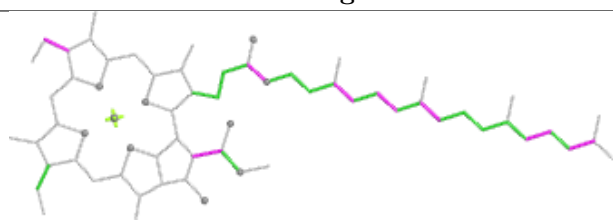
Ligand CLA A 826



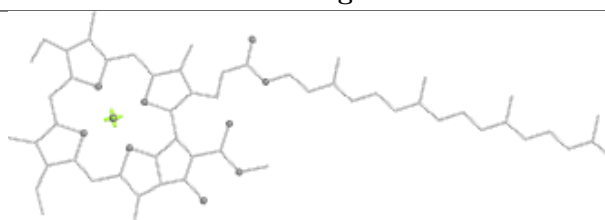
Bond lengths



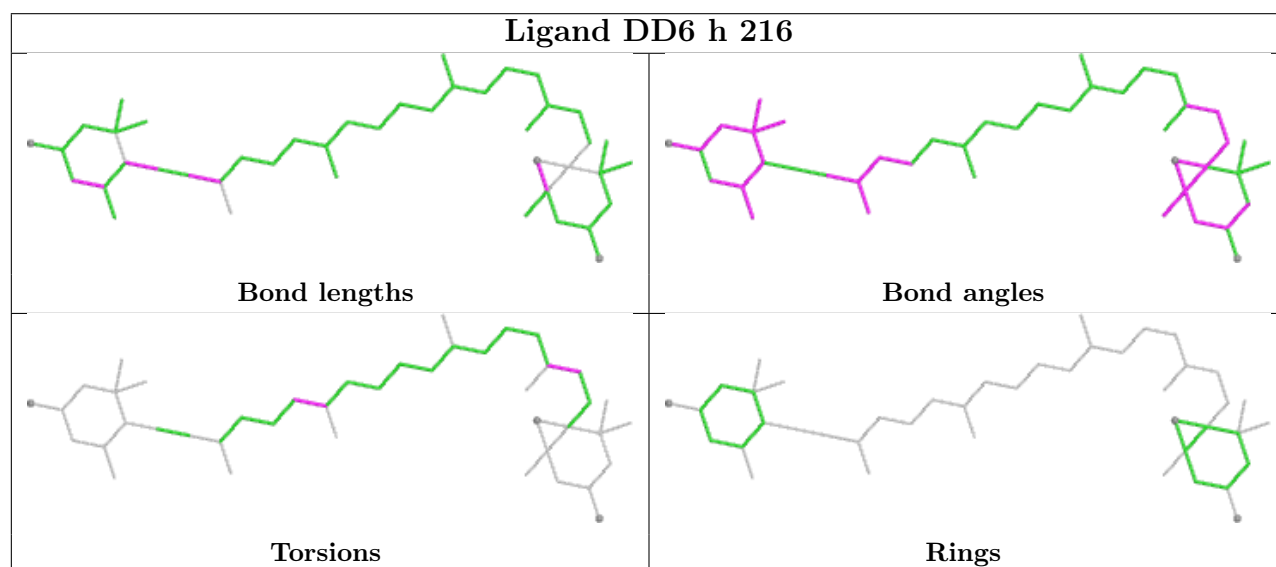
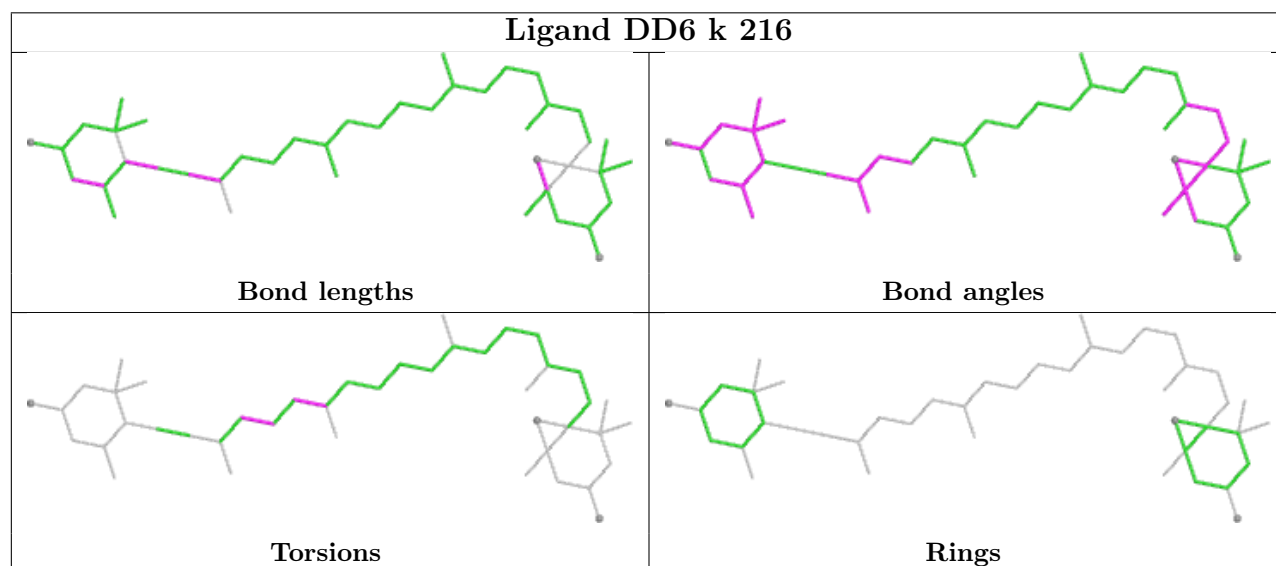
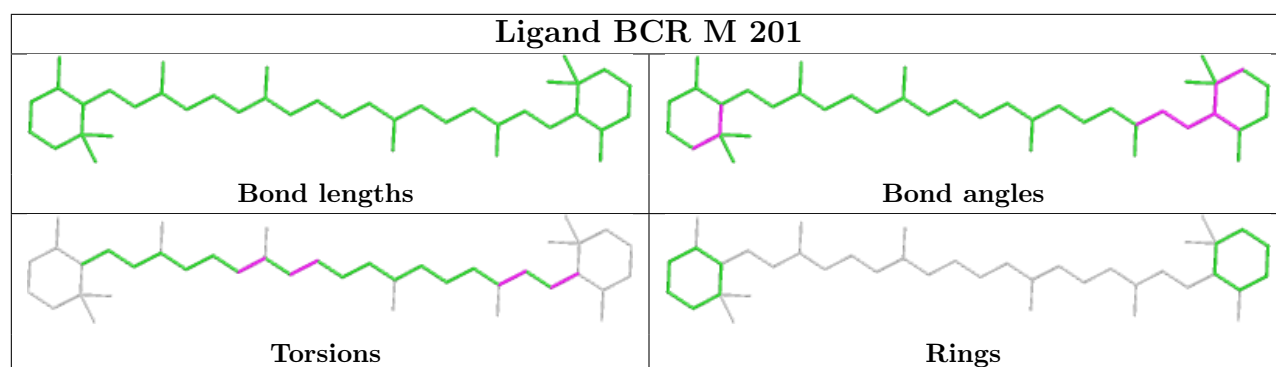
Bond angles

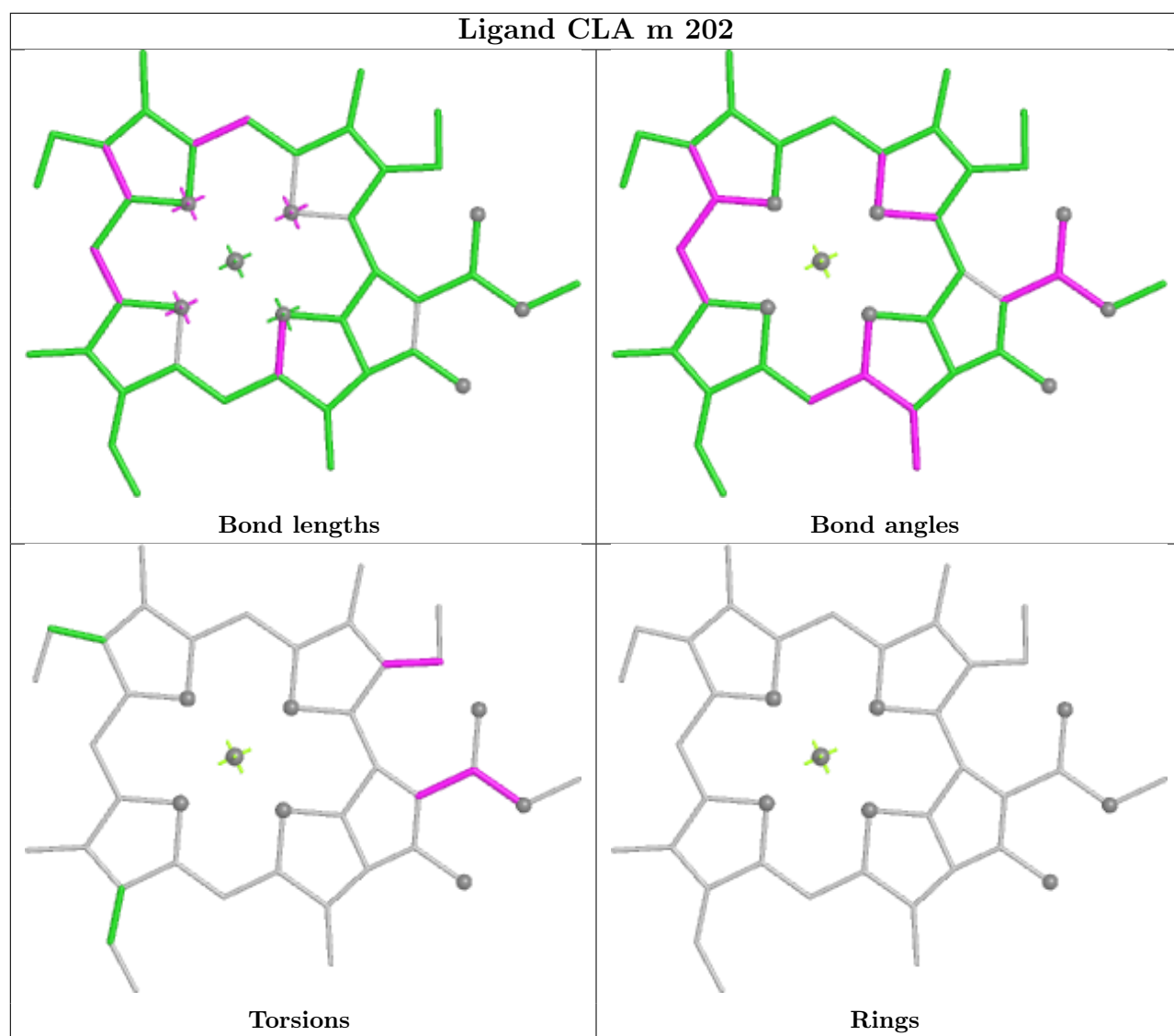


Torsions

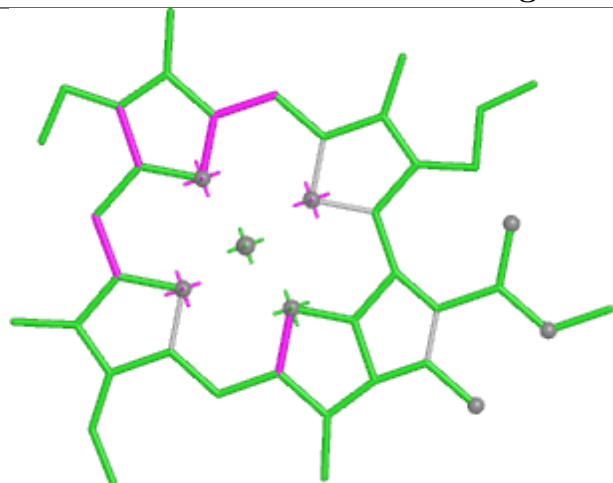


Rings

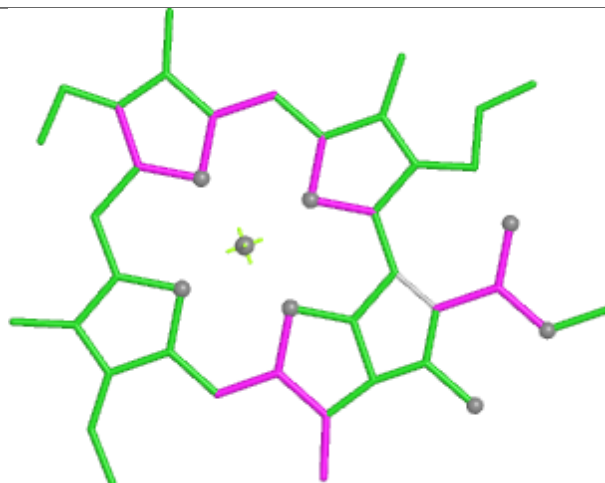




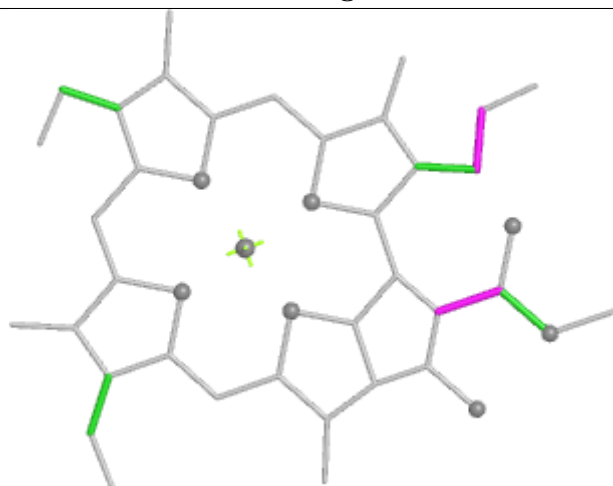
Ligand CLA e 215



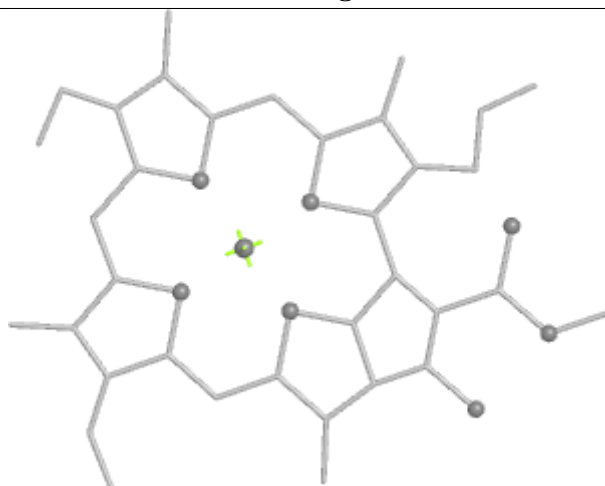
Bond lengths



Bond angles

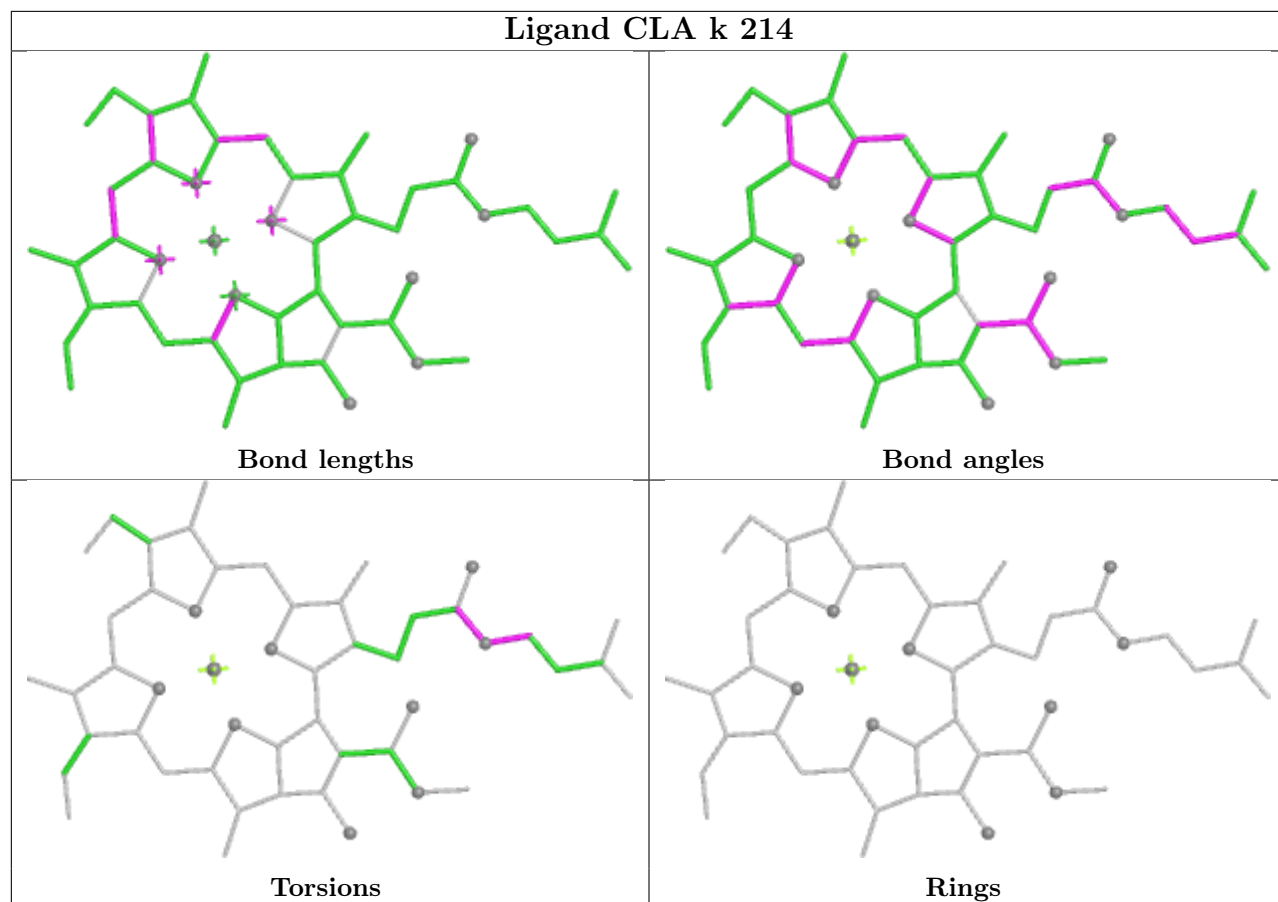


Torsions

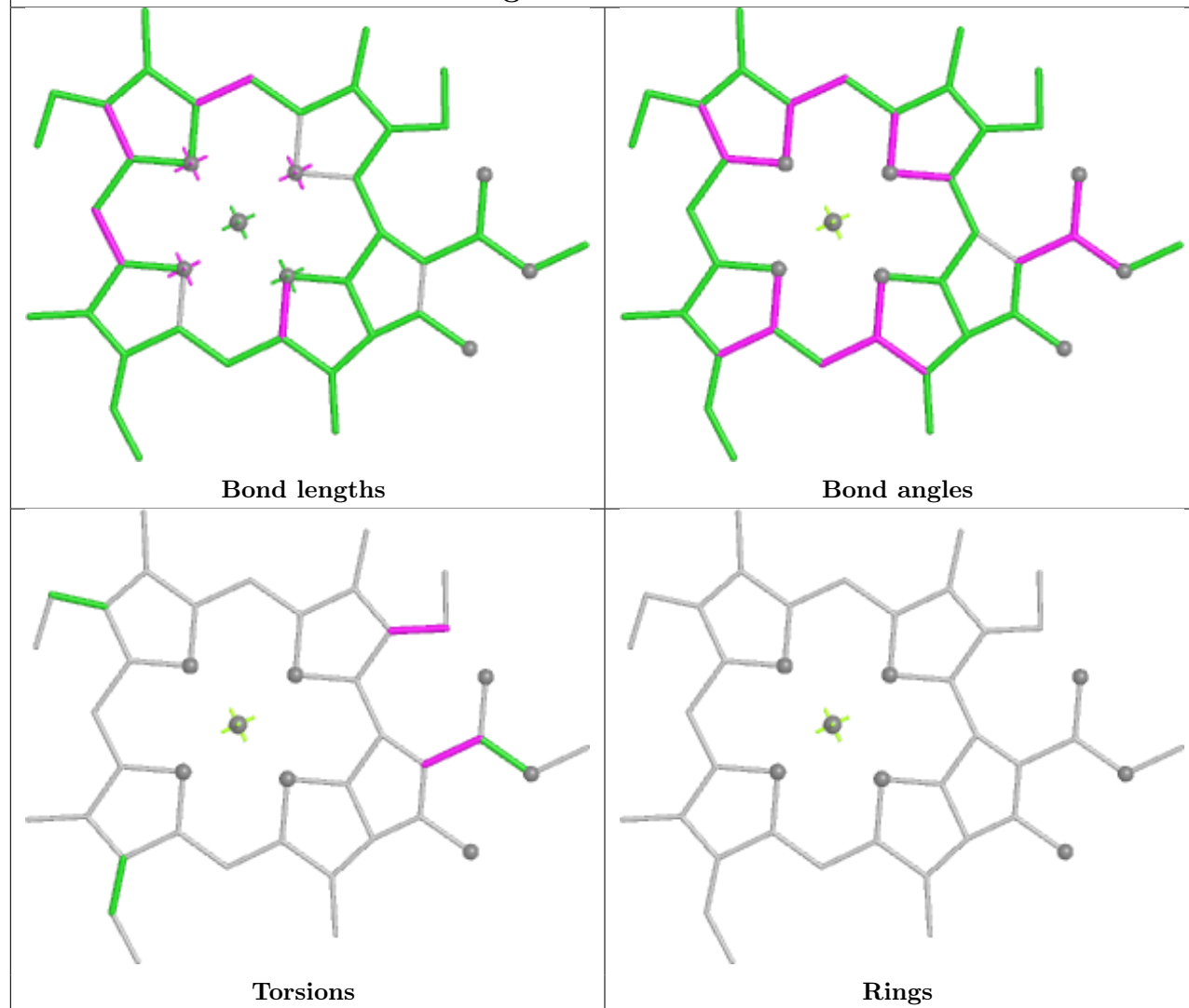


Rings

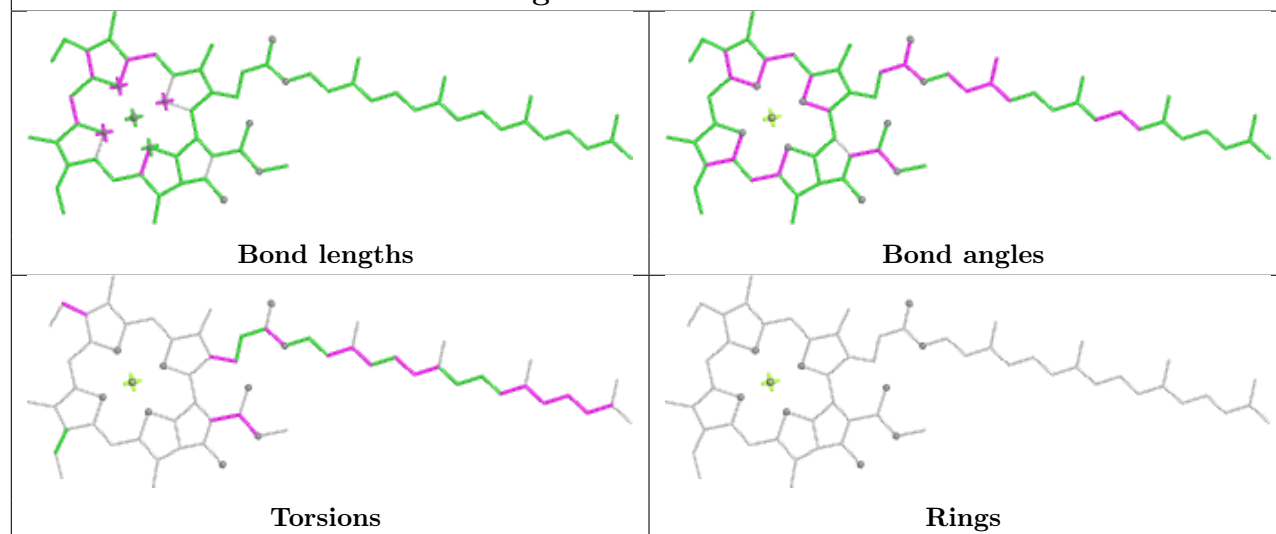
Ligand CLA k 214



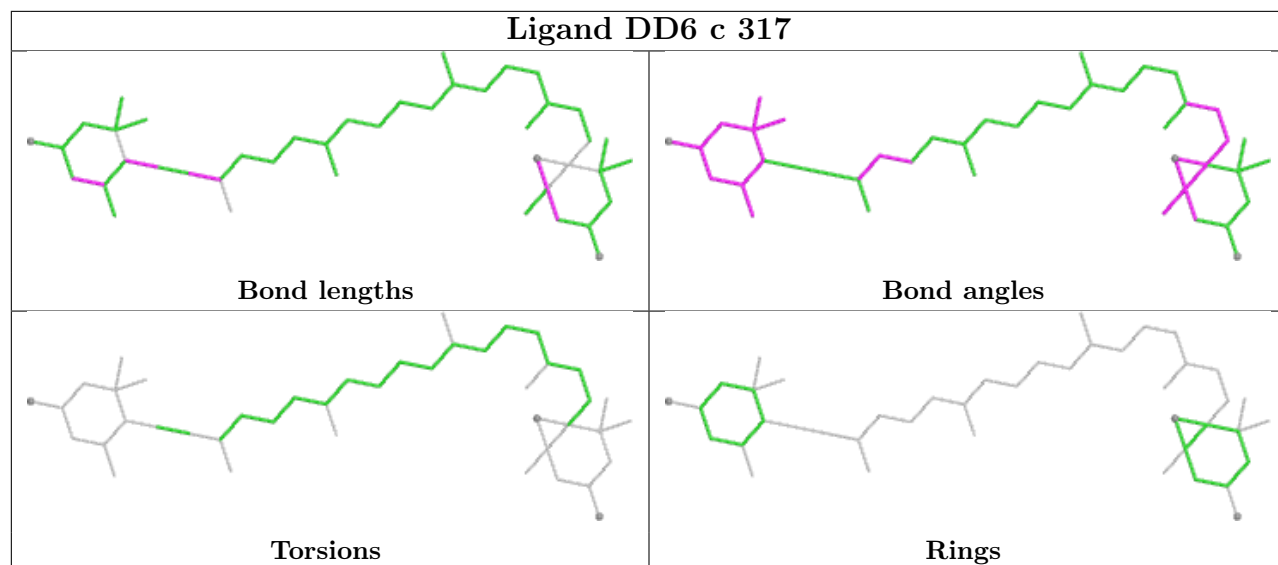
Ligand CLA i 212



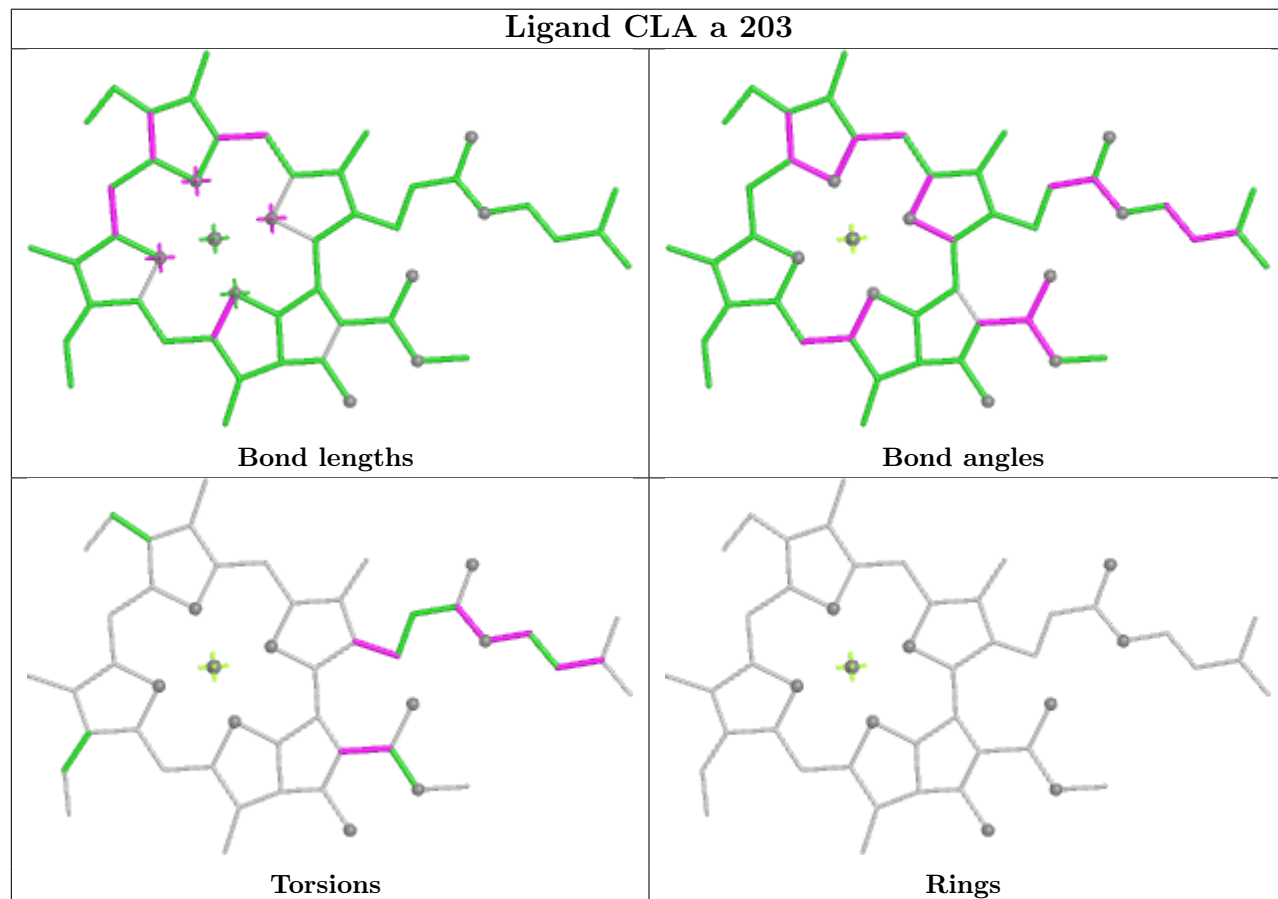
Ligand CLA B 824



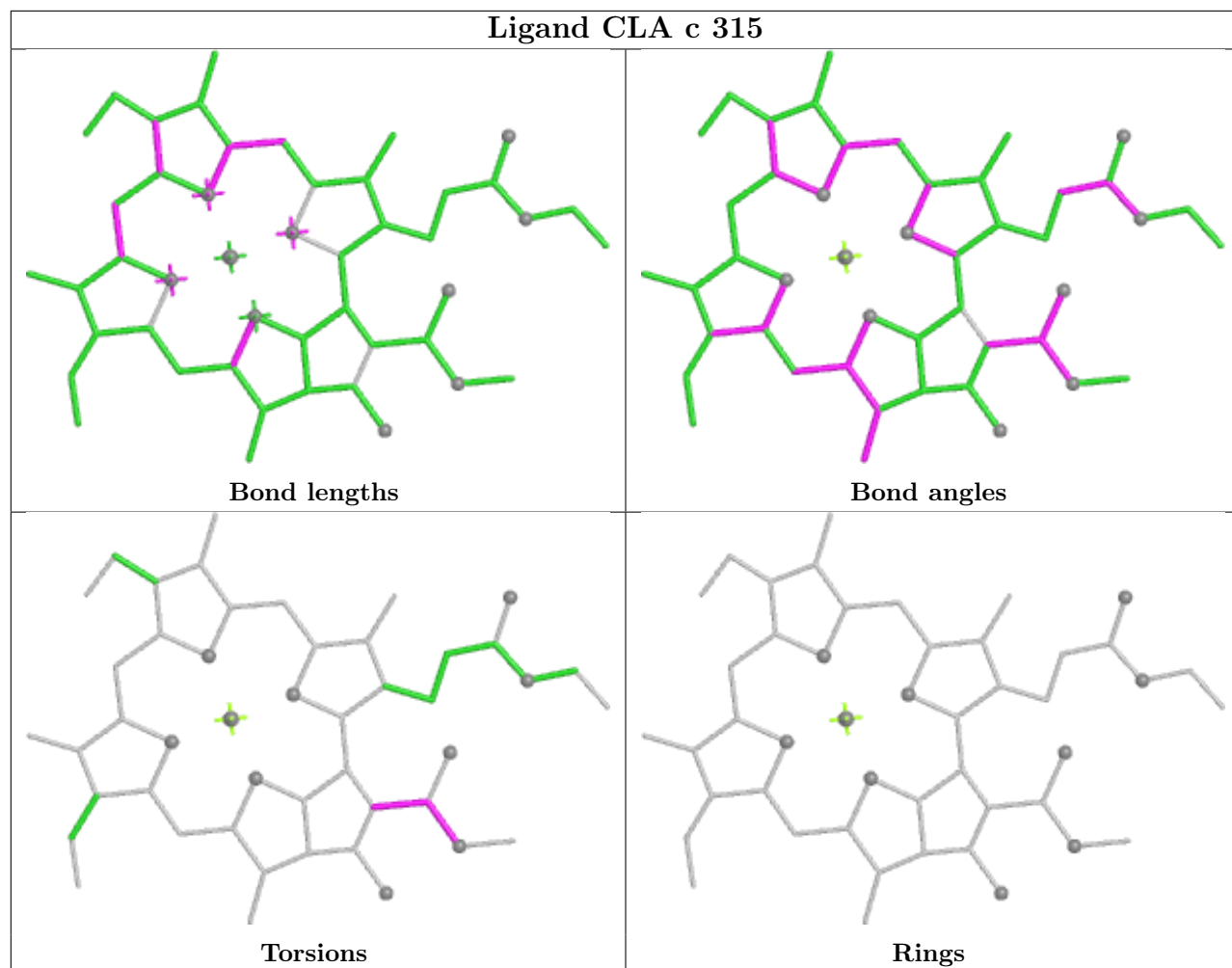
Ligand DD6 c 317



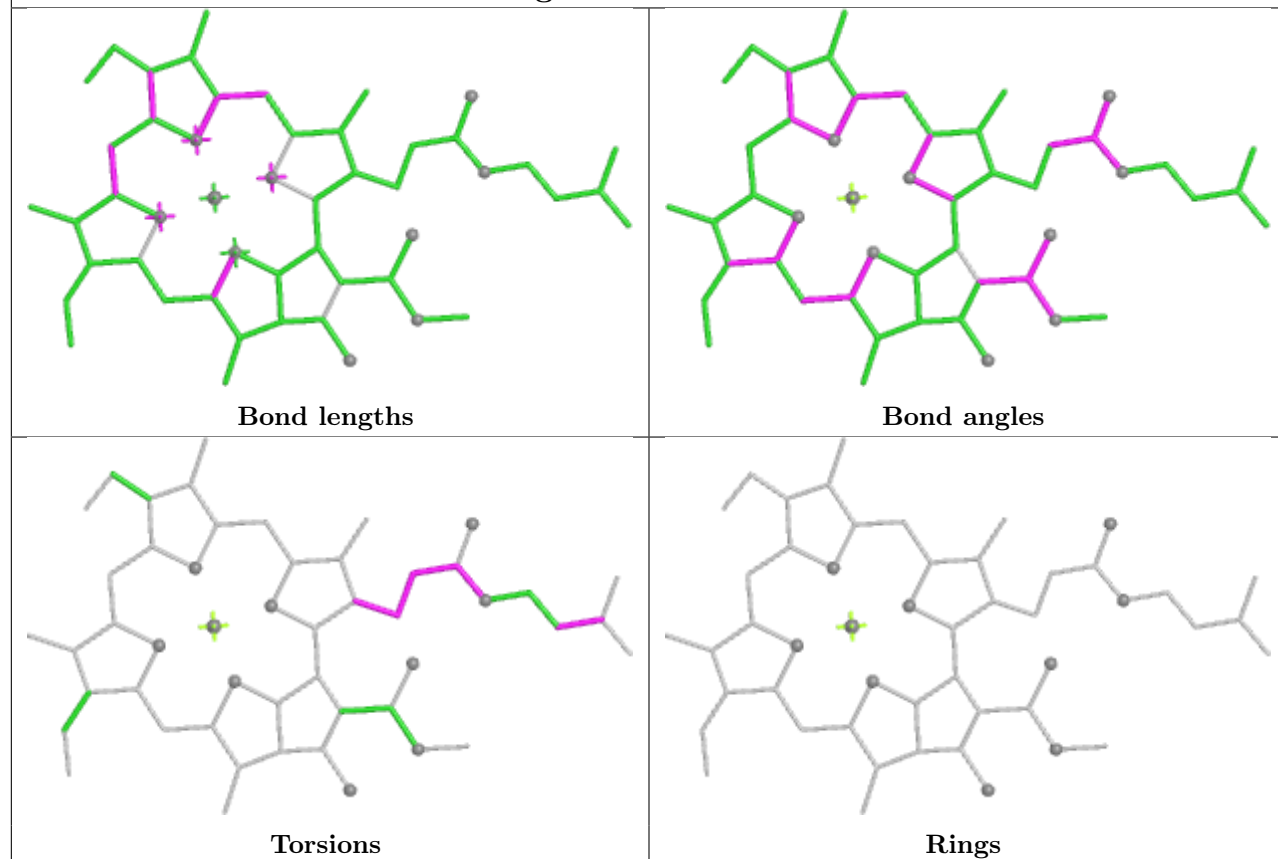
Ligand CLA a 203



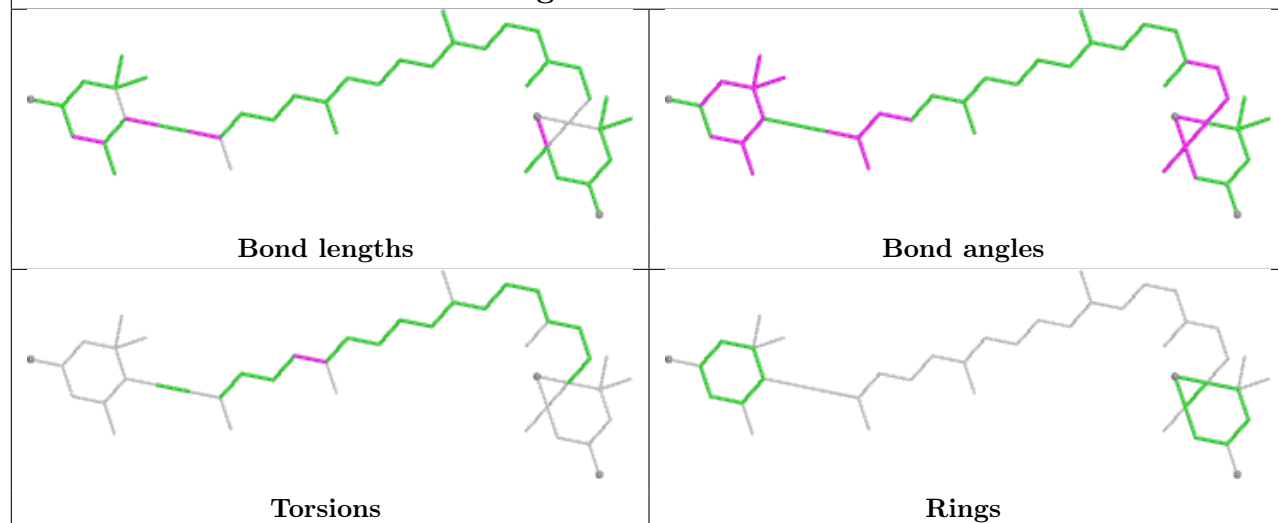
Ligand CLA c 315



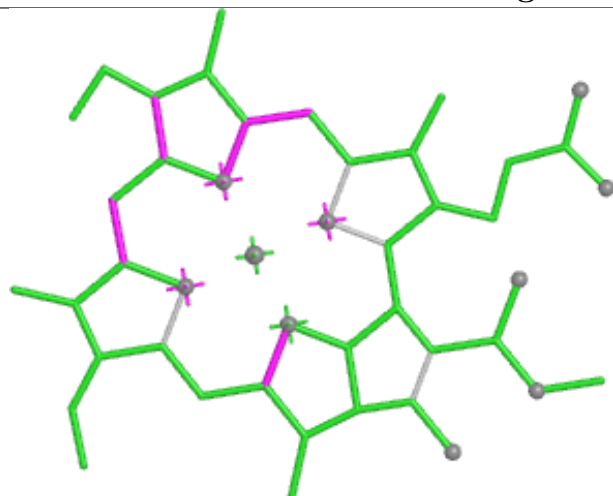
Ligand CLA h 208



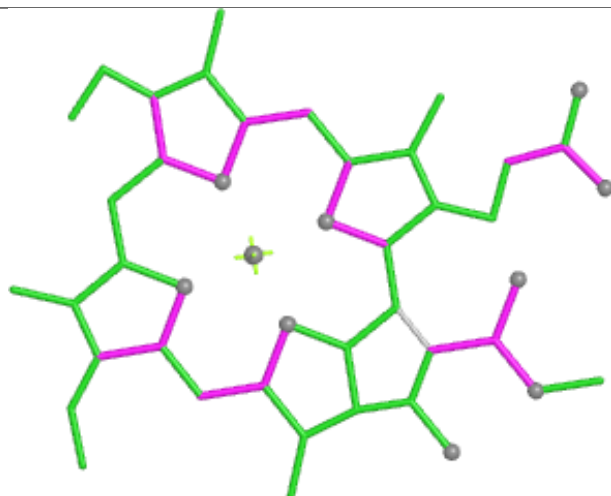
Ligand DD6 k 215



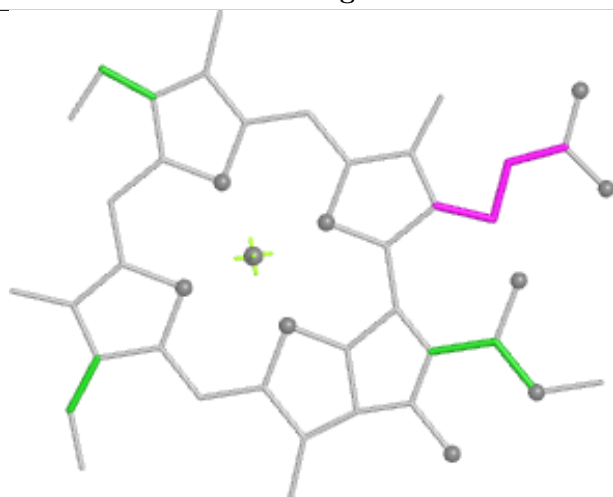
Ligand CLA d 313



Bond lengths



Bond angles

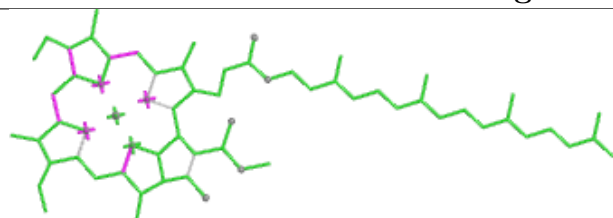


Torsions

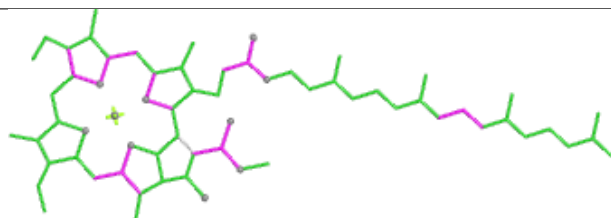


Rings

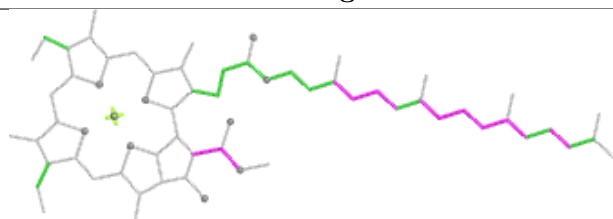
Ligand CLA B 807



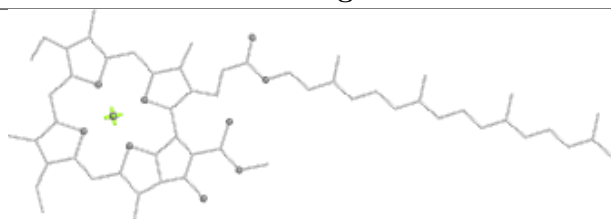
Bond lengths



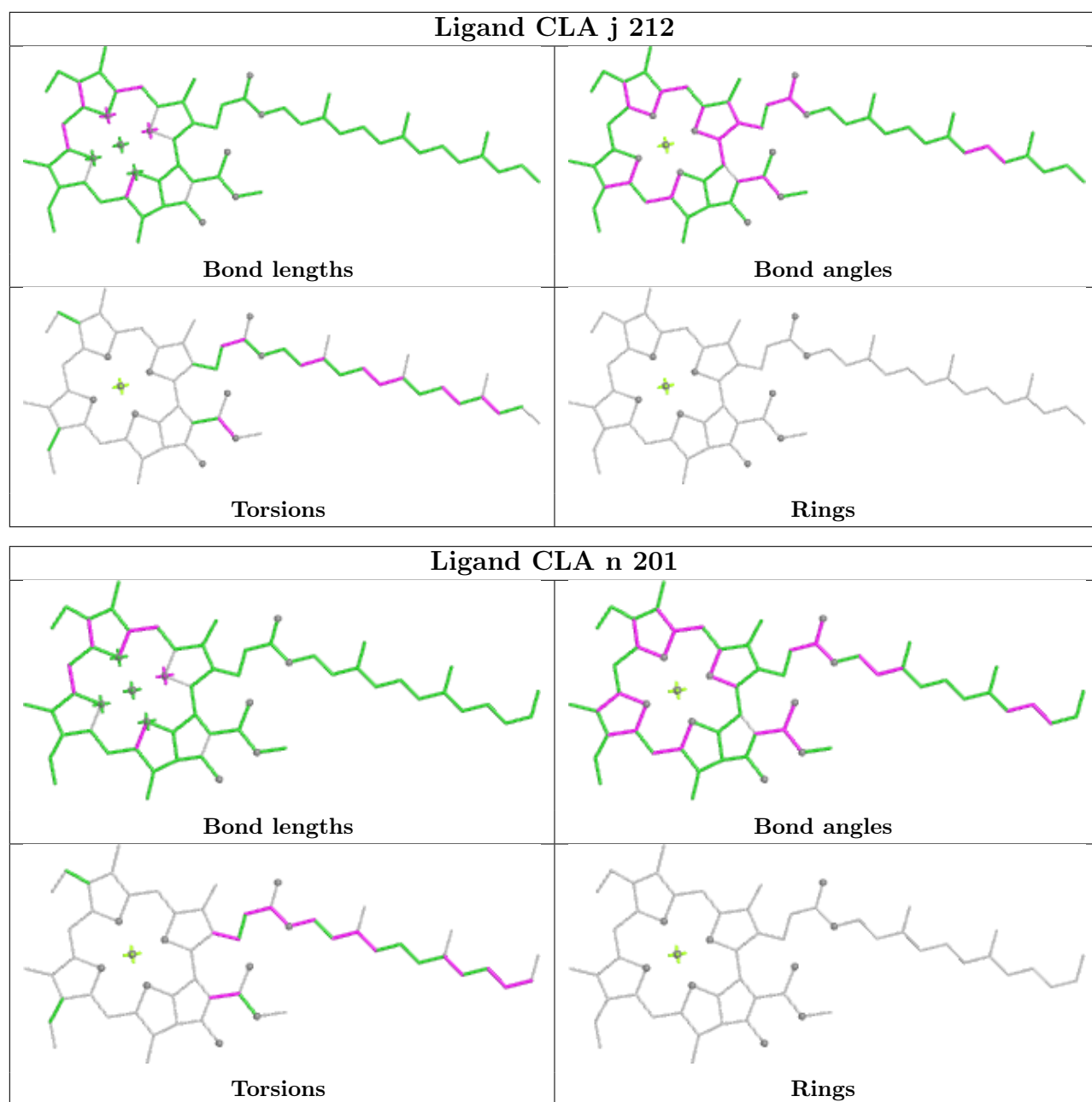
Bond angles



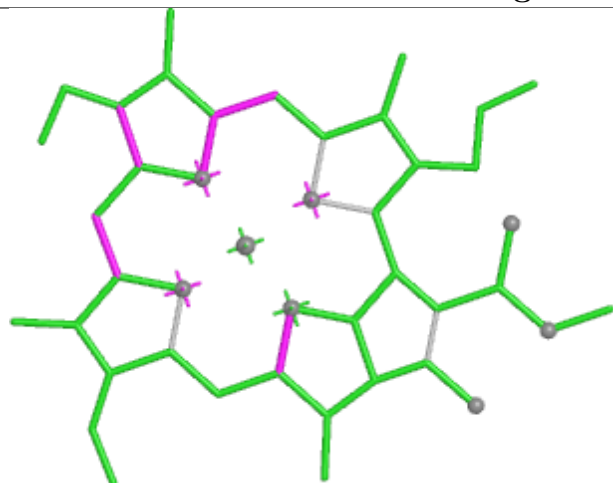
Torsions



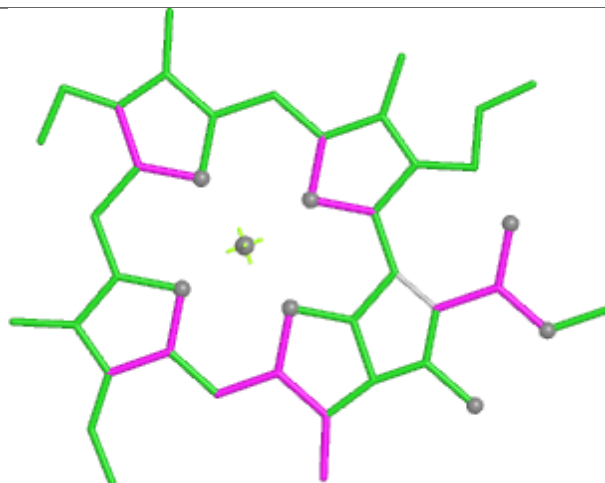
Rings



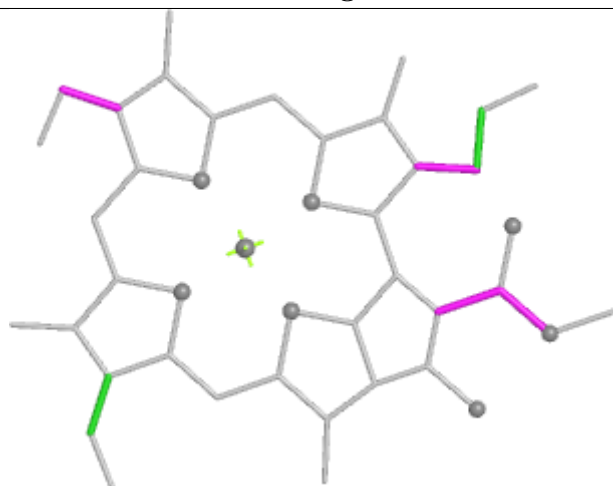
Ligand CLA A 828



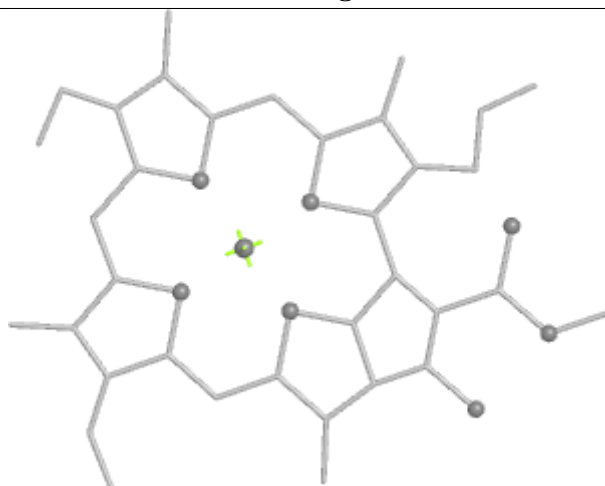
Bond lengths



Bond angles

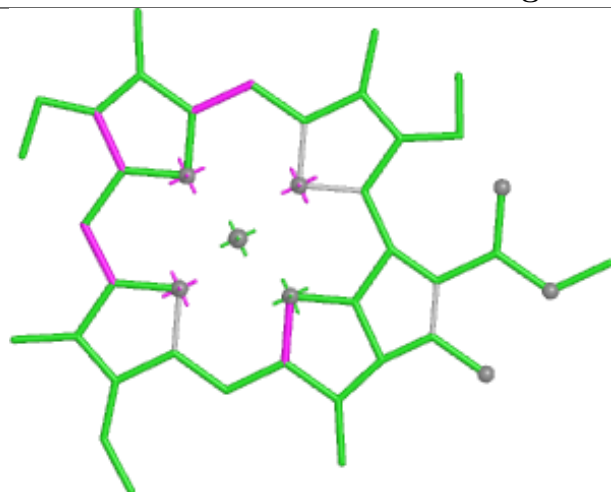


Torsions

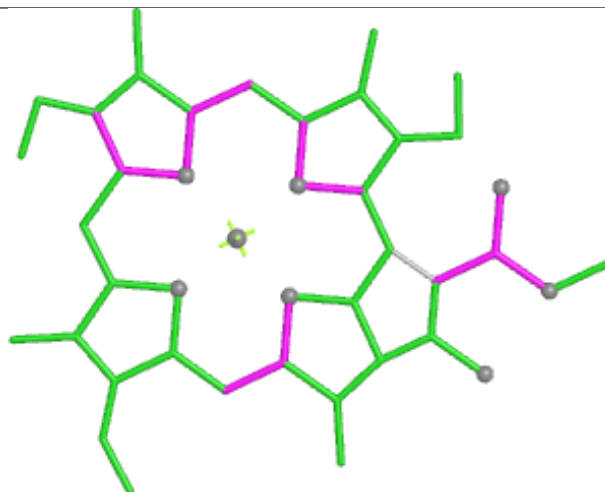


Rings

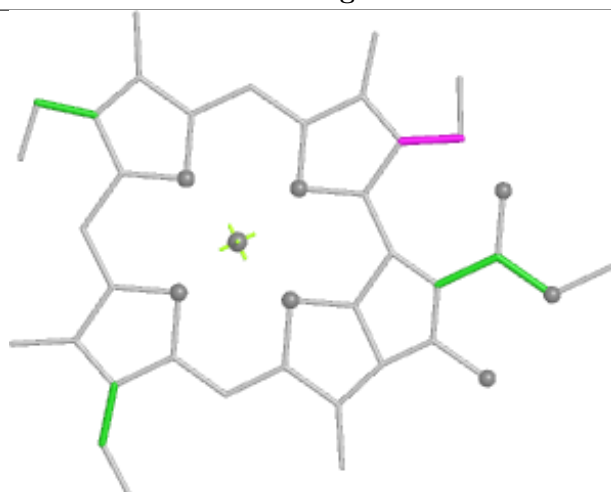
Ligand CLA f 608



Bond lengths



Bond angles

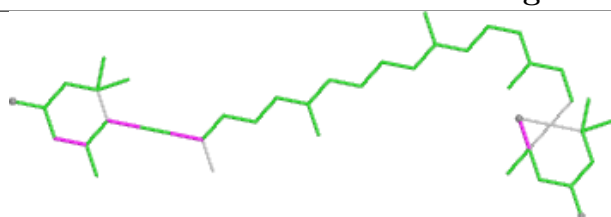


Torsions

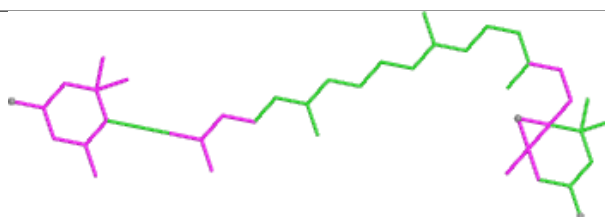


Rings

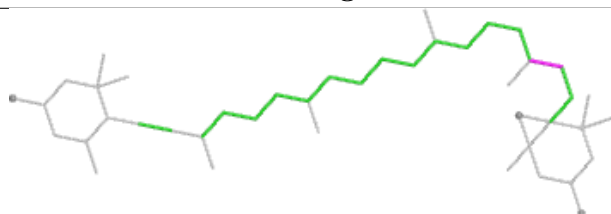
Ligand DD6 l 613



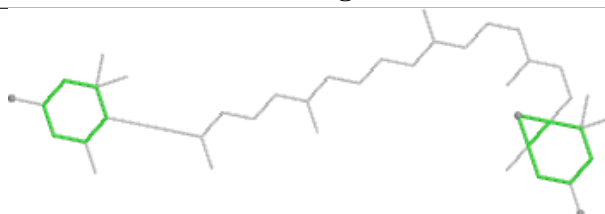
Bond lengths



Bond angles

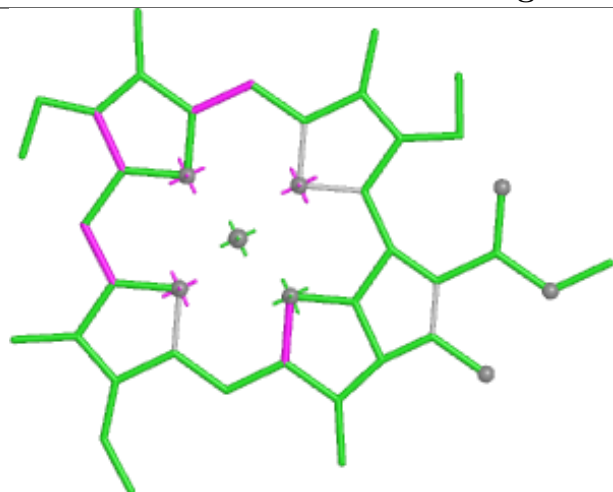


Torsions

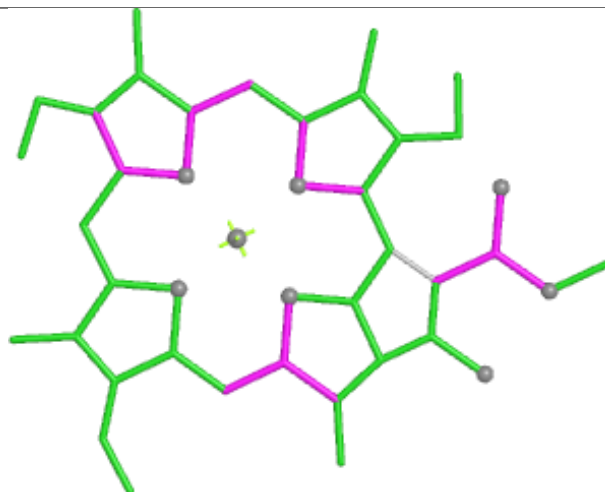


Rings

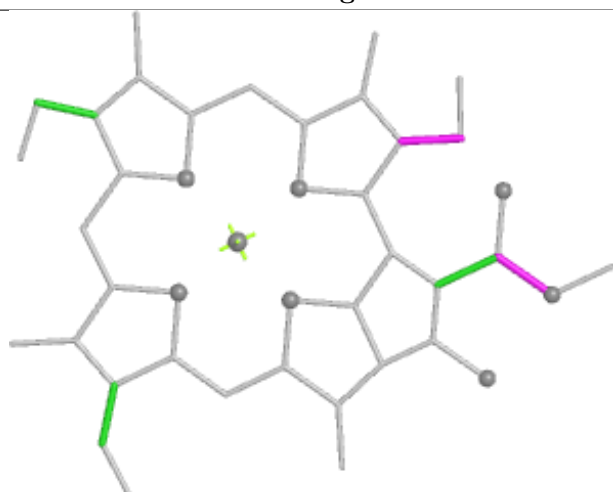
Ligand CLA d 316



Bond lengths



Bond angles

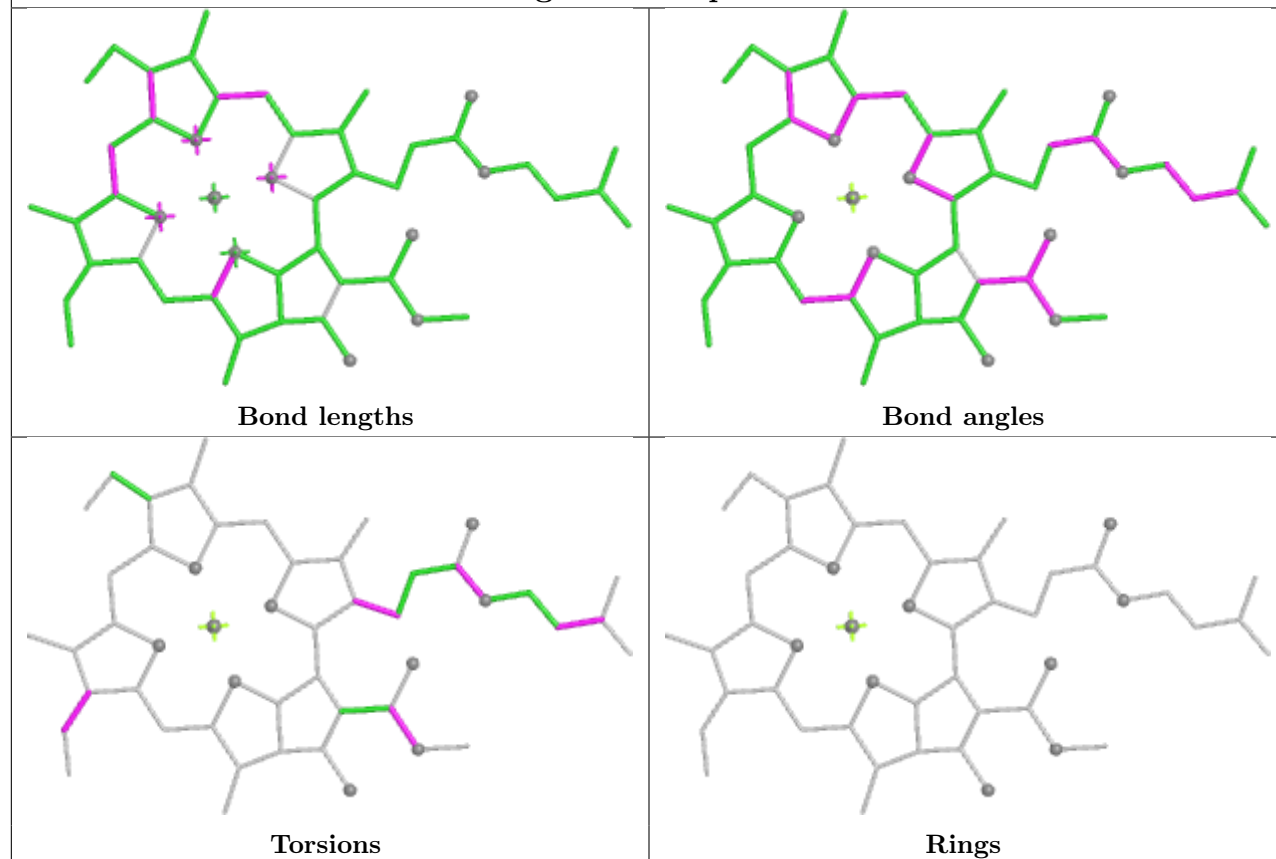


Torsions

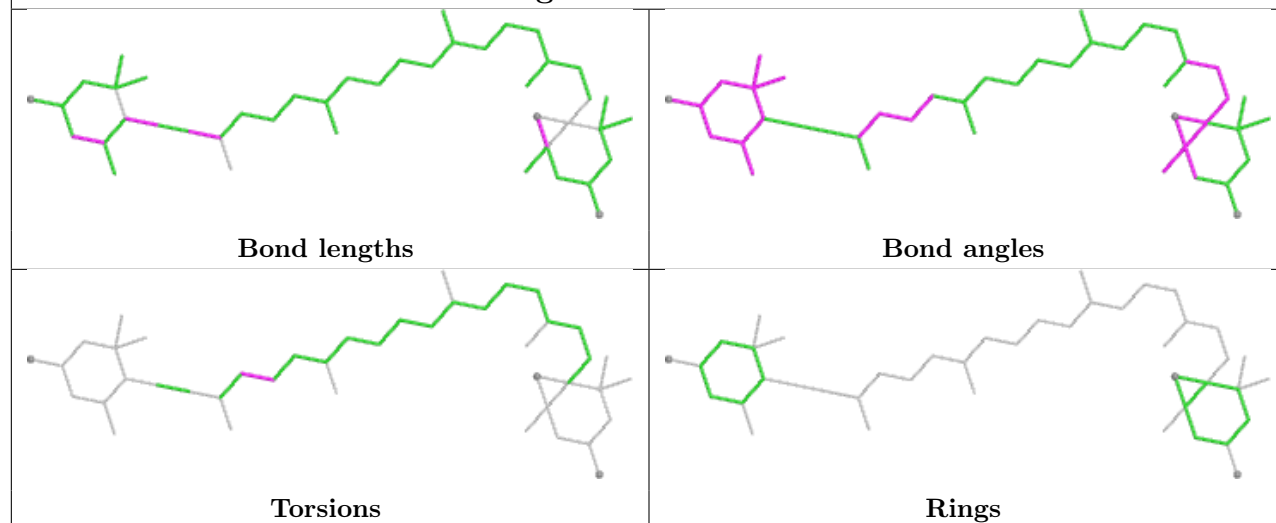


Rings

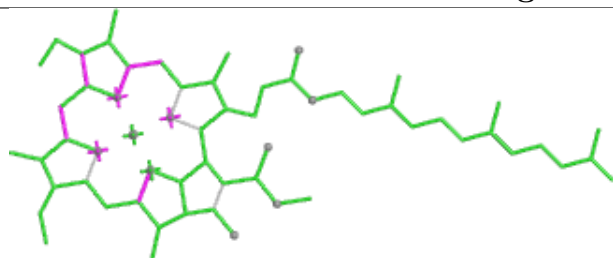
Ligand CLA p 606



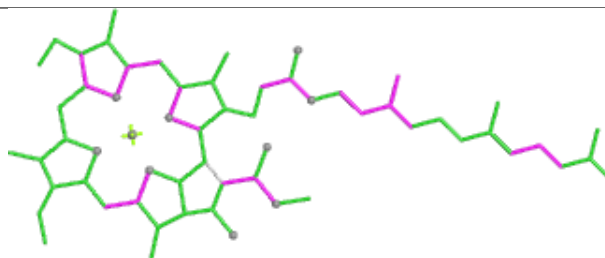
Ligand DD6 b 215



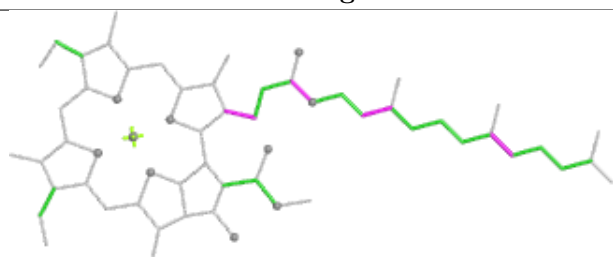
Ligand CLA h 206



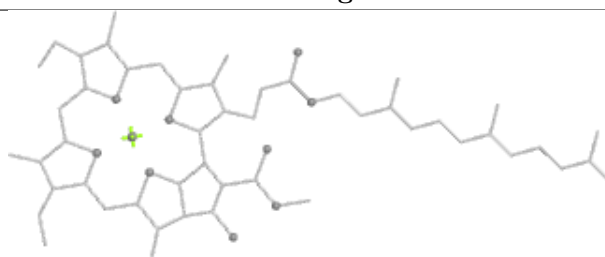
Bond lengths



Bond angles

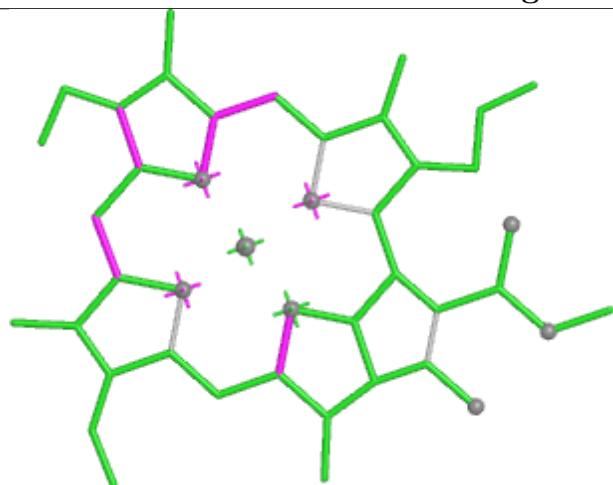


Torsions

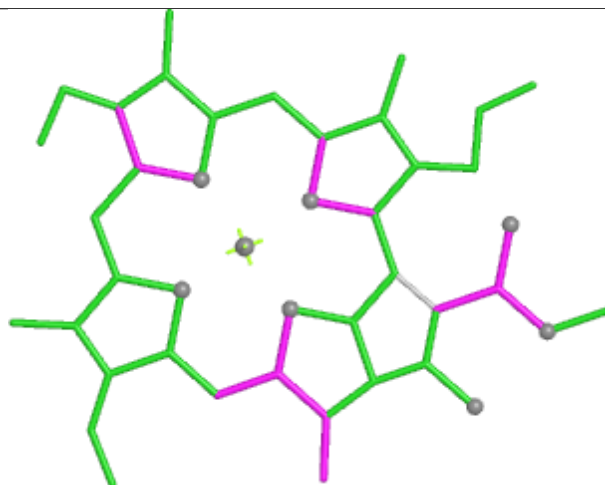


Rings

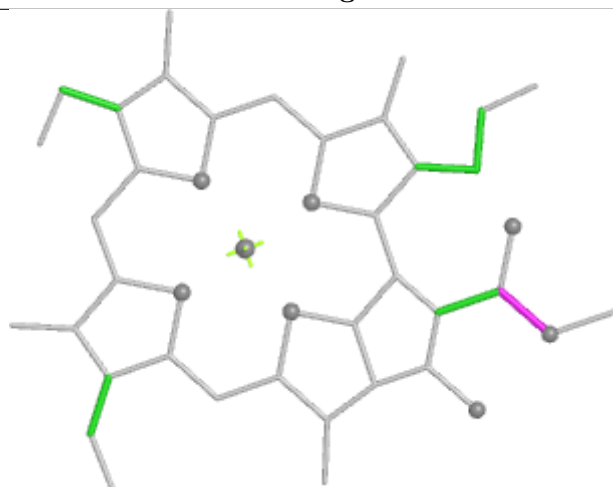
Ligand CLA f 603



Bond lengths



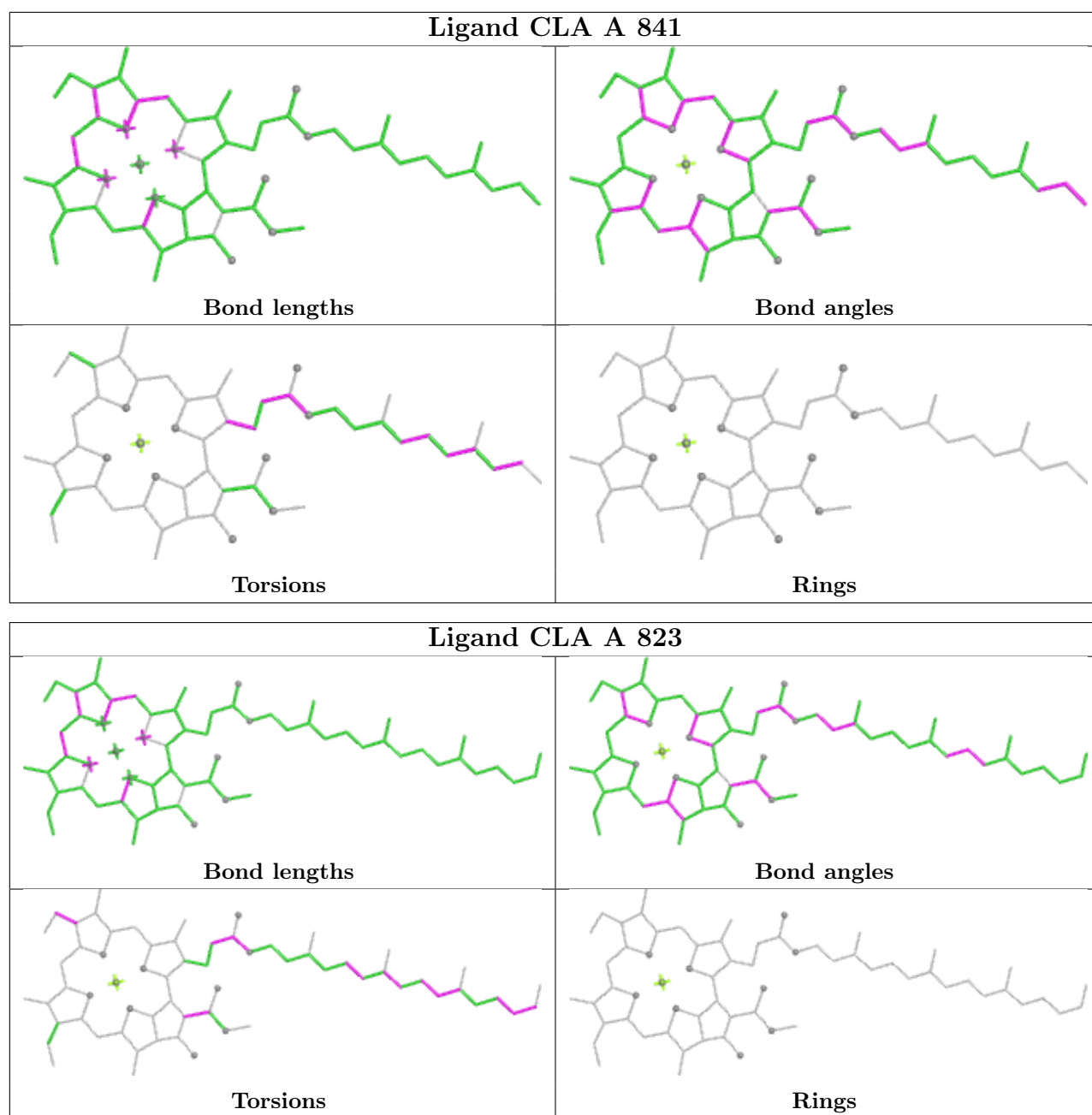
Bond angles



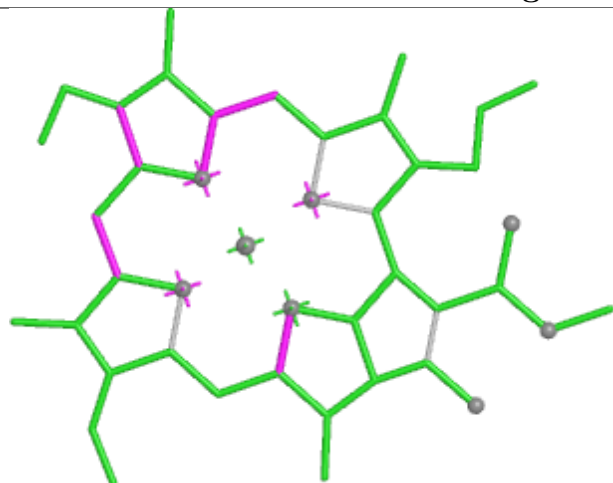
Torsions



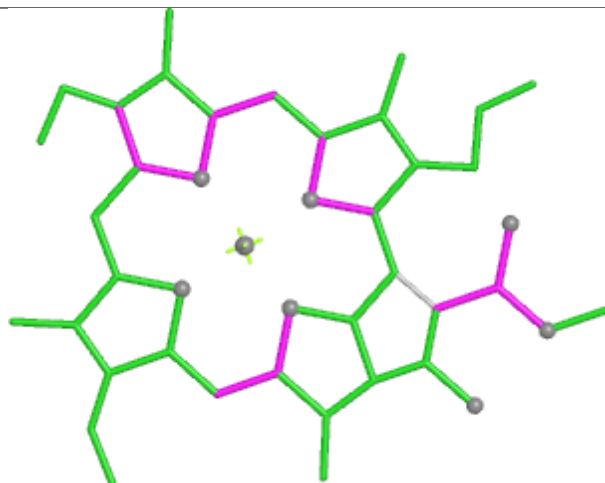
Rings



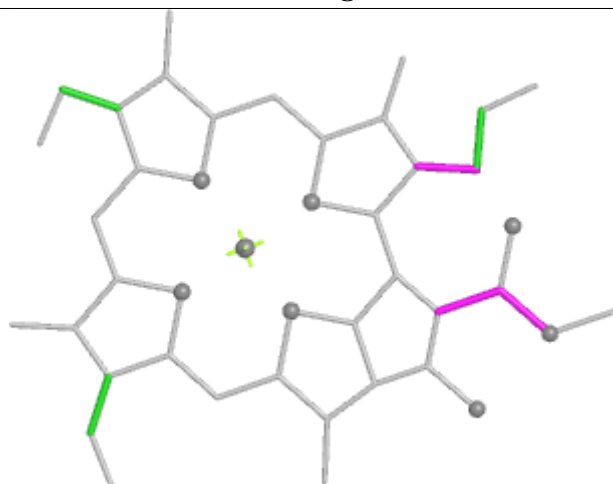
Ligand CLA i 209



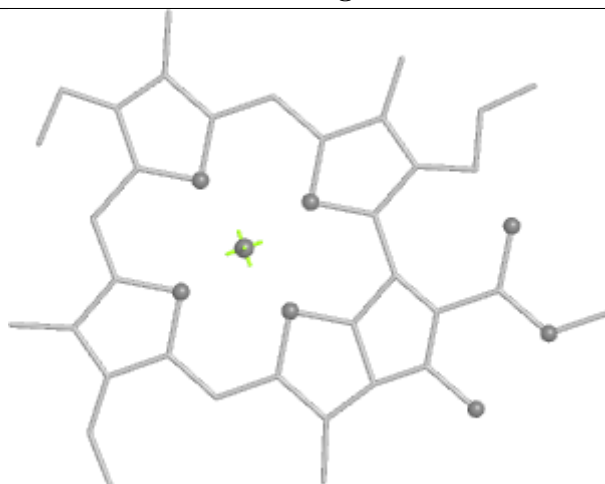
Bond lengths



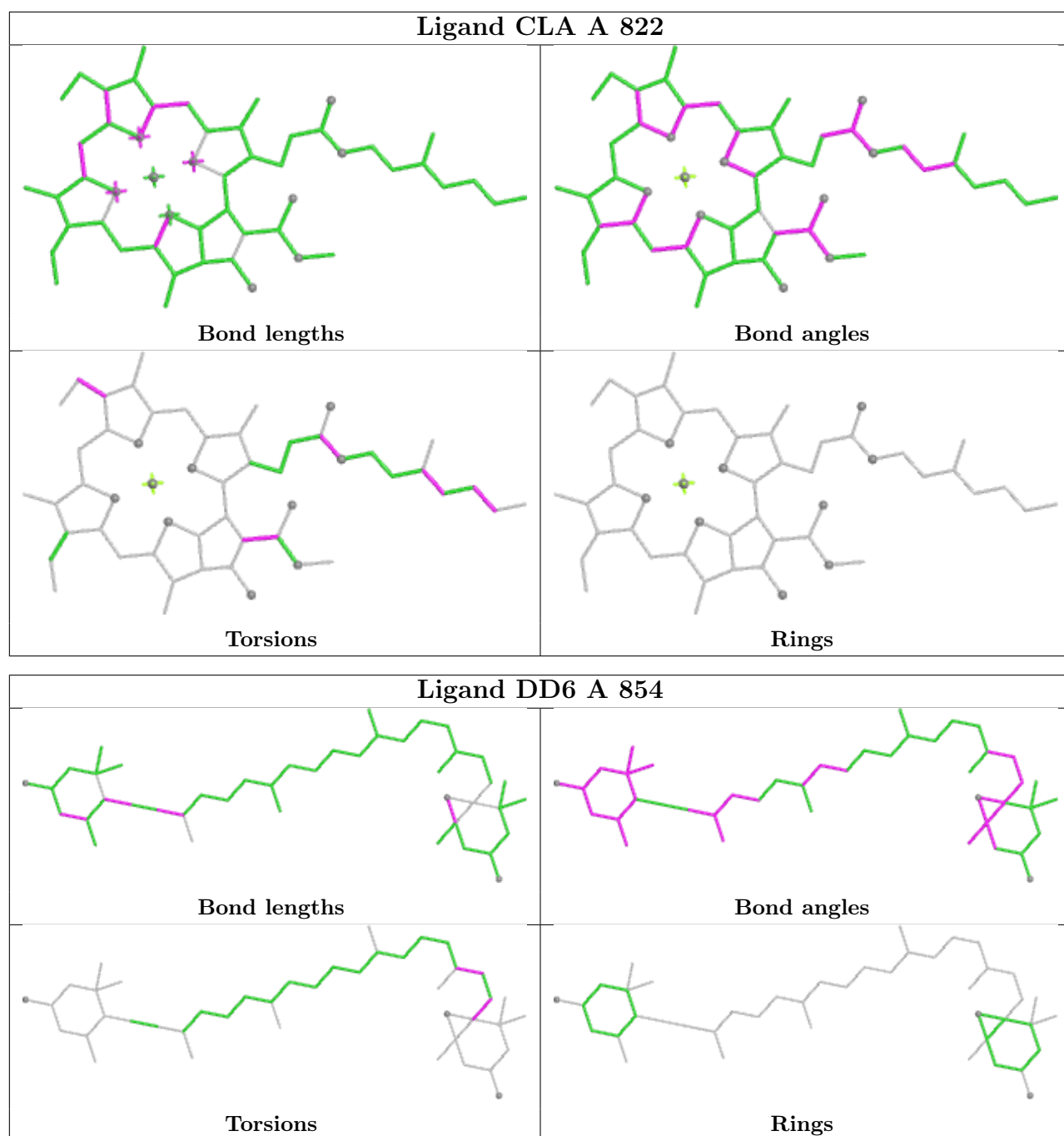
Bond angles



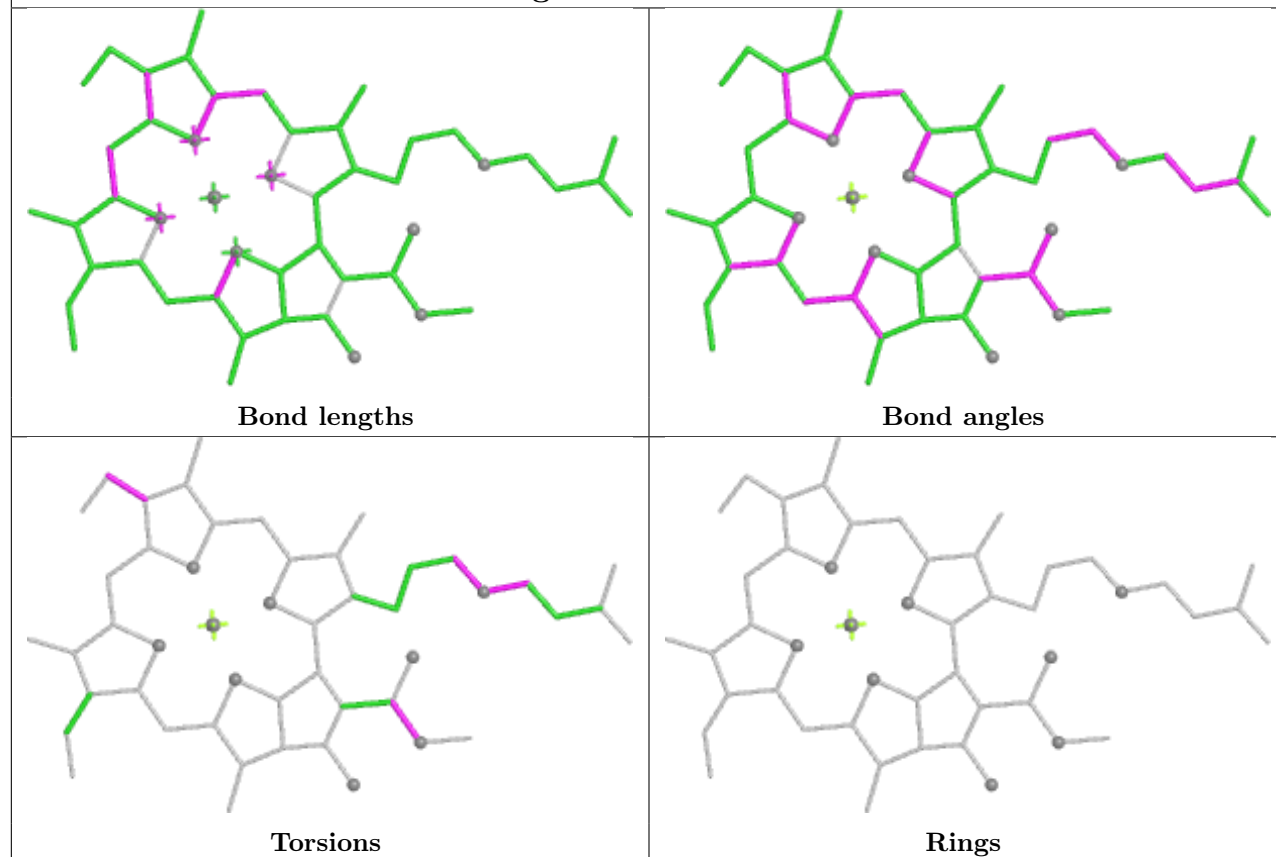
Torsions



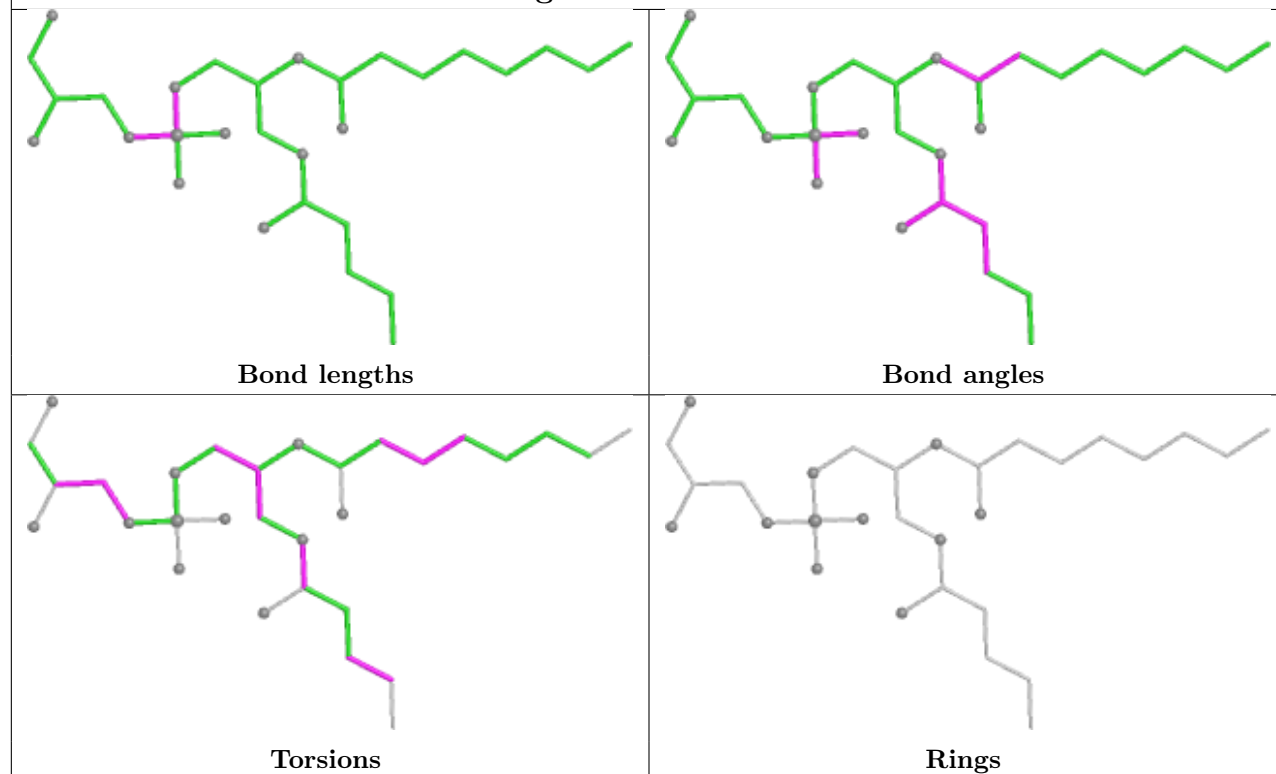
Rings



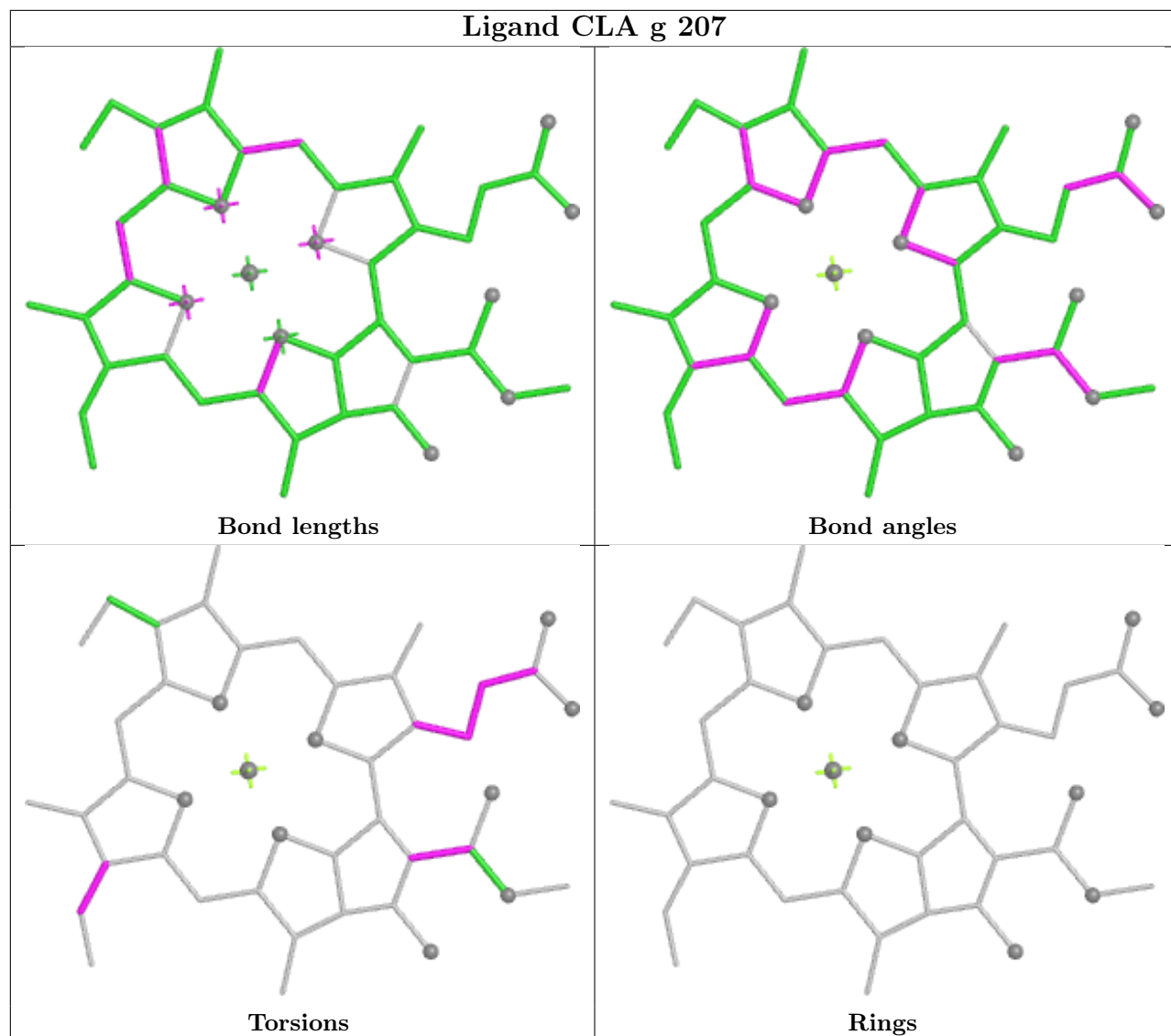
Ligand CLA B 813



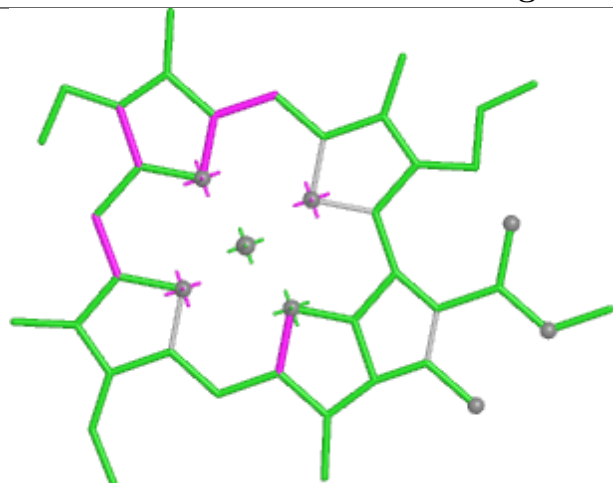
Ligand LHG c 301



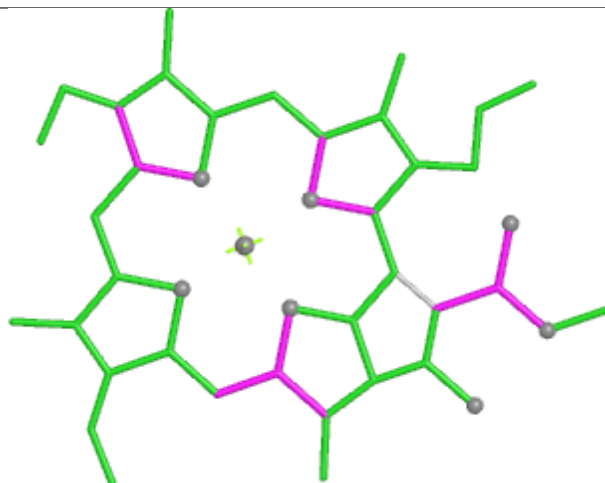
Ligand CLA g 207



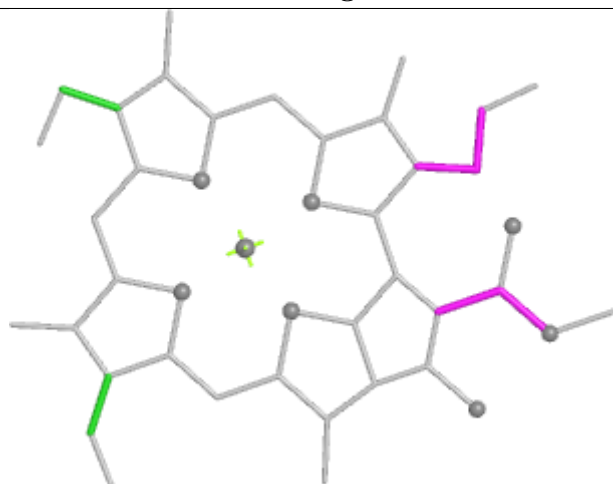
Ligand CLA a 211



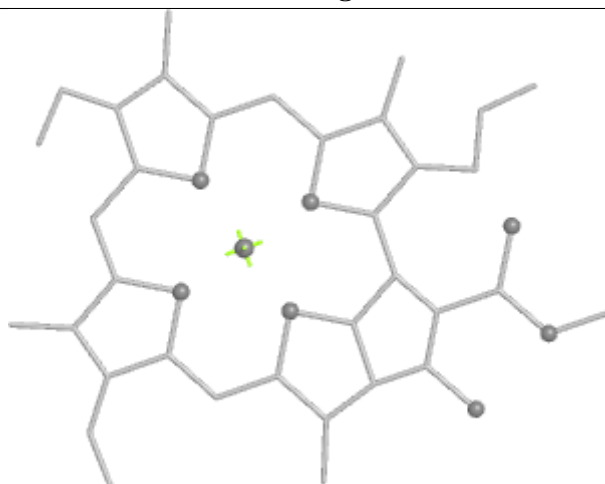
Bond lengths



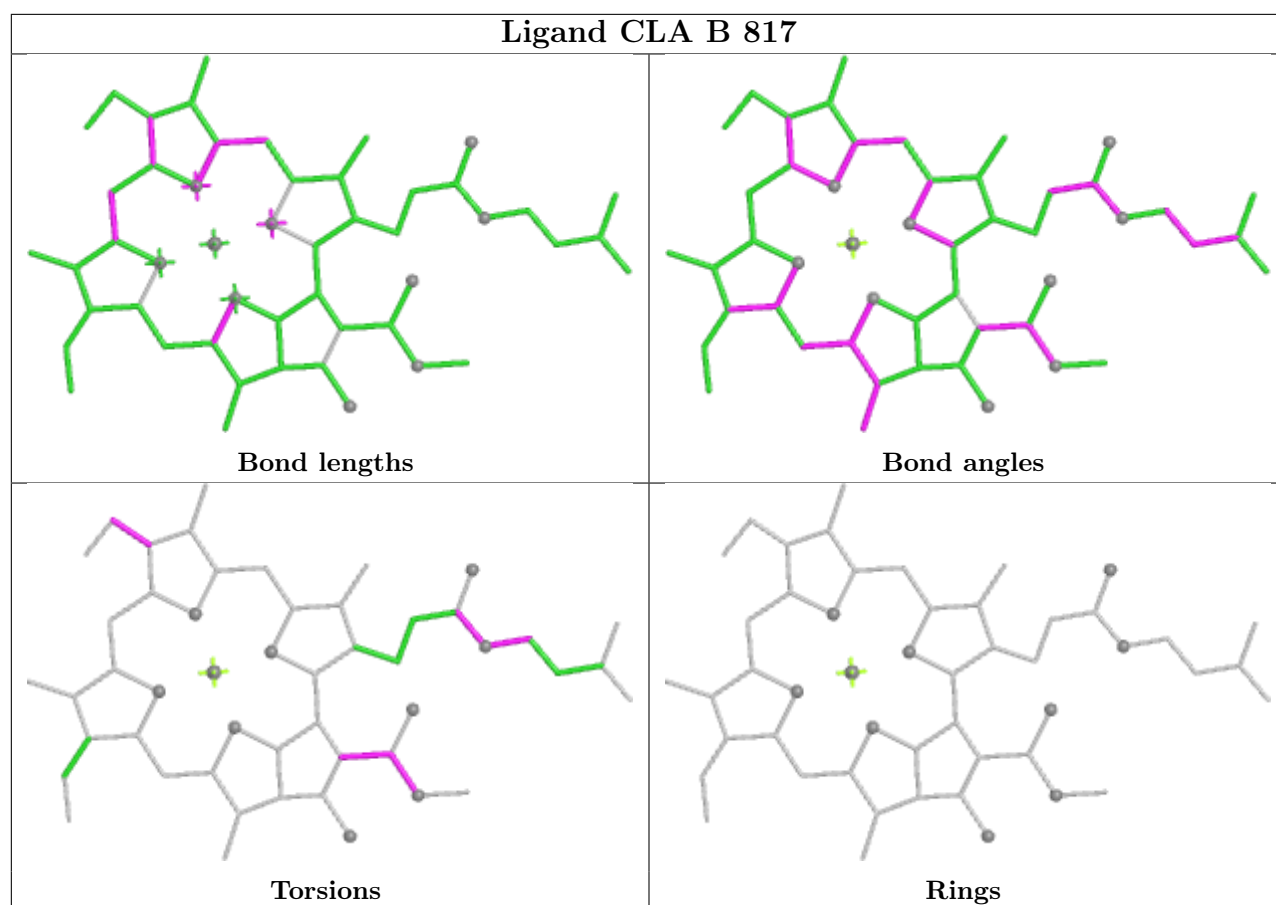
Bond angles



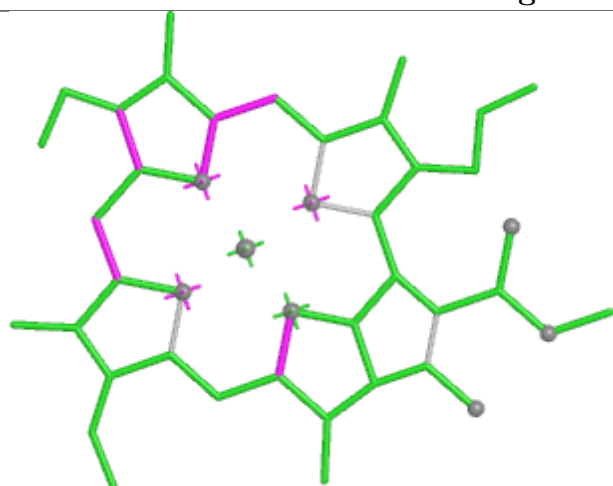
Torsions



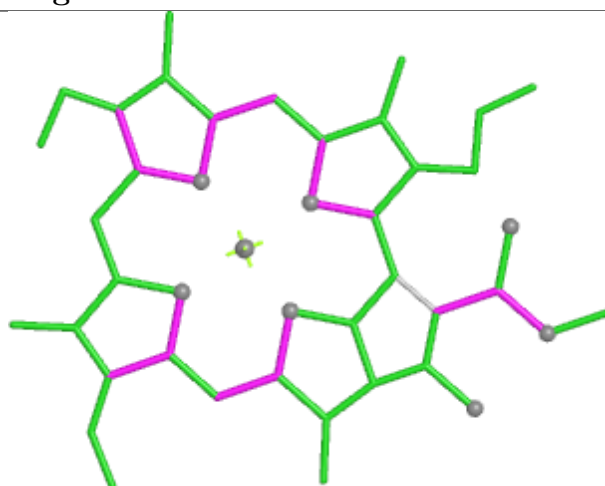
Rings



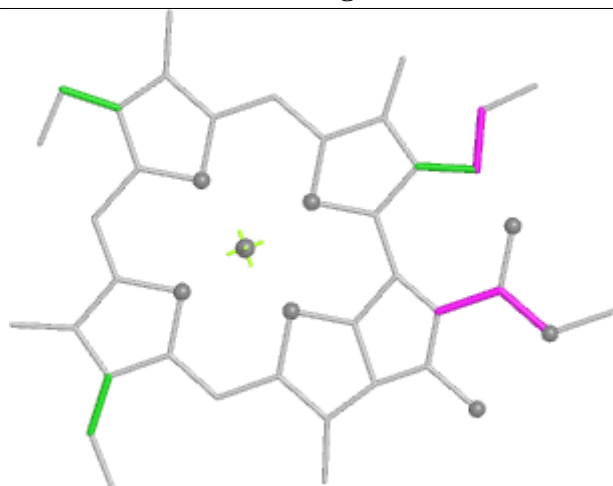
Ligand CLA g 206



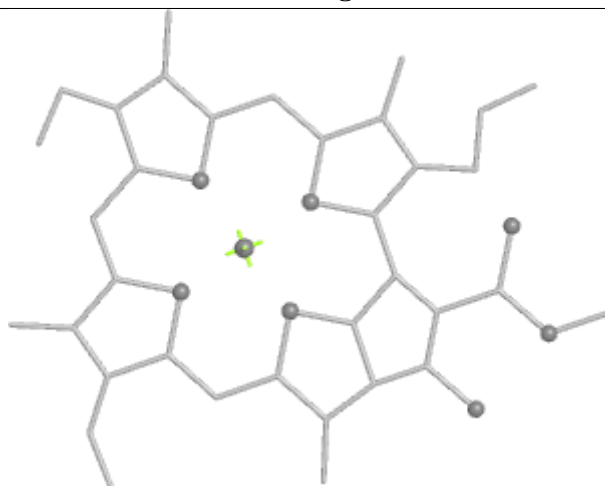
Bond lengths



Bond angles

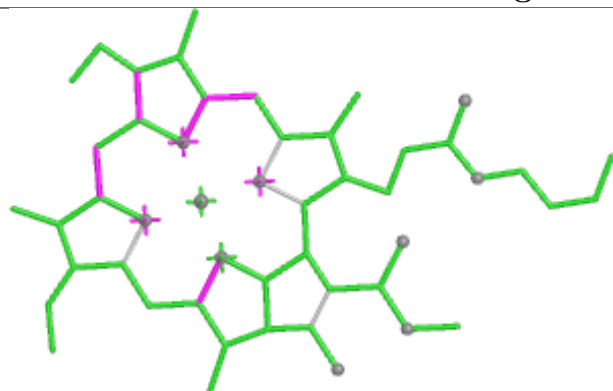


Torsions

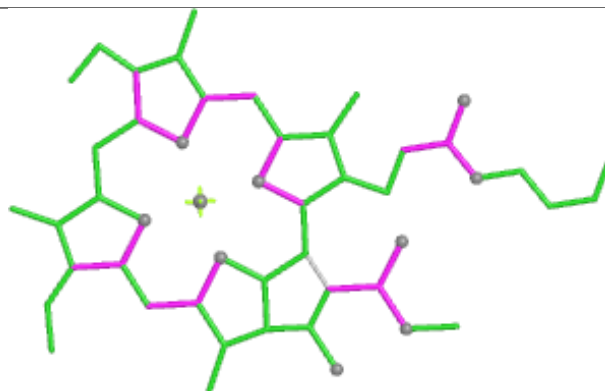


Rings

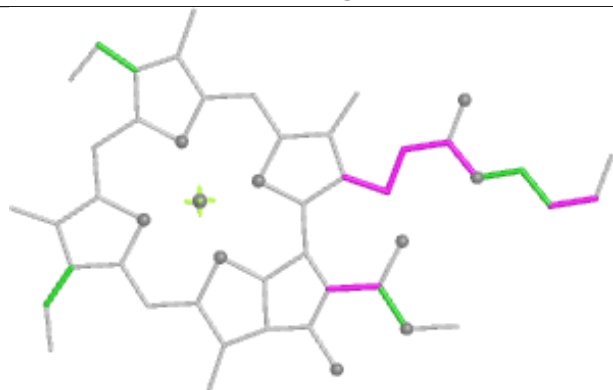
Ligand CLA B 815



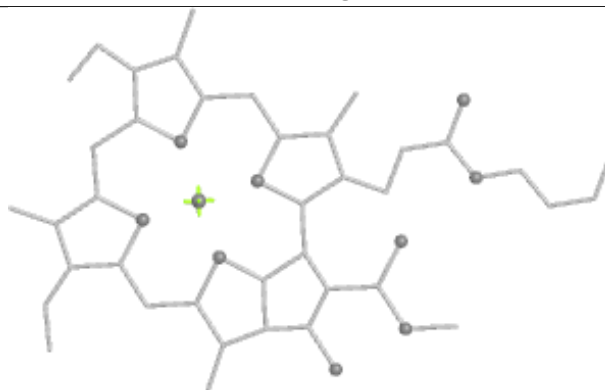
Bond lengths



Bond angles

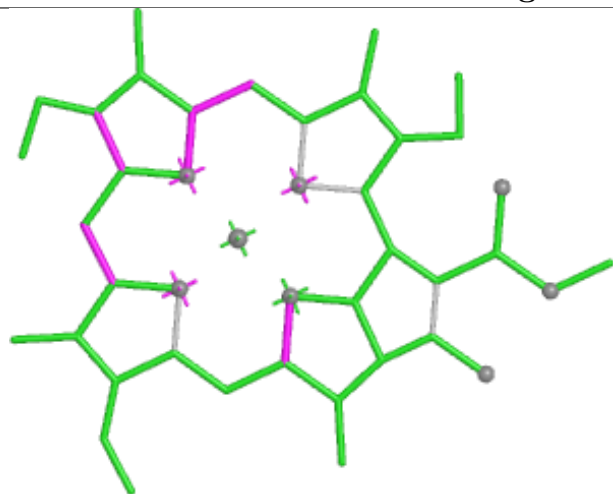


Torsions

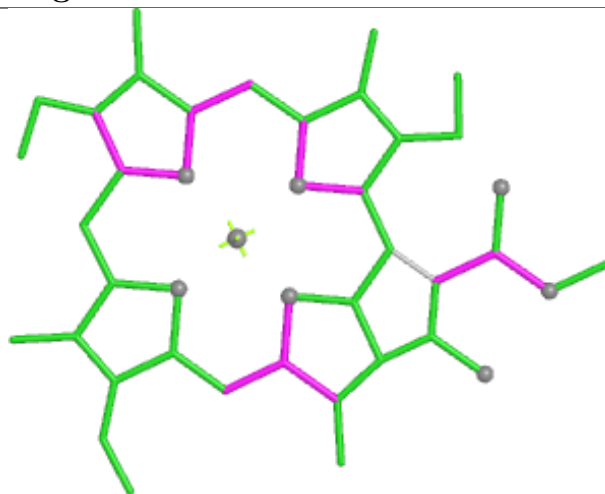


Rings

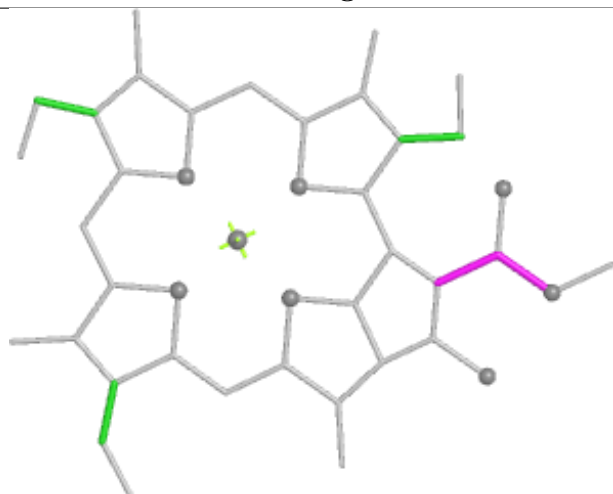
Ligand CLA g 211



Bond lengths



Bond angles

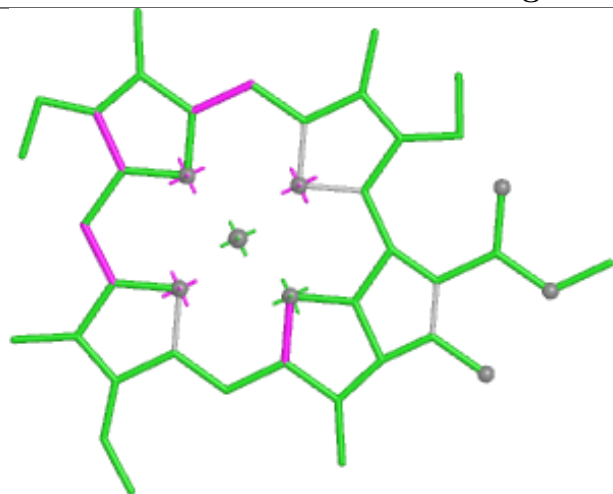


Torsions

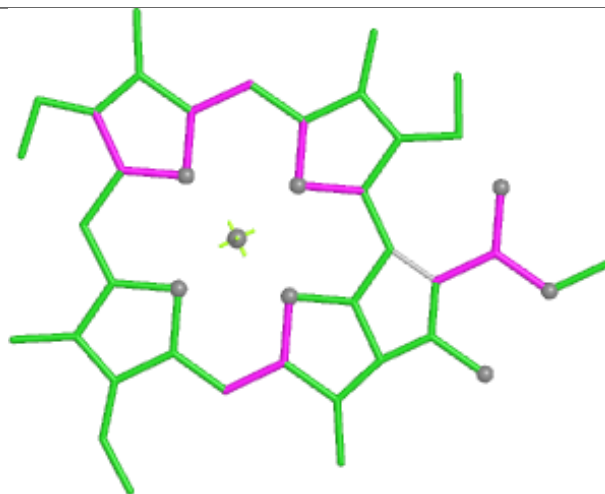


Rings

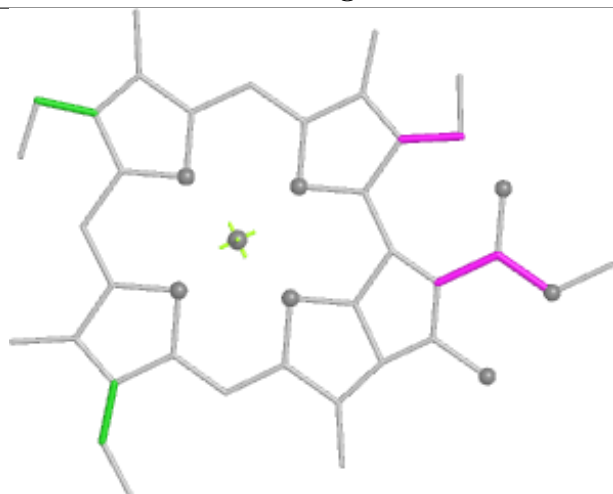
Ligand CLA 1 601



Bond lengths



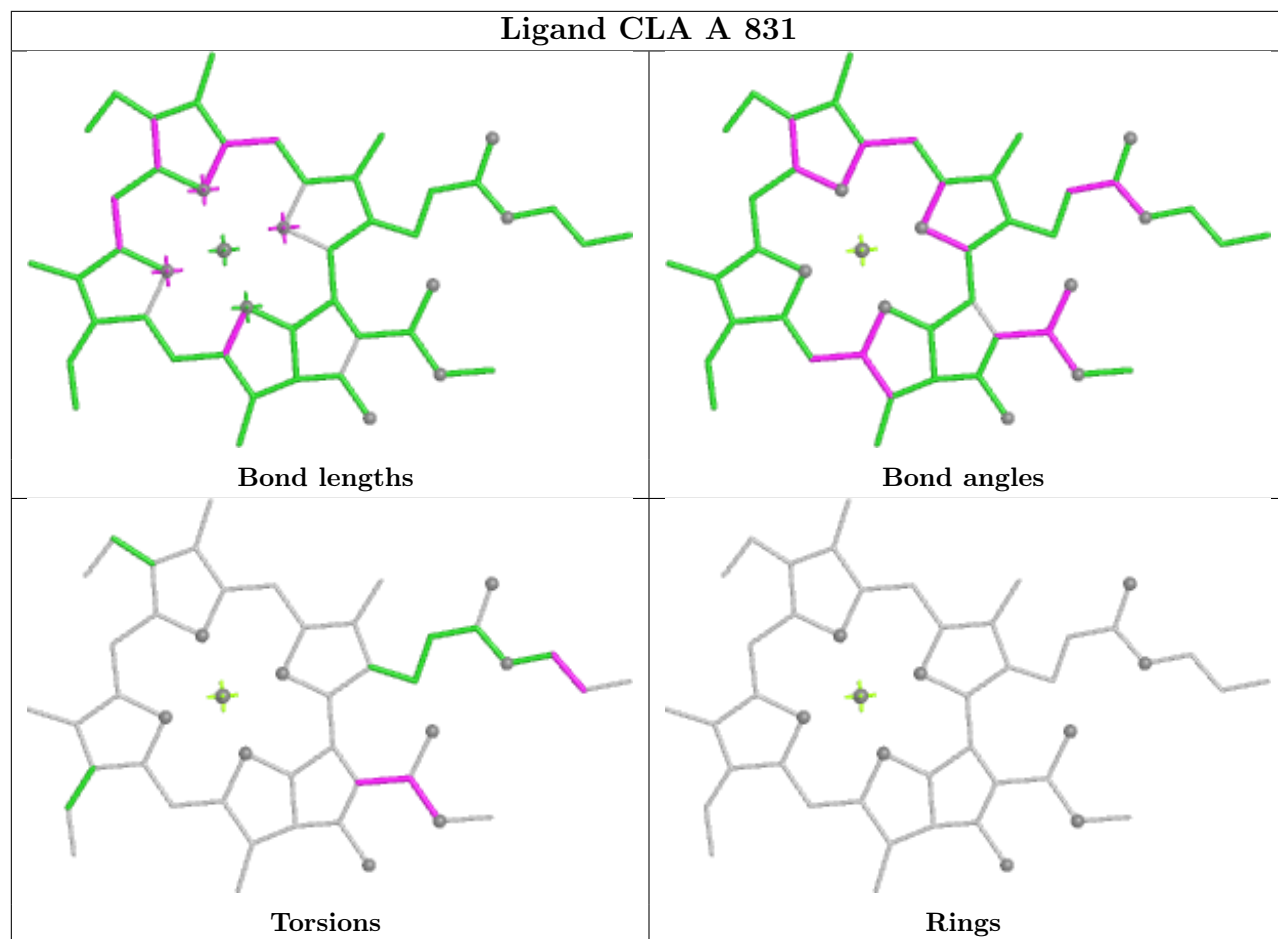
Bond angles



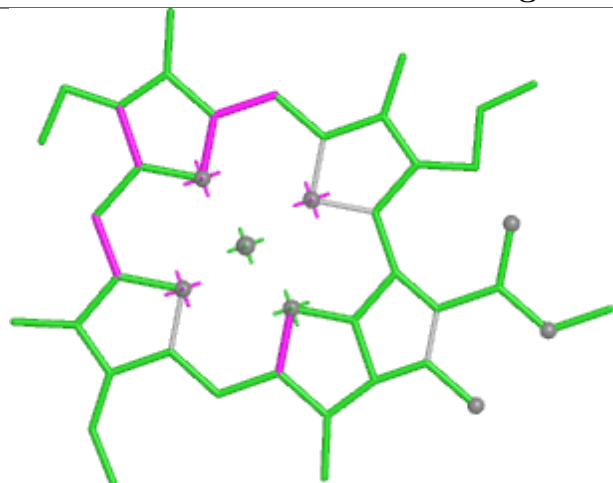
Torsions



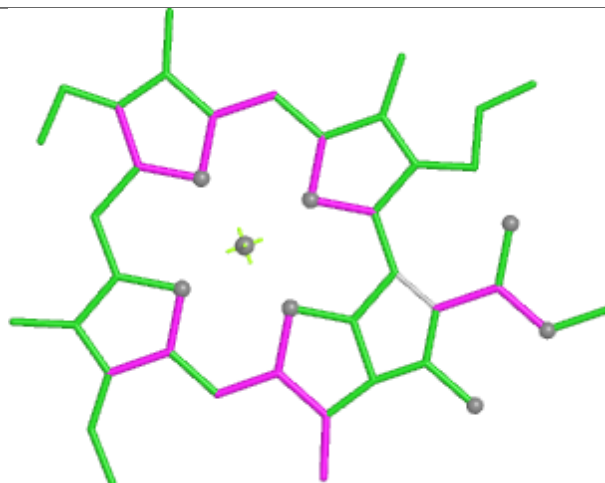
Rings



Ligand CLA e 210



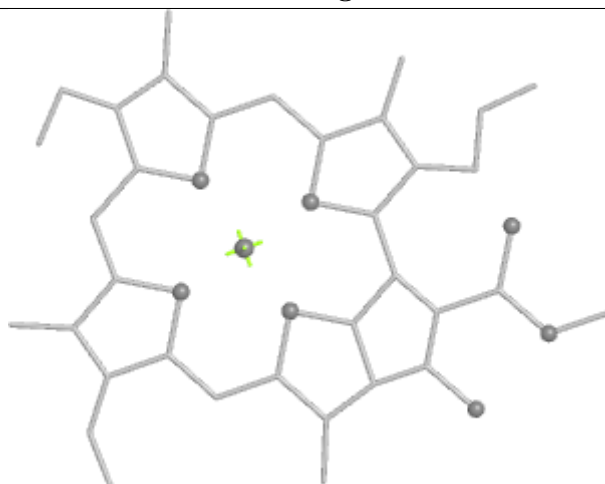
Bond lengths



Bond angles

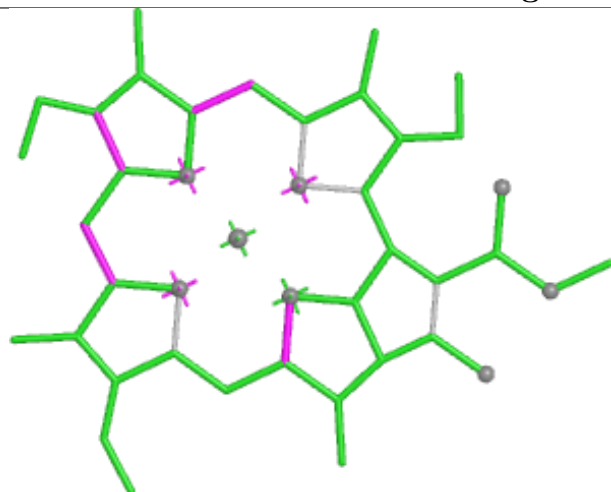


Torsions

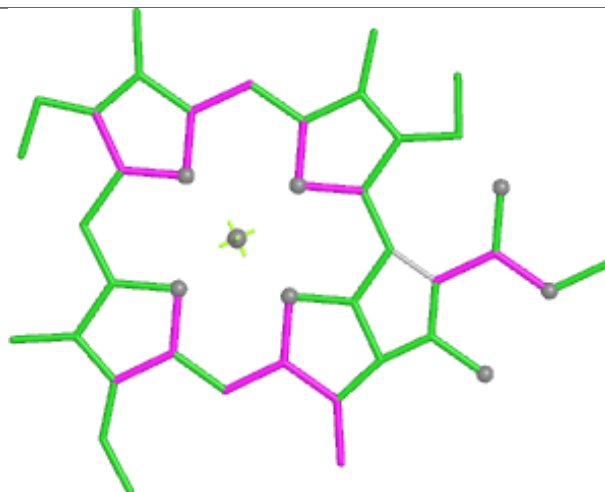


Rings

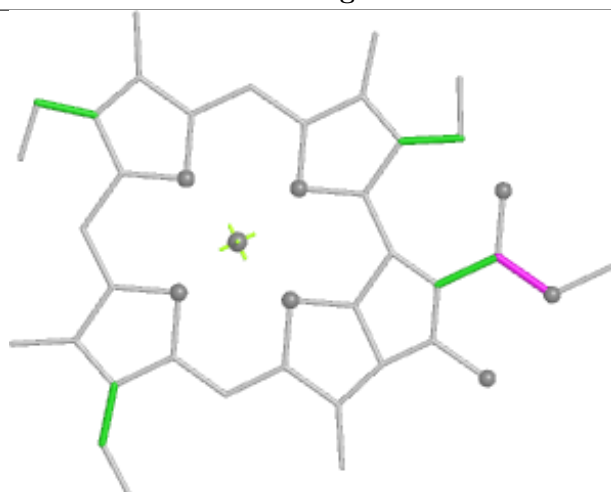
Ligand CLA f 605



Bond lengths



Bond angles

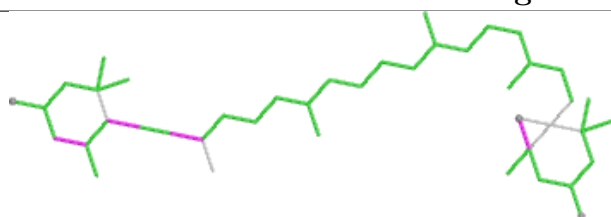


Torsions

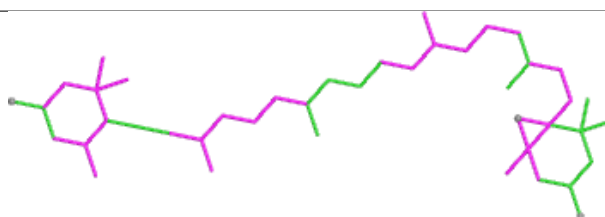


Rings

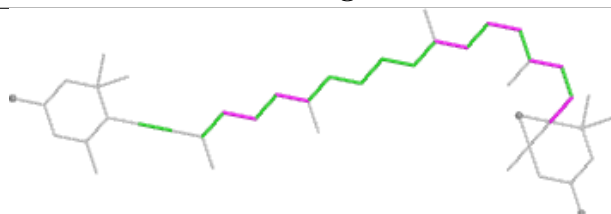
Ligand DD6 A 855



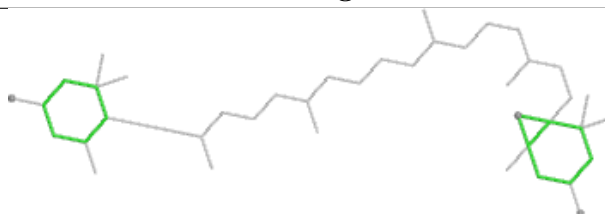
Bond lengths



Bond angles

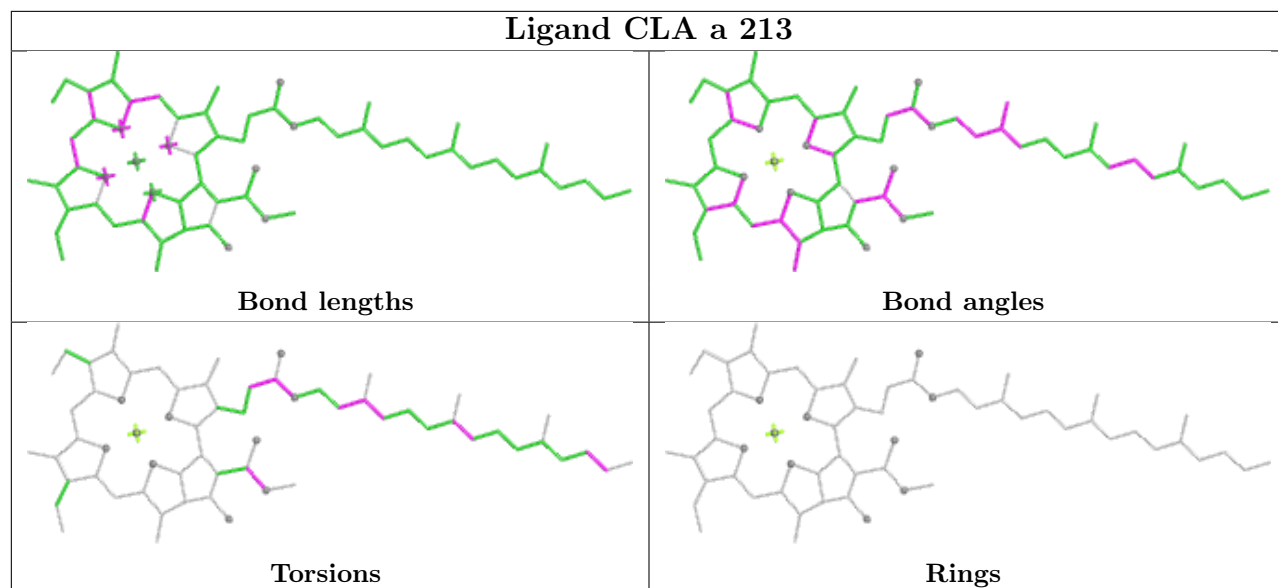


Torsions

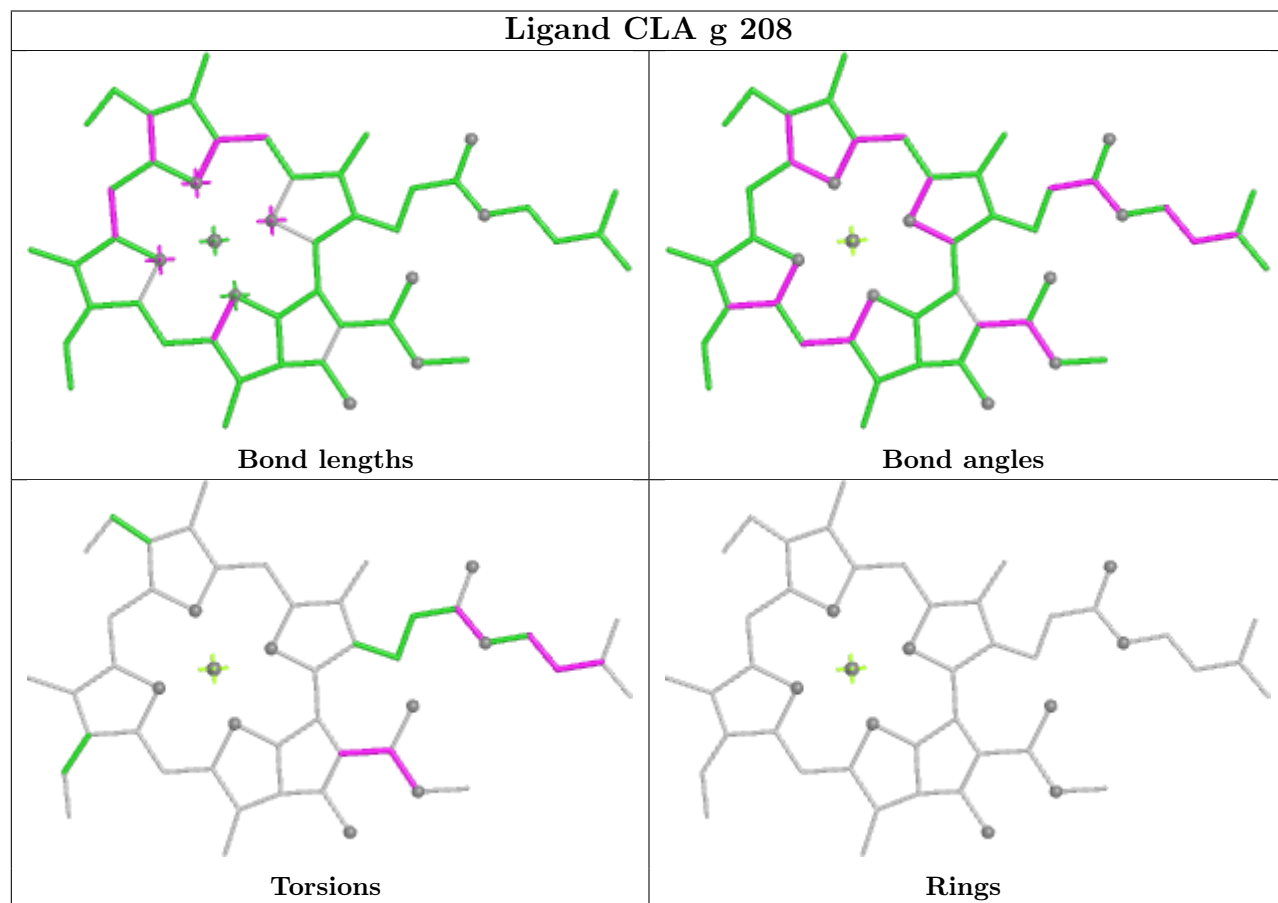


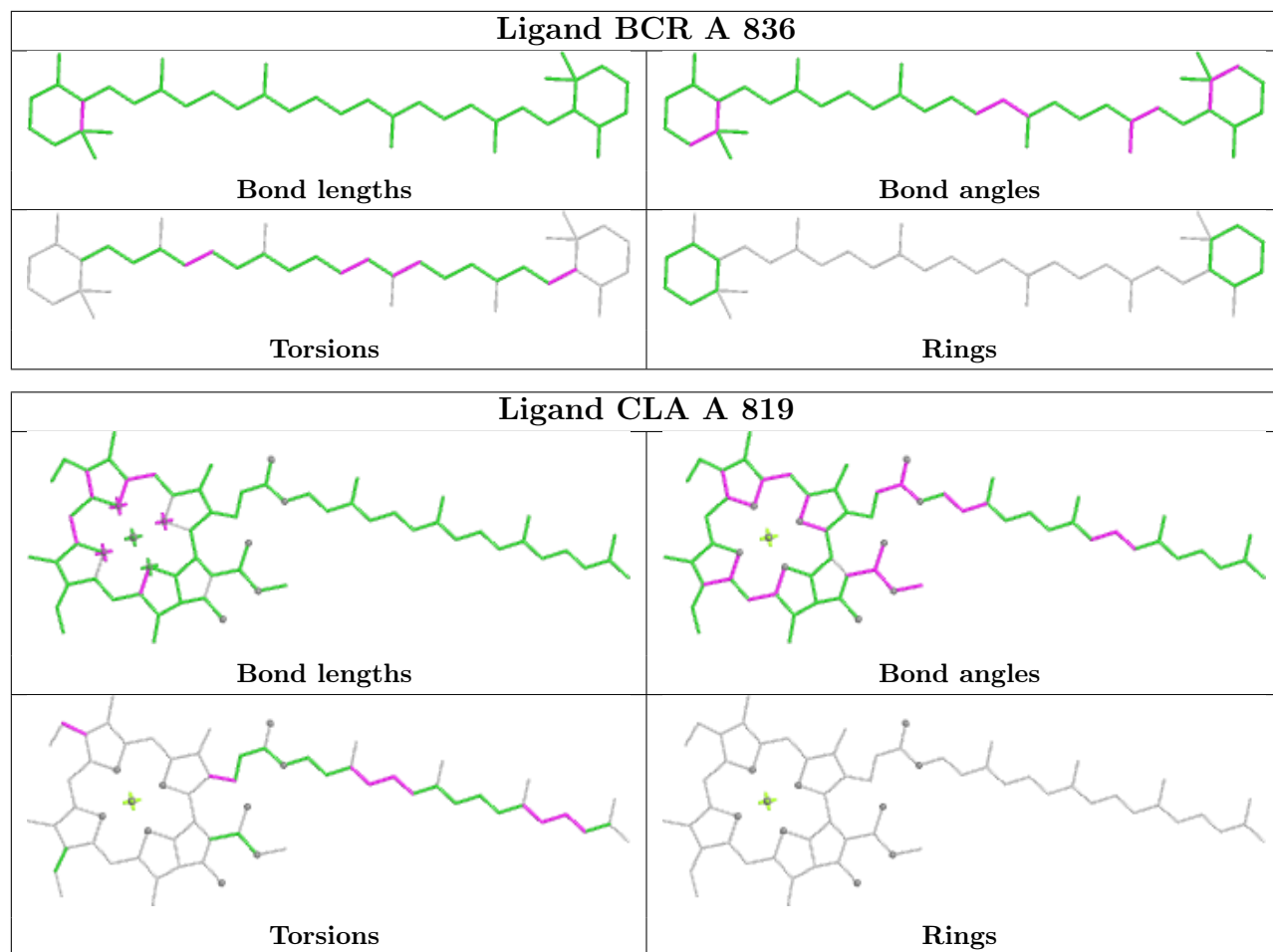
Rings

Ligand CLA a 213

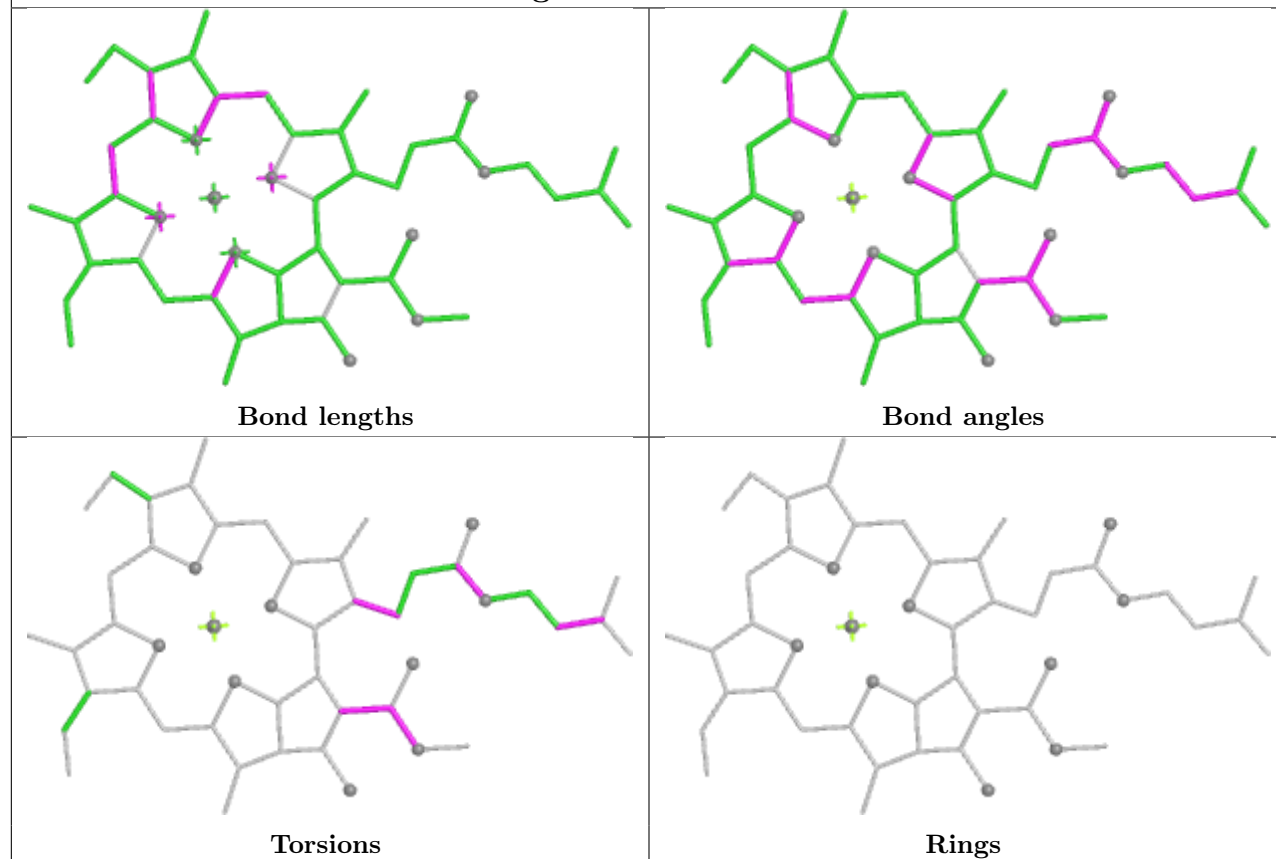


Ligand CLA g 208

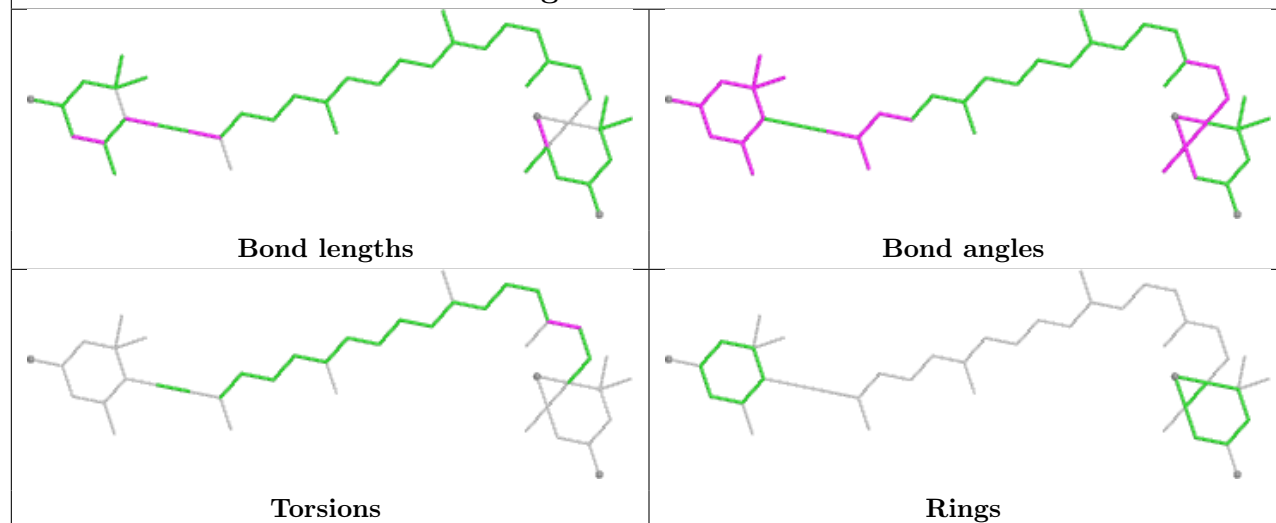


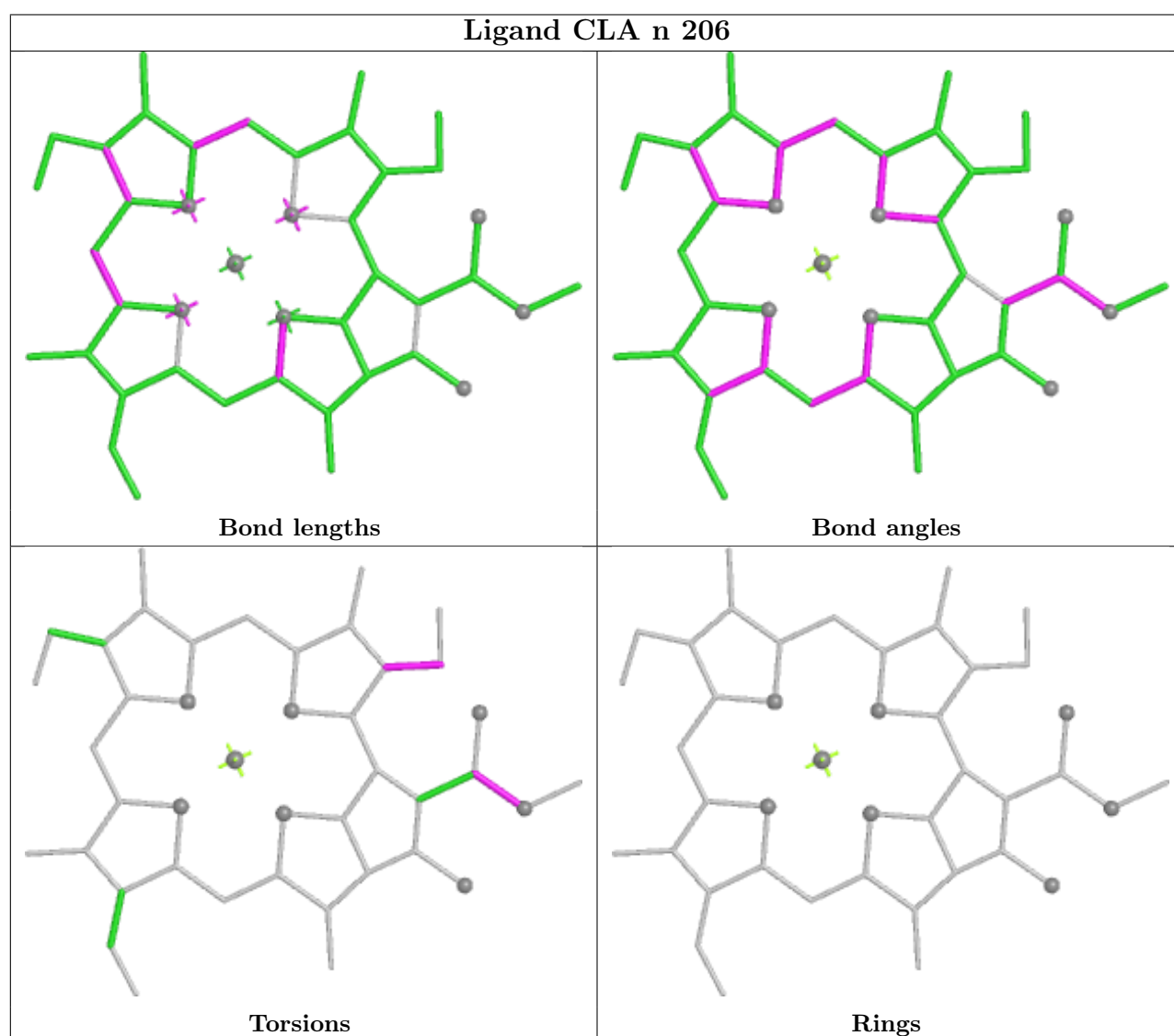
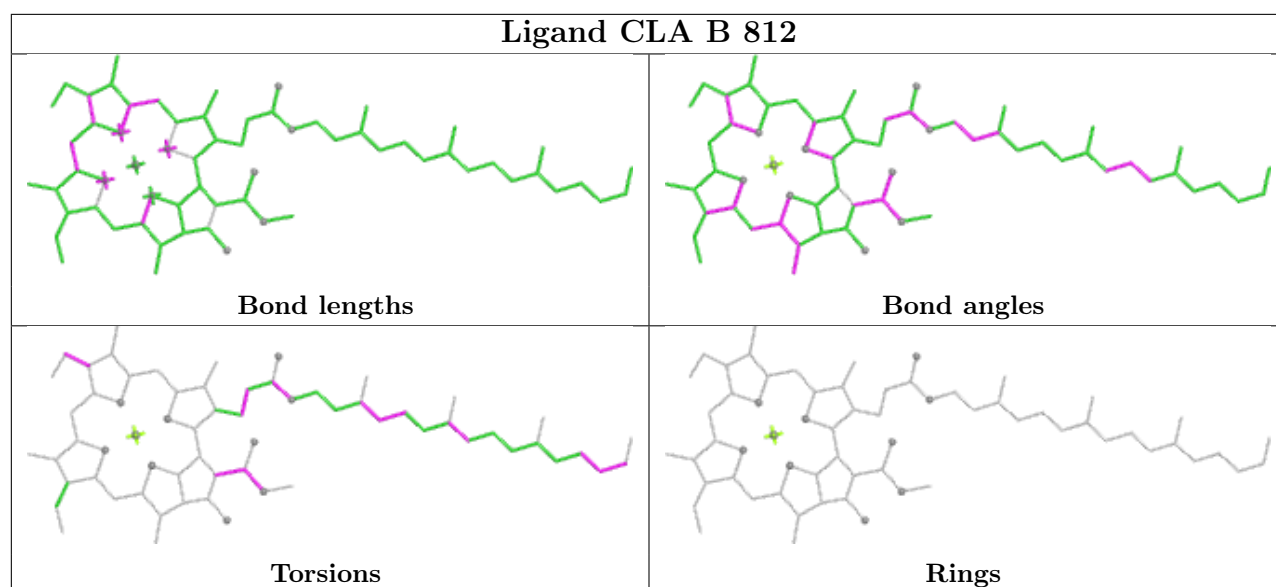


Ligand CLA B 840

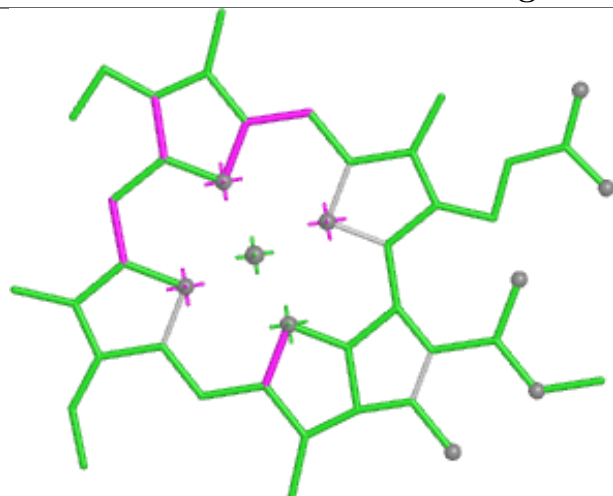


Ligand DD6 i 216

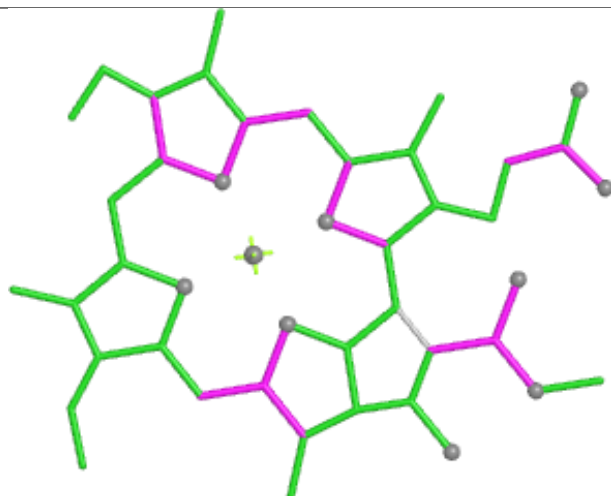




Ligand CLA a 210



Bond lengths



Bond angles

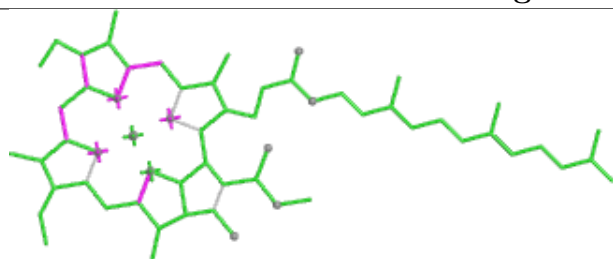


Torsions

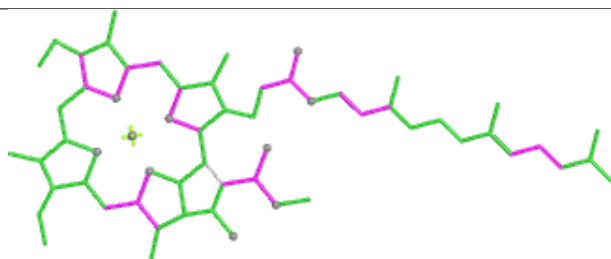


Rings

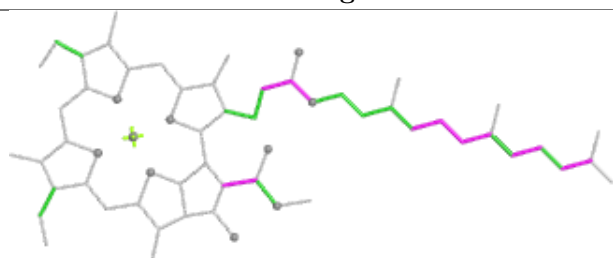
Ligand CLA A 808



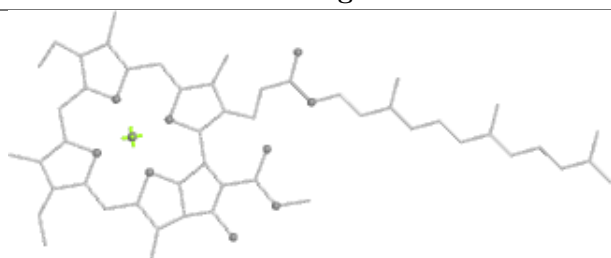
Bond lengths



Bond angles

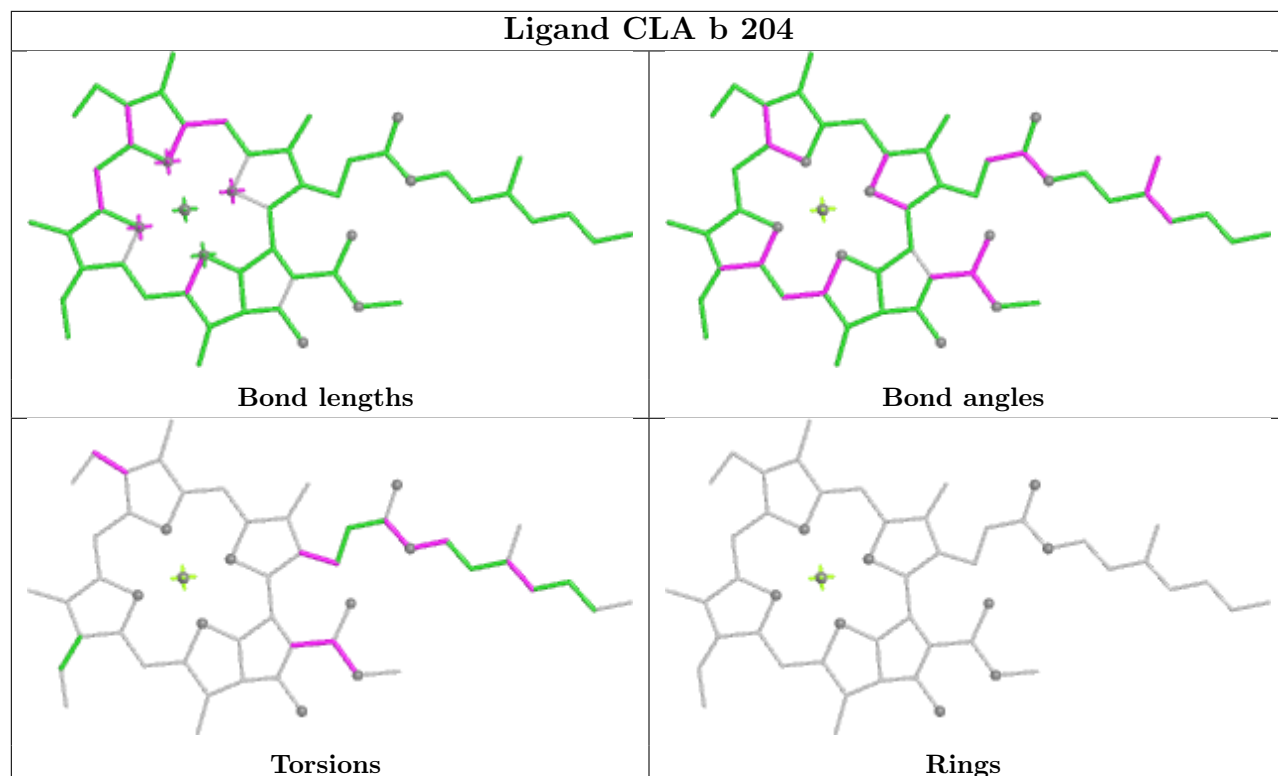


Torsions

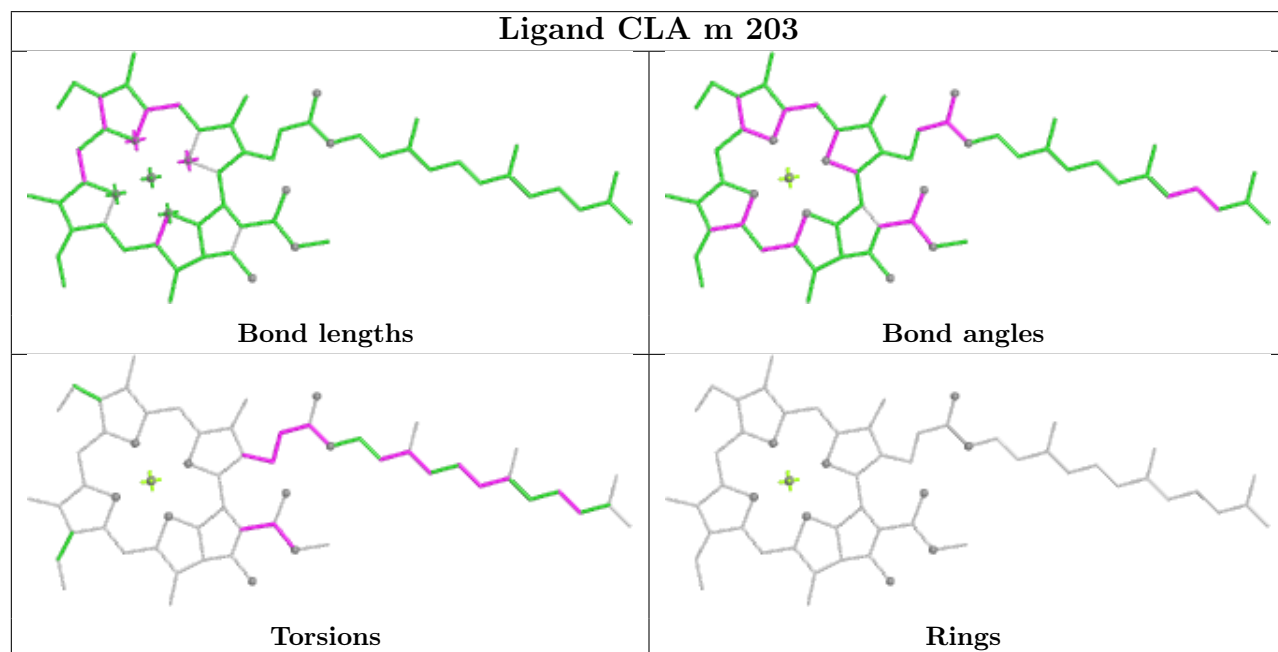


Rings

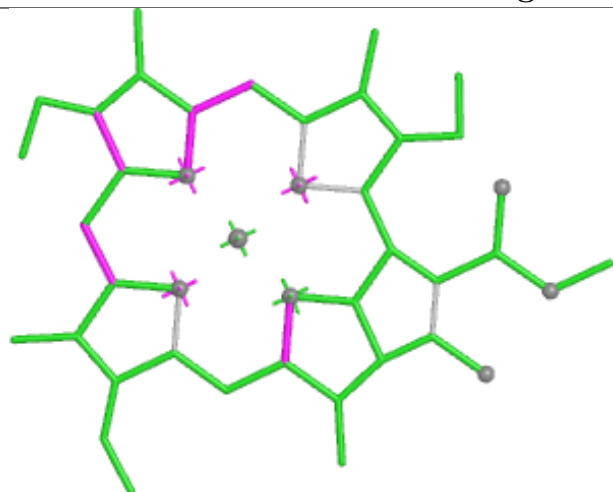
Ligand CLA b 204



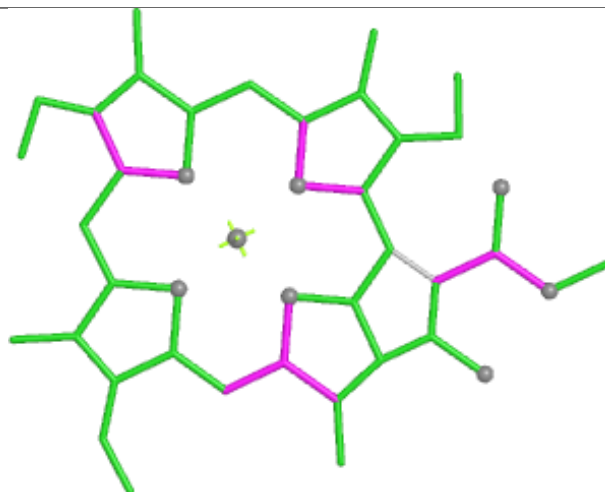
Ligand CLA m 203



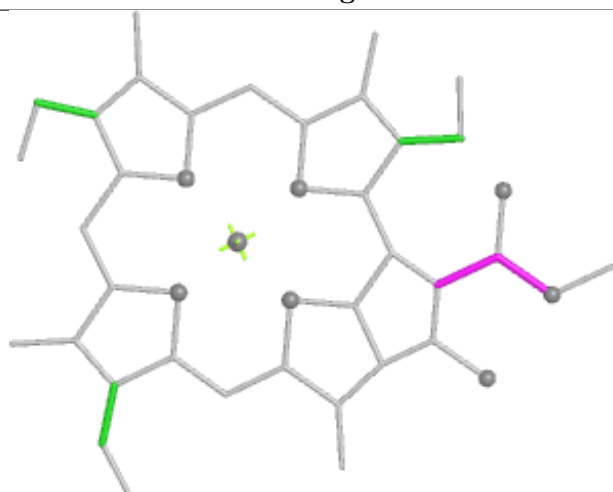
Ligand CLA d 314



Bond lengths



Bond angles

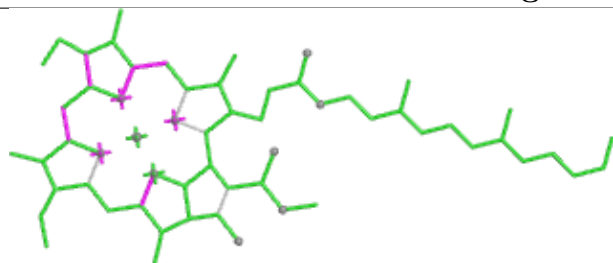


Torsions

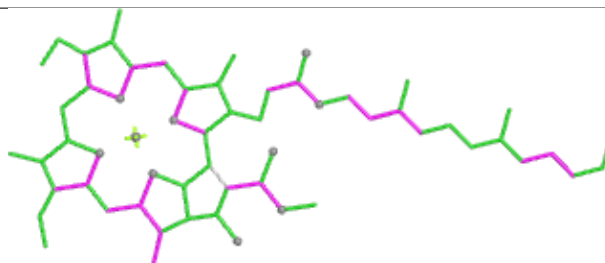


Rings

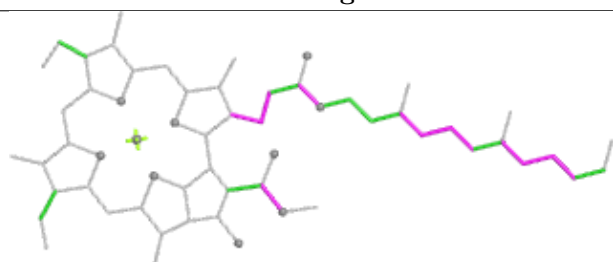
Ligand CLA f 610



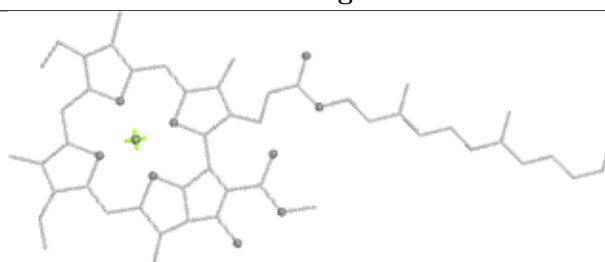
Bond lengths



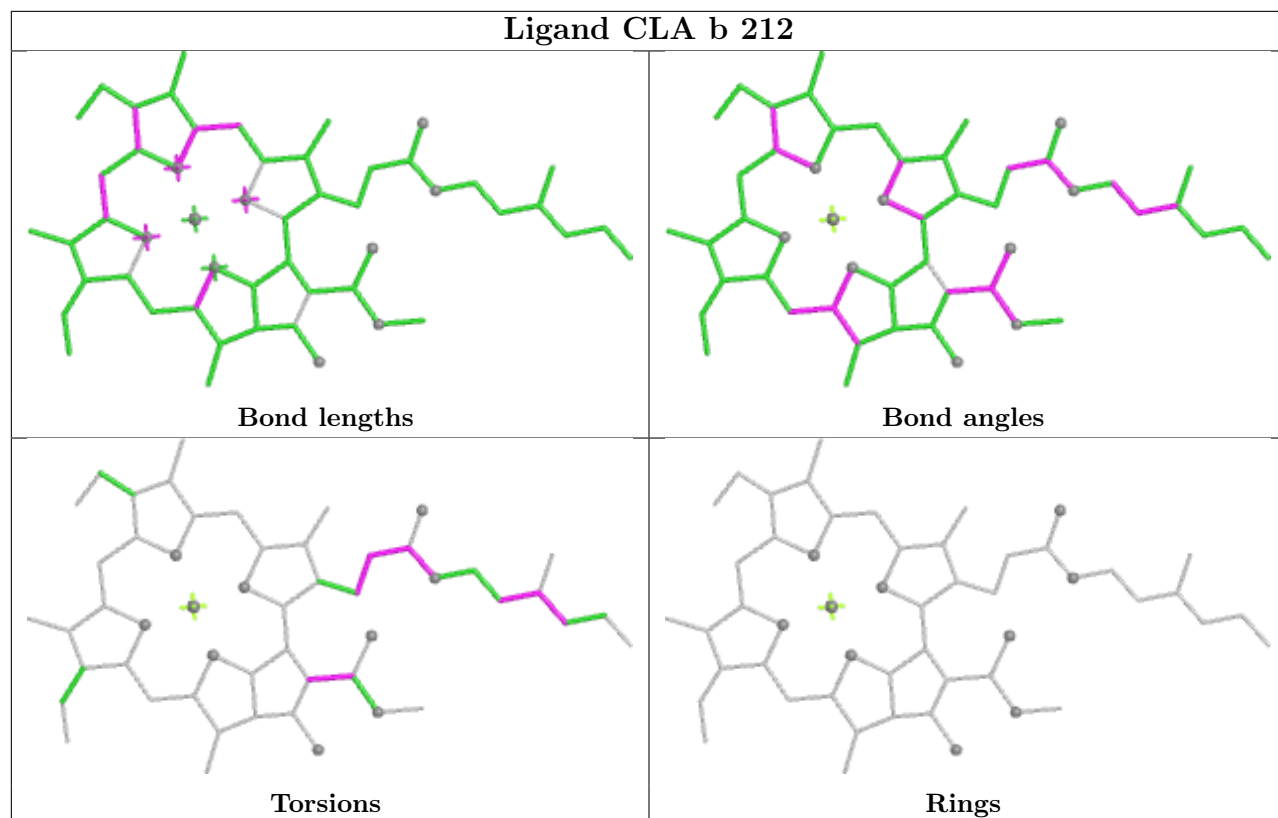
Bond angles



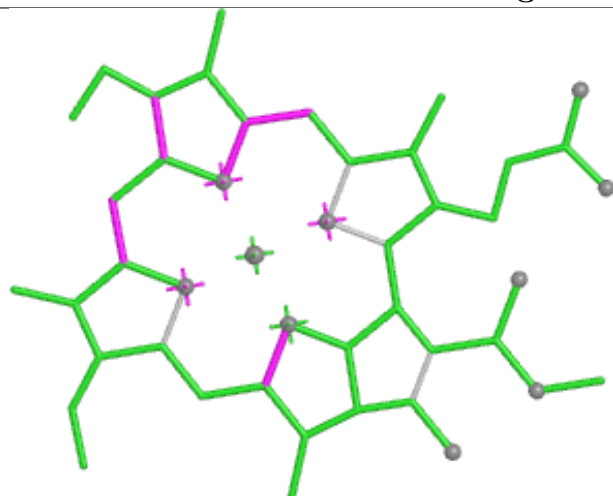
Torsions



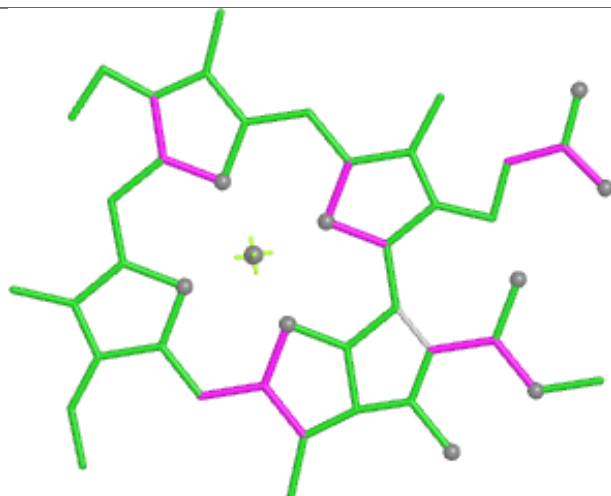
Rings



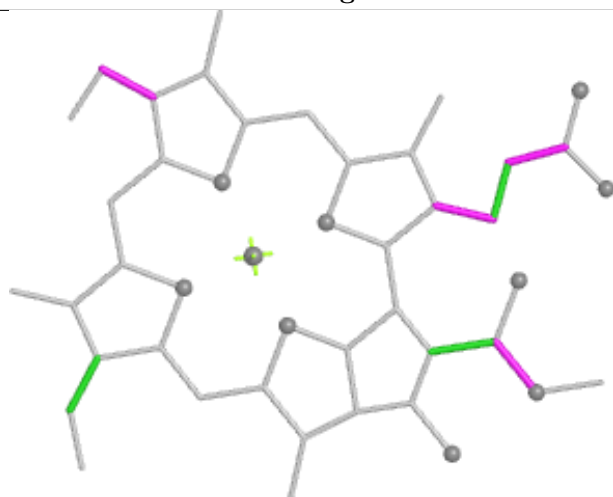
Ligand CLA n 208



Bond lengths



Bond angles

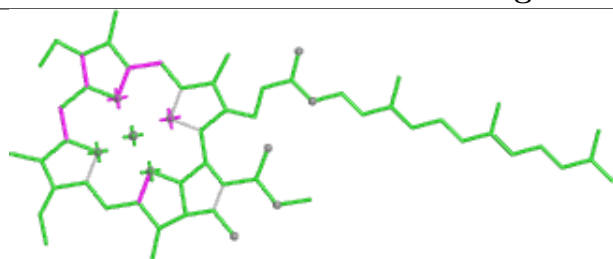


Torsions

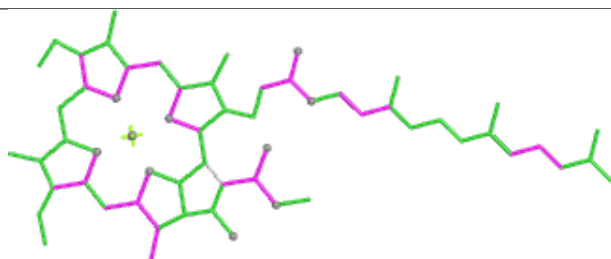


Rings

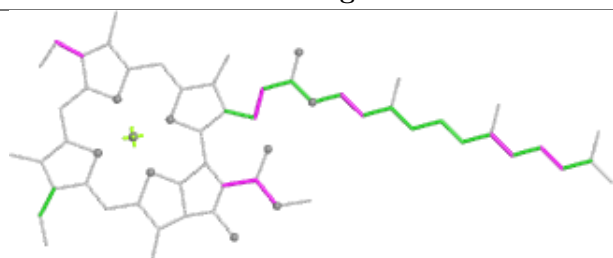
Ligand CLA B 816



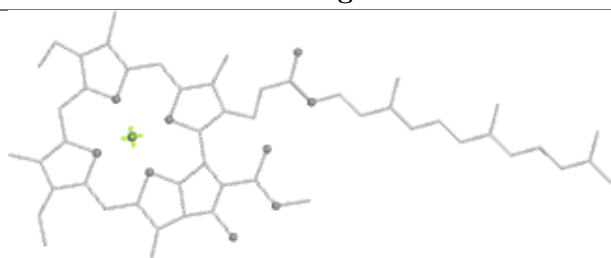
Bond lengths



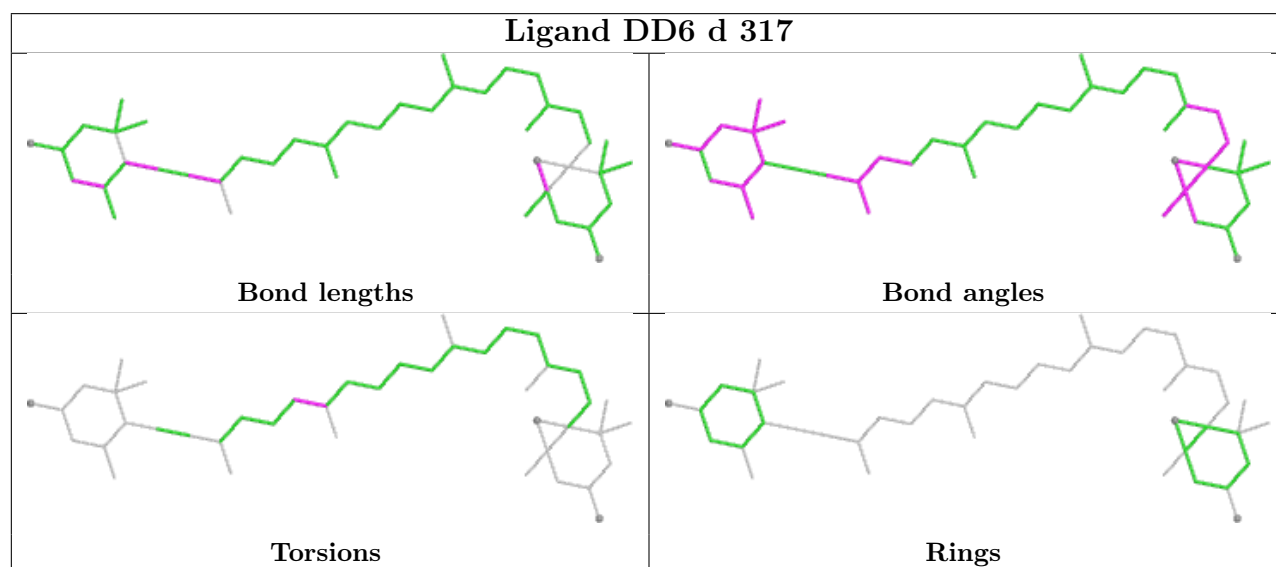
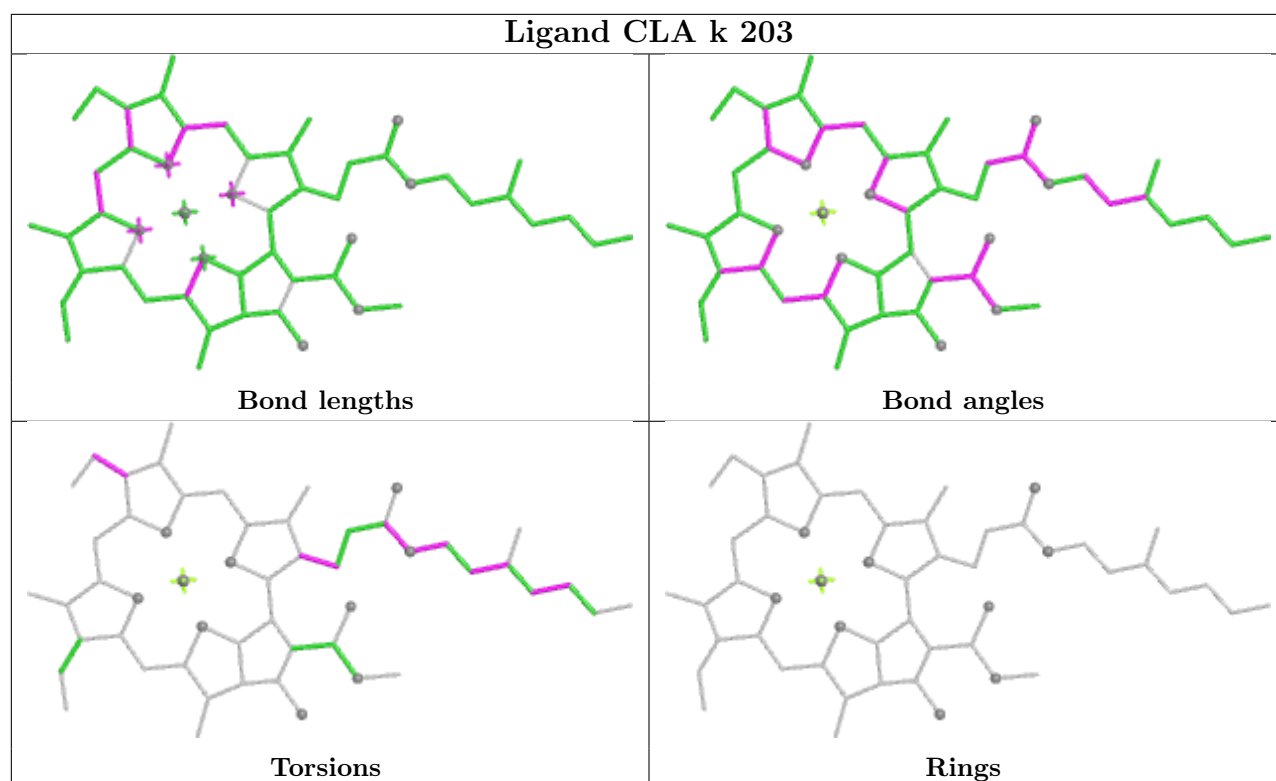
Bond angles



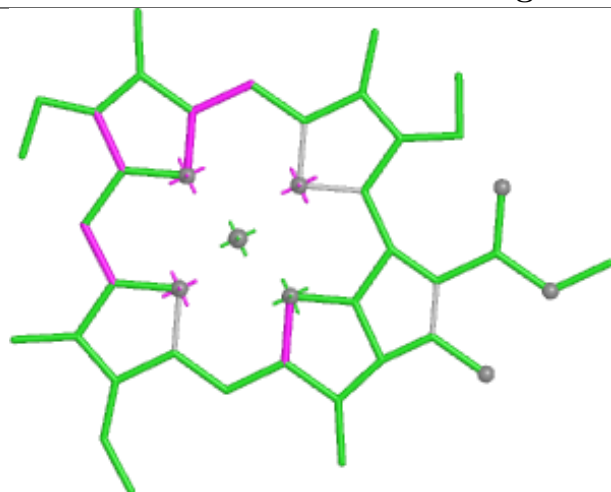
Torsions



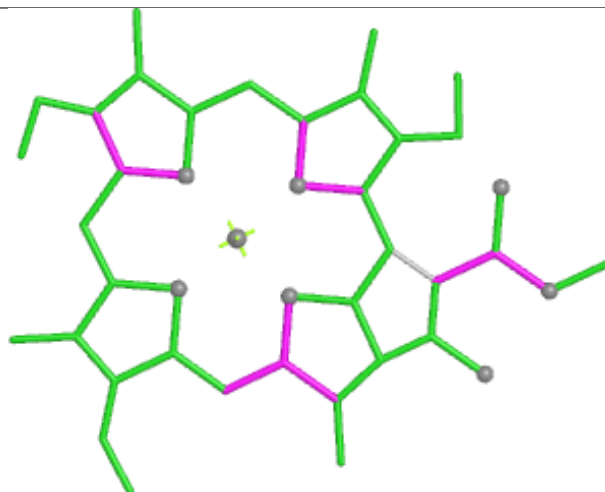
Rings



Ligand CLA F 201



Bond lengths



Bond angles

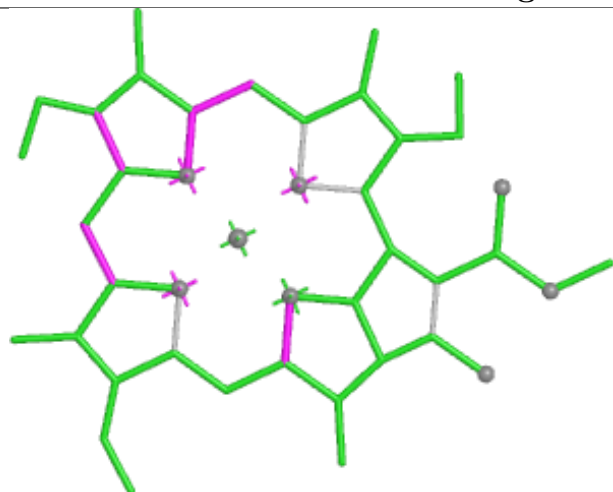


Torsions

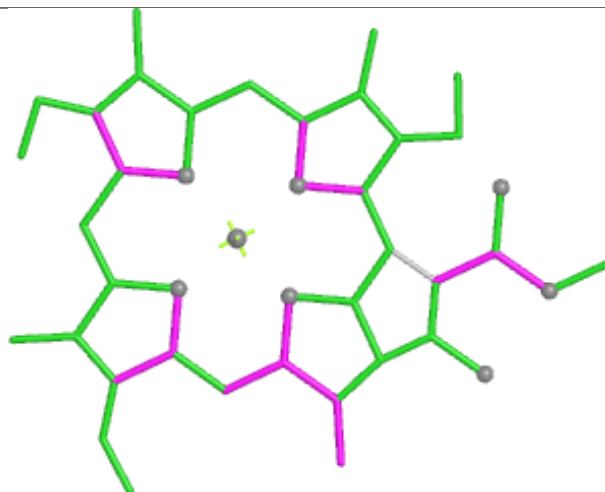


Rings

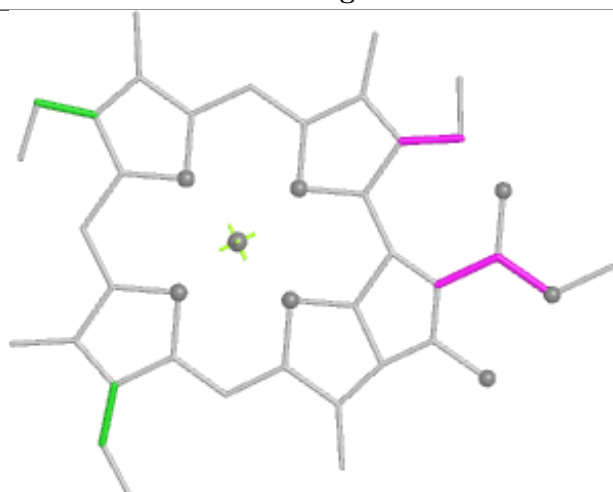
Ligand CLA k 204



Bond lengths



Bond angles

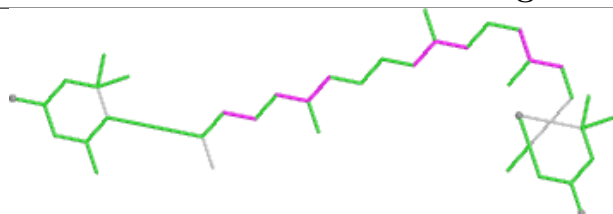


Torsions

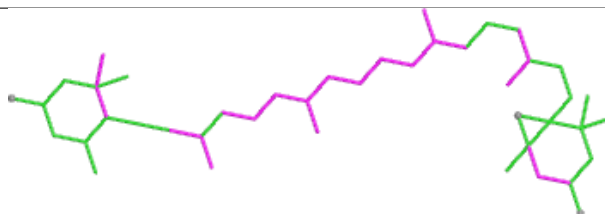


Rings

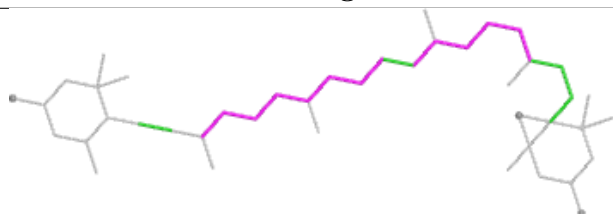
Ligand DD6 F 203



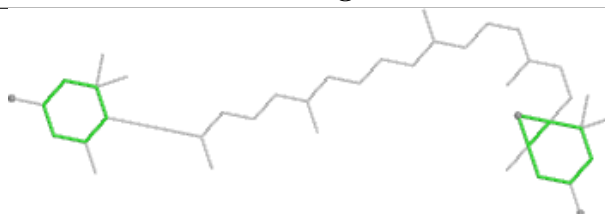
Bond lengths



Bond angles

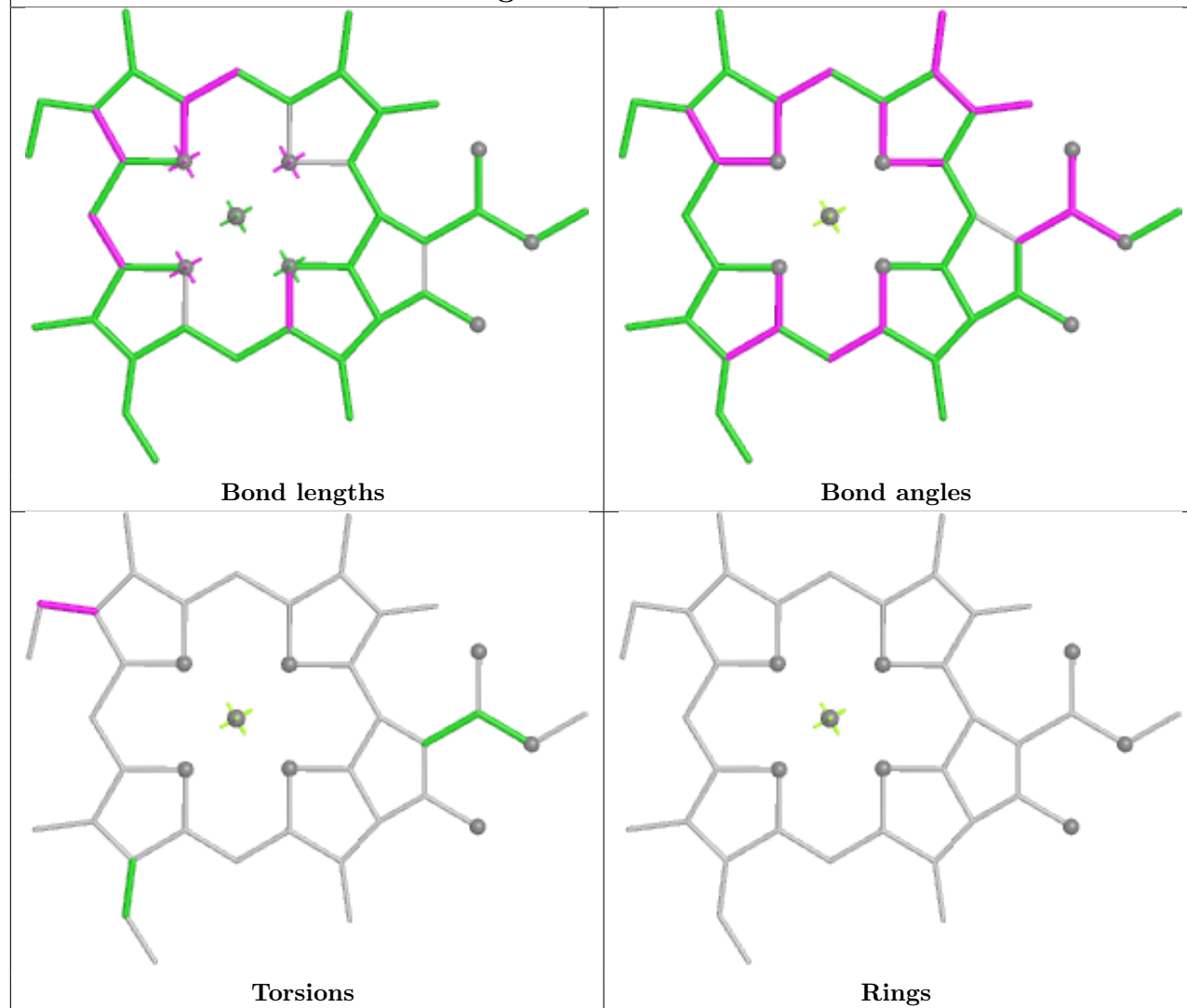


Torsions

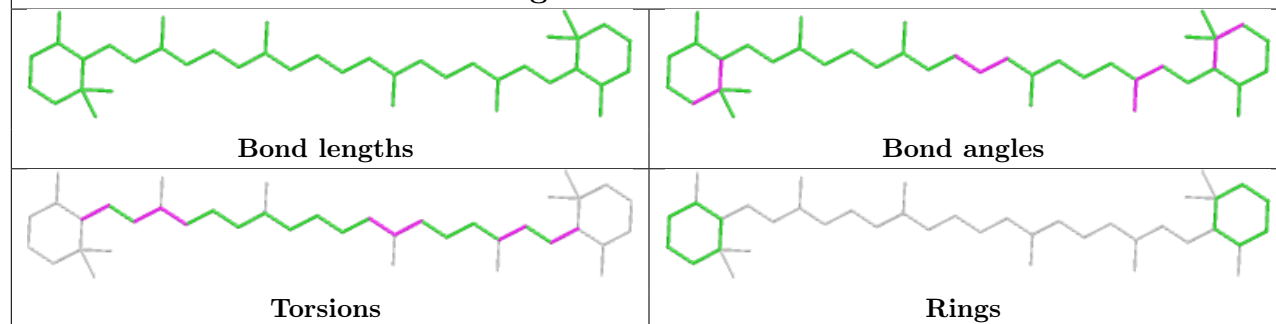


Rings

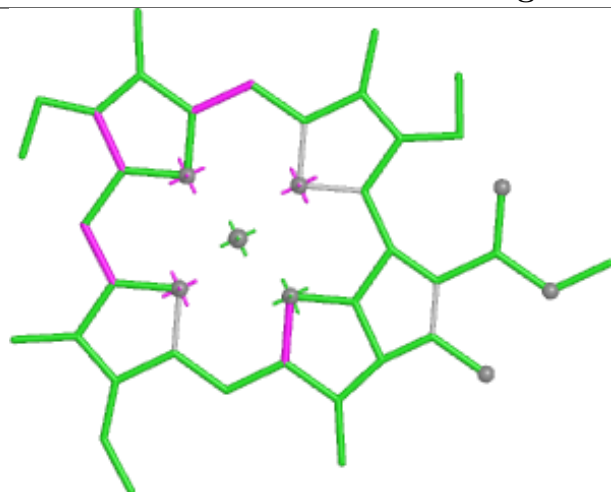
Ligand CLA b 208



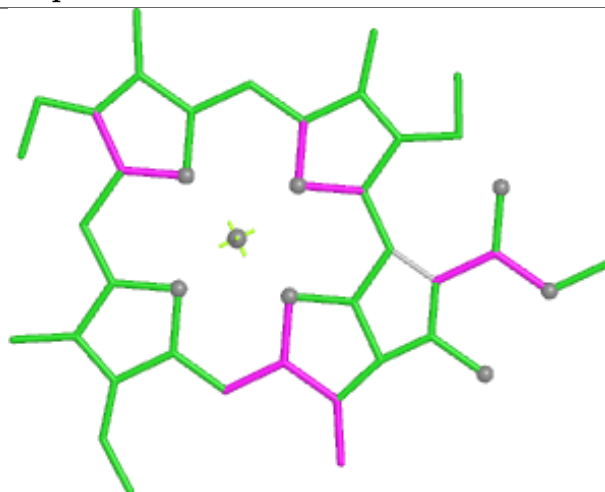
Ligand BCR A 839



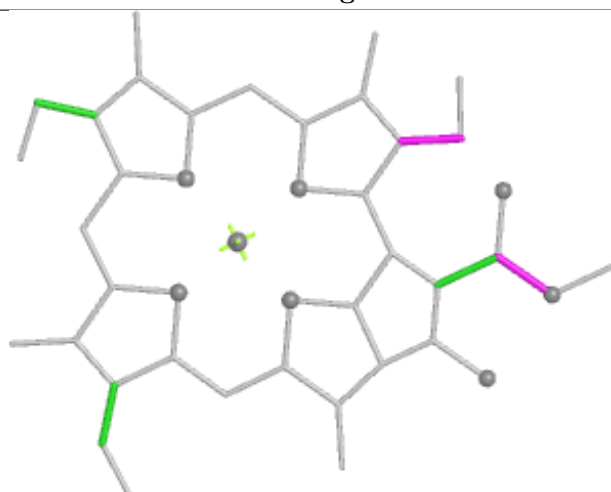
Ligand CLA p 603



Bond lengths



Bond angles

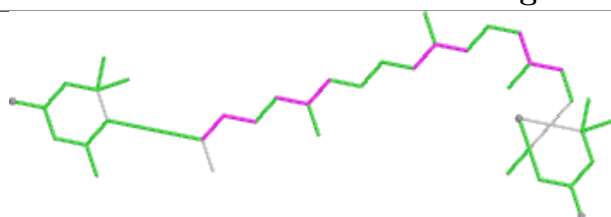


Torsions

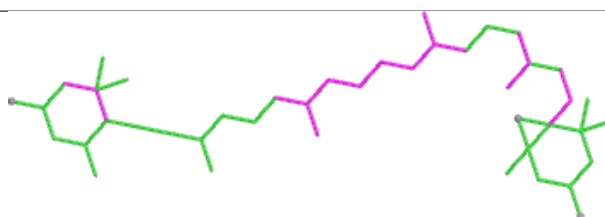


Rings

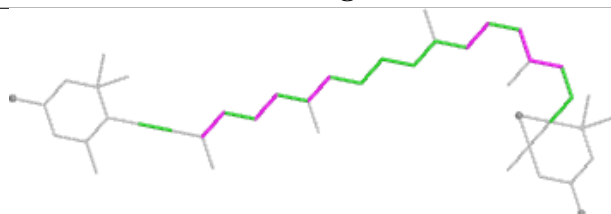
Ligand DD6 e 218



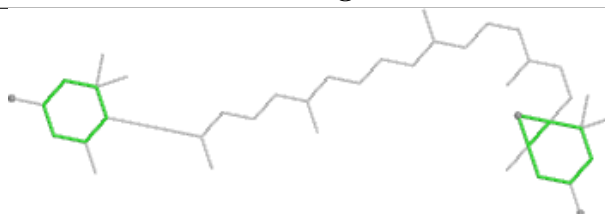
Bond lengths



Bond angles

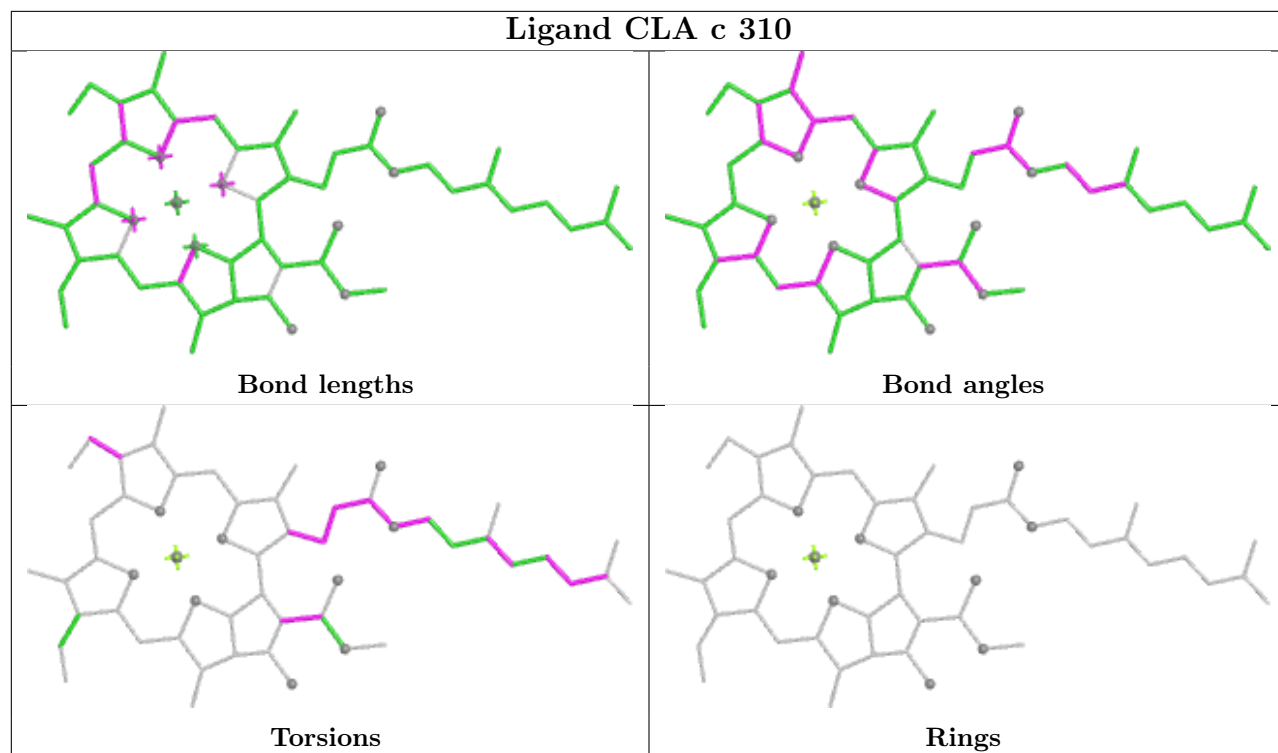


Torsions

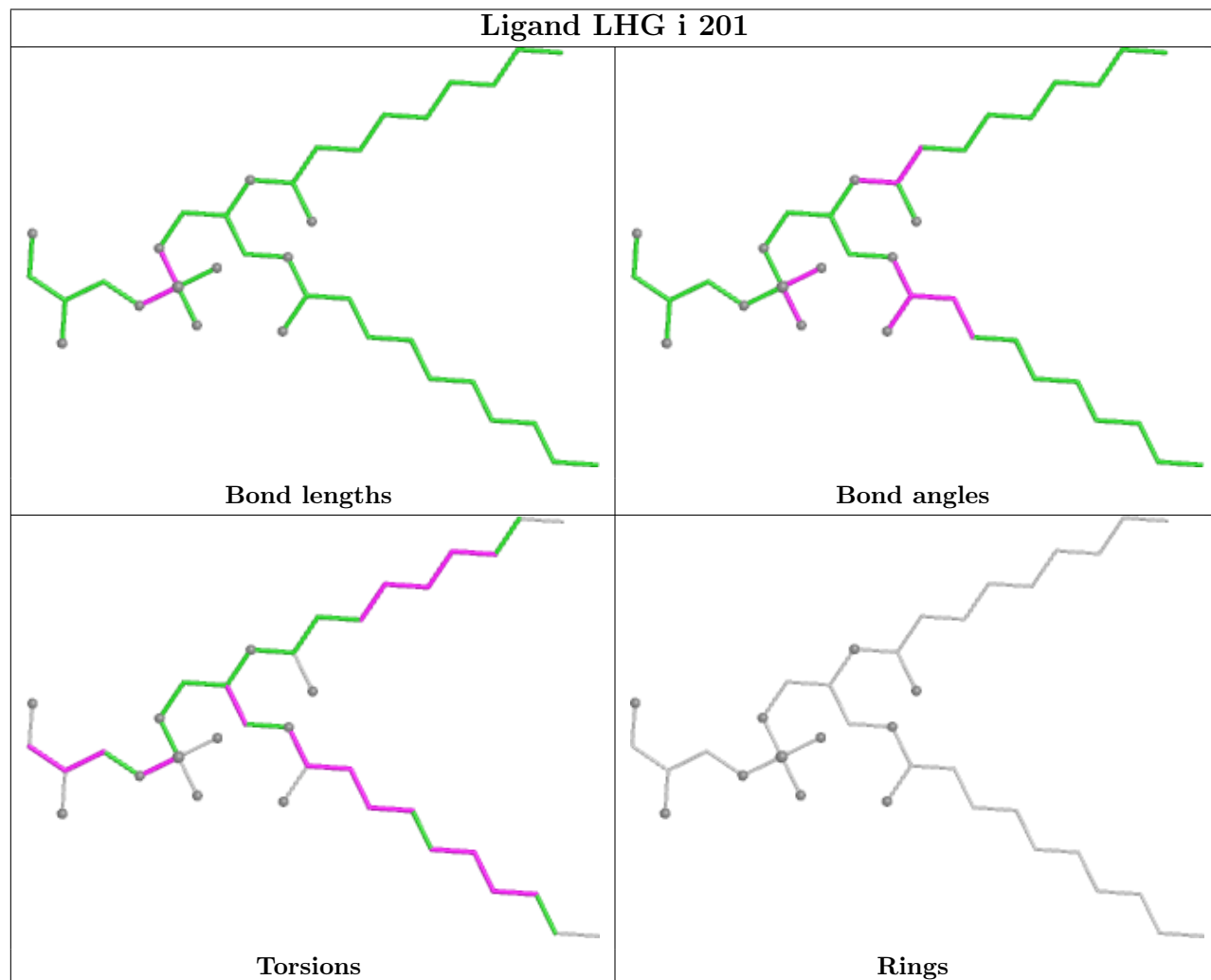


Rings

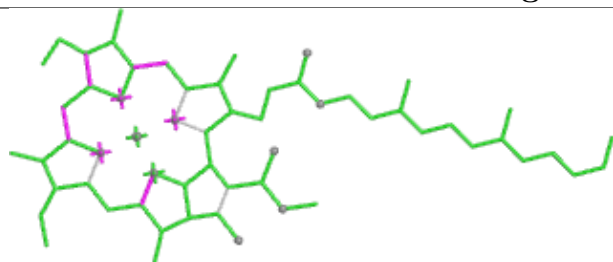
Ligand CLA c 310



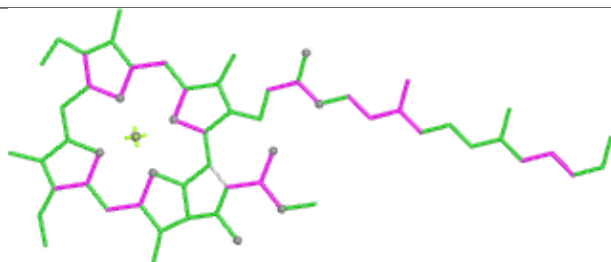
Ligand LHG i 201



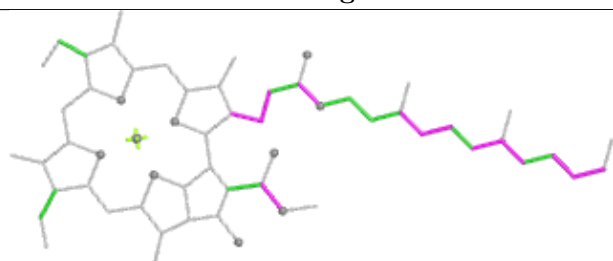
Ligand CLA f 602



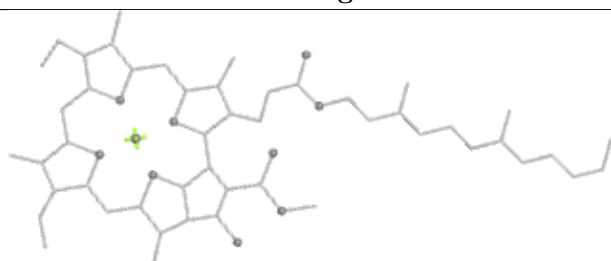
Bond lengths



Bond angles

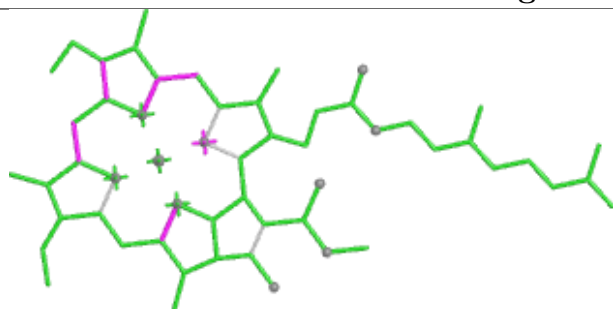


Torsions

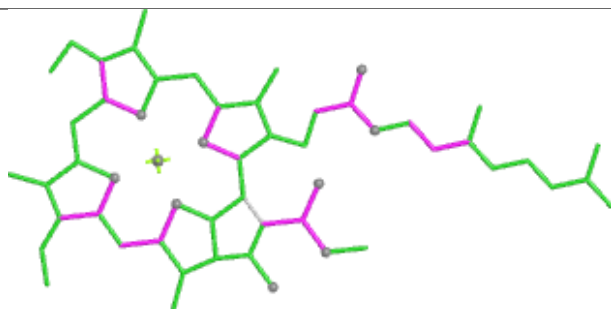


Rings

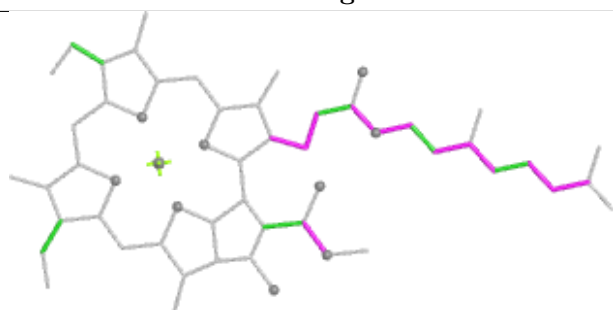
Ligand CLA a 212



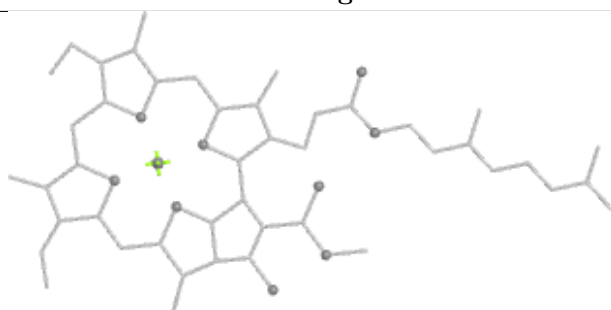
Bond lengths



Bond angles

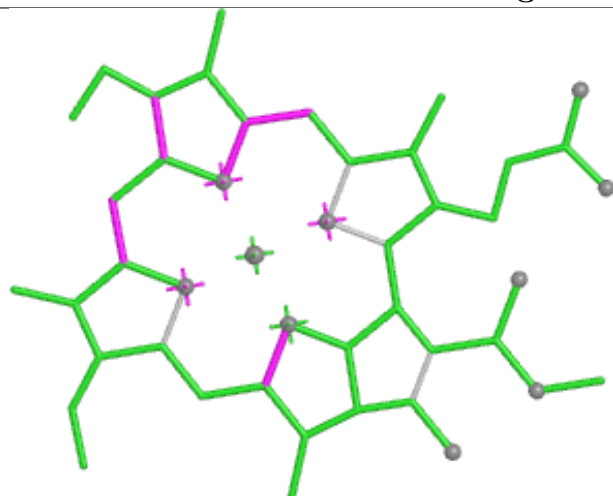


Torsions

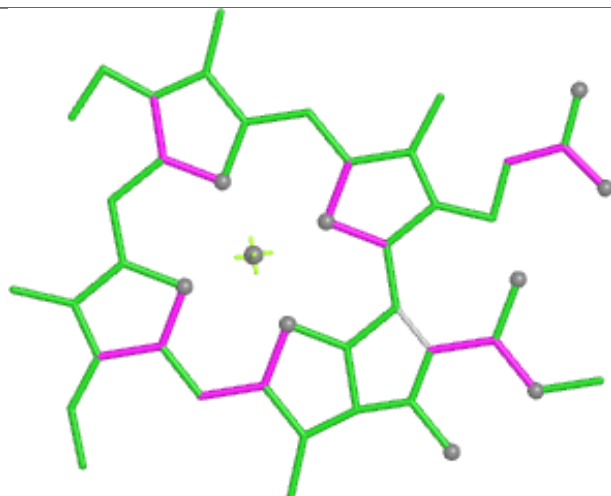


Rings

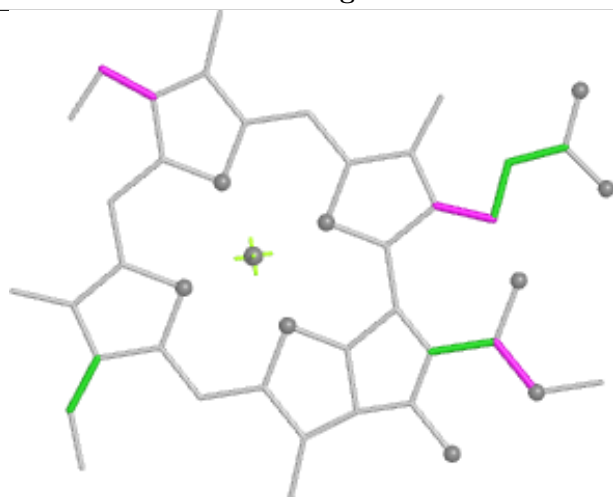
Ligand CLA b 206



Bond lengths



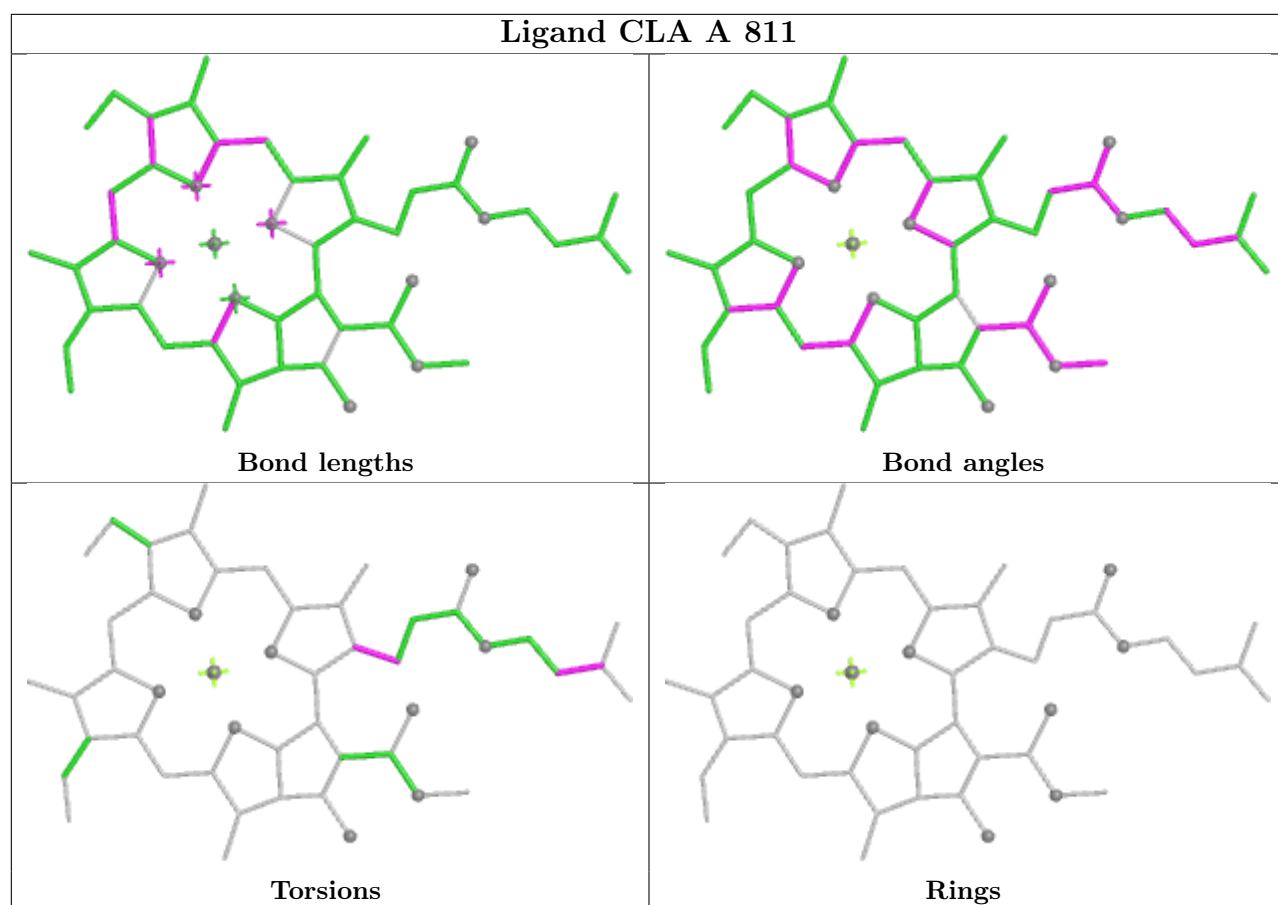
Bond angles



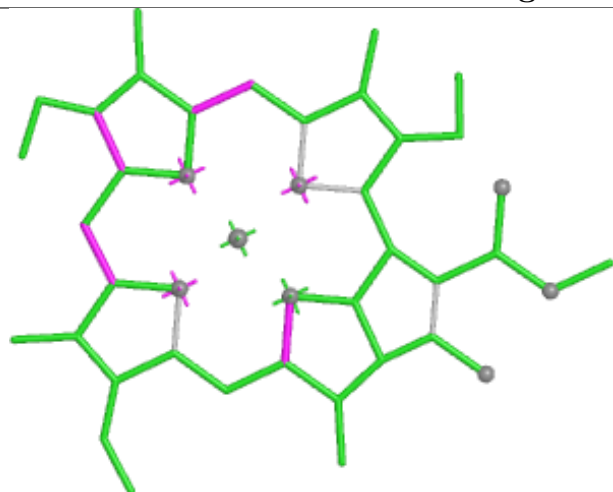
Torsions



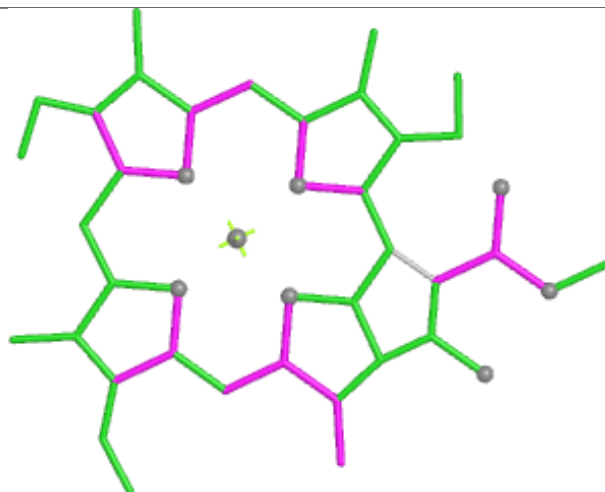
Rings



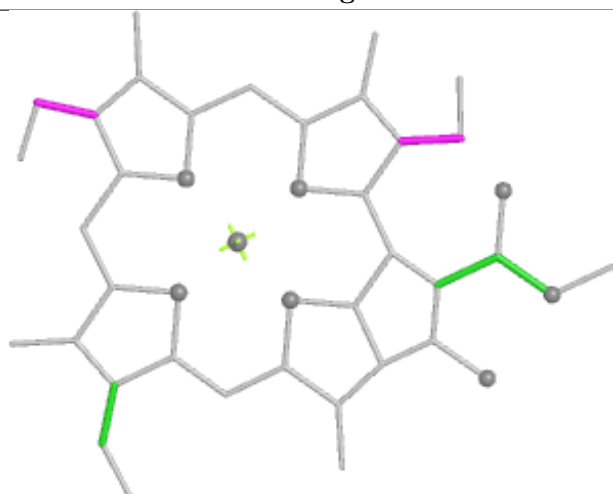
Ligand CLA o 604



Bond lengths



Bond angles

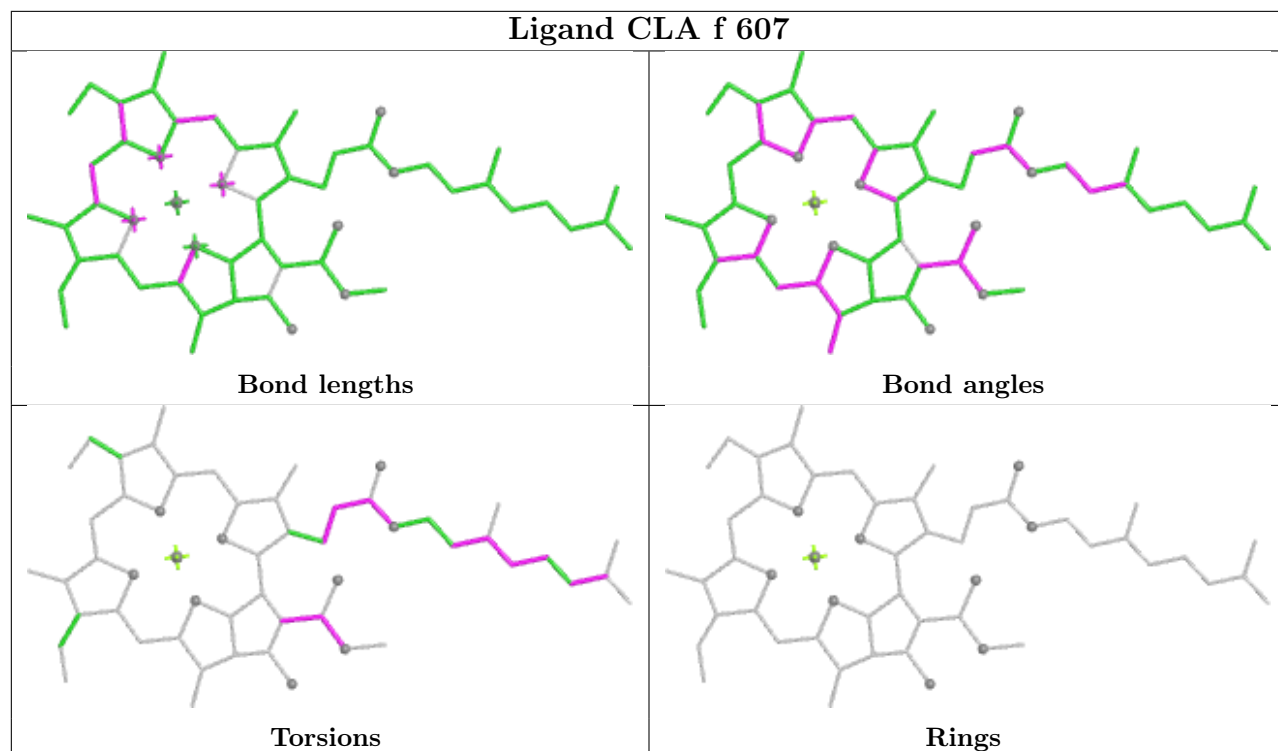


Torsions

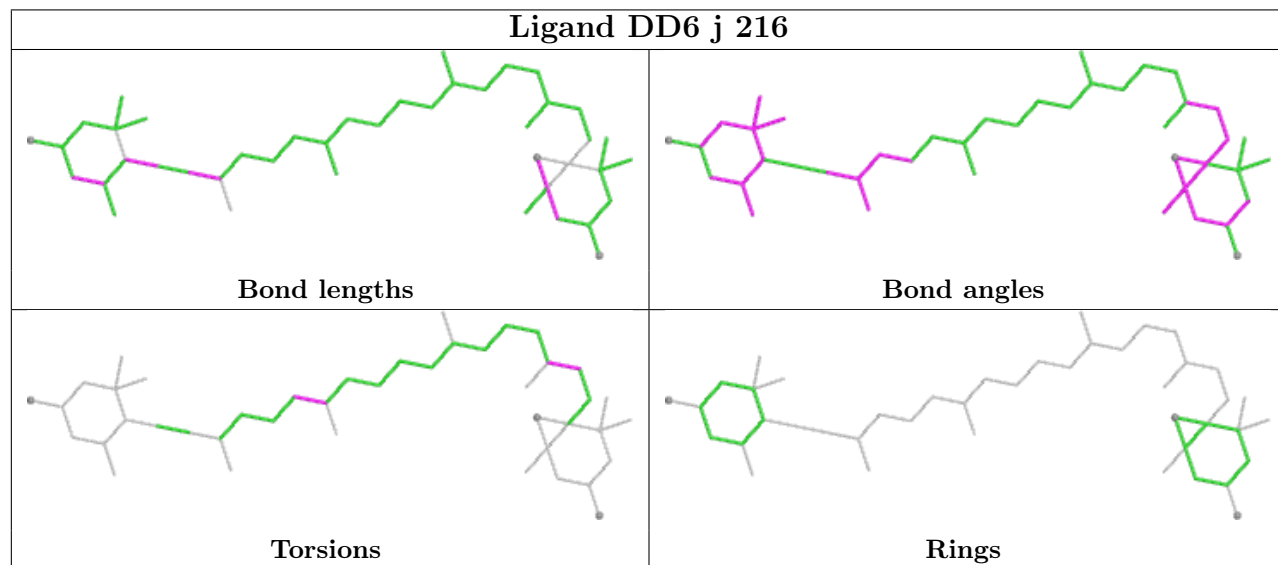


Rings

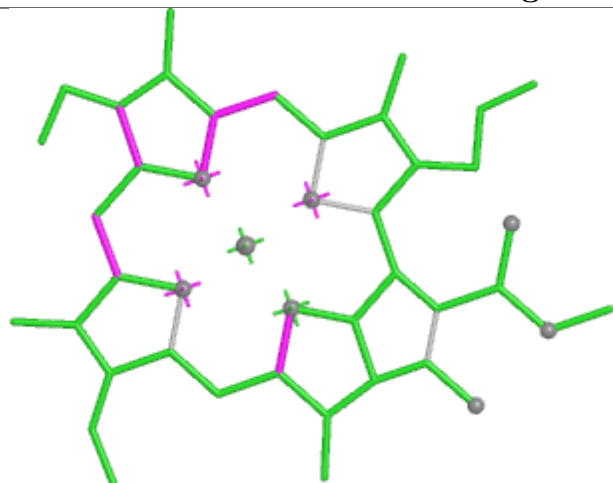
Ligand CLA f 607



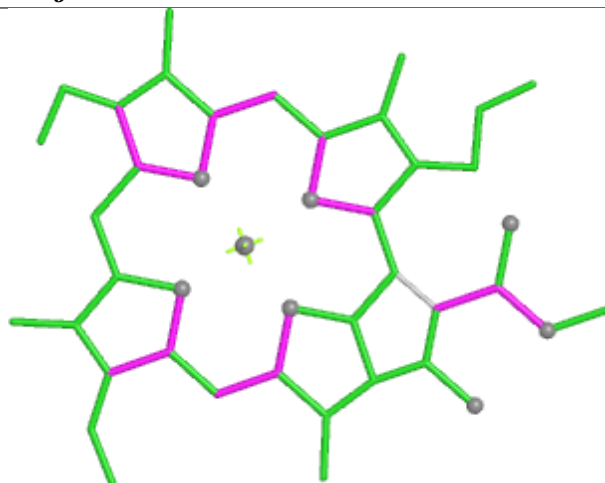
Ligand DD6 j 216



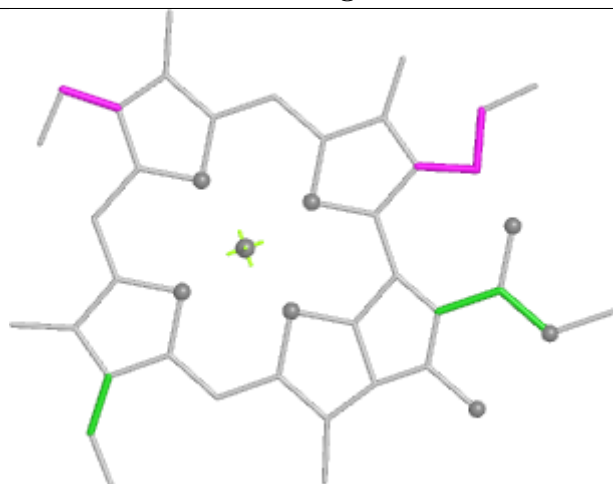
Ligand CLA j 214



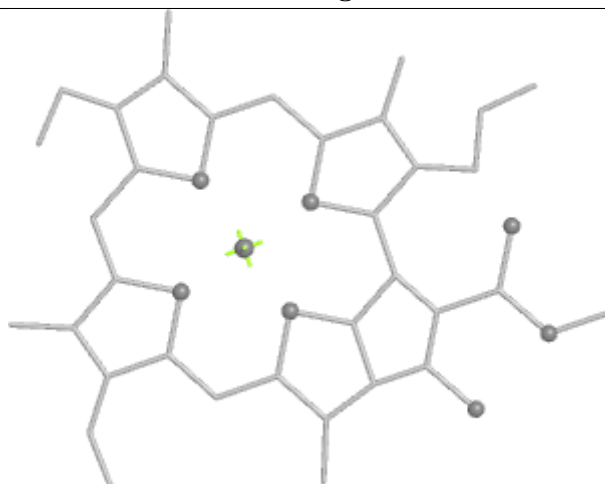
Bond lengths



Bond angles

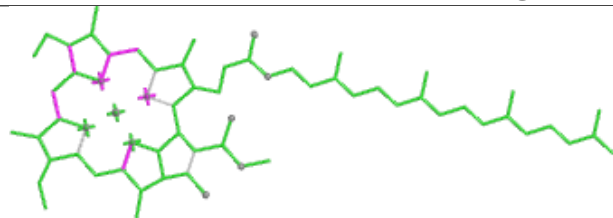


Torsions

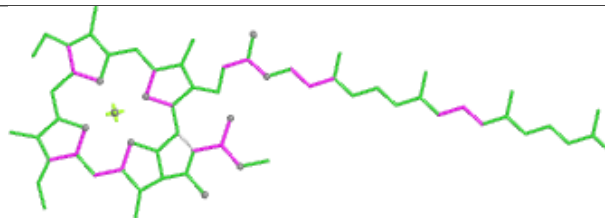


Rings

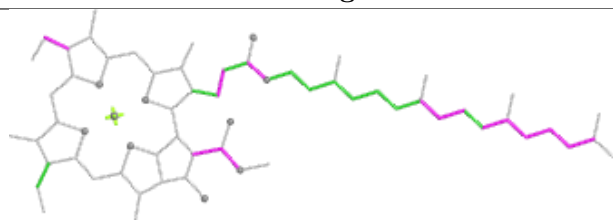
Ligand CLA A 812



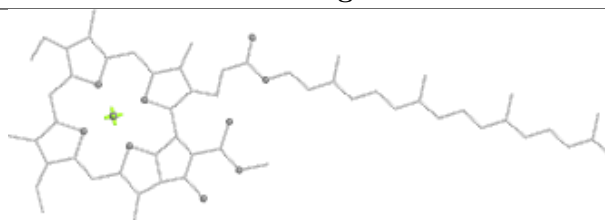
Bond lengths



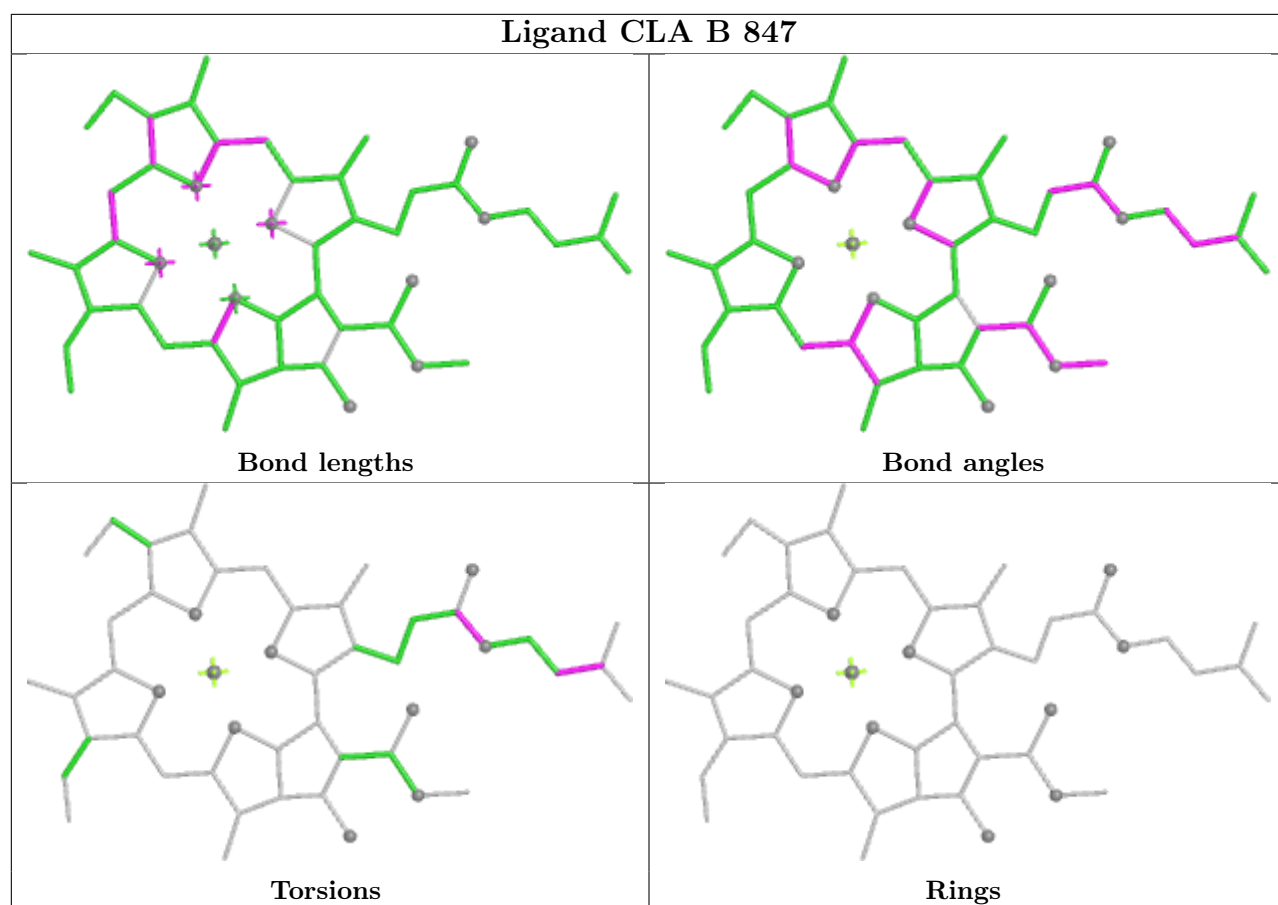
Bond angles



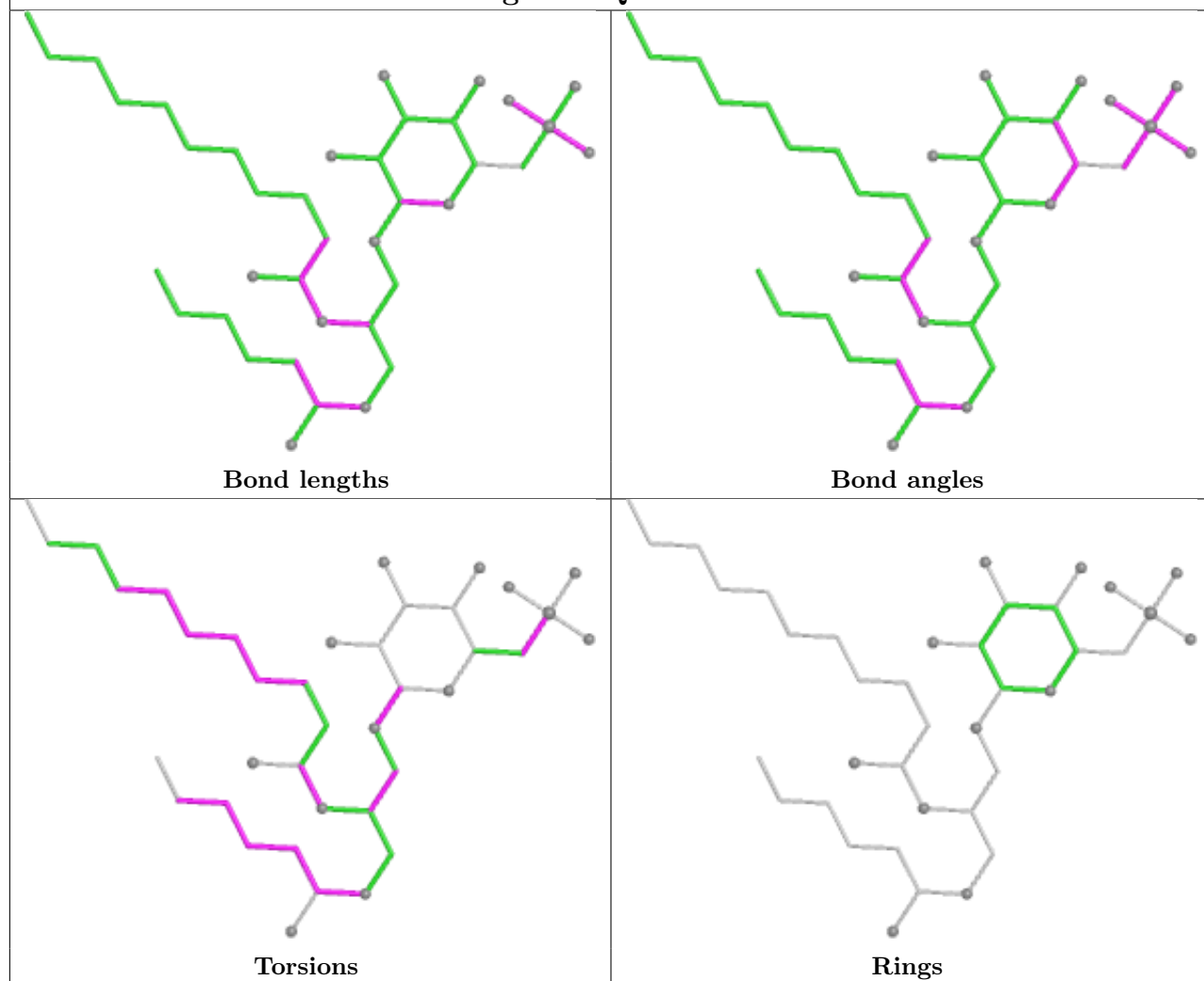
Torsions



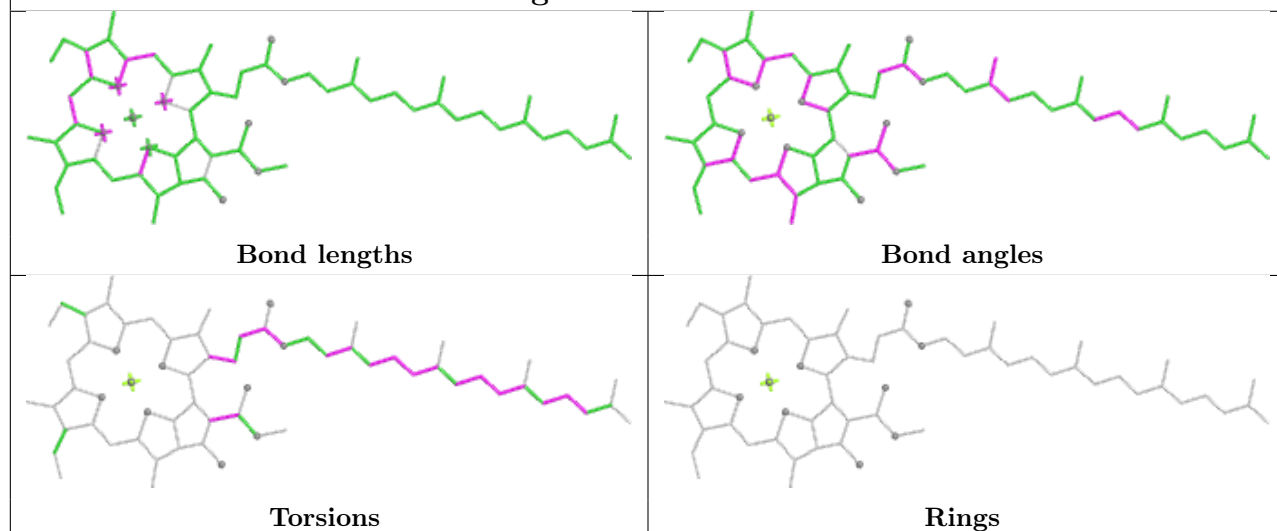
Rings



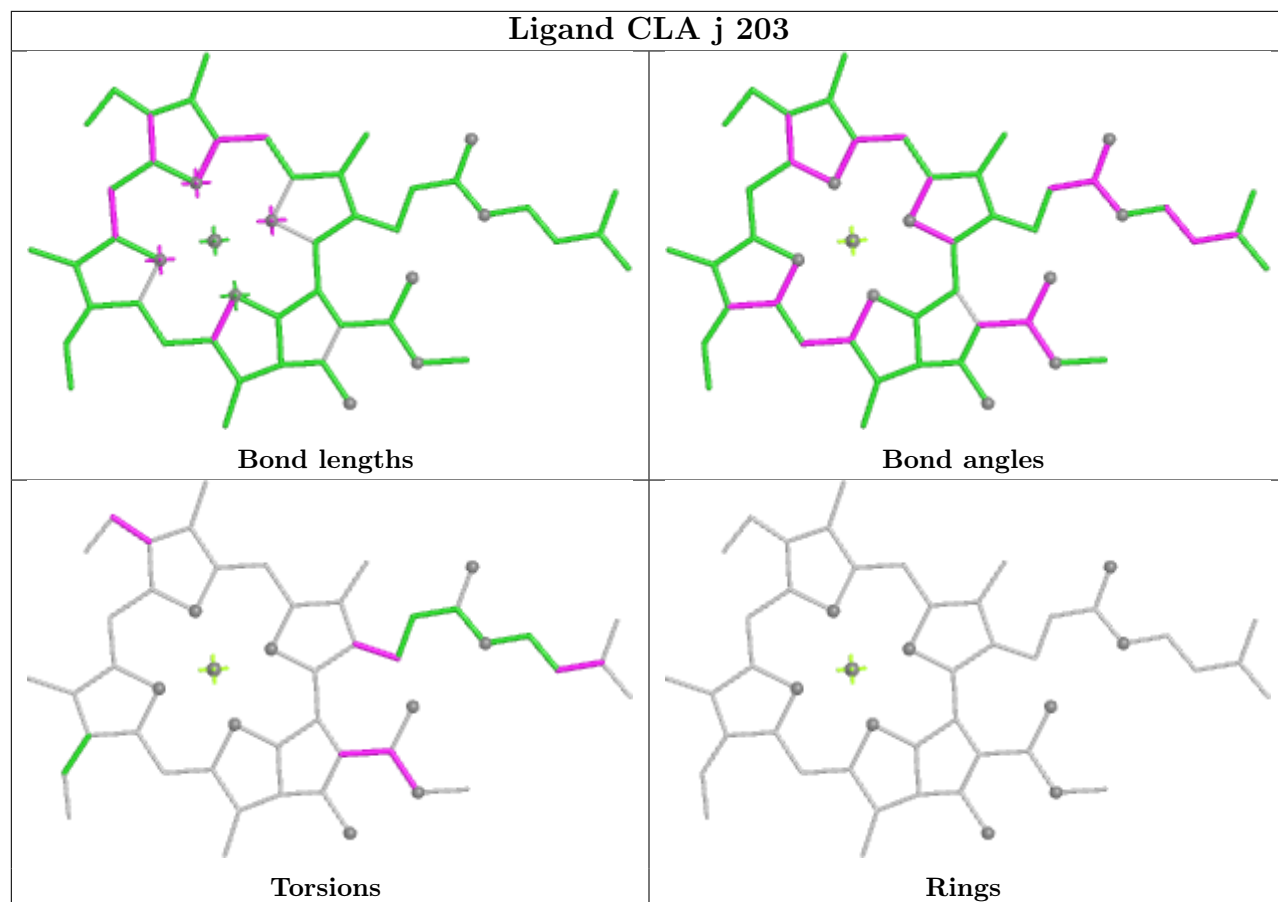
Ligand SQD F 204



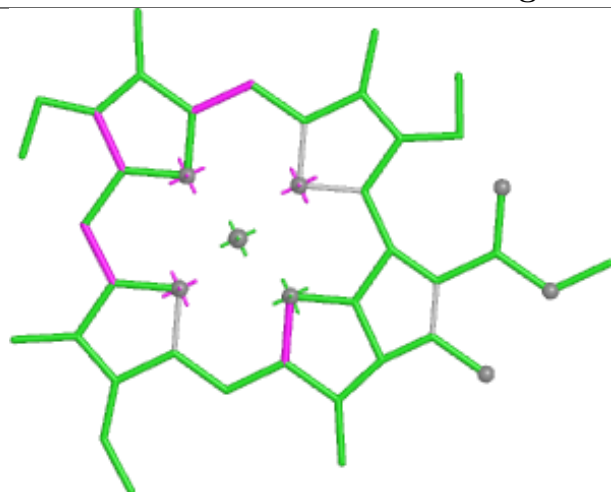
Ligand CLA B 848



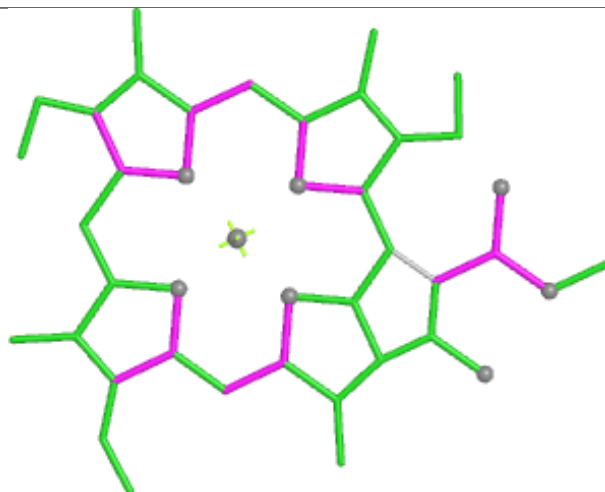
Ligand CLA j 203



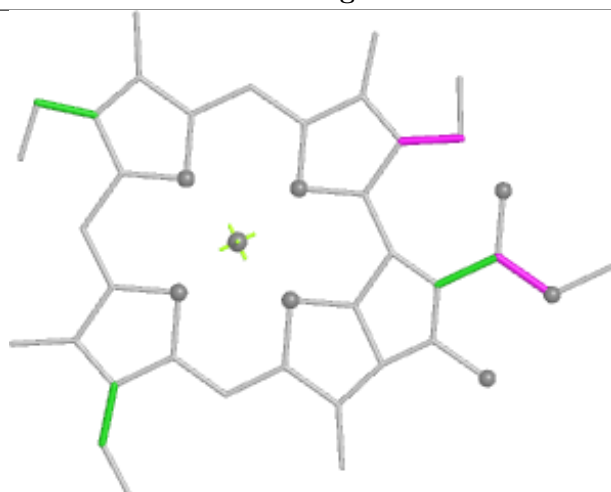
Ligand CLA e 214



Bond lengths



Bond angles

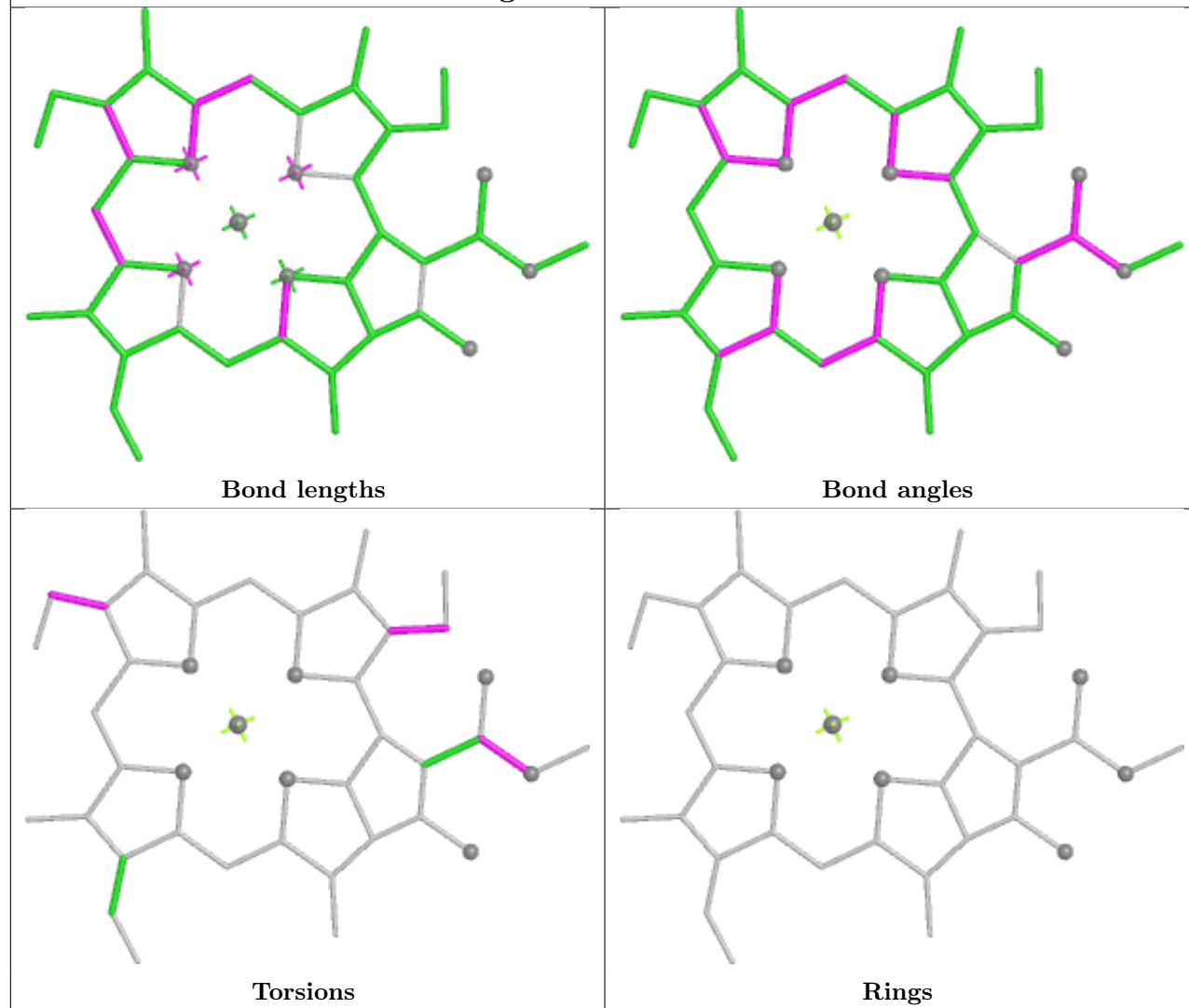


Torsions

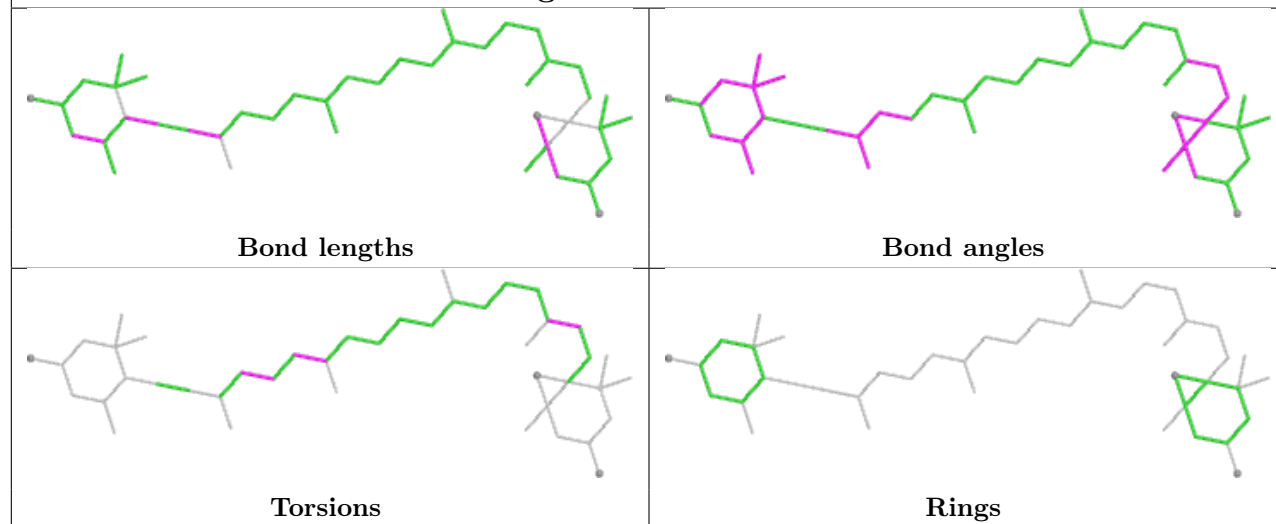


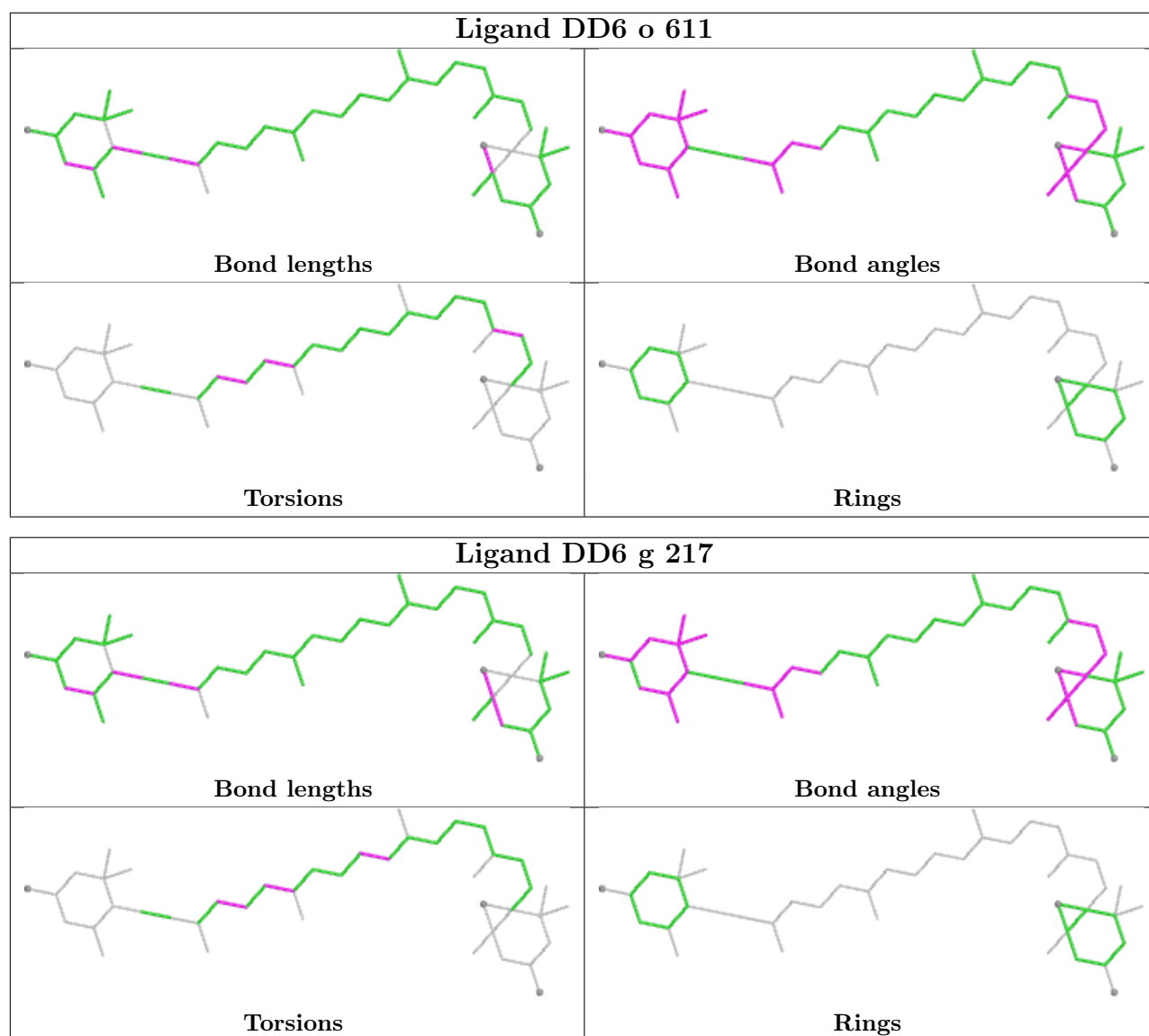
Rings

Ligand CLA k 213



Ligand DD6 e 219





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.

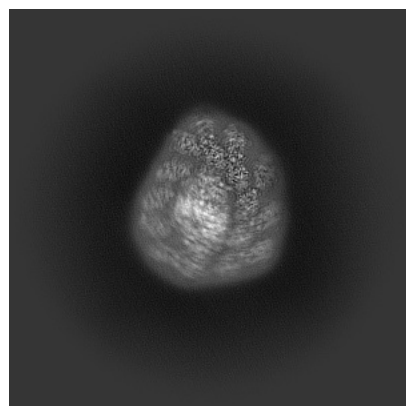
6 Map visualisation [i](#)

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.

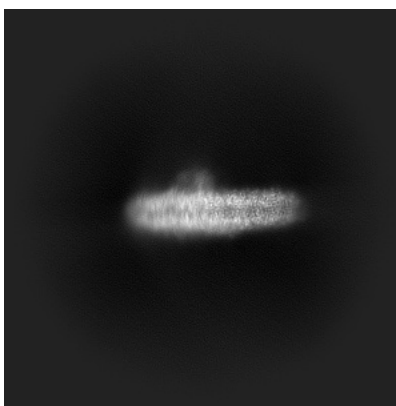
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

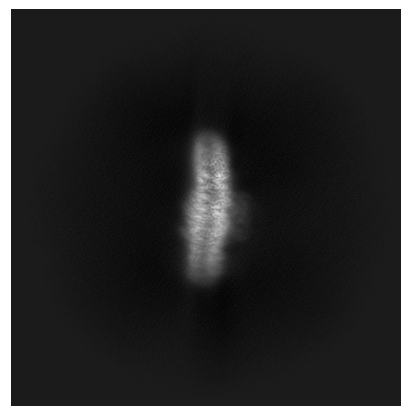
6.1.1 Primary map



X

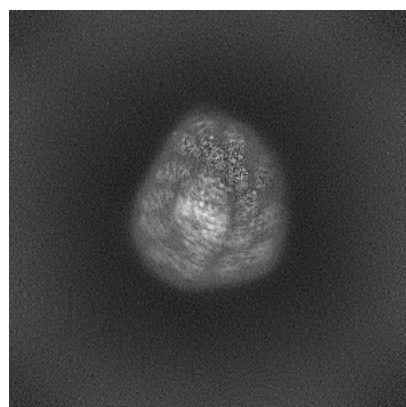


Y

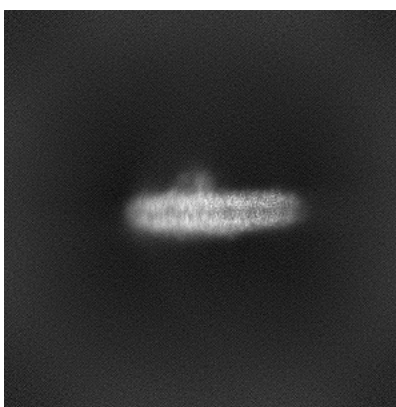


Z

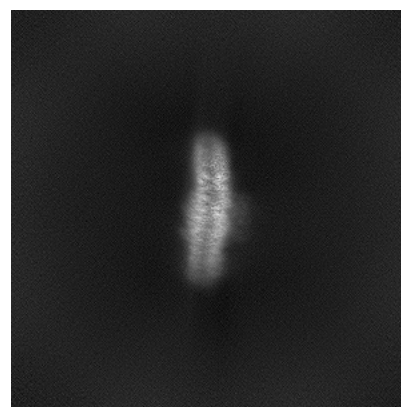
6.1.2 Raw map



X



Y

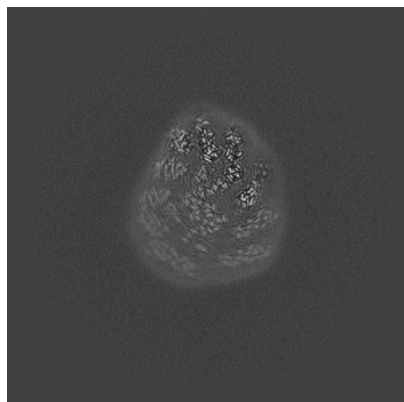


Z

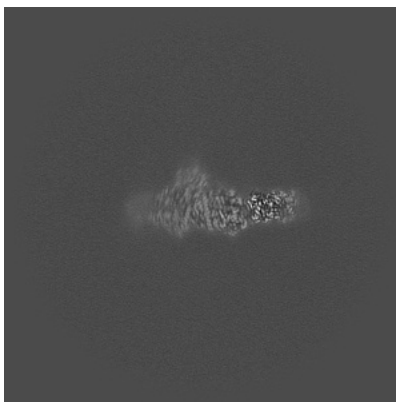
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

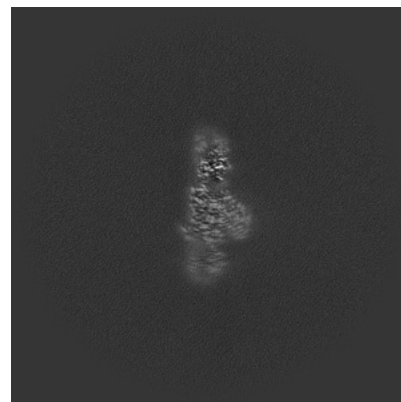
6.2.1 Primary map



X Index: 256

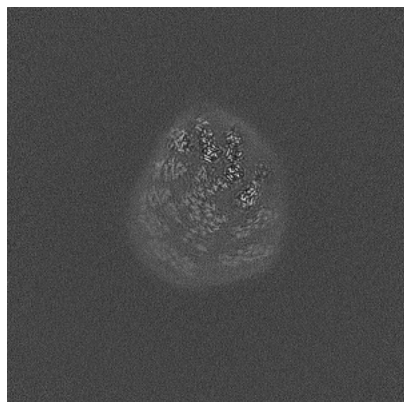


Y Index: 256

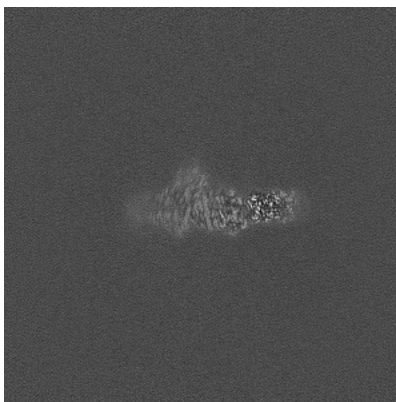


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

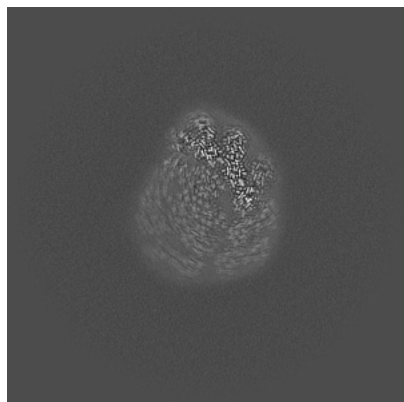


Z Index: 256

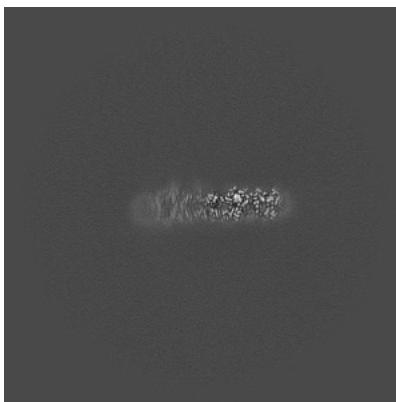
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

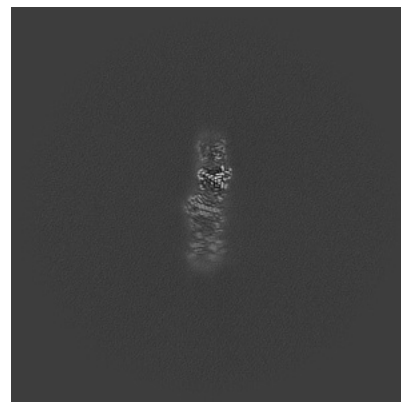
6.3.1 Primary map



X Index: 265

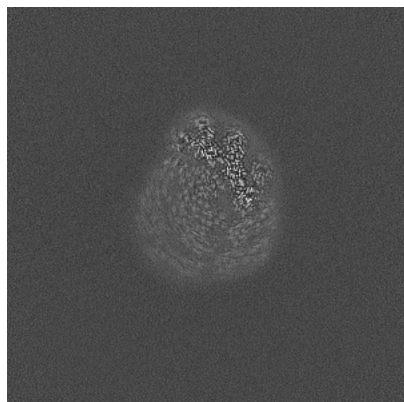


Y Index: 298

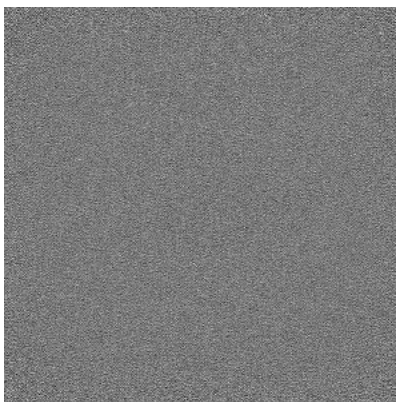


Z Index: 296

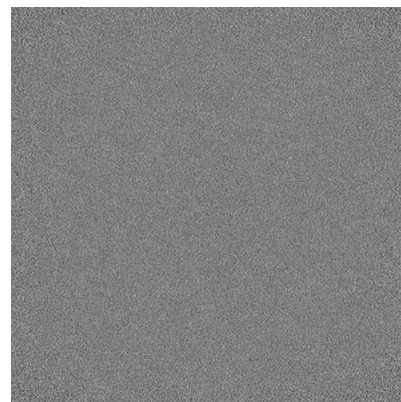
6.3.2 Raw map



X Index: 265



Y Index: 0

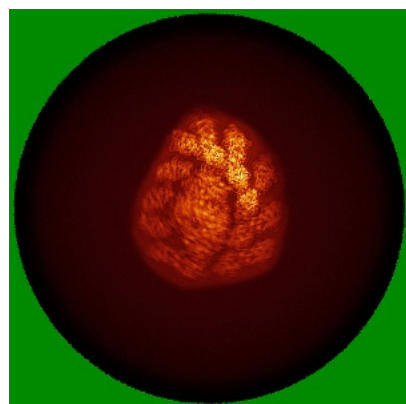


Z Index: 0

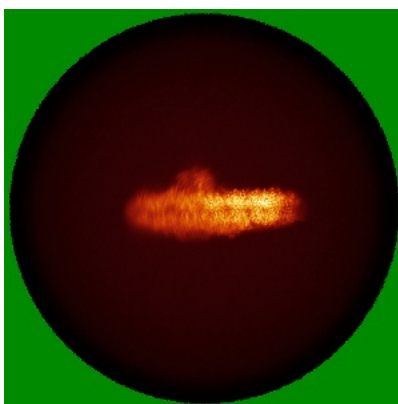
The images above show the largest variance slices of the map in three orthogonal directions.

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

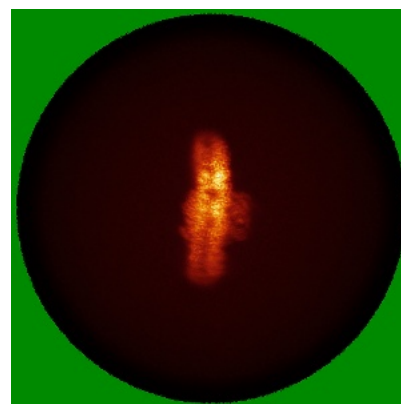
6.4.1 Primary map



X

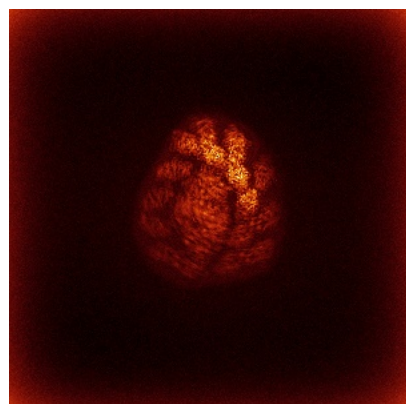


Y

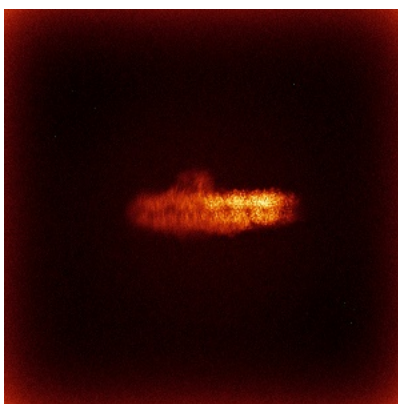


Z

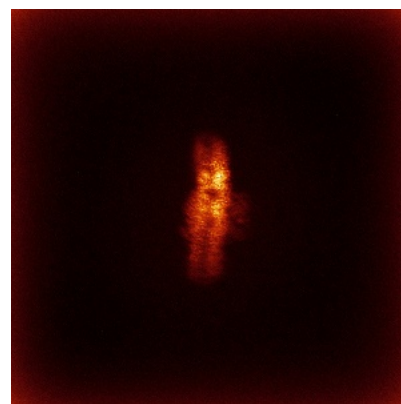
6.4.2 Raw map



X



Y

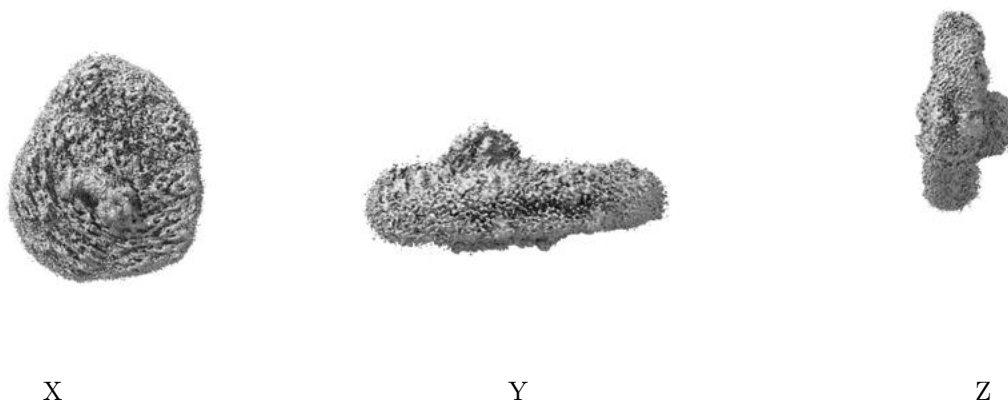


Z

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.

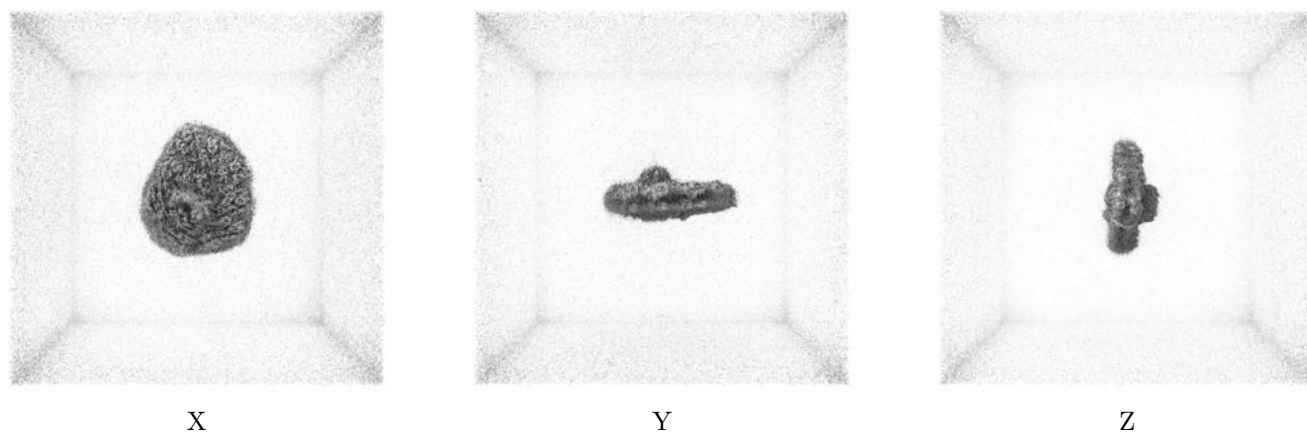
6.5 Orthogonal surface views [i](#)

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.

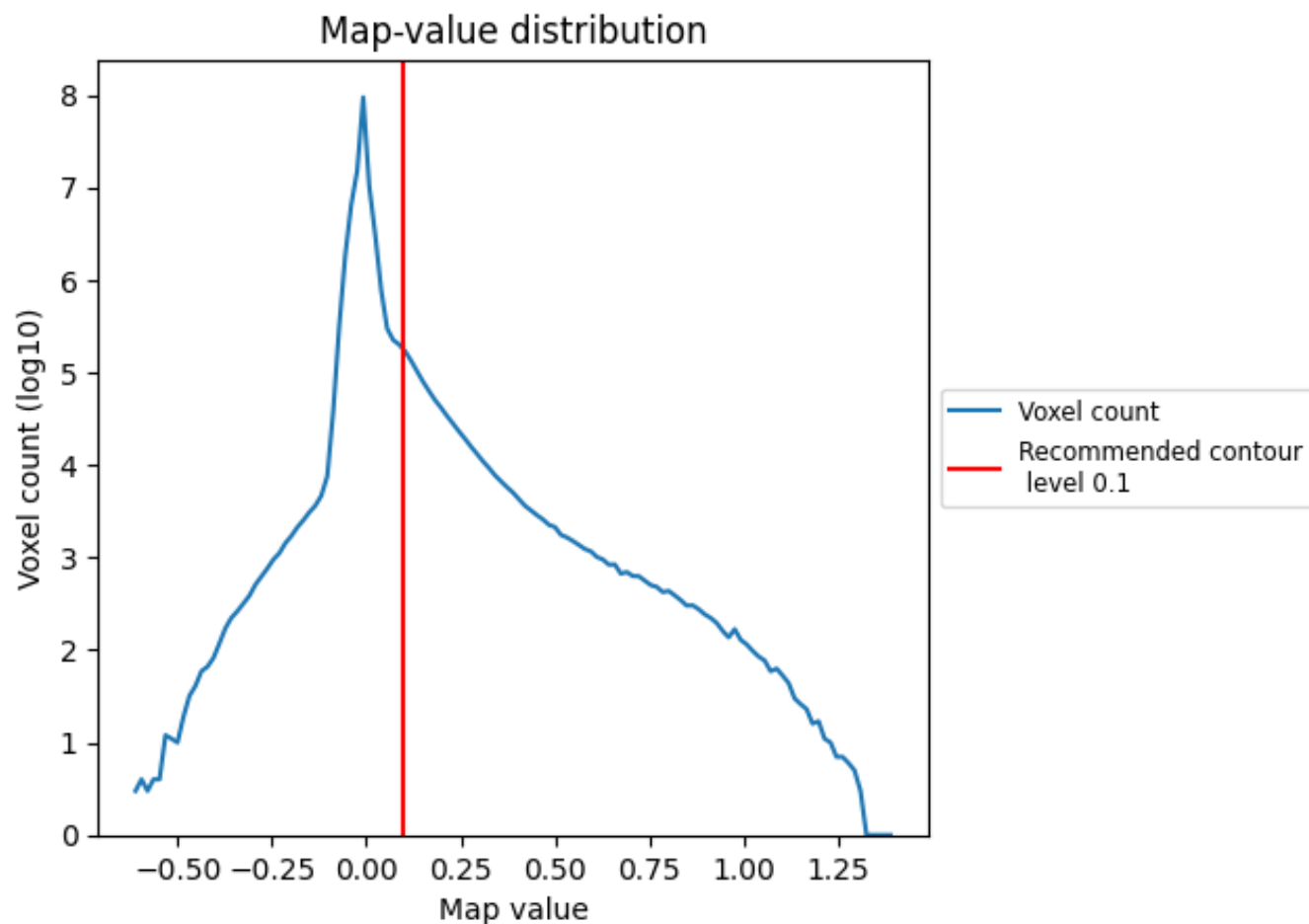
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

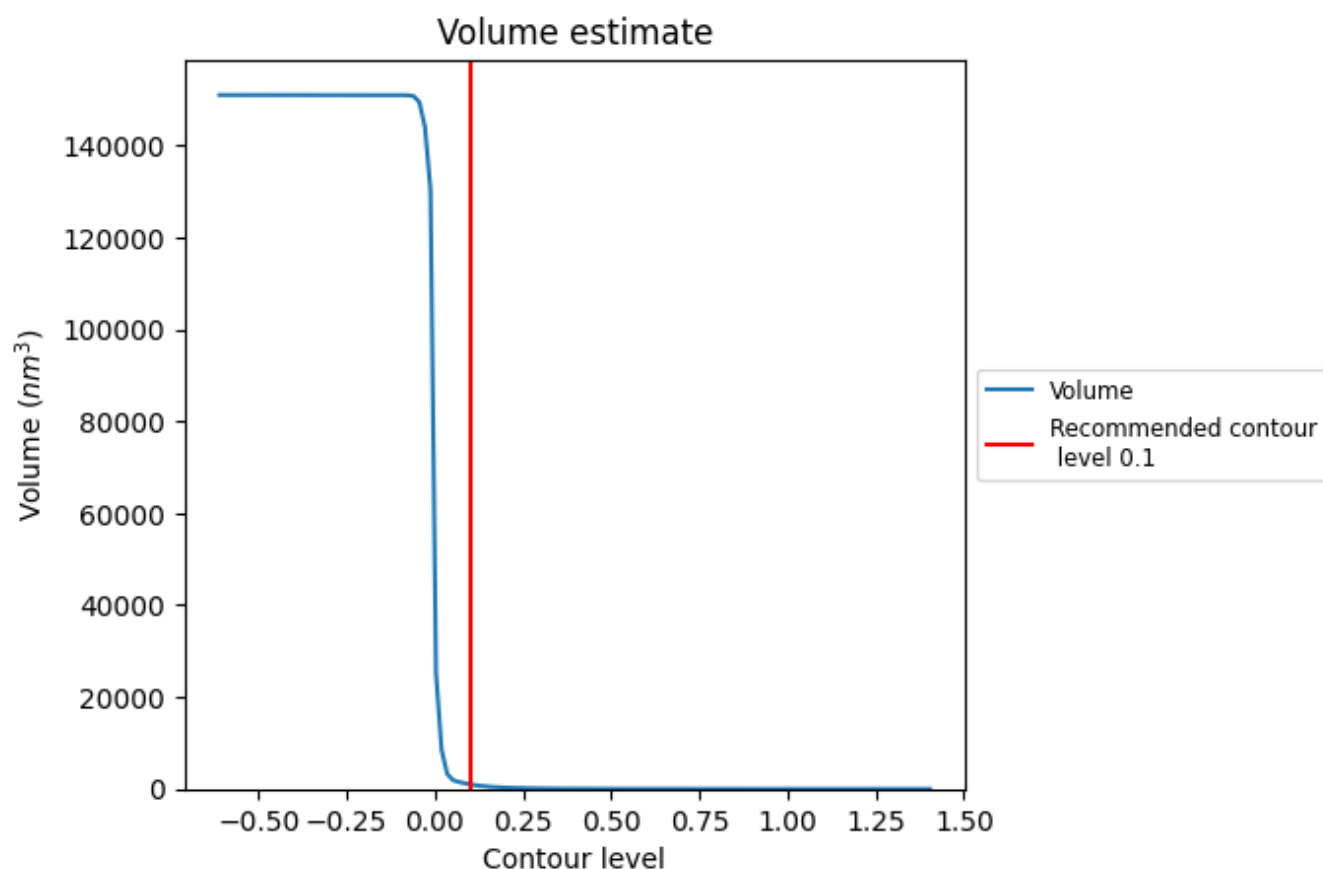
This section contains the results of statistical analysis of the map.

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.

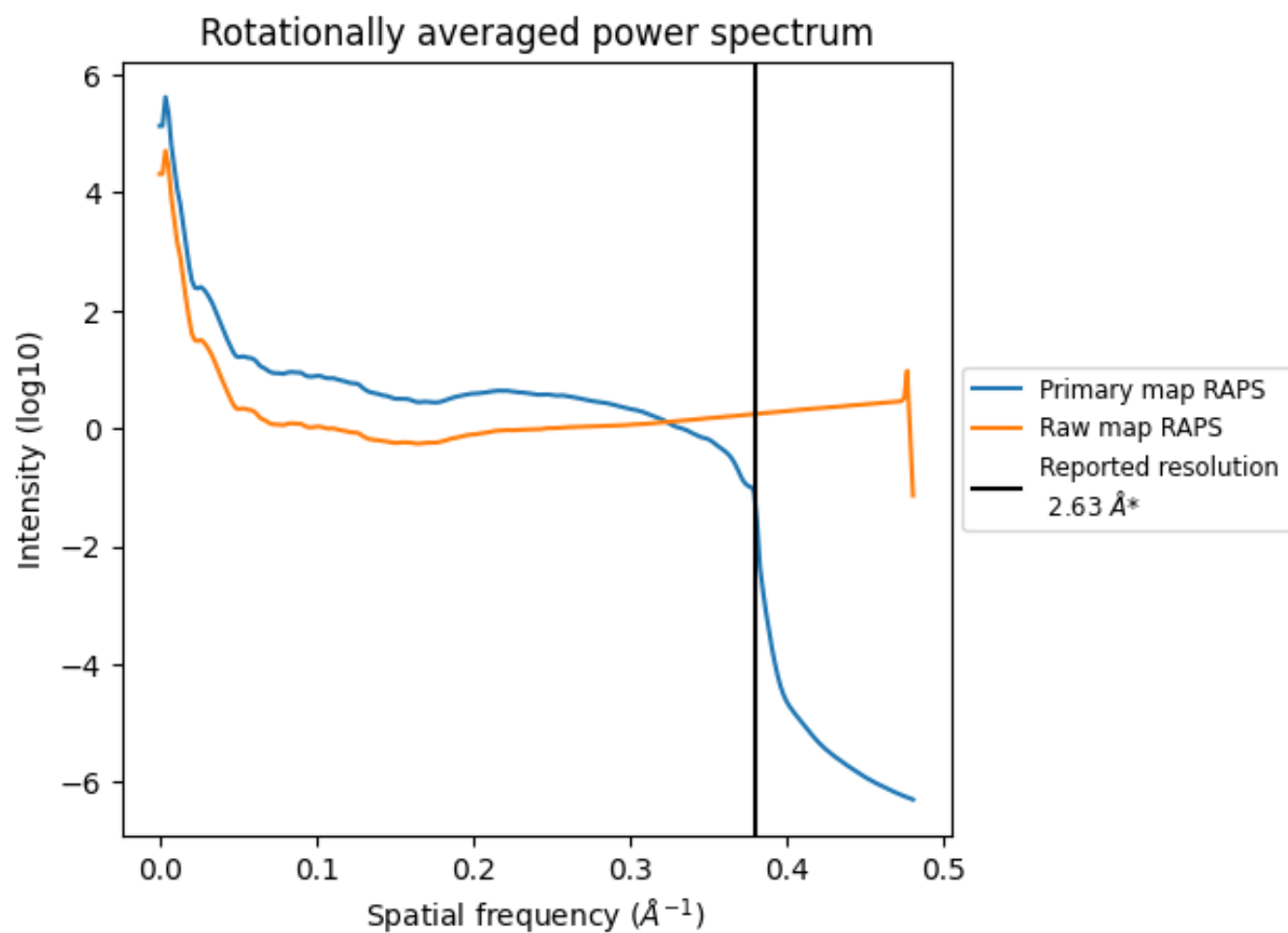
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1012 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 ⓘ

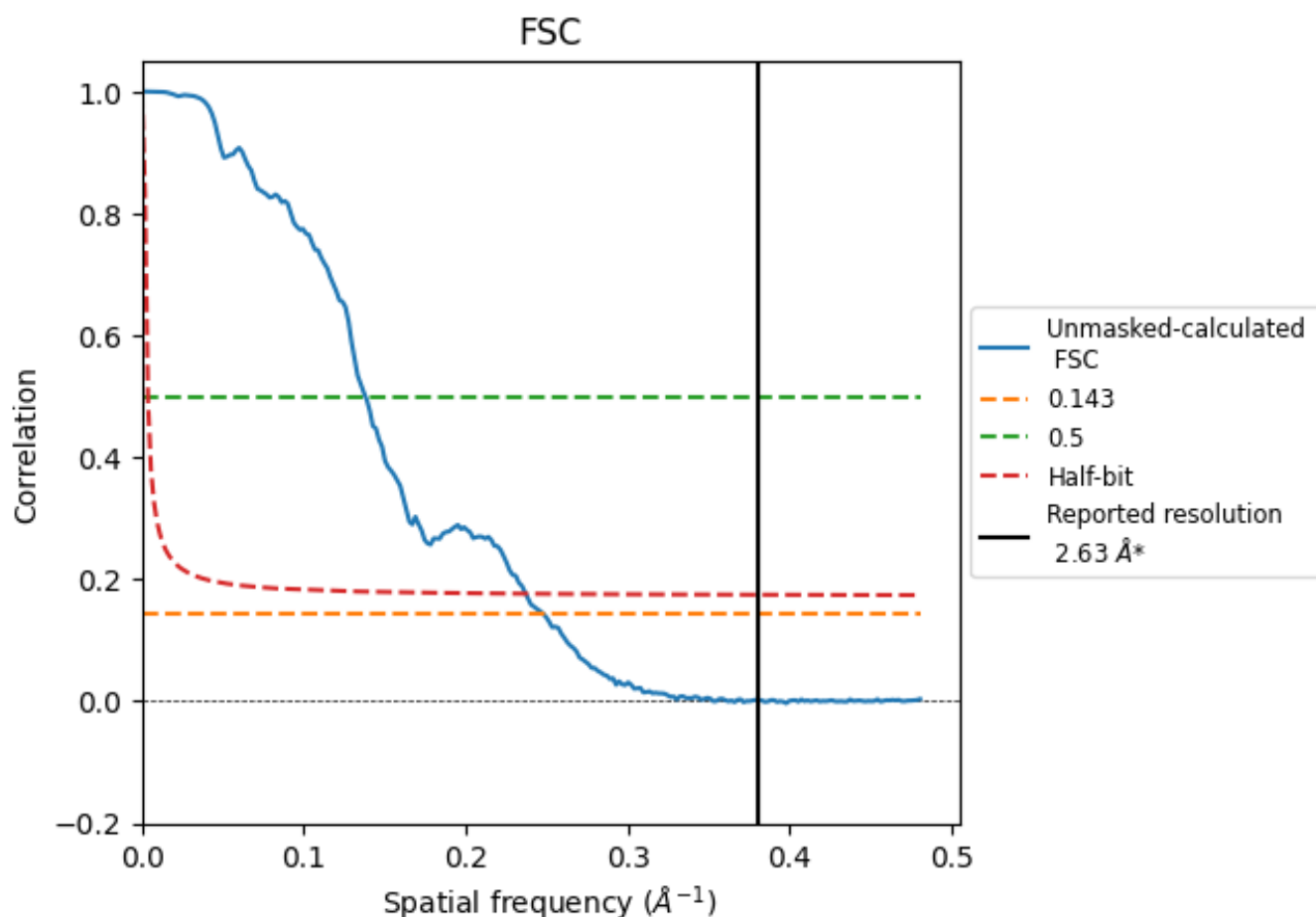


*Reported resolution corresponds to spatial frequency of 0.380 $\text{\AA}^{-1}$

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⁻¹

8.2 Resolution estimates [i](#)

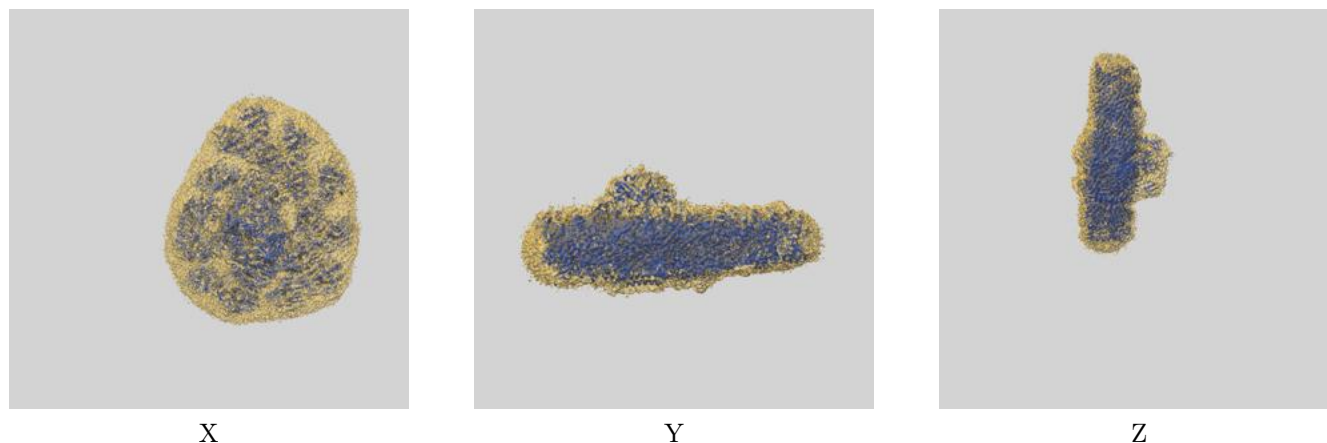
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	7.25	4.22

*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](#)

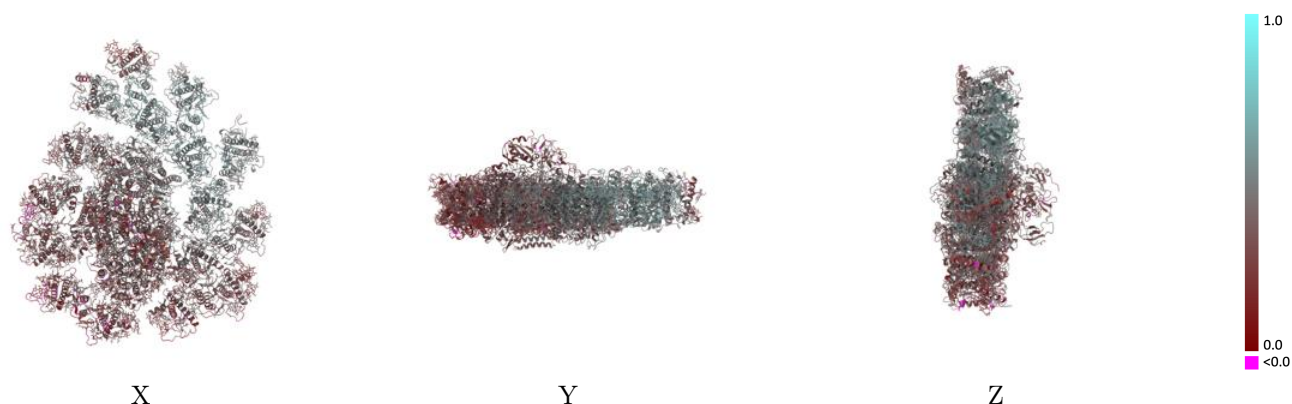
This section contains information regarding the fit between EMDB map EMD-64824 and PDB model 9V7U. Per-residue inclusion information can be found in section [3](#) on page [31](#).

9.1 Map-model overlay [i](#)



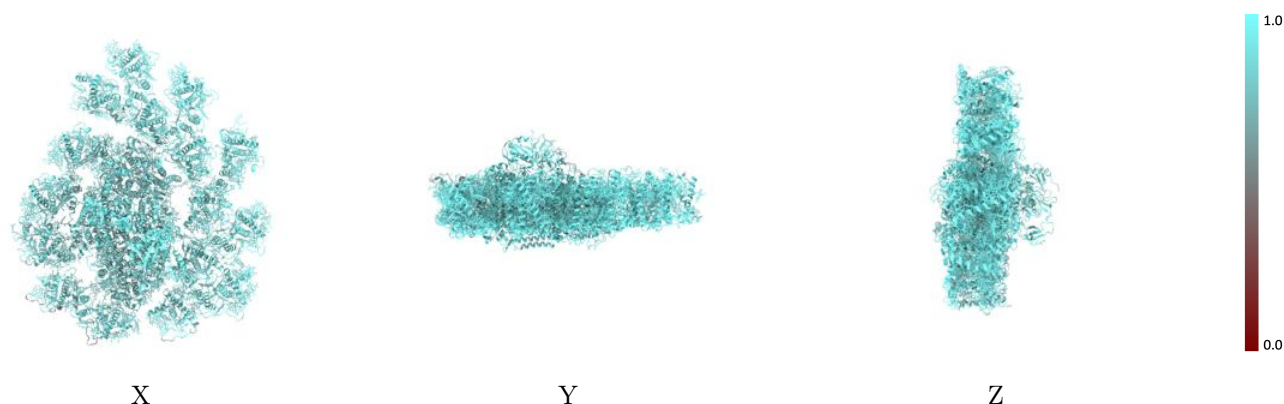
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



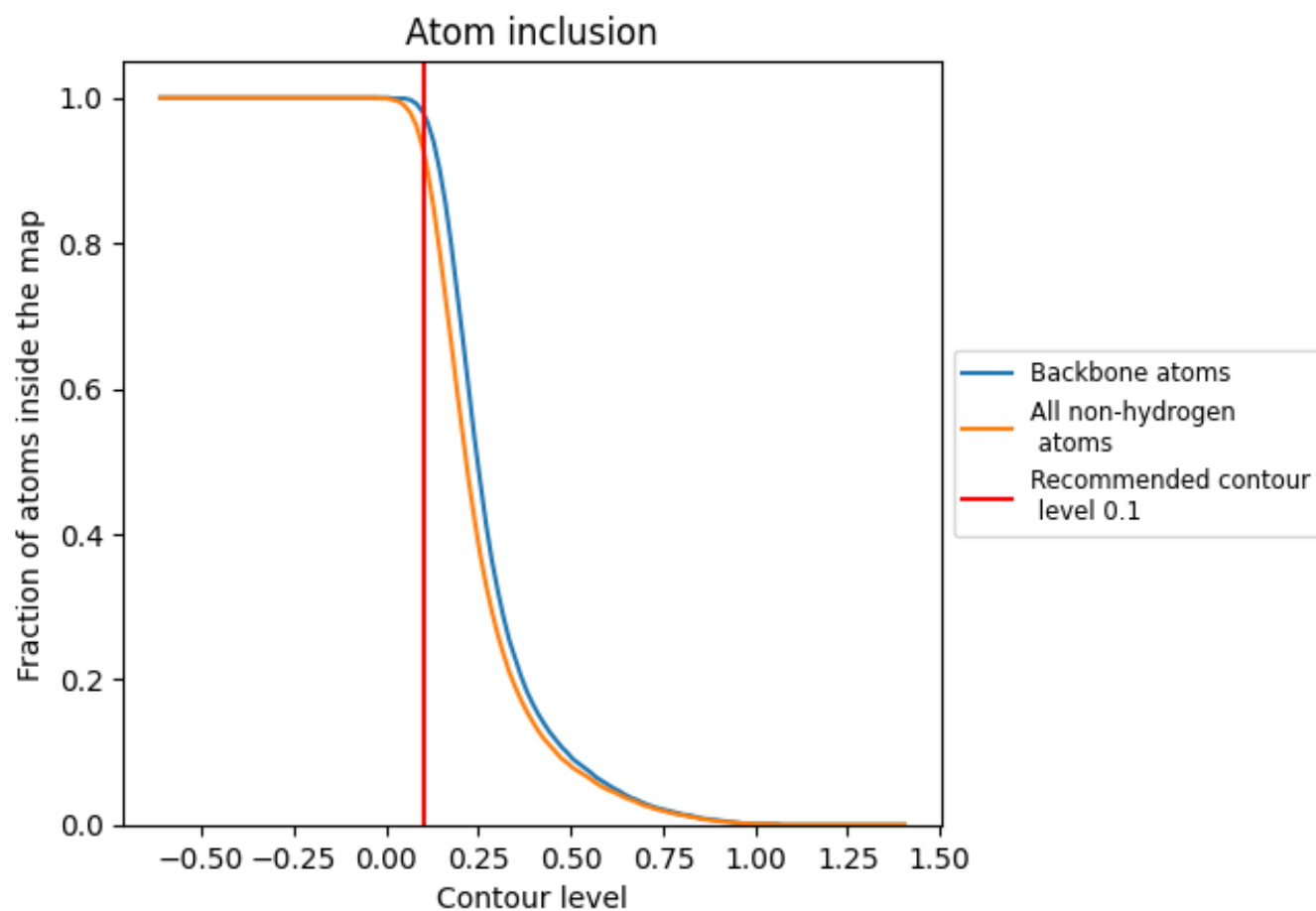
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

