



wwPDB EM Validation Summary Report ⓘ

Aug 9, 2026 – 05:45 AM JST

PDB ID : 9M4F / pdb_00009m4f
EMDB ID : EMD-63625
Title : Photosystem I from the eukaryotic filamentous algae
Authors : Shao, R.Q.; Pan, X.W.
Deposited on : 2025-03-04
Resolution : 2.82 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

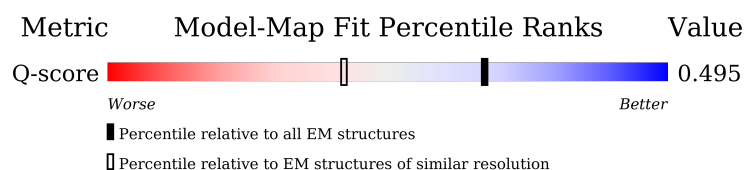
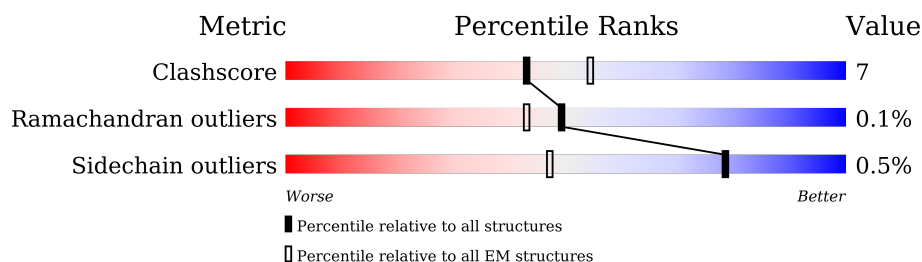
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.82 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	11795 (2.32 - 3.32)

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	1	220	
2	2	194	
3	3	205	
4	4	231	

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Mol	Chain	Length	Quality of chain
5	5	216	
6	6	212	
6	h	212	
7	7	207	
8	8	179	
9	9	215	
9	k	215	
10	c	210	
11	t	228	
12	A	749	
13	B	734	
14	C	81	
15	D	139	
16	E	61	
17	F	185	
18	I	36	
19	J	42	
20	L	149	
21	M	30	
22	R	87	
23	S	134	

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 50344 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 Light-harvesting protein XLH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	176	Total	C	N	O	S	0	0
			1328	865	221	237	5		

- Molecule 2 is a protein called light-harvesting protein XLH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	137	Total	C	N	O	S	0	0
			1080	695	187	191	7		

- Molecule 3 is a protein called light-harvesting protein XLH3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	158	Total	C	N	O	S	0	0
			1206	775	204	221	6		

- Molecule 4 is a protein called light-harvesting protein XLH4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	188	Total	C	N	O	S	0	0
			1396	894	240	251	11		

- Molecule 5 is a protein called light-harvesting protein XLH5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	167	Total	C	N	O	S	0	0
			1249	798	210	234	7		

- Molecule 6 is a protein called light-harvesting protein XLH6/10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	163	Total	C	N	O	S	0	0
			1228	790	206	226	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	165	Total	C	N	O	S	0	0
			1244	801	209	228	6		

- Molecule 7 is a protein called light-harvesting protein XLH7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	166	Total	C	N	O	S	0	0
			1268	816	210	230	12		

- Molecule 8 is a protein called light-harvesting protein XLH8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	161	Total	C	N	O	S	0	0
			1240	794	208	229	9		

- Molecule 9 is a protein called light-harvesting protein XLH9/13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	149	Total	C	N	O	S	0	0
			1171	761	195	206	9		
9	k	154	Total	C	N	O	S	0	0
			1201	777	200	215	9		

- Molecule 10 is a protein called light-harvesting protein XLH11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	165	Total	C	N	O	S	0	0
			1231	787	209	225	10		

- Molecule 11 is a protein called light-harvesting protein XLH12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	t	159	Total	C	N	O	S	0	0
			1253	799	212	235	7		

- Molecule 12 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	741	Total	C	N	O	S	0	0
			5835	3825	992	996	22		

- Molecule 13 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	733	Total	C	N	O	S	0	0
			5822	3830	976	997	19		

- Molecule 14 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	80	Total	C	N	O	S	0	0
			592	363	103	115	11		

- Molecule 15 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D	132	Total	C	N	O	S	0	0
			1030	668	171	188	3		

- Molecule 16 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	60	Total	C	N	O	S	0	0
			484	307	82	94	1		

- Molecule 17 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	161	Total	C	N	O	S	0	0
			1267	818	215	230	4		

- Molecule 18 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	33	Total	C	N	O	S	0	0
			252	174	34	43	1		

- Molecule 19 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	40	Total	C	N	O	S	0	0
			320	217	47	55	1		

- Molecule 20 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	137	Total	C	N	O	S	0	0
			1027	674	165	186	2		

- Molecule 21 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	30	Total	C	N	O	S	0	0
			227	153	35	38	1		

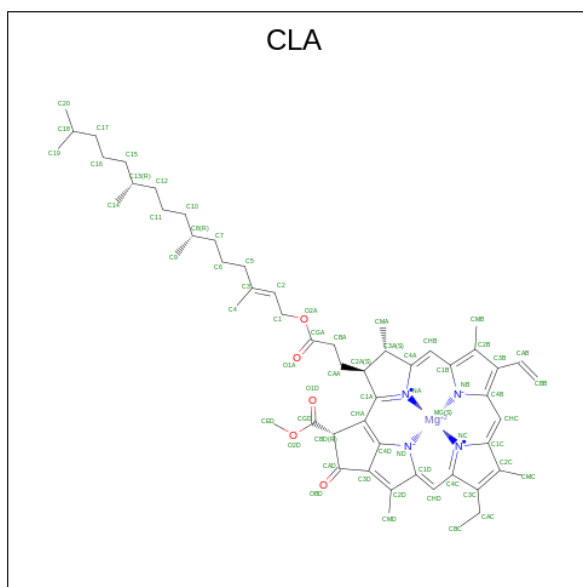
- Molecule 22 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	81	Total	C	N	O	S	0	0
			608	397	99	111	1		

- Molecule 23 is a protein called PsaS.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	82	Total	C	N	O		0	0
			410	246	82	82			

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	3	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	5	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	6	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 44	C 34	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
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24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	c	1	Total 43	C 35	Mg 1	N 4	O 3	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	c	1	Total 44	C 34	Mg 1	N 4	O 5	0
24	c	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	k	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	k	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	k	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
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24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
24	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 54	C 44	Mg 1	N 4	O 5	0

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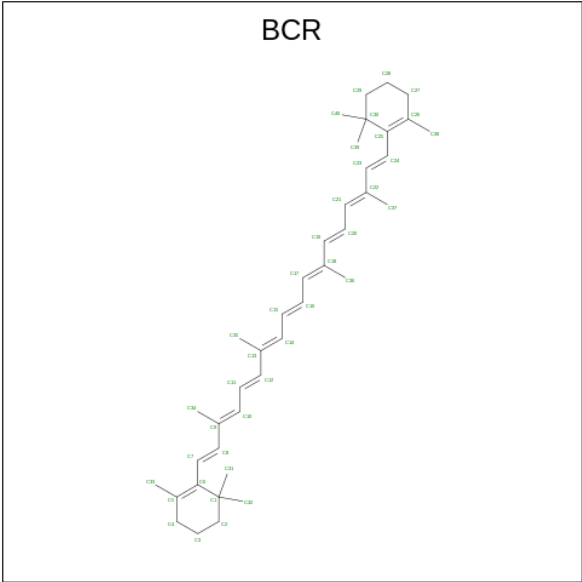
Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	F	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
24	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



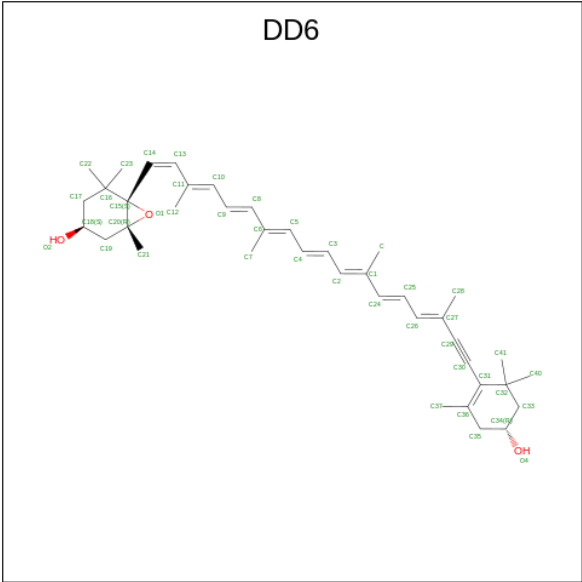
Mol	Chain	Residues	Atoms	AltConf
25	1	1	Total C 40 40	0
25	1	1	Total C 40 40	0
25	2	1	Total C 40 40	0
25	4	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	9	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	t	1	Total C 40 40	0
25	k	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 39 39	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	M	1	Total C 40 40	0
25	R	1	Total C 40 40	0
25	R	1	Total C 40 40	0

- Molecule 26 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			43	40	3	
26	1	1	Total	C	O	0
			43	40	3	
26	1	1	Total	C	O	0
			43	40	3	
26	2	1	Total	C	O	0
			43	40	3	
26	2	1	Total	C	O	0
			43	40	3	
26	3	1	Total	C	O	0
			43	40	3	
26	3	1	Total	C	O	0
			43	40	3	
26	3	1	Total	C	O	0
			43	40	3	
26	4	1	Total	C	O	0
			43	40	3	
26	4	1	Total	C	O	0
			43	40	3	
26	4	1	Total	C	O	0
			43	40	3	
26	4	1	Total	C	O	0
			43	40	3	
26	5	1	Total	C	O	0
			43	40	3	
26	5	1	Total	C	O	0
			43	40	3	

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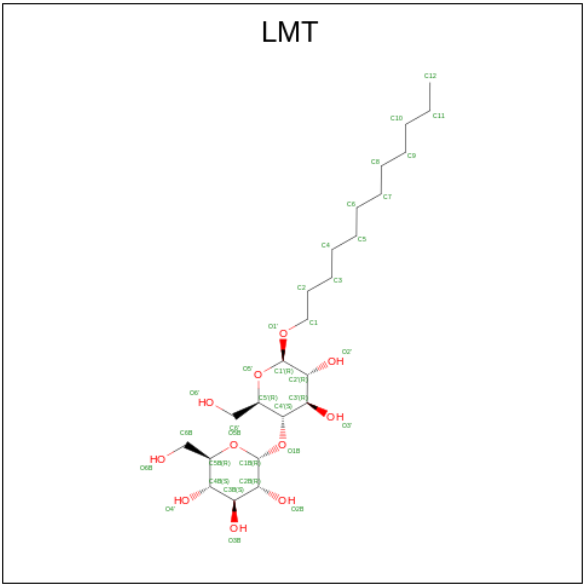
Mol	Chain	Residues	Atoms			AltConf
26	6	1	Total	C	O	0
			43	40	3	
26	6	1	Total	C	O	0
			43	40	3	
26	6	1	Total	C	O	0
			43	40	3	
26	6	1	Total	C	O	0
			43	40	3	
26	6	1	Total	C	O	0
			43	40	3	
26	7	1	Total	C	O	0
			43	40	3	
26	7	1	Total	C	O	0
			43	40	3	
26	7	1	Total	C	O	0
			43	40	3	
26	7	1	Total	C	O	0
			43	40	3	
26	8	1	Total	C	O	0
			43	40	3	
26	8	1	Total	C	O	0
			43	40	3	
26	8	1	Total	C	O	0
			43	40	3	
26	9	1	Total	C	O	0
			43	40	3	
26	9	1	Total	C	O	0
			43	40	3	
26	9	1	Total	C	O	0
			43	40	3	
26	9	1	Total	C	O	0
			43	40	3	
26	h	1	Total	C	O	0
			43	40	3	
26	h	1	Total	C	O	0
			43	40	3	
26	h	1	Total	C	O	0
			43	40	3	
26	h	1	Total	C	O	0
			43	40	3	
26	c	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
26	c	1	Total	C	O	0
			43	40	3	
26	c	1	Total	C	O	0
			43	40	3	
26	t	1	Total	C	O	0
			43	40	3	
26	t	1	Total	C	O	0
			43	40	3	
26	k	1	Total	C	O	0
			43	40	3	
26	k	1	Total	C	O	0
			43	40	3	
26	k	1	Total	C	O	0
			43	40	3	
26	A	1	Total	C	O	0
			43	40	3	
26	J	1	Total	C	O	0
			43	40	3	
26	R	1	Total	C	O	0
			43	40	3	

- Molecule 27 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



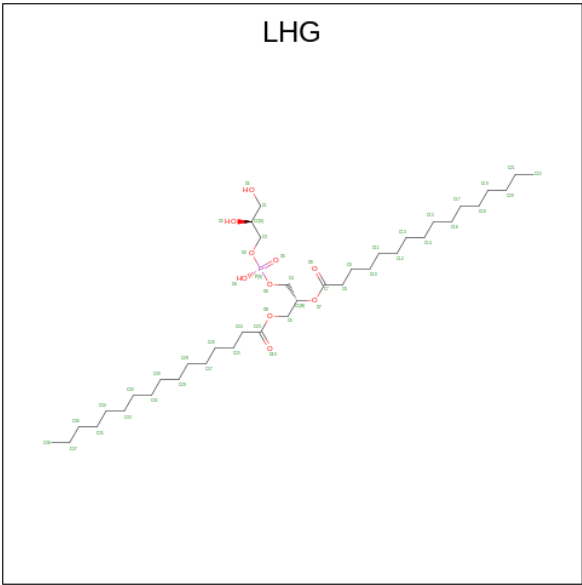
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			35	24	11	
27	3	1	Total	C	O	0
			30	19	11	
27	h	1	Total	C	O	0
			28	17	11	
27	A	1	Total	C	O	0
			35	24	11	
27	A	1	Total	C	O	0
			25	14	11	
27	A	1	Total	C	O	0
			35	24	11	

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



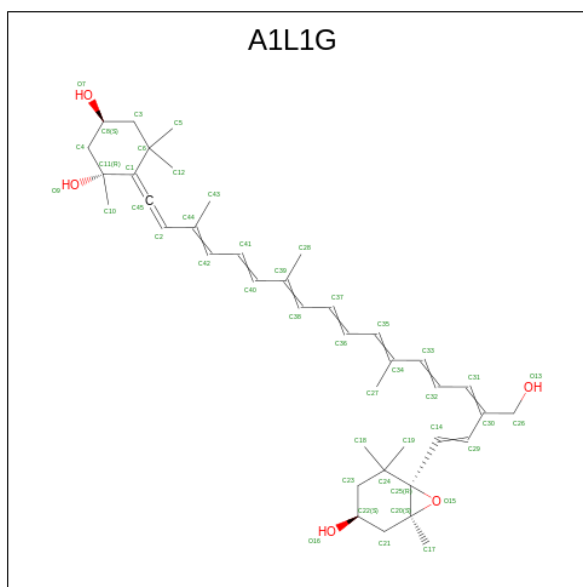
Mol	Chain	Residues	Atoms				AltConf
28	1	1	Total	C	O	P	0
			43	32	10	1	
28	2	1	Total	C	O	P	0
			31	20	10	1	
28	3	1	Total	C	O	P	0
			43	32	10	1	
28	4	1	Total	C	O	P	0
			39	28	10	1	
28	8	1	Total	C	O	P	0
			31	20	10	1	

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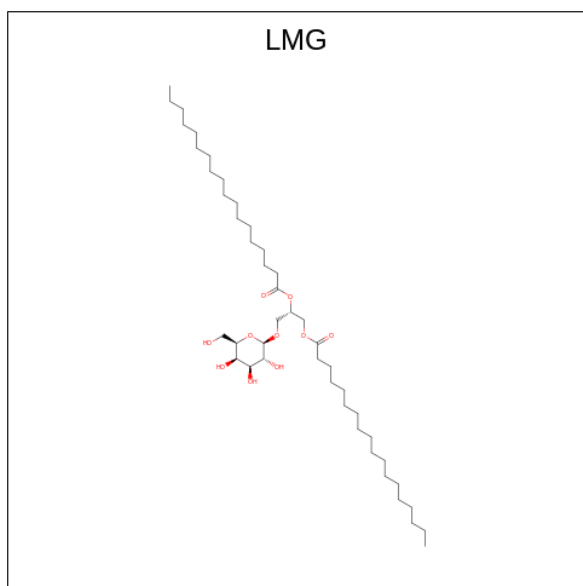
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			48	37	10	1	
28	A	1	Total	C	O	P	0
			42	31	10	1	
28	A	1	Total	C	O	P	0
			41	30	10	1	
28	A	1	Total	C	O	P	0
			37	26	10	1	
28	B	1	Total	C	O	P	0
			49	38	10	1	
28	B	1	Total	C	O	P	0
			41	30	10	1	
28	I	1	Total	C	O	P	0
			40	29	10	1	
28	J	1	Total	C	O	P	0
			38	27	10	1	
28	L	1	Total	C	O	P	0
			29	18	10	1	

- Molecule 29 is (1 {R},3 {S})-6-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {Z},17 {E})-16-(hydroxymethyl)-3,7,12-trimethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]-1,5,5-trimethyl-cyclohexane-1,3-diol (CCD ID: A1L1G) (formula: C₄₀H₅₆O₅) (labeled as "Ligand of Interest" by depositor).



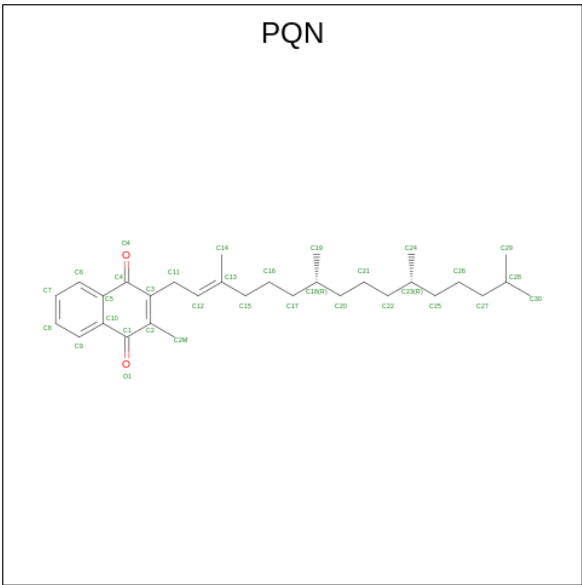
Mol	Chain	Residues	Atoms			AltConf
29	2	1	Total	C	O	0
			45	40	5	
29	3	1	Total	C	O	0
			45	40	5	
29	7	1	Total	C	O	0
			45	40	5	
29	9	1	Total	C	O	0
			45	40	5	
29	k	1	Total	C	O	0
			45	40	5	

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



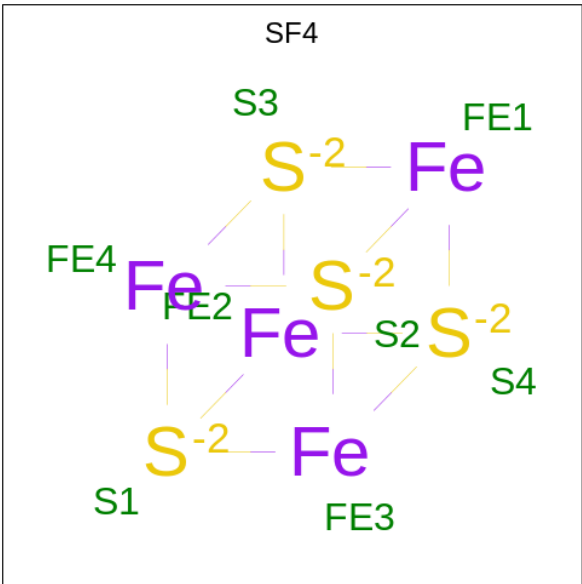
Mol	Chain	Residues	Atoms			AltConf
30	2	1	Total	C	O	0
			45	35	10	
30	t	1	Total	C	O	0
			34	24	10	
30	A	1	Total	C	O	0
			38	28	10	

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



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

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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

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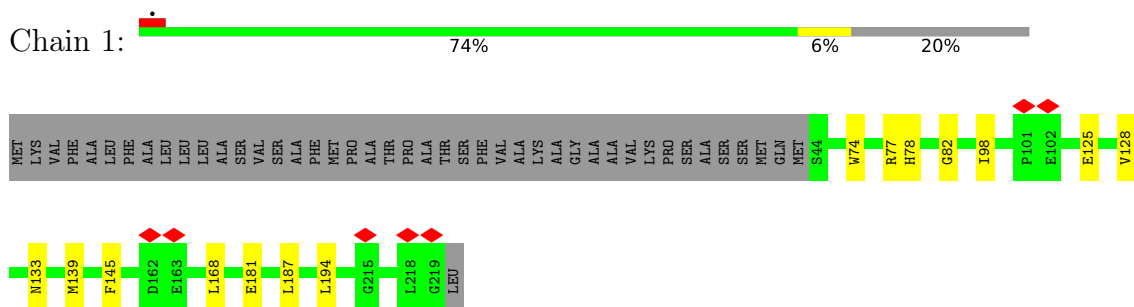
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Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	Fe	S	0
			8	4	4	
32	C	1	Total	Fe	S	0
			8	4	4	

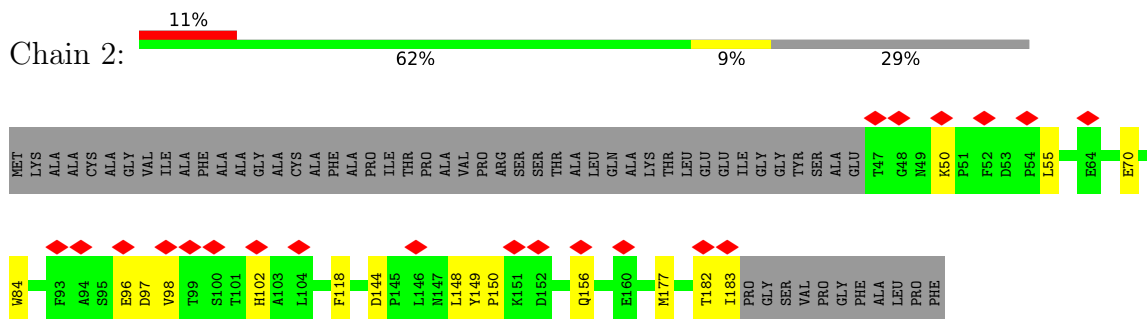
3 Residue-property plots [i](#)

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

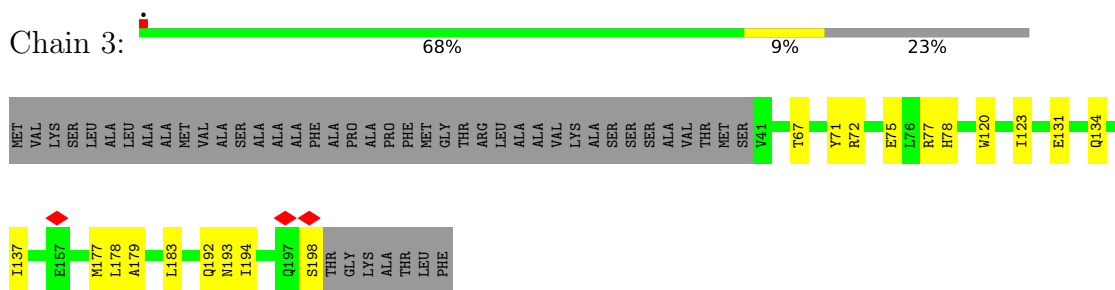
- Molecule 1: Light-harvesting protein XLH1



- Molecule 2: light-harvesting protein XLH2

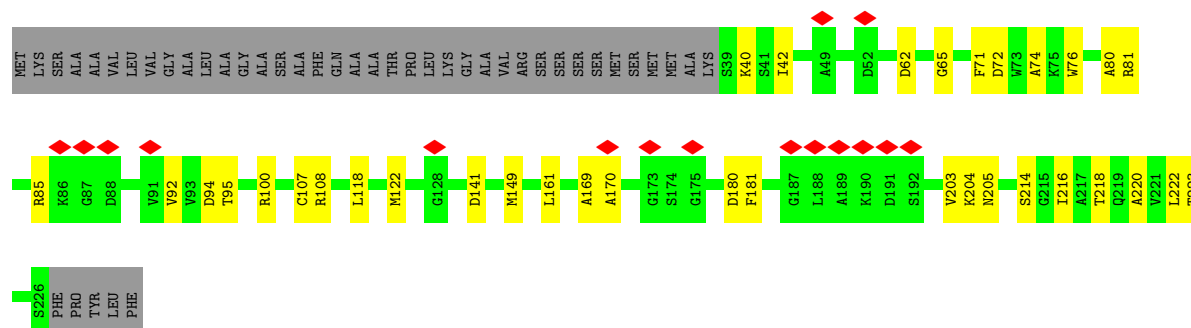


- Molecule 3: light-harvesting protein XLH3

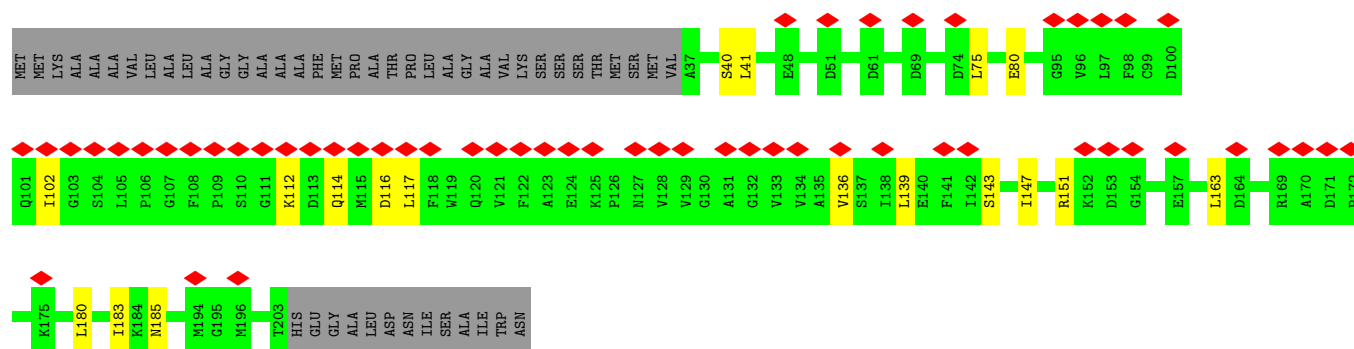


- Molecule 4: light-harvesting protein XLH4

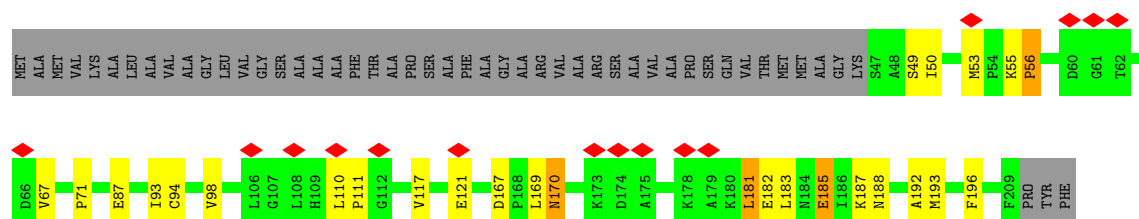




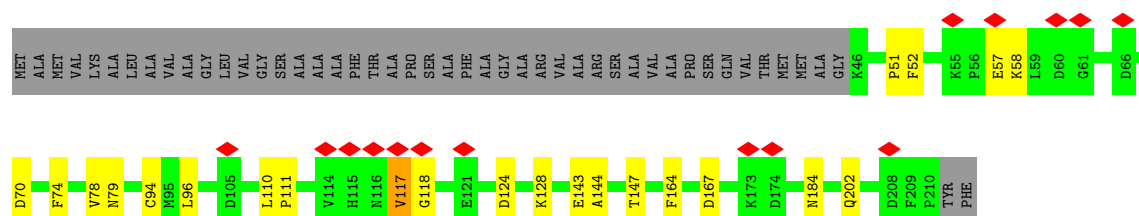
- Molecule 5: light-harvesting protein XLH5



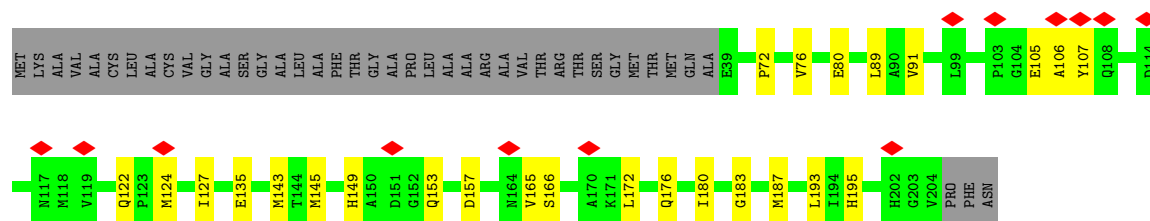
- Molecule 6: light-harvesting protein XLH6/10



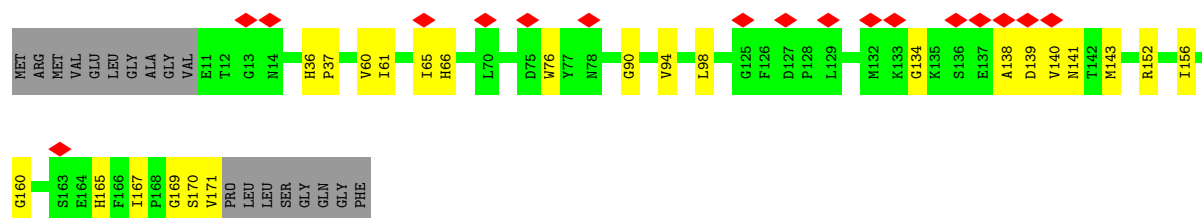
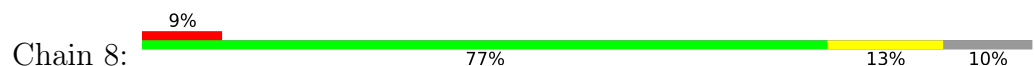
- Molecule 6: light-harvesting protein XLH6/10



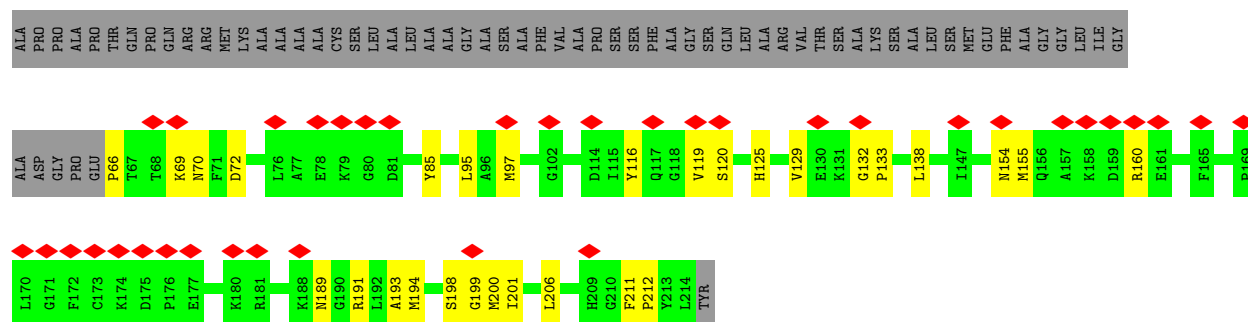
- Molecule 7: light-harvesting protein XLH7



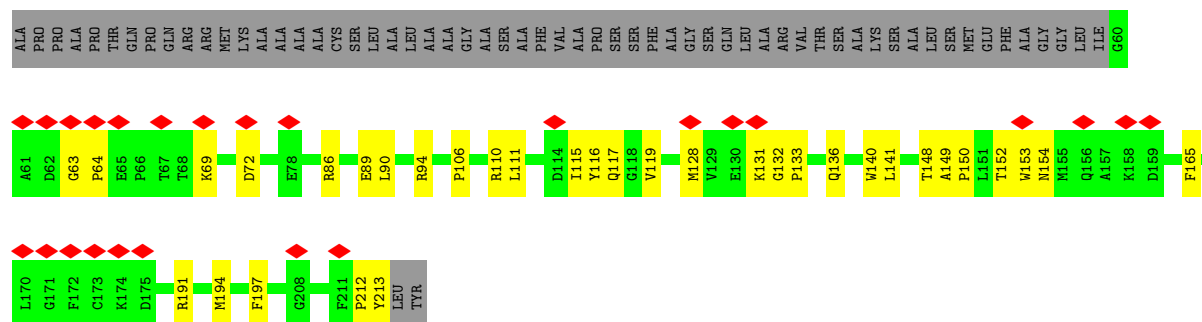
- Molecule 8: light-harvesting protein XLH8



- Molecule 9: light-harvesting protein XLH9/13

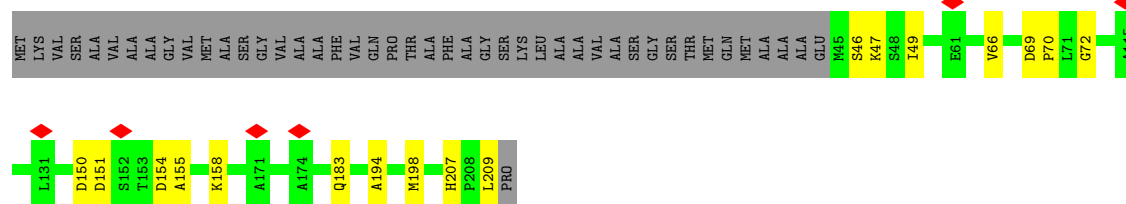


- Molecule 9: light-harvesting protein XLH9/13

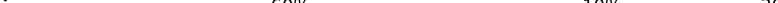


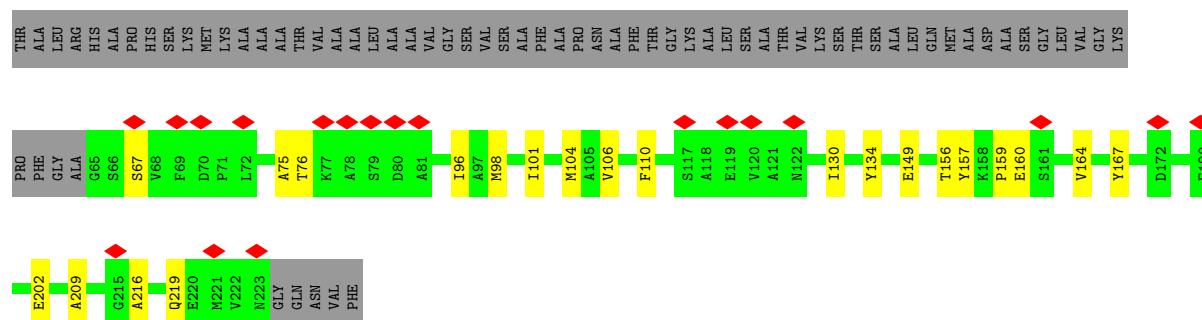
- Molecule 10: light-harvesting protein XLH11

Chain c: 70% 8% 21%

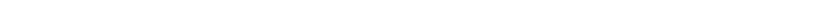


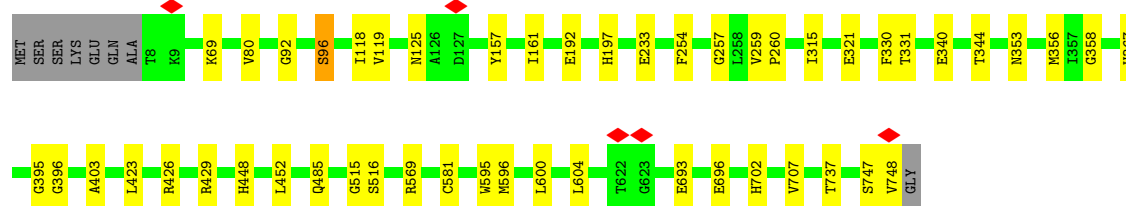
- Molecule 11: light-harvesting protein XLH12

Chain t: 



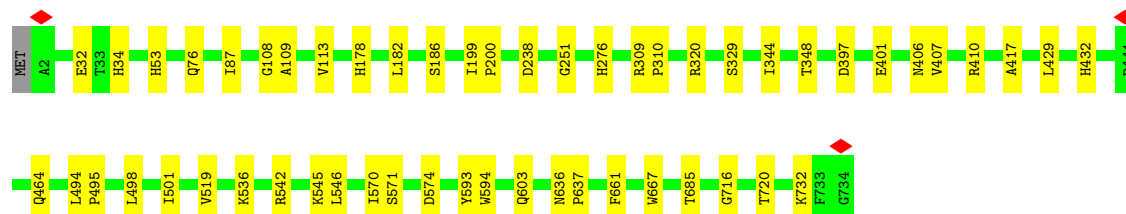
- Molecule 12: PsaA

Chain A:  92% 7%

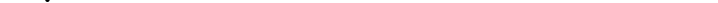


- Molecule 13: PsaB

Chain B:  93% 7%

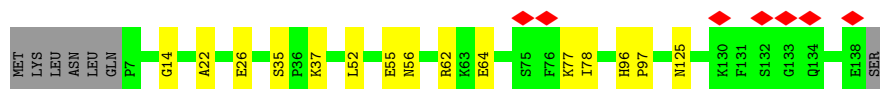
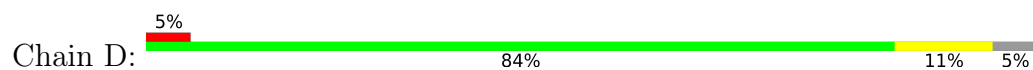


- Molecule 14: PsaC

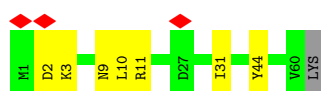
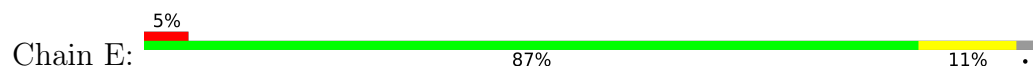
Chain C:  89% 10%



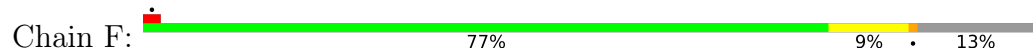
- Molecule 15: PsaD



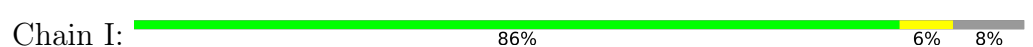
- Molecule 16: PsaE



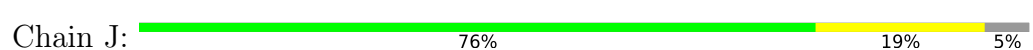
- Molecule 17: PsaF



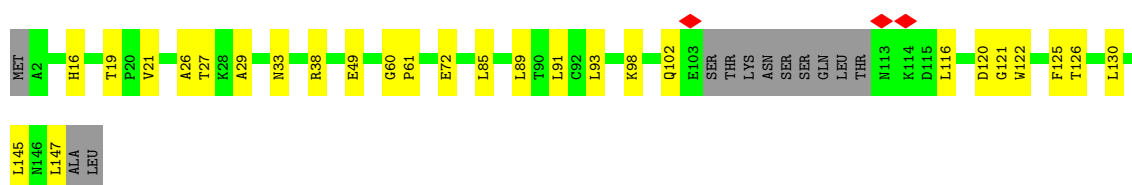
- Molecule 18: PsaI



- Molecule 19: PsaJ



- Molecule 20: PsaL



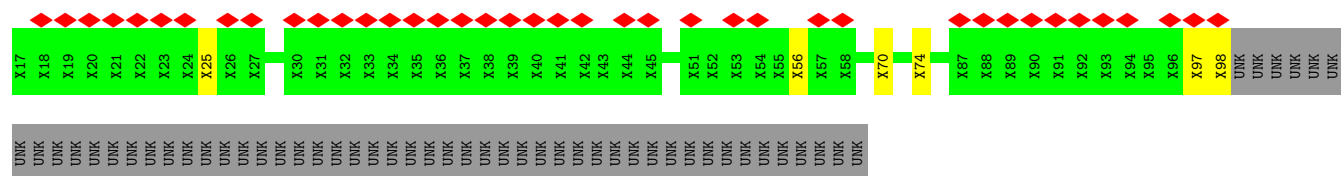
- Molecule 21: PsaM



Chain R: 85% 8% 7%



Chain S: 30% 57% . 39%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60389	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI SPIRIT	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.857	Depositor
Minimum map value	-0.484	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	457.59998, 457.59998, 457.59998	wwPDB
Map dimensions	440, 440, 440	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DD6, CLA, LMT, LHG, PQN, BCR, A1L1G, LMG, SF4

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	1	0.18	0/1363	0.30	0/1859
2	2	0.36	0/1109	0.60	0/1504
3	3	0.16	0/1238	0.31	0/1677
4	4	0.24	0/1427	0.38	0/1934
5	5	0.23	0/1274	0.43	0/1722
6	6	0.39	0/1257	0.64	0/1704
6	h	0.27	0/1274	0.46	0/1727
7	7	0.18	0/1298	0.36	0/1752
8	8	0.22	0/1276	0.41	0/1730
9	9	0.31	0/1200	0.48	0/1622
9	k	0.38	0/1231	0.57	0/1666
10	c	0.16	0/1255	0.32	0/1697
11	t	0.20	0/1285	0.37	0/1741
12	A	0.19	0/6030	0.33	0/8219
13	B	0.18	0/6034	0.31	0/8236
14	C	0.28	0/602	0.55	0/816
15	D	0.19	0/1059	0.36	0/1432
16	E	0.29	0/492	0.48	0/662
17	F	0.25	0/1297	0.44	0/1761
18	I	0.21	0/258	0.32	0/353
19	J	0.31	0/331	0.49	0/453
20	L	0.30	0/1051	0.45	0/1428
21	M	0.26	0/228	0.44	0/310
22	R	0.15	0/627	0.27	0/864
All	All	0.24	0/34496	0.40	0/46869

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1328	0	1344	24	0
2	2	1080	0	1061	16	0
3	3	1206	0	1171	18	0
4	4	1396	0	1415	32	0
5	5	1249	0	1255	15	0
6	6	1228	0	1215	41	0
6	h	1244	0	1236	16	0
7	7	1268	0	1265	27	0
8	8	1240	0	1195	17	0
9	9	1171	0	1187	28	0
9	k	1201	0	1207	30	0
10	c	1231	0	1259	12	0
11	t	1253	0	1213	15	0
12	A	5835	0	5718	48	0
13	B	5822	0	5629	43	0
14	C	592	0	569	5	0
15	D	1030	0	1028	11	0
16	E	484	0	486	5	0
17	F	1267	0	1290	14	0
18	I	252	0	272	1	0
19	J	320	0	313	9	0
20	L	1027	0	1037	27	0
21	M	227	0	262	5	0
22	R	608	0	612	5	0
23	S	410	0	86	3	0
24	1	507	0	427	16	0
24	2	440	0	345	13	0
24	3	468	0	413	8	0
24	4	607	0	454	27	0
24	5	328	0	247	7	0
24	6	554	0	401	12	0
24	7	564	0	428	23	0
24	8	409	0	299	9	0
24	9	505	0	363	18	0
24	A	2651	0	2720	33	0
24	B	2471	0	2526	59	0
24	F	161	0	144	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	J	42	0	31	1	0
24	L	166	0	154	6	0
24	R	110	0	105	1	0
24	c	548	0	460	7	0
24	h	553	0	405	5	0
24	k	513	0	387	10	0
24	t	477	0	369	8	0
25	1	80	0	112	7	0
25	2	40	0	56	4	0
25	4	40	0	56	7	0
25	7	40	0	56	2	0
25	9	40	0	56	9	0
25	A	199	0	277	8	0
25	B	200	0	280	11	0
25	F	40	0	56	2	0
25	I	80	0	112	3	0
25	J	80	0	112	5	0
25	L	80	0	112	2	0
25	M	40	0	56	2	0
25	R	80	0	112	2	0
25	c	40	0	56	7	0
25	k	40	0	56	2	0
25	t	40	0	56	2	0
26	1	129	0	0	7	0
26	2	86	0	0	2	0
26	3	129	0	0	1	0
26	4	172	0	0	2	0
26	5	86	0	0	3	0
26	6	215	0	0	2	0
26	7	172	0	0	3	0
26	8	129	0	0	2	0
26	9	172	0	0	6	0
26	A	43	0	0	0	0
26	J	43	0	0	0	0
26	R	43	0	0	0	0
26	c	129	0	0	3	0
26	h	172	0	0	1	0
26	k	129	0	0	4	0
26	t	86	0	0	0	0
27	1	70	0	92	2	0
27	3	30	0	33	1	0
27	A	95	0	115	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	h	28	0	29	1	0
28	1	43	0	56	2	0
28	2	31	0	32	0	0
28	3	43	0	59	1	0
28	4	39	0	48	1	0
28	8	31	0	32	1	0
28	A	168	0	222	2	0
28	B	90	0	129	0	0
28	I	40	0	50	1	0
28	J	38	0	46	1	0
28	L	29	0	28	4	0
29	2	45	0	0	0	0
29	3	45	0	0	2	0
29	7	45	0	0	0	0
29	9	45	0	0	1	0
29	k	45	0	0	2	0
30	2	45	0	60	1	0
30	A	38	0	46	0	0
30	t	34	0	38	0	0
31	A	33	0	46	1	0
31	B	33	0	46	0	0
32	A	8	0	0	0	0
32	C	16	0	0	0	0
All	All	50344	0	46831	640	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 7.

The worst 5 of 640 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)
20:L:147:LEU:HD23	24:L:205:CLA:C1	1.56	1.33
3:3:194:ILE:HD13	3:3:198:SER:OG	1.43	1.16
1:1:98:ILE:HG23	1:1:128:VAL:HG11	1.21	1.15
20:L:147:LEU:CD2	24:L:205:CLA:C1	2.31	1.07
6:6:50:ILE:HG21	6:6:53:MET:HG3	1.37	1.04

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	174/220 (79%)	169 (97%)	5 (3%)	0	100	100
2	2	135/194 (70%)	121 (90%)	13 (10%)	1 (1%)	18	45
3	3	156/205 (76%)	147 (94%)	9 (6%)	0	100	100
4	4	186/231 (80%)	172 (92%)	14 (8%)	0	100	100
5	5	165/216 (76%)	153 (93%)	12 (7%)	0	100	100
6	6	161/212 (76%)	148 (92%)	12 (8%)	1 (1%)	21	48
6	h	163/212 (77%)	154 (94%)	8 (5%)	1 (1%)	21	48
7	7	164/207 (79%)	149 (91%)	15 (9%)	0	100	100
8	8	159/179 (89%)	146 (92%)	13 (8%)	0	100	100
9	9	147/215 (68%)	142 (97%)	5 (3%)	0	100	100
9	k	152/215 (71%)	144 (95%)	7 (5%)	1 (1%)	18	45
10	c	163/210 (78%)	154 (94%)	9 (6%)	0	100	100
11	t	157/228 (69%)	143 (91%)	14 (9%)	0	100	100
12	A	739/749 (99%)	715 (97%)	24 (3%)	0	100	100
13	B	731/734 (100%)	706 (97%)	25 (3%)	0	100	100
14	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
15	D	130/139 (94%)	120 (92%)	10 (8%)	0	100	100
16	E	58/61 (95%)	56 (97%)	1 (2%)	1 (2%)	7	23
17	F	159/185 (86%)	153 (96%)	5 (3%)	1 (1%)	21	48
18	I	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
19	J	38/42 (90%)	38 (100%)	0	0	100	100
20	L	133/149 (89%)	130 (98%)	3 (2%)	0	100	100
21	M	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
22	R	79/87 (91%)	77 (98%)	2 (2%)	0	100	100
All	All	4286/5037 (85%)	4069 (95%)	211 (5%)	6 (0%)	49	75

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	6	56	PRO
16	E	31	ILE
9	k	119	VAL
6	h	117	VAL
17	F	26	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	1	137/169 (81%)	137 (100%)	0	100	100
2	2	112/149 (75%)	110 (98%)	2 (2%)	51	80
3	3	121/152 (80%)	121 (100%)	0	100	100
4	4	143/173 (83%)	142 (99%)	1 (1%)	76	91
5	5	130/162 (80%)	130 (100%)	0	100	100
6	6	129/159 (81%)	125 (97%)	4 (3%)	35	69
6	h	131/159 (82%)	131 (100%)	0	100	100
7	7	137/163 (84%)	135 (98%)	2 (2%)	57	83
8	8	127/141 (90%)	126 (99%)	1 (1%)	73	90
9	9	125/168 (74%)	124 (99%)	1 (1%)	73	90
9	k	128/168 (76%)	127 (99%)	1 (1%)	73	90
10	c	129/156 (83%)	128 (99%)	1 (1%)	73	90
11	t	133/178 (75%)	132 (99%)	1 (1%)	73	90
12	A	603/609 (99%)	601 (100%)	2 (0%)	86	95
13	B	597/598 (100%)	597 (100%)	0	100	100
14	C	66/67 (98%)	66 (100%)	0	100	100
15	D	110/117 (94%)	110 (100%)	0	100	100
16	E	55/56 (98%)	55 (100%)	0	100	100
17	F	138/159 (87%)	138 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	I	28/31 (90%)	28 (100%)	0	100	100
19	J	32/34 (94%)	32 (100%)	0	100	100
20	L	108/119 (91%)	106 (98%)	2 (2%)	50	79
21	M	25/25 (100%)	25 (100%)	0	100	100
22	R	68/73 (93%)	67 (98%)	1 (2%)	57	83
All	All	3512/3985 (88%)	3493 (100%)	19 (0%)	78	93

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	A	96	SER
20	L	91	LEU
22	R	76	HIS
20	L	16	HIS
7	7	195	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
13	B	432	HIS
13	B	598	HIS
22	R	48	ASN
6	h	123	HIS
9	9	92	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

338 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$
24	CLA	A	835	12	55,59,73	1.39	6 (10%)	66,96,113	1.28	7 (10%)
26	DD6	6	616	-	39,45,45	1.54	8 (20%)	52,67,67	2.05	12 (23%)
26	DD6	t	313	-	39,45,45	1.46	8 (20%)	52,67,67	1.72	11 (21%)
24	CLA	A	822	12	59,63,73	1.37	7 (11%)	71,101,113	1.21	7 (9%)
25	BCR	B	842	-	41,41,41	0.75	0	56,56,56	2.12	14 (25%)
24	CLA	A	836	12	69,73,73	1.25	6 (8%)	83,113,113	1.10	5 (6%)
24	CLA	7	601	7	49,53,73	1.48	7 (14%)	59,89,113	1.24	5 (8%)
24	CLA	6	609	-	54,58,73	1.41	7 (12%)	65,95,113	1.32	6 (9%)
29	A1L1G	2	213	-	38,47,47	1.51	8 (21%)	49,71,71	1.03	5 (10%)
26	DD6	h	616	-	39,45,45	1.56	8 (20%)	52,67,67	1.72	9 (17%)
24	CLA	t	301	11	49,53,73	1.50	6 (12%)	59,89,113	1.45	7 (11%)
28	LHG	2	215	-	30,30,48	1.16	2 (6%)	33,36,54	1.13	3 (9%)
24	CLA	h	605	6	50,54,73	1.47	7 (14%)	60,90,113	1.23	7 (11%)
25	BCR	t	312	-	41,41,41	0.76	0	56,56,56	1.79	9 (16%)
25	BCR	1	310	-	41,41,41	0.76	0	56,56,56	2.17	21 (37%)
26	DD6	k	315	-	39,45,45	1.50	8 (20%)	52,67,67	2.04	12 (23%)
24	CLA	2	204	2	64,68,73	1.29	6 (9%)	77,107,113	1.24	6 (7%)
24	CLA	k	303	-	59,63,73	1.34	6 (10%)	71,101,113	1.39	10 (14%)
24	CLA	A	834	12	49,53,73	1.50	7 (14%)	59,89,113	1.31	7 (11%)
24	CLA	A	817	12	69,73,73	1.24	7 (10%)	83,113,113	1.18	7 (8%)
24	CLA	A	816	12	69,73,73	1.23	6 (8%)	83,113,113	1.16	6 (7%)
24	CLA	A	825	-	69,73,73	1.23	5 (7%)	83,113,113	1.17	6 (7%)
25	BCR	1	314	-	41,41,41	0.74	0	56,56,56	2.16	18 (32%)
24	CLA	B	848	13	69,73,73	1.25	6 (8%)	83,113,113	1.15	5 (6%)
24	CLA	6	607	6	50,54,73	1.45	6 (12%)	60,90,113	1.21	6 (10%)
29	A1L1G	9	312	-	38,47,47	1.54	8 (21%)	49,71,71	1.24	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	t	304	-	50,54,73	1.45	7 (14%)	60,90,113	1.22	4 (6%)
24	CLA	A	820	-	69,73,73	1.25	7 (10%)	83,113,113	1.20	9 (10%)
24	CLA	A	829	12	69,73,73	1.25	6 (8%)	83,113,113	1.15	6 (7%)
24	CLA	7	611	7	50,54,73	1.45	6 (12%)	60,90,113	1.23	4 (6%)
26	DD6	6	615	-	39,45,45	1.45	8 (20%)	52,67,67	1.88	15 (28%)
24	CLA	B	829	13	69,73,73	1.23	9 (13%)	83,113,113	1.37	11 (13%)
24	CLA	A	811	12	50,54,73	1.45	6 (12%)	60,90,113	1.23	5 (8%)
26	DD6	7	618	-	39,45,45	1.72	6 (15%)	52,67,67	1.72	13 (25%)
24	CLA	h	607	6	50,54,73	1.45	7 (14%)	60,90,113	1.18	6 (10%)
24	CLA	3	301	3	69,73,73	1.25	7 (10%)	83,113,113	1.23	5 (6%)
24	CLA	6	601	6	49,53,73	1.49	5 (10%)	59,89,113	1.27	5 (8%)
24	CLA	A	823	12	69,73,73	1.25	6 (8%)	83,113,113	1.11	6 (7%)
26	DD6	7	615	-	39,45,45	1.49	8 (20%)	52,67,67	1.82	12 (23%)
24	CLA	A	860	12	69,73,73	1.23	8 (11%)	83,113,113	1.37	11 (13%)
24	CLA	4	610	4	45,49,73	1.54	6 (13%)	54,84,113	1.28	4 (7%)
25	BCR	I	102	-	41,41,41	0.72	0	56,56,56	2.32	26 (46%)
24	CLA	B	819	13	50,54,73	1.47	6 (12%)	60,90,113	1.21	4 (6%)
24	CLA	c	610	10	47,52,73	1.52	6 (12%)	56,88,113	1.19	5 (8%)
24	CLA	8	202	8	50,54,73	1.46	5 (10%)	60,90,113	1.28	6 (10%)
27	LMT	A	854	-	36,36,36	0.68	0	47,47,47	0.88	0
24	CLA	1	305	1	49,53,73	1.47	7 (14%)	59,89,113	1.68	7 (11%)
24	CLA	2	203	-	54,58,73	1.41	6 (11%)	65,95,113	1.23	5 (7%)
24	CLA	h	606	6	50,54,73	1.46	7 (14%)	60,90,113	1.20	4 (6%)
26	DD6	7	616	-	39,45,45	1.63	8 (20%)	52,67,67	1.71	8 (15%)
24	CLA	4	613	4	50,54,73	1.45	5 (10%)	60,90,113	1.20	4 (6%)
27	LMT	3	314	-	31,31,36	0.70	0	42,42,47	1.19	3 (7%)
30	LMG	t	314	-	34,34,55	1.12	2 (5%)	42,42,63	1.21	4 (9%)
26	DD6	k	313	-	39,45,45	1.48	8 (20%)	52,67,67	1.70	11 (21%)
24	CLA	B	815	13	59,63,73	1.34	6 (10%)	71,101,113	1.24	7 (9%)
24	CLA	F	202	-	50,54,73	1.47	7 (14%)	60,90,113	1.23	6 (10%)
25	BCR	R	101	-	41,41,41	0.79	1 (2%)	56,56,56	2.02	22 (39%)
24	CLA	c	605	10	50,54,73	1.47	6 (12%)	60,90,113	1.22	3 (5%)
28	LHG	3	315	-	42,42,48	0.99	2 (4%)	45,48,54	1.03	4 (8%)
24	CLA	8	206	8	50,54,73	1.44	6 (12%)	60,90,113	1.24	4 (6%)
26	DD6	8	212	-	39,45,45	1.50	8 (20%)	52,67,67	1.64	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	c	612	-	39,45,45	1.48	8 (20%)	52,67,67	2.07	11 (21%)
26	DD6	1	311	24	39,45,45	1.59	8 (20%)	52,67,67	1.61	12 (23%)
24	CLA	A	838	12	69,73,73	1.25	7 (10%)	83,113,113	1.15	7 (8%)
24	CLA	5	602	5	59,63,73	1.35	6 (10%)	71,101,113	1.25	10 (14%)
24	CLA	B	824	13	69,73,73	1.27	7 (10%)	83,113,113	1.28	10 (12%)
25	BCR	A	859	-	41,41,41	0.71	0	56,56,56	1.81	14 (25%)
24	CLA	9	301	9	50,54,73	1.48	7 (14%)	60,90,113	1.36	8 (13%)
24	CLA	L	204	20	69,73,73	1.25	7 (10%)	83,113,113	1.17	7 (8%)
28	LHG	I	103	-	39,39,48	1.03	2 (5%)	42,45,54	1.15	4 (9%)
24	CLA	6	604	-	50,54,73	1.45	7 (14%)	60,90,113	1.19	4 (6%)
24	CLA	B	805	13	69,73,73	1.24	6 (8%)	83,113,113	1.19	6 (7%)
26	DD6	3	313	-	39,45,45	1.54	8 (20%)	52,67,67	1.61	10 (19%)
24	CLA	A	821	12	53,57,73	1.40	6 (11%)	62,93,113	1.24	5 (8%)
26	DD6	9	313	-	39,45,45	1.56	8 (20%)	52,67,67	1.61	8 (15%)
24	CLA	B	821	13	57,61,73	1.36	7 (12%)	68,98,113	1.25	9 (13%)
24	CLA	8	208	8	49,53,73	1.47	6 (12%)	59,89,113	1.37	5 (8%)
26	DD6	6	613	-	39,45,45	1.52	8 (20%)	52,67,67	1.66	8 (15%)
24	CLA	A	827	12	66,70,73	1.25	6 (9%)	79,109,113	1.16	7 (8%)
26	DD6	4	616	-	39,45,45	1.51	8 (20%)	52,67,67	1.83	13 (25%)
24	CLA	t	303	11	69,73,73	1.24	6 (8%)	83,113,113	1.20	6 (7%)
24	CLA	4	609	4	50,54,73	1.46	6 (12%)	60,90,113	1.22	5 (8%)
24	CLA	4	604	-	50,54,73	1.48	7 (14%)	60,90,113	1.17	5 (8%)
24	CLA	c	609	-	64,68,73	1.31	5 (7%)	77,107,113	1.32	7 (9%)
24	CLA	6	608	6	50,54,73	1.44	6 (12%)	60,90,113	1.23	6 (10%)
24	CLA	F	203	17	54,58,73	1.40	6 (11%)	65,95,113	1.29	4 (6%)
27	LMT	1	316	-	36,36,36	0.69	0	47,47,47	0.94	2 (4%)
24	CLA	k	308	-	45,49,73	1.51	5 (11%)	54,84,113	1.48	7 (12%)
24	CLA	h	610	6	50,54,73	1.47	6 (12%)	60,90,113	1.17	6 (10%)
24	CLA	4	603	4	50,54,73	1.47	7 (14%)	60,90,113	1.27	7 (11%)
24	CLA	B	835	13	51,55,73	1.45	6 (11%)	61,91,113	1.39	8 (13%)
24	CLA	4	607	4	50,54,73	1.45	6 (12%)	60,90,113	1.24	6 (10%)
24	CLA	B	836	-	69,73,73	1.25	7 (10%)	83,113,113	1.09	6 (7%)
26	DD6	6	614	-	39,45,45	1.61	8 (20%)	52,67,67	1.46	6 (11%)
24	CLA	A	818	12	69,73,73	1.24	7 (10%)	83,113,113	1.18	10 (12%)
31	PQN	A	839	-	34,34,34	0.35	0	42,45,45	0.61	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LHG	L	201	-	28,28,48	1.22	2 (7%)	31,34,54	1.13	2 (6%)
24	CLA	B	833	13	62,66,73	1.31	7 (11%)	74,104,113	1.30	7 (9%)
26	DD6	t	311	-	39,45,45	1.56	8 (20%)	52,67,67	1.54	7 (13%)
24	CLA	A	832	12	69,73,73	1.25	6 (8%)	83,113,113	1.17	7 (8%)
24	CLA	c	606	10	50,54,73	1.46	6 (12%)	60,90,113	1.23	3 (5%)
24	CLA	B	807	13	69,73,73	1.25	7 (10%)	83,113,113	1.20	6 (7%)
24	CLA	4	601	4	45,50,73	1.51	7 (15%)	53,85,113	1.11	4 (7%)
24	CLA	t	305	11	50,54,73	1.45	7 (14%)	60,90,113	1.24	7 (11%)
24	CLA	B	832	-	49,53,73	1.50	7 (14%)	59,89,113	1.23	5 (8%)
29	A1L1G	k	312	-	38,47,47	1.48	8 (21%)	49,71,71	1.08	4 (8%)
24	CLA	c	601	10	47,51,73	1.51	6 (12%)	56,86,113	1.26	7 (12%)
24	CLA	A	828	12	69,73,73	1.25	7 (10%)	83,113,113	1.16	7 (8%)
28	LHG	A	842	24	41,41,48	1.09	2 (4%)	44,47,54	1.28	5 (11%)
24	CLA	B	823	-	68,72,73	1.25	7 (10%)	81,111,113	1.17	10 (12%)
24	CLA	9	305	-	50,54,73	1.46	6 (12%)	60,90,113	1.40	6 (10%)
24	CLA	c	603	10	50,54,73	1.43	6 (12%)	60,90,113	1.33	7 (11%)
24	CLA	c	607	10	50,54,73	1.41	6 (12%)	60,90,113	1.31	7 (11%)
24	CLA	5	605	5	50,54,73	1.45	6 (12%)	60,90,113	1.25	6 (10%)
24	CLA	k	307	9	50,54,73	1.47	7 (14%)	60,90,113	1.22	4 (6%)
32	SF4	A	858	13,12	0,12,12	-	-	-	-	-
24	CLA	h	612	-	49,53,73	1.48	6 (12%)	59,89,113	1.30	7 (11%)
26	DD6	1	313	-	39,45,45	1.52	8 (20%)	52,67,67	1.56	8 (15%)
24	CLA	A	837	12	59,63,73	1.35	6 (10%)	71,101,113	1.28	8 (11%)
24	CLA	B	808	13	69,73,73	1.24	8 (11%)	83,113,113	1.18	9 (10%)
24	CLA	h	608	6	50,54,73	1.45	7 (14%)	60,90,113	1.19	4 (6%)
24	CLA	c	604	-	50,54,73	1.46	6 (12%)	60,90,113	1.19	3 (5%)
28	LHG	8	213	-	30,30,48	1.19	2 (6%)	33,36,54	1.47	4 (12%)
24	CLA	7	604	-	49,53,73	1.46	8 (16%)	59,89,113	1.36	6 (10%)
24	CLA	B	834	13	69,73,73	1.24	6 (8%)	83,113,113	1.11	5 (6%)
24	CLA	B	817	13	69,73,73	1.24	6 (8%)	83,113,113	1.15	8 (9%)
24	CLA	A	804	12	69,73,73	1.25	6 (8%)	83,113,113	1.18	6 (7%)
24	CLA	7	606	7	64,68,73	1.31	6 (9%)	77,107,113	1.28	8 (10%)
26	DD6	6	617	-	39,45,45	1.55	9 (23%)	52,67,67	1.63	9 (17%)
26	DD6	9	317	-	39,45,45	1.48	8 (20%)	52,67,67	2.09	16 (30%)
24	CLA	9	311	-	49,53,73	1.47	8 (16%)	59,89,113	1.29	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	4	618	-	41,41,41	0.79	0	56,56,56	2.38	20 (35%)
24	CLA	k	305	9	50,54,73	1.45	6 (12%)	60,90,113	1.25	3 (5%)
24	CLA	B	822	-	69,73,73	1.25	6 (8%)	83,113,113	1.27	9 (10%)
24	CLA	3	305	3	64,68,73	1.28	6 (9%)	77,107,113	1.12	7 (9%)
24	CLA	L	205	-	50,54,73	1.44	6 (12%)	60,90,113	1.18	6 (10%)
28	LHG	4	619	-	38,38,48	1.05	2 (5%)	41,44,54	0.99	2 (4%)
27	LMT	1	315	-	36,36,36	0.67	0	47,47,47	0.79	1 (2%)
24	CLA	6	611	6	47,52,73	1.51	7 (14%)	56,88,113	1.31	5 (8%)
24	CLA	8	209	-	45,49,73	1.52	6 (13%)	54,84,113	1.28	4 (7%)
24	CLA	h	604	-	50,54,73	1.45	6 (12%)	60,90,113	1.21	4 (6%)
24	CLA	A	802	-	69,73,73	1.23	8 (11%)	83,113,113	1.31	8 (9%)
24	CLA	B	846	13	59,63,73	1.33	7 (11%)	71,101,113	1.17	5 (7%)
24	CLA	B	811	13	59,63,73	1.35	7 (11%)	71,101,113	1.26	9 (12%)
24	CLA	t	306	11	49,53,73	1.48	6 (12%)	59,89,113	1.28	5 (8%)
29	A1L1G	3	310	-	38,47,47	1.49	8 (21%)	49,71,71	0.99	3 (6%)
26	DD6	3	311	-	39,45,45	1.51	8 (20%)	52,67,67	1.63	10 (19%)
24	CLA	B	827	13	69,73,73	1.24	7 (10%)	83,113,113	1.15	6 (7%)
24	CLA	h	603	6	48,53,73	1.48	6 (12%)	57,89,113	1.27	9 (15%)
24	CLA	8	207	-	49,53,73	1.51	6 (12%)	59,89,113	1.25	4 (6%)
26	DD6	k	314	-	39,45,45	1.53	9 (23%)	52,67,67	1.75	7 (13%)
25	BCR	c	615	-	41,41,41	0.71	0	56,56,56	2.64	21 (37%)
26	DD6	7	613	-	39,45,45	1.48	8 (20%)	52,67,67	1.86	11 (21%)
26	DD6	4	615	-	39,45,45	1.56	9 (23%)	52,67,67	1.60	7 (13%)
24	CLA	B	826	13	69,73,73	1.26	8 (11%)	83,113,113	1.12	7 (8%)
24	CLA	9	306	9	50,54,73	1.47	7 (14%)	60,90,113	1.33	5 (8%)
24	CLA	A	815	-	49,53,73	1.50	6 (12%)	59,89,113	1.27	6 (10%)
24	CLA	B	806	13	69,73,73	1.25	6 (8%)	83,113,113	1.18	5 (6%)
29	A1L1G	7	614	-	38,47,47	1.53	8 (21%)	49,71,71	1.10	2 (4%)
24	CLA	A	814	12	54,58,73	1.41	6 (11%)	65,95,113	1.27	5 (7%)
25	BCR	A	846	-	41,41,41	0.74	1 (2%)	56,56,56	2.38	27 (48%)
24	CLA	t	308	11	50,54,73	1.48	6 (12%)	60,90,113	1.14	4 (6%)
30	LMG	2	214	-	45,45,55	0.95	2 (4%)	53,53,63	1.37	5 (9%)
27	LMT	h	617	-	29,29,36	0.74	0	40,40,47	0.85	2 (5%)
25	BCR	L	206	-	41,41,41	0.73	0	56,56,56	2.09	18 (32%)
24	CLA	2	202	2	59,63,73	1.37	6 (10%)	71,101,113	1.21	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	820	13	59,63,73	1.34	7 (11%)	71,101,113	1.26	9 (12%)
24	CLA	7	610	7	49,53,73	1.48	6 (12%)	59,89,113	1.21	4 (6%)
24	CLA	2	209	-	50,54,73	1.46	6 (12%)	60,90,113	1.21	4 (6%)
28	LHG	1	318	-	42,42,48	0.97	3 (7%)	45,48,54	1.39	4 (8%)
26	DD6	5	608	-	39,45,45	1.53	8 (20%)	52,67,67	1.77	11 (21%)
25	BCR	A	843	-	41,41,41	0.72	0	56,56,56	2.34	21 (37%)
24	CLA	A	831	12	69,73,73	1.24	6 (8%)	83,113,113	1.13	7 (8%)
26	DD6	4	617	-	39,45,45	1.50	8 (20%)	52,67,67	1.85	12 (23%)
26	DD6	c	614	-	39,45,45	1.50	8 (20%)	52,67,67	2.15	11 (21%)
24	CLA	A	840	28	69,73,73	1.24	6 (8%)	83,113,113	1.19	7 (8%)
24	CLA	B	814	13	54,58,73	1.42	7 (12%)	65,95,113	1.27	9 (13%)
27	LMT	A	851	-	26,26,36	0.82	0	37,37,47	1.05	5 (13%)
28	LHG	B	844	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
24	CLA	A	833	12	69,73,73	1.26	7 (10%)	83,113,113	1.16	6 (7%)
24	CLA	B	838	28	69,73,73	1.24	7 (10%)	83,113,113	1.31	9 (10%)
24	CLA	3	306	3	69,73,73	1.24	6 (8%)	83,113,113	1.11	5 (6%)
24	CLA	h	602	6	59,63,73	1.36	7 (11%)	71,101,113	1.86	12 (16%)
25	BCR	B	840	-	41,41,41	0.79	0	56,56,56	2.01	23 (41%)
24	CLA	7	608	-	49,53,73	1.50	6 (12%)	59,89,113	1.34	7 (11%)
25	BCR	A	844	-	41,41,41	0.84	0	56,56,56	2.12	18 (32%)
24	CLA	5	601	5	49,53,73	1.49	6 (12%)	59,89,113	1.23	5 (8%)
24	CLA	k	301	9	50,54,73	1.44	5 (10%)	60,90,113	1.25	4 (6%)
24	CLA	A	819	12	49,53,73	1.47	5 (10%)	59,89,113	1.28	5 (8%)
24	CLA	8	201	8	50,54,73	1.46	6 (12%)	60,90,113	1.20	4 (6%)
24	CLA	B	804	13	69,73,73	1.30	6 (8%)	83,113,113	1.34	12 (14%)
25	BCR	B	849	-	41,41,41	0.64	0	56,56,56	2.24	20 (35%)
24	CLA	h	601	6	49,53,73	1.48	5 (10%)	59,89,113	1.32	5 (8%)
28	LHG	A	852	-	36,36,48	1.07	2 (5%)	39,42,54	1.02	2 (5%)
24	CLA	t	302	11	50,54,73	1.47	5 (10%)	60,90,113	1.20	4 (6%)
24	CLA	B	828	13	54,58,73	1.41	8 (14%)	65,95,113	1.21	5 (7%)
32	SF4	C	102	14	0,12,12	-	-	-	-	-
24	CLA	4	602	4	64,68,73	1.28	6 (9%)	77,107,113	1.21	7 (9%)
24	CLA	t	307	-	50,54,73	1.45	6 (12%)	60,90,113	1.17	3 (5%)
25	BCR	B	841	-	41,41,41	0.75	0	56,56,56	2.08	22 (39%)
24	CLA	5	604	5	50,54,73	1.46	6 (12%)	60,90,113	1.19	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	1	301	1	69,73,73	1.24	7 (10%)	83,113,113	1.12	4 (4%)
24	CLA	k	309	9	49,53,73	1.48	6 (12%)	59,89,113	1.23	5 (8%)
27	LMT	A	850	-	36,36,36	0.68	0	47,47,47	0.64	0
26	DD6	8	210	-	39,45,45	1.68	8 (20%)	52,67,67	2.09	12 (23%)
26	DD6	c	613	-	39,45,45	1.50	8 (20%)	52,67,67	1.70	8 (15%)
24	CLA	4	608	-	54,58,73	1.41	6 (11%)	65,95,113	1.39	9 (13%)
24	CLA	B	847	13	69,73,73	1.26	7 (10%)	83,113,113	1.14	6 (7%)
24	CLA	1	306	1	54,58,73	1.39	5 (9%)	65,95,113	1.26	7 (10%)
24	CLA	A	847	-	59,63,73	1.34	6 (10%)	71,101,113	1.27	9 (12%)
24	CLA	k	311	-	59,63,73	1.35	6 (10%)	71,101,113	1.22	6 (8%)
26	DD6	2	212	-	39,45,45	1.53	8 (20%)	52,67,67	1.67	8 (15%)
24	CLA	t	309	-	50,54,73	1.47	6 (12%)	60,90,113	1.20	4 (6%)
24	CLA	L	203	20	59,63,73	1.34	7 (11%)	71,101,113	1.33	8 (11%)
24	CLA	A	806	12	69,73,73	1.26	6 (8%)	83,113,113	1.12	5 (6%)
24	CLA	7	607	7	49,53,73	1.49	6 (12%)	59,89,113	1.29	8 (13%)
24	CLA	2	205	2	50,54,73	1.46	6 (12%)	60,90,113	1.23	5 (8%)
24	CLA	J	103	19	46,50,73	1.50	6 (13%)	55,85,113	1.27	5 (9%)
24	CLA	5	606	-	50,54,73	1.46	6 (12%)	60,90,113	1.24	4 (6%)
26	DD6	J	102	-	39,45,45	1.53	8 (20%)	52,67,67	1.65	11 (21%)
24	CLA	c	602	10	69,73,73	1.23	6 (8%)	83,113,113	1.16	7 (8%)
24	CLA	1	308	1	50,54,73	1.48	7 (14%)	60,90,113	1.17	4 (6%)
26	DD6	h	614	-	39,45,45	1.53	8 (20%)	52,67,67	1.59	10 (19%)
26	DD6	1	312	-	39,45,45	1.57	9 (23%)	52,67,67	1.51	7 (13%)
24	CLA	A	803	12	59,63,73	1.34	7 (11%)	71,101,113	1.29	8 (11%)
24	CLA	9	302	9	50,54,73	1.45	8 (16%)	60,90,113	1.39	7 (11%)
24	CLA	A	812	12	69,73,73	1.25	7 (10%)	83,113,113	1.22	7 (8%)
24	CLA	8	204	8	49,53,73	1.49	6 (12%)	59,89,113	1.33	5 (8%)
24	CLA	3	303	-	59,63,73	1.35	7 (11%)	71,101,113	1.22	6 (8%)
24	CLA	9	303	-	50,54,73	1.46	8 (16%)	60,90,113	1.36	6 (10%)
26	DD6	9	315	-	39,45,45	1.58	9 (23%)	52,67,67	1.74	10 (19%)
30	LMG	A	855	-	38,38,55	1.07	2 (5%)	46,46,63	1.08	2 (4%)
24	CLA	k	306	9	50,54,73	1.43	7 (14%)	60,90,113	1.22	6 (10%)
31	PQN	B	839	-	34,34,34	0.35	0	42,45,45	0.60	1 (2%)
25	BCR	2	211	-	41,41,41	0.76	0	56,56,56	2.12	22 (39%)
25	BCR	I	101	-	41,41,41	0.78	1 (2%)	56,56,56	2.28	25 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	9	316	-	41,41,41	0.76	0	56,56,56	2.36	18 (32%)
24	CLA	B	831	-	69,73,73	1.26	7 (10%)	83,113,113	1.15	7 (8%)
24	CLA	9	309	9	50,54,73	1.45	5 (10%)	60,90,113	1.32	6 (10%)
24	CLA	A	856	-	69,73,73	1.25	6 (8%)	83,113,113	1.20	8 (9%)
24	CLA	A	824	-	69,73,73	1.24	7 (10%)	83,113,113	1.17	7 (8%)
24	CLA	6	606	6	50,54,73	1.46	5 (10%)	60,90,113	1.18	4 (6%)
24	CLA	2	208	-	50,54,73	1.47	5 (10%)	60,90,113	1.22	3 (5%)
24	CLA	B	802	13	69,73,73	1.23	6 (8%)	83,113,113	1.11	6 (7%)
24	CLA	4	605	4	50,54,73	1.43	6 (12%)	60,90,113	1.22	5 (8%)
24	CLA	4	606	4	50,54,73	1.44	6 (12%)	60,90,113	1.23	7 (11%)
28	LHG	J	105	-	37,37,48	1.05	2 (5%)	40,43,54	1.11	3 (7%)
24	CLA	A	810	12	66,70,73	1.27	6 (9%)	79,109,113	1.11	5 (6%)
24	CLA	1	302	1	49,53,73	1.46	7 (14%)	59,89,113	1.27	7 (11%)
24	CLA	A	830	12	59,63,73	1.34	8 (13%)	71,101,113	1.75	12 (16%)
24	CLA	c	611	10	45,49,73	1.52	7 (15%)	54,84,113	1.31	4 (7%)
24	CLA	F	201	-	69,73,73	1.25	6 (8%)	83,113,113	1.14	6 (7%)
24	CLA	A	857	12	69,73,73	1.21	8 (11%)	83,113,113	1.33	7 (8%)
24	CLA	9	307	9	50,54,73	1.42	7 (14%)	60,90,113	1.35	5 (8%)
24	CLA	1	303	1	50,54,73	1.44	6 (12%)	60,90,113	1.24	5 (8%)
24	CLA	7	603	7	49,53,73	1.49	6 (12%)	59,89,113	1.30	9 (15%)
26	DD6	8	211	-	39,45,45	1.51	8 (20%)	52,67,67	1.78	9 (17%)
25	BCR	B	843	-	41,41,41	0.84	1 (2%)	56,56,56	2.37	20 (35%)
24	CLA	3	309	3	45,49,73	1.51	6 (13%)	54,84,113	1.31	5 (9%)
24	CLA	8	203	-	54,58,73	1.41	8 (14%)	65,95,113	1.30	7 (10%)
24	CLA	A	805	12	69,73,73	1.25	6 (8%)	83,113,113	1.19	7 (8%)
28	LHG	A	841	-	47,47,48	0.93	2 (4%)	50,53,54	0.98	3 (6%)
24	CLA	B	830	13	62,66,73	1.32	6 (9%)	74,104,113	1.20	5 (6%)
25	BCR	A	845	-	40,40,41	0.81	0	52,54,56	2.22	18 (34%)
26	DD6	4	614	-	39,45,45	1.52	8 (20%)	52,67,67	1.80	11 (21%)
24	CLA	2	207	-	50,54,73	1.46	6 (12%)	60,90,113	1.26	6 (10%)
24	CLA	4	612	4	50,54,73	1.44	6 (12%)	60,90,113	1.30	7 (11%)
26	DD6	R	105	-	39,45,45	1.55	10 (25%)	52,67,67	1.87	12 (23%)
26	DD6	2	210	-	39,45,45	1.50	8 (20%)	52,67,67	1.73	8 (15%)
24	CLA	9	308	-	50,54,73	1.45	7 (14%)	60,90,113	1.21	5 (8%)
25	BCR	7	617	-	41,41,41	0.77	0	56,56,56	1.98	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	9	314	-	39,45,45	1.65	7 (17%)	52,67,67	2.20	11 (21%)
25	BCR	J	101	-	41,41,41	0.88	0	56,56,56	2.37	19 (33%)
24	CLA	k	310	9	45,49,73	1.53	6 (13%)	54,84,113	1.33	6 (11%)
24	CLA	B	837	13	69,73,73	1.24	6 (8%)	83,113,113	1.26	6 (7%)
24	CLA	B	818	-	69,73,73	1.25	7 (10%)	83,113,113	1.12	9 (10%)
24	CLA	c	608	10	69,73,73	1.24	6 (8%)	83,113,113	1.13	7 (8%)
24	CLA	1	317	-	69,73,73	1.25	7 (10%)	83,113,113	1.09	5 (6%)
26	DD6	5	609	-	39,45,45	1.50	8 (20%)	52,67,67	1.77	9 (17%)
24	CLA	B	809	13	69,73,73	1.25	6 (8%)	83,113,113	1.23	9 (10%)
24	CLA	1	309	1	48,53,73	1.48	7 (14%)	57,89,113	1.20	4 (7%)
25	BCR	F	204	-	41,41,41	0.75	0	56,56,56	2.01	16 (28%)
32	SF4	C	101	14	0,12,12	-	-	-	-	-
24	CLA	7	605	7	50,54,73	1.46	5 (10%)	60,90,113	1.25	4 (6%)
24	CLA	A	853	12	59,63,73	1.35	7 (11%)	71,101,113	1.26	7 (9%)
24	CLA	6	610	6	50,54,73	1.46	5 (10%)	60,90,113	1.12	4 (6%)
24	CLA	6	605	6	50,54,73	1.46	6 (12%)	60,90,113	1.25	7 (11%)
24	CLA	k	304	9	50,54,73	1.46	6 (12%)	60,90,113	1.32	3 (5%)
24	CLA	3	304	3	50,54,73	1.45	4 (8%)	60,90,113	1.44	10 (16%)
24	CLA	9	310	9	50,54,73	1.46	7 (14%)	60,90,113	1.30	3 (5%)
24	CLA	5	603	5	49,53,73	1.50	6 (12%)	59,89,113	1.29	6 (10%)
26	DD6	A	848	-	39,45,45	1.46	8 (20%)	52,67,67	1.92	10 (19%)
24	CLA	B	803	-	69,73,73	1.22	9 (13%)	83,113,113	1.32	6 (7%)
24	CLA	A	808	12	69,73,73	1.26	6 (8%)	83,113,113	1.14	4 (4%)
24	CLA	7	609	7	50,54,73	1.46	5 (10%)	60,90,113	1.30	7 (11%)
28	LHG	A	849	-	40,40,48	1.03	2 (5%)	43,46,54	1.05	2 (4%)
24	CLA	7	612	7	50,54,73	1.50	6 (12%)	60,90,113	1.28	7 (11%)
24	CLA	k	302	9	50,54,73	1.45	6 (12%)	60,90,113	1.39	7 (11%)
24	CLA	B	810	13	58,62,73	1.40	8 (13%)	73,100,113	1.33	11 (15%)
25	BCR	M	101	-	41,41,41	0.74	0	56,56,56	2.14	16 (28%)
24	CLA	A	813	12	69,73,73	1.25	8 (11%)	83,113,113	1.12	7 (8%)
24	CLA	B	801	-	69,73,73	1.25	7 (10%)	83,113,113	1.24	6 (7%)
26	DD6	3	312	-	39,45,45	1.47	8 (20%)	52,67,67	1.84	9 (17%)
24	CLA	B	813	13	50,54,73	1.44	6 (12%)	60,90,113	1.30	5 (8%)
25	BCR	J	104	-	41,41,41	0.69	0	56,56,56	2.28	23 (41%)
24	CLA	1	307	1	49,53,73	1.50	6 (12%)	59,89,113	1.24	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	3	308	3	50,54,73	1.45	9 (18%)	60,90,113	1.30	7 (11%)
25	BCR	k	316	-	41,41,41	0.73	0	56,56,56	2.32	20 (35%)
24	CLA	B	825	13	59,63,73	1.33	6 (10%)	71,101,113	1.20	7 (9%)
25	BCR	R	102	-	41,41,41	0.75	0	56,56,56	2.15	21 (37%)
24	CLA	6	612	-	50,54,73	1.46	6 (12%)	60,90,113	1.24	4 (6%)
24	CLA	5	607	5	49,53,73	1.50	6 (12%)	59,89,113	1.40	6 (10%)
24	CLA	1	304	26	59,63,73	1.33	7 (11%)	71,101,113	1.10	5 (7%)
24	CLA	A	826	12	69,73,73	1.24	6 (8%)	83,113,113	1.23	9 (10%)
24	CLA	6	603	6	50,54,73	1.46	6 (12%)	60,90,113	1.18	4 (6%)
24	CLA	2	206	2	50,54,73	1.45	6 (12%)	60,90,113	1.30	6 (10%)
24	CLA	8	205	8	49,53,73	1.47	5 (10%)	59,89,113	1.20	5 (8%)
24	CLA	h	611	6	45,49,73	1.46	6 (13%)	54,84,113	1.56	7 (12%)
24	CLA	9	304	9	50,54,73	1.43	7 (14%)	60,90,113	1.43	7 (11%)
24	CLA	h	609	-	50,54,73	1.47	6 (12%)	60,90,113	1.21	5 (8%)
24	CLA	B	812	13	69,73,73	1.25	6 (8%)	83,113,113	1.18	6 (7%)
25	BCR	L	202	-	41,41,41	0.68	0	56,56,56	2.28	24 (42%)
24	CLA	7	602	7	54,58,73	1.42	6 (11%)	65,95,113	1.49	13 (20%)
24	CLA	2	201	2	49,53,73	1.48	6 (12%)	59,89,113	1.38	8 (13%)
24	CLA	B	816	13	69,73,73	1.23	5 (7%)	83,113,113	1.26	6 (7%)
26	DD6	h	615	-	39,45,45	1.50	8 (20%)	52,67,67	1.71	10 (19%)
24	CLA	A	809	12	50,54,73	1.44	6 (12%)	60,90,113	1.23	5 (8%)
24	CLA	3	302	3	49,53,73	1.47	6 (12%)	59,89,113	1.37	7 (11%)
24	CLA	3	307	-	49,53,73	1.47	6 (12%)	59,89,113	1.30	4 (6%)
24	CLA	4	611	-	50,54,73	1.46	6 (12%)	60,90,113	1.24	5 (8%)
24	CLA	A	807	12	69,73,73	1.23	6 (8%)	83,113,113	1.17	7 (8%)
24	CLA	t	310	-	50,54,73	1.46	6 (12%)	60,90,113	1.23	4 (6%)
24	CLA	R	103	22	69,73,73	1.24	7 (10%)	83,113,113	1.15	4 (4%)
28	LHG	B	845	24	40,40,48	1.02	2 (5%)	43,46,54	0.97	1 (2%)
24	CLA	6	602	6	51,55,73	1.44	6 (11%)	61,91,113	1.25	7 (11%)
24	CLA	A	801	12	69,73,73	1.24	6 (8%)	83,113,113	1.34	9 (10%)
24	CLA	R	104	22	49,53,73	1.45	8 (16%)	59,89,113	1.39	4 (6%)
26	DD6	h	613	-	39,45,45	1.50	8 (20%)	52,67,67	1.56	9 (17%)

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
24	CLA	A	835	12	-	6/23/99/115	-
26	DD6	6	616	-	-	4/26/80/80	0/3/3/3
26	DD6	t	313	-	-	0/26/80/80	0/3/3/3
24	CLA	A	822	12	-	16/27/103/115	-
25	BCR	B	842	-	-	3/29/63/63	0/2/2/2
24	CLA	A	836	12	-	15/39/115/115	-
24	CLA	7	601	7	-	8/15/91/115	-
24	CLA	6	609	-	-	9/21/97/115	-
29	A1L1G	2	213	-	-	19/29/85/85	0/3/3/3
26	DD6	h	616	-	-	2/26/80/80	0/3/3/3
24	CLA	t	301	11	-	4/15/91/115	-
28	LHG	2	215	-	-	9/35/35/53	-
24	CLA	h	605	6	-	4/17/93/115	-
25	BCR	t	312	-	-	8/29/63/63	0/2/2/2
25	BCR	1	310	-	-	3/29/63/63	0/2/2/2
26	DD6	k	315	-	-	3/26/80/80	0/3/3/3
24	CLA	2	204	2	-	12/33/109/115	-
24	CLA	k	303	-	-	10/27/103/115	-
24	CLA	A	834	12	-	5/15/91/115	-
24	CLA	A	817	12	-	13/39/115/115	-
24	CLA	A	816	12	-	13/39/115/115	-
24	CLA	A	825	-	-	6/39/115/115	-
25	BCR	1	314	-	-	8/29/63/63	0/2/2/2
24	CLA	B	848	13	-	10/39/115/115	-
24	CLA	6	607	6	-	6/17/93/115	-
29	A1L1G	9	312	-	-	13/29/85/85	0/3/3/3
24	CLA	t	304	-	-	5/17/93/115	-
24	CLA	A	820	-	-	10/39/115/115	-
24	CLA	A	829	12	-	8/39/115/115	-
24	CLA	7	611	7	-	7/17/93/115	-
26	DD6	6	615	-	-	4/26/80/80	0/3/3/3
24	CLA	B	829	13	-	9/39/115/115	-
24	CLA	A	811	12	-	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DD6	7	618	-	-	3/26/80/80	0/3/3/3
24	CLA	h	607	6	-	6/17/93/115	-
24	CLA	3	301	3	-	15/39/115/115	-
24	CLA	6	601	6	-	6/15/91/115	-
24	CLA	A	823	12	-	21/39/115/115	-
26	DD6	7	615	-	-	3/26/80/80	0/3/3/3
24	CLA	A	860	12	-	6/39/115/115	-
24	CLA	4	610	4	-	2/10/86/115	-
25	BCR	I	102	-	-	0/29/63/63	0/2/2/2
24	CLA	B	819	13	-	4/17/93/115	-
24	CLA	c	610	10	-	3/13/89/115	-
24	CLA	8	202	8	-	9/17/93/115	-
27	LMT	A	854	-	-	9/21/61/61	0/2/2/2
24	CLA	1	305	1	-	7/15/91/115	-
24	CLA	2	203	-	-	5/21/97/115	-
24	CLA	h	606	6	-	5/17/93/115	-
26	DD6	7	616	-	-	2/26/80/80	0/3/3/3
24	CLA	4	613	4	-	13/17/93/115	-
27	LMT	3	314	-	-	9/16/56/61	0/2/2/2
30	LMG	t	314	-	-	6/29/49/70	0/1/1/1
26	DD6	k	313	-	-	1/26/80/80	0/3/3/3
24	CLA	B	815	13	-	11/27/103/115	-
24	CLA	F	202	-	-	3/17/93/115	-
25	BCR	R	101	-	-	4/29/63/63	0/2/2/2
24	CLA	c	605	10	-	10/17/93/115	-
28	LHG	3	315	-	-	26/47/47/53	-
24	CLA	8	206	8	-	8/17/93/115	-
26	DD6	8	212	-	-	2/26/80/80	0/3/3/3
26	DD6	c	612	-	-	1/26/80/80	0/3/3/3
26	DD6	1	311	24	-	0/26/80/80	0/3/3/3
24	CLA	A	838	12	-	10/39/115/115	-
24	CLA	5	602	5	-	10/27/103/115	-
24	CLA	B	824	13	-	9/39/115/115	-
25	BCR	A	859	-	-	4/29/63/63	0/2/2/2
24	CLA	9	301	9	-	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	L	204	20	-	11/39/115/115	-
28	LHG	I	103	-	-	13/44/44/53	-
24	CLA	6	604	-	-	4/17/93/115	-
24	CLA	B	805	13	-	11/39/115/115	-
26	DD6	3	313	-	-	3/26/80/80	0/3/3/3
24	CLA	A	821	12	-	2/20/96/115	-
26	DD6	9	313	-	-	3/26/80/80	0/3/3/3
24	CLA	B	821	13	-	13/25/101/115	-
24	CLA	8	208	8	-	5/15/91/115	-
26	DD6	6	613	-	-	2/26/80/80	0/3/3/3
24	CLA	A	827	12	-	11/36/112/115	-
26	DD6	4	616	-	-	4/26/80/80	0/3/3/3
24	CLA	t	303	11	-	15/39/115/115	-
24	CLA	4	609	4	-	6/17/93/115	-
24	CLA	4	604	-	-	8/17/93/115	-
24	CLA	c	609	-	-	12/33/109/115	-
24	CLA	6	608	6	-	4/17/93/115	-
24	CLA	F	203	17	-	7/21/97/115	-
27	LMT	1	316	-	-	8/21/61/61	0/2/2/2
24	CLA	k	308	-	-	7/10/86/115	-
24	CLA	h	610	6	-	9/17/93/115	-
24	CLA	4	603	4	-	4/17/93/115	-
24	CLA	B	835	13	-	7/18/94/115	-
24	CLA	4	607	4	-	8/17/93/115	-
24	CLA	B	836	-	-	14/39/115/115	-
26	DD6	6	614	-	-	1/26/80/80	0/3/3/3
24	CLA	A	818	12	-	15/39/115/115	-
31	PQN	A	839	-	-	5/23/43/43	0/2/2/2
28	LHG	L	201	-	-	15/33/33/53	-
24	CLA	B	833	13	-	6/31/107/115	-
26	DD6	t	311	-	-	2/26/80/80	0/3/3/3
24	CLA	A	832	12	-	14/39/115/115	-
24	CLA	c	606	10	-	6/17/93/115	-
24	CLA	B	807	13	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	4	601	4	-	5/11/87/115	-
24	CLA	t	305	11	-	6/17/93/115	-
24	CLA	B	832	-	-	11/15/91/115	-
29	A1L1G	k	312	-	-	8/29/85/85	0/3/3/3
24	CLA	c	601	10	-	5/13/89/115	-
24	CLA	A	828	12	-	12/39/115/115	-
28	LHG	A	842	24	-	10/46/46/53	-
24	CLA	B	823	-	-	7/38/114/115	-
24	CLA	9	305	-	-	10/17/93/115	-
24	CLA	c	603	10	-	11/17/93/115	-
24	CLA	c	607	10	-	3/17/93/115	-
24	CLA	5	605	5	-	11/17/93/115	-
24	CLA	k	307	9	-	8/17/93/115	-
32	SF4	A	858	13,12	-	-	0/6/5/5
24	CLA	h	612	-	-	8/15/91/115	-
26	DD6	1	313	-	-	1/26/80/80	0/3/3/3
24	CLA	A	837	12	-	8/27/103/115	-
24	CLA	B	808	13	-	10/39/115/115	-
24	CLA	h	608	6	-	7/17/93/115	-
24	CLA	c	604	-	-	8/17/93/115	-
28	LHG	8	213	-	-	17/35/35/53	-
24	CLA	7	604	-	-	6/15/91/115	-
24	CLA	B	834	13	-	10/39/115/115	-
24	CLA	B	817	13	-	18/39/115/115	-
24	CLA	A	804	12	-	15/39/115/115	-
24	CLA	7	606	7	-	12/33/109/115	-
26	DD6	6	617	-	-	1/26/80/80	0/3/3/3
26	DD6	9	317	-	-	2/26/80/80	0/3/3/3
24	CLA	9	311	-	-	6/15/91/115	-
25	BCR	4	618	-	-	1/29/63/63	0/2/2/2
24	CLA	k	305	9	-	6/17/93/115	-
24	CLA	B	822	-	-	12/39/115/115	-
24	CLA	3	305	3	-	8/33/109/115	-
24	CLA	L	205	-	-	6/17/93/115	-
28	LHG	4	619	-	-	8/43/43/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMT	1	315	-	-	12/21/61/61	0/2/2/2
24	CLA	6	611	6	-	4/13/89/115	-
24	CLA	8	209	-	-	5/10/86/115	-
24	CLA	h	604	-	-	5/17/93/115	-
24	CLA	A	802	-	-	6/39/115/115	-
24	CLA	B	846	13	-	10/27/103/115	-
24	CLA	B	811	13	-	5/27/103/115	-
24	CLA	t	306	11	-	8/15/91/115	-
29	A1L1G	3	310	-	-	16/29/85/85	0/3/3/3
26	DD6	3	311	-	-	1/26/80/80	0/3/3/3
24	CLA	B	827	13	-	12/39/115/115	-
24	CLA	h	603	6	-	4/15/91/115	-
24	CLA	8	207	-	-	9/15/91/115	-
26	DD6	k	314	-	-	2/26/80/80	0/3/3/3
25	BCR	c	615	-	-	10/29/63/63	0/2/2/2
26	DD6	7	613	-	-	0/26/80/80	0/3/3/3
26	DD6	4	615	-	-	1/26/80/80	0/3/3/3
24	CLA	B	826	13	-	8/39/115/115	-
24	CLA	9	306	9	-	7/17/93/115	-
24	CLA	A	815	-	-	7/15/91/115	-
24	CLA	B	806	13	-	9/39/115/115	-
29	A1L1G	7	614	-	-	12/29/85/85	0/3/3/3
24	CLA	A	814	12	-	7/21/97/115	-
25	BCR	A	846	-	-	2/29/63/63	0/2/2/2
24	CLA	t	308	11	-	6/17/93/115	-
30	LMG	2	214	-	-	8/40/60/70	0/1/1/1
27	LMT	h	617	-	-	7/14/54/61	0/2/2/2
25	BCR	L	206	-	-	4/29/63/63	0/2/2/2
24	CLA	2	202	2	-	6/27/103/115	-
24	CLA	B	820	13	-	10/27/103/115	-
24	CLA	7	610	7	-	8/15/91/115	-
24	CLA	2	209	-	-	7/17/93/115	-
28	LHG	1	318	-	-	15/47/47/53	-
26	DD6	5	608	-	-	4/26/80/80	0/3/3/3
25	BCR	A	843	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	831	12	-	12/39/115/115	-
26	DD6	4	617	-	-	1/26/80/80	0/3/3/3
26	DD6	c	614	-	-	1/26/80/80	0/3/3/3
24	CLA	A	840	28	-	11/39/115/115	-
24	CLA	B	814	13	-	3/21/97/115	-
27	LMT	A	851	-	-	4/11/51/61	0/2/2/2
28	LHG	B	844	-	-	16/53/53/53	-
24	CLA	A	833	12	-	5/39/115/115	-
24	CLA	B	838	28	-	9/39/115/115	-
24	CLA	3	306	3	-	10/39/115/115	-
24	CLA	h	602	6	-	7/27/103/115	-
25	BCR	B	840	-	-	4/29/63/63	0/2/2/2
24	CLA	7	608	-	-	6/15/91/115	-
25	BCR	A	844	-	-	6/29/63/63	0/2/2/2
24	CLA	5	601	5	-	4/15/91/115	-
24	CLA	k	301	9	-	4/17/93/115	-
24	CLA	A	819	12	-	4/15/91/115	-
24	CLA	8	201	8	-	6/17/93/115	-
24	CLA	B	804	13	-	13/39/115/115	-
25	BCR	B	849	-	-	4/29/63/63	0/2/2/2
24	CLA	h	601	6	-	7/15/91/115	-
28	LHG	A	852	-	-	9/41/41/53	-
24	CLA	t	302	11	-	12/17/93/115	-
24	CLA	B	828	13	-	11/21/97/115	-
32	SF4	C	102	14	-	-	0/6/5/5
24	CLA	4	602	4	-	11/33/109/115	-
24	CLA	t	307	-	-	9/17/93/115	-
25	BCR	B	841	-	-	2/29/63/63	0/2/2/2
24	CLA	5	604	5	-	3/17/93/115	-
24	CLA	1	301	1	-	11/39/115/115	-
24	CLA	k	309	9	-	5/15/91/115	-
27	LMT	A	850	-	-	10/21/61/61	0/2/2/2
26	DD6	8	210	-	-	3/26/80/80	0/3/3/3
26	DD6	c	613	-	-	0/26/80/80	0/3/3/3
24	CLA	4	608	-	-	9/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	847	13	-	14/39/115/115	-
24	CLA	1	306	1	-	4/21/97/115	-
24	CLA	A	847	-	-	10/27/103/115	-
24	CLA	k	311	-	-	7/27/103/115	-
26	DD6	2	212	-	-	1/26/80/80	0/3/3/3
24	CLA	t	309	-	-	4/17/93/115	-
24	CLA	L	203	20	-	12/27/103/115	-
24	CLA	A	806	12	-	10/39/115/115	-
24	CLA	7	607	7	-	3/15/91/115	-
24	CLA	2	205	2	-	4/17/93/115	-
24	CLA	J	103	19	-	8/12/88/115	-
24	CLA	5	606	-	-	6/17/93/115	-
26	DD6	J	102	-	-	2/26/80/80	0/3/3/3
24	CLA	c	602	10	-	12/39/115/115	-
24	CLA	1	308	1	-	7/17/93/115	-
26	DD6	h	614	-	-	4/26/80/80	0/3/3/3
26	DD6	1	312	-	-	0/26/80/80	0/3/3/3
24	CLA	A	803	12	-	6/27/103/115	-
24	CLA	9	302	9	-	7/17/93/115	-
24	CLA	A	812	12	-	15/39/115/115	-
24	CLA	8	204	8	-	6/15/91/115	-
24	CLA	3	303	-	-	7/27/103/115	-
24	CLA	9	303	-	-	10/17/93/115	-
26	DD6	9	315	-	-	4/26/80/80	0/3/3/3
30	LMG	A	855	-	-	5/33/53/70	0/1/1/1
24	CLA	k	306	9	-	5/17/93/115	-
31	PQN	B	839	-	-	10/23/43/43	0/2/2/2
25	BCR	2	211	-	-	4/29/63/63	0/2/2/2
25	BCR	I	101	-	-	4/29/63/63	0/2/2/2
25	BCR	9	316	-	-	2/29/63/63	0/2/2/2
24	CLA	B	831	-	-	19/39/115/115	-
24	CLA	9	309	9	-	9/17/93/115	-
24	CLA	A	856	-	-	11/39/115/115	-
24	CLA	A	824	-	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	6	606	6	-	9/17/93/115	-
24	CLA	2	208	-	-	6/17/93/115	-
24	CLA	B	802	13	-	19/39/115/115	-
24	CLA	4	605	4	-	6/17/93/115	-
24	CLA	4	606	4	-	2/17/93/115	-
28	LHG	J	105	-	-	12/42/42/53	-
24	CLA	A	810	12	-	15/36/112/115	-
24	CLA	1	302	1	-	7/15/91/115	-
24	CLA	A	830	12	-	10/27/103/115	-
24	CLA	c	611	10	-	4/10/86/115	-
24	CLA	F	201	-	-	12/39/115/115	-
24	CLA	A	857	12	-	9/39/115/115	-
24	CLA	9	307	9	-	7/17/93/115	-
24	CLA	1	303	1	-	8/17/93/115	-
24	CLA	7	603	7	-	2/15/91/115	-
26	DD6	8	211	-	-	3/26/80/80	0/3/3/3
25	BCR	B	843	-	-	4/29/63/63	0/2/2/2
24	CLA	3	309	3	-	2/10/86/115	-
24	CLA	8	203	-	-	10/21/97/115	-
24	CLA	A	805	12	-	11/39/115/115	-
28	LHG	A	841	-	-	19/52/52/53	-
24	CLA	B	830	13	-	10/31/107/115	-
25	BCR	A	845	-	-	5/29/60/63	0/2/2/2
26	DD6	4	614	-	-	1/26/80/80	0/3/3/3
24	CLA	2	207	-	-	6/17/93/115	-
24	CLA	4	612	4	-	5/17/93/115	-
26	DD6	R	105	-	-	6/26/80/80	0/3/3/3
26	DD6	2	210	-	-	1/26/80/80	0/3/3/3
24	CLA	9	308	-	-	8/17/93/115	-
25	BCR	7	617	-	-	2/29/63/63	0/2/2/2
26	DD6	9	314	-	-	2/26/80/80	0/3/3/3
25	BCR	J	101	-	-	2/29/63/63	0/2/2/2
24	CLA	k	310	9	-	2/10/86/115	-
24	CLA	B	837	13	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	818	-	-	14/39/115/115	-
24	CLA	c	608	10	-	14/39/115/115	-
24	CLA	1	317	-	-	15/39/115/115	-
26	DD6	5	609	-	-	1/26/80/80	0/3/3/3
24	CLA	B	809	13	-	10/39/115/115	-
24	CLA	1	309	1	-	3/15/91/115	-
25	BCR	F	204	-	-	2/29/63/63	0/2/2/2
32	SF4	C	101	14	-	-	0/6/5/5
24	CLA	7	605	7	-	4/17/93/115	-
24	CLA	A	853	12	-	7/27/103/115	-
24	CLA	6	610	6	-	6/17/93/115	-
24	CLA	6	605	6	-	4/17/93/115	-
24	CLA	k	304	9	-	9/17/93/115	-
24	CLA	3	304	3	-	6/17/93/115	-
24	CLA	9	310	9	-	8/17/93/115	-
24	CLA	5	603	5	-	4/15/91/115	-
26	DD6	A	848	-	-	1/26/80/80	0/3/3/3
24	CLA	B	803	-	-	10/39/115/115	-
24	CLA	A	808	12	-	10/39/115/115	-
24	CLA	7	609	7	-	7/17/93/115	-
28	LHG	A	849	-	-	13/45/45/53	-
24	CLA	7	612	7	-	10/17/93/115	-
24	CLA	k	302	9	-	9/17/93/115	-
24	CLA	B	810	13	-	8/25/101/115	-
25	BCR	M	101	-	-	9/29/63/63	0/2/2/2
24	CLA	A	813	12	-	12/39/115/115	-
24	CLA	B	801	-	-	15/39/115/115	-
26	DD6	3	312	-	-	1/26/80/80	0/3/3/3
24	CLA	B	813	13	-	8/17/93/115	-
25	BCR	J	104	-	-	2/29/63/63	0/2/2/2
24	CLA	1	307	1	-	4/15/91/115	-
24	CLA	3	308	3	-	8/17/93/115	-
25	BCR	k	316	-	-	3/29/63/63	0/2/2/2
24	CLA	B	825	13	-	8/27/103/115	-
25	BCR	R	102	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	6	612	-	-	3/17/93/115	-
24	CLA	5	607	5	-	5/15/91/115	-
24	CLA	1	304	26	-	13/27/103/115	-
24	CLA	A	826	12	-	11/39/115/115	-
24	CLA	6	603	6	-	8/17/93/115	-
24	CLA	2	206	2	-	7/17/93/115	-
24	CLA	8	205	8	-	9/15/91/115	-
24	CLA	h	611	6	-	4/10/86/115	-
24	CLA	9	304	9	-	7/17/93/115	-
24	CLA	h	609	-	-	7/17/93/115	-
24	CLA	B	812	13	-	16/39/115/115	-
25	BCR	L	202	-	-	6/29/63/63	0/2/2/2
24	CLA	7	602	7	-	9/21/97/115	-
24	CLA	2	201	2	-	9/15/91/115	-
24	CLA	B	816	13	-	14/39/115/115	-
26	DD6	h	615	-	-	3/26/80/80	0/3/3/3
24	CLA	A	809	12	-	6/17/93/115	-
24	CLA	3	302	3	-	5/15/91/115	-
24	CLA	3	307	-	-	4/15/91/115	-
24	CLA	4	611	-	-	6/17/93/115	-
24	CLA	A	807	12	-	16/39/115/115	-
24	CLA	t	310	-	-	8/17/93/115	-
24	CLA	R	103	22	-	9/39/115/115	-
28	LHG	B	845	24	-	9/45/45/53	-
24	CLA	6	602	6	-	8/18/94/115	-
24	CLA	A	801	12	-	18/39/115/115	-
24	CLA	R	104	22	-	3/15/91/115	-
26	DD6	h	613	-	-	1/26/80/80	0/3/3/3

The worst 5 of 1906 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	618	DD6	C10-C11	4.87	1.42	1.35
26	7	618	DD6	C5-C6	4.86	1.42	1.35
28	A	842	LHG	O7-C7	4.82	1.47	1.34
26	7	618	DD6	C2-C1	4.75	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	9	314	DD6	C2-C1	4.65	1.41	1.35

The worst 5 of 2545 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	830	CLA	C4A-NA-C1A	9.33	110.90	106.71
26	9	314	DD6	C3-C2-C1	-8.92	114.58	127.31
26	8	210	DD6	C14-C13-C11	-8.74	111.97	125.53
25	c	615	BCR	C20-C21-C22	-8.66	114.95	127.31
26	k	315	DD6	C3-C2-C1	-8.60	115.04	127.31

There are no chirality outliers.

5 of 2475 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	1	301	CLA	C1A-C2A-CAA-CBA
24	1	301	CLA	C3A-C2A-CAA-CBA
24	1	301	CLA	CBD-CGD-O2D-CED
24	1	303	CLA	CHA-CBD-CGD-O1D
24	1	303	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

205 monomers are involved in 358 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	835	CLA	1	0
25	B	842	BCR	2	0
24	7	601	CLA	1	0
25	t	312	BCR	2	0
25	1	310	BCR	4	0
26	k	315	DD6	3	0
24	2	204	CLA	1	0
24	A	834	CLA	1	0
24	A	817	CLA	2	0
24	A	816	CLA	1	0
25	1	314	BCR	3	0
24	B	848	CLA	1	0
24	6	607	CLA	2	0
29	9	312	A1L1G	1	0
24	A	829	CLA	2	0
24	7	611	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	6	615	DD6	1	0
24	B	829	CLA	4	0
26	7	618	DD6	1	0
24	6	601	CLA	3	0
24	A	823	CLA	1	0
26	7	615	DD6	1	0
25	I	102	BCR	2	0
24	c	610	CLA	1	0
27	A	854	LMT	3	0
24	1	305	CLA	4	0
24	4	613	CLA	2	0
27	3	314	LMT	1	0
26	k	313	DD6	1	0
24	B	815	CLA	1	0
24	F	202	CLA	1	0
28	3	315	LHG	1	0
24	8	206	CLA	2	0
26	8	212	DD6	1	0
26	c	612	DD6	2	0
26	1	311	DD6	5	0
24	A	838	CLA	1	0
24	B	824	CLA	2	0
25	A	859	BCR	1	0
24	9	301	CLA	8	0
24	L	204	CLA	1	0
28	I	103	LHG	1	0
24	B	805	CLA	3	0
26	9	313	DD6	2	0
24	B	821	CLA	1	0
26	6	613	DD6	1	0
24	4	609	CLA	2	0
24	6	608	CLA	1	0
27	1	316	LMT	2	0
24	k	308	CLA	2	0
24	h	610	CLA	1	0
24	B	835	CLA	1	0
24	4	607	CLA	4	0
24	A	818	CLA	3	0
31	A	839	PQN	1	0
28	L	201	LHG	4	0
24	B	833	CLA	2	0
24	A	832	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	807	CLA	1	0
24	t	305	CLA	3	0
24	B	832	CLA	3	0
29	k	312	A1L1G	2	0
24	c	601	CLA	2	0
28	A	842	LHG	2	0
24	B	823	CLA	1	0
24	9	305	CLA	3	0
24	c	603	CLA	1	0
24	c	607	CLA	1	0
24	5	605	CLA	2	0
24	k	307	CLA	1	0
24	h	612	CLA	2	0
26	1	313	DD6	1	0
24	B	808	CLA	2	0
24	h	608	CLA	2	0
28	8	213	LHG	1	0
24	B	834	CLA	2	0
24	B	817	CLA	2	0
24	A	804	CLA	1	0
24	7	606	CLA	4	0
26	9	317	DD6	1	0
24	9	311	CLA	1	0
25	4	618	BCR	7	0
24	k	305	CLA	1	0
24	B	822	CLA	1	0
24	3	305	CLA	1	0
24	L	205	CLA	5	0
28	4	619	LHG	1	0
24	6	611	CLA	1	0
24	8	209	CLA	1	0
24	A	802	CLA	2	0
24	B	846	CLA	1	0
24	B	811	CLA	1	0
24	t	306	CLA	1	0
29	3	310	A1L1G	2	0
24	B	827	CLA	1	0
25	c	615	BCR	7	0
26	7	613	DD6	1	0
26	4	615	DD6	1	0
24	B	806	CLA	1	0
24	A	814	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	846	BCR	2	0
24	t	308	CLA	1	0
30	2	214	LMG	1	0
27	h	617	LMT	1	0
24	2	202	CLA	1	0
24	7	610	CLA	2	0
24	2	209	CLA	4	0
28	1	318	LHG	2	0
26	5	608	DD6	2	0
25	A	843	BCR	2	0
24	A	840	CLA	1	0
27	A	851	LMT	1	0
24	B	838	CLA	2	0
25	B	840	BCR	1	0
25	A	844	BCR	3	0
24	k	301	CLA	4	0
24	A	819	CLA	1	0
24	8	201	CLA	2	0
24	B	804	CLA	6	0
25	B	849	BCR	1	0
24	t	302	CLA	1	0
24	B	828	CLA	1	0
24	4	602	CLA	3	0
24	t	307	CLA	2	0
25	B	841	BCR	2	0
24	5	604	CLA	2	0
24	1	301	CLA	2	0
24	k	309	CLA	1	0
26	c	613	DD6	1	0
24	4	608	CLA	4	0
24	B	847	CLA	1	0
24	1	306	CLA	1	0
24	A	847	CLA	1	0
26	2	212	DD6	1	0
24	7	607	CLA	4	0
24	2	205	CLA	1	0
24	J	103	CLA	1	0
24	5	606	CLA	1	0
24	c	602	CLA	2	0
26	h	614	DD6	1	0
26	1	312	DD6	1	0
24	9	302	CLA	2	0

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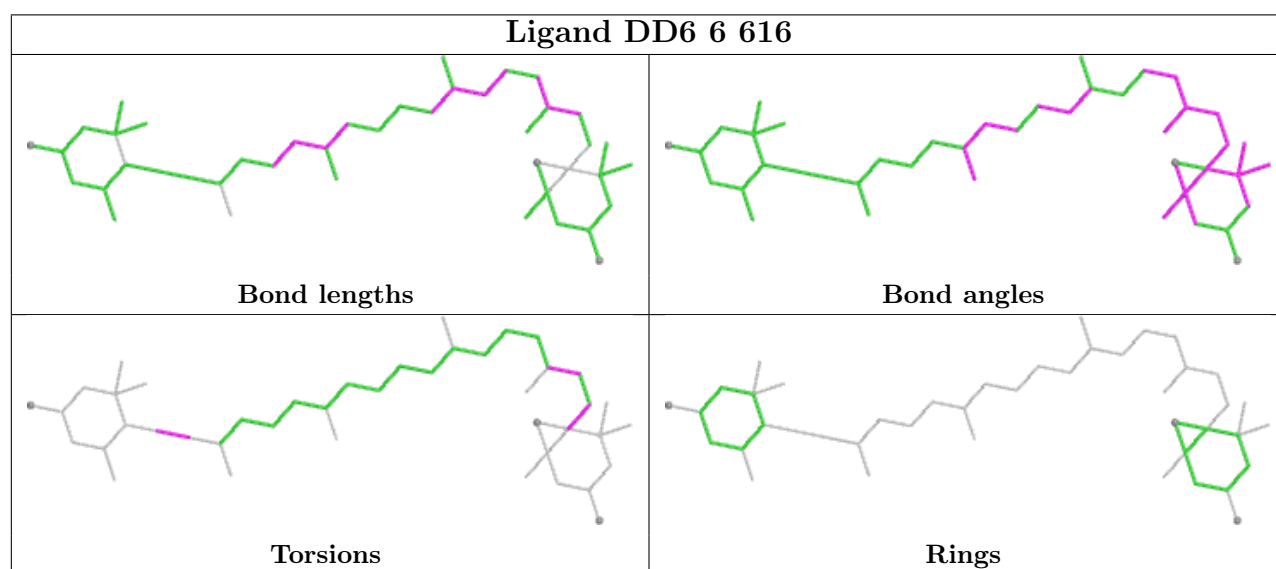
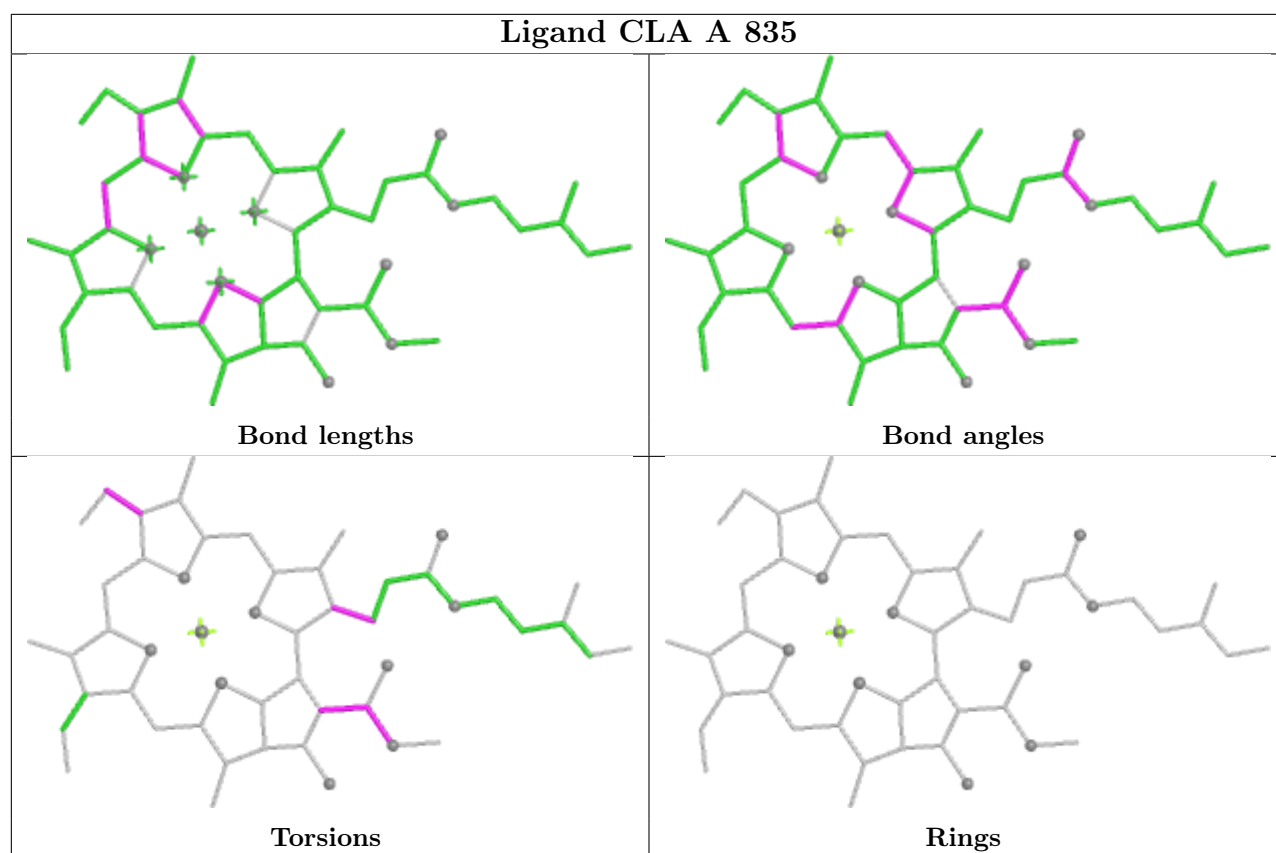
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24	A	812	CLA	1	0
24	8	204	CLA	2	0
24	9	303	CLA	1	0
26	9	315	DD6	3	0
25	2	211	BCR	4	0
25	I	101	BCR	1	0
25	9	316	BCR	9	0
24	B	831	CLA	3	0
24	A	824	CLA	1	0
24	6	606	CLA	1	0
24	B	802	CLA	2	0
24	4	605	CLA	1	0
24	4	606	CLA	1	0
28	J	105	LHG	1	0
24	A	810	CLA	1	0
24	1	302	CLA	1	0
24	A	830	CLA	6	0
24	1	303	CLA	1	0
26	8	211	DD6	1	0
25	B	843	BCR	5	0
24	8	203	CLA	2	0
24	A	805	CLA	1	0
24	B	830	CLA	7	0
25	A	845	BCR	1	0
26	4	614	DD6	1	0
24	2	207	CLA	1	0
24	4	612	CLA	2	0
26	2	210	DD6	1	0
24	9	308	CLA	2	0
25	7	617	BCR	2	0
25	J	101	BCR	4	0
24	1	317	CLA	2	0
26	5	609	DD6	1	0
25	F	204	BCR	2	0
24	A	853	CLA	2	0
24	k	304	CLA	2	0
24	3	304	CLA	5	0
24	9	310	CLA	2	0
24	B	803	CLA	4	0
24	7	612	CLA	2	0
24	B	810	CLA	1	0
25	M	101	BCR	2	0

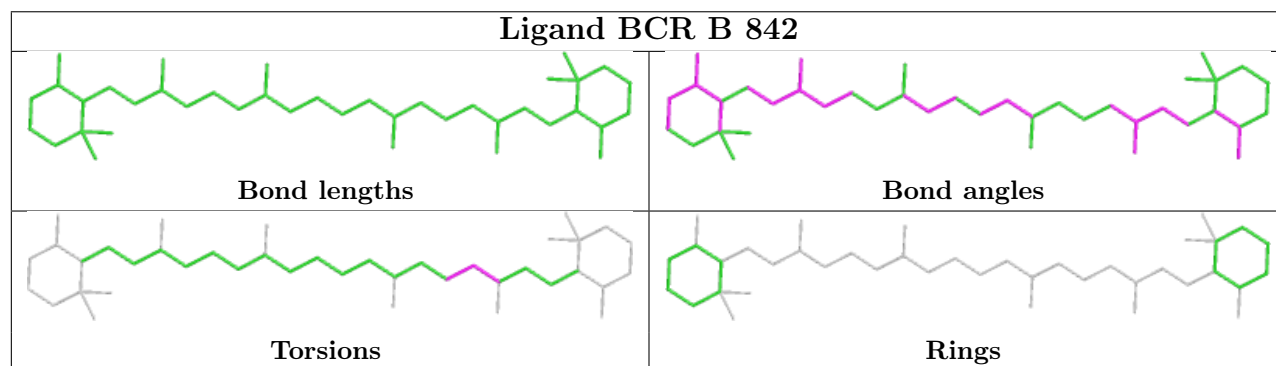
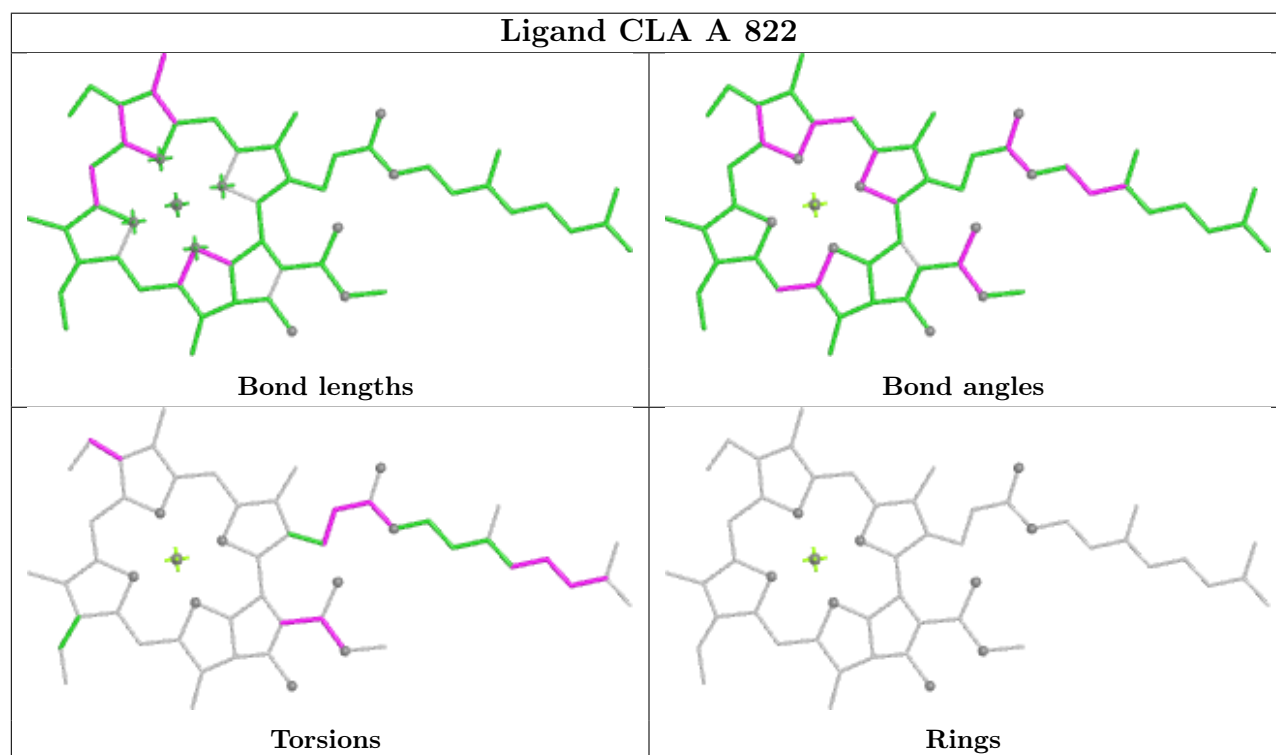
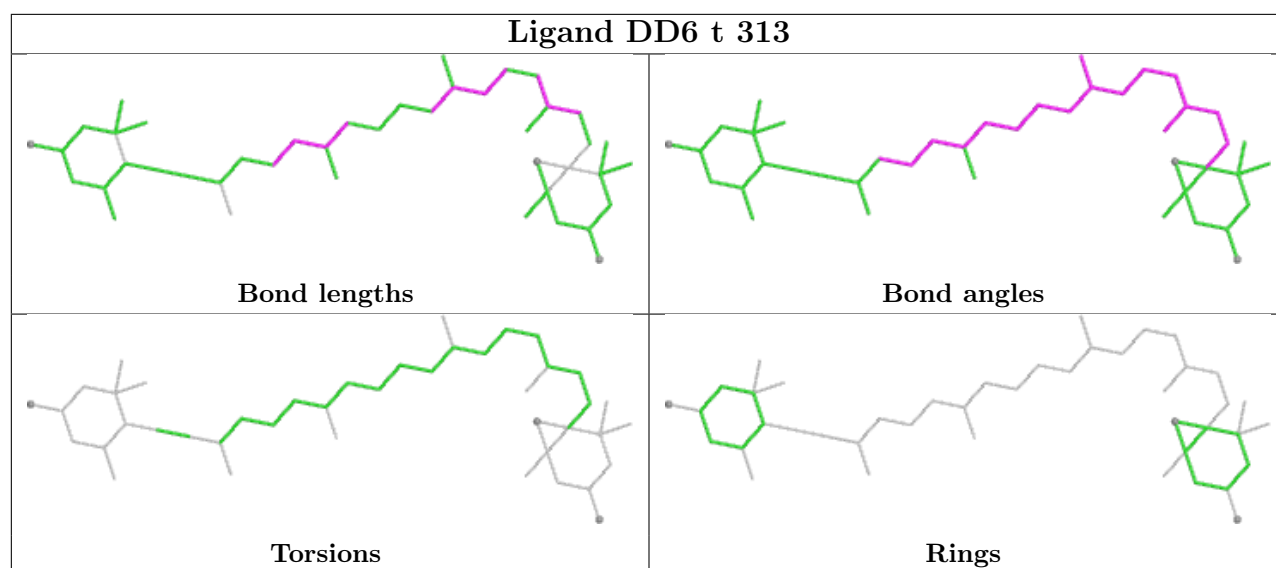
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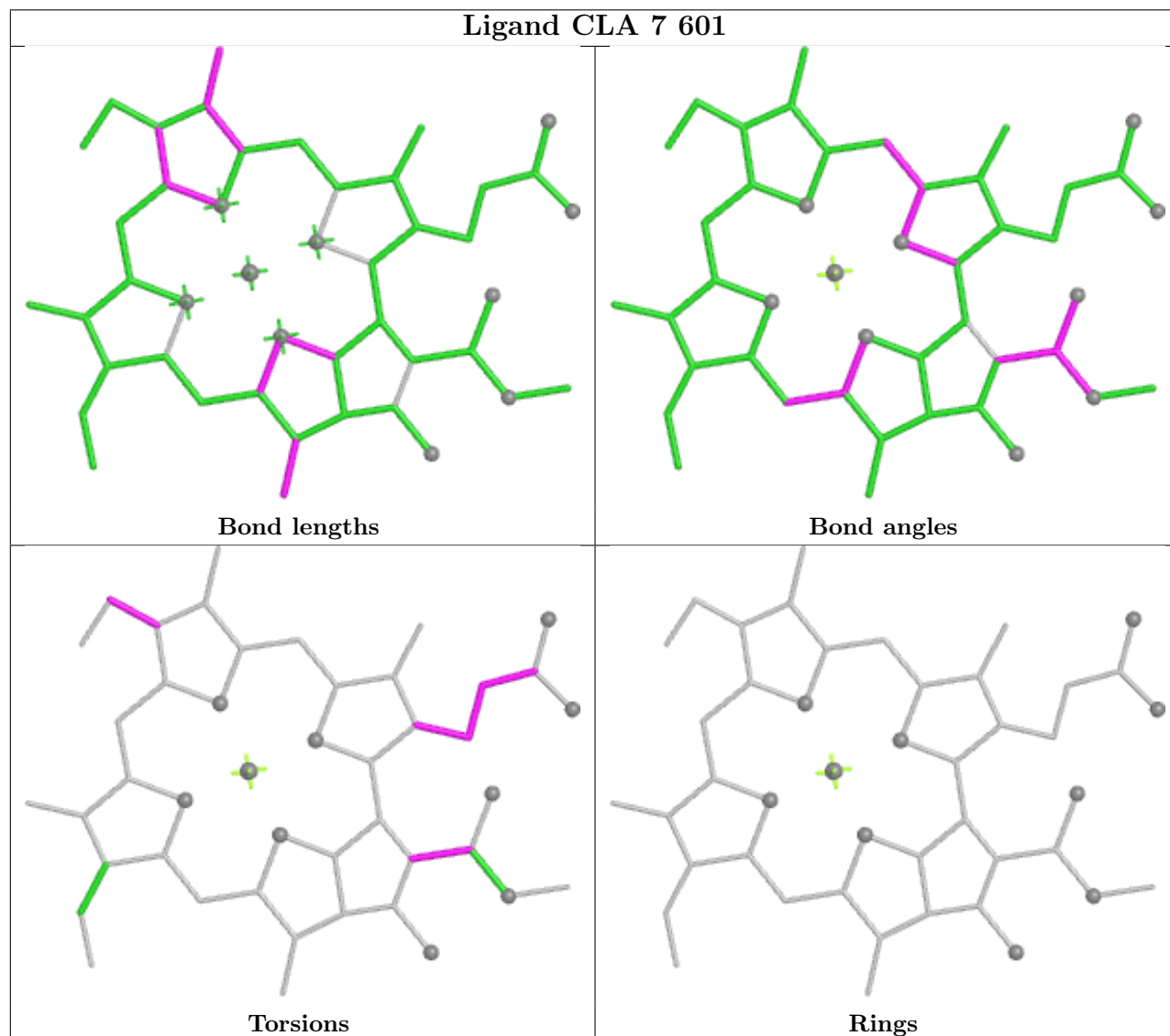
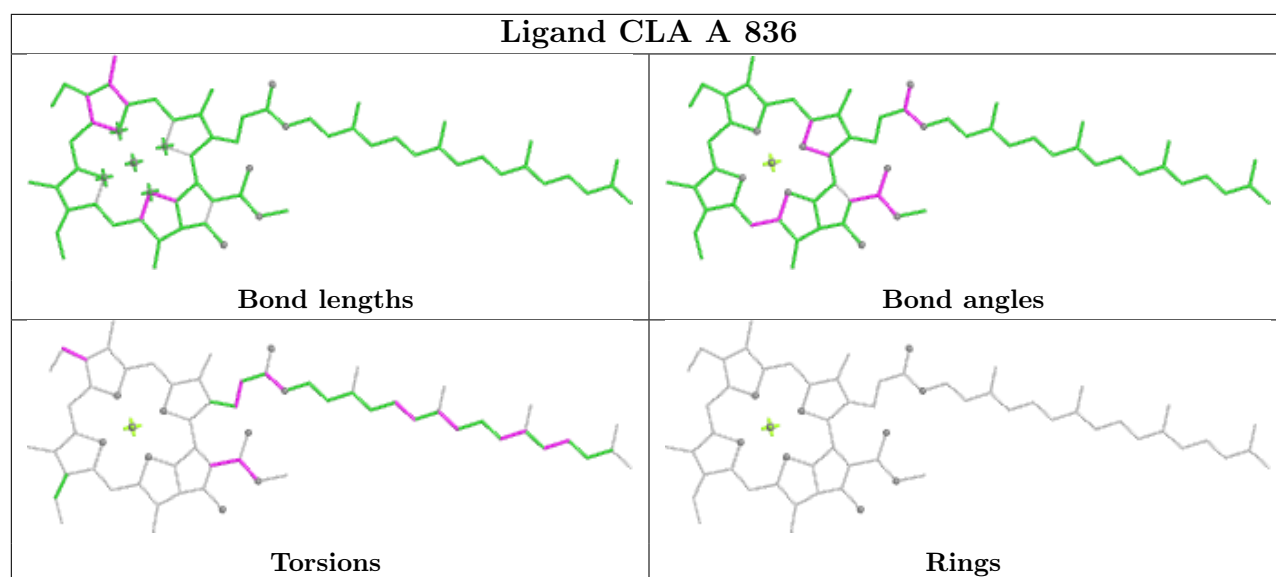
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	801	CLA	1	0
26	3	312	DD6	1	0
25	J	104	BCR	1	0
24	1	307	CLA	2	0
24	3	308	CLA	2	0
25	k	316	BCR	2	0
24	B	825	CLA	1	0
25	R	102	BCR	2	0
24	5	607	CLA	2	0
24	1	304	CLA	3	0
24	A	826	CLA	2	0
24	6	603	CLA	3	0
24	2	206	CLA	2	0
24	B	812	CLA	3	0
25	L	202	BCR	2	0
24	7	602	CLA	9	0
24	2	201	CLA	3	0
24	4	611	CLA	10	0
24	R	103	CLA	1	0
24	6	602	CLA	2	0
24	A	801	CLA	1	0

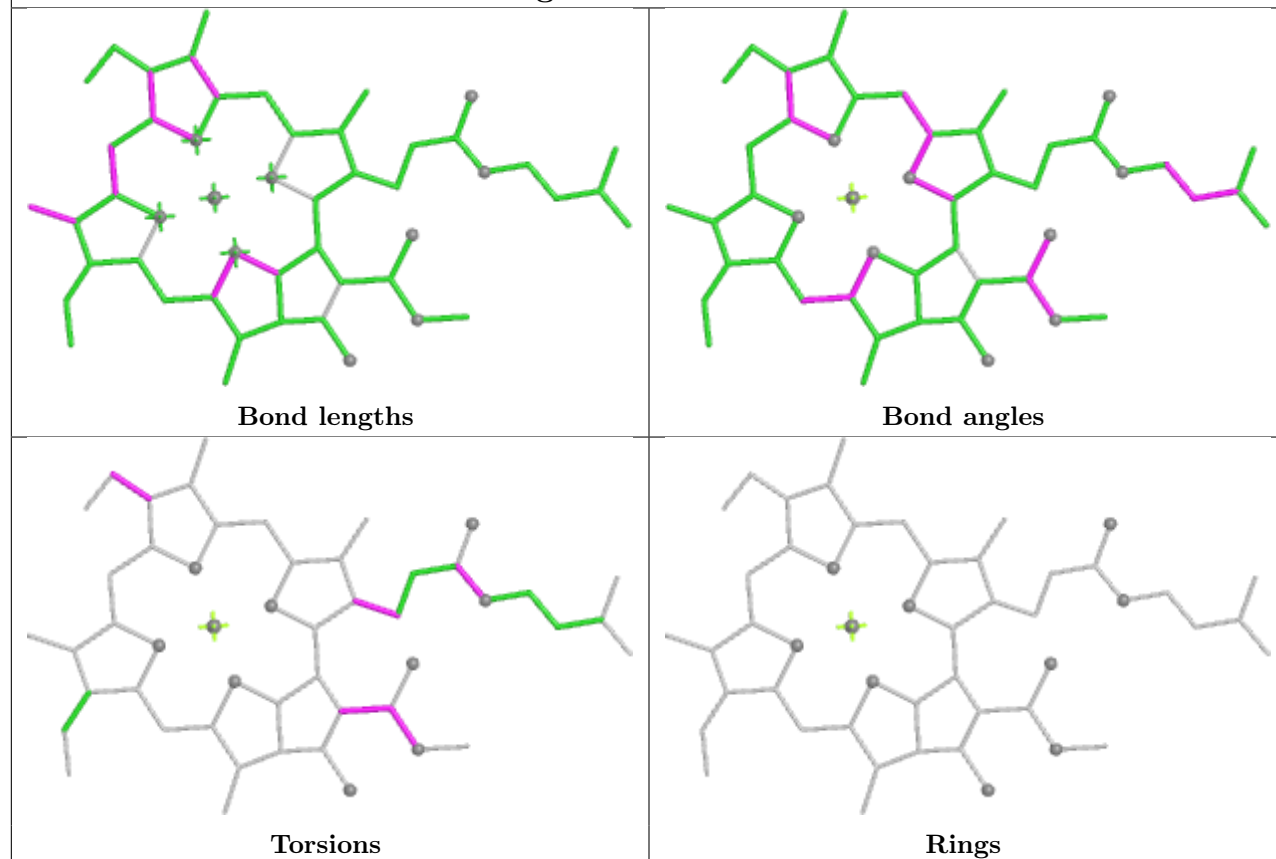
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



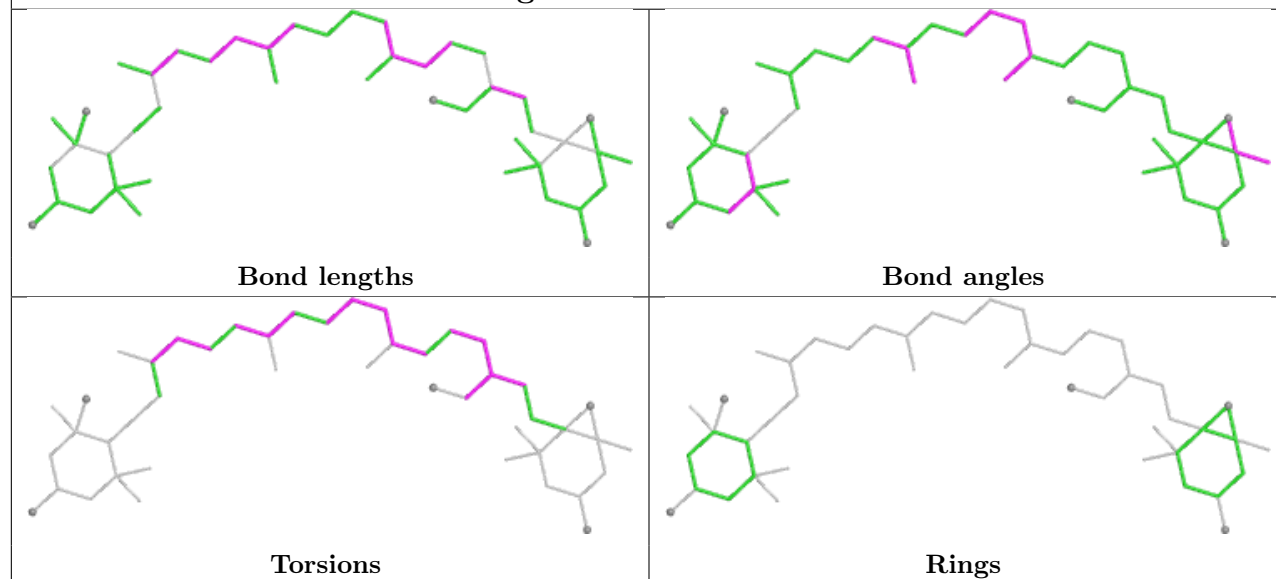


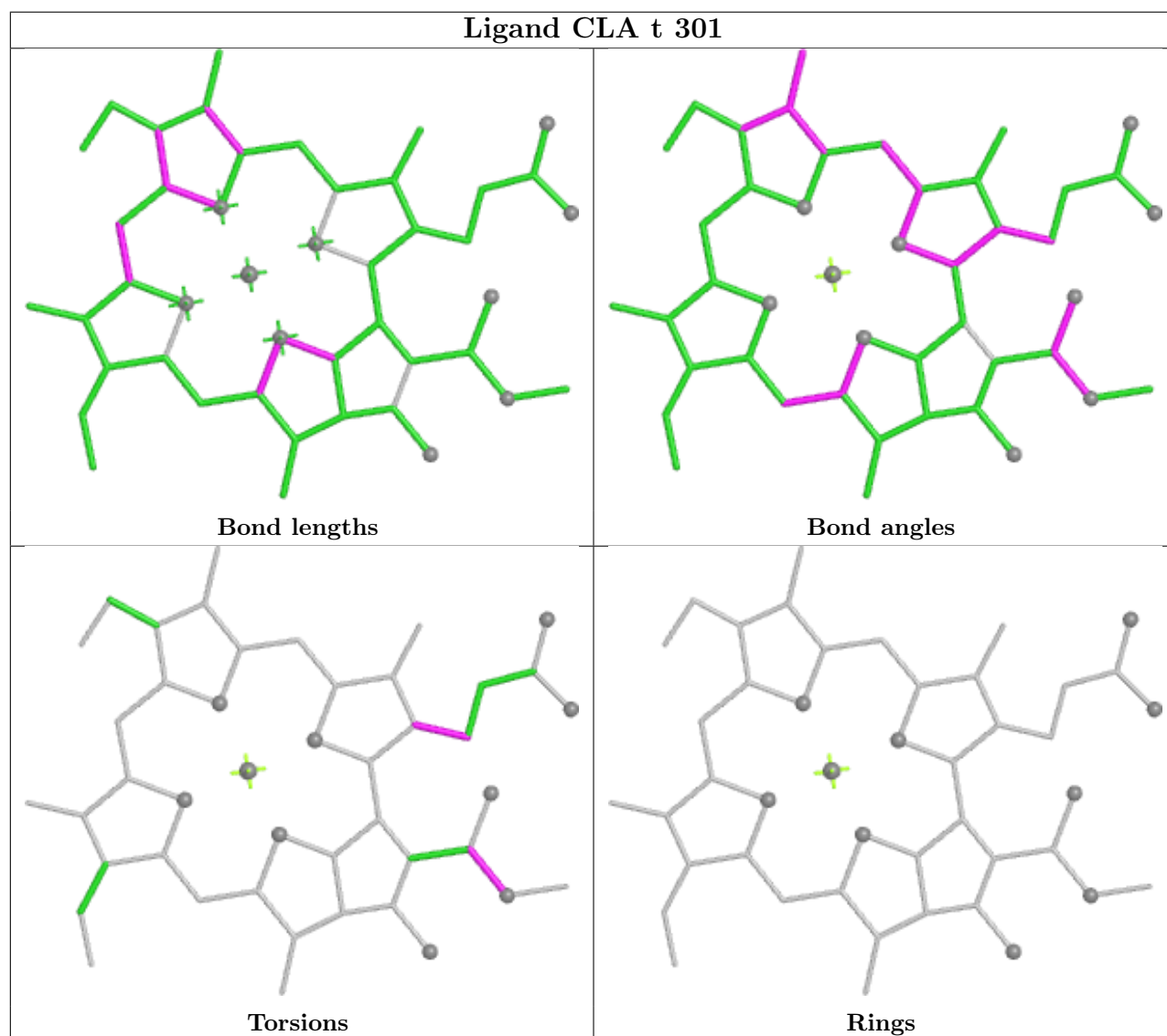
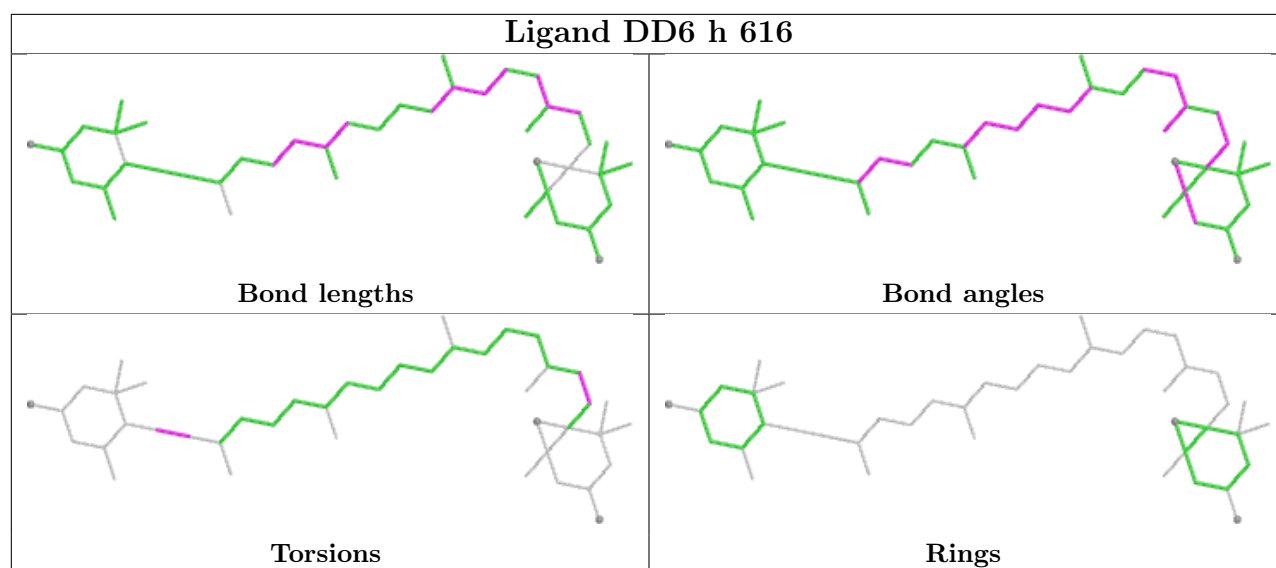


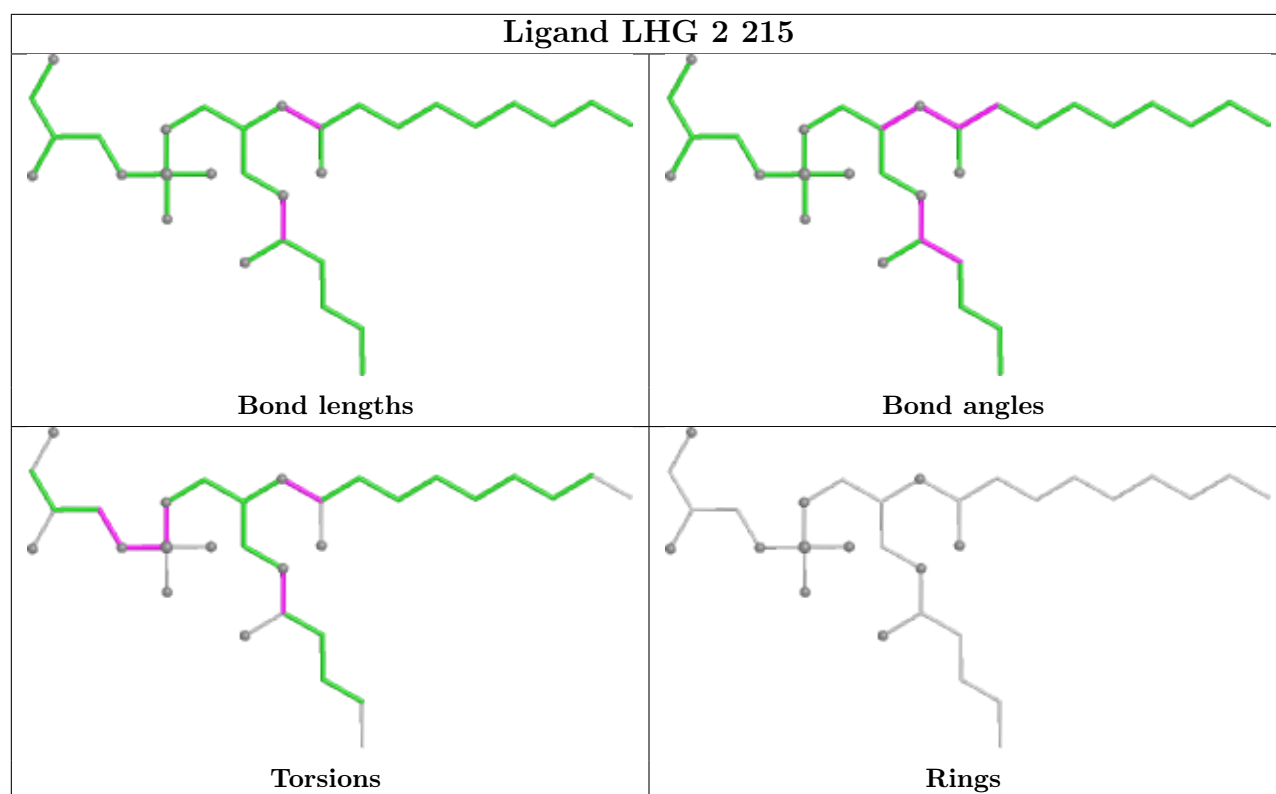
Ligand CLA 6 609

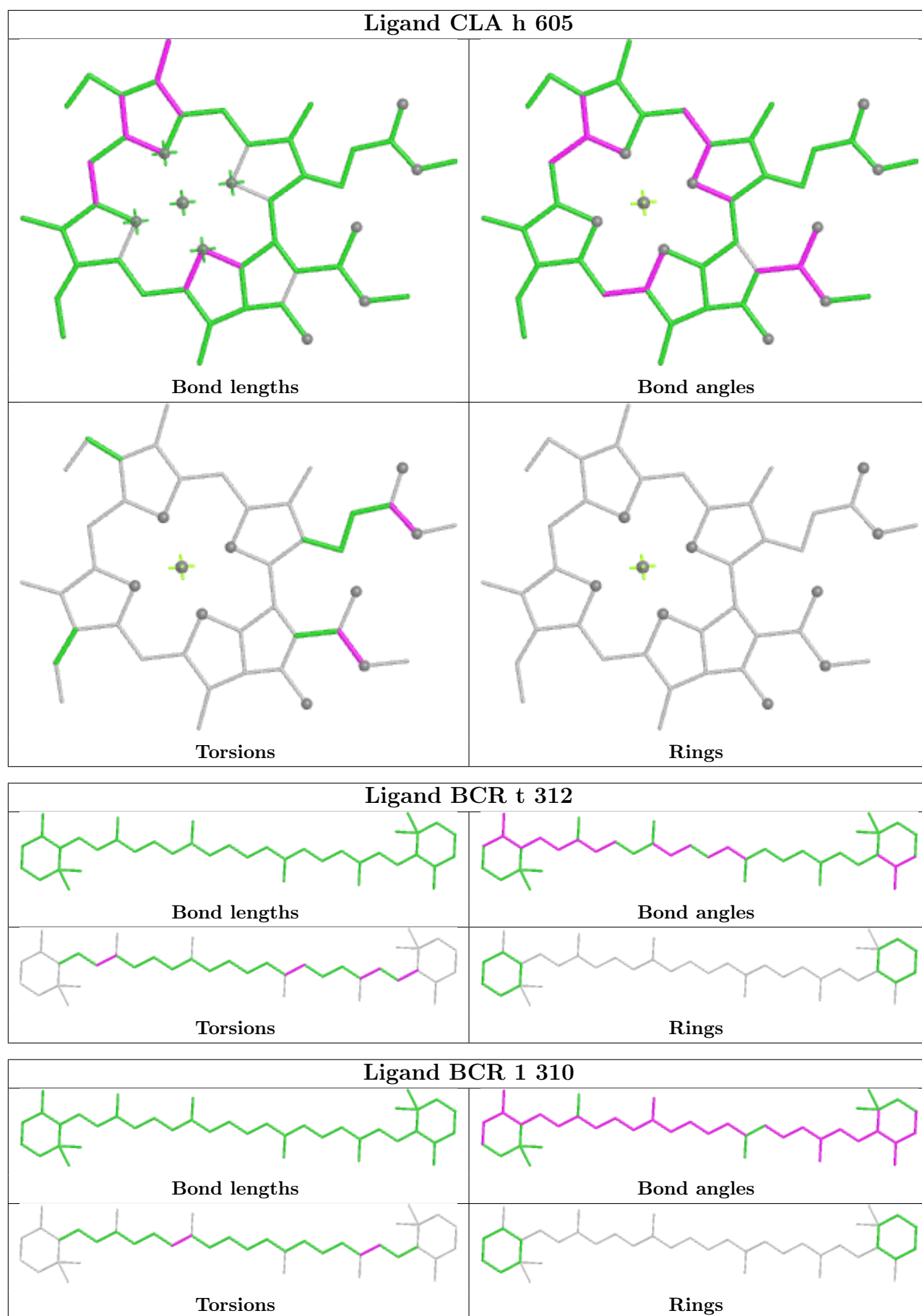


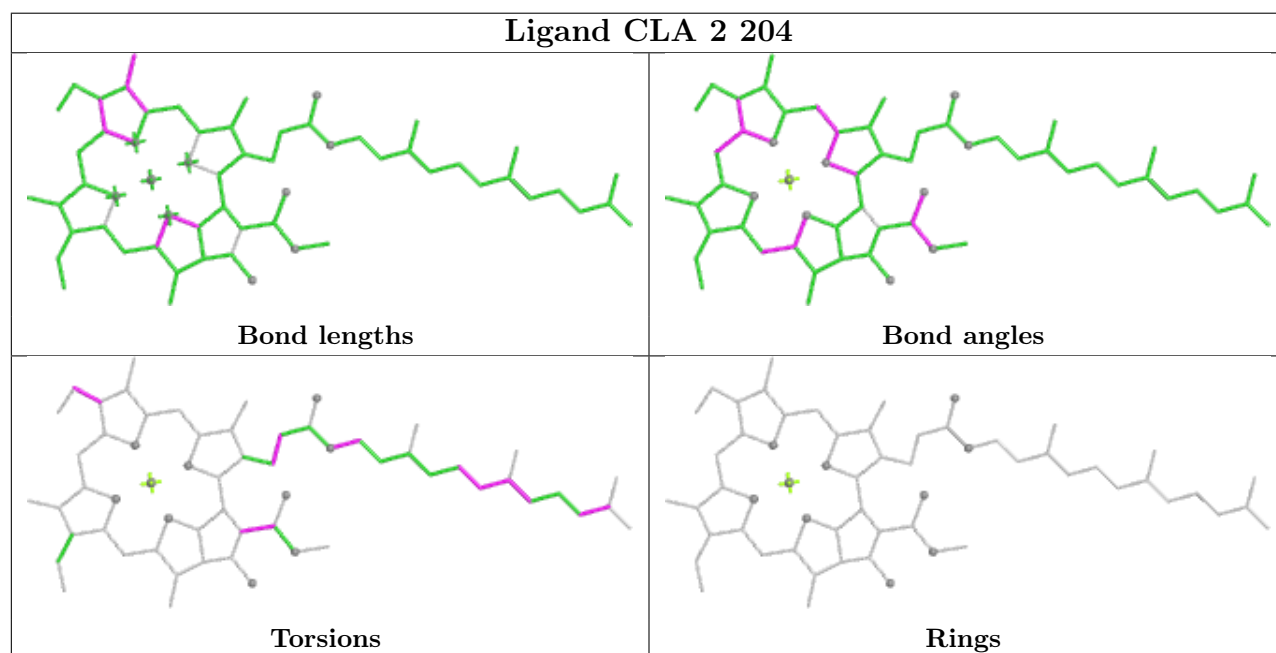
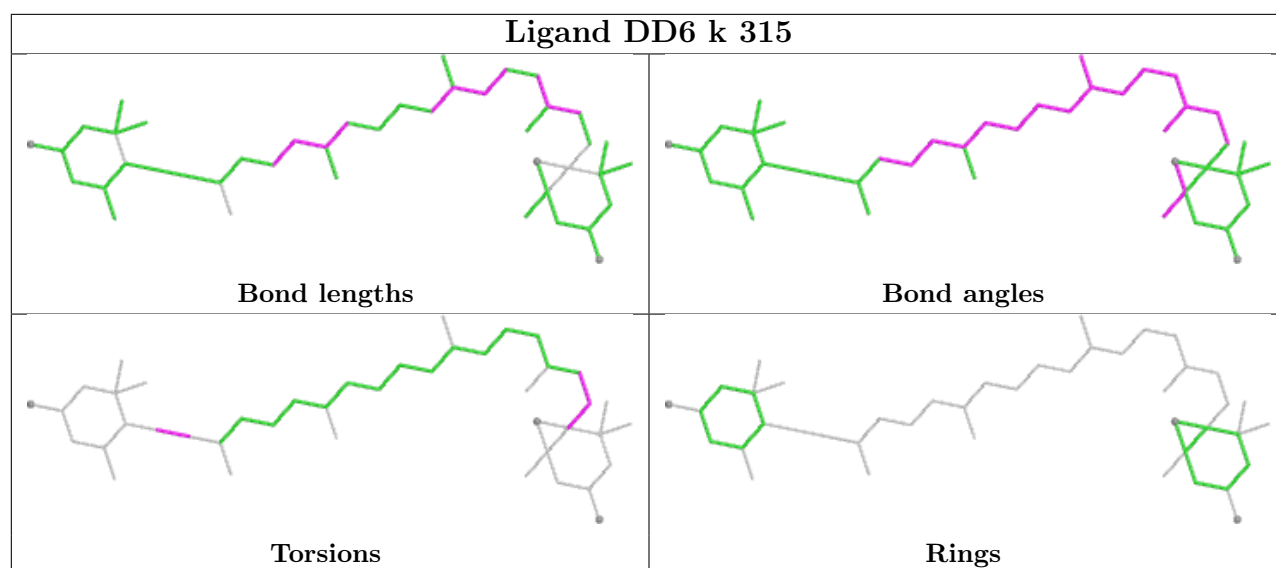
Ligand A1L1G 2 213

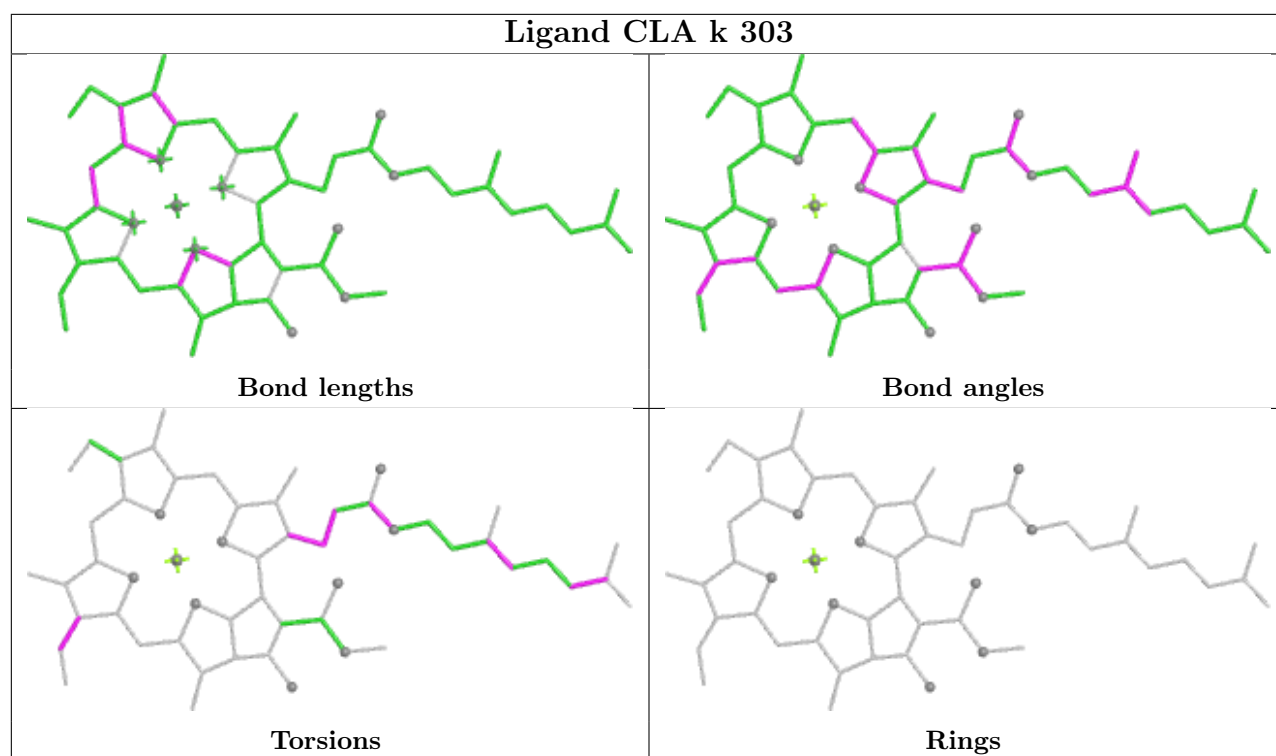


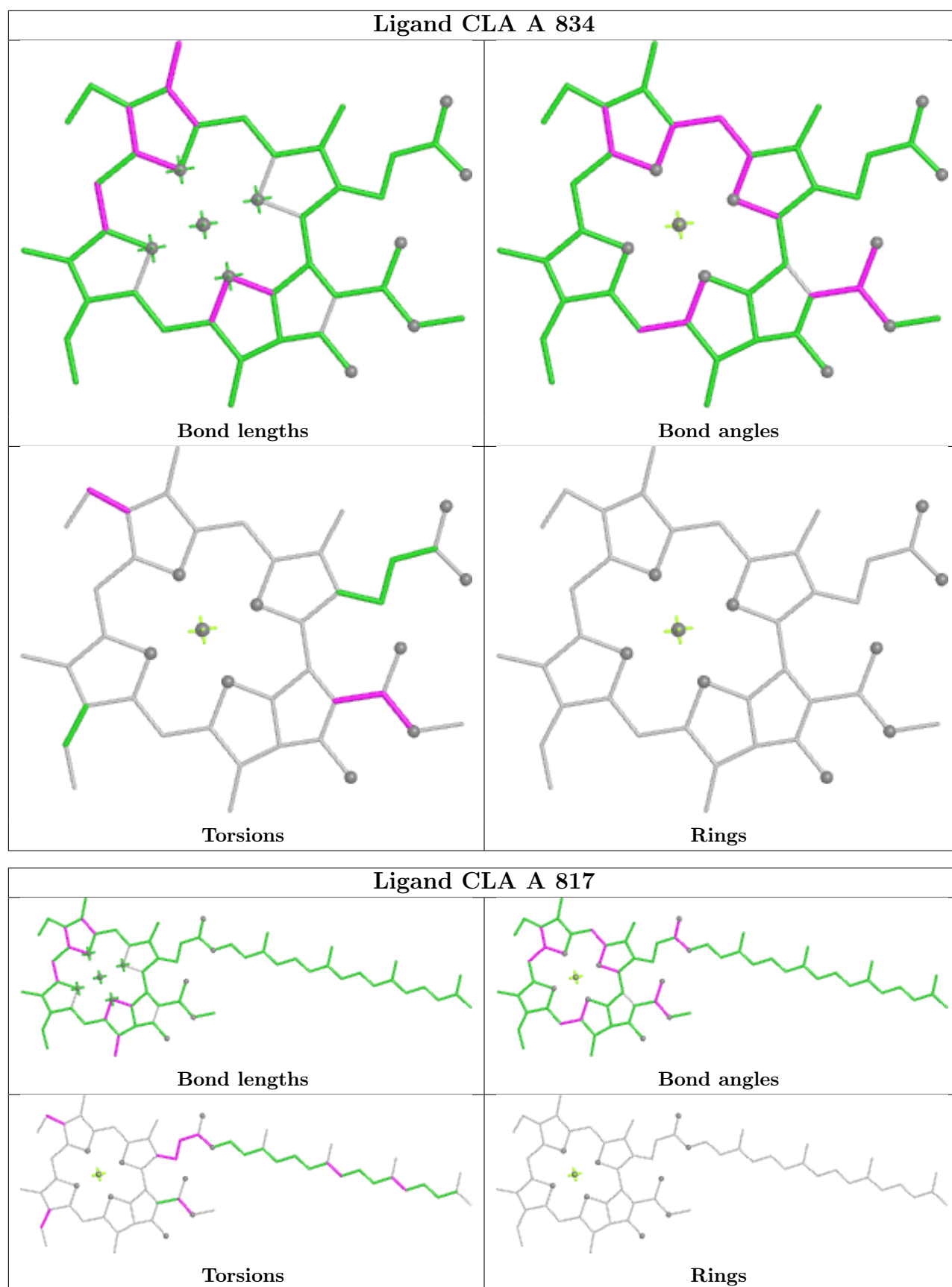


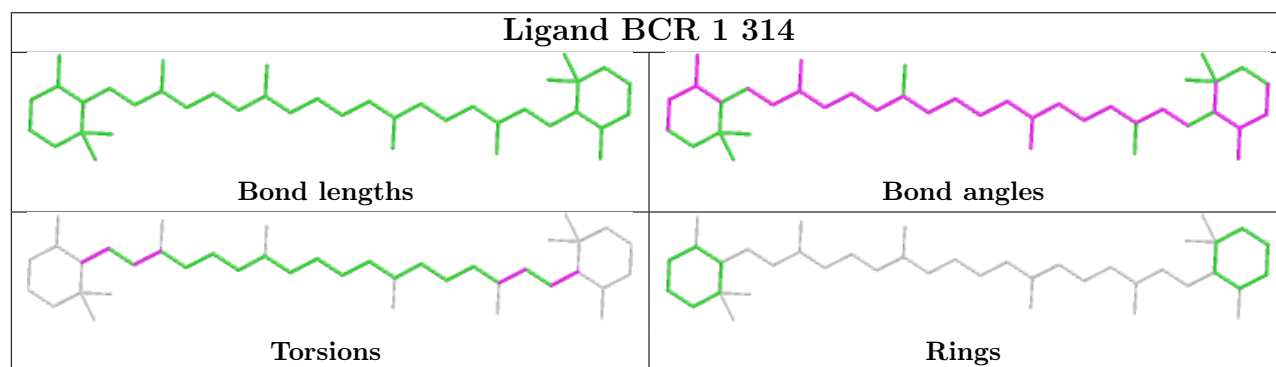
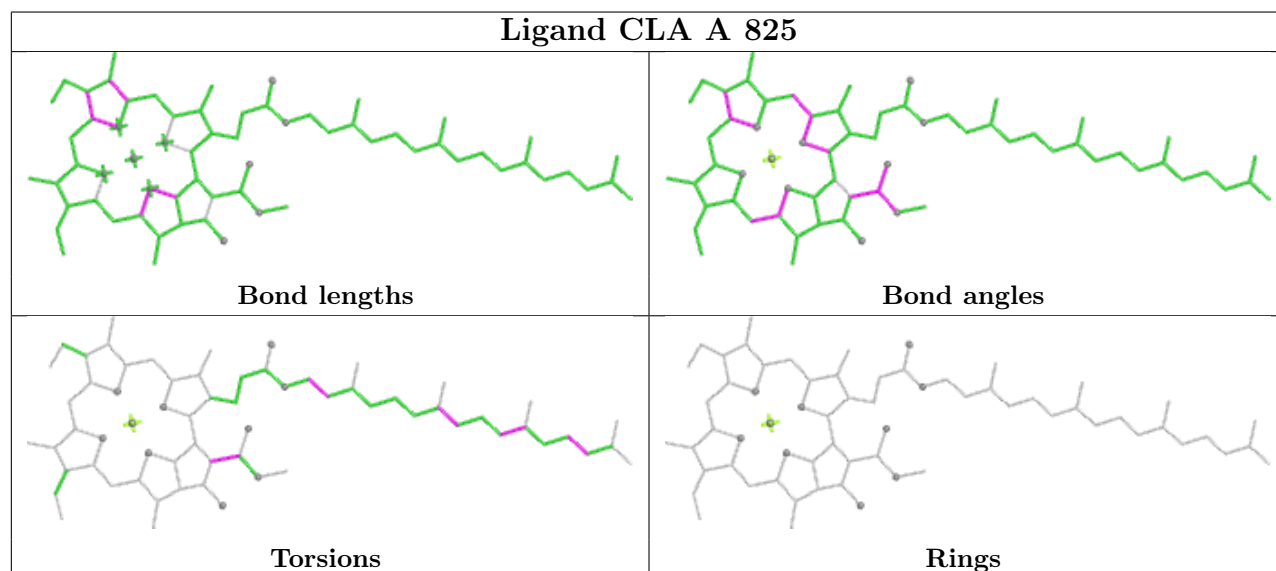
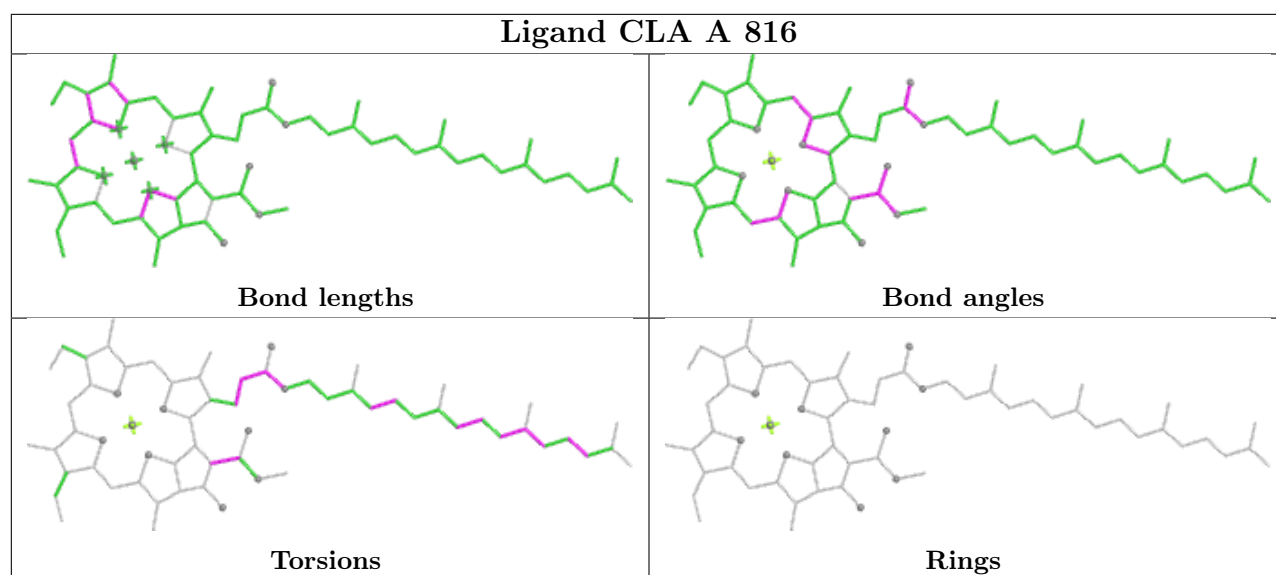


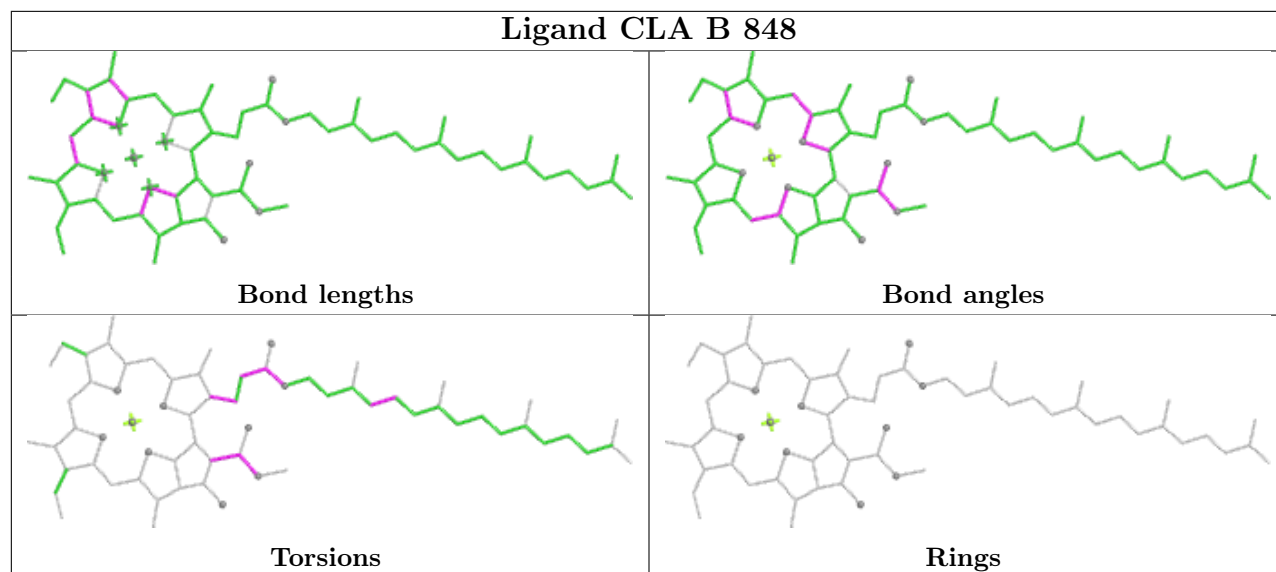
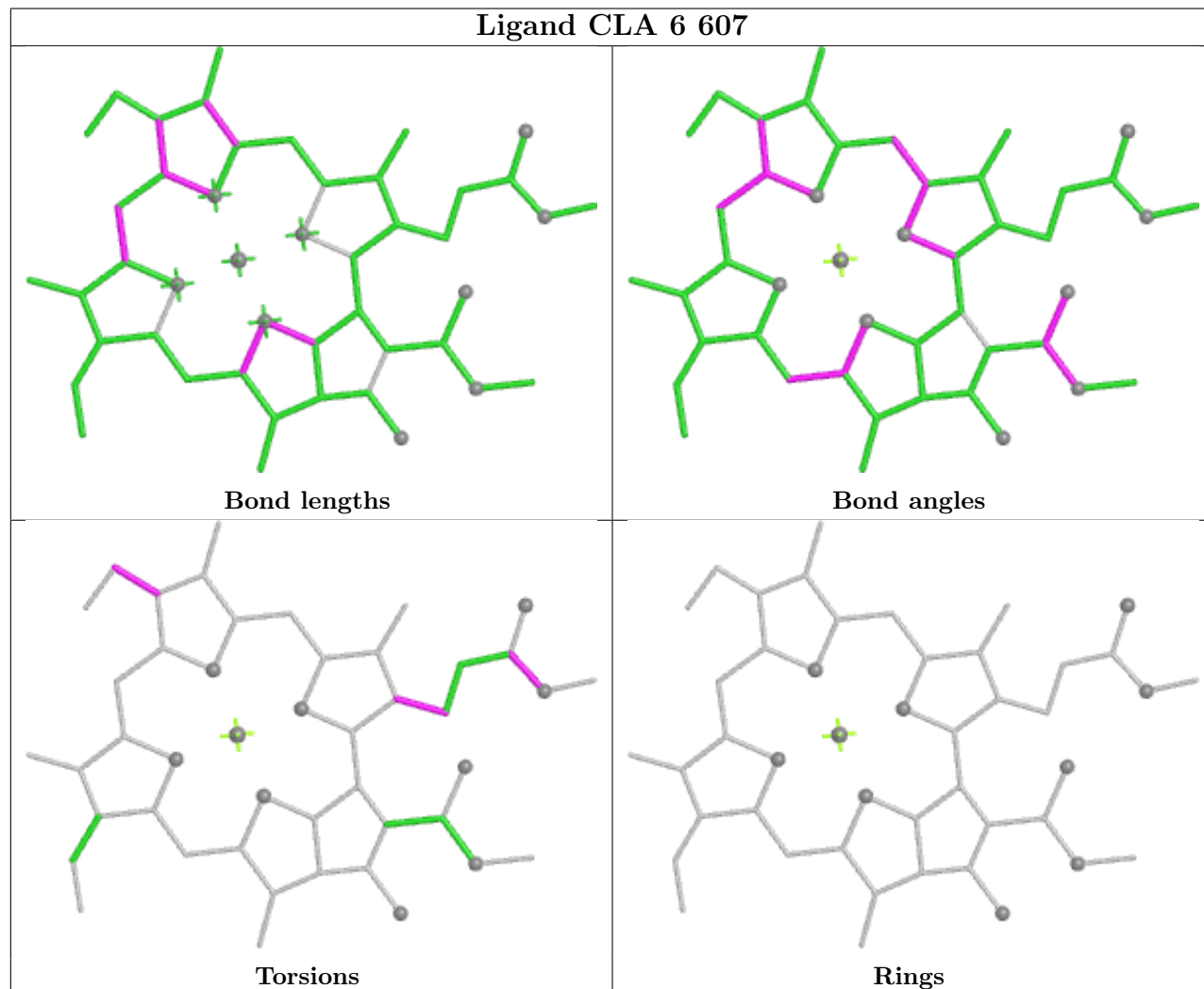


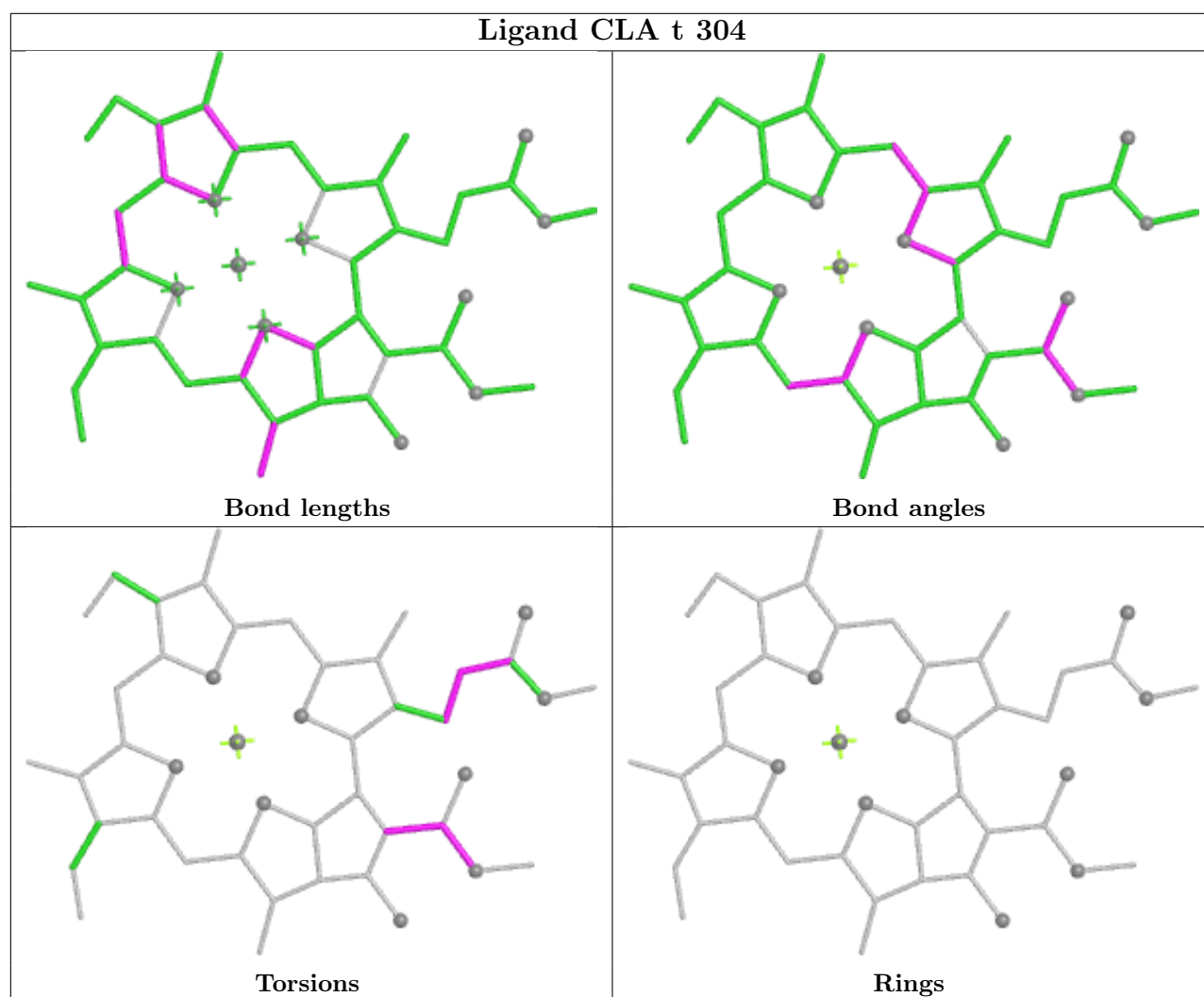
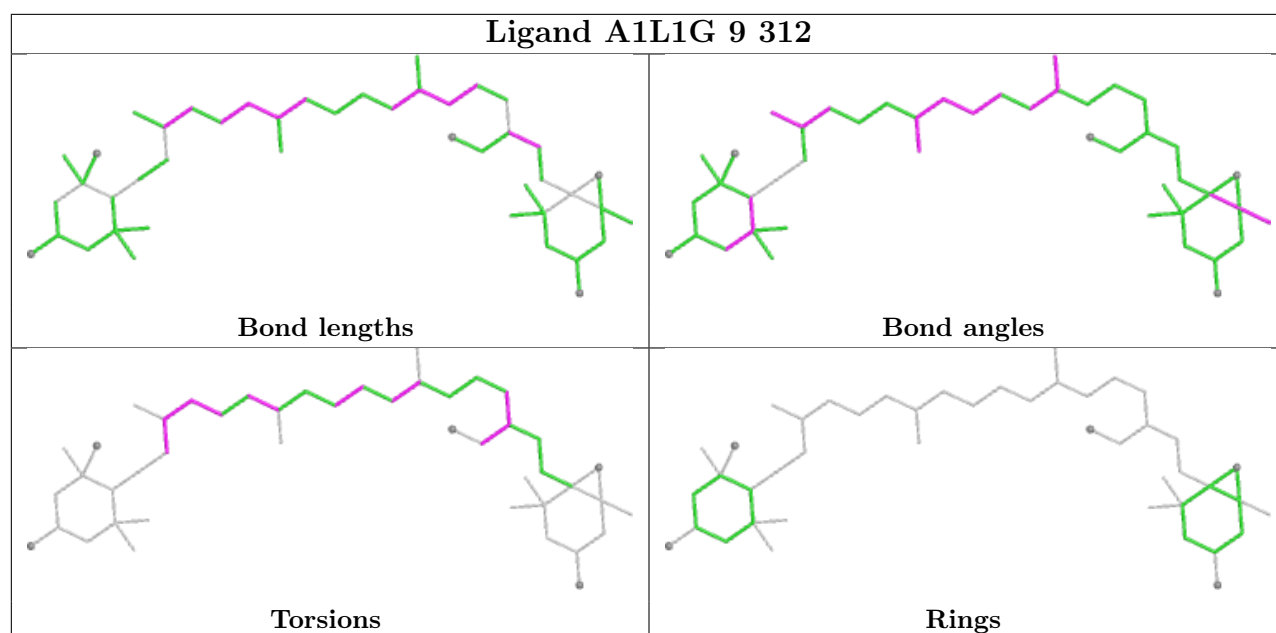


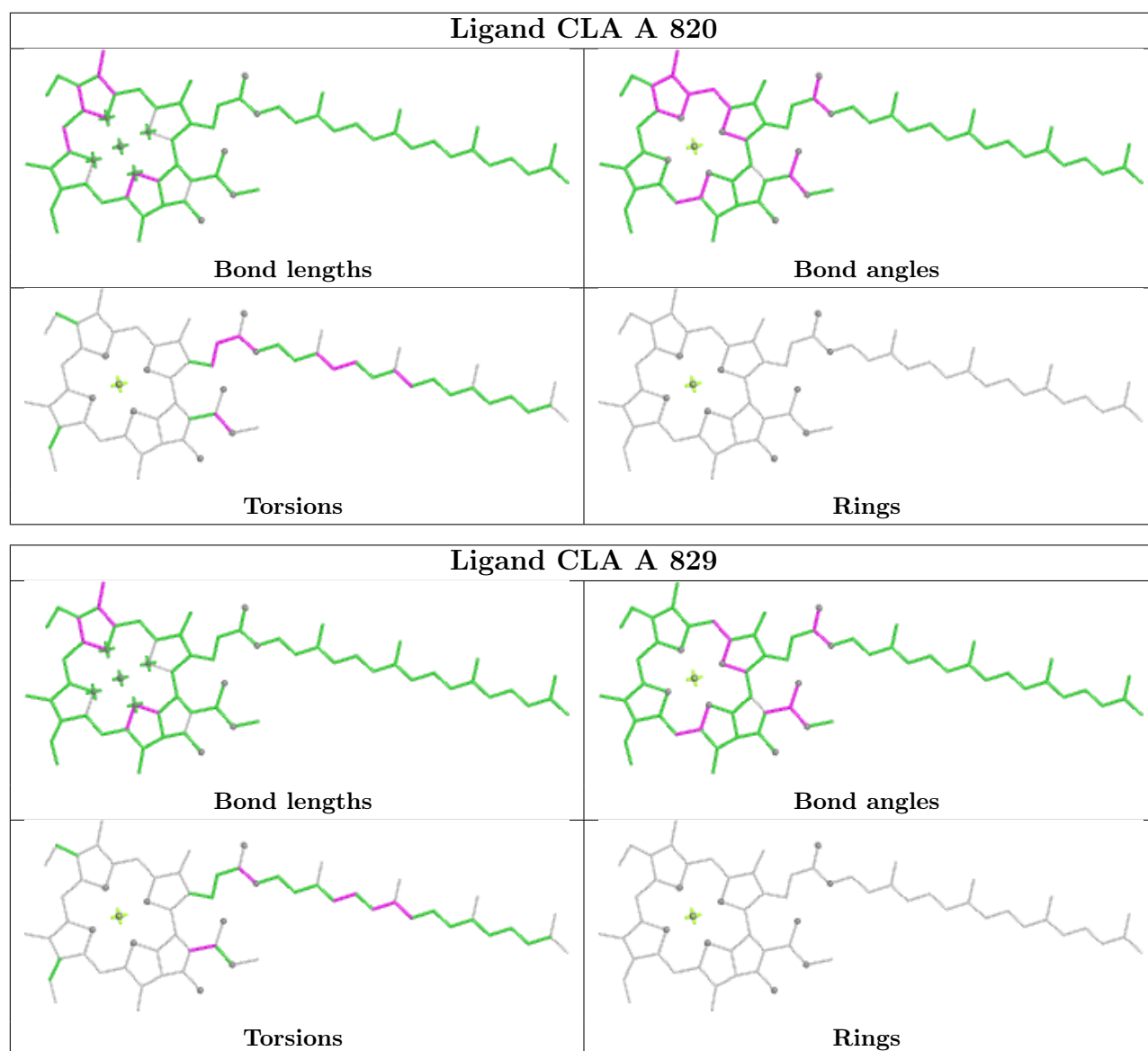




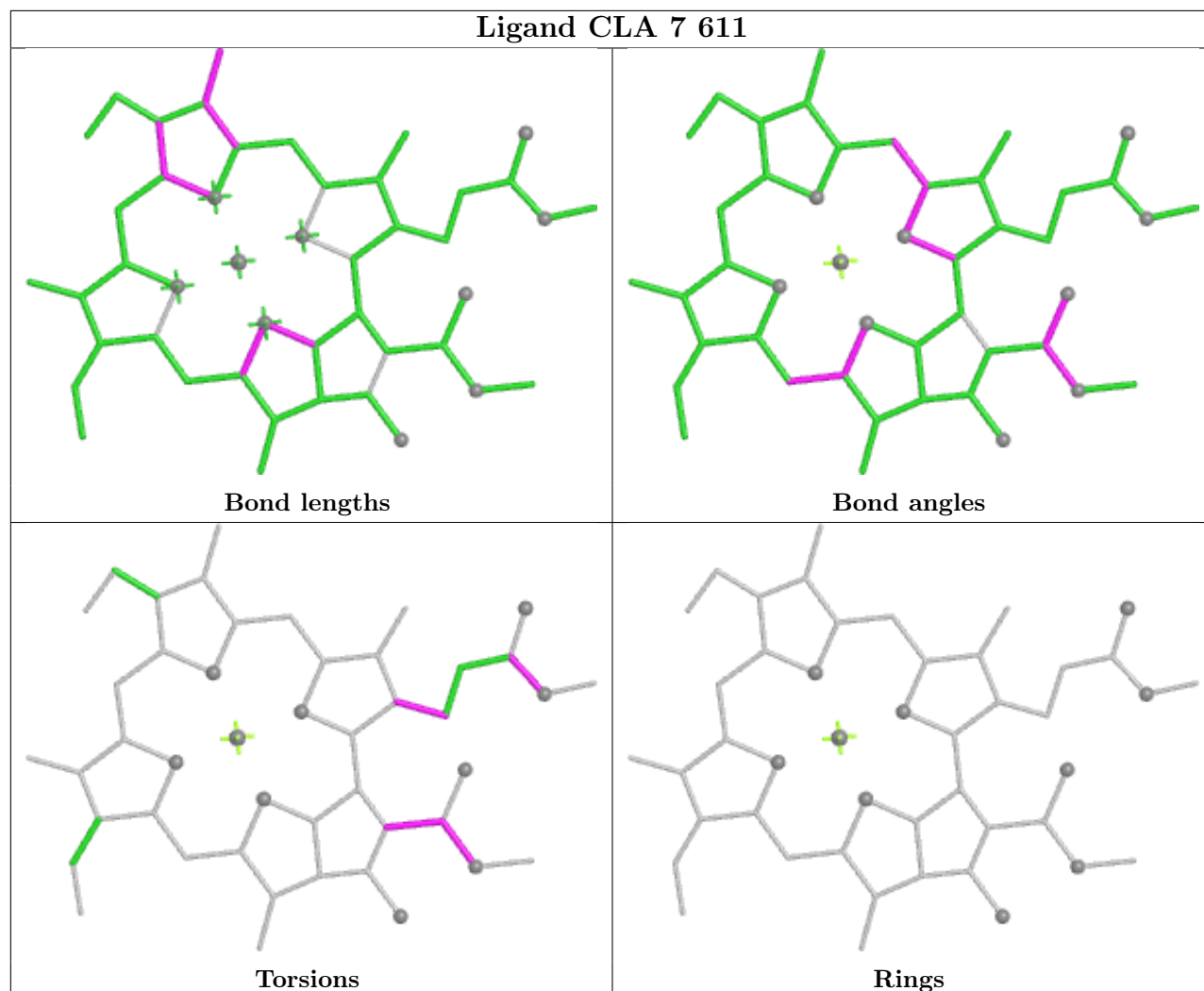


Ligand CLA B 848**Ligand CLA 6 607**

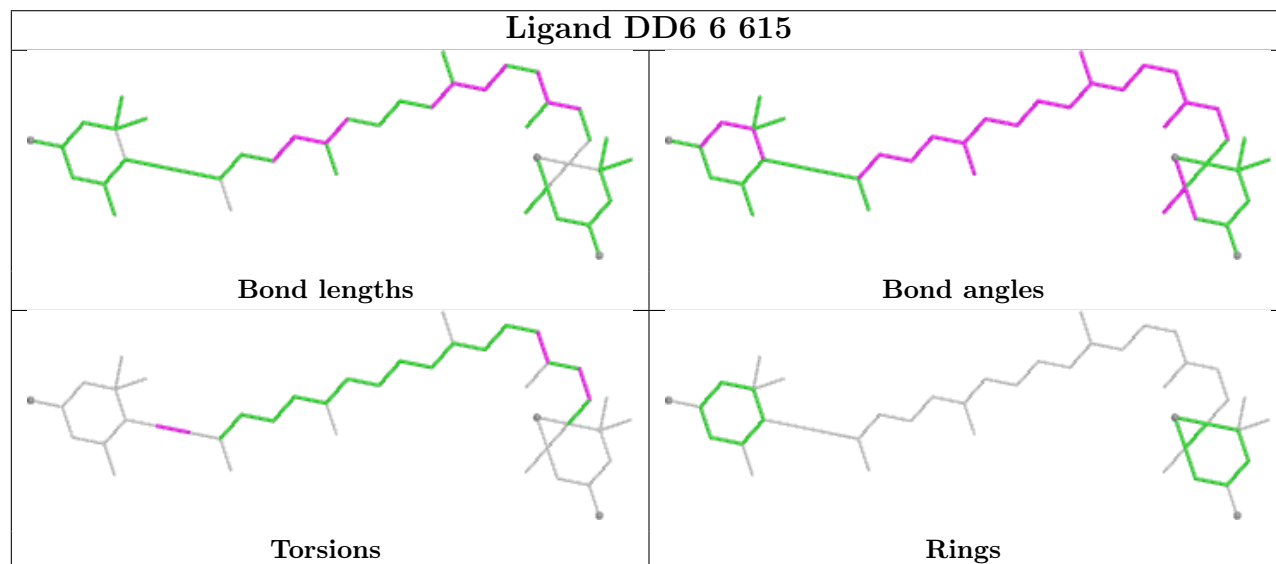


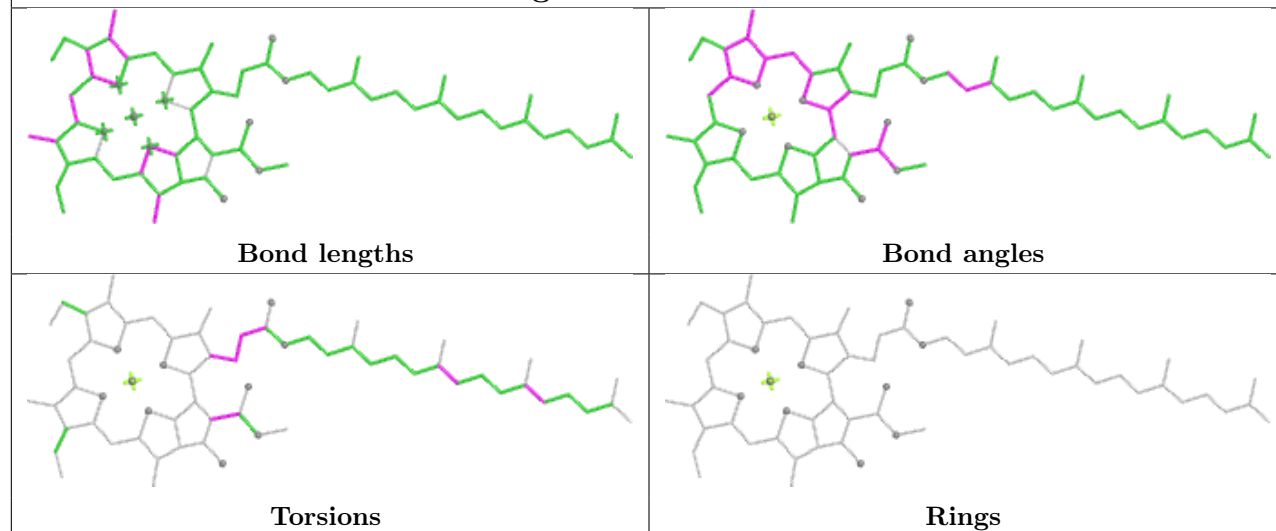
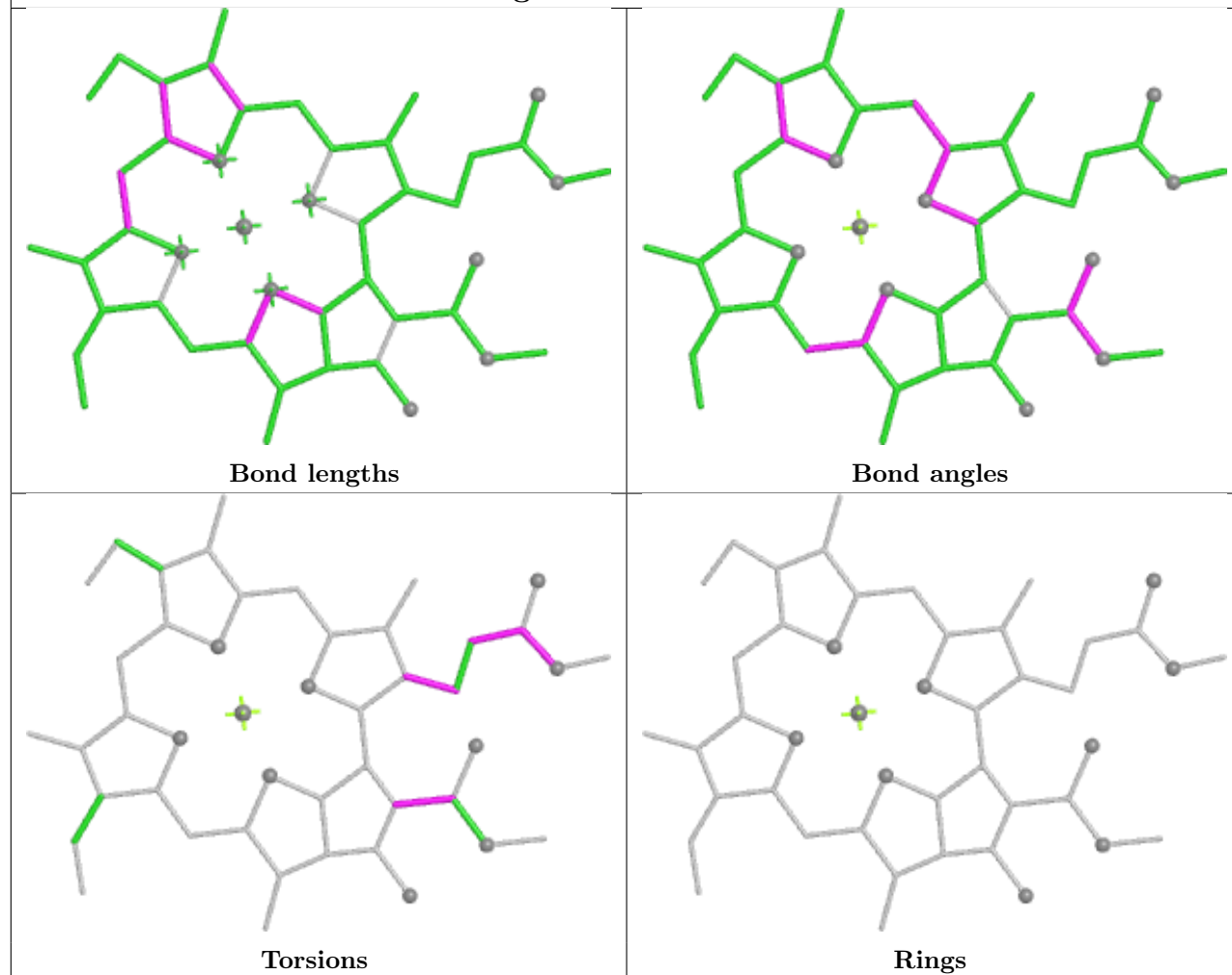


Ligand CLA 7 611

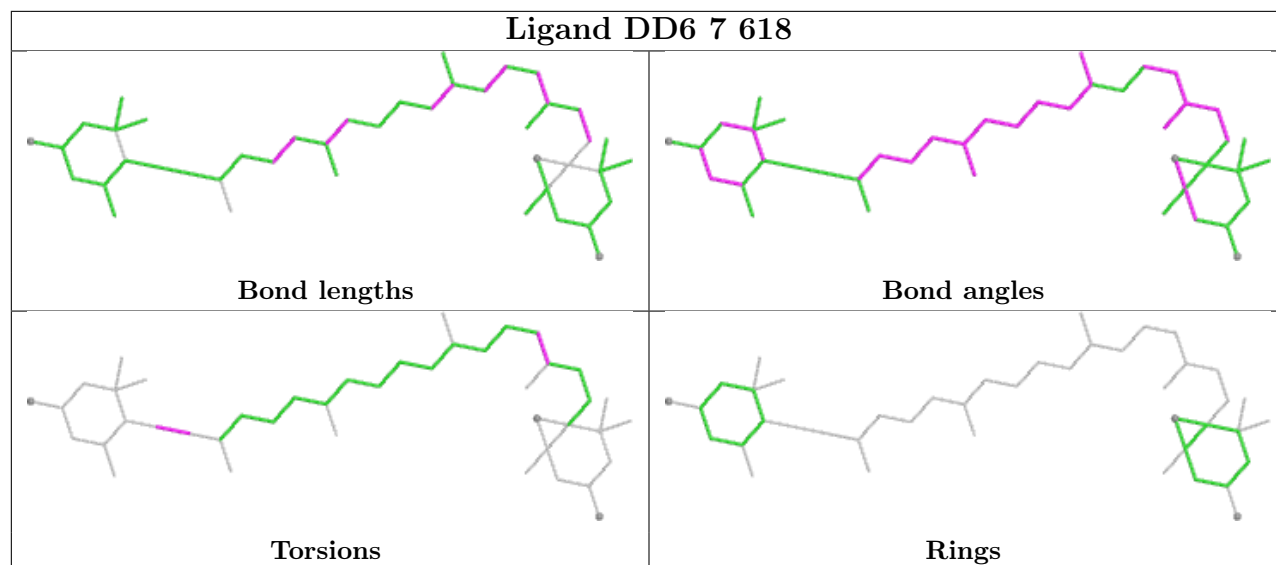


Ligand DD6 6 615

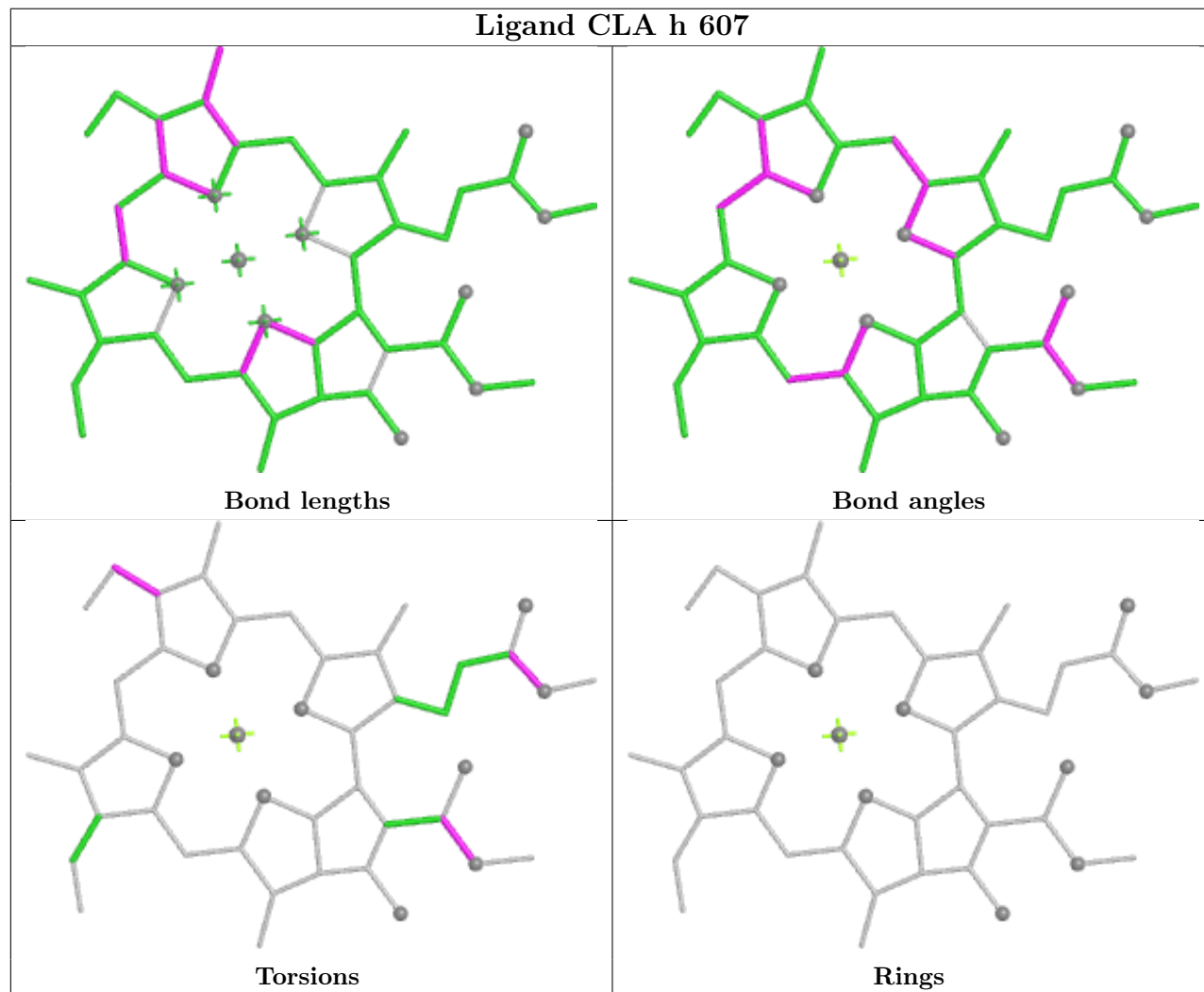


Ligand CLA B 829**Ligand CLA A 811**

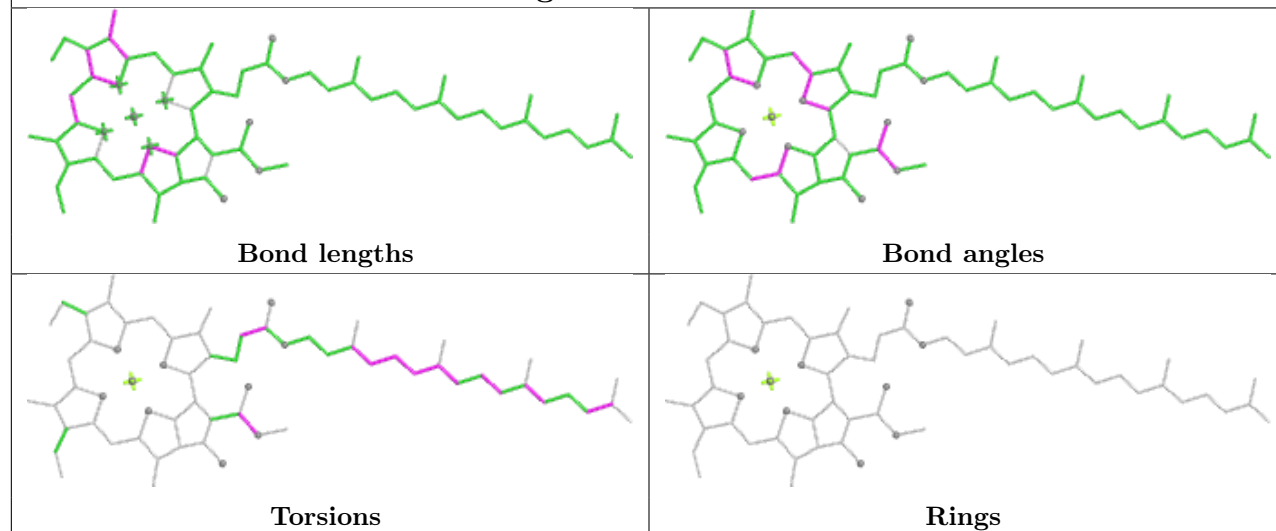
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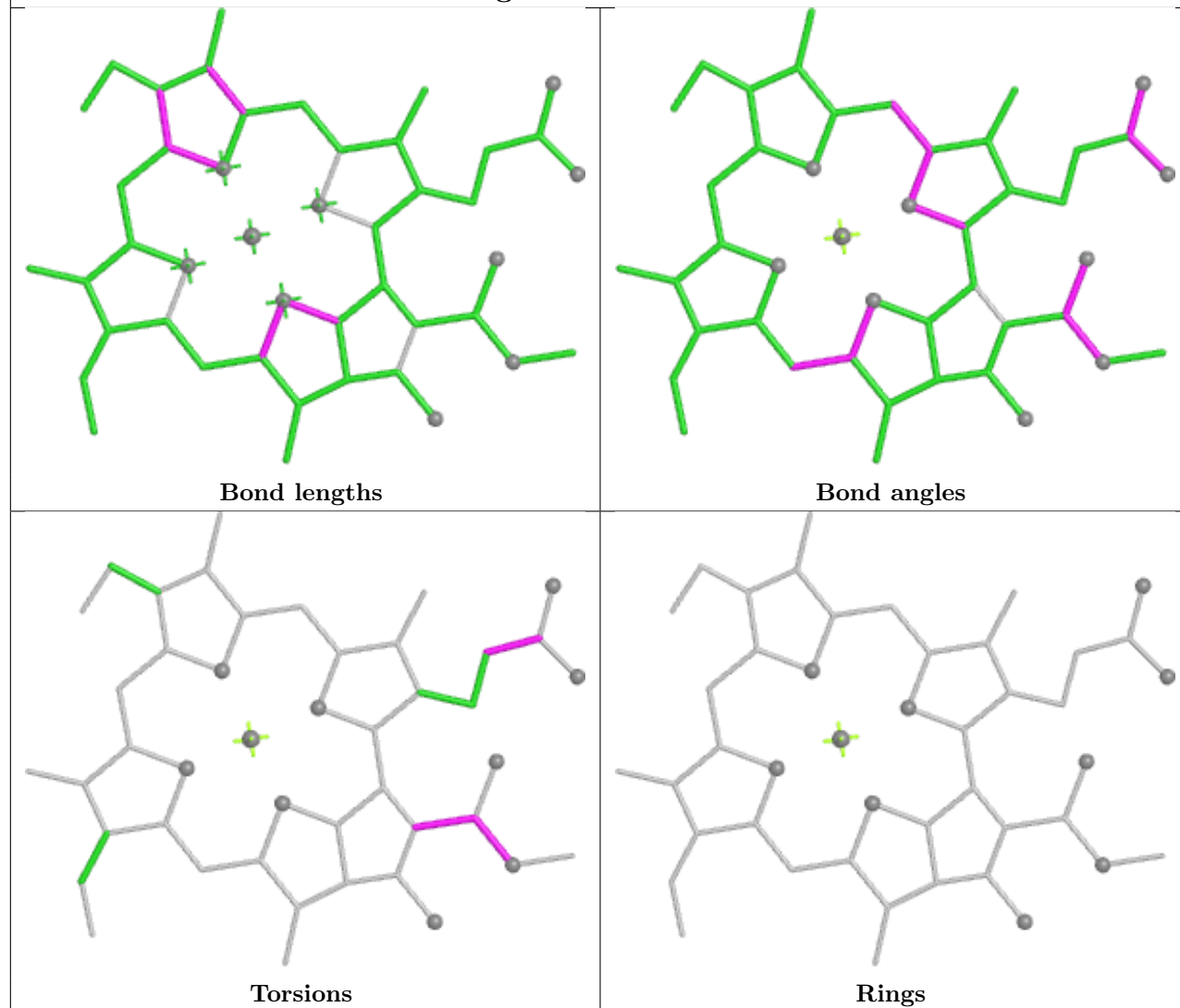
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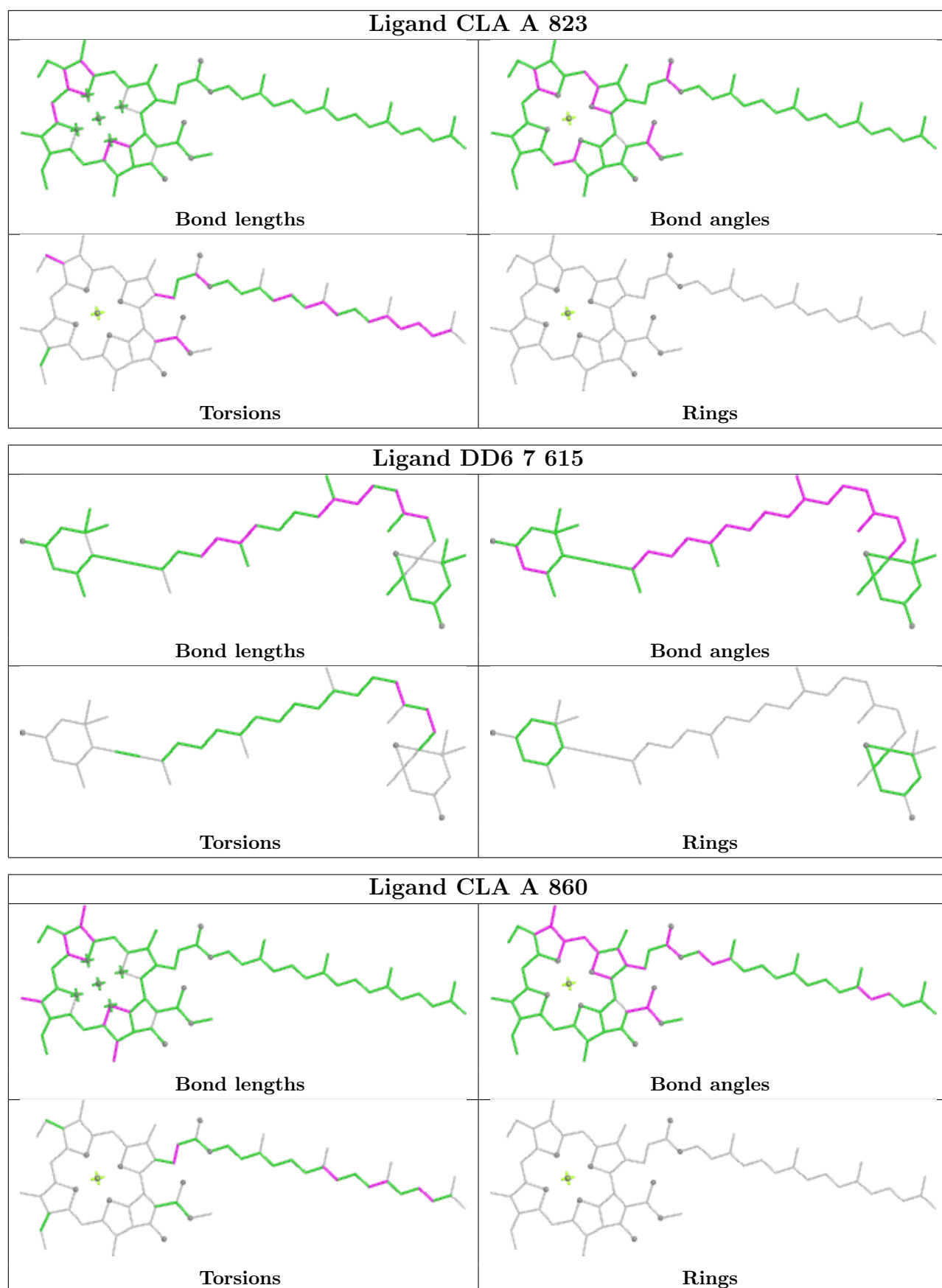


Ligand CLA 3 301

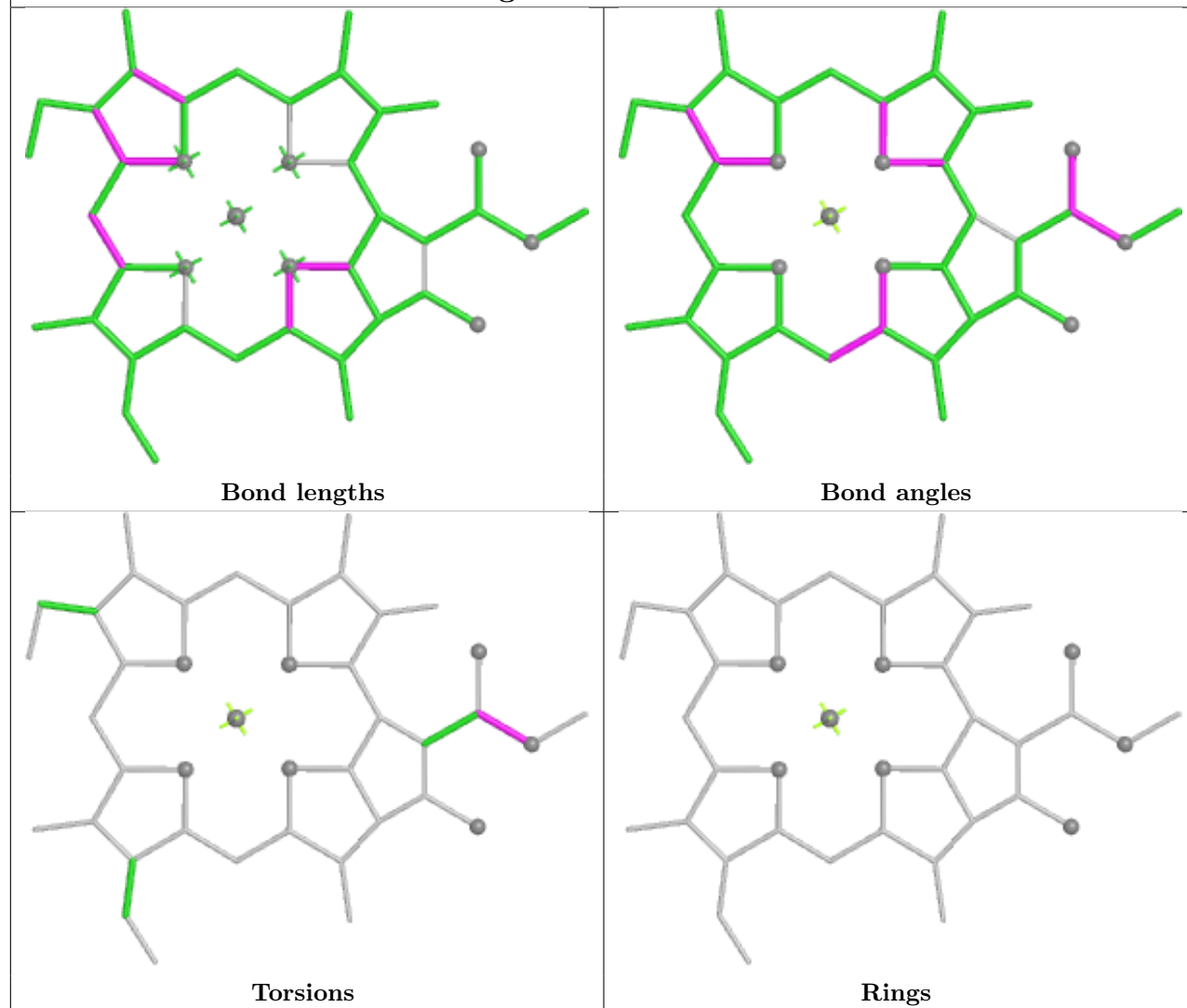


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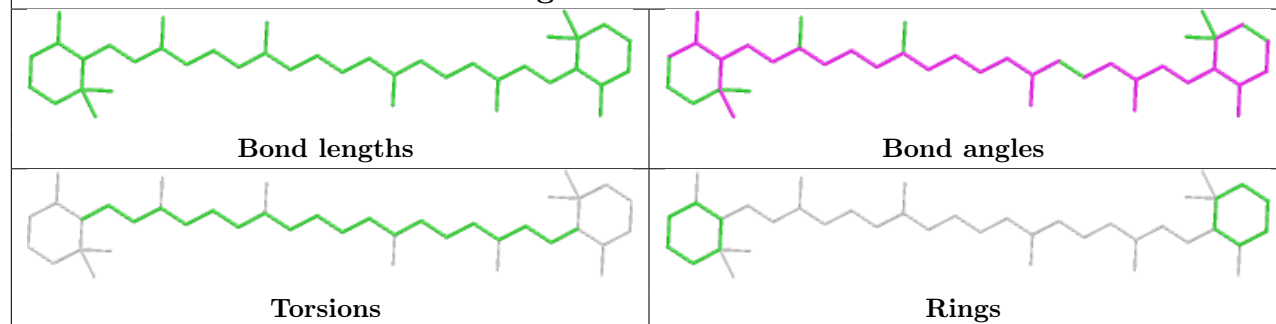




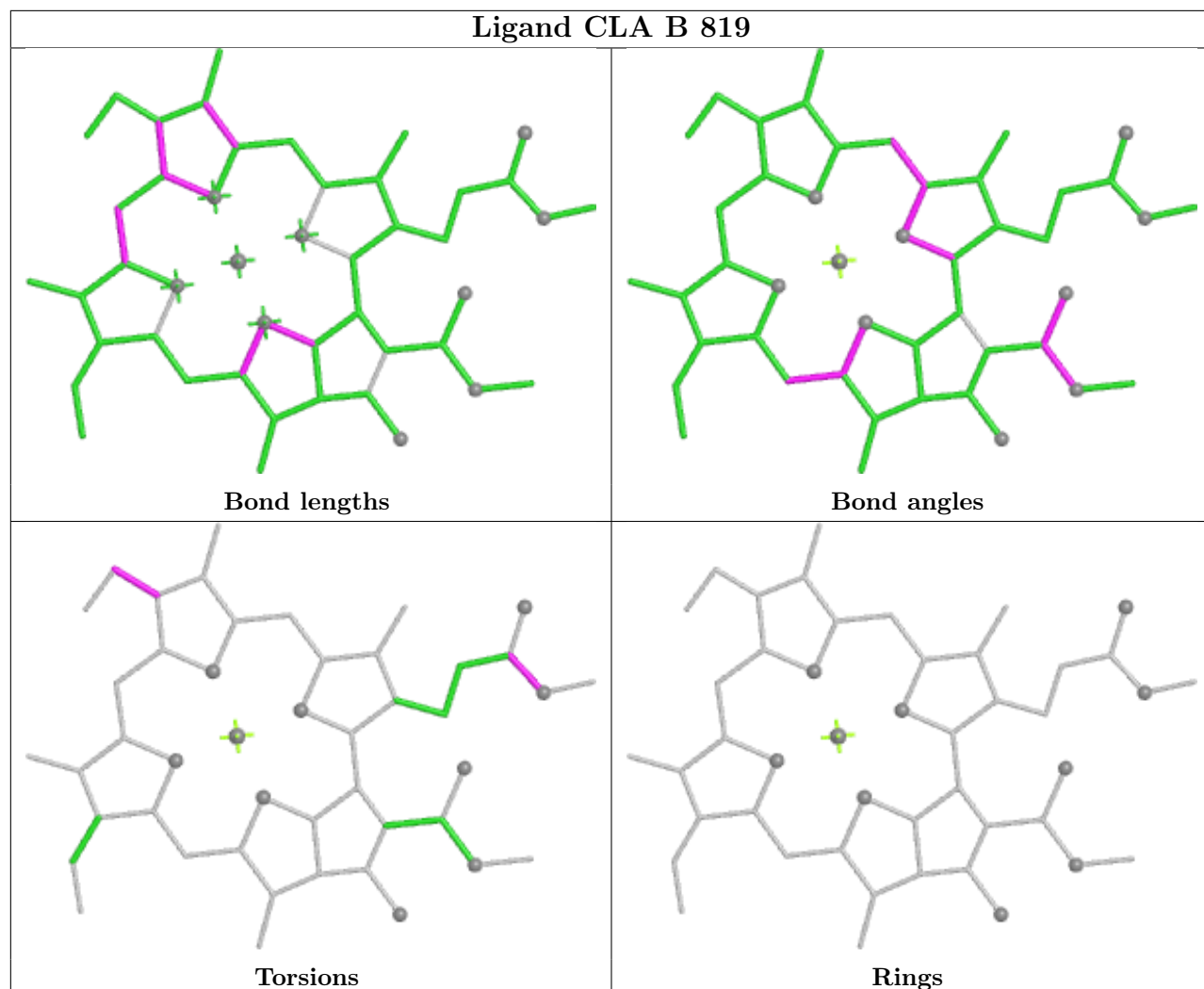
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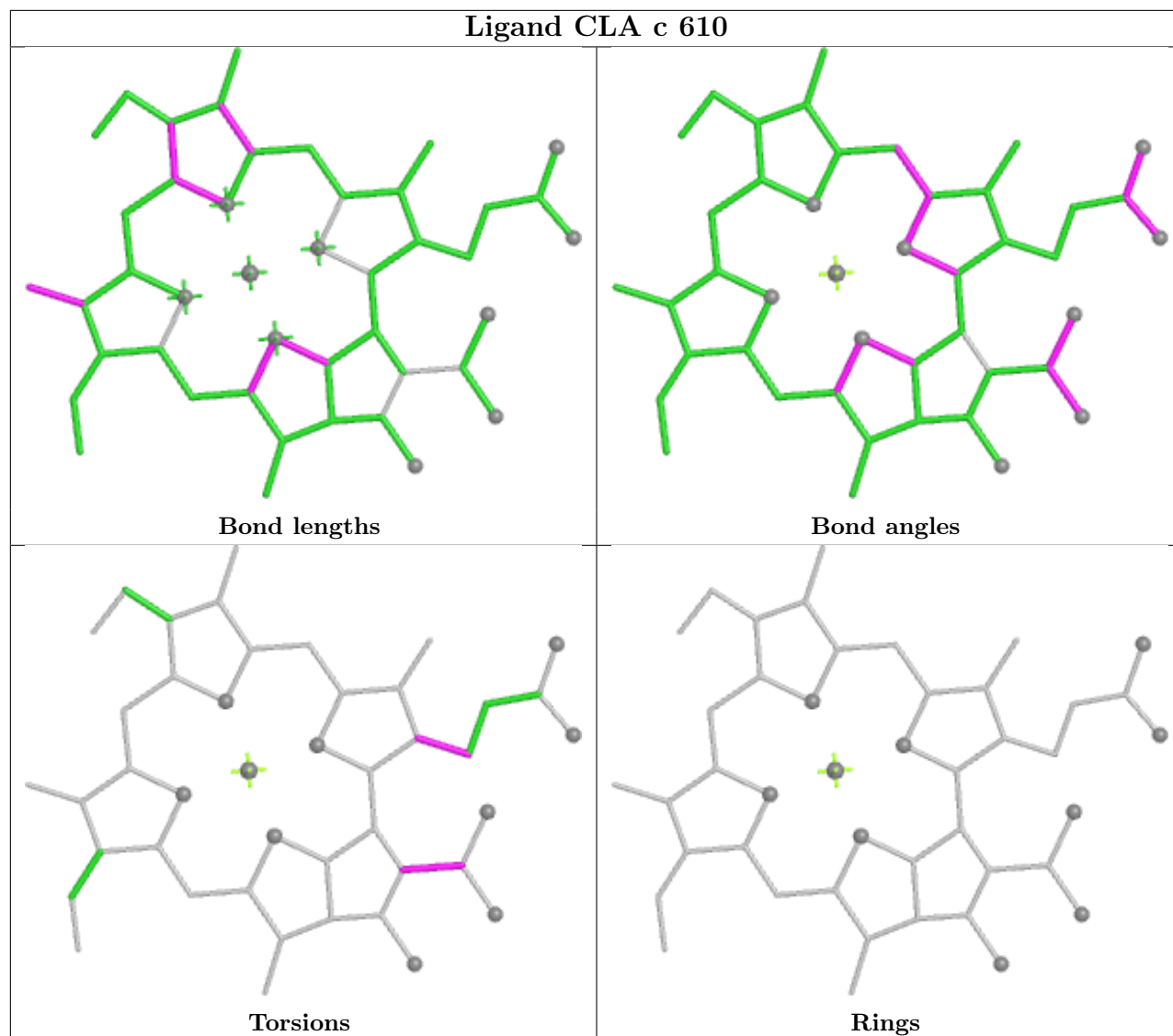
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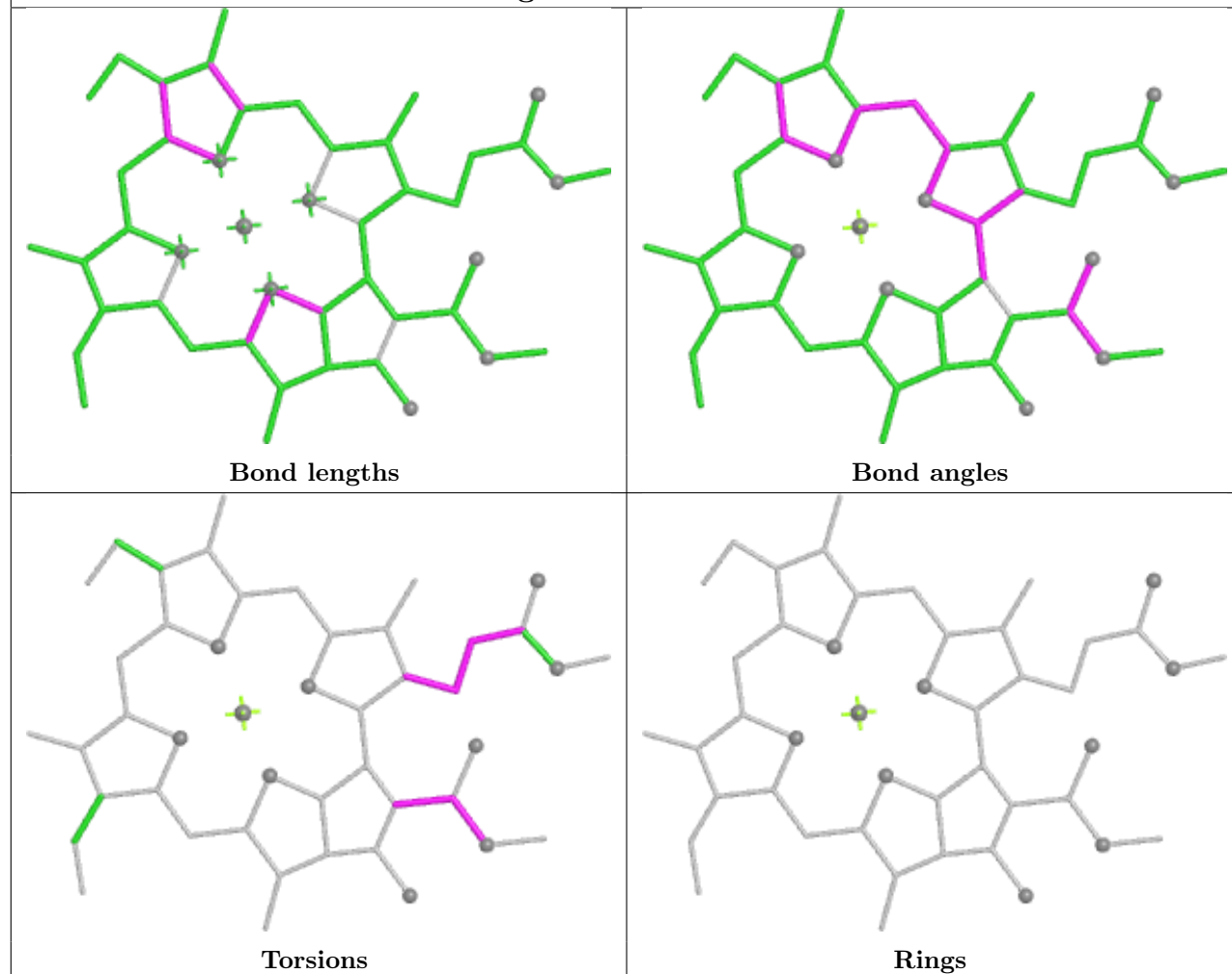
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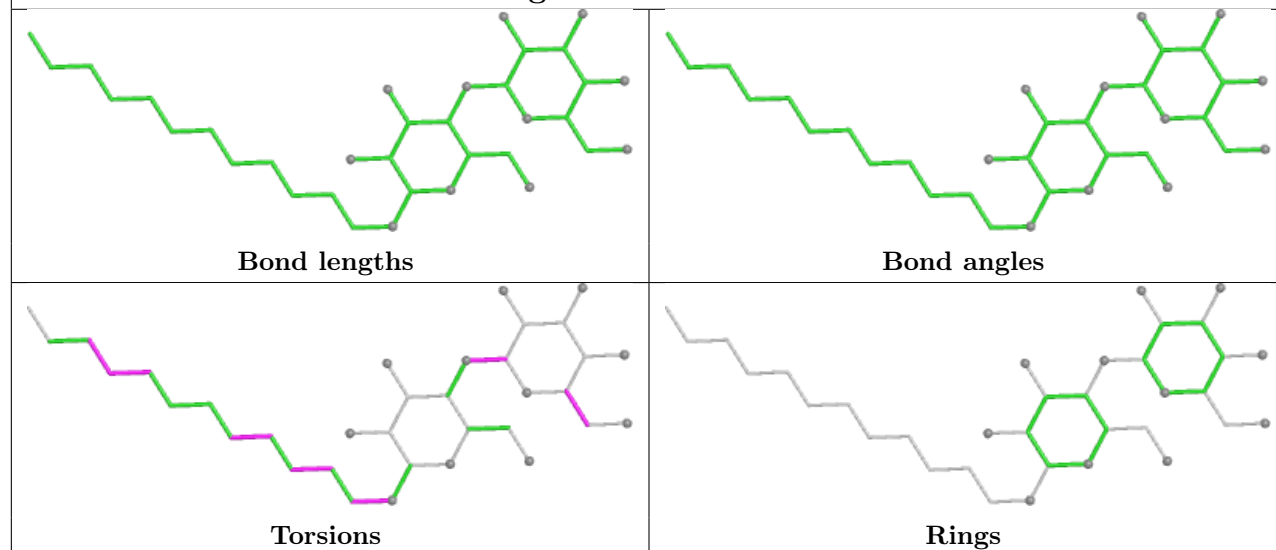
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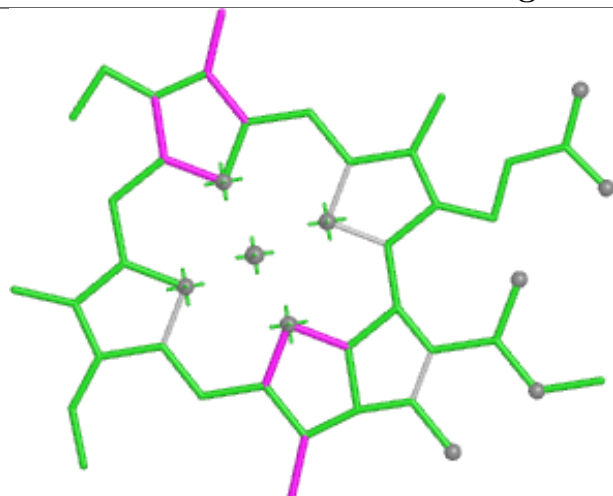
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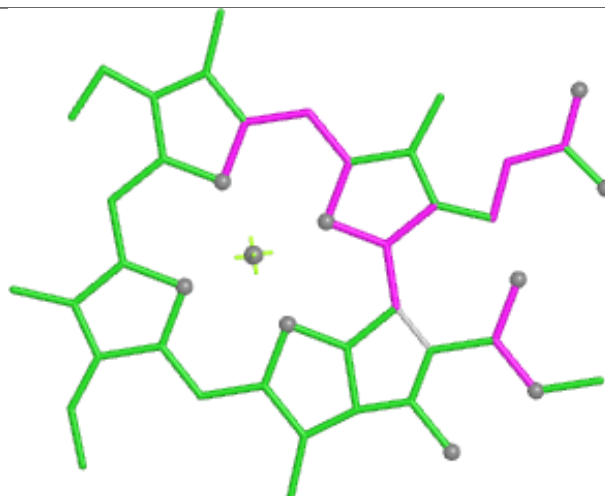
Ligand LMT A 854



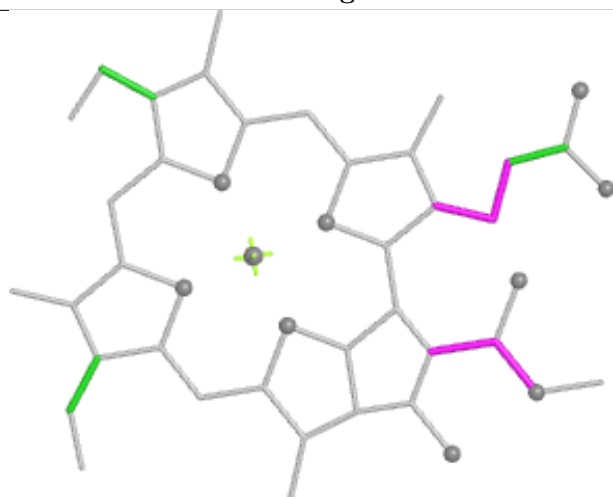
Ligand CLA 1 305



Bond lengths



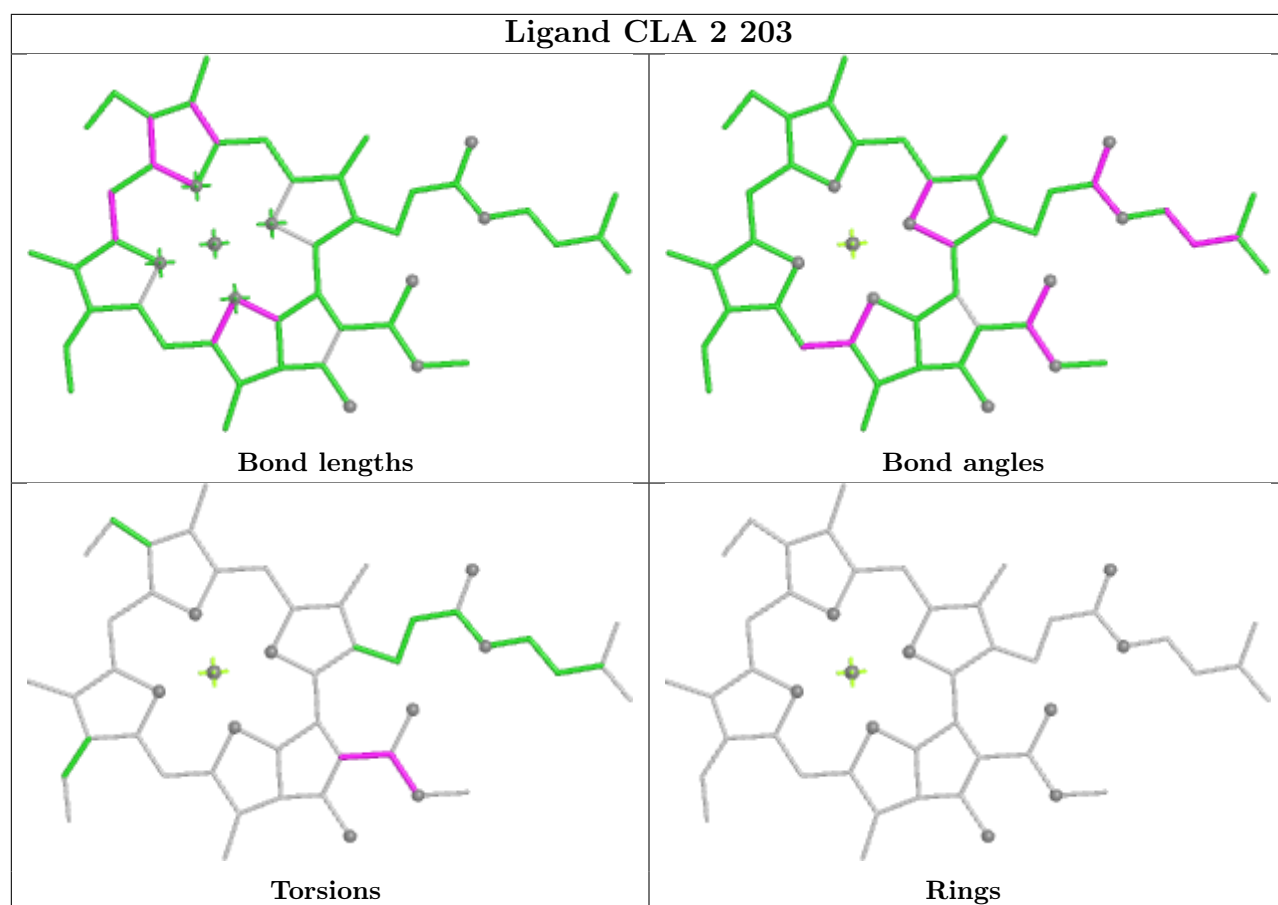
Bond angles



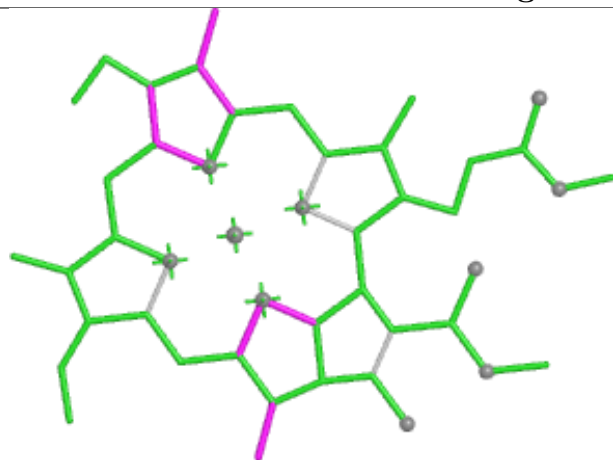
Torsions



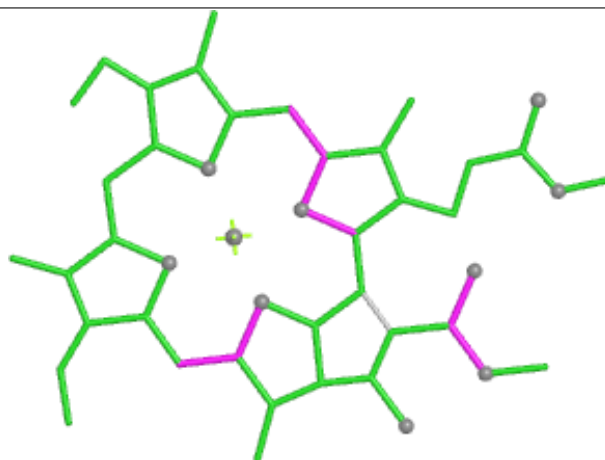
Rings



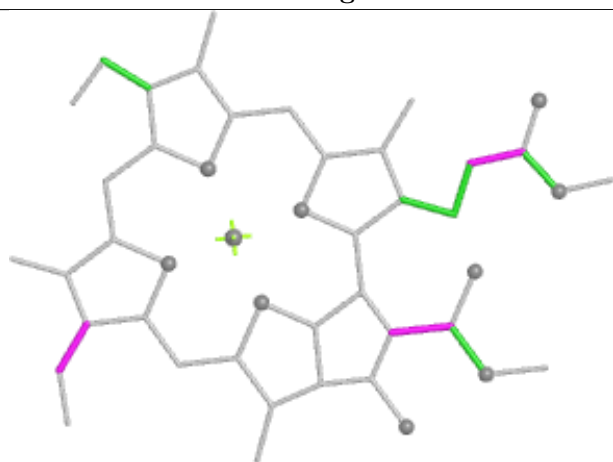
Ligand CLA h 606



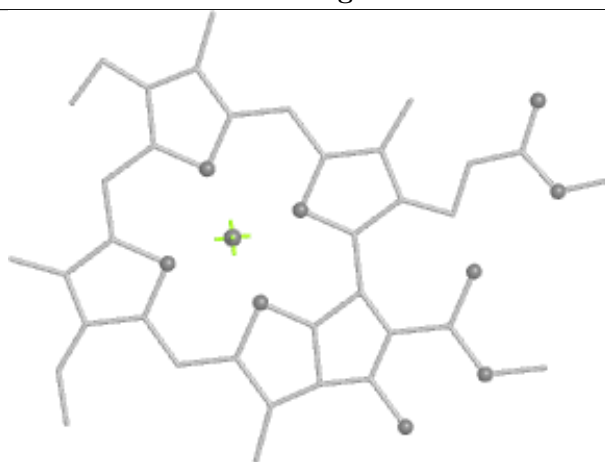
Bond lengths



Bond angles

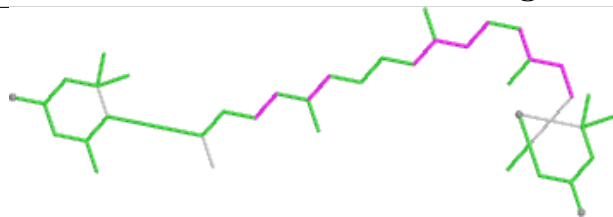


Torsions

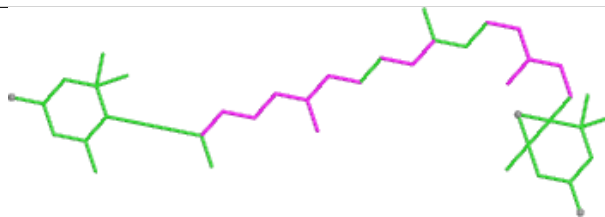


Rings

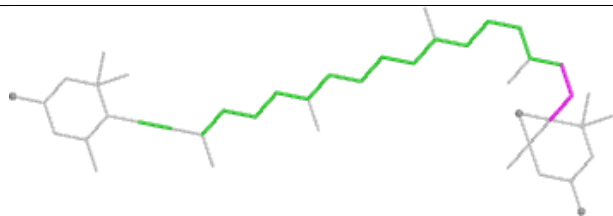
Ligand DD6 7 616



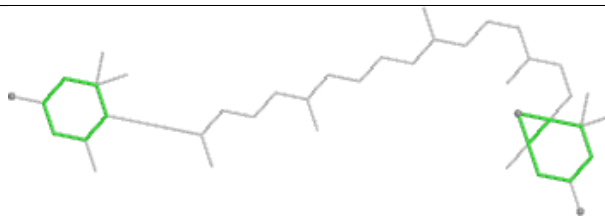
Bond lengths



Bond angles

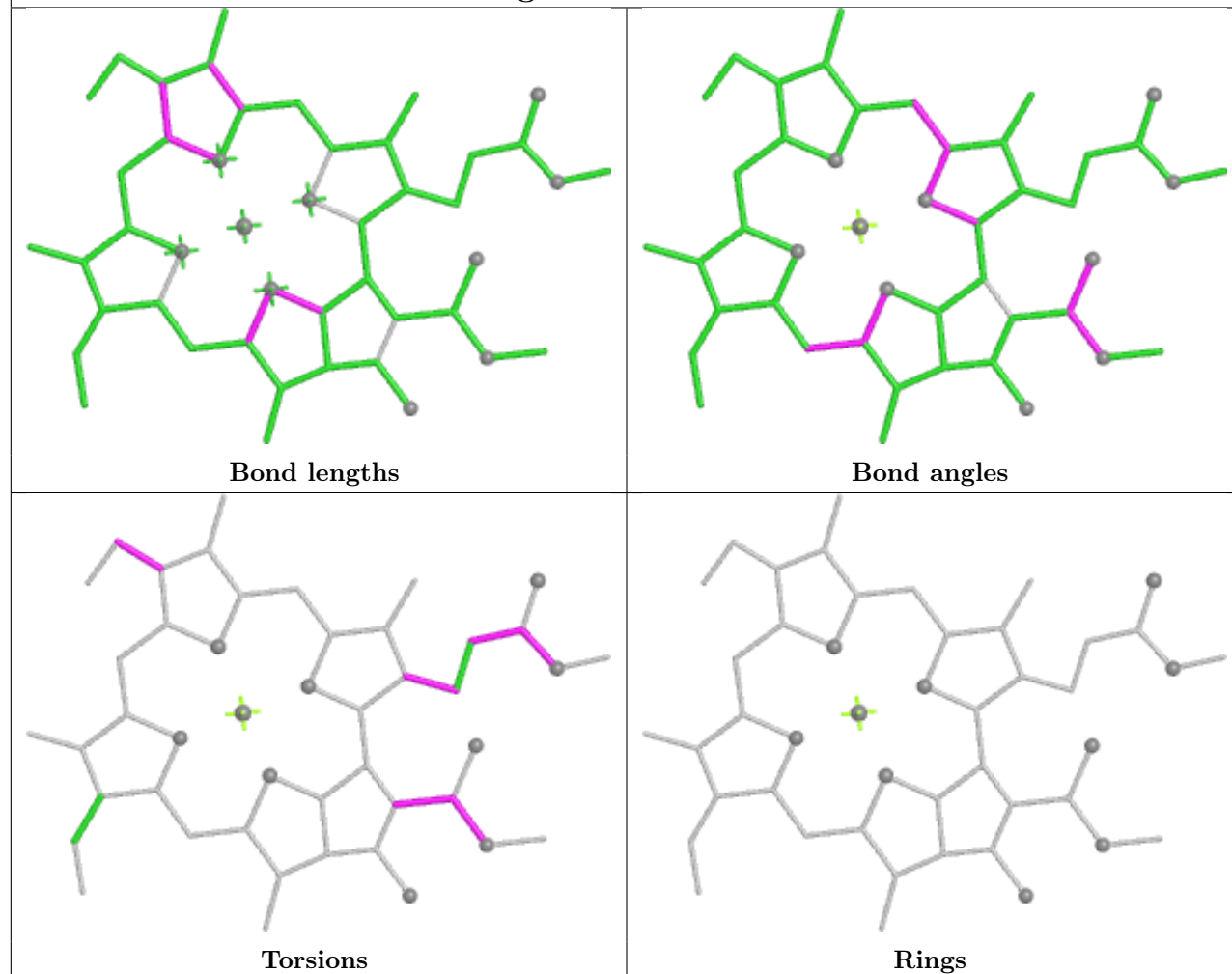


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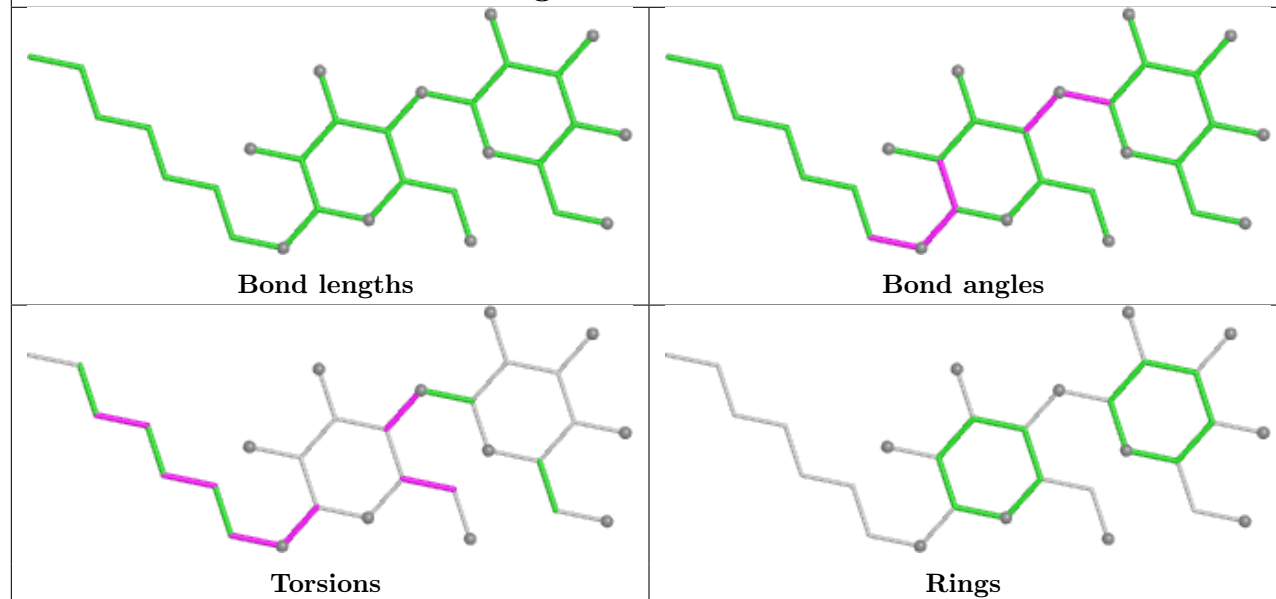


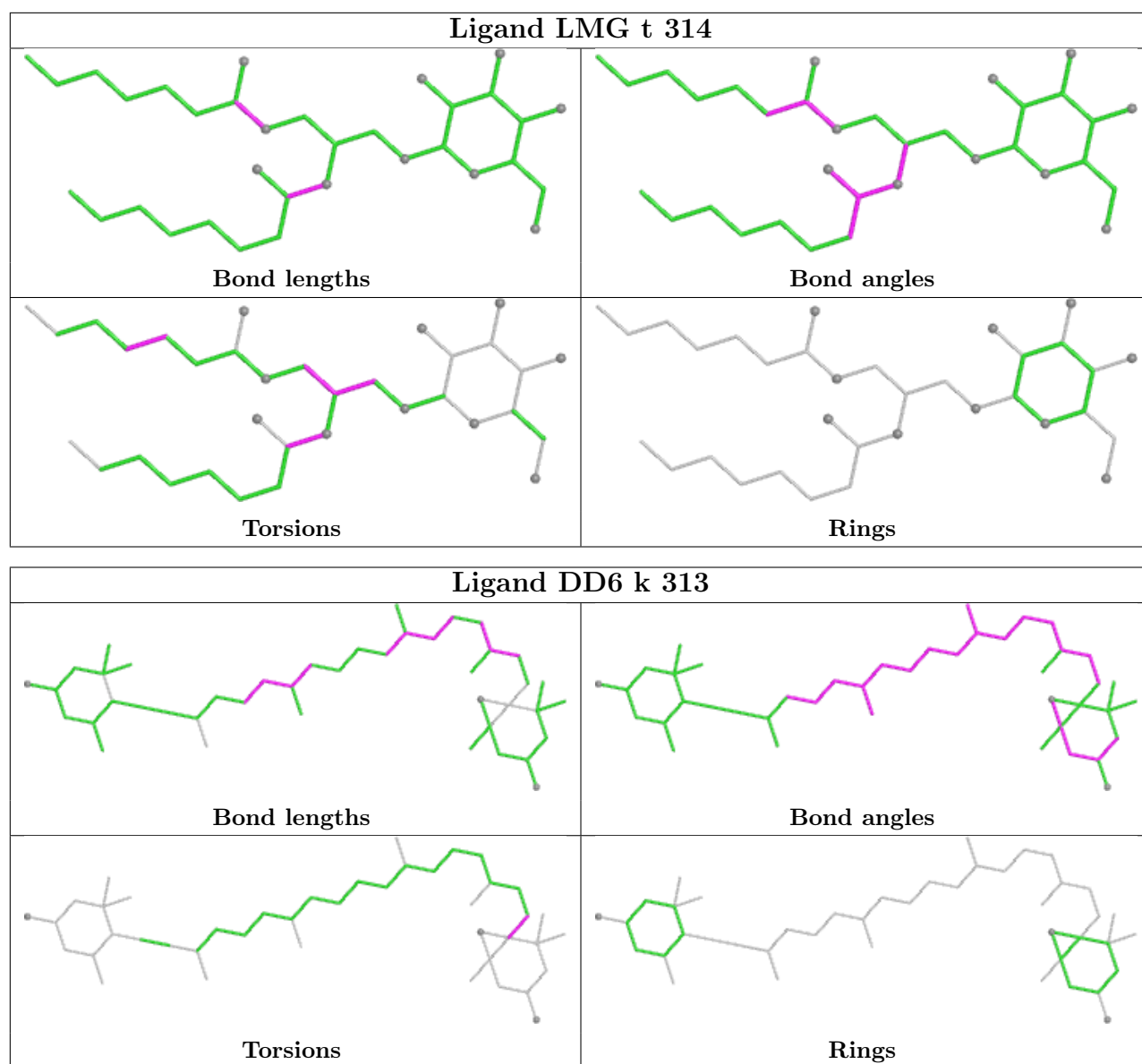
Rings

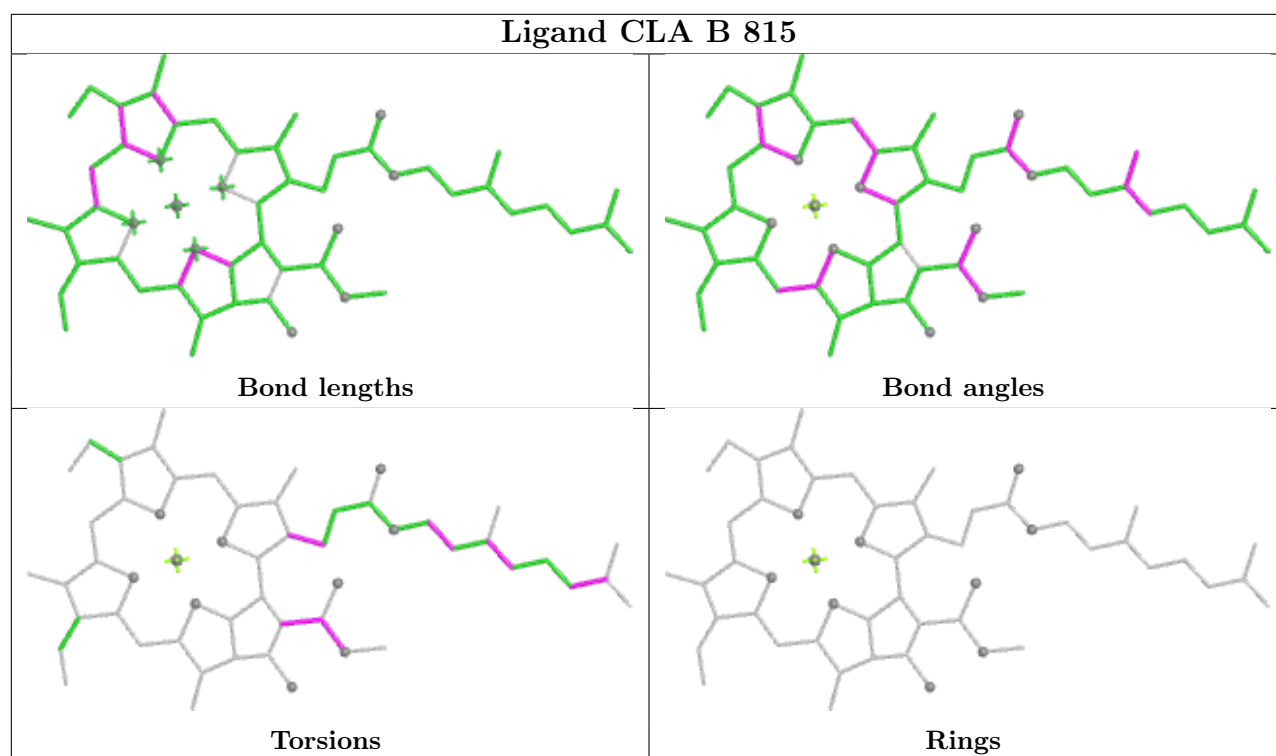
Ligand CLA 4 613



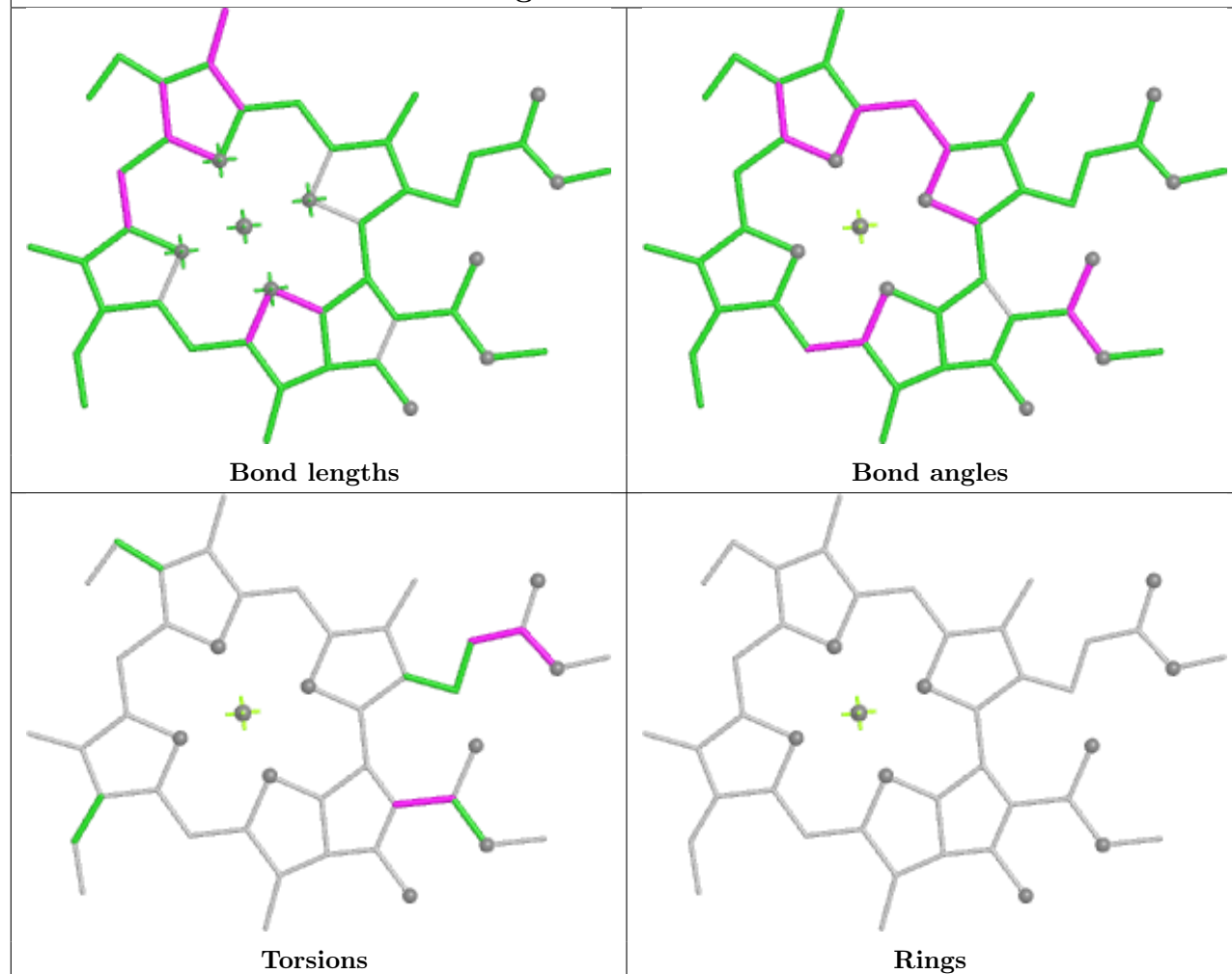
Ligand LMT 3 314



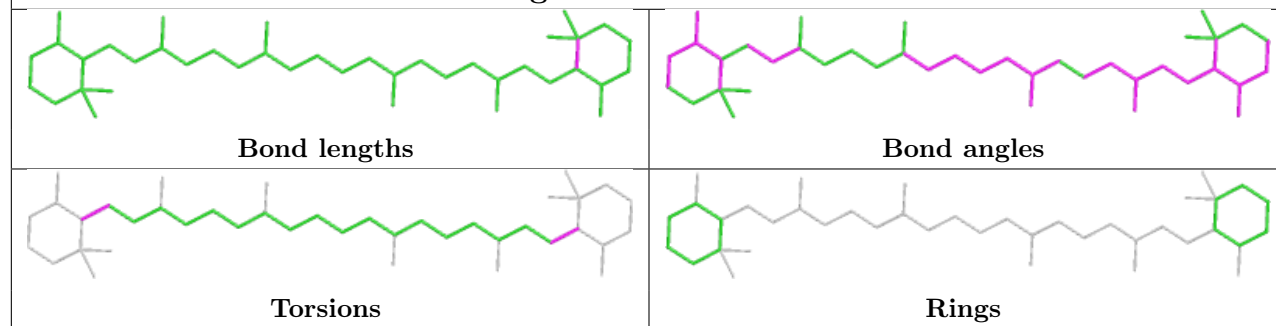




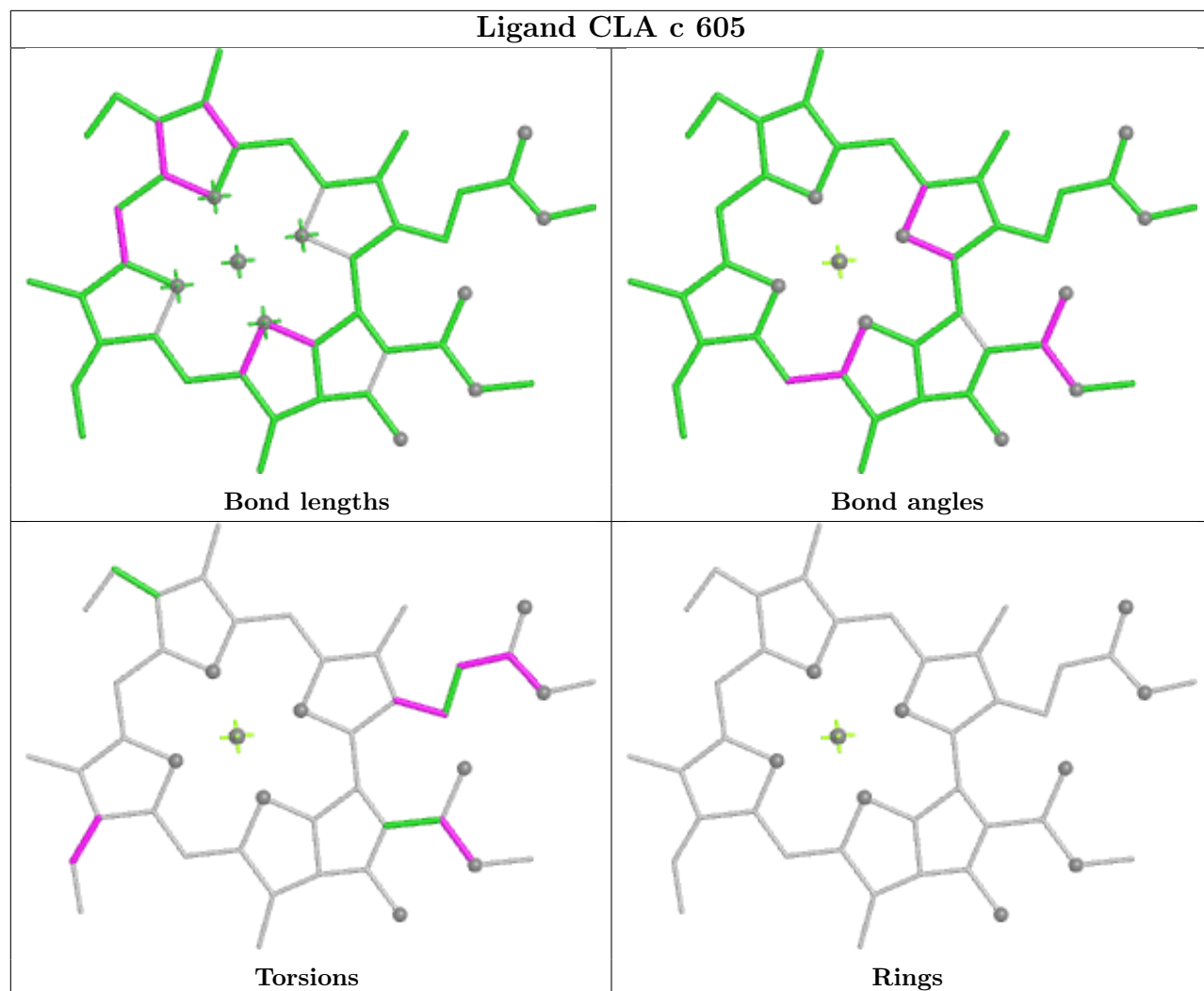
Ligand CLA F 202

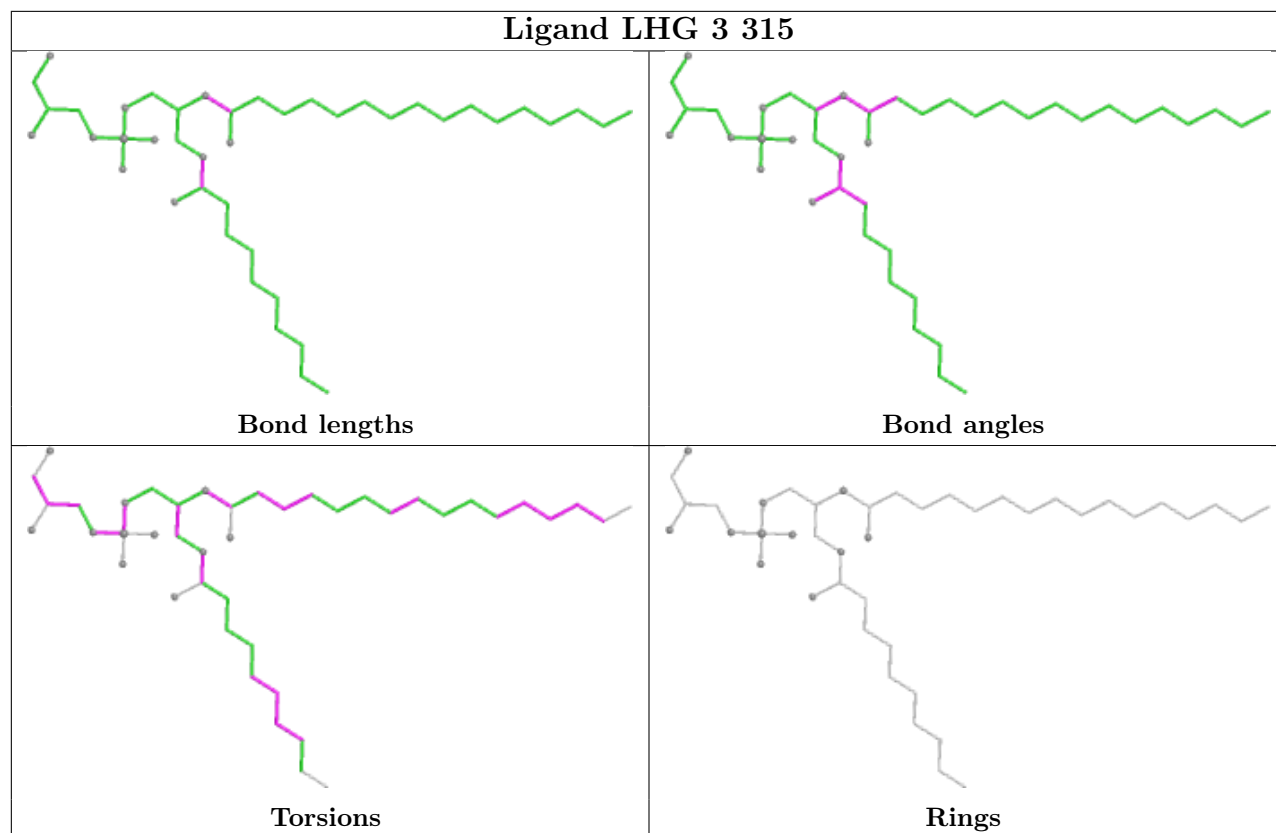


Ligand BCR R 101

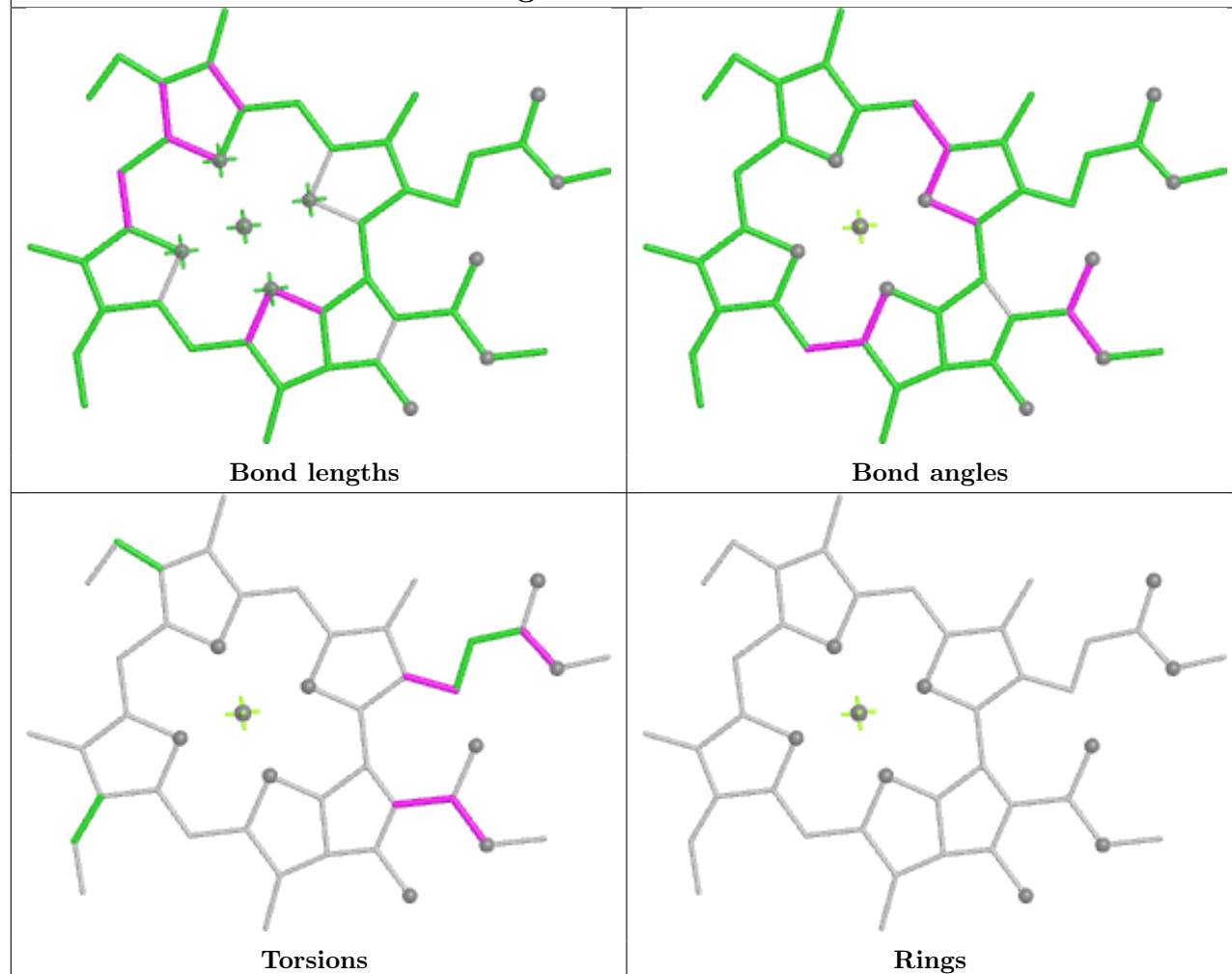


Ligand CLA c 605

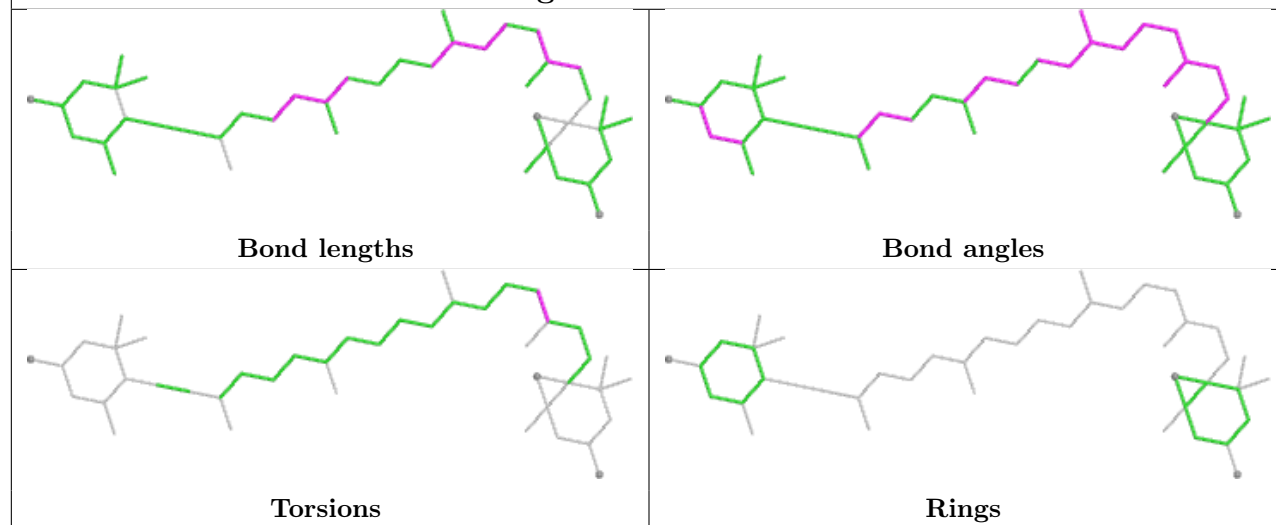


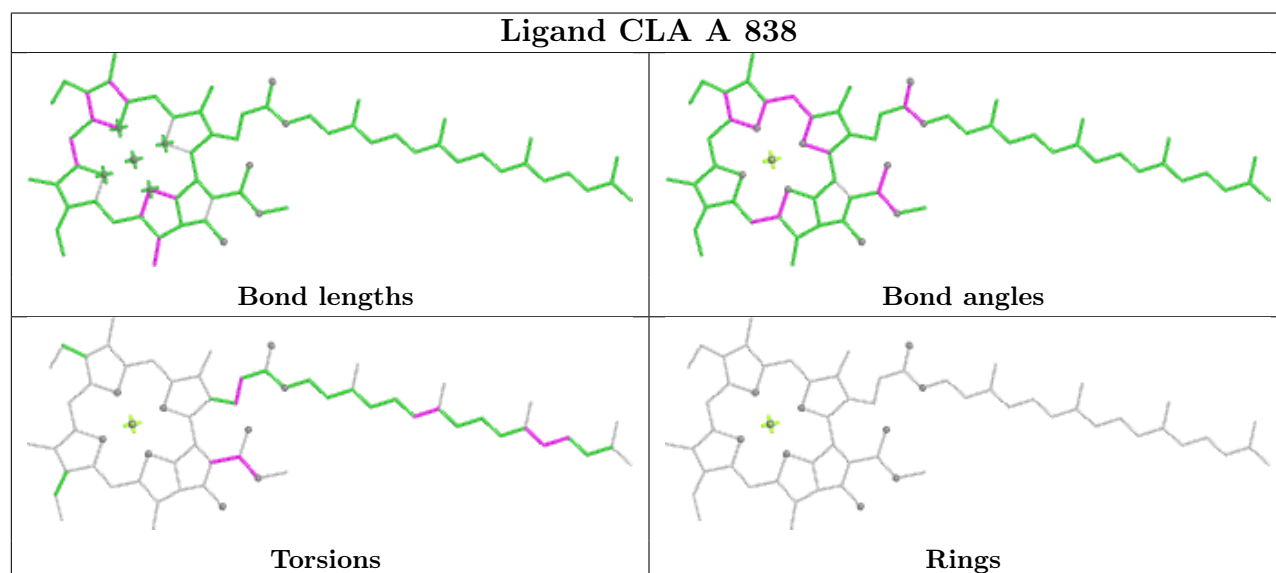
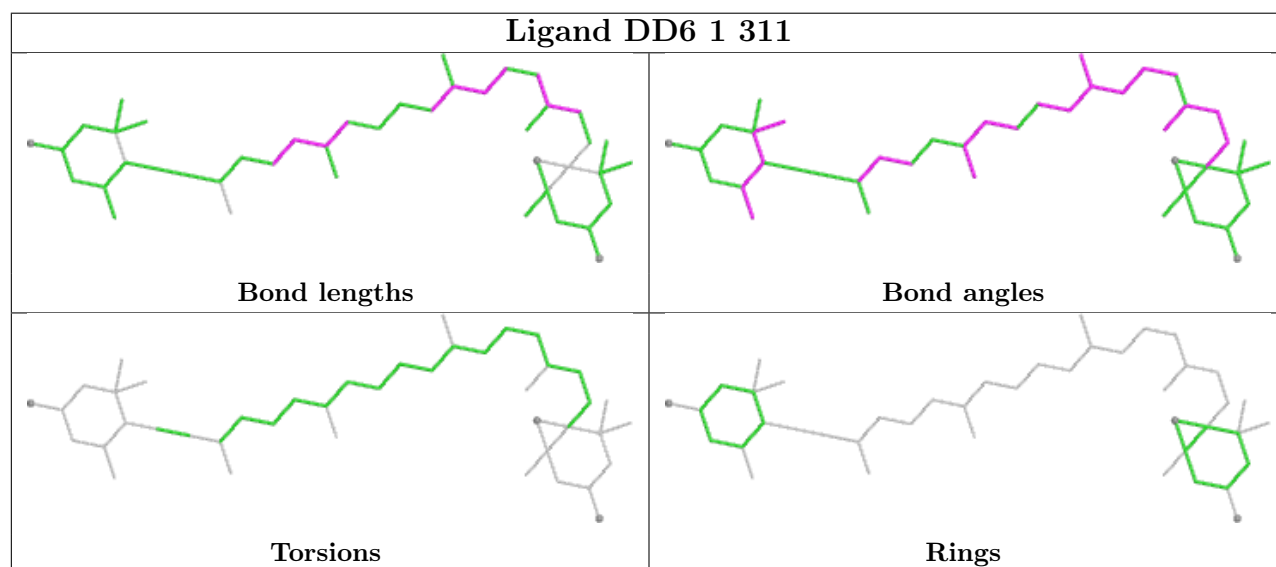
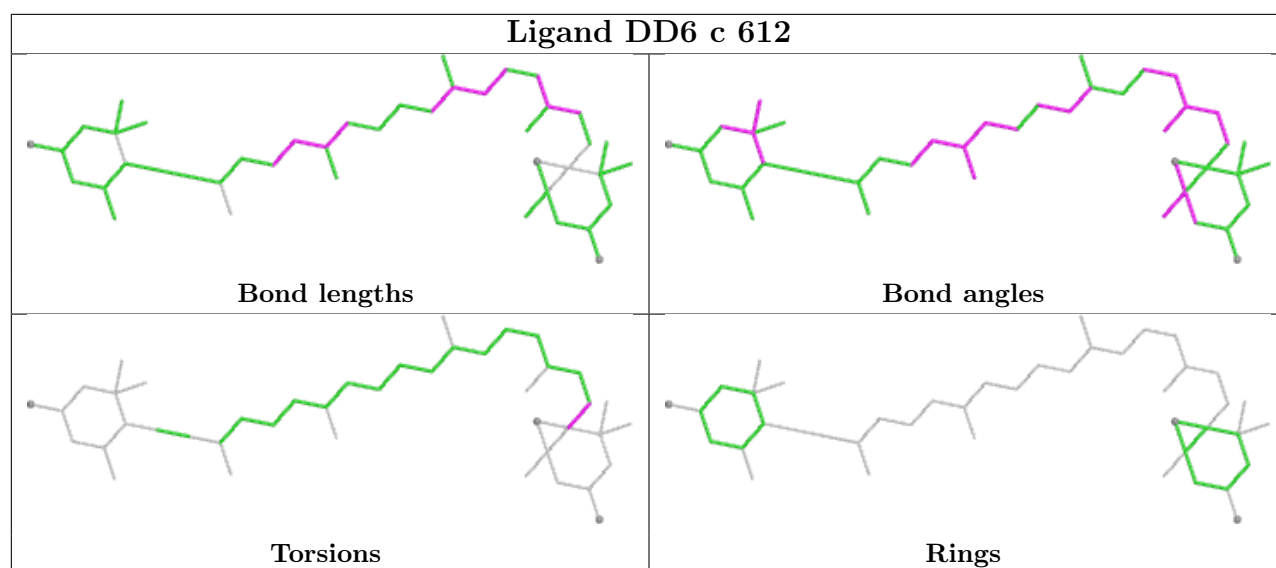


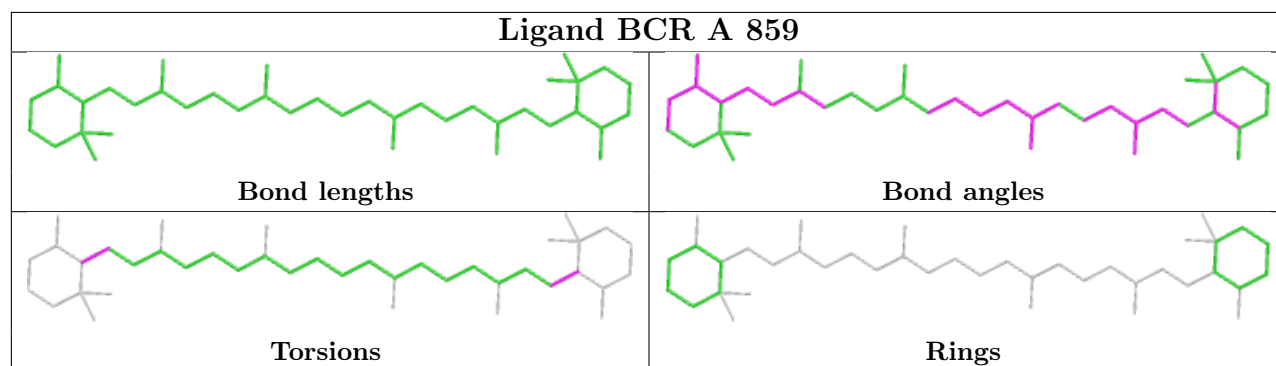
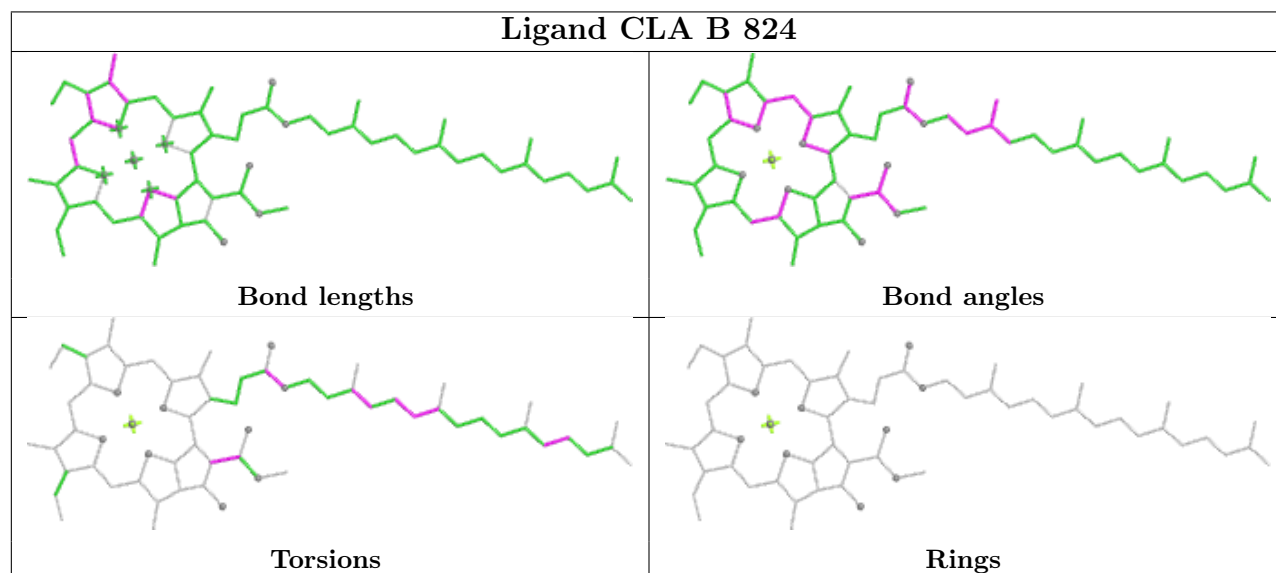
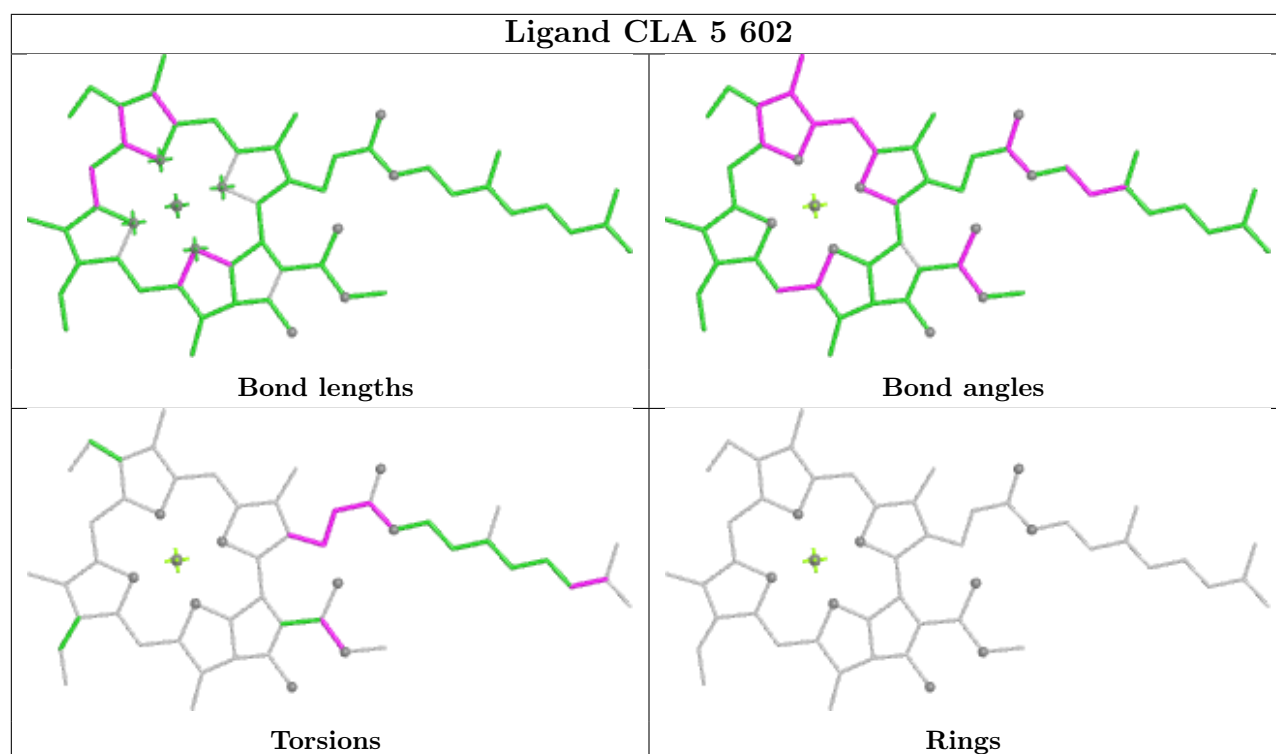
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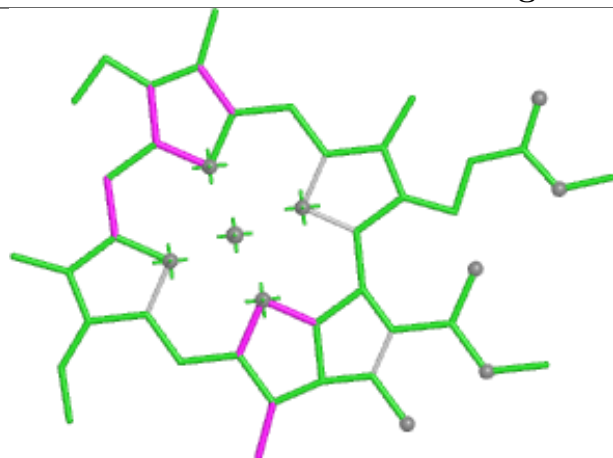
Ligand DD6 8 212



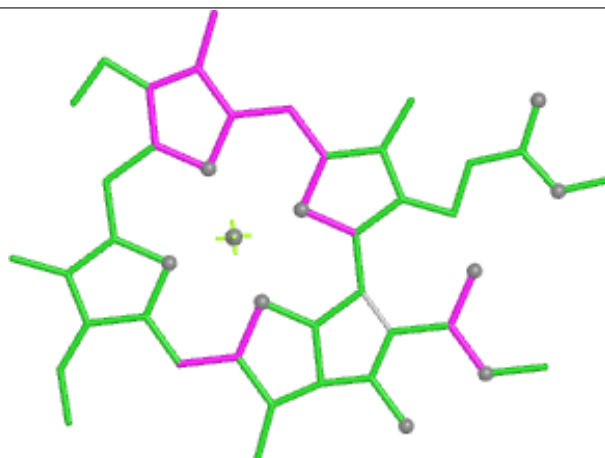




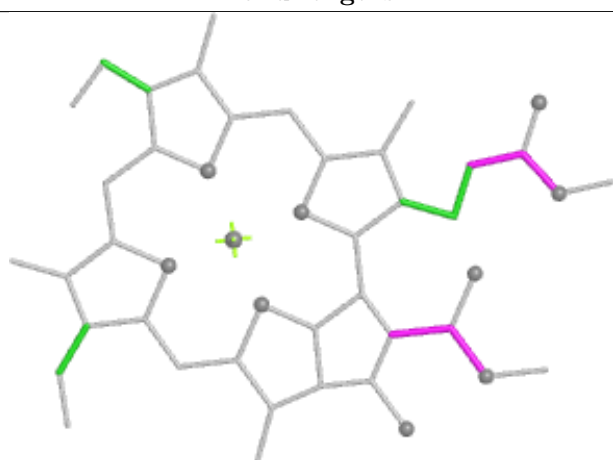
Ligand CLA 9 301



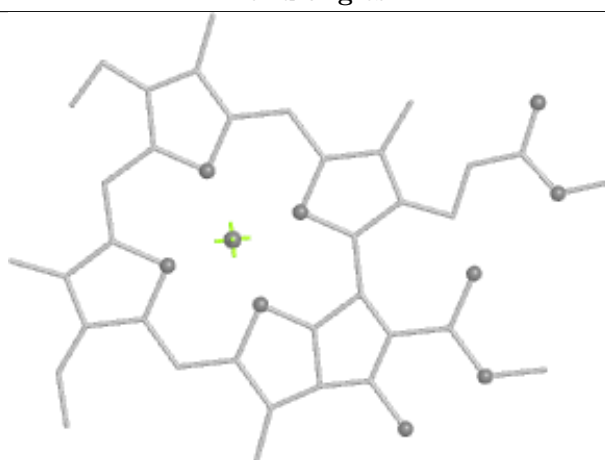
Bond lengths



Bond angles

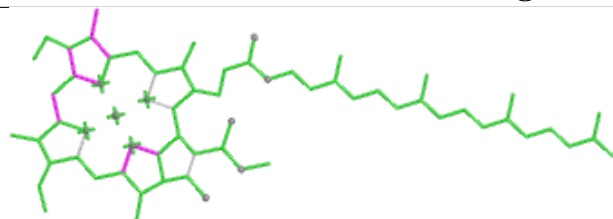


Torsions

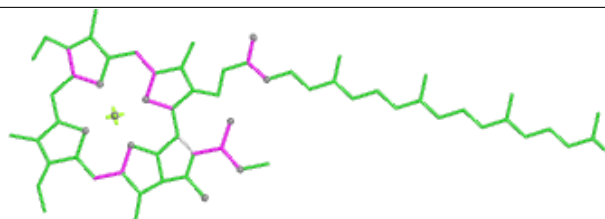


Rings

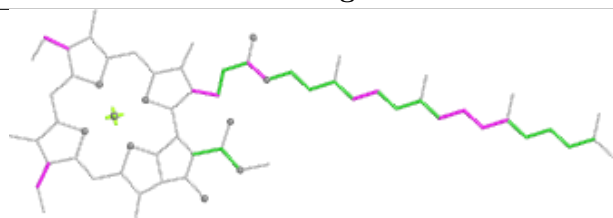
Ligand CLA L 204



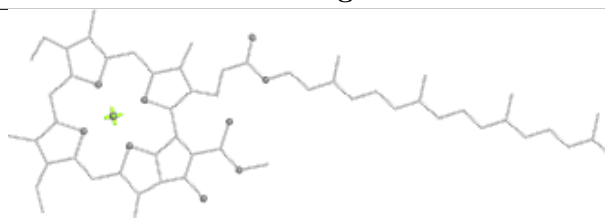
Bond lengths



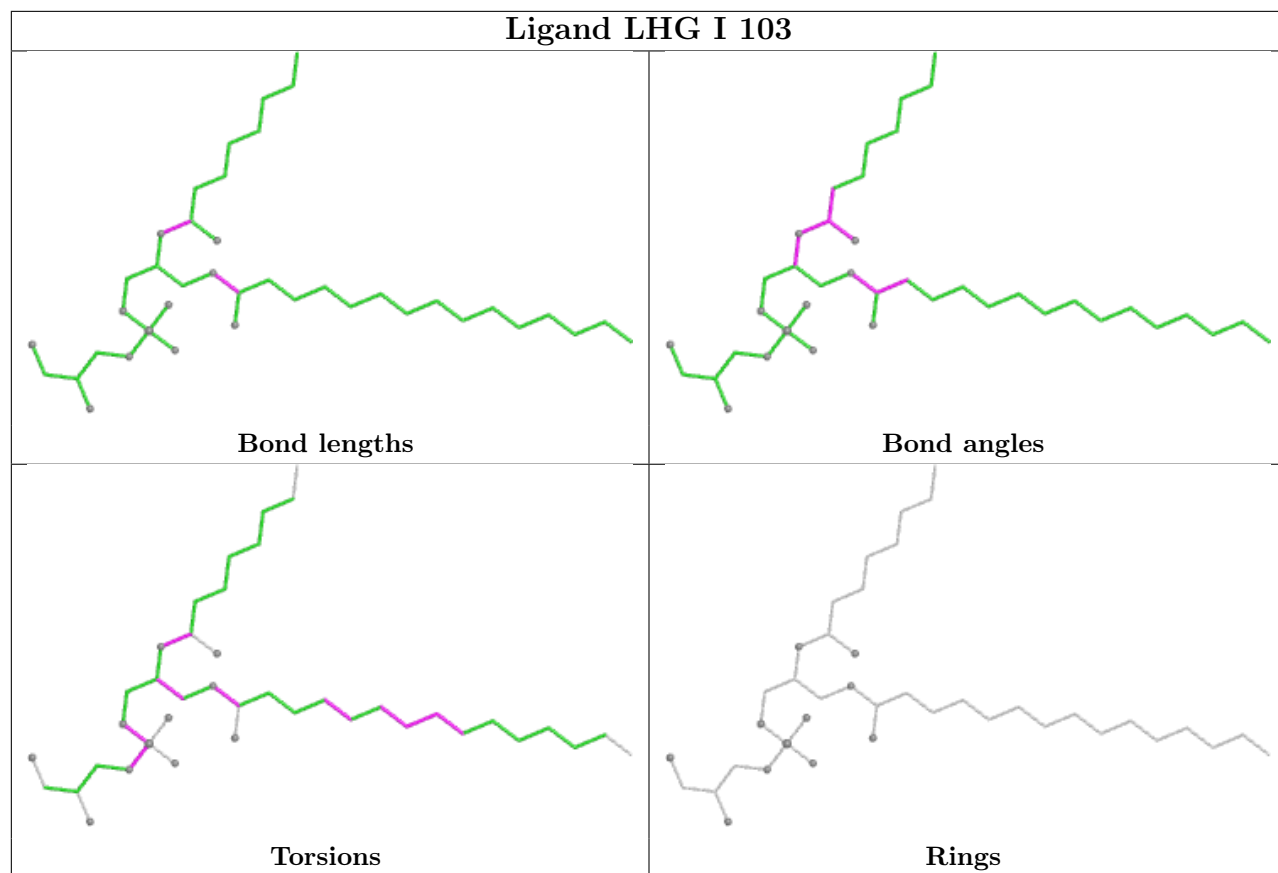
Bond angles



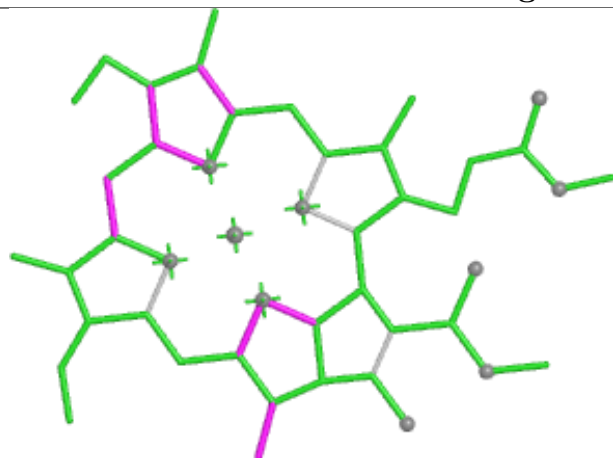
Torsions



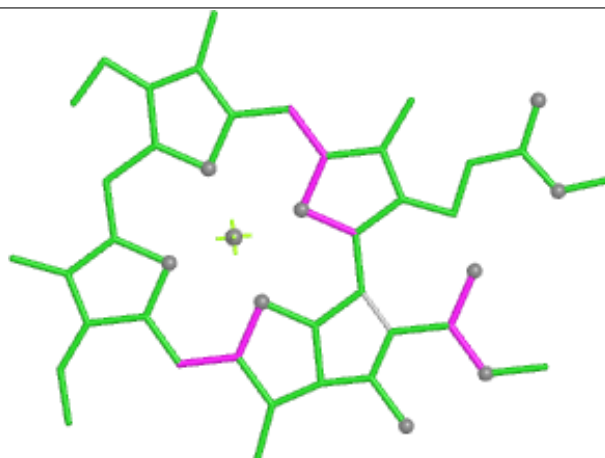
Rings



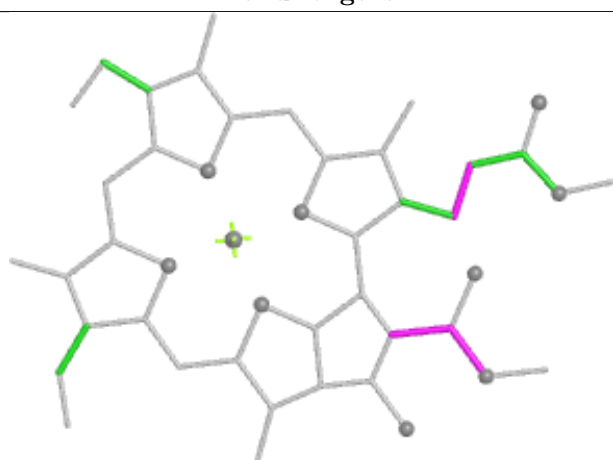
Ligand CLA 6 604



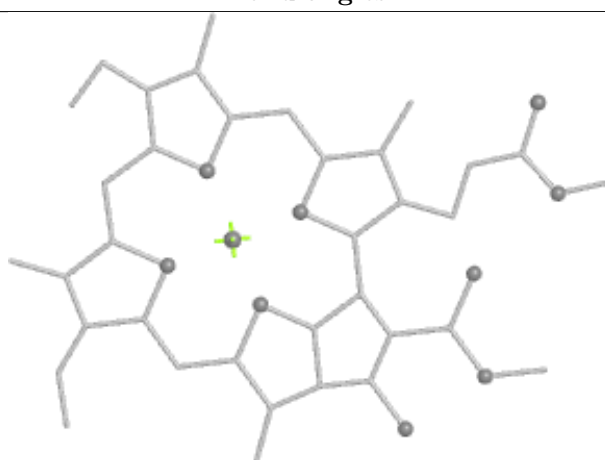
Bond lengths



Bond angles

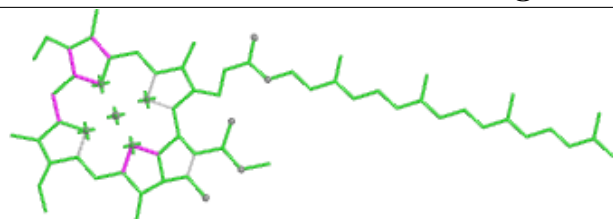


Torsions

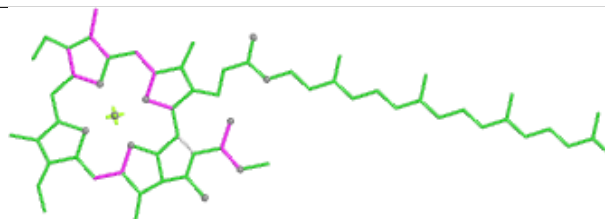


Rings

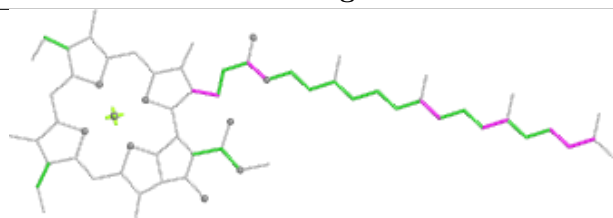
Ligand CLA B 805



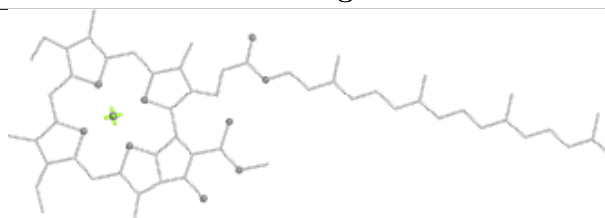
Bond lengths



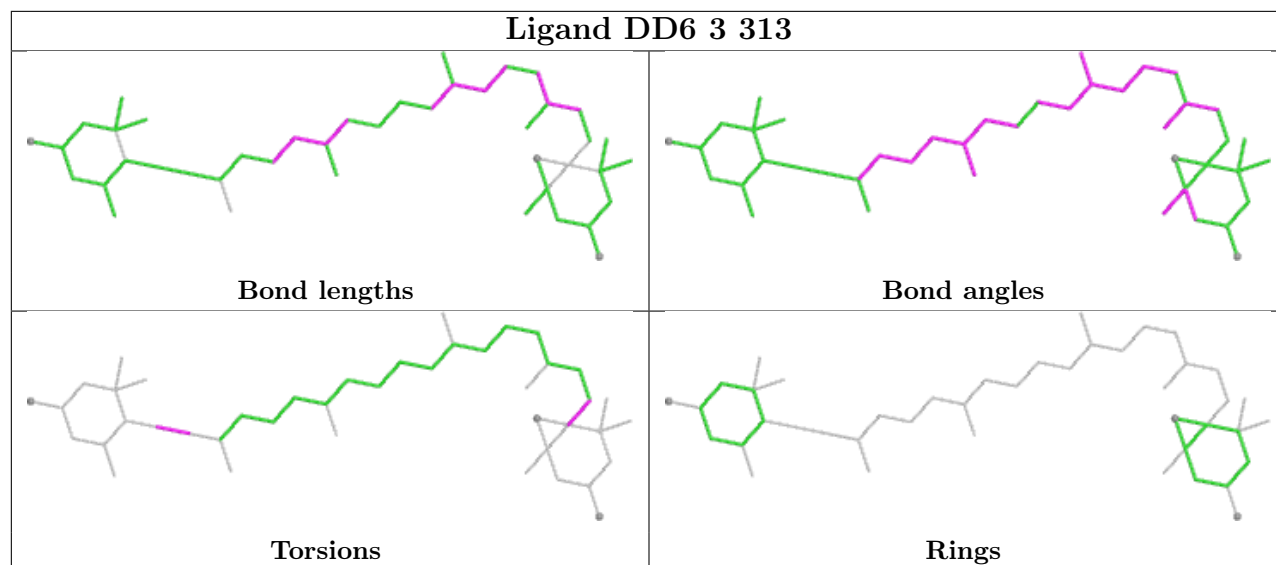
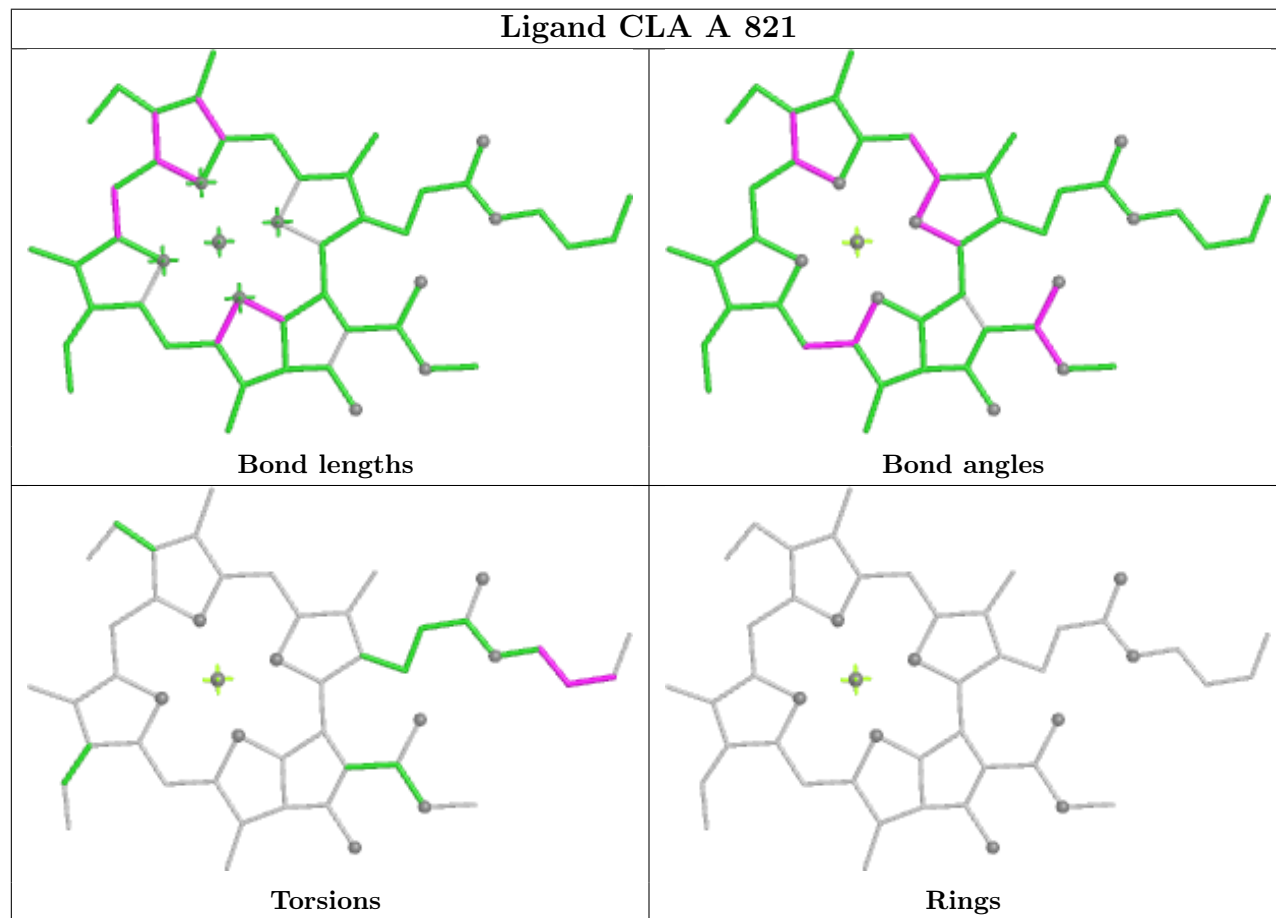
Bond angles

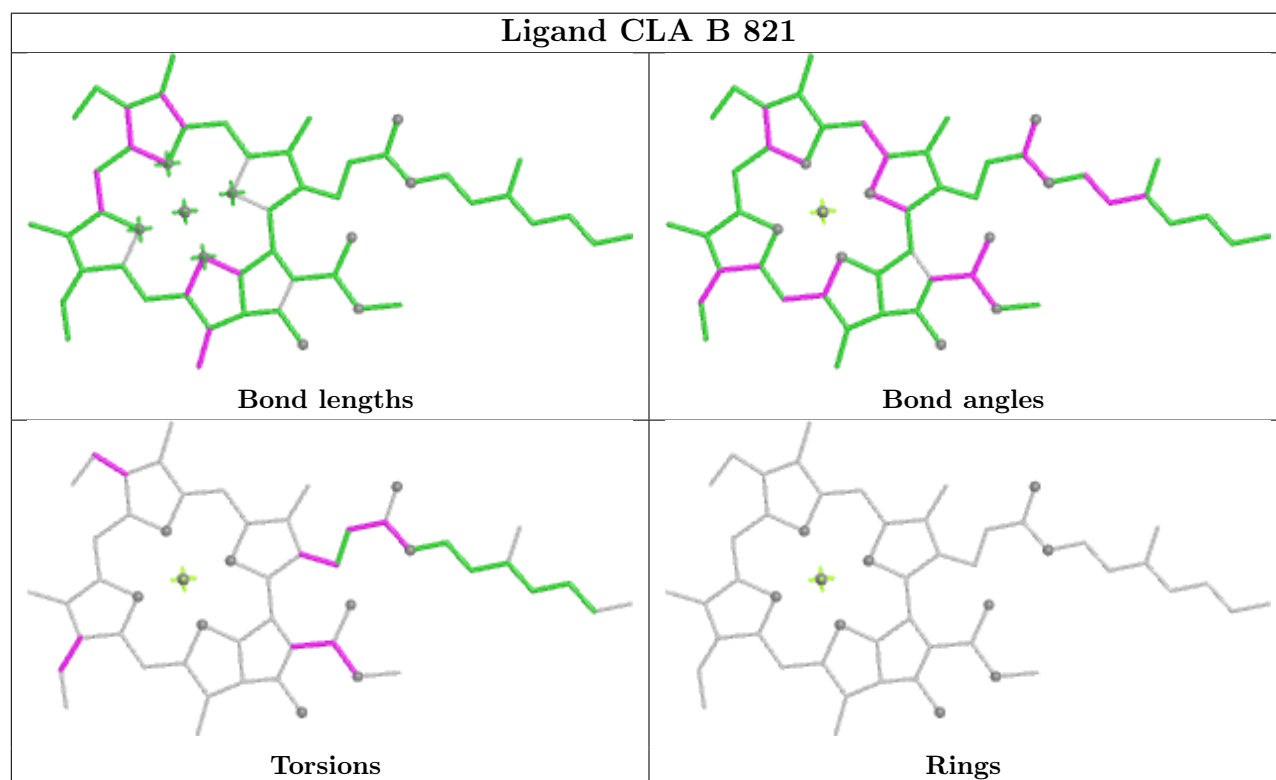
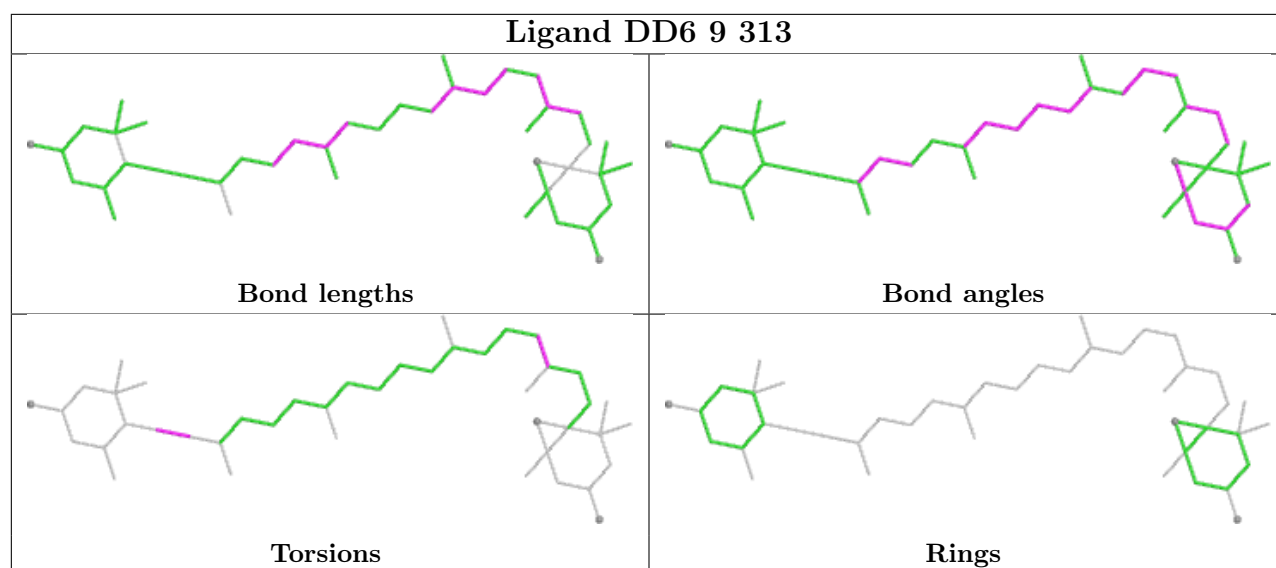


Torsions

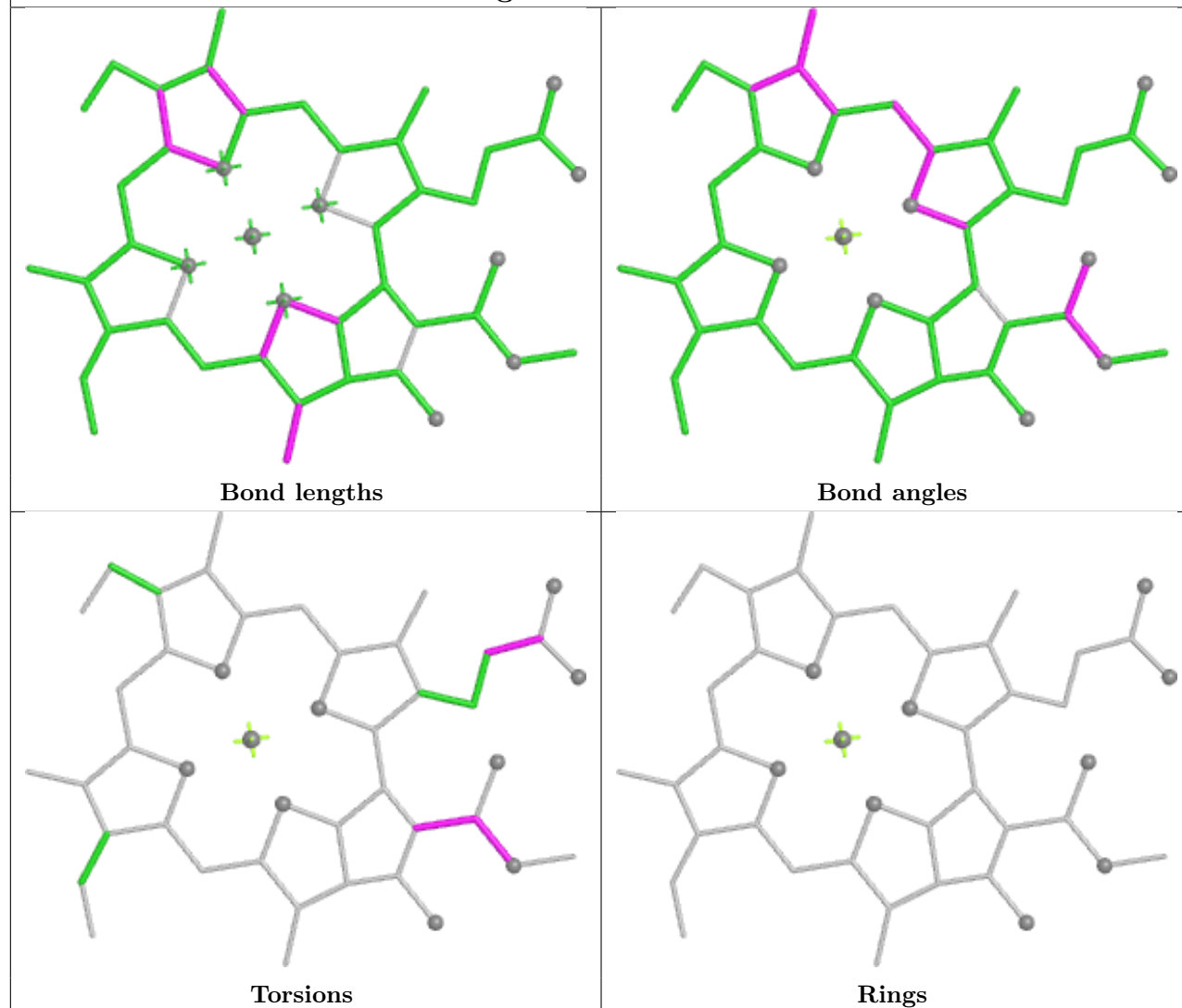


Rings

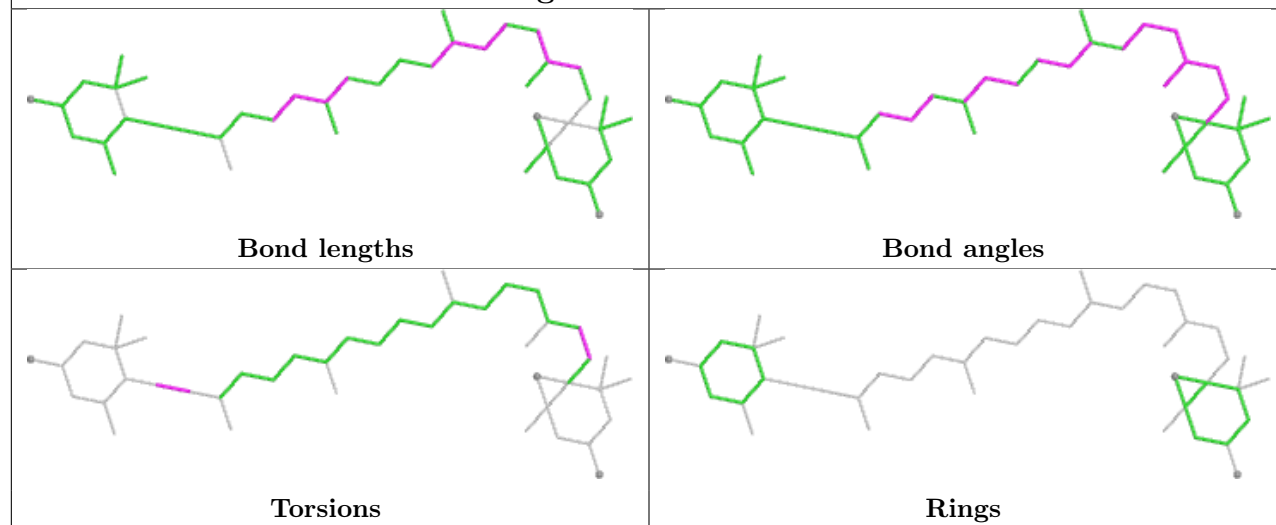
Ligand DD6 3 313**Ligand CLA A 821**

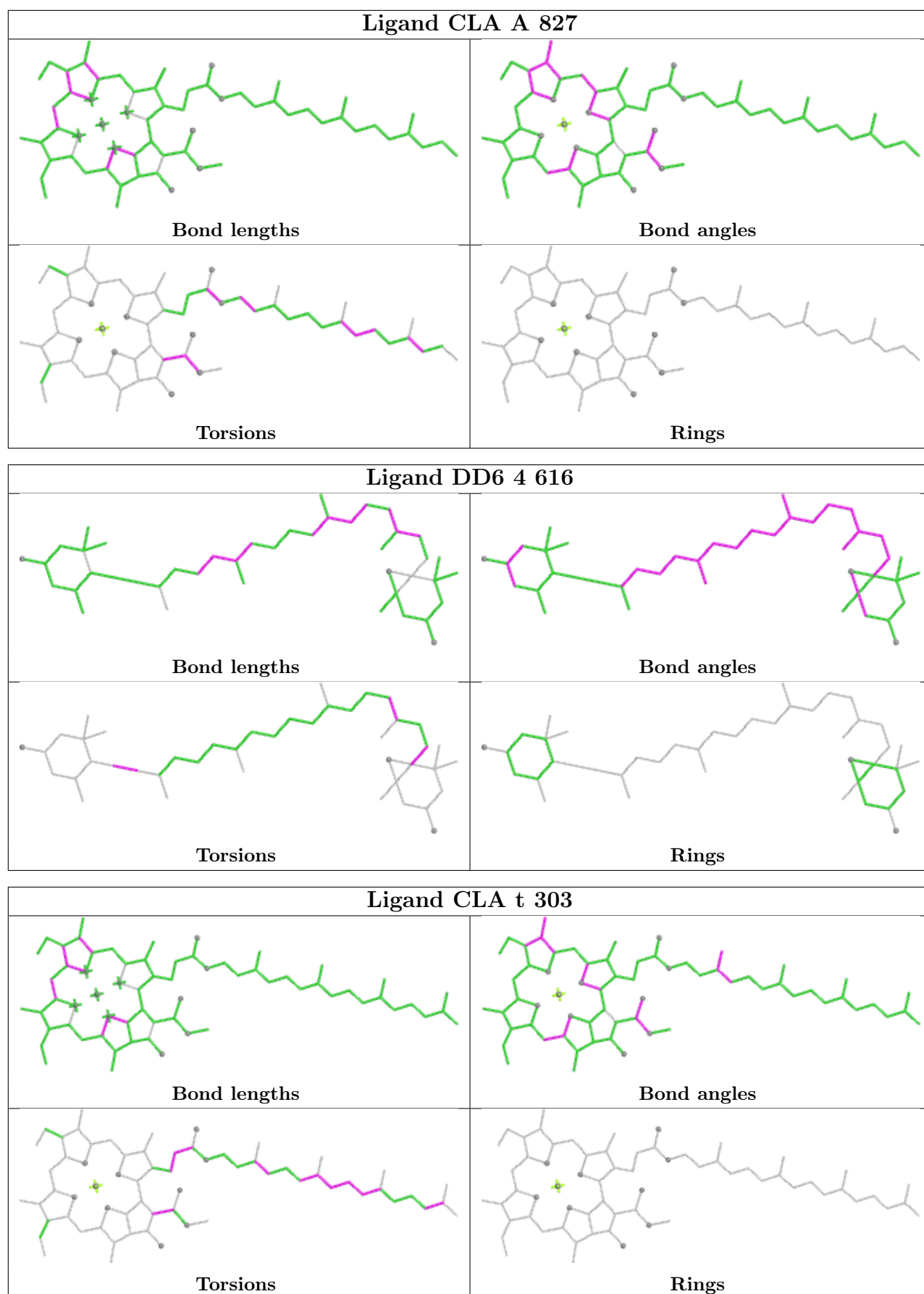


Ligand CLA 8 208

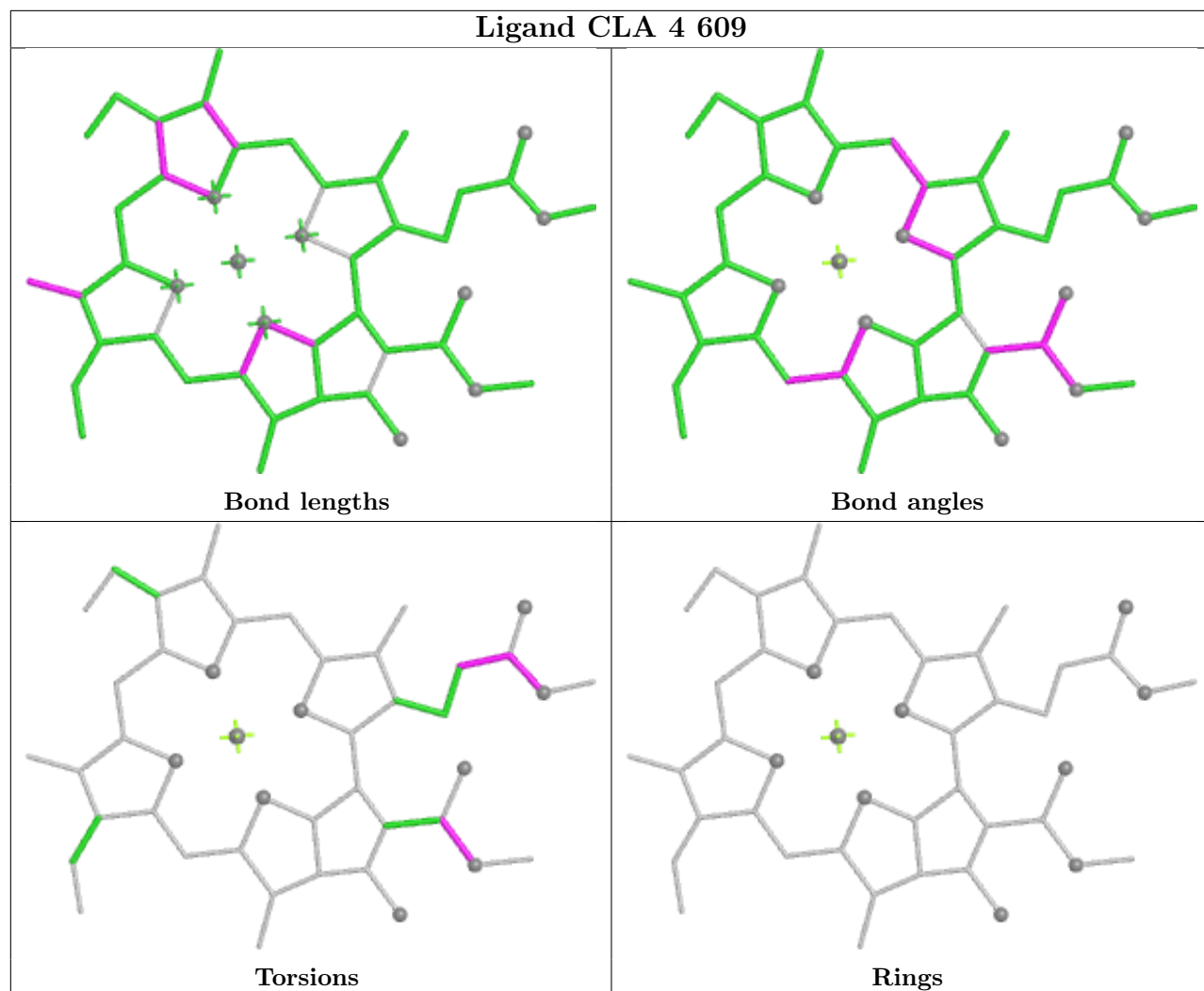


Ligand DD6 6 613

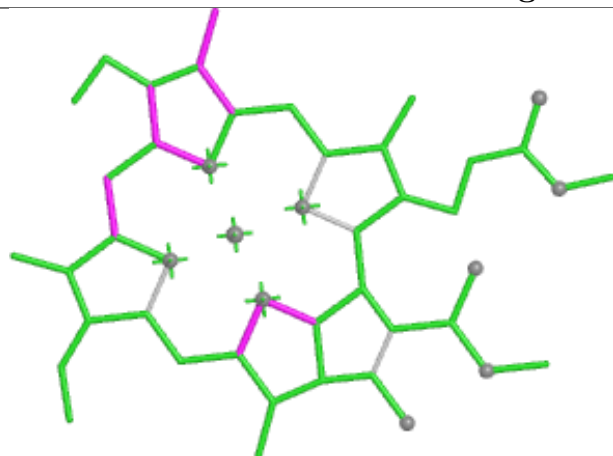




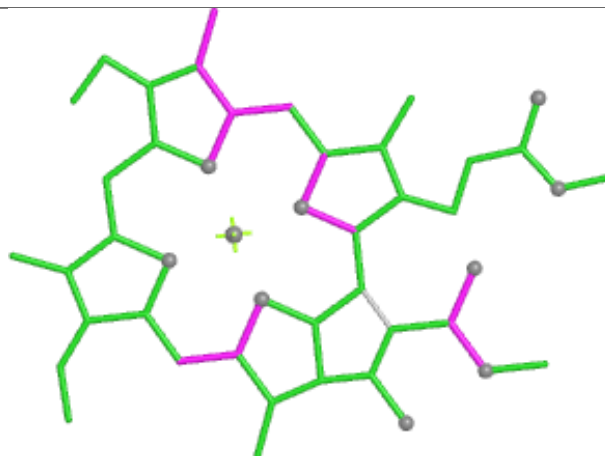
Ligand CLA 4 609



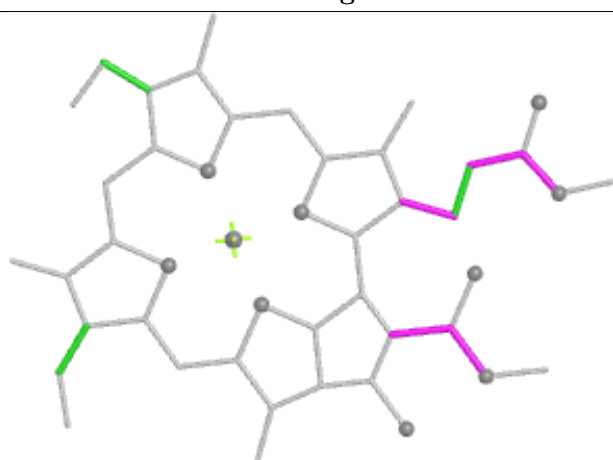
Ligand CLA 4 604



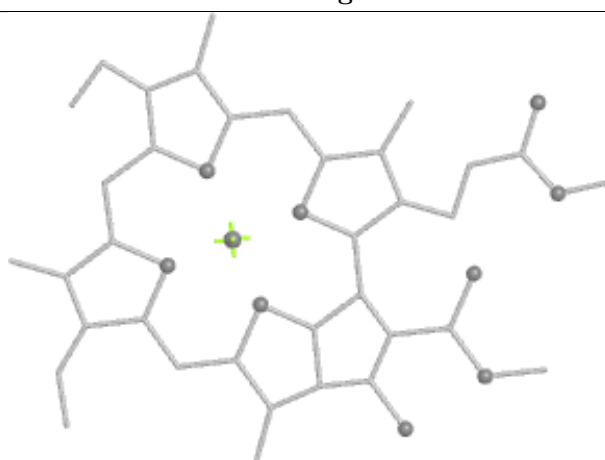
Bond lengths



Bond angles

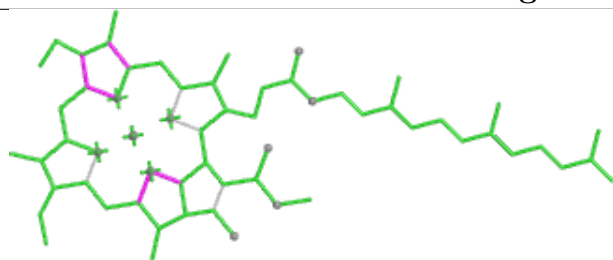


Torsions

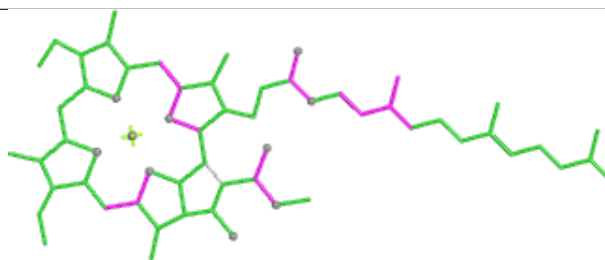


Rings

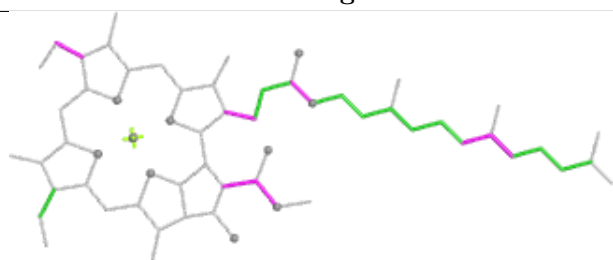
Ligand CLA c 609



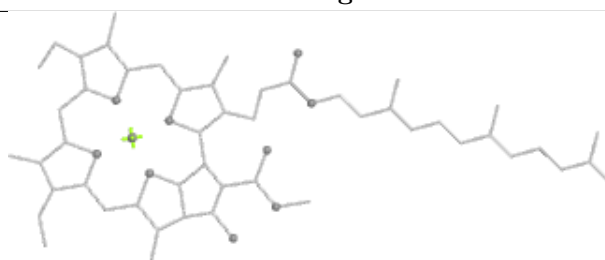
Bond lengths



Bond angles

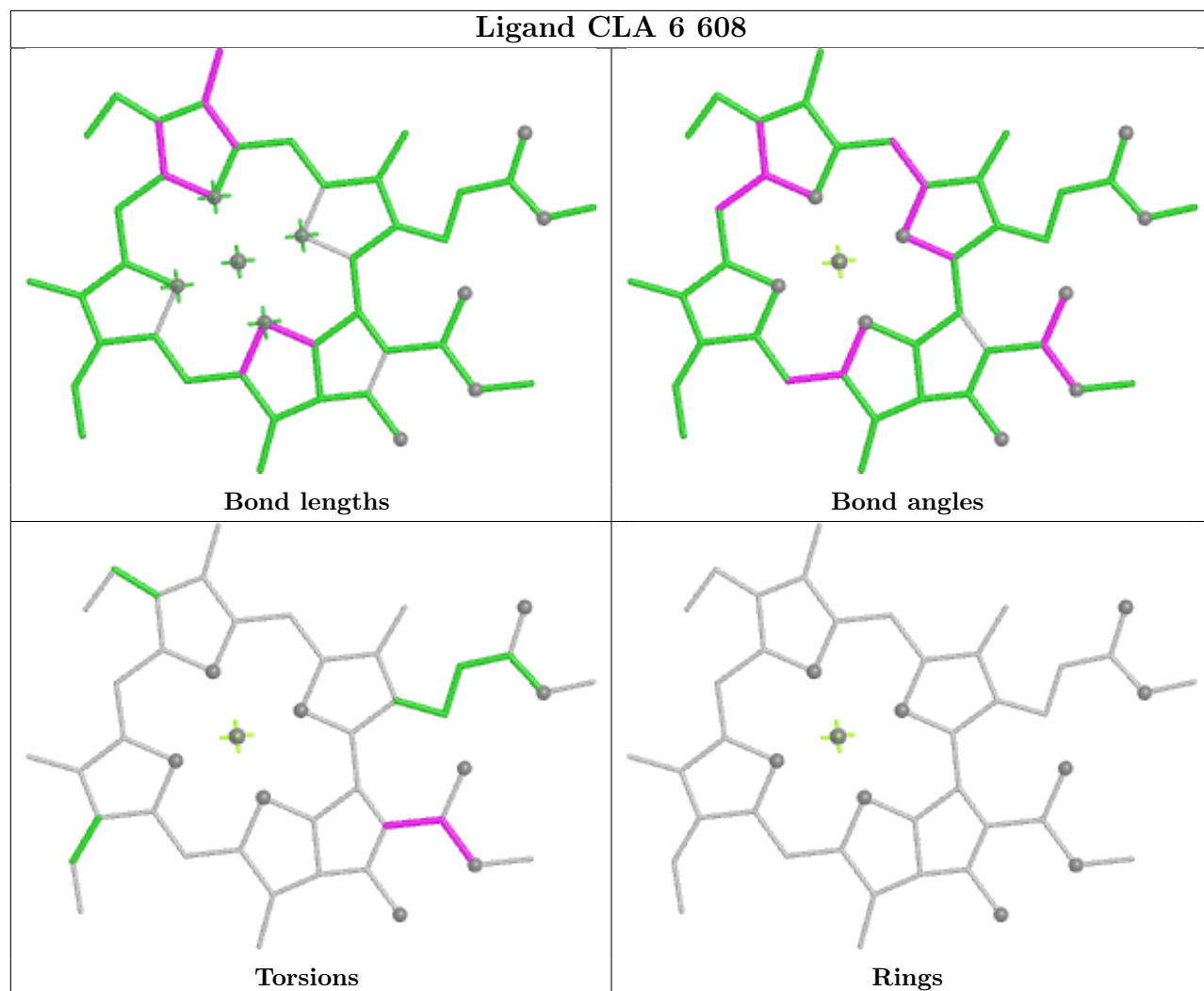


Torsions

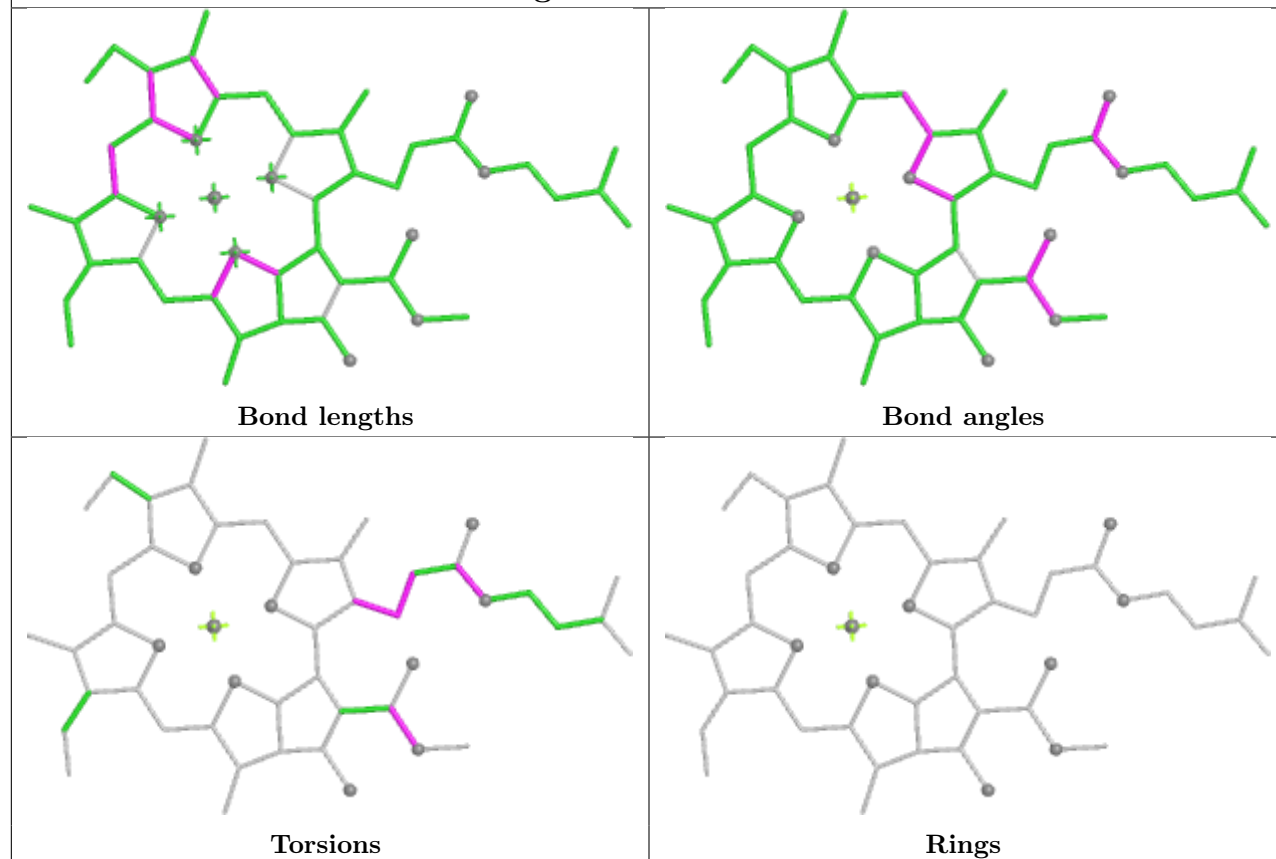


Rings

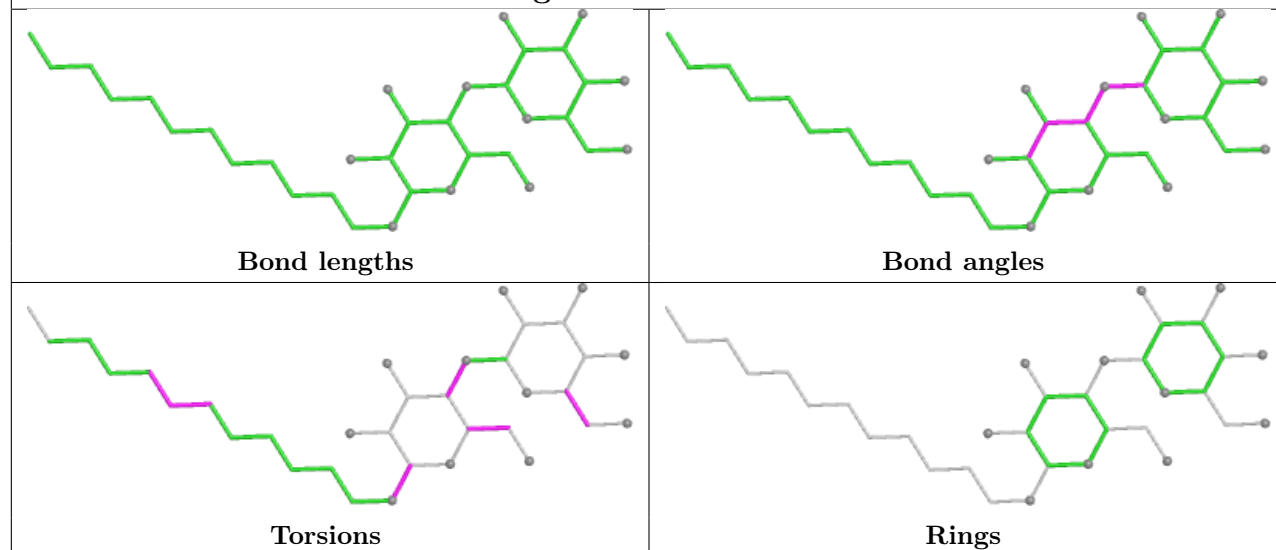
Ligand CLA 6 608



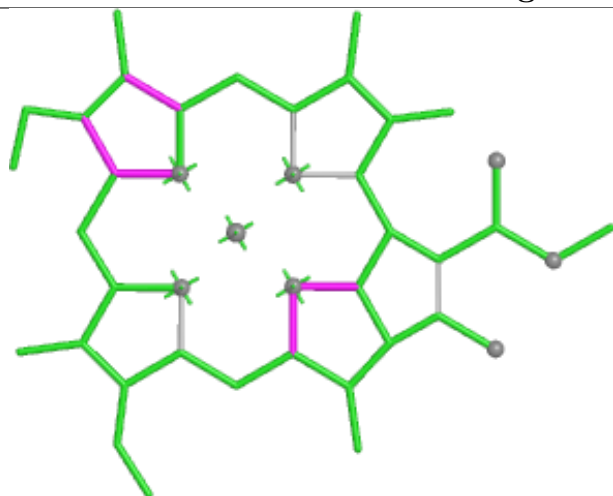
Ligand CLA F 203



Ligand LMT 1 316



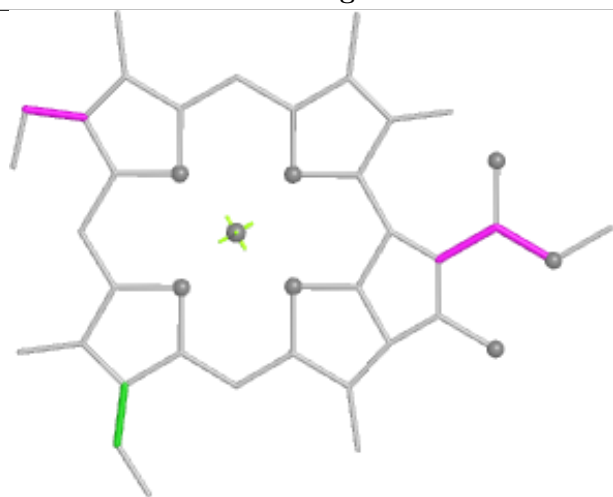
Ligand CLA k 308



Bond lengths



Bond angles

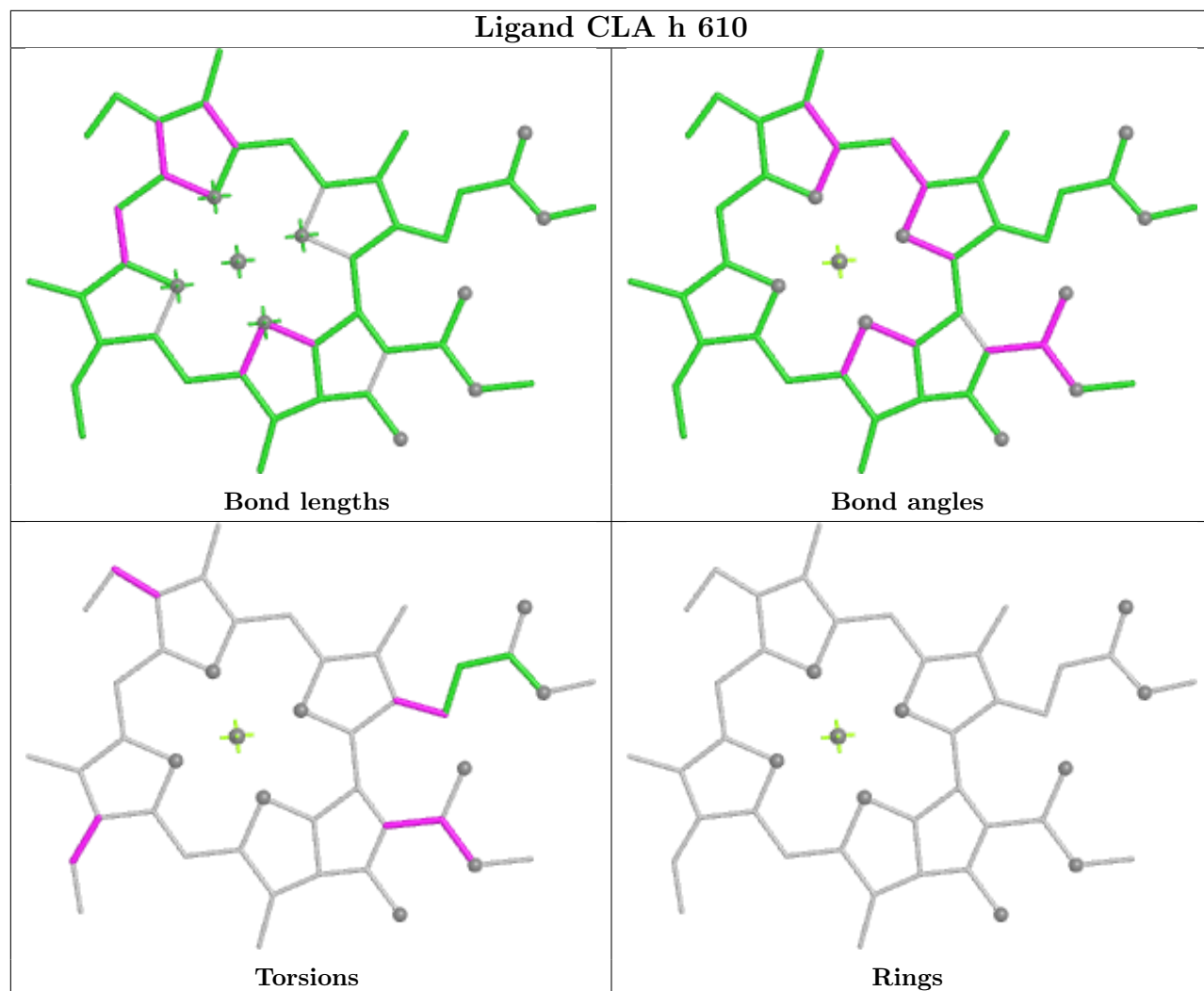


Torsions

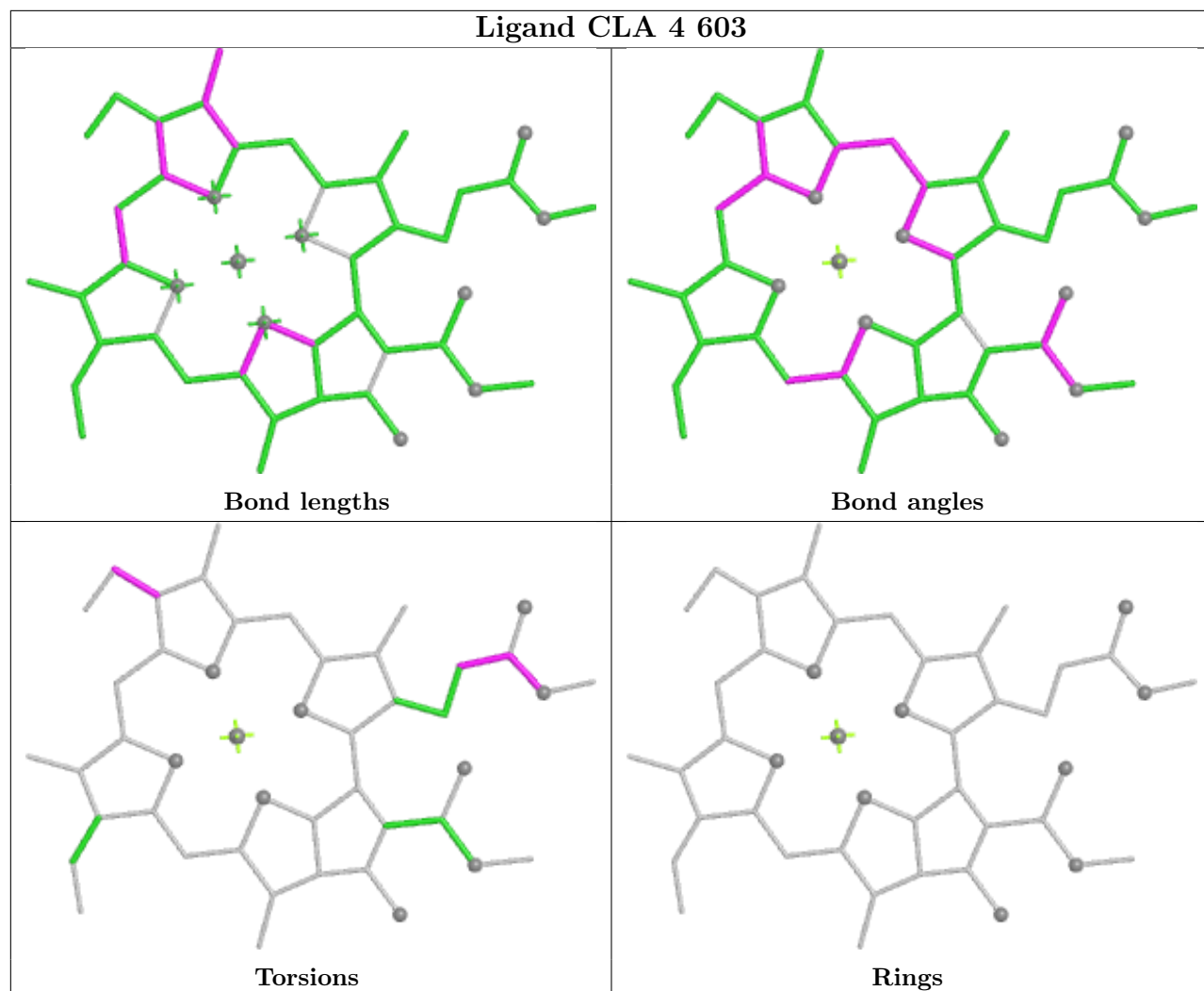


Rings

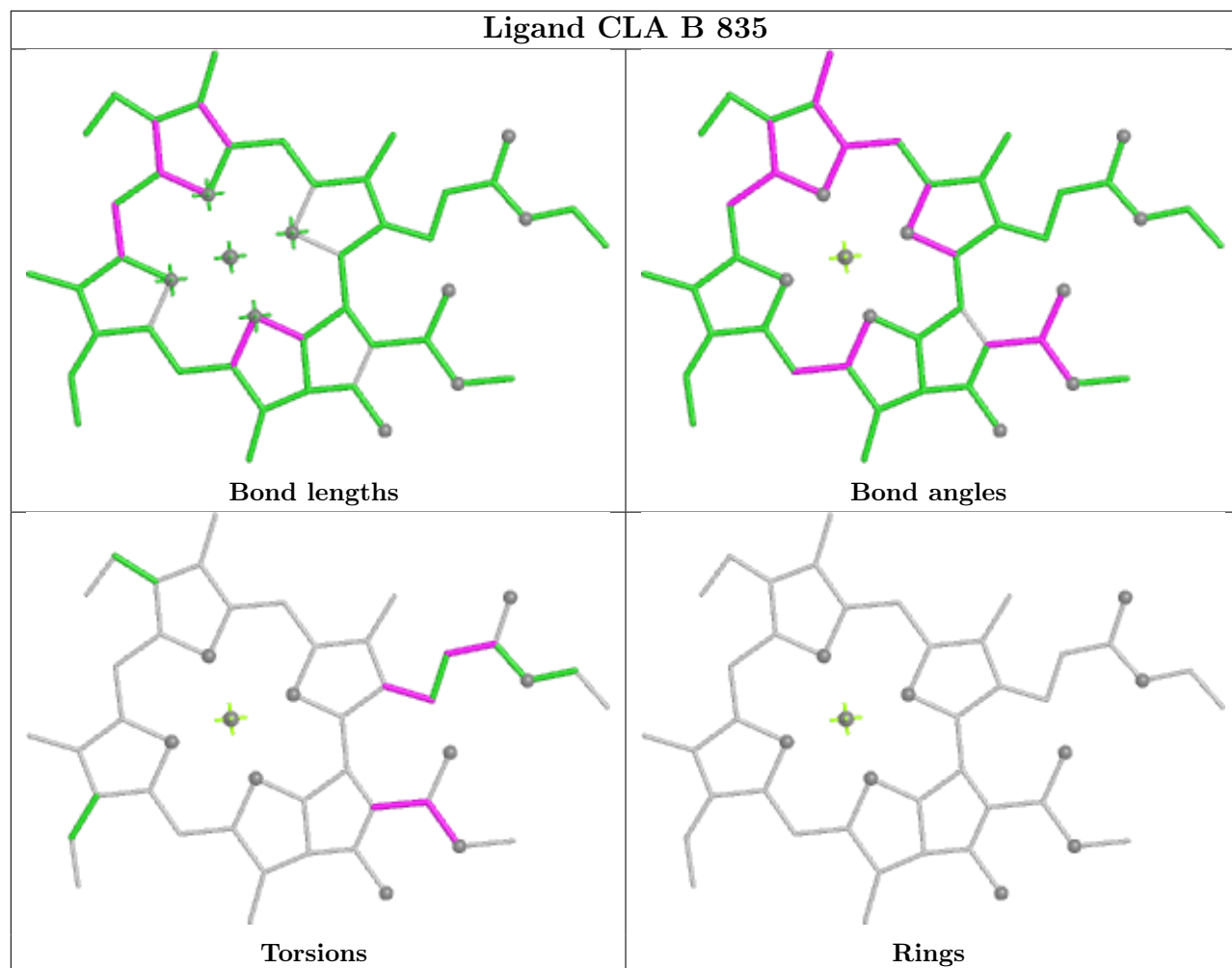
Ligand CLA h 610



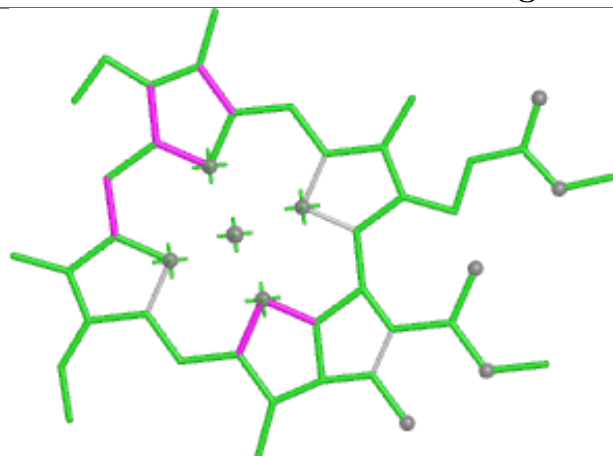
Ligand CLA 4 603



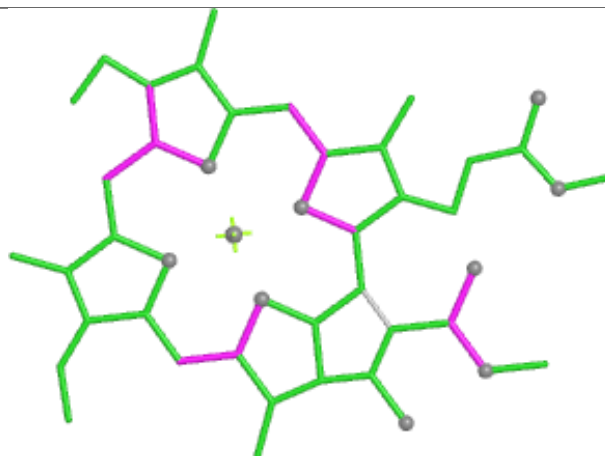
Ligand CLA B 835



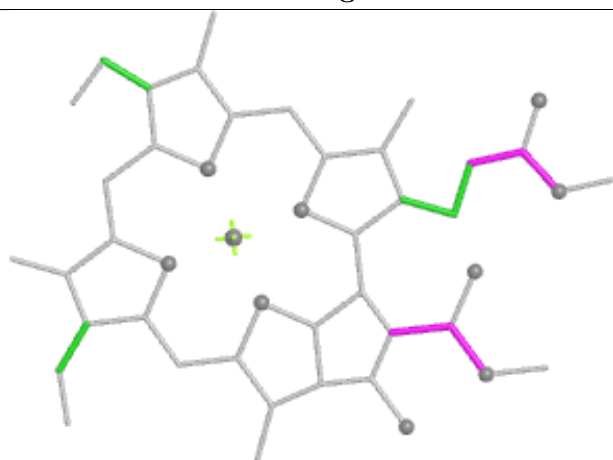
Ligand CLA 4 607



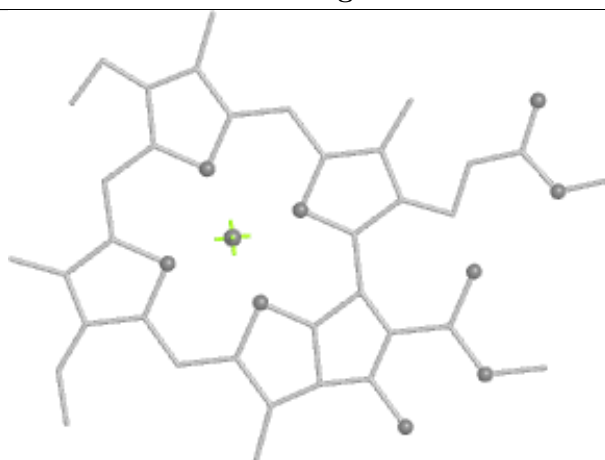
Bond lengths



Bond angles

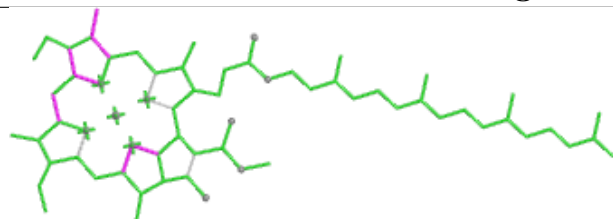


Torsions

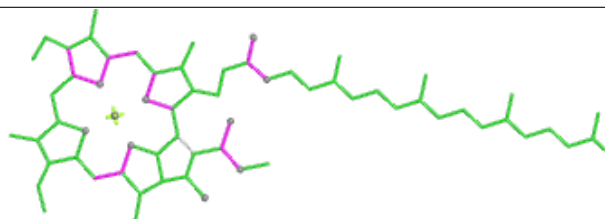


Rings

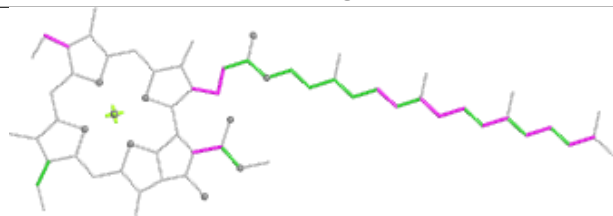
Ligand CLA B 836



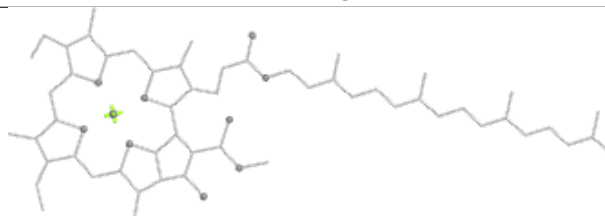
Bond lengths



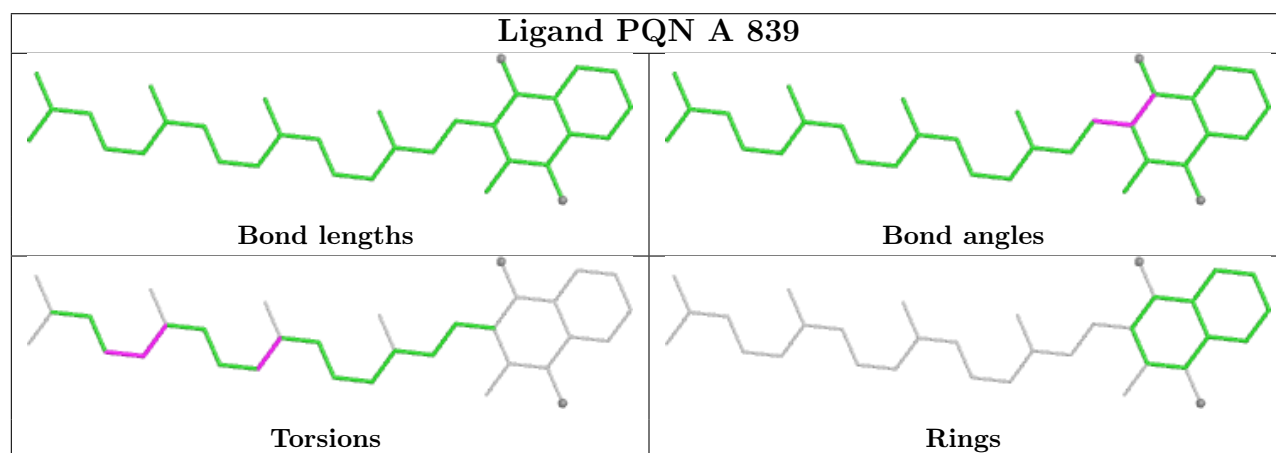
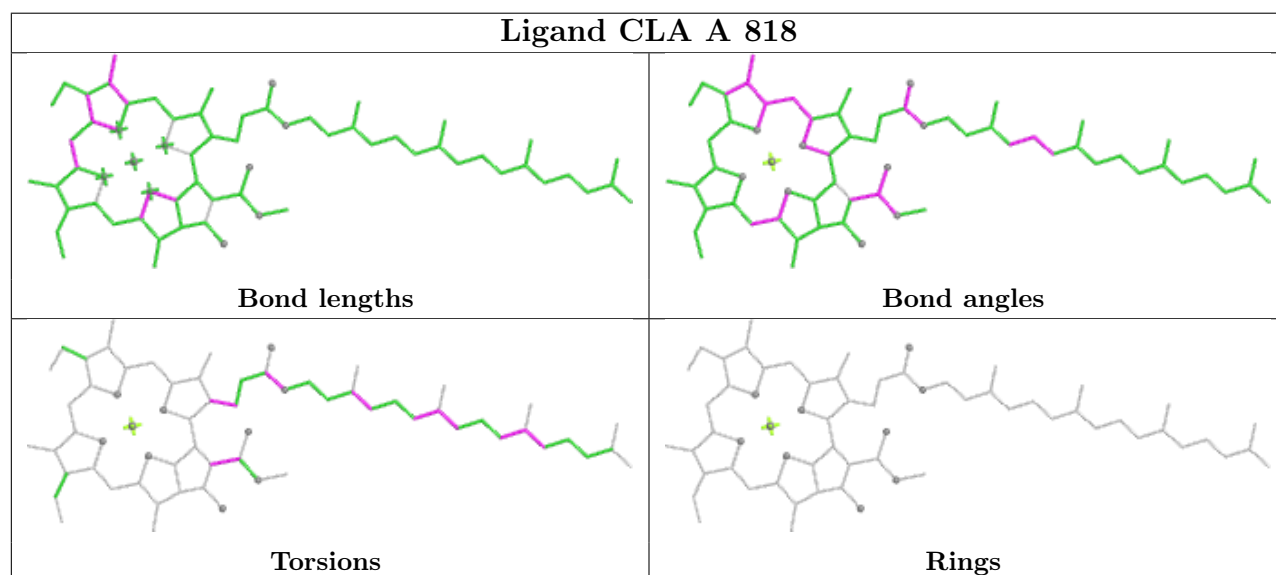
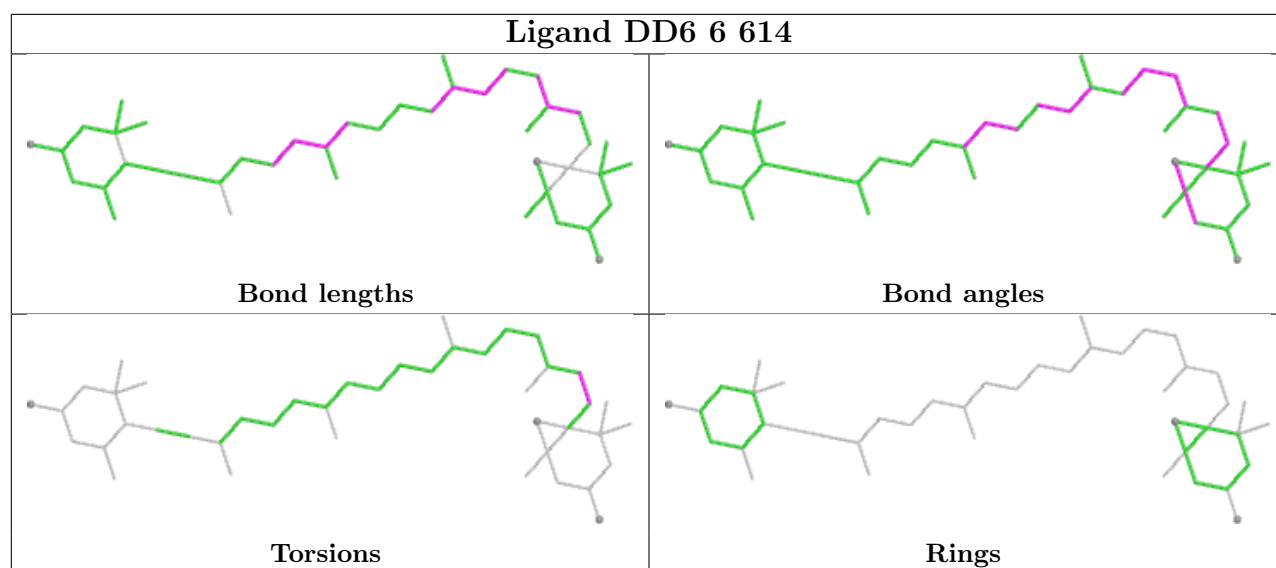
Bond angles

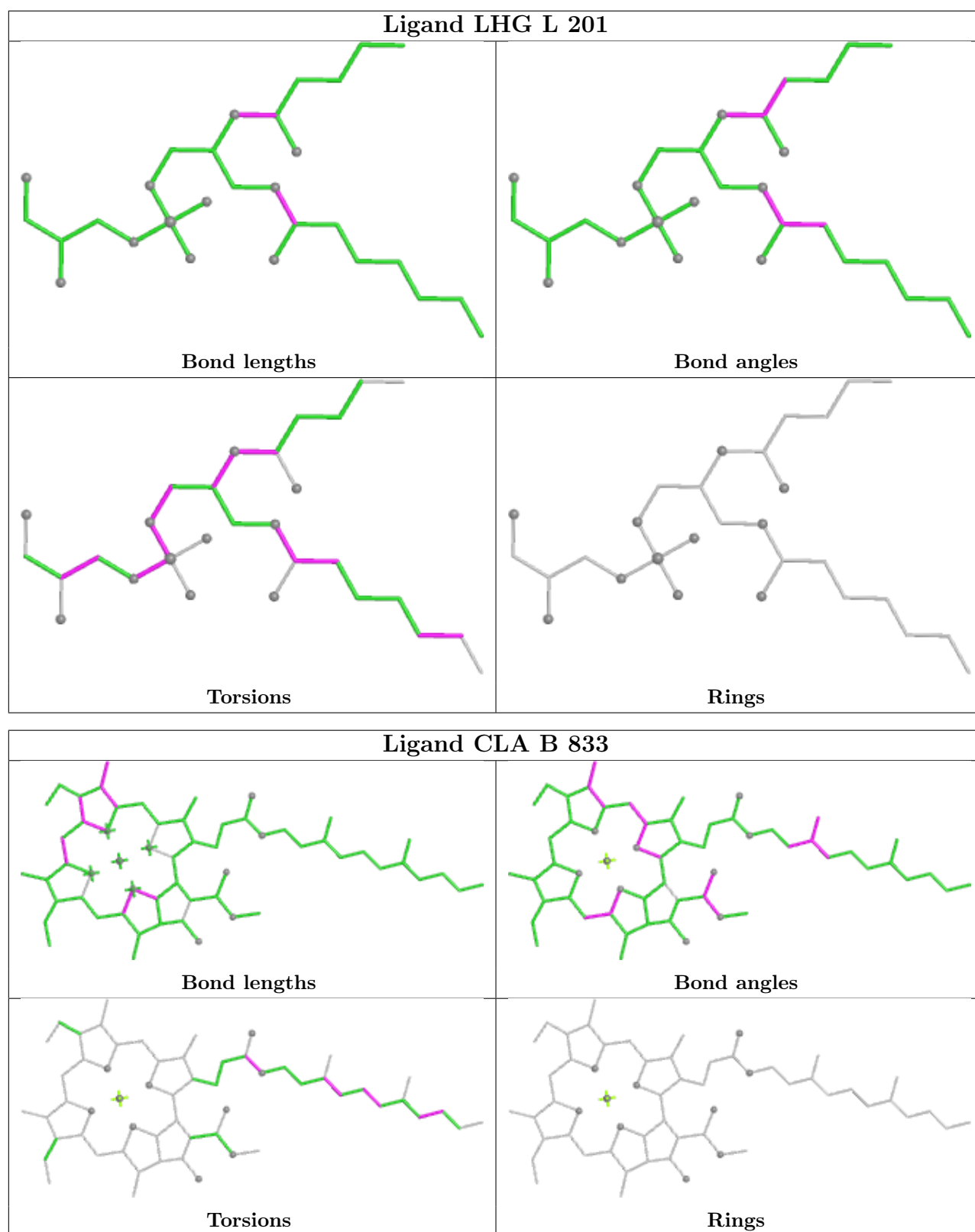


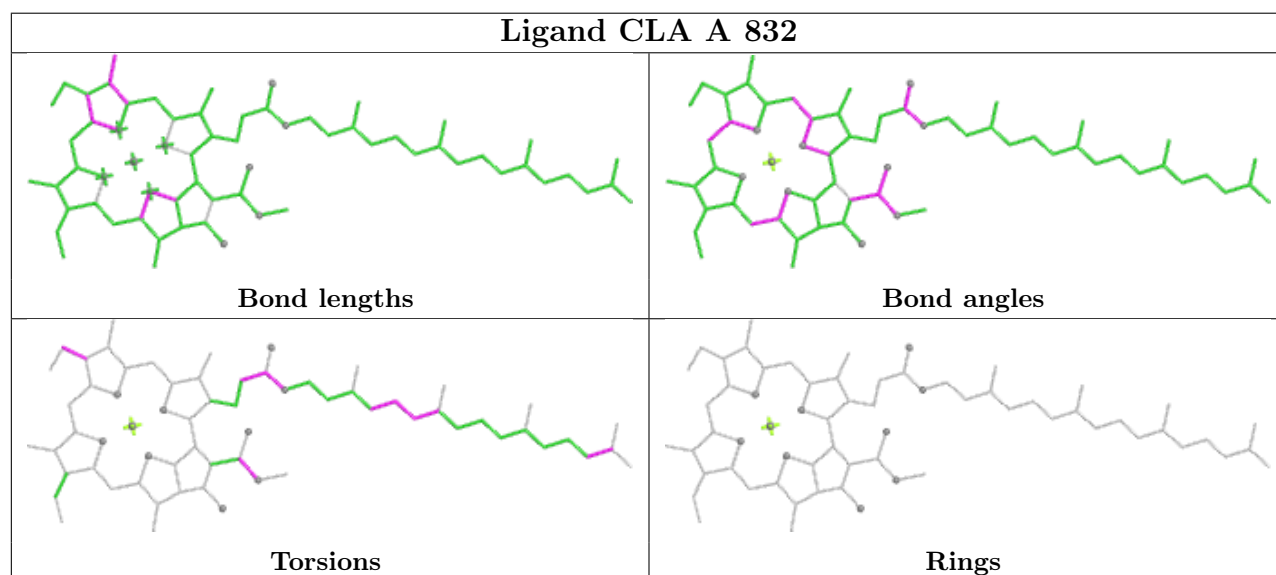
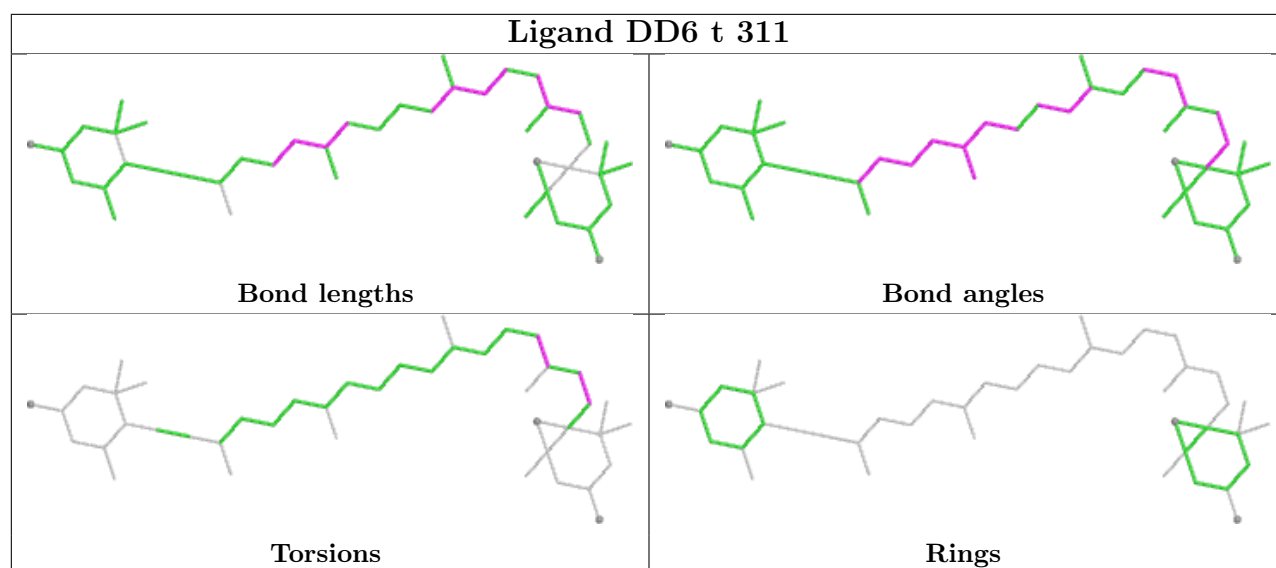
Torsions



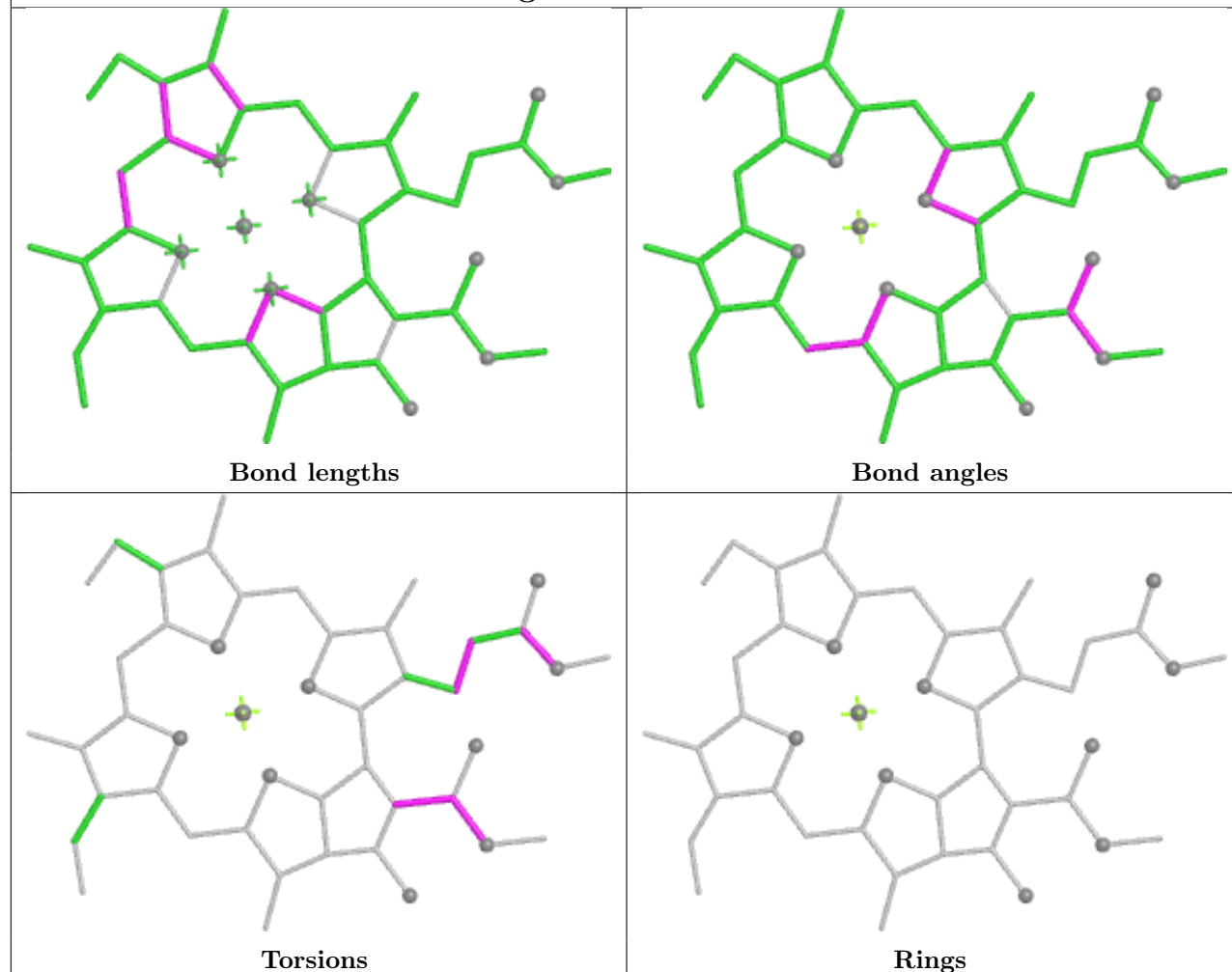
Rings



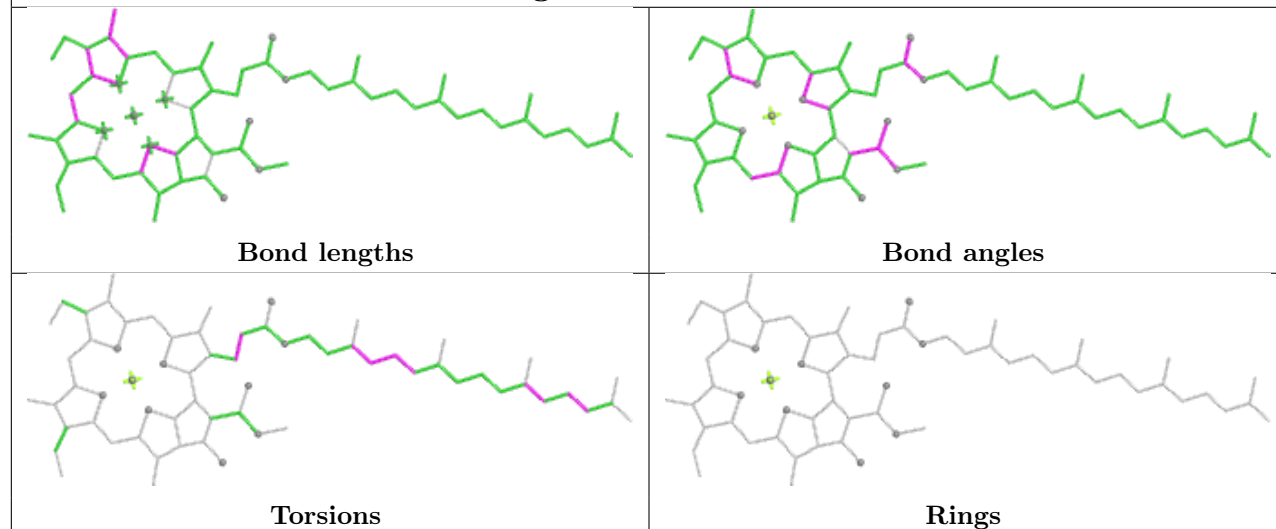




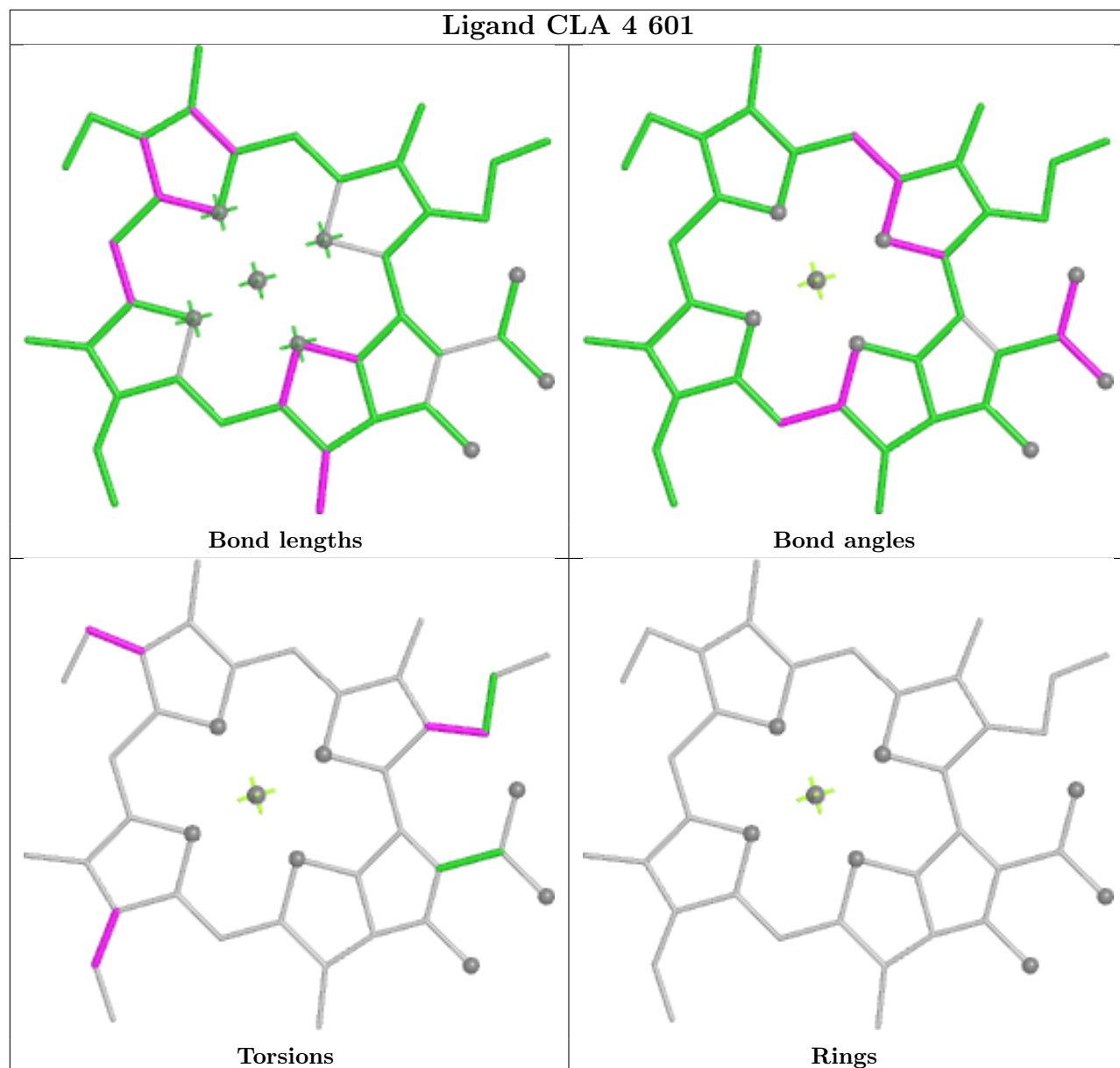
Ligand CLA c 606



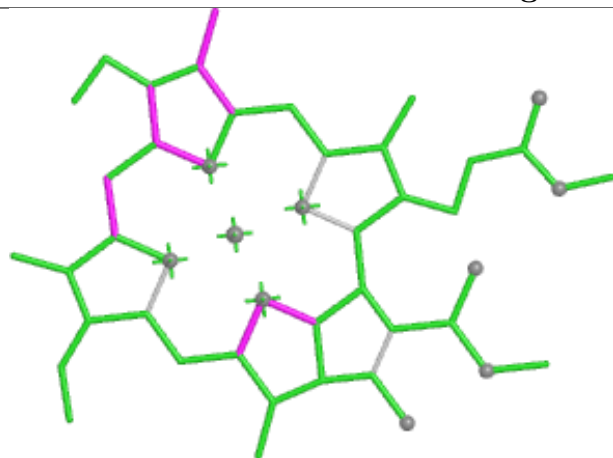
Ligand CLA B 807



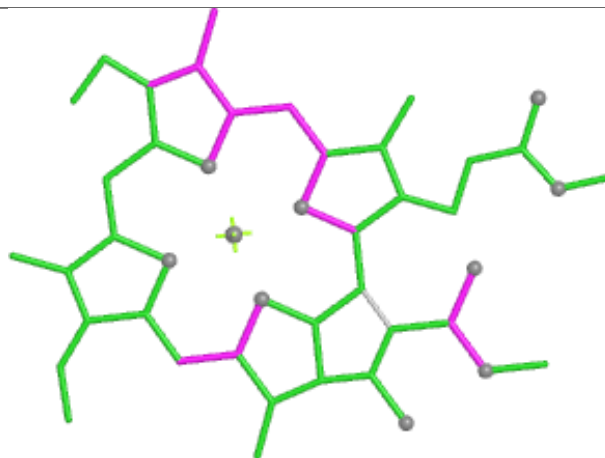
Ligand CLA 4 601



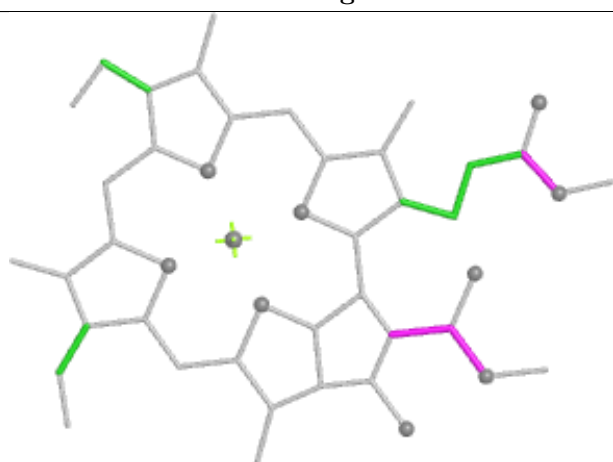
Ligand CLA t 305



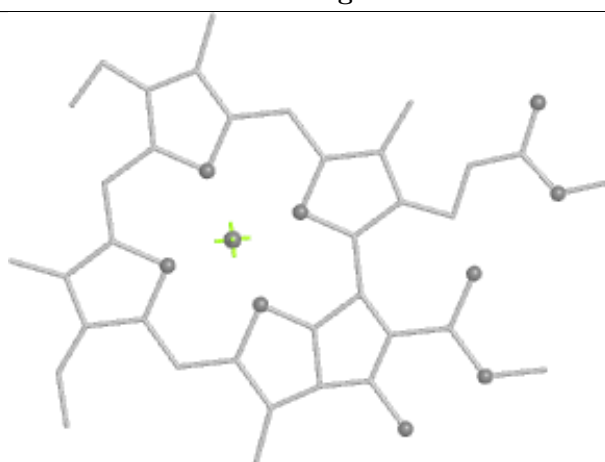
Bond lengths



Bond angles

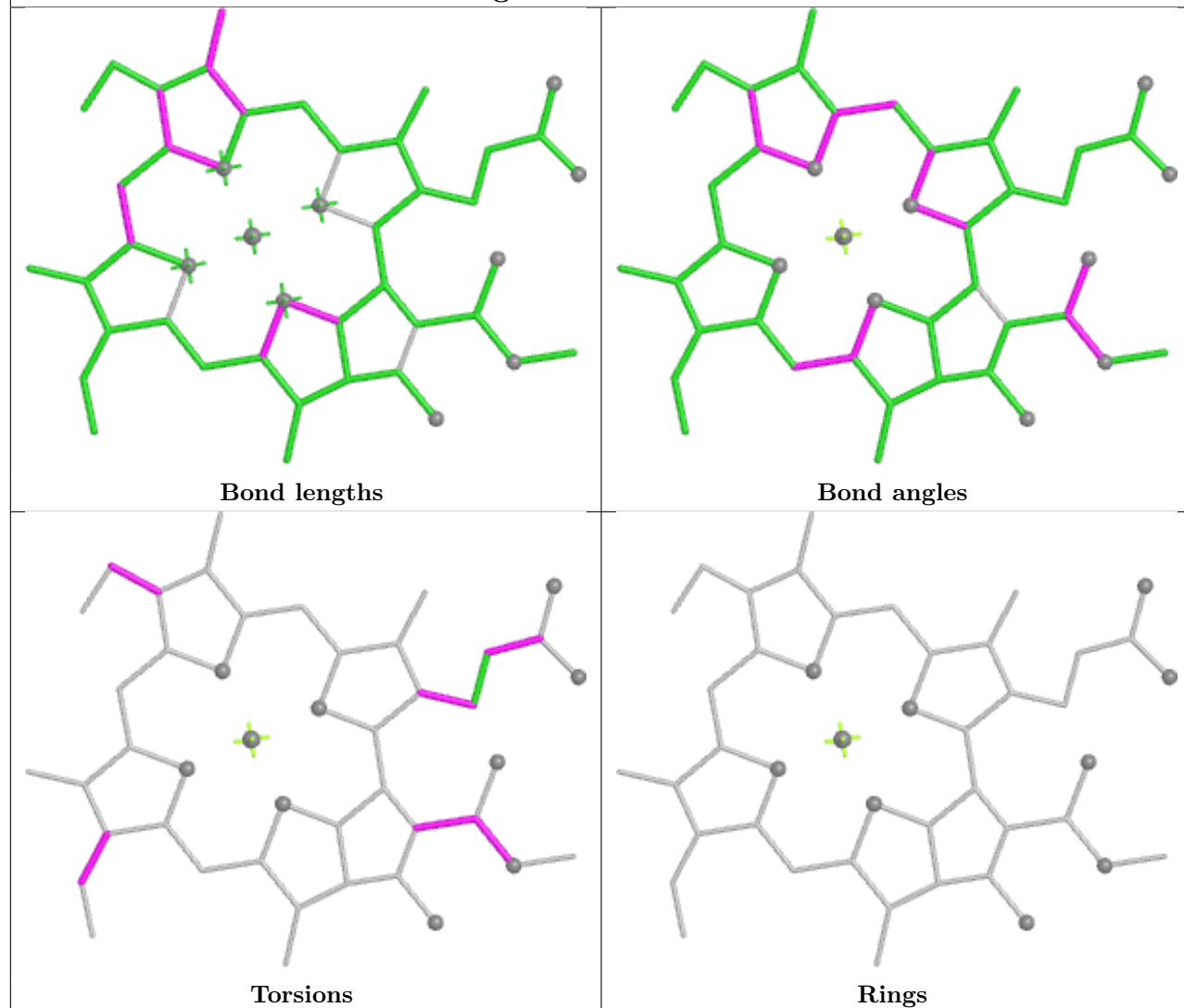


Torsions

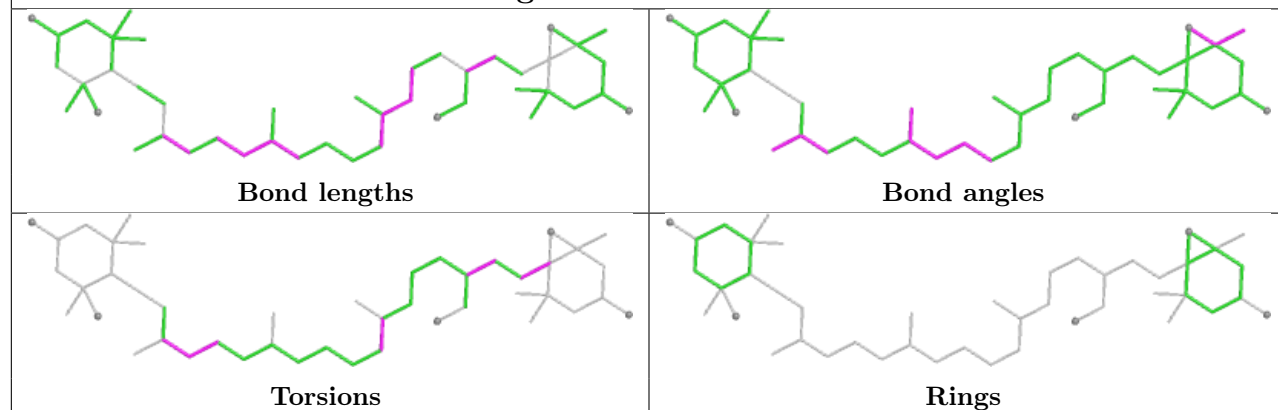


Rings

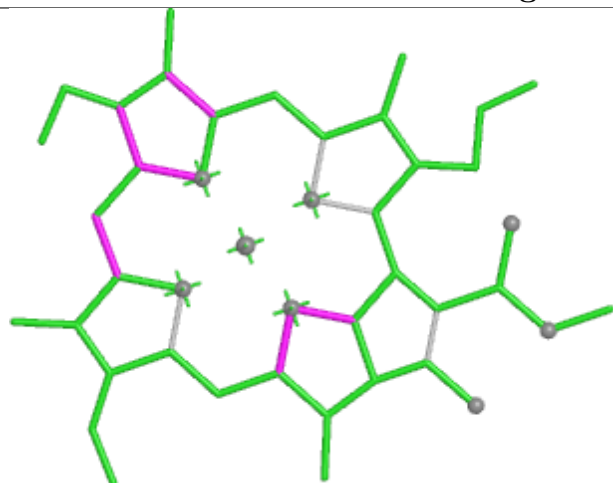
Ligand CLA B 832



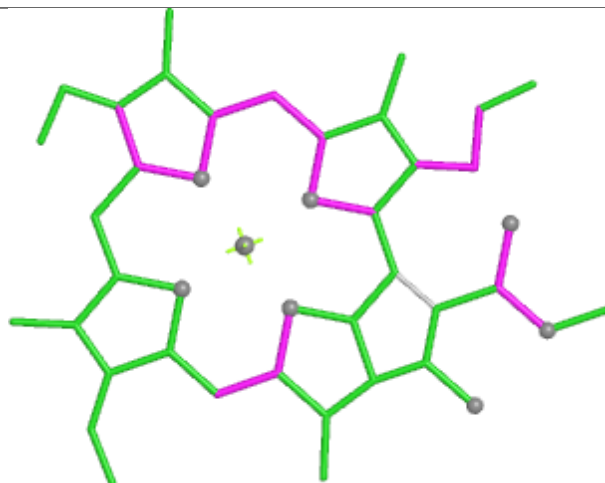
Ligand A1L1G k 312



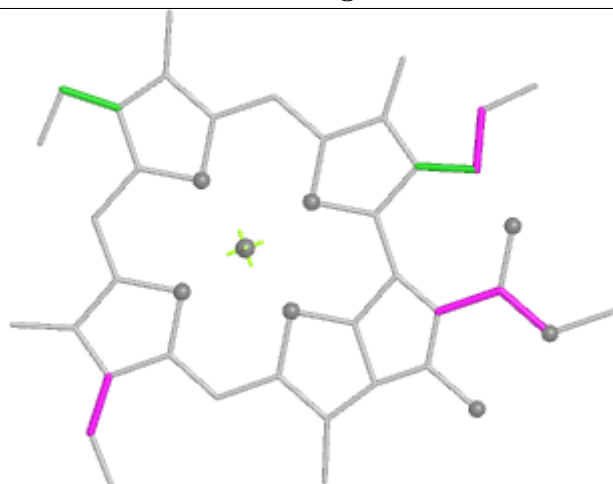
Ligand CLA c 601



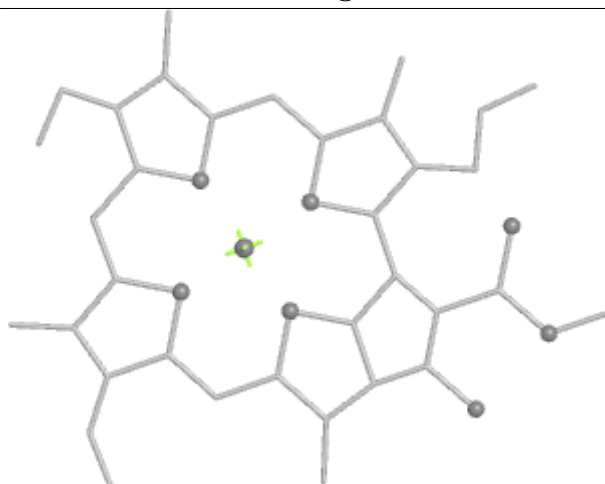
Bond lengths



Bond angles

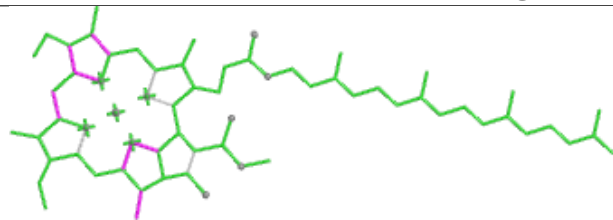


Torsions

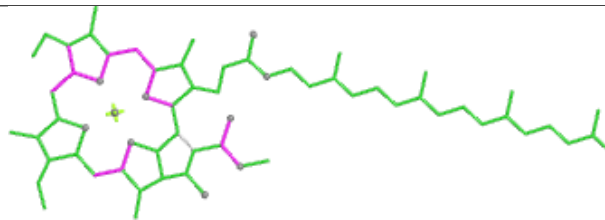


Rings

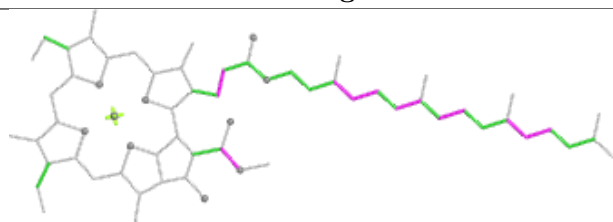
Ligand CLA A 828



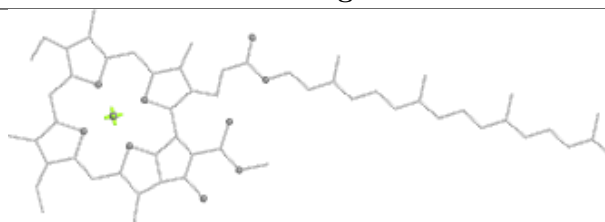
Bond lengths



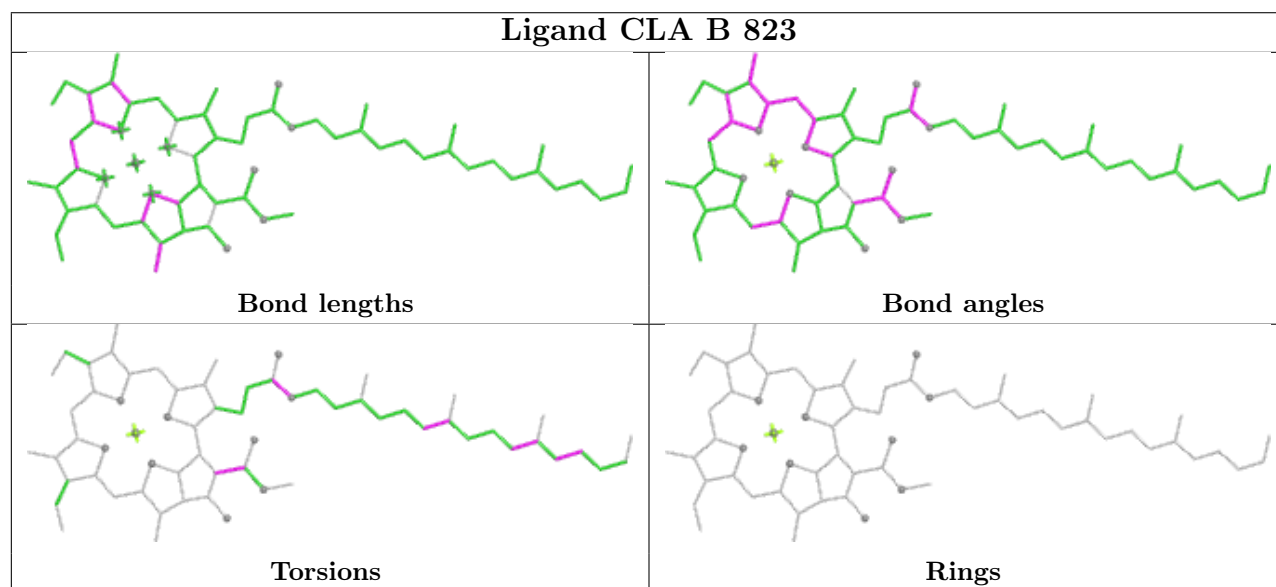
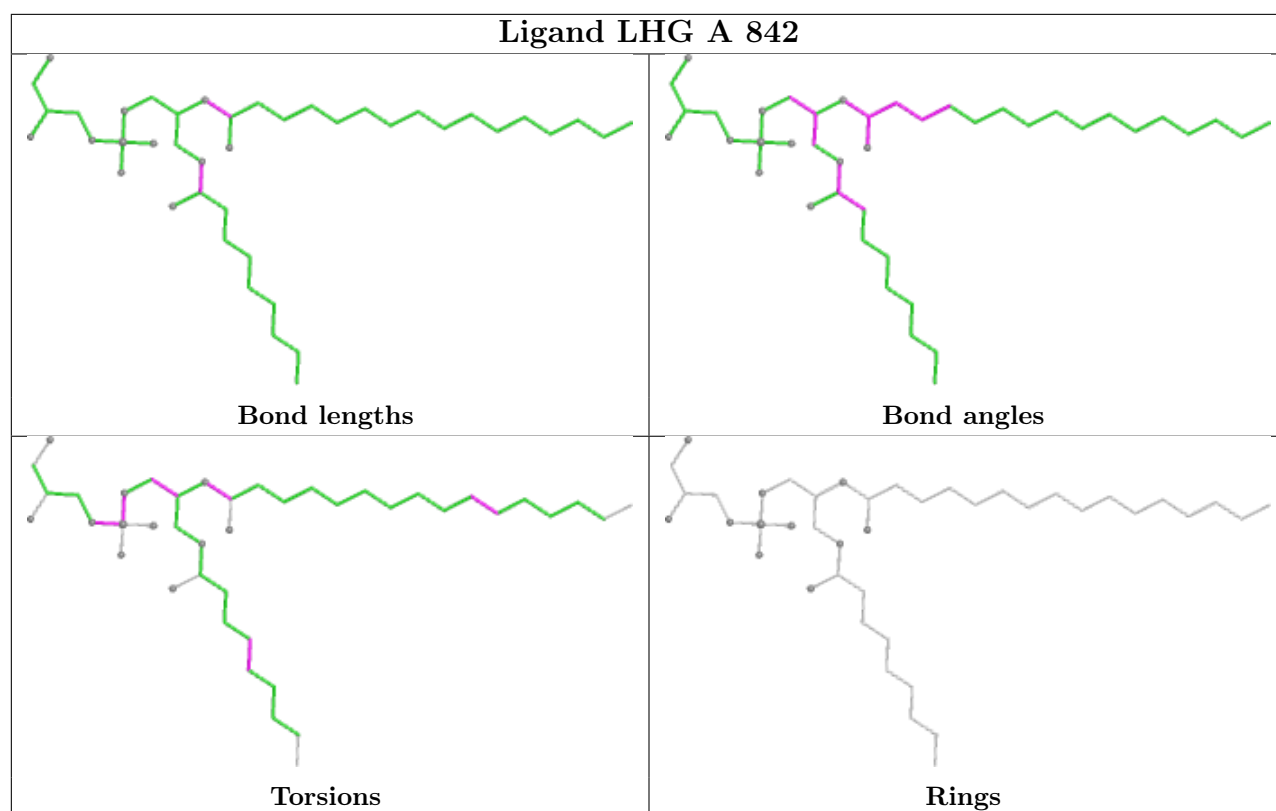
Bond angles



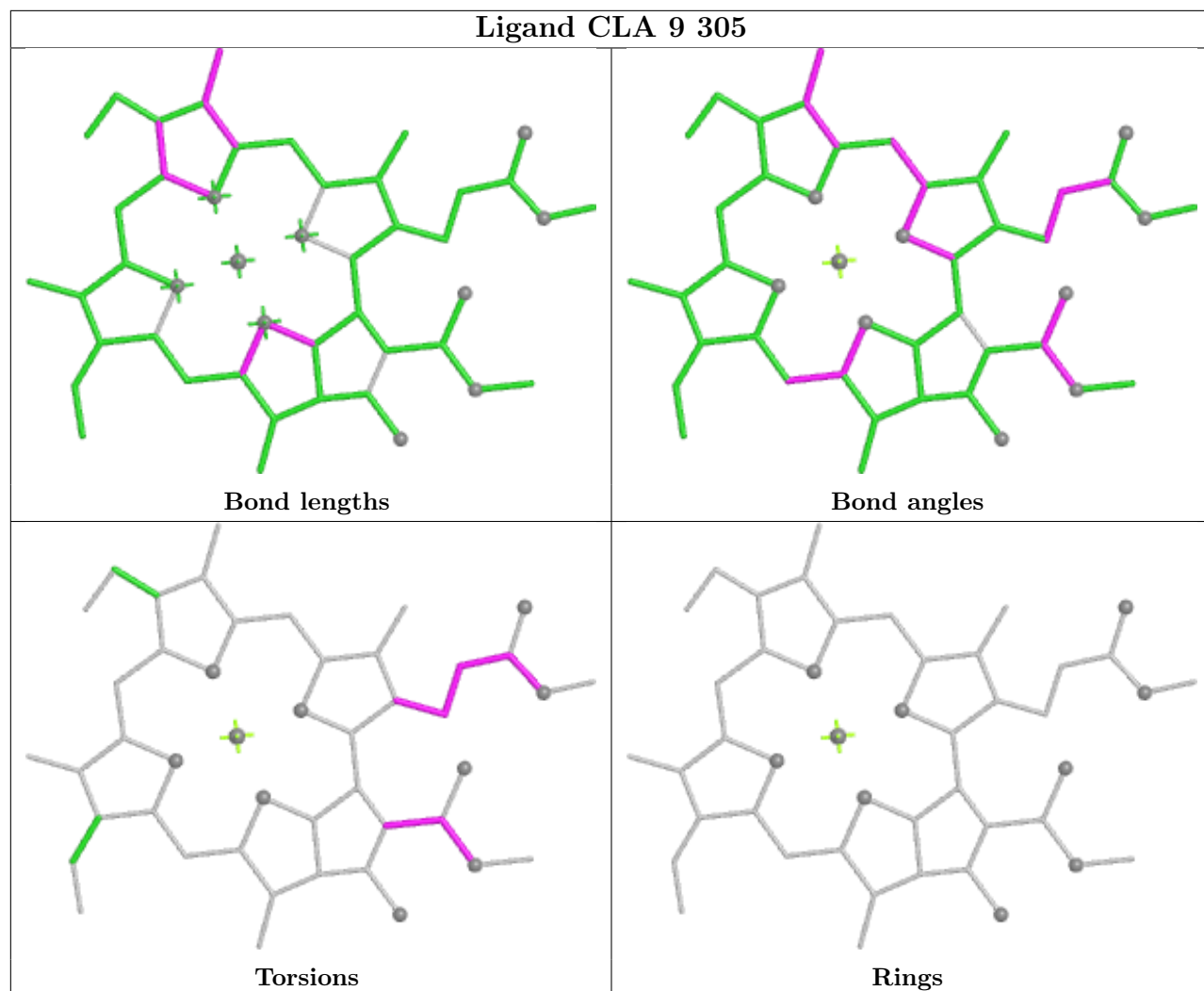
Torsions



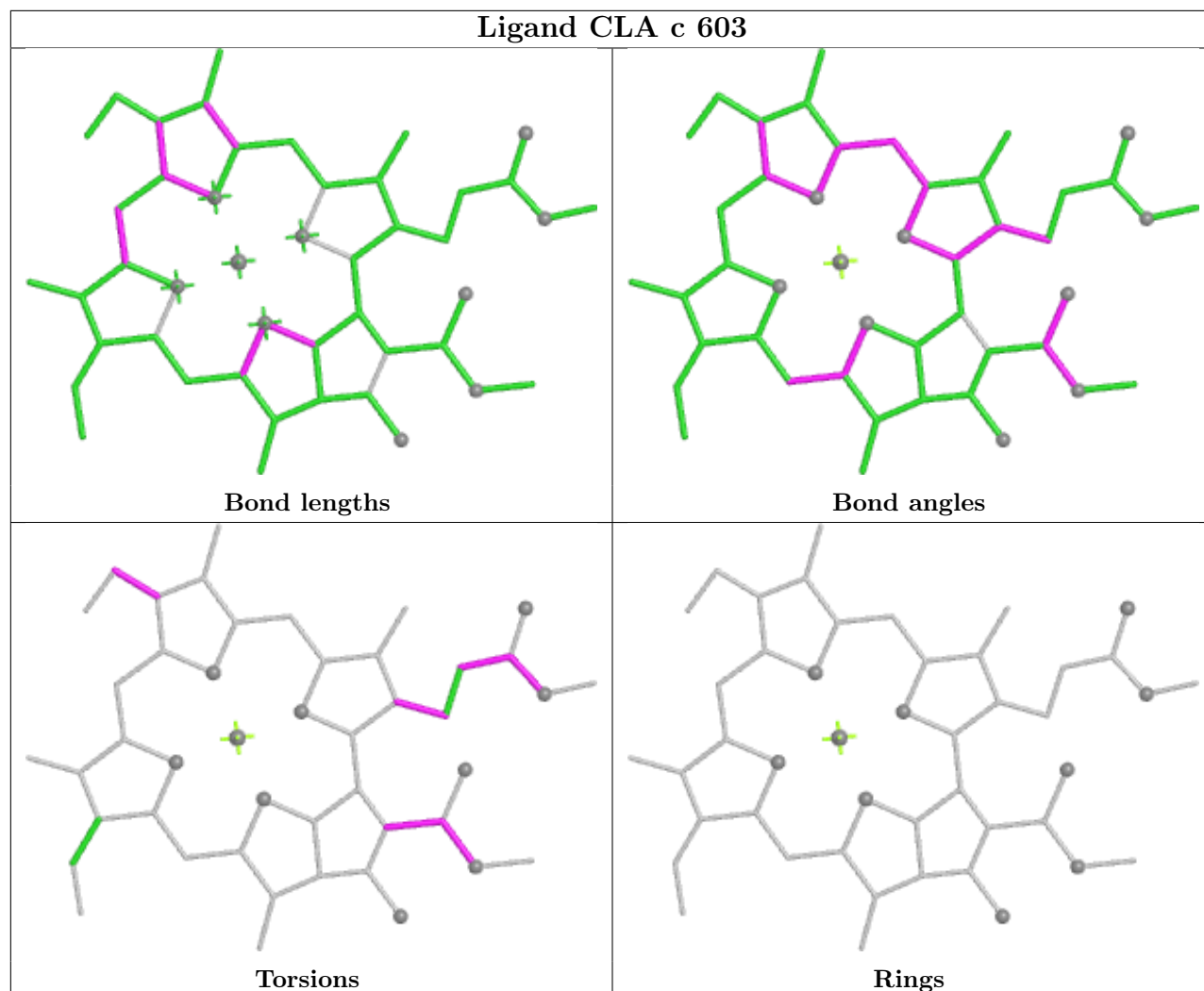
Rings



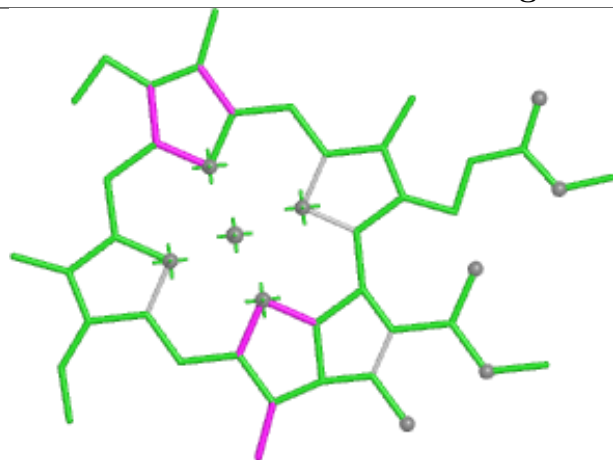
Ligand CLA 9 305



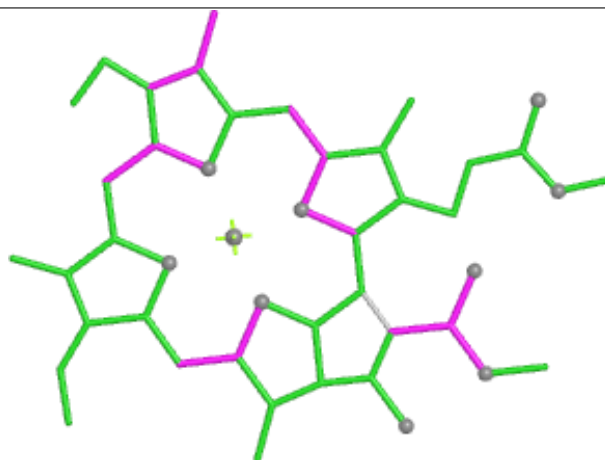
Ligand CLA c 603



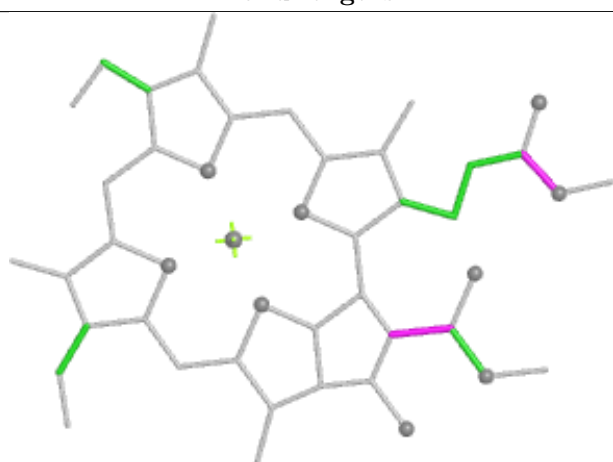
Ligand CLA c 607



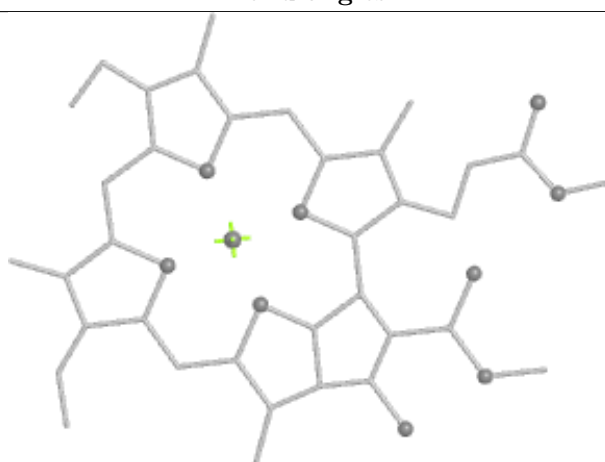
Bond lengths



Bond angles

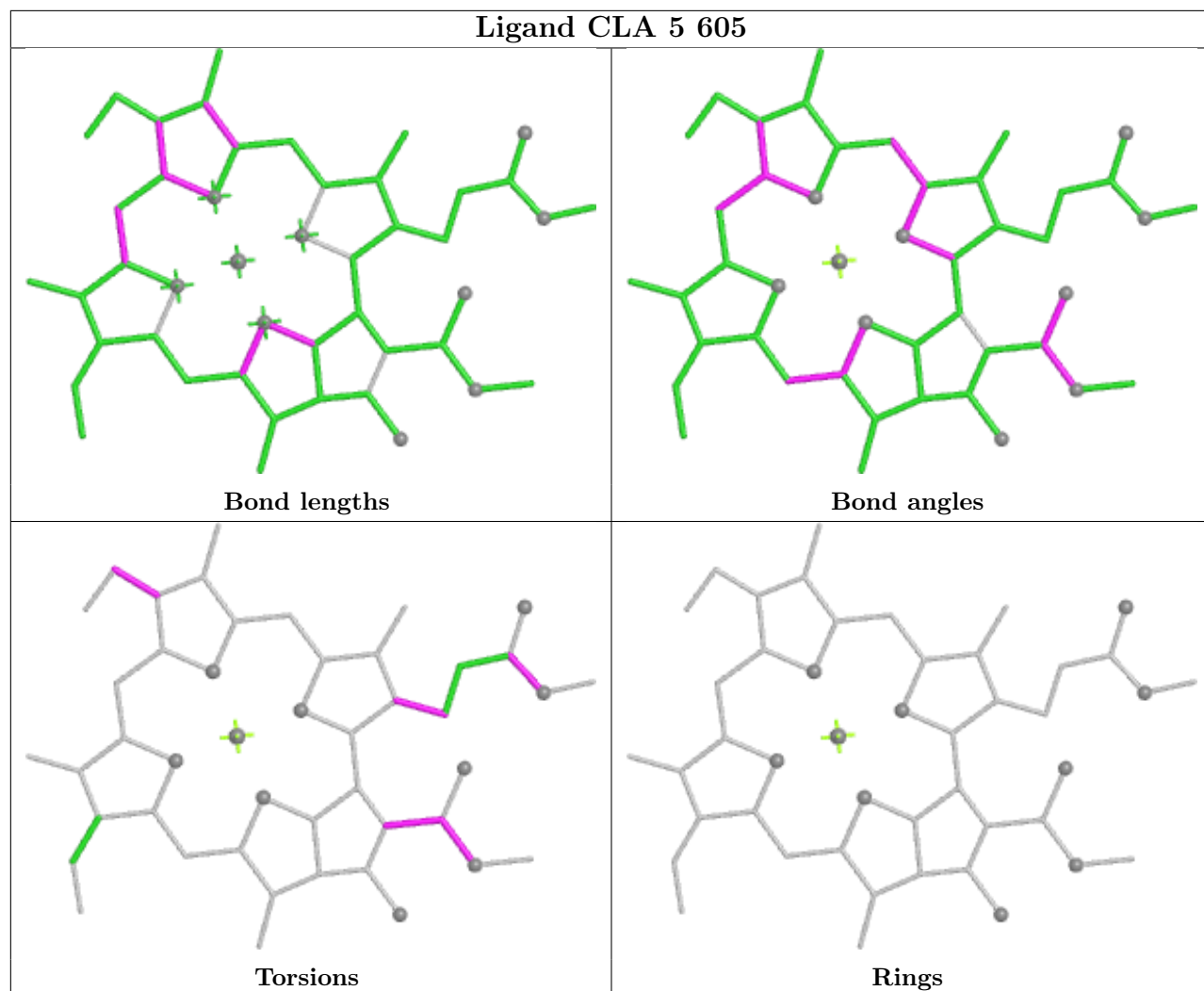


Torsions

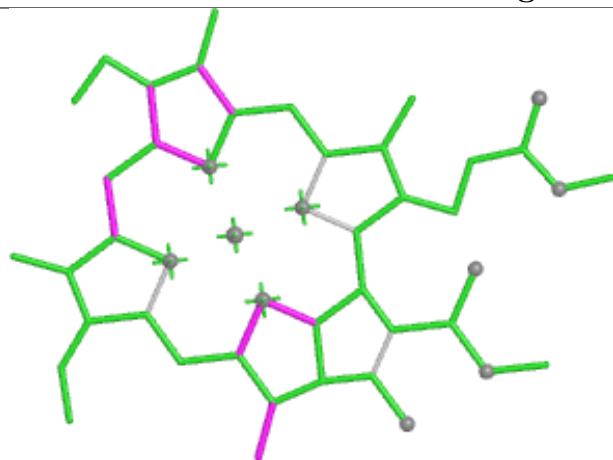


Rings

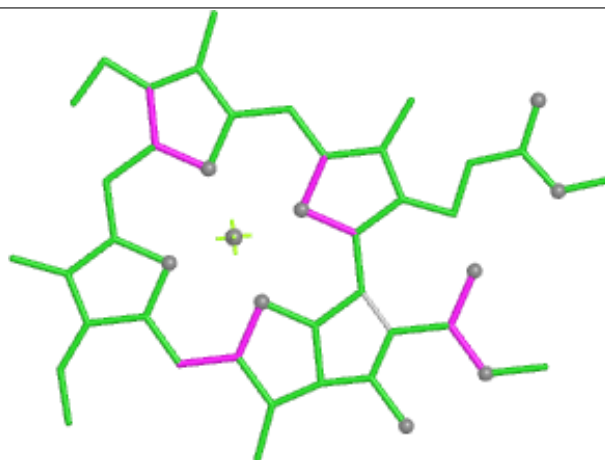
Ligand CLA 5 605



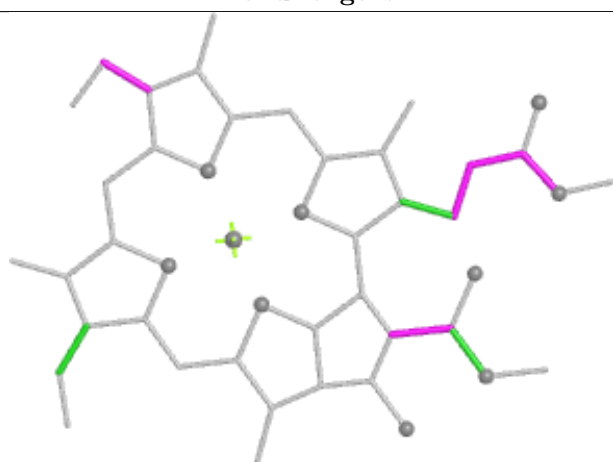
Ligand CLA k 307



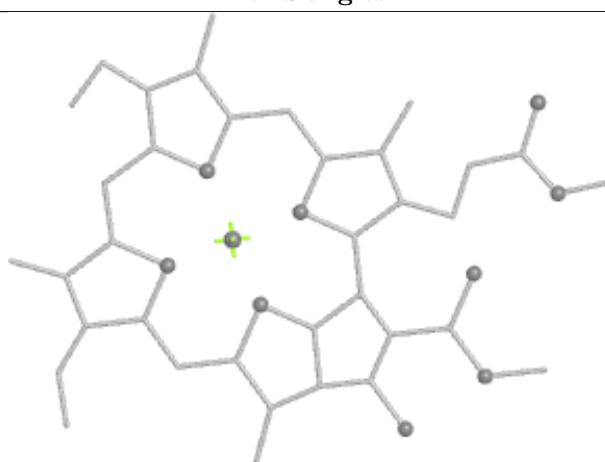
Bond lengths



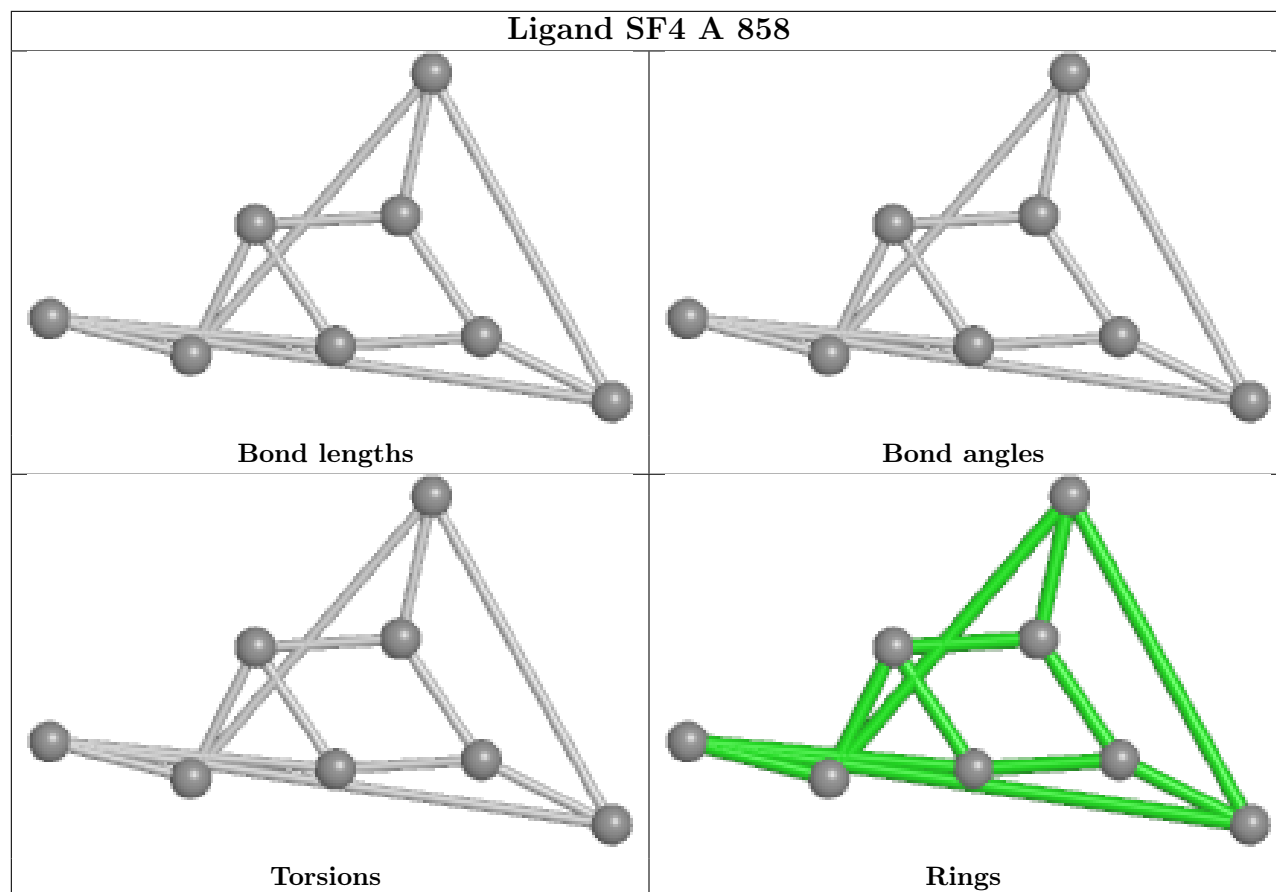
Bond angles



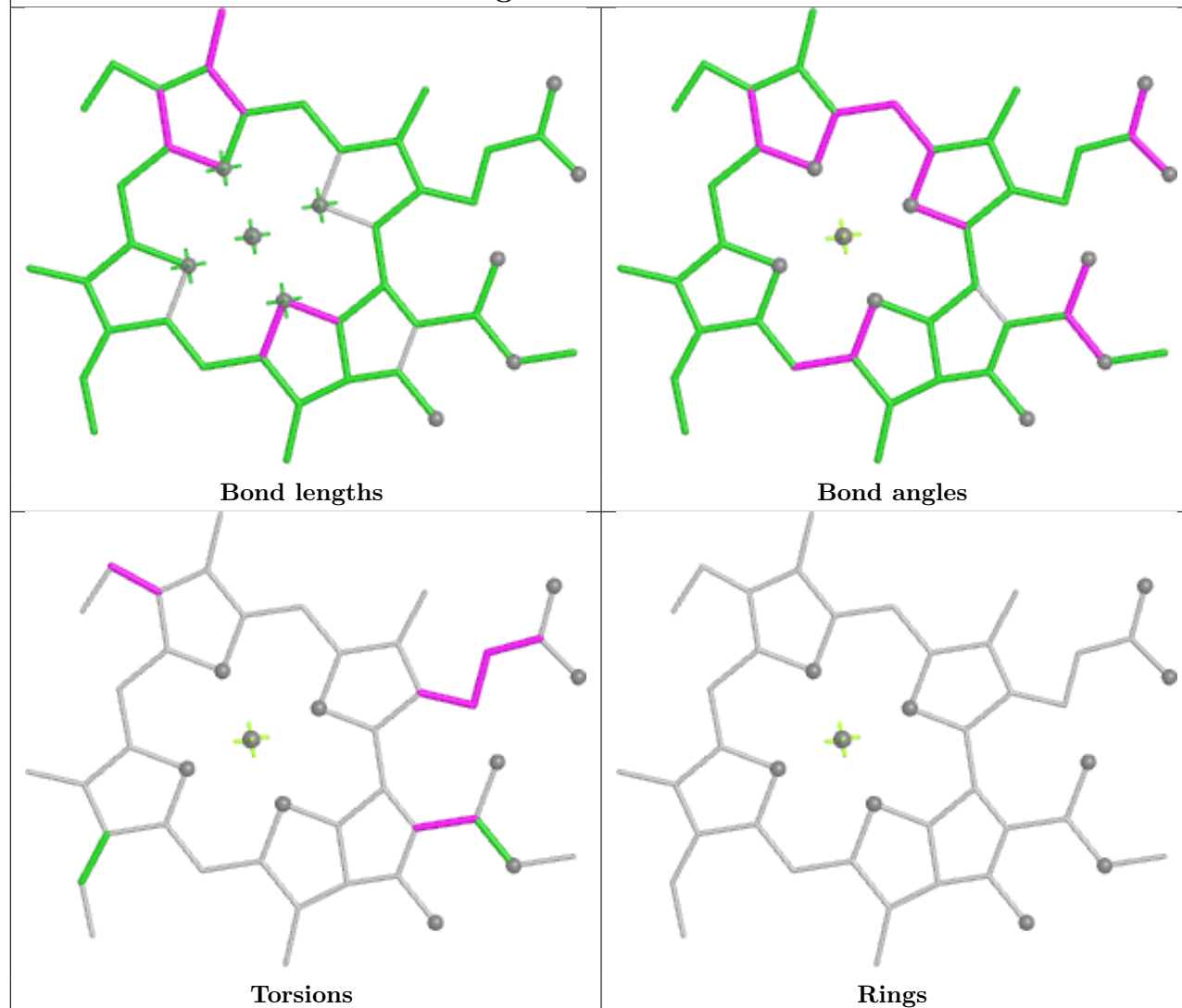
Torsions



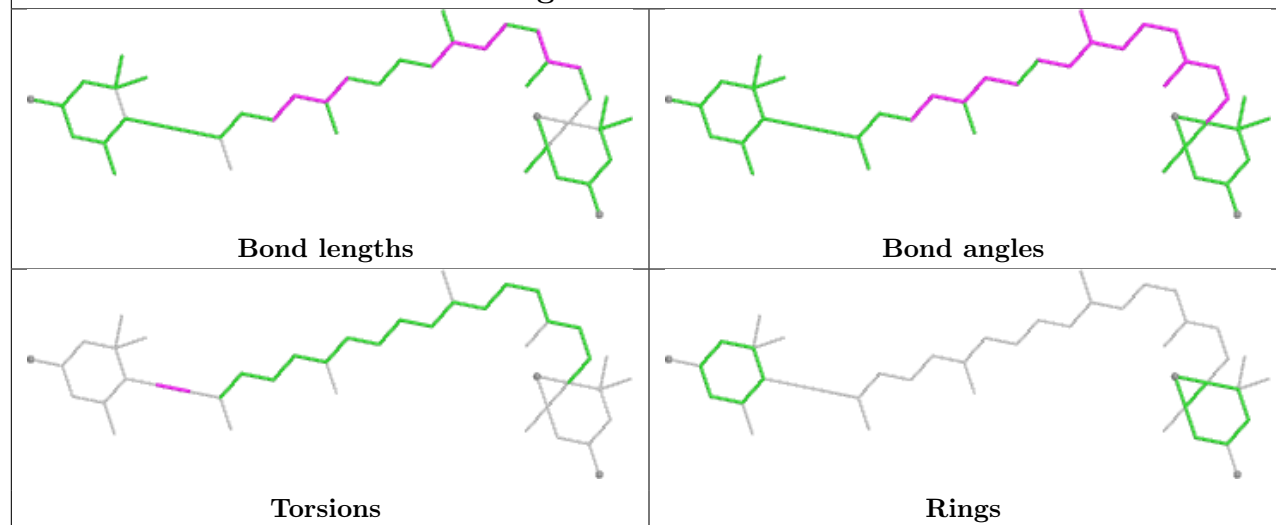
Rings

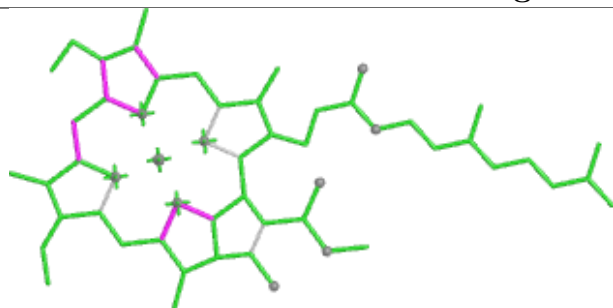


Ligand CLA h 612

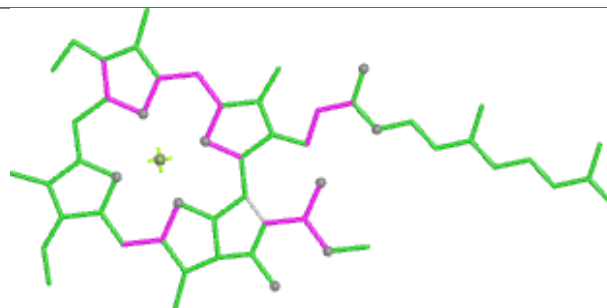


Ligand DD6 1 313

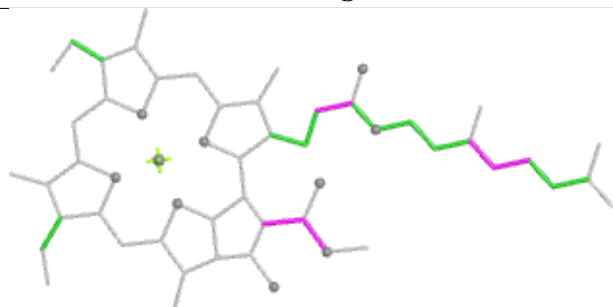


Ligand CLA A 837

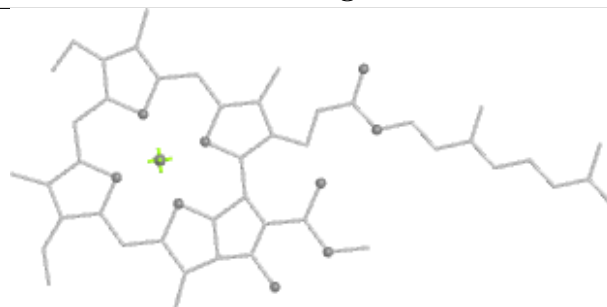
Bond lengths



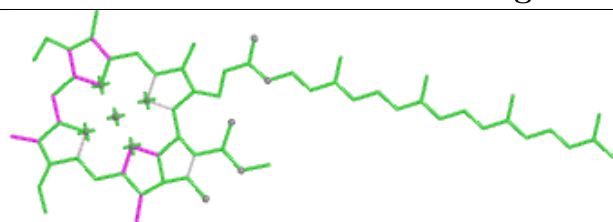
Bond angles



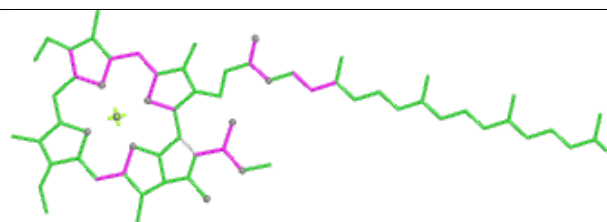
Torsions



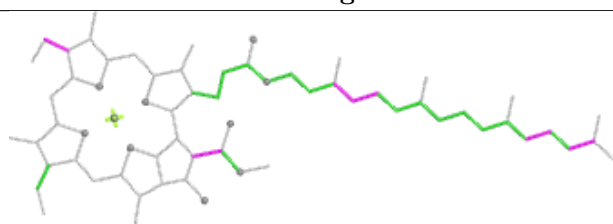
Rings

Ligand CLA B 808

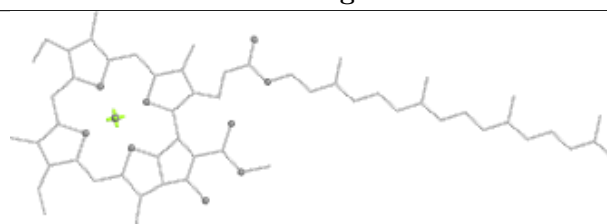
Bond lengths



Bond angles

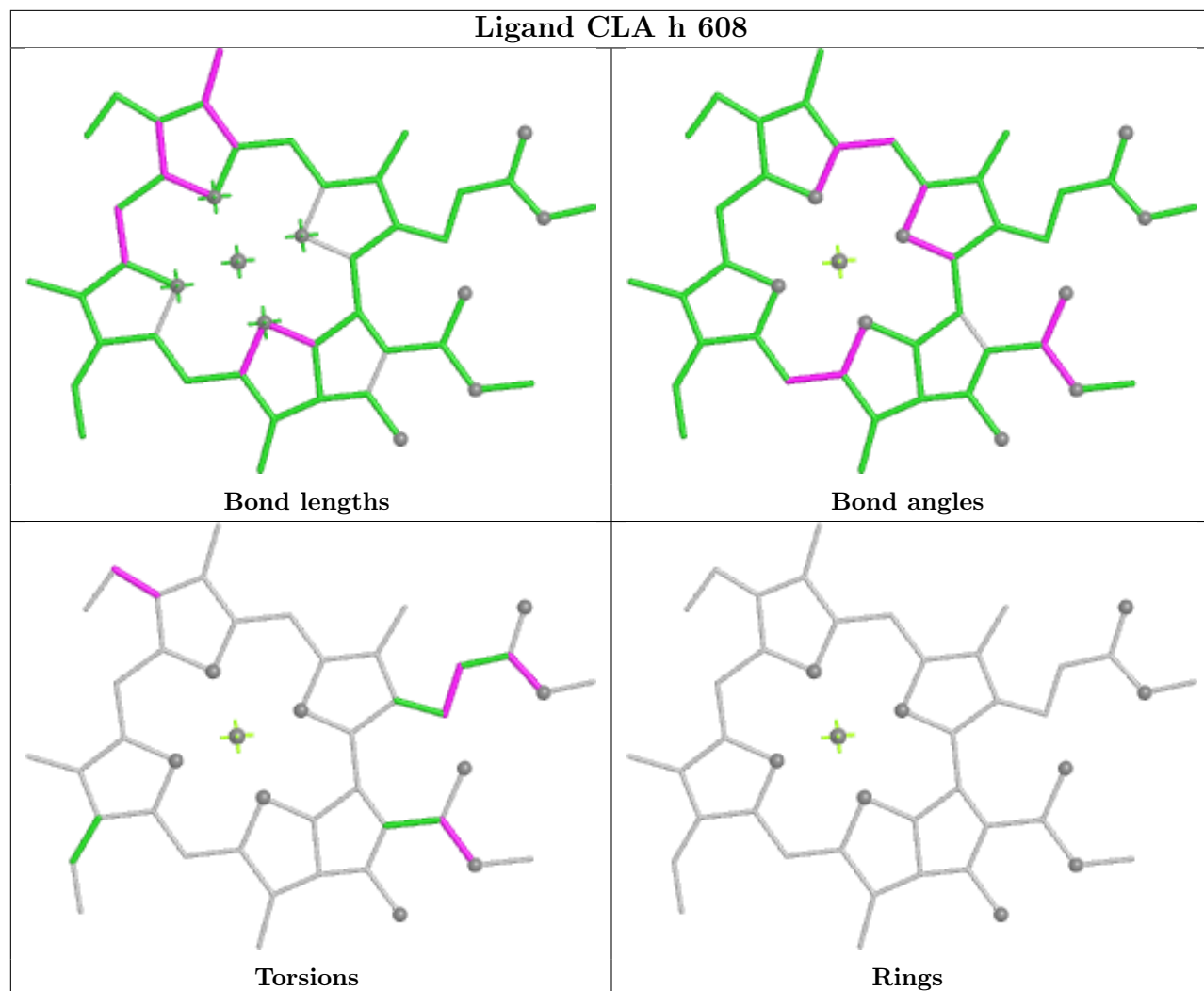


Torsions

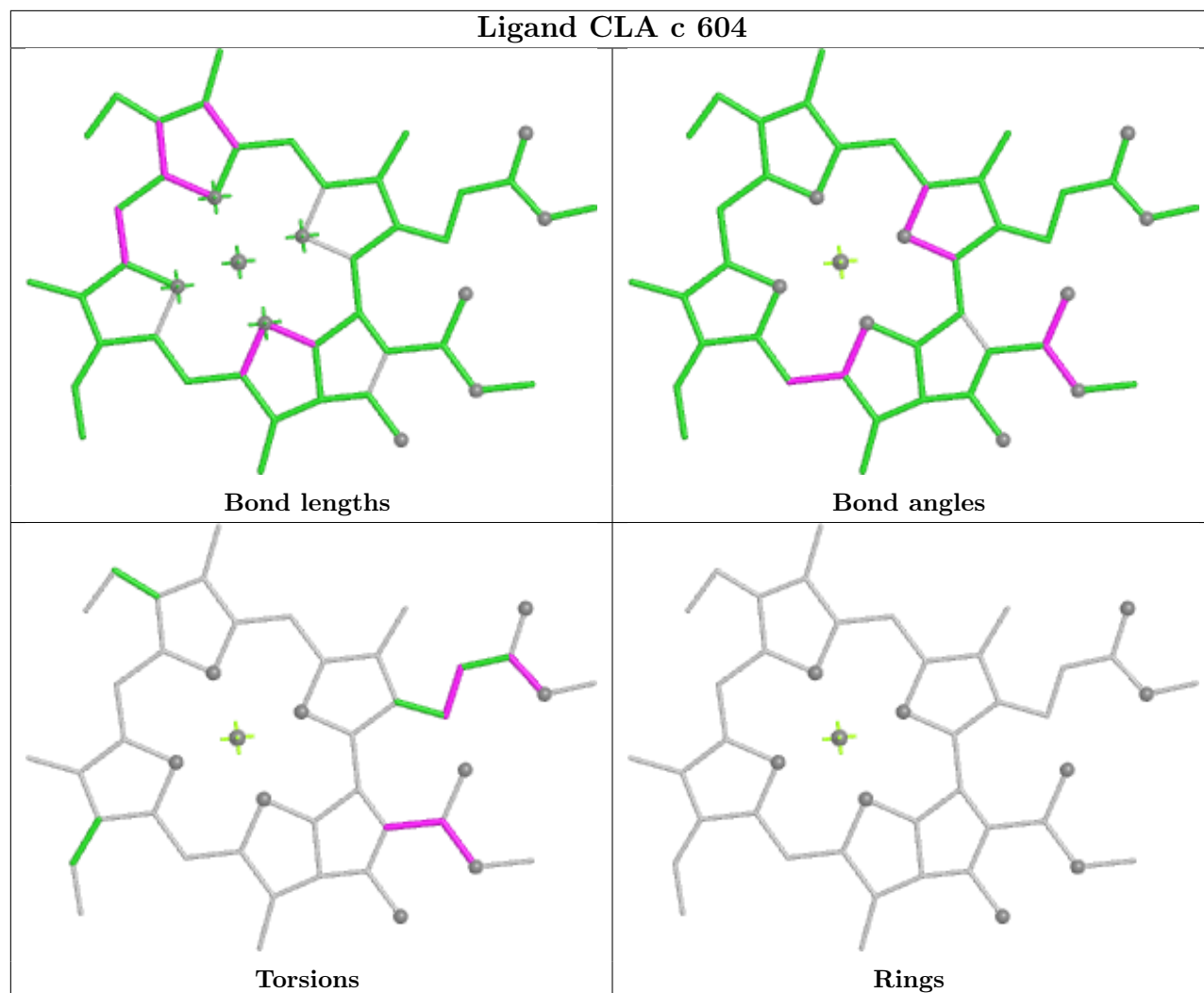


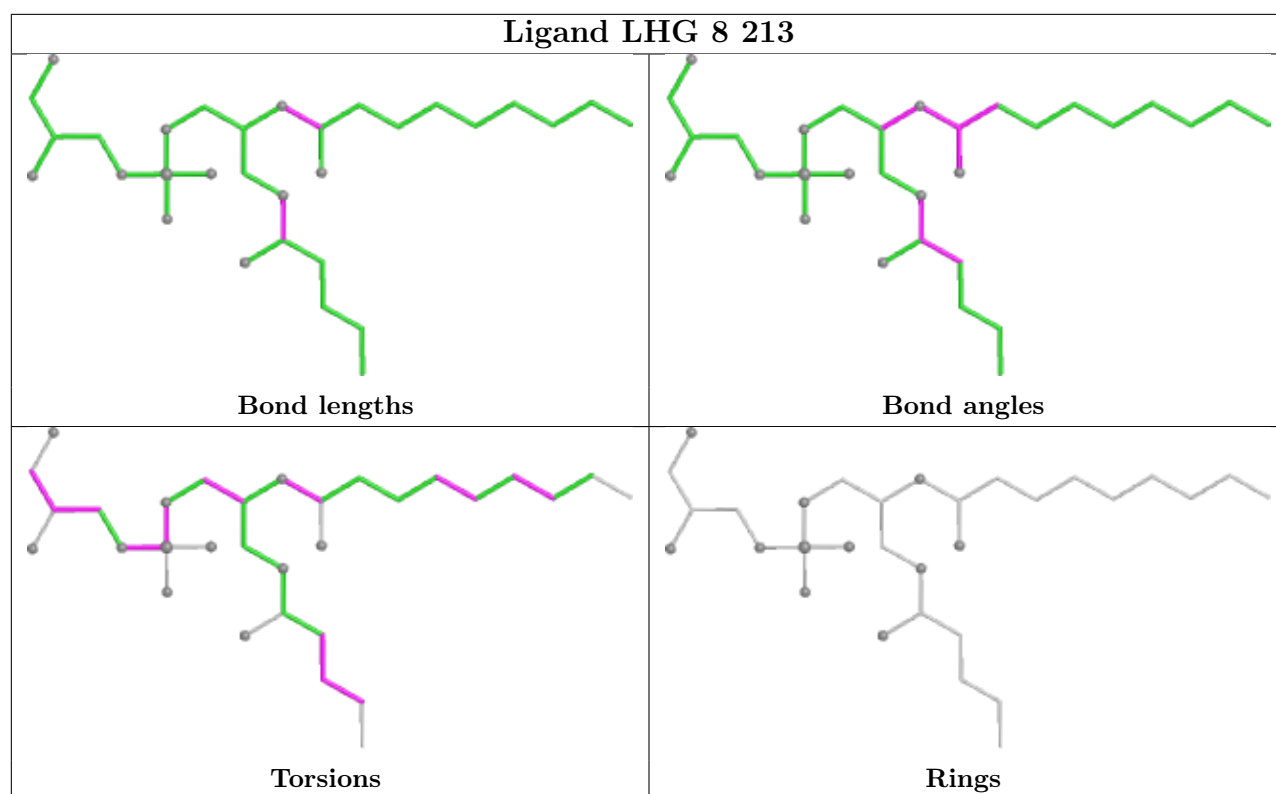
Rings

Ligand CLA h 608

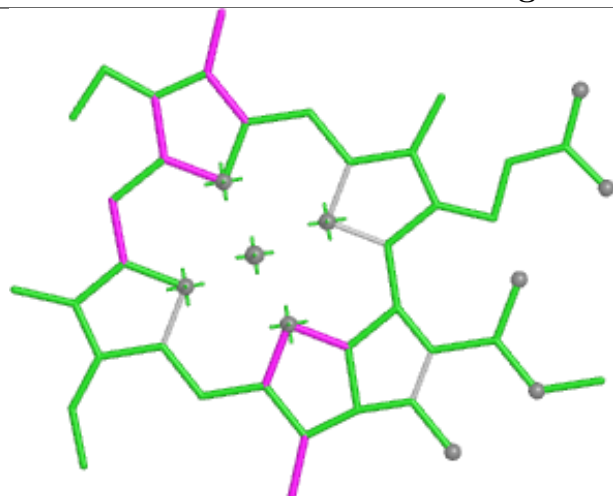


Ligand CLA c 604

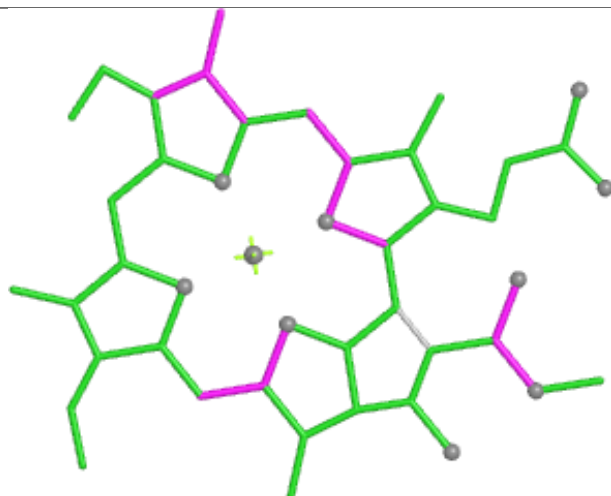




Ligand CLA 7 604



Bond lengths



Bond angles

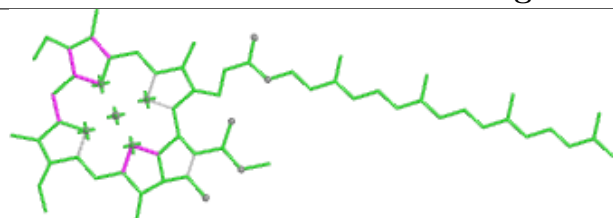


Torsions

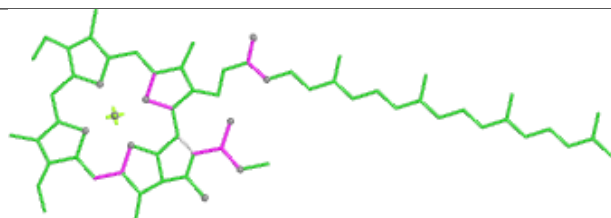


Rings

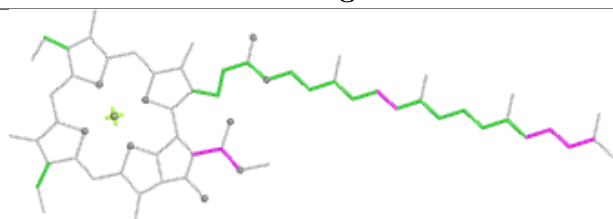
Ligand CLA B 834



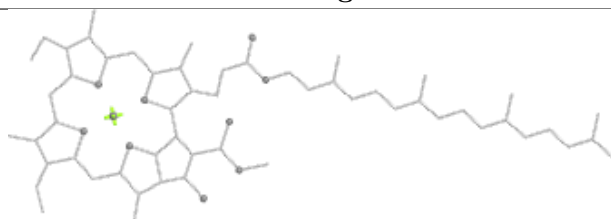
Bond lengths



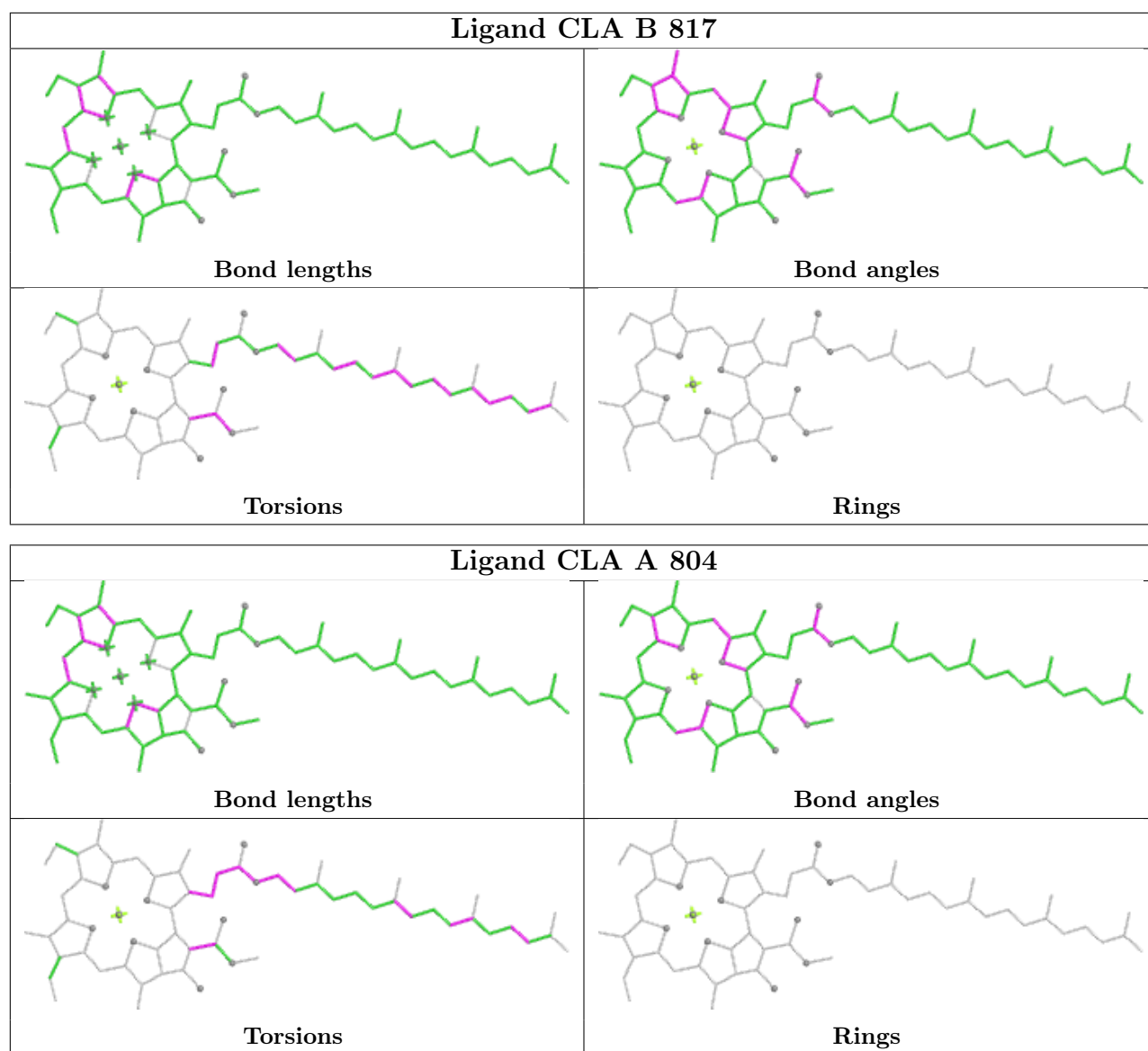
Bond angles

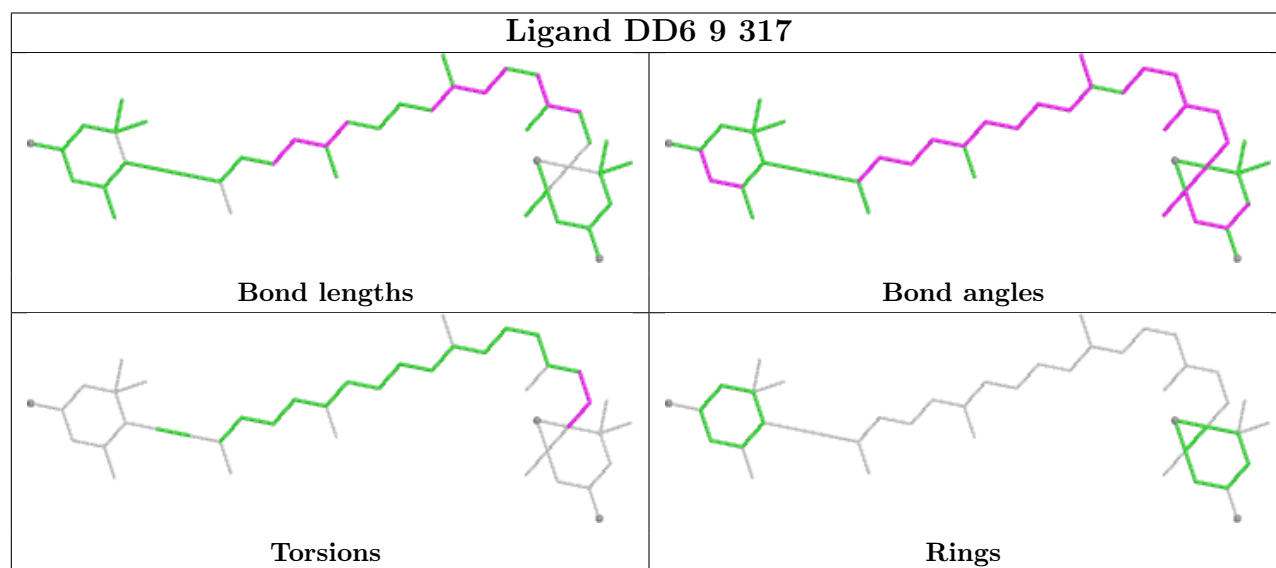
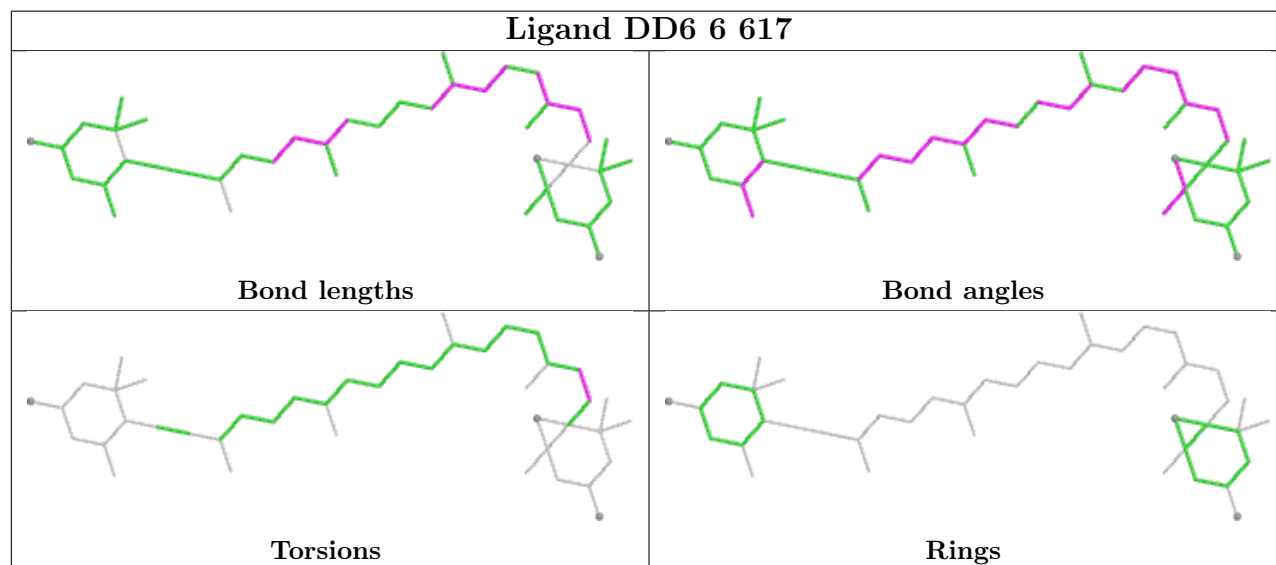
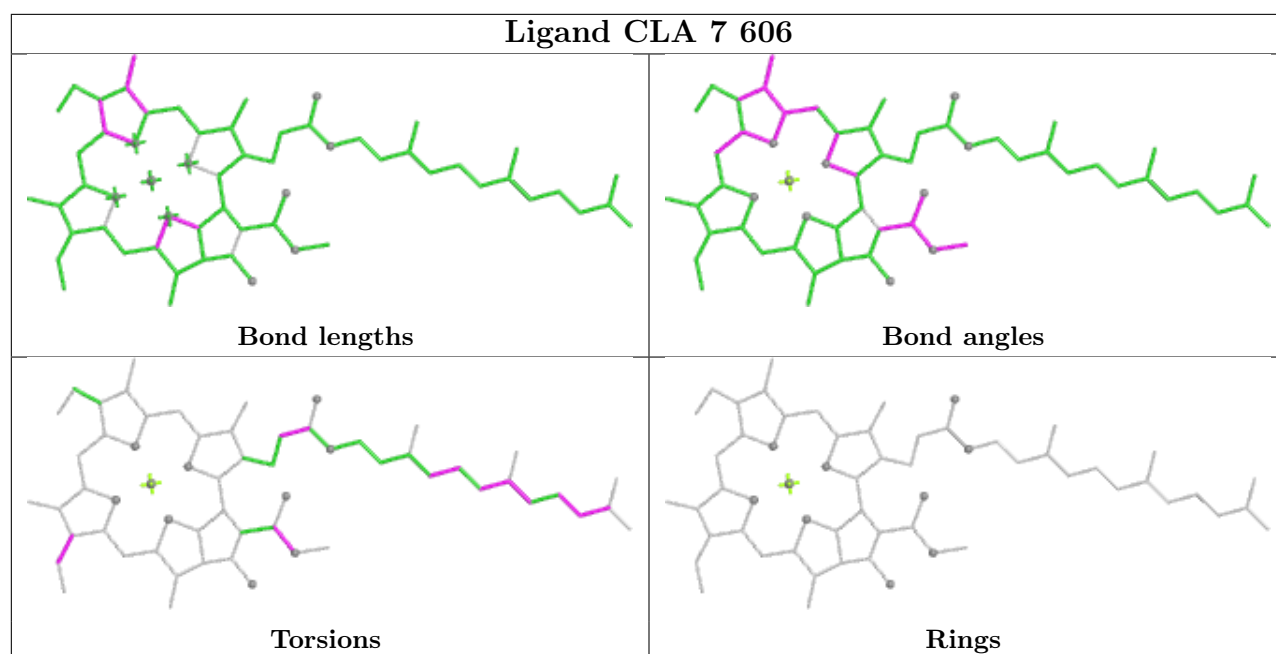


Torsions

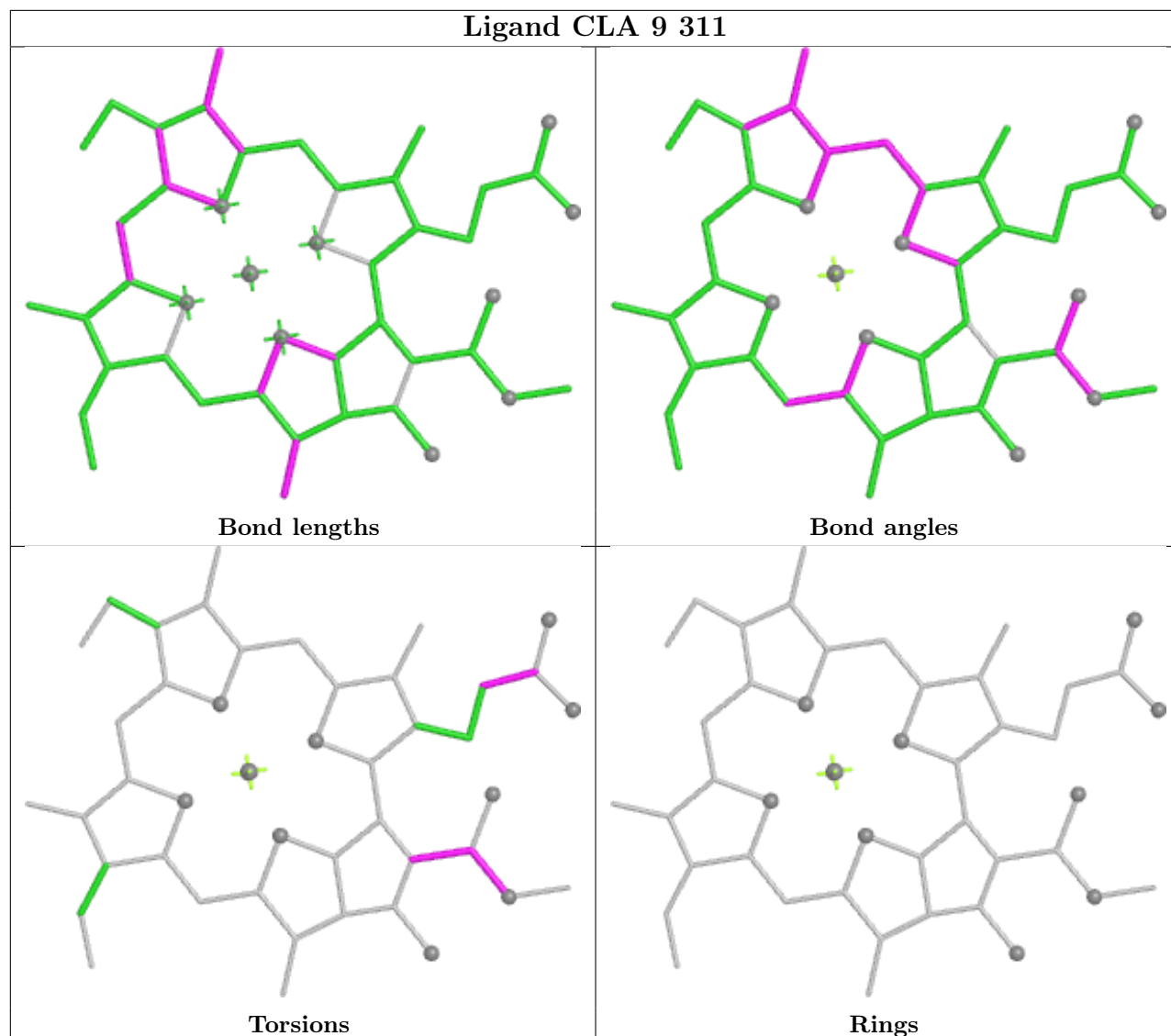


Rings

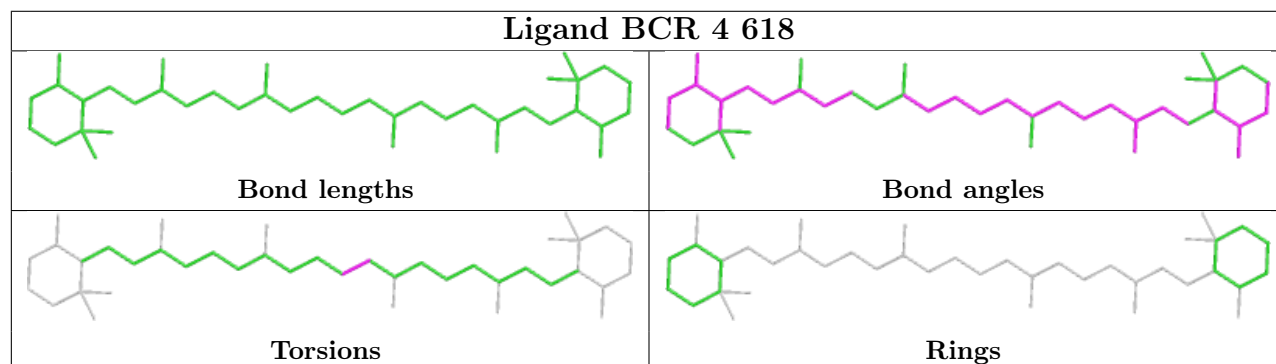




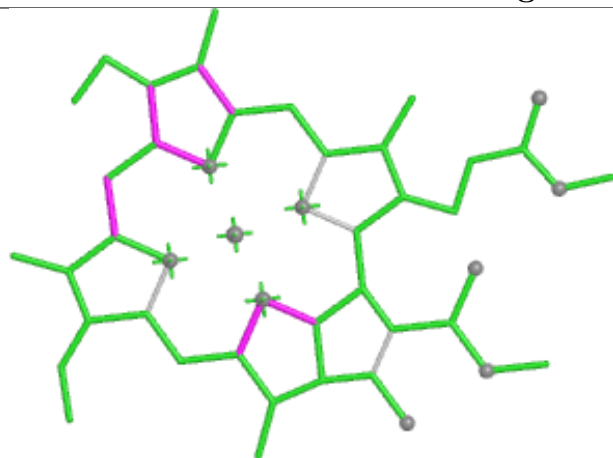
Ligand CLA 9 311



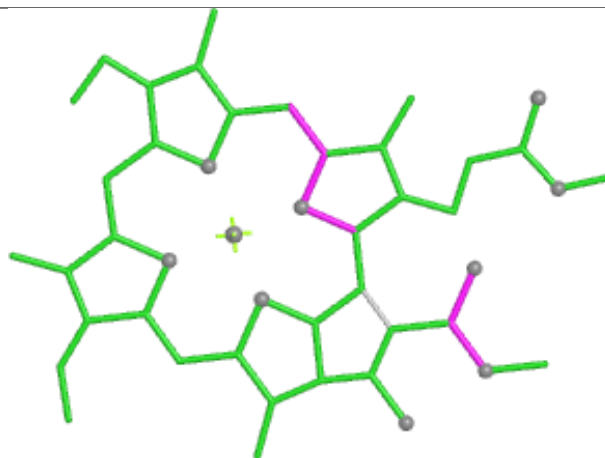
Ligand BCR 4 618



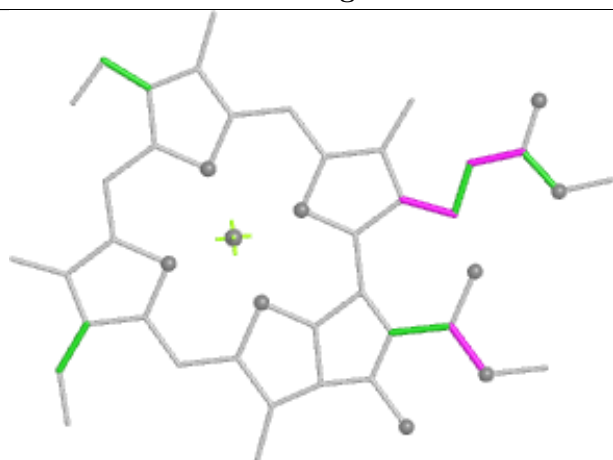
Ligand CLA k 305



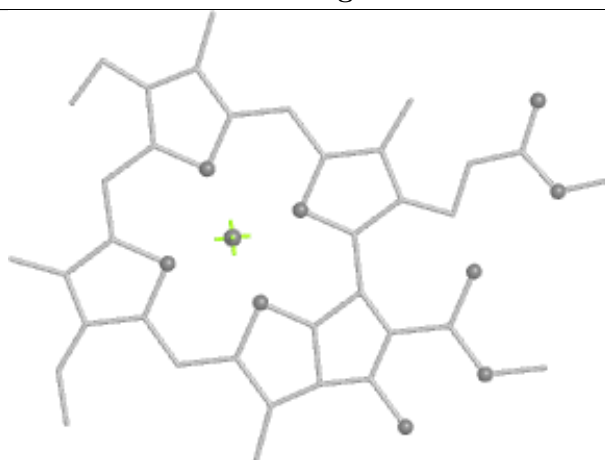
Bond lengths



Bond angles

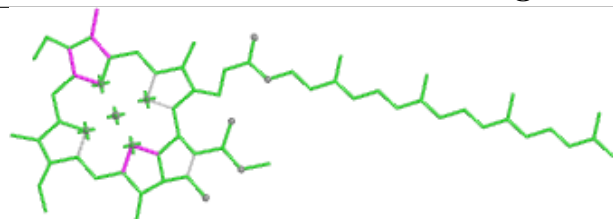


Torsions

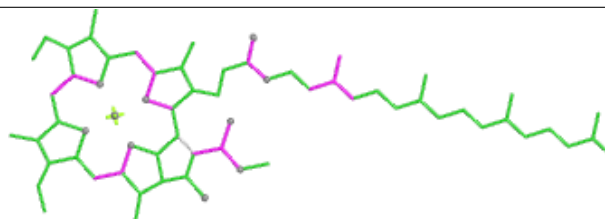


Rings

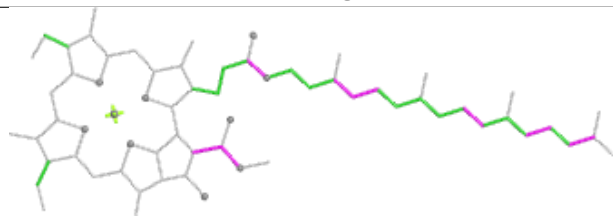
Ligand CLA B 822



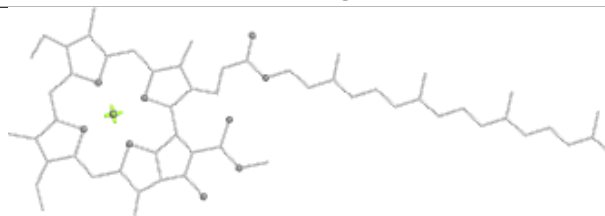
Bond lengths



Bond angles

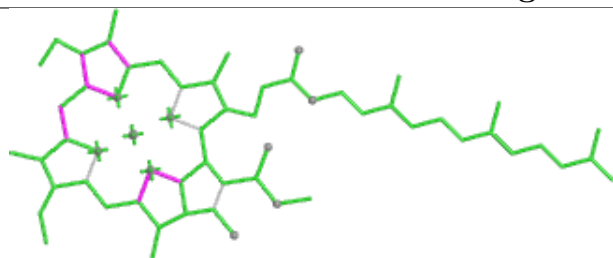


Torsions

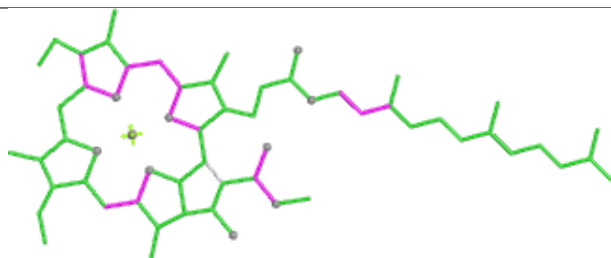


Rings

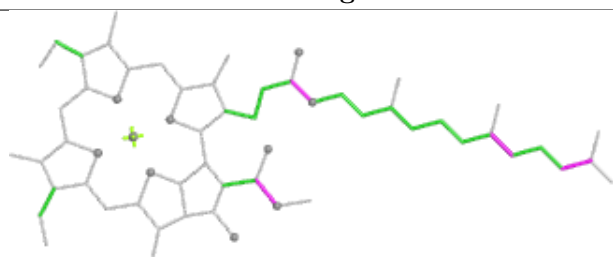
Ligand CLA 3 305



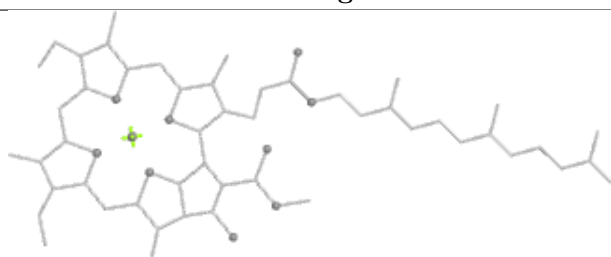
Bond lengths



Bond angles

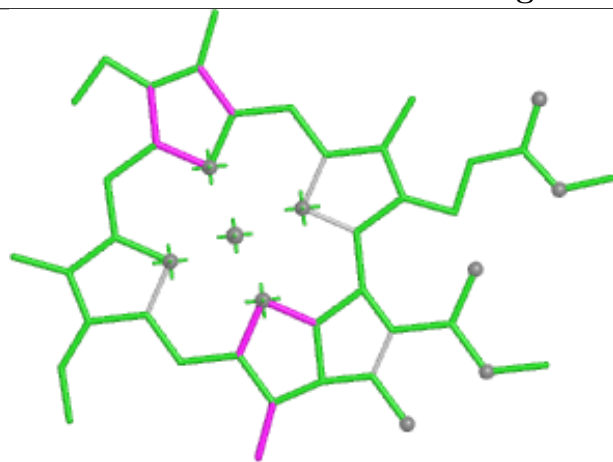


Torsions

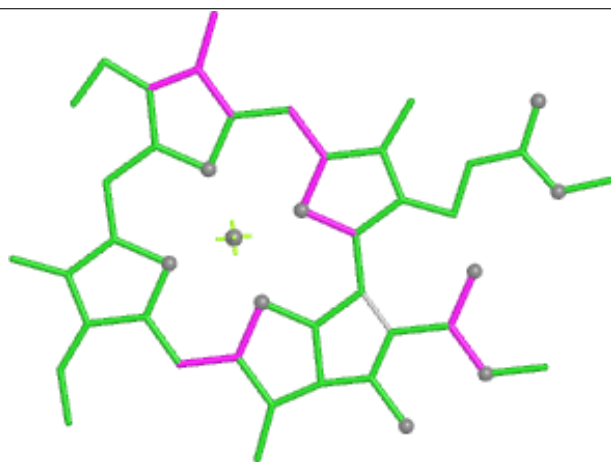


Rings

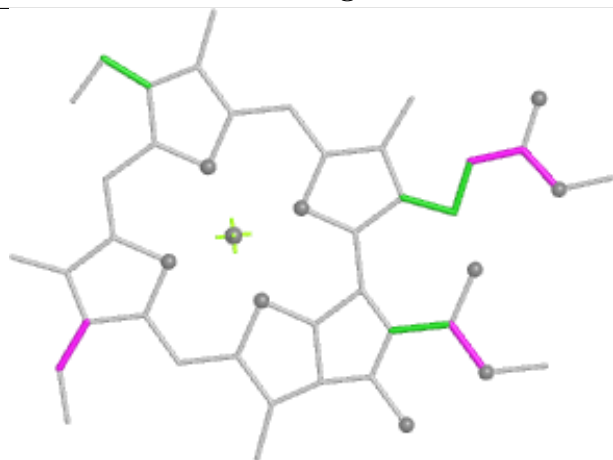
Ligand CLA L 205



Bond lengths



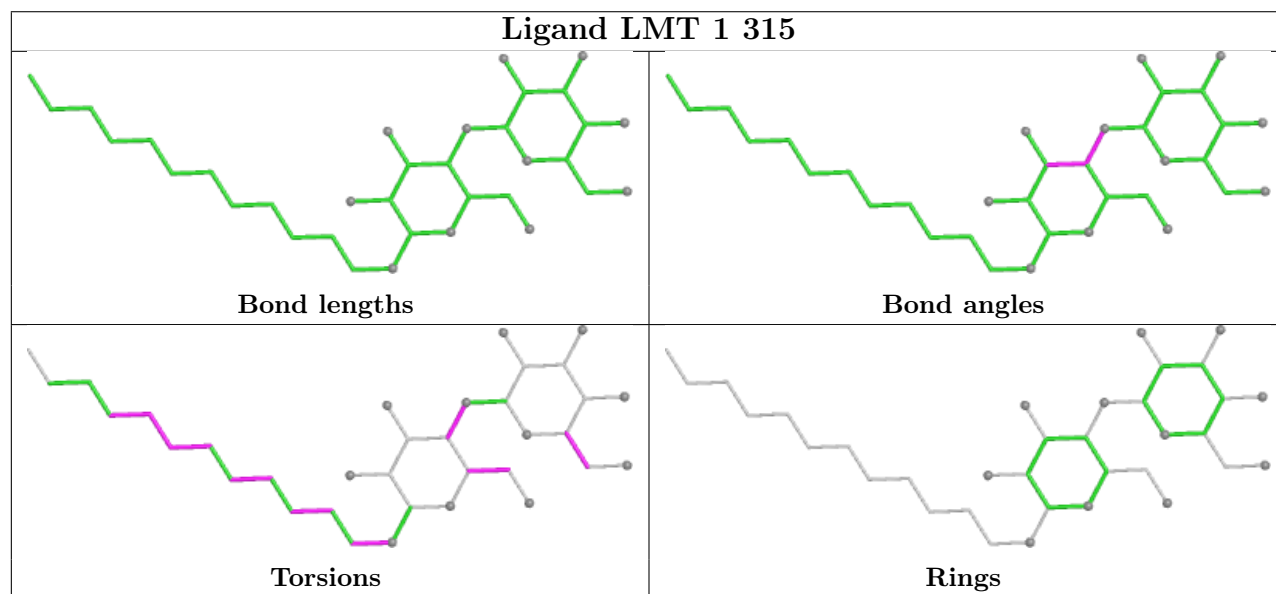
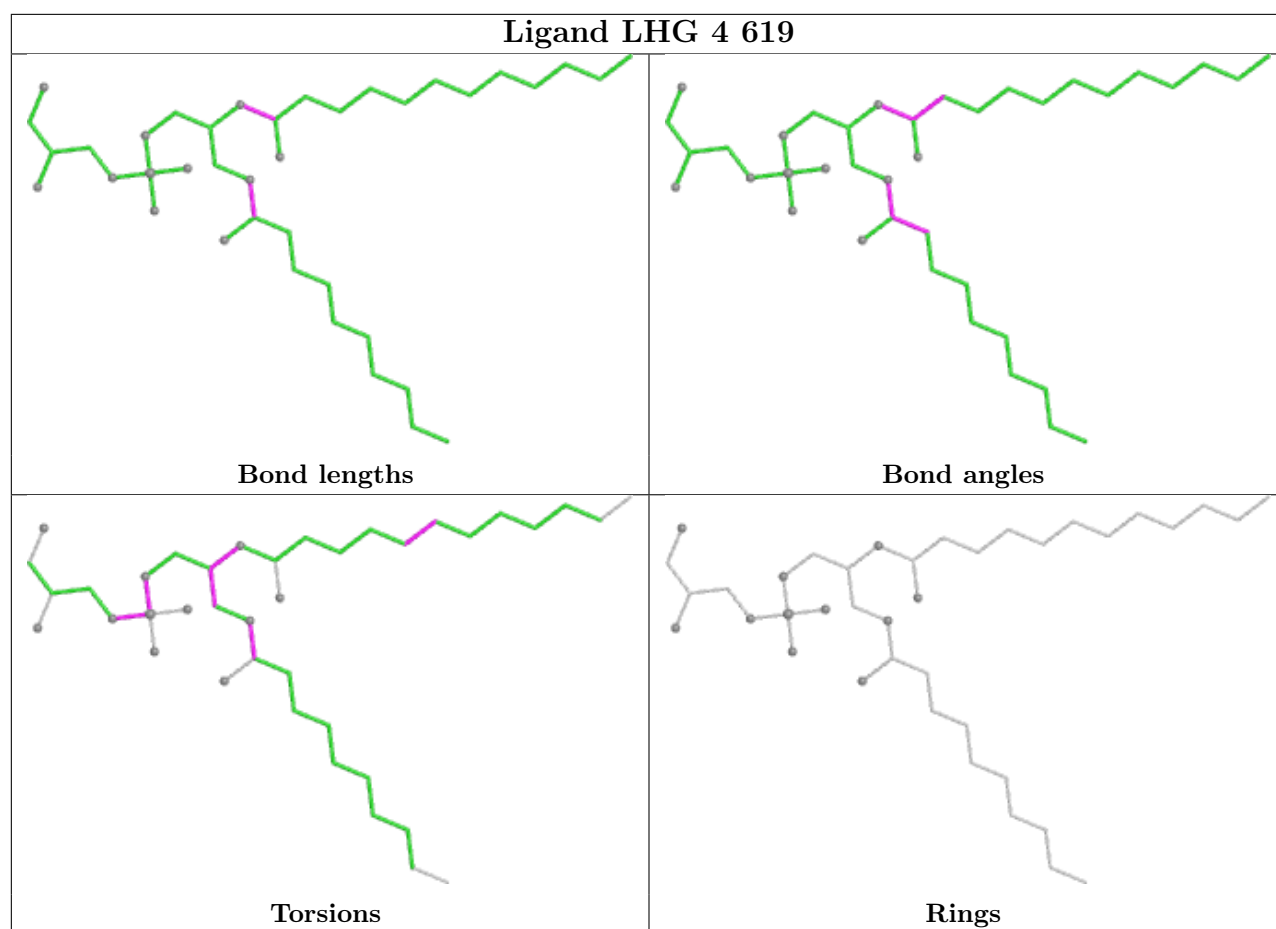
Bond angles



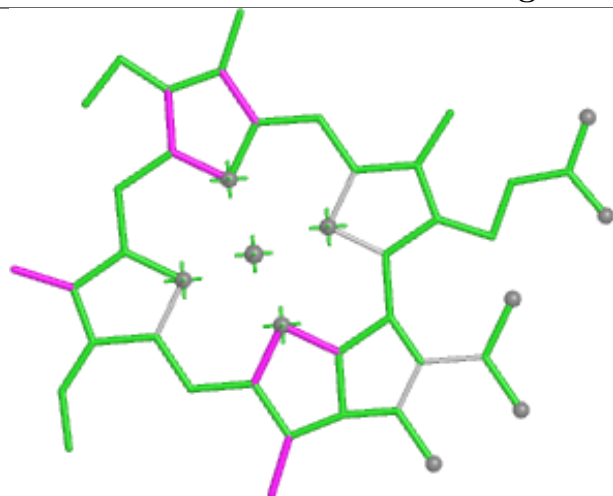
Torsions



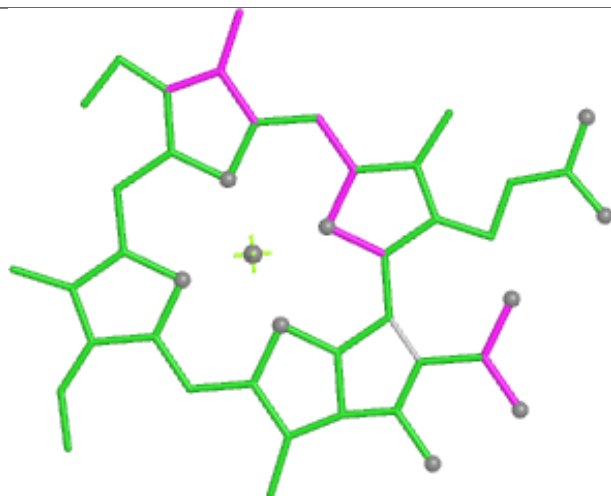
Rings



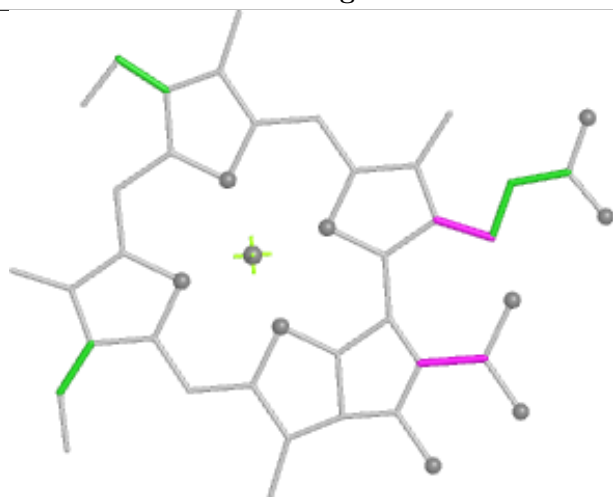
Ligand CLA 6 611



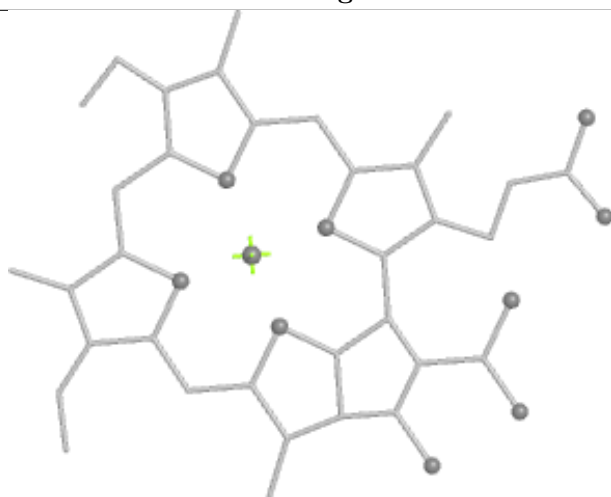
Bond lengths



Bond angles

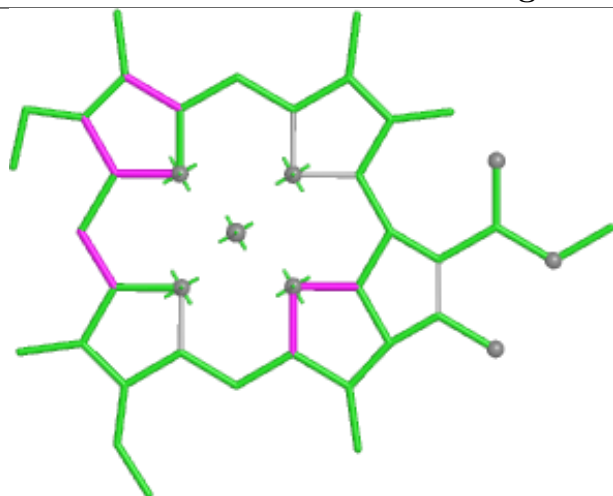


Torsions



Rings

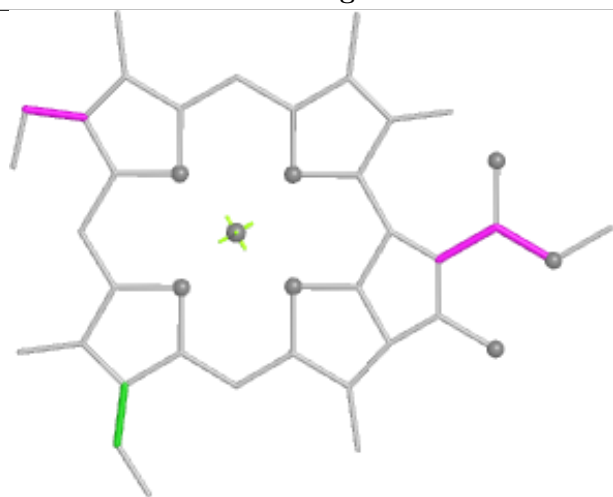
Ligand CLA 8 209



Bond lengths



Bond angles

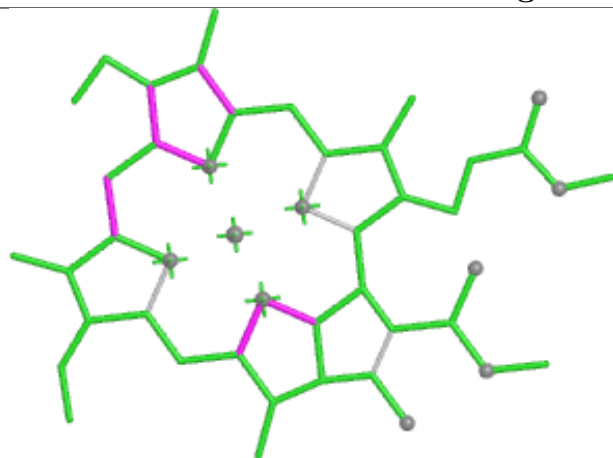


Torsions

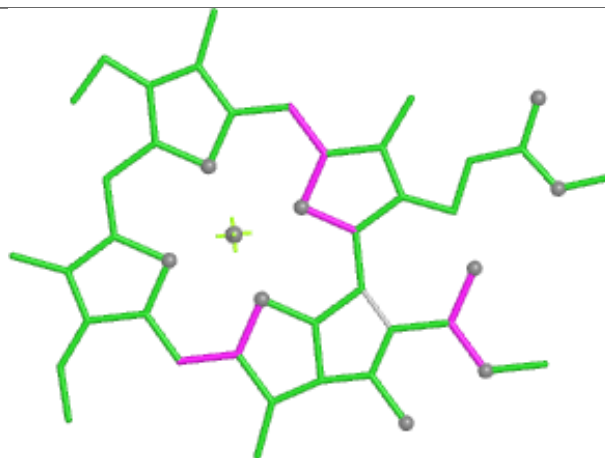


Rings

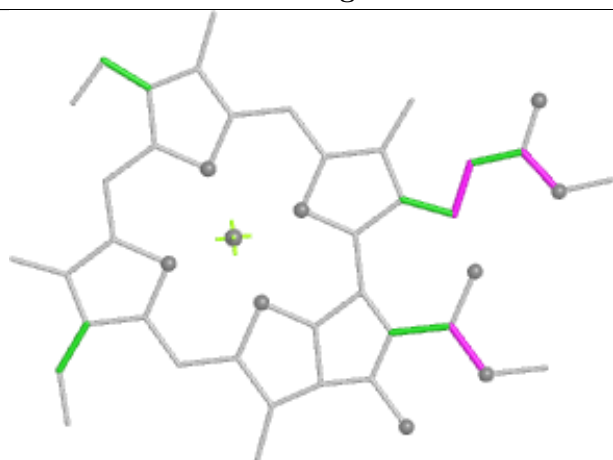
Ligand CLA h 604



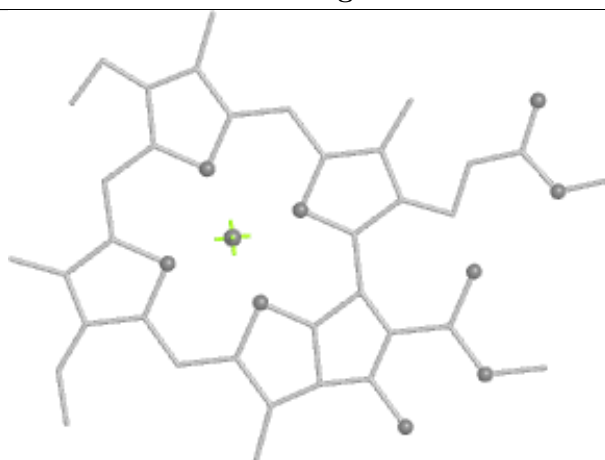
Bond lengths



Bond angles

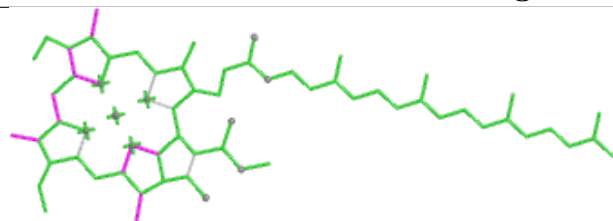


Torsions

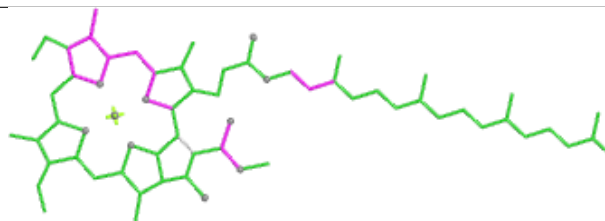


Rings

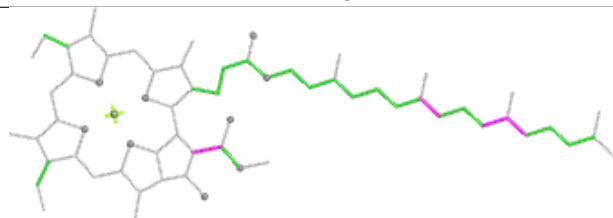
Ligand CLA A 802



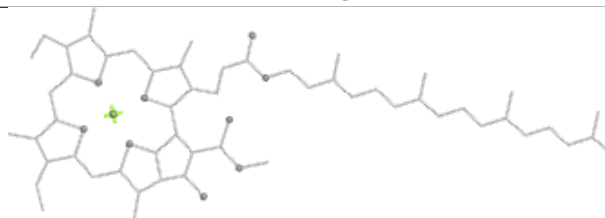
Bond lengths



Bond angles

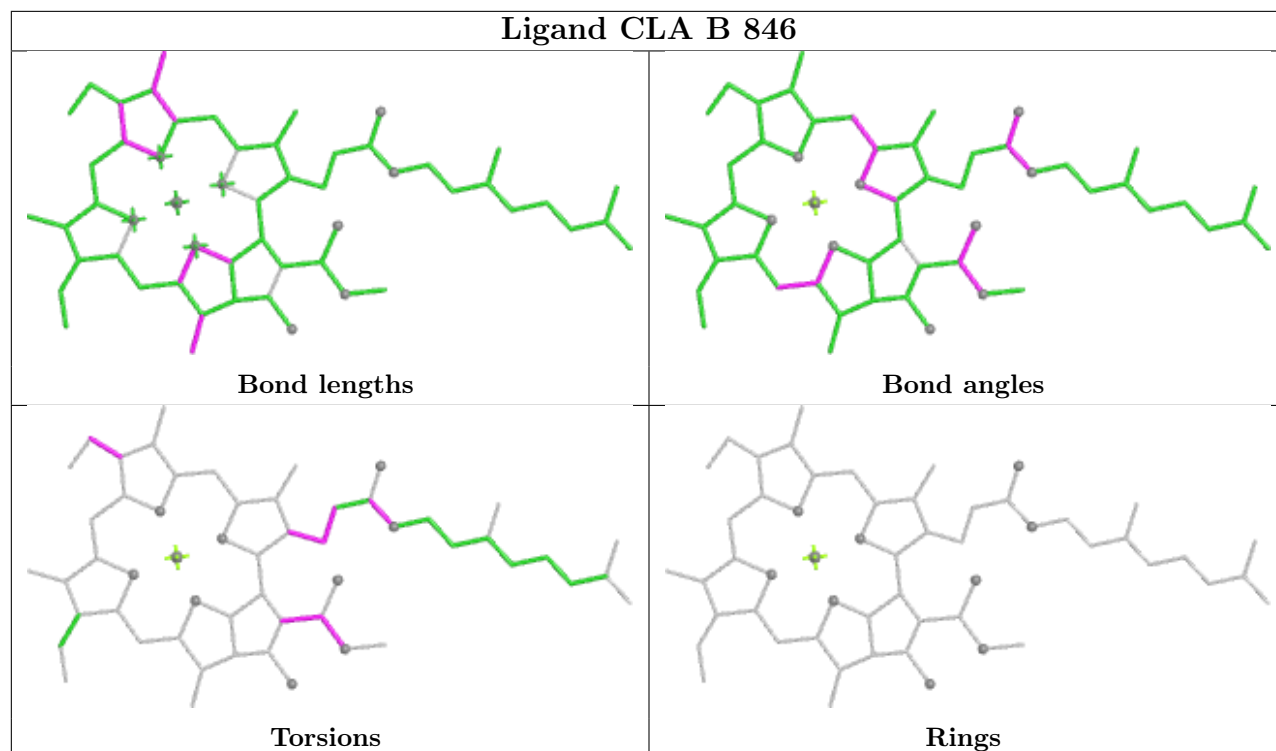


Torsions

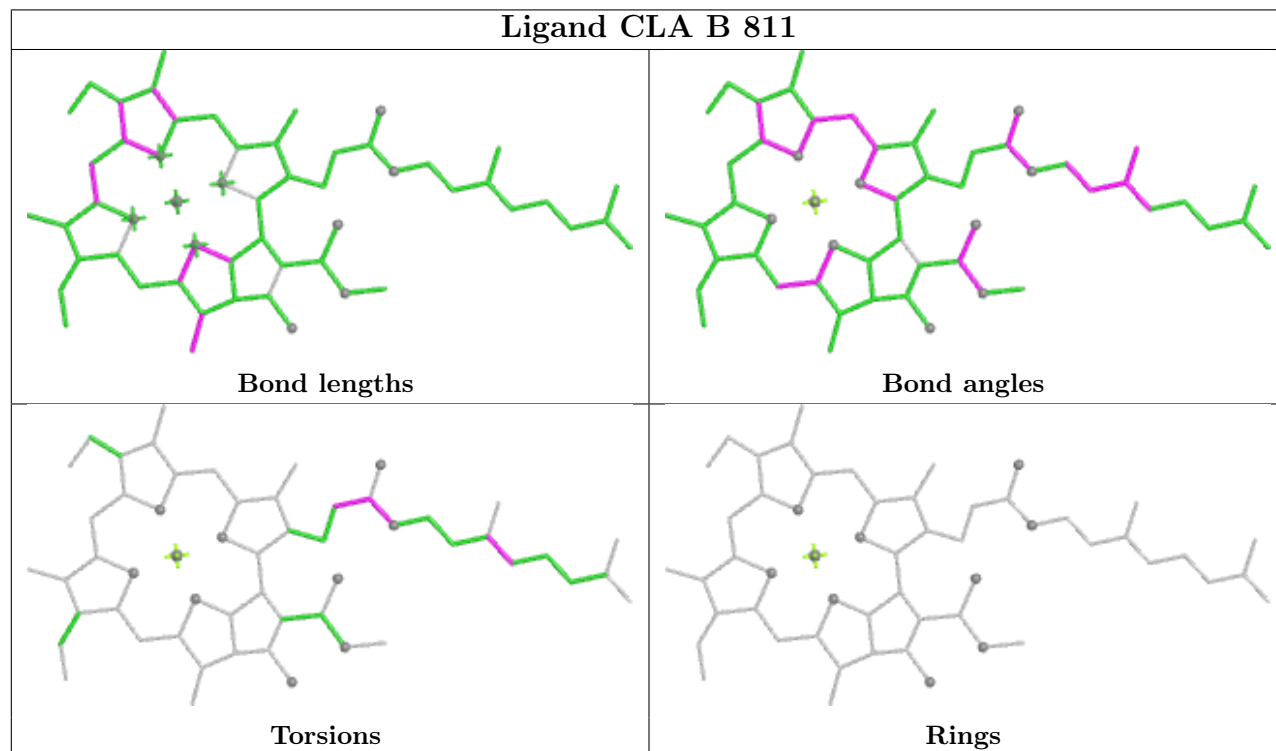


Rings

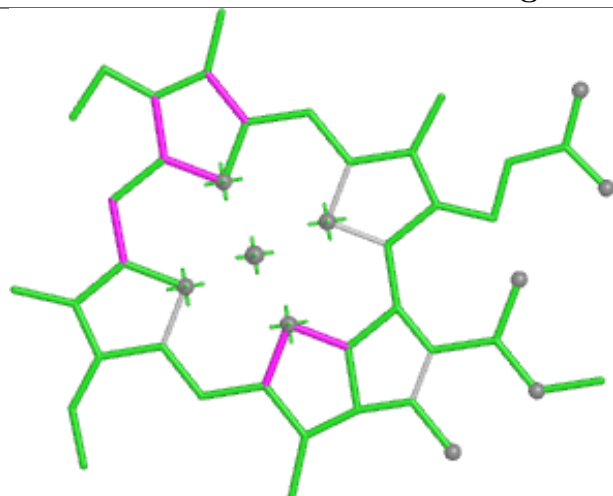
Ligand CLA B 846



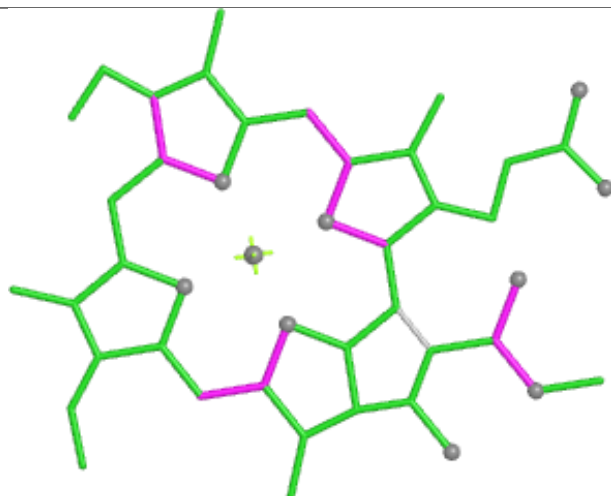
Ligand CLA B 811



Ligand CLA t 306



Bond lengths



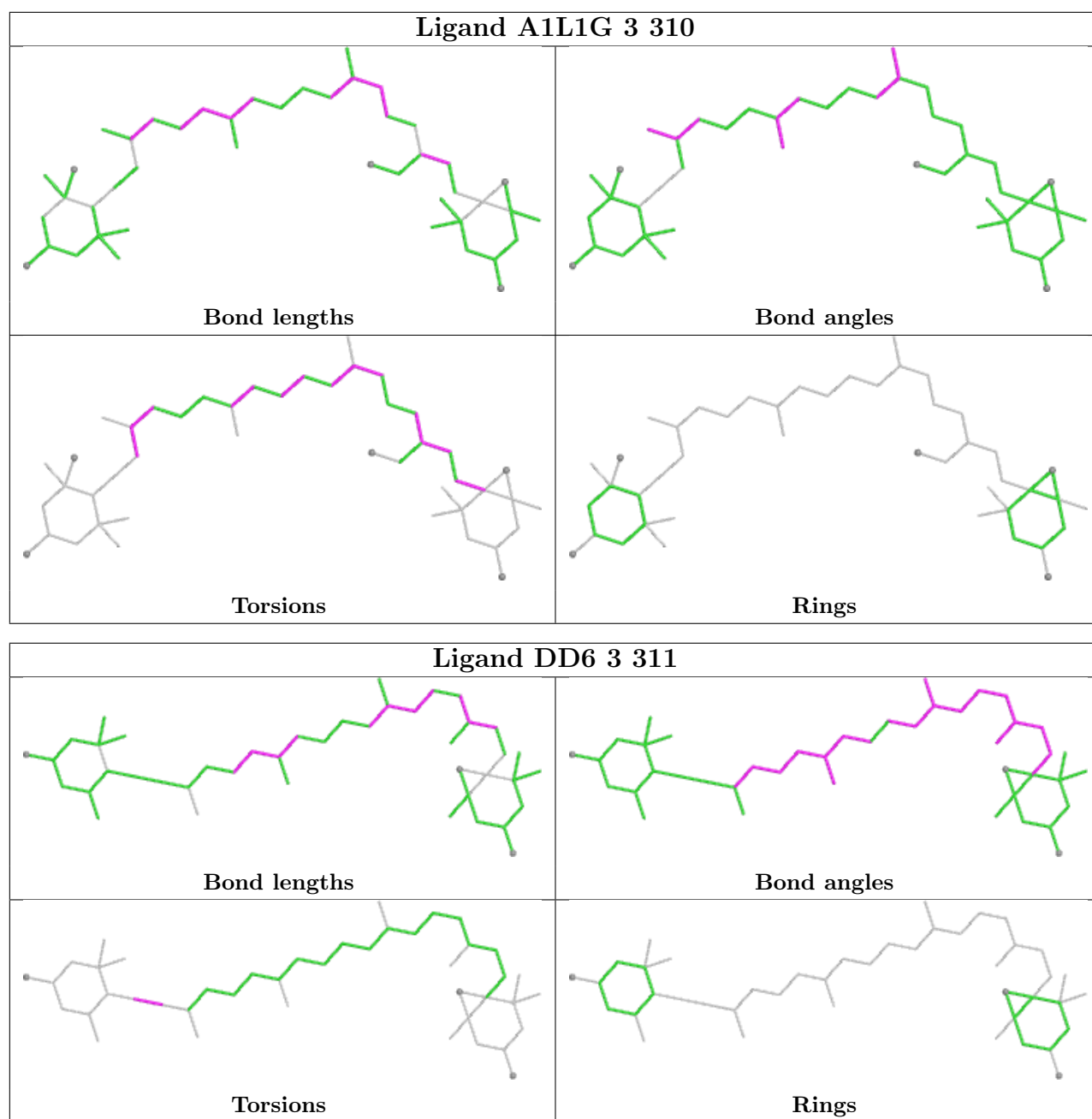
Bond angles

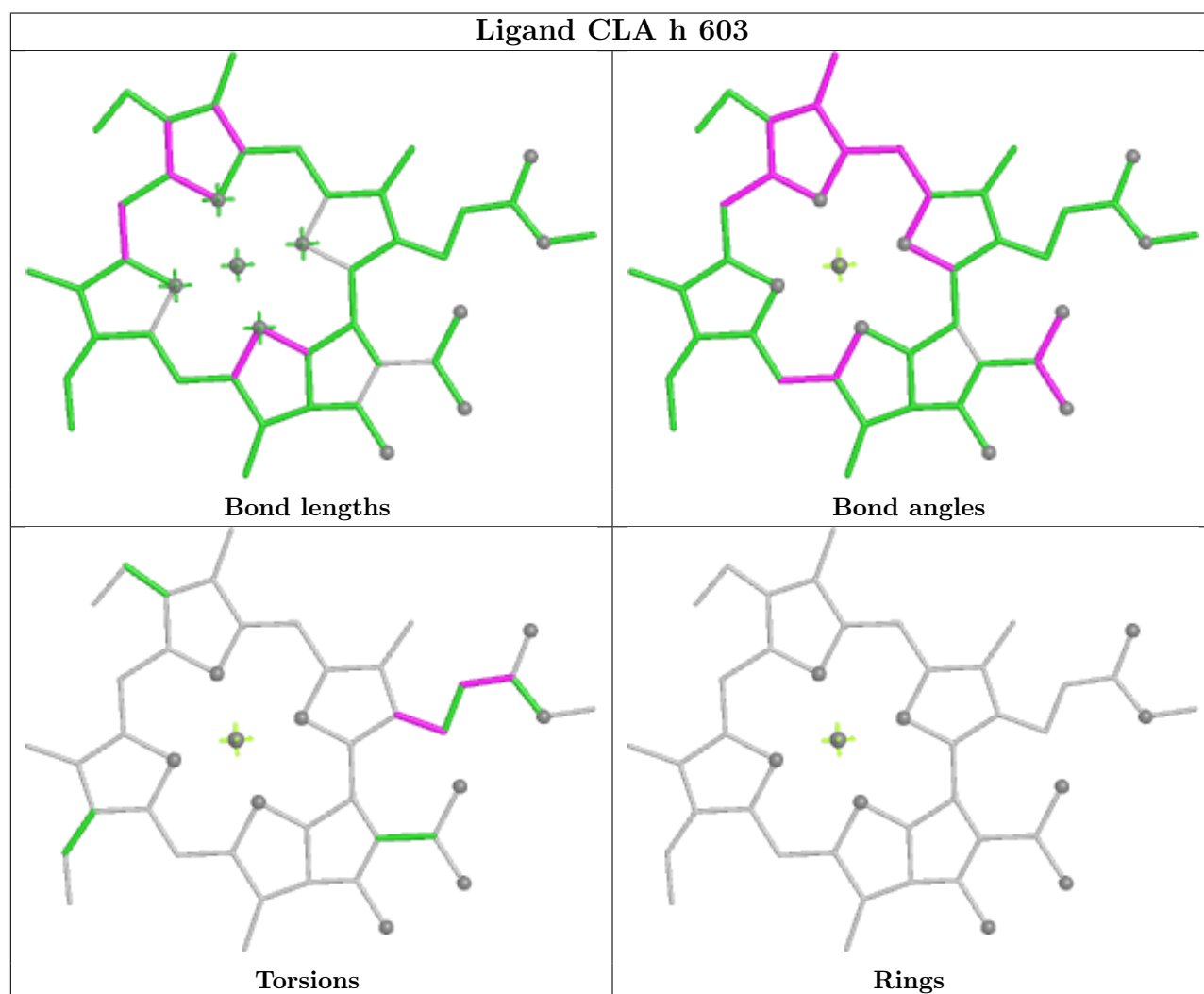
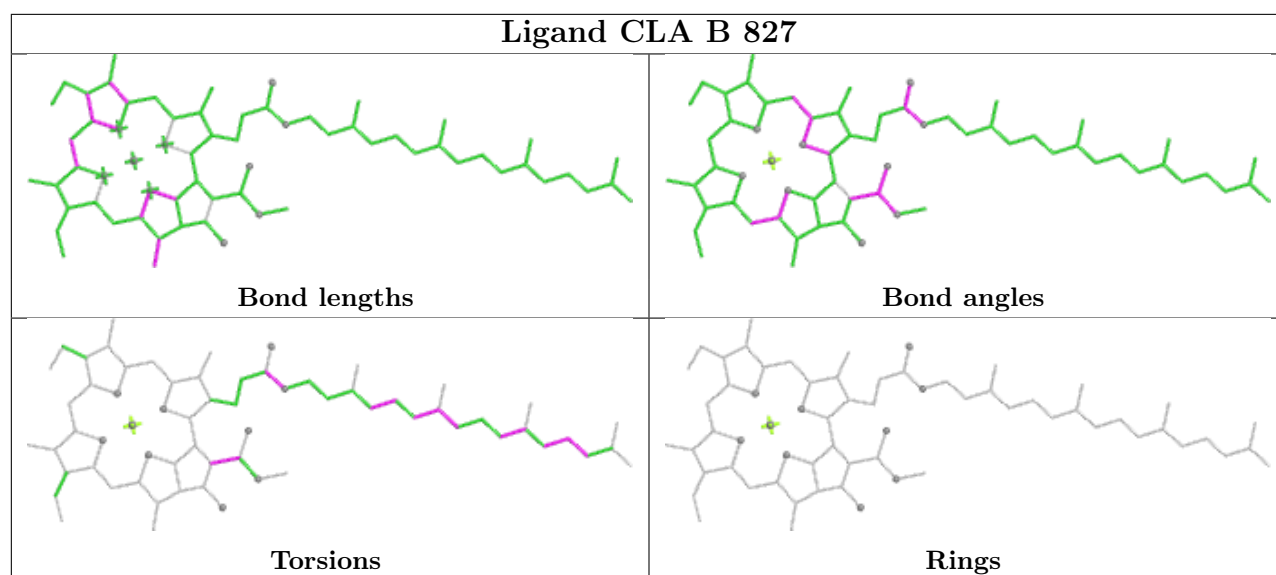


Torsions

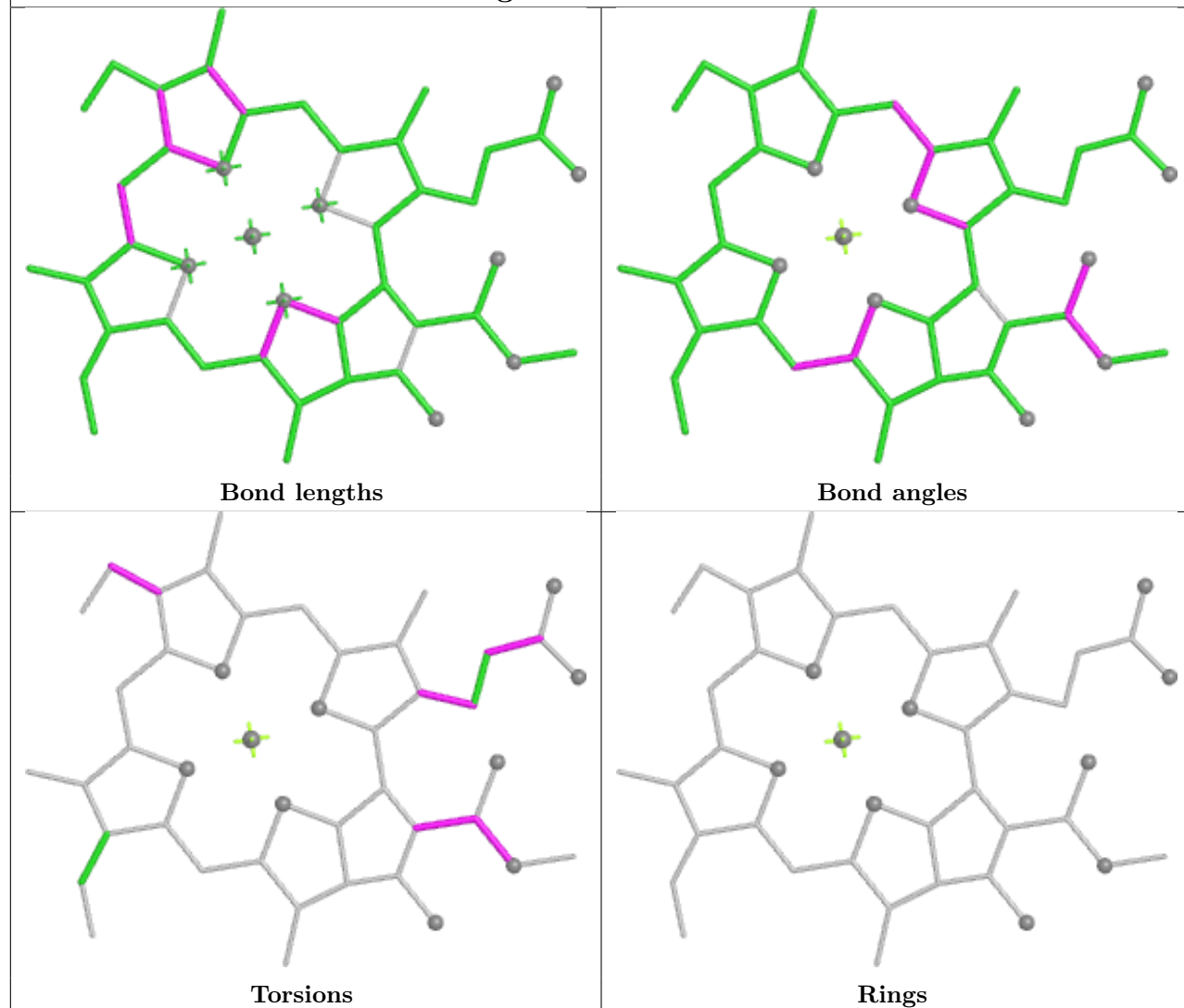


Rings

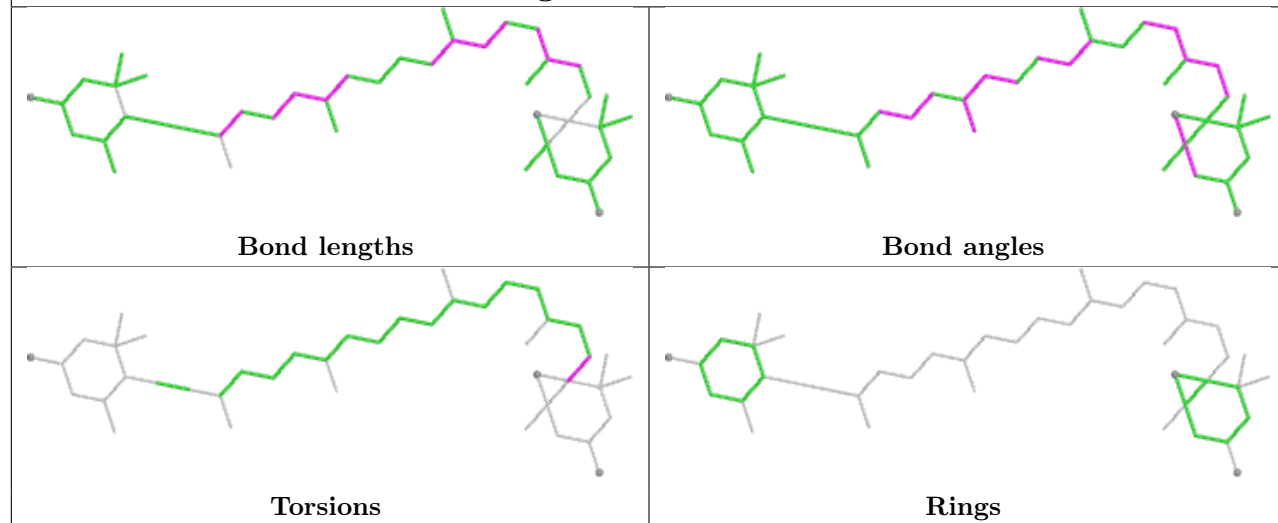


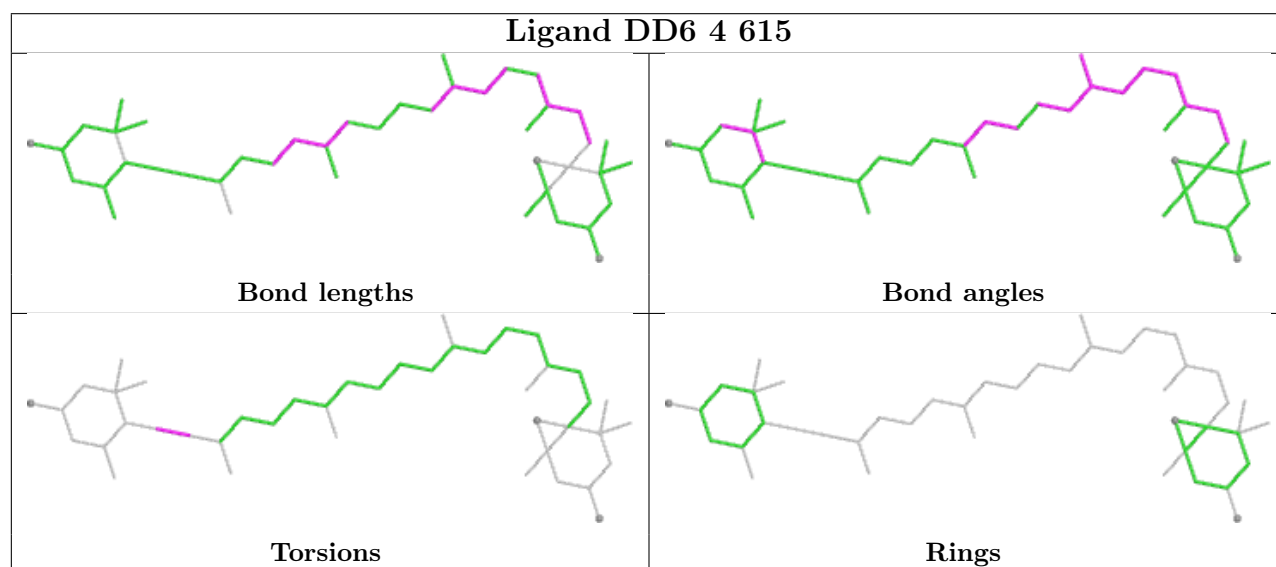
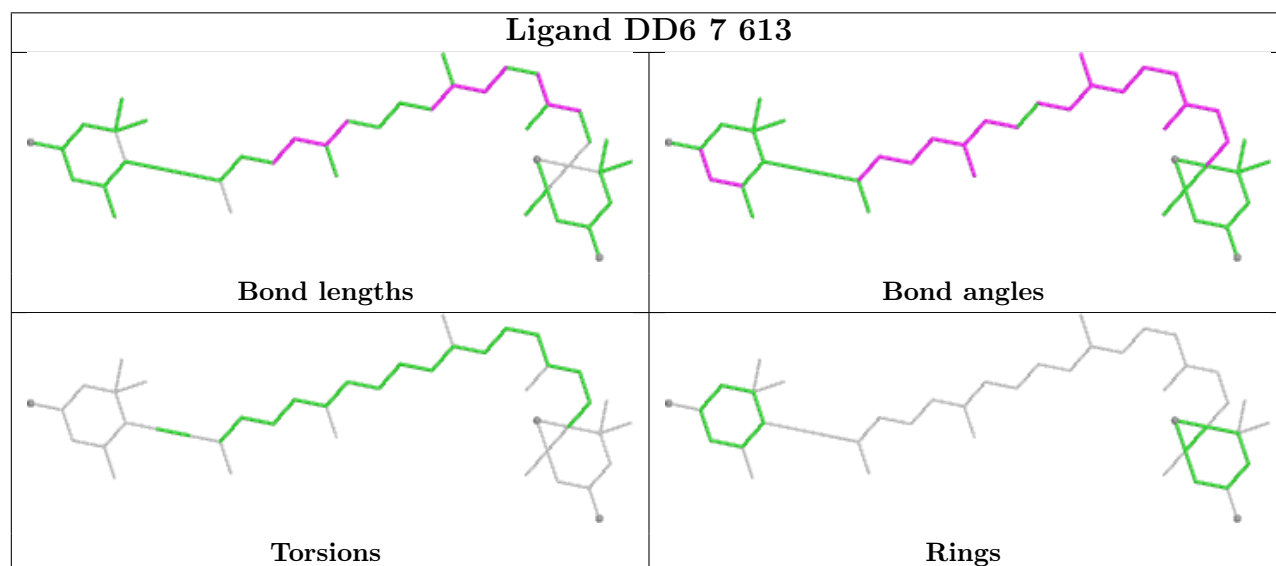
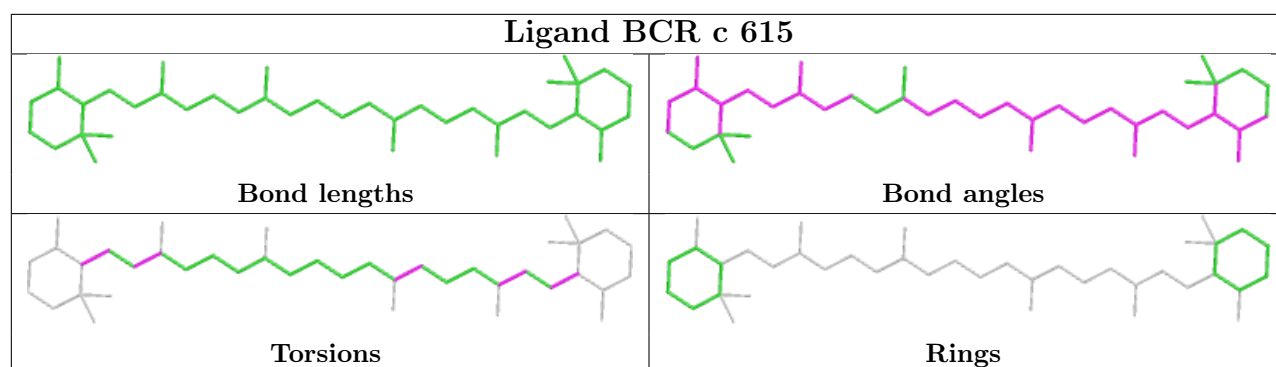


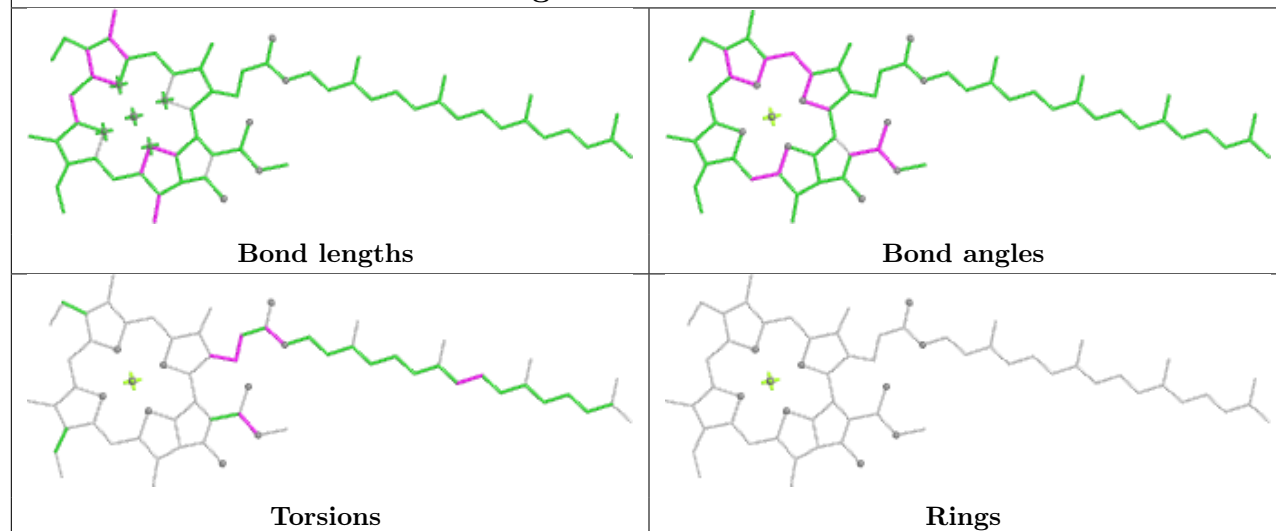
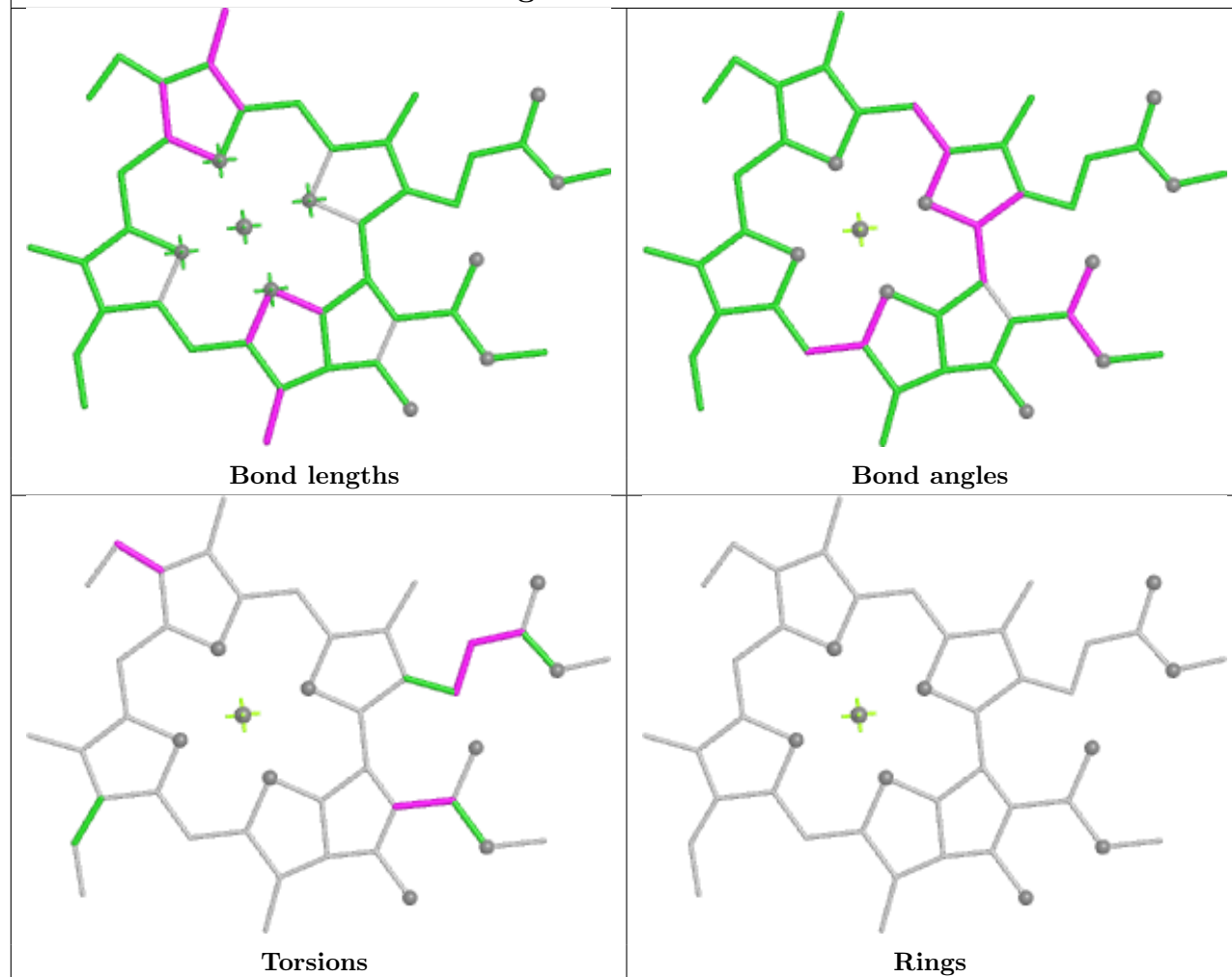
Ligand CLA 8 207



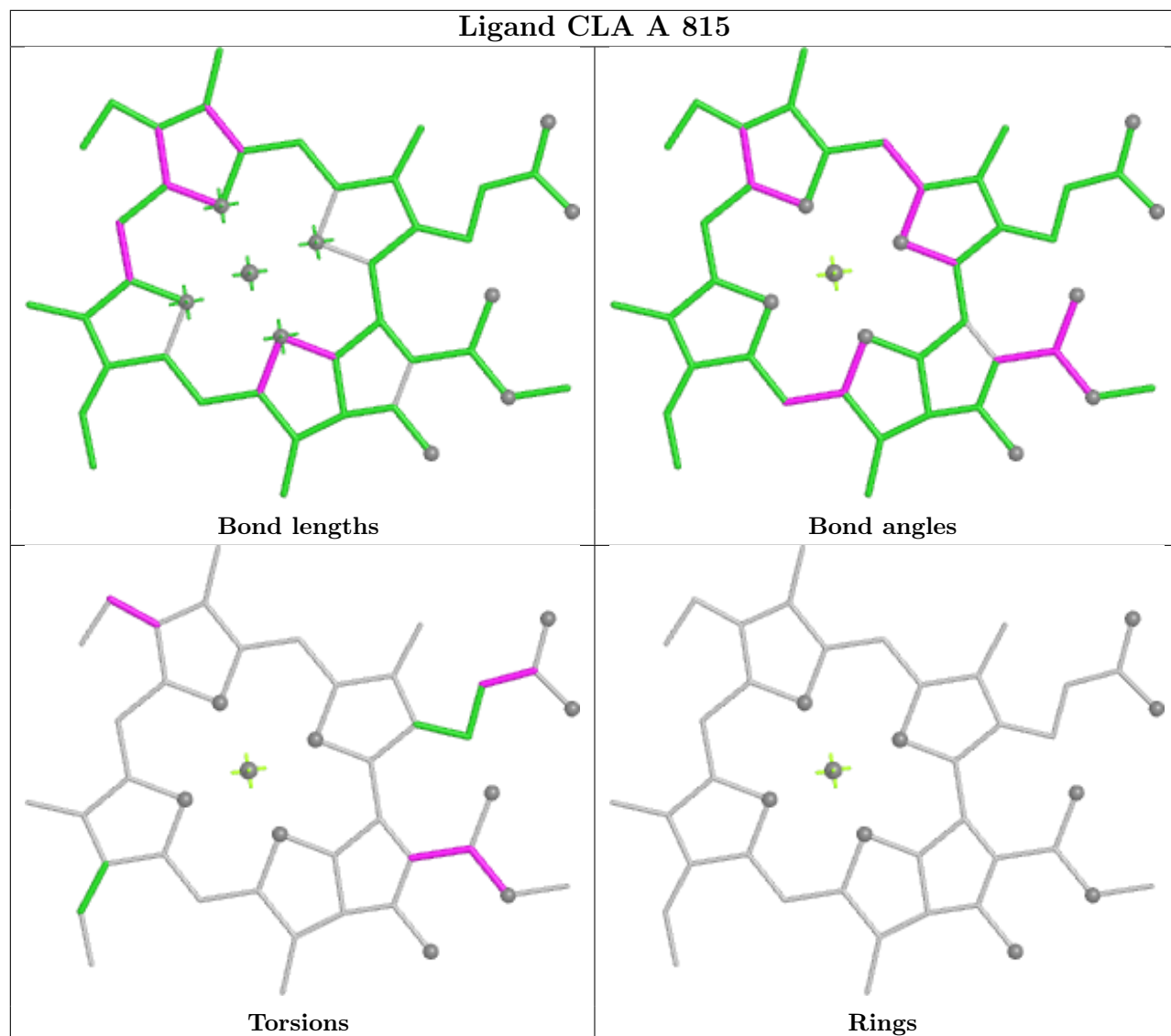
Ligand DD6 k 314



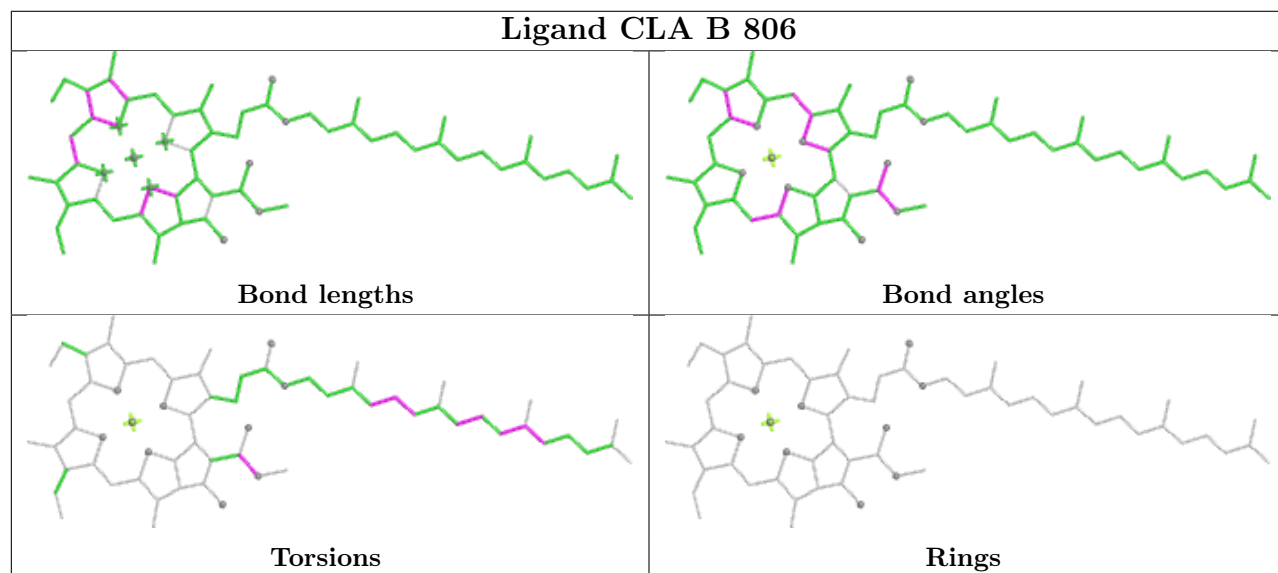


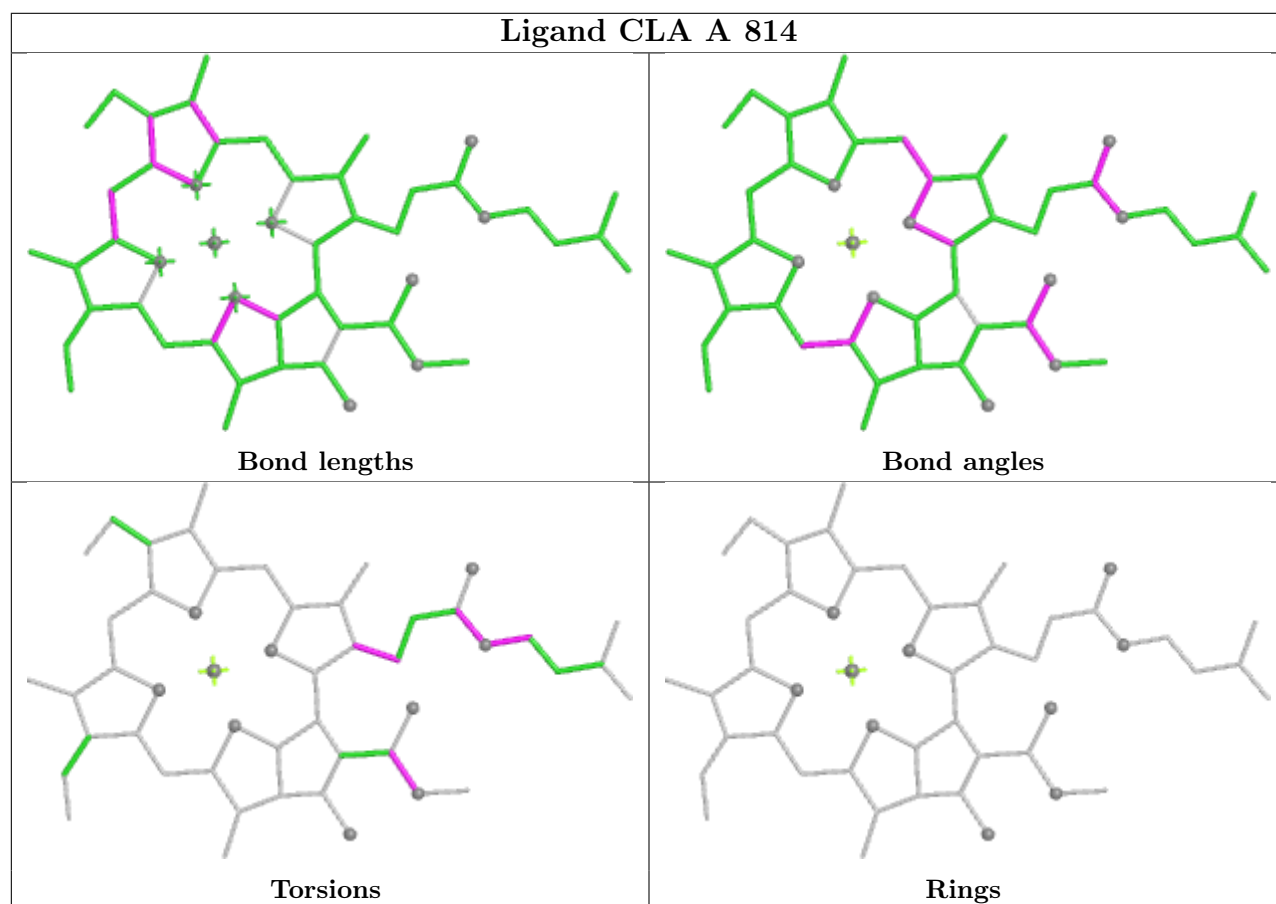
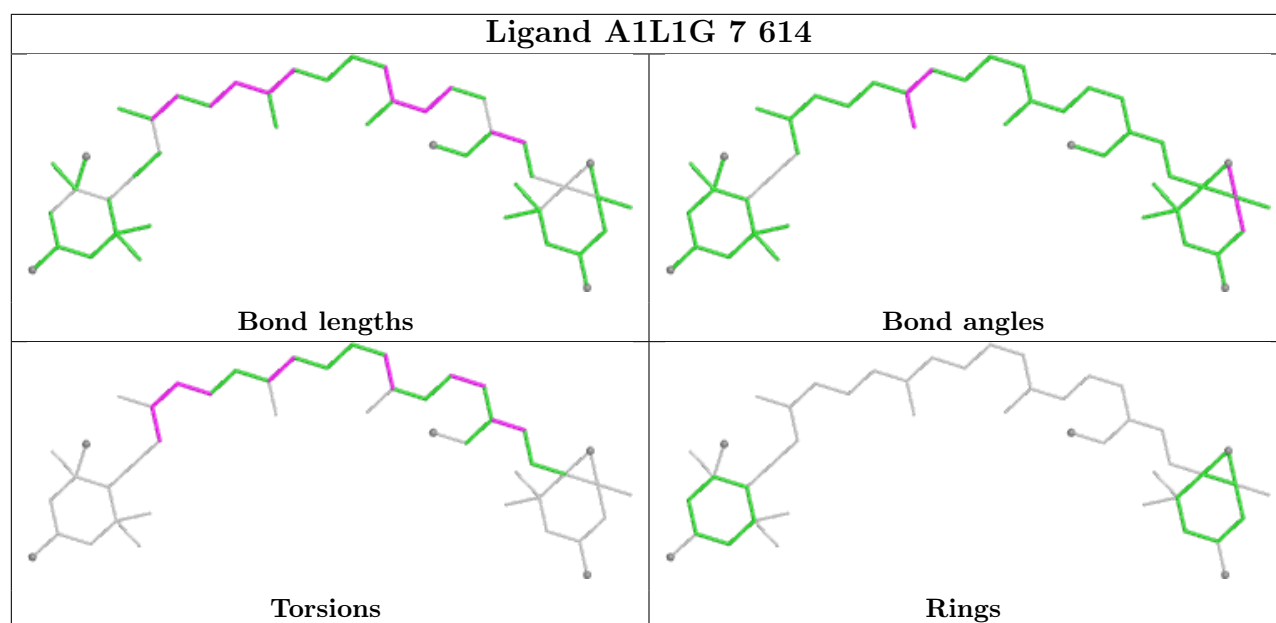
Ligand CLA B 826**Ligand CLA 9 306**

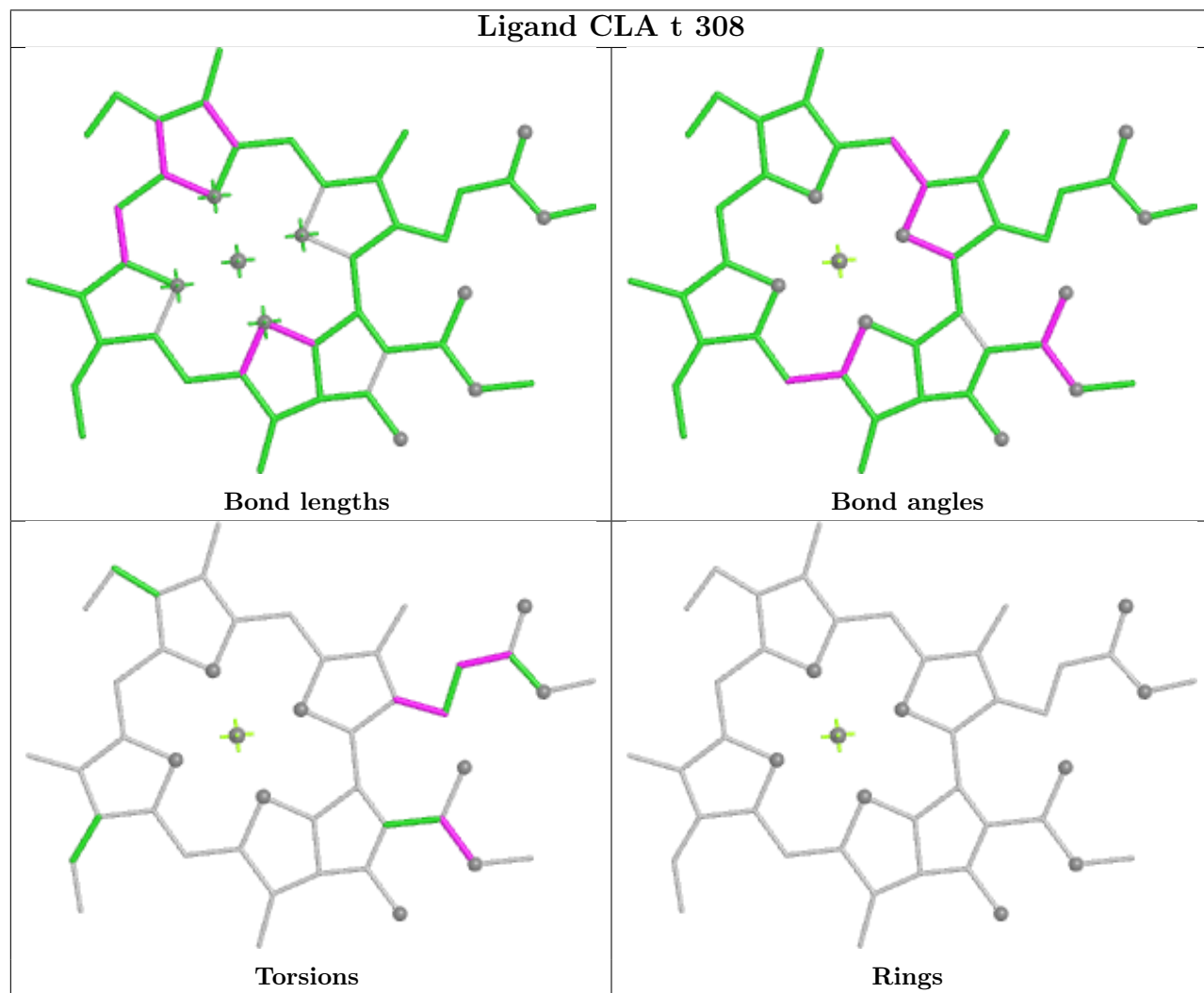
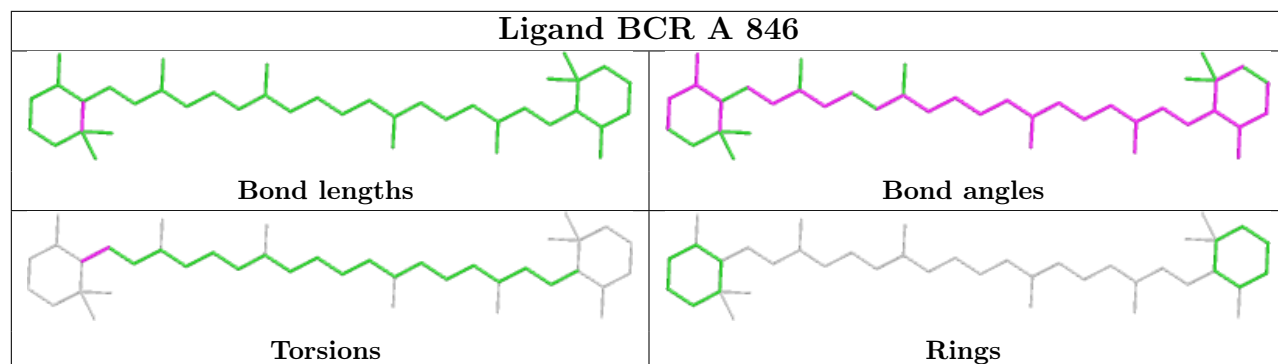
Ligand CLA A 815

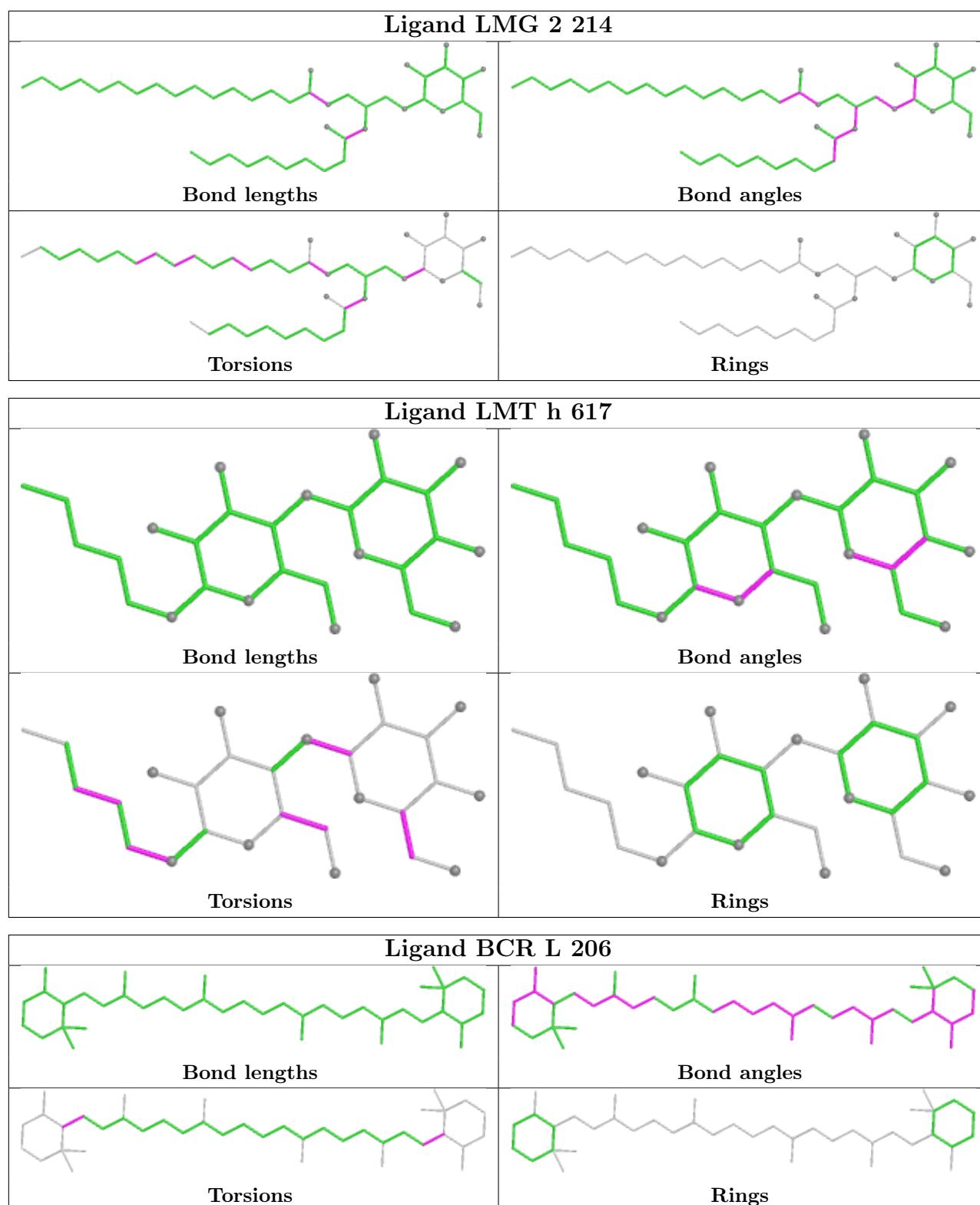


Ligand CLA B 806

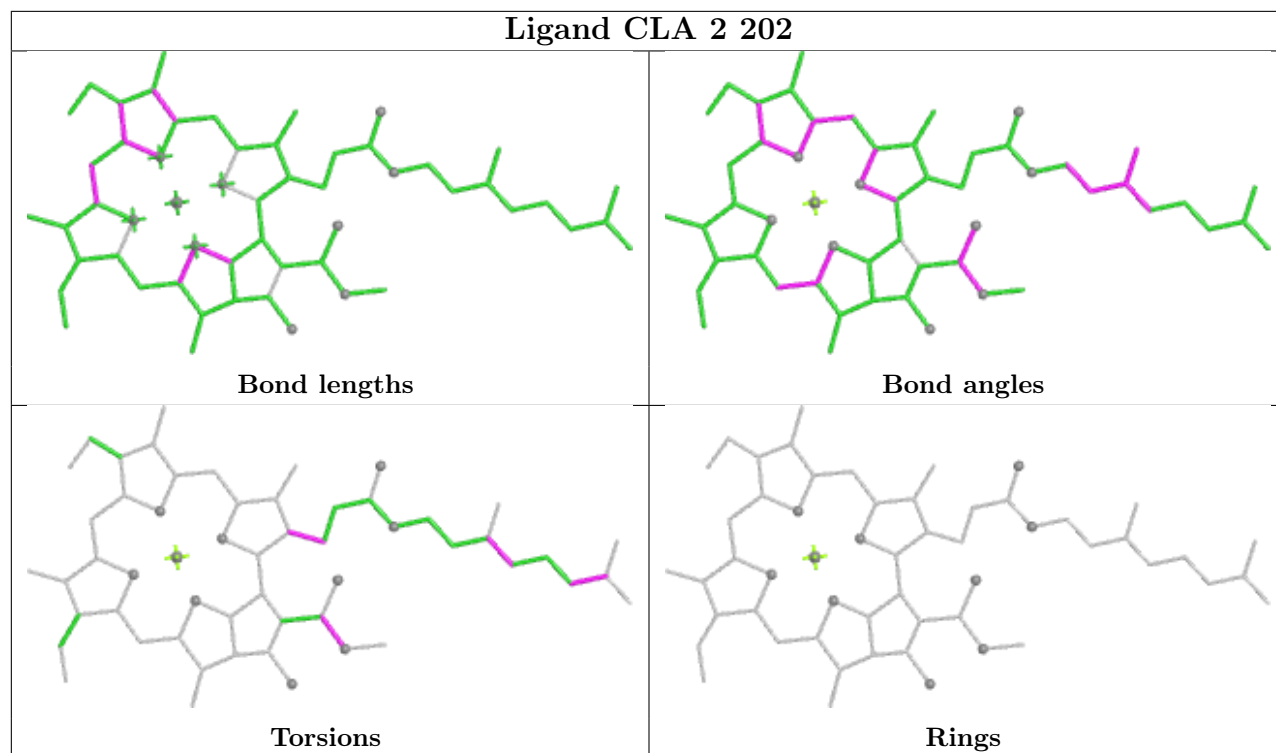




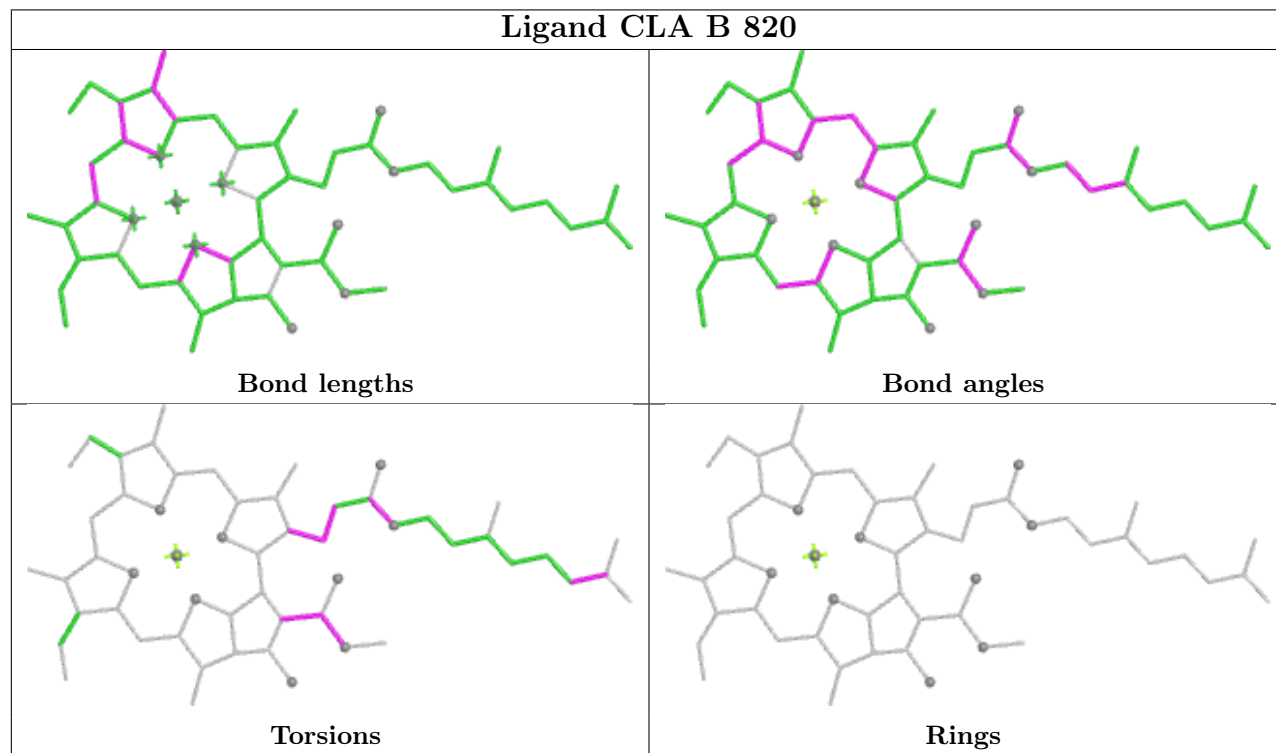




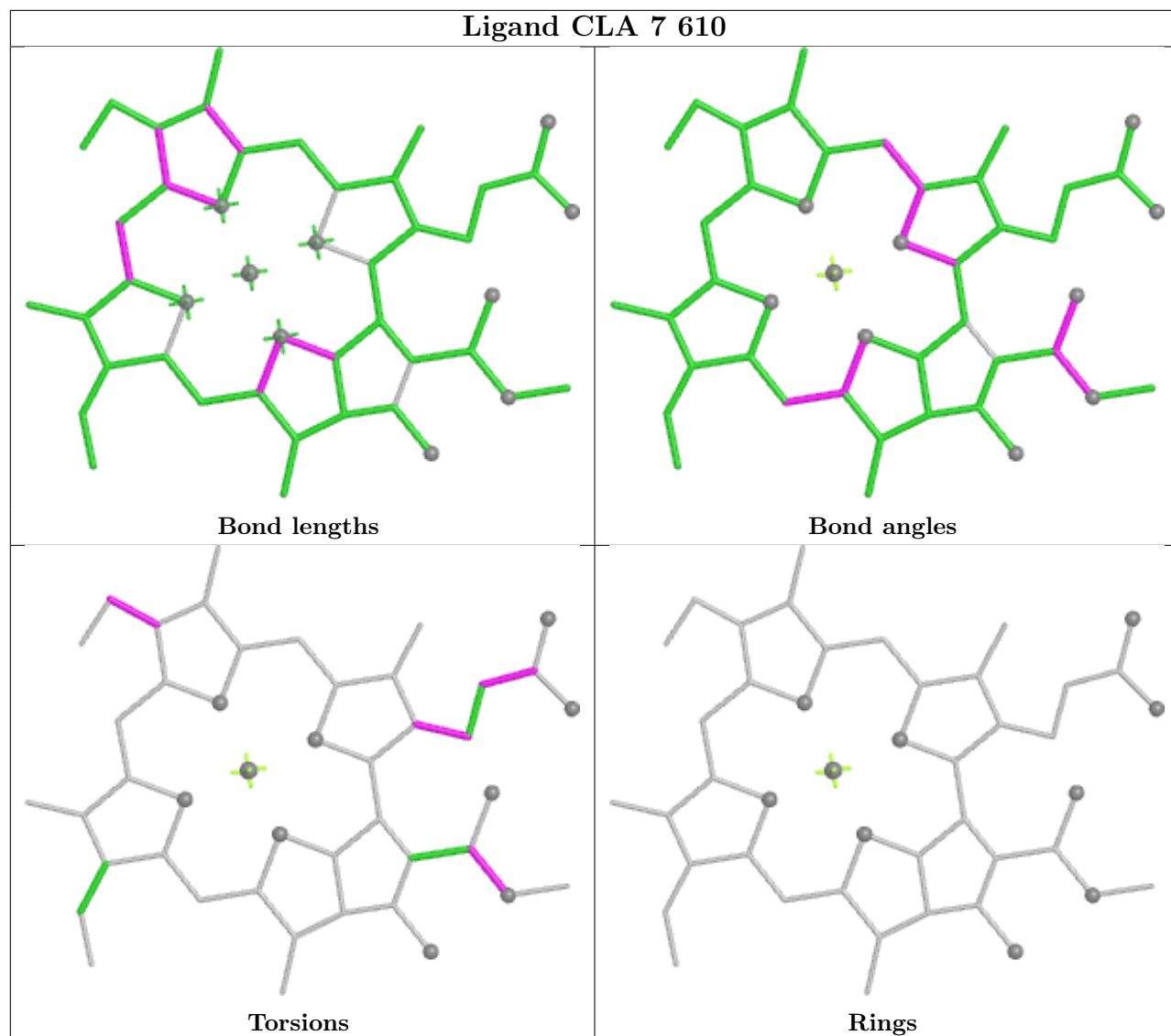
Ligand CLA 2 202



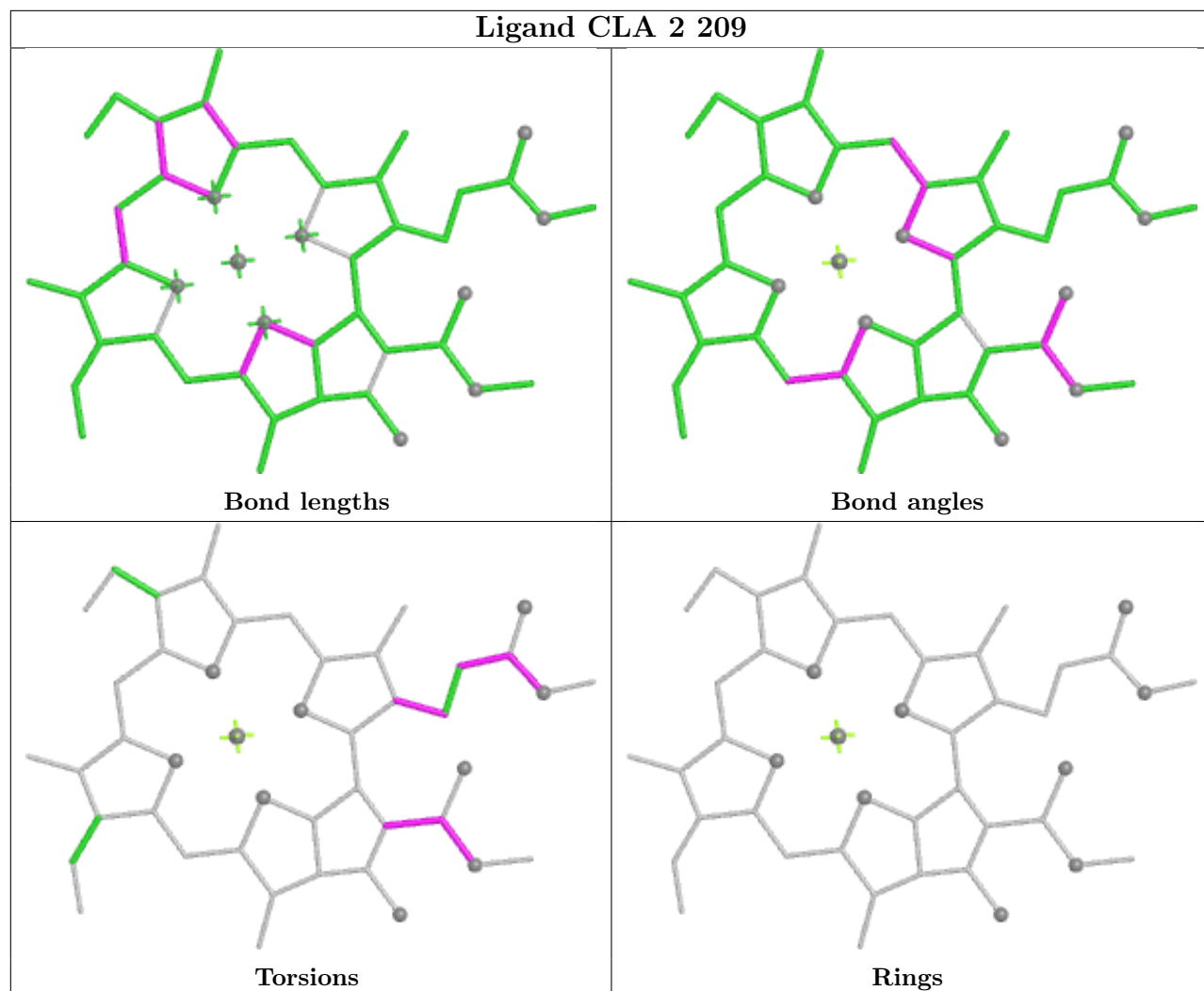
Ligand CLA B 820

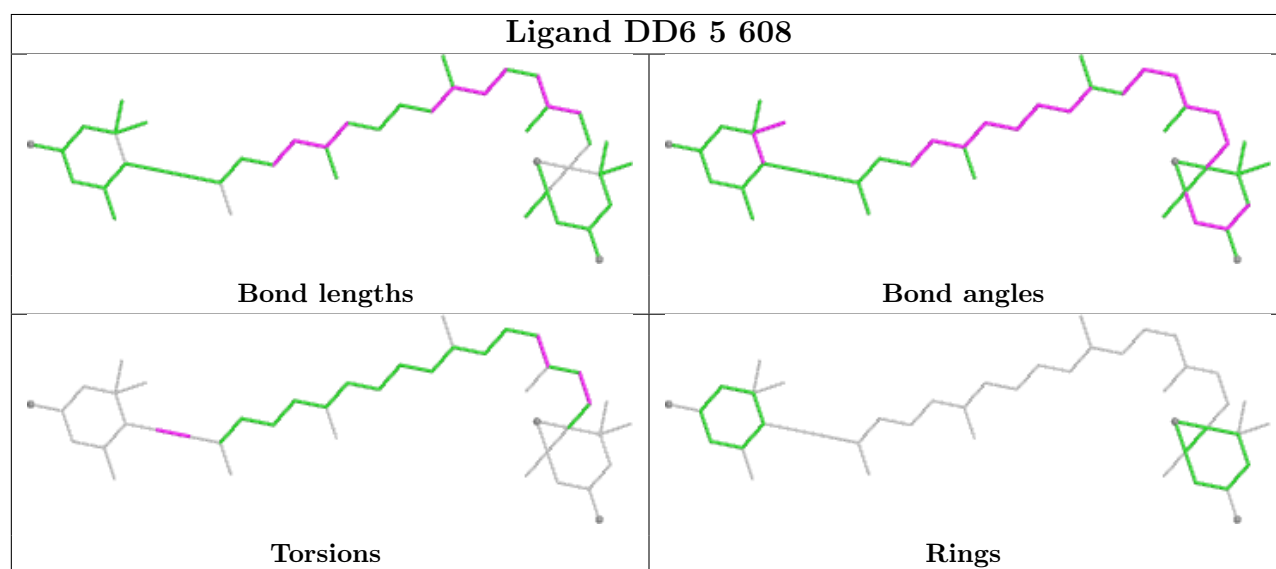
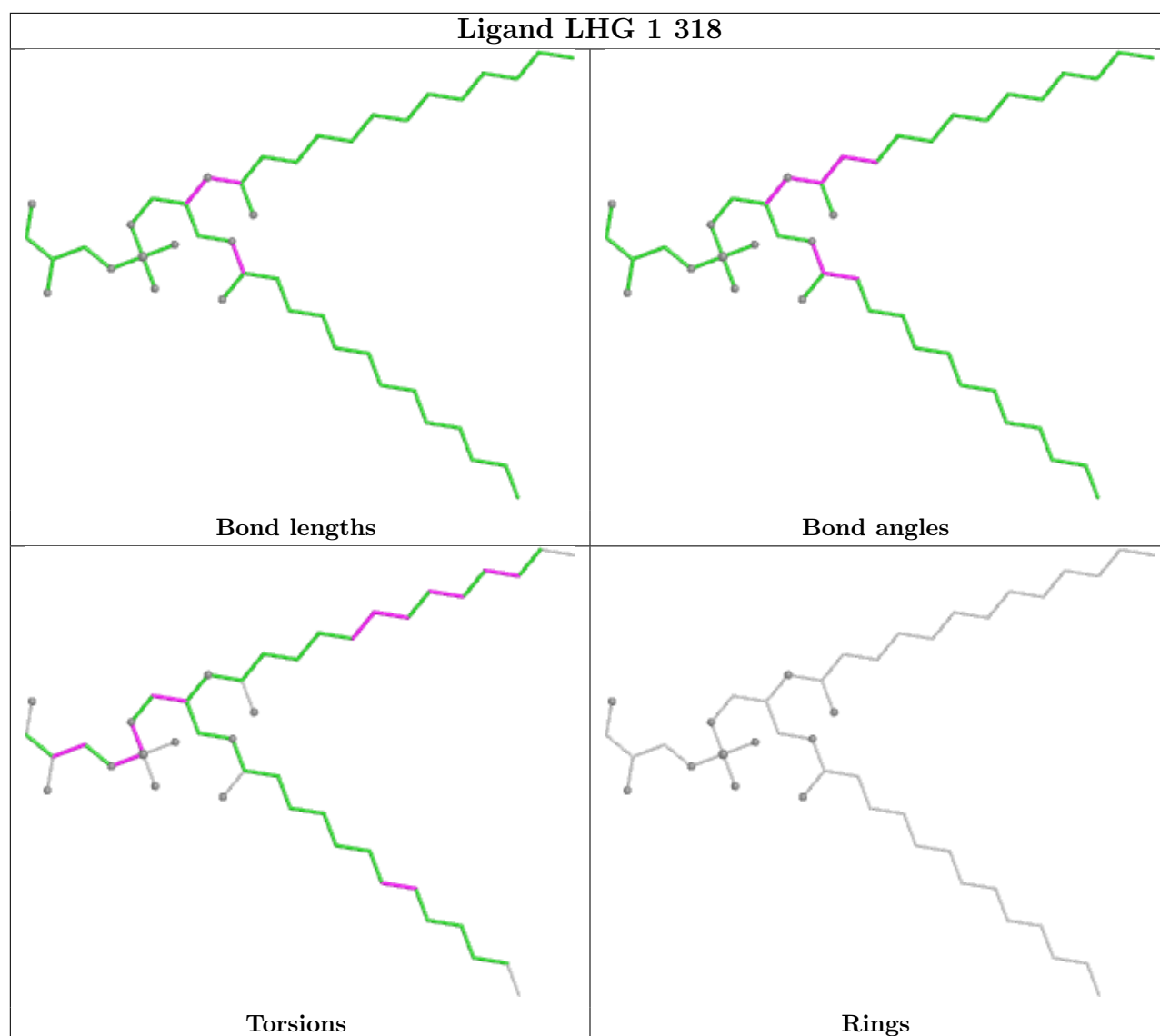


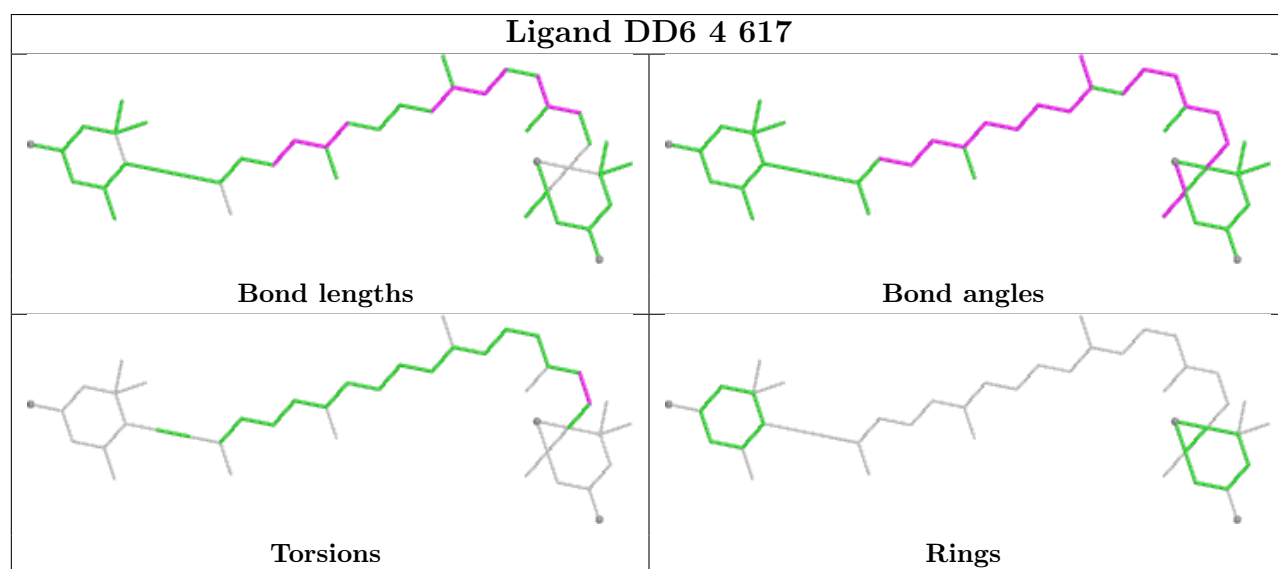
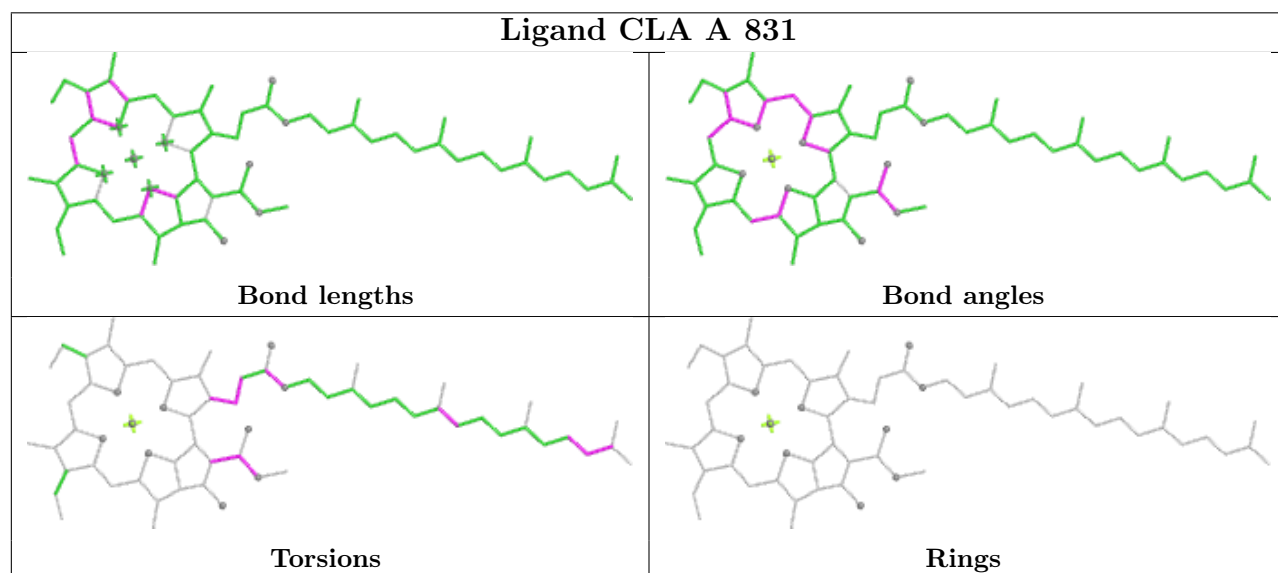
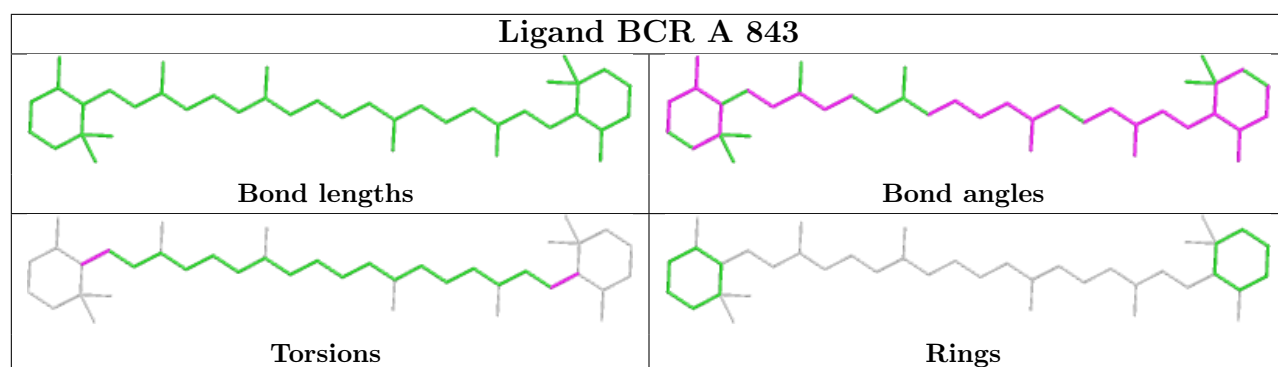
Ligand CLA 7 610

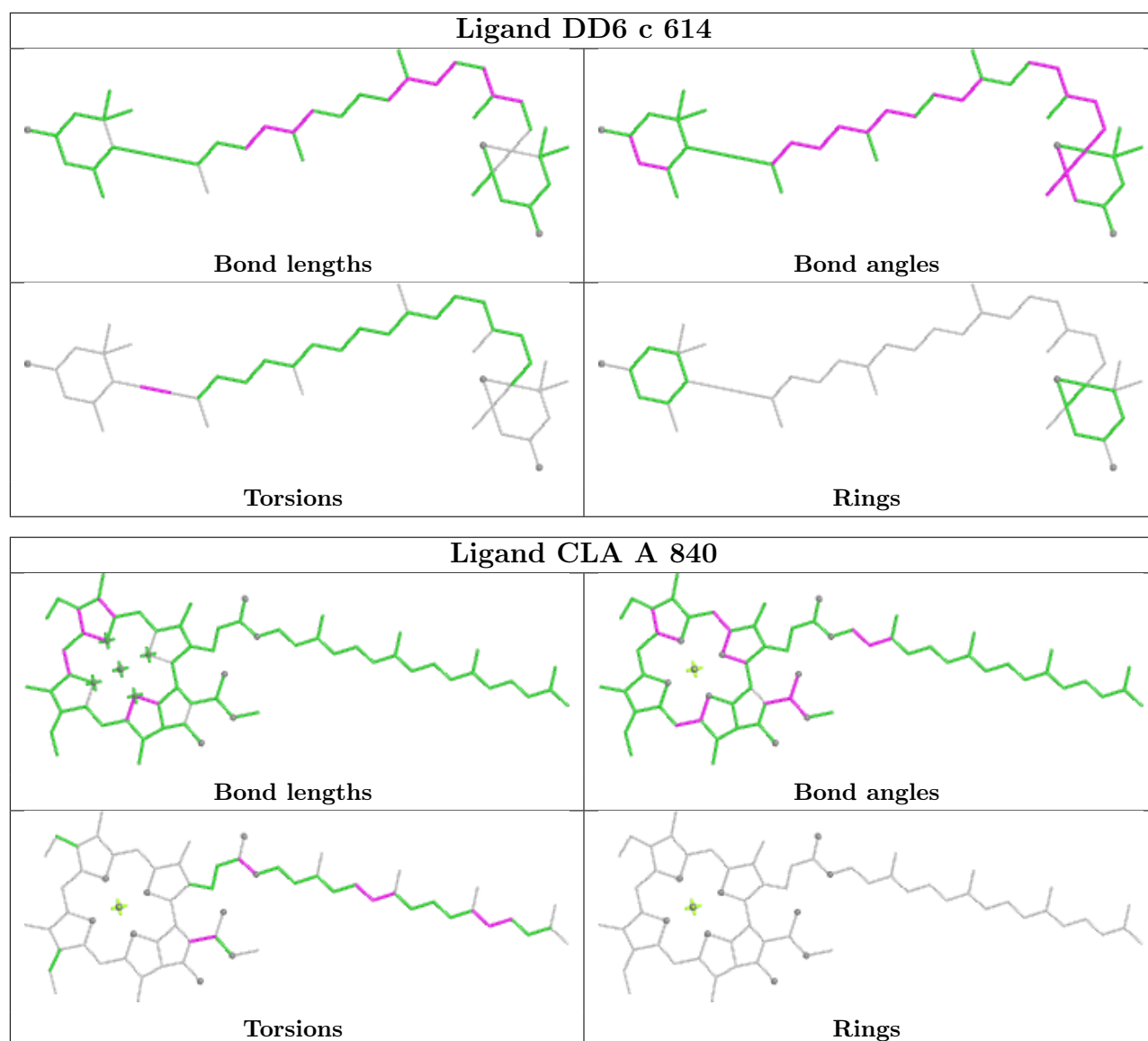


Ligand CLA 2 209

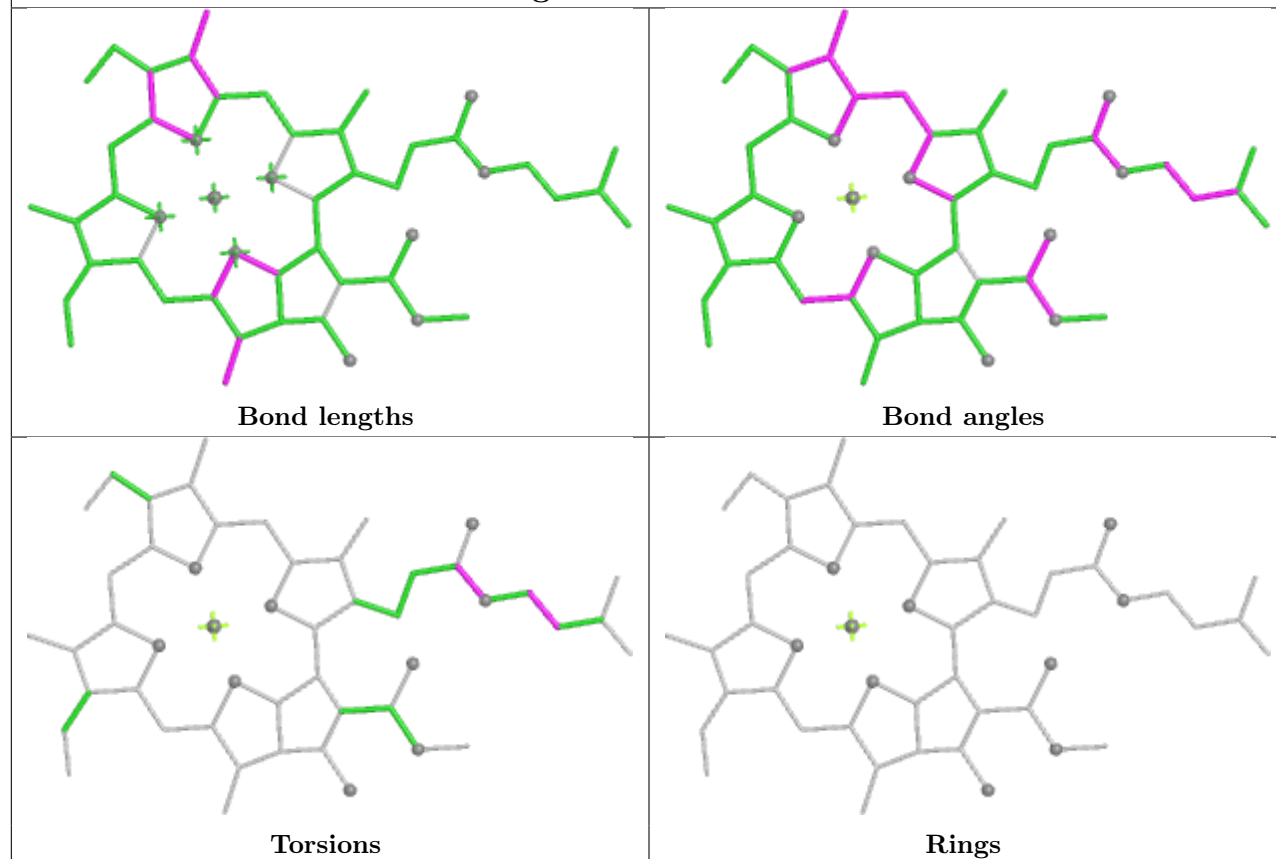




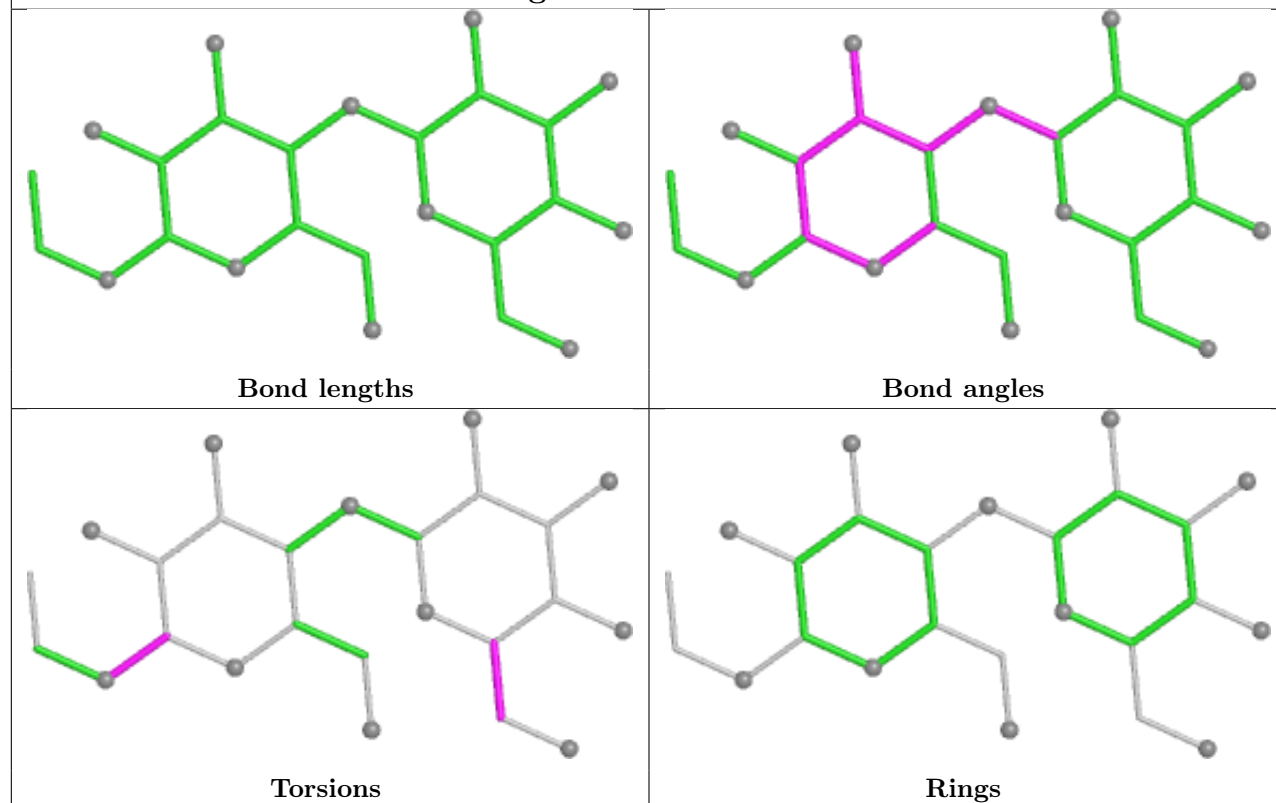


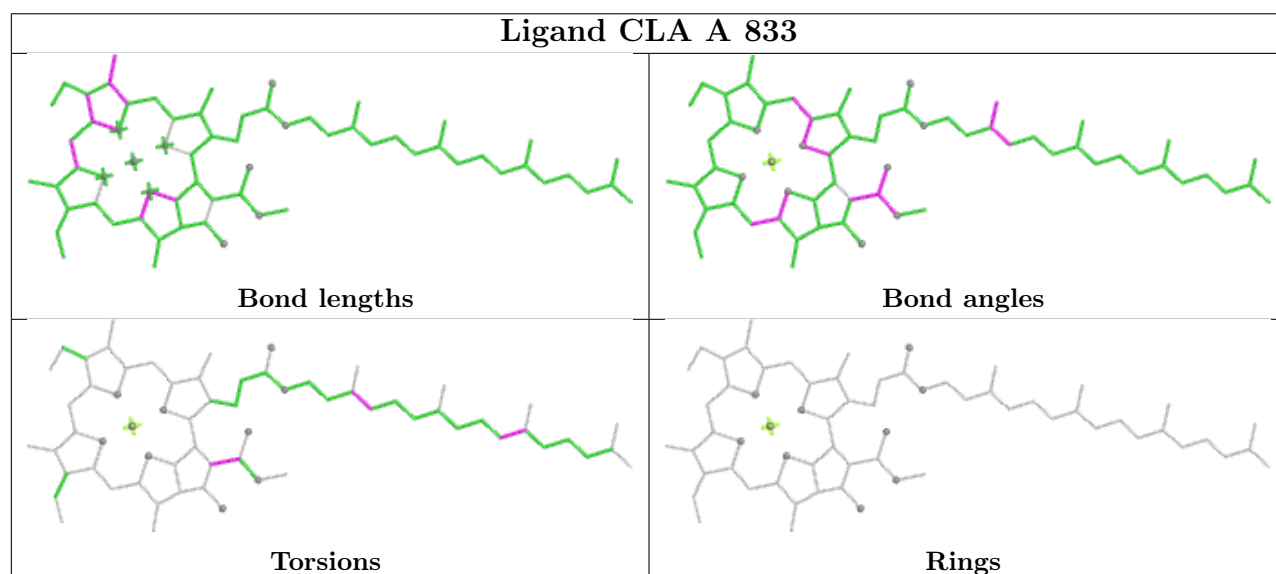
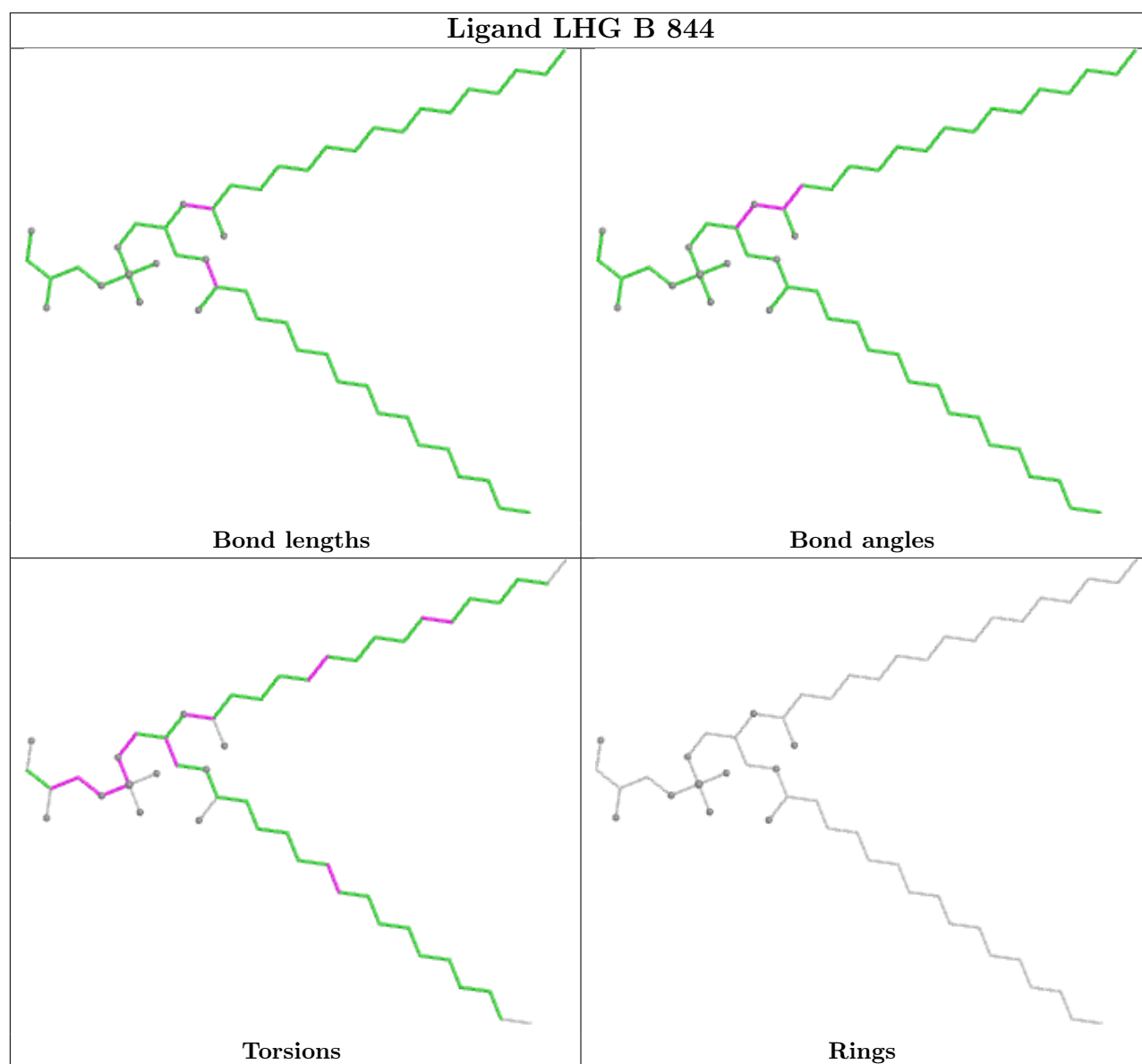


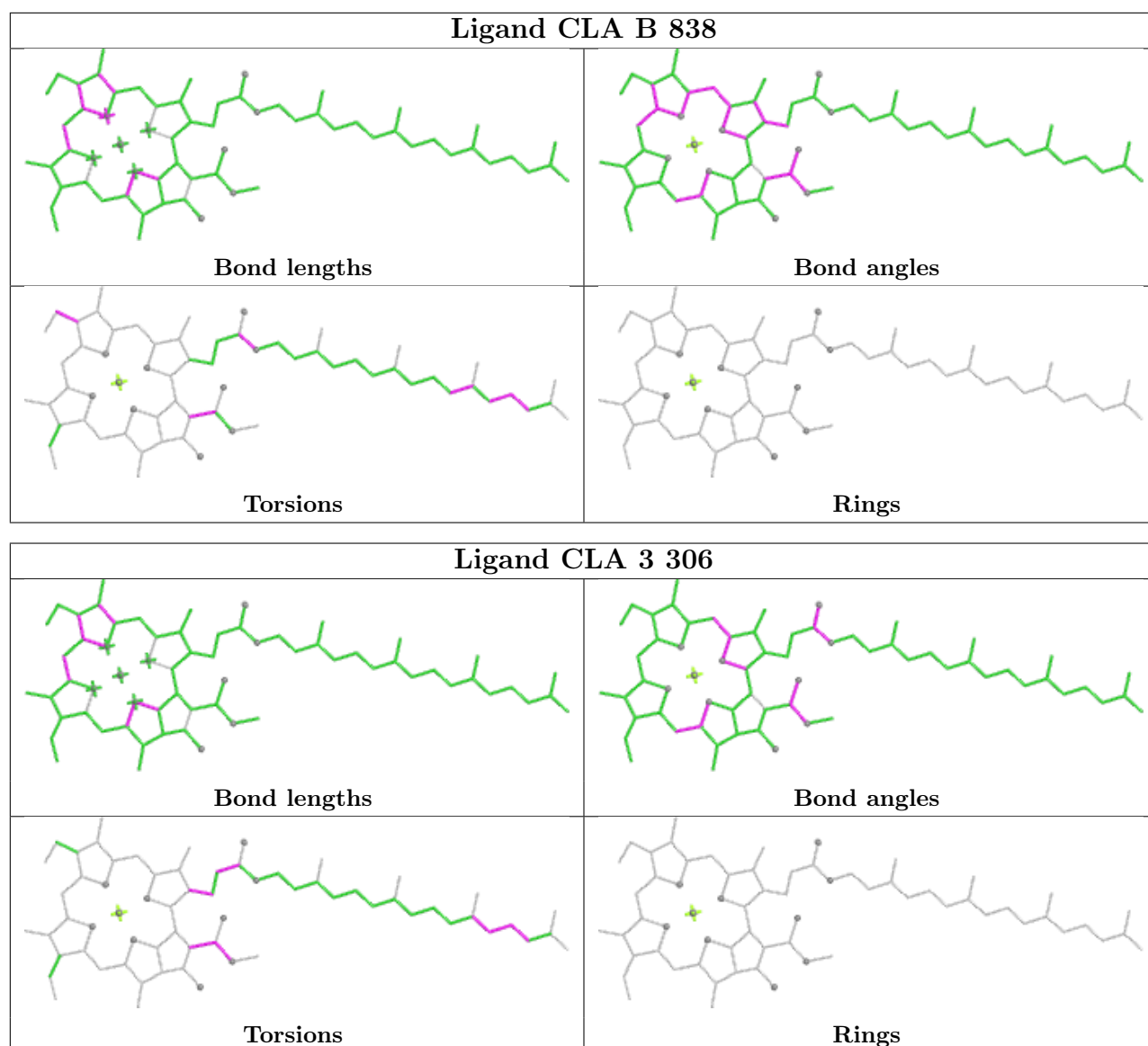
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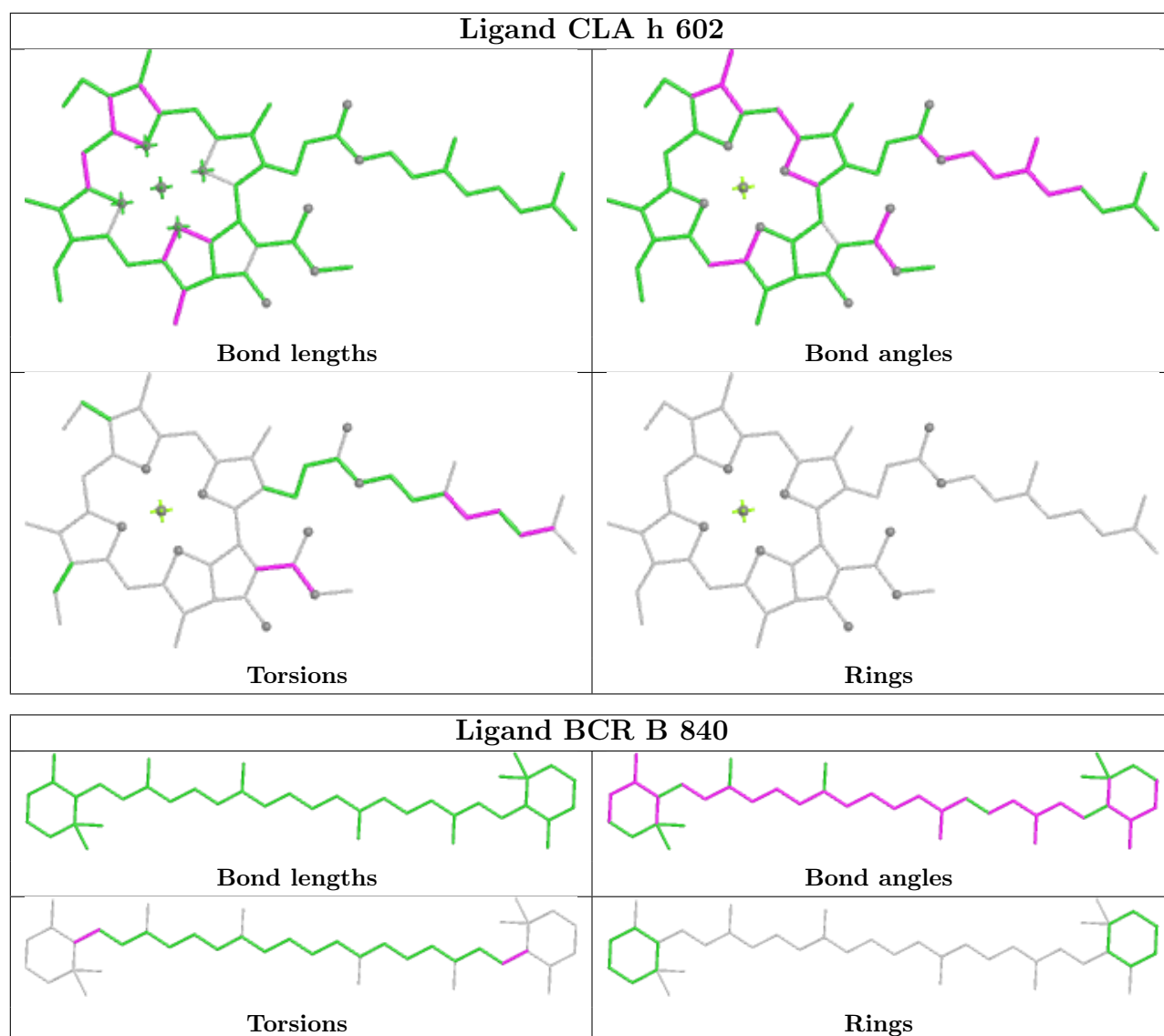


Ligand LMT A 851

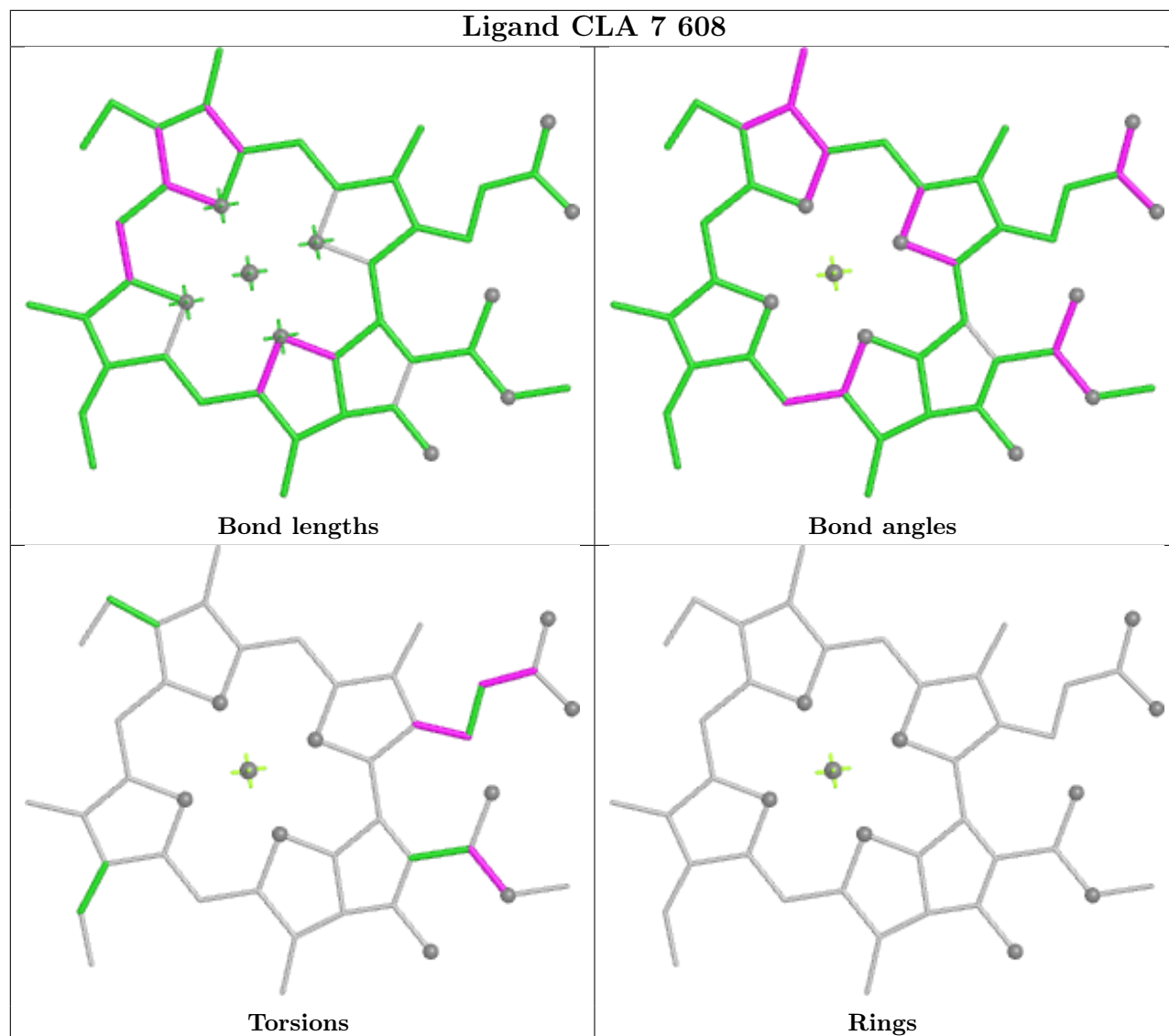




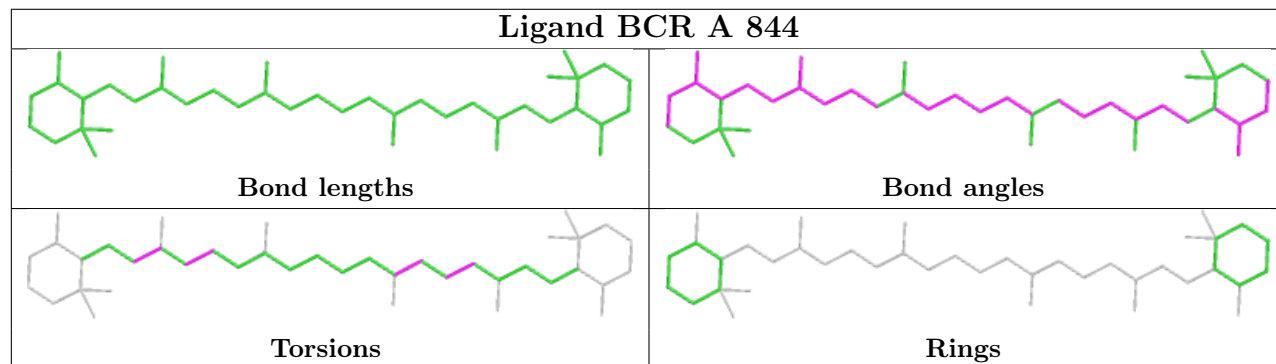




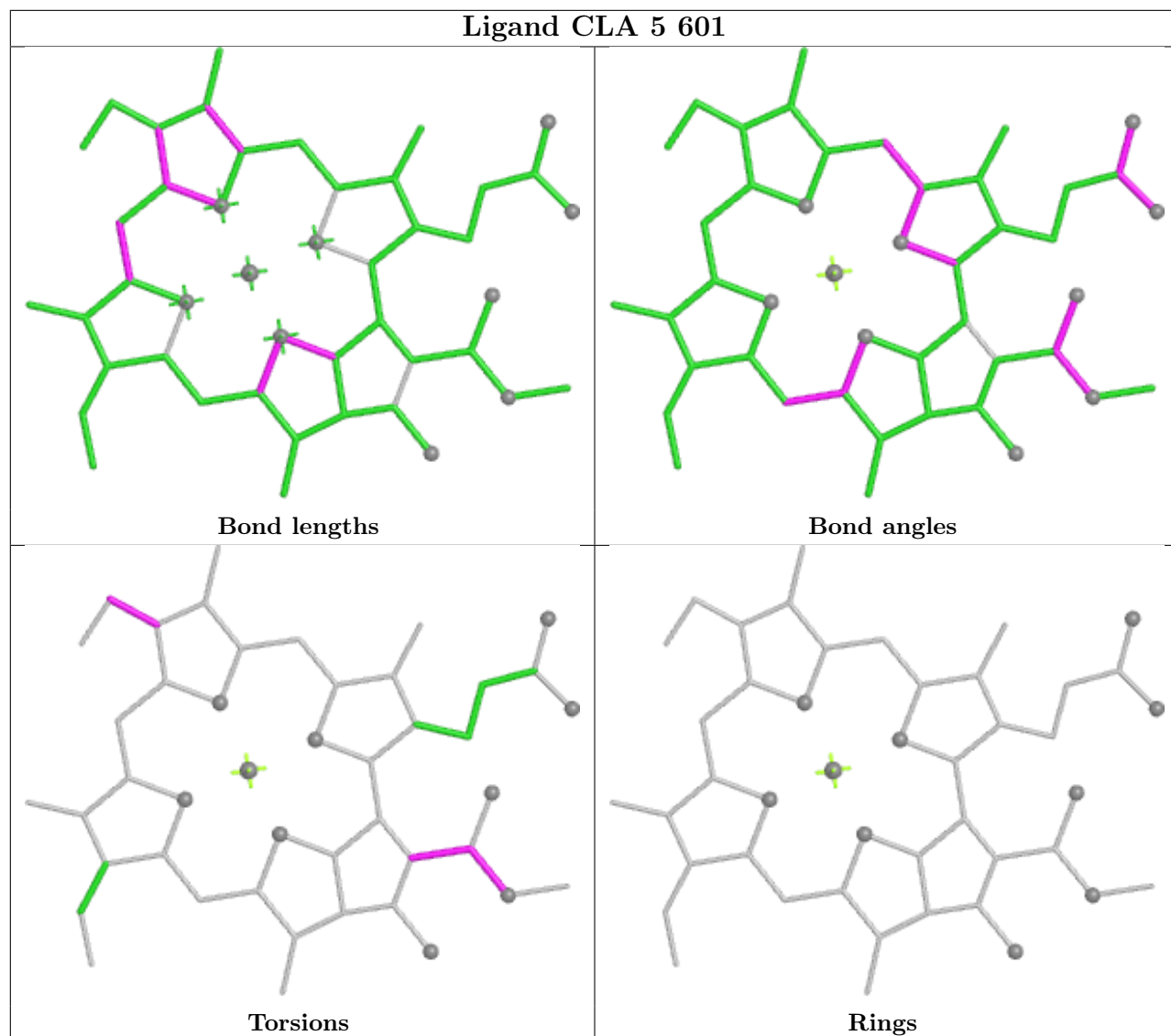
Ligand CLA 7 608



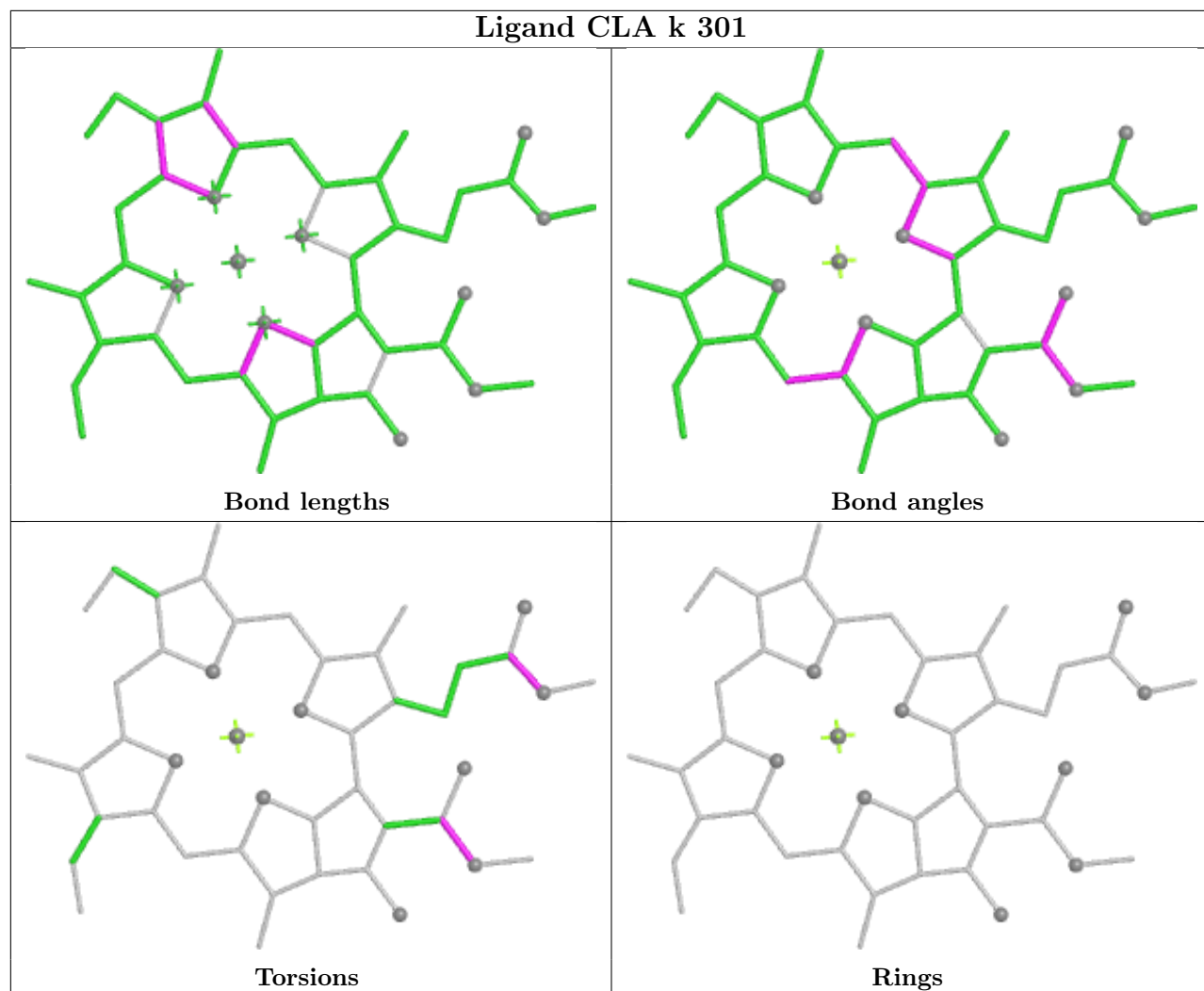
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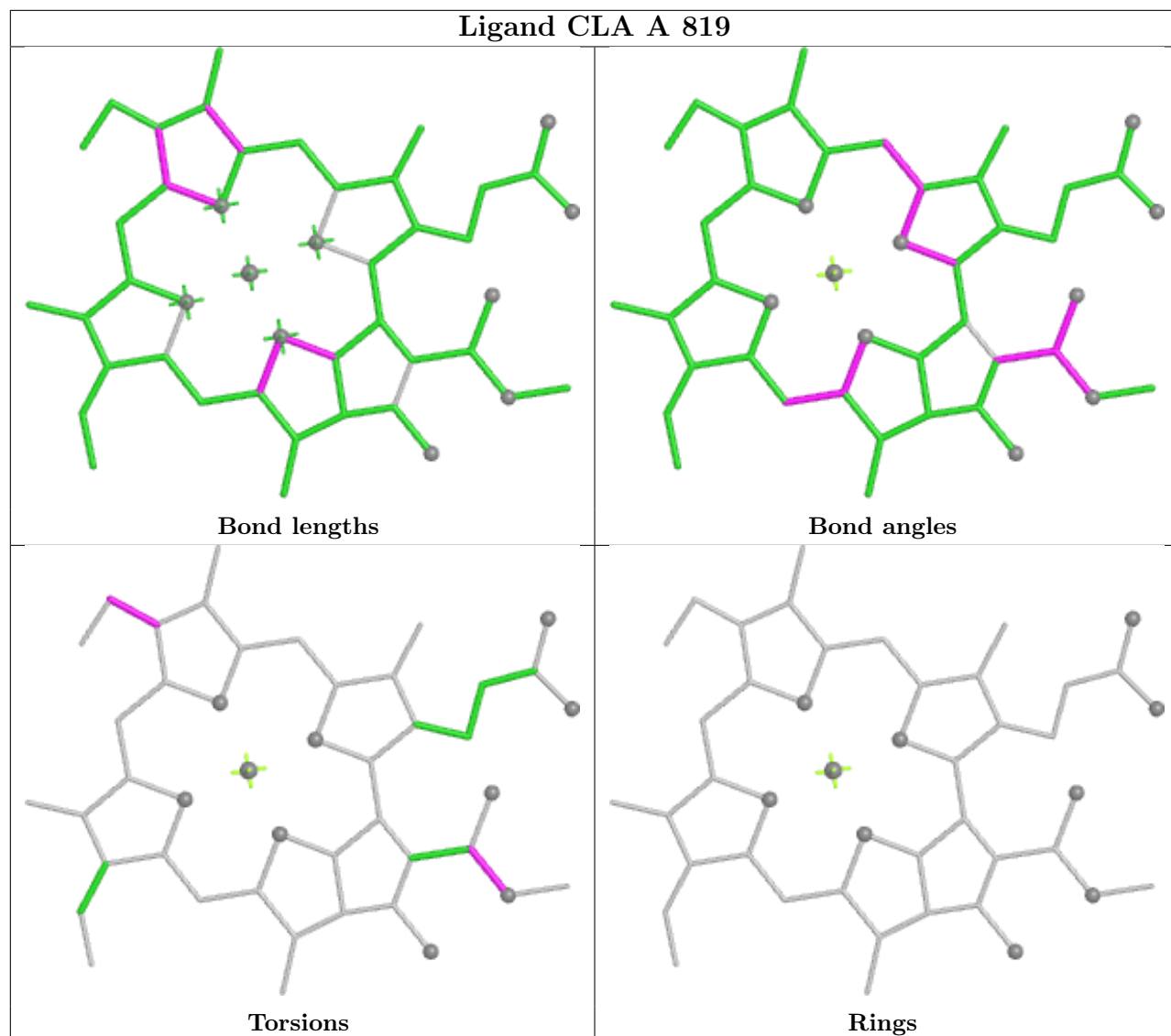
Ligand CLA 5 601



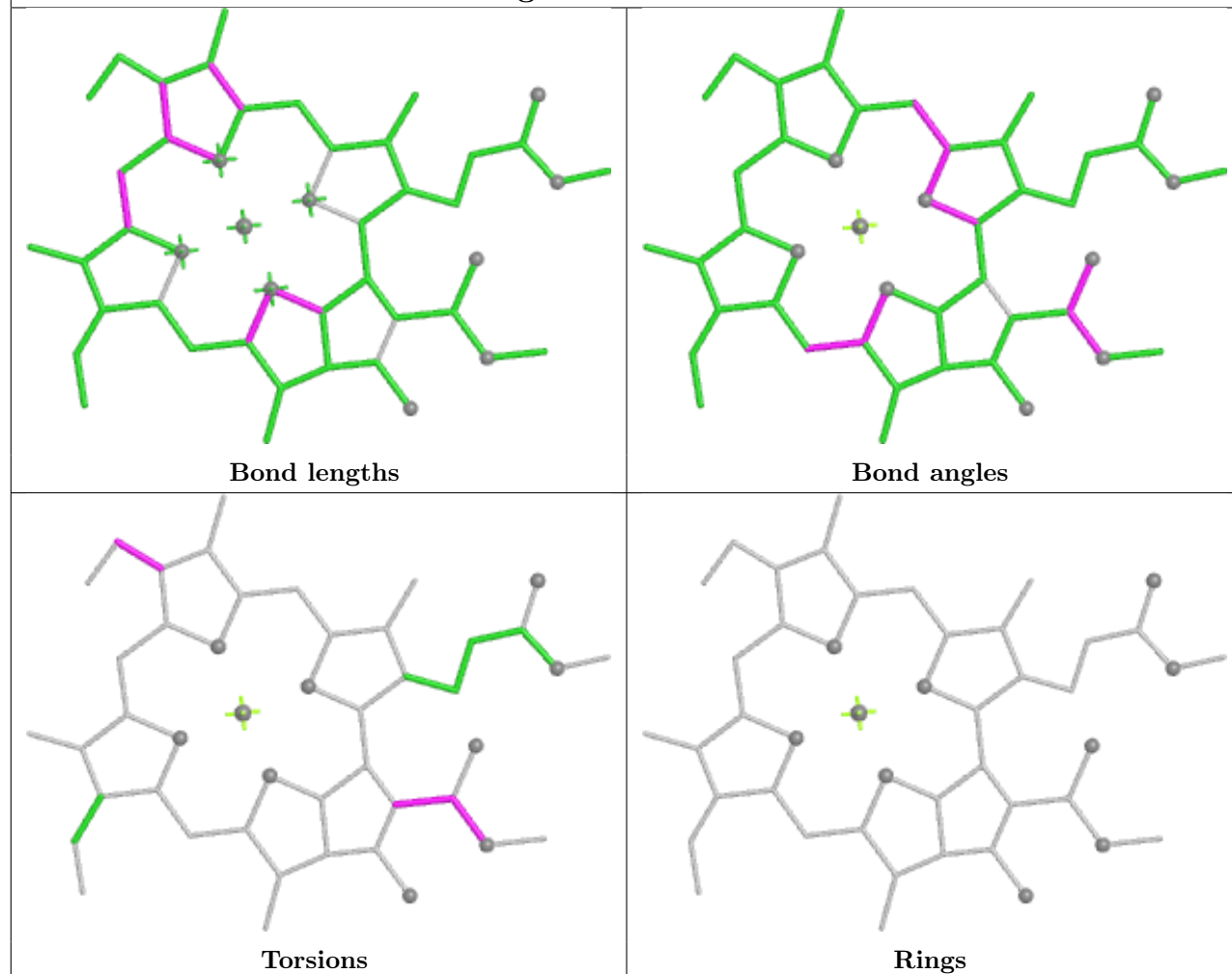
Ligand CLA k 301



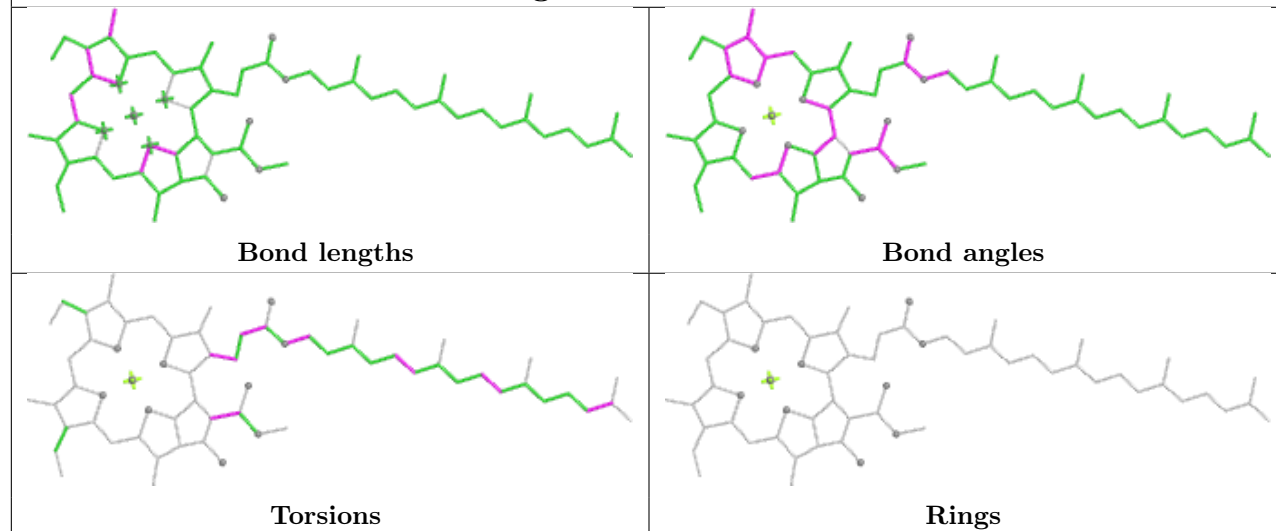
Ligand CLA A 819

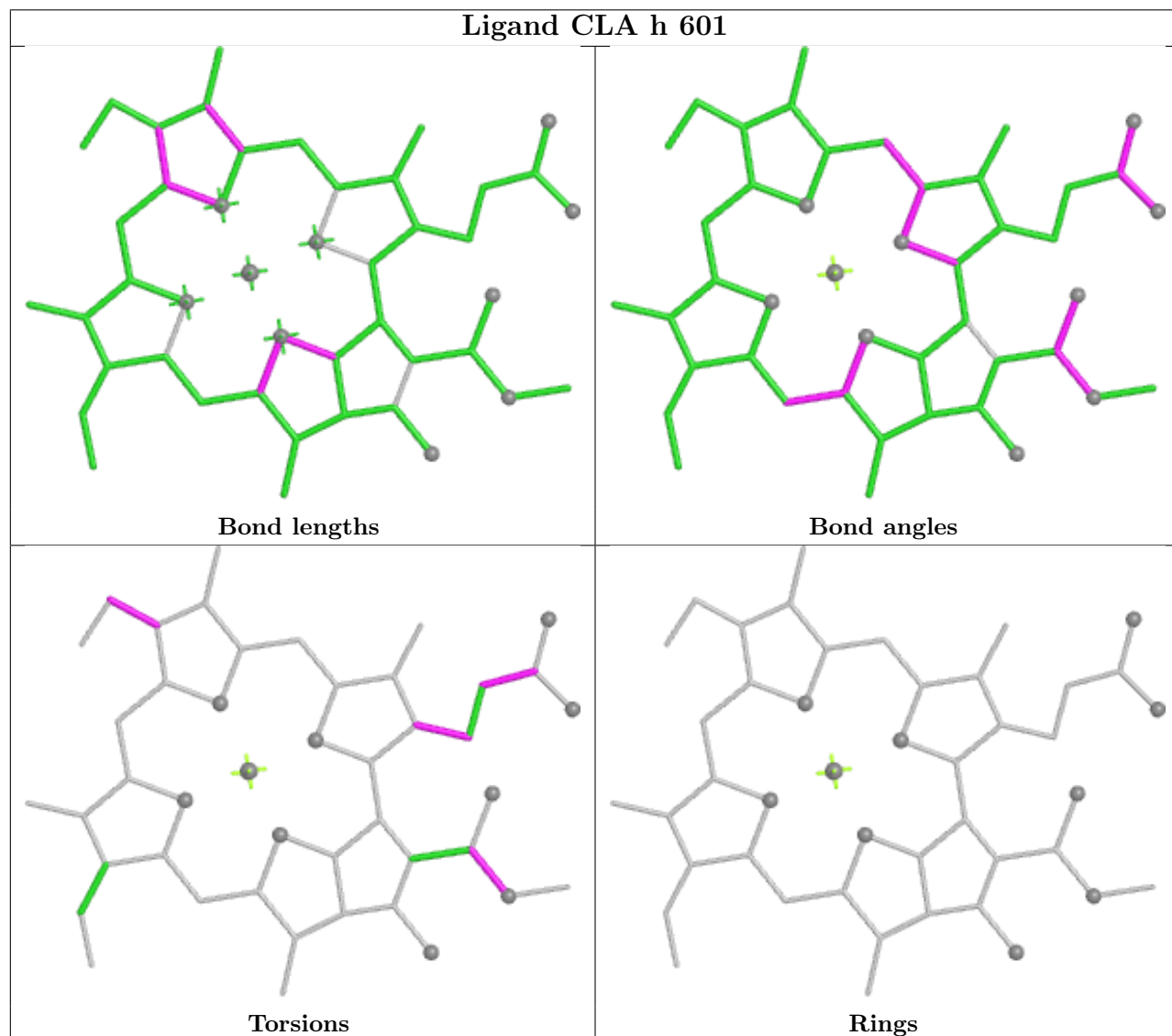
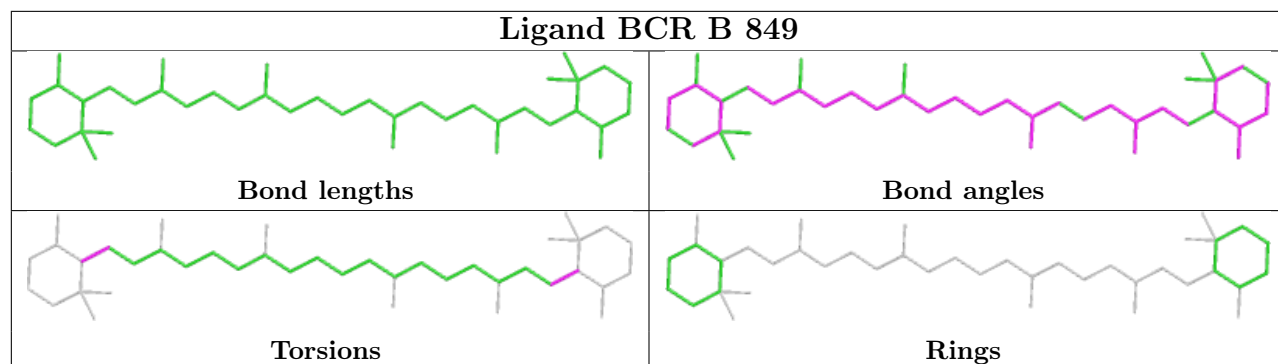


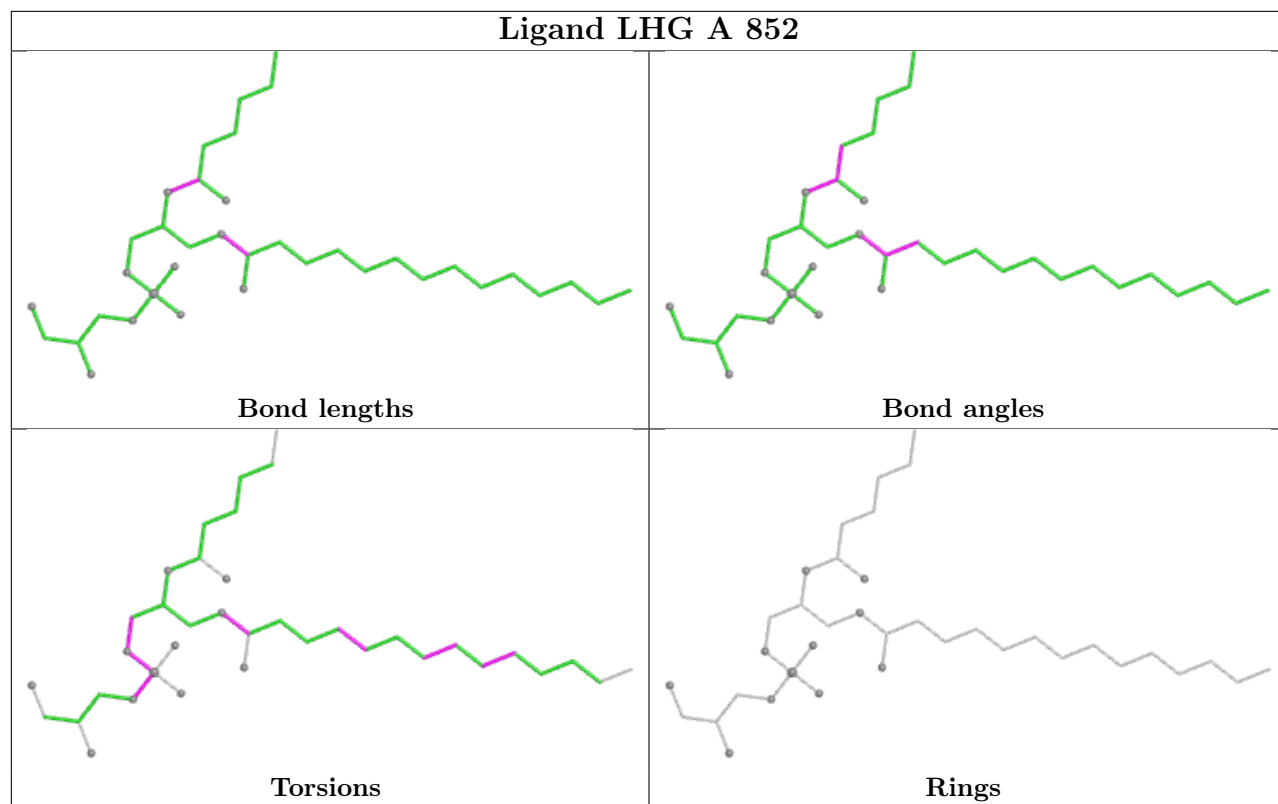
Ligand CLA 8 201



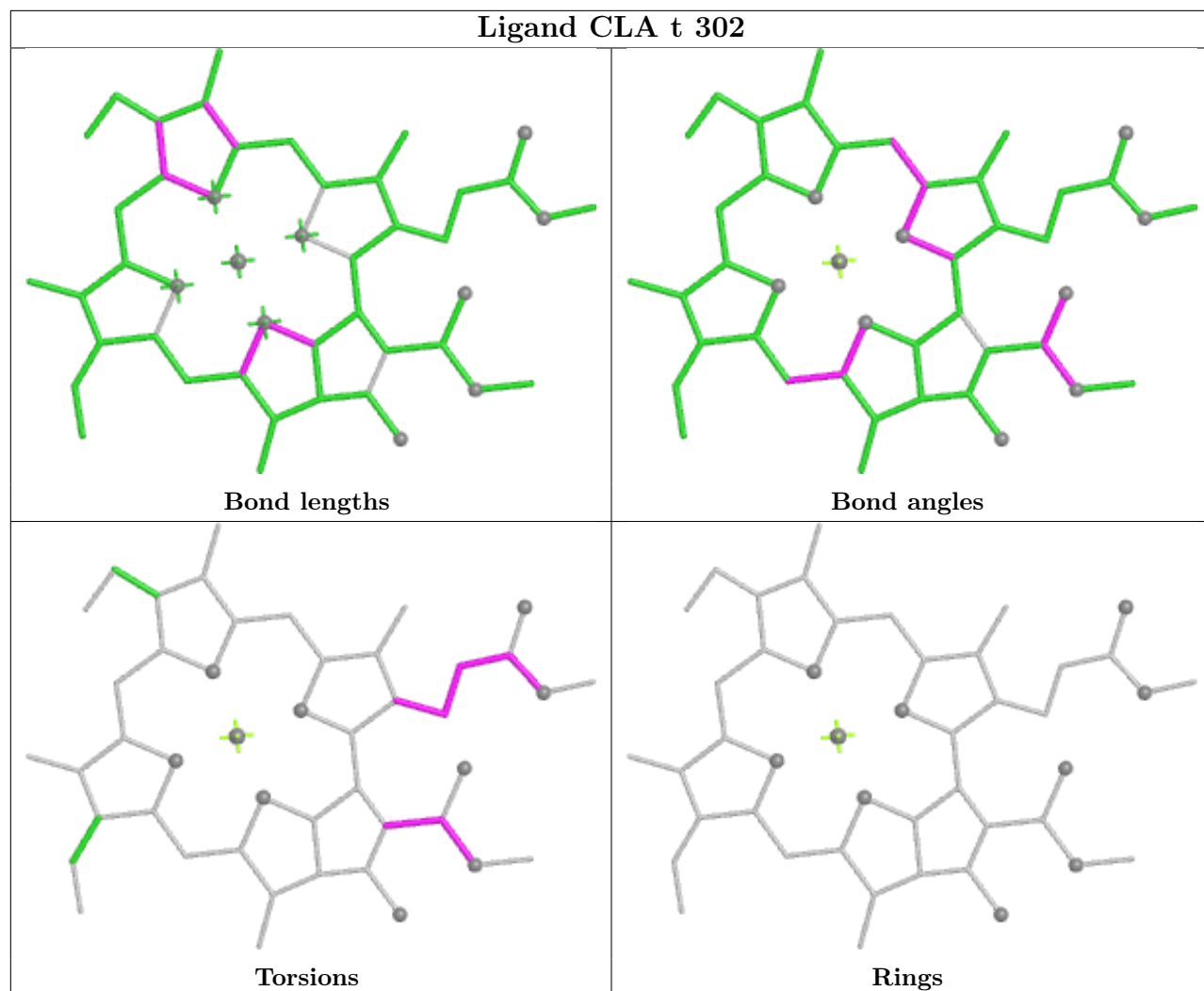
Ligand CLA B 804



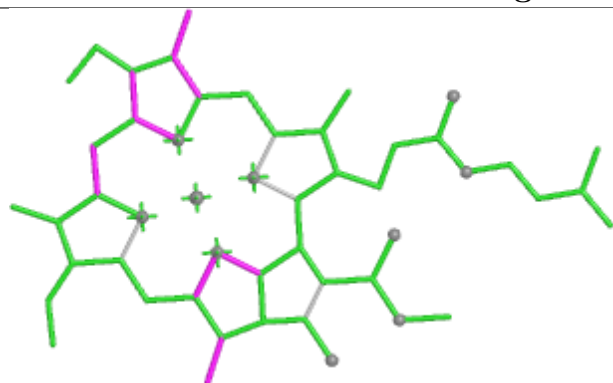




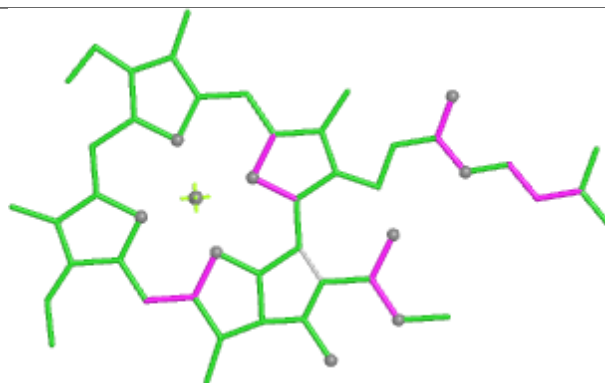
Ligand CLA t 302



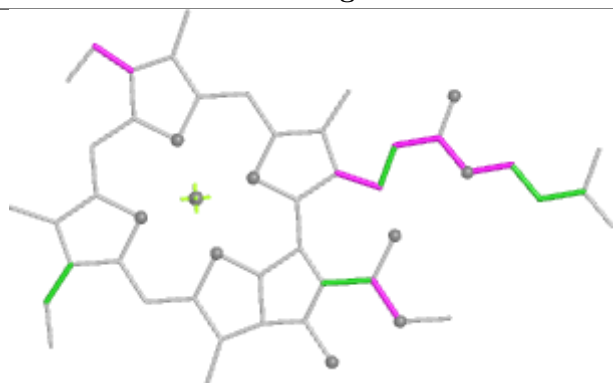
Ligand CLA B 828



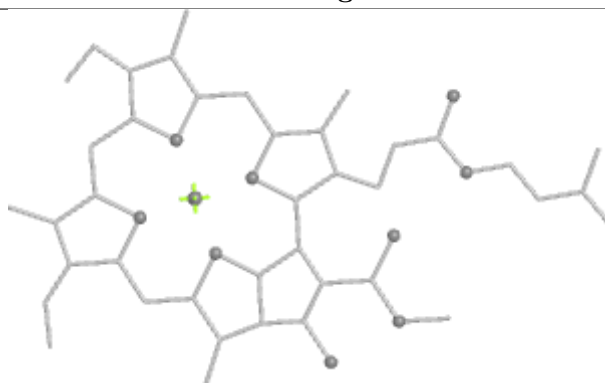
Bond lengths



Bond angles

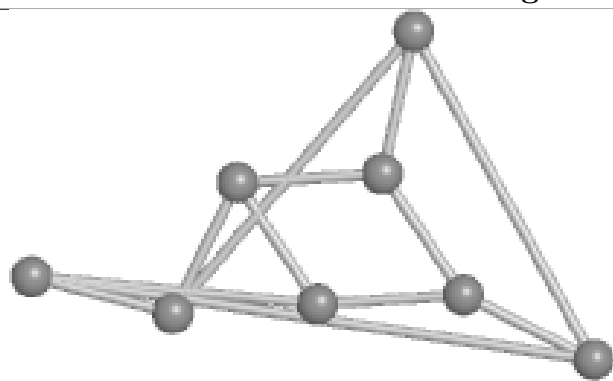


Torsions

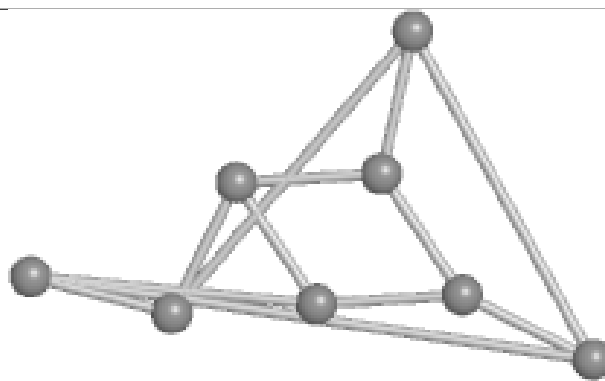


Rings

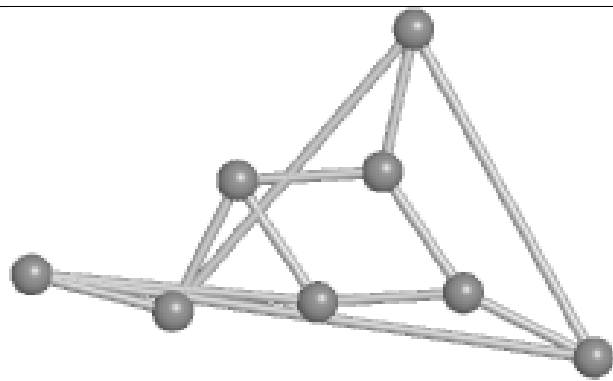
Ligand SF4 C 102



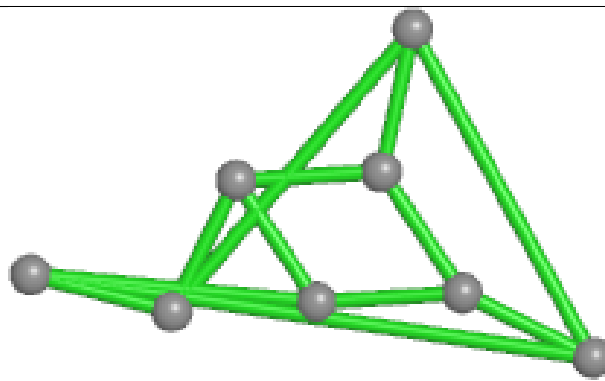
Bond lengths



Bond angles

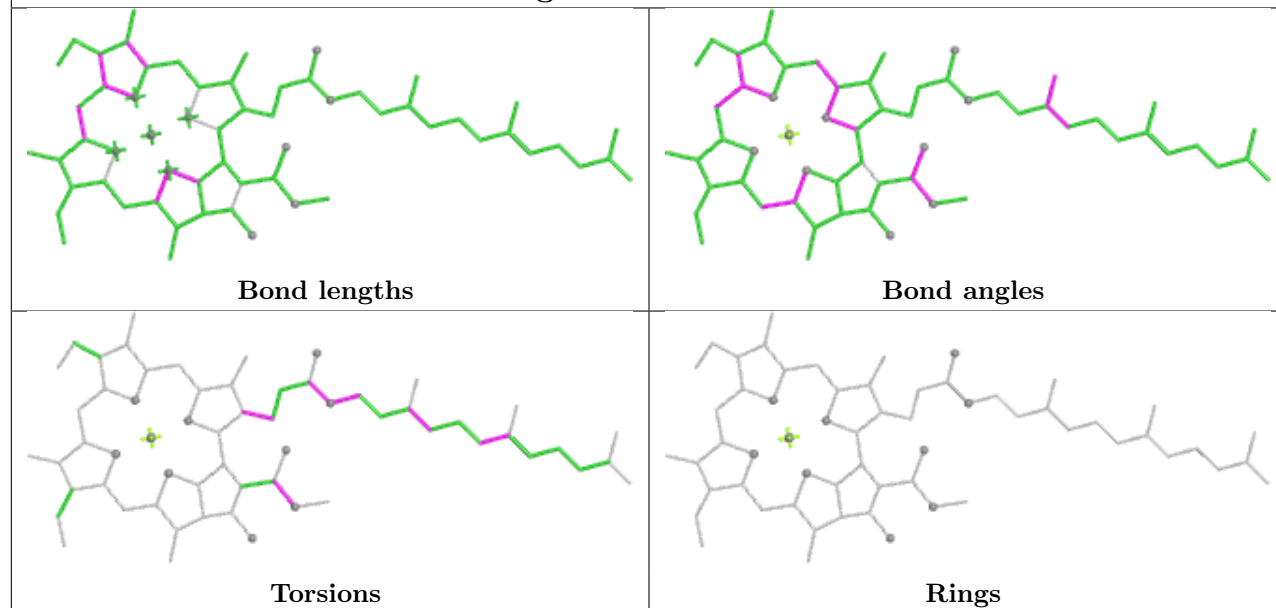


Torsions

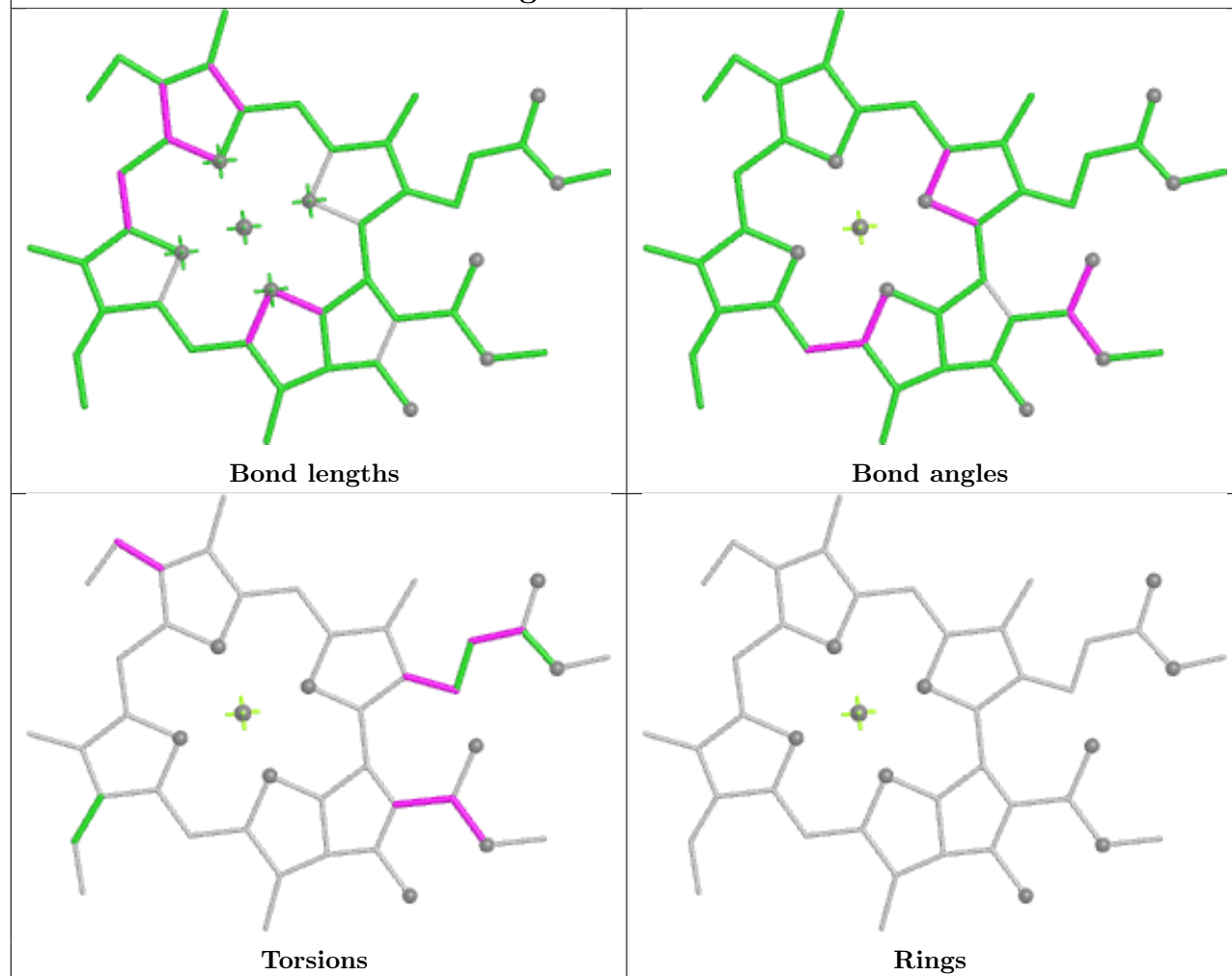


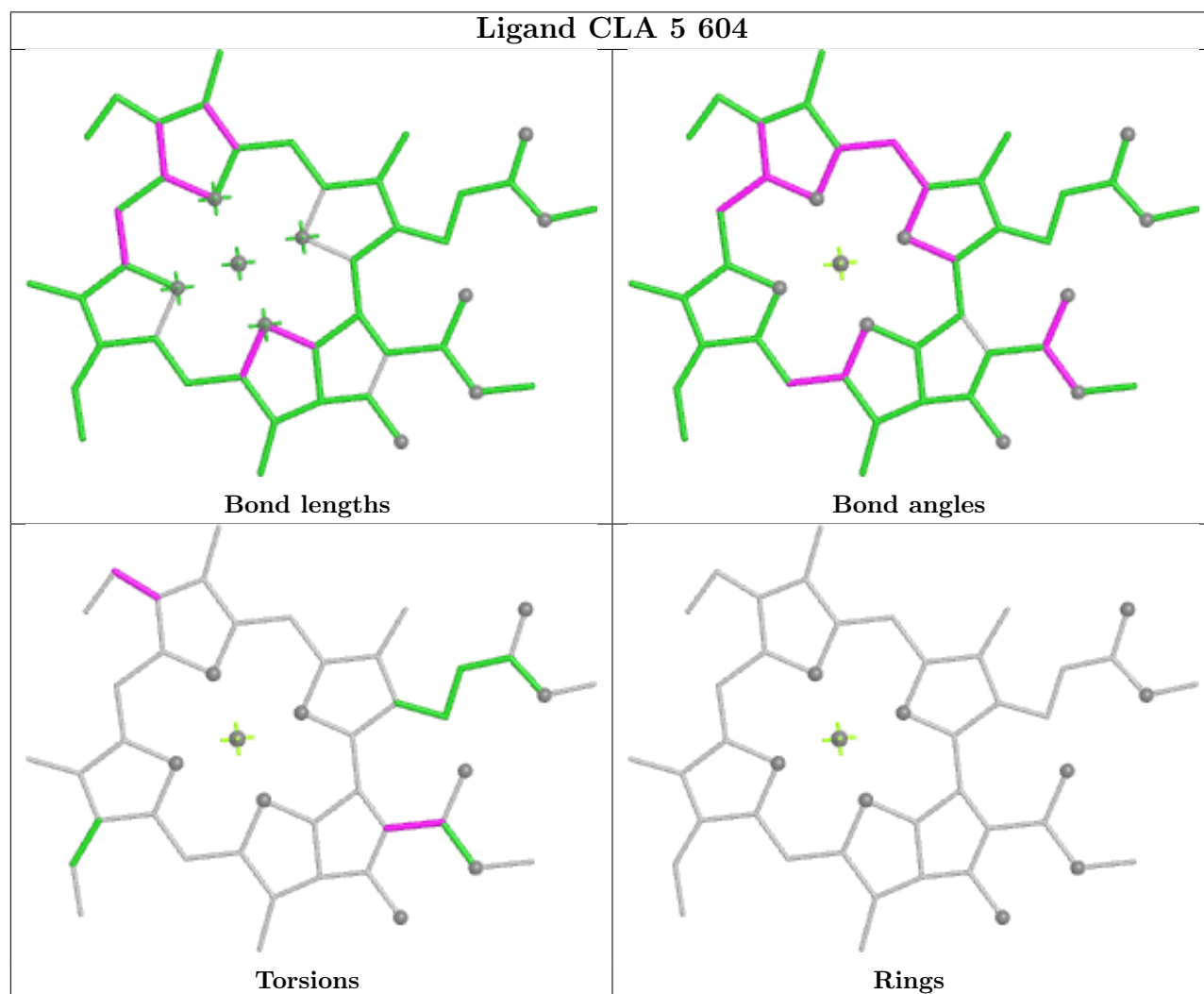
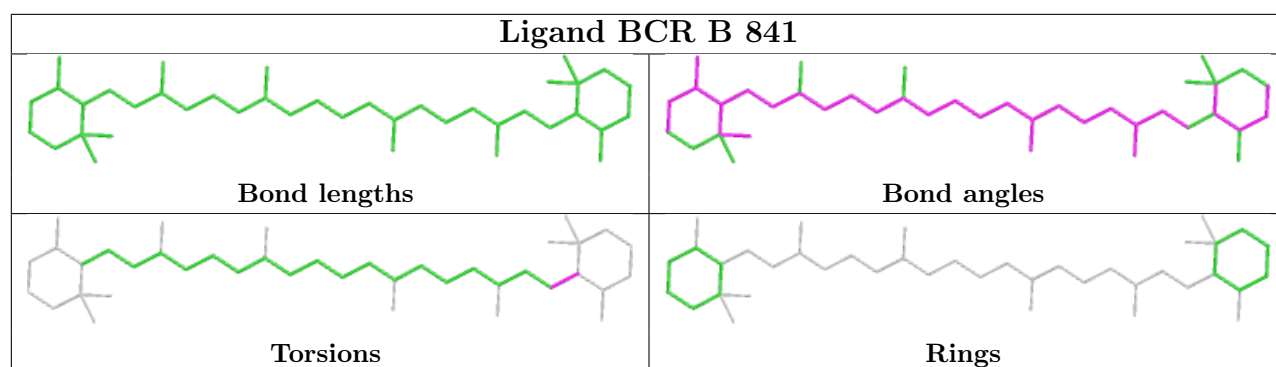
Rings

Ligand CLA 4 602

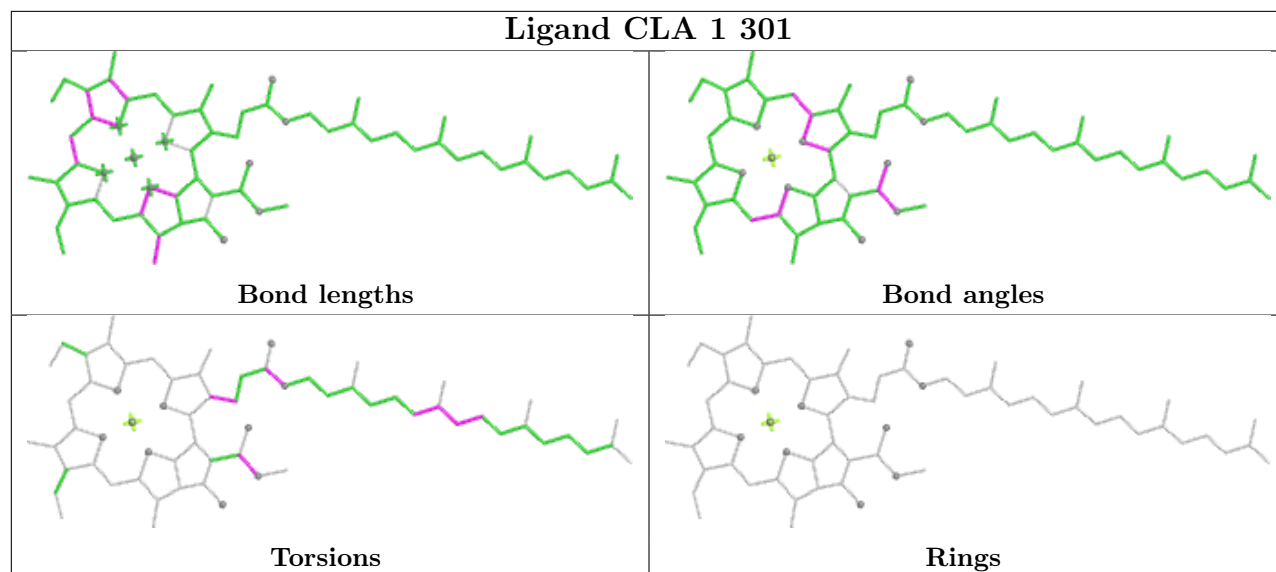


Ligand CLA t 307

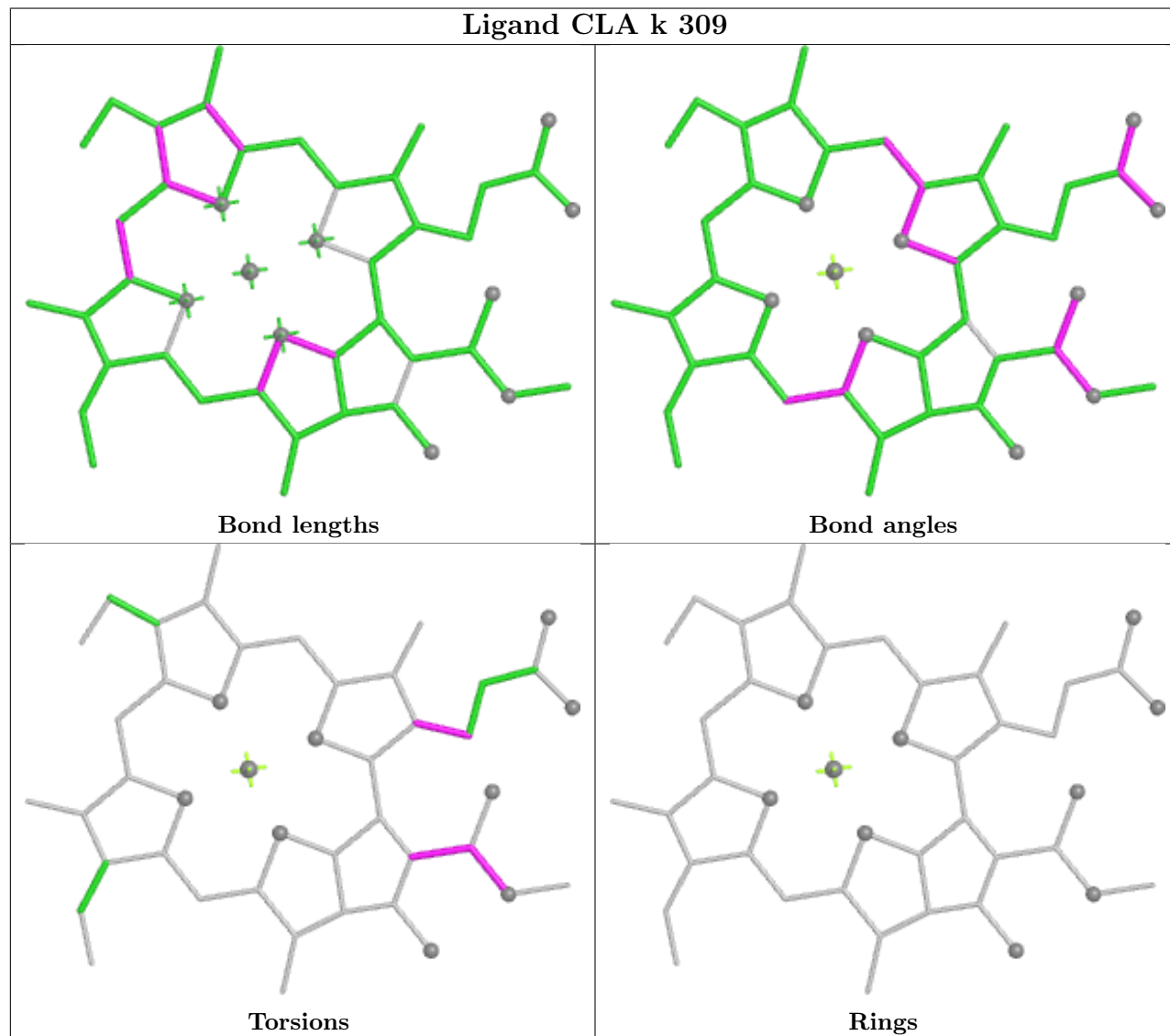


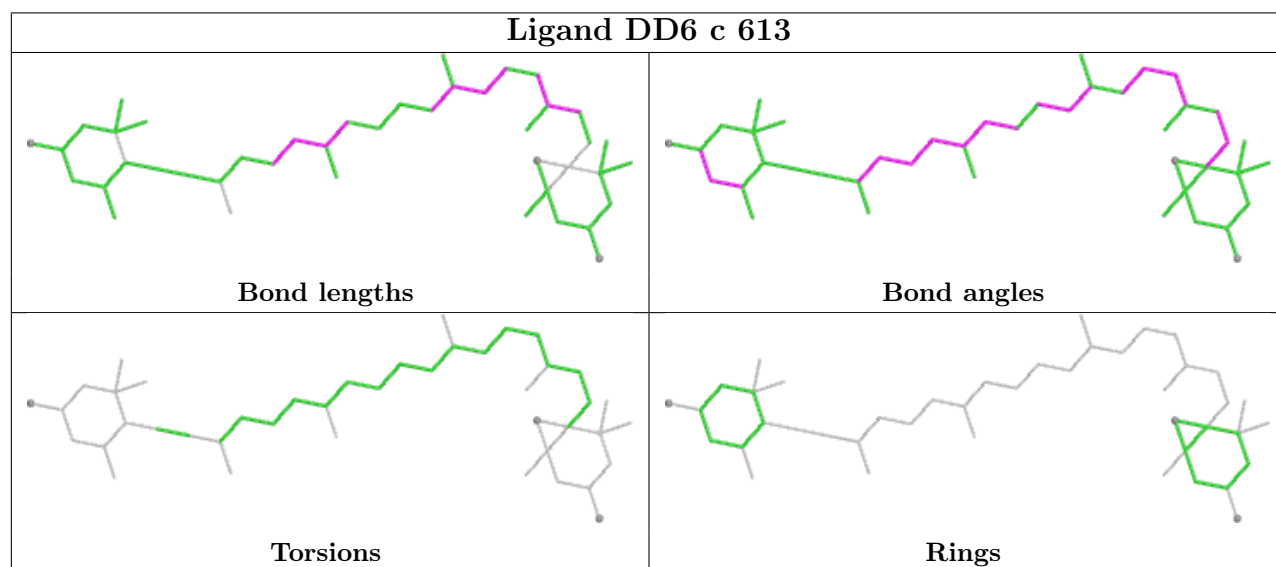
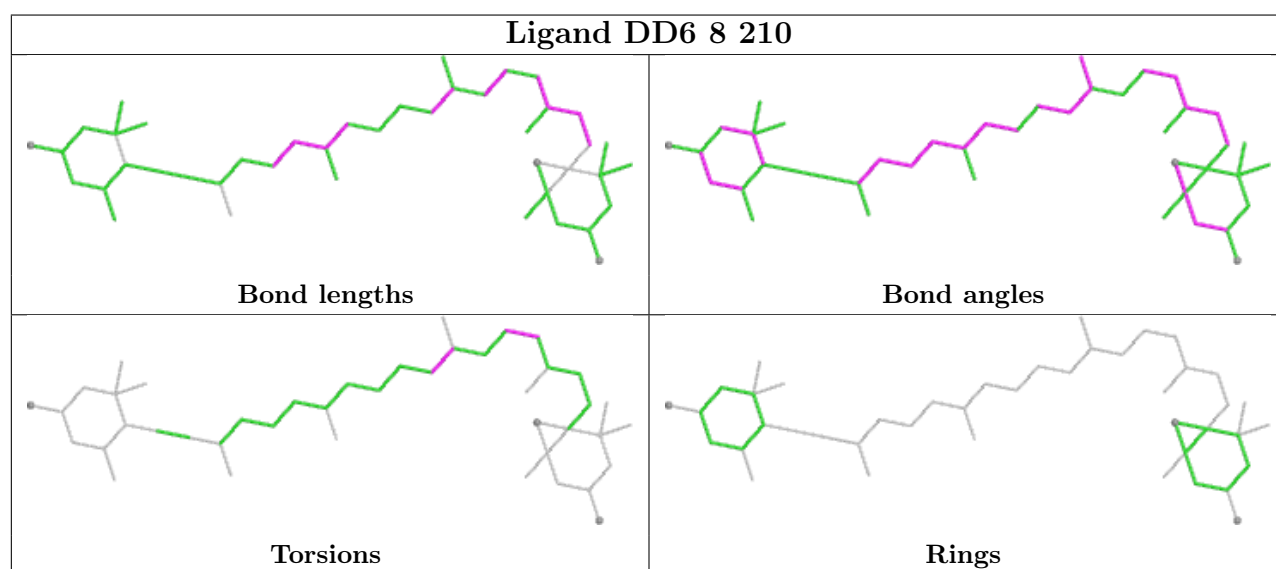
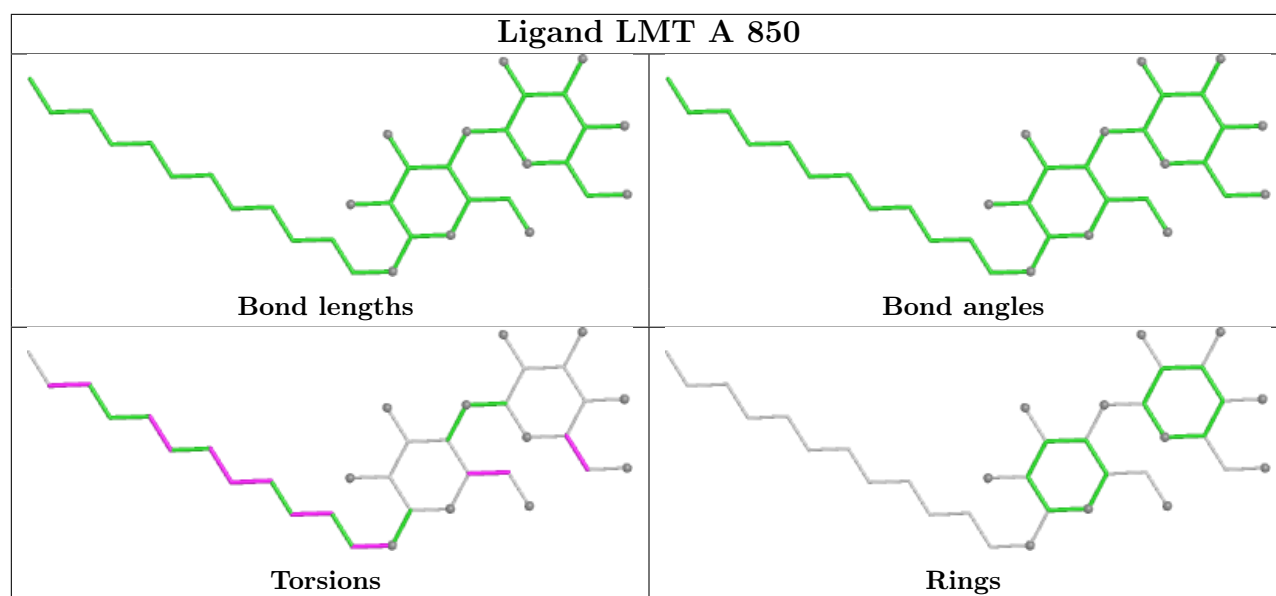


Ligand CLA 1 301

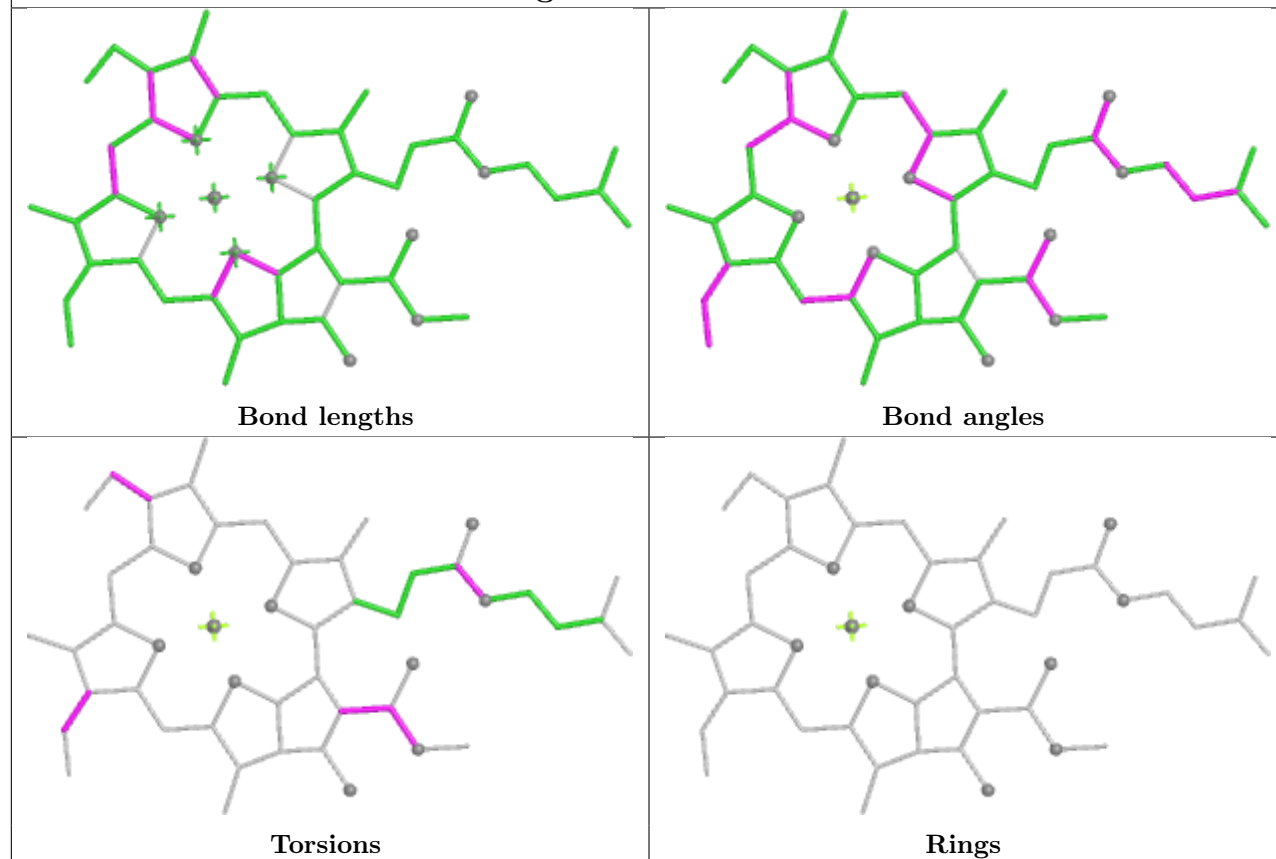


Ligand CLA k 309

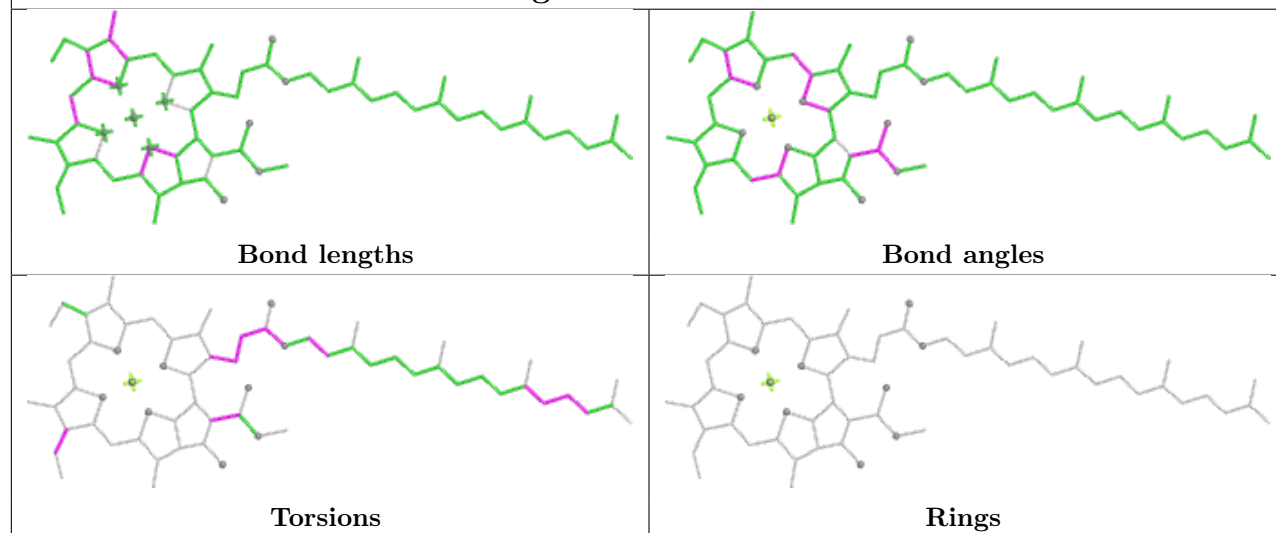




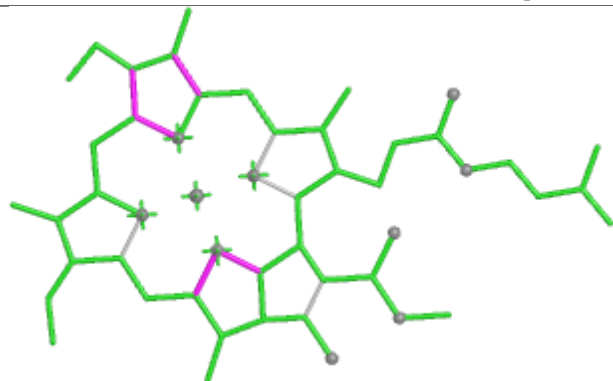
Ligand CLA 4 608



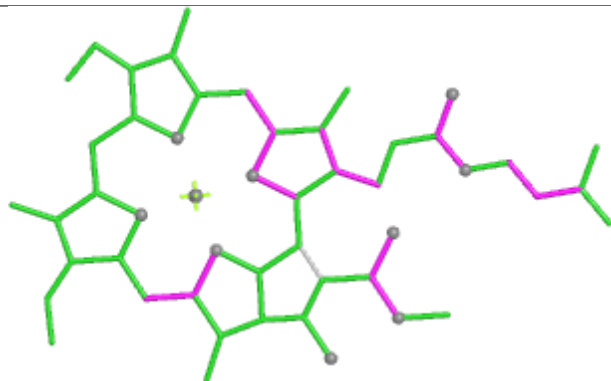
Ligand CLA B 847



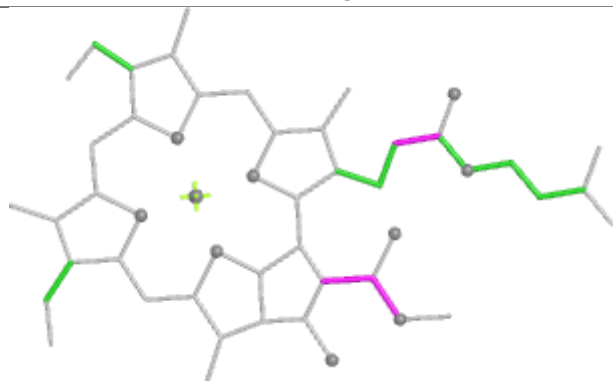
Ligand CLA 1 306



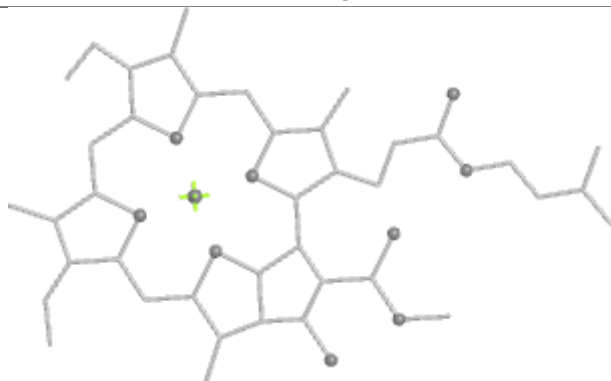
Bond lengths



Bond angles

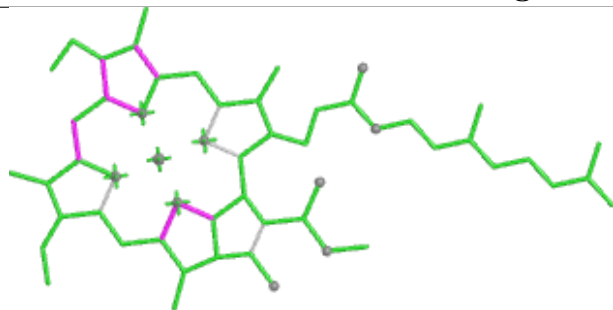


Torsions

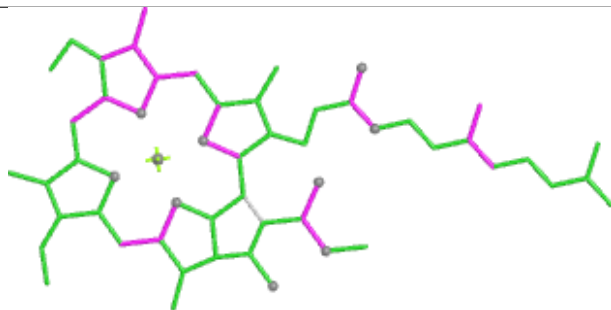


Rings

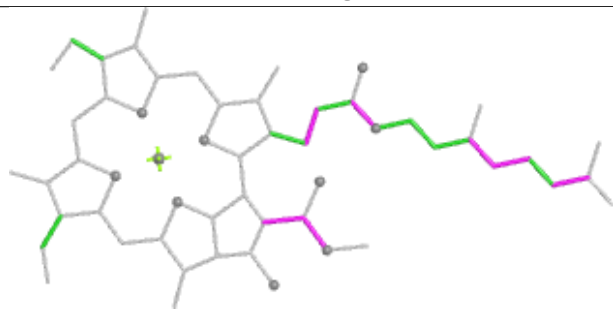
Ligand CLA A 847



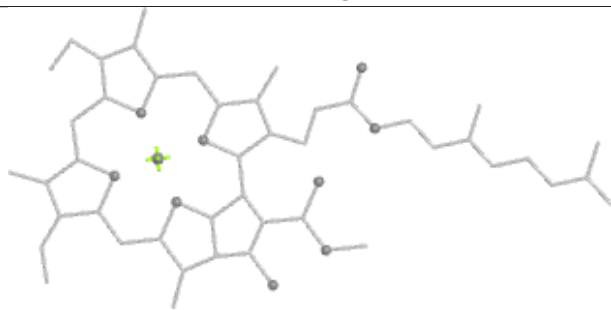
Bond lengths



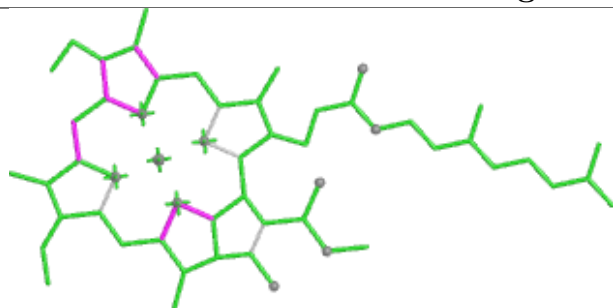
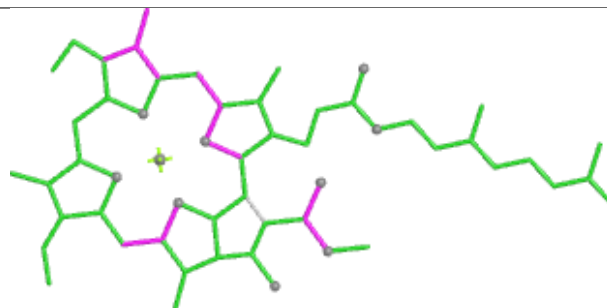
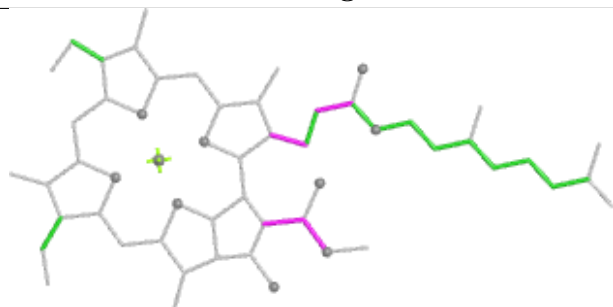
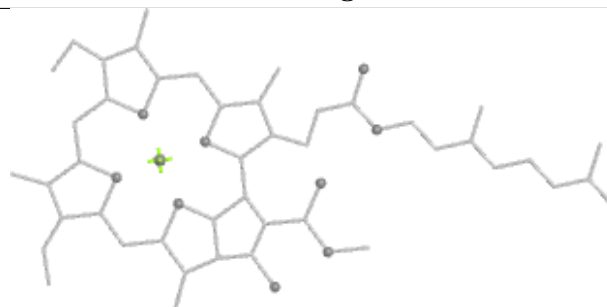
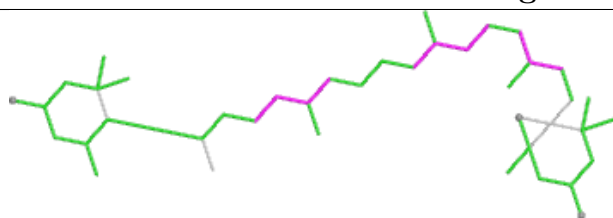
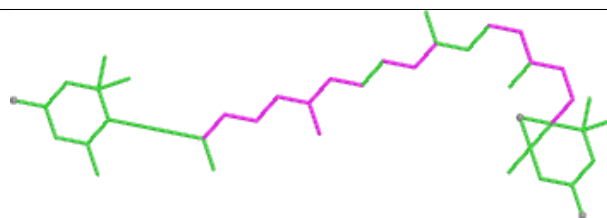
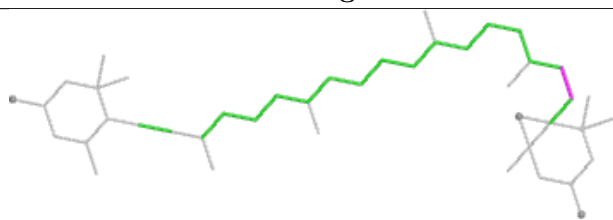
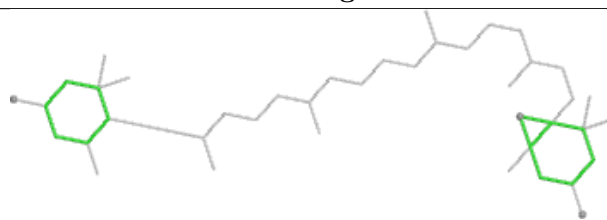
Bond angles



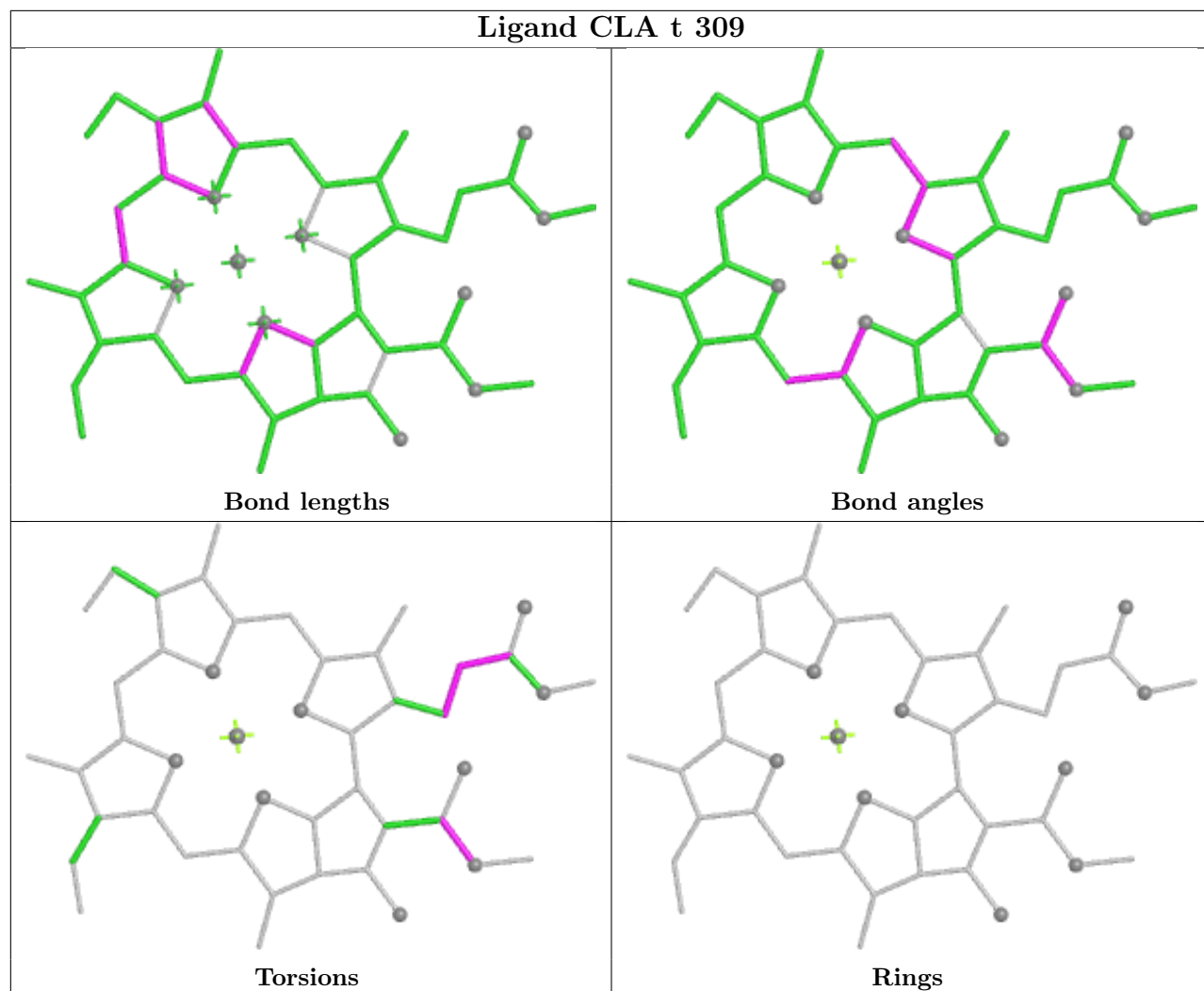
Torsions

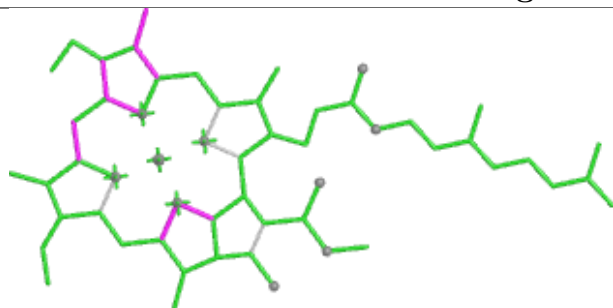


Rings

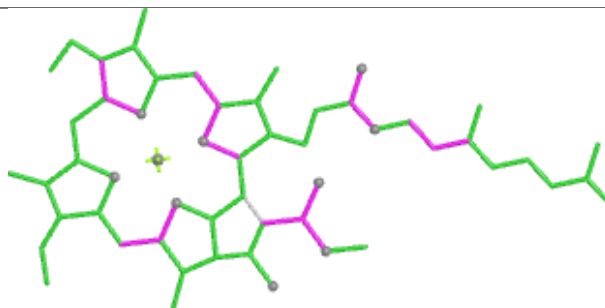
Ligand CLA k 311**Bond lengths****Bond angles****Torsions****Rings****Ligand DD6 2 212****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA t 309

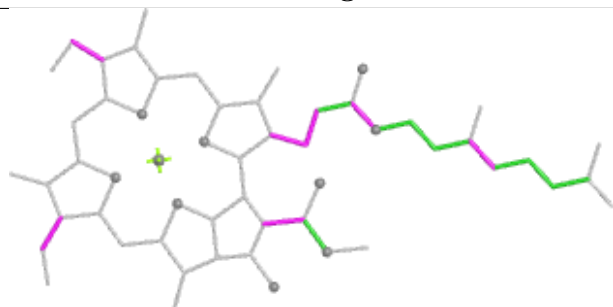


Ligand CLA L 203

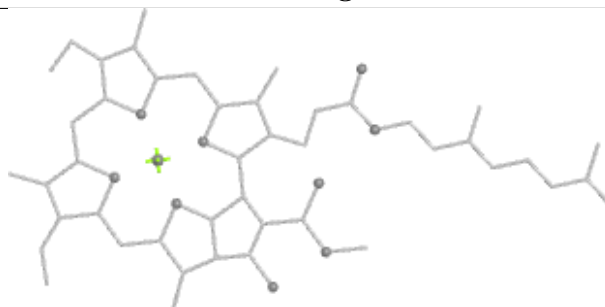
Bond lengths



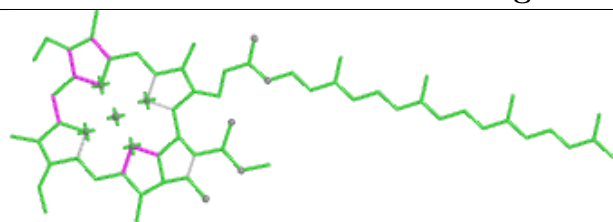
Bond angles



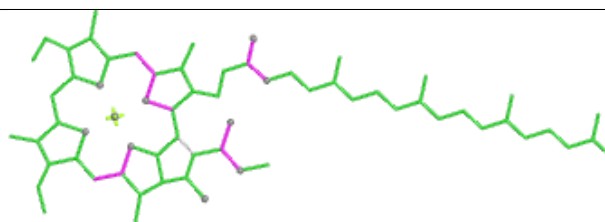
Torsions



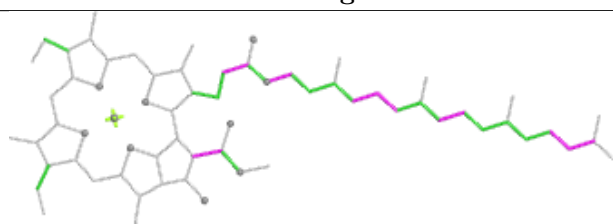
Rings

Ligand CLA A 806

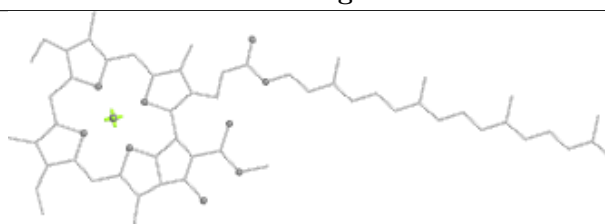
Bond lengths



Bond angles

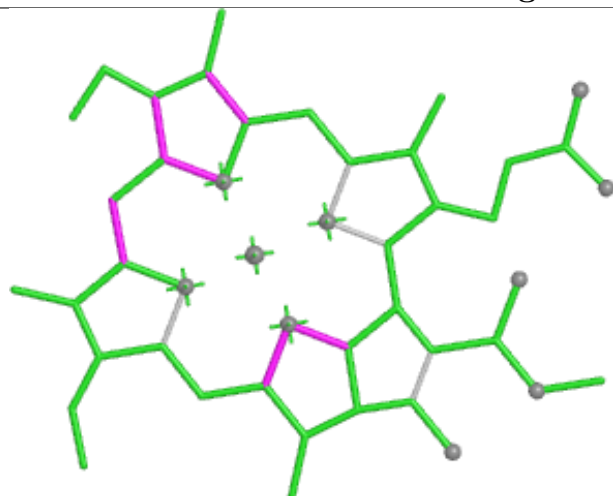


Torsions

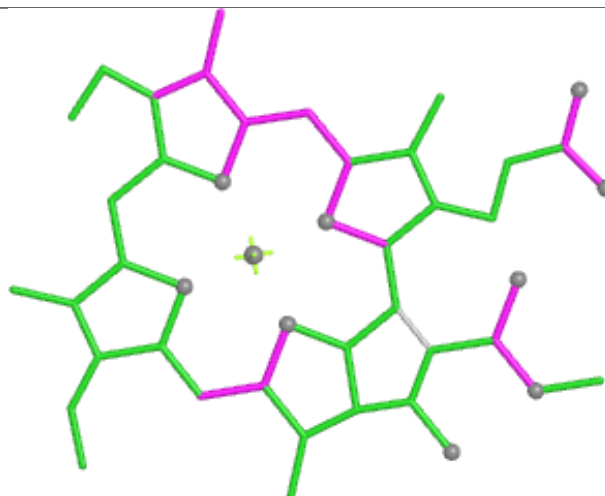


Rings

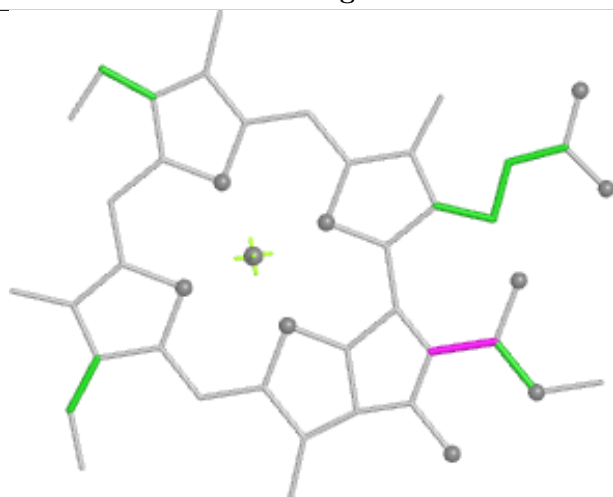
Ligand CLA 7 607



Bond lengths



Bond angles

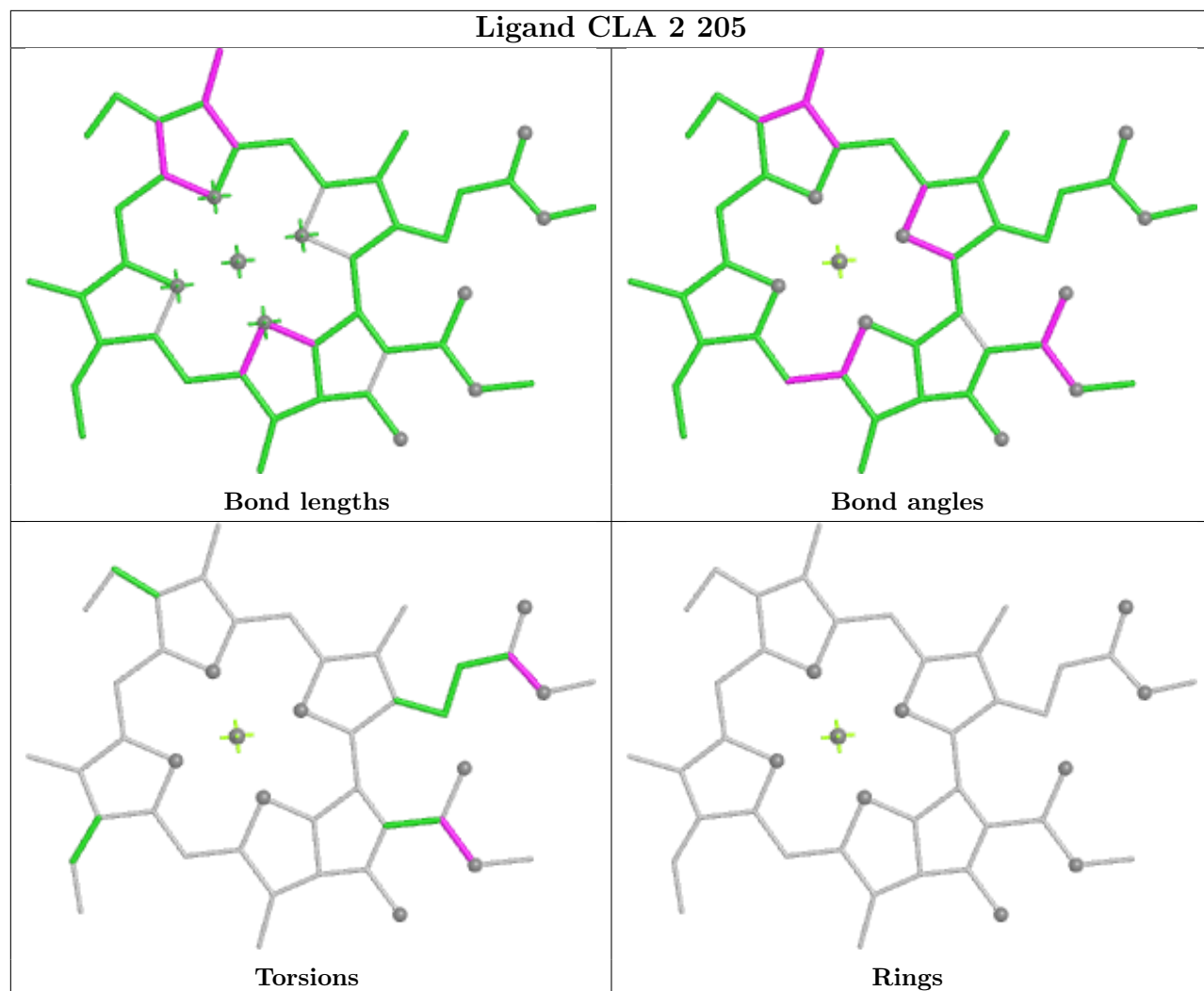


Torsions

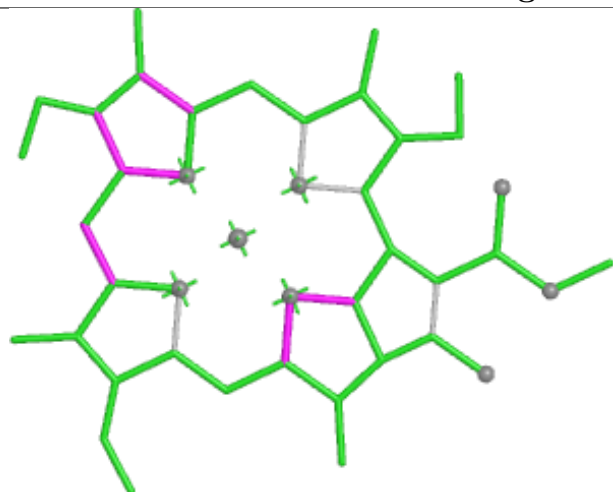


Rings

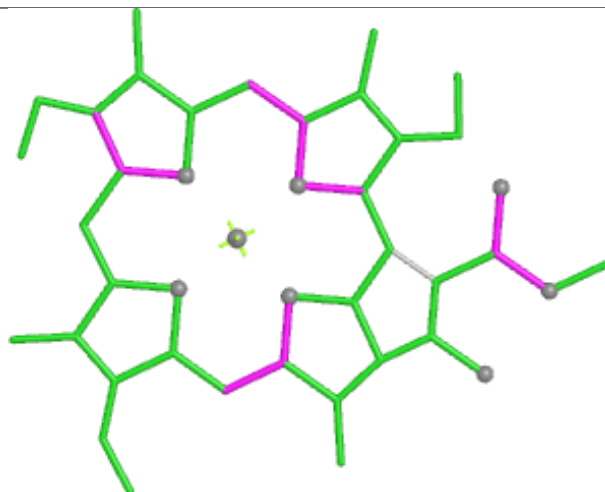
Ligand CLA 2 205



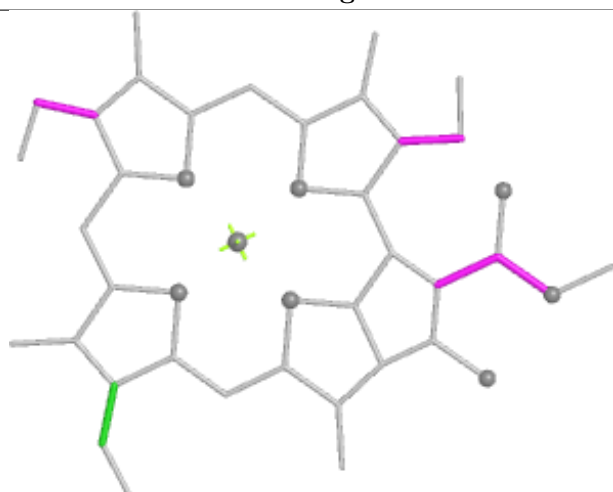
Ligand CLA J 103



Bond lengths



Bond angles

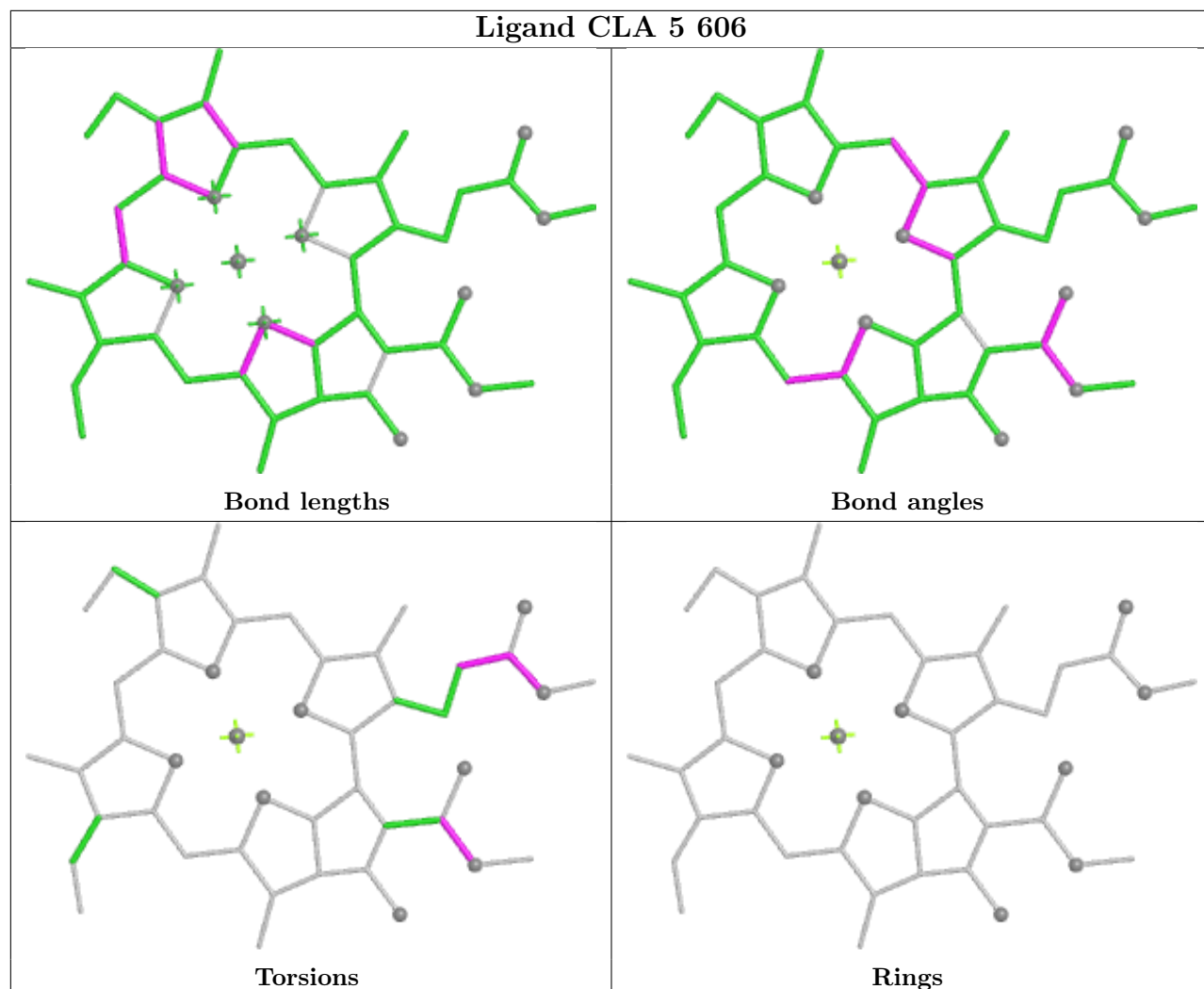


Torsions

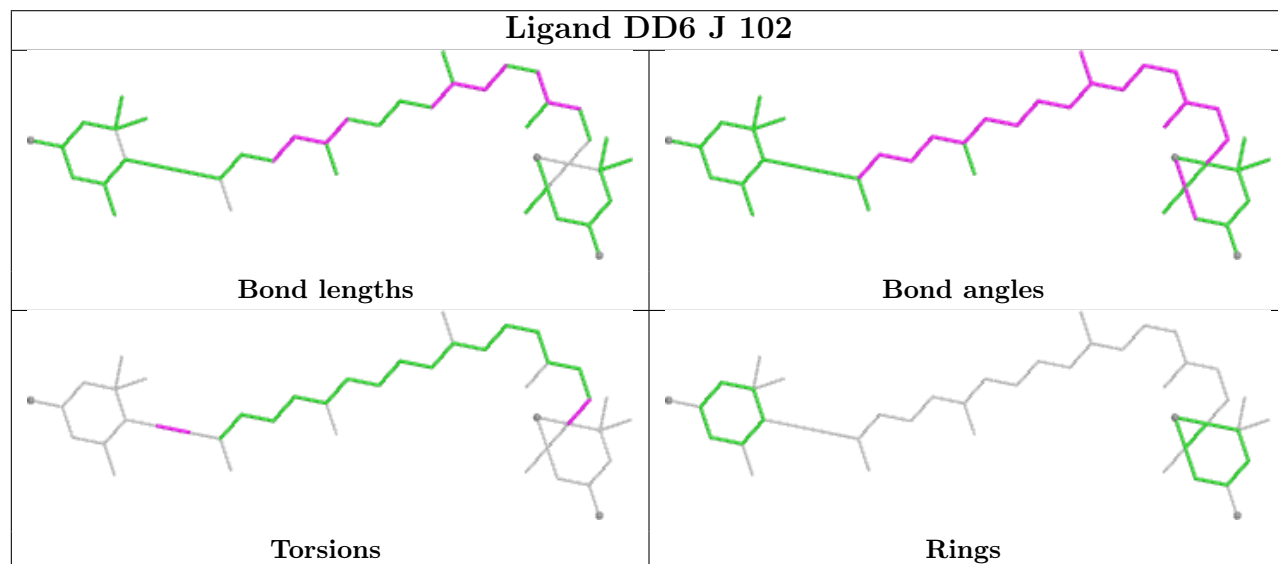


Rings

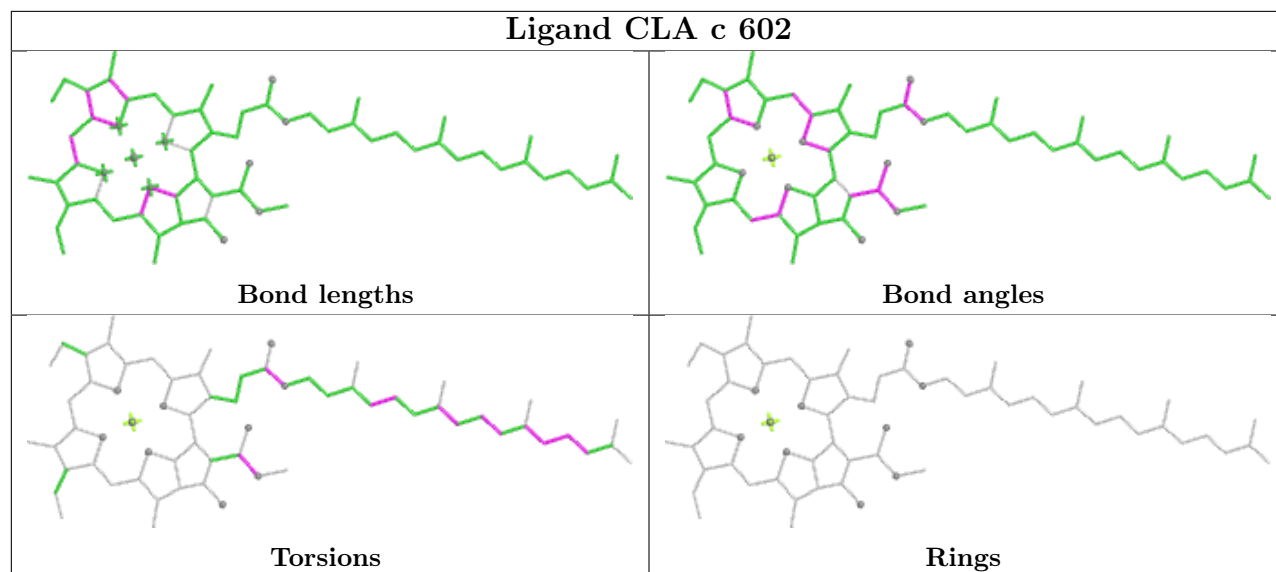
Ligand CLA 5 606



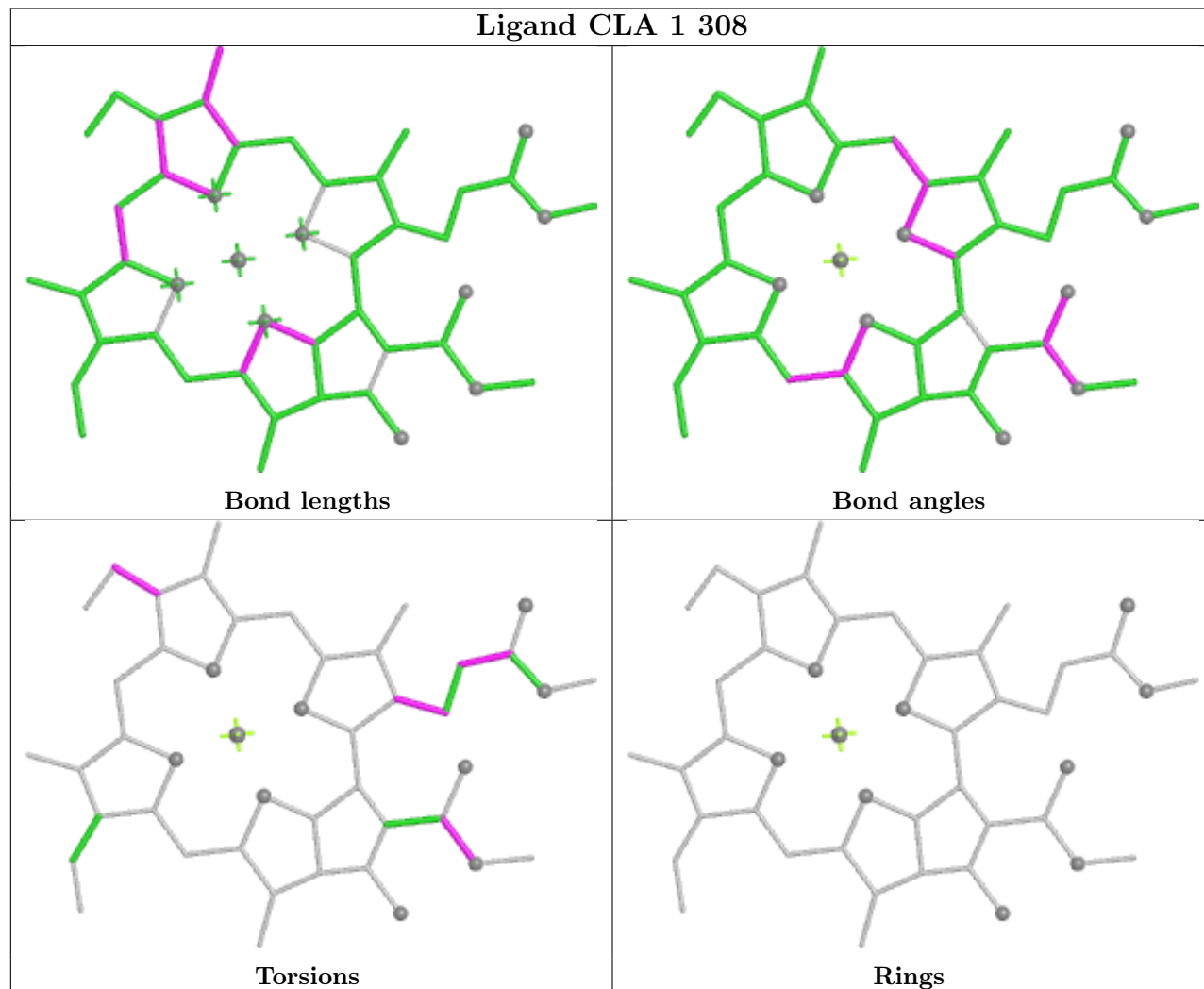
Ligand DD6 J 102

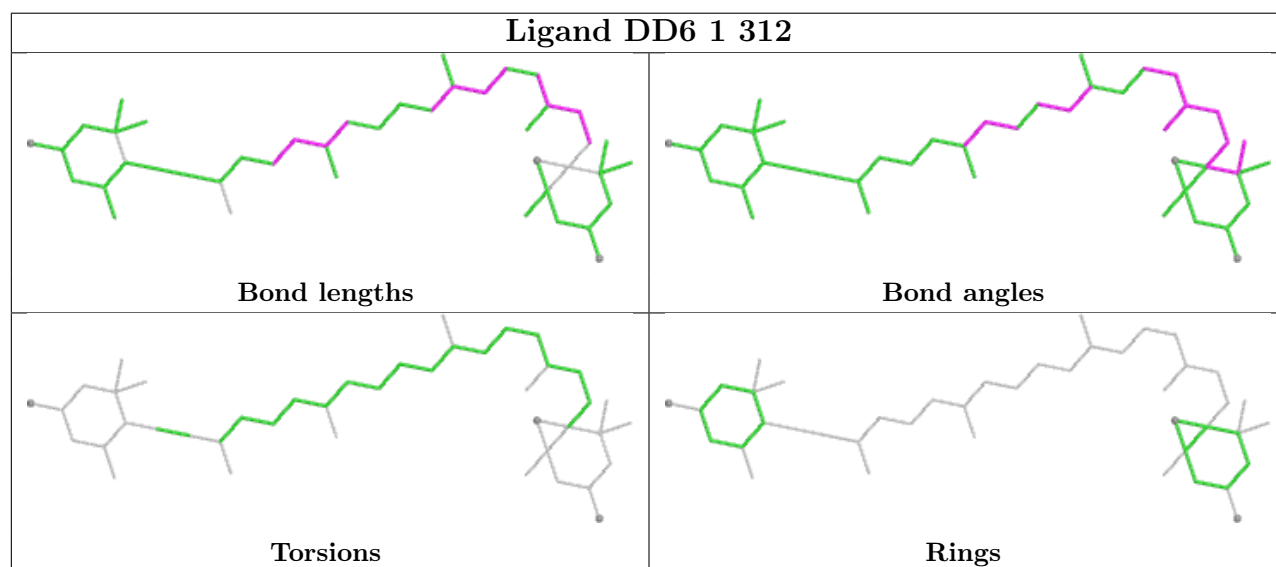
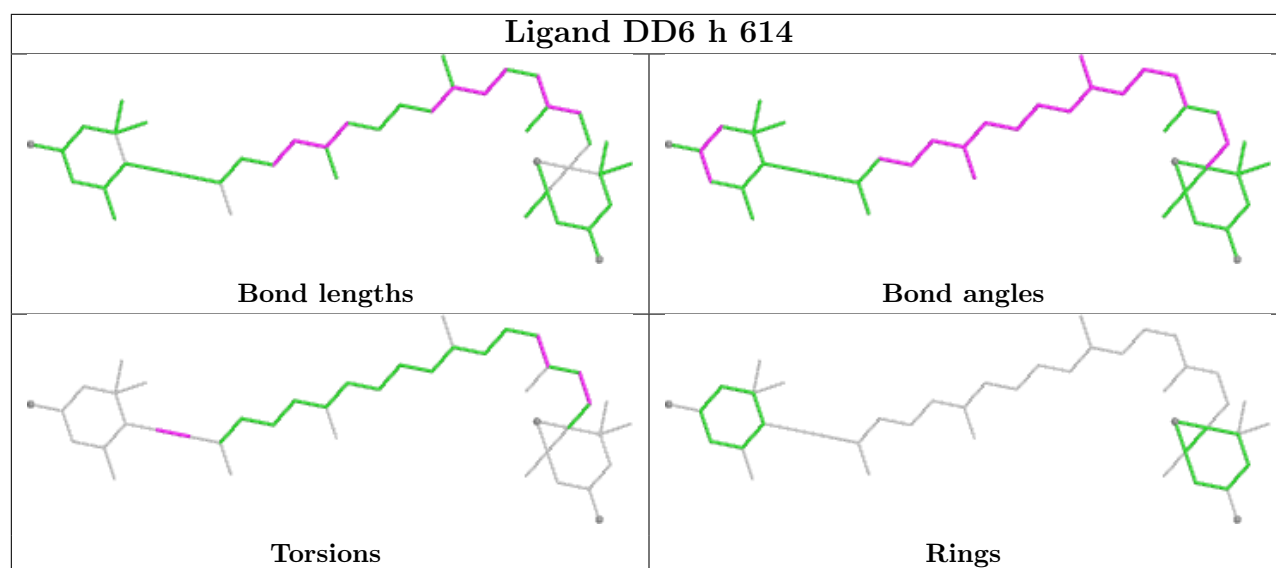


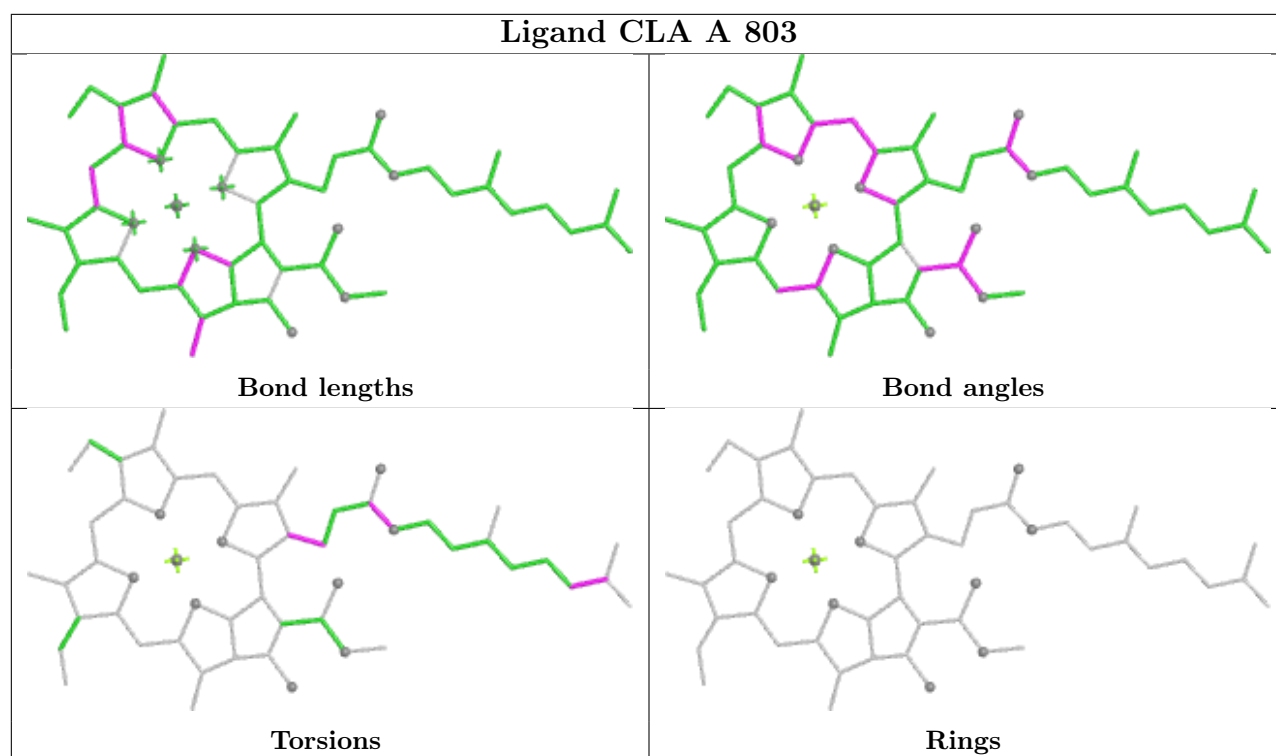
Ligand CLA c 602



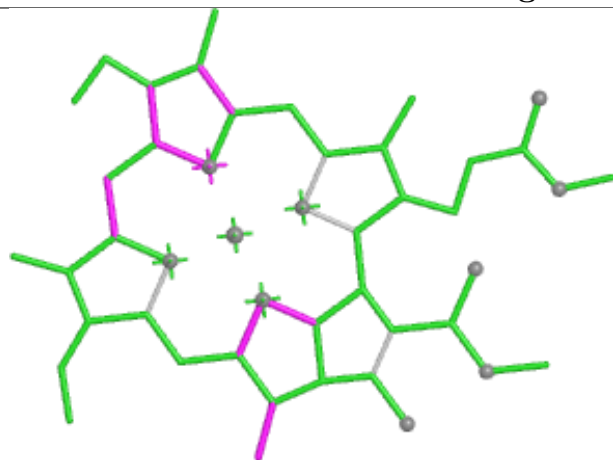
Ligand CLA 1 308



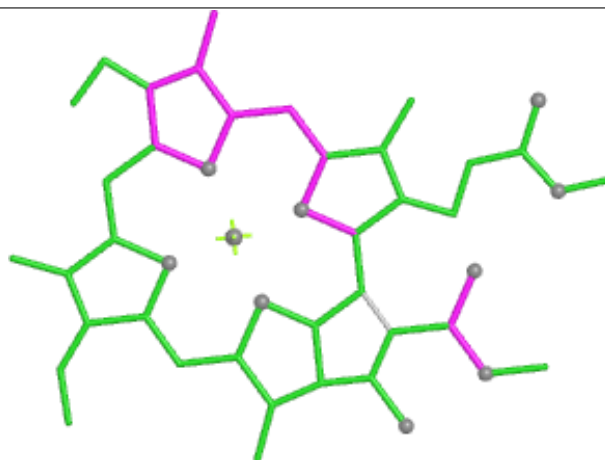




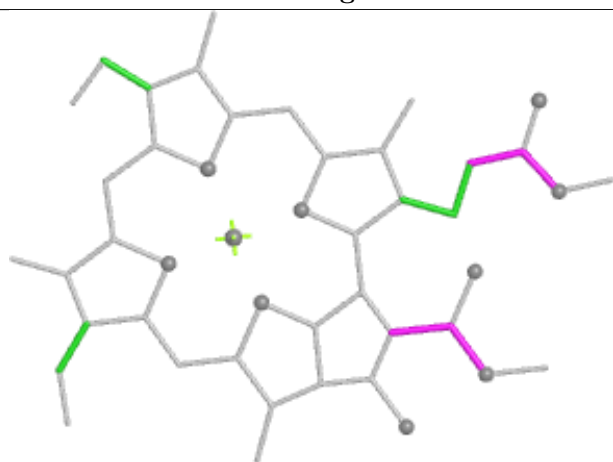
Ligand CLA 9 302



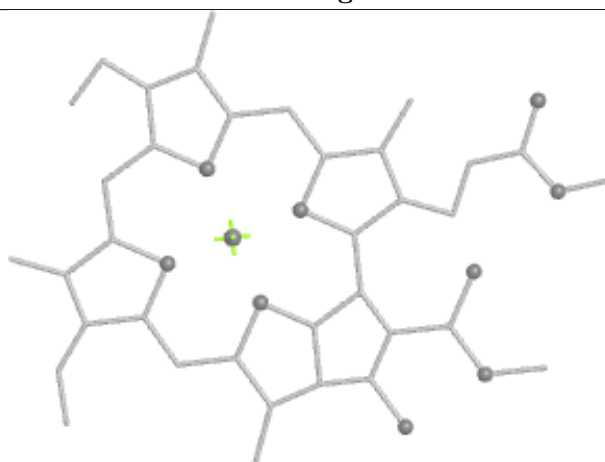
Bond lengths



Bond angles

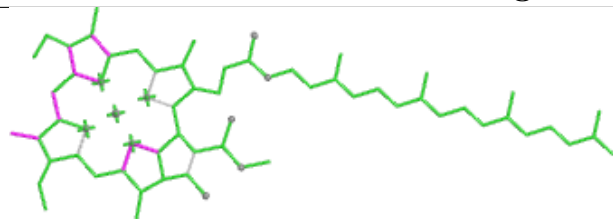


Torsions

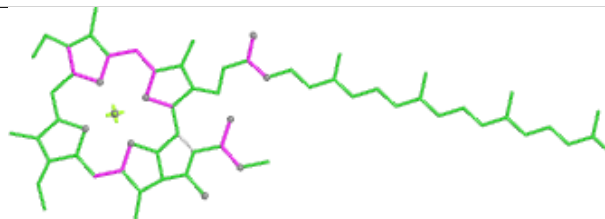


Rings

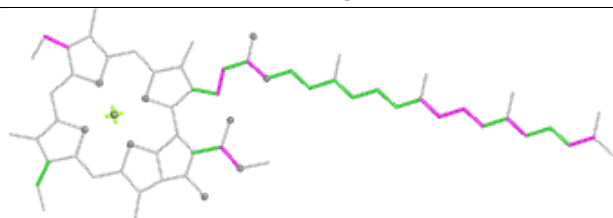
Ligand CLA A 812



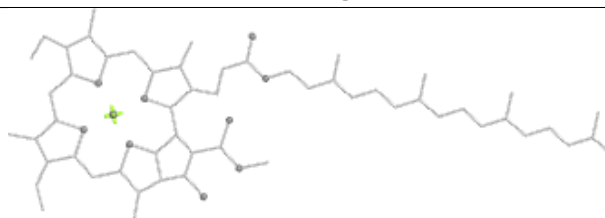
Bond lengths



Bond angles

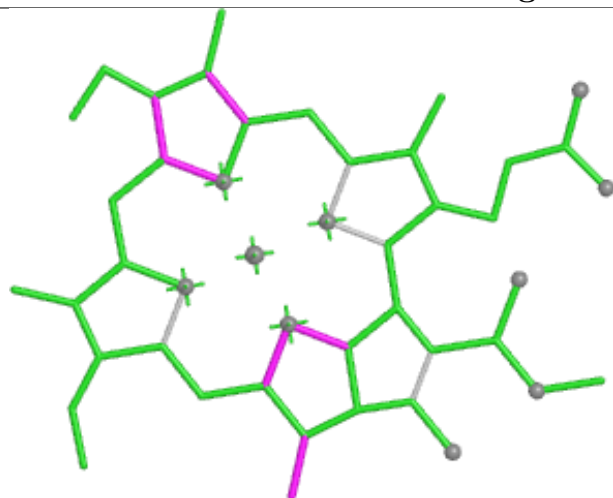


Torsions

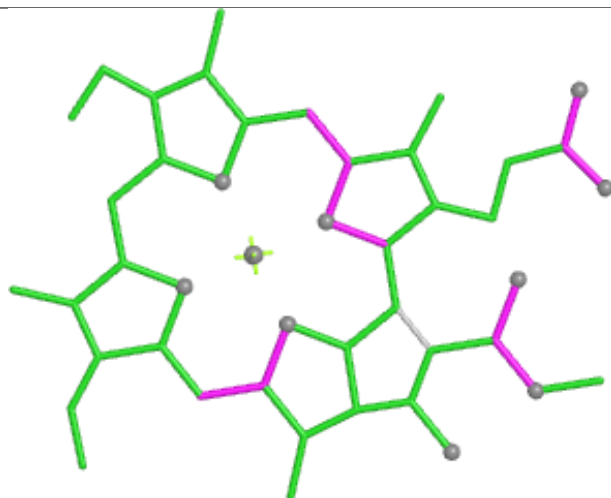


Rings

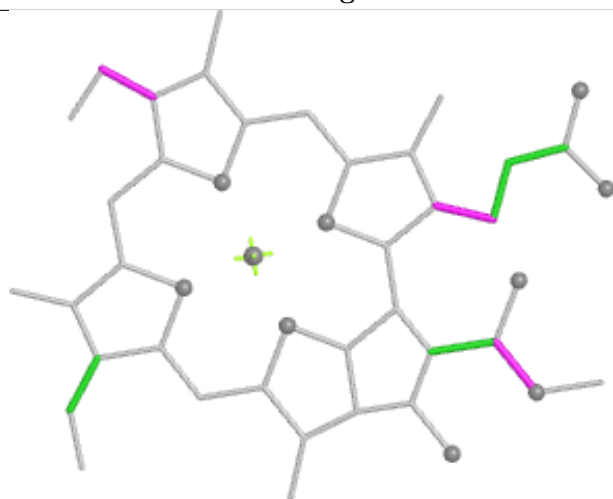
Ligand CLA 8 204



Bond lengths



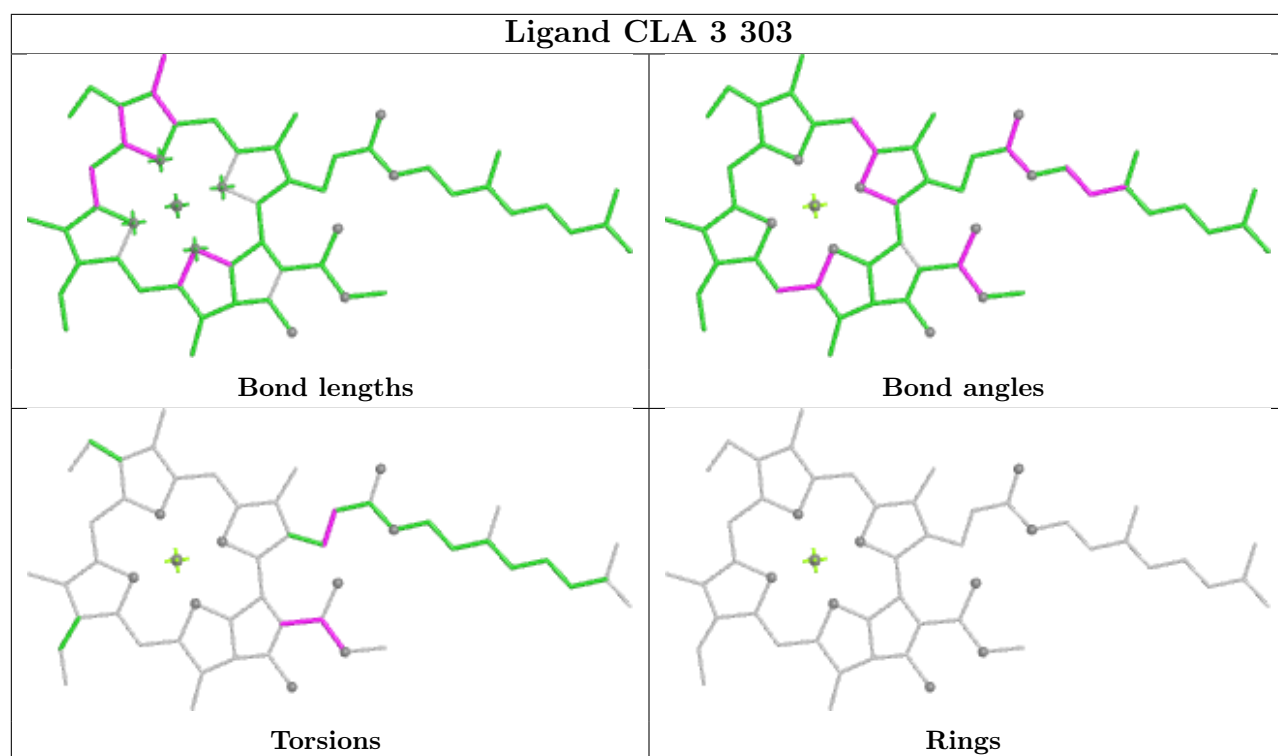
Bond angles



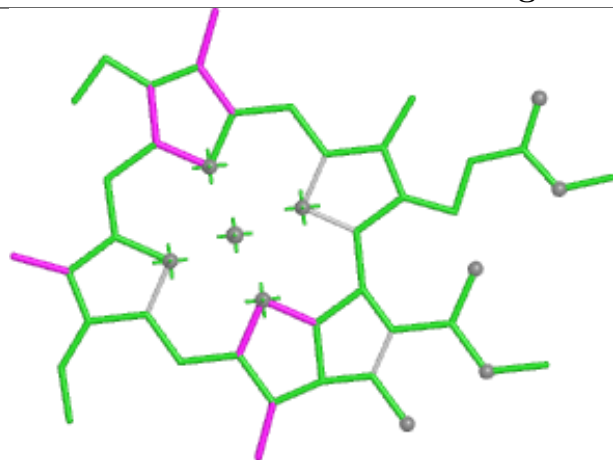
Torsions



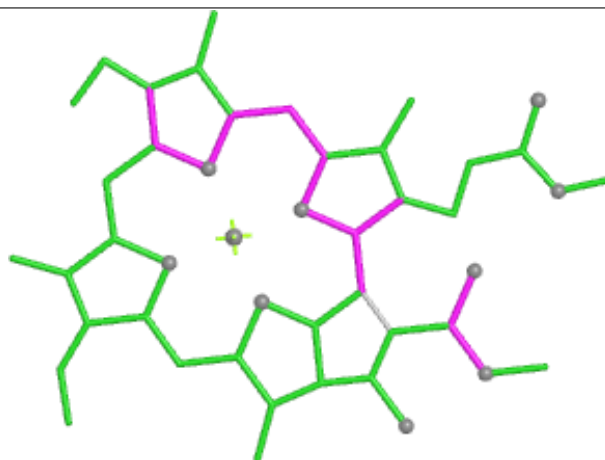
Rings



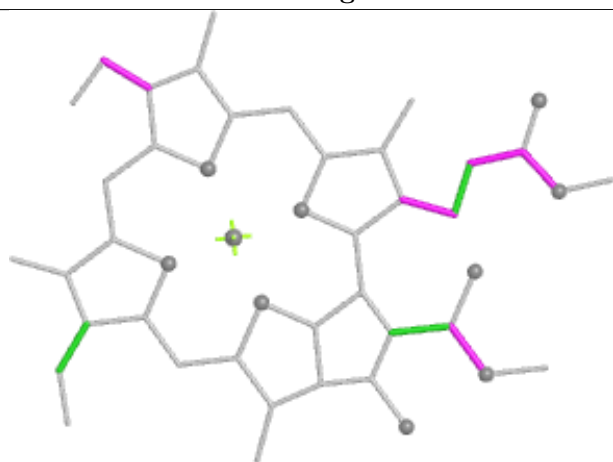
Ligand CLA 9 303



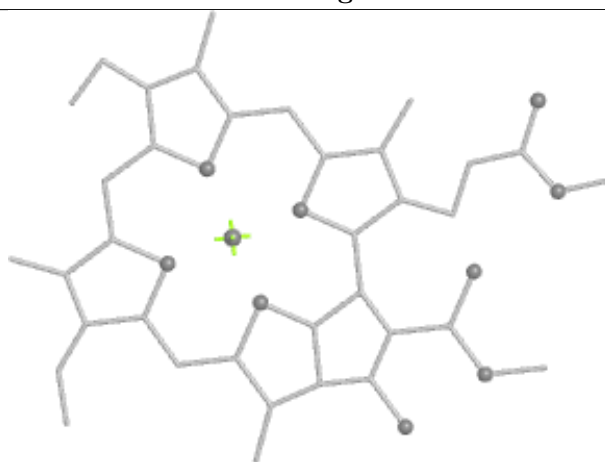
Bond lengths



Bond angles

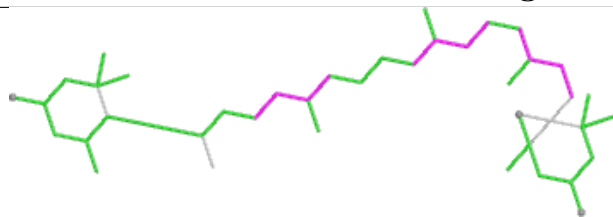


Torsions

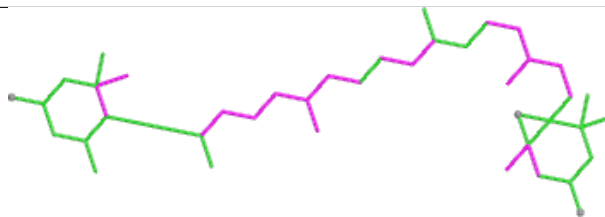


Rings

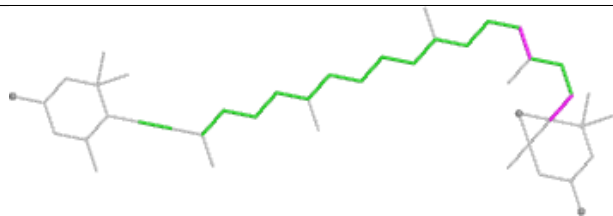
Ligand DD6 9 315



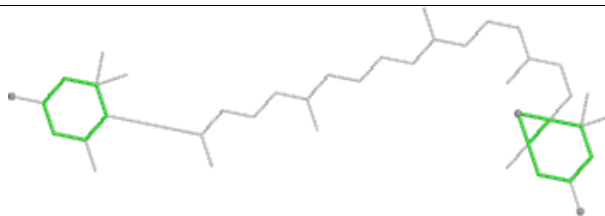
Bond lengths



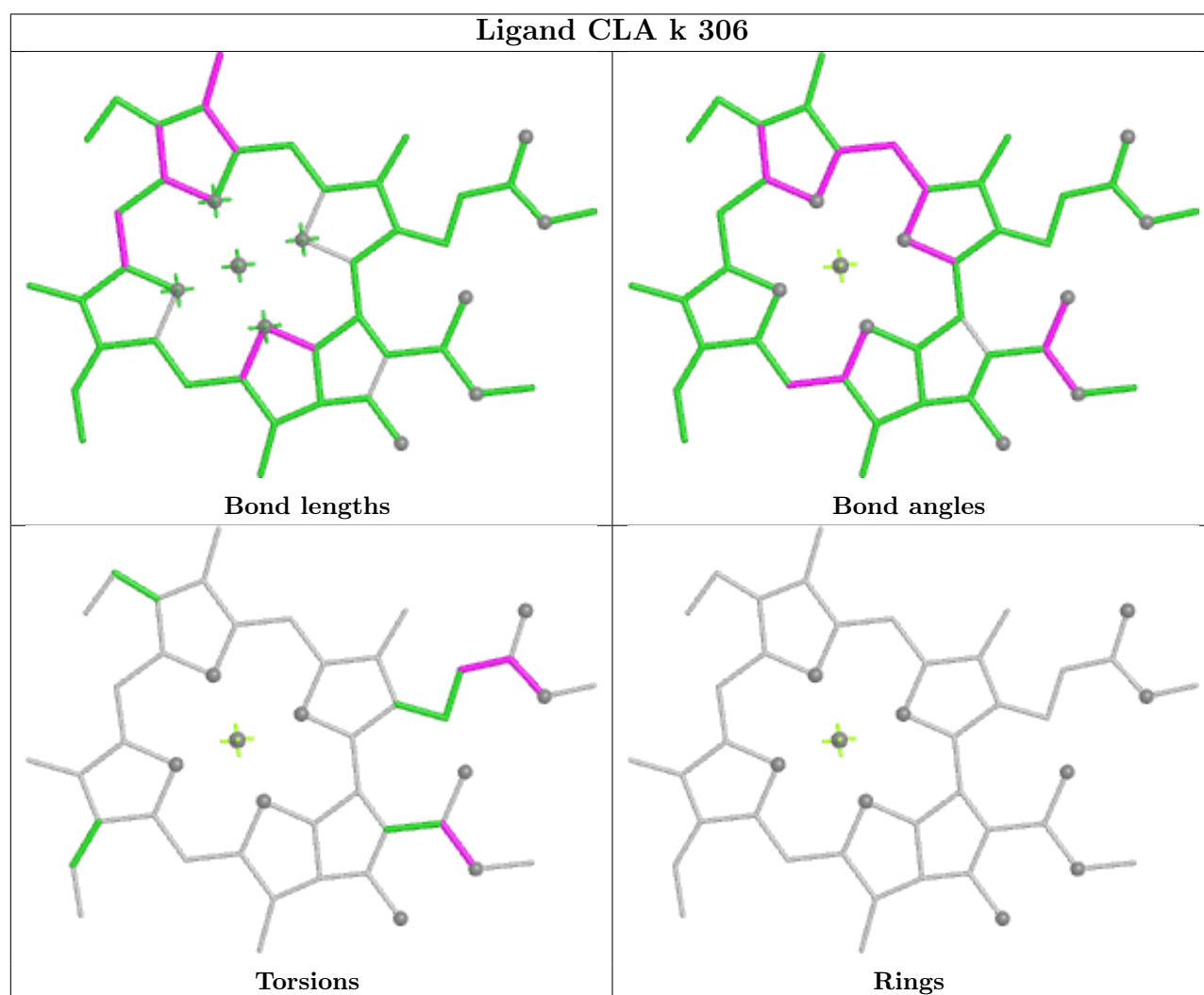
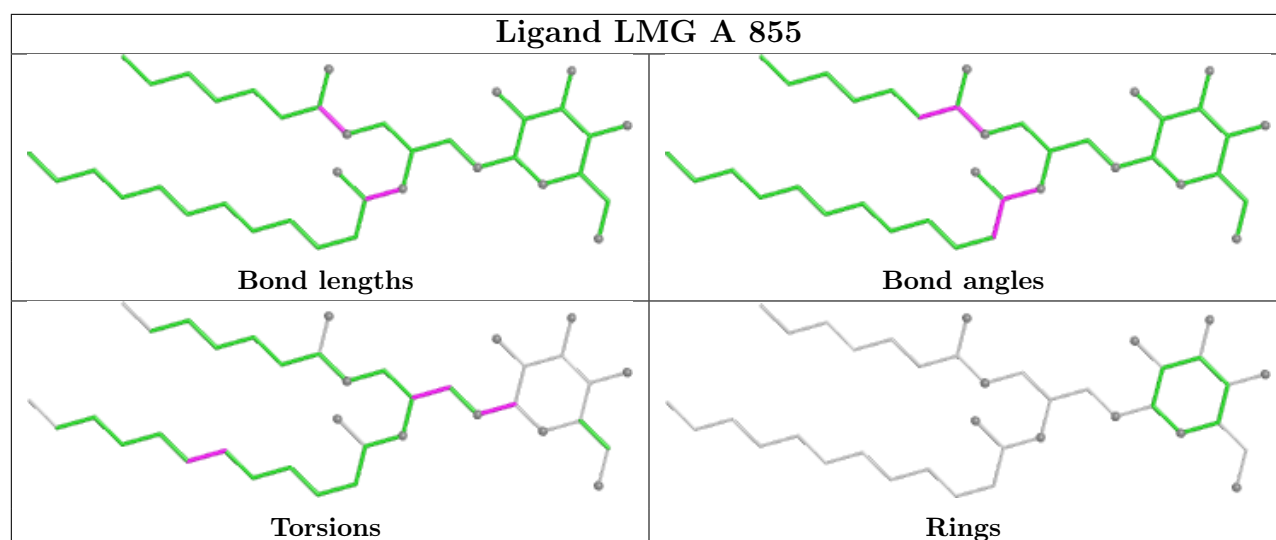
Bond angles

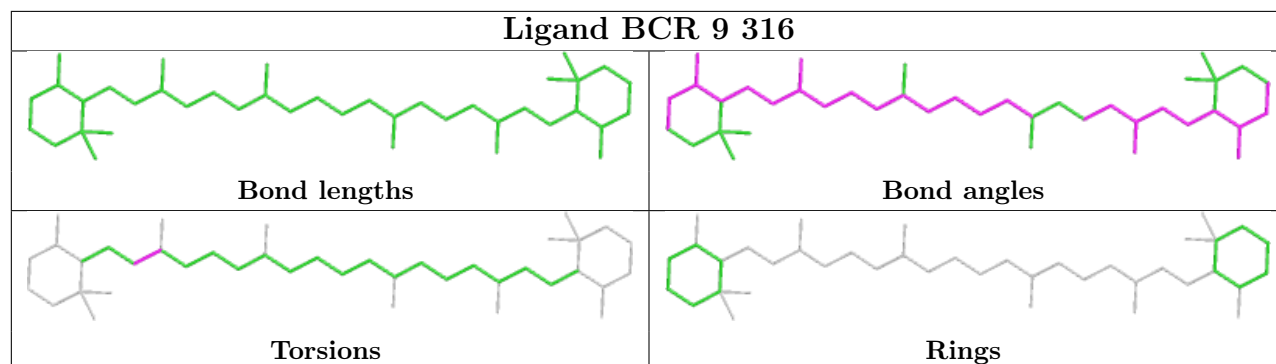
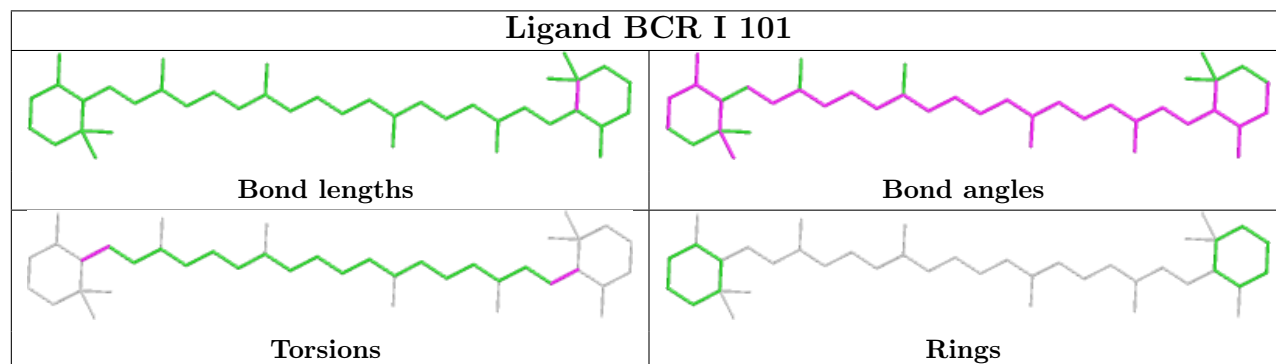
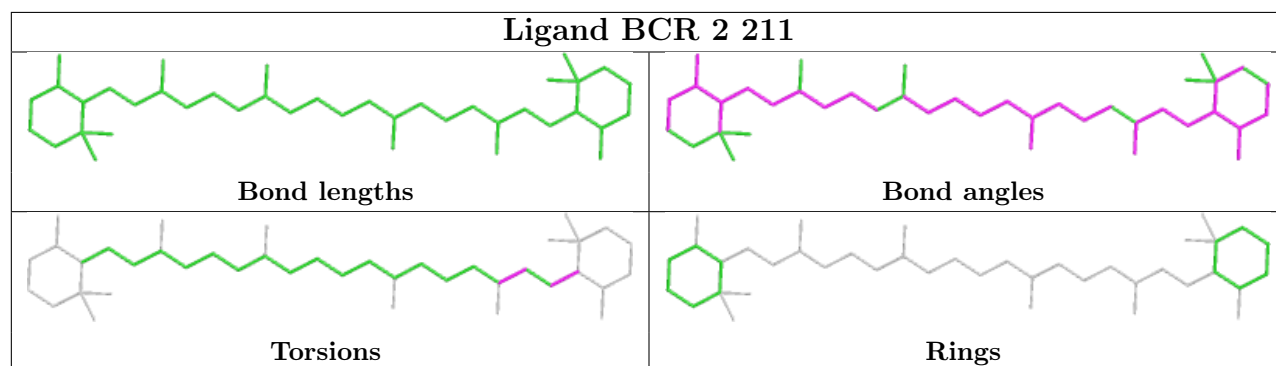
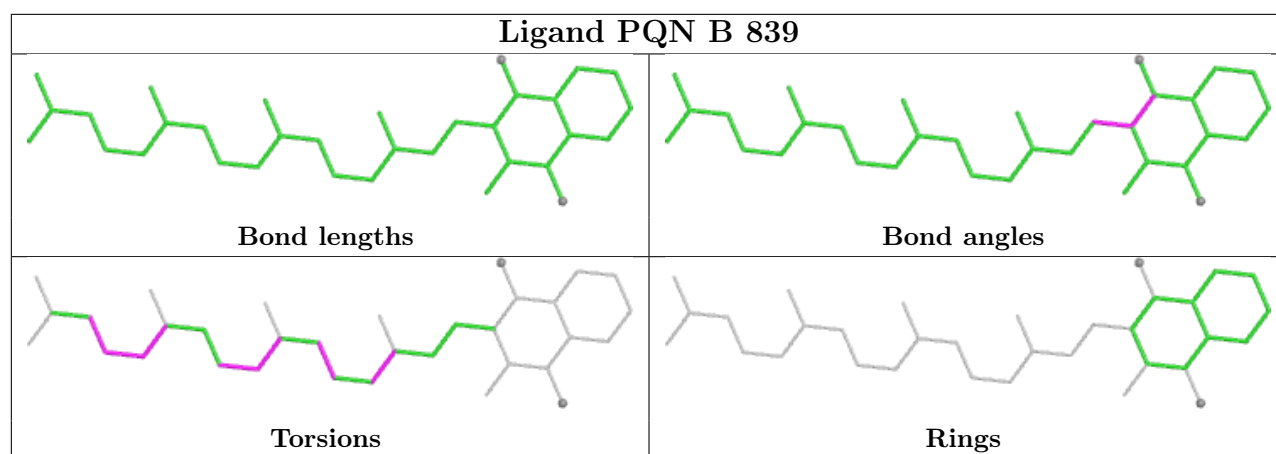


Torsions

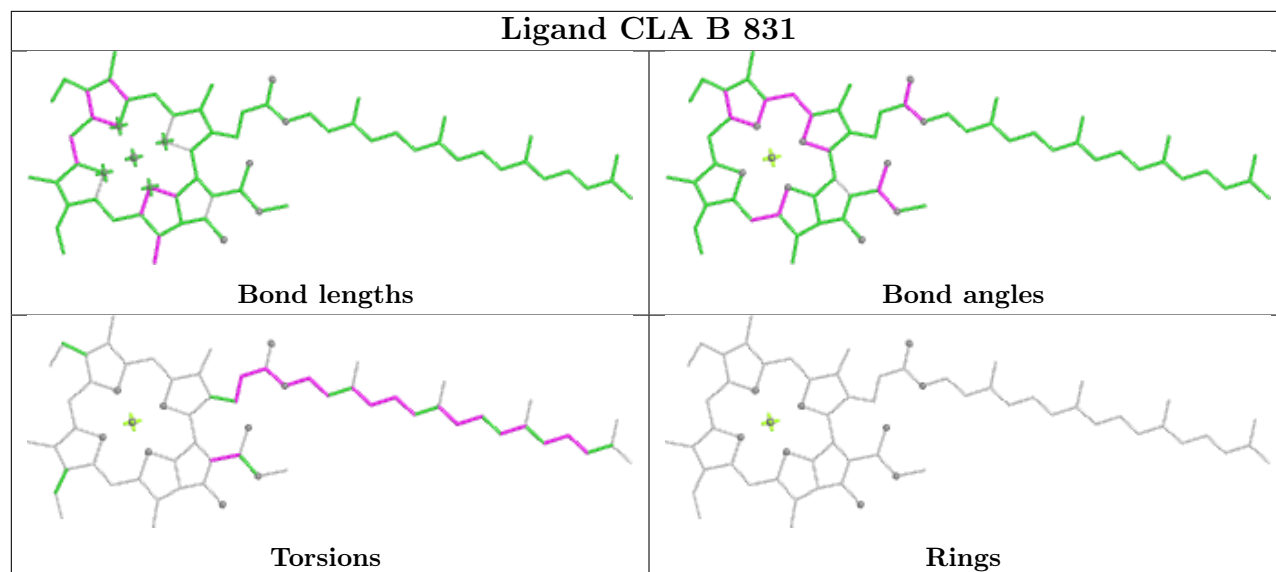


Rings

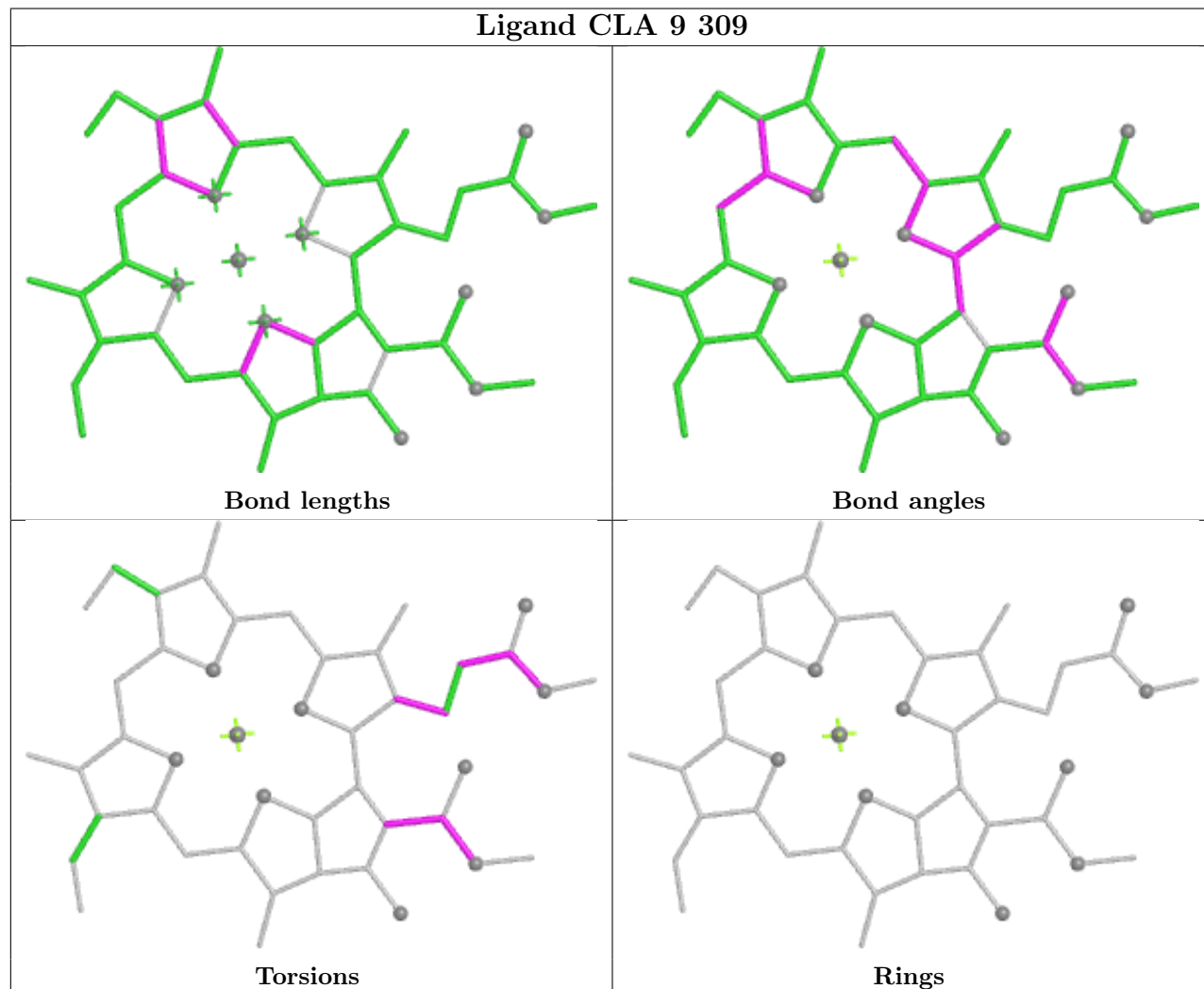


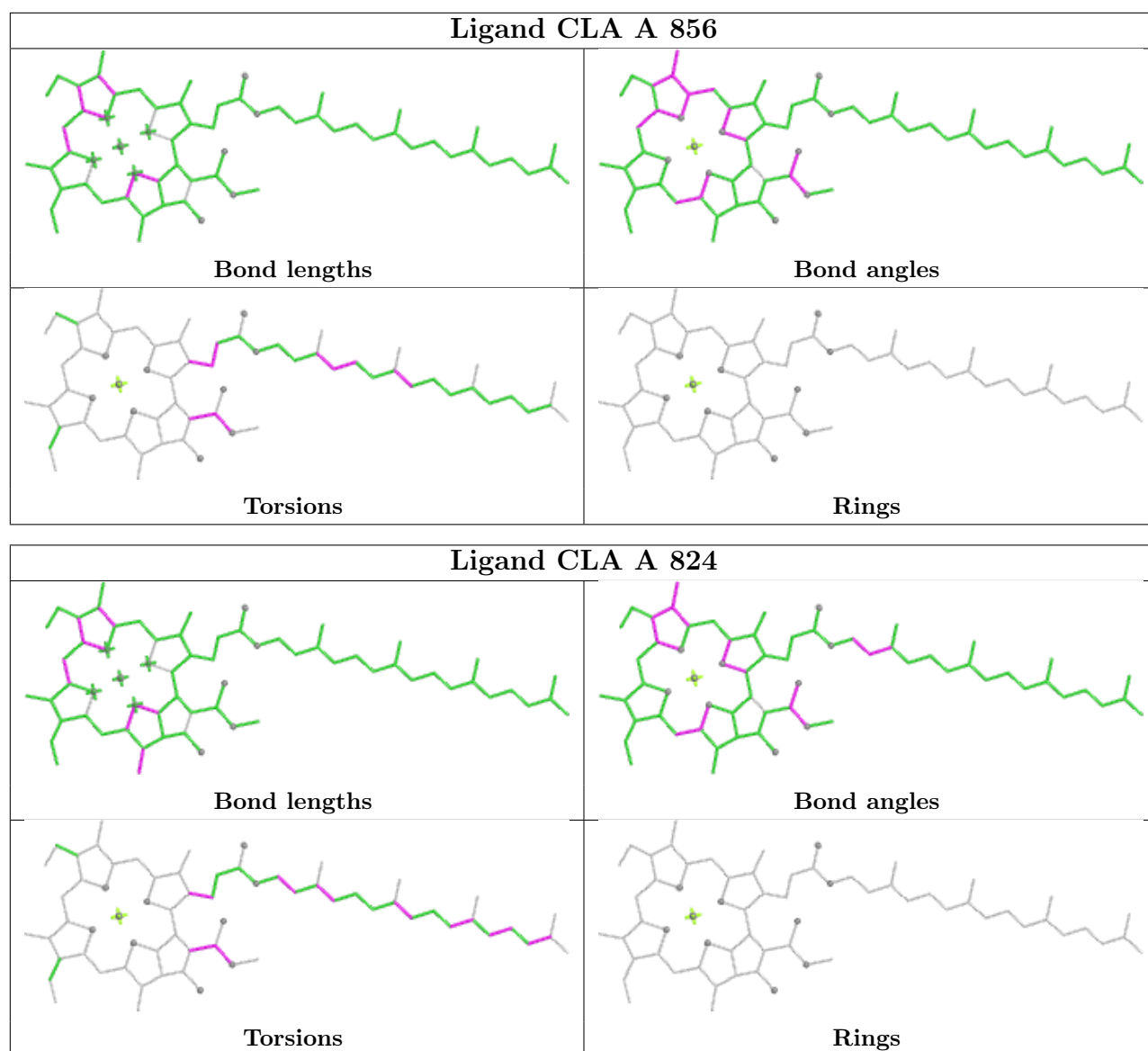


Ligand CLA B 831

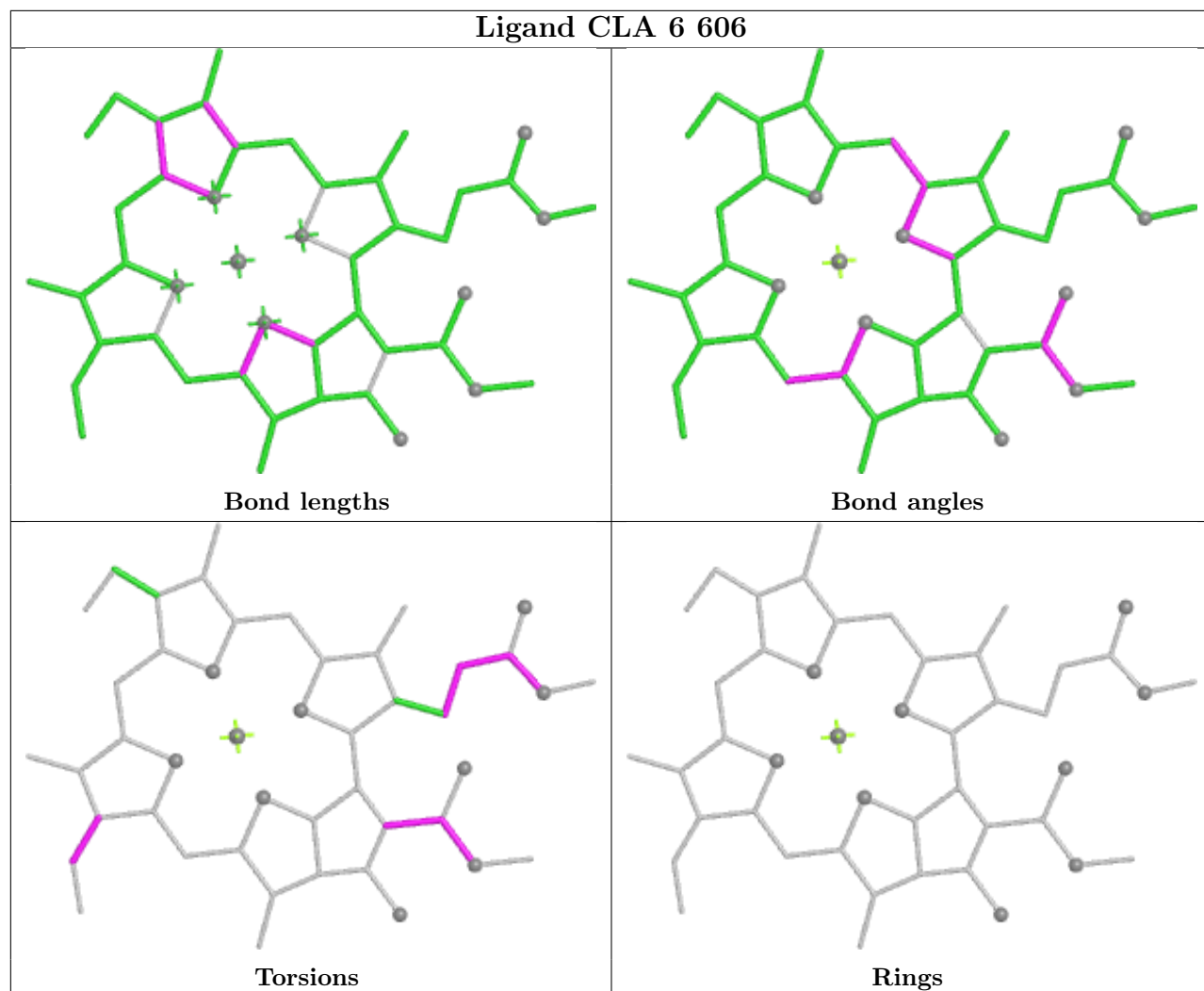


Ligand CLA 9 309

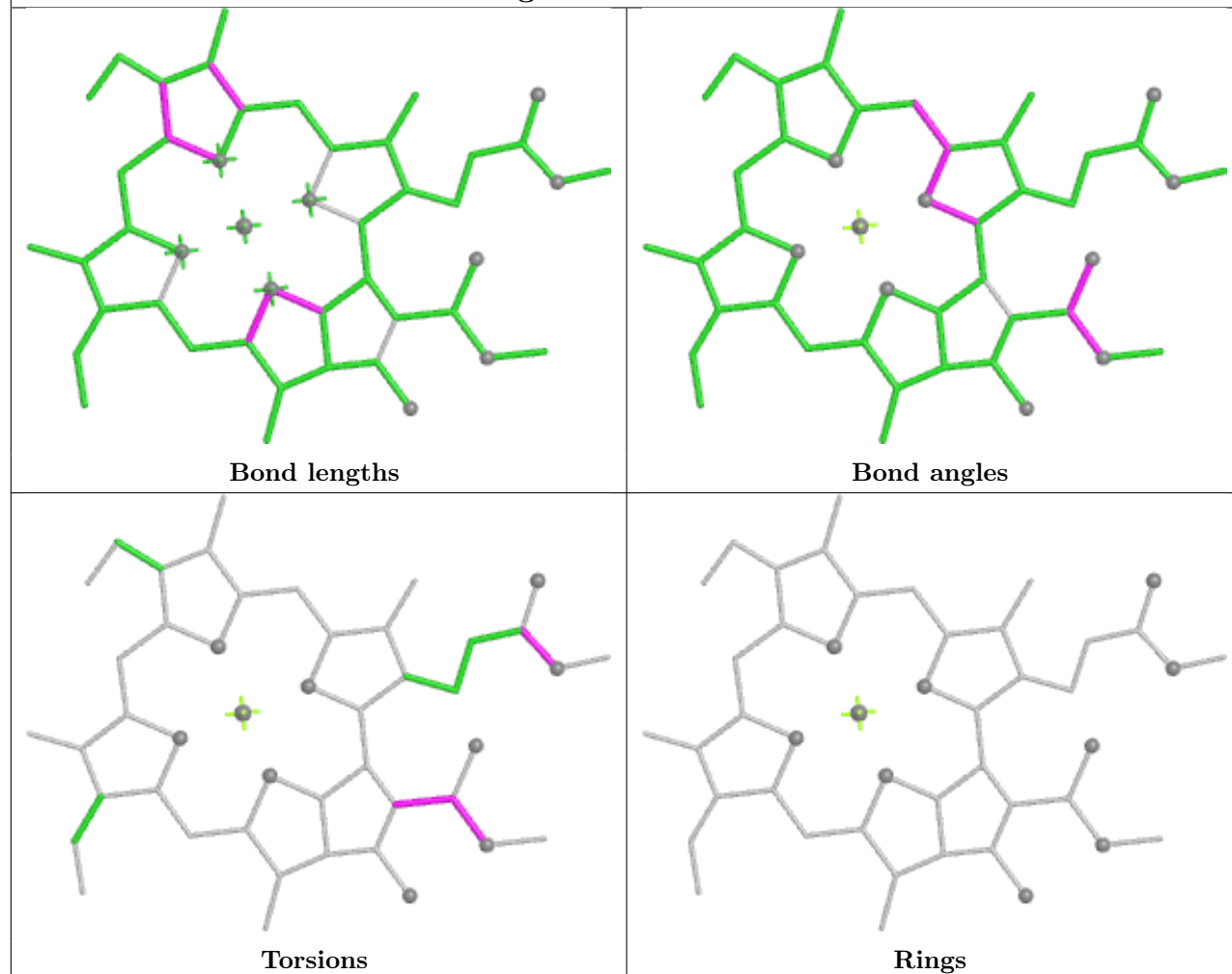




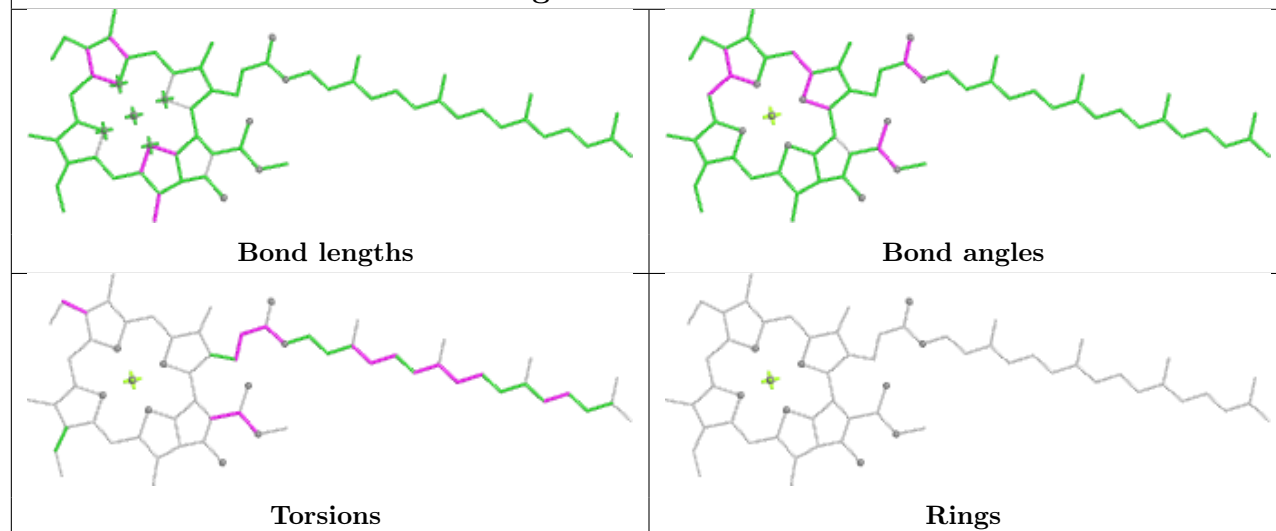
Ligand CLA 6 606



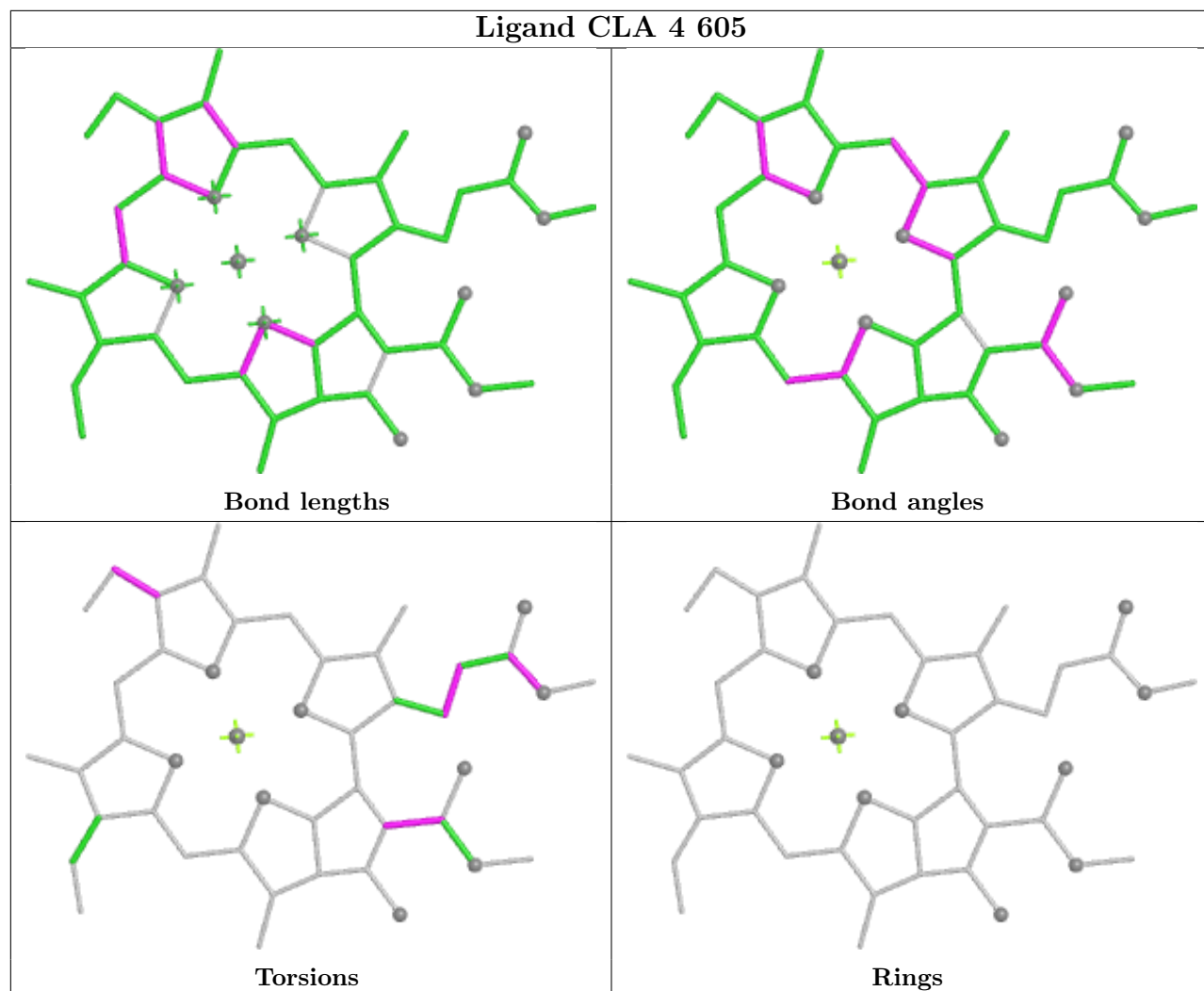
Ligand CLA 2 208



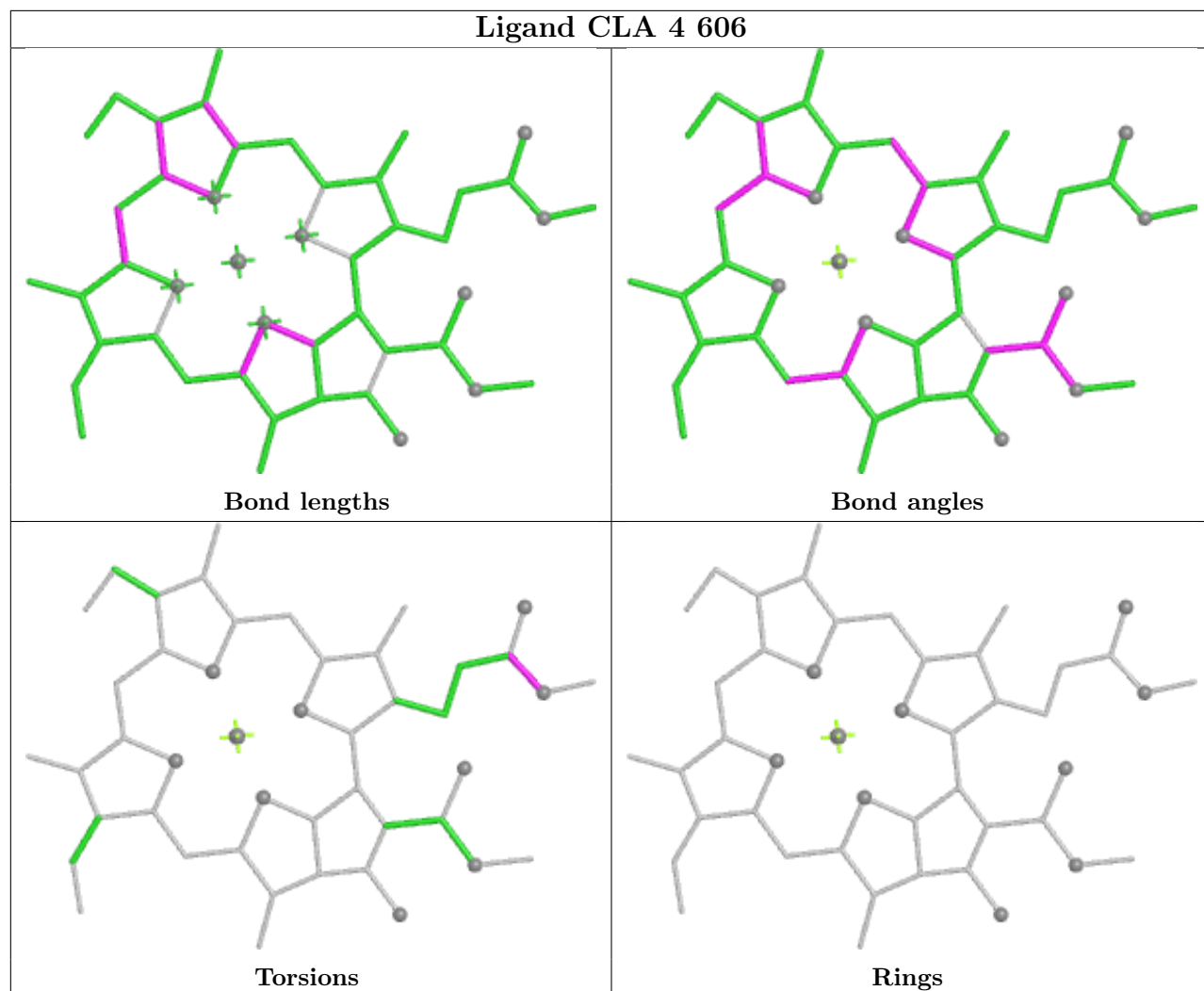
Ligand CLA B 802

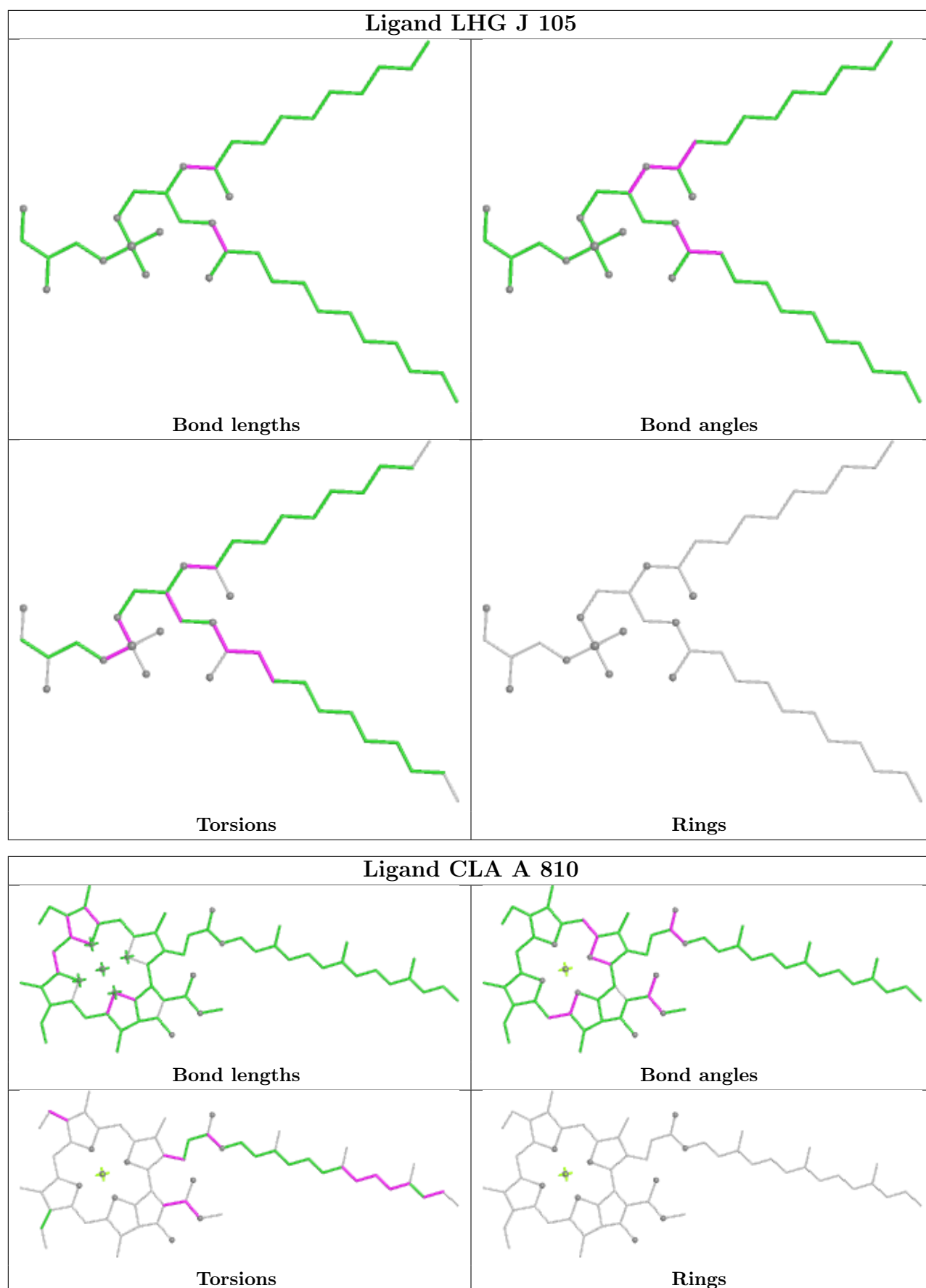


Ligand CLA 4 605

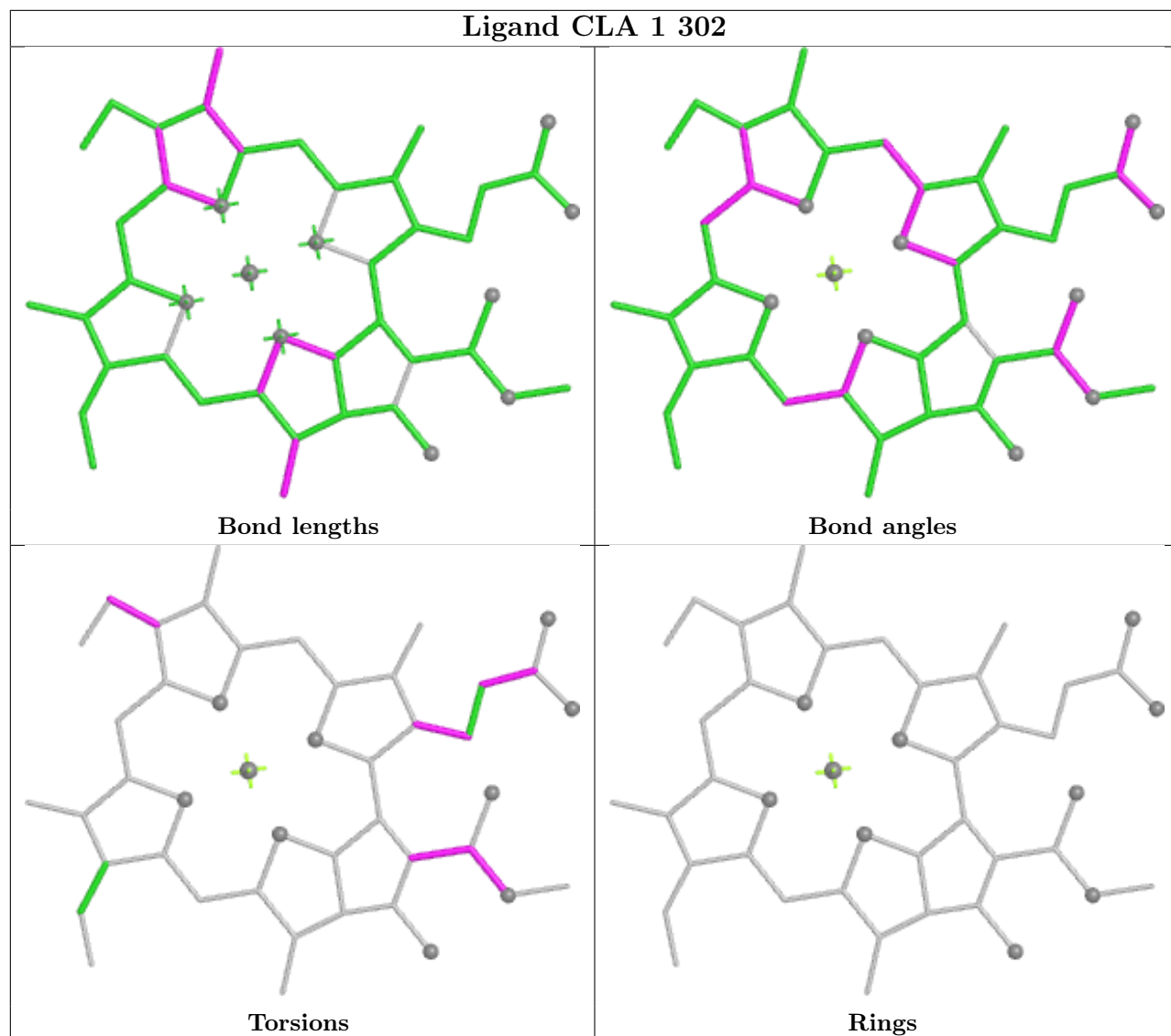


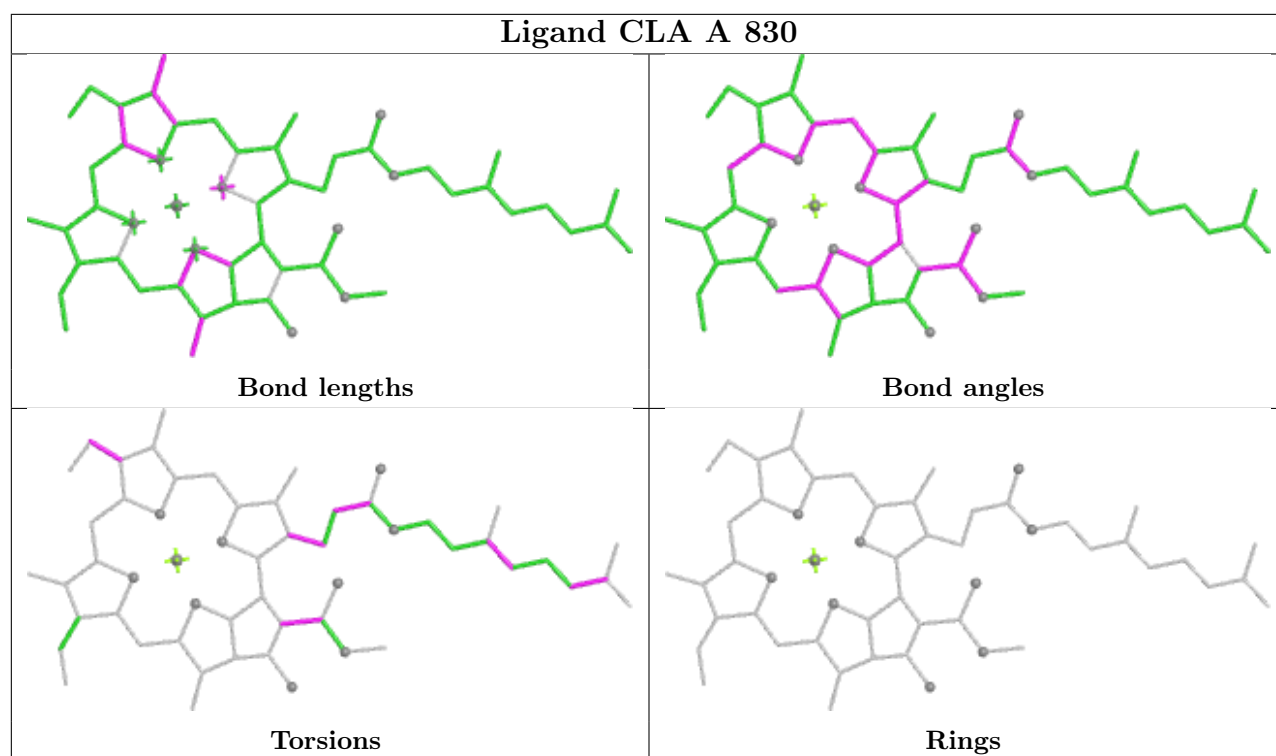
Ligand CLA 4 606



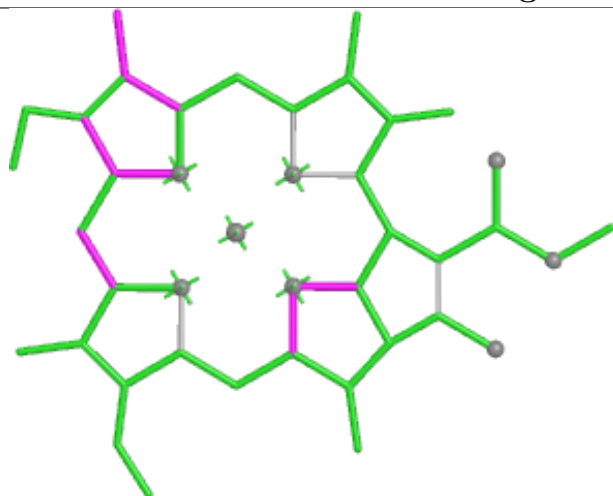


Ligand CLA 1 302





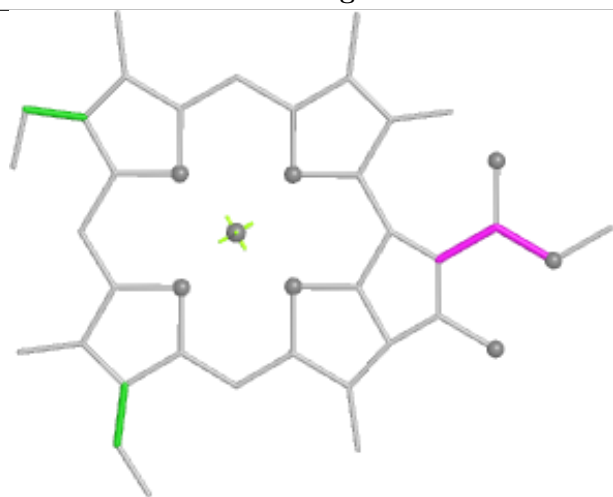
Ligand CLA c 611



Bond lengths



Bond angles

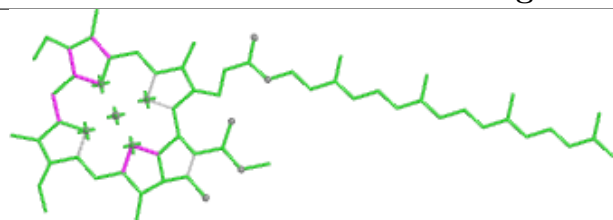


Torsions

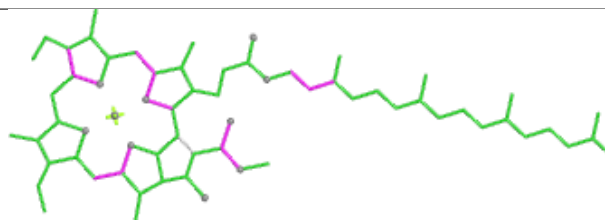


Rings

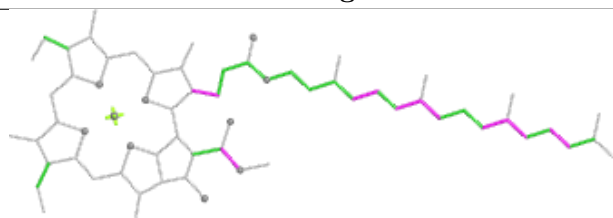
Ligand CLA F 201



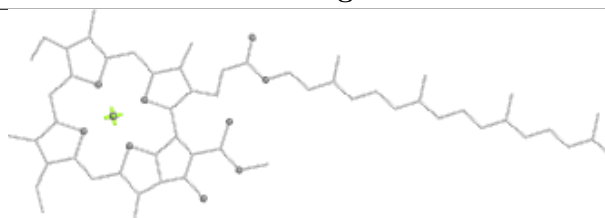
Bond lengths



Bond angles

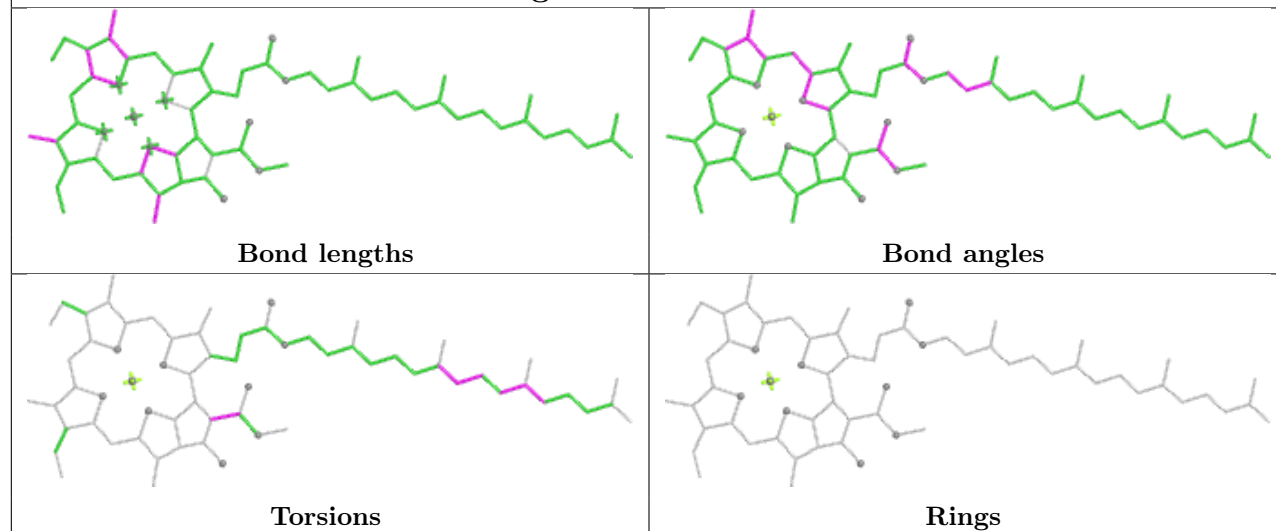


Torsions

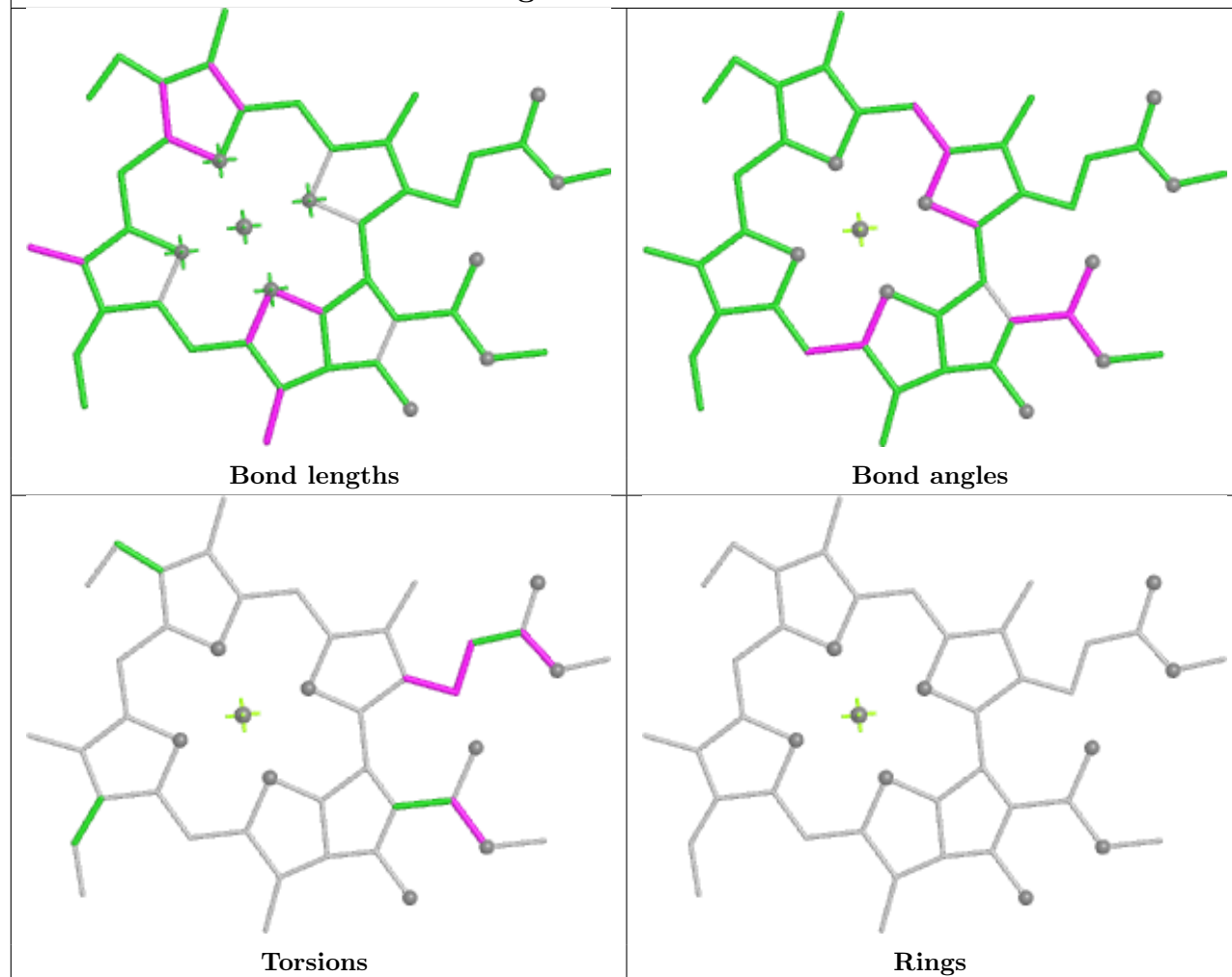


Rings

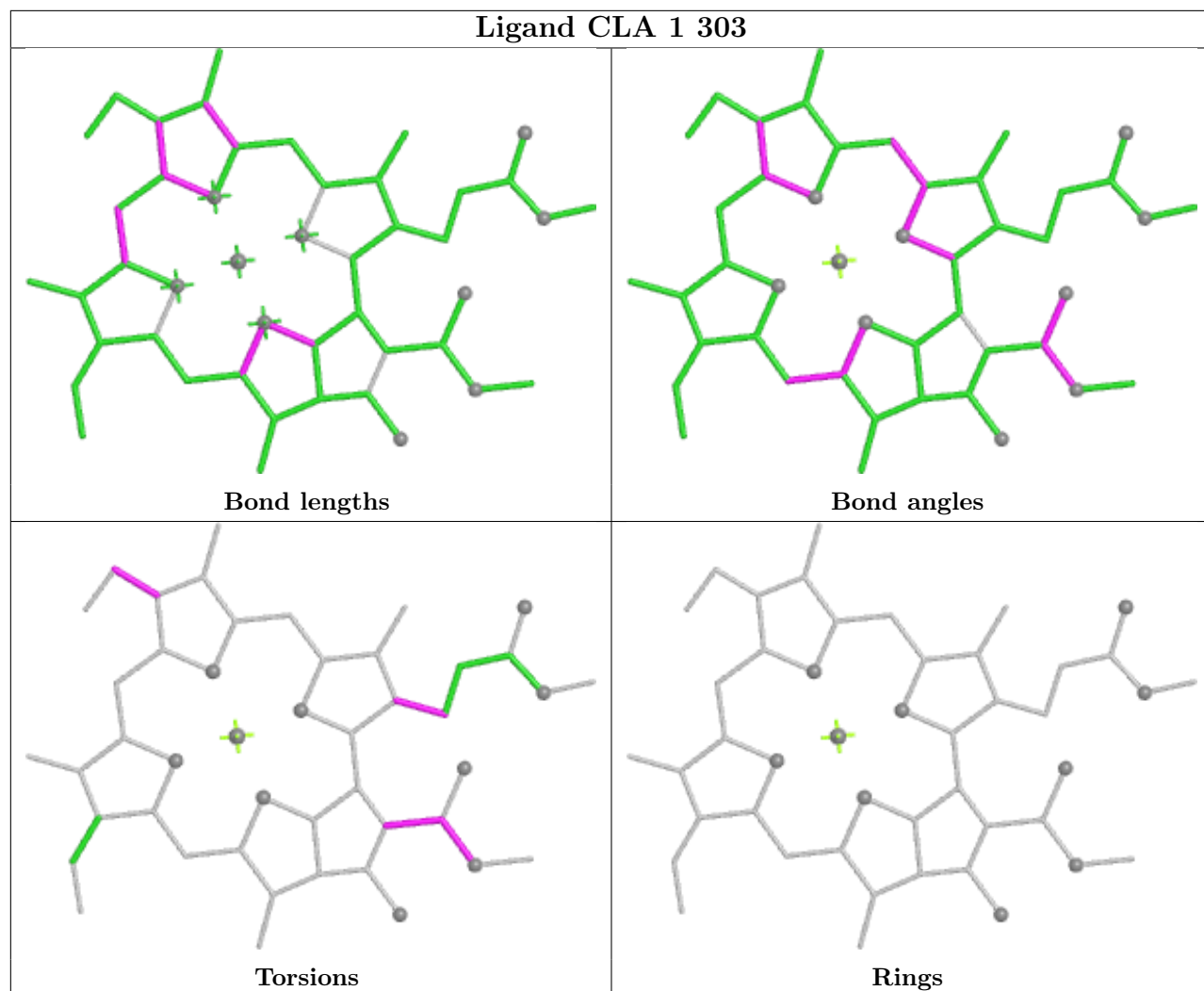
Ligand CLA A 857



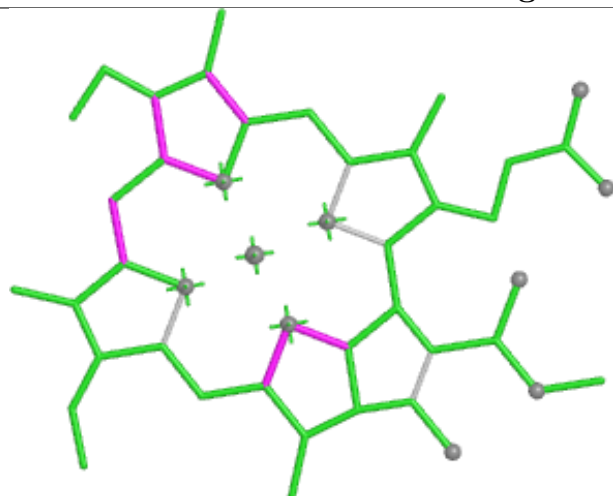
Ligand CLA 9 307



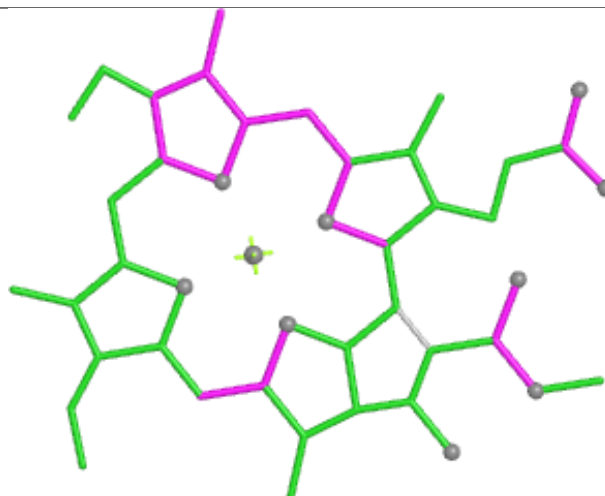
Ligand CLA 1 303



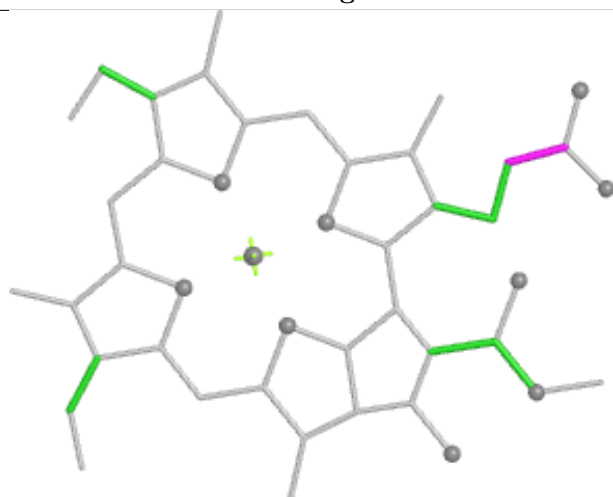
Ligand CLA 7 603



Bond lengths



Bond angles

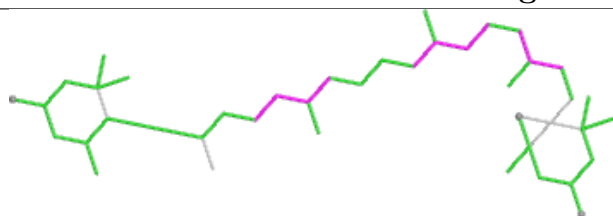


Torsions

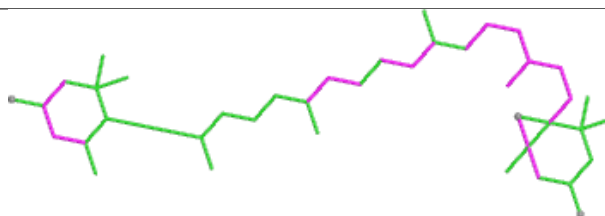


Rings

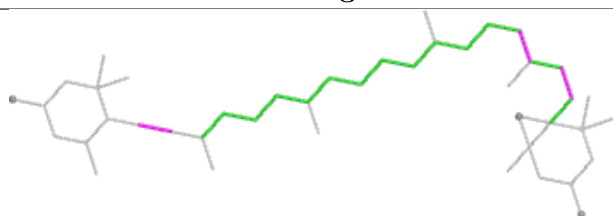
Ligand DD6 8 211



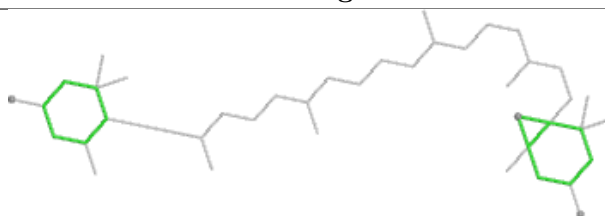
Bond lengths



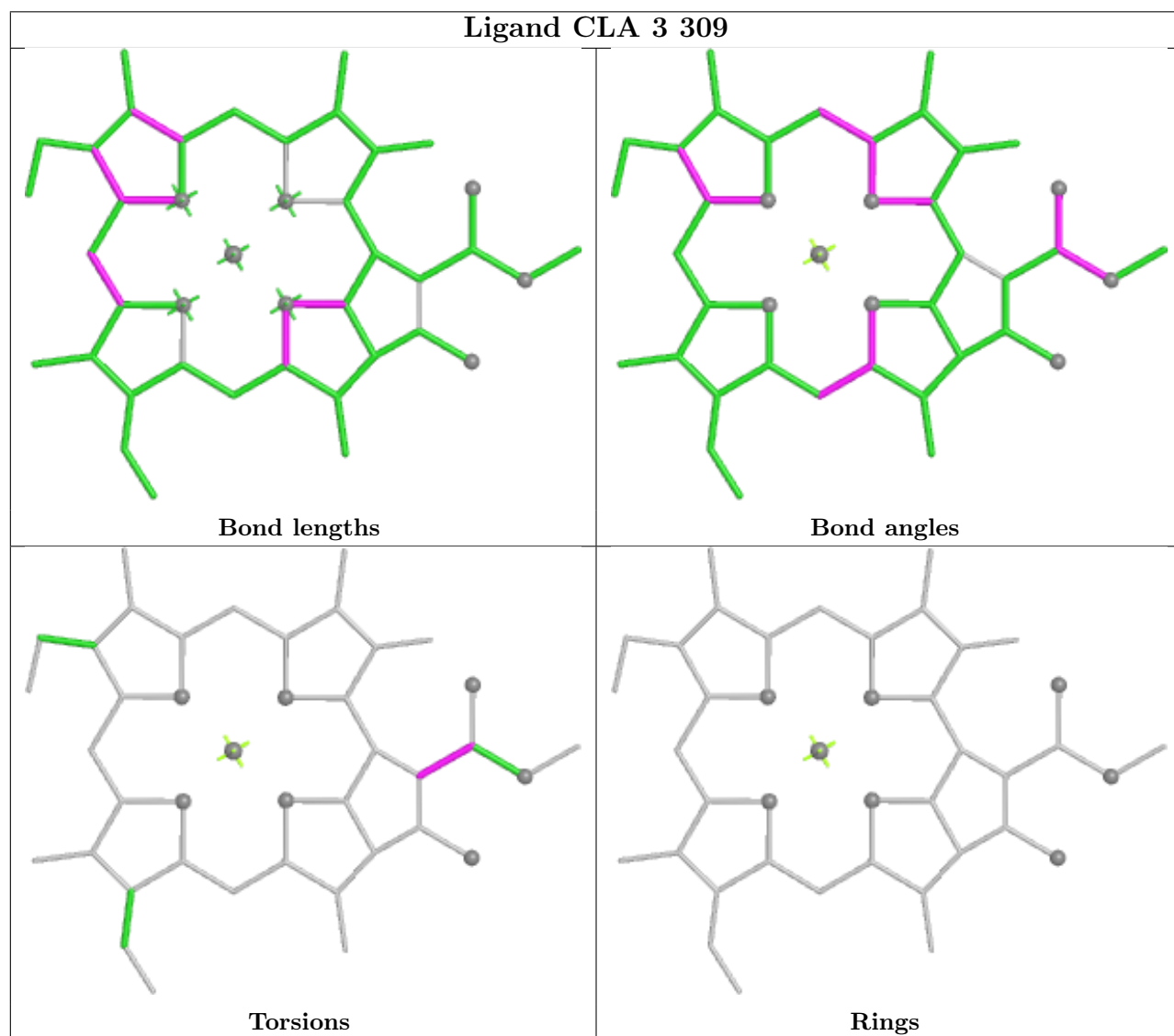
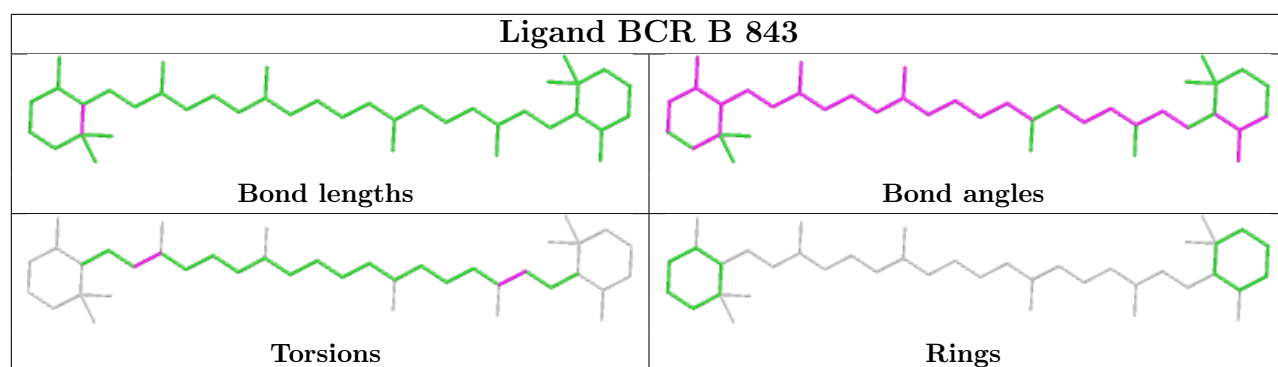
Bond angles



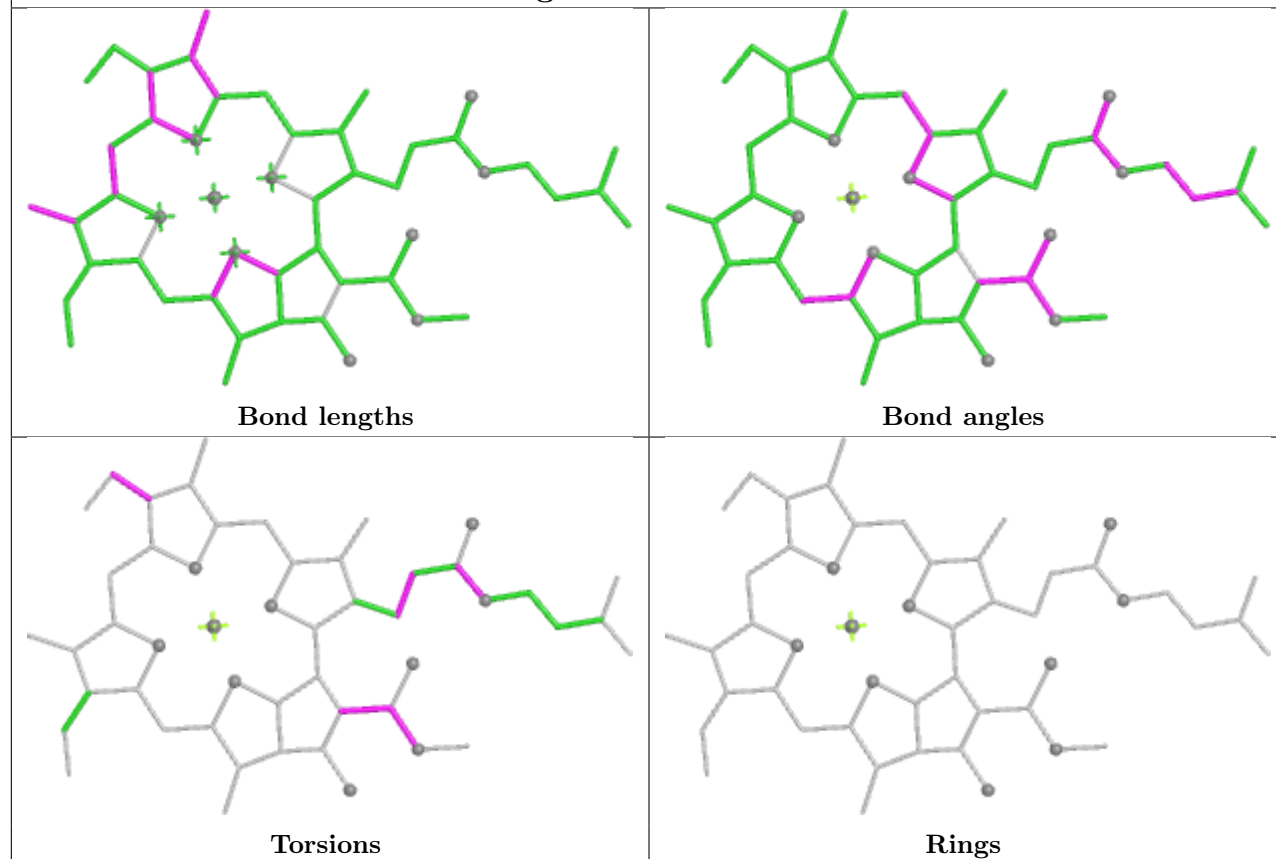
Torsions



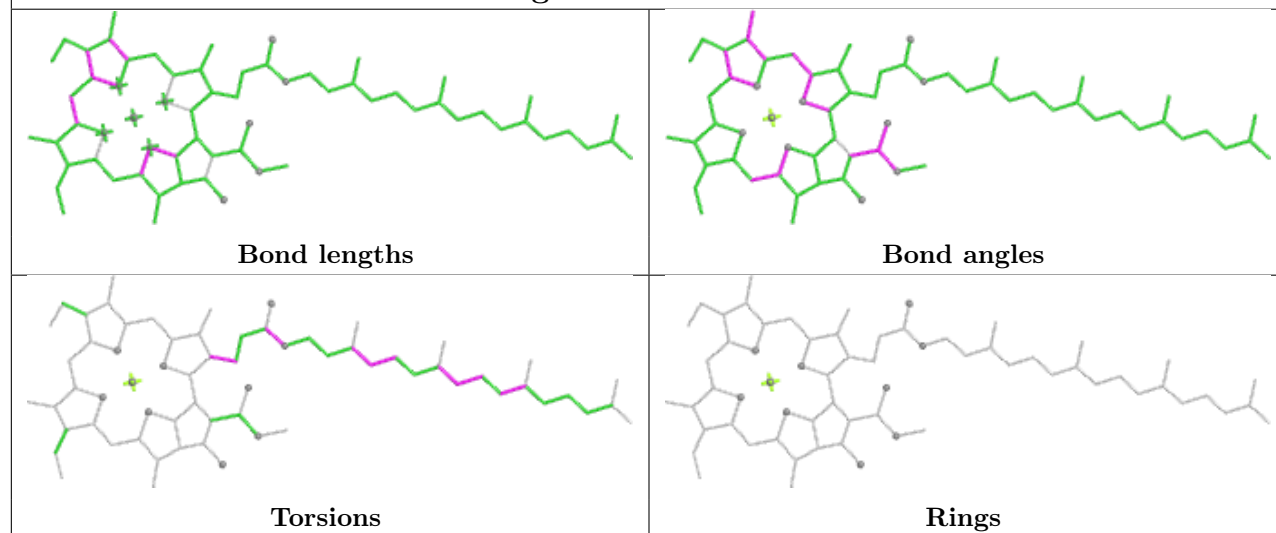
Rings

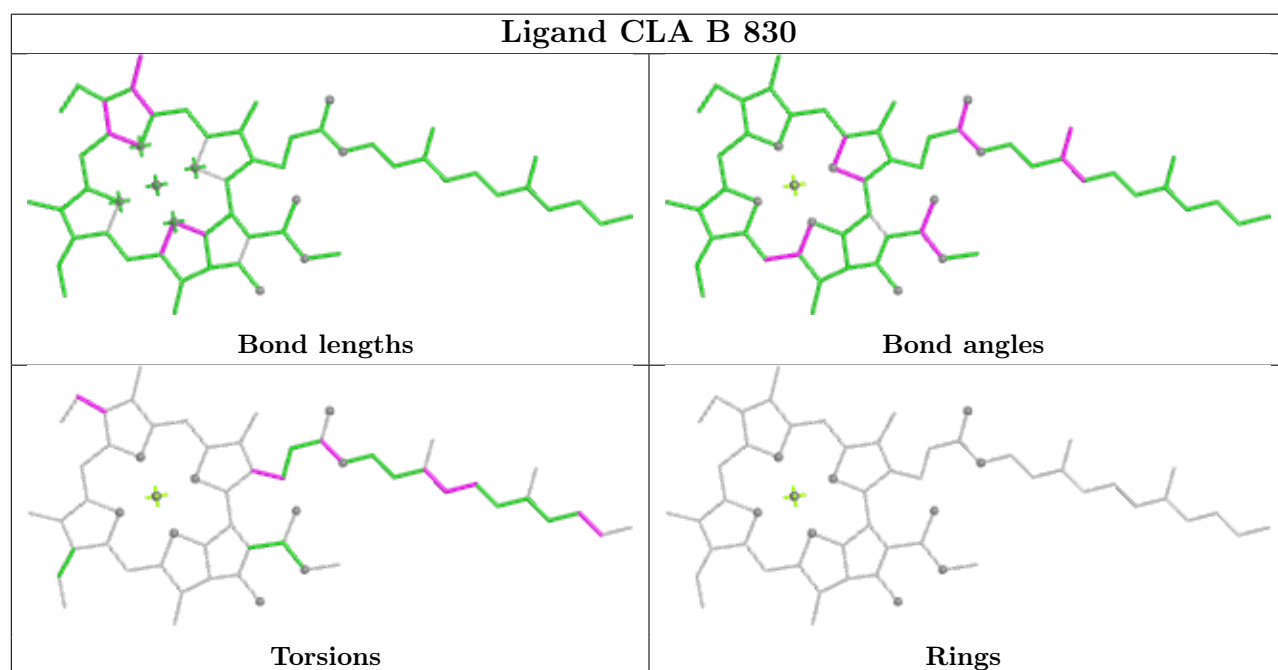
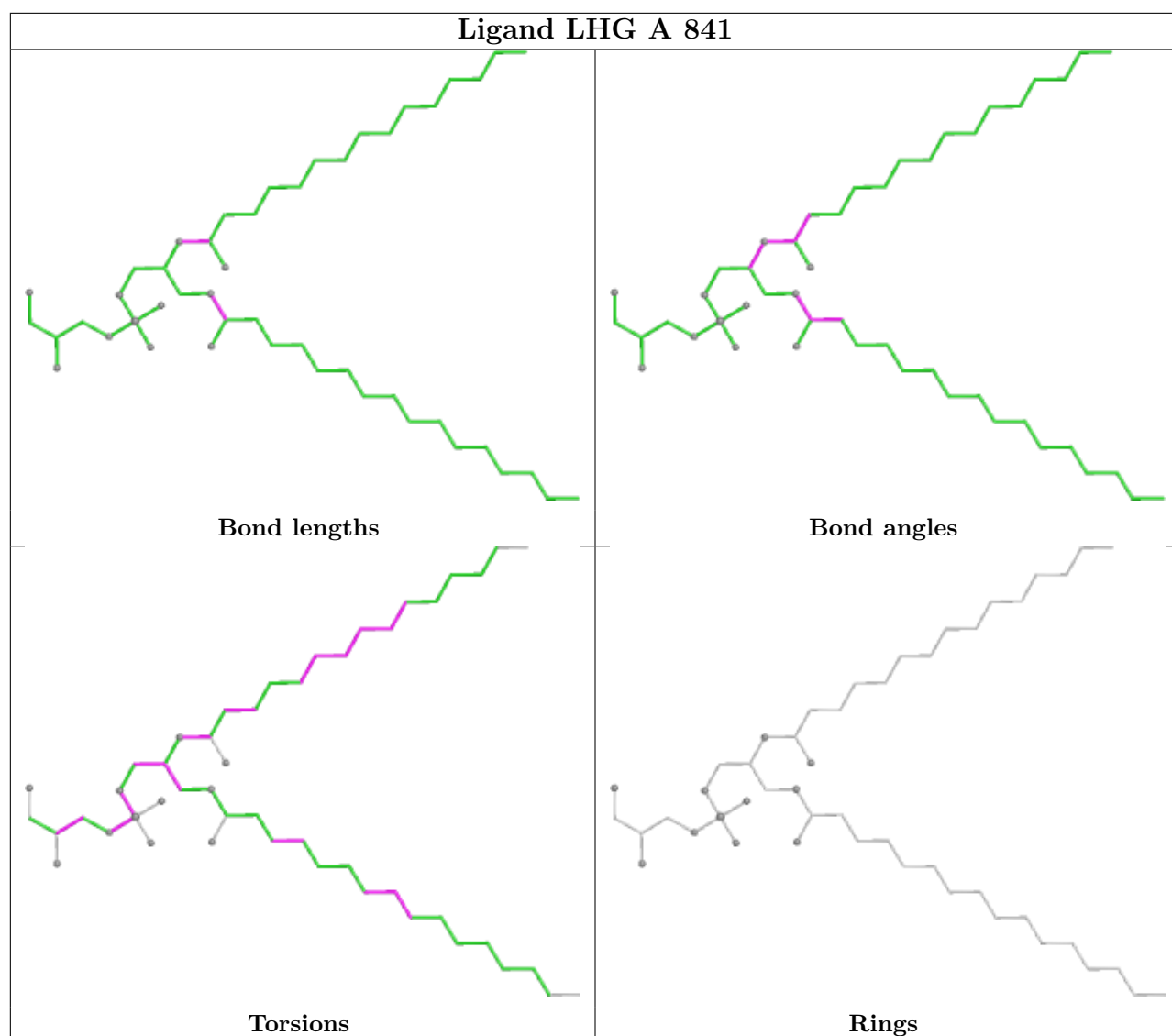


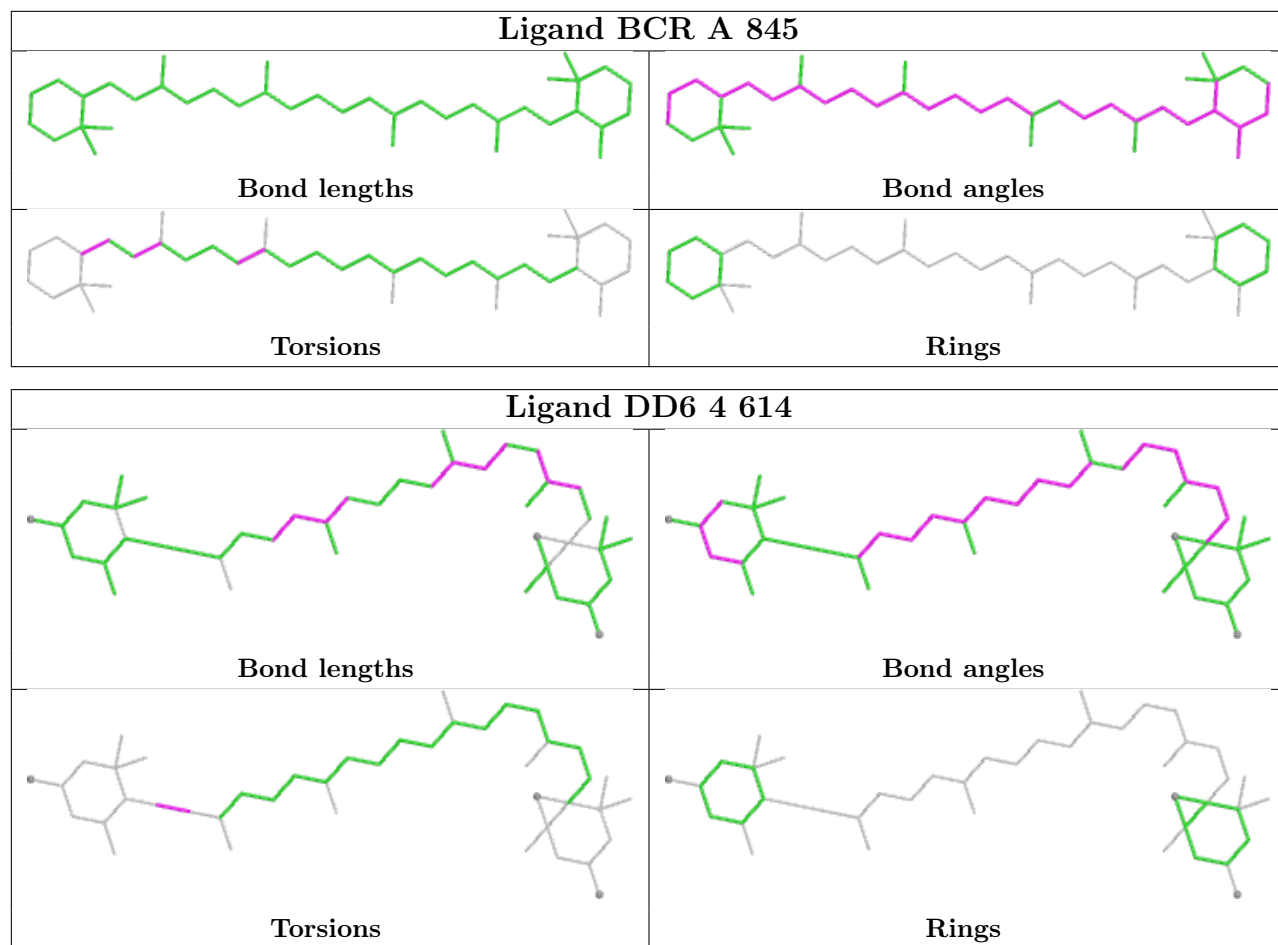
Ligand CLA 8 203



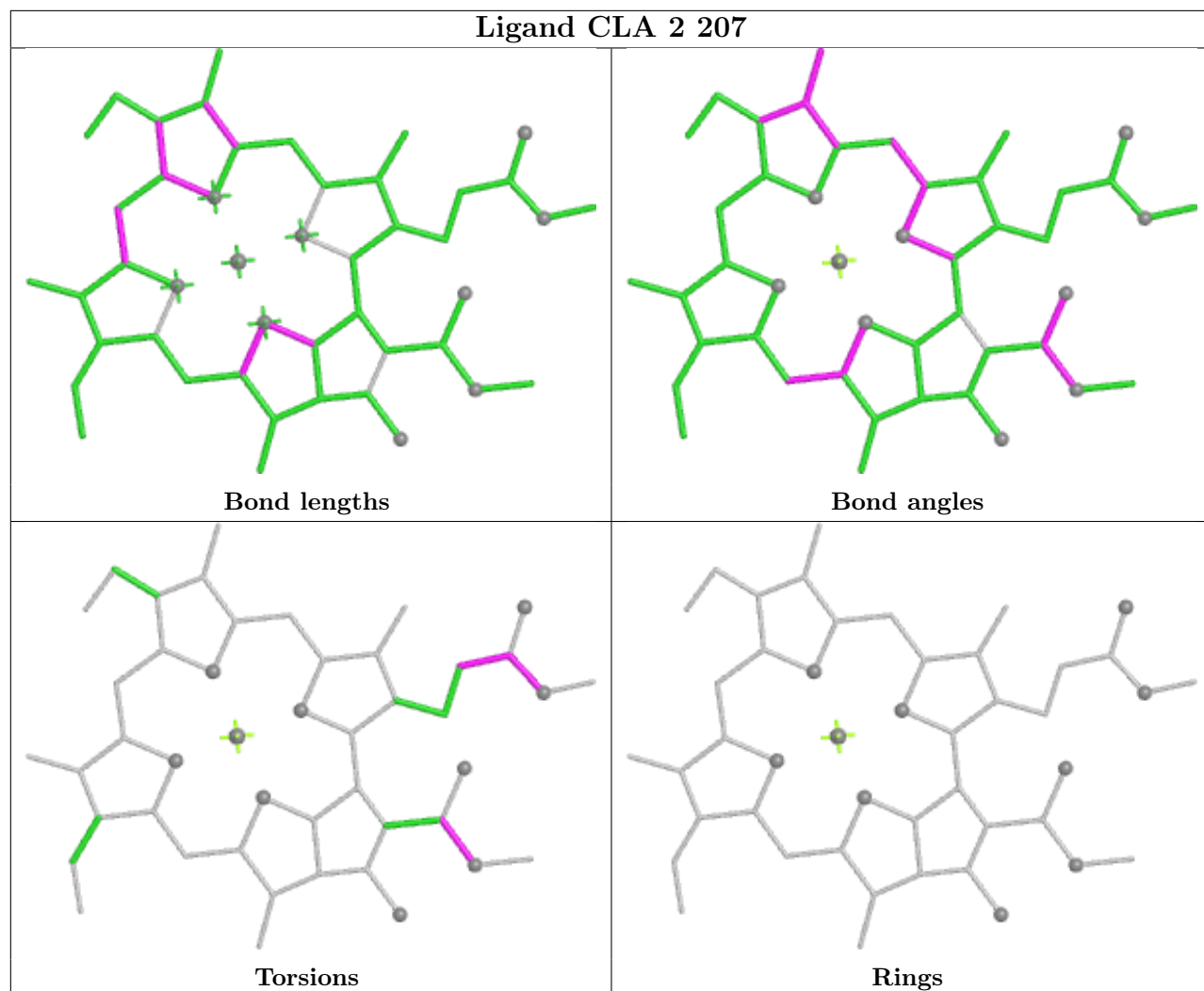
Ligand CLA A 805



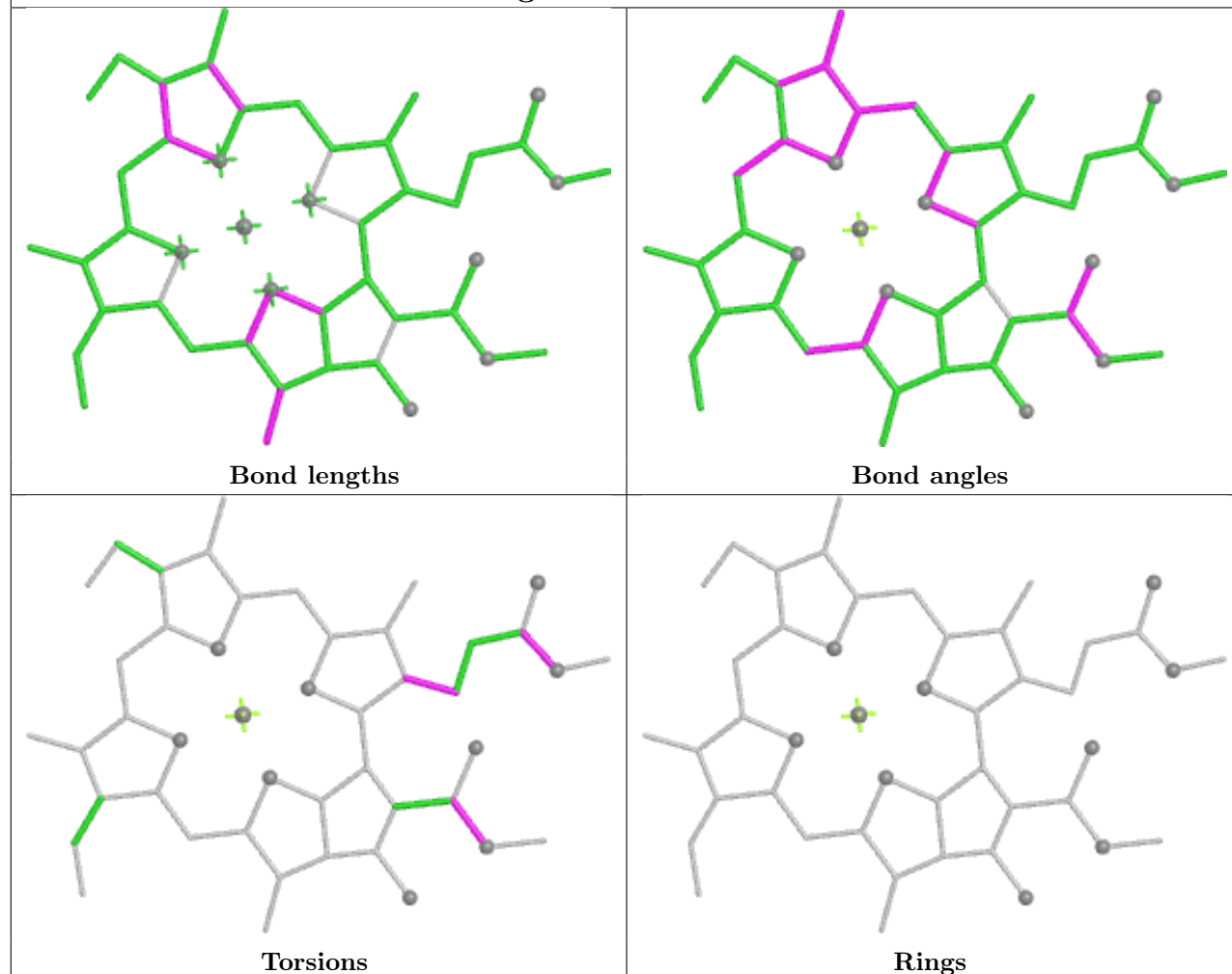




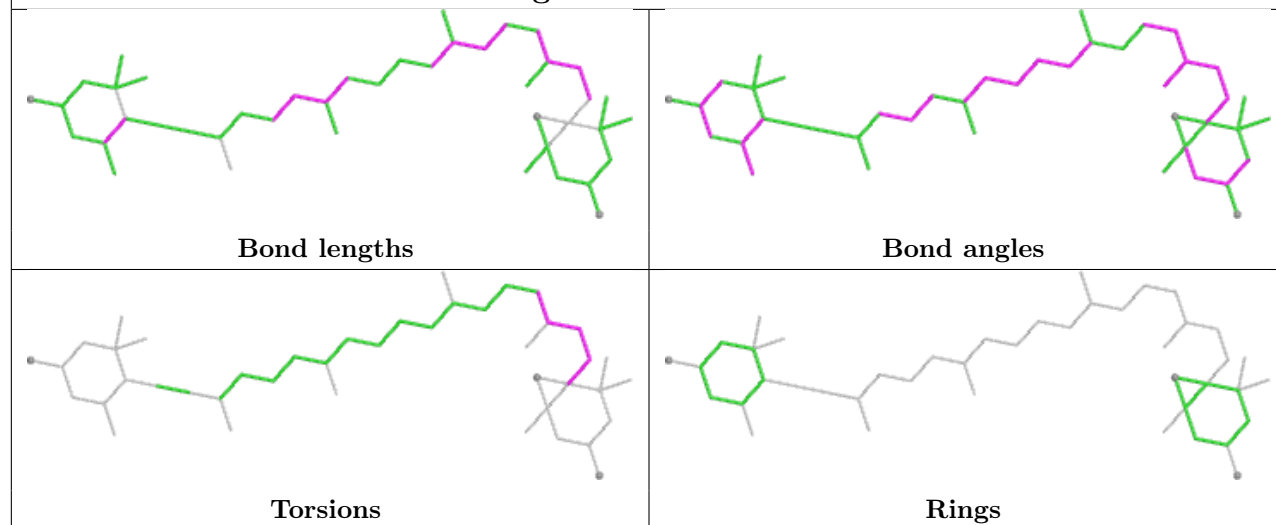
Ligand CLA 2 207

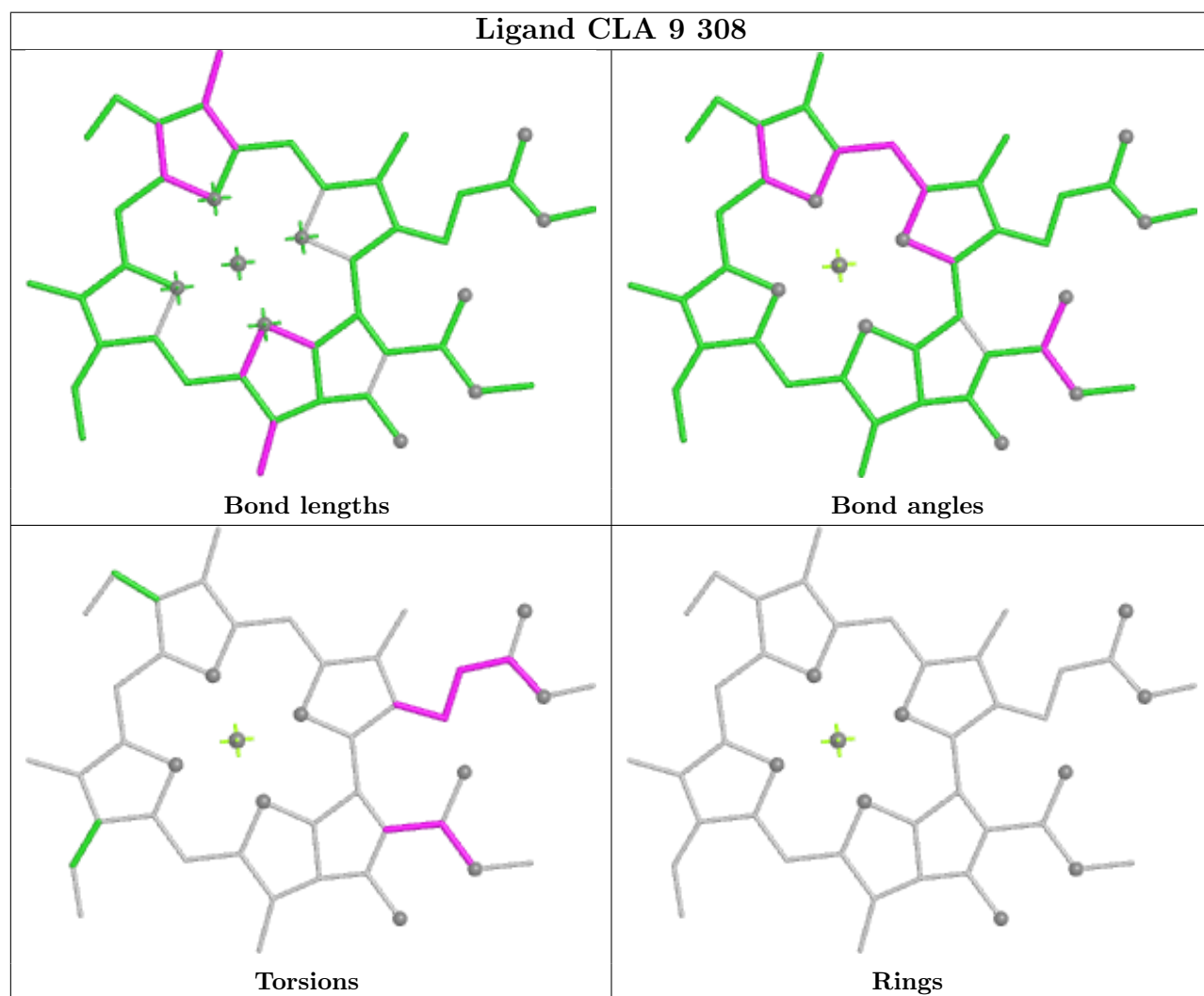
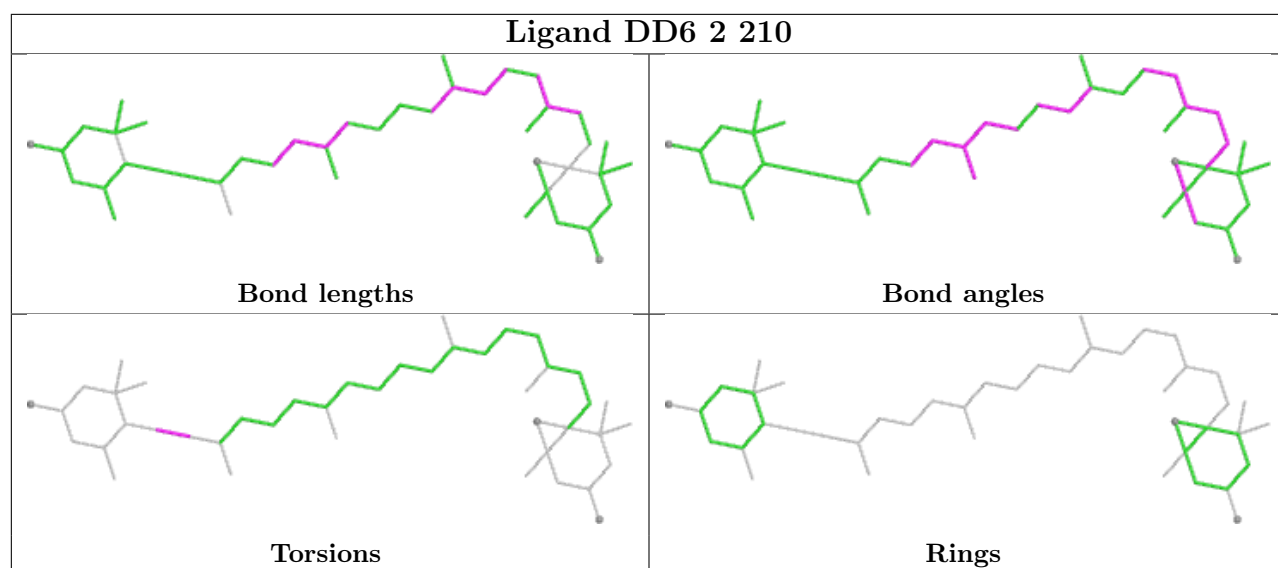


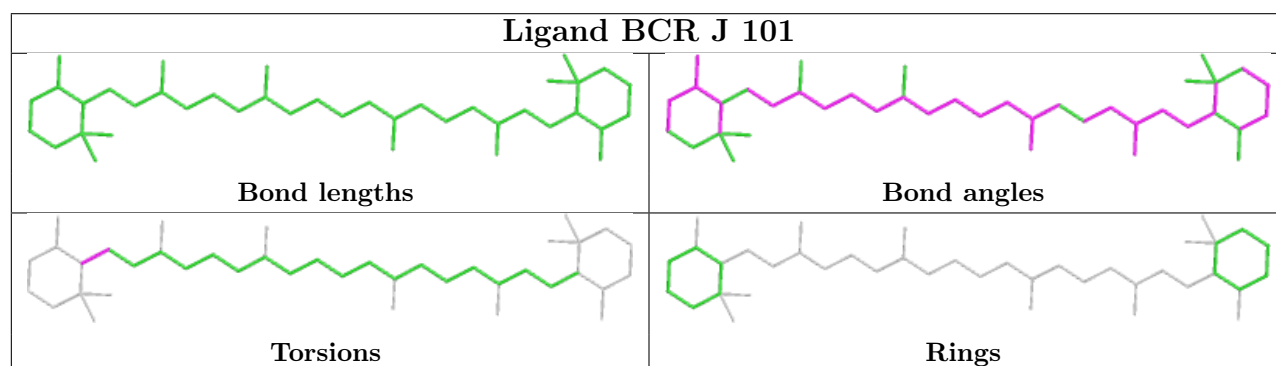
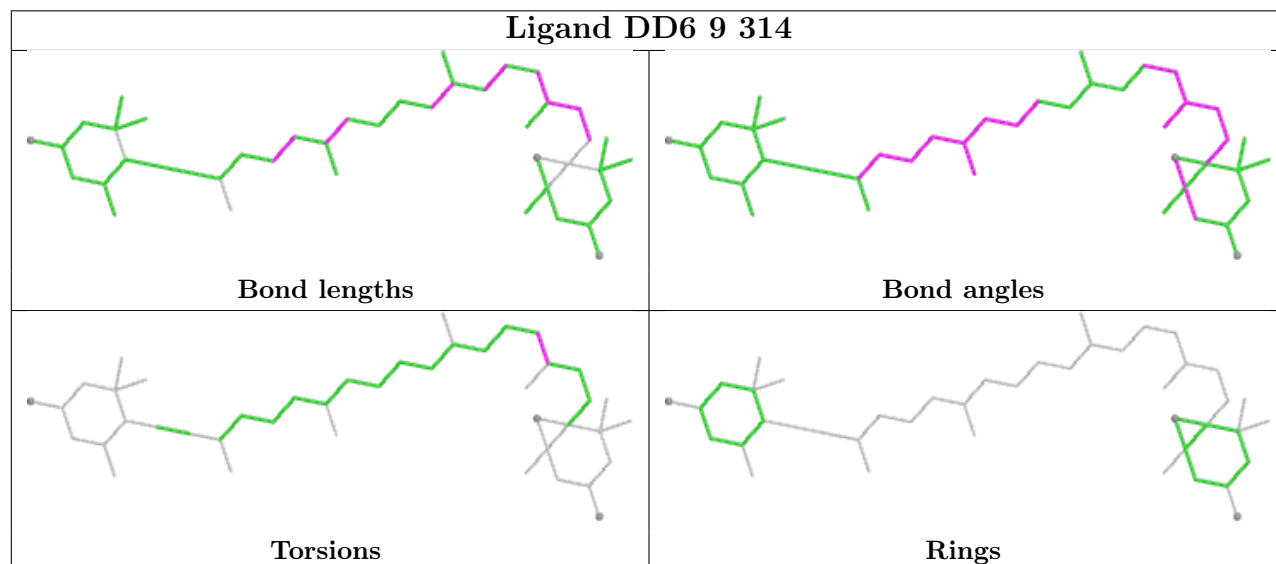
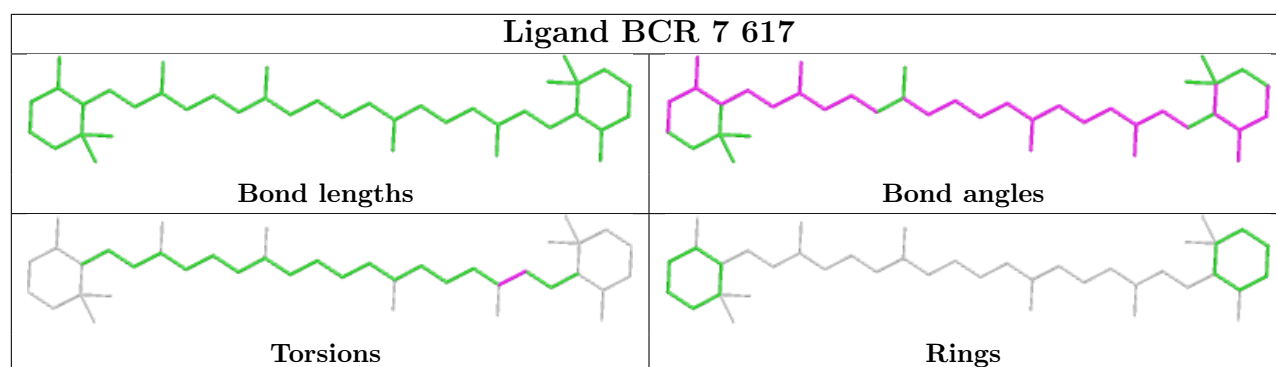
Ligand CLA 4 612



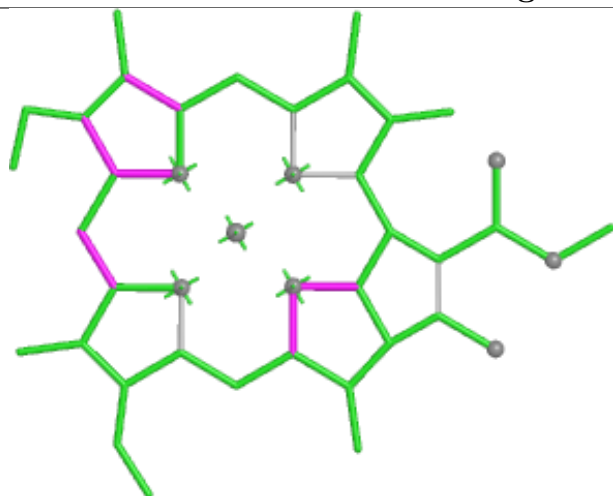
Ligand DD6 R 105







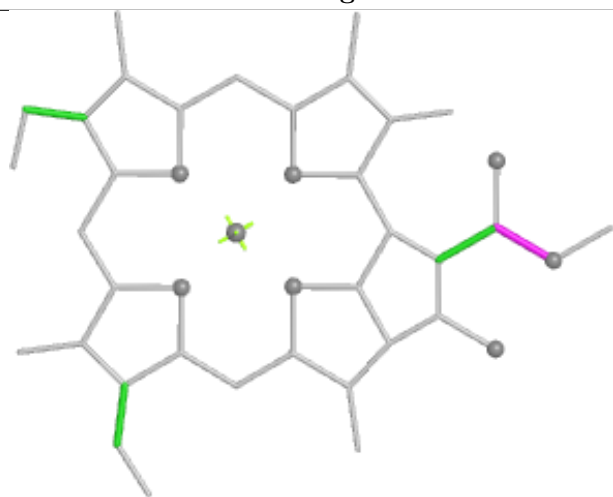
Ligand CLA k 310



Bond lengths



Bond angles

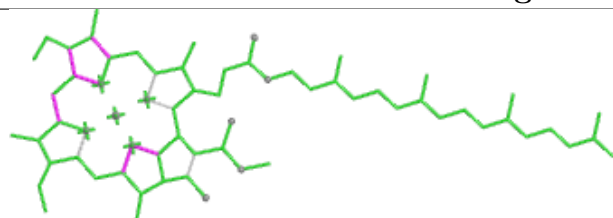


Torsions

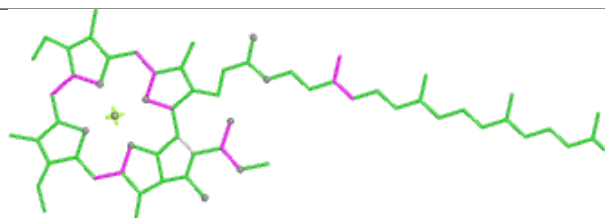


Rings

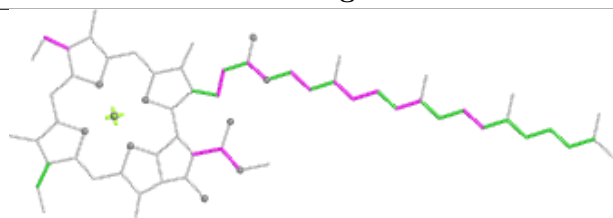
Ligand CLA B 837



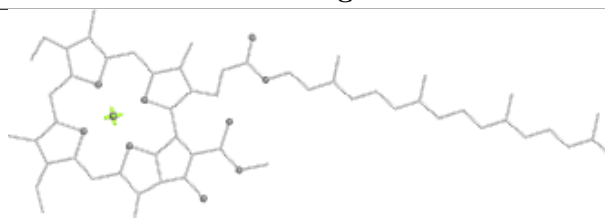
Bond lengths



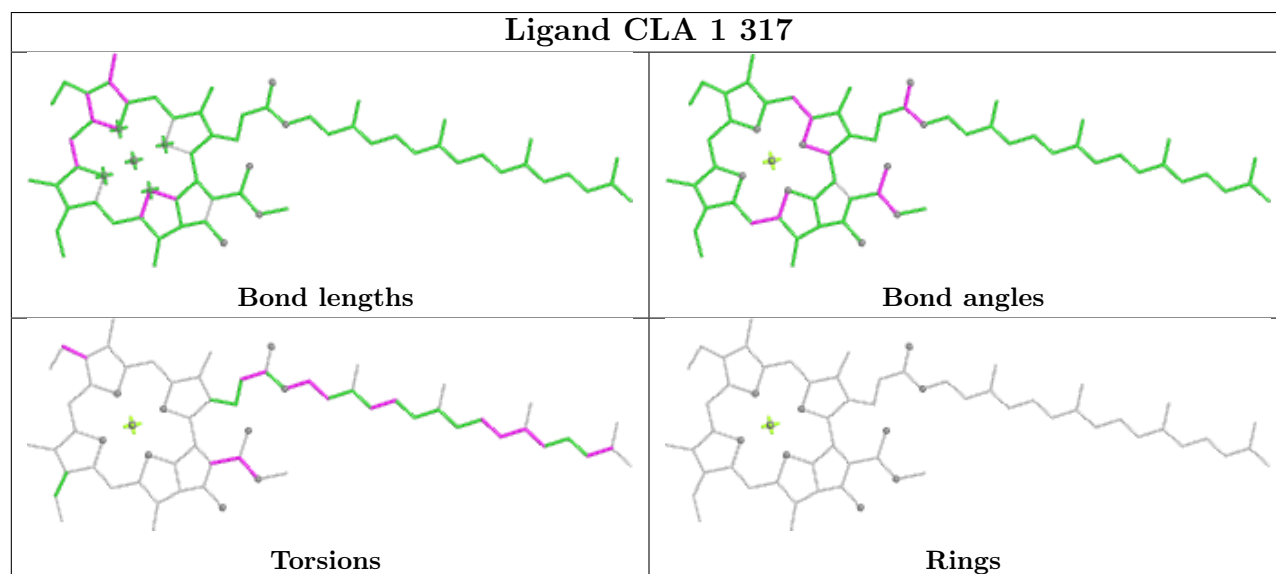
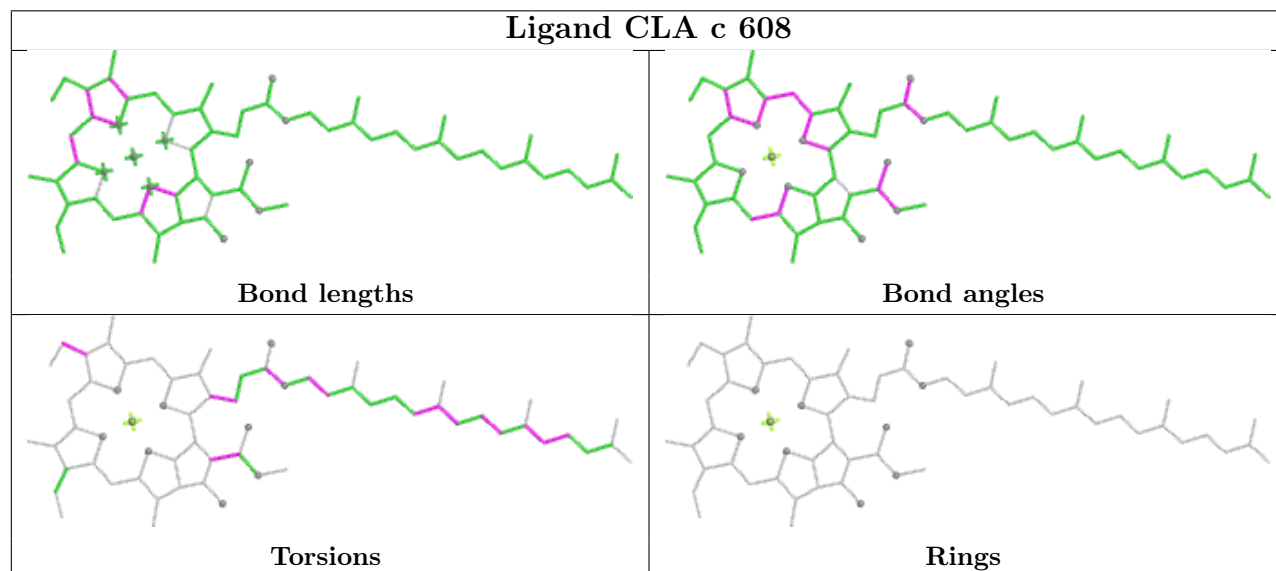
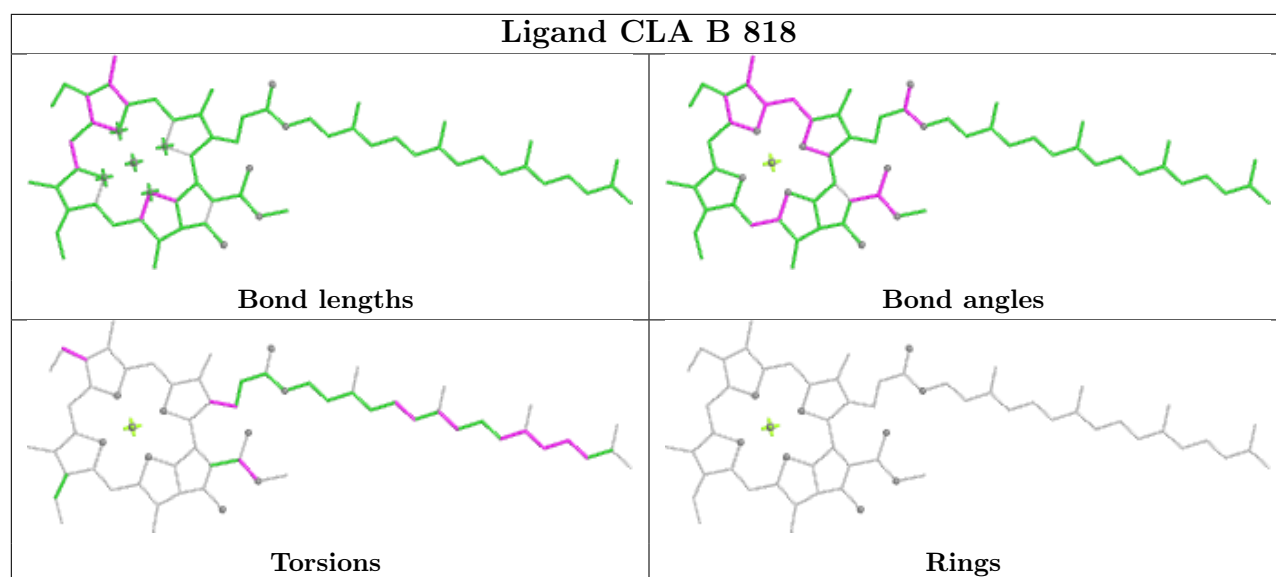
Bond angles

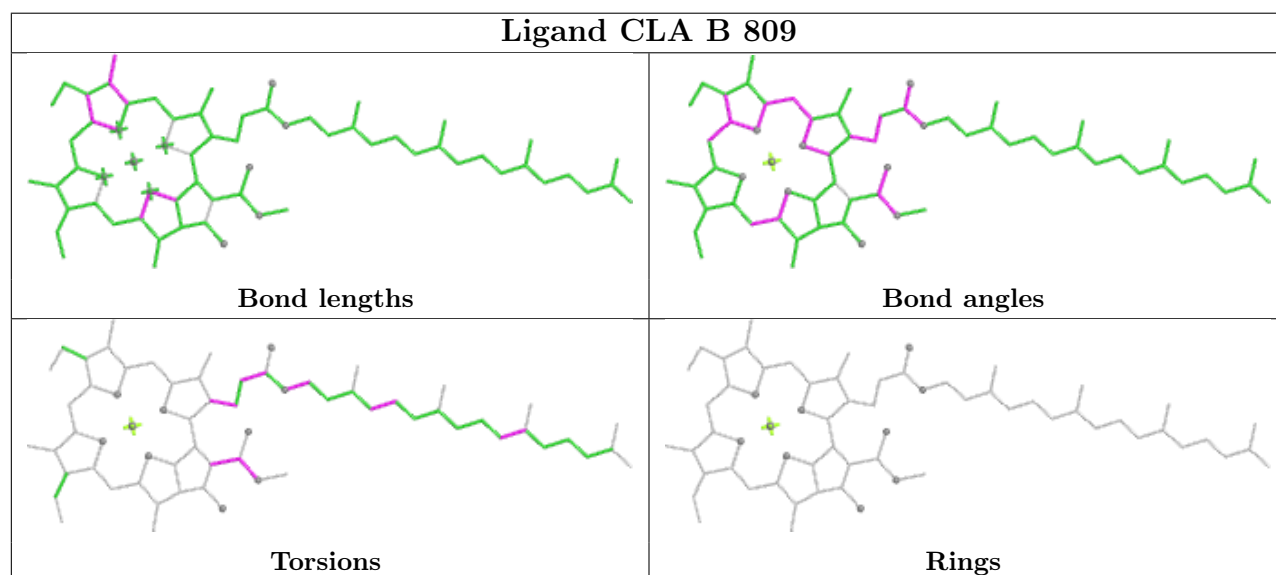
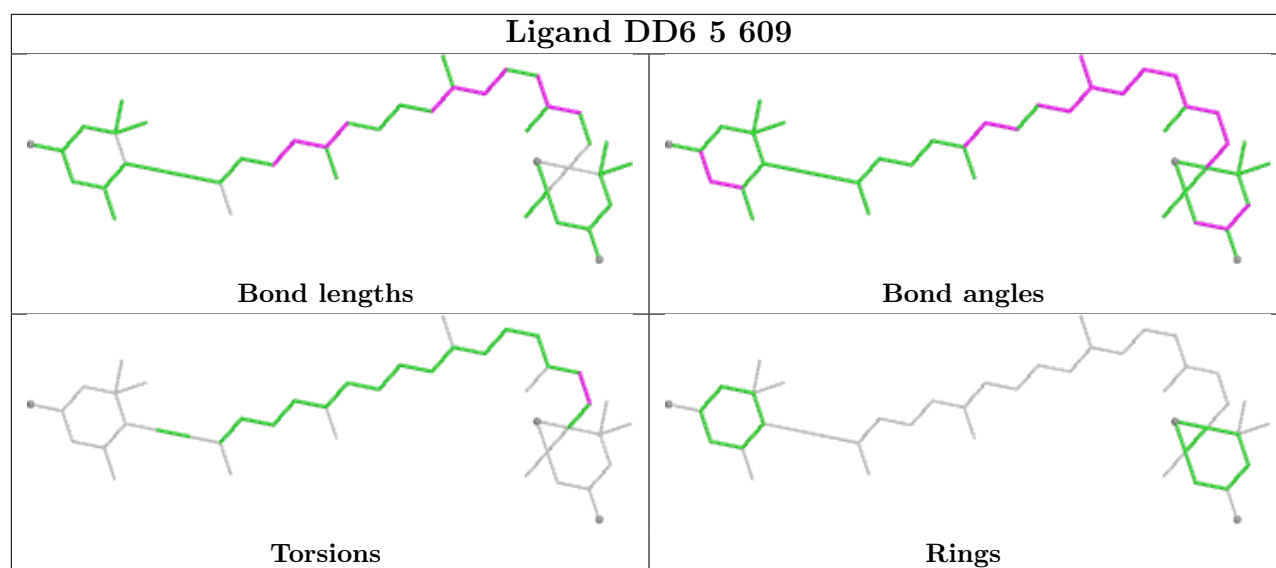


Torsions

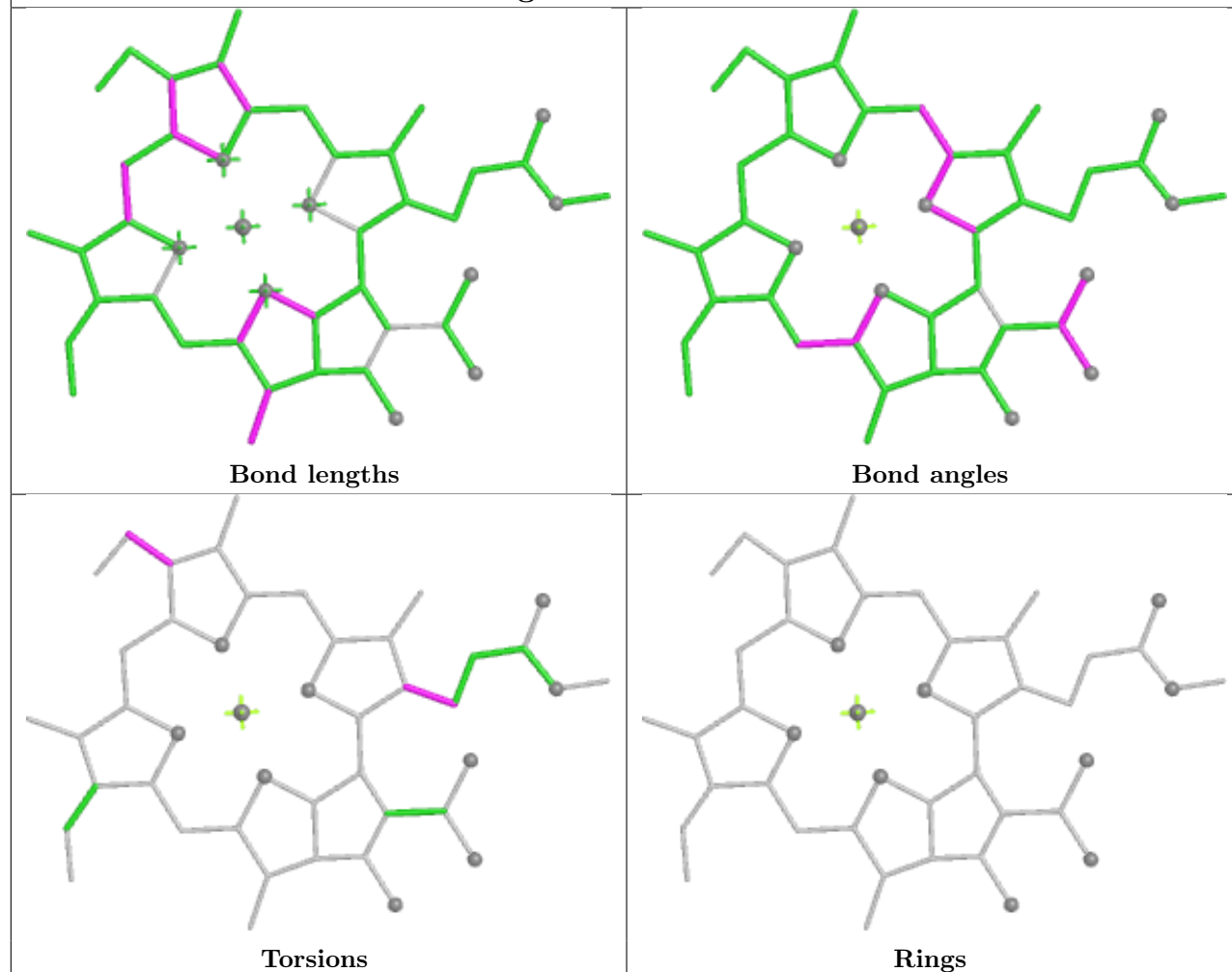


Rings

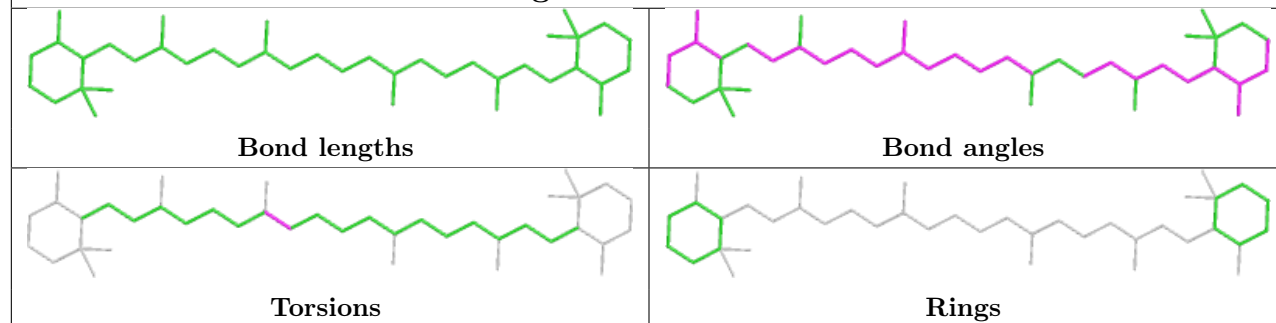


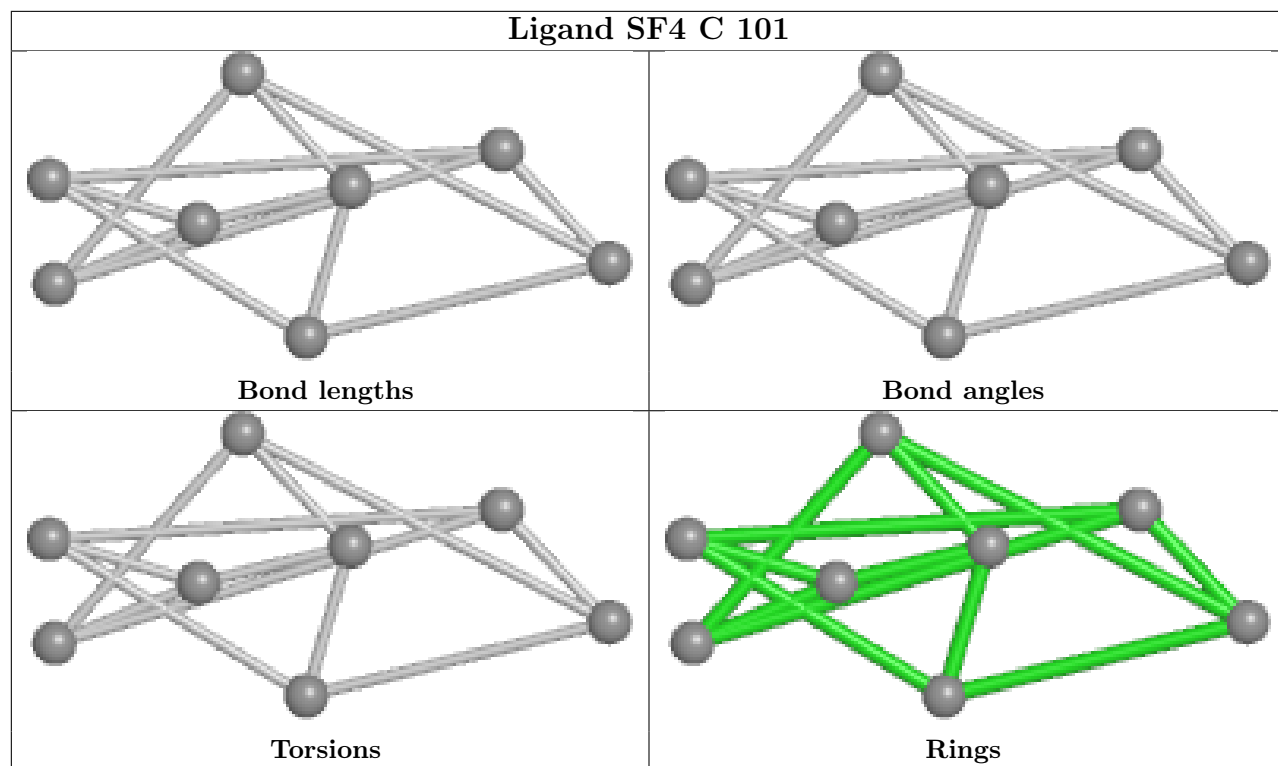


Ligand CLA 1 309

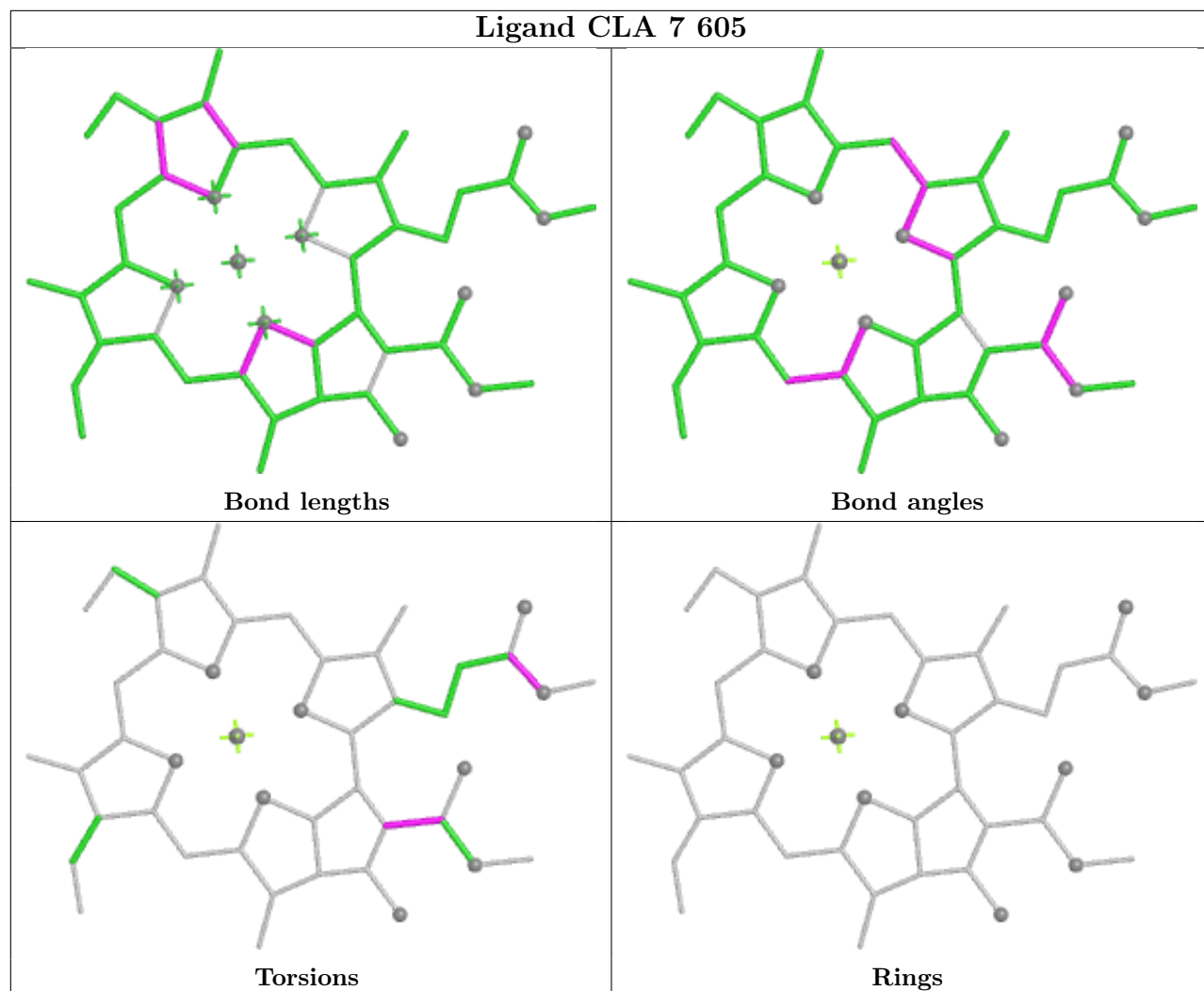


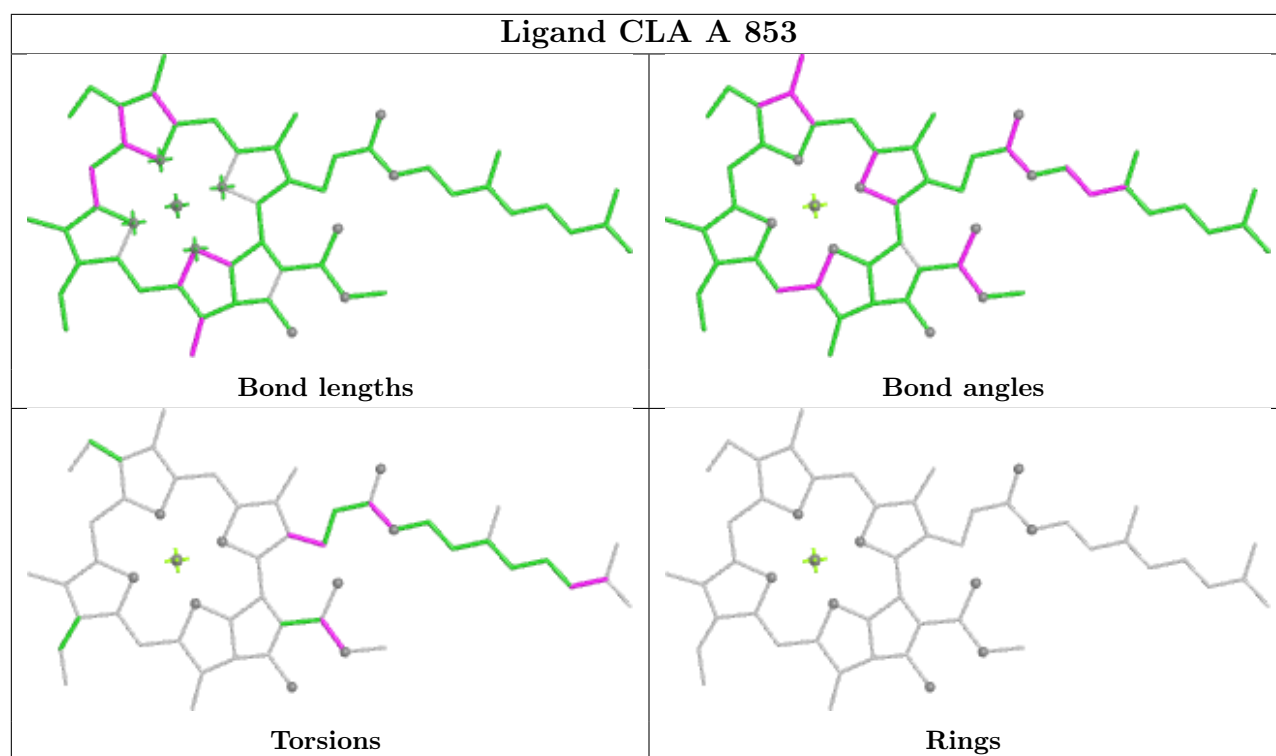
Ligand BCR F 204



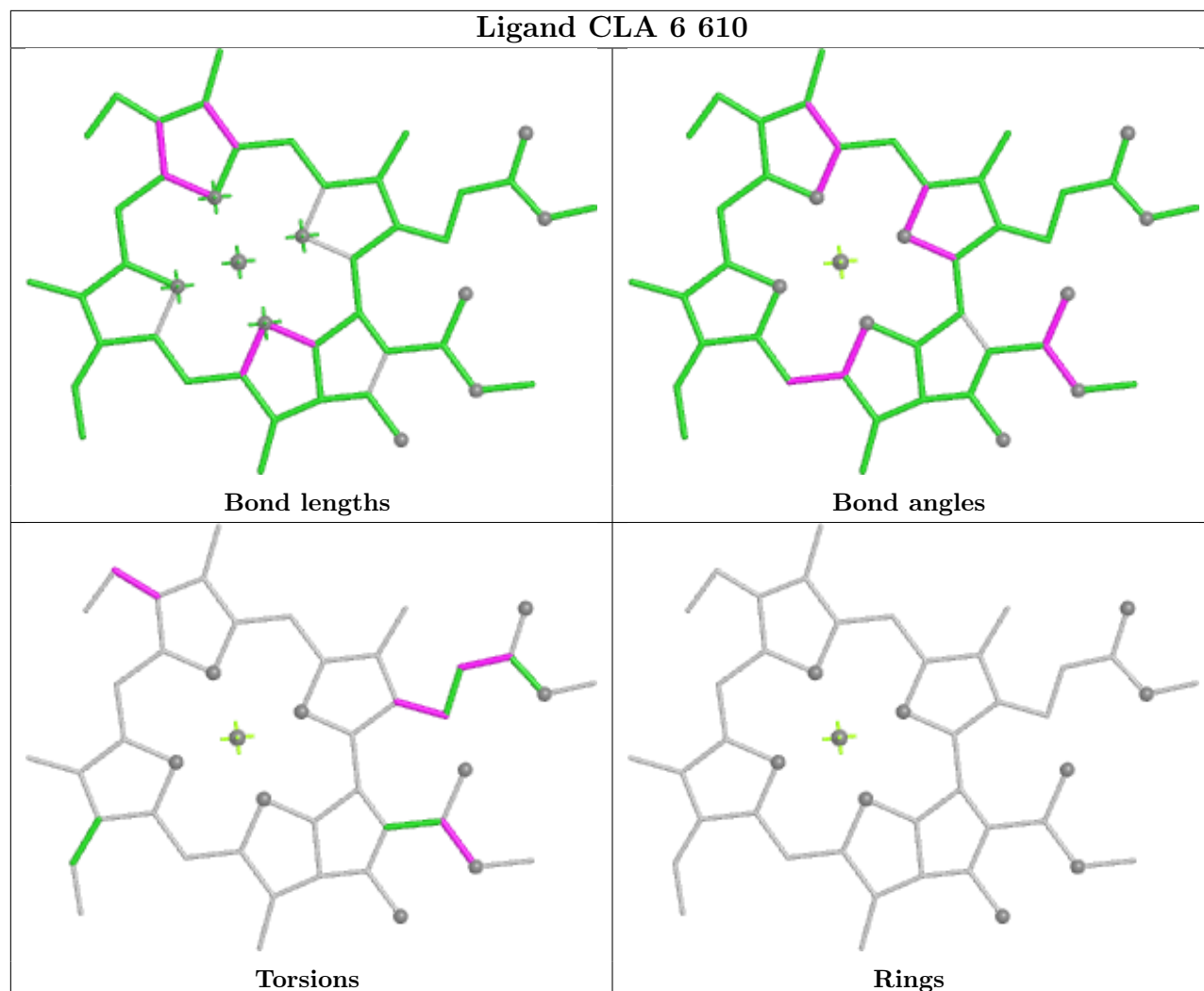


Ligand CLA 7 605

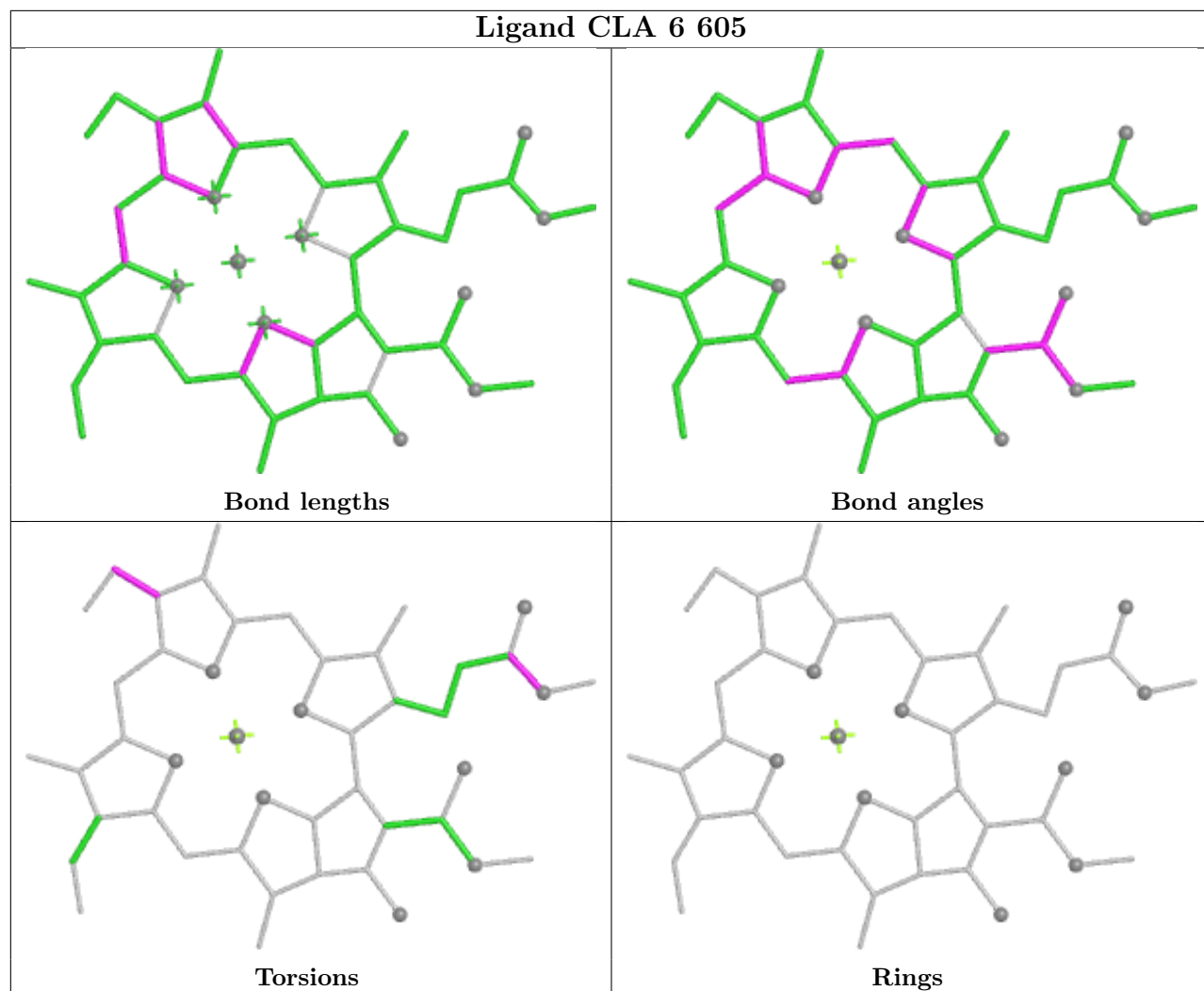




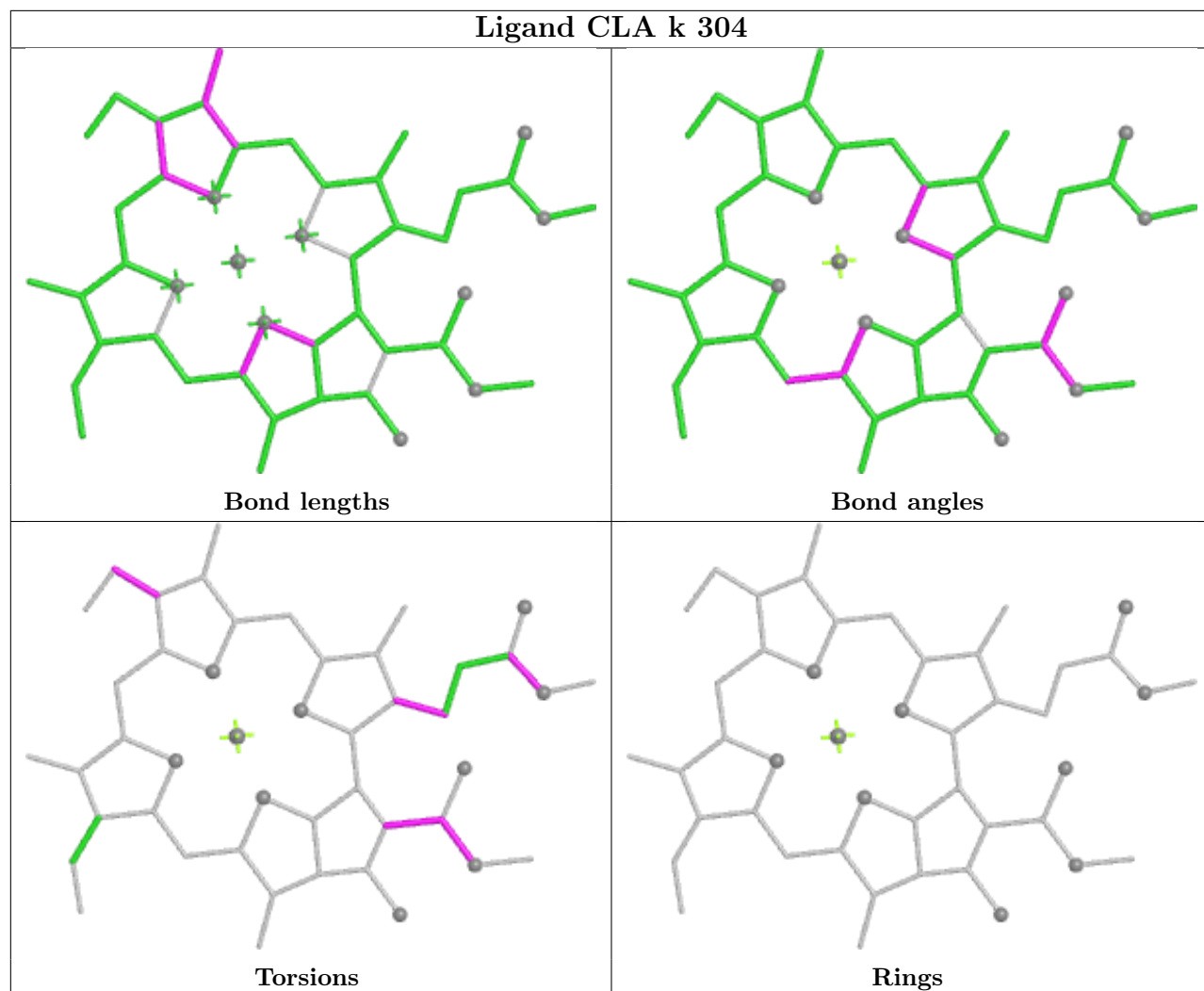
Ligand CLA 6 610



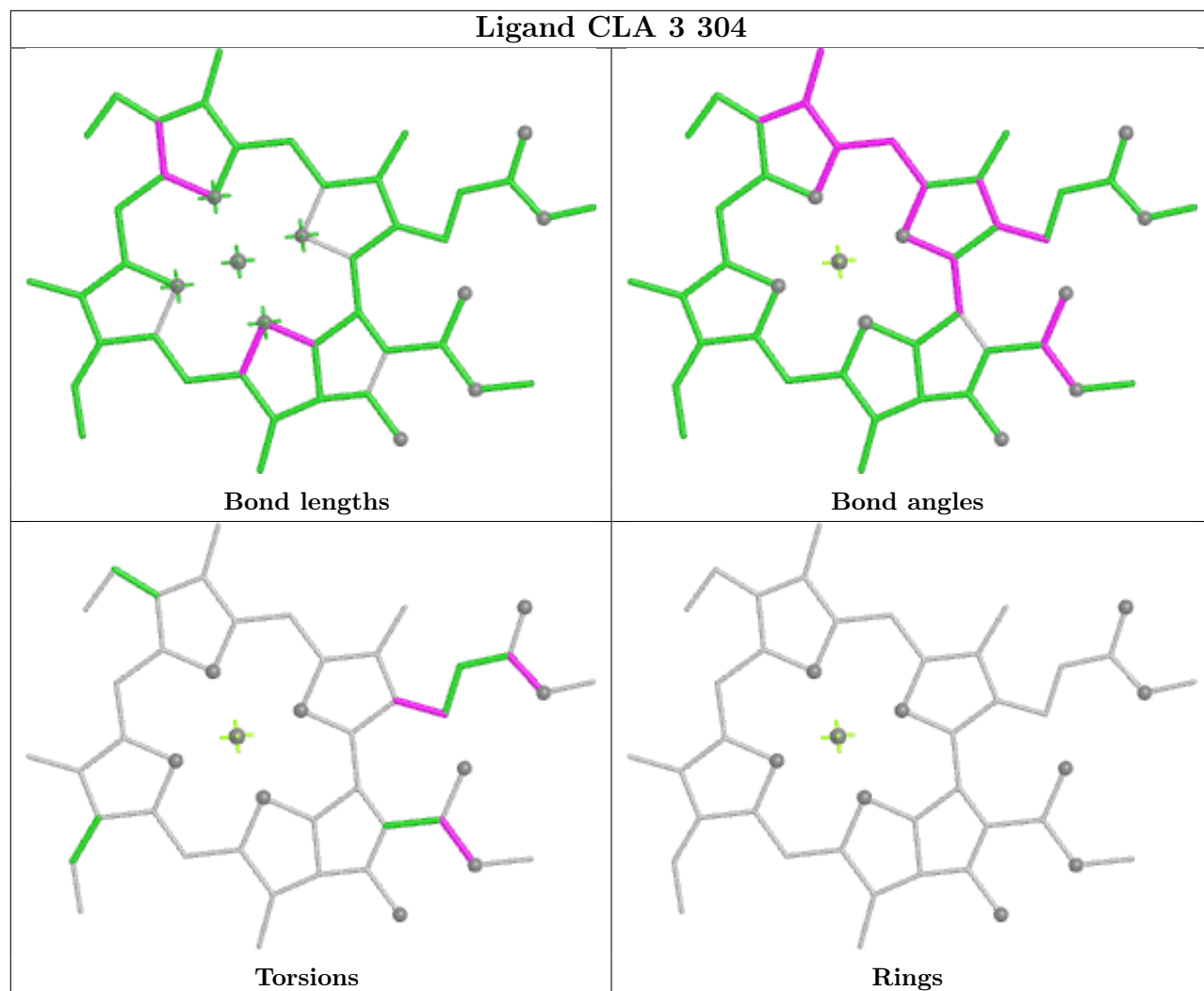
Ligand CLA 6 605



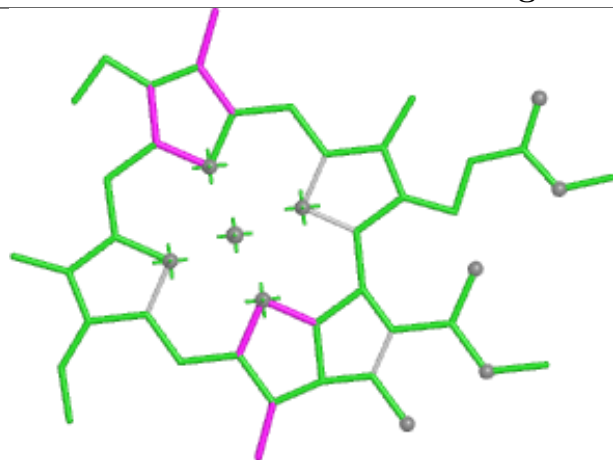
Ligand CLA k 304



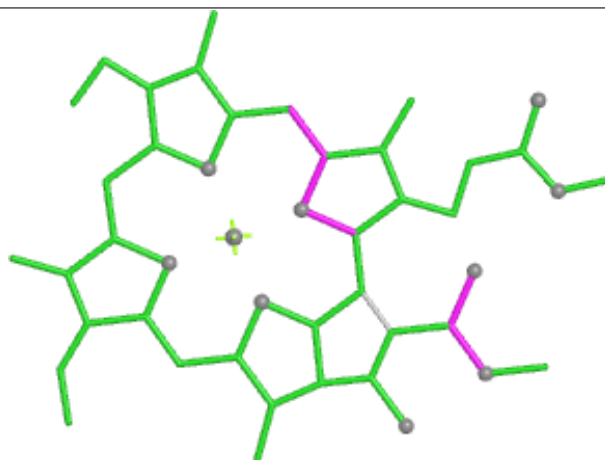
Ligand CLA 3 304



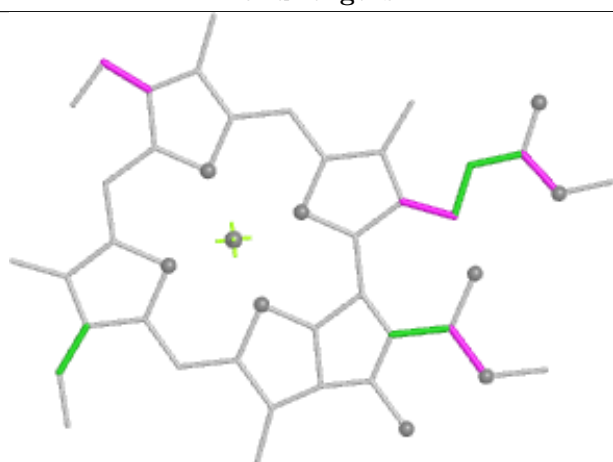
Ligand CLA 9 310



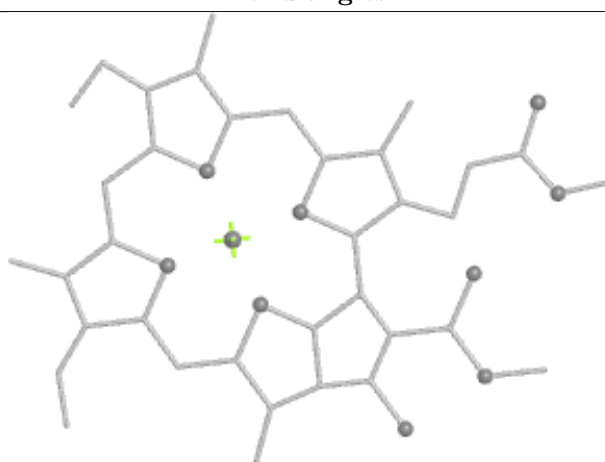
Bond lengths



Bond angles

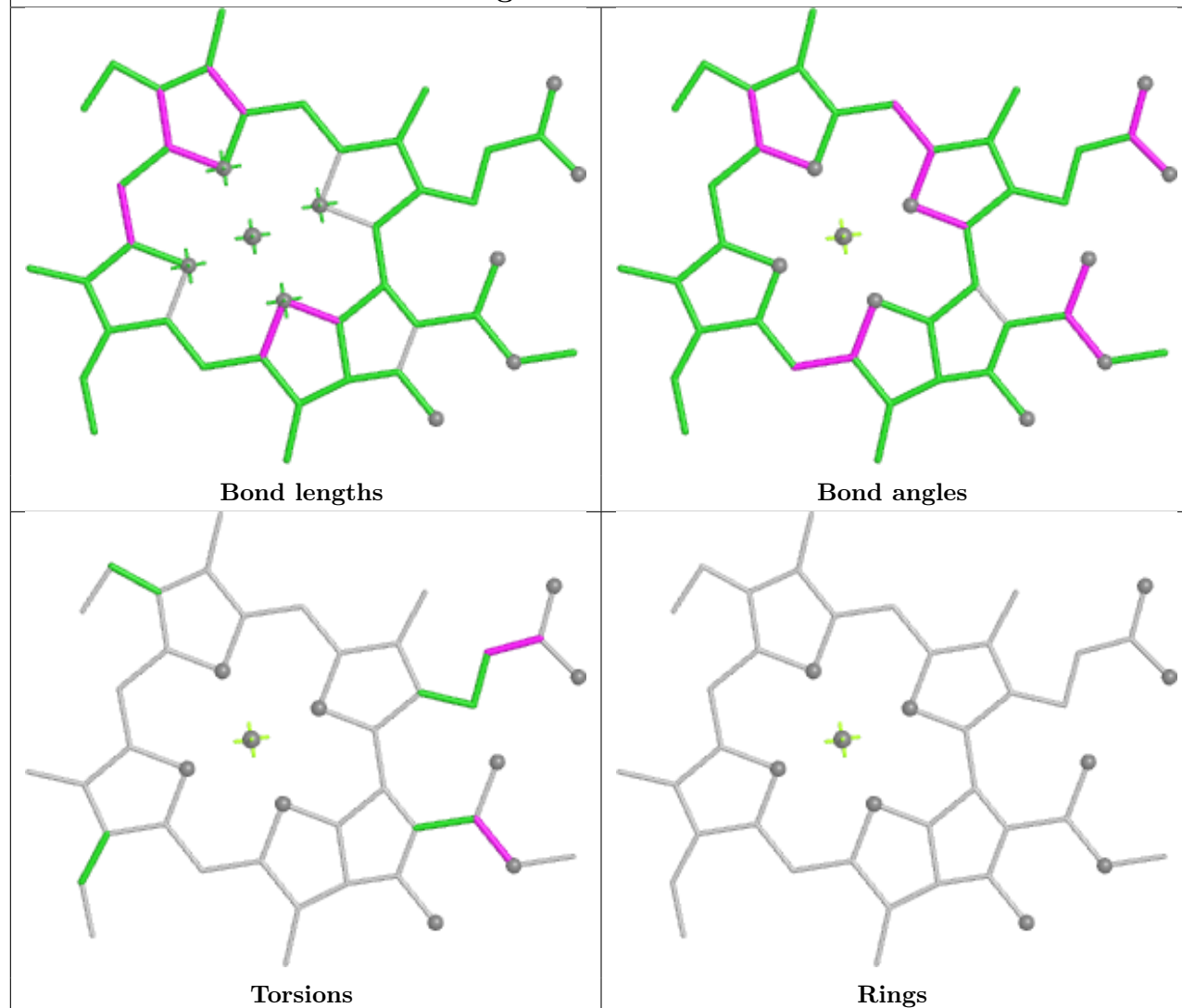


Torsions

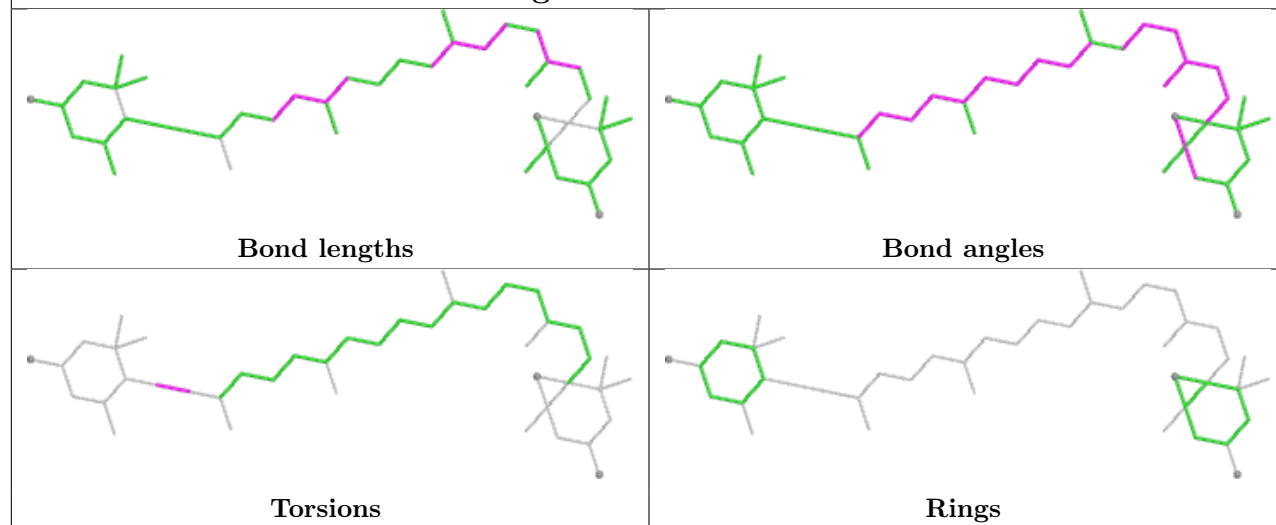


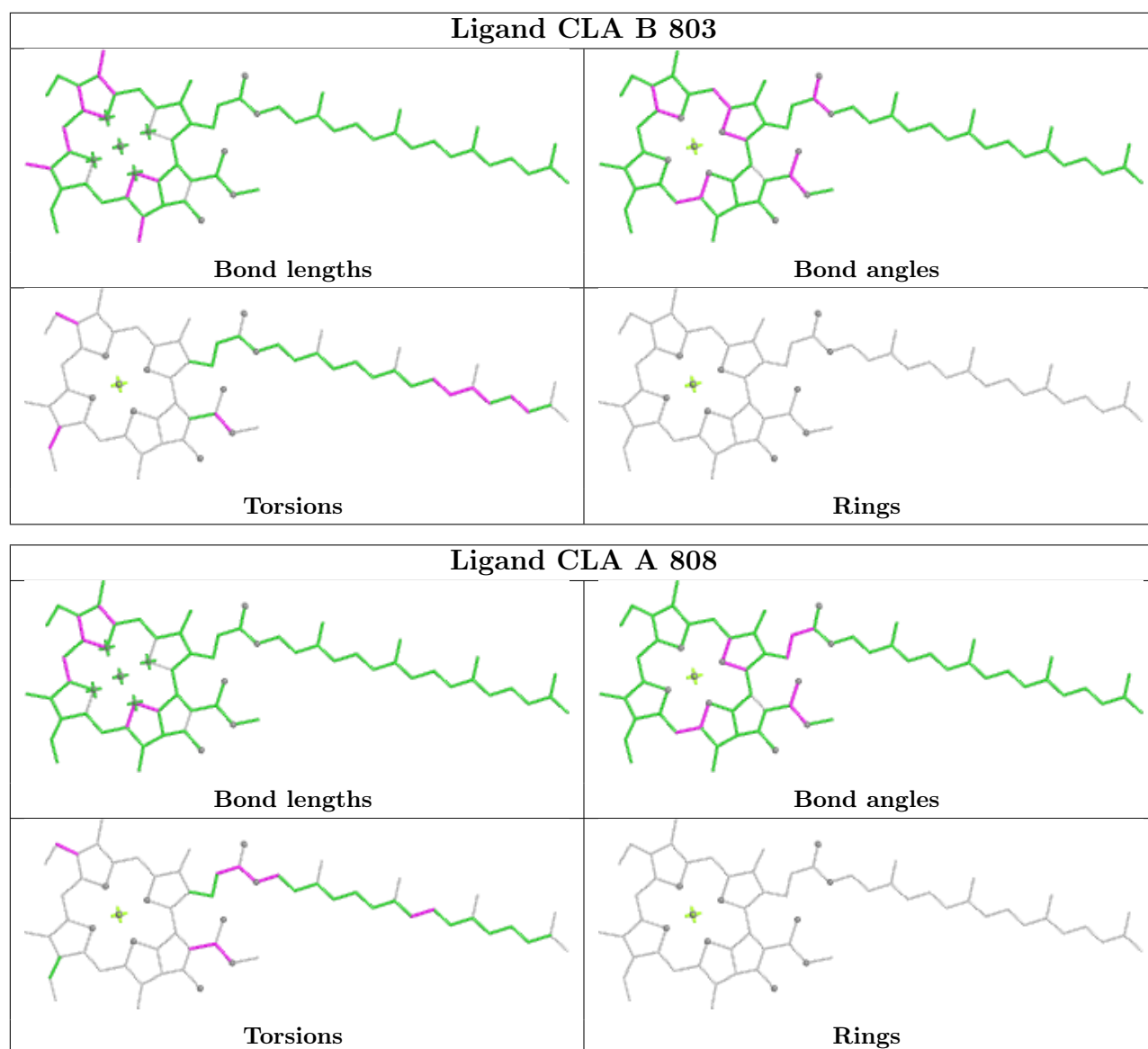
Rings

Ligand CLA 5 603

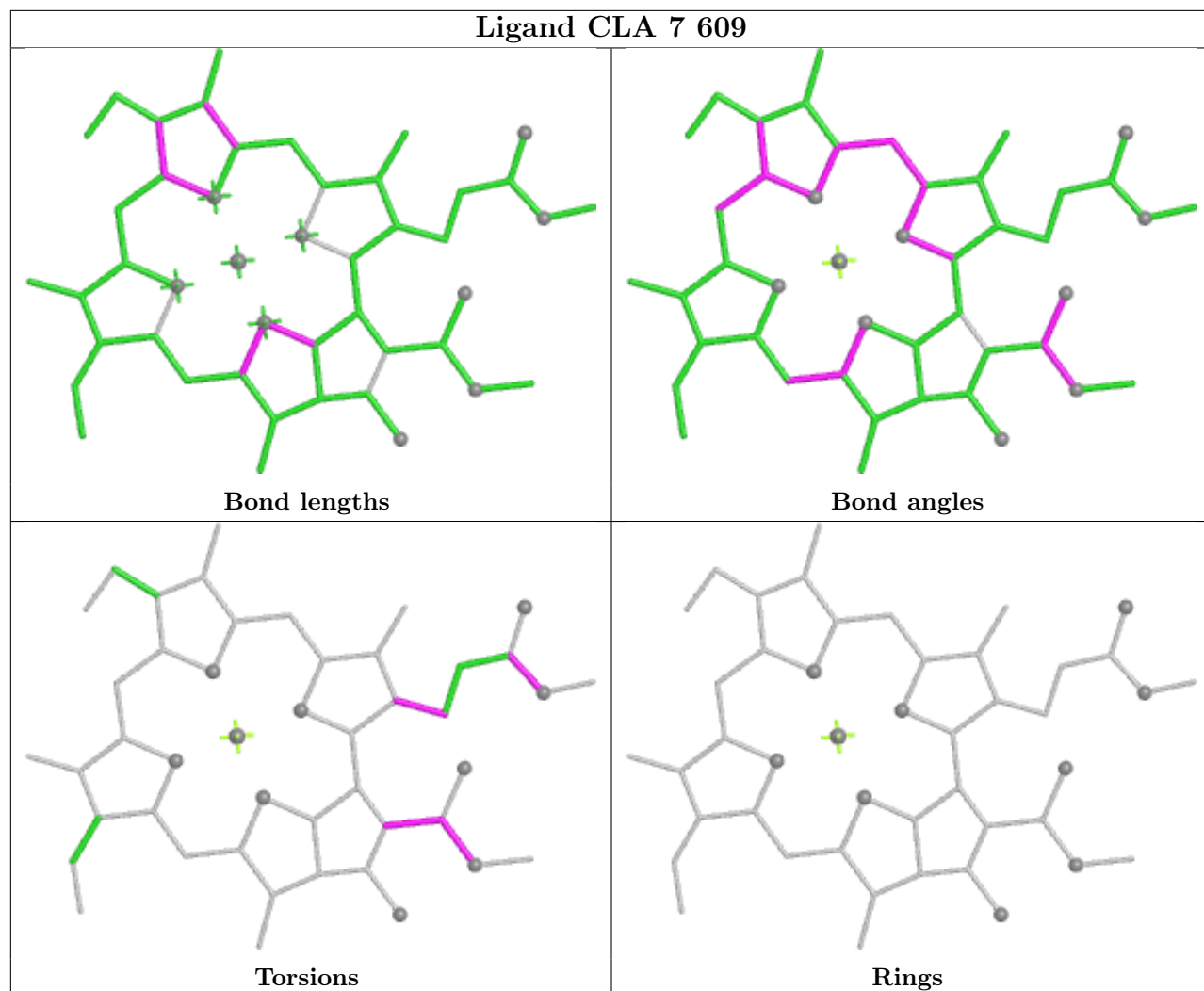


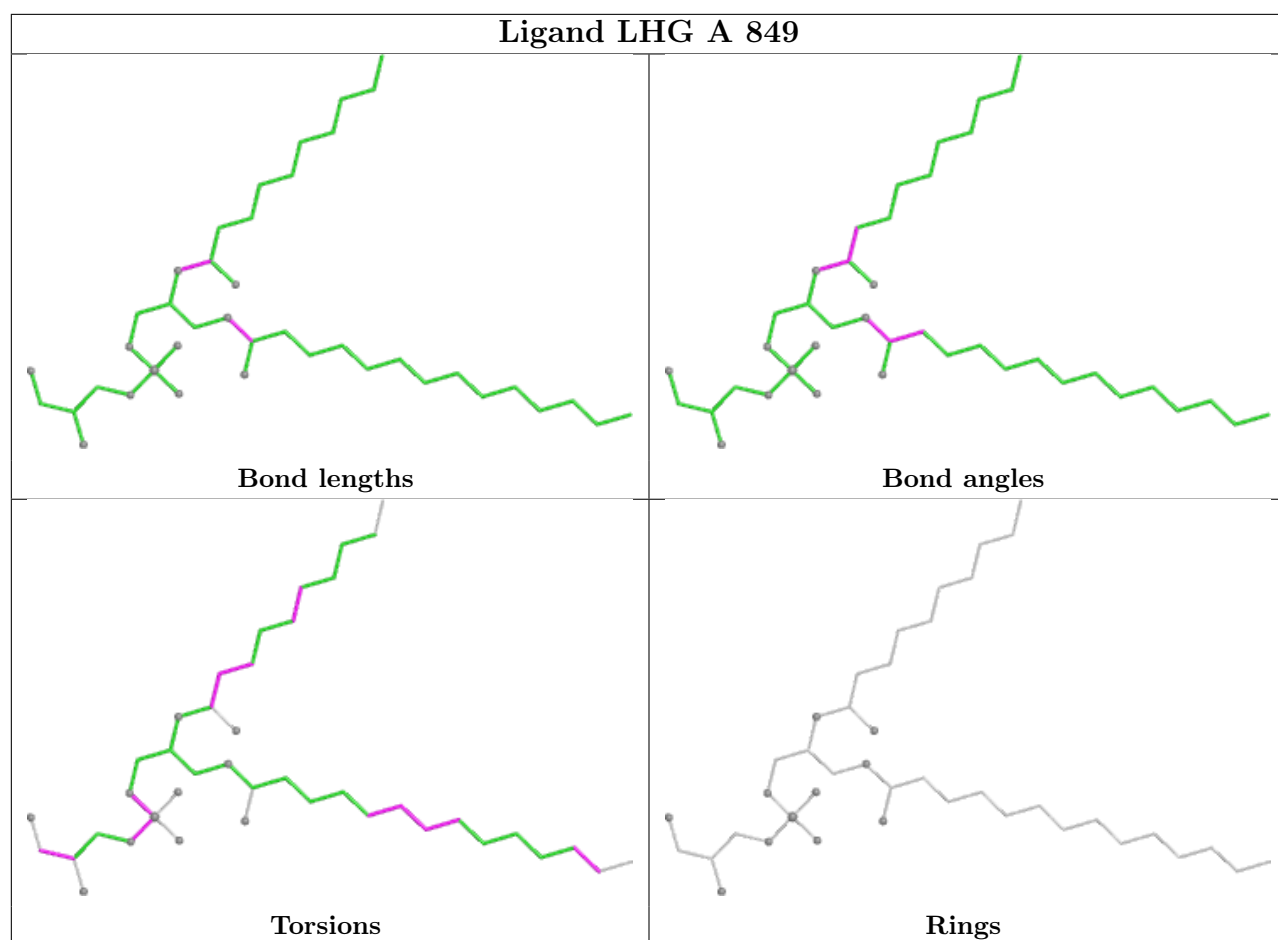
Ligand DD6 A 848



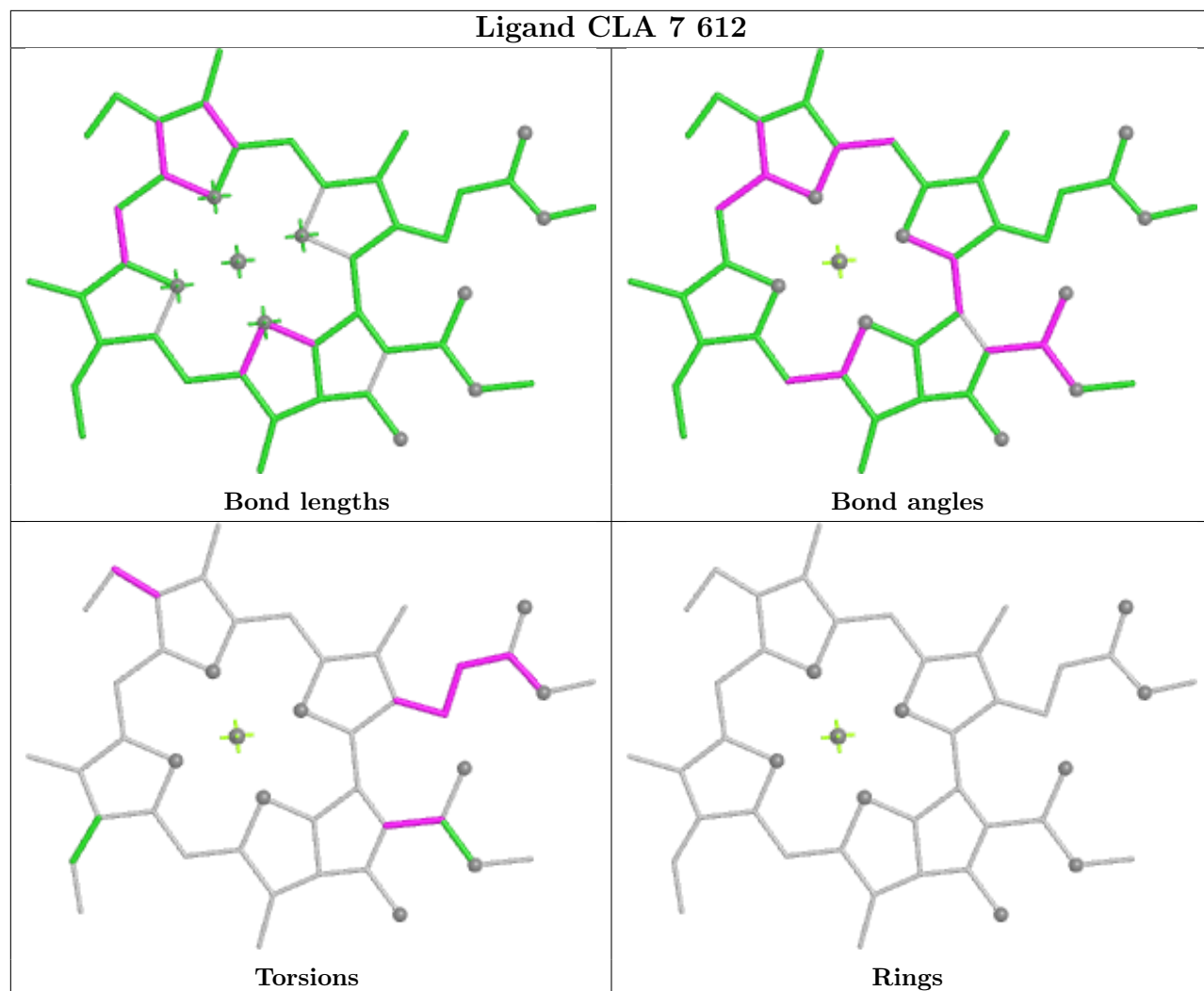


Ligand CLA 7 609

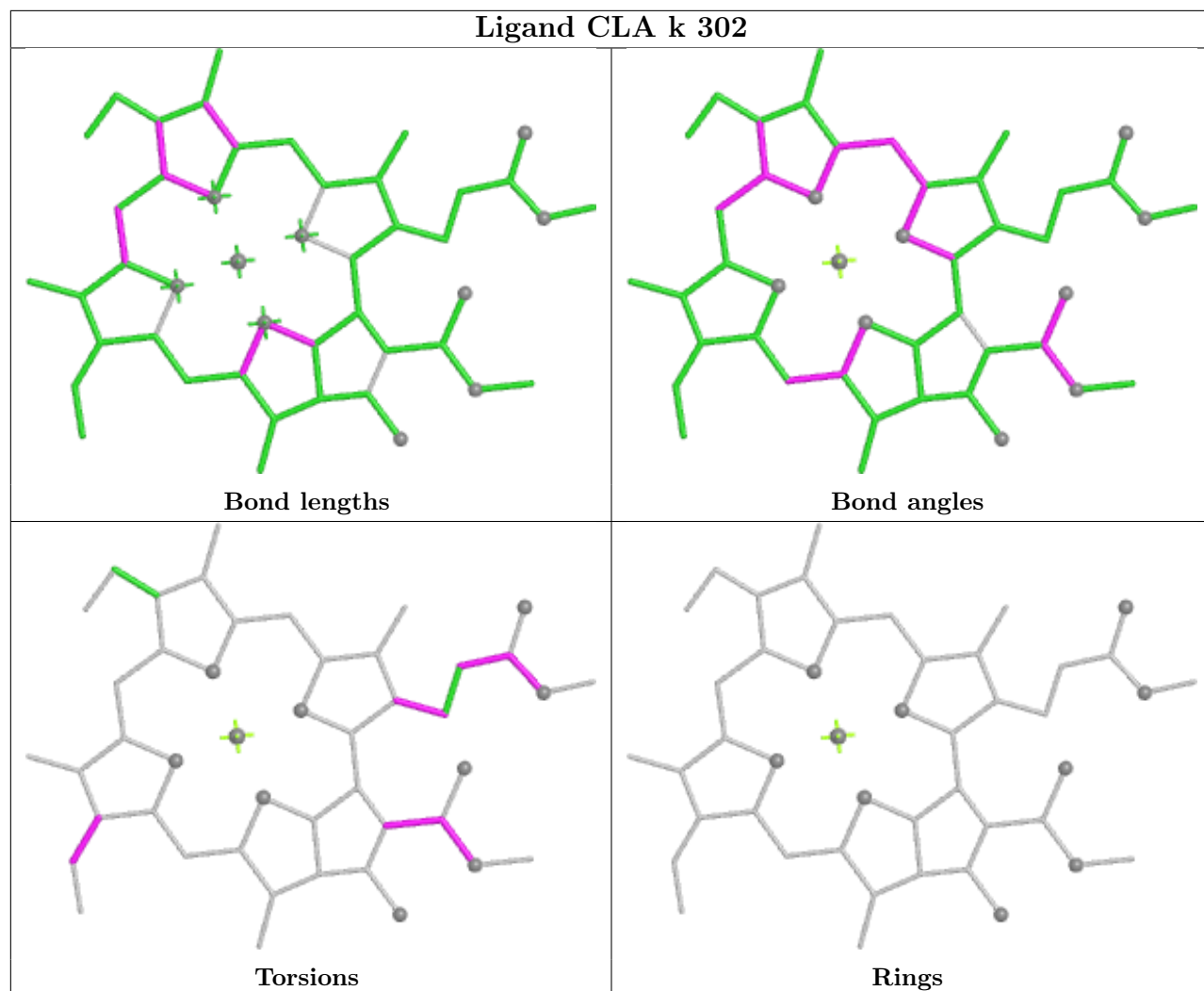


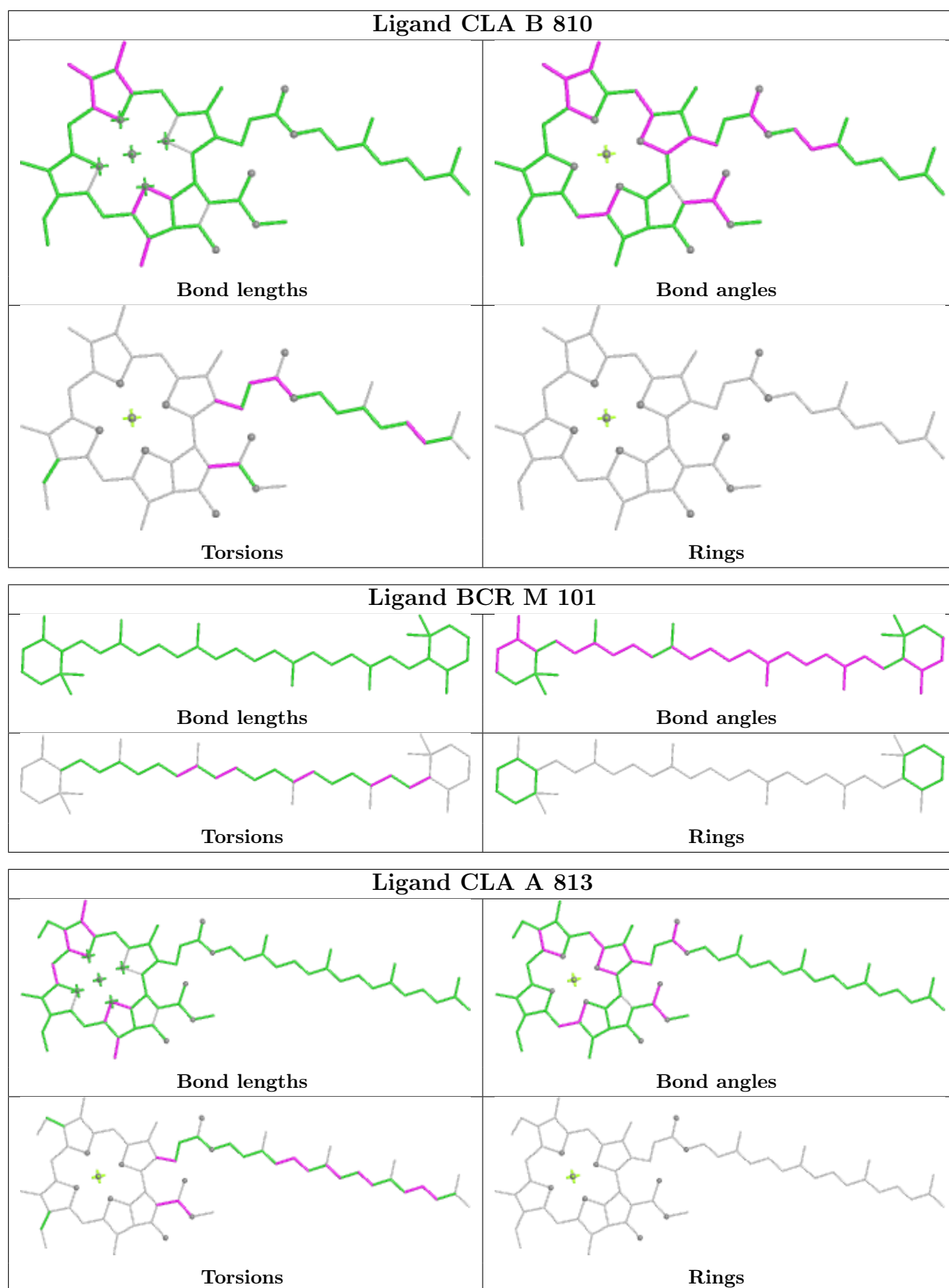


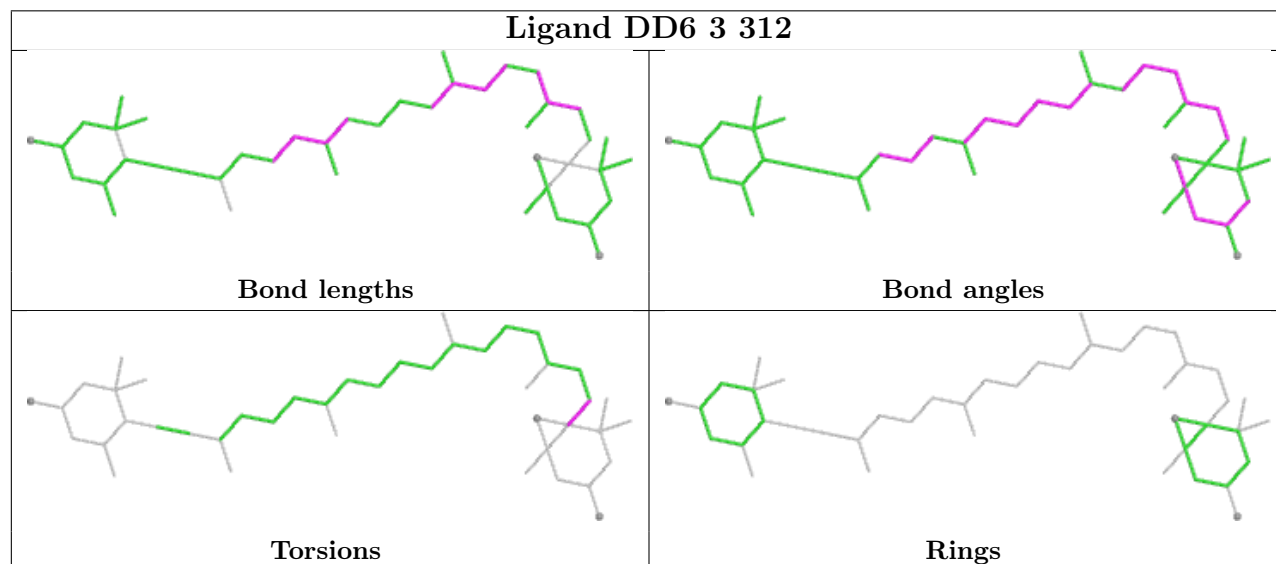
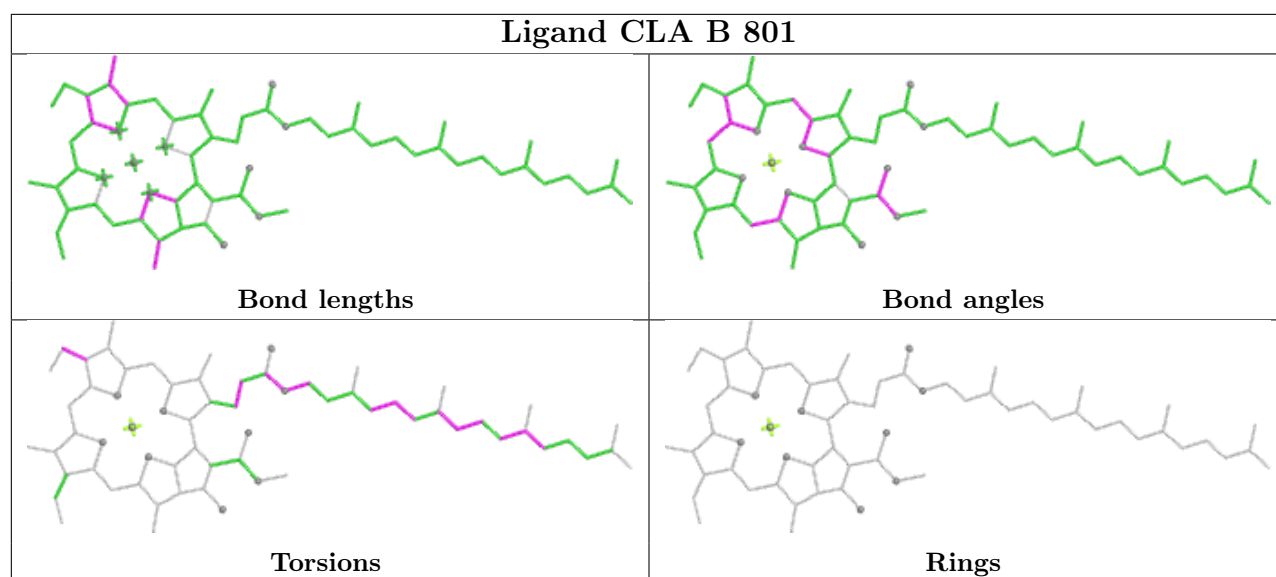
Ligand CLA 7 612

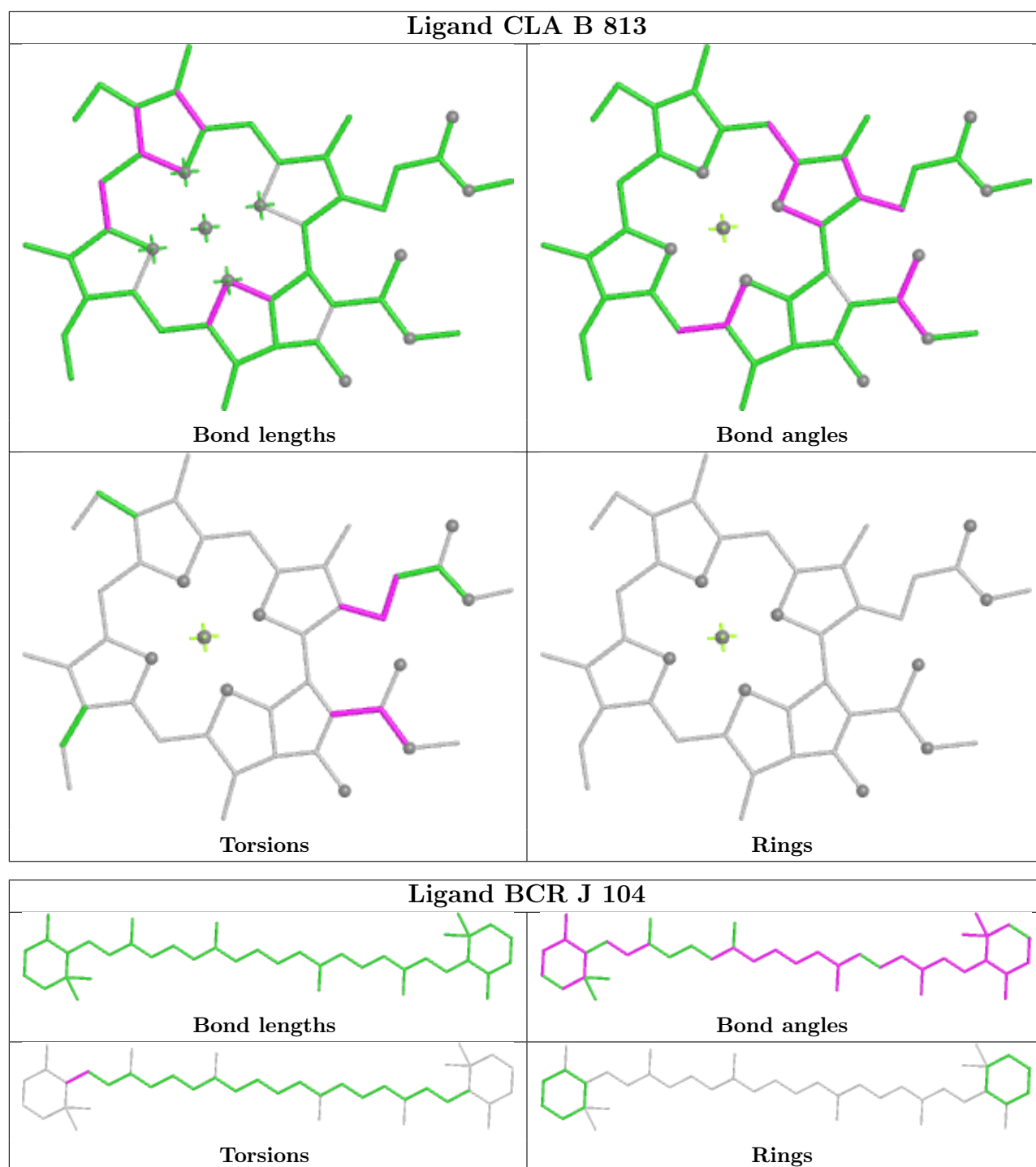


Ligand CLA k 302

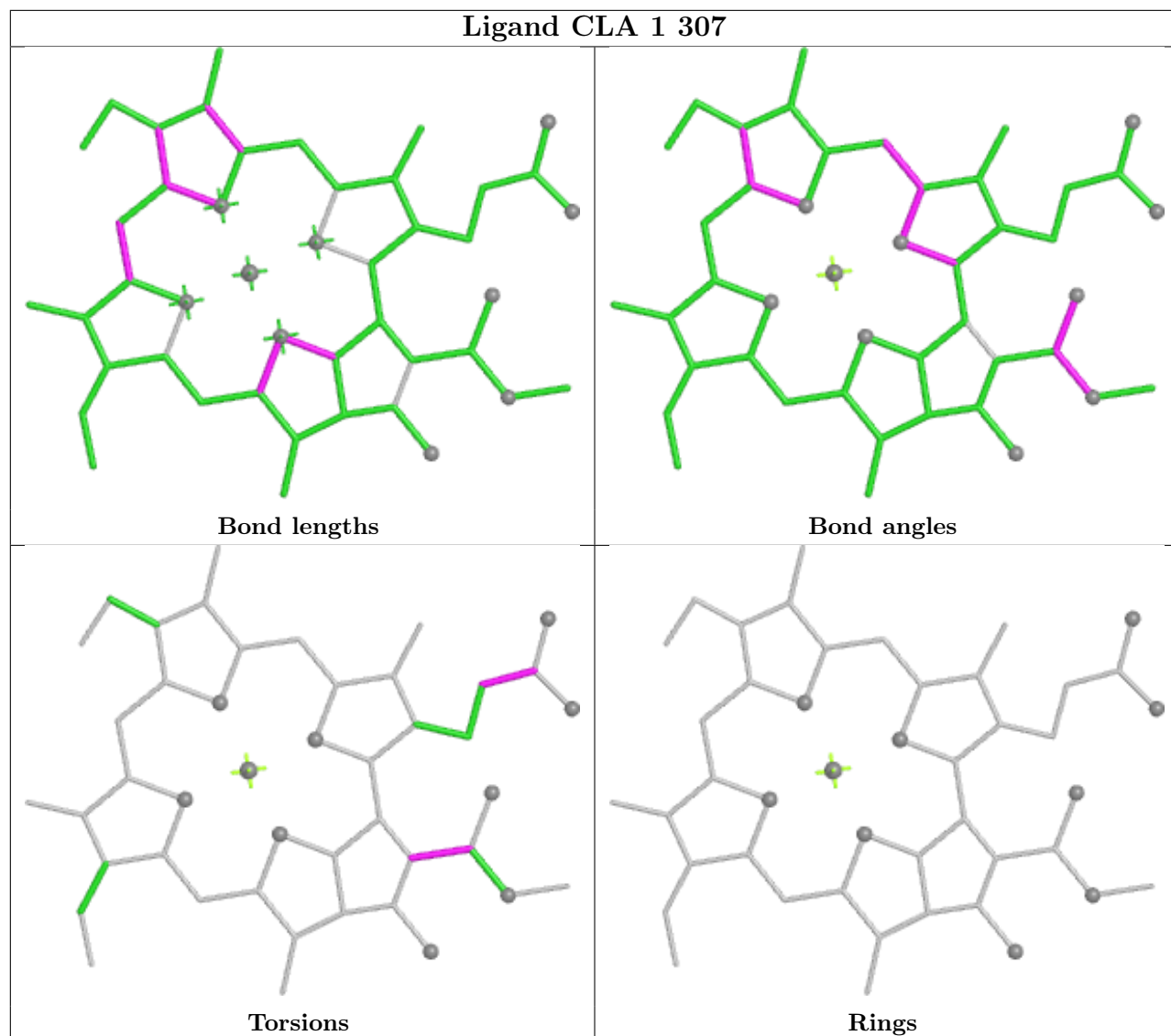




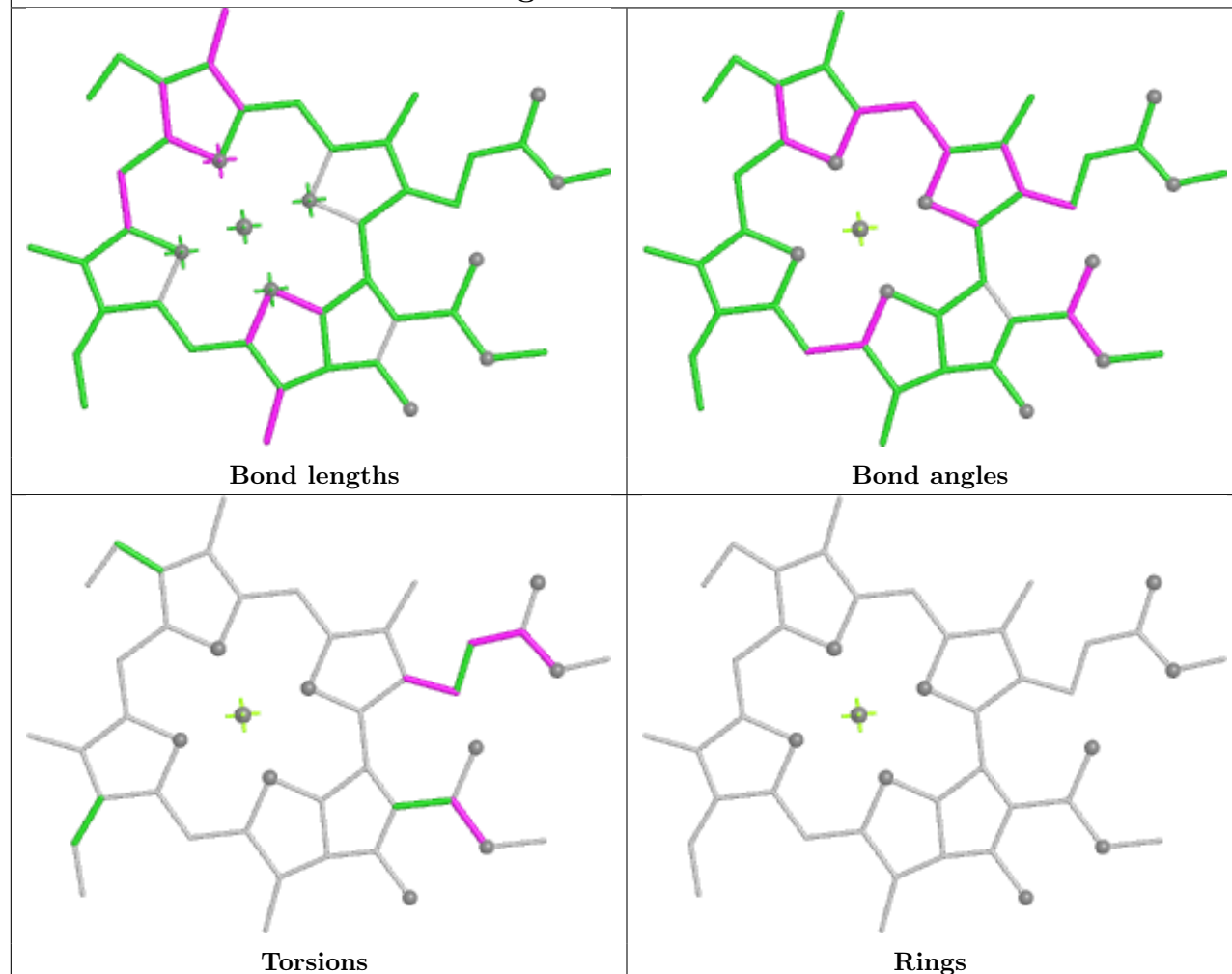




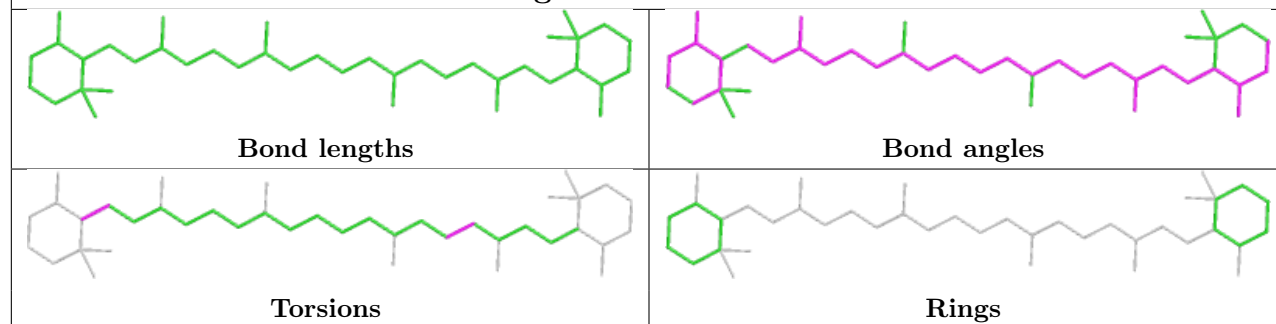
Ligand CLA 1 307

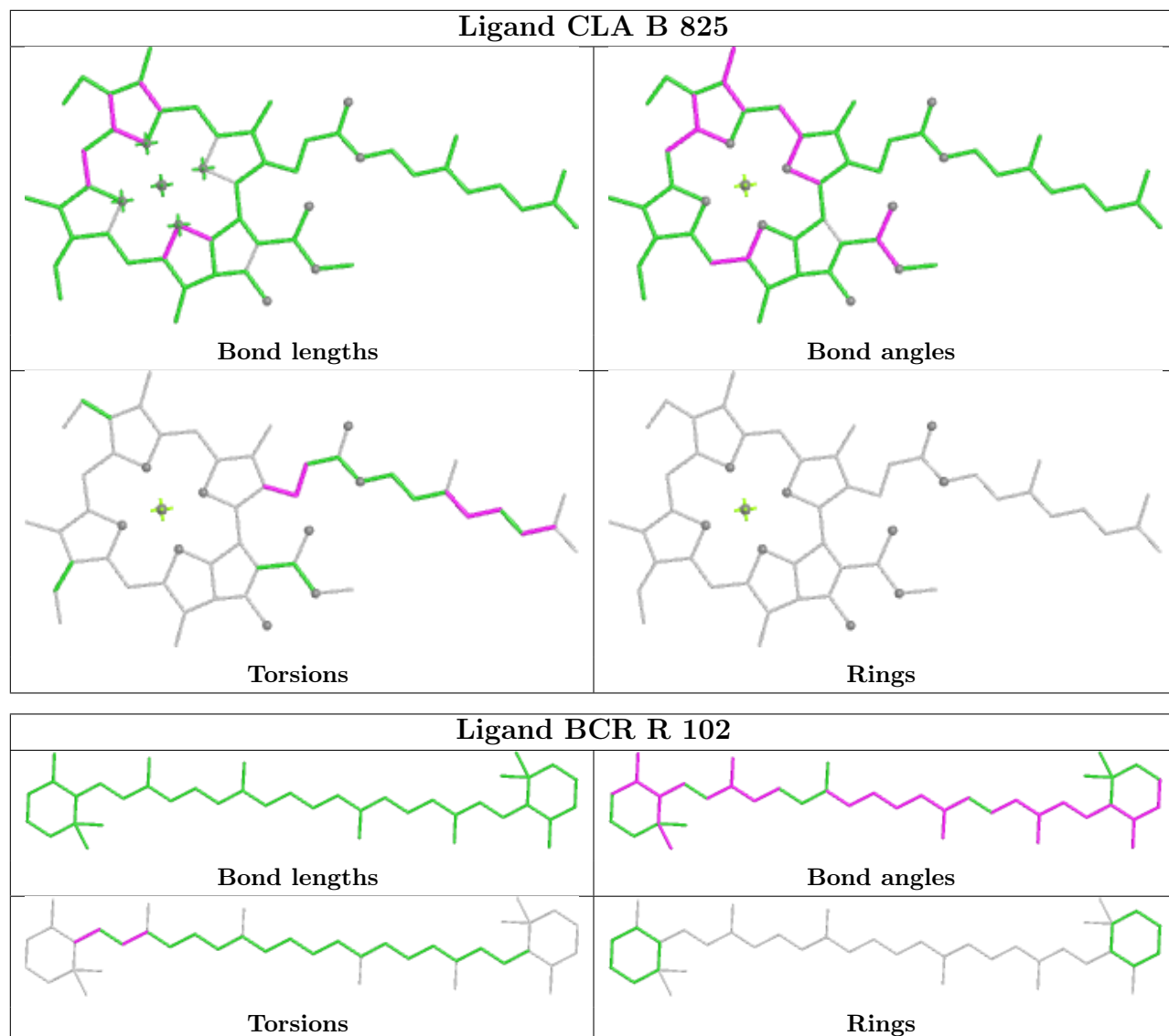


Ligand CLA 3 308

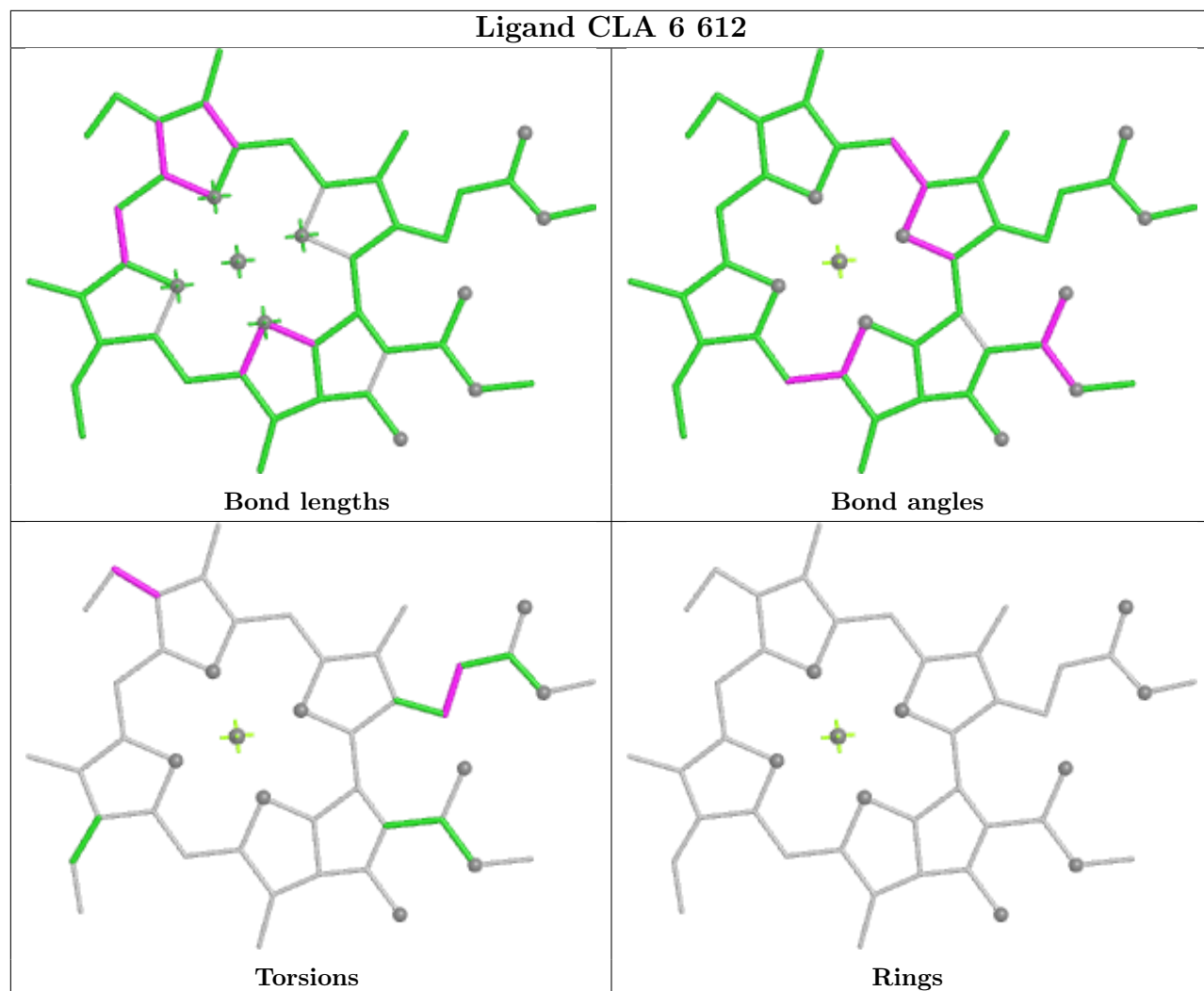


Ligand BCR k 316

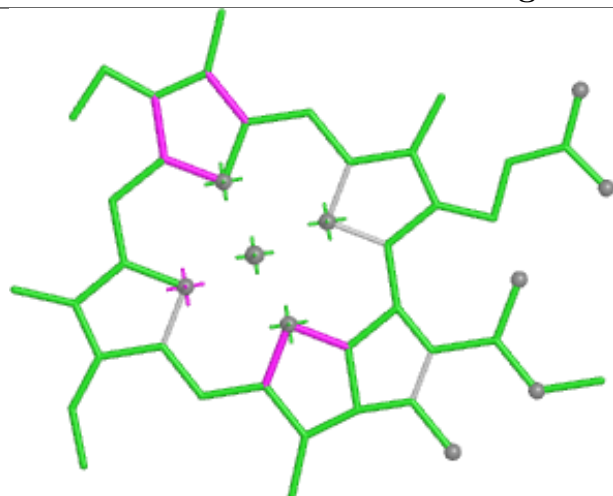




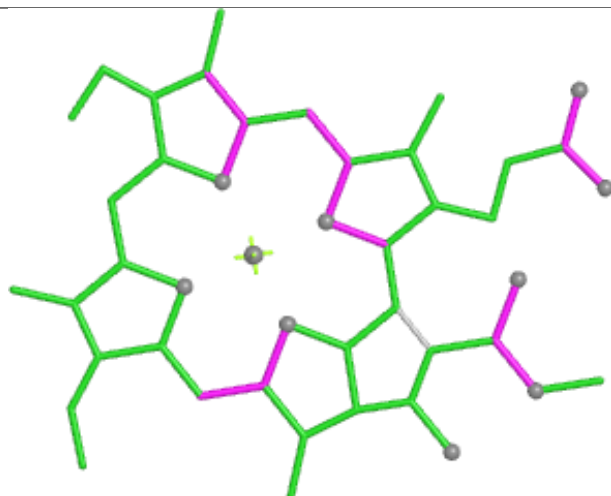
Ligand CLA 6 612



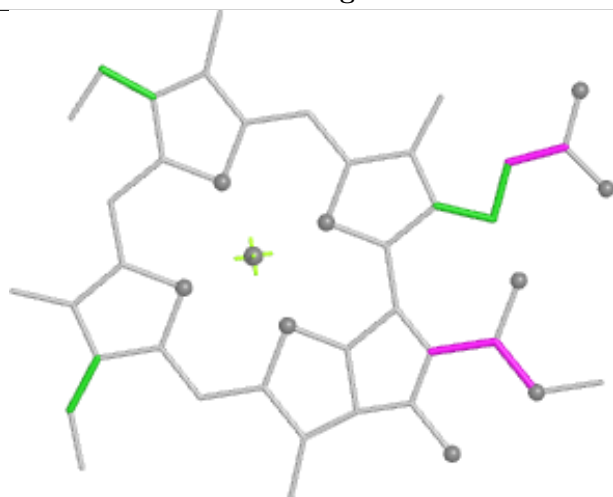
Ligand CLA 5 607



Bond lengths



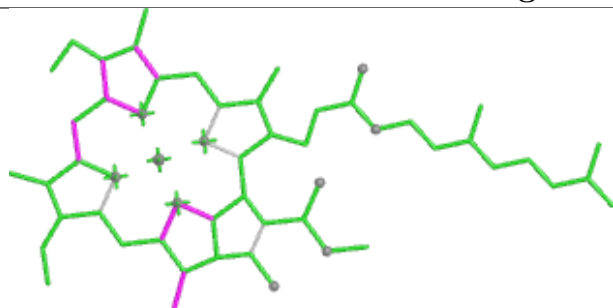
Bond angles



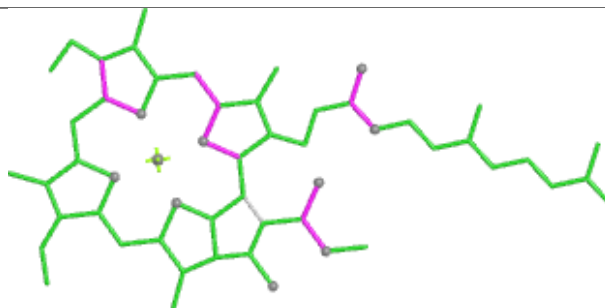
Torsions



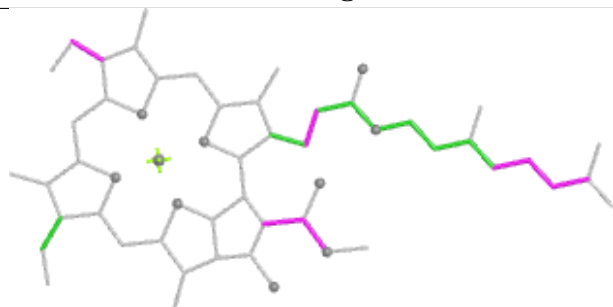
Rings

Ligand CLA 1 304

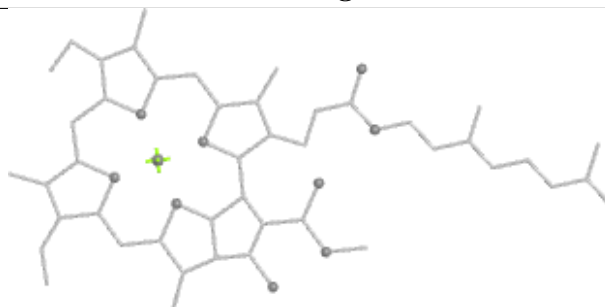
Bond lengths



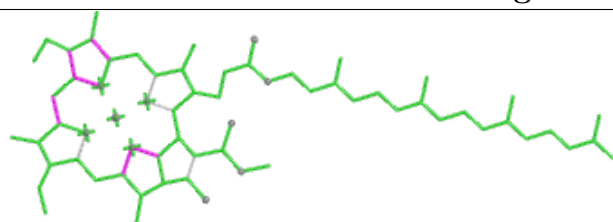
Bond angles



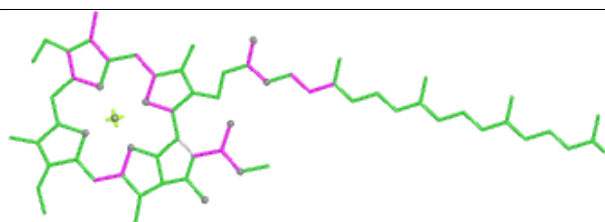
Torsions



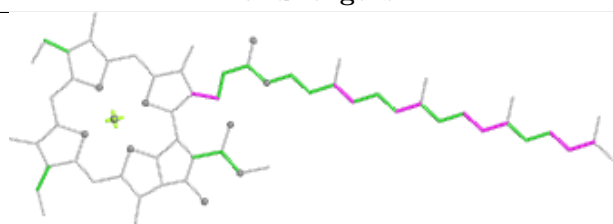
Rings

Ligand CLA A 826

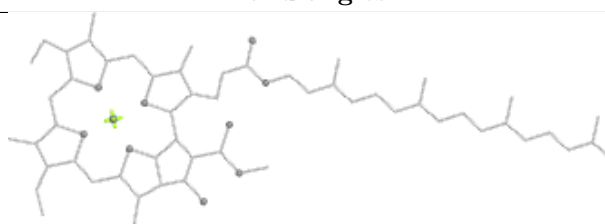
Bond lengths



Bond angles

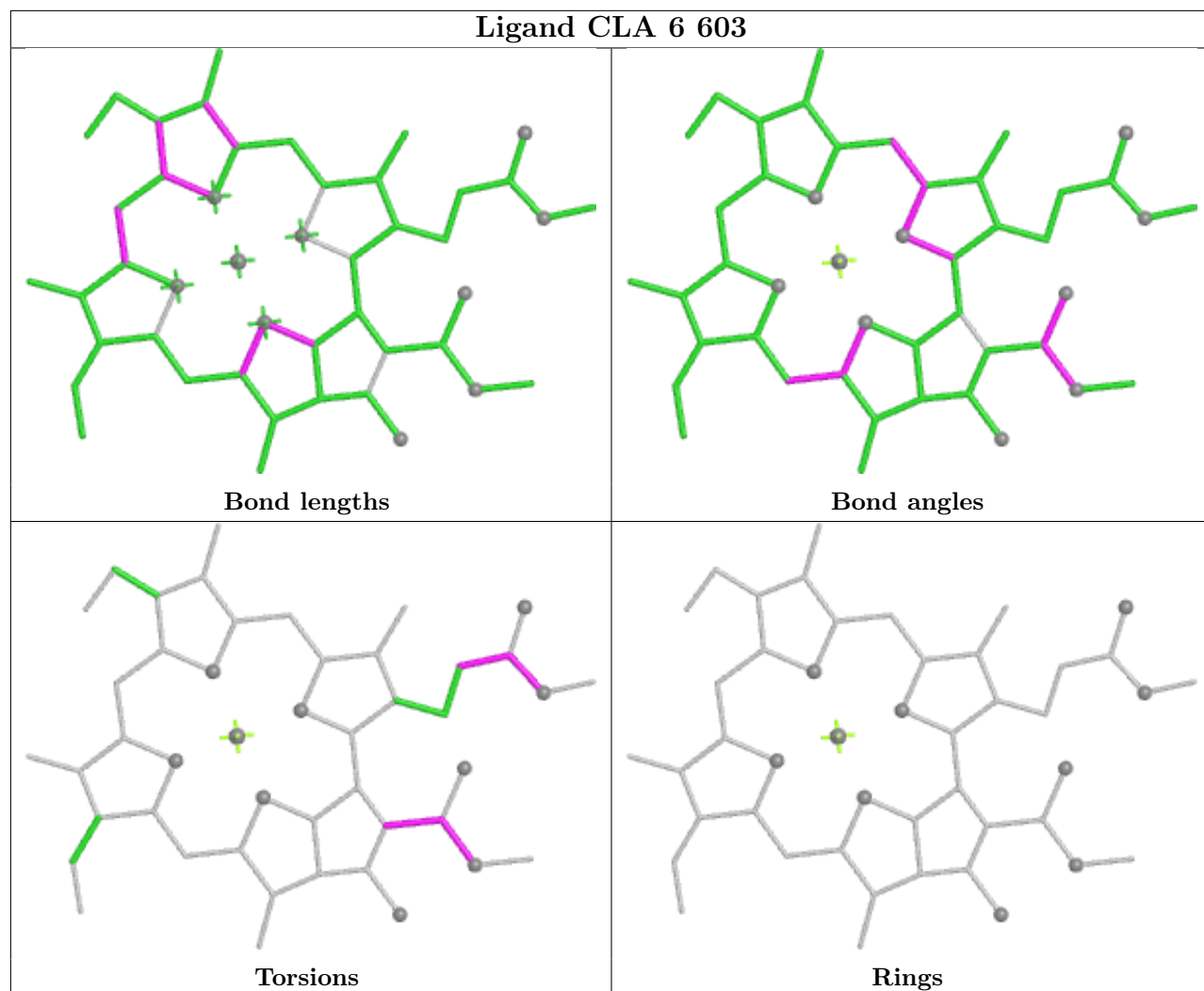


Torsions

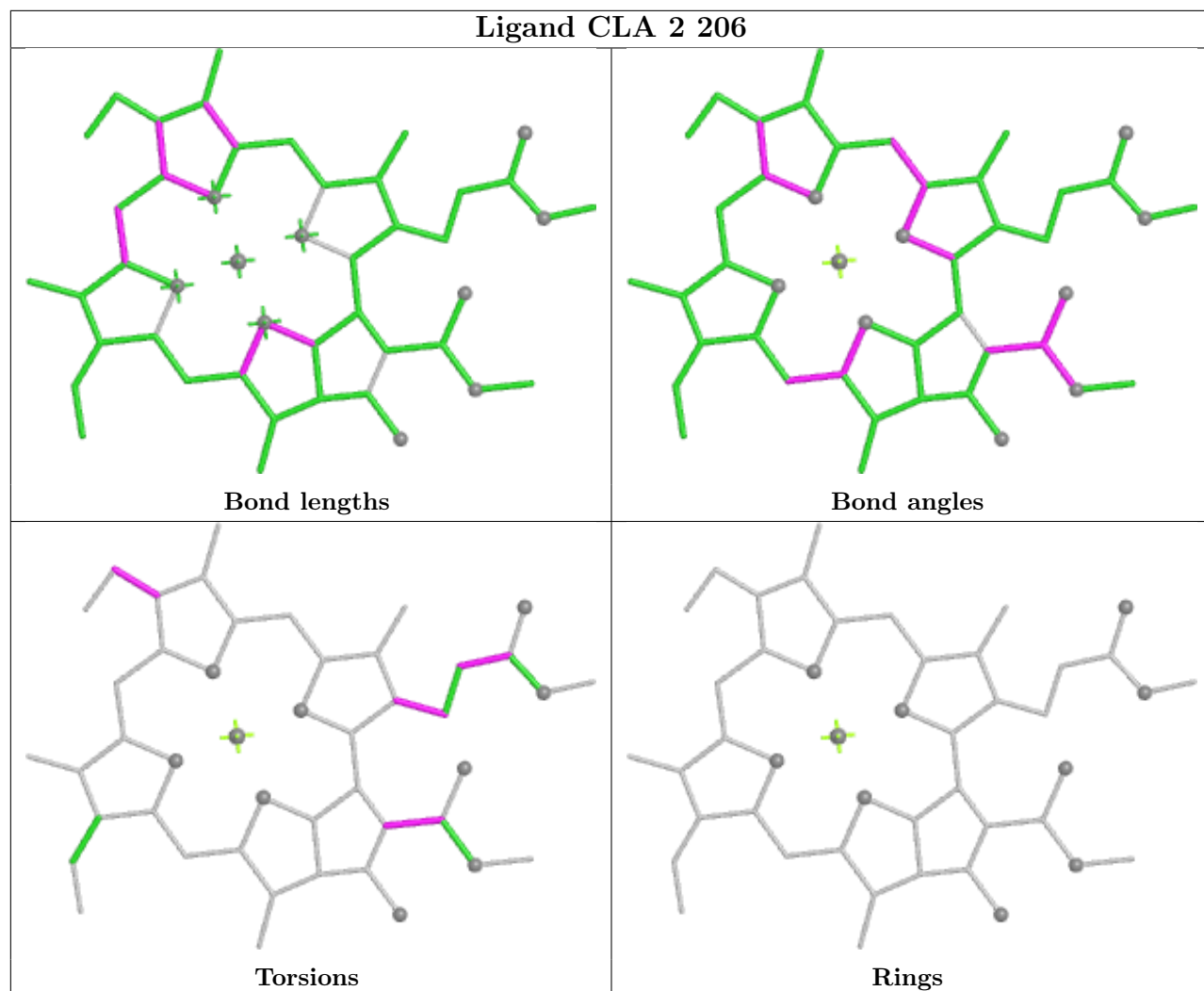


Rings

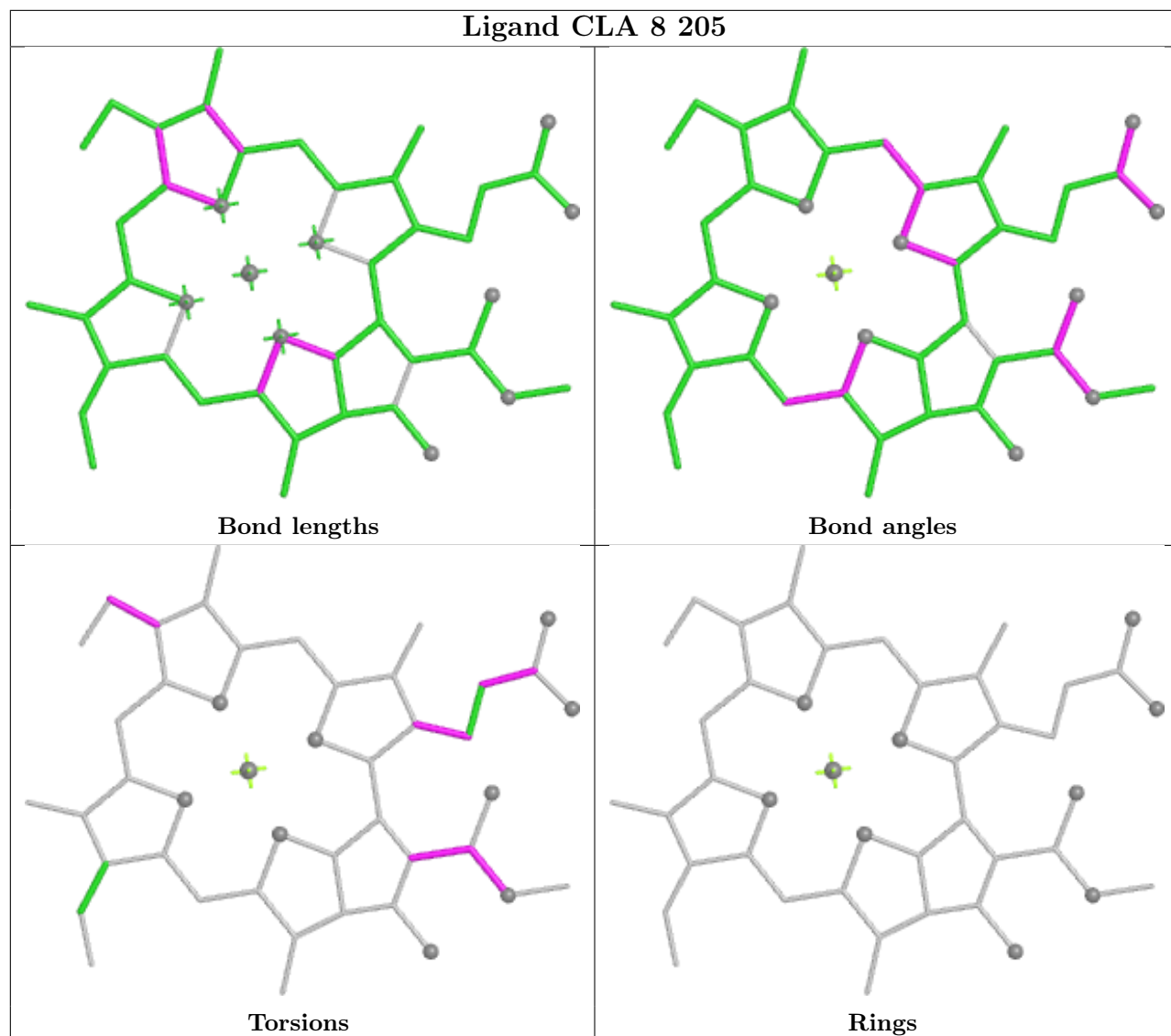
Ligand CLA 6 603



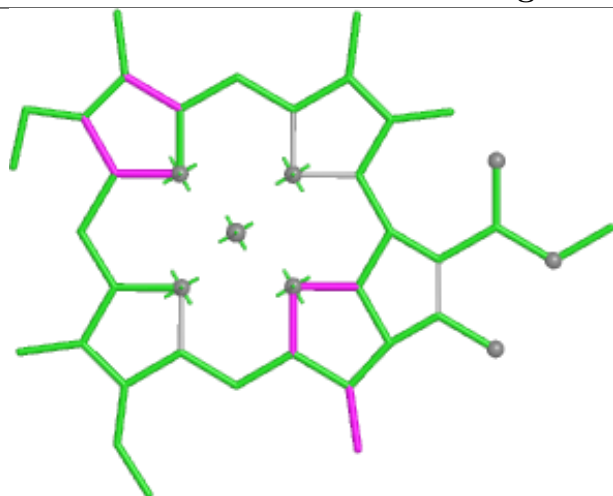
Ligand CLA 2 206



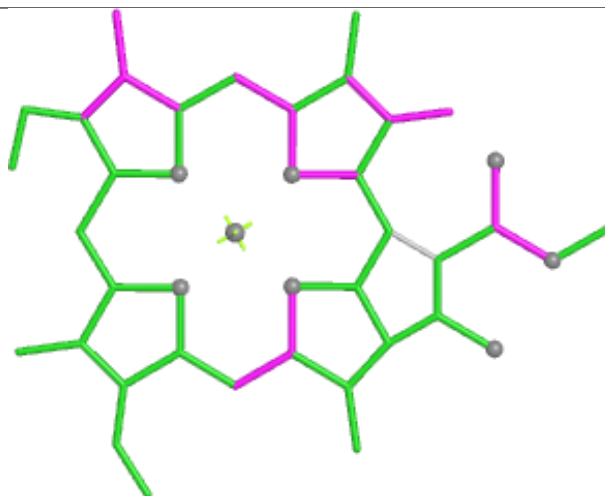
Ligand CLA 8 205



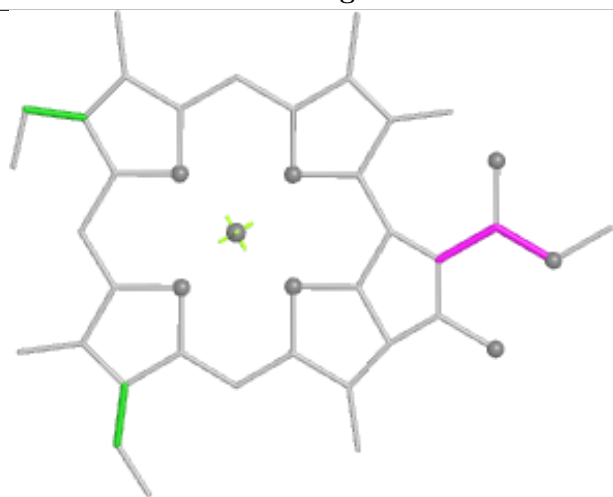
Ligand CLA h 611



Bond lengths



Bond angles

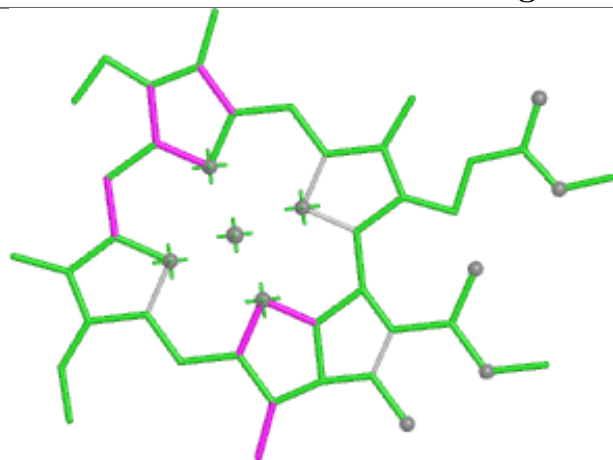


Torsions

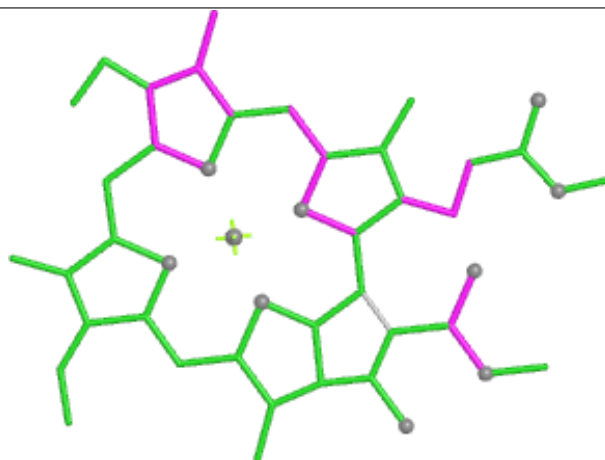


Rings

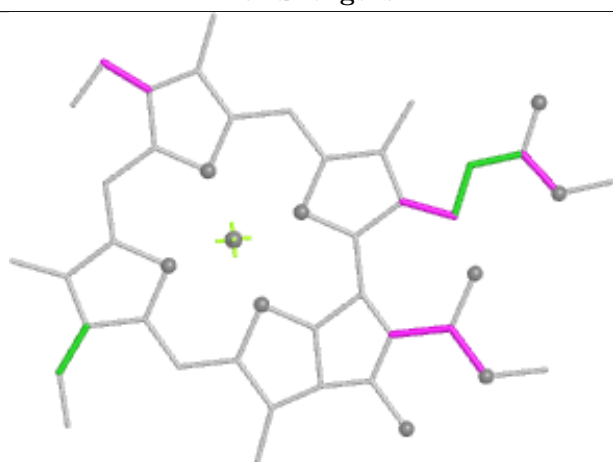
Ligand CLA 9 304



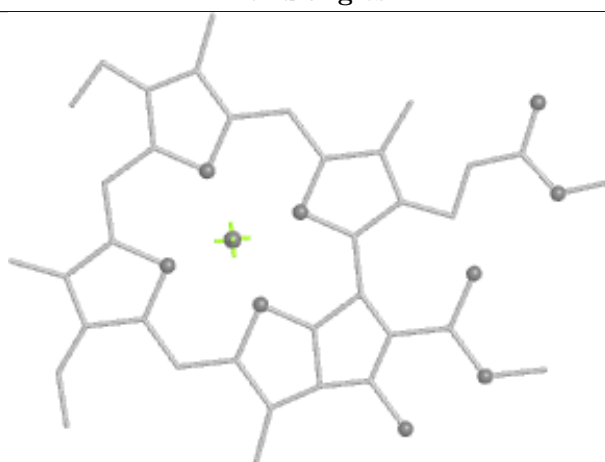
Bond lengths



Bond angles

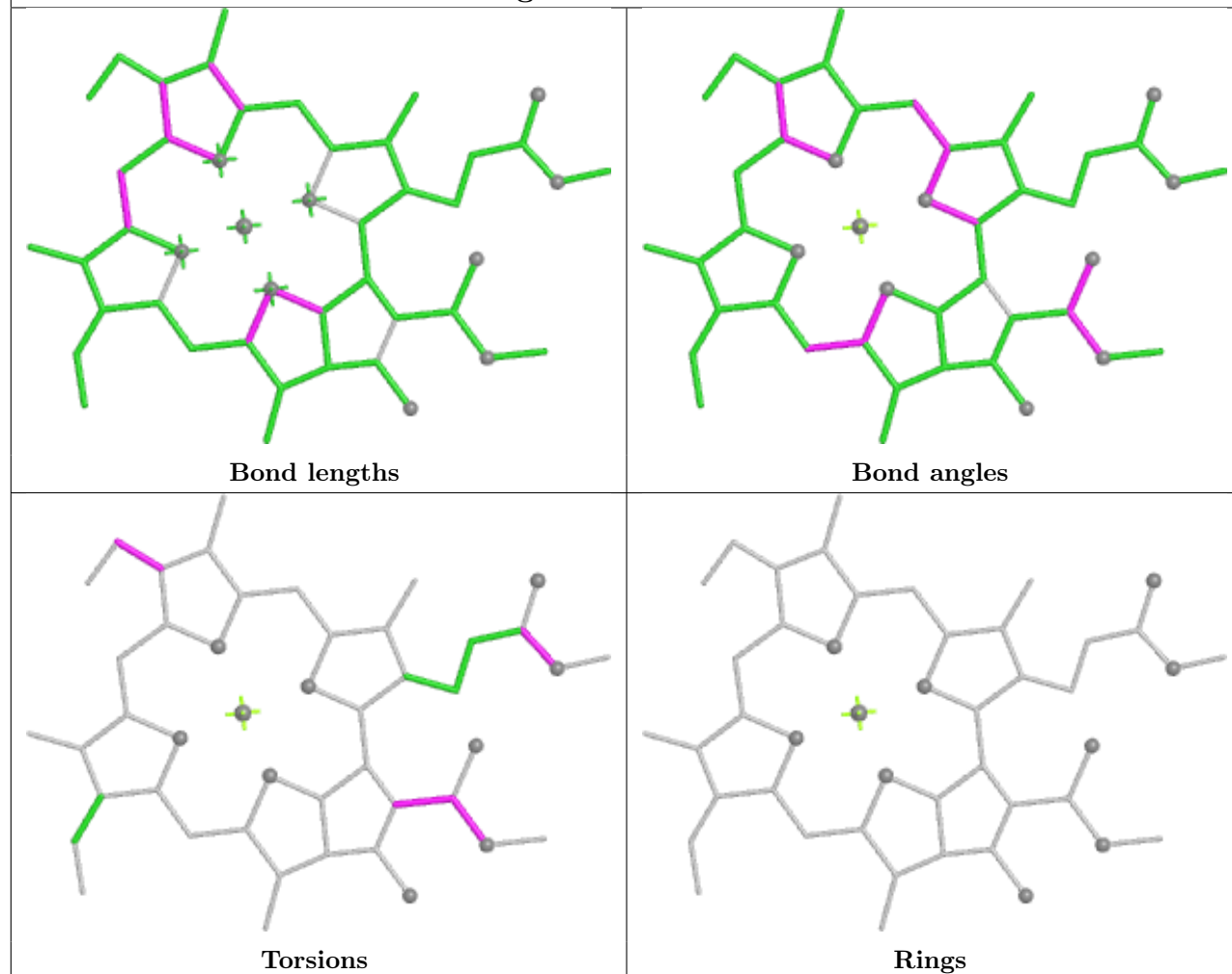


Torsions

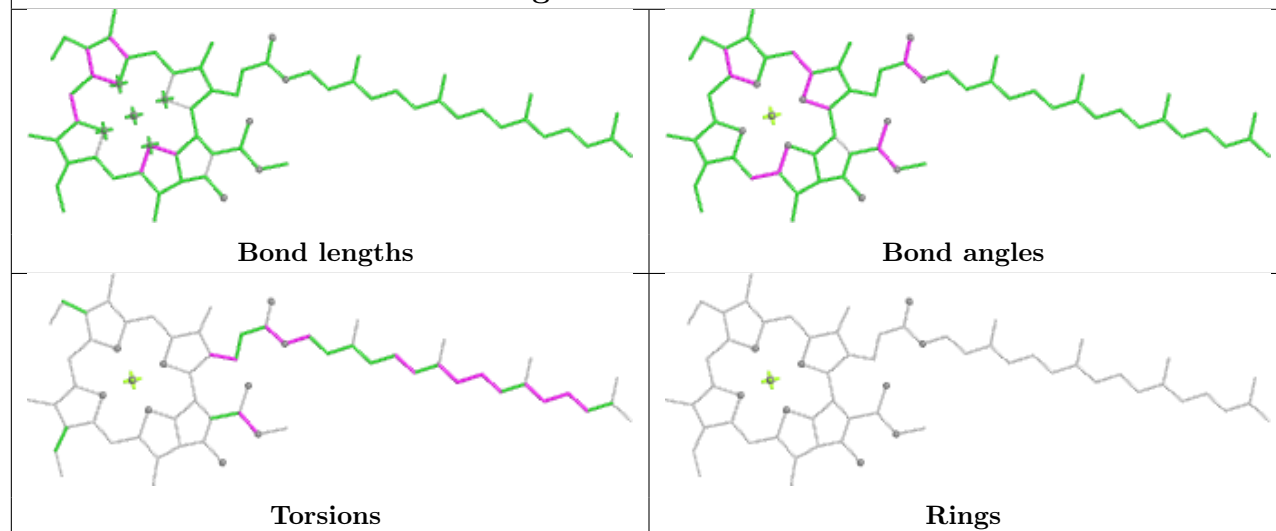


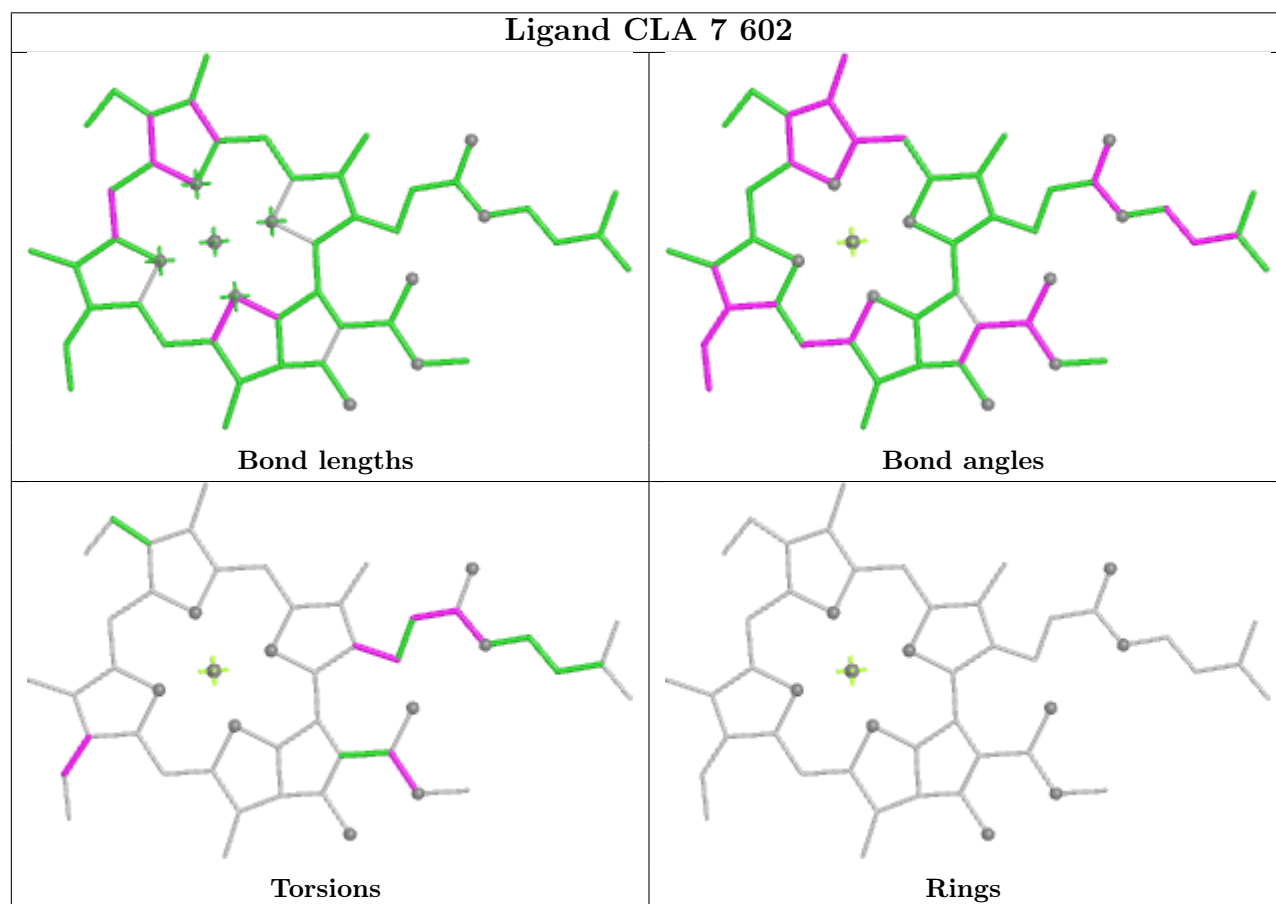
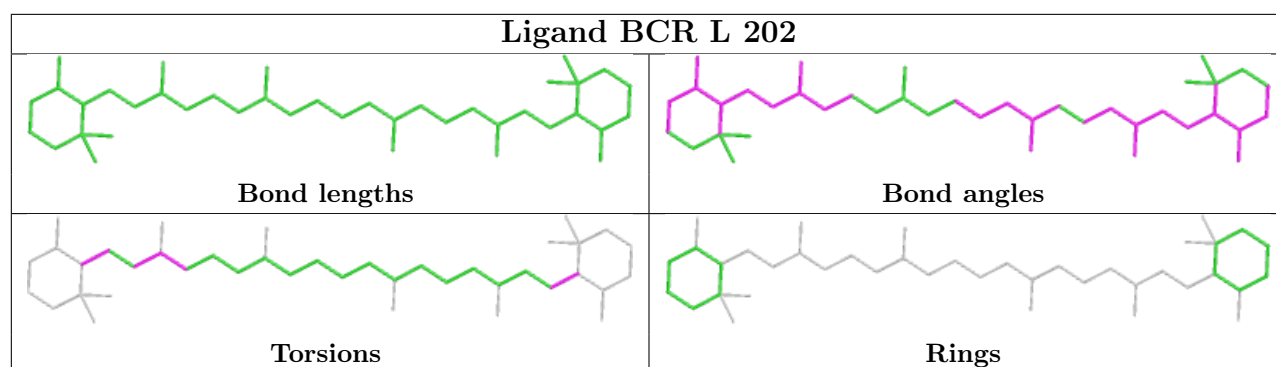
Rings

Ligand CLA h 609

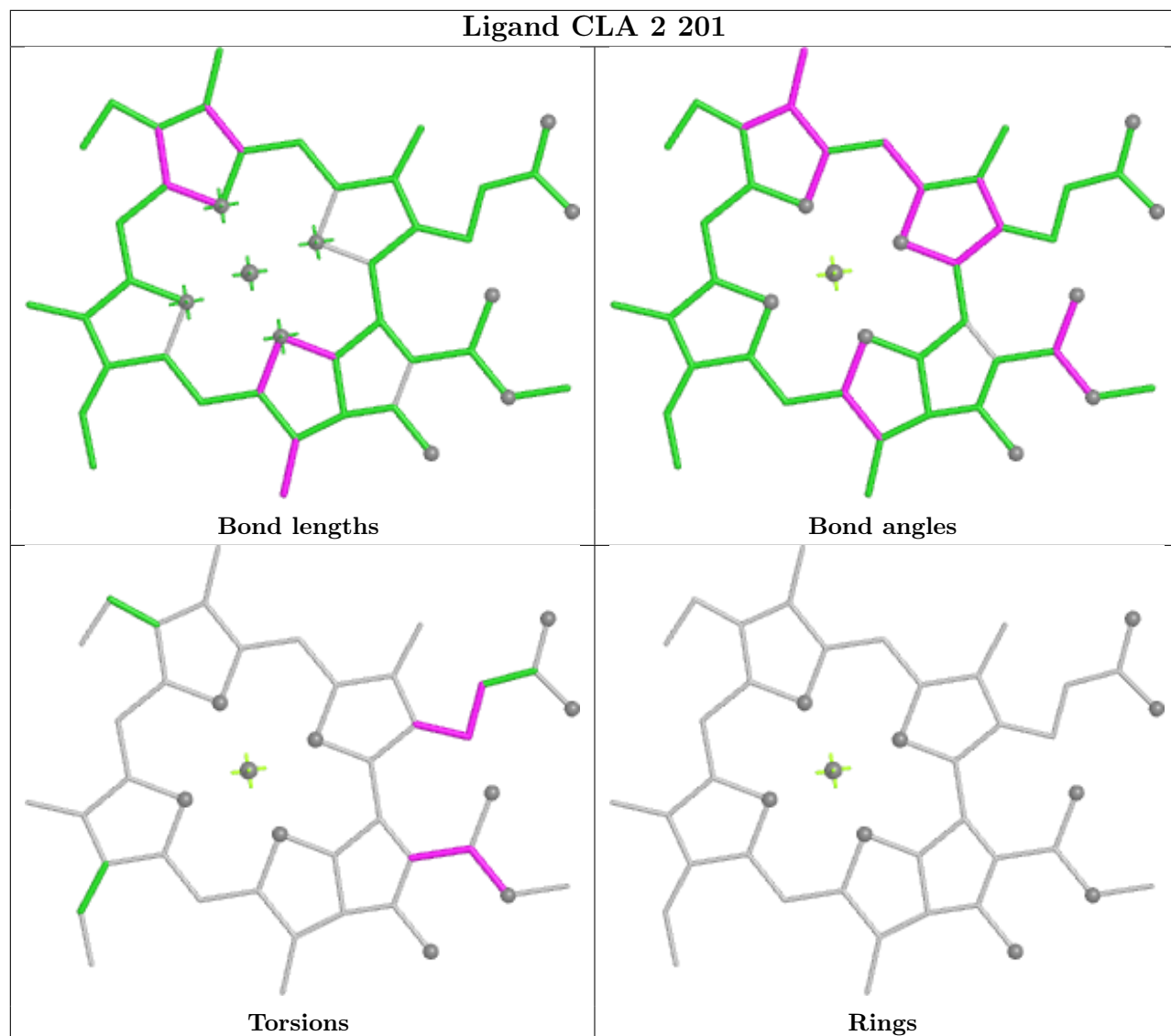


Ligand CLA B 812

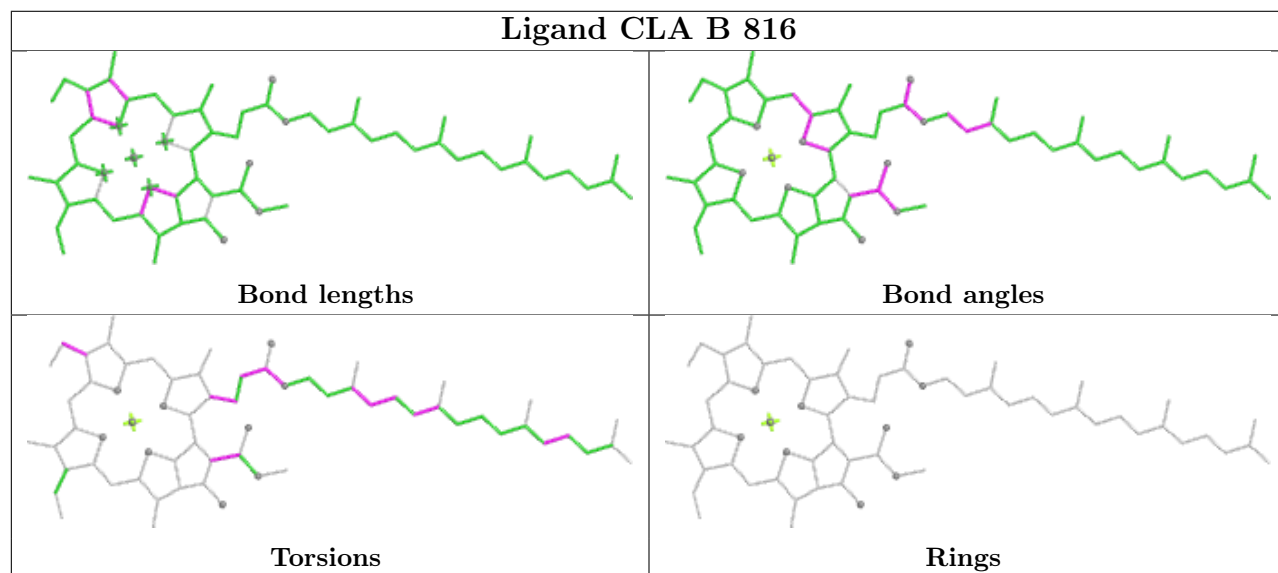


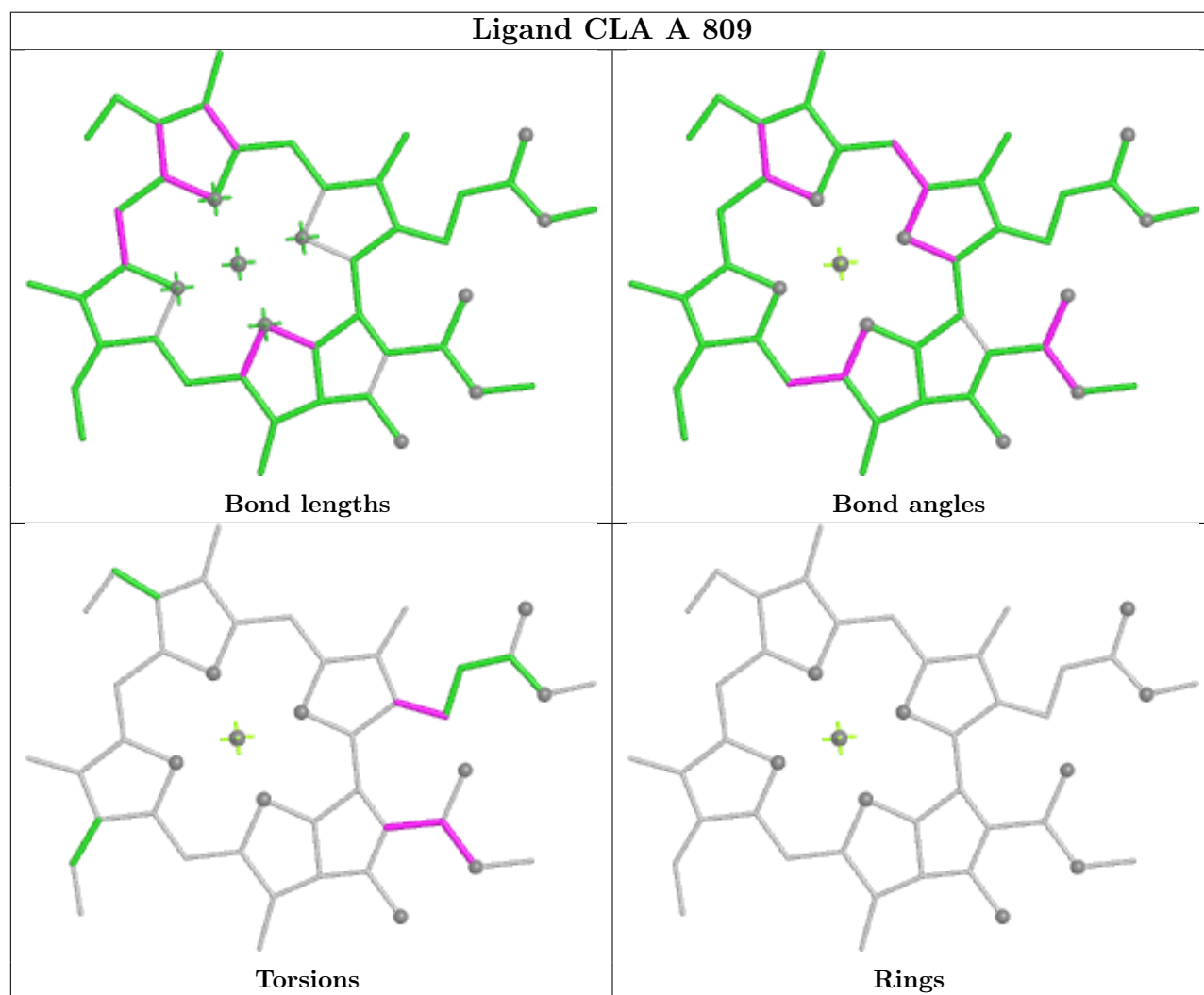
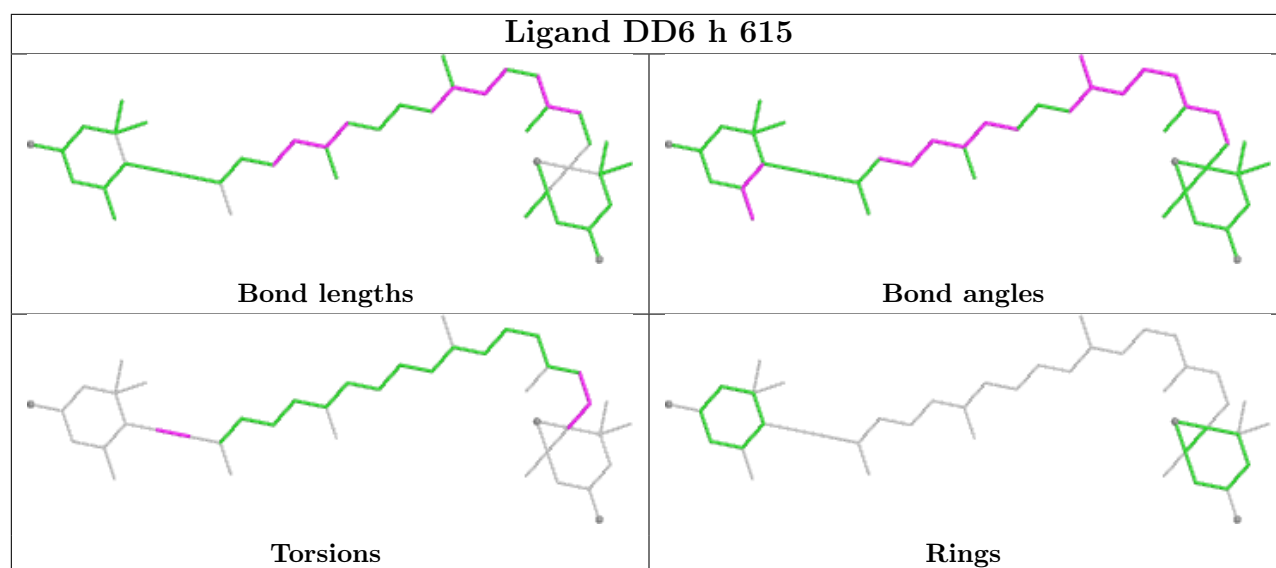


Ligand CLA 2 201

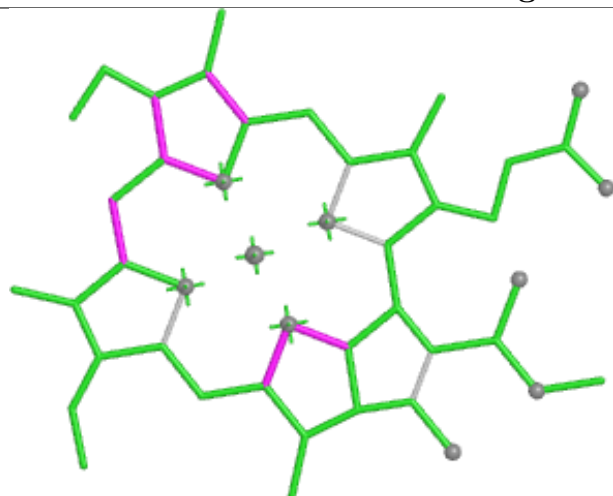


Ligand CLA B 816

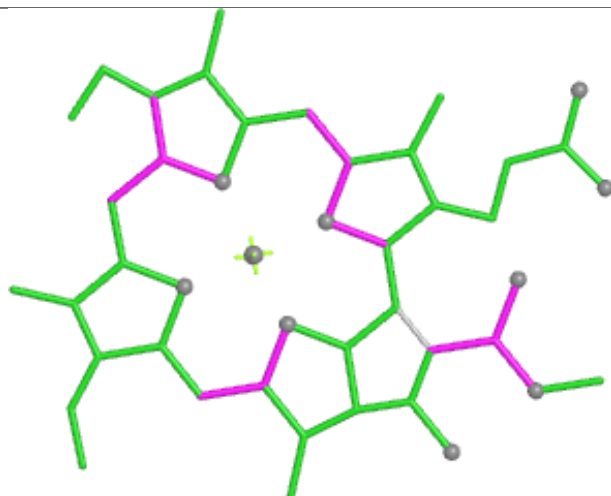




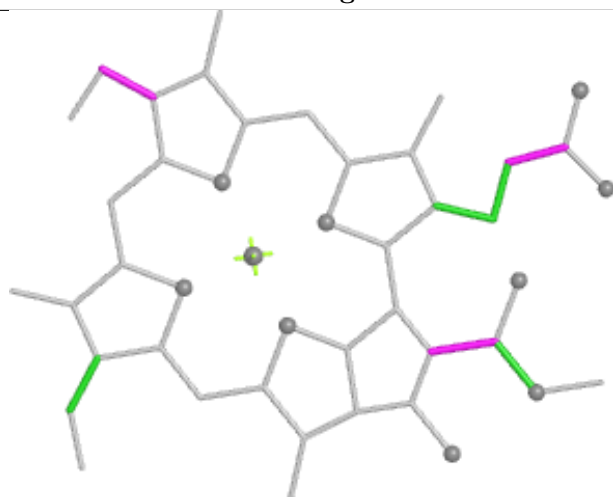
Ligand CLA 3 302



Bond lengths



Bond angles

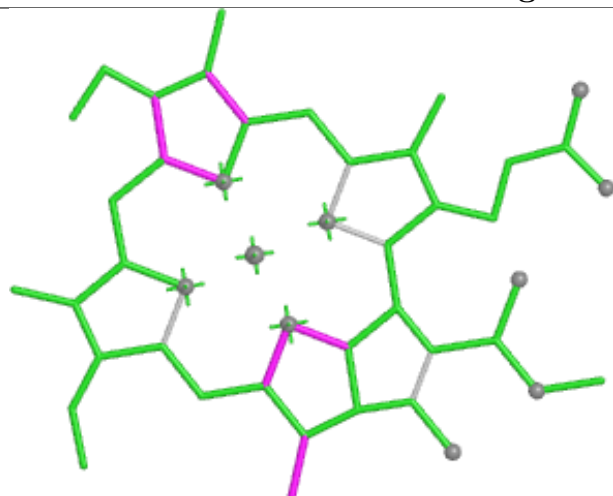


Torsions

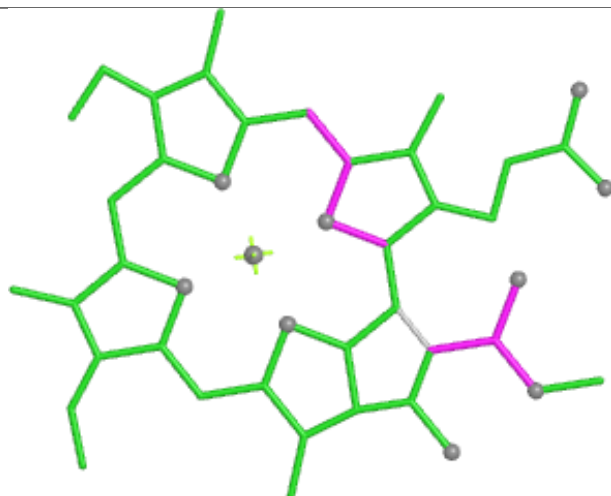


Rings

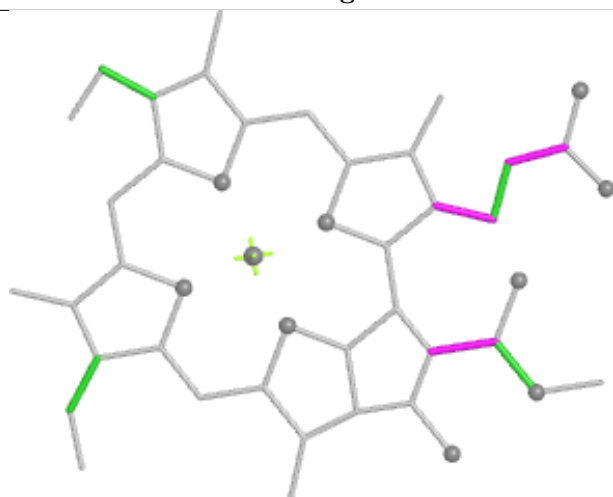
Ligand CLA 3 307



Bond lengths



Bond angles

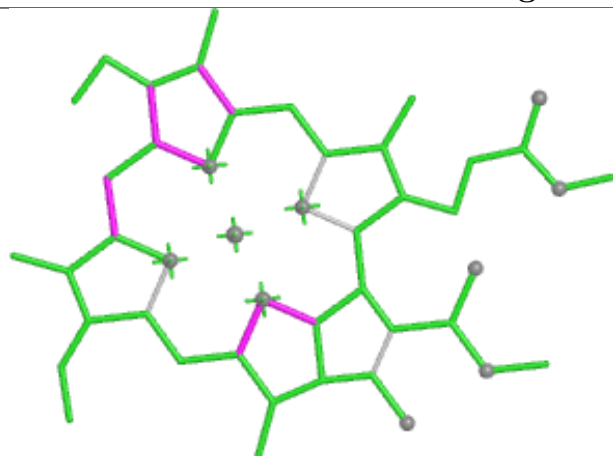


Torsions

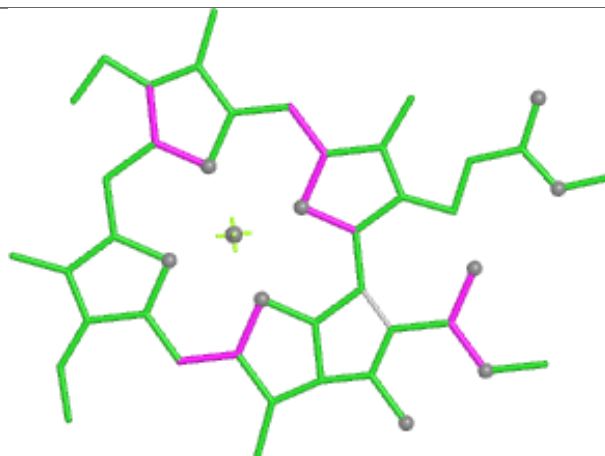


Rings

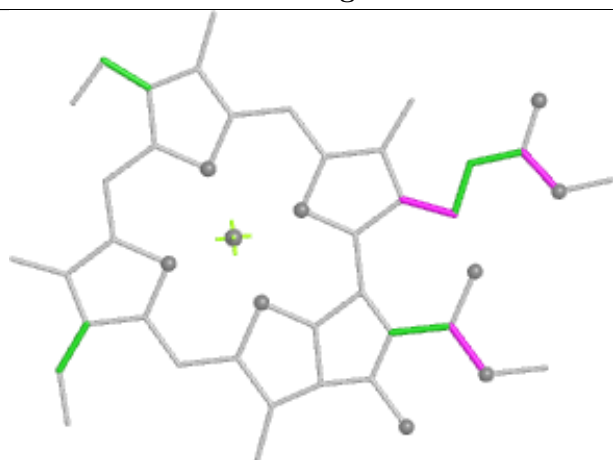
Ligand CLA 4 611



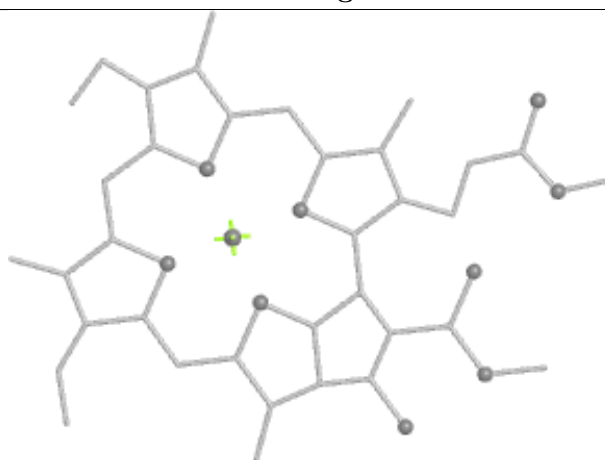
Bond lengths



Bond angles

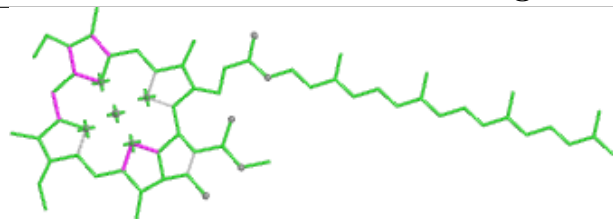


Torsions

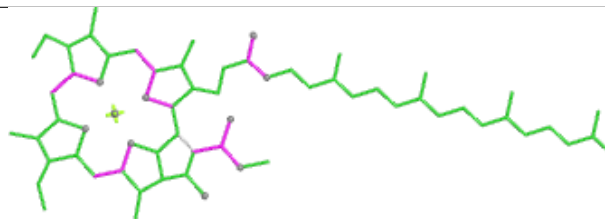


Rings

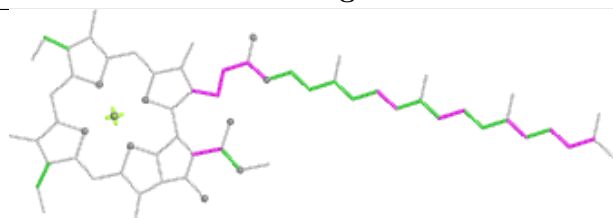
Ligand CLA A 807



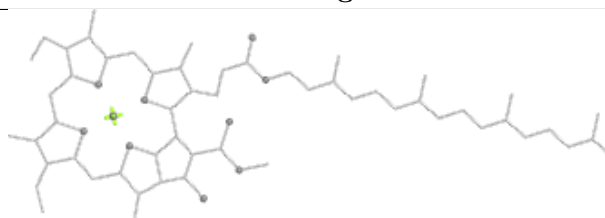
Bond lengths



Bond angles

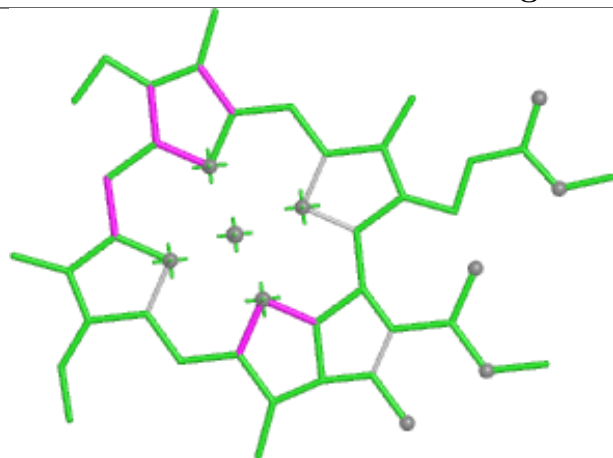


Torsions

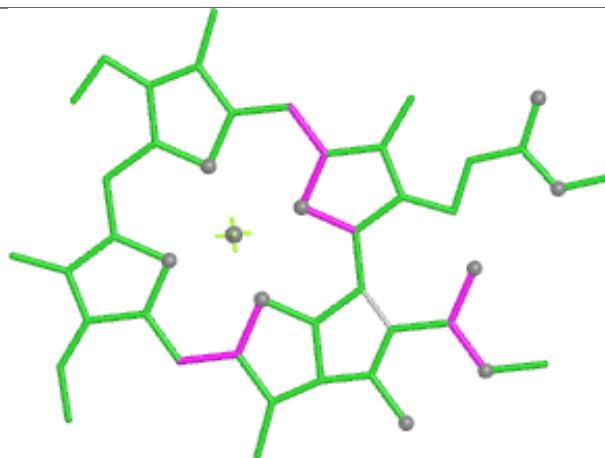


Rings

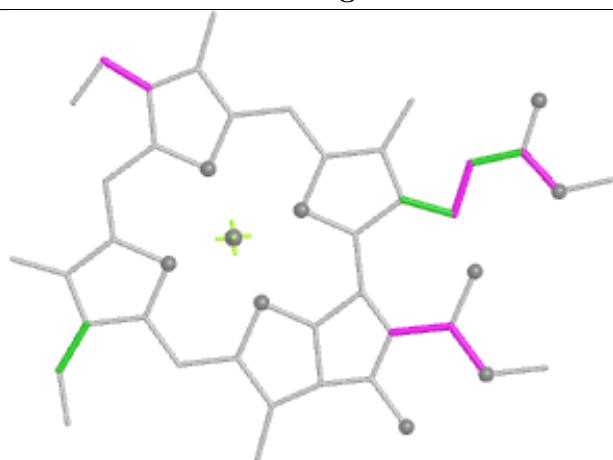
Ligand CLA t 310



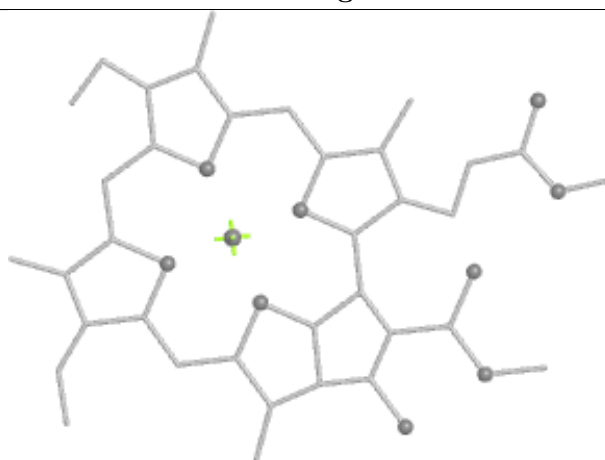
Bond lengths



Bond angles

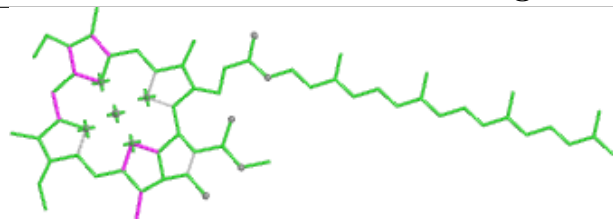


Torsions

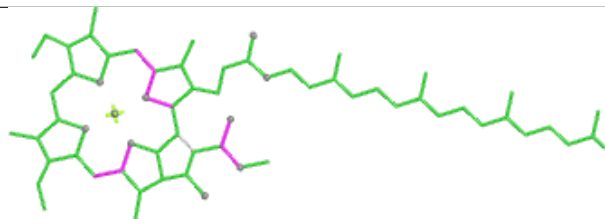


Rings

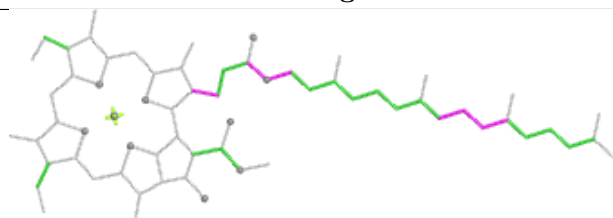
Ligand CLA R 103



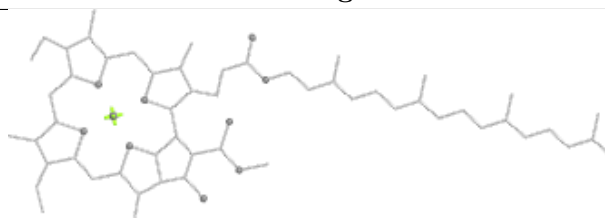
Bond lengths



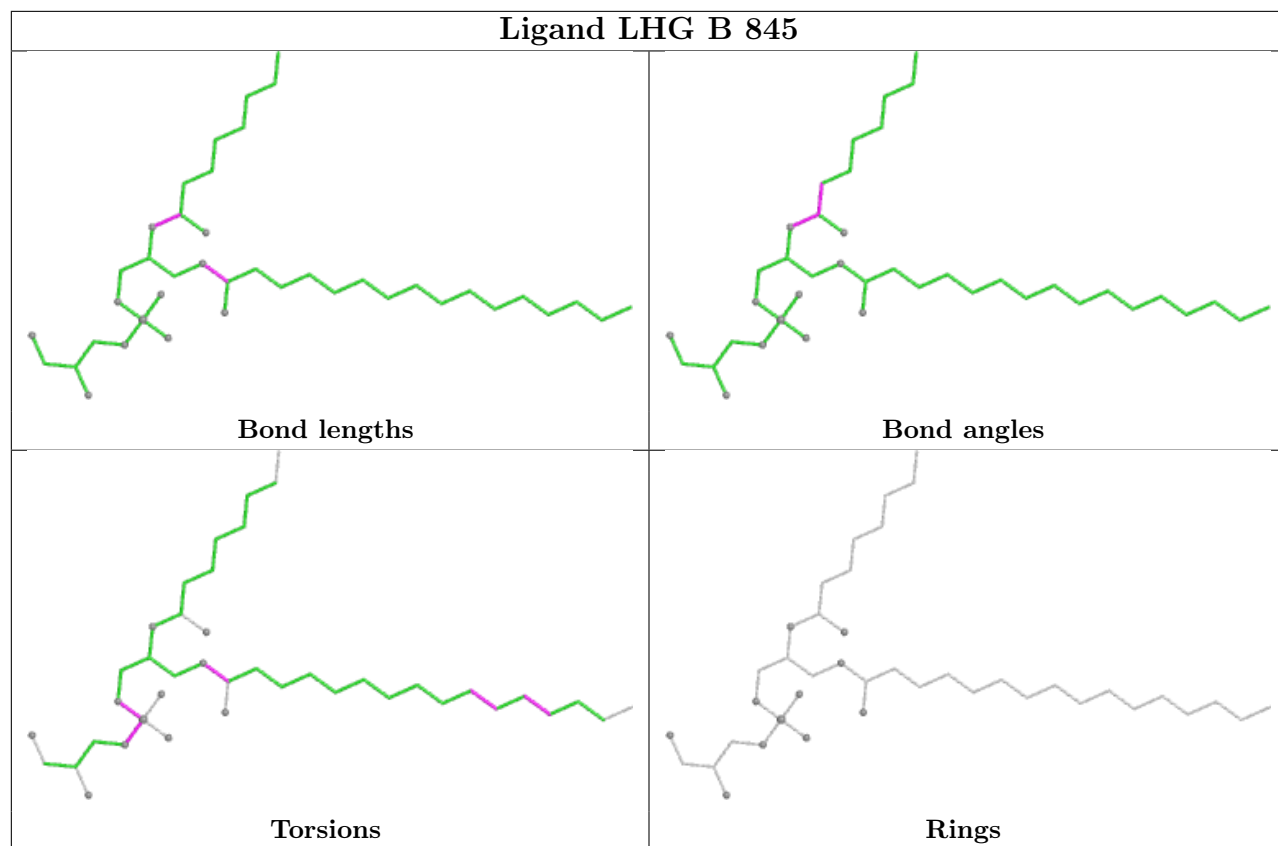
Bond angles



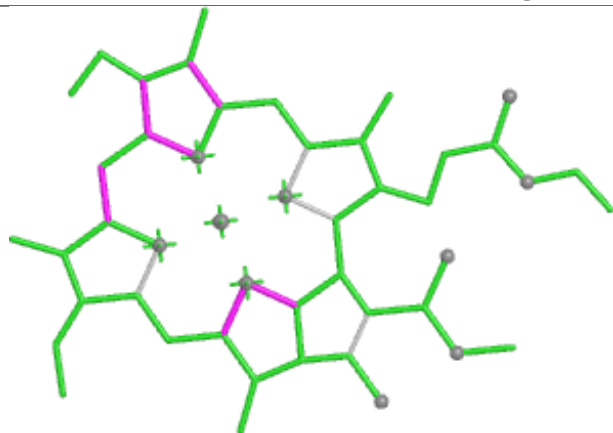
Torsions



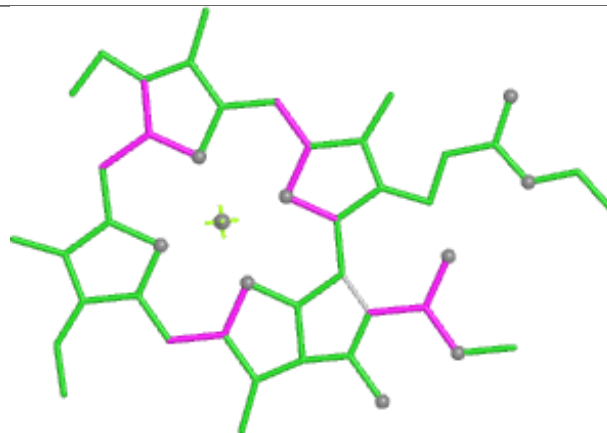
Rings



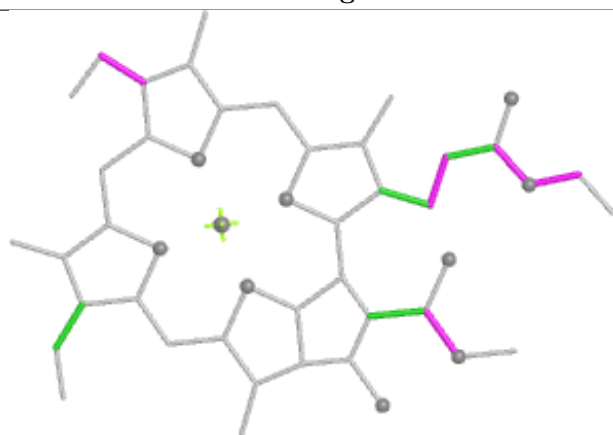
Ligand CLA 6 602



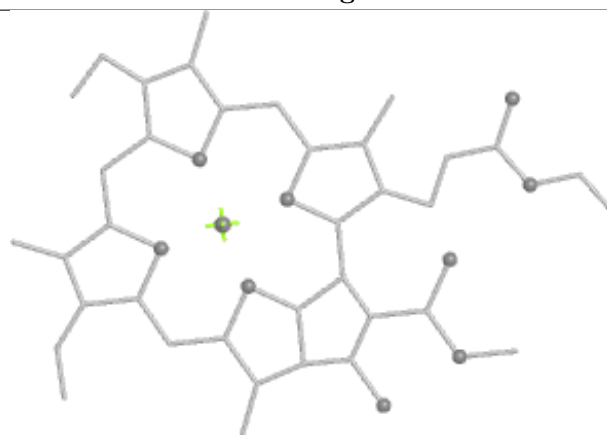
Bond lengths



Bond angles

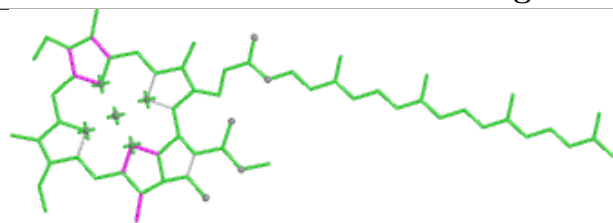


Torsions

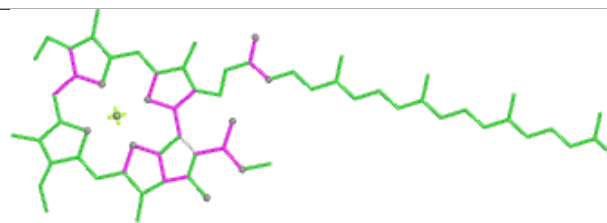


Rings

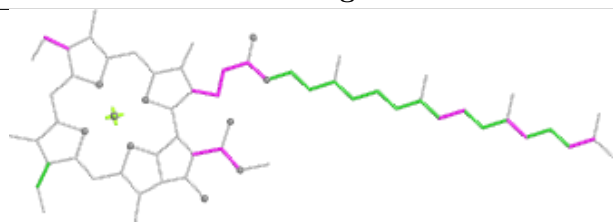
Ligand CLA A 801



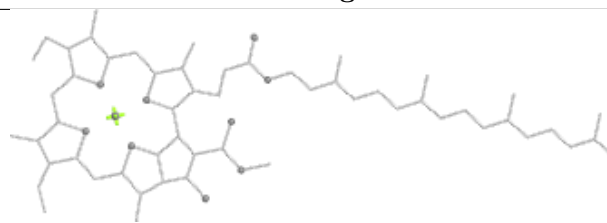
Bond lengths



Bond angles

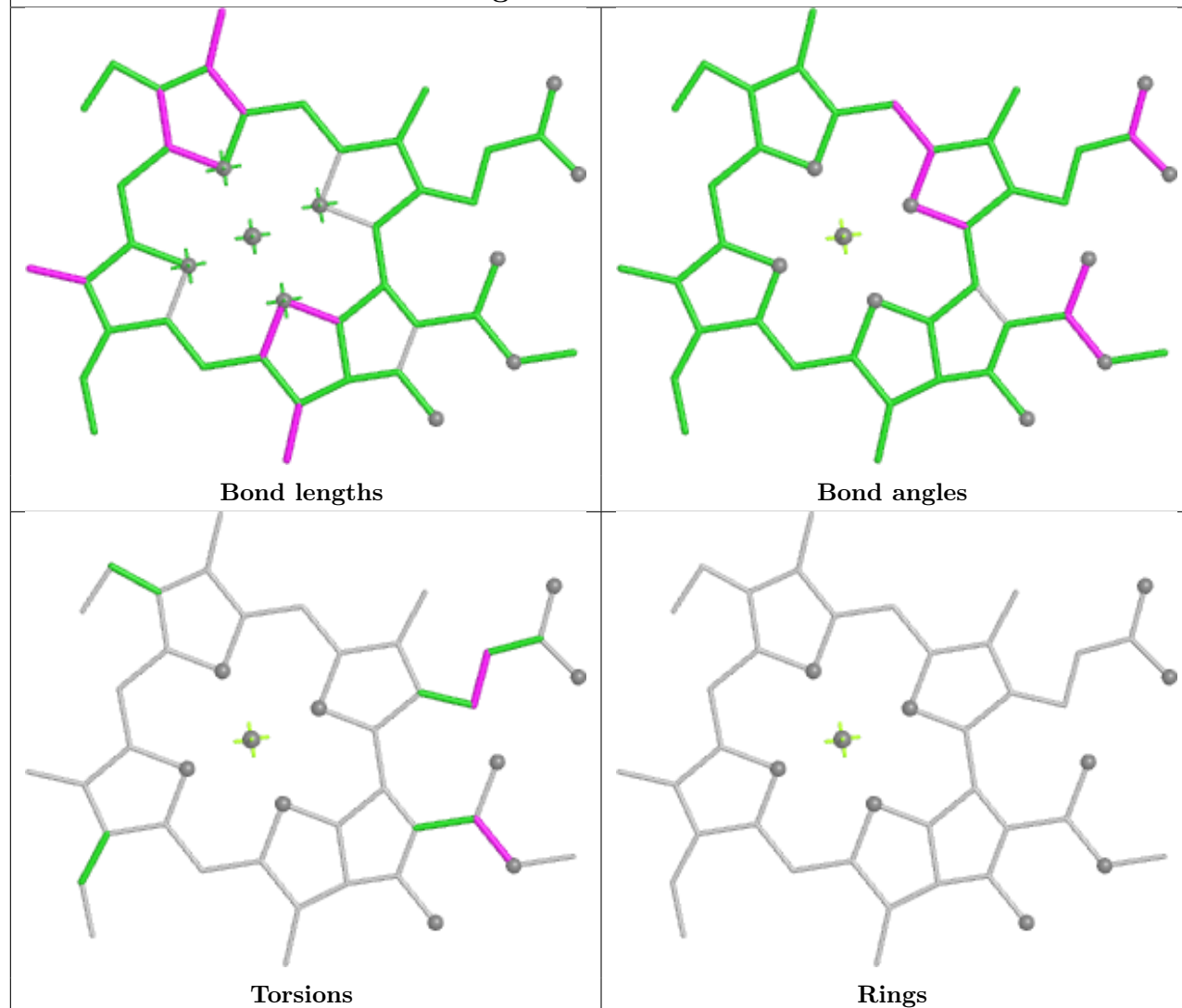


Torsions

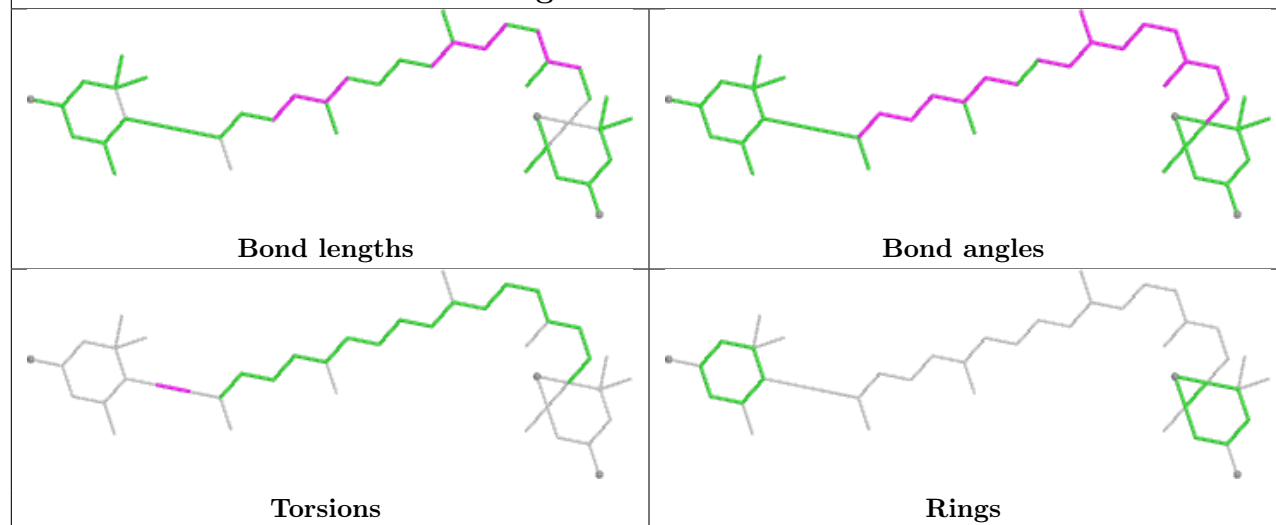


Rings

Ligand CLA R 104



Ligand DD6 h 613



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.

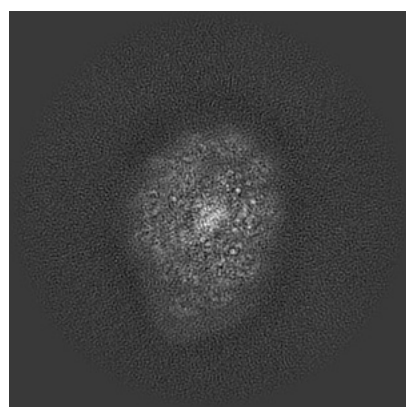
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63625. These allow visual inspection of the internal detail of the map and identification of artifacts.

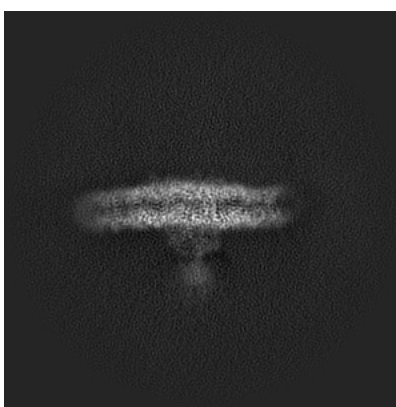
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

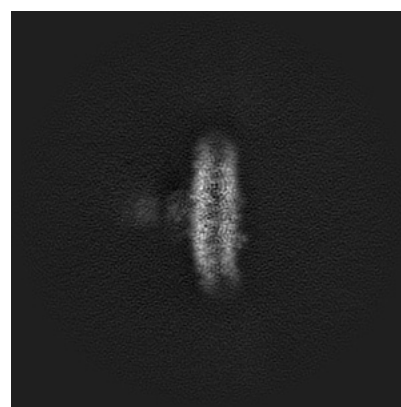
6.1.1 Primary map



X



Y

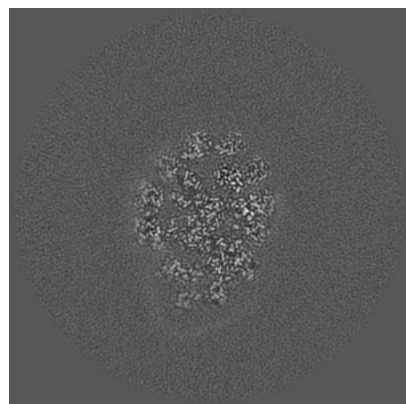


Z

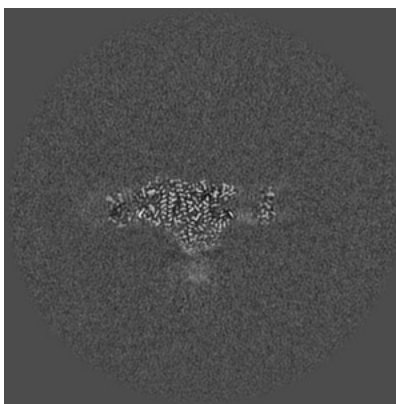
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

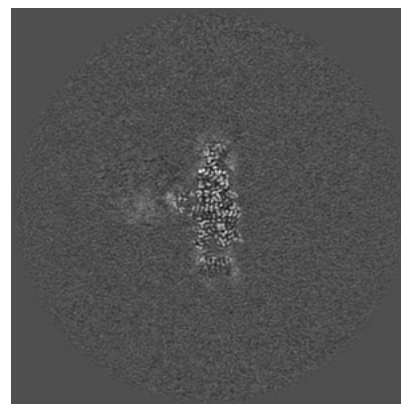
6.2.1 Primary map



X Index: 220



Y Index: 220

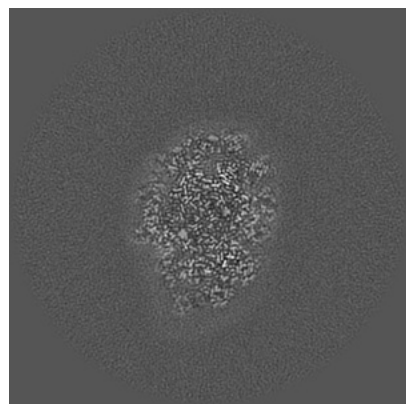


Z Index: 220

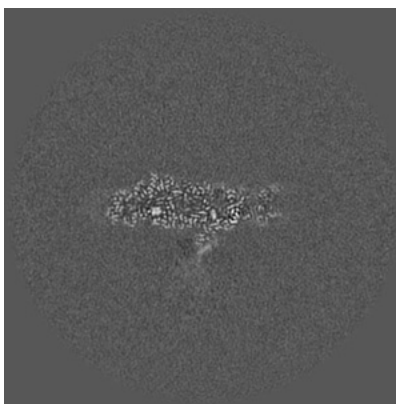
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

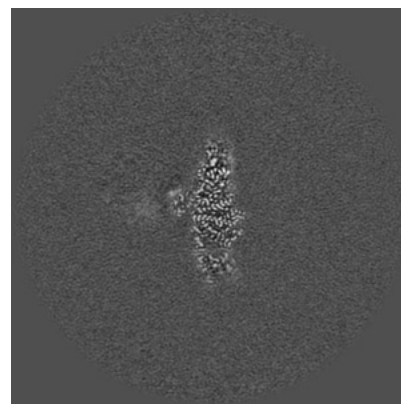
6.3.1 Primary map



X Index: 213



Y Index: 234

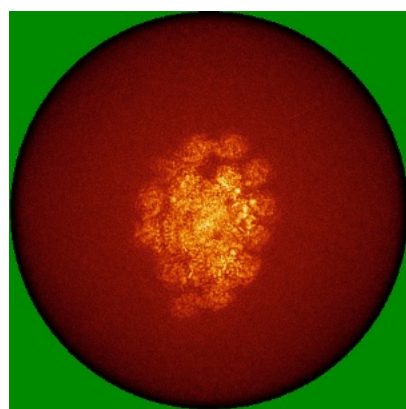


Z Index: 224

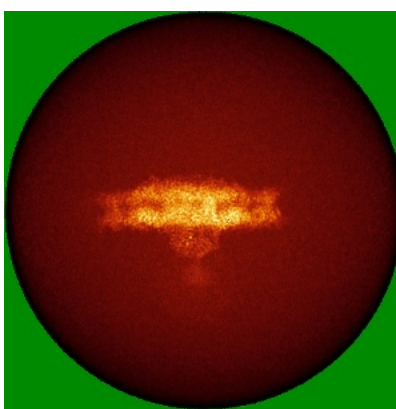
The images above show the largest variance slices of the map in three orthogonal directions.

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

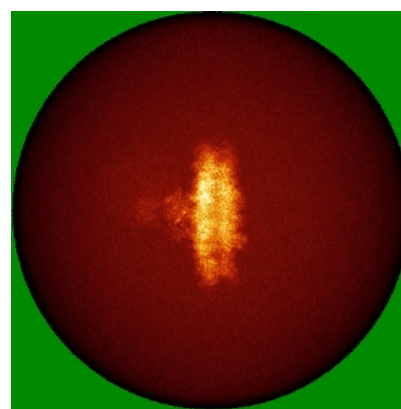
6.4.1 Primary map



X



Y

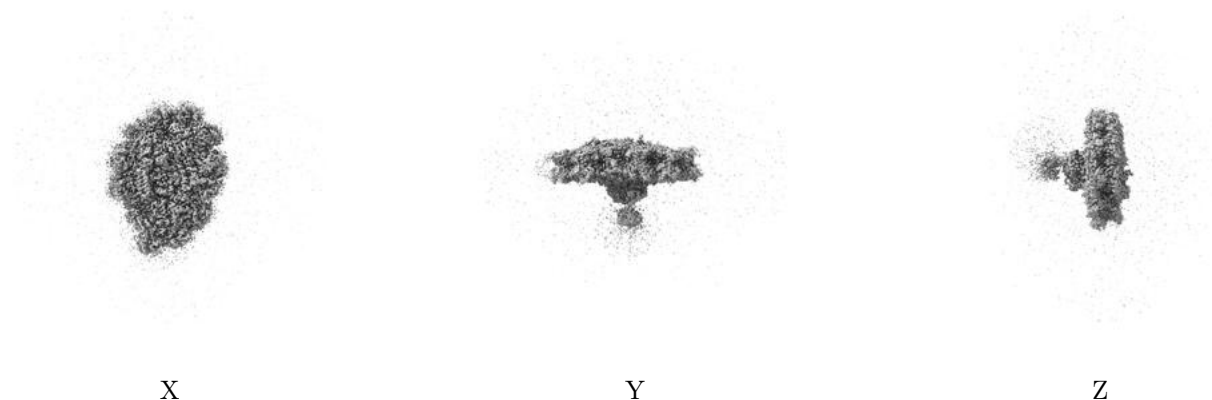


Z

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.

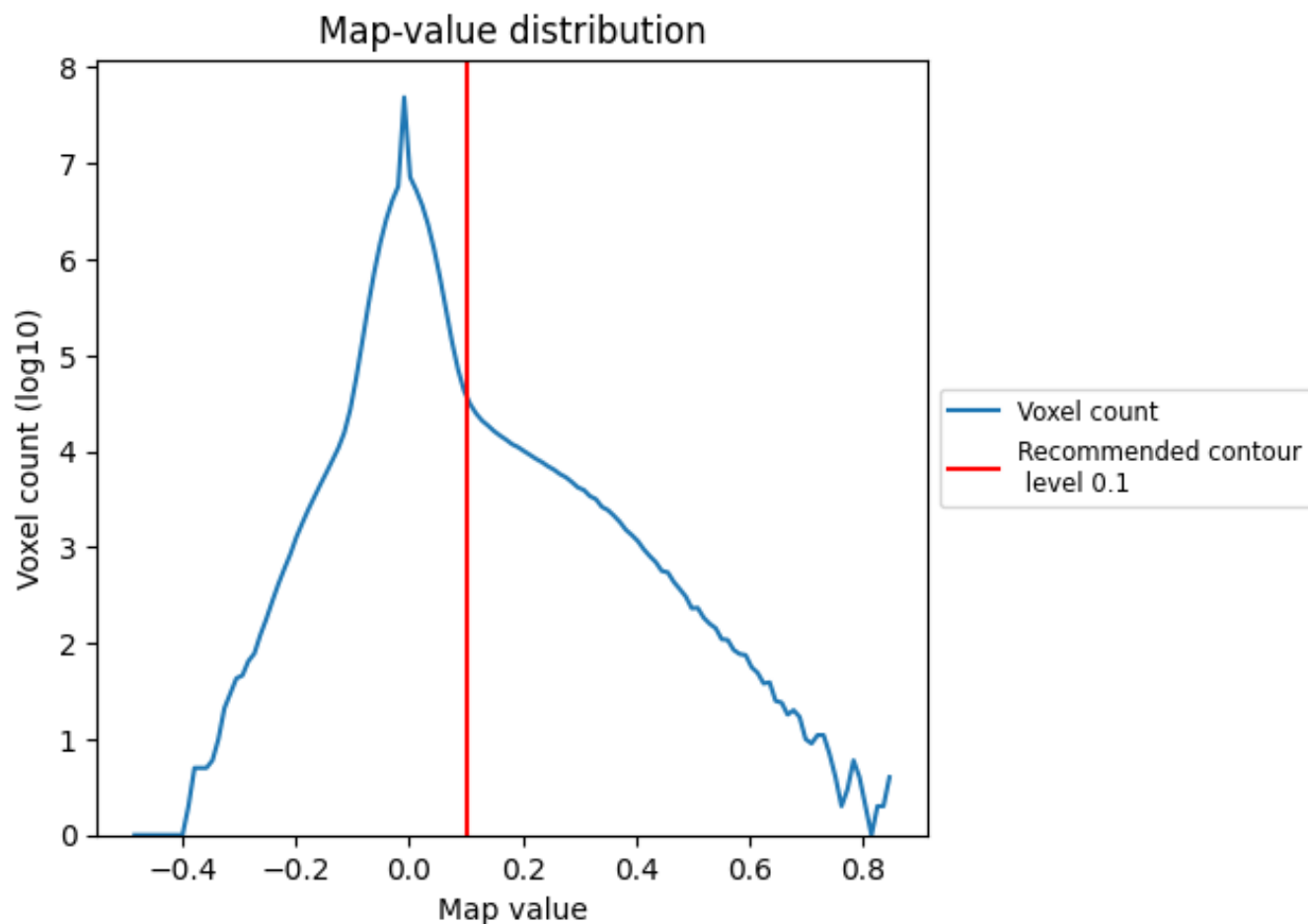
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

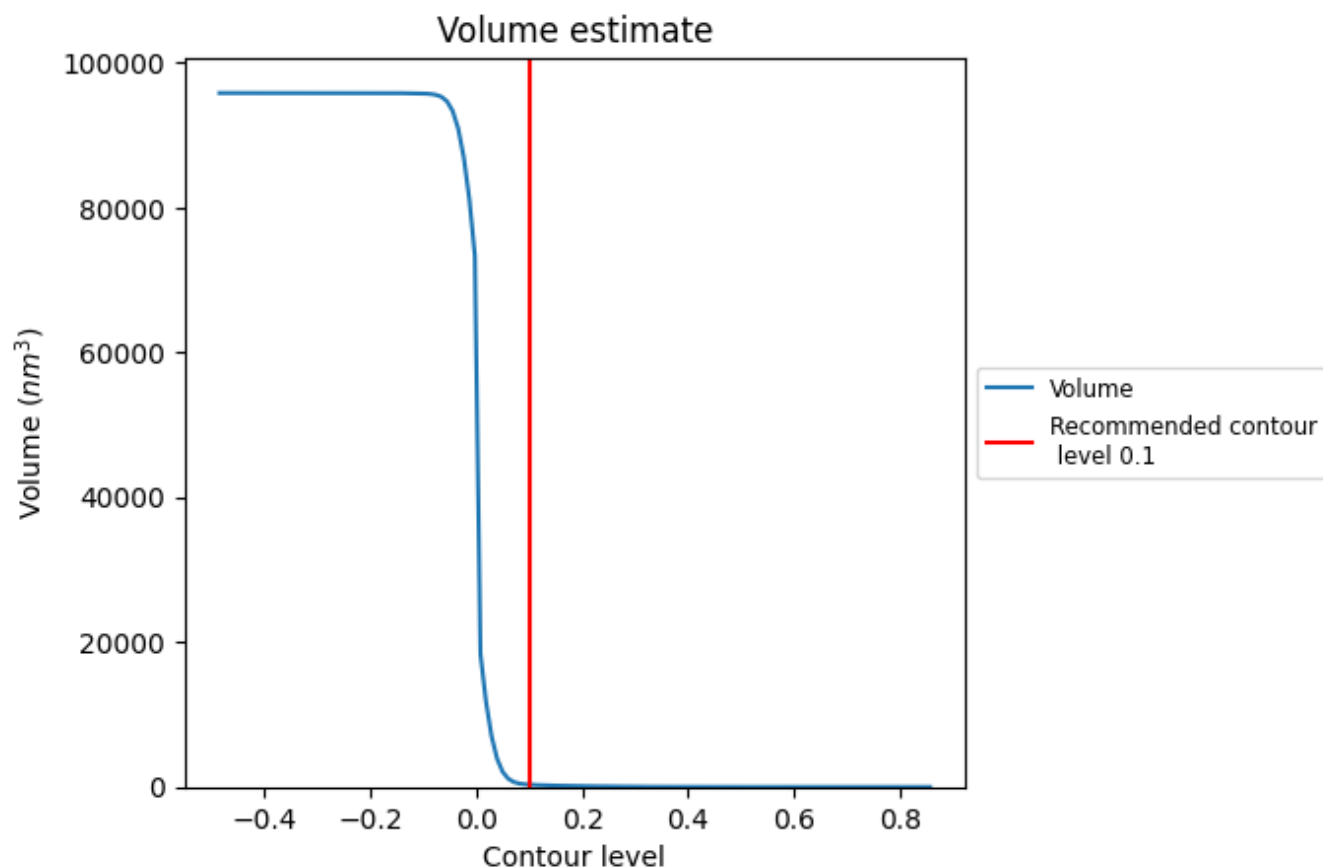
This section contains the results of statistical analysis of the map.

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.

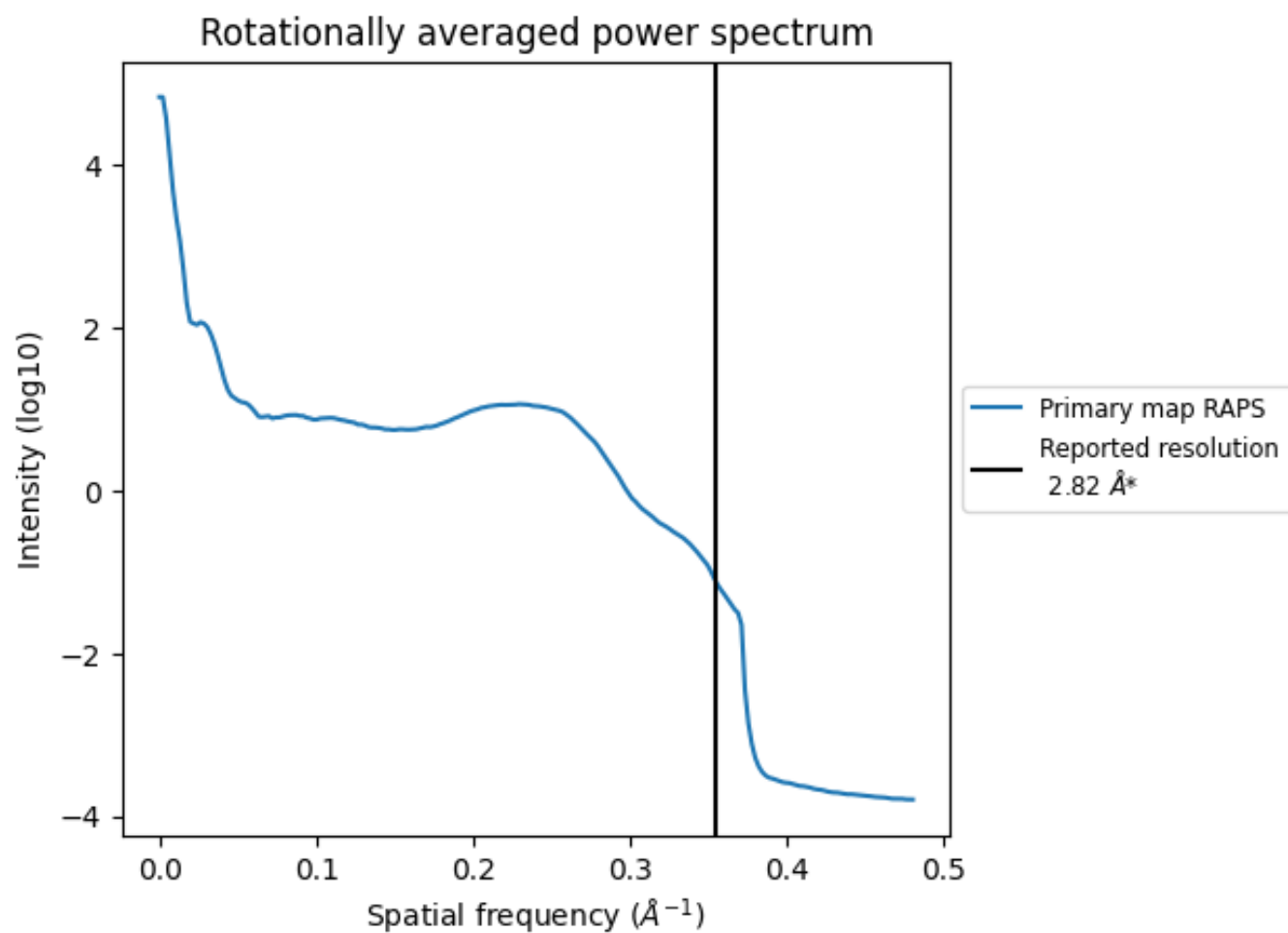
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 326 nm³; this corresponds to an approximate mass of 295 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 0.355 Å⁻¹

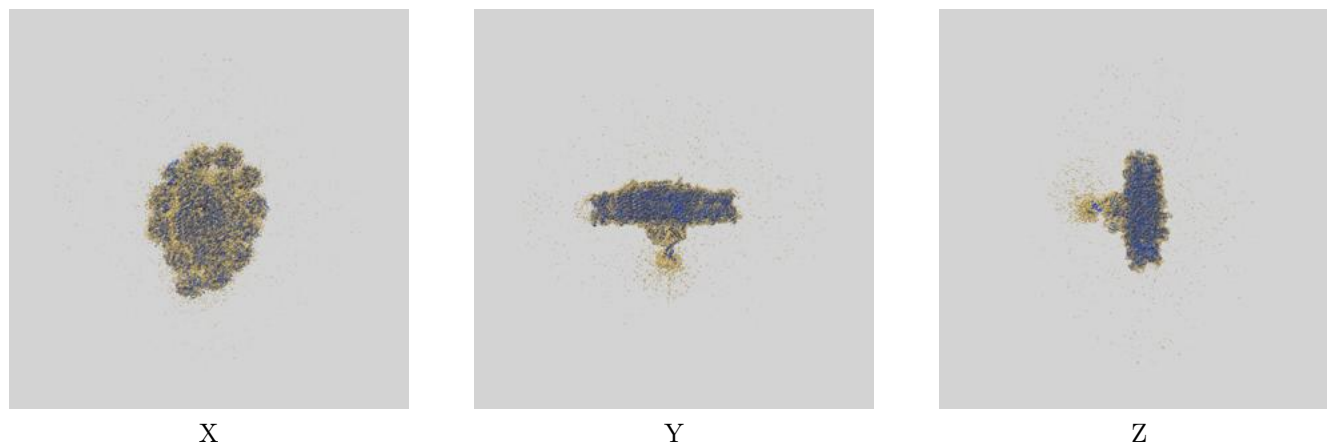
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

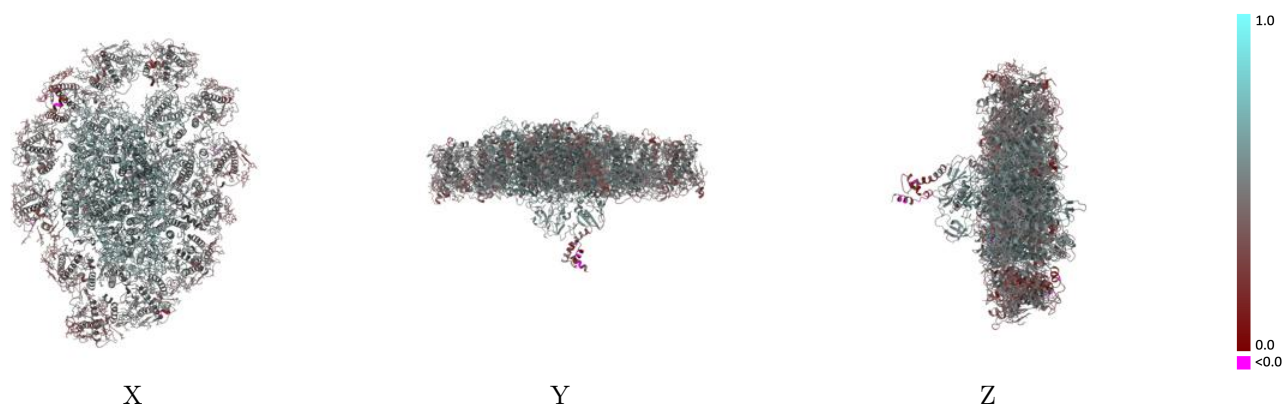
This section contains information regarding the fit between EMDB map EMD-63625 and PDB model 9M4F. Per-residue inclusion information can be found in section [3](#) on page [29](#).

9.1 Map-model overlay [i](#)



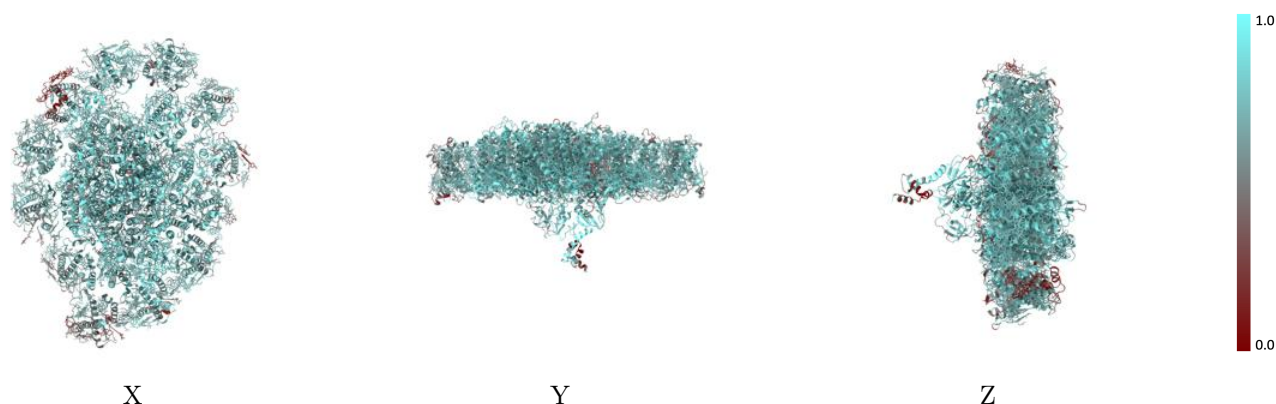
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



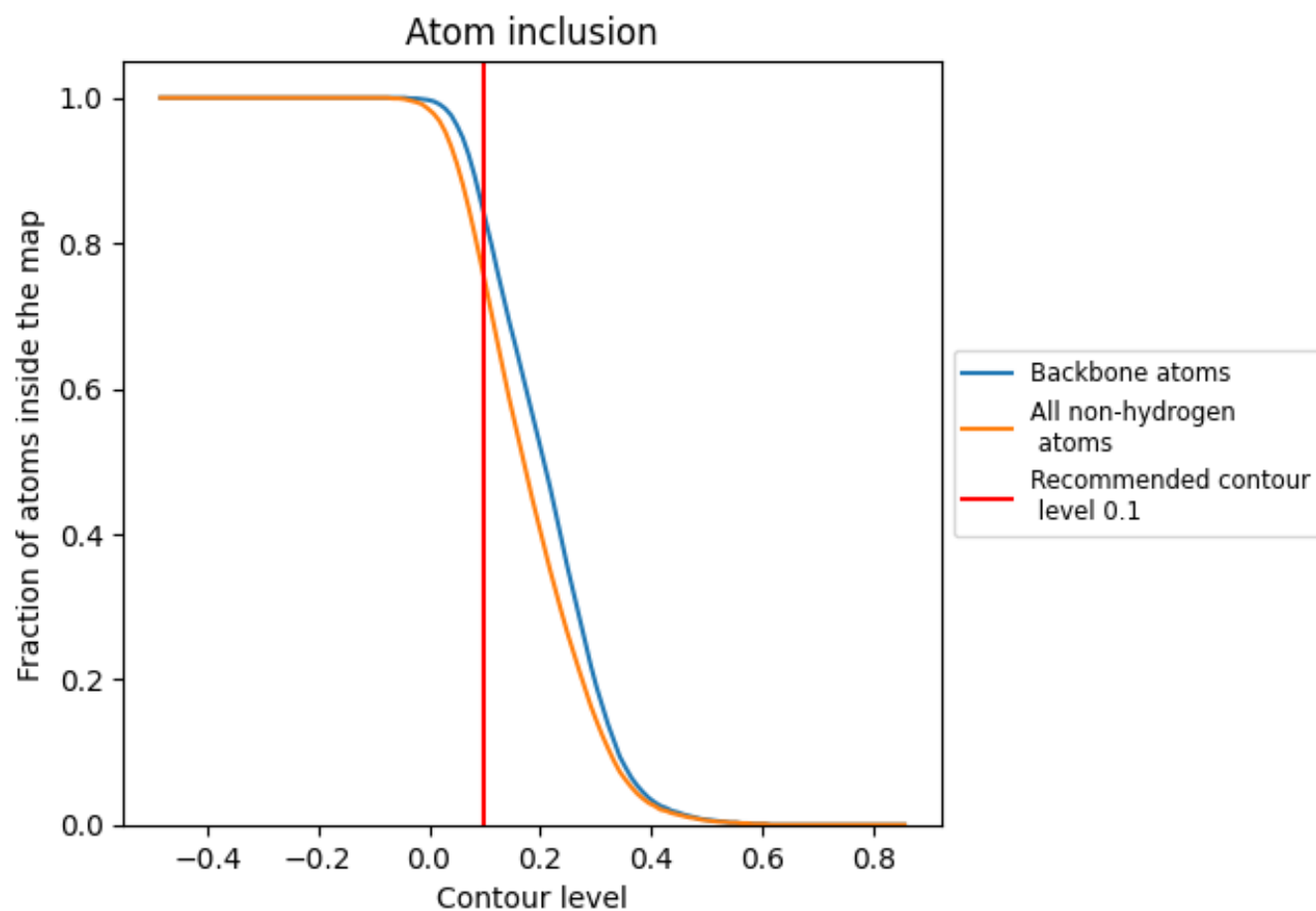
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 84% of all backbone atoms, 75% 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	 0.7490	 0.4950
1	 0.7410	 0.4690
2	 0.6780	 0.4260
3	 0.8430	 0.5220
4	 0.7210	 0.4510
5	 0.5160	 0.3670
6	 0.6820	 0.4370
7	 0.6840	 0.4260
8	 0.6740	 0.4200
9	 0.5030	 0.3820
A	 0.8250	 0.5720
B	 0.8350	 0.5690
C	 0.8540	 0.5490
D	 0.7810	 0.5150
E	 0.7450	 0.5250
F	 0.7860	 0.5220
I	 0.7860	 0.5260
J	 0.8270	 0.5420
L	 0.8760	 0.5340
M	 0.8330	 0.5030
R	 0.7510	 0.4920
S	 0.5070	 0.2720
c	 0.7410	 0.4640
h	 0.7040	 0.4590
k	 0.6510	 0.4290
t	 0.6750	 0.4380

