



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 04:56 AM JST

PDB ID : 6KIG / pdb_00006kig
EMDB ID : EMD-9995
Title : Structure of cyanobacterial photosystem I-IsiA supercomplex
Authors : Cao, P.; Cao, D.F.; Si, L.; Su, X.D.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on : 2019-07-18
Resolution : 2.90 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

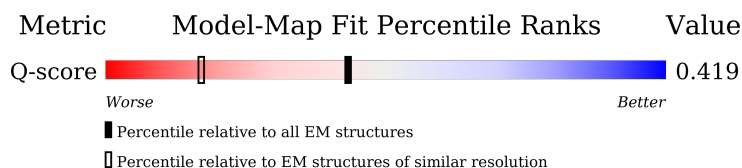
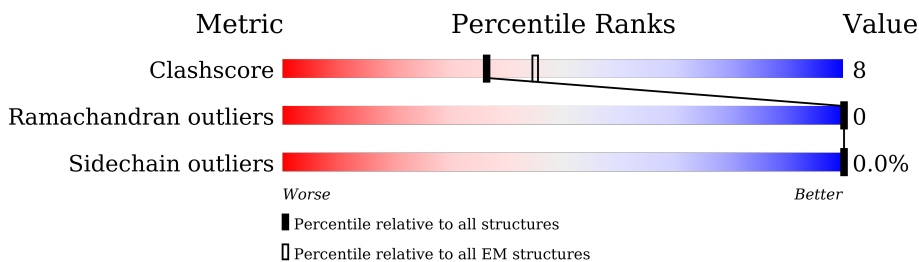
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



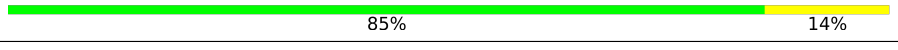
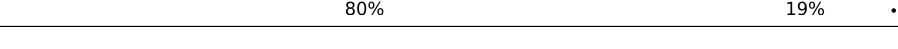
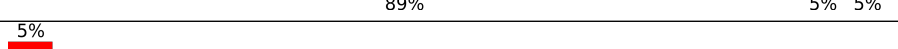
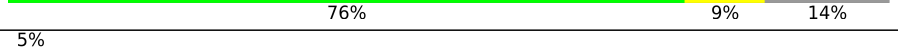
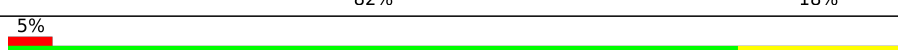
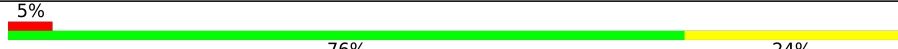
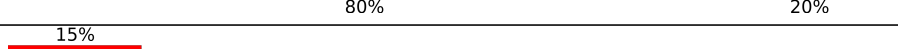
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	763	
1	G	763	
1	e	763	
2	B	734	

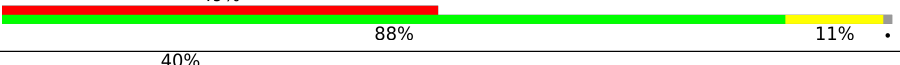
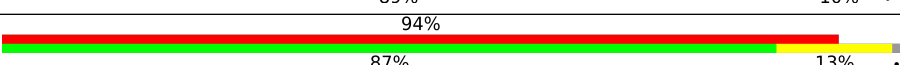
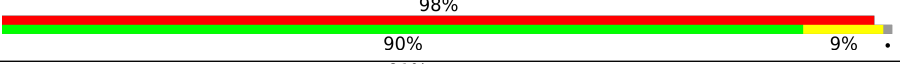
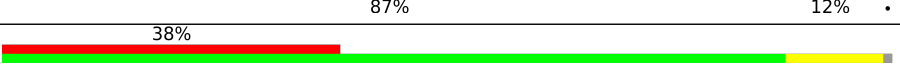
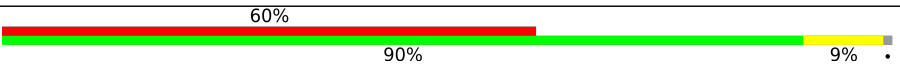
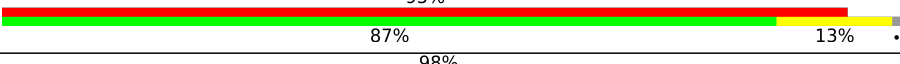
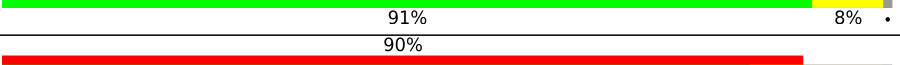
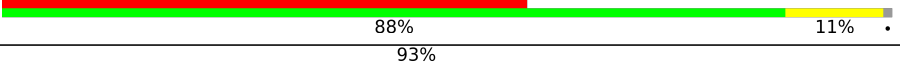
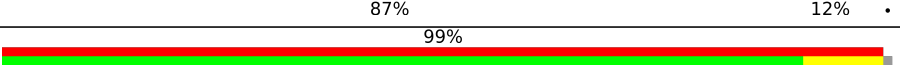
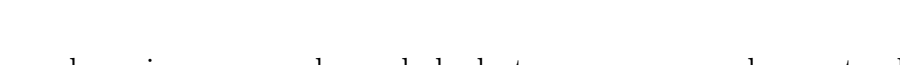
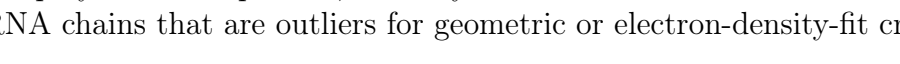
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Mol	Chain	Length	Quality of chain
2	H	734	
2	f	734	
3	C	81	
3	N	81	
3	g	81	
4	D	141	
4	O	141	
4	h	141	
5	E	75	
5	Q	75	
5	i	75	
6	F	159	
6	R	159	
6	j	159	
7	I	38	
7	S	38	
7	k	38	
8	J	41	
8	T	41	
8	l	41	
9	K	84	
9	U	84	
9	m	84	
10	L	166	
10	V	166	

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Mol	Chain	Length	Quality of chain
10	n	166	
11	M	29	
11	W	29	
11	o	29	
12	1	342	
12	2	342	
12	3	342	
12	4	342	
12	5	342	
12	6	342	
12	Y	342	
12	Z	342	
12	a	342	
12	b	342	
12	c	342	
12	d	342	
12	q	342	
12	r	342	
12	s	342	
12	t	342	
12	u	342	
12	v	342	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	q	505	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 143022 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		
1	G	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		
1	e	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5789	3811	970	994	14		
2	H	733	Total	C	N	O	S	0	0
			5789	3811	970	994	14		
2	f	733	Total	C	N	O	S	0	0
			5789	3811	970	994	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			598	368	103	116	11		
3	N	80	Total	C	N	O	S	0	0
			598	368	103	116	11		
3	g	80	Total	C	N	O	S	0	0
			598	368	103	116	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	141	Total	C	N	O	S	0	0
			1098	702	187	208	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	141	Total	C	N	O	S	0	0
			1098	702	187	208	1		
4	h	141	Total	C	N	O	S	0	0
			1098	702	187	208	1		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	71	Total	C	N	O		0	0
			543	343	95	105			
5	Q	71	Total	C	N	O		0	0
			543	343	95	105			
5	i	71	Total	C	N	O		0	0
			543	343	95	105			

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	136	Total	C	N	O	S	0	0
			1036	670	174	190	2		
6	R	136	Total	C	N	O	S	0	0
			1036	670	174	190	2		
6	j	136	Total	C	N	O	S	0	0
			1036	670	174	190	2		

- Molecule 7 is a protein called Photosystem I PsaI protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			282	191	38	51	2		
7	S	38	Total	C	N	O	S	0	0
			282	191	38	51	2		
7	k	38	Total	C	N	O	S	0	0
			282	191	38	51	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			335	228	52	54	1		
8	T	41	Total	C	N	O	S	0	0
			335	228	52	54	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	l	41	Total	C	N	O	S	0	0
			335	228	52	54	1		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	78	Total	C	N	O	S	0	0
			549	364	91	93	1		
9	U	78	Total	C	N	O	S	0	0
			549	364	91	93	1		
9	m	78	Total	C	N	O	S	0	0
			549	364	91	93	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	164	Total	C	N	O	S	0	0
			1210	782	201	225	2		
10	V	164	Total	C	N	O	S	0	0
			1210	782	201	225	2		
10	n	164	Total	C	N	O	S	0	0
			1210	782	201	225	2		

- Molecule 11 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	29	Total	C	N	O	S	0	0
			228	151	36	40	1		
11	W	29	Total	C	N	O	S	0	0
			228	151	36	40	1		
11	o	29	Total	C	N	O	S	0	0
			228	151	36	40	1		

- Molecule 12 is a protein called Iron stress-induced chlorophyll-binding protein.

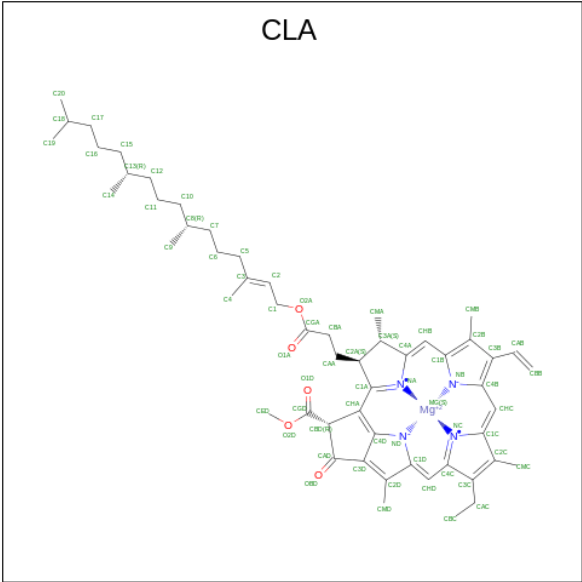
Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	2	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	3	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	4	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	5	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	6	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	Y	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	Z	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	a	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	b	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	c	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	d	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	q	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	r	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	s	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	t	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	u	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	v	339	Total 2605	C 1722	N 428	O 448	S 7	0	0

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	J	1	Total 58	C 48	Mg 1	N 4	O 5	0
13	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	1	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	6	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	G	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	T	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	U	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	V	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	Y	1	Total 64	C 54	Mg 1	N 4	O 5	0
13	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	Y	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 53	C 43	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 61	C 51	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	d	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	e	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 53	C 43	Mg 1	N 4	O 5	0
13	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	e	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	e	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	e	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	f	1	Total 57	C 47	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	l	1	Total 58	C 48	Mg 1	N 4	O 5	0
13	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	m	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	m	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	m	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	q	1	Total 64	C 54	Mg 1	N 4	O 5	0
13	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	q	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	q	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	q	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	r	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	r	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	t	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	t	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	t	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	t	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	t	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	t	1	Total 55	C 45	Mg 1	N 4	O 5	0

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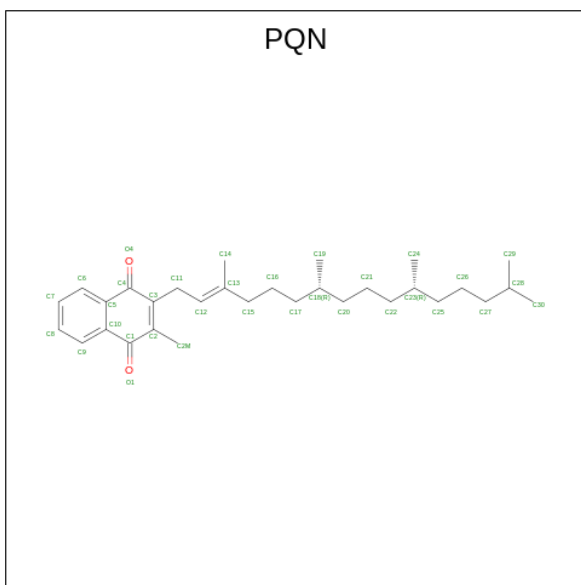
Mol	Chain	Residues	Atoms					AltConf
13	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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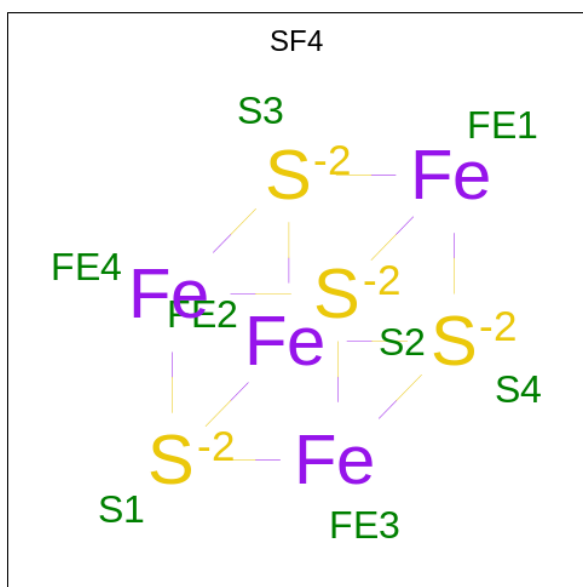
Mol	Chain	Residues	Atoms					AltConf
13	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



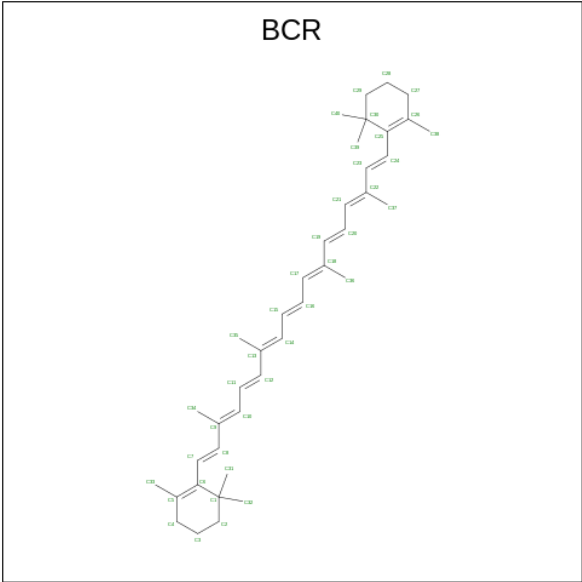
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			33	31	2	
14	B	1	Total	C	O	0
			33	31	2	
14	G	1	Total	C	O	0
			33	31	2	
14	H	1	Total	C	O	0
			33	31	2	
14	e	1	Total	C	O	0
			33	31	2	
14	f	1	Total	C	O	0
			33	31	2	

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	Fe	S	0
			8	4	4	
15	C	1	Total	Fe	S	0
			8	4	4	
15	C	1	Total	Fe	S	0
			8	4	4	
15	G	1	Total	Fe	S	0
			8	4	4	
15	N	1	Total	Fe	S	0
			8	4	4	
15	N	1	Total	Fe	S	0
			8	4	4	
15	e	1	Total	Fe	S	0
			8	4	4	
15	g	1	Total	Fe	S	0
			8	4	4	
15	g	1	Total	Fe	S	0
			8	4	4	

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	F	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
16	I	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	K	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	M	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	3	1	Total C 40 40	0
16	3	1	Total C 40 40	0
16	3	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	3	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	R	1	Total C 40 40	0
16	S	1	Total C 40 40	0
16	T	1	Total C 40 40	0
16	T	1	Total C 40 40	0
16	T	1	Total C 40 40	0
16	U	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	W	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Z	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	Z	1	Total C 40 40	0
16	Z	1	Total C 40 40	0
16	Z	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	k	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	m	1	Total C 40 40	0
16	n	1	Total C 40 40	0
16	n	1	Total C 40 40	0
16	n	1	Total C 40 40	0
16	n	1	Total C 40 40	0

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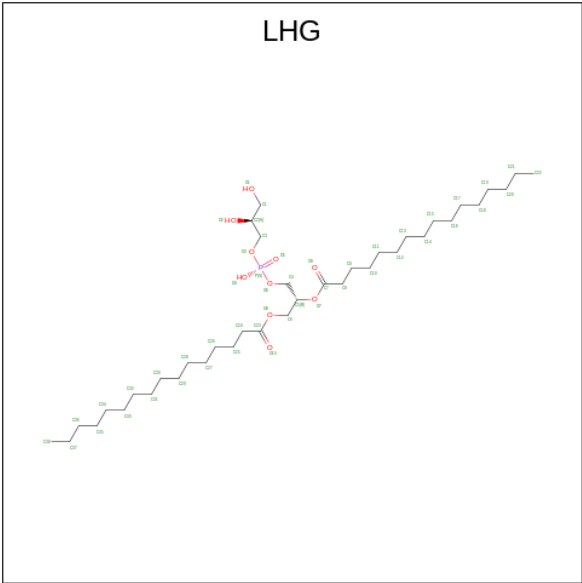
Mol	Chain	Residues	Atoms	AltConf
16	o	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	u	1	Total C 40 40	0
16	u	1	Total C 40 40	0
16	u	1	Total C 40 40	0
16	u	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
16	v	1	Total	C	0
			40	40	
16	v	1	Total	C	0
			40	40	
16	v	1	Total	C	0
			40	40	
16	v	1	Total	C	0
			40	40	

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			39	28	10	1	
17	A	1	Total	C	O	P	0
			36	25	10	1	
17	A	1	Total	C	O	P	0
			45	34	10	1	
17	A	1	Total	C	O	P	0
			45	34	10	1	
17	A	1	Total	C	O	P	0
			47	36	10	1	
17	A	1	Total	C	O	P	0
			35	24	10	1	
17	A	1	Total	C	O	P	0
			49	38	10	1	

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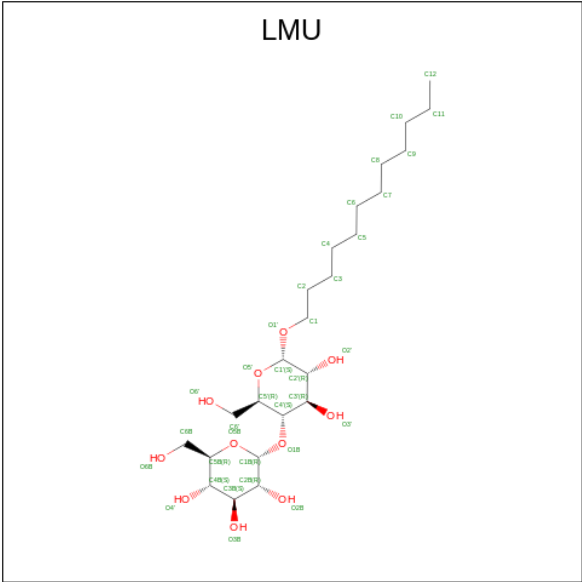
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total 49	C 38	O 10	P 1	0
17	A	1	Total 41	C 30	O 10	P 1	0
17	B	1	Total 39	C 28	O 10	P 1	0
17	B	1	Total 44	C 33	O 10	P 1	0
17	I	1	Total 44	C 33	O 10	P 1	0
17	L	1	Total 38	C 27	O 10	P 1	0
17	L	1	Total 41	C 30	O 10	P 1	0
17	L	1	Total 49	C 38	O 10	P 1	0
17	G	1	Total 39	C 28	O 10	P 1	0
17	G	1	Total 36	C 25	O 10	P 1	0
17	G	1	Total 45	C 34	O 10	P 1	0
17	G	1	Total 45	C 34	O 10	P 1	0
17	G	1	Total 47	C 36	O 10	P 1	0
17	G	1	Total 35	C 24	O 10	P 1	0
17	G	1	Total 49	C 38	O 10	P 1	0
17	G	1	Total 49	C 38	O 10	P 1	0
17	G	1	Total 41	C 30	O 10	P 1	0
17	H	1	Total 39	C 28	O 10	P 1	0
17	H	1	Total 44	C 33	O 10	P 1	0
17	S	1	Total 44	C 33	O 10	P 1	0
17	V	1	Total 38	C 27	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
17	V	1	Total	C	O	P	0
			41	30	10	1	
17	V	1	Total	C	O	P	0
			49	38	10	1	
17	e	1	Total	C	O	P	0
			39	28	10	1	
17	e	1	Total	C	O	P	0
			36	25	10	1	
17	e	1	Total	C	O	P	0
			45	34	10	1	
17	e	1	Total	C	O	P	0
			45	34	10	1	
17	e	1	Total	C	O	P	0
			47	36	10	1	
17	e	1	Total	C	O	P	0
			35	24	10	1	
17	e	1	Total	C	O	P	0
			49	38	10	1	
17	e	1	Total	C	O	P	0
			49	38	10	1	
17	e	1	Total	C	O	P	0
			41	30	10	1	
17	f	1	Total	C	O	P	0
			39	28	10	1	
17	f	1	Total	C	O	P	0
			44	33	10	1	
17	k	1	Total	C	O	P	0
			44	33	10	1	
17	n	1	Total	C	O	P	0
			38	27	10	1	
17	n	1	Total	C	O	P	0
			41	30	10	1	
17	n	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 18 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



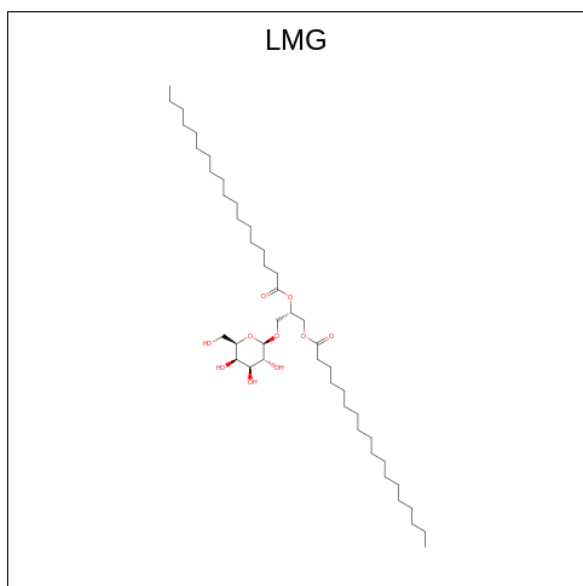
Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			35	24	11	
18	A	1	Total	C	O	0
			23	17	6	
18	B	1	Total	C	O	0
			35	24	11	
18	J	1	Total	C	O	0
			22	16	6	
18	1	1	Total	C	O	0
			19	13	6	
18	2	1	Total	C	O	0
			23	17	6	
18	G	1	Total	C	O	0
			35	24	11	
18	G	1	Total	C	O	0
			23	17	6	
18	H	1	Total	C	O	0
			35	24	11	
18	T	1	Total	C	O	0
			22	16	6	
18	Y	1	Total	C	O	0
			19	13	6	
18	Z	1	Total	C	O	0
			23	17	6	
18	e	1	Total	C	O	0
			35	24	11	
18	e	1	Total	C	O	0
			23	17	6	

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Mol	Chain	Residues	Atoms			AltConf
18	f	1	Total	C	O	0
			35	24	11	
18	l	1	Total	C	O	0
			22	16	6	
18	q	1	Total	C	O	0
			19	13	6	
18	r	1	Total	C	O	0
			23	17	6	

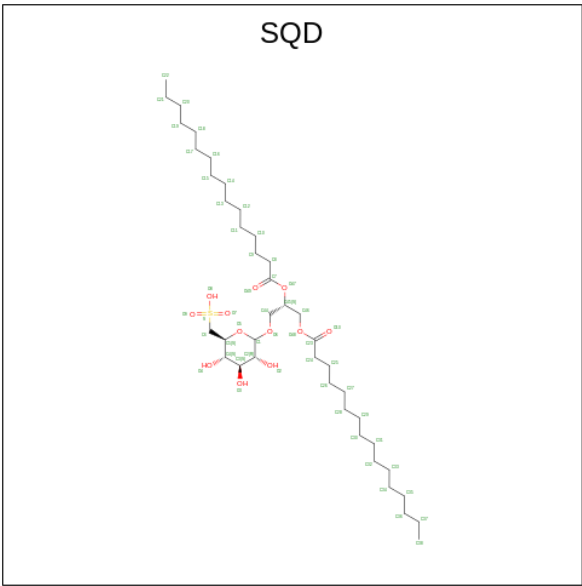
- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
19	B	1	Total	C	O	0
			54	44	10	
19	J	1	Total	C	O	0
			35	25	10	
19	H	1	Total	C	O	0
			54	44	10	
19	T	1	Total	C	O	0
			35	25	10	
19	f	1	Total	C	O	0
			54	44	10	
19	l	1	Total	C	O	0
			35	25	10	

- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				AltConf
20	B	1	Total	C	O	S	0
			45	32	12	1	
20	L	1	Total	C	O	S	0
			51	38	12	1	
20	1	1	Total	C	O	S	0
			48	35	12	1	
20	2	1	Total	C	O	S	0
			43	30	12	1	
20	3	1	Total	C	O	S	0
			43	30	12	1	
20	4	1	Total	C	O	S	0
			26	13	12	1	
20	5	1	Total	C	O	S	0
			29	16	12	1	
20	6	1	Total	C	O	S	0
			26	13	12	1	
20	H	1	Total	C	O	S	0
			45	32	12	1	
20	V	1	Total	C	O	S	0
			51	38	12	1	
20	Y	1	Total	C	O	S	0
			48	35	12	1	
20	Z	1	Total	C	O	S	0
			43	30	12	1	
20	a	1	Total	C	O	S	0
			43	30	12	1	

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Mol	Chain	Residues	Atoms				AltConf
20	b	1	Total	C	O	S	0
			26	13	12	1	
20	c	1	Total	C	O	S	0
			29	16	12	1	
20	d	1	Total	C	O	S	0
			26	13	12	1	
20	f	1	Total	C	O	S	0
			45	32	12	1	
20	n	1	Total	C	O	S	0
			51	38	12	1	
20	q	1	Total	C	O	S	0
			48	35	12	1	
20	r	1	Total	C	O	S	0
			43	30	12	1	
20	s	1	Total	C	O	S	0
			43	30	12	1	
20	t	1	Total	C	O	S	0
			26	13	12	1	
20	u	1	Total	C	O	S	0
			29	16	12	1	
20	v	1	Total	C	O	S	0
			26	13	12	1	

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	A	9	Total	O	0
			9	9	
21	B	7	Total	O	0
			7	7	
21	F	1	Total	O	0
			1	1	
21	L	1	Total	O	0
			1	1	
21	G	9	Total	O	0
			9	9	
21	H	7	Total	O	0
			7	7	
21	R	1	Total	O	0
			1	1	
21	V	1	Total	O	0
			1	1	

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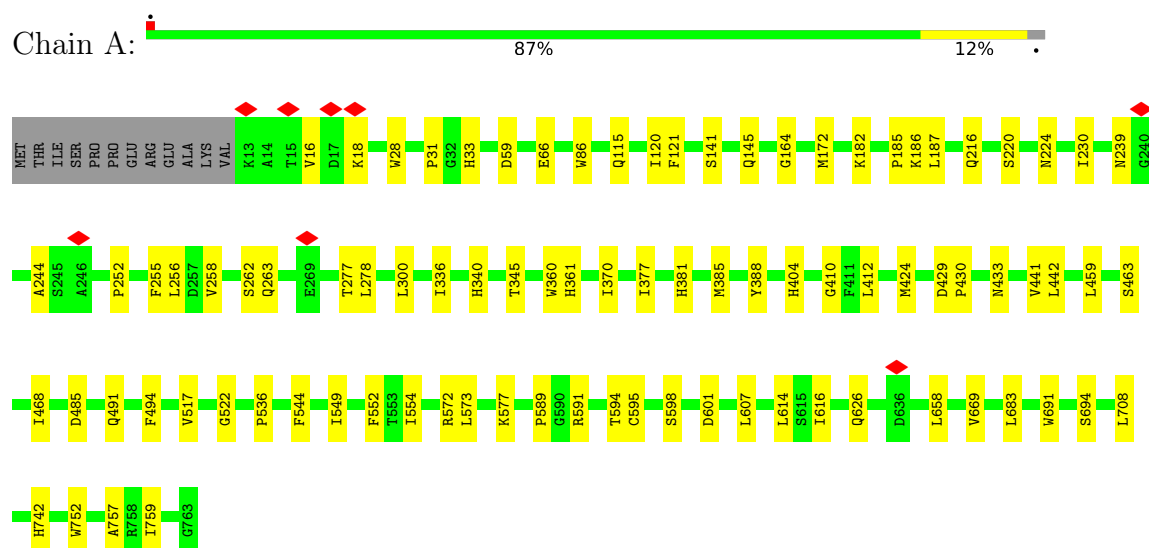
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Mol	Chain	Residues	Atoms		AltConf
21	e	9	Total 9	O 9	0
21	f	7	Total 7	O 7	0
21	j	1	Total 1	O 1	0
21	n	1	Total 1	O 1	0

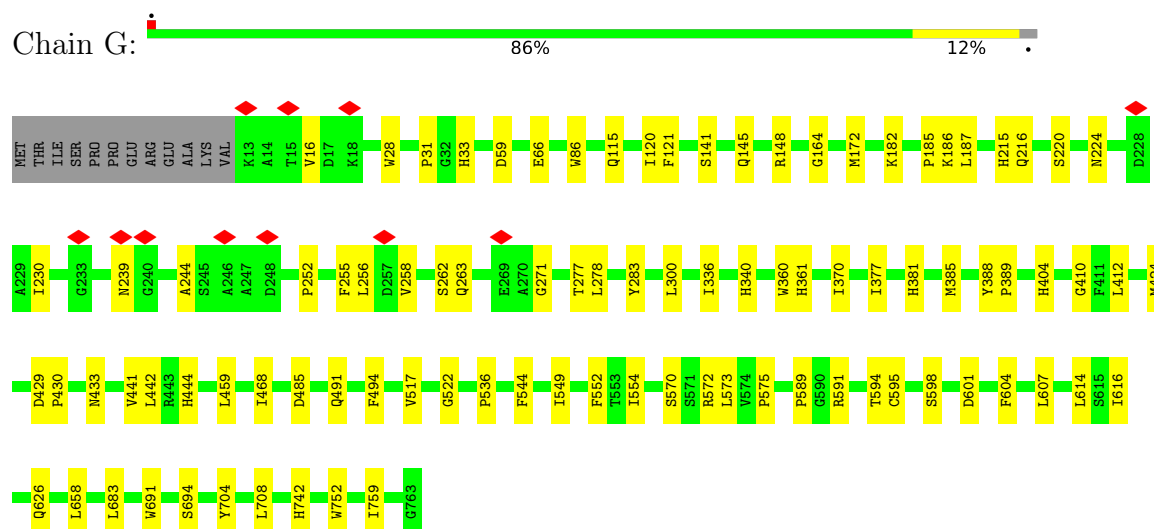
3 Residue-property plots

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

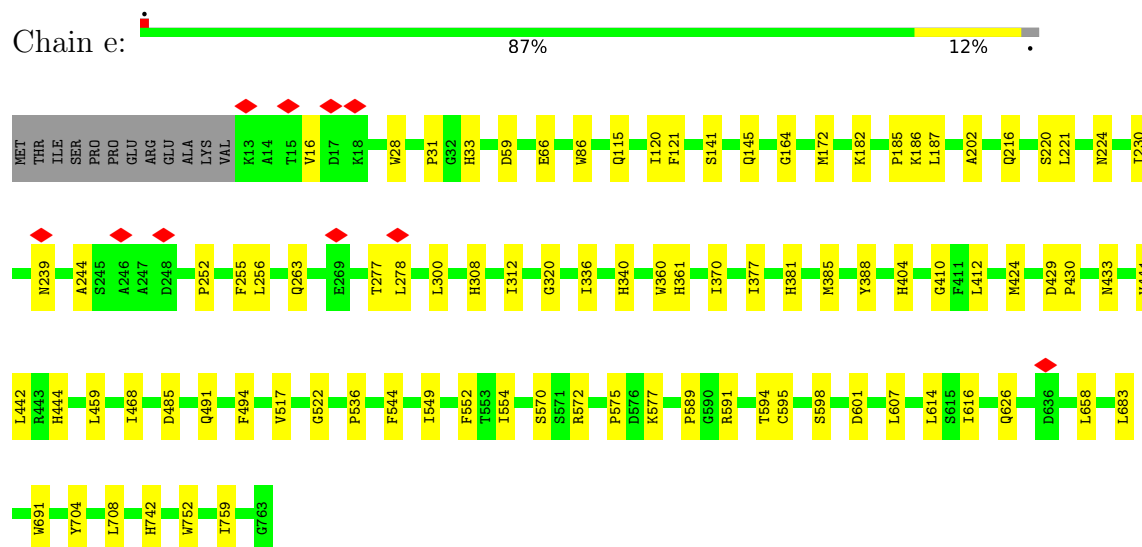
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



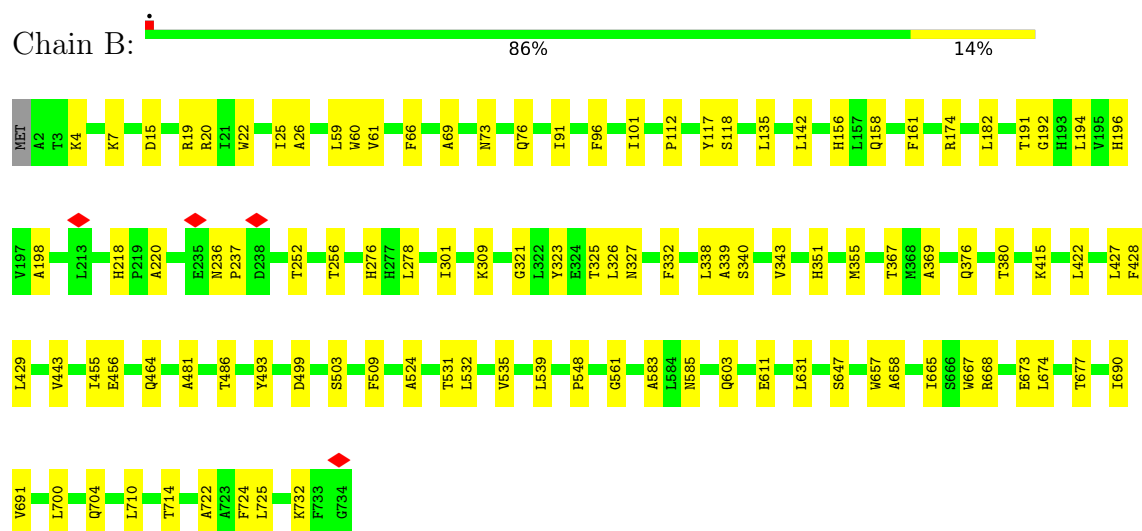
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



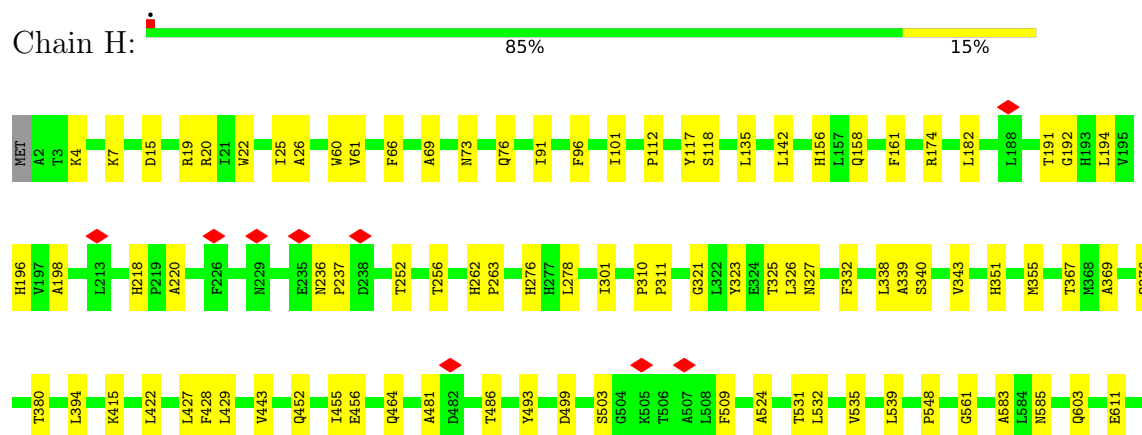
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain f: 85% 14%



- Molecule 3: Photosystem I iron-sulfur center

Chain C: 80% 19%



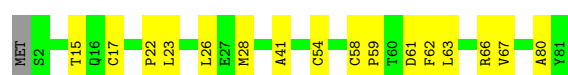
- Molecule 3: Photosystem I iron-sulfur center

Chain N: 81% 17%



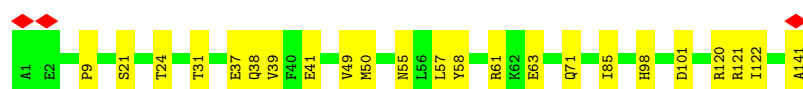
- Molecule 3: Photosystem I iron-sulfur center

Chain g: 79% 20%



- Molecule 4: Photosystem I reaction center subunit II

Chain D: 84% 16%



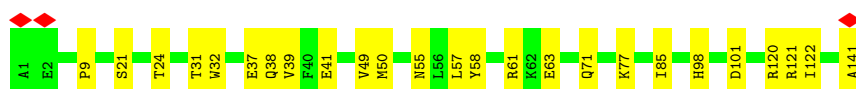
- Molecule 4: Photosystem I reaction center subunit II

Chain O:  84% 16%



- Molecule 4: Photosystem I reaction center subunit II

Chain h:  82% 18%



- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  5% 89% 5% 5%



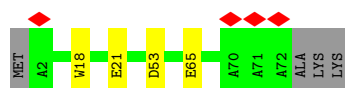
- Molecule 5: Photosystem I reaction center subunit IV

Chain Q:  5% 89% 5% 5%



- Molecule 5: Photosystem I reaction center subunit IV

Chain i:  5% 89% 5% 5%



- Molecule 6: Photosystem I reaction center subunit III

Chain F:  76% 9% 14%

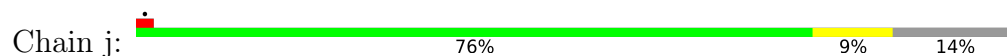


- Molecule 6: Photosystem I reaction center subunit III

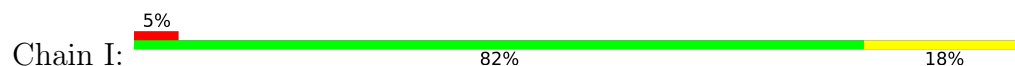
Chain R:  76% 9% 14%



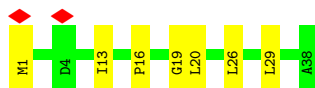
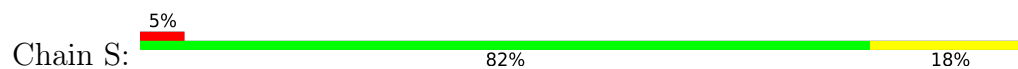
- Molecule 6: Photosystem I reaction center subunit III



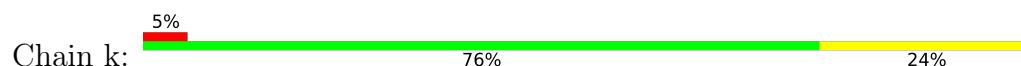
- Molecule 7: Photosystem I PsaI protein



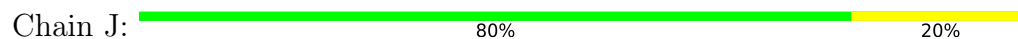
- Molecule 7: Photosystem I PsaI protein



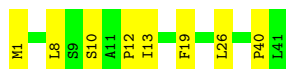
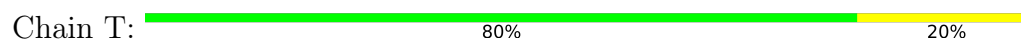
- Molecule 7: Photosystem I PsaI protein



- Molecule 8: Photosystem I reaction center subunit IX

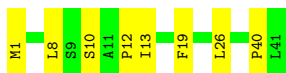


- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX

Chain l:  80% 20%



- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:  15% 75% 18% 7%



- Molecule 9: Photosystem I reaction center subunit PsaK

Chain U:  13% 75% 18% 7%



- Molecule 9: Photosystem I reaction center subunit PsaK

Chain m:  14% 74% 19% 7%



- Molecule 10: Photosystem I reaction center subunit XI

Chain L:  89% 10%



- Molecule 10: Photosystem I reaction center subunit XI

Chain V:  87% 12%



- Molecule 10: Photosystem I reaction center subunit XI

Chain n:  87% 12%



- Molecule 11: PsaM

Chain M:  86% 14%



- Molecule 11: PsaM

Chain W:  86% 14%



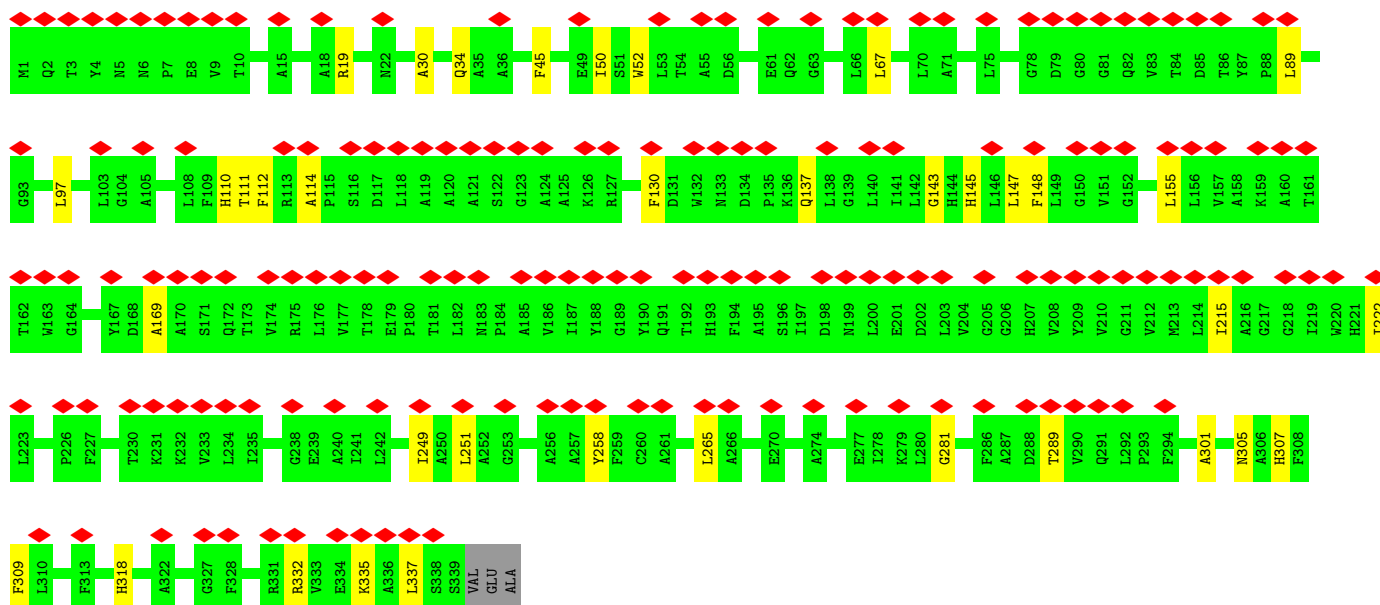
- Molecule 11: PsaM

Chain o:  86% 14%



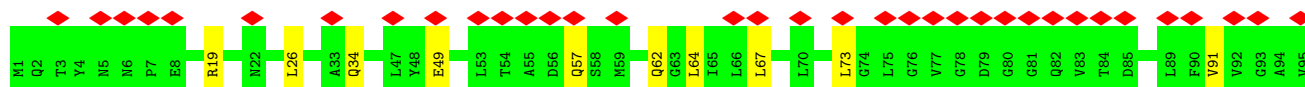
- Molecule 12: Iron stress-induced chlorophyll-binding protein

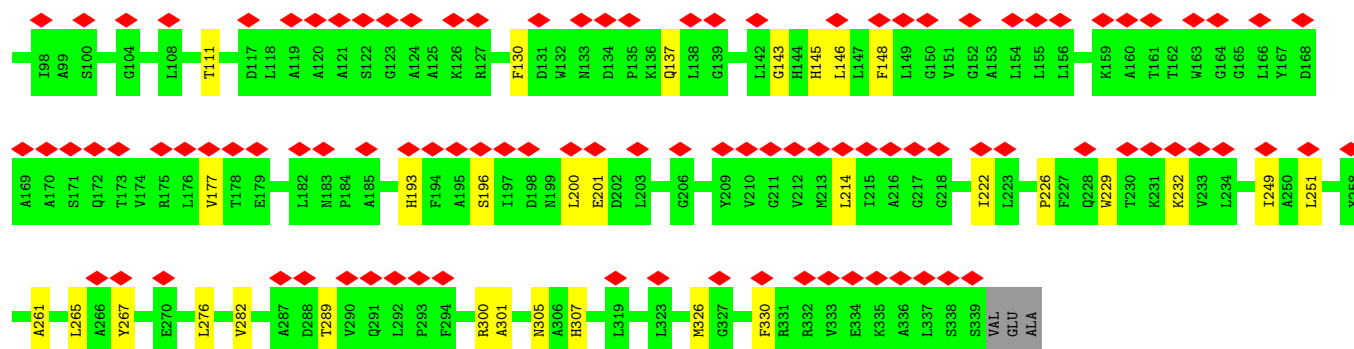
Chain 1:  49% 88% 11%



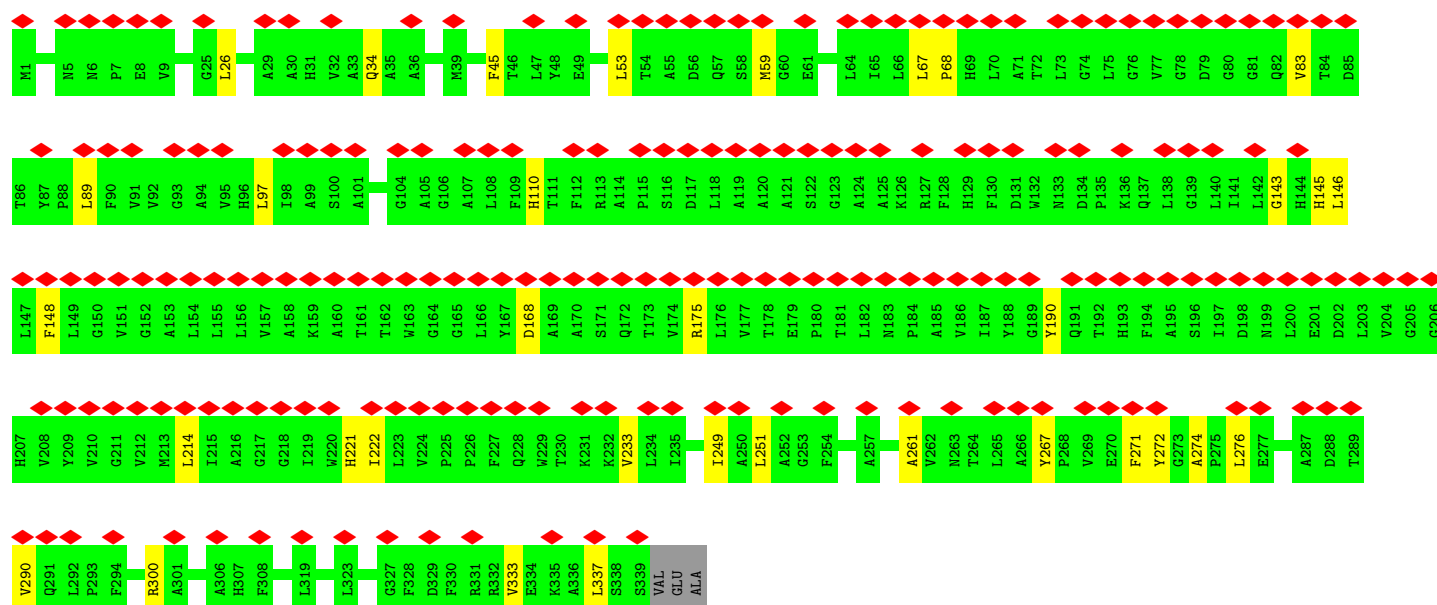
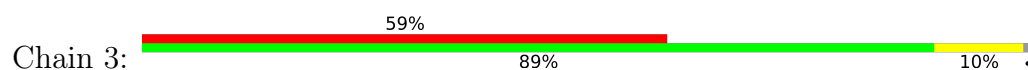
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain 2:  40% 87% 12%

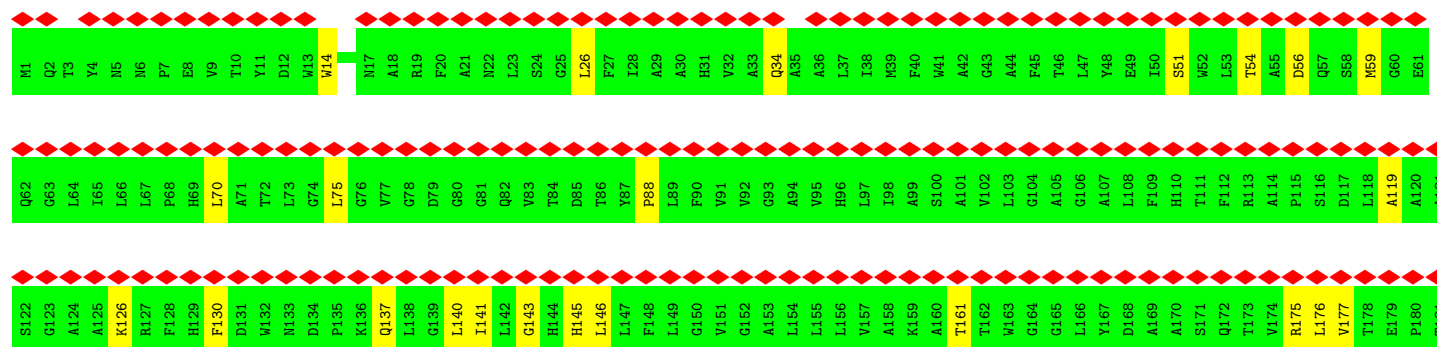
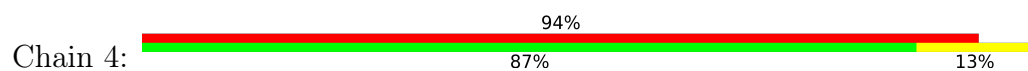


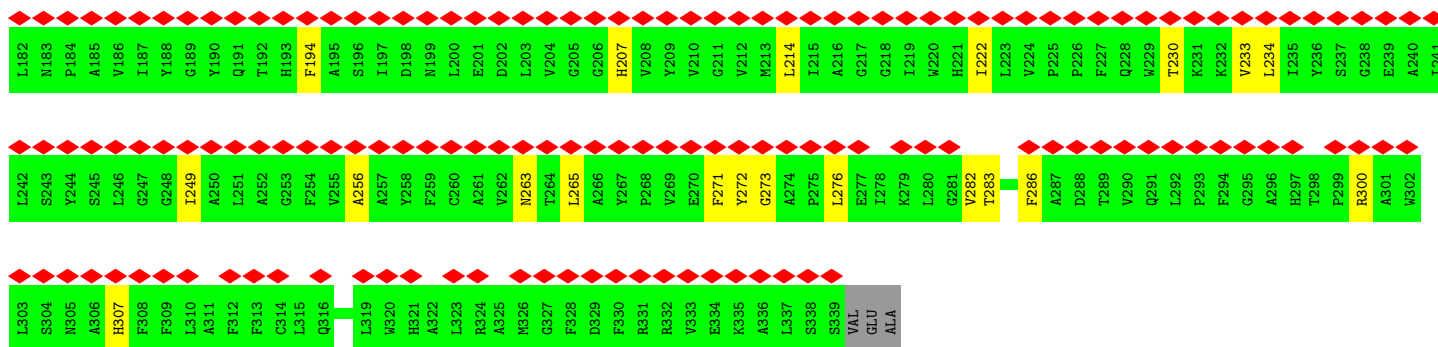


• Molecule 12: Iron stress-induced chlorophyll-binding protein



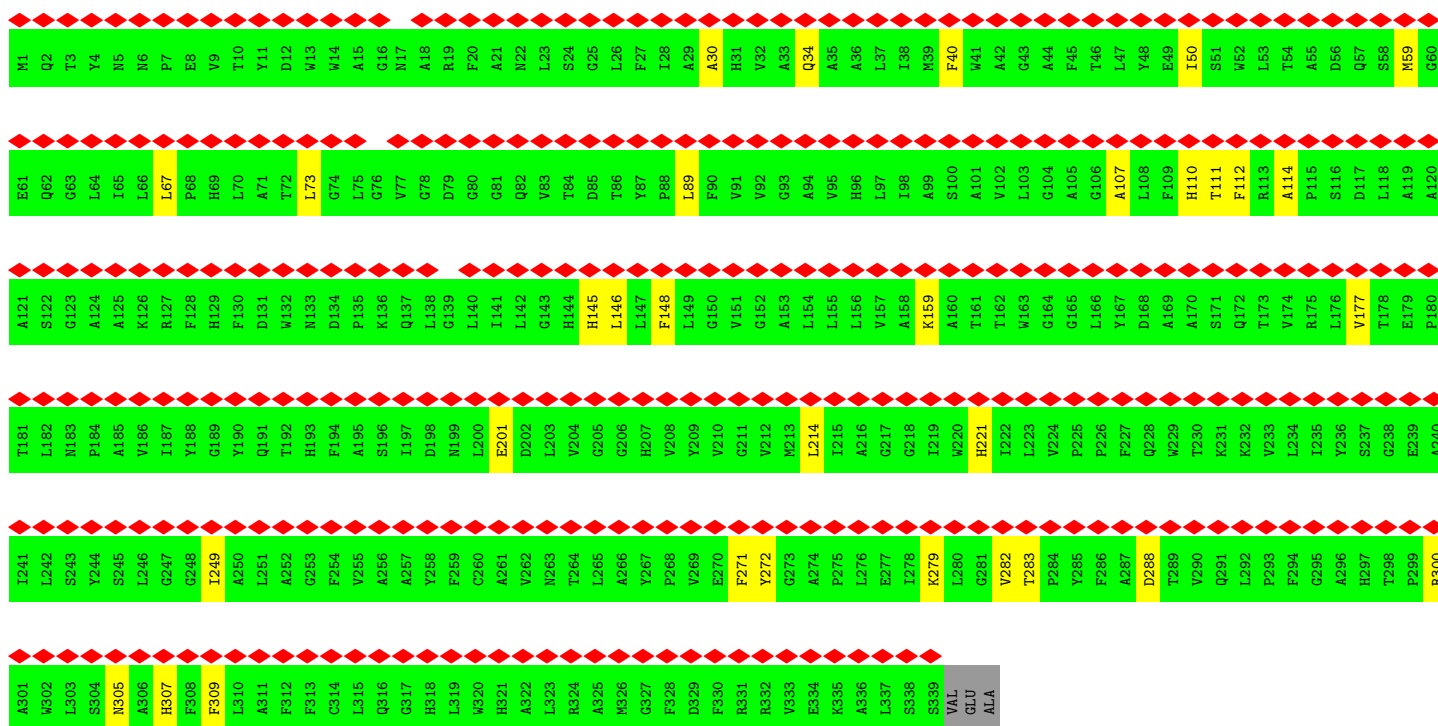
• Molecule 12: Iron stress-induced chlorophyll-binding protein





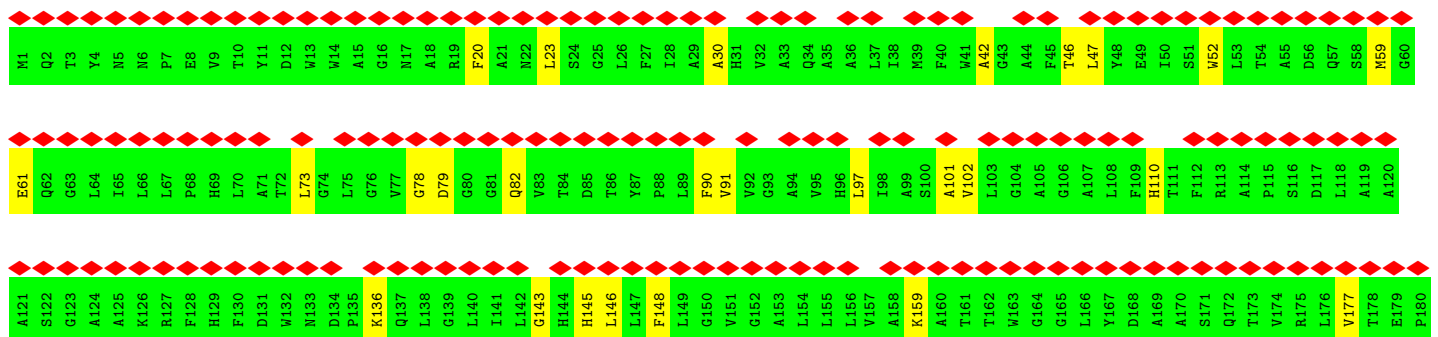
• Molecule 12: Iron stress-induced chlorophyll-binding protein

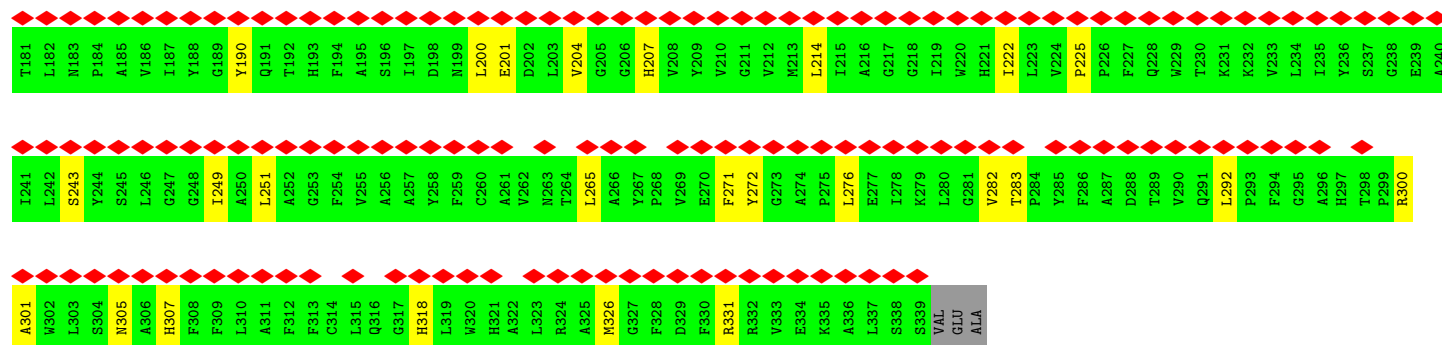
Chain 5: .



• Molecule 12: Iron stress-induced chlorophyll-binding protein

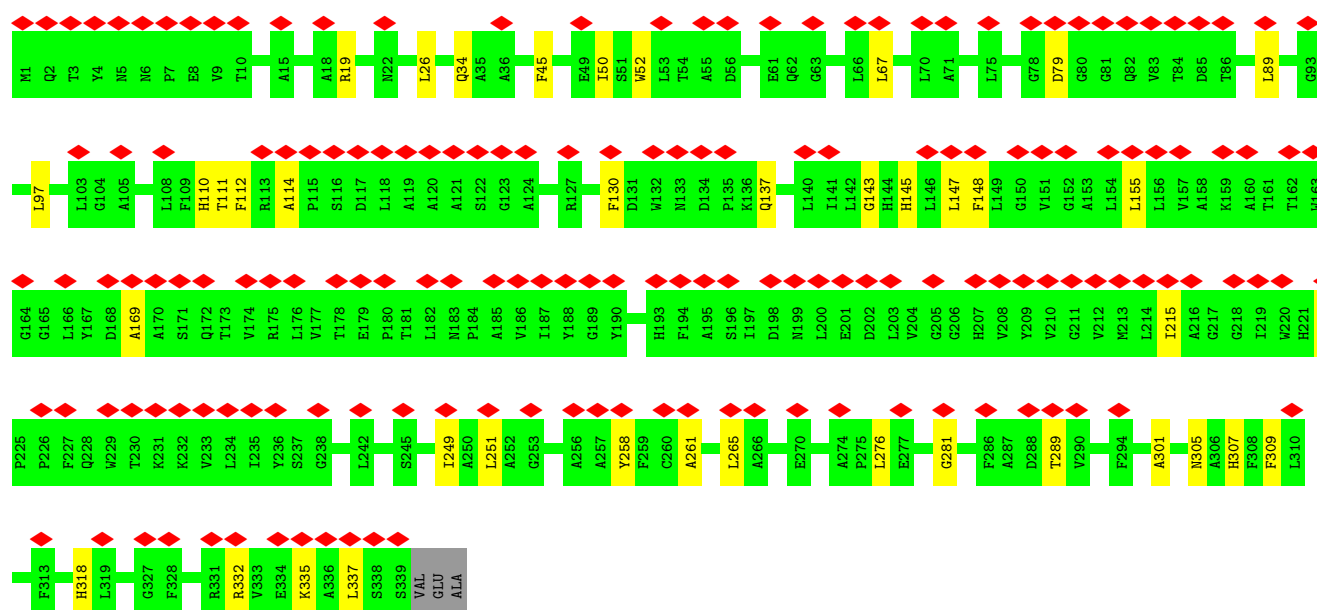
Chain 6: .





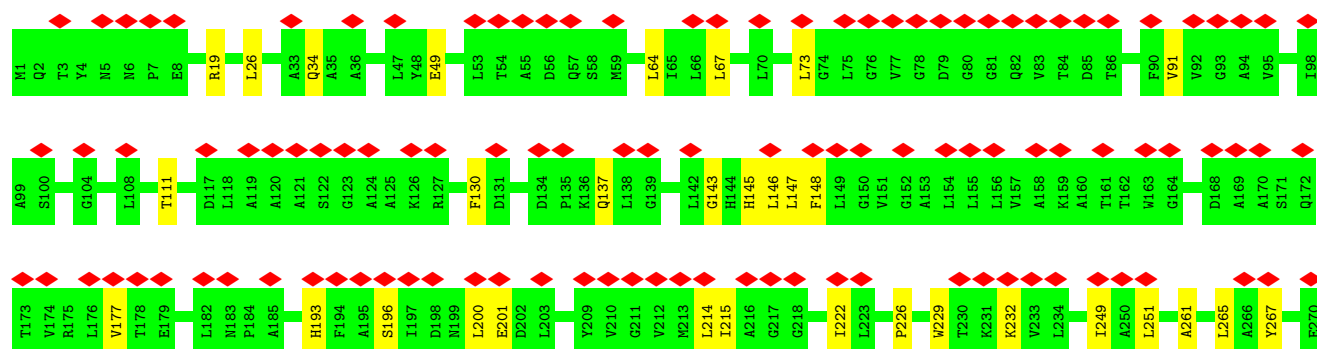
• Molecule 12: Iron stress-induced chlorophyll-binding protein

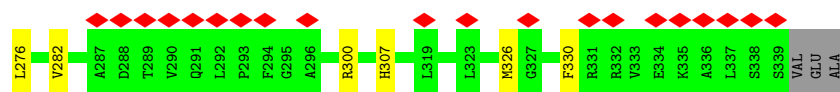
Chain Y: 49% 87% 12% .



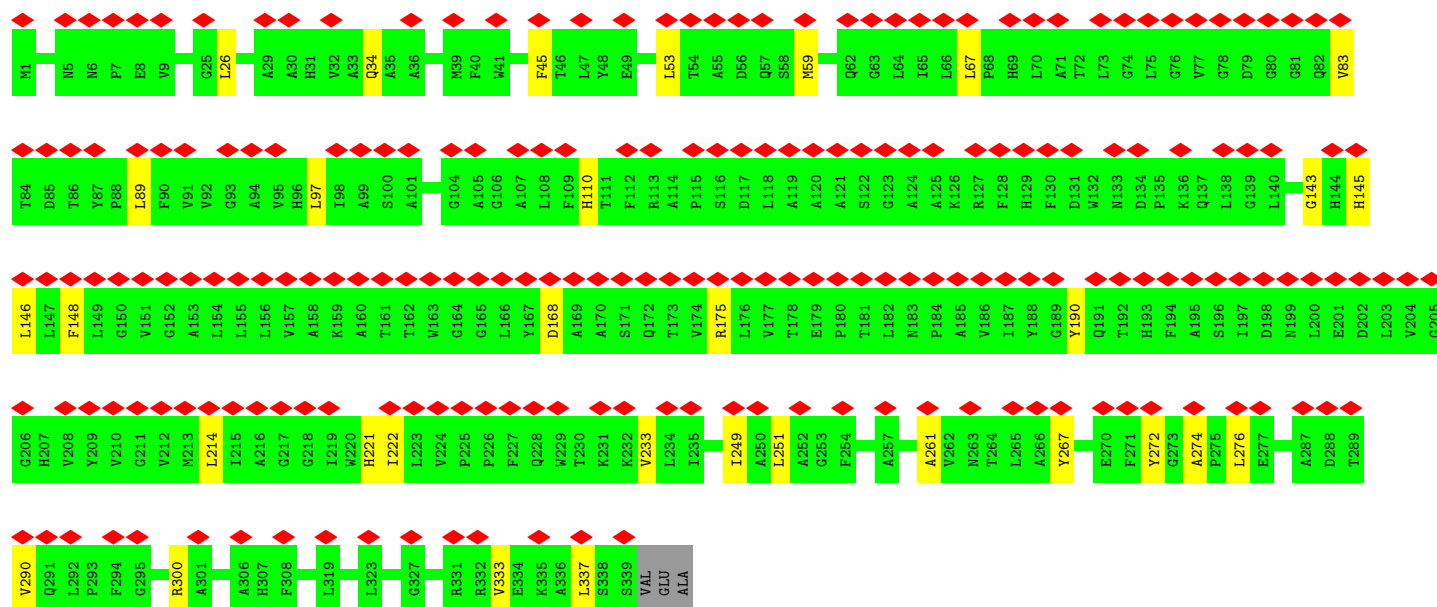
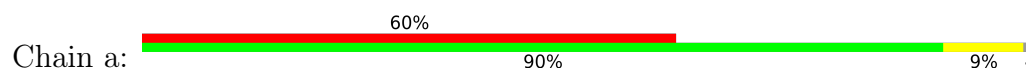
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain Z: 38% 88% 11% .

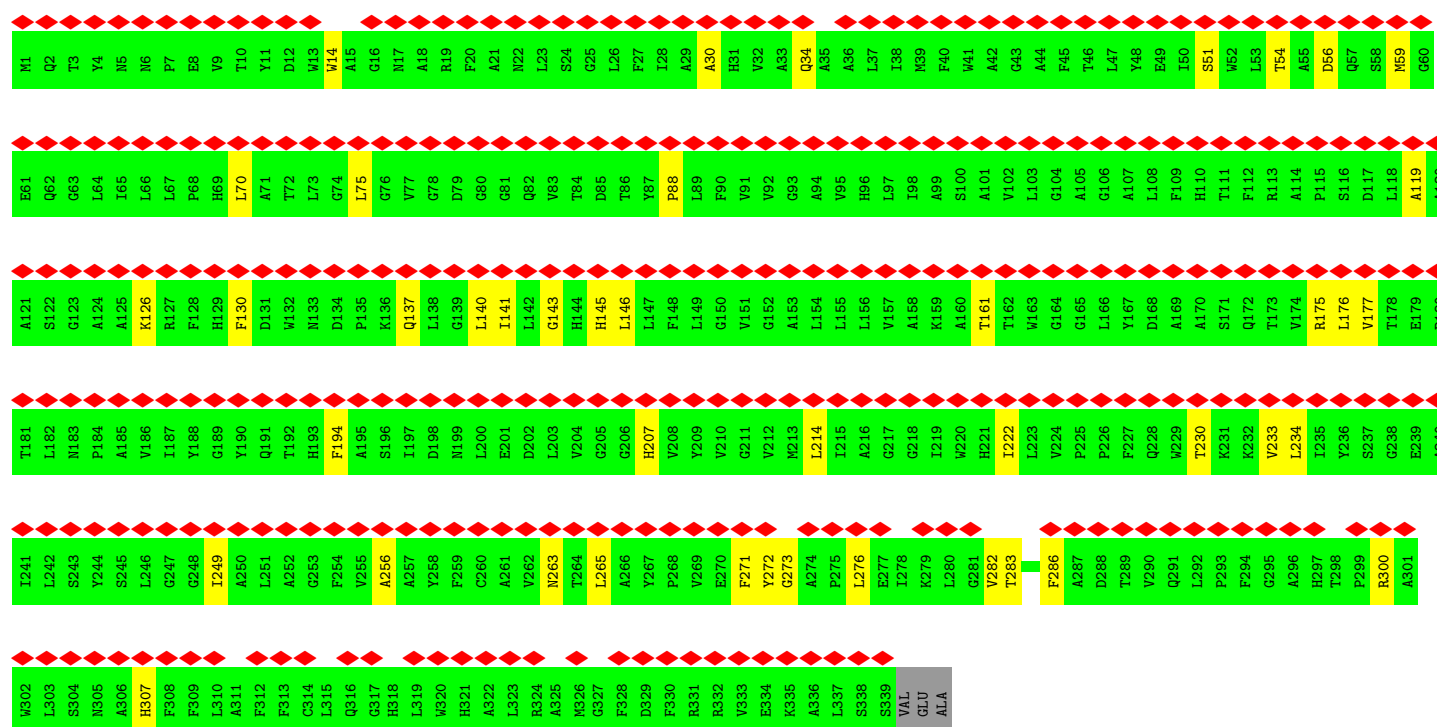
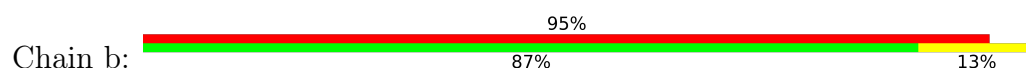




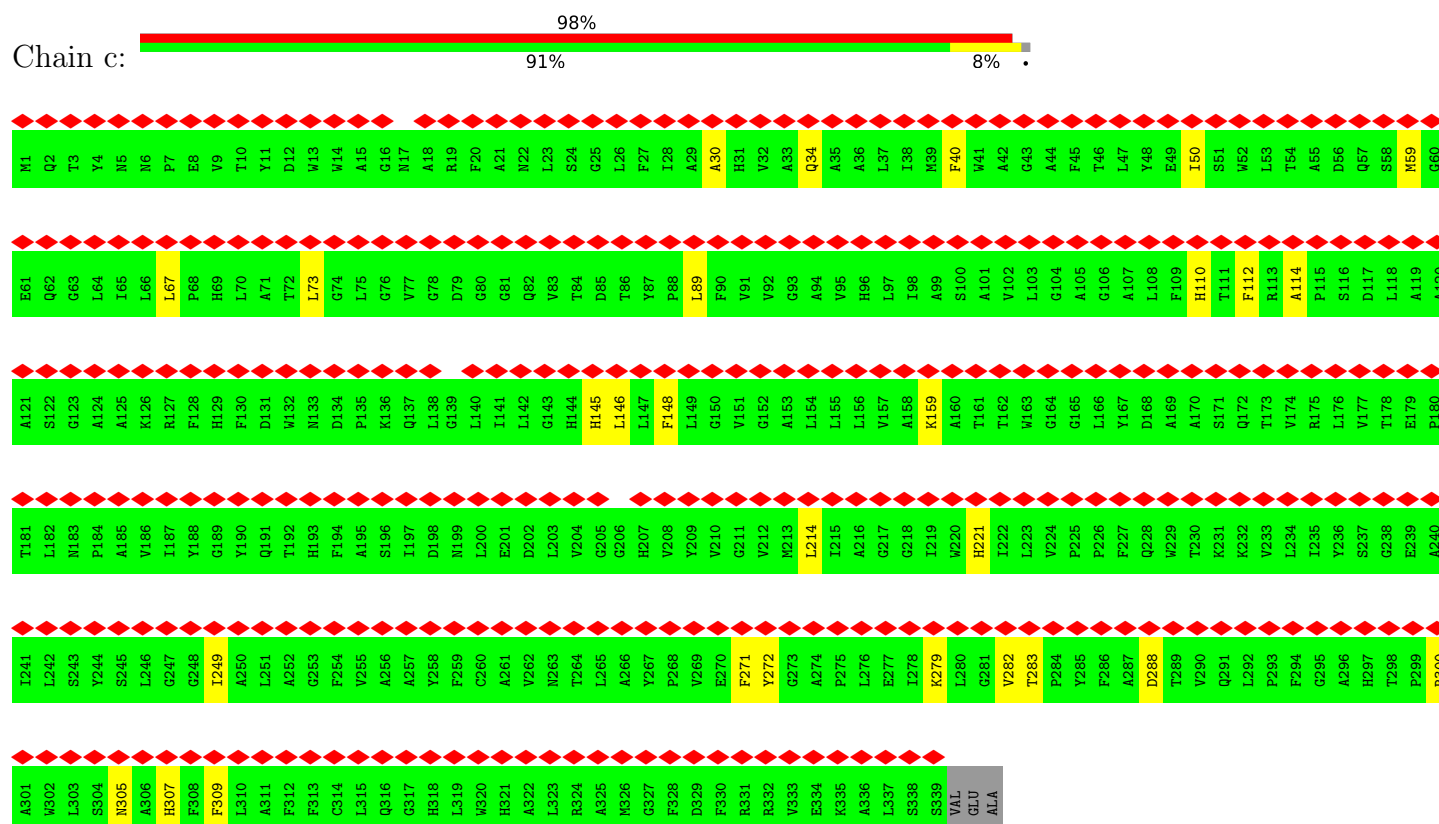
• Molecule 12: Iron stress-induced chlorophyll-binding protein



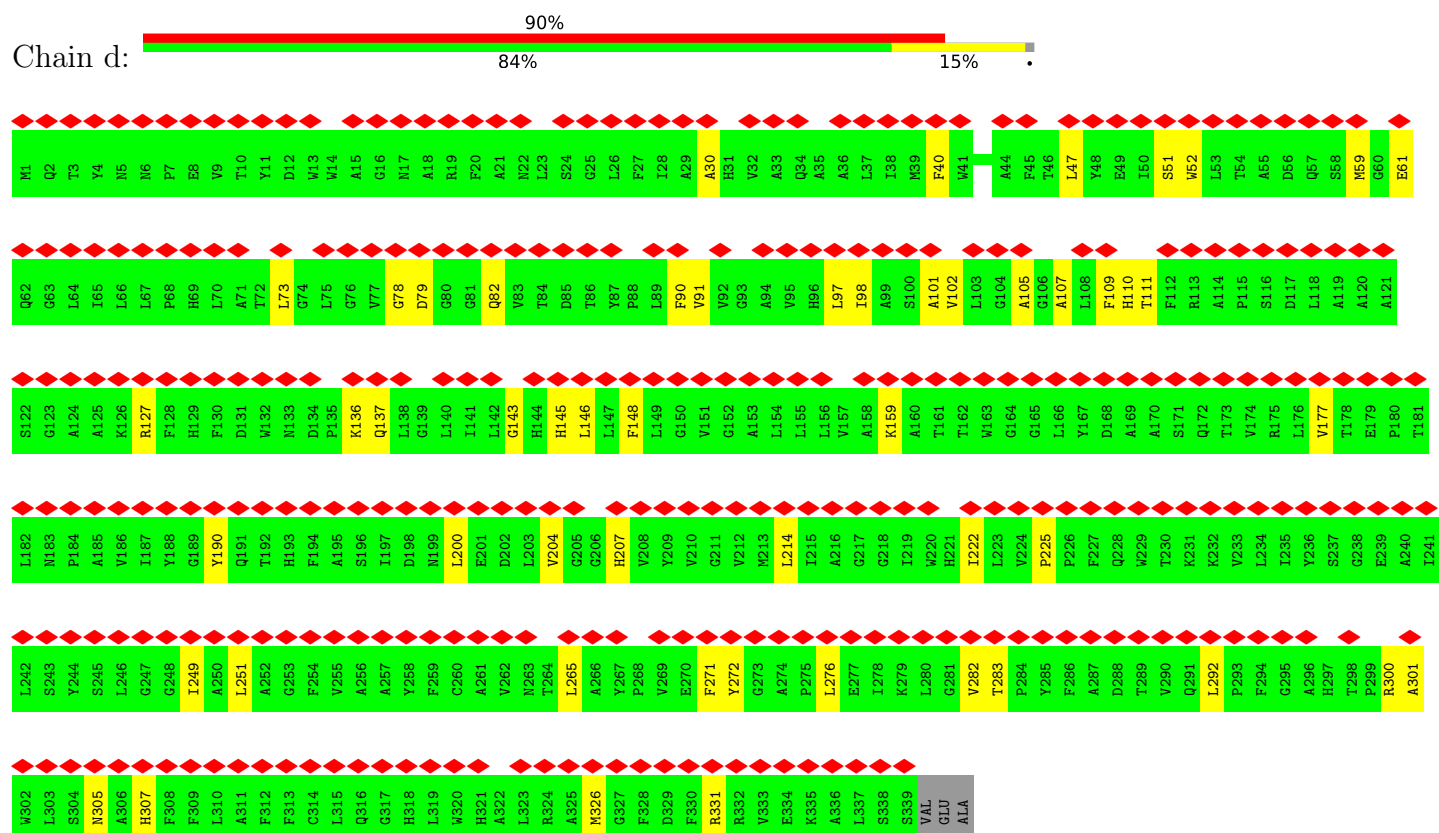
• Molecule 12: Iron stress-induced chlorophyll-binding protein



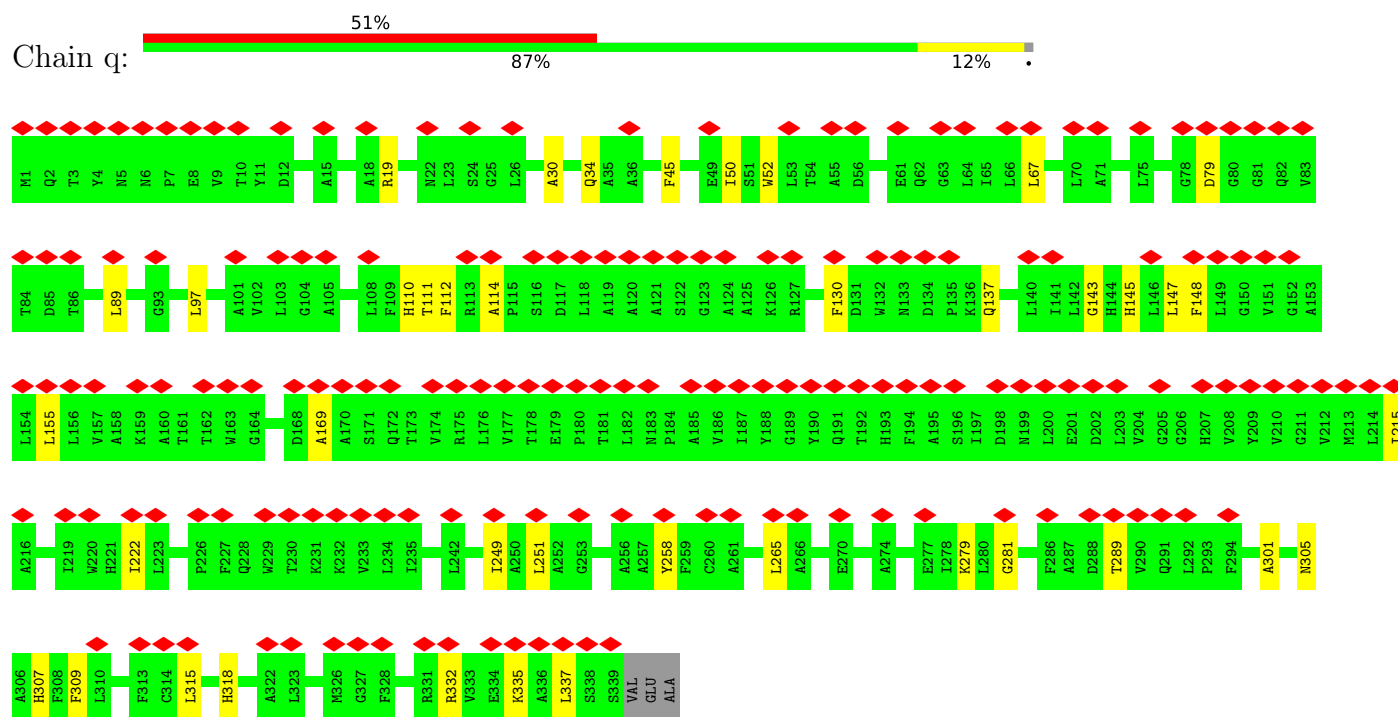
• Molecule 12: Iron stress-induced chlorophyll-binding protein



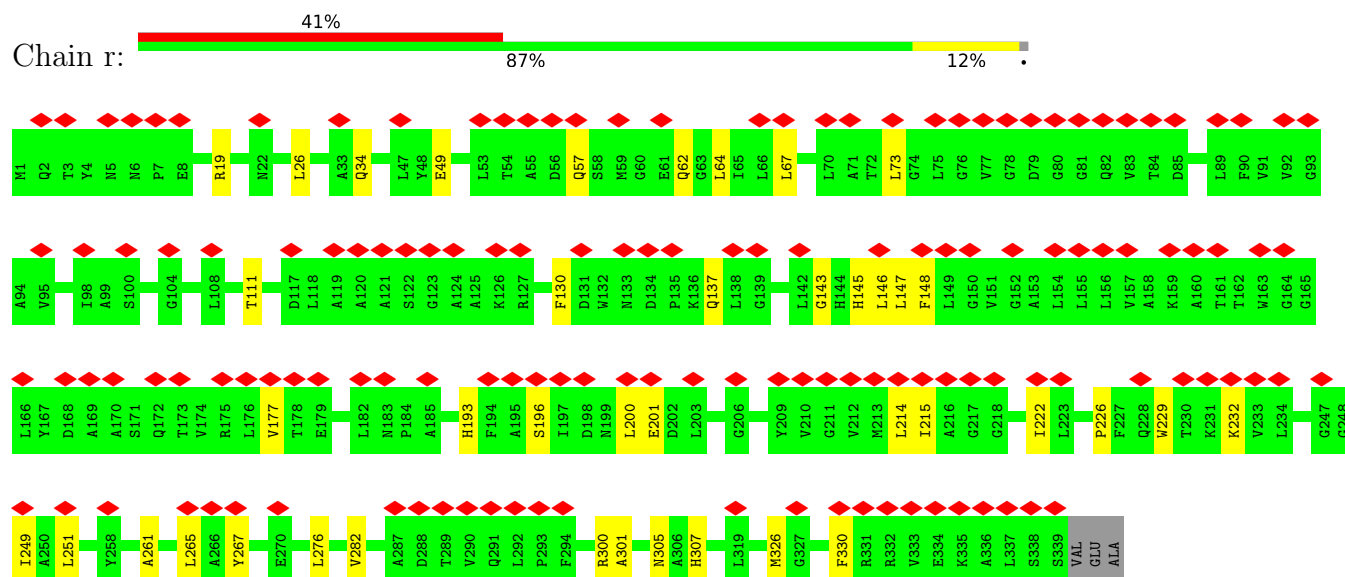
• Molecule 12: Iron stress-induced chlorophyll-binding protein



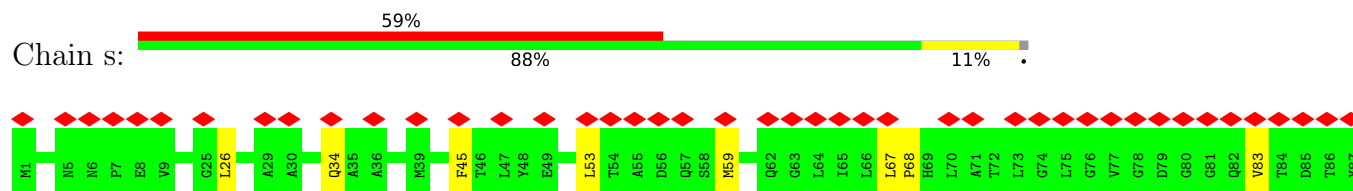
• Molecule 12: Iron stress-induced chlorophyll-binding protein

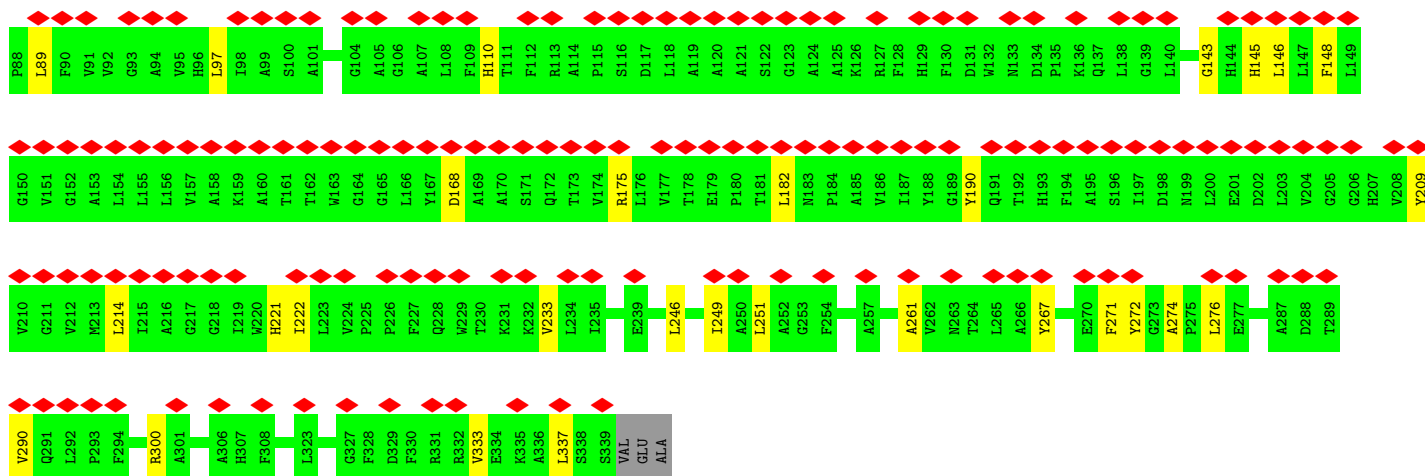


• Molecule 12: Iron stress-induced chlorophyll-binding protein

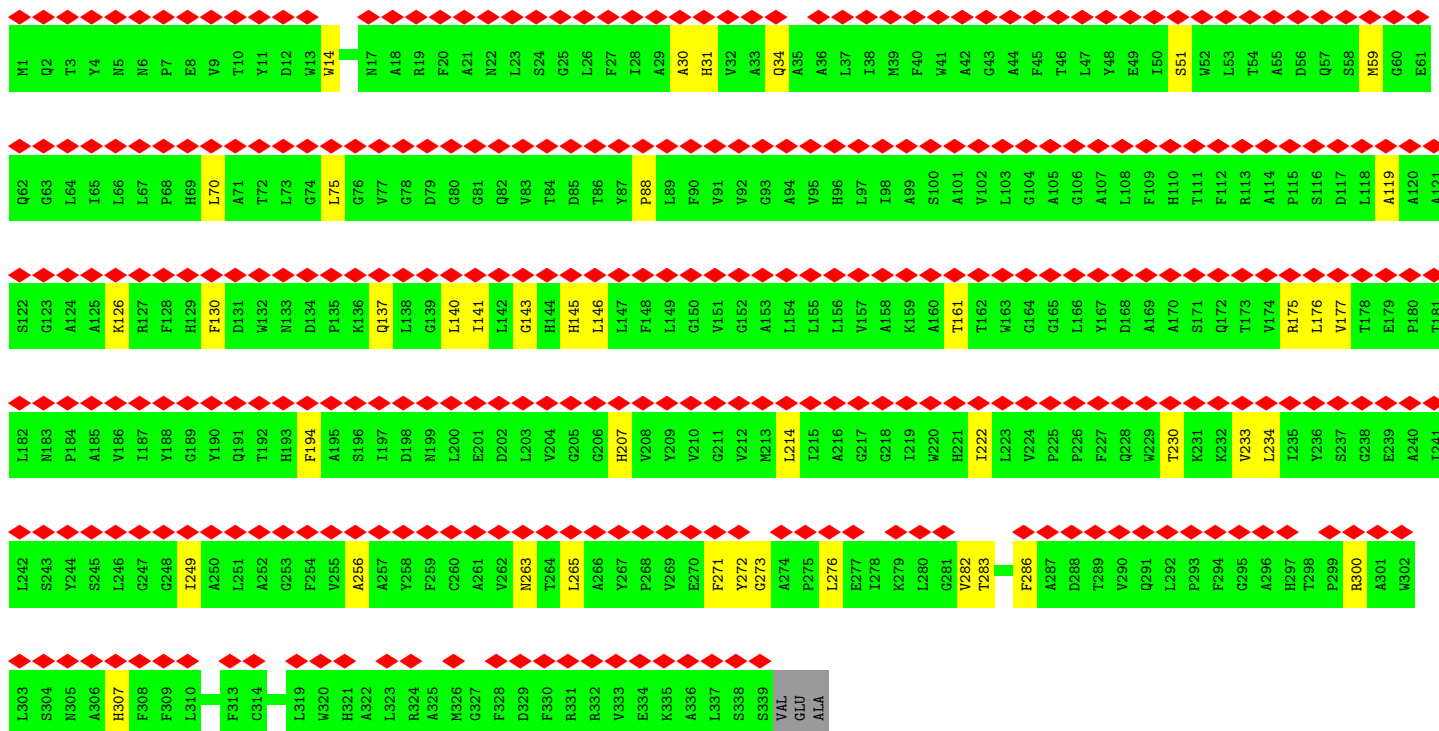
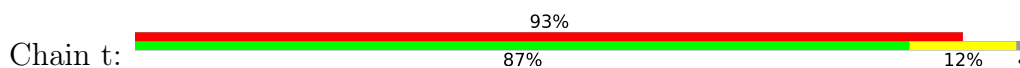


• Molecule 12: Iron stress-induced chlorophyll-binding protein

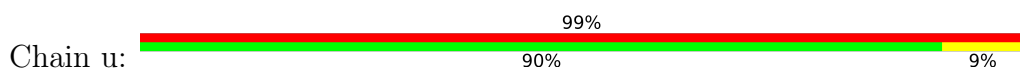


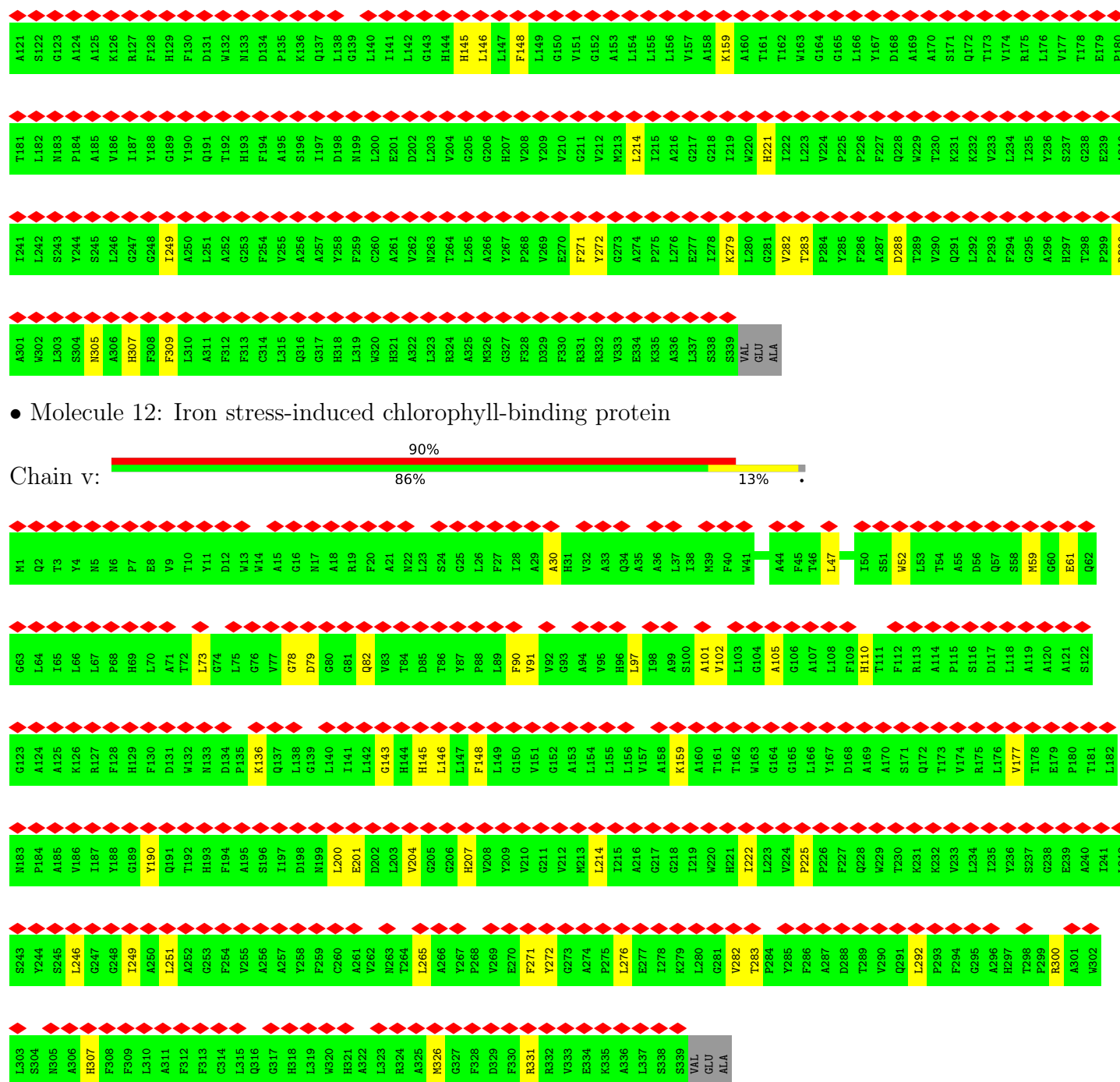


• Molecule 12: Iron stress-induced chlorophyll-binding protein



• Molecule 12: Iron stress-induced chlorophyll-binding protein





- Molecule 12: Iron stress-induced chlorophyll-binding protein

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	63332	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.170	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/6064	0.51	0/8274
1	G	0.37	0/6064	0.51	0/8274
1	e	0.37	0/6064	0.51	0/8274
2	B	0.37	0/5999	0.53	2/8199 (0.0%)
2	H	0.37	0/5999	0.53	2/8199 (0.0%)
2	f	0.37	0/5999	0.53	2/8199 (0.0%)
3	C	0.38	0/608	0.57	0/823
3	N	0.39	0/608	0.56	0/823
3	g	0.39	0/608	0.56	0/823
4	D	0.29	0/1124	0.47	0/1516
4	O	0.30	0/1124	0.47	0/1516
4	h	0.30	0/1124	0.47	0/1516
5	E	0.27	0/553	0.41	0/750
5	Q	0.27	0/553	0.41	0/750
5	i	0.27	0/553	0.42	0/750
6	F	0.30	0/1062	0.50	0/1442
6	R	0.30	0/1062	0.50	0/1442
6	j	0.30	0/1062	0.50	0/1442
7	I	0.33	0/289	0.60	0/393
7	S	0.33	0/289	0.60	0/393
7	k	0.33	0/289	0.60	0/393
8	J	0.37	0/346	0.51	0/469
8	T	0.37	0/346	0.51	0/469
8	l	0.37	0/346	0.51	0/469
9	K	0.27	0/560	0.54	0/765
9	U	0.27	0/560	0.54	0/765
9	m	0.27	0/560	0.54	0/765
10	L	0.28	0/1242	0.49	0/1696
10	V	0.28	0/1242	0.49	0/1696
10	n	0.28	0/1242	0.49	0/1696
11	M	0.33	0/231	0.53	0/314
11	W	0.33	0/231	0.53	0/314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	o	0.33	0/231	0.53	0/314
12	1	0.20	0/2689	0.42	0/3678
12	2	0.19	0/2689	0.41	0/3678
12	3	0.18	0/2689	0.39	0/3678
12	4	0.18	0/2689	0.41	0/3678
12	5	0.17	0/2689	0.40	2/3678 (0.1%)
12	6	0.16	0/2689	0.39	0/3678
12	Y	0.21	0/2689	0.42	0/3678
12	Z	0.20	0/2689	0.41	0/3678
12	a	0.18	0/2689	0.39	0/3678
12	b	0.18	0/2689	0.41	0/3678
12	c	0.17	0/2689	0.40	2/3678 (0.1%)
12	d	0.17	0/2689	0.39	0/3678
12	q	0.21	0/2689	0.42	0/3678
12	r	0.20	0/2689	0.41	0/3678
12	s	0.18	0/2689	0.39	0/3678
12	t	0.18	0/2689	0.40	0/3678
12	u	0.17	0/2689	0.40	2/3678 (0.1%)
12	v	0.17	0/2689	0.39	0/3678
All	All	0.28	0/102636	0.46	12/140127 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	665	ILE	N-CA-C	9.10	119.65	110.82
2	f	665	ILE	N-CA-C	9.10	119.65	110.82
2	H	665	ILE	N-CA-C	9.07	119.62	110.82
2	B	668	ARG	N-CA-C	8.15	120.16	111.28
2	f	668	ARG	N-CA-C	8.13	120.14	111.28

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	A	5865	0	5744	70	0
1	G	5865	0	5744	73	0
1	e	5865	0	5744	71	0
2	B	5789	0	5575	83	0
2	H	5789	0	5575	83	0
2	f	5789	0	5575	83	0
3	C	598	0	579	10	0
3	N	598	0	579	9	0
3	g	598	0	579	11	0
4	D	1098	0	1099	16	0
4	O	1098	0	1099	16	0
4	h	1098	0	1099	17	0
5	E	543	0	525	3	0
5	Q	543	0	525	3	0
5	i	543	0	525	3	0
6	F	1036	0	1031	12	0
6	R	1036	0	1031	12	0
6	j	1036	0	1031	12	0
7	I	282	0	291	10	0
7	S	282	0	291	11	0
7	k	282	0	291	11	0
8	J	335	0	344	8	0
8	T	335	0	344	8	0
8	l	335	0	344	8	0
9	K	549	0	597	13	0
9	U	549	0	597	13	0
9	m	549	0	597	13	0
10	L	1210	0	1206	15	0
10	V	1210	0	1206	17	0
10	n	1210	0	1206	16	0
11	M	228	0	246	4	0
11	W	228	0	246	4	0
11	o	228	0	246	4	0
12	1	2605	0	2564	34	0
12	2	2605	0	2564	34	0
12	3	2605	0	2564	26	0
12	4	2605	0	2564	35	0
12	5	2605	0	2564	28	0
12	6	2605	0	2564	38	0
12	Y	2605	0	2564	36	0
12	Z	2605	0	2564	32	0
12	a	2605	0	2564	25	0
12	b	2605	0	2564	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	c	2605	0	2564	26	0
12	d	2605	0	2564	54	0
12	q	2605	0	2564	36	0
12	r	2605	0	2564	33	0
12	s	2605	0	2564	28	0
12	t	2605	0	2564	35	0
12	u	2605	0	2564	27	0
12	v	2605	0	2564	38	0
13	1	951	0	894	39	0
13	2	993	0	981	34	0
13	3	950	0	900	24	0
13	4	860	0	725	20	0
13	5	857	0	721	20	0
13	6	823	0	658	21	0
13	A	2728	0	2800	99	0
13	B	2550	0	2680	93	0
13	F	110	0	105	4	0
13	G	2728	0	2800	102	0
13	H	2550	0	2680	97	0
13	J	123	0	127	5	0
13	K	150	0	121	4	0
13	L	190	0	203	10	0
13	R	110	0	105	3	0
13	T	123	0	127	3	0
13	U	150	0	121	4	0
13	V	190	0	203	11	0
13	Y	951	0	894	36	0
13	Z	993	0	981	35	0
13	a	950	0	900	23	0
13	b	860	0	725	18	0
13	c	857	0	721	21	0
13	d	823	0	658	20	0
13	e	2728	0	2800	110	0
13	f	2550	0	2680	95	0
13	j	110	0	105	4	0
13	l	123	0	127	4	0
13	m	150	0	121	4	0
13	n	190	0	203	11	0
13	q	951	0	894	57	0
13	r	993	0	981	37	0
13	s	950	0	900	22	0
13	t	860	0	725	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	u	857	0	721	23	0
13	v	823	0	658	18	0
14	A	33	0	46	3	0
14	B	33	0	46	2	0
14	G	33	0	46	3	0
14	H	33	0	46	4	0
14	e	33	0	46	2	0
14	f	33	0	46	3	0
15	A	8	0	0	0	0
15	C	16	0	0	1	0
15	G	8	0	0	0	0
15	N	16	0	0	1	0
15	e	8	0	0	0	0
15	g	16	0	0	1	0
16	1	160	0	224	11	0
16	2	160	0	224	13	0
16	3	160	0	224	14	0
16	4	160	0	224	6	0
16	5	160	0	224	9	0
16	6	160	0	224	16	0
16	A	240	0	336	18	0
16	B	280	0	392	29	0
16	F	40	0	56	5	0
16	G	240	0	336	17	0
16	H	280	0	392	23	0
16	I	40	0	56	3	0
16	J	120	0	168	12	0
16	K	40	0	56	7	0
16	L	160	0	224	12	0
16	M	40	0	56	2	0
16	R	40	0	56	4	0
16	S	40	0	56	5	0
16	T	120	0	168	16	0
16	U	40	0	56	6	0
16	V	160	0	224	15	0
16	W	40	0	56	4	0
16	Y	160	0	224	13	0
16	Z	160	0	224	10	0
16	a	160	0	224	13	0
16	b	160	0	224	8	0
16	c	160	0	224	11	0
16	d	160	0	224	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	e	240	0	336	17	0
16	f	280	0	392	26	0
16	j	40	0	56	3	0
16	k	40	0	56	4	0
16	l	120	0	168	14	0
16	m	40	0	56	5	0
16	n	160	0	224	15	0
16	o	40	0	56	4	0
16	q	160	0	224	11	0
16	r	160	0	224	13	0
16	s	160	0	224	11	0
16	t	160	0	224	9	0
16	u	160	0	224	12	0
16	v	160	0	224	15	0
17	A	386	0	520	19	0
17	B	83	0	109	4	0
17	G	386	0	520	17	0
17	H	83	0	109	5	0
17	I	44	0	58	1	0
17	L	128	0	172	13	0
17	S	44	0	58	0	0
17	V	128	0	172	11	0
17	e	386	0	520	20	0
17	f	83	0	109	4	0
17	k	44	0	58	1	0
17	n	128	0	172	12	0
18	1	19	0	22	0	0
18	2	23	0	30	0	0
18	A	58	0	76	1	0
18	B	35	0	46	0	0
18	G	58	0	76	0	0
18	H	35	0	46	0	0
18	J	22	0	28	2	0
18	T	22	0	28	2	0
18	Y	19	0	22	0	0
18	Z	23	0	30	0	0
18	e	58	0	76	1	0
18	f	35	0	46	0	0
18	l	22	0	28	2	0
18	q	19	0	22	0	0
18	r	23	0	30	0	0
19	B	54	0	81	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	H	54	0	81	7	0
19	J	35	0	40	0	0
19	T	35	0	40	0	0
19	f	54	0	81	7	0
19	l	35	0	40	0	0
20	1	48	0	63	4	0
20	2	43	0	49	1	0
20	3	43	0	50	1	0
20	4	26	0	16	0	0
20	5	29	0	22	0	0
20	6	26	0	16	1	0
20	B	45	0	53	7	0
20	H	45	0	53	10	0
20	L	51	0	69	4	0
20	V	51	0	69	3	0
20	Y	48	0	63	5	0
20	Z	43	0	49	1	0
20	a	43	0	50	1	0
20	b	26	0	16	0	0
20	c	29	0	22	0	0
20	d	26	0	16	1	0
20	f	45	0	53	8	0
20	n	51	0	69	4	0
20	q	48	0	63	4	0
20	r	43	0	49	1	0
20	s	43	0	50	1	0
20	t	26	0	16	0	0
20	u	29	0	22	0	0
20	v	26	0	16	1	0
21	A	9	0	0	0	0
21	B	7	0	0	0	0
21	F	1	0	0	0	0
21	G	9	0	0	0	0
21	H	7	0	0	0	0
21	L	1	0	0	0	0
21	R	1	0	0	0	0
21	V	1	0	0	0	0
21	e	9	0	0	0	0
21	f	7	0	0	0	0
21	j	1	0	0	0	0
21	n	1	0	0	0	0
All	All	143022	0	143508	2193	0

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

The worst 5 of 2193 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:H:1852:SQD:H91	17:e:5002:LHG:C23	2.07	0.84
17:L:5221:LHG:H252	13:f:1207:CLA:H42	1.60	0.83
13:B:1207:CLA:H42	17:V:5221:LHG:H252	1.58	0.83
13:H:1207:CLA:H42	17:n:5221:LHG:H252	1.59	0.83
20:H:1852:SQD:H91	17:e:5002:LHG:O10	1.81	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	749/763 (98%)	723 (96%)	26 (4%)	0	100	100
1	G	749/763 (98%)	723 (96%)	26 (4%)	0	100	100
1	e	749/763 (98%)	723 (96%)	26 (4%)	0	100	100
2	B	731/734 (100%)	711 (97%)	20 (3%)	0	100	100
2	H	731/734 (100%)	711 (97%)	20 (3%)	0	100	100
2	f	731/734 (100%)	711 (97%)	20 (3%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	N	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	g	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
4	O	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
4	h	139/141 (99%)	132 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
5	Q	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
5	i	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
6	F	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
6	R	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
6	j	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
7	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	S	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	k	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
8	T	39/41 (95%)	39 (100%)	0	0	100	100
8	l	39/41 (95%)	39 (100%)	0	0	100	100
9	K	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
9	U	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
9	m	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
10	L	162/166 (98%)	157 (97%)	5 (3%)	0	100	100
10	V	162/166 (98%)	157 (97%)	5 (3%)	0	100	100
10	n	162/166 (98%)	157 (97%)	5 (3%)	0	100	100
11	M	27/29 (93%)	27 (100%)	0	0	100	100
11	W	27/29 (93%)	27 (100%)	0	0	100	100
11	o	27/29 (93%)	27 (100%)	0	0	100	100
12	1	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	2	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	3	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	4	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
12	5	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	6	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	Y	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	Z	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	a	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	b	337/342 (98%)	327 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	c	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	d	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	q	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	r	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	s	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	t	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
12	u	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	v	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
All	All	12786/13089 (98%)	12420 (97%)	366 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	600/611 (98%)	600 (100%)	0	100	100
1	G	600/611 (98%)	600 (100%)	0	100	100
1	e	600/611 (98%)	600 (100%)	0	100	100
2	B	583/584 (100%)	582 (100%)	1 (0%)	87	96
2	H	583/584 (100%)	582 (100%)	1 (0%)	87	96
2	f	583/584 (100%)	582 (100%)	1 (0%)	87	96
3	C	67/68 (98%)	67 (100%)	0	100	100
3	N	67/68 (98%)	67 (100%)	0	100	100
3	g	67/68 (98%)	67 (100%)	0	100	100
4	D	114/114 (100%)	114 (100%)	0	100	100
4	O	114/114 (100%)	114 (100%)	0	100	100
4	h	114/114 (100%)	114 (100%)	0	100	100
5	E	56/59 (95%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Q	56/59 (95%)	56 (100%)	0	100	100
5	i	56/59 (95%)	56 (100%)	0	100	100
6	F	105/121 (87%)	105 (100%)	0	100	100
6	R	105/121 (87%)	105 (100%)	0	100	100
6	j	105/121 (87%)	105 (100%)	0	100	100
7	I	30/30 (100%)	30 (100%)	0	100	100
7	S	30/30 (100%)	30 (100%)	0	100	100
7	k	30/30 (100%)	30 (100%)	0	100	100
8	J	35/35 (100%)	35 (100%)	0	100	100
8	T	35/35 (100%)	35 (100%)	0	100	100
8	l	35/35 (100%)	35 (100%)	0	100	100
9	K	56/61 (92%)	56 (100%)	0	100	100
9	U	56/61 (92%)	56 (100%)	0	100	100
9	m	56/61 (92%)	56 (100%)	0	100	100
10	L	127/128 (99%)	127 (100%)	0	100	100
10	V	127/128 (99%)	127 (100%)	0	100	100
10	n	127/128 (99%)	127 (100%)	0	100	100
11	M	24/24 (100%)	24 (100%)	0	100	100
11	W	24/24 (100%)	24 (100%)	0	100	100
11	o	24/24 (100%)	24 (100%)	0	100	100
12	1	257/259 (99%)	257 (100%)	0	100	100
12	2	257/259 (99%)	257 (100%)	0	100	100
12	3	257/259 (99%)	257 (100%)	0	100	100
12	4	257/259 (99%)	257 (100%)	0	100	100
12	5	257/259 (99%)	257 (100%)	0	100	100
12	6	257/259 (99%)	257 (100%)	0	100	100
12	Y	257/259 (99%)	257 (100%)	0	100	100
12	Z	257/259 (99%)	257 (100%)	0	100	100
12	a	257/259 (99%)	257 (100%)	0	100	100
12	b	257/259 (99%)	257 (100%)	0	100	100
12	c	257/259 (99%)	257 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	d	257/259 (99%)	257 (100%)	0	100	100
12	q	257/259 (99%)	257 (100%)	0	100	100
12	r	257/259 (99%)	257 (100%)	0	100	100
12	s	257/259 (99%)	257 (100%)	0	100	100
12	t	257/259 (99%)	257 (100%)	0	100	100
12	u	257/259 (99%)	257 (100%)	0	100	100
12	v	257/259 (99%)	257 (100%)	0	100	100
All	All	10017/10167 (98%)	10014 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	443	VAL
2	H	443	VAL
2	f	443	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 116 such sidechains are listed below:

Mol	Chain	Res	Type
8	T	39	HIS
12	u	207	HIS
12	c	291	GLN
12	u	133	ASN
12	q	207	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

846 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$
13	CLA	Y	501	12	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)
20	SQD	b	822	-	25,26,54	1.31	4 (16%)	34,37,65	1.85	9 (26%)
13	CLA	l	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.44	8 (11%)
13	CLA	f	1232	21	54,58,73	1.39	11 (20%)	65,95,113	1.60	7 (10%)
17	LHG	I	5001	-	43,43,48	0.64	0	46,49,54	1.22	4 (8%)
16	BCR	n	4022	-	41,41,41	0.75	0	56,56,56	1.90	15 (26%)
13	CLA	f	1205	2	69,73,73	1.24	10 (14%)	83,113,113	1.42	8 (9%)
16	BCR	F	4016	-	41,41,41	0.74	0	56,56,56	1.78	13 (23%)
13	CLA	G	1129	1	55,59,73	1.38	9 (16%)	66,96,113	1.53	10 (15%)
16	BCR	r	521	-	41,41,41	0.66	0	56,56,56	1.86	11 (19%)
13	CLA	c	505	12	65,69,73	1.28	8 (12%)	78,108,113	1.27	4 (5%)
13	CLA	A	1117	1	69,73,73	1.22	11 (15%)	83,113,113	1.56	12 (14%)
18	LMU	A	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.00	1 (3%)
13	CLA	u	516	12	49,53,73	1.48	8 (16%)	59,89,113	1.45	4 (6%)
16	BCR	4	522	-	41,41,41	0.74	0	56,56,56	1.85	18 (32%)
13	CLA	Y	505	12	69,73,73	1.24	8 (11%)	83,113,113	1.27	5 (6%)
17	LHG	e	5009	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
16	BCR	v	523	-	41,41,41	0.70	0	56,56,56	1.73	14 (25%)
13	CLA	5	512	12	49,53,73	1.47	9 (18%)	59,89,113	1.46	5 (8%)
13	CLA	B	1223	2	69,73,73	1.25	9 (13%)	83,113,113	1.40	6 (7%)
13	CLA	d	510	12	49,53,73	1.49	8 (16%)	59,89,113	1.41	5 (8%)
13	CLA	a	511	12	54,58,73	1.43	9 (16%)	65,95,113	1.49	5 (7%)
13	CLA	A	1107	1	69,73,73	1.25	11 (15%)	83,113,113	1.35	10 (12%)
16	BCR	f	4005	-	41,41,41	0.70	0	56,56,56	1.78	11 (19%)
13	CLA	d	519	12	50,54,73	1.47	8 (16%)	60,90,113	1.45	4 (6%)
13	CLA	Y	510	12	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	Z	522	-	41,41,41	0.71	0	56,56,56	1.75	18 (32%)
13	CLA	A	1112	1	54,58,73	1.37	9 (16%)	65,95,113	1.58	10 (15%)
13	CLA	5	513	12	49,53,73	1.49	10 (20%)	59,89,113	1.43	4 (6%)
17	LHG	G	5003	13	40,40,48	0.74	0	43,46,54	1.34	6 (13%)
13	CLA	A	1122	1	64,68,73	1.28	9 (14%)	77,107,113	1.43	8 (10%)
13	CLA	H	1210	2	69,73,73	1.25	9 (13%)	83,113,113	1.41	11 (13%)
13	CLA	v	506	12	49,53,73	1.50	10 (20%)	59,89,113	1.48	6 (10%)
16	BCR	T	4015	-	41,41,41	0.78	0	56,56,56	1.82	14 (25%)
13	CLA	4	504	-	49,53,73	1.48	7 (14%)	59,89,113	1.47	5 (8%)
13	CLA	4	517	-	49,53,73	1.50	8 (16%)	59,89,113	1.51	6 (10%)
18	LMU	T	5105	-	22,22,36	1.14	1 (4%)	27,27,47	0.81	0
13	CLA	e	1115	1	64,68,73	1.25	9 (14%)	77,107,113	1.47	9 (11%)
16	BCR	a	521	-	41,41,41	0.68	0	56,56,56	1.75	10 (17%)
13	CLA	f	1228	2	59,63,73	1.31	9 (15%)	71,101,113	1.49	9 (12%)
13	CLA	A	1123	21	69,73,73	1.23	9 (13%)	83,113,113	1.36	9 (10%)
13	CLA	B	1218	2	64,68,73	1.27	9 (14%)	77,107,113	1.38	6 (7%)
13	CLA	G	1131	1	69,73,73	1.22	9 (13%)	83,113,113	1.35	7 (8%)
16	BCR	s	523	-	41,41,41	0.69	0	56,56,56	1.76	15 (26%)
13	CLA	6	502	12	54,58,73	1.41	8 (14%)	65,95,113	1.48	5 (7%)
13	CLA	G	1105	1	59,63,73	1.30	10 (16%)	71,101,113	1.52	10 (14%)
13	CLA	G	1114	21	54,58,73	1.42	9 (16%)	65,95,113	1.50	7 (10%)
13	CLA	e	1104	1	69,73,73	1.23	10 (14%)	83,113,113	1.38	10 (12%)
13	CLA	q	505	12	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
17	LHG	e	5008	-	34,34,48	0.77	1 (2%)	37,40,54	1.28	4 (10%)
20	SQD	4	822	-	25,26,54	1.31	4 (16%)	34,37,65	1.84	9 (26%)
16	BCR	f	4006	-	41,41,41	0.72	0	56,56,56	1.98	20 (35%)
20	SQD	V	5216	-	50,51,54	0.97	5 (10%)	59,62,65	1.64	10 (16%)
13	CLA	v	502	12	54,58,73	1.41	8 (14%)	65,95,113	1.47	4 (6%)
13	CLA	m	1401	-	59,63,73	1.35	10 (16%)	71,101,113	1.46	7 (9%)
13	CLA	H	1219	2	69,73,73	1.25	8 (11%)	83,113,113	1.26	8 (9%)
13	CLA	q	506	12	49,53,73	1.48	8 (16%)	59,89,113	1.47	5 (8%)
13	CLA	Z	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.48	4 (6%)
13	CLA	u	501	12	69,73,73	1.24	9 (13%)	83,113,113	1.37	5 (6%)
13	CLA	V	1502	10	69,73,73	1.23	10 (14%)	83,113,113	1.39	6 (7%)
20	SQD	2	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.61	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	6	509	12	49,53,73	1.49	8 (16%)	59,89,113	1.46	5 (8%)
13	CLA	A	1129	1	55,59,73	1.38	9 (16%)	66,96,113	1.53	10 (15%)
13	CLA	d	508	12	49,53,73	1.48	10 (20%)	59,89,113	1.50	7 (11%)
16	BCR	j	4016	-	41,41,41	0.74	0	56,56,56	1.79	13 (23%)
16	BCR	b	523	-	41,41,41	0.70	0	56,56,56	1.65	12 (21%)
13	CLA	G	1109	1	69,73,73	1.23	9 (13%)	83,113,113	1.41	5 (6%)
13	CLA	e	1106	1	69,73,73	1.21	11 (15%)	83,113,113	1.43	11 (13%)
13	CLA	H	1216	21	64,68,73	1.31	10 (15%)	77,107,113	1.38	5 (6%)
13	CLA	t	511	12	49,53,73	1.51	9 (18%)	59,89,113	1.54	7 (11%)
13	CLA	G	1101	1	69,73,73	1.27	10 (14%)	83,113,113	1.40	8 (9%)
13	CLA	u	512	12	49,53,73	1.48	9 (18%)	59,89,113	1.47	5 (8%)
16	BCR	r	522	-	41,41,41	0.70	0	56,56,56	1.75	17 (30%)
20	SQD	u	822	-	28,29,54	1.26	5 (17%)	37,40,65	1.92	13 (35%)
13	CLA	q	516	12	49,53,73	1.48	8 (16%)	59,89,113	1.65	8 (13%)
19	LMG	l	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.24	7 (16%)
13	CLA	3	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.44	4 (6%)
16	BCR	c	521	-	41,41,41	0.69	0	56,56,56	1.94	16 (28%)
13	CLA	b	506	12	49,53,73	1.49	9 (18%)	59,89,113	1.49	4 (6%)
16	BCR	e	4001	-	41,41,41	0.76	0	56,56,56	1.72	11 (19%)
16	BCR	t	524	-	41,41,41	0.68	0	56,56,56	1.84	15 (26%)
13	CLA	3	510	12	69,73,73	1.25	8 (11%)	83,113,113	1.35	9 (10%)
13	CLA	G	1110	1	55,59,73	1.40	10 (18%)	66,96,113	1.48	6 (9%)
13	CLA	f	1021	2	69,73,73	1.24	10 (14%)	83,113,113	1.36	8 (9%)
16	BCR	r	524	-	41,41,41	0.73	0	56,56,56	1.67	12 (21%)
16	BCR	Y	523	-	41,41,41	0.71	0	56,56,56	1.64	16 (28%)
13	CLA	m	1103	9	54,58,73	1.40	9 (16%)	65,95,113	1.56	11 (16%)
13	CLA	2	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.49	4 (6%)
13	CLA	e	1140	1	69,73,73	1.27	10 (14%)	83,113,113	1.39	11 (13%)
13	CLA	4	505	12	69,73,73	1.24	8 (11%)	83,113,113	1.27	5 (6%)
13	CLA	b	504	-	49,53,73	1.47	7 (14%)	59,89,113	1.47	5 (8%)
13	CLA	4	513	12	49,53,73	1.50	9 (18%)	59,89,113	1.47	4 (6%)
16	BCR	b	521	-	41,41,41	0.64	0	56,56,56	1.78	11 (19%)
16	BCR	V	4019	-	41,41,41	0.74	0	56,56,56	1.92	14 (25%)
13	CLA	B	1012	21	69,73,73	1.27	11 (15%)	83,113,113	1.38	9 (10%)
13	CLA	6	517	-	49,53,73	1.48	9 (18%)	59,89,113	1.45	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	H	1231	21	69,73,73	1.20	9 (13%)	83,113,113	1.40	8 (9%)
13	CLA	2	512	12	57,61,73	1.36	8 (14%)	68,98,113	1.37	4 (5%)
13	CLA	f	1211	2	60,64,73	1.32	8 (13%)	72,102,113	1.58	5 (6%)
16	BCR	S	4018	-	41,41,41	0.77	0	56,56,56	1.84	15 (26%)
13	CLA	q	504	-	49,53,73	1.49	10 (20%)	59,89,113	1.49	6 (10%)
13	CLA	G	1139	21	69,73,73	1.24	10 (14%)	83,113,113	1.27	8 (9%)
13	CLA	1	507	-	64,68,73	1.29	8 (12%)	77,107,113	1.40	8 (10%)
13	CLA	b	502	12	54,58,73	1.41	9 (16%)	65,95,113	1.48	5 (7%)
16	BCR	n	4219	-	41,41,41	0.78	0	56,56,56	1.81	12 (21%)
17	LHG	f	1842	13	38,38,48	0.65	0	41,44,54	1.23	4 (9%)
16	BCR	a	524	-	41,41,41	0.74	0	56,56,56	1.81	17 (30%)
13	CLA	d	509	12	49,53,73	1.50	8 (16%)	59,89,113	1.46	5 (8%)
16	BCR	5	522	-	41,41,41	0.74	0	56,56,56	1.93	20 (35%)
20	SQD	6	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.91	10 (29%)
13	CLA	B	1239	2	69,73,73	1.25	8 (11%)	83,113,113	1.53	11 (13%)
13	CLA	u	505	12	65,69,73	1.28	7 (10%)	78,108,113	1.27	4 (5%)
16	BCR	r	523	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
17	LHG	A	5005	-	44,44,48	0.67	1 (2%)	47,50,54	1.27	6 (12%)
17	LHG	A	5001	-	48,48,48	0.78	1 (2%)	51,54,54	1.26	6 (11%)
16	BCR	G	4003	-	41,41,41	0.78	0	56,56,56	1.73	11 (19%)
13	CLA	v	519	12	50,54,73	1.47	8 (16%)	60,90,113	1.45	4 (6%)
16	BCR	W	4021	-	41,41,41	0.71	0	56,56,56	1.82	14 (25%)
13	CLA	c	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.40	7 (9%)
13	CLA	1	505	12	69,73,73	1.25	8 (11%)	83,113,113	1.27	5 (6%)
13	CLA	s	509	12	69,73,73	1.25	10 (14%)	83,113,113	1.37	8 (9%)
13	CLA	s	502	12	54,58,73	1.41	8 (14%)	65,95,113	1.50	6 (9%)
17	LHG	V	5221	-	48,48,48	0.65	2 (4%)	51,54,54	1.30	6 (11%)
13	CLA	2	516	12	49,53,73	1.48	8 (16%)	59,89,113	1.51	5 (8%)
13	CLA	G	1103	1	69,73,73	1.24	8 (11%)	83,113,113	1.50	8 (9%)
13	CLA	a	507	-	69,73,73	1.25	8 (11%)	83,113,113	1.34	7 (8%)
13	CLA	b	519	12	59,63,73	1.35	10 (16%)	71,101,113	1.40	5 (7%)
13	CLA	G	1126	1	69,73,73	1.20	9 (13%)	83,113,113	1.40	8 (9%)
13	CLA	Z	503	12	69,73,73	1.26	8 (11%)	83,113,113	1.32	7 (8%)
13	CLA	2	501	12	69,73,73	1.24	10 (14%)	83,113,113	1.37	6 (7%)
17	LHG	f	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.22	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	2	523	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
16	BCR	J	4015	-	41,41,41	0.78	0	56,56,56	1.82	14 (25%)
13	CLA	5	504	-	49,53,73	1.48	8 (16%)	59,89,113	1.49	6 (10%)
13	CLA	u	502	12	54,58,73	1.42	10 (18%)	65,95,113	1.47	6 (9%)
13	CLA	c	501	12	69,73,73	1.24	9 (13%)	83,113,113	1.37	5 (6%)
20	SQD	v	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.91	10 (29%)
13	CLA	3	518	12	59,63,73	1.36	10 (16%)	71,101,113	1.38	5 (7%)
13	CLA	Y	508	12	59,63,73	1.36	10 (16%)	71,101,113	1.54	10 (14%)
16	BCR	n	4019	-	41,41,41	0.73	0	56,56,56	1.92	14 (25%)
13	CLA	5	509	12	69,73,73	1.25	10 (14%)	83,113,113	1.33	8 (9%)
20	SQD	t	822	-	25,26,54	1.31	4 (16%)	34,37,65	1.84	9 (26%)
17	LHG	G	5002	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	5 (12%)
13	CLA	3	506	12	54,58,73	1.43	9 (16%)	65,95,113	1.47	6 (9%)
13	CLA	1	502	12	64,68,73	1.31	8 (12%)	77,107,113	1.37	7 (9%)
13	CLA	G	1137	1	69,73,73	1.23	8 (11%)	83,113,113	1.43	7 (8%)
16	BCR	G	4007	-	41,41,41	0.75	0	56,56,56	2.10	18 (32%)
13	CLA	H	1213	2	69,73,73	1.22	11 (15%)	83,113,113	1.42	11 (13%)
13	CLA	d	517	-	49,53,73	1.48	9 (18%)	59,89,113	1.44	4 (6%)
13	CLA	G	1124	21	60,64,73	1.36	9 (15%)	72,102,113	1.49	13 (18%)
13	CLA	2	505	12	69,73,73	1.23	7 (10%)	83,113,113	1.28	6 (7%)
16	BCR	4	521	-	41,41,41	0.64	0	56,56,56	1.78	11 (19%)
13	CLA	Z	505	12	69,73,73	1.23	7 (10%)	83,113,113	1.28	6 (7%)
16	BCR	u	523	-	41,41,41	0.74	0	56,56,56	1.78	16 (28%)
13	CLA	2	506	12	59,63,73	1.36	10 (16%)	71,101,113	1.40	6 (8%)
16	BCR	Y	522	-	41,41,41	0.73	0	56,56,56	1.91	20 (35%)
13	CLA	G	1133	1	69,73,73	1.20	8 (11%)	83,113,113	1.39	6 (7%)
13	CLA	3	501	12	69,73,73	1.24	9 (13%)	83,113,113	1.38	6 (7%)
13	CLA	H	1227	2	69,73,73	1.22	10 (14%)	83,113,113	1.40	8 (9%)
16	BCR	c	524	-	41,41,41	0.69	0	56,56,56	1.67	15 (26%)
16	BCR	e	4002	-	41,41,41	0.81	0	56,56,56	1.85	14 (25%)
13	CLA	6	513	12	49,53,73	1.50	7 (14%)	59,89,113	1.41	5 (8%)
16	BCR	o	4021	-	41,41,41	0.71	0	56,56,56	1.81	14 (25%)
13	CLA	G	1022	21	69,73,73	1.27	10 (14%)	83,113,113	1.32	9 (10%)
20	SQD	r	822	-	42,43,54	1.07	5 (11%)	51,54,65	1.61	10 (19%)
13	CLA	H	1209	2	56,60,73	1.38	9 (16%)	67,97,113	1.56	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	e	1108	1	58,62,73	1.36	10 (17%)	69,99,113	1.36	6 (8%)
16	BCR	1	523	-	41,41,41	0.71	0	56,56,56	1.63	16 (28%)
13	CLA	6	510	12	49,53,73	1.48	9 (18%)	59,89,113	1.42	5 (8%)
13	CLA	f	1212	2	59,63,73	1.32	9 (15%)	71,101,113	1.48	6 (8%)
17	LHG	G	5009	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
19	LMG	T	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.25	7 (16%)
16	BCR	A	4003	-	41,41,41	0.78	0	56,56,56	1.73	11 (19%)
13	CLA	e	1011	1	69,73,73	1.25	8 (11%)	83,113,113	1.54	11 (13%)
13	CLA	A	1134	1	60,64,73	1.31	9 (15%)	72,102,113	1.44	6 (8%)
13	CLA	Y	512	12	56,60,73	1.39	9 (16%)	67,97,113	1.44	5 (7%)
13	CLA	B	1216	21	64,68,73	1.31	10 (15%)	77,107,113	1.38	6 (7%)
13	CLA	F	1302	6	49,53,73	1.46	8 (16%)	59,89,113	1.47	4 (6%)
13	CLA	l	1302	8	62,66,73	1.29	9 (14%)	74,104,113	1.43	6 (8%)
13	CLA	B	1202	2	69,73,73	1.23	10 (14%)	83,113,113	1.49	9 (10%)
16	BCR	L	4022	-	41,41,41	0.76	0	56,56,56	1.90	14 (25%)
13	CLA	a	512	12	49,53,73	1.48	9 (18%)	59,89,113	1.50	4 (6%)
13	CLA	f	1225	2	69,73,73	1.22	11 (15%)	83,113,113	1.31	8 (9%)
13	CLA	s	511	12	54,58,73	1.43	9 (16%)	65,95,113	1.49	5 (7%)
13	CLA	1	504	-	49,53,73	1.48	10 (20%)	59,89,113	1.49	6 (10%)
13	CLA	3	513	12	69,73,73	1.24	9 (13%)	83,113,113	1.33	5 (6%)
20	SQD	a	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.59	12 (23%)
13	CLA	5	517	-	49,53,73	1.50	9 (18%)	59,89,113	1.40	4 (6%)
13	CLA	H	1207	2	69,73,73	1.25	10 (14%)	83,113,113	1.31	4 (4%)
18	LMU	r	901	-	23,23,36	1.10	1 (4%)	28,28,47	0.94	0
13	CLA	G	1115	1	64,68,73	1.26	9 (14%)	77,107,113	1.47	9 (11%)
13	CLA	3	507	-	69,73,73	1.24	8 (11%)	83,113,113	1.33	7 (8%)
16	BCR	V	4022	-	41,41,41	0.76	0	56,56,56	1.90	14 (25%)
13	CLA	4	511	12	49,53,73	1.50	9 (18%)	59,89,113	1.53	7 (11%)
13	CLA	Y	509	12	69,73,73	1.25	10 (14%)	83,113,113	1.37	7 (8%)
13	CLA	Z	516	12	49,53,73	1.48	10 (20%)	59,89,113	1.51	5 (8%)
13	CLA	B	1021	2	69,73,73	1.24	10 (14%)	83,113,113	1.37	8 (9%)
13	CLA	4	507	-	49,53,73	1.48	7 (14%)	59,89,113	1.54	7 (11%)
17	LHG	e	5007	-	46,46,48	0.66	1 (2%)	49,52,54	1.24	5 (10%)
13	CLA	e	1130	1	69,73,73	1.24	10 (14%)	83,113,113	1.40	11 (13%)
13	CLA	B	1212	2	59,63,73	1.32	9 (15%)	71,101,113	1.47	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	LHG	L	5220	-	40,40,48	0.65	0	43,46,54	1.23	4 (9%)
13	CLA	f	1219	2	69,73,73	1.25	8 (11%)	83,113,113	1.26	8 (9%)
16	BCR	5	523	-	41,41,41	0.75	0	56,56,56	1.78	16 (28%)
16	BCR	3	521	-	41,41,41	0.67	0	56,56,56	1.76	10 (17%)
16	BCR	m	4104	-	41,41,41	0.74	0	56,56,56	1.86	15 (26%)
13	CLA	f	1202	2	69,73,73	1.24	10 (14%)	83,113,113	1.48	10 (12%)
13	CLA	f	1229	2	69,73,73	1.24	10 (14%)	83,113,113	1.42	11 (13%)
13	CLA	6	506	12	49,53,73	1.49	8 (16%)	59,89,113	1.49	6 (10%)
13	CLA	2	504	-	54,58,73	1.40	10 (18%)	65,95,113	1.46	7 (10%)
13	CLA	f	1023	-	69,73,73	1.25	11 (15%)	83,113,113	1.69	15 (18%)
16	BCR	2	521	-	41,41,41	0.66	0	56,56,56	1.87	11 (19%)
16	BCR	G	4002	-	41,41,41	0.81	1 (2%)	56,56,56	1.85	14 (25%)
16	BCR	f	4004	-	41,41,41	0.72	0	56,56,56	1.85	13 (23%)
13	CLA	f	1224	2	64,68,73	1.28	9 (14%)	77,107,113	1.42	8 (10%)
13	CLA	H	1222	21	64,68,73	1.28	10 (15%)	77,107,113	1.39	10 (12%)
13	CLA	A	1139	21	69,73,73	1.24	10 (14%)	83,113,113	1.27	8 (9%)
16	BCR	B	4017	-	41,41,41	0.80	0	56,56,56	1.57	11 (19%)
13	CLA	e	1135	1	56,60,73	1.37	9 (16%)	67,97,113	1.55	11 (16%)
18	LMU	1	902	-	19,19,36	1.22	1 (5%)	24,24,47	1.10	3 (12%)
13	CLA	U	1401	-	59,63,73	1.35	10 (16%)	71,101,113	1.45	8 (11%)
13	CLA	q	502	12	64,68,73	1.31	8 (12%)	77,107,113	1.37	7 (9%)
16	BCR	H	4006	-	41,41,41	0.73	0	56,56,56	1.98	19 (33%)
13	CLA	a	518	12	59,63,73	1.36	10 (16%)	71,101,113	1.37	5 (7%)
13	CLA	4	519	12	59,63,73	1.35	10 (16%)	71,101,113	1.41	5 (7%)
13	CLA	f	1216	21	64,68,73	1.31	10 (15%)	77,107,113	1.39	5 (6%)
17	LHG	A	5008	-	34,34,48	0.76	1 (2%)	37,40,54	1.28	4 (10%)
13	CLA	Y	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.44	9 (12%)
13	CLA	B	1232	21	54,58,73	1.39	11 (20%)	65,95,113	1.60	7 (10%)
13	CLA	e	1109	1	69,73,73	1.23	9 (13%)	83,113,113	1.40	5 (6%)
13	CLA	t	516	12	49,53,73	1.50	8 (16%)	59,89,113	1.44	5 (8%)
17	LHG	V	5218	-	37,37,48	0.75	2 (5%)	40,43,54	1.23	4 (10%)
13	CLA	a	501	12	69,73,73	1.24	9 (13%)	83,113,113	1.39	6 (7%)
16	BCR	e	4008	-	41,41,41	0.84	1 (2%)	56,56,56	2.02	17 (30%)
13	CLA	r	516	12	49,53,73	1.47	9 (18%)	59,89,113	1.52	5 (8%)
16	BCR	n	4020	-	41,41,41	0.82	0	56,56,56	1.95	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	G	1104	1	69,73,73	1.23	10 (14%)	83,113,113	1.39	10 (12%)
13	CLA	A	1138	1	69,73,73	1.21	10 (14%)	83,113,113	1.35	7 (8%)
13	CLA	3	519	12	59,63,73	1.35	10 (16%)	71,101,113	1.40	5 (7%)
13	CLA	e	1126	1	69,73,73	1.20	10 (14%)	83,113,113	1.41	8 (9%)
13	CLA	s	507	-	69,73,73	1.25	8 (11%)	83,113,113	1.32	7 (8%)
13	CLA	H	1204	2	69,73,73	1.22	9 (13%)	83,113,113	1.30	7 (8%)
13	CLA	d	501	12	64,68,73	1.29	8 (12%)	77,107,113	1.40	5 (6%)
13	CLA	3	511	12	54,58,73	1.43	9 (16%)	65,95,113	1.49	5 (7%)
16	BCR	c	523	-	41,41,41	0.74	0	56,56,56	1.78	16 (28%)
13	CLA	B	1228	2	59,63,73	1.30	9 (15%)	71,101,113	1.49	9 (12%)
13	CLA	f	1214	2	69,73,73	1.25	10 (14%)	83,113,113	1.43	6 (7%)
13	CLA	5	507	-	49,53,73	1.46	7 (14%)	59,89,113	1.53	7 (11%)
16	BCR	L	4020	-	41,41,41	0.83	0	56,56,56	1.95	16 (28%)
17	LHG	H	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.21	5 (10%)
13	CLA	Z	519	12	59,63,73	1.35	10 (16%)	71,101,113	1.39	8 (11%)
18	LMU	e	1849	-	23,23,36	1.16	1 (4%)	28,28,47	1.00	2 (7%)
13	CLA	5	502	12	54,58,73	1.42	10 (18%)	65,95,113	1.46	5 (7%)
17	LHG	A	5009	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
13	CLA	A	1106	1	69,73,73	1.22	11 (15%)	83,113,113	1.44	11 (13%)
13	CLA	f	1208	2	69,73,73	1.21	8 (11%)	83,113,113	1.32	7 (8%)
13	CLA	u	513	12	49,53,73	1.49	10 (20%)	59,89,113	1.43	6 (10%)
13	CLA	v	505	12	69,73,73	1.25	8 (11%)	83,113,113	1.30	5 (6%)
16	BCR	B	4009	-	41,41,41	0.81	0	56,56,56	1.91	21 (37%)
13	CLA	e	1124	21	60,64,73	1.36	9 (15%)	72,102,113	1.47	13 (18%)
16	BCR	k	4018	-	41,41,41	0.77	0	56,56,56	1.84	15 (26%)
14	PQN	e	2001	-	34,34,34	2.88	11 (32%)	42,45,45	2.11	7 (16%)
13	CLA	q	519	12	54,58,73	1.40	10 (18%)	65,95,113	1.45	8 (12%)
16	BCR	5	521	-	41,41,41	0.68	0	56,56,56	1.94	16 (28%)
16	BCR	V	4219	-	41,41,41	0.77	0	56,56,56	1.80	12 (21%)
13	CLA	f	1206	2	69,73,73	1.25	11 (15%)	83,113,113	1.45	6 (7%)
13	CLA	r	506	12	59,63,73	1.35	9 (15%)	71,101,113	1.40	6 (8%)
16	BCR	e	4007	-	41,41,41	0.74	0	56,56,56	2.11	18 (32%)
13	CLA	d	511	12	49,53,73	1.49	9 (18%)	59,89,113	1.50	4 (6%)
13	CLA	e	1131	1	69,73,73	1.22	9 (13%)	83,113,113	1.34	7 (8%)
13	CLA	f	1230	2	64,68,73	1.30	9 (14%)	77,107,113	1.44	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	1115	1	64,68,73	1.26	10 (15%)	77,107,113	1.47	9 (11%)
13	CLA	G	1132	1	69,73,73	1.23	10 (14%)	83,113,113	1.38	9 (10%)
13	CLA	s	512	12	49,53,73	1.47	9 (18%)	59,89,113	1.50	4 (6%)
16	BCR	G	4011	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
13	CLA	b	509	12	69,73,73	1.25	7 (10%)	83,113,113	1.38	6 (7%)
13	CLA	u	504	-	49,53,73	1.49	9 (18%)	59,89,113	1.49	5 (8%)
13	CLA	T	1302	8	62,66,73	1.30	9 (14%)	74,104,113	1.41	6 (8%)
16	BCR	d	521	-	41,41,41	0.66	0	56,56,56	1.91	12 (21%)
16	BCR	3	522	-	41,41,41	0.67	0	56,56,56	1.91	16 (28%)
17	LHG	V	5220	-	40,40,48	0.64	0	43,46,54	1.23	4 (9%)
13	CLA	4	508	12	49,53,73	1.51	9 (18%)	59,89,113	1.58	9 (15%)
13	CLA	A	1022	21	69,73,73	1.26	10 (14%)	83,113,113	1.32	9 (10%)
13	CLA	3	503	12	69,73,73	1.27	9 (13%)	83,113,113	1.32	7 (8%)
13	CLA	f	1217	2	61,65,73	1.30	10 (16%)	73,103,113	1.43	8 (10%)
13	CLA	v	503	12	56,60,73	1.39	8 (14%)	67,97,113	1.45	7 (10%)
13	CLA	A	1140	1	69,73,73	1.27	10 (14%)	83,113,113	1.39	11 (13%)
13	CLA	a	506	12	54,58,73	1.43	9 (16%)	65,95,113	1.47	6 (9%)
13	CLA	B	1235	2	69,73,73	1.23	10 (14%)	83,113,113	1.43	8 (9%)
13	CLA	3	505	12	69,73,73	1.24	8 (11%)	83,113,113	1.26	4 (4%)
13	CLA	A	1103	1	69,73,73	1.24	8 (11%)	83,113,113	1.49	8 (9%)
13	CLA	B	1225	2	69,73,73	1.23	11 (15%)	83,113,113	1.30	8 (9%)
13	CLA	f	1240	17	69,73,73	1.25	9 (13%)	83,113,113	1.34	8 (9%)
17	LHG	k	5001	-	43,43,48	0.64	0	46,49,54	1.22	4 (8%)
18	LMU	H	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.10	3 (6%)
13	CLA	1	516	12	49,53,73	1.49	9 (18%)	59,89,113	1.65	8 (13%)
13	CLA	B	1227	2	69,73,73	1.22	10 (14%)	83,113,113	1.40	8 (9%)
13	CLA	b	503	12	59,63,73	1.38	8 (13%)	71,101,113	1.42	9 (12%)
13	CLA	Y	507	-	64,68,73	1.29	8 (12%)	77,107,113	1.39	8 (10%)
13	CLA	f	1238	21	69,73,73	1.23	10 (14%)	83,113,113	1.42	11 (13%)
13	CLA	Z	508	12	59,63,73	1.36	10 (16%)	71,101,113	1.44	9 (12%)
13	CLA	e	1127	1	69,73,73	1.24	9 (13%)	83,113,113	1.35	9 (10%)
13	CLA	v	516	12	49,53,73	1.49	7 (14%)	59,89,113	1.46	6 (10%)
16	BCR	H	4005	-	41,41,41	0.70	0	56,56,56	1.78	11 (19%)
16	BCR	H	4017	-	41,41,41	0.79	0	56,56,56	1.58	11 (19%)
20	SQD	c	822	-	28,29,54	1.25	5 (17%)	37,40,65	1.92	13 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	c	508	12	49,53,73	1.48	9 (18%)	59,89,113	1.55	5 (8%)
15	SF4	G	3001	1,2	0,12,12	-	-	-		
17	LHG	e	5002	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	5 (12%)
13	CLA	5	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.40	6 (8%)
13	CLA	q	503	12	68,72,73	1.27	8 (11%)	81,111,113	1.34	6 (7%)
13	CLA	f	1210	2	69,73,73	1.25	9 (13%)	83,113,113	1.41	11 (13%)
13	CLA	e	1137	1	69,73,73	1.24	8 (11%)	83,113,113	1.42	7 (8%)
13	CLA	F	1301	21	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)
13	CLA	B	1219	2	69,73,73	1.25	8 (11%)	83,113,113	1.26	8 (9%)
13	CLA	a	502	12	54,58,73	1.40	8 (14%)	65,95,113	1.51	6 (9%)
13	CLA	u	506	12	49,53,73	1.49	9 (18%)	59,89,113	1.51	5 (8%)
13	CLA	l	508	12	59,63,73	1.36	9 (15%)	71,101,113	1.54	9 (12%)
13	CLA	Z	504	-	54,58,73	1.40	9 (16%)	65,95,113	1.46	7 (10%)
13	CLA	B	1229	2	69,73,73	1.24	10 (14%)	83,113,113	1.42	11 (13%)
13	CLA	e	1133	1	69,73,73	1.20	9 (13%)	83,113,113	1.38	6 (7%)
13	CLA	n	1502	10	69,73,73	1.23	10 (14%)	83,113,113	1.38	6 (7%)
16	BCR	J	4013	-	41,41,41	0.76	0	56,56,56	1.96	15 (26%)
16	BCR	R	4016	-	41,41,41	0.75	0	56,56,56	1.78	13 (23%)
13	CLA	b	505	12	69,73,73	1.25	8 (11%)	83,113,113	1.27	4 (4%)
13	CLA	r	507	-	69,73,73	1.23	9 (13%)	83,113,113	1.38	6 (7%)
13	CLA	t	503	12	59,63,73	1.38	7 (11%)	71,101,113	1.41	10 (14%)
13	CLA	B	1023	-	69,73,73	1.25	11 (15%)	83,113,113	1.70	15 (18%)
13	CLA	l	510	12	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
13	CLA	L	1502	10	69,73,73	1.23	10 (14%)	83,113,113	1.39	6 (7%)
13	CLA	B	1224	2	64,68,73	1.28	9 (14%)	77,107,113	1.43	8 (10%)
13	CLA	r	512	12	57,61,73	1.37	8 (14%)	68,98,113	1.37	4 (5%)
16	BCR	d	524	-	41,41,41	0.75	0	56,56,56	1.87	13 (23%)
16	BCR	s	524	-	41,41,41	0.73	0	56,56,56	1.82	17 (30%)
13	CLA	4	502	12	54,58,73	1.41	9 (16%)	65,95,113	1.48	5 (7%)
13	CLA	e	1801	17	49,53,73	1.51	10 (20%)	59,89,113	1.61	8 (13%)
13	CLA	e	1118	1	64,68,73	1.28	9 (14%)	77,107,113	1.41	8 (10%)
16	BCR	B	4005	-	41,41,41	0.70	0	56,56,56	1.78	11 (19%)
16	BCR	Y	524	-	41,41,41	0.73	0	56,56,56	1.82	15 (26%)
13	CLA	H	1217	2	61,65,73	1.31	10 (16%)	73,103,113	1.43	9 (12%)
13	CLA	R	1302	6	49,53,73	1.46	8 (16%)	59,89,113	1.47	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	e	1102	1	69,73,73	1.21	10 (14%)	83,113,113	1.34	7 (8%)
13	CLA	H	1218	2	64,68,73	1.27	9 (14%)	77,107,113	1.38	5 (6%)
17	LHG	G	5007	-	46,46,48	0.67	1 (2%)	49,52,54	1.24	5 (10%)
13	CLA	R	1301	21	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)
13	CLA	6	518	12	59,63,73	1.35	9 (15%)	71,101,113	1.38	6 (8%)
13	CLA	H	1203	2	69,73,73	1.26	12 (17%)	83,113,113	1.34	8 (9%)
13	CLA	2	508	12	59,63,73	1.36	10 (16%)	71,101,113	1.44	9 (12%)
13	CLA	a	519	12	59,63,73	1.35	10 (16%)	71,101,113	1.40	5 (7%)
13	CLA	f	1226	2	69,73,73	1.34	11 (15%)	83,113,113	1.67	16 (19%)
15	SF4	g	3003	3	0,12,12	-	-	-	-	-
17	LHG	e	5004	-	35,35,48	0.74	1 (2%)	38,41,54	1.25	4 (10%)
13	CLA	2	509	12	69,73,73	1.26	10 (14%)	83,113,113	1.35	7 (8%)
13	CLA	5	519	12	50,54,73	1.46	9 (18%)	60,90,113	1.45	5 (8%)
13	CLA	v	501	12	64,68,73	1.29	9 (14%)	77,107,113	1.40	5 (6%)
13	CLA	c	513	12	49,53,73	1.49	10 (20%)	59,89,113	1.44	5 (8%)
13	CLA	3	504	-	49,53,73	1.47	9 (18%)	59,89,113	1.52	7 (11%)
13	CLA	c	509	12	69,73,73	1.25	9 (13%)	83,113,113	1.34	8 (9%)
16	BCR	H	4014	-	41,41,41	0.74	0	56,56,56	1.84	13 (23%)
16	BCR	d	523	-	41,41,41	0.70	0	56,56,56	1.73	14 (25%)
13	CLA	B	1214	2	69,73,73	1.25	10 (14%)	83,113,113	1.42	6 (7%)
13	CLA	K	1105	9	49,53,73	1.50	9 (18%)	59,89,113	1.70	9 (15%)
13	CLA	Y	504	-	49,53,73	1.49	10 (20%)	59,89,113	1.49	6 (10%)
13	CLA	b	516	12	49,53,73	1.49	8 (16%)	59,89,113	1.43	5 (8%)
13	CLA	K	1103	9	54,58,73	1.40	9 (16%)	65,95,113	1.56	12 (18%)
13	CLA	Y	517	-	49,53,73	1.47	10 (20%)	59,89,113	1.44	4 (6%)
16	BCR	d	522	-	41,41,41	0.70	0	56,56,56	1.84	14 (25%)
13	CLA	b	501	12	64,68,73	1.31	8 (12%)	77,107,113	1.35	4 (5%)
17	LHG	S	5001	-	43,43,48	0.64	0	46,49,54	1.22	4 (8%)
13	CLA	u	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.53	7 (11%)
13	CLA	6	503	12	56,60,73	1.39	8 (14%)	67,97,113	1.44	7 (10%)
13	CLA	A	1113	1	49,53,73	1.43	9 (18%)	59,89,113	1.56	6 (10%)
13	CLA	f	1213	2	69,73,73	1.22	10 (14%)	83,113,113	1.42	11 (13%)
15	SF4	N	3003	3	0,12,12	-	-	-	-	-
13	CLA	q	501	12	69,73,73	1.26	10 (14%)	83,113,113	1.34	7 (8%)
13	CLA	Y	518	12	64,68,73	1.28	9 (14%)	77,107,113	1.42	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	q	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.43	4 (6%)
13	CLA	u	510	12	49,53,73	1.49	9 (18%)	59,89,113	1.46	5 (8%)
17	LHG	G	5005	-	44,44,48	0.67	1 (2%)	47,50,54	1.27	6 (12%)
13	CLA	B	1230	2	64,68,73	1.30	9 (14%)	77,107,113	1.44	8 (10%)
13	CLA	e	1120	1	57,61,73	1.35	11 (19%)	68,98,113	1.52	7 (10%)
13	CLA	r	518	12	69,73,73	1.24	10 (14%)	83,113,113	1.36	7 (8%)
13	CLA	l	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.44	4 (6%)
13	CLA	e	1132	1	69,73,73	1.23	11 (15%)	83,113,113	1.38	9 (10%)
18	LMU	e	1848	-	36,36,36	1.14	2 (5%)	47,47,47	1.07	2 (4%)
13	CLA	G	1134	1	60,64,73	1.31	8 (13%)	72,102,113	1.44	6 (8%)
13	CLA	v	510	12	49,53,73	1.48	9 (18%)	59,89,113	1.42	5 (8%)
13	CLA	f	1221	21	69,73,73	1.29	11 (15%)	83,113,113	1.49	13 (15%)
16	BCR	a	522	-	41,41,41	0.67	0	56,56,56	1.91	16 (28%)
16	BCR	A	4001	-	41,41,41	0.76	0	56,56,56	1.72	11 (19%)
13	CLA	e	1237	21	69,73,73	1.25	9 (13%)	83,113,113	1.43	10 (12%)
17	LHG	n	5220	-	40,40,48	0.65	0	43,46,54	1.23	4 (9%)
18	LMU	Z	901	-	23,23,36	1.10	1 (4%)	28,28,47	0.94	0
13	CLA	6	511	12	49,53,73	1.49	9 (18%)	59,89,113	1.51	4 (6%)
13	CLA	2	513	12	69,73,73	1.26	10 (14%)	83,113,113	1.29	5 (6%)
13	CLA	4	509	12	69,73,73	1.25	8 (11%)	83,113,113	1.39	6 (7%)
13	CLA	b	511	12	49,53,73	1.50	9 (18%)	59,89,113	1.53	6 (10%)
13	CLA	c	517	-	49,53,73	1.50	8 (16%)	59,89,113	1.40	4 (6%)
17	LHG	A	5007	-	46,46,48	0.67	1 (2%)	49,52,54	1.24	5 (10%)
13	CLA	B	1203	2	69,73,73	1.26	12 (17%)	83,113,113	1.34	8 (9%)
13	CLA	H	1202	2	69,73,73	1.23	10 (14%)	83,113,113	1.49	9 (10%)
13	CLA	H	1230	2	64,68,73	1.30	9 (14%)	77,107,113	1.44	8 (10%)
16	BCR	q	521	-	41,41,41	0.65	0	56,56,56	1.80	11 (19%)
13	CLA	B	1234	2	69,73,73	1.28	11 (15%)	83,113,113	1.54	14 (16%)
13	CLA	G	1138	1	69,73,73	1.22	10 (14%)	83,113,113	1.35	7 (8%)
13	CLA	c	506	12	49,53,73	1.49	8 (16%)	59,89,113	1.50	5 (8%)
13	CLA	Z	518	12	69,73,73	1.24	9 (13%)	83,113,113	1.36	7 (8%)
16	BCR	4	523	-	41,41,41	0.69	0	56,56,56	1.65	12 (21%)
16	BCR	U	4104	-	41,41,41	0.74	0	56,56,56	1.86	15 (26%)
13	CLA	q	510	12	69,73,73	1.26	7 (10%)	83,113,113	1.31	7 (8%)
13	CLA	t	504	-	49,53,73	1.48	8 (16%)	59,89,113	1.48	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	K	1401	-	59,63,73	1.36	10 (16%)	71,101,113	1.45	7 (9%)
20	SQD	d	822	-	25,26,54	1.30	4 (16%)	34,37,65	1.91	10 (29%)
16	BCR	f	4017	-	41,41,41	0.80	0	56,56,56	1.57	11 (19%)
13	CLA	B	1207	2	69,73,73	1.25	10 (14%)	83,113,113	1.30	4 (4%)
13	CLA	e	1128	1	69,73,73	1.32	10 (14%)	83,113,113	1.53	9 (10%)
13	CLA	4	506	12	49,53,73	1.49	9 (18%)	59,89,113	1.50	4 (6%)
13	CLA	G	1106	1	69,73,73	1.22	11 (15%)	83,113,113	1.44	11 (13%)
16	BCR	A	4002	-	41,41,41	0.81	1 (2%)	56,56,56	1.85	15 (26%)
13	CLA	e	1125	1	69,73,73	1.24	10 (14%)	83,113,113	1.43	9 (10%)
13	CLA	u	518	12	59,63,73	1.35	9 (15%)	71,101,113	1.34	5 (7%)
20	SQD	s	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.59	12 (23%)
13	CLA	H	1238	21	69,73,73	1.23	9 (13%)	83,113,113	1.42	11 (13%)
13	CLA	G	1121	1	59,63,73	1.34	10 (16%)	71,101,113	1.48	10 (14%)
13	CLA	1	513	12	59,63,73	1.35	10 (16%)	71,101,113	1.36	5 (7%)
15	SF4	C	3002	3	0,12,12	-	-	-	-	-
13	CLA	6	516	12	49,53,73	1.49	8 (16%)	59,89,113	1.46	6 (10%)
14	PQN	B	2002	-	34,34,34	2.88	11 (32%)	42,45,45	2.18	4 (9%)
13	CLA	e	1105	1	59,63,73	1.30	10 (16%)	71,101,113	1.51	10 (14%)
13	CLA	B	1215	2	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
13	CLA	H	1206	2	69,73,73	1.25	11 (15%)	83,113,113	1.45	6 (7%)
13	CLA	e	1119	21	69,73,73	1.26	10 (14%)	83,113,113	1.40	10 (12%)
16	BCR	3	523	-	41,41,41	0.69	0	56,56,56	1.76	15 (26%)
13	CLA	A	1011	1	69,73,73	1.25	8 (11%)	83,113,113	1.54	11 (13%)
13	CLA	6	519	12	50,54,73	1.46	8 (16%)	60,90,113	1.45	4 (6%)
14	PQN	G	2001	-	34,34,34	2.87	11 (32%)	42,45,45	2.12	7 (16%)
13	CLA	e	1114	21	54,58,73	1.43	9 (16%)	65,95,113	1.50	7 (10%)
17	LHG	G	5008	-	34,34,48	0.76	1 (2%)	37,40,54	1.28	4 (10%)
13	CLA	G	1107	1	69,73,73	1.24	11 (15%)	83,113,113	1.35	10 (12%)
13	CLA	4	503	12	59,63,73	1.38	7 (11%)	71,101,113	1.41	9 (12%)
13	CLA	q	512	12	56,60,73	1.38	9 (16%)	67,97,113	1.44	5 (7%)
13	CLA	B	1201	2	64,68,73	1.27	10 (15%)	77,107,113	1.50	9 (11%)
13	CLA	2	518	12	69,73,73	1.24	9 (13%)	83,113,113	1.36	7 (8%)
13	CLA	f	1231	21	69,73,73	1.21	9 (13%)	83,113,113	1.42	8 (9%)
13	CLA	1	506	12	49,53,73	1.48	7 (14%)	59,89,113	1.47	6 (10%)
13	CLA	v	508	12	49,53,73	1.48	10 (20%)	59,89,113	1.50	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	a	513	12	69,73,73	1.25	8 (11%)	83,113,113	1.33	5 (6%)
13	CLA	B	1238	21	69,73,73	1.23	10 (14%)	83,113,113	1.42	11 (13%)
13	CLA	r	502	12	64,68,73	1.31	8 (12%)	77,107,113	1.39	7 (9%)
13	CLA	A	1130	1	69,73,73	1.24	10 (14%)	83,113,113	1.41	11 (13%)
13	CLA	c	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.53	7 (11%)
13	CLA	q	508	12	59,63,73	1.36	10 (16%)	71,101,113	1.54	9 (12%)
13	CLA	d	513	12	49,53,73	1.51	6 (12%)	59,89,113	1.41	4 (6%)
13	CLA	s	505	12	69,73,73	1.25	8 (11%)	83,113,113	1.26	4 (4%)
15	SF4	e	3001	1,2	0,12,12	-	-	-	-	-
13	CLA	s	506	12	54,58,73	1.42	9 (16%)	65,95,113	1.47	6 (9%)
13	CLA	G	1123	21	69,73,73	1.24	9 (13%)	83,113,113	1.35	9 (10%)
13	CLA	3	502	12	54,58,73	1.40	8 (14%)	65,95,113	1.51	6 (9%)
13	CLA	A	1108	1	58,62,73	1.36	10 (17%)	69,99,113	1.36	6 (8%)
13	CLA	Z	501	12	69,73,73	1.25	10 (14%)	83,113,113	1.37	6 (7%)
16	BCR	B	4004	-	41,41,41	0.72	0	56,56,56	1.85	13 (23%)
20	SQD	Y	822	-	47,48,54	0.99	5 (10%)	56,59,65	1.74	13 (23%)
16	BCR	5	524	-	41,41,41	0.68	0	56,56,56	1.67	14 (25%)
13	CLA	B	1217	2	61,65,73	1.30	10 (16%)	73,103,113	1.42	8 (10%)
13	CLA	A	1135	1	56,60,73	1.37	9 (16%)	67,97,113	1.55	11 (16%)
13	CLA	B	1213	2	69,73,73	1.22	11 (15%)	83,113,113	1.42	11 (13%)
13	CLA	4	512	12	49,53,73	1.49	8 (16%)	59,89,113	1.50	4 (6%)
13	CLA	Y	502	12	64,68,73	1.31	8 (12%)	77,107,113	1.38	7 (9%)
19	LMG	B	5002	-	54,54,55	0.79	2 (3%)	62,62,63	1.43	10 (16%)
13	CLA	H	1012	21	69,73,73	1.27	11 (15%)	83,113,113	1.38	9 (10%)
13	CLA	1	518	12	64,68,73	1.28	10 (15%)	77,107,113	1.43	8 (10%)
13	CLA	3	508	12	59,63,73	1.38	10 (16%)	71,101,113	1.44	9 (12%)
13	CLA	f	1234	2	69,73,73	1.28	11 (15%)	83,113,113	1.54	14 (16%)
16	BCR	q	523	-	41,41,41	0.71	0	56,56,56	1.64	16 (28%)
13	CLA	r	503	12	69,73,73	1.26	9 (13%)	83,113,113	1.33	7 (8%)
13	CLA	d	516	12	49,53,73	1.50	8 (16%)	59,89,113	1.46	6 (10%)
16	BCR	A	4008	-	41,41,41	0.84	1 (2%)	56,56,56	2.03	17 (30%)
13	CLA	B	1206	2	69,73,73	1.25	11 (15%)	83,113,113	1.45	6 (7%)
13	CLA	J	1303	8	69,73,73	1.24	9 (13%)	83,113,113	1.39	10 (12%)
13	CLA	a	510	12	69,73,73	1.25	8 (11%)	83,113,113	1.35	9 (10%)
13	CLA	G	1127	1	69,73,73	1.23	9 (13%)	83,113,113	1.35	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	1240	17	69,73,73	1.26	9 (13%)	83,113,113	1.34	9 (10%)
13	CLA	B	1222	21	64,68,73	1.28	10 (15%)	77,107,113	1.39	10 (12%)
16	BCR	Y	521	-	41,41,41	0.65	0	56,56,56	1.80	11 (19%)
13	CLA	e	1116	1	64,68,73	1.30	10 (15%)	77,107,113	1.34	8 (10%)
13	CLA	r	519	12	59,63,73	1.35	9 (15%)	71,101,113	1.39	8 (11%)
13	CLA	r	505	12	69,73,73	1.23	8 (11%)	83,113,113	1.27	6 (7%)
16	BCR	e	4011	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
16	BCR	V	4020	-	41,41,41	0.83	0	56,56,56	1.95	16 (28%)
13	CLA	A	1109	1	69,73,73	1.23	9 (13%)	83,113,113	1.41	5 (6%)
13	CLA	U	1105	9	49,53,73	1.50	9 (18%)	59,89,113	1.69	9 (15%)
13	CLA	s	516	12	49,53,73	1.50	8 (16%)	59,89,113	1.69	10 (16%)
15	SF4	g	3002	3	0,12,12	-	-	-	-	-
13	CLA	U	1103	9	54,58,73	1.40	9 (16%)	65,95,113	1.57	11 (16%)
17	LHG	e	5006	-	44,44,48	0.62	0	47,50,54	1.26	5 (10%)
17	LHG	n	5221	-	48,48,48	0.65	2 (4%)	51,54,54	1.30	6 (11%)
13	CLA	B	1226	2	69,73,73	1.34	11 (15%)	83,113,113	1.67	16 (19%)
13	CLA	A	1110	1	55,59,73	1.40	10 (18%)	66,96,113	1.48	6 (9%)
13	CLA	B	1210	2	69,73,73	1.25	9 (13%)	83,113,113	1.41	11 (13%)
17	LHG	L	5218	-	37,37,48	0.75	2 (5%)	40,43,54	1.23	4 (10%)
13	CLA	A	1137	1	69,73,73	1.24	8 (11%)	83,113,113	1.42	7 (8%)
13	CLA	f	1215	2	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
13	CLA	e	1013	-	69,73,73	1.27	11 (15%)	83,113,113	1.56	10 (12%)
18	LMU	G	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.00	2 (7%)
16	BCR	2	524	-	41,41,41	0.73	0	56,56,56	1.67	12 (21%)
16	BCR	1	521	-	41,41,41	0.66	0	56,56,56	1.81	11 (19%)
17	LHG	L	5221	-	48,48,48	0.65	2 (4%)	51,54,54	1.30	6 (11%)
13	CLA	q	509	12	69,73,73	1.24	10 (14%)	83,113,113	1.36	7 (8%)
14	PQN	H	2002	-	34,34,34	2.87	11 (32%)	42,45,45	2.17	4 (9%)
13	CLA	c	512	12	49,53,73	1.47	9 (18%)	59,89,113	1.47	6 (10%)
13	CLA	H	1228	2	59,63,73	1.30	9 (15%)	71,101,113	1.50	10 (14%)
13	CLA	Z	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.43	7 (9%)
13	CLA	G	1013	-	69,73,73	1.28	11 (15%)	83,113,113	1.56	10 (12%)
13	CLA	2	519	12	59,63,73	1.35	10 (16%)	71,101,113	1.39	8 (11%)
13	CLA	a	505	12	69,73,73	1.24	8 (11%)	83,113,113	1.26	4 (4%)
13	CLA	b	508	12	49,53,73	1.50	9 (18%)	59,89,113	1.57	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	d	506	12	49,53,73	1.50	9 (18%)	59,89,113	1.48	6 (10%)
13	CLA	t	518	12	59,63,73	1.36	9 (15%)	71,101,113	1.39	5 (7%)
16	BCR	L	4219	-	41,41,41	0.78	0	56,56,56	1.80	12 (21%)
16	BCR	f	4014	-	41,41,41	0.74	0	56,56,56	1.84	13 (23%)
13	CLA	J	1302	8	62,66,73	1.29	9 (14%)	74,104,113	1.41	6 (8%)
13	CLA	t	501	12	64,68,73	1.31	7 (10%)	77,107,113	1.34	4 (5%)
13	CLA	2	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.43	7 (9%)
13	CLA	Z	507	-	69,73,73	1.23	8 (11%)	83,113,113	1.38	6 (7%)
16	BCR	Z	521	-	41,41,41	0.66	0	56,56,56	1.86	11 (19%)
13	CLA	H	1021	2	69,73,73	1.24	10 (14%)	83,113,113	1.36	8 (9%)
13	CLA	H	1236	2	59,63,73	1.35	8 (13%)	71,101,113	1.30	6 (8%)
13	CLA	s	504	-	49,53,73	1.47	9 (18%)	59,89,113	1.53	7 (11%)
13	CLA	Z	510	12	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)
13	CLA	n	1501	10	69,73,73	1.24	9 (13%)	83,113,113	1.40	8 (9%)
18	LMU	G	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.07	2 (4%)
13	CLA	H	1201	2	64,68,73	1.27	10 (15%)	77,107,113	1.50	9 (11%)
16	BCR	A	4007	-	41,41,41	0.74	0	56,56,56	2.11	18 (32%)
13	CLA	n	1503	21	64,68,73	1.28	10 (15%)	77,107,113	1.39	6 (7%)
13	CLA	s	510	12	69,73,73	1.25	8 (11%)	83,113,113	1.34	9 (10%)
13	CLA	A	1131	1	69,73,73	1.22	9 (13%)	83,113,113	1.34	7 (8%)
13	CLA	Y	513	12	59,63,73	1.35	10 (16%)	71,101,113	1.36	5 (7%)
13	CLA	e	1121	1	59,63,73	1.35	9 (15%)	71,101,113	1.47	10 (14%)
16	BCR	T	4012	-	41,41,41	0.70	0	56,56,56	1.66	13 (23%)
16	BCR	v	522	-	41,41,41	0.69	0	56,56,56	1.84	15 (26%)
13	CLA	c	518	12	59,63,73	1.34	9 (15%)	71,101,113	1.34	5 (7%)
13	CLA	3	512	12	49,53,73	1.47	9 (18%)	59,89,113	1.49	4 (6%)
13	CLA	L	1503	21	64,68,73	1.28	10 (15%)	77,107,113	1.39	6 (7%)
13	CLA	t	505	12	69,73,73	1.24	8 (11%)	83,113,113	1.27	4 (4%)
13	CLA	A	1136	1	64,68,73	1.29	8 (12%)	77,107,113	1.47	10 (12%)
13	CLA	A	1111	1	69,73,73	1.26	10 (14%)	83,113,113	1.37	8 (9%)
13	CLA	e	1110	1	55,59,73	1.40	10 (18%)	66,96,113	1.49	6 (9%)
16	BCR	l	4015	-	41,41,41	0.79	0	56,56,56	1.82	14 (25%)
13	CLA	G	1118	1	64,68,73	1.28	9 (14%)	77,107,113	1.40	8 (10%)
16	BCR	1	524	-	41,41,41	0.73	0	56,56,56	1.82	15 (26%)
13	CLA	A	1127	1	69,73,73	1.23	9 (13%)	83,113,113	1.35	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	b	522	-	41,41,41	0.74	0	56,56,56	1.85	18 (32%)
13	CLA	Z	512	12	57,61,73	1.37	8 (14%)	68,98,113	1.38	4 (5%)
13	CLA	1	519	12	54,58,73	1.40	10 (18%)	65,95,113	1.45	8 (12%)
13	CLA	f	1222	21	64,68,73	1.28	10 (15%)	77,107,113	1.39	10 (12%)
13	CLA	5	506	12	49,53,73	1.49	9 (18%)	59,89,113	1.50	5 (8%)
13	CLA	A	1126	1	69,73,73	1.20	10 (14%)	83,113,113	1.40	8 (9%)
20	SQD	B	1852	-	44,45,54	1.02	4 (9%)	53,56,65	1.84	14 (26%)
16	BCR	q	522	-	41,41,41	0.74	0	56,56,56	1.90	19 (33%)
13	CLA	2	503	12	69,73,73	1.26	8 (11%)	83,113,113	1.33	7 (8%)
13	CLA	r	504	-	54,58,73	1.40	10 (18%)	65,95,113	1.45	7 (10%)
16	BCR	4	524	-	41,41,41	0.67	0	56,56,56	1.84	15 (26%)
19	LMG	f	5002	-	54,54,55	0.80	3 (5%)	62,62,63	1.43	10 (16%)
13	CLA	B	1231	21	69,73,73	1.20	9 (13%)	83,113,113	1.41	8 (9%)
13	CLA	2	507	-	69,73,73	1.22	8 (11%)	83,113,113	1.38	6 (7%)
16	BCR	B	4006	-	41,41,41	0.72	0	56,56,56	1.99	19 (33%)
13	CLA	3	516	12	49,53,73	1.49	8 (16%)	59,89,113	1.69	10 (16%)
13	CLA	H	1211	2	60,64,73	1.32	7 (11%)	72,102,113	1.60	5 (6%)
13	CLA	H	1232	21	54,58,73	1.39	11 (20%)	65,95,113	1.60	7 (10%)
13	CLA	Z	502	12	64,68,73	1.30	8 (12%)	77,107,113	1.39	8 (10%)
17	LHG	A	5002	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	5 (12%)
13	CLA	v	513	12	49,53,73	1.50	6 (12%)	59,89,113	1.42	5 (8%)
13	CLA	d	507	-	49,53,73	1.47	8 (16%)	59,89,113	1.51	7 (11%)
13	CLA	f	1227	2	69,73,73	1.23	10 (14%)	83,113,113	1.40	8 (9%)
13	CLA	v	509	12	49,53,73	1.50	8 (16%)	59,89,113	1.46	5 (8%)
13	CLA	A	1124	21	60,64,73	1.36	9 (15%)	72,102,113	1.48	13 (18%)
13	CLA	e	1111	1	69,73,73	1.26	10 (14%)	83,113,113	1.37	8 (9%)
13	CLA	1	501	12	69,73,73	1.25	10 (14%)	83,113,113	1.35	7 (8%)
13	CLA	5	503	12	59,63,73	1.36	8 (13%)	71,101,113	1.40	6 (8%)
13	CLA	a	504	-	49,53,73	1.47	9 (18%)	59,89,113	1.52	7 (11%)
13	CLA	H	1221	21	69,73,73	1.29	11 (15%)	83,113,113	1.50	13 (15%)
13	CLA	A	1133	1	69,73,73	1.20	9 (13%)	83,113,113	1.38	6 (7%)
13	CLA	G	1135	1	56,60,73	1.36	9 (16%)	67,97,113	1.55	11 (16%)
13	CLA	G	1237	21	69,73,73	1.25	9 (13%)	83,113,113	1.44	10 (12%)
15	SF4	N	3002	3	0,12,12	-	-	-	-	-
16	BCR	M	4021	-	41,41,41	0.71	0	56,56,56	1.82	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	5	505	12	65,69,73	1.28	7 (10%)	78,108,113	1.26	4 (5%)
13	CLA	e	1101	1	69,73,73	1.27	10 (14%)	83,113,113	1.40	8 (9%)
16	BCR	l	4012	-	41,41,41	0.70	0	56,56,56	1.66	13 (23%)
13	CLA	H	1240	17	69,73,73	1.26	9 (13%)	83,113,113	1.34	9 (10%)
13	CLA	l	503	12	68,72,73	1.27	8 (11%)	81,111,113	1.34	5 (6%)
13	CLA	s	517	-	49,53,73	1.47	10 (20%)	59,89,113	1.44	4 (6%)
13	CLA	q	513	12	59,63,73	1.34	10 (16%)	71,101,113	1.37	5 (7%)
16	BCR	6	522	-	41,41,41	0.70	0	56,56,56	1.84	14 (25%)
13	CLA	t	512	12	49,53,73	1.49	8 (16%)	59,89,113	1.49	4 (6%)
16	BCR	K	4104	-	41,41,41	0.74	0	56,56,56	1.86	15 (26%)
16	BCR	6	523	-	41,41,41	0.70	0	56,56,56	1.73	14 (25%)
17	LHG	A	5004	-	35,35,48	0.74	1 (2%)	38,41,54	1.25	4 (10%)
17	LHG	e	5003	13	40,40,48	0.74	1 (2%)	43,46,54	1.33	6 (13%)
16	BCR	l	4013	-	41,41,41	0.76	0	56,56,56	1.96	15 (26%)
13	CLA	A	1118	1	64,68,73	1.28	9 (14%)	77,107,113	1.41	8 (10%)
13	CLA	G	1011	1	69,73,73	1.25	8 (11%)	83,113,113	1.54	11 (13%)
13	CLA	e	1123	21	69,73,73	1.23	9 (13%)	83,113,113	1.36	9 (10%)
13	CLA	f	1239	2	69,73,73	1.25	8 (11%)	83,113,113	1.52	11 (13%)
13	CLA	l	1303	8	69,73,73	1.23	9 (13%)	83,113,113	1.39	9 (10%)
16	BCR	Z	523	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
16	BCR	u	521	-	41,41,41	0.68	0	56,56,56	1.94	16 (28%)
13	CLA	A	1104	1	69,73,73	1.23	10 (14%)	83,113,113	1.39	10 (12%)
13	CLA	e	1117	1	69,73,73	1.22	11 (15%)	83,113,113	1.56	12 (14%)
13	CLA	e	1103	1	69,73,73	1.24	8 (11%)	83,113,113	1.49	8 (9%)
13	CLA	H	1223	2	69,73,73	1.25	9 (13%)	83,113,113	1.40	6 (7%)
16	BCR	2	522	-	41,41,41	0.71	0	56,56,56	1.75	18 (32%)
13	CLA	B	1236	2	59,63,73	1.35	8 (13%)	71,101,113	1.30	6 (8%)
13	CLA	A	1128	1	69,73,73	1.32	10 (14%)	83,113,113	1.53	9 (10%)
16	BCR	f	4009	-	41,41,41	0.81	0	56,56,56	1.91	21 (37%)
13	CLA	a	503	12	69,73,73	1.27	9 (13%)	83,113,113	1.33	7 (8%)
13	CLA	B	1221	21	69,73,73	1.28	11 (15%)	83,113,113	1.50	13 (15%)
13	CLA	u	503	12	59,63,73	1.37	8 (13%)	71,101,113	1.40	6 (8%)
18	LMU	Y	902	-	19,19,36	1.22	1 (5%)	24,24,47	1.10	3 (12%)
13	CLA	e	1136	1	64,68,73	1.29	8 (12%)	77,107,113	1.47	10 (12%)
13	CLA	B	1211	2	60,64,73	1.32	8 (13%)	72,102,113	1.59	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	SQD	5	822	-	28,29,54	1.25	5 (17%)	37,40,65	1.92	13 (35%)
13	CLA	d	512	12	49,53,73	1.47	9 (18%)	59,89,113	1.48	4 (6%)
13	CLA	v	518	12	59,63,73	1.35	9 (15%)	71,101,113	1.38	6 (8%)
13	CLA	f	1236	2	59,63,73	1.35	8 (13%)	71,101,113	1.30	6 (8%)
13	CLA	5	516	12	49,53,73	1.49	9 (18%)	59,89,113	1.45	4 (6%)
13	CLA	b	517	-	49,53,73	1.49	8 (16%)	59,89,113	1.51	6 (10%)
14	PQN	f	2002	-	34,34,34	2.87	11 (32%)	42,45,45	2.18	4 (9%)
13	CLA	d	518	12	59,63,73	1.36	9 (15%)	71,101,113	1.38	6 (8%)
16	BCR	t	521	-	41,41,41	0.65	0	56,56,56	1.78	11 (19%)
16	BCR	t	523	-	41,41,41	0.69	0	56,56,56	1.65	13 (23%)
13	CLA	b	513	12	49,53,73	1.50	9 (18%)	59,89,113	1.48	4 (6%)
13	CLA	c	519	12	50,54,73	1.46	9 (18%)	60,90,113	1.46	5 (8%)
16	BCR	u	522	-	41,41,41	0.74	0	56,56,56	1.93	20 (35%)
17	LHG	B	1842	13	38,38,48	0.66	0	41,44,54	1.23	4 (9%)
13	CLA	e	1112	1	54,58,73	1.37	9 (16%)	65,95,113	1.58	9 (13%)
13	CLA	t	510	12	54,58,73	1.41	8 (14%)	65,95,113	1.49	5 (7%)
13	CLA	G	1116	1	64,68,73	1.30	10 (15%)	77,107,113	1.35	8 (10%)
13	CLA	m	1105	9	49,53,73	1.50	9 (18%)	59,89,113	1.69	9 (15%)
13	CLA	q	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.43	8 (11%)
13	CLA	r	510	12	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
13	CLA	H	1212	2	59,63,73	1.33	10 (16%)	71,101,113	1.47	7 (9%)
13	CLA	e	1113	1	49,53,73	1.42	9 (18%)	59,89,113	1.56	6 (10%)
20	SQD	Z	822	-	42,43,54	1.07	5 (11%)	51,54,65	1.61	10 (19%)
13	CLA	t	519	12	59,63,73	1.36	10 (16%)	71,101,113	1.42	5 (7%)
16	BCR	l	522	-	41,41,41	0.73	0	56,56,56	1.91	19 (33%)
13	CLA	f	1201	2	64,68,73	1.27	10 (15%)	77,107,113	1.50	9 (11%)
13	CLA	c	502	12	54,58,73	1.42	10 (18%)	65,95,113	1.46	6 (9%)
13	CLA	u	511	12	59,63,73	1.36	9 (15%)	71,101,113	1.40	7 (9%)
13	CLA	A	1801	17	49,53,73	1.51	10 (20%)	59,89,113	1.60	8 (13%)
13	CLA	f	1235	2	69,73,73	1.23	9 (13%)	83,113,113	1.43	8 (9%)
16	BCR	J	4012	-	41,41,41	0.70	0	56,56,56	1.66	13 (23%)
13	CLA	H	1229	2	69,73,73	1.24	10 (14%)	83,113,113	1.42	11 (13%)
18	LMU	A	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.07	2 (4%)
13	CLA	6	508	12	49,53,73	1.48	10 (20%)	59,89,113	1.50	7 (11%)
13	CLA	A	1102	1	69,73,73	1.21	9 (13%)	83,113,113	1.35	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	s	518	12	59,63,73	1.36	10 (16%)	71,101,113	1.38	5 (7%)
16	BCR	s	521	-	41,41,41	0.66	0	56,56,56	1.76	10 (17%)
13	CLA	f	1204	2	69,73,73	1.22	9 (13%)	83,113,113	1.30	7 (8%)
13	CLA	H	1224	2	64,68,73	1.27	9 (14%)	77,107,113	1.42	8 (10%)
13	CLA	H	1239	2	69,73,73	1.25	9 (13%)	83,113,113	1.54	12 (14%)
13	CLA	s	508	12	59,63,73	1.37	10 (16%)	71,101,113	1.44	9 (12%)
13	CLA	v	512	12	49,53,73	1.48	9 (18%)	59,89,113	1.47	4 (6%)
17	LHG	B	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.21	5 (10%)
13	CLA	f	1223	2	69,73,73	1.26	9 (13%)	83,113,113	1.40	6 (7%)
15	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
13	CLA	A	1132	1	69,73,73	1.23	11 (15%)	83,113,113	1.38	9 (10%)
16	BCR	H	4010	-	41,41,41	0.94	3 (7%)	56,56,56	2.28	23 (41%)
13	CLA	l	512	12	56,60,73	1.39	9 (16%)	67,97,113	1.44	5 (7%)
13	CLA	c	503	12	59,63,73	1.37	8 (13%)	71,101,113	1.40	6 (8%)
13	CLA	e	1129	1	55,59,73	1.38	9 (16%)	66,96,113	1.52	10 (15%)
18	LMU	f	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.11	3 (6%)
13	CLA	v	507	-	49,53,73	1.47	9 (18%)	59,89,113	1.51	7 (11%)
13	CLA	V	1503	21	64,68,73	1.28	10 (15%)	77,107,113	1.40	6 (7%)
13	CLA	v	511	12	49,53,73	1.49	9 (18%)	59,89,113	1.51	4 (6%)
16	BCR	s	522	-	41,41,41	0.68	0	56,56,56	1.91	15 (26%)
16	BCR	T	4013	-	41,41,41	0.76	0	56,56,56	1.96	15 (26%)
13	CLA	T	1303	8	69,73,73	1.24	9 (13%)	83,113,113	1.39	8 (9%)
13	CLA	G	1130	1	69,73,73	1.24	10 (14%)	83,113,113	1.40	11 (13%)
13	CLA	t	508	12	49,53,73	1.51	9 (18%)	59,89,113	1.57	9 (15%)
16	BCR	H	4004	-	41,41,41	0.72	0	56,56,56	1.85	13 (23%)
20	SQD	l	822	-	47,48,54	0.99	5 (10%)	56,59,65	1.74	13 (23%)
13	CLA	4	518	12	59,63,73	1.35	9 (15%)	71,101,113	1.39	5 (7%)
13	CLA	b	518	12	59,63,73	1.36	9 (15%)	71,101,113	1.40	5 (7%)
13	CLA	H	1214	2	69,73,73	1.25	10 (14%)	83,113,113	1.43	6 (7%)
13	CLA	e	1107	1	69,73,73	1.24	11 (15%)	83,113,113	1.36	11 (13%)
13	CLA	j	1301	21	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
13	CLA	G	1111	1	69,73,73	1.26	10 (14%)	83,113,113	1.37	8 (9%)
13	CLA	G	1119	21	69,73,73	1.27	10 (14%)	83,113,113	1.40	10 (12%)
13	CLA	r	508	12	59,63,73	1.36	10 (16%)	71,101,113	1.44	9 (12%)
13	CLA	u	519	12	50,54,73	1.46	9 (18%)	60,90,113	1.46	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	1120	1	57,61,73	1.34	11 (19%)	68,98,113	1.51	7 (10%)
13	CLA	A	1116	1	64,68,73	1.30	9 (14%)	77,107,113	1.35	8 (10%)
13	CLA	Z	513	12	69,73,73	1.26	10 (14%)	83,113,113	1.29	6 (7%)
13	CLA	Z	509	12	69,73,73	1.26	10 (14%)	83,113,113	1.34	7 (8%)
13	CLA	s	519	12	59,63,73	1.34	10 (16%)	71,101,113	1.40	5 (7%)
16	BCR	v	521	-	41,41,41	0.66	0	56,56,56	1.91	12 (21%)
13	CLA	A	1105	1	59,63,73	1.30	10 (16%)	71,101,113	1.51	10 (14%)
13	CLA	G	1108	1	58,62,73	1.36	10 (17%)	69,99,113	1.35	6 (8%)
13	CLA	e	1122	1	64,68,73	1.28	9 (14%)	77,107,113	1.43	8 (10%)
13	CLA	q	507	-	64,68,73	1.29	8 (12%)	77,107,113	1.41	8 (10%)
13	CLA	A	1237	21	69,73,73	1.25	9 (13%)	83,113,113	1.44	10 (12%)
13	CLA	H	1023	-	69,73,73	1.24	11 (15%)	83,113,113	1.70	16 (19%)
16	BCR	t	522	-	41,41,41	0.73	0	56,56,56	1.85	18 (32%)
17	LHG	A	5006	-	44,44,48	0.62	0	47,50,54	1.26	5 (10%)
13	CLA	d	502	12	54,58,73	1.41	8 (14%)	65,95,113	1.48	5 (7%)
15	SF4	C	3003	3	0,12,12	-	-	-	-	-
13	CLA	H	1220	2	59,63,73	1.31	9 (15%)	71,101,113	1.54	9 (12%)
13	CLA	f	1207	2	69,73,73	1.25	10 (14%)	83,113,113	1.30	4 (4%)
16	BCR	G	4008	-	41,41,41	0.84	1 (2%)	56,56,56	2.03	16 (28%)
13	CLA	a	508	12	59,63,73	1.38	9 (15%)	71,101,113	1.45	9 (12%)
13	CLA	Y	506	12	49,53,73	1.48	7 (14%)	59,89,113	1.47	6 (10%)
13	CLA	6	501	12	64,68,73	1.29	8 (12%)	77,107,113	1.40	5 (6%)
16	BCR	3	524	-	41,41,41	0.74	0	56,56,56	1.81	17 (30%)
16	BCR	v	524	-	41,41,41	0.76	0	56,56,56	1.87	13 (23%)
13	CLA	b	512	12	49,53,73	1.48	8 (16%)	59,89,113	1.50	4 (6%)
13	CLA	G	1117	1	69,73,73	1.22	11 (15%)	83,113,113	1.56	12 (14%)
13	CLA	t	502	12	54,58,73	1.41	8 (14%)	65,95,113	1.48	5 (7%)
16	BCR	B	4010	-	41,41,41	0.94	3 (7%)	56,56,56	2.28	23 (41%)
16	BCR	c	522	-	41,41,41	0.74	0	56,56,56	1.93	20 (35%)
18	LMU	J	5105	-	22,22,36	1.14	1 (4%)	27,27,47	0.81	0
16	BCR	L	4019	-	41,41,41	0.73	0	56,56,56	1.92	14 (25%)
13	CLA	3	509	12	69,73,73	1.25	10 (14%)	83,113,113	1.37	8 (9%)
13	CLA	5	510	12	49,53,73	1.48	9 (18%)	59,89,113	1.46	5 (8%)
17	LHG	e	5005	-	44,44,48	0.67	1 (2%)	47,50,54	1.27	6 (12%)
17	LHG	e	5001	-	48,48,48	0.78	1 (2%)	51,54,54	1.26	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	u	508	12	49,53,73	1.49	9 (18%)	59,89,113	1.55	6 (10%)
13	CLA	s	503	12	69,73,73	1.27	9 (13%)	83,113,113	1.32	7 (8%)
13	CLA	6	505	12	69,73,73	1.24	8 (11%)	83,113,113	1.30	4 (4%)
13	CLA	A	1125	1	69,73,73	1.24	10 (14%)	83,113,113	1.43	9 (10%)
13	CLA	c	516	12	49,53,73	1.50	9 (18%)	59,89,113	1.45	4 (6%)
13	CLA	r	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.50	4 (6%)
13	CLA	b	507	-	49,53,73	1.47	7 (14%)	59,89,113	1.53	7 (11%)
13	CLA	t	509	12	69,73,73	1.26	8 (11%)	83,113,113	1.38	6 (7%)
16	BCR	q	524	-	41,41,41	0.73	0	56,56,56	1.82	15 (26%)
16	BCR	B	4014	-	41,41,41	0.74	0	56,56,56	1.85	13 (23%)
13	CLA	r	509	12	69,73,73	1.26	10 (14%)	83,113,113	1.35	7 (8%)
13	CLA	Z	506	12	59,63,73	1.36	10 (16%)	71,101,113	1.40	6 (8%)
13	CLA	s	513	12	69,73,73	1.25	9 (13%)	83,113,113	1.34	5 (6%)
20	SQD	H	1852	-	44,45,54	1.02	4 (9%)	53,56,65	1.84	14 (26%)
13	CLA	A	1119	21	69,73,73	1.26	10 (14%)	83,113,113	1.40	10 (12%)
13	CLA	f	1220	2	59,63,73	1.31	9 (15%)	71,101,113	1.54	9 (12%)
13	CLA	b	510	12	54,58,73	1.41	8 (14%)	65,95,113	1.48	5 (7%)
13	CLA	2	502	12	64,68,73	1.31	8 (12%)	77,107,113	1.39	7 (9%)
13	CLA	H	1208	2	69,73,73	1.21	9 (13%)	83,113,113	1.32	7 (8%)
13	CLA	f	1209	2	56,60,73	1.38	9 (16%)	67,97,113	1.56	7 (10%)
13	CLA	H	1205	2	69,73,73	1.24	10 (14%)	83,113,113	1.44	8 (9%)
13	CLA	G	1122	1	64,68,73	1.28	9 (14%)	77,107,113	1.43	8 (10%)
13	CLA	f	1218	2	64,68,73	1.27	9 (14%)	77,107,113	1.39	5 (6%)
13	CLA	f	1203	2	69,73,73	1.26	12 (17%)	83,113,113	1.34	8 (9%)
13	CLA	A	1114	21	54,58,73	1.42	10 (18%)	65,95,113	1.50	7 (10%)
13	CLA	4	501	12	64,68,73	1.31	8 (12%)	77,107,113	1.34	4 (5%)
13	CLA	r	511	12	59,63,73	1.37	9 (15%)	71,101,113	1.43	7 (9%)
19	LMG	H	5002	-	54,54,55	0.79	2 (3%)	62,62,63	1.43	10 (16%)
16	BCR	I	4018	-	41,41,41	0.77	0	56,56,56	1.84	15 (26%)
16	BCR	A	4011	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
17	LHG	G	5004	-	35,35,48	0.74	1 (2%)	38,41,54	1.25	4 (10%)
13	CLA	2	510	12	69,73,73	1.25	8 (11%)	83,113,113	1.31	7 (8%)
13	CLA	a	509	12	69,73,73	1.26	10 (14%)	83,113,113	1.36	8 (9%)
13	CLA	G	1136	1	64,68,73	1.29	8 (12%)	77,107,113	1.47	10 (12%)
13	CLA	G	1125	1	69,73,73	1.24	10 (14%)	83,113,113	1.43	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	LMG	J	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.25	7 (16%)
13	CLA	u	517	-	49,53,73	1.49	10 (20%)	59,89,113	1.40	4 (6%)
13	CLA	A	1013	-	69,73,73	1.27	11 (15%)	83,113,113	1.56	10 (12%)
13	CLA	H	1225	2	69,73,73	1.23	11 (15%)	83,113,113	1.30	8 (9%)
13	CLA	c	510	12	49,53,73	1.48	9 (18%)	59,89,113	1.46	5 (8%)
20	SQD	n	5216	-	50,51,54	0.97	5 (10%)	59,62,65	1.63	11 (18%)
16	BCR	b	524	-	41,41,41	0.67	0	56,56,56	1.85	15 (26%)
13	CLA	4	516	12	49,53,73	1.49	8 (16%)	59,89,113	1.43	5 (8%)
13	CLA	G	1128	1	69,73,73	1.32	10 (14%)	83,113,113	1.53	8 (9%)
13	CLA	v	504	-	49,53,73	1.48	7 (14%)	59,89,113	1.51	8 (13%)
13	CLA	B	1209	2	56,60,73	1.38	9 (16%)	67,97,113	1.56	7 (10%)
13	CLA	a	517	-	49,53,73	1.47	10 (20%)	59,89,113	1.45	4 (6%)
13	CLA	t	517	-	49,53,73	1.49	9 (18%)	59,89,113	1.51	6 (10%)
16	BCR	f	4010	-	41,41,41	0.94	3 (7%)	56,56,56	2.28	23 (41%)
13	CLA	5	508	12	49,53,73	1.49	9 (18%)	59,89,113	1.55	5 (8%)
13	CLA	d	503	12	56,60,73	1.39	9 (16%)	67,97,113	1.44	7 (10%)
13	CLA	V	1501	10	69,73,73	1.24	9 (13%)	83,113,113	1.40	8 (9%)
20	SQD	L	5216	-	50,51,54	0.97	5 (10%)	59,62,65	1.63	11 (18%)
18	LMU	B	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.11	3 (6%)
13	CLA	t	513	12	49,53,73	1.50	10 (20%)	59,89,113	1.47	4 (6%)
18	LMU	2	901	-	23,23,36	1.10	1 (4%)	28,28,47	0.94	0
13	CLA	u	509	12	69,73,73	1.25	10 (14%)	83,113,113	1.34	8 (9%)
13	CLA	B	1208	2	69,73,73	1.21	8 (11%)	83,113,113	1.32	7 (8%)
13	CLA	6	512	12	49,53,73	1.47	9 (18%)	59,89,113	1.47	4 (6%)
13	CLA	Y	503	12	68,72,73	1.27	9 (13%)	81,111,113	1.34	6 (7%)
13	CLA	t	506	12	49,53,73	1.50	9 (18%)	59,89,113	1.50	5 (8%)
13	CLA	d	505	12	69,73,73	1.25	8 (11%)	83,113,113	1.30	4 (4%)
16	BCR	e	4003	-	41,41,41	0.78	0	56,56,56	1.73	11 (19%)
13	CLA	a	516	12	49,53,73	1.49	8 (16%)	59,89,113	1.69	10 (16%)
13	CLA	B	1220	2	59,63,73	1.31	9 (15%)	71,101,113	1.54	9 (12%)
20	SQD	3	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.59	12 (23%)
13	CLA	A	1121	1	59,63,73	1.34	9 (15%)	71,101,113	1.48	10 (14%)
17	LHG	G	5006	-	44,44,48	0.62	0	47,50,54	1.25	5 (10%)
13	CLA	e	1134	1	60,64,73	1.31	9 (15%)	72,102,113	1.44	6 (8%)
13	CLA	H	1234	2	69,73,73	1.28	11 (15%)	83,113,113	1.53	14 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	1	509	12	69,73,73	1.25	10 (14%)	83,113,113	1.36	7 (8%)
13	CLA	6	504	-	49,53,73	1.49	7 (14%)	59,89,113	1.51	9 (15%)
16	BCR	a	523	-	41,41,41	0.69	0	56,56,56	1.76	15 (26%)
17	LHG	A	5003	13	40,40,48	0.74	1 (2%)	43,46,54	1.34	6 (13%)
20	SQD	f	1852	-	44,45,54	1.01	4 (9%)	53,56,65	1.84	14 (26%)
13	CLA	c	504	-	49,53,73	1.48	8 (16%)	59,89,113	1.48	5 (8%)
13	CLA	5	518	12	59,63,73	1.35	9 (15%)	71,101,113	1.34	5 (7%)
13	CLA	s	501	12	69,73,73	1.25	9 (13%)	83,113,113	1.38	6 (7%)
13	CLA	H	1215	2	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
13	CLA	r	513	12	69,73,73	1.26	10 (14%)	83,113,113	1.30	5 (6%)
17	LHG	n	5218	-	37,37,48	0.75	2 (5%)	40,43,54	1.23	4 (10%)
13	CLA	q	518	12	64,68,73	1.28	9 (14%)	77,107,113	1.43	8 (10%)
14	PQN	A	2001	-	34,34,34	2.88	11 (32%)	42,45,45	2.11	7 (16%)
13	CLA	4	510	12	54,58,73	1.41	8 (14%)	65,95,113	1.48	5 (7%)
13	CLA	G	1801	17	49,53,73	1.51	10 (20%)	59,89,113	1.60	8 (13%)
13	CLA	5	501	12	69,73,73	1.24	8 (11%)	83,113,113	1.37	5 (6%)
13	CLA	6	507	-	49,53,73	1.47	8 (16%)	59,89,113	1.51	7 (11%)
13	CLA	G	1140	1	69,73,73	1.27	10 (14%)	83,113,113	1.40	11 (13%)
16	BCR	H	4009	-	41,41,41	0.81	0	56,56,56	1.91	21 (37%)
13	CLA	Y	519	12	54,58,73	1.40	10 (18%)	65,95,113	1.45	8 (12%)
16	BCR	u	524	-	41,41,41	0.68	0	56,56,56	1.67	14 (25%)
13	CLA	G	1102	1	69,73,73	1.21	9 (13%)	83,113,113	1.35	7 (8%)
13	CLA	L	1501	10	69,73,73	1.24	9 (13%)	83,113,113	1.40	8 (9%)
13	CLA	e	1138	1	69,73,73	1.21	10 (14%)	83,113,113	1.35	7 (8%)
13	CLA	f	1012	21	69,73,73	1.26	11 (15%)	83,113,113	1.38	9 (10%)
20	SQD	q	822	-	47,48,54	0.99	5 (10%)	56,59,65	1.74	13 (23%)
13	CLA	H	1226	2	69,73,73	1.34	11 (15%)	83,113,113	1.67	15 (18%)
13	CLA	G	1112	1	54,58,73	1.37	9 (16%)	65,95,113	1.58	10 (15%)
13	CLA	j	1302	6	49,53,73	1.47	8 (16%)	59,89,113	1.47	4 (6%)
16	BCR	6	521	-	41,41,41	0.66	0	56,56,56	1.91	12 (21%)
17	LHG	H	1842	13	38,38,48	0.66	0	41,44,54	1.23	4 (9%)
13	CLA	G	1113	1	49,53,73	1.43	9 (18%)	59,89,113	1.56	6 (10%)
16	BCR	G	4001	-	41,41,41	0.76	0	56,56,56	1.72	11 (19%)
13	CLA	r	501	12	69,73,73	1.25	10 (14%)	83,113,113	1.37	6 (7%)
13	CLA	B	1205	2	69,73,73	1.24	10 (14%)	83,113,113	1.43	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	e	1139	21	69,73,73	1.25	10 (14%)	83,113,113	1.28	8 (9%)
13	CLA	H	1235	2	69,73,73	1.24	9 (13%)	83,113,113	1.43	8 (9%)
13	CLA	t	507	-	49,53,73	1.48	7 (14%)	59,89,113	1.55	7 (11%)
13	CLA	v	517	-	49,53,73	1.48	8 (16%)	59,89,113	1.45	4 (6%)
18	LMU	q	902	-	19,19,36	1.22	1 (5%)	24,24,47	1.10	3 (12%)
16	BCR	6	524	-	41,41,41	0.75	0	56,56,56	1.86	13 (23%)
17	LHG	G	5001	-	48,48,48	0.78	1 (2%)	51,54,54	1.26	6 (11%)
13	CLA	A	1101	1	69,73,73	1.27	10 (14%)	83,113,113	1.40	8 (9%)
18	LMU	l	5105	-	22,22,36	1.14	1 (4%)	27,27,47	0.81	0
13	CLA	d	504	-	49,53,73	1.49	7 (14%)	59,89,113	1.51	8 (13%)
13	CLA	Y	516	12	49,53,73	1.49	9 (18%)	59,89,113	1.65	8 (13%)
13	CLA	e	1022	21	69,73,73	1.27	10 (14%)	83,113,113	1.32	9 (10%)
13	CLA	B	1204	2	69,73,73	1.22	9 (13%)	83,113,113	1.31	7 (8%)
13	CLA	G	1120	1	57,61,73	1.34	11 (19%)	68,98,113	1.52	7 (10%)
16	BCR	Z	524	-	41,41,41	0.74	0	56,56,56	1.67	12 (21%)

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
13	CLA	Y	501	12	-	20/39/115/115	-
20	SQD	b	822	-	-	8/19/39/69	0/1/1/1
13	CLA	l	511	12	-	4/27/103/115	-
13	CLA	f	1232	21	-	6/21/97/115	-
17	LHG	I	5001	-	-	22/48/48/53	-
16	BCR	n	4022	-	-	2/29/63/63	0/2/2/2
13	CLA	f	1205	2	-	12/39/115/115	-
16	BCR	F	4016	-	-	2/29/63/63	0/2/2/2
13	CLA	G	1129	1	-	7/23/99/115	-
16	BCR	r	521	-	-	4/29/63/63	0/2/2/2
13	CLA	c	505	12	-	16/35/111/115	-
13	CLA	A	1117	1	-	13/39/115/115	-
18	LMU	A	1849	-	-	6/14/34/61	0/1/1/2
13	CLA	u	516	12	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	4	522	-	-	4/29/63/63	0/2/2/2
13	CLA	Y	505	12	-	11/39/115/115	-
17	LHG	e	5009	-	-	28/53/53/53	-
16	BCR	v	523	-	-	4/29/63/63	0/2/2/2
13	CLA	5	512	12	-	7/15/91/115	-
13	CLA	B	1223	2	-	14/39/115/115	-
13	CLA	d	510	12	-	9/15/91/115	-
13	CLA	a	511	12	-	7/21/97/115	-
13	CLA	A	1107	1	-	16/39/115/115	-
16	BCR	f	4005	-	-	6/29/63/63	0/2/2/2
13	CLA	d	519	12	-	8/17/93/115	-
13	CLA	Y	510	12	-	13/39/115/115	-
16	BCR	Z	522	-	-	6/29/63/63	0/2/2/2
13	CLA	A	1112	1	-	5/21/97/115	-
13	CLA	5	513	12	-	6/15/91/115	-
17	LHG	G	5003	13	-	16/45/45/53	-
13	CLA	A	1122	1	-	16/33/109/115	-
13	CLA	H	1210	2	-	21/39/115/115	-
13	CLA	v	506	12	-	7/15/91/115	-
16	BCR	T	4015	-	-	5/29/63/63	0/2/2/2
13	CLA	4	504	-	-	7/15/91/115	-
13	CLA	4	517	-	-	7/15/91/115	-
18	LMU	T	5105	-	-	8/13/33/61	0/1/1/2
13	CLA	e	1115	1	-	12/33/109/115	-
16	BCR	a	521	-	-	7/29/63/63	0/2/2/2
13	CLA	f	1228	2	-	8/27/103/115	-
13	CLA	A	1123	21	-	11/39/115/115	-
13	CLA	B	1218	2	-	7/33/109/115	-
13	CLA	G	1131	1	-	8/39/115/115	-
16	BCR	s	523	-	-	4/29/63/63	0/2/2/2
13	CLA	6	502	12	-	7/21/97/115	-
13	CLA	G	1105	1	-	6/27/103/115	-
13	CLA	G	1114	21	-	2/21/97/115	-
13	CLA	e	1104	1	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	q	505	12	-	11/39/115/115	-
17	LHG	e	5008	-	-	19/39/39/53	-
20	SQD	4	822	-	-	8/19/39/69	0/1/1/1
16	BCR	f	4006	-	-	4/29/63/63	0/2/2/2
20	SQD	V	5216	-	-	17/46/66/69	0/1/1/1
13	CLA	v	502	12	-	7/21/97/115	-
13	CLA	m	1401	-	-	10/27/103/115	-
13	CLA	H	1219	2	-	19/39/115/115	-
13	CLA	q	506	12	-	6/15/91/115	-
13	CLA	Z	517	-	-	6/15/91/115	-
13	CLA	u	501	12	-	21/39/115/115	-
13	CLA	V	1502	10	-	10/39/115/115	-
20	SQD	2	822	-	-	13/38/58/69	0/1/1/1
13	CLA	6	509	12	-	5/15/91/115	-
13	CLA	A	1129	1	-	7/23/99/115	-
13	CLA	d	508	12	-	5/15/91/115	-
16	BCR	j	4016	-	-	2/29/63/63	0/2/2/2
16	BCR	b	523	-	-	5/29/63/63	0/2/2/2
13	CLA	G	1109	1	-	11/39/115/115	-
13	CLA	e	1106	1	-	23/39/115/115	-
13	CLA	H	1216	21	-	7/33/109/115	-
13	CLA	t	511	12	-	5/15/91/115	-
13	CLA	G	1101	1	-	13/39/115/115	-
13	CLA	u	512	12	-	7/15/91/115	-
16	BCR	r	522	-	-	6/29/63/63	0/2/2/2
20	SQD	u	822	-	-	7/24/44/69	0/1/1/1
13	CLA	q	516	12	-	15/15/91/115	-
19	LMG	l	5104	-	-	17/30/50/70	0/1/1/1
13	CLA	3	517	-	-	9/15/91/115	-
16	BCR	c	521	-	-	7/29/63/63	0/2/2/2
13	CLA	b	506	12	-	4/15/91/115	-
16	BCR	e	4001	-	-	8/29/63/63	0/2/2/2
16	BCR	t	524	-	-	4/29/63/63	0/2/2/2
13	CLA	3	510	12	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	G	1110	1	-	11/23/99/115	-
13	CLA	f	1021	2	-	13/39/115/115	-
16	BCR	r	524	-	-	2/29/63/63	0/2/2/2
16	BCR	Y	523	-	-	6/29/63/63	0/2/2/2
13	CLA	m	1103	9	-	9/21/97/115	-
13	CLA	2	517	-	-	6/15/91/115	-
13	CLA	e	1140	1	-	13/39/115/115	-
13	CLA	4	505	12	-	13/39/115/115	-
13	CLA	b	504	-	-	7/15/91/115	-
13	CLA	4	513	12	-	9/15/91/115	-
16	BCR	b	521	-	-	10/29/63/63	0/2/2/2
16	BCR	V	4019	-	-	6/29/63/63	0/2/2/2
13	CLA	B	1012	21	-	16/39/115/115	-
13	CLA	6	517	-	-	11/15/91/115	-
13	CLA	H	1231	21	-	8/39/115/115	-
13	CLA	2	512	12	-	7/25/101/115	-
13	CLA	f	1211	2	-	4/29/105/115	-
16	BCR	S	4018	-	-	1/29/63/63	0/2/2/2
13	CLA	q	504	-	-	7/15/91/115	-
13	CLA	G	1139	21	-	14/39/115/115	-
13	CLA	1	507	-	-	16/33/109/115	-
13	CLA	b	502	12	-	7/21/97/115	-
16	BCR	n	4219	-	-	2/29/63/63	0/2/2/2
17	LHG	f	1842	13	-	22/43/43/53	-
16	BCR	a	524	-	-	5/29/63/63	0/2/2/2
13	CLA	d	509	12	-	6/15/91/115	-
16	BCR	5	522	-	-	5/29/63/63	0/2/2/2
20	SQD	6	822	-	-	9/19/39/69	0/1/1/1
13	CLA	B	1239	2	-	17/39/115/115	-
13	CLA	u	505	12	-	16/35/111/115	-
16	BCR	r	523	-	-	6/29/63/63	0/2/2/2
17	LHG	A	5005	-	-	29/49/49/53	-
17	LHG	A	5001	-	-	25/53/53/53	-
16	BCR	G	4003	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	v	519	12	-	8/17/93/115	-
16	BCR	W	4021	-	-	7/29/63/63	0/2/2/2
13	CLA	c	511	12	-	7/27/103/115	-
13	CLA	1	505	12	-	11/39/115/115	-
13	CLA	s	509	12	-	4/39/115/115	-
13	CLA	s	502	12	-	6/21/97/115	-
17	LHG	V	5221	-	-	30/53/53/53	-
13	CLA	2	516	12	-	10/15/91/115	-
13	CLA	G	1103	1	-	20/39/115/115	-
13	CLA	a	507	-	-	15/39/115/115	-
13	CLA	b	519	12	-	14/27/103/115	-
13	CLA	G	1126	1	-	18/39/115/115	-
13	CLA	Z	503	12	-	9/39/115/115	-
13	CLA	2	501	12	-	14/39/115/115	-
17	LHG	f	1855	-	-	28/48/48/53	-
16	BCR	2	523	-	-	6/29/63/63	0/2/2/2
16	BCR	J	4015	-	-	5/29/63/63	0/2/2/2
13	CLA	5	504	-	-	5/15/91/115	-
13	CLA	u	502	12	-	7/21/97/115	-
13	CLA	c	501	12	-	21/39/115/115	-
20	SQD	v	822	-	-	9/19/39/69	0/1/1/1
13	CLA	3	518	12	-	12/27/103/115	-
13	CLA	Y	508	12	-	11/27/103/115	-
16	BCR	n	4019	-	-	6/29/63/63	0/2/2/2
13	CLA	5	509	12	-	12/39/115/115	-
20	SQD	t	822	-	-	8/19/39/69	0/1/1/1
17	LHG	G	5002	-	-	26/43/43/53	-
13	CLA	3	506	12	-	5/21/97/115	-
13	CLA	1	502	12	-	16/33/109/115	-
13	CLA	G	1137	1	-	19/39/115/115	-
16	BCR	G	4007	-	-	0/29/63/63	0/2/2/2
13	CLA	H	1213	2	-	14/39/115/115	-
13	CLA	d	517	-	-	11/15/91/115	-
13	CLA	G	1124	21	-	13/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	2	505	12	-	14/39/115/115	-
16	BCR	4	521	-	-	10/29/63/63	0/2/2/2
13	CLA	Z	505	12	-	14/39/115/115	-
16	BCR	u	523	-	-	4/29/63/63	0/2/2/2
13	CLA	2	506	12	-	8/27/103/115	-
16	BCR	Y	522	-	-	6/29/63/63	0/2/2/2
13	CLA	G	1133	1	-	17/39/115/115	-
13	CLA	3	501	12	-	6/39/115/115	-
13	CLA	H	1227	2	-	14/39/115/115	-
16	BCR	c	524	-	-	2/29/63/63	0/2/2/2
16	BCR	e	4002	-	-	0/29/63/63	0/2/2/2
13	CLA	6	513	12	-	5/15/91/115	-
16	BCR	o	4021	-	-	7/29/63/63	0/2/2/2
13	CLA	G	1022	21	-	8/39/115/115	-
20	SQD	r	822	-	-	13/38/58/69	0/1/1/1
13	CLA	H	1209	2	-	8/24/100/115	-
13	CLA	e	1108	1	-	18/26/102/115	-
16	BCR	1	523	-	-	6/29/63/63	0/2/2/2
13	CLA	6	510	12	-	9/15/91/115	-
13	CLA	f	1212	2	-	11/27/103/115	-
17	LHG	G	5009	-	-	28/53/53/53	-
19	LMG	T	5104	-	-	17/30/50/70	0/1/1/1
16	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
13	CLA	e	1011	1	-	11/39/115/115	-
13	CLA	A	1134	1	-	13/29/105/115	-
13	CLA	Y	512	12	-	11/24/100/115	-
13	CLA	B	1216	21	-	7/33/109/115	-
13	CLA	F	1302	6	-	10/15/91/115	-
13	CLA	l	1302	8	-	15/31/107/115	-
13	CLA	B	1202	2	-	13/39/115/115	-
16	BCR	L	4022	-	-	2/29/63/63	0/2/2/2
13	CLA	a	512	12	-	5/15/91/115	-
13	CLA	f	1225	2	-	7/39/115/115	-
13	CLA	s	511	12	-	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	1	504	-	-	7/15/91/115	-
13	CLA	3	513	12	-	15/39/115/115	-
20	SQD	a	822	-	-	21/38/58/69	0/1/1/1
13	CLA	5	517	-	-	11/15/91/115	-
13	CLA	H	1207	2	-	16/39/115/115	-
18	LMU	r	901	-	-	8/14/34/61	0/1/1/2
13	CLA	G	1115	1	-	12/33/109/115	-
13	CLA	3	507	-	-	15/39/115/115	-
16	BCR	V	4022	-	-	2/29/63/63	0/2/2/2
13	CLA	4	511	12	-	5/15/91/115	-
13	CLA	Y	509	12	-	6/39/115/115	-
13	CLA	Z	516	12	-	10/15/91/115	-
13	CLA	B	1021	2	-	12/39/115/115	-
13	CLA	4	507	-	-	8/15/91/115	-
17	LHG	e	5007	-	-	24/51/51/53	-
13	CLA	e	1130	1	-	9/39/115/115	-
13	CLA	B	1212	2	-	11/27/103/115	-
17	LHG	L	5220	-	-	24/45/45/53	-
13	CLA	f	1219	2	-	19/39/115/115	-
16	BCR	5	523	-	-	4/29/63/63	0/2/2/2
16	BCR	3	521	-	-	7/29/63/63	0/2/2/2
16	BCR	m	4104	-	-	2/29/63/63	0/2/2/2
13	CLA	f	1202	2	-	13/39/115/115	-
13	CLA	f	1229	2	-	13/39/115/115	-
13	CLA	6	506	12	-	7/15/91/115	-
13	CLA	2	504	-	-	7/21/97/115	-
13	CLA	f	1023	-	-	10/39/115/115	-
16	BCR	2	521	-	-	4/29/63/63	0/2/2/2
16	BCR	G	4002	-	-	0/29/63/63	0/2/2/2
16	BCR	f	4004	-	-	8/29/63/63	0/2/2/2
13	CLA	f	1224	2	-	13/33/109/115	-
13	CLA	H	1222	21	-	7/33/109/115	-
13	CLA	A	1139	21	-	14/39/115/115	-
16	BCR	B	4017	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	e	1135	1	-	10/24/100/115	-
18	LMU	1	902	-	-	6/10/30/61	0/1/1/2
13	CLA	U	1401	-	-	10/27/103/115	-
13	CLA	q	502	12	-	16/33/109/115	-
16	BCR	H	4006	-	-	4/29/63/63	0/2/2/2
13	CLA	a	518	12	-	12/27/103/115	-
13	CLA	4	519	12	-	14/27/103/115	-
13	CLA	f	1216	21	-	7/33/109/115	-
17	LHG	A	5008	-	-	19/39/39/53	-
13	CLA	Y	511	12	-	4/27/103/115	-
13	CLA	B	1232	21	-	6/21/97/115	-
13	CLA	e	1109	1	-	11/39/115/115	-
13	CLA	t	516	12	-	9/15/91/115	-
17	LHG	V	5218	-	-	23/42/42/53	-
13	CLA	a	501	12	-	6/39/115/115	-
16	BCR	e	4008	-	-	7/29/63/63	0/2/2/2
13	CLA	r	516	12	-	10/15/91/115	-
16	BCR	n	4020	-	-	4/29/63/63	0/2/2/2
13	CLA	G	1104	1	-	12/39/115/115	-
13	CLA	A	1138	1	-	14/39/115/115	-
13	CLA	3	519	12	-	10/27/103/115	-
13	CLA	e	1126	1	-	18/39/115/115	-
13	CLA	s	507	-	-	15/39/115/115	-
13	CLA	H	1204	2	-	13/39/115/115	-
13	CLA	d	501	12	-	18/33/109/115	-
13	CLA	3	511	12	-	7/21/97/115	-
16	BCR	c	523	-	-	4/29/63/63	0/2/2/2
13	CLA	B	1228	2	-	8/27/103/115	-
13	CLA	f	1214	2	-	15/39/115/115	-
13	CLA	5	507	-	-	7/15/91/115	-
16	BCR	L	4020	-	-	4/29/63/63	0/2/2/2
17	LHG	H	1855	-	-	28/48/48/53	-
13	CLA	Z	519	12	-	11/27/103/115	-
18	LMU	e	1849	-	-	6/14/34/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	5	502	12	-	7/21/97/115	-
17	LHG	A	5009	-	-	28/53/53/53	-
13	CLA	A	1106	1	-	23/39/115/115	-
13	CLA	f	1208	2	-	17/39/115/115	-
13	CLA	u	513	12	-	6/15/91/115	-
13	CLA	v	505	12	-	15/39/115/115	-
16	BCR	B	4009	-	-	1/29/63/63	0/2/2/2
13	CLA	e	1124	21	-	13/29/105/115	-
16	BCR	k	4018	-	-	1/29/63/63	0/2/2/2
14	PQN	e	2001	-	-	14/23/43/43	0/2/2/2
13	CLA	q	519	12	-	8/21/97/115	-
16	BCR	5	521	-	-	7/29/63/63	0/2/2/2
16	BCR	V	4219	-	-	2/29/63/63	0/2/2/2
13	CLA	f	1206	2	-	15/39/115/115	-
13	CLA	r	506	12	-	8/27/103/115	-
16	BCR	e	4007	-	-	0/29/63/63	0/2/2/2
13	CLA	d	511	12	-	6/15/91/115	-
13	CLA	e	1131	1	-	8/39/115/115	-
13	CLA	f	1230	2	-	12/33/109/115	-
13	CLA	A	1115	1	-	12/33/109/115	-
13	CLA	G	1132	1	-	17/39/115/115	-
13	CLA	s	512	12	-	5/15/91/115	-
16	BCR	G	4011	-	-	12/29/63/63	0/2/2/2
13	CLA	b	509	12	-	7/39/115/115	-
13	CLA	u	504	-	-	5/15/91/115	-
13	CLA	T	1302	8	-	15/31/107/115	-
16	BCR	d	521	-	-	5/29/63/63	0/2/2/2
16	BCR	3	522	-	-	5/29/63/63	0/2/2/2
17	LHG	V	5220	-	-	24/45/45/53	-
13	CLA	4	508	12	-	6/15/91/115	-
13	CLA	A	1022	21	-	8/39/115/115	-
13	CLA	3	503	12	-	9/39/115/115	-
13	CLA	f	1217	2	-	14/30/106/115	-
13	CLA	v	503	12	-	10/24/100/115	-
13	CLA	A	1140	1	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	a	506	12	-	5/21/97/115	-
13	CLA	B	1235	2	-	8/39/115/115	-
13	CLA	3	505	12	-	19/39/115/115	-
13	CLA	A	1103	1	-	20/39/115/115	-
13	CLA	B	1225	2	-	8/39/115/115	-
13	CLA	f	1240	17	-	15/39/115/115	-
17	LHG	k	5001	-	-	22/48/48/53	-
18	LMU	H	1843	-	-	12/21/61/61	0/2/2/2
13	CLA	1	516	12	-	15/15/91/115	-
13	CLA	B	1227	2	-	14/39/115/115	-
13	CLA	b	503	12	-	3/27/103/115	-
13	CLA	Y	507	-	-	16/33/109/115	-
13	CLA	f	1238	21	-	4/39/115/115	-
13	CLA	Z	508	12	-	8/27/103/115	-
13	CLA	e	1127	1	-	12/39/115/115	-
13	CLA	v	516	12	-	10/15/91/115	-
16	BCR	H	4005	-	-	6/29/63/63	0/2/2/2
16	BCR	H	4017	-	-	2/29/63/63	0/2/2/2
20	SQD	c	822	-	-	7/24/44/69	0/1/1/1
13	CLA	c	508	12	-	6/15/91/115	-
15	SF4	G	3001	1,2	-	-	0/6/5/5
17	LHG	e	5002	-	-	26/43/43/53	-
13	CLA	5	511	12	-	7/27/103/115	-
13	CLA	q	503	12	-	11/38/114/115	-
13	CLA	f	1210	2	-	21/39/115/115	-
13	CLA	e	1137	1	-	19/39/115/115	-
13	CLA	F	1301	21	-	12/39/115/115	-
13	CLA	B	1219	2	-	19/39/115/115	-
13	CLA	a	502	12	-	6/21/97/115	-
13	CLA	u	506	12	-	7/15/91/115	-
13	CLA	1	508	12	-	11/27/103/115	-
13	CLA	Z	504	-	-	7/21/97/115	-
13	CLA	B	1229	2	-	13/39/115/115	-
13	CLA	e	1133	1	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	n	1502	10	-	10/39/115/115	-
16	BCR	J	4013	-	-	4/29/63/63	0/2/2/2
16	BCR	R	4016	-	-	2/29/63/63	0/2/2/2
13	CLA	b	505	12	-	13/39/115/115	-
13	CLA	r	507	-	-	16/39/115/115	-
13	CLA	t	503	12	-	3/27/103/115	-
13	CLA	B	1023	-	-	10/39/115/115	-
13	CLA	l	510	12	-	13/39/115/115	-
13	CLA	L	1502	10	-	10/39/115/115	-
13	CLA	B	1224	2	-	13/33/109/115	-
13	CLA	r	512	12	-	7/25/101/115	-
16	BCR	d	524	-	-	5/29/63/63	0/2/2/2
16	BCR	s	524	-	-	5/29/63/63	0/2/2/2
13	CLA	4	502	12	-	7/21/97/115	-
13	CLA	e	1801	17	-	5/15/91/115	-
13	CLA	e	1118	1	-	14/33/109/115	-
16	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
16	BCR	Y	524	-	-	2/29/63/63	0/2/2/2
13	CLA	H	1217	2	-	14/30/106/115	-
13	CLA	R	1302	6	-	10/15/91/115	-
13	CLA	e	1102	1	-	11/39/115/115	-
13	CLA	H	1218	2	-	7/33/109/115	-
17	LHG	G	5007	-	-	24/51/51/53	-
13	CLA	R	1301	21	-	12/39/115/115	-
13	CLA	6	518	12	-	12/27/103/115	-
13	CLA	H	1203	2	-	18/39/115/115	-
13	CLA	2	508	12	-	8/27/103/115	-
13	CLA	a	519	12	-	10/27/103/115	-
13	CLA	f	1226	2	-	12/39/115/115	-
17	LHG	e	5004	-	-	21/40/40/53	-
15	SF4	g	3003	3	-	-	0/6/5/5
13	CLA	2	509	12	-	6/39/115/115	-
13	CLA	5	519	12	-	10/17/93/115	-
13	CLA	v	501	12	-	18/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	c	513	12	-	6/15/91/115	-
13	CLA	3	504	-	-	6/15/91/115	-
13	CLA	c	509	12	-	12/39/115/115	-
16	BCR	H	4014	-	-	9/29/63/63	0/2/2/2
16	BCR	d	523	-	-	4/29/63/63	0/2/2/2
13	CLA	B	1214	2	-	15/39/115/115	-
13	CLA	K	1105	9	-	11/15/91/115	-
13	CLA	Y	504	-	-	7/15/91/115	-
13	CLA	b	516	12	-	9/15/91/115	-
13	CLA	K	1103	9	-	9/21/97/115	-
13	CLA	Y	517	-	-	6/15/91/115	-
16	BCR	d	522	-	-	5/29/63/63	0/2/2/2
13	CLA	b	501	12	-	14/33/109/115	-
17	LHG	S	5001	-	-	22/48/48/53	-
13	CLA	u	507	-	-	7/15/91/115	-
13	CLA	6	503	12	-	10/24/100/115	-
13	CLA	A	1113	1	-	5/15/91/115	-
13	CLA	f	1213	2	-	14/39/115/115	-
15	SF4	N	3003	3	-	-	0/6/5/5
13	CLA	q	501	12	-	20/39/115/115	-
13	CLA	Y	518	12	-	17/33/109/115	-
13	CLA	q	517	-	-	6/15/91/115	-
13	CLA	u	510	12	-	9/15/91/115	-
17	LHG	G	5005	-	-	29/49/49/53	-
13	CLA	B	1230	2	-	12/33/109/115	-
13	CLA	e	1120	1	-	4/25/101/115	-
13	CLA	r	518	12	-	16/39/115/115	-
13	CLA	l	517	-	-	6/15/91/115	-
13	CLA	e	1132	1	-	17/39/115/115	-
18	LMU	e	1848	-	-	7/21/61/61	0/2/2/2
13	CLA	G	1134	1	-	13/29/105/115	-
13	CLA	v	510	12	-	9/15/91/115	-
13	CLA	f	1221	21	-	14/39/115/115	-
16	BCR	a	522	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	A	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	e	1237	21	-	21/39/115/115	-
17	LHG	n	5220	-	-	24/45/45/53	-
18	LMU	Z	901	-	-	8/14/34/61	0/1/1/2
13	CLA	6	511	12	-	6/15/91/115	-
13	CLA	2	513	12	-	17/39/115/115	-
13	CLA	4	509	12	-	7/39/115/115	-
13	CLA	b	511	12	-	5/15/91/115	-
13	CLA	c	517	-	-	11/15/91/115	-
17	LHG	A	5007	-	-	24/51/51/53	-
13	CLA	B	1203	2	-	18/39/115/115	-
13	CLA	H	1202	2	-	13/39/115/115	-
13	CLA	H	1230	2	-	12/33/109/115	-
16	BCR	q	521	-	-	7/29/63/63	0/2/2/2
13	CLA	B	1234	2	-	13/39/115/115	-
13	CLA	G	1138	1	-	14/39/115/115	-
13	CLA	c	506	12	-	7/15/91/115	-
13	CLA	Z	518	12	-	16/39/115/115	-
16	BCR	4	523	-	-	5/29/63/63	0/2/2/2
16	BCR	U	4104	-	-	2/29/63/63	0/2/2/2
13	CLA	q	510	12	-	13/39/115/115	-
13	CLA	t	504	-	-	7/15/91/115	-
13	CLA	K	1401	-	-	10/27/103/115	-
20	SQD	d	822	-	-	9/19/39/69	0/1/1/1
16	BCR	f	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1207	2	-	16/39/115/115	-
13	CLA	e	1128	1	-	12/39/115/115	-
13	CLA	4	506	12	-	4/15/91/115	-
13	CLA	G	1106	1	-	23/39/115/115	-
16	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
13	CLA	e	1125	1	-	14/39/115/115	-
13	CLA	u	518	12	-	13/27/103/115	-
20	SQD	s	822	-	-	21/38/58/69	0/1/1/1
13	CLA	H	1238	21	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	G	1121	1	-	8/27/103/115	-
13	CLA	1	513	12	-	4/27/103/115	-
15	SF4	C	3002	3	-	-	0/6/5/5
13	CLA	6	516	12	-	10/15/91/115	-
14	PQN	B	2002	-	-	9/23/43/43	0/2/2/2
13	CLA	e	1105	1	-	6/27/103/115	-
13	CLA	B	1215	2	-	19/39/115/115	-
13	CLA	H	1206	2	-	15/39/115/115	-
13	CLA	e	1119	21	-	15/39/115/115	-
16	BCR	3	523	-	-	4/29/63/63	0/2/2/2
13	CLA	A	1011	1	-	11/39/115/115	-
13	CLA	6	519	12	-	8/17/93/115	-
14	PQN	G	2001	-	-	14/23/43/43	0/2/2/2
13	CLA	e	1114	21	-	2/21/97/115	-
17	LHG	G	5008	-	-	19/39/39/53	-
13	CLA	G	1107	1	-	16/39/115/115	-
13	CLA	4	503	12	-	3/27/103/115	-
13	CLA	q	512	12	-	12/24/100/115	-
13	CLA	B	1201	2	-	11/33/109/115	-
13	CLA	2	518	12	-	16/39/115/115	-
13	CLA	f	1231	21	-	8/39/115/115	-
13	CLA	l	506	12	-	6/15/91/115	-
13	CLA	v	508	12	-	5/15/91/115	-
13	CLA	a	513	12	-	15/39/115/115	-
13	CLA	B	1238	21	-	4/39/115/115	-
13	CLA	r	502	12	-	13/33/109/115	-
13	CLA	A	1130	1	-	9/39/115/115	-
13	CLA	c	507	-	-	7/15/91/115	-
13	CLA	q	508	12	-	11/27/103/115	-
13	CLA	d	513	12	-	5/15/91/115	-
13	CLA	s	505	12	-	20/39/115/115	-
15	SF4	e	3001	1,2	-	-	0/6/5/5
13	CLA	s	506	12	-	5/21/97/115	-
13	CLA	G	1123	21	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	3	502	12	-	6/21/97/115	-
13	CLA	A	1108	1	-	18/26/102/115	-
13	CLA	Z	501	12	-	14/39/115/115	-
16	BCR	B	4004	-	-	8/29/63/63	0/2/2/2
20	SQD	Y	822	-	-	20/43/63/69	0/1/1/1
16	BCR	5	524	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1217	2	-	14/30/106/115	-
13	CLA	A	1135	1	-	10/24/100/115	-
13	CLA	B	1213	2	-	14/39/115/115	-
13	CLA	4	512	12	-	5/15/91/115	-
13	CLA	Y	502	12	-	16/33/109/115	-
19	LMG	B	5002	-	-	24/49/69/70	0/1/1/1
13	CLA	H	1012	21	-	16/39/115/115	-
13	CLA	1	518	12	-	17/33/109/115	-
13	CLA	3	508	12	-	7/27/103/115	-
13	CLA	f	1234	2	-	13/39/115/115	-
16	BCR	q	523	-	-	6/29/63/63	0/2/2/2
13	CLA	r	503	12	-	9/39/115/115	-
13	CLA	d	516	12	-	10/15/91/115	-
16	BCR	A	4008	-	-	7/29/63/63	0/2/2/2
13	CLA	B	1206	2	-	15/39/115/115	-
13	CLA	J	1303	8	-	18/39/115/115	-
13	CLA	a	510	12	-	19/39/115/115	-
13	CLA	G	1127	1	-	12/39/115/115	-
13	CLA	B	1240	17	-	15/39/115/115	-
13	CLA	B	1222	21	-	7/33/109/115	-
16	BCR	Y	521	-	-	6/29/63/63	0/2/2/2
13	CLA	e	1116	1	-	15/33/109/115	-
13	CLA	r	519	12	-	11/27/103/115	-
13	CLA	r	505	12	-	14/39/115/115	-
16	BCR	e	4011	-	-	13/29/63/63	0/2/2/2
16	BCR	V	4020	-	-	4/29/63/63	0/2/2/2
13	CLA	A	1109	1	-	11/39/115/115	-
13	CLA	U	1105	9	-	11/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	s	516	12	-	11/15/91/115	-
17	LHG	e	5006	-	-	24/49/49/53	-
13	CLA	U	1103	9	-	9/21/97/115	-
15	SF4	g	3002	3	-	-	0/6/5/5
17	LHG	n	5221	-	-	30/53/53/53	-
13	CLA	B	1226	2	-	12/39/115/115	-
13	CLA	A	1110	1	-	11/23/99/115	-
13	CLA	B	1210	2	-	21/39/115/115	-
17	LHG	L	5218	-	-	23/42/42/53	-
13	CLA	A	1137	1	-	19/39/115/115	-
13	CLA	f	1215	2	-	19/39/115/115	-
13	CLA	e	1013	-	-	11/39/115/115	-
18	LMU	G	1849	-	-	6/14/34/61	0/1/1/2
16	BCR	2	524	-	-	2/29/63/63	0/2/2/2
16	BCR	1	521	-	-	7/29/63/63	0/2/2/2
17	LHG	L	5221	-	-	30/53/53/53	-
13	CLA	q	509	12	-	6/39/115/115	-
14	PQN	H	2002	-	-	9/23/43/43	0/2/2/2
13	CLA	c	512	12	-	7/15/91/115	-
13	CLA	H	1228	2	-	8/27/103/115	-
13	CLA	Z	511	12	-	6/27/103/115	-
13	CLA	G	1013	-	-	11/39/115/115	-
13	CLA	2	519	12	-	11/27/103/115	-
13	CLA	a	505	12	-	19/39/115/115	-
13	CLA	b	508	12	-	6/15/91/115	-
13	CLA	d	506	12	-	7/15/91/115	-
13	CLA	t	518	12	-	10/27/103/115	-
16	BCR	L	4219	-	-	2/29/63/63	0/2/2/2
16	BCR	f	4014	-	-	9/29/63/63	0/2/2/2
13	CLA	J	1302	8	-	15/31/107/115	-
13	CLA	t	501	12	-	14/33/109/115	-
13	CLA	2	511	12	-	6/27/103/115	-
13	CLA	Z	507	-	-	16/39/115/115	-
16	BCR	Z	521	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	H	1021	2	-	13/39/115/115	-
13	CLA	H	1236	2	-	5/27/103/115	-
13	CLA	s	504	-	-	6/15/91/115	-
13	CLA	Z	510	12	-	9/39/115/115	-
13	CLA	n	1501	10	-	20/39/115/115	-
18	LMU	G	1848	-	-	7/21/61/61	0/2/2/2
13	CLA	H	1201	2	-	11/33/109/115	-
16	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
13	CLA	n	1503	21	-	10/33/109/115	-
13	CLA	s	510	12	-	19/39/115/115	-
13	CLA	A	1131	1	-	8/39/115/115	-
13	CLA	Y	513	12	-	4/27/103/115	-
13	CLA	e	1121	1	-	8/27/103/115	-
16	BCR	T	4012	-	-	9/29/63/63	0/2/2/2
16	BCR	v	522	-	-	5/29/63/63	0/2/2/2
13	CLA	c	518	12	-	13/27/103/115	-
13	CLA	3	512	12	-	5/15/91/115	-
13	CLA	L	1503	21	-	10/33/109/115	-
13	CLA	t	505	12	-	13/39/115/115	-
13	CLA	A	1136	1	-	5/33/109/115	-
13	CLA	A	1111	1	-	16/39/115/115	-
13	CLA	e	1110	1	-	11/23/99/115	-
16	BCR	l	4015	-	-	5/29/63/63	0/2/2/2
13	CLA	G	1118	1	-	14/33/109/115	-
16	BCR	1	524	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1127	1	-	12/39/115/115	-
16	BCR	b	522	-	-	4/29/63/63	0/2/2/2
13	CLA	Z	512	12	-	7/25/101/115	-
13	CLA	1	519	12	-	8/21/97/115	-
13	CLA	f	1222	21	-	7/33/109/115	-
13	CLA	5	506	12	-	7/15/91/115	-
13	CLA	A	1126	1	-	18/39/115/115	-
20	SQD	B	1852	-	-	19/40/60/69	0/1/1/1
16	BCR	q	522	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	2	503	12	-	9/39/115/115	-
13	CLA	r	504	-	-	7/21/97/115	-
16	BCR	4	524	-	-	4/29/63/63	0/2/2/2
19	LMG	f	5002	-	-	24/49/69/70	0/1/1/1
13	CLA	B	1231	21	-	8/39/115/115	-
13	CLA	2	507	-	-	16/39/115/115	-
16	BCR	B	4006	-	-	4/29/63/63	0/2/2/2
13	CLA	3	516	12	-	11/15/91/115	-
13	CLA	H	1211	2	-	4/29/105/115	-
13	CLA	H	1232	21	-	6/21/97/115	-
13	CLA	Z	502	12	-	13/33/109/115	-
17	LHG	A	5002	-	-	26/43/43/53	-
13	CLA	v	513	12	-	5/15/91/115	-
13	CLA	d	507	-	-	6/15/91/115	-
13	CLA	f	1227	2	-	14/39/115/115	-
13	CLA	v	509	12	-	6/15/91/115	-
13	CLA	A	1124	21	-	13/29/105/115	-
13	CLA	e	1111	1	-	16/39/115/115	-
13	CLA	1	501	12	-	20/39/115/115	-
13	CLA	5	503	12	-	12/27/103/115	-
13	CLA	a	504	-	-	6/15/91/115	-
13	CLA	H	1221	21	-	14/39/115/115	-
13	CLA	A	1133	1	-	17/39/115/115	-
13	CLA	G	1135	1	-	10/24/100/115	-
13	CLA	G	1237	21	-	20/39/115/115	-
15	SF4	N	3002	3	-	-	0/6/5/5
16	BCR	M	4021	-	-	7/29/63/63	0/2/2/2
13	CLA	5	505	12	-	16/35/111/115	-
13	CLA	e	1101	1	-	13/39/115/115	-
16	BCR	l	4012	-	-	9/29/63/63	0/2/2/2
13	CLA	H	1240	17	-	15/39/115/115	-
13	CLA	1	503	12	-	11/38/114/115	-
13	CLA	s	517	-	-	9/15/91/115	-
13	CLA	q	513	12	-	4/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	6	522	-	-	5/29/63/63	0/2/2/2
13	CLA	t	512	12	-	5/15/91/115	-
16	BCR	K	4104	-	-	2/29/63/63	0/2/2/2
16	BCR	6	523	-	-	4/29/63/63	0/2/2/2
17	LHG	A	5004	-	-	21/40/40/53	-
17	LHG	e	5003	13	-	17/45/45/53	-
16	BCR	l	4013	-	-	4/29/63/63	0/2/2/2
13	CLA	A	1118	1	-	14/33/109/115	-
13	CLA	G	1011	1	-	12/39/115/115	-
13	CLA	e	1123	21	-	11/39/115/115	-
13	CLA	f	1239	2	-	17/39/115/115	-
13	CLA	l	1303	8	-	18/39/115/115	-
16	BCR	Z	523	-	-	6/29/63/63	0/2/2/2
16	BCR	u	521	-	-	7/29/63/63	0/2/2/2
13	CLA	A	1104	1	-	12/39/115/115	-
13	CLA	e	1117	1	-	13/39/115/115	-
13	CLA	e	1103	1	-	20/39/115/115	-
13	CLA	H	1223	2	-	14/39/115/115	-
16	BCR	2	522	-	-	6/29/63/63	0/2/2/2
13	CLA	B	1236	2	-	5/27/103/115	-
13	CLA	A	1128	1	-	12/39/115/115	-
16	BCR	f	4009	-	-	1/29/63/63	0/2/2/2
13	CLA	a	503	12	-	9/39/115/115	-
13	CLA	B	1221	21	-	14/39/115/115	-
13	CLA	u	503	12	-	12/27/103/115	-
18	LMU	Y	902	-	-	6/10/30/61	0/1/1/2
13	CLA	e	1136	1	-	5/33/109/115	-
13	CLA	B	1211	2	-	4/29/105/115	-
20	SQD	5	822	-	-	7/24/44/69	0/1/1/1
13	CLA	d	512	12	-	8/15/91/115	-
13	CLA	v	518	12	-	12/27/103/115	-
13	CLA	f	1236	2	-	5/27/103/115	-
13	CLA	5	516	12	-	4/15/91/115	-
13	CLA	b	517	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PQN	f	2002	-	-	9/23/43/43	0/2/2/2
13	CLA	d	518	12	-	12/27/103/115	-
16	BCR	t	521	-	-	10/29/63/63	0/2/2/2
16	BCR	t	523	-	-	5/29/63/63	0/2/2/2
13	CLA	b	513	12	-	9/15/91/115	-
13	CLA	c	519	12	-	10/17/93/115	-
16	BCR	u	522	-	-	5/29/63/63	0/2/2/2
17	LHG	B	1842	13	-	22/43/43/53	-
13	CLA	e	1112	1	-	5/21/97/115	-
13	CLA	t	510	12	-	7/21/97/115	-
13	CLA	G	1116	1	-	15/33/109/115	-
13	CLA	m	1105	9	-	11/15/91/115	-
13	CLA	q	511	12	-	4/27/103/115	-
13	CLA	r	510	12	-	9/39/115/115	-
13	CLA	H	1212	2	-	11/27/103/115	-
13	CLA	e	1113	1	-	5/15/91/115	-
20	SQD	Z	822	-	-	13/38/58/69	0/1/1/1
13	CLA	t	519	12	-	14/27/103/115	-
16	BCR	l	522	-	-	6/29/63/63	0/2/2/2
13	CLA	f	1201	2	-	11/33/109/115	-
13	CLA	c	502	12	-	7/21/97/115	-
13	CLA	u	511	12	-	7/27/103/115	-
13	CLA	A	1801	17	-	5/15/91/115	-
13	CLA	f	1235	2	-	8/39/115/115	-
16	BCR	J	4012	-	-	9/29/63/63	0/2/2/2
13	CLA	H	1229	2	-	13/39/115/115	-
18	LMU	A	1848	-	-	7/21/61/61	0/2/2/2
13	CLA	6	508	12	-	5/15/91/115	-
13	CLA	A	1102	1	-	11/39/115/115	-
13	CLA	s	518	12	-	12/27/103/115	-
16	BCR	s	521	-	-	7/29/63/63	0/2/2/2
13	CLA	f	1204	2	-	13/39/115/115	-
13	CLA	H	1224	2	-	13/33/109/115	-
13	CLA	H	1239	2	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	s	508	12	-	7/27/103/115	-
13	CLA	v	512	12	-	8/15/91/115	-
17	LHG	B	1855	-	-	28/48/48/53	-
13	CLA	f	1223	2	-	14/39/115/115	-
15	SF4	A	3001	1,2	-	-	0/6/5/5
13	CLA	A	1132	1	-	17/39/115/115	-
16	BCR	H	4010	-	-	5/29/63/63	0/2/2/2
13	CLA	l	512	12	-	12/24/100/115	-
13	CLA	c	503	12	-	12/27/103/115	-
13	CLA	e	1129	1	-	7/23/99/115	-
18	LMU	f	1843	-	-	12/21/61/61	0/2/2/2
13	CLA	v	507	-	-	6/15/91/115	-
13	CLA	V	1503	21	-	10/33/109/115	-
13	CLA	v	511	12	-	6/15/91/115	-
16	BCR	s	522	-	-	5/29/63/63	0/2/2/2
16	BCR	T	4013	-	-	4/29/63/63	0/2/2/2
13	CLA	T	1303	8	-	18/39/115/115	-
13	CLA	G	1130	1	-	9/39/115/115	-
13	CLA	t	508	12	-	6/15/91/115	-
16	BCR	H	4004	-	-	8/29/63/63	0/2/2/2
20	SQD	l	822	-	-	20/43/63/69	0/1/1/1
13	CLA	4	518	12	-	10/27/103/115	-
13	CLA	b	518	12	-	10/27/103/115	-
13	CLA	H	1214	2	-	15/39/115/115	-
13	CLA	e	1107	1	-	16/39/115/115	-
13	CLA	j	1301	21	-	12/39/115/115	-
13	CLA	G	1111	1	-	16/39/115/115	-
13	CLA	G	1119	21	-	15/39/115/115	-
13	CLA	r	508	12	-	8/27/103/115	-
13	CLA	u	519	12	-	10/17/93/115	-
13	CLA	A	1120	1	-	4/25/101/115	-
13	CLA	A	1116	1	-	15/33/109/115	-
13	CLA	Z	513	12	-	17/39/115/115	-
13	CLA	Z	509	12	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	s	519	12	-	10/27/103/115	-
16	BCR	v	521	-	-	5/29/63/63	0/2/2/2
13	CLA	A	1105	1	-	6/27/103/115	-
13	CLA	G	1108	1	-	18/26/102/115	-
13	CLA	e	1122	1	-	16/33/109/115	-
13	CLA	q	507	-	-	16/33/109/115	-
13	CLA	A	1237	21	-	21/39/115/115	-
13	CLA	H	1023	-	-	10/39/115/115	-
16	BCR	t	522	-	-	4/29/63/63	0/2/2/2
17	LHG	A	5006	-	-	24/49/49/53	-
13	CLA	d	502	12	-	7/21/97/115	-
15	SF4	C	3003	3	-	-	0/6/5/5
13	CLA	H	1220	2	-	11/27/103/115	-
13	CLA	f	1207	2	-	16/39/115/115	-
16	BCR	G	4008	-	-	7/29/63/63	0/2/2/2
13	CLA	a	508	12	-	7/27/103/115	-
13	CLA	Y	506	12	-	6/15/91/115	-
13	CLA	6	501	12	-	18/33/109/115	-
16	BCR	3	524	-	-	5/29/63/63	0/2/2/2
16	BCR	v	524	-	-	5/29/63/63	0/2/2/2
13	CLA	b	512	12	-	5/15/91/115	-
13	CLA	G	1117	1	-	13/39/115/115	-
13	CLA	t	502	12	-	7/21/97/115	-
16	BCR	B	4010	-	-	5/29/63/63	0/2/2/2
16	BCR	c	522	-	-	5/29/63/63	0/2/2/2
18	LMU	J	5105	-	-	8/13/33/61	0/1/1/2
16	BCR	L	4019	-	-	6/29/63/63	0/2/2/2
13	CLA	3	509	12	-	4/39/115/115	-
13	CLA	5	510	12	-	9/15/91/115	-
17	LHG	e	5005	-	-	29/49/49/53	-
17	LHG	e	5001	-	-	25/53/53/53	-
13	CLA	u	508	12	-	6/15/91/115	-
13	CLA	s	503	12	-	9/39/115/115	-
13	CLA	6	505	12	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1125	1	-	14/39/115/115	-
13	CLA	c	516	12	-	4/15/91/115	-
13	CLA	r	517	-	-	6/15/91/115	-
13	CLA	b	507	-	-	8/15/91/115	-
13	CLA	t	509	12	-	7/39/115/115	-
16	BCR	q	524	-	-	2/29/63/63	0/2/2/2
16	BCR	B	4014	-	-	9/29/63/63	0/2/2/2
13	CLA	r	509	12	-	6/39/115/115	-
13	CLA	Z	506	12	-	8/27/103/115	-
13	CLA	s	513	12	-	15/39/115/115	-
20	SQD	H	1852	-	-	19/40/60/69	0/1/1/1
13	CLA	A	1119	21	-	15/39/115/115	-
13	CLA	f	1220	2	-	11/27/103/115	-
13	CLA	b	510	12	-	7/21/97/115	-
13	CLA	2	502	12	-	13/33/109/115	-
13	CLA	H	1208	2	-	17/39/115/115	-
13	CLA	f	1209	2	-	8/24/100/115	-
13	CLA	H	1205	2	-	12/39/115/115	-
13	CLA	G	1122	1	-	16/33/109/115	-
13	CLA	f	1218	2	-	7/33/109/115	-
13	CLA	f	1203	2	-	18/39/115/115	-
13	CLA	A	1114	21	-	2/21/97/115	-
13	CLA	4	501	12	-	14/33/109/115	-
13	CLA	r	511	12	-	6/27/103/115	-
19	LMG	H	5002	-	-	24/49/69/70	0/1/1/1
16	BCR	I	4018	-	-	1/29/63/63	0/2/2/2
16	BCR	A	4011	-	-	12/29/63/63	0/2/2/2
17	LHG	G	5004	-	-	21/40/40/53	-
13	CLA	2	510	12	-	9/39/115/115	-
13	CLA	a	509	12	-	4/39/115/115	-
13	CLA	G	1136	1	-	5/33/109/115	-
13	CLA	G	1125	1	-	15/39/115/115	-
19	LMG	J	5104	-	-	17/30/50/70	0/1/1/1
13	CLA	u	517	-	-	11/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1013	-	-	11/39/115/115	-
13	CLA	H	1225	2	-	7/39/115/115	-
13	CLA	c	510	12	-	9/15/91/115	-
20	SQD	n	5216	-	-	17/46/66/69	0/1/1/1
16	BCR	b	524	-	-	4/29/63/63	0/2/2/2
13	CLA	4	516	12	-	9/15/91/115	-
13	CLA	G	1128	1	-	12/39/115/115	-
13	CLA	v	504	-	-	8/15/91/115	-
13	CLA	B	1209	2	-	8/24/100/115	-
13	CLA	a	517	-	-	9/15/91/115	-
13	CLA	t	517	-	-	7/15/91/115	-
16	BCR	f	4010	-	-	5/29/63/63	0/2/2/2
13	CLA	5	508	12	-	6/15/91/115	-
13	CLA	d	503	12	-	10/24/100/115	-
13	CLA	V	1501	10	-	20/39/115/115	-
20	SQD	L	5216	-	-	17/46/66/69	0/1/1/1
18	LMU	B	1843	-	-	12/21/61/61	0/2/2/2
13	CLA	t	513	12	-	9/15/91/115	-
18	LMU	2	901	-	-	8/14/34/61	0/1/1/2
13	CLA	u	509	12	-	12/39/115/115	-
13	CLA	B	1208	2	-	17/39/115/115	-
13	CLA	6	512	12	-	8/15/91/115	-
13	CLA	Y	503	12	-	11/38/114/115	-
13	CLA	t	506	12	-	4/15/91/115	-
13	CLA	d	505	12	-	15/39/115/115	-
16	BCR	e	4003	-	-	0/29/63/63	0/2/2/2
13	CLA	a	516	12	-	11/15/91/115	-
13	CLA	B	1220	2	-	11/27/103/115	-
20	SQD	3	822	-	-	21/38/58/69	0/1/1/1
13	CLA	A	1121	1	-	8/27/103/115	-
17	LHG	G	5006	-	-	24/49/49/53	-
13	CLA	e	1134	1	-	13/29/105/115	-
13	CLA	H	1234	2	-	13/39/115/115	-
13	CLA	1	509	12	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	6	504	-	-	8/15/91/115	-
16	BCR	a	523	-	-	4/29/63/63	0/2/2/2
17	LHG	A	5003	13	-	17/45/45/53	-
20	SQD	f	1852	-	-	19/40/60/69	0/1/1/1
13	CLA	c	504	-	-	5/15/91/115	-
13	CLA	5	518	12	-	13/27/103/115	-
13	CLA	s	501	12	-	6/39/115/115	-
13	CLA	H	1215	2	-	19/39/115/115	-
13	CLA	r	513	12	-	17/39/115/115	-
17	LHG	n	5218	-	-	23/42/42/53	-
13	CLA	q	518	12	-	17/33/109/115	-
14	PQN	A	2001	-	-	14/23/43/43	0/2/2/2
13	CLA	4	510	12	-	7/21/97/115	-
13	CLA	G	1801	17	-	5/15/91/115	-
13	CLA	5	501	12	-	21/39/115/115	-
13	CLA	6	507	-	-	6/15/91/115	-
13	CLA	G	1140	1	-	13/39/115/115	-
16	BCR	H	4009	-	-	1/29/63/63	0/2/2/2
13	CLA	Y	519	12	-	8/21/97/115	-
16	BCR	u	524	-	-	2/29/63/63	0/2/2/2
13	CLA	G	1102	1	-	11/39/115/115	-
13	CLA	L	1501	10	-	20/39/115/115	-
13	CLA	e	1138	1	-	14/39/115/115	-
13	CLA	f	1012	21	-	16/39/115/115	-
20	SQD	q	822	-	-	20/43/63/69	0/1/1/1
13	CLA	H	1226	2	-	12/39/115/115	-
13	CLA	G	1112	1	-	5/21/97/115	-
13	CLA	j	1302	6	-	10/15/91/115	-
16	BCR	6	521	-	-	5/29/63/63	0/2/2/2
17	LHG	H	1842	13	-	22/43/43/53	-
13	CLA	G	1113	1	-	5/15/91/115	-
16	BCR	G	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	r	501	12	-	14/39/115/115	-
13	CLA	B	1205	2	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	e	1139	21	-	14/39/115/115	-
13	CLA	H	1235	2	-	8/39/115/115	-
13	CLA	t	507	-	-	8/15/91/115	-
13	CLA	v	517	-	-	11/15/91/115	-
18	LMU	q	902	-	-	6/10/30/61	0/1/1/2
16	BCR	6	524	-	-	5/29/63/63	0/2/2/2
17	LHG	G	5001	-	-	25/53/53/53	-
13	CLA	A	1101	1	-	13/39/115/115	-
18	LMU	l	5105	-	-	8/13/33/61	0/1/1/2
13	CLA	d	504	-	-	8/15/91/115	-
13	CLA	Y	516	12	-	15/15/91/115	-
13	CLA	e	1022	21	-	8/39/115/115	-
13	CLA	B	1204	2	-	13/39/115/115	-
13	CLA	G	1120	1	-	4/25/101/115	-
16	BCR	Z	524	-	-	2/29/63/63	0/2/2/2

The worst 5 of 5705 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	2002	PQN	C12-C13	8.71	1.53	1.33
14	f	2002	PQN	C12-C13	8.70	1.53	1.33
14	H	2002	PQN	C12-C13	8.70	1.53	1.33
14	G	2001	PQN	C12-C13	8.66	1.53	1.33
14	e	2001	PQN	C12-C13	8.66	1.53	1.33

The worst 5 of 6991 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	f	2002	PQN	C11-C12-C13	-9.00	111.81	126.79
14	B	2002	PQN	C11-C12-C13	-9.00	111.81	126.79
13	H	1211	CLA	C4A-NA-C1A	8.99	110.75	106.71
14	H	2002	PQN	C11-C12-C13	-8.98	111.85	126.79
13	B	1211	CLA	C4A-NA-C1A	8.88	110.70	106.71

There are no chirality outliers.

5 of 8852 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1011	CLA	CHA-CBD-CGD-O1D
13	A	1102	CLA	C3A-C2A-CAA-CBA
13	A	1103	CLA	C1A-C2A-CAA-CBA
13	A	1103	CLA	CHA-CBD-CGD-O1D
13	A	1103	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

704 monomers are involved in 1558 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Y	501	CLA	4	0
13	l	511	CLA	3	0
17	I	5001	LHG	1	0
16	n	4022	BCR	6	0
16	F	4016	BCR	5	0
13	G	1129	CLA	1	0
16	r	521	BCR	2	0
13	c	505	CLA	1	0
13	A	1117	CLA	2	0
18	A	1849	LMU	1	0
13	Y	505	CLA	5	0
17	e	5009	LHG	4	0
16	v	523	BCR	3	0
13	5	512	CLA	4	0
13	B	1223	CLA	1	0
13	a	511	CLA	1	0
13	A	1107	CLA	1	0
16	f	4005	BCR	1	0
13	d	519	CLA	2	0
13	Y	510	CLA	1	0
16	Z	522	BCR	2	0
13	5	513	CLA	1	0
17	G	5003	LHG	1	0
13	A	1122	CLA	2	0
13	H	1210	CLA	4	0
13	v	506	CLA	1	0
16	T	4015	BCR	5	0
13	4	517	CLA	2	0
18	T	5105	LMU	2	0
13	e	1115	CLA	1	0
16	a	521	BCR	3	0
13	f	1228	CLA	3	0
13	A	1123	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1218	CLA	1	0
13	G	1131	CLA	1	0
16	s	523	BCR	3	0
13	6	502	CLA	2	0
13	G	1105	CLA	2	0
13	G	1114	CLA	1	0
13	e	1104	CLA	7	0
13	q	505	CLA	24	0
17	e	5008	LHG	2	0
16	f	4006	BCR	3	0
20	V	5216	SQD	3	0
13	v	502	CLA	2	0
13	m	1401	CLA	1	0
13	H	1219	CLA	5	0
13	Z	517	CLA	2	0
13	u	501	CLA	4	0
13	V	1502	CLA	2	0
20	2	822	SQD	1	0
13	A	1129	CLA	2	0
16	j	4016	BCR	3	0
16	b	523	BCR	2	0
13	G	1109	CLA	3	0
13	e	1106	CLA	2	0
13	H	1216	CLA	2	0
13	t	511	CLA	1	0
13	G	1101	CLA	4	0
13	u	512	CLA	4	0
16	r	522	BCR	2	0
13	q	516	CLA	2	0
13	3	517	CLA	1	0
16	c	521	BCR	5	0
13	b	506	CLA	1	0
16	e	4001	BCR	2	0
16	t	524	BCR	5	0
13	3	510	CLA	3	0
13	G	1110	CLA	1	0
13	f	1021	CLA	1	0
16	r	524	BCR	7	0
16	Y	523	BCR	1	0
13	m	1103	CLA	2	0
13	2	517	CLA	1	0
13	e	1140	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	4	505	CLA	1	0
13	4	513	CLA	1	0
16	b	521	BCR	2	0
16	V	4019	BCR	1	0
13	B	1012	CLA	3	0
13	6	517	CLA	3	0
13	H	1231	CLA	3	0
13	2	512	CLA	5	0
16	S	4018	BCR	5	0
13	q	504	CLA	1	0
13	G	1139	CLA	2	0
13	1	507	CLA	3	0
13	b	502	CLA	2	0
16	n	4219	BCR	4	0
17	f	1842	LHG	2	0
16	a	524	BCR	6	0
16	5	522	BCR	2	0
20	6	822	SQD	1	0
13	B	1239	CLA	2	0
13	u	505	CLA	2	0
16	r	523	BCR	2	0
17	A	5005	LHG	1	0
17	A	5001	LHG	4	0
16	G	4003	BCR	3	0
13	v	519	CLA	2	0
16	W	4021	BCR	4	0
13	c	511	CLA	1	0
13	1	505	CLA	8	0
13	s	509	CLA	1	0
13	s	502	CLA	2	0
17	V	5221	LHG	9	0
13	G	1103	CLA	4	0
13	a	507	CLA	2	0
13	b	519	CLA	2	0
13	G	1126	CLA	8	0
13	Z	503	CLA	4	0
13	2	501	CLA	4	0
17	f	1855	LHG	2	0
16	2	523	BCR	1	0
16	J	4015	BCR	3	0
13	u	502	CLA	3	0
13	c	501	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	v	822	SQD	1	0
13	3	518	CLA	1	0
13	Y	508	CLA	1	0
16	n	4019	BCR	2	0
17	G	5002	LHG	2	0
13	3	506	CLA	1	0
13	1	502	CLA	7	0
13	G	1137	CLA	2	0
16	G	4007	BCR	5	0
13	H	1213	CLA	1	0
13	d	517	CLA	3	0
13	G	1124	CLA	1	0
13	2	505	CLA	3	0
16	4	521	BCR	1	0
13	Z	505	CLA	2	0
16	u	523	BCR	2	0
13	2	506	CLA	5	0
16	Y	522	BCR	5	0
13	G	1133	CLA	1	0
13	3	501	CLA	2	0
13	H	1227	CLA	3	0
16	c	524	BCR	3	0
16	e	4002	BCR	3	0
13	6	513	CLA	1	0
16	o	4021	BCR	4	0
13	G	1022	CLA	3	0
20	r	822	SQD	1	0
13	H	1209	CLA	2	0
13	e	1108	CLA	2	0
16	1	523	BCR	1	0
13	f	1212	CLA	1	0
17	G	5009	LHG	4	0
16	A	4003	BCR	2	0
13	e	1011	CLA	3	0
13	Y	512	CLA	6	0
13	B	1216	CLA	1	0
13	F	1302	CLA	2	0
13	l	1302	CLA	1	0
13	B	1202	CLA	2	0
16	L	4022	BCR	5	0
13	a	512	CLA	2	0
13	f	1225	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	s	511	CLA	1	0
13	1	504	CLA	1	0
13	3	513	CLA	3	0
20	a	822	SQD	1	0
13	H	1207	CLA	6	0
13	3	507	CLA	2	0
16	V	4022	BCR	6	0
13	4	511	CLA	1	0
13	Y	509	CLA	4	0
13	B	1021	CLA	1	0
17	e	5007	LHG	1	0
13	e	1130	CLA	4	0
13	B	1212	CLA	1	0
17	L	5220	LHG	2	0
13	f	1219	CLA	4	0
16	3	521	BCR	2	0
16	m	4104	BCR	5	0
13	f	1202	CLA	3	0
13	f	1229	CLA	4	0
13	6	506	CLA	1	0
13	f	1023	CLA	4	0
16	2	521	BCR	4	0
16	G	4002	BCR	3	0
16	f	4004	BCR	3	0
13	f	1224	CLA	6	0
13	H	1222	CLA	4	0
13	A	1139	CLA	3	0
16	B	4017	BCR	6	0
13	e	1135	CLA	3	0
13	U	1401	CLA	1	0
13	q	502	CLA	7	0
16	H	4006	BCR	1	0
13	a	518	CLA	1	0
13	4	519	CLA	2	0
13	f	1216	CLA	1	0
17	A	5008	LHG	2	0
13	Y	511	CLA	3	0
13	e	1109	CLA	3	0
13	t	516	CLA	1	0
13	a	501	CLA	2	0
16	e	4008	BCR	1	0
16	n	4020	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	1104	CLA	7	0
13	A	1138	CLA	2	0
13	3	519	CLA	1	0
13	e	1126	CLA	9	0
13	s	507	CLA	2	0
13	H	1204	CLA	1	0
13	d	501	CLA	3	0
13	3	511	CLA	2	0
16	c	523	BCR	1	0
13	B	1228	CLA	4	0
13	f	1214	CLA	2	0
13	5	507	CLA	1	0
16	L	4020	BCR	3	0
17	H	1855	LHG	3	0
13	Z	519	CLA	1	0
18	e	1849	LMU	1	0
13	5	502	CLA	3	0
17	A	5009	LHG	4	0
13	A	1106	CLA	2	0
13	f	1208	CLA	1	0
13	u	513	CLA	1	0
13	v	505	CLA	4	0
16	B	4009	BCR	5	0
13	e	1124	CLA	1	0
16	k	4018	BCR	4	0
14	e	2001	PQN	2	0
13	q	519	CLA	1	0
16	5	521	BCR	4	0
16	V	4219	BCR	5	0
13	f	1206	CLA	1	0
13	r	506	CLA	5	0
16	e	4007	BCR	4	0
13	d	511	CLA	1	0
13	e	1131	CLA	1	0
13	A	1115	CLA	1	0
13	s	512	CLA	2	0
16	G	4011	BCR	3	0
13	b	509	CLA	2	0
16	d	521	BCR	2	0
16	3	522	BCR	5	0
17	V	5220	LHG	2	0
13	A	1022	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	3	503	CLA	4	0
13	f	1217	CLA	4	0
13	A	1140	CLA	6	0
13	a	506	CLA	1	0
13	B	1235	CLA	3	0
13	3	505	CLA	2	0
13	A	1103	CLA	4	0
13	B	1225	CLA	3	0
17	k	5001	LHG	1	0
13	1	516	CLA	2	0
13	B	1227	CLA	4	0
13	b	503	CLA	1	0
13	Y	507	CLA	3	0
13	f	1238	CLA	1	0
16	H	4005	BCR	2	0
16	H	4017	BCR	3	0
17	e	5002	LHG	4	0
13	5	511	CLA	1	0
13	q	503	CLA	4	0
13	f	1210	CLA	4	0
13	e	1137	CLA	4	0
13	F	1301	CLA	2	0
13	B	1219	CLA	5	0
13	a	502	CLA	2	0
13	u	506	CLA	3	0
13	1	508	CLA	2	0
13	B	1229	CLA	5	0
13	e	1133	CLA	1	0
13	n	1502	CLA	2	0
16	J	4013	BCR	6	0
16	R	4016	BCR	4	0
13	r	507	CLA	3	0
13	t	503	CLA	1	0
13	B	1023	CLA	3	0
13	1	510	CLA	2	0
13	L	1502	CLA	2	0
13	B	1224	CLA	6	0
13	r	512	CLA	5	0
16	d	524	BCR	8	0
16	s	524	BCR	4	0
13	4	502	CLA	2	0
13	e	1801	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	e	1118	CLA	2	0
16	B	4005	BCR	3	0
16	Y	524	BCR	5	0
13	H	1217	CLA	4	0
13	R	1302	CLA	2	0
13	e	1102	CLA	2	0
13	H	1218	CLA	2	0
17	G	5007	LHG	1	0
13	R	1301	CLA	1	0
13	H	1203	CLA	3	0
13	a	519	CLA	1	0
13	f	1226	CLA	6	0
17	e	5004	LHG	1	0
13	2	509	CLA	1	0
13	v	501	CLA	3	0
13	c	513	CLA	1	0
13	c	509	CLA	1	0
16	H	4014	BCR	4	0
16	d	523	BCR	2	0
13	B	1214	CLA	2	0
13	K	1105	CLA	1	0
13	Y	504	CLA	1	0
13	b	516	CLA	1	0
13	K	1103	CLA	2	0
13	Y	517	CLA	1	0
16	d	522	BCR	9	0
13	b	501	CLA	2	0
13	u	507	CLA	1	0
13	f	1213	CLA	1	0
13	q	501	CLA	4	0
13	Y	518	CLA	2	0
13	u	510	CLA	1	0
17	G	5005	LHG	1	0
13	e	1120	CLA	2	0
13	r	518	CLA	2	0
13	G	1134	CLA	1	0
13	f	1221	CLA	6	0
16	a	522	BCR	2	0
16	A	4001	BCR	1	0
13	e	1237	CLA	3	0
17	n	5220	LHG	2	0
13	6	511	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	4	509	CLA	3	0
13	b	511	CLA	1	0
17	A	5007	LHG	1	0
13	B	1203	CLA	2	0
13	H	1202	CLA	2	0
16	q	521	BCR	1	0
13	B	1234	CLA	2	0
13	G	1138	CLA	2	0
13	c	506	CLA	3	0
13	Z	518	CLA	2	0
16	4	523	BCR	1	0
16	U	4104	BCR	6	0
13	q	510	CLA	2	0
13	K	1401	CLA	1	0
20	d	822	SQD	1	0
16	f	4017	BCR	5	0
13	B	1207	CLA	6	0
13	e	1128	CLA	5	0
13	4	506	CLA	1	0
13	G	1106	CLA	2	0
16	A	4002	BCR	4	0
20	s	822	SQD	1	0
13	H	1238	CLA	1	0
13	G	1121	CLA	2	0
13	1	513	CLA	1	0
15	C	3002	SF4	1	0
14	B	2002	PQN	2	0
13	e	1105	CLA	2	0
13	B	1215	CLA	3	0
13	H	1206	CLA	2	0
13	e	1119	CLA	5	0
16	3	523	BCR	1	0
13	A	1011	CLA	4	0
13	6	519	CLA	2	0
14	G	2001	PQN	3	0
13	e	1114	CLA	1	0
17	G	5008	LHG	2	0
13	G	1107	CLA	2	0
13	4	503	CLA	1	0
13	q	512	CLA	6	0
13	B	1201	CLA	2	0
13	2	518	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	f	1231	CLA	3	0
13	a	513	CLA	3	0
13	B	1238	CLA	1	0
13	r	502	CLA	5	0
13	A	1130	CLA	4	0
13	c	507	CLA	1	0
13	q	508	CLA	2	0
13	d	513	CLA	1	0
13	s	505	CLA	2	0
13	s	506	CLA	1	0
13	G	1123	CLA	2	0
13	3	502	CLA	2	0
13	A	1108	CLA	2	0
13	Z	501	CLA	4	0
16	B	4004	BCR	4	0
20	Y	822	SQD	5	0
16	5	524	BCR	3	0
13	B	1217	CLA	3	0
13	A	1135	CLA	2	0
13	B	1213	CLA	1	0
13	4	512	CLA	2	0
13	Y	502	CLA	7	0
19	B	5002	LMG	7	0
13	H	1012	CLA	2	0
13	1	518	CLA	1	0
13	f	1234	CLA	4	0
16	q	523	BCR	1	0
13	r	503	CLA	4	0
16	A	4008	BCR	2	0
13	B	1206	CLA	2	0
13	J	1303	CLA	4	0
13	a	510	CLA	3	0
13	B	1240	CLA	1	0
13	B	1222	CLA	4	0
16	Y	521	BCR	2	0
13	e	1116	CLA	4	0
13	r	519	CLA	1	0
13	r	505	CLA	4	0
16	e	4011	BCR	3	0
16	V	4020	BCR	3	0
13	A	1109	CLA	3	0
13	U	1105	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	s	516	CLA	1	0
15	g	3002	SF4	1	0
13	U	1103	CLA	2	0
17	e	5006	LHG	1	0
17	n	5221	LHG	10	0
13	B	1226	CLA	5	0
13	B	1210	CLA	4	0
13	A	1137	CLA	3	0
13	f	1215	CLA	2	0
13	e	1013	CLA	8	0
16	2	524	BCR	6	0
16	1	521	BCR	1	0
17	L	5221	LHG	11	0
13	q	509	CLA	3	0
14	H	2002	PQN	4	0
13	c	512	CLA	4	0
13	H	1228	CLA	4	0
13	Z	511	CLA	4	0
13	G	1013	CLA	8	0
13	2	519	CLA	1	0
13	a	505	CLA	3	0
13	d	506	CLA	1	0
13	t	518	CLA	1	0
16	L	4219	BCR	4	0
16	f	4014	BCR	4	0
13	J	1302	CLA	1	0
13	t	501	CLA	2	0
13	2	511	CLA	3	0
13	Z	507	CLA	2	0
16	Z	521	BCR	2	0
13	H	1021	CLA	2	0
13	H	1236	CLA	4	0
13	Z	510	CLA	2	0
13	n	1501	CLA	9	0
13	H	1201	CLA	3	0
16	A	4007	BCR	5	0
13	n	1503	CLA	2	0
13	s	510	CLA	4	0
13	Y	513	CLA	1	0
13	e	1121	CLA	3	0
16	T	4012	BCR	6	0
16	v	522	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	3	512	CLA	2	0
13	L	1503	CLA	1	0
13	t	505	CLA	1	0
13	A	1136	CLA	1	0
13	A	1111	CLA	1	0
13	e	1110	CLA	1	0
16	l	4015	BCR	4	0
13	G	1118	CLA	2	0
16	1	524	BCR	5	0
13	Z	512	CLA	5	0
13	1	519	CLA	1	0
13	f	1222	CLA	4	0
13	5	506	CLA	3	0
13	A	1126	CLA	8	0
20	B	1852	SQD	7	0
16	q	522	BCR	4	0
13	2	503	CLA	4	0
16	4	524	BCR	4	0
19	f	5002	LMG	7	0
13	B	1231	CLA	3	0
13	2	507	CLA	3	0
16	B	4006	BCR	1	0
13	3	516	CLA	1	0
13	Z	502	CLA	5	0
17	A	5002	LHG	3	0
13	v	513	CLA	1	0
13	f	1227	CLA	3	0
13	A	1124	CLA	1	0
13	e	1111	CLA	1	0
13	1	501	CLA	4	0
13	5	503	CLA	3	0
13	H	1221	CLA	6	0
13	A	1133	CLA	1	0
13	G	1135	CLA	3	0
13	G	1237	CLA	4	0
15	N	3002	SF4	1	0
16	M	4021	BCR	2	0
13	5	505	CLA	1	0
13	e	1101	CLA	3	0
16	l	4012	BCR	5	0
13	1	503	CLA	4	0
13	s	517	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	q	513	CLA	1	0
16	6	522	BCR	4	0
13	t	512	CLA	2	0
16	K	4104	BCR	7	0
16	6	523	BCR	2	0
17	A	5004	LHG	1	0
17	e	5003	LHG	1	0
16	l	4013	BCR	6	0
13	A	1118	CLA	2	0
13	G	1011	CLA	3	0
13	e	1123	CLA	2	0
13	f	1239	CLA	3	0
13	l	1303	CLA	3	0
16	Z	523	BCR	1	0
16	u	521	BCR	4	0
13	A	1104	CLA	6	0
13	e	1117	CLA	3	0
13	e	1103	CLA	4	0
13	H	1223	CLA	1	0
16	2	522	BCR	2	0
13	B	1236	CLA	5	0
13	A	1128	CLA	5	0
16	f	4009	BCR	5	0
13	a	503	CLA	3	0
13	B	1221	CLA	7	0
13	u	503	CLA	3	0
13	e	1136	CLA	2	0
13	d	512	CLA	4	0
13	f	1236	CLA	4	0
13	b	517	CLA	2	0
14	f	2002	PQN	3	0
16	t	521	BCR	1	0
16	t	523	BCR	3	0
13	b	513	CLA	1	0
16	u	522	BCR	3	0
17	B	1842	LHG	2	0
13	t	510	CLA	1	0
13	G	1116	CLA	3	0
13	m	1105	CLA	1	0
13	q	511	CLA	3	0
13	r	510	CLA	3	0
13	H	1212	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	Z	822	SQD	1	0
13	t	519	CLA	2	0
16	l	522	BCR	4	0
13	f	1201	CLA	3	0
13	c	502	CLA	3	0
13	u	511	CLA	1	0
13	A	1801	CLA	3	0
13	f	1235	CLA	4	0
16	J	4012	BCR	4	0
13	H	1229	CLA	4	0
13	A	1102	CLA	4	0
13	s	518	CLA	1	0
16	s	521	BCR	3	0
13	f	1204	CLA	2	0
13	H	1224	CLA	6	0
13	H	1239	CLA	2	0
13	v	512	CLA	3	0
17	B	1855	LHG	2	0
13	f	1223	CLA	2	0
16	H	4010	BCR	6	0
13	l	512	CLA	6	0
13	c	503	CLA	3	0
13	e	1129	CLA	2	0
13	V	1503	CLA	3	0
13	v	511	CLA	1	0
16	s	522	BCR	1	0
16	T	4013	BCR	6	0
13	T	1303	CLA	3	0
13	G	1130	CLA	4	0
16	H	4004	BCR	3	0
20	l	822	SQD	4	0
13	4	518	CLA	1	0
13	b	518	CLA	1	0
13	H	1214	CLA	2	0
13	e	1107	CLA	2	0
13	j	1301	CLA	3	0
13	G	1111	CLA	1	0
13	G	1119	CLA	4	0
13	A	1120	CLA	2	0
13	A	1116	CLA	2	0
13	Z	513	CLA	1	0
13	Z	509	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	s	519	CLA	1	0
16	v	521	BCR	2	0
13	A	1105	CLA	2	0
13	G	1108	CLA	1	0
13	e	1122	CLA	3	0
13	q	507	CLA	3	0
13	A	1237	CLA	3	0
13	H	1023	CLA	2	0
17	A	5006	LHG	1	0
13	d	502	CLA	2	0
13	H	1220	CLA	3	0
13	f	1207	CLA	8	0
16	G	4008	BCR	1	0
13	6	501	CLA	4	0
16	3	524	BCR	6	0
16	v	524	BCR	6	0
13	b	512	CLA	2	0
13	G	1117	CLA	3	0
13	t	502	CLA	2	0
16	B	4010	BCR	6	0
16	c	522	BCR	2	0
18	J	5105	LMU	2	0
13	3	509	CLA	1	0
13	5	510	CLA	1	0
17	e	5005	LHG	1	0
17	e	5001	LHG	5	0
13	s	503	CLA	3	0
13	6	505	CLA	4	0
13	r	517	CLA	1	0
13	t	509	CLA	3	0
16	q	524	BCR	5	0
16	B	4014	BCR	4	0
13	r	509	CLA	1	0
13	Z	506	CLA	5	0
13	s	513	CLA	2	0
20	H	1852	SQD	10	0
13	A	1119	CLA	4	0
13	f	1220	CLA	4	0
13	b	510	CLA	1	0
13	2	502	CLA	5	0
13	H	1208	CLA	2	0
13	f	1209	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	H	1205	CLA	1	0
13	G	1122	CLA	3	0
13	f	1218	CLA	2	0
13	f	1203	CLA	3	0
13	A	1114	CLA	1	0
13	4	501	CLA	2	0
13	r	511	CLA	3	0
19	H	5002	LMG	7	0
16	I	4018	BCR	3	0
16	A	4011	BCR	4	0
17	G	5004	LHG	1	0
13	2	510	CLA	2	0
13	a	509	CLA	1	0
13	G	1136	CLA	2	0
13	G	1125	CLA	1	0
13	A	1013	CLA	7	0
13	H	1225	CLA	3	0
13	c	510	CLA	1	0
20	n	5216	SQD	4	0
16	b	524	BCR	4	0
13	4	516	CLA	1	0
13	G	1128	CLA	3	0
13	B	1209	CLA	1	0
13	a	517	CLA	1	0
13	t	517	CLA	2	0
16	f	4010	BCR	5	0
13	V	1501	CLA	8	0
20	L	5216	SQD	4	0
13	t	513	CLA	1	0
13	u	509	CLA	2	0
13	B	1208	CLA	2	0
13	6	512	CLA	4	0
13	Y	503	CLA	4	0
13	t	506	CLA	1	0
13	d	505	CLA	4	0
16	e	4003	BCR	4	0
13	a	516	CLA	1	0
13	B	1220	CLA	4	0
20	3	822	SQD	1	0
13	A	1121	CLA	3	0
17	G	5006	LHG	1	0
13	H	1234	CLA	4	0

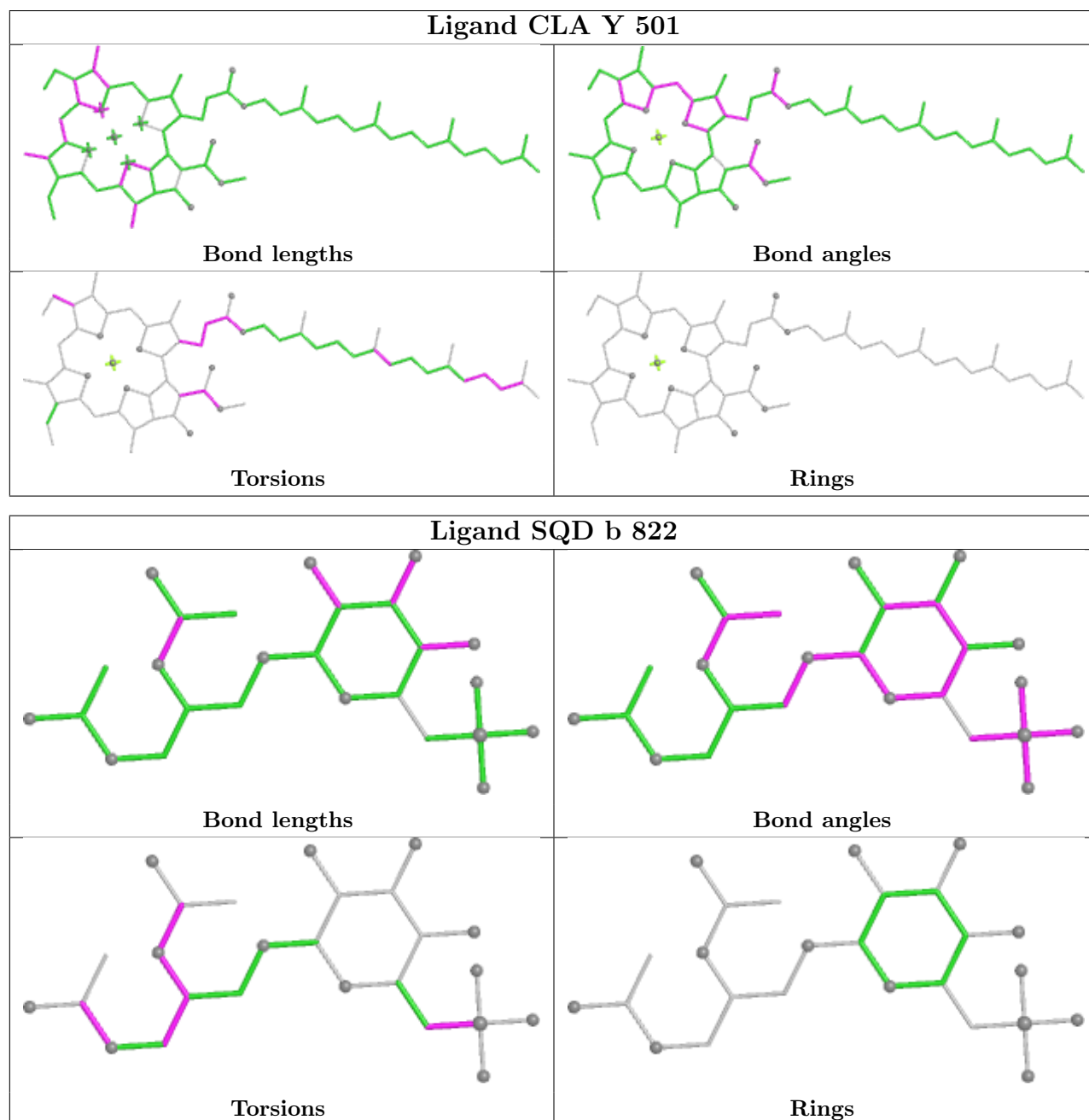
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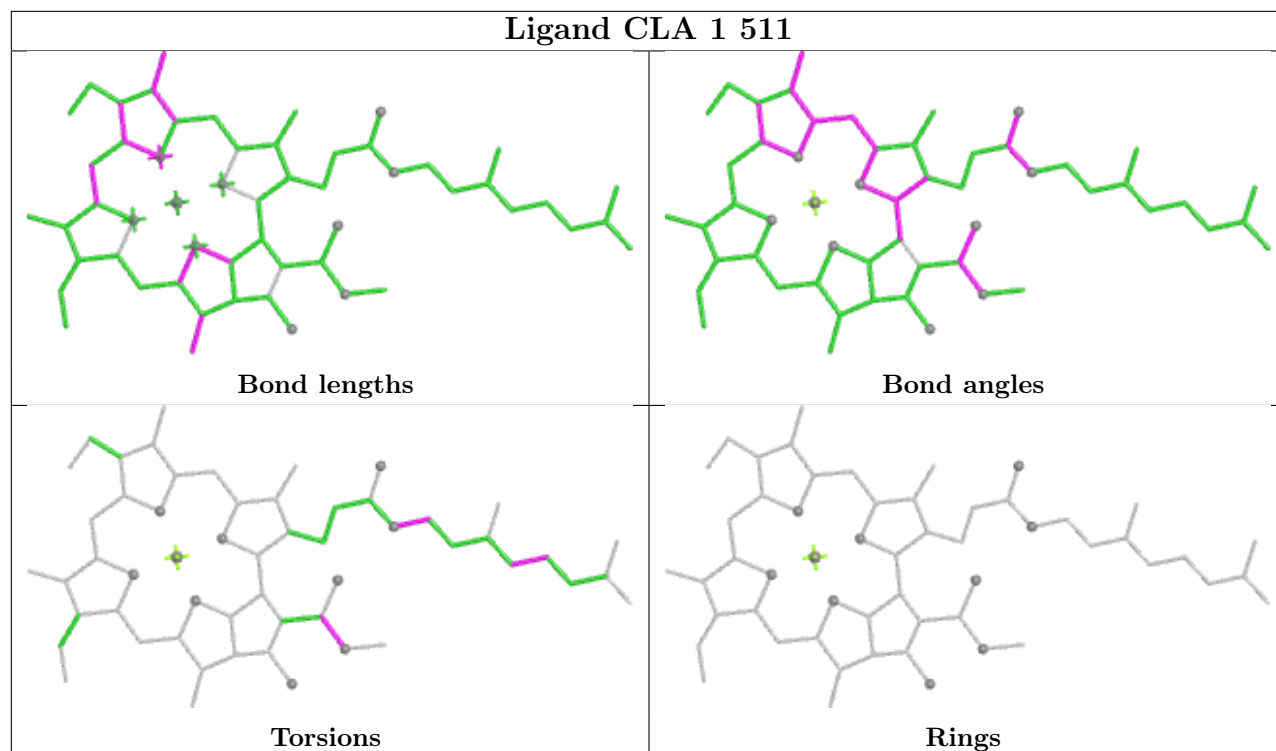
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	1	509	CLA	4	0
16	a	523	BCR	2	0
17	A	5003	LHG	2	0
20	f	1852	SQD	8	0
13	s	501	CLA	2	0
13	H	1215	CLA	4	0
13	r	513	CLA	1	0
13	q	518	CLA	4	0
14	A	2001	PQN	3	0
13	4	510	CLA	1	0
13	G	1801	CLA	2	0
13	5	501	CLA	4	0
13	G	1140	CLA	6	0
16	H	4009	BCR	4	0
13	Y	519	CLA	1	0
16	u	524	BCR	3	0
13	G	1102	CLA	3	0
13	L	1501	CLA	8	0
13	e	1138	CLA	2	0
13	f	1012	CLA	2	0
20	q	822	SQD	4	0
13	H	1226	CLA	7	0
13	G	1112	CLA	1	0
13	j	1302	CLA	1	0
16	6	521	BCR	2	0
17	H	1842	LHG	2	0
16	G	4001	BCR	2	0
13	r	501	CLA	4	0
13	B	1205	CLA	1	0
13	e	1139	CLA	2	0
13	H	1235	CLA	4	0
13	v	517	CLA	2	0
16	6	524	BCR	8	0
17	G	5001	LHG	4	0
13	A	1101	CLA	3	0
18	l	5105	LMU	2	0
13	Y	516	CLA	2	0
13	e	1022	CLA	4	0
13	B	1204	CLA	1	0
13	G	1120	CLA	2	0
16	Z	524	BCR	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

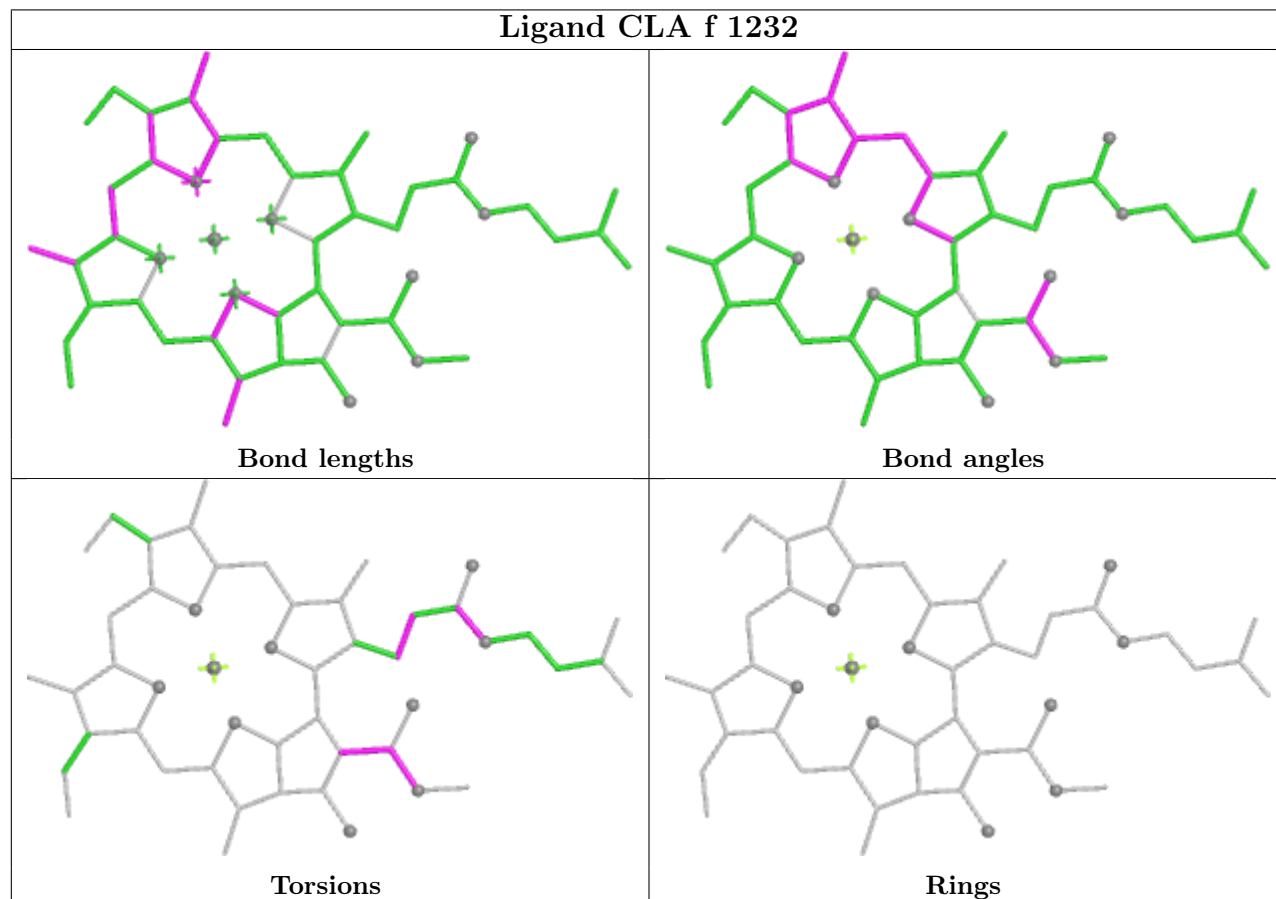
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

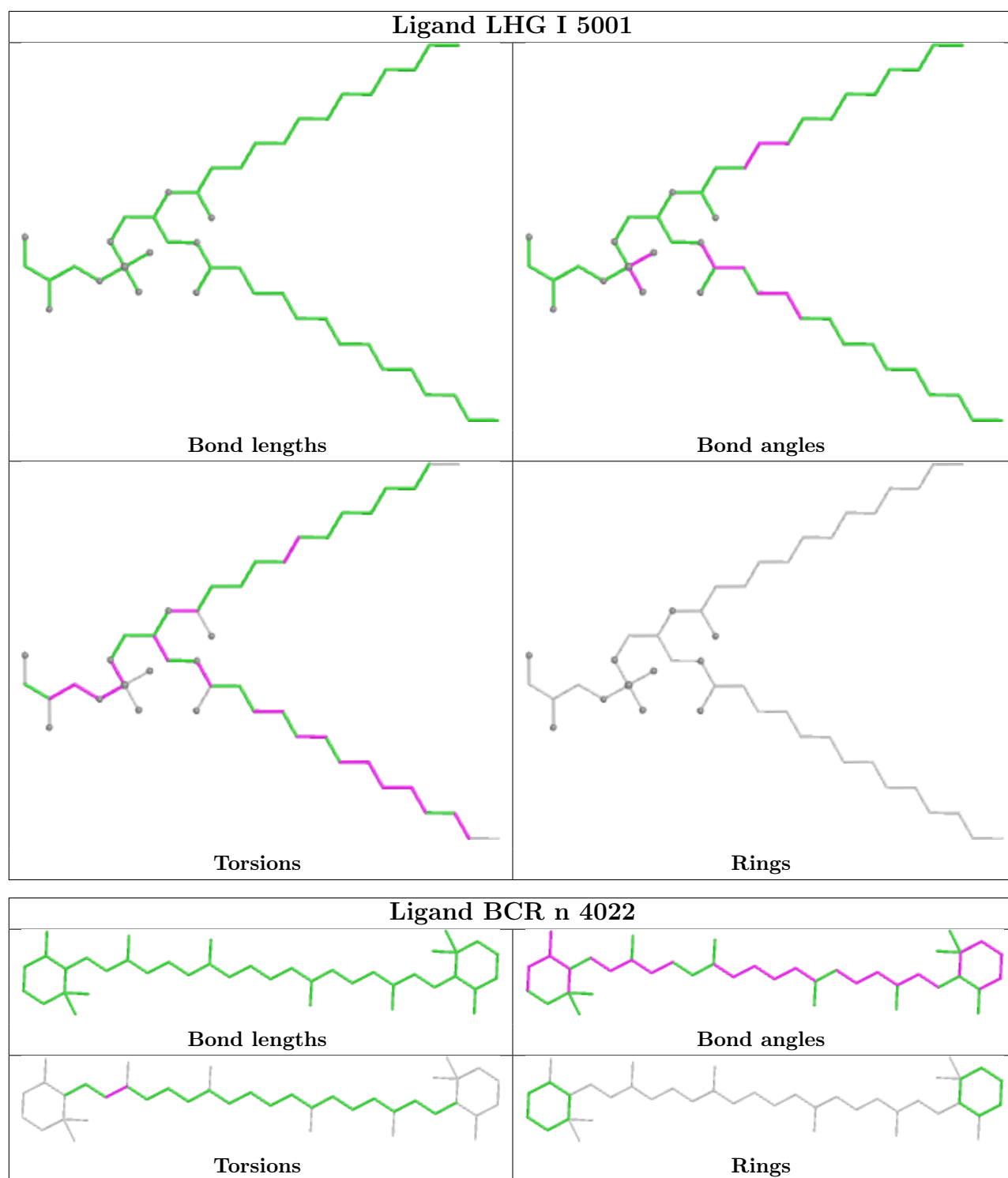


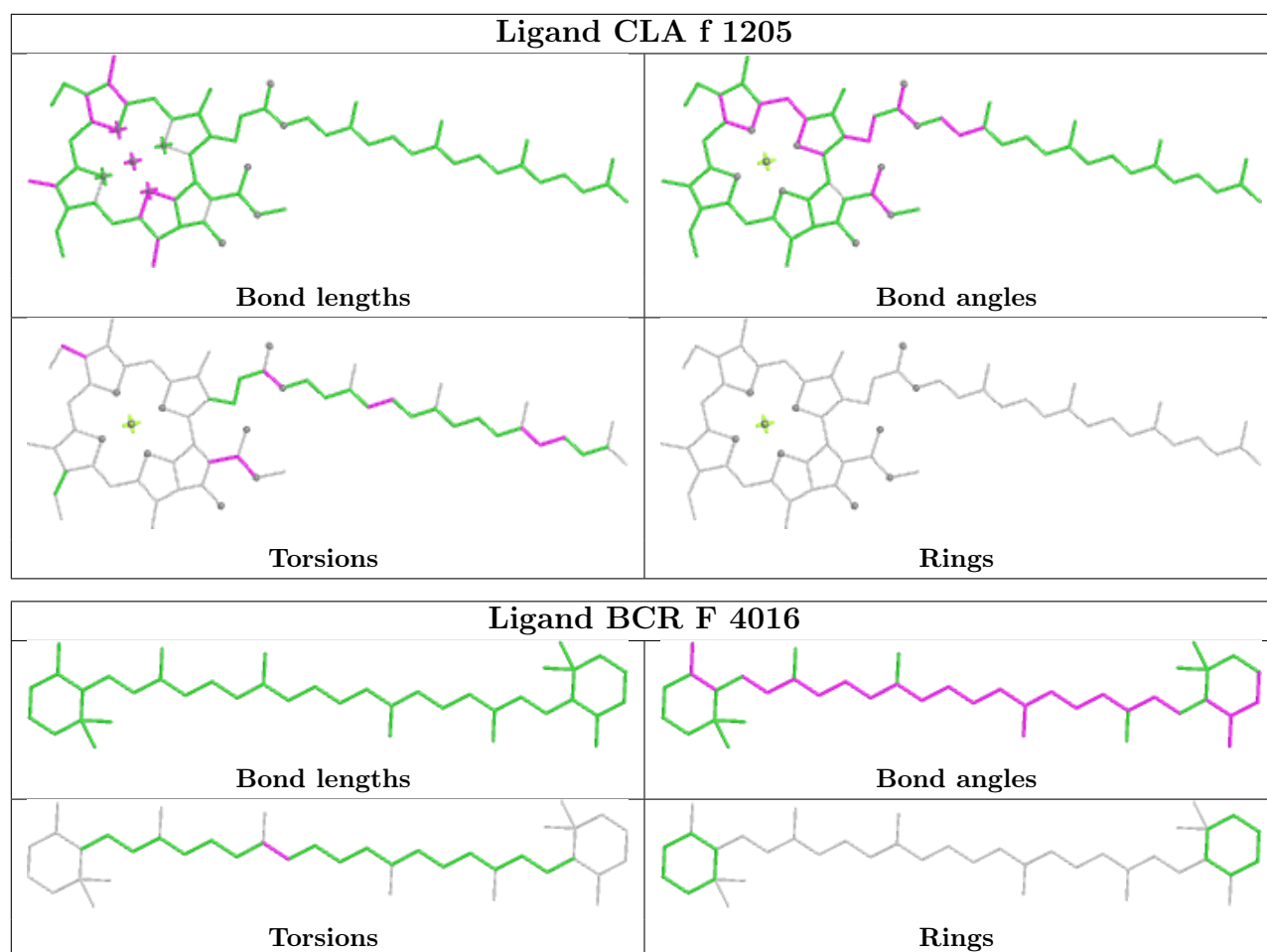
Ligand CLA 1 511



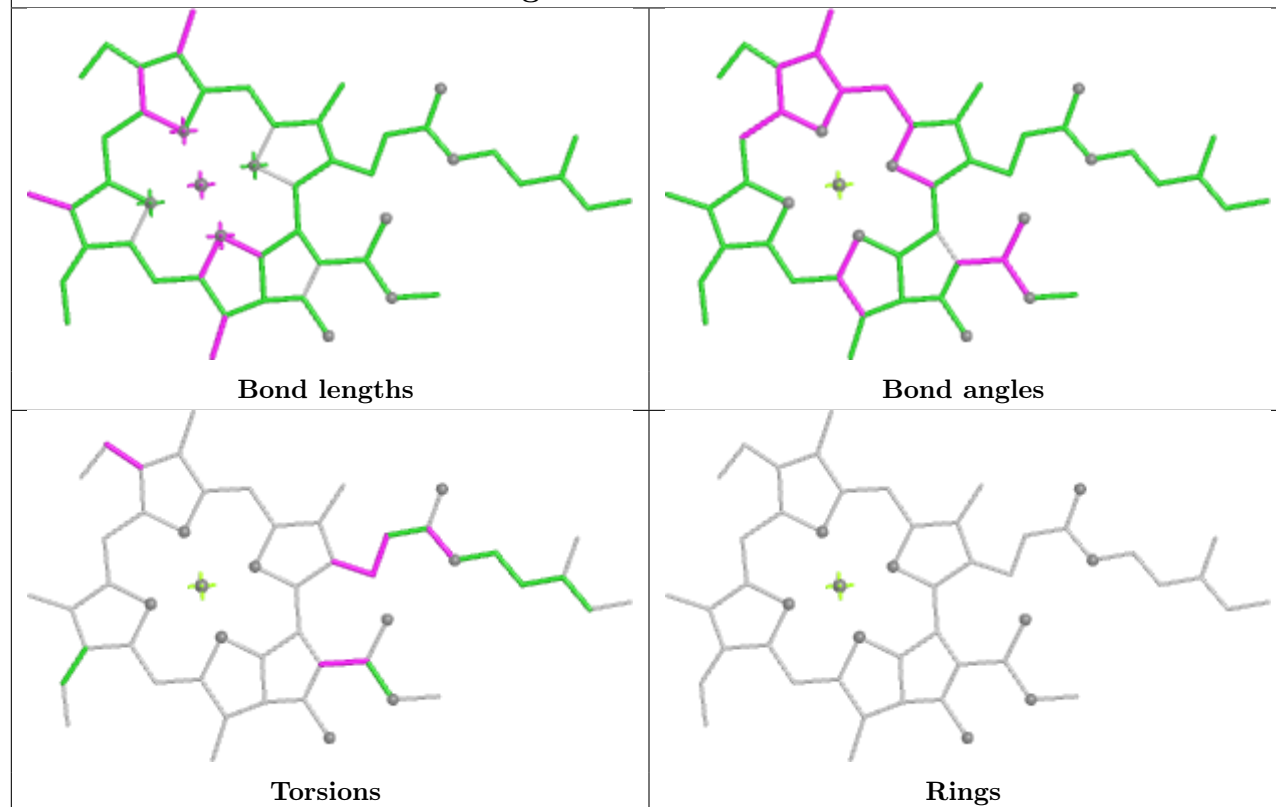
Ligand CLA f 1232



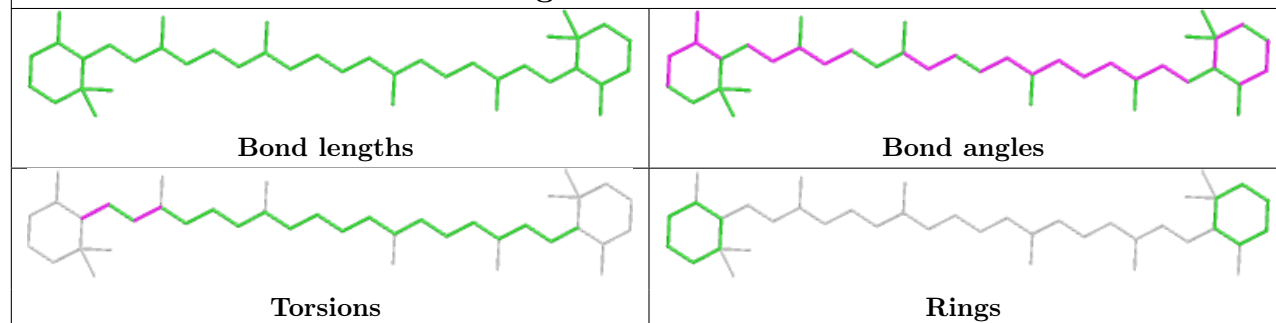


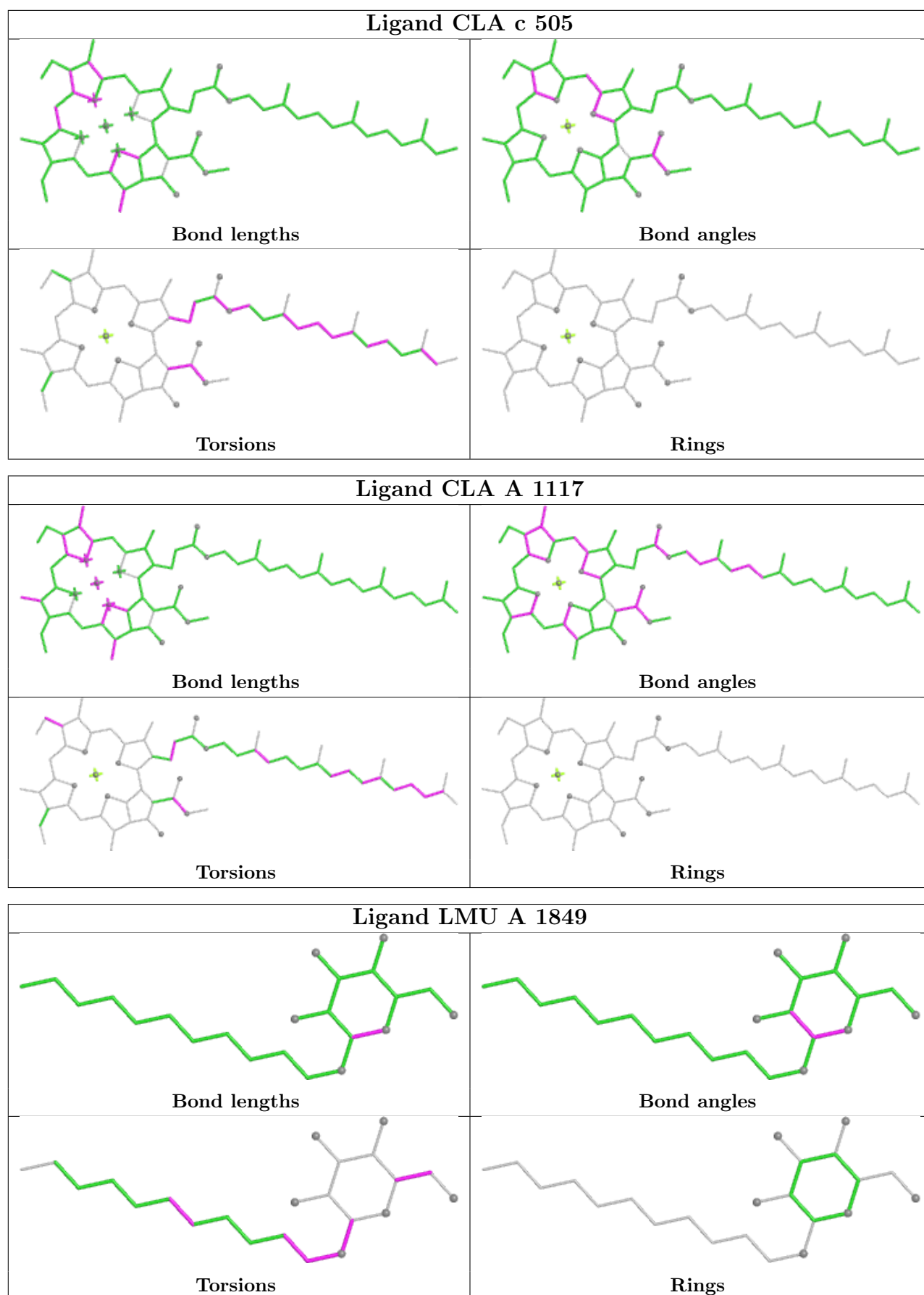


Ligand CLA G 1129

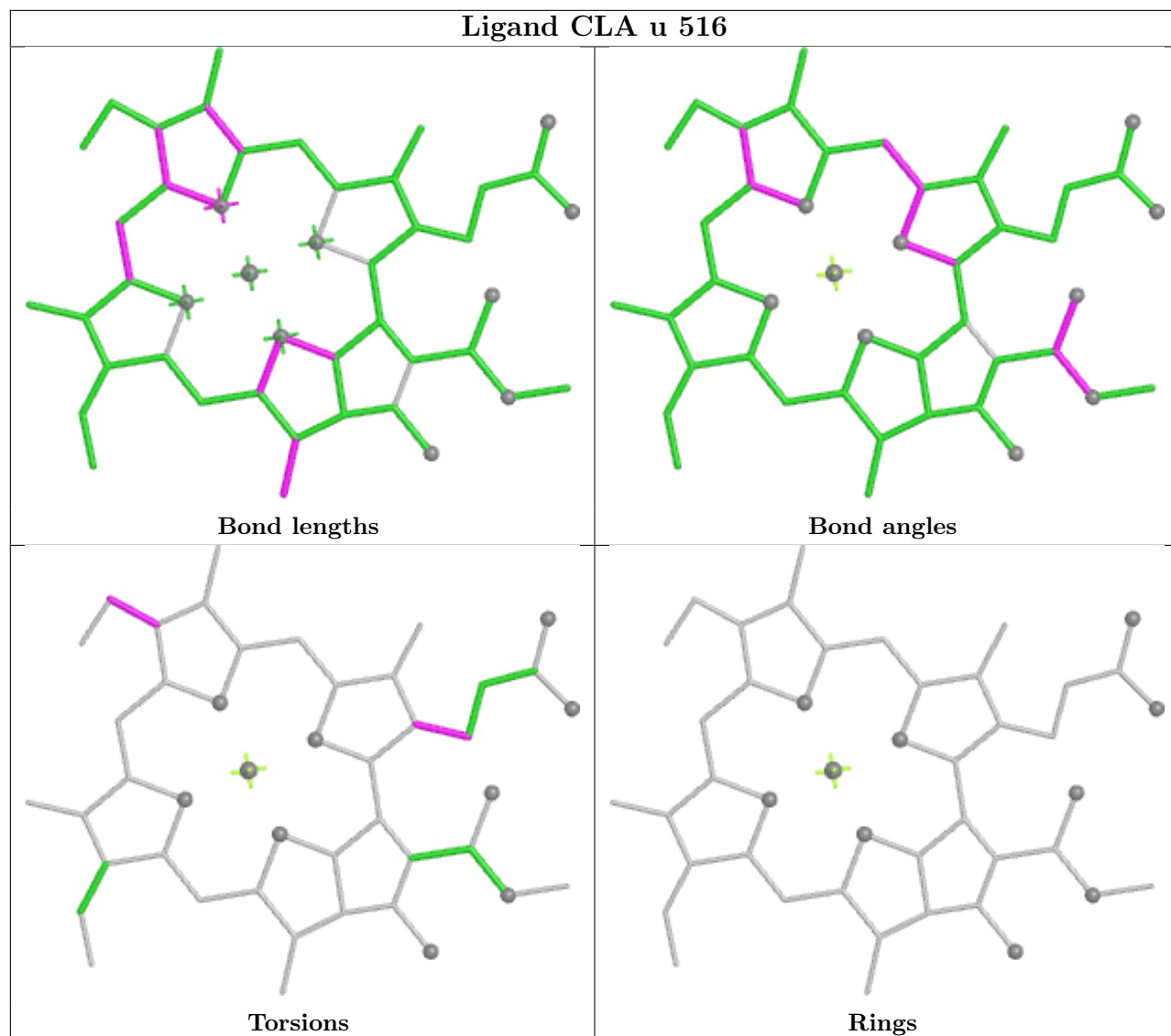


Ligand BCR r 521

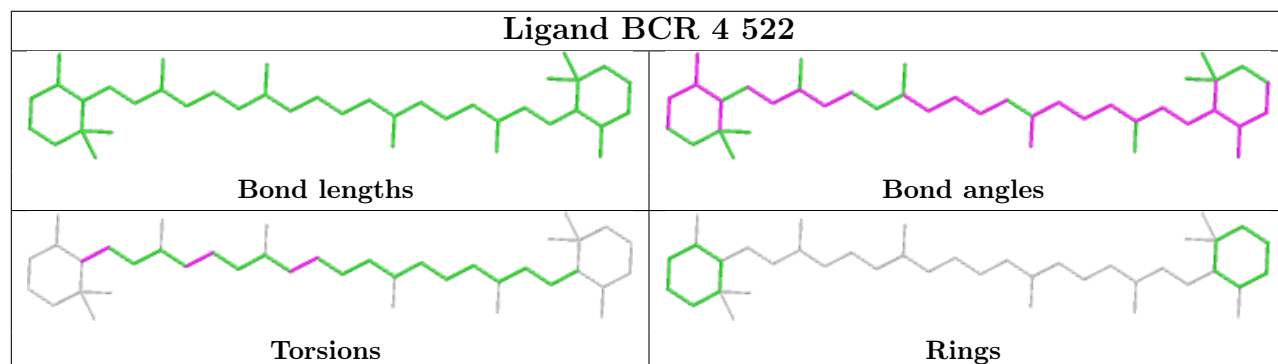


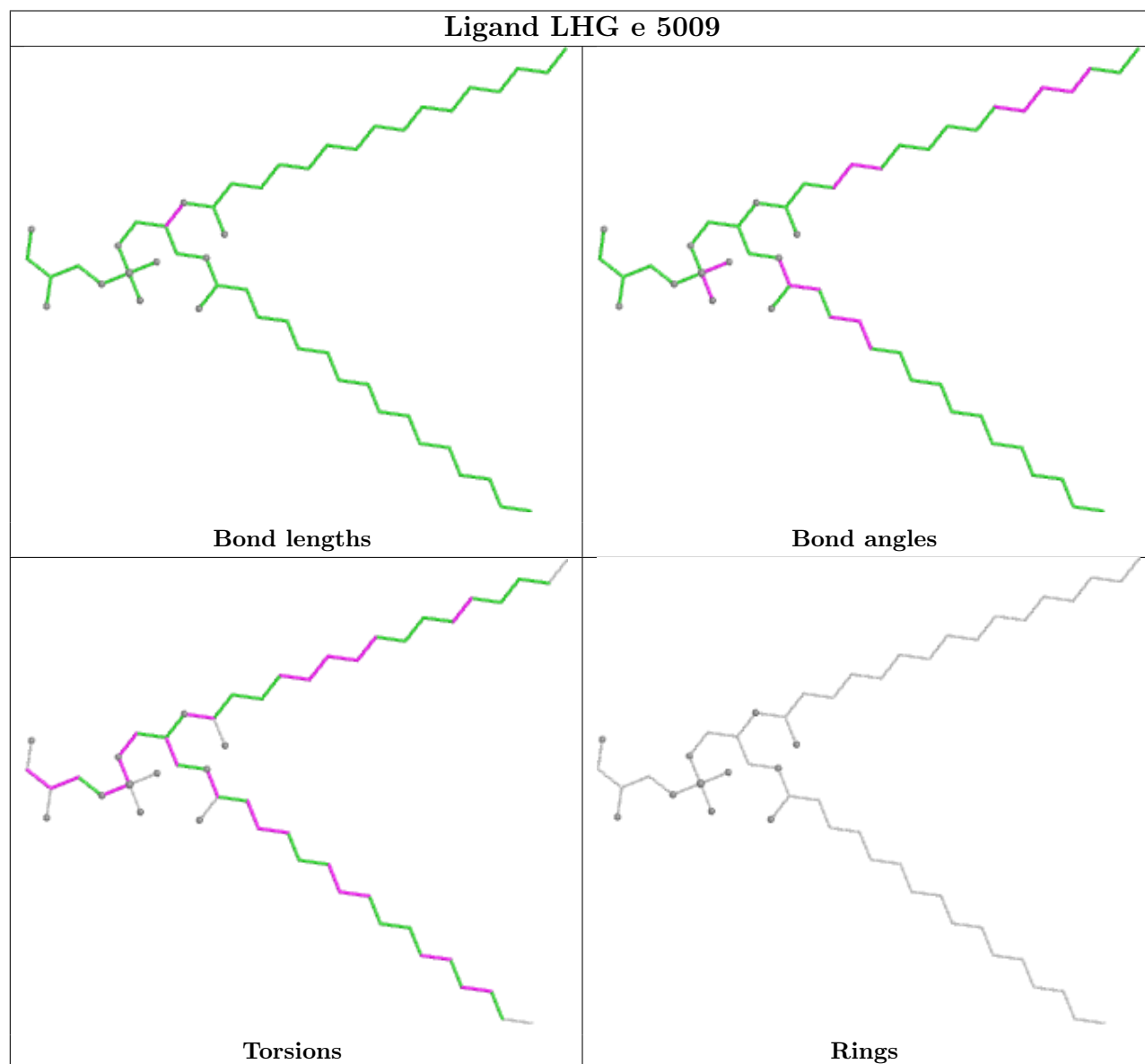
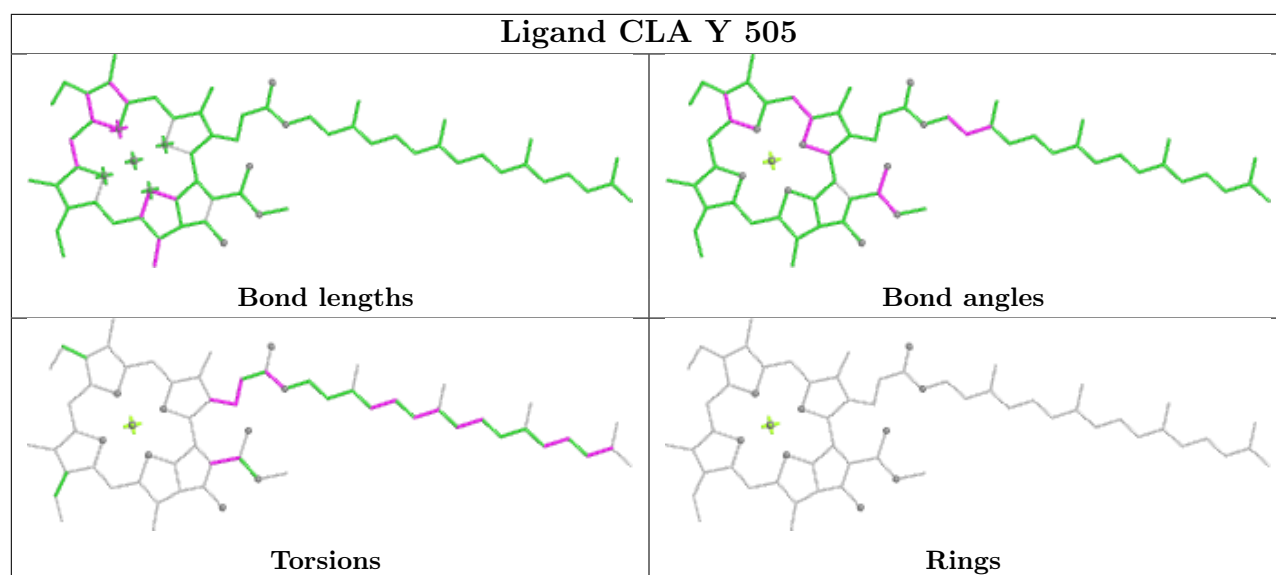


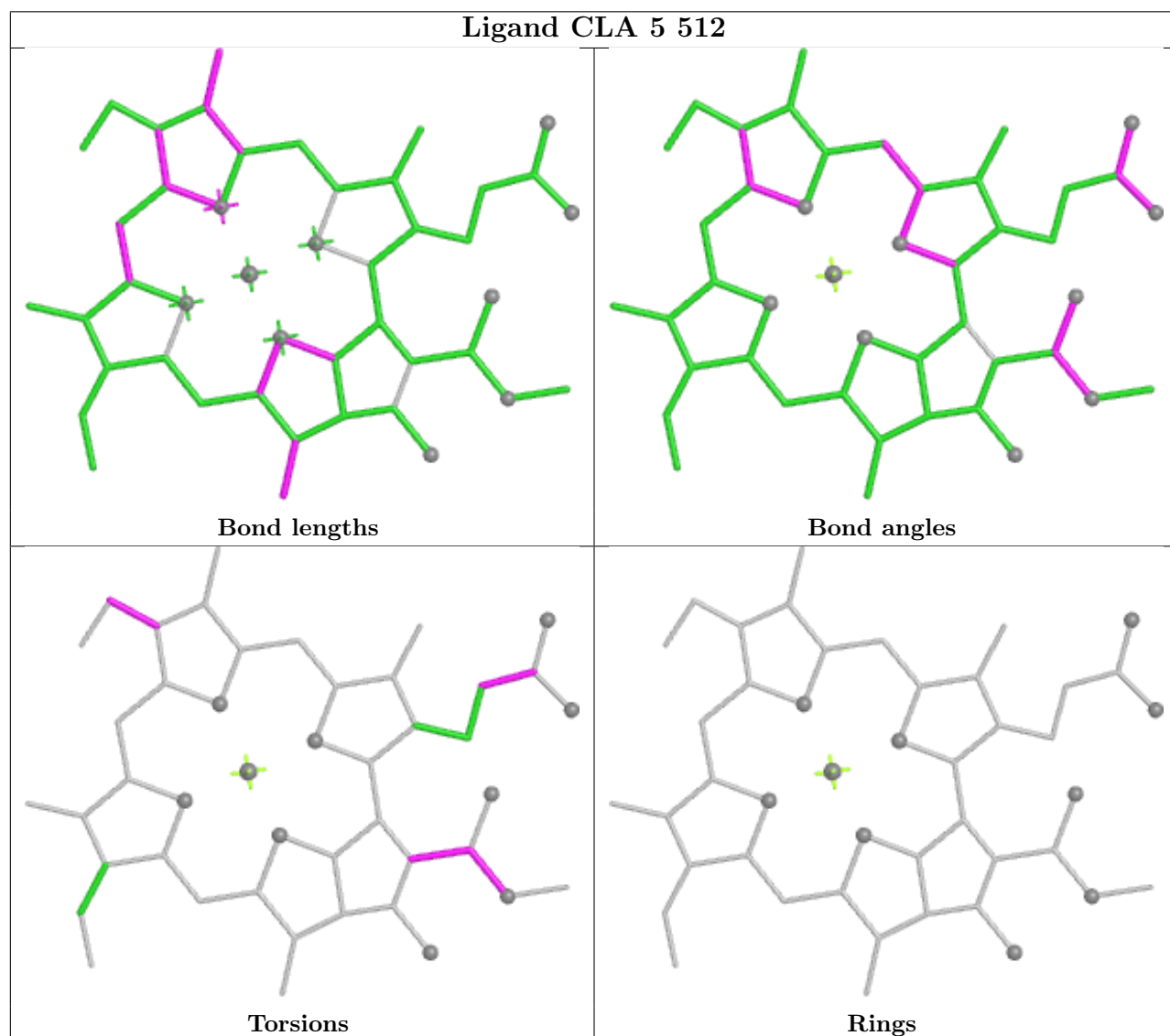
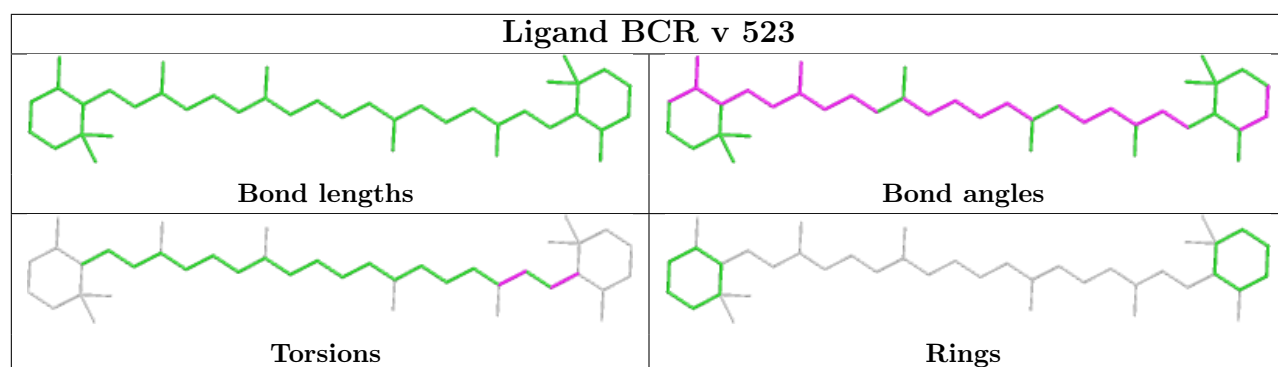
Ligand CLA u 516



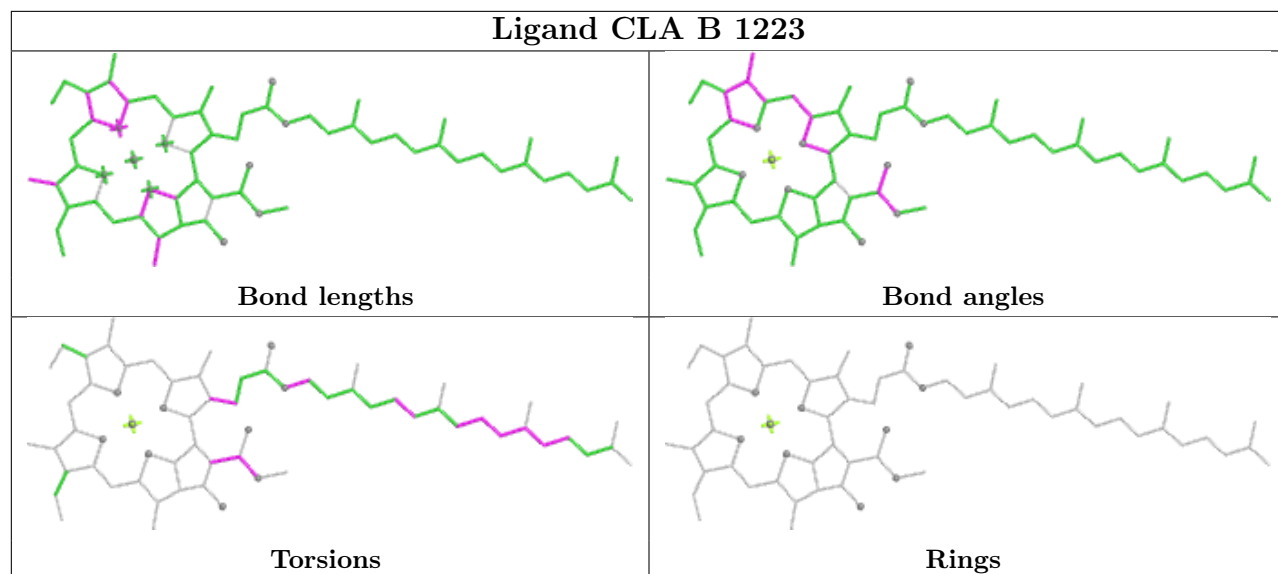
Ligand BCR 4 522



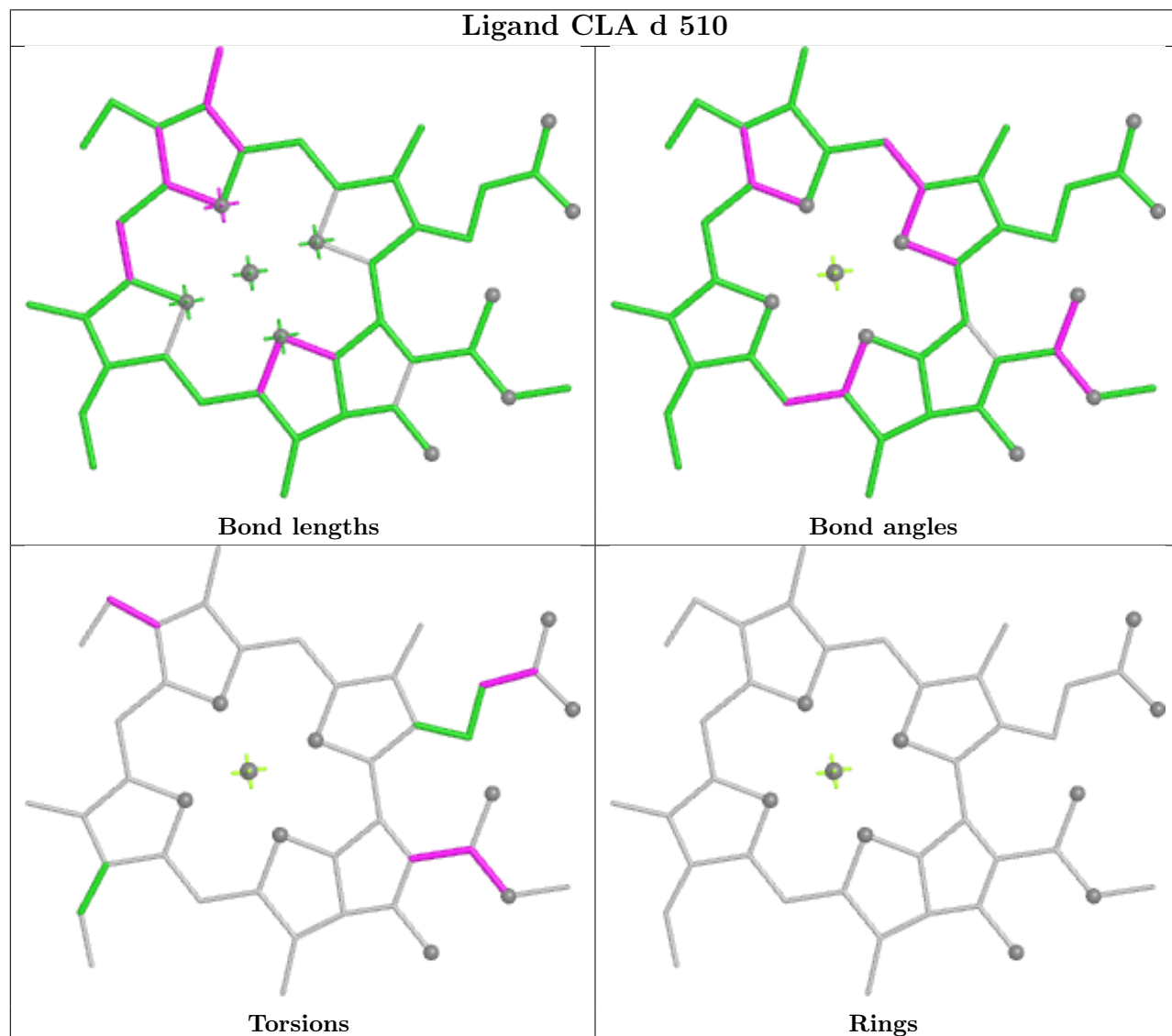




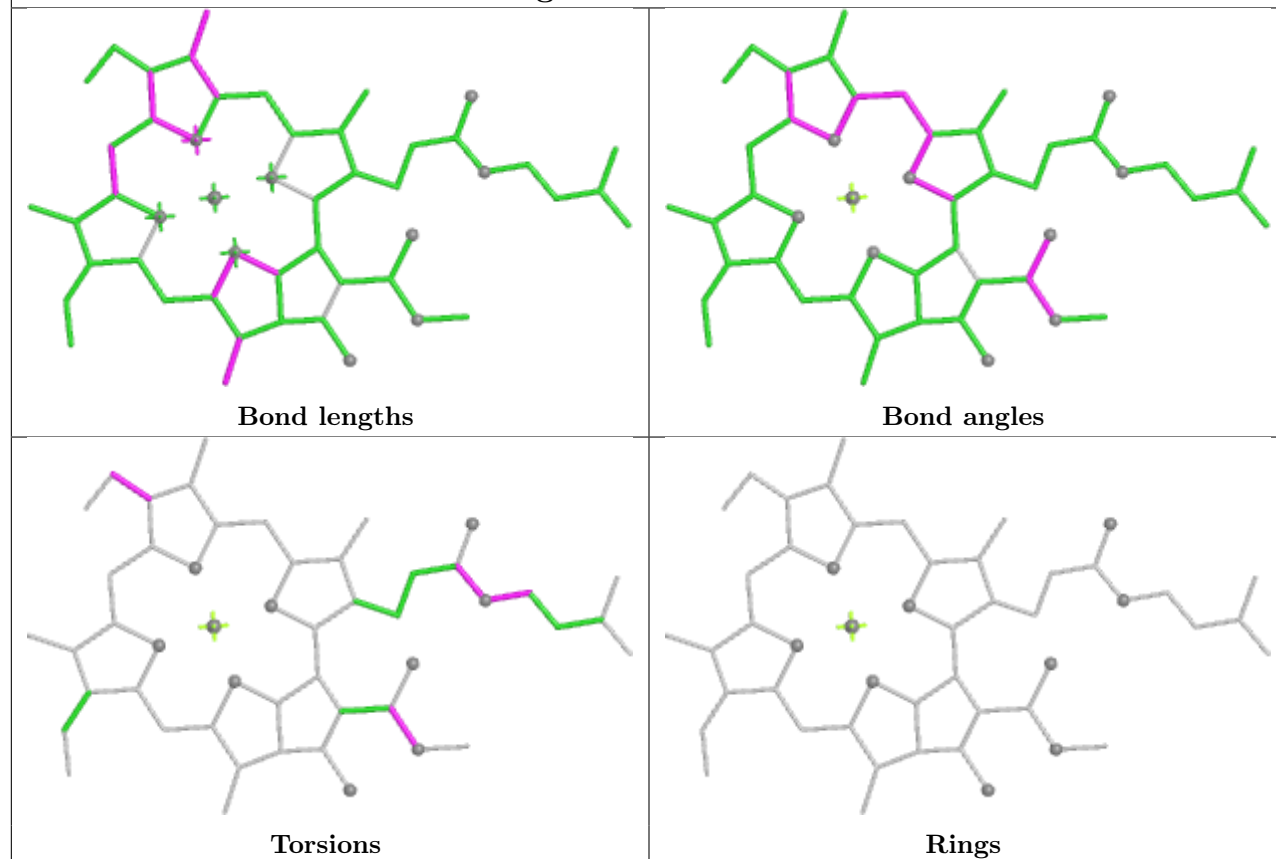
Ligand CLA B 1223



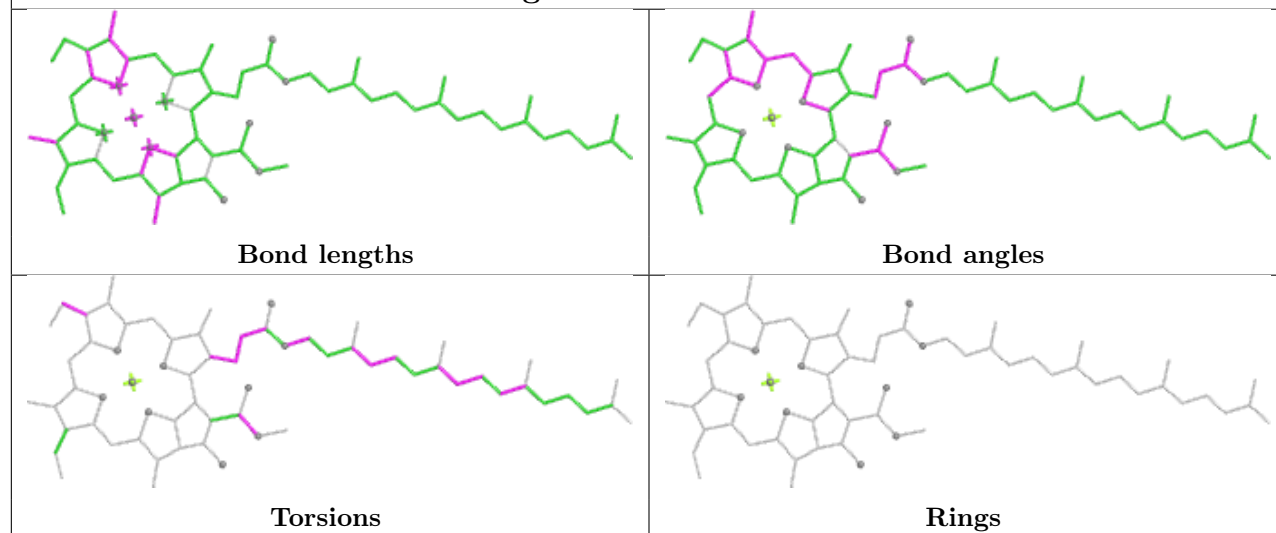
Ligand CLA d 510

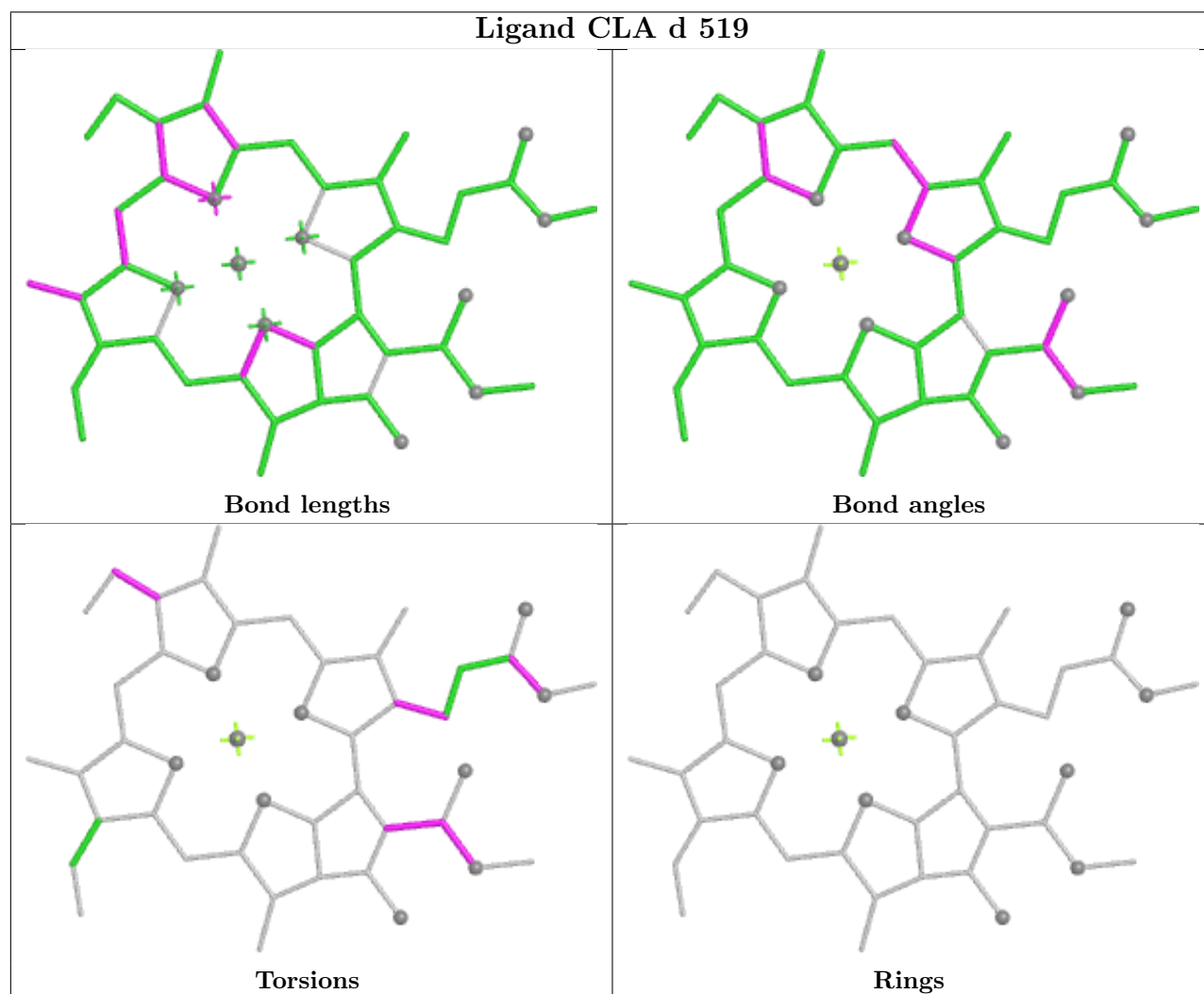
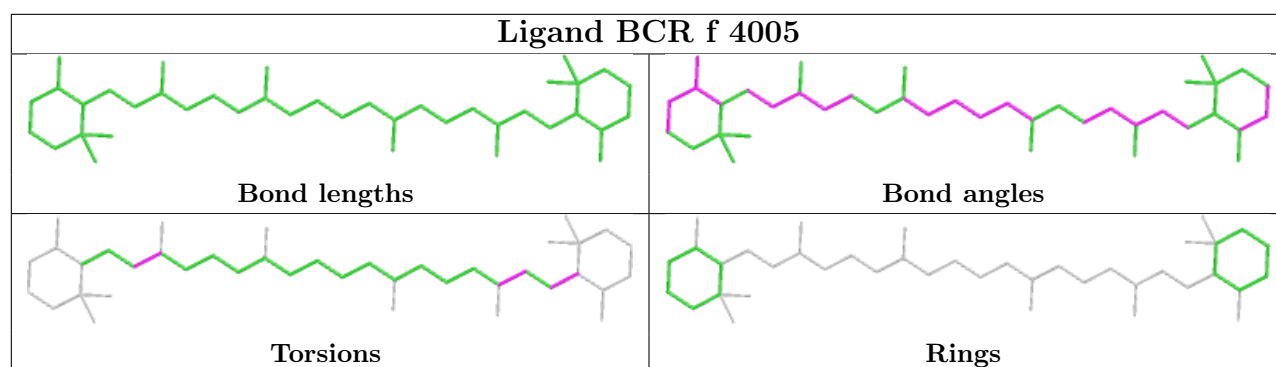


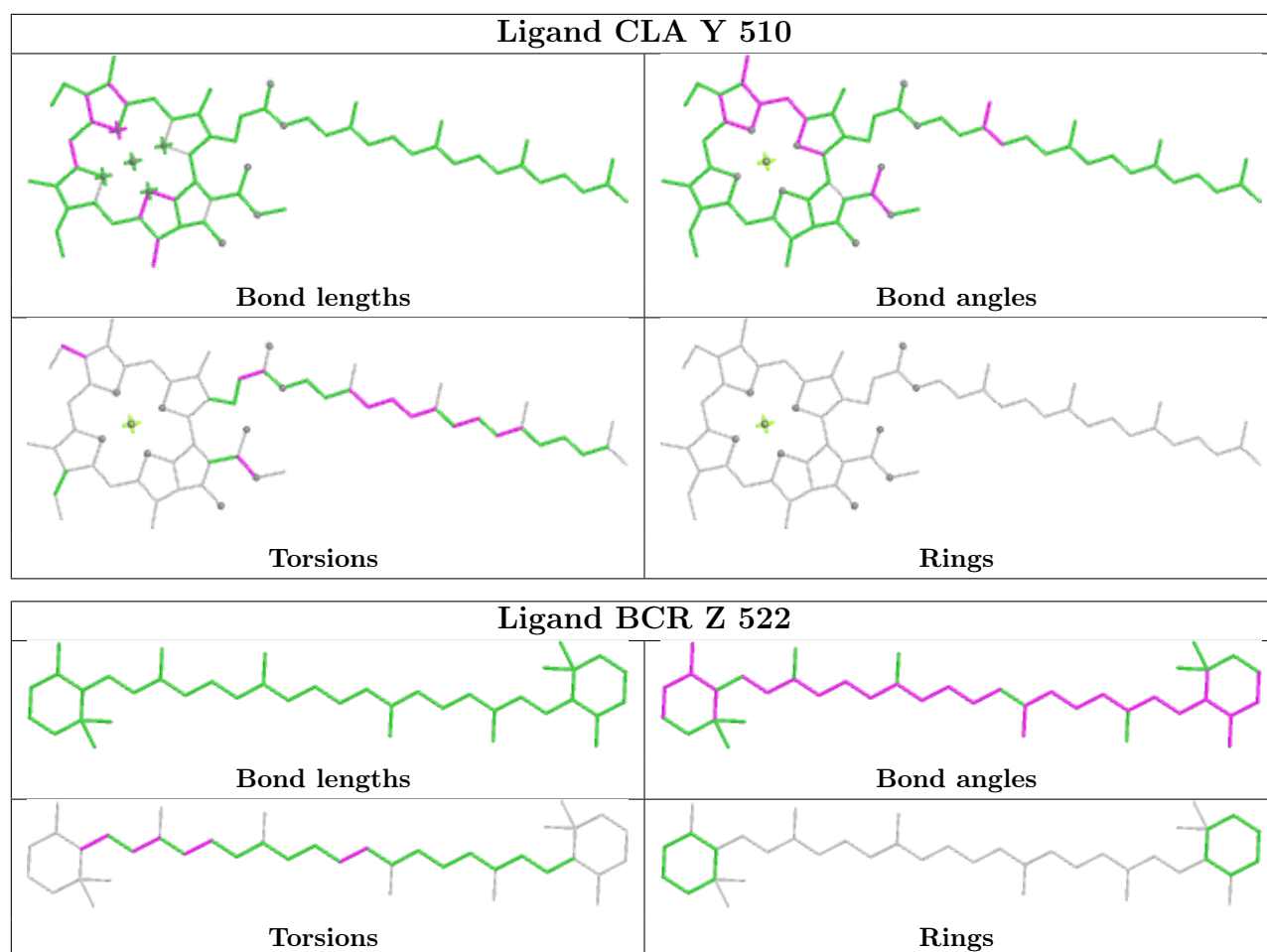
Ligand CLA a 511



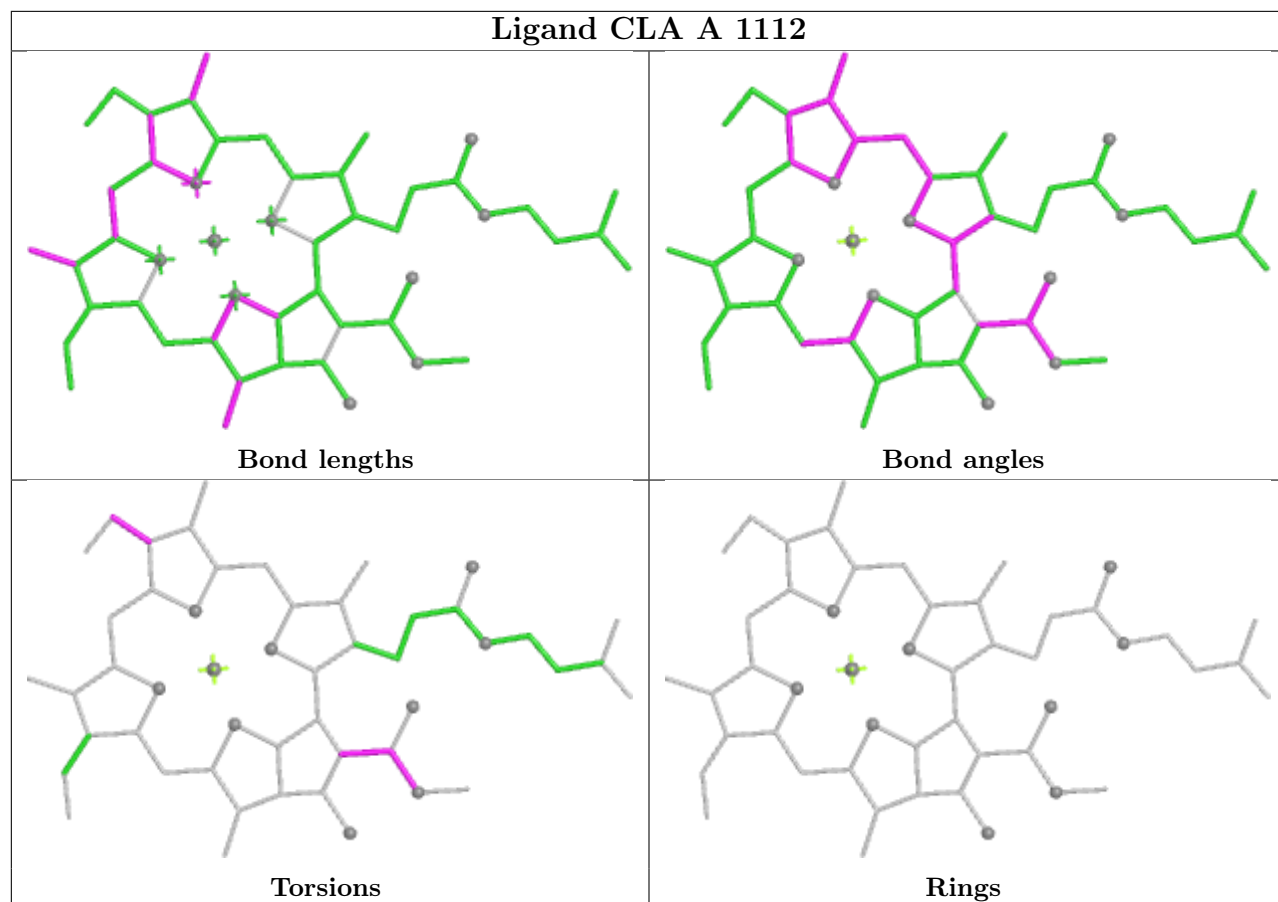
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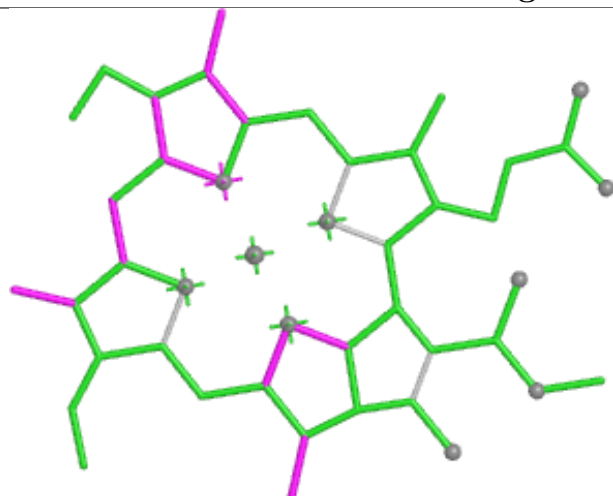




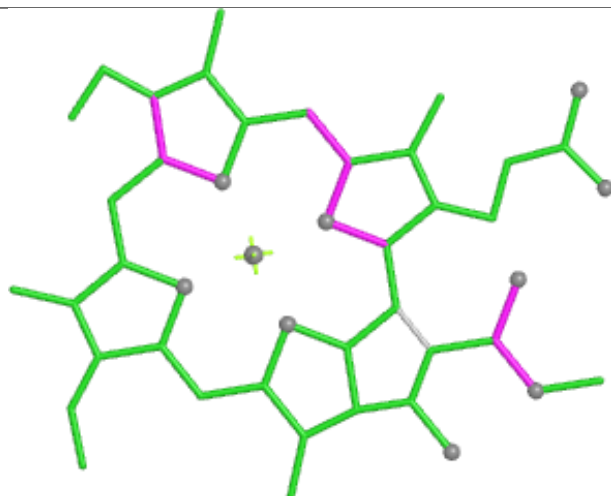
Ligand CLA A 1112



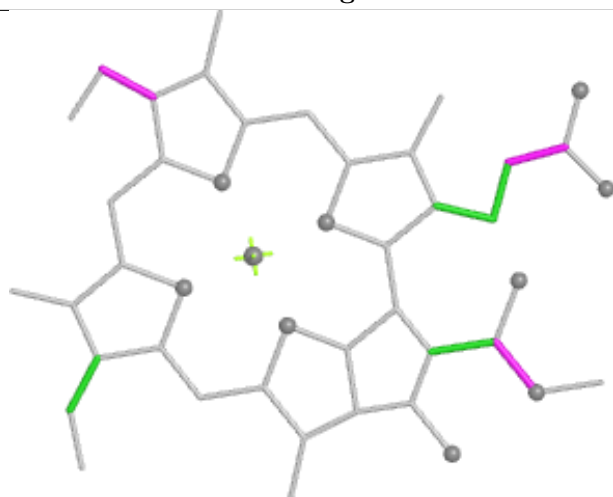
Ligand CLA 5 513



Bond lengths



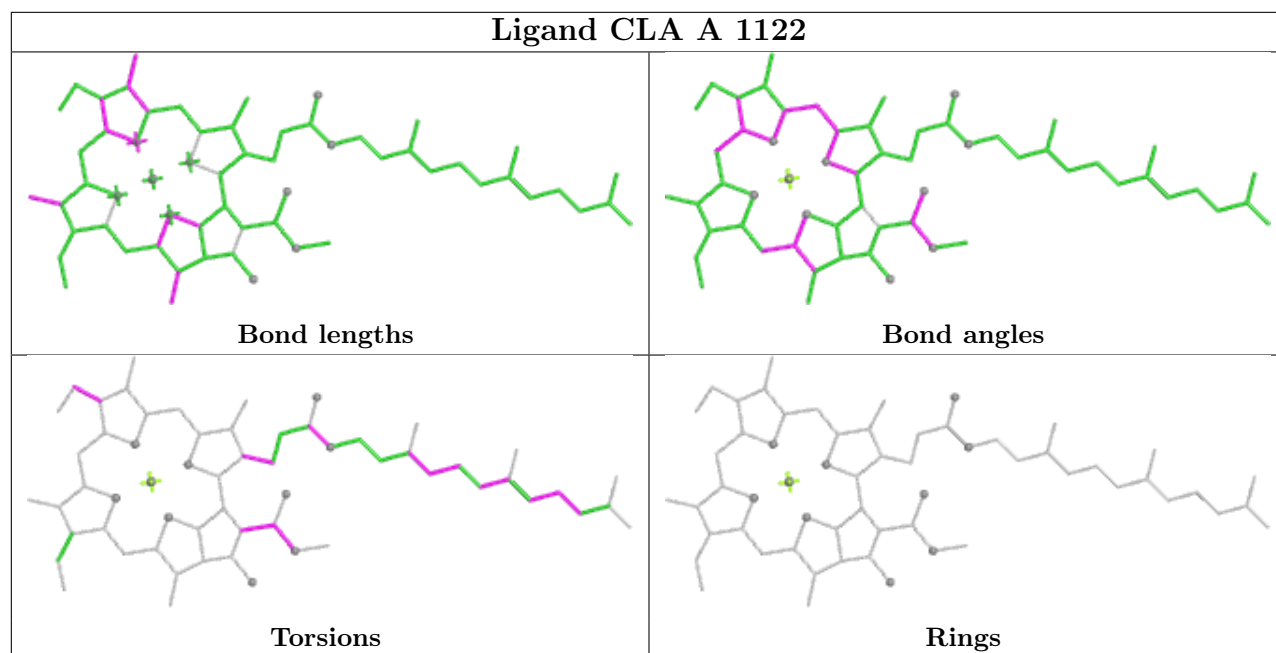
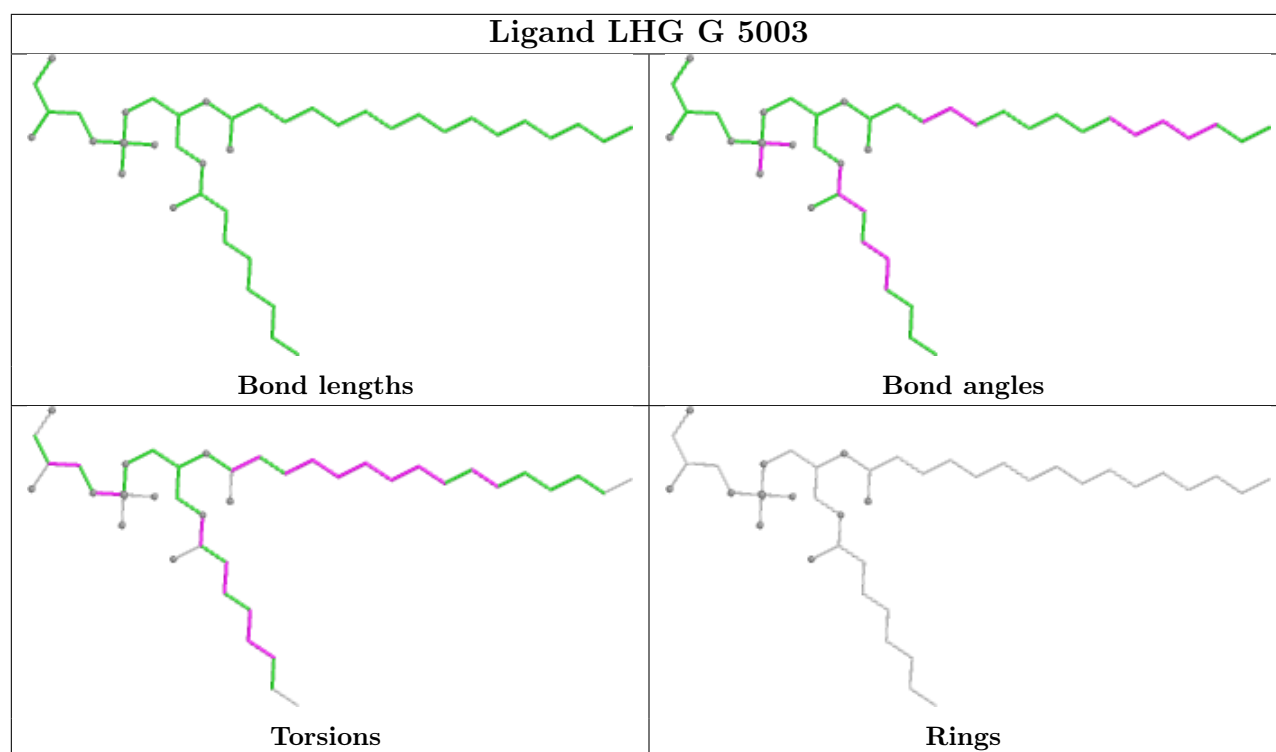
Bond angles



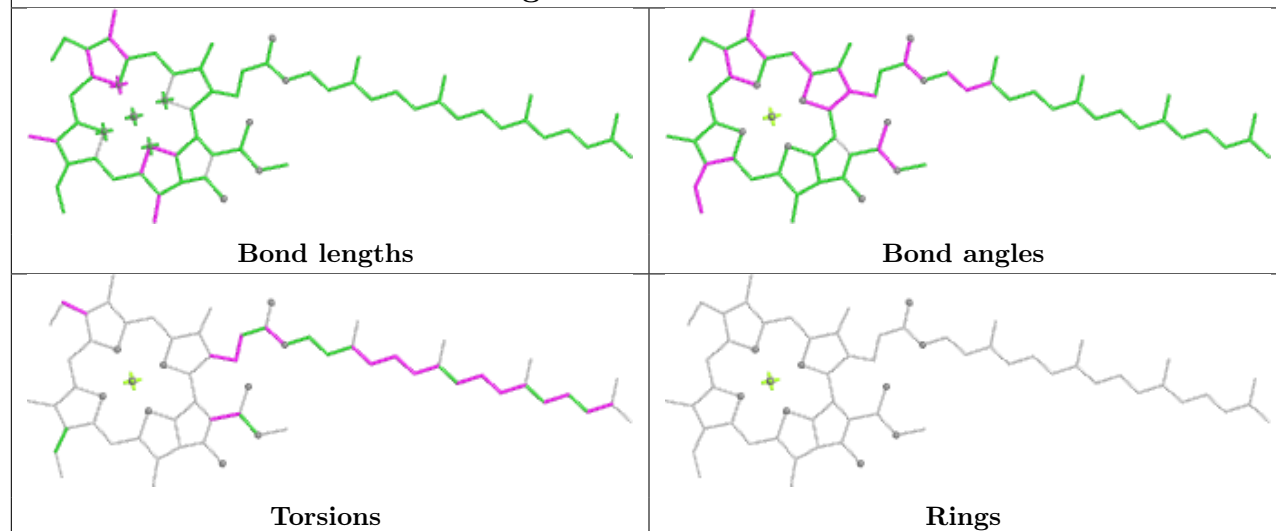
Torsions



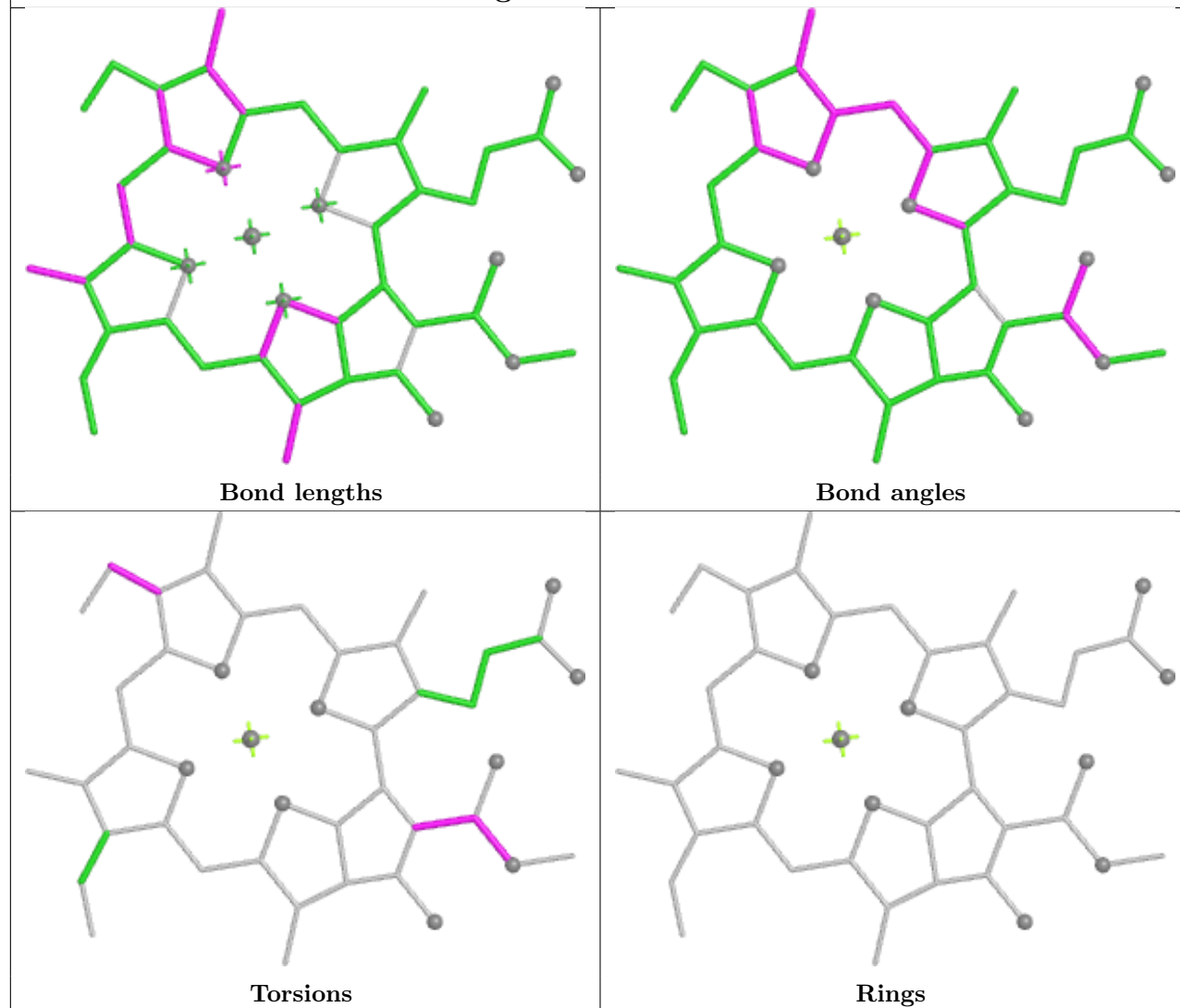
Rings

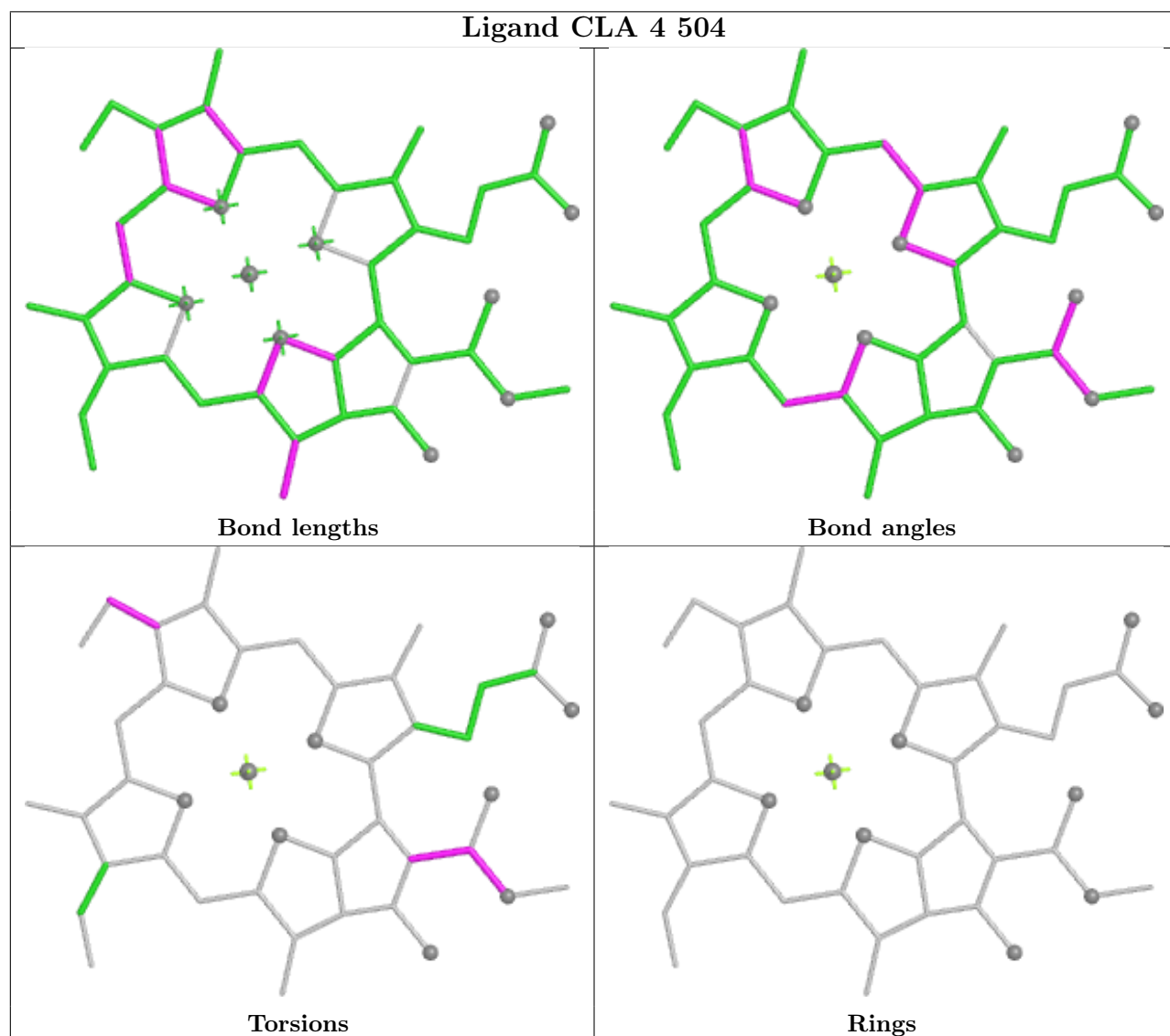
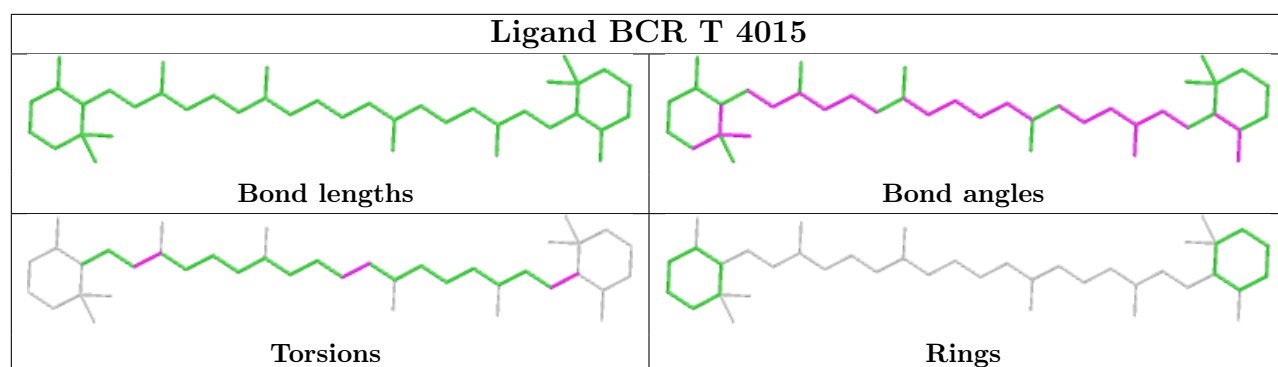


Ligand CLA H 1210

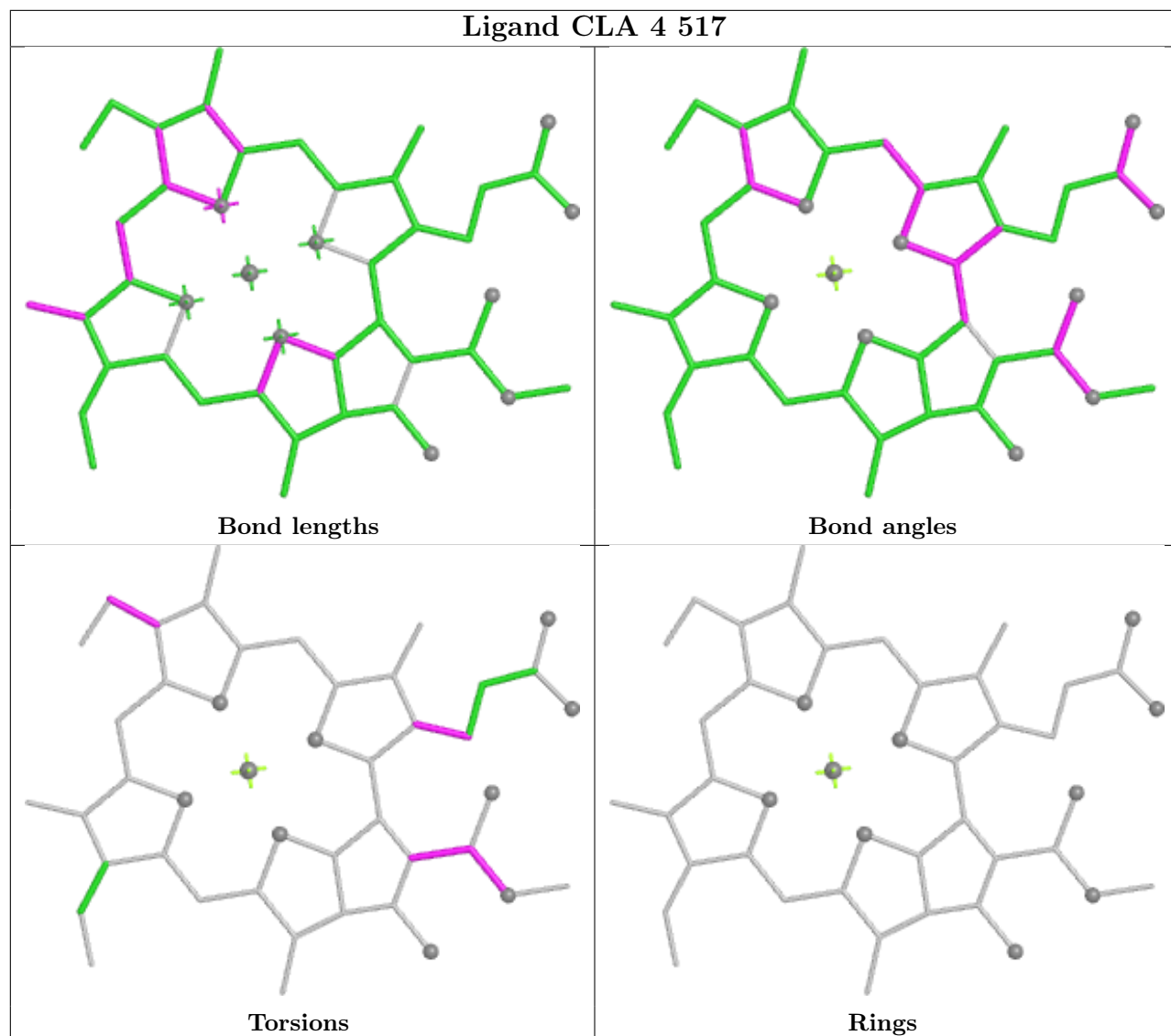


Ligand CLA v 506

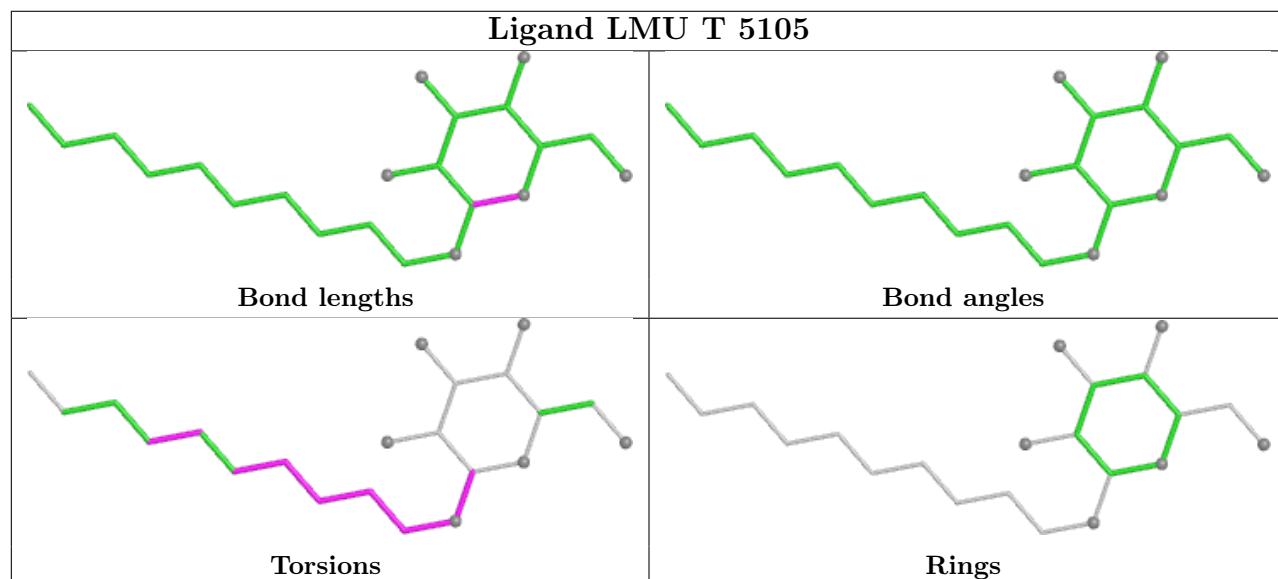


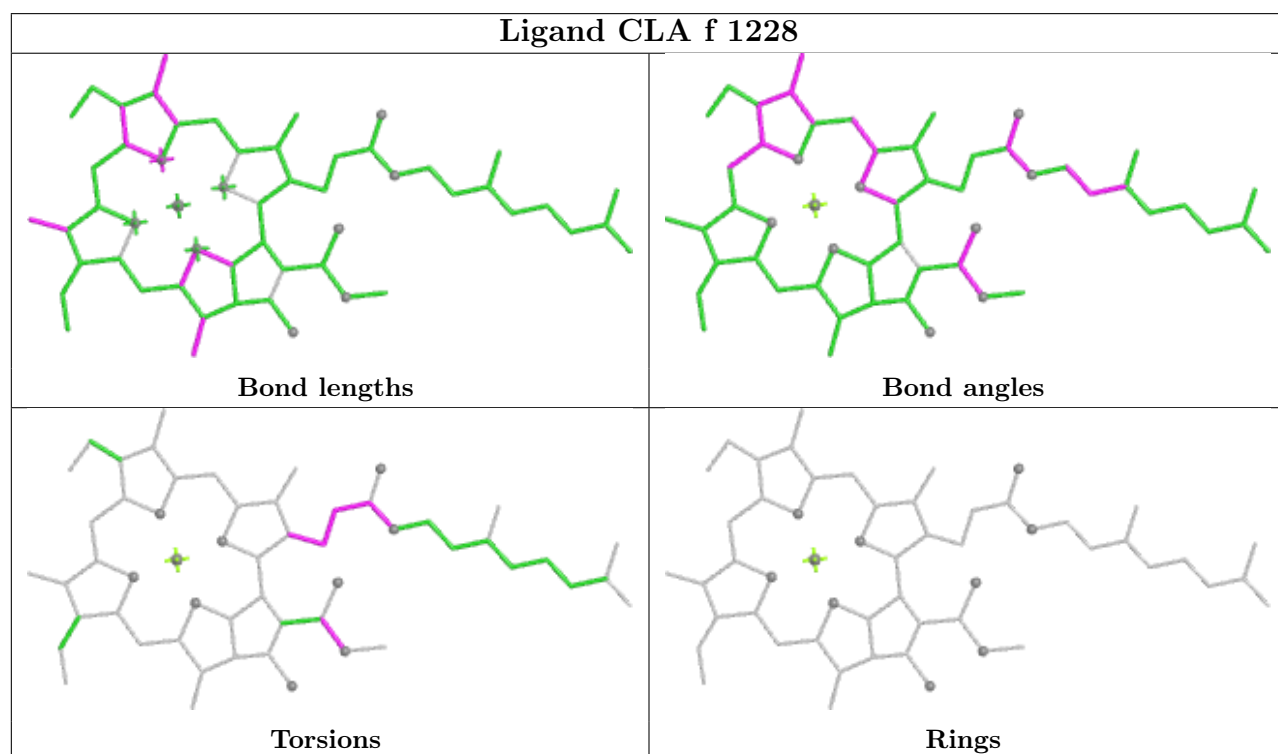
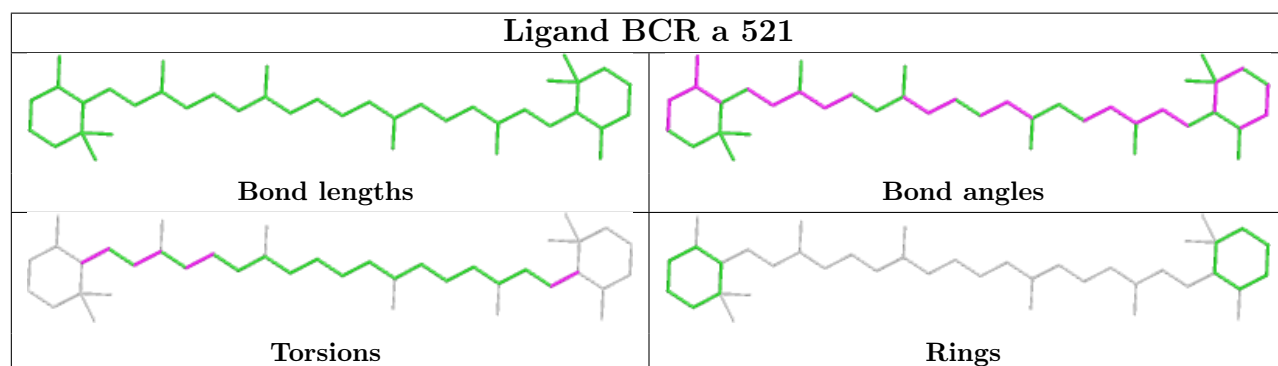
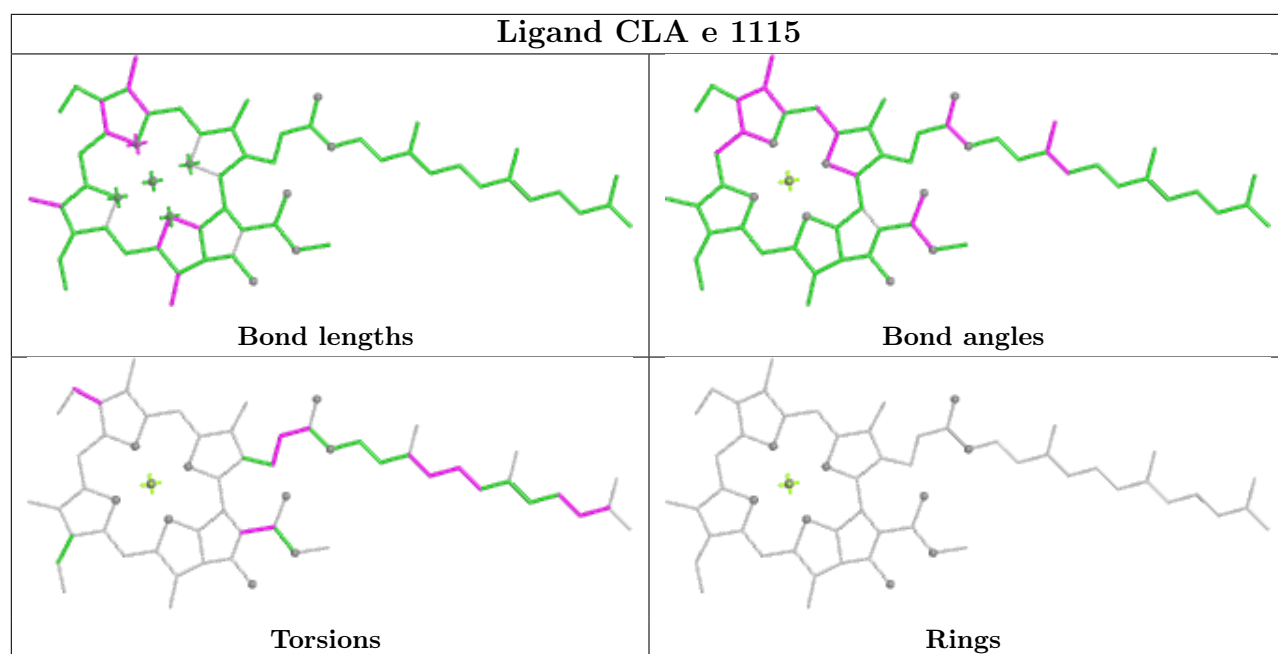


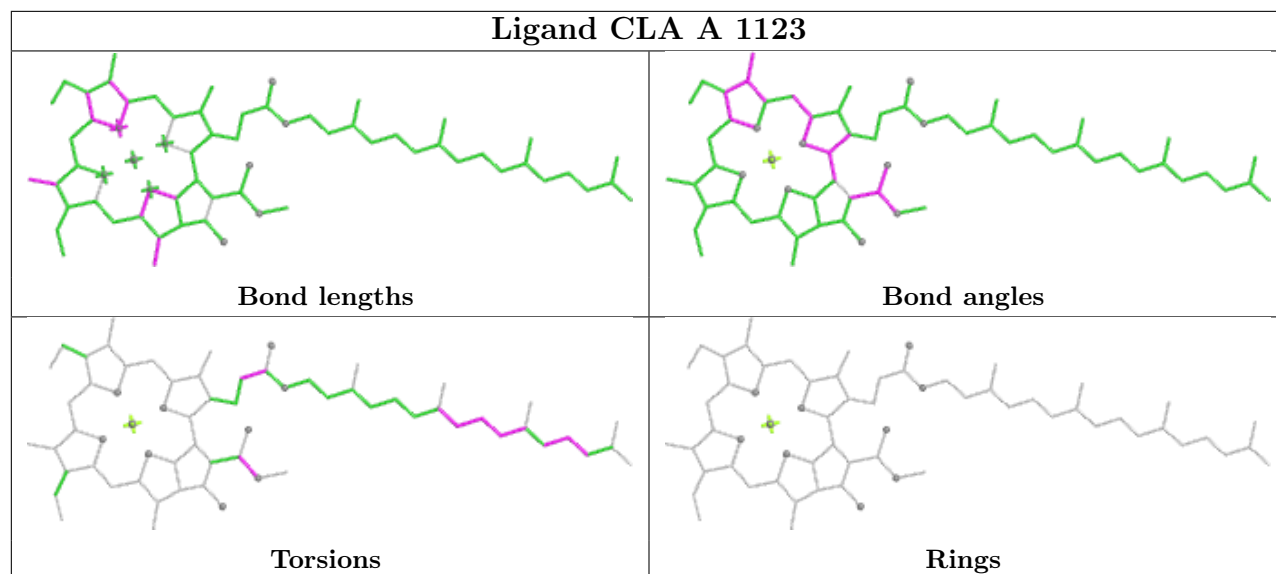
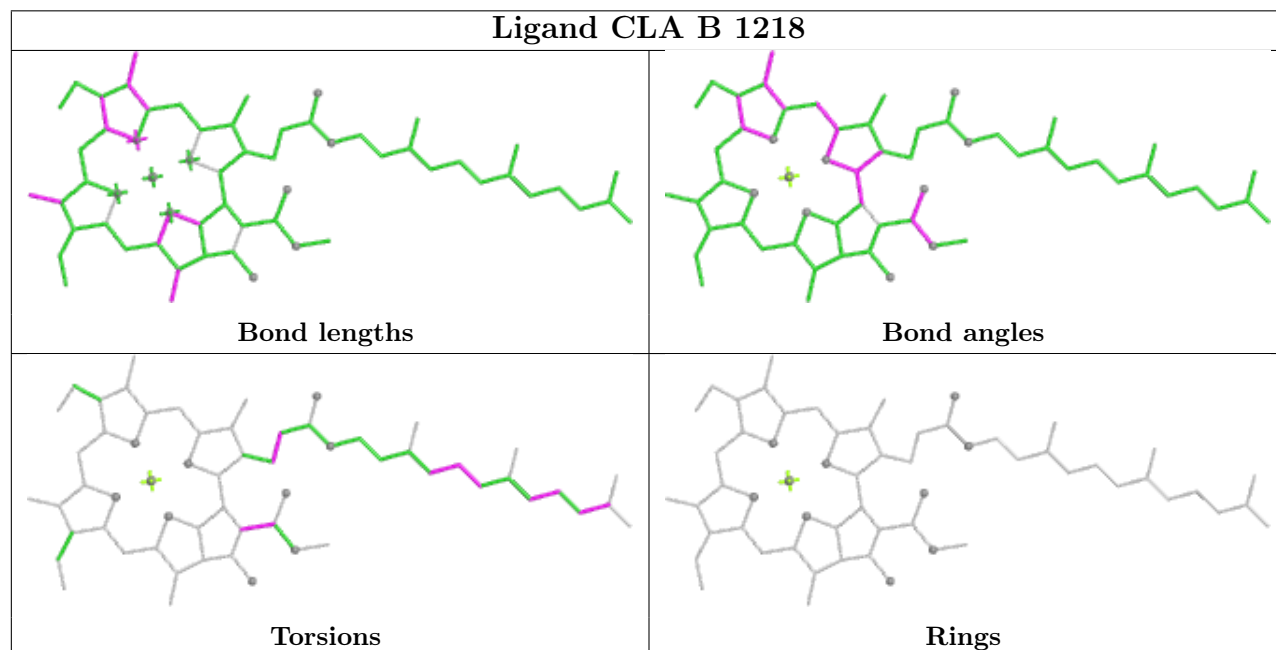
Ligand CLA 4 517

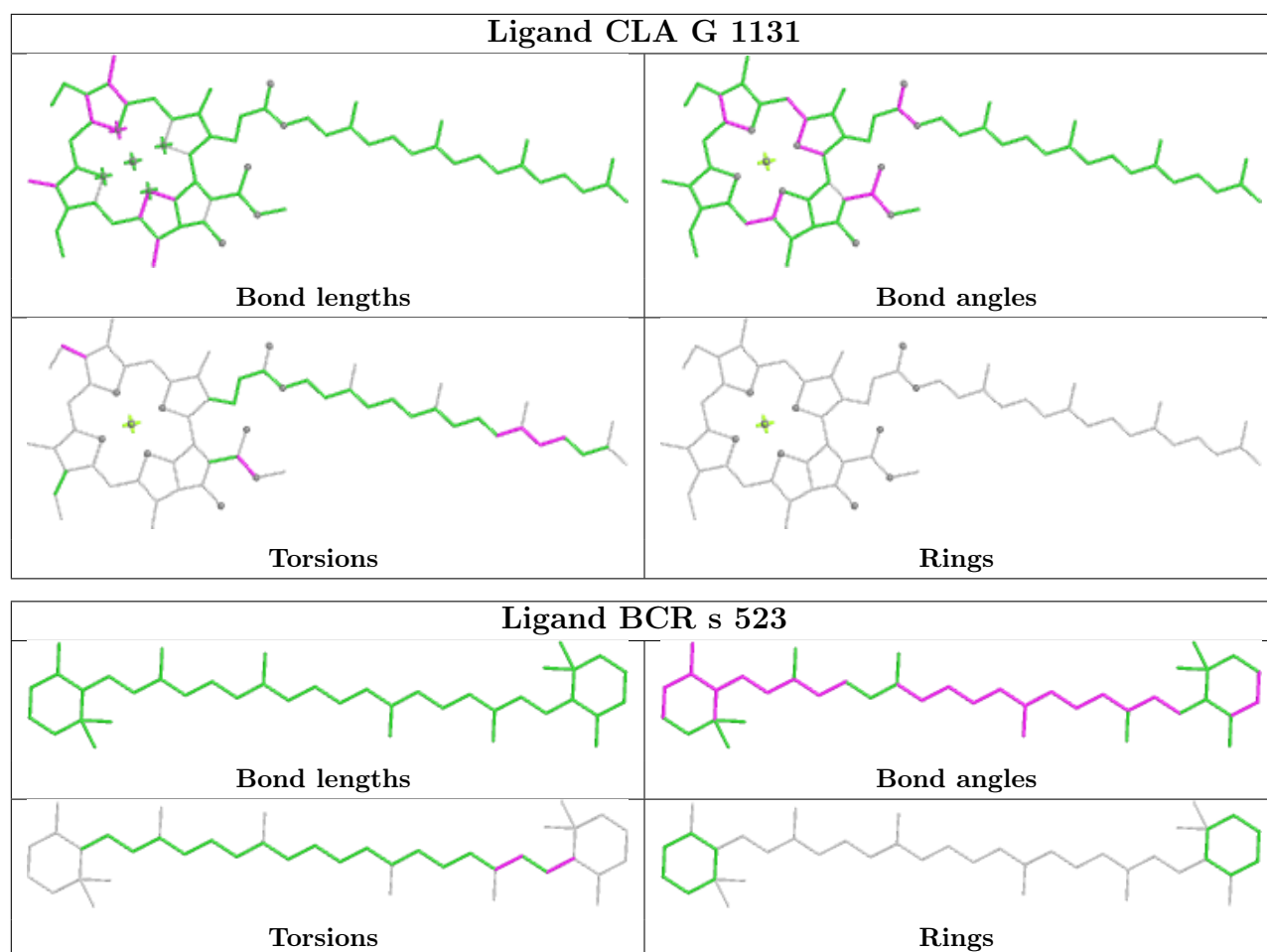


Ligand LMU T 5105

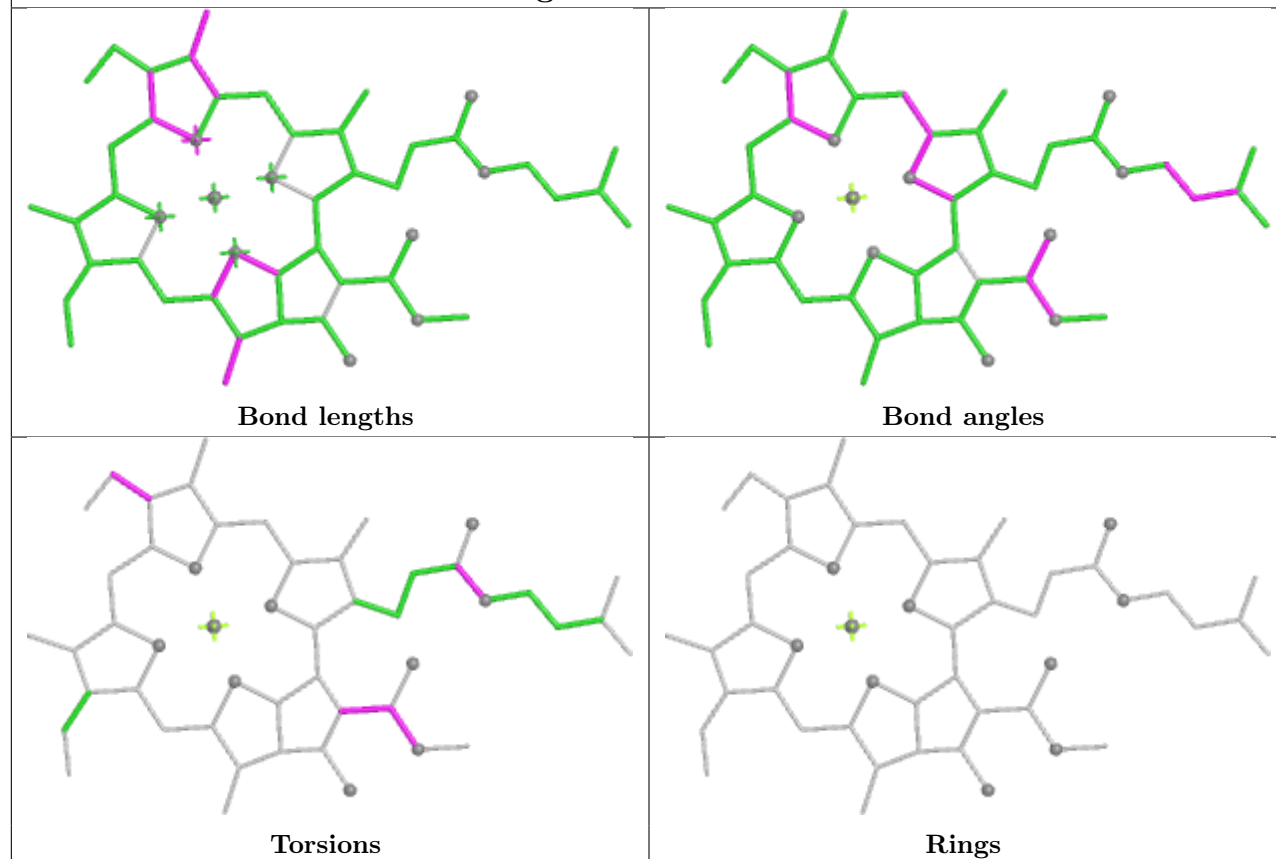




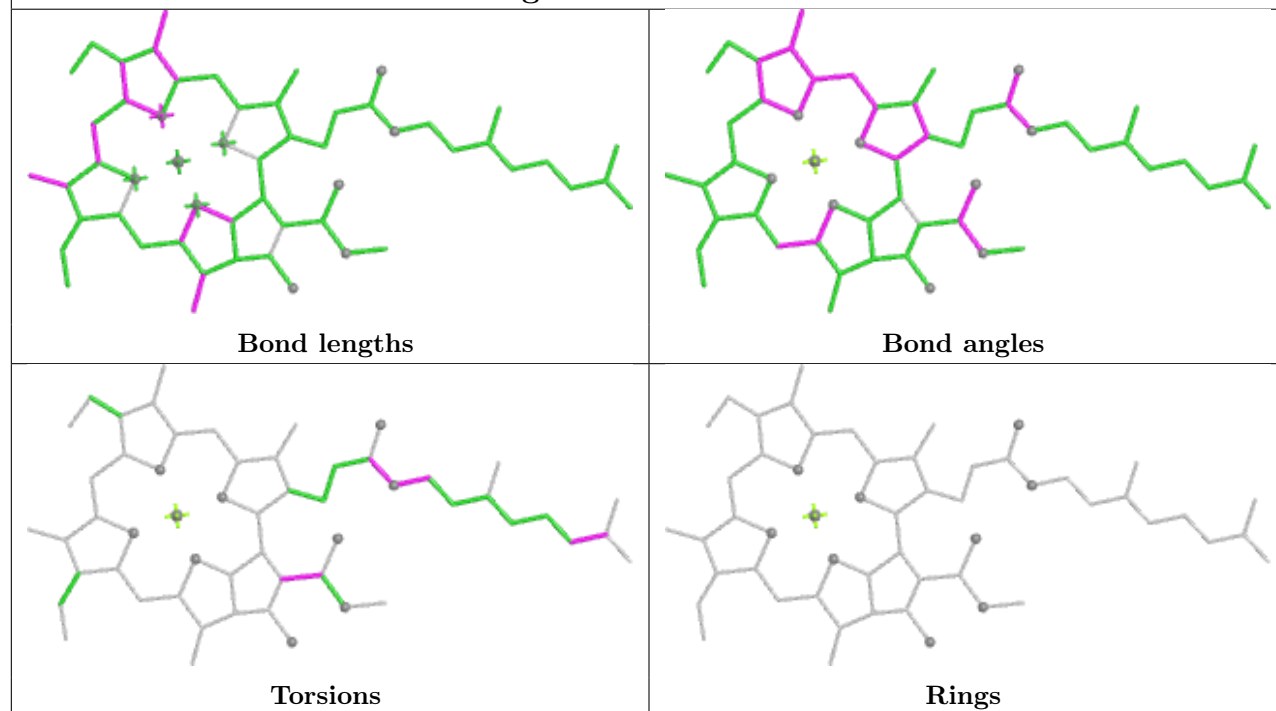
Ligand CLA A 1123**Ligand CLA B 1218**



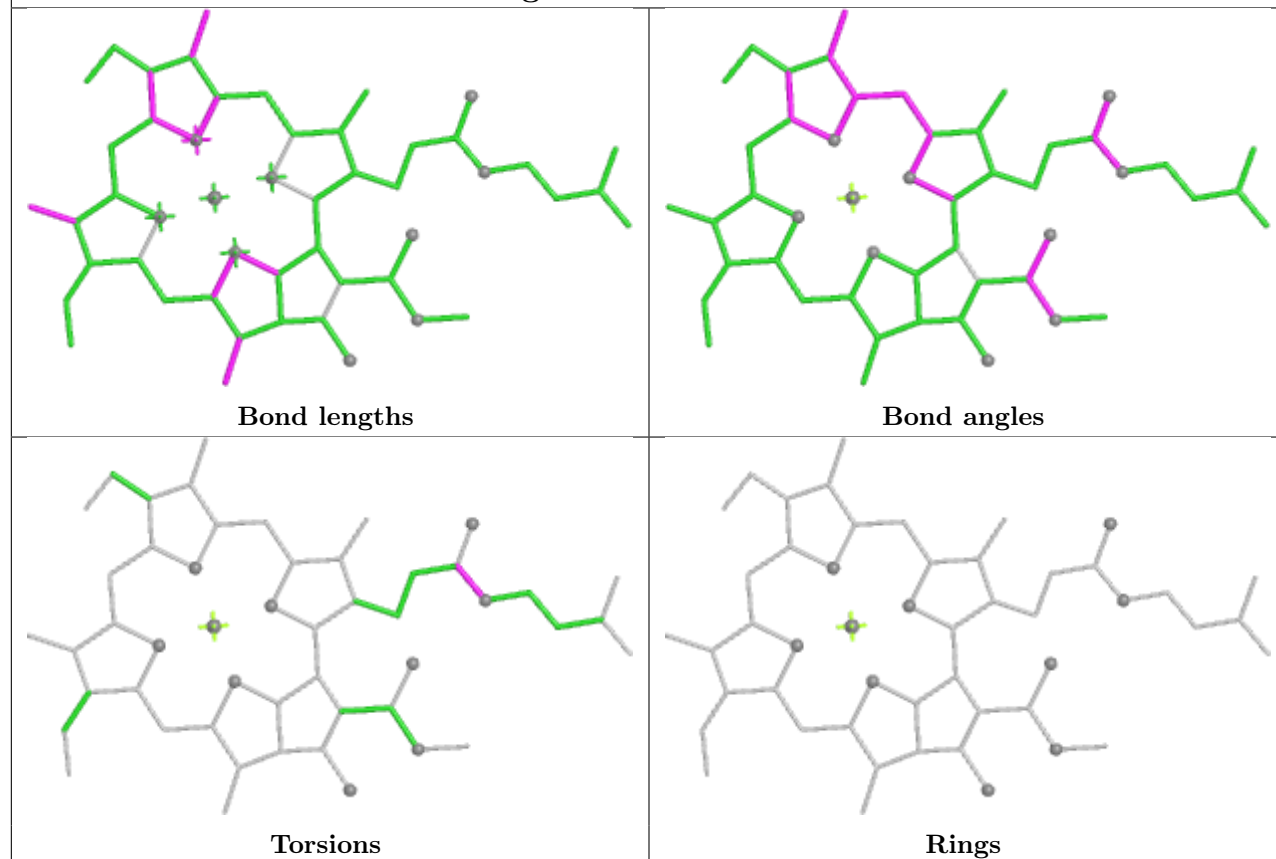
Ligand CLA 6 502



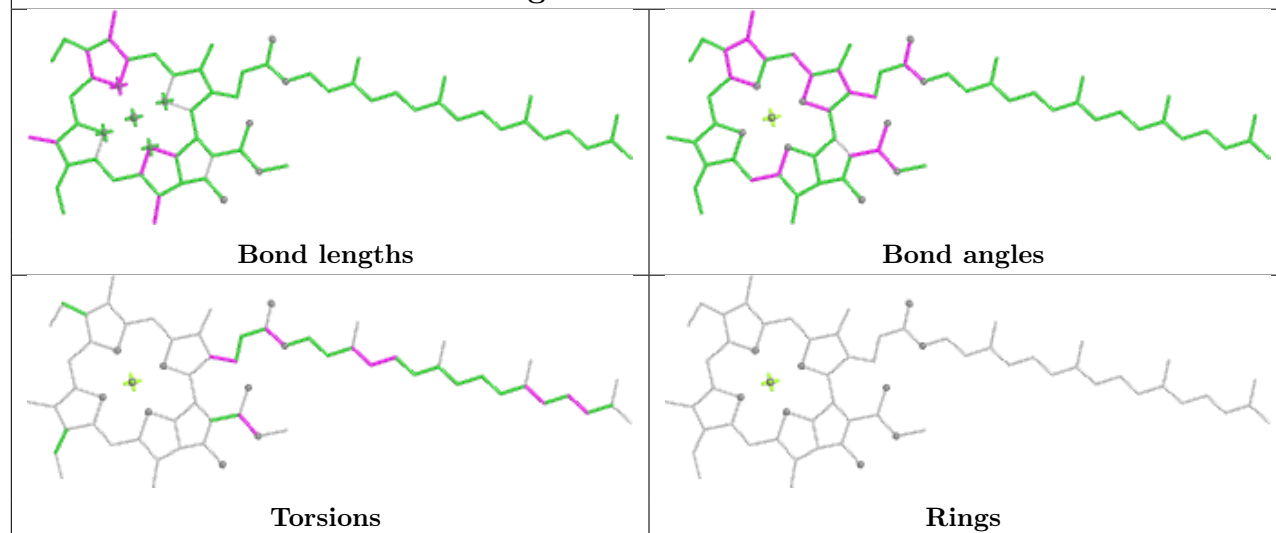
Ligand CLA G 1105

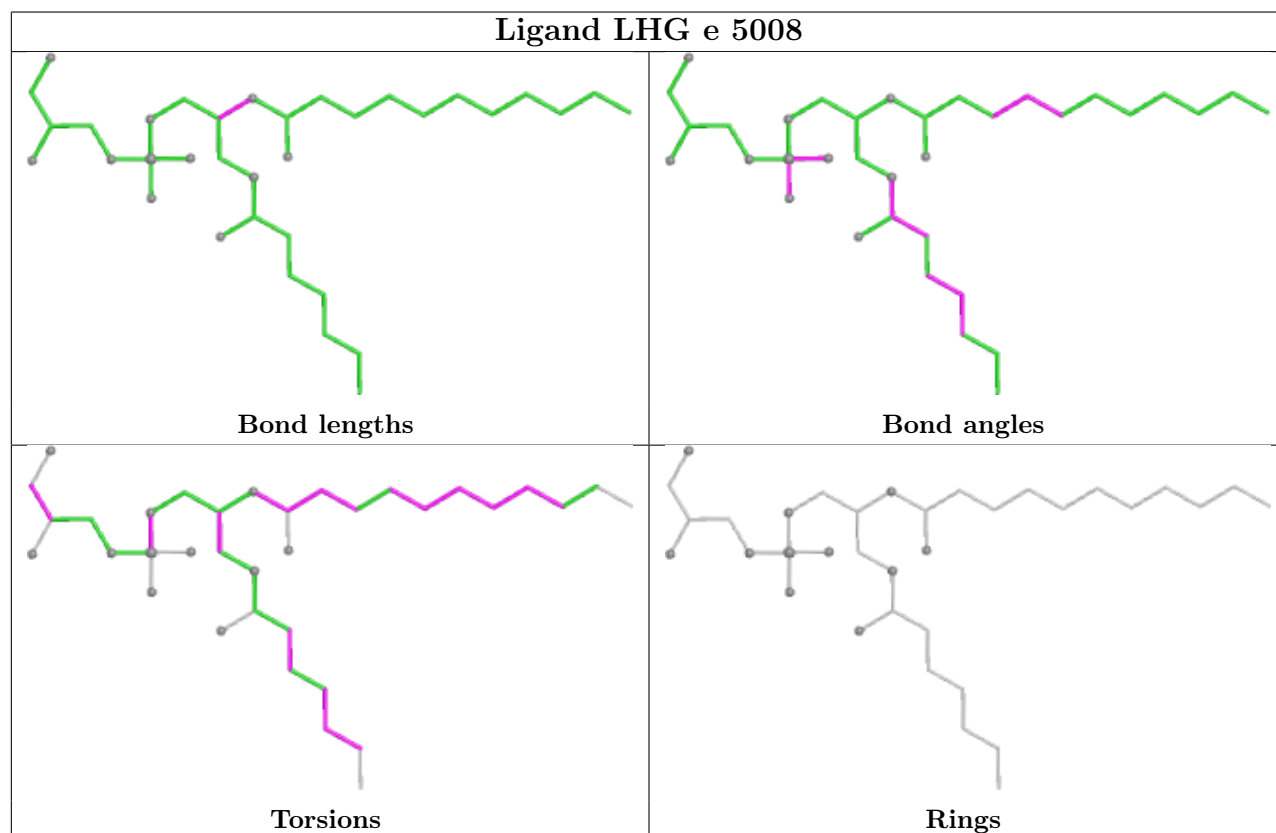
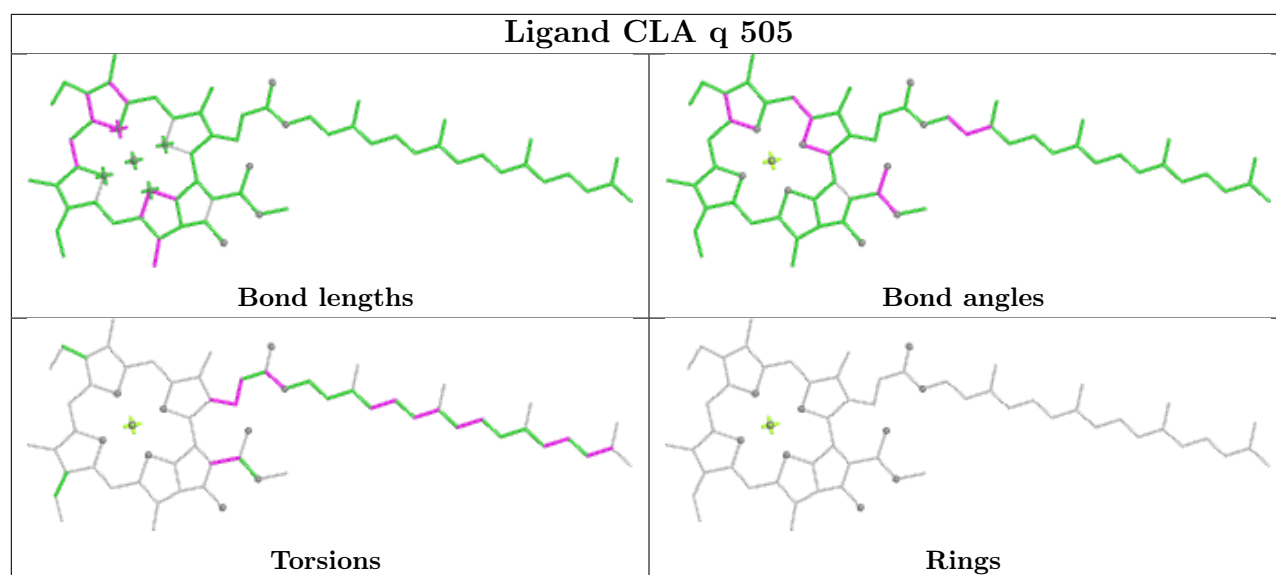


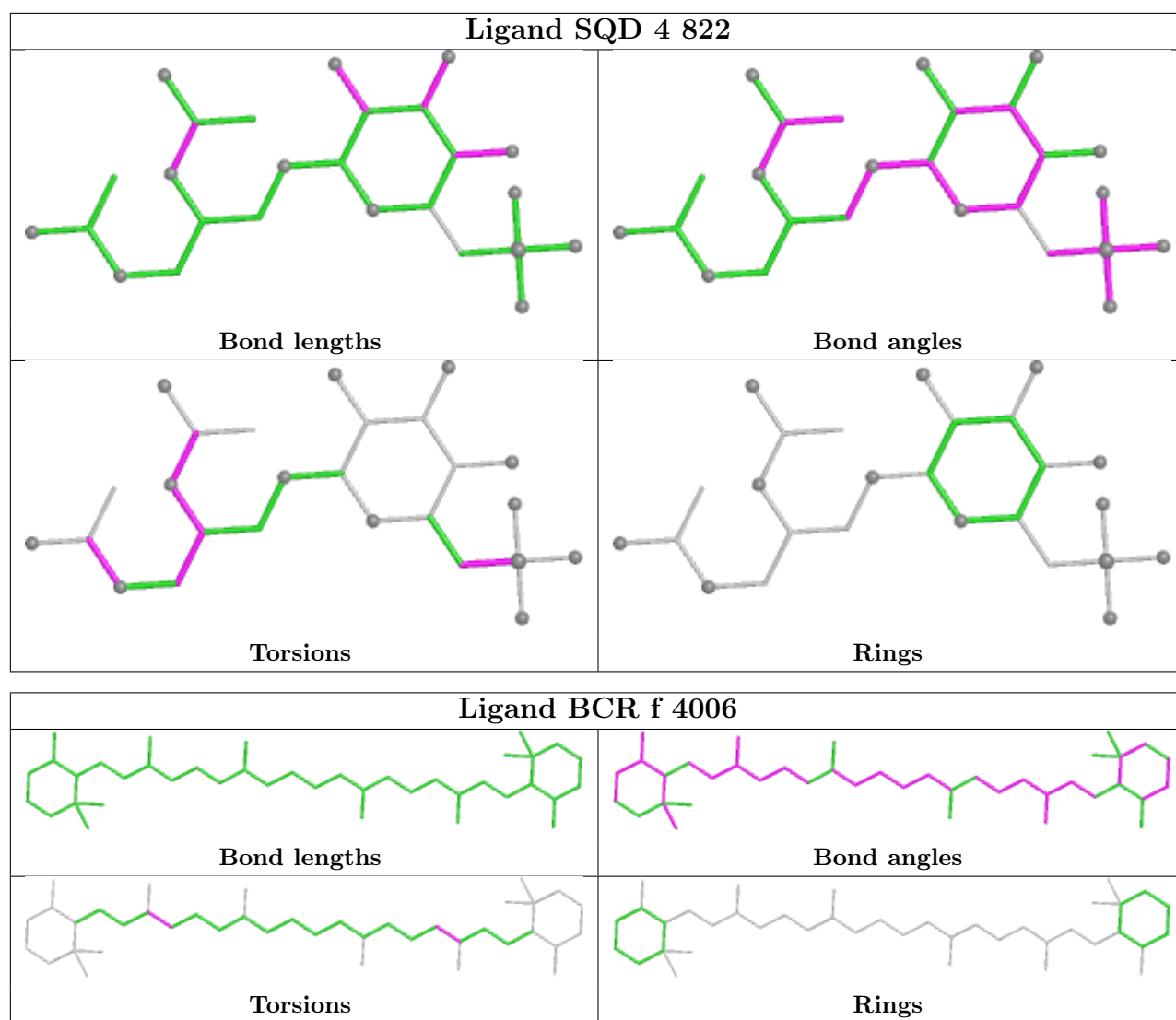
Ligand CLA G 1114

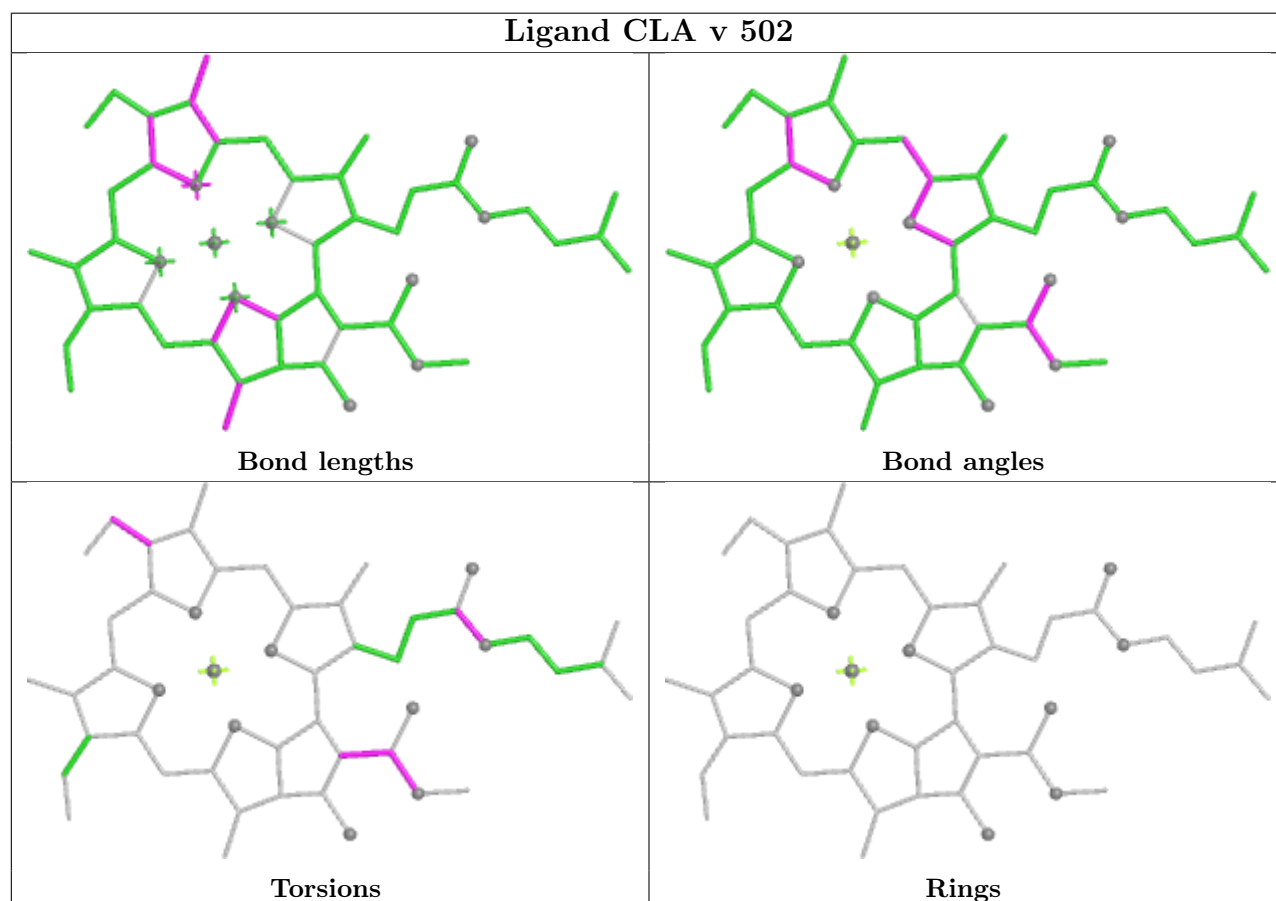
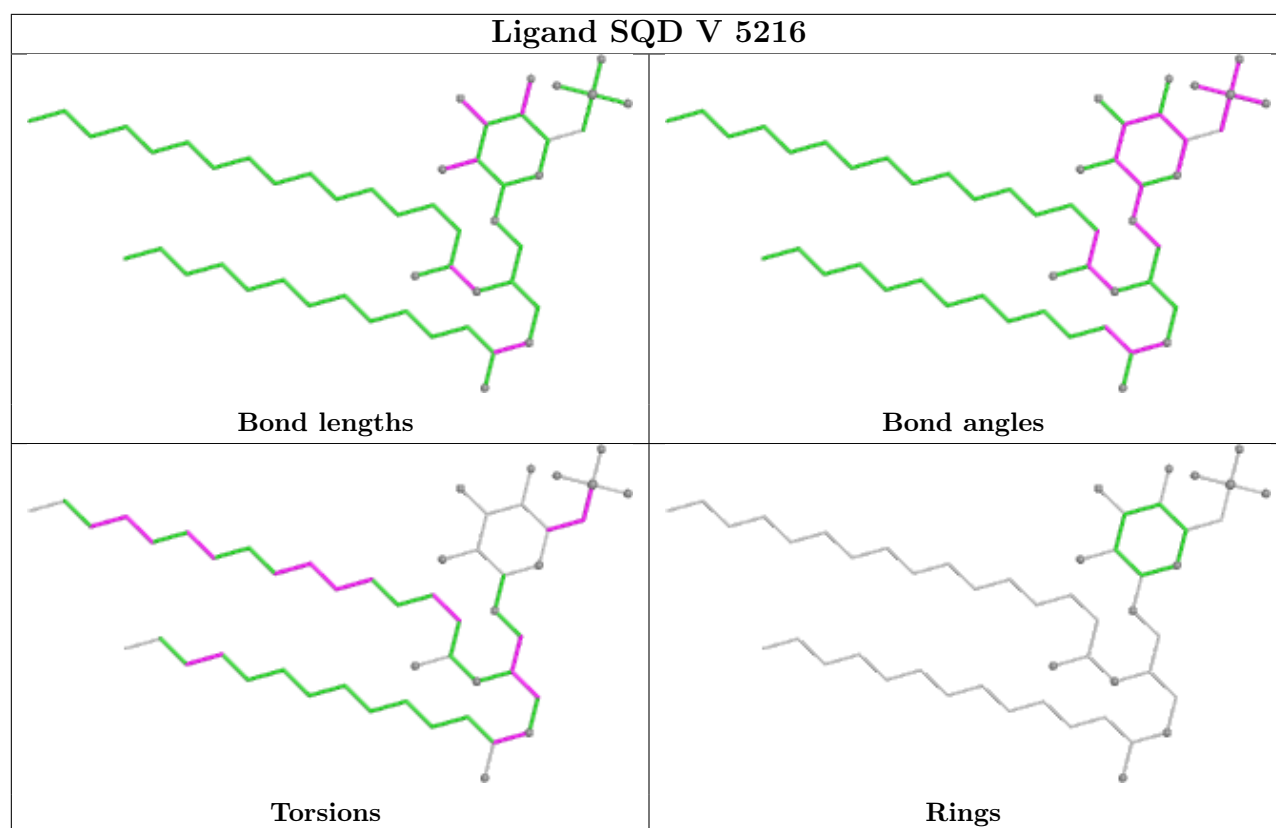


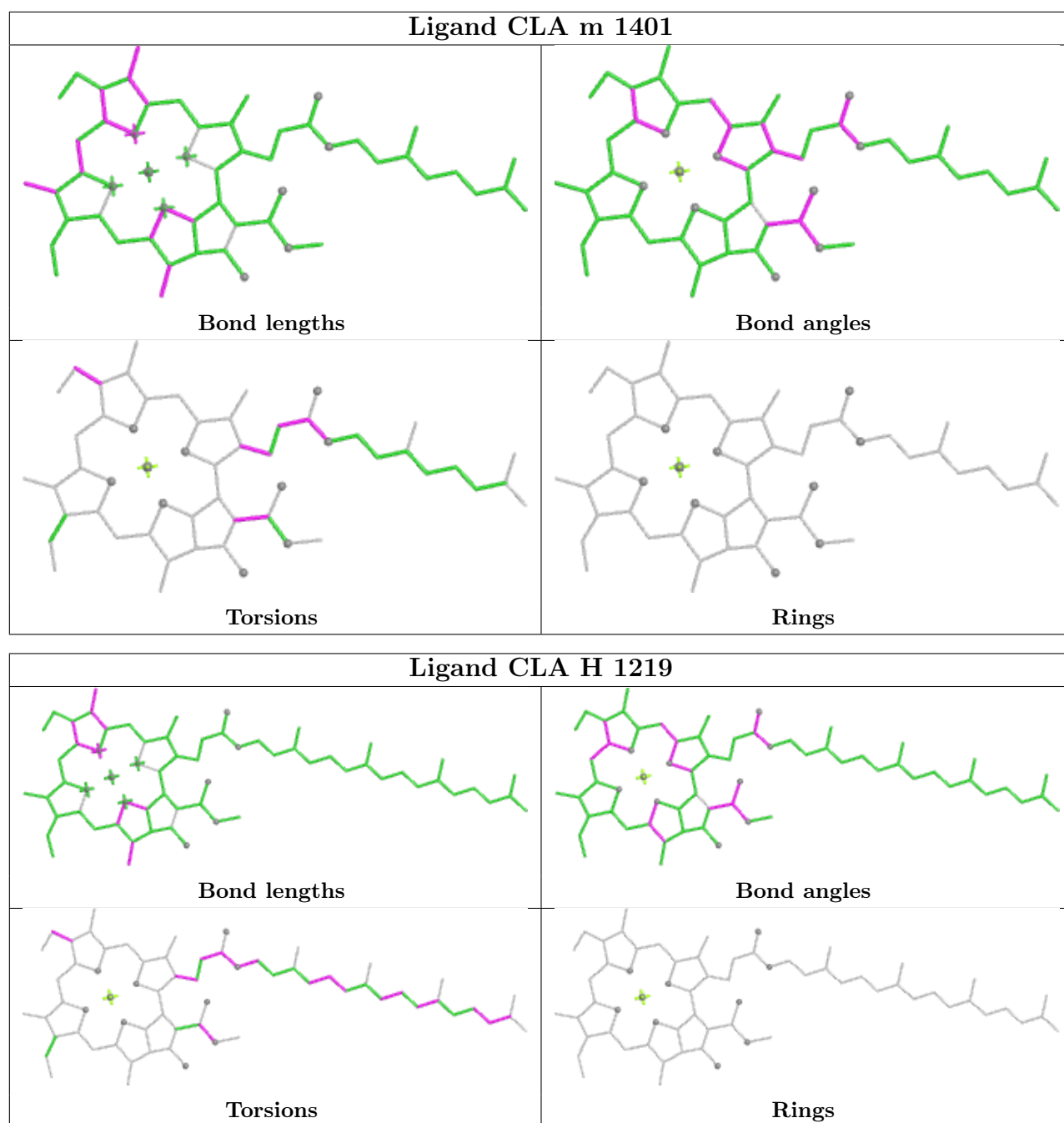
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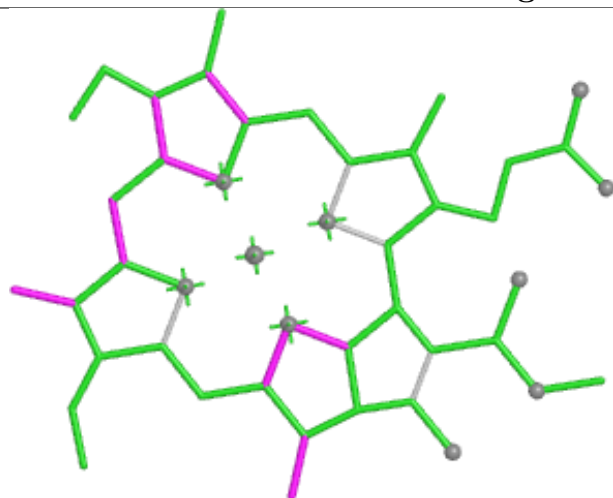




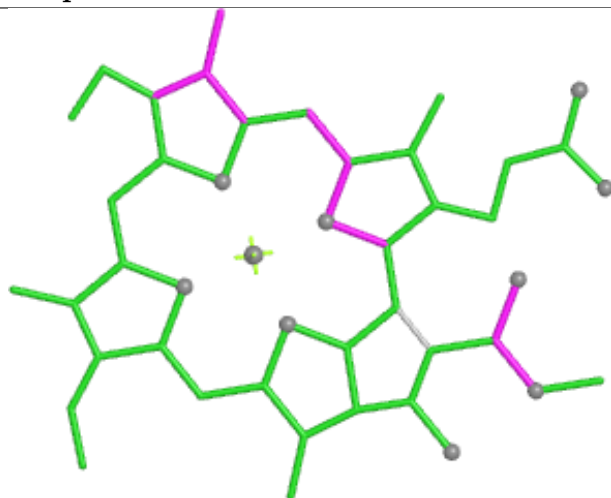




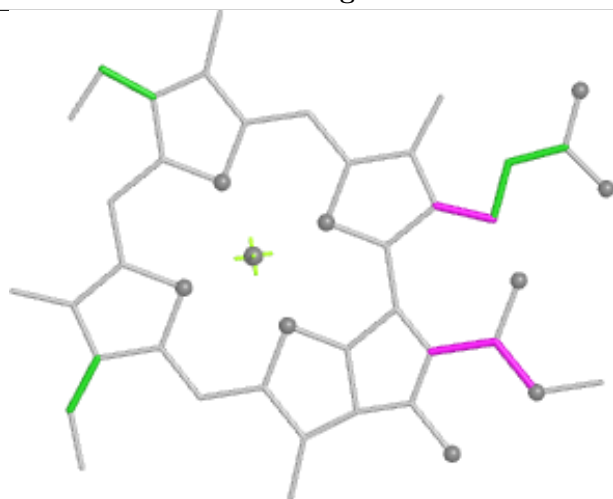
Ligand CLA q 506



Bond lengths



Bond angles

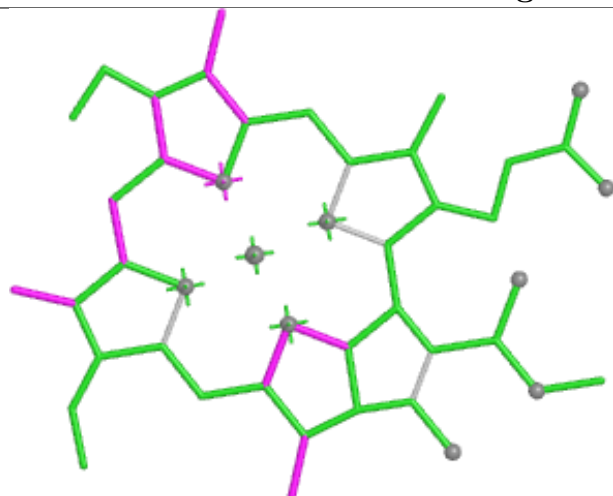


Torsions

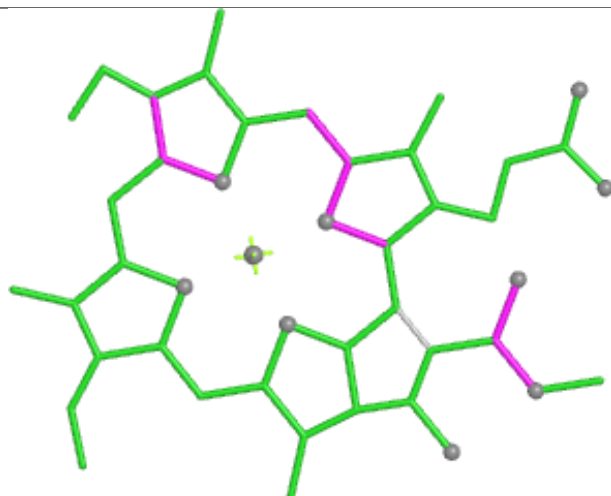


Rings

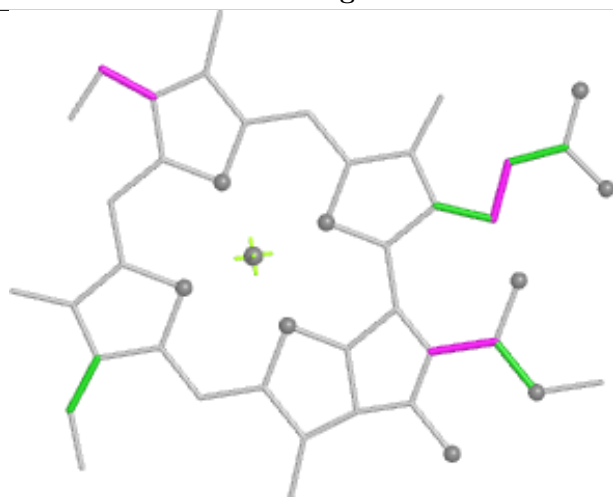
Ligand CLA Z 517



Bond lengths



Bond angles

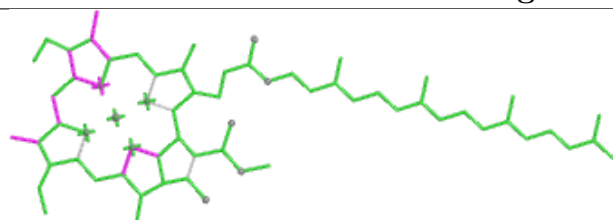


Torsions

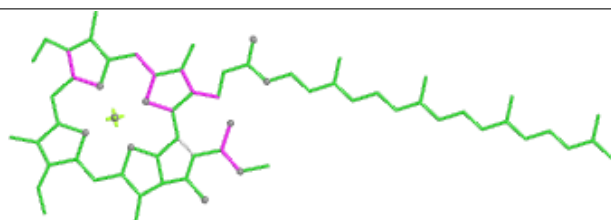


Rings

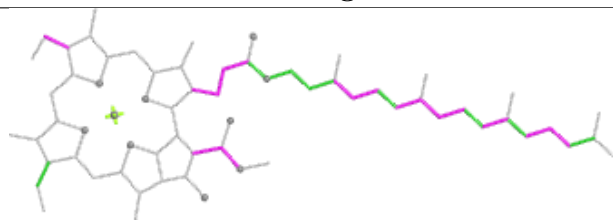
Ligand CLA u 501



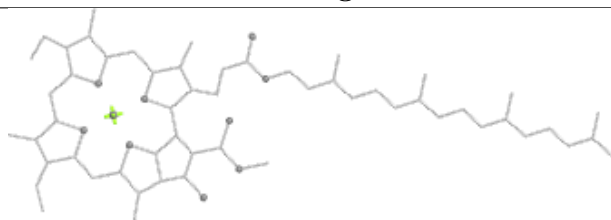
Bond lengths



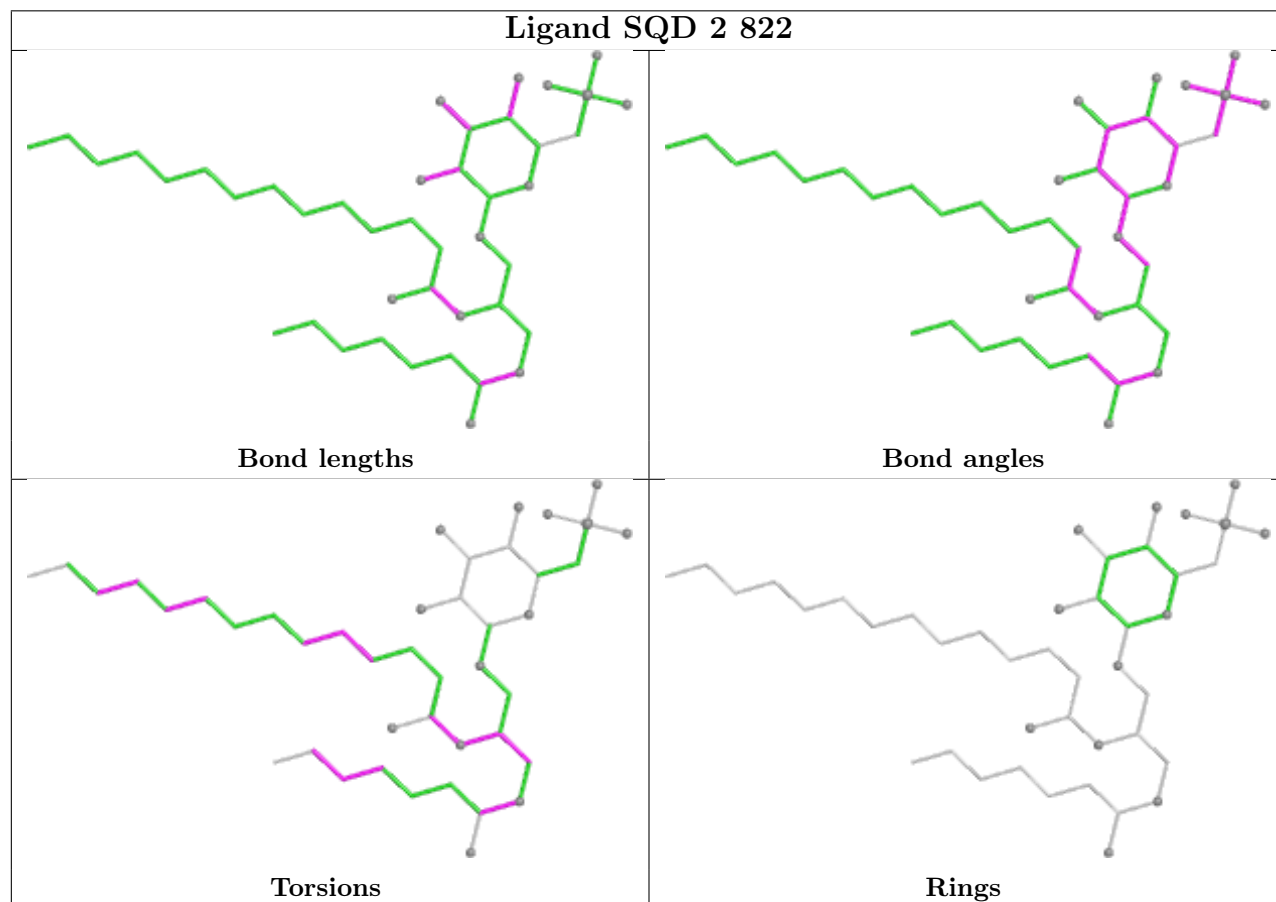
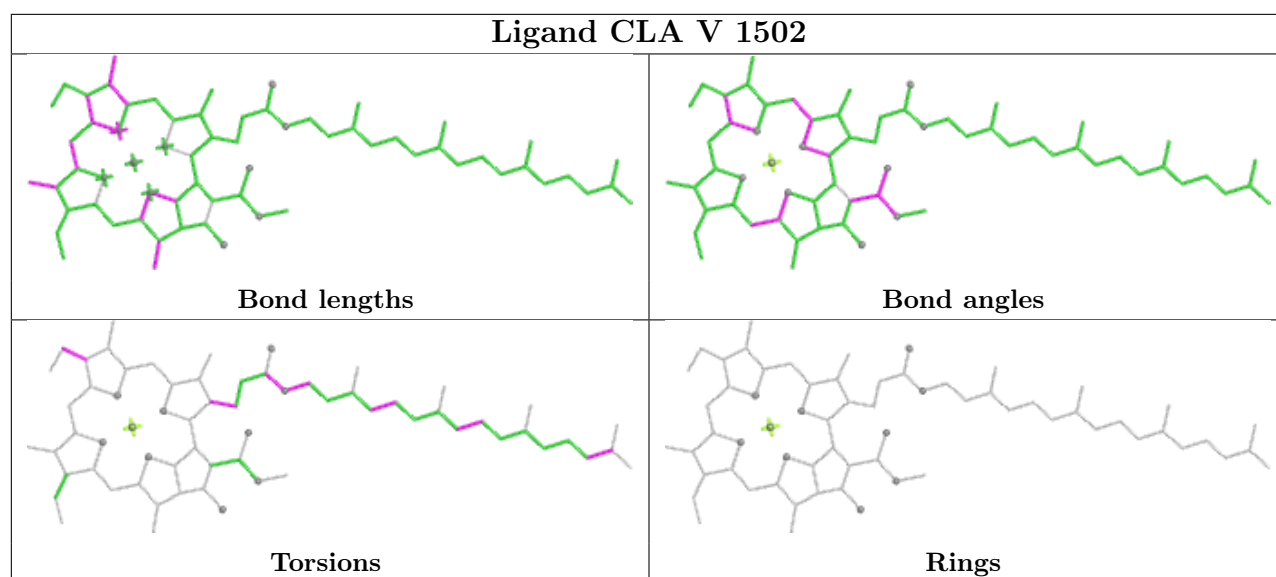
Bond angles



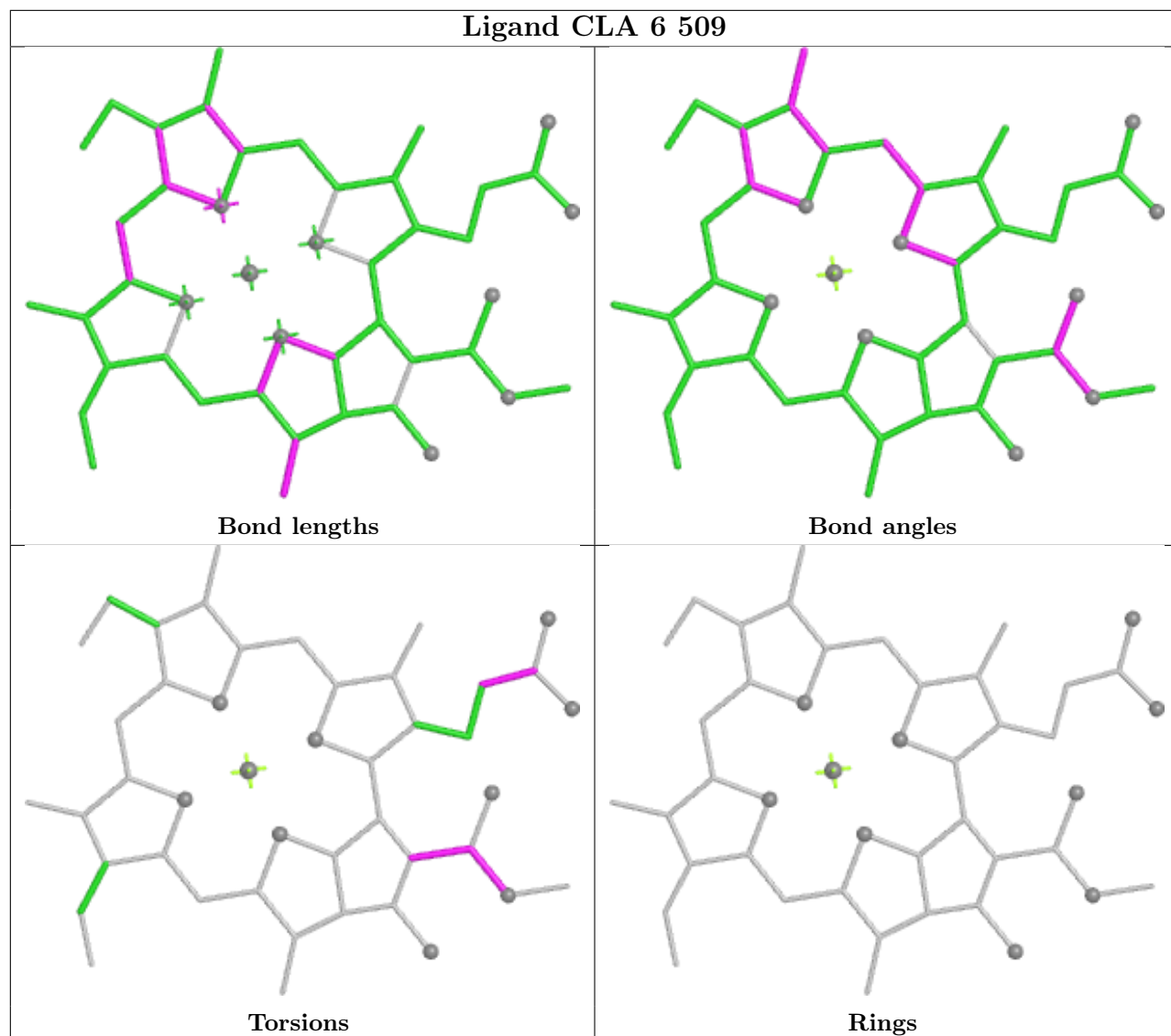
Torsions

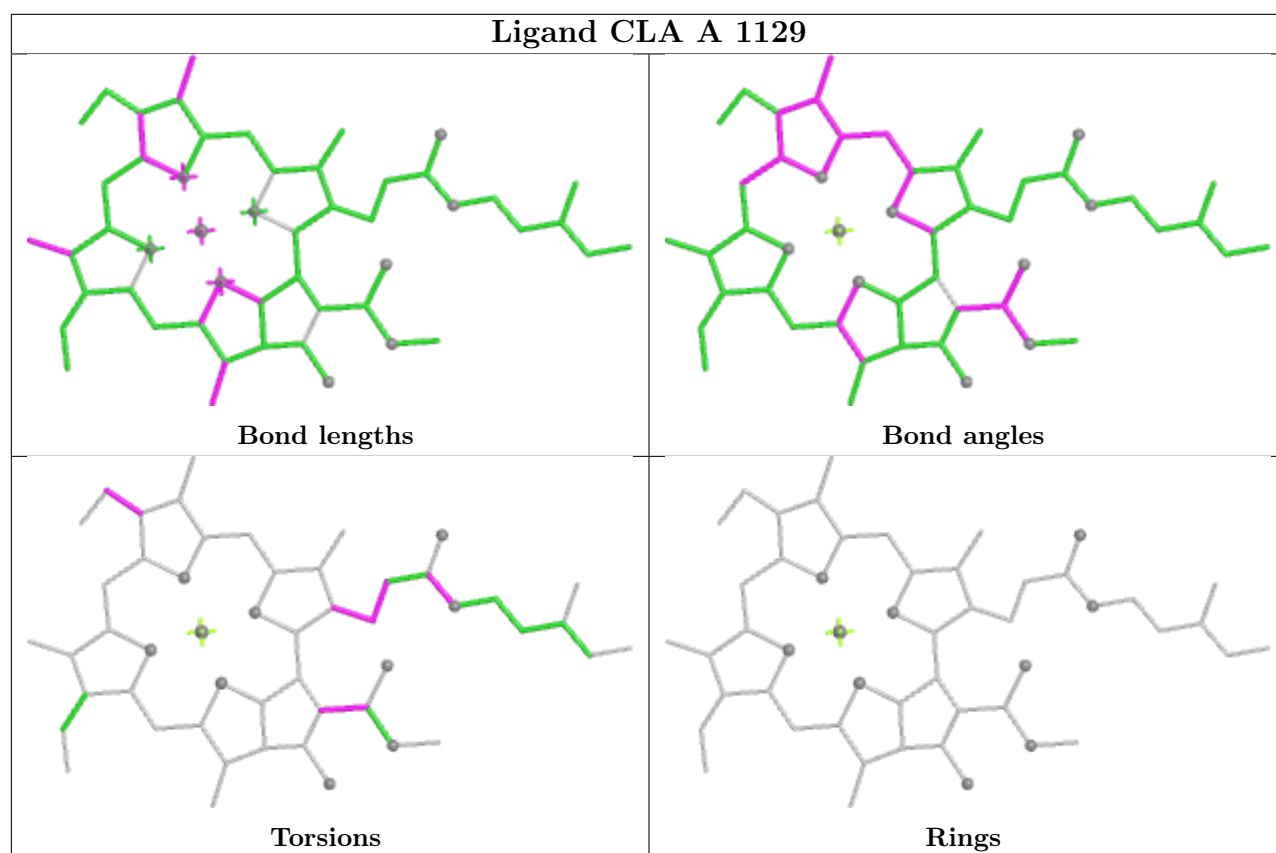


Rings

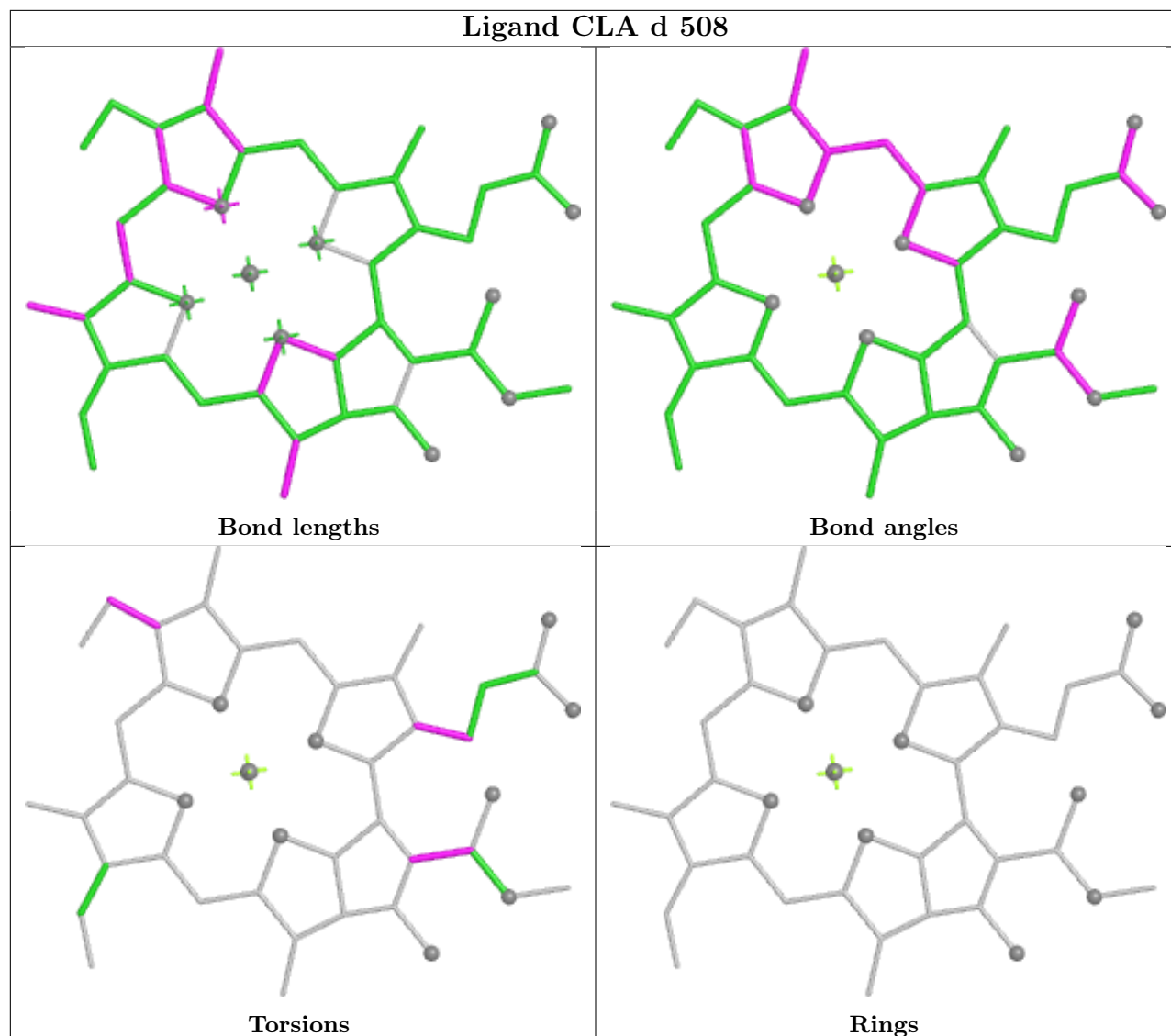


Ligand CLA 6 509

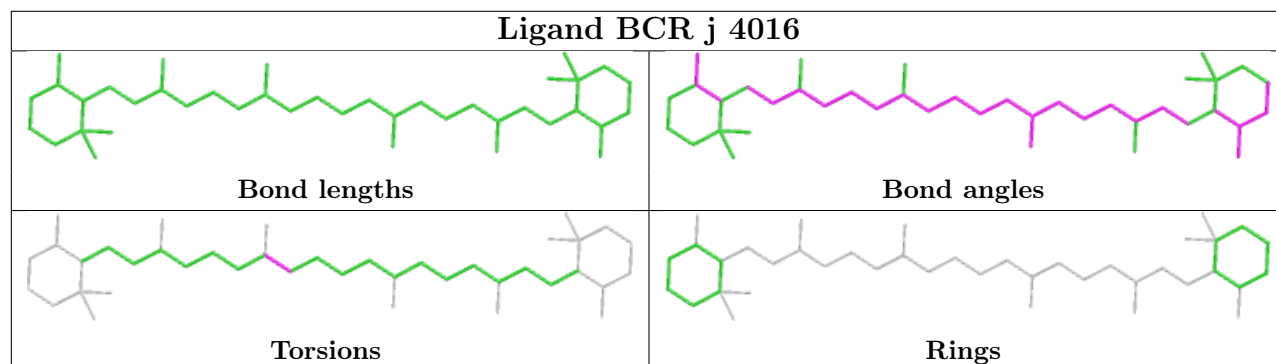


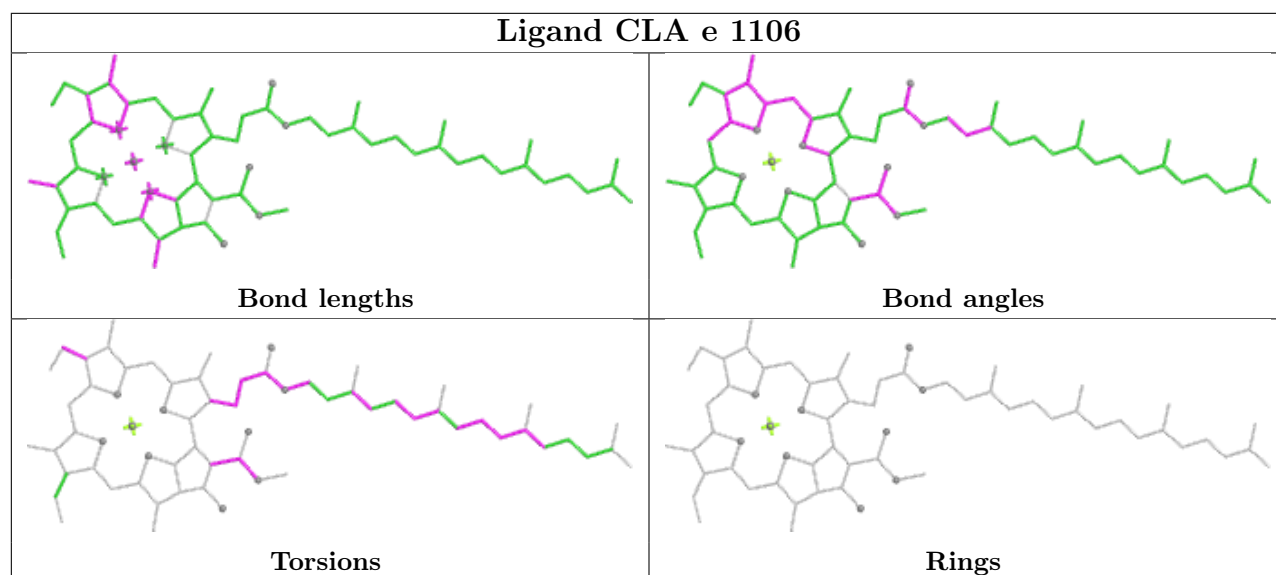
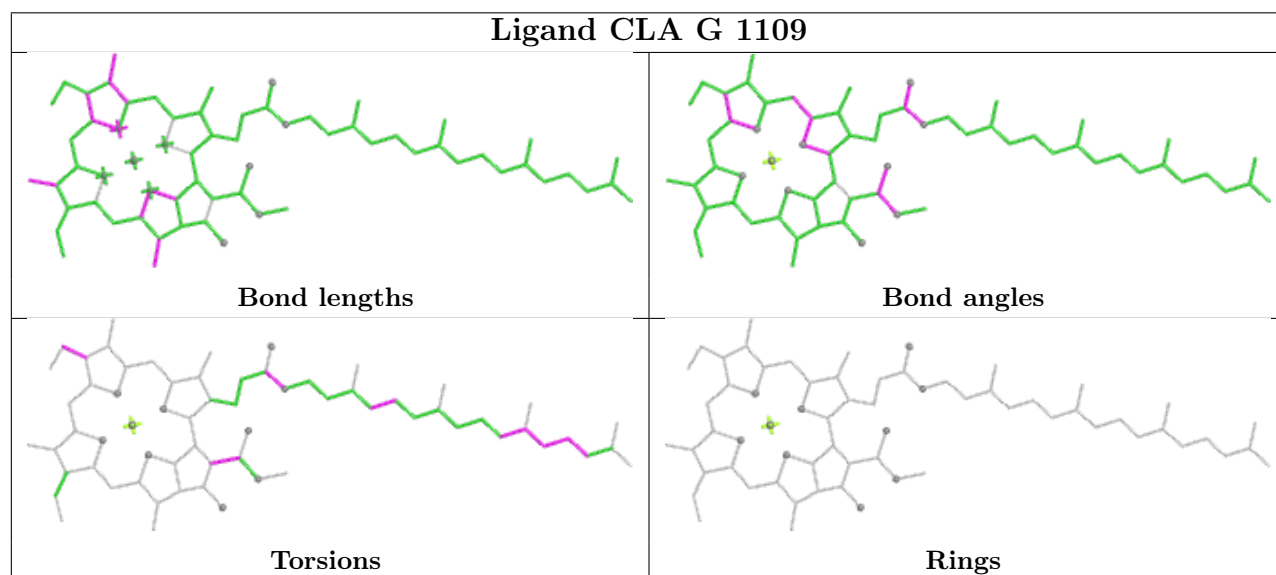
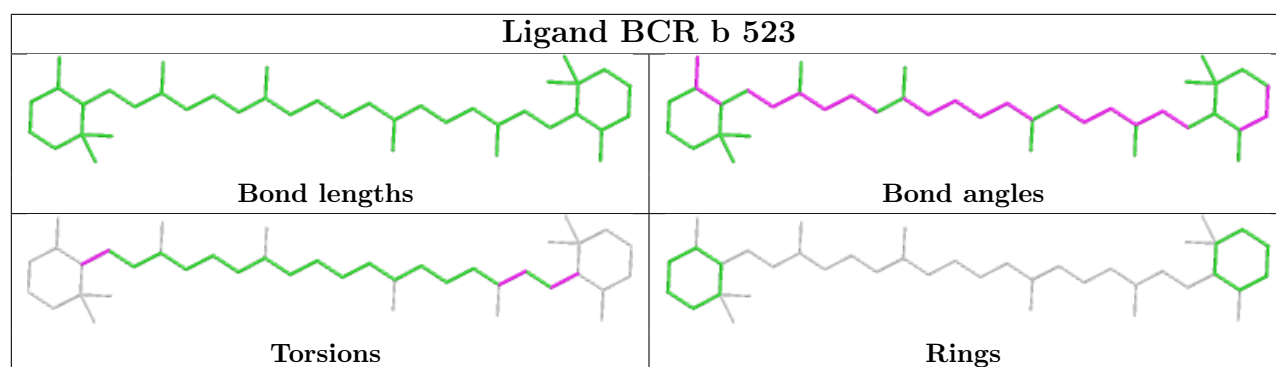


Ligand CLA d 508

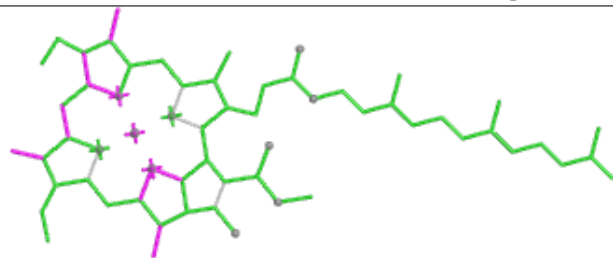


Ligand BCR j 4016

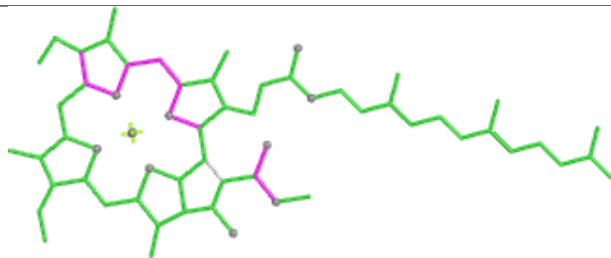




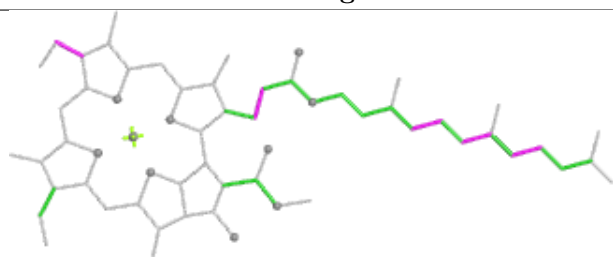
Ligand CLA H 1216



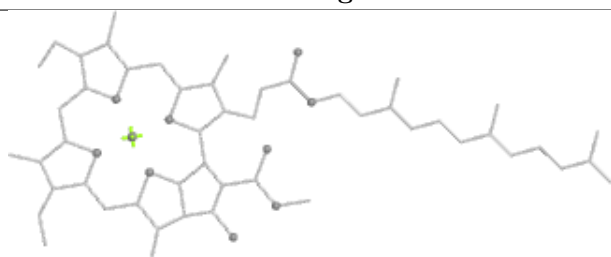
Bond lengths



Bond angles

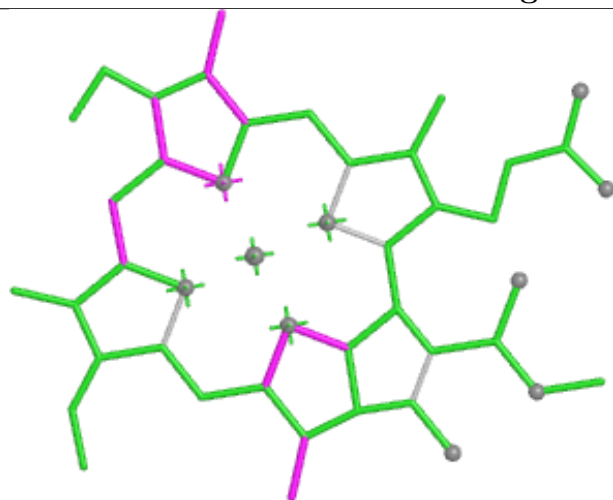


Torsions

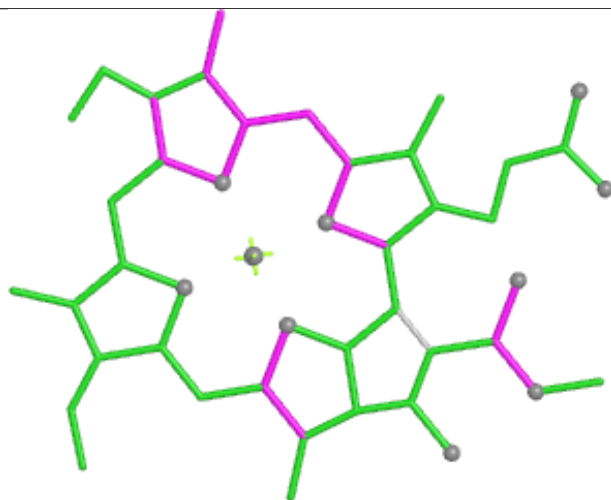


Rings

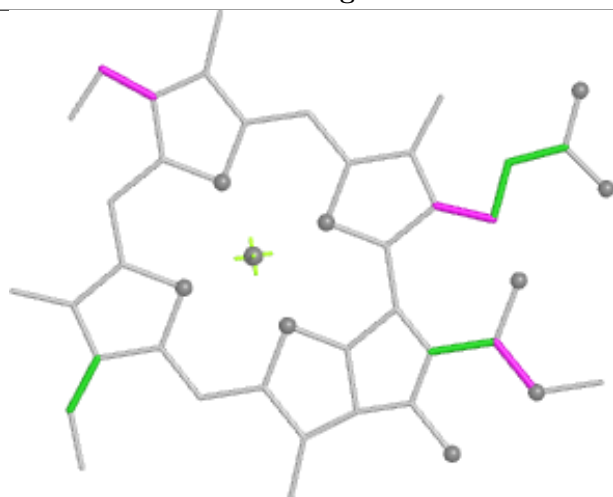
Ligand CLA t 511



Bond lengths



Bond angles

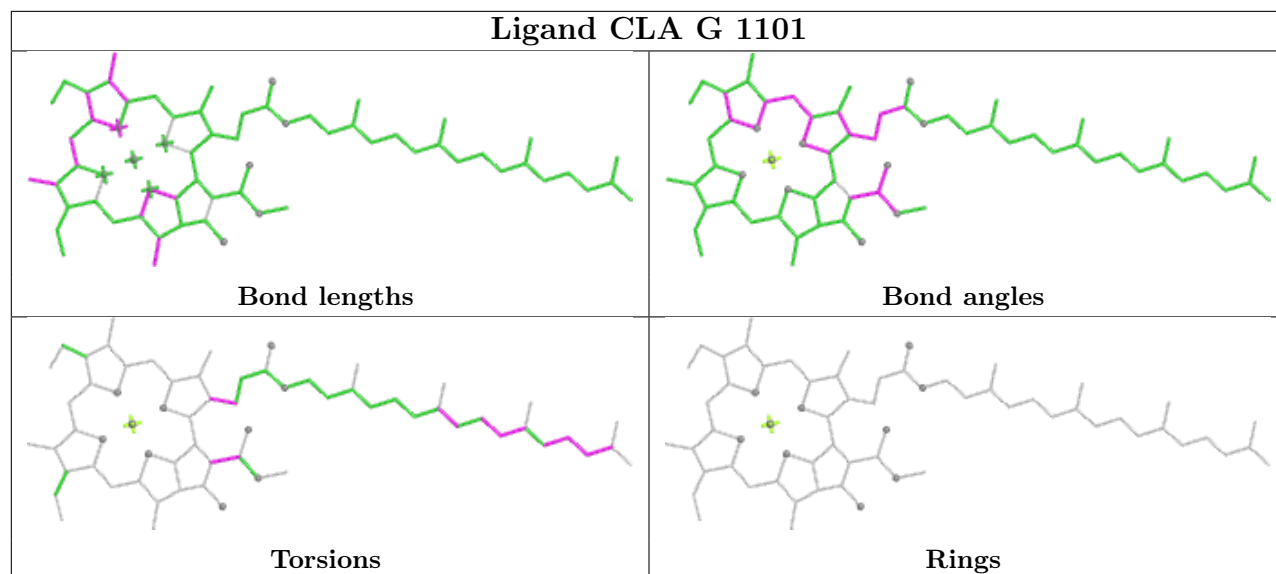


Torsions

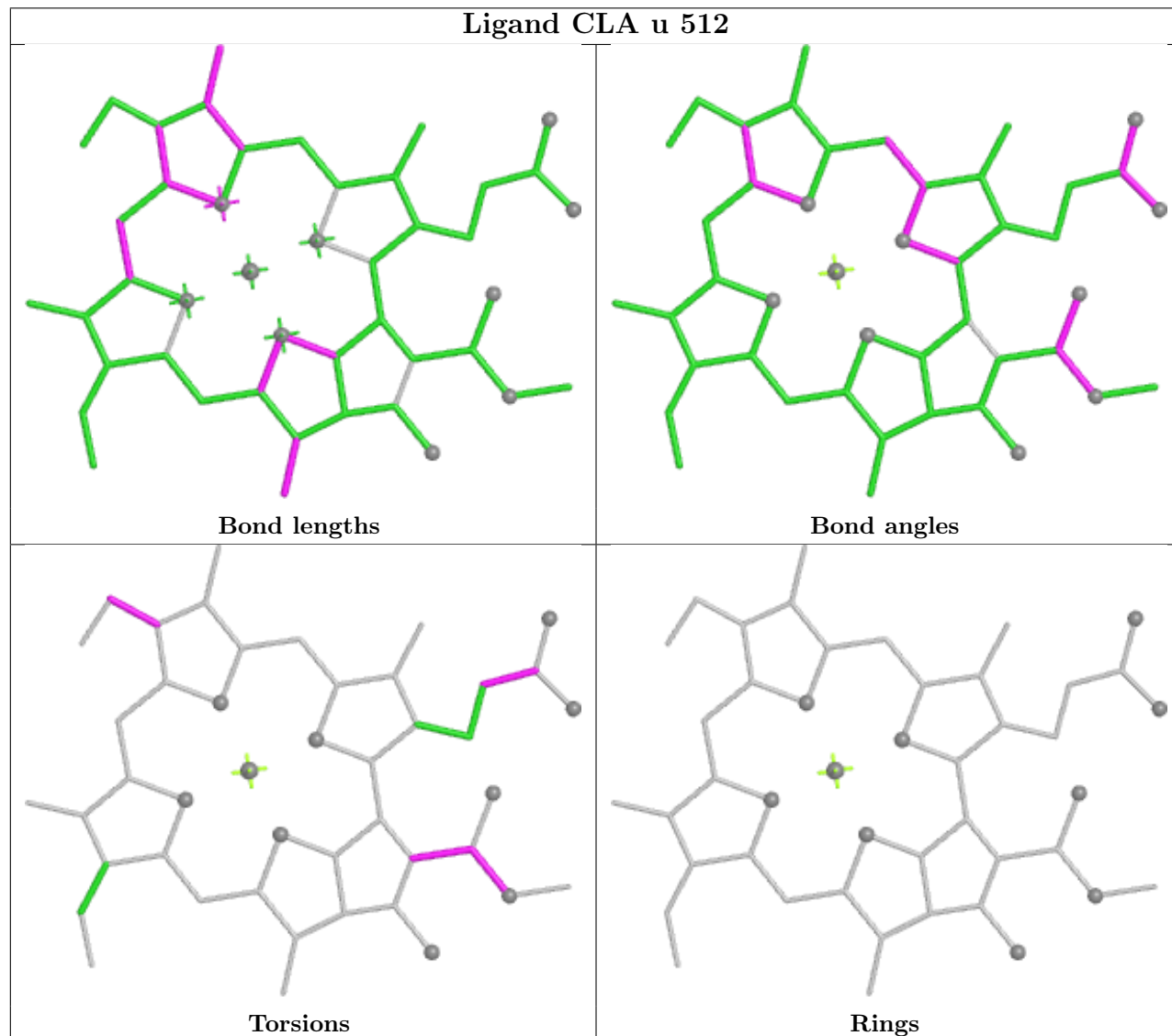


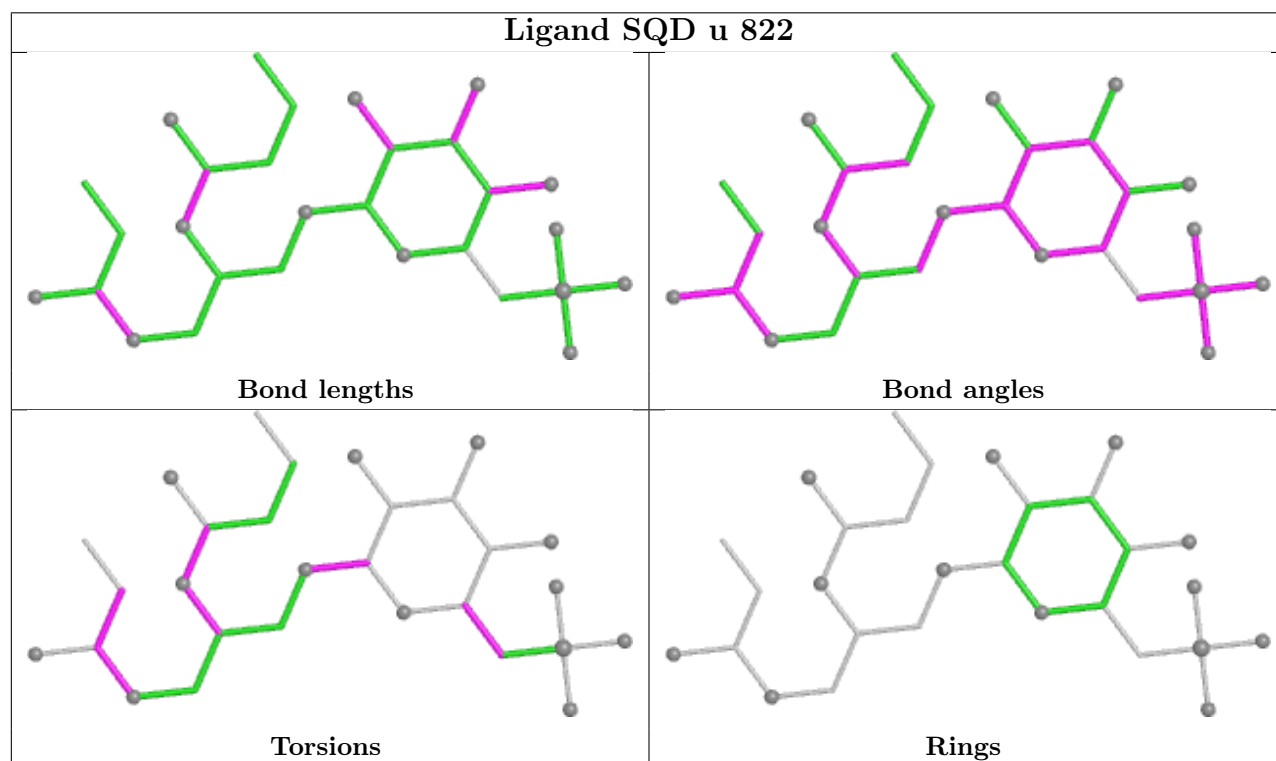
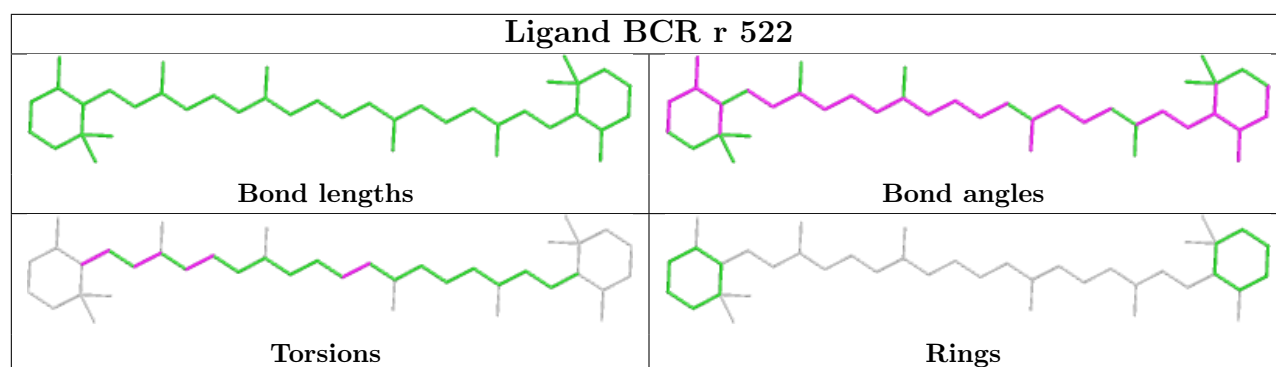
Rings

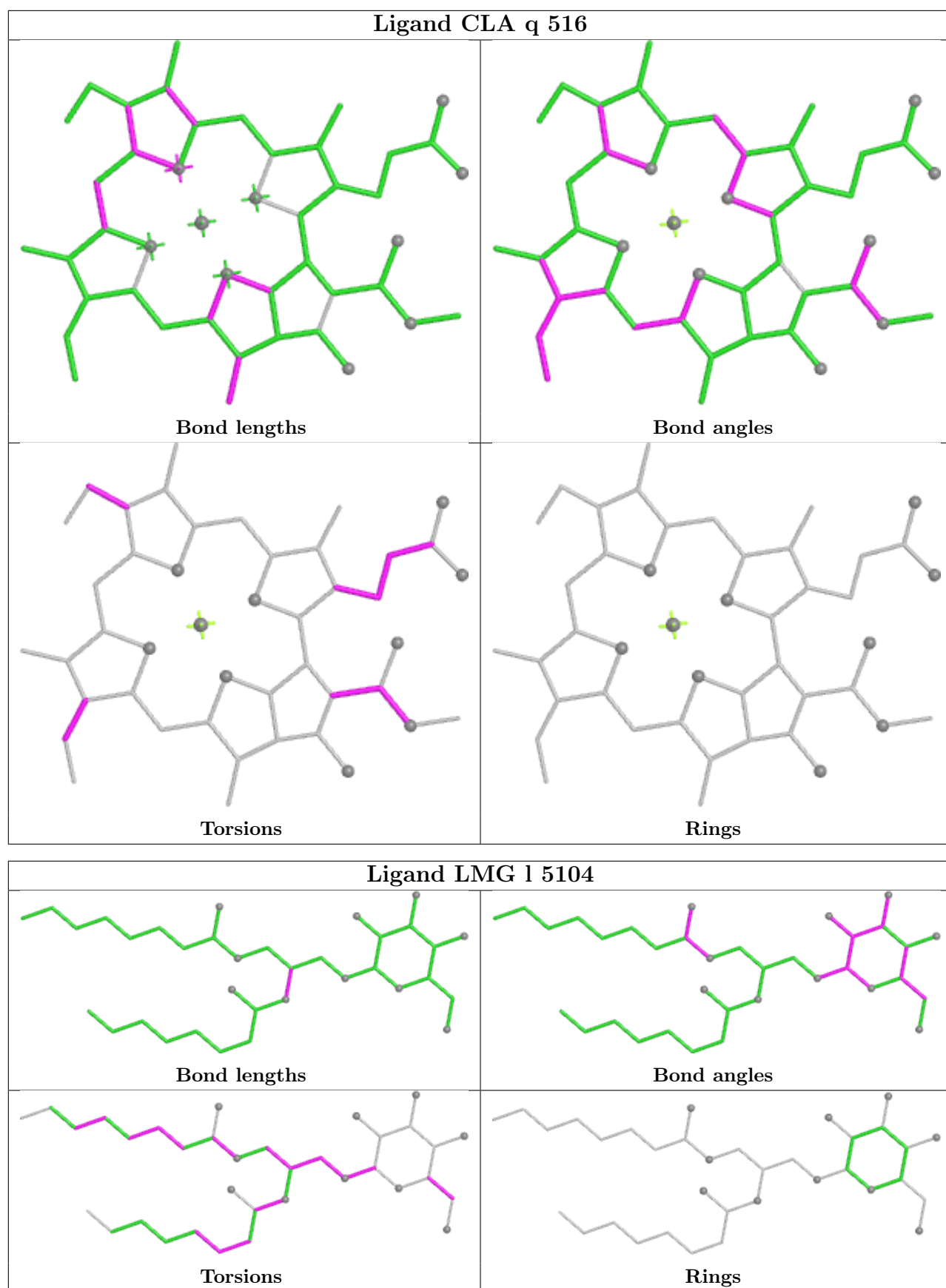
Ligand CLA G 1101



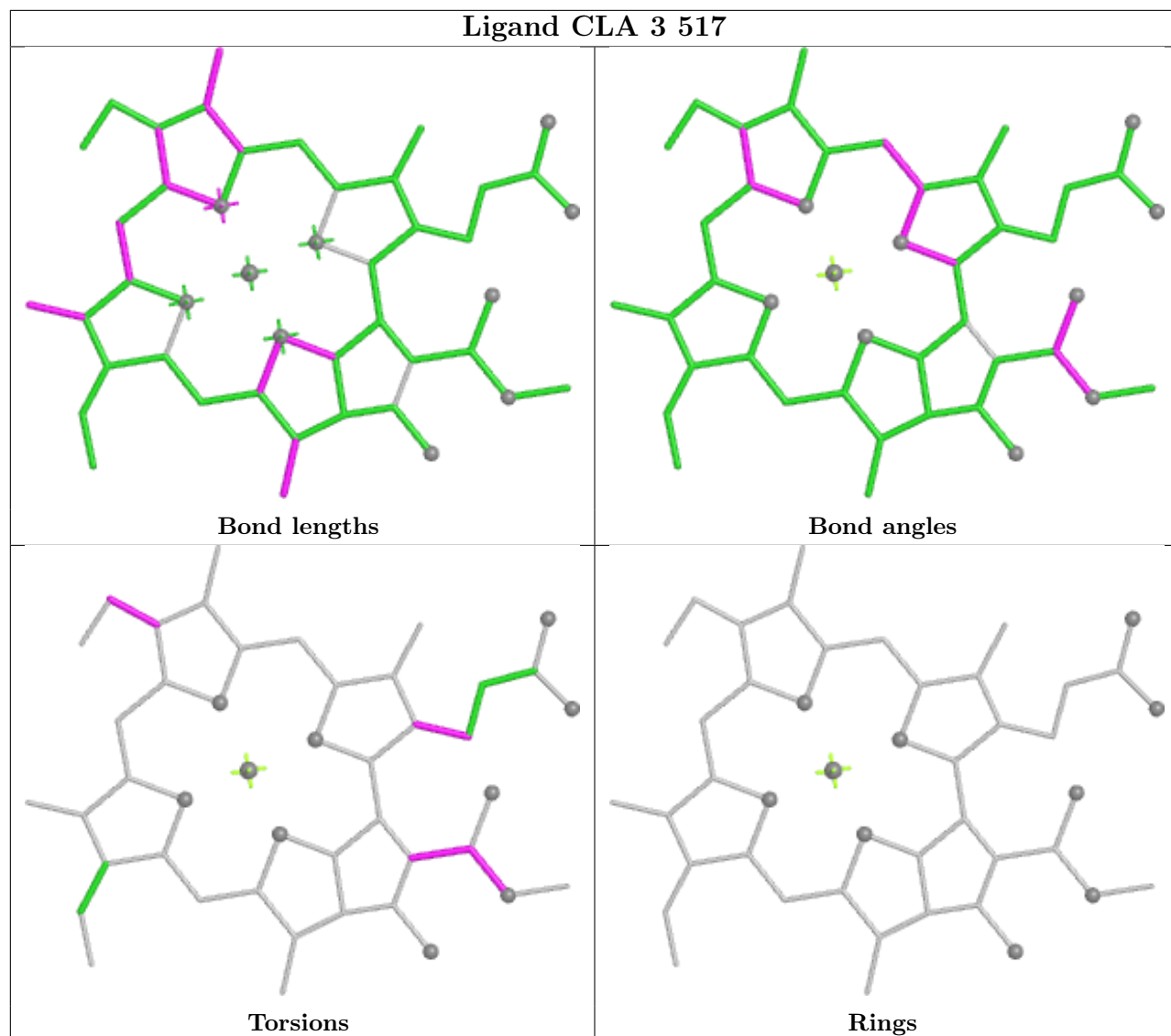
Ligand CLA u 512



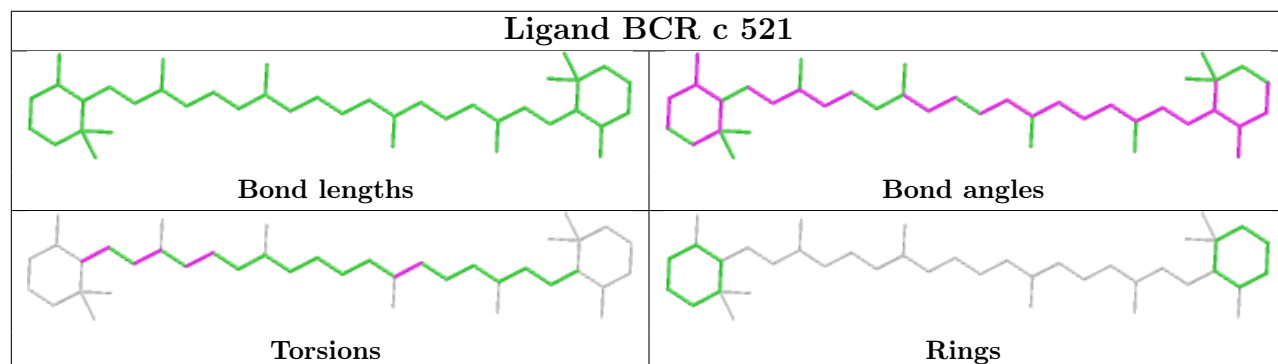


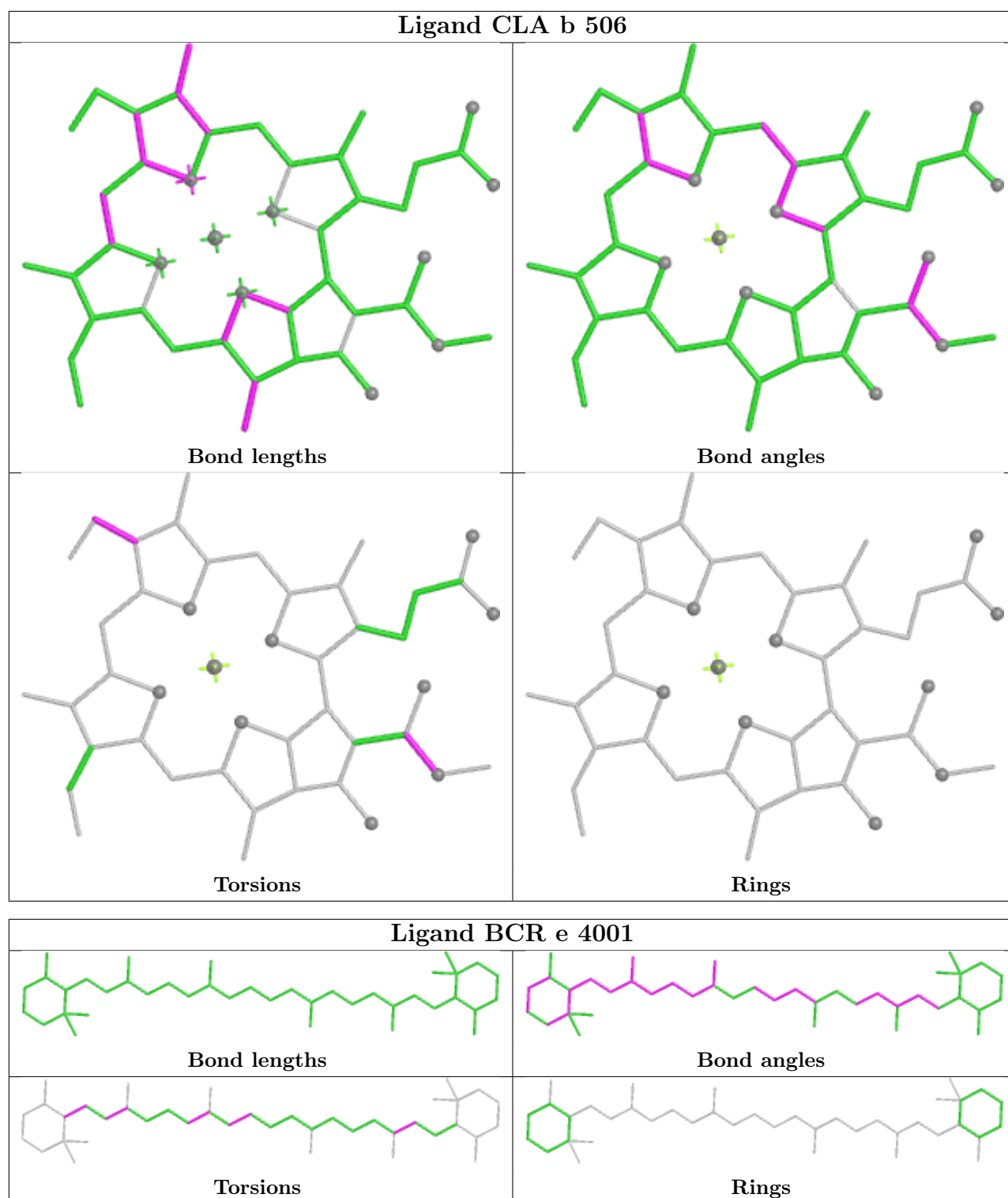


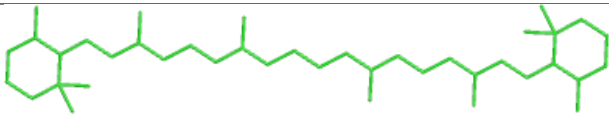
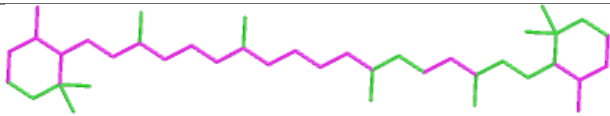
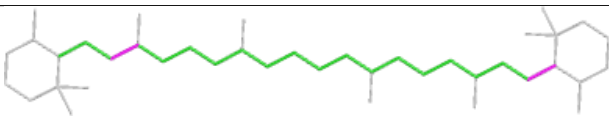
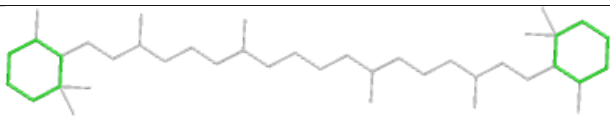
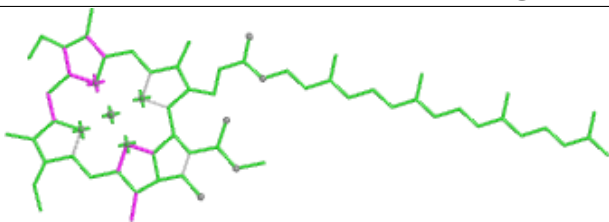
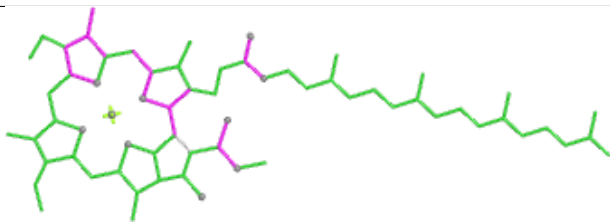
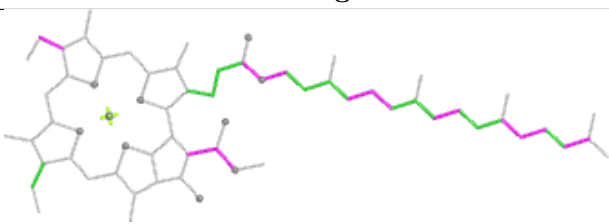
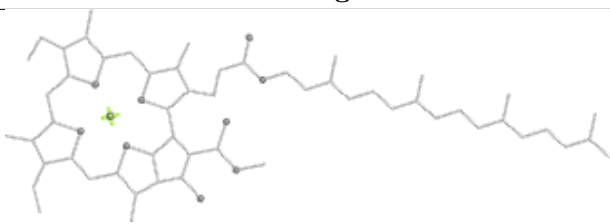
Ligand CLA 3 517



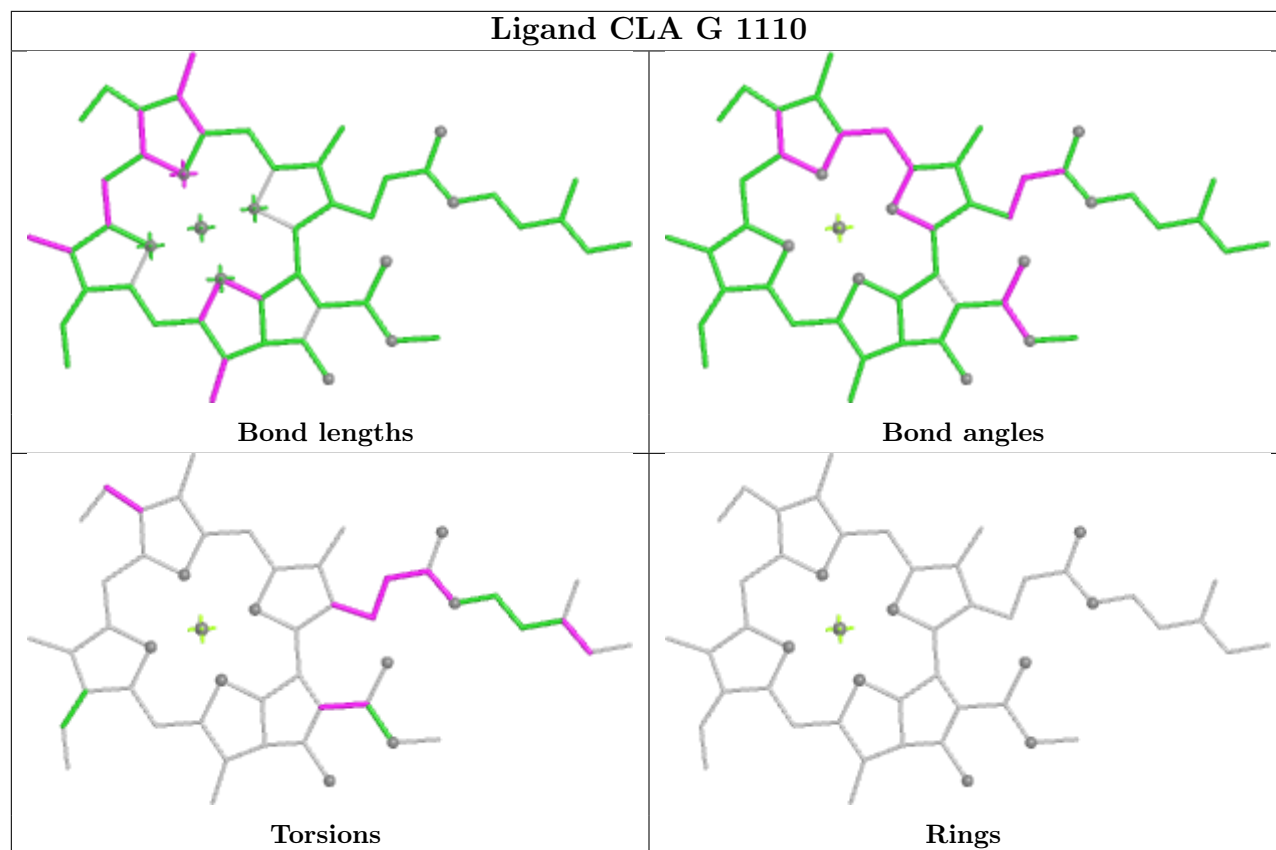
Ligand BCR c 521



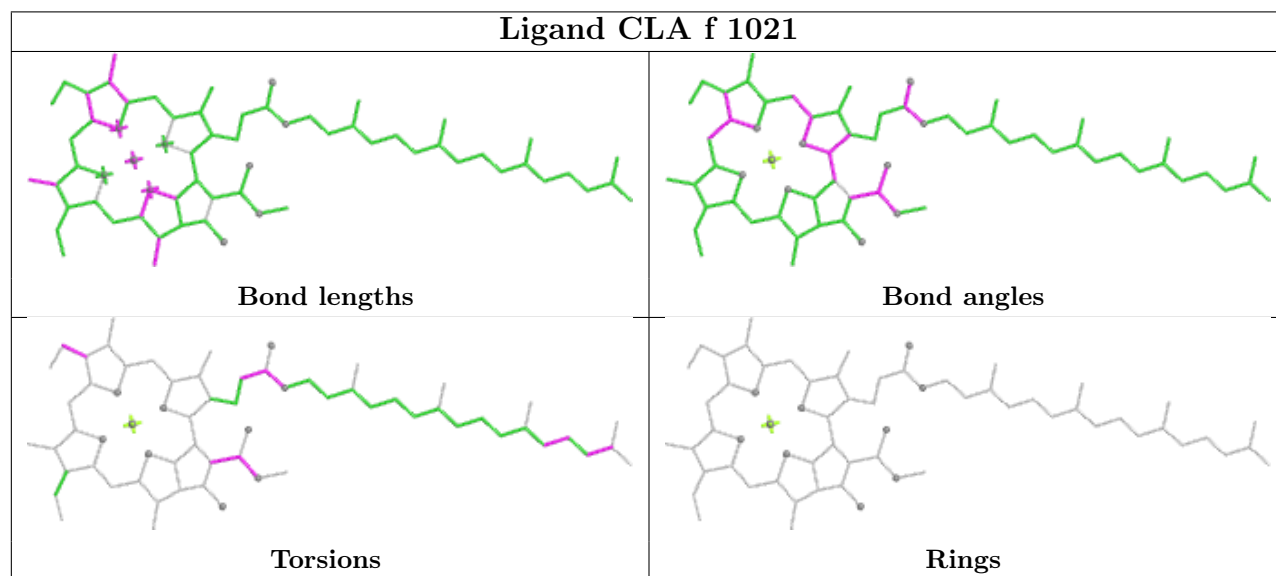


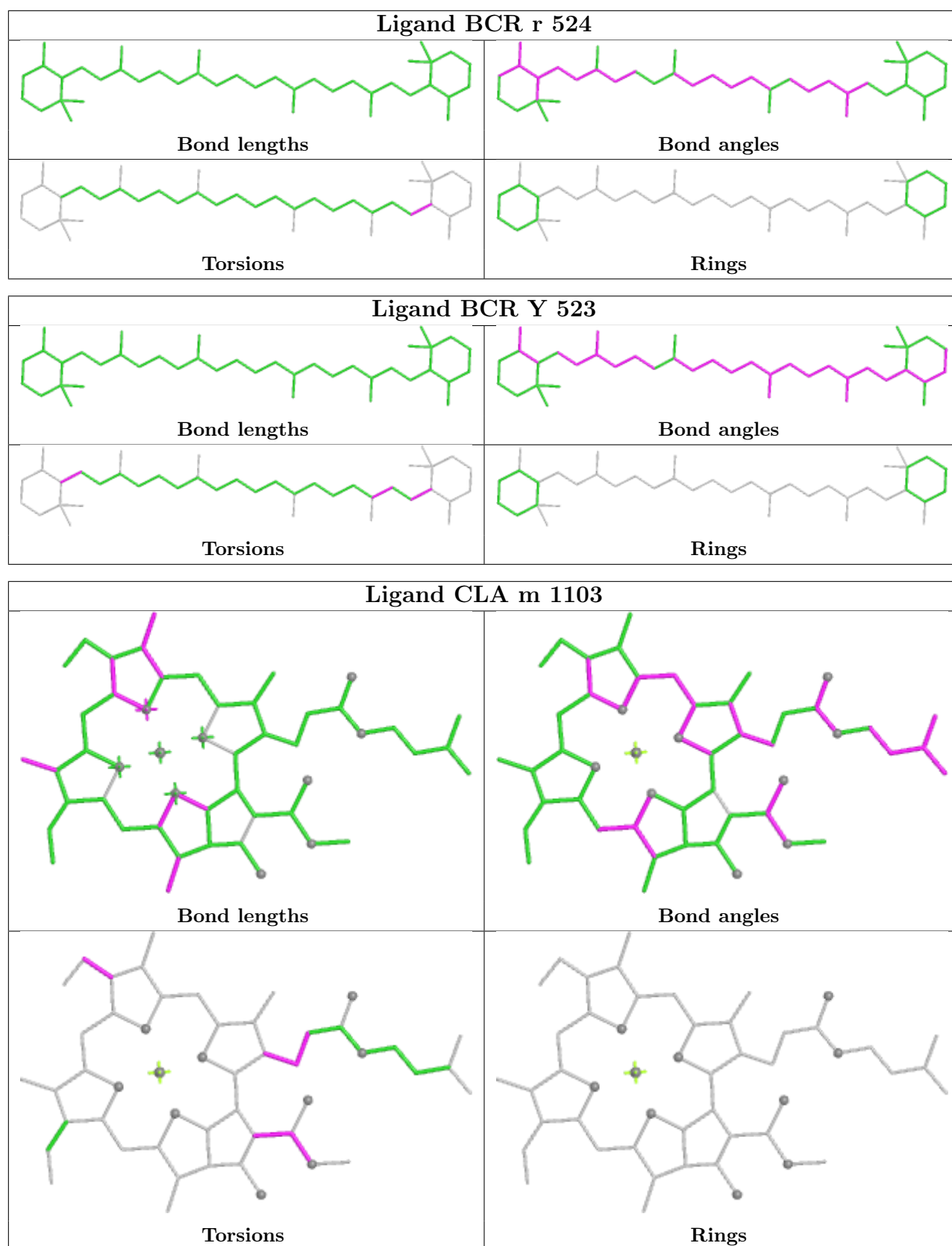
Ligand BCR t 524	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA 3 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1110

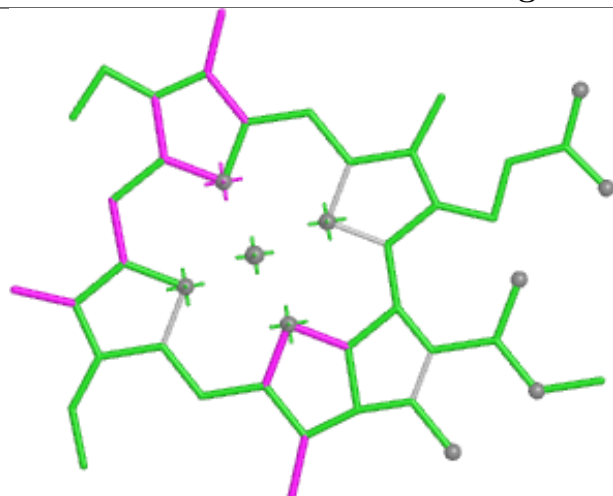


Ligand CLA f 1021

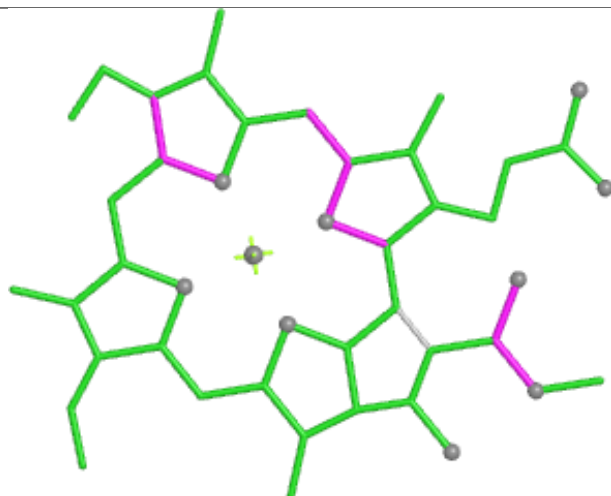




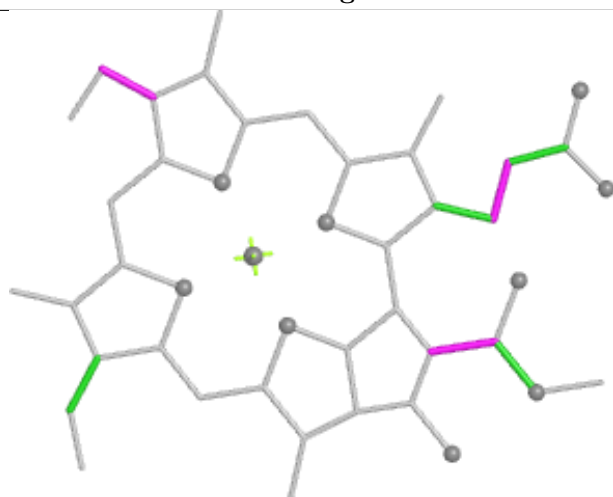
Ligand CLA 2 517



Bond lengths



Bond angles

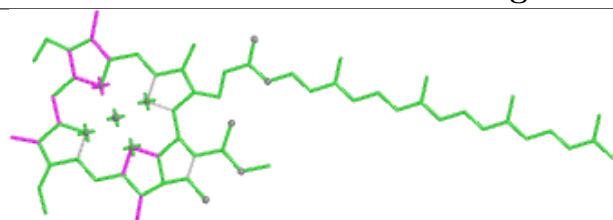


Torsions

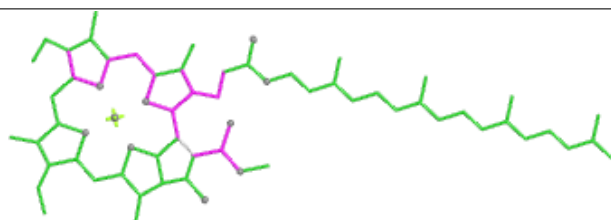


Rings

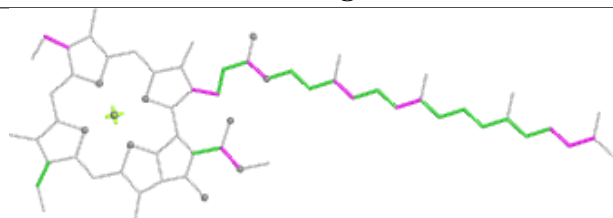
Ligand CLA e 1140



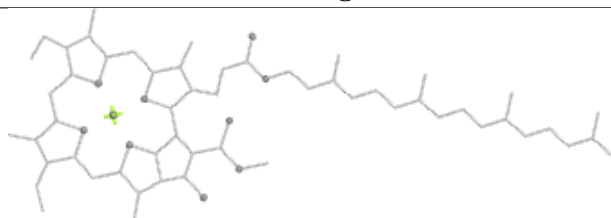
Bond lengths



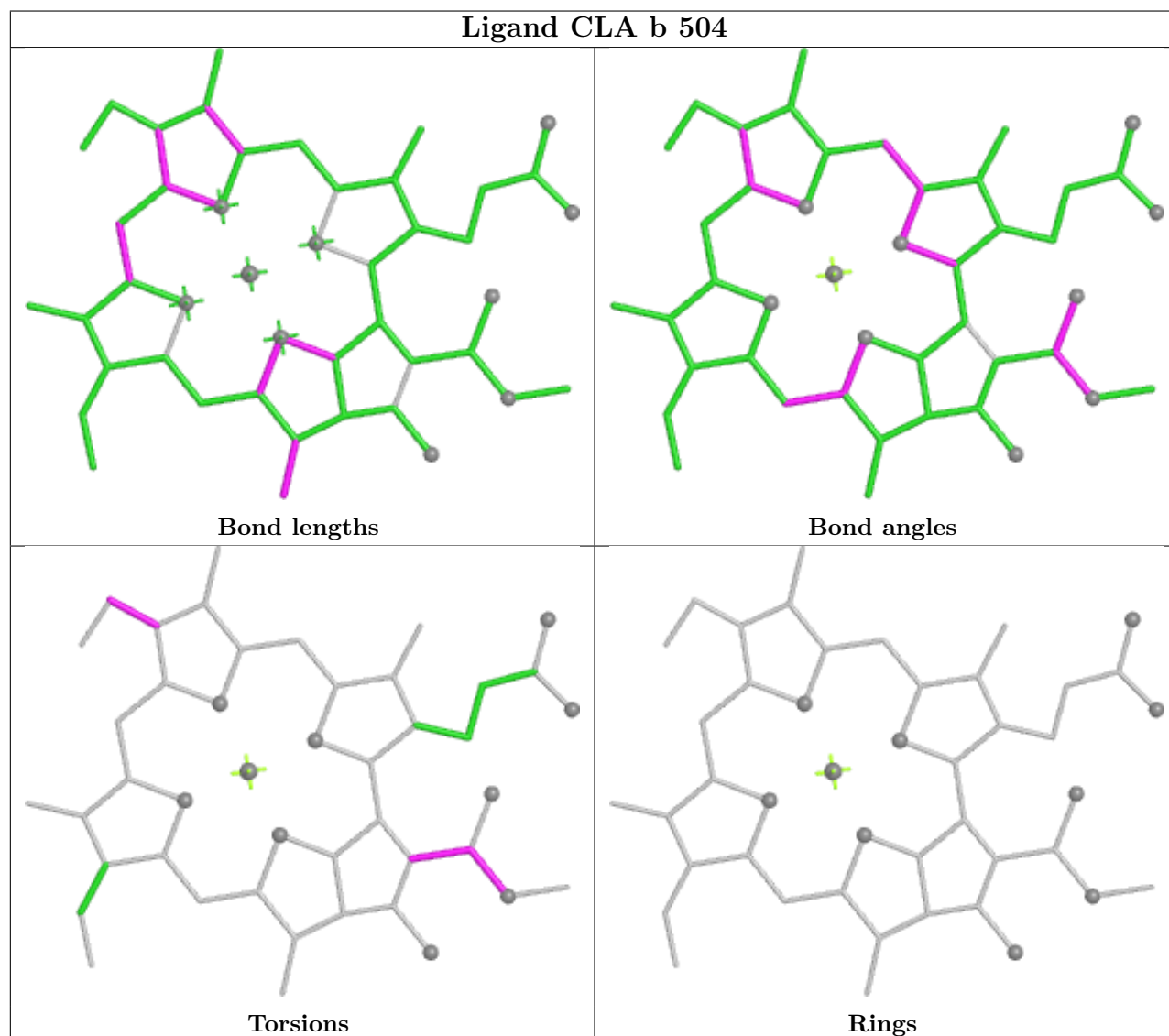
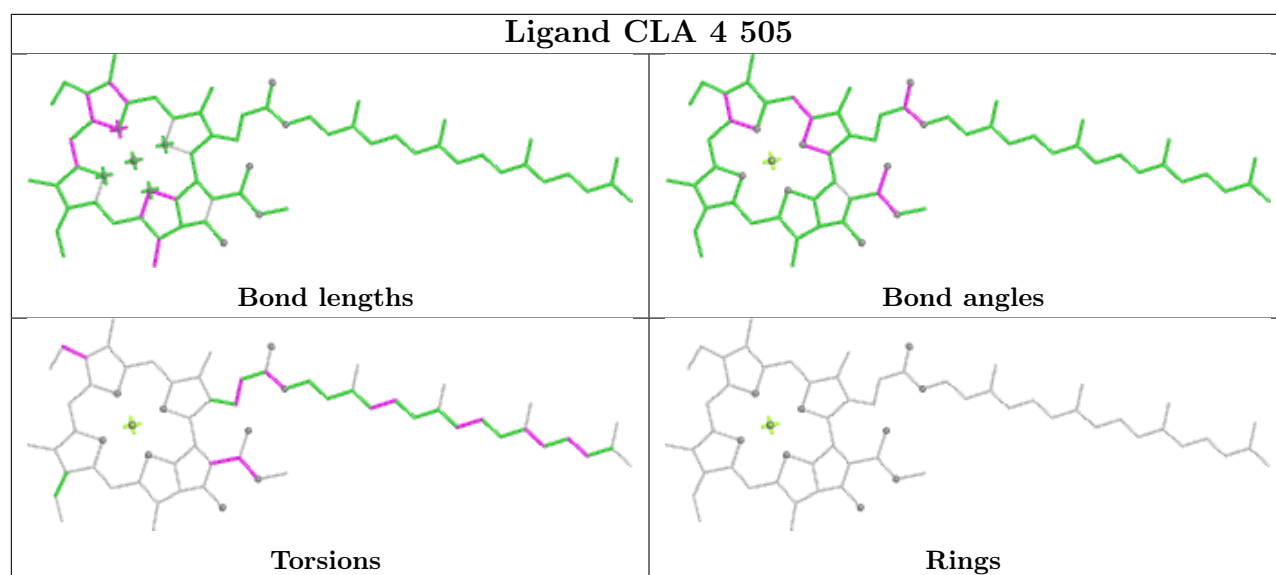
Bond angles



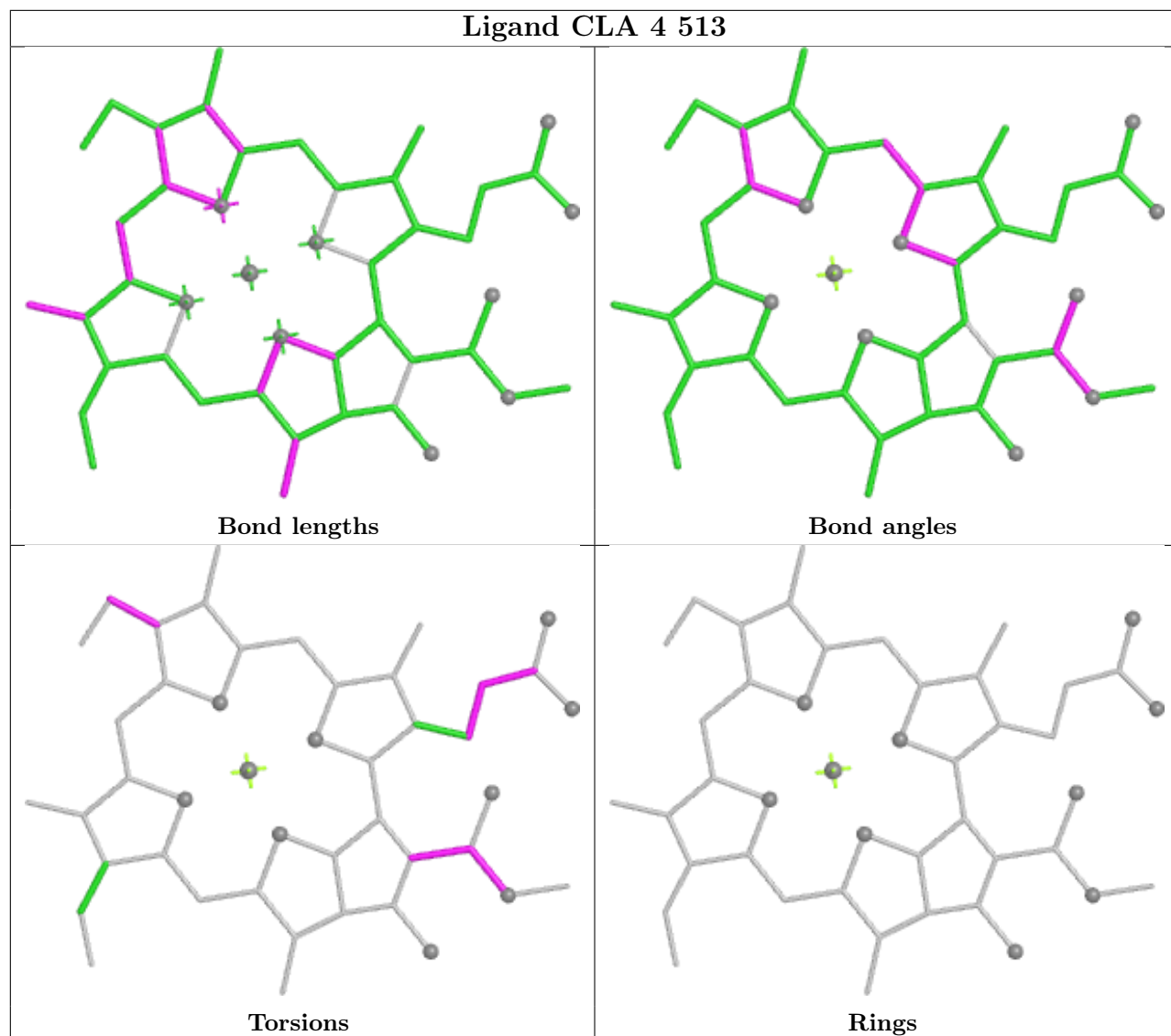
Torsions



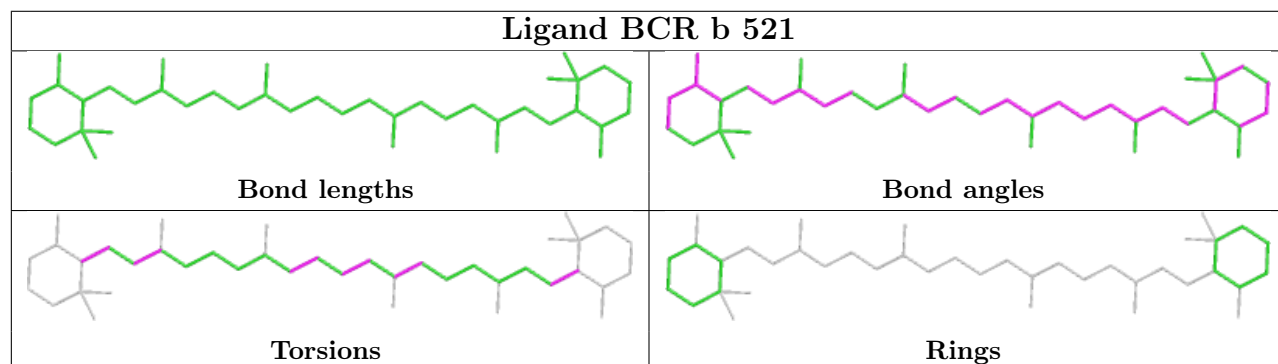
Rings

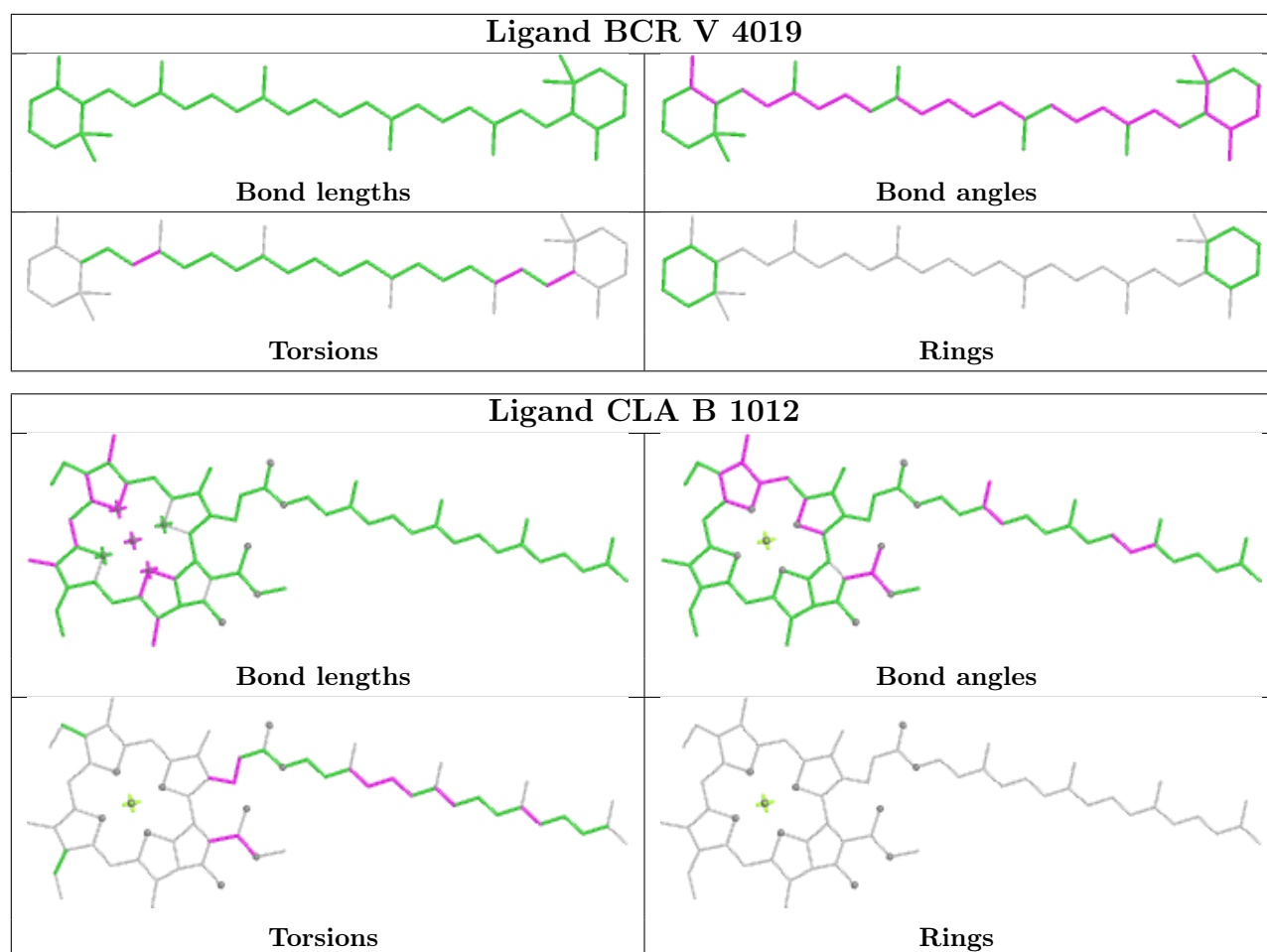


Ligand CLA 4 513

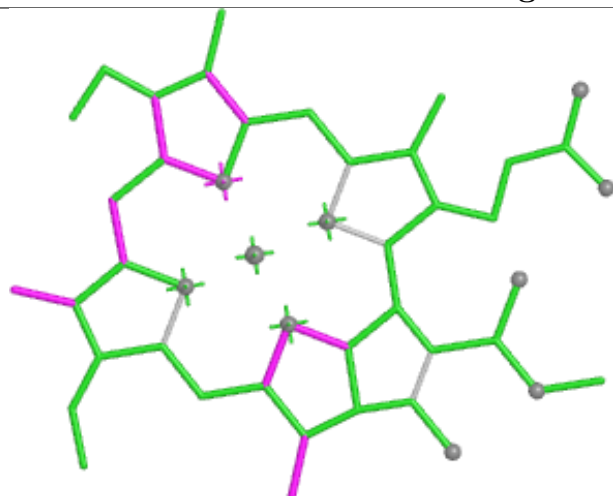


Ligand BCR b 521

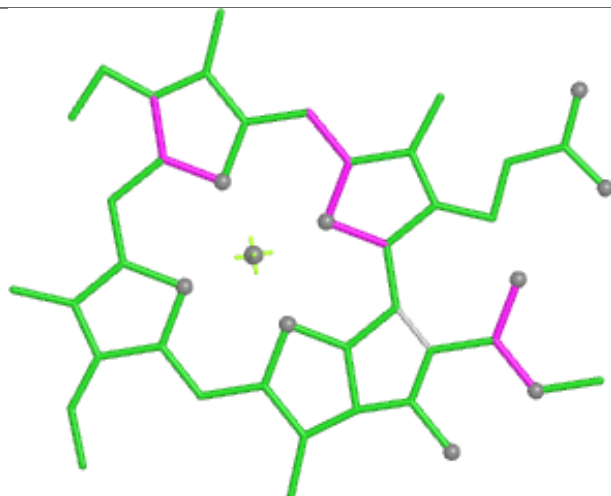




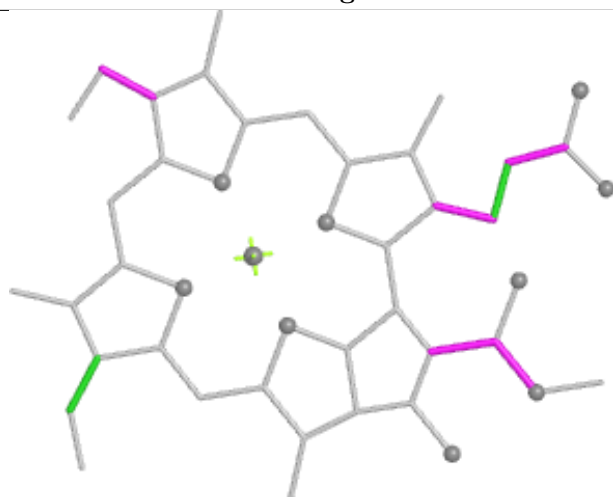
Ligand CLA 6 517



Bond lengths



Bond angles

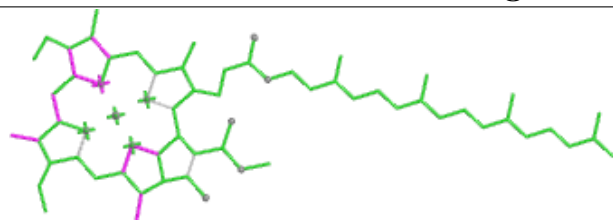


Torsions

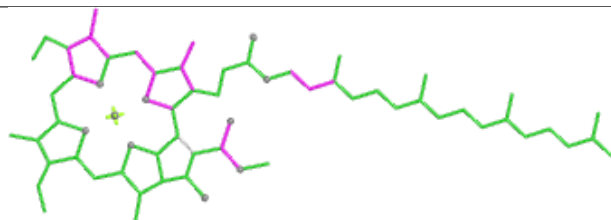


Rings

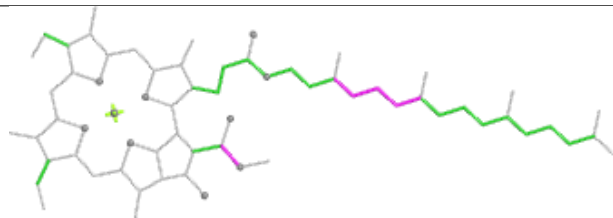
Ligand CLA H 1231



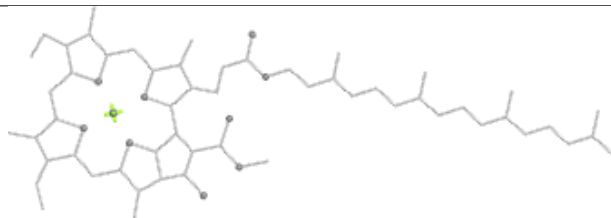
Bond lengths



Bond angles

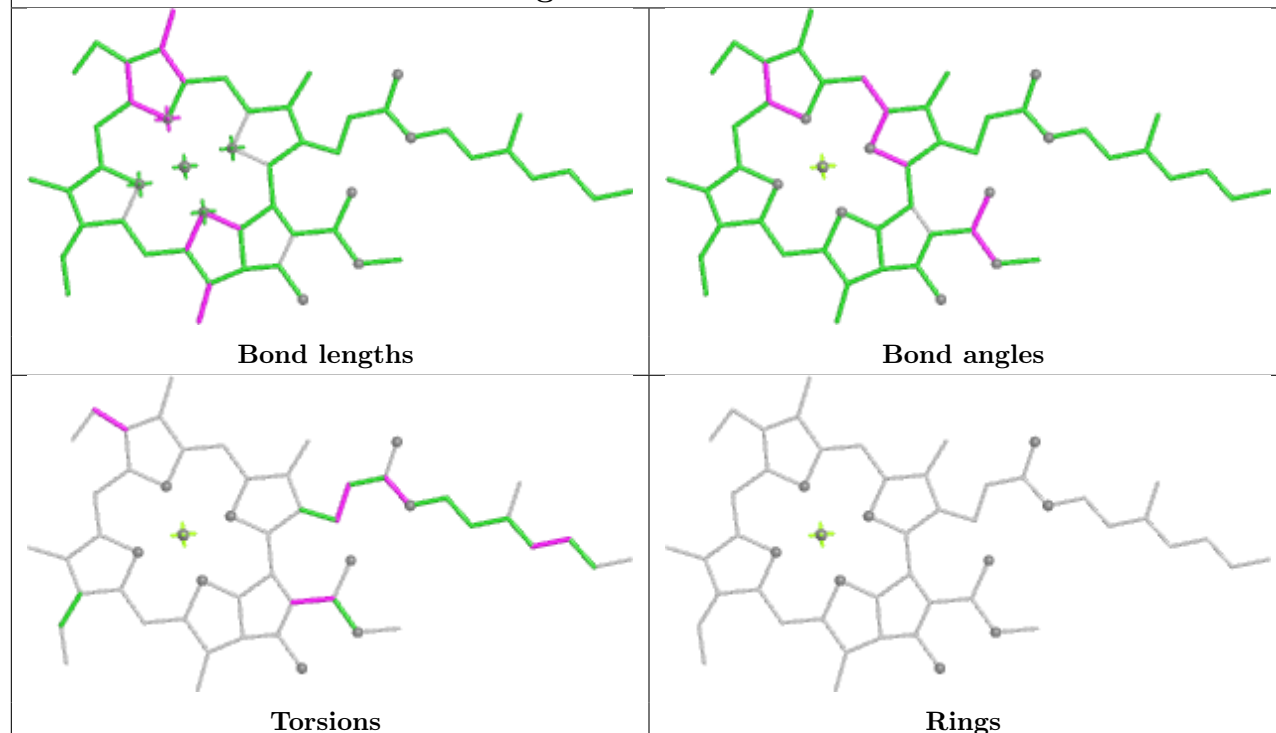


Torsions

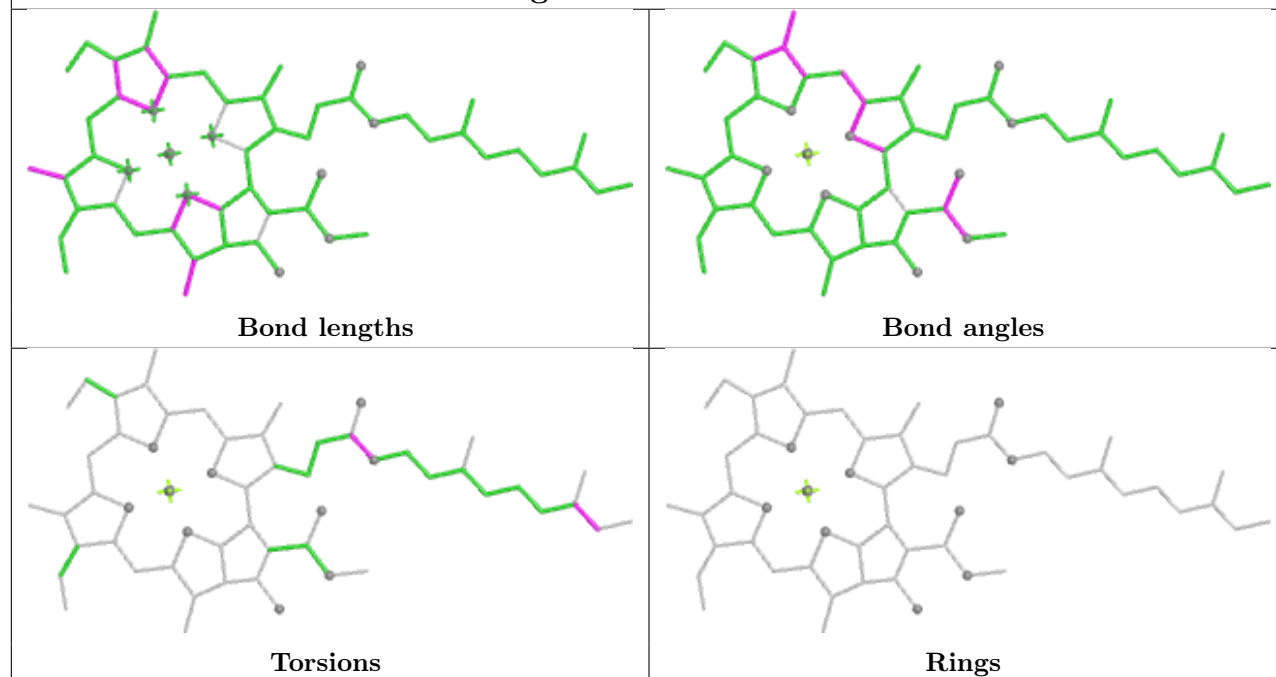


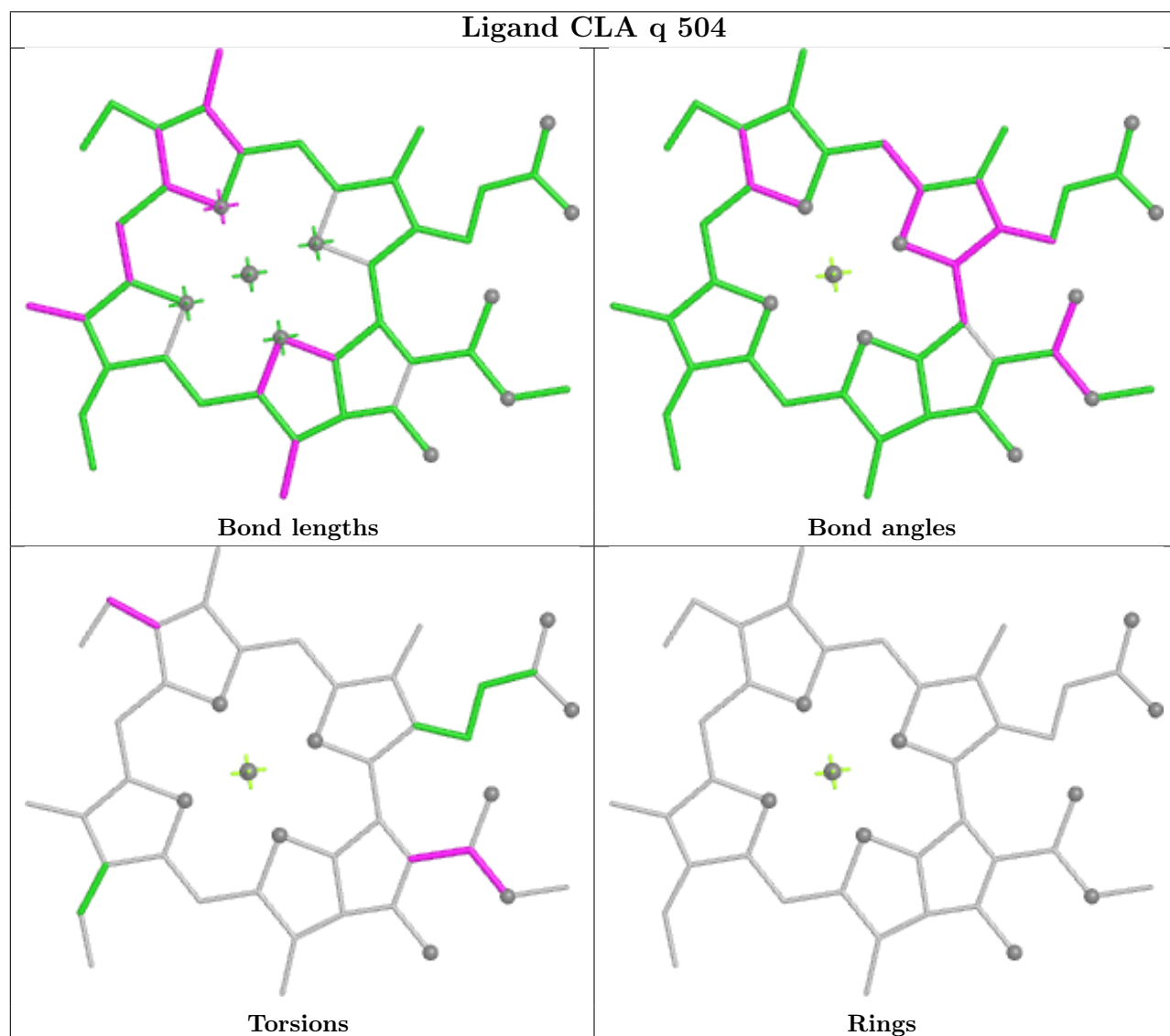
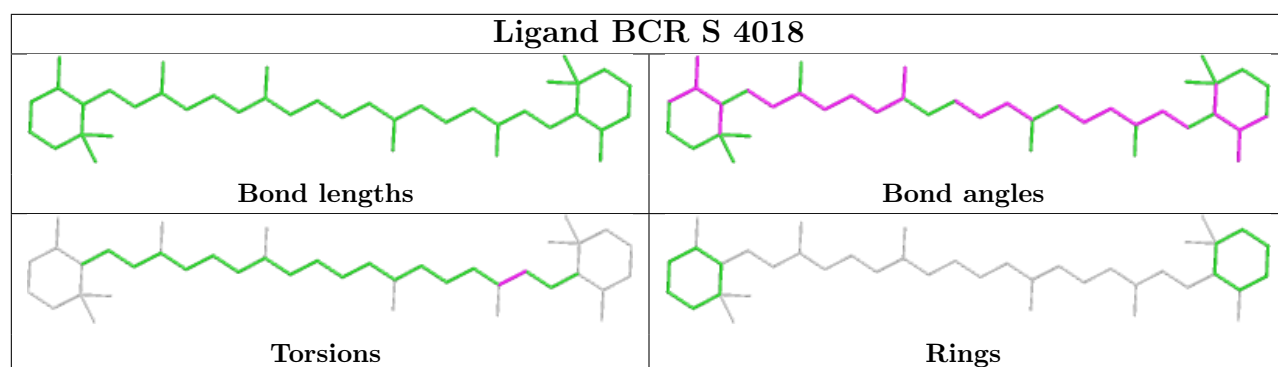
Rings

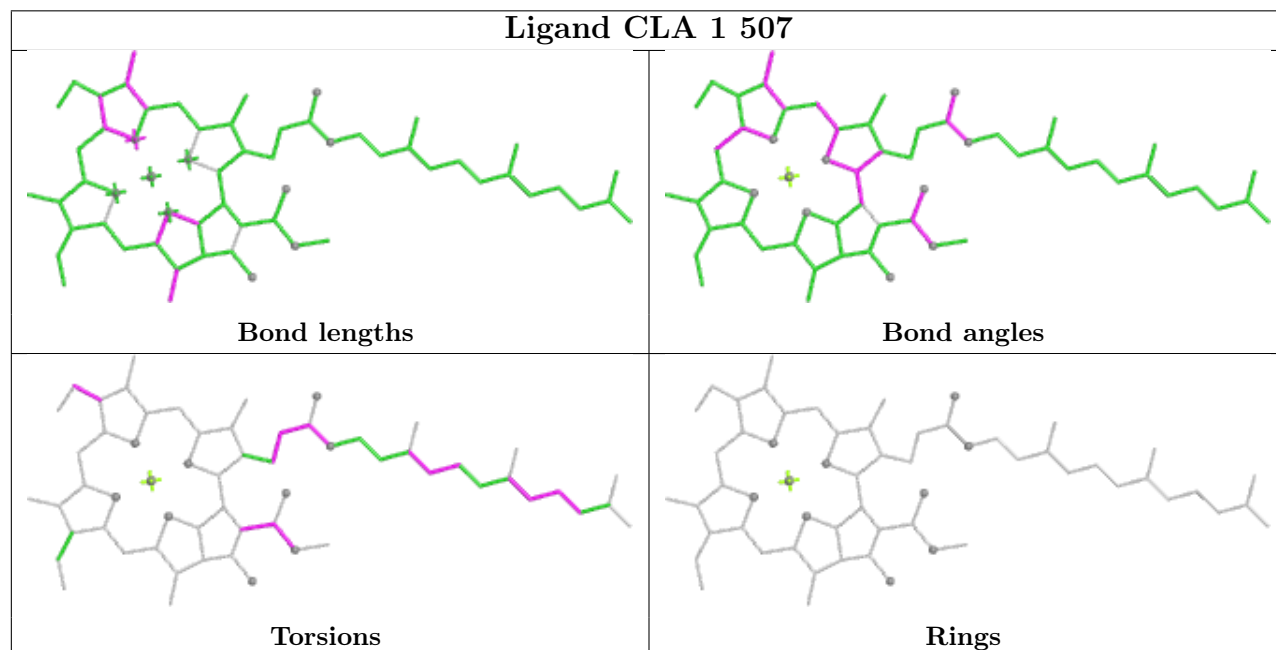
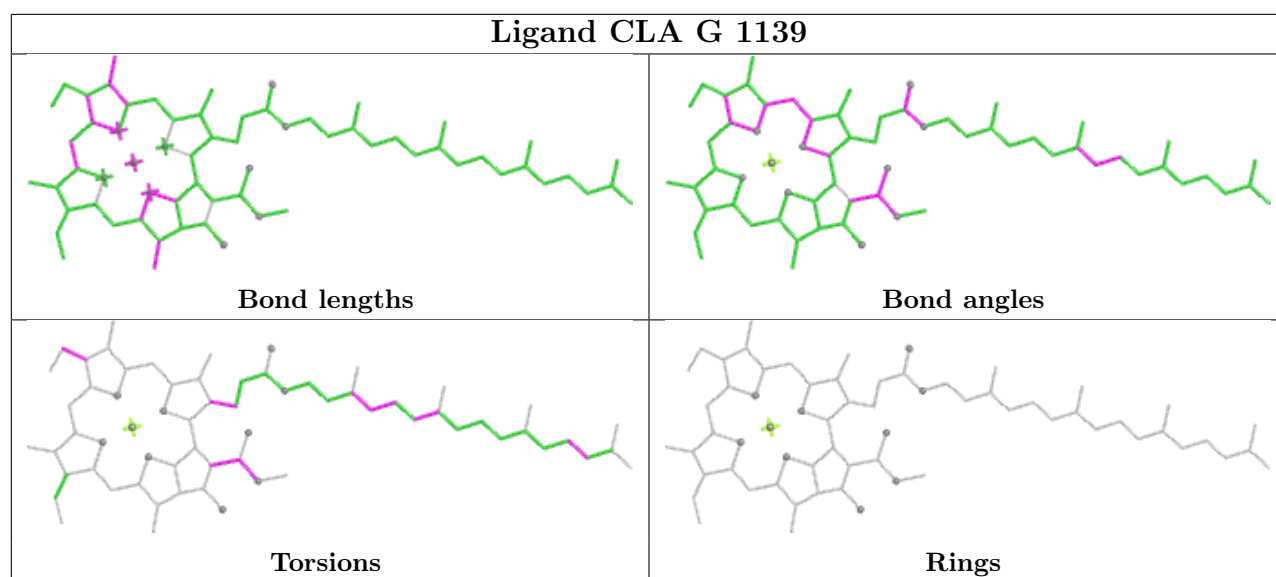
Ligand CLA 2 512

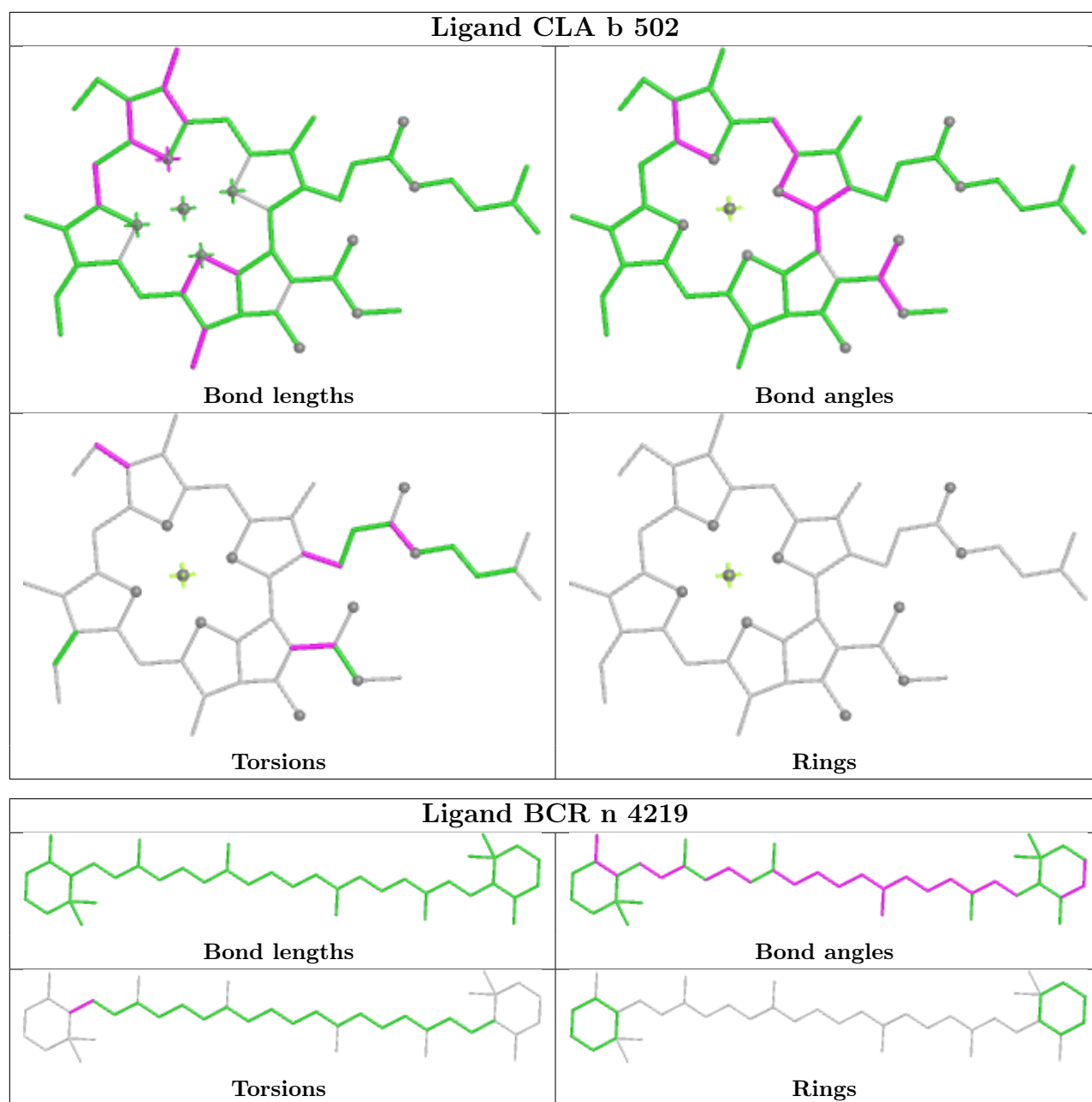


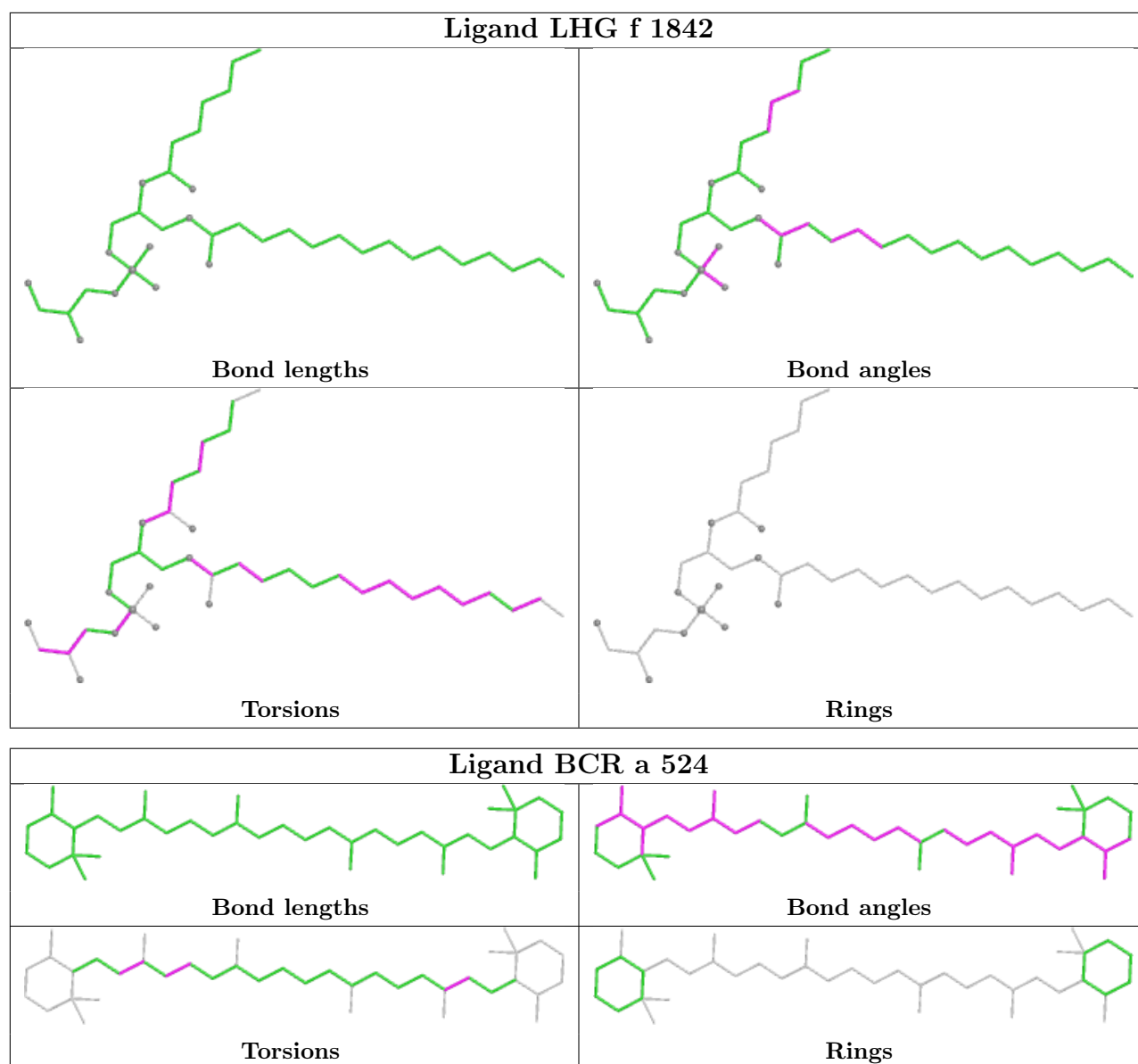
Ligand CLA f 1211



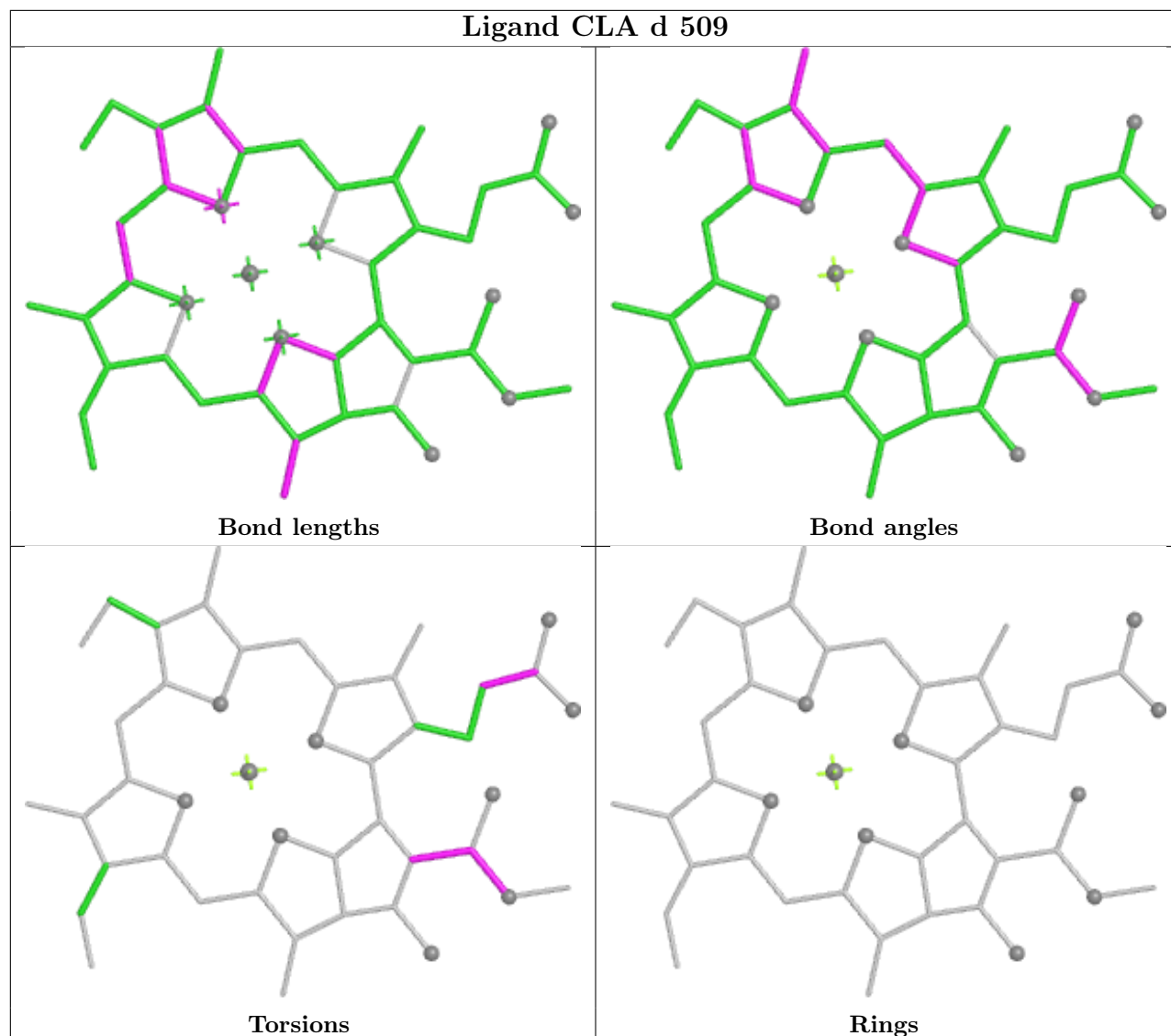




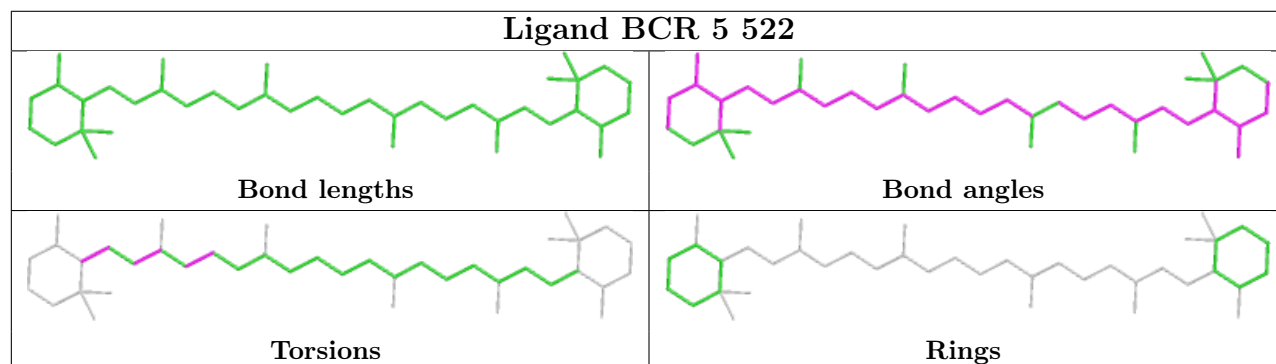


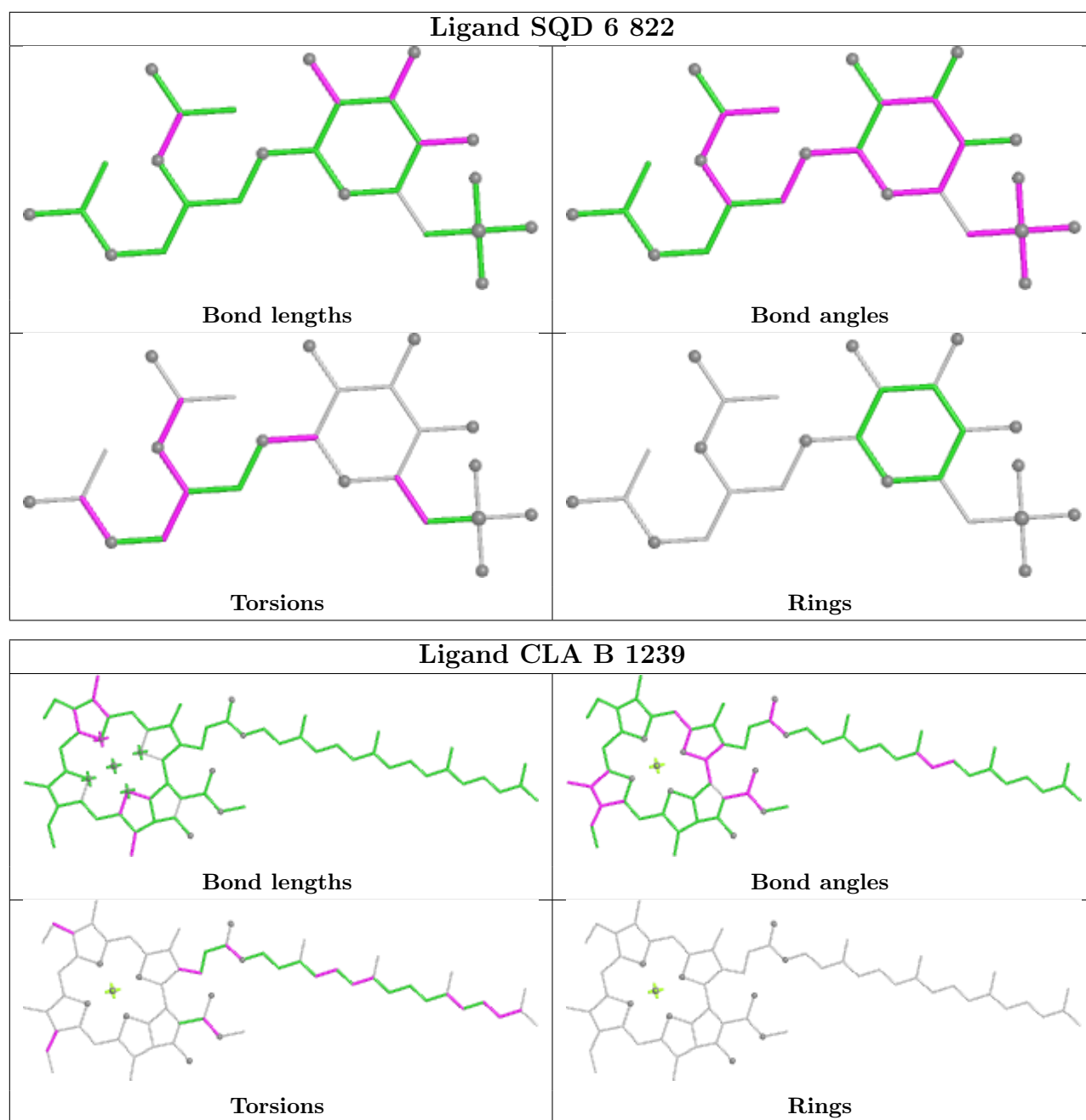


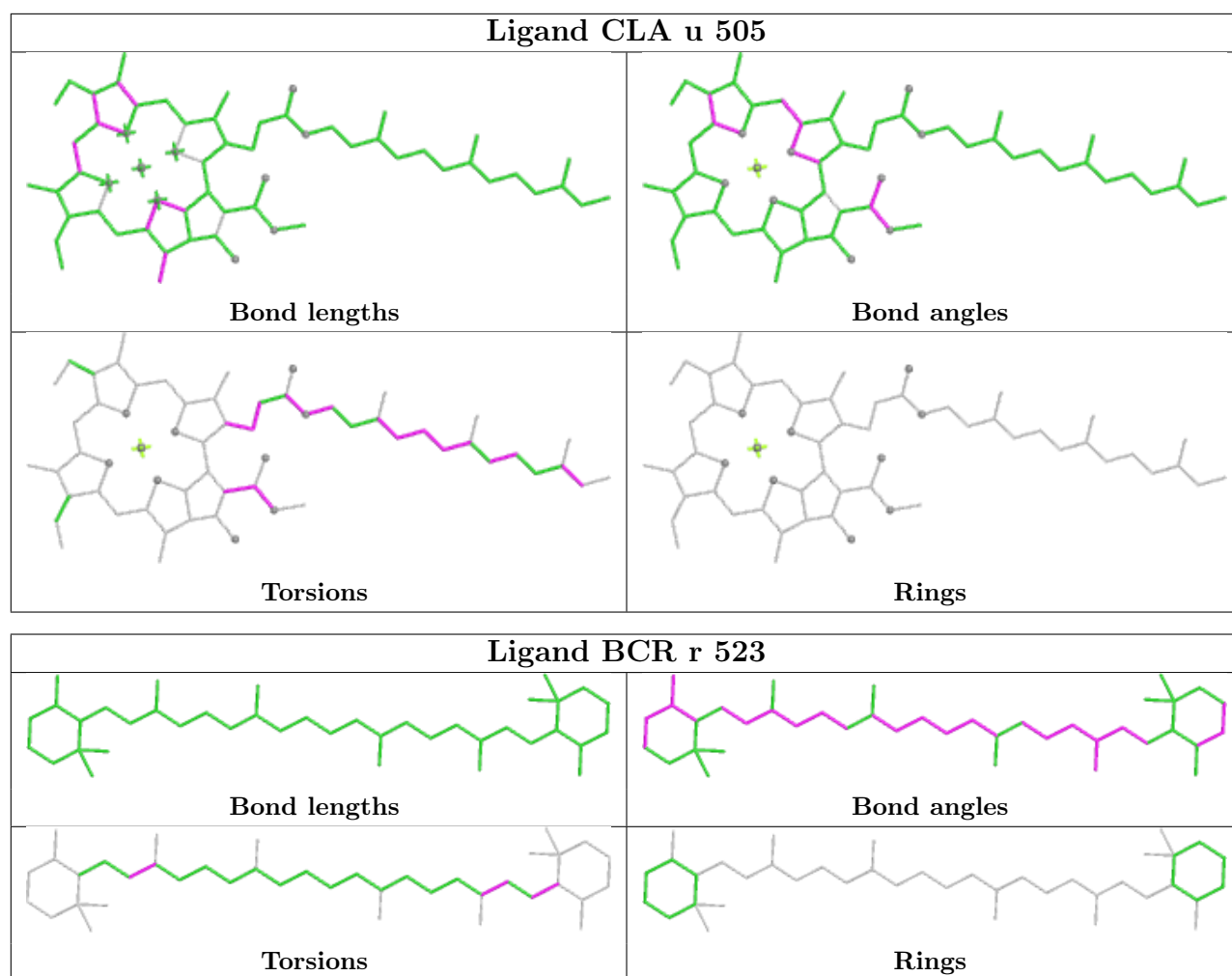
Ligand CLA d 509

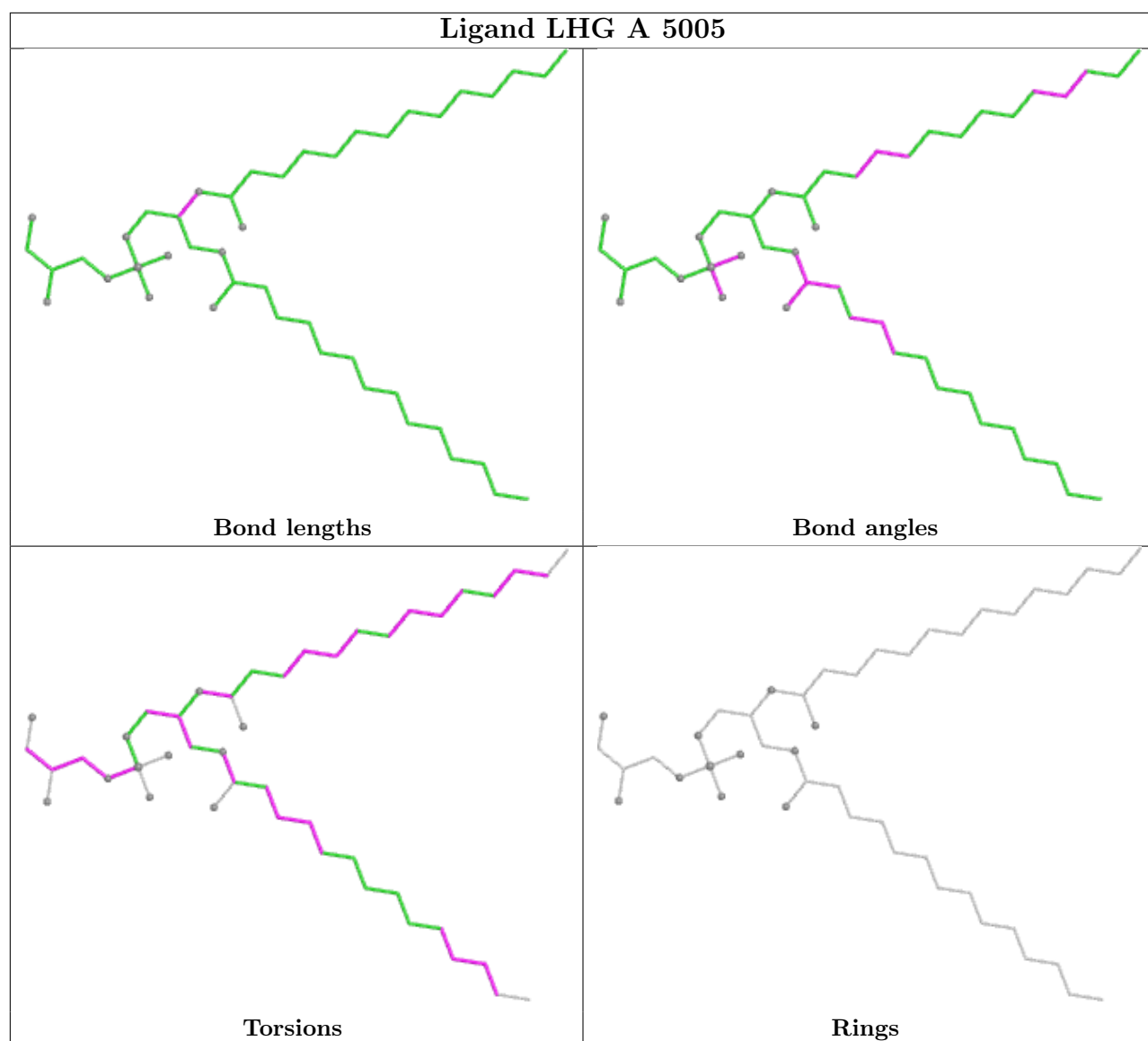


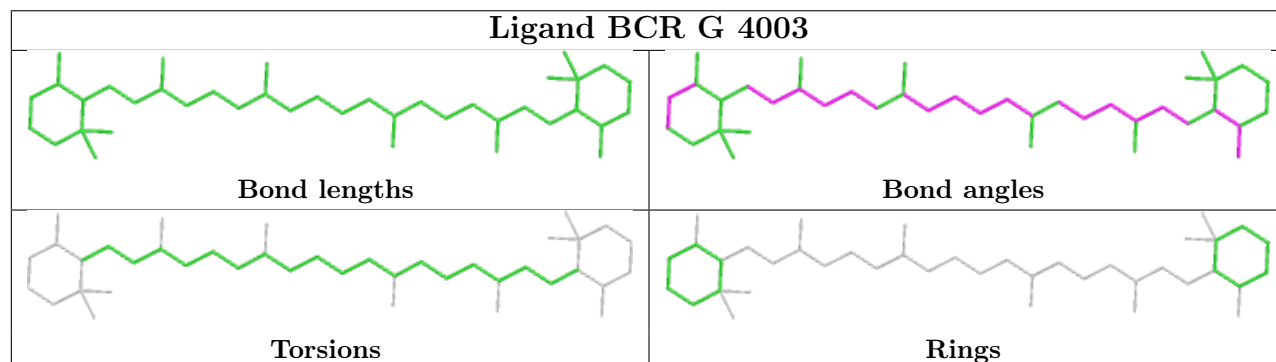
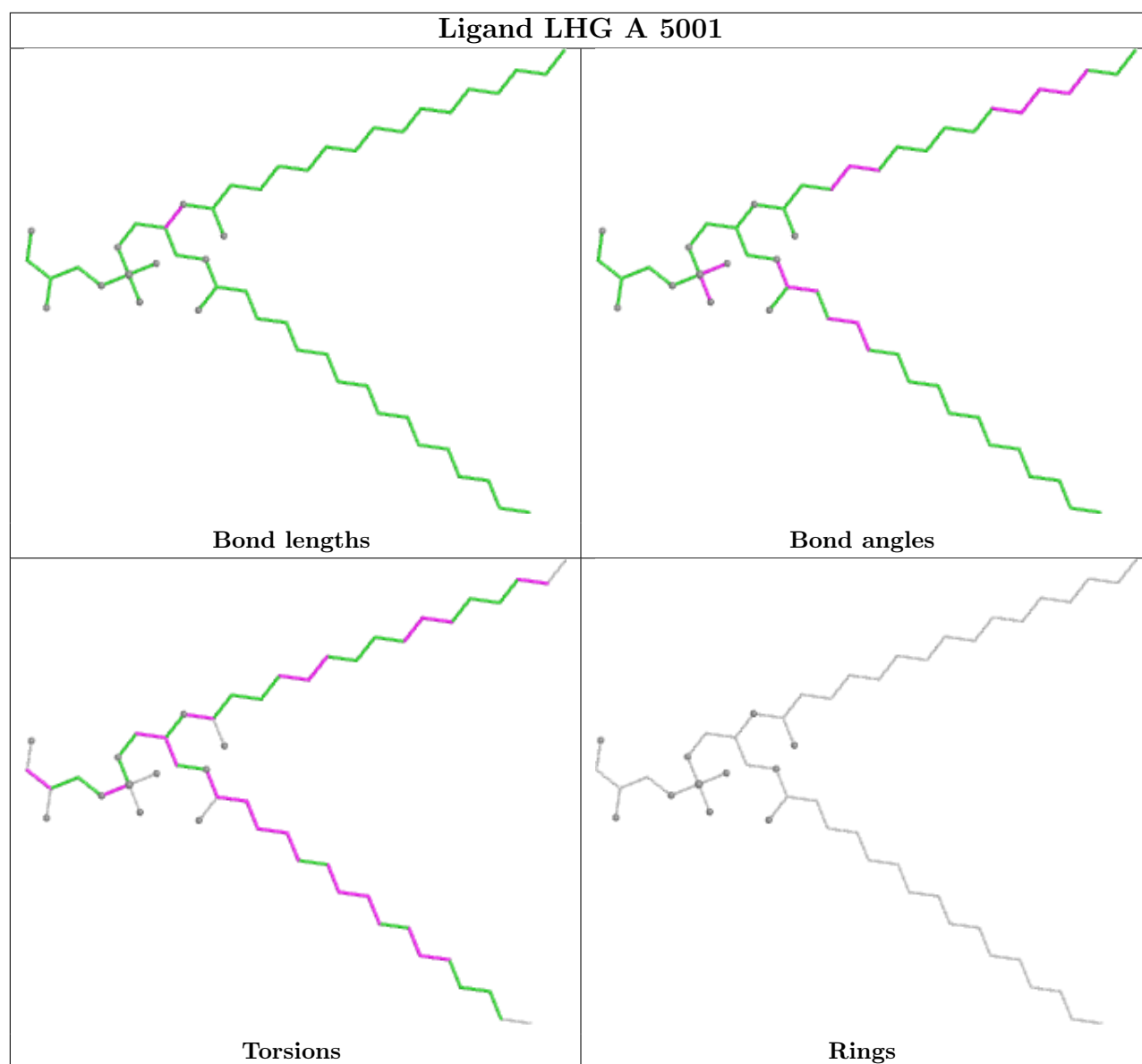
Ligand BCR 5 522

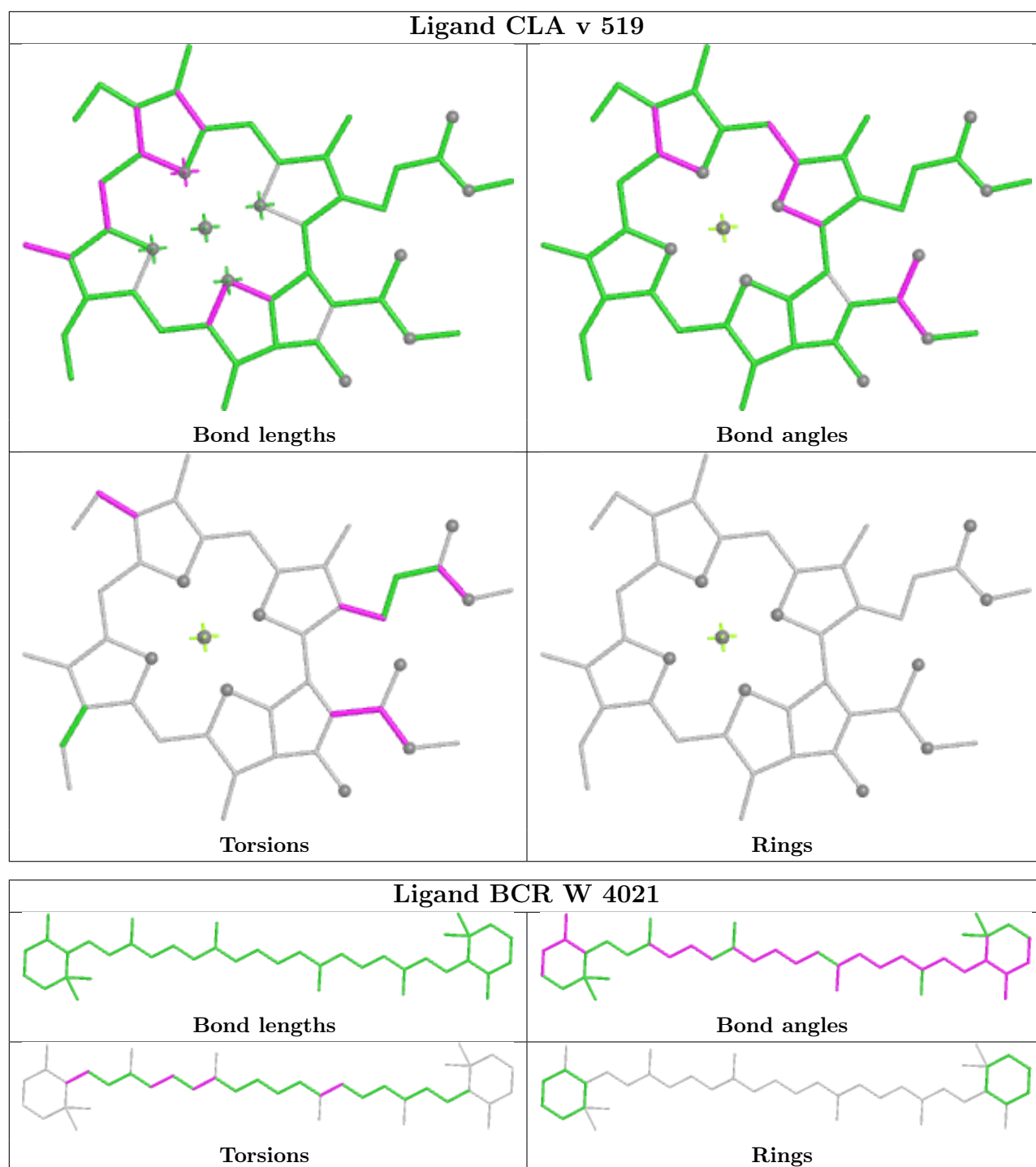




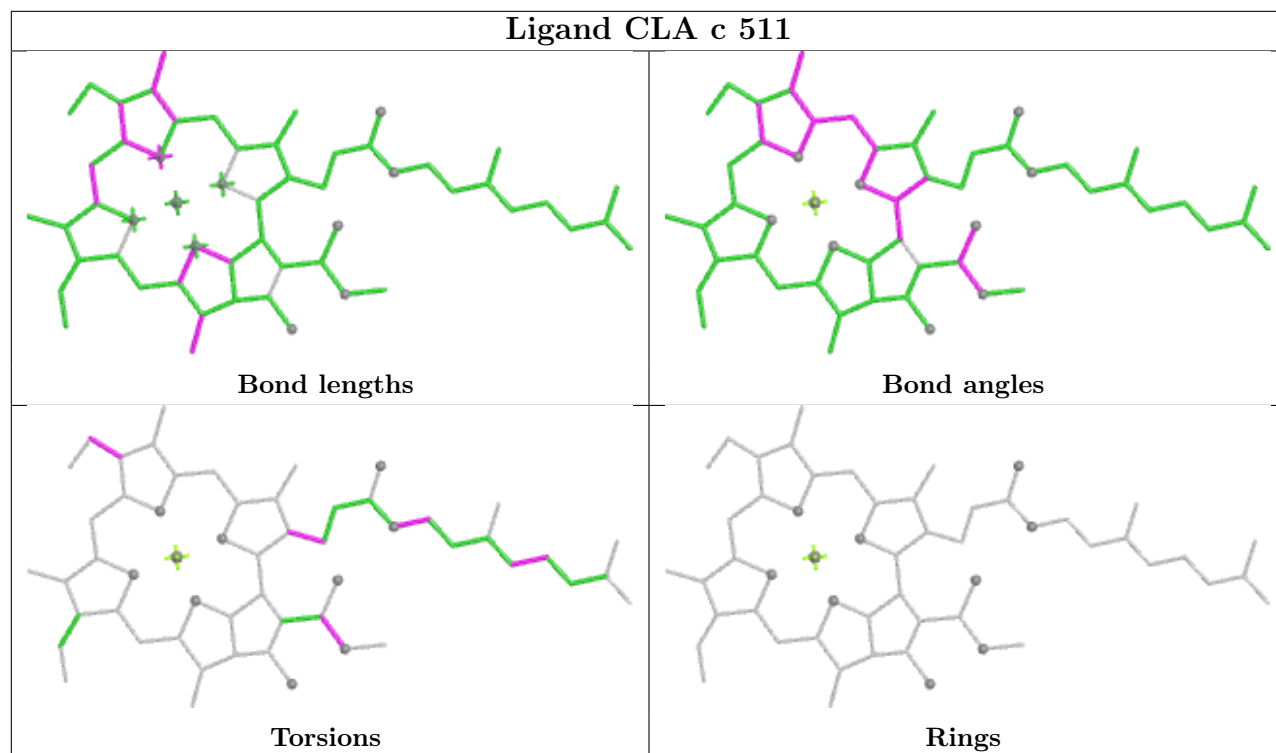




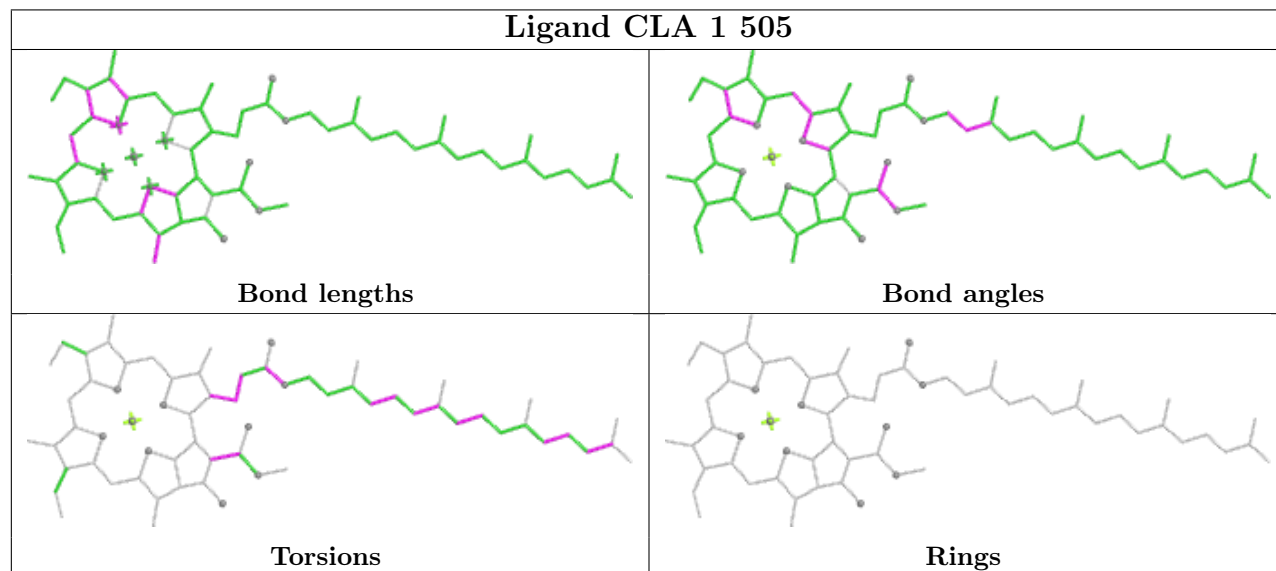




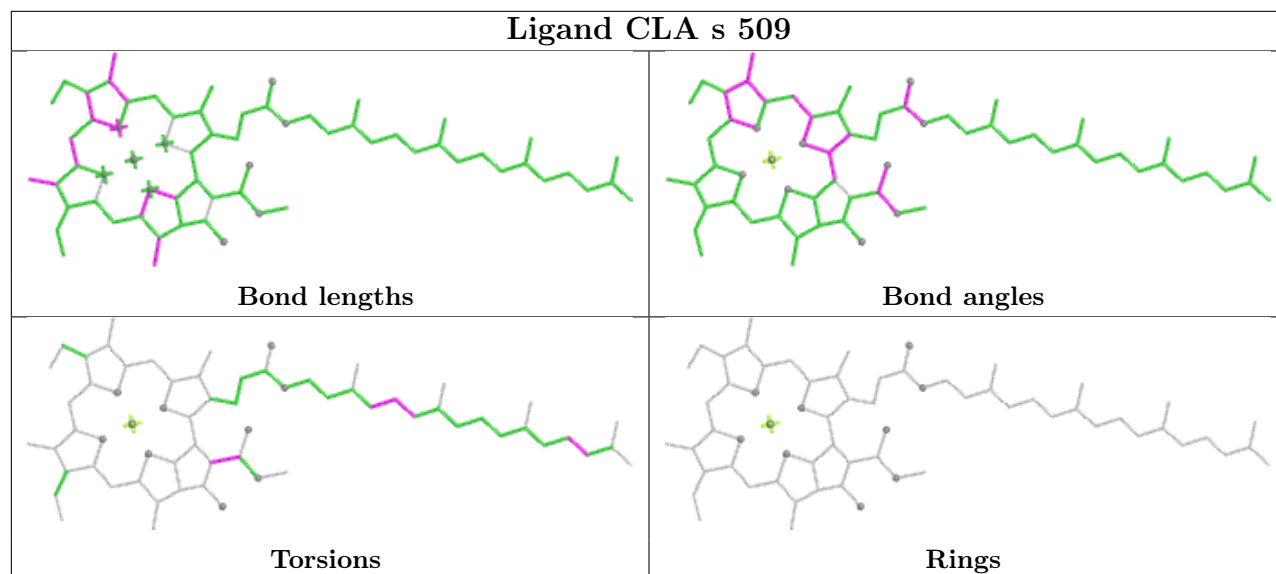
Ligand CLA c 511



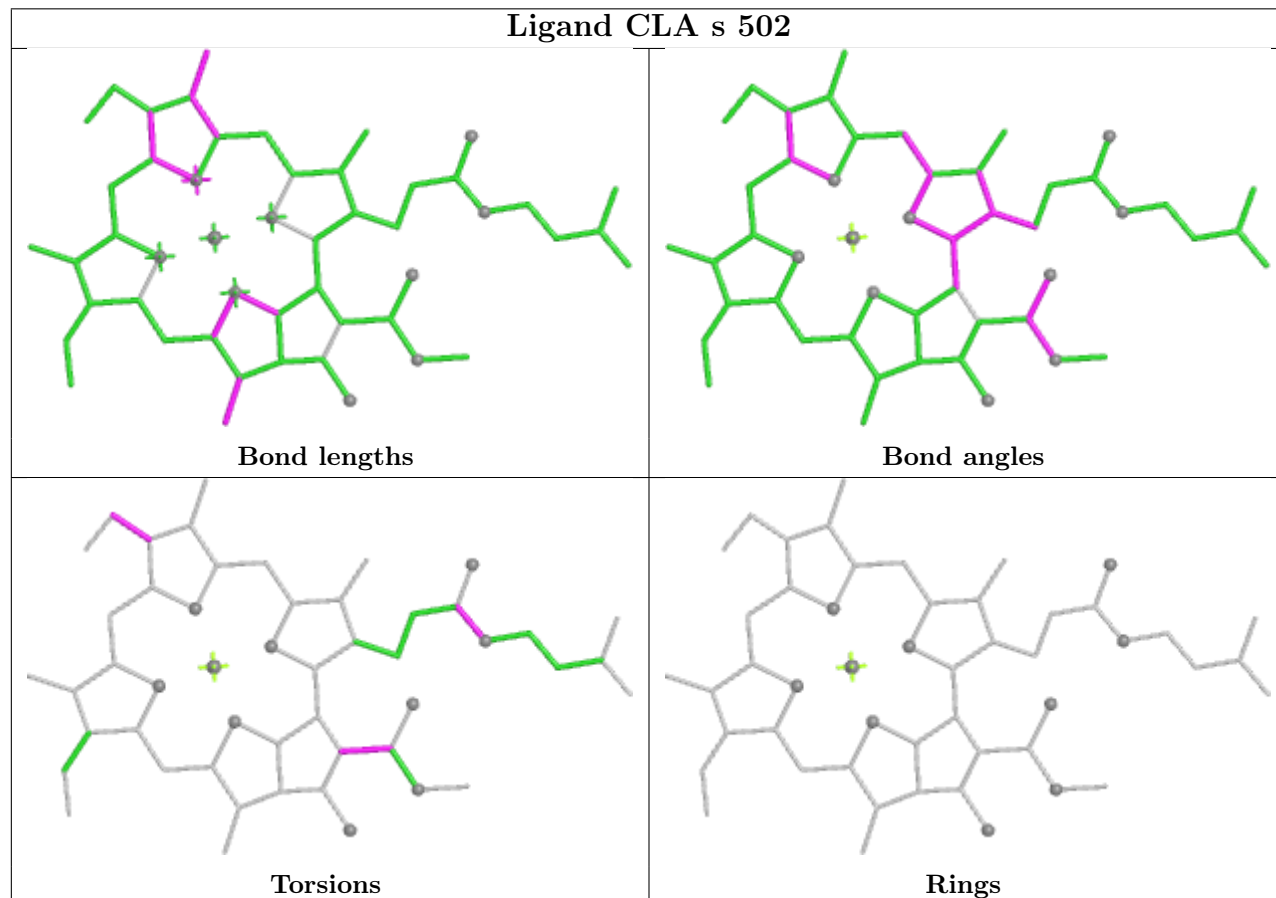
Ligand CLA 1 505

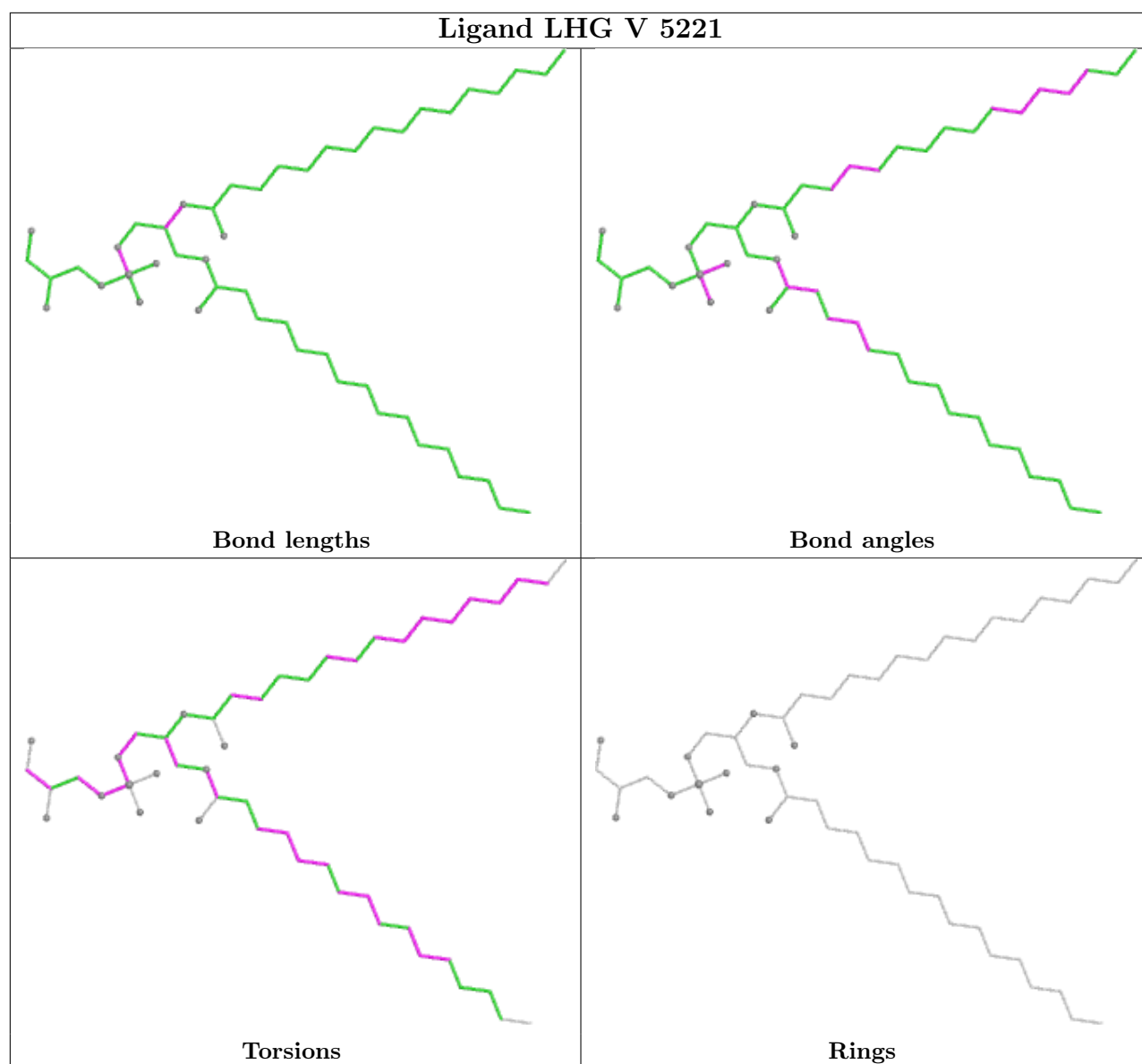


Ligand CLA s 509

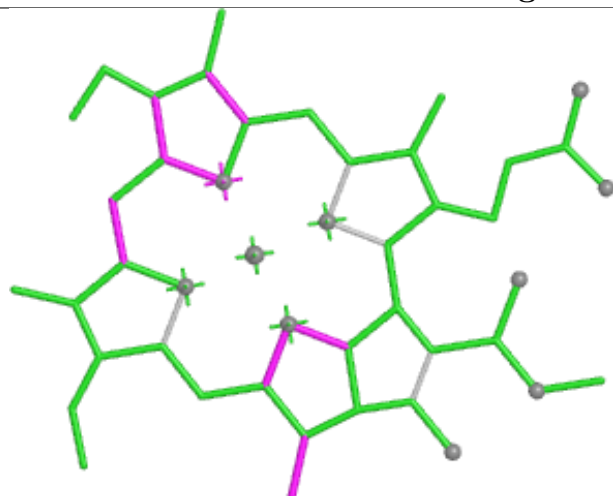


Ligand CLA s 502

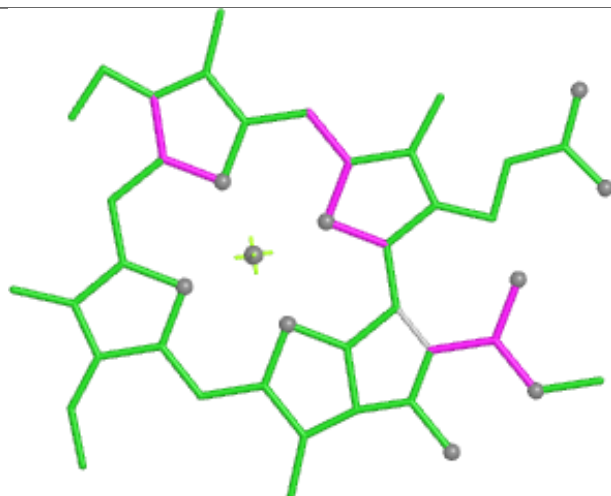




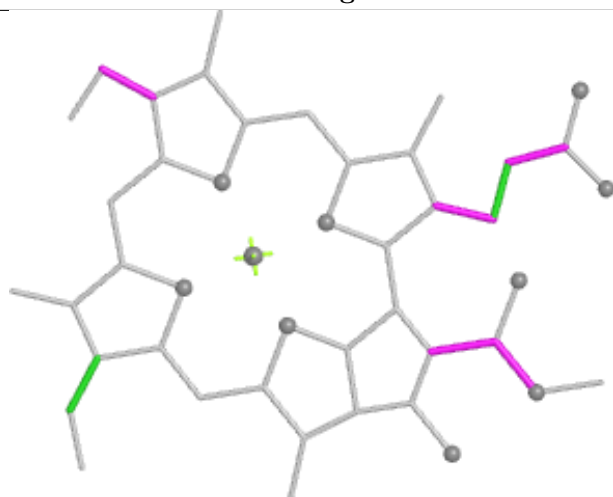
Ligand CLA 2 516



Bond lengths



Bond angles

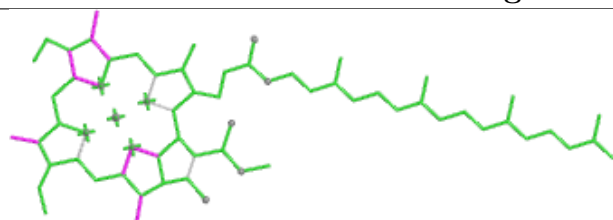


Torsions

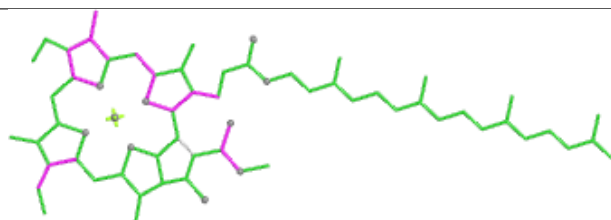


Rings

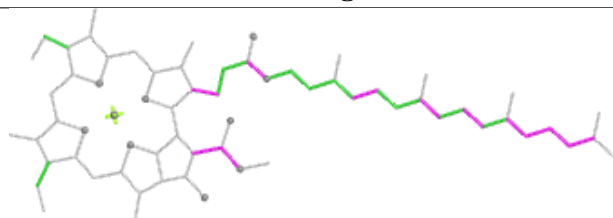
Ligand CLA G 1103



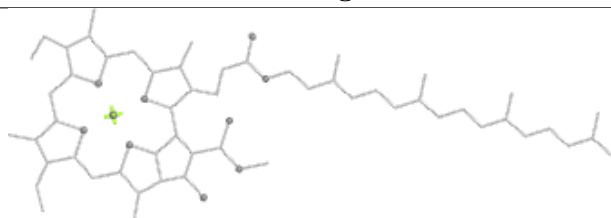
Bond lengths



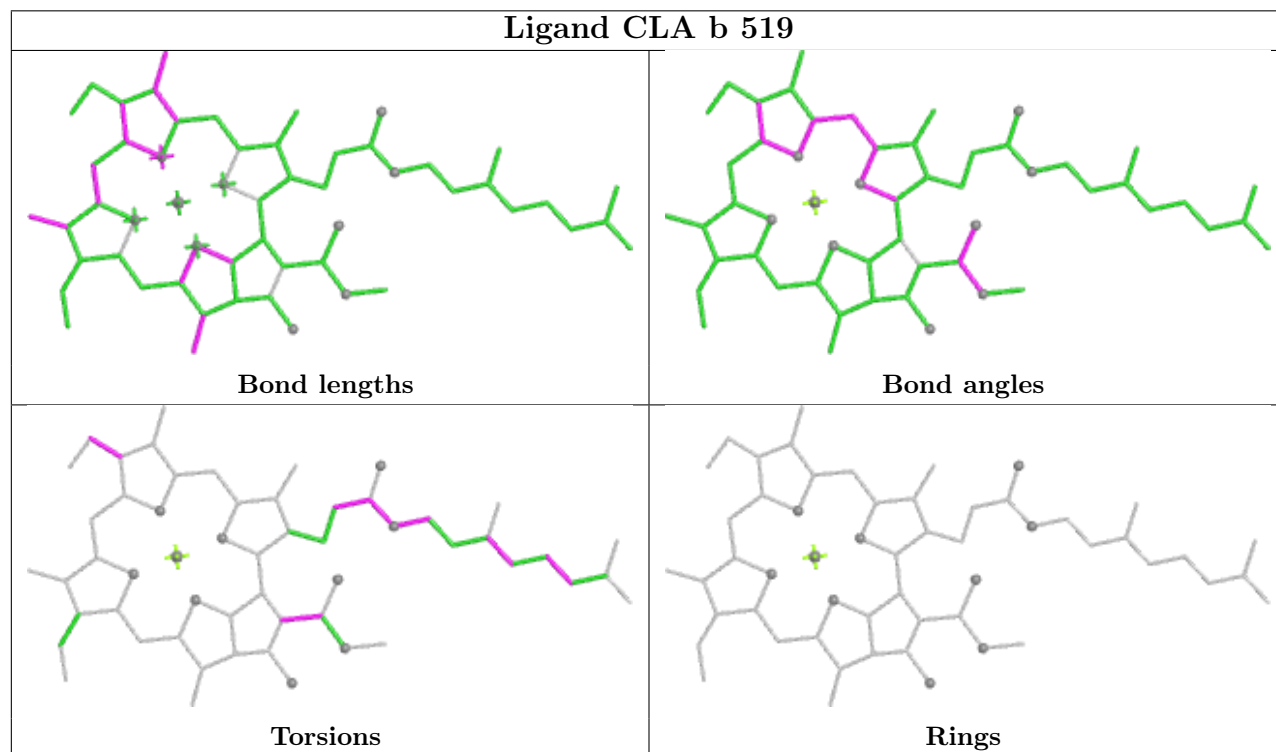
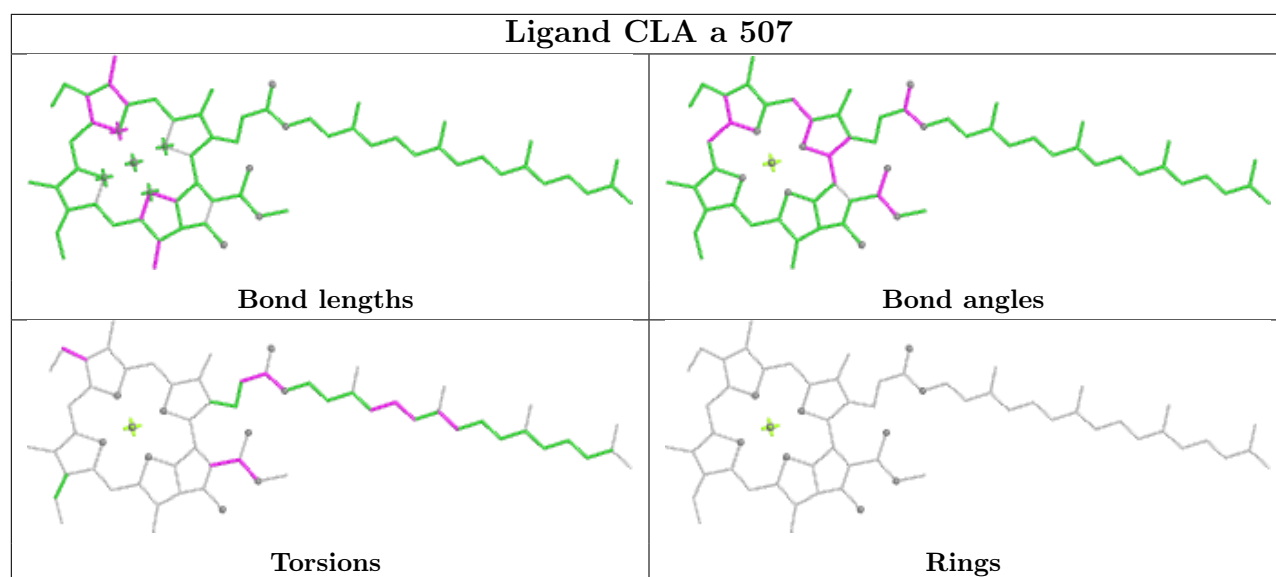
Bond angles

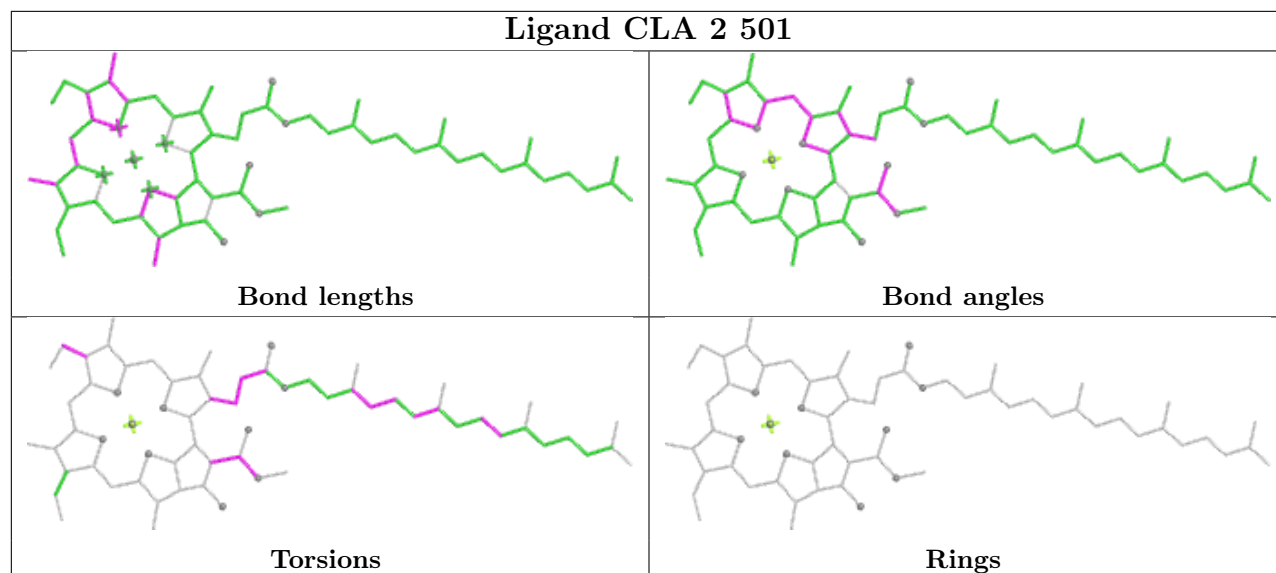
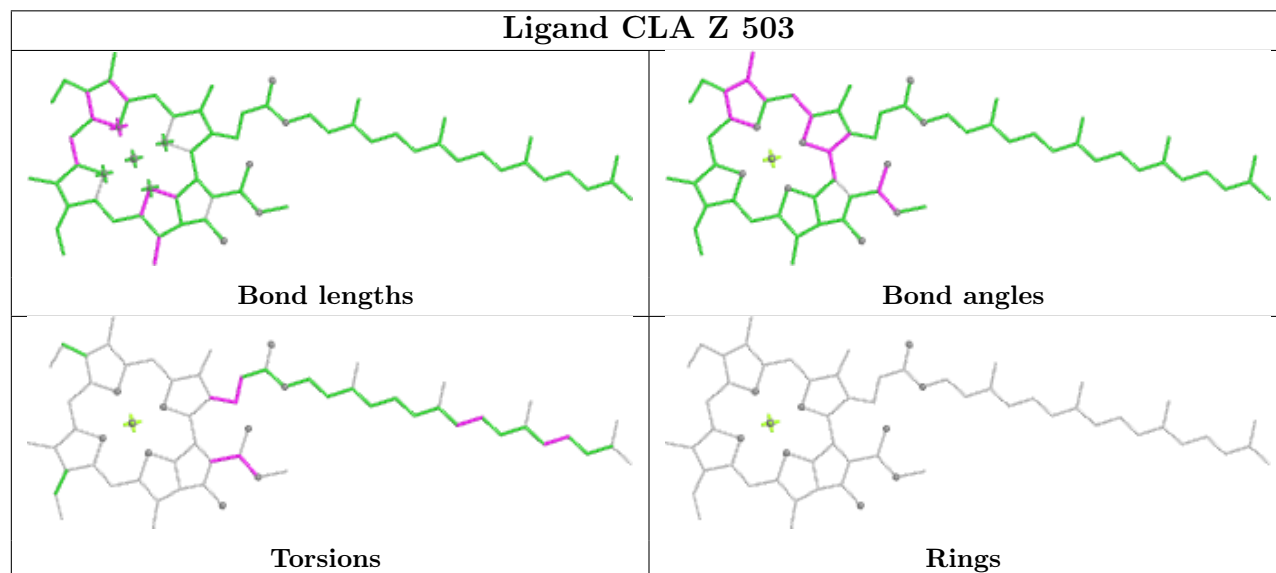
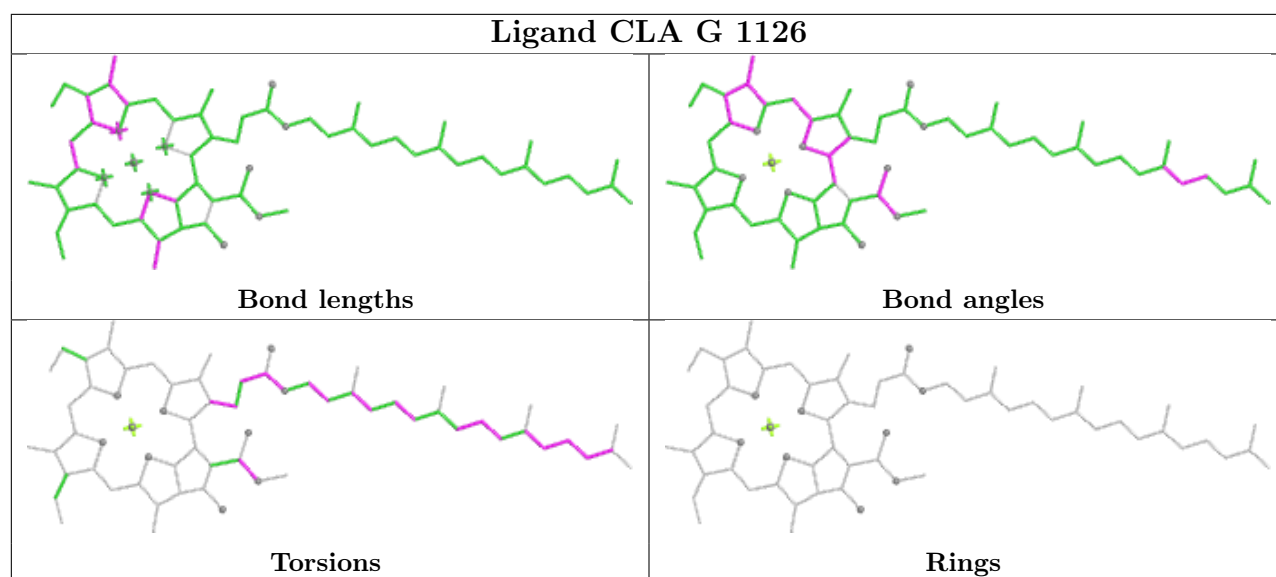


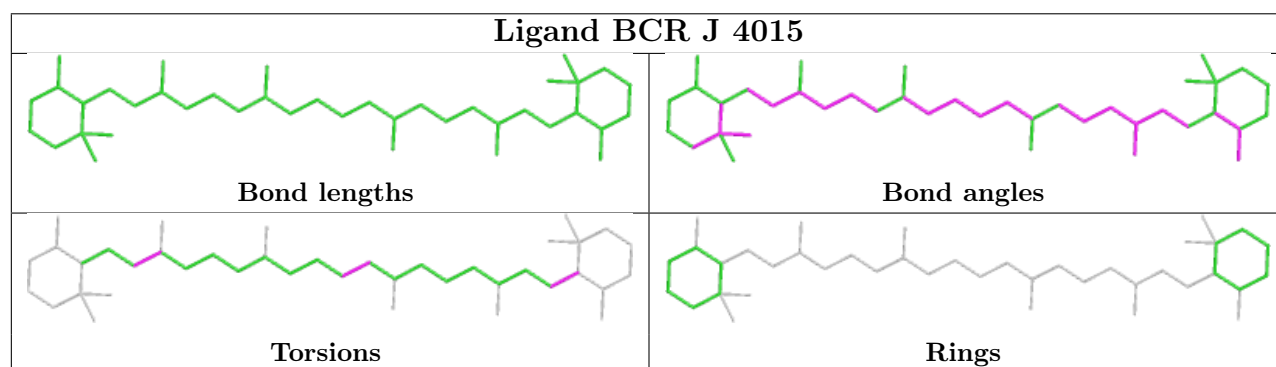
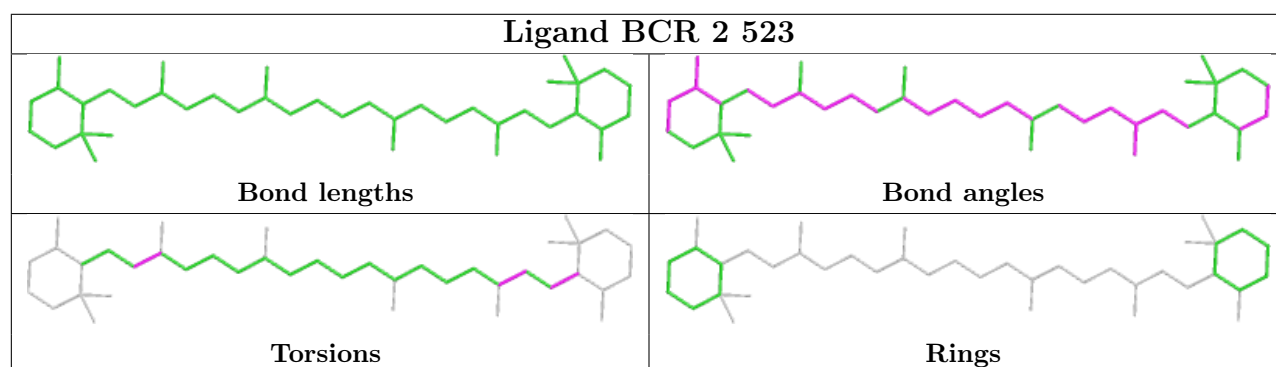
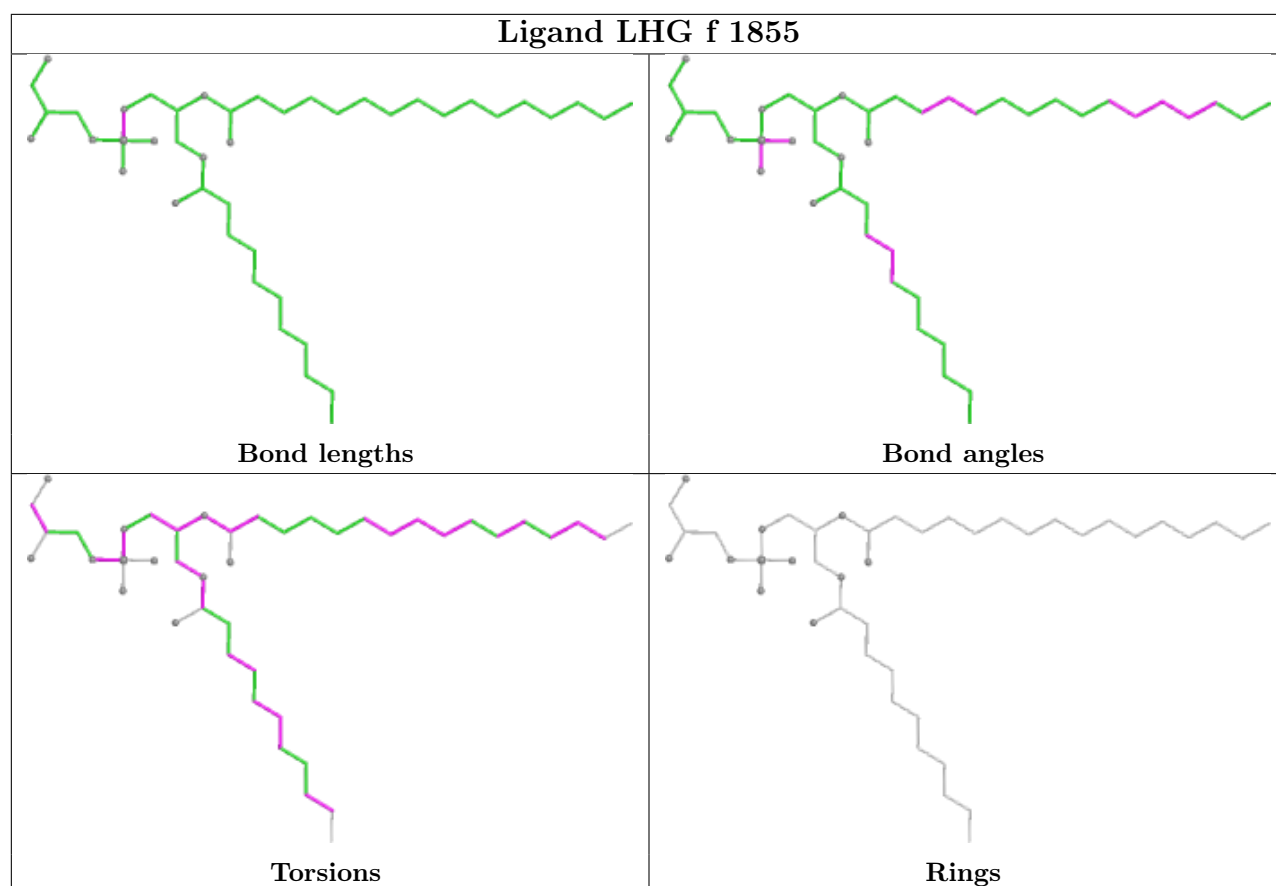
Torsions



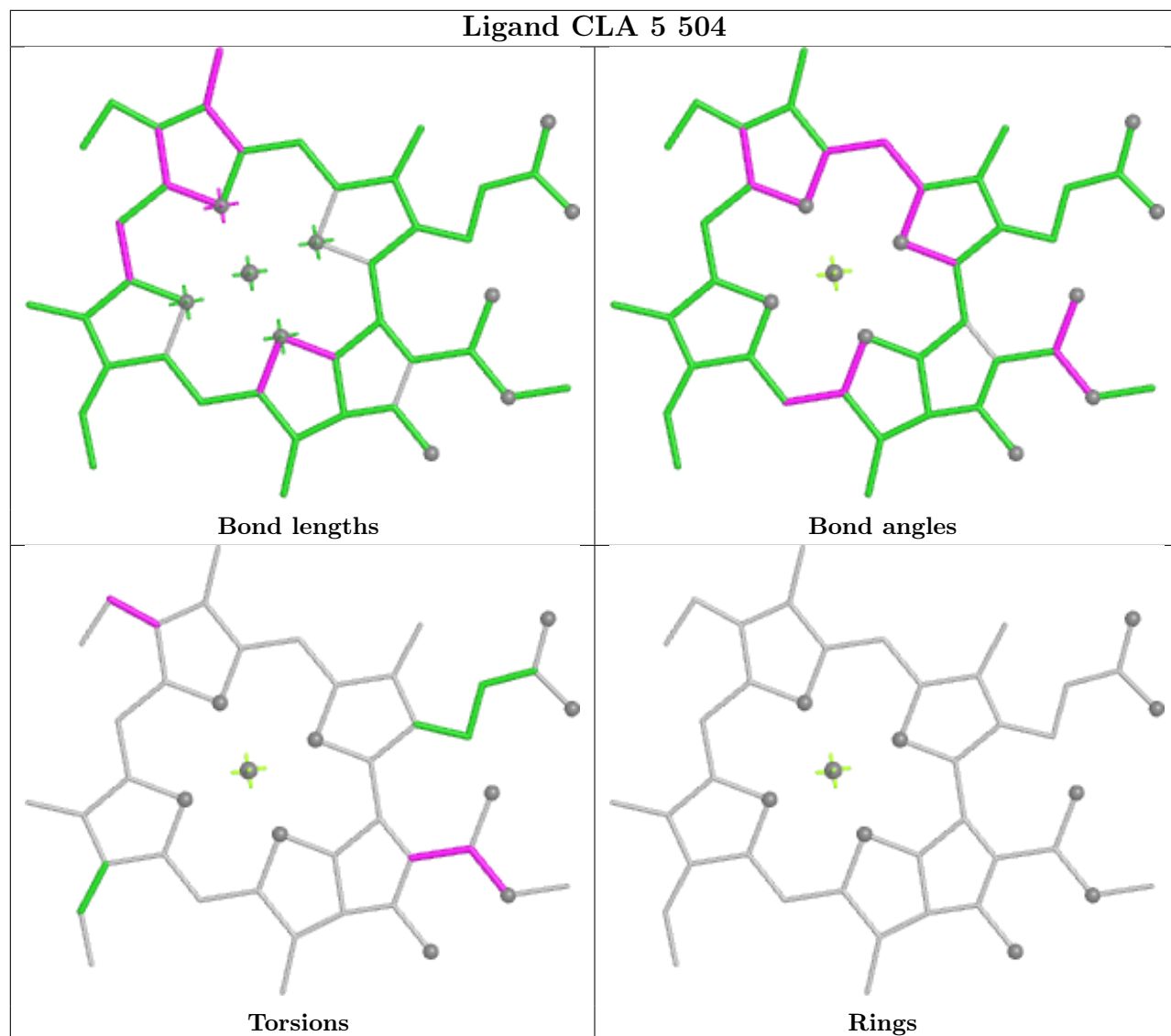
Rings



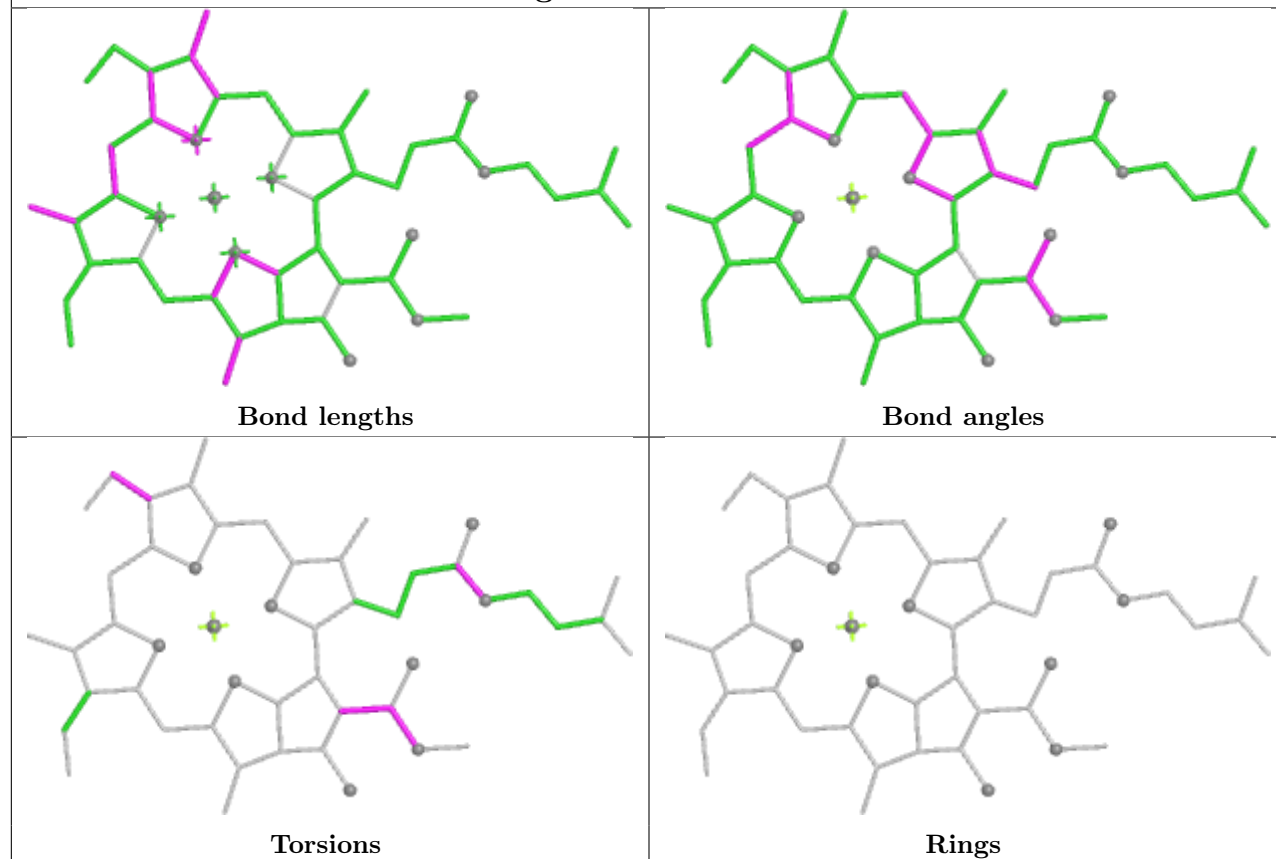




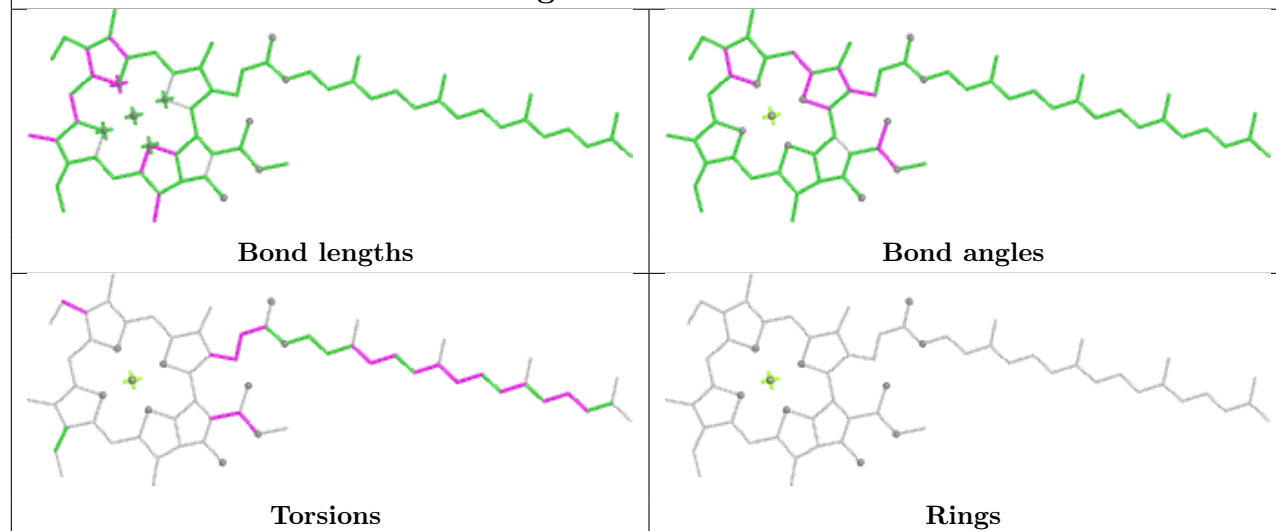
Ligand CLA 5 504

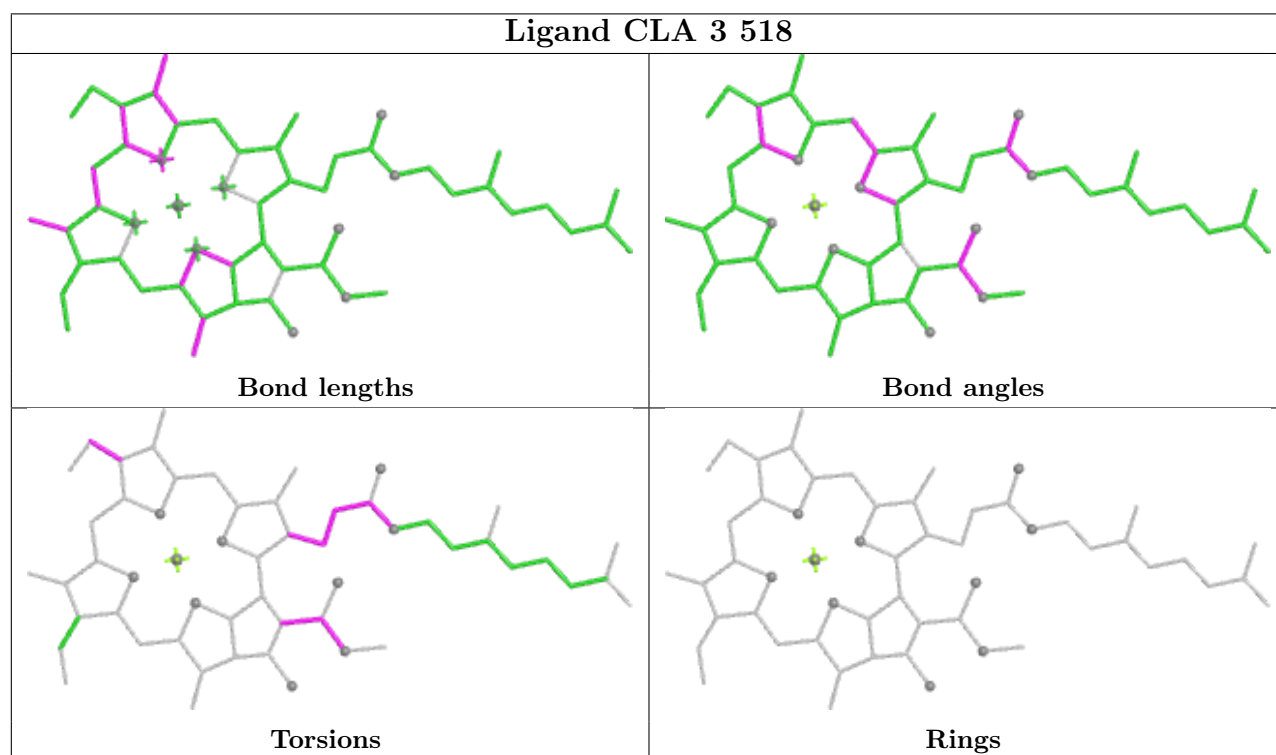
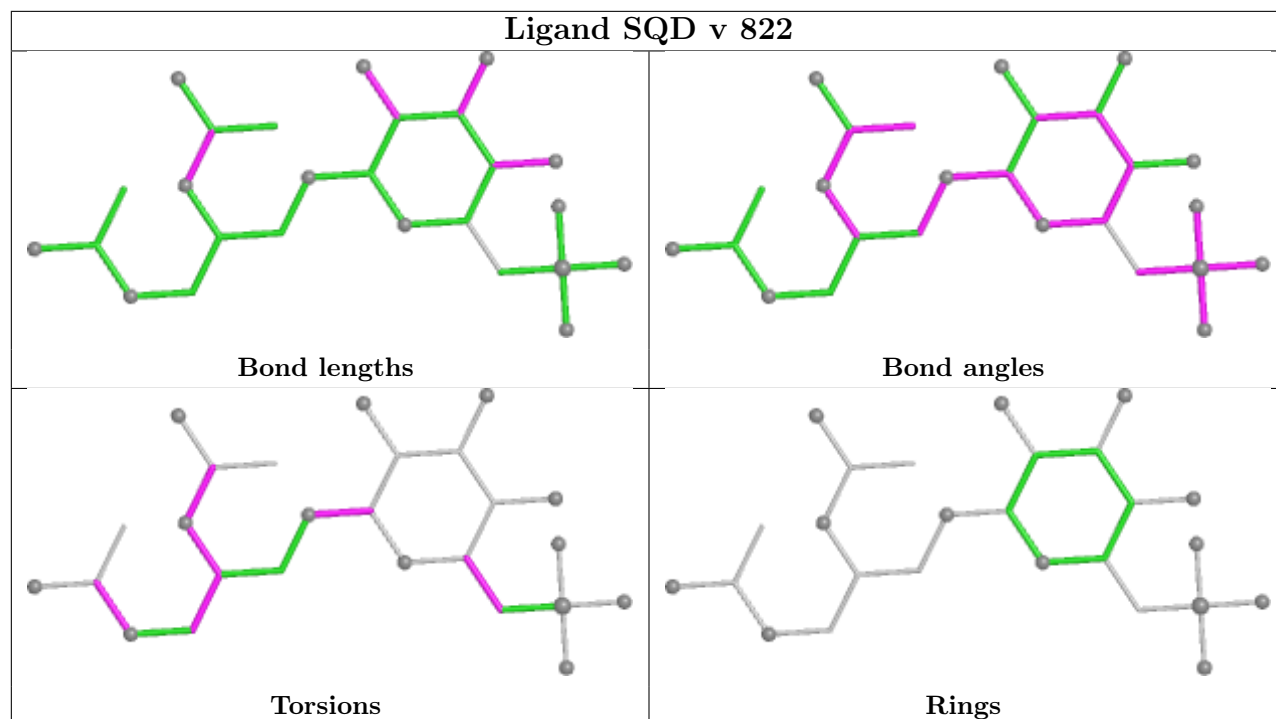


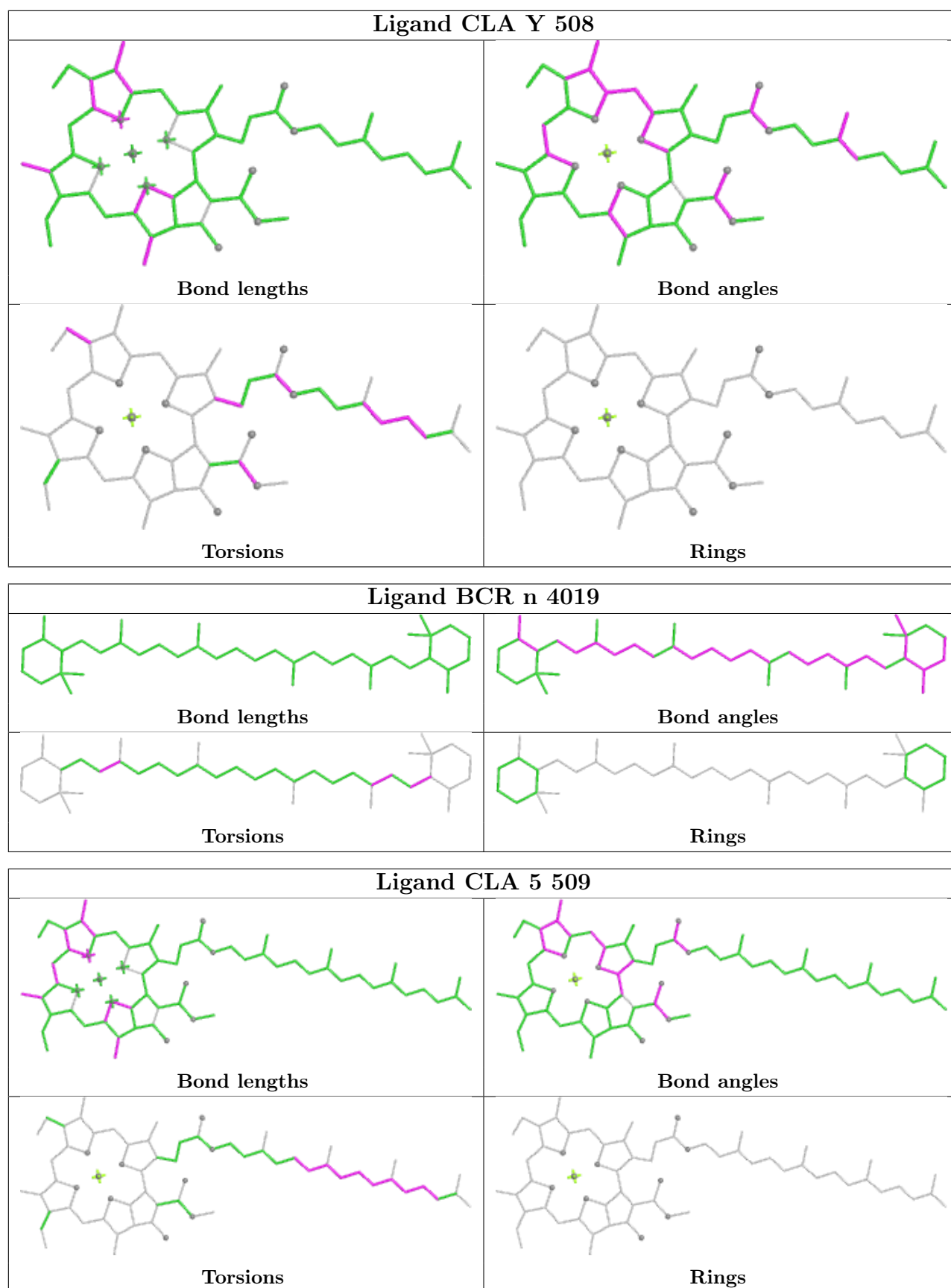
Ligand CLA u 502

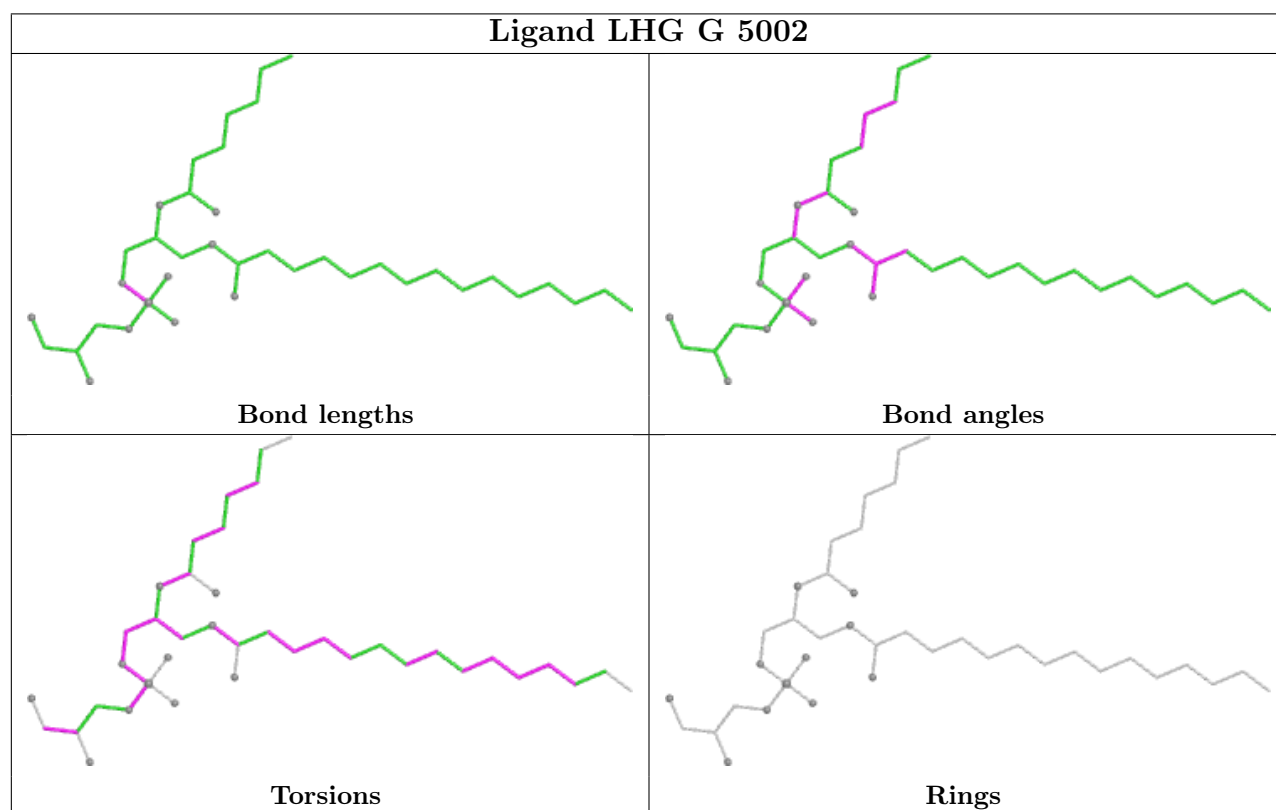
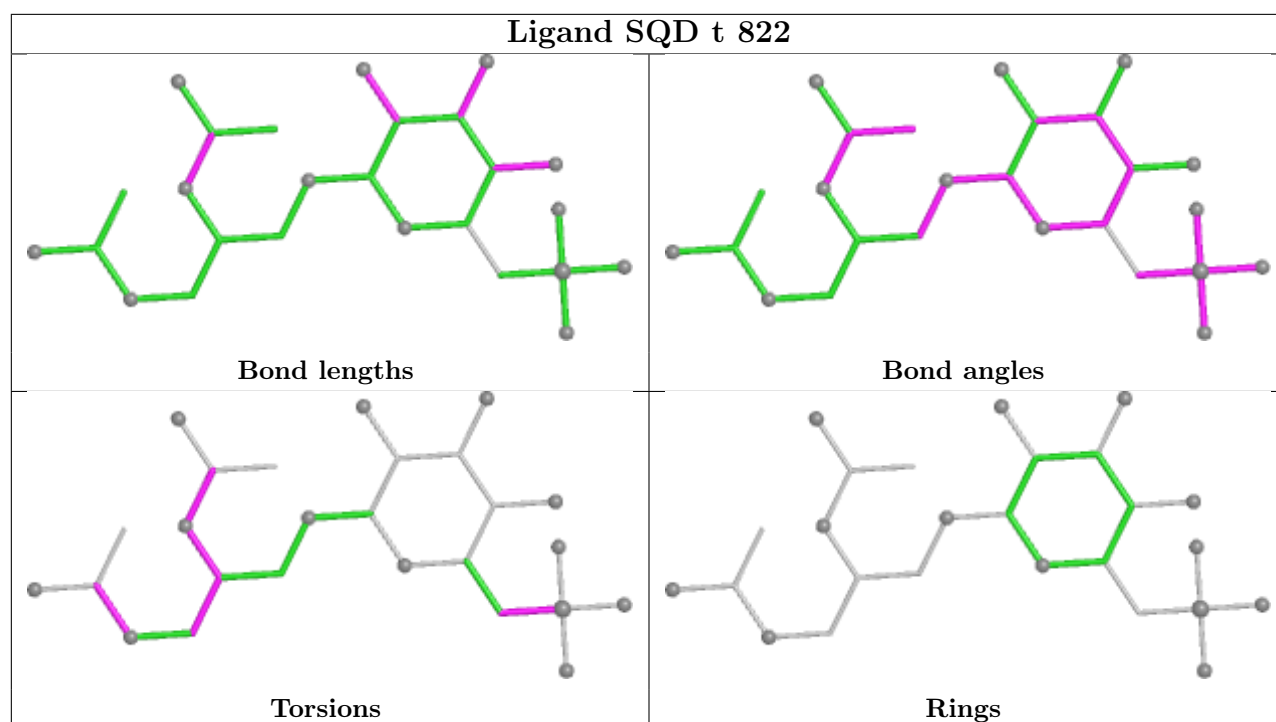


Ligand CLA c 501

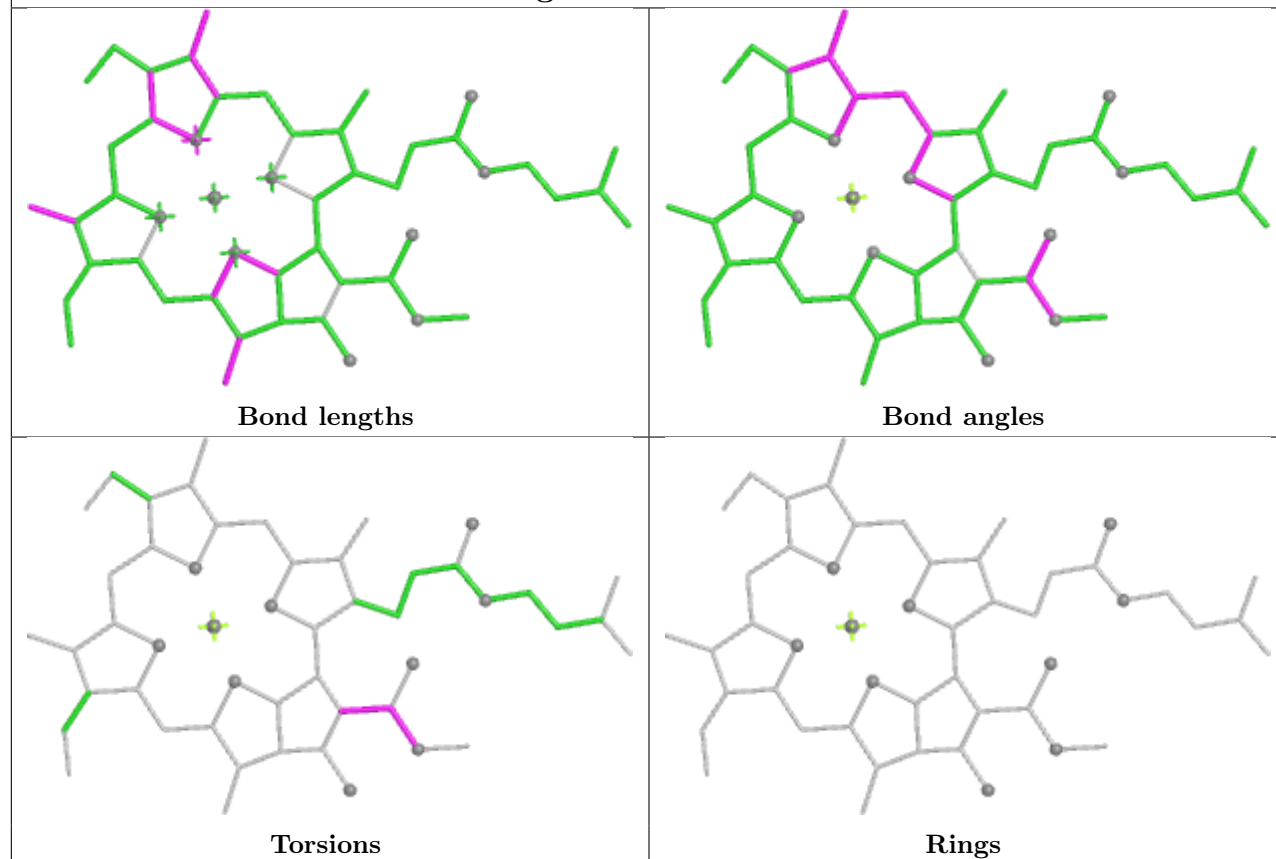




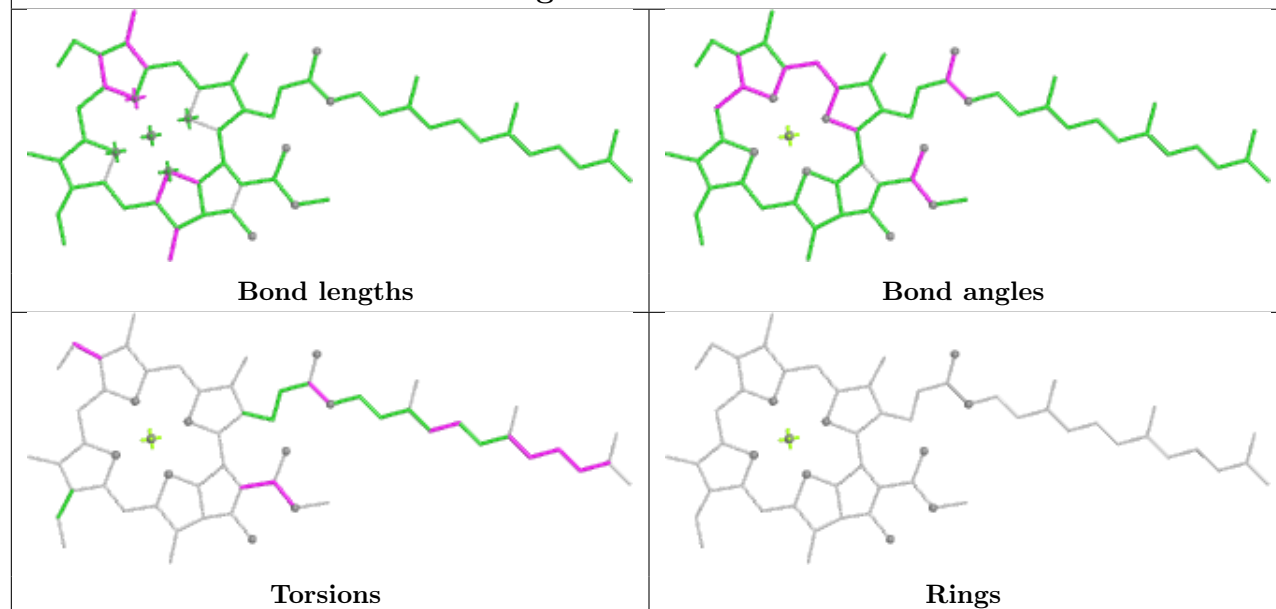


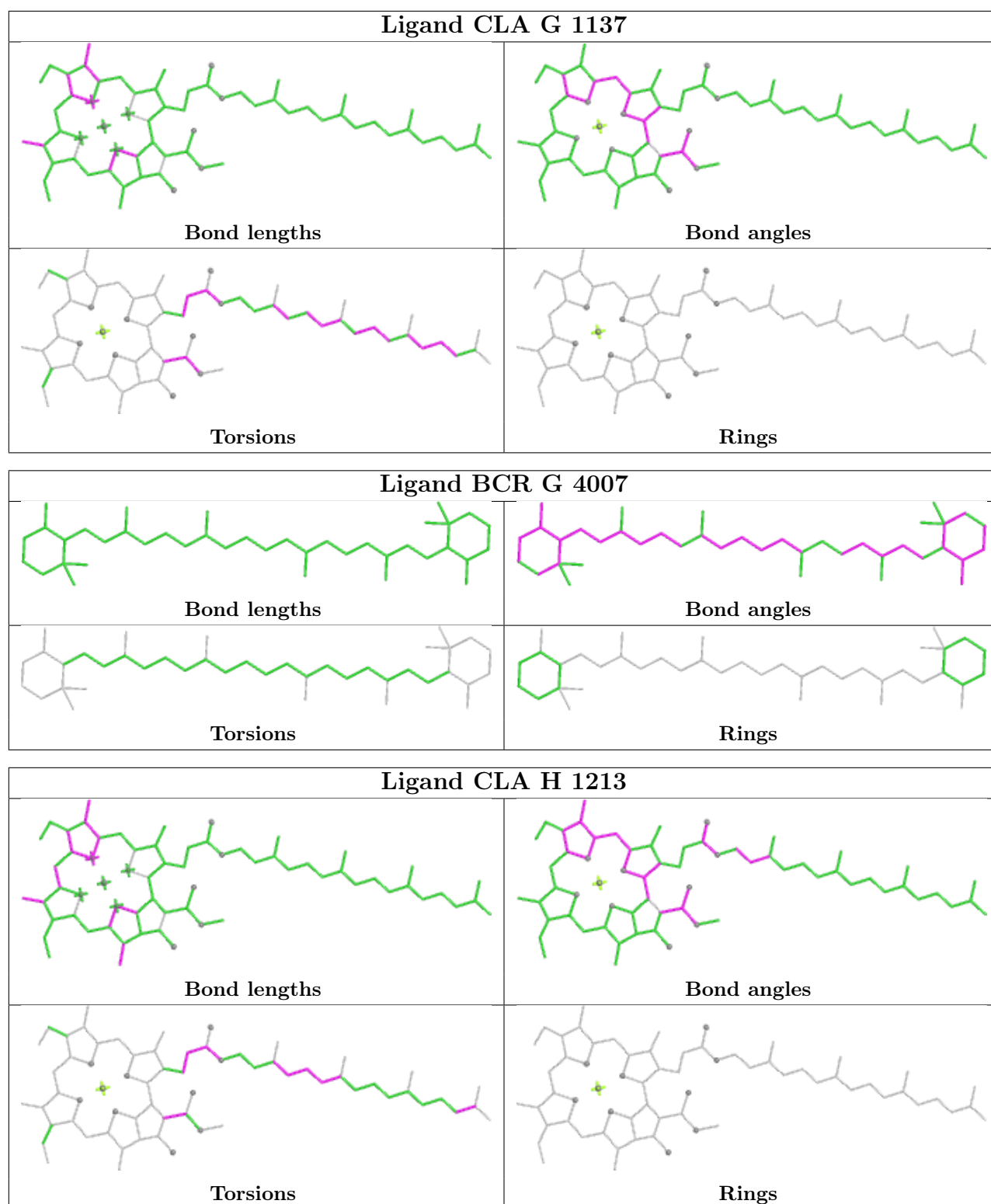


Ligand CLA 3 506

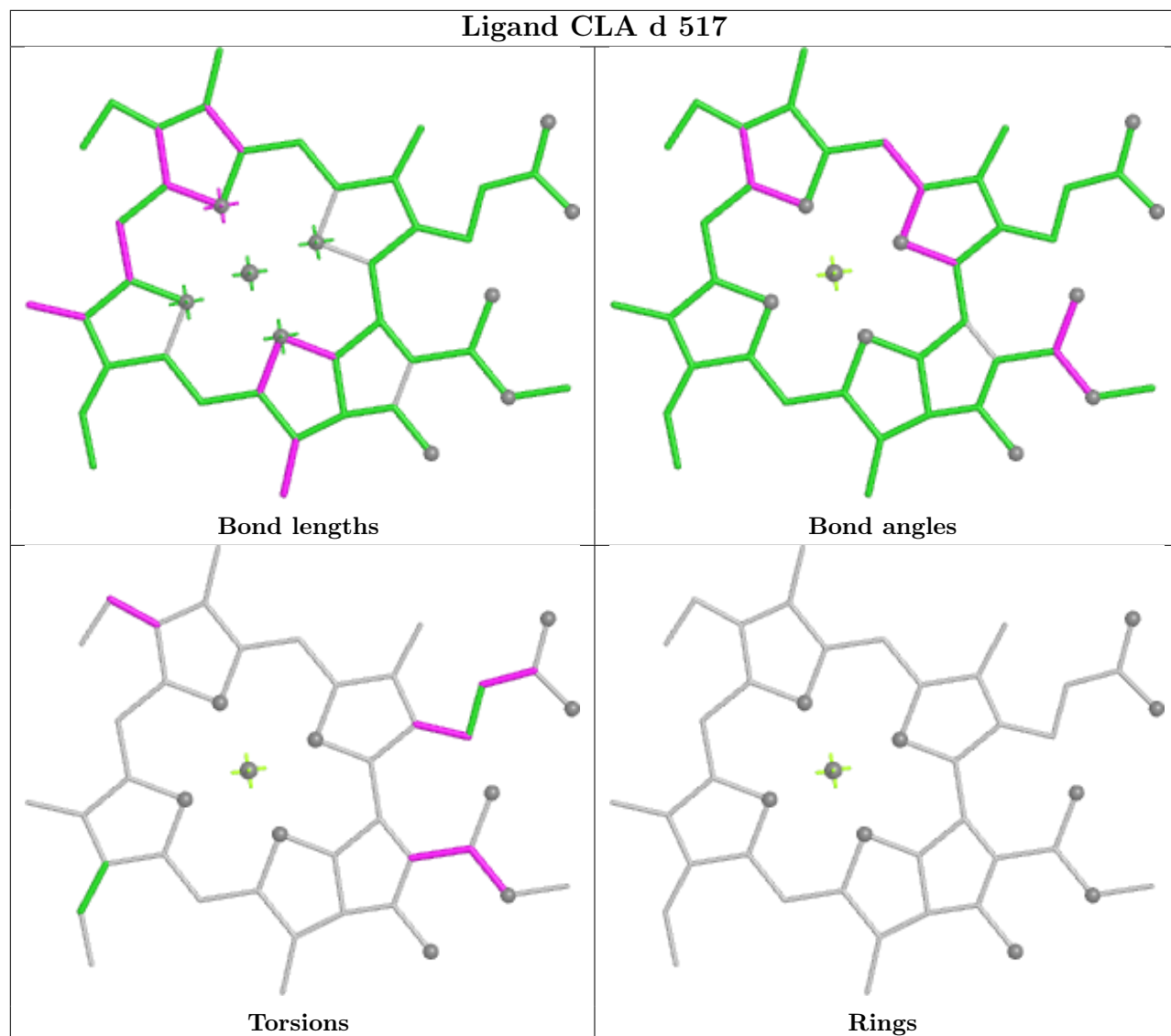


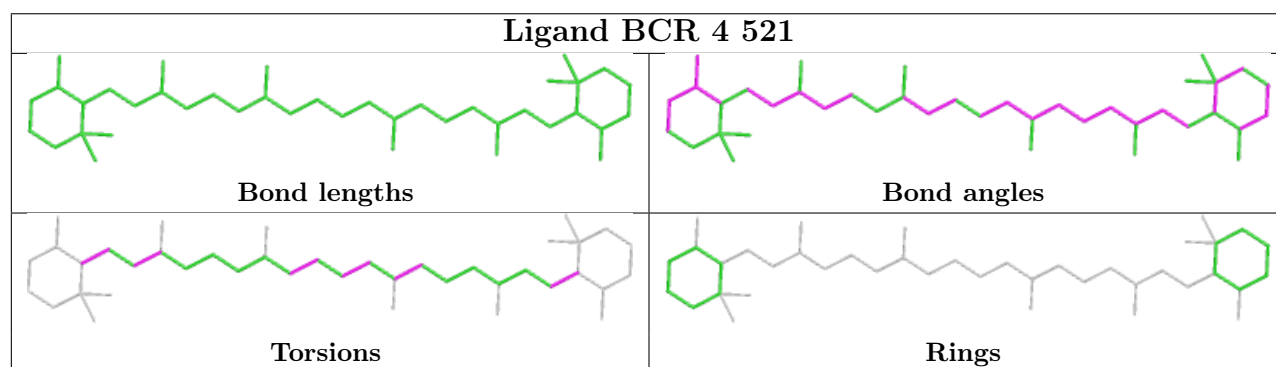
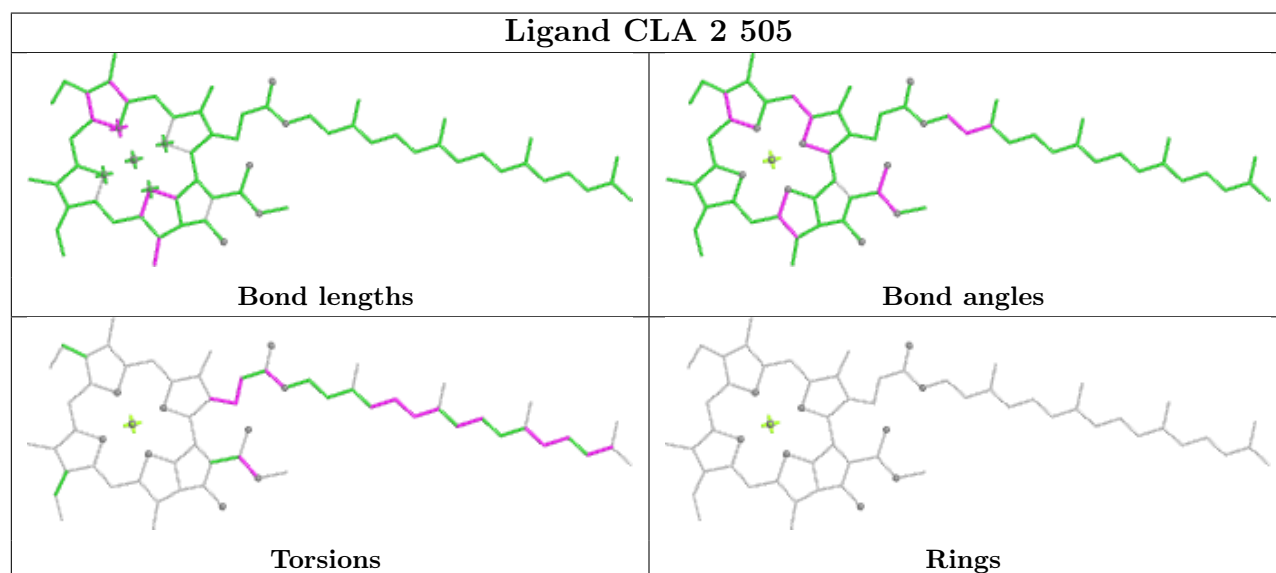
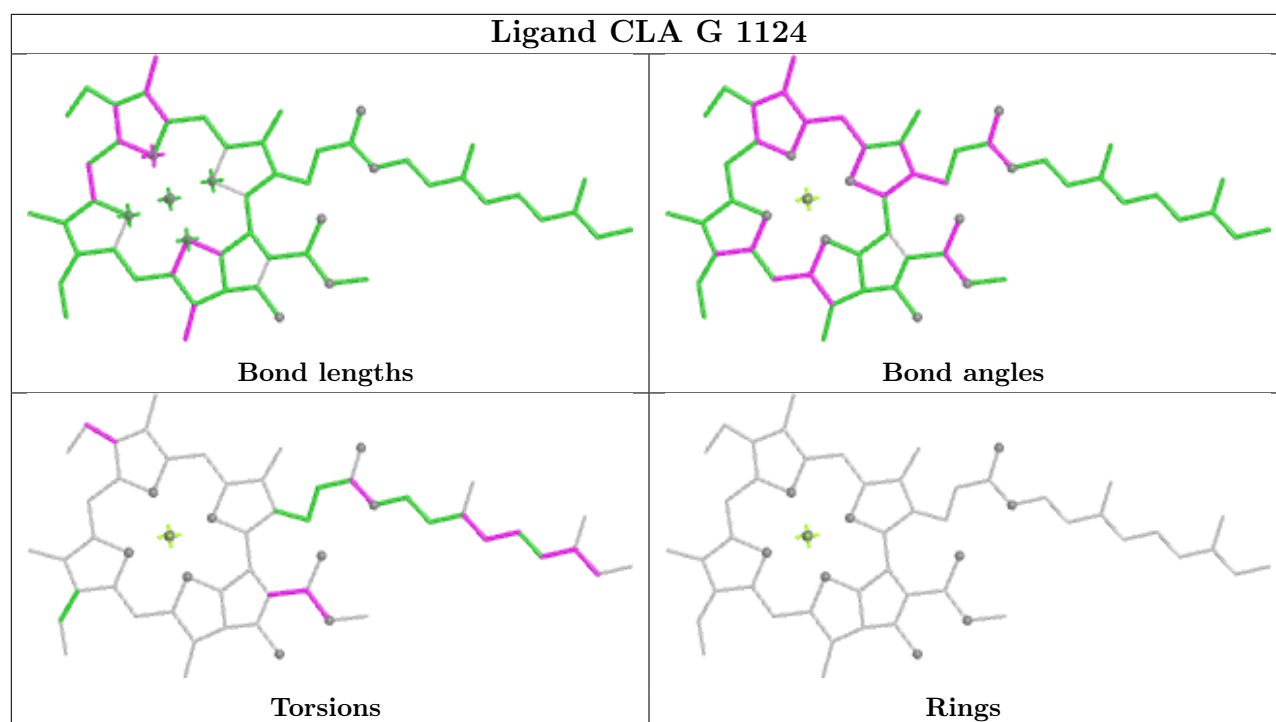
Ligand CLA 1 502

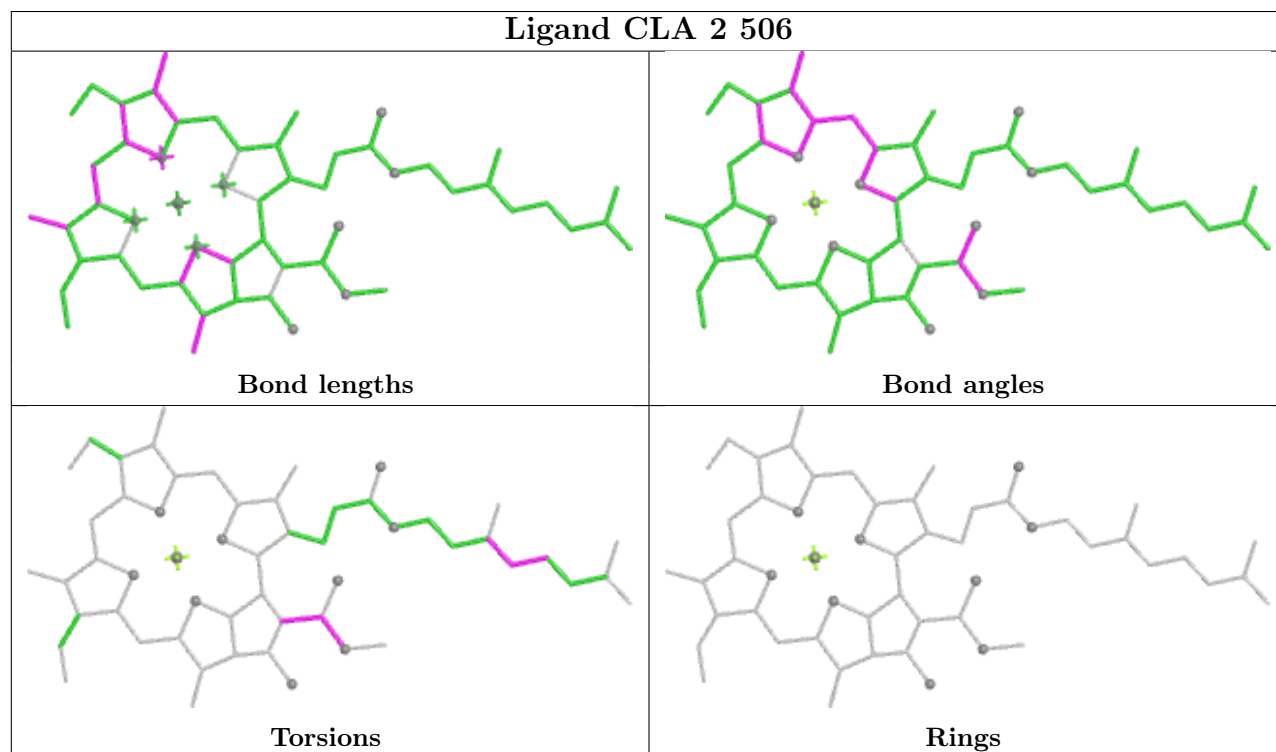
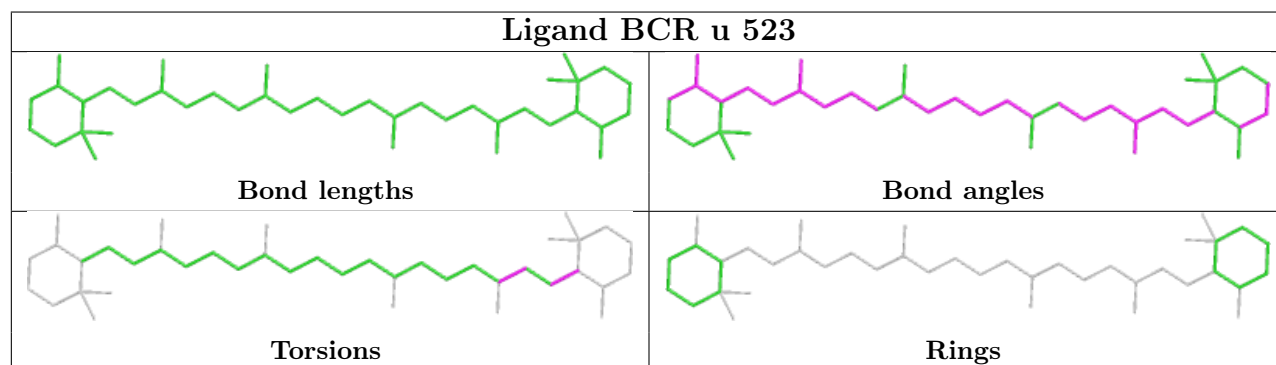
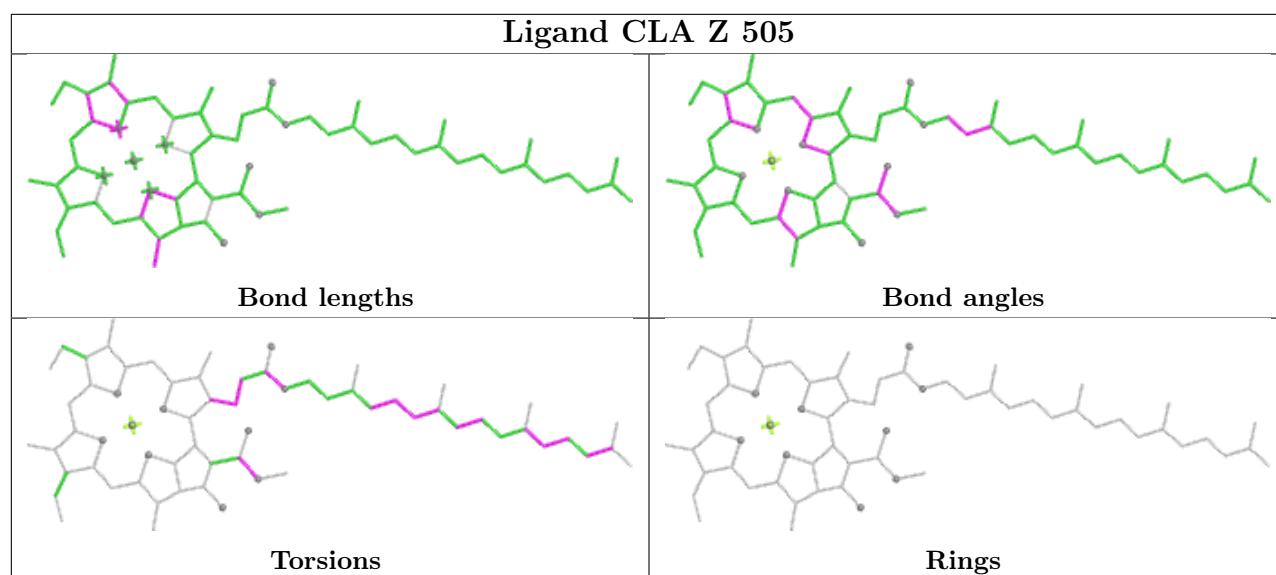


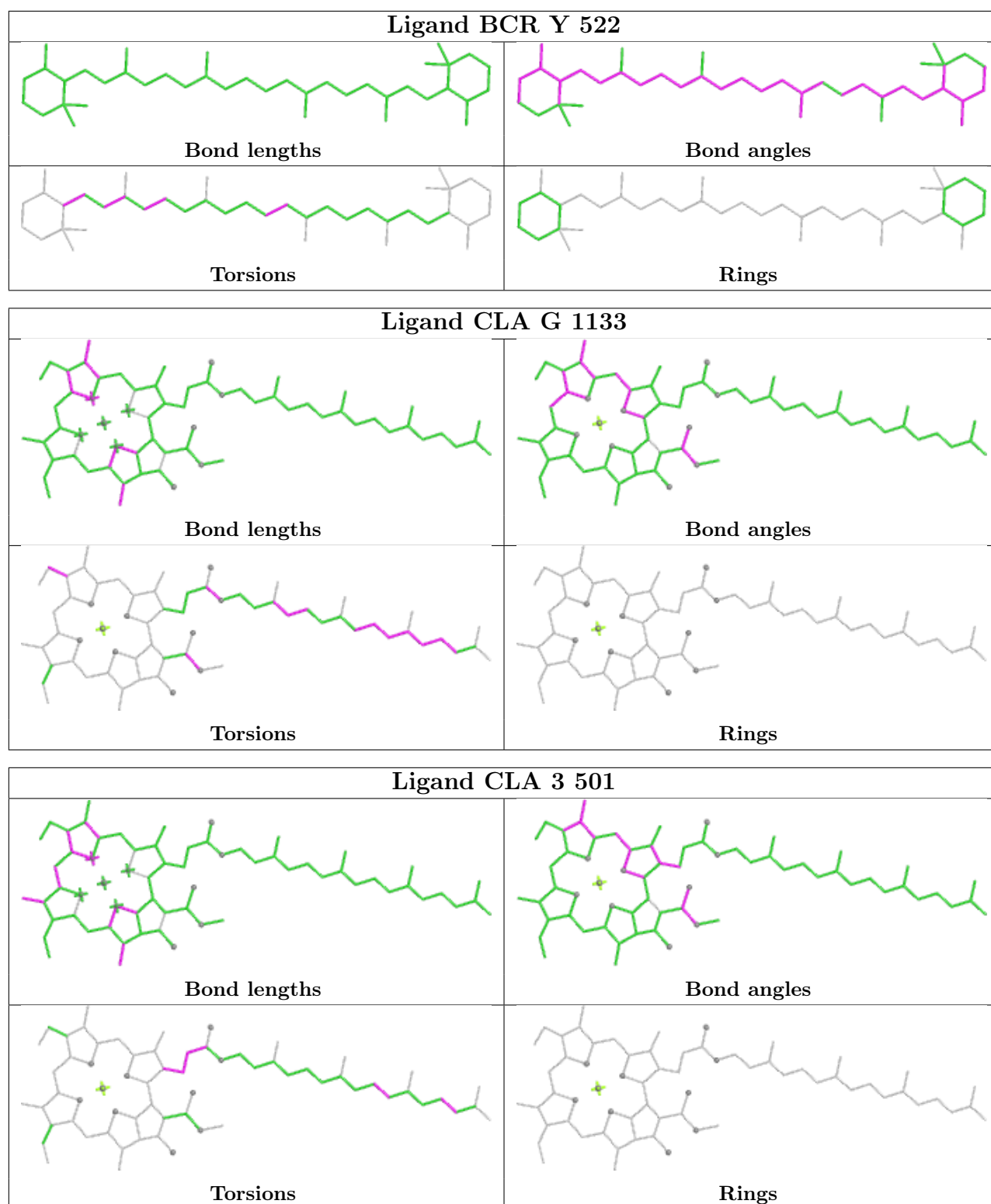


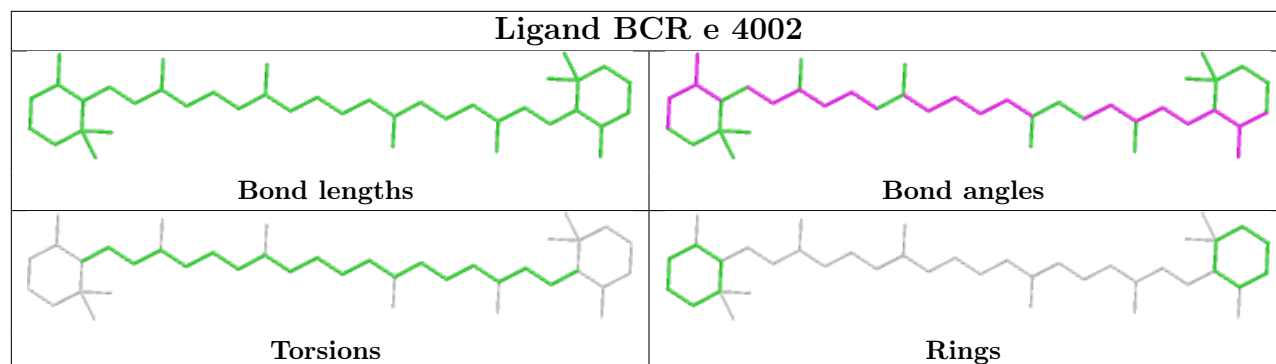
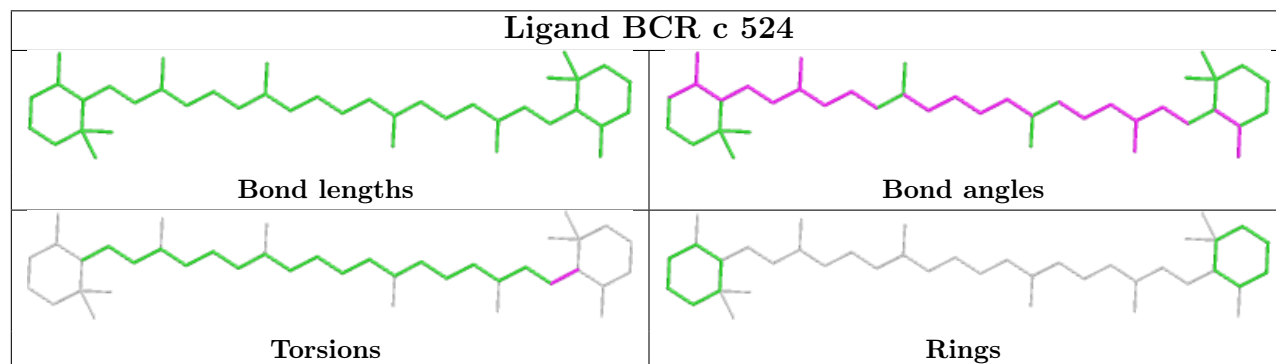
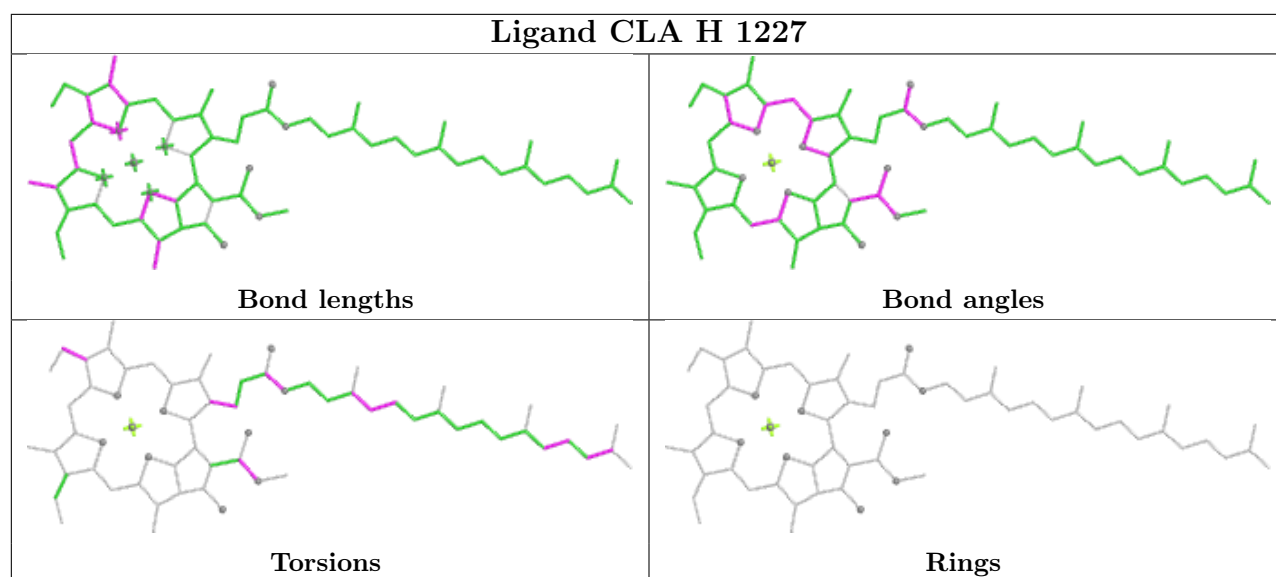
Ligand CLA d 517



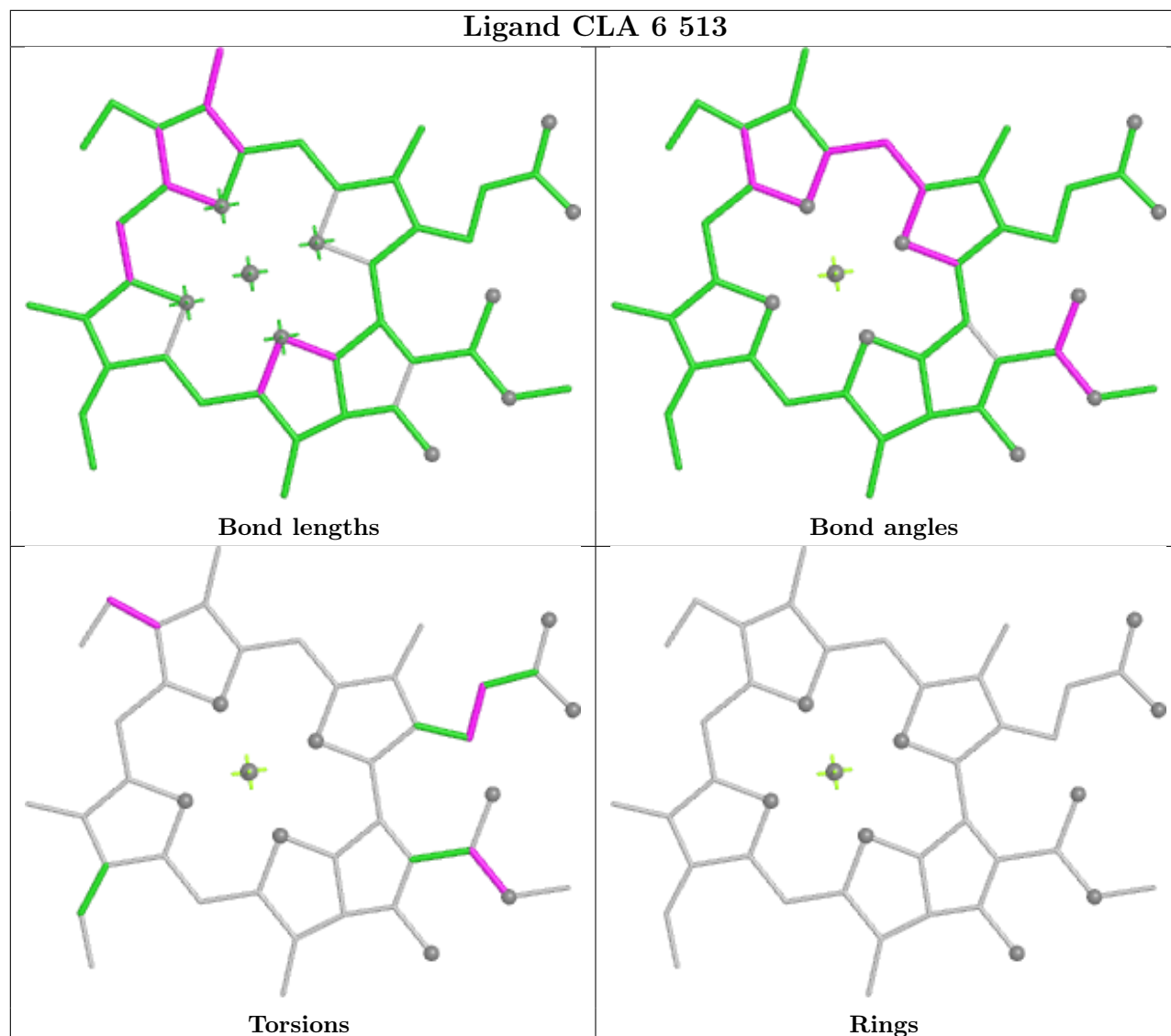




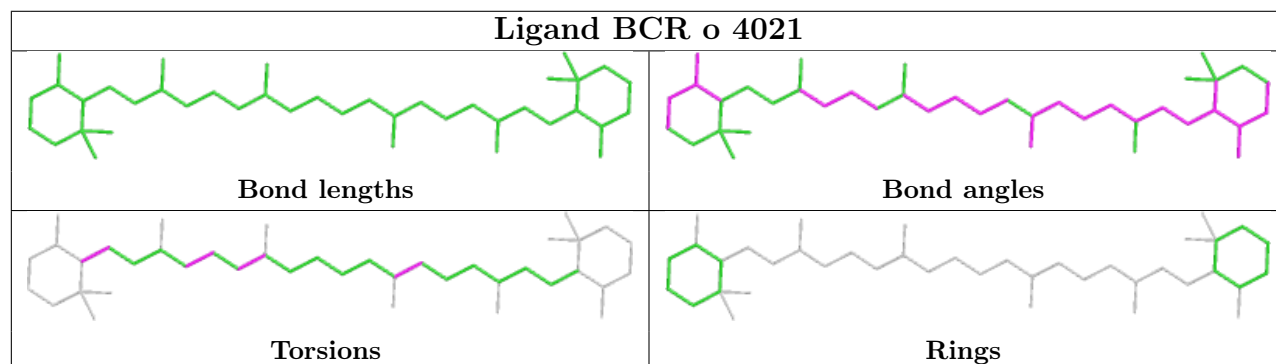


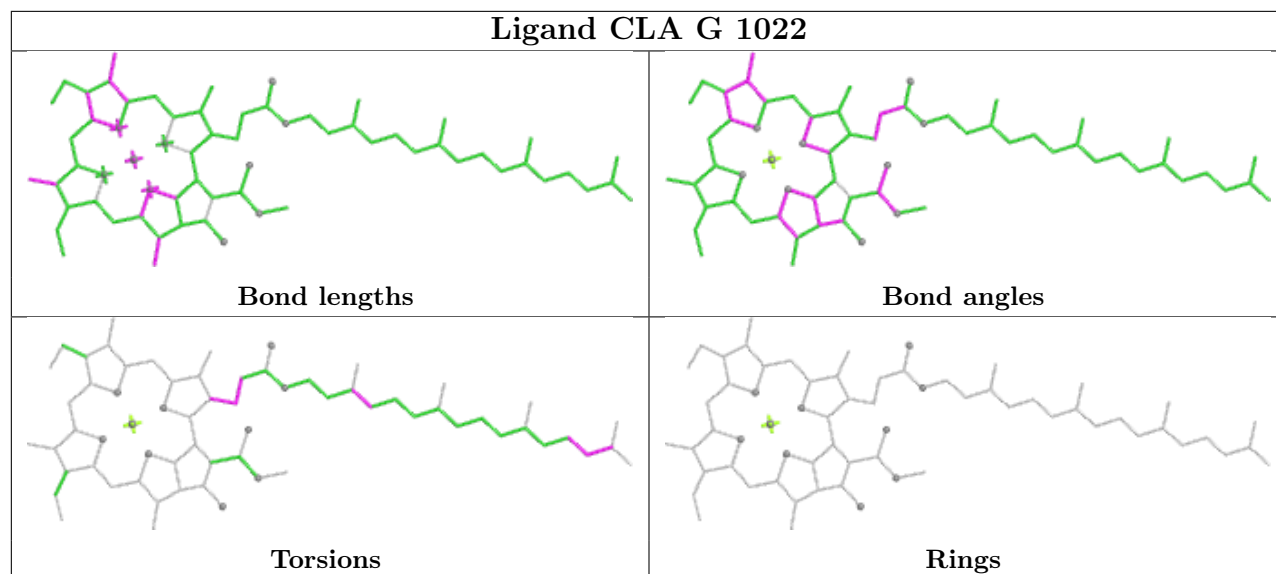
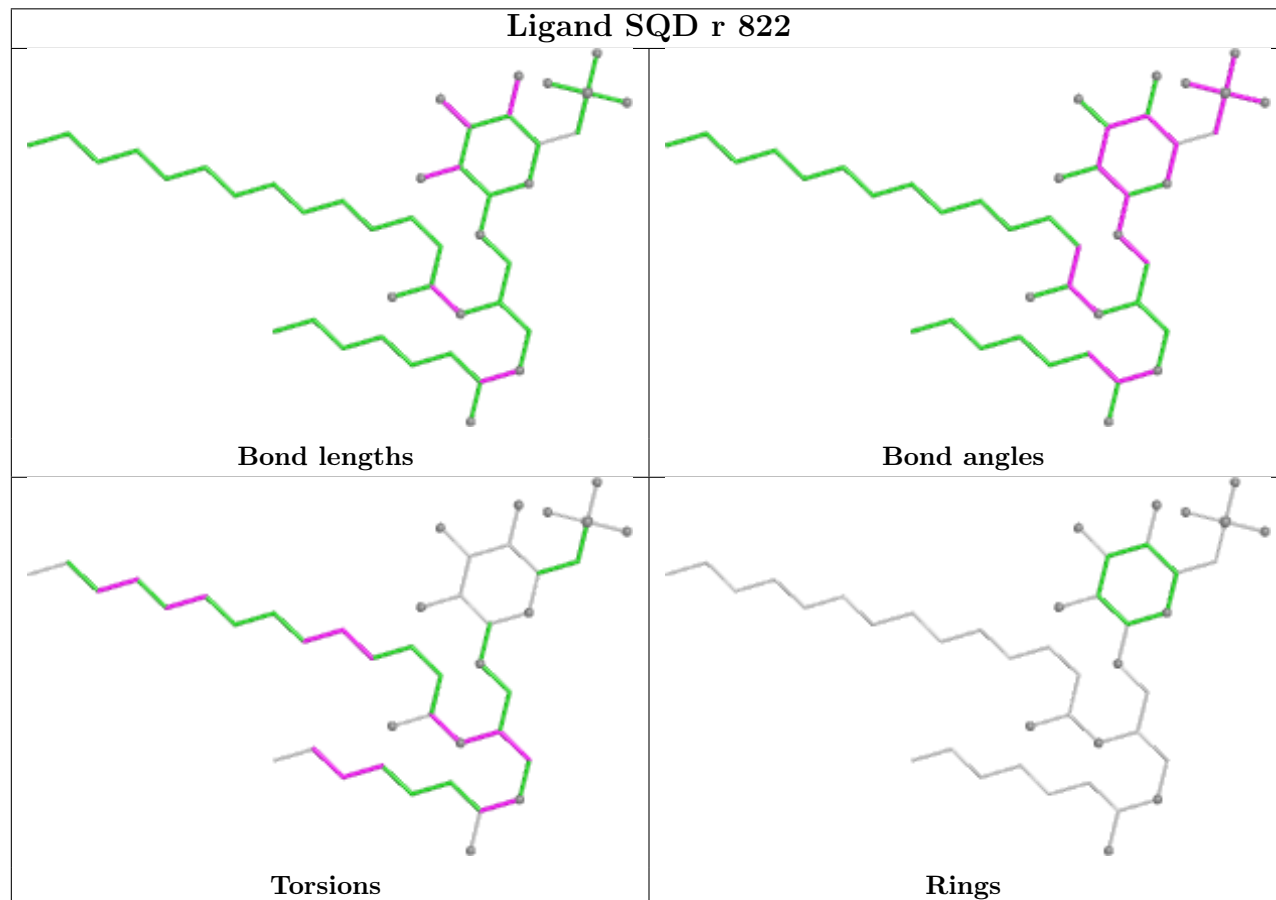


Ligand CLA 6 513

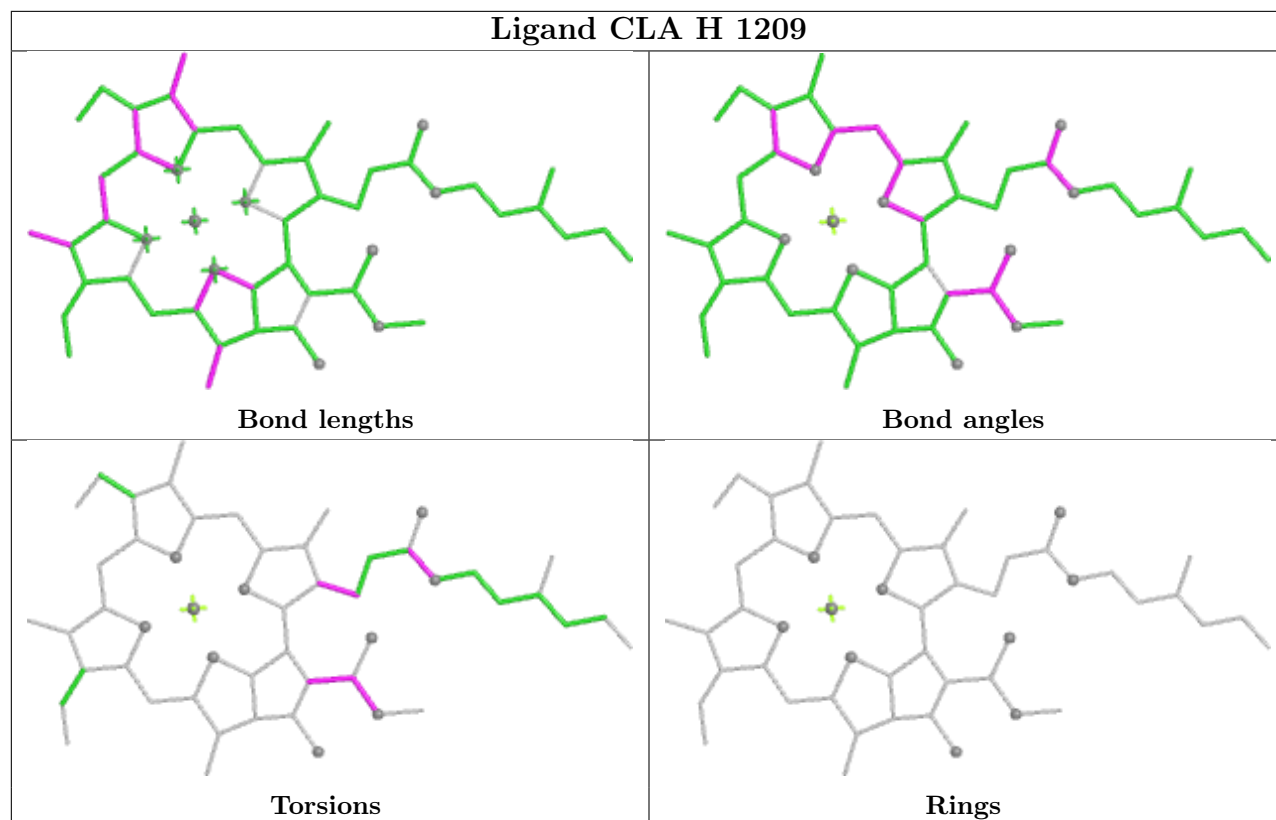


Ligand BCR o 4021

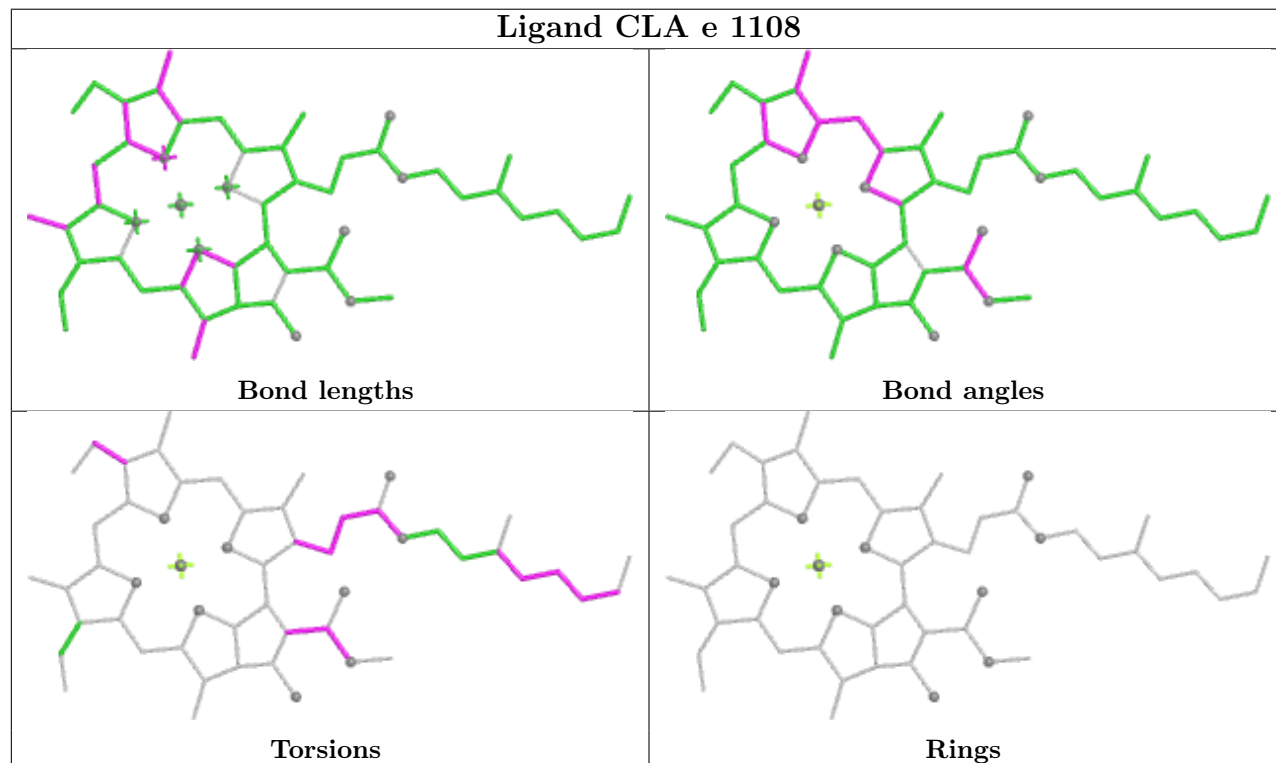


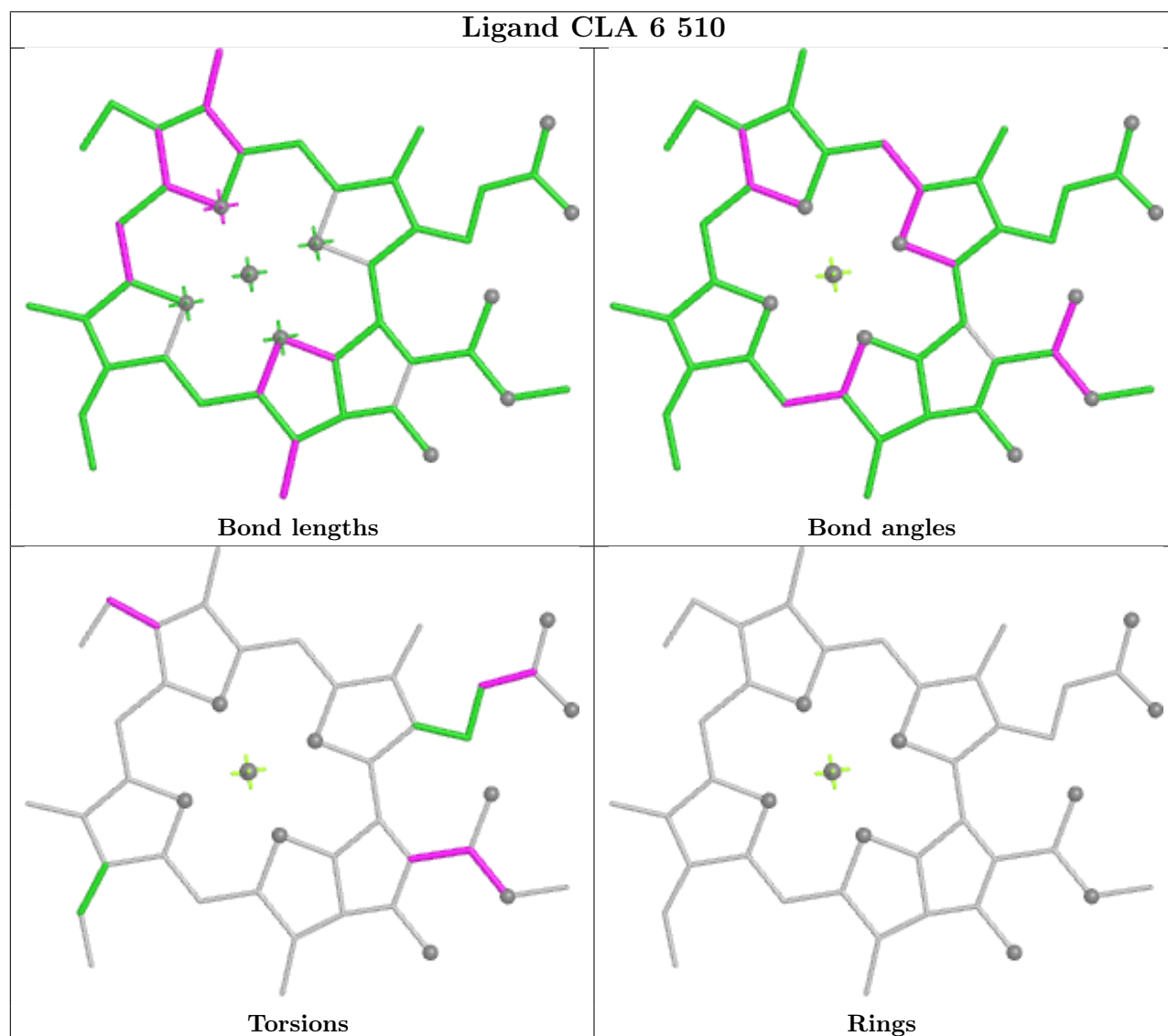
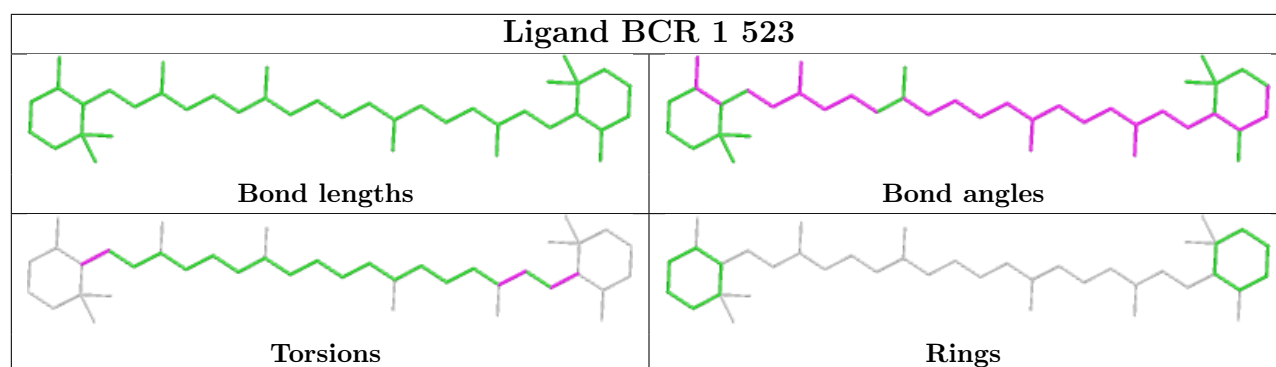
Ligand CLA G 1022**Ligand SQD r 822**

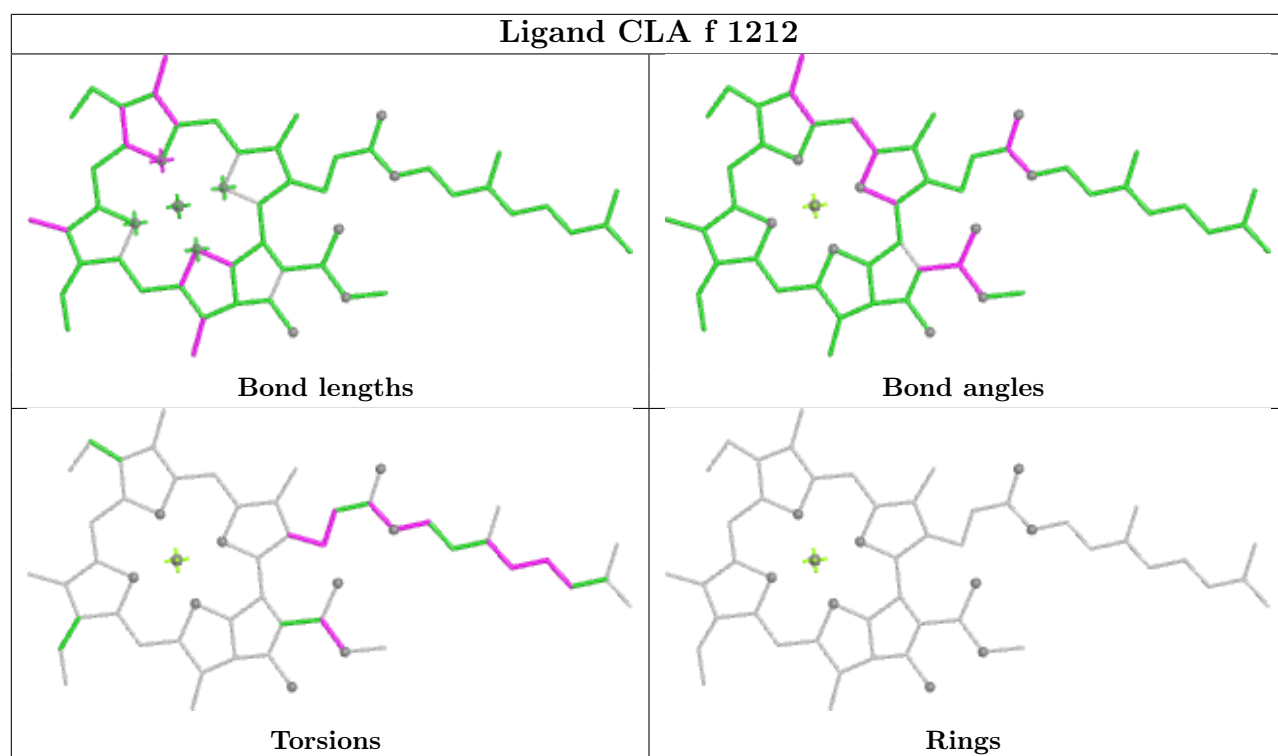
Ligand CLA H 1209

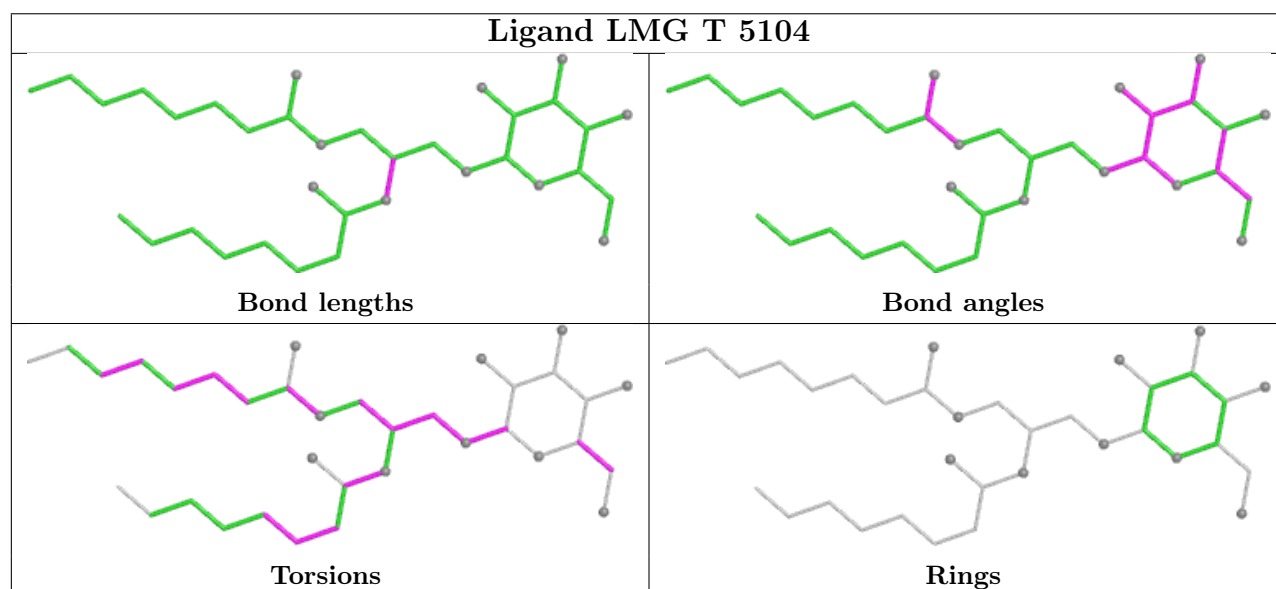
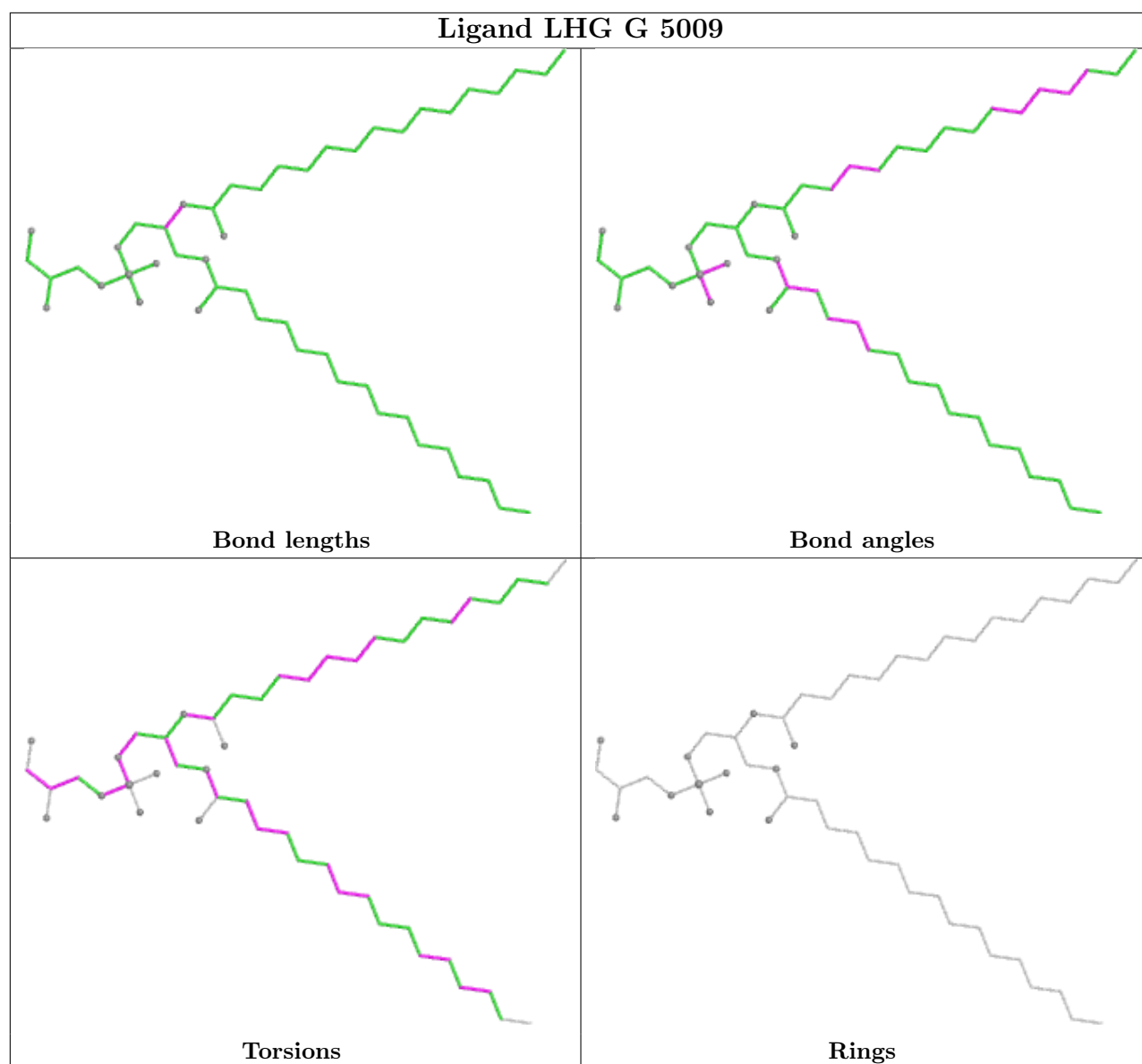


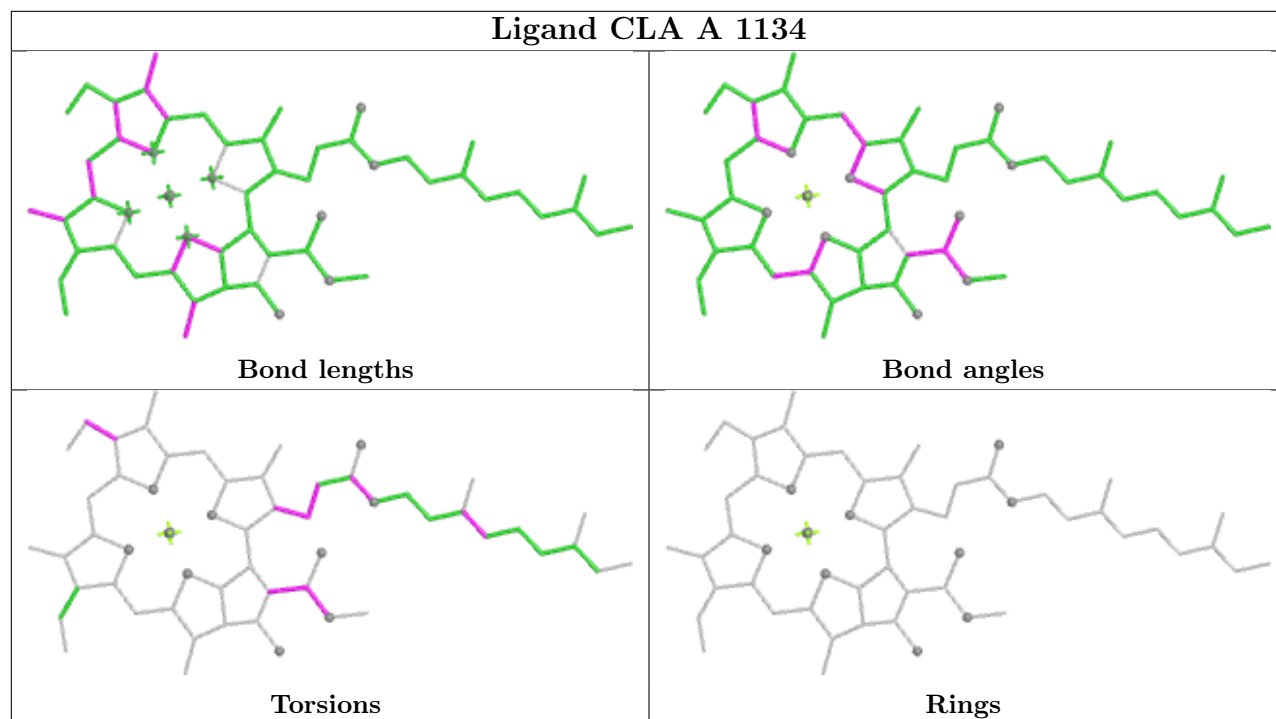
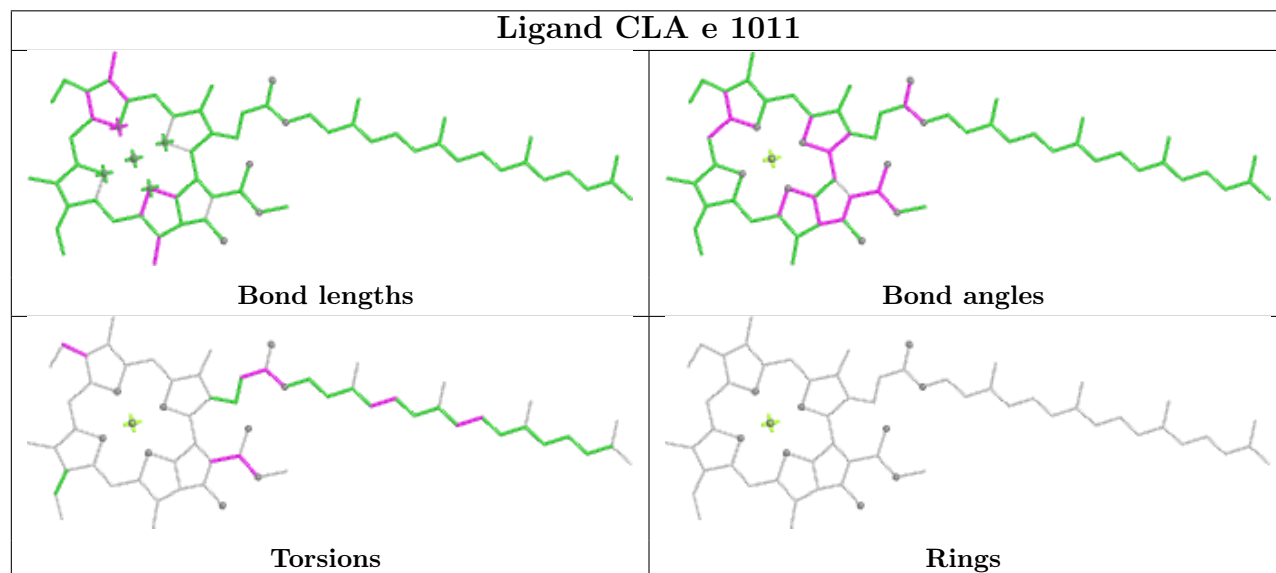
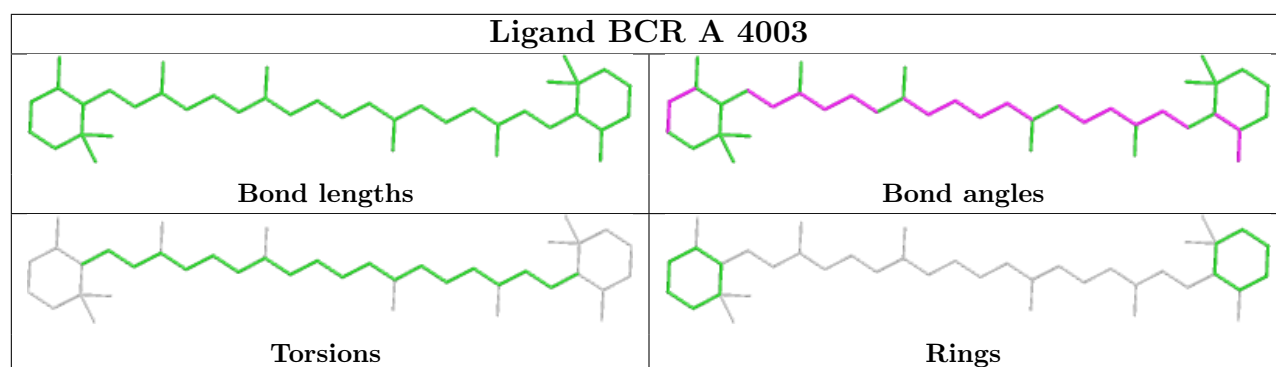
Ligand CLA e 1108



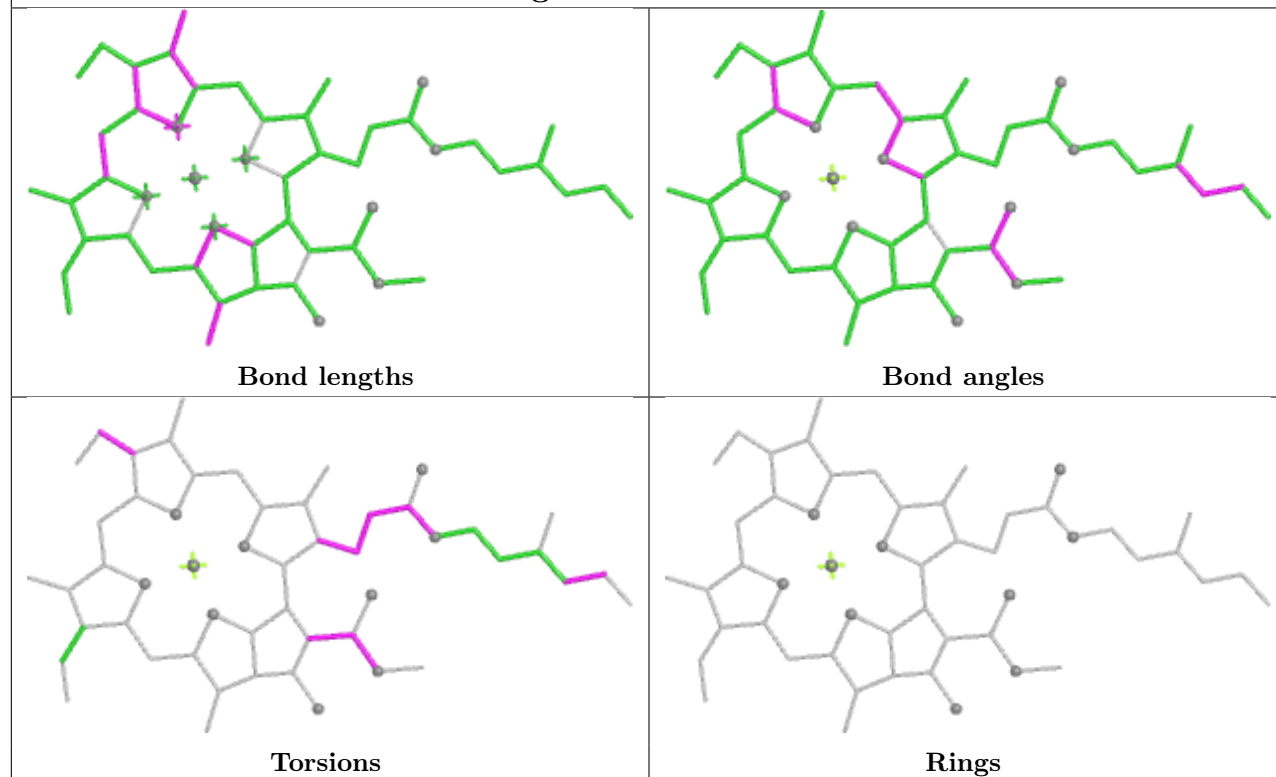




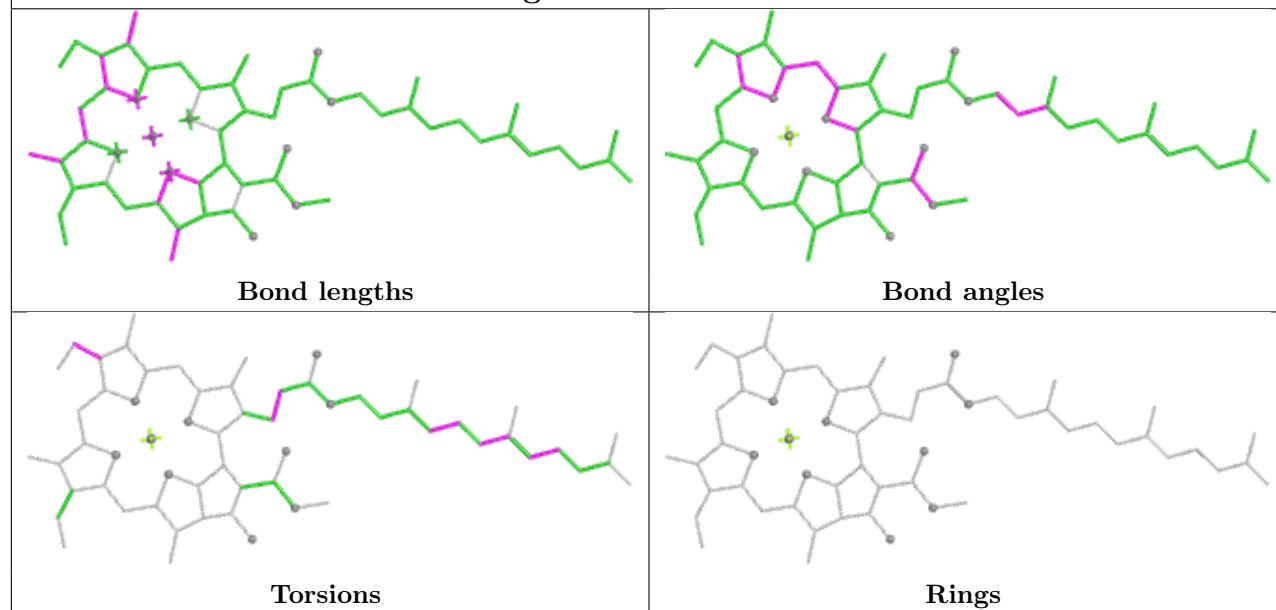


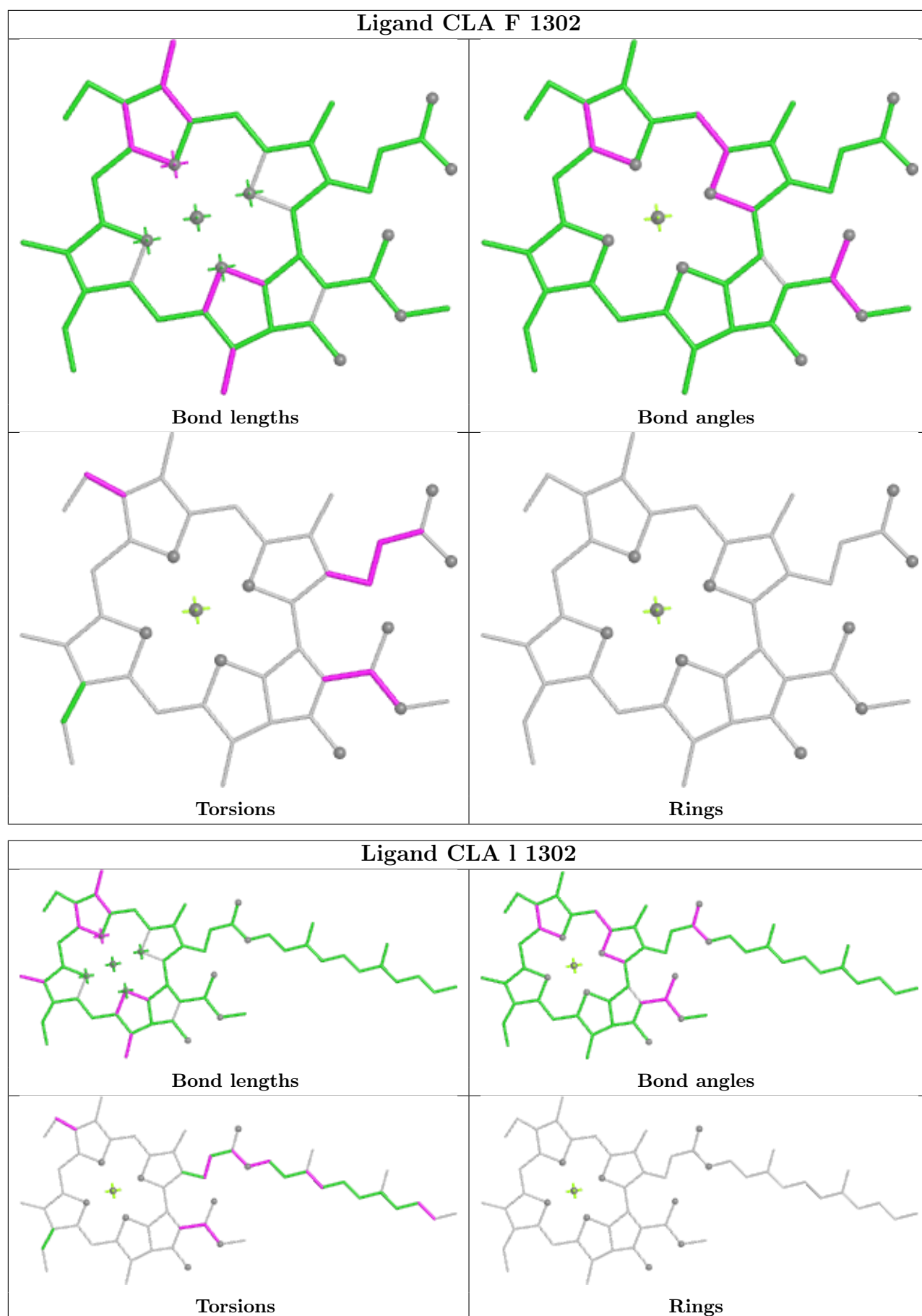


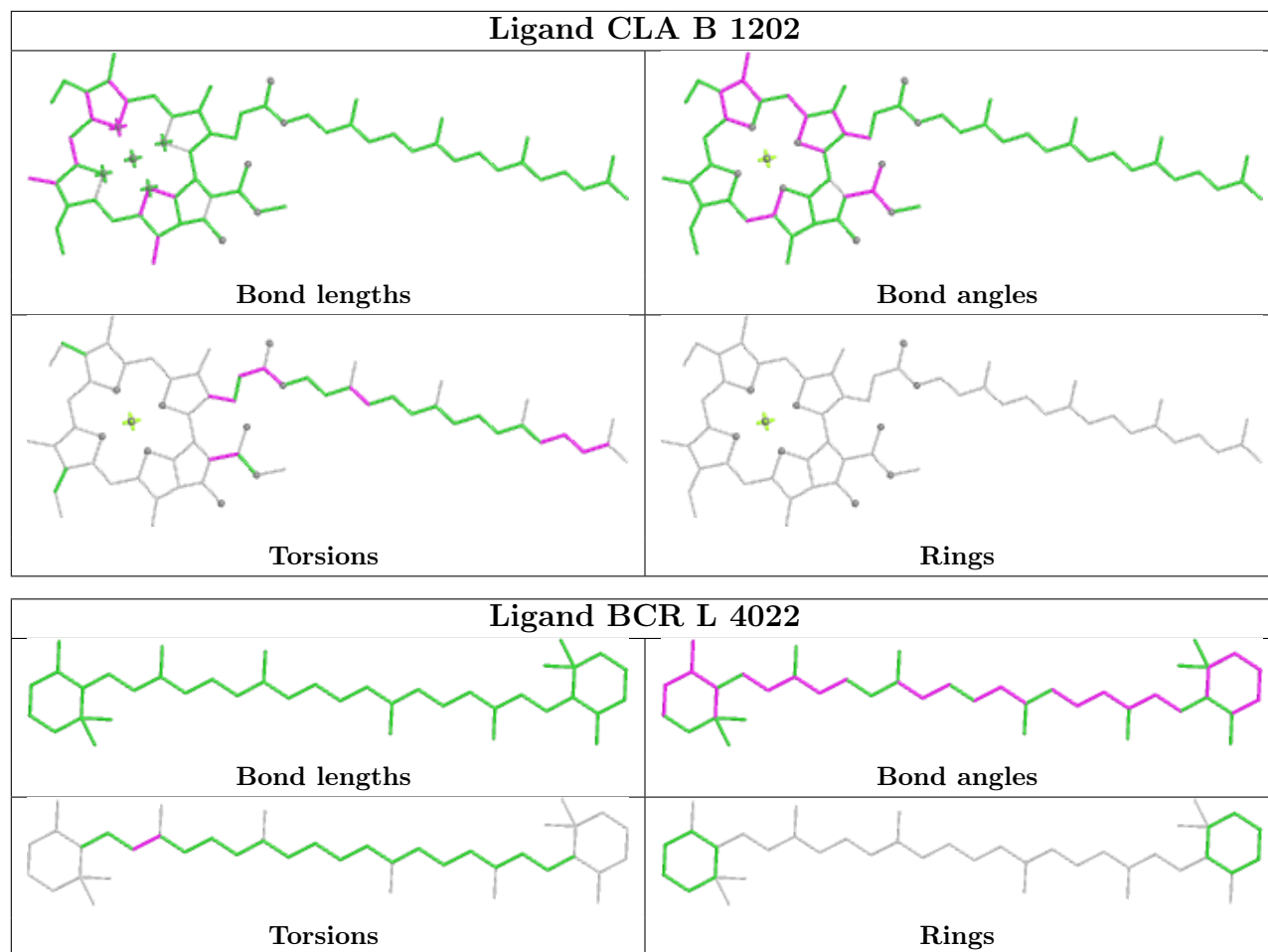
Ligand CLA Y 512



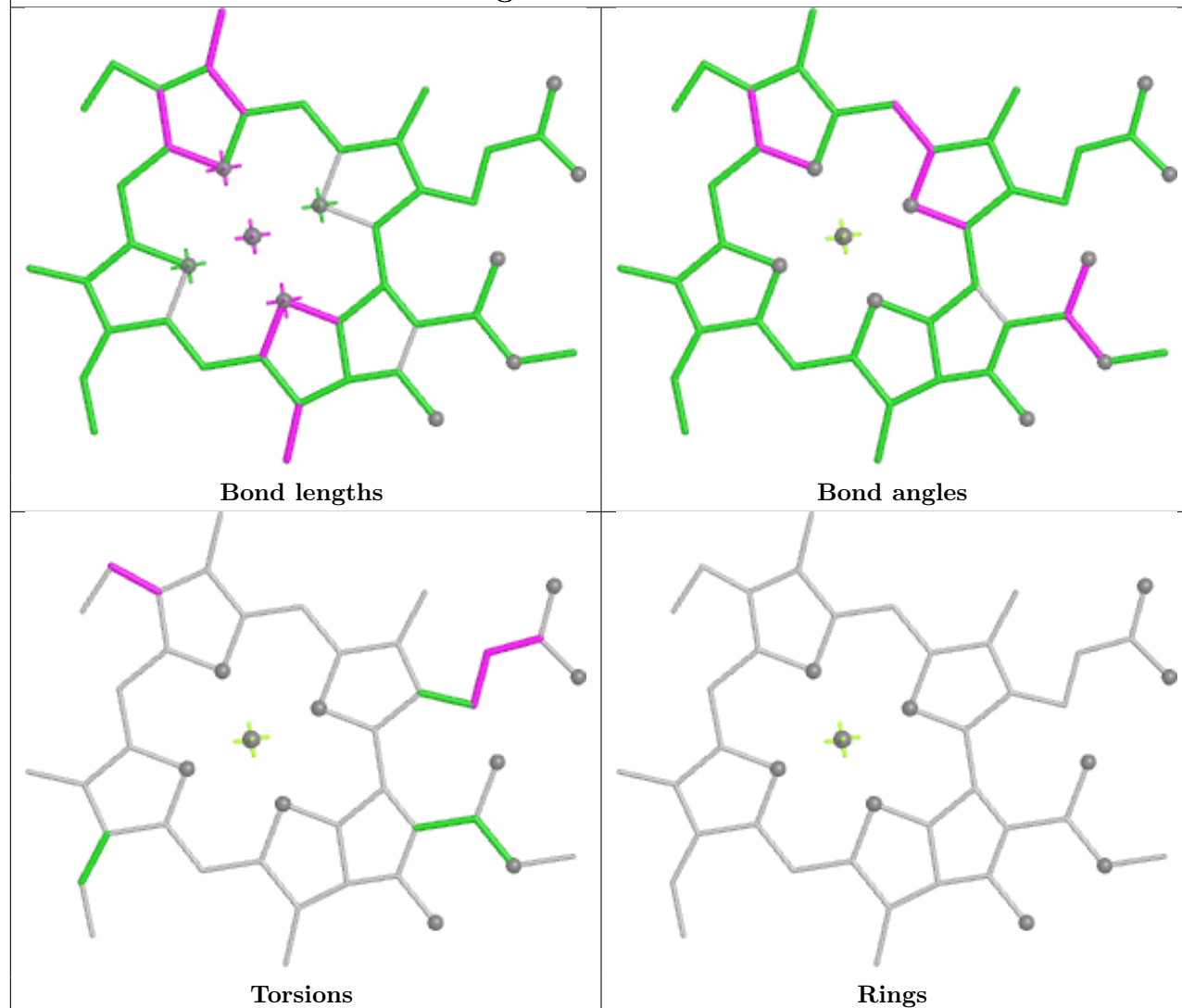
Ligand CLA B 1216



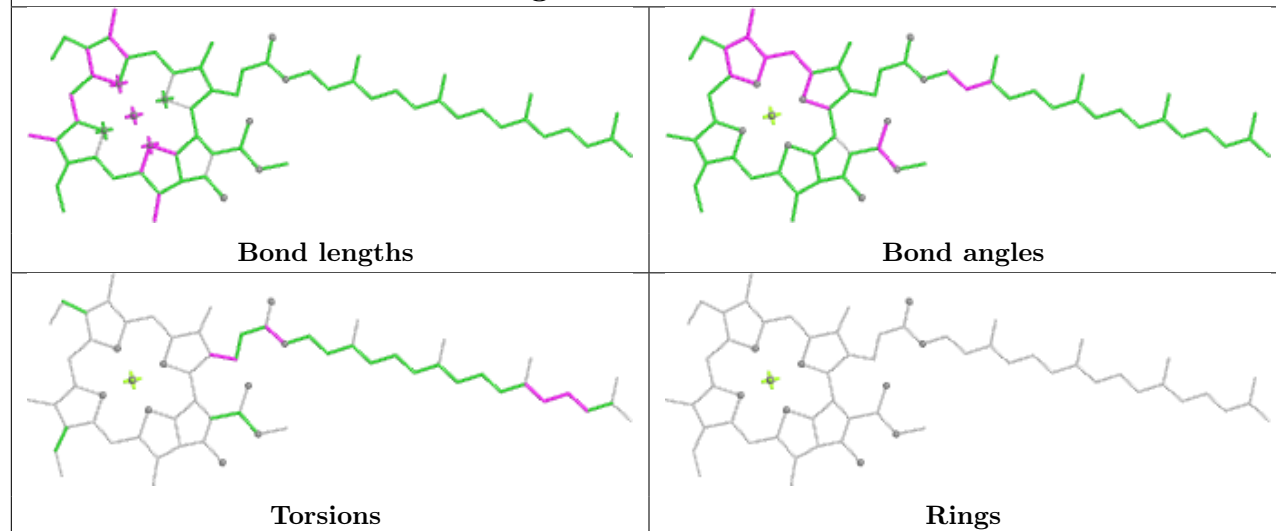




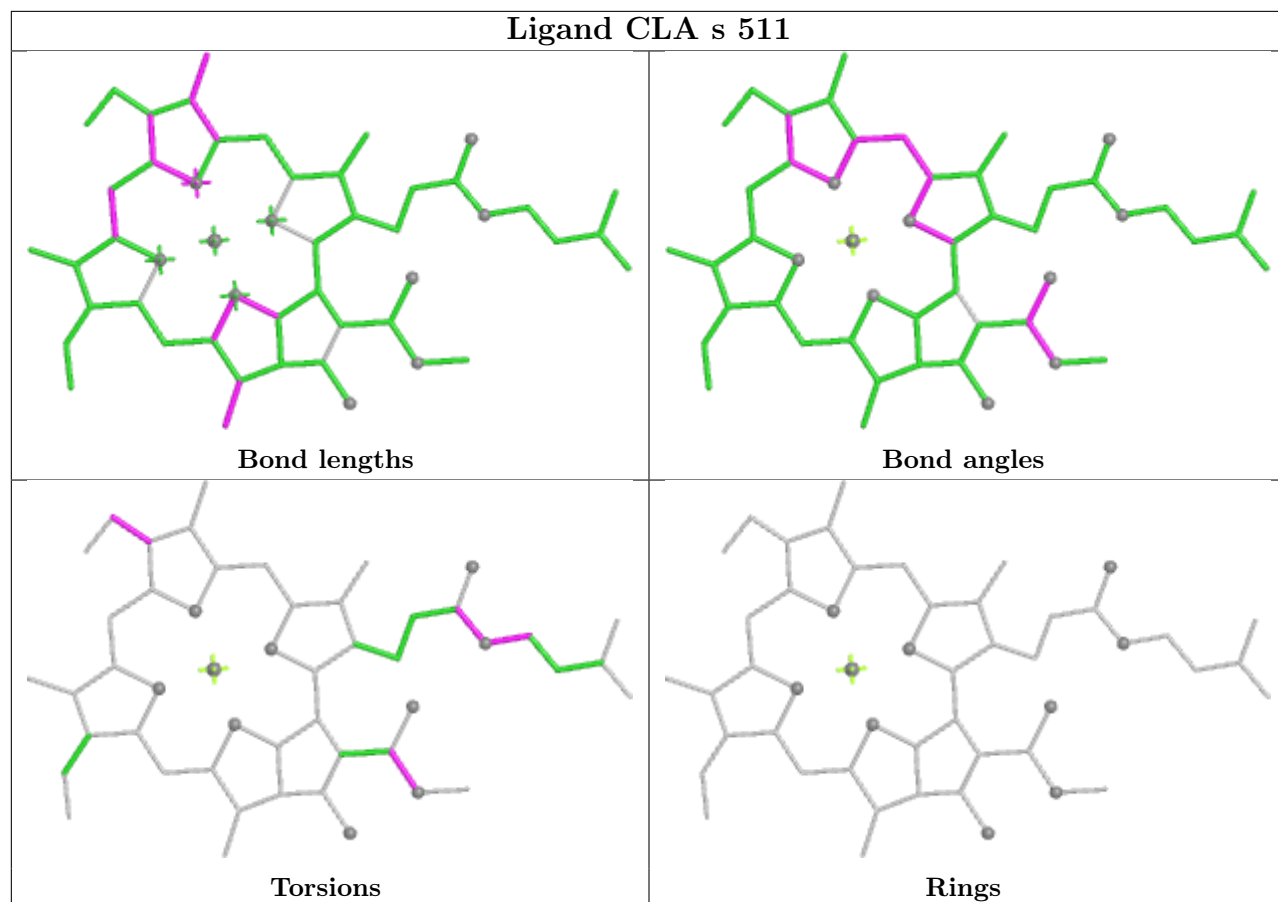
Ligand CLA a 512



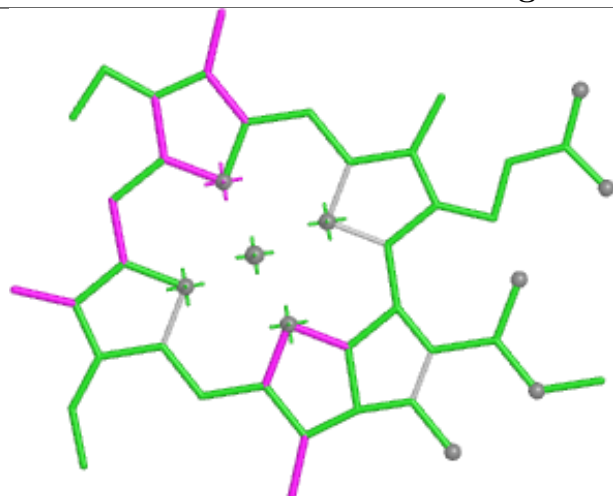
Ligand CLA f 1225



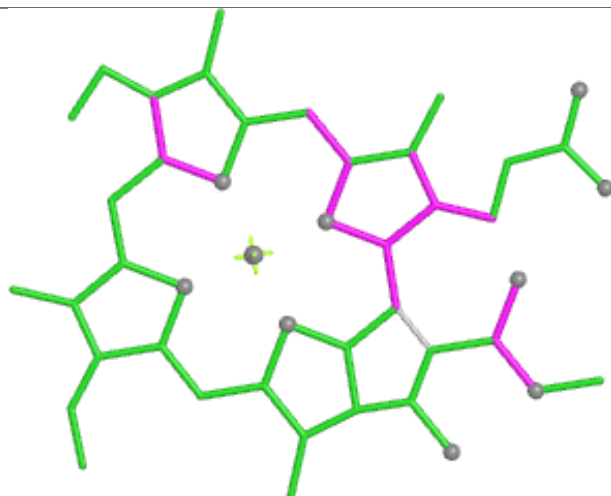
Ligand CLA s 511



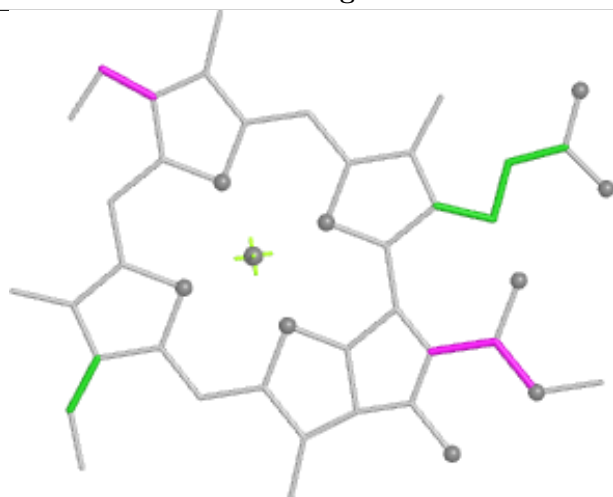
Ligand CLA 1 504



Bond lengths



Bond angles

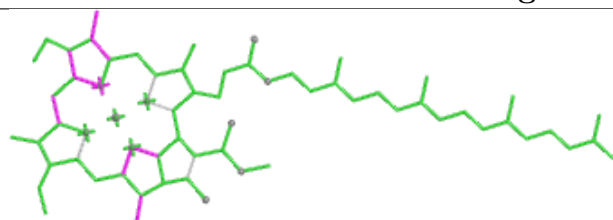


Torsions

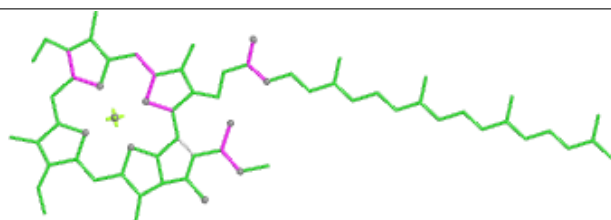


Rings

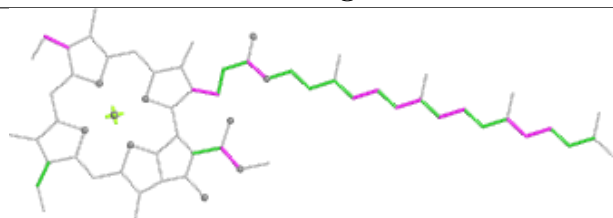
Ligand CLA 3 513



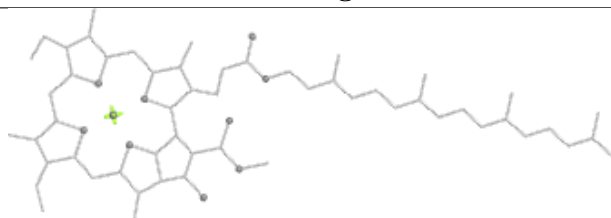
Bond lengths



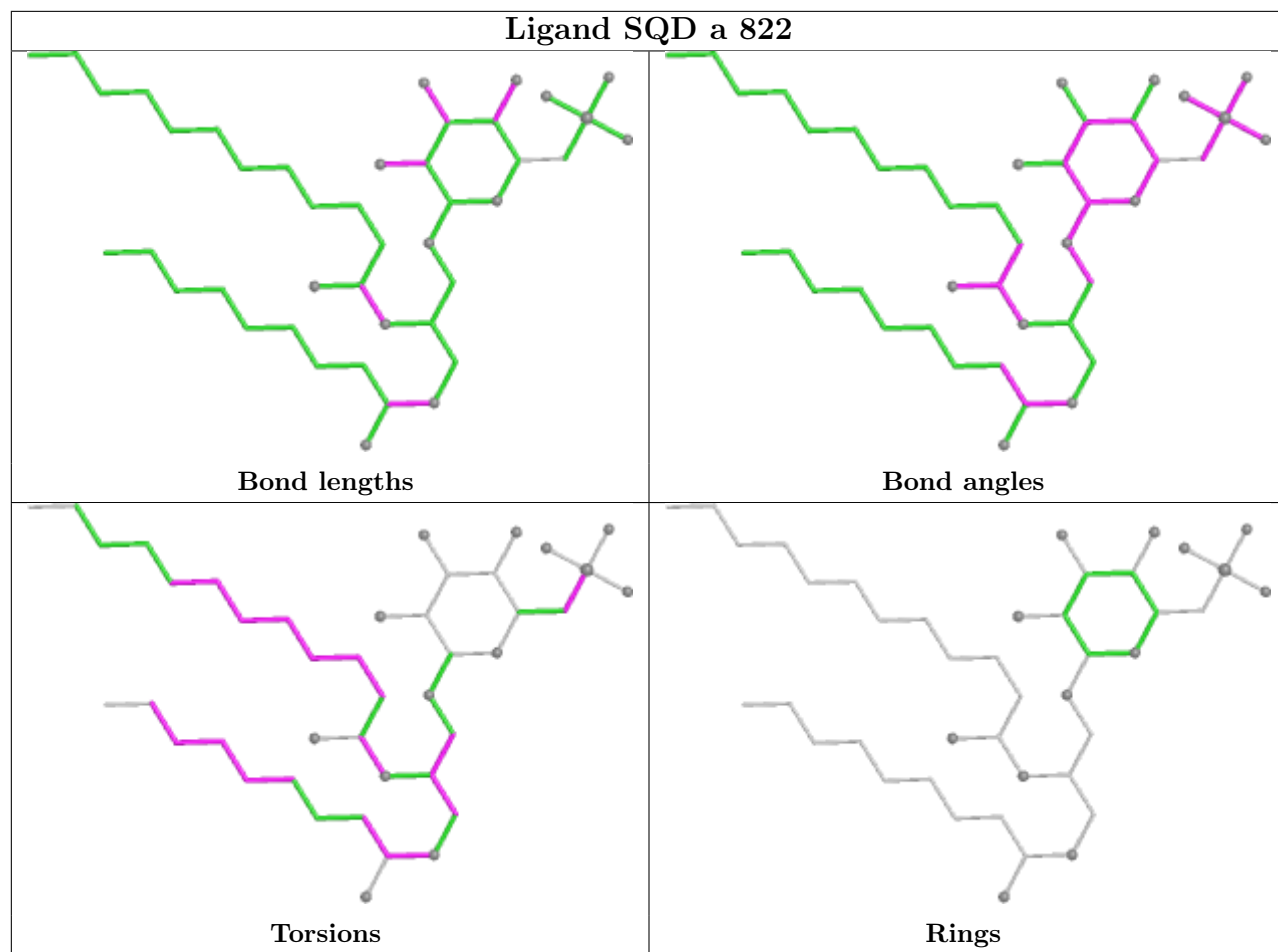
Bond angles



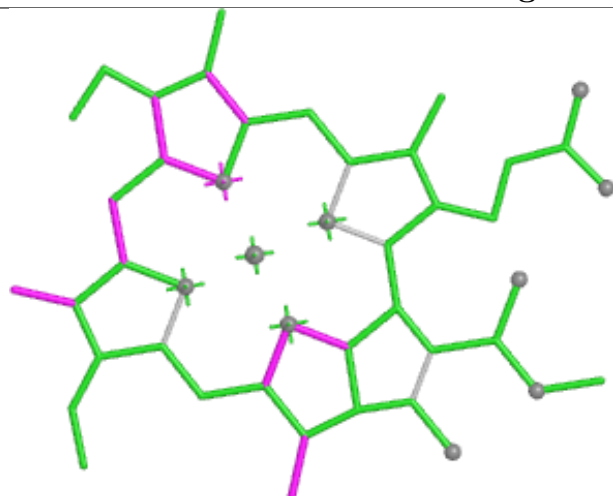
Torsions



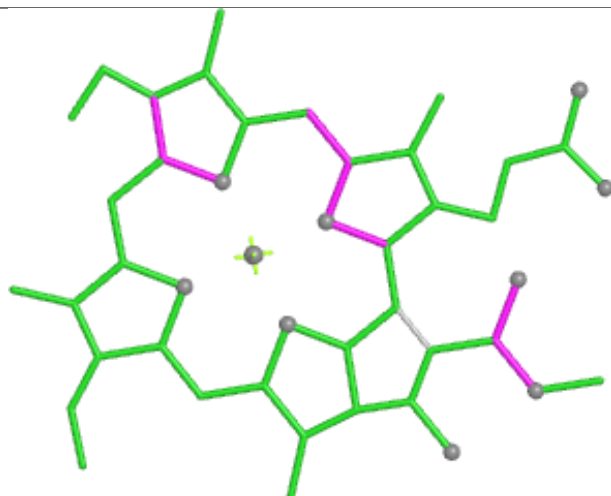
Rings



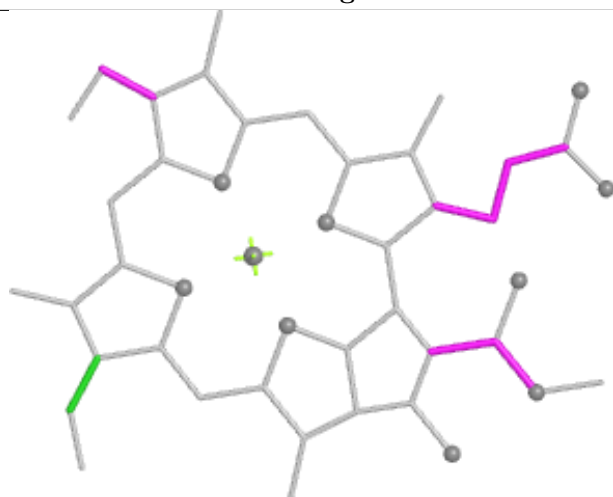
Ligand CLA 5 517



Bond lengths



Bond angles

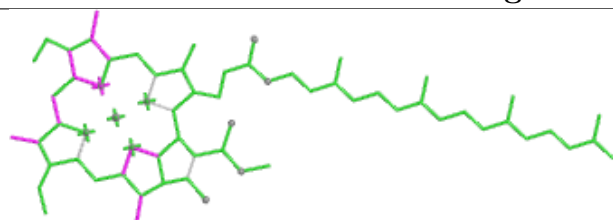


Torsions

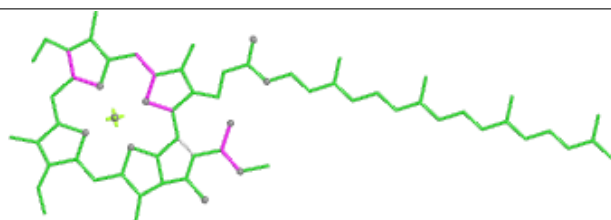


Rings

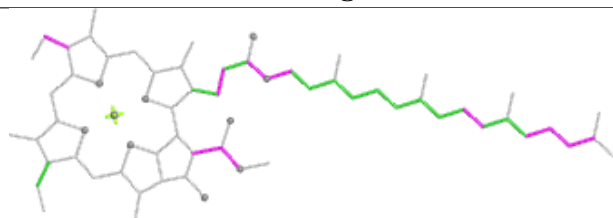
Ligand CLA H 1207



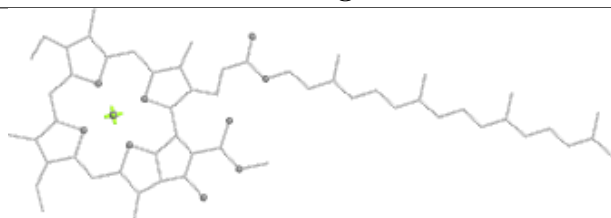
Bond lengths



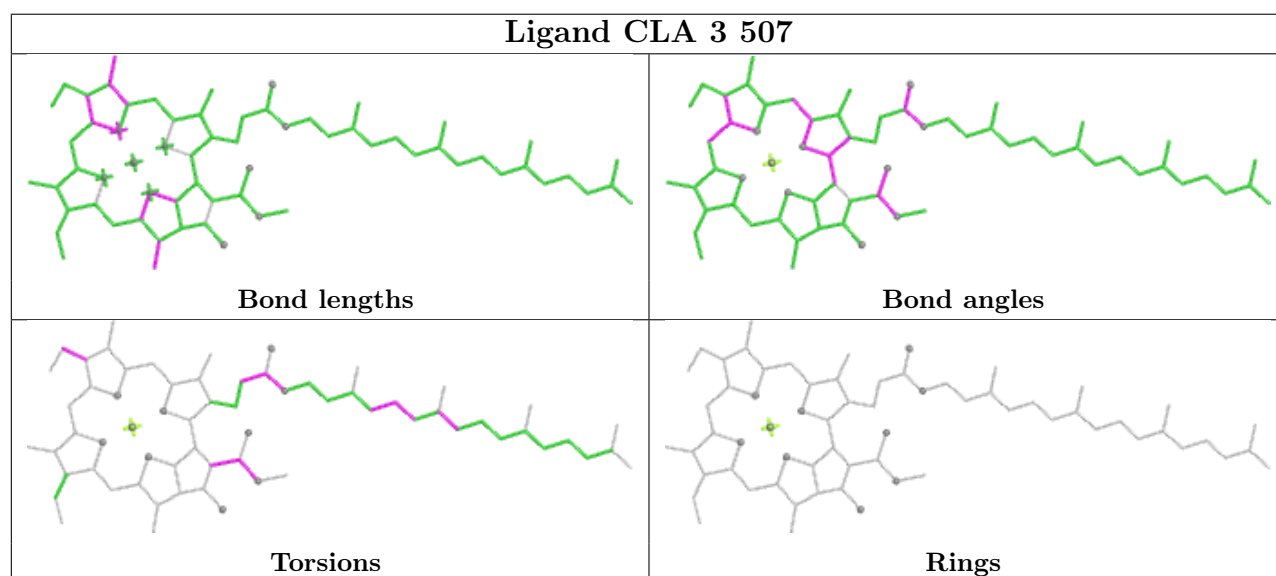
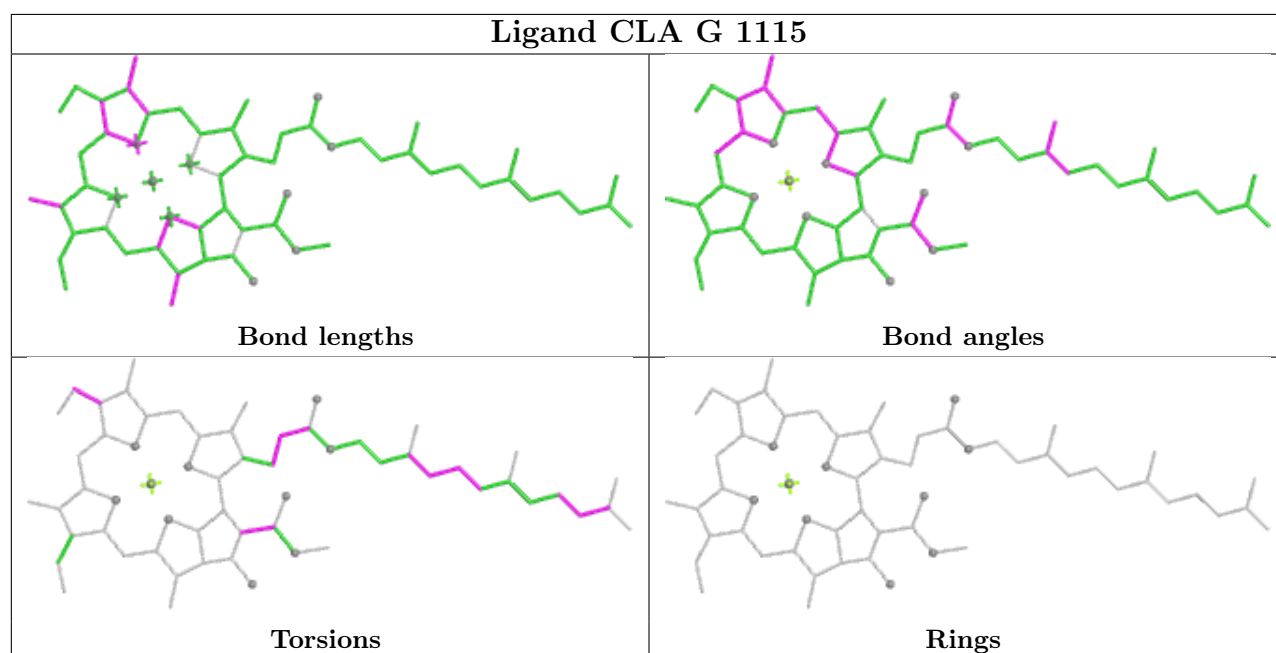
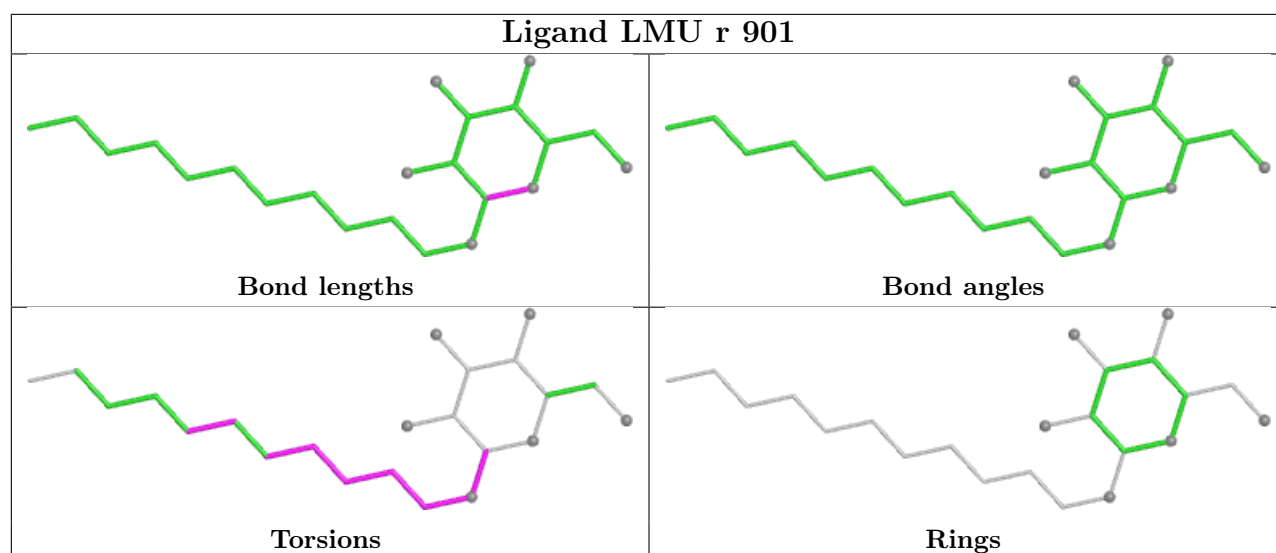
Bond angles

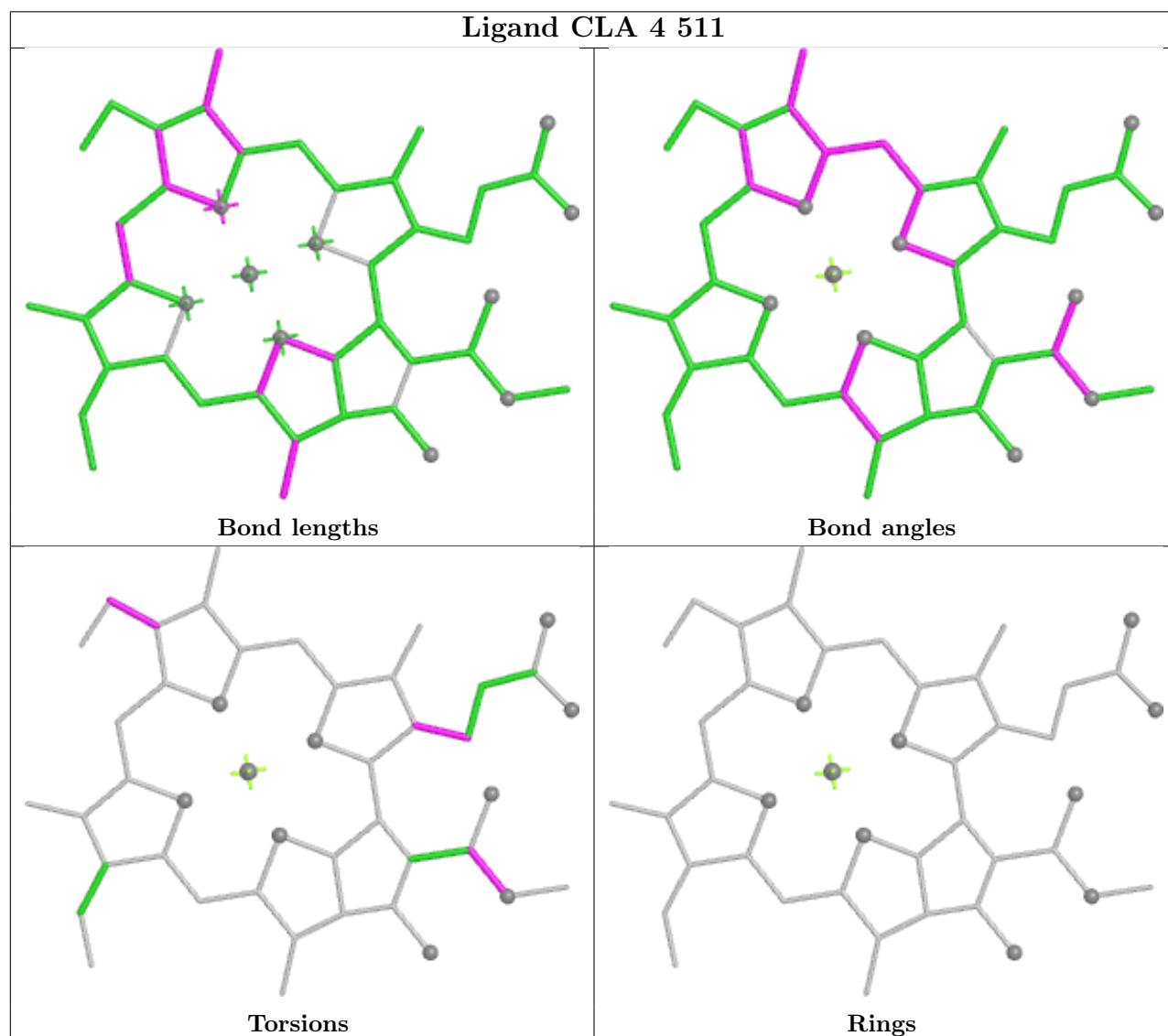
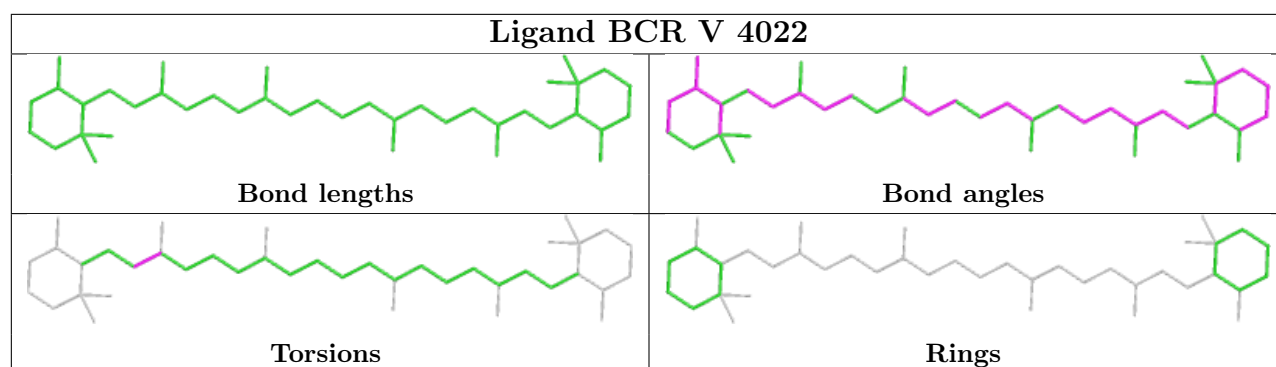


Torsions

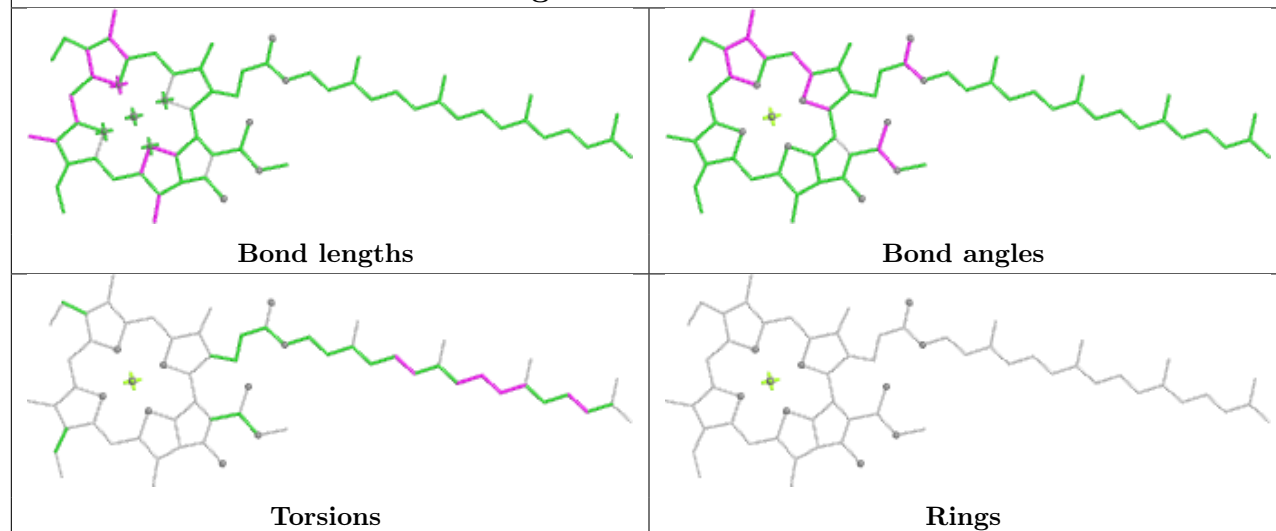


Rings

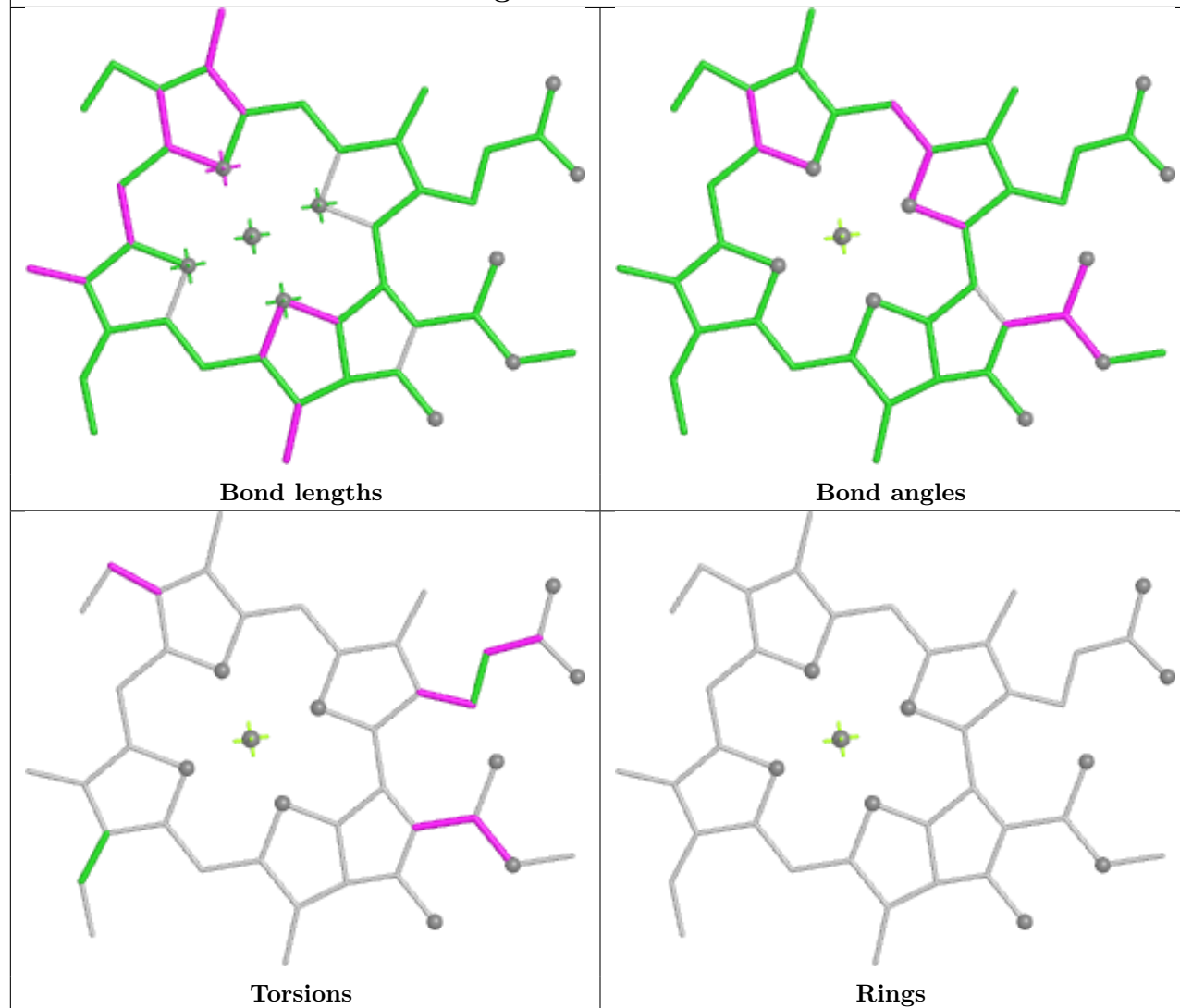




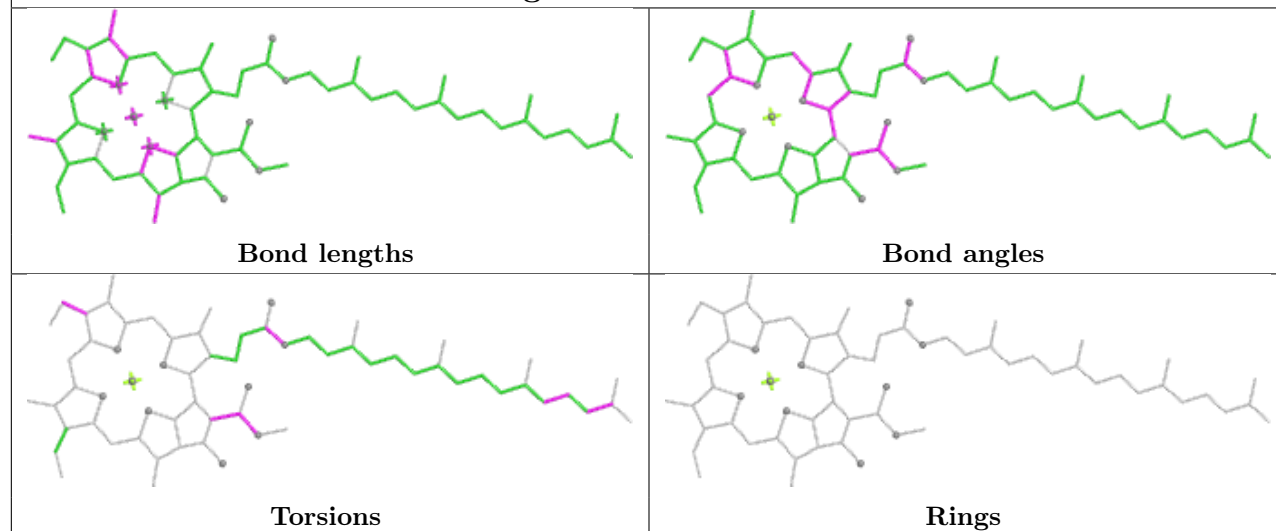
Ligand CLA Y 509



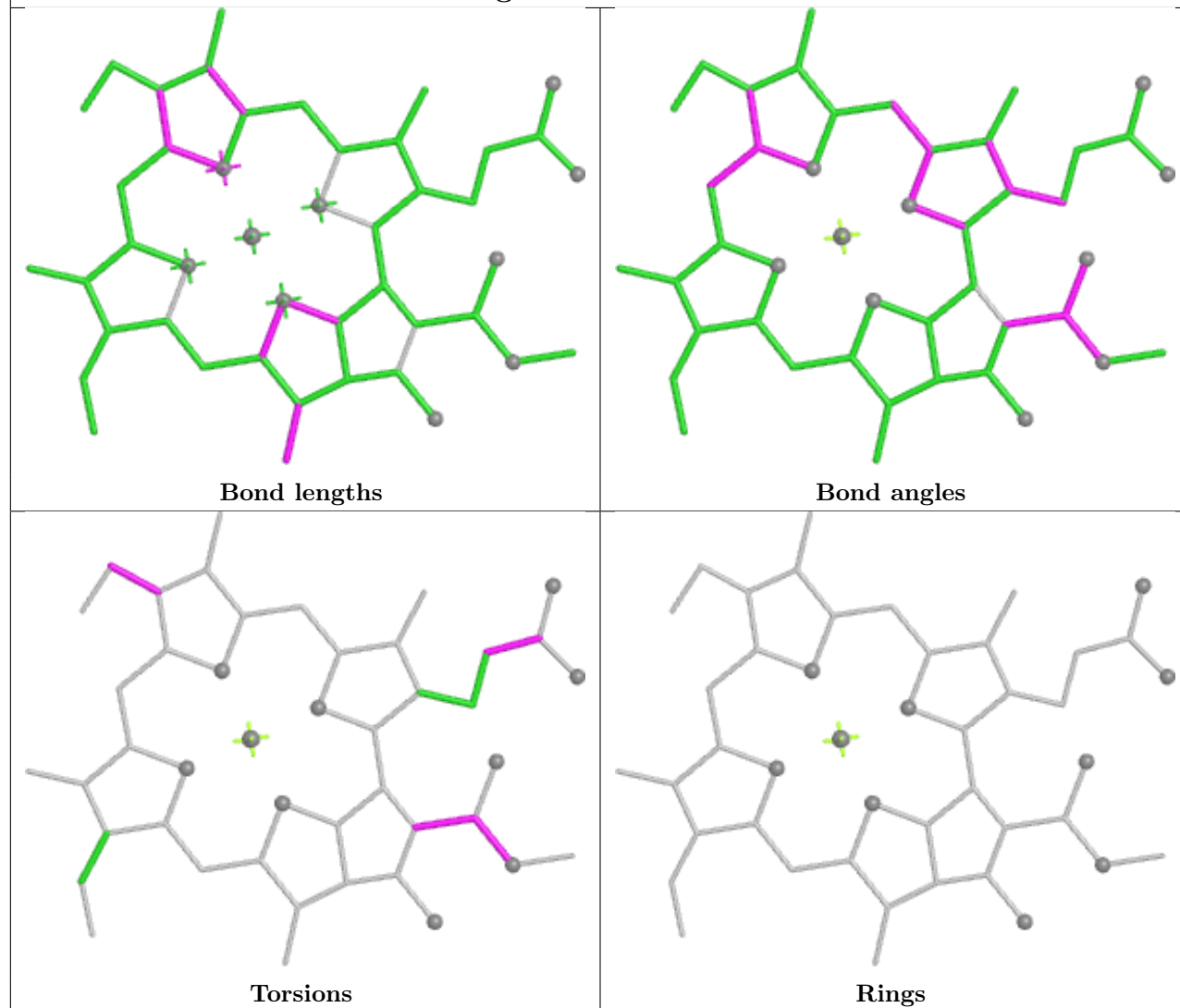
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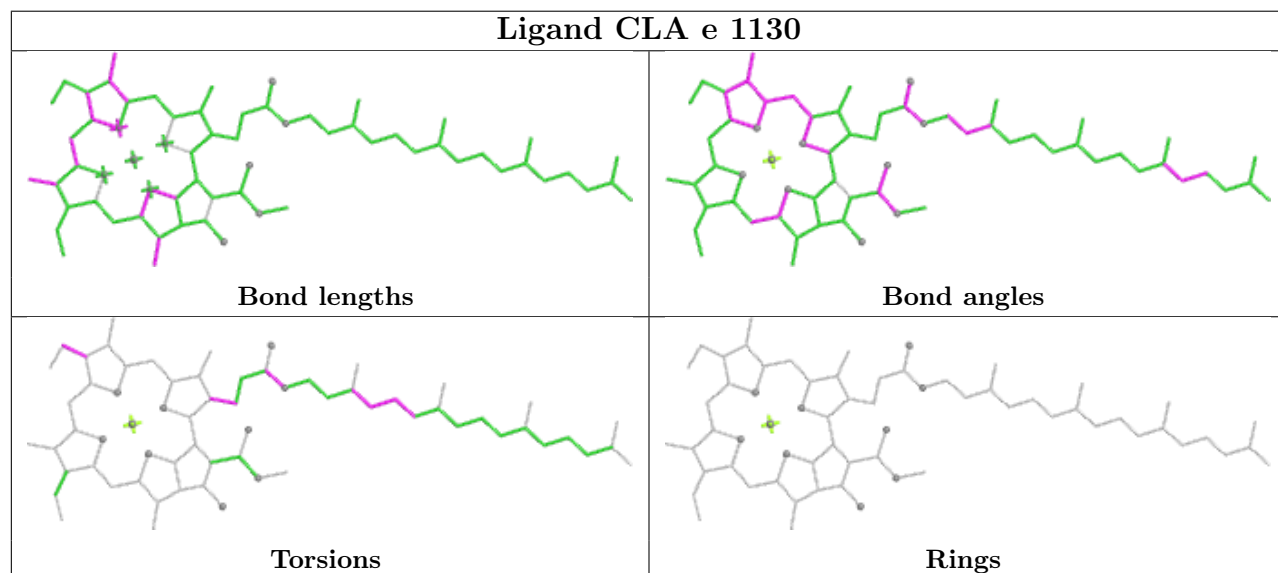
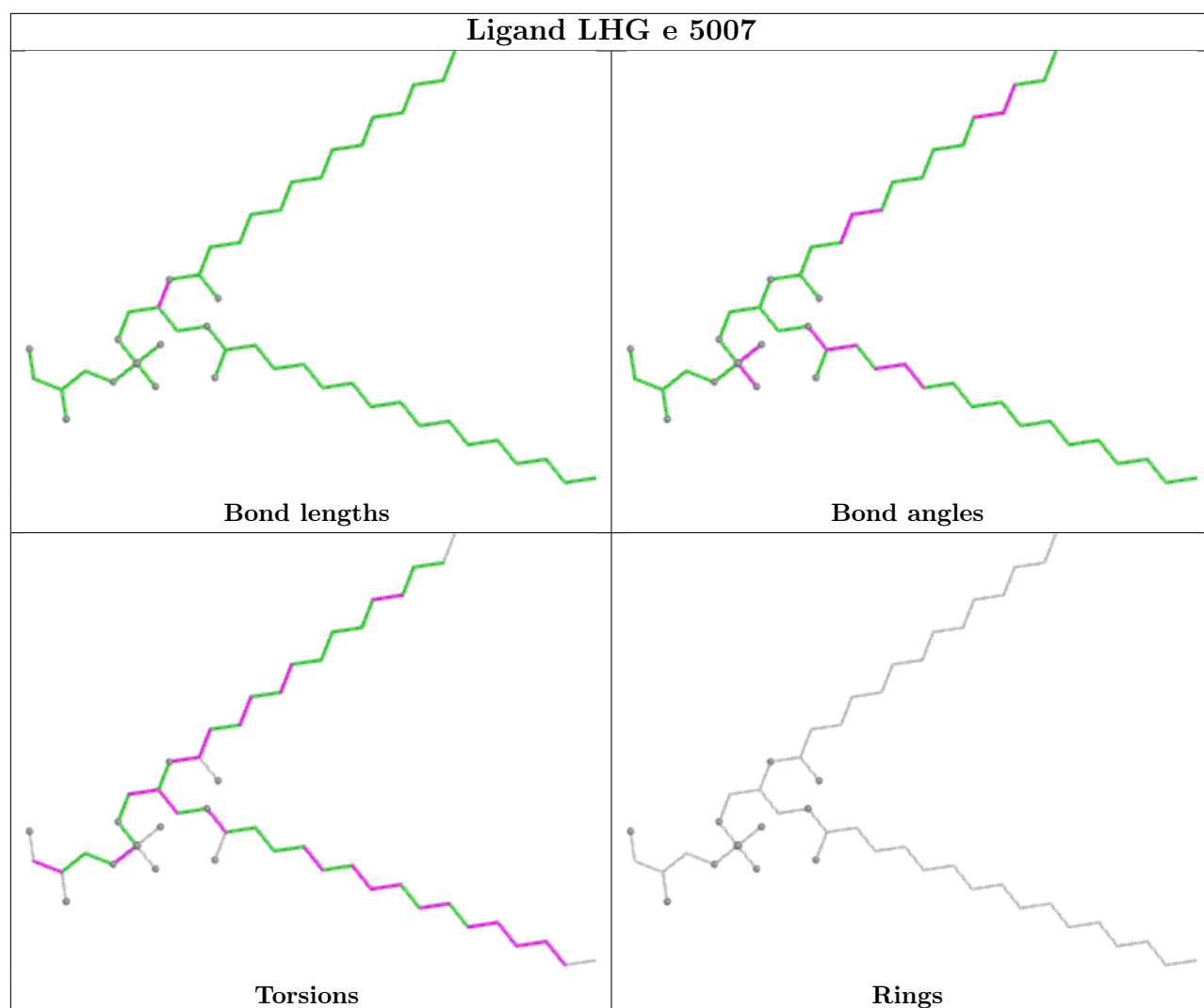


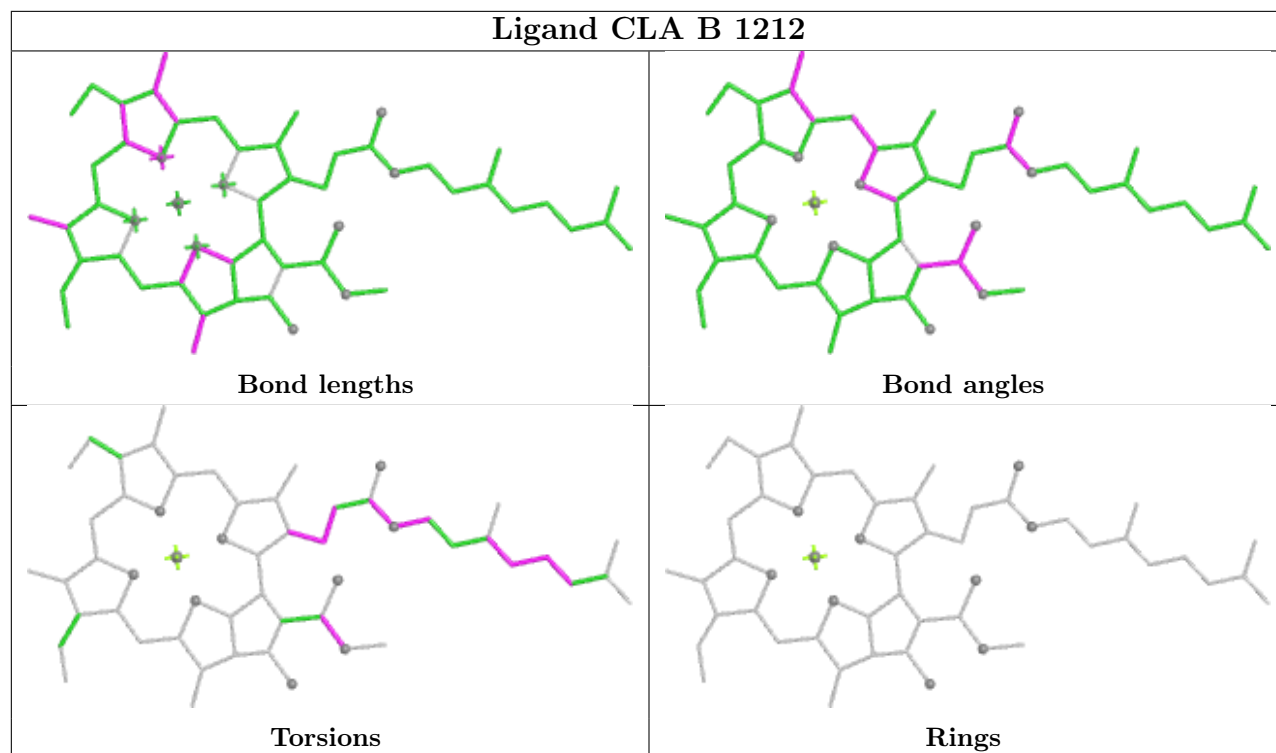
Ligand CLA B 1021

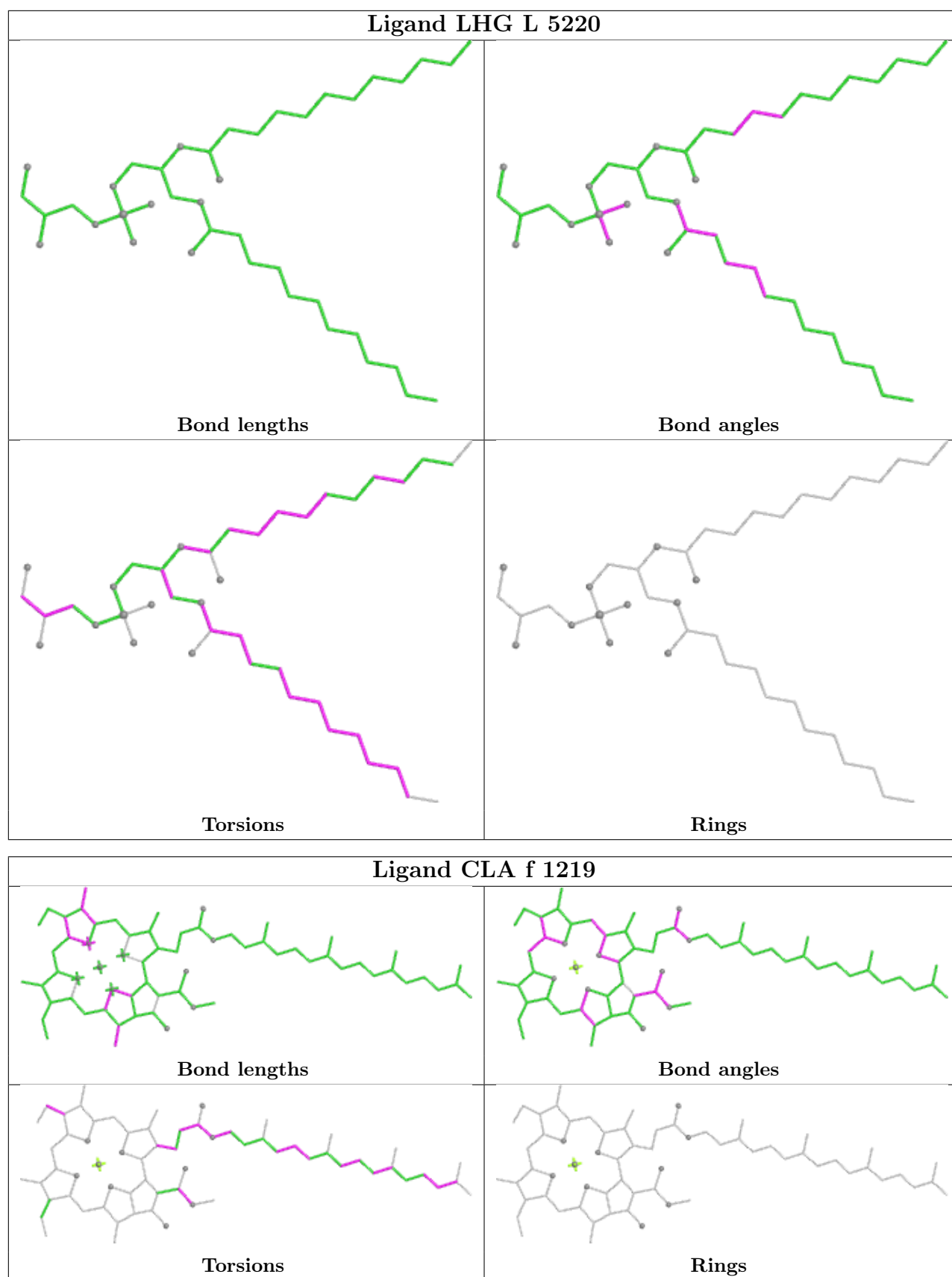


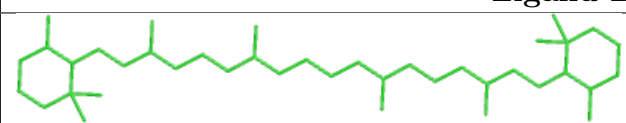
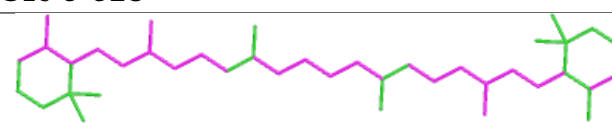
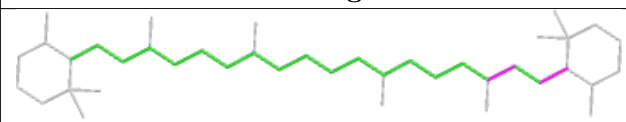
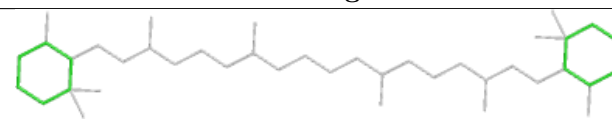
Ligand CLA 4 507

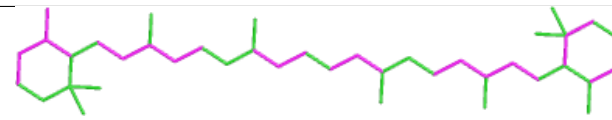
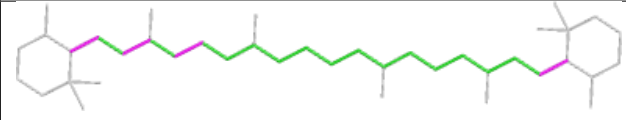
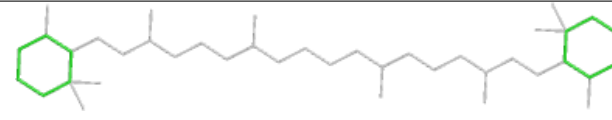


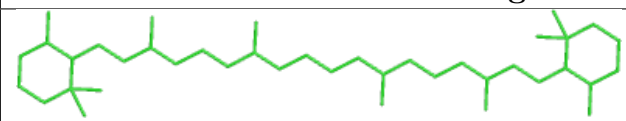
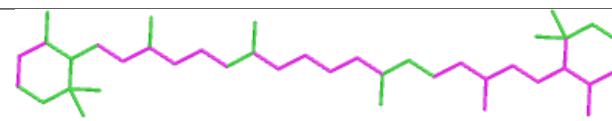
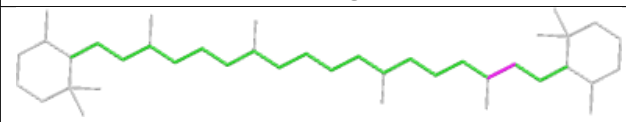
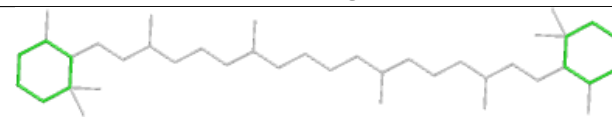


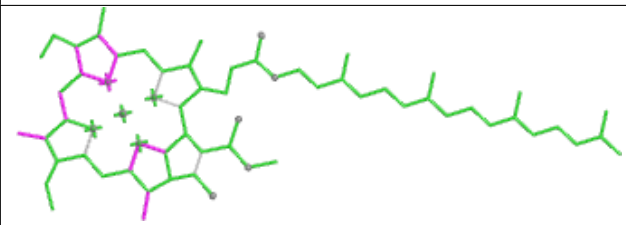
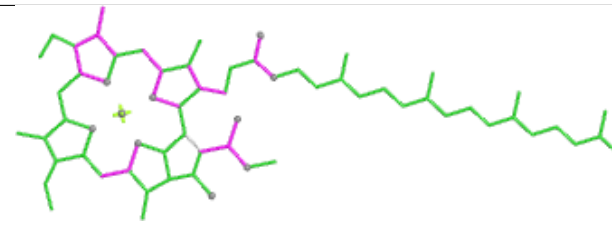
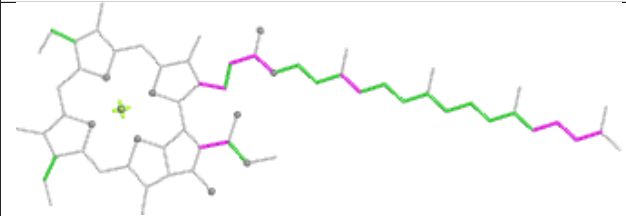
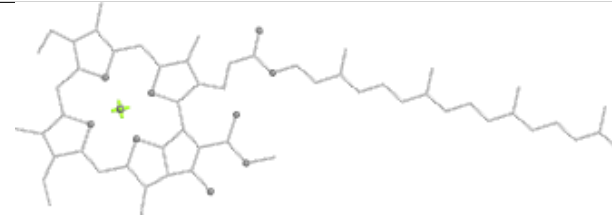




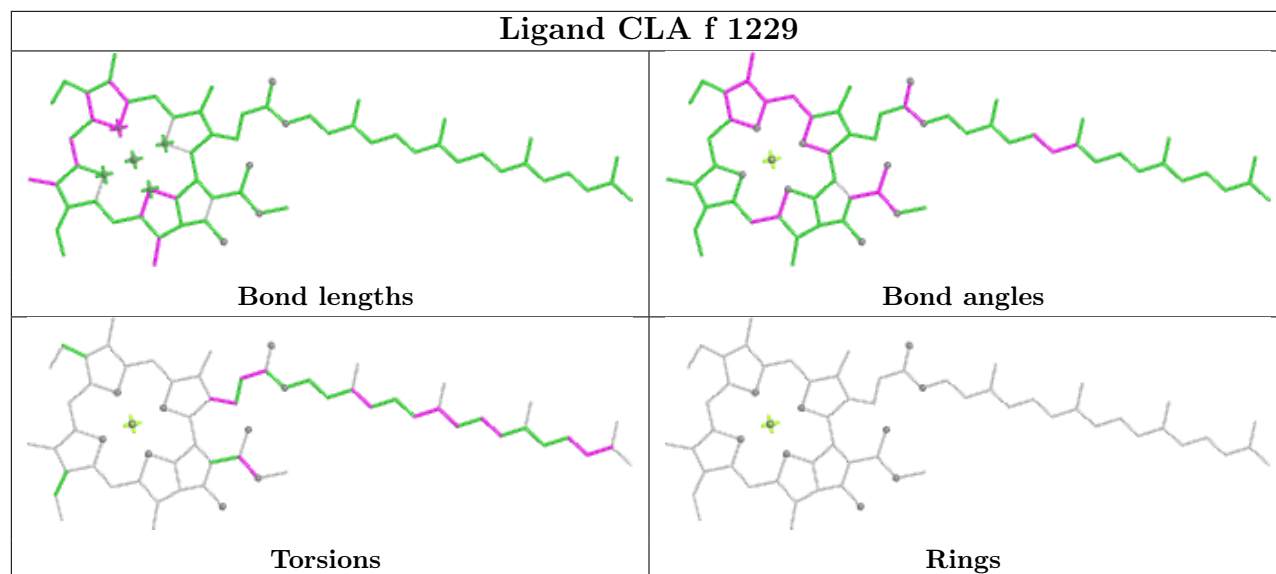
Ligand BCR 5 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 3 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

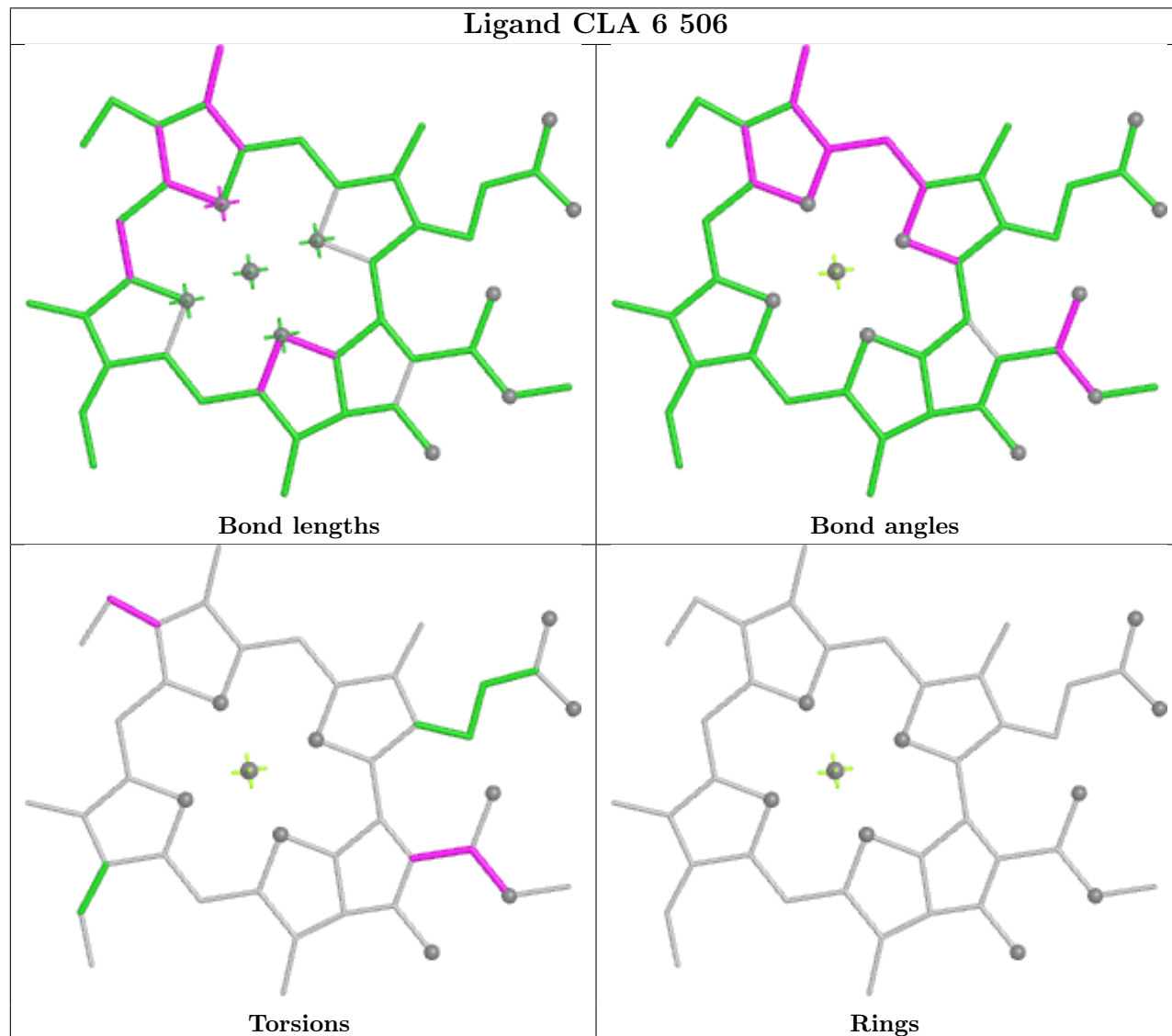
Ligand BCR m 4104	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA f 1202	
	
Bond lengths	Bond angles
	
Torsions	Rings

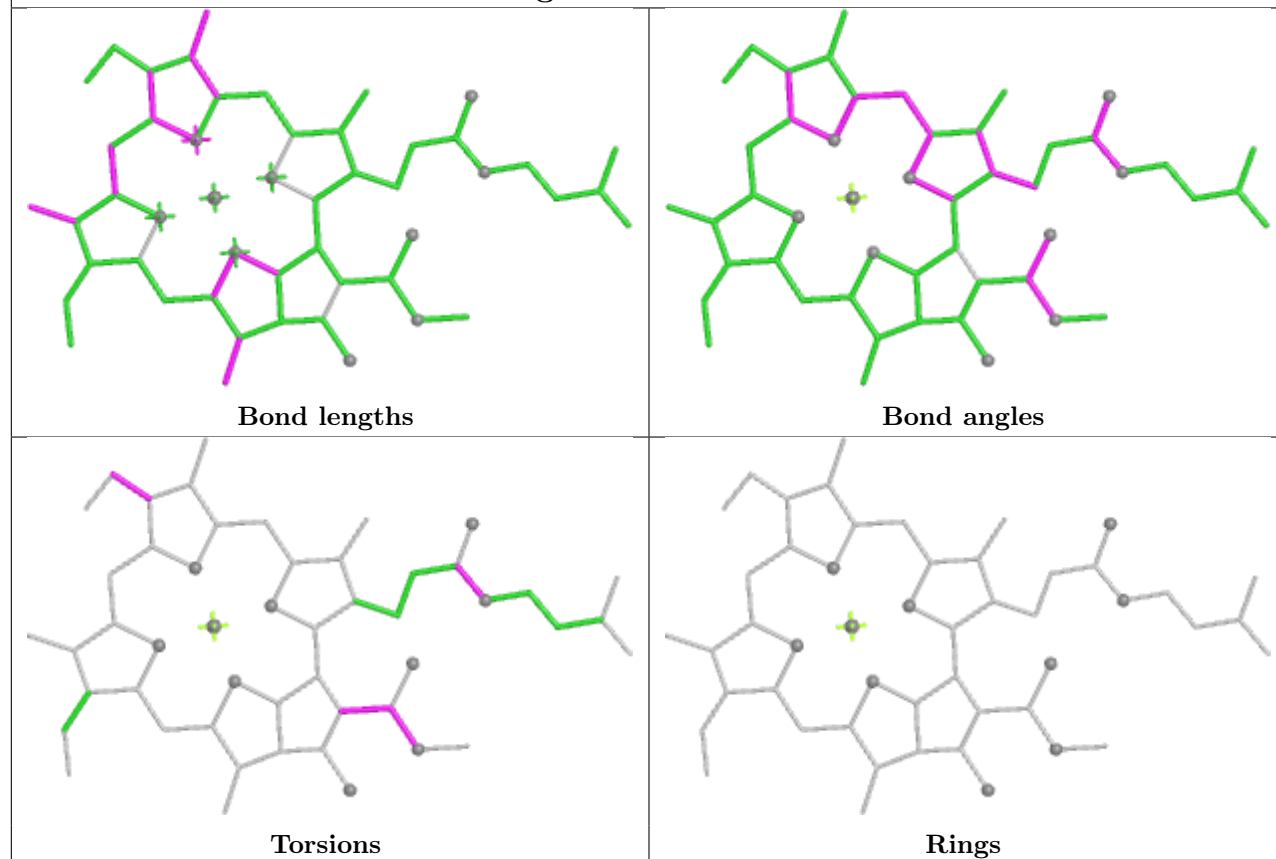
Ligand CLA f 1229



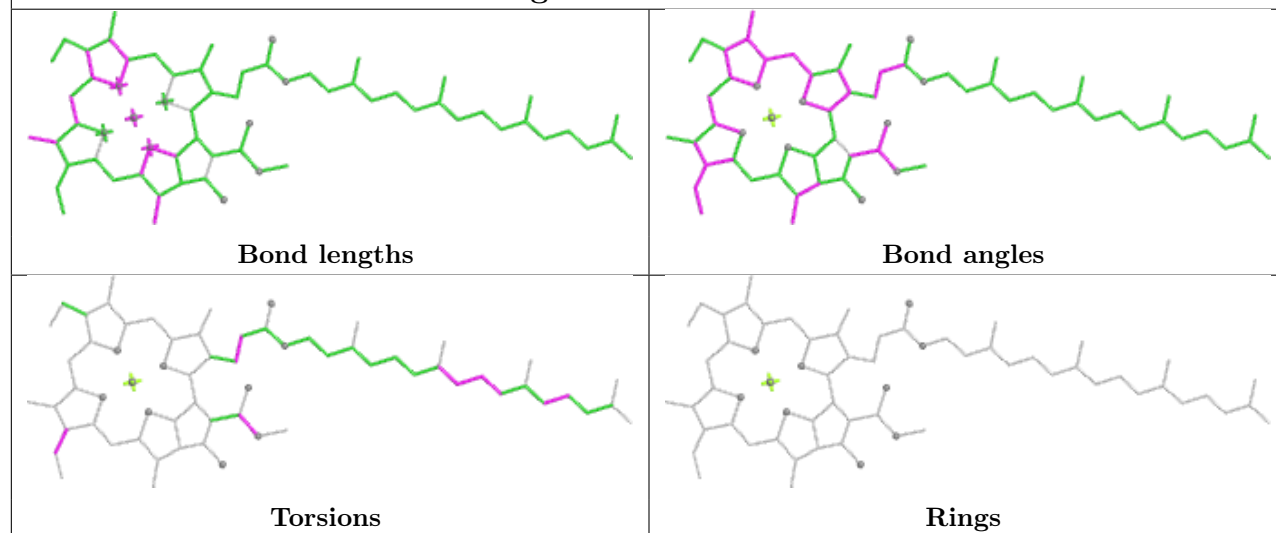
Ligand CLA 6 506

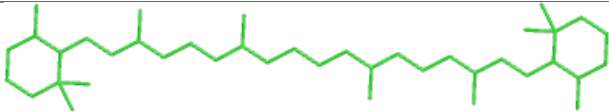
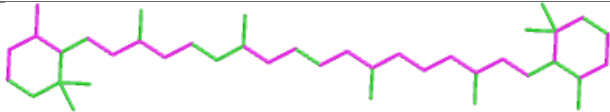
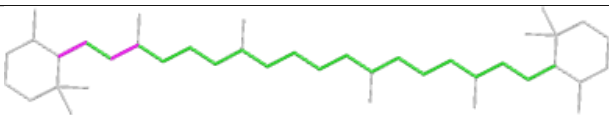
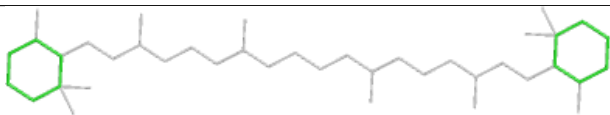


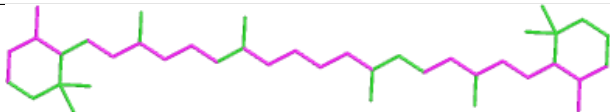
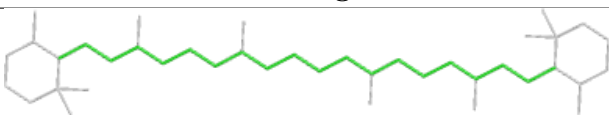
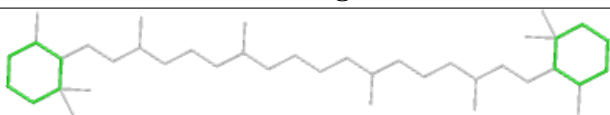
Ligand CLA 2 504

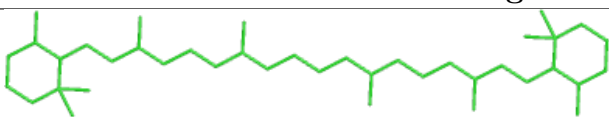
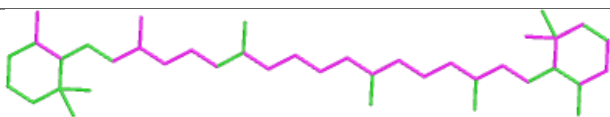
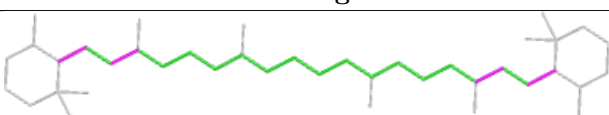
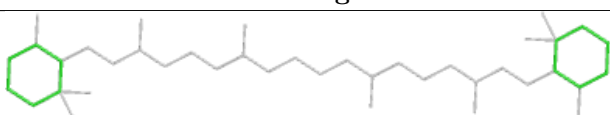


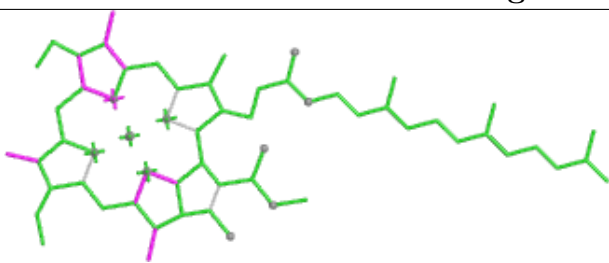
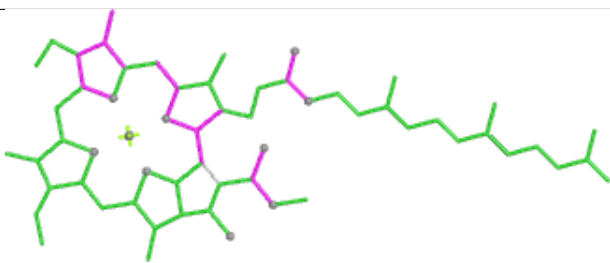
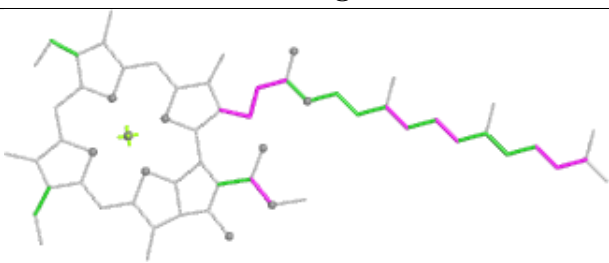
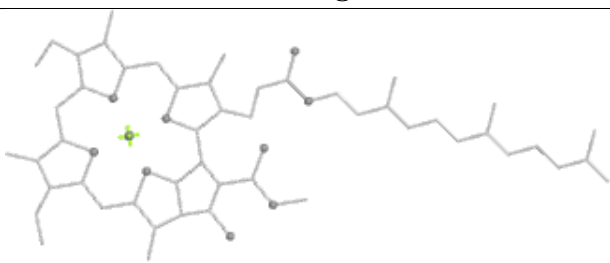
Ligand CLA f 1023

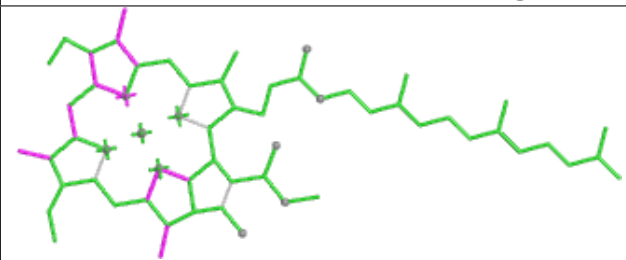
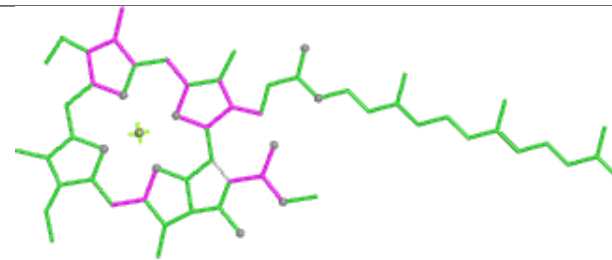
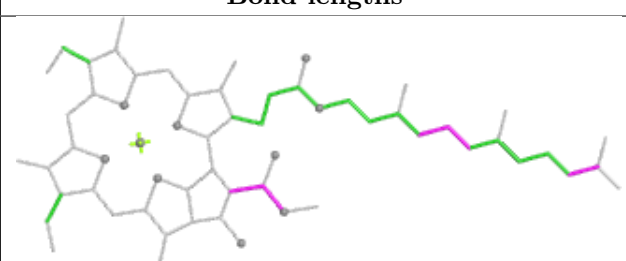
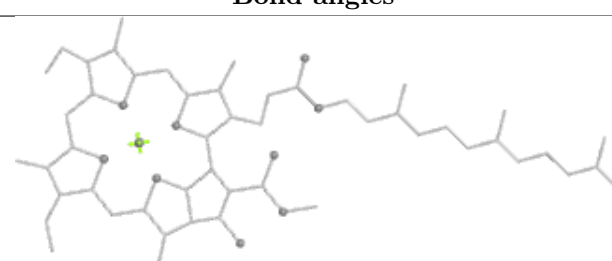


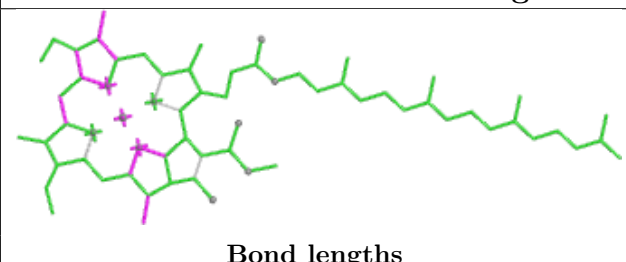
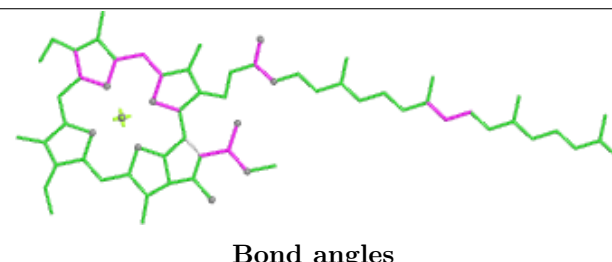
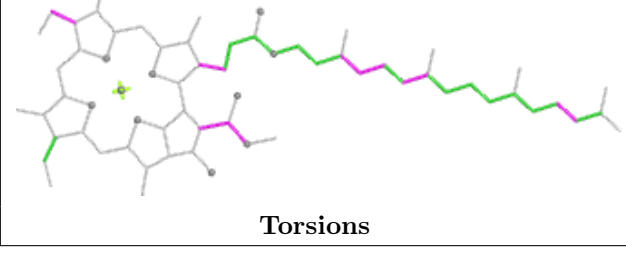
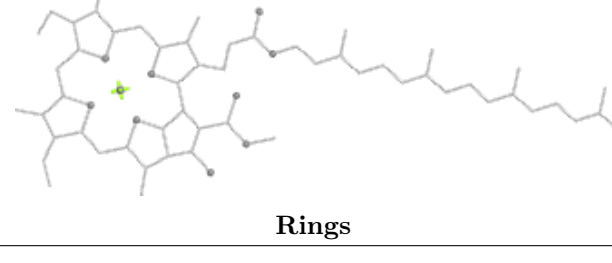
Ligand BCR 2 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

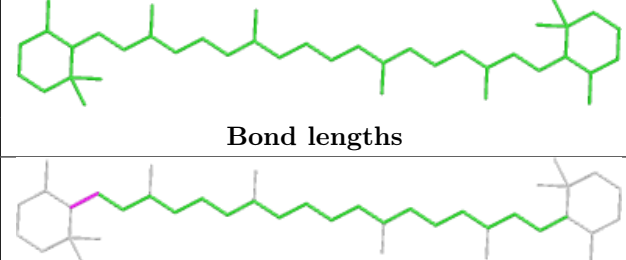
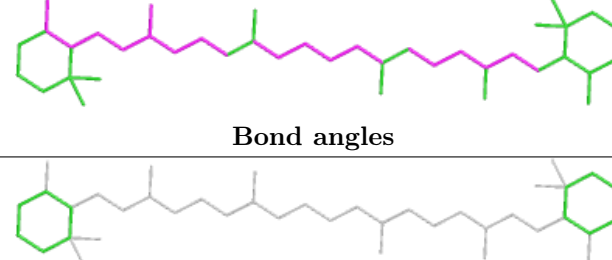
Ligand BCR G 4002	
	
Bond lengths	Bond angles
	
Torsions	Rings

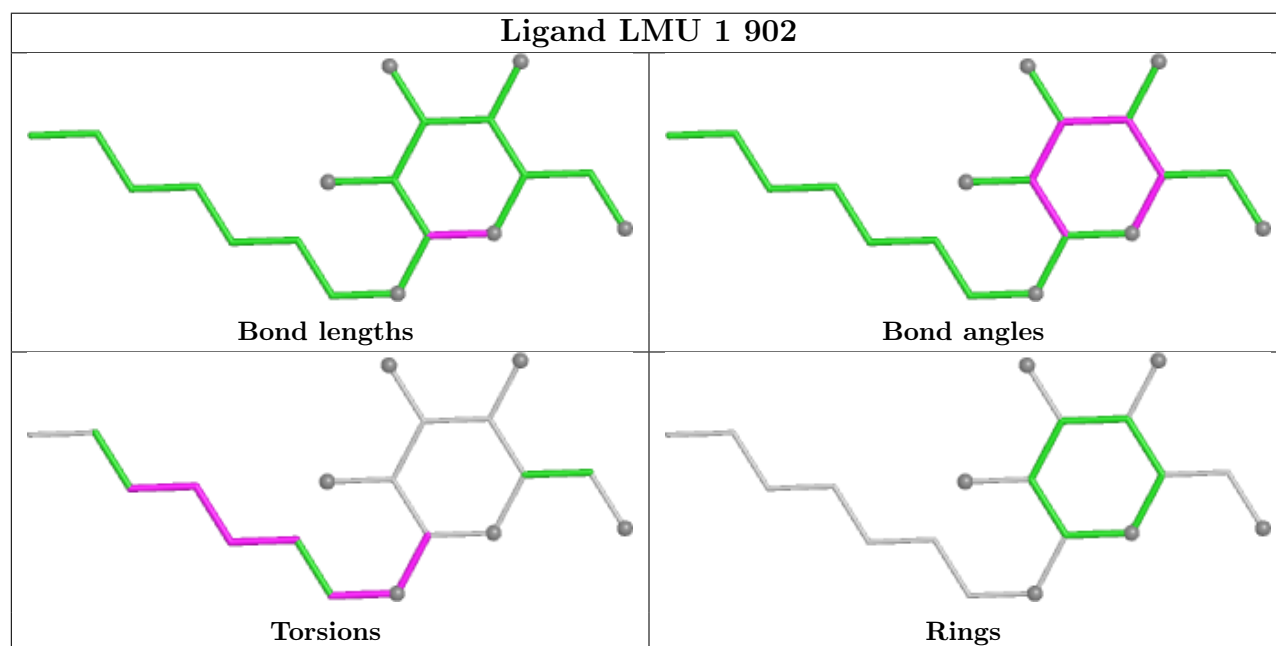
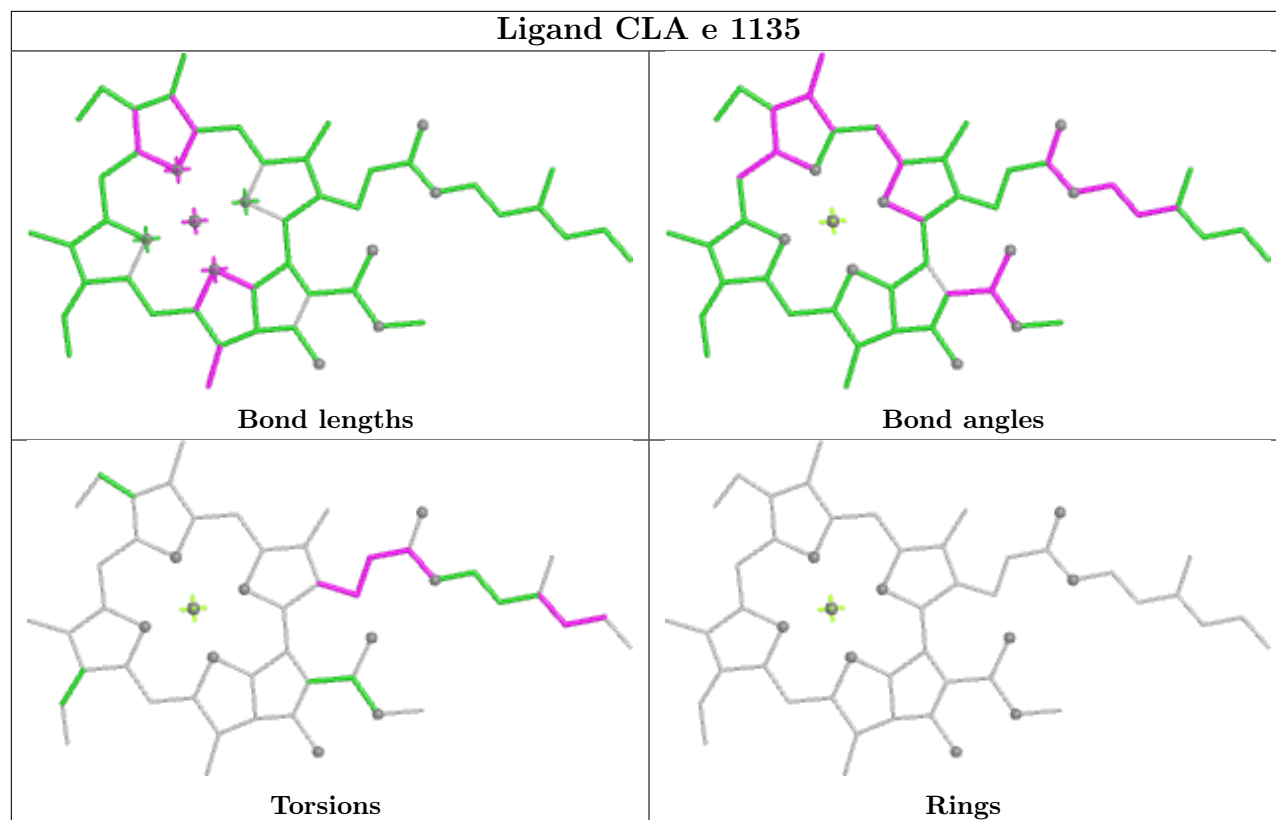
Ligand BCR f 4004	
	
Bond lengths	Bond angles
	
Torsions	Rings

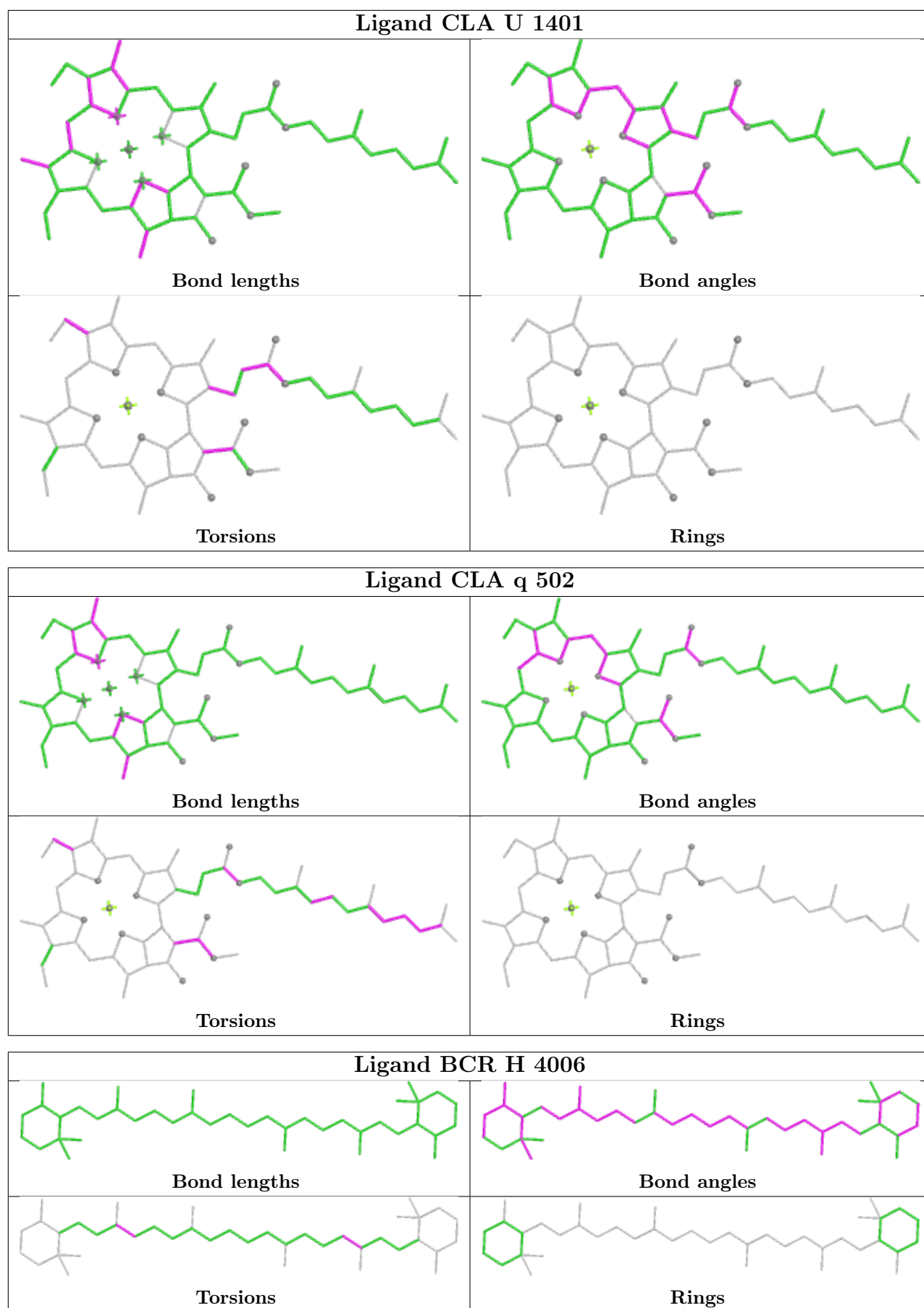
Ligand CLA f 1224	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1222	
	
Bond lengths	Bond angles
	
Torsions	Rings

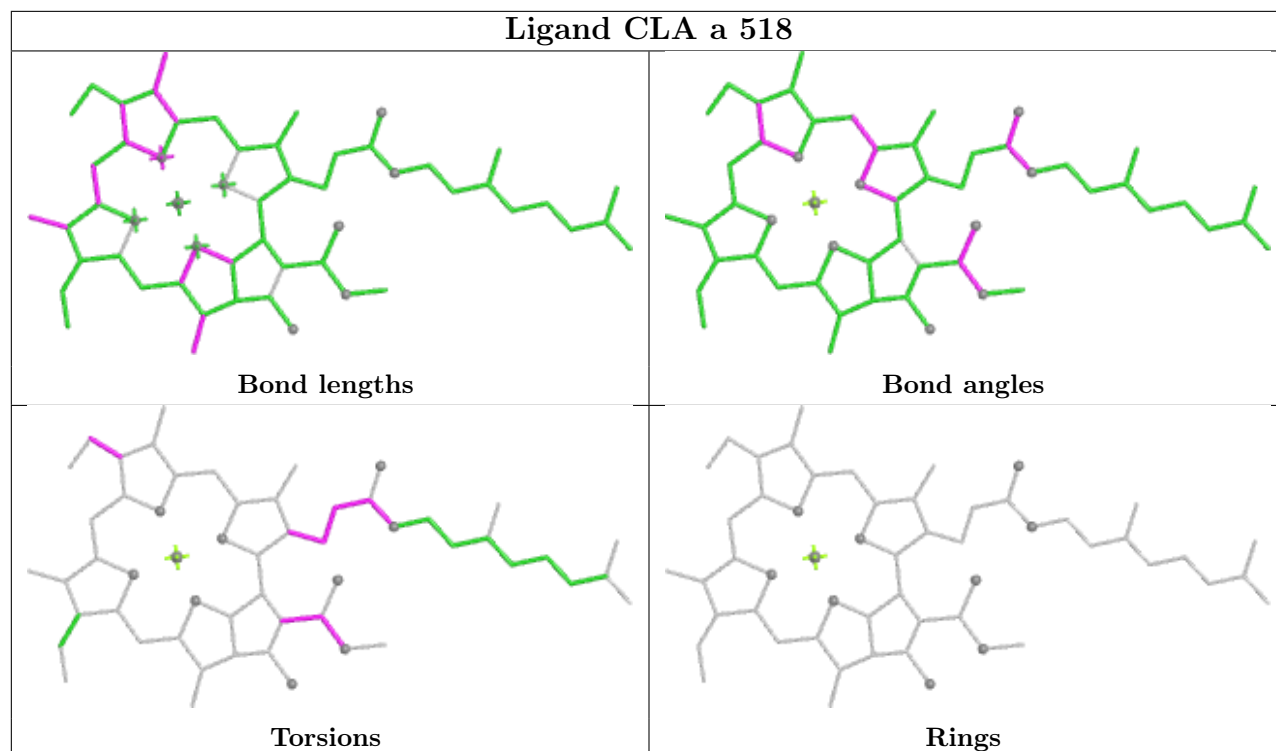
Ligand CLA A 1139	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 4017	
	
Bond lengths	Bond angles
	
Torsions	Rings

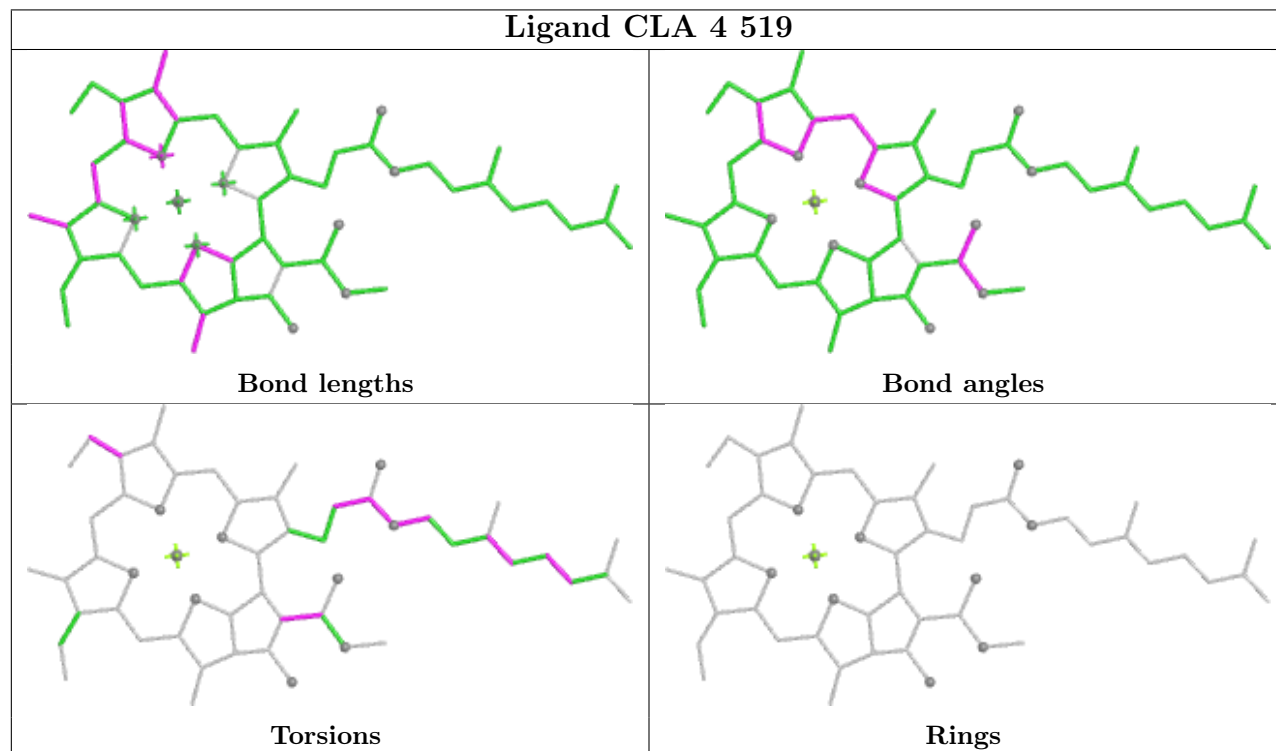


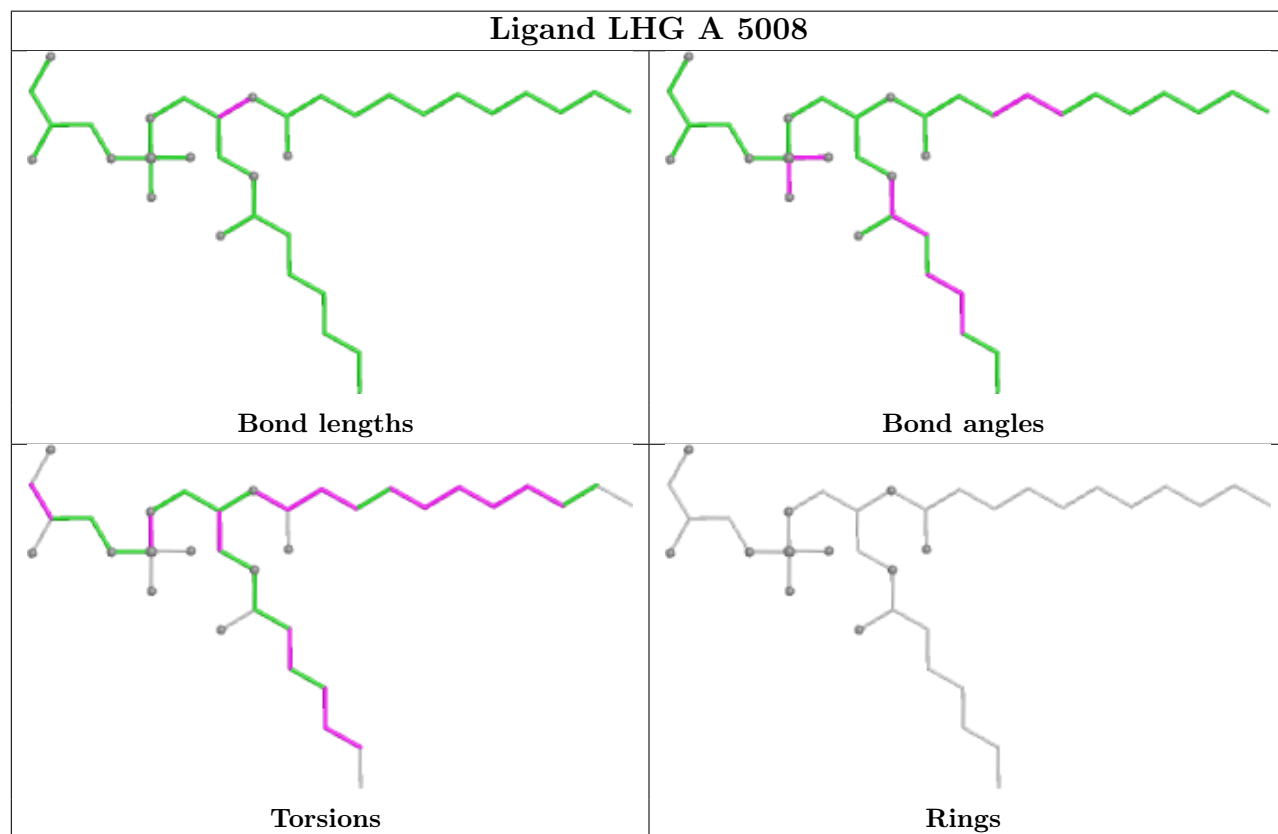
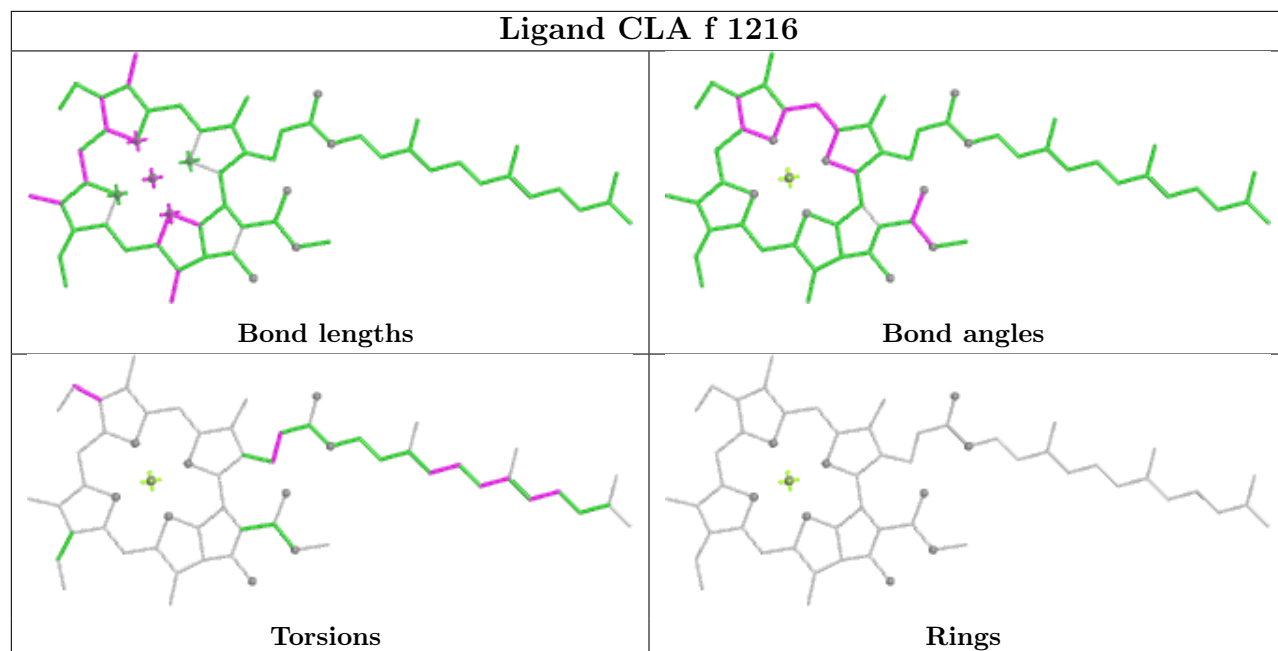


Ligand CLA a 518

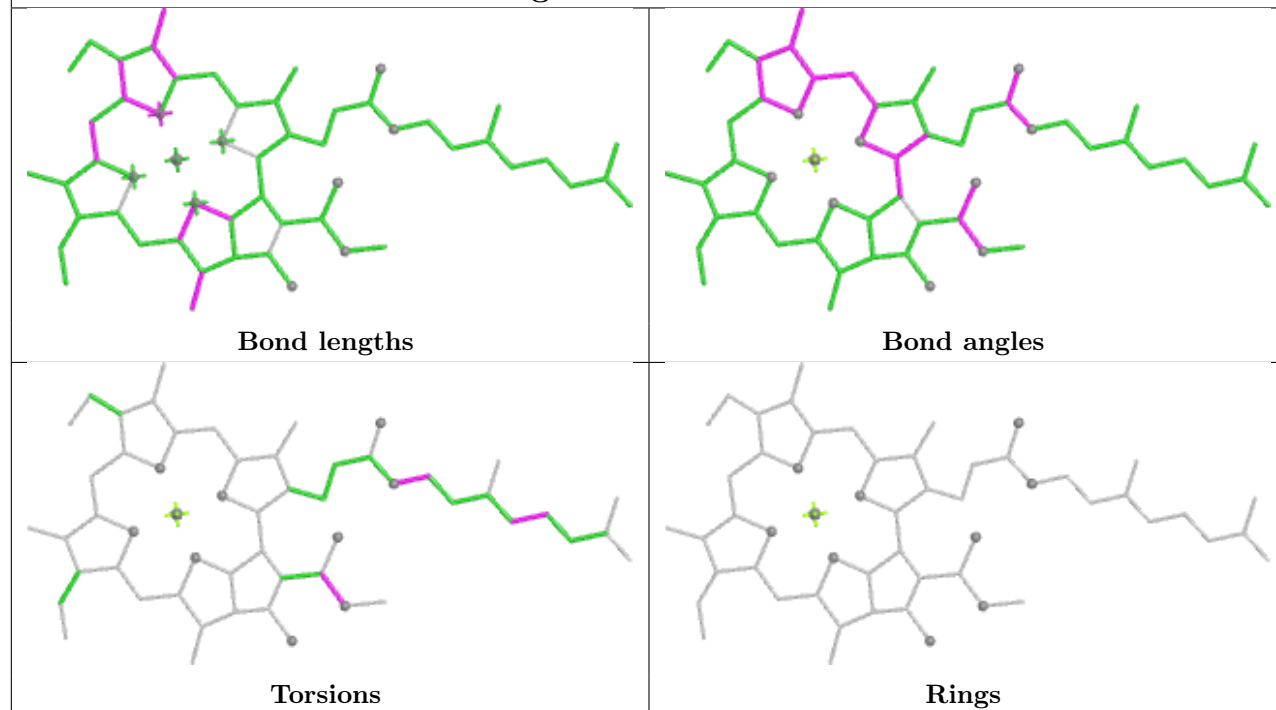


Ligand CLA 4 519

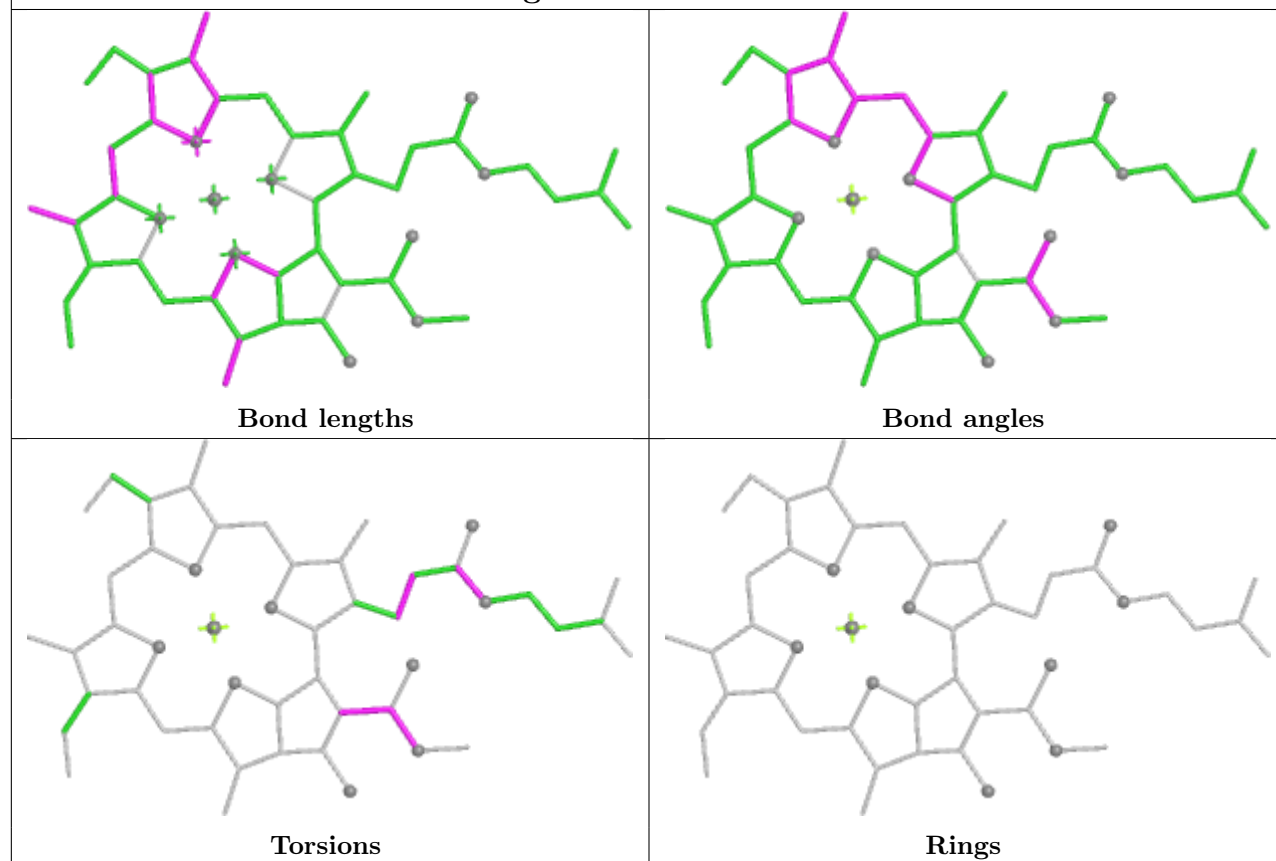


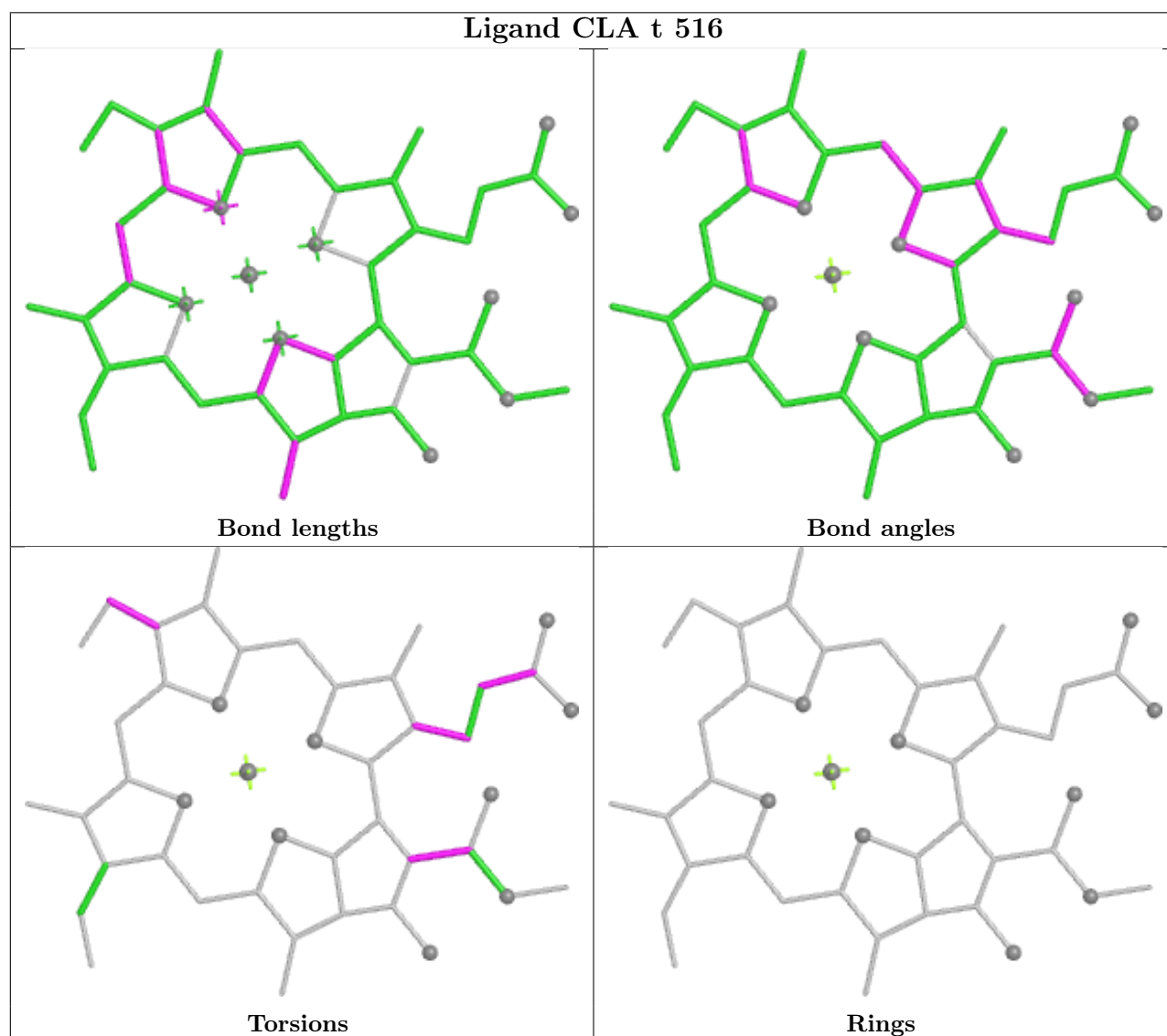
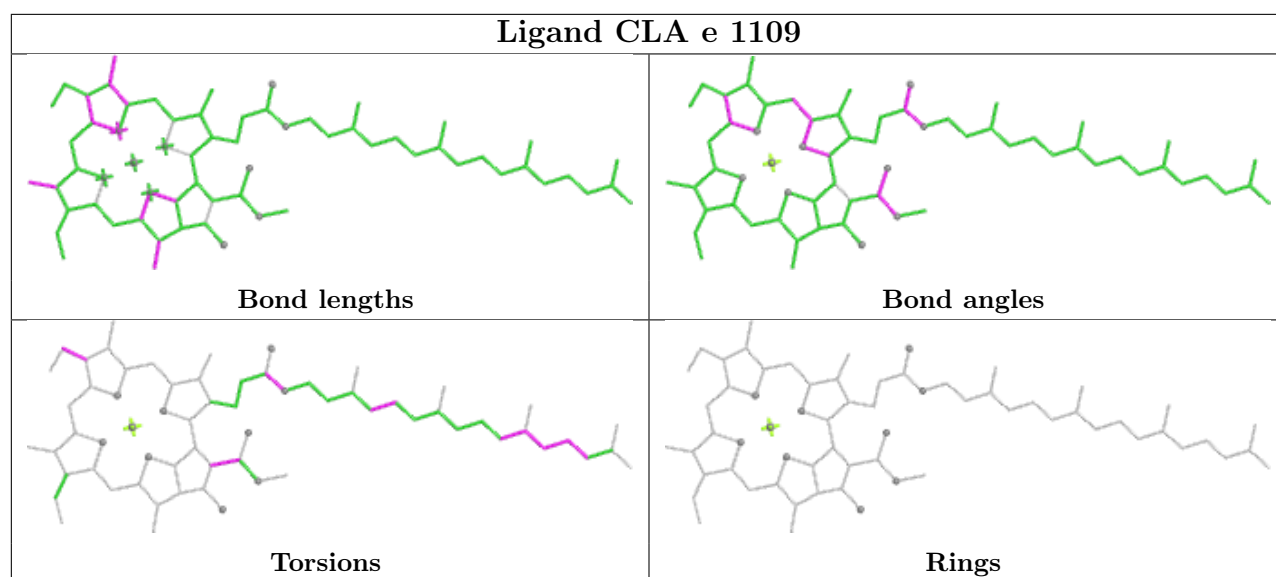


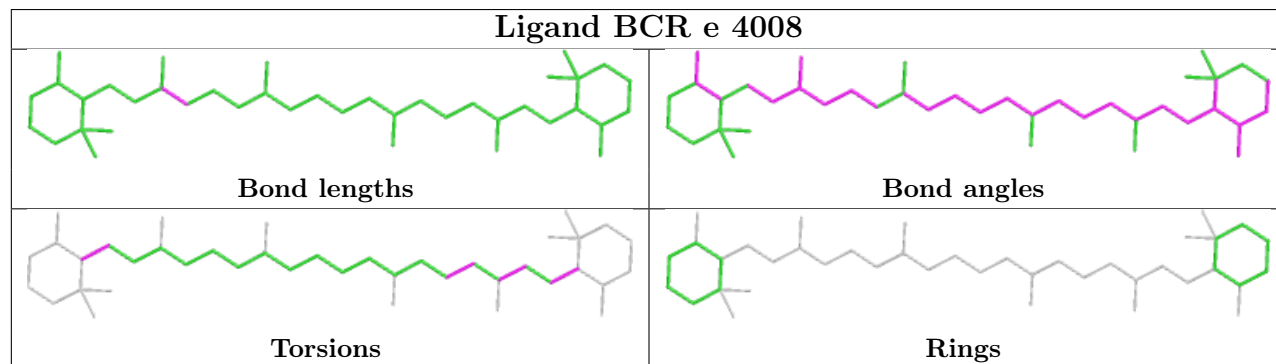
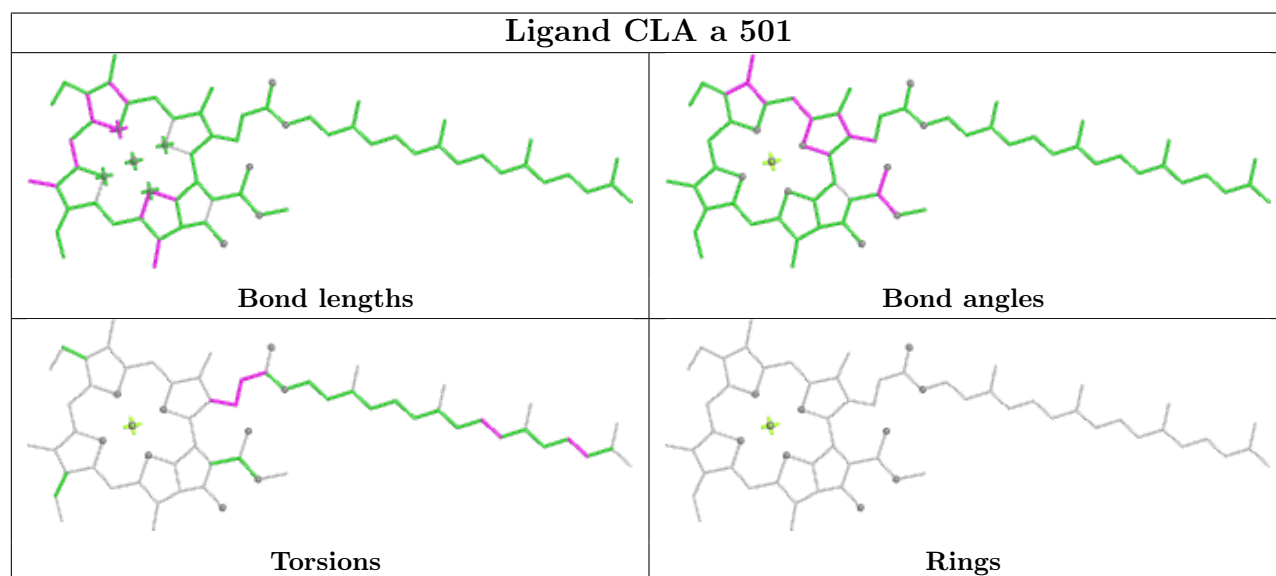
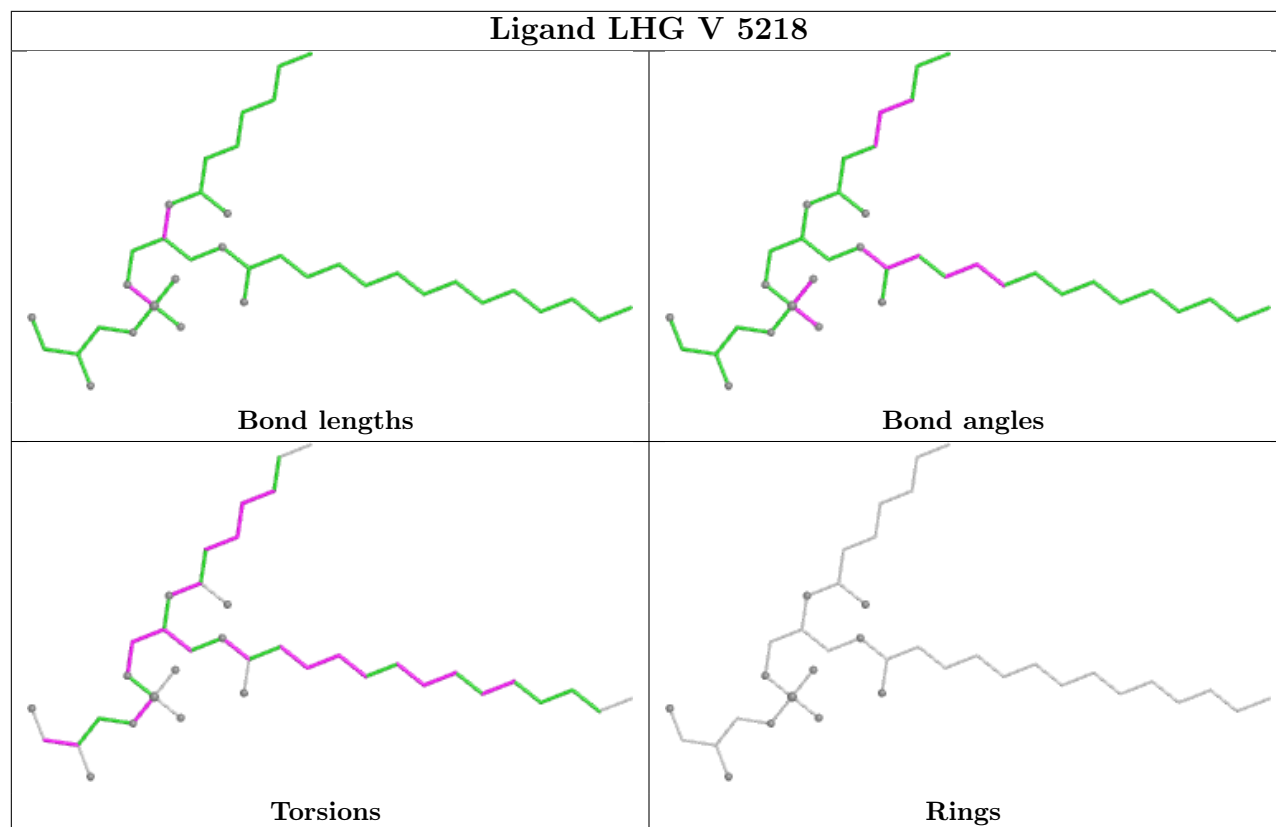
Ligand CLA Y 511



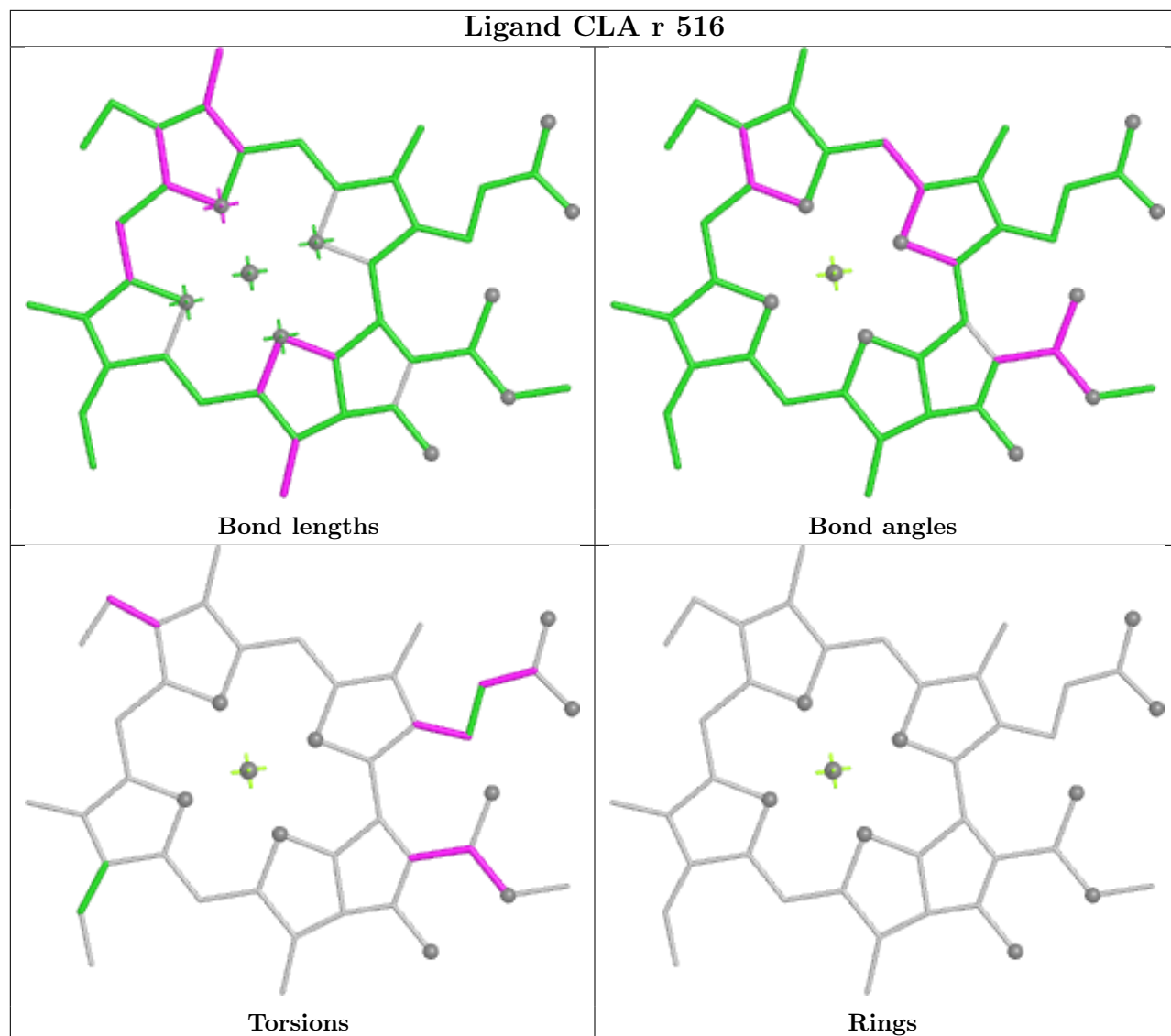
Ligand CLA B 1232



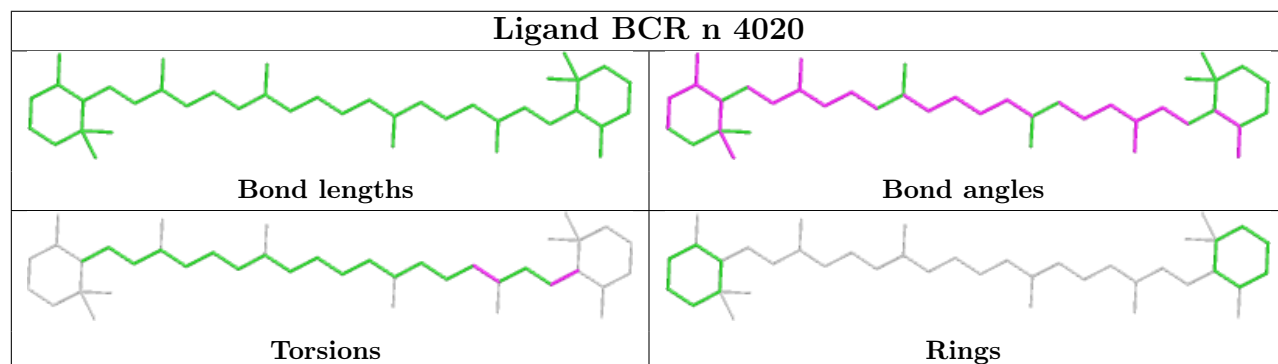


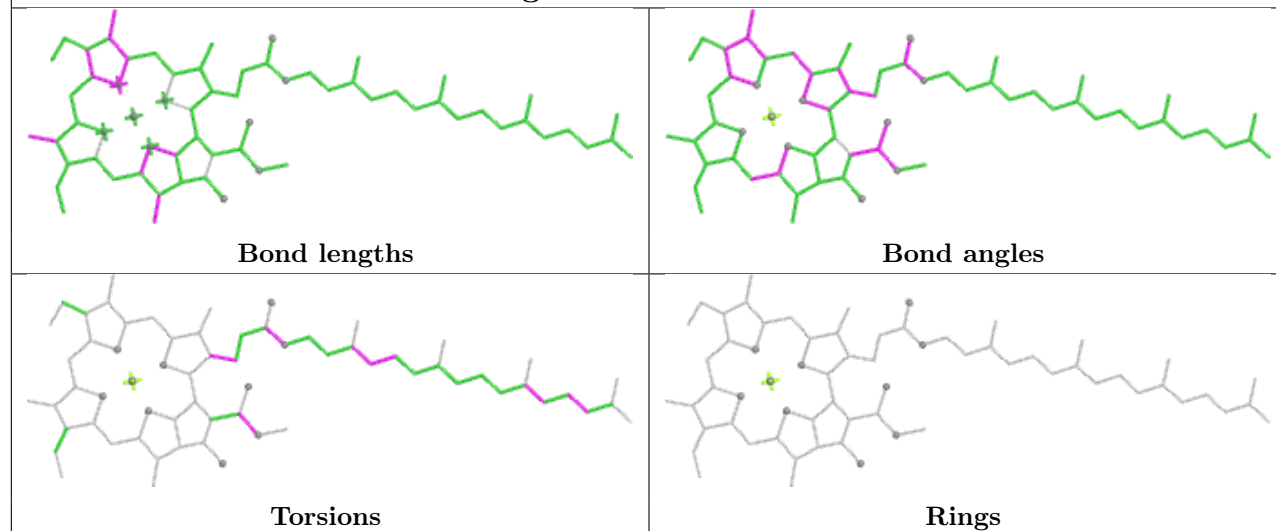
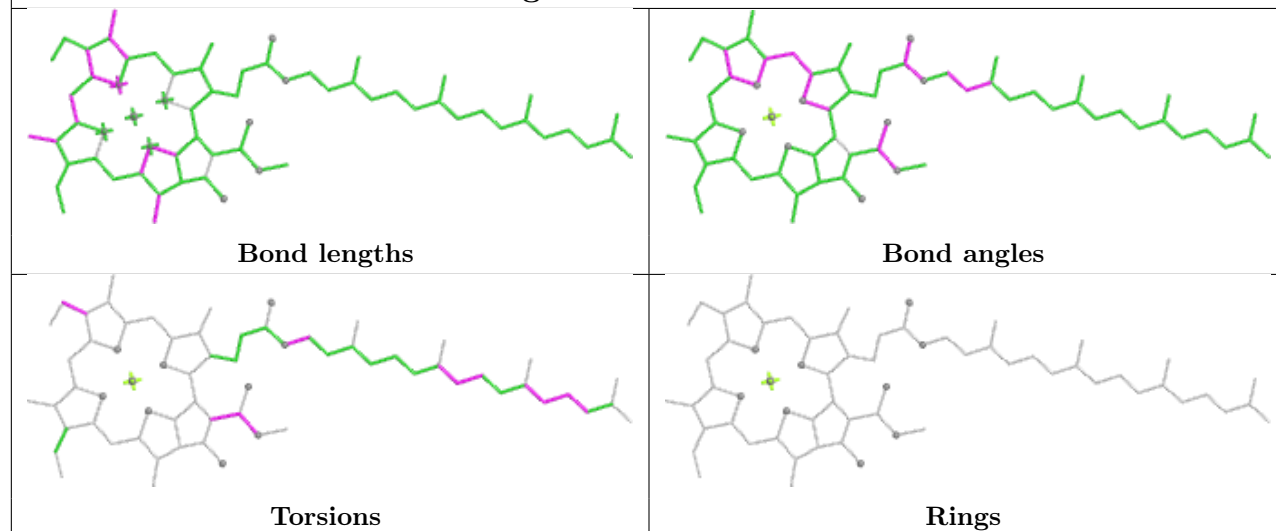


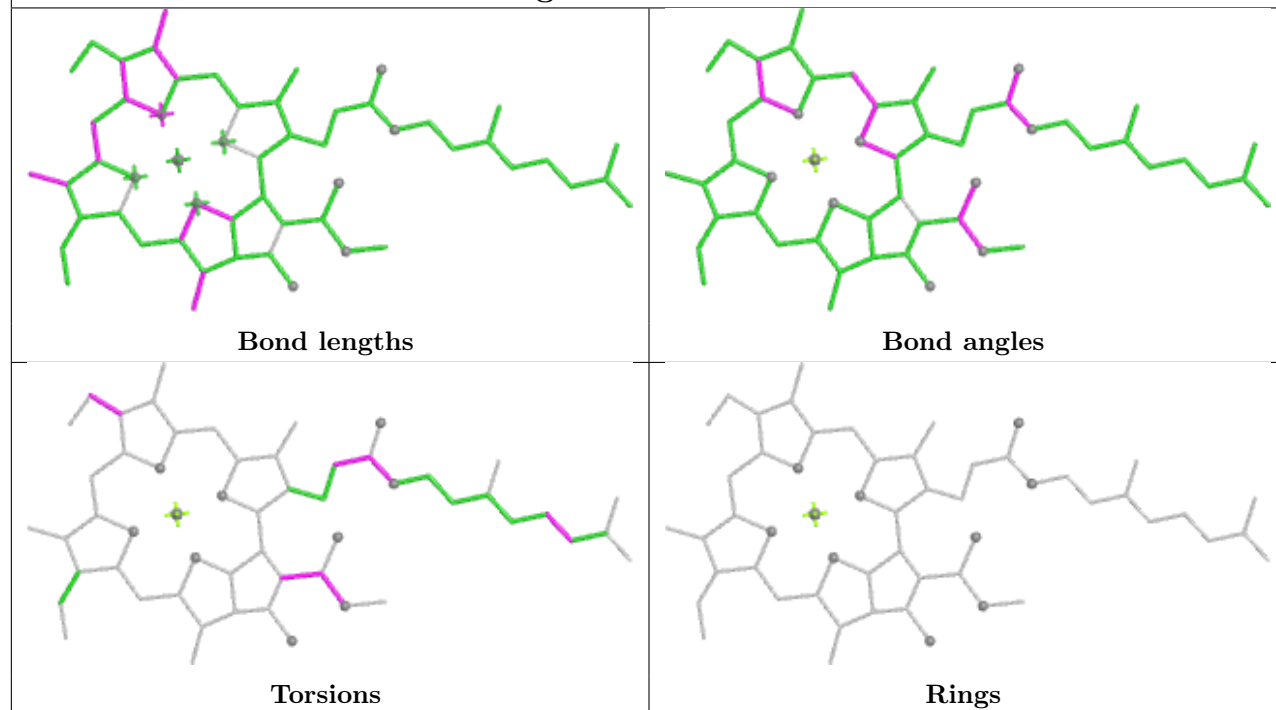
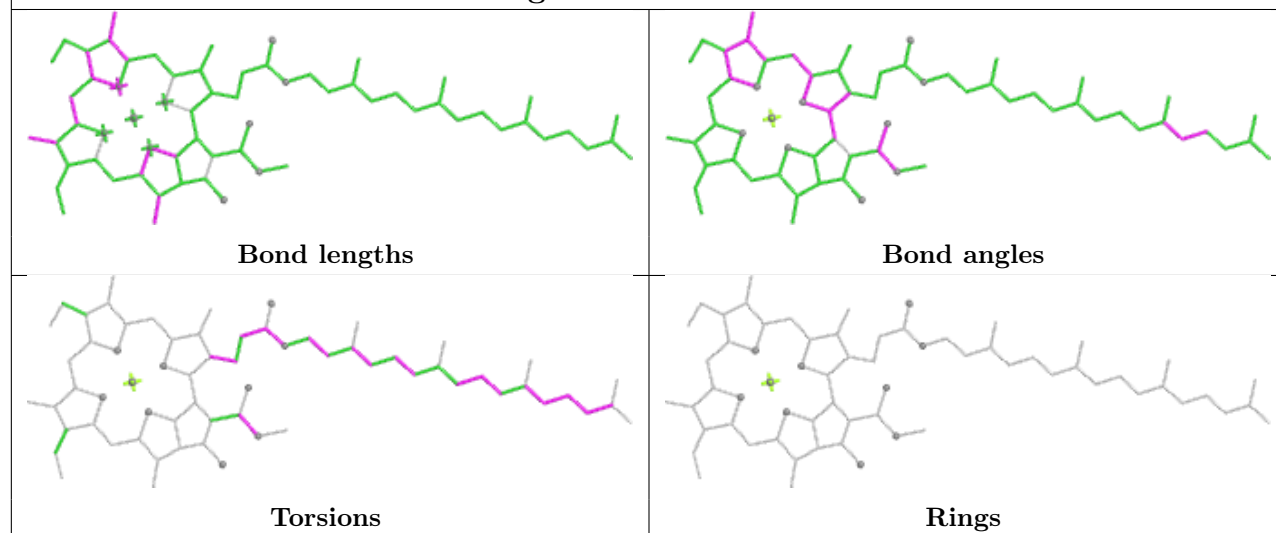
Ligand CLA r 516

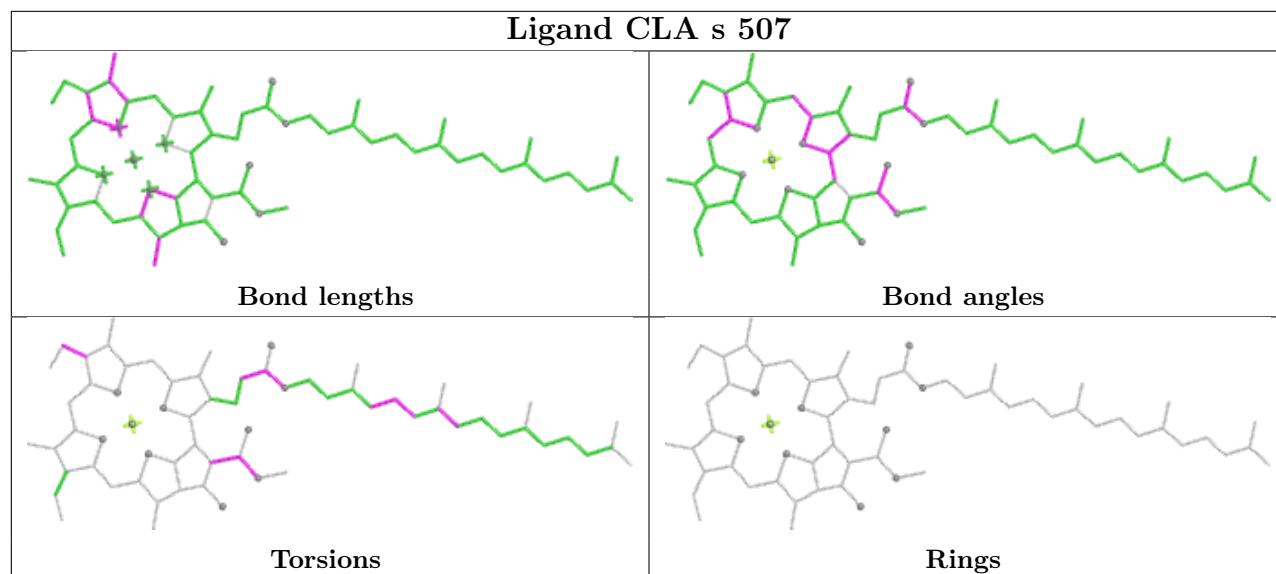
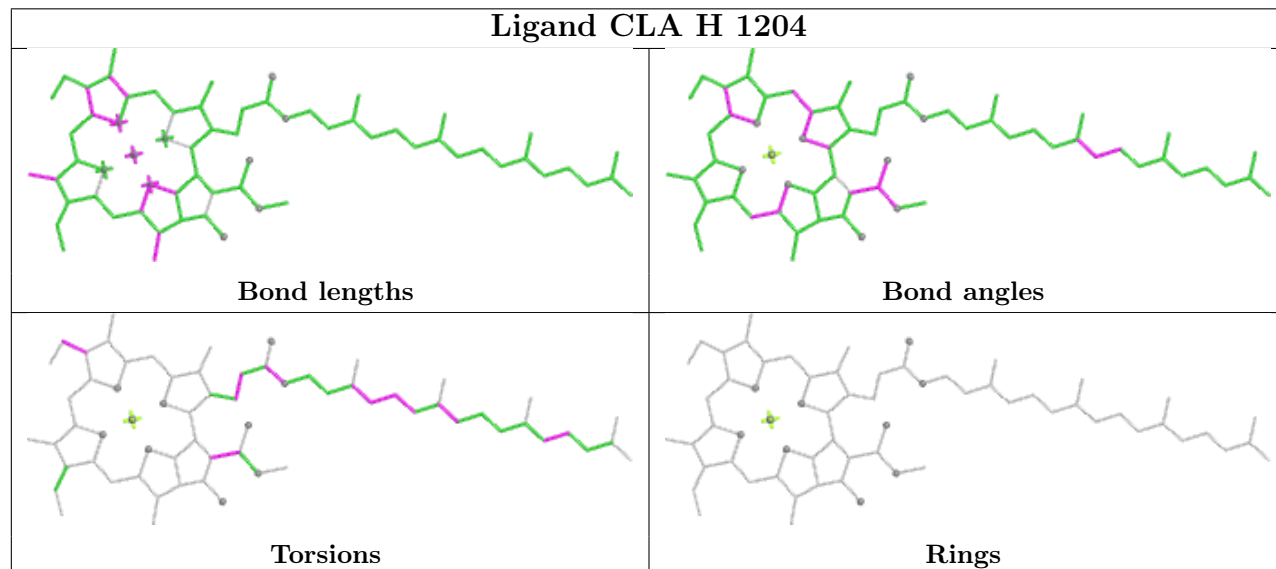


Ligand BCR n 4020

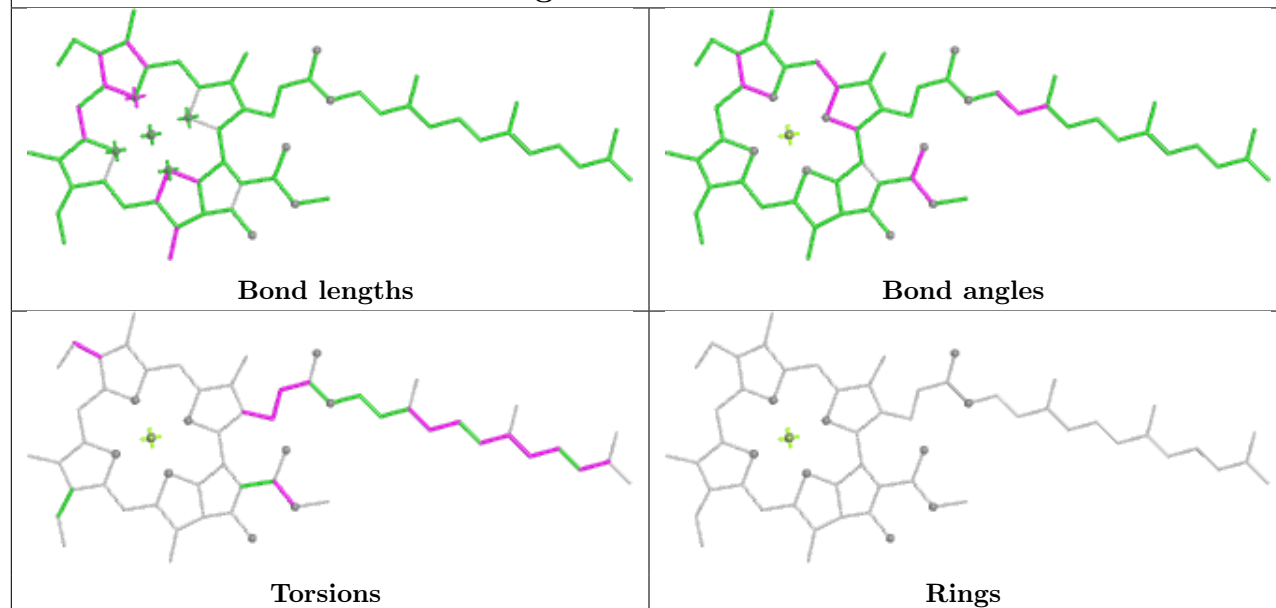


Ligand CLA G 1104**Ligand CLA A 1138**

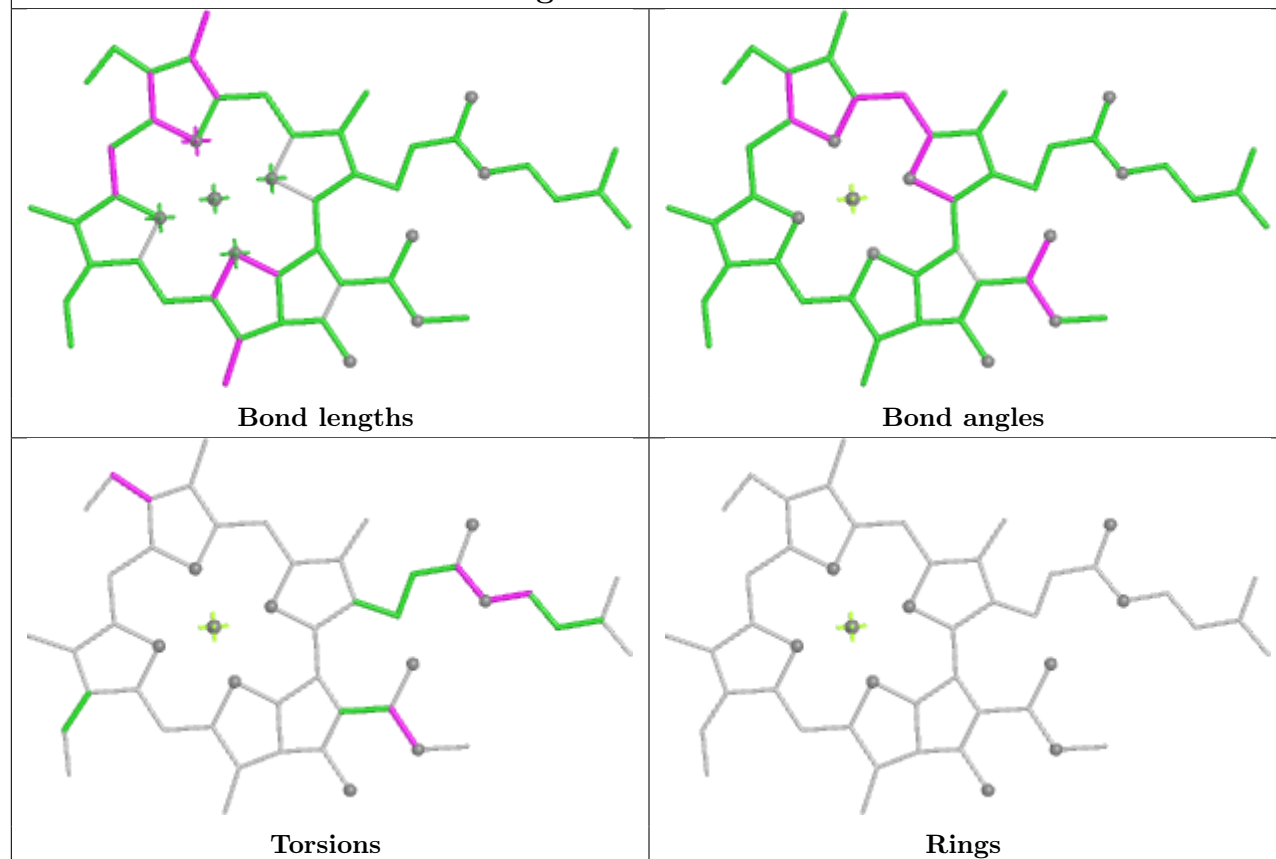
Ligand CLA 3 519**Ligand CLA e 1126**

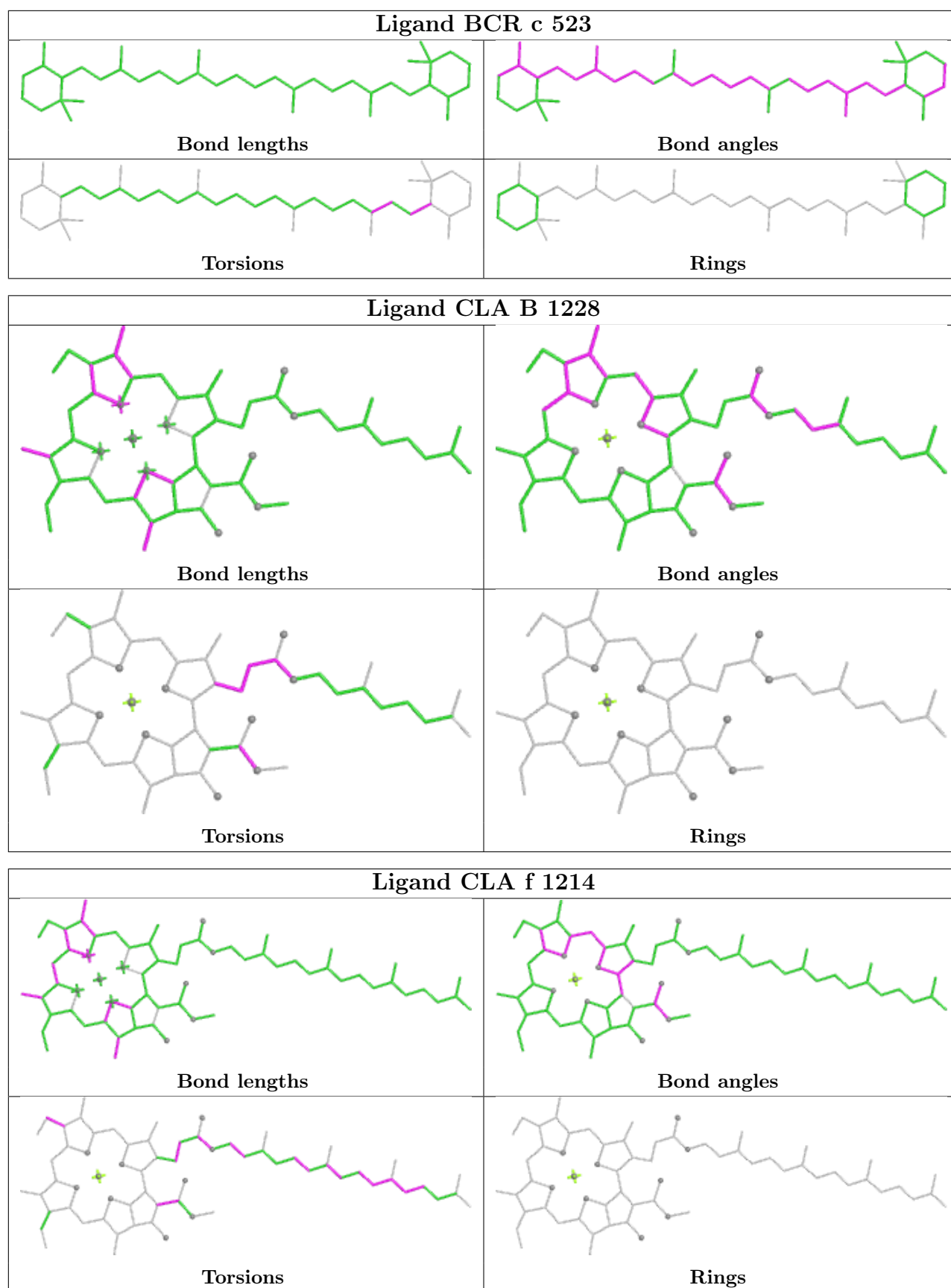
Ligand CLA s 507**Ligand CLA H 1204**

Ligand CLA d 501

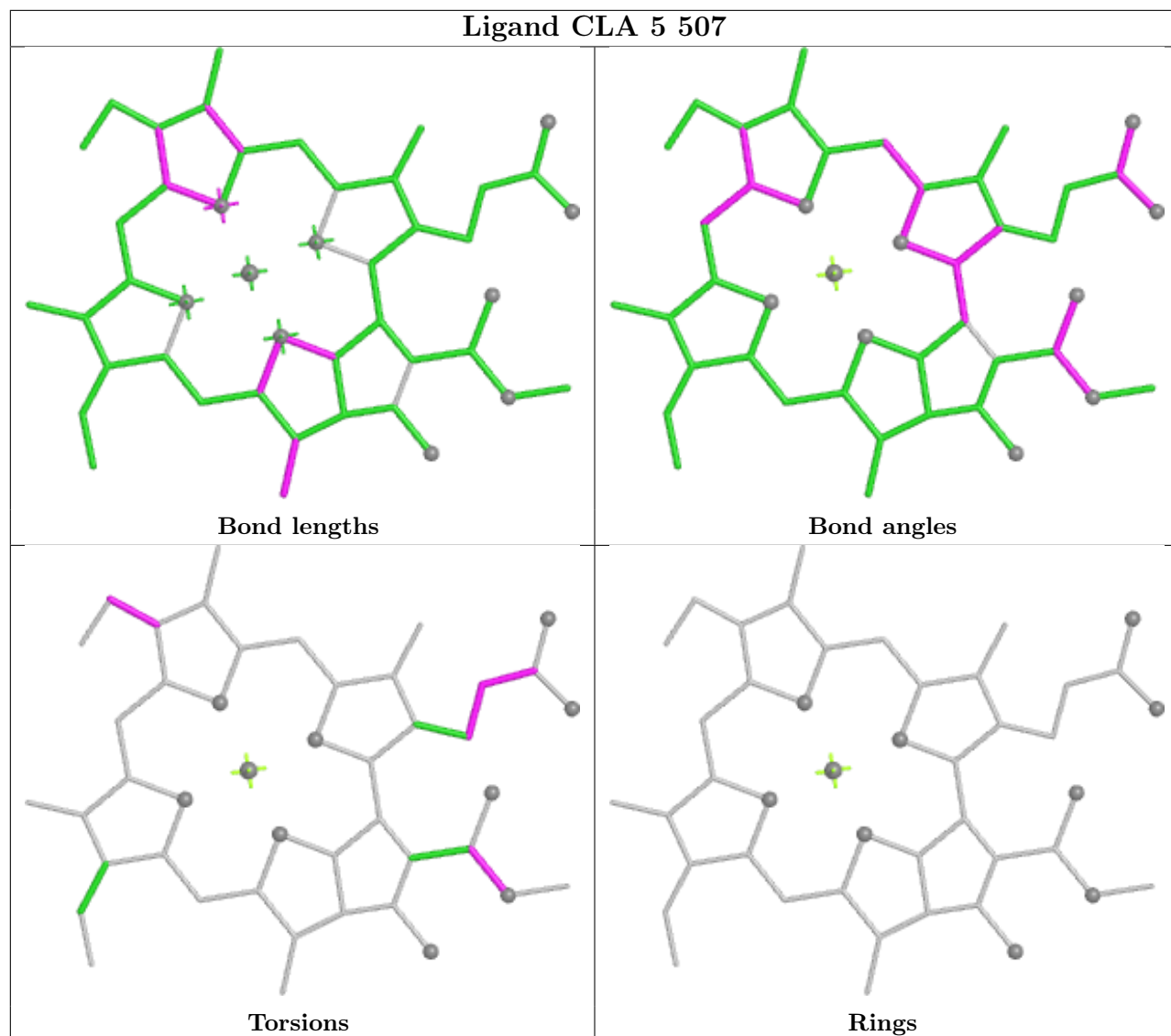


Ligand CLA 3 511

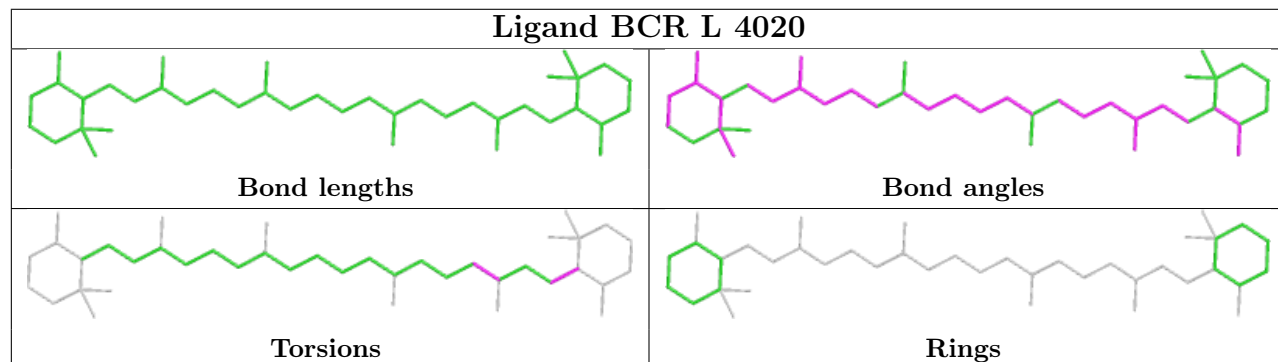


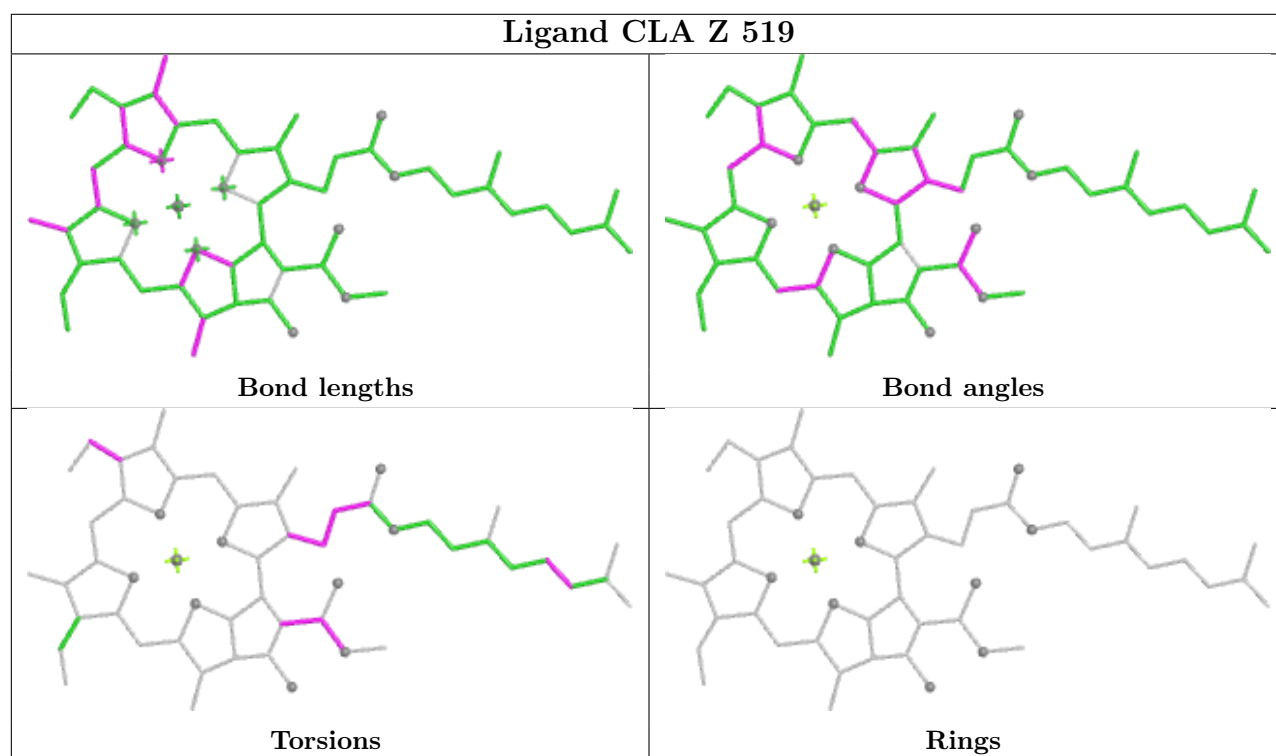
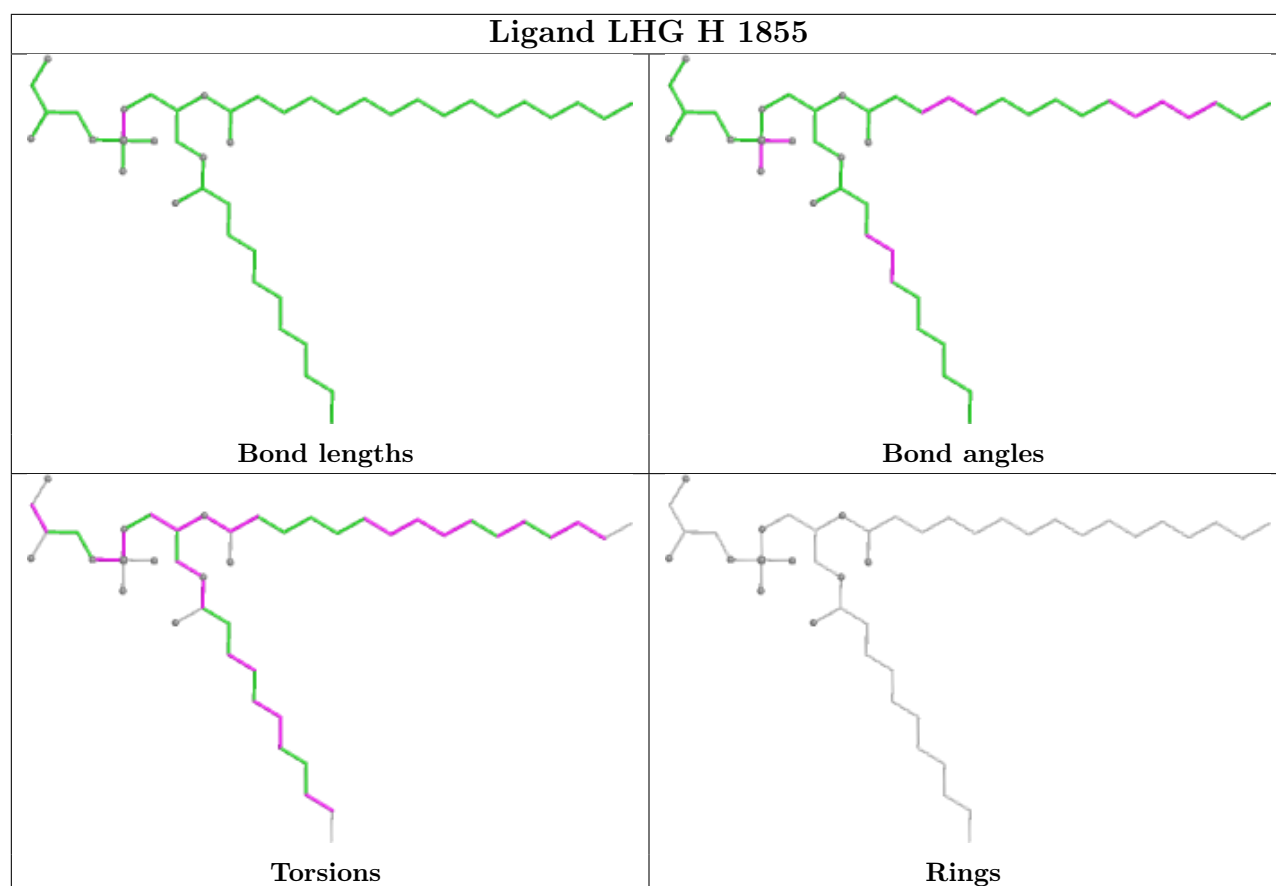


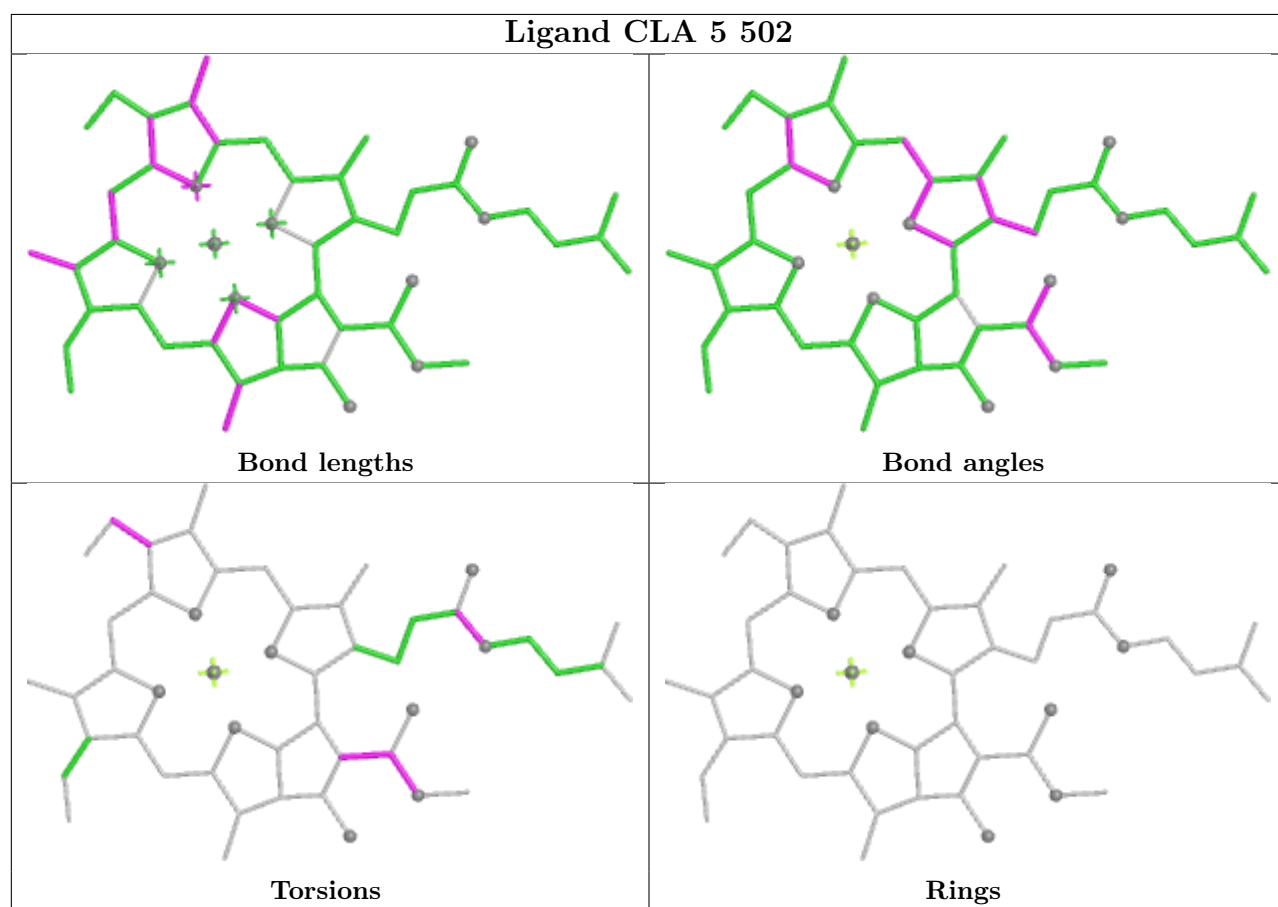
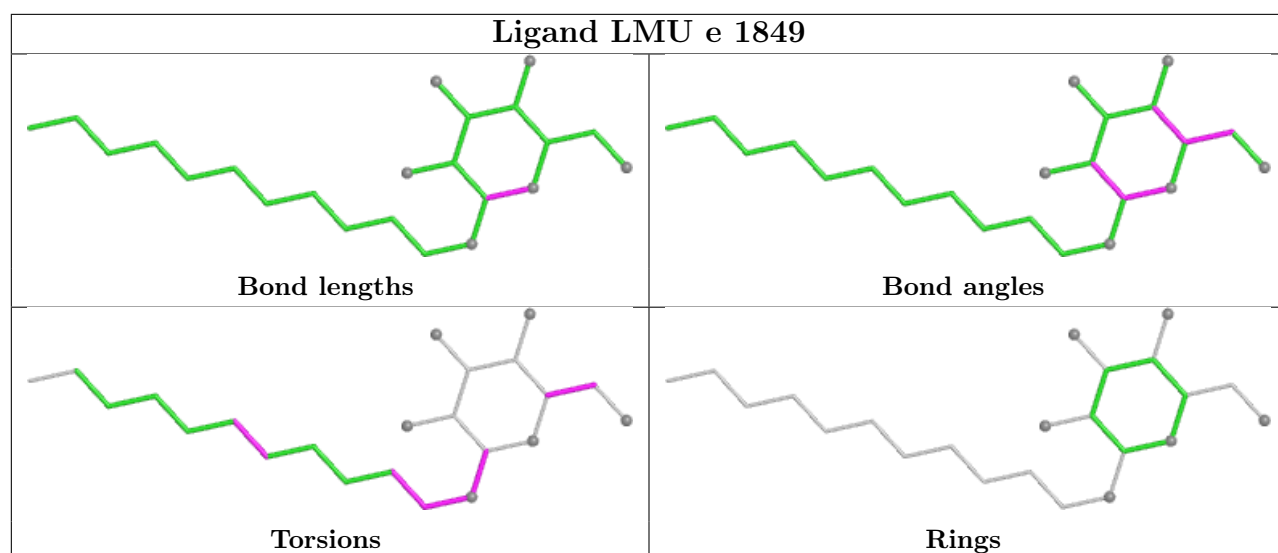
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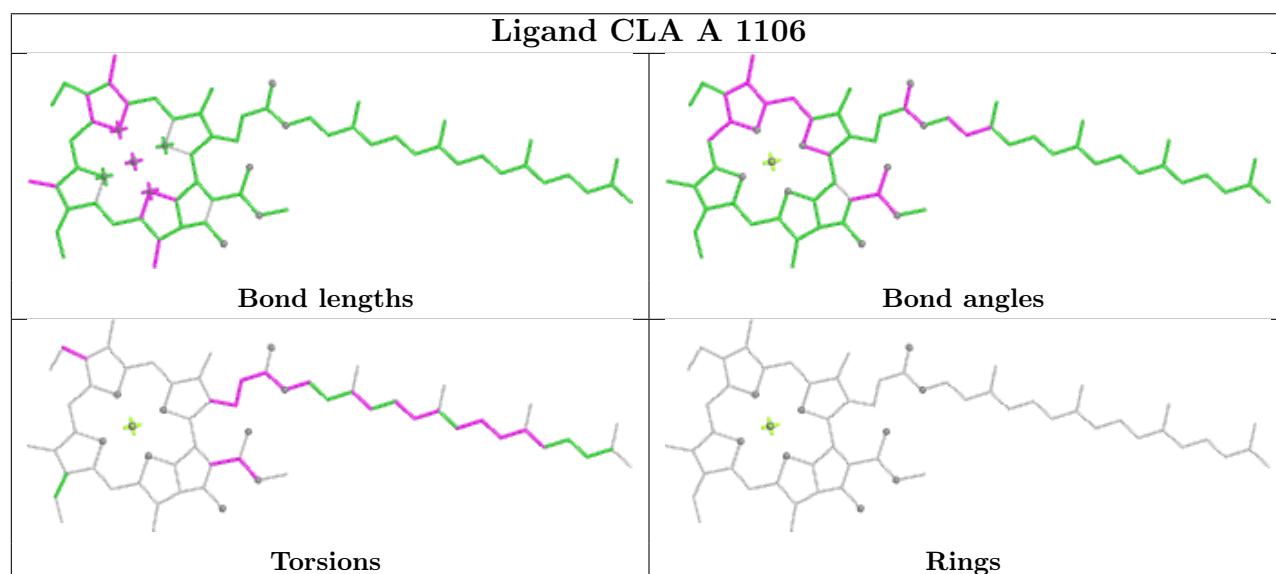
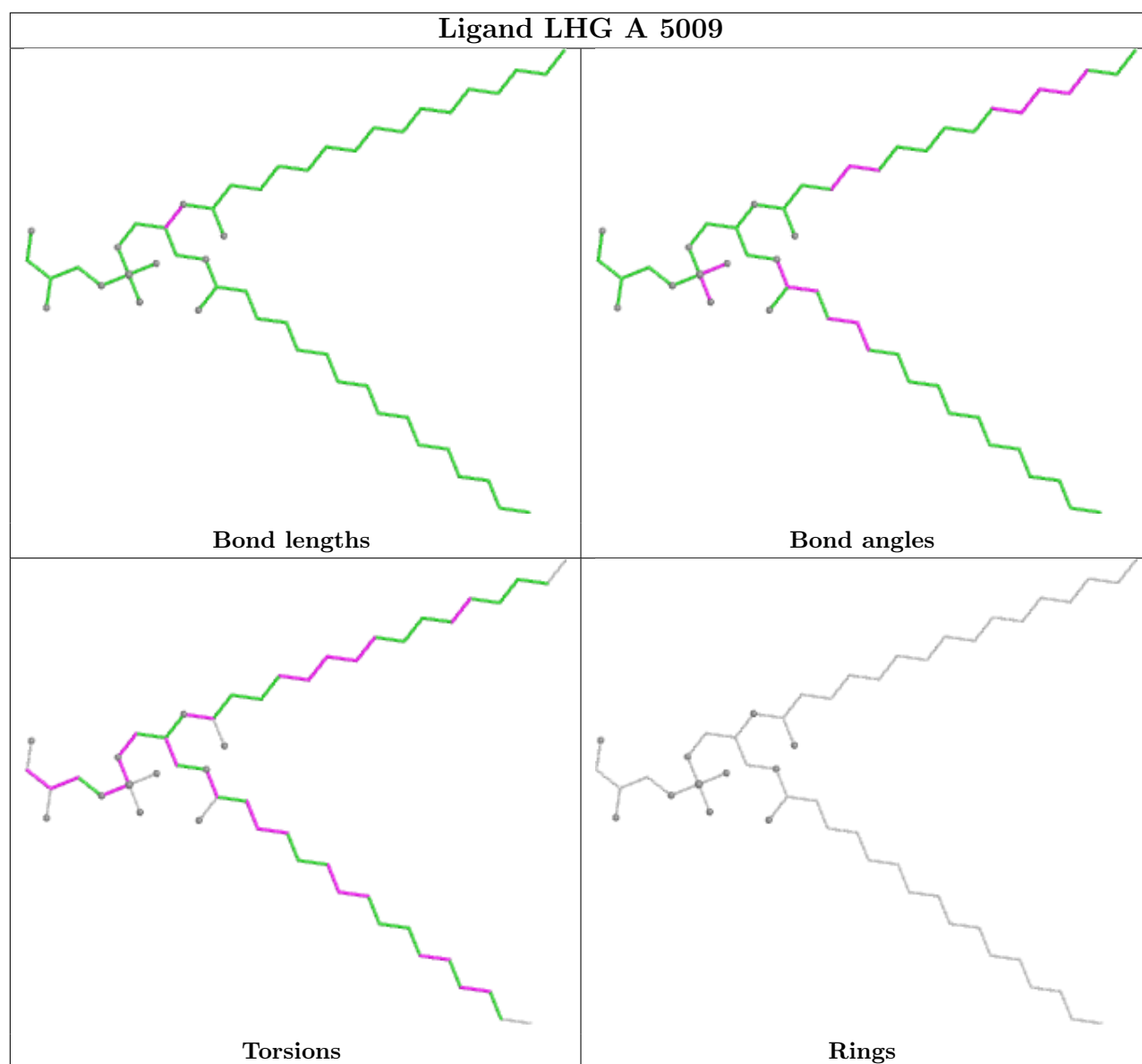


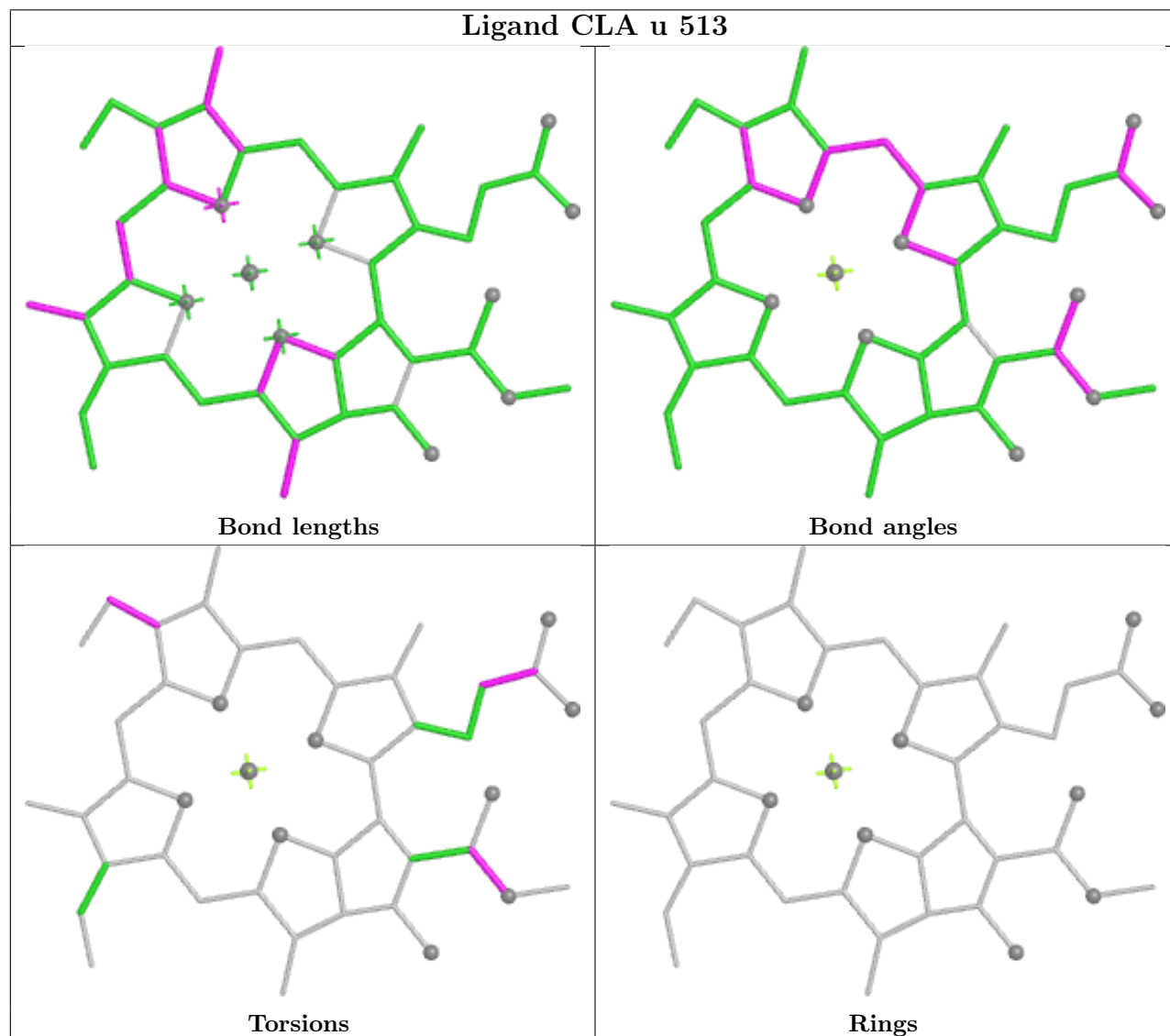
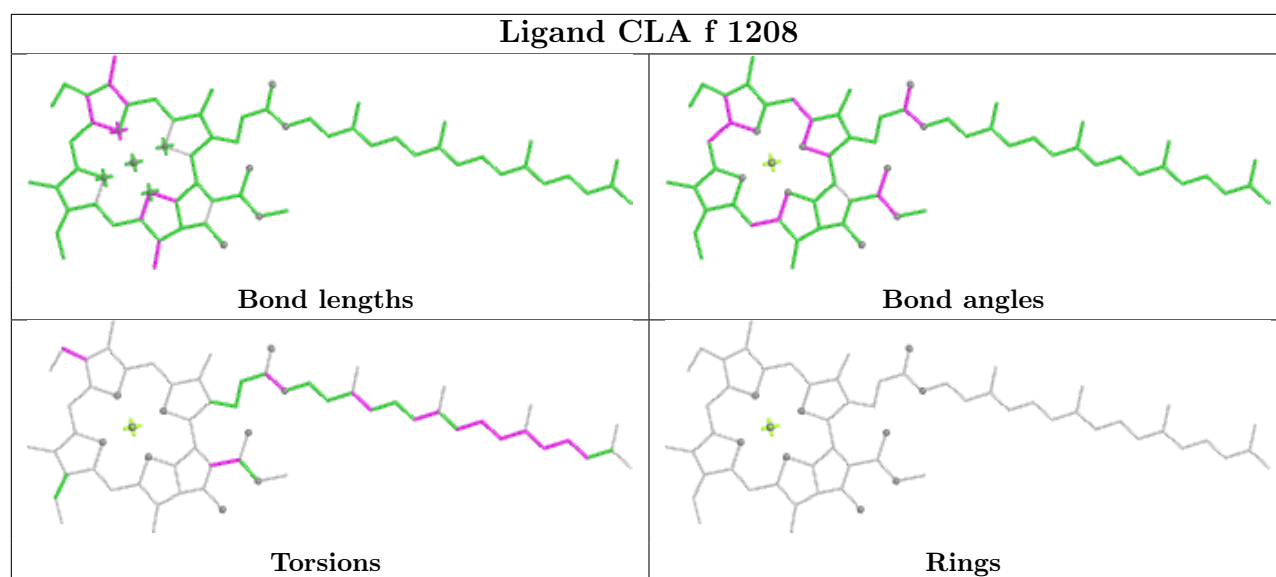
Ligand BCR L 4020

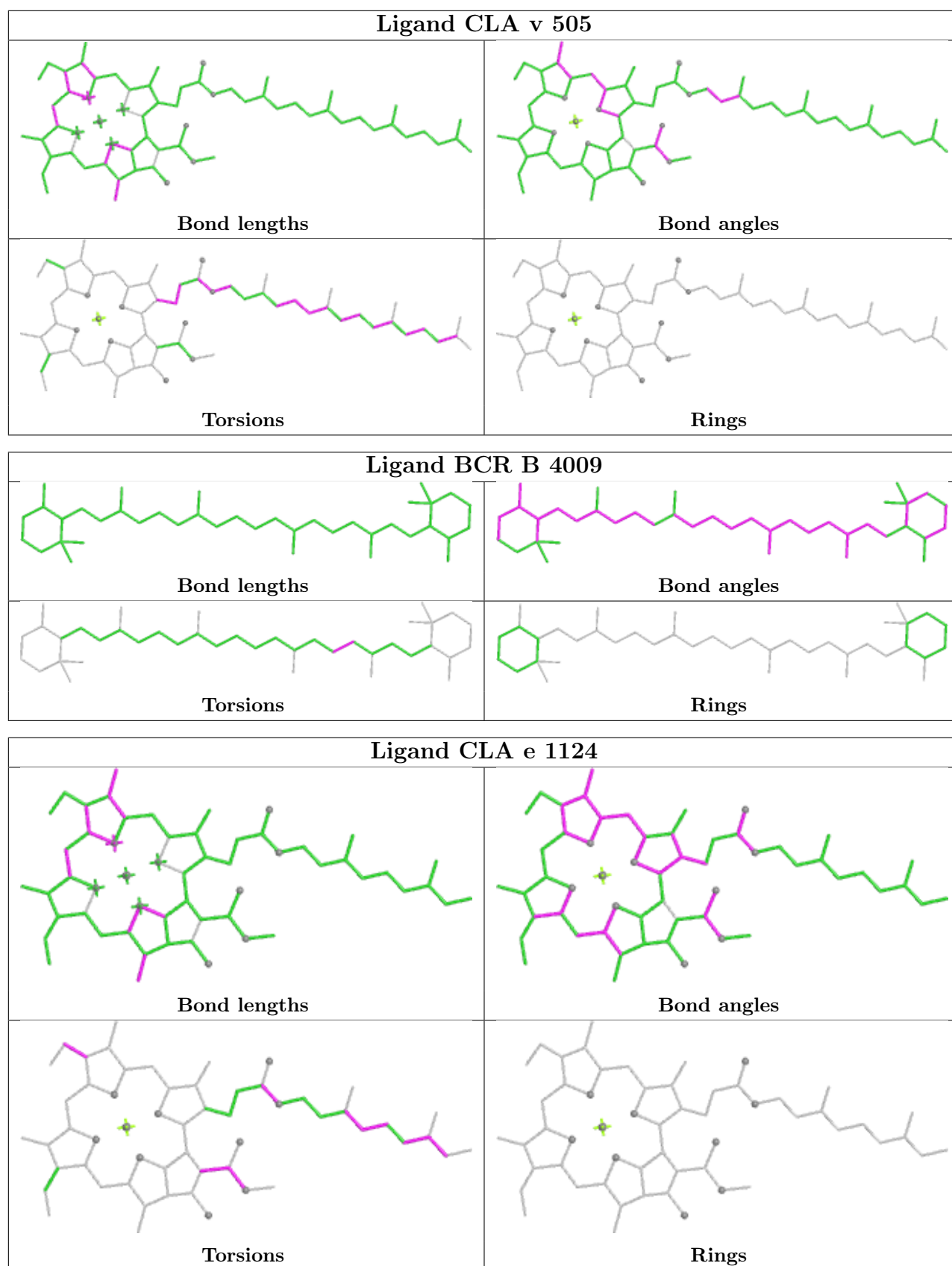


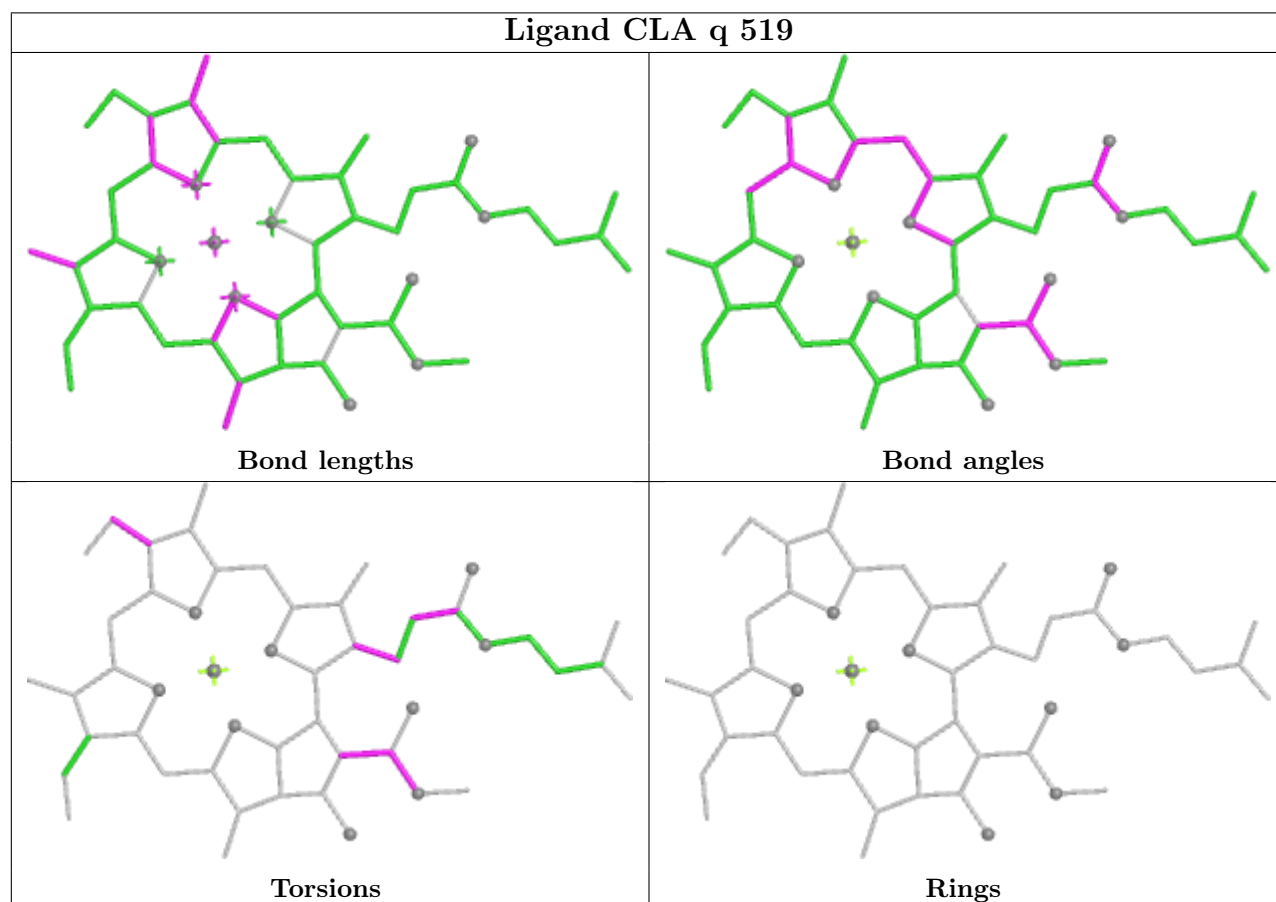
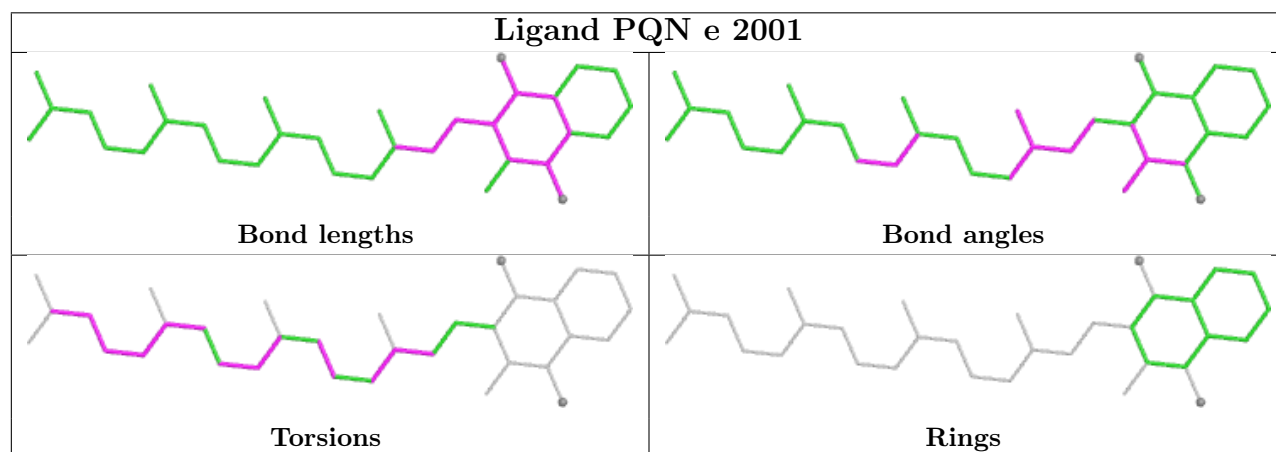
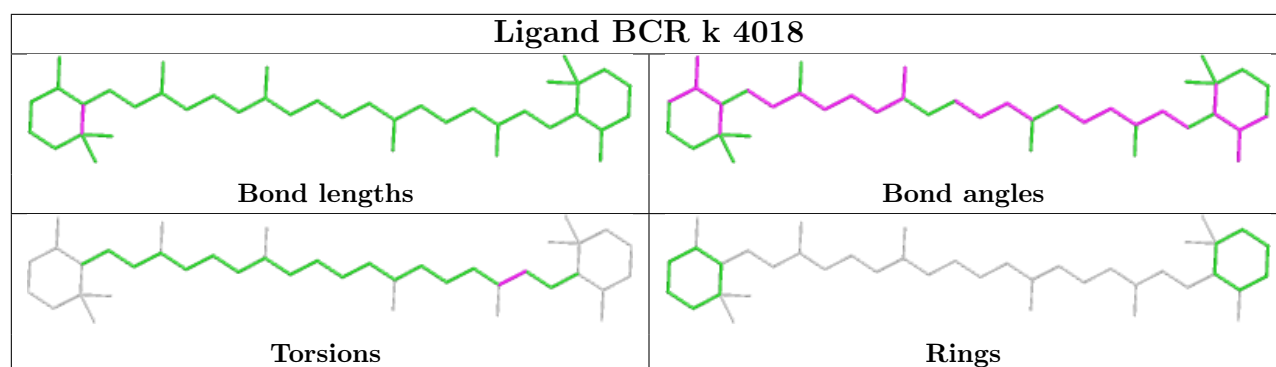


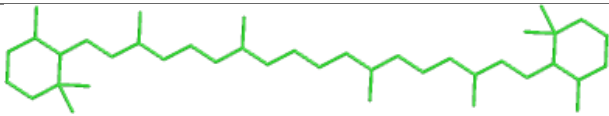
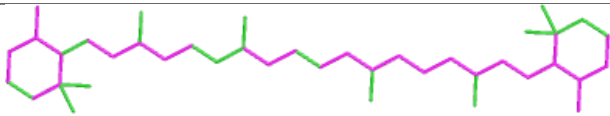
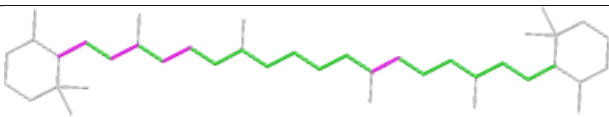
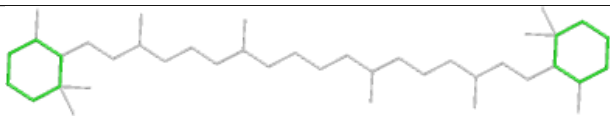
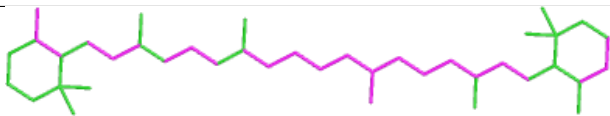
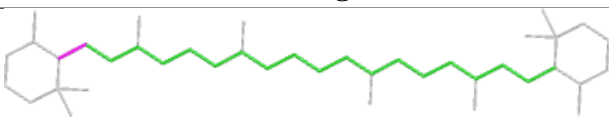
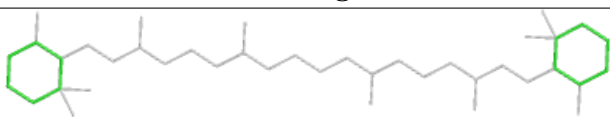
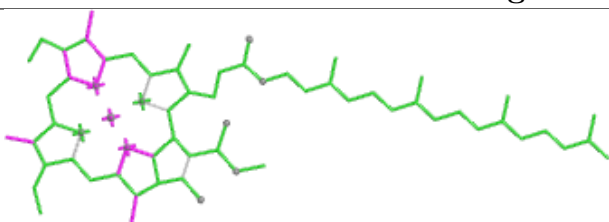
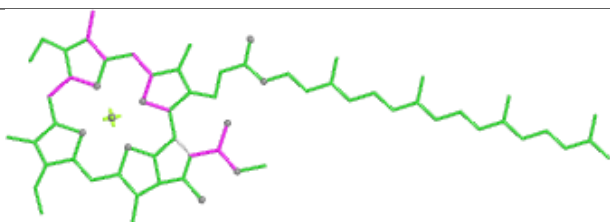
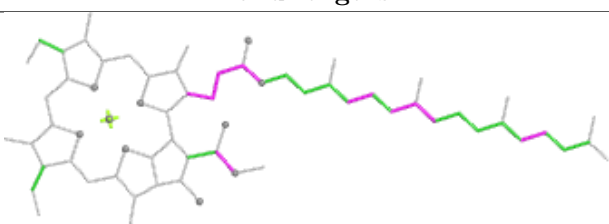
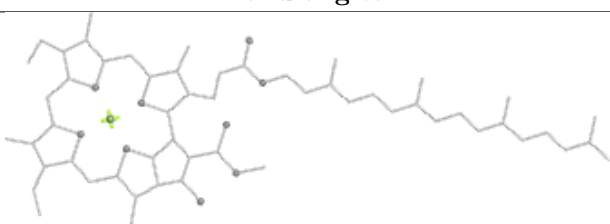


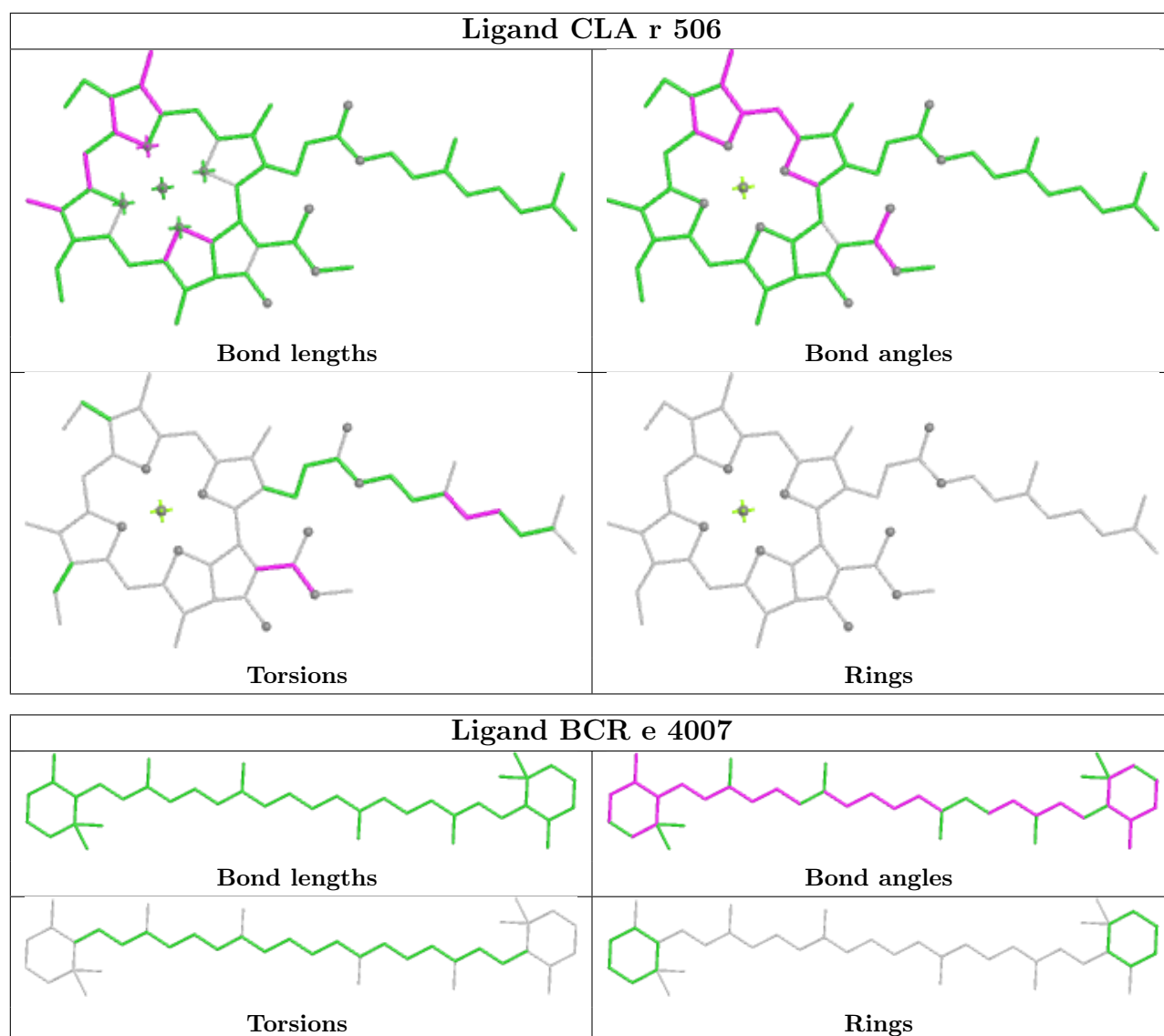




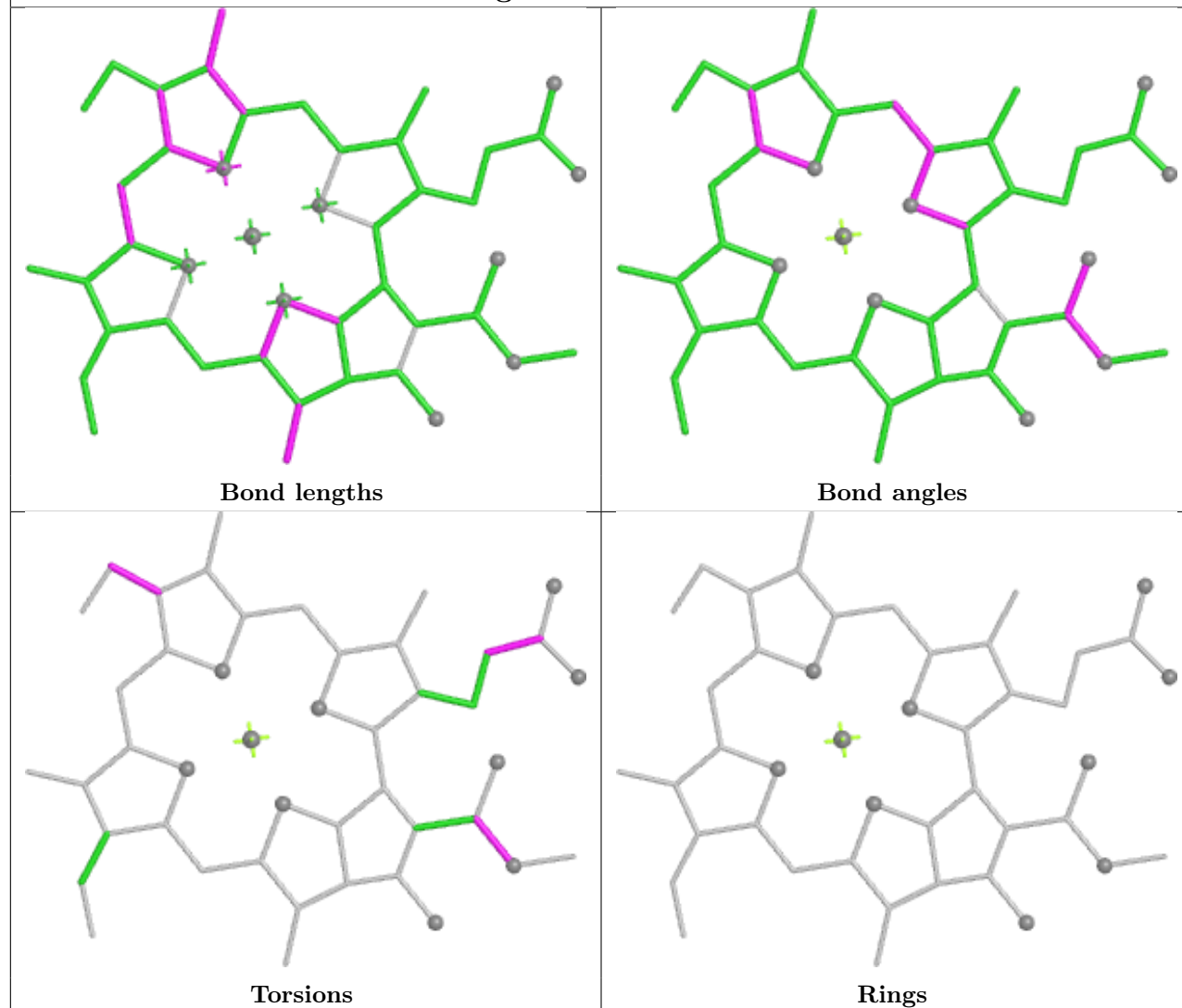




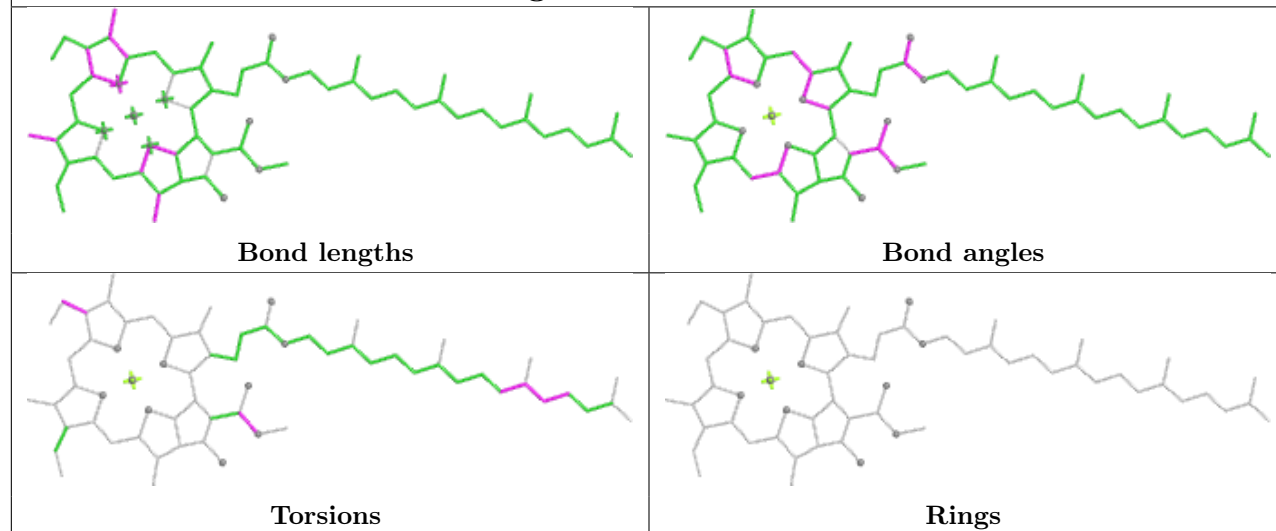
Ligand BCR 5 521	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR V 4219	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA f 1206	
	
Bond lengths	Bond angles
	
Torsions	Rings

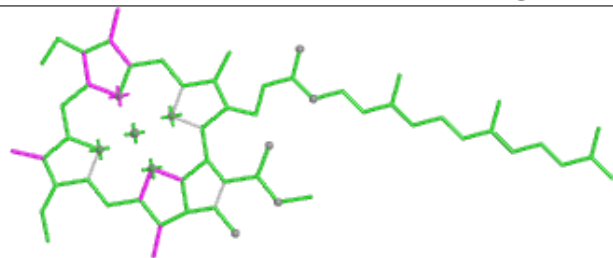
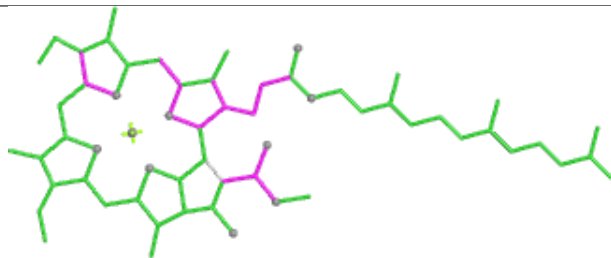
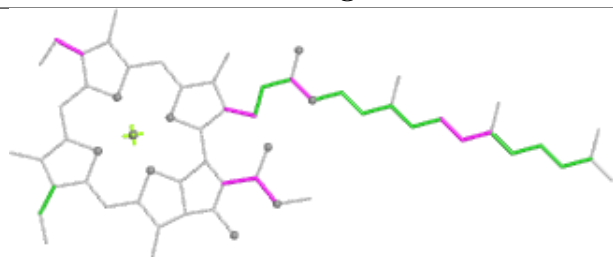
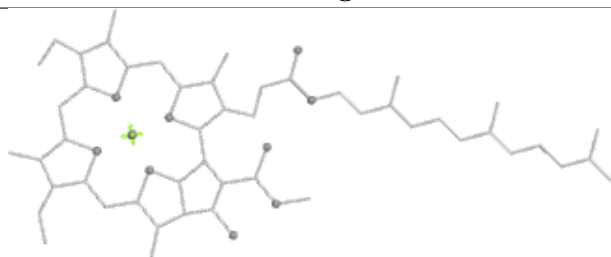
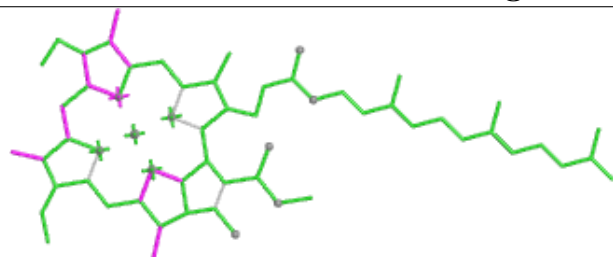
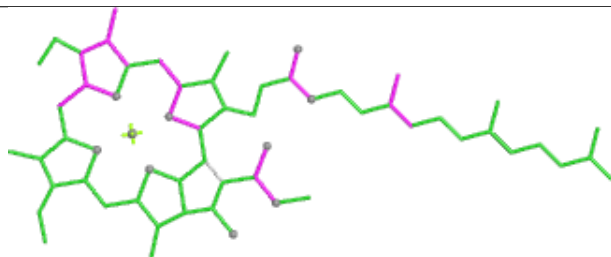
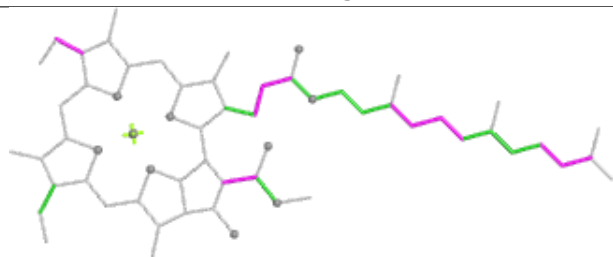
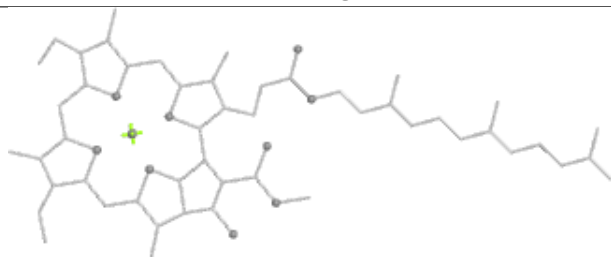


Ligand CLA d 511

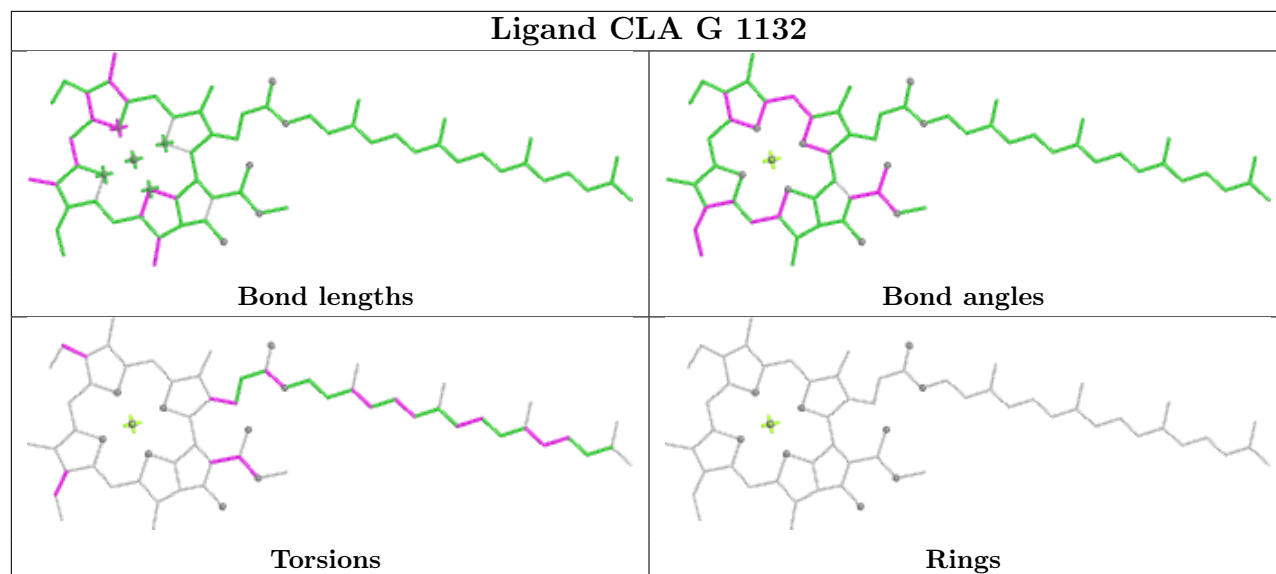


Ligand CLA e 1131

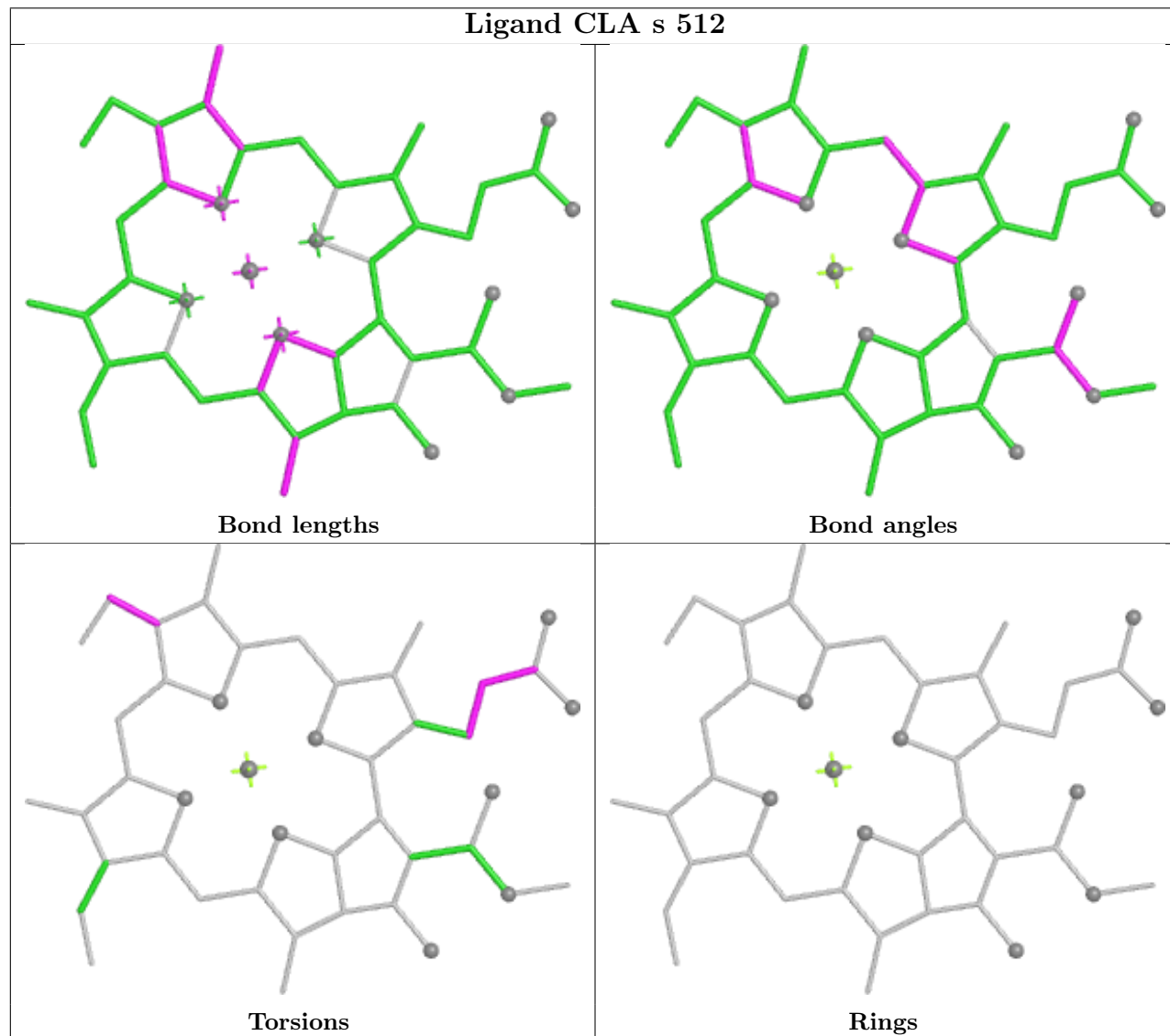


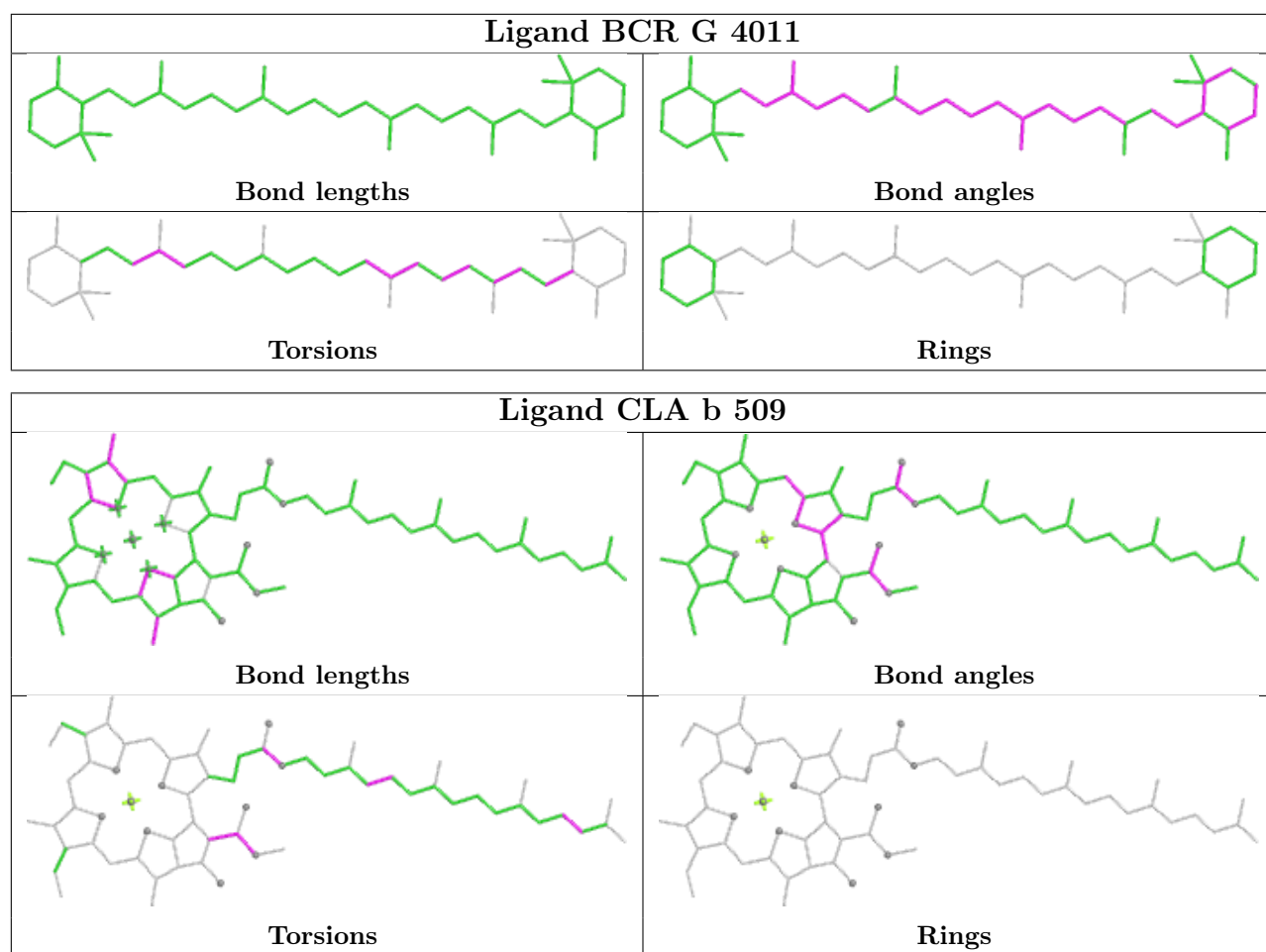
Ligand CLA f 1230**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 1115****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA G 1132

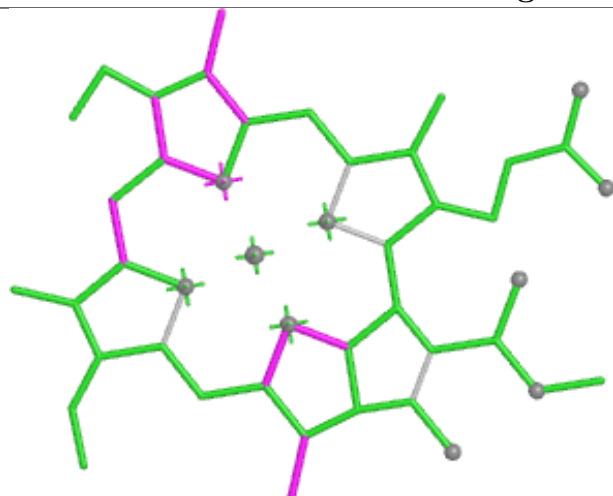


Ligand CLA s 512

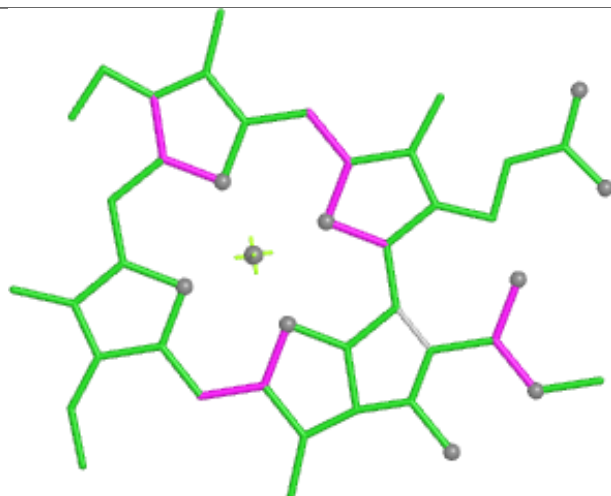




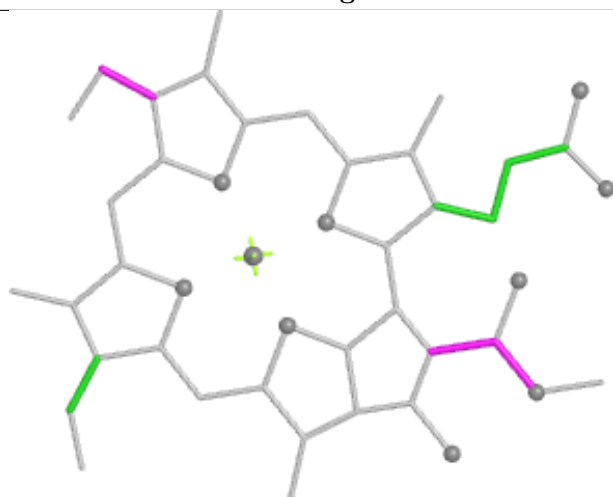
Ligand CLA u 504



Bond lengths



Bond angles

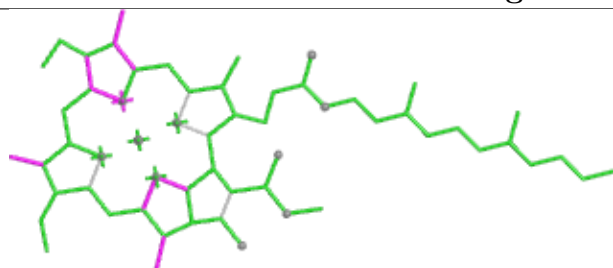


Torsions

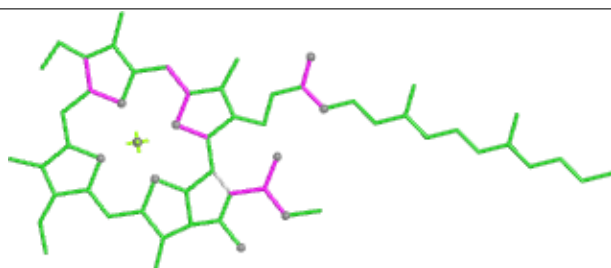


Rings

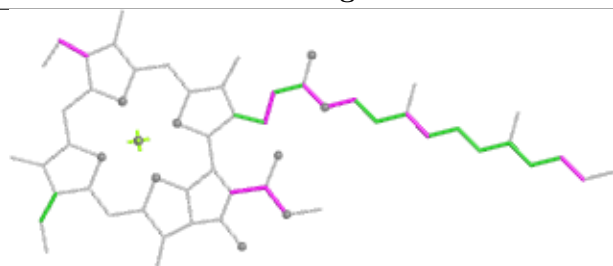
Ligand CLA T 1302



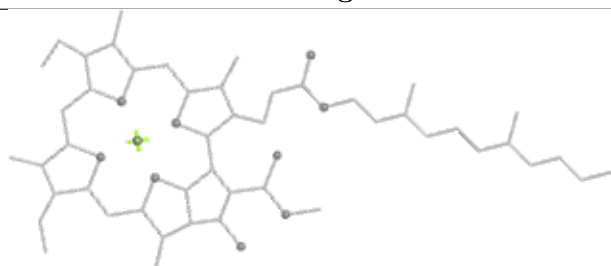
Bond lengths



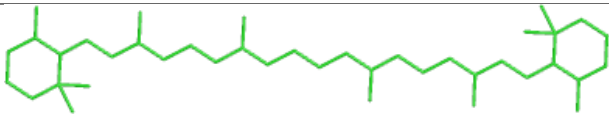
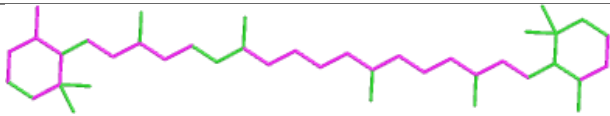
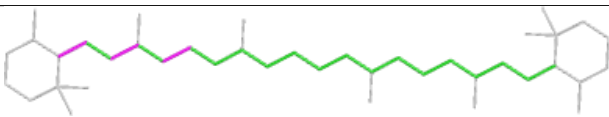
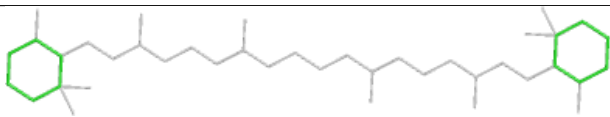
Bond angles

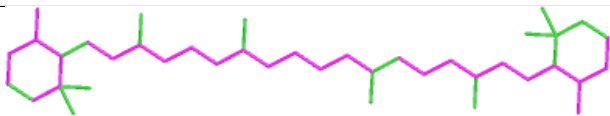
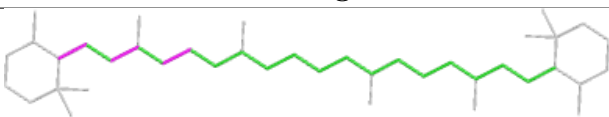
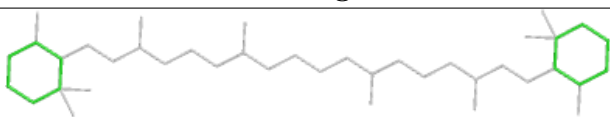


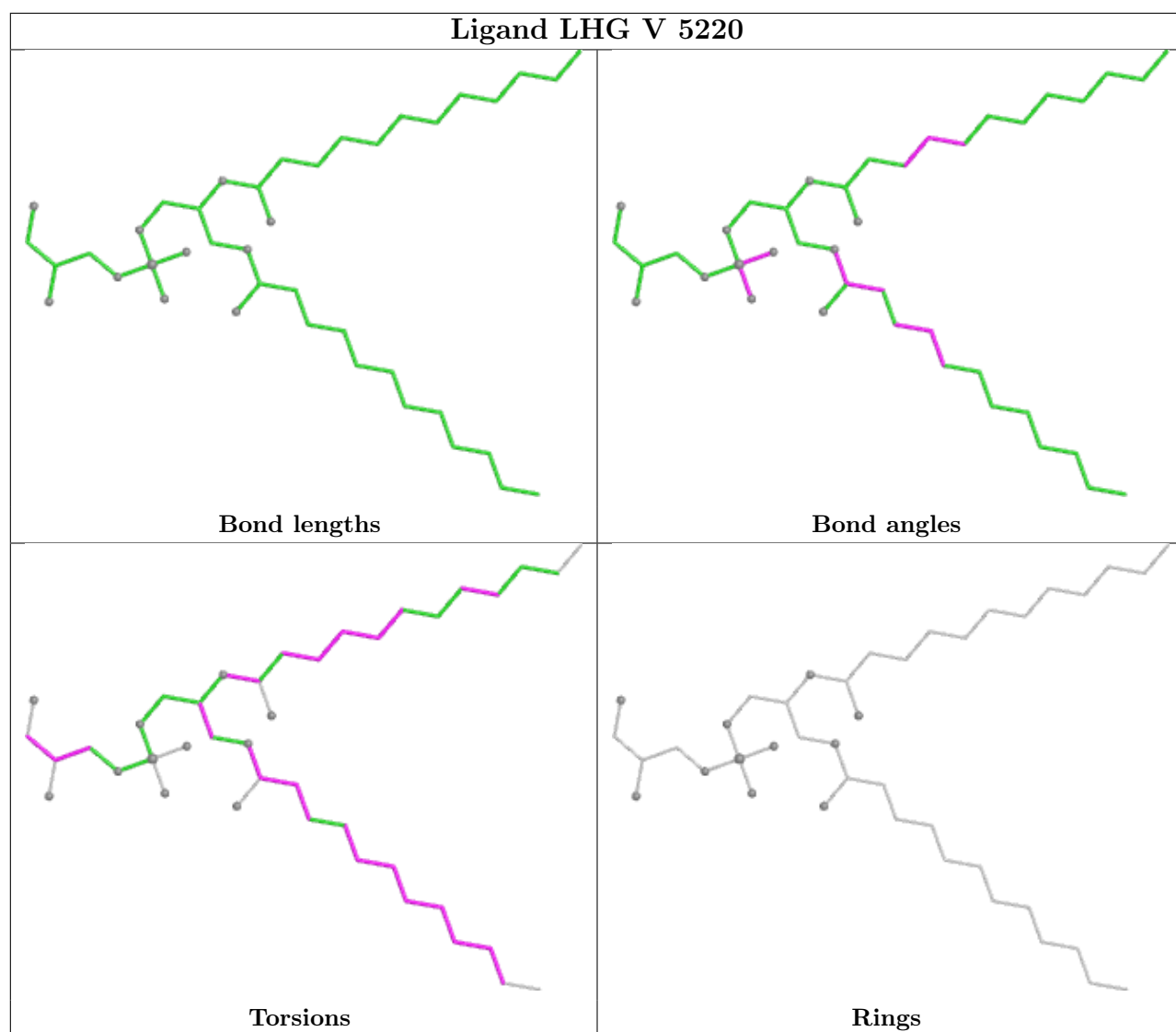
Torsions



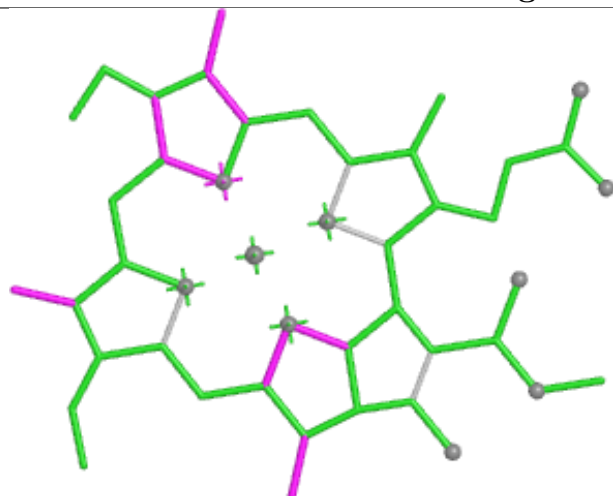
Rings

Ligand BCR d 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

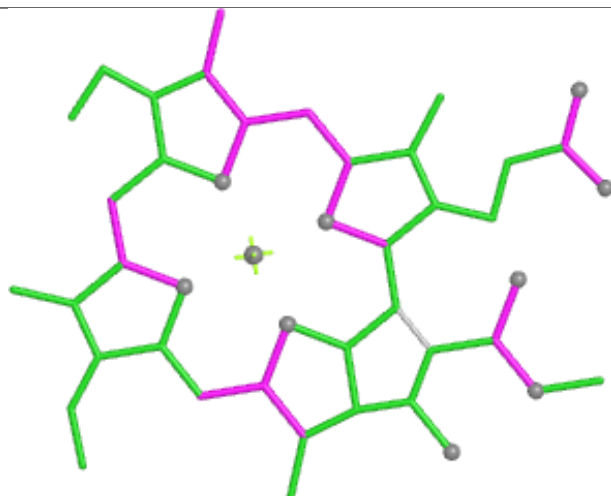
Ligand BCR 3 522	
	
Bond lengths	Bond angles
	
Torsions	Rings



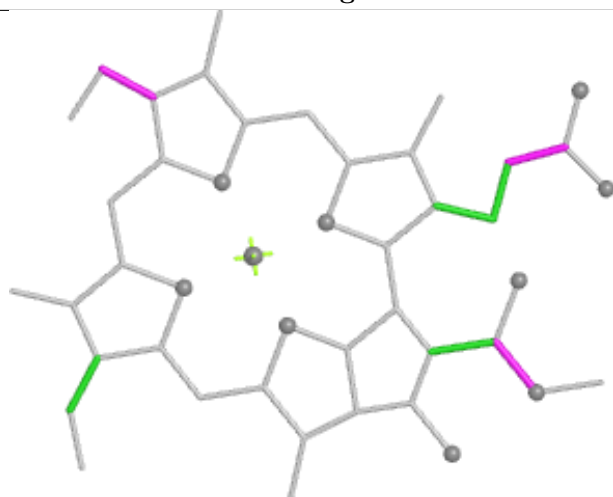
Ligand CLA 4 508



Bond lengths



Bond angles

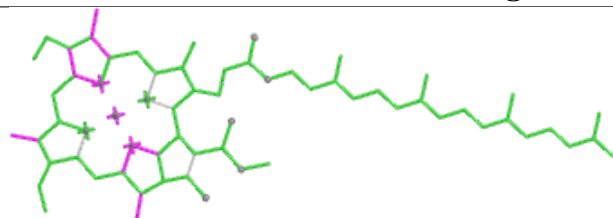


Torsions

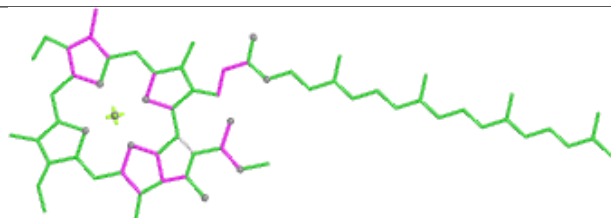


Rings

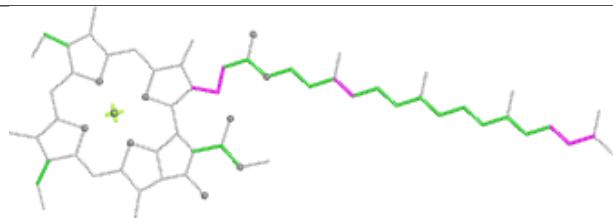
Ligand CLA A 1022



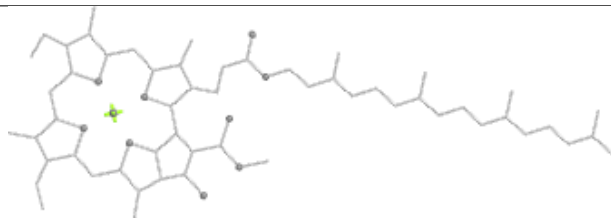
Bond lengths



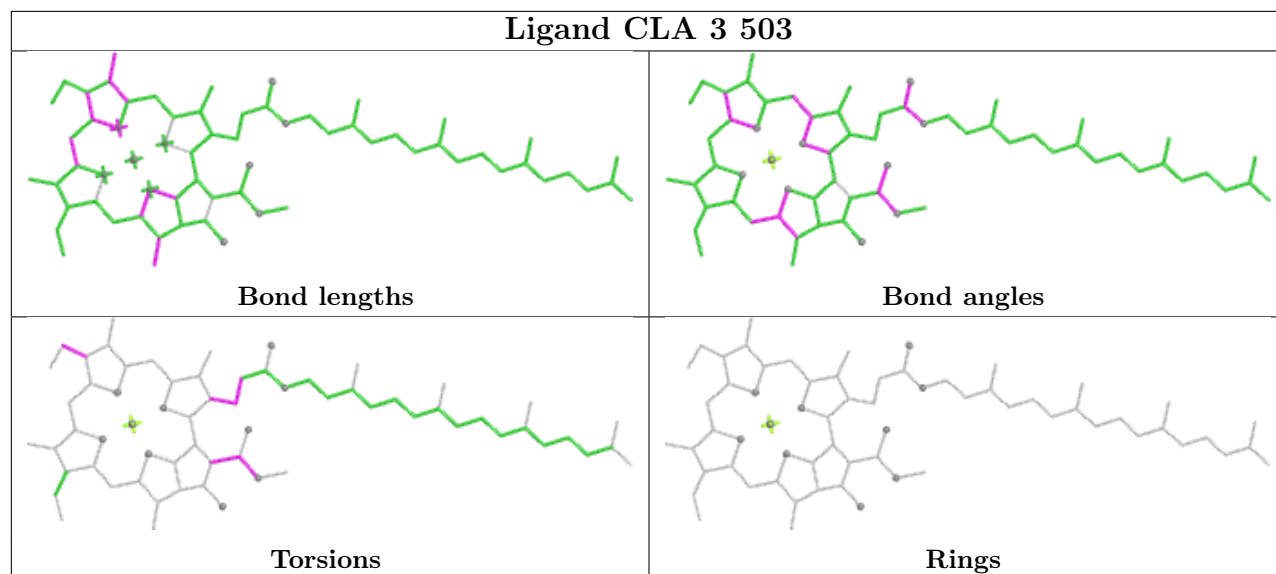
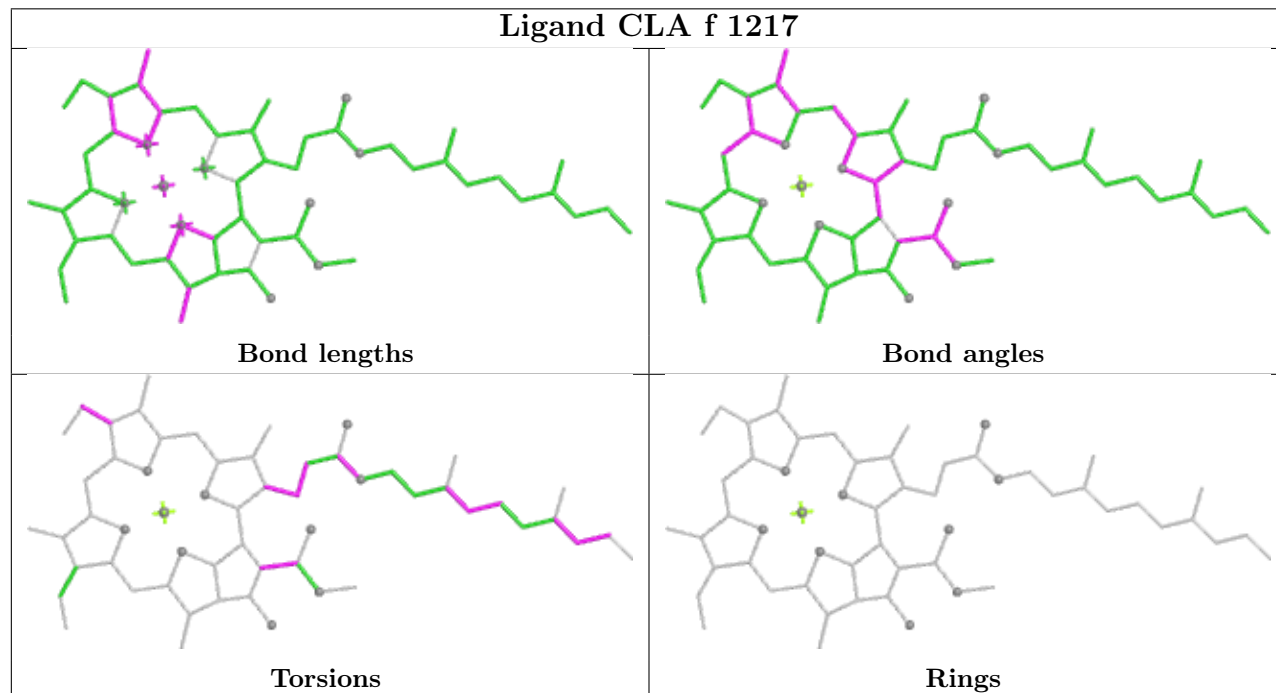
Bond angles



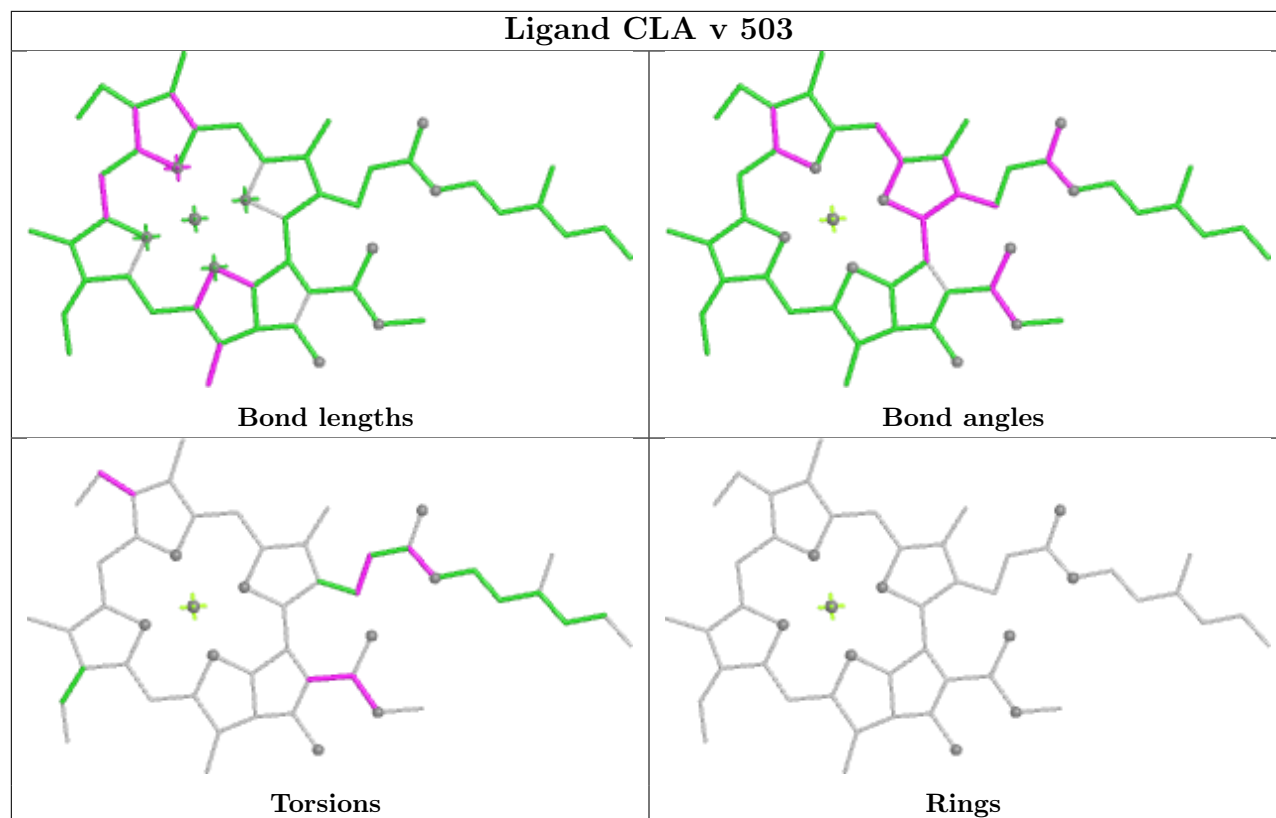
Torsions



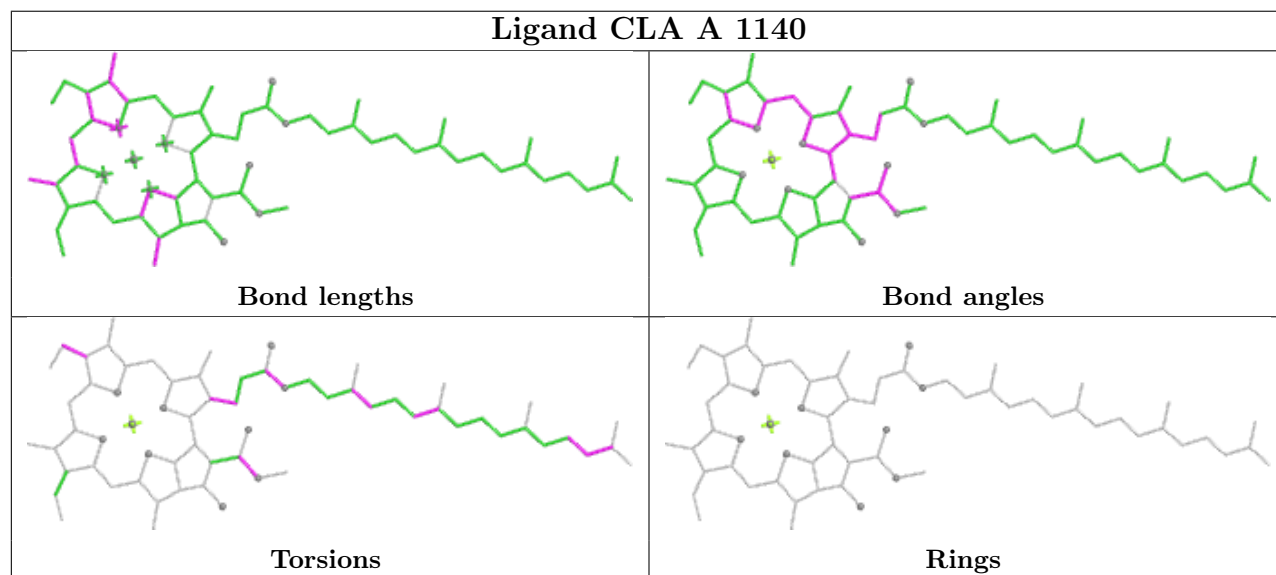
Rings

Ligand CLA 3 503**Ligand CLA f 1217**

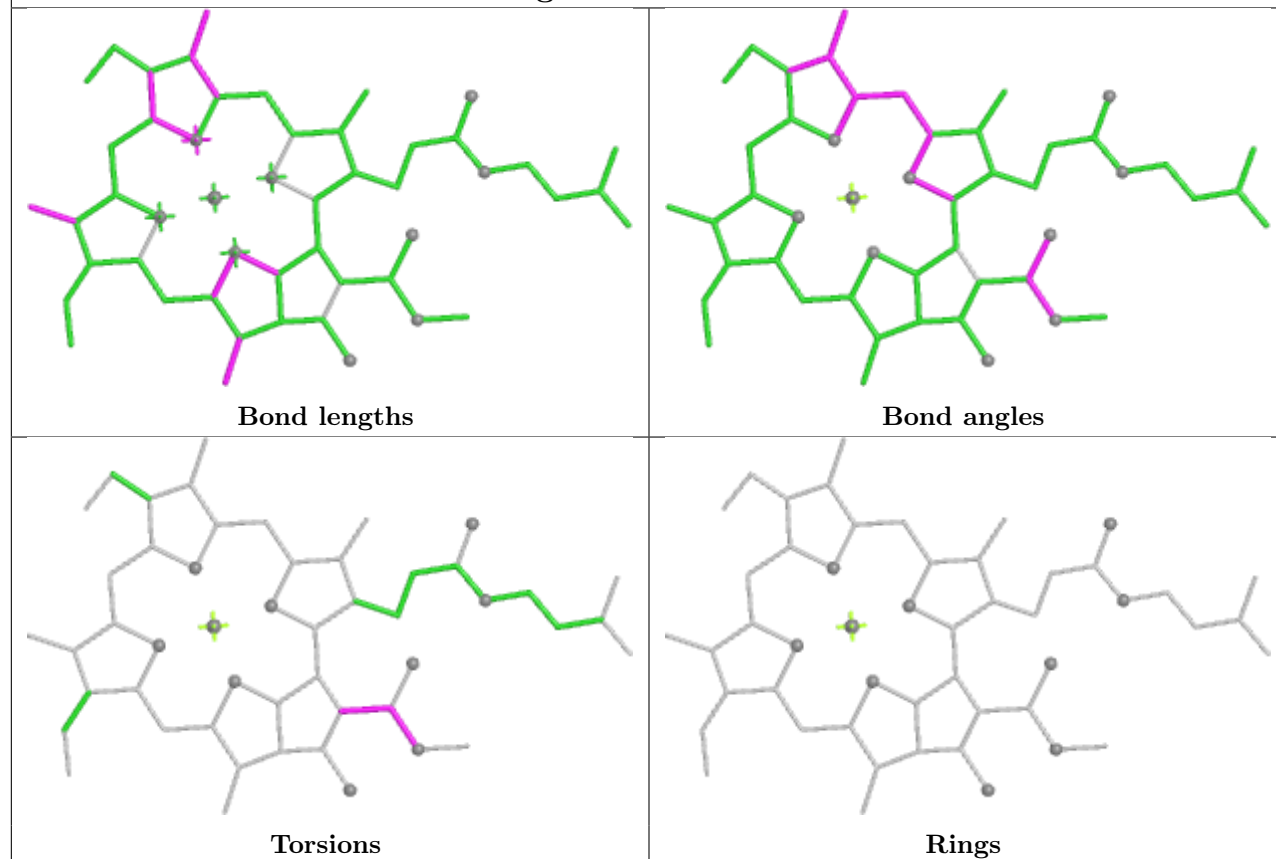
Ligand CLA v 503



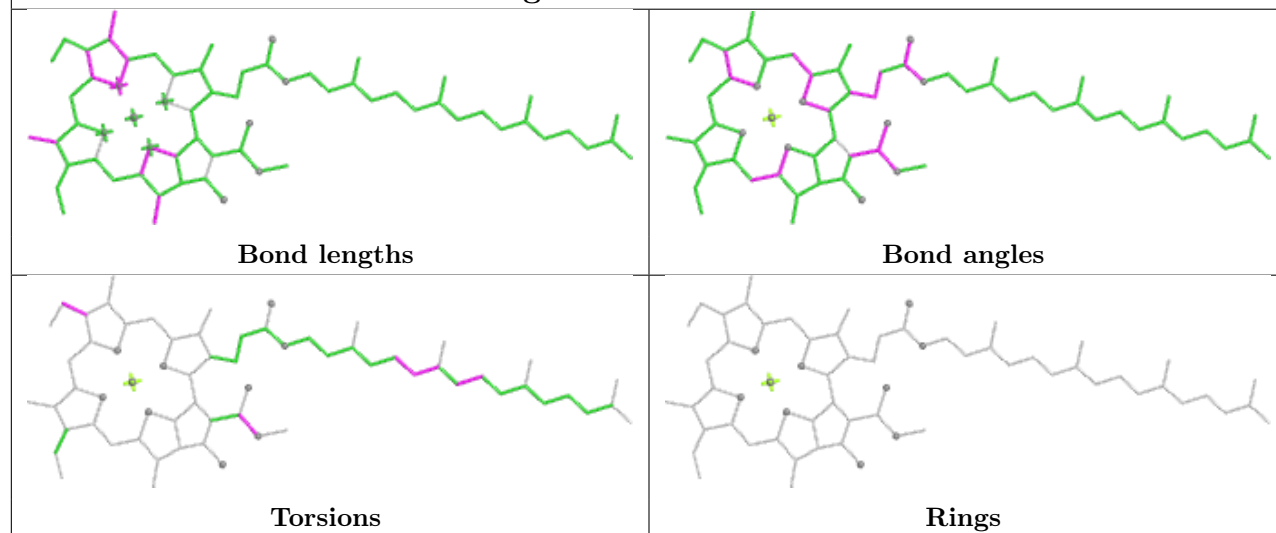
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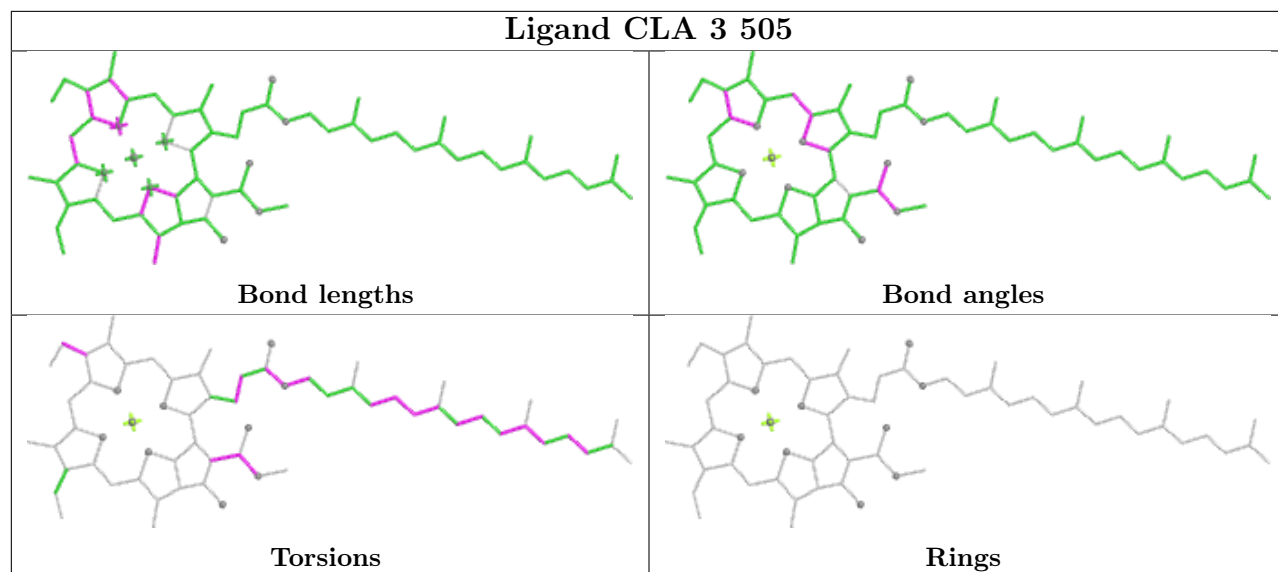
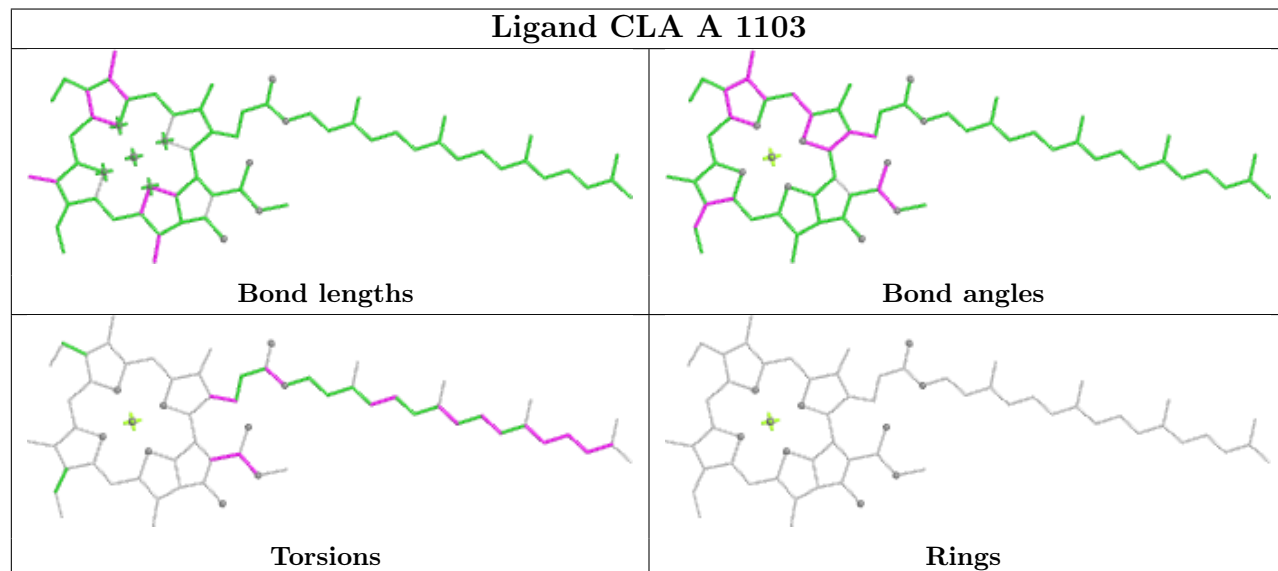
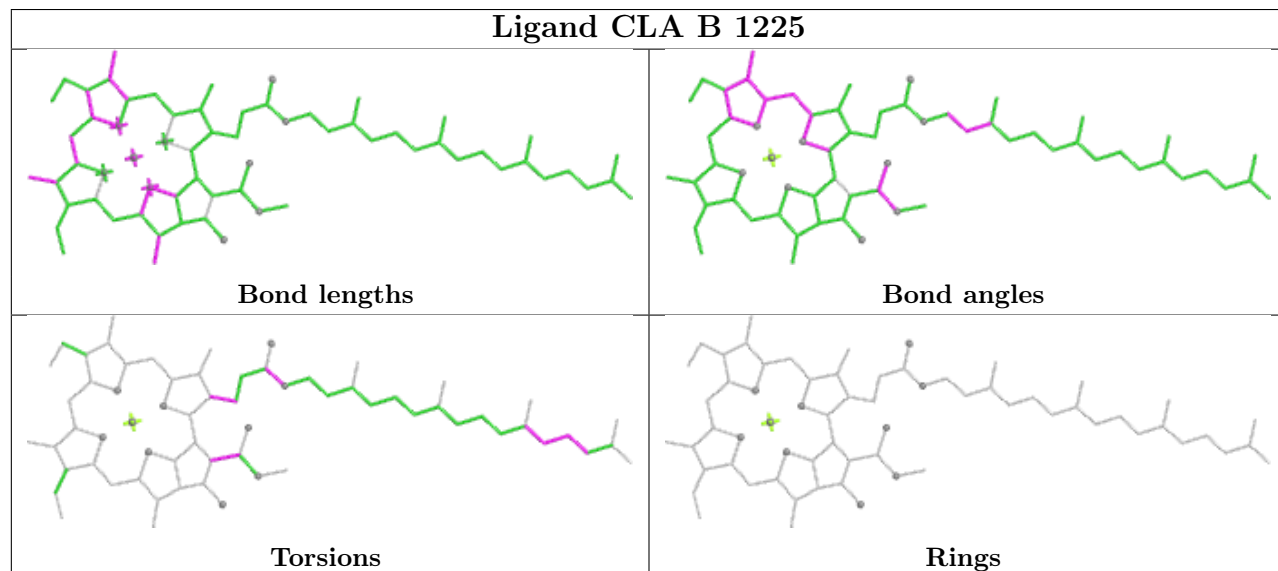


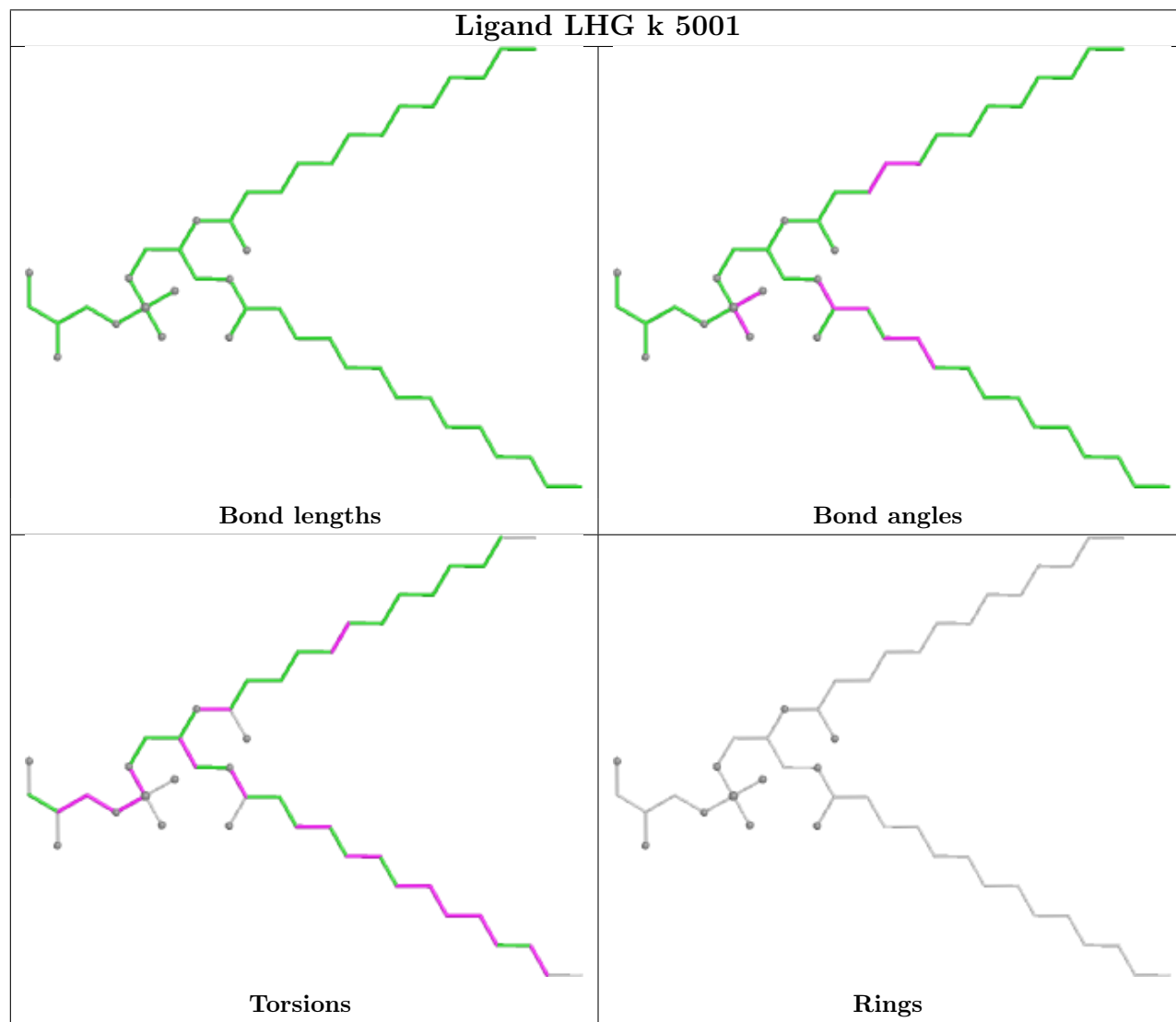
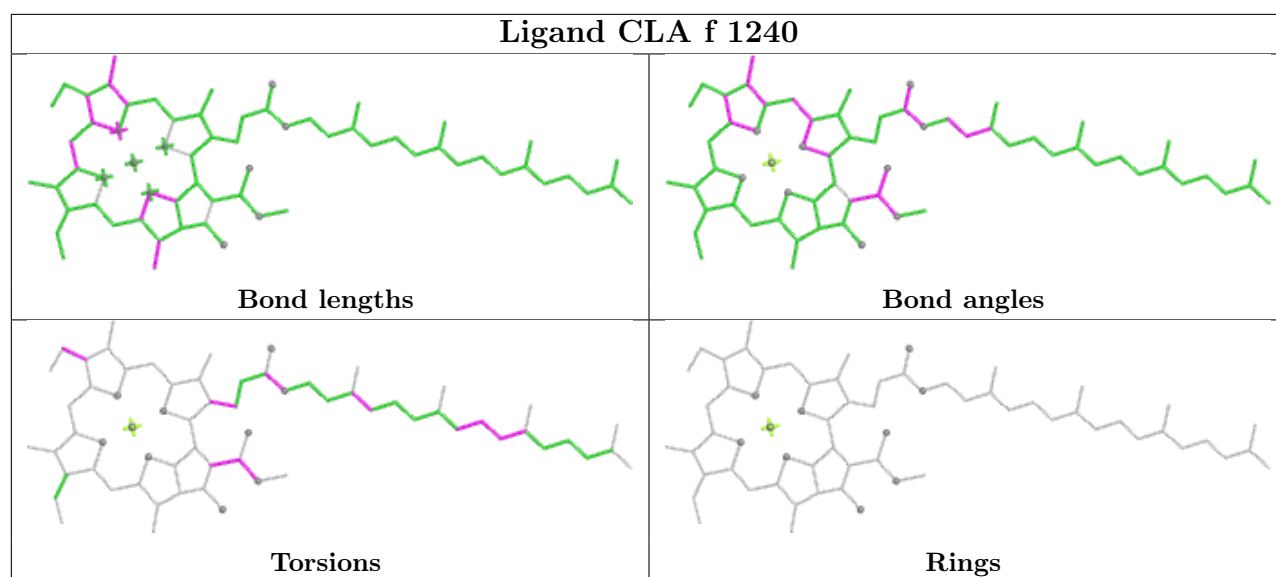
Ligand CLA a 506

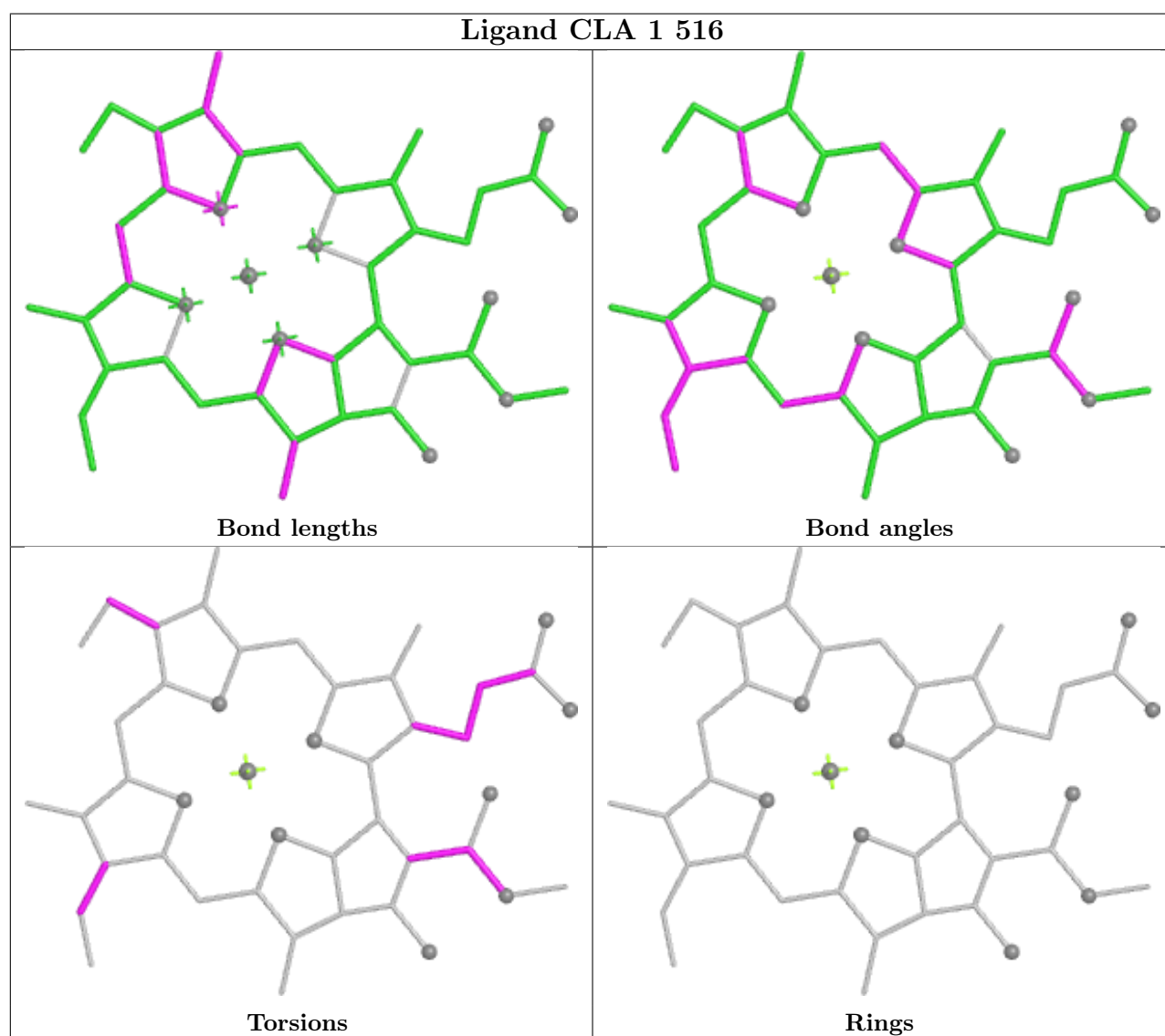
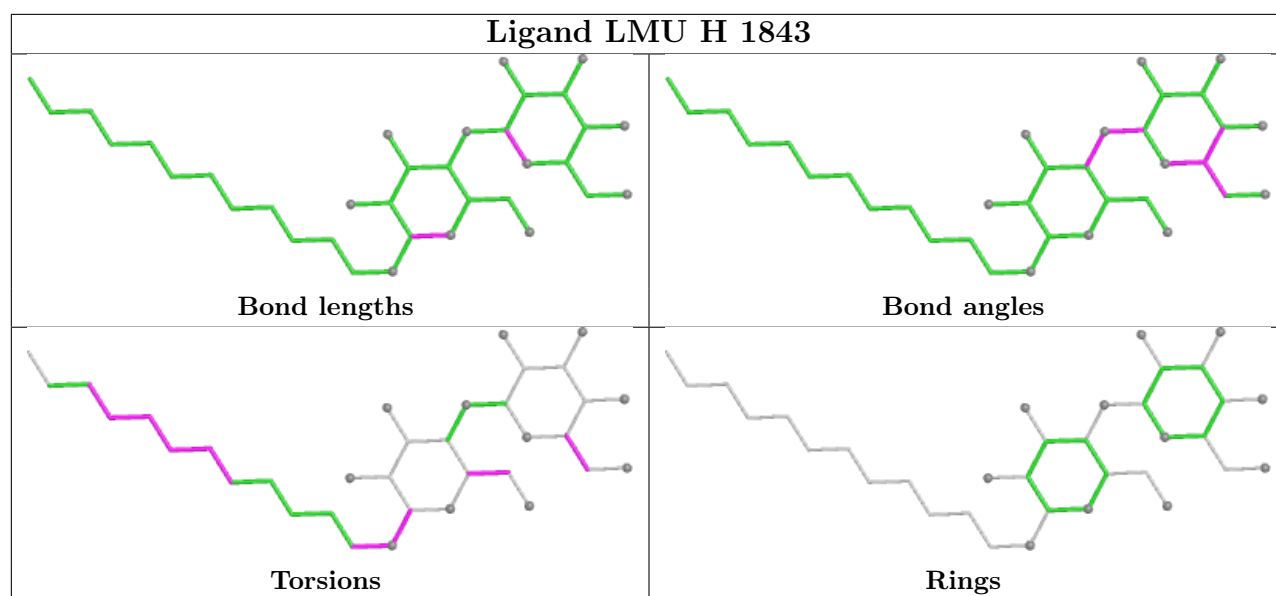


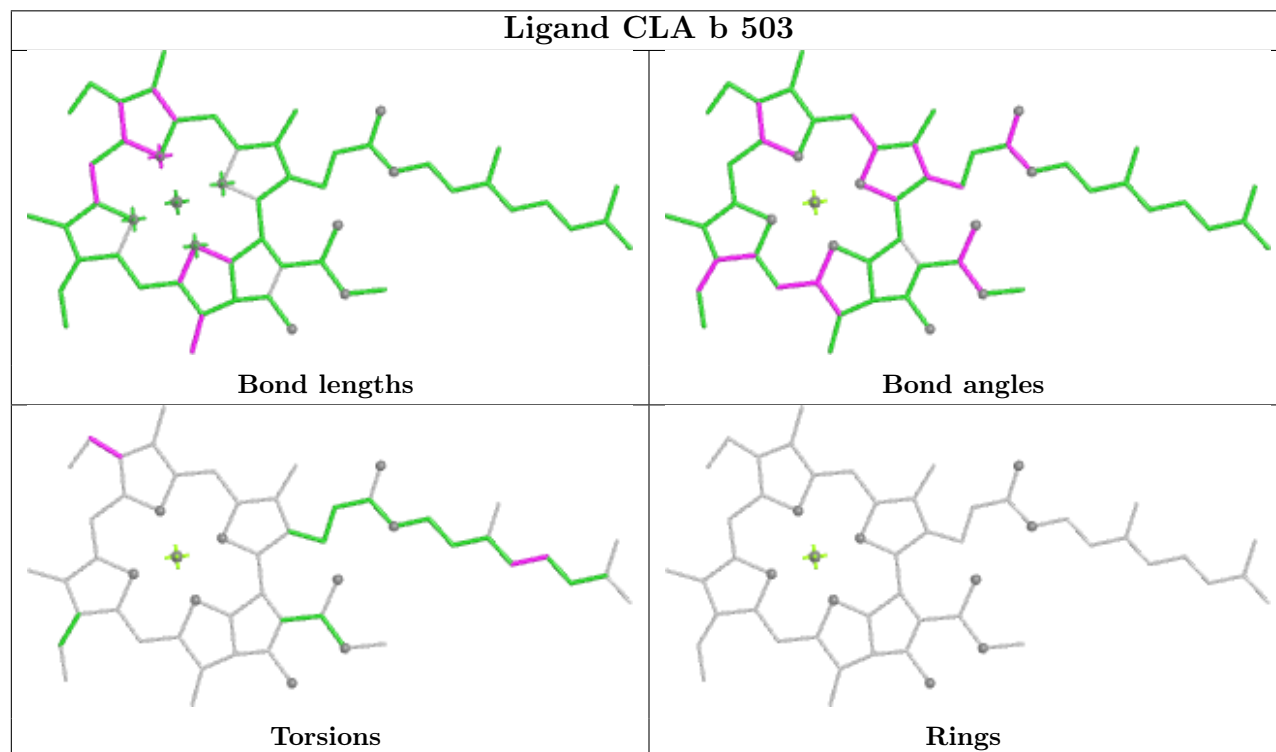
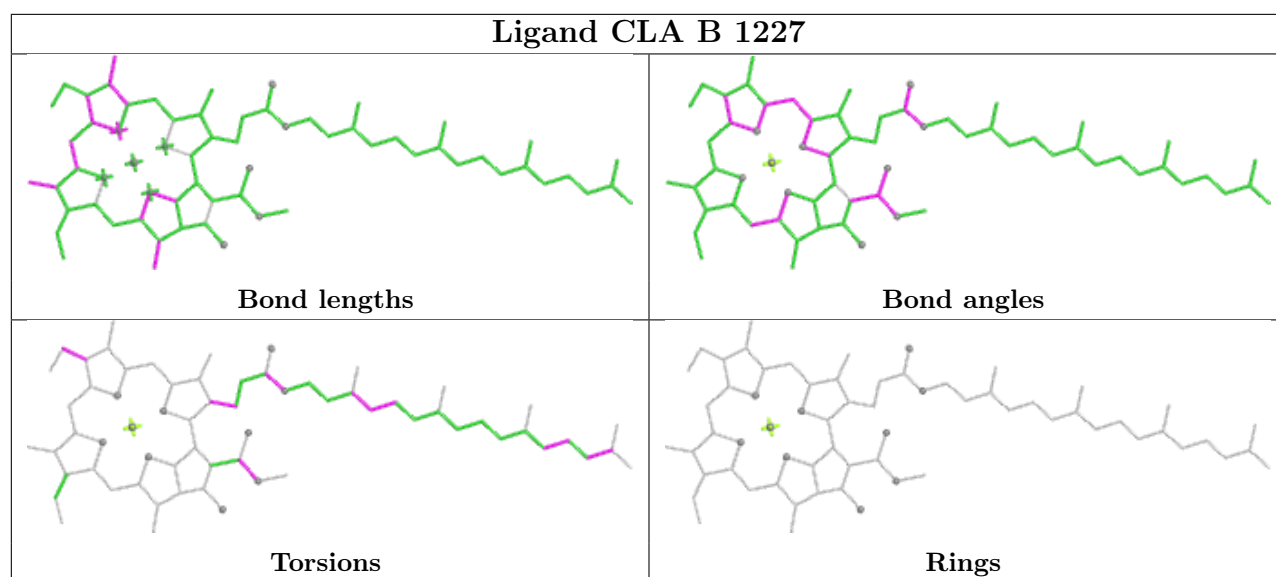
Ligand CLA B 1235

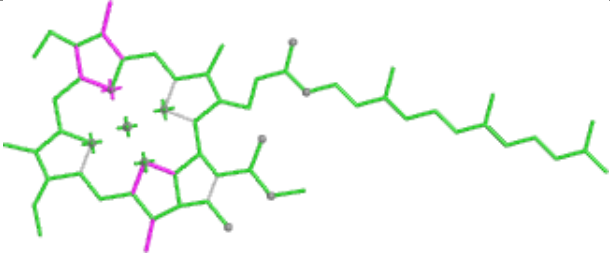
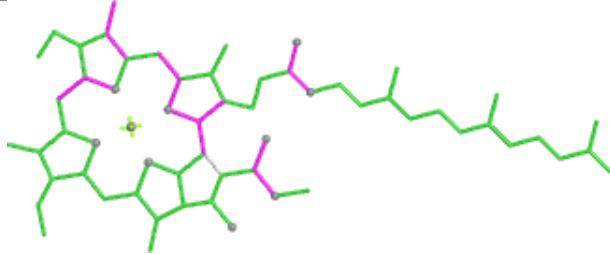
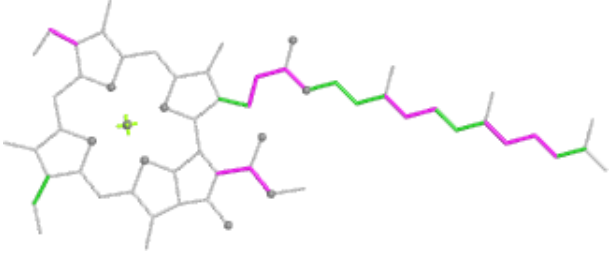
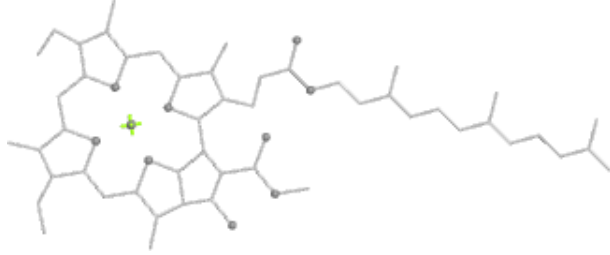
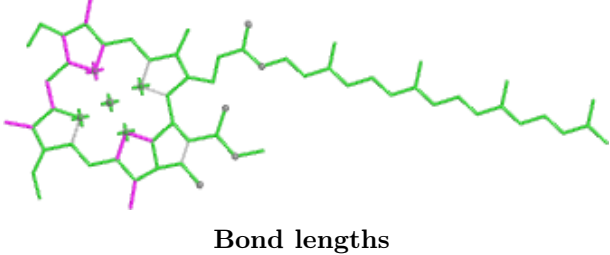
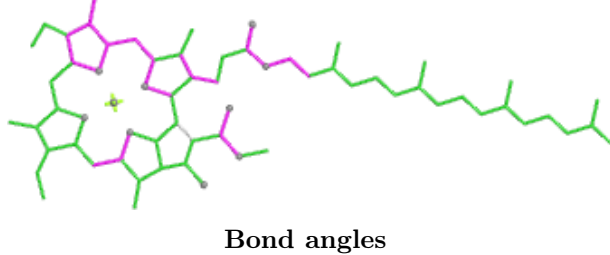
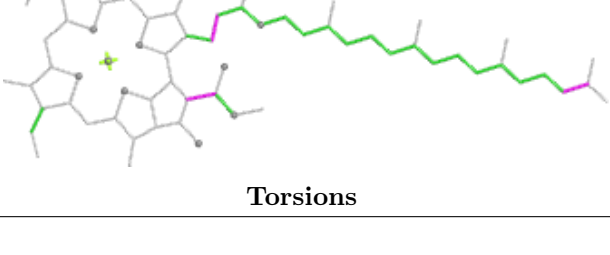
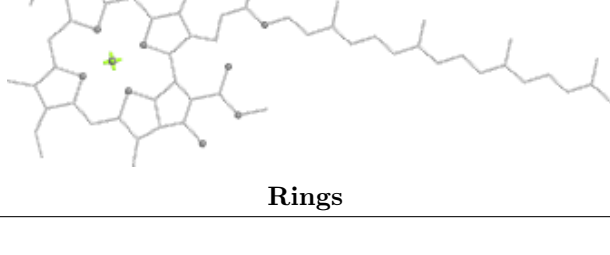


Ligand CLA 3 505**Ligand CLA A 1103****Ligand CLA B 1225**

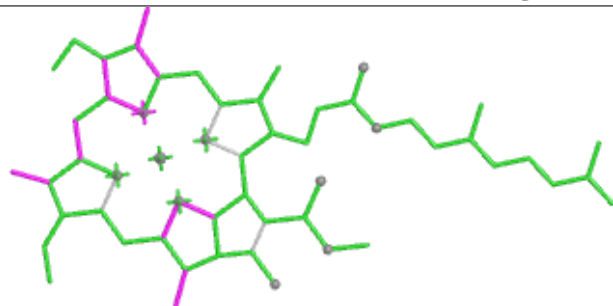




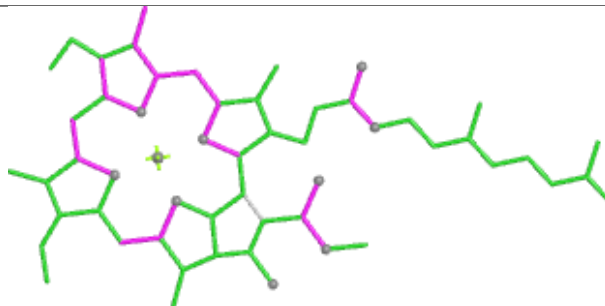


Ligand CLA Y 507	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA f 1238	
 Bond lengths	 Bond angles
 Torsions	 Rings

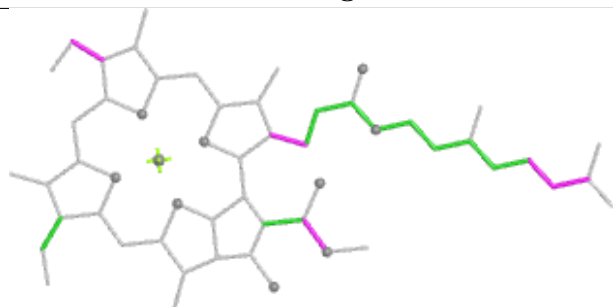
Ligand CLA Z 508



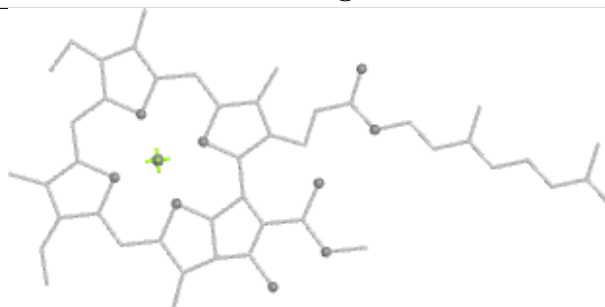
Bond lengths



Bond angles

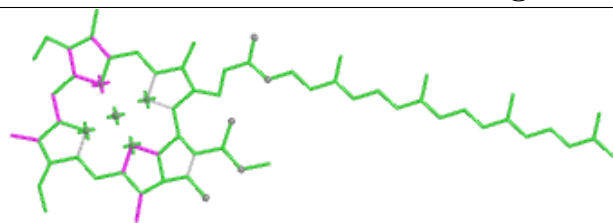


Torsions

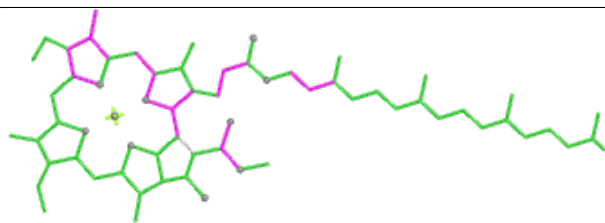


Rings

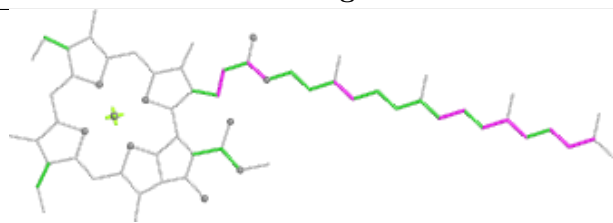
Ligand CLA e 1127



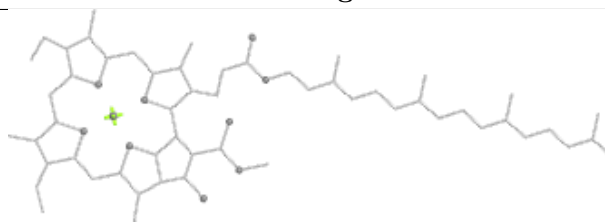
Bond lengths



Bond angles

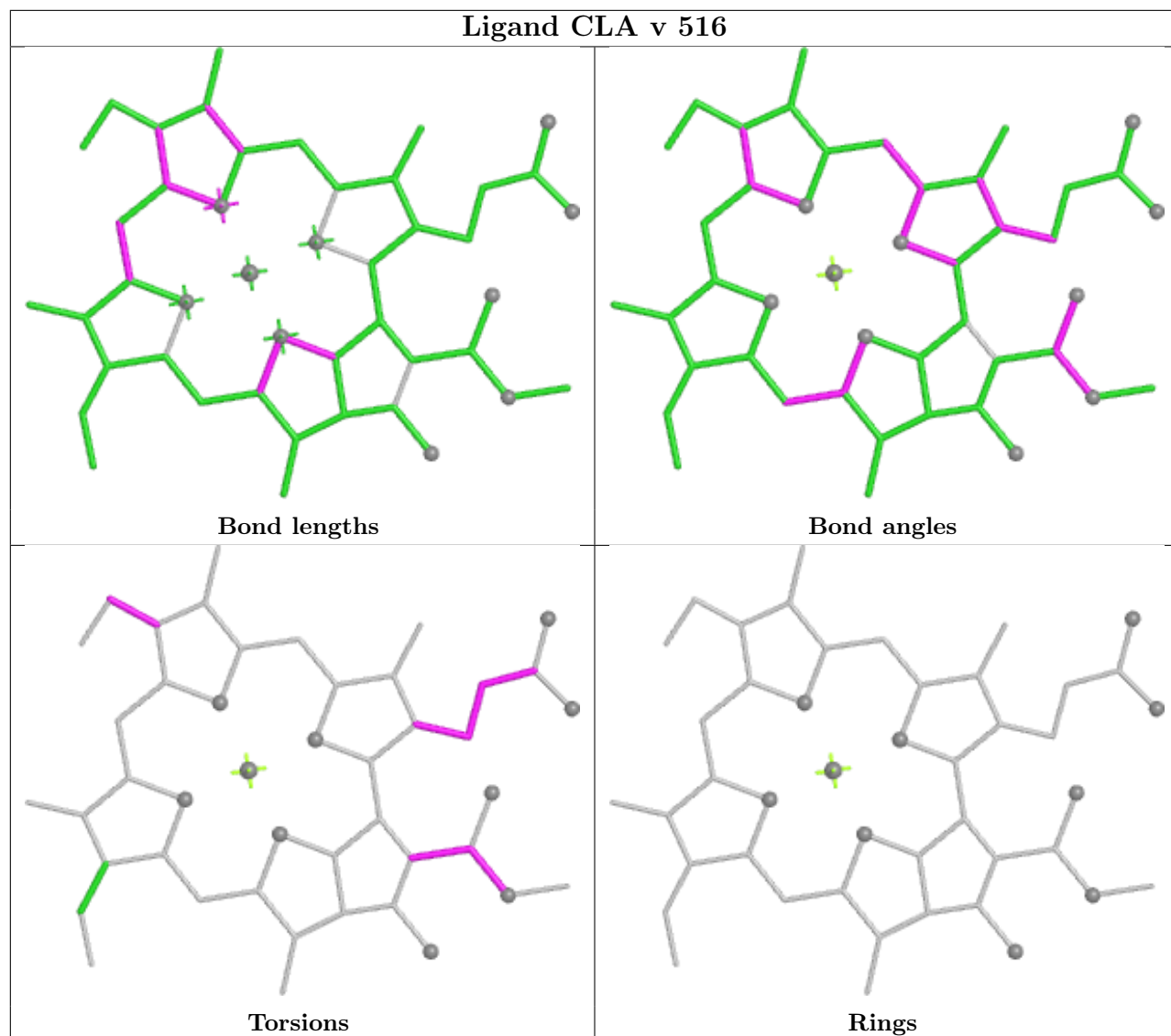


Torsions

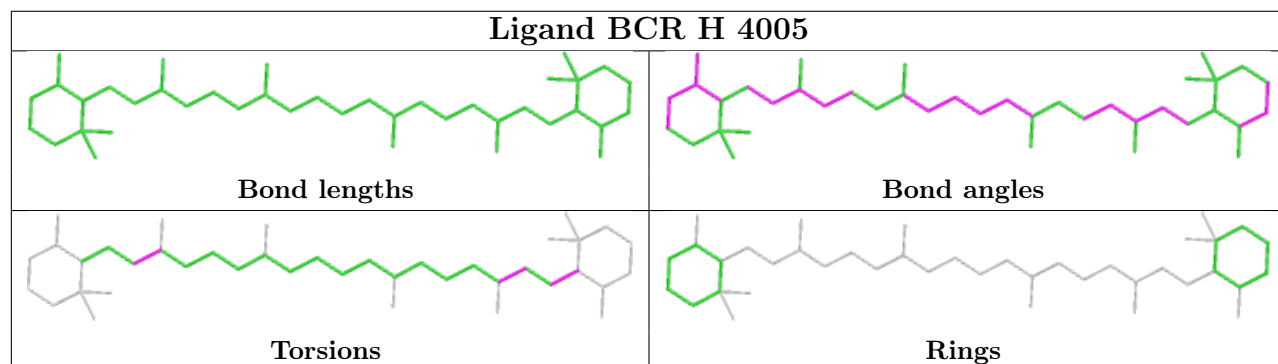


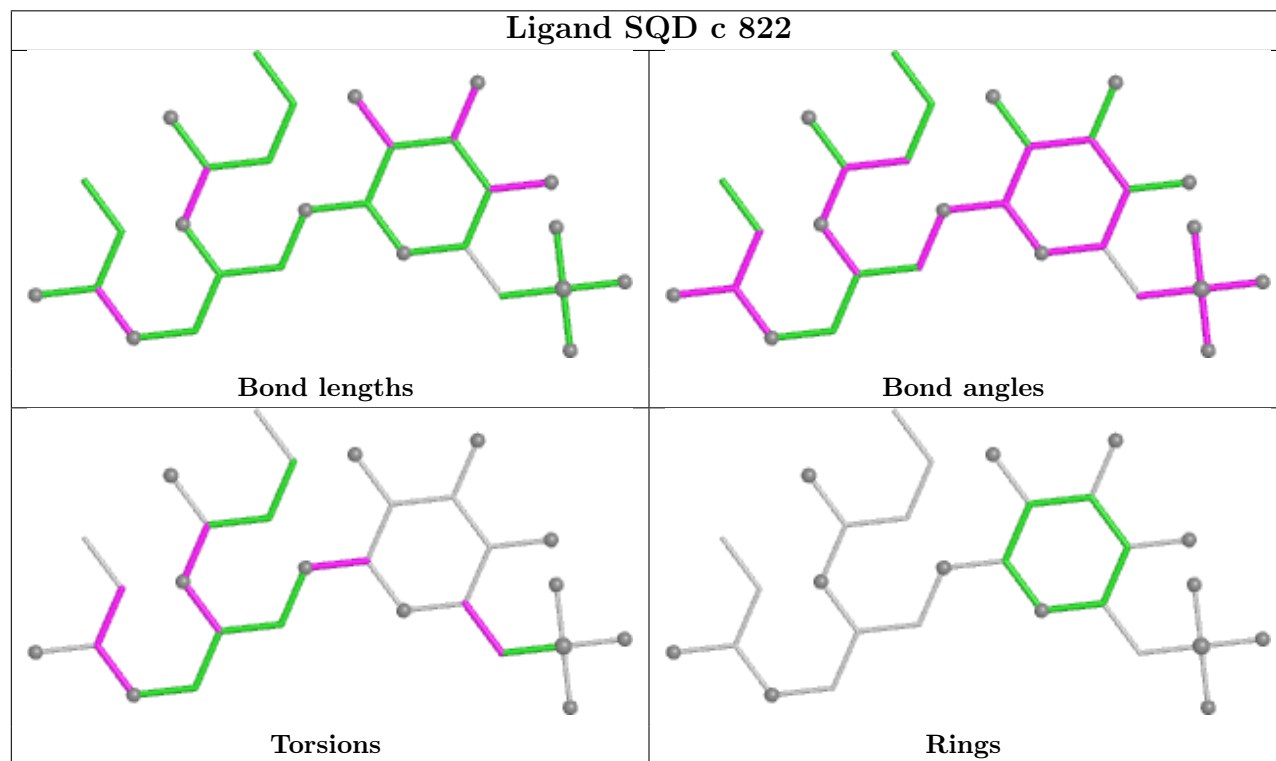
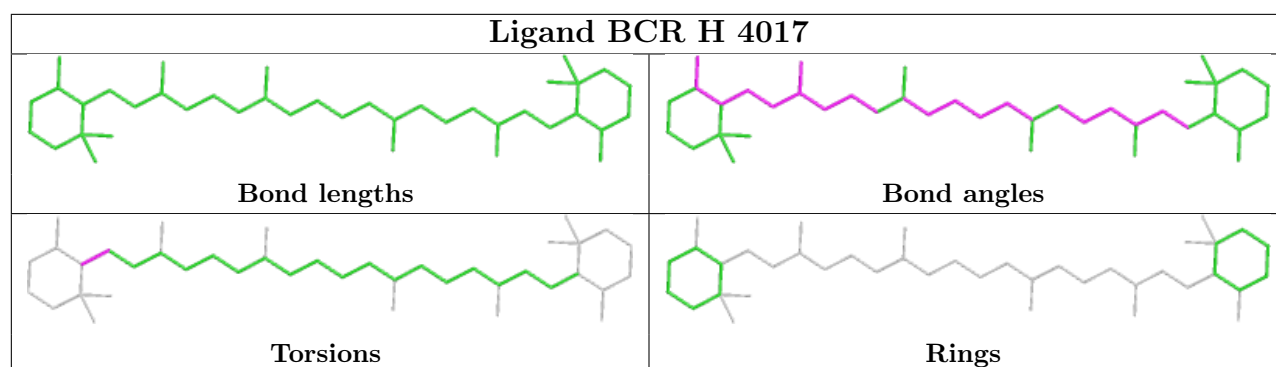
Rings

Ligand CLA v 516

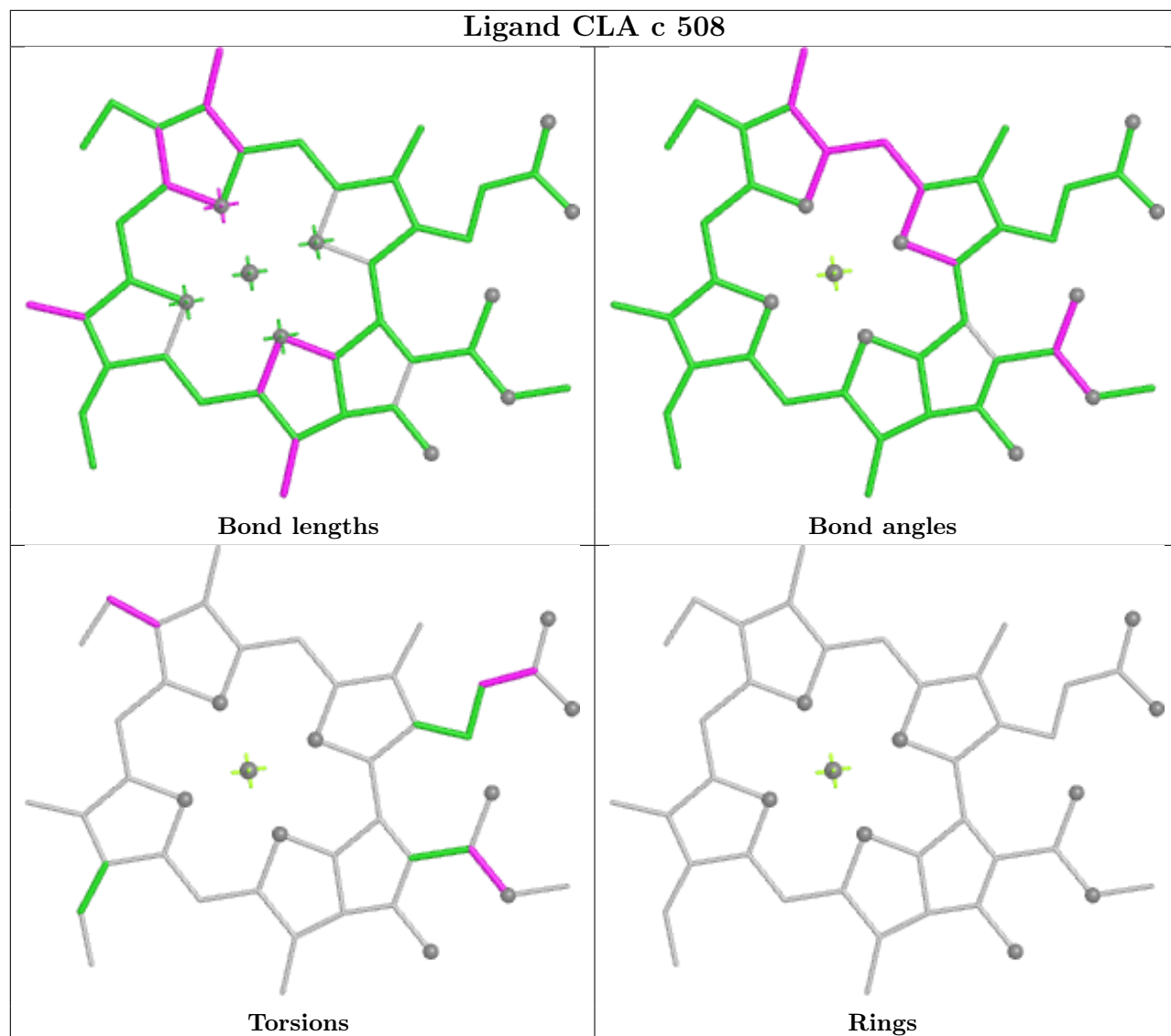


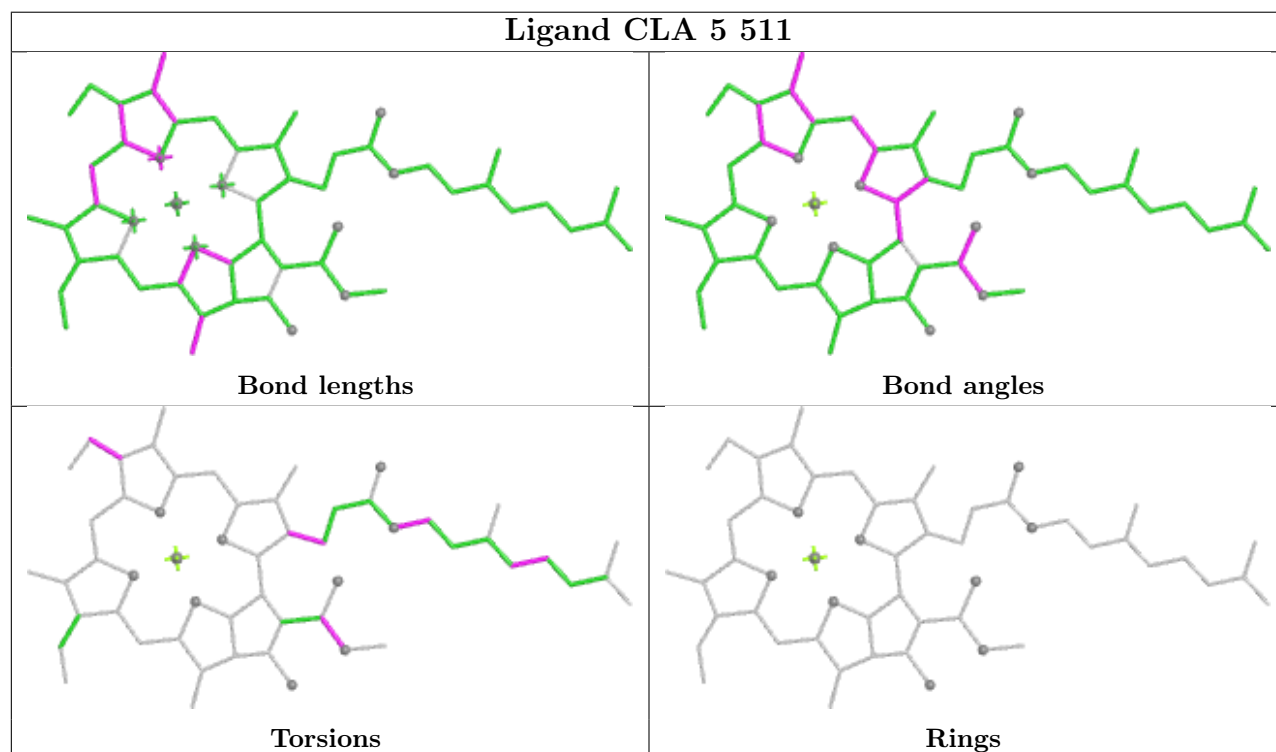
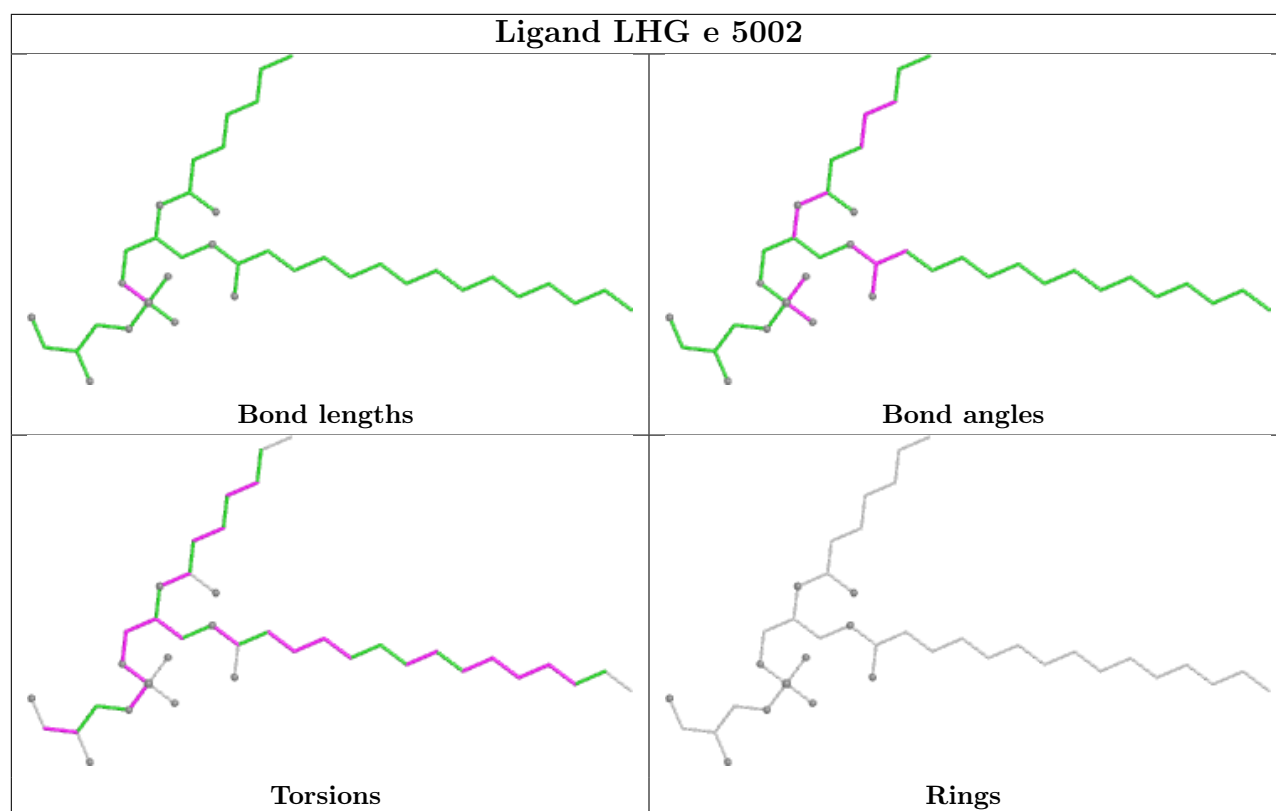
Ligand BCR H 4005

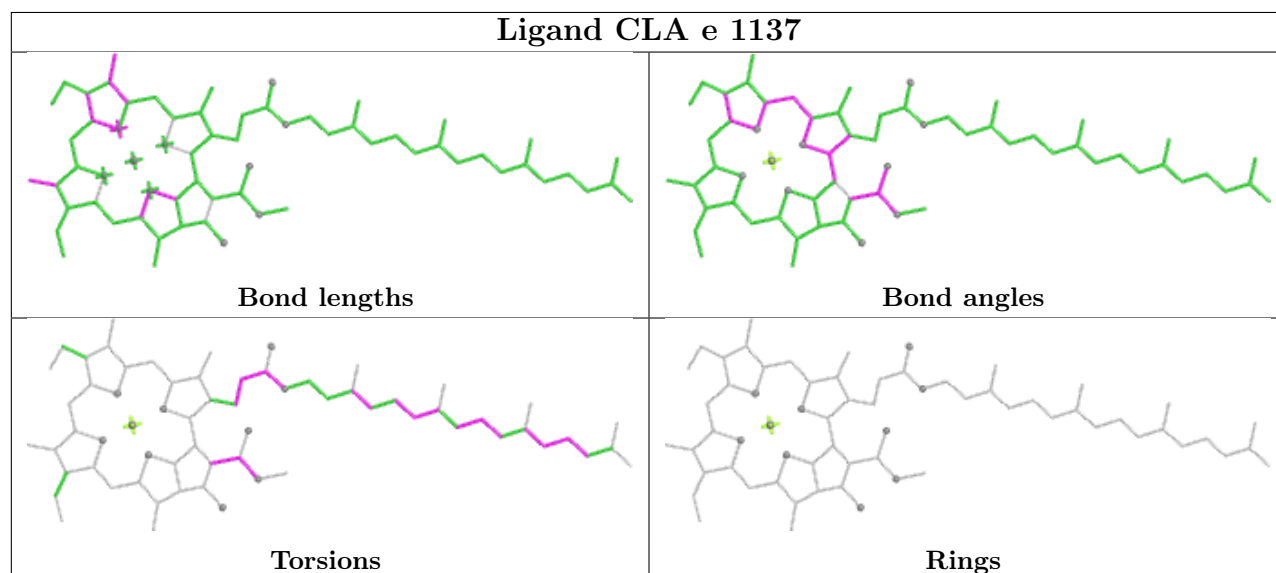
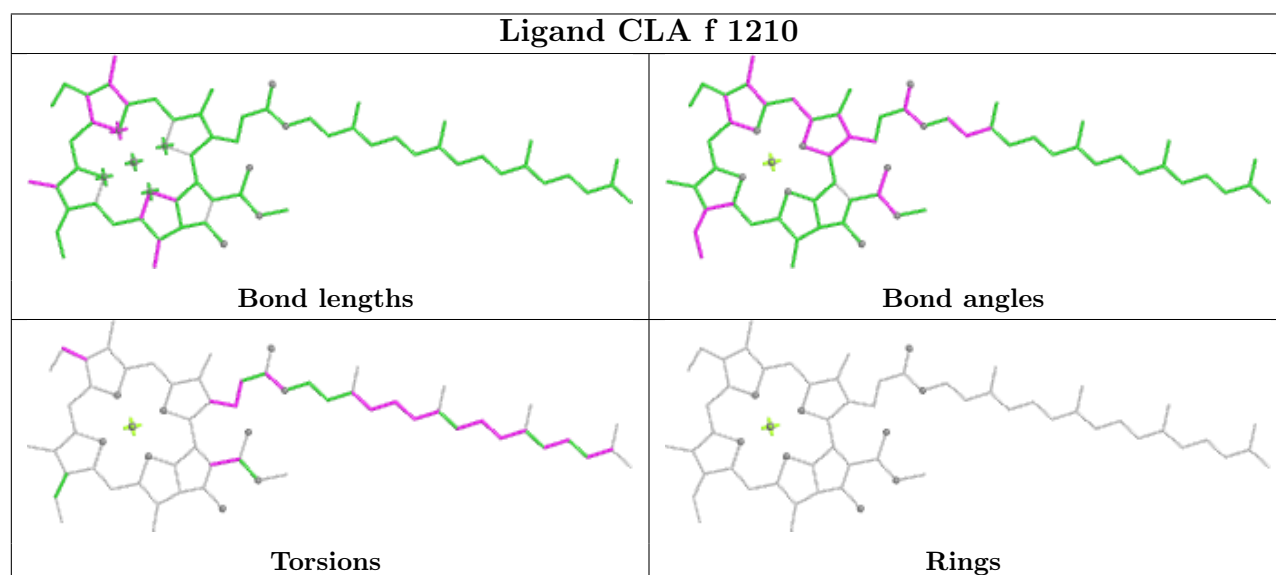
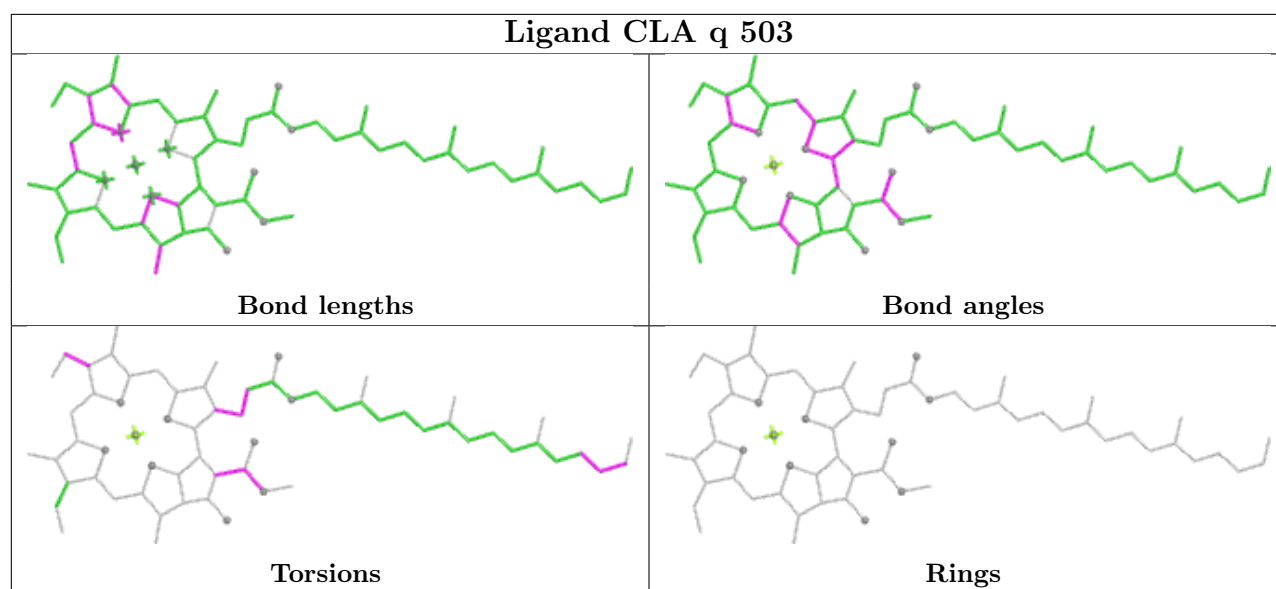


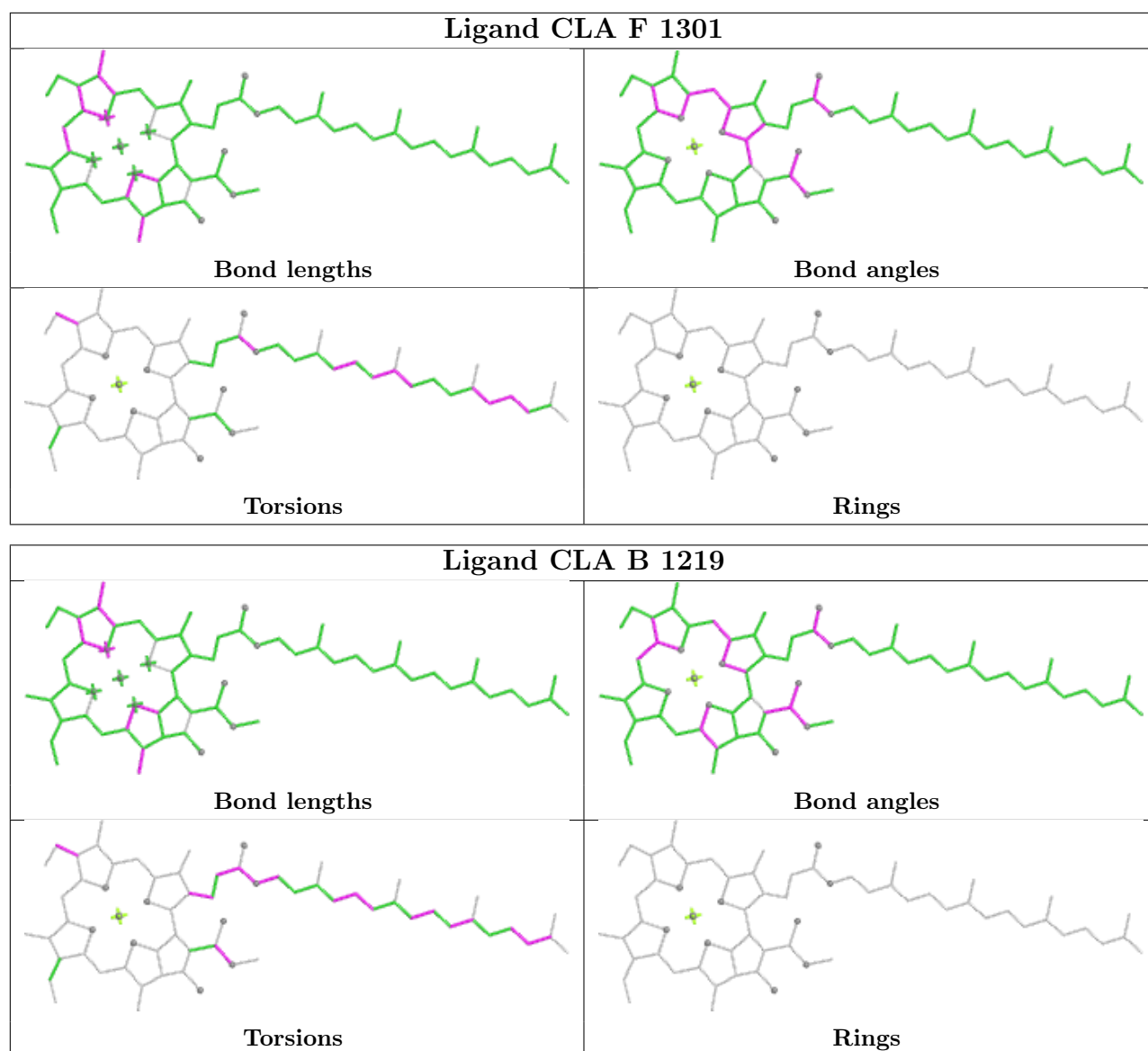


Ligand CLA c 508

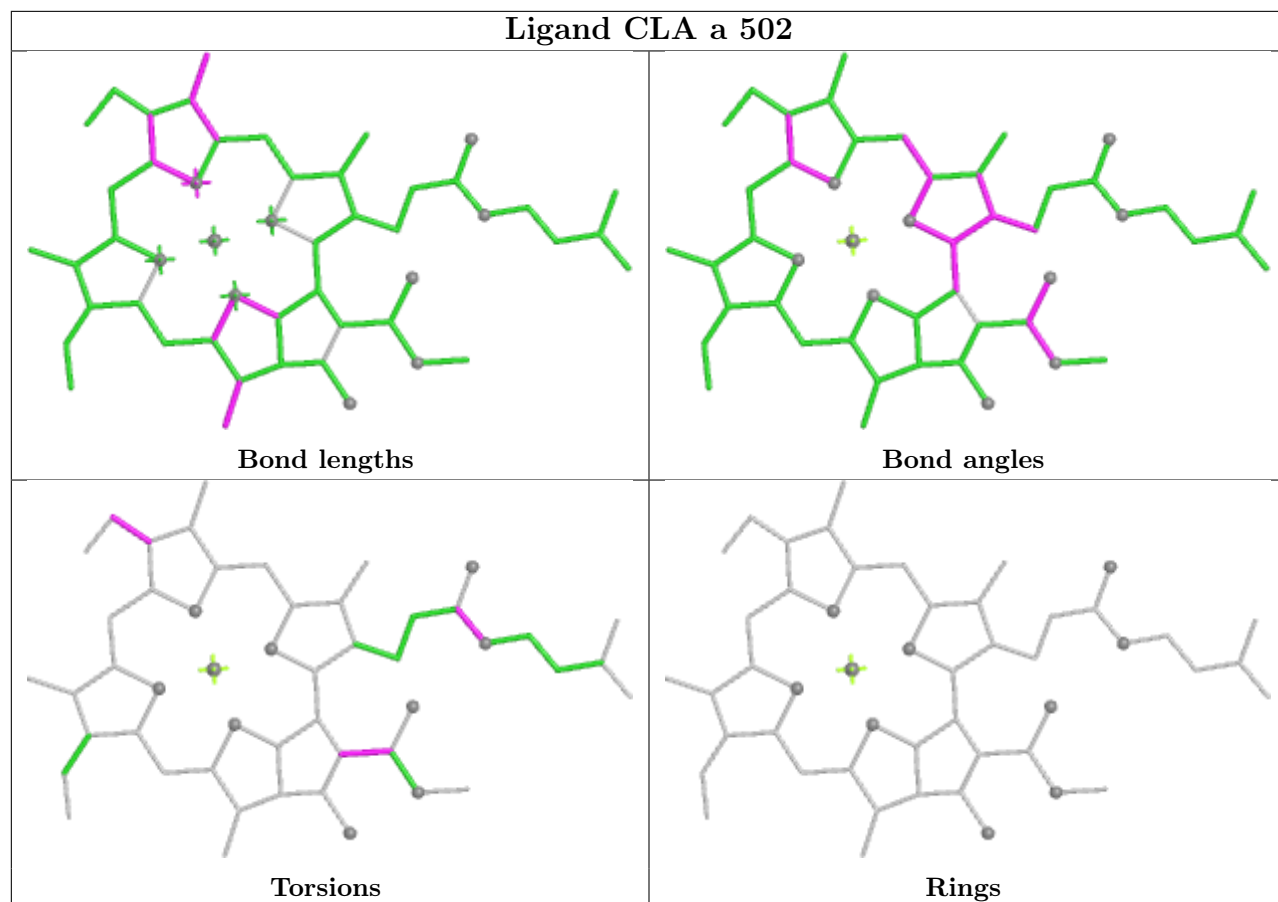




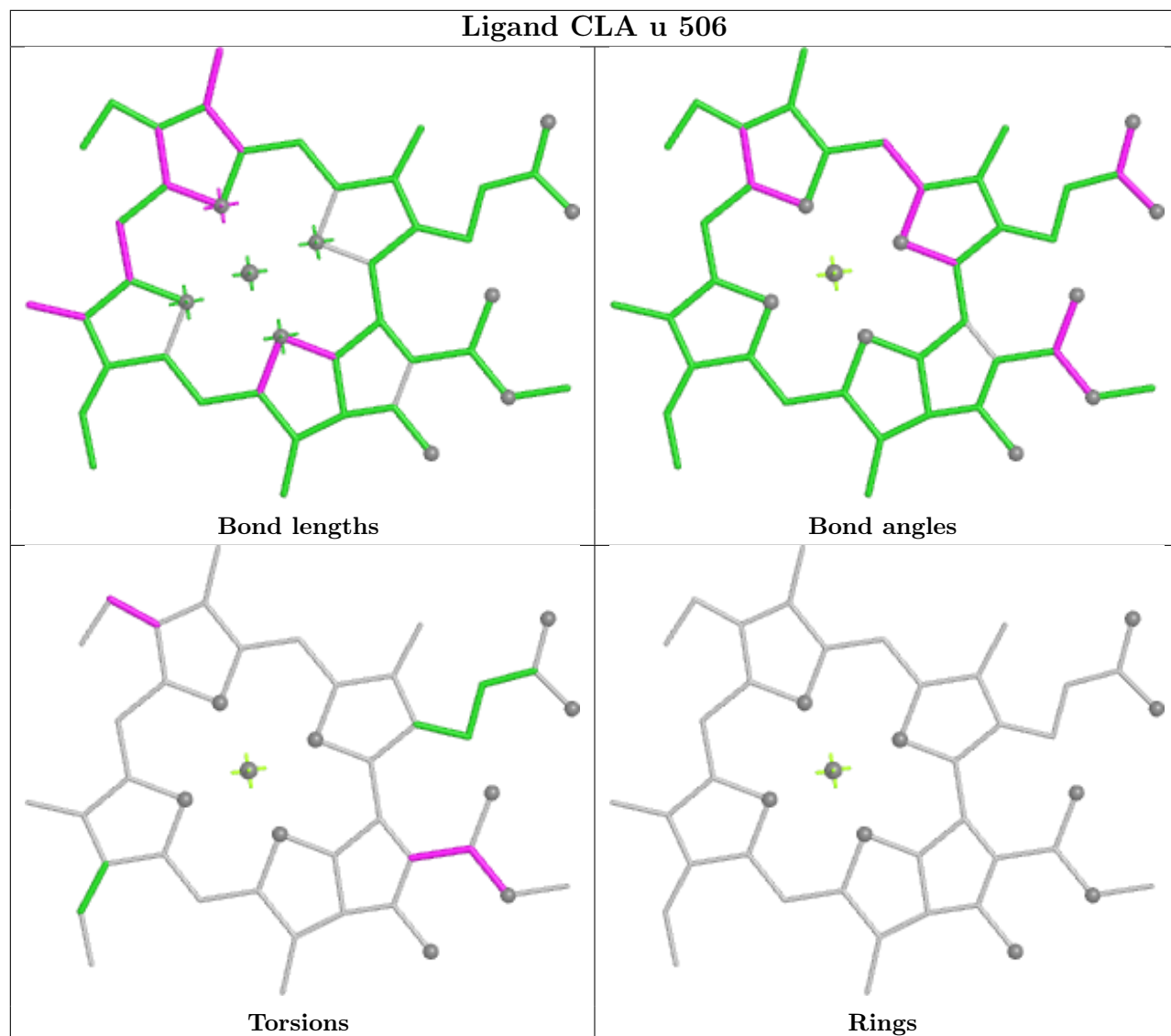




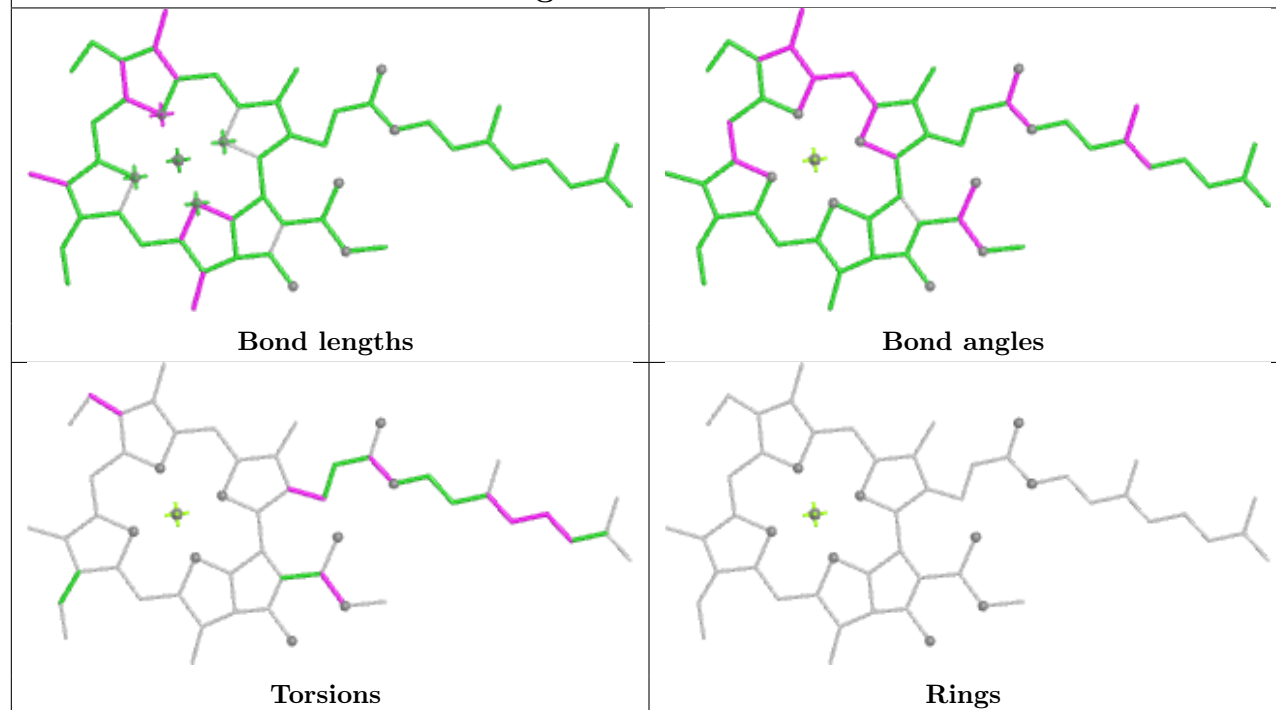
Ligand CLA a 502



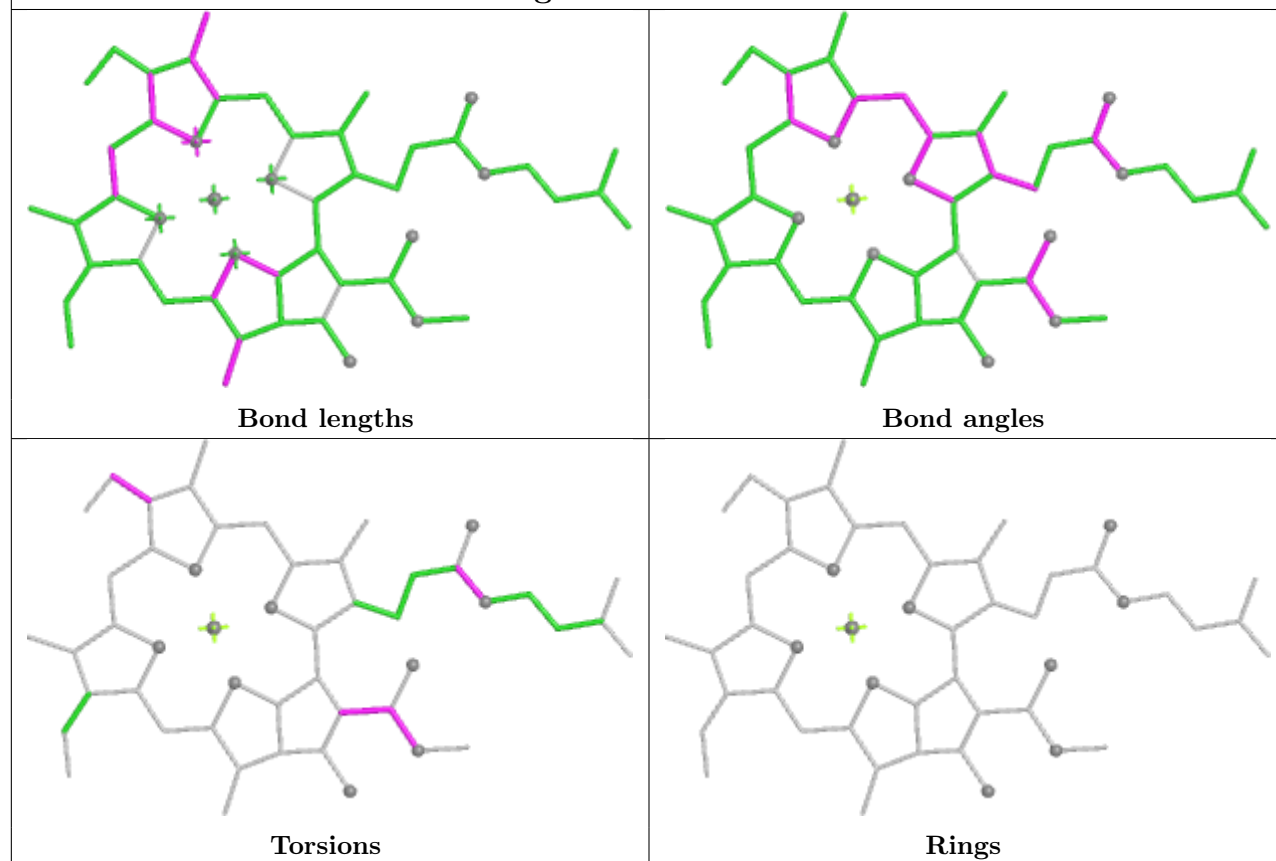
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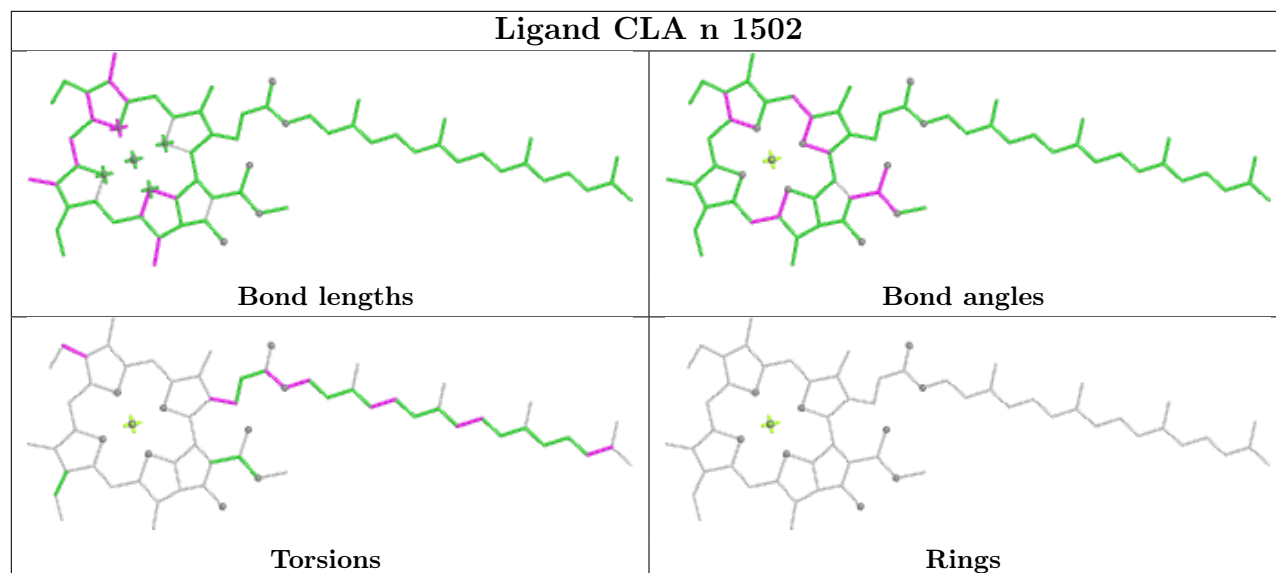
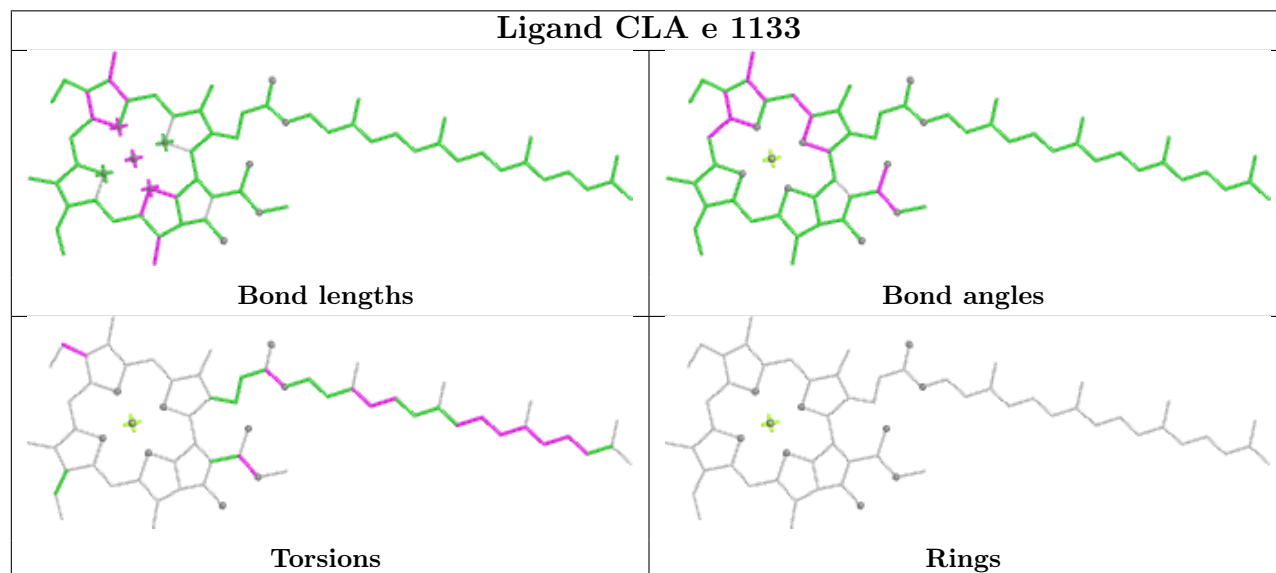
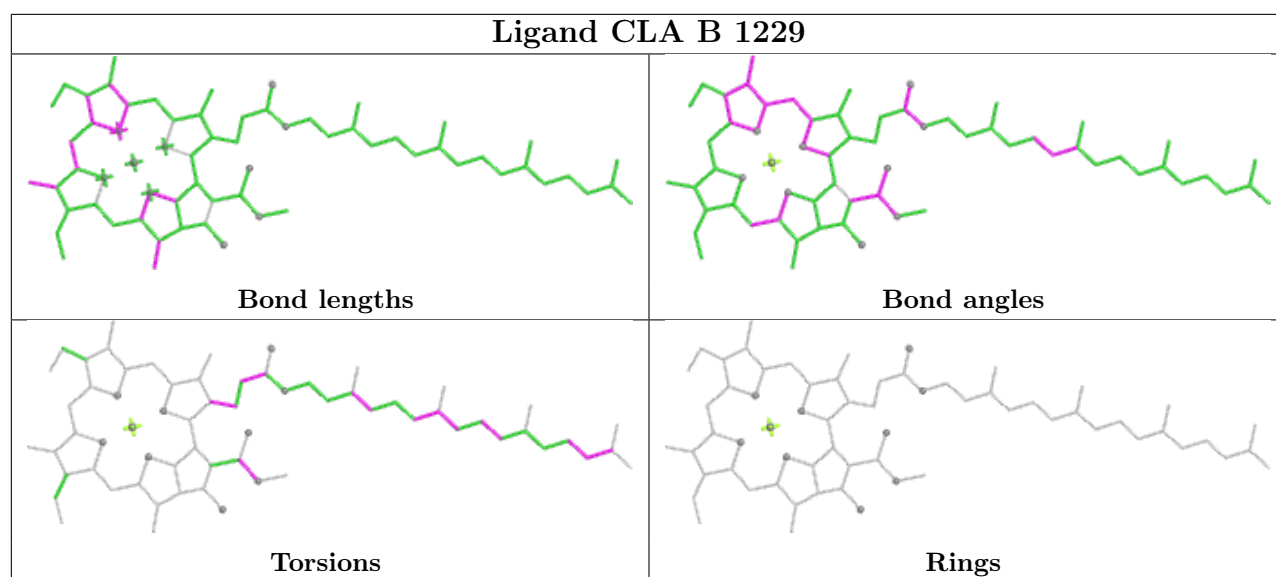


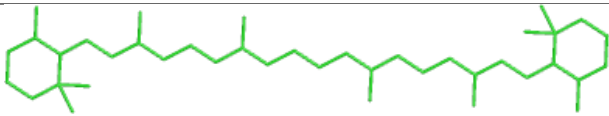
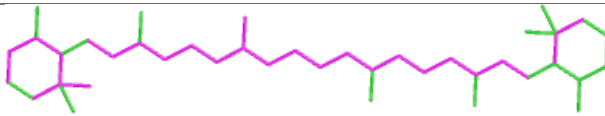
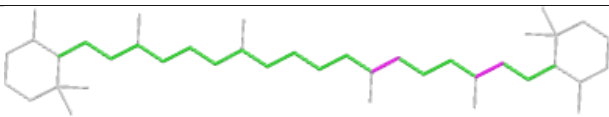
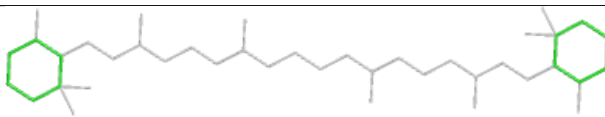
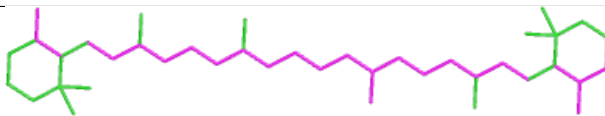
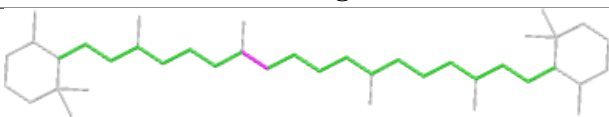
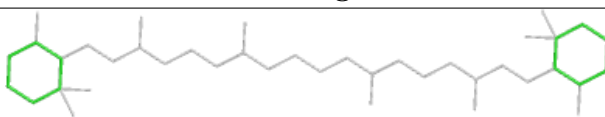
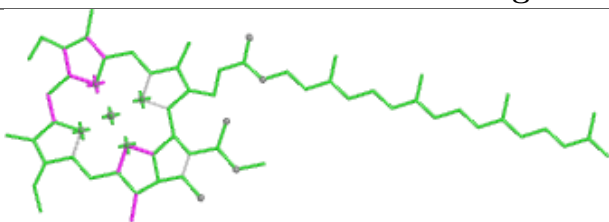
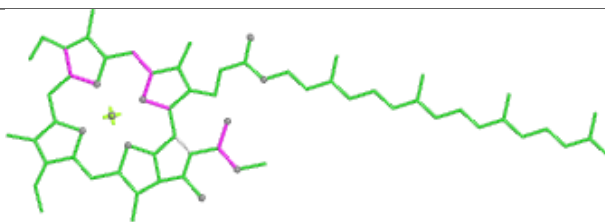
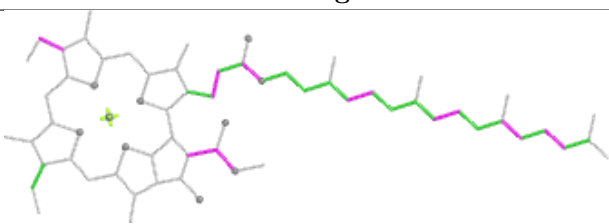
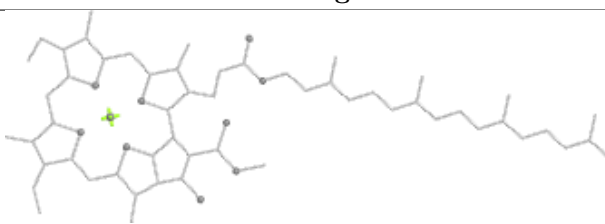
Ligand CLA 1 508



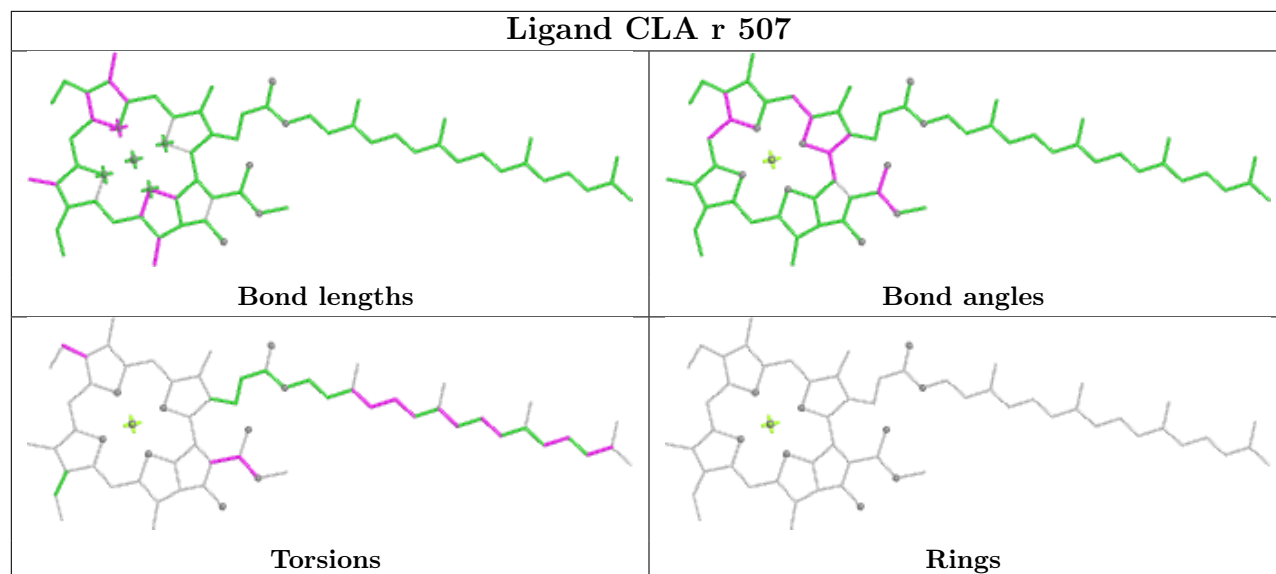
Ligand CLA Z 504



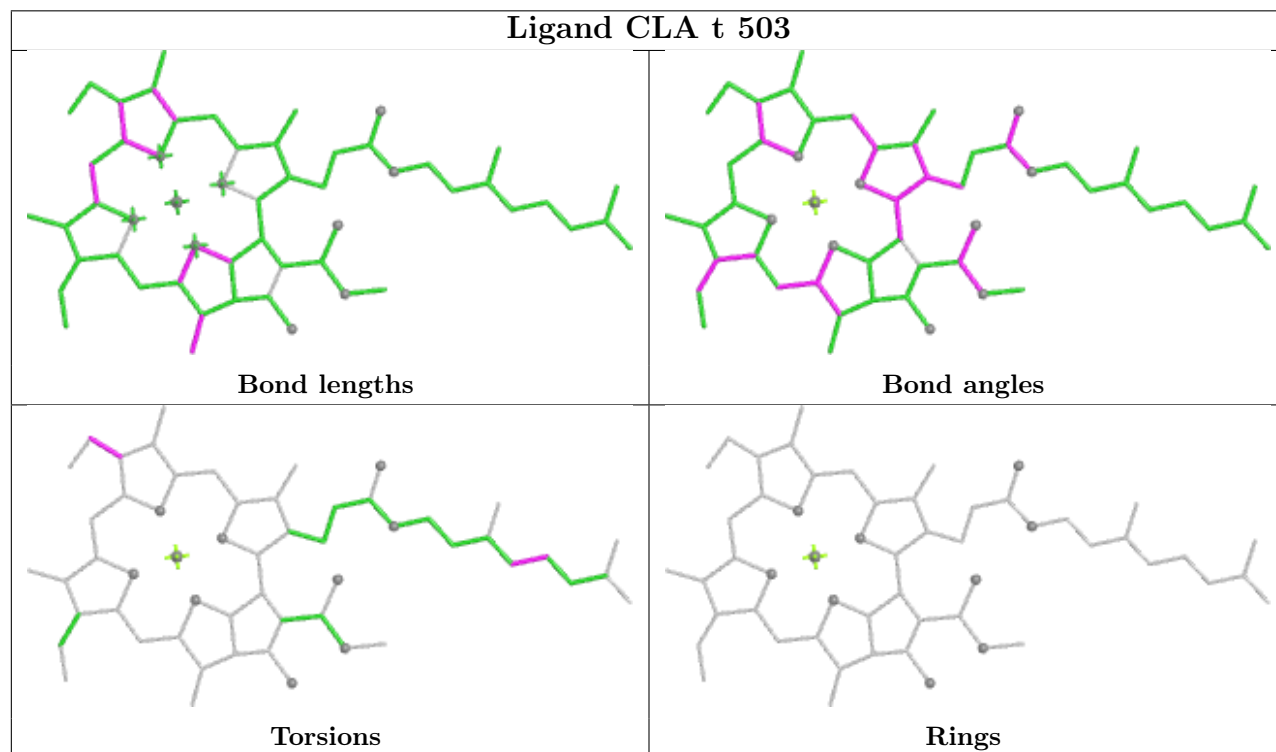


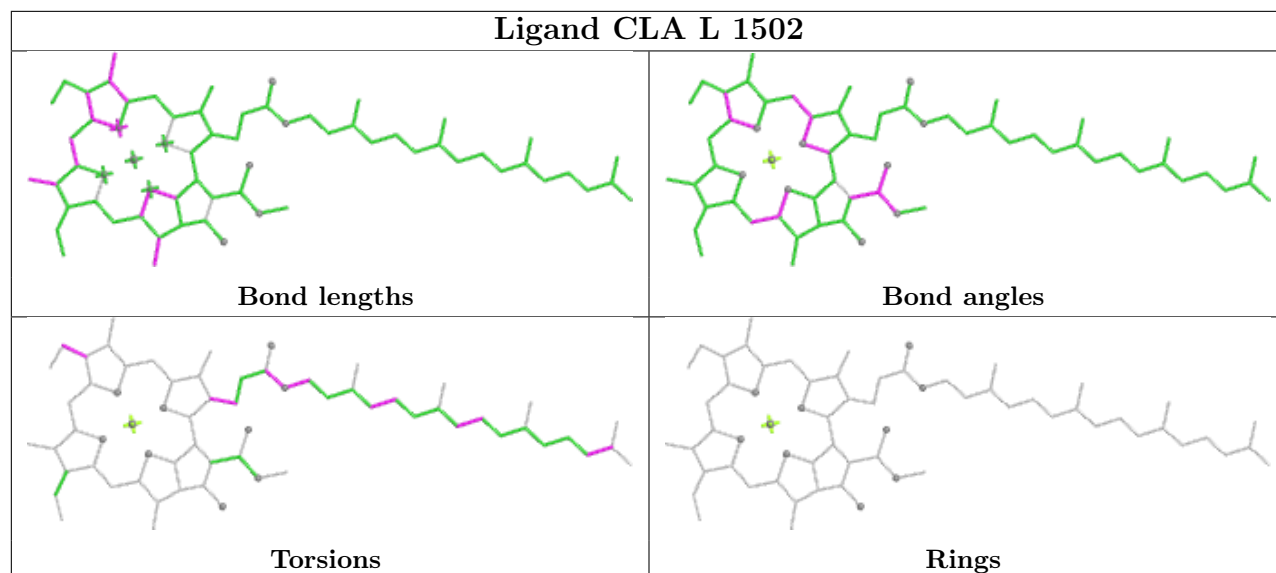
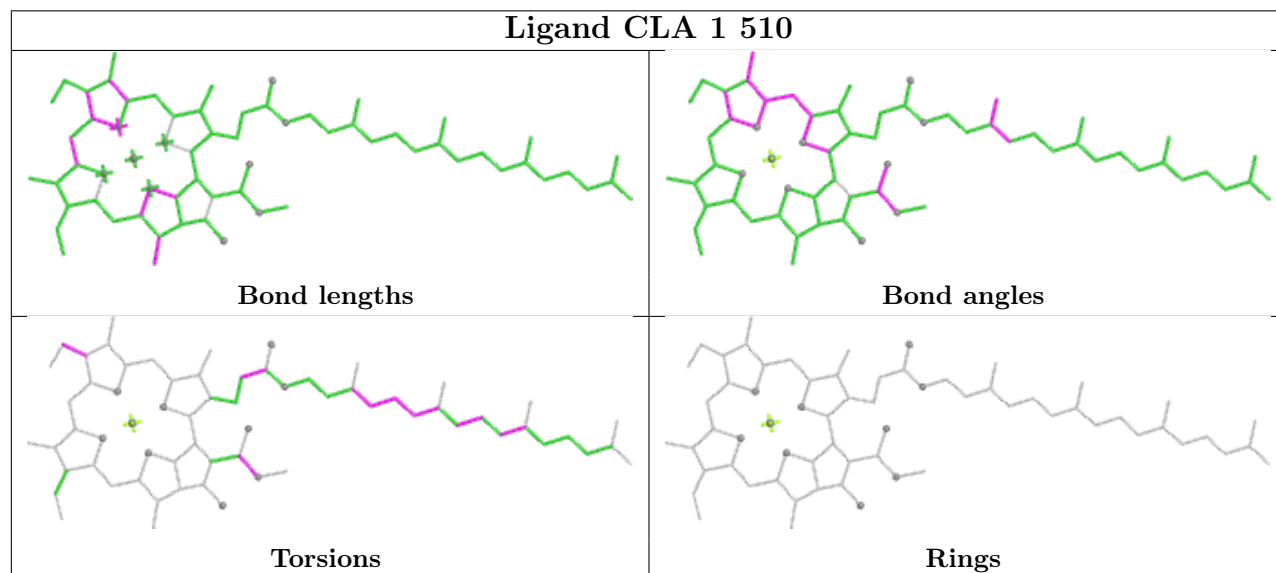
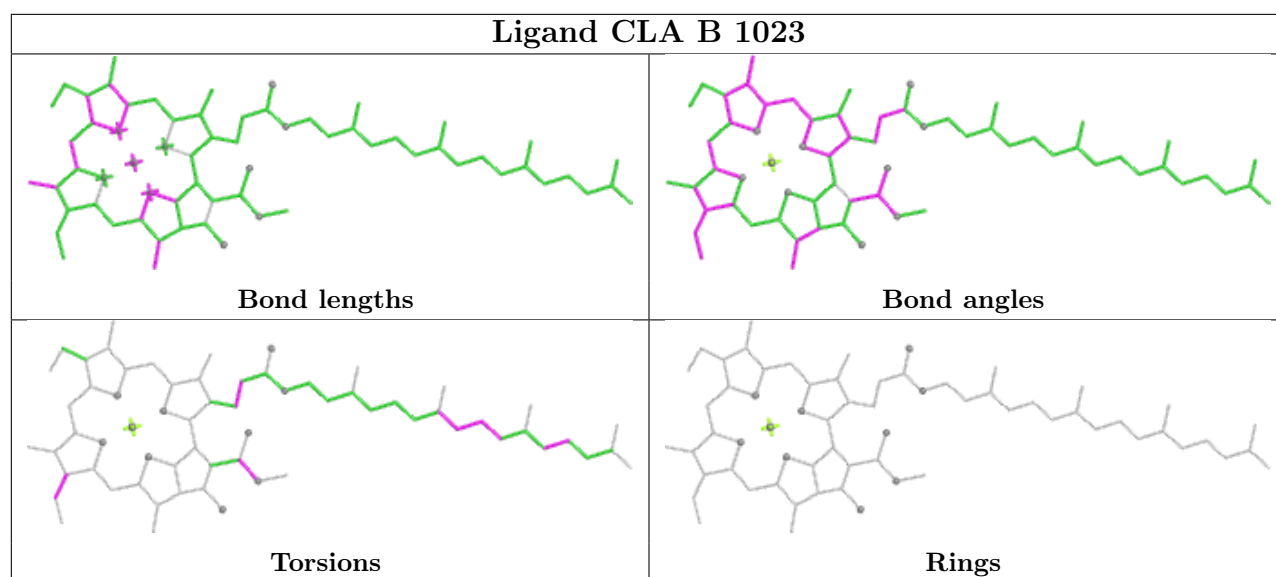
Ligand BCR J 4013	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR R 4016	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA b 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

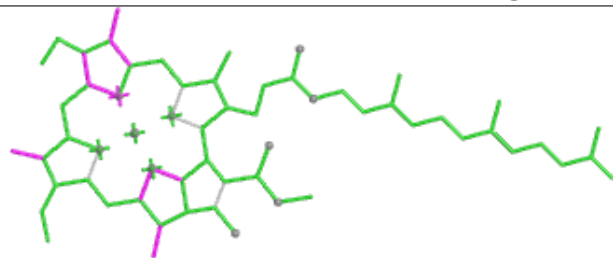
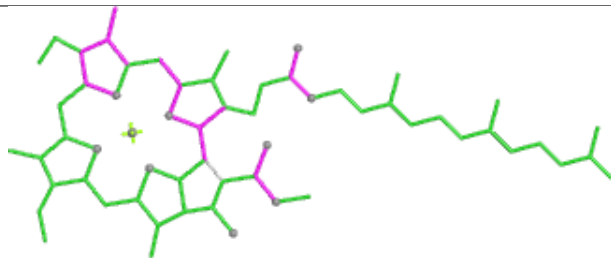
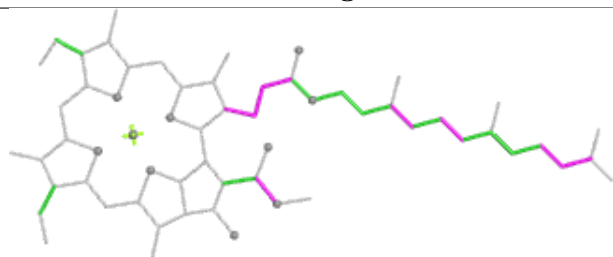
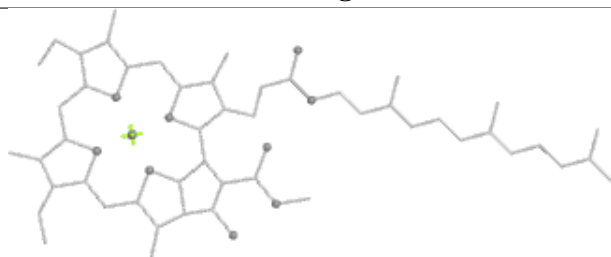
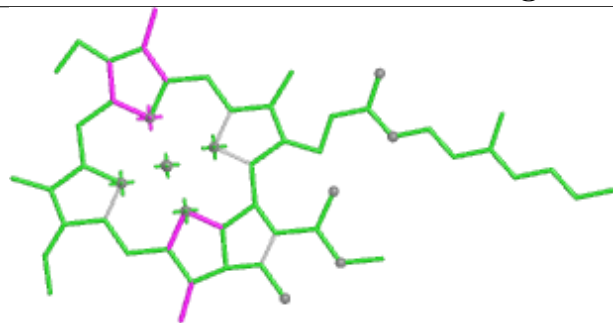
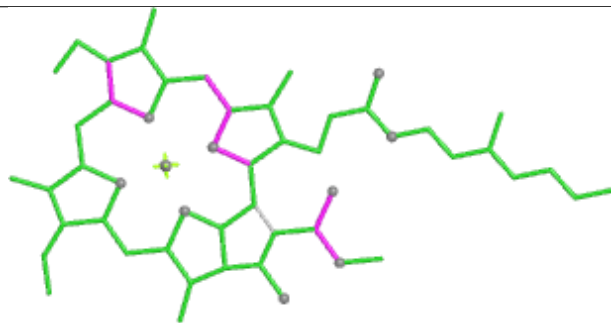
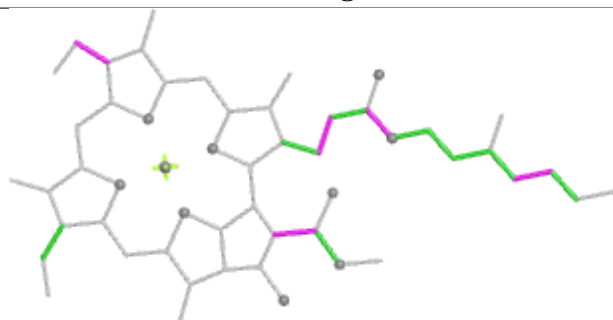
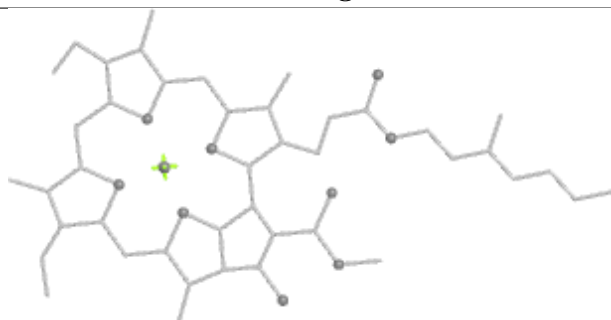
Ligand CLA r 507

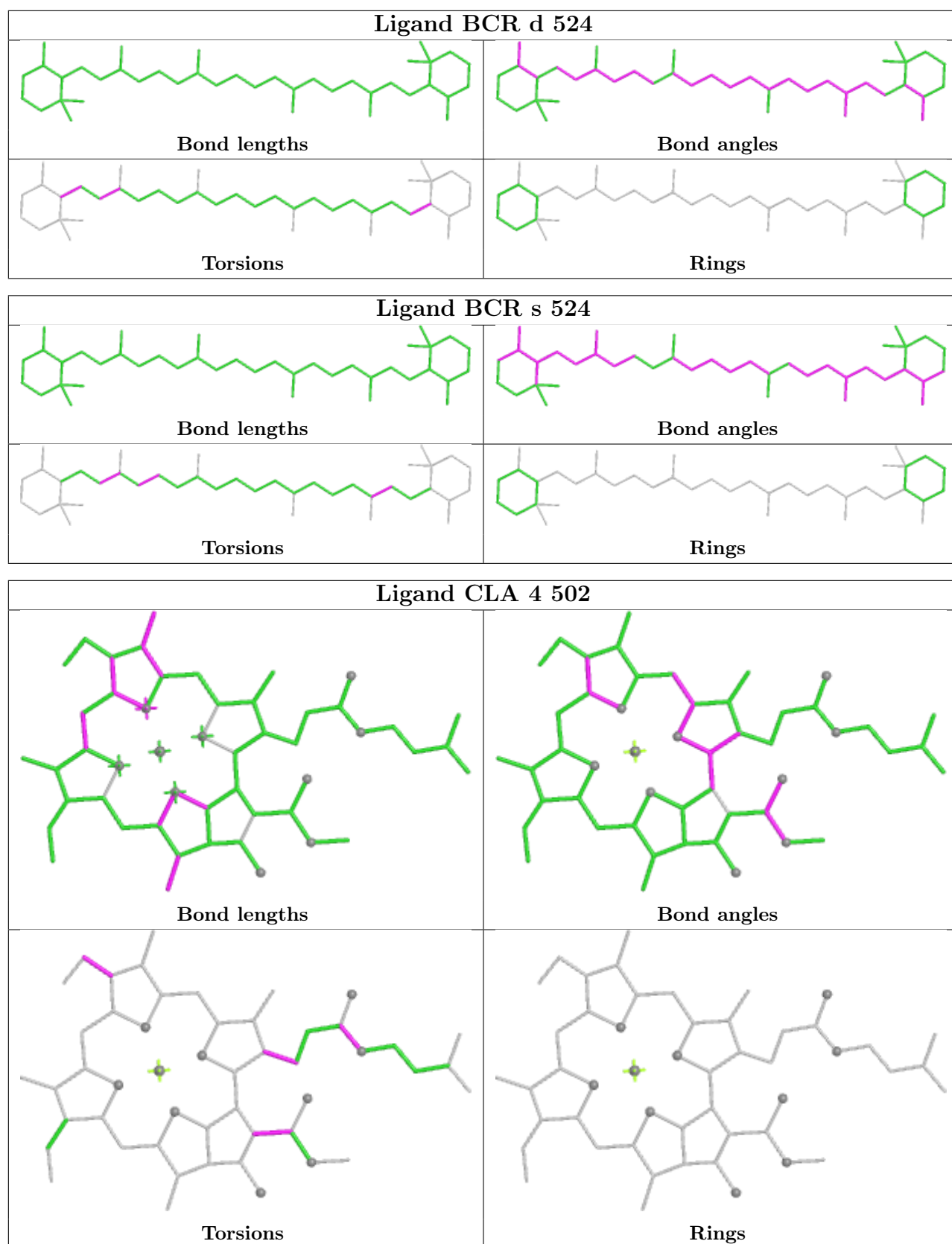


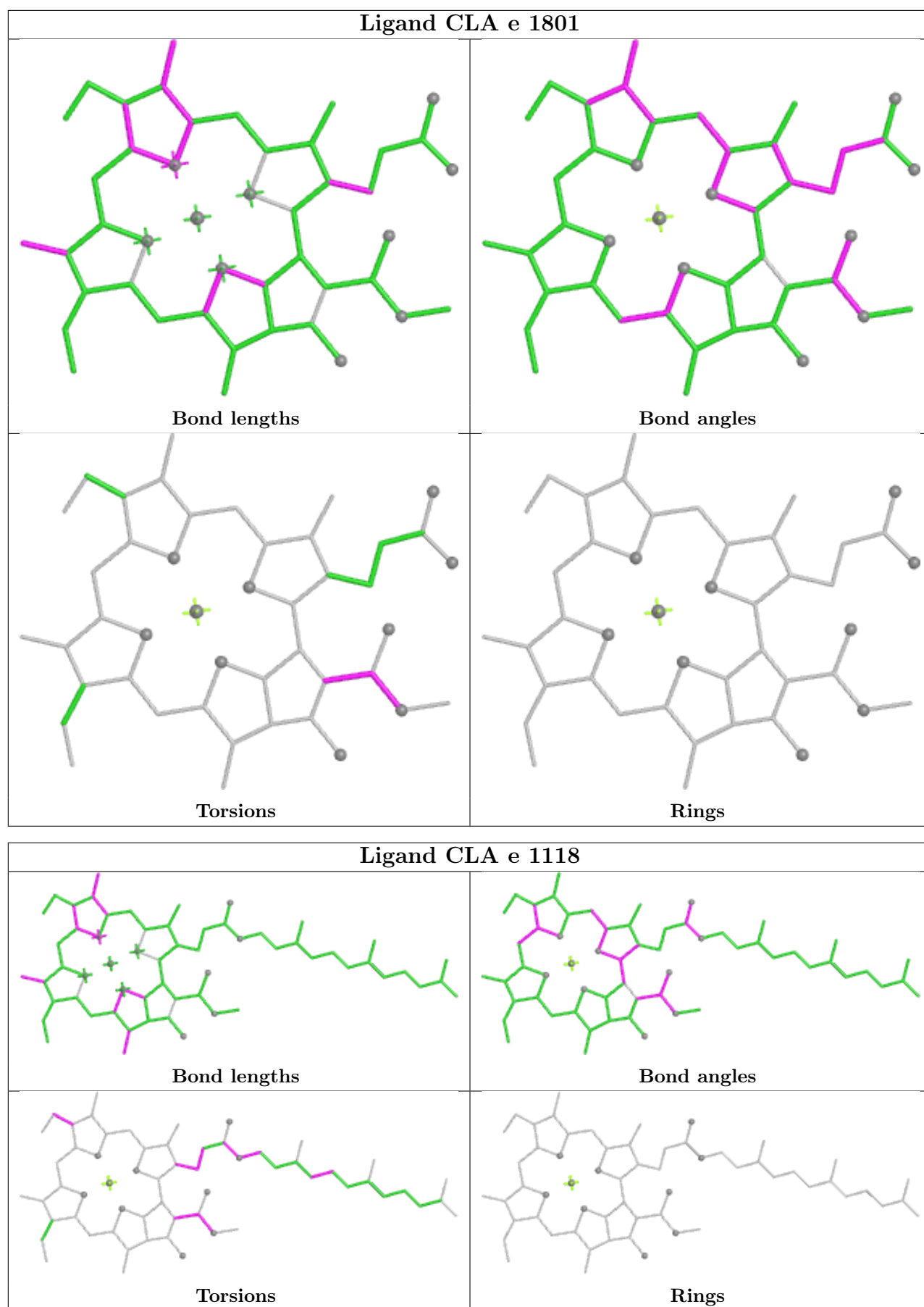
Ligand CLA t 503

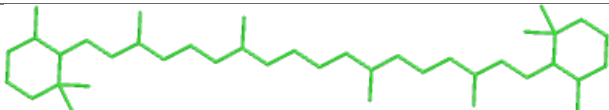
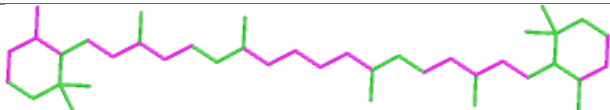
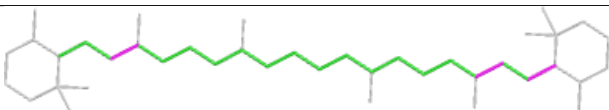
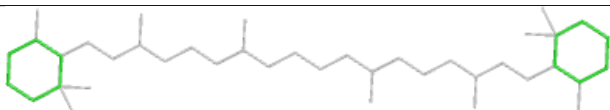


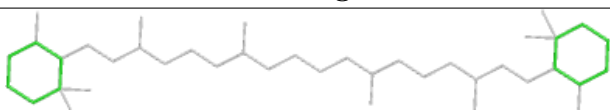


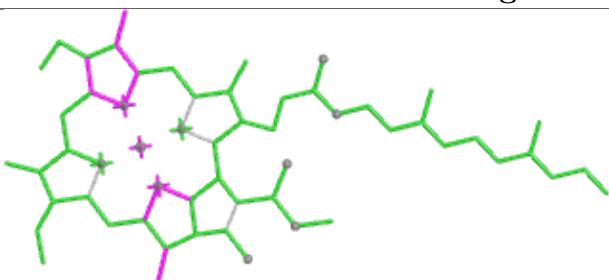
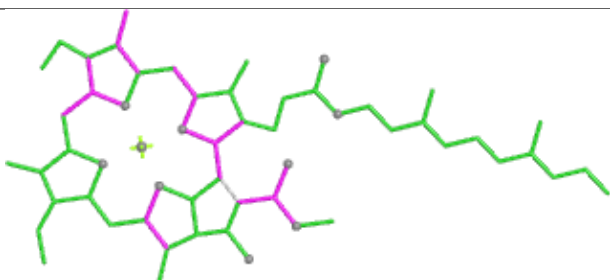
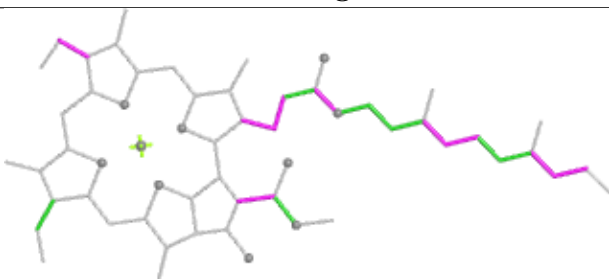
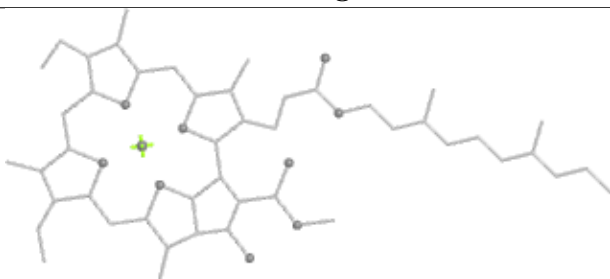
Ligand CLA B 1224**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA r 512****Bond lengths****Bond angles****Torsions****Rings**



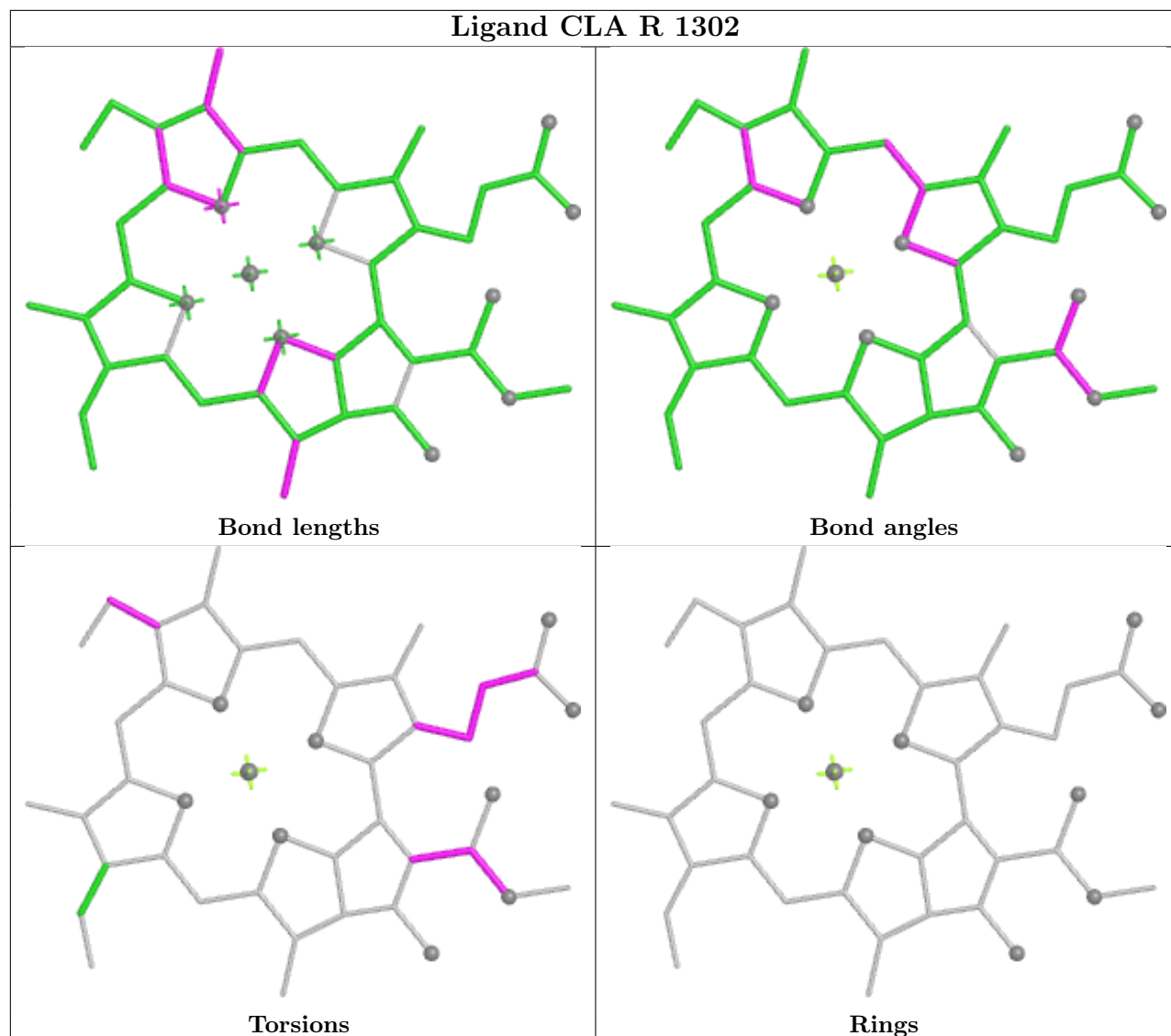


Ligand BCR B 4005	
	
Bond lengths	Bond angles
	
Torsions	Rings

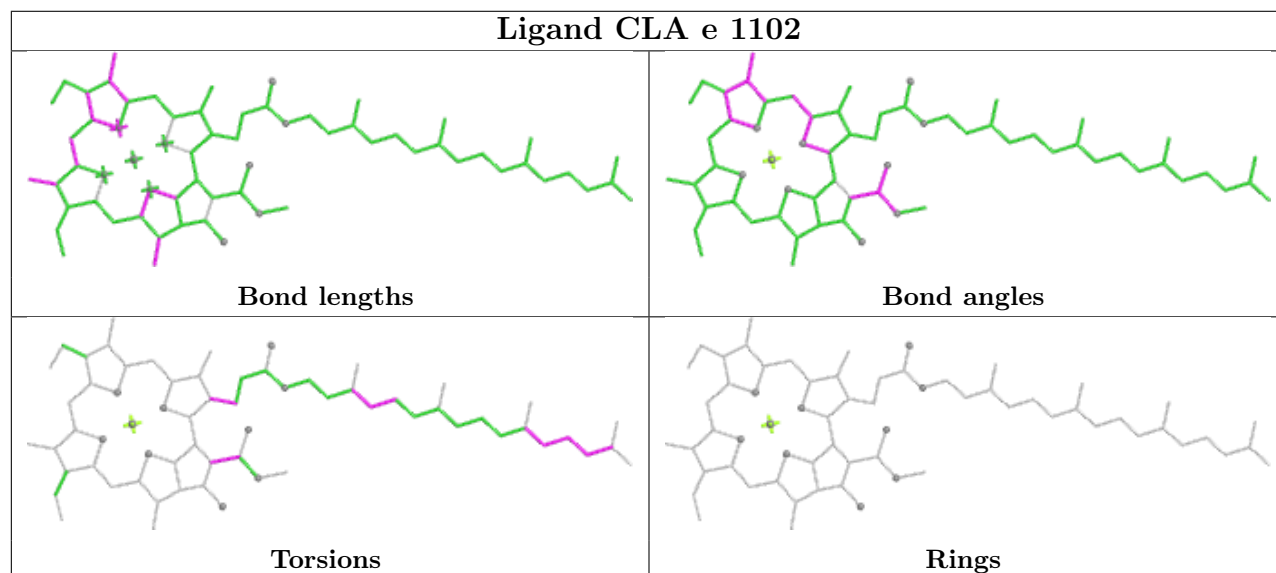
Ligand BCR Y 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

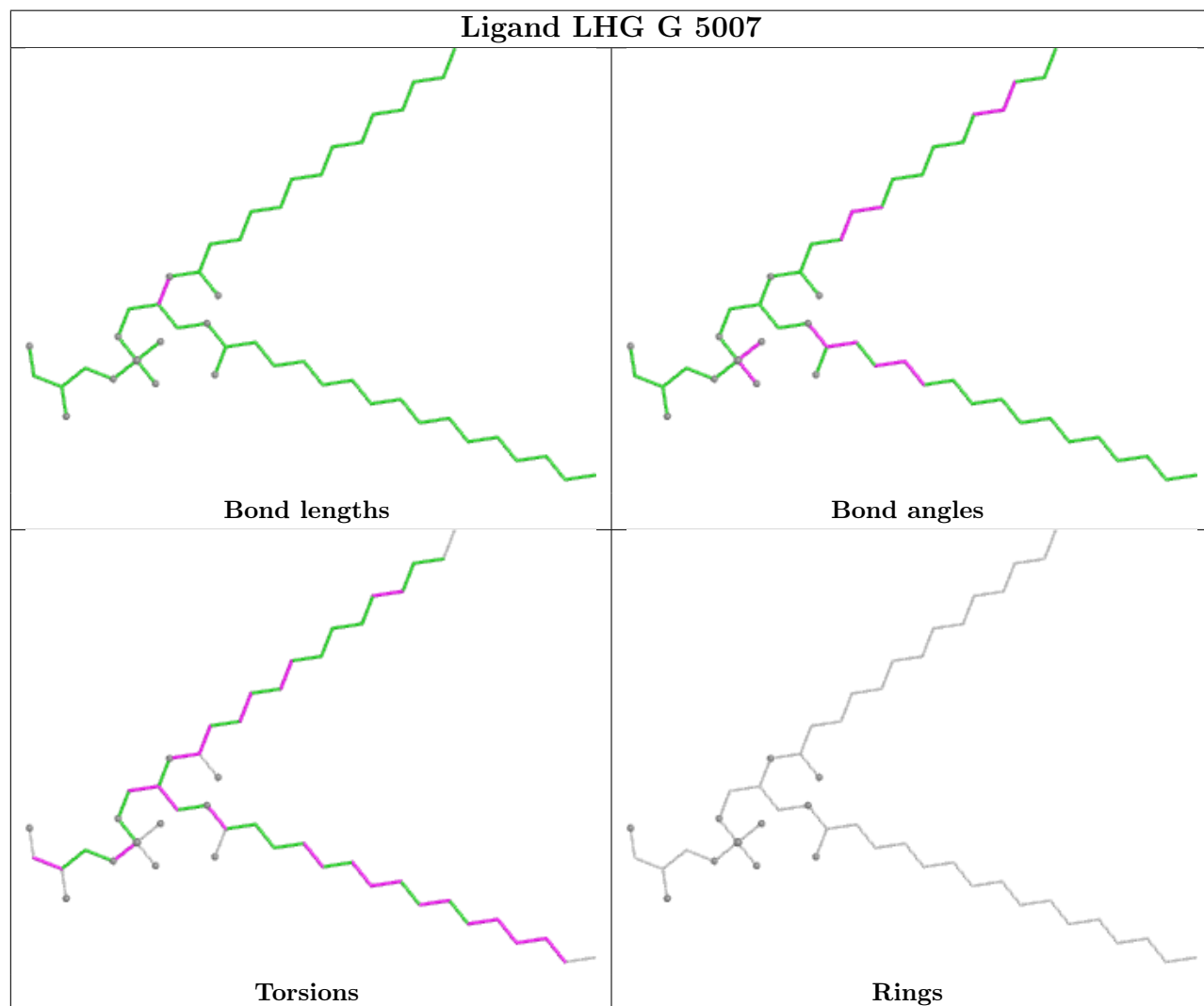
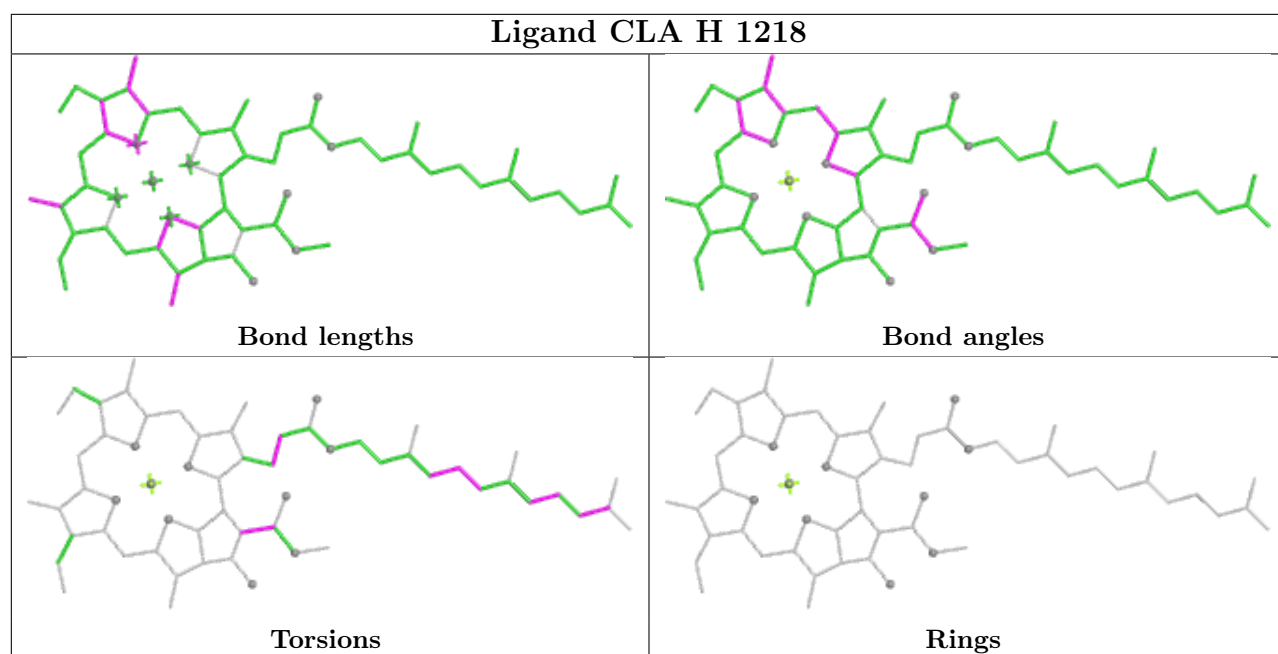
Ligand CLA H 1217	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R 1302

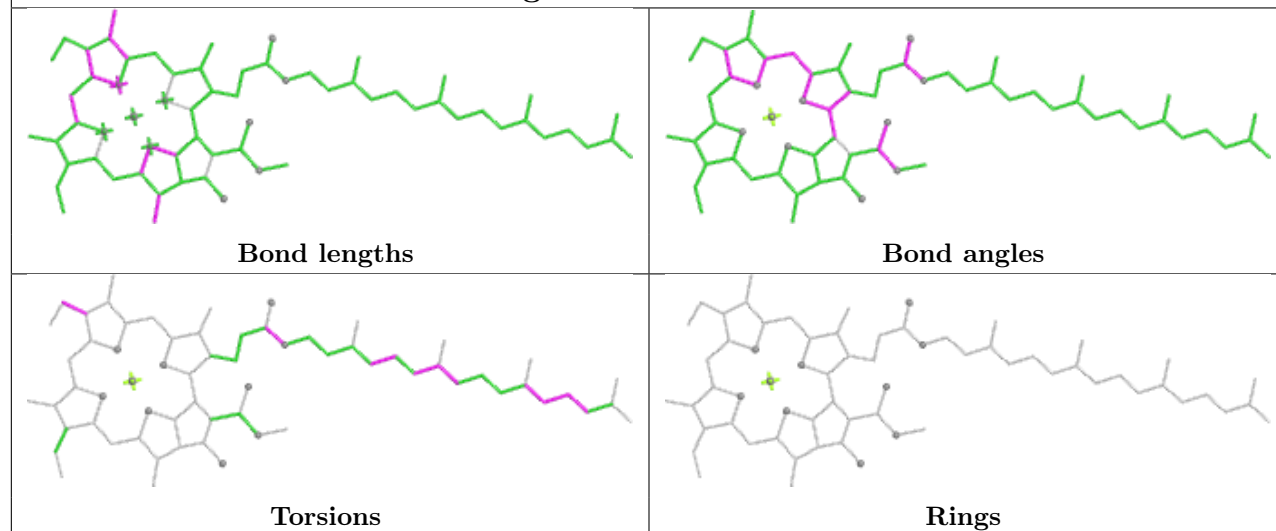


Ligand CLA e 1102

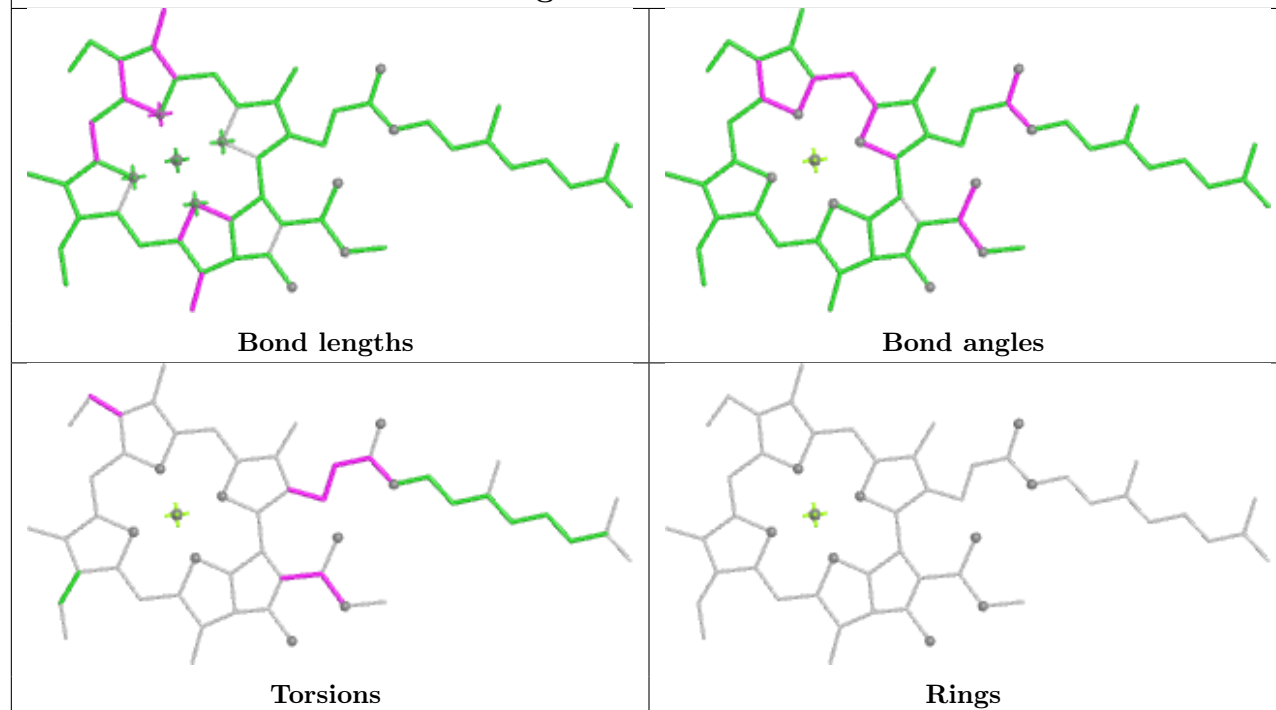


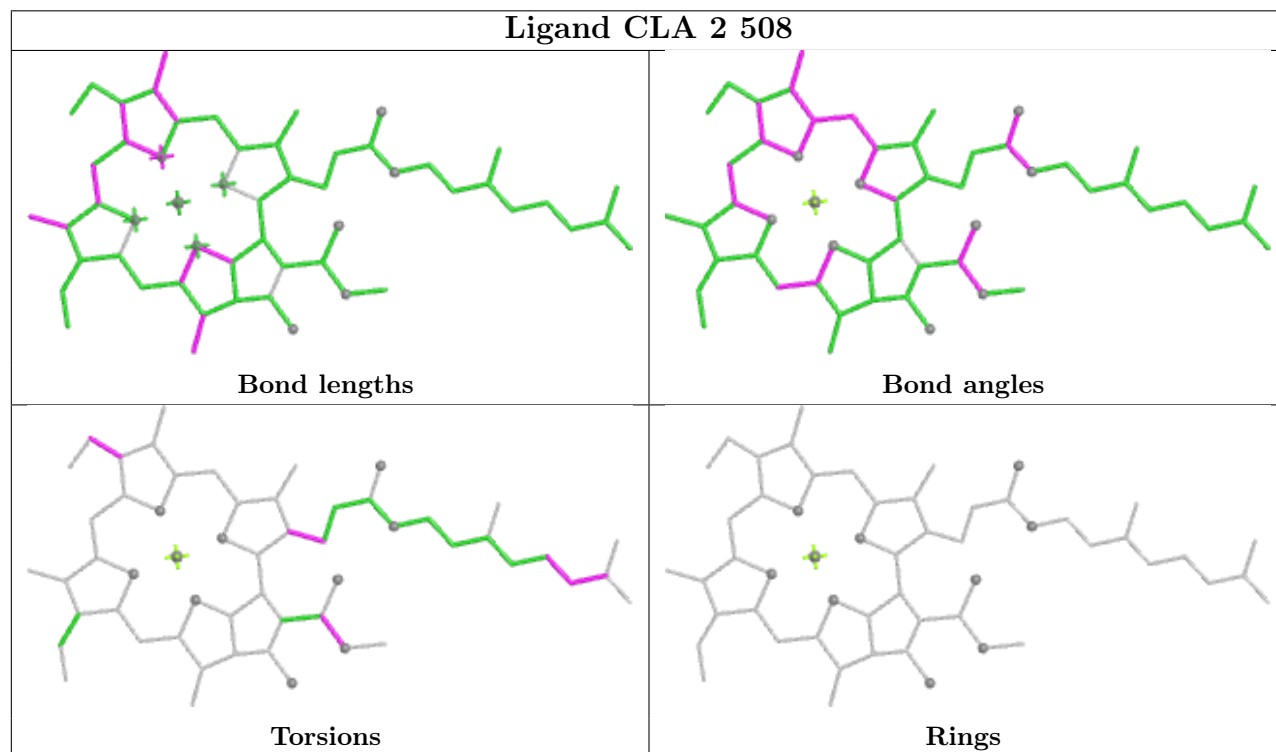
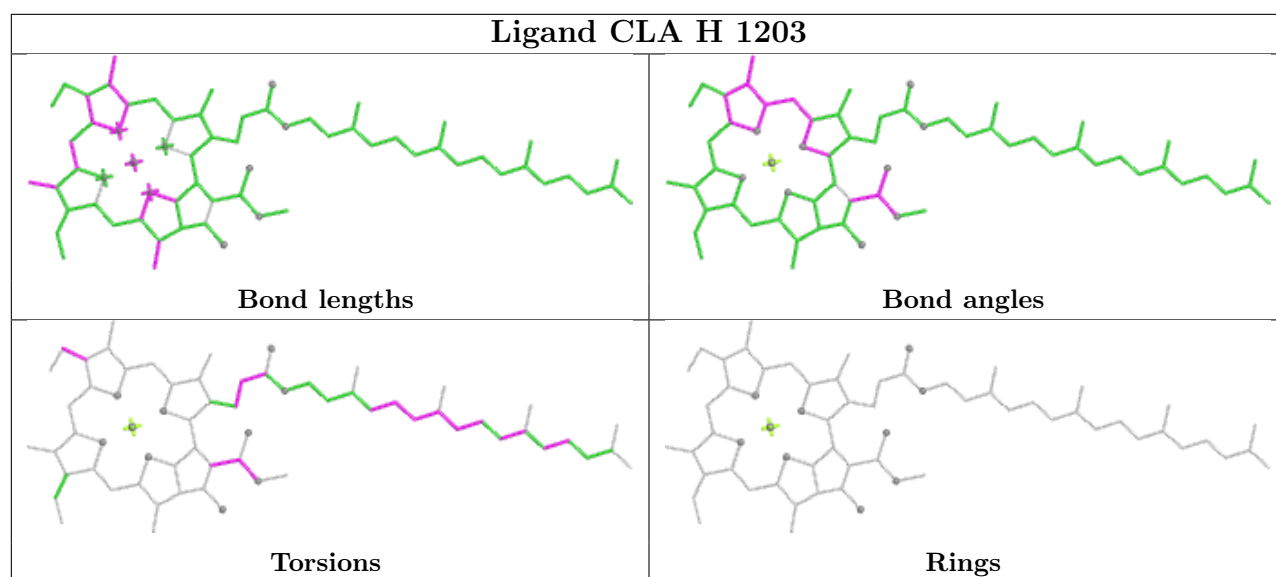


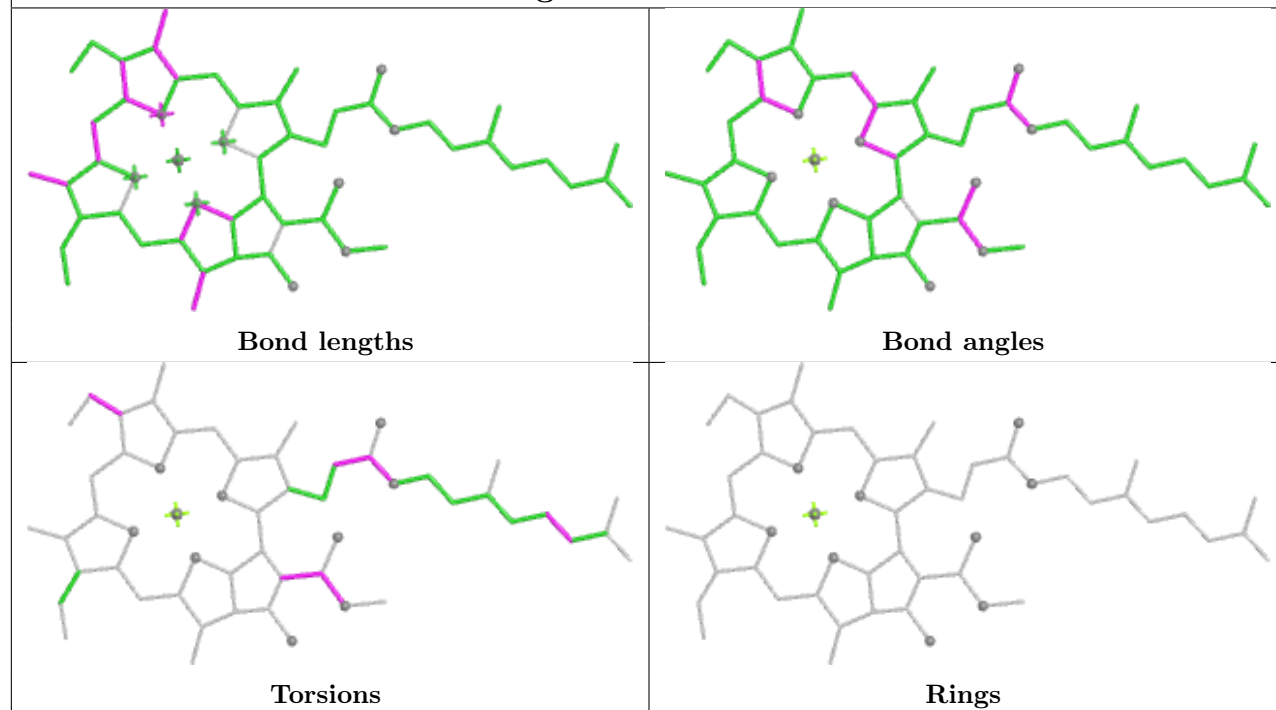
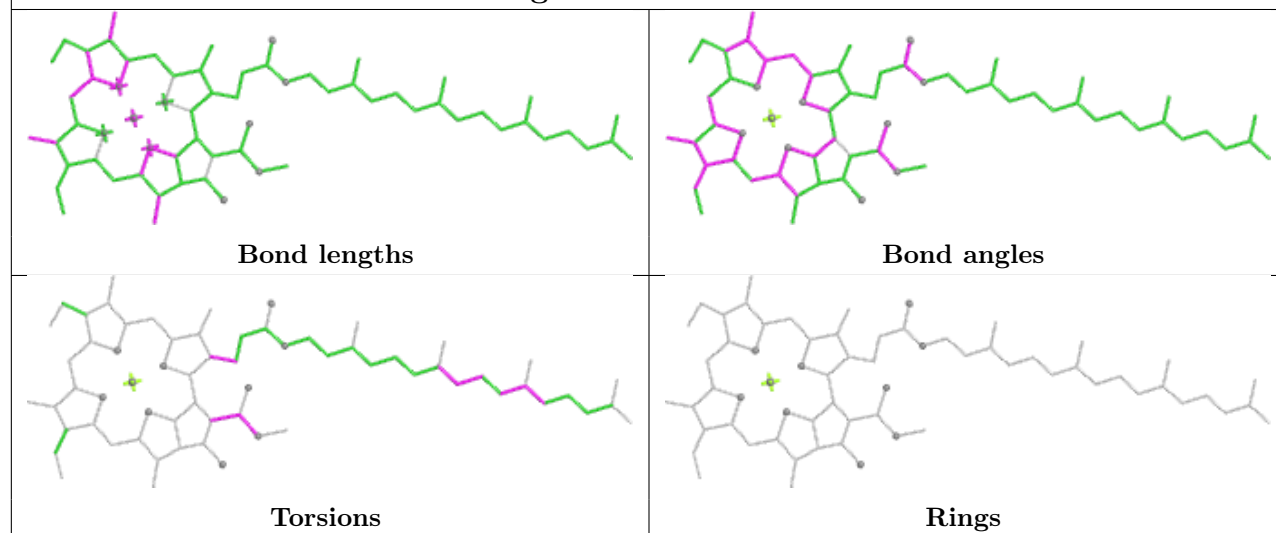
Ligand CLA R 1301

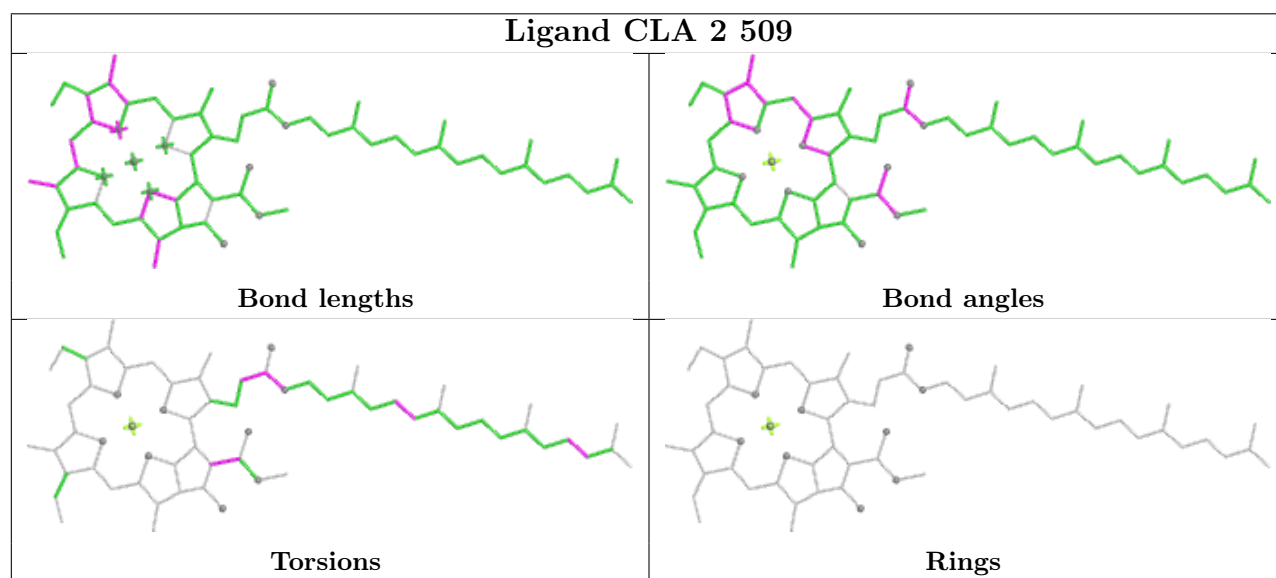
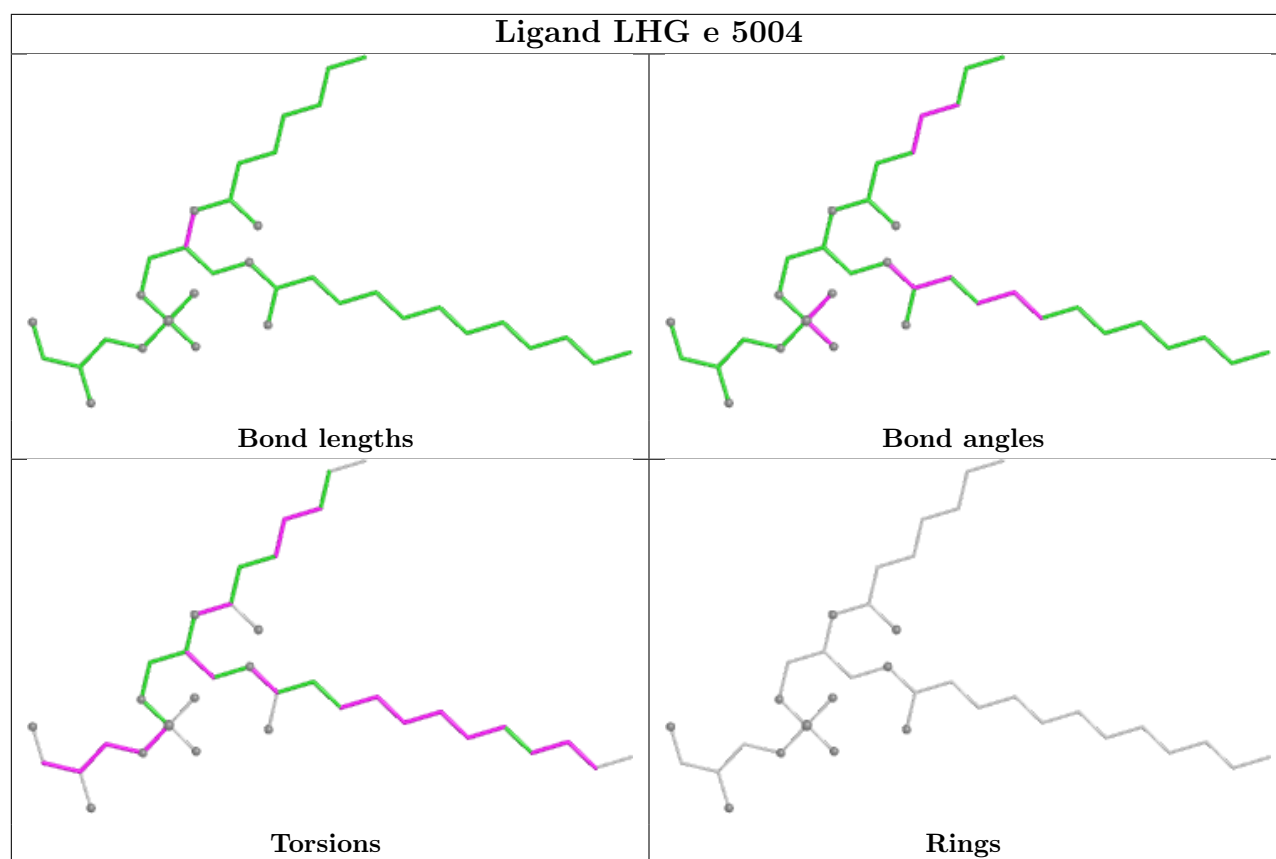


Ligand CLA 6 518

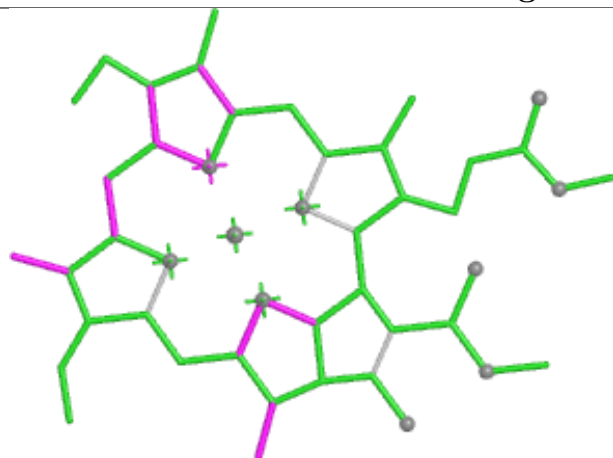




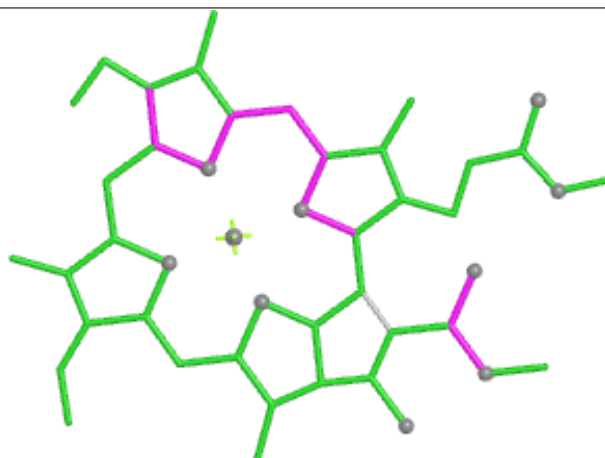
Ligand CLA a 519**Ligand CLA f 1226**



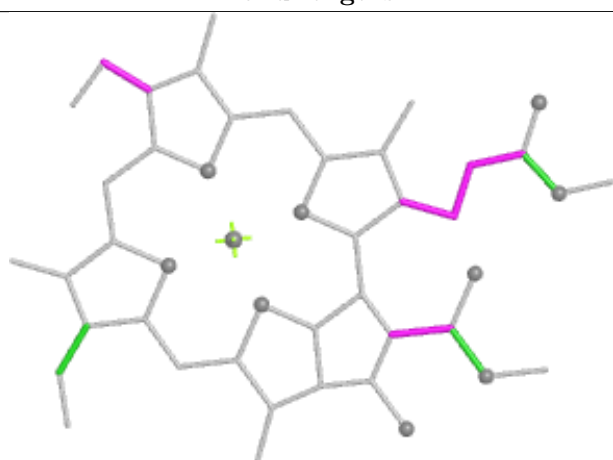
Ligand CLA 5 519



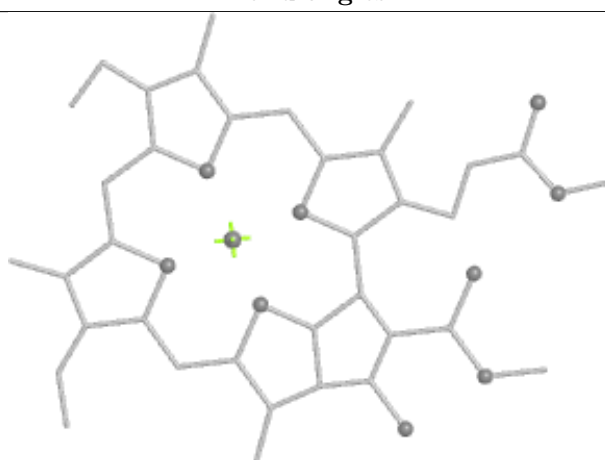
Bond lengths



Bond angles

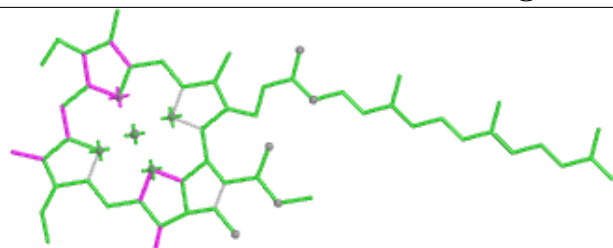


Torsions

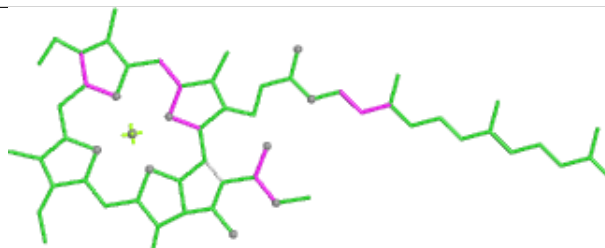


Rings

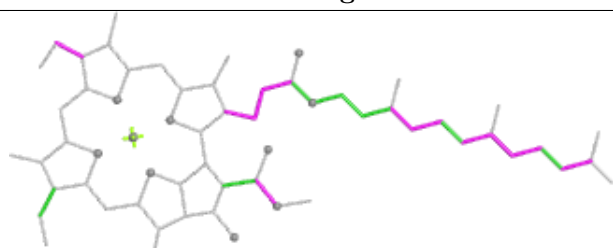
Ligand CLA v 501



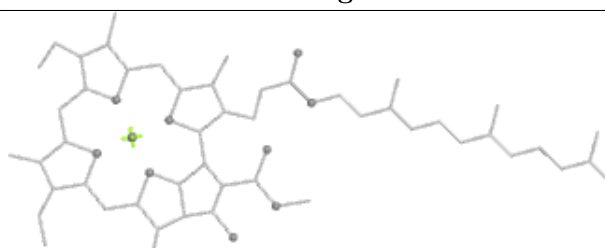
Bond lengths



Bond angles

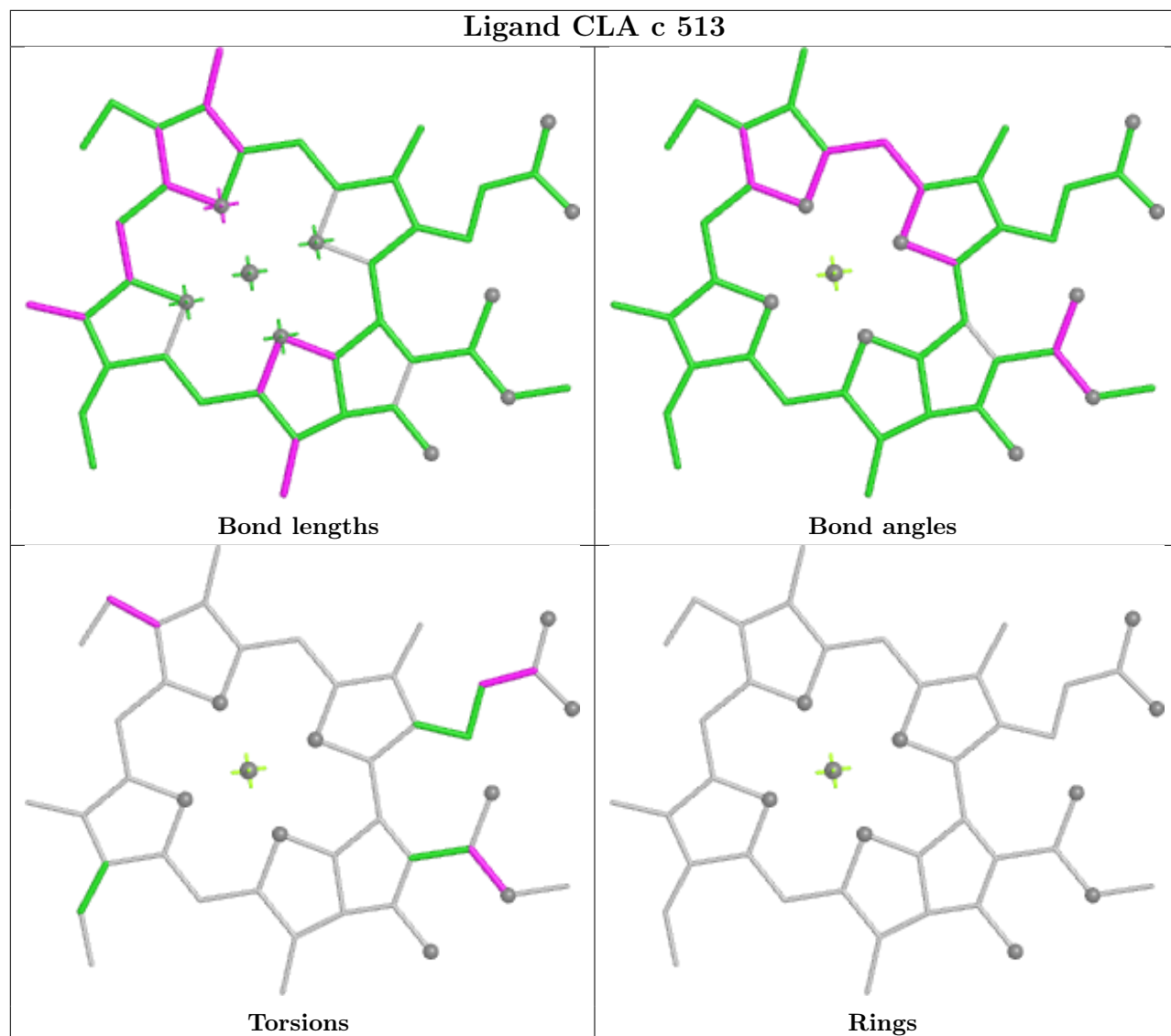


Torsions

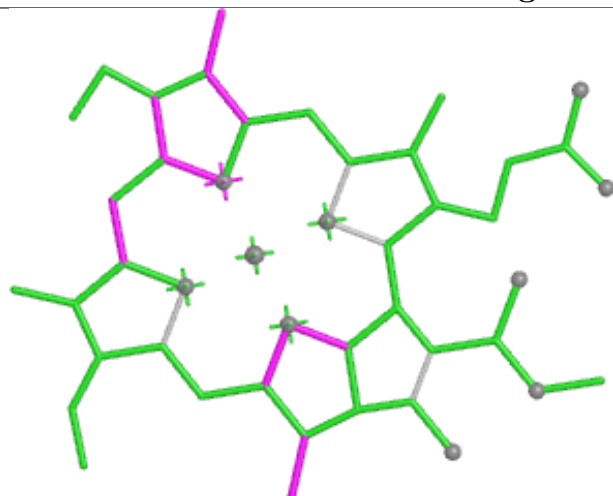


Rings

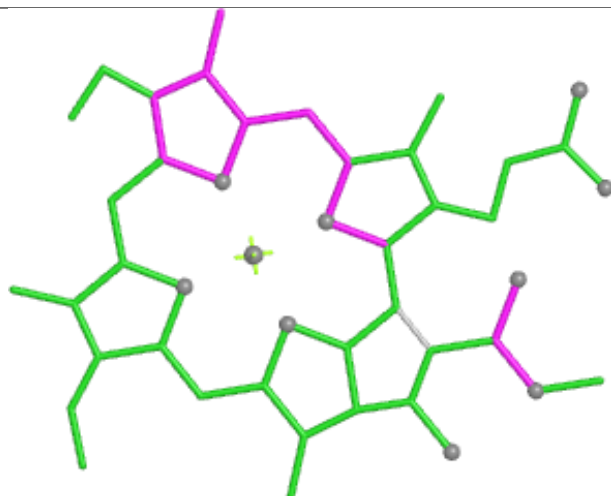
Ligand CLA c 513



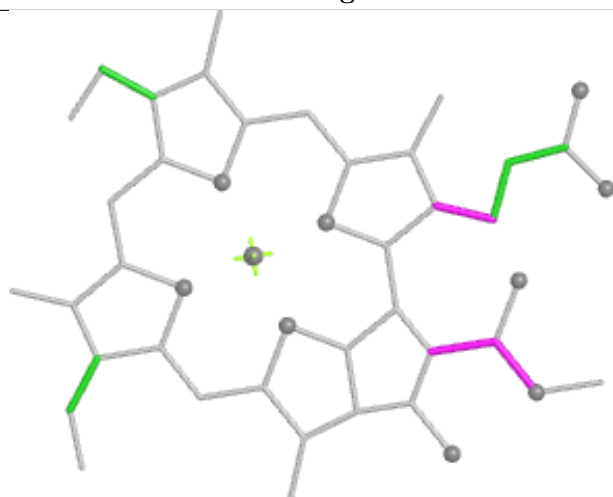
Ligand CLA 3 504



Bond lengths



Bond angles

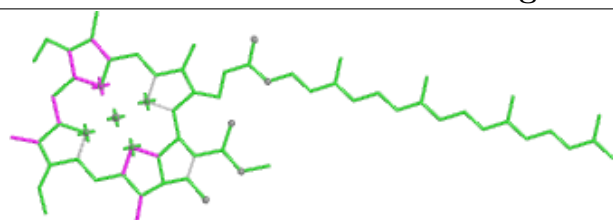


Torsions

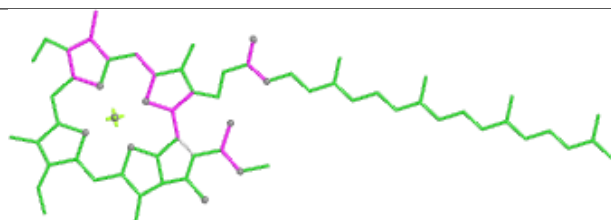


Rings

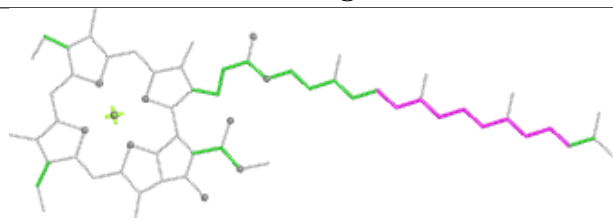
Ligand CLA c 509



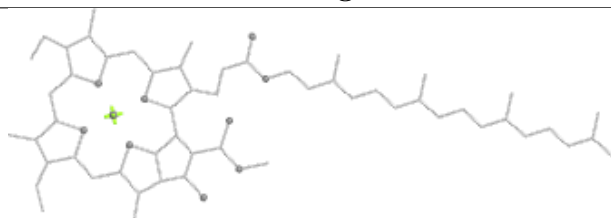
Bond lengths



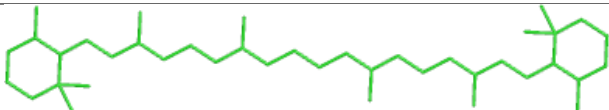
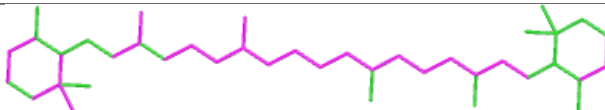
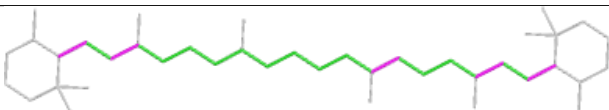
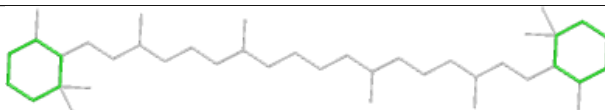
Bond angles

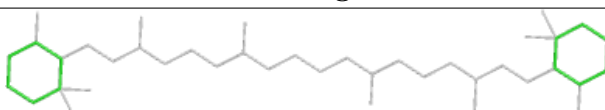


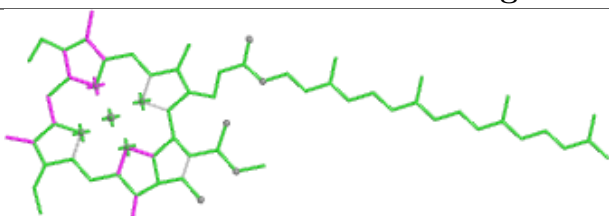
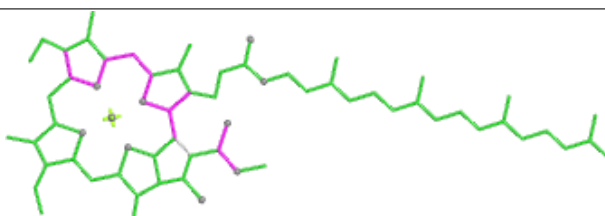
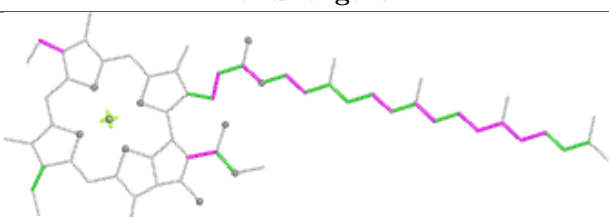
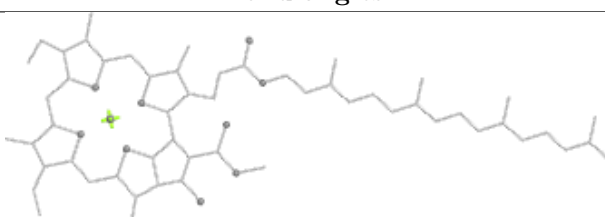
Torsions



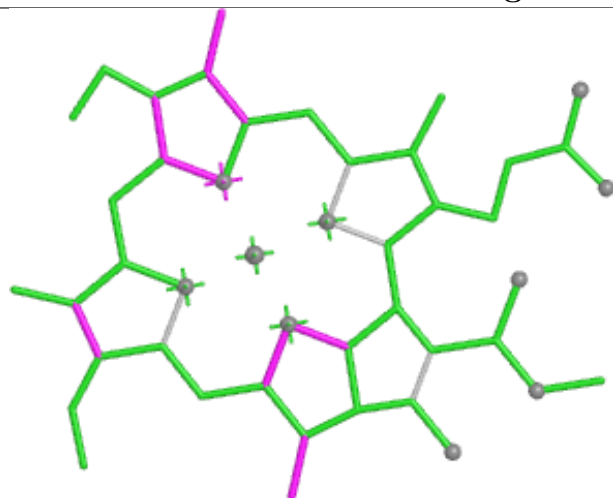
Rings

Ligand BCR H 4014	
	
Bond lengths	Bond angles
	
Torsions	Rings

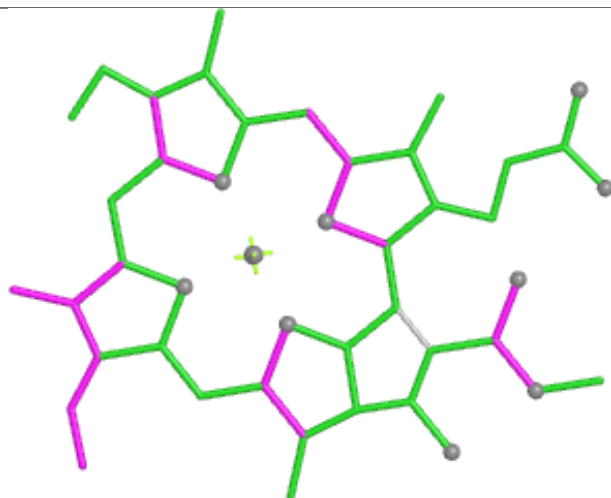
Ligand BCR d 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1214	
	
Bond lengths	Bond angles
	
Torsions	Rings

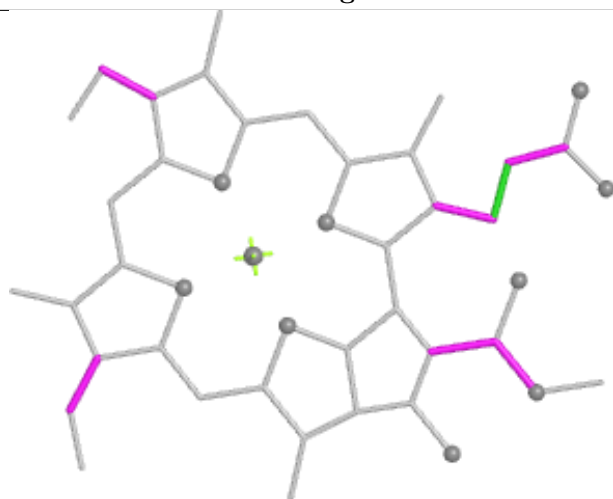
Ligand CLA K 1105



Bond lengths



Bond angles

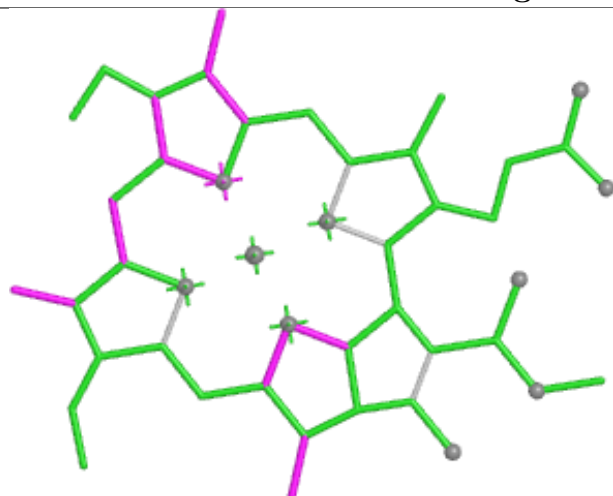


Torsions

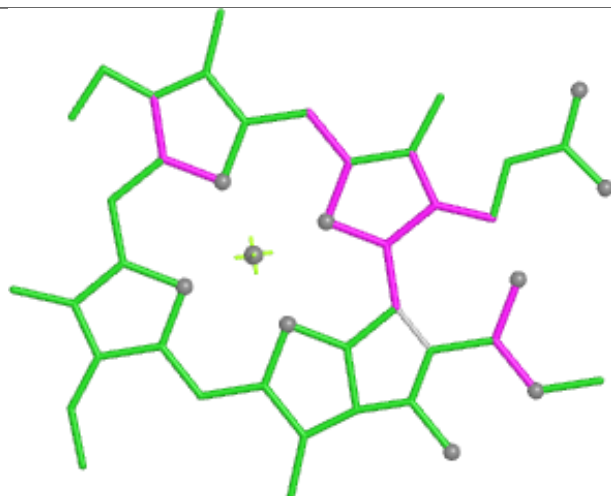


Rings

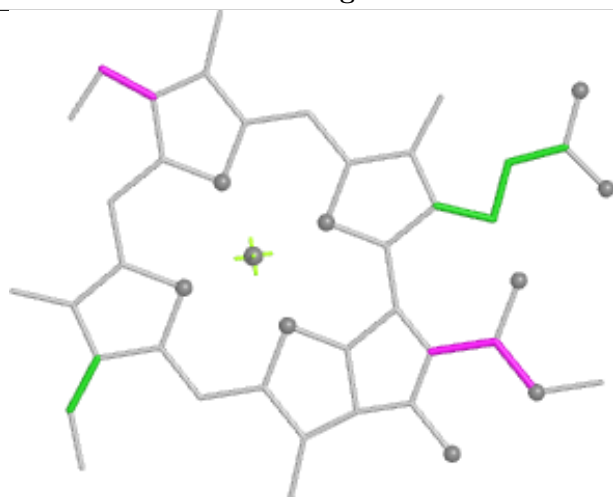
Ligand CLA Y 504



Bond lengths



Bond angles

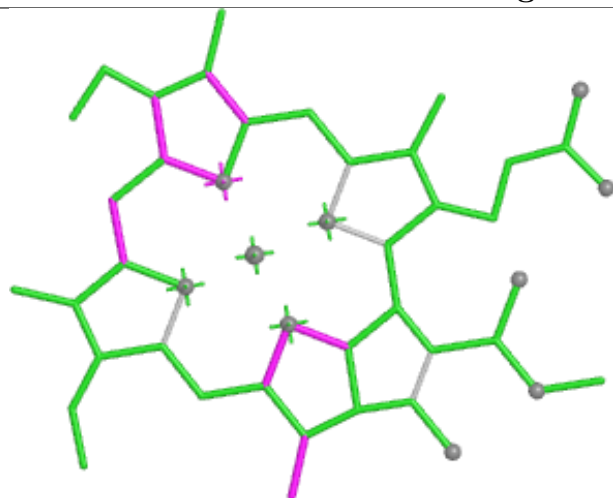


Torsions

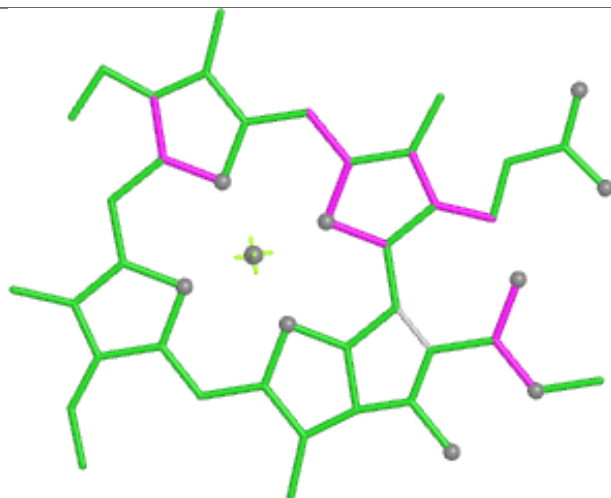


Rings

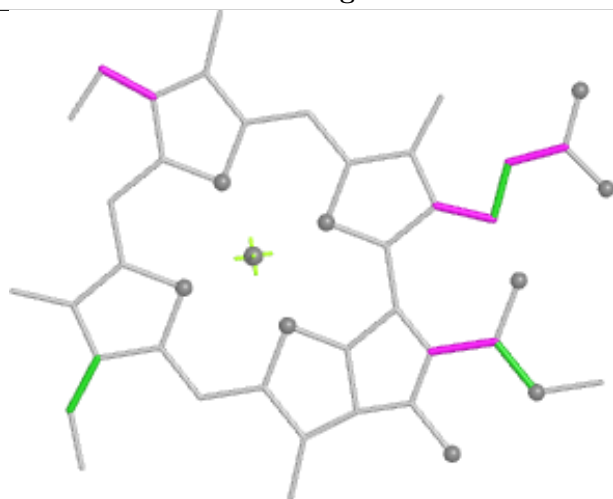
Ligand CLA b 516



Bond lengths



Bond angles

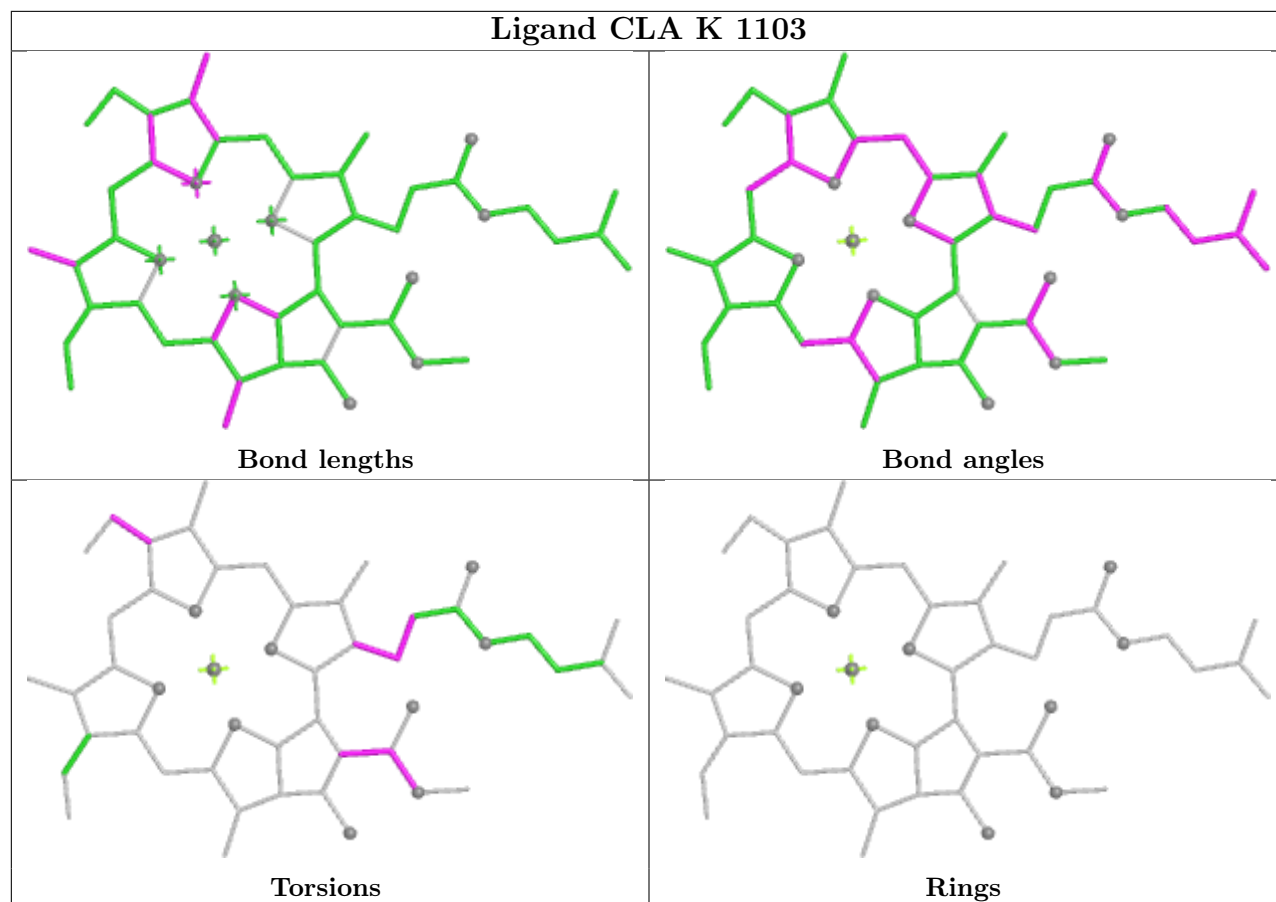


Torsions

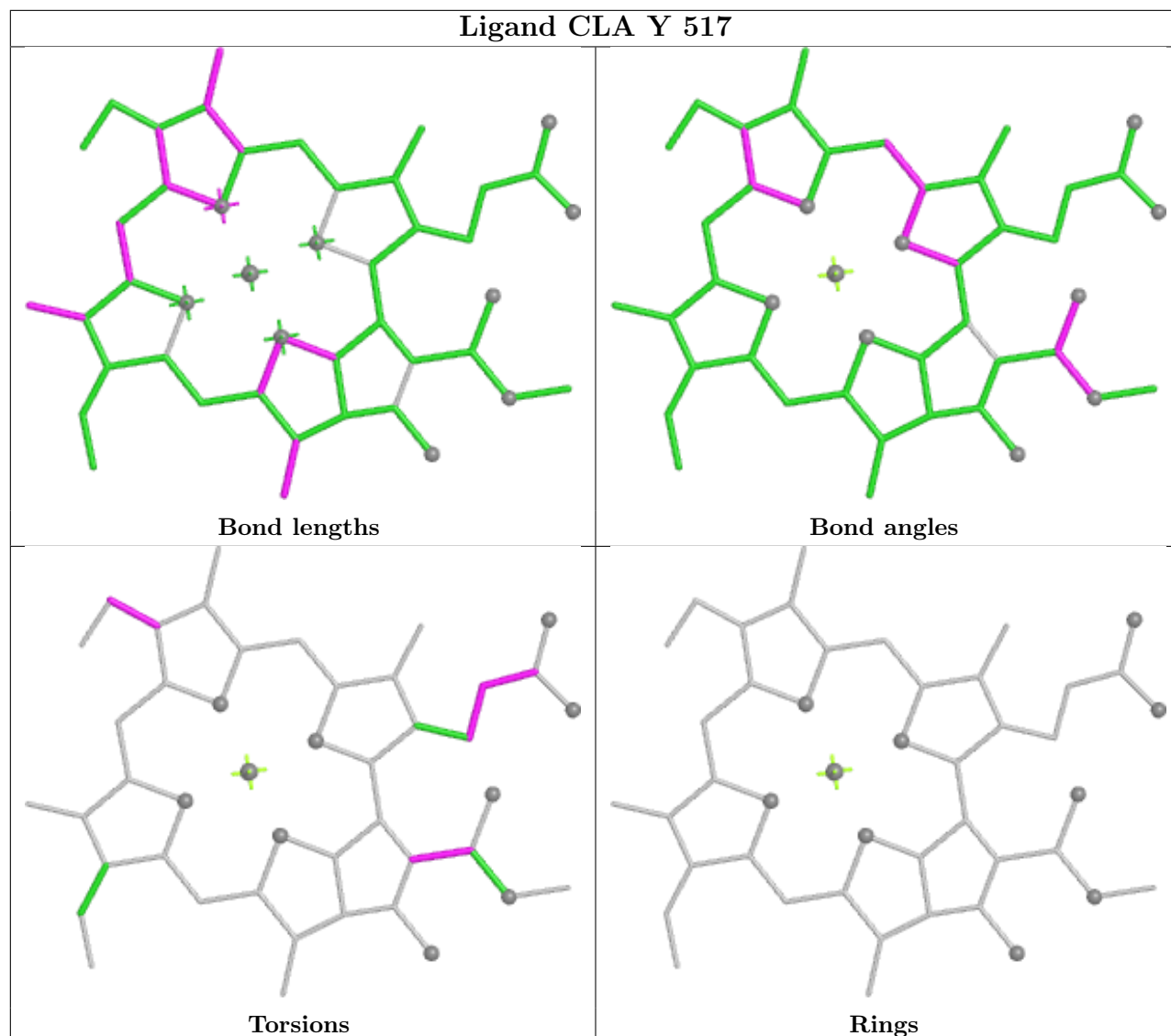


Rings

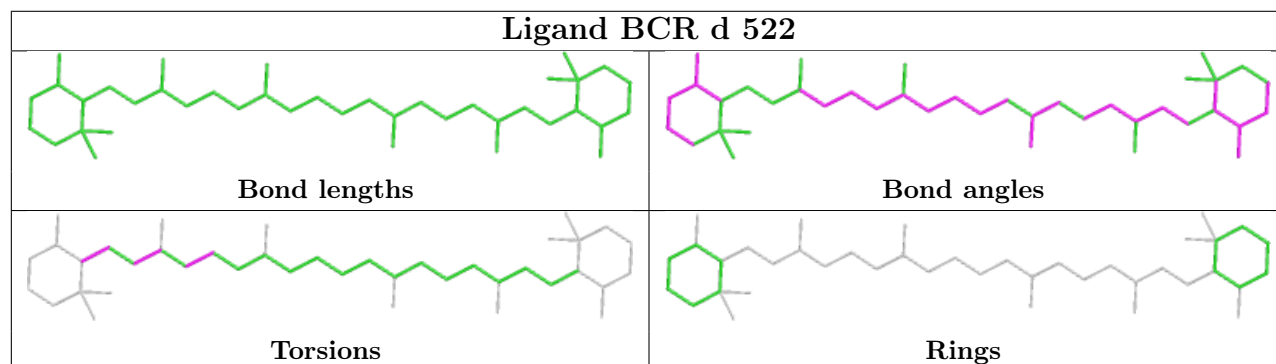
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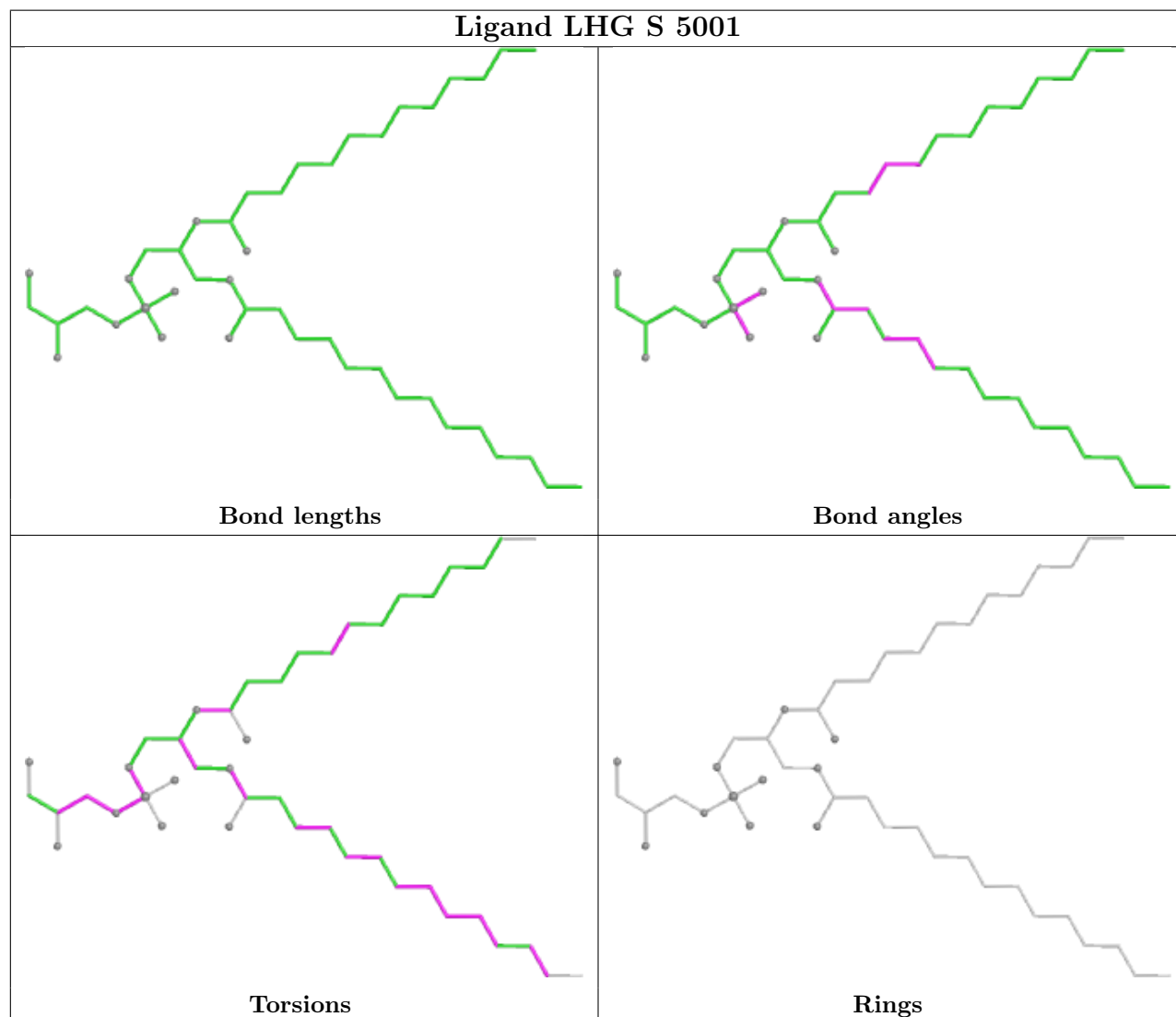
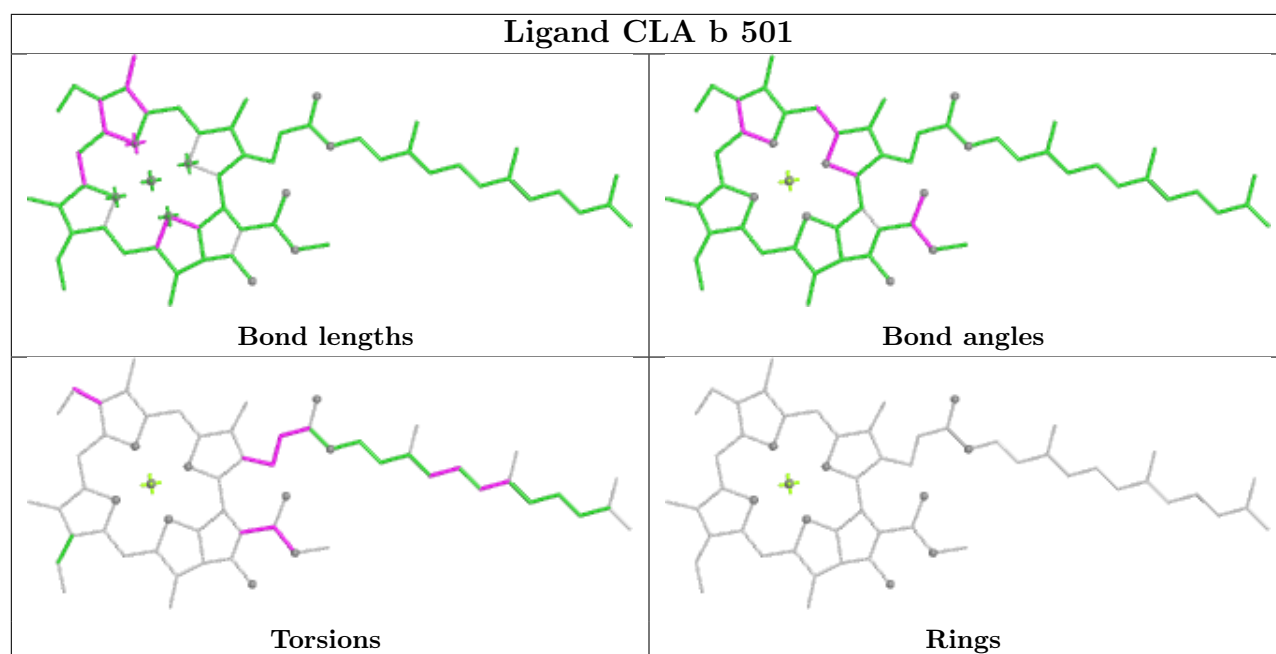


Ligand CLA Y 517

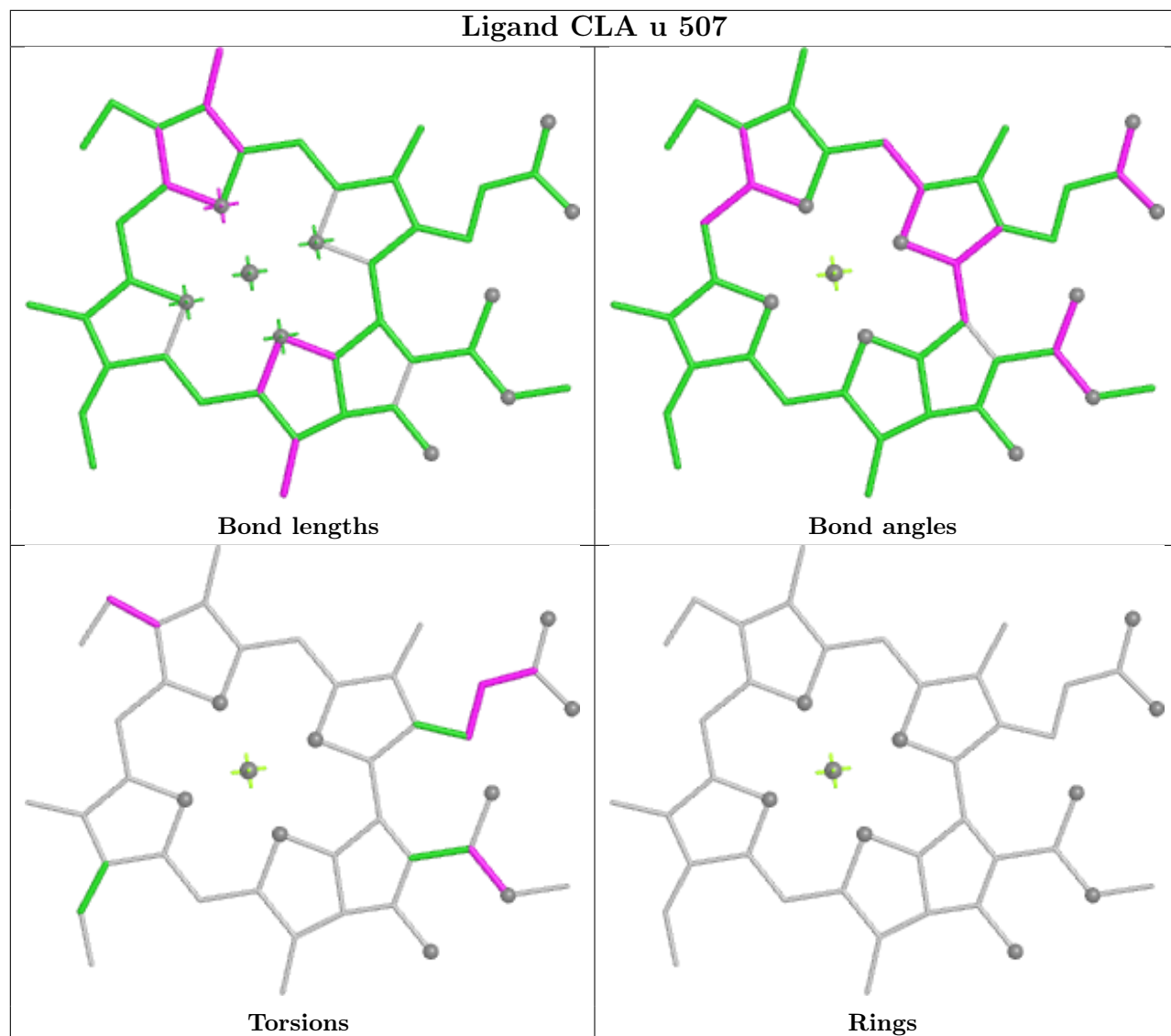


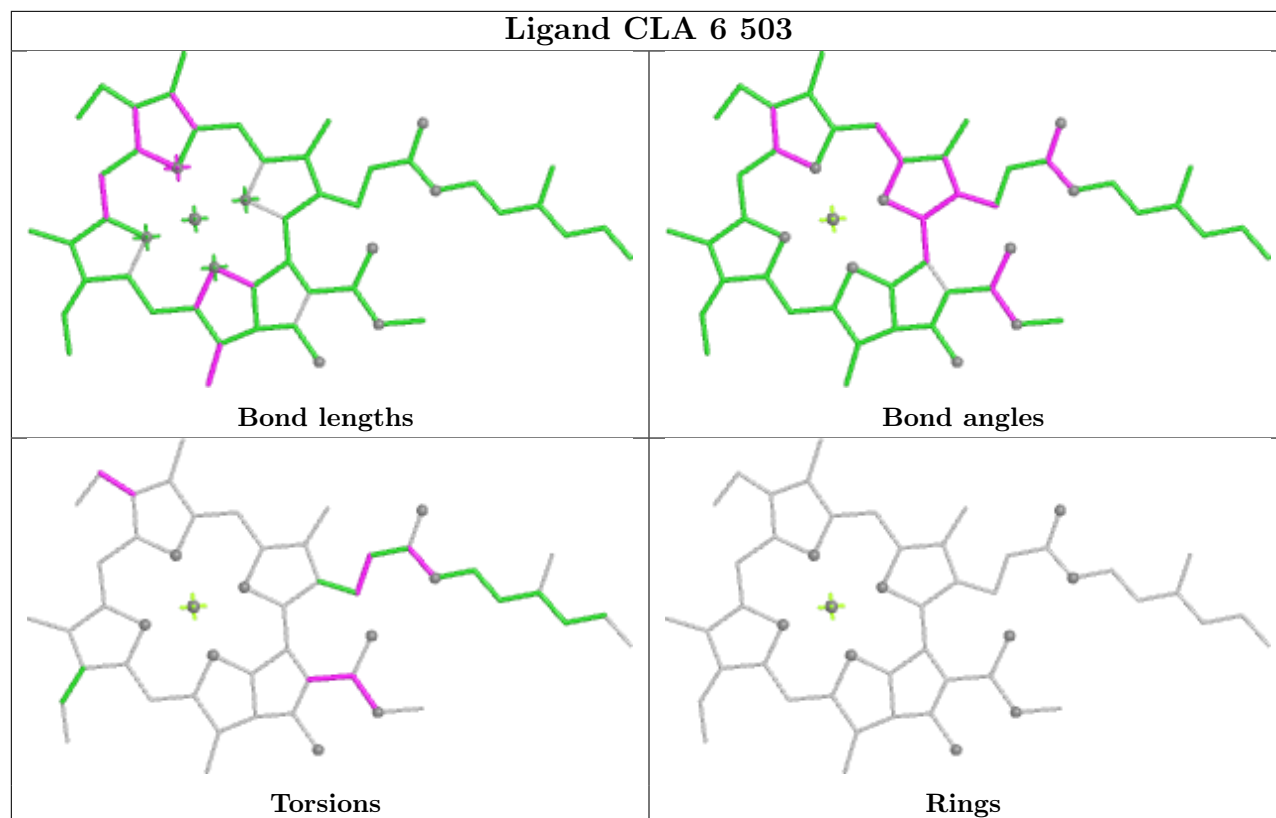
Ligand BCR d 522



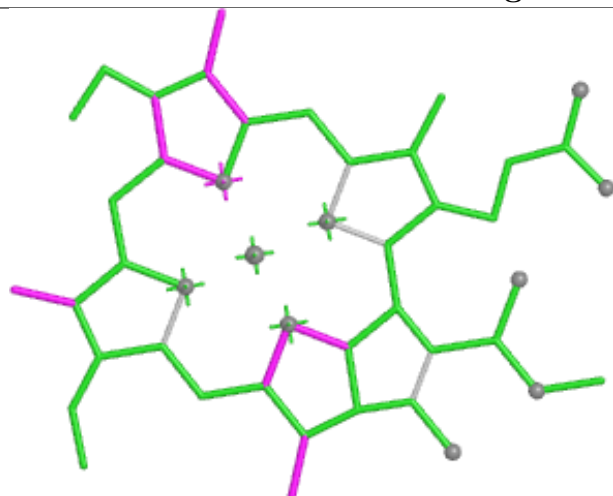


Ligand CLA u 507

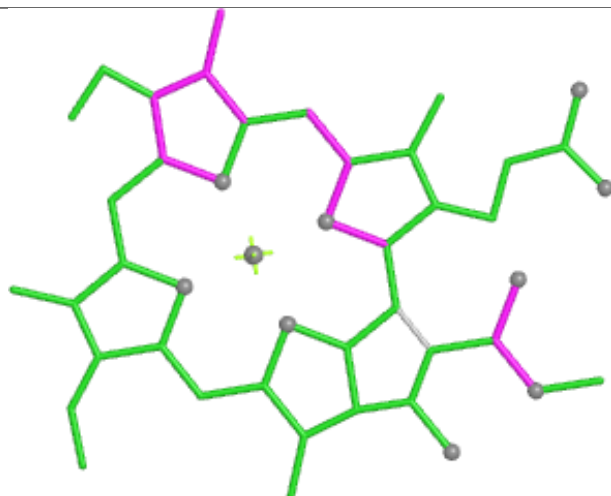




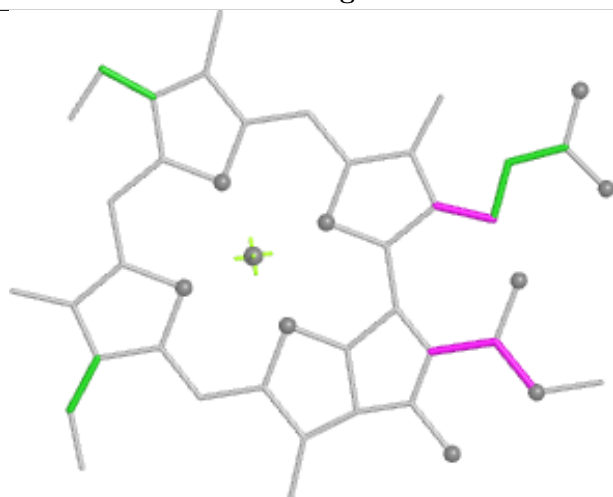
Ligand CLA A 1113



Bond lengths



Bond angles

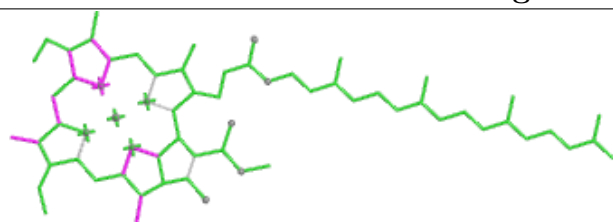


Torsions

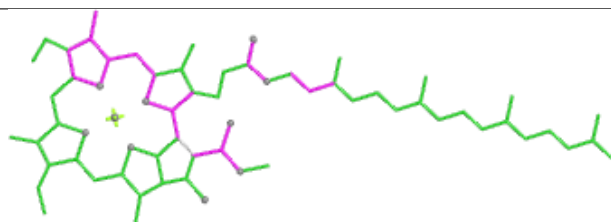


Rings

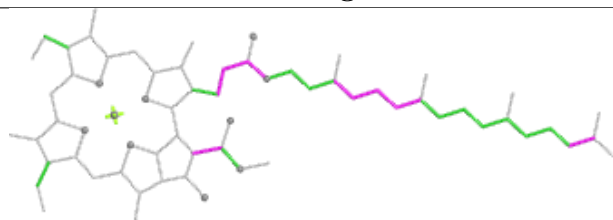
Ligand CLA f 1213



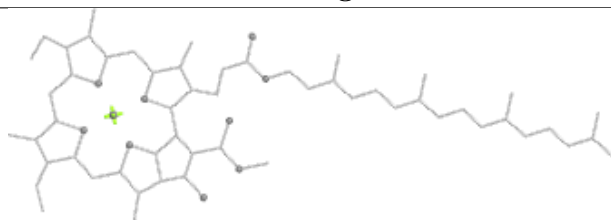
Bond lengths



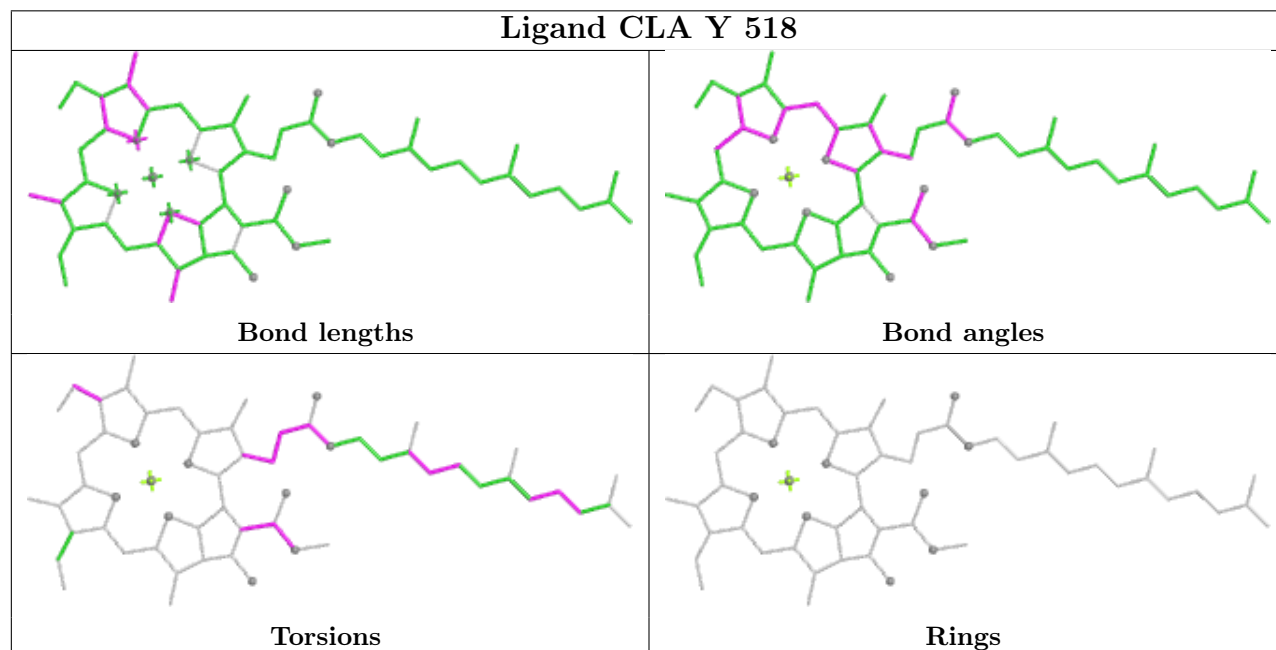
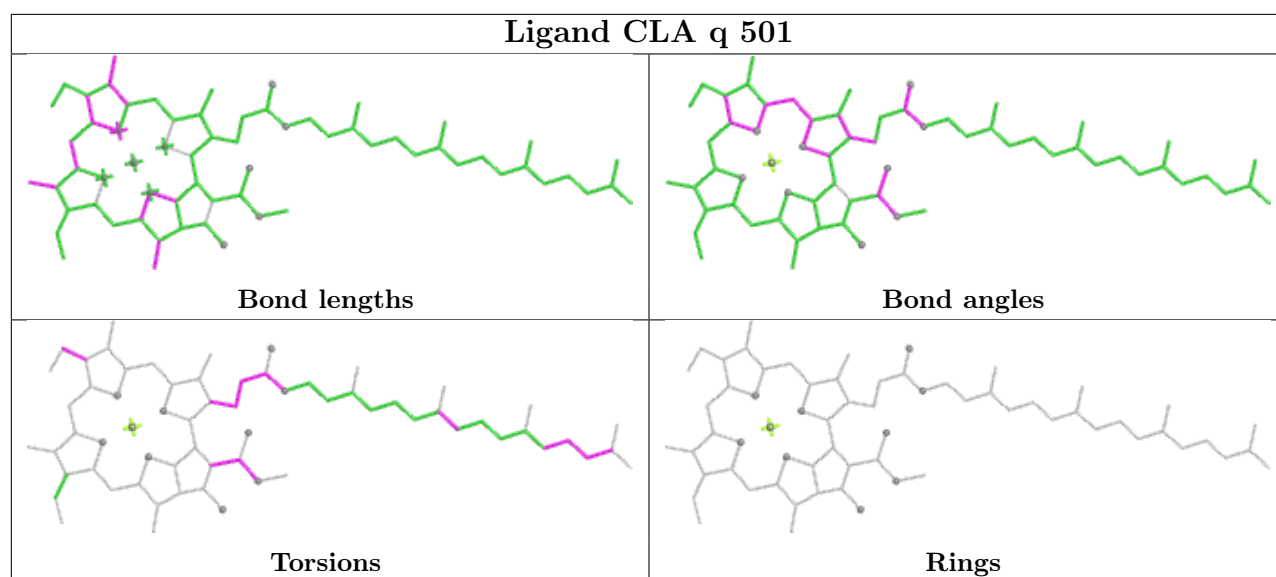
Bond angles



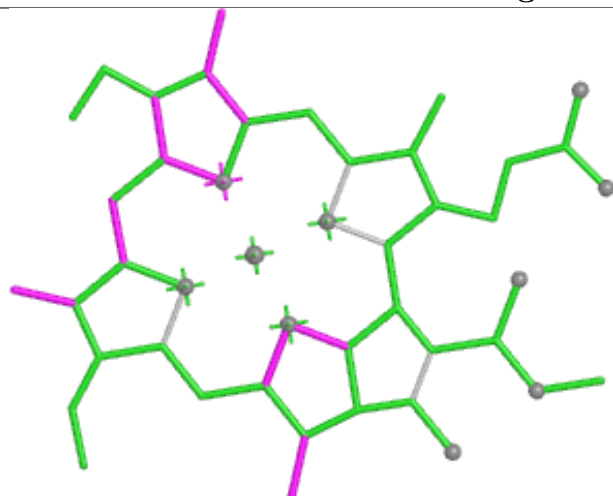
Torsions



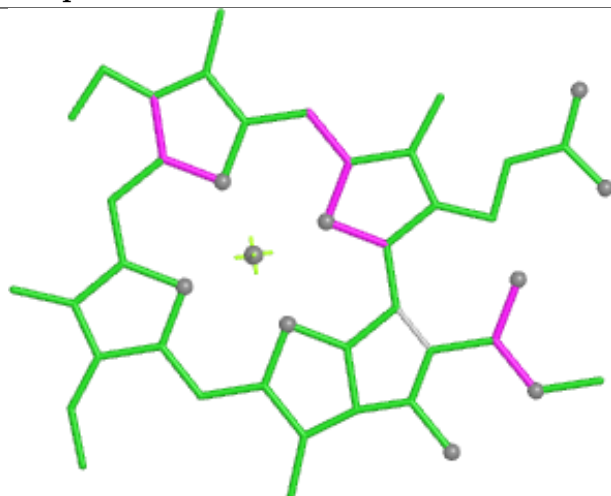
Rings



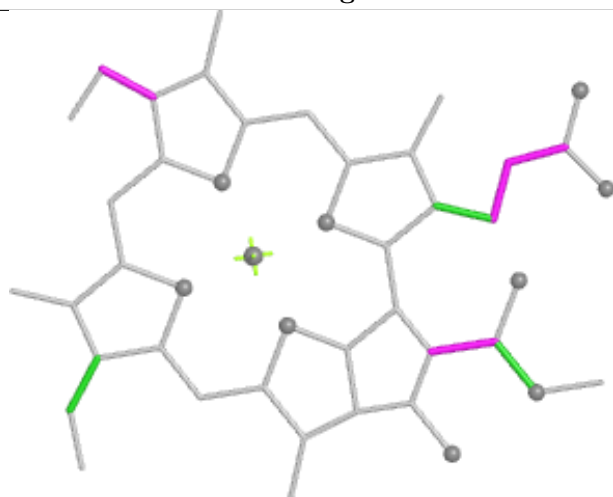
Ligand CLA q 517



Bond lengths



Bond angles

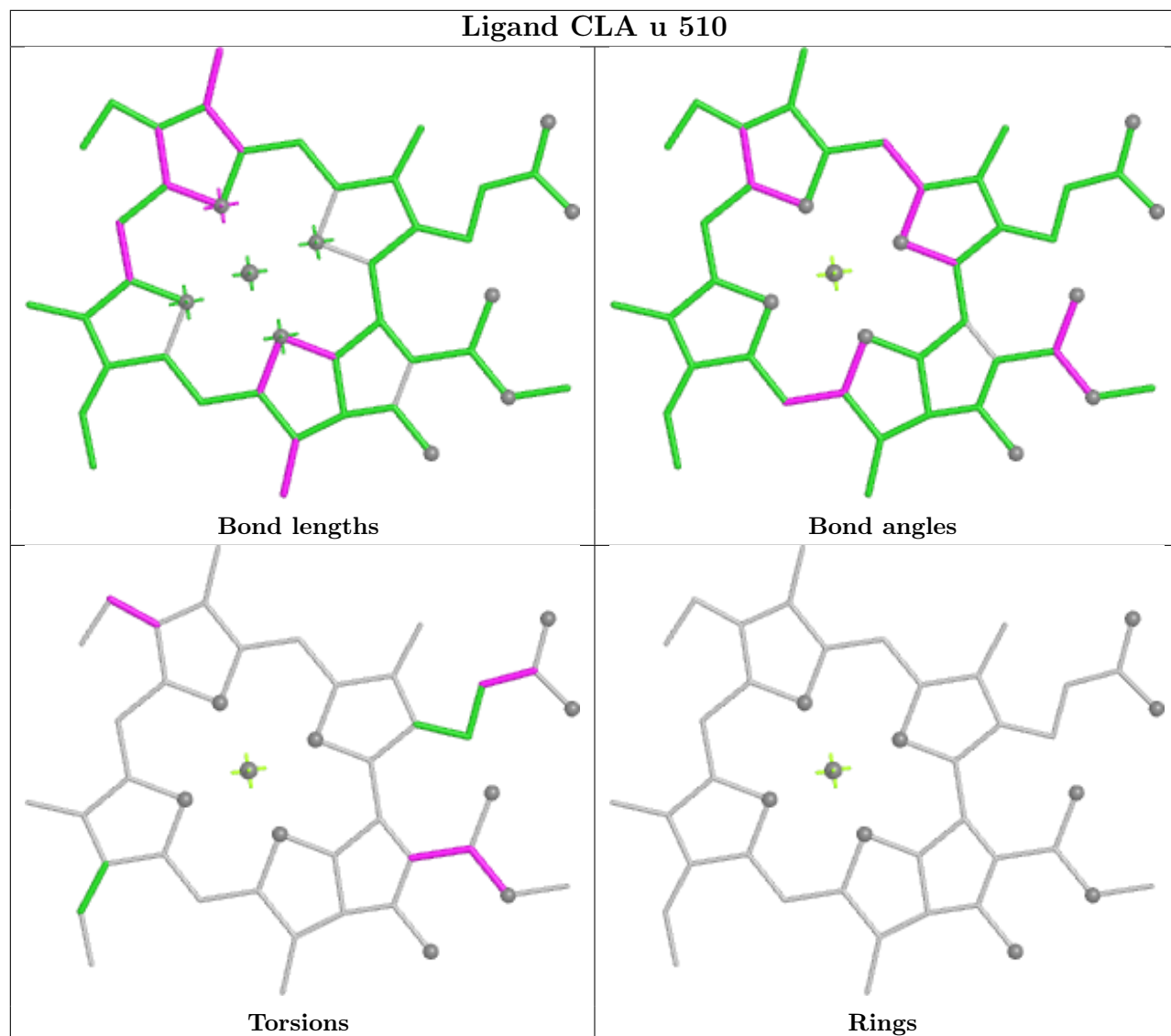


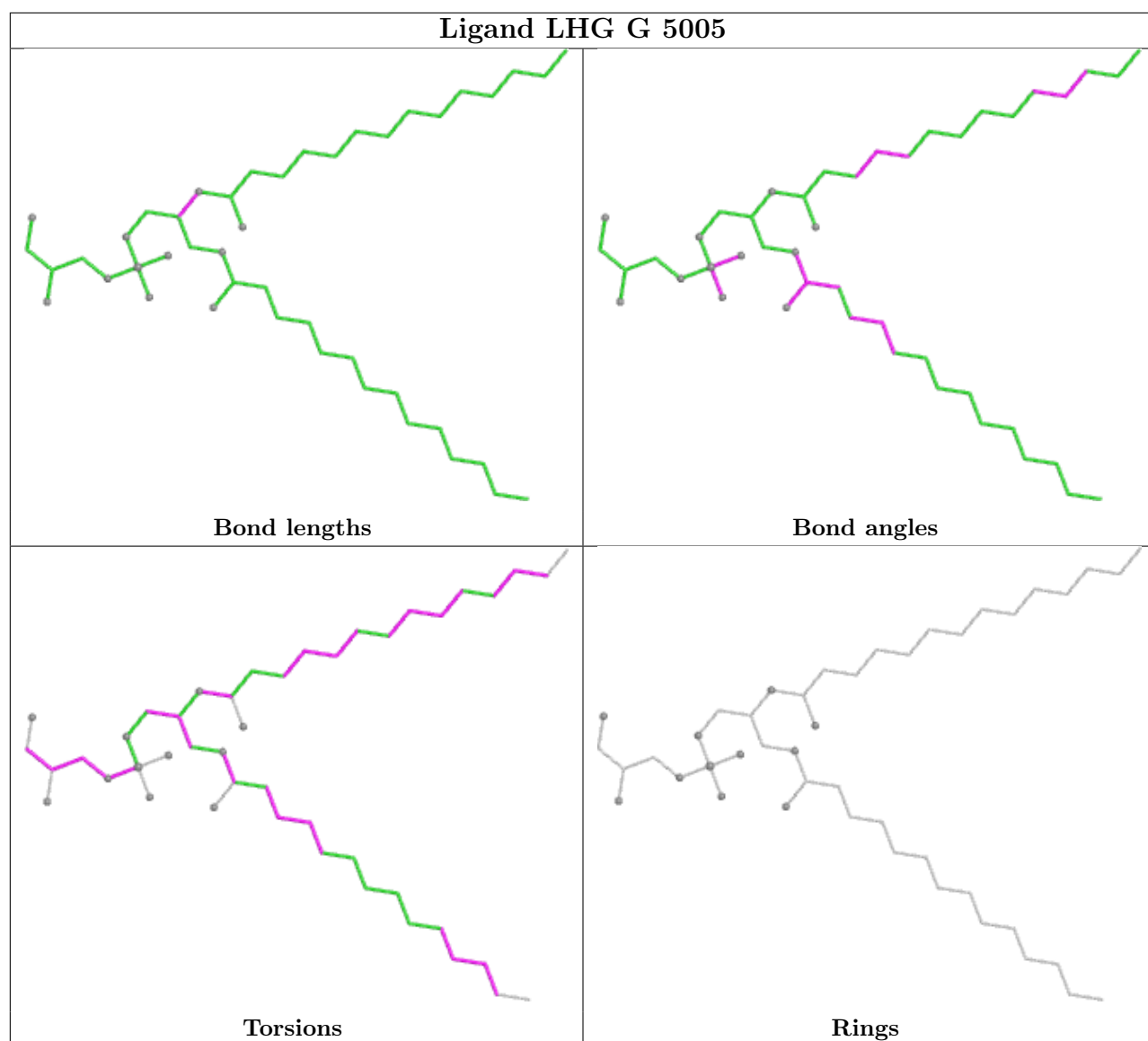
Torsions

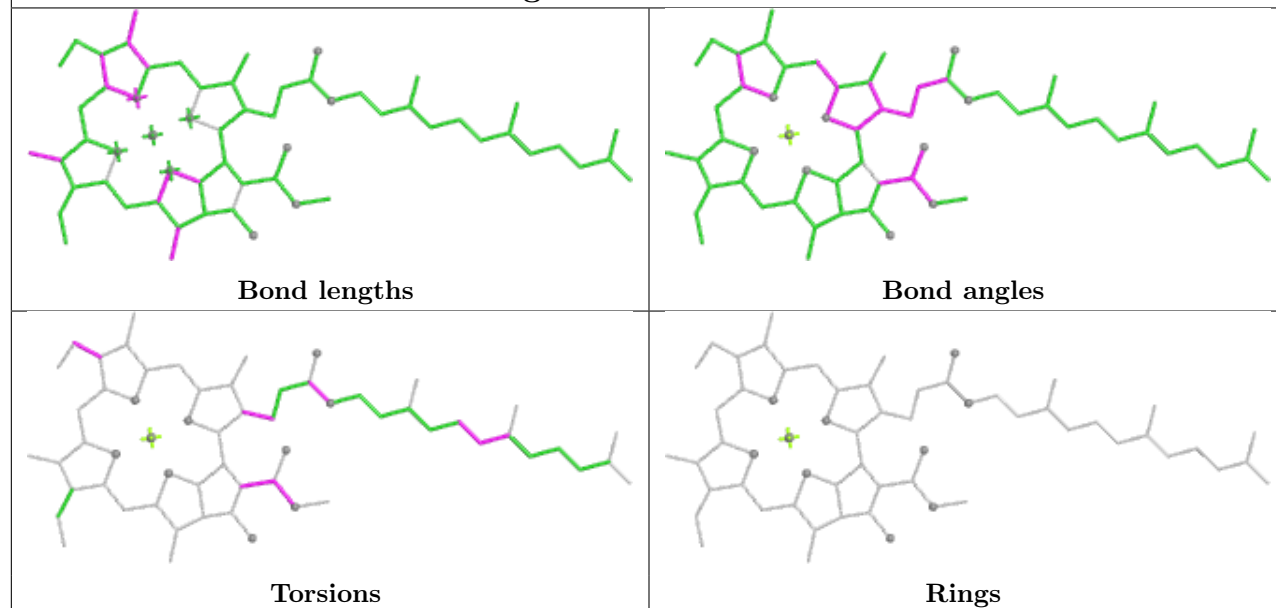
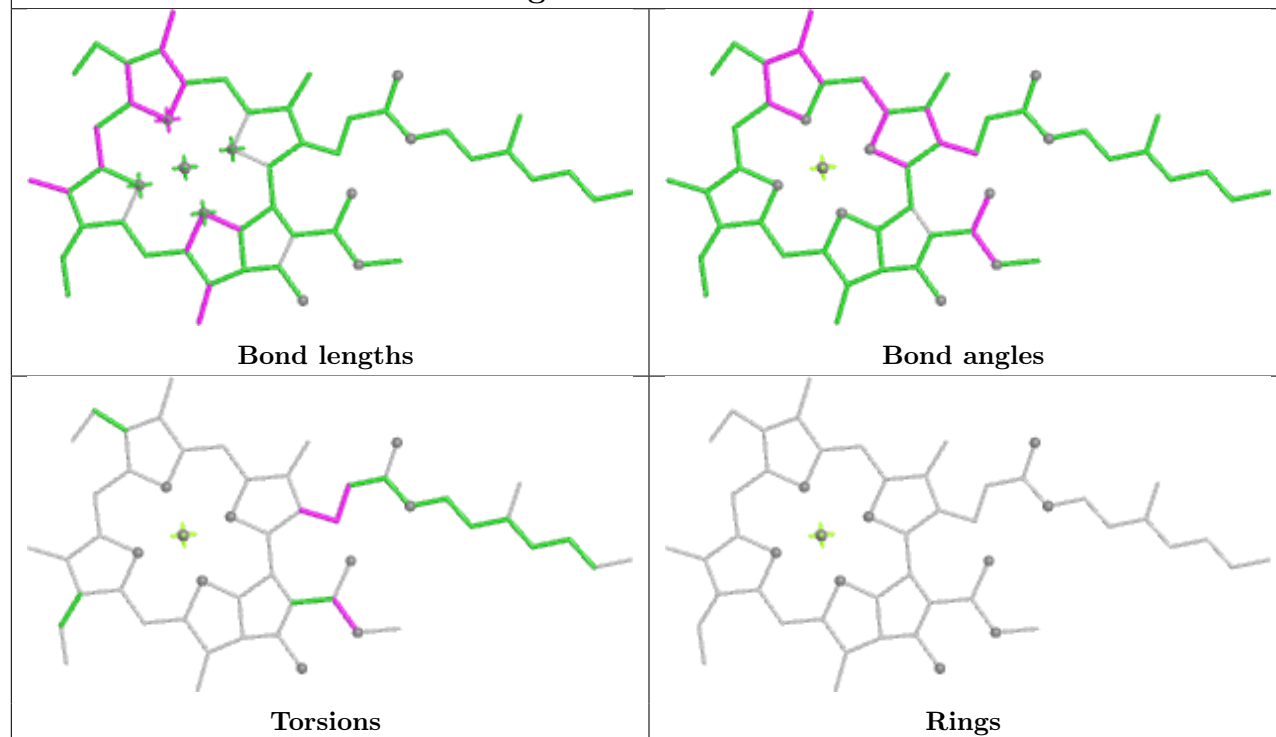


Rings

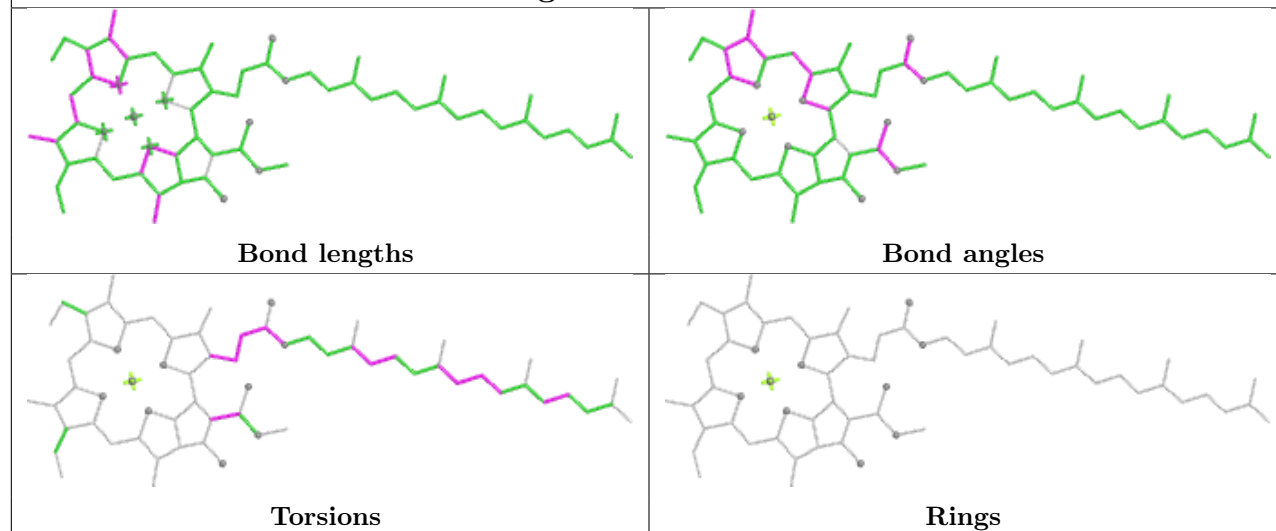
Ligand CLA u 510



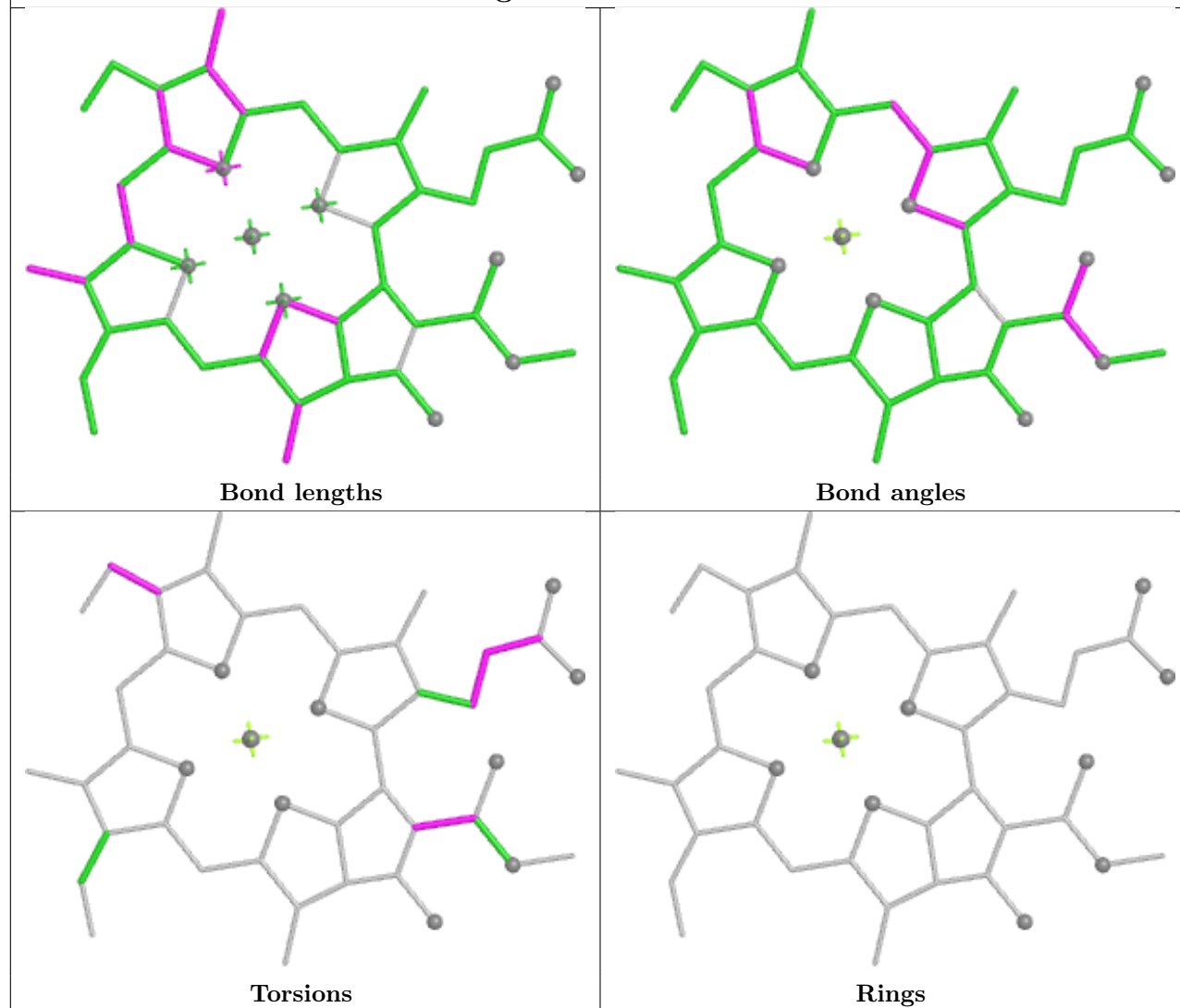


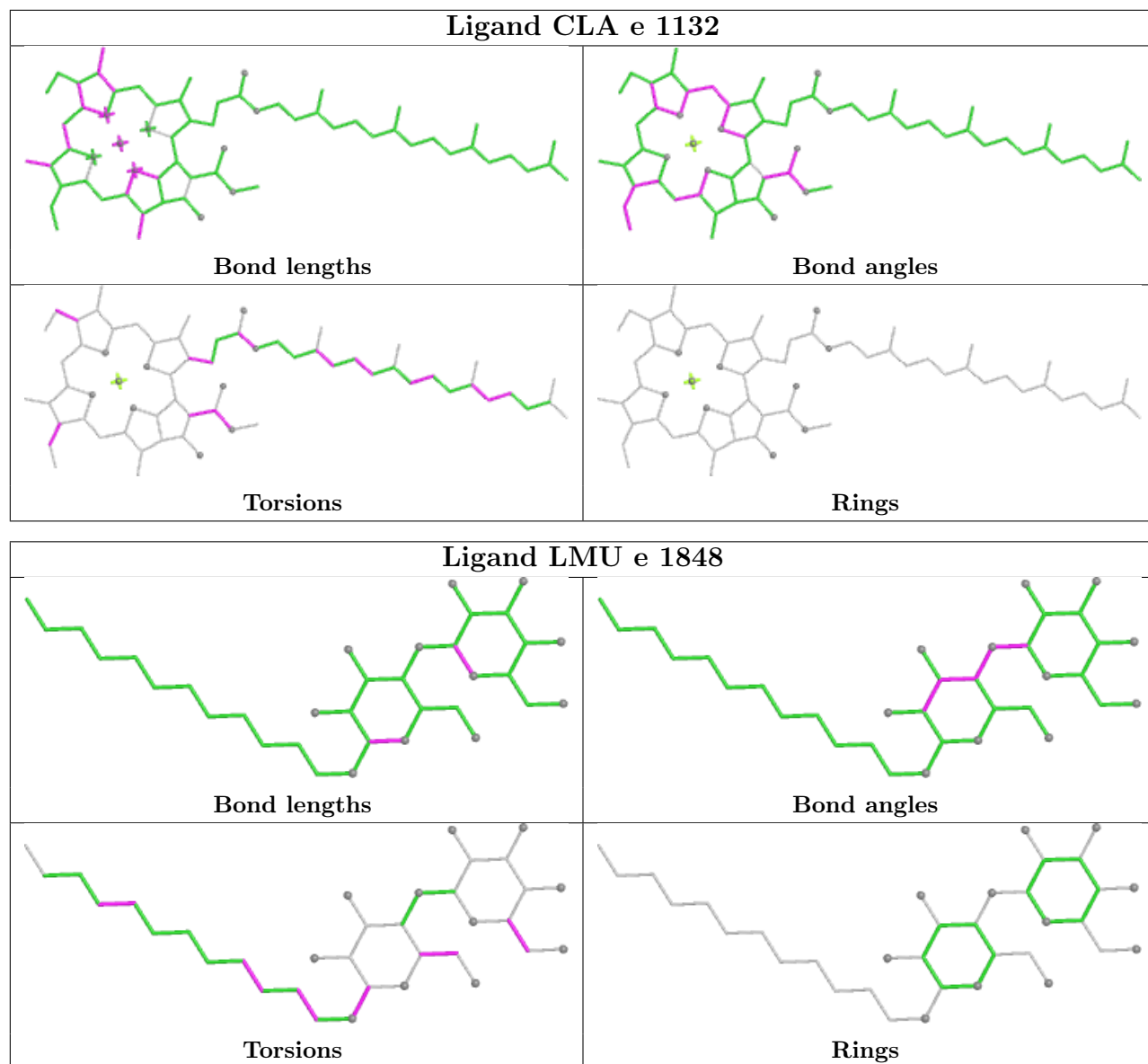
Ligand CLA B 1230**Ligand CLA e 1120**

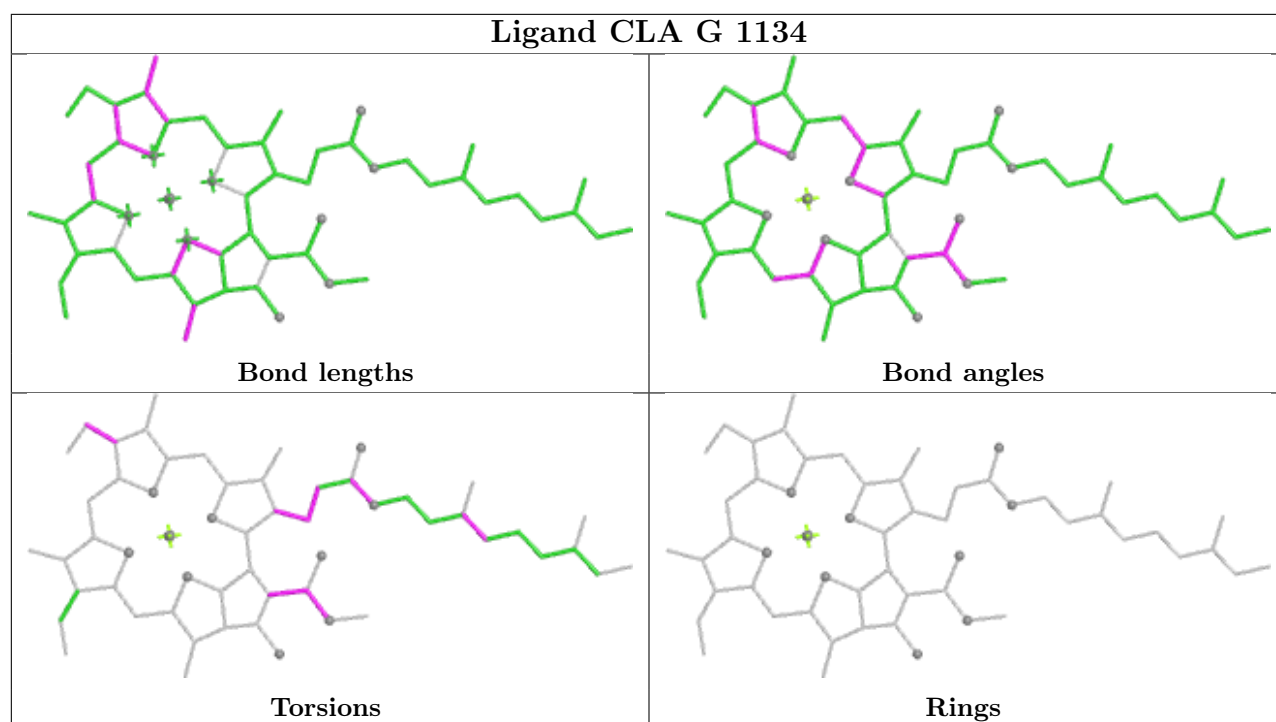
Ligand CLA r 518



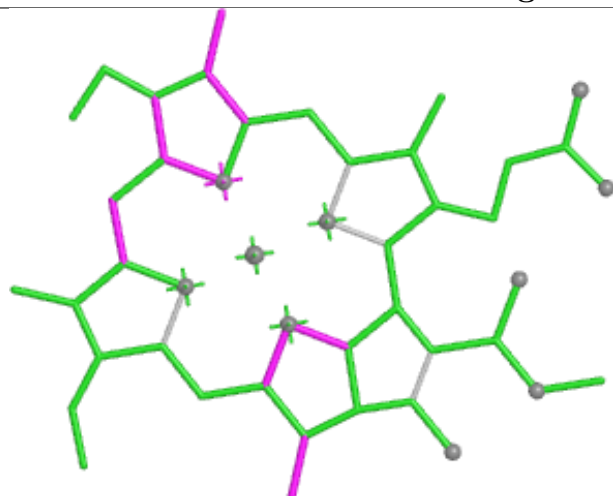
Ligand CLA 1 517



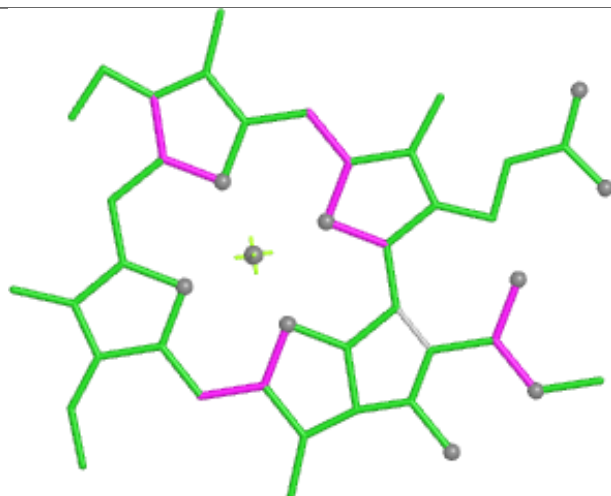




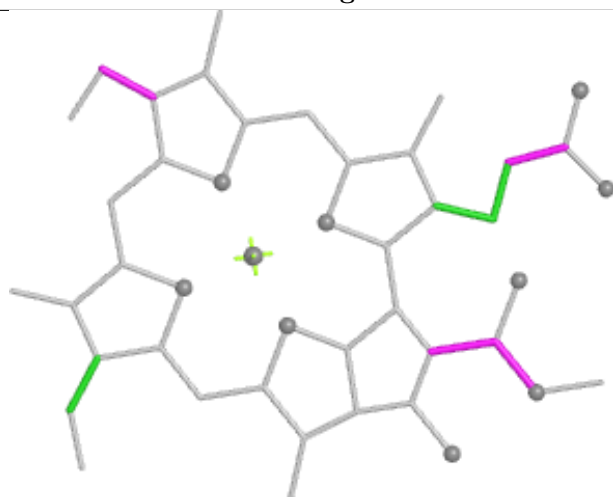
Ligand CLA v 510



Bond lengths



Bond angles

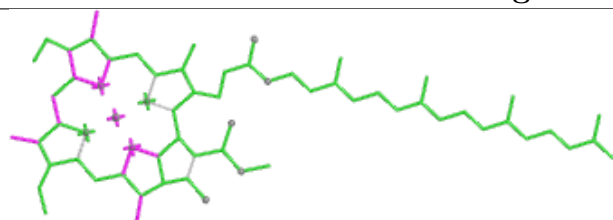


Torsions

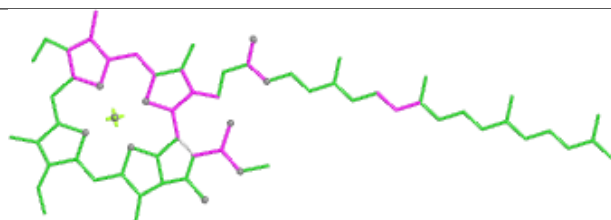


Rings

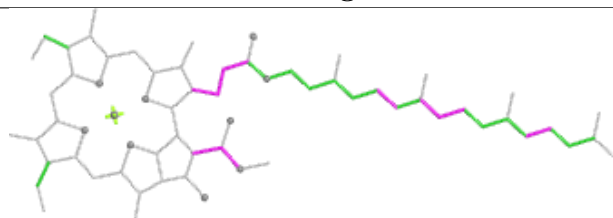
Ligand CLA f 1221



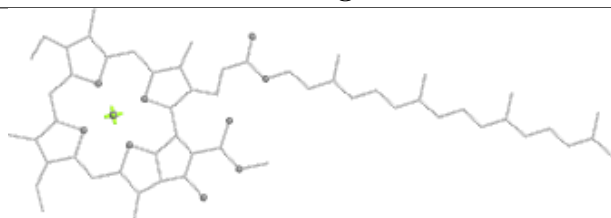
Bond lengths



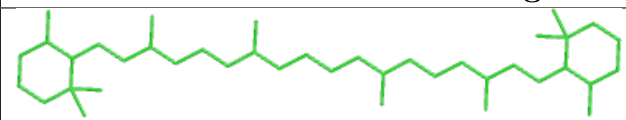
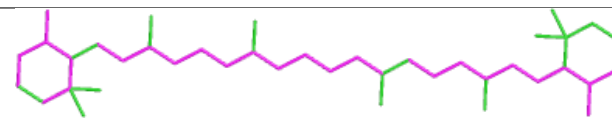
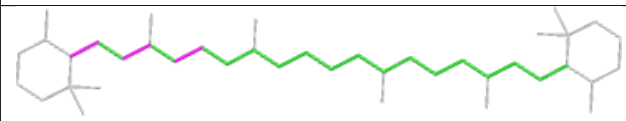
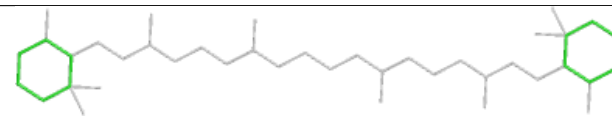
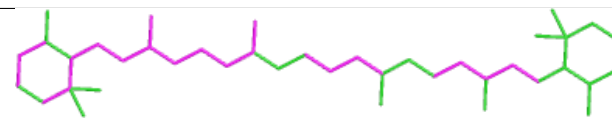
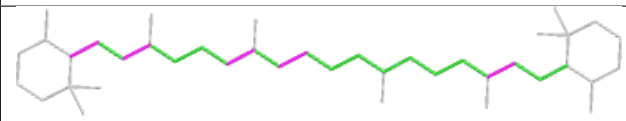
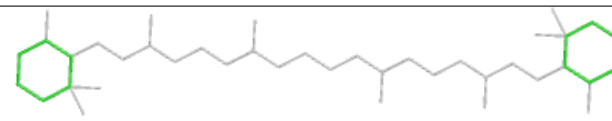
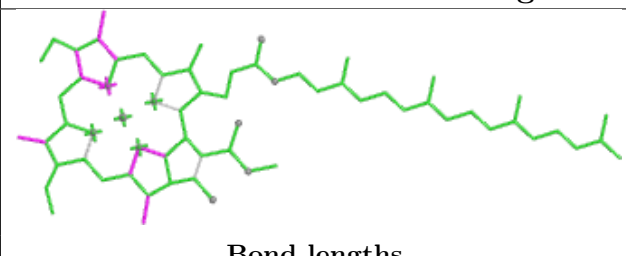
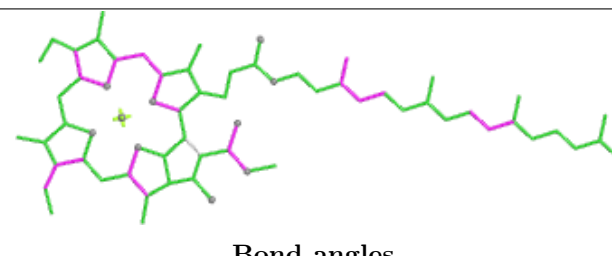
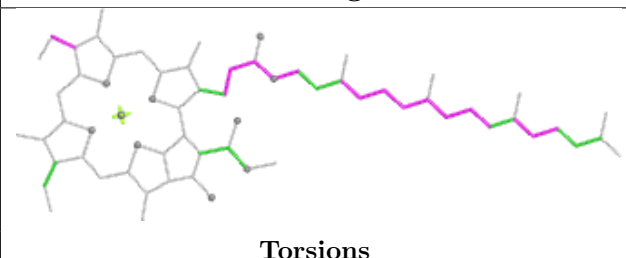
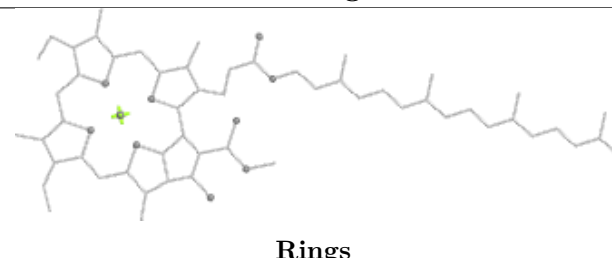
Bond angles

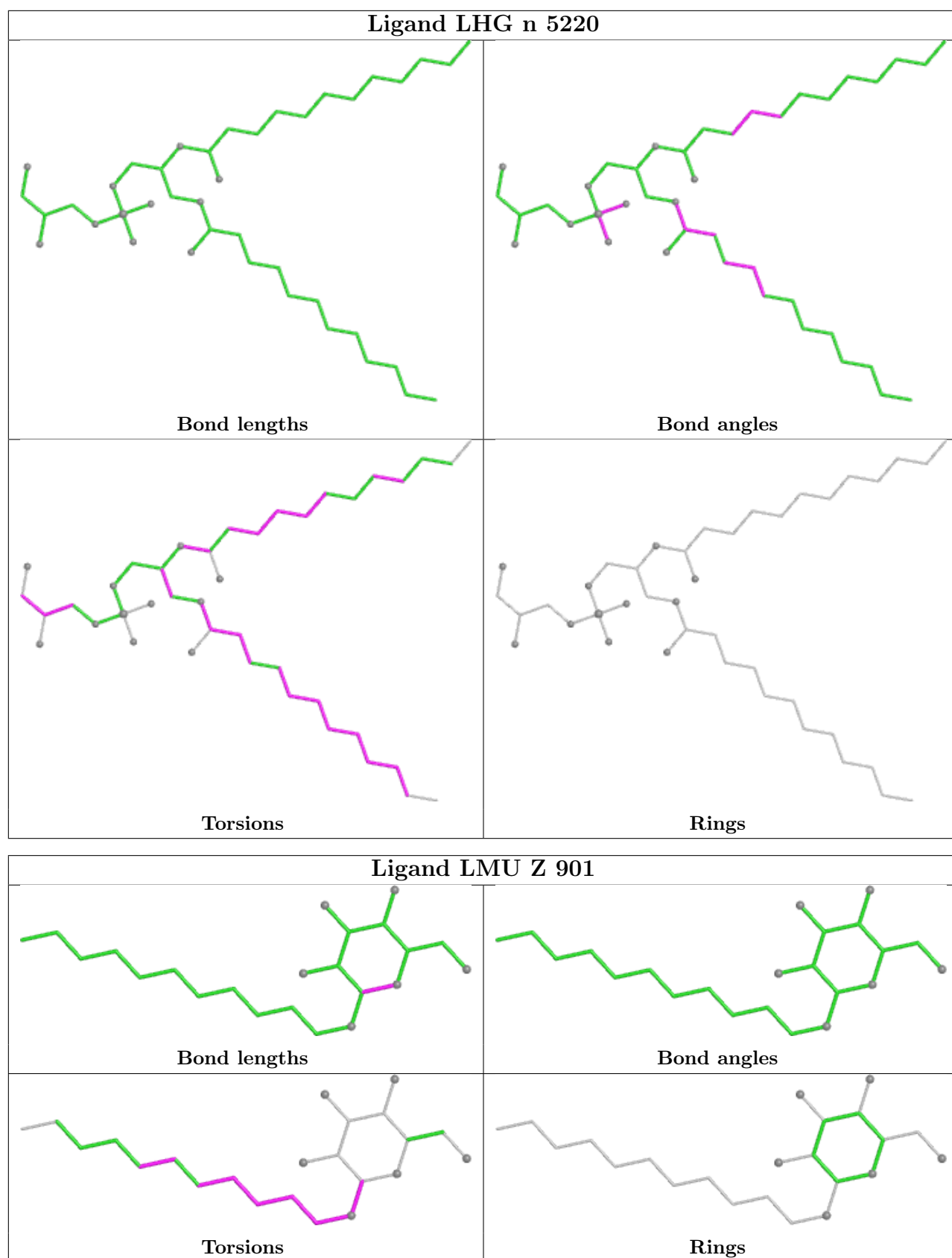


Torsions

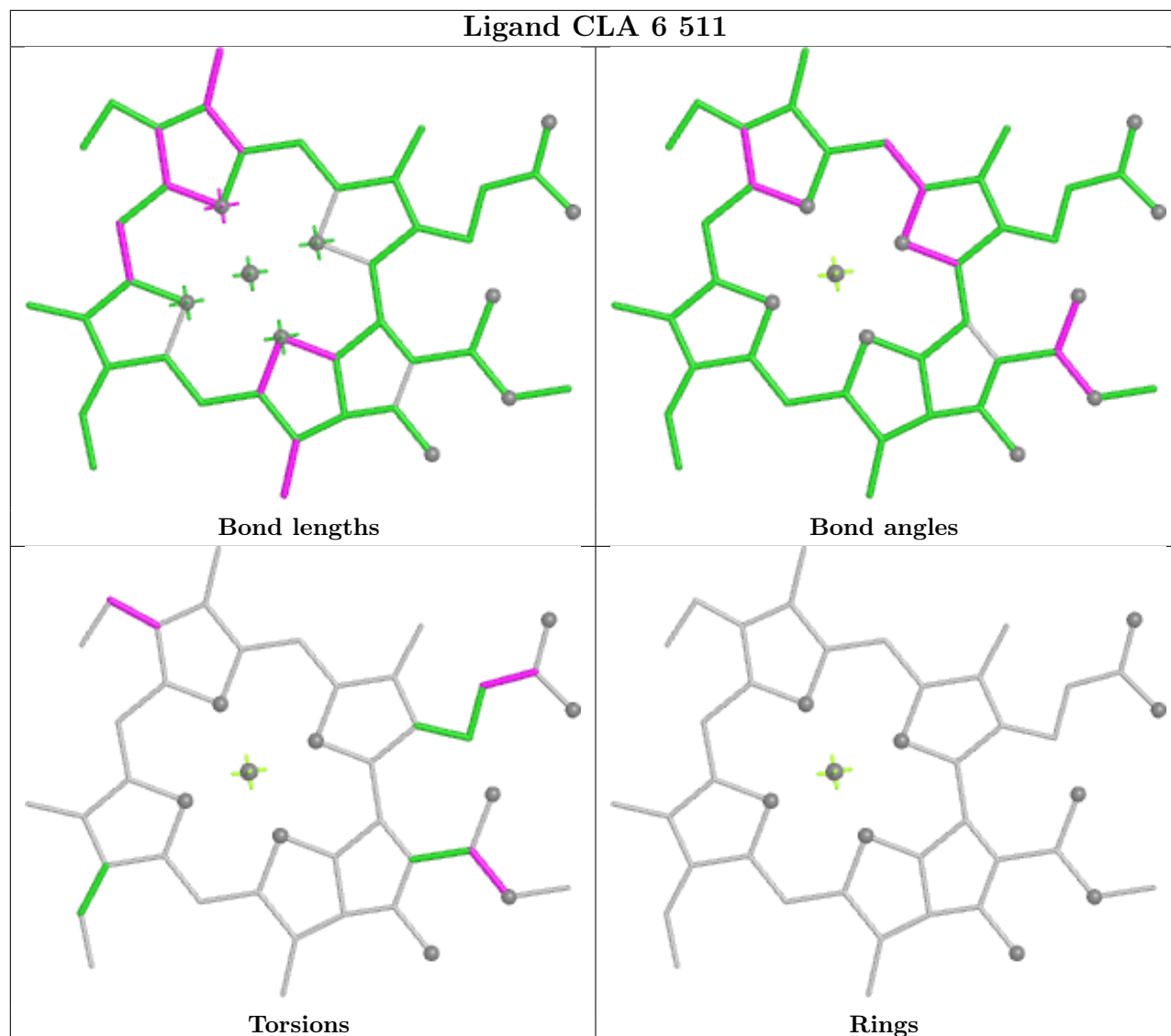


Rings

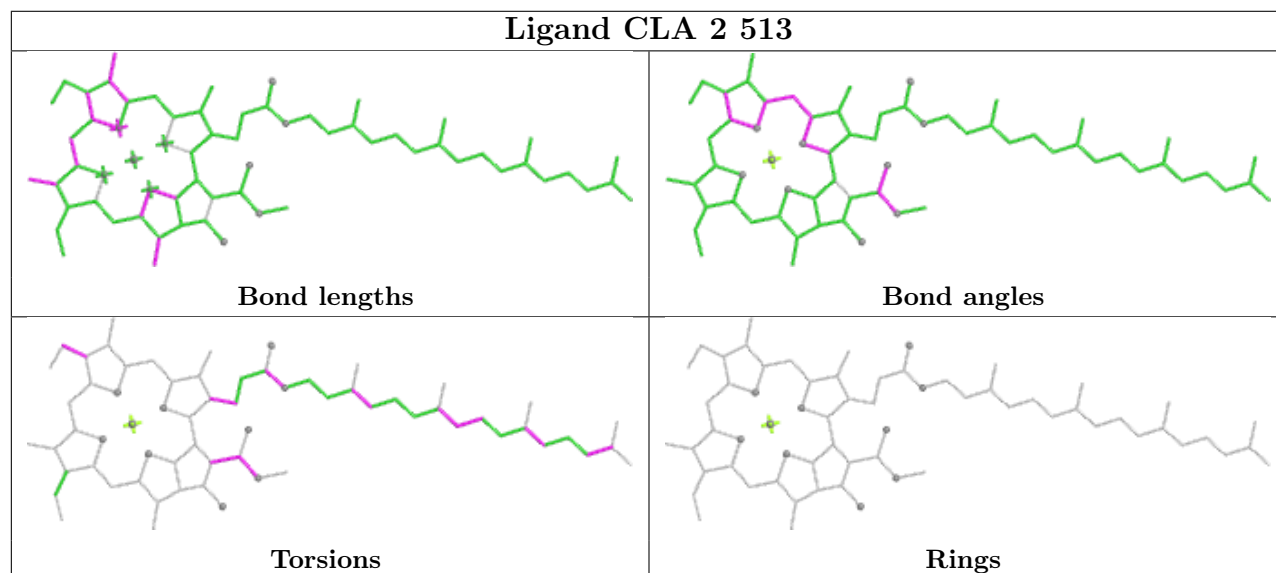
Ligand BCR a 522	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR A 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA e 1237	
	
Bond lengths	Bond angles
	
Torsions	Rings



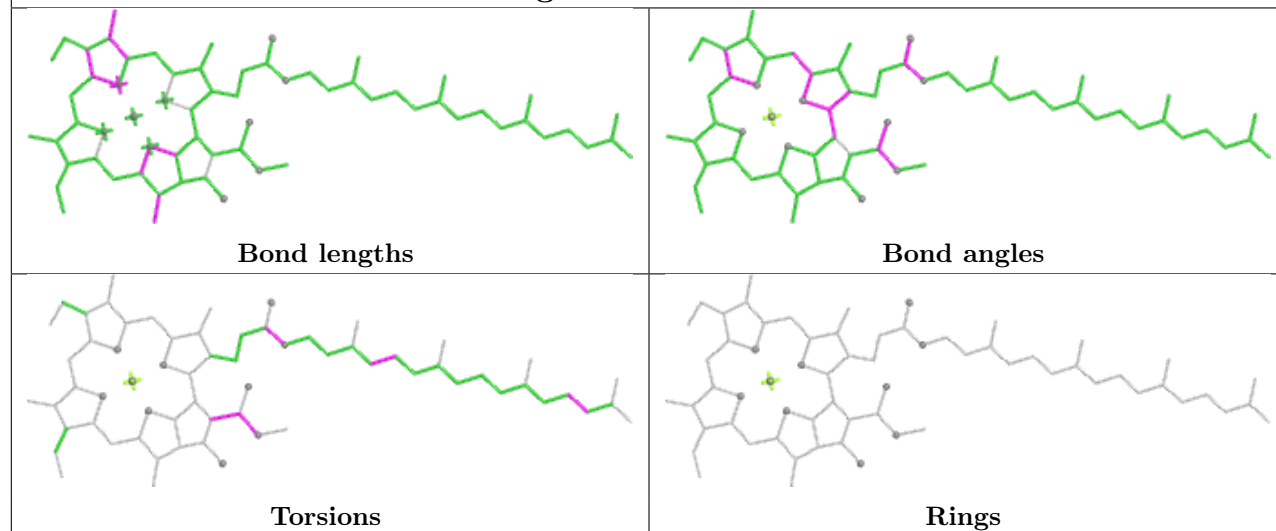
Ligand CLA 6 511



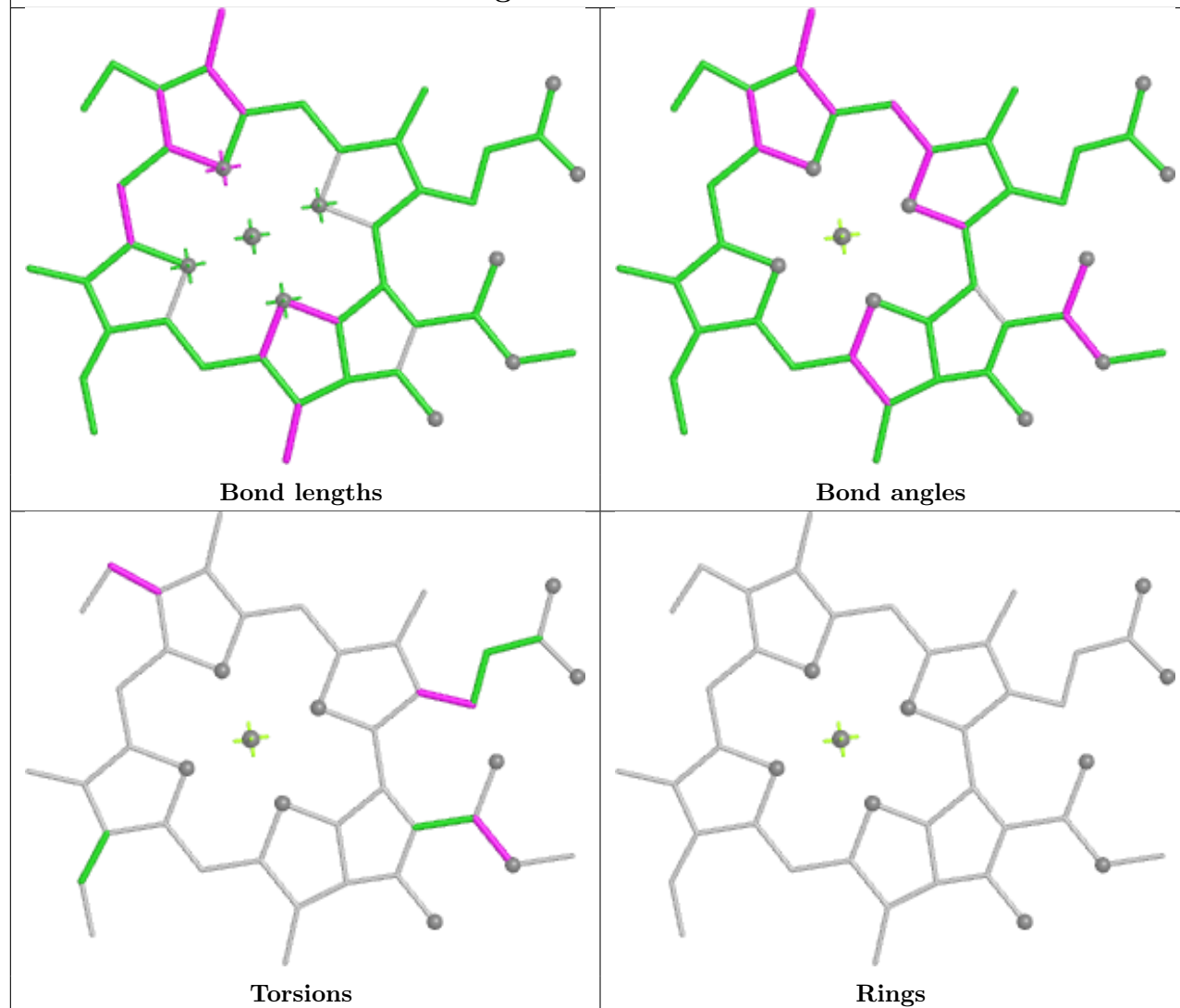
Ligand CLA 2 513



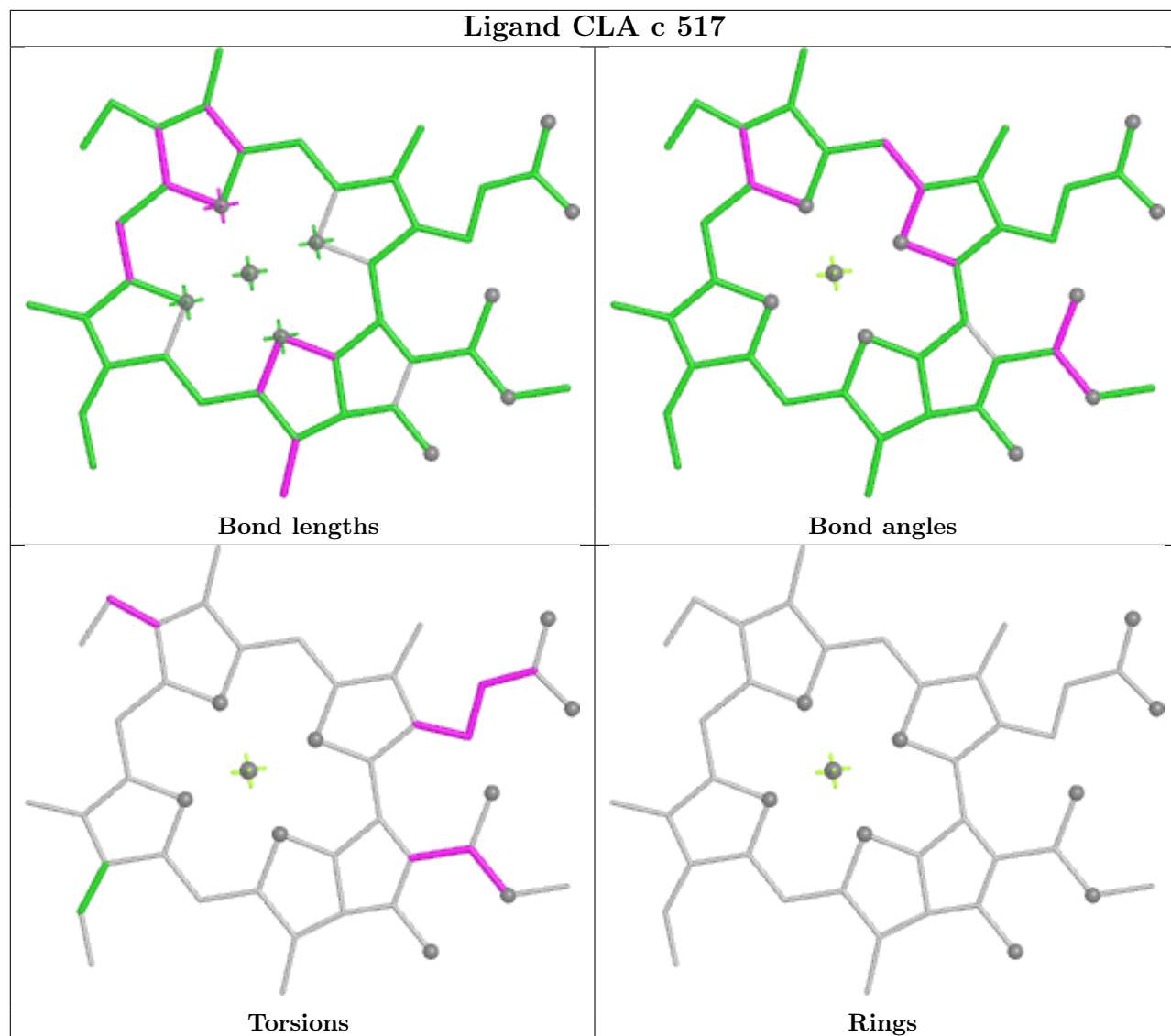
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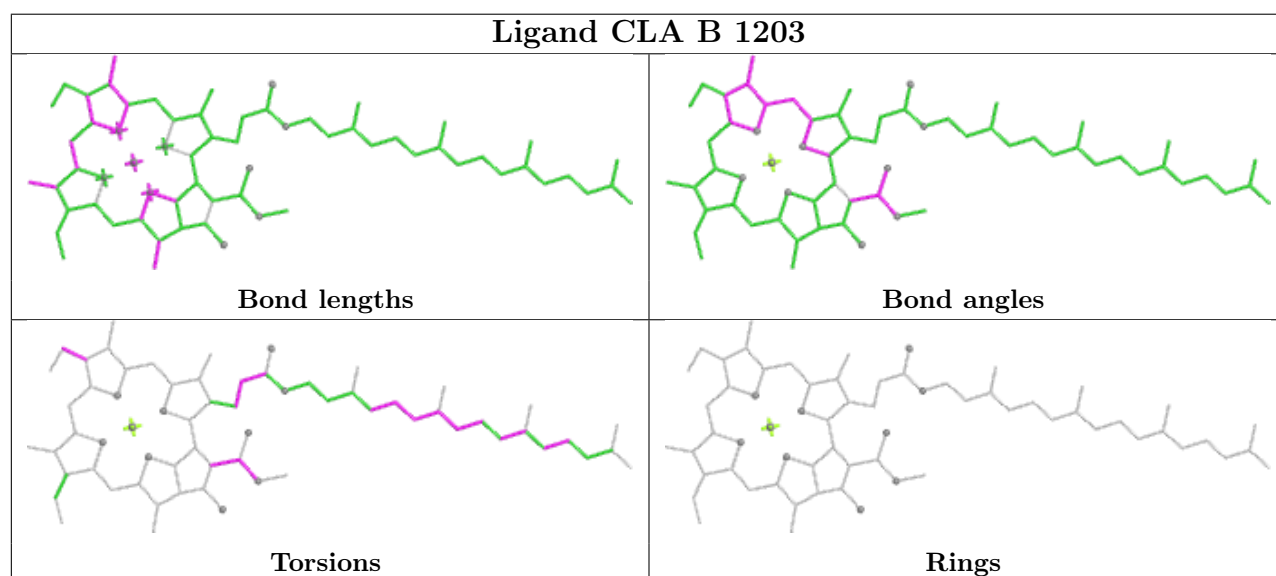
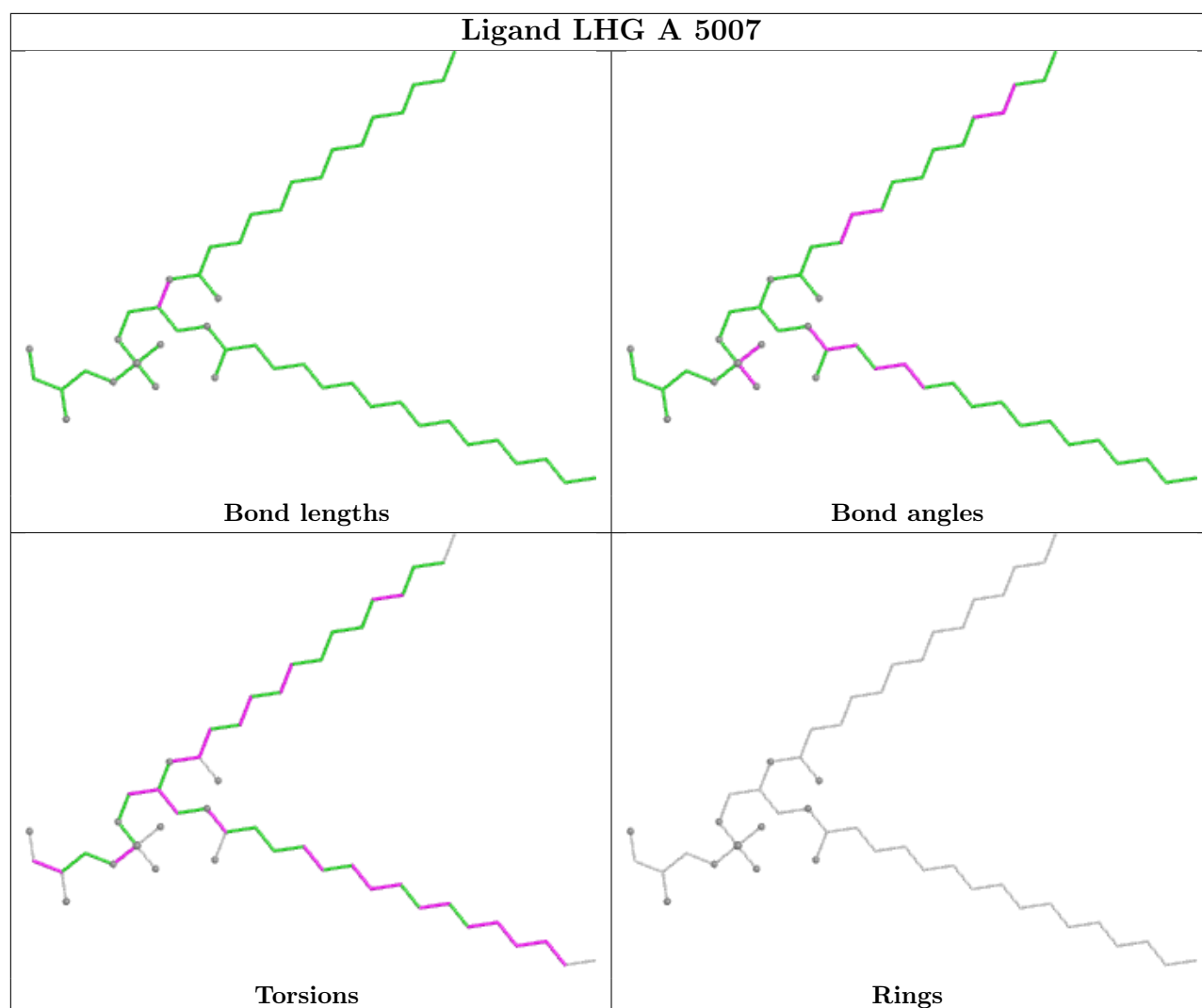


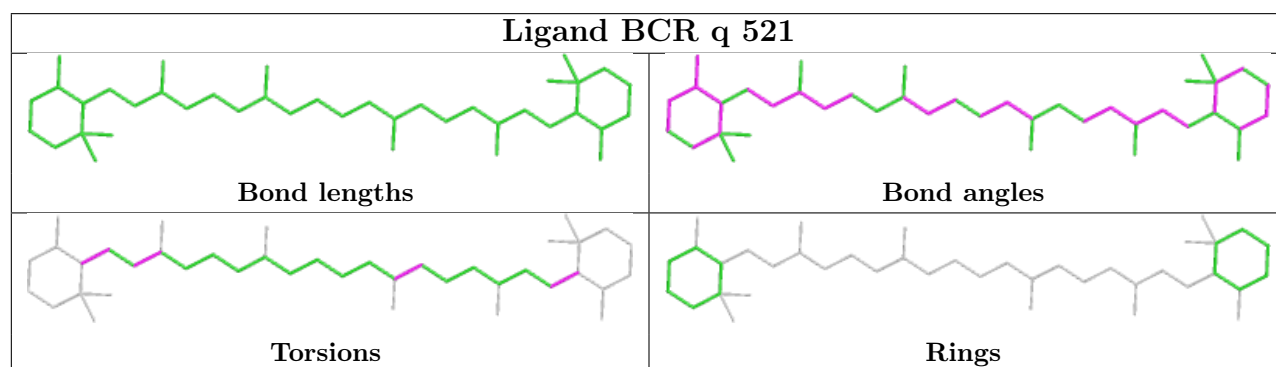
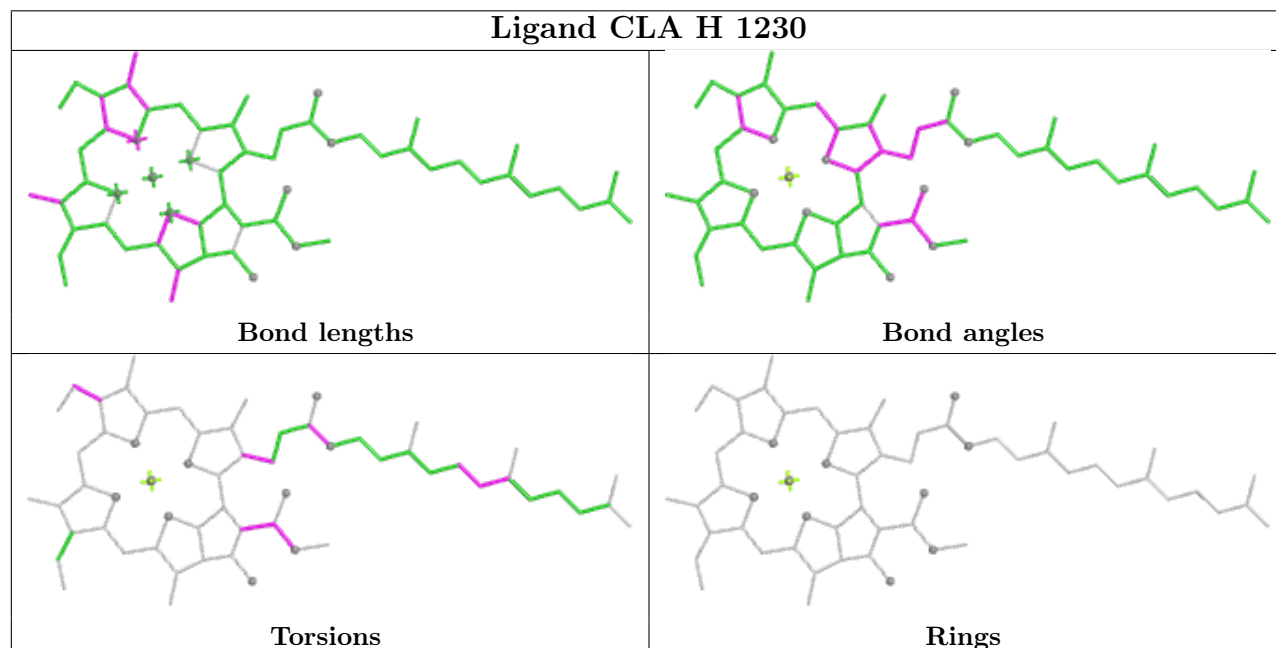
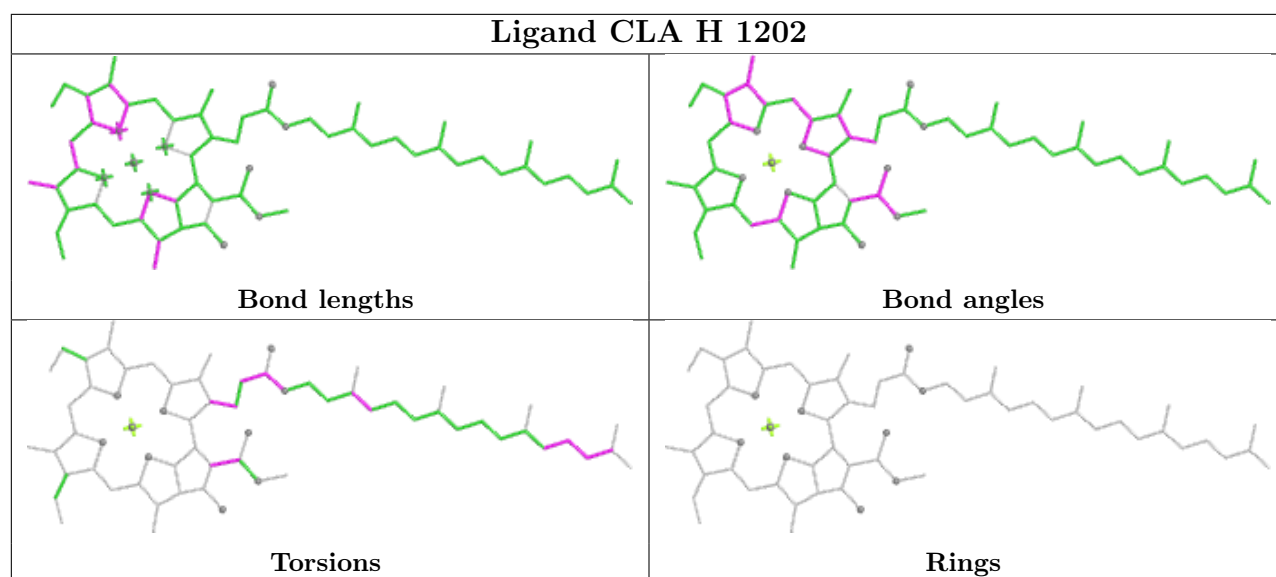
Ligand CLA b 511

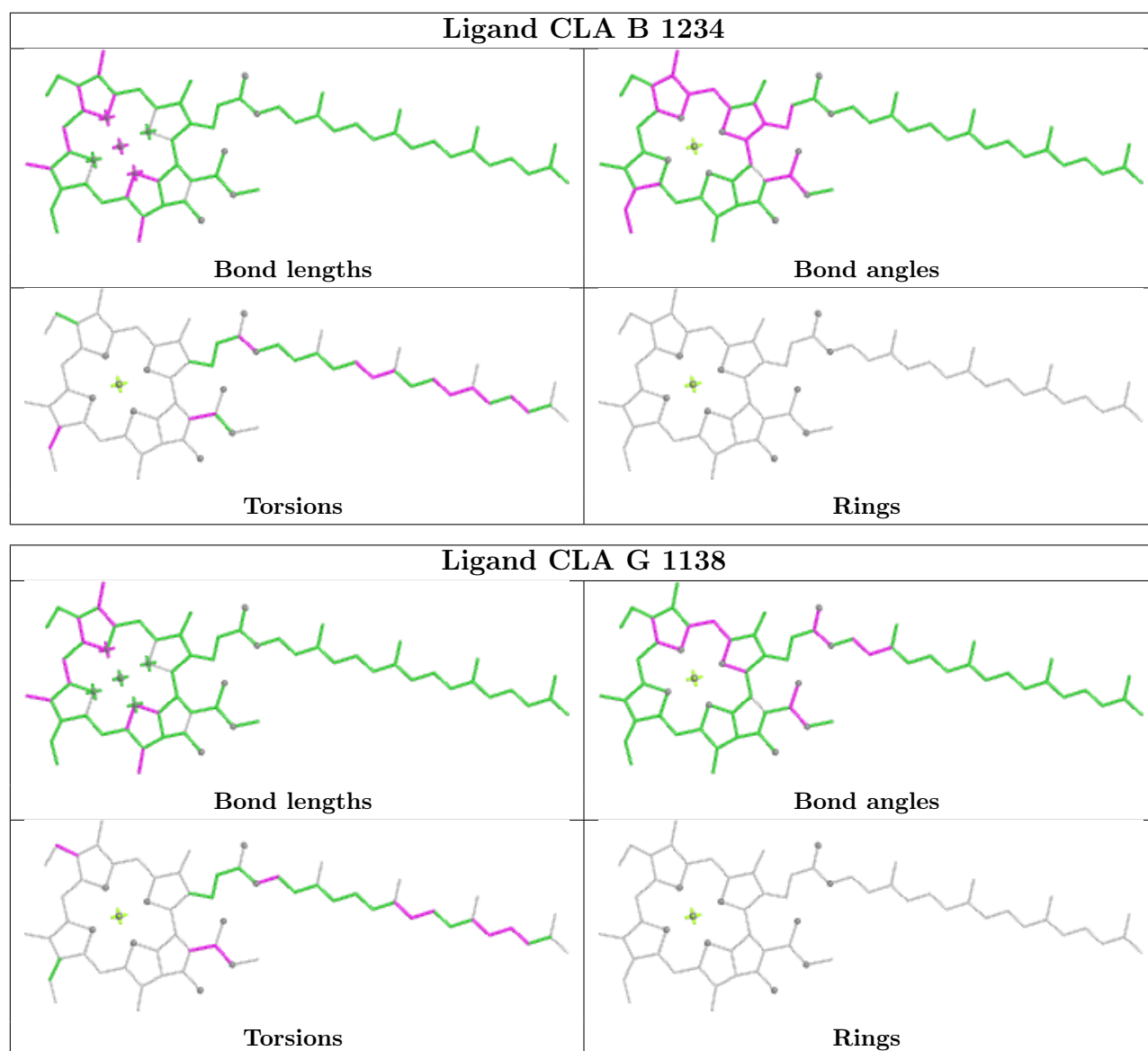


Ligand CLA c 517

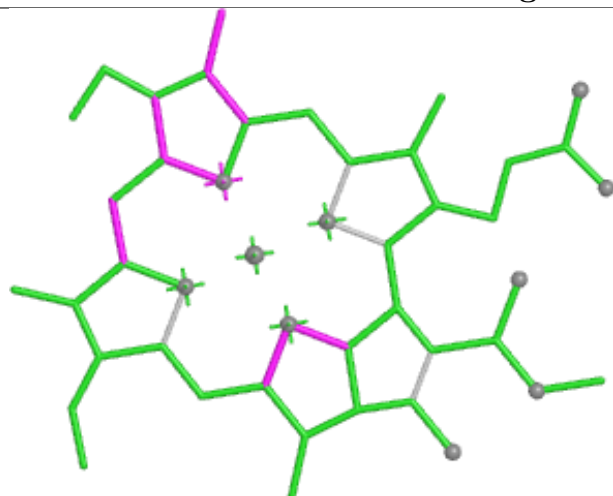




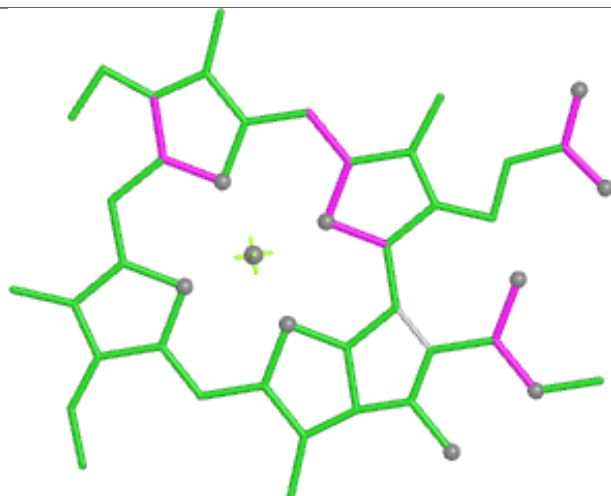




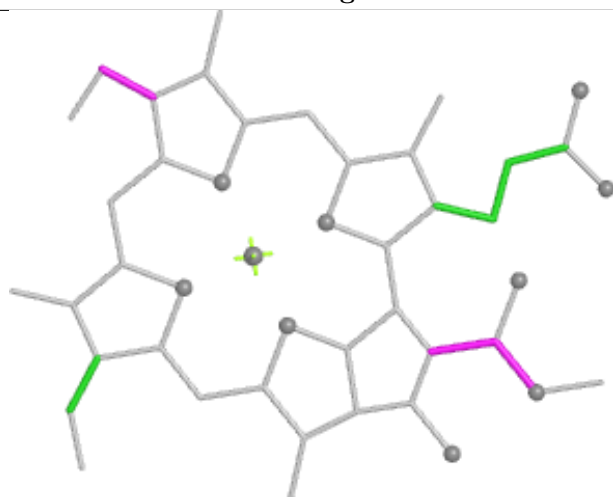
Ligand CLA c 506



Bond lengths



Bond angles

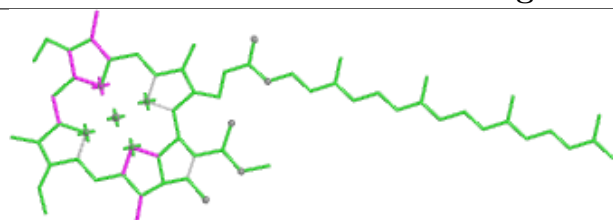


Torsions

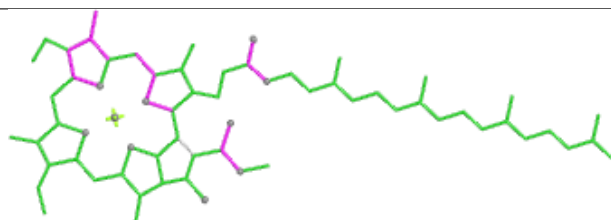


Rings

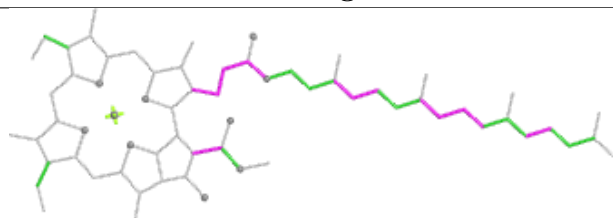
Ligand CLA Z 518



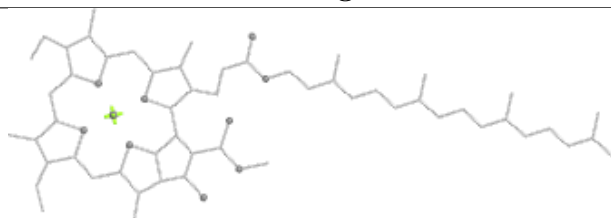
Bond lengths



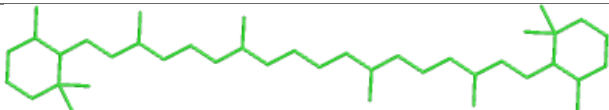
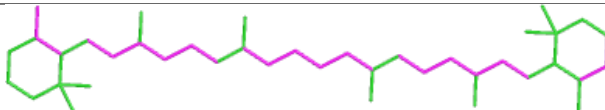
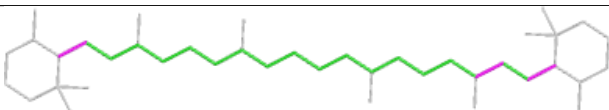
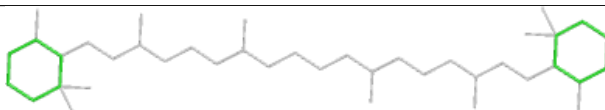
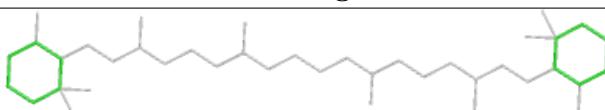
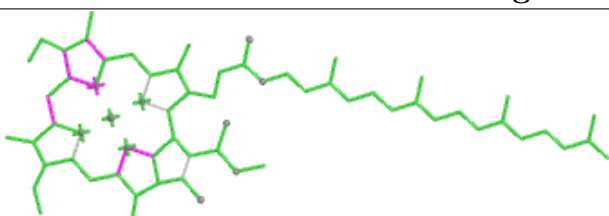
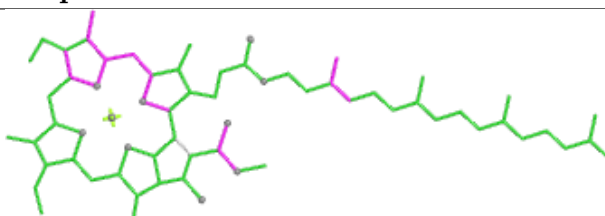
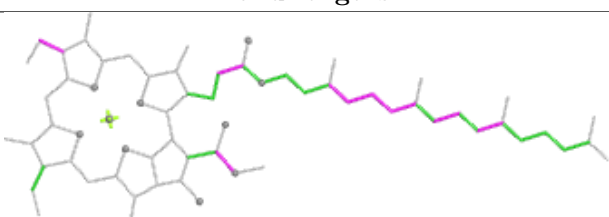
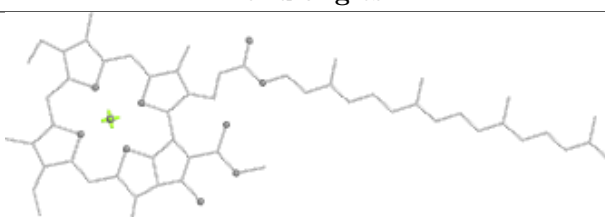
Bond angles



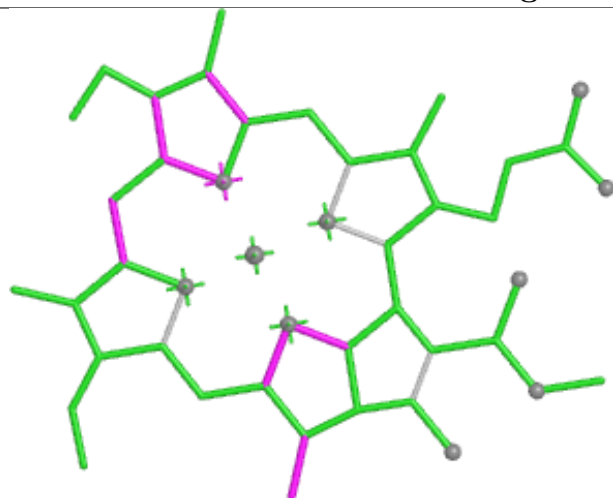
Torsions



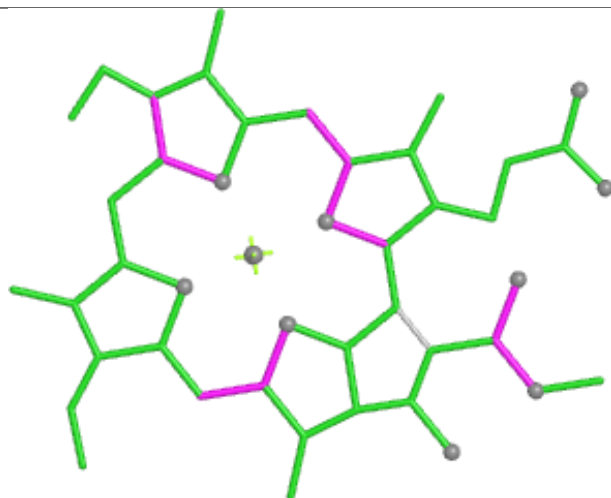
Rings

Ligand BCR 4 523	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR U 4104	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA q 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

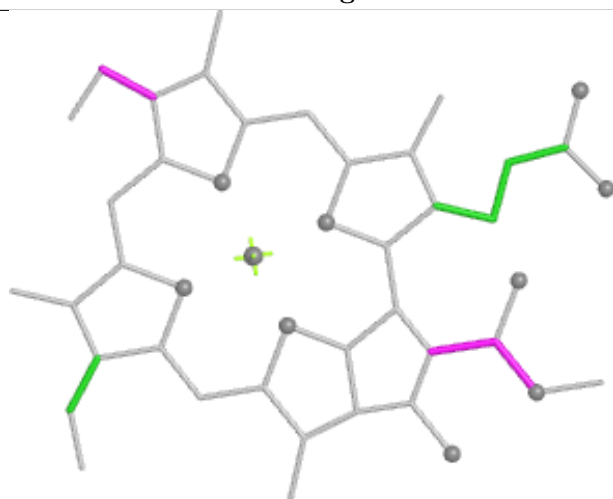
Ligand CLA t 504



Bond lengths



Bond angles

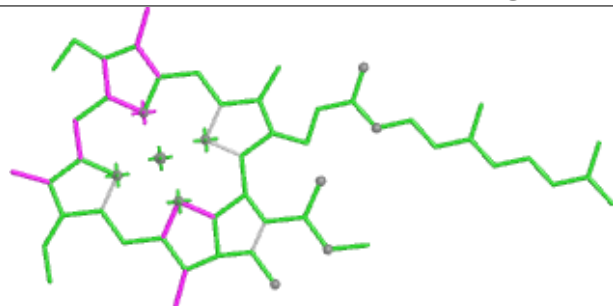


Torsions

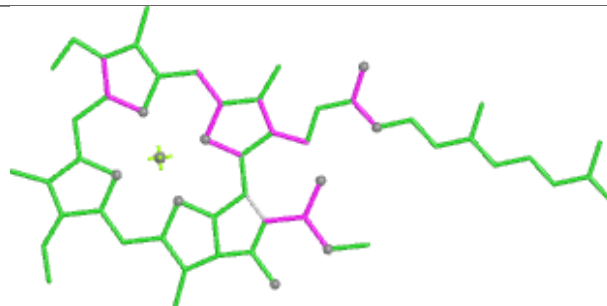


Rings

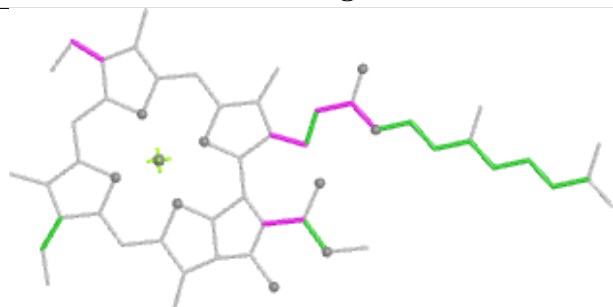
Ligand CLA K 1401



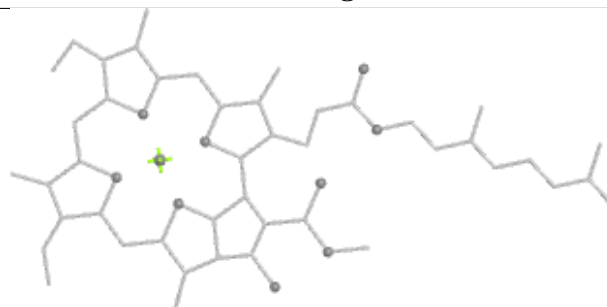
Bond lengths



Bond angles

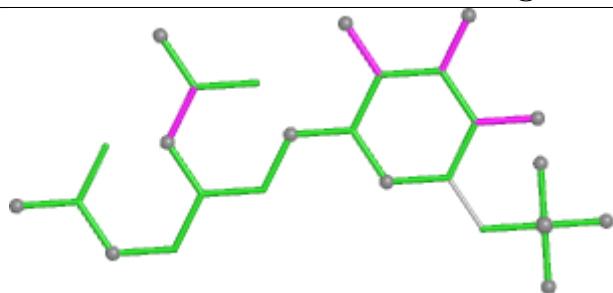


Torsions

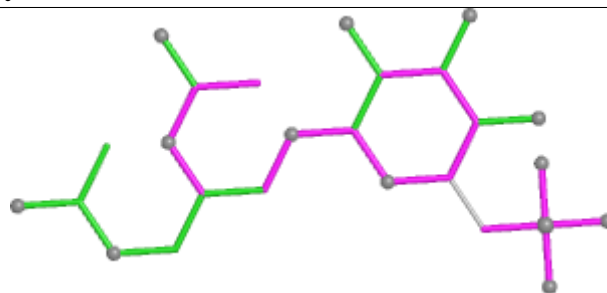


Rings

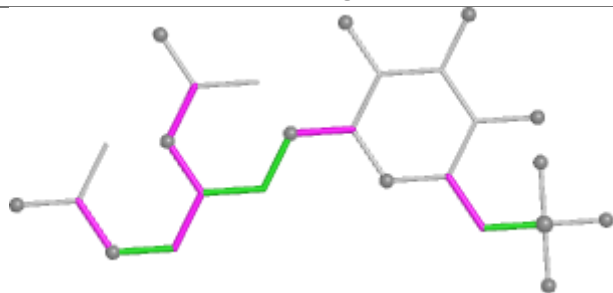
Ligand SQD d 822



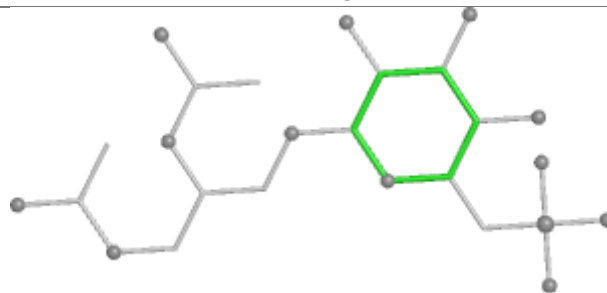
Bond lengths



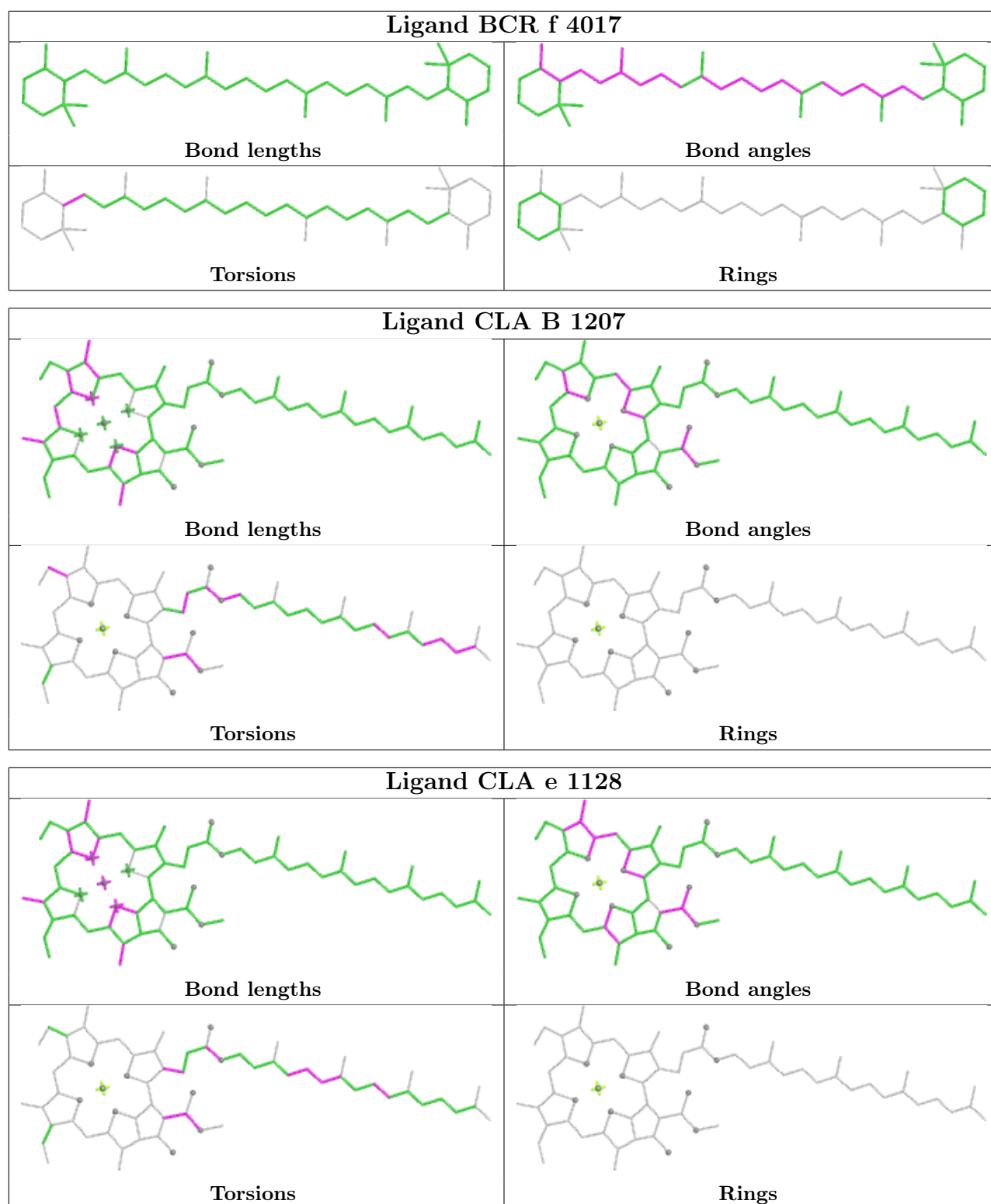
Bond angles



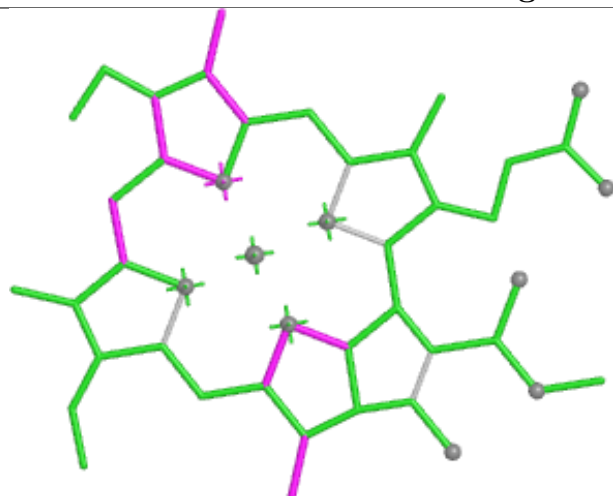
Torsions



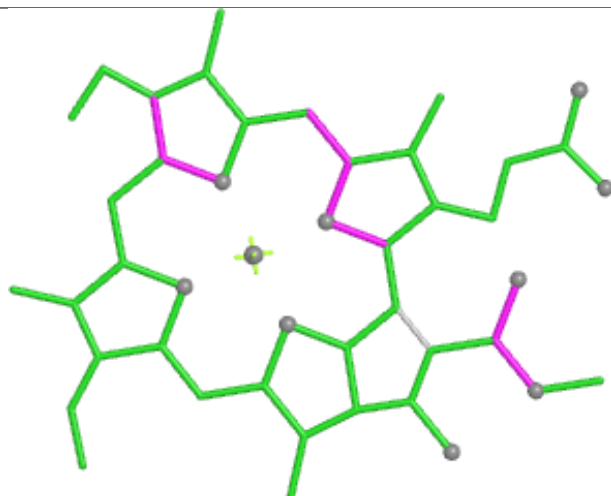
Rings



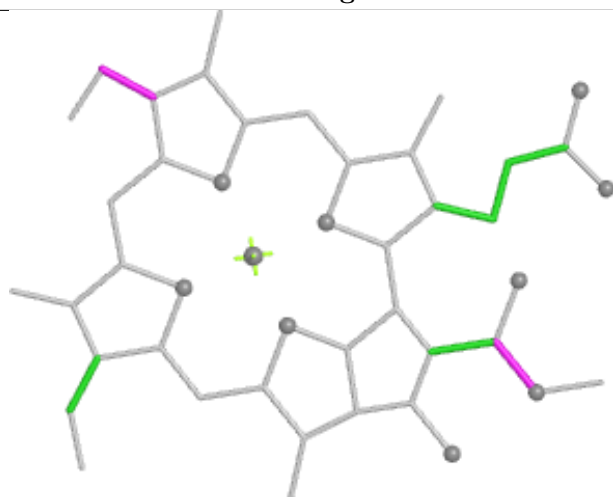
Ligand CLA 4 506



Bond lengths



Bond angles

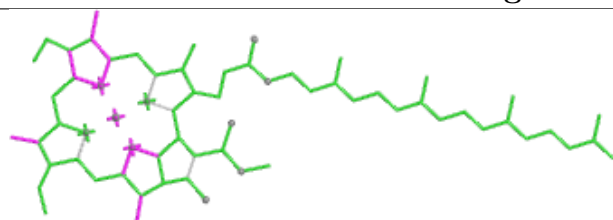


Torsions

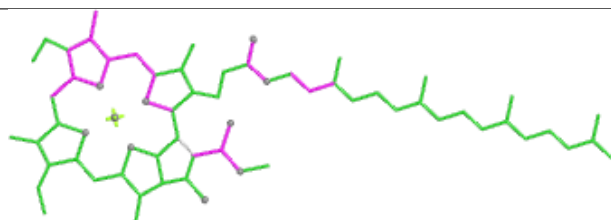


Rings

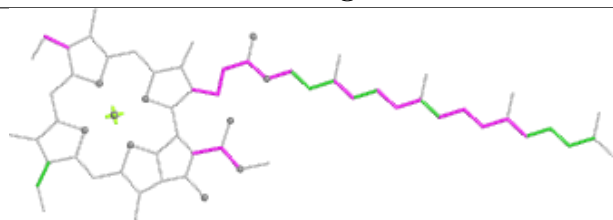
Ligand CLA G 1106



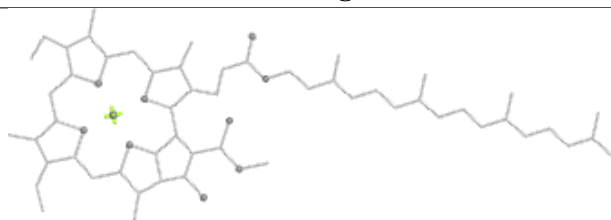
Bond lengths



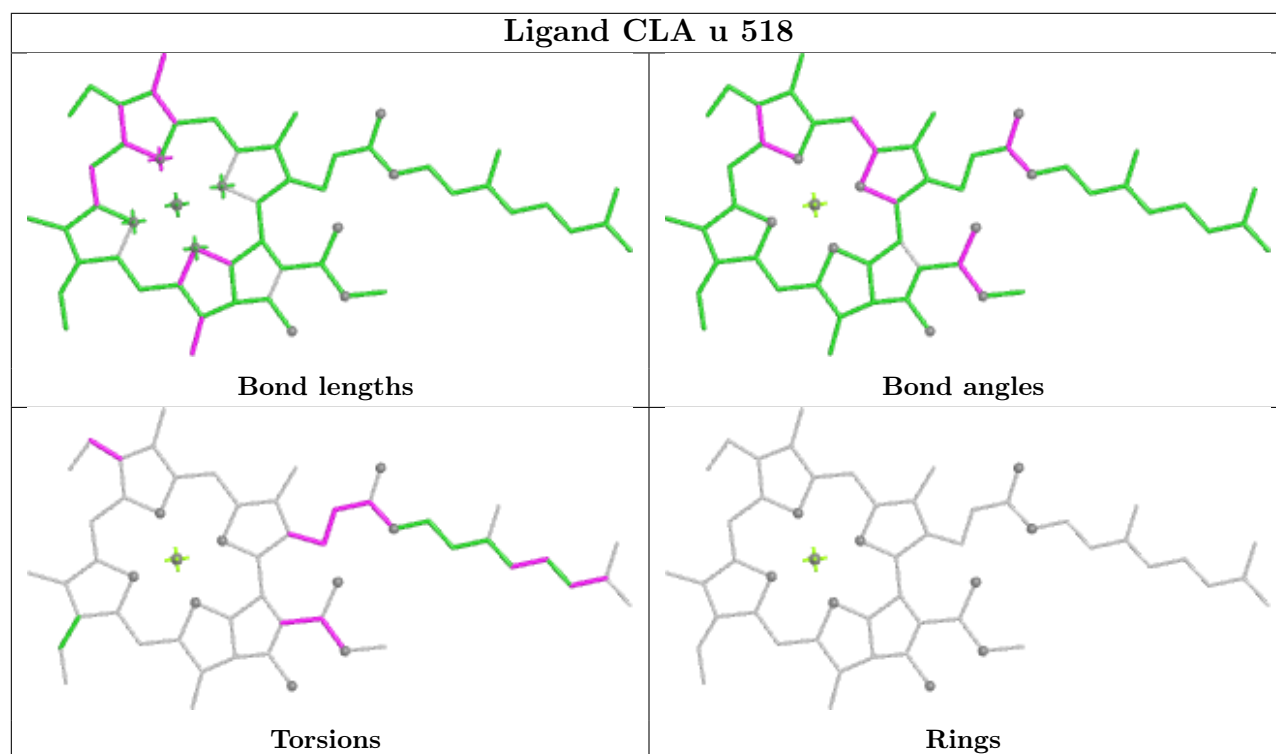
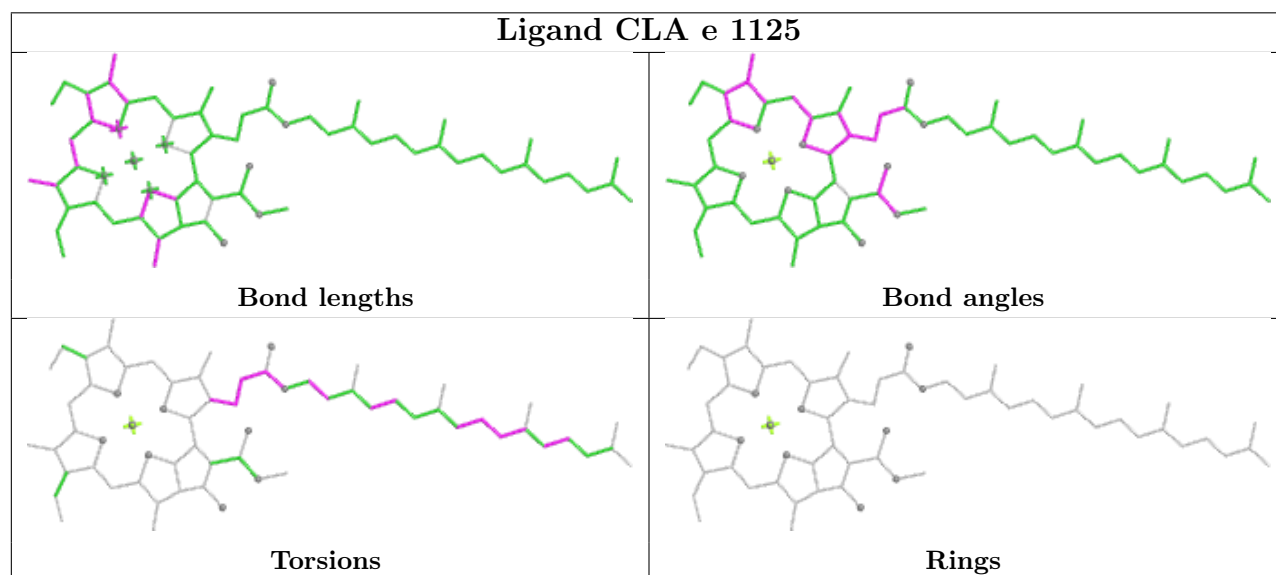
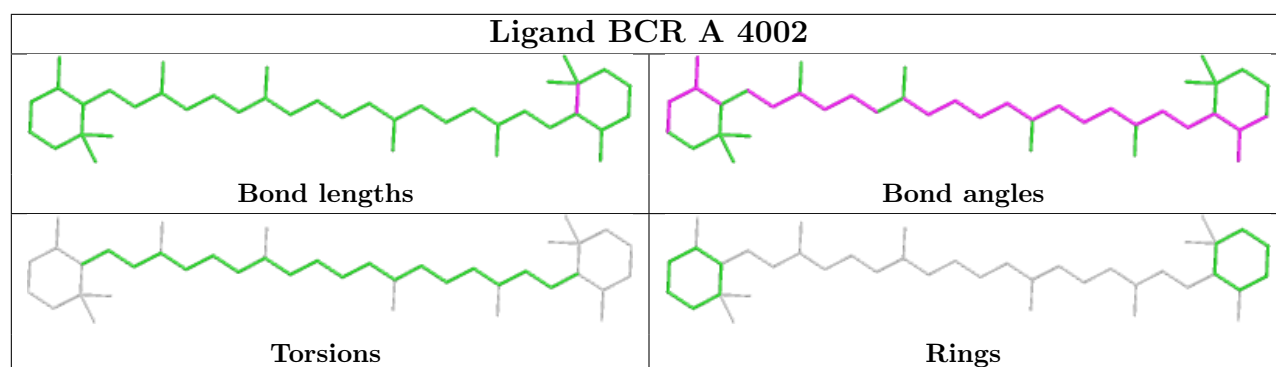
Bond angles

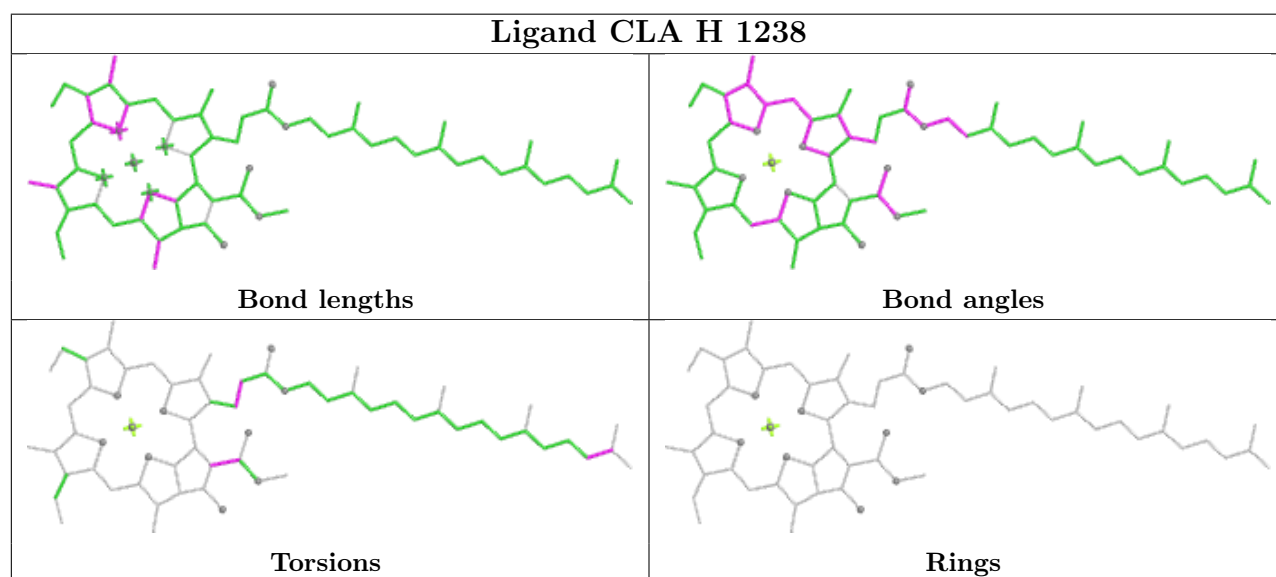
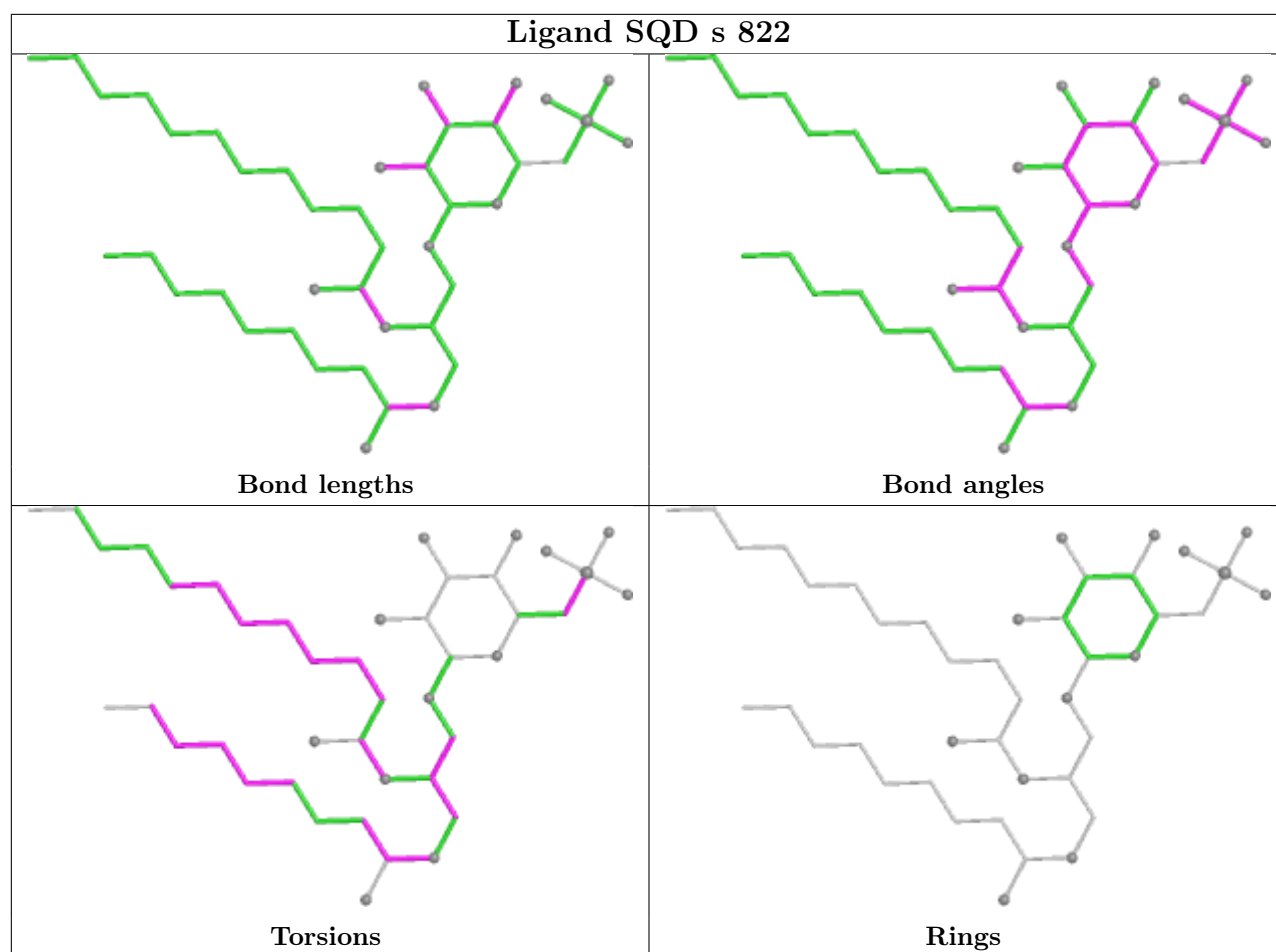


Torsions

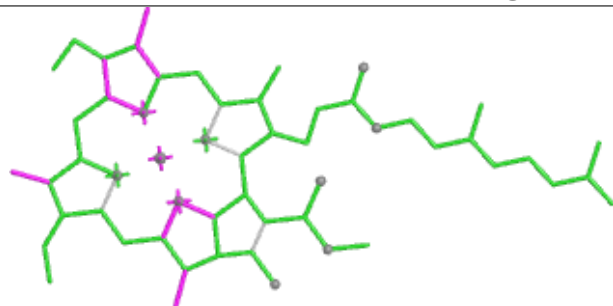


Rings

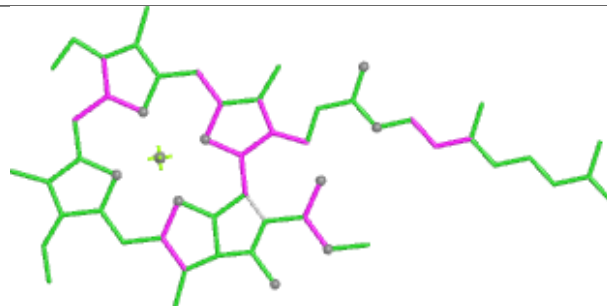




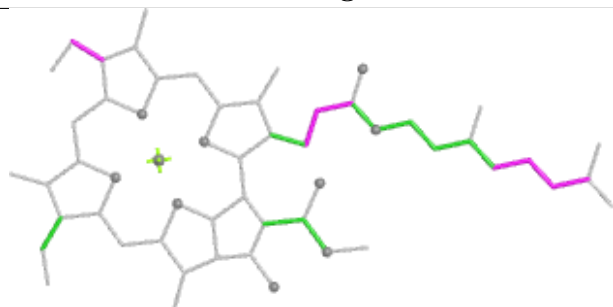
Ligand CLA G 1121



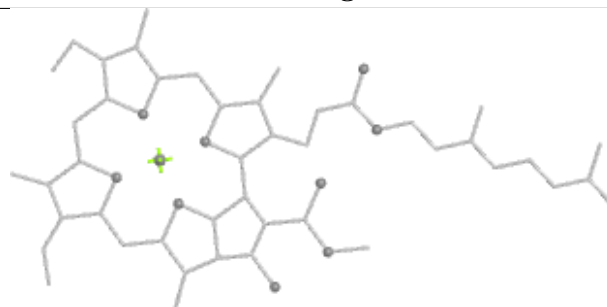
Bond lengths



Bond angles

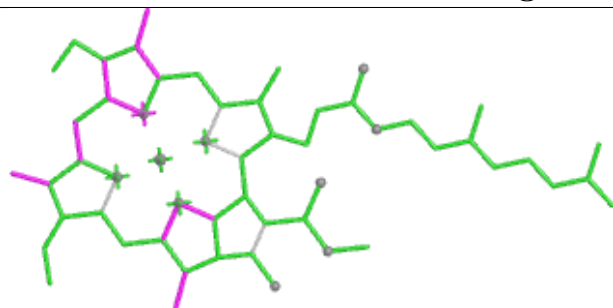


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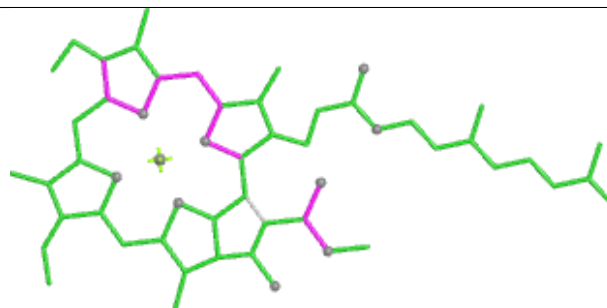


Rings

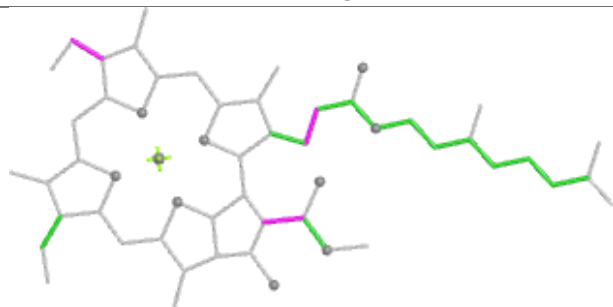
Ligand CLA 1 513



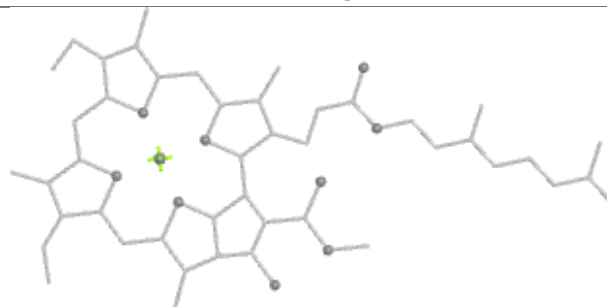
Bond lengths



Bond angles

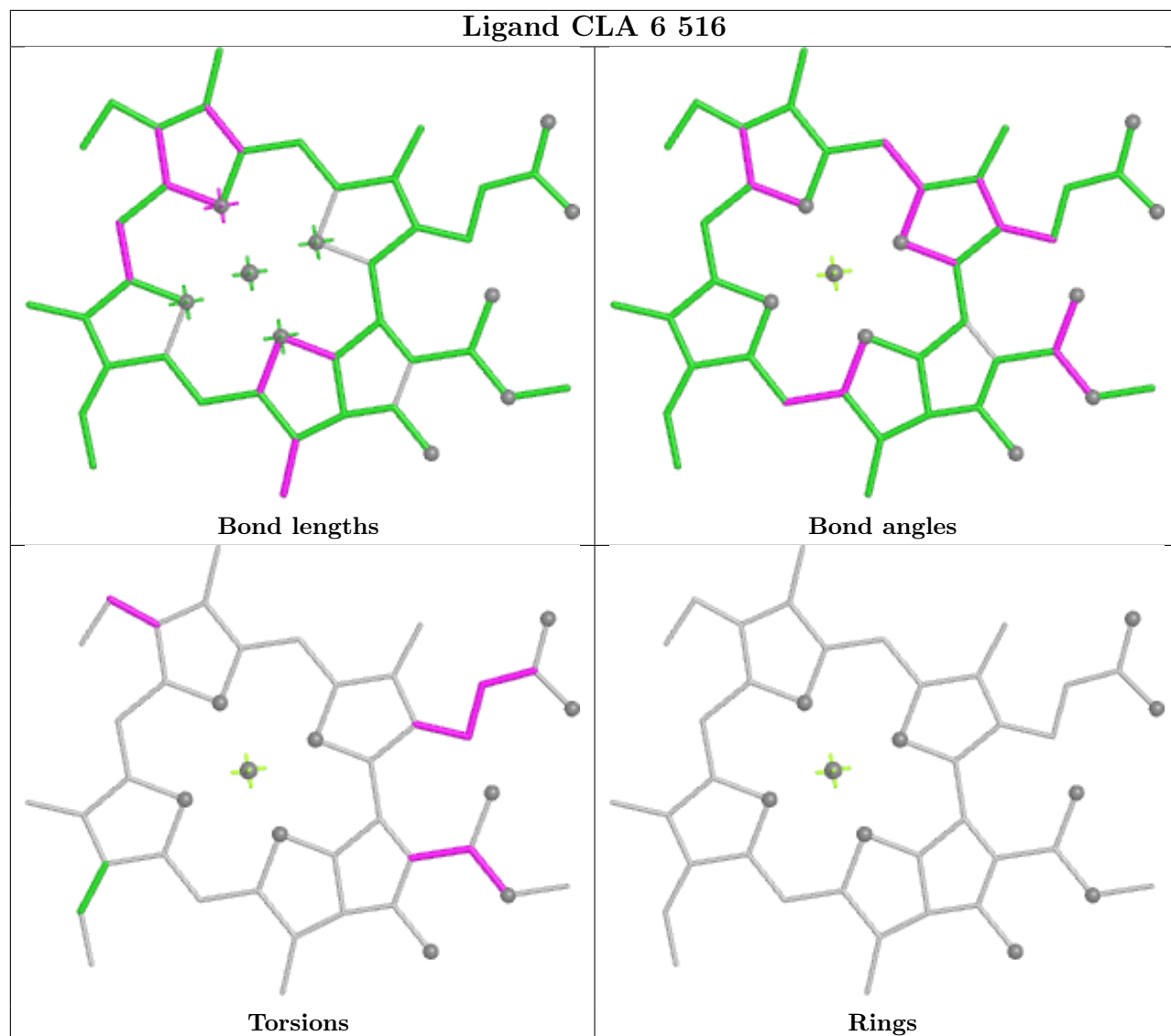


Torsions

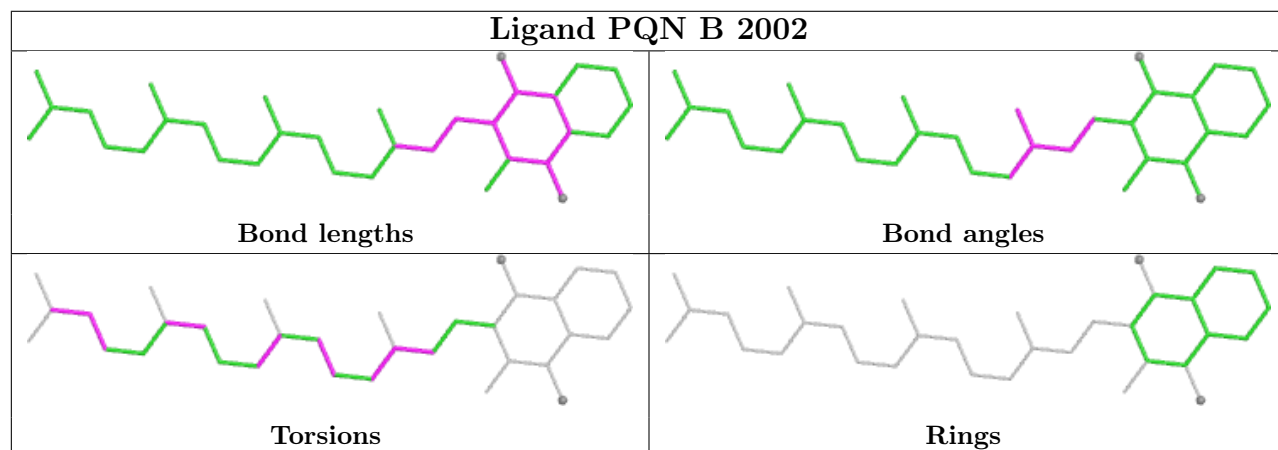


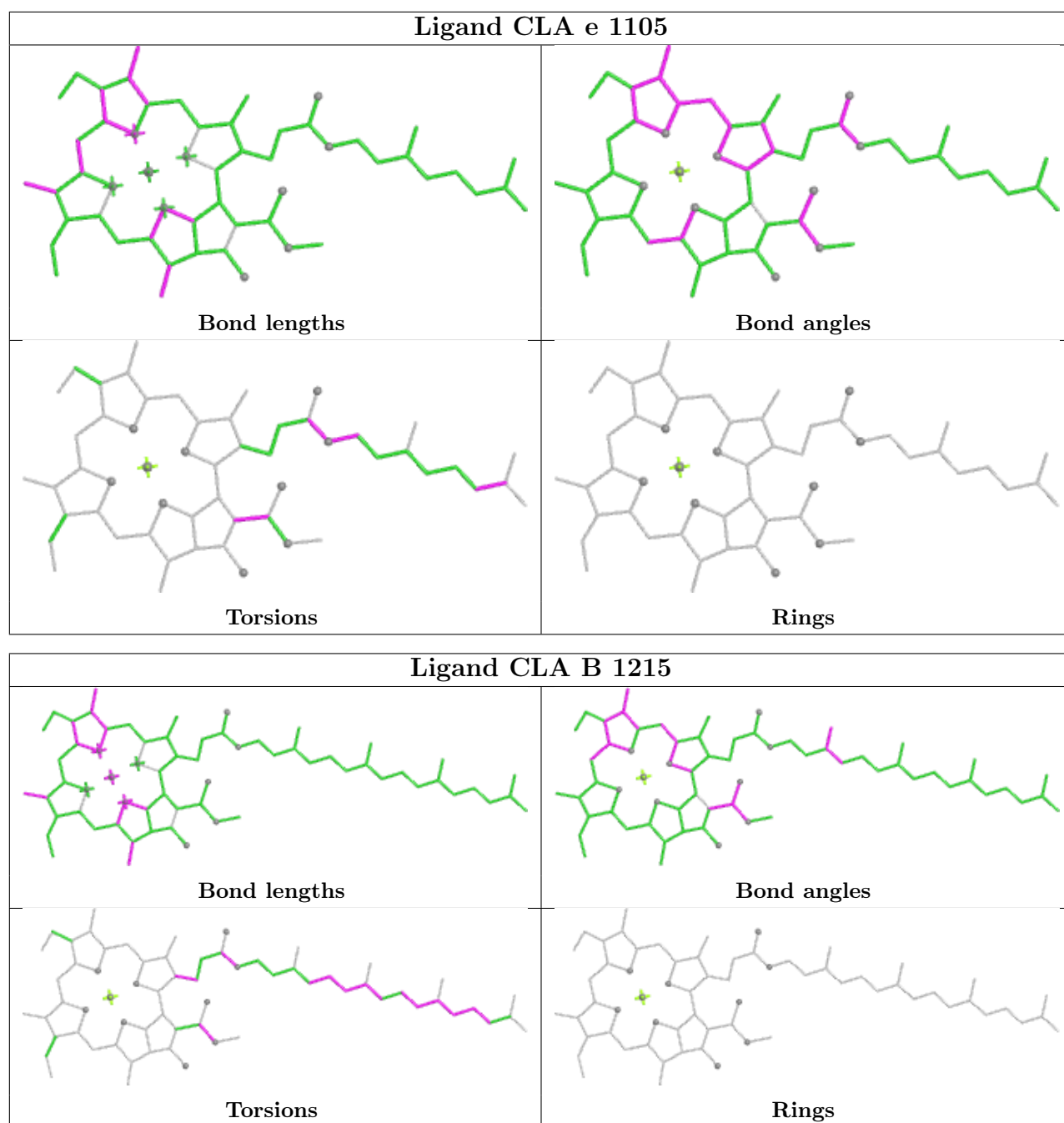
Rings

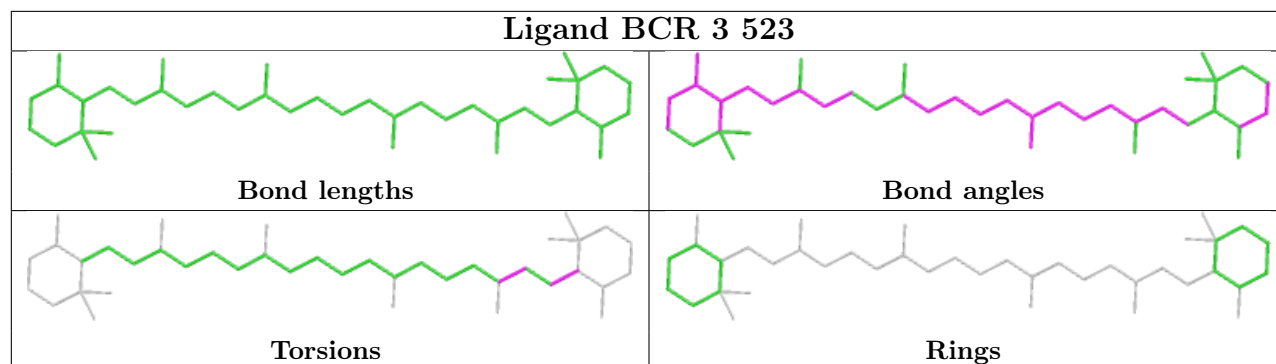
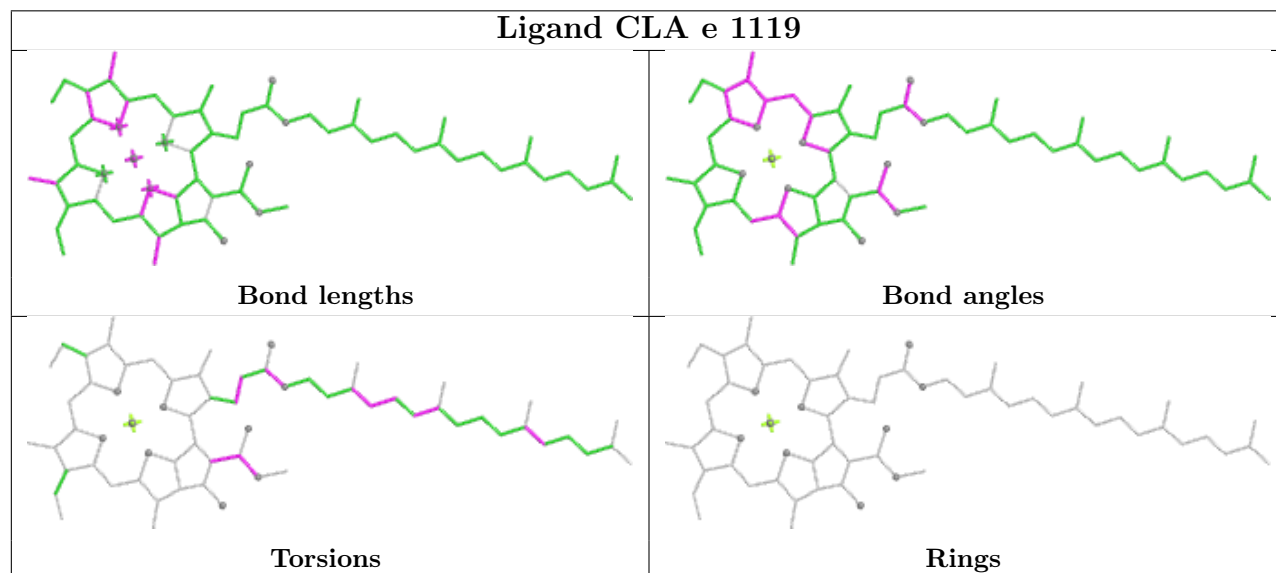
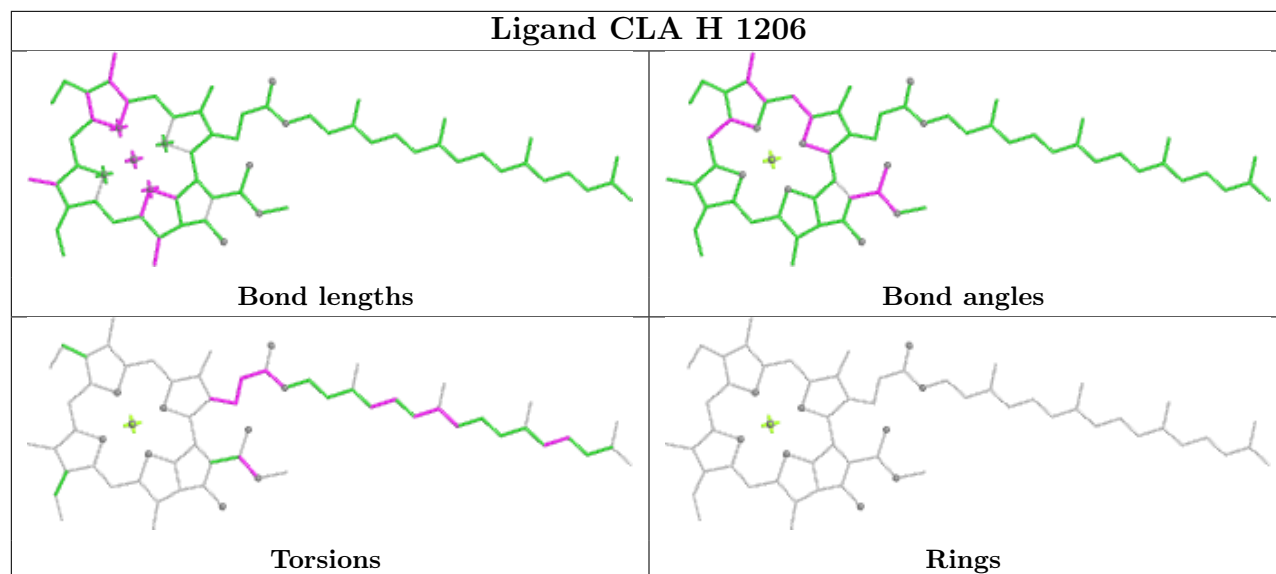
Ligand CLA 6 516

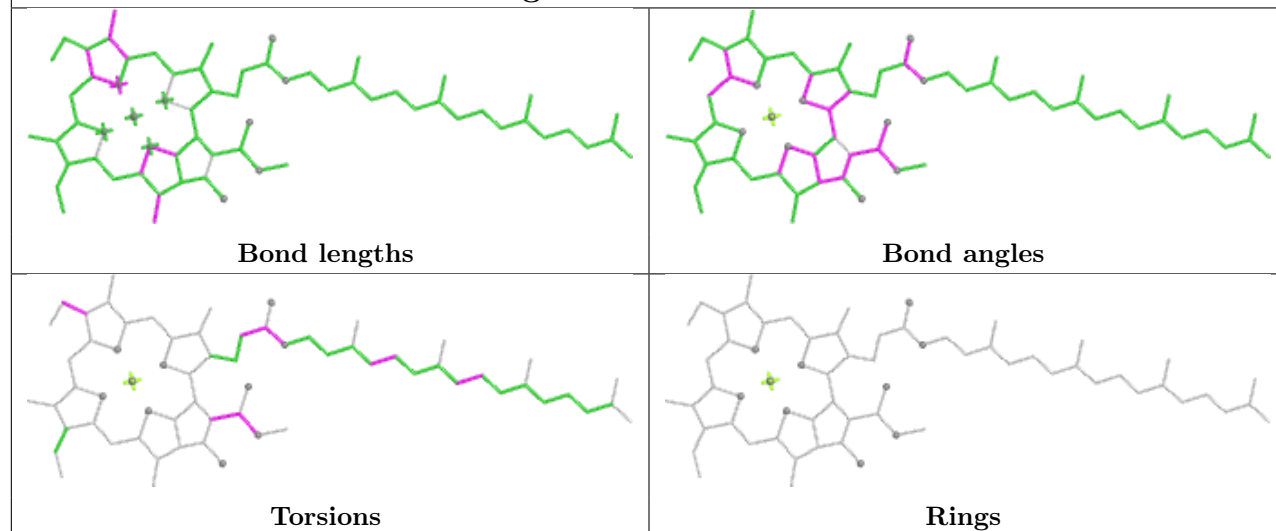
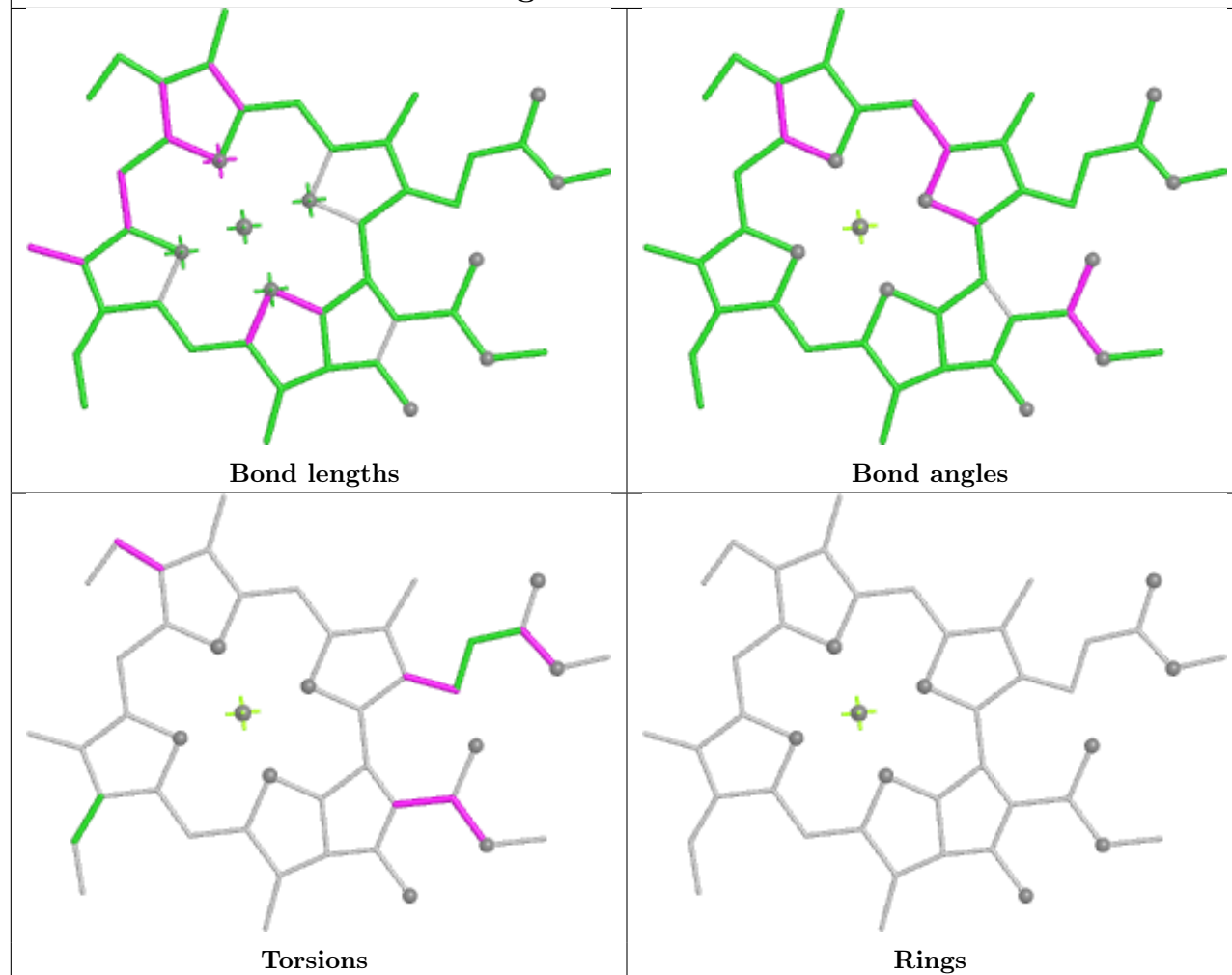


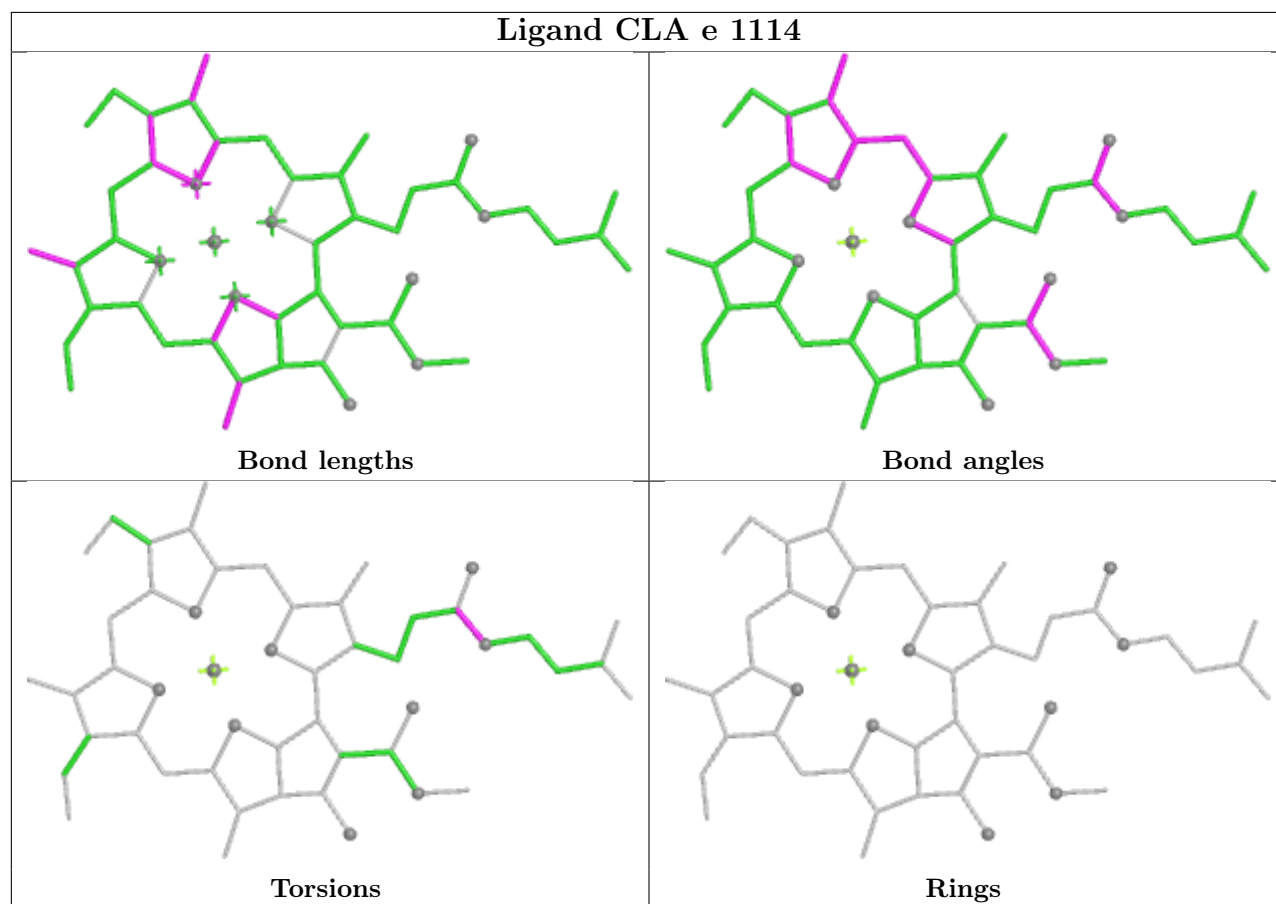
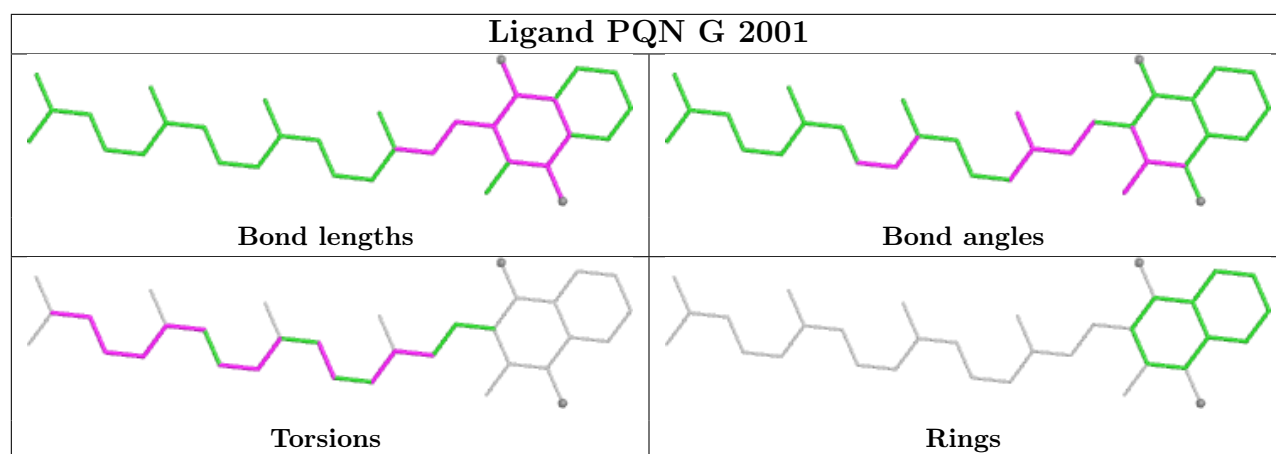
Ligand PQN B 2002

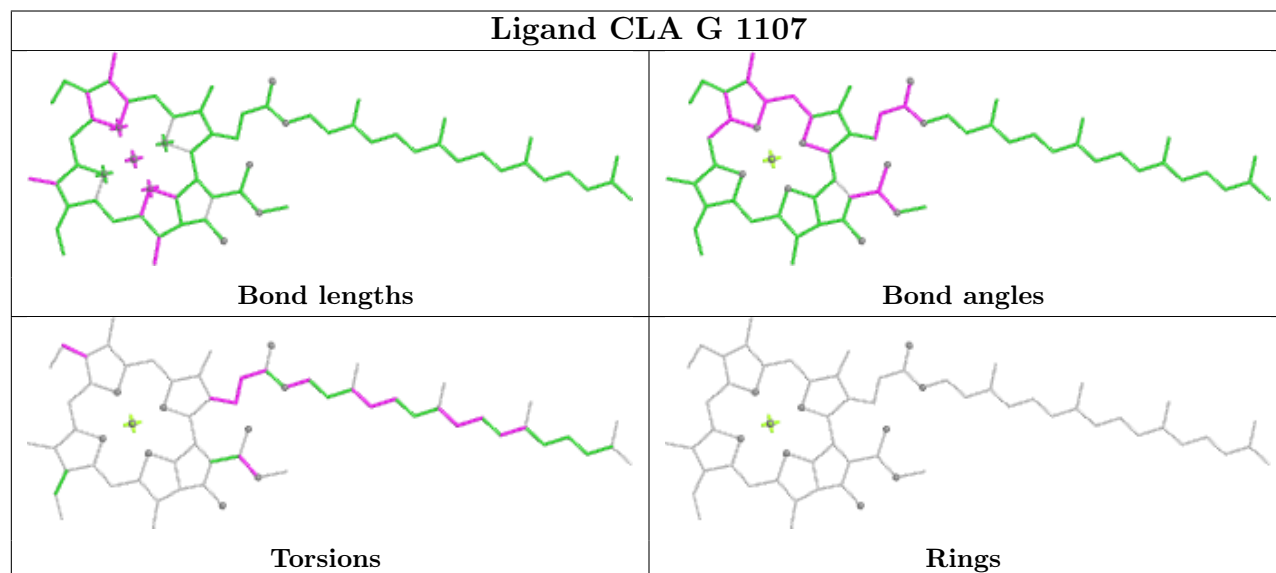
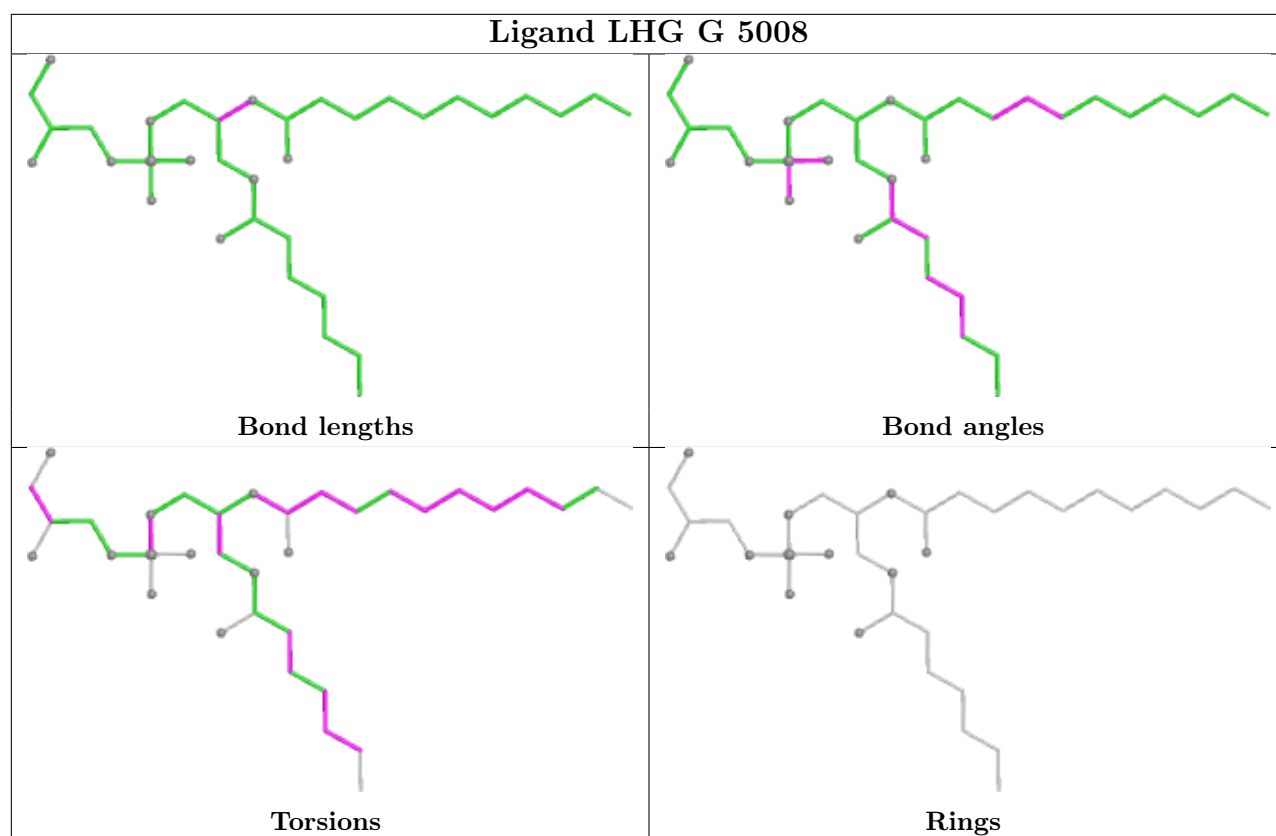


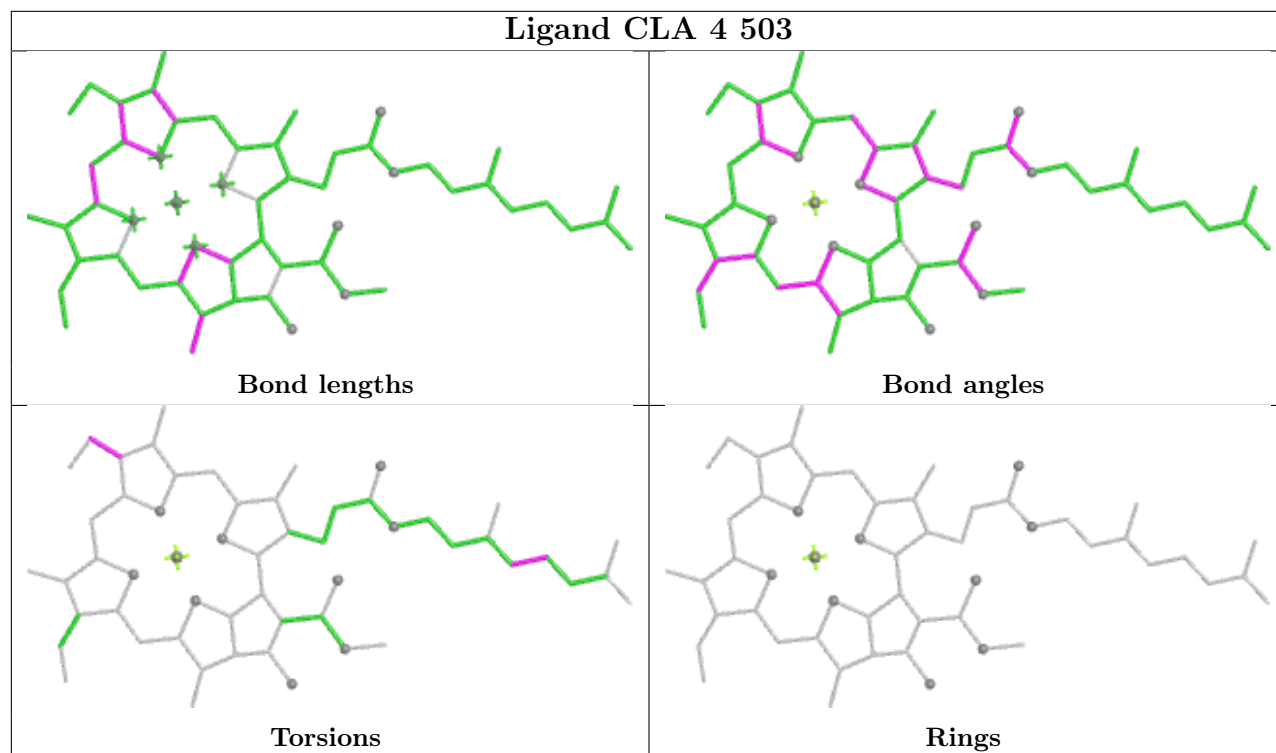
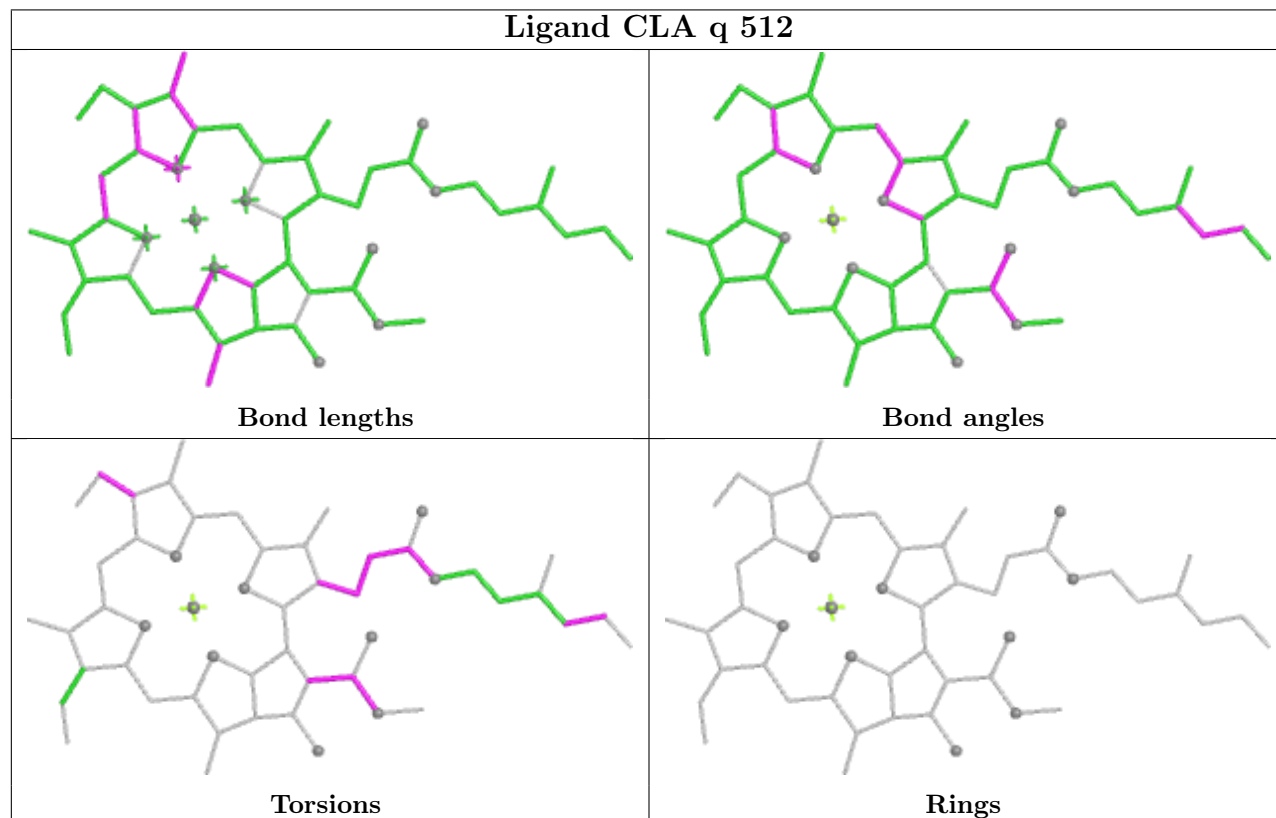


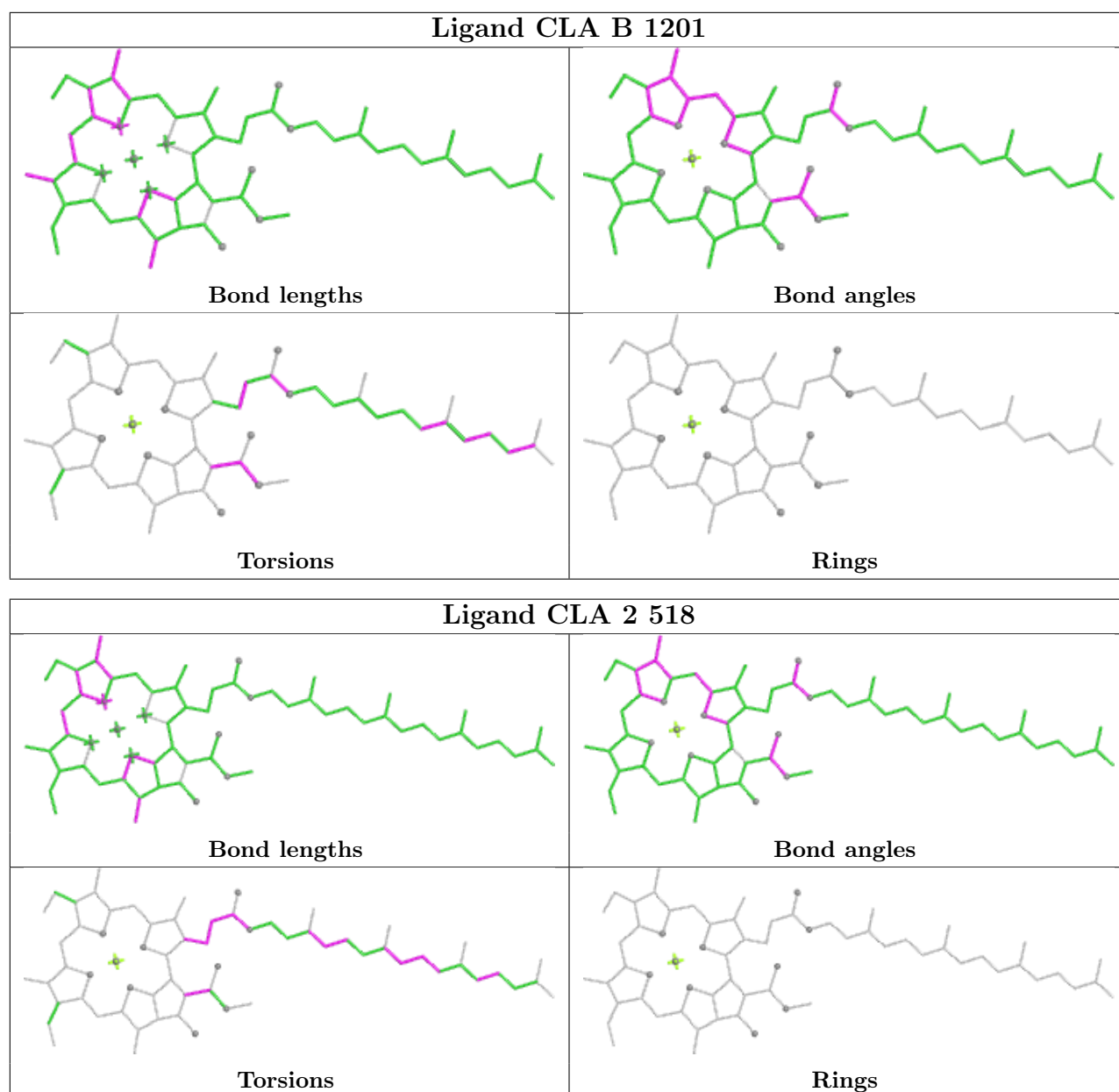


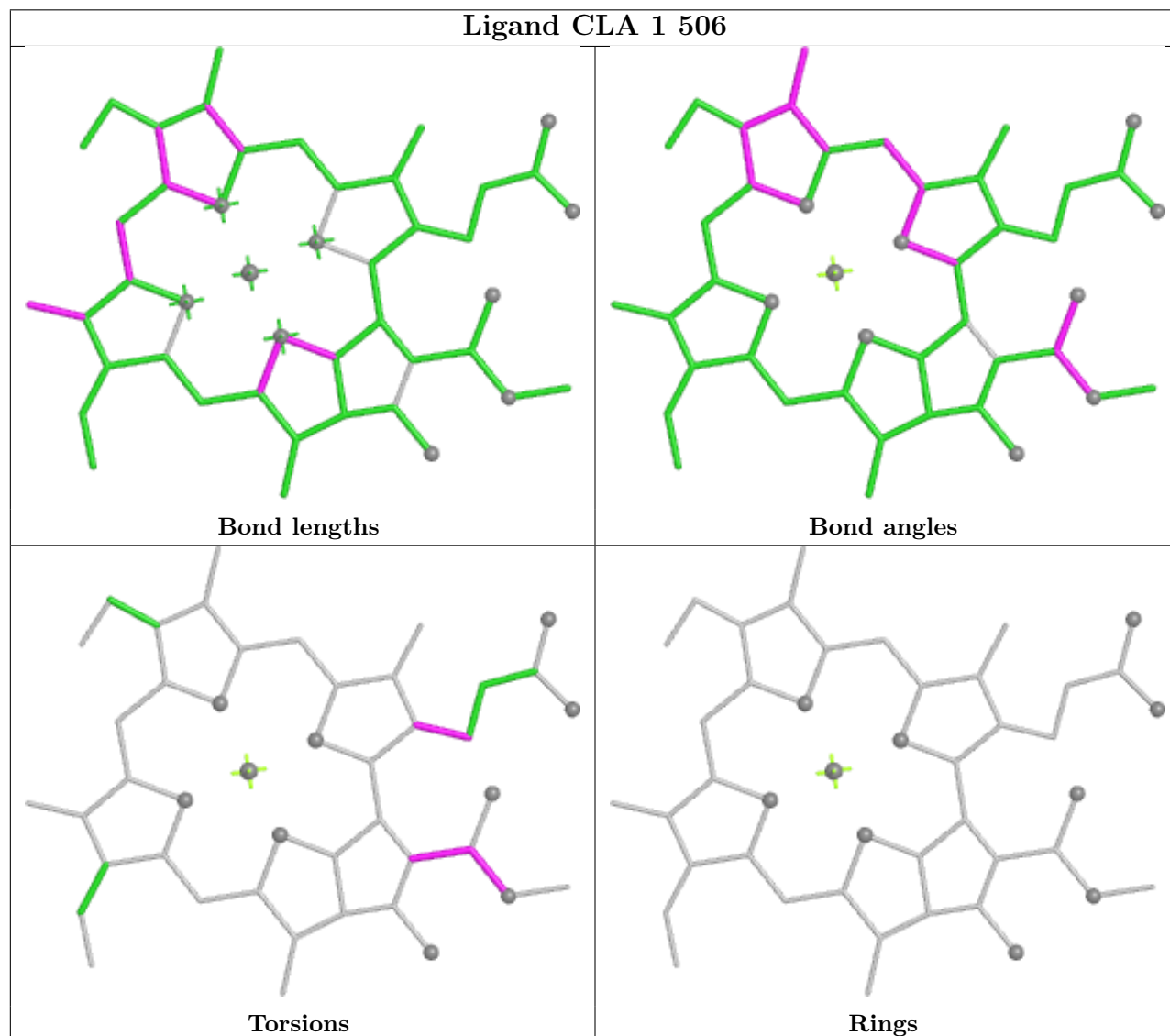
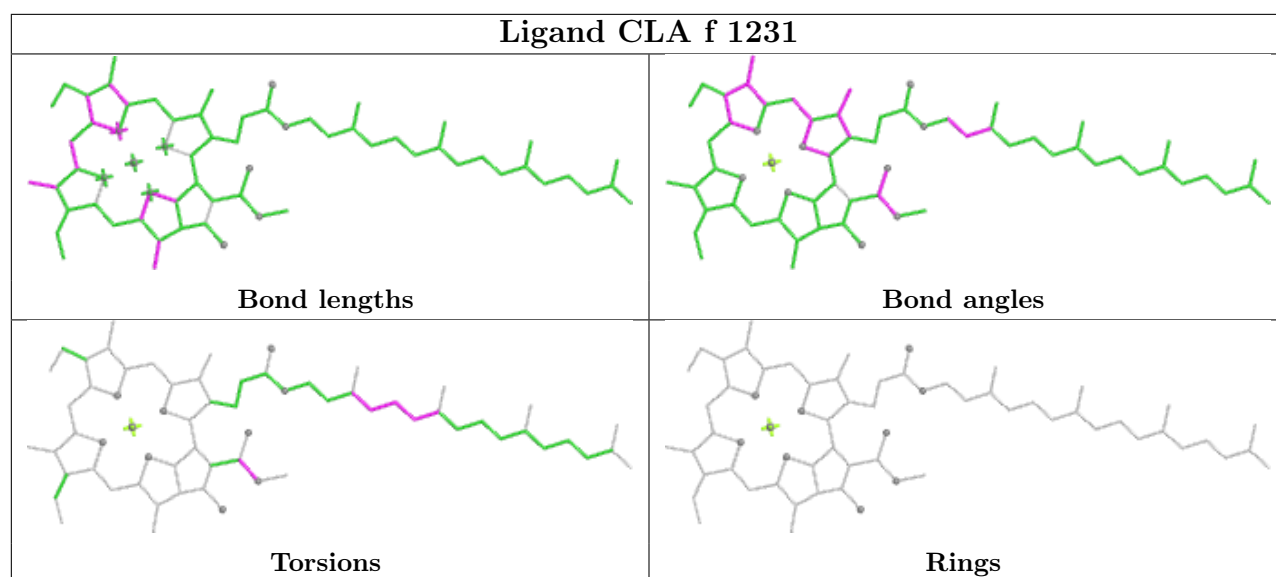
Ligand CLA A 1011**Ligand CLA 6 519**



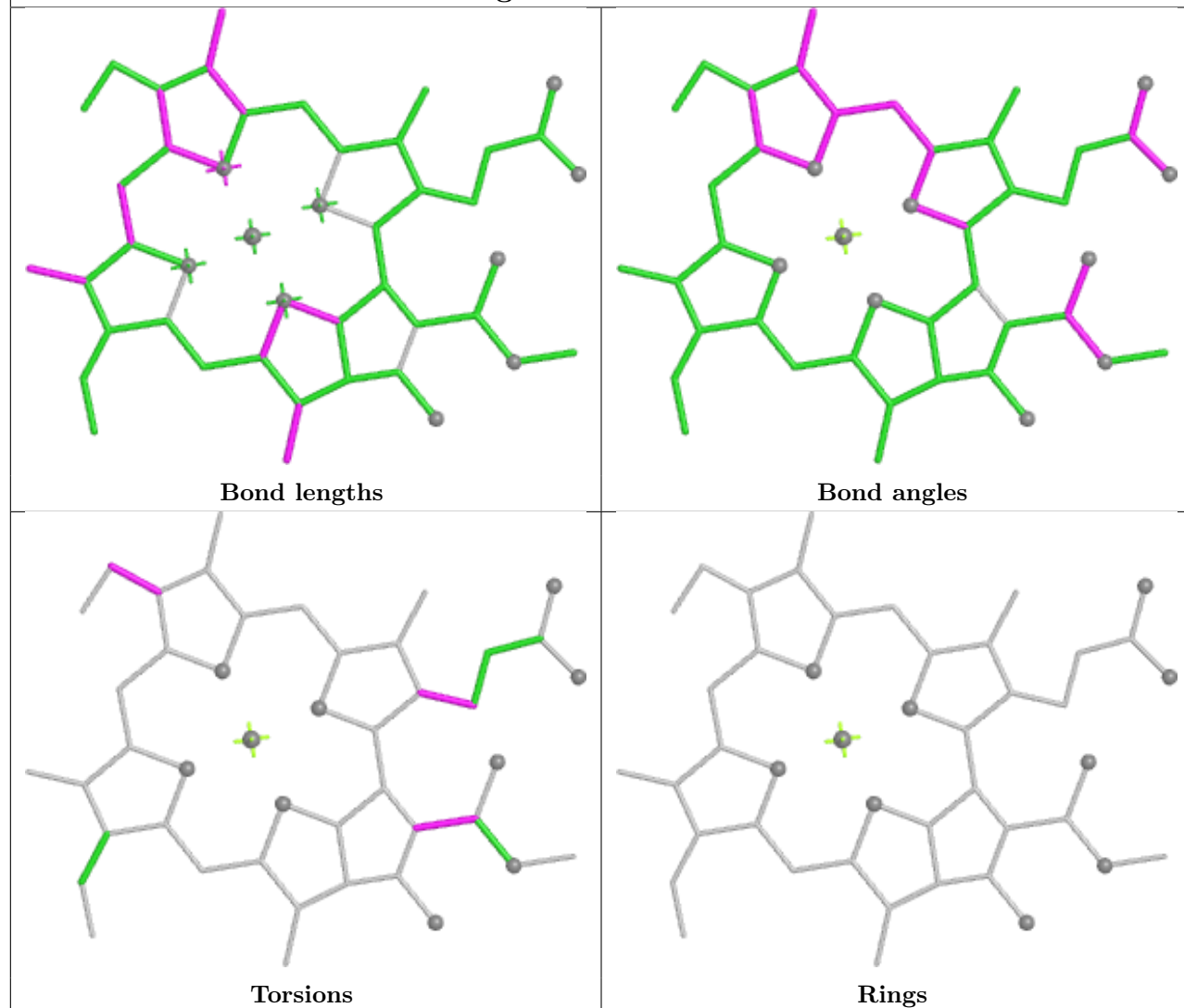


Ligand CLA 4 503**Ligand CLA q 512**

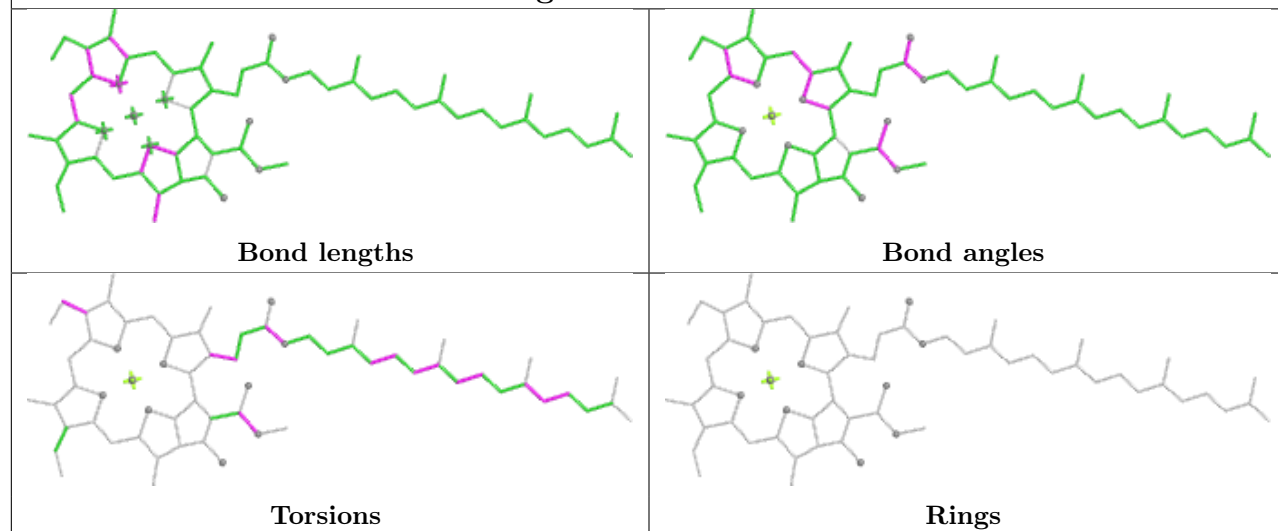


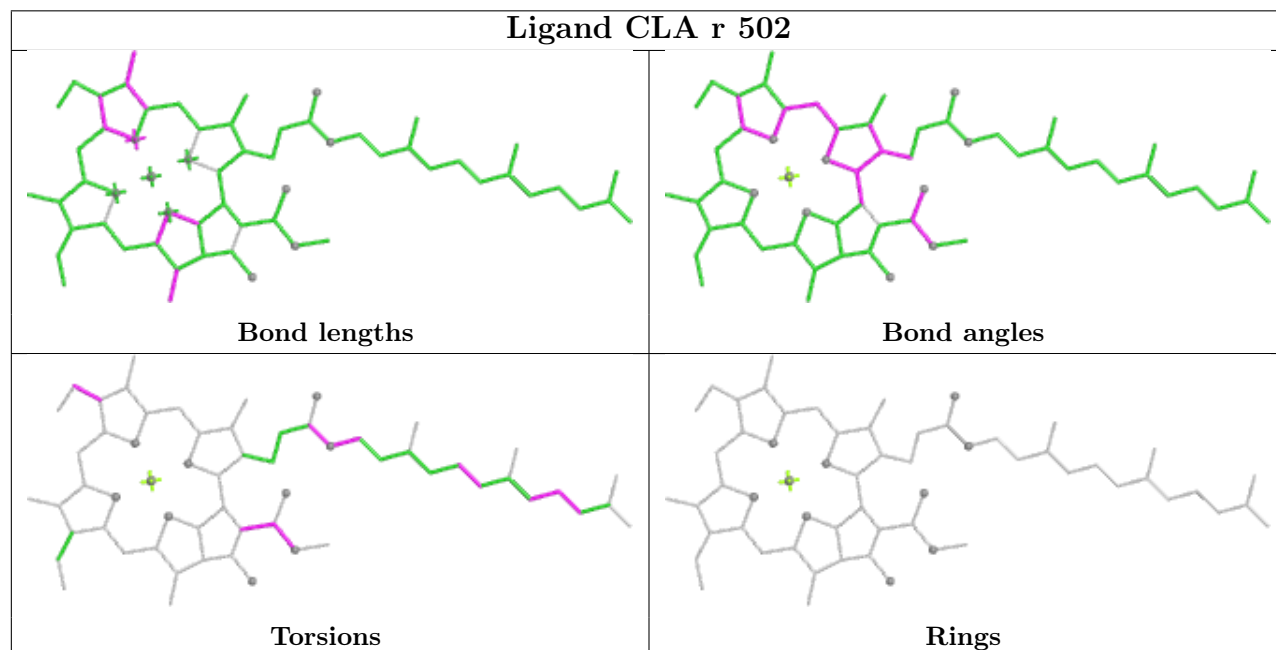
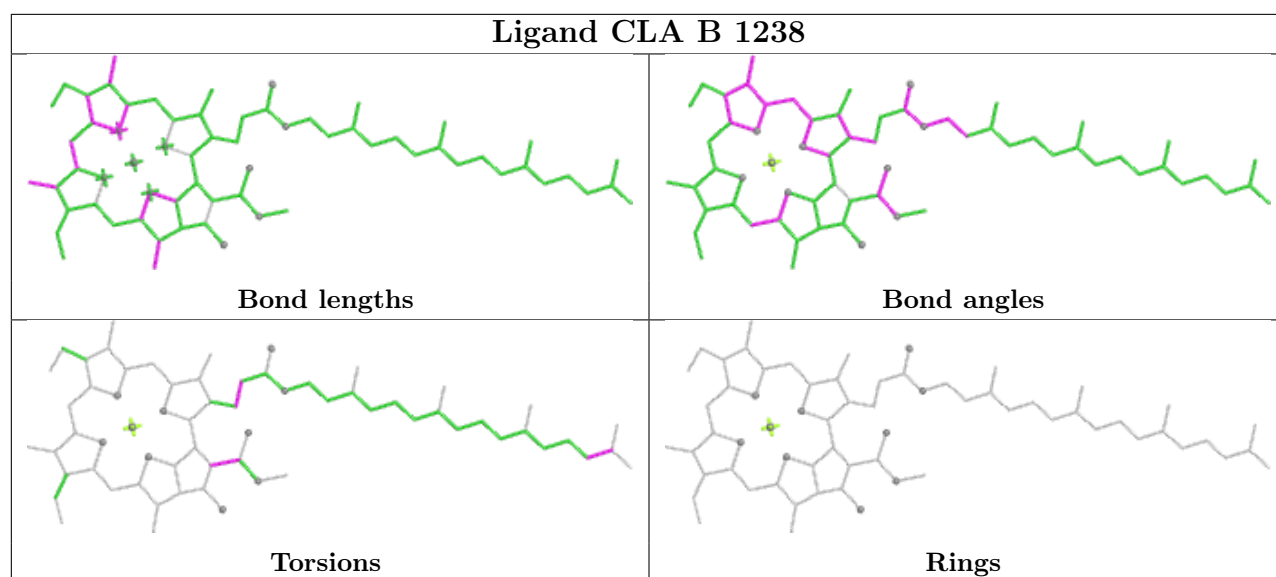


Ligand CLA v 508

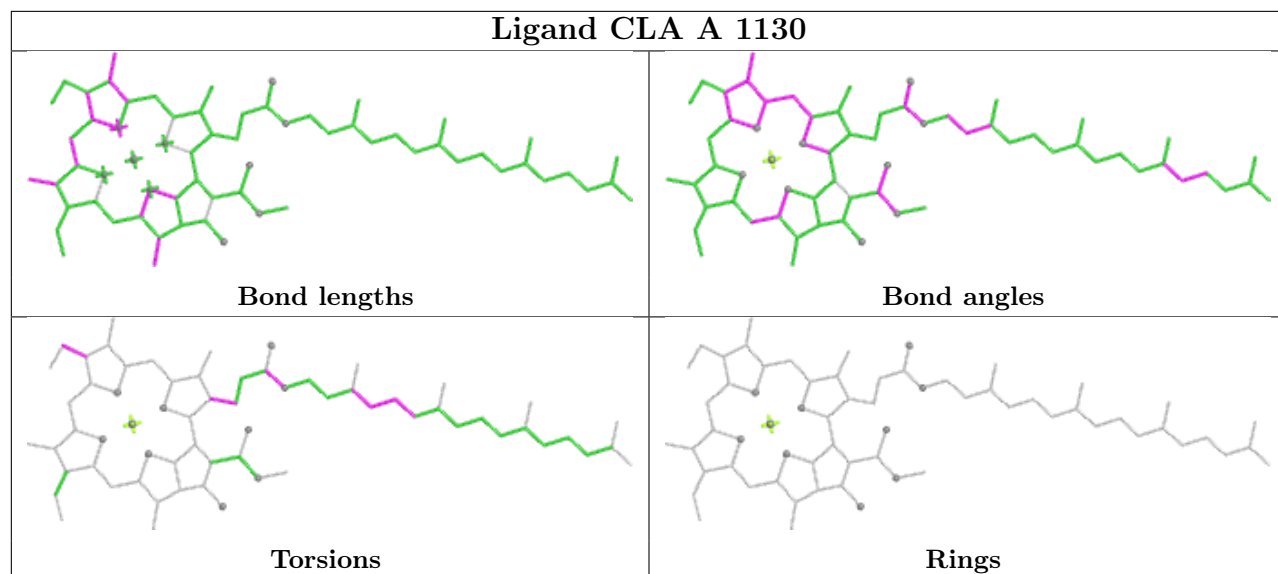


Ligand CLA a 513

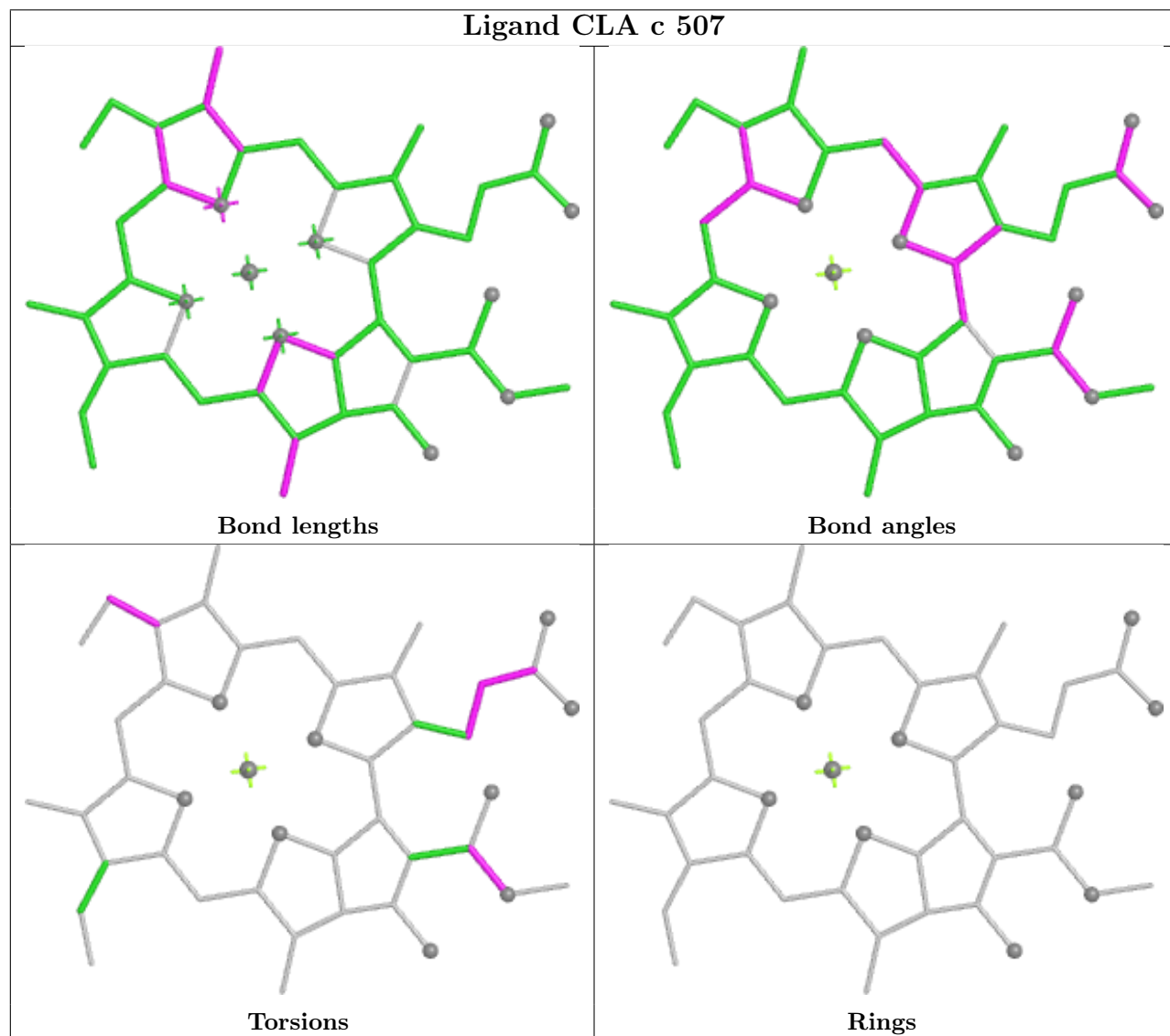


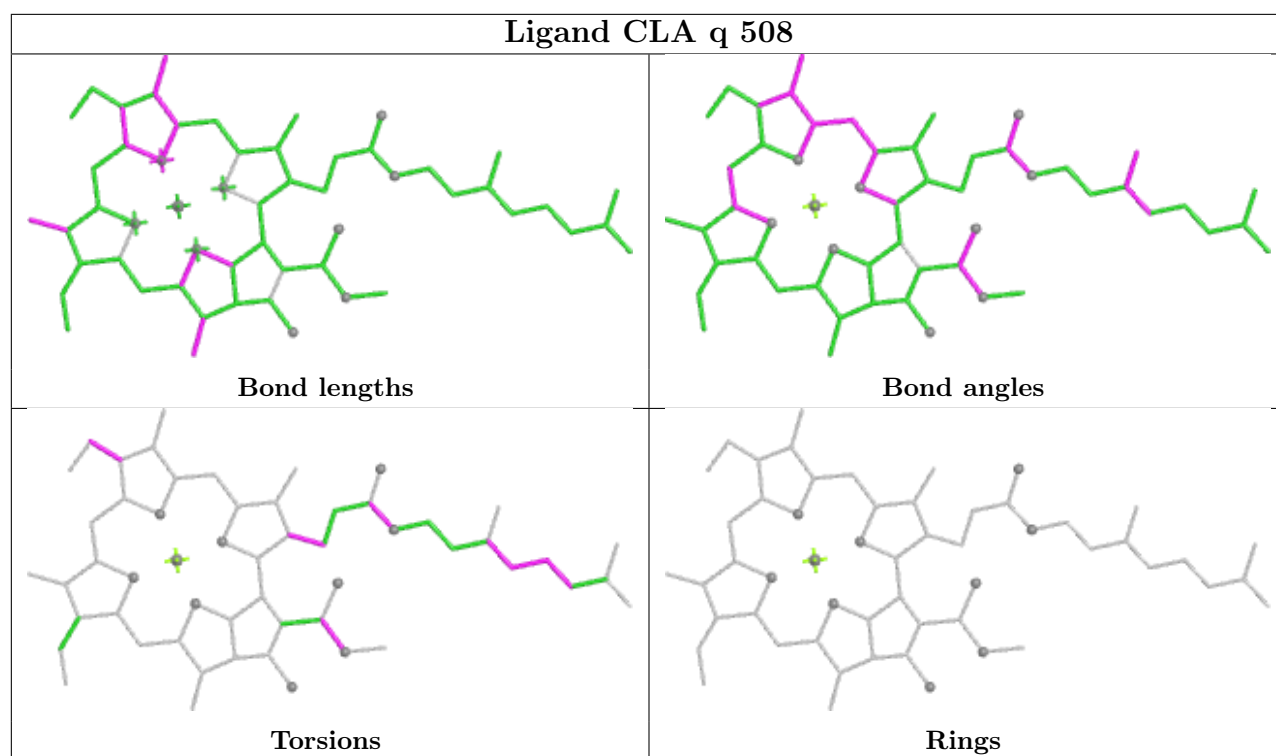


Ligand CLA A 1130

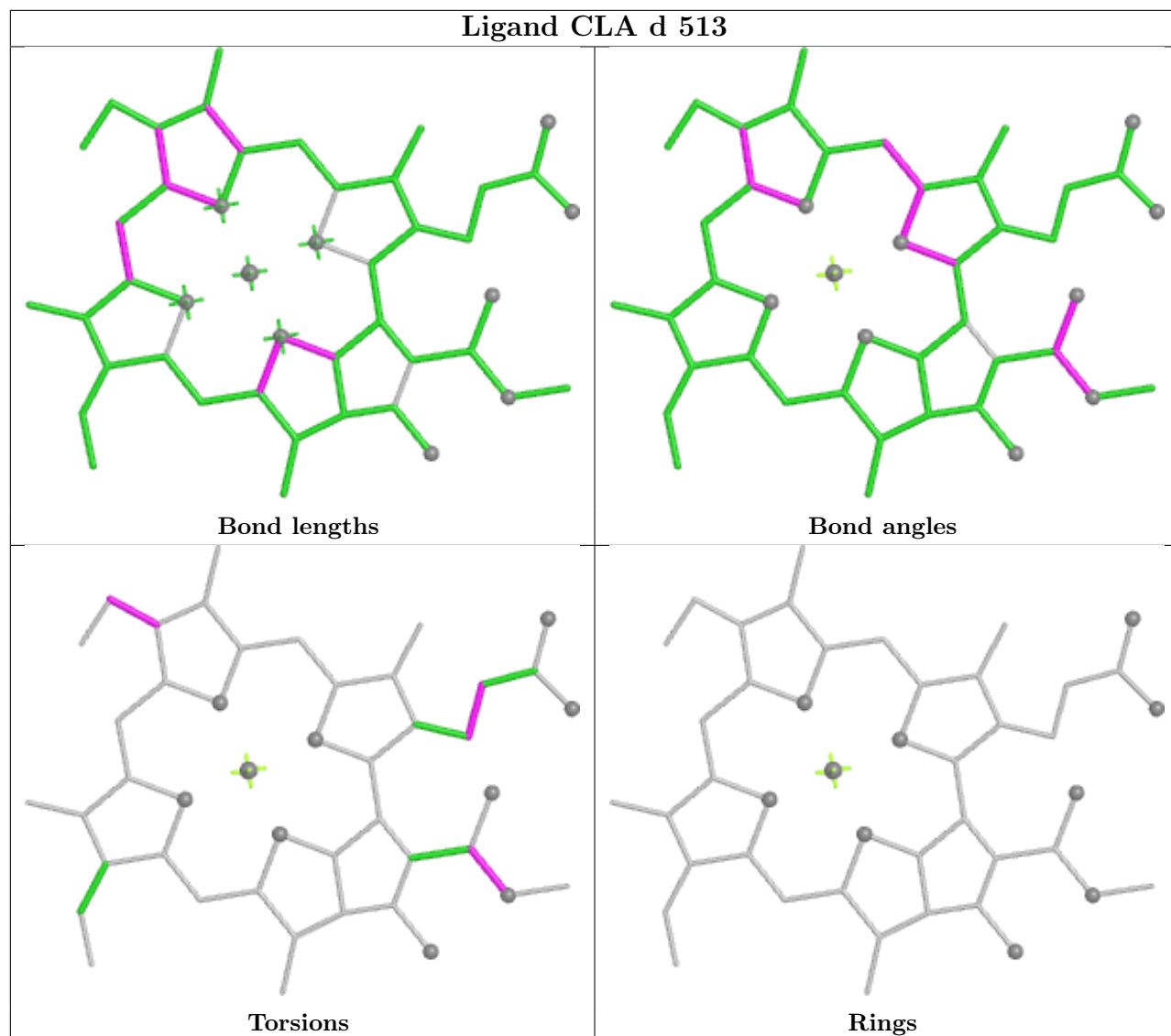


Ligand CLA c 507

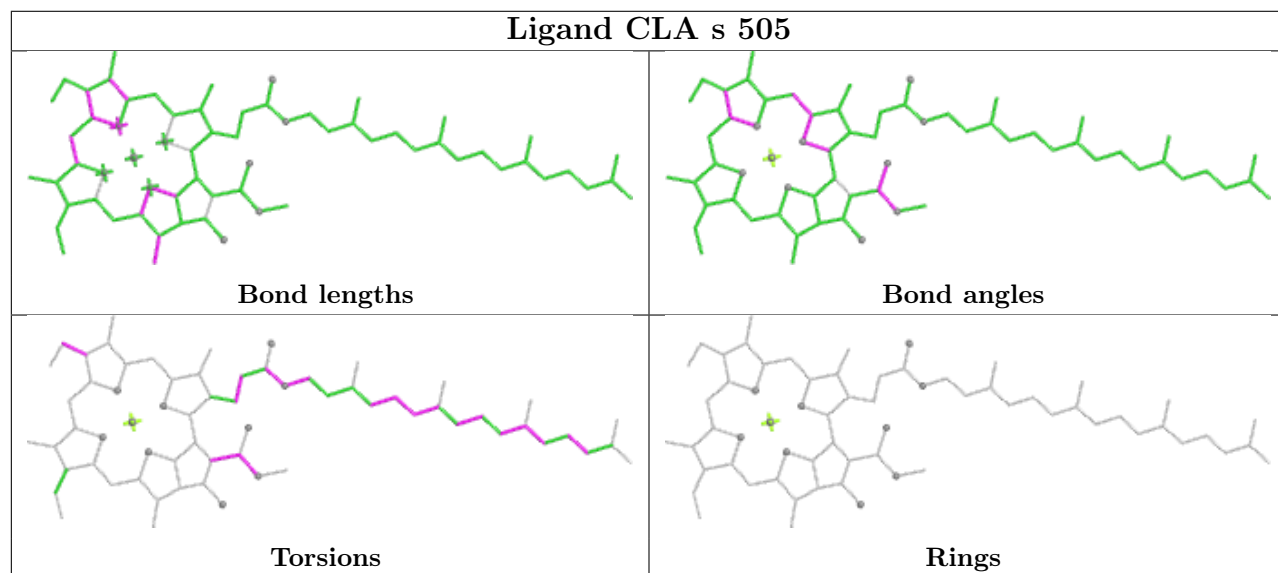




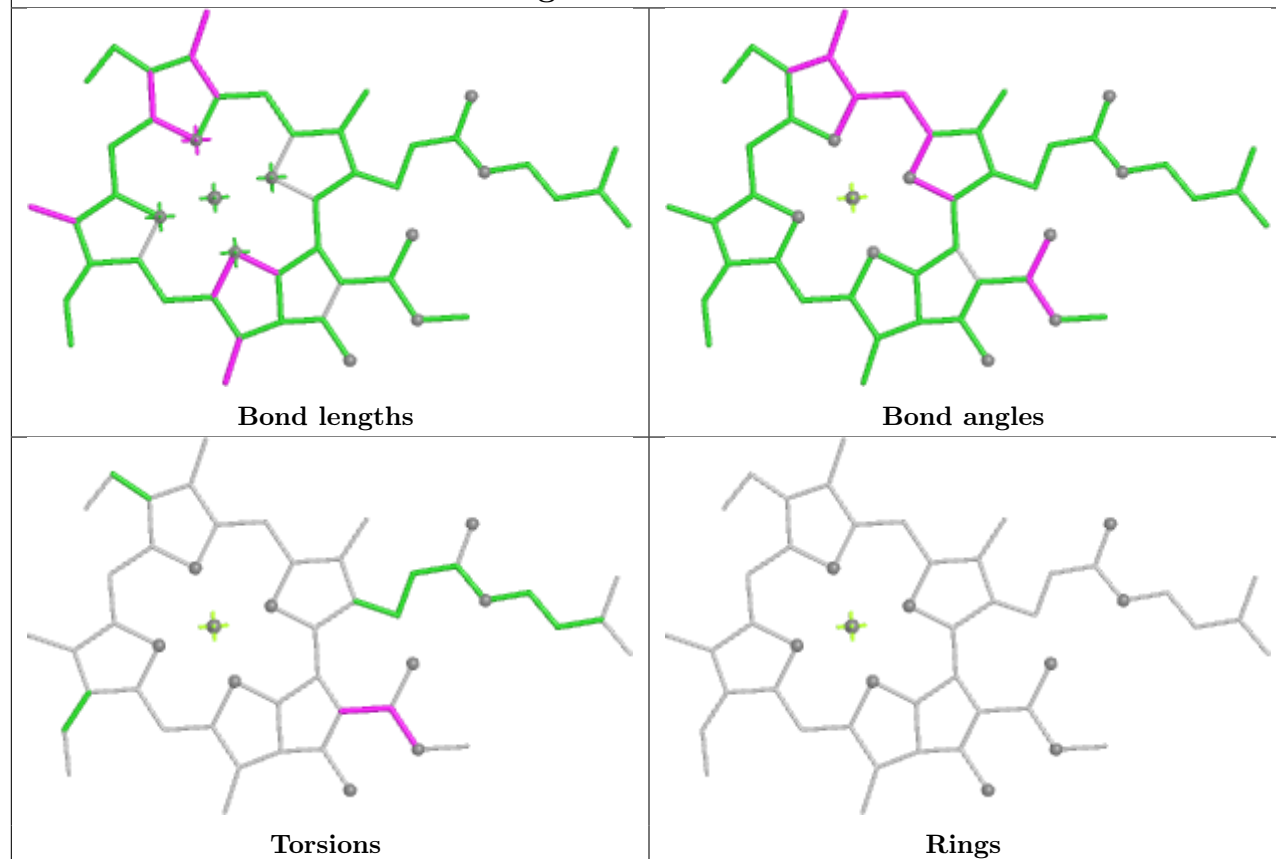
Ligand CLA d 513



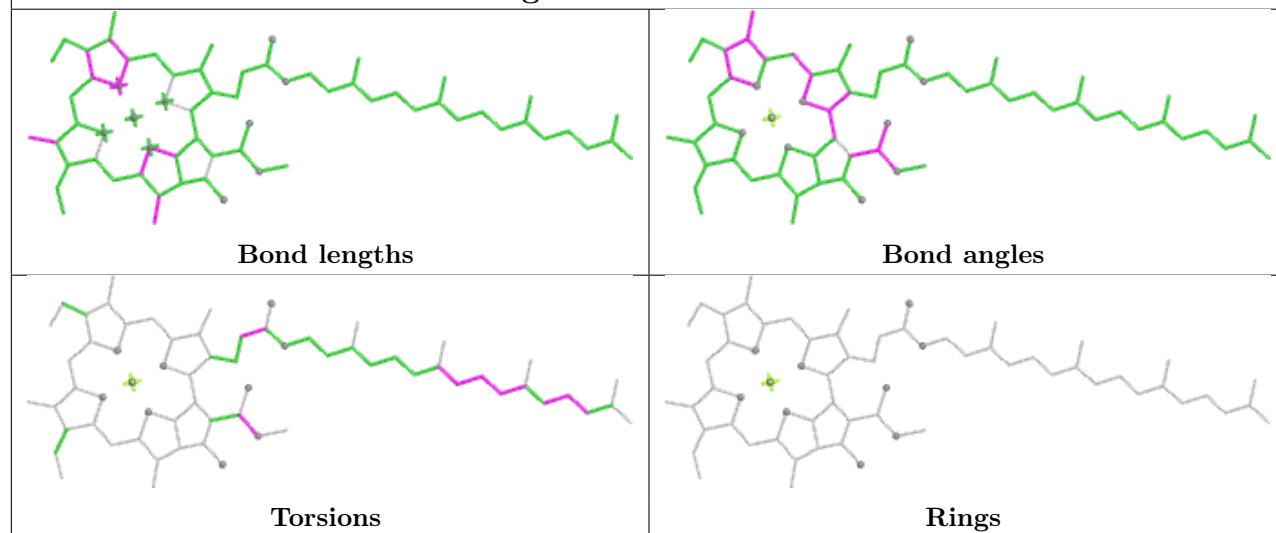
Ligand CLA s 505



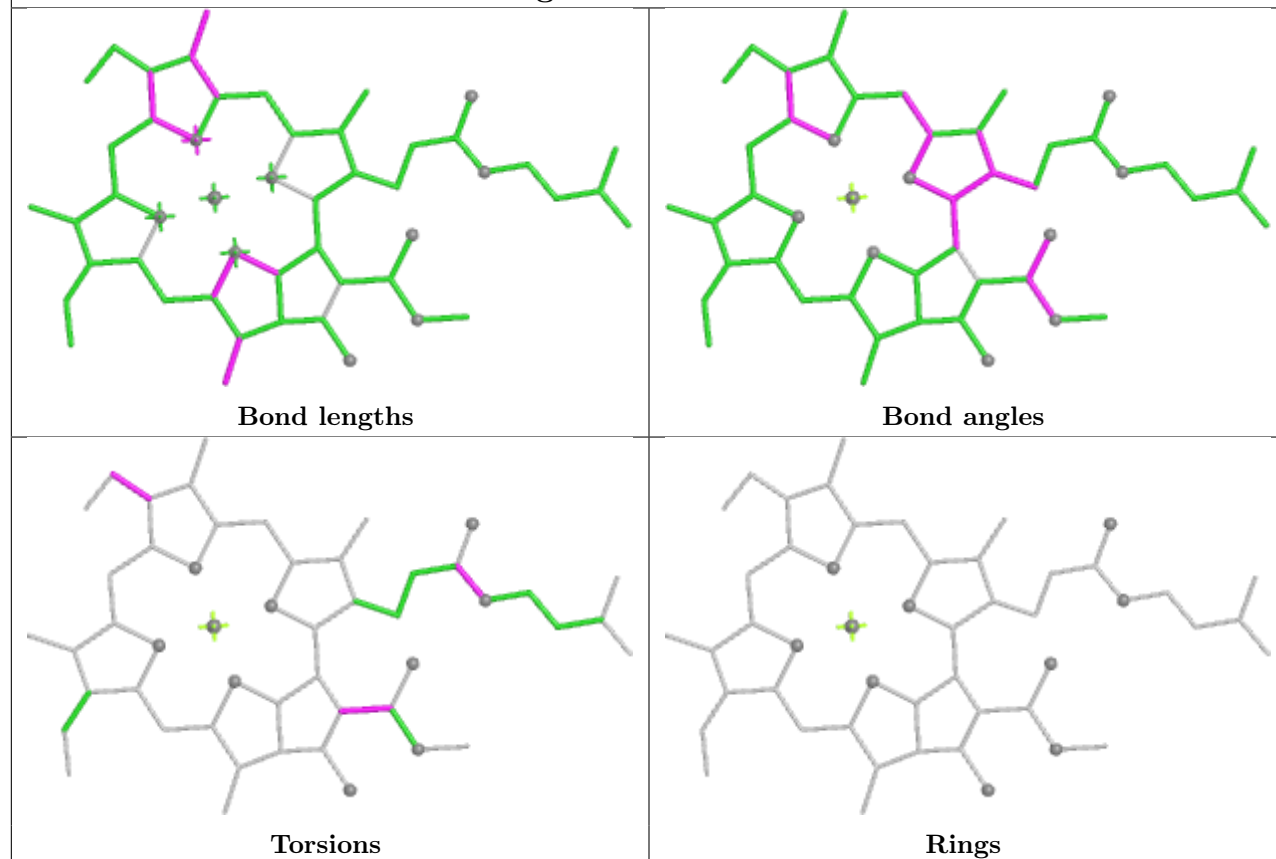
Ligand CLA s 506



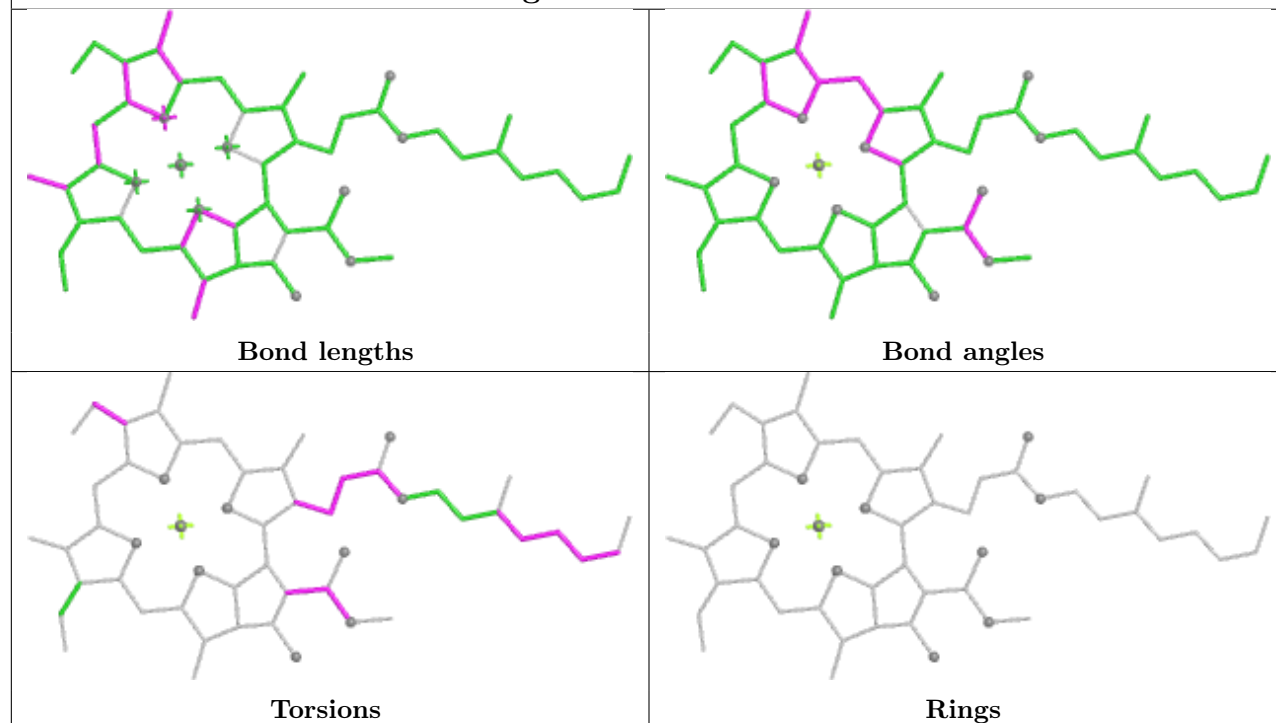
Ligand CLA G 1123

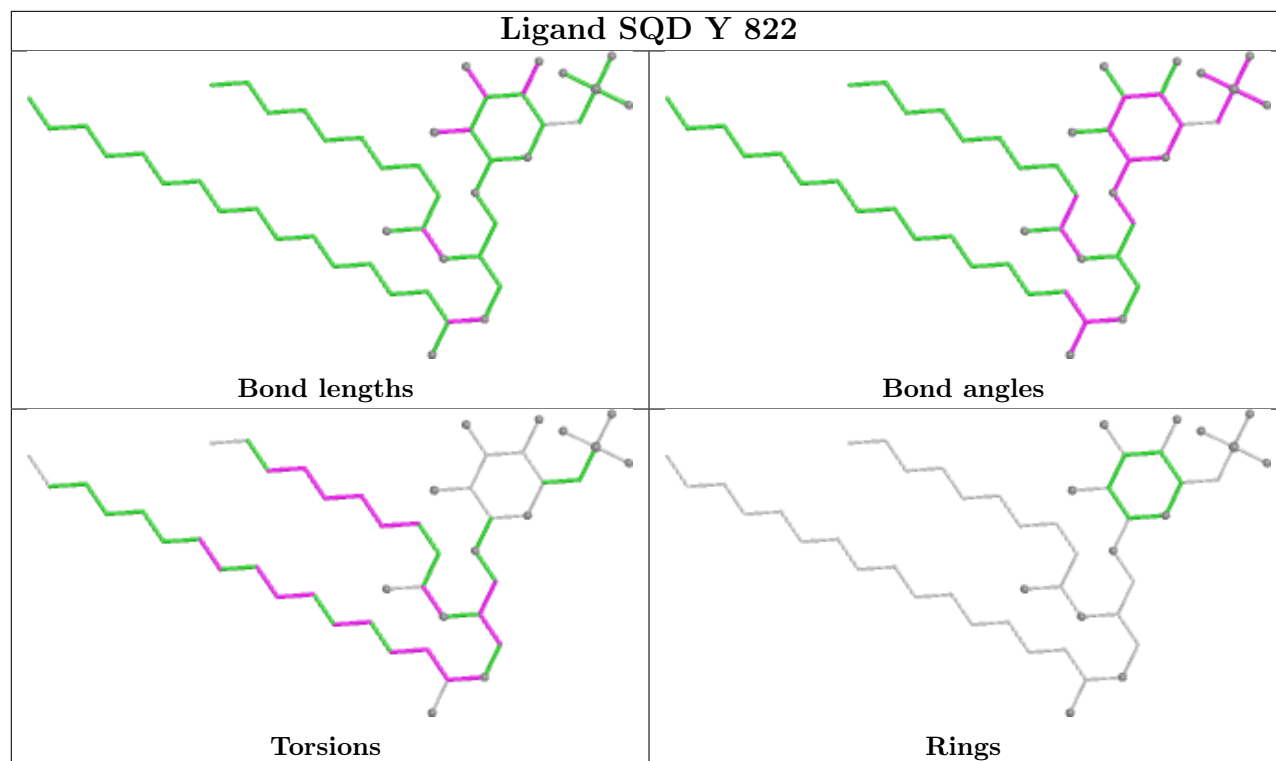
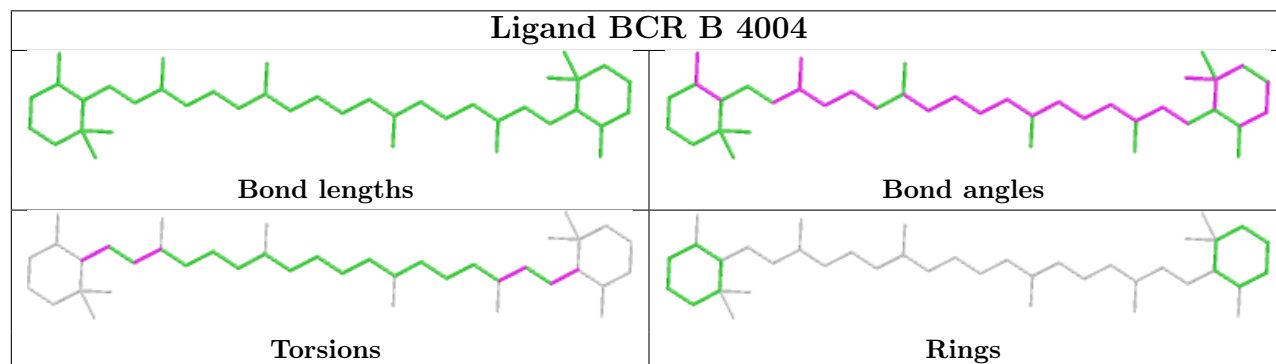
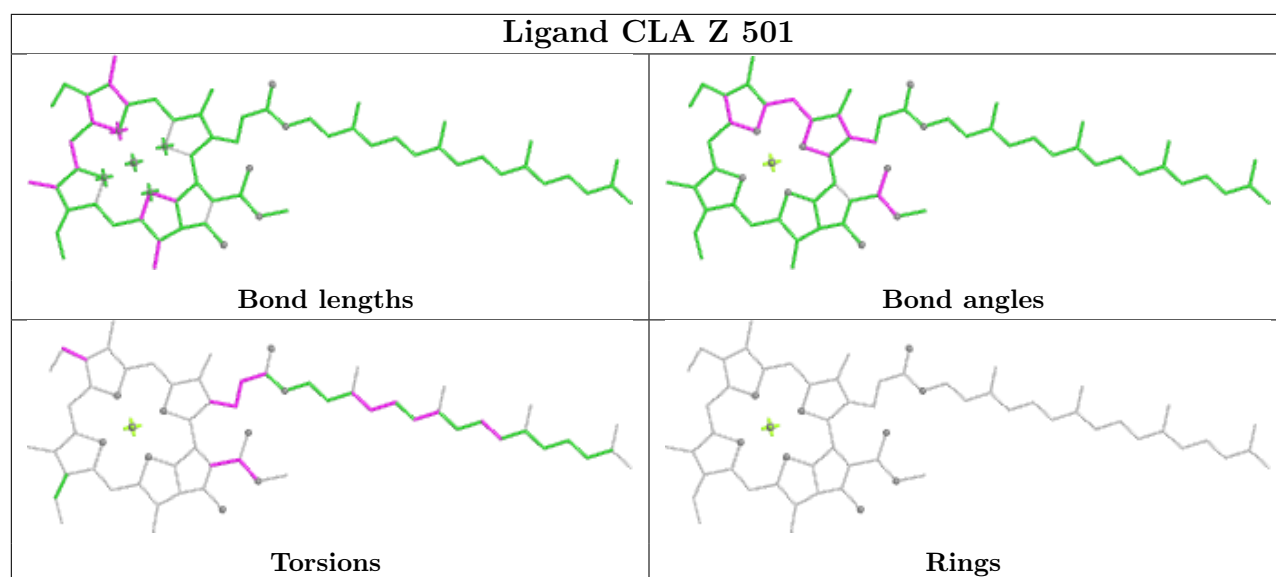


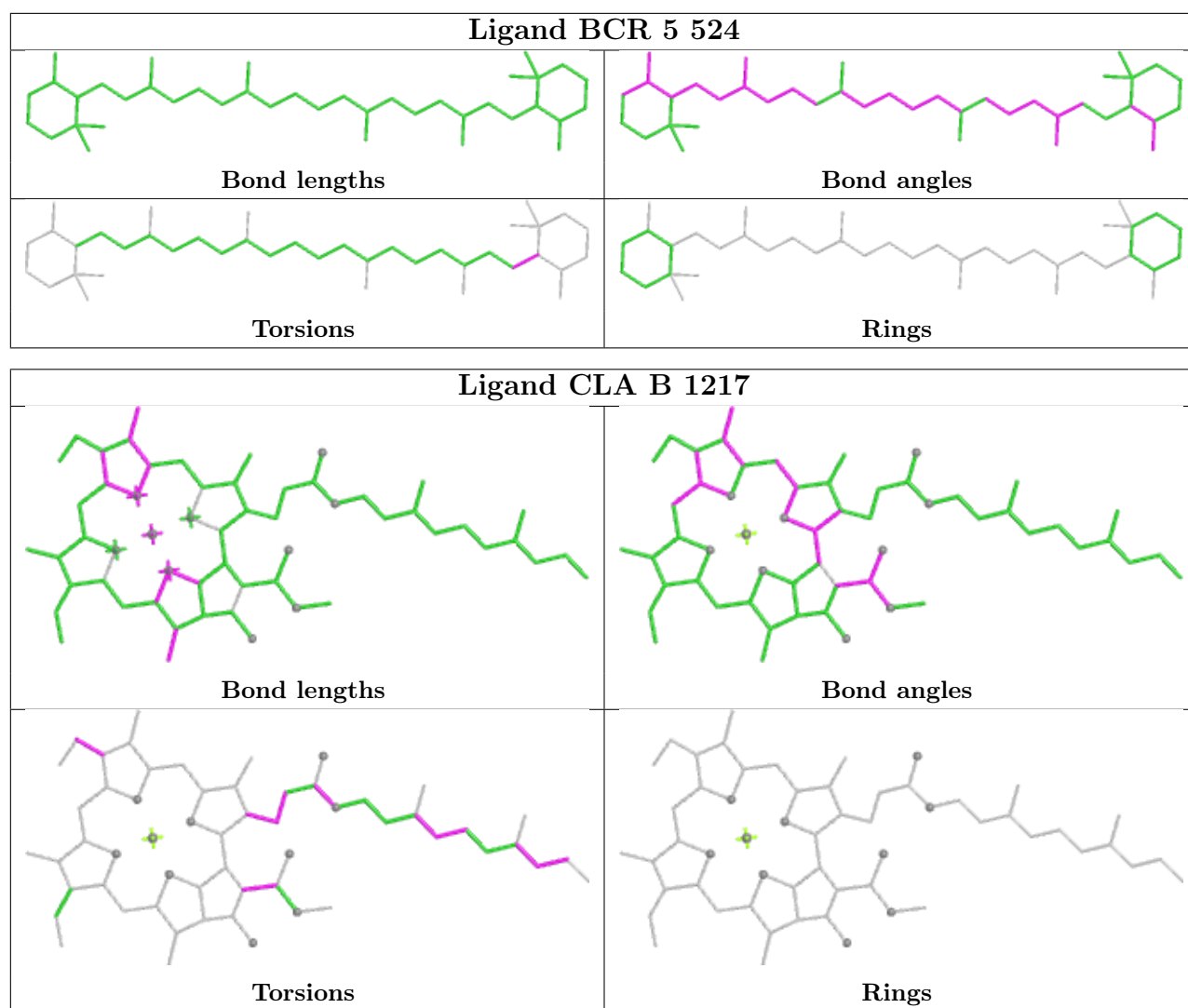
Ligand CLA 3 502

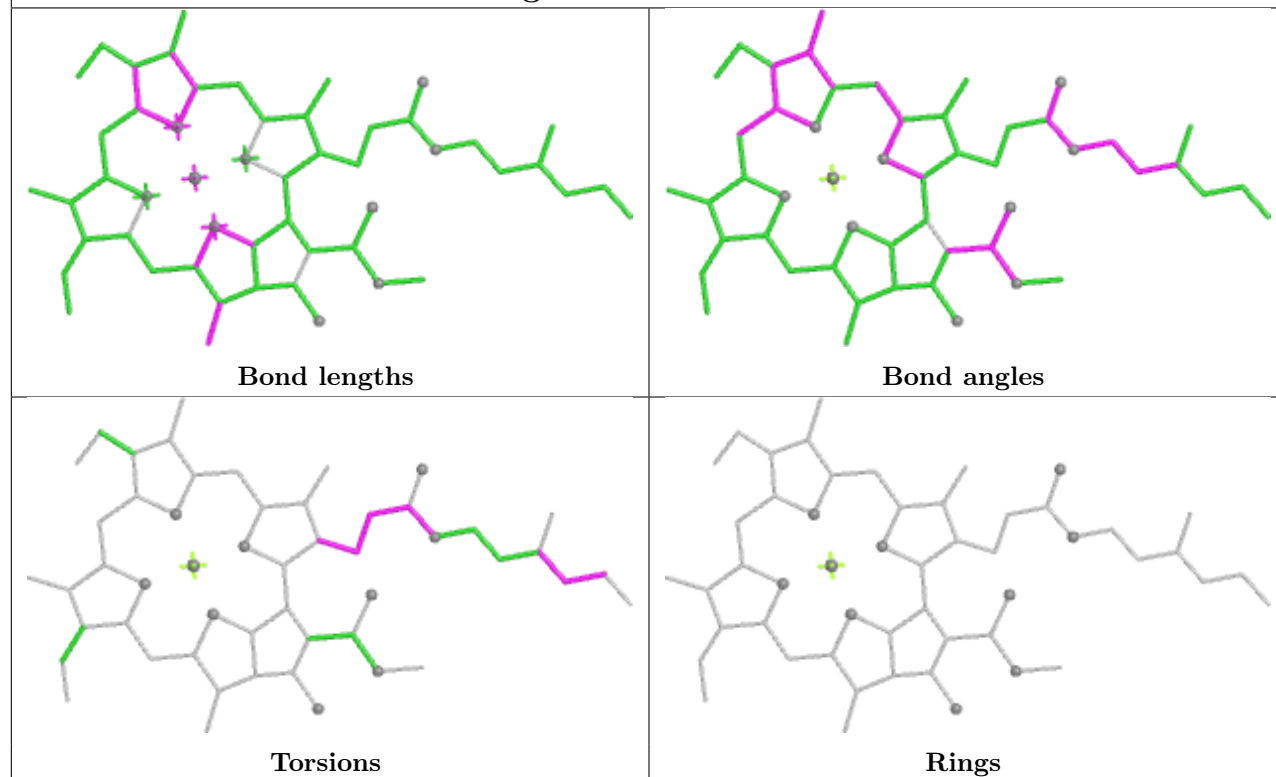
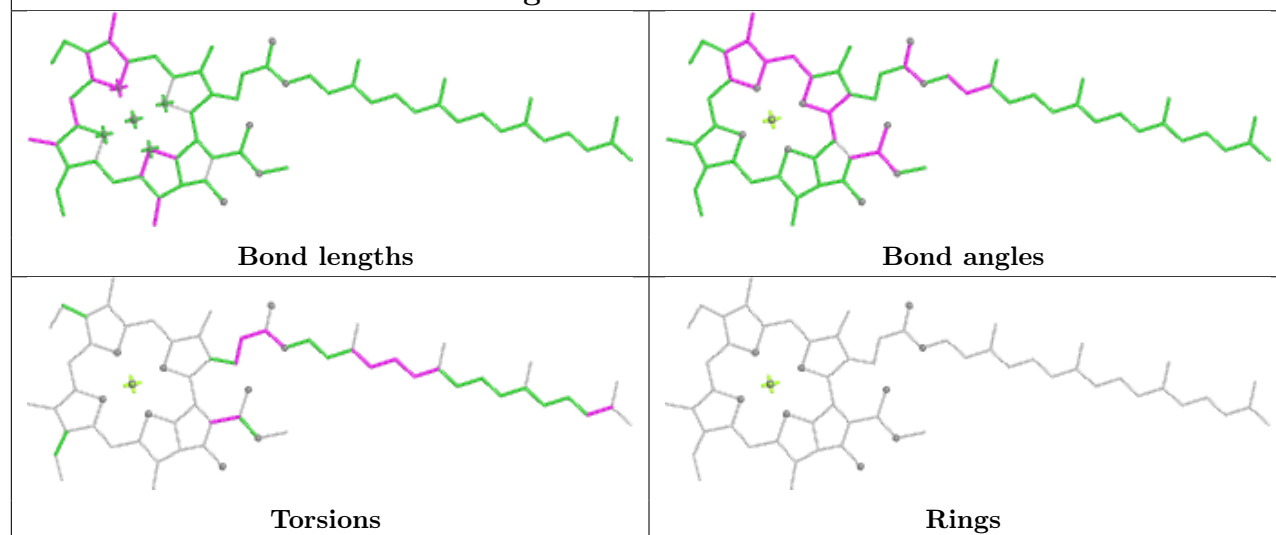


Ligand CLA A 1108

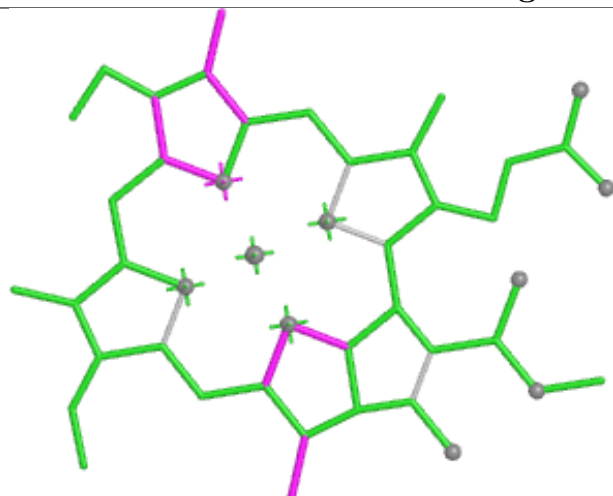




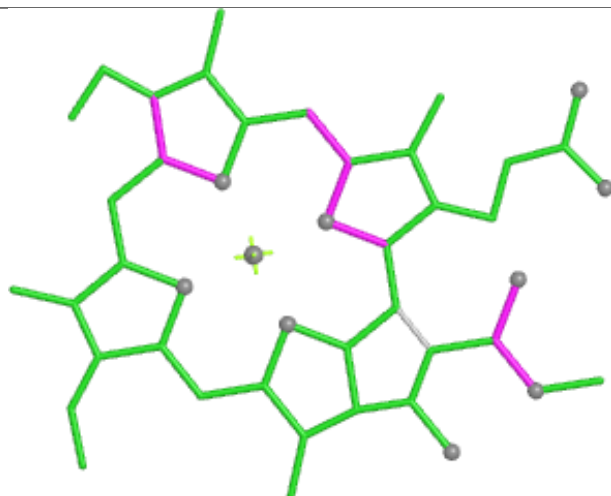


Ligand CLA A 1135**Ligand CLA B 1213**

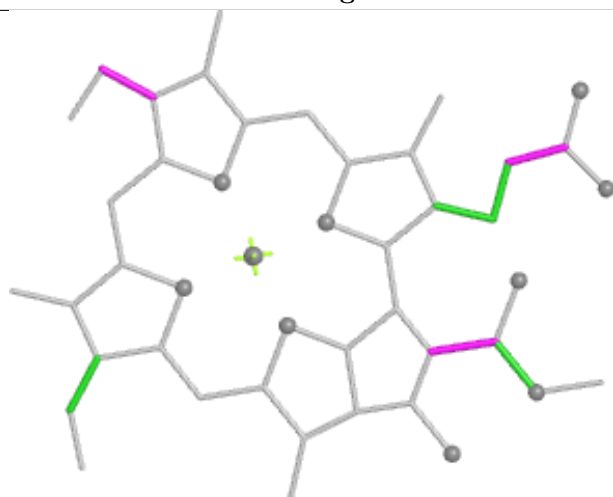
Ligand CLA 4 512



Bond lengths



Bond angles

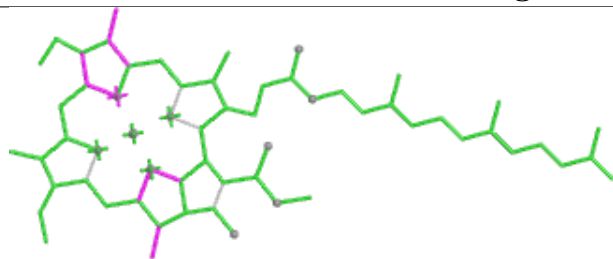


Torsions

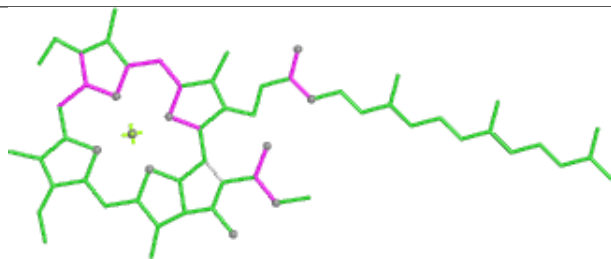


Rings

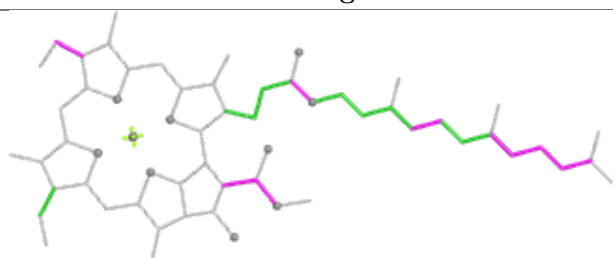
Ligand CLA Y 502



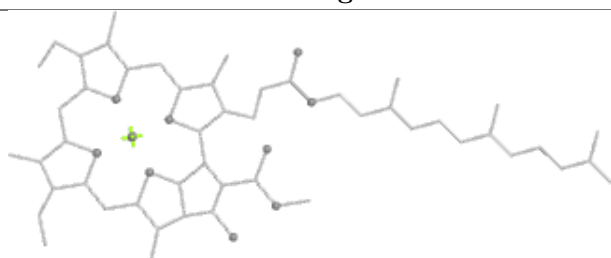
Bond lengths



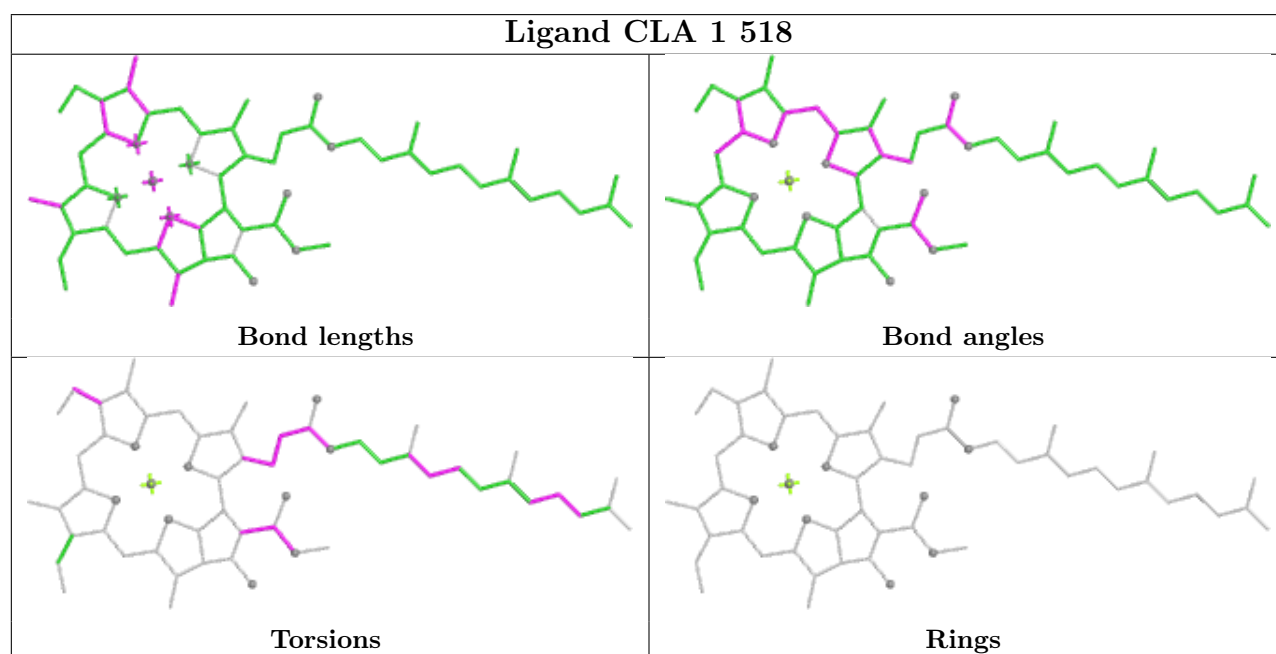
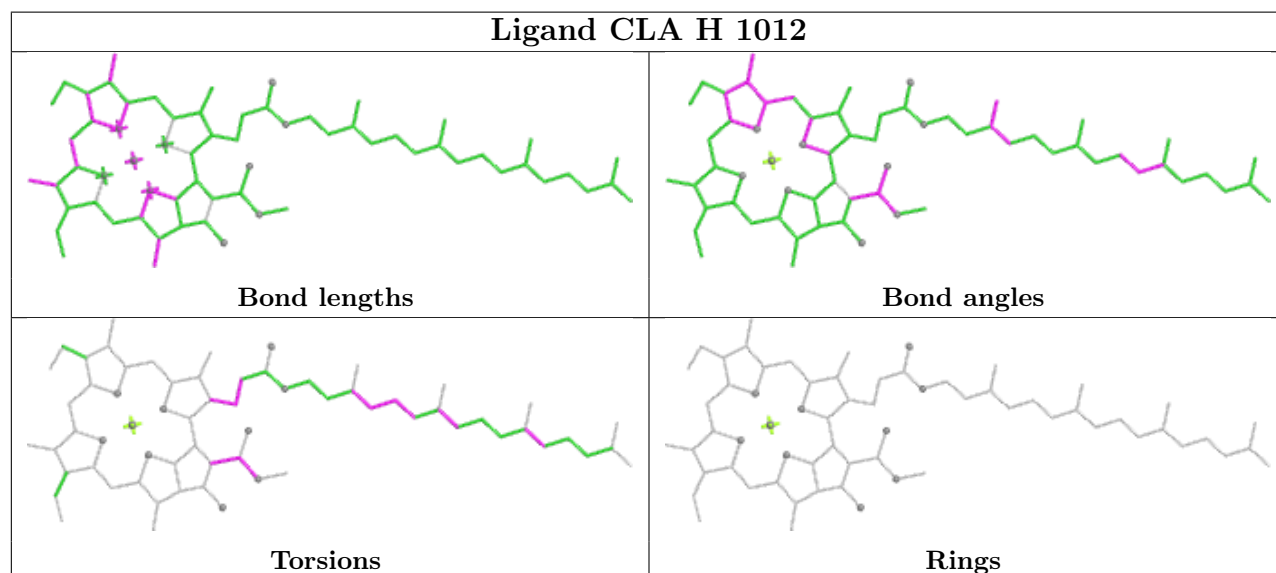
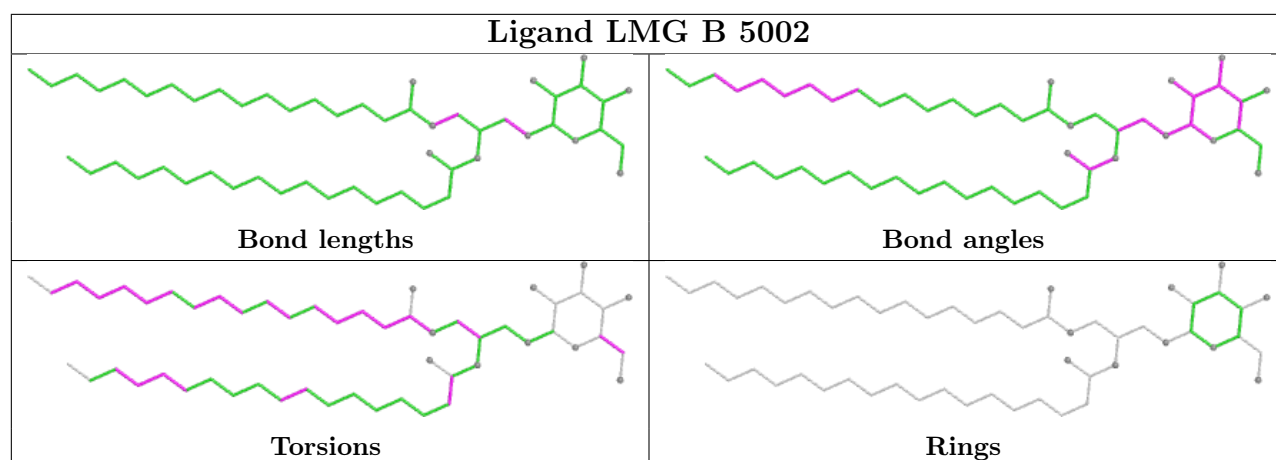
Bond angles

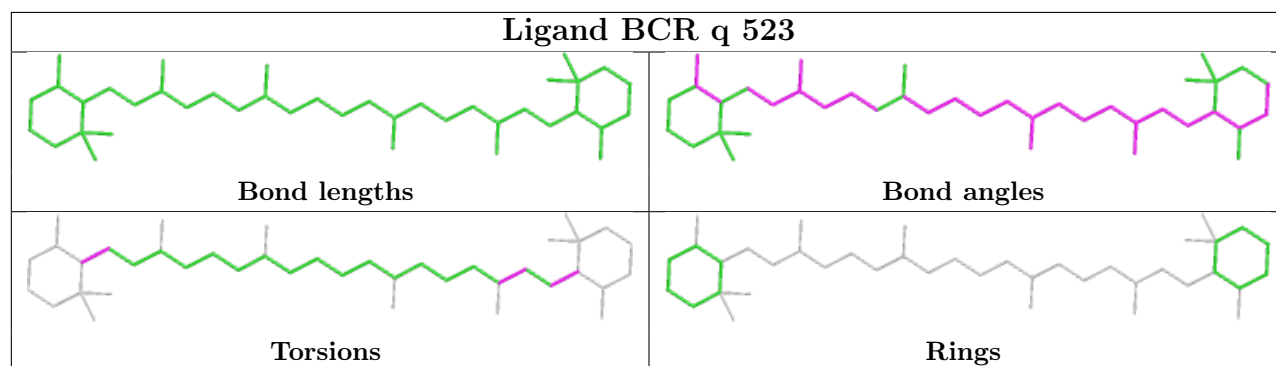
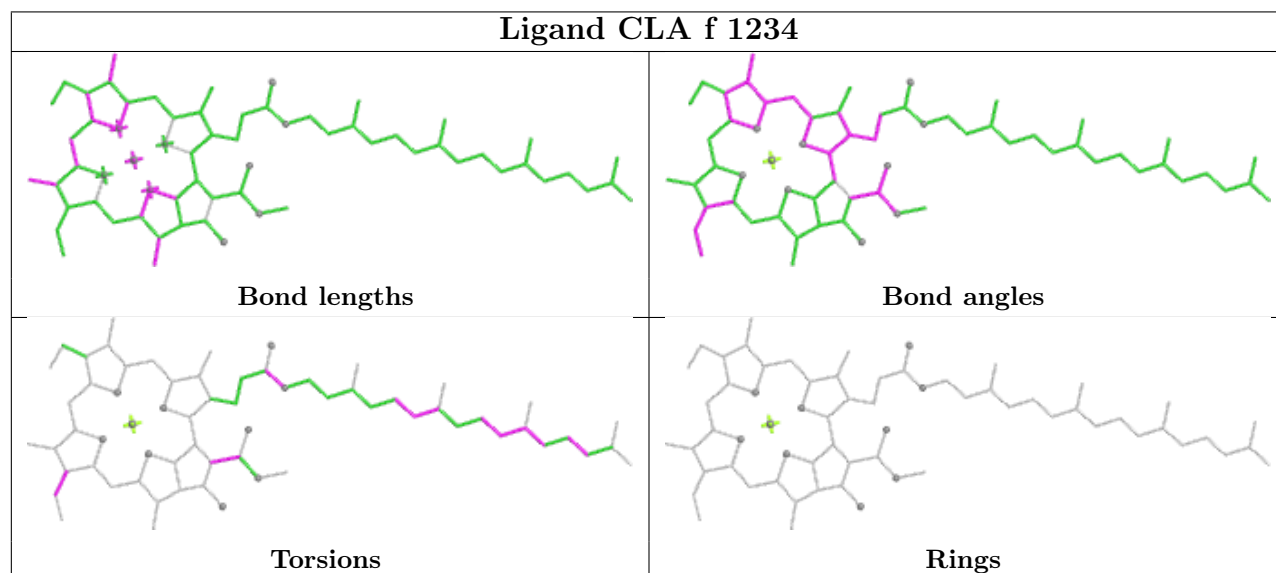
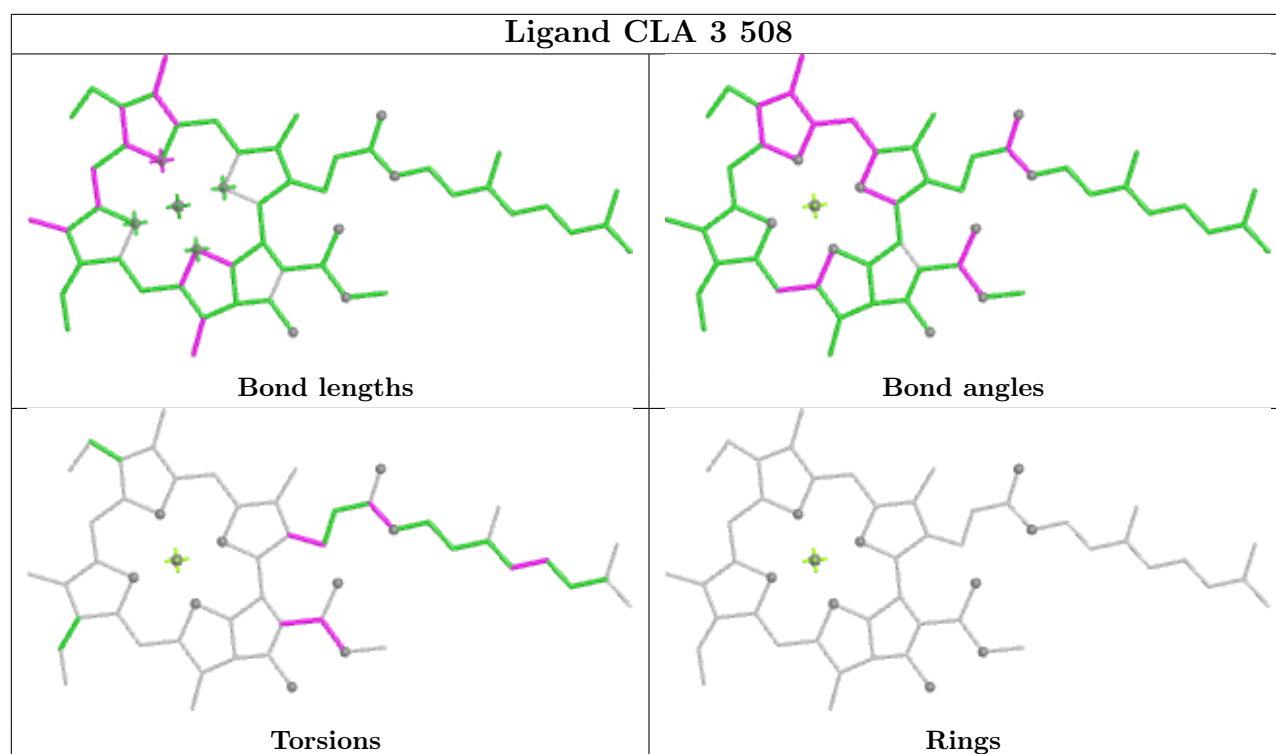


Torsions

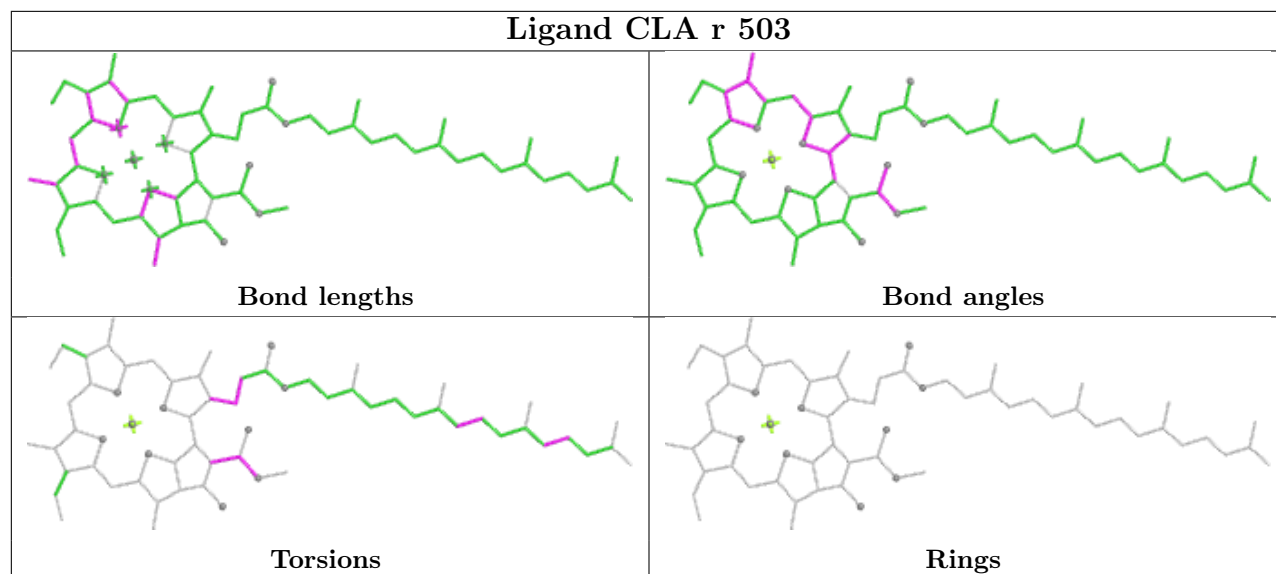


Rings

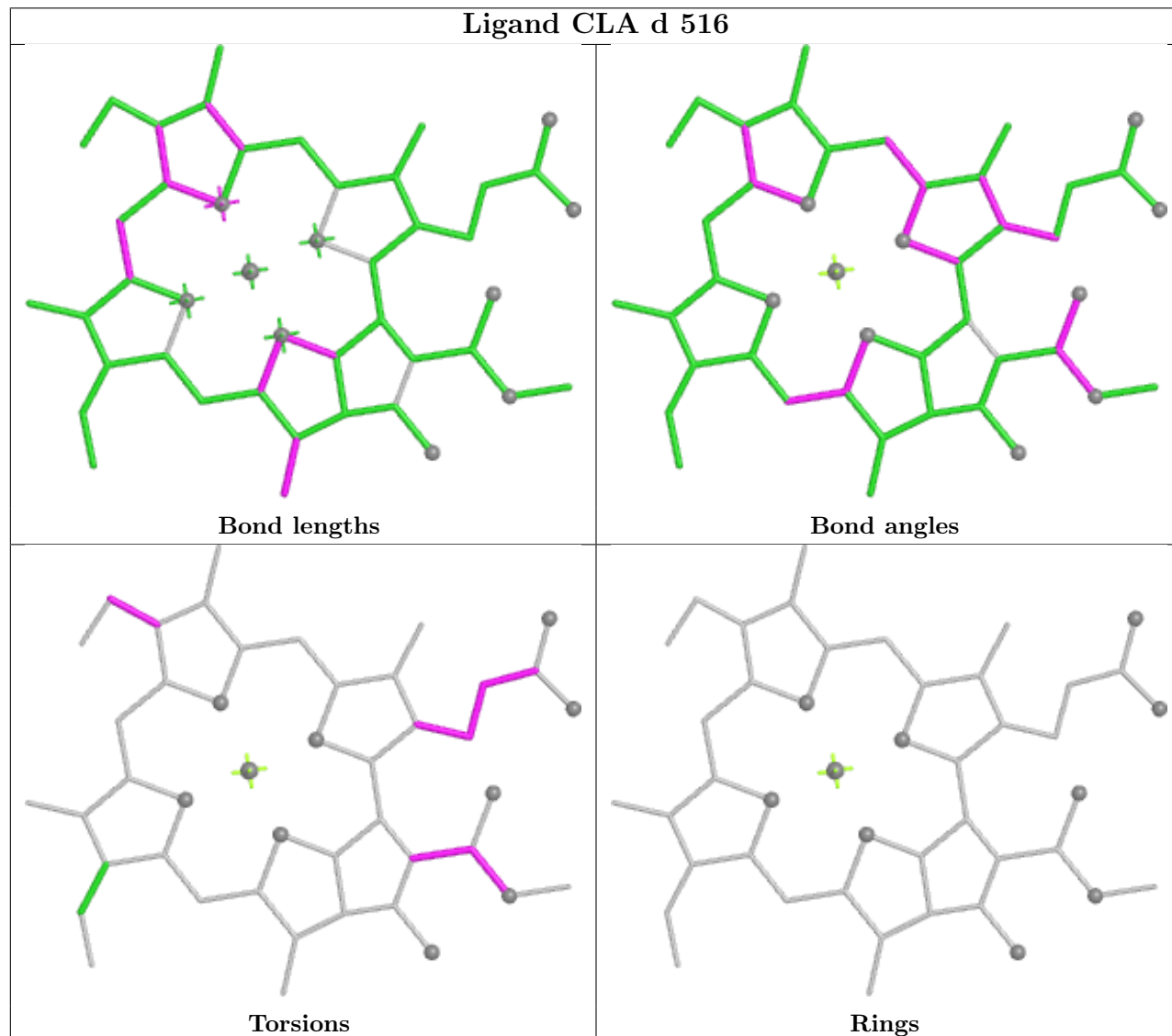


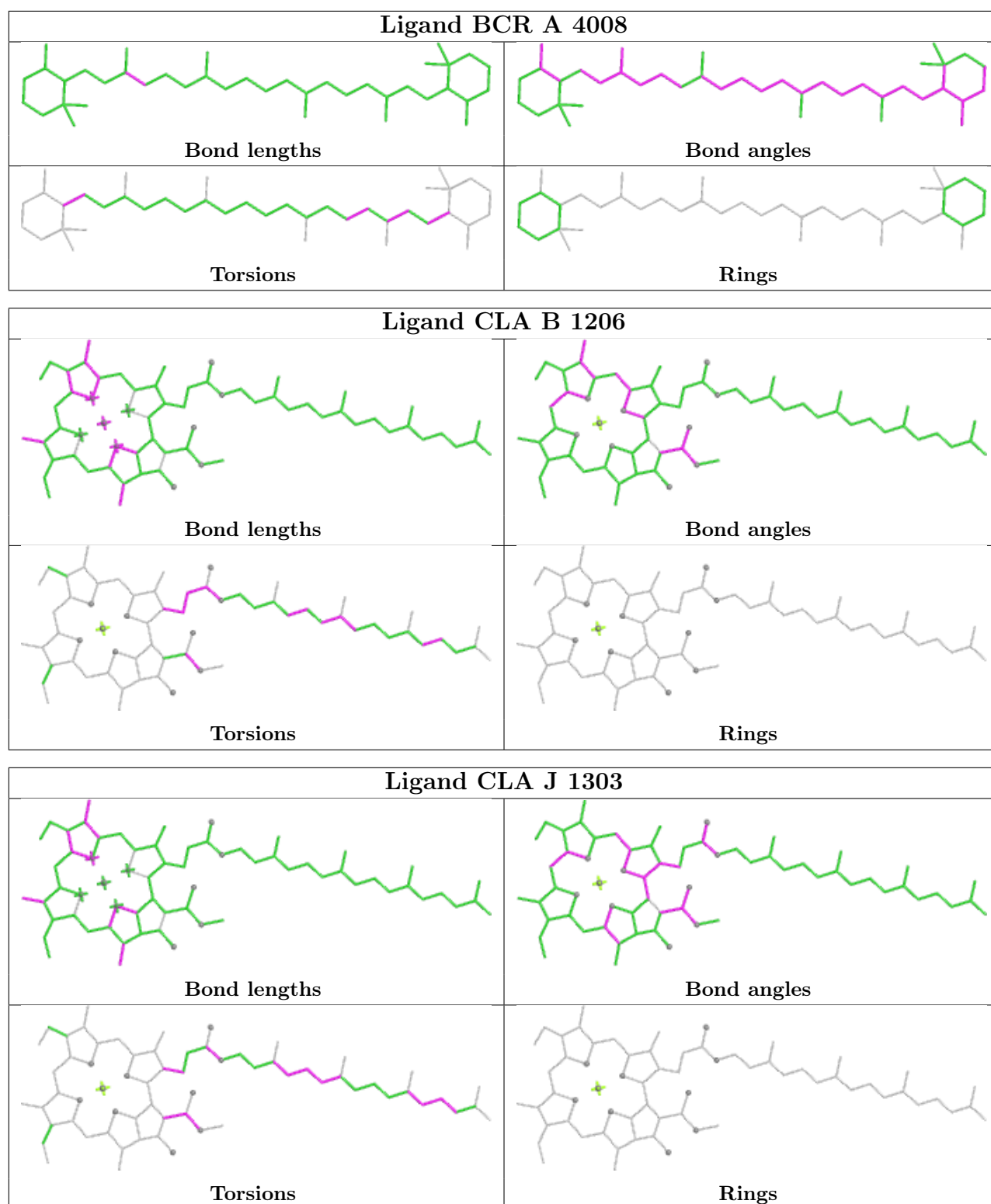


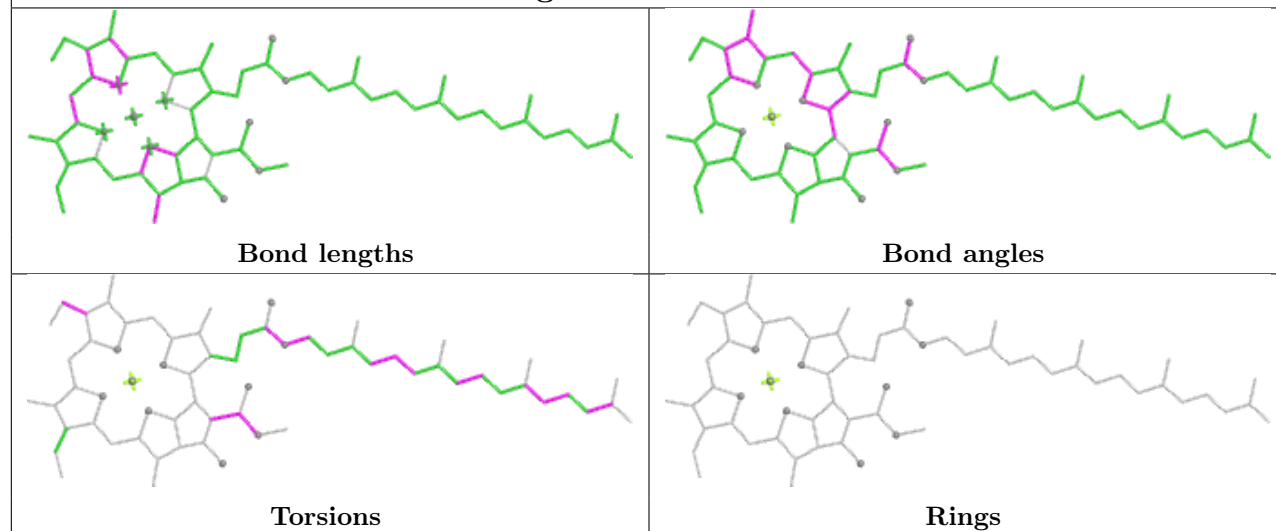
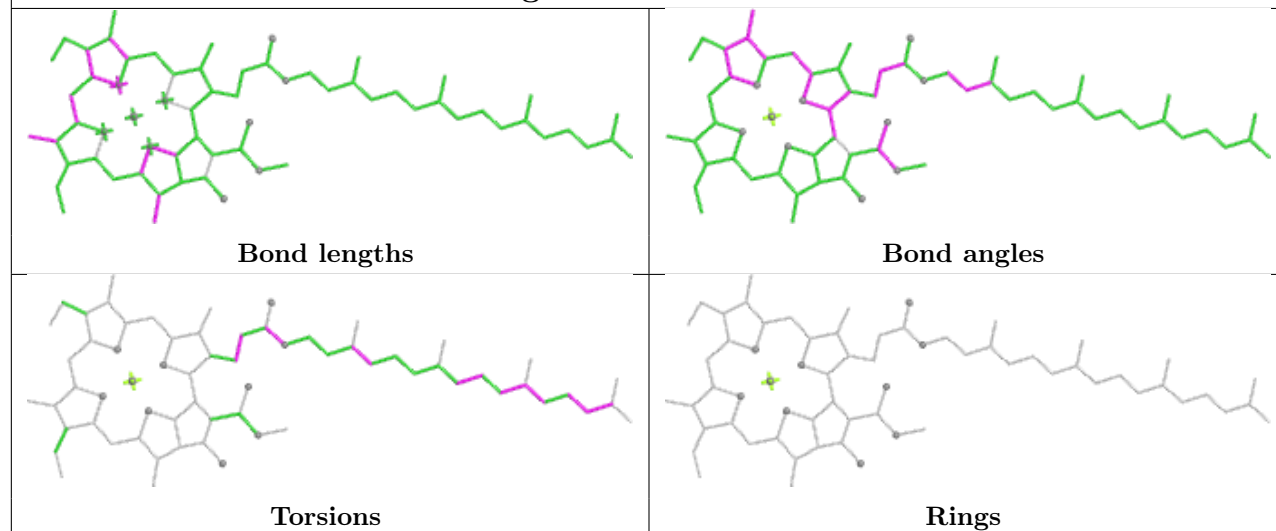
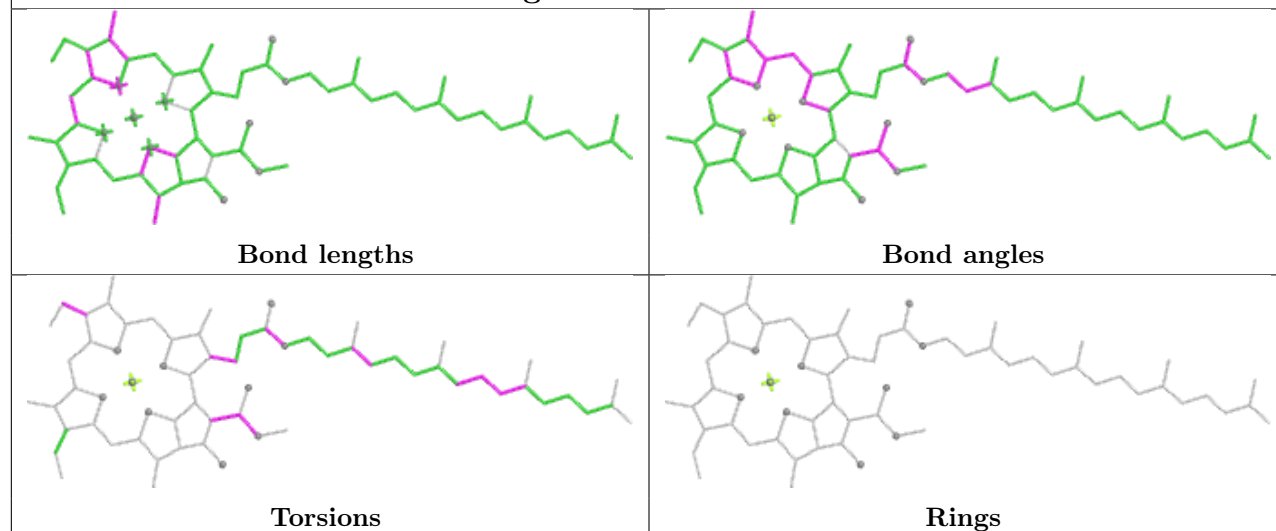
Ligand CLA r 503

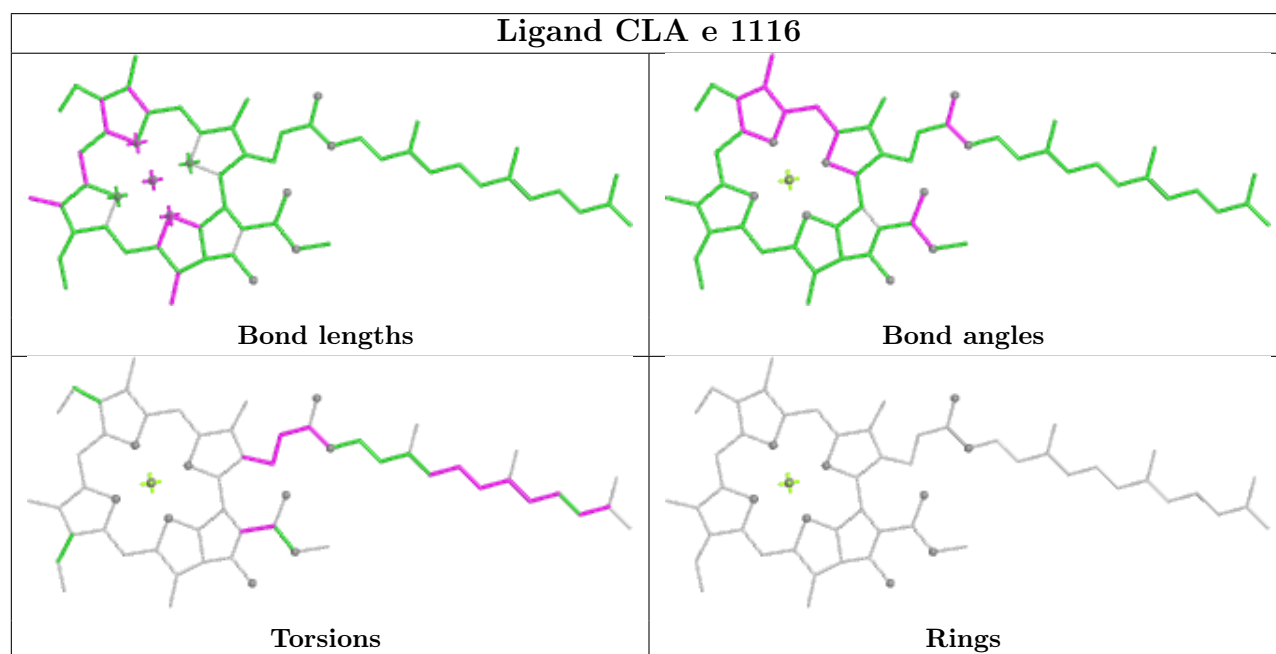
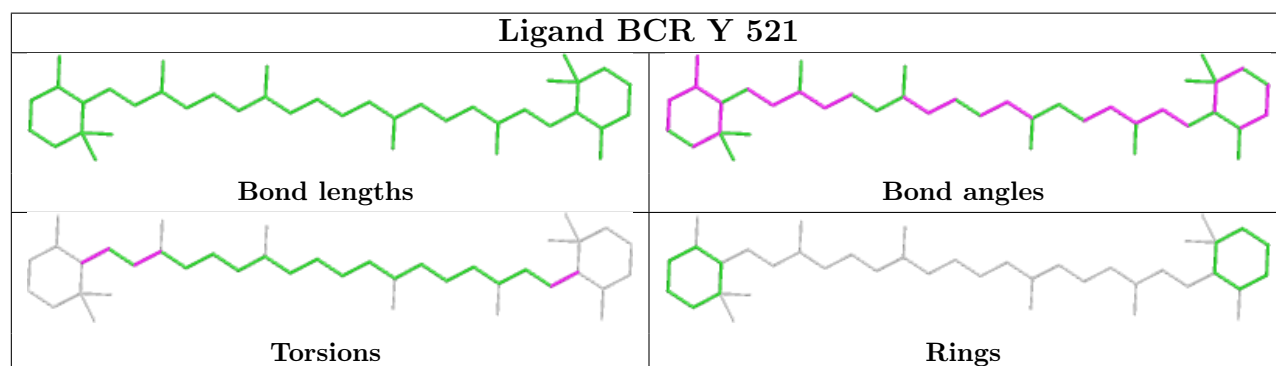
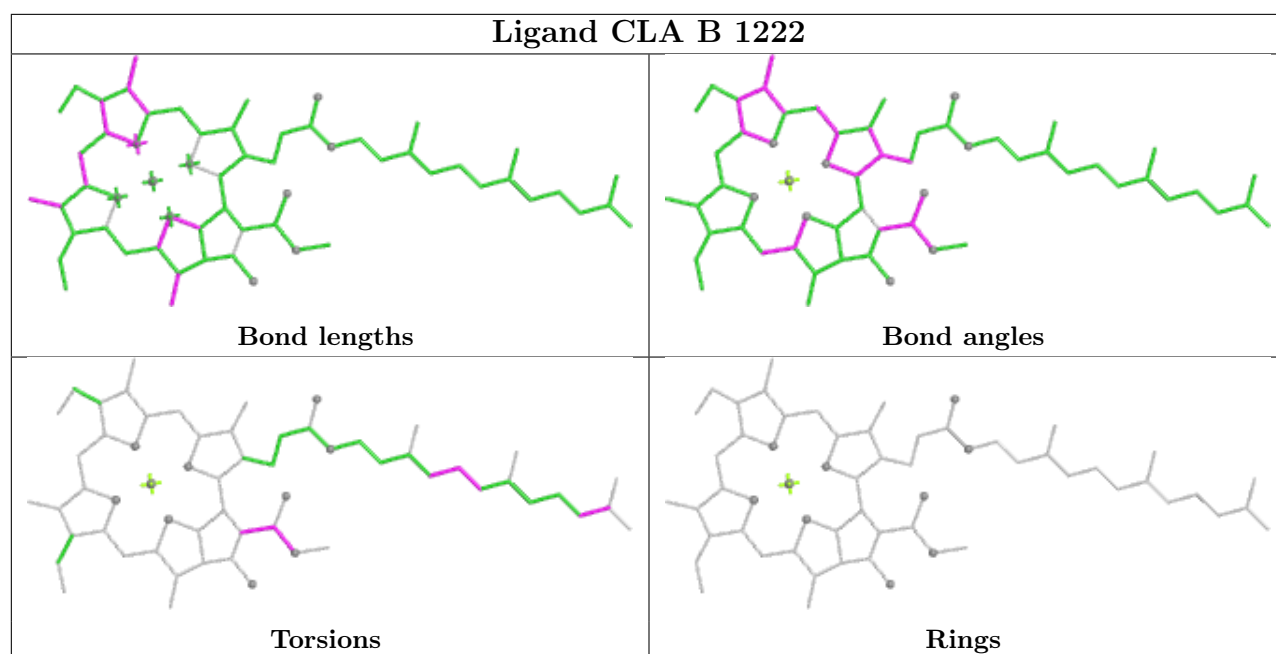


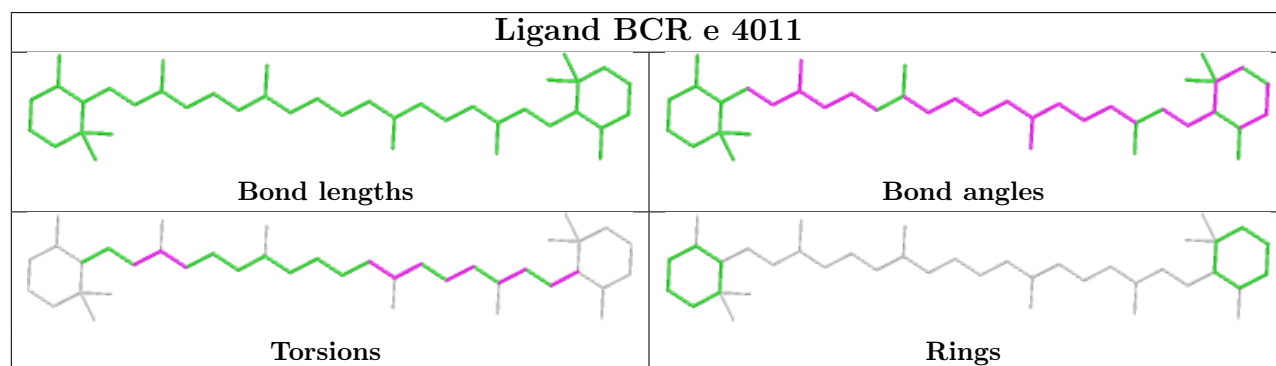
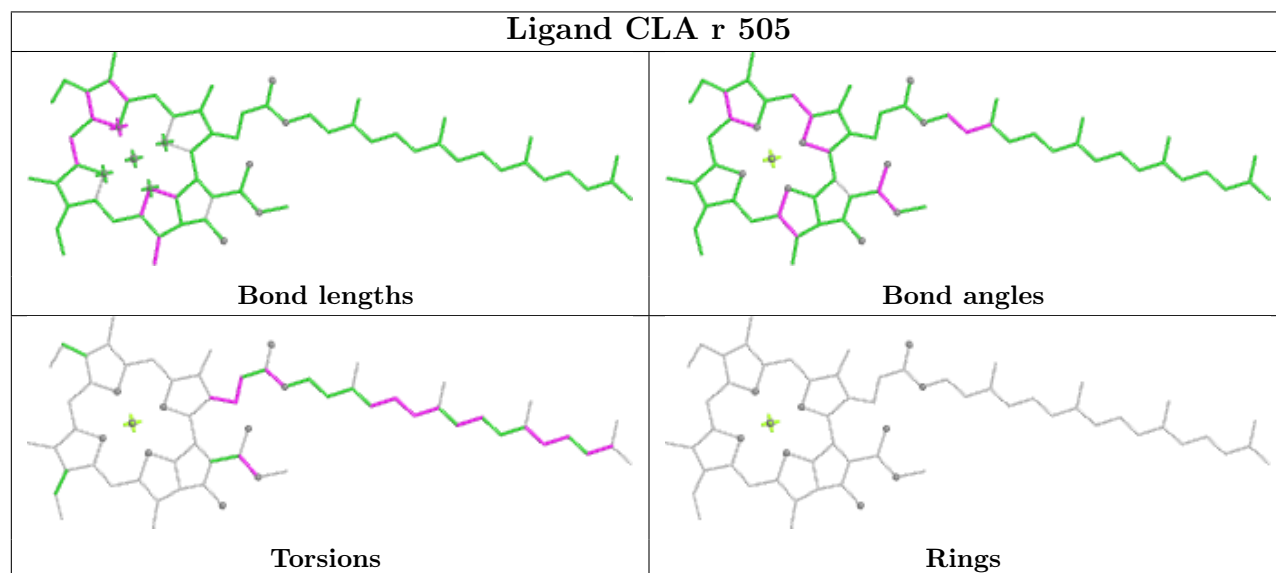
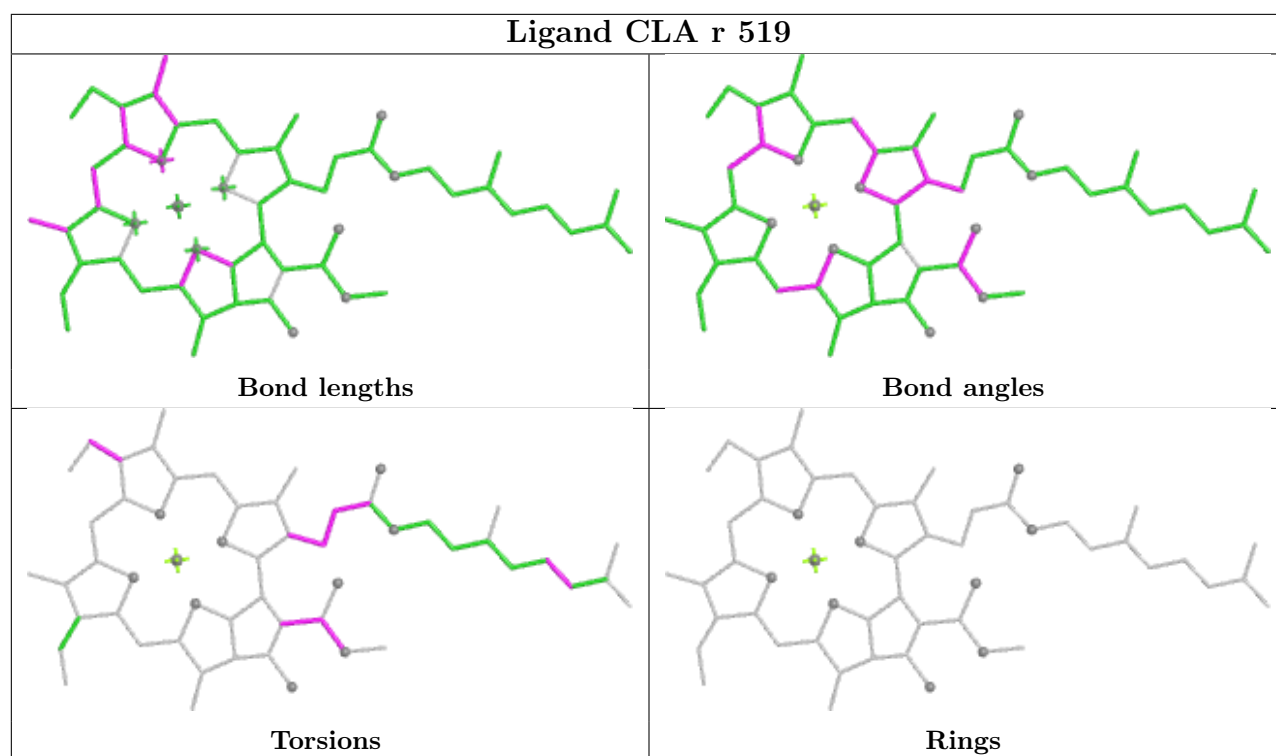
Ligand CLA d 516

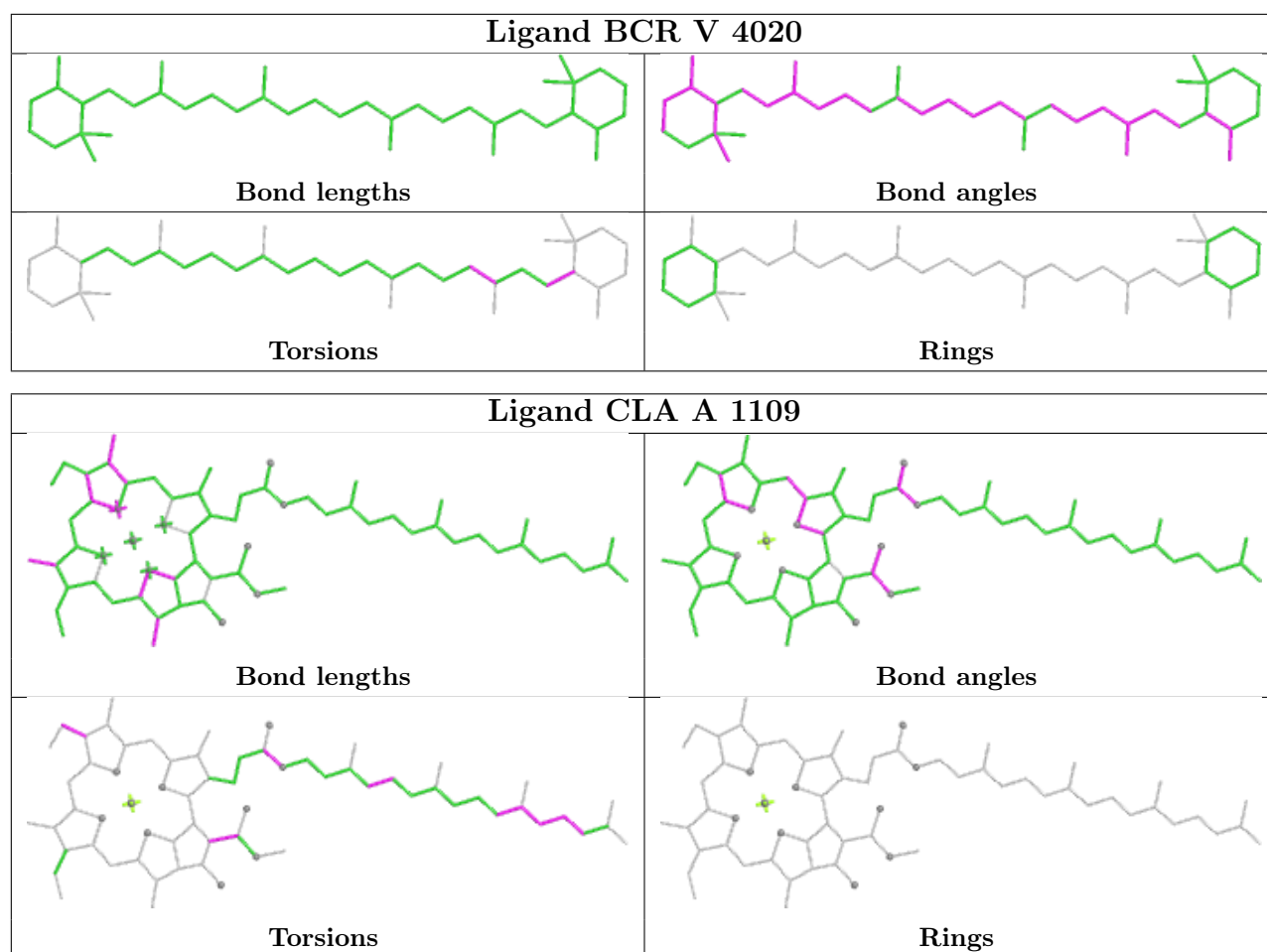




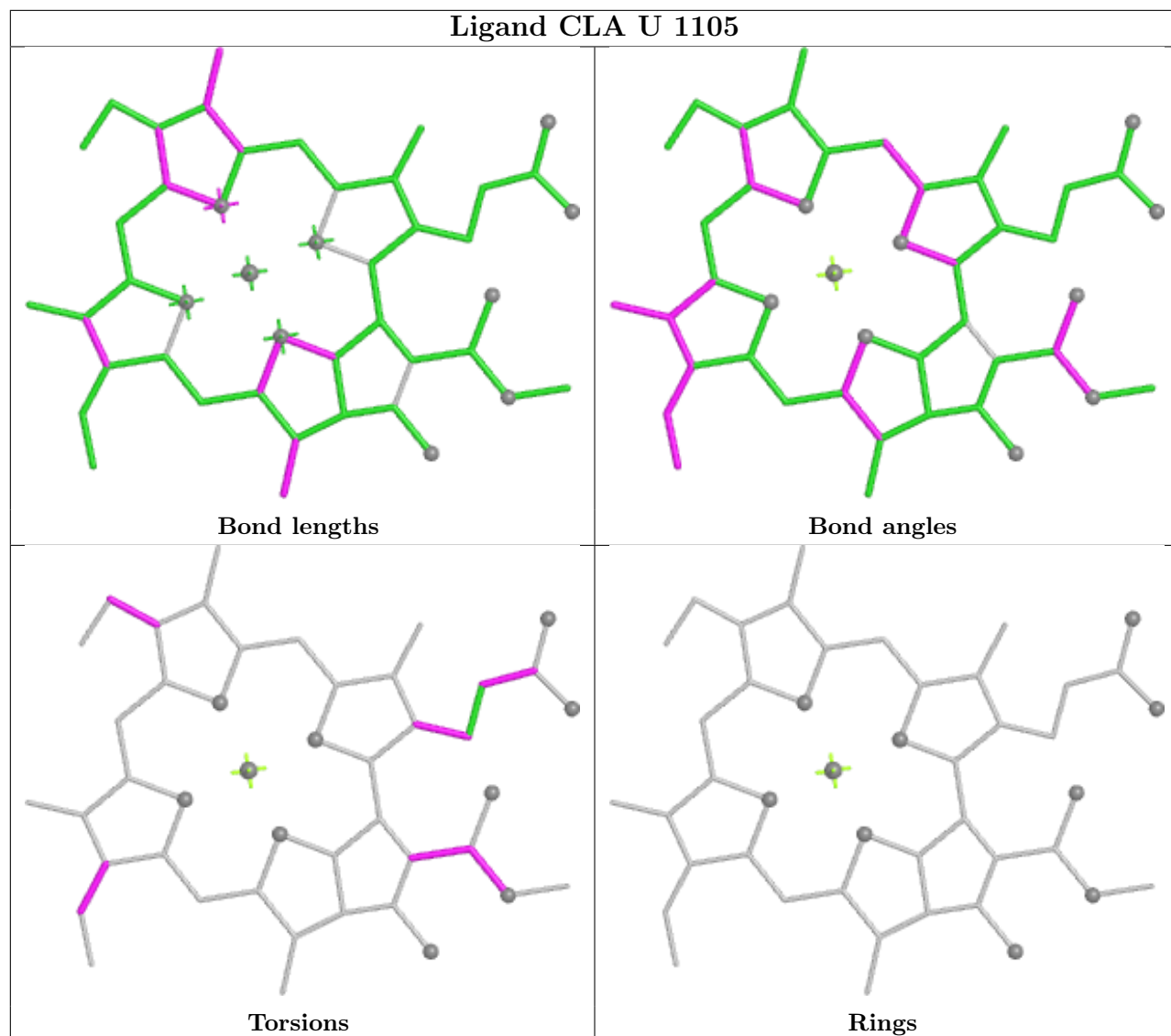
Ligand CLA a 510**Ligand CLA G 1127****Ligand CLA B 1240**



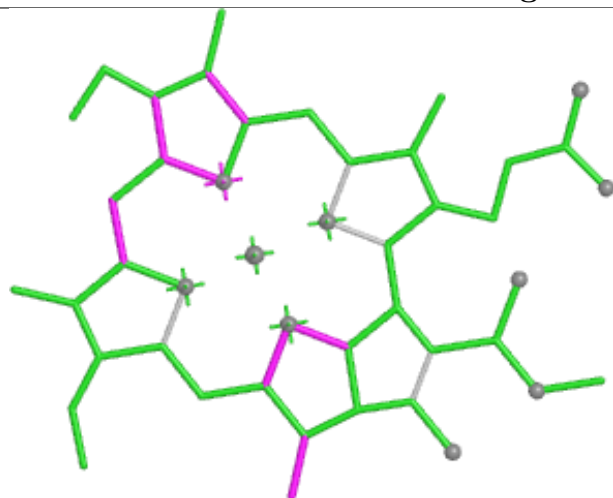




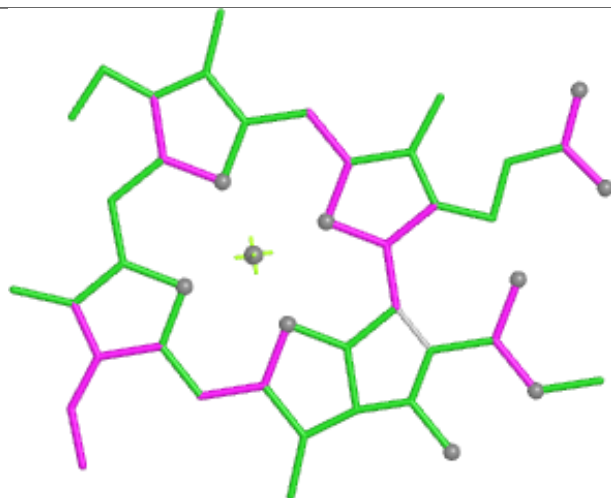
Ligand CLA U 1105



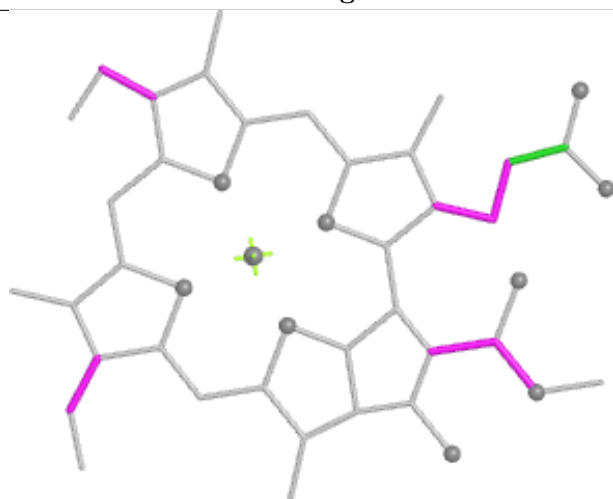
Ligand CLA s 516



Bond lengths



Bond angles

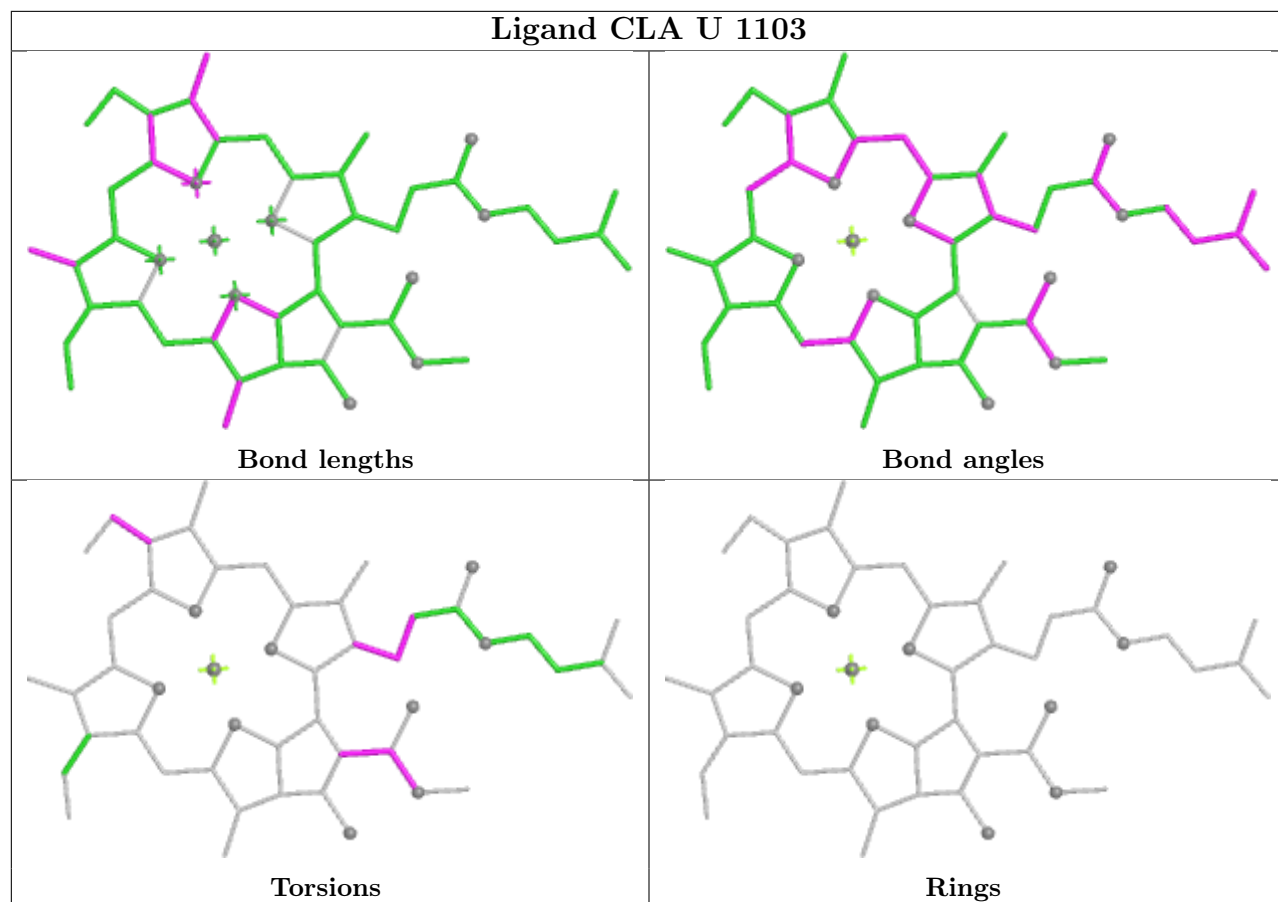


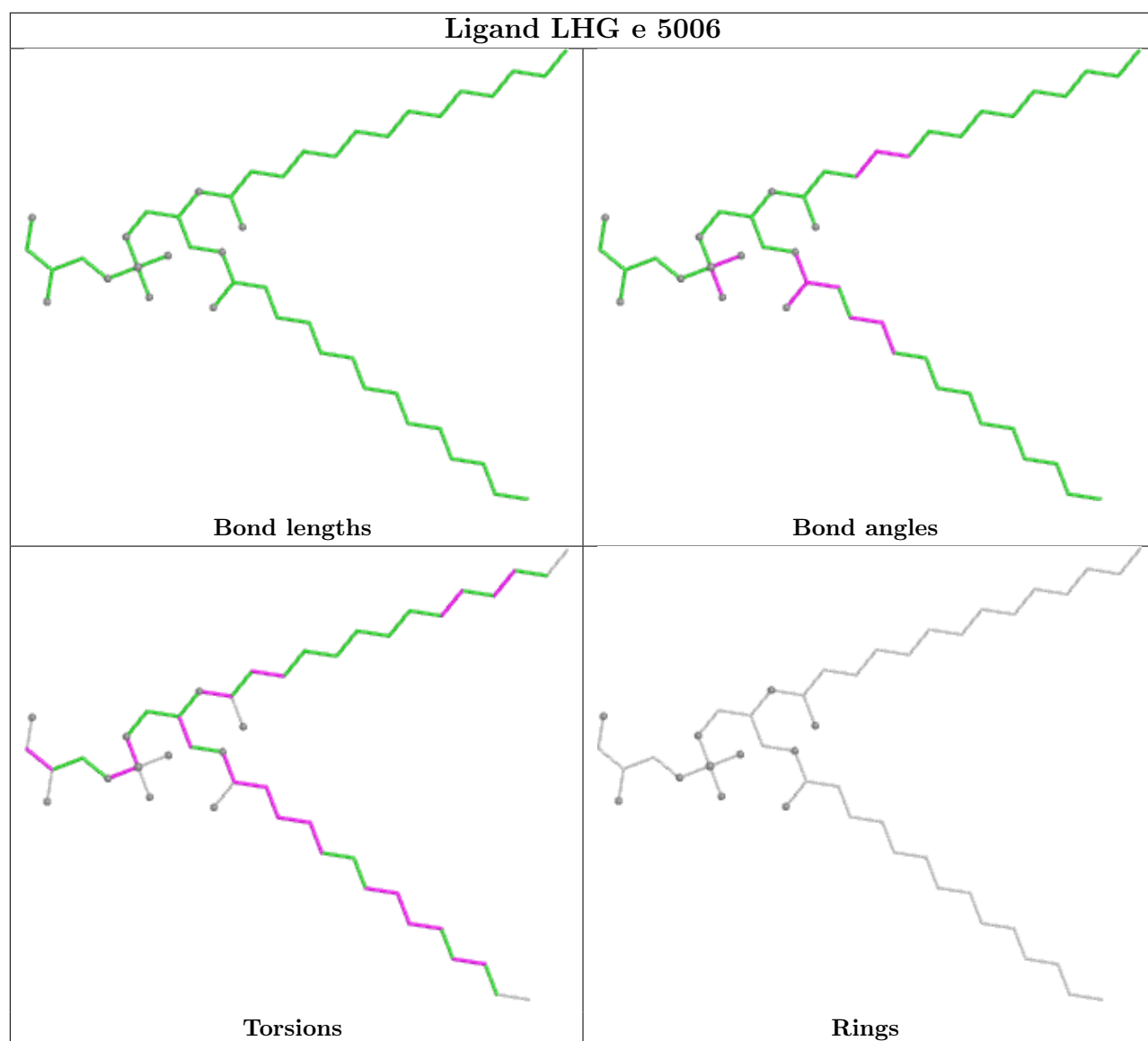
Torsions

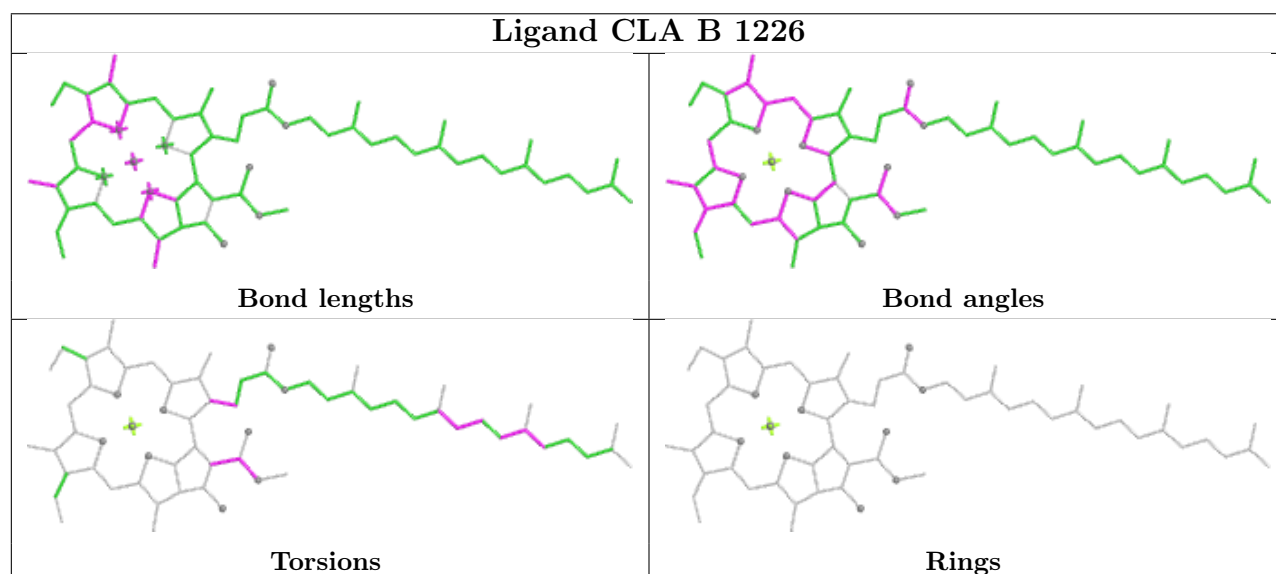
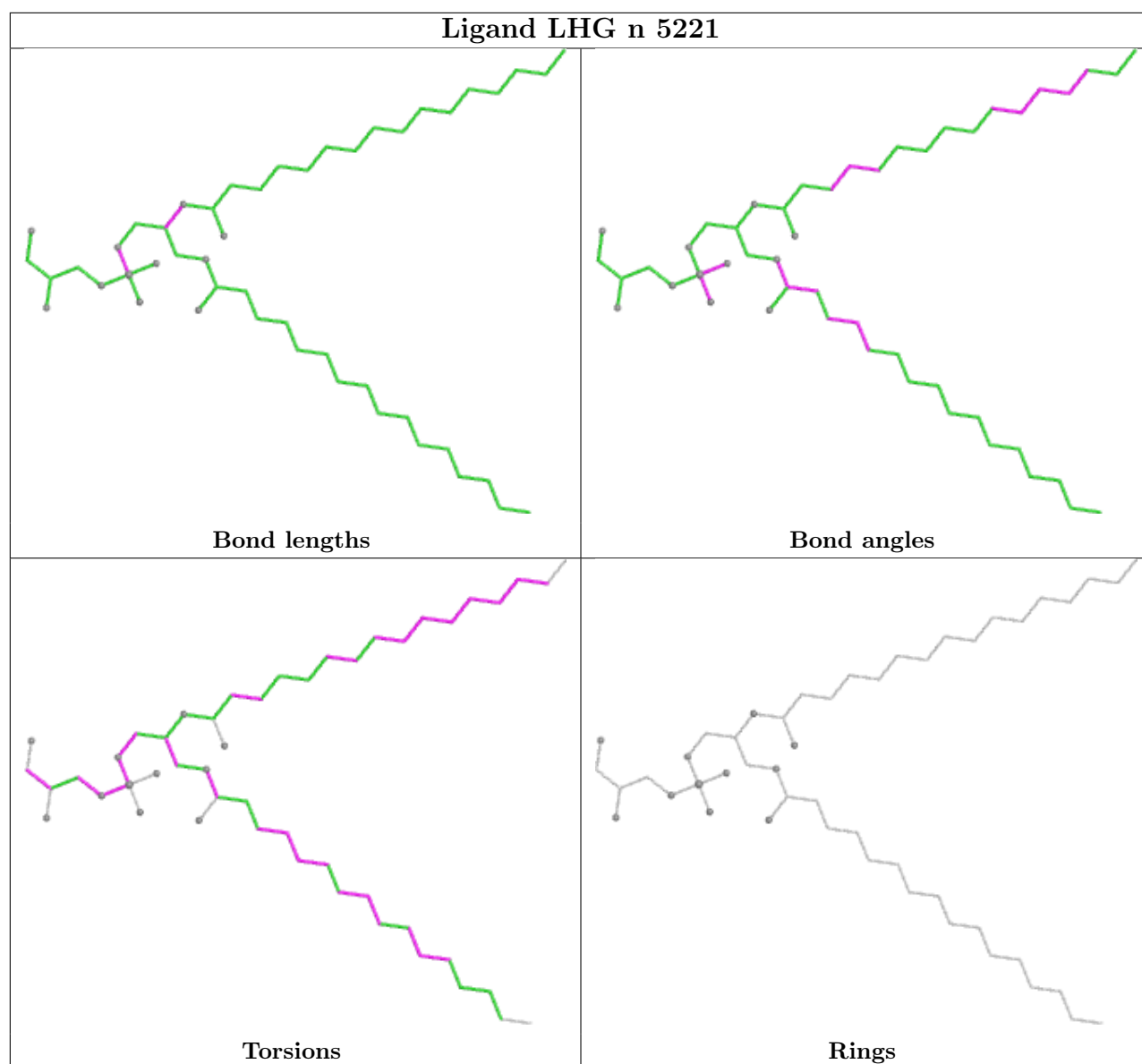


Rings

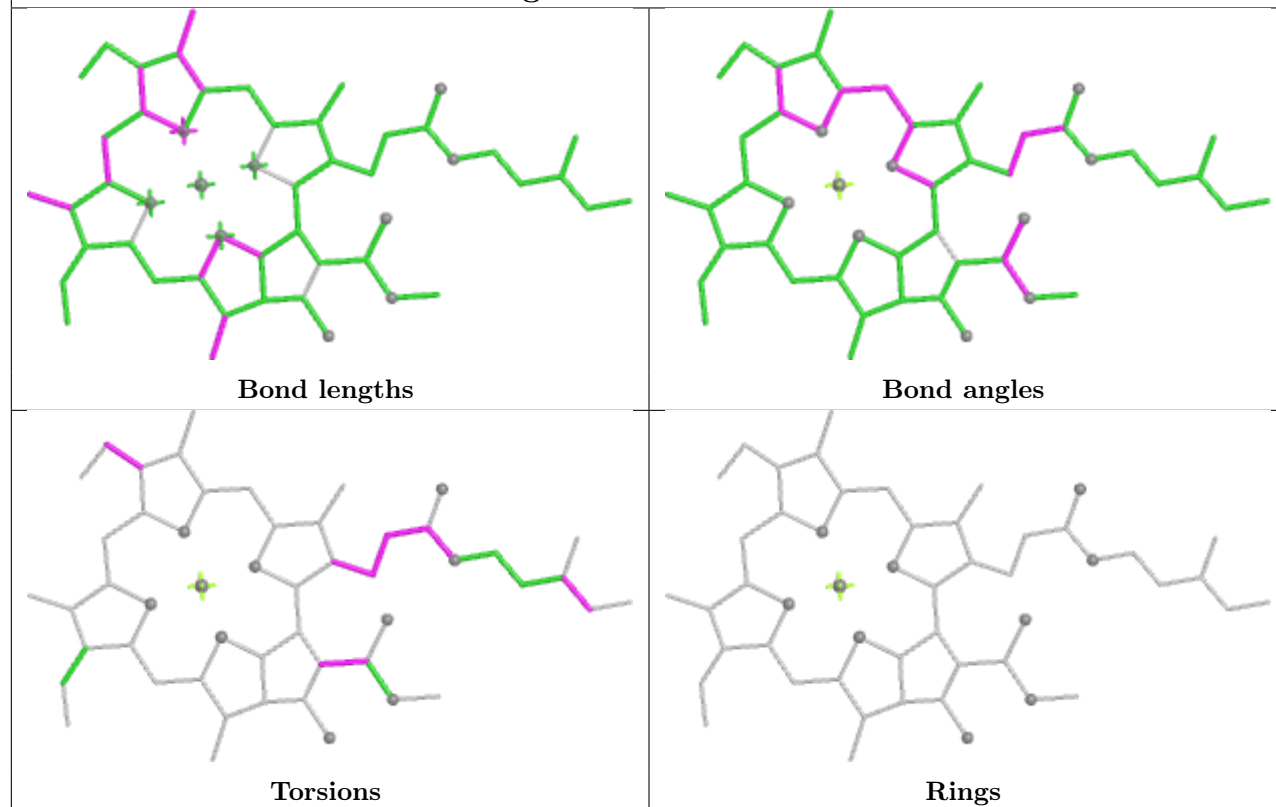
Ligand CLA U 1103



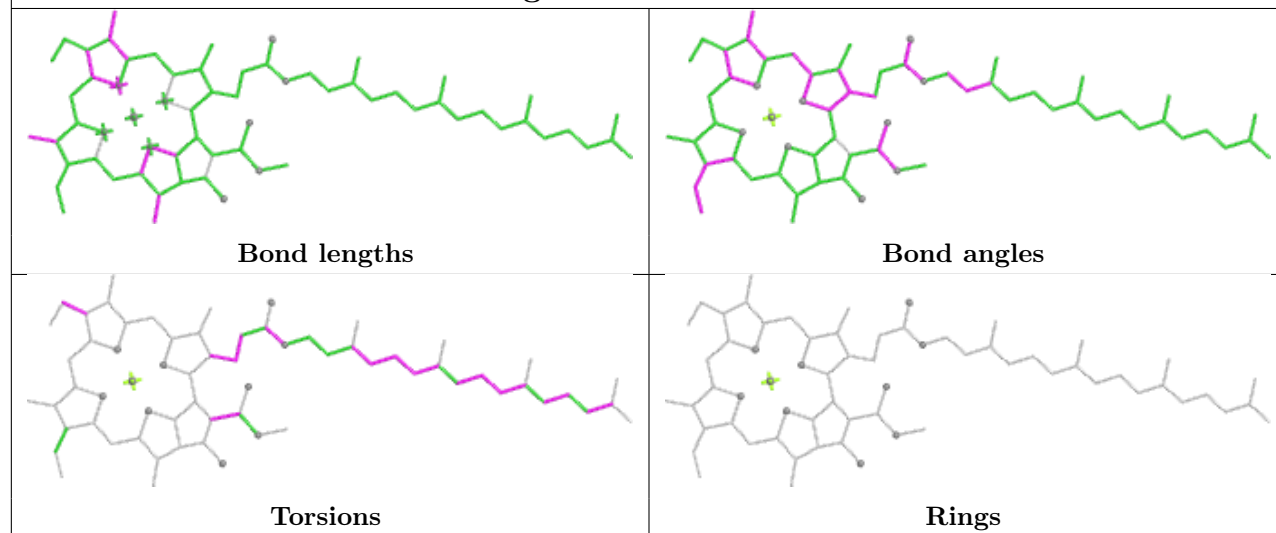


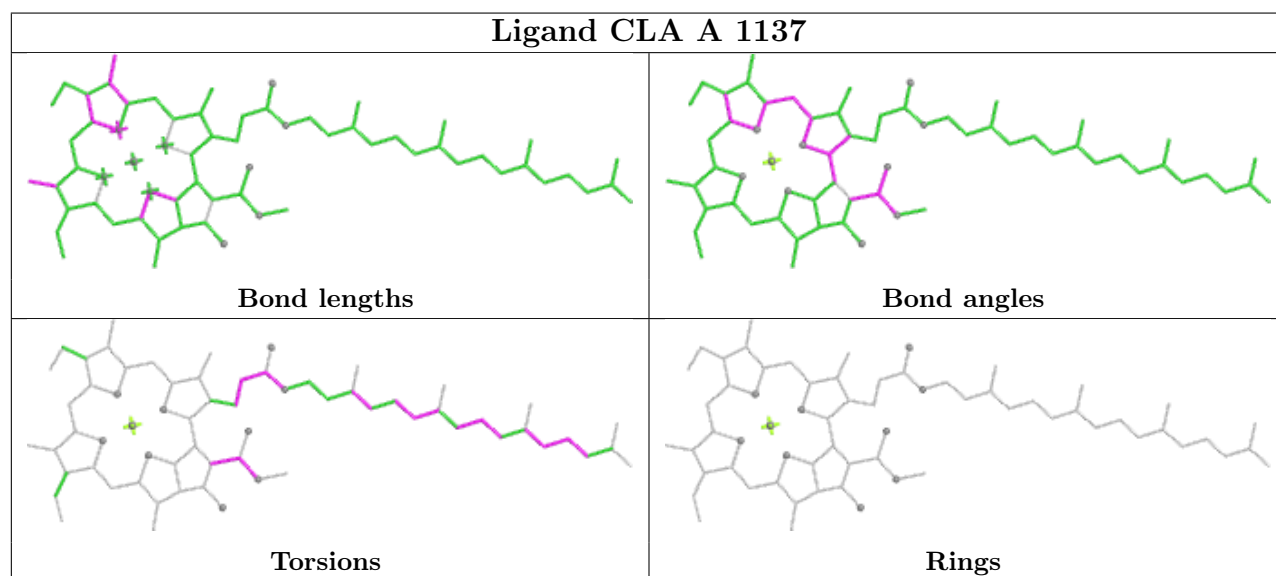
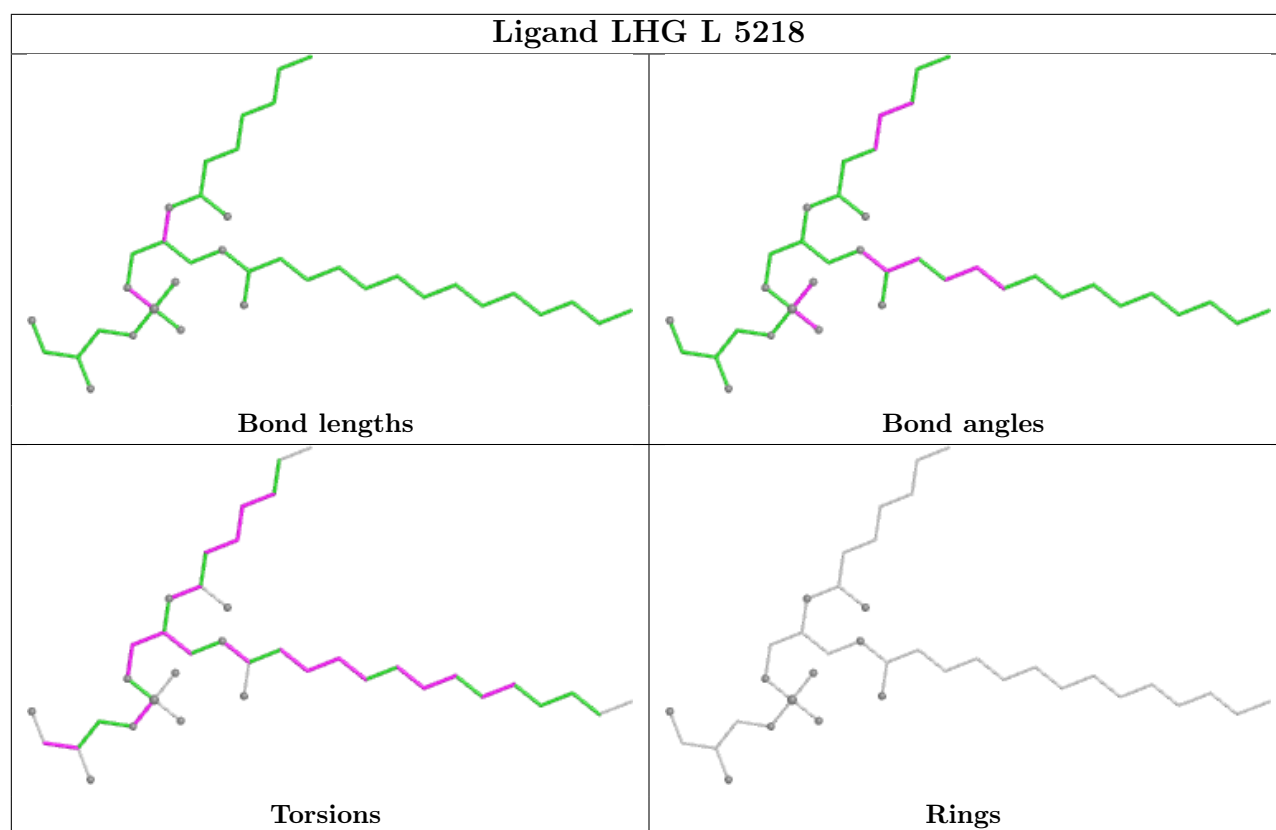


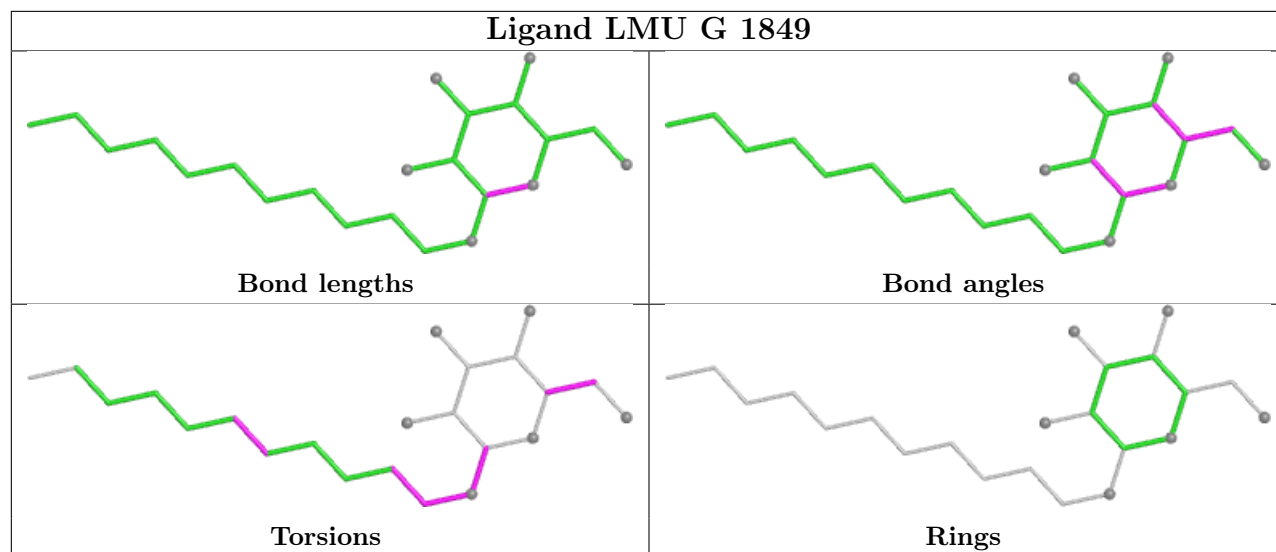
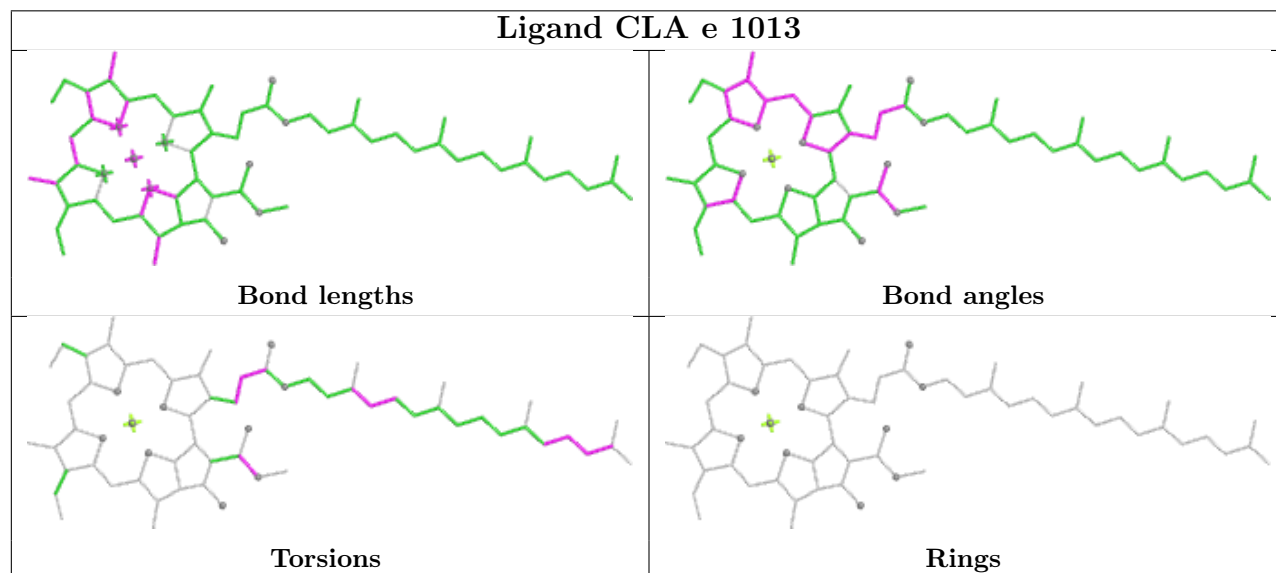
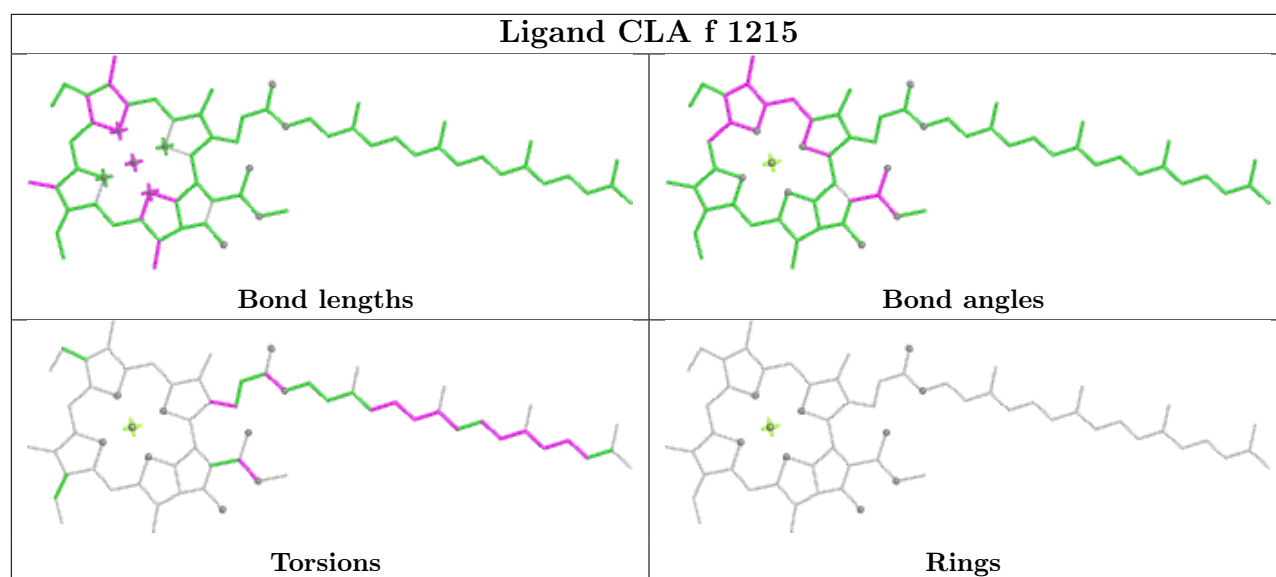
Ligand CLA A 1110

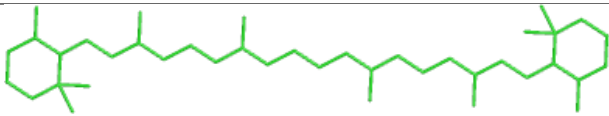
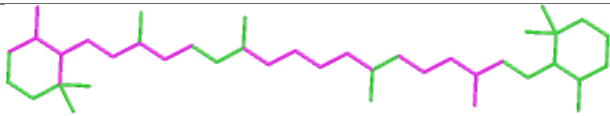
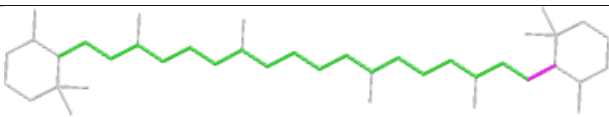
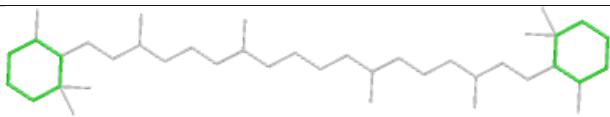


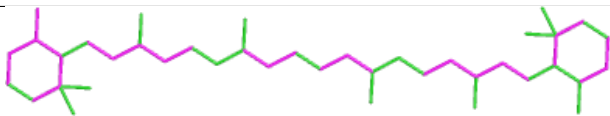
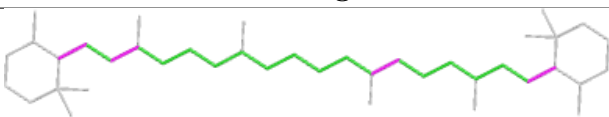
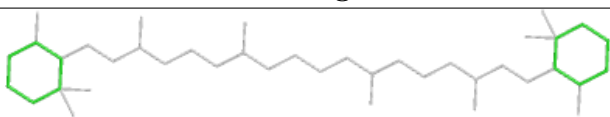
Ligand CLA B 1210

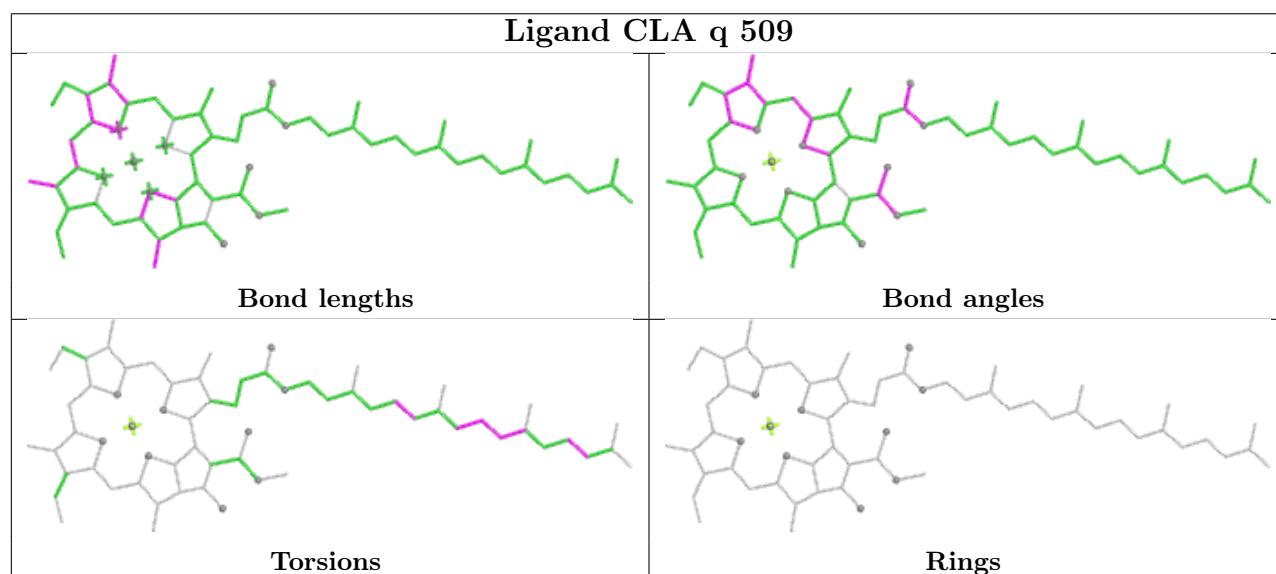
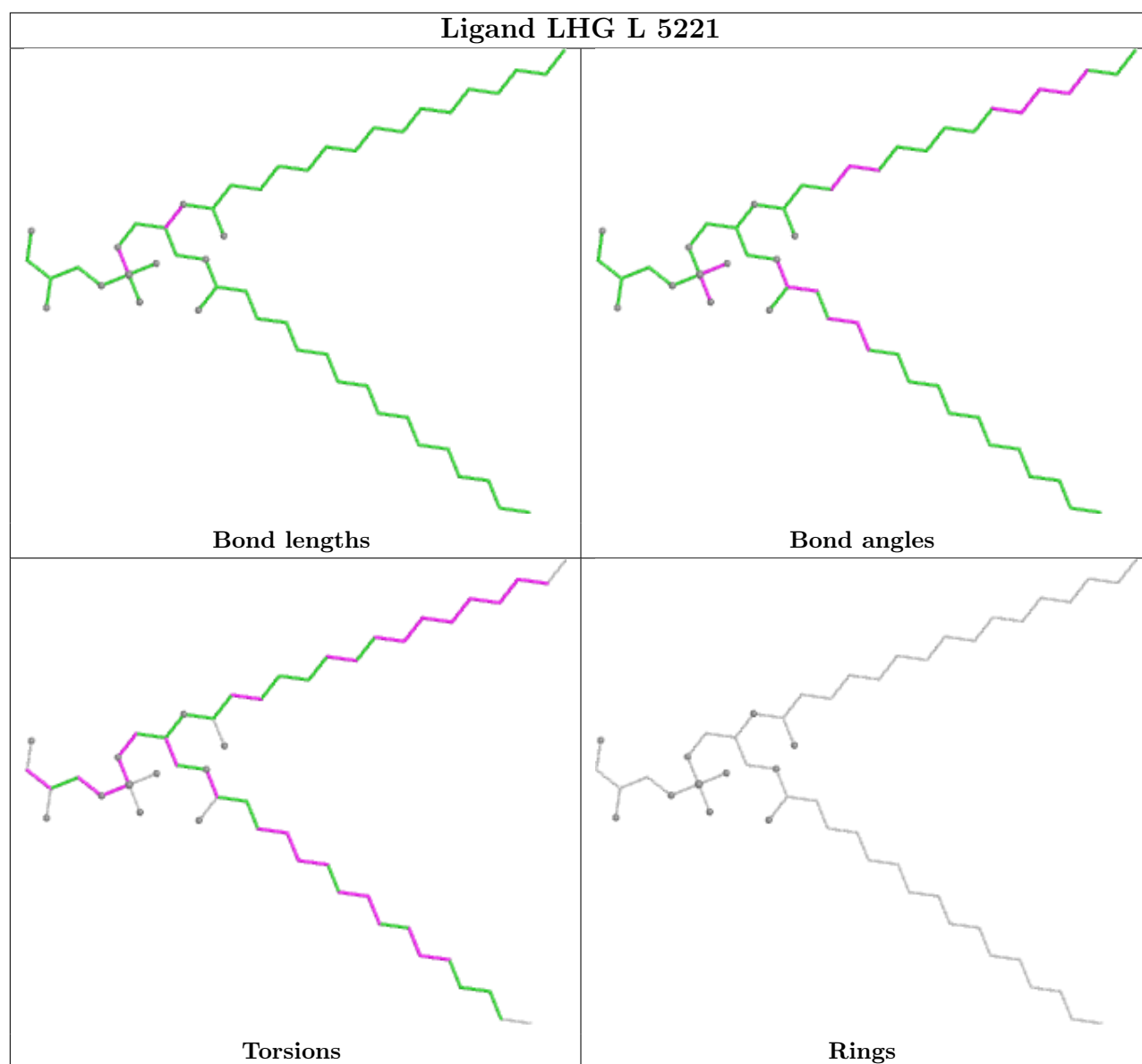


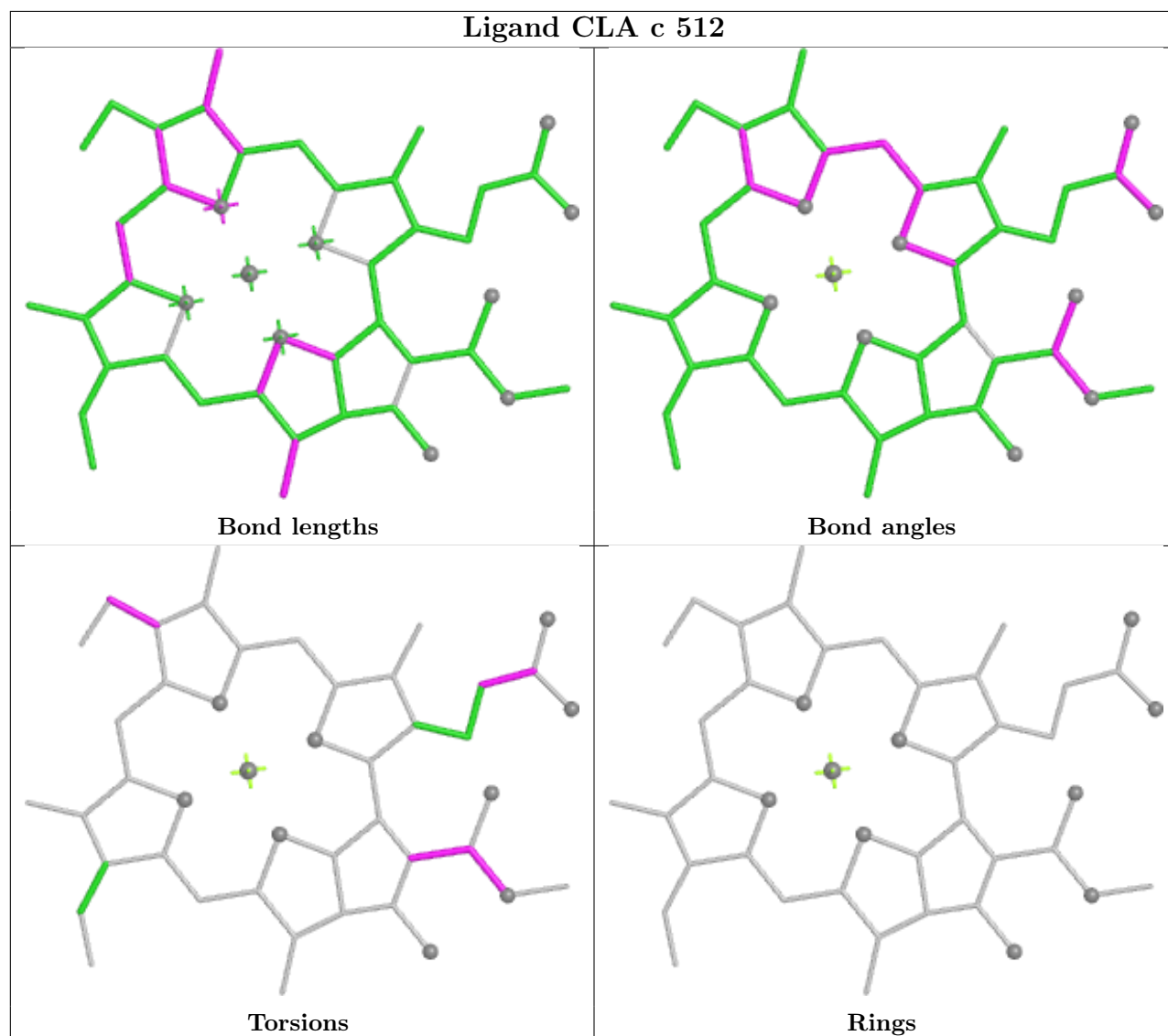
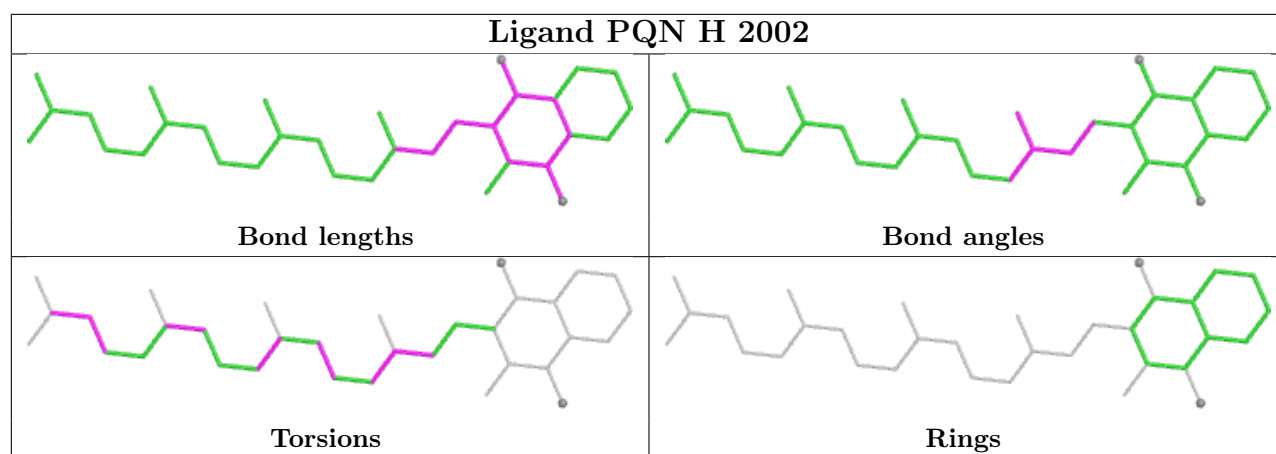




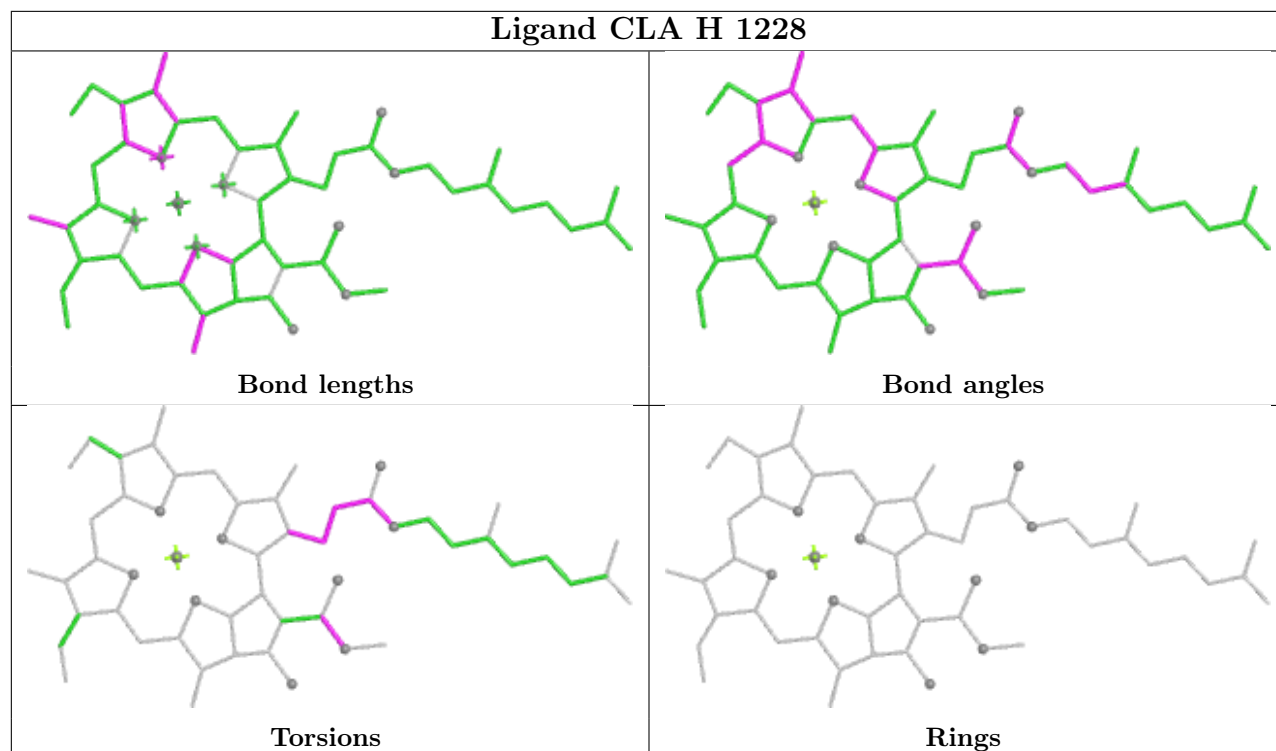
Ligand BCR 2 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 1 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

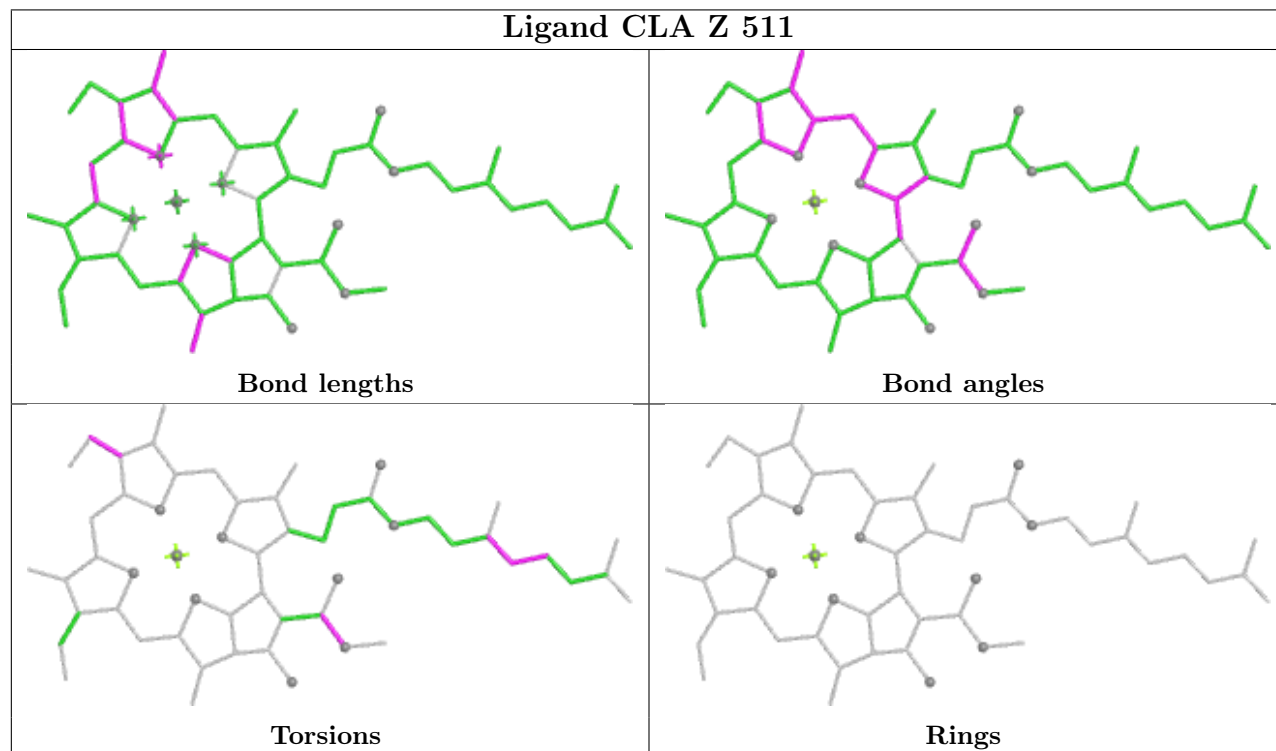


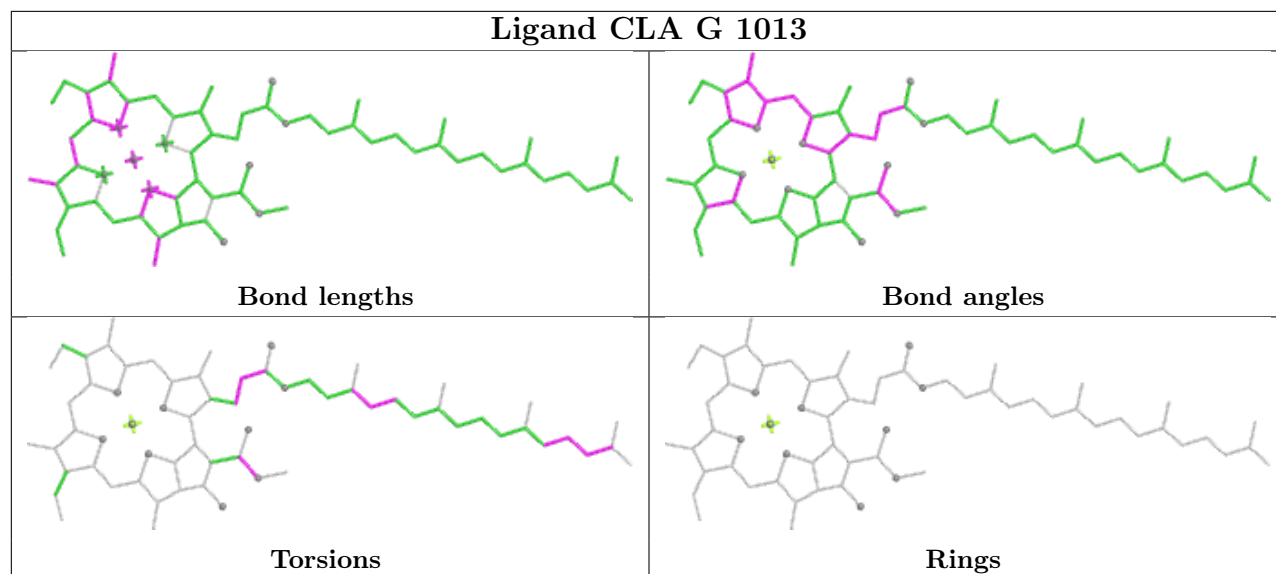
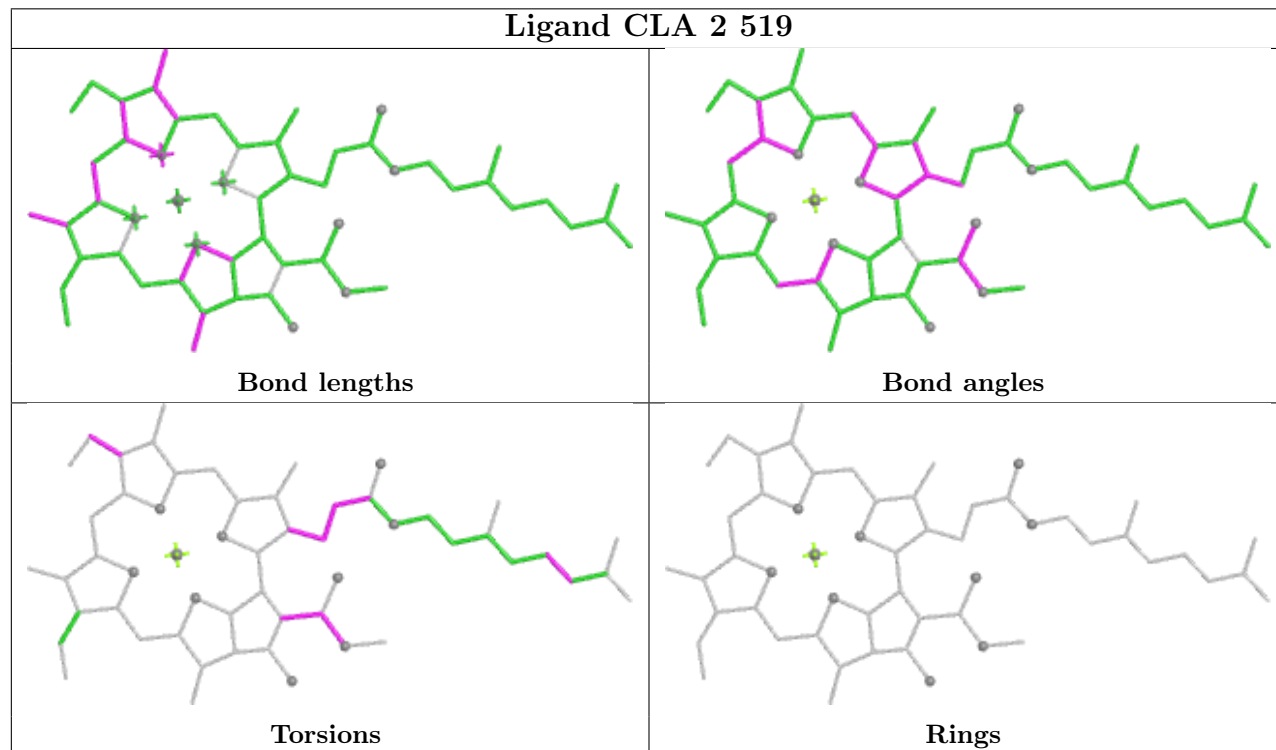


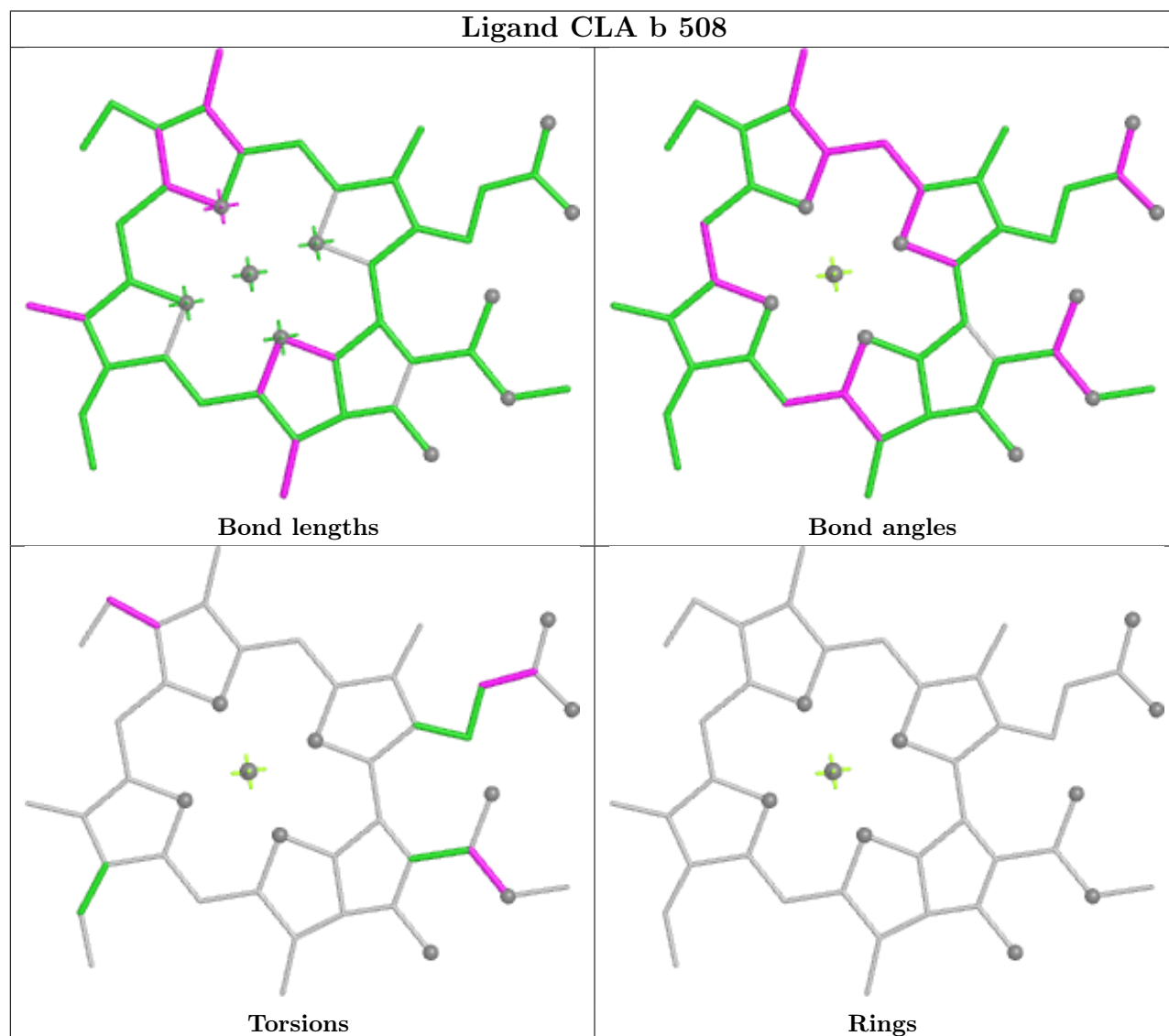
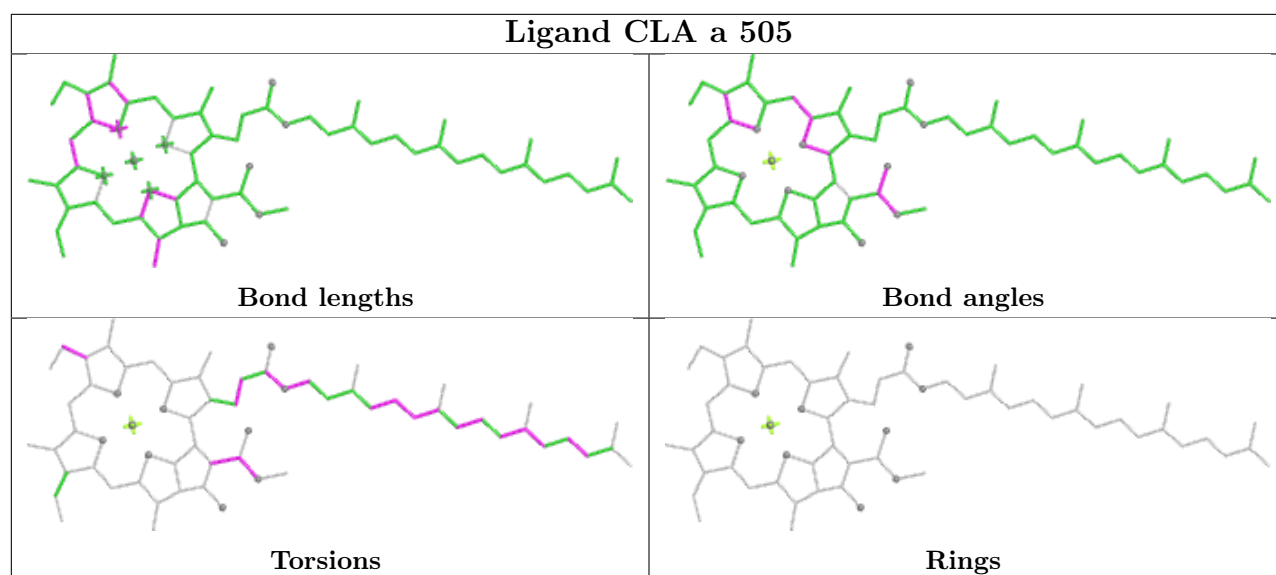
Ligand CLA H 1228



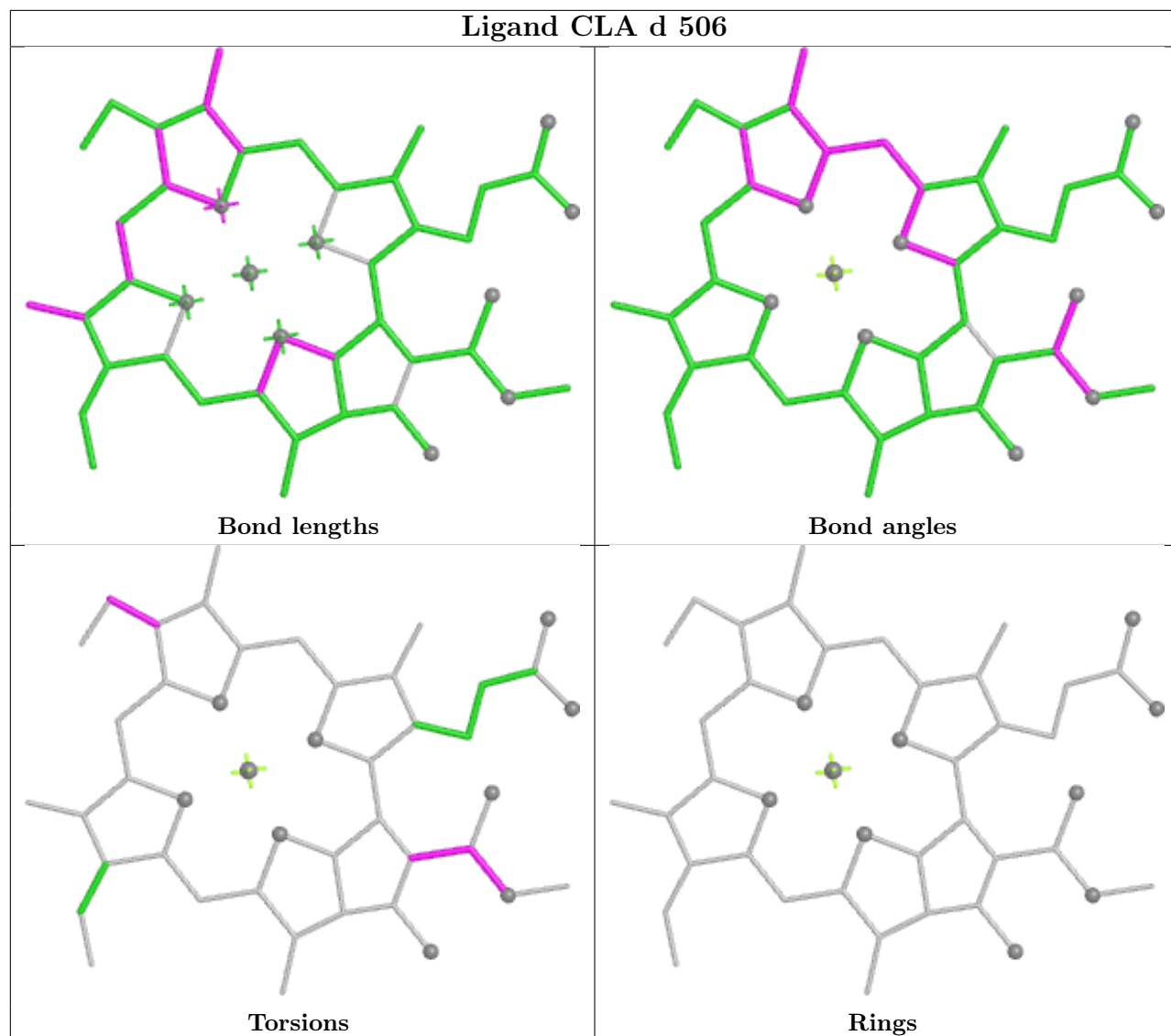
Ligand CLA Z 511

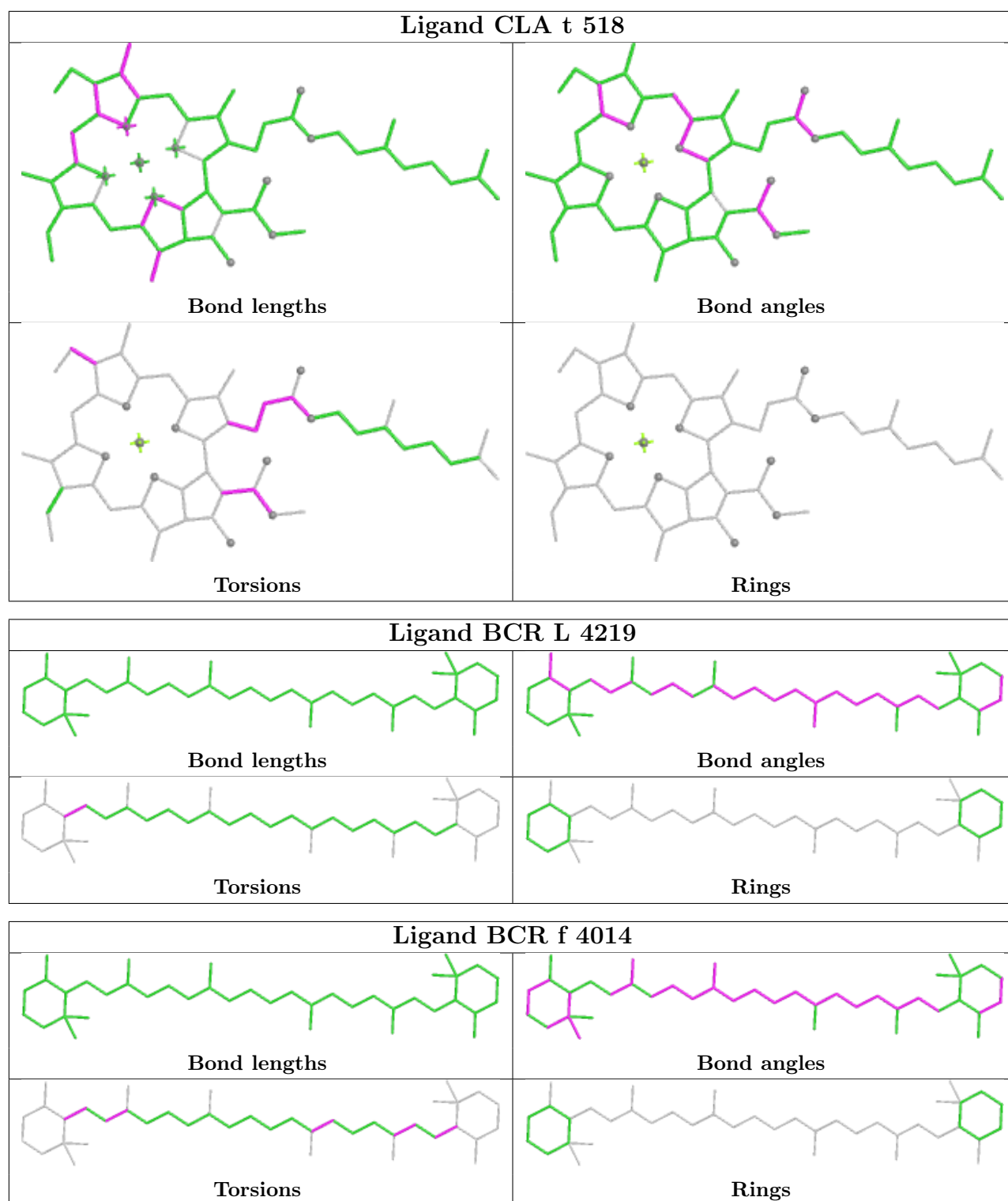


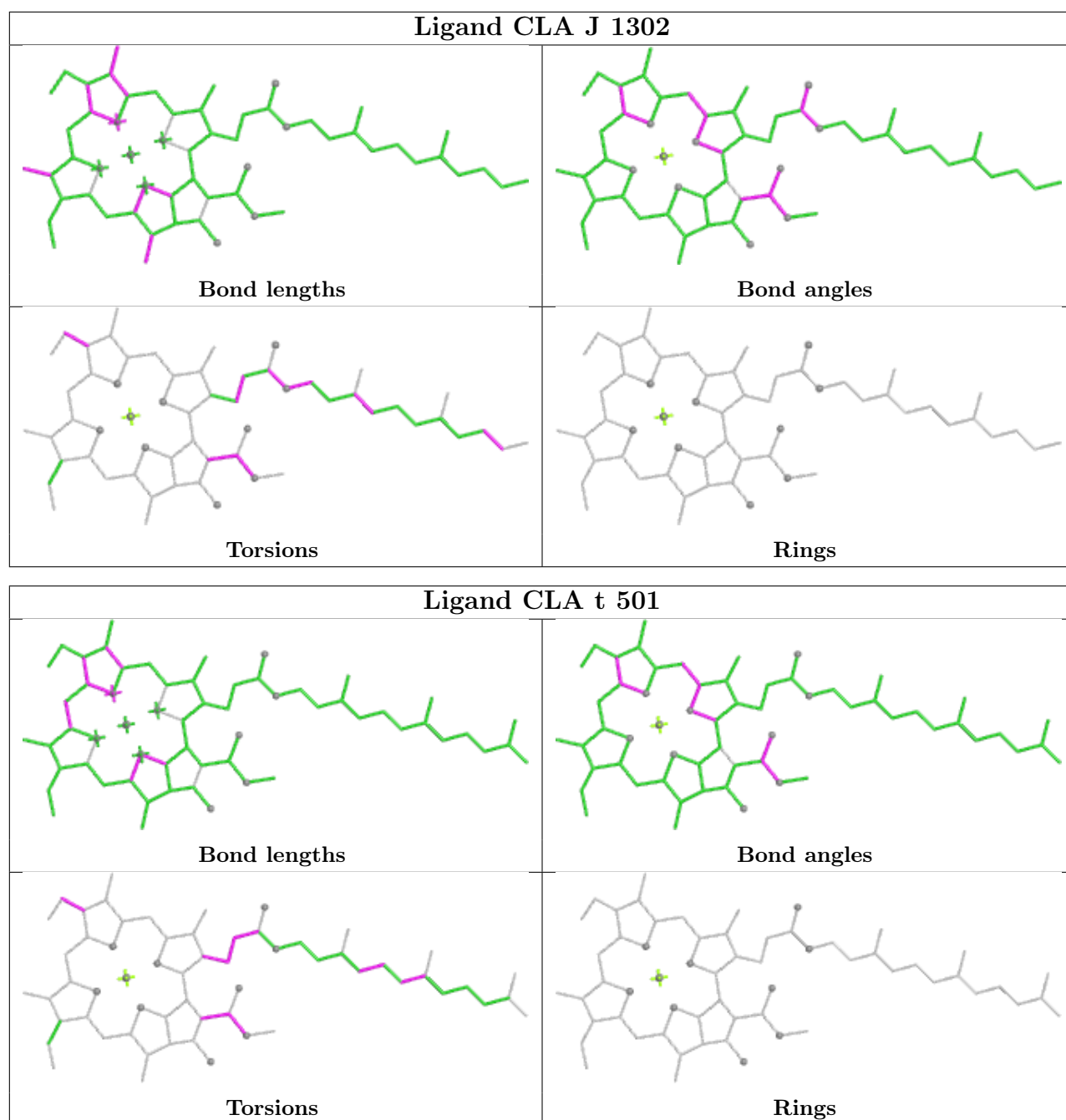
Ligand CLA G 1013**Ligand CLA 2 519**

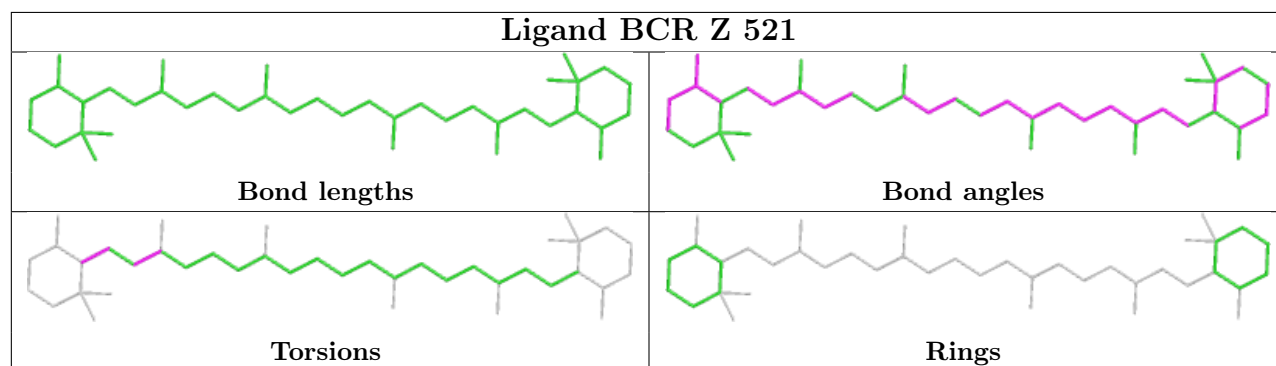
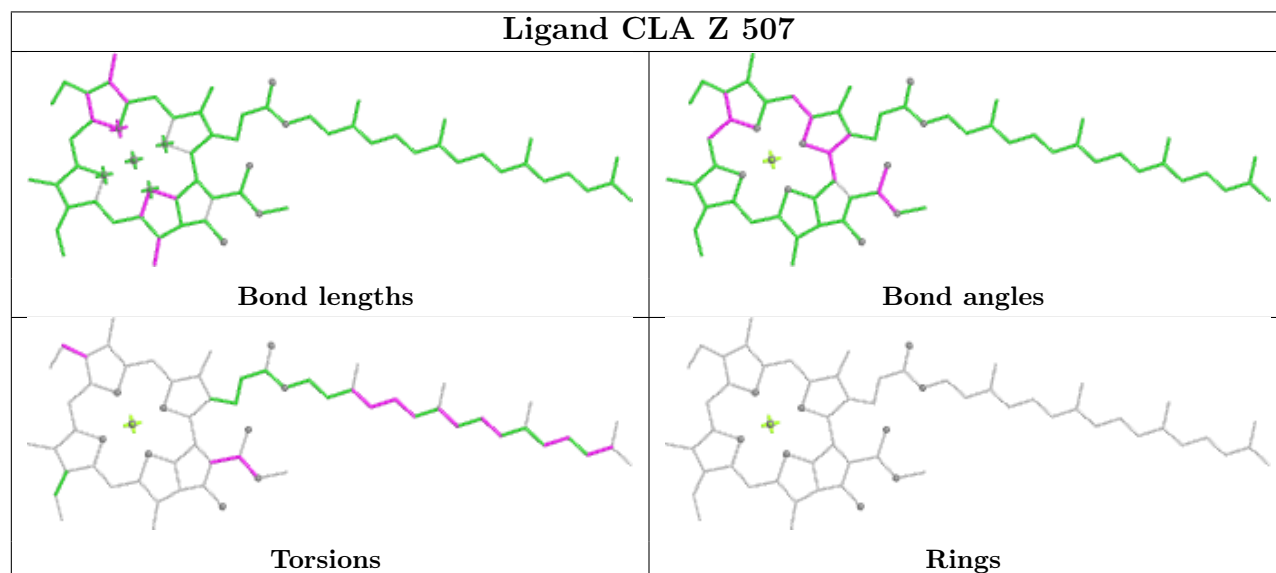
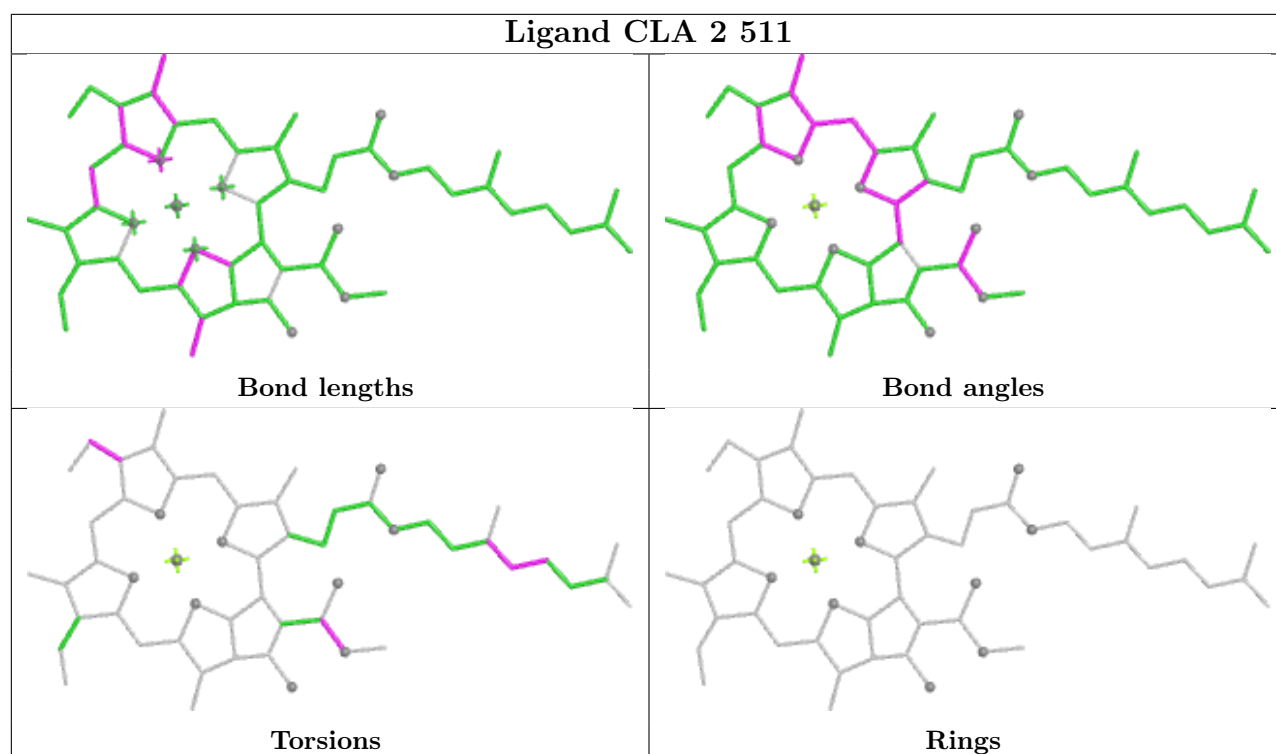


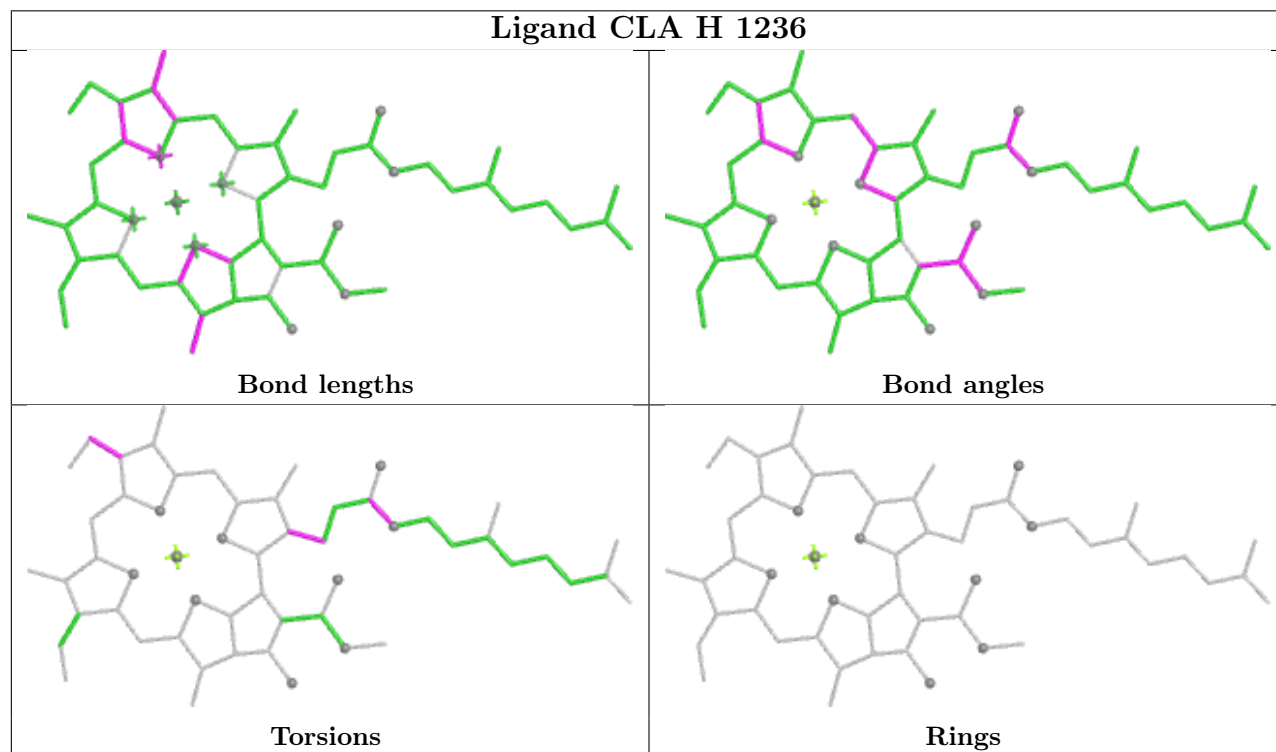
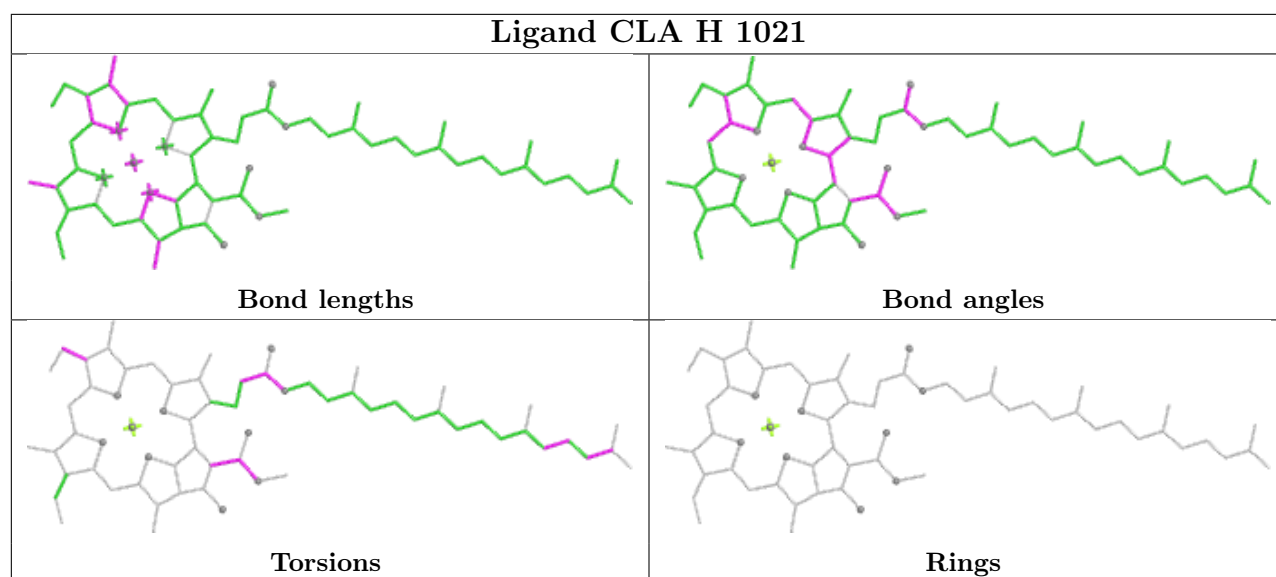
Ligand CLA d 506

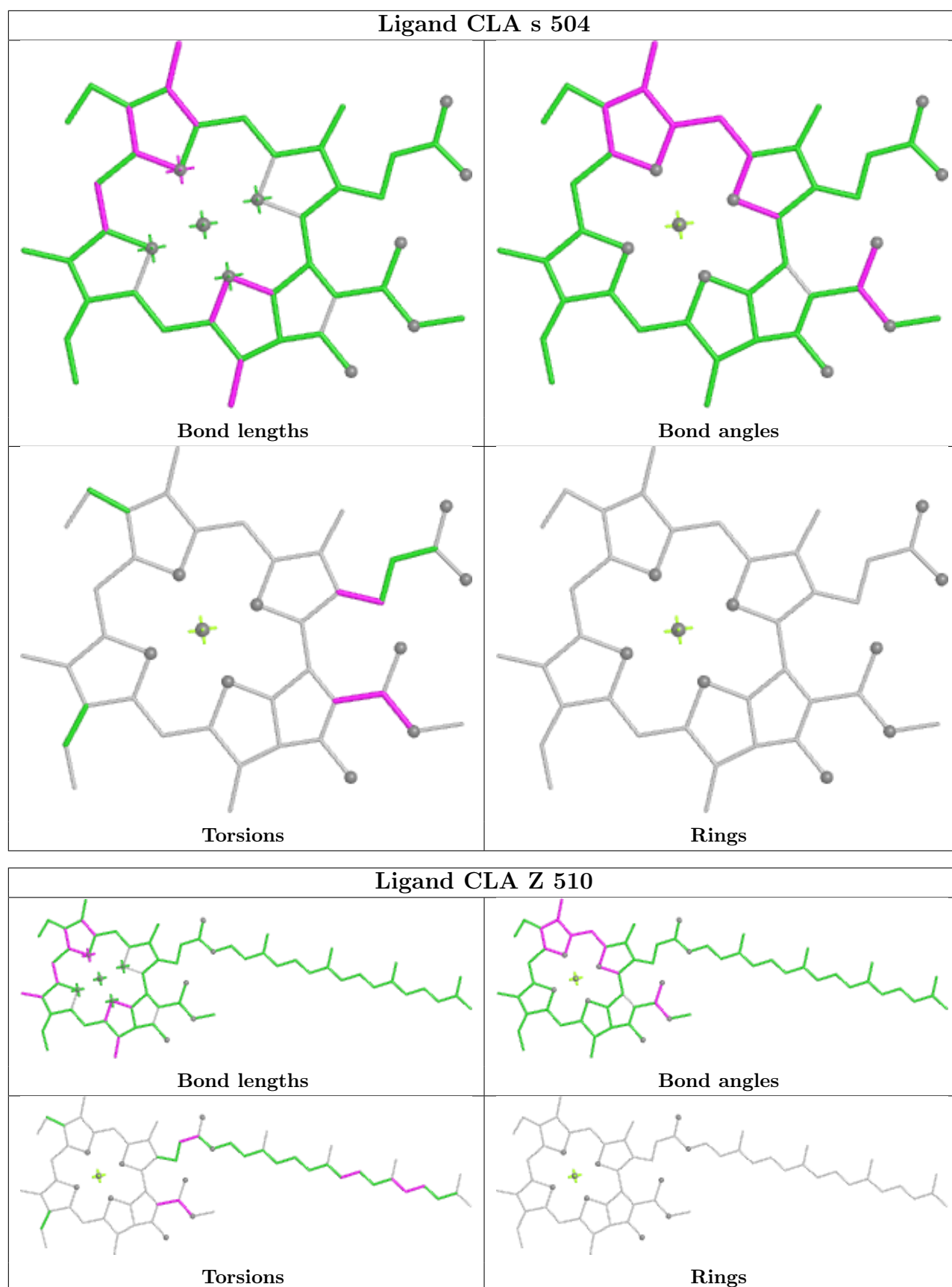


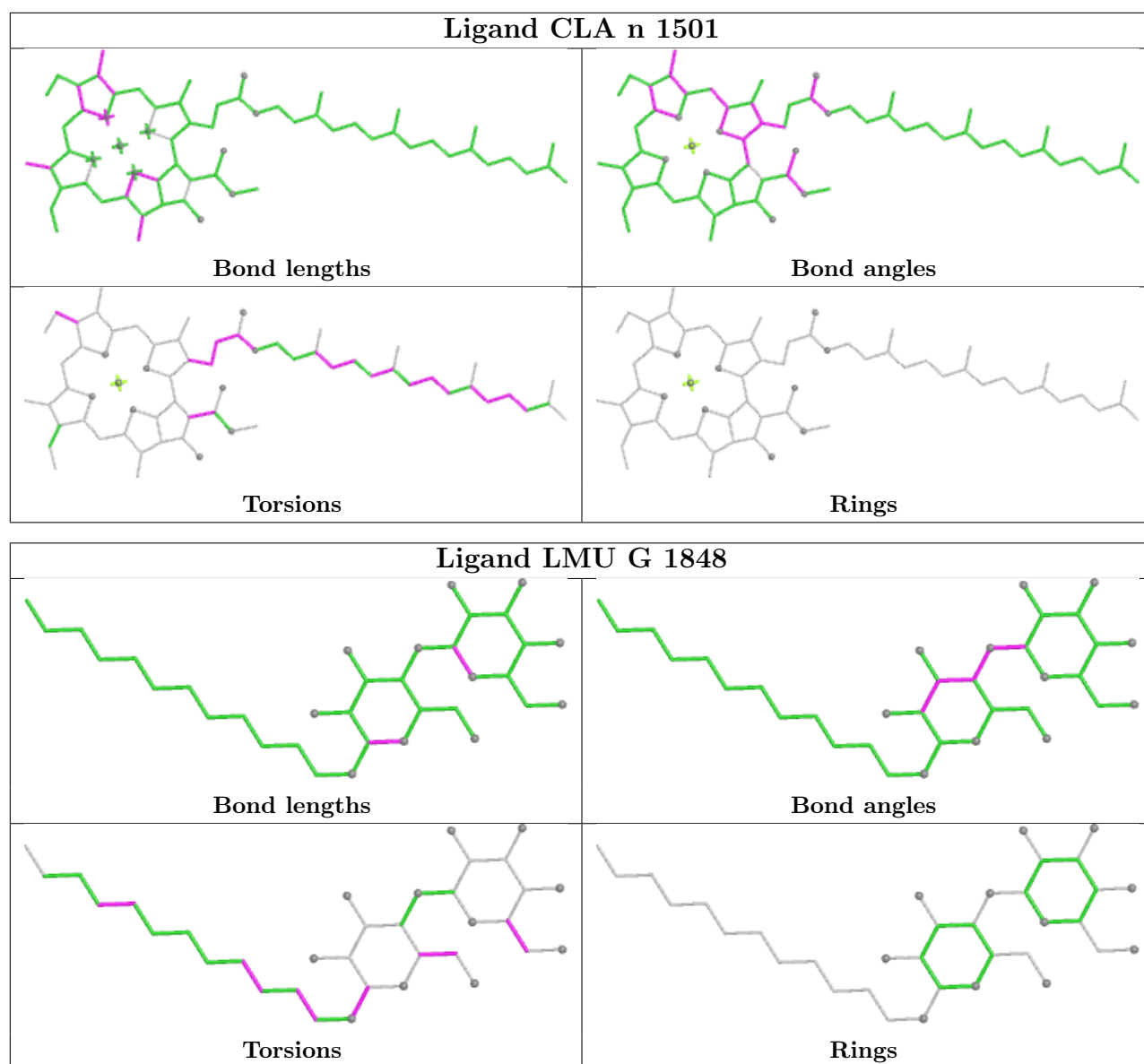


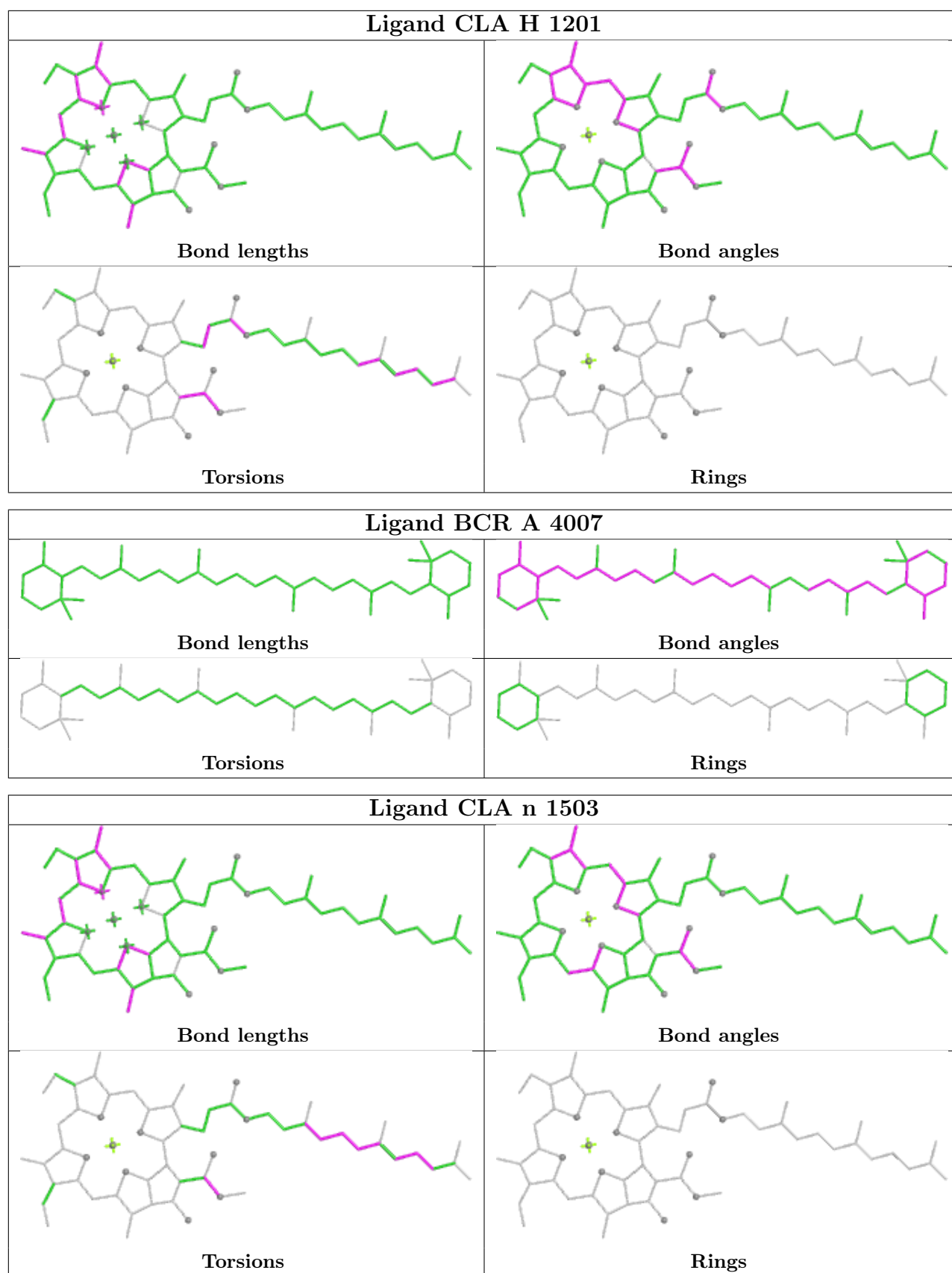


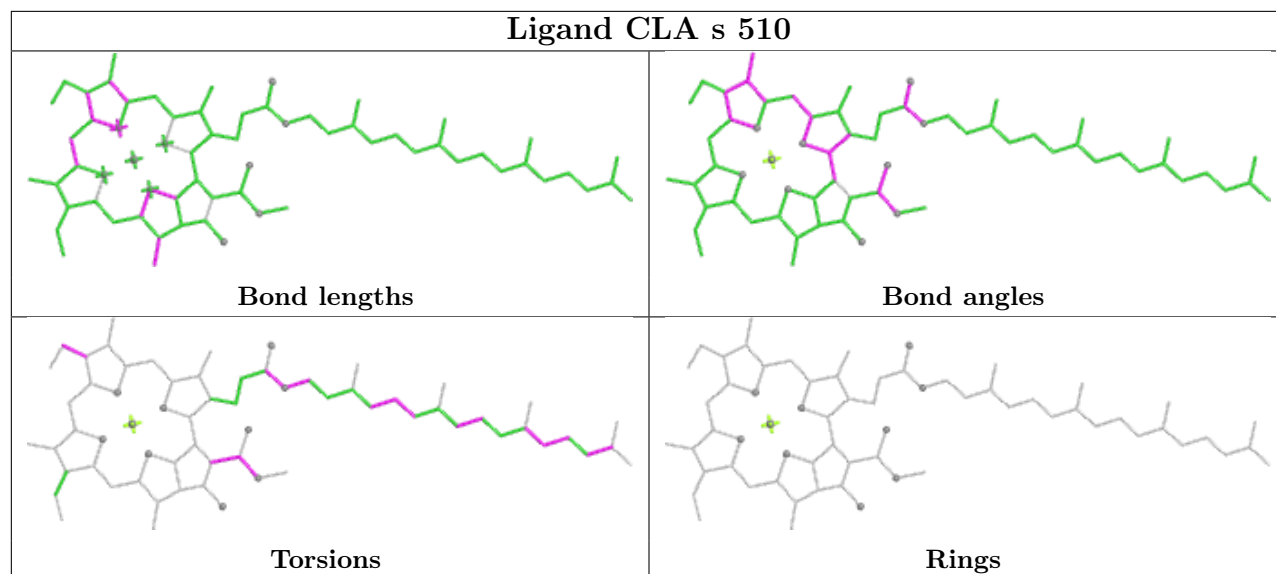
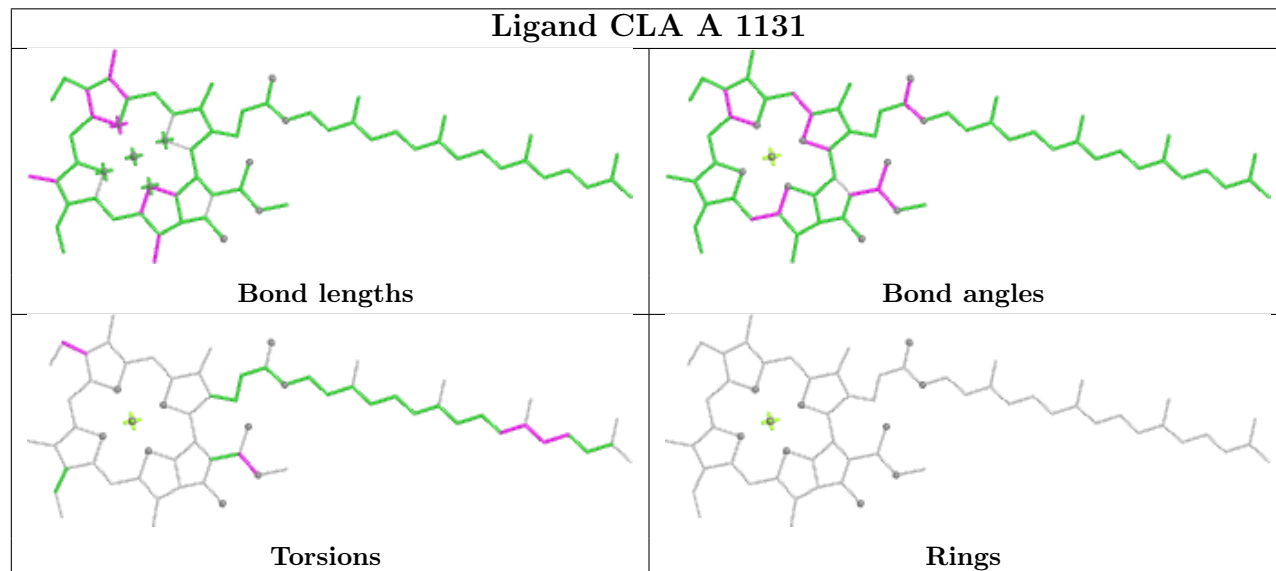


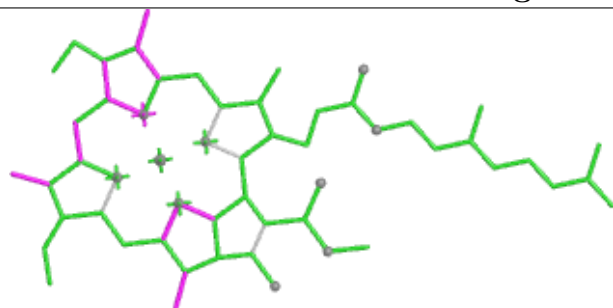




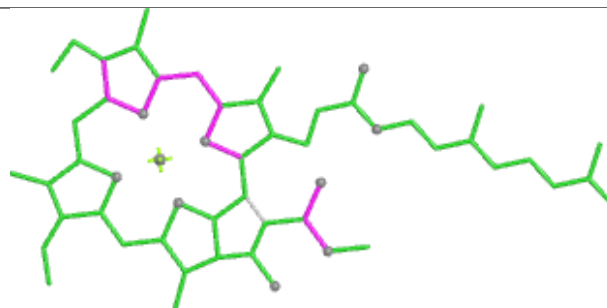




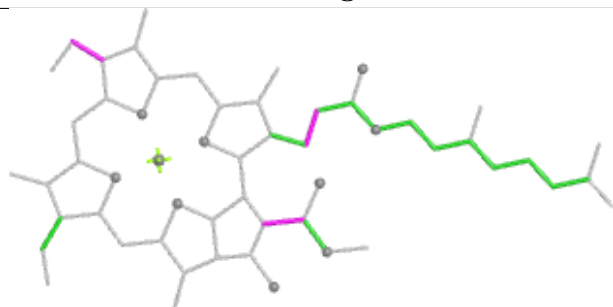
Ligand CLA s 510**Ligand CLA A 1131**

Ligand CLA Y 513

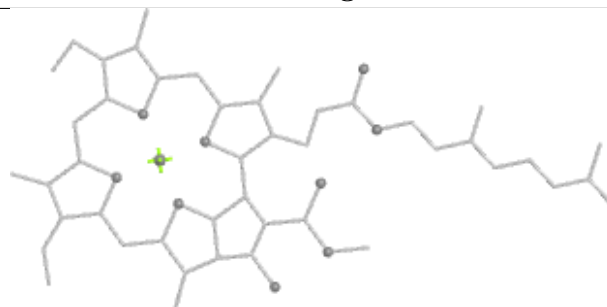
Bond lengths



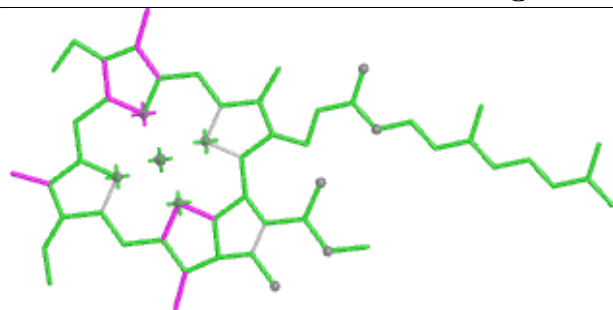
Bond angles



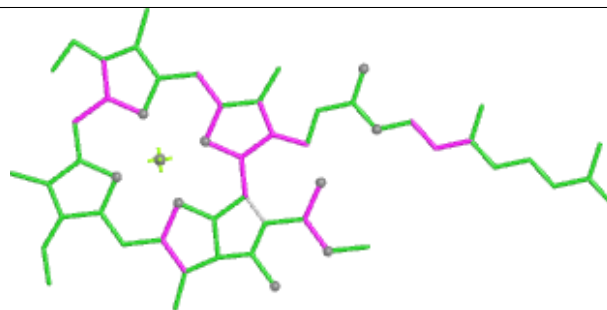
Torsions



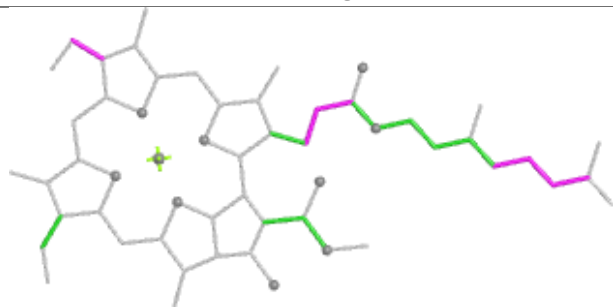
Rings

Ligand CLA e 1121

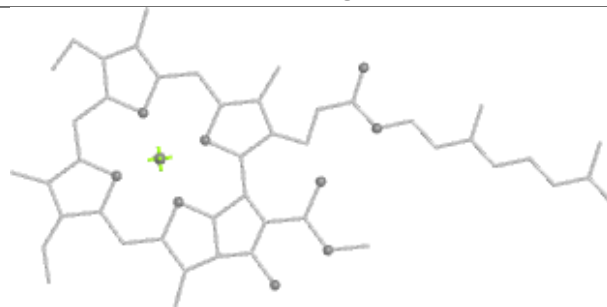
Bond lengths



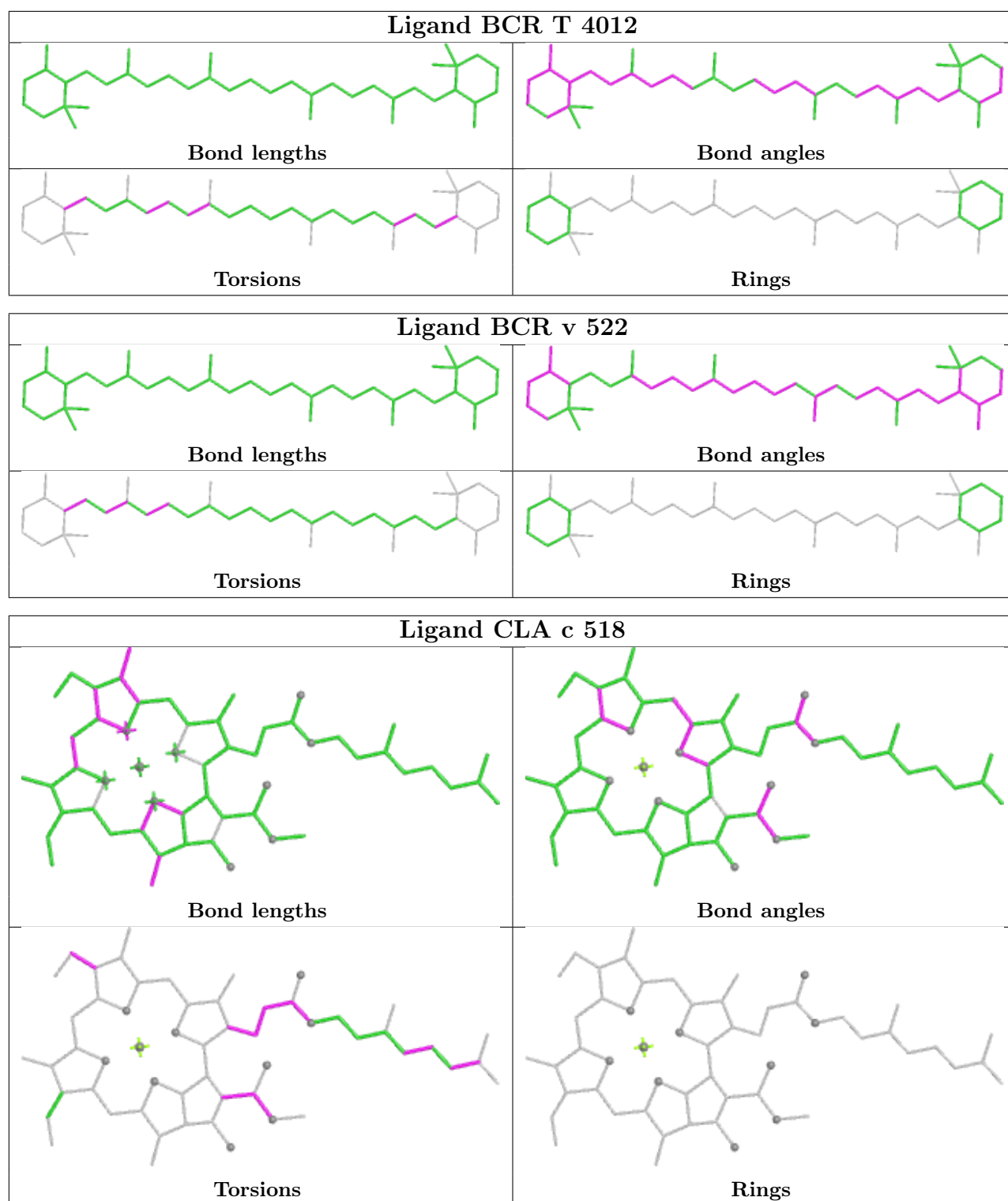
Bond angles



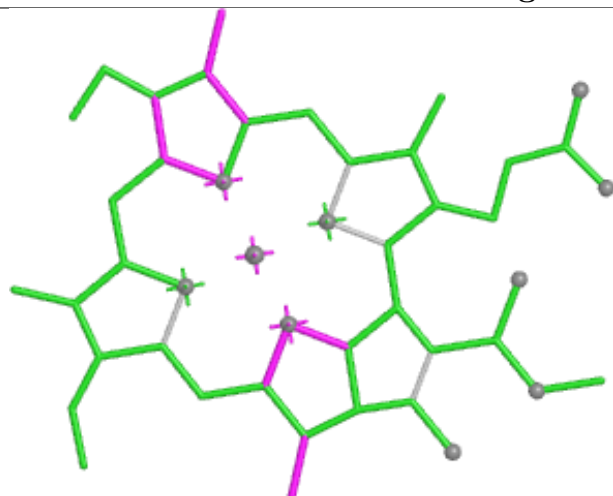
Torsions



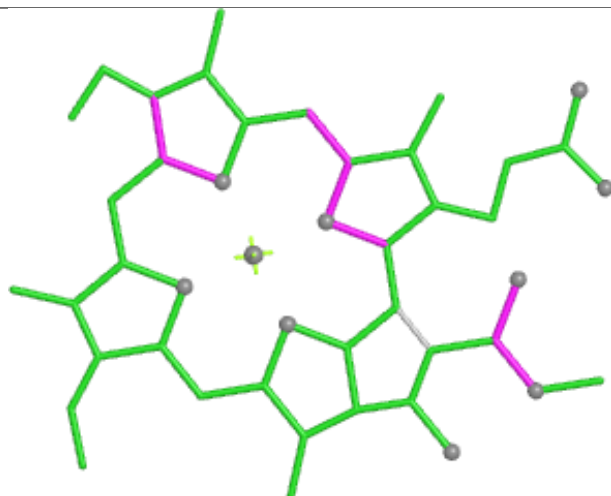
Rings



Ligand CLA 3 512



Bond lengths



Bond angles

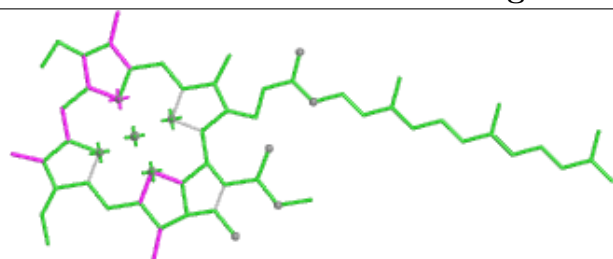


Torsions

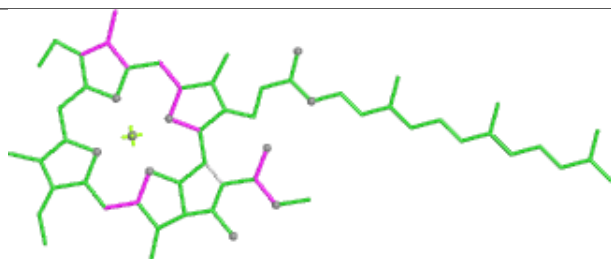


Rings

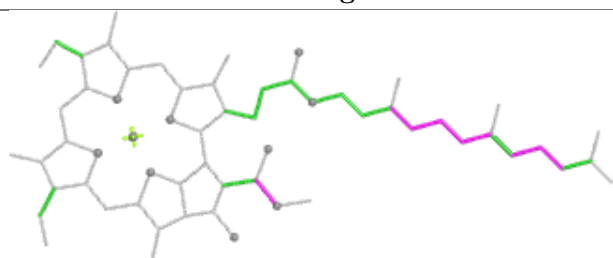
Ligand CLA L 1503



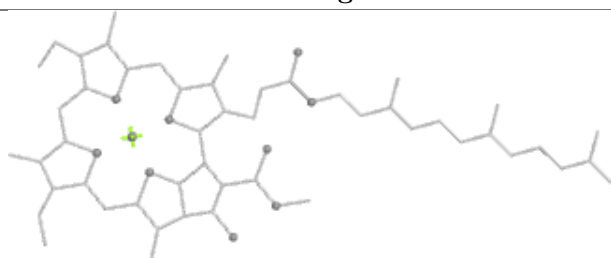
Bond lengths



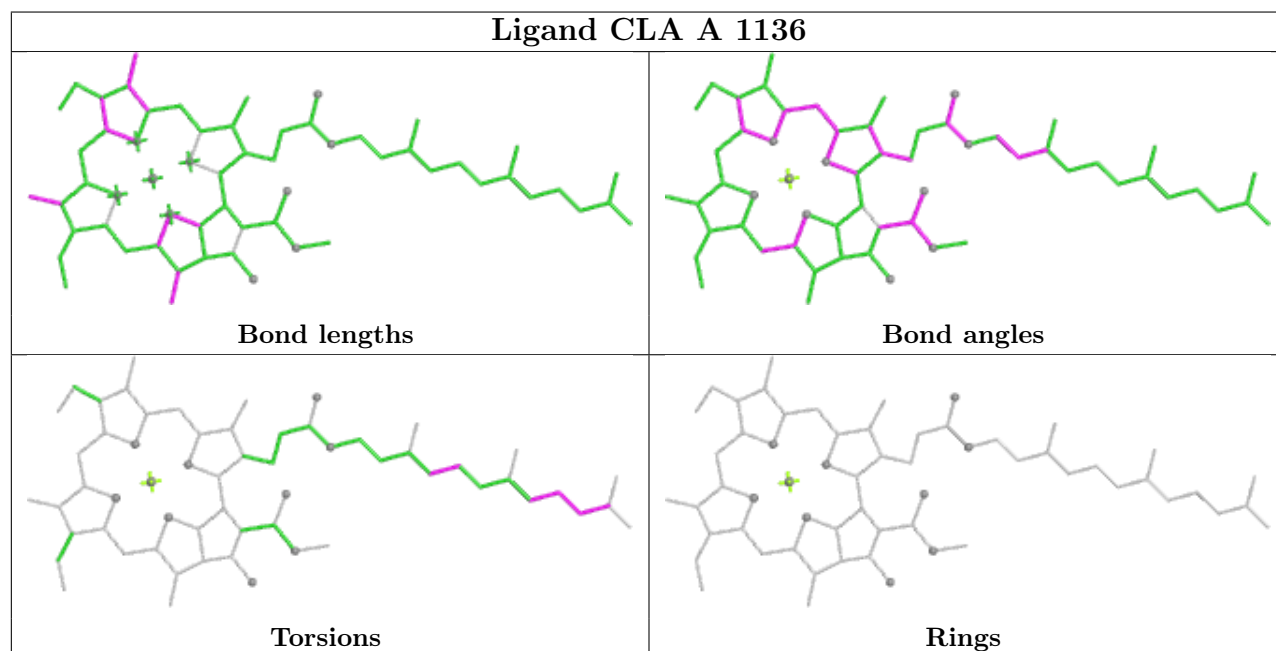
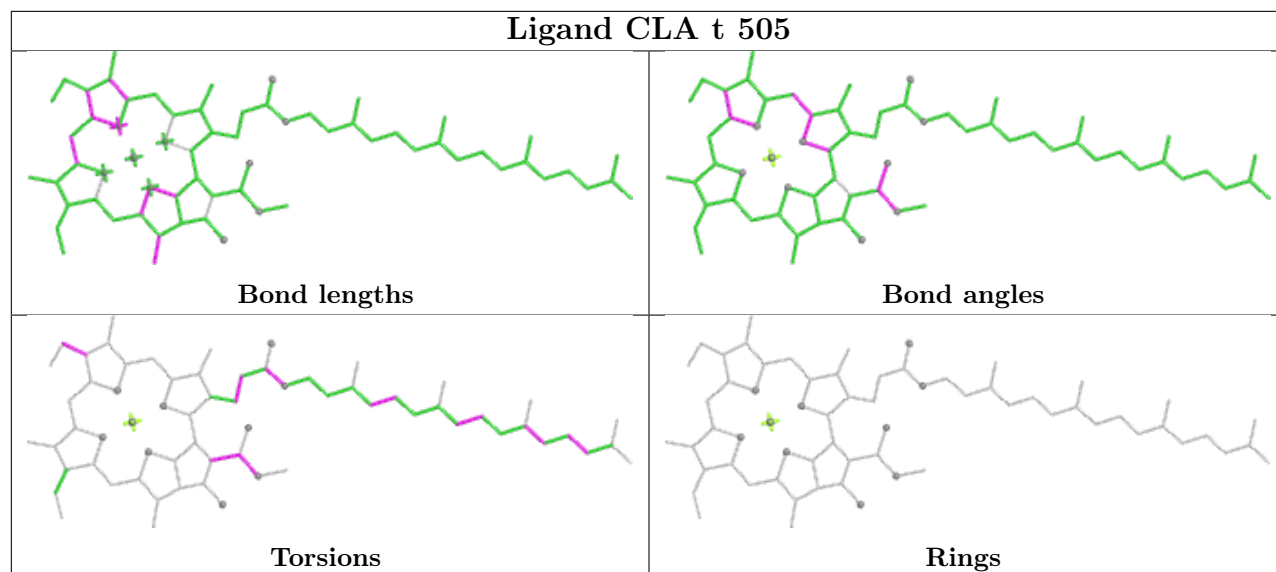
Bond angles



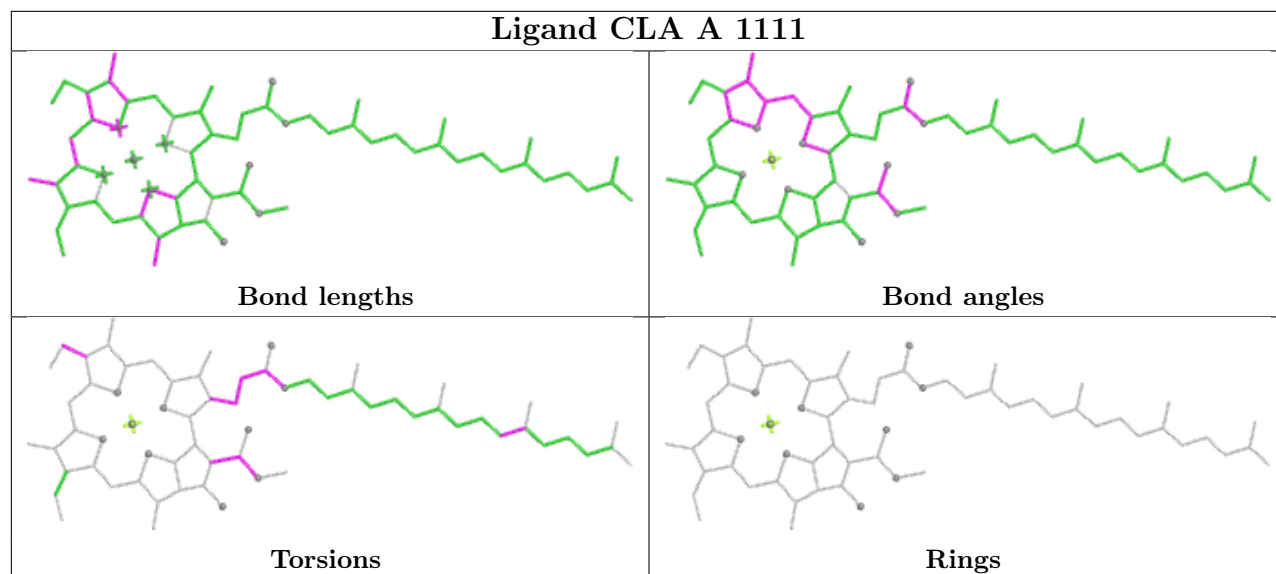
Torsions



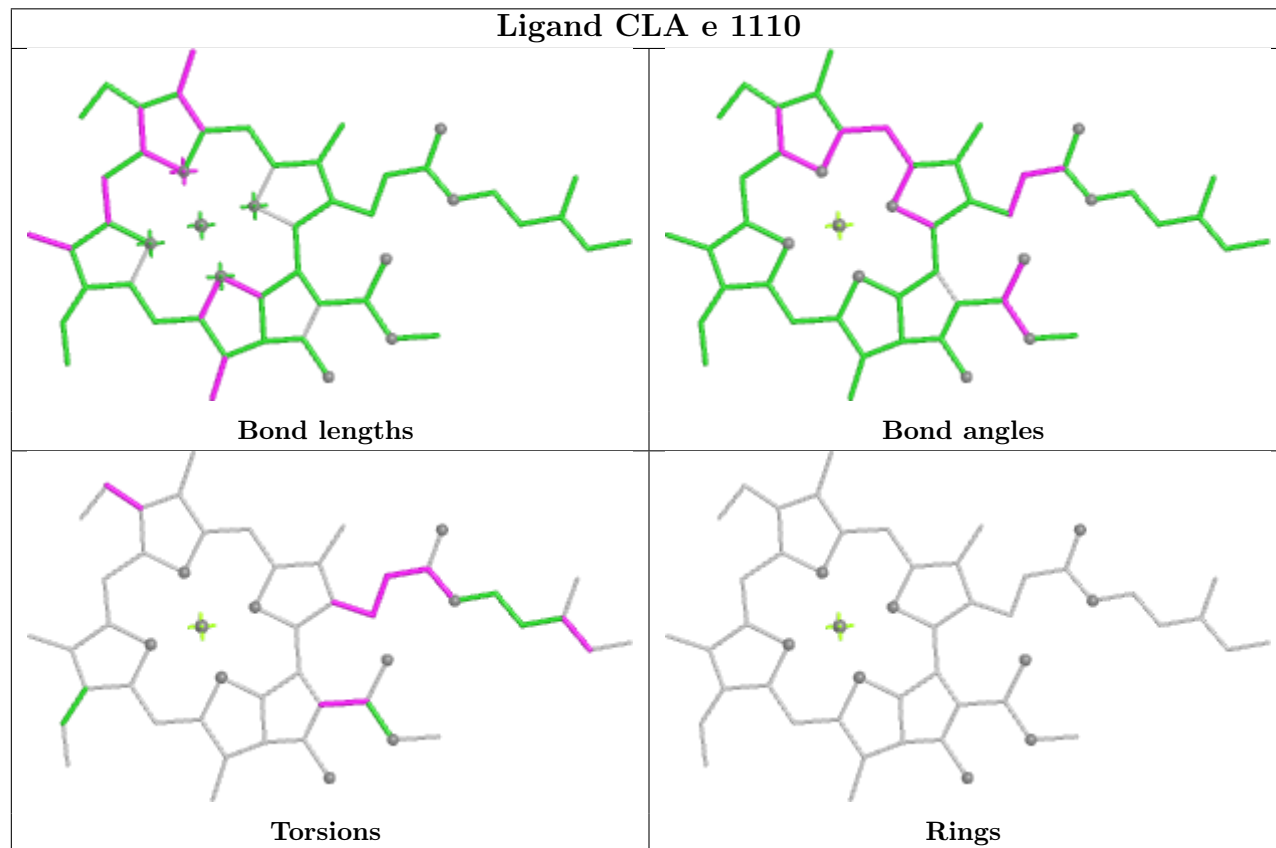
Rings

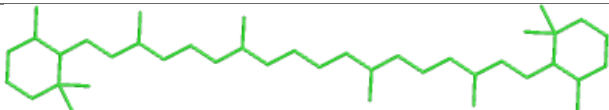
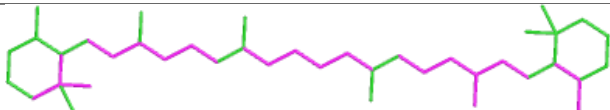
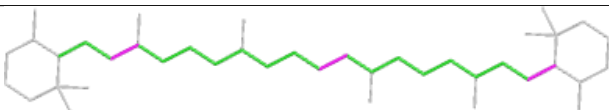
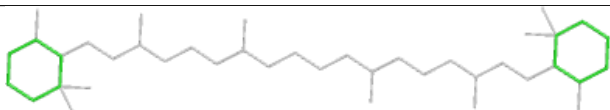


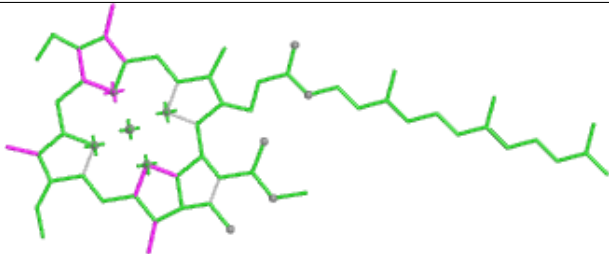
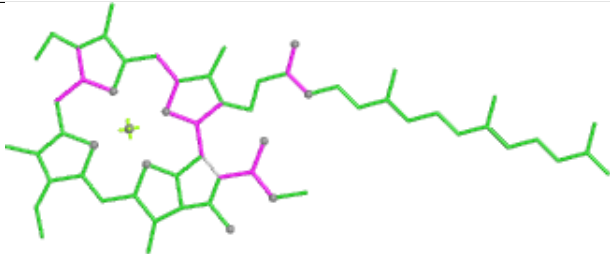
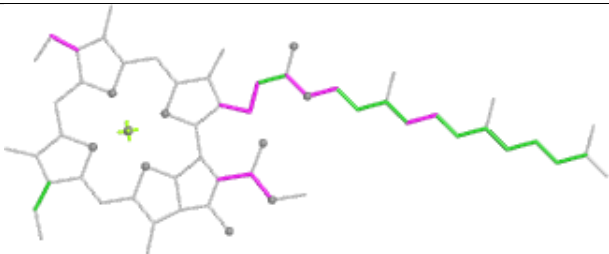
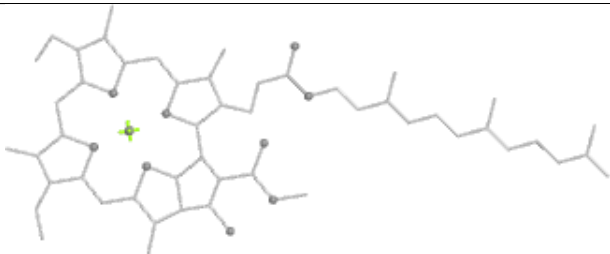
Ligand CLA A 1111

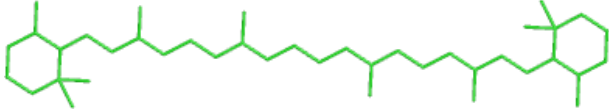
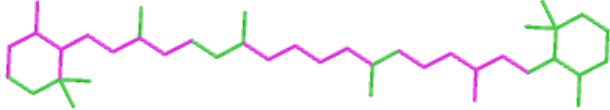
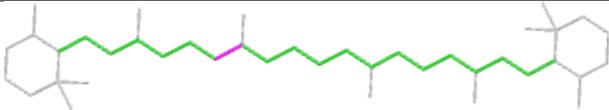
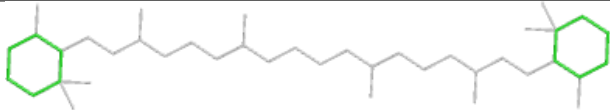


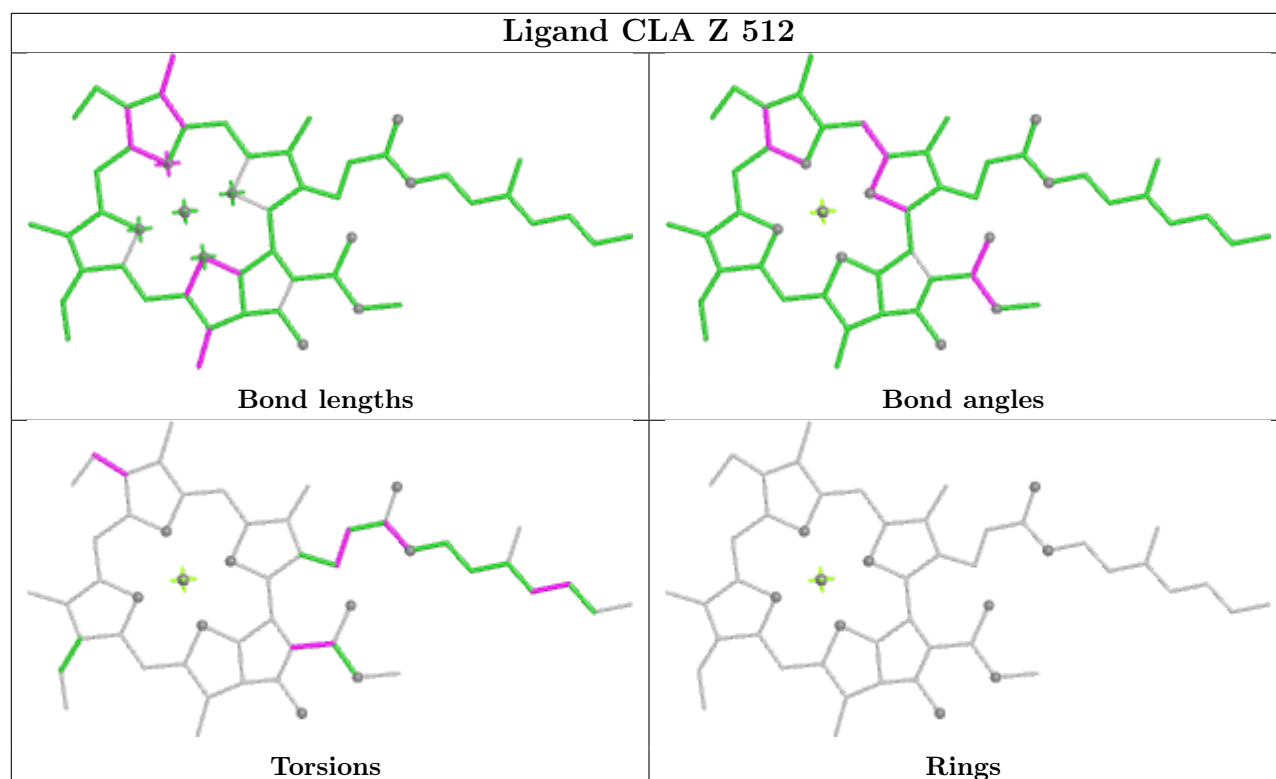
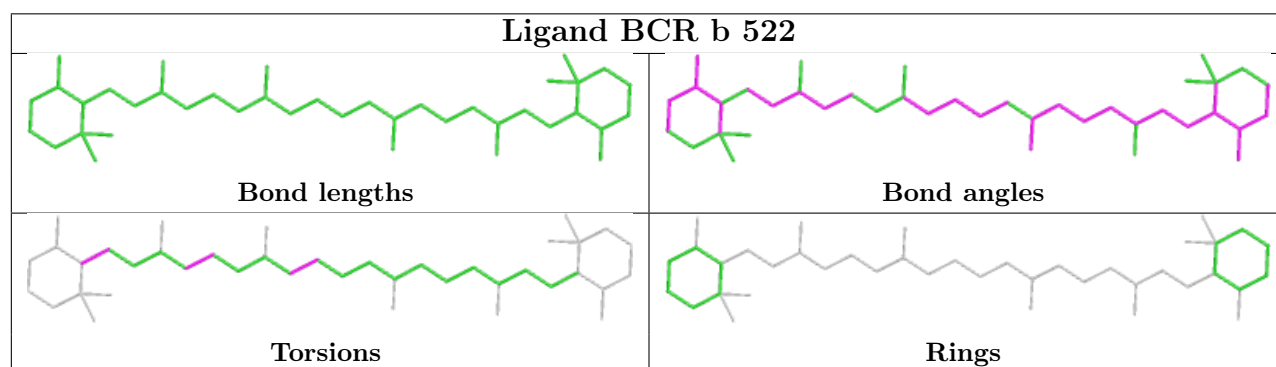
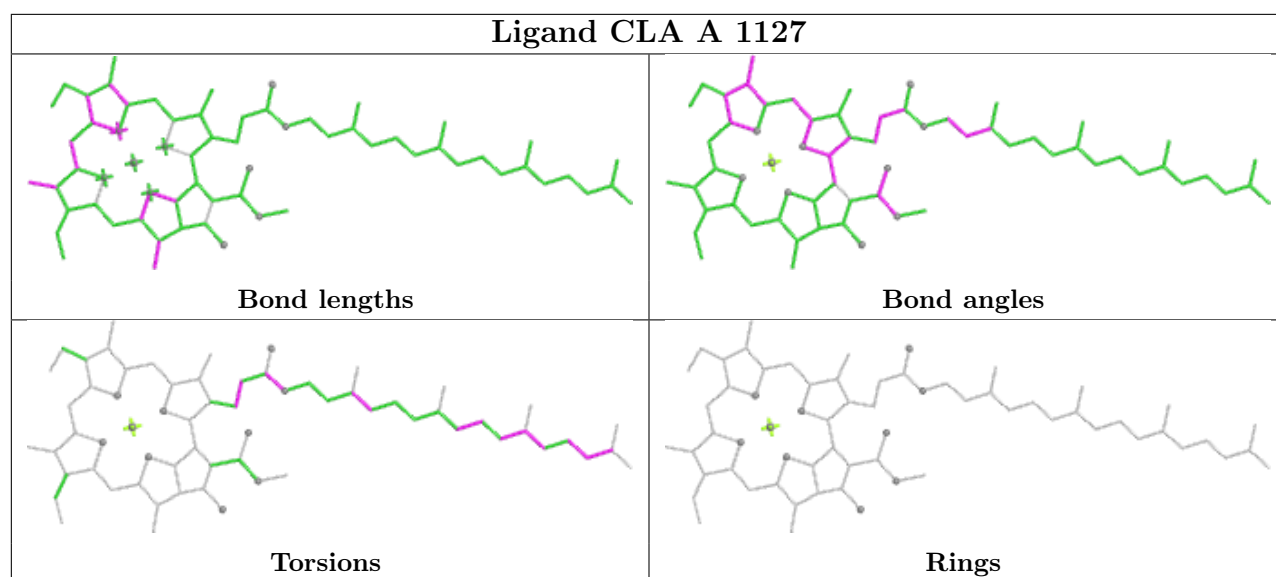
Ligand CLA e 1110



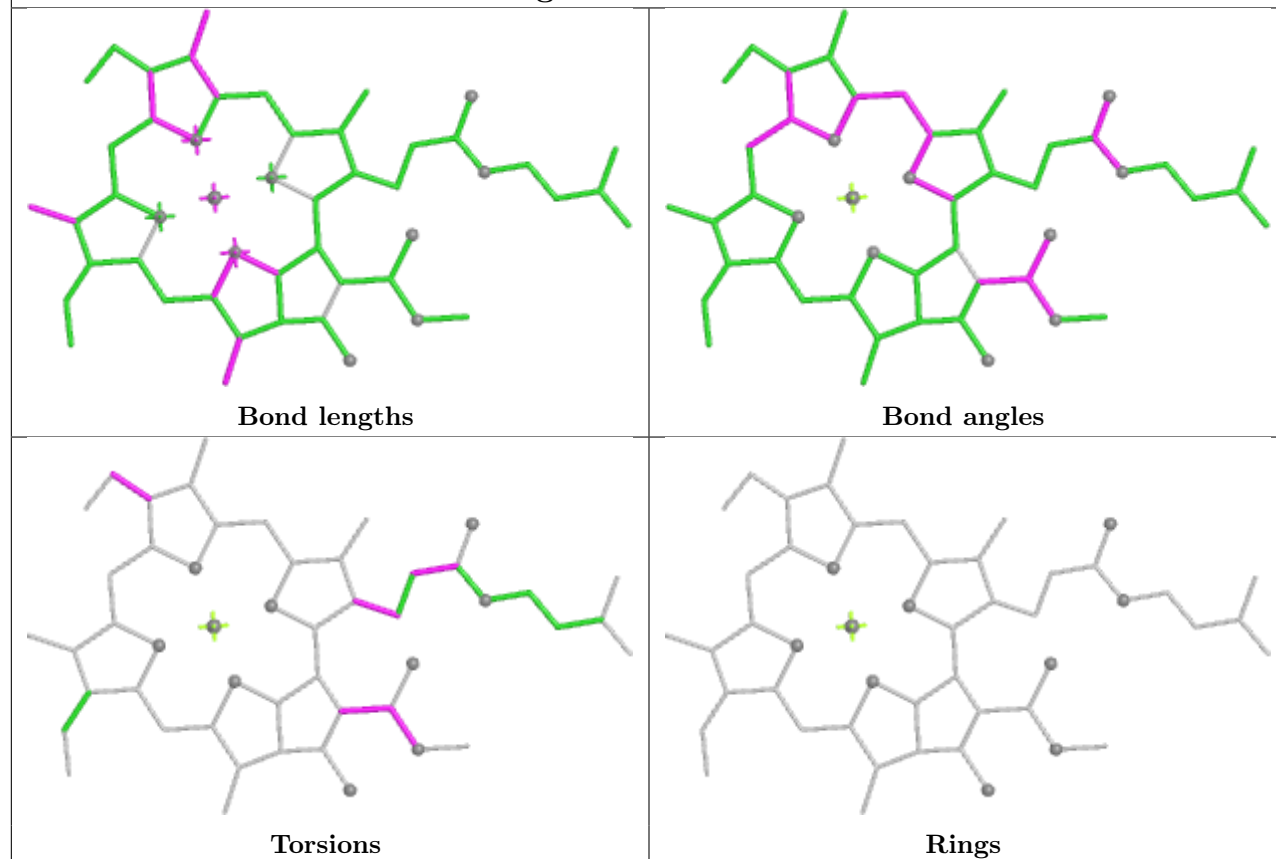
Ligand BCR 1 4015	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1118	
	
Bond lengths	Bond angles
	
Torsions	Rings

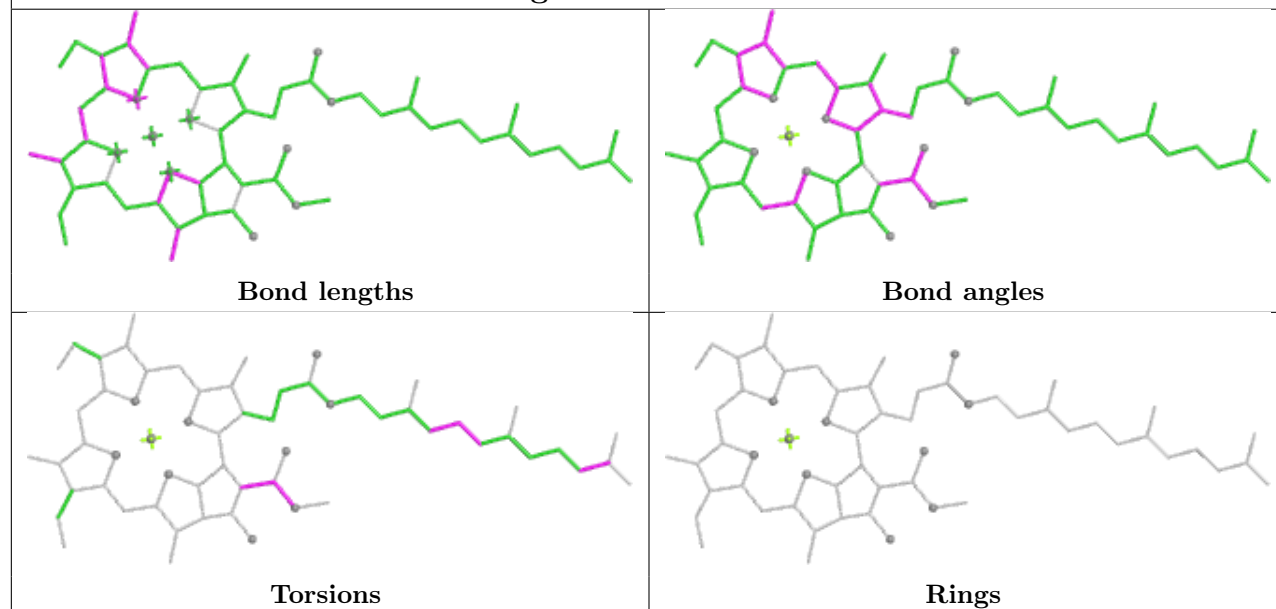
Ligand BCR 1 524	
	
Bond lengths	Bond angles
	
Torsions	Rings



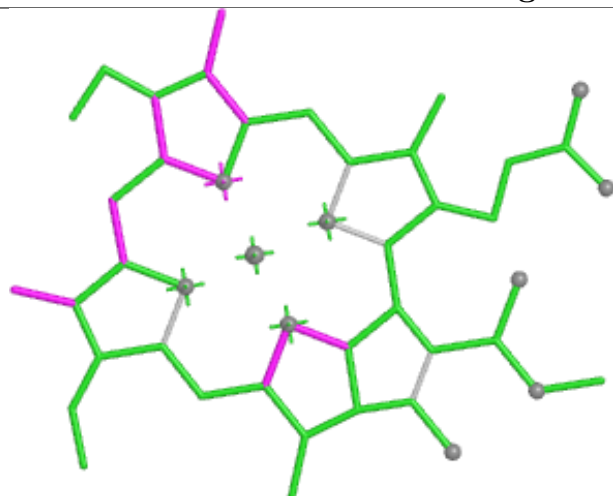
Ligand CLA 1 519



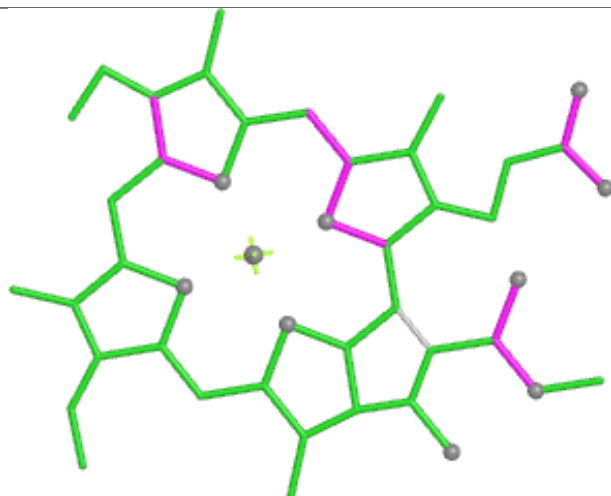
Ligand CLA f 1222



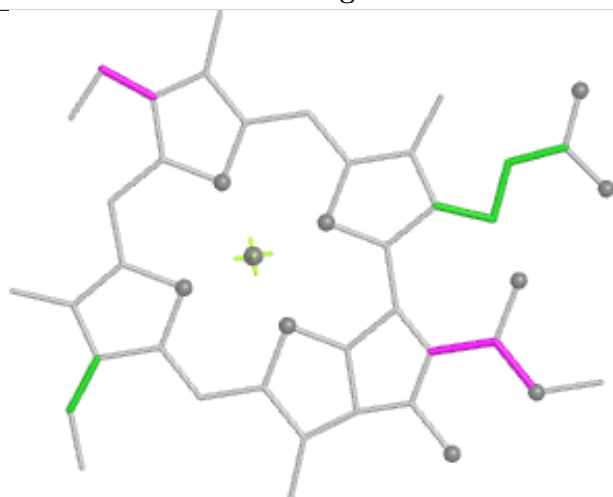
Ligand CLA 5 506



Bond lengths



Bond angles

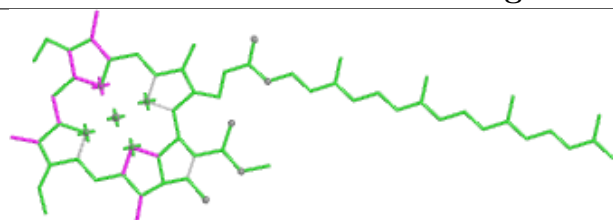


Torsions

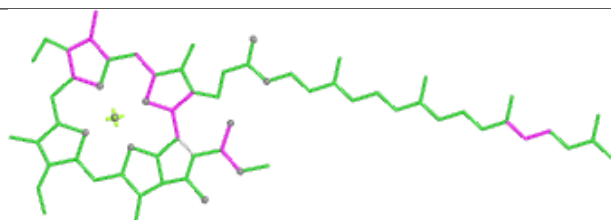


Rings

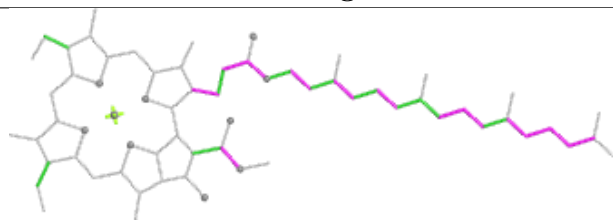
Ligand CLA A 1126



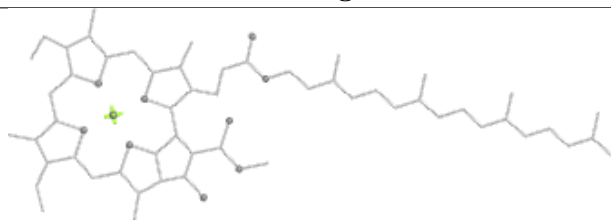
Bond lengths



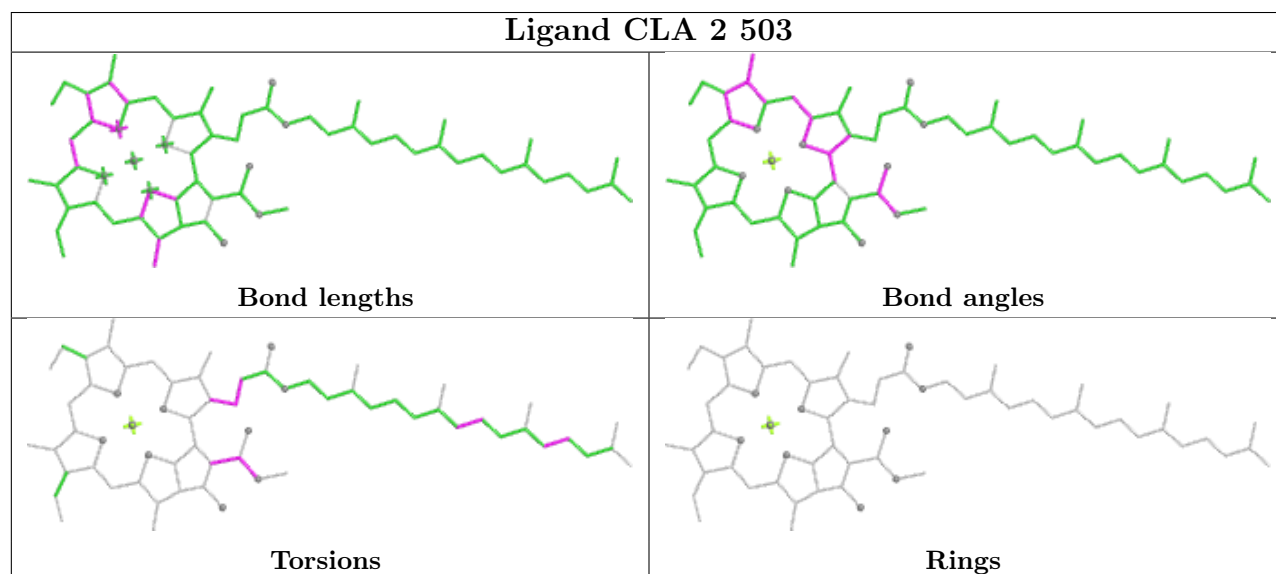
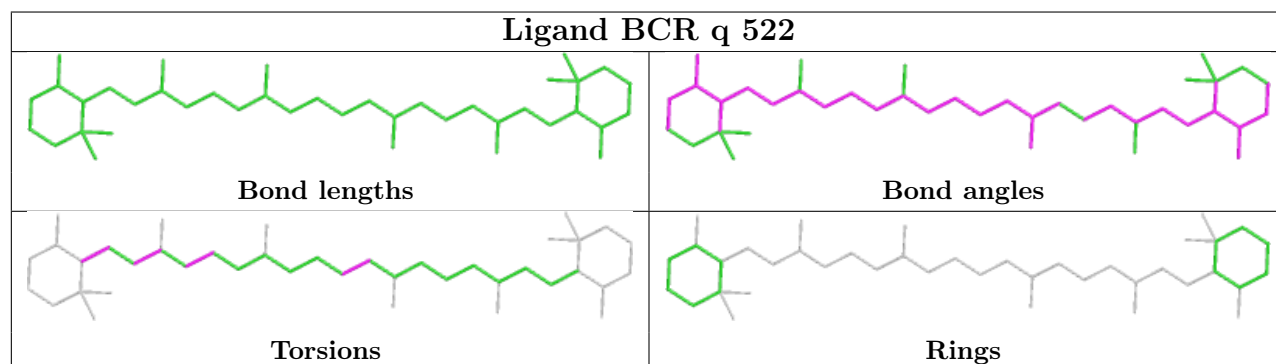
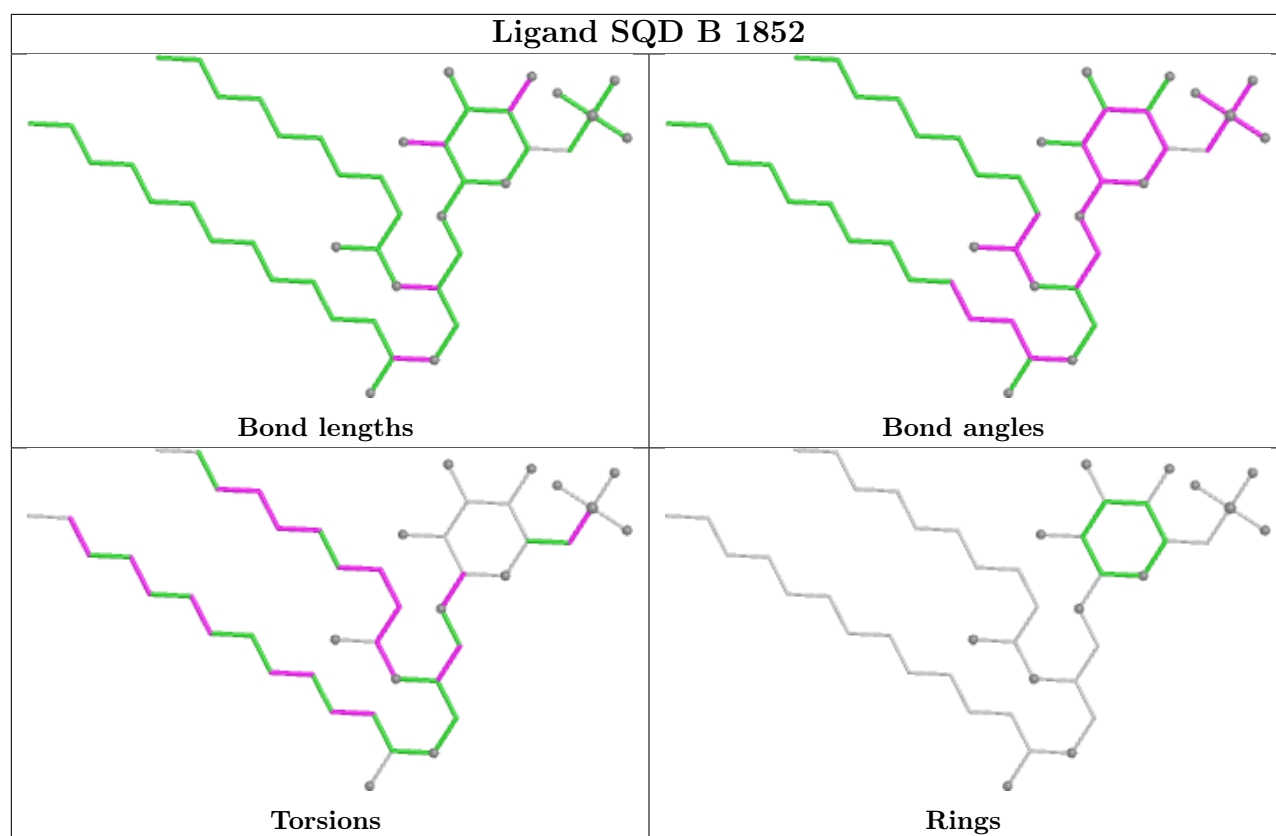
Bond angles

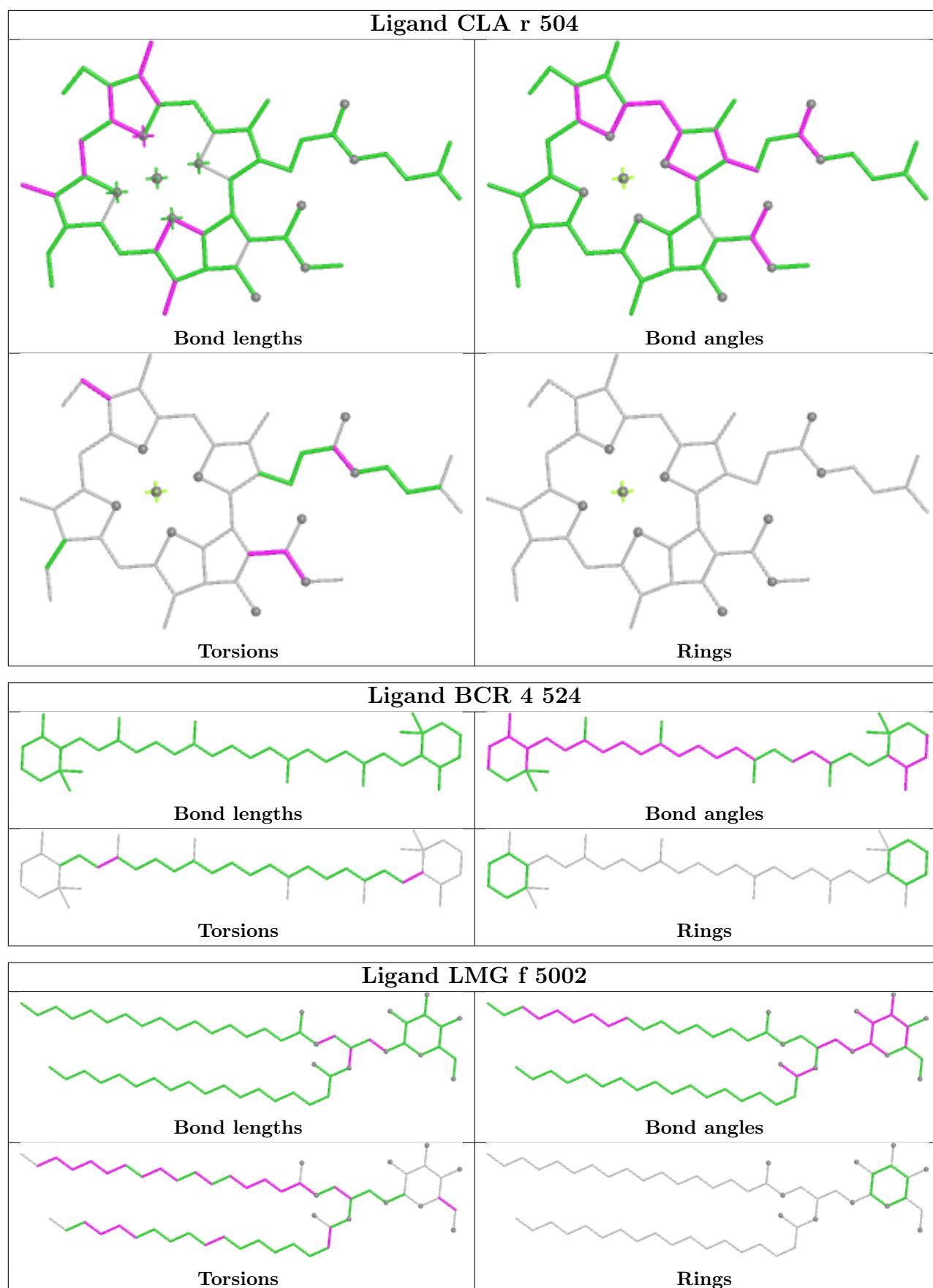


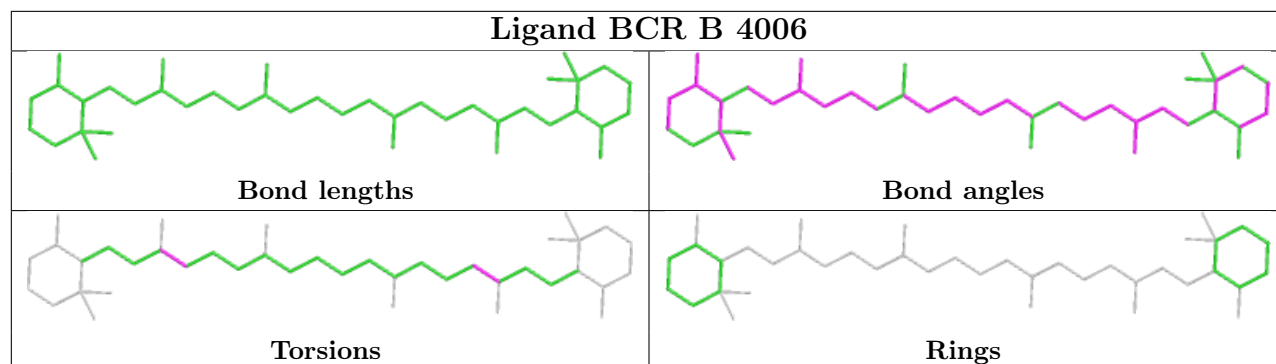
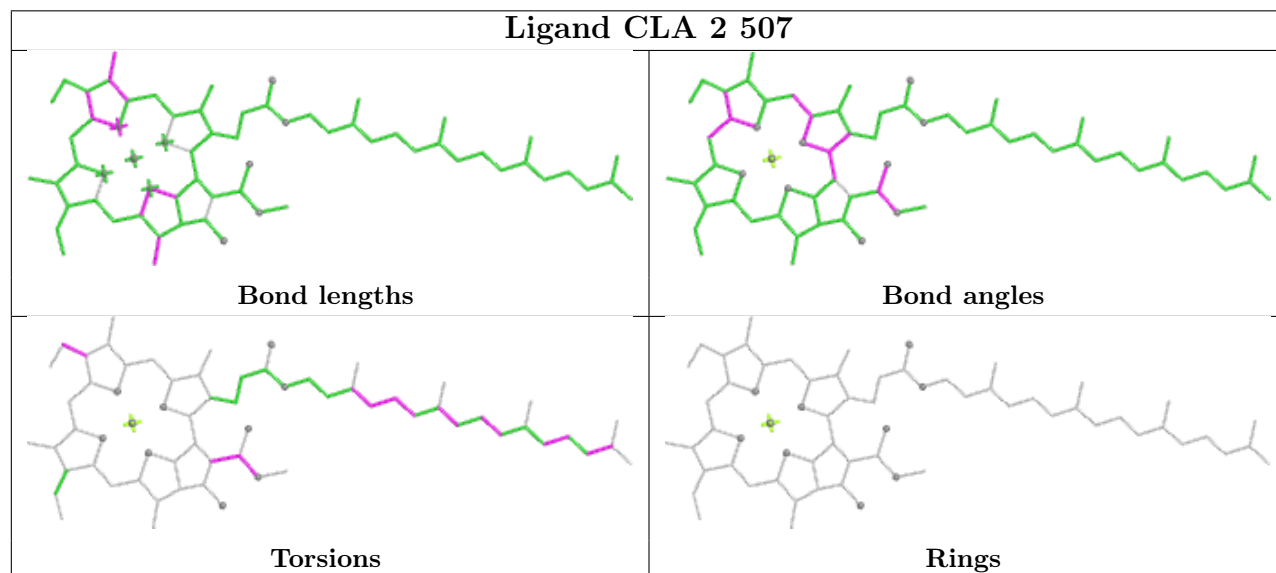
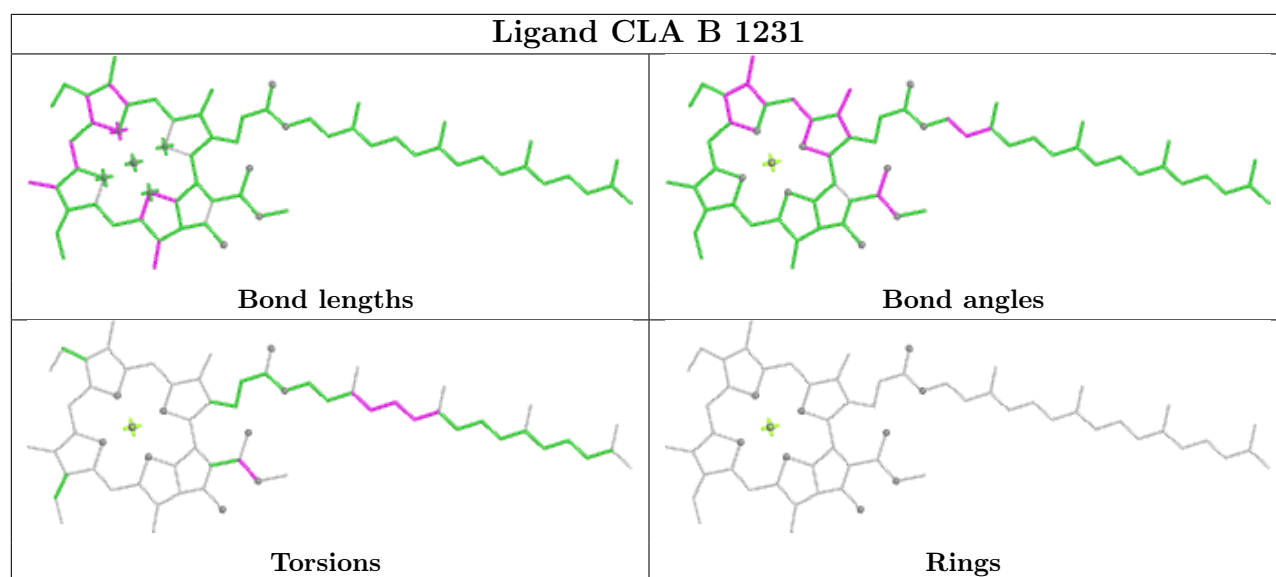
Torsions



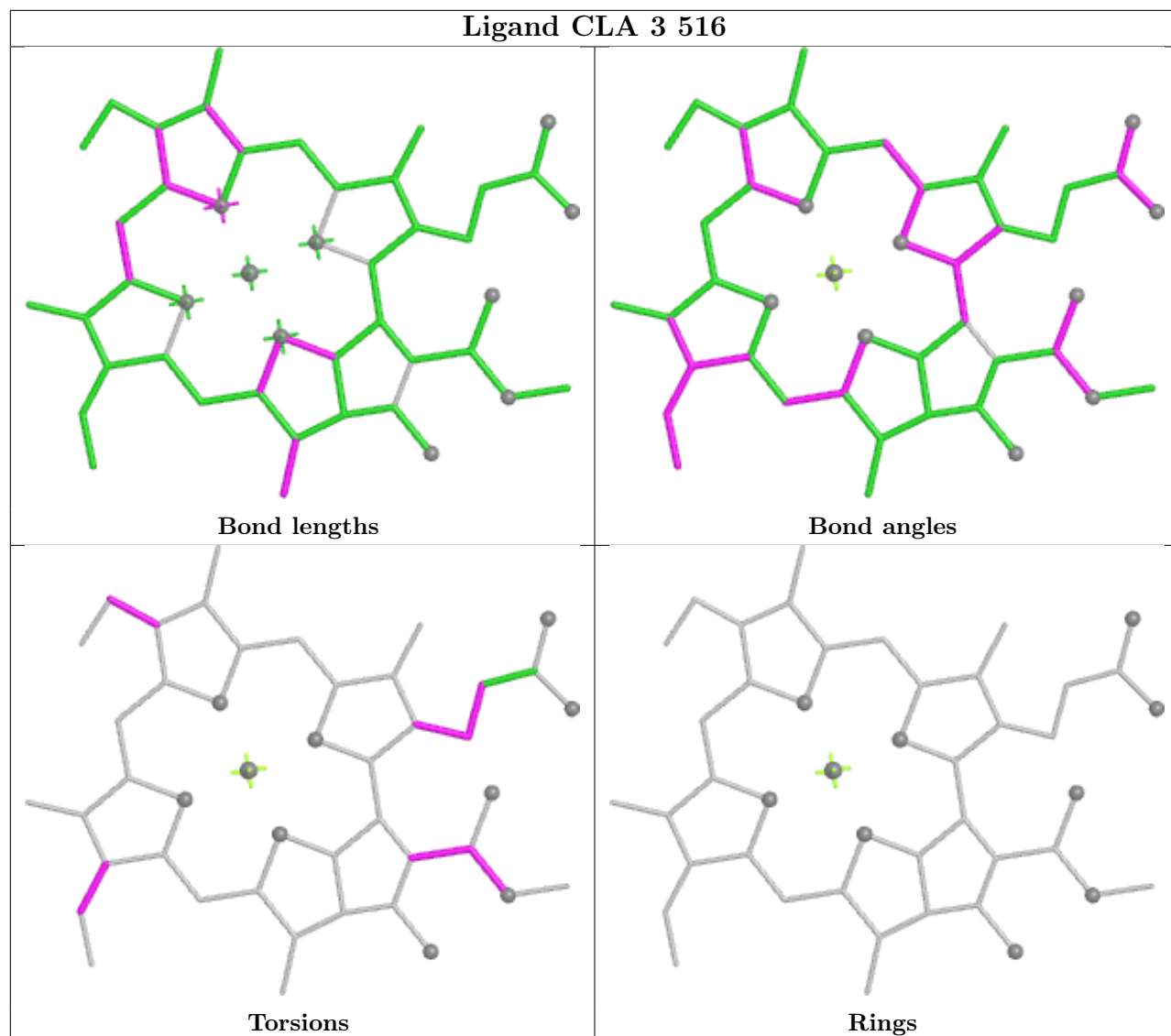
Rings



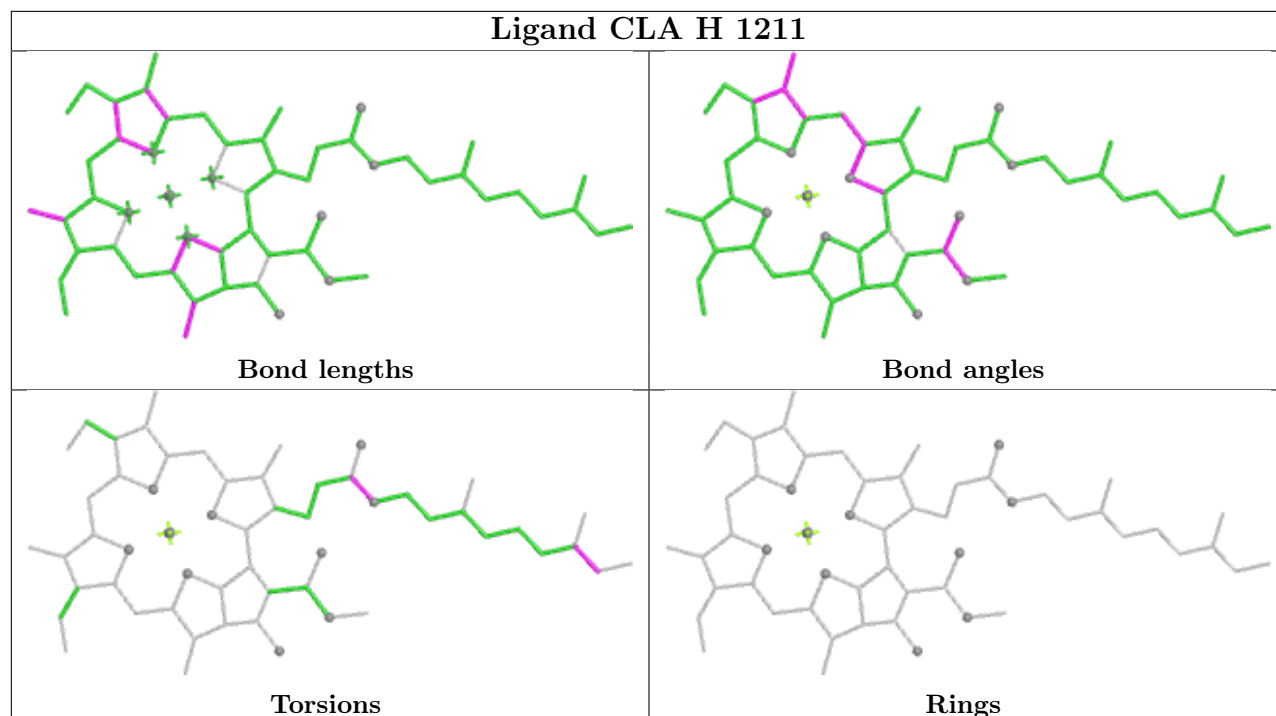




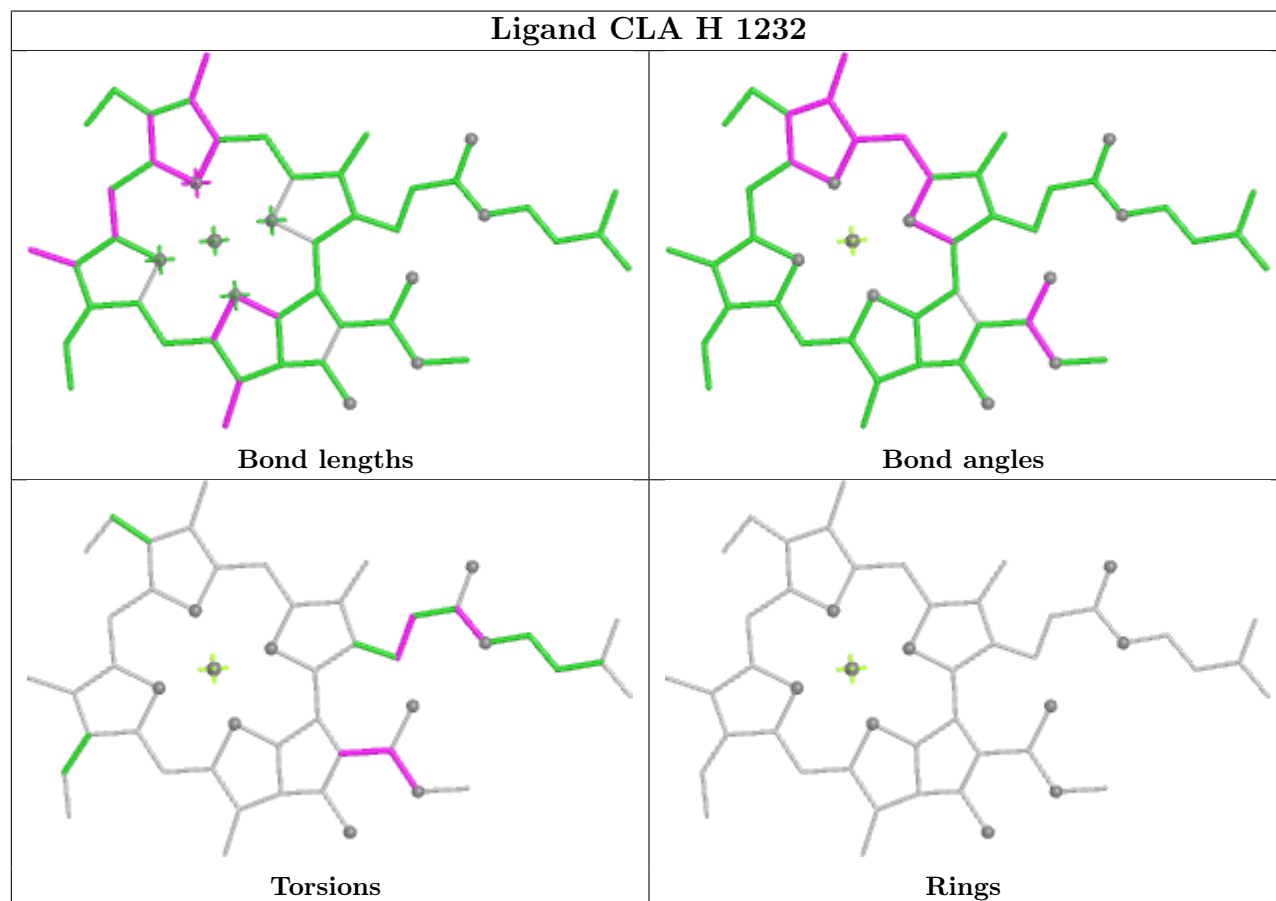
Ligand CLA 3 516

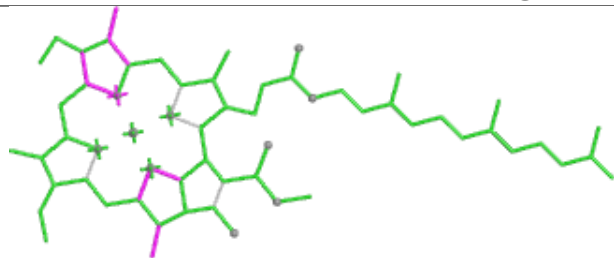
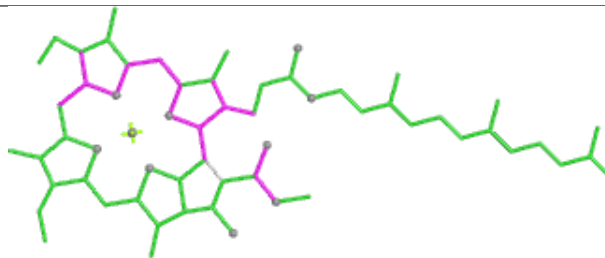
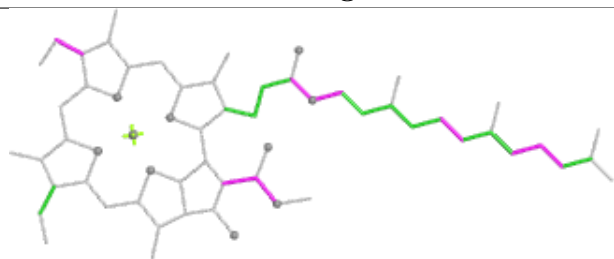
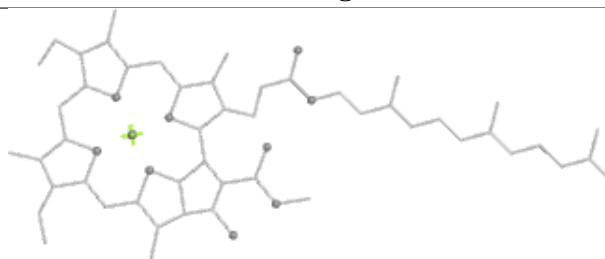
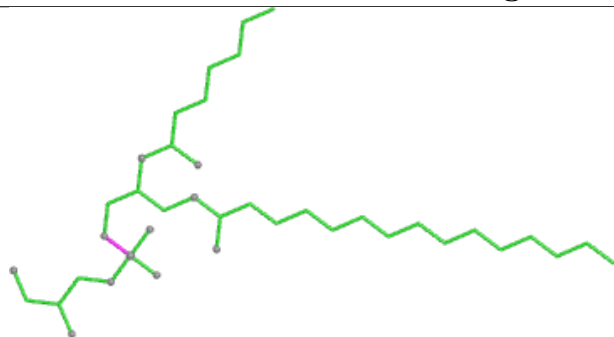
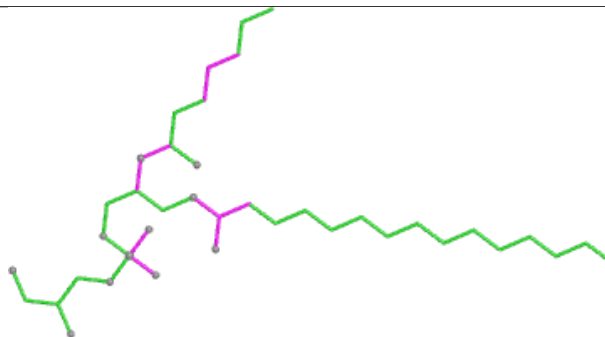
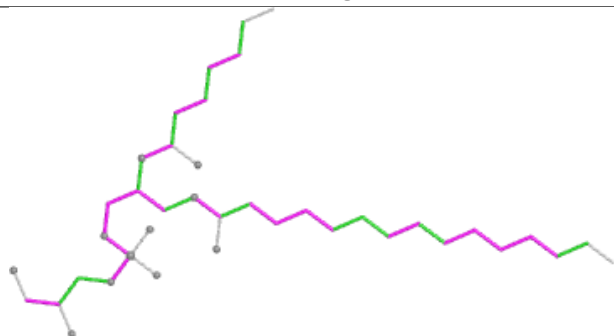
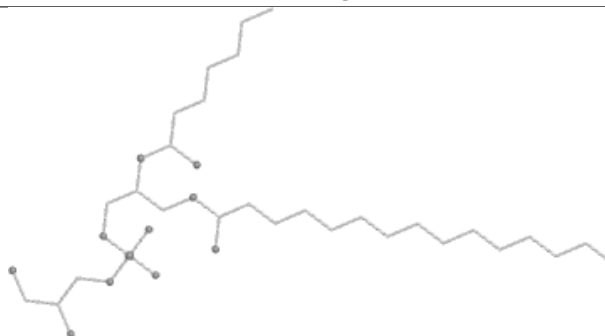


Ligand CLA H 1211

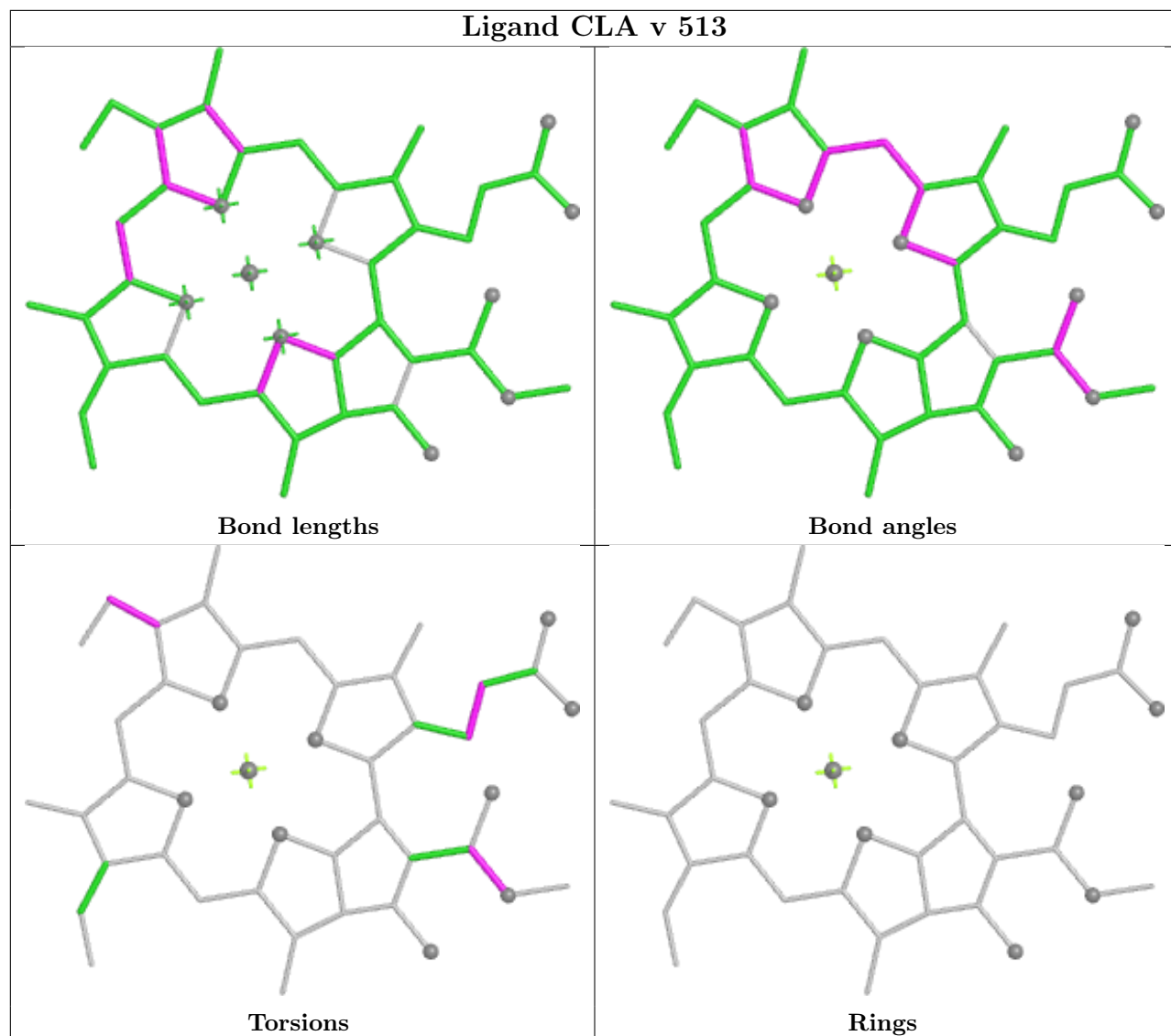


Ligand CLA H 1232

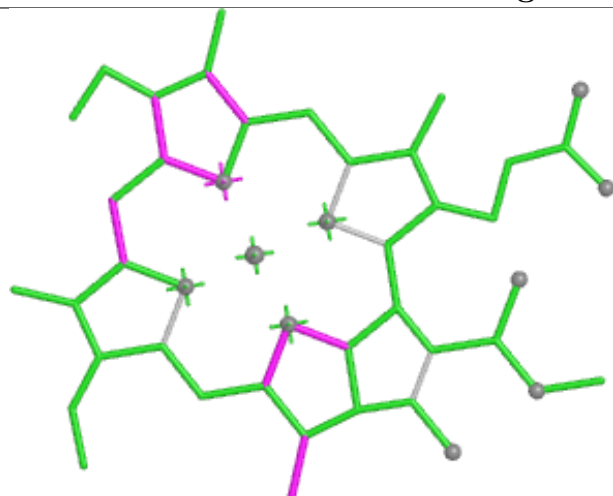


Ligand CLA Z 502**Bond lengths****Bond angles****Torsions****Rings****Ligand LHG A 5002****Bond lengths****Bond angles****Torsions****Rings**

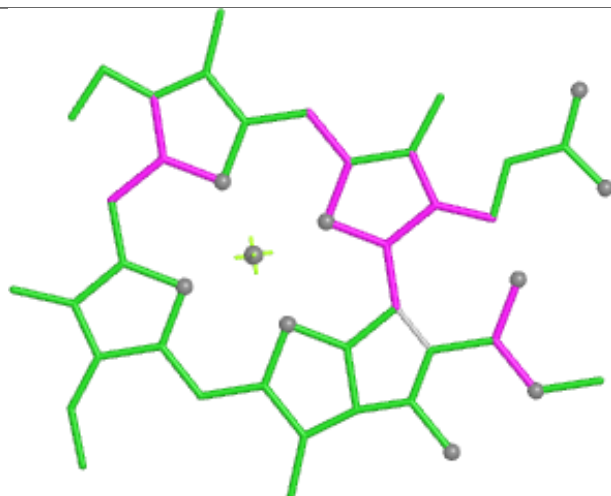
Ligand CLA v 513



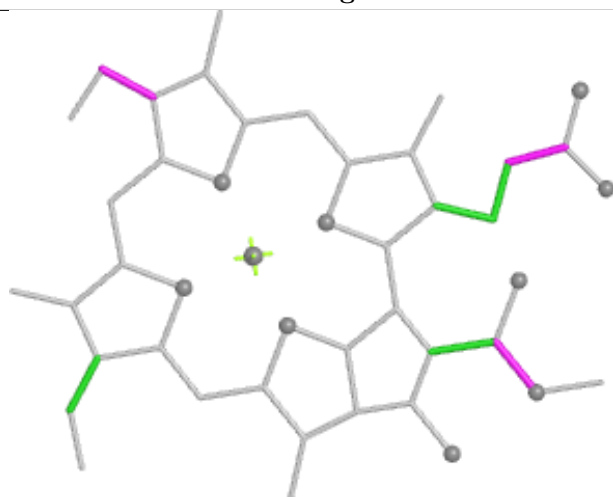
Ligand CLA d 507



Bond lengths



Bond angles

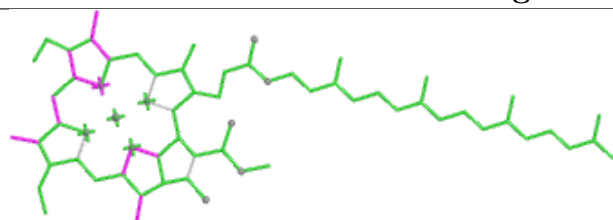


Torsions

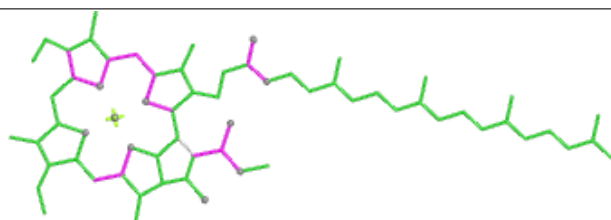


Rings

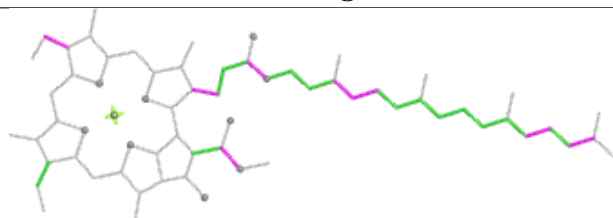
Ligand CLA f 1227



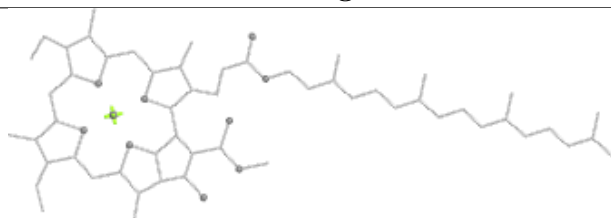
Bond lengths



Bond angles

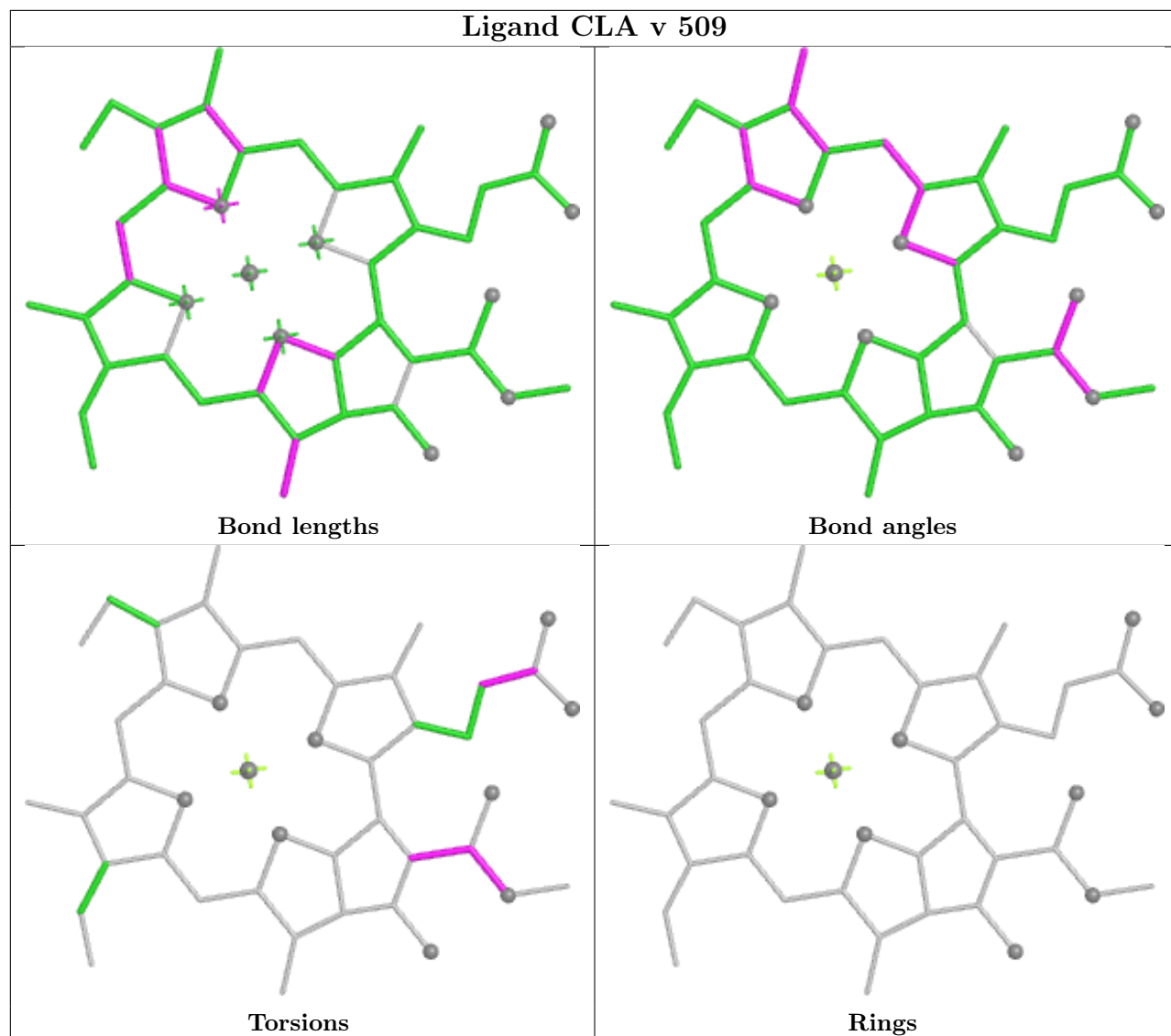


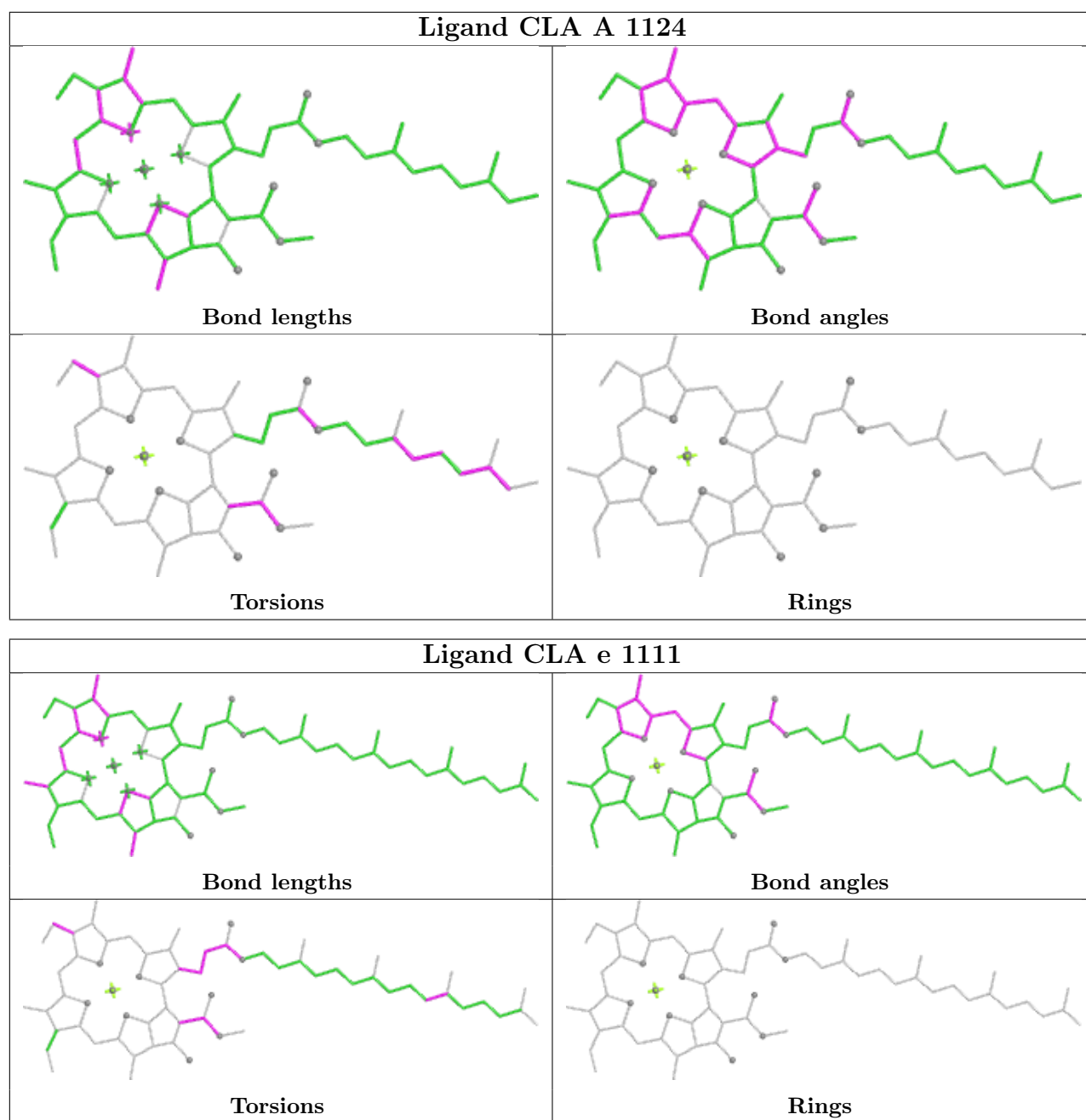
Torsions

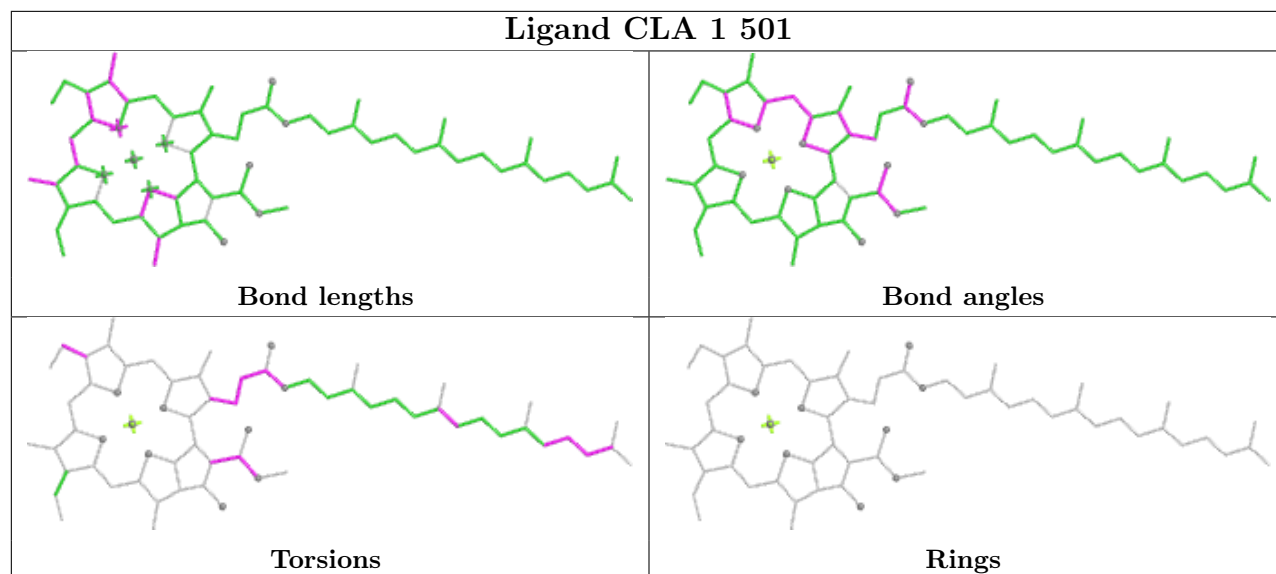
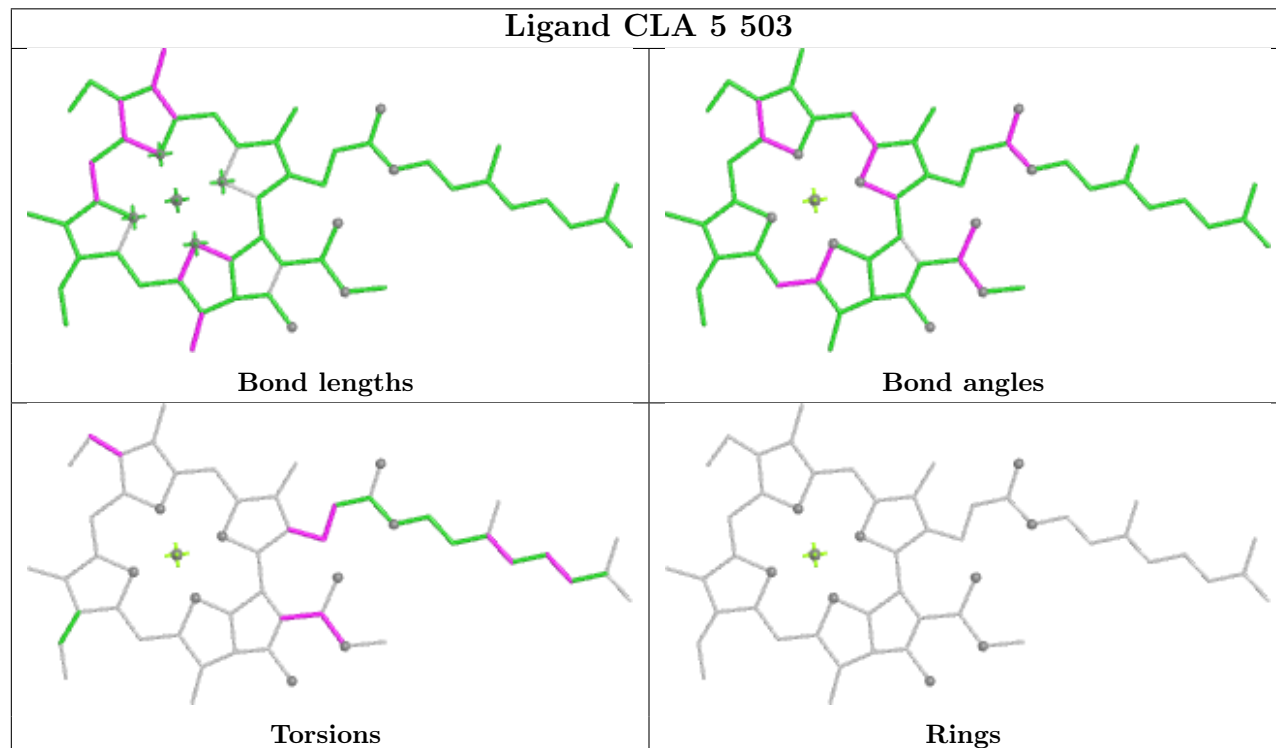


Rings

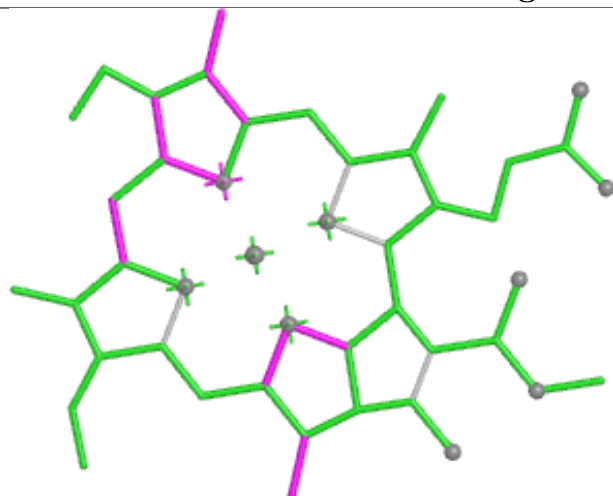
Ligand CLA v 509



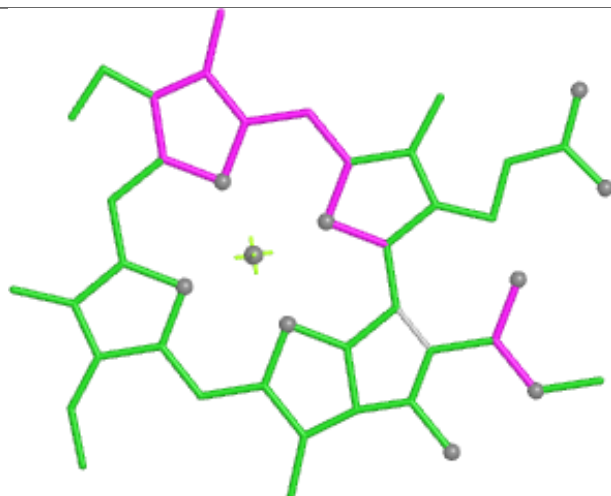


Ligand CLA 1 501**Ligand CLA 5 503**

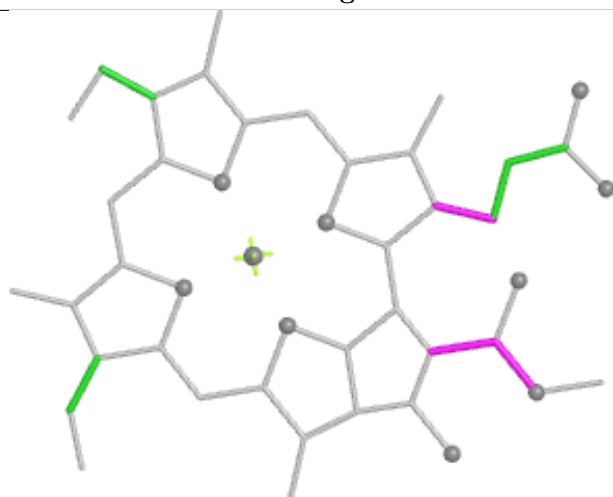
Ligand CLA a 504



Bond lengths



Bond angles

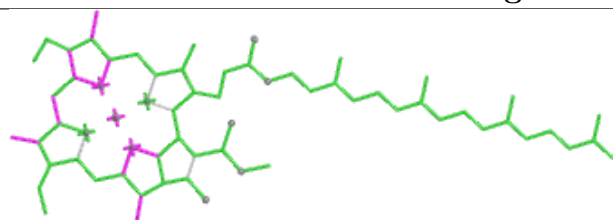


Torsions

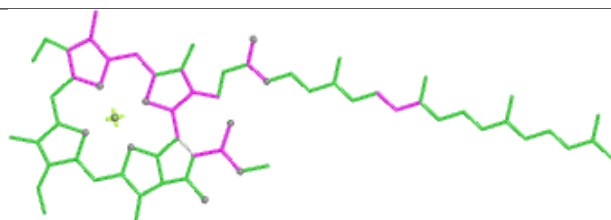


Rings

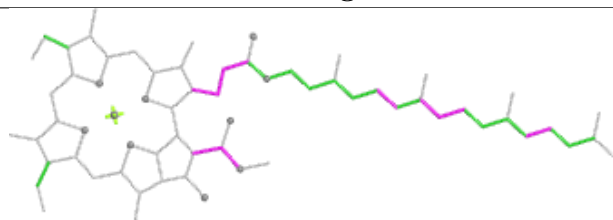
Ligand CLA H 1221



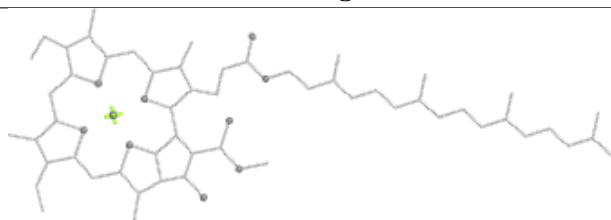
Bond lengths



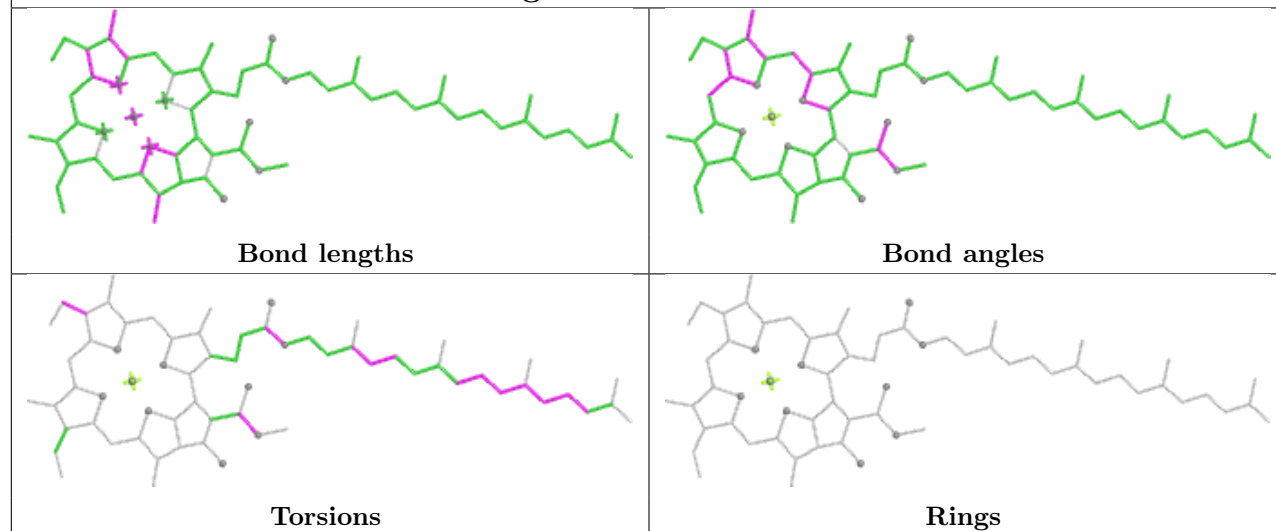
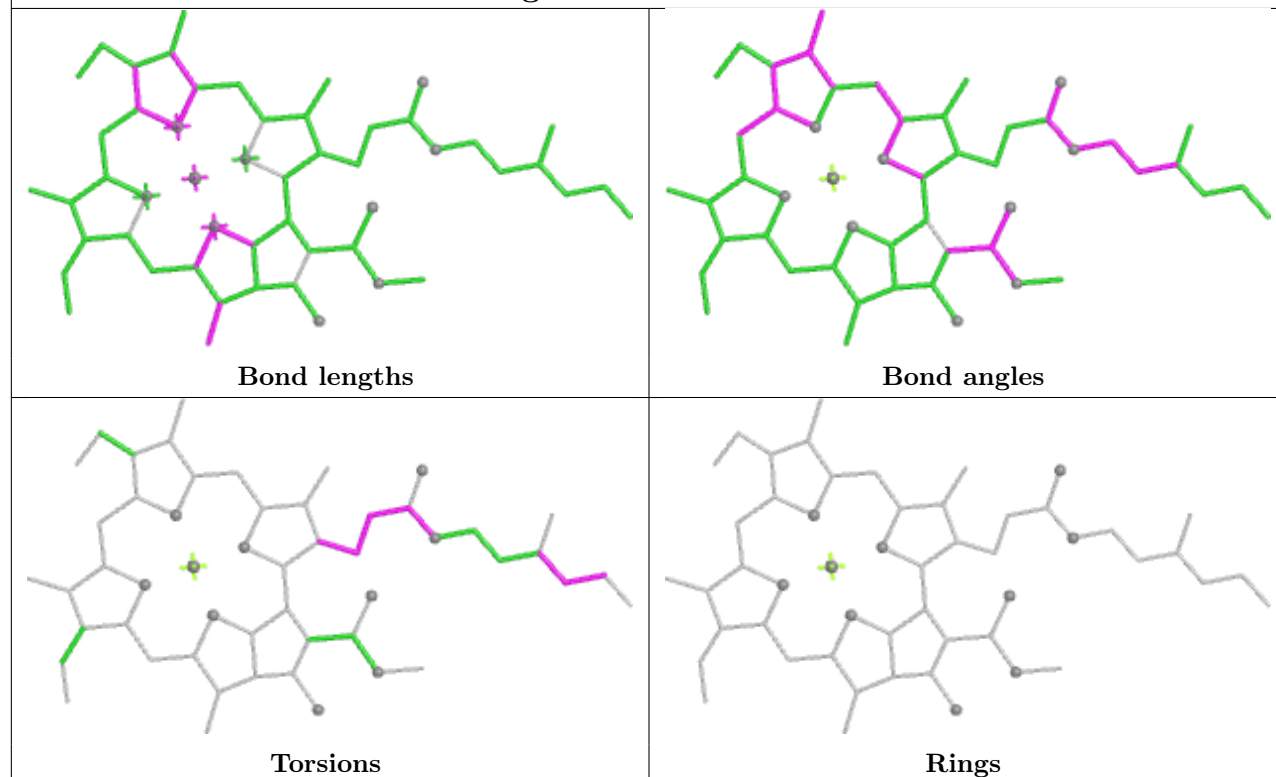
Bond angles

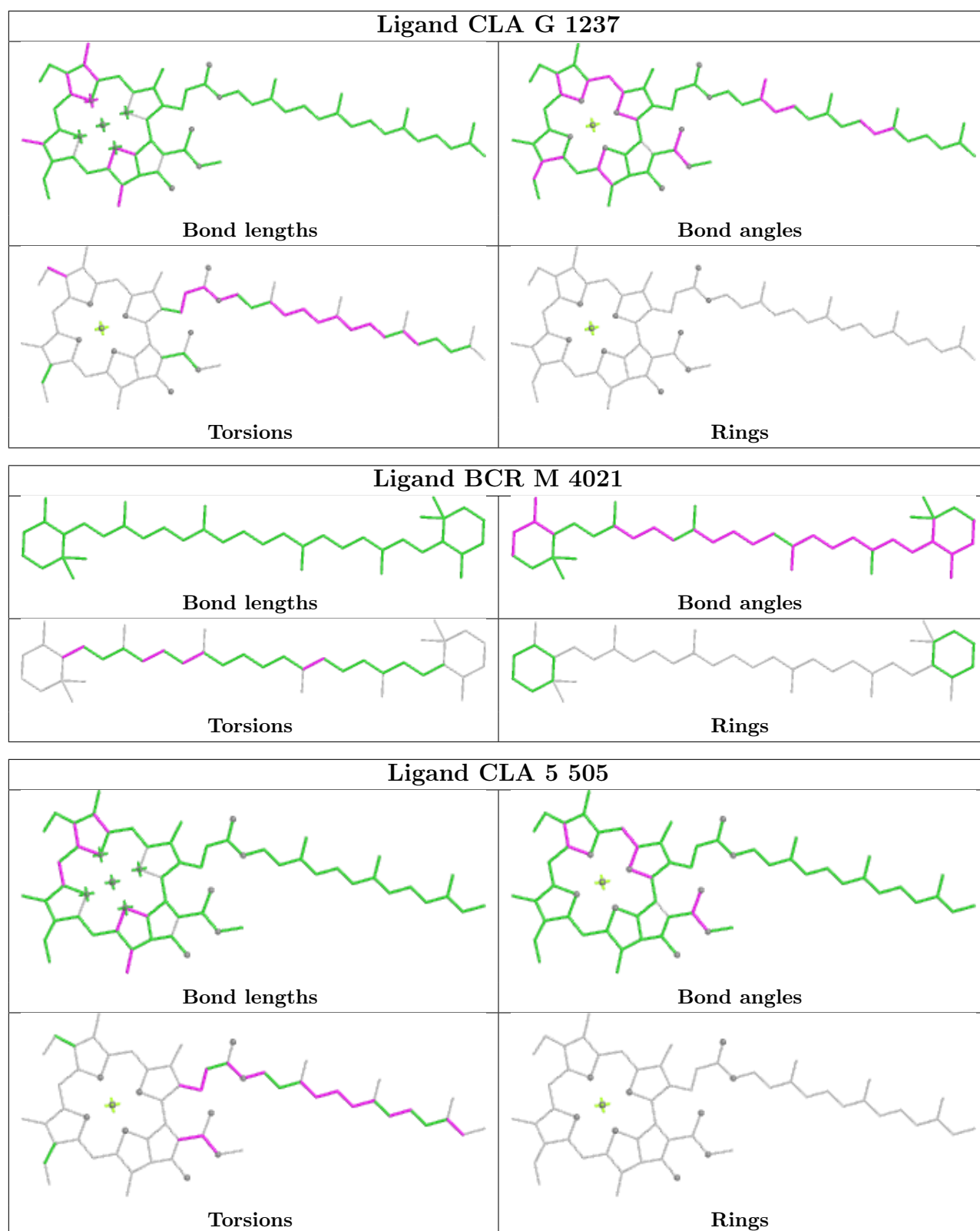


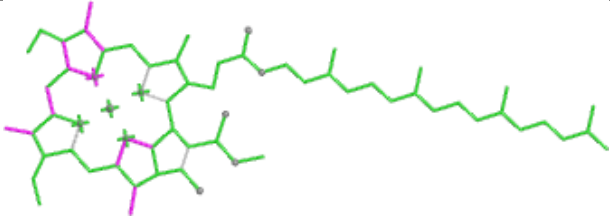
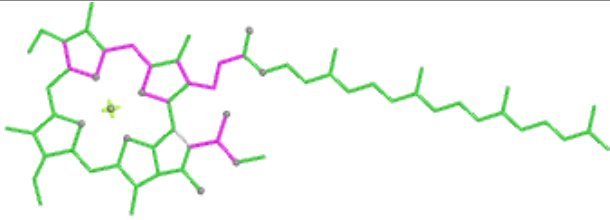
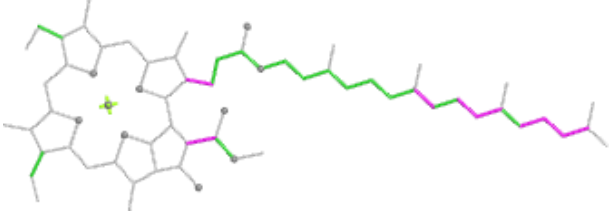
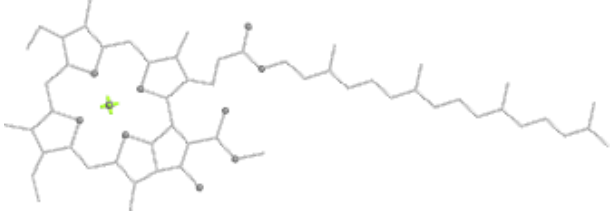
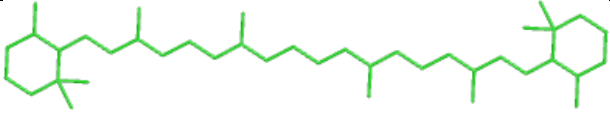
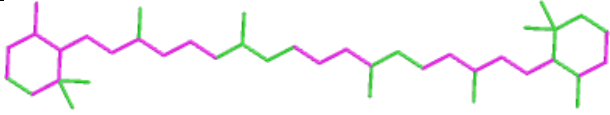
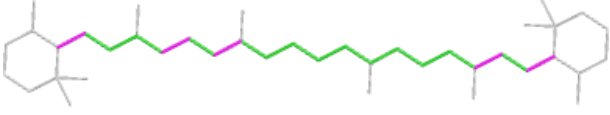
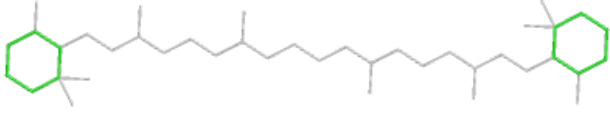
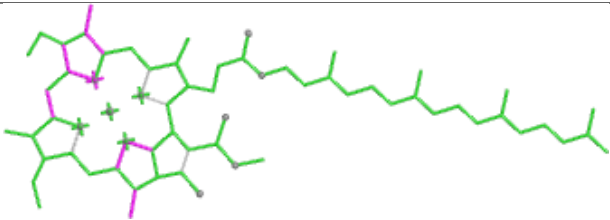
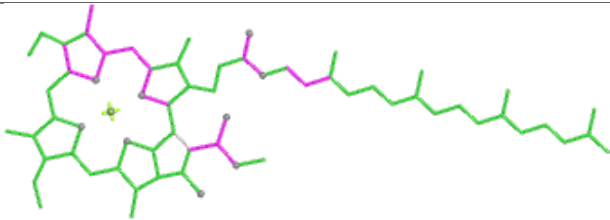
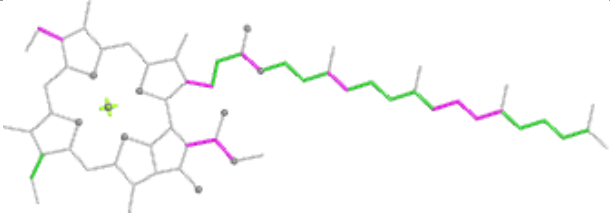
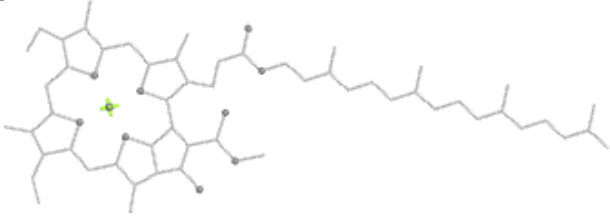
Torsions

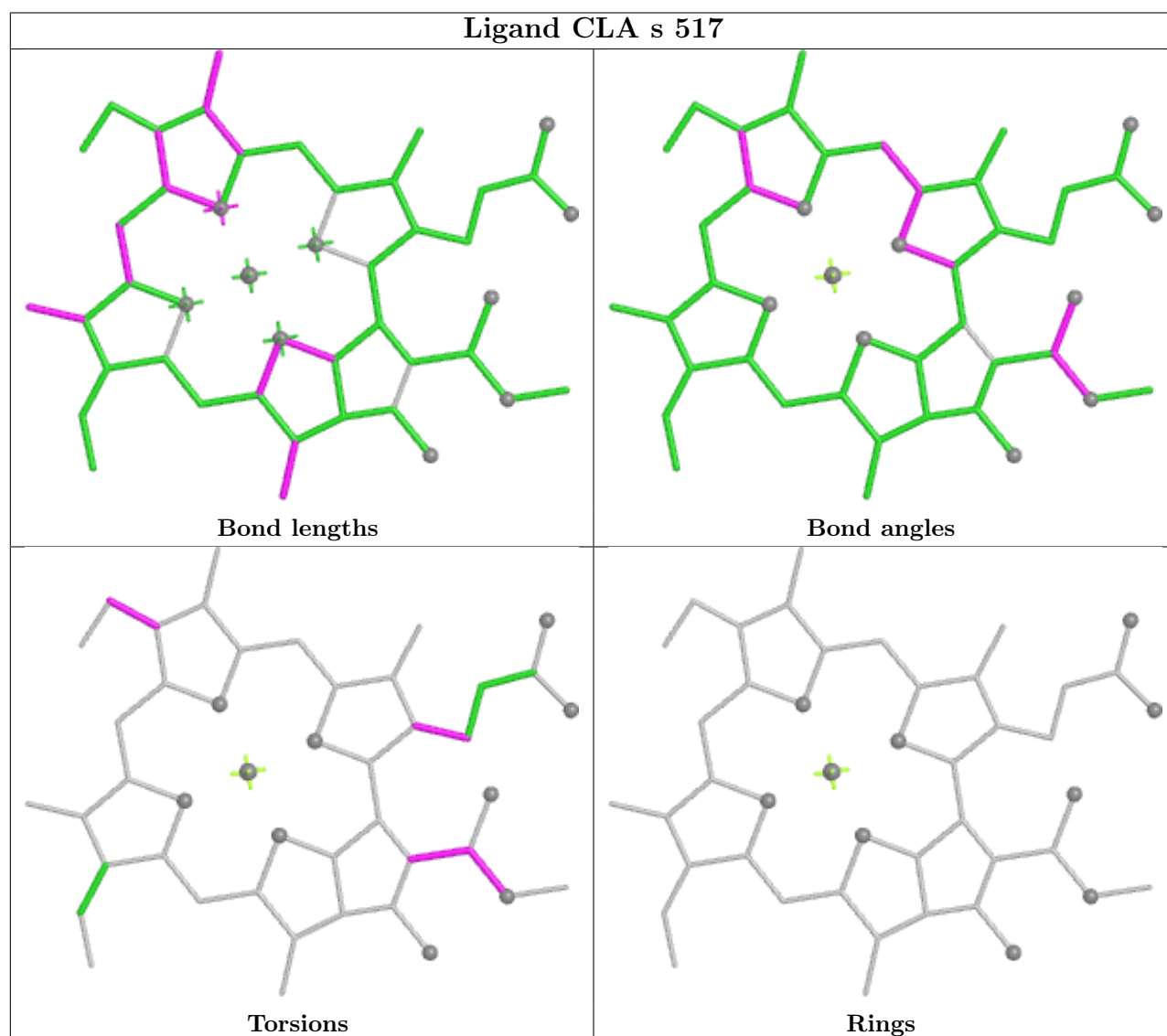
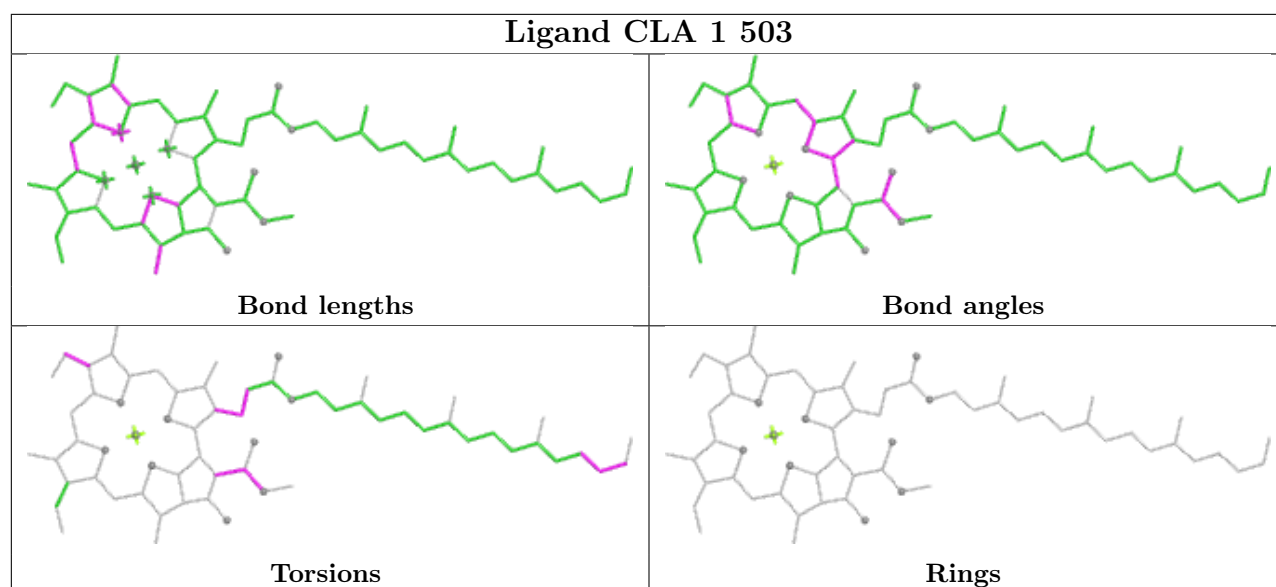


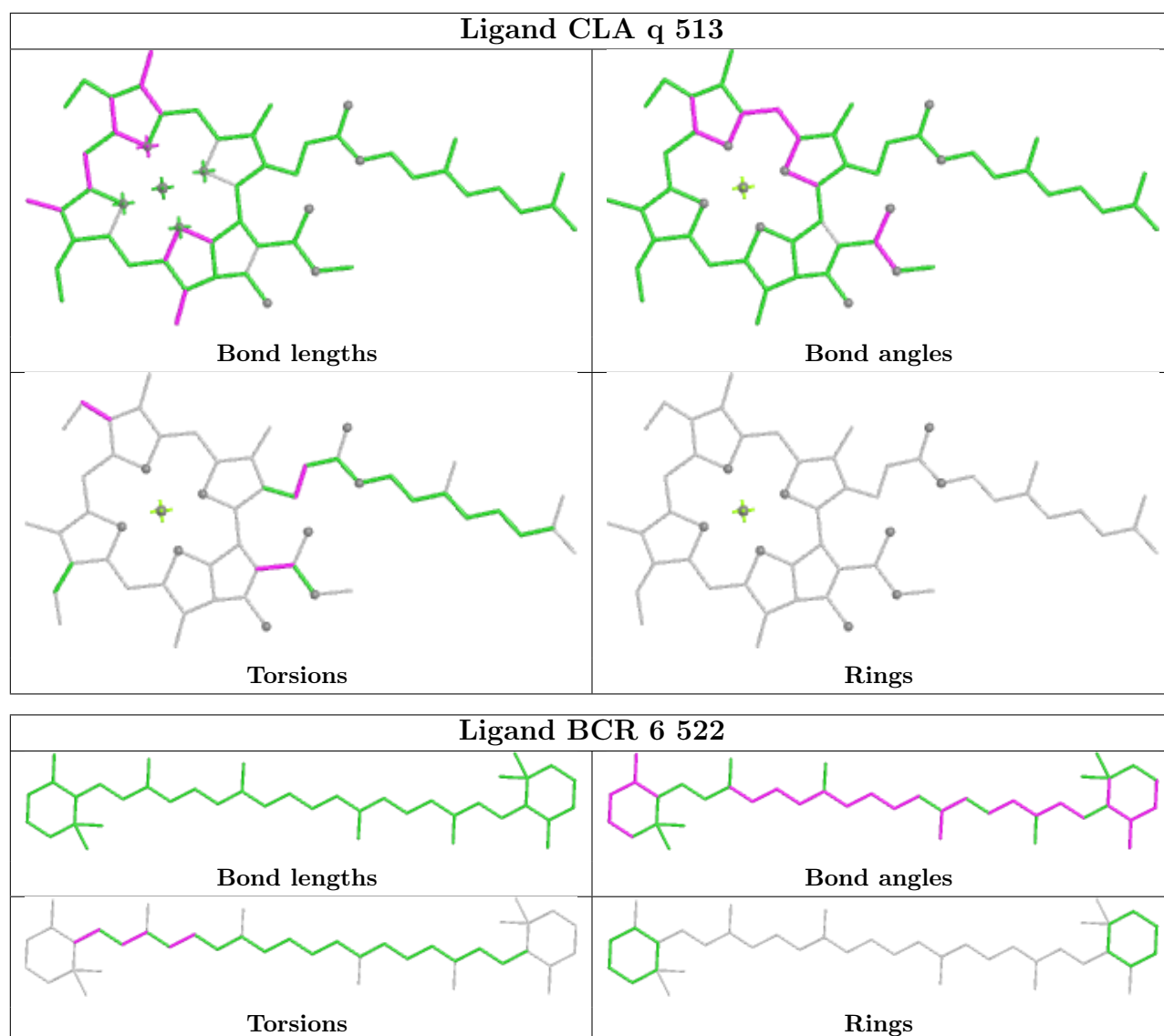
Rings

Ligand CLA A 1133**Ligand CLA G 1135**

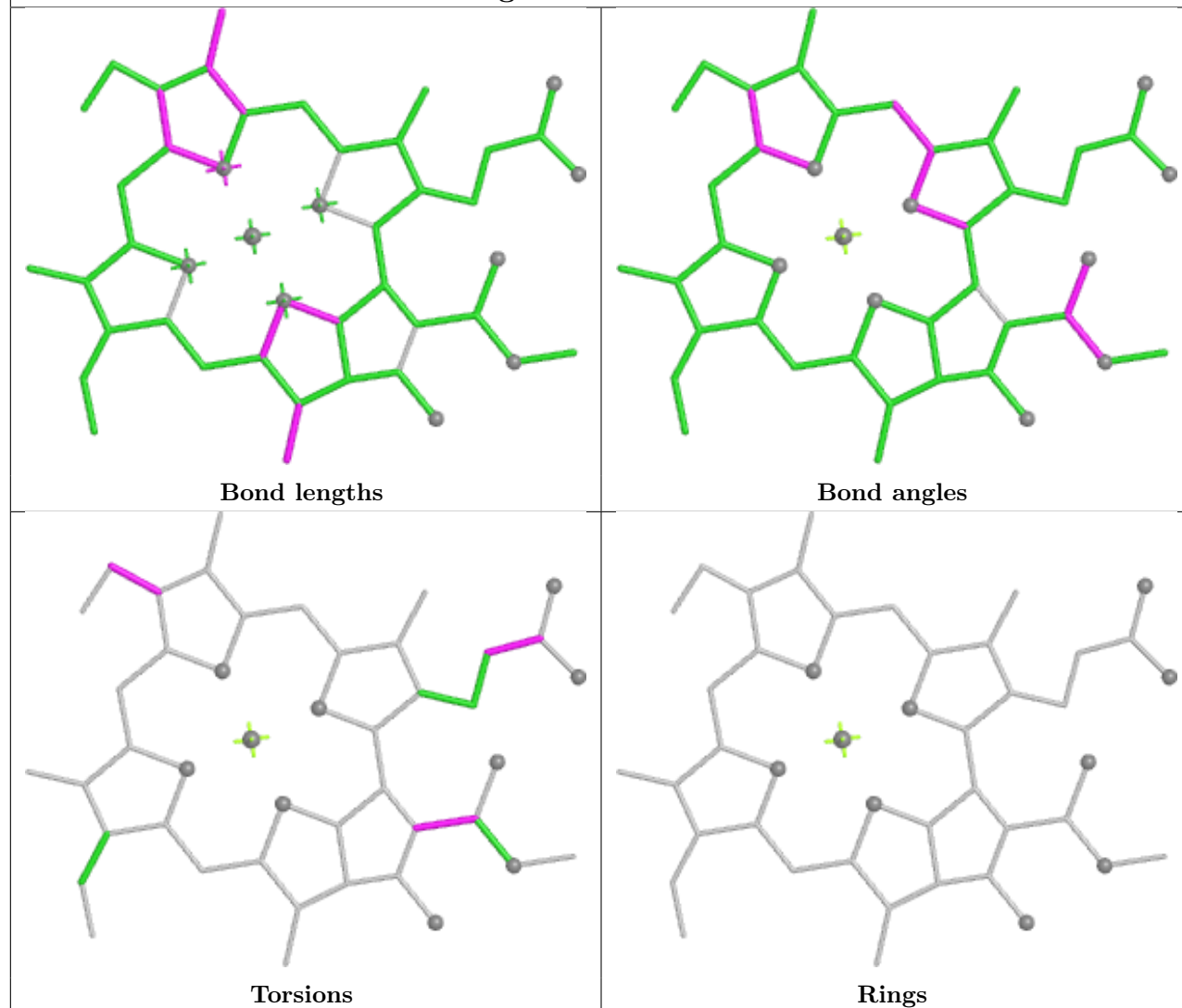


Ligand CLA e 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 1 4012	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA H 1240	
 Bond lengths	 Bond angles
 Torsions	 Rings

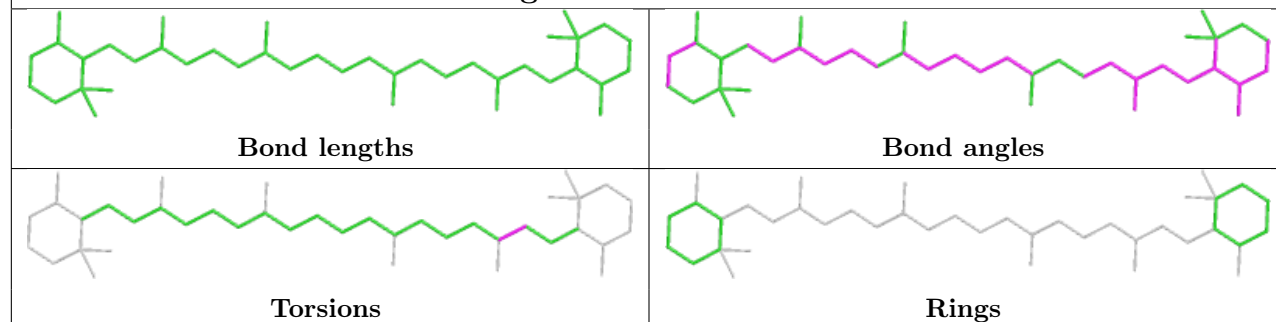


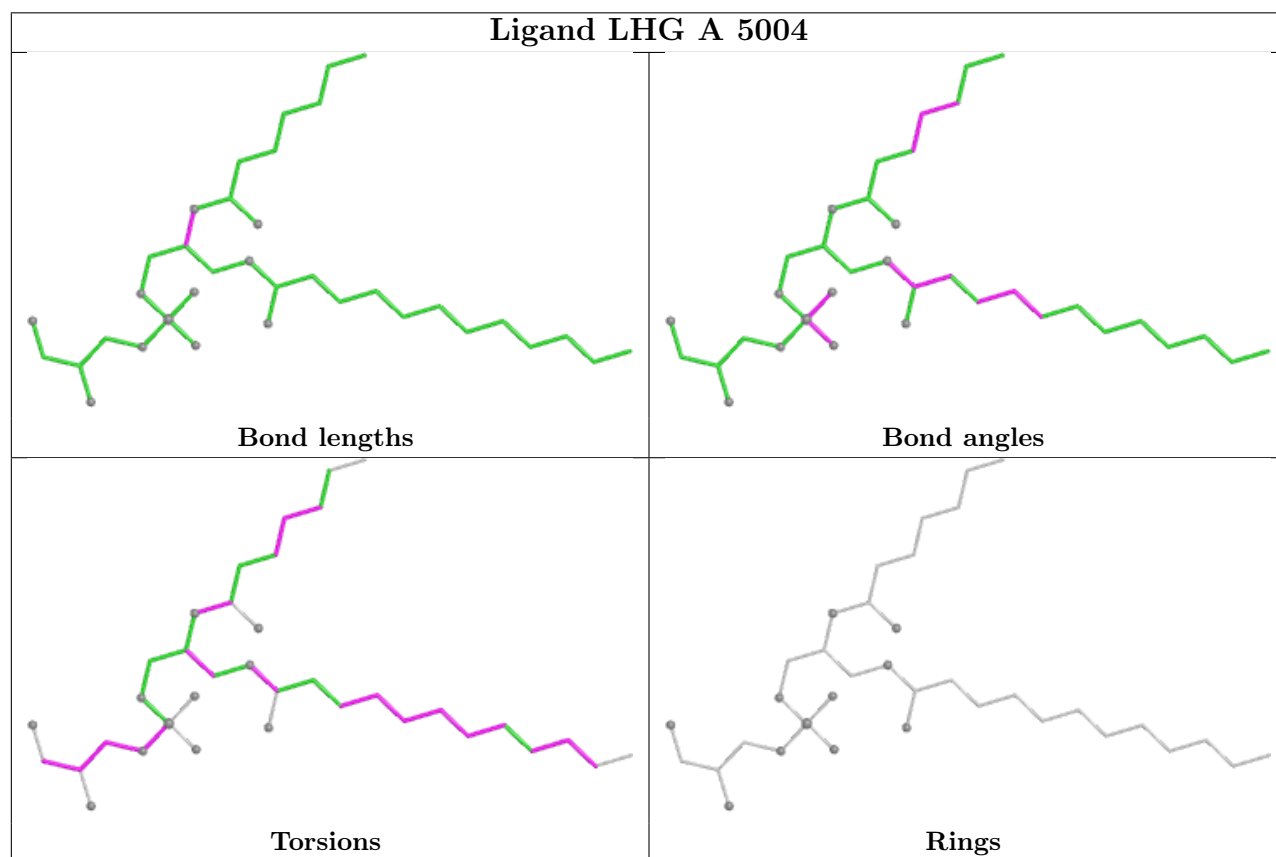
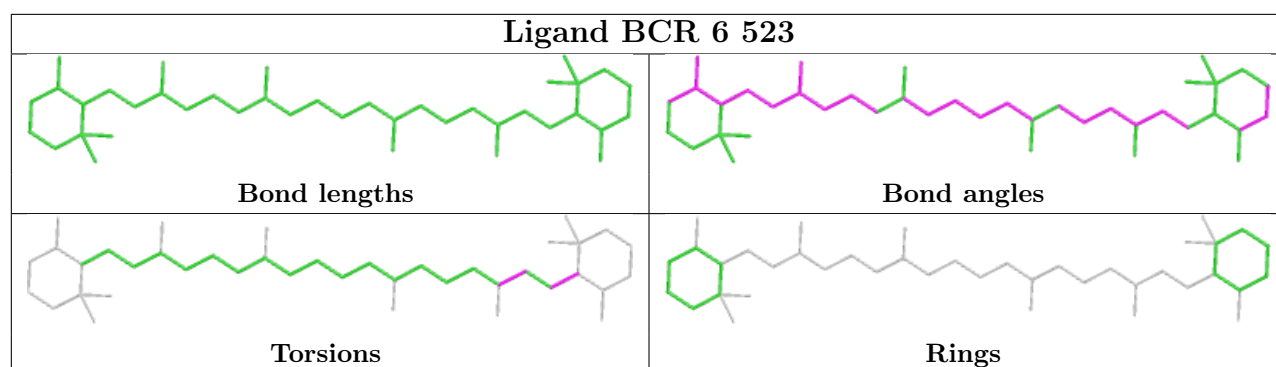


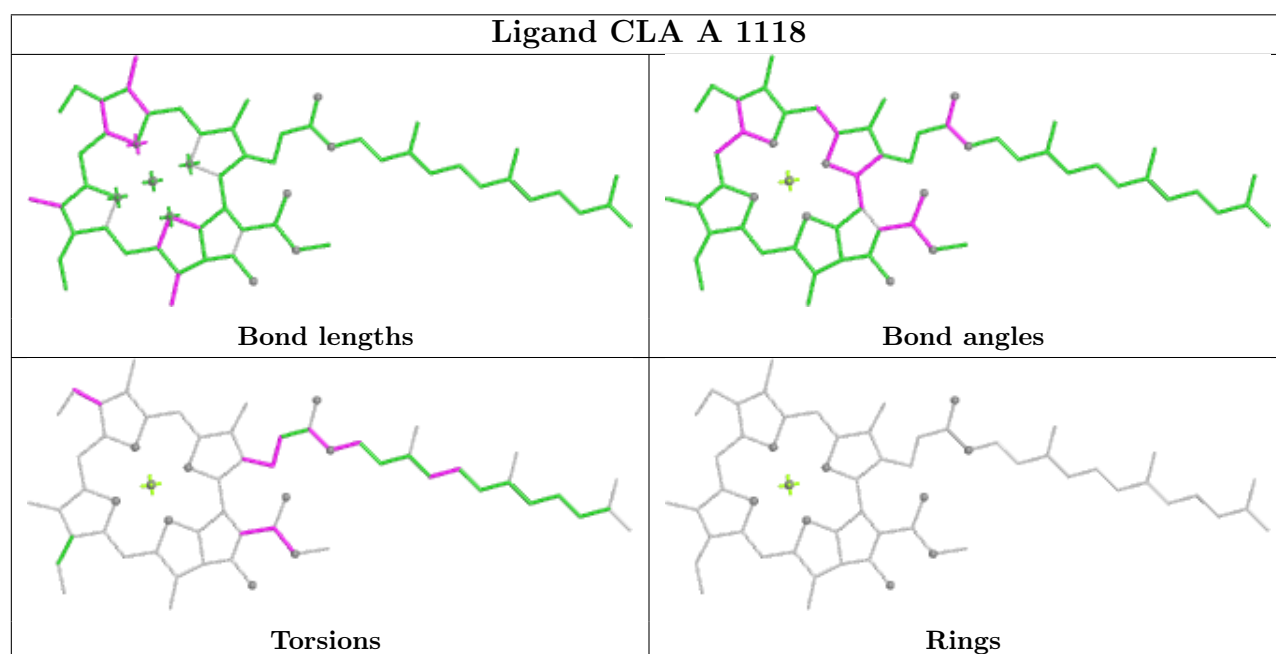
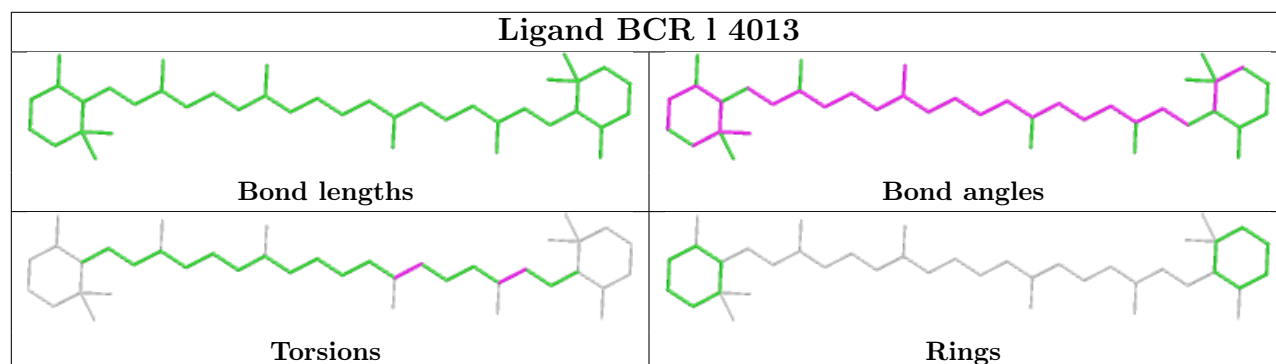
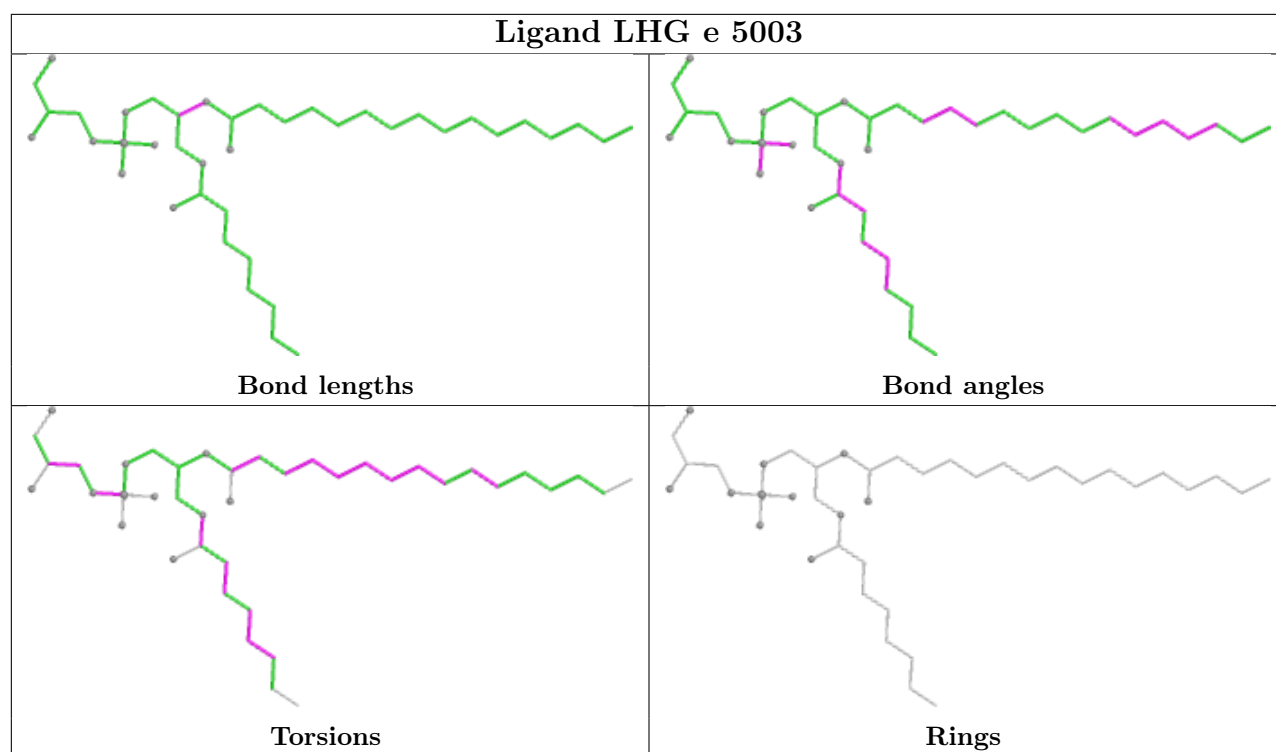
Ligand CLA t 512

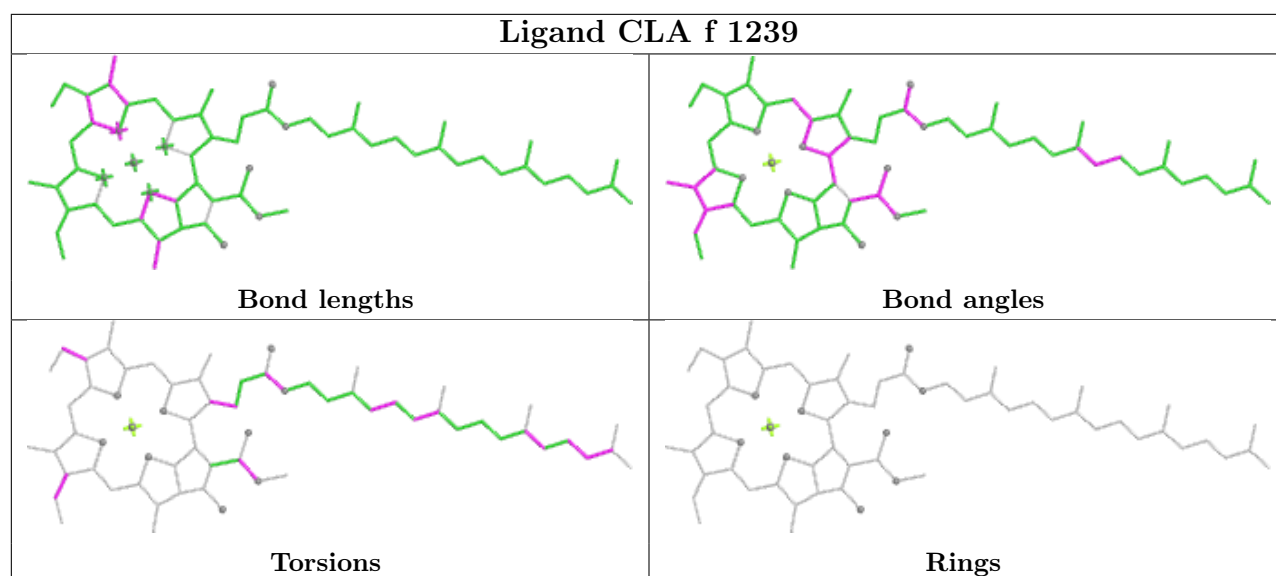
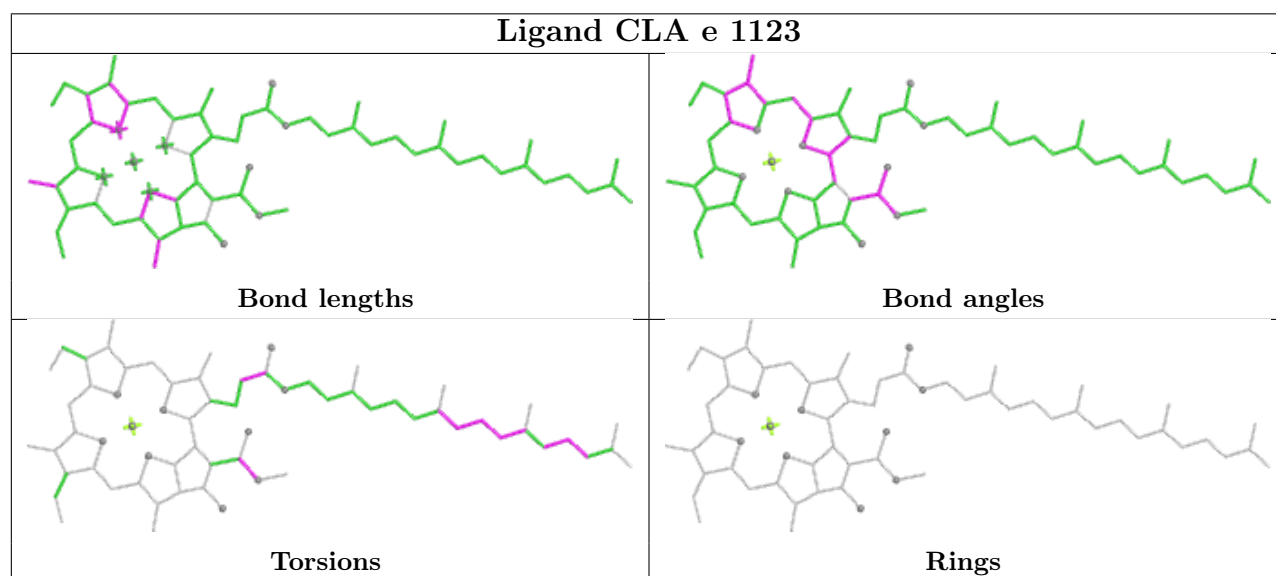
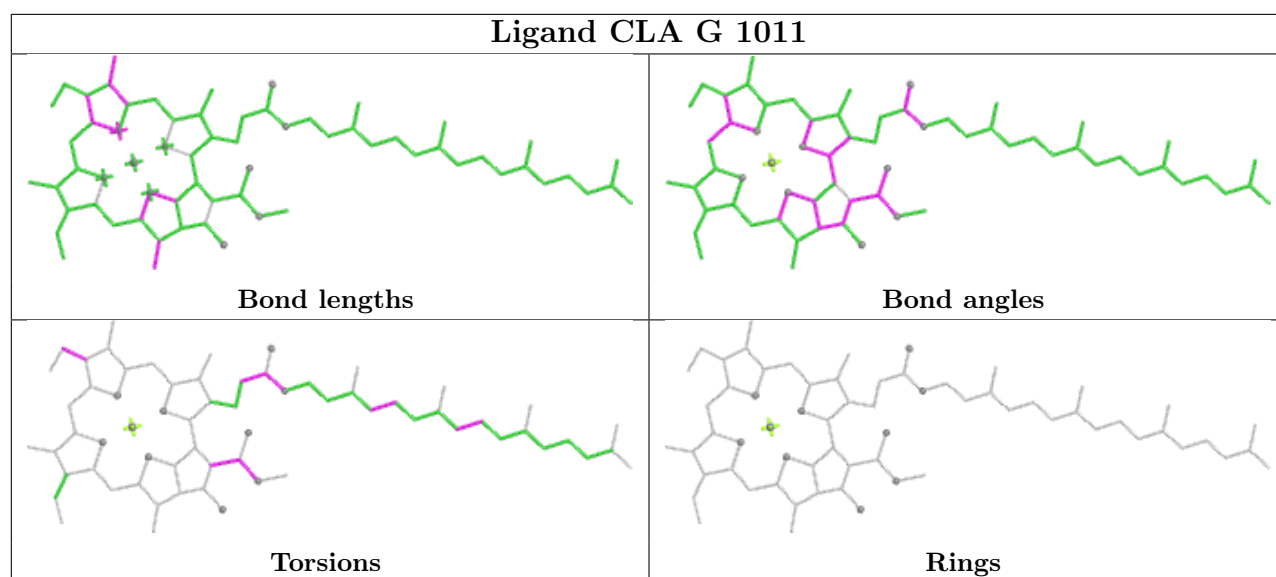


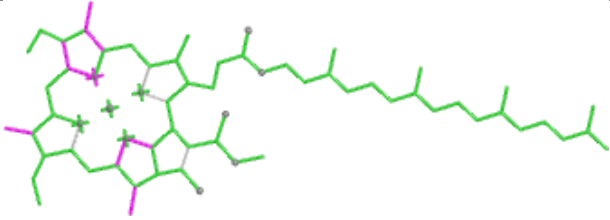
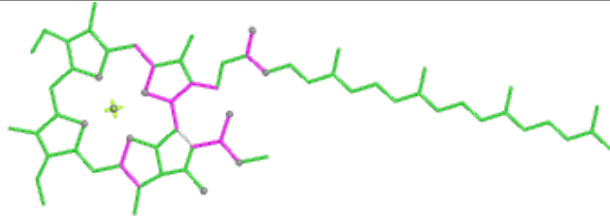
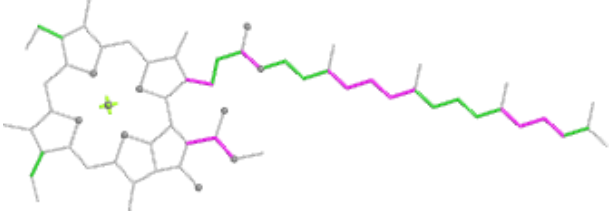
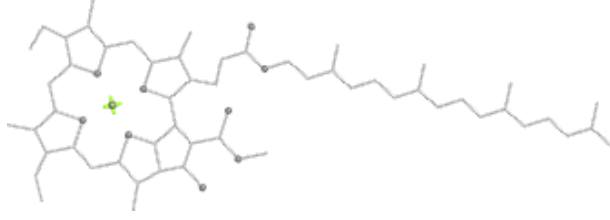
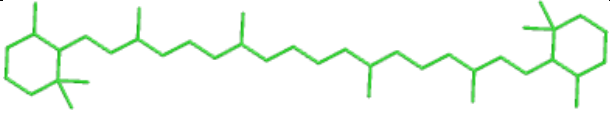
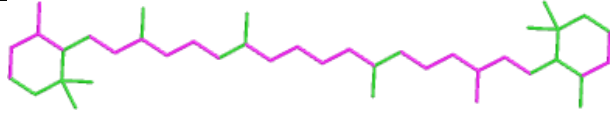
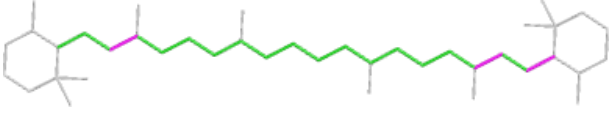
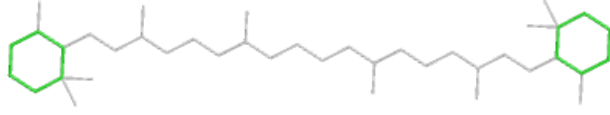
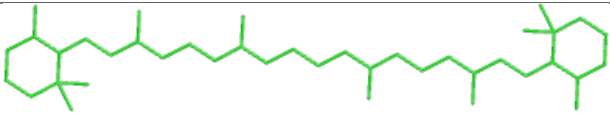
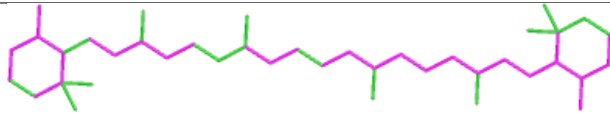
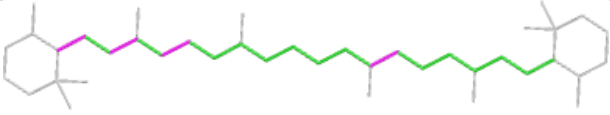
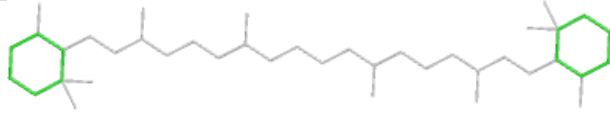
Ligand BCR K 4104

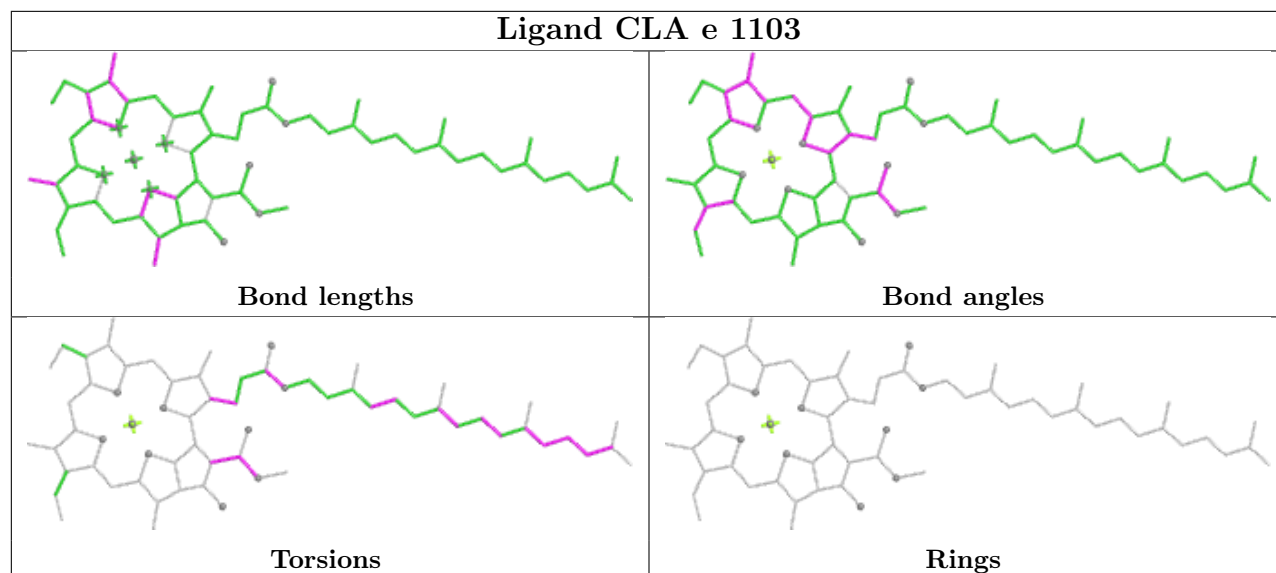
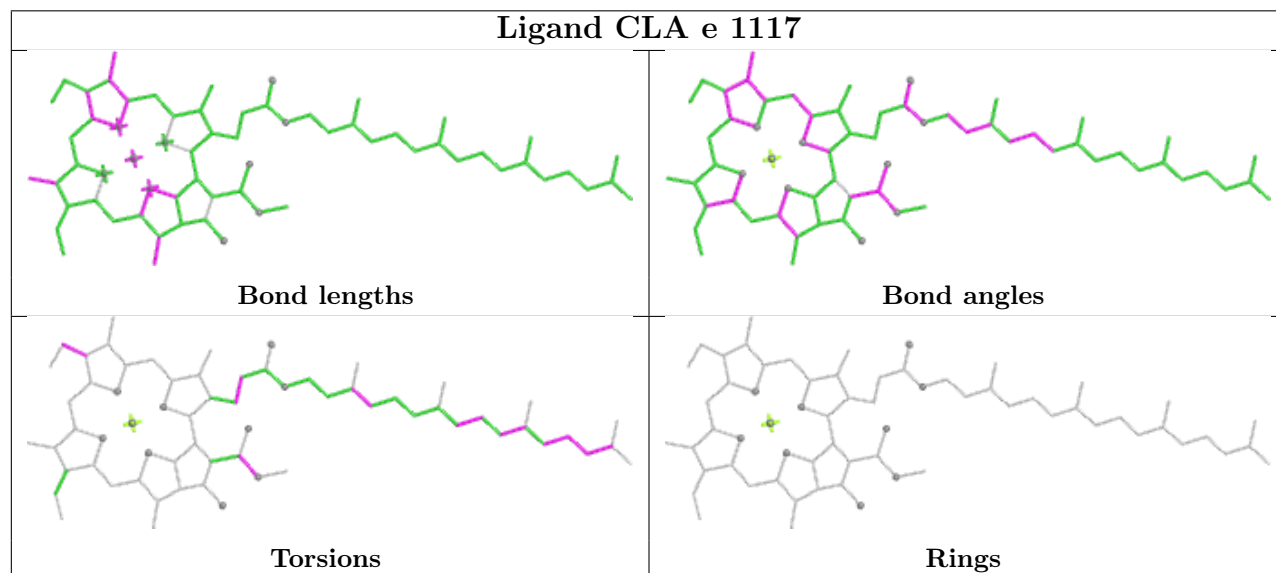
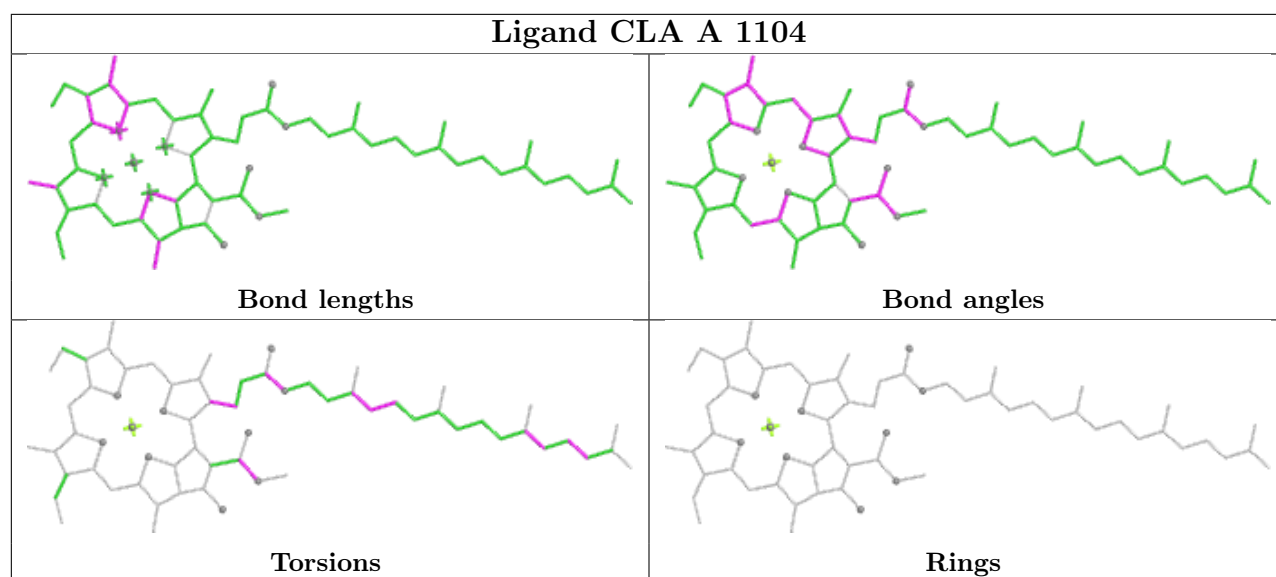


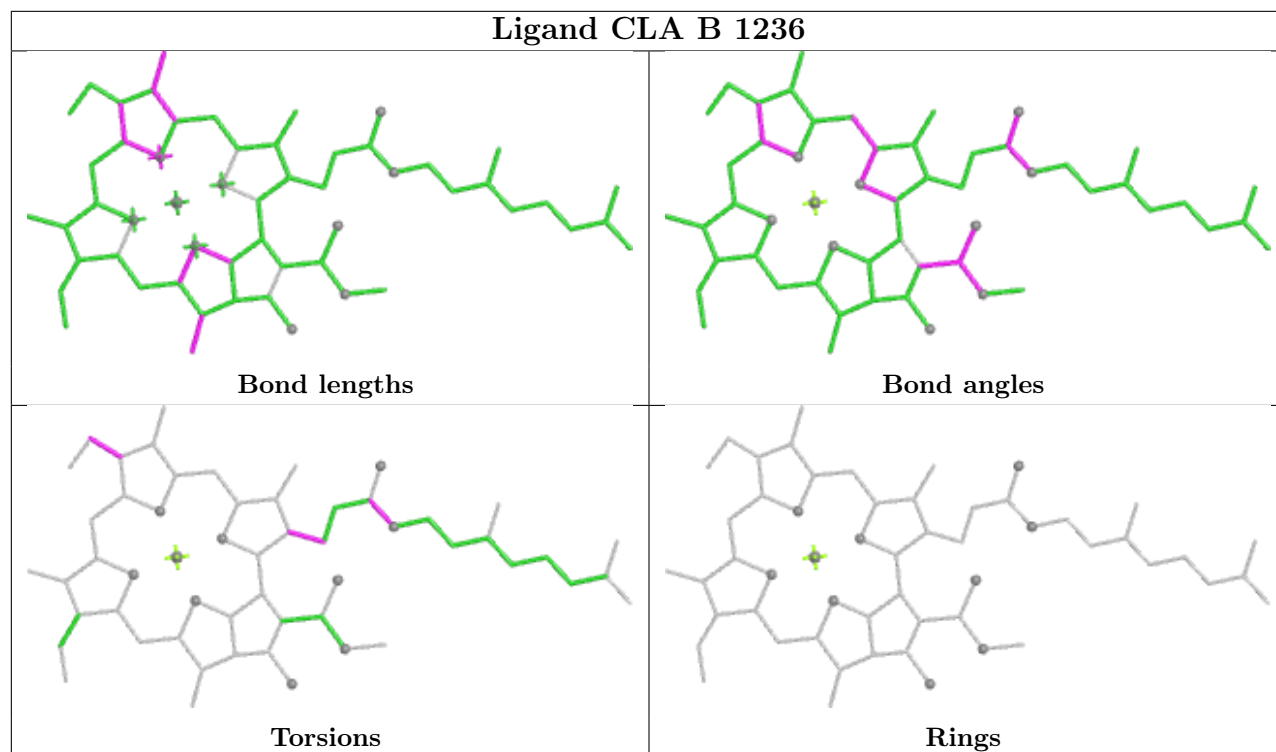
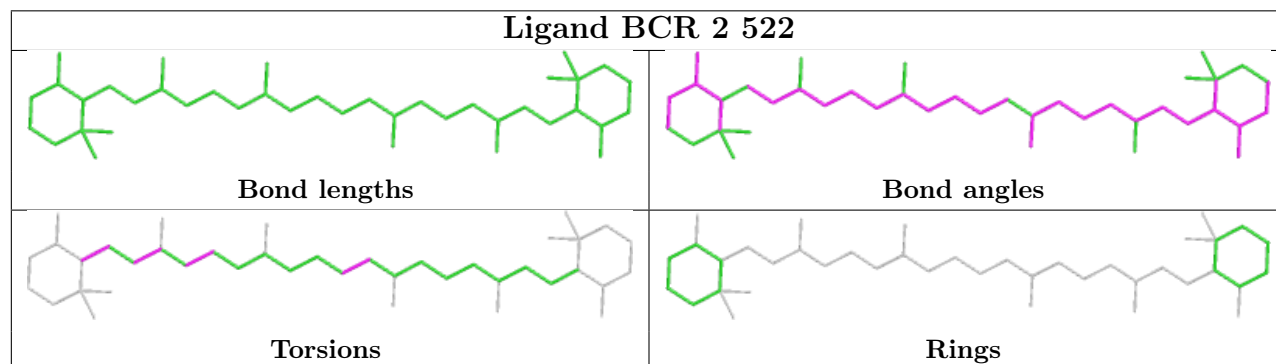
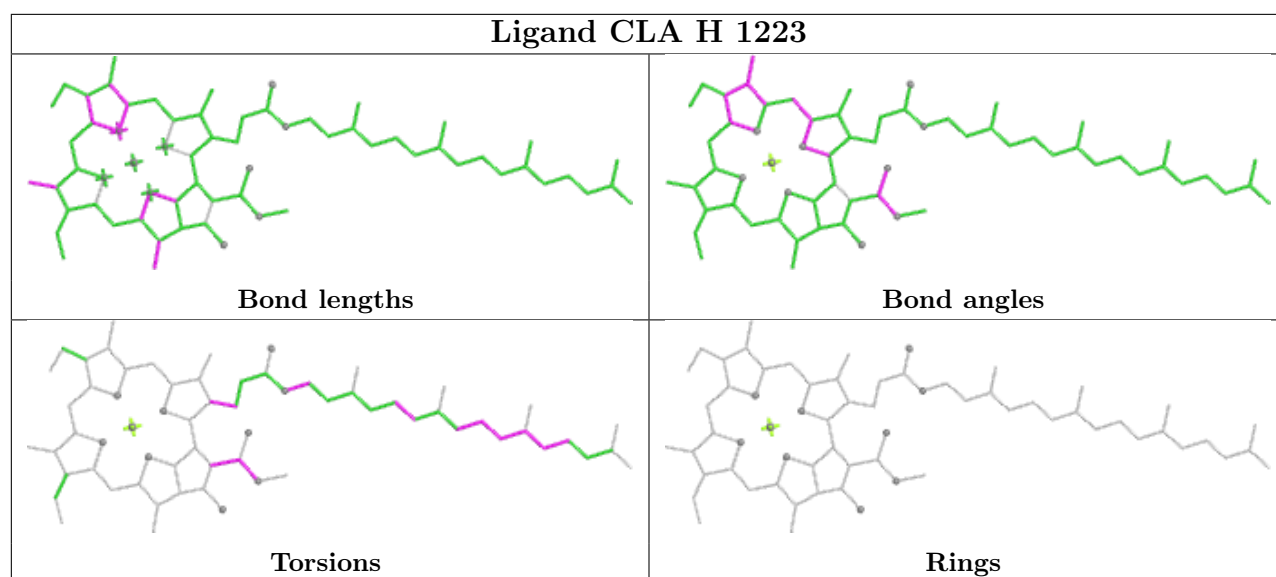


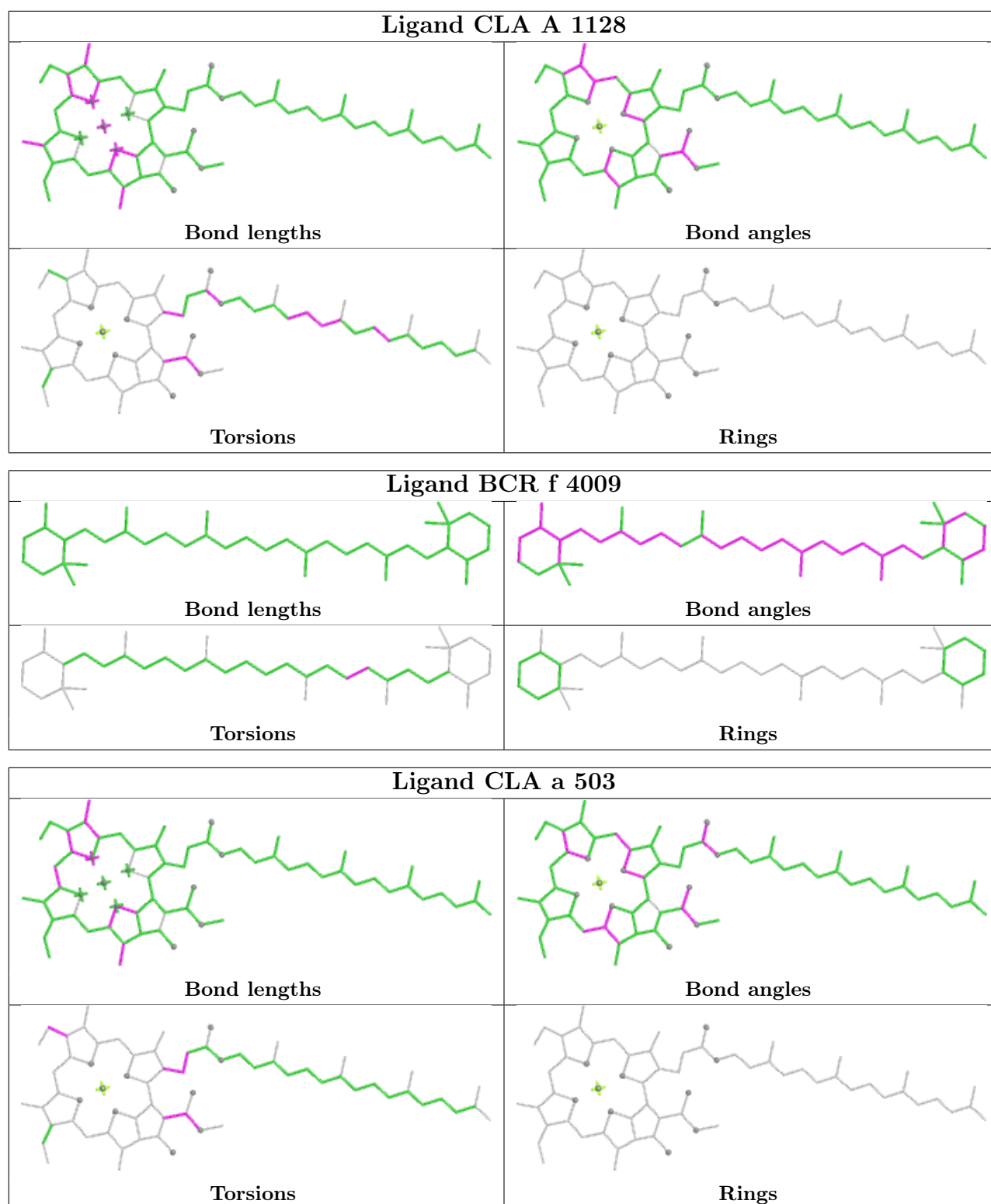




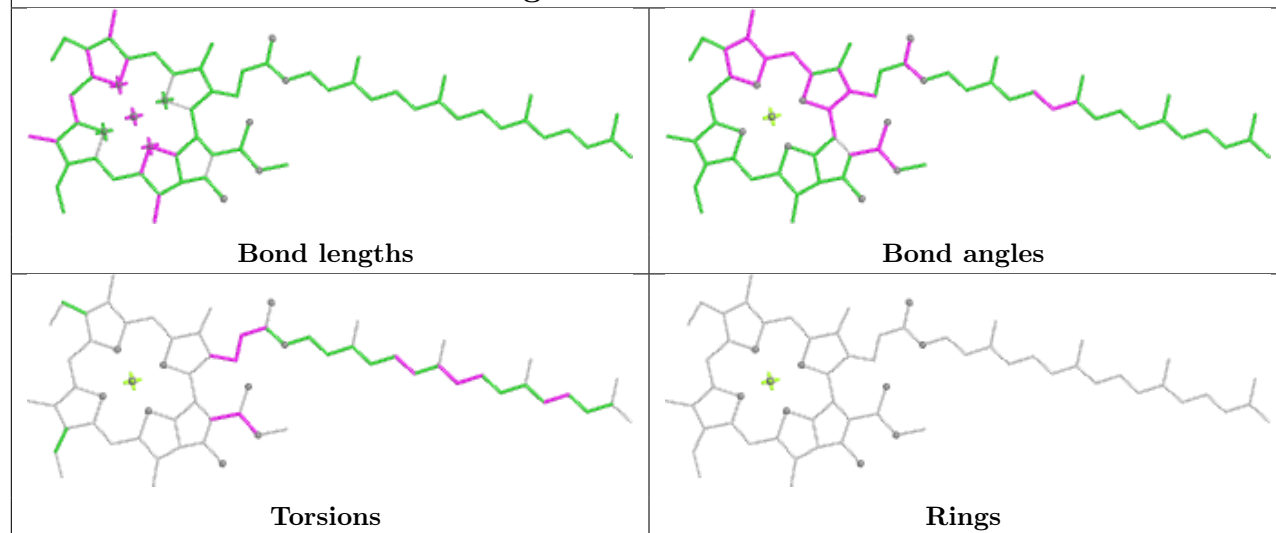
Ligand CLA l 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR Z 523	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR u 521	
 Bond lengths	 Bond angles
 Torsions	 Rings



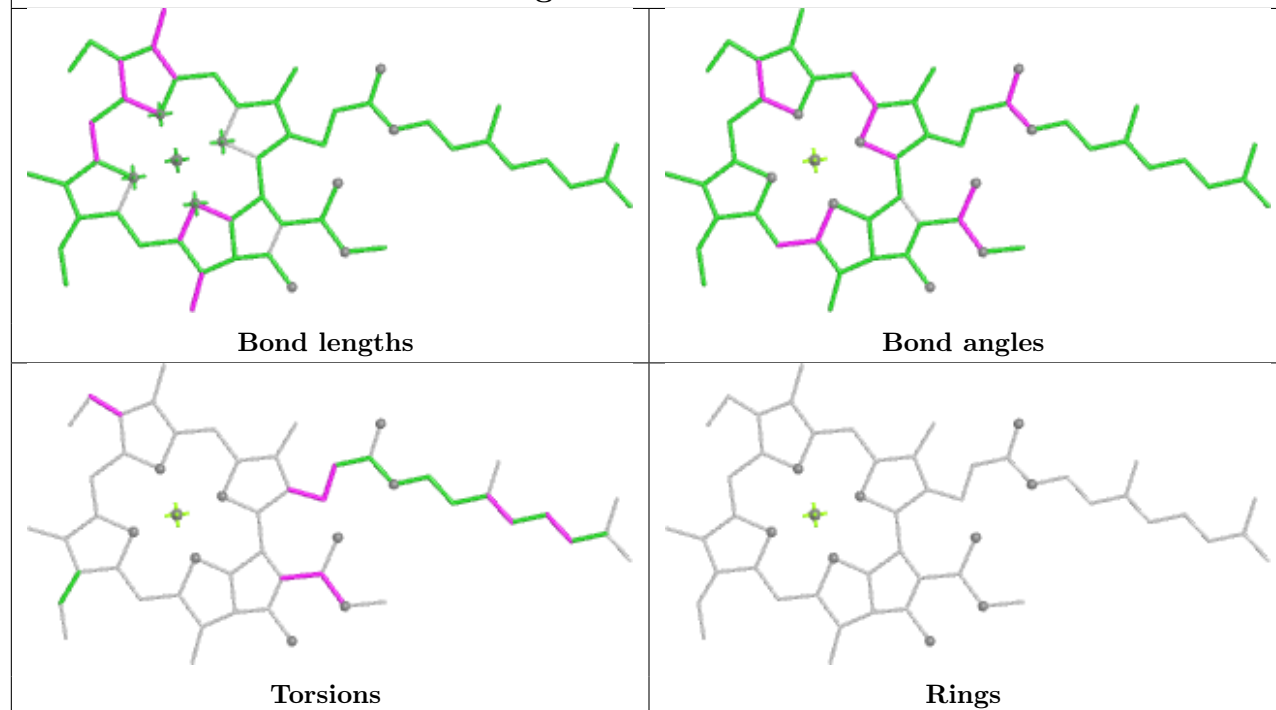


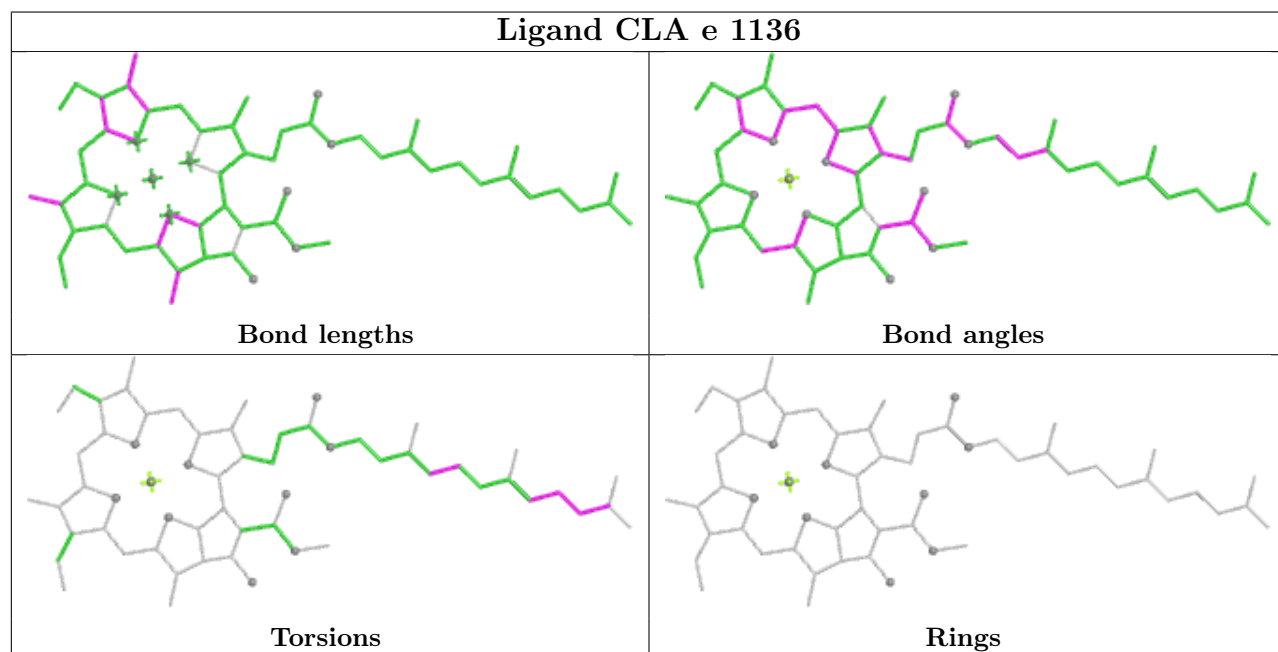
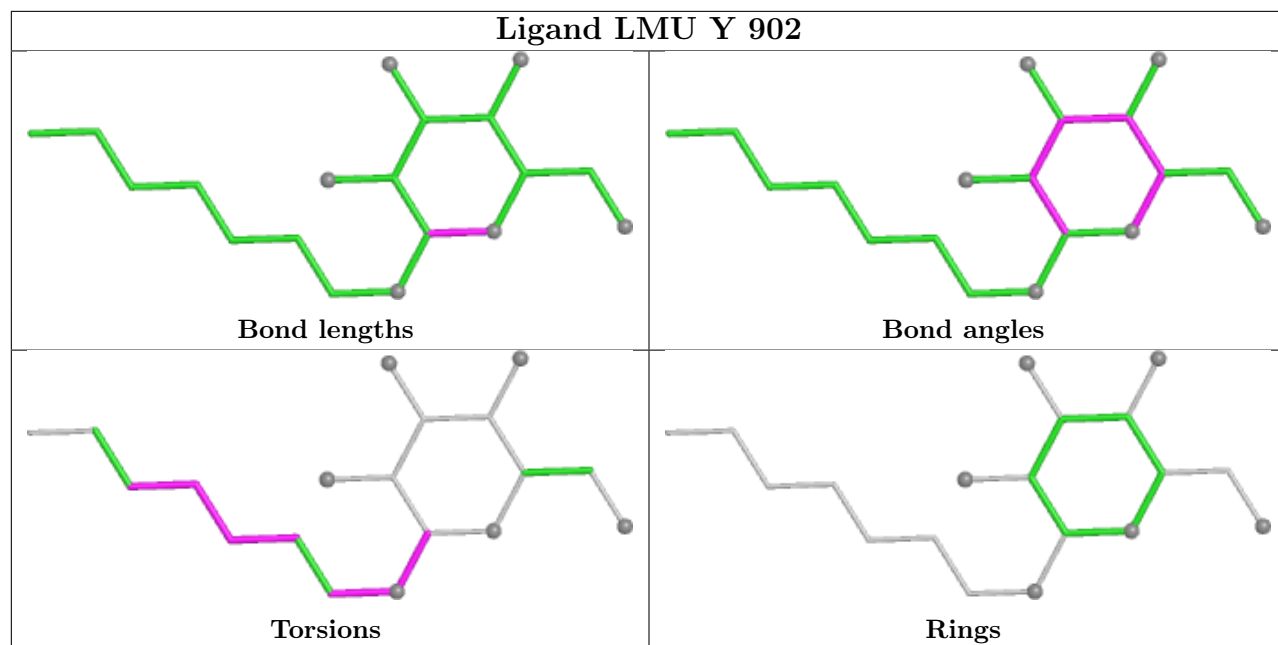


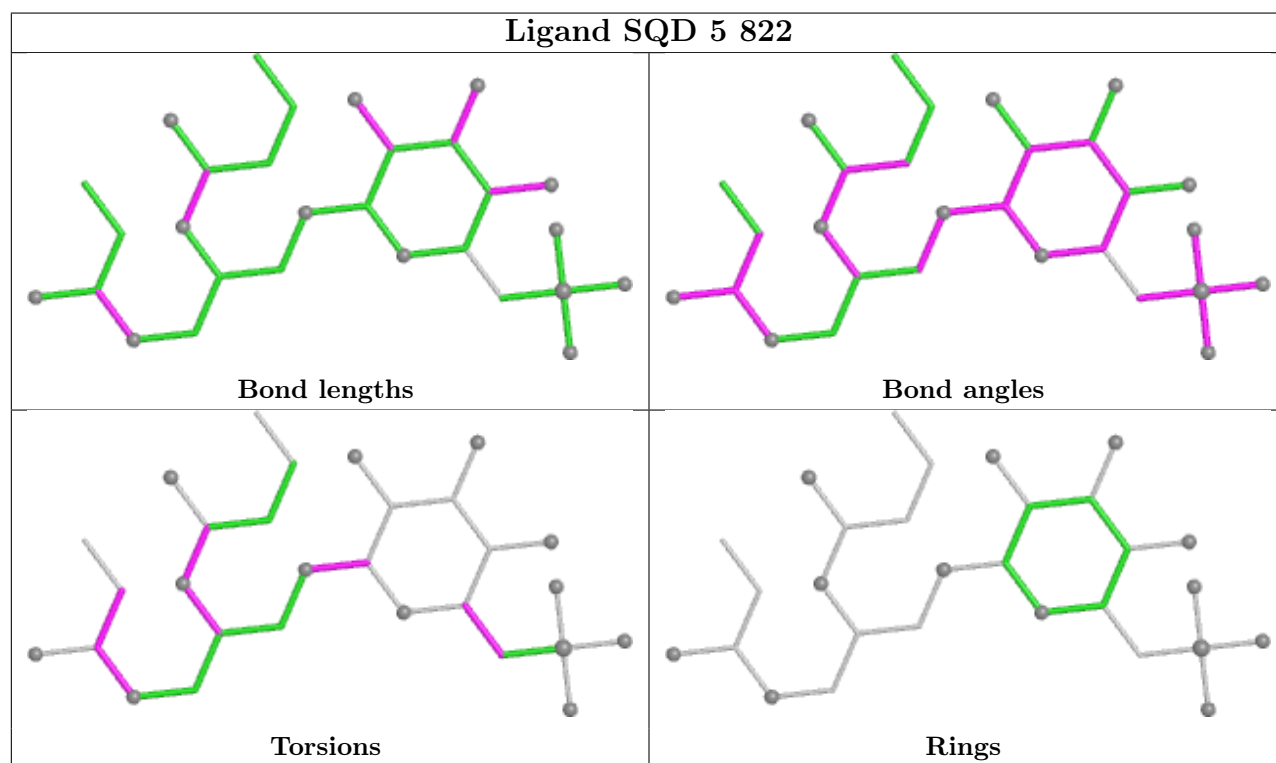
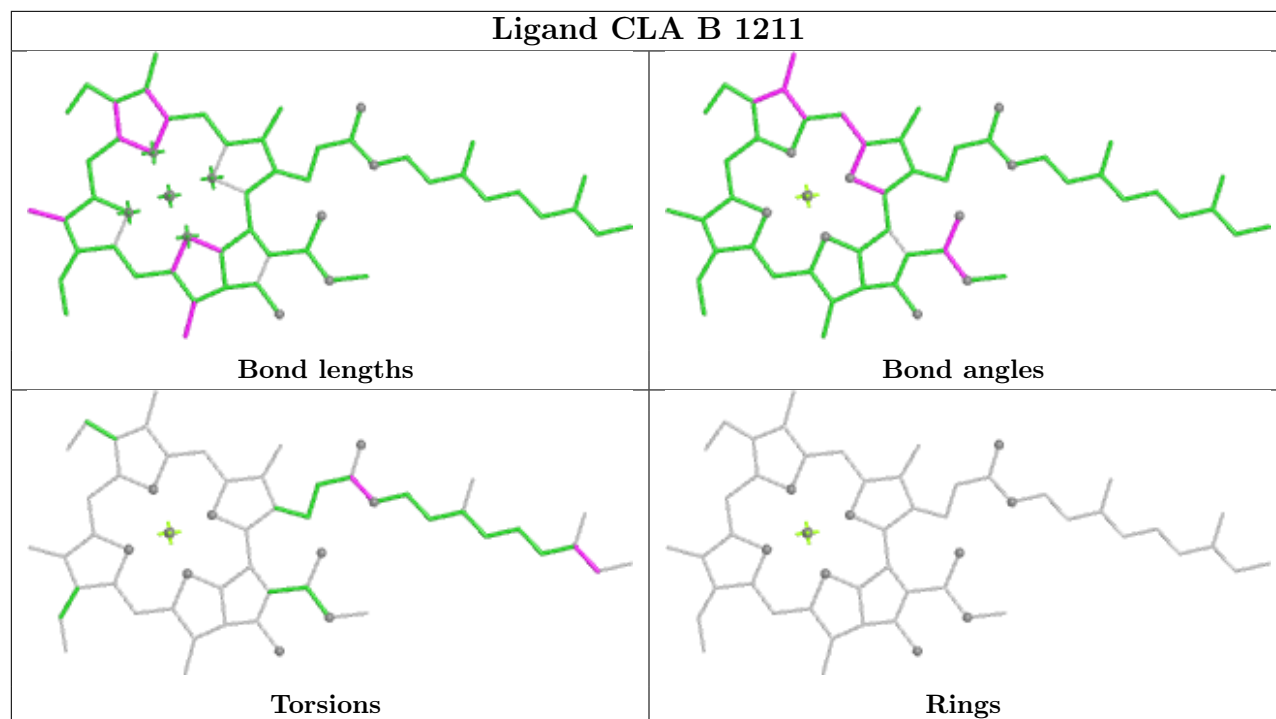
Ligand CLA B 1221



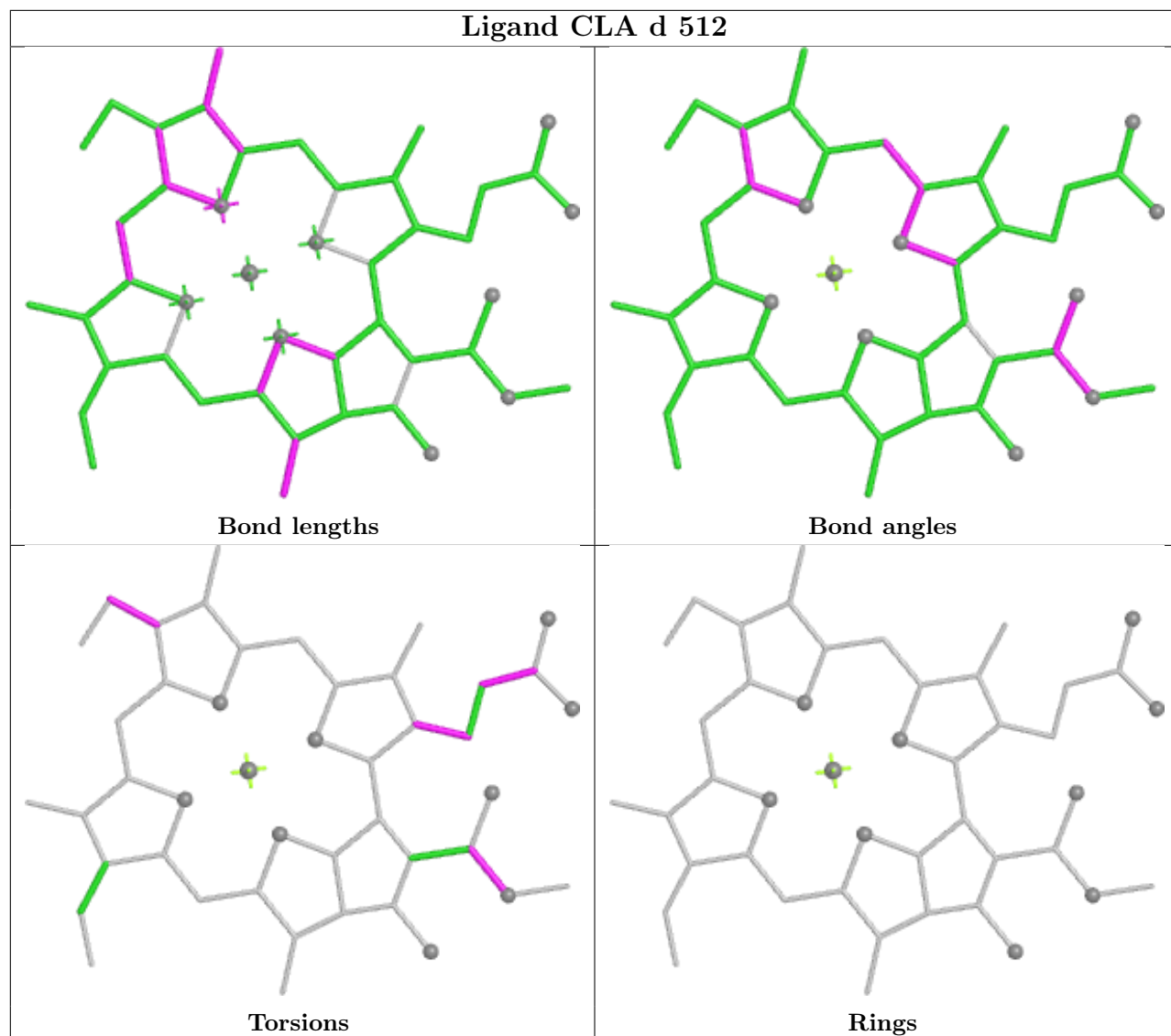
Ligand CLA u 503



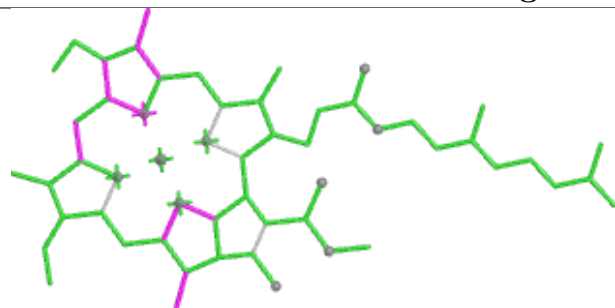




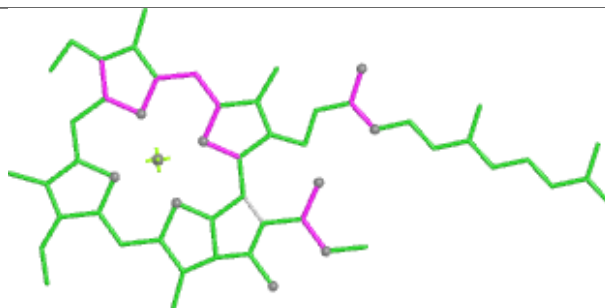
Ligand CLA d 512



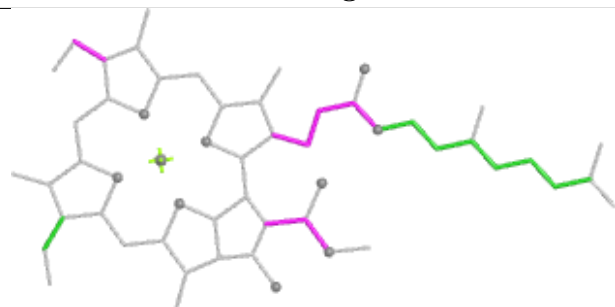
Ligand CLA v 518



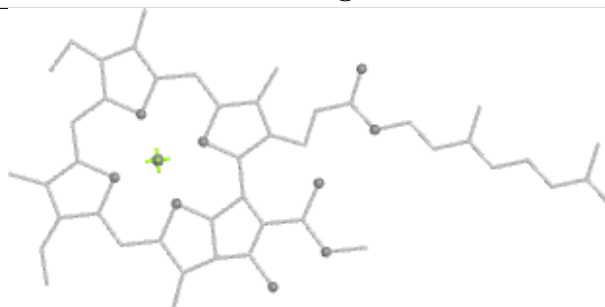
Bond lengths



Bond angles

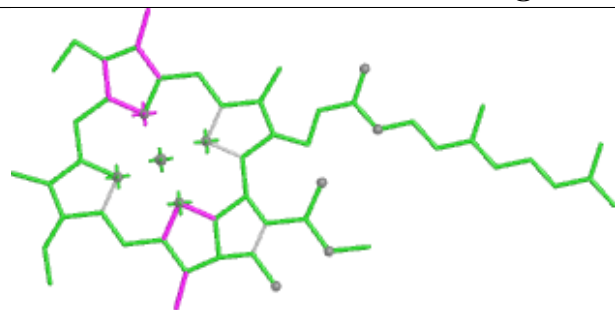


Torsions

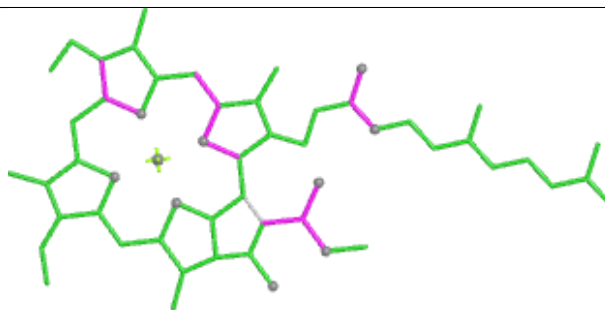


Rings

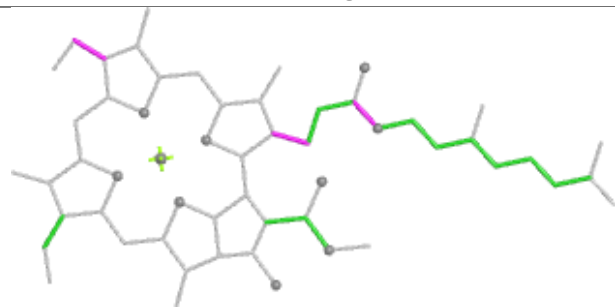
Ligand CLA f 1236



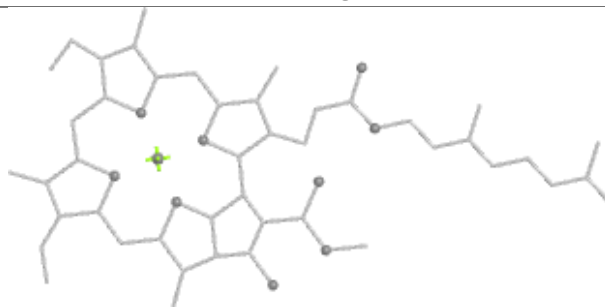
Bond lengths



Bond angles

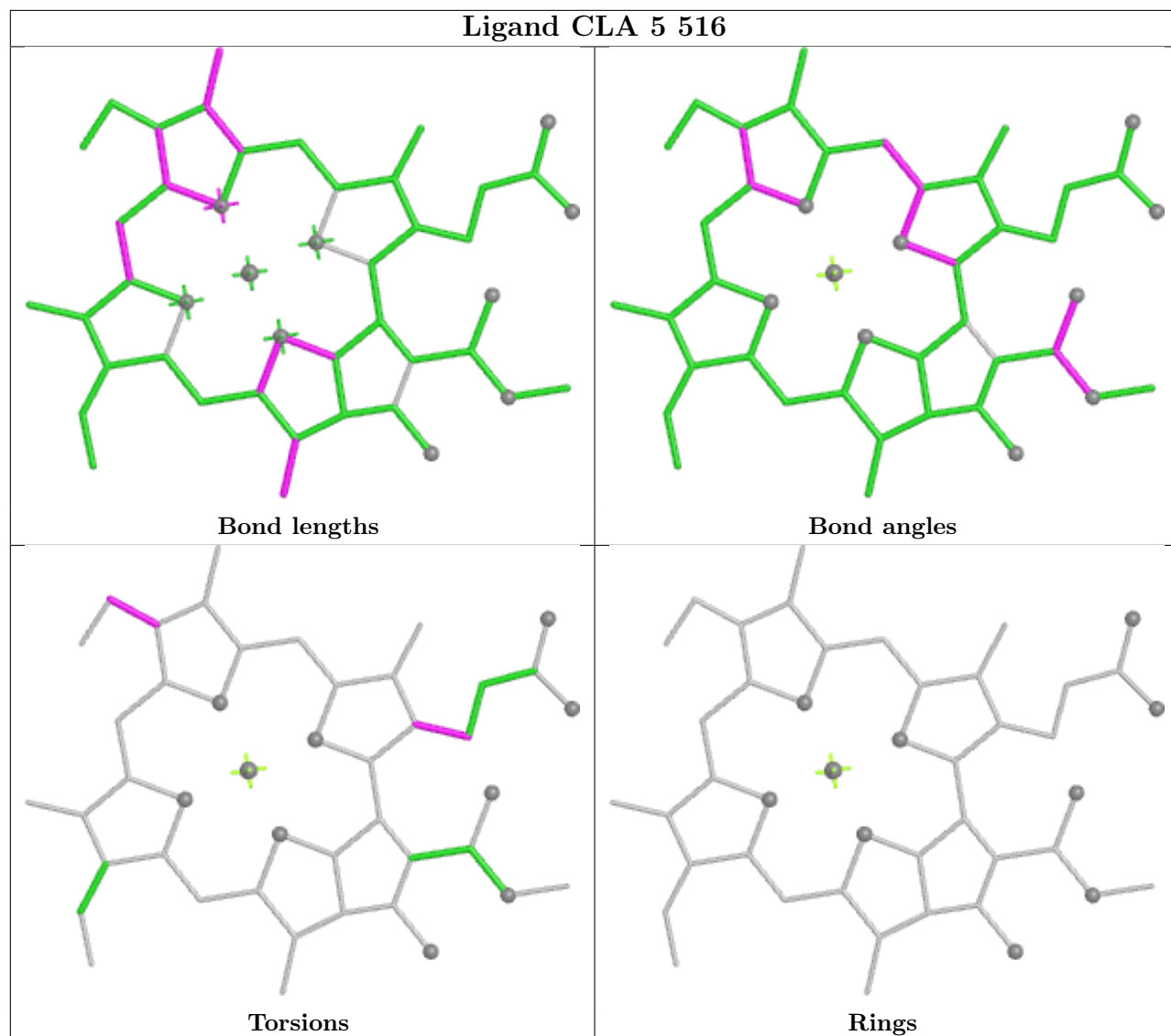


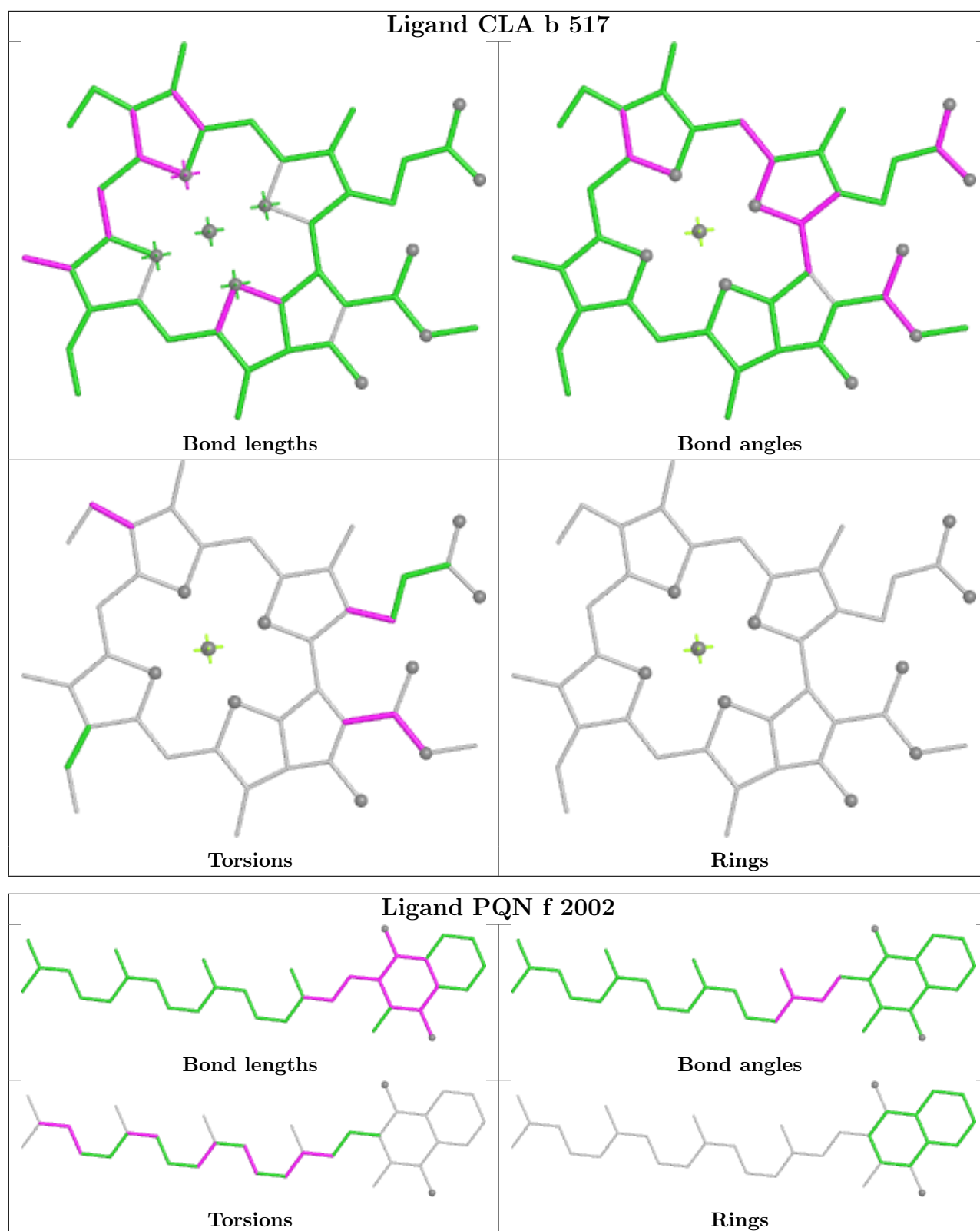
Torsions

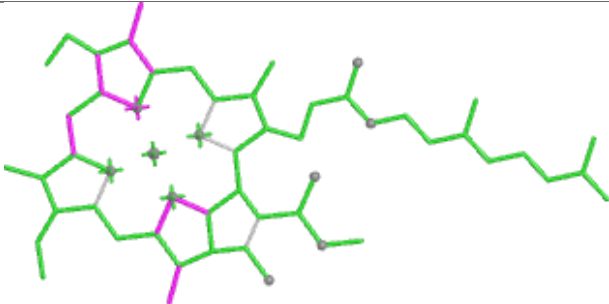
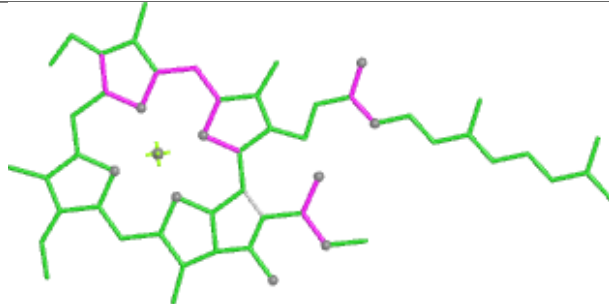
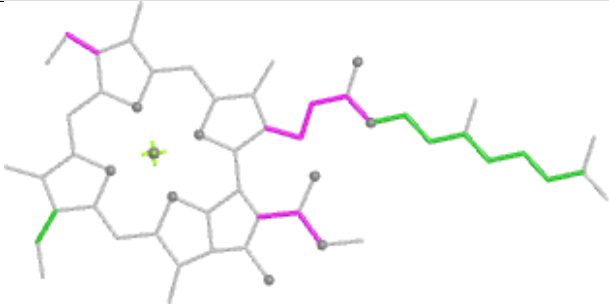
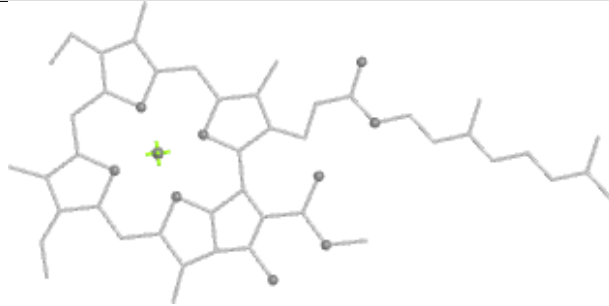


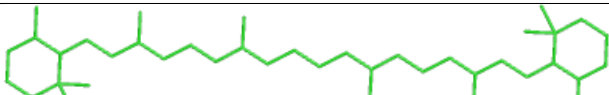
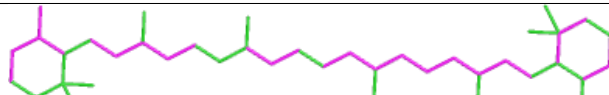
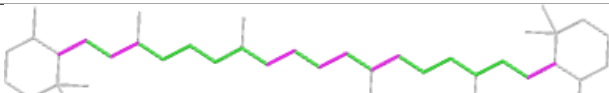
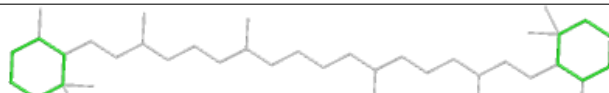
Rings

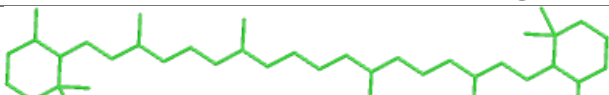
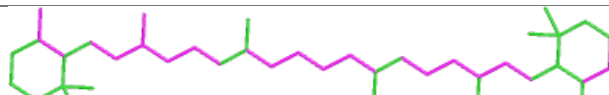
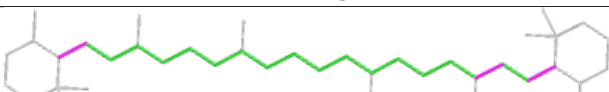
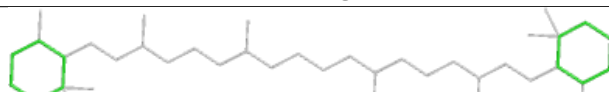
Ligand CLA 5 516



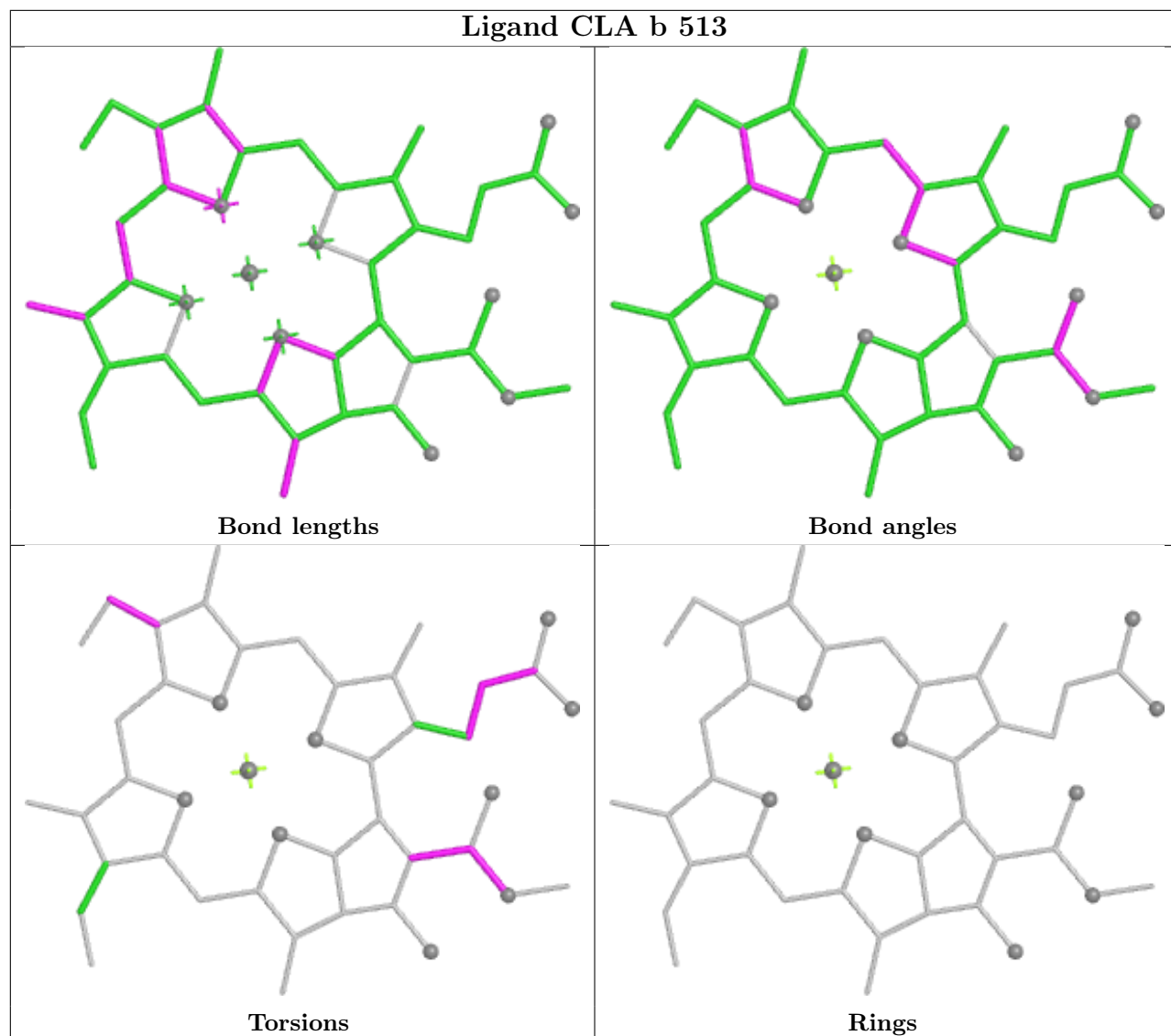


Ligand CLA d 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

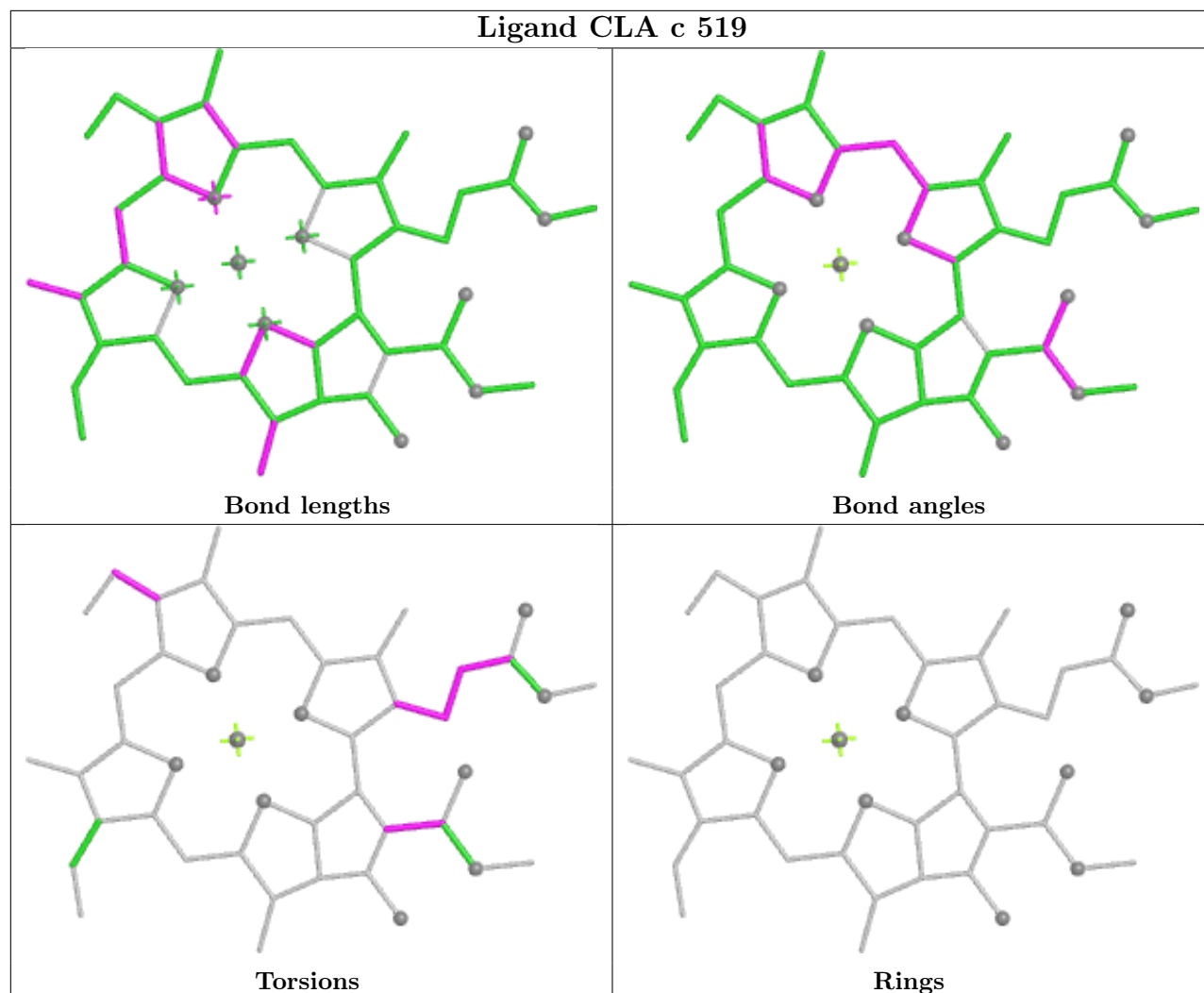
Ligand BCR t 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR t 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

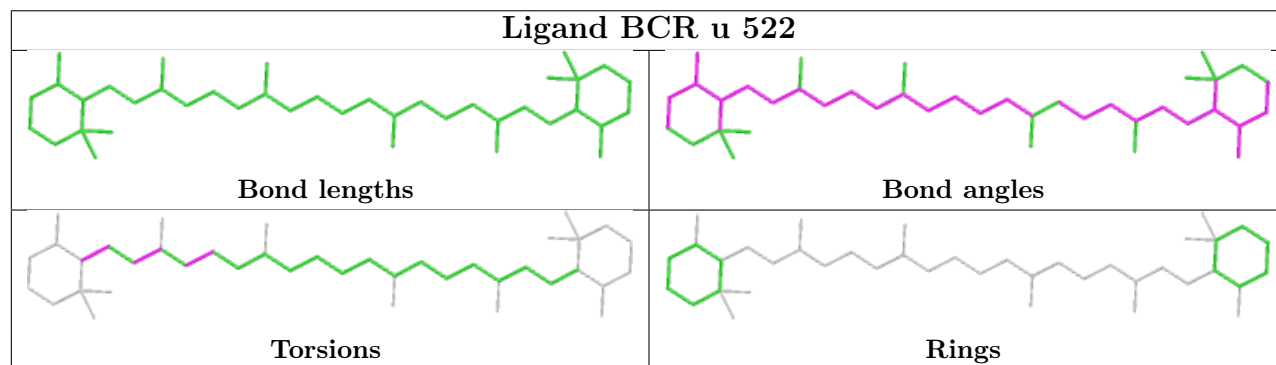
Ligand CLA b 513

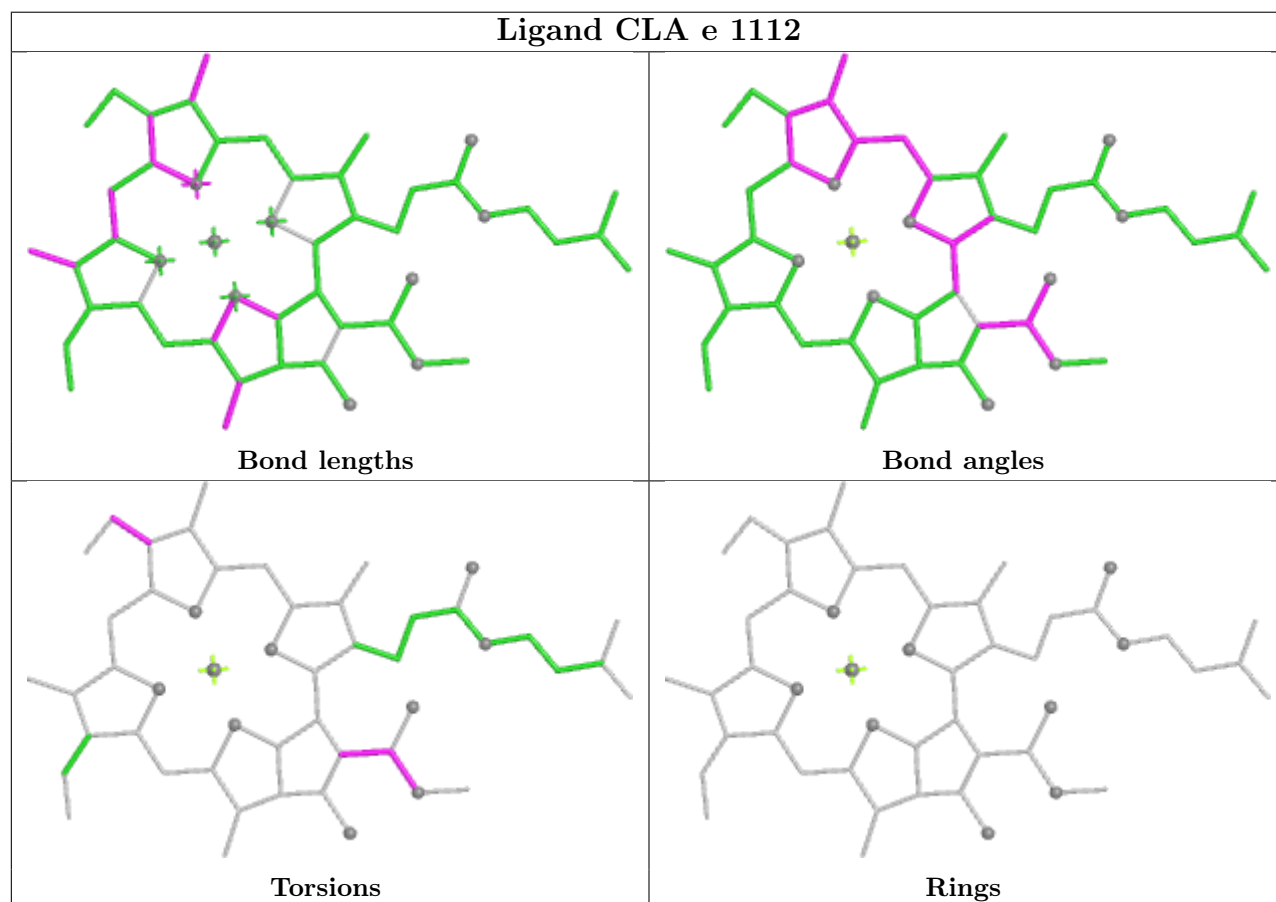
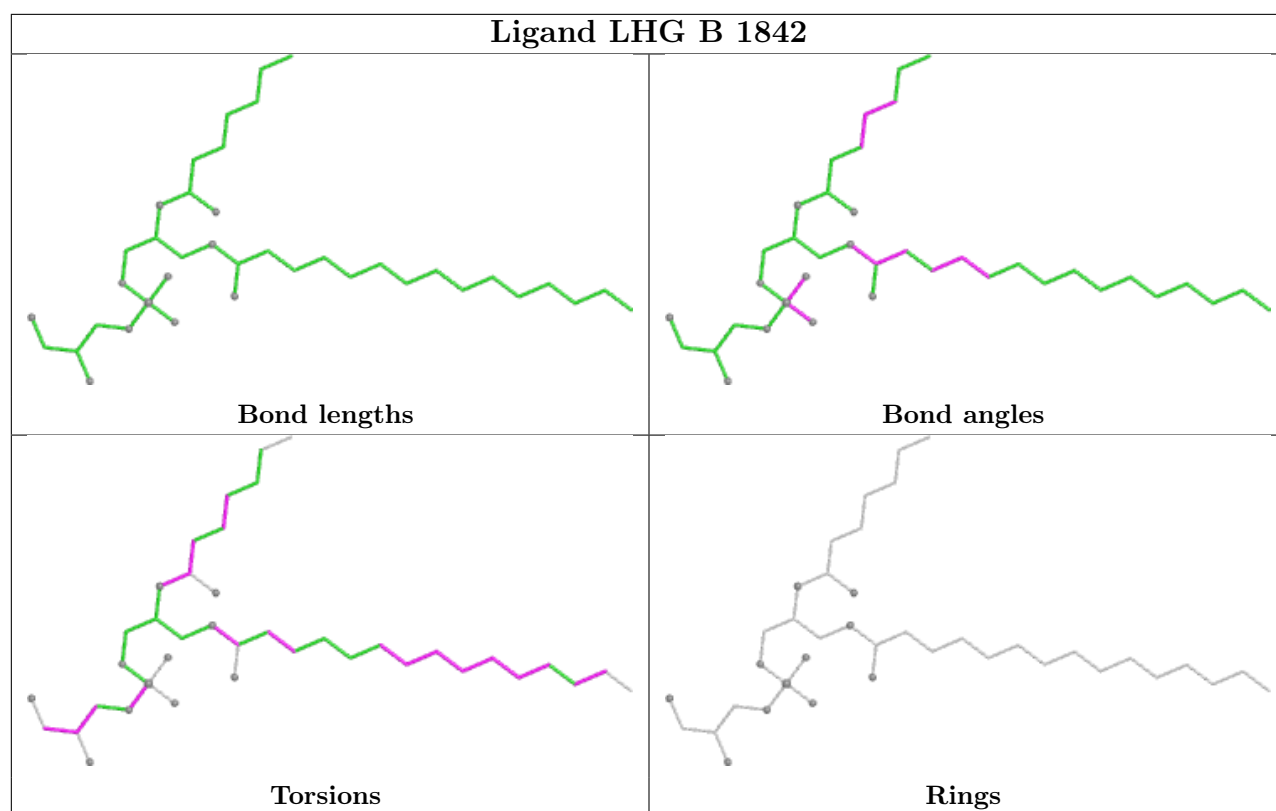


Ligand CLA c 519

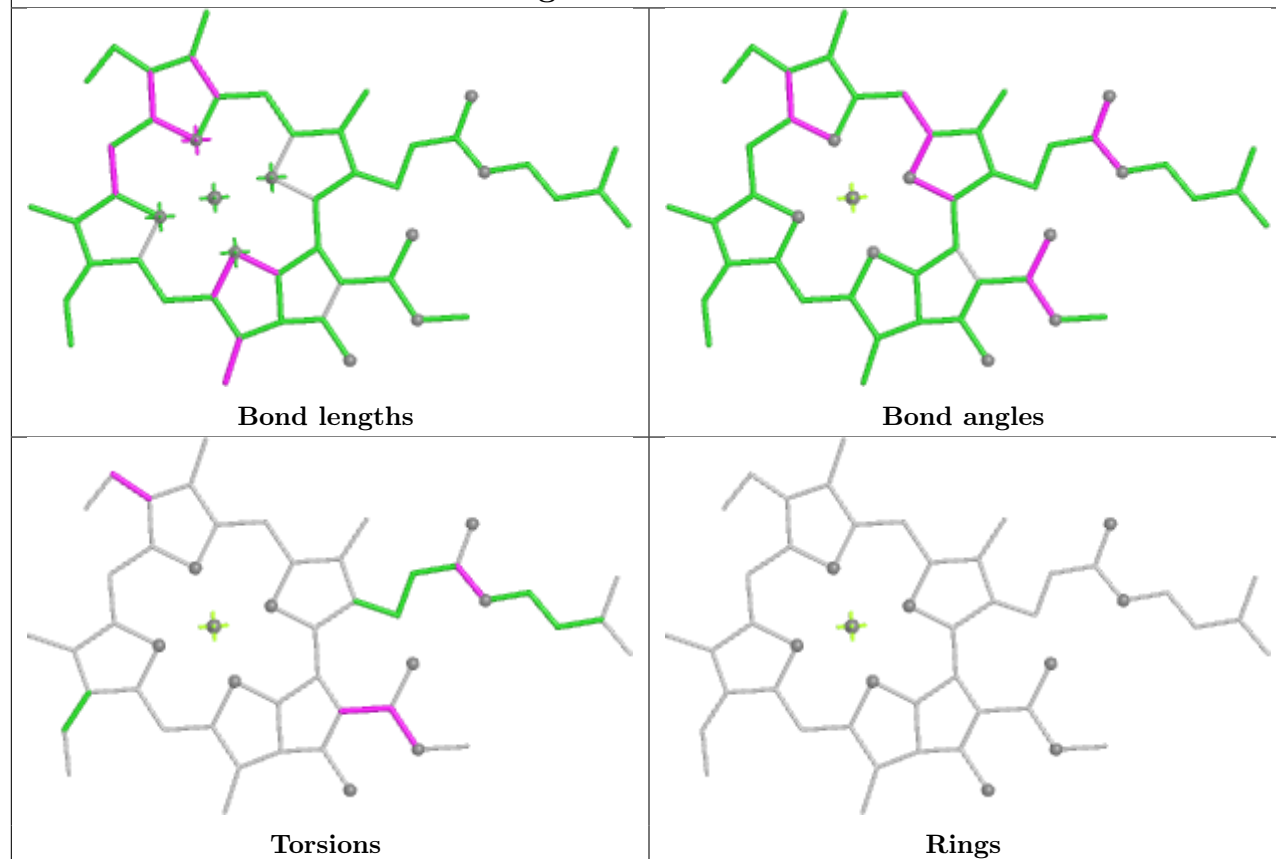


Ligand BCR u 522

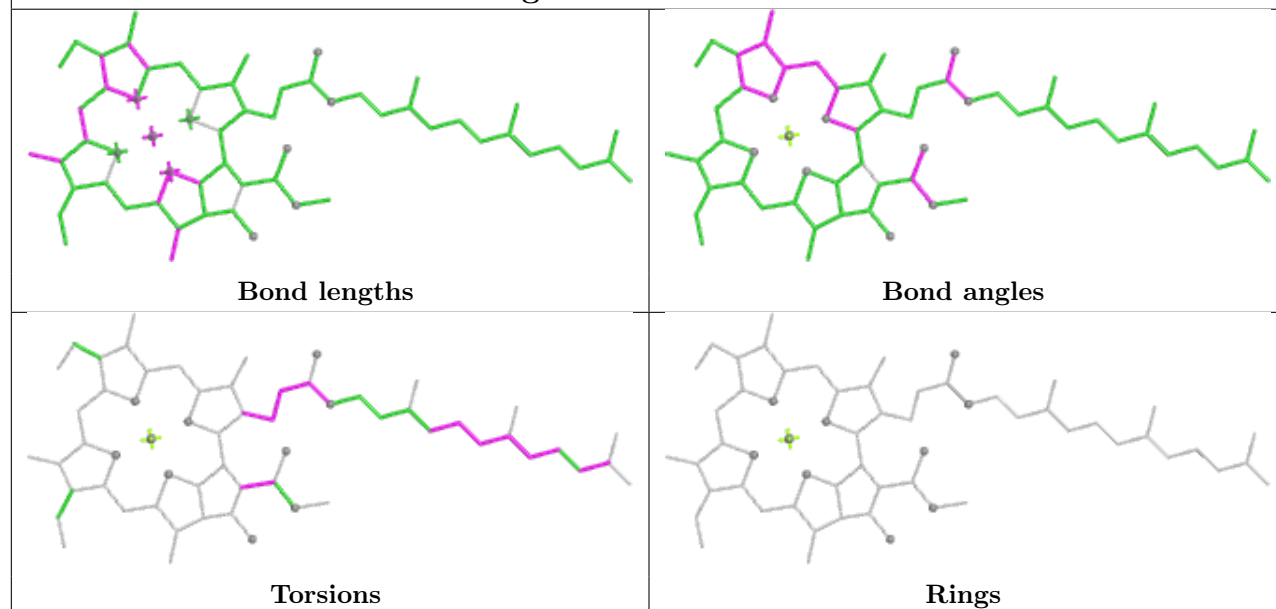




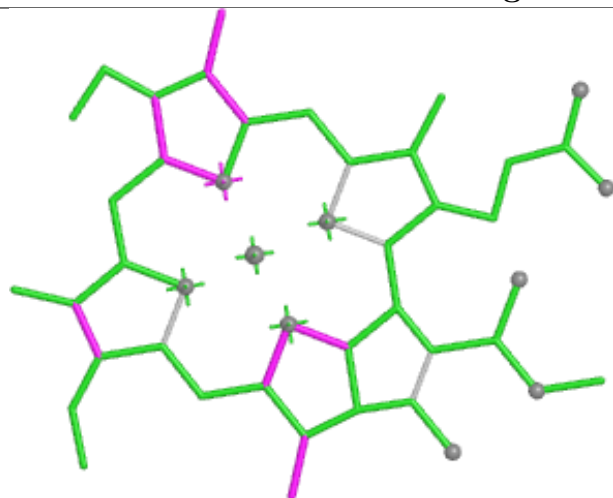
Ligand CLA t 510



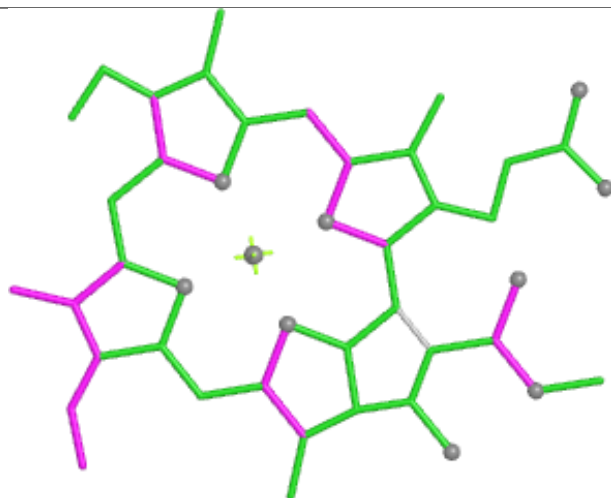
Ligand CLA G 1116



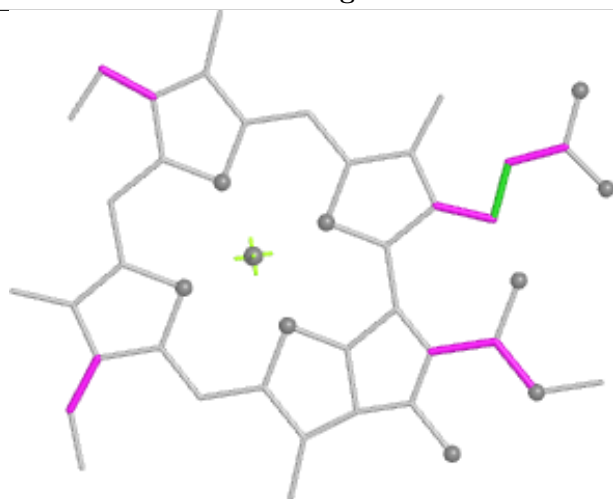
Ligand CLA m 1105



Bond lengths



Bond angles

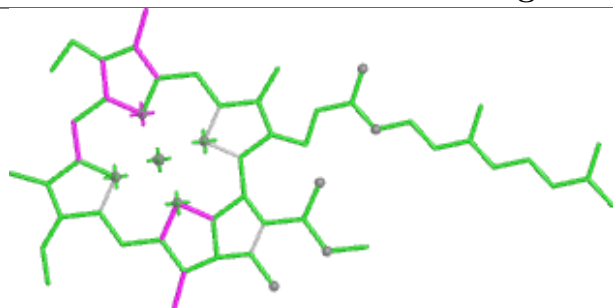


Torsions

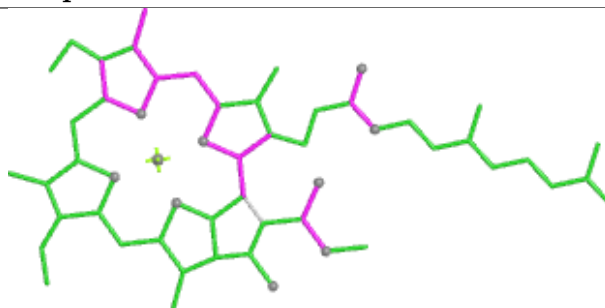


Rings

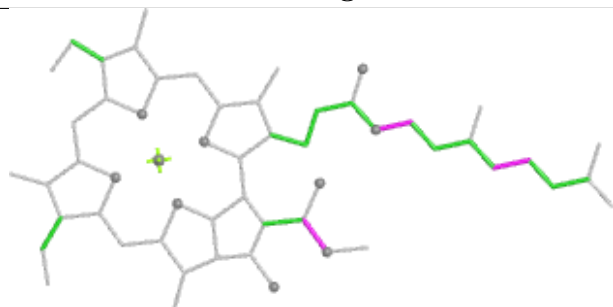
Ligand CLA q 511



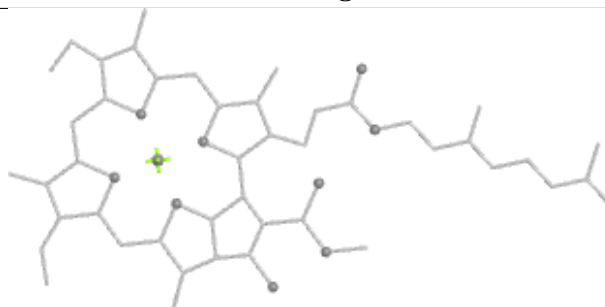
Bond lengths



Bond angles

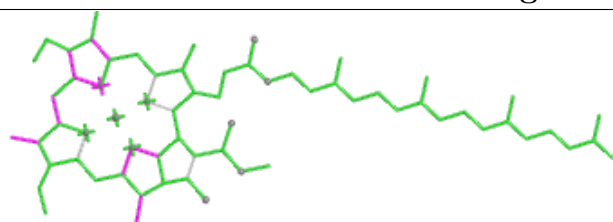


Torsions

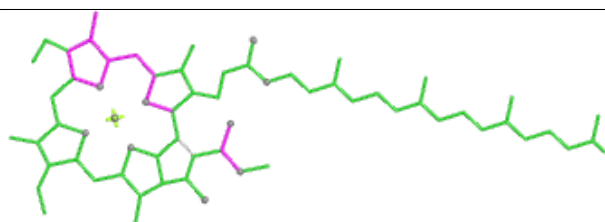


Rings

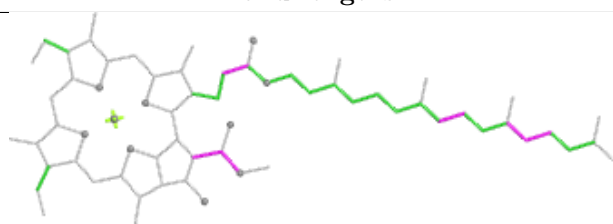
Ligand CLA r 510



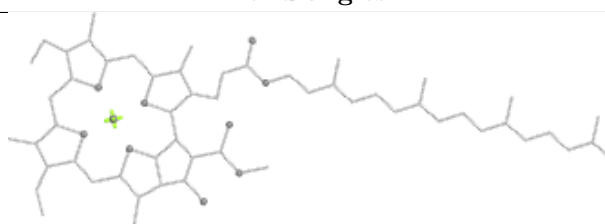
Bond lengths



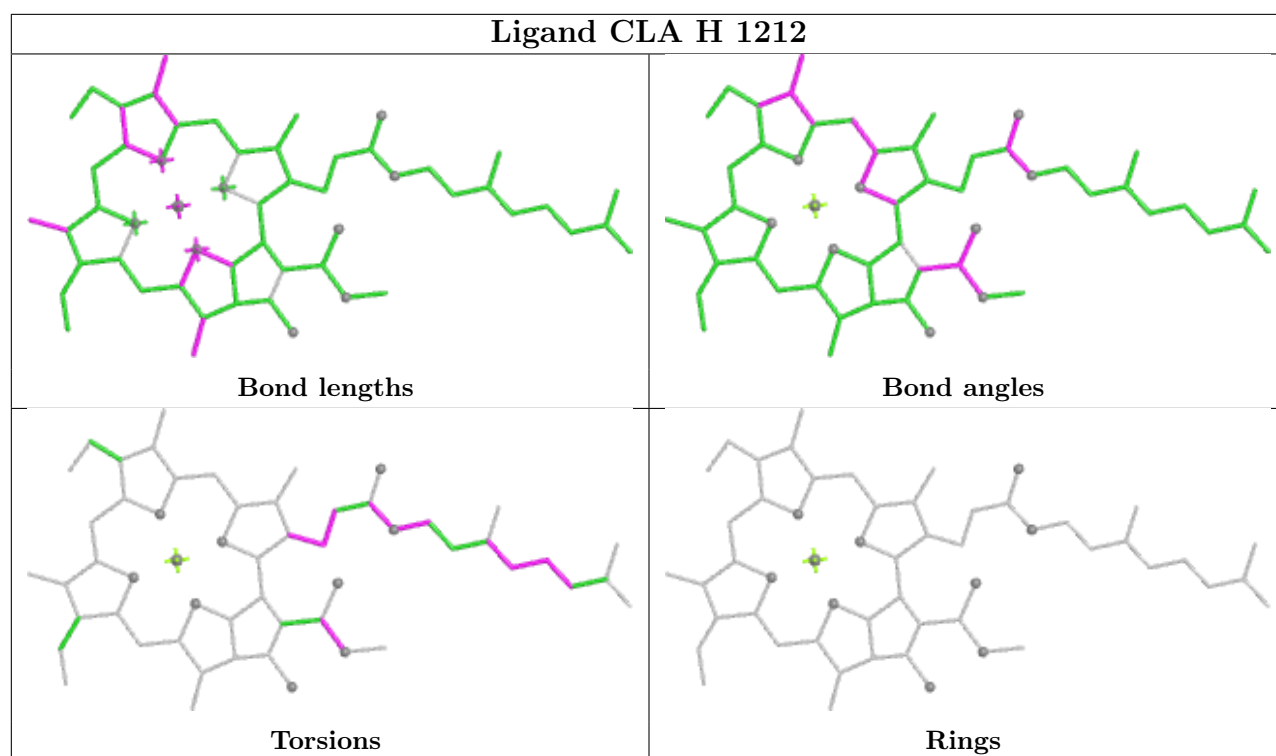
Bond angles

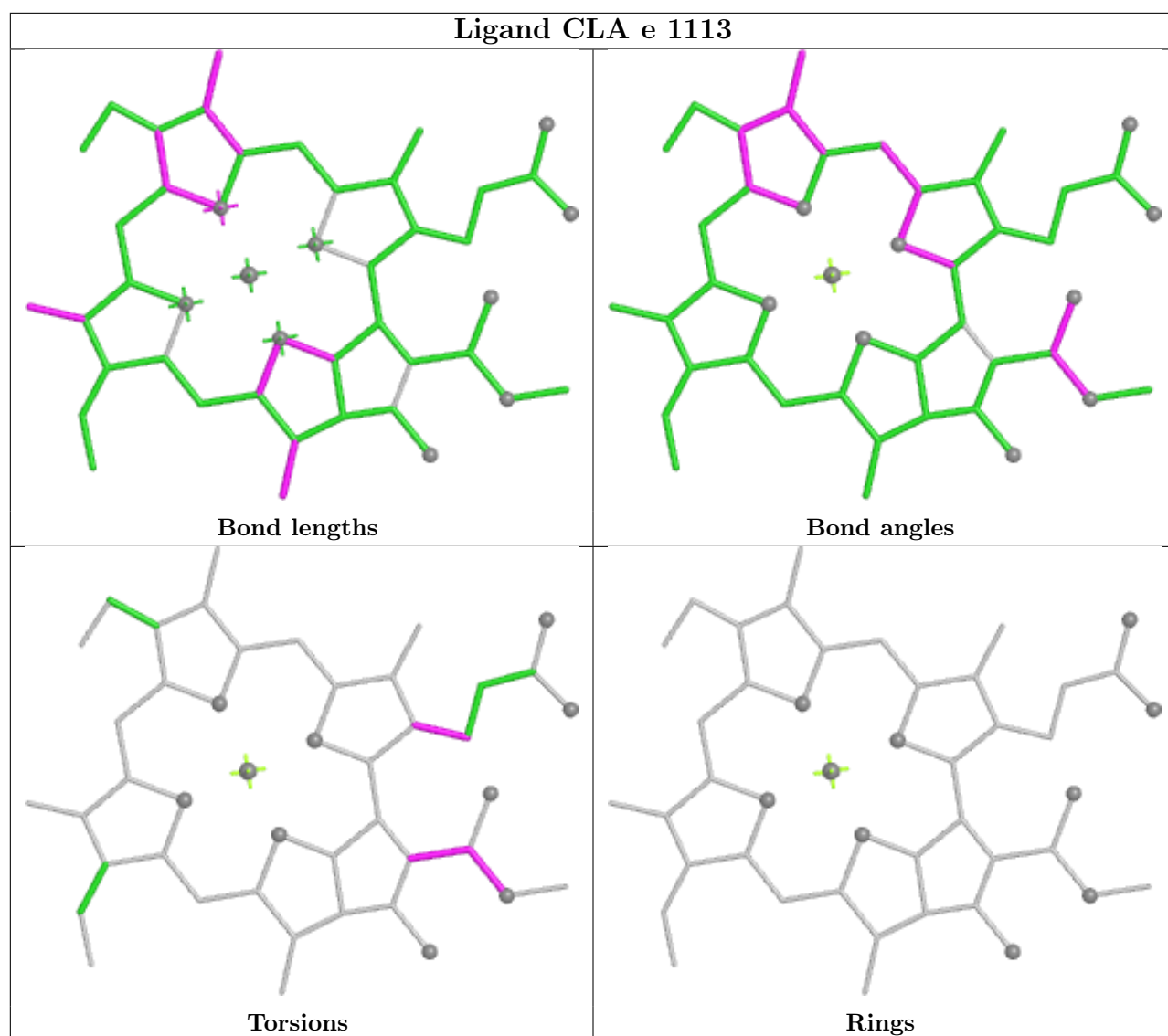


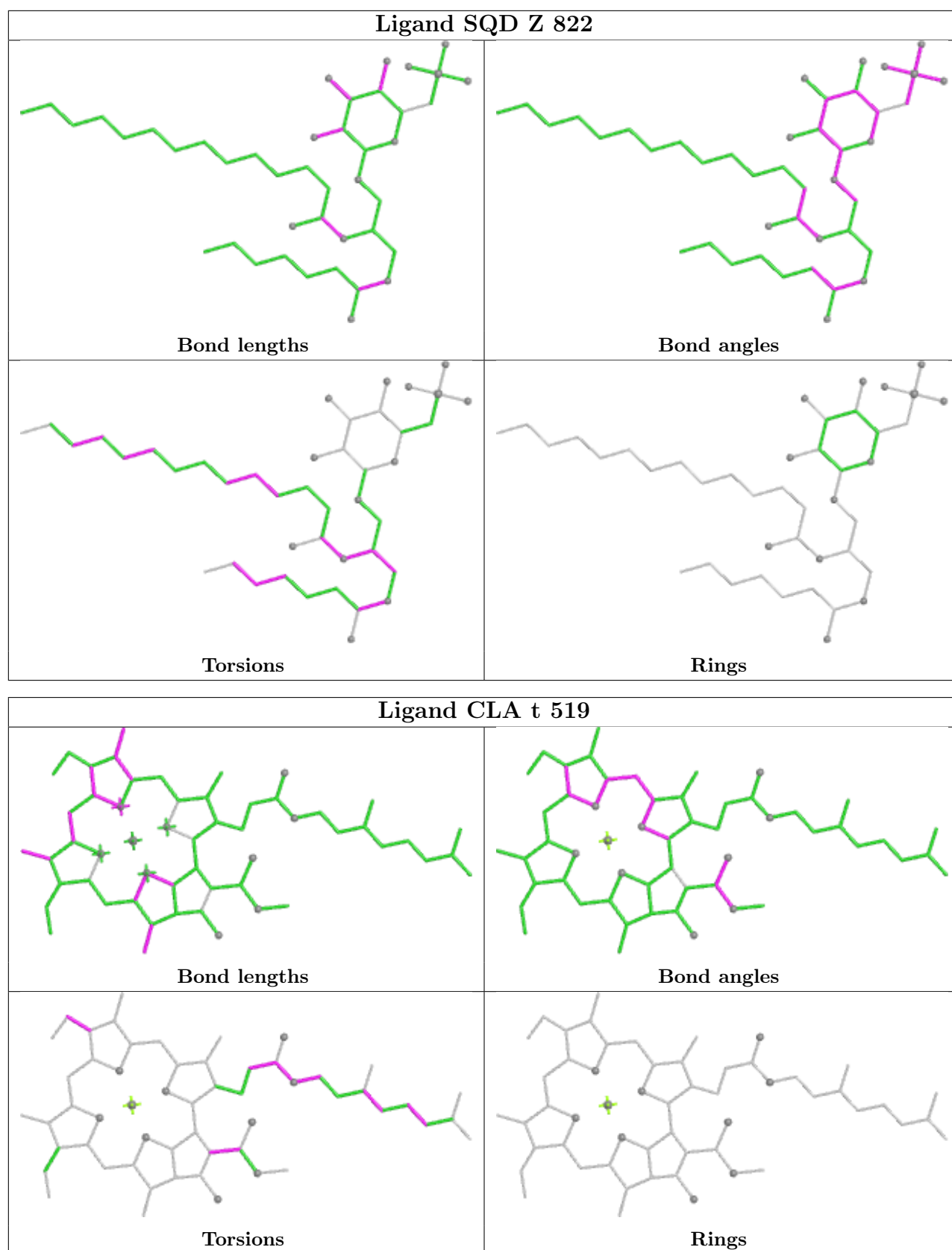
Torsions

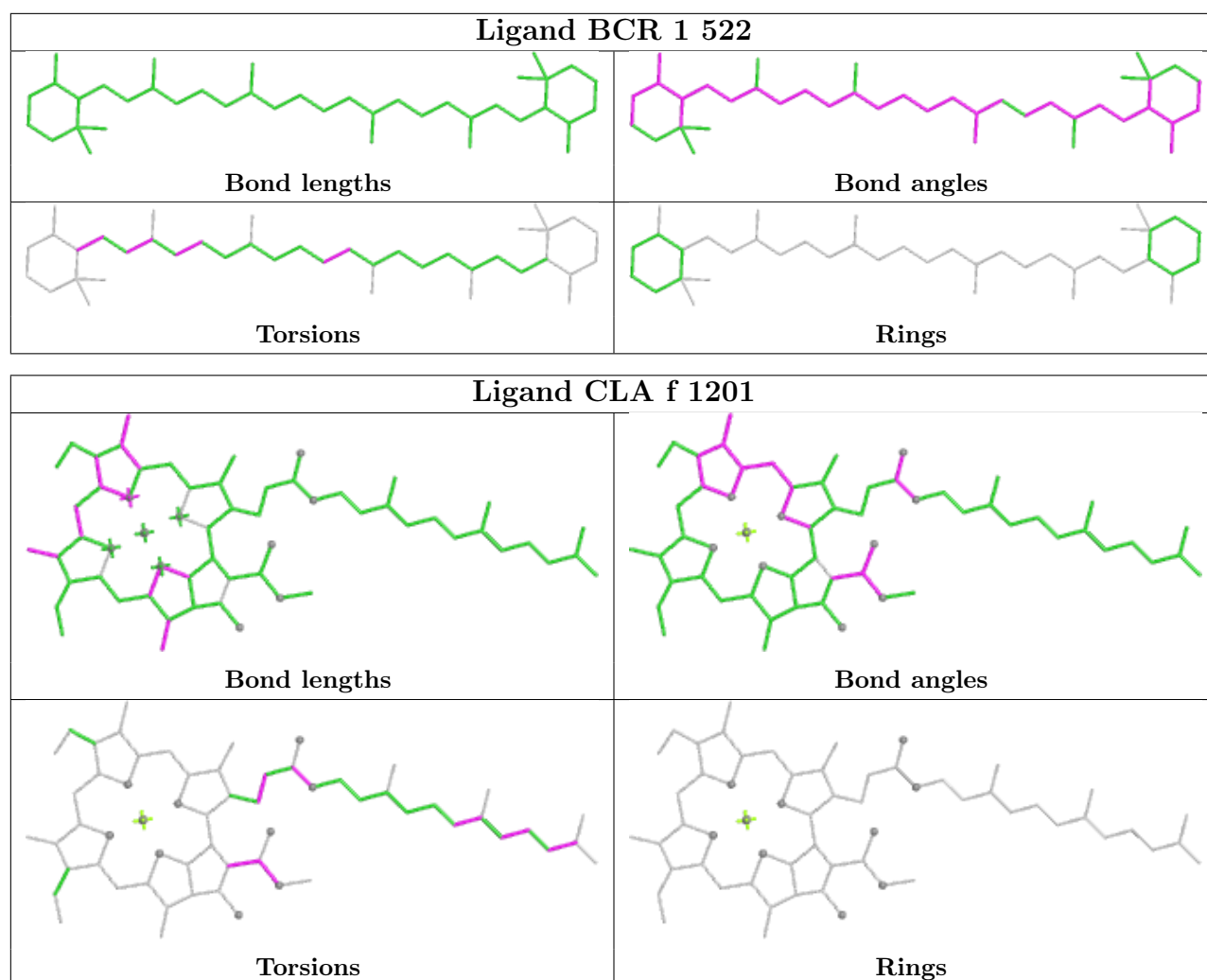


Rings

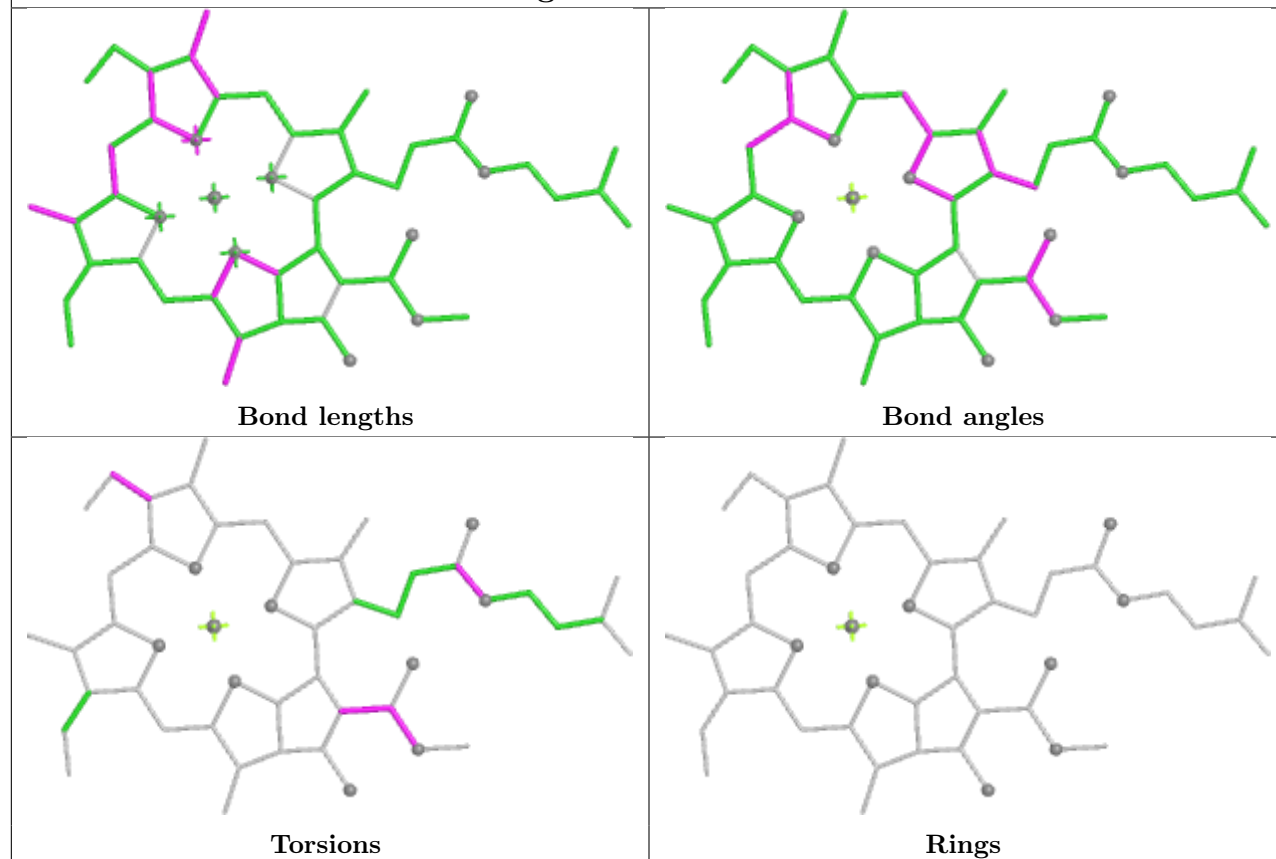




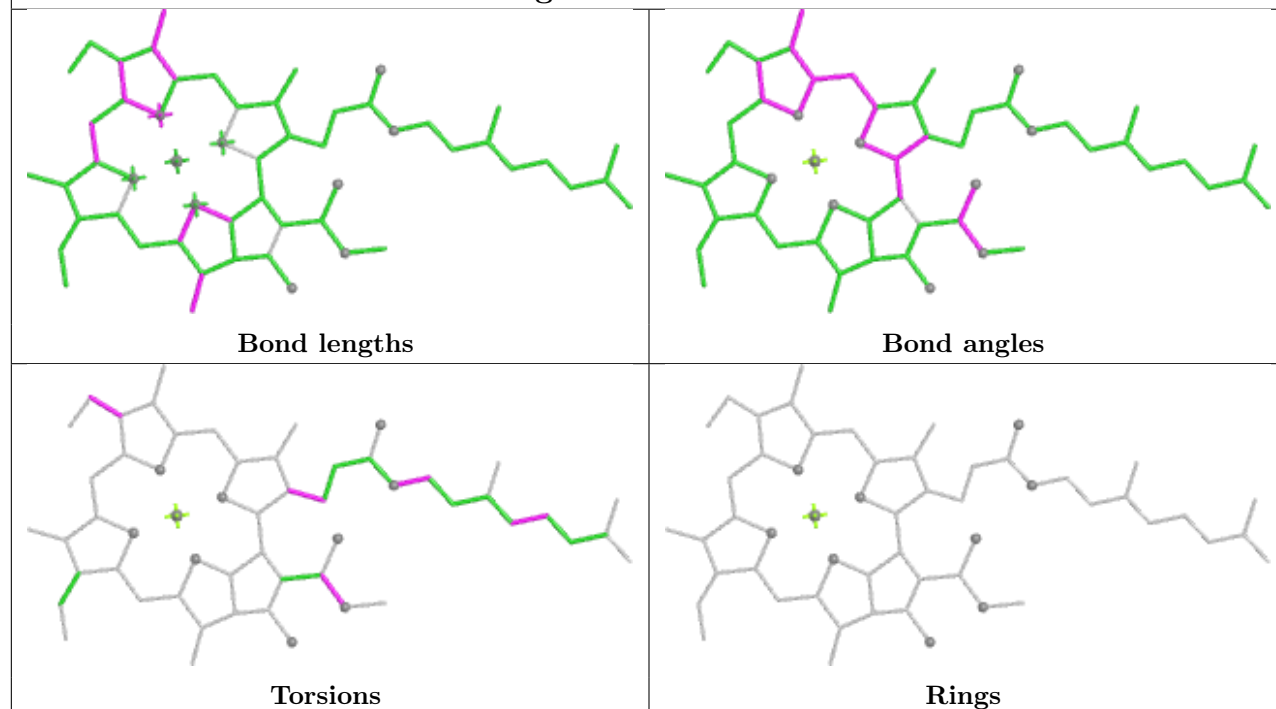




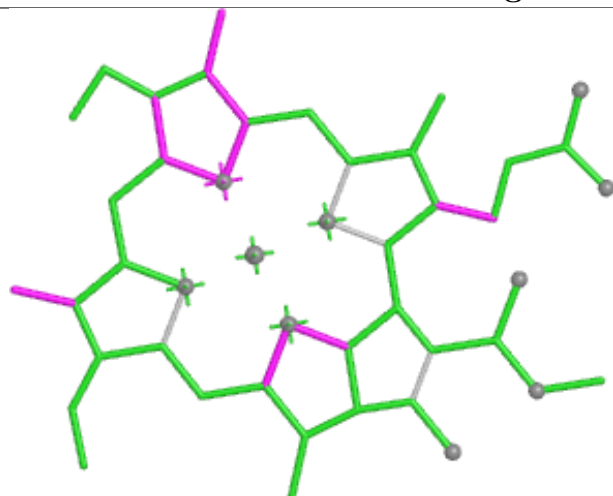
Ligand CLA c 502



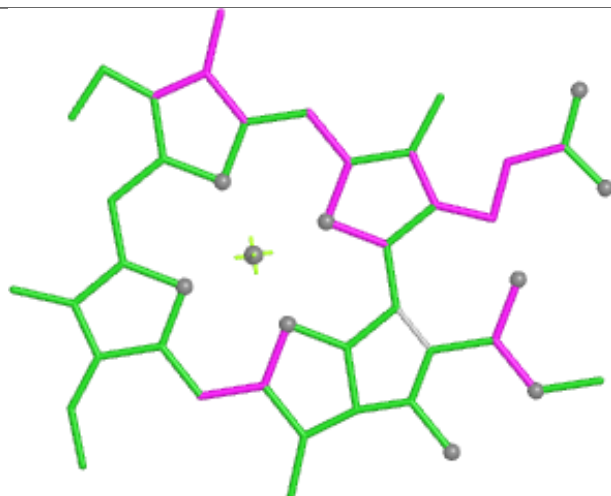
Ligand CLA u 511



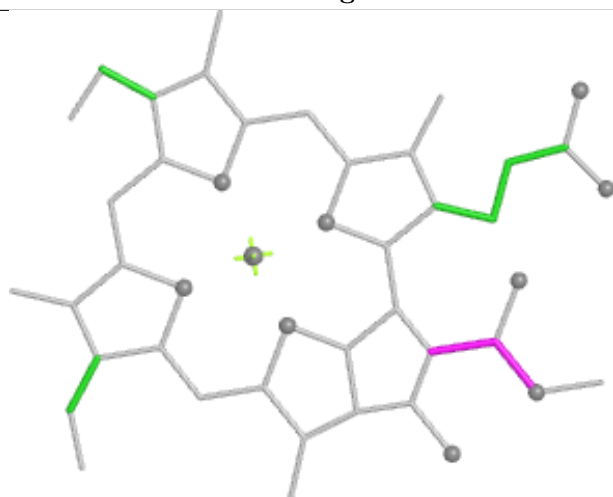
Ligand CLA A 1801



Bond lengths



Bond angles

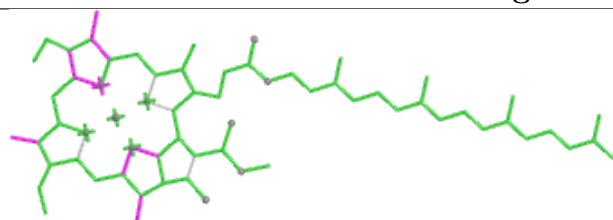


Torsions

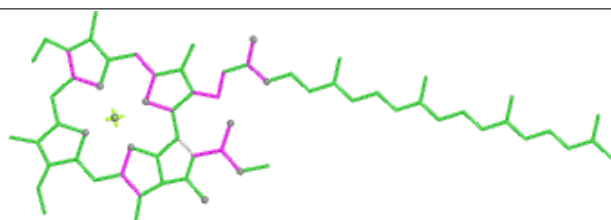


Rings

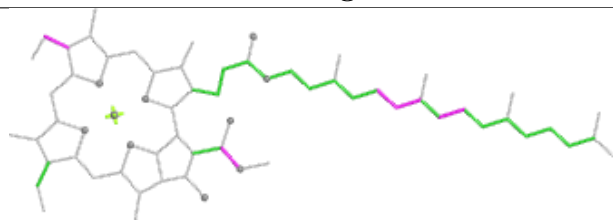
Ligand CLA f 1235



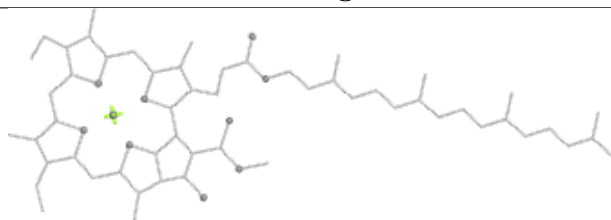
Bond lengths



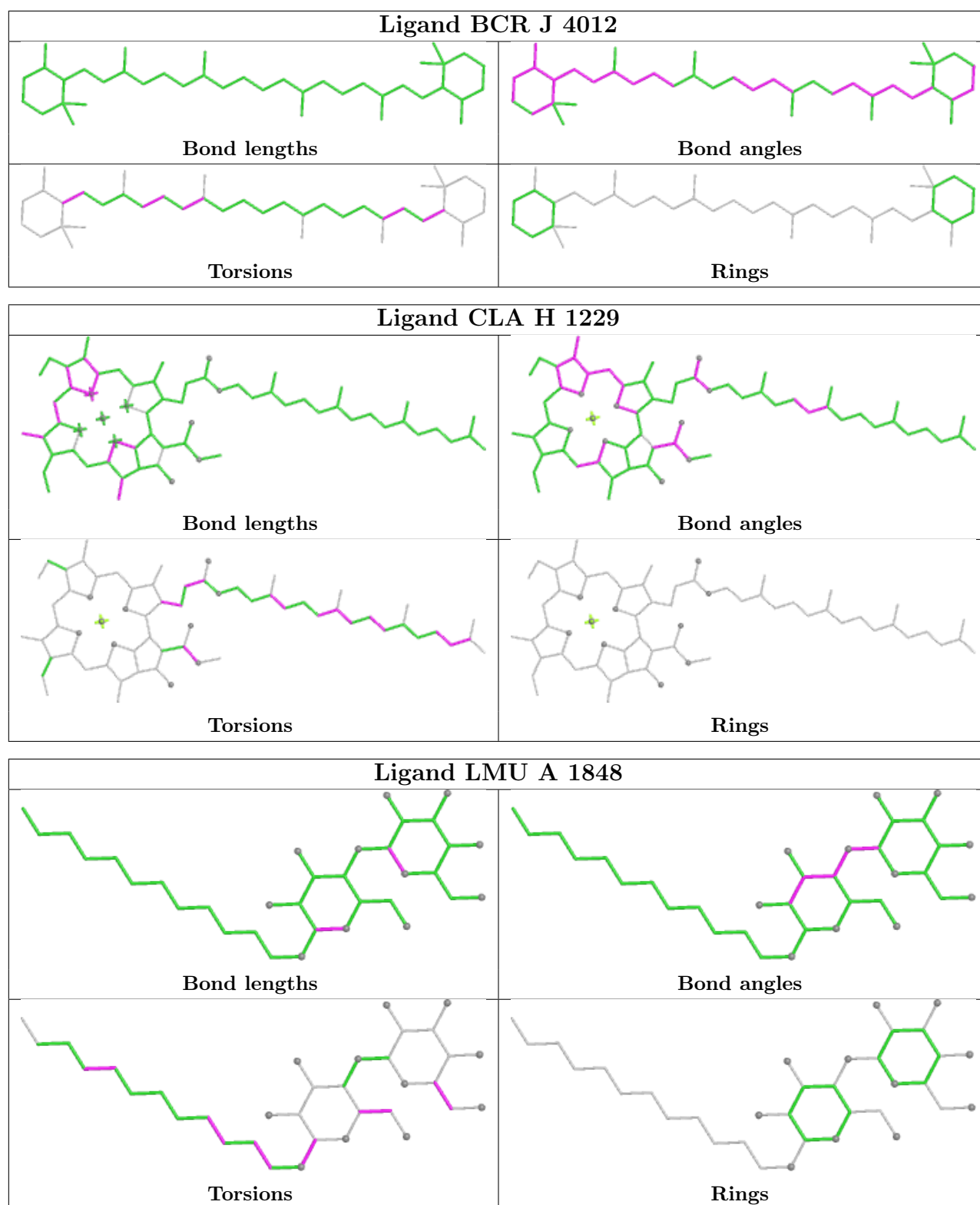
Bond angles



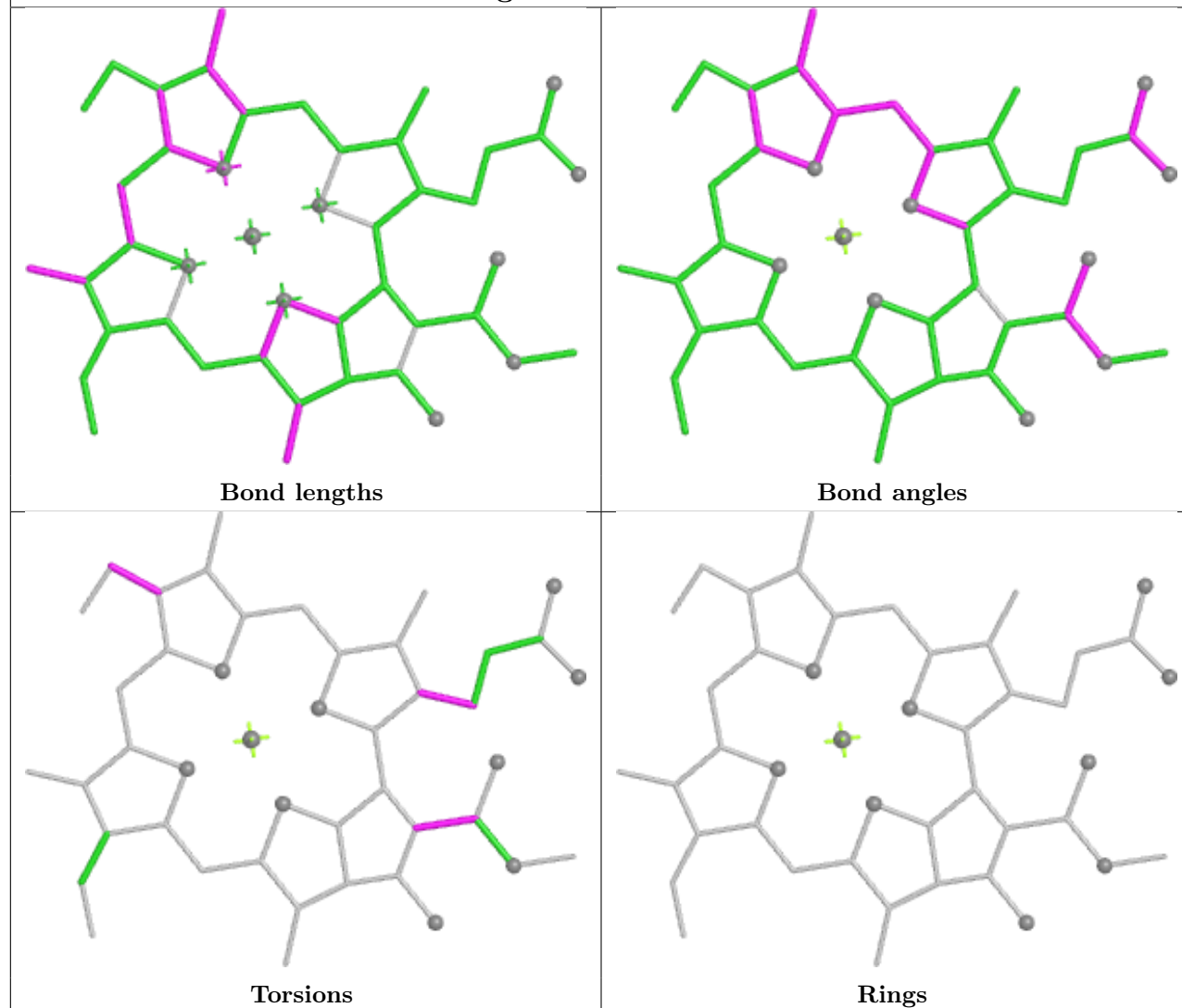
Torsions



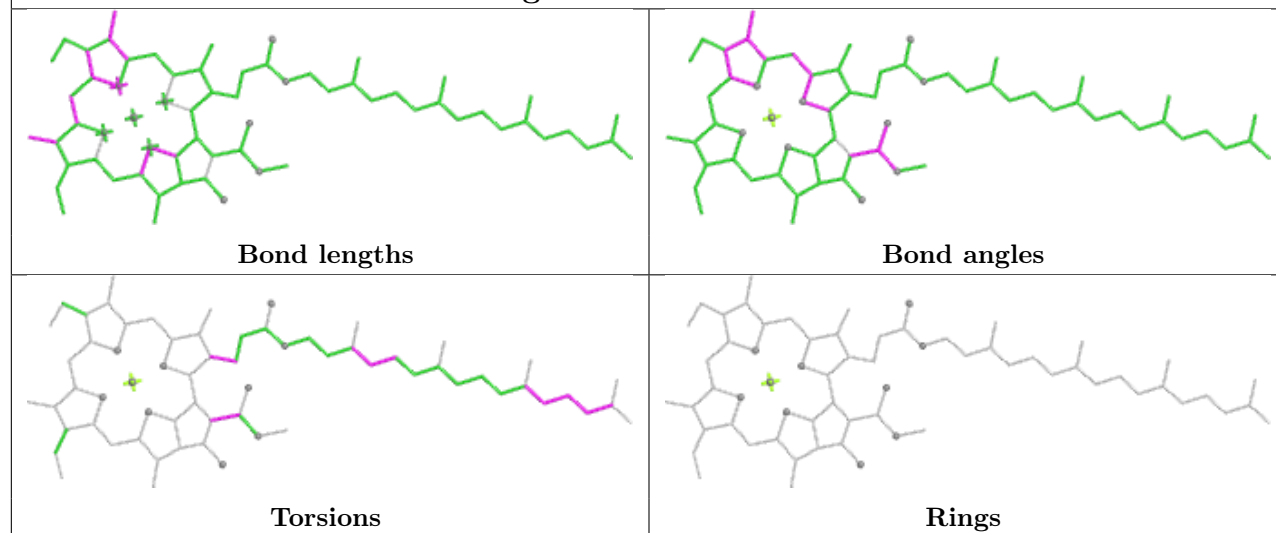
Rings

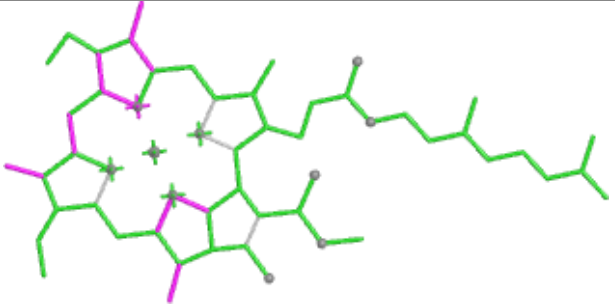
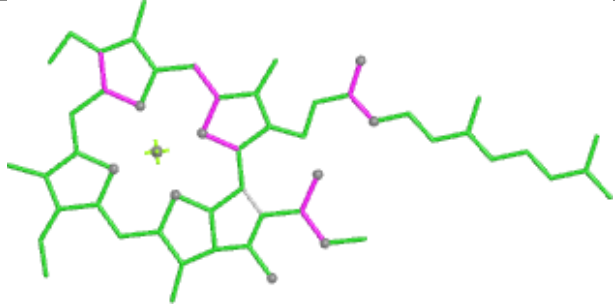
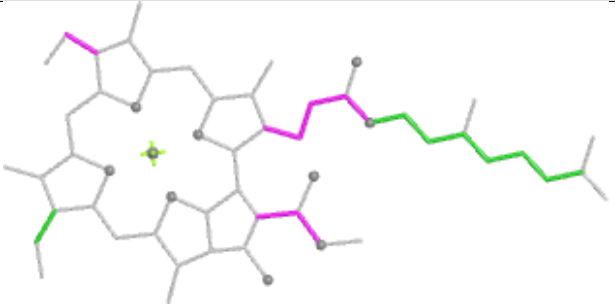
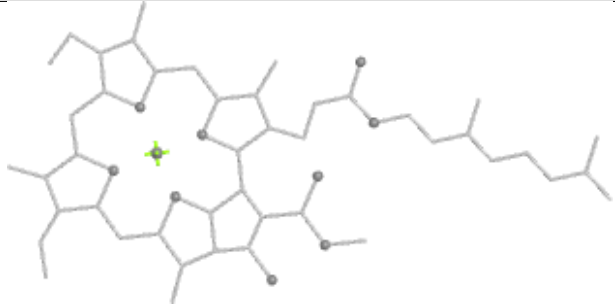
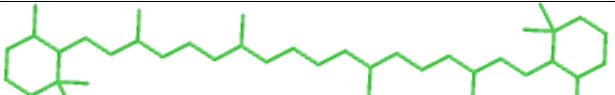
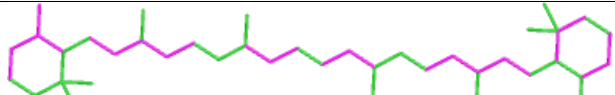
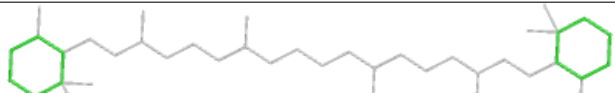
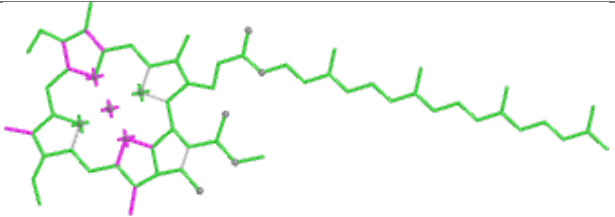
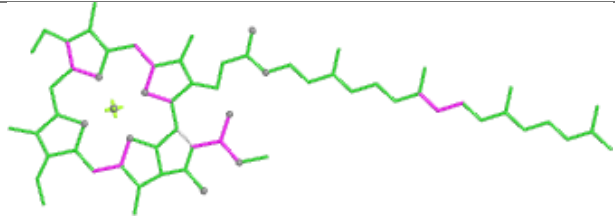
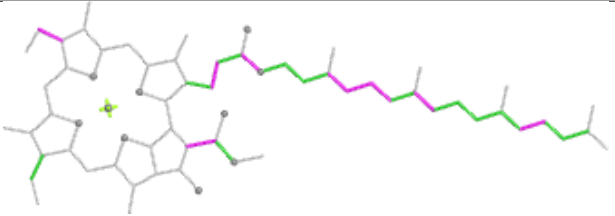
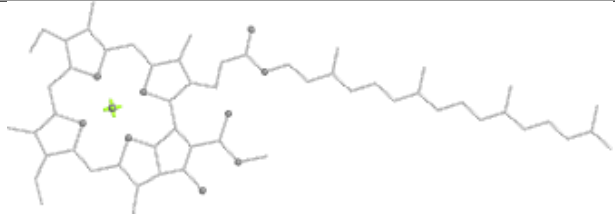


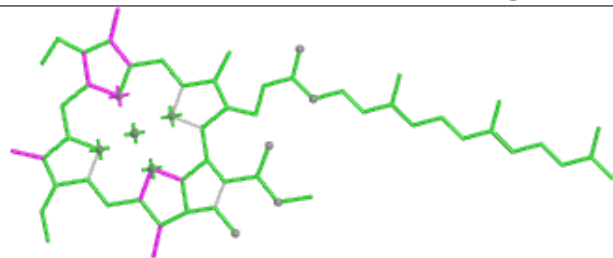
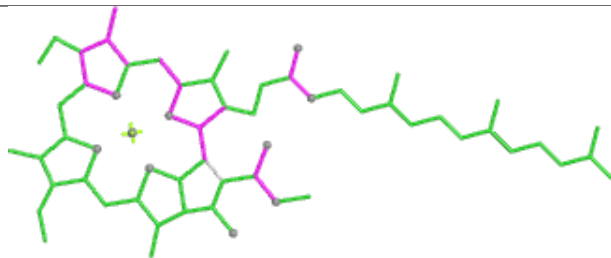
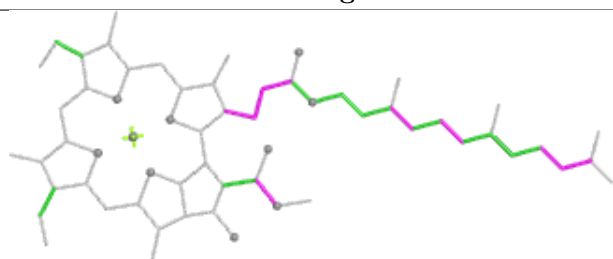
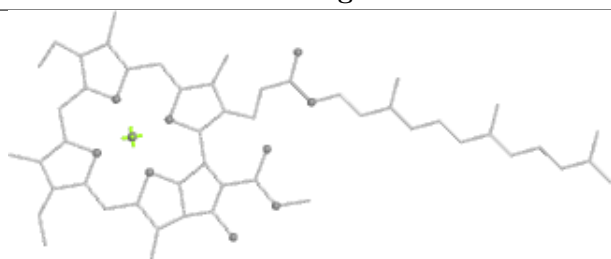
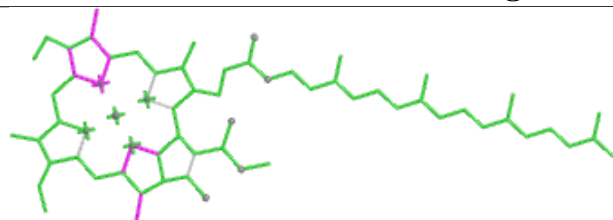
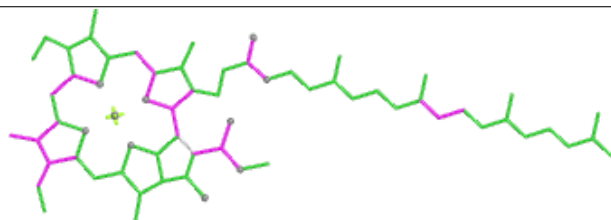
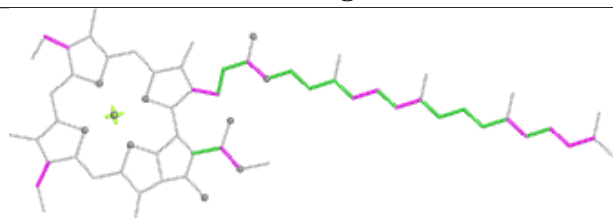
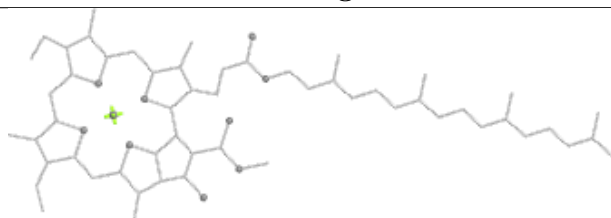
Ligand CLA 6 508

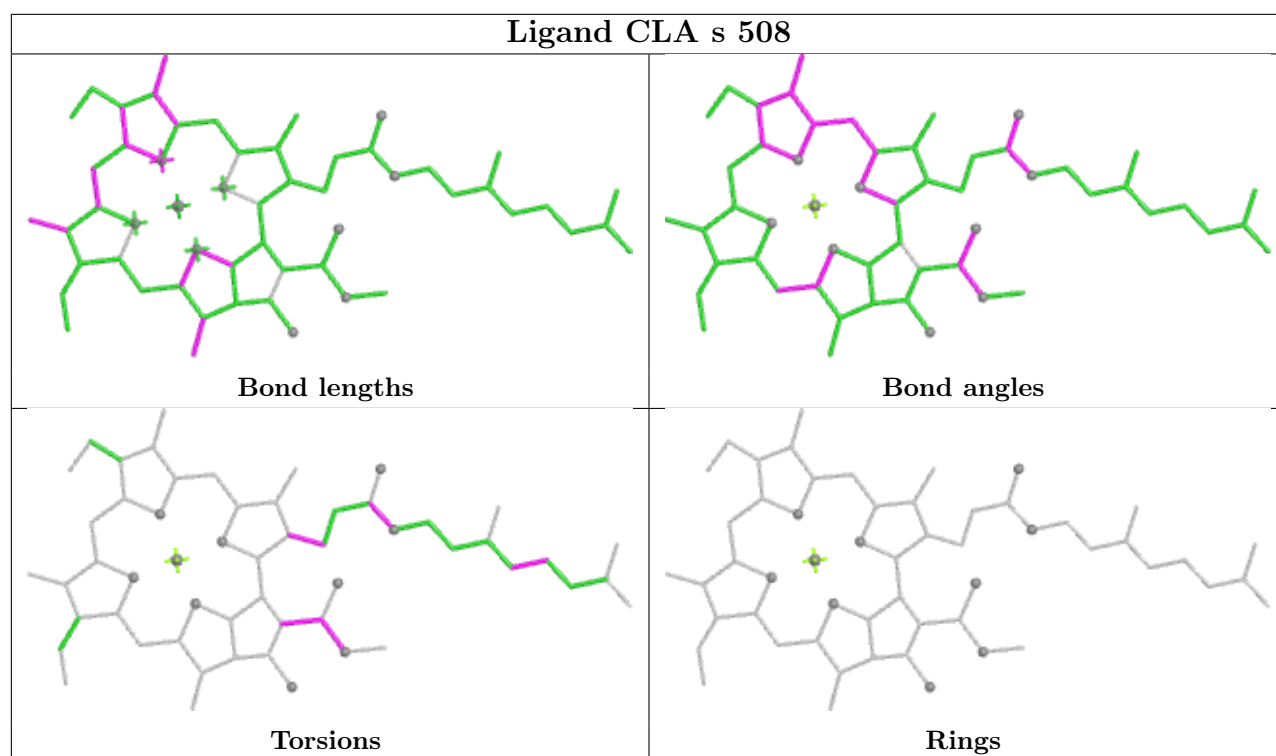


Ligand CLA A 1102

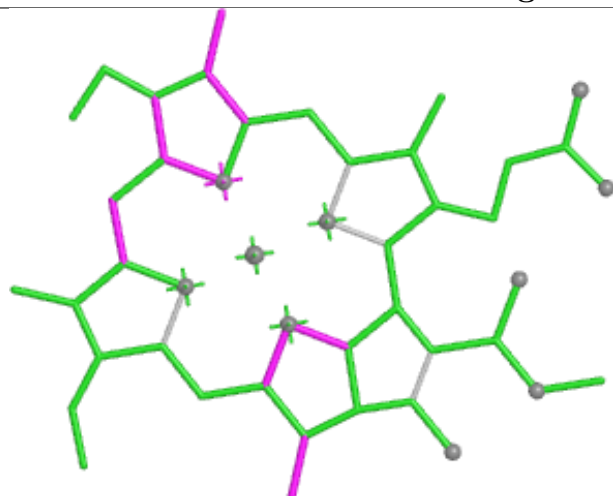


Ligand CLA s 518	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR s 521	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA f 1204	
	
Bond lengths	Bond angles
	
Torsions	Rings

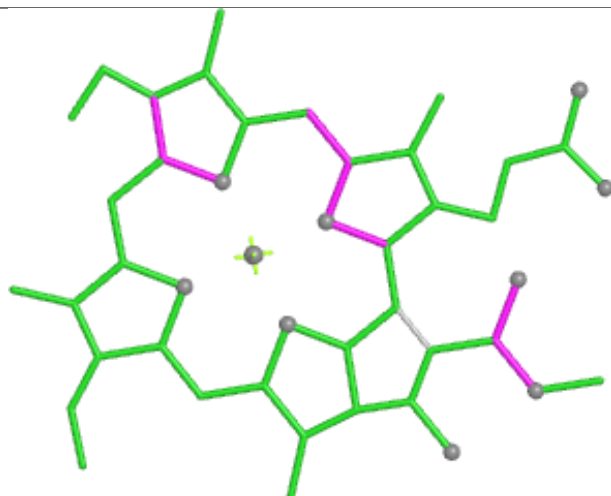
Ligand CLA H 1224**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA H 1239****Bond lengths****Bond angles****Torsions****Rings**



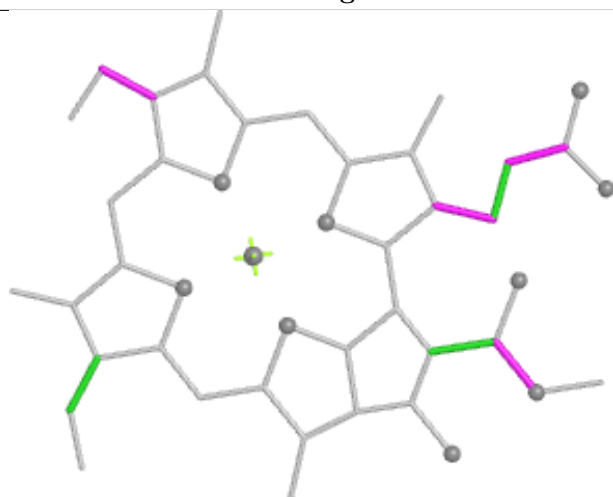
Ligand CLA v 512



Bond lengths



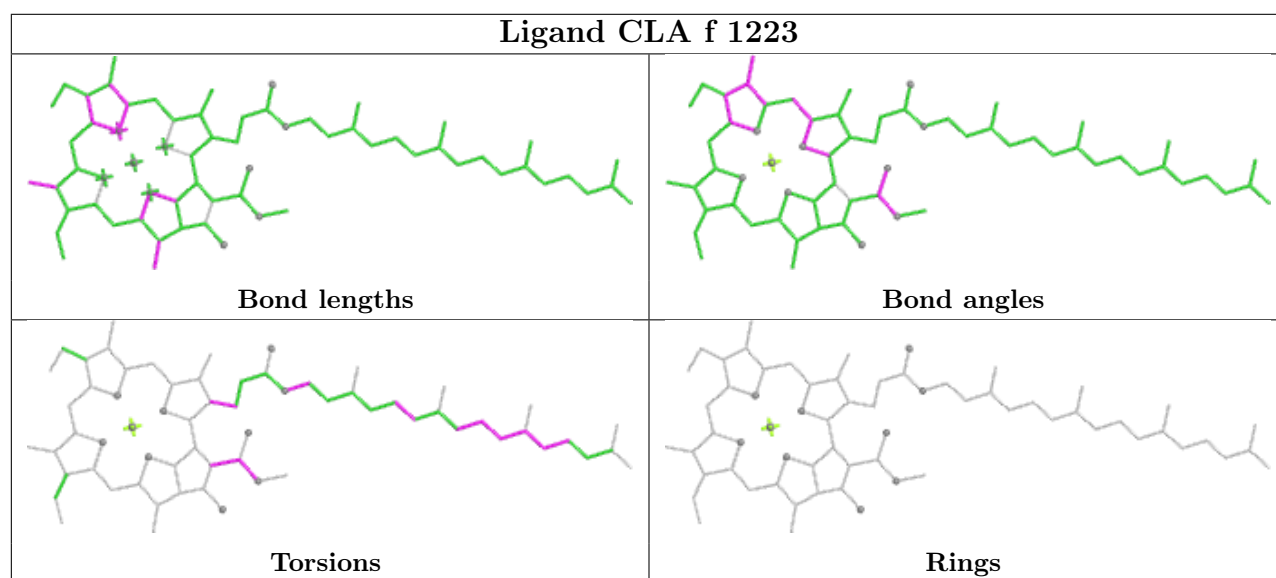
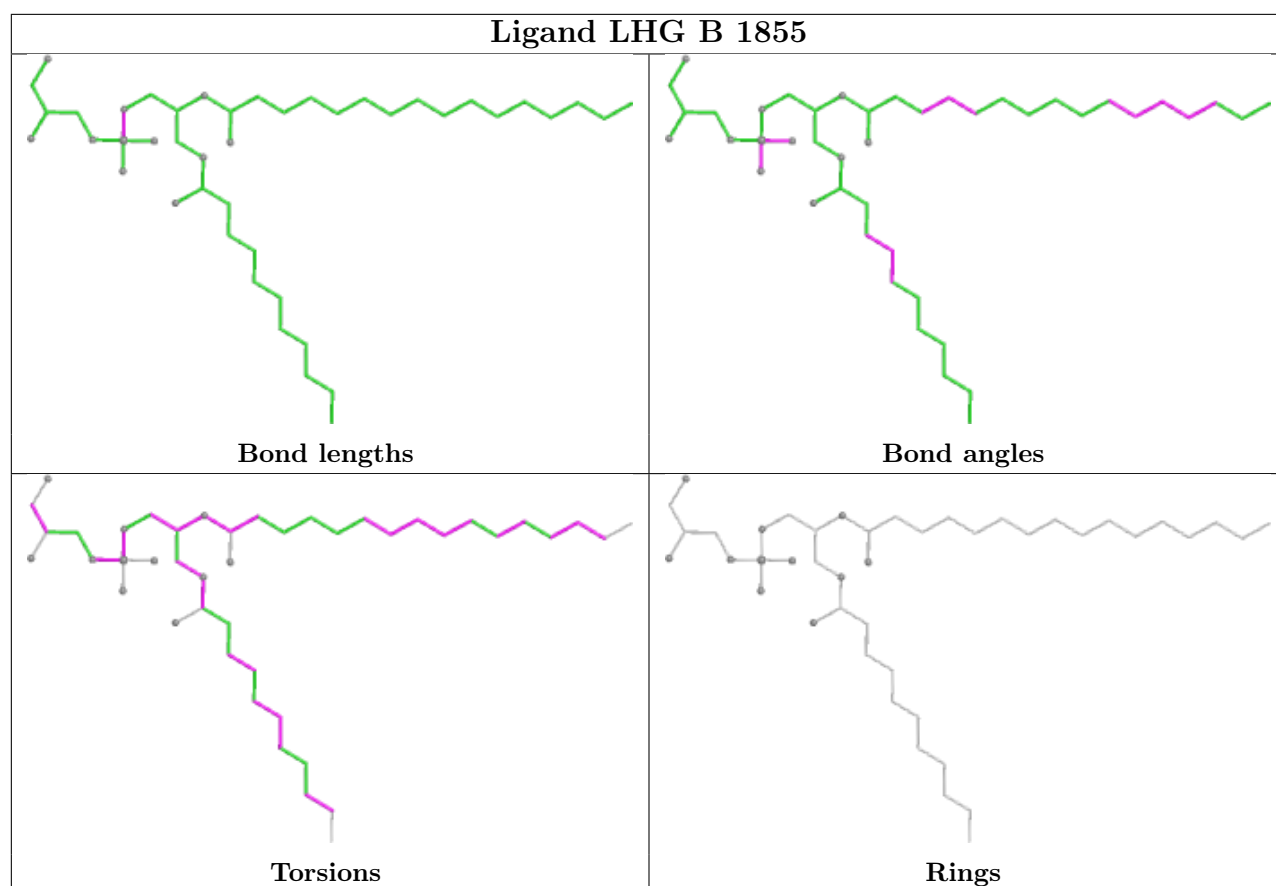
Bond angles

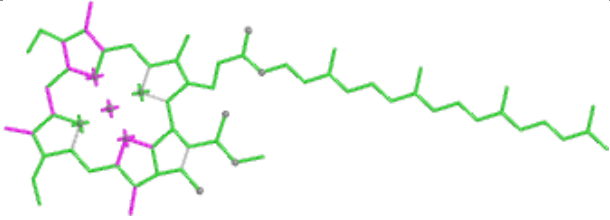
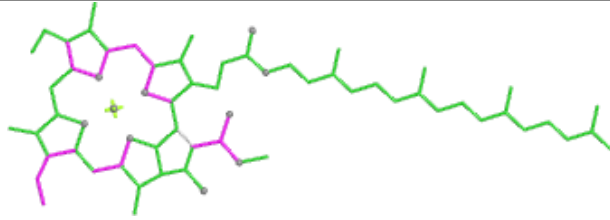
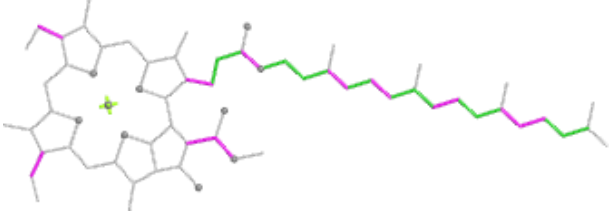
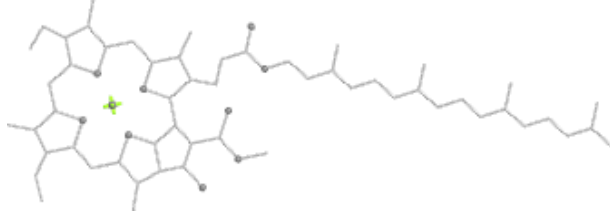
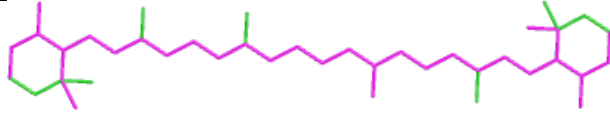
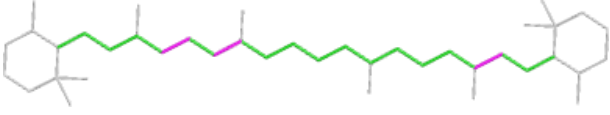
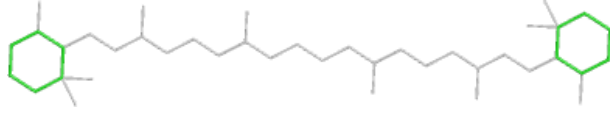
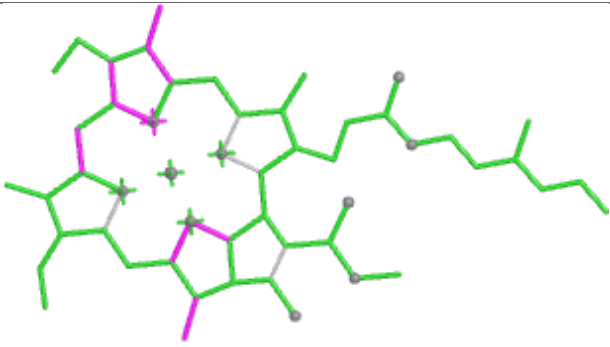
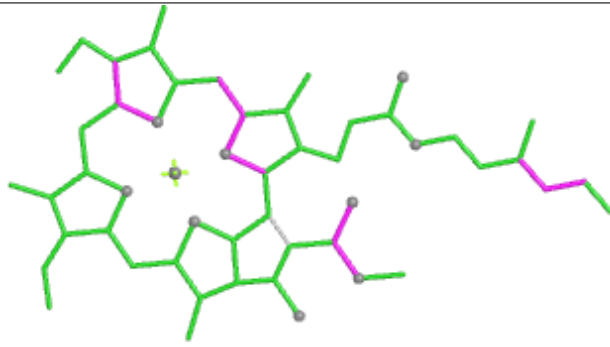
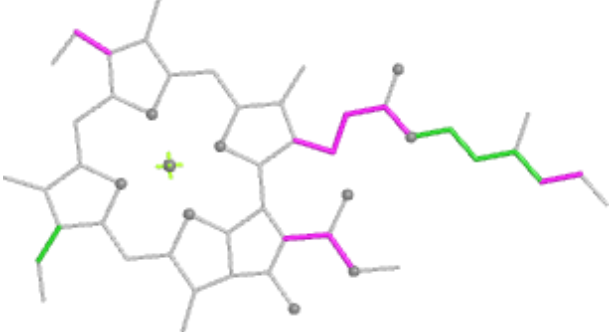
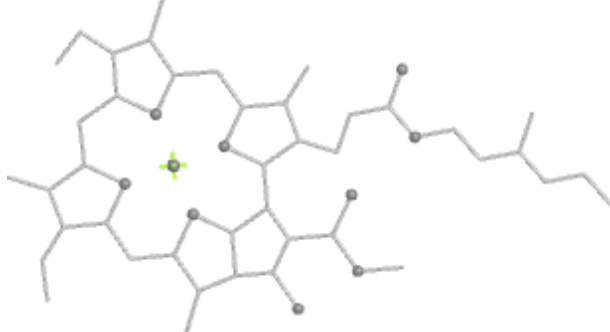


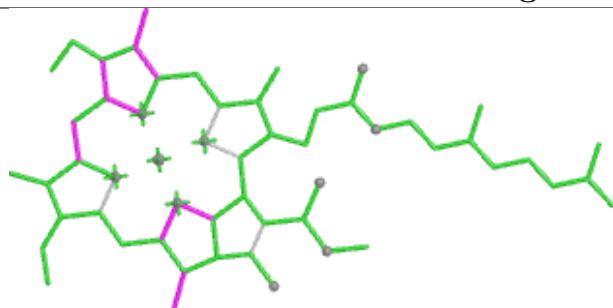
Torsions



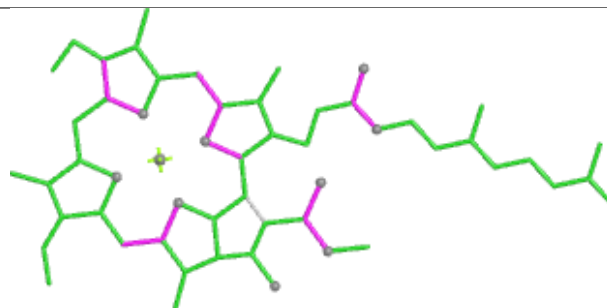
Rings



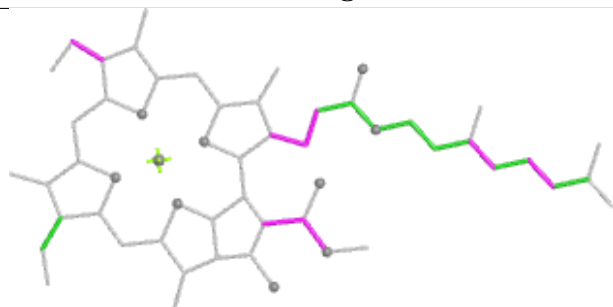
Ligand CLA A 1132	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 4010	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 1 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 503

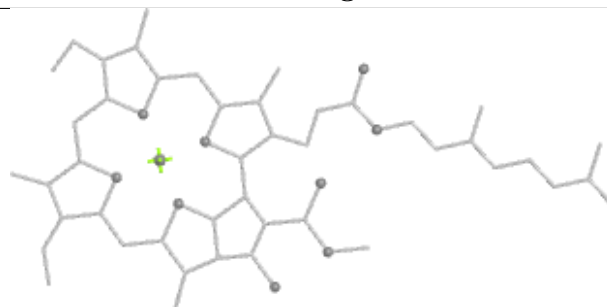
Bond lengths



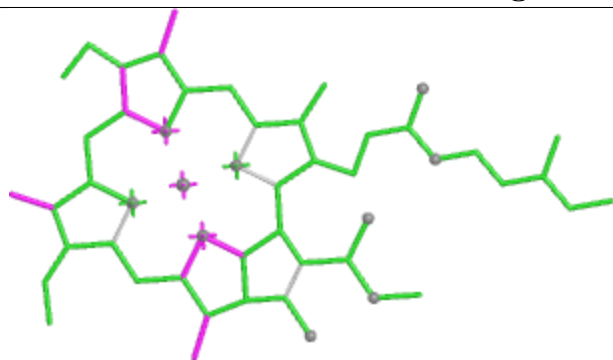
Bond angles



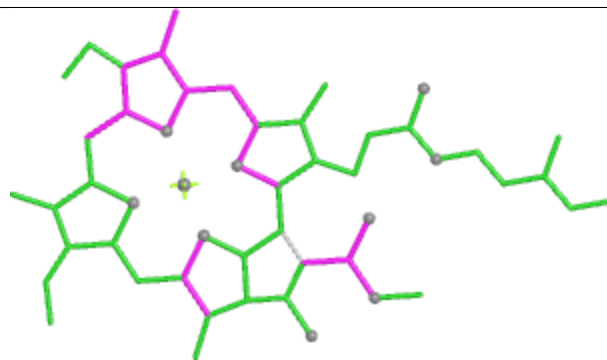
Torsions



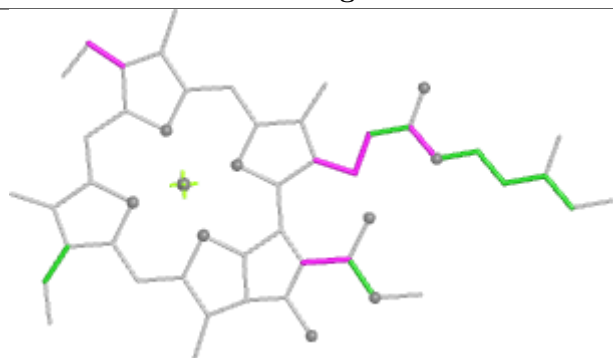
Rings

Ligand CLA e 1129

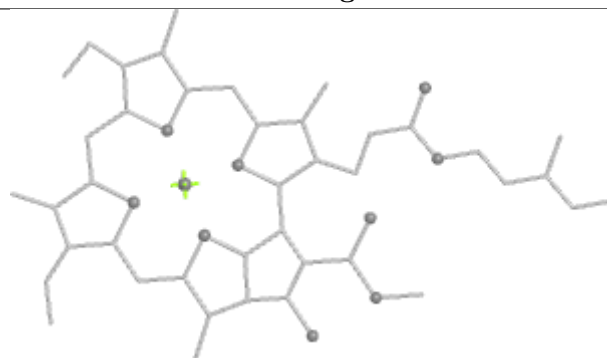
Bond lengths



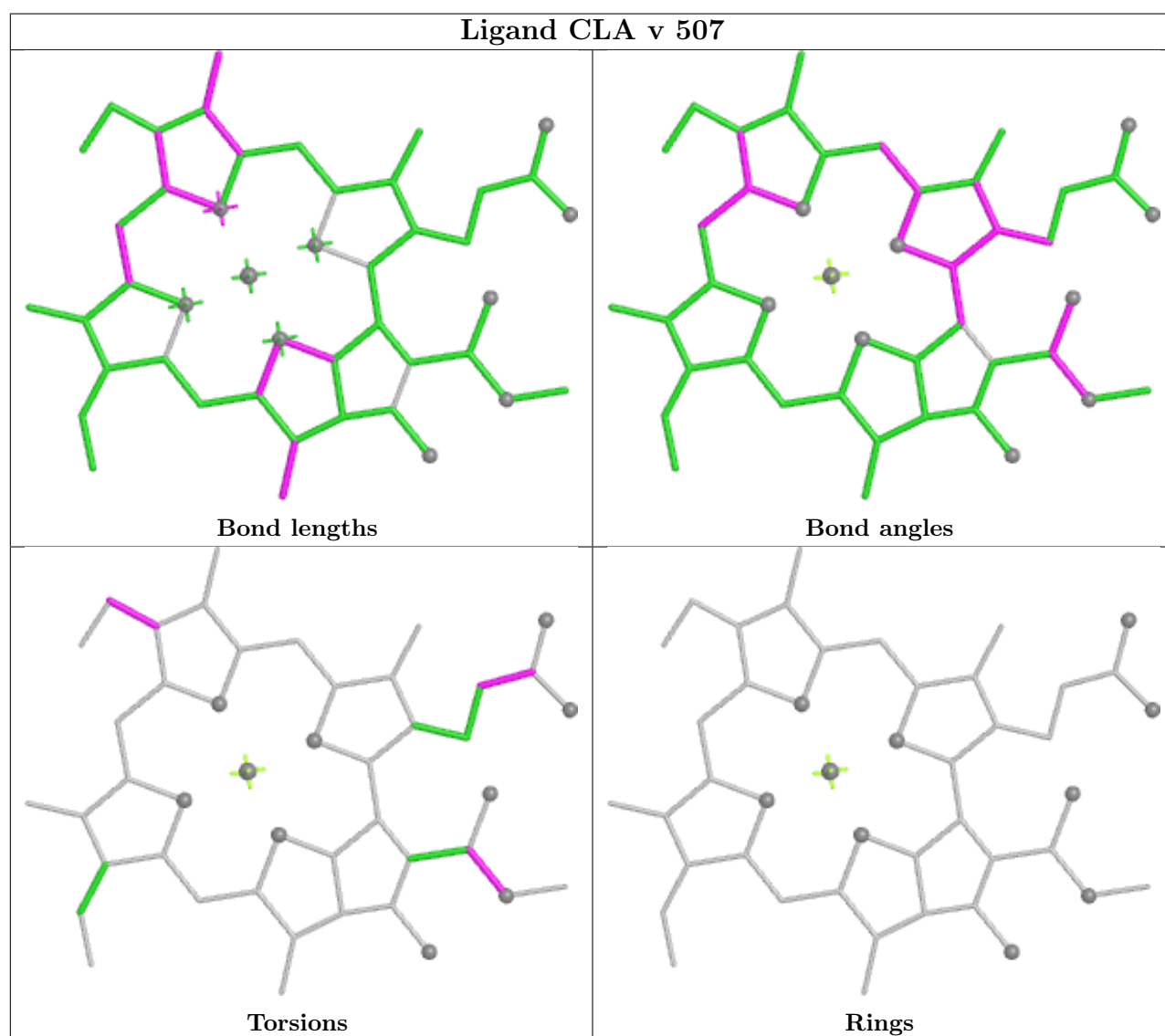
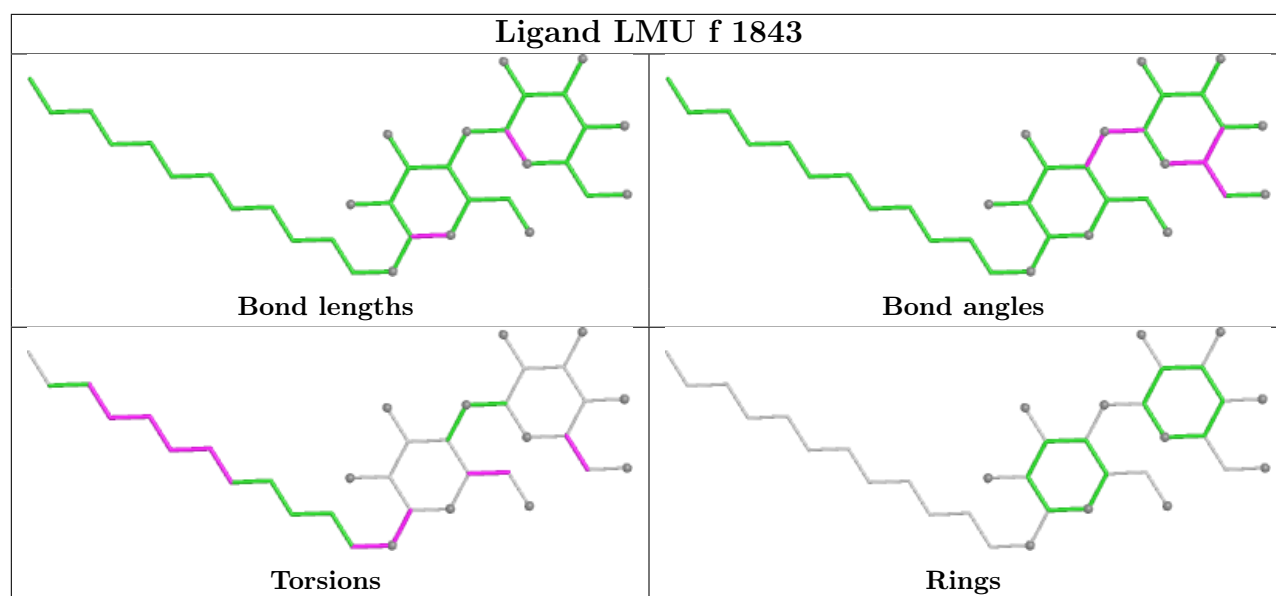
Bond angles



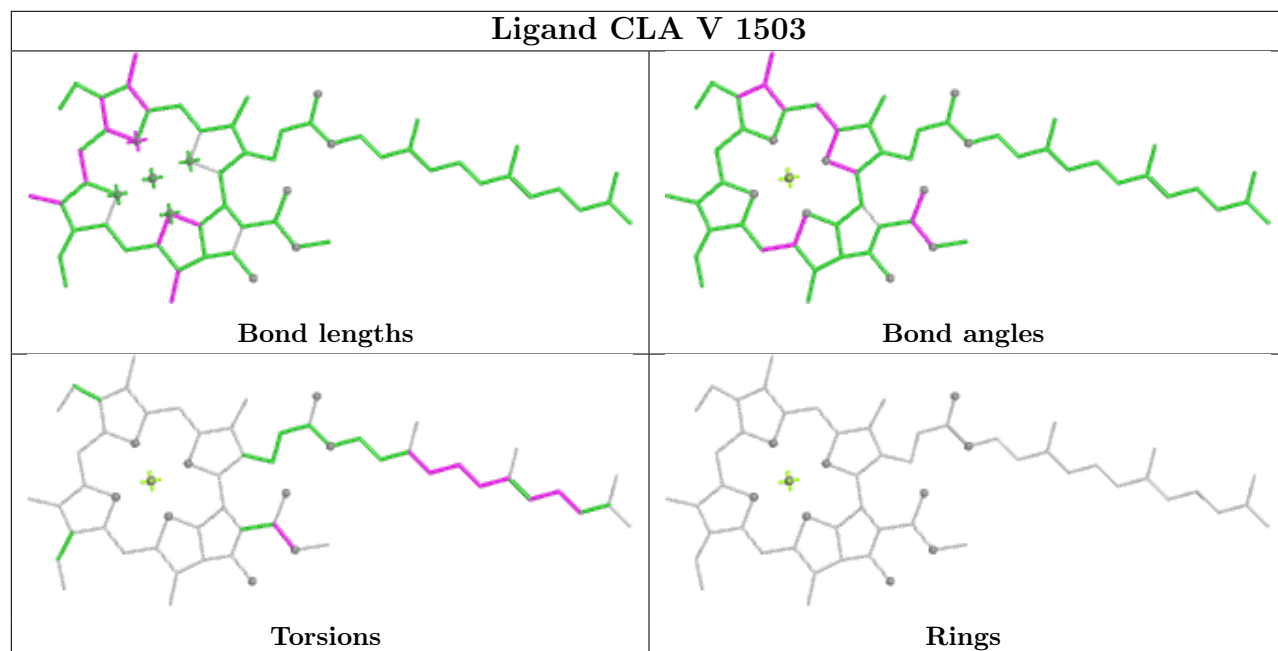
Torsions



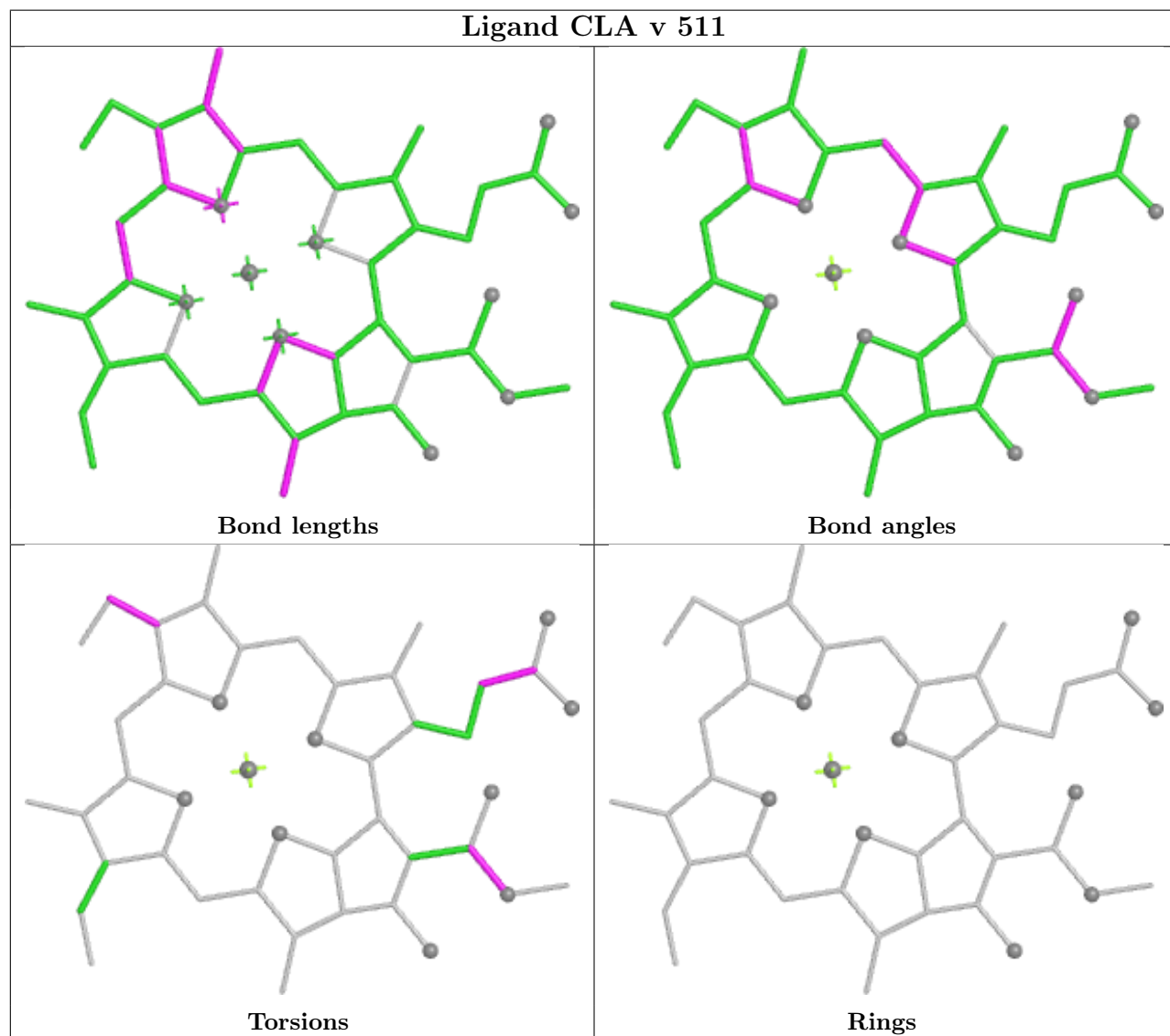
Rings

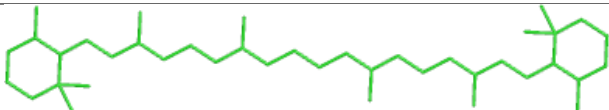
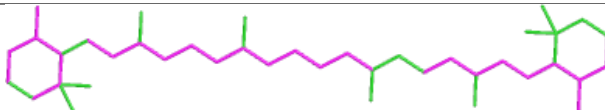
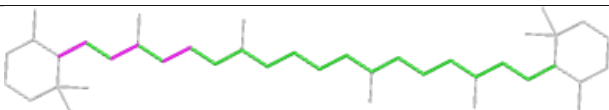
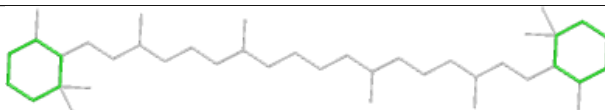


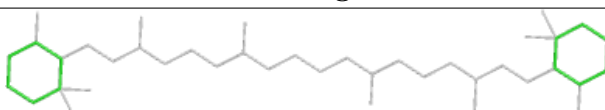
Ligand CLA V 1503

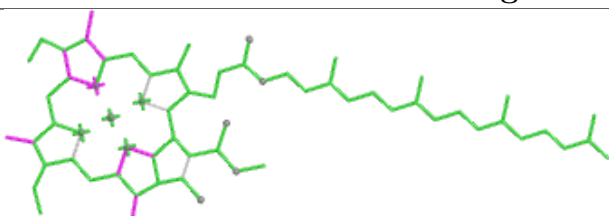
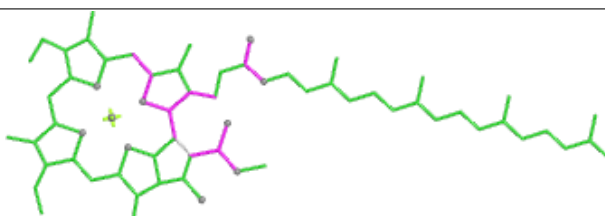
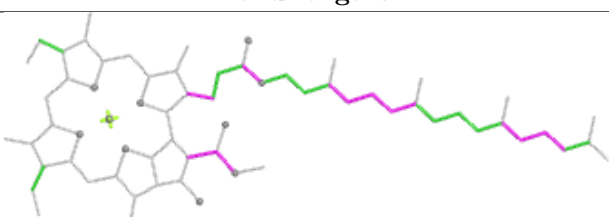
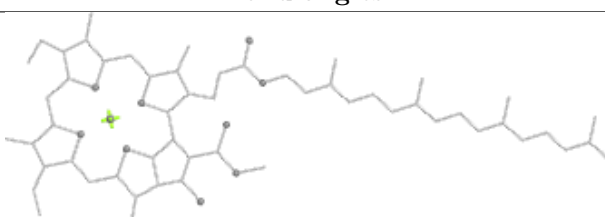


Ligand CLA v 511

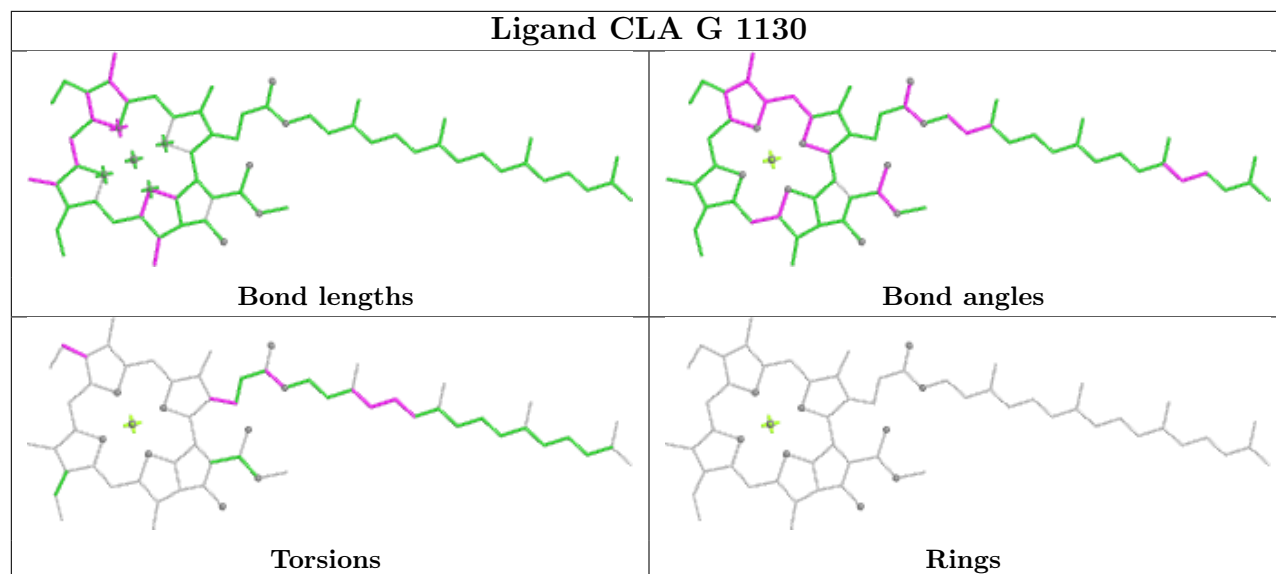


Ligand BCR s 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

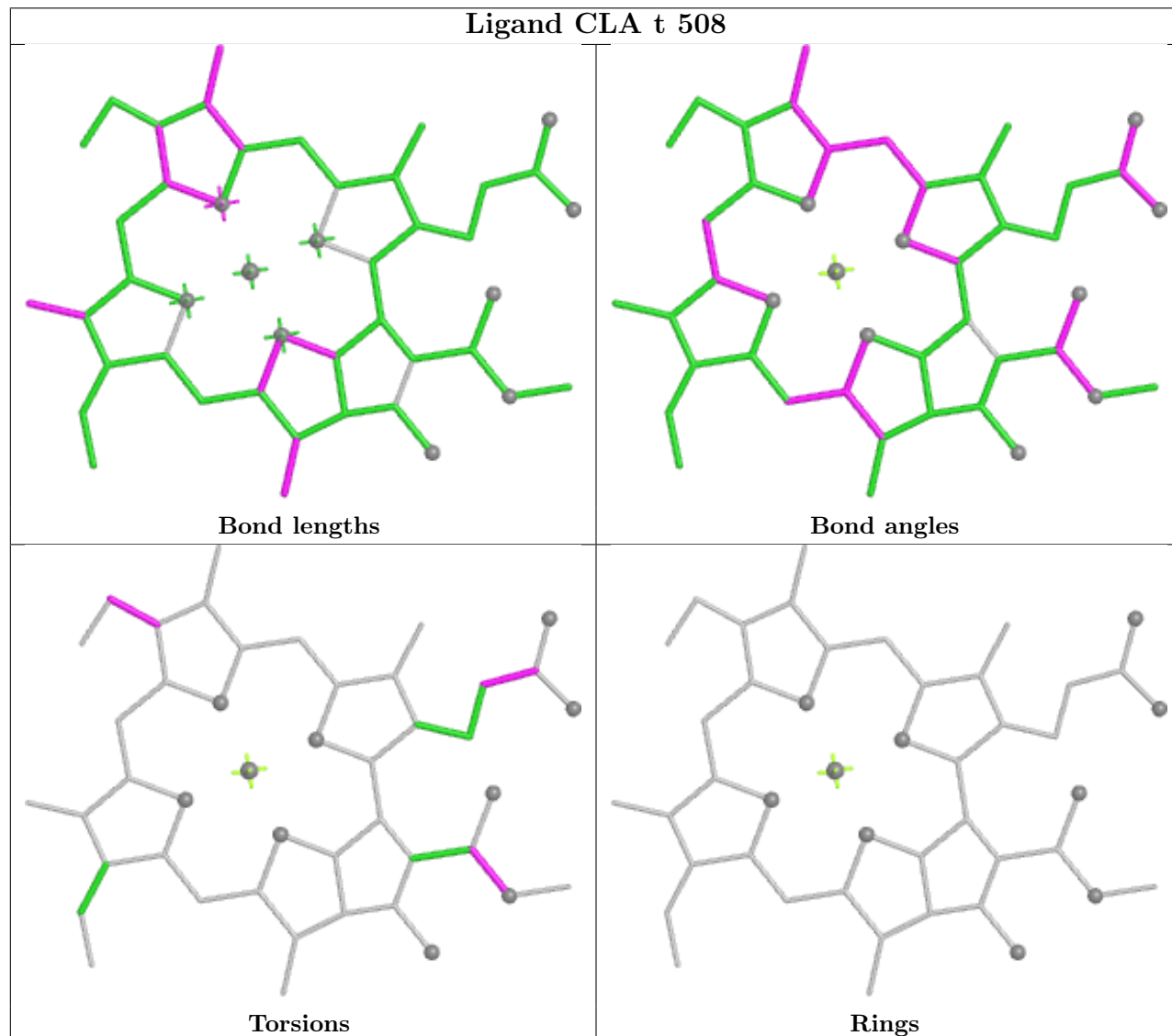
Ligand BCR T 4013	
	
Bond lengths	Bond angles
	
Torsions	Rings

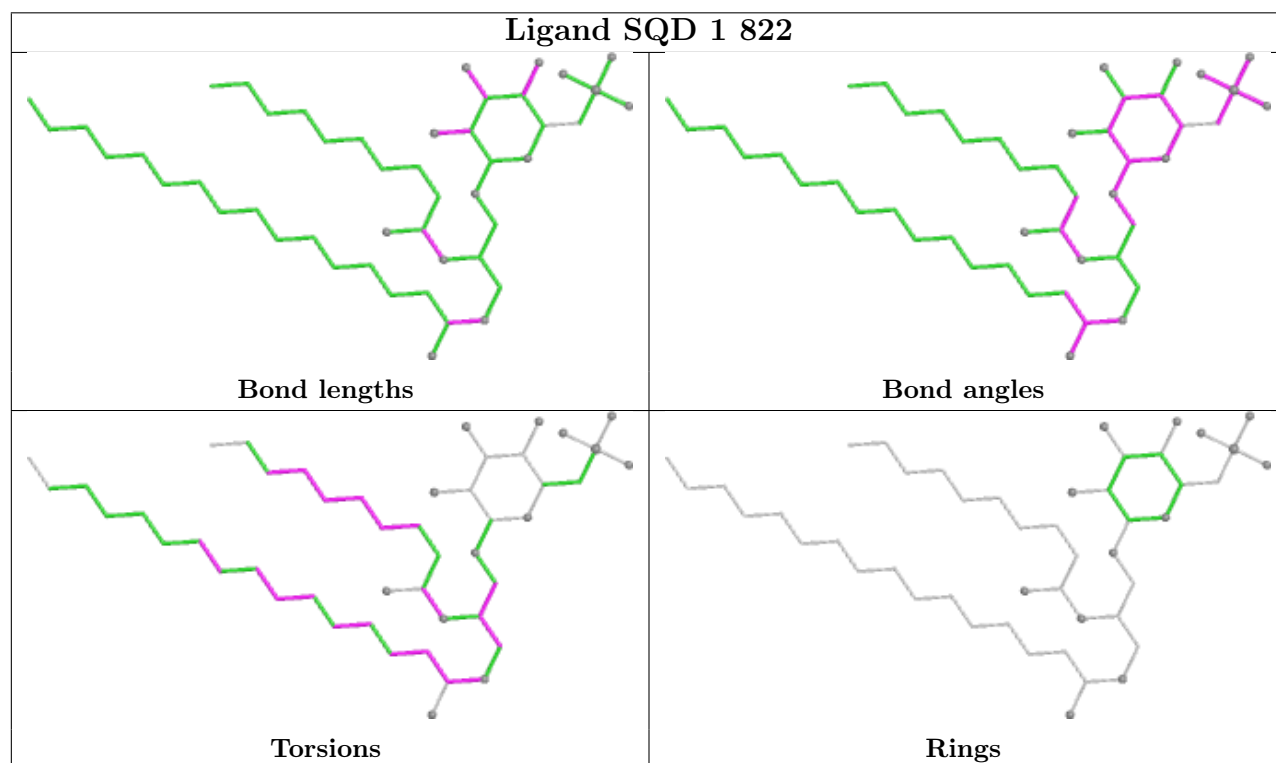
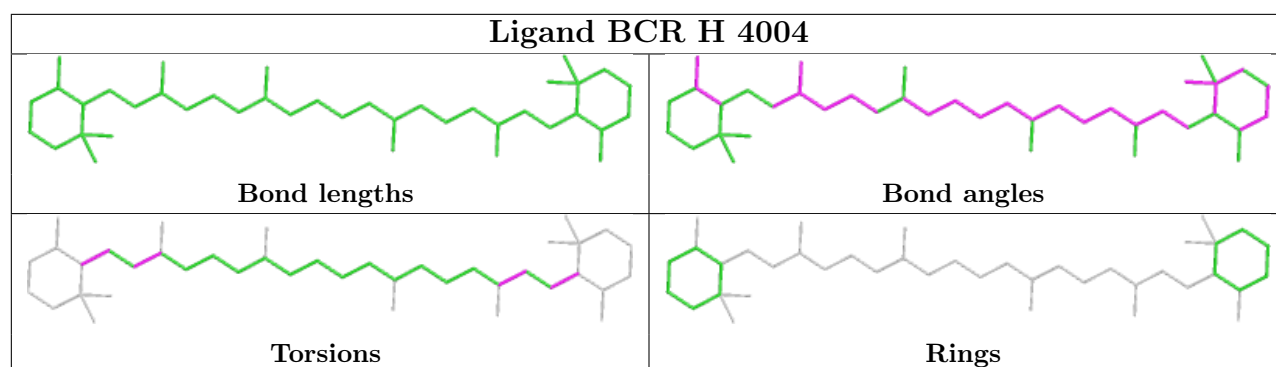
Ligand CLA T 1303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1130

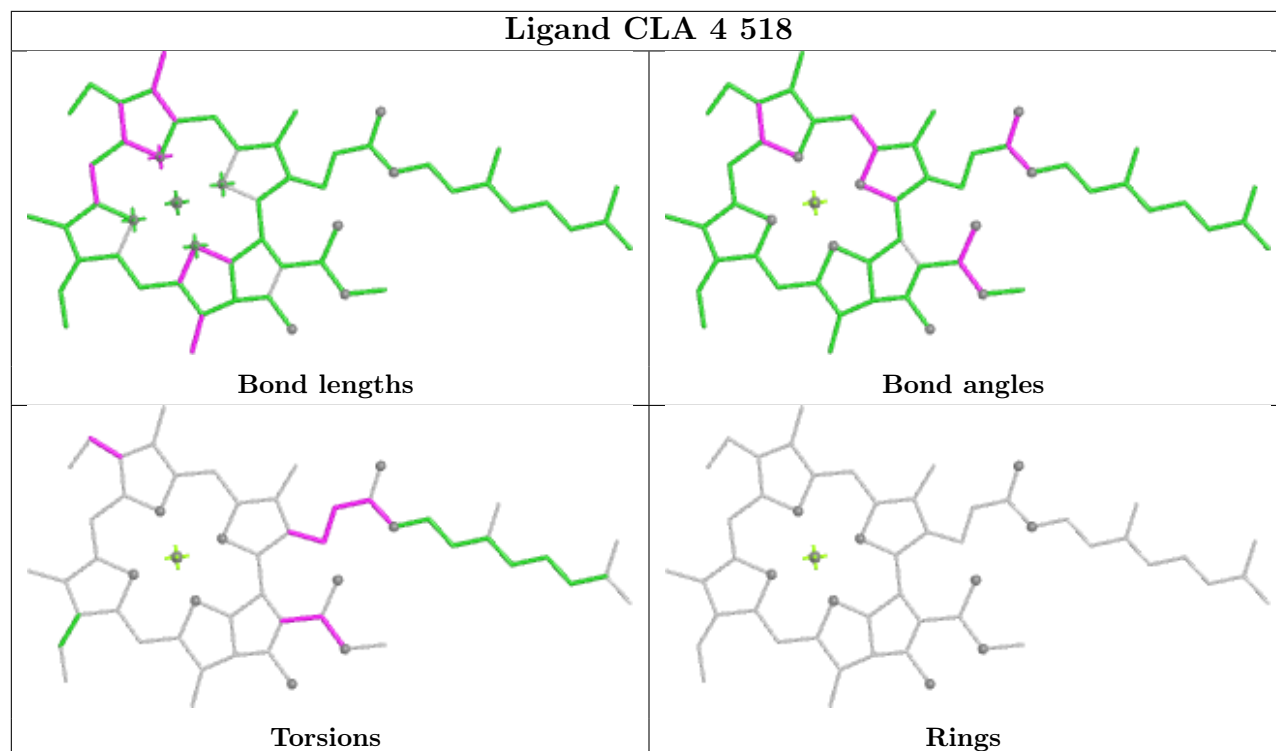


Ligand CLA t 508

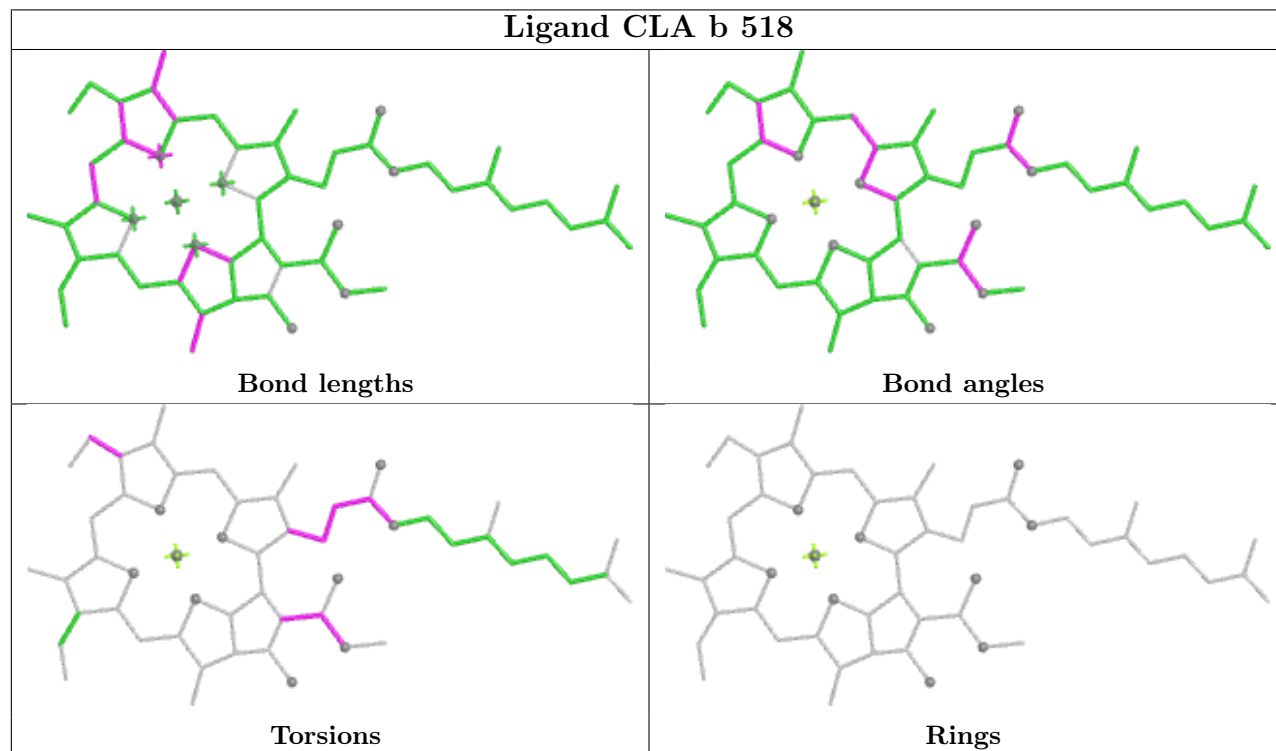


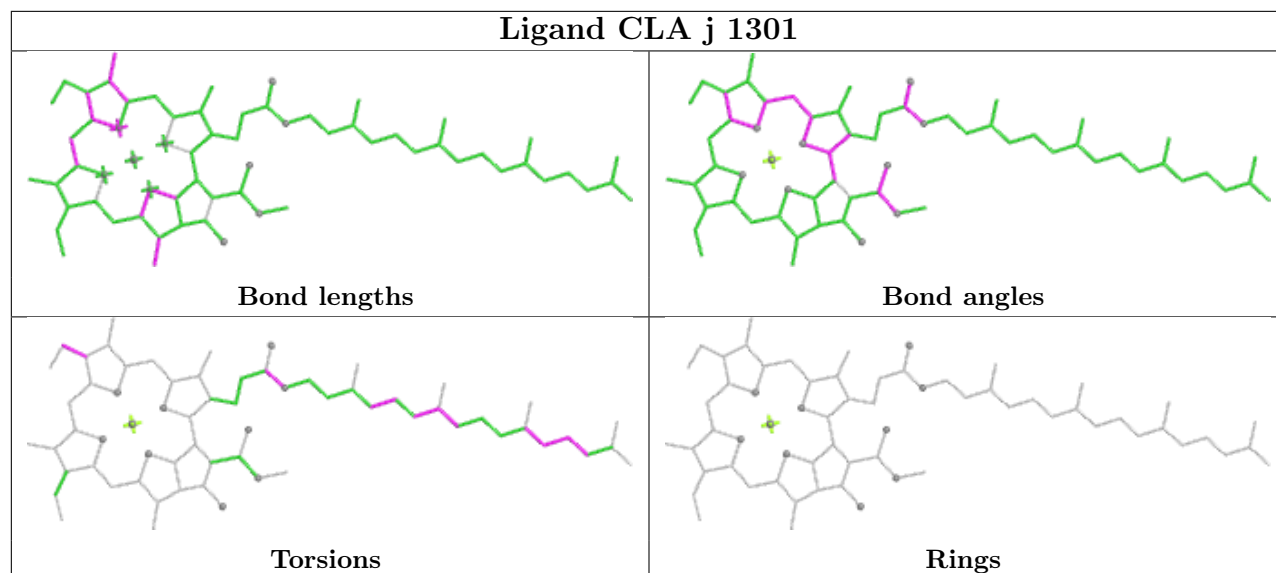
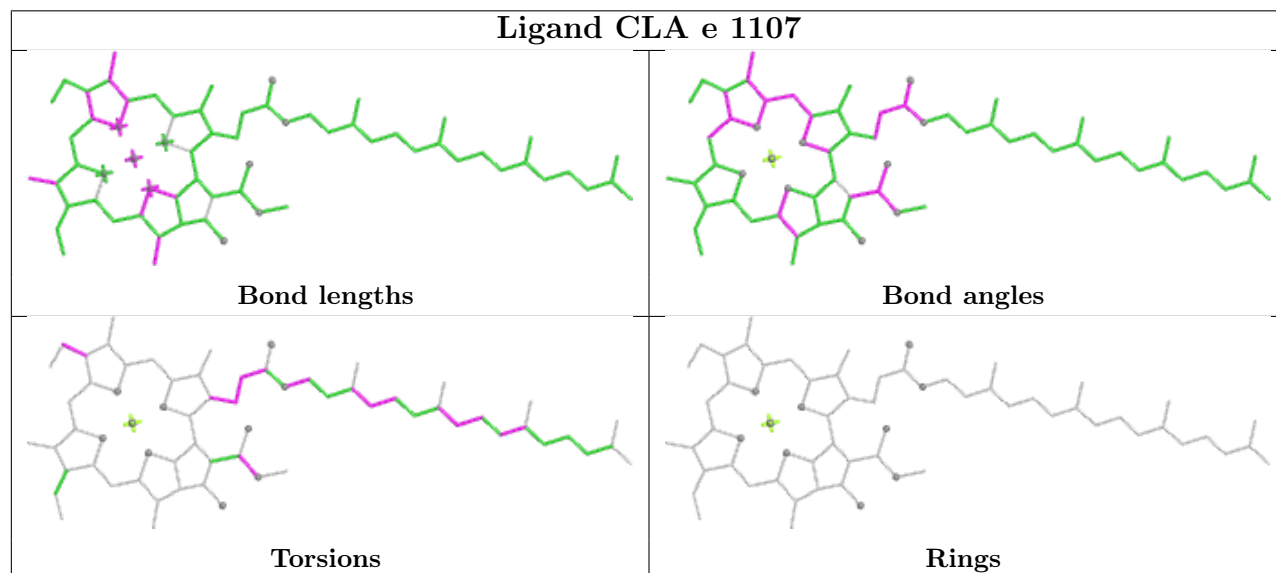
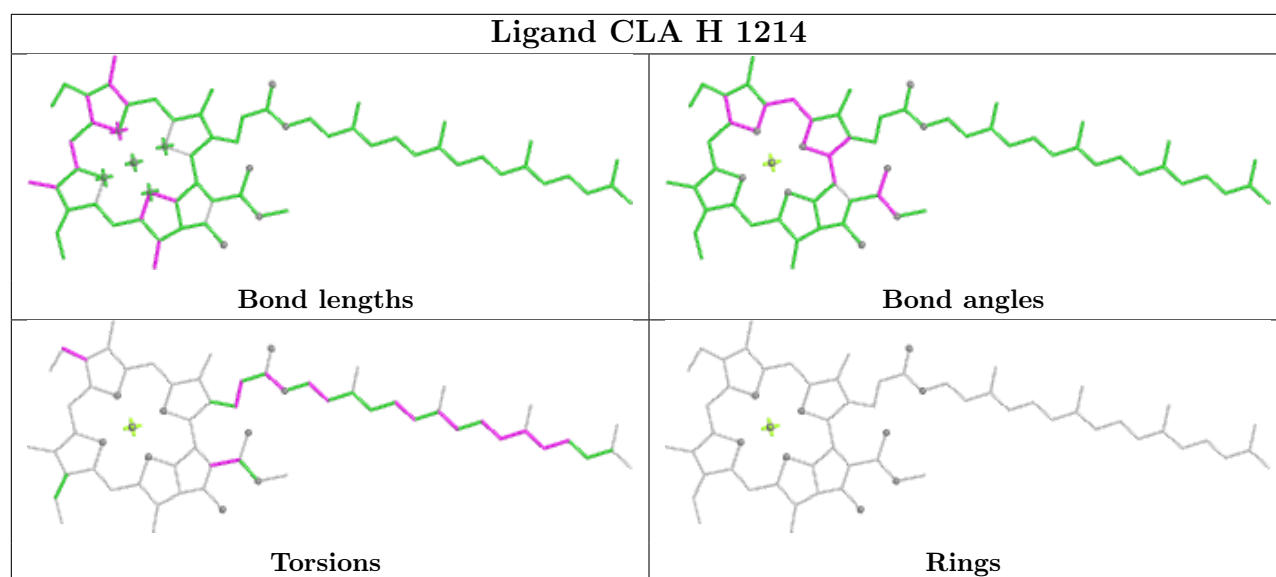


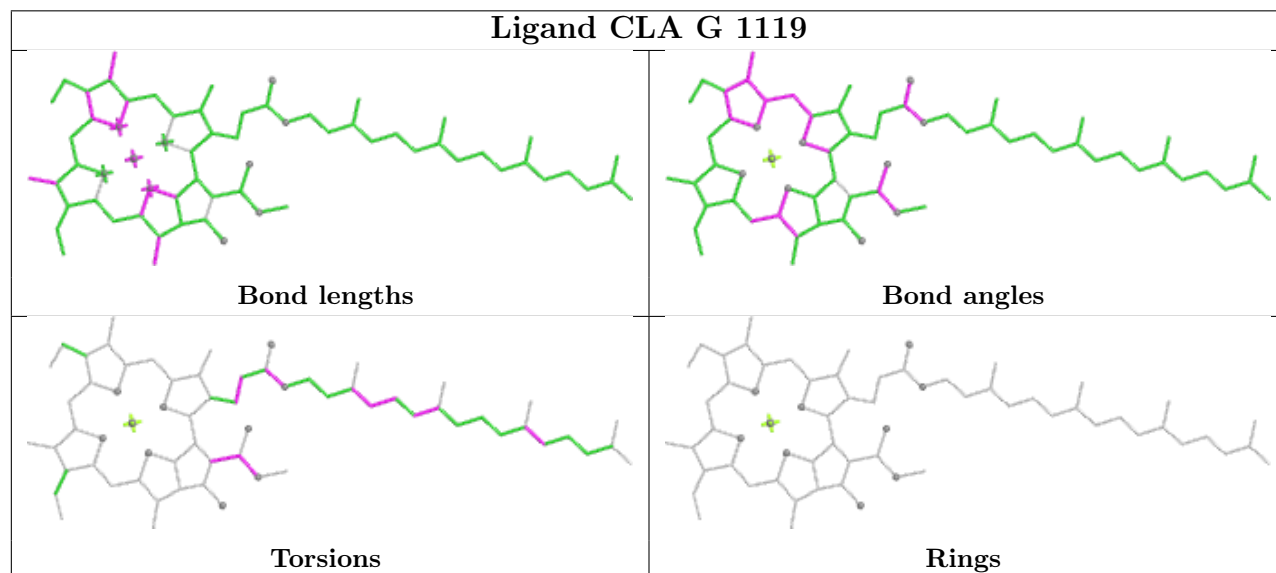
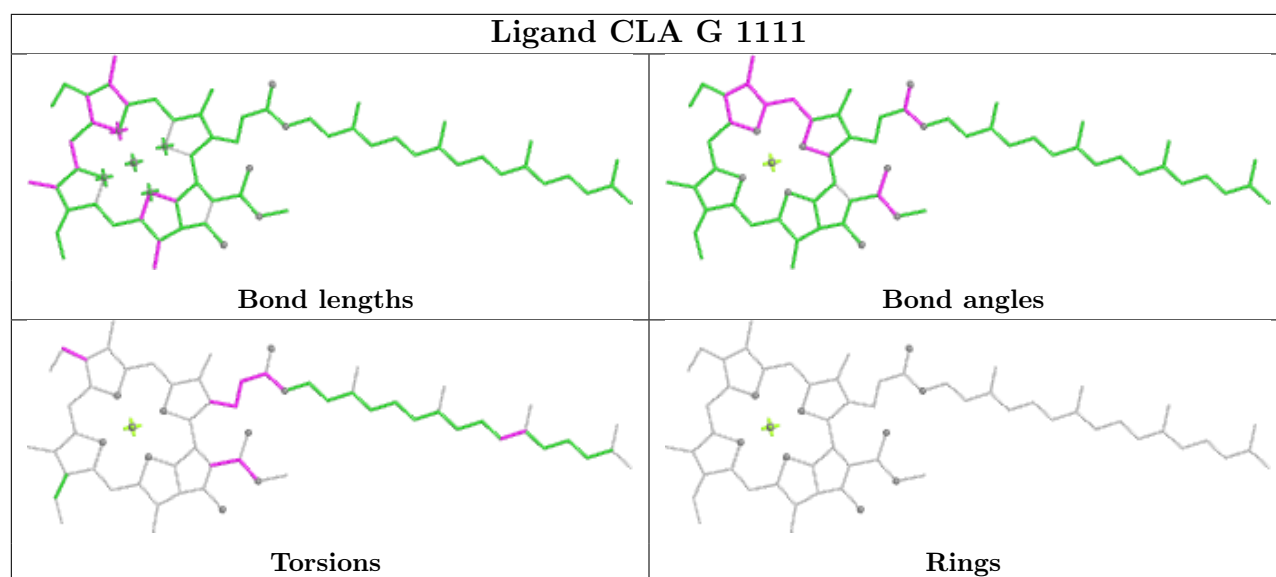
Ligand CLA 4 518

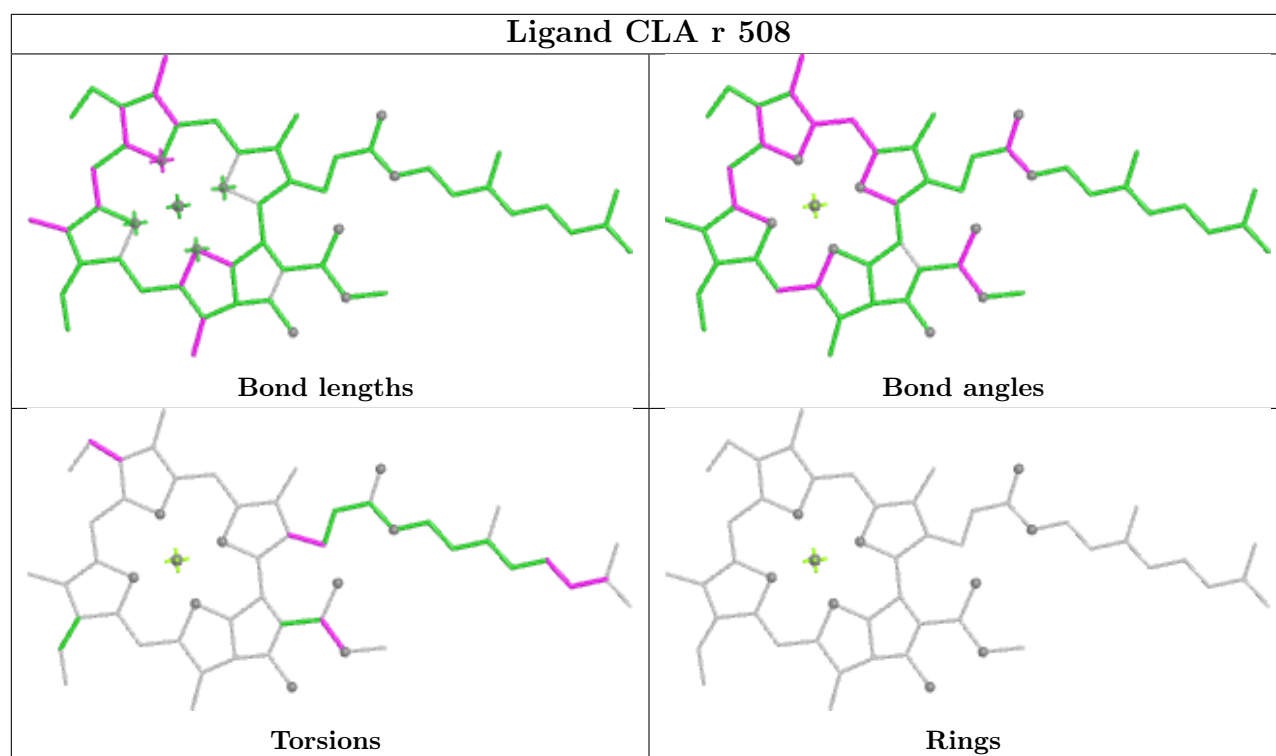


Ligand CLA b 518

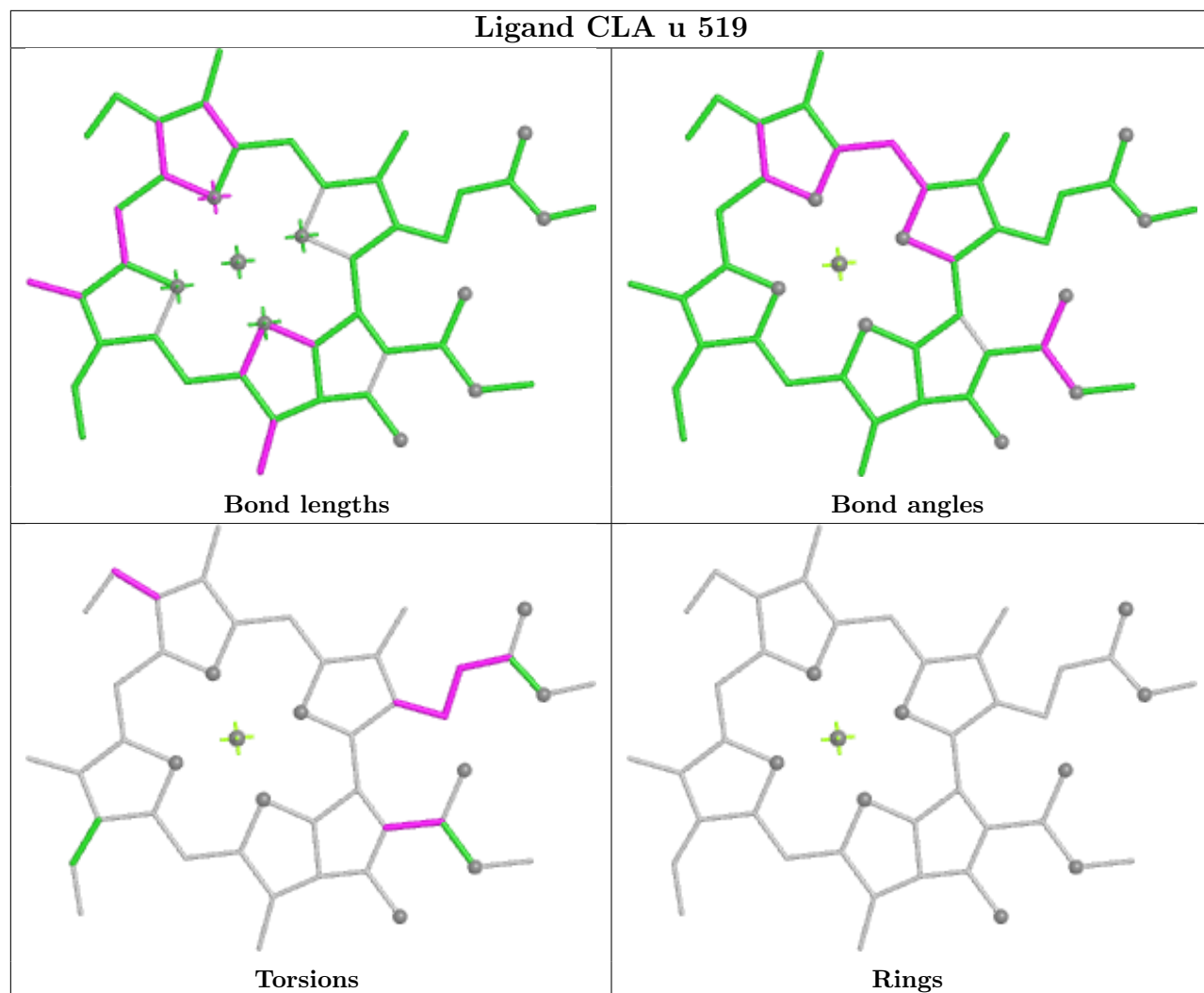


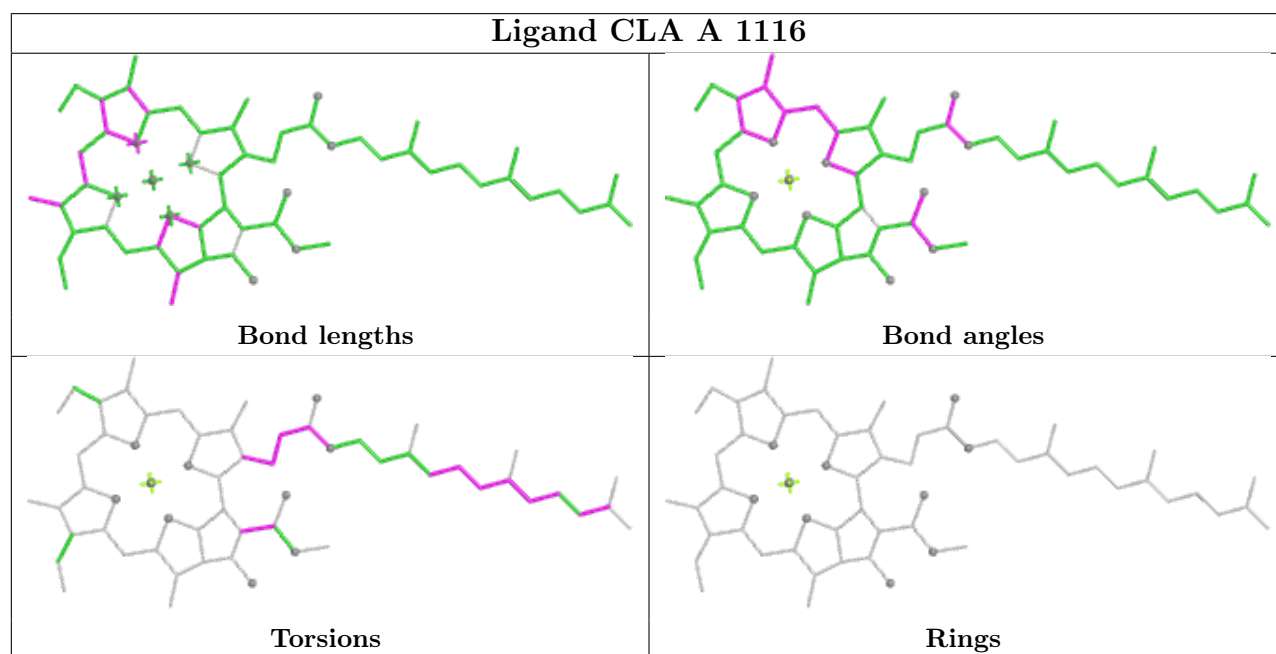
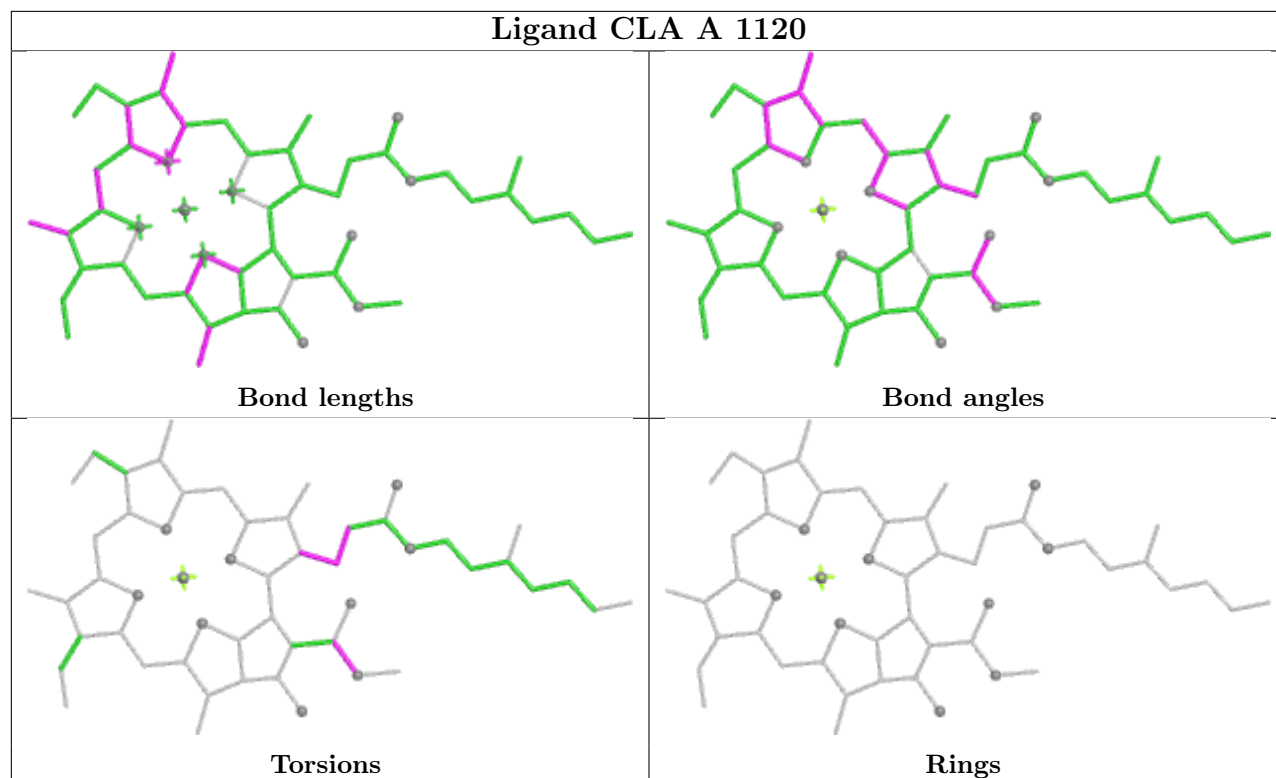


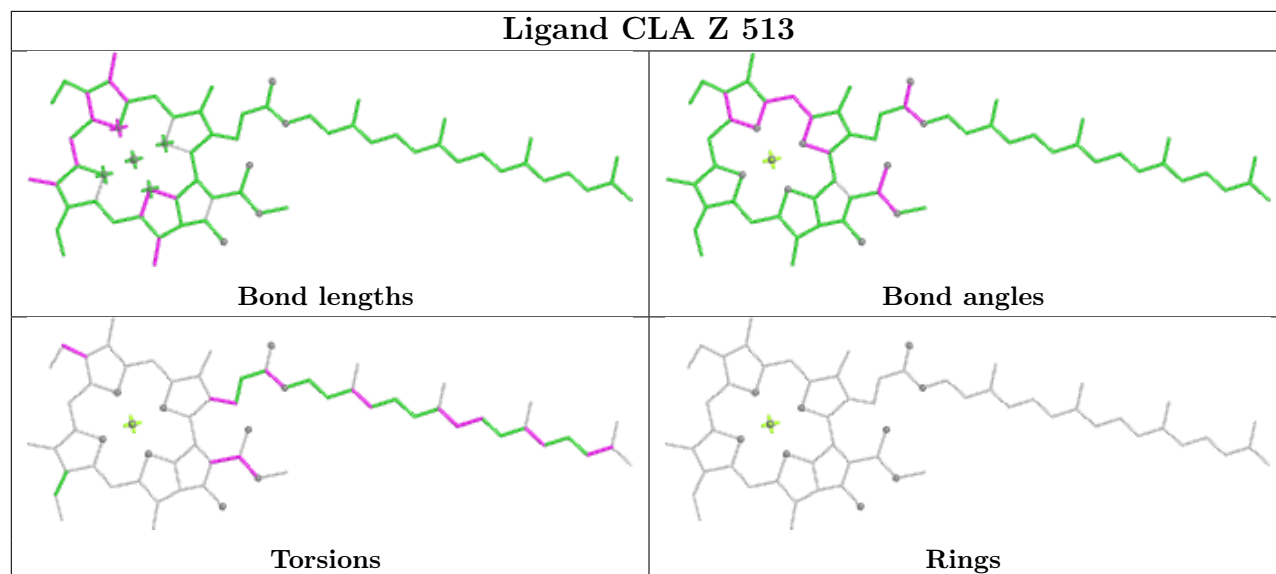
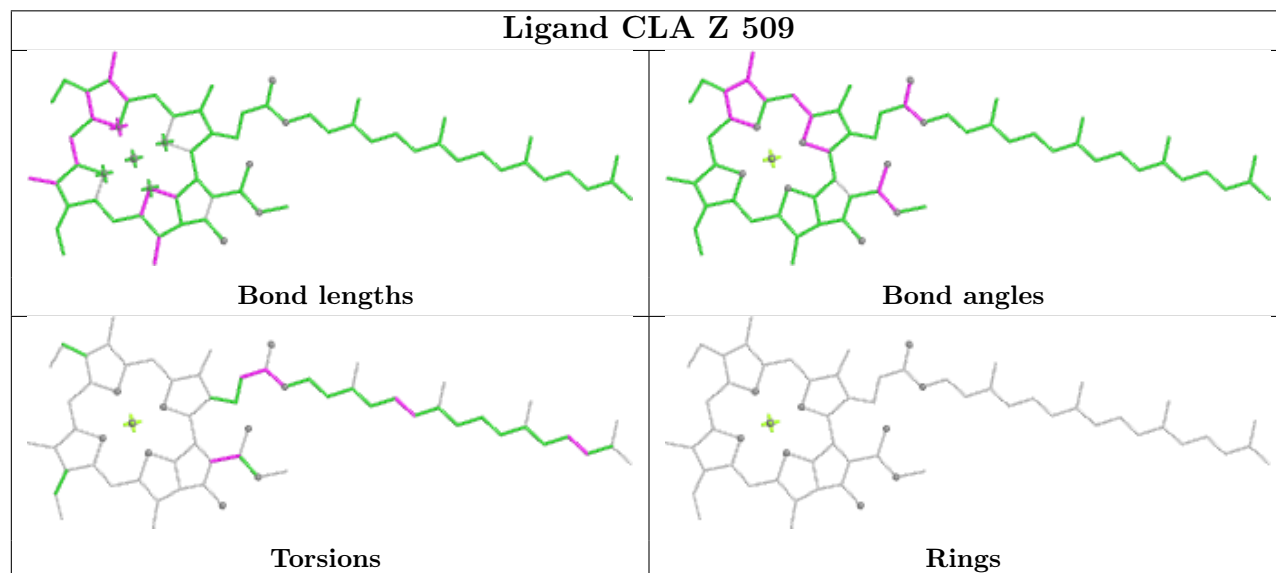


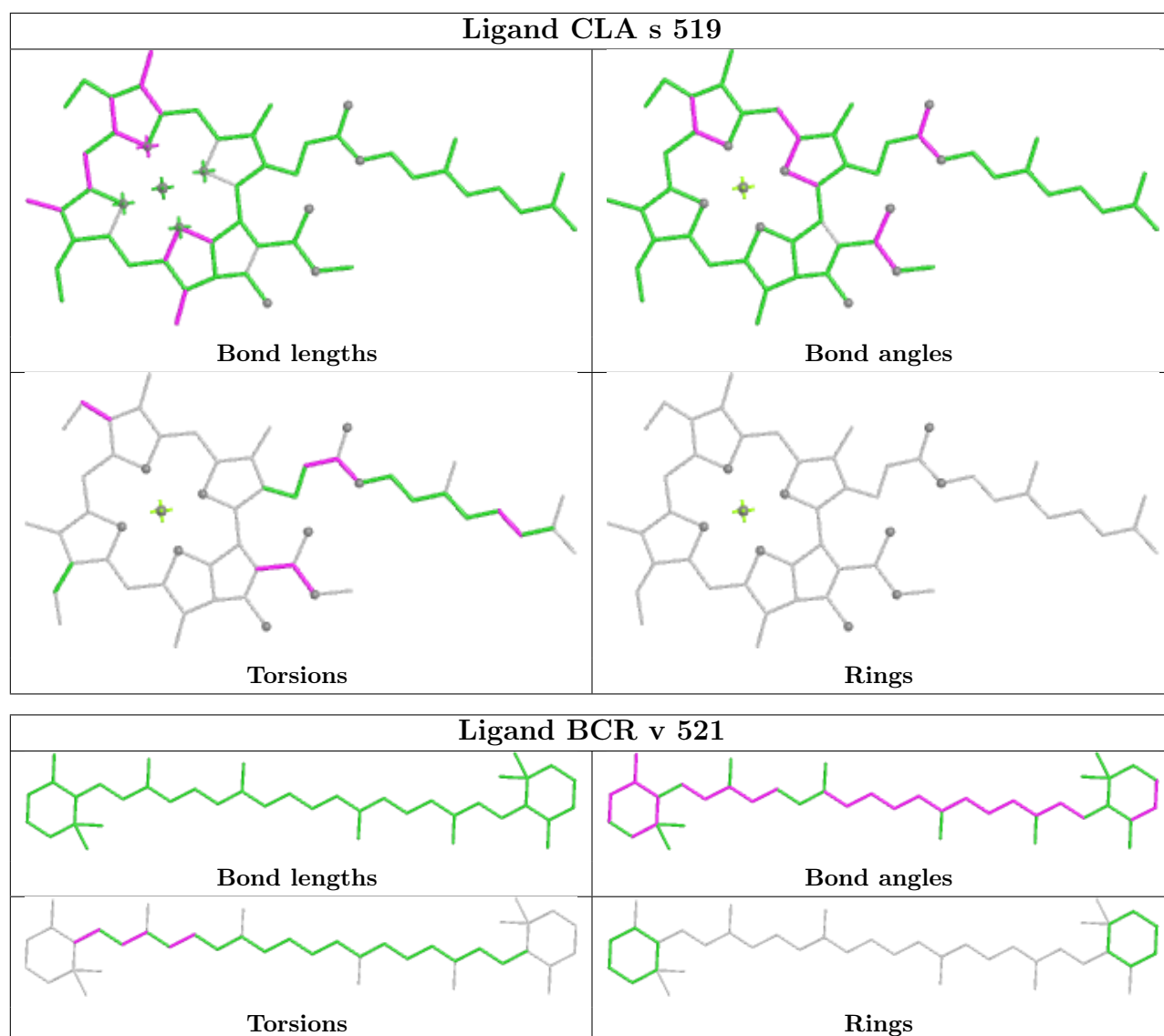


Ligand CLA u 519

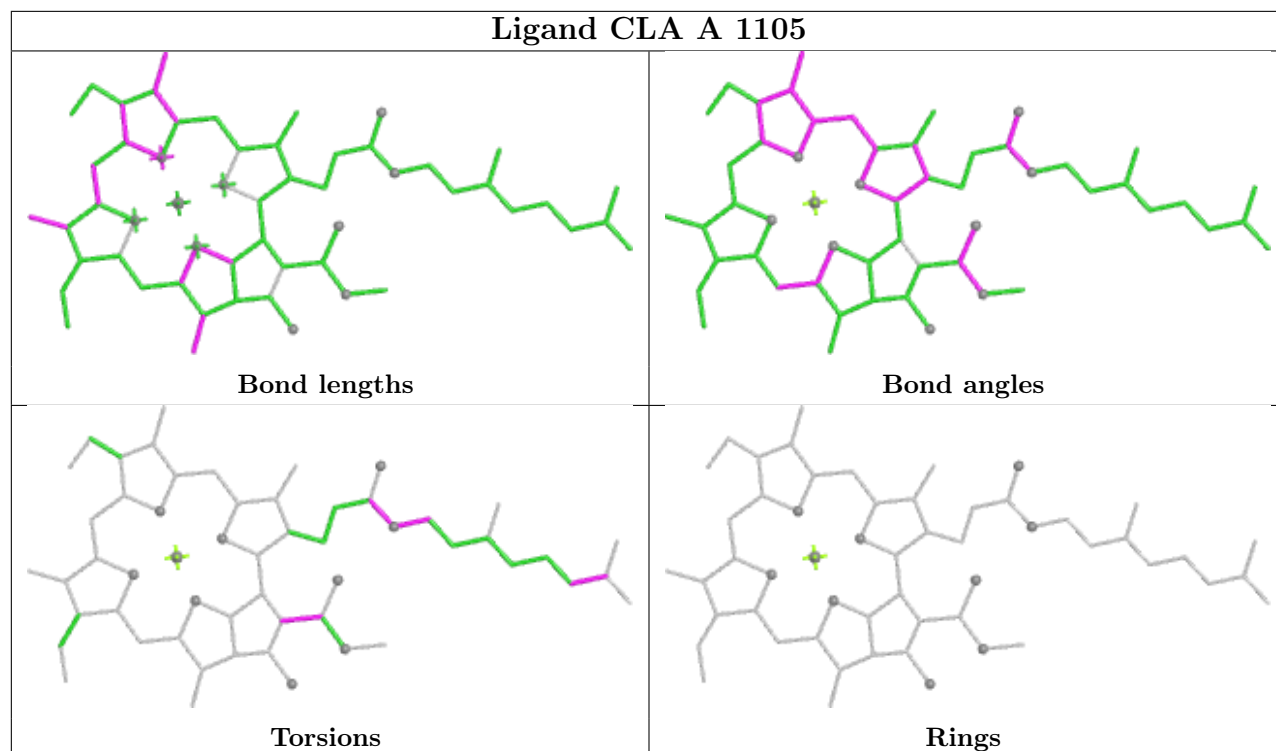




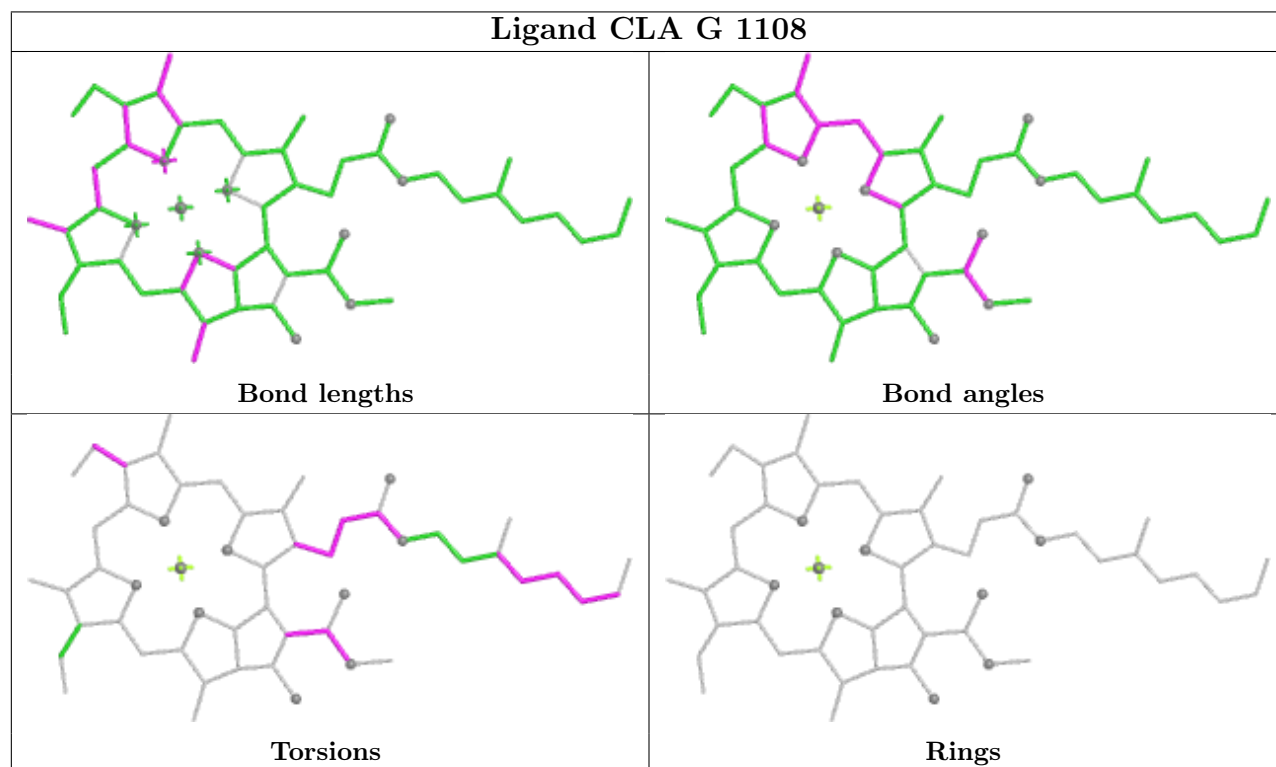
Ligand CLA Z 513**Ligand CLA Z 509**

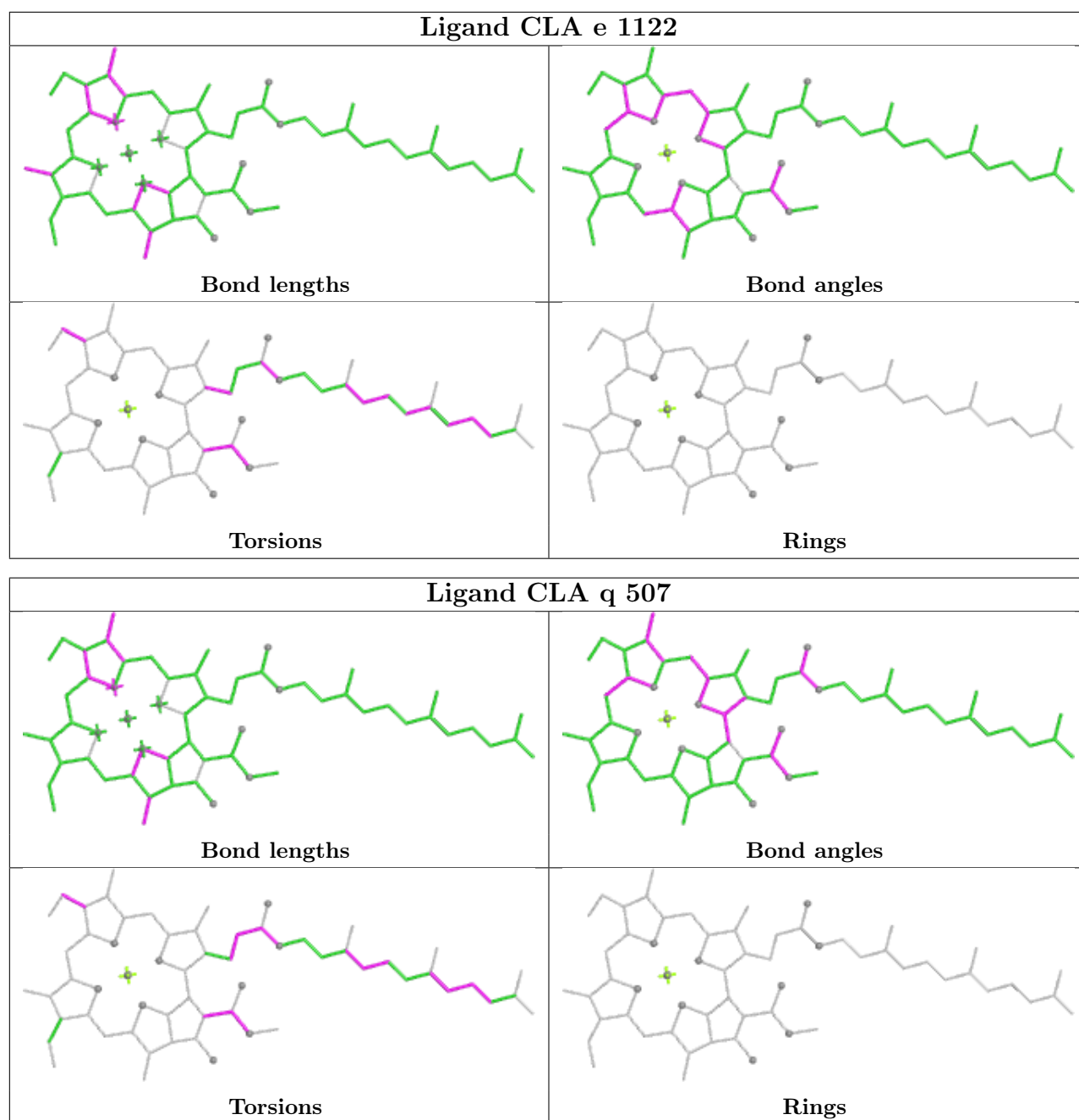


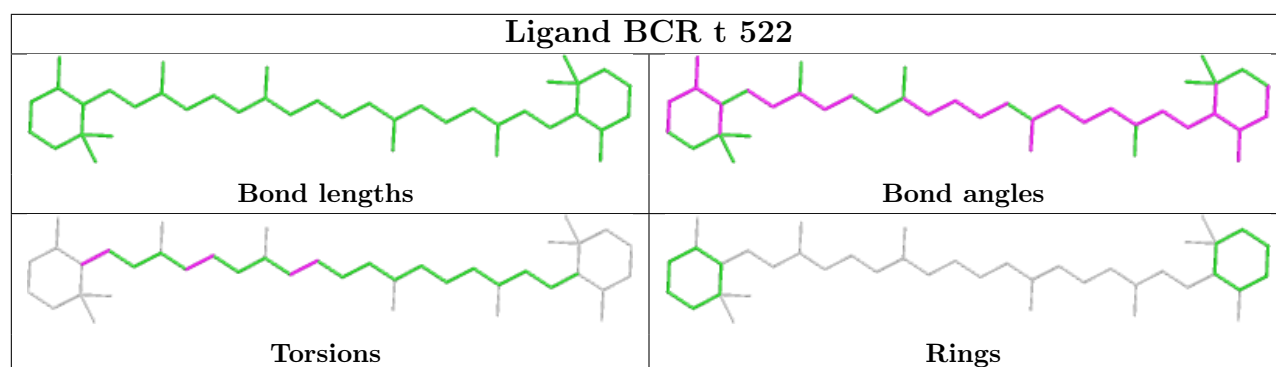
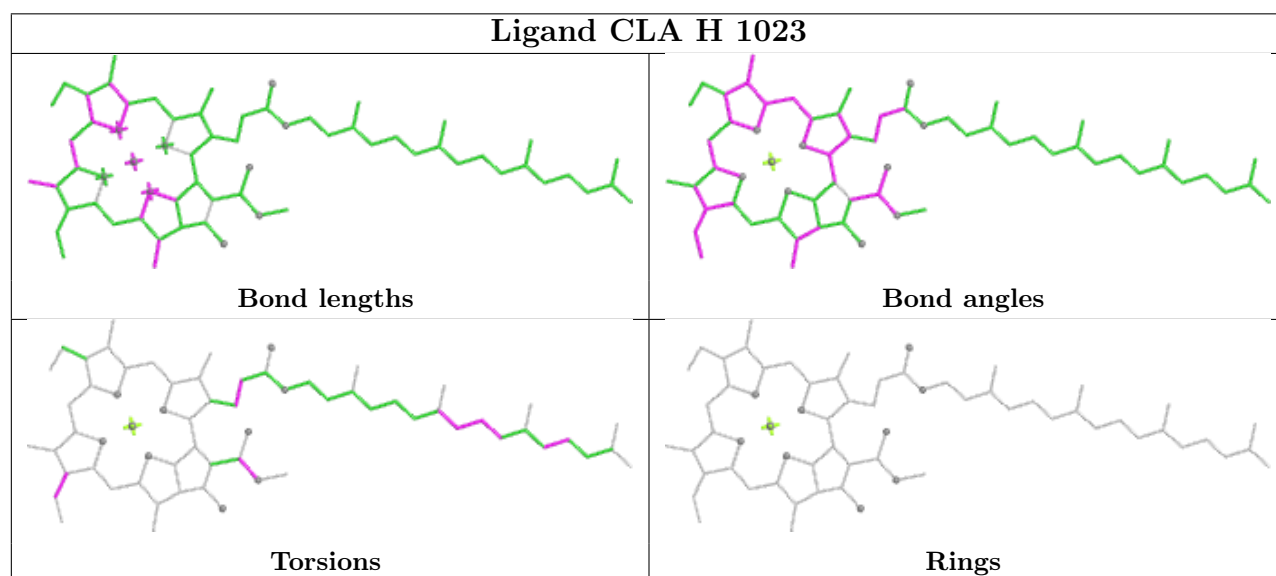
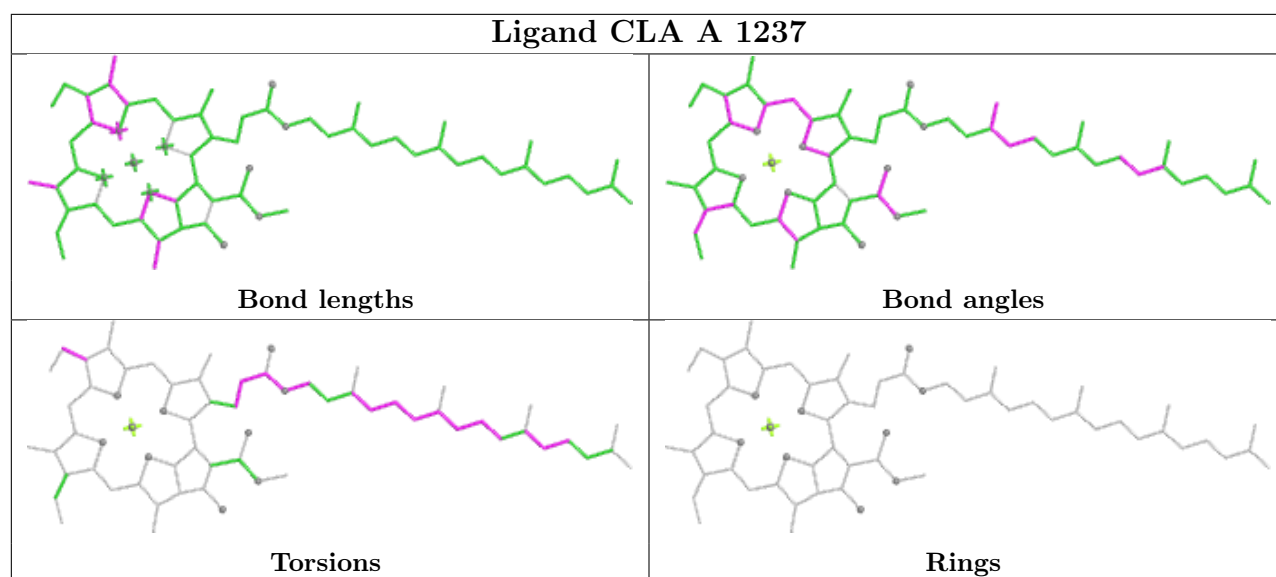
Ligand CLA A 1105

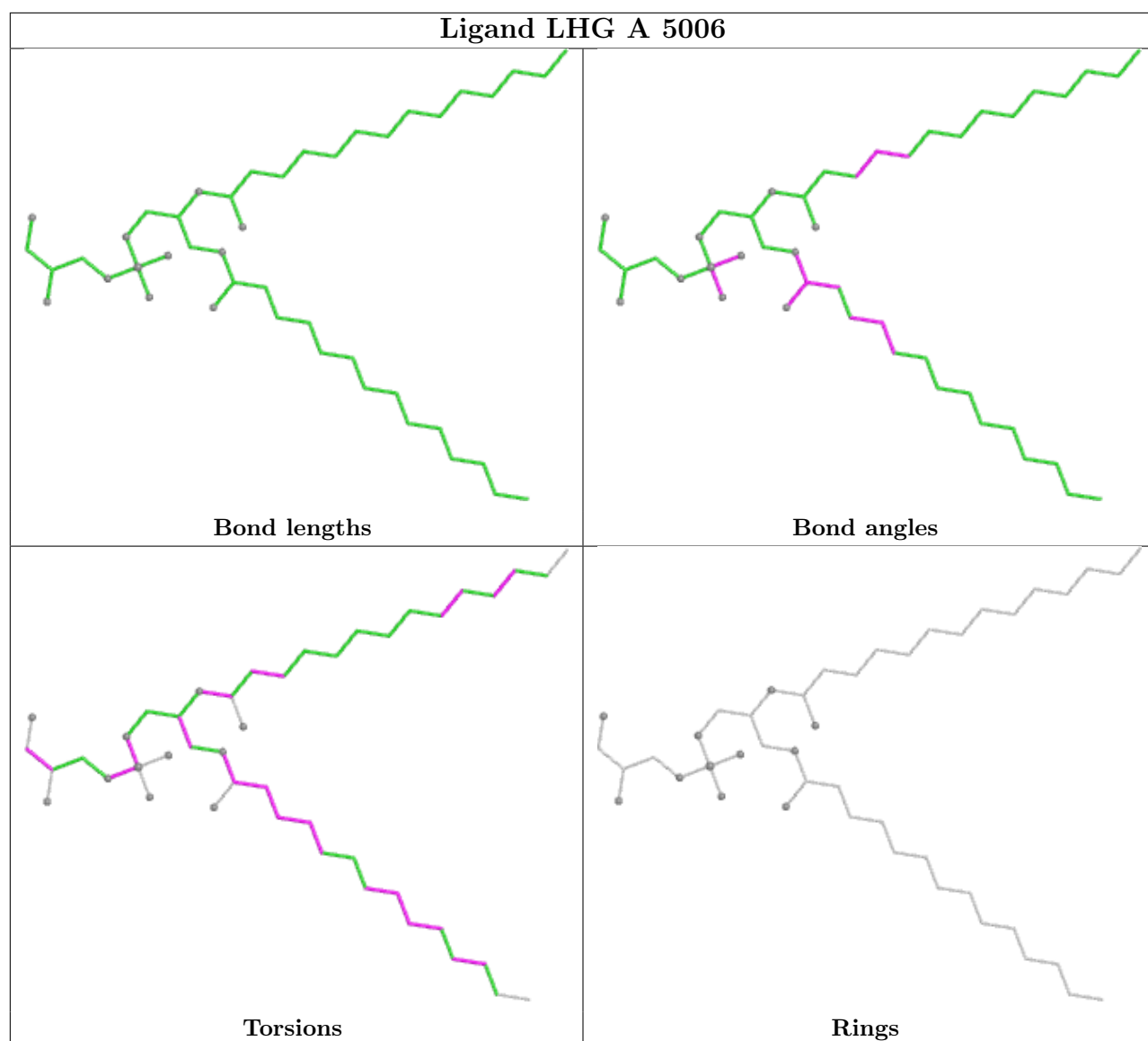


Ligand CLA G 1108

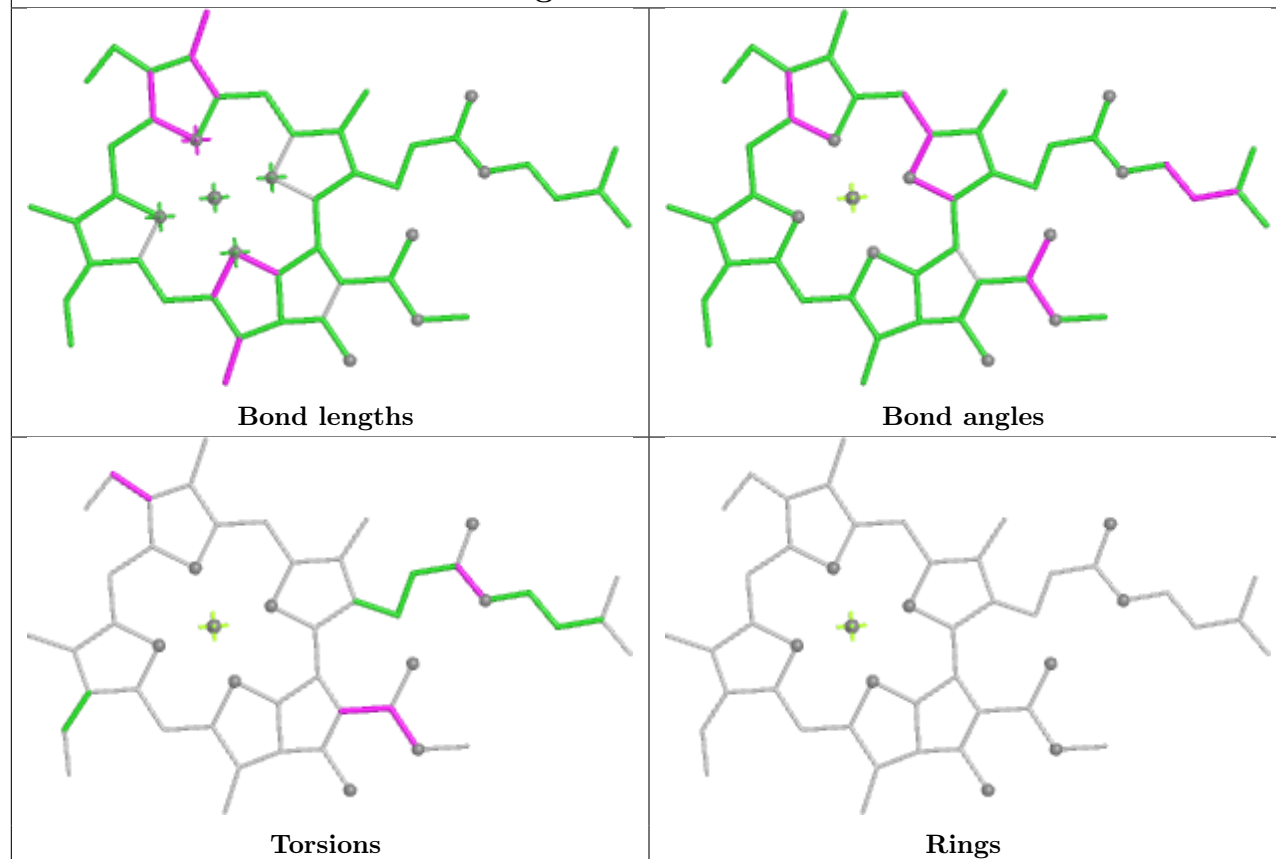




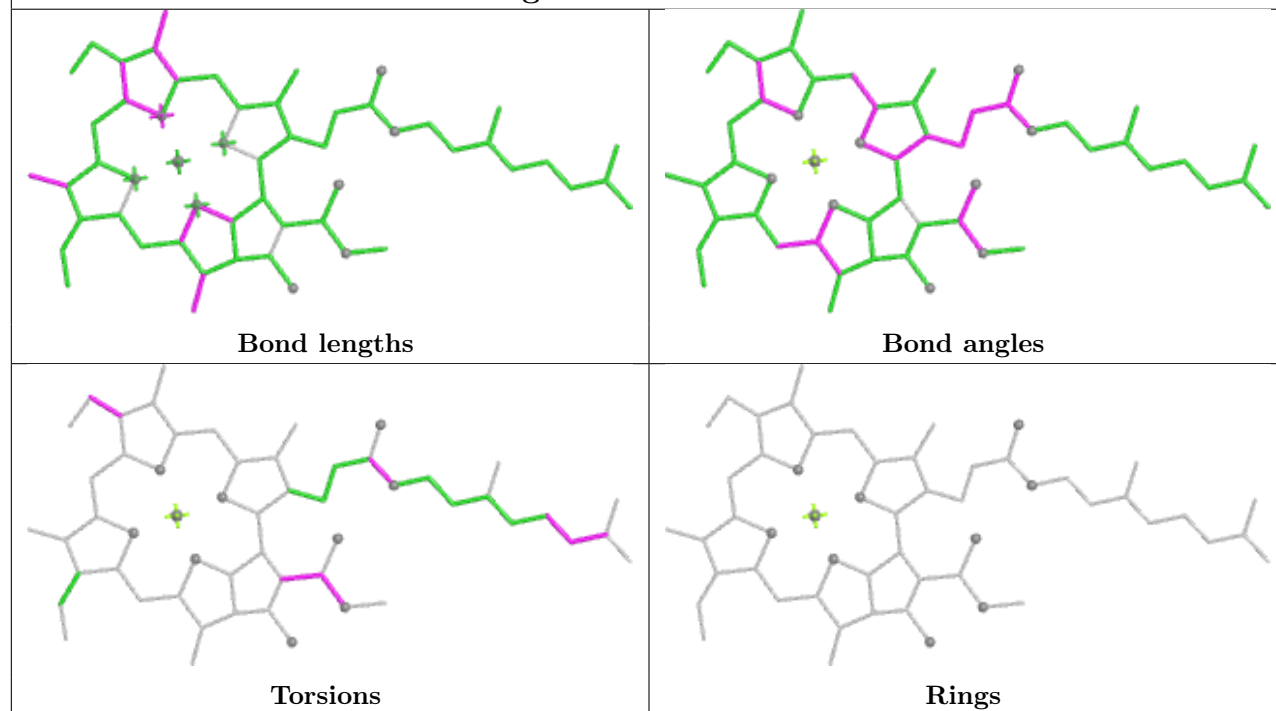


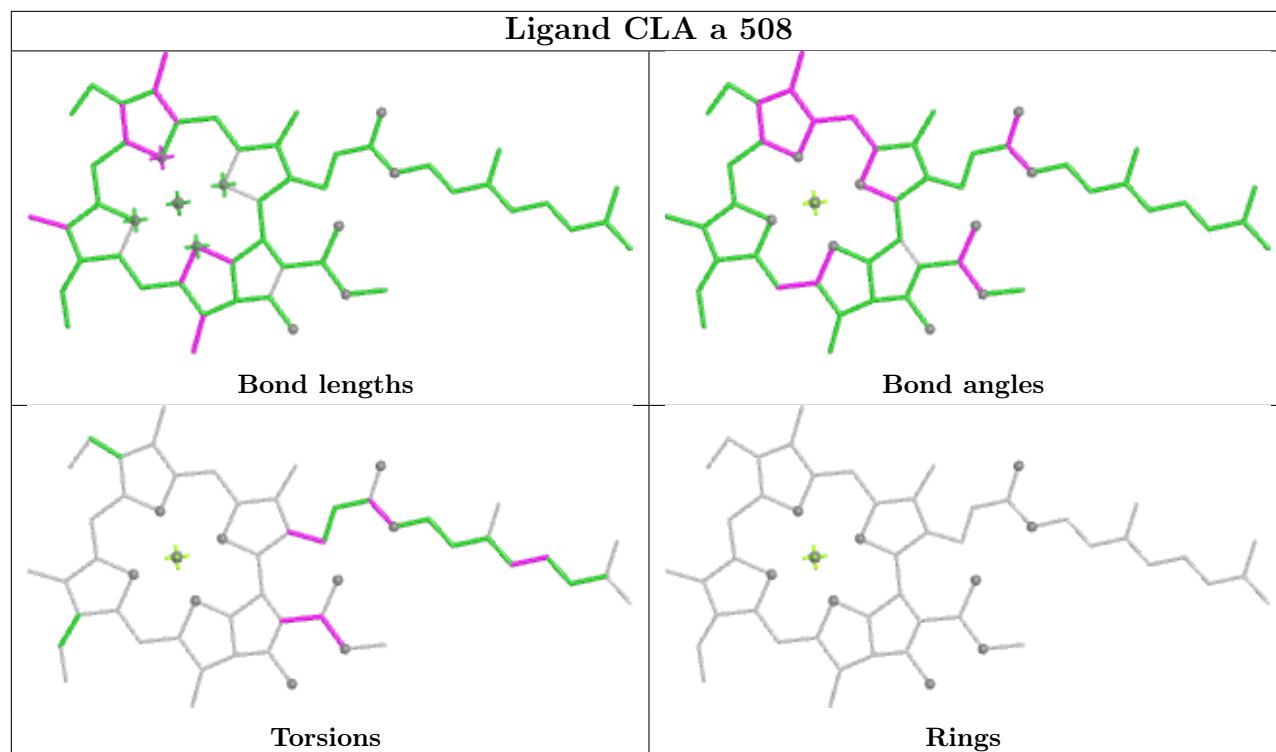
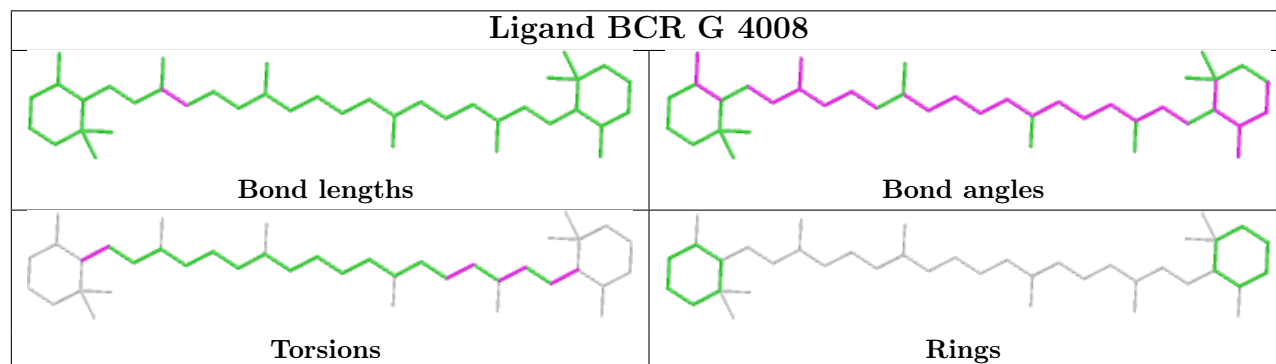
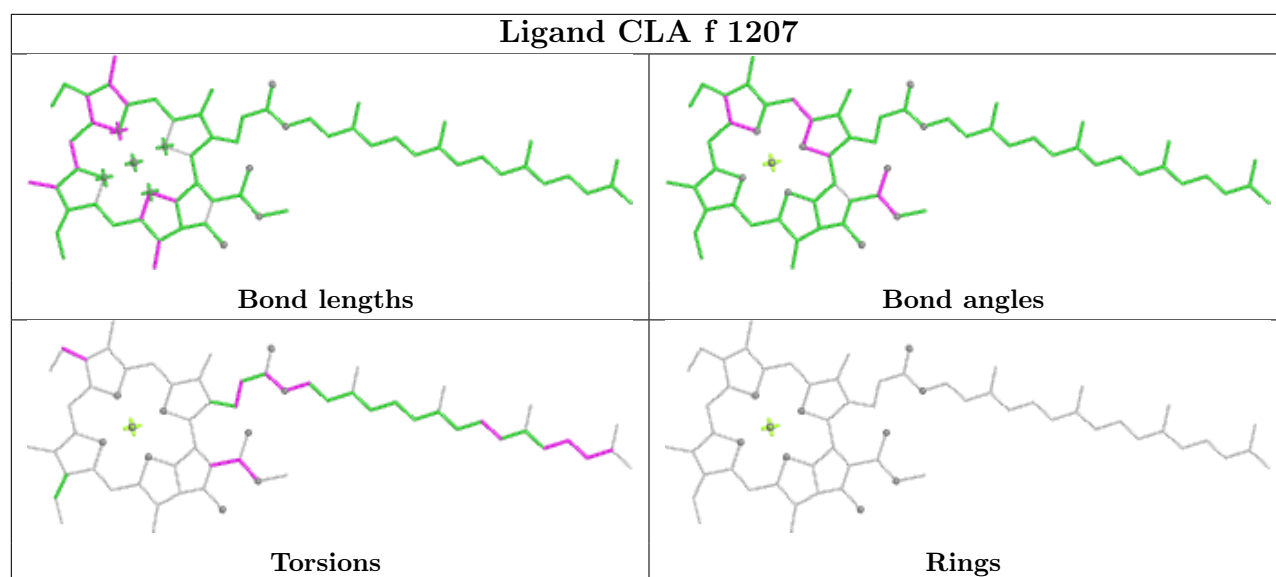


Ligand CLA d 502

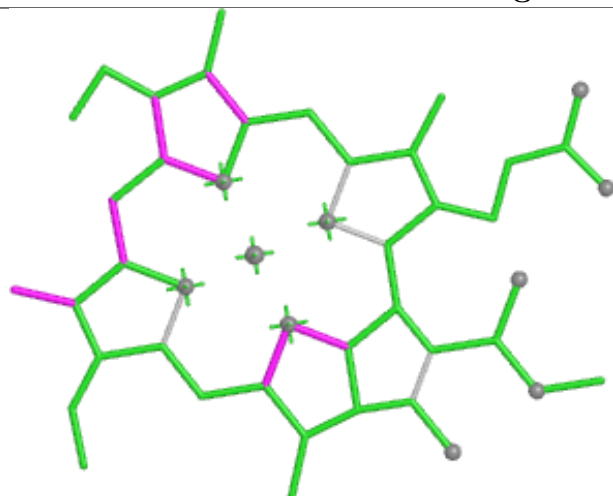


Ligand CLA H 1220

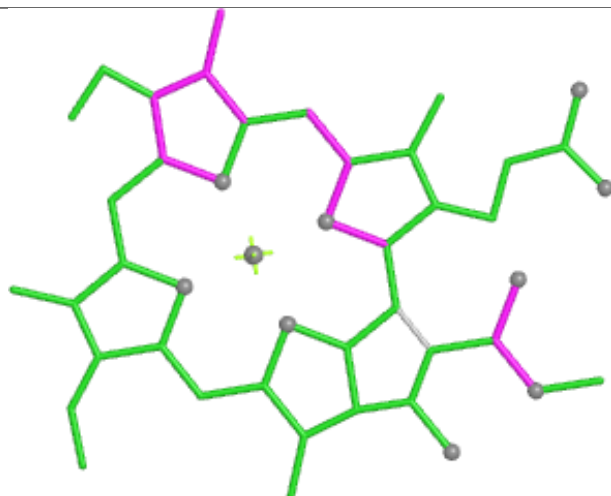




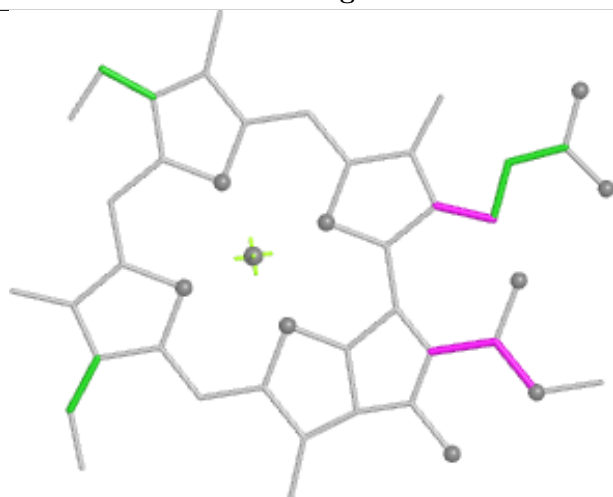
Ligand CLA Y 506



Bond lengths



Bond angles

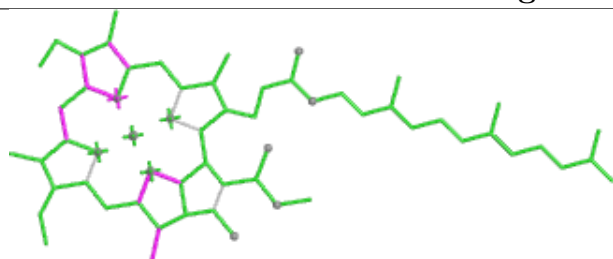


Torsions

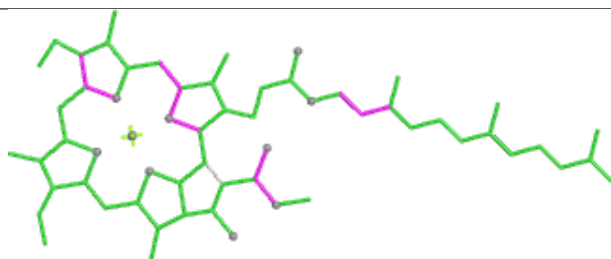


Rings

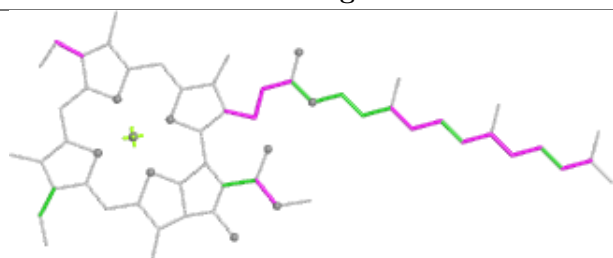
Ligand CLA 6 501



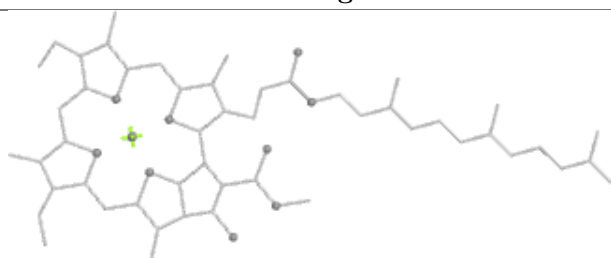
Bond lengths



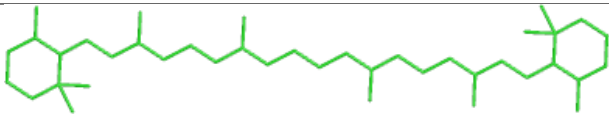
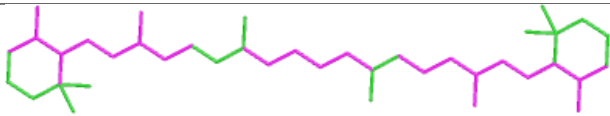
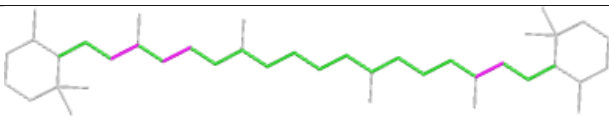
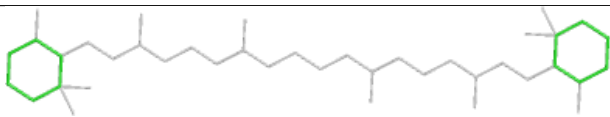
Bond angles

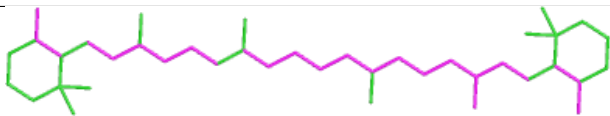
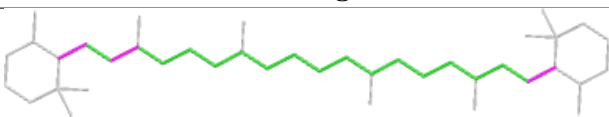
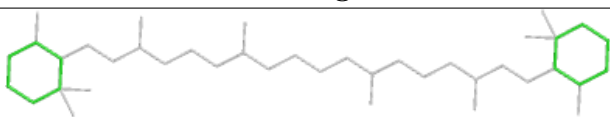


Torsions

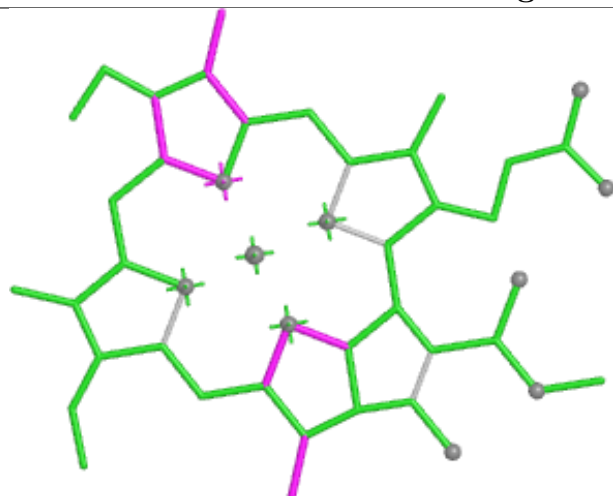


Rings

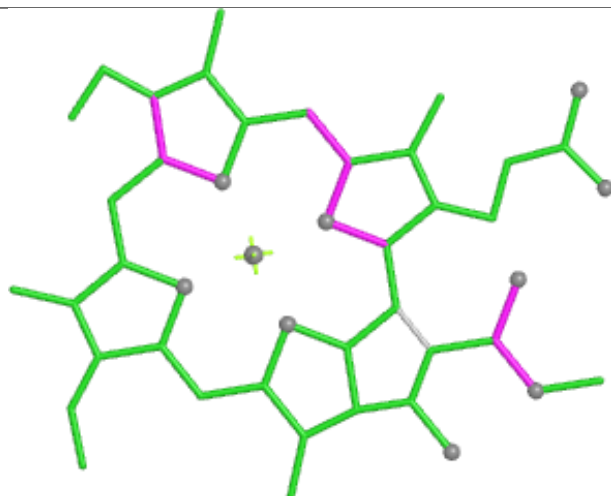
Ligand BCR 3 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR v 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

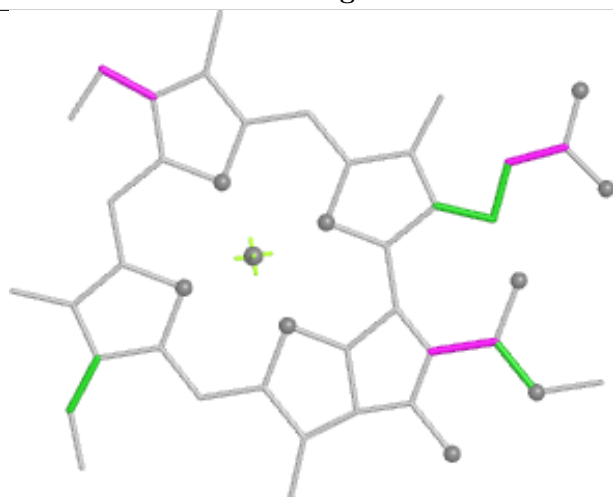
Ligand CLA b 512



Bond lengths



Bond angles

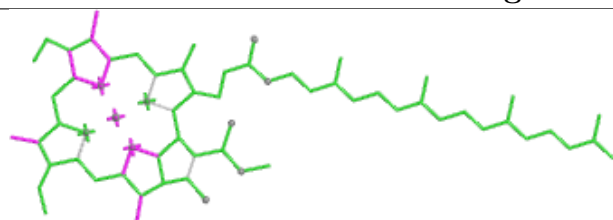


Torsions

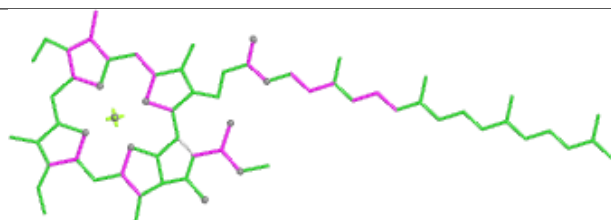


Rings

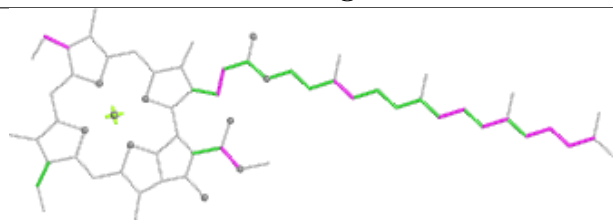
Ligand CLA G 1117



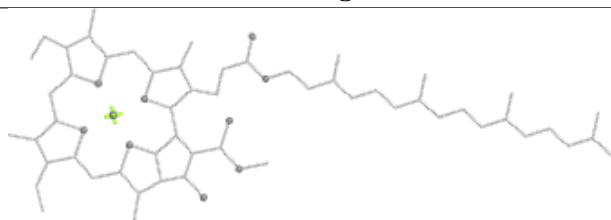
Bond lengths



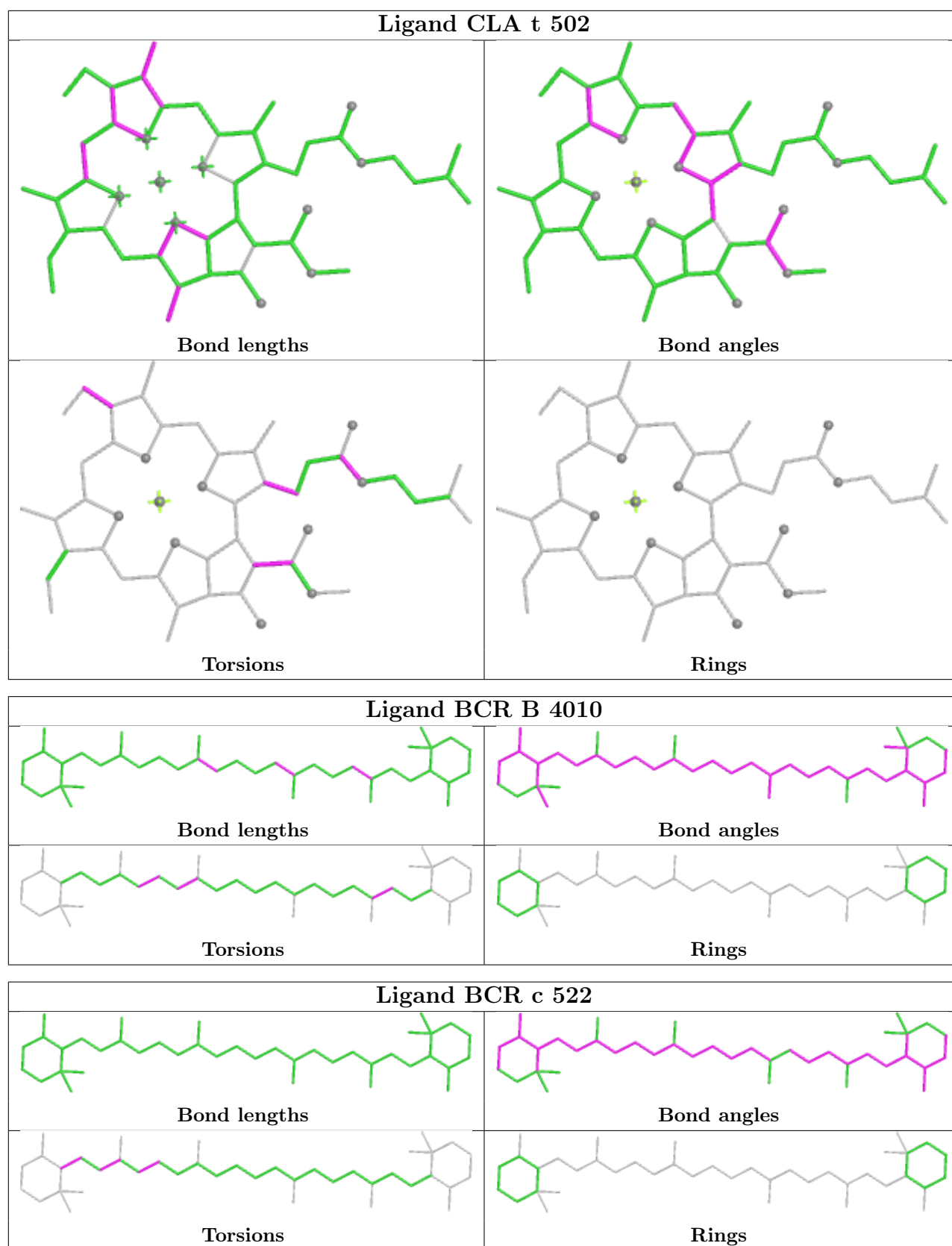
Bond angles

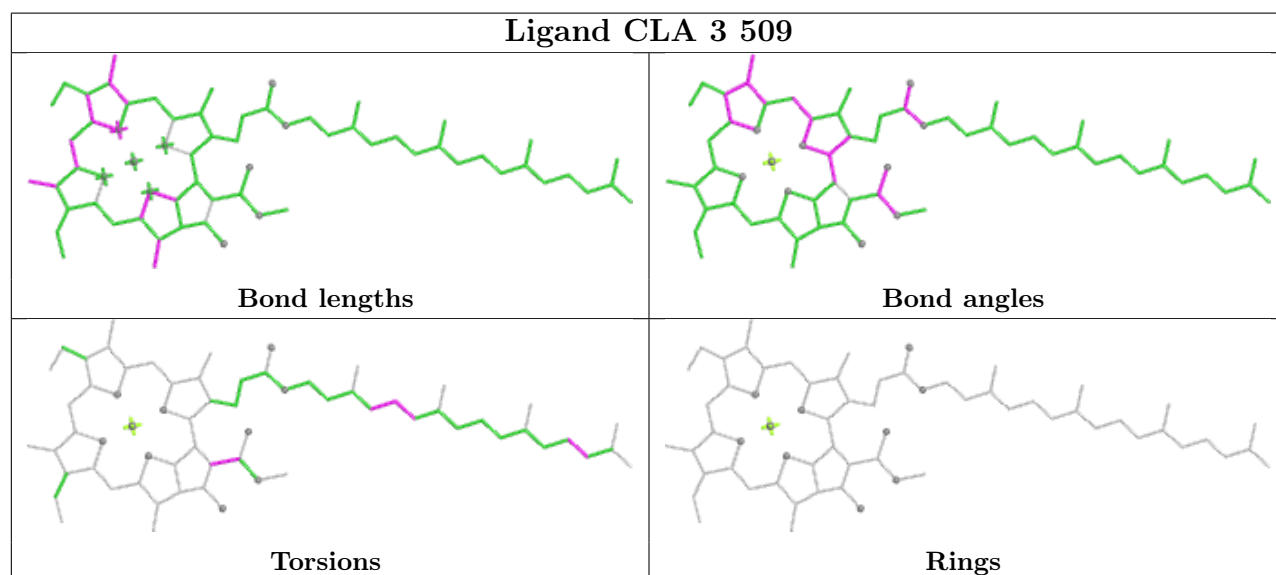
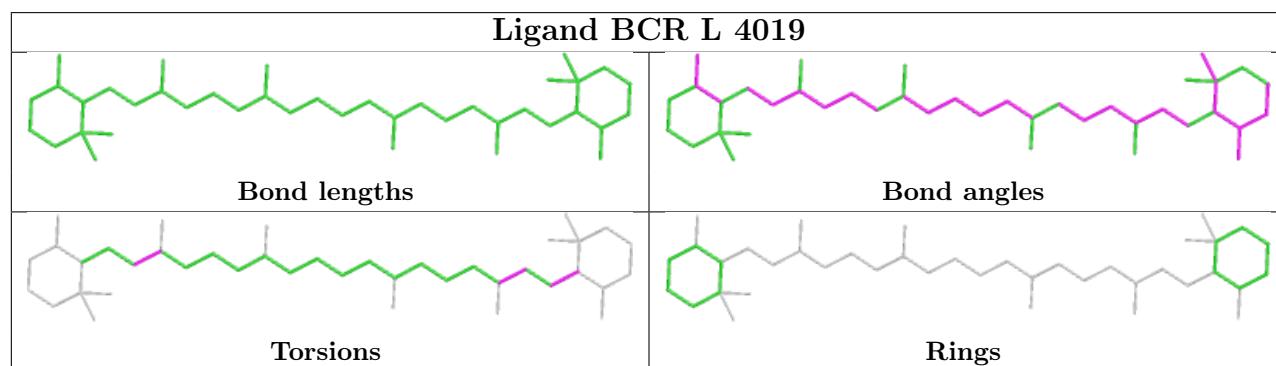
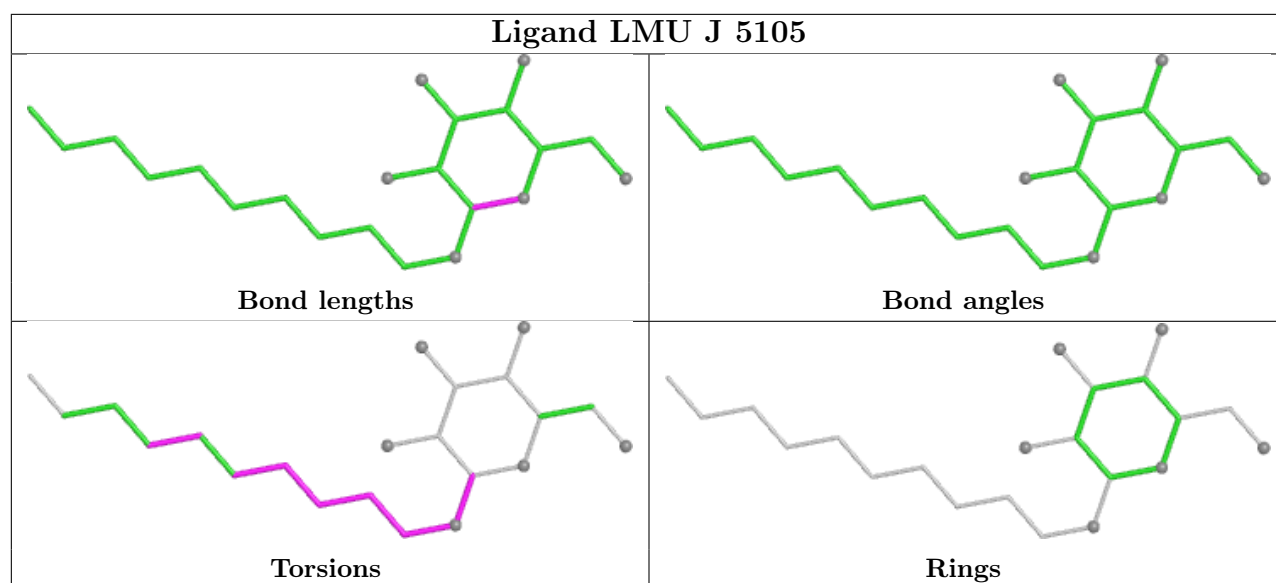


Torsions

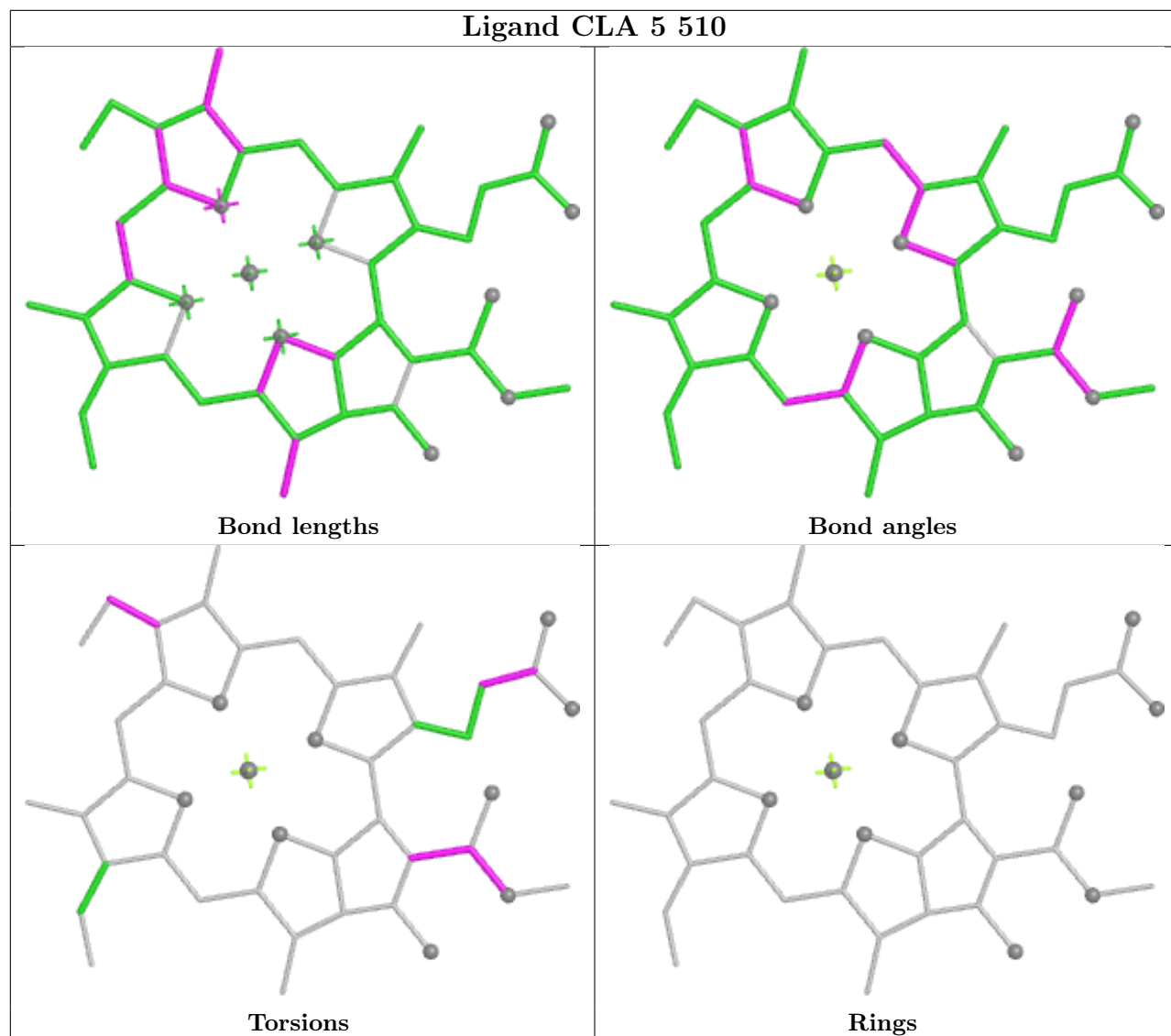


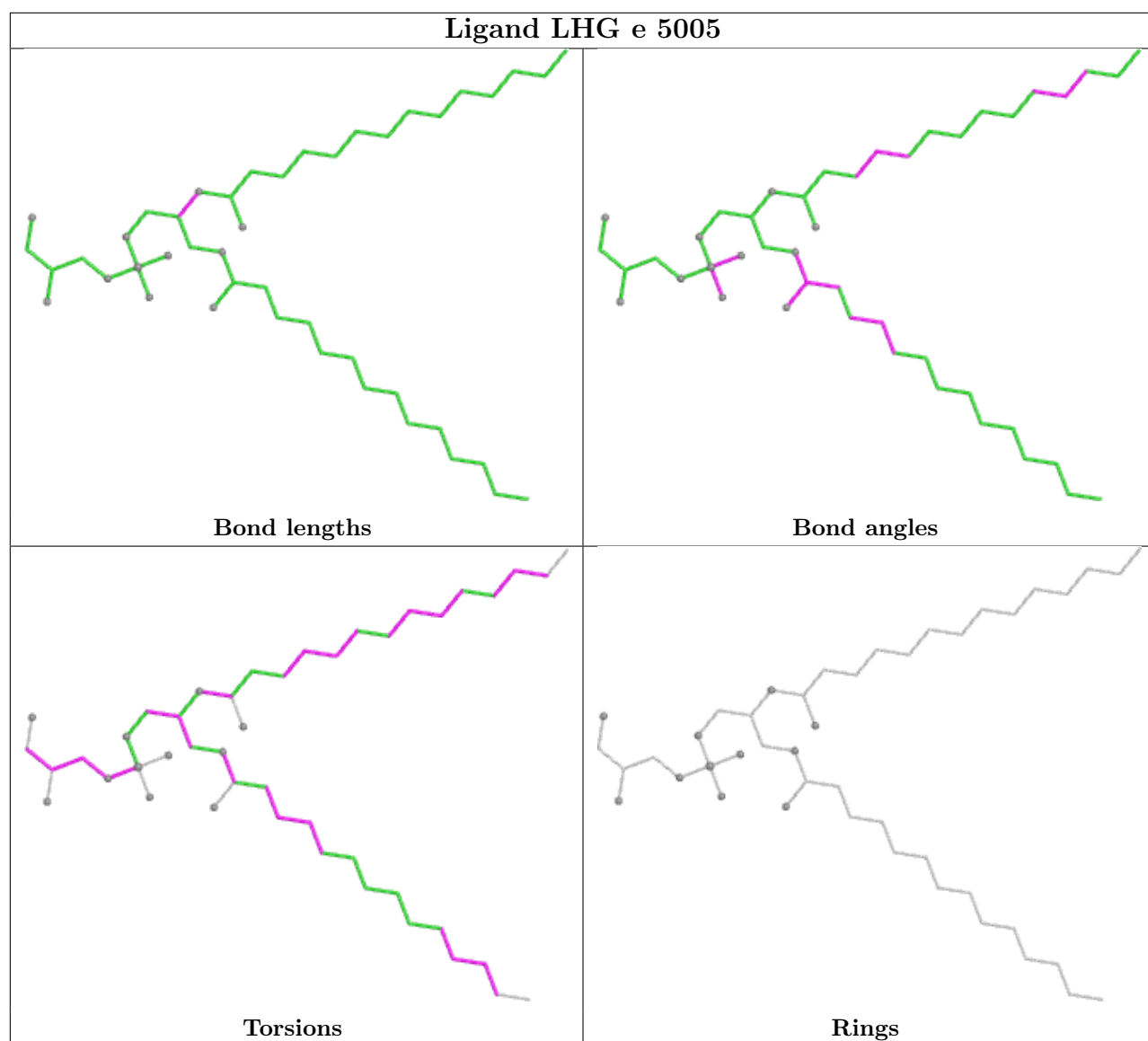
Rings

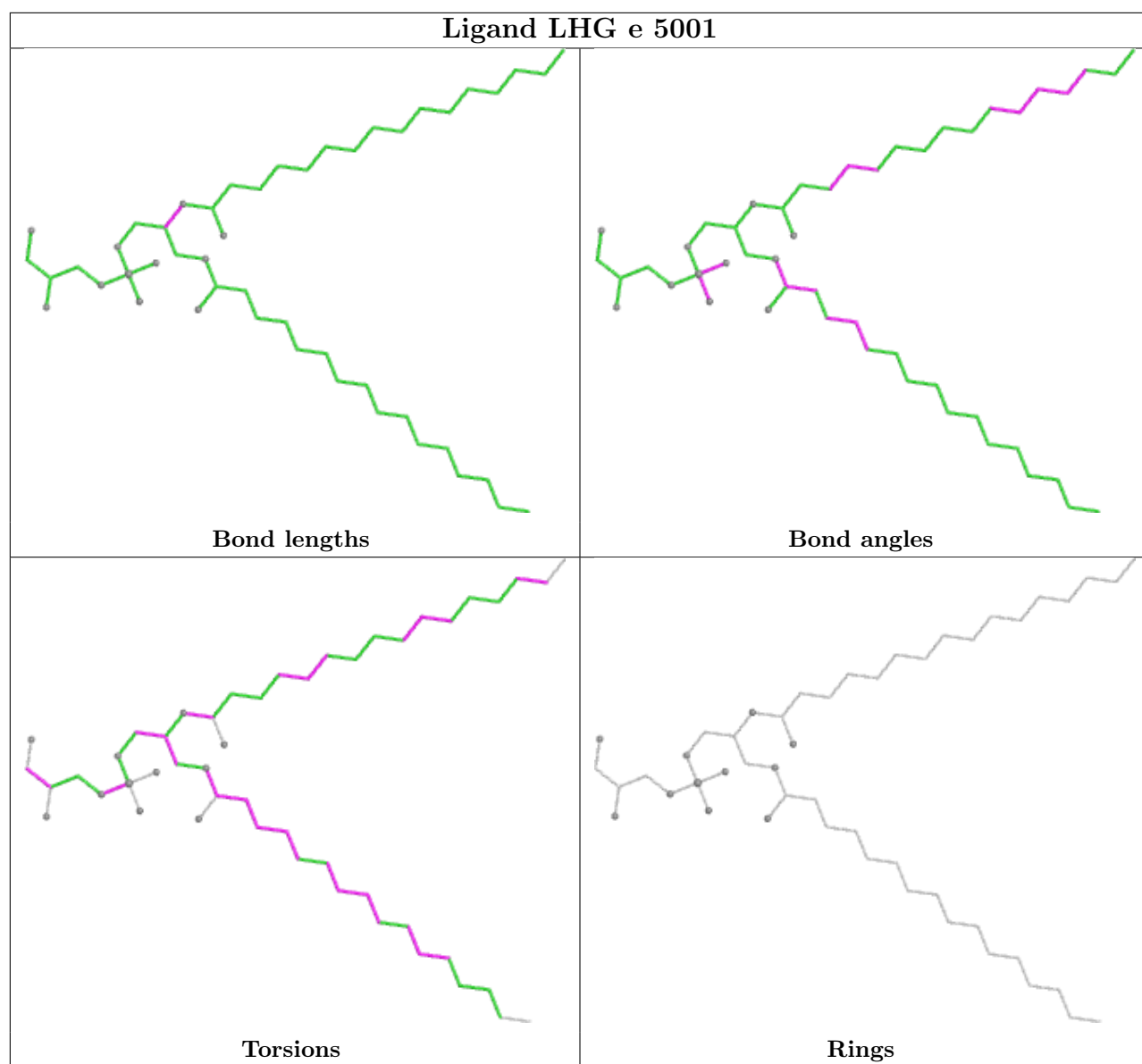




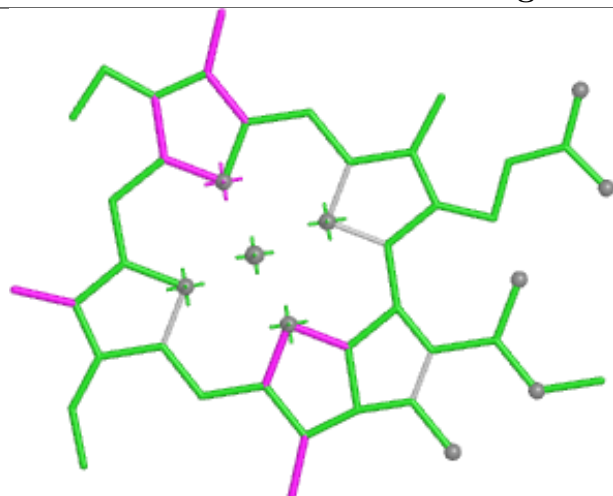
Ligand CLA 5 510



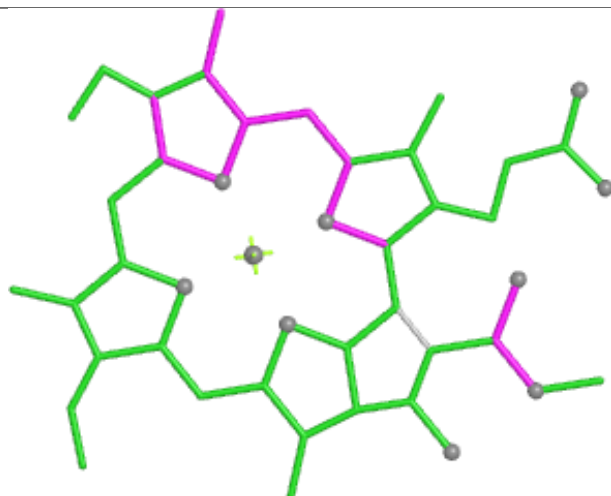




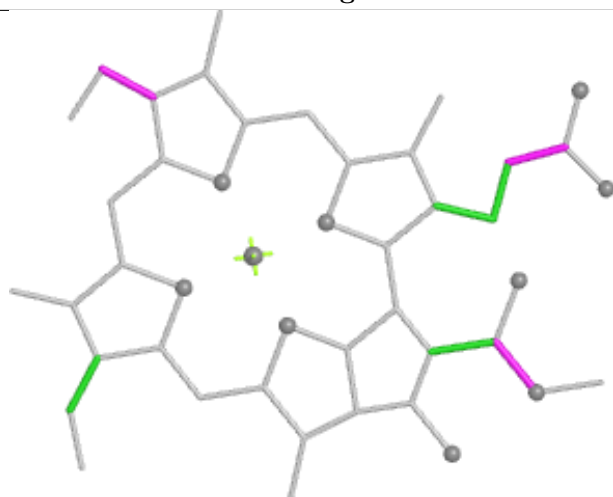
Ligand CLA u 508



Bond lengths



Bond angles

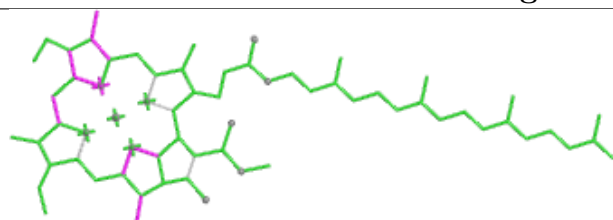


Torsions

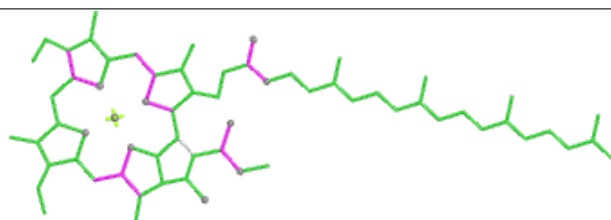


Rings

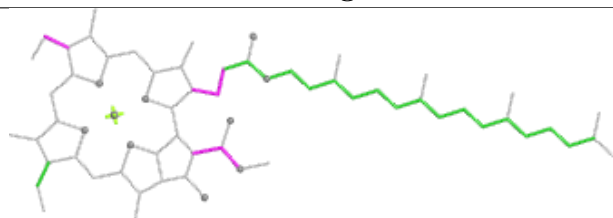
Ligand CLA s 503



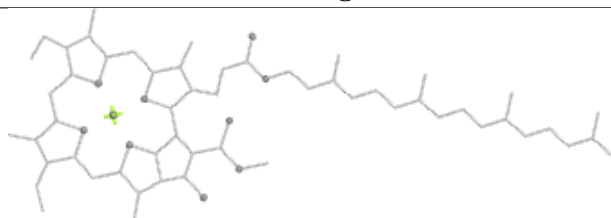
Bond lengths



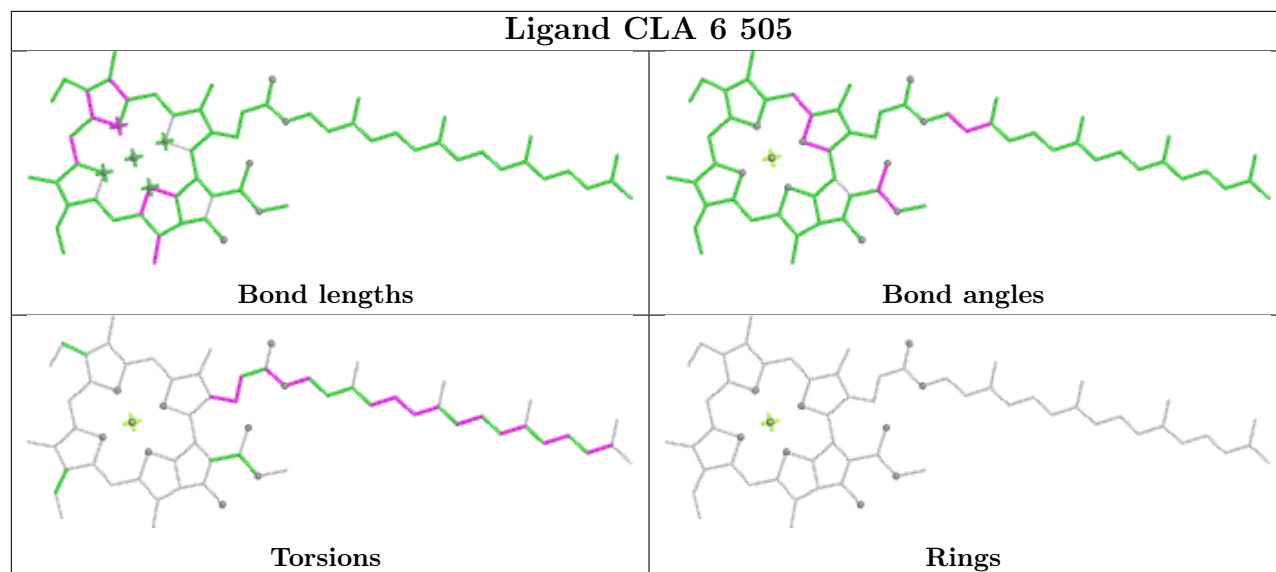
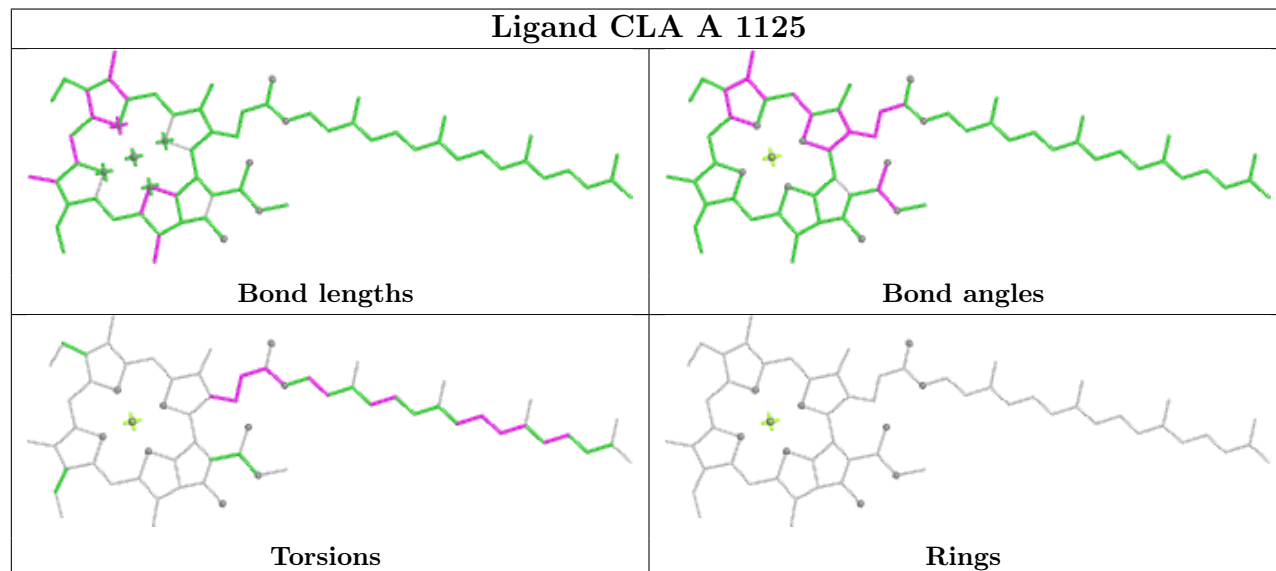
Bond angles



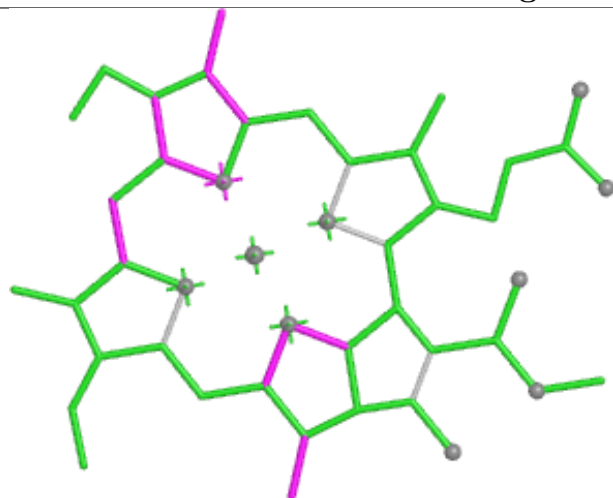
Torsions



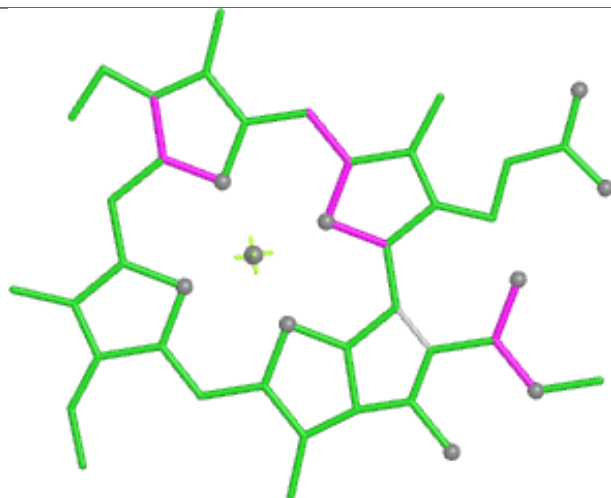
Rings

Ligand CLA 6 505**Ligand CLA A 1125**

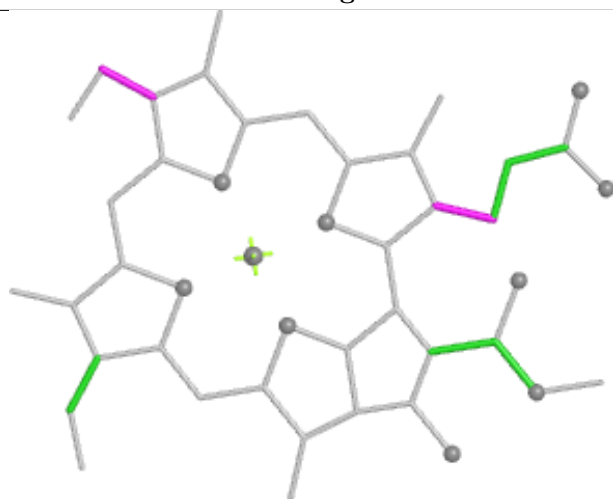
Ligand CLA c 516



Bond lengths



Bond angles

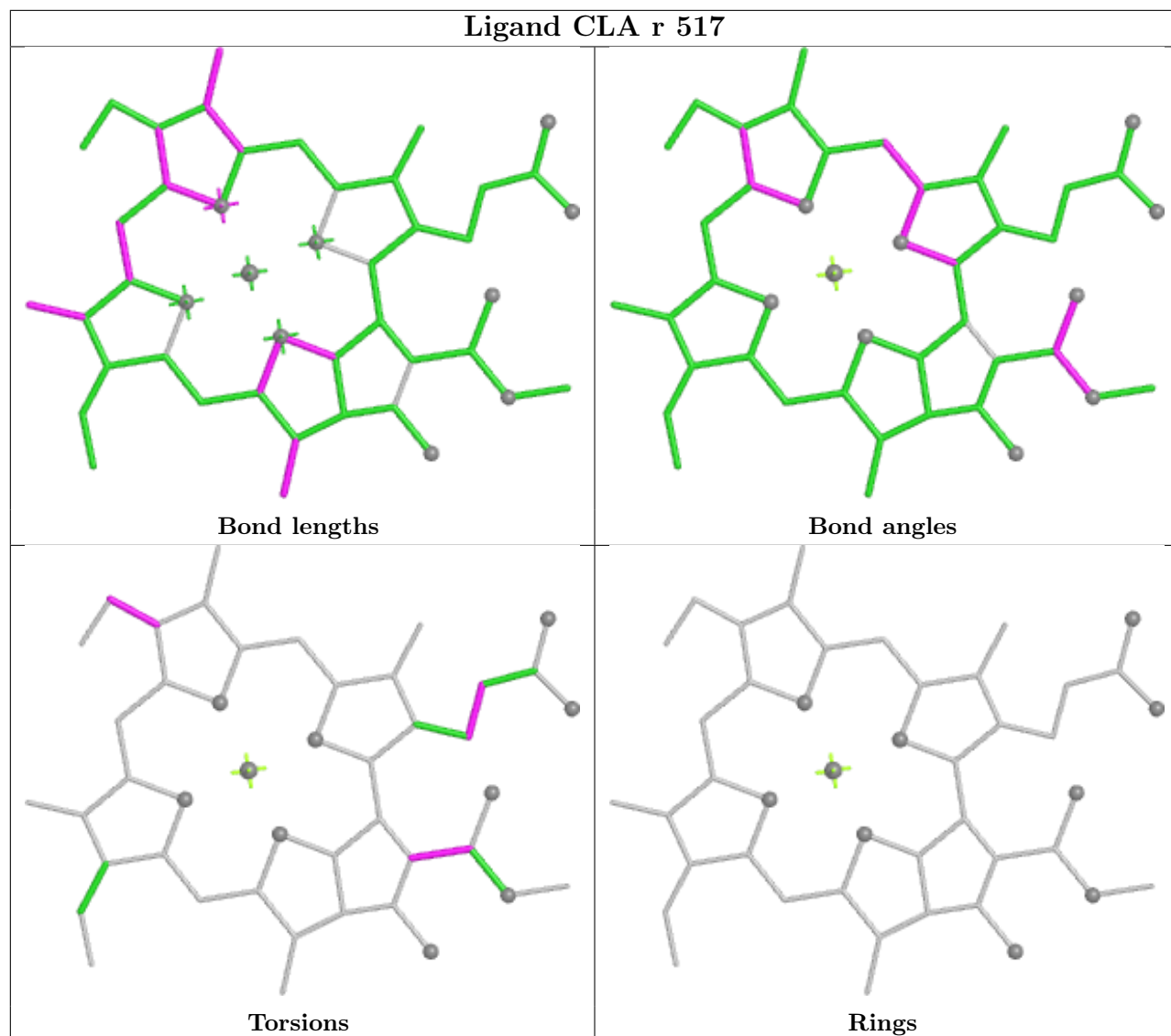


Torsions

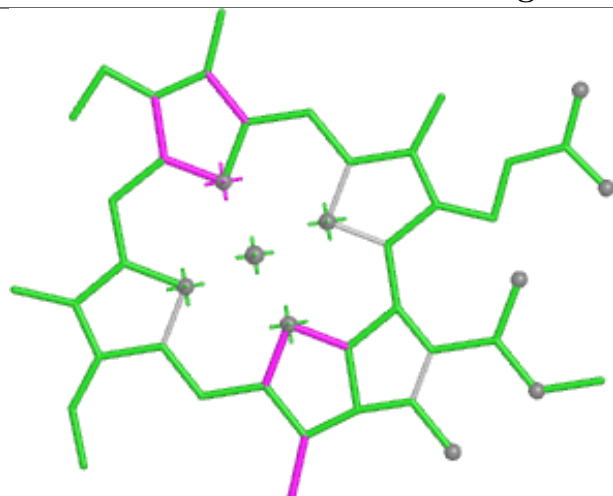


Rings

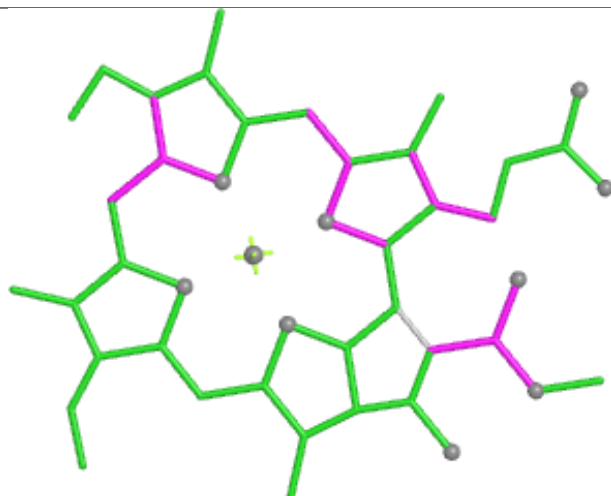
Ligand CLA r 517



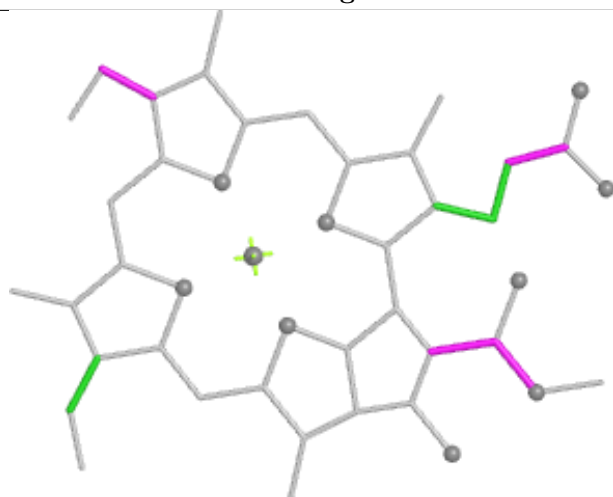
Ligand CLA b 507



Bond lengths



Bond angles

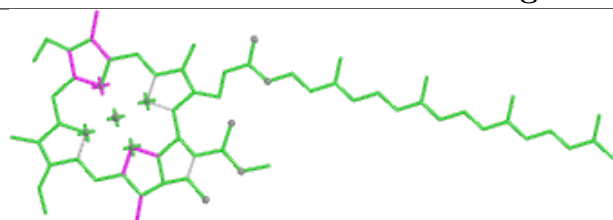


Torsions

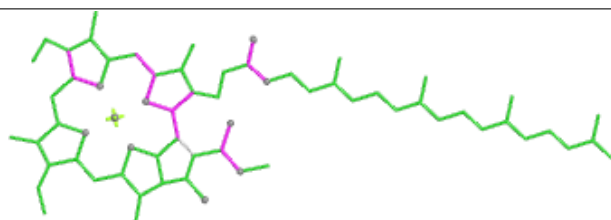


Rings

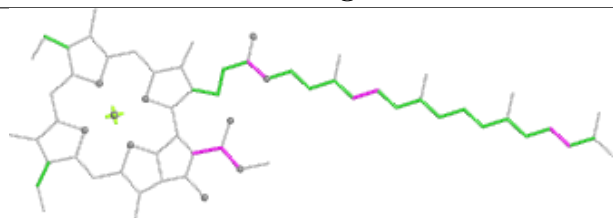
Ligand CLA t 509



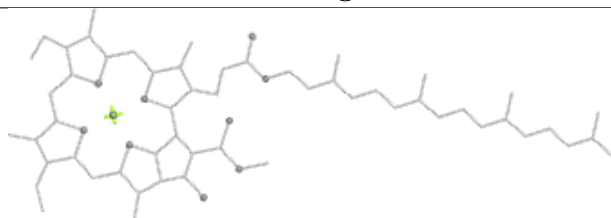
Bond lengths



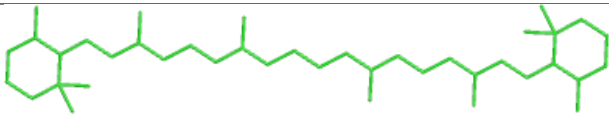
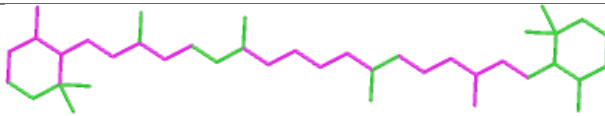
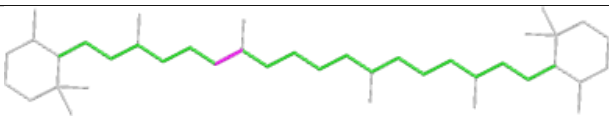
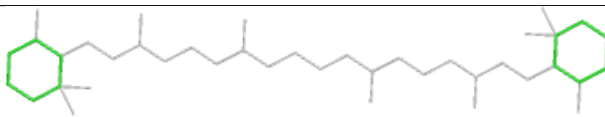
Bond angles

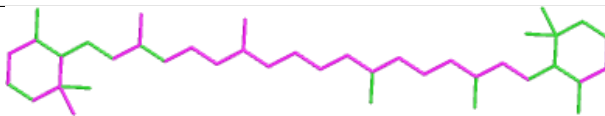
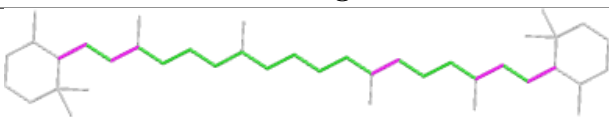
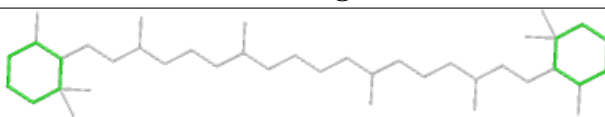


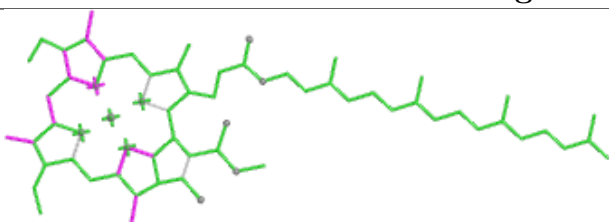
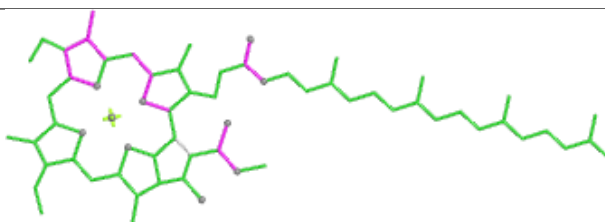
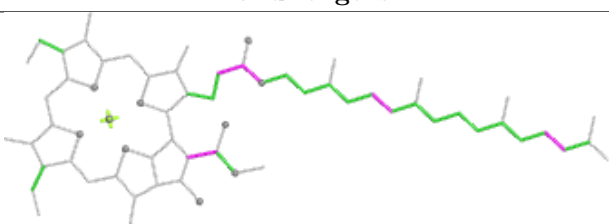
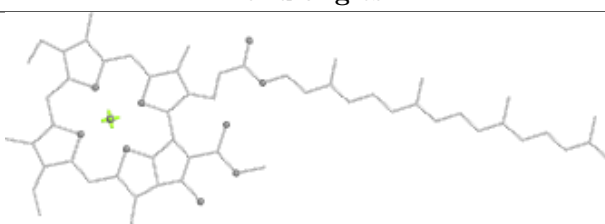
Torsions



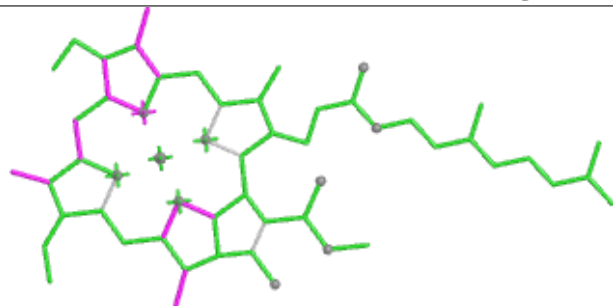
Rings

Ligand BCR q 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

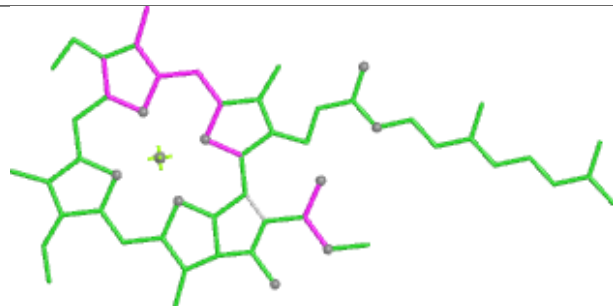
Ligand BCR B 4014	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA r 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

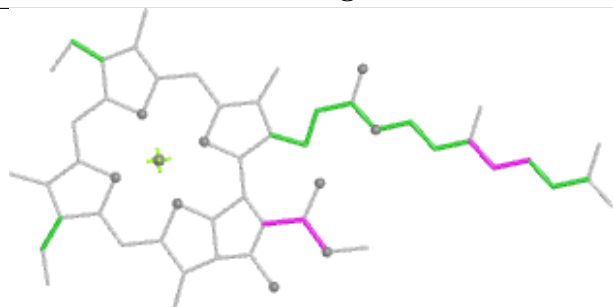
Ligand CLA Z 506



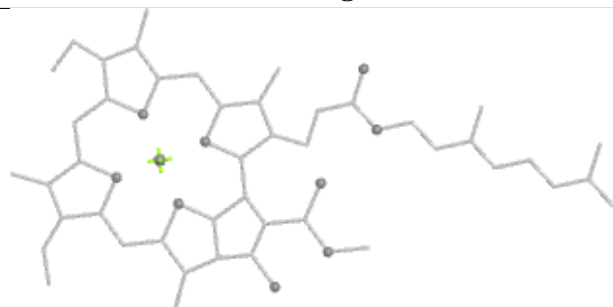
Bond lengths



Bond angles

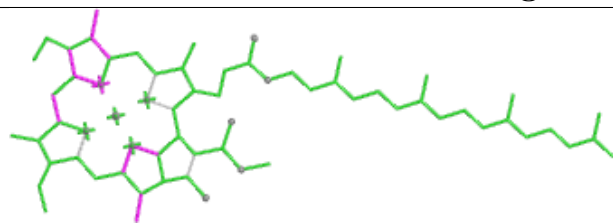


Torsions

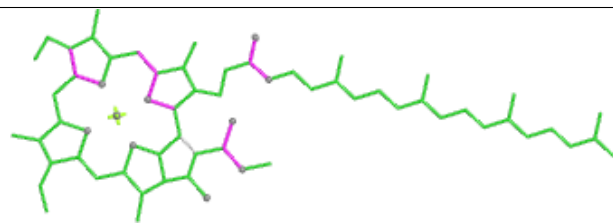


Rings

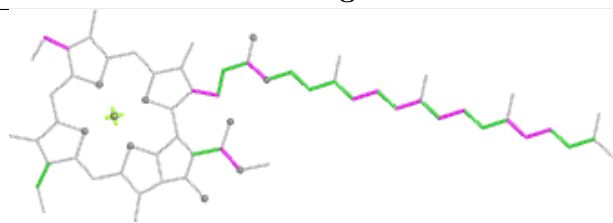
Ligand CLA s 513



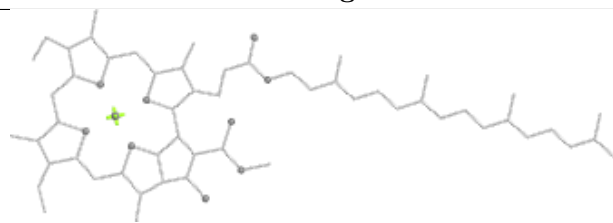
Bond lengths



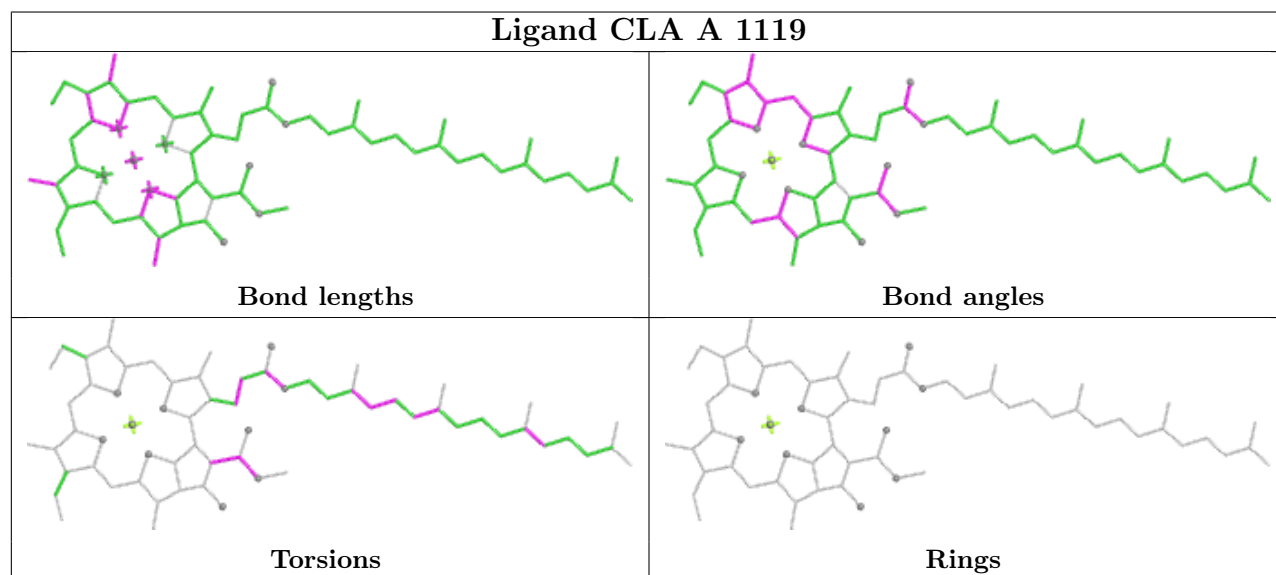
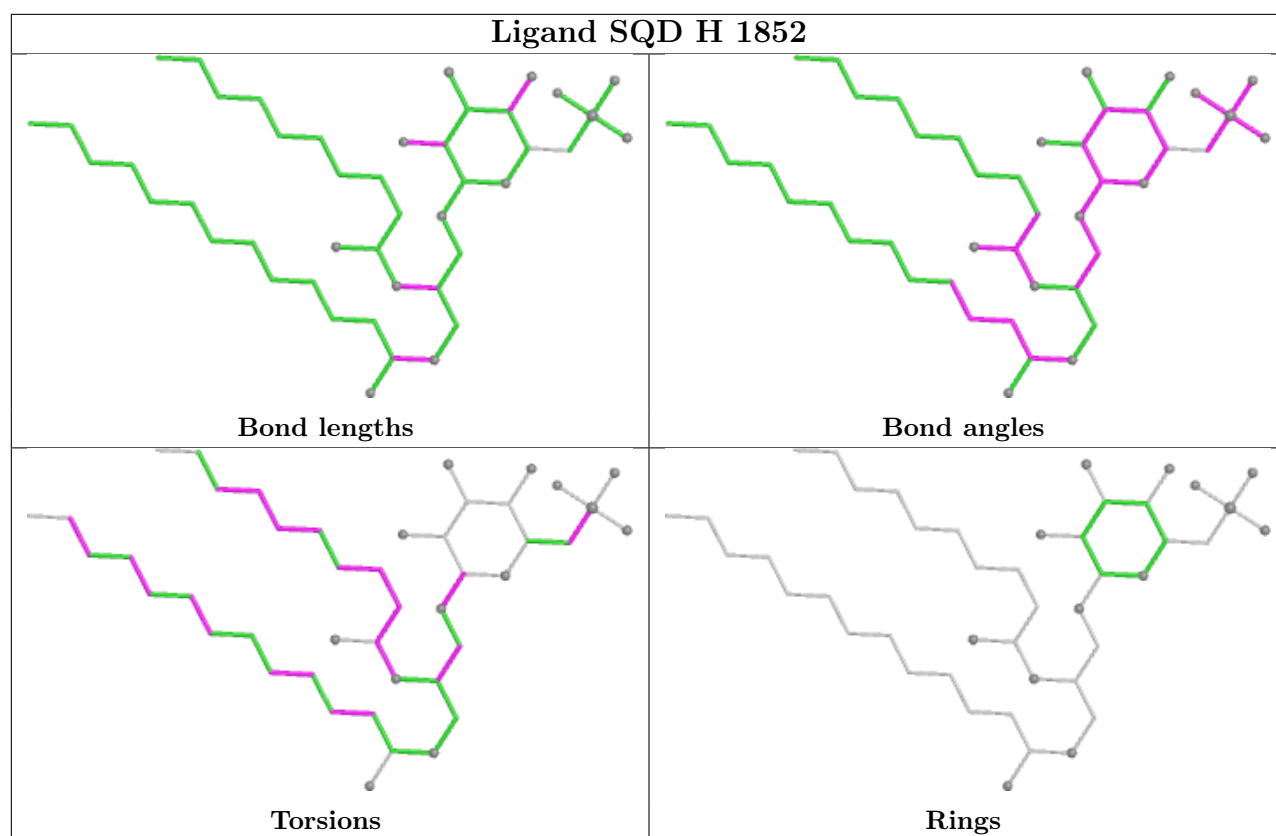
Bond angles

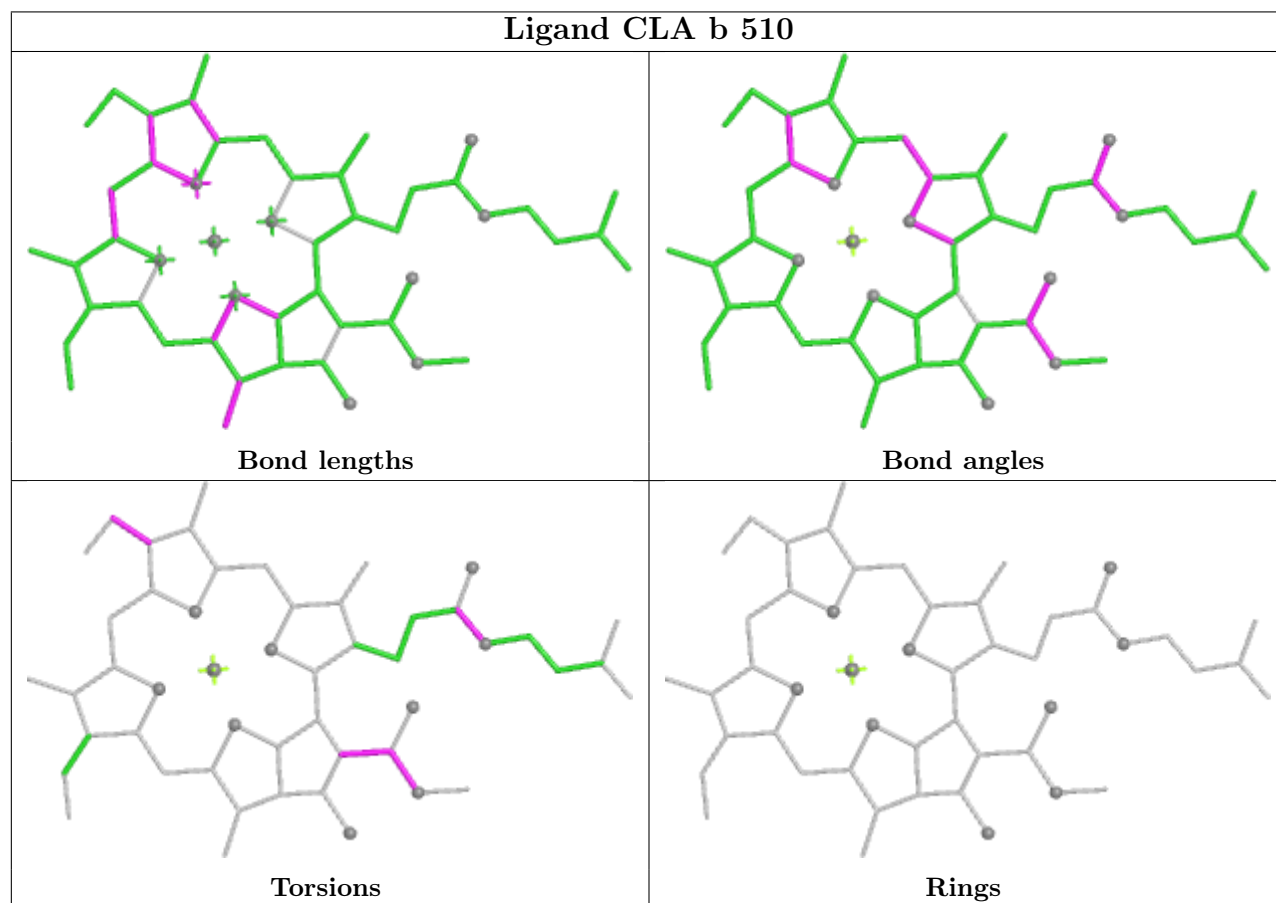
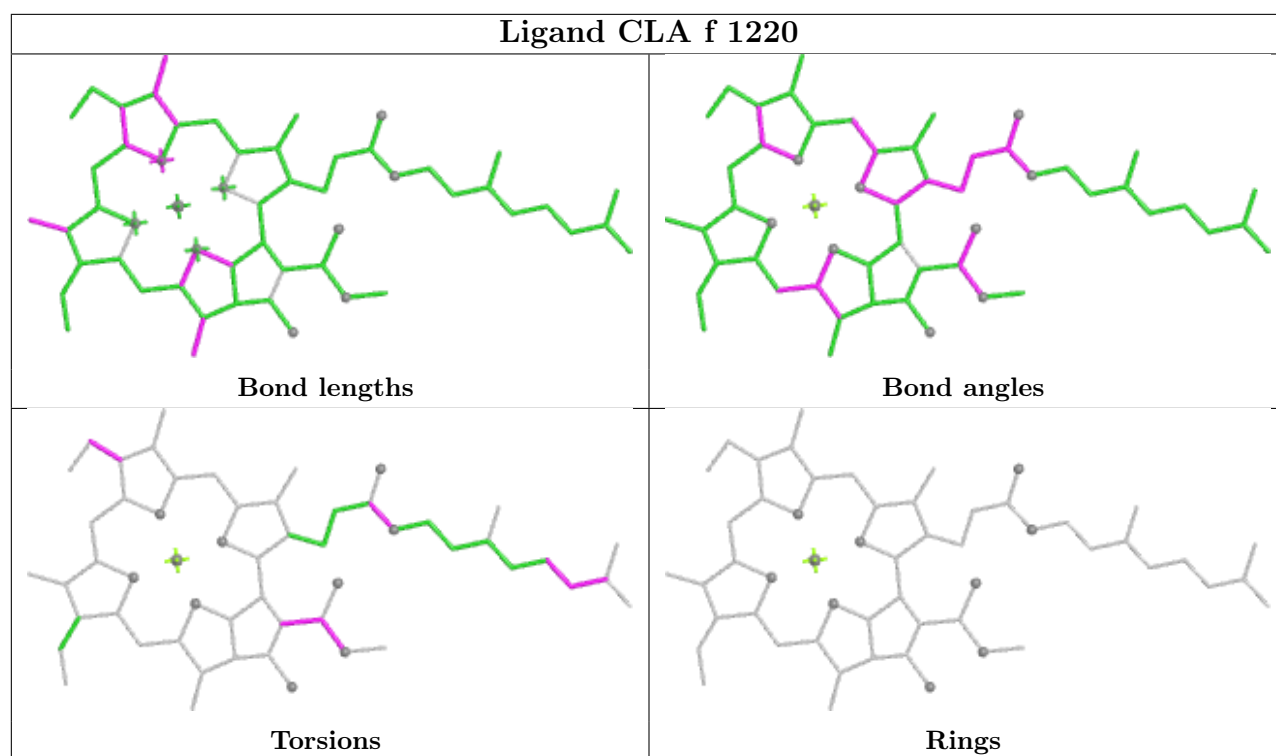


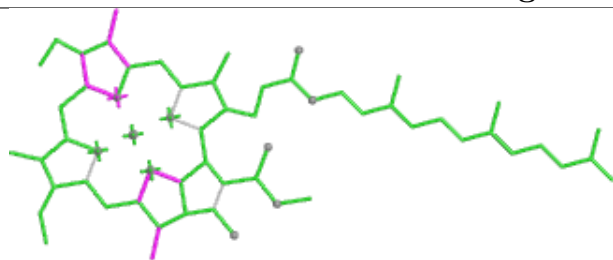
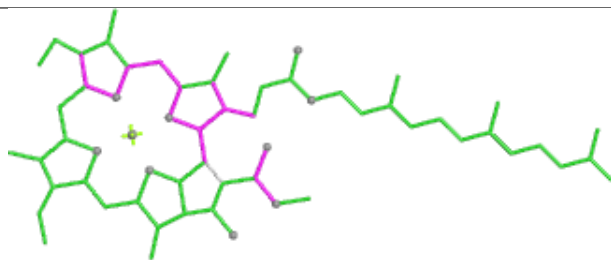
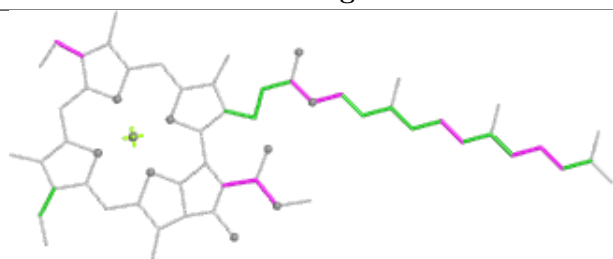
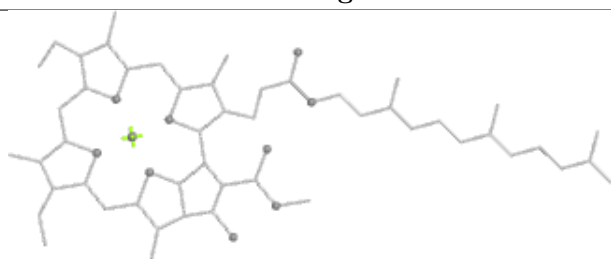
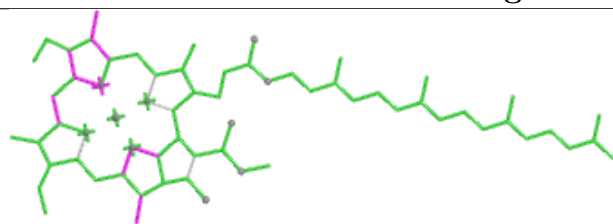
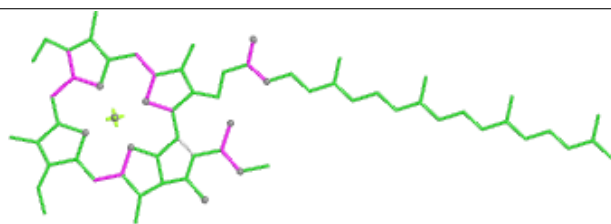
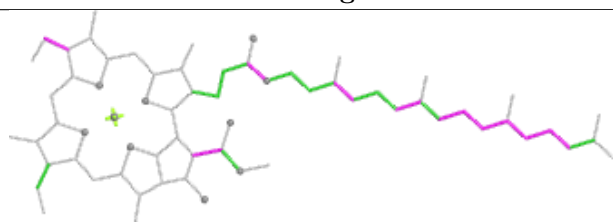
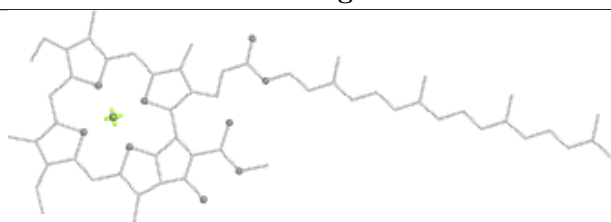
Torsions

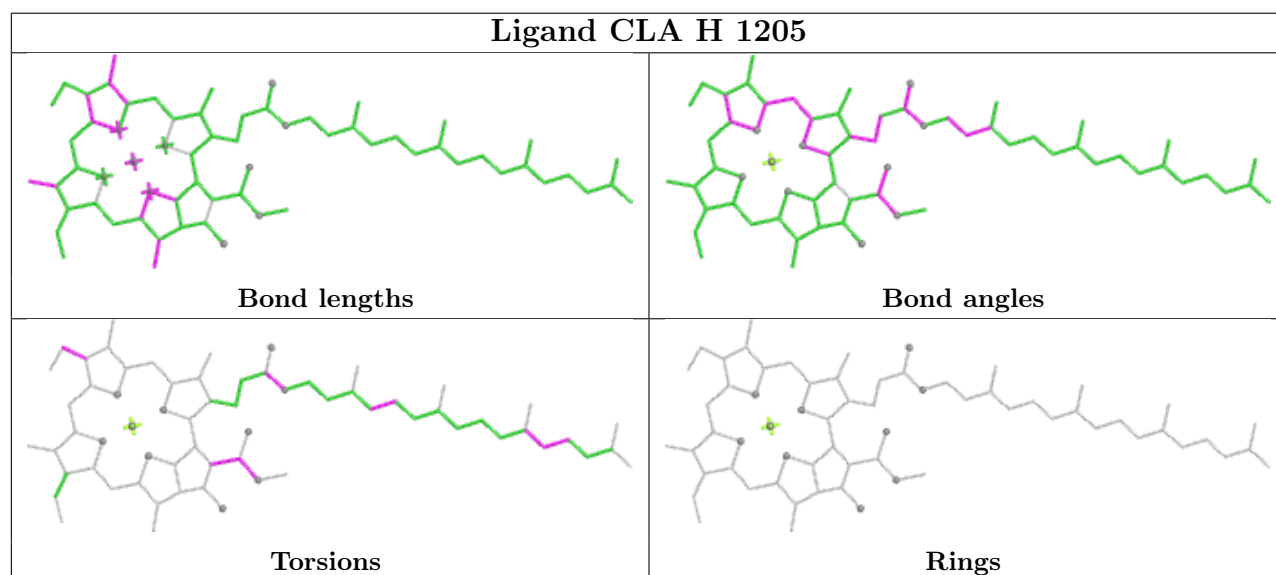
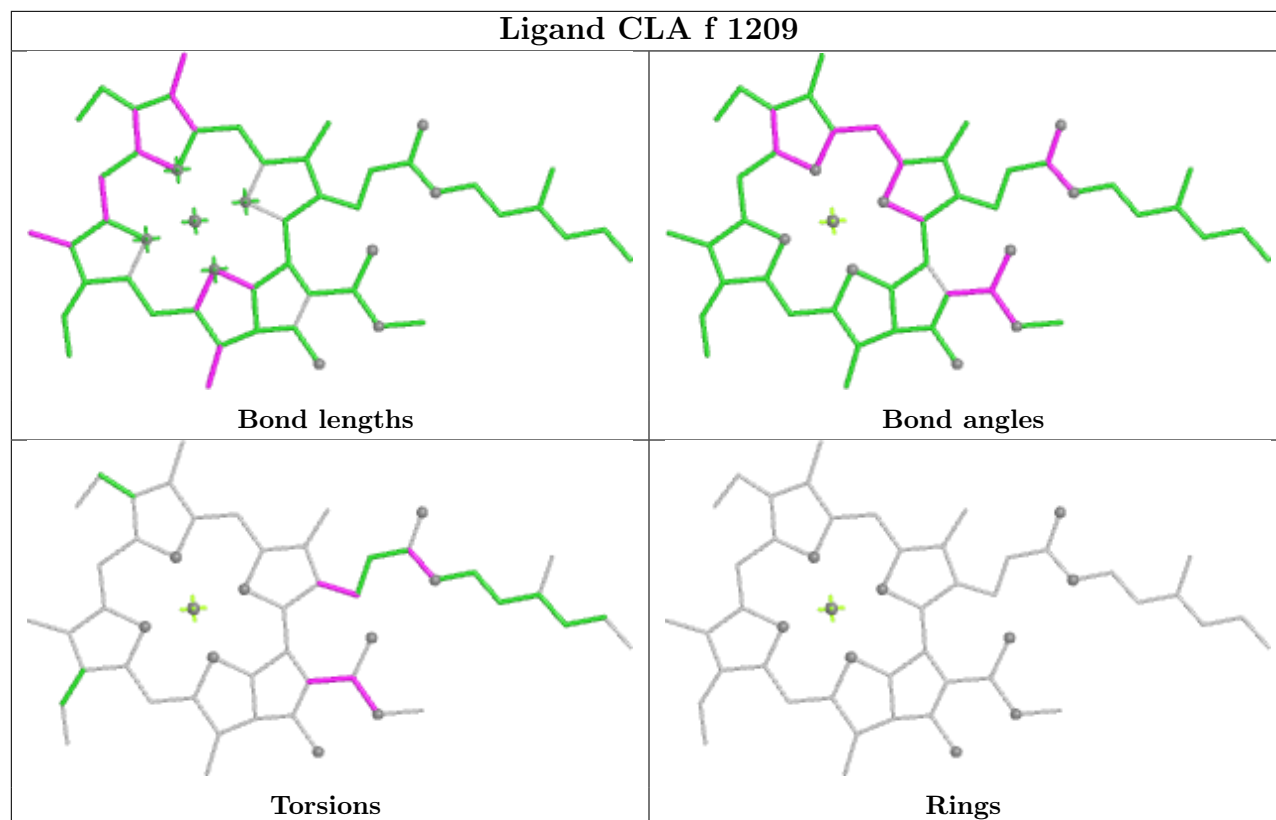


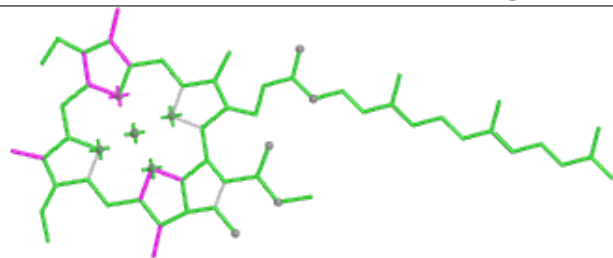
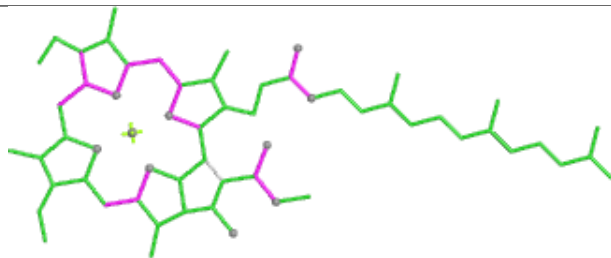
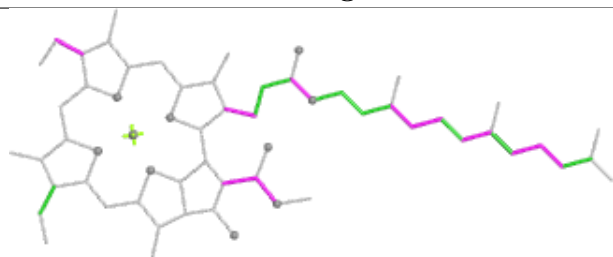
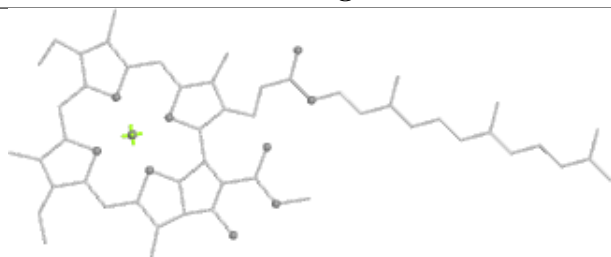
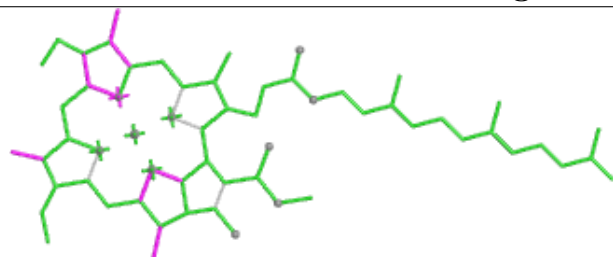
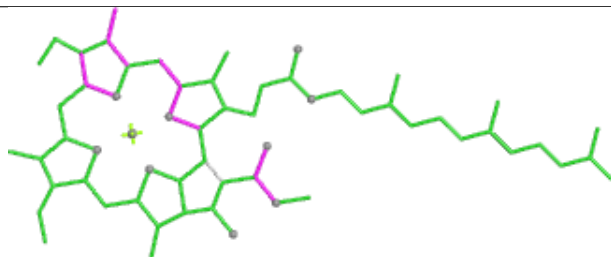
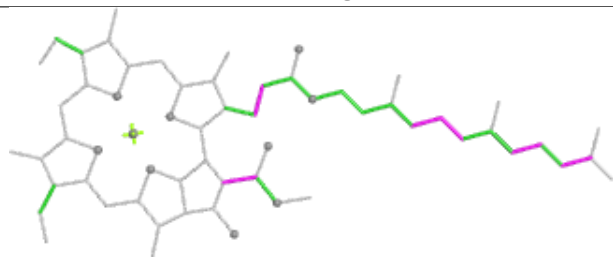
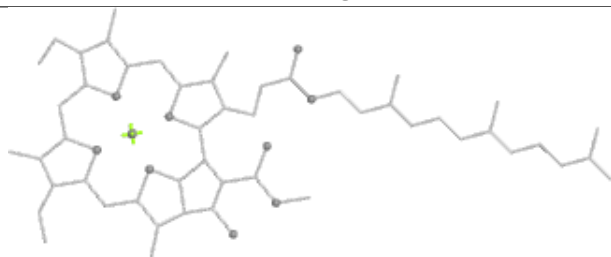
Rings

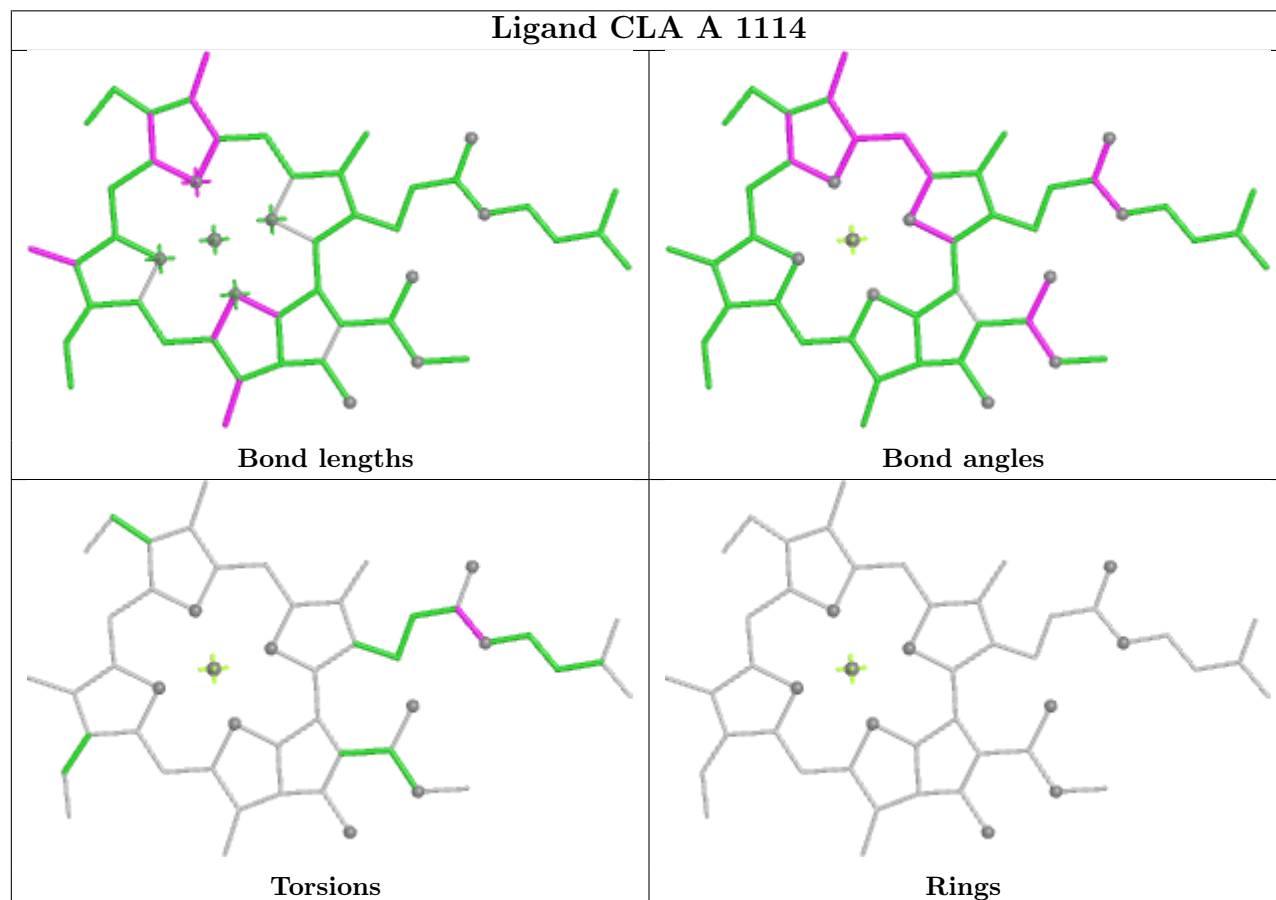
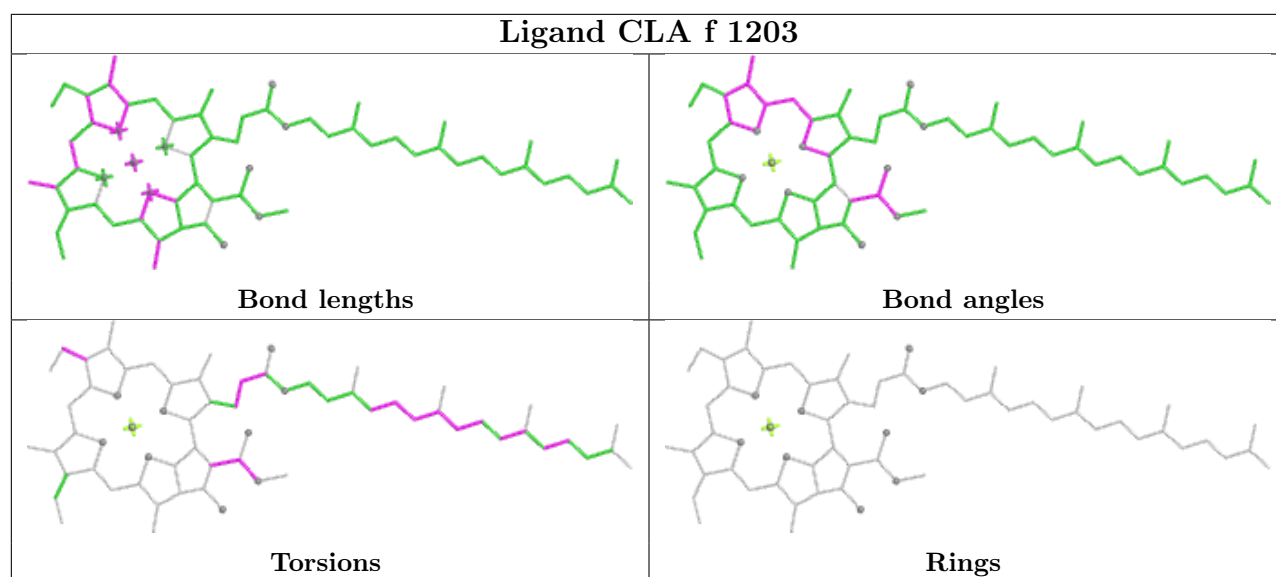


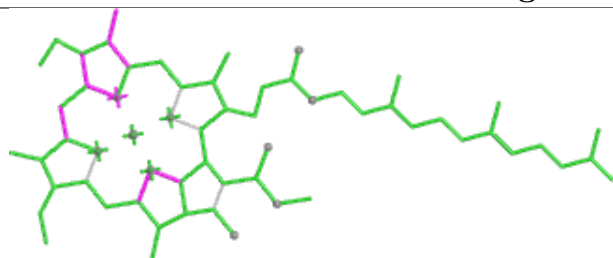
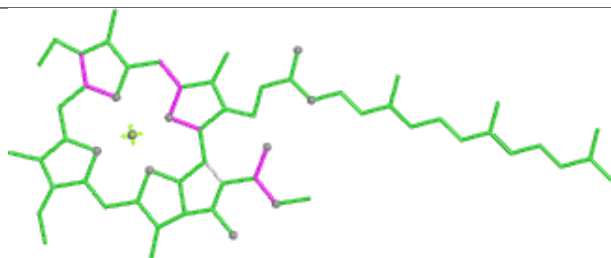
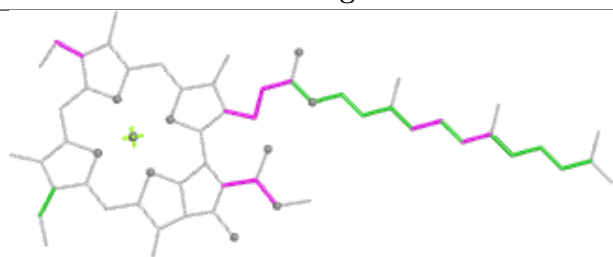
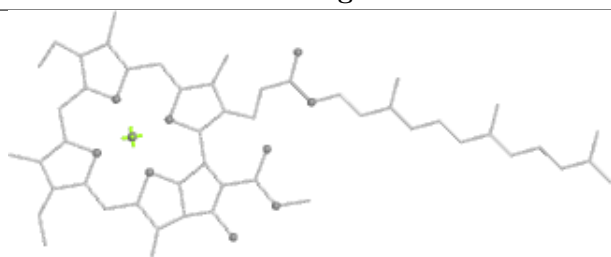
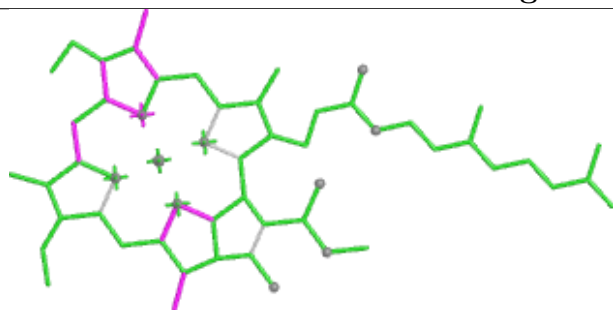
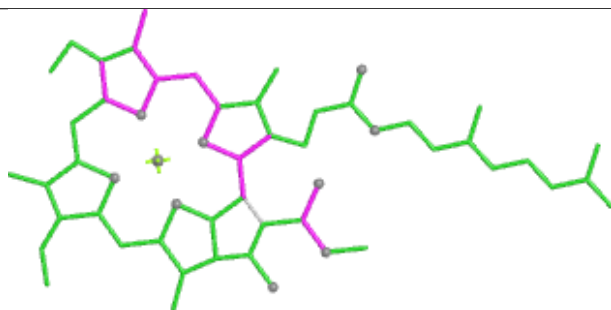
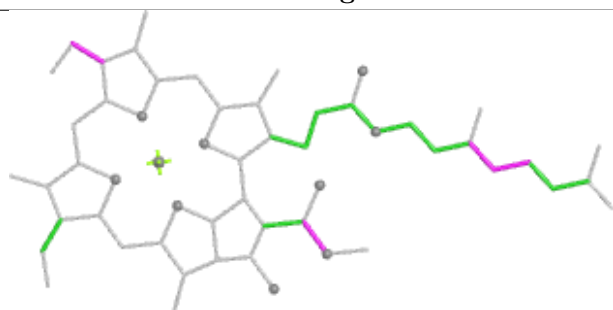
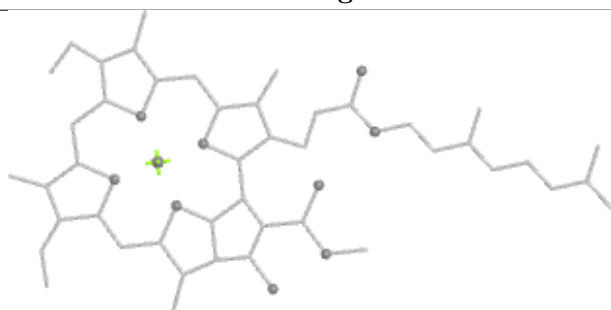


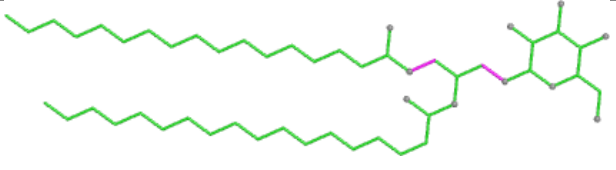
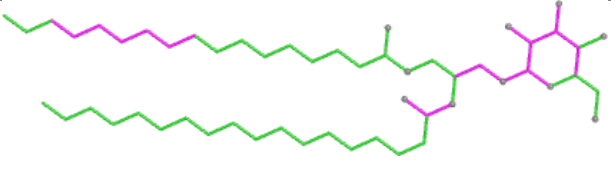
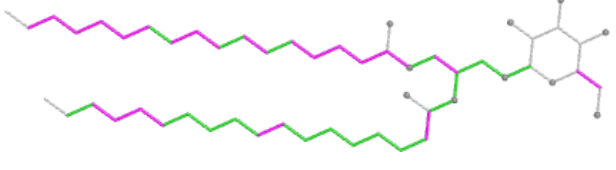
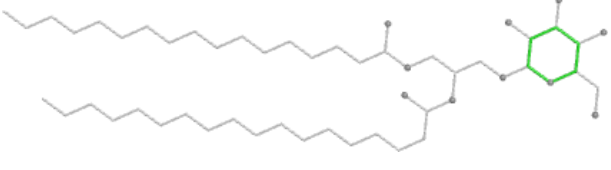
Ligand CLA 2 502**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA H 1208****Bond lengths****Bond angles****Torsions****Rings**

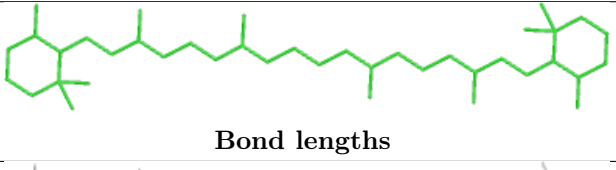
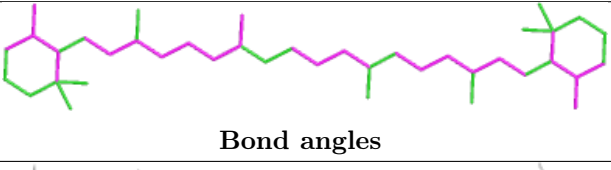
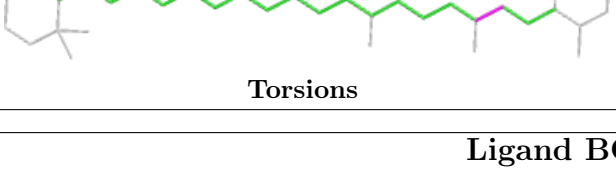
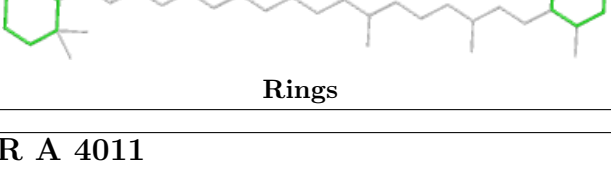


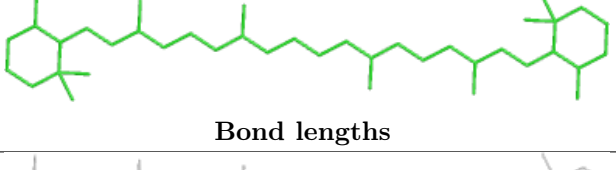
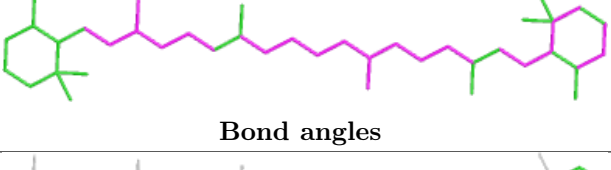
Ligand CLA G 1122**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA f 1218****Bond lengths****Bond angles****Torsions****Rings**

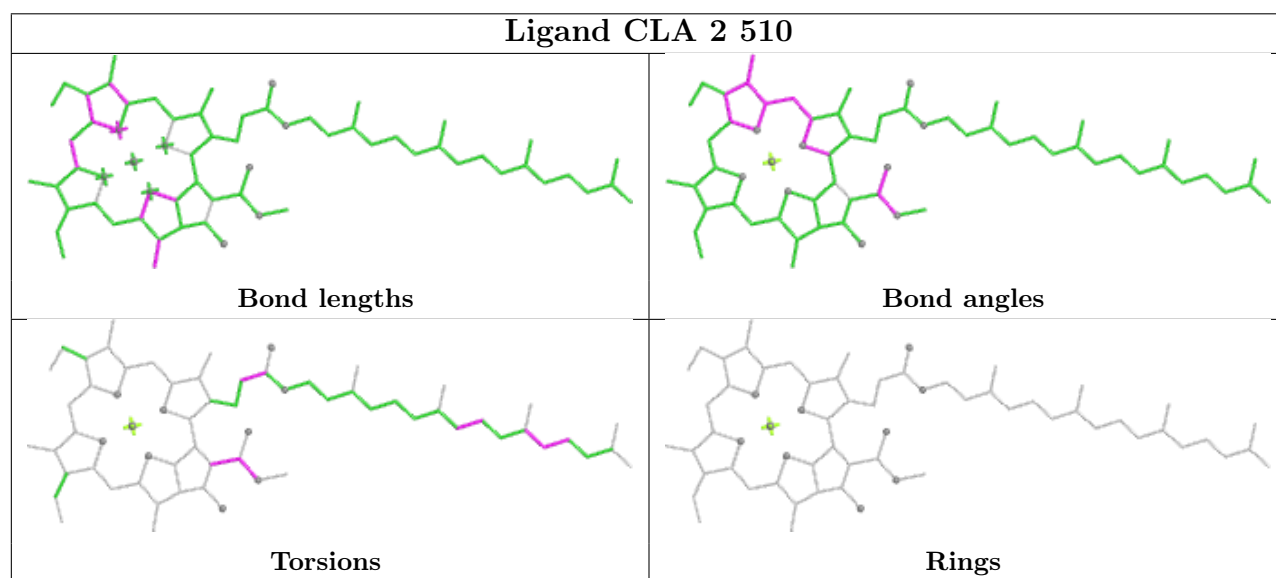
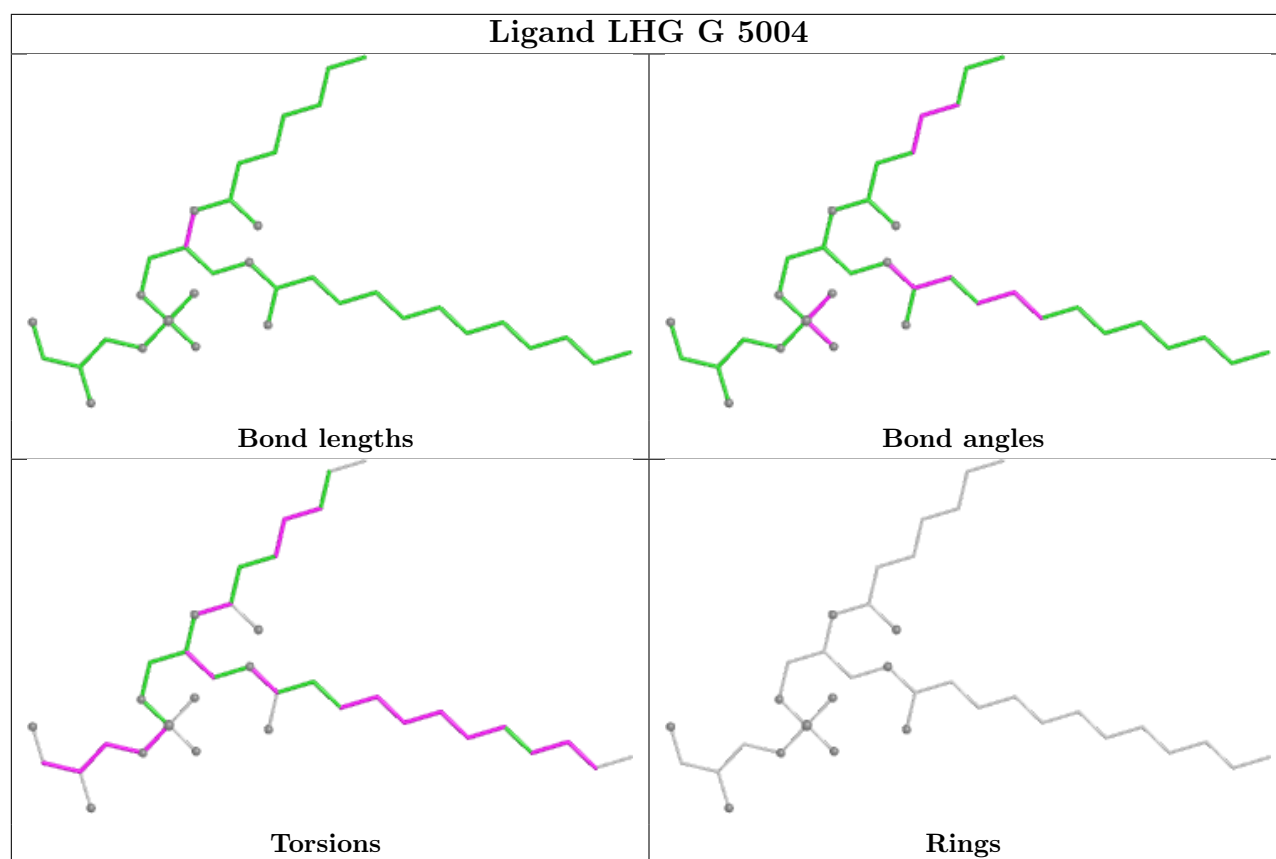


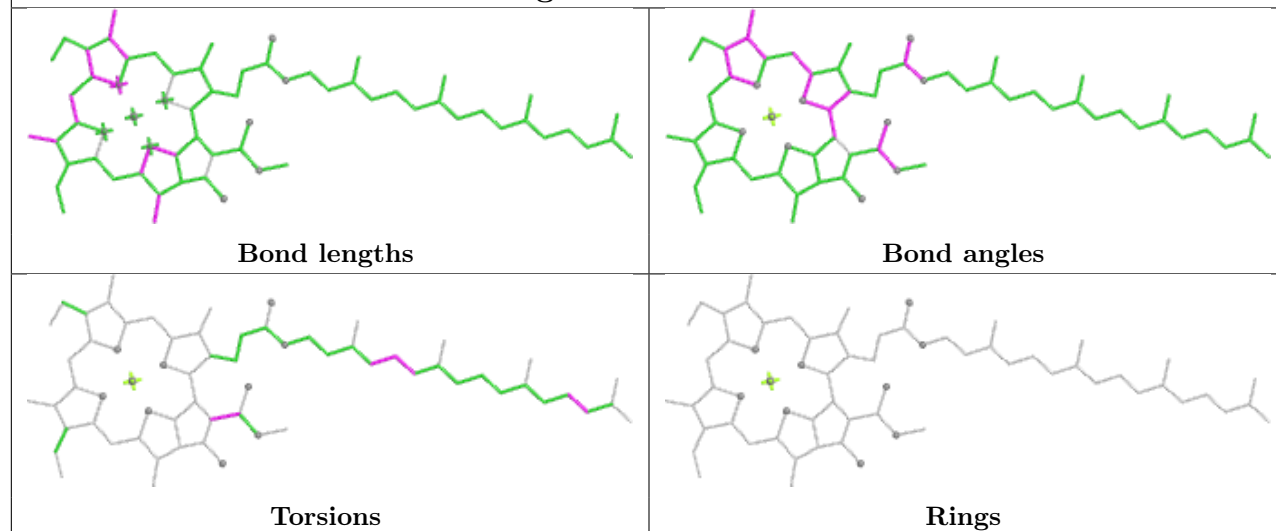
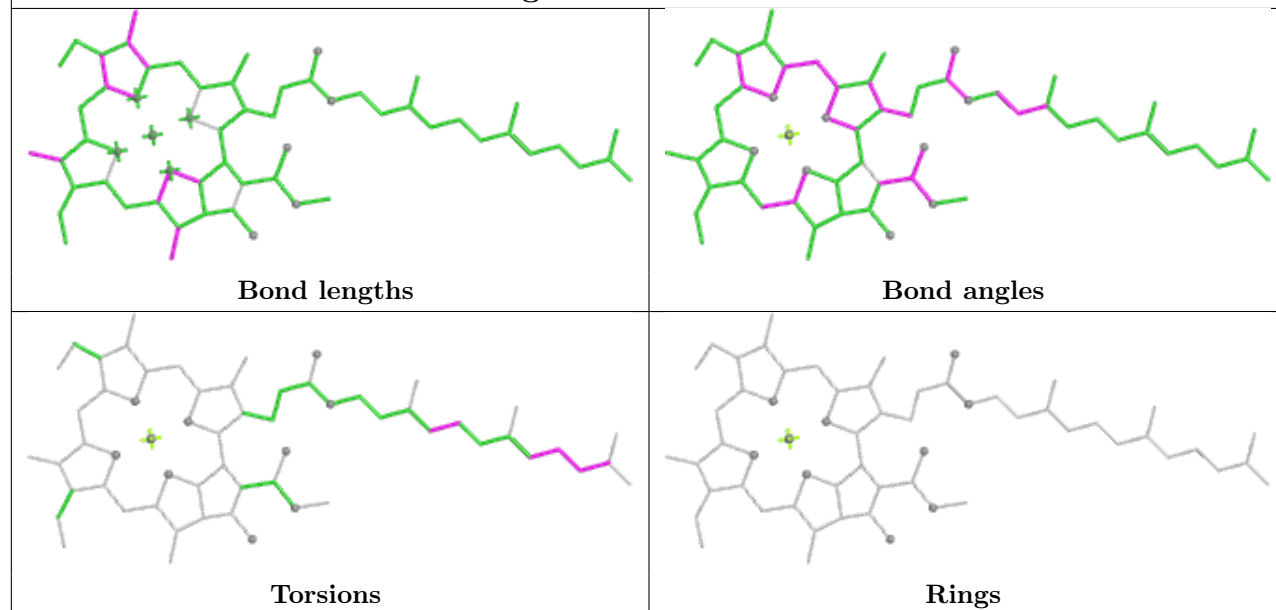
Ligand CLA 4 501**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA r 511****Bond lengths****Bond angles****Torsions****Rings**

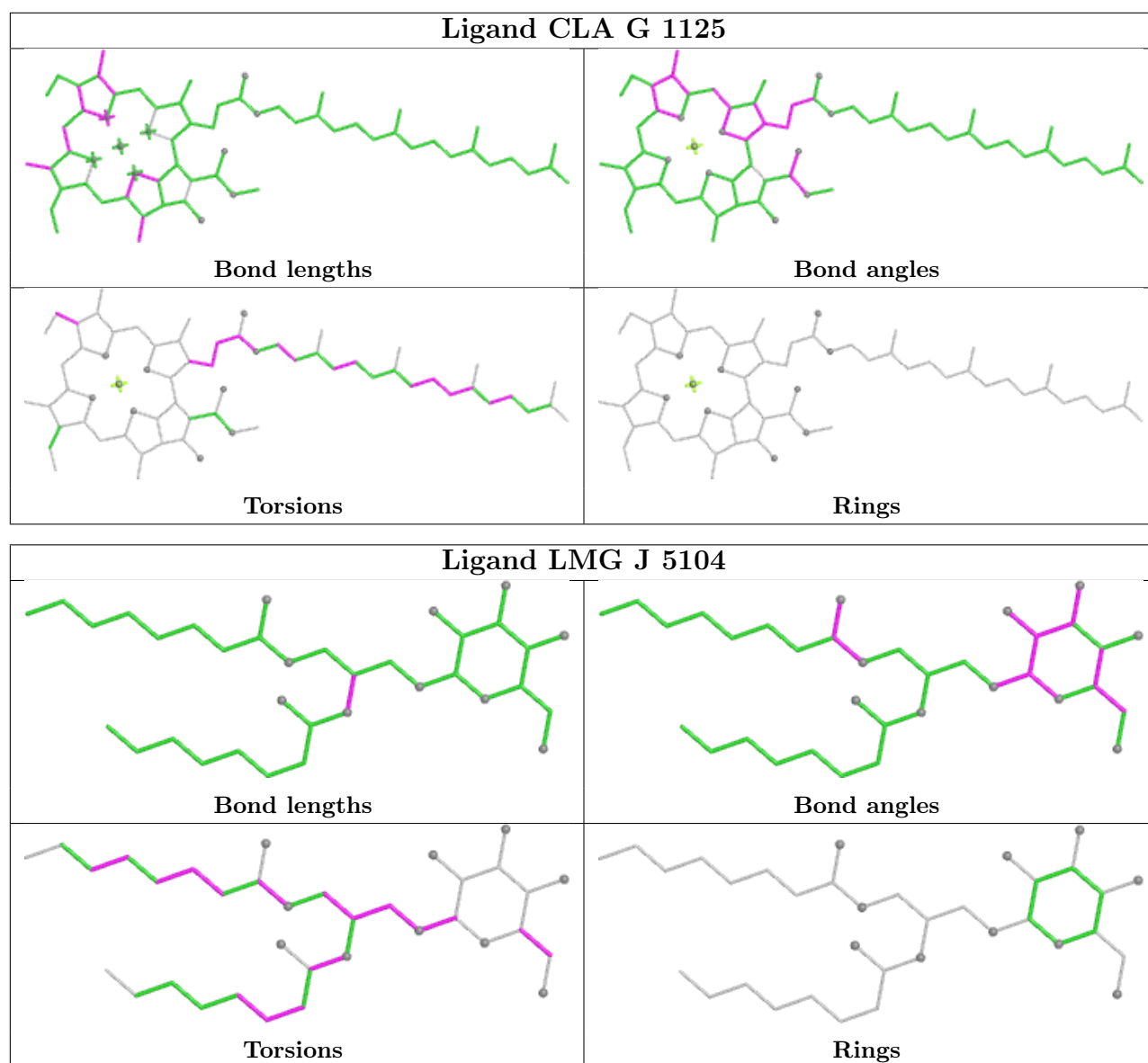
Ligand LMG H 5002	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR I 4018	
	
Bond lengths	Bond angles
	
Torsions	Rings

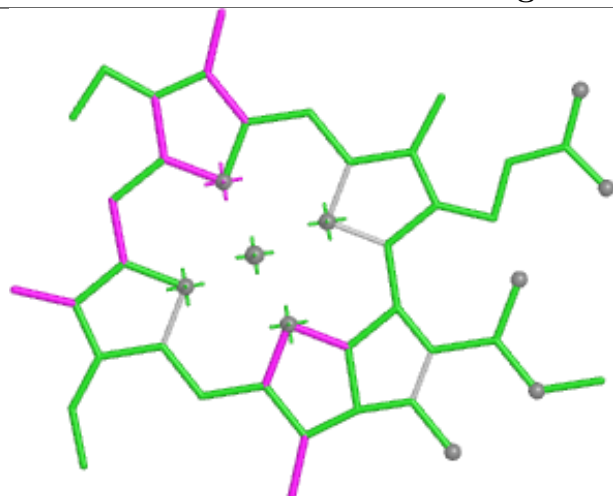
Ligand BCR A 4011	
	
Bond lengths	Bond angles
	
Torsions	Rings



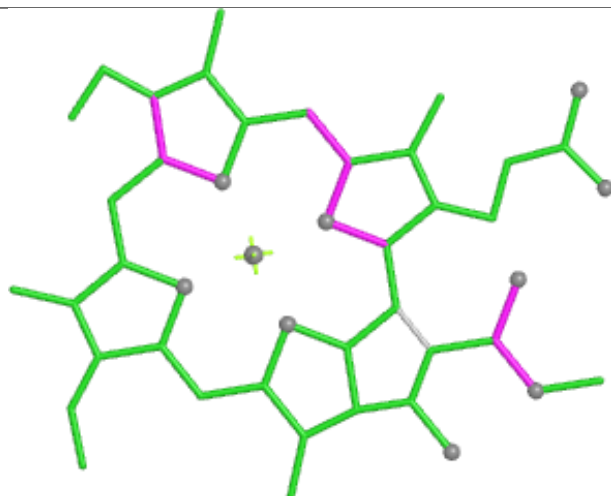
Ligand CLA a 509**Ligand CLA G 1136**



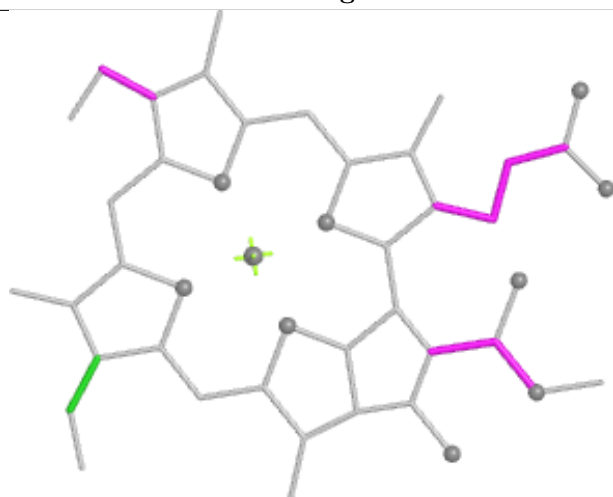
Ligand CLA u 517



Bond lengths



Bond angles

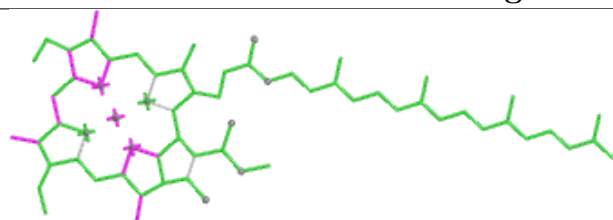


Torsions

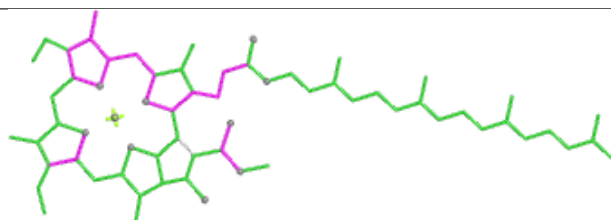


Rings

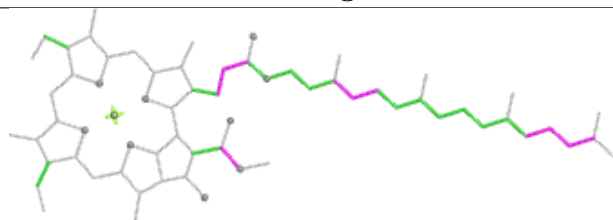
Ligand CLA A 1013



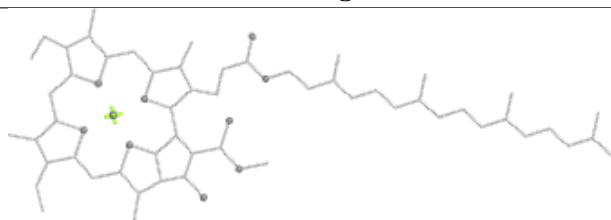
Bond lengths



Bond angles

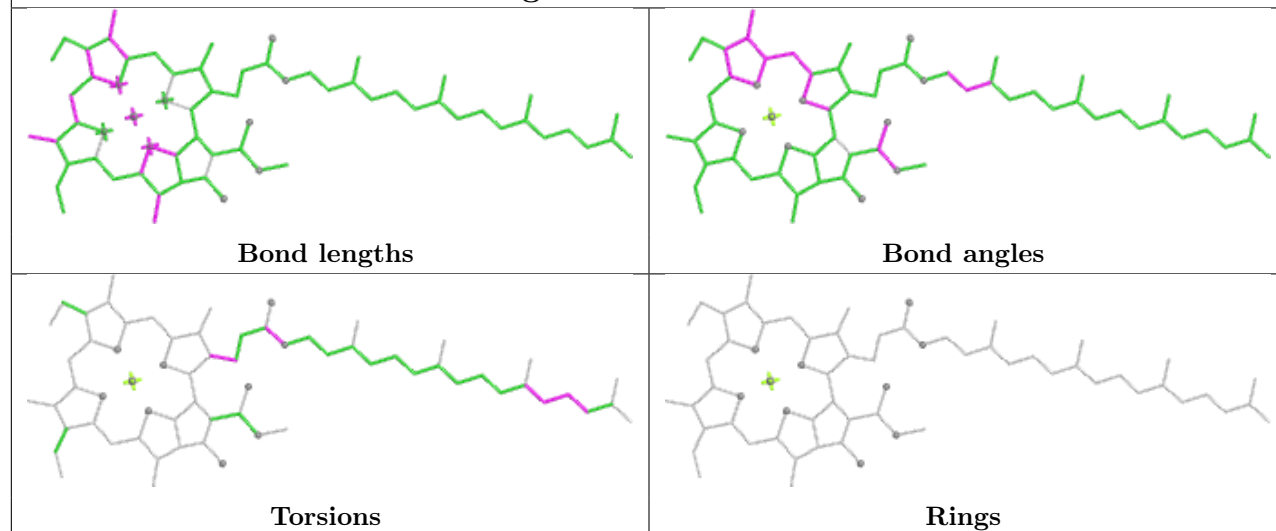


Torsions

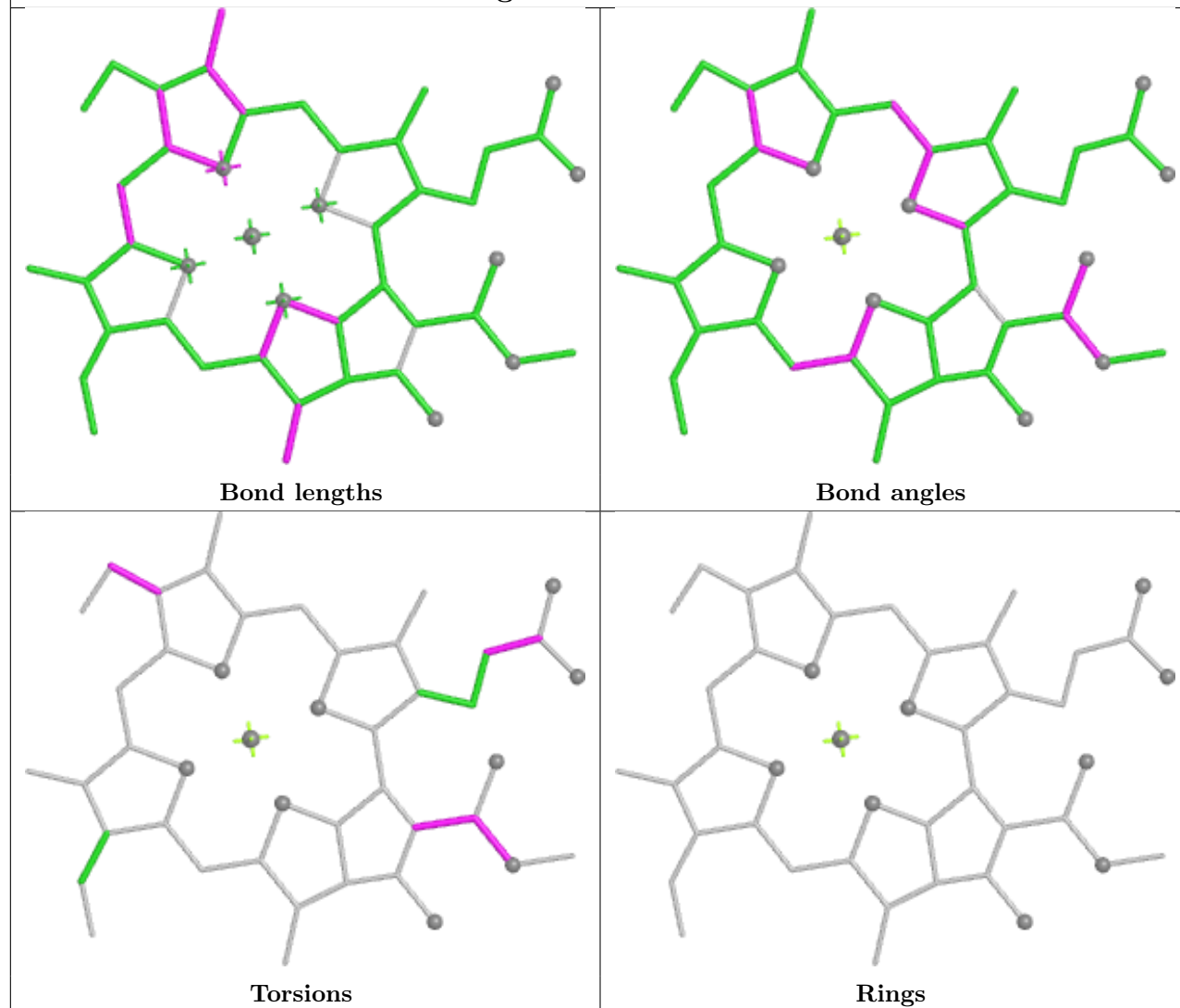


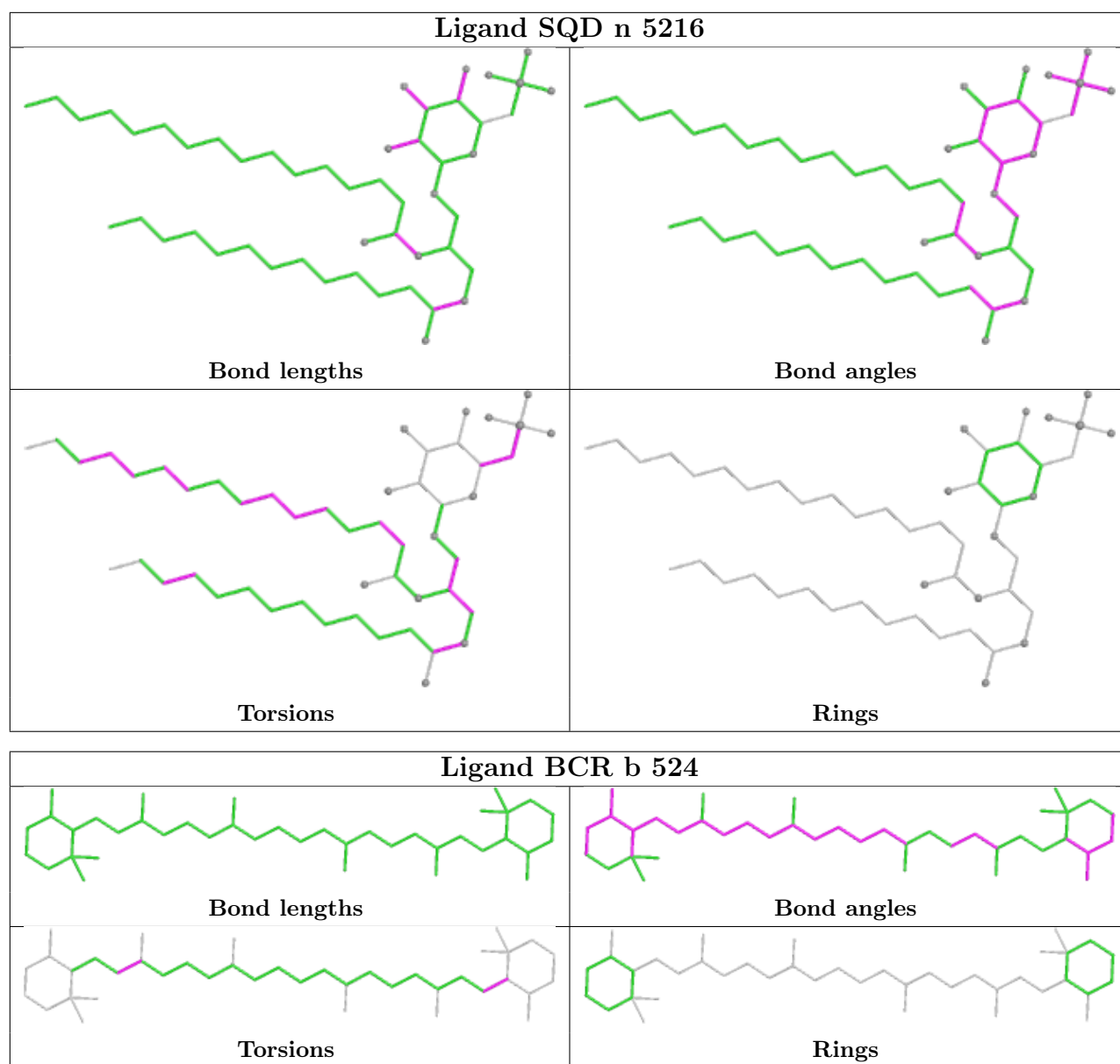
Rings

Ligand CLA H 1225

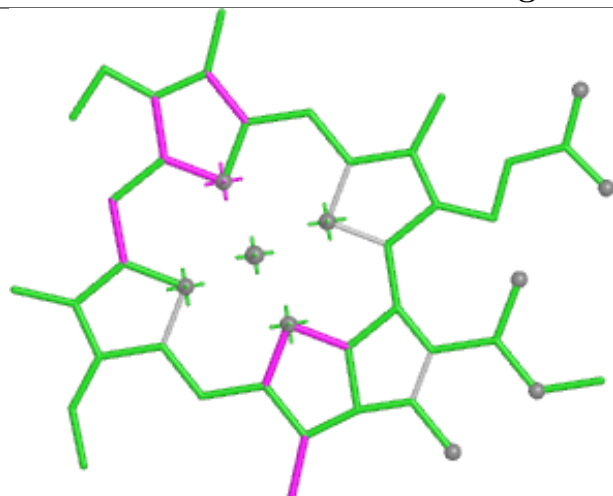


Ligand CLA c 510

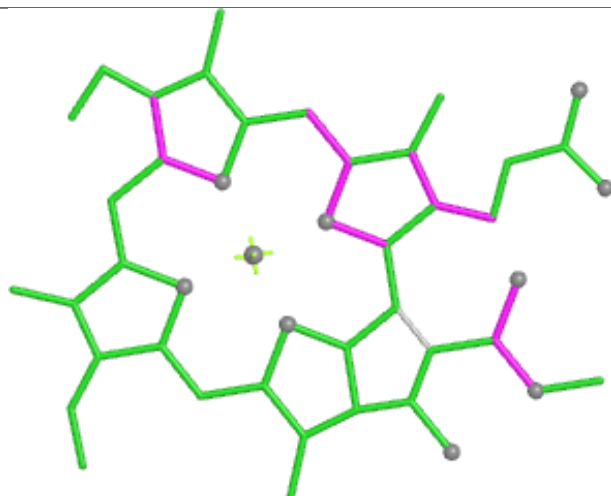




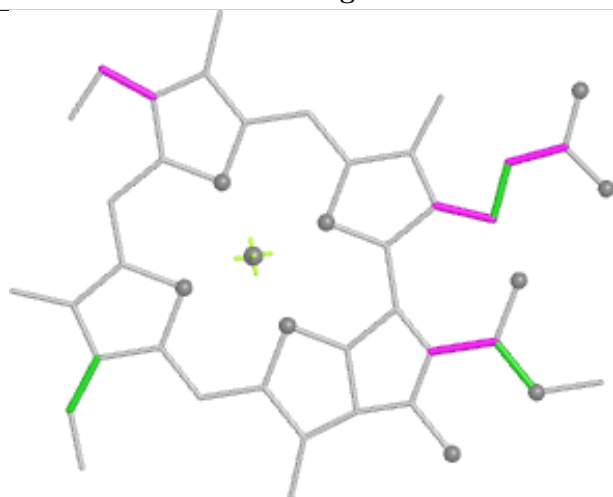
Ligand CLA 4 516



Bond lengths



Bond angles

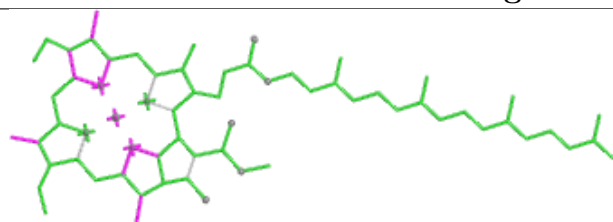


Torsions

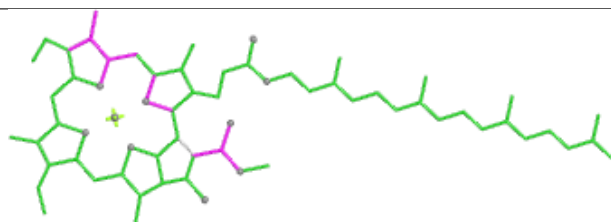


Rings

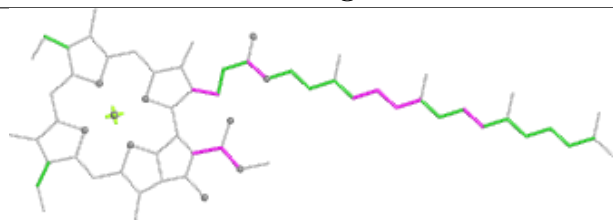
Ligand CLA G 1128



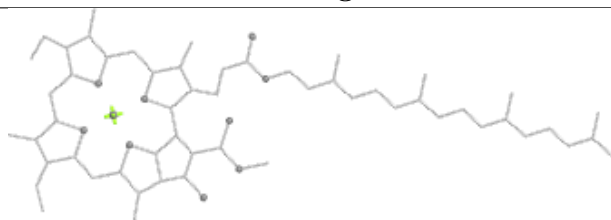
Bond lengths



Bond angles

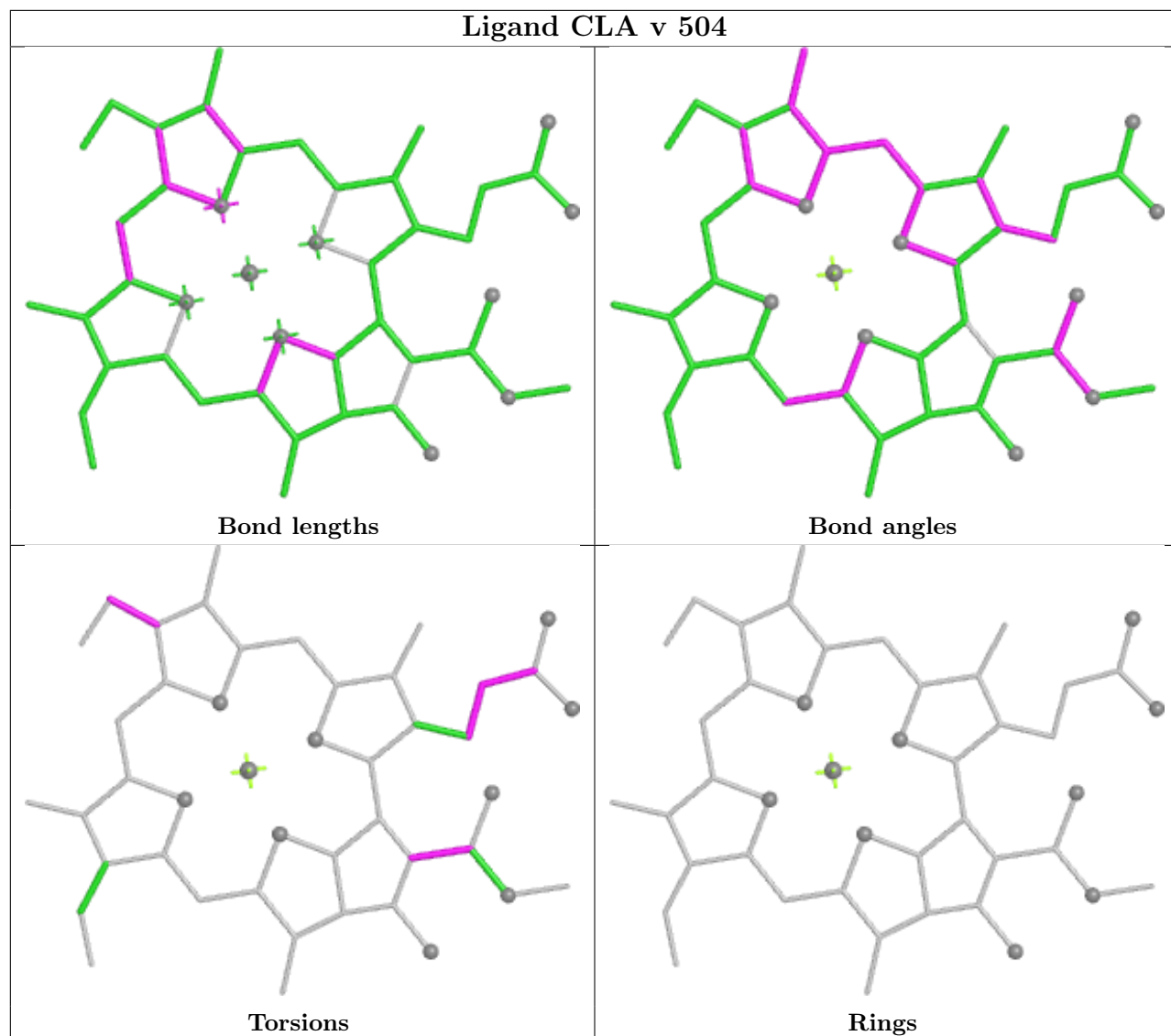


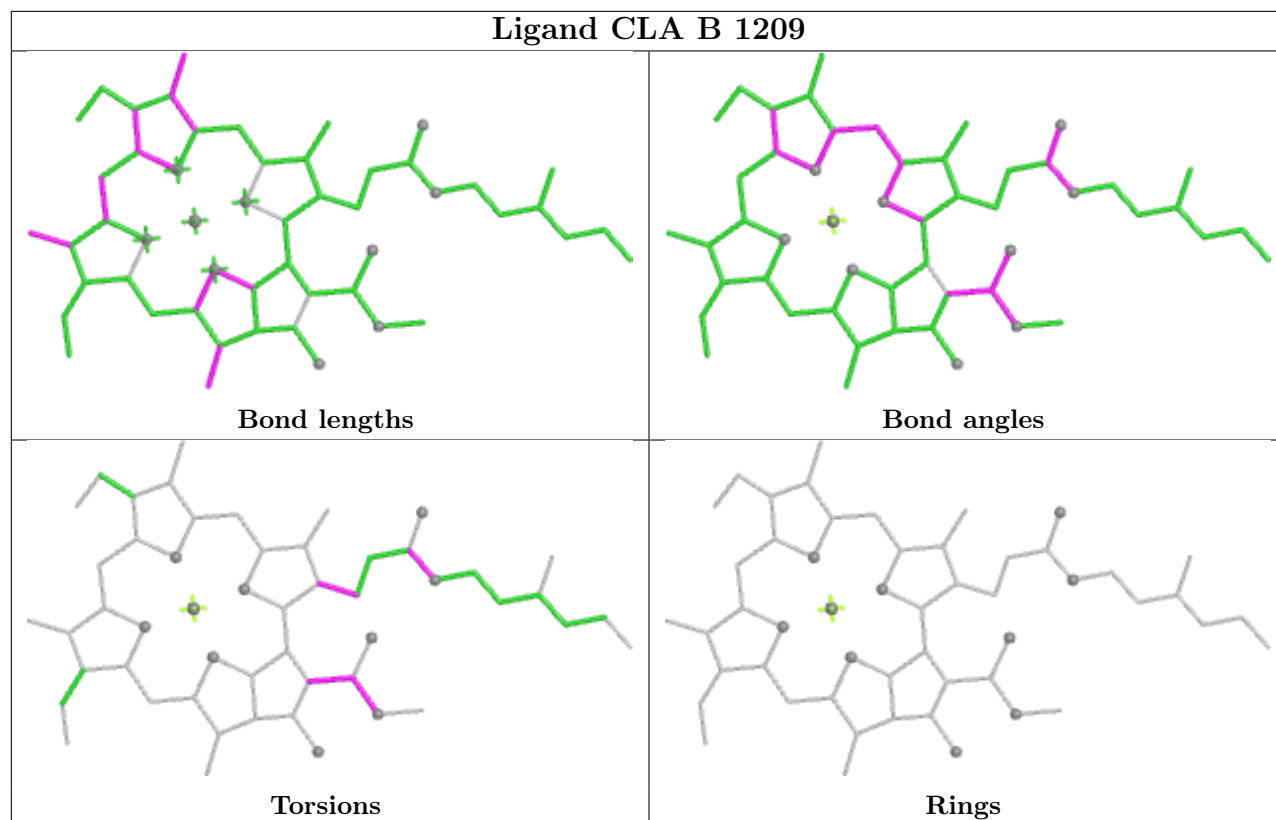
Torsions



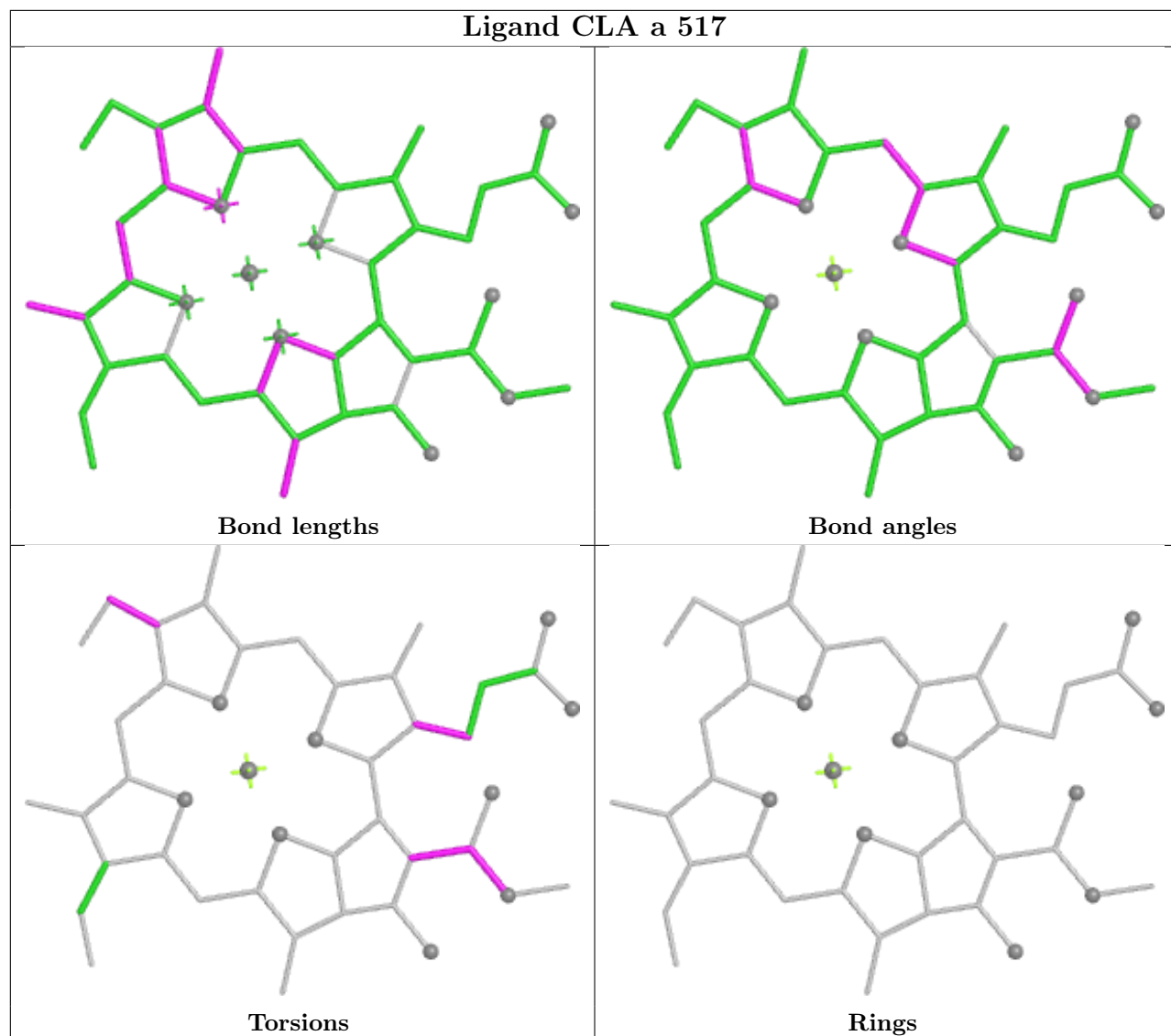
Rings

Ligand CLA v 504

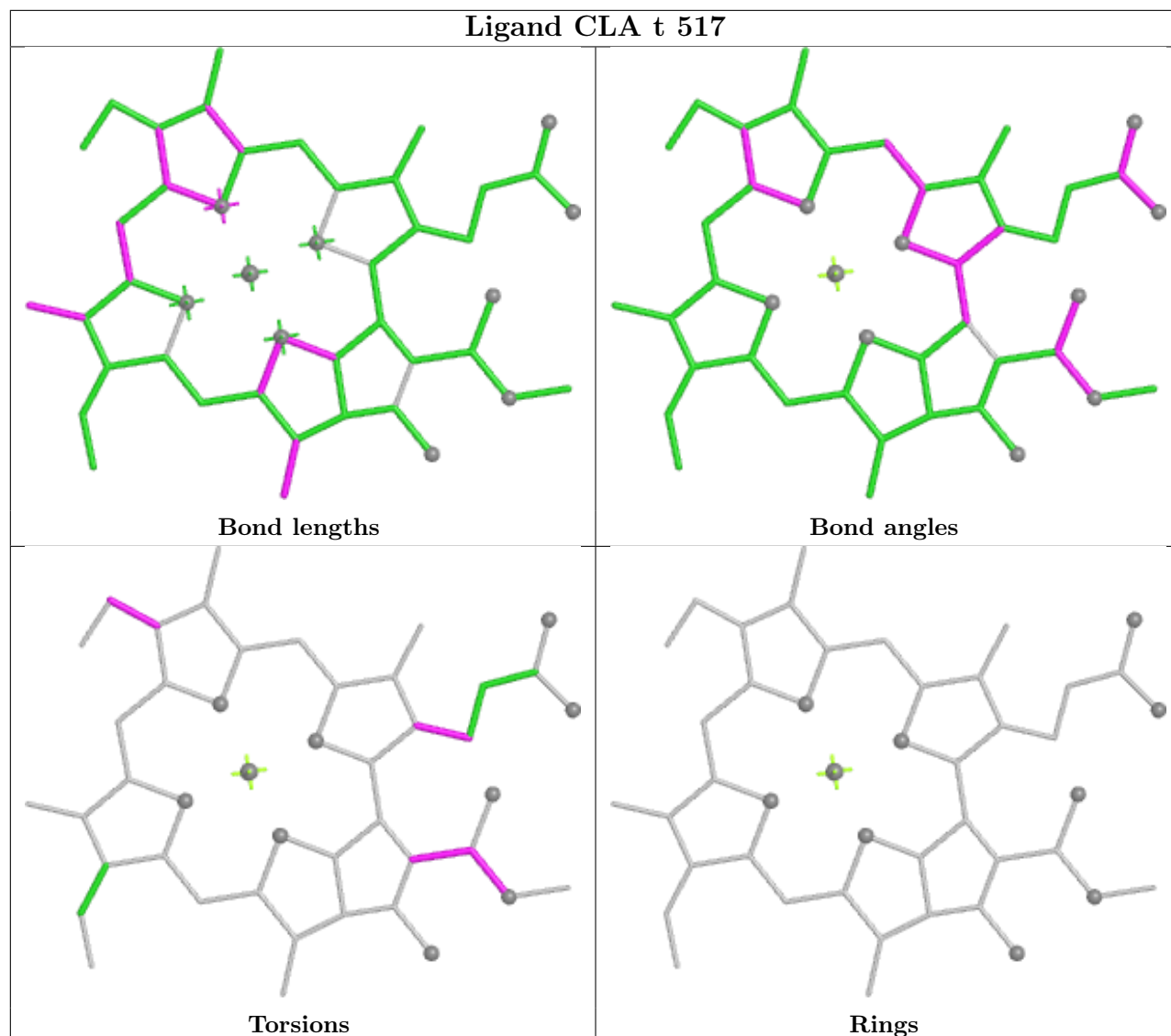




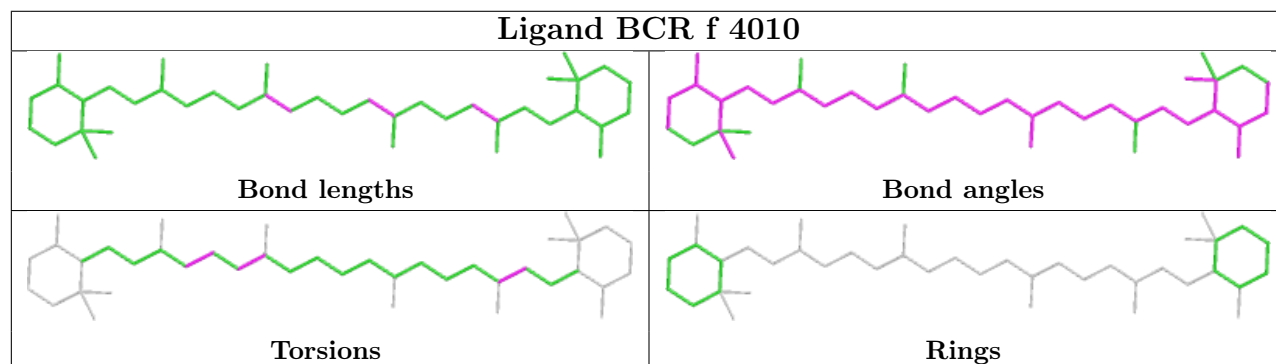
Ligand CLA a 517



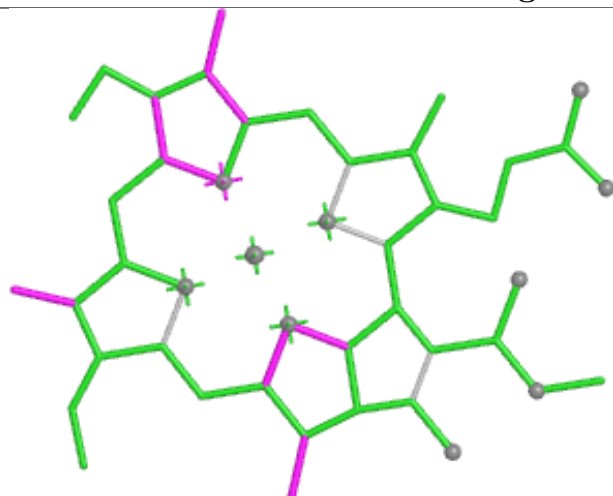
Ligand CLA t 517



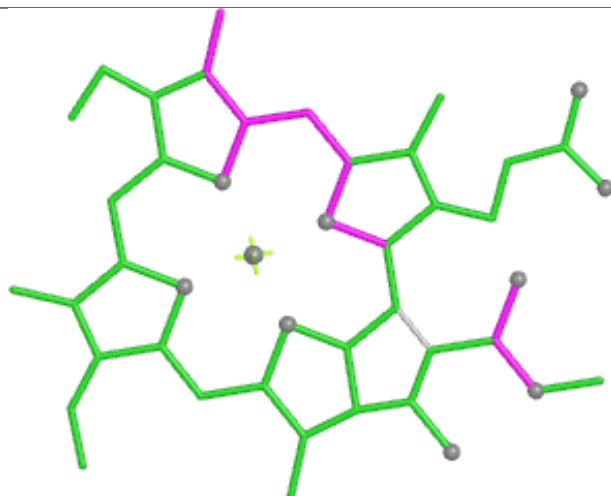
Ligand BCR f 4010



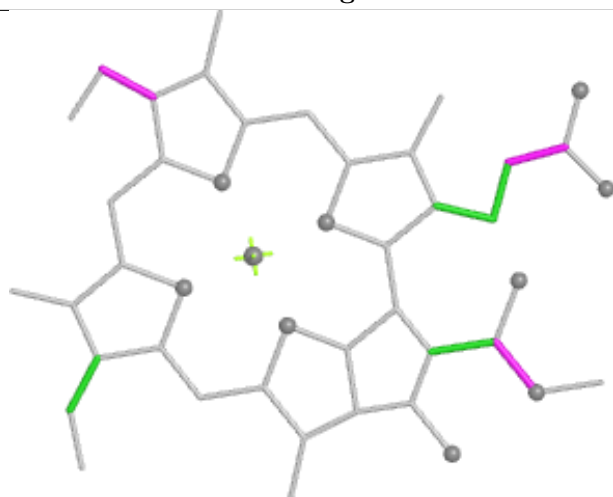
Ligand CLA 5 508



Bond lengths



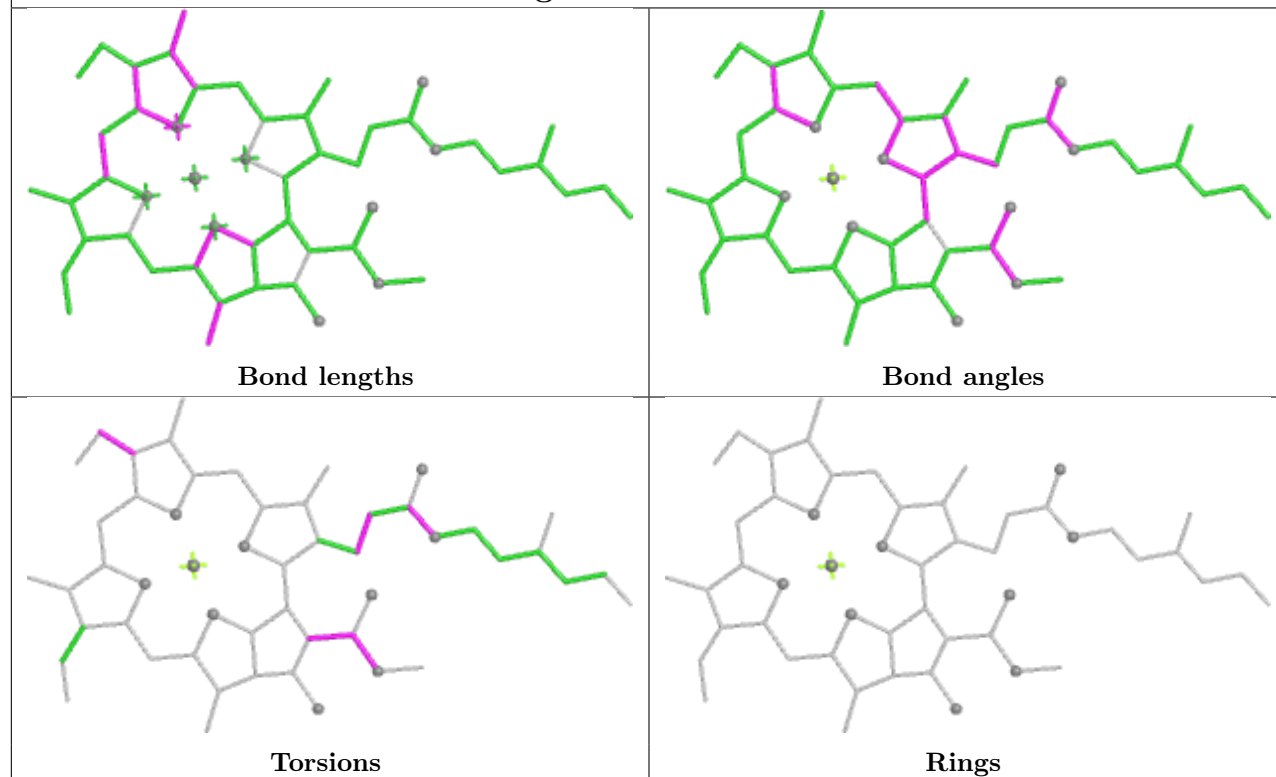
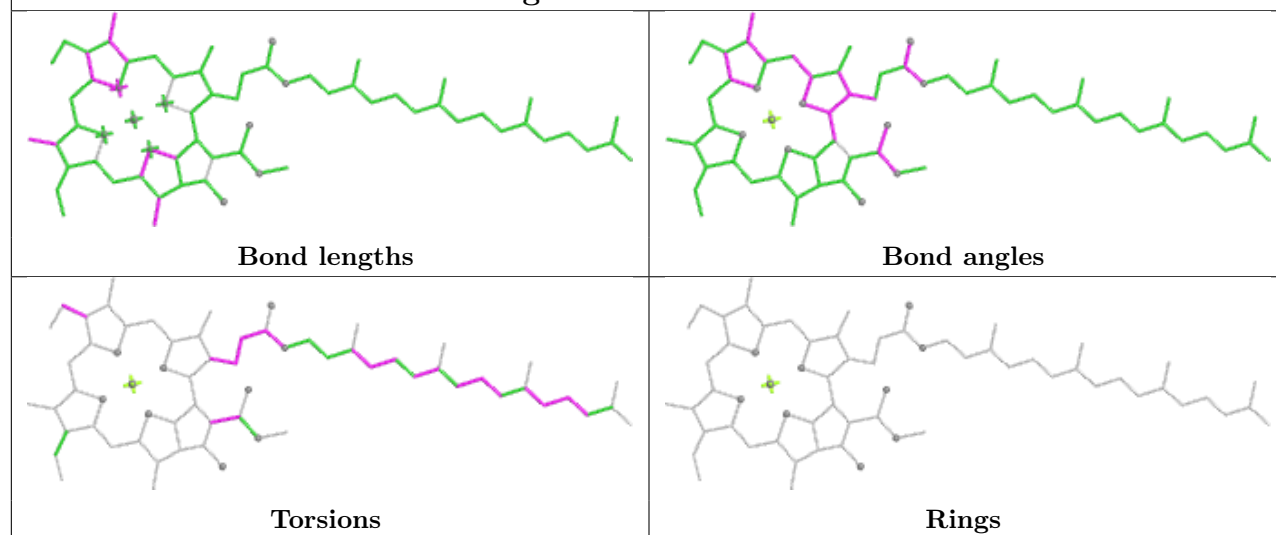
Bond angles

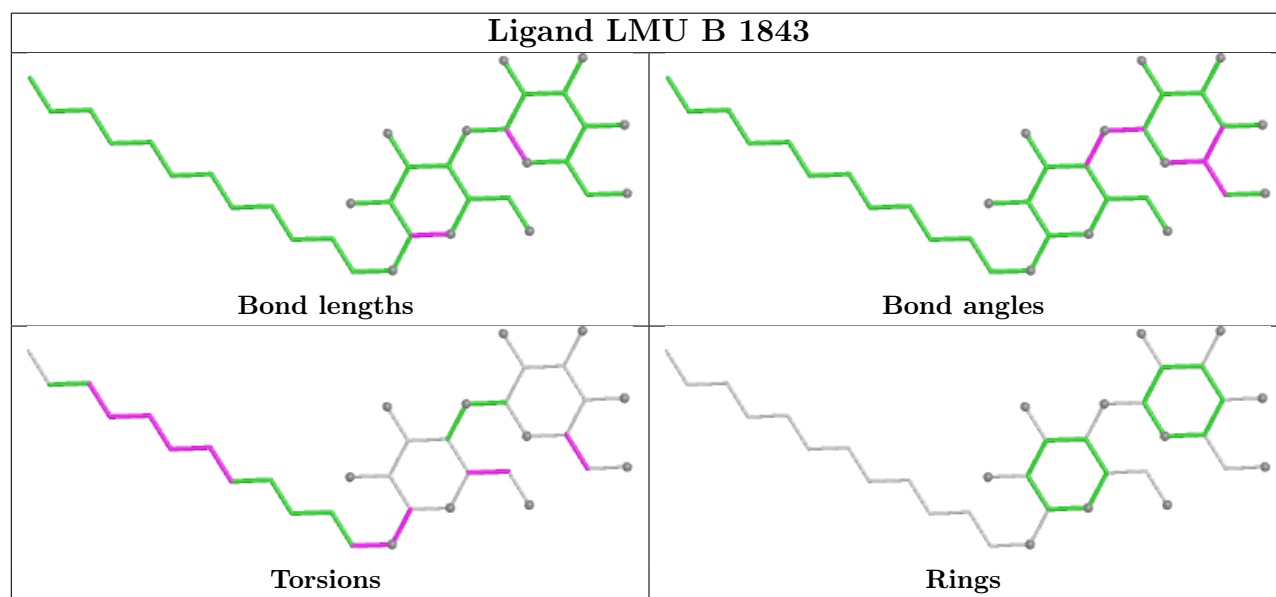
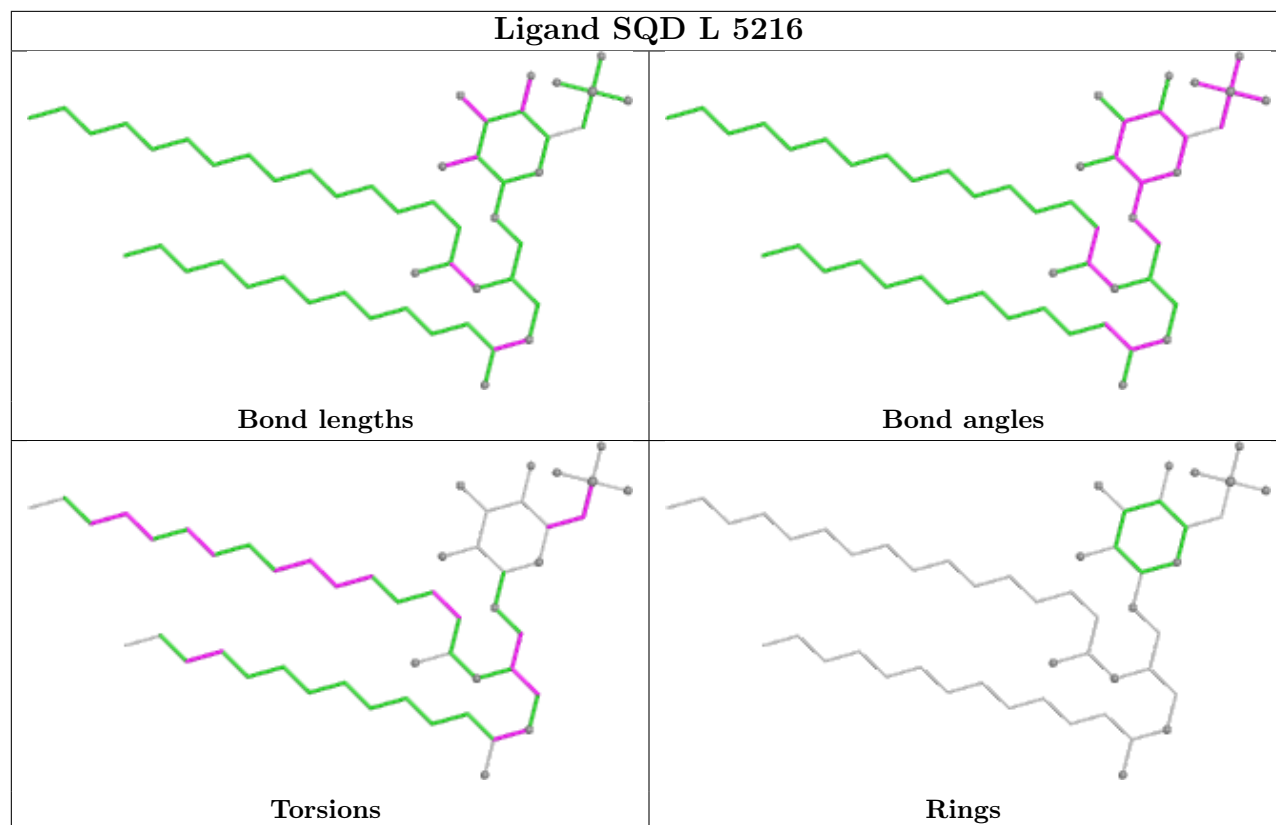


Torsions

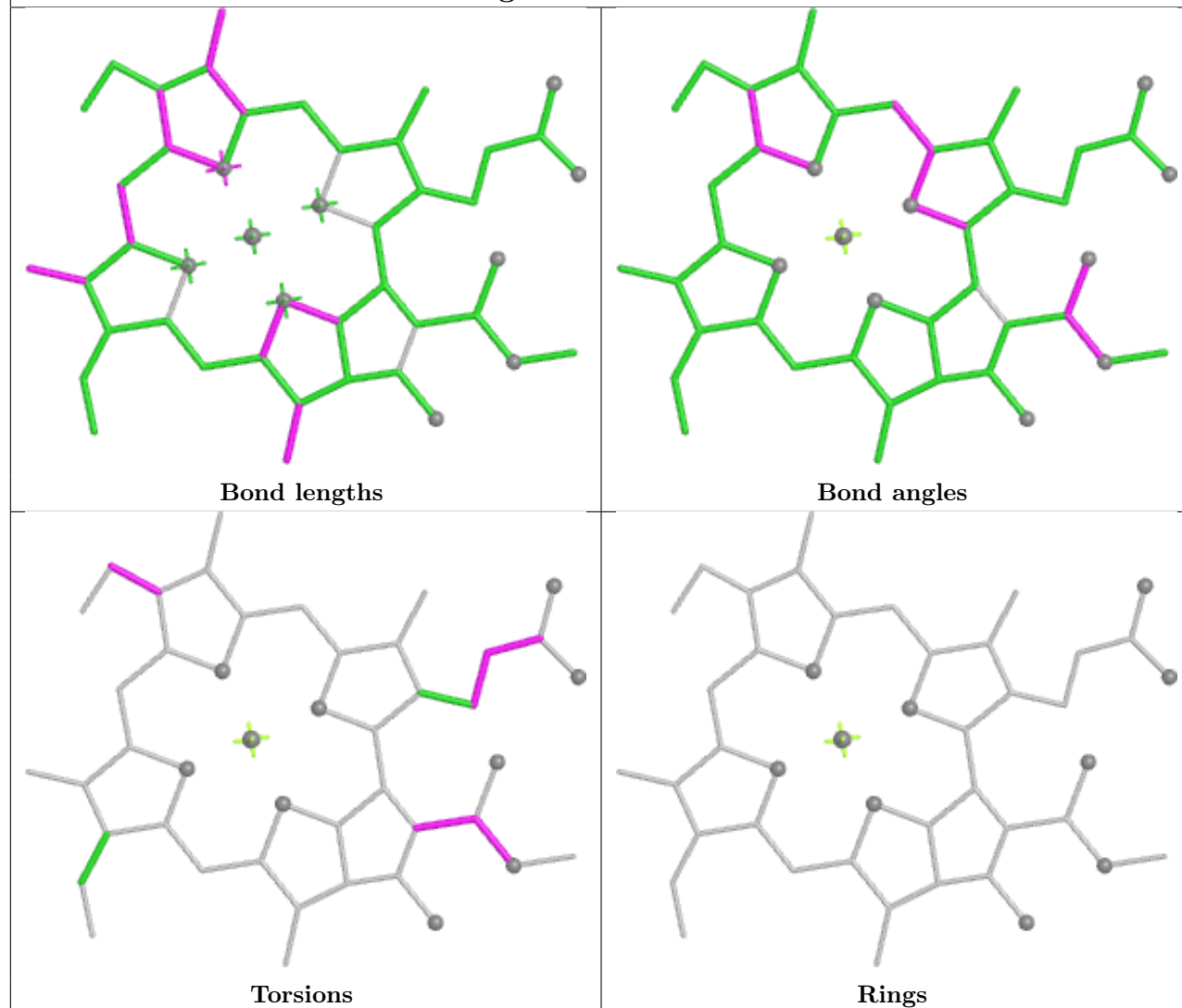


Rings

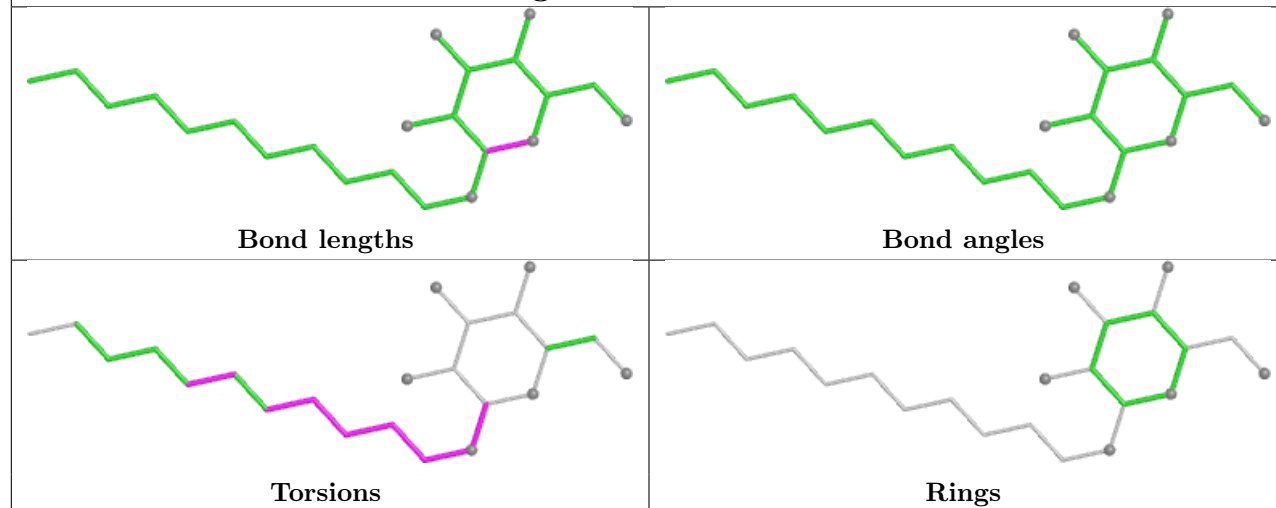
Ligand CLA d 503**Ligand CLA V 1501**

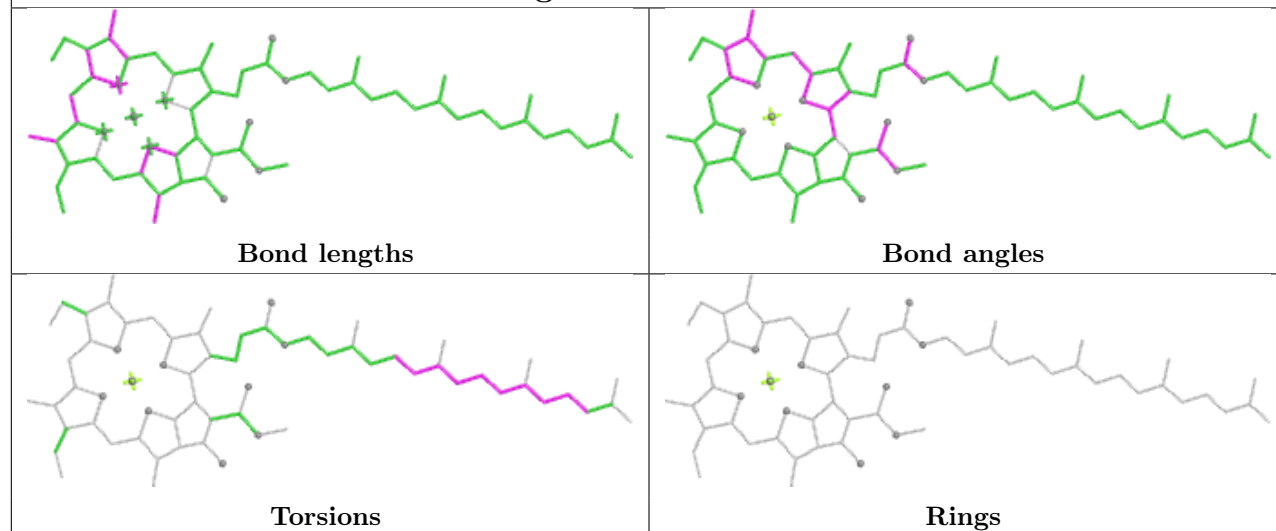
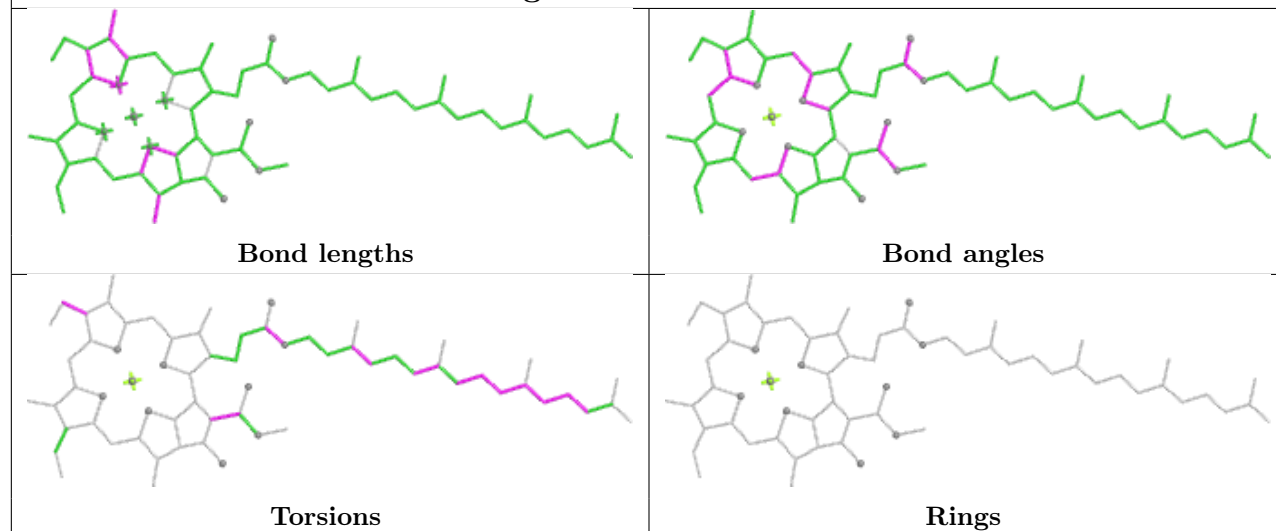


Ligand CLA t 513

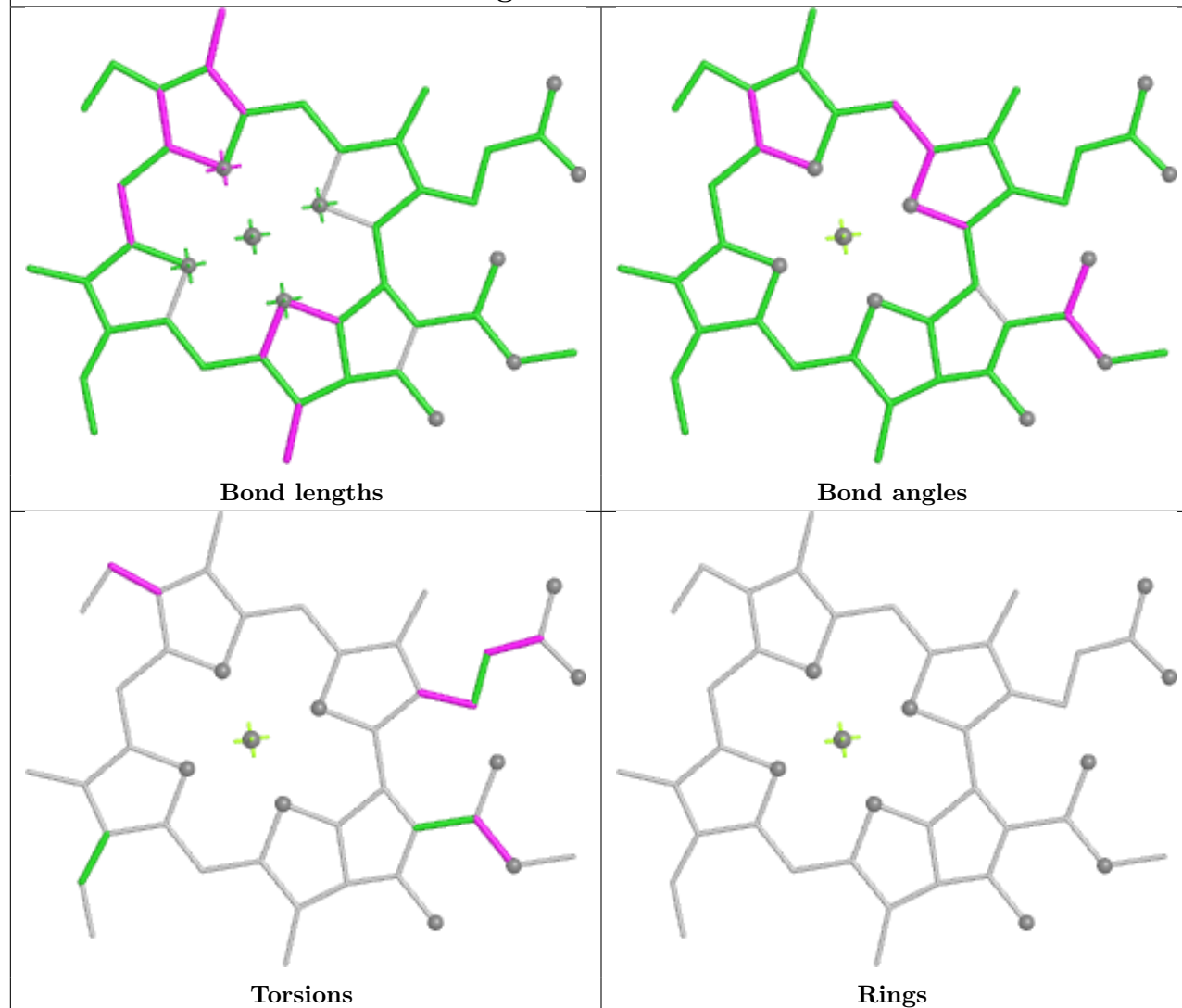


Ligand LMU 2 901

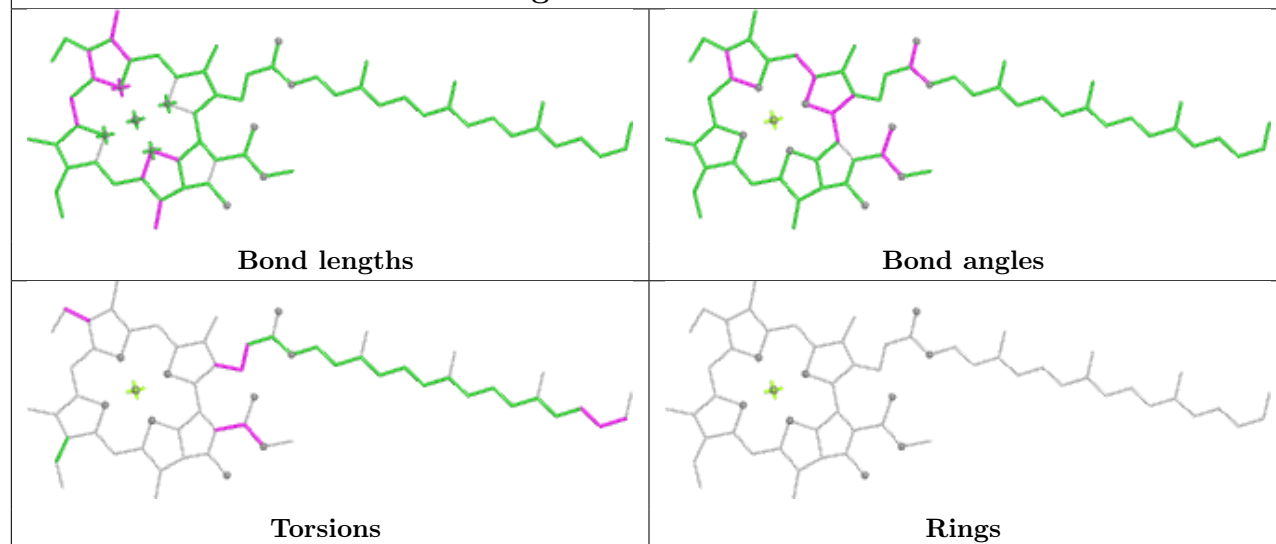


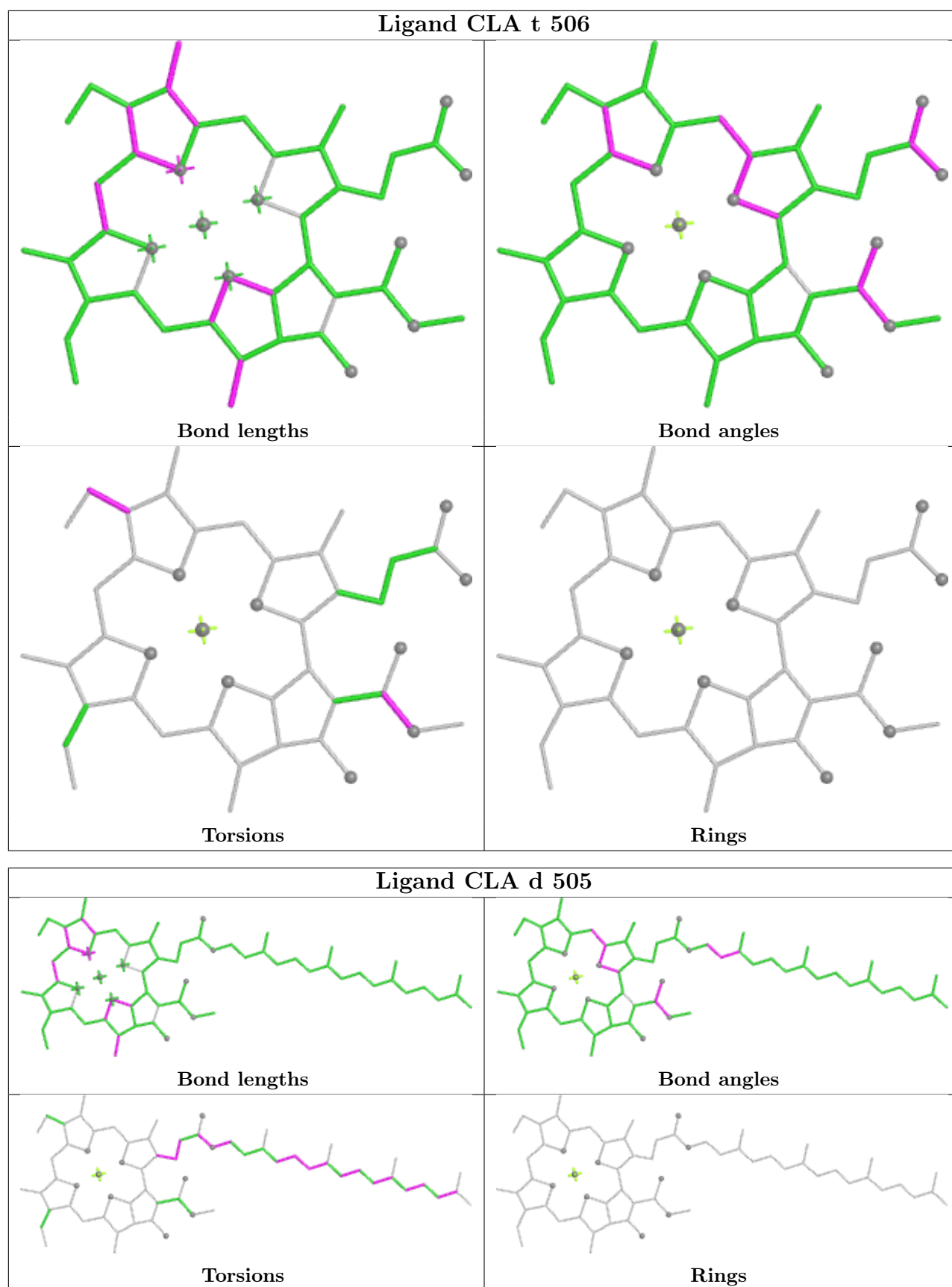
Ligand CLA u 509**Ligand CLA B 1208**

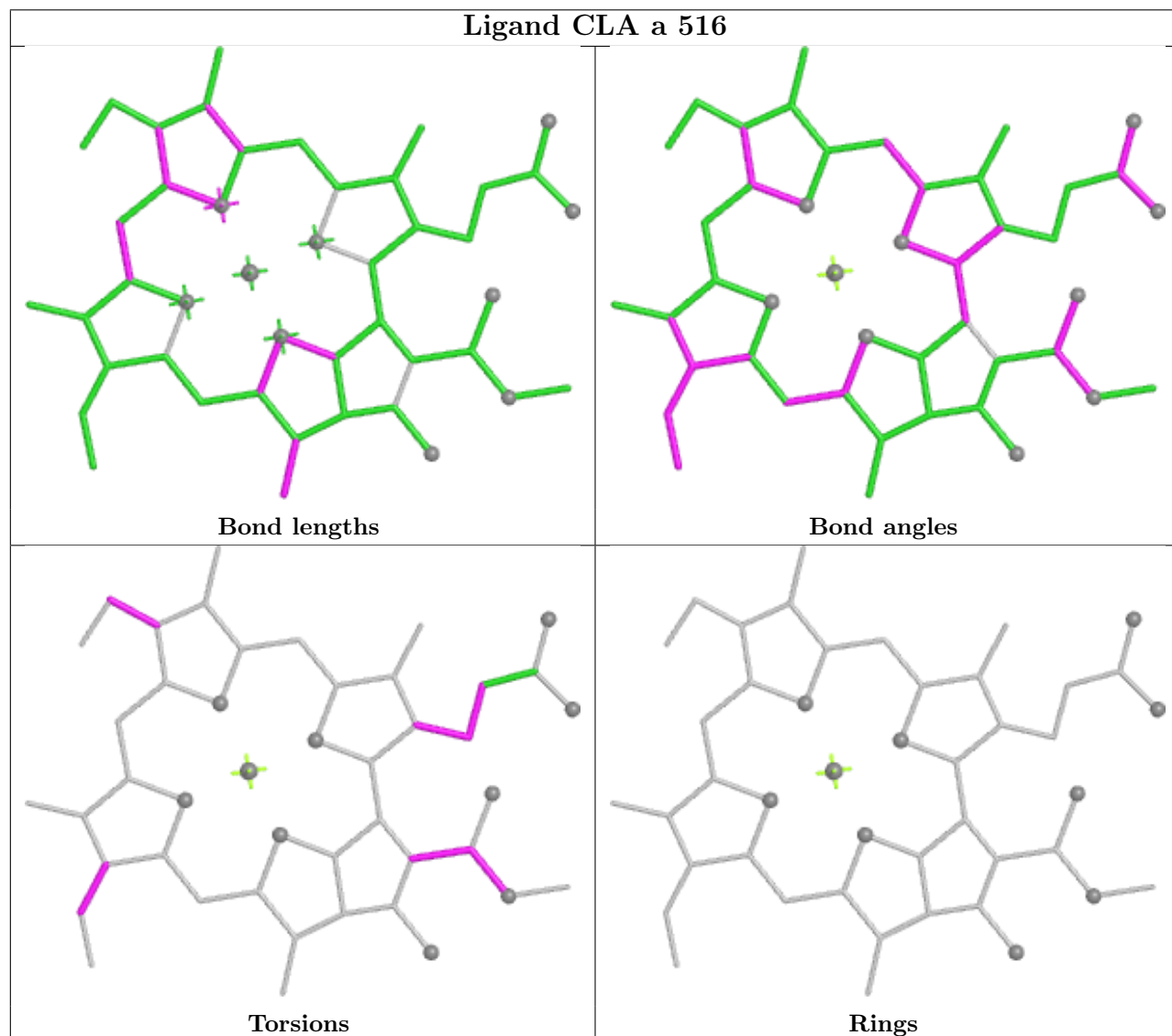
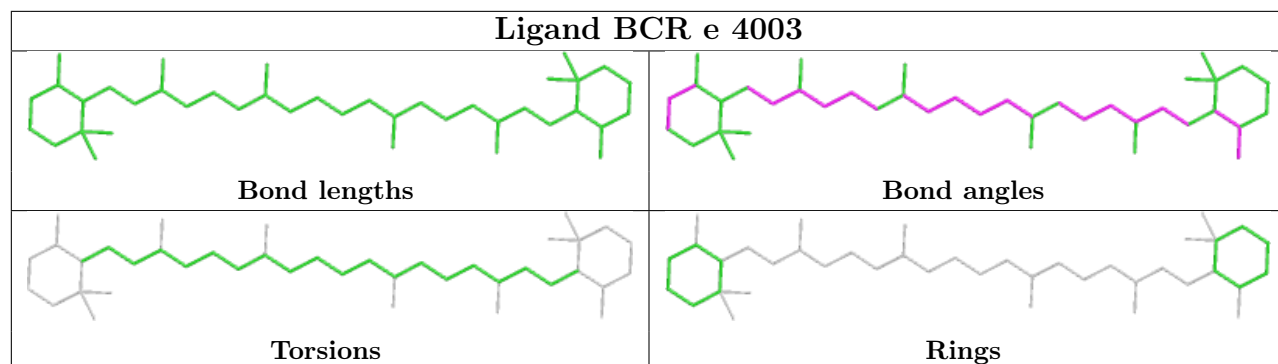
Ligand CLA 6 512

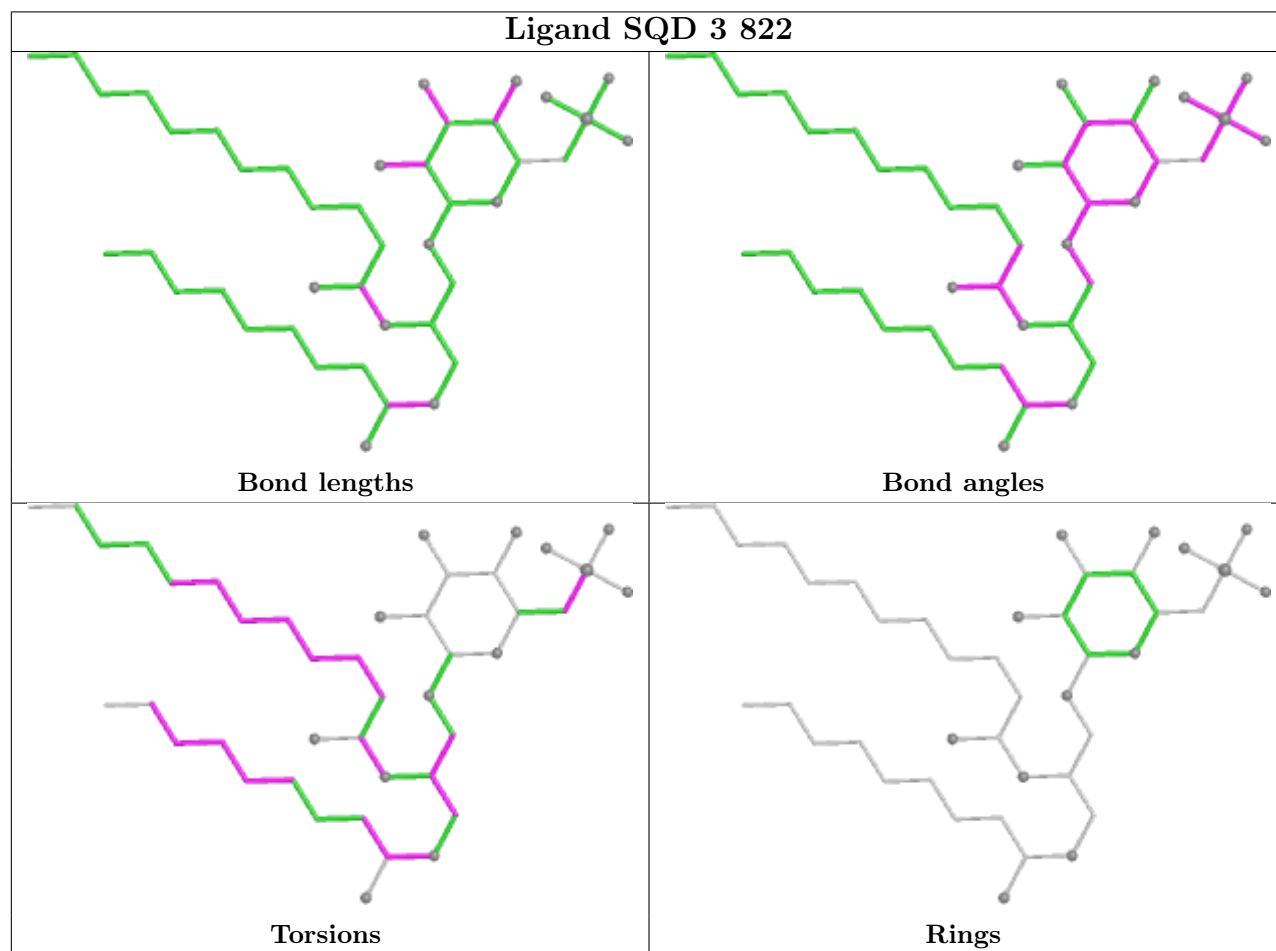
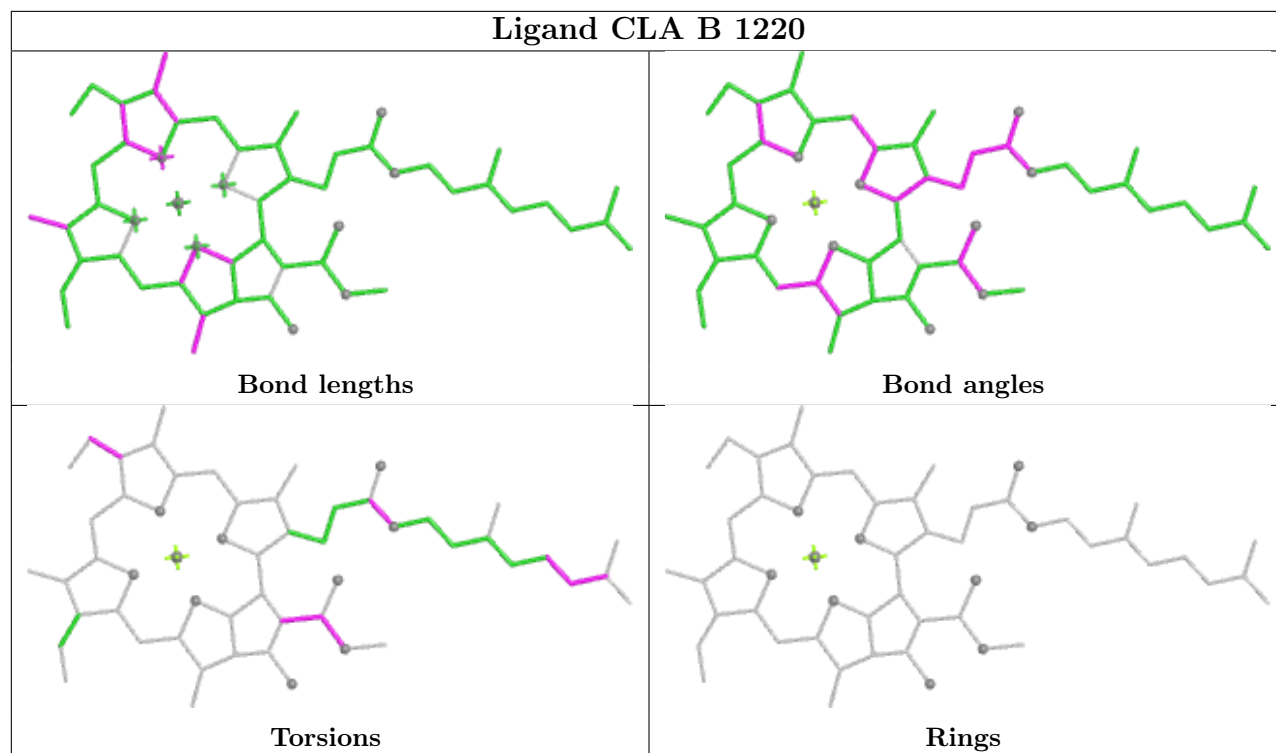


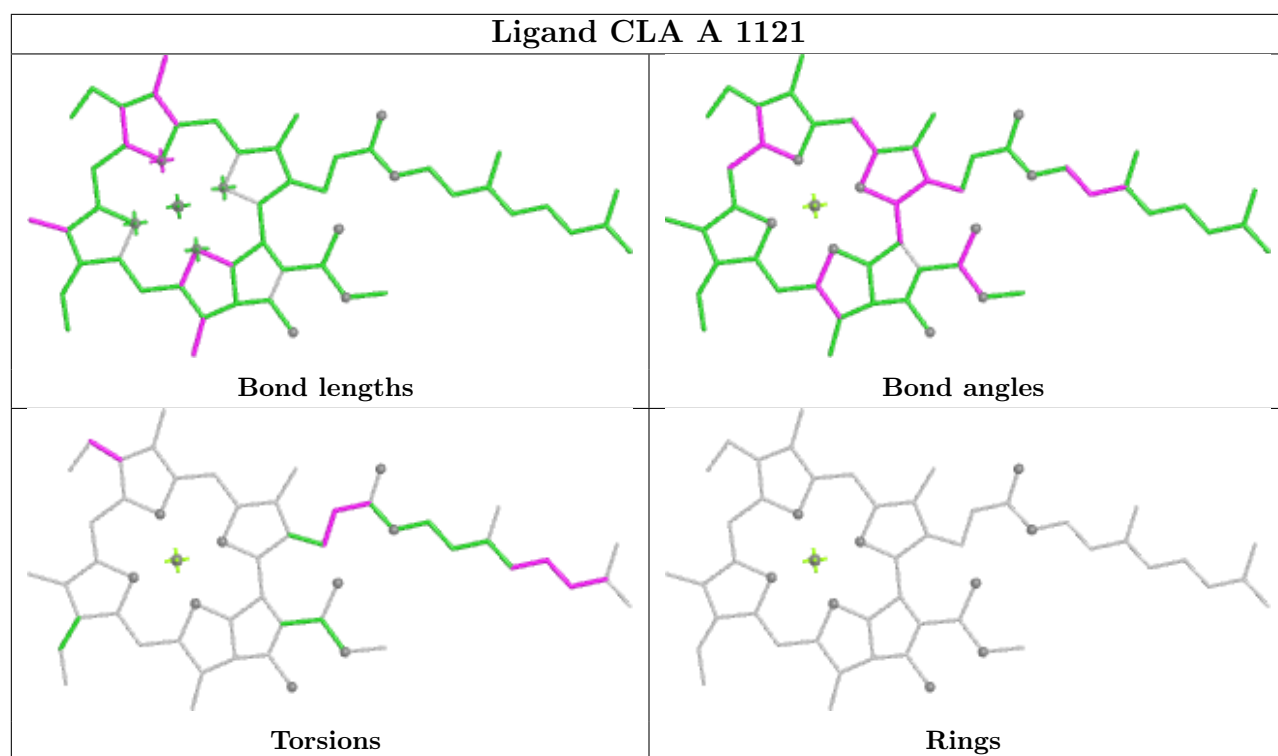
Ligand CLA Y 503

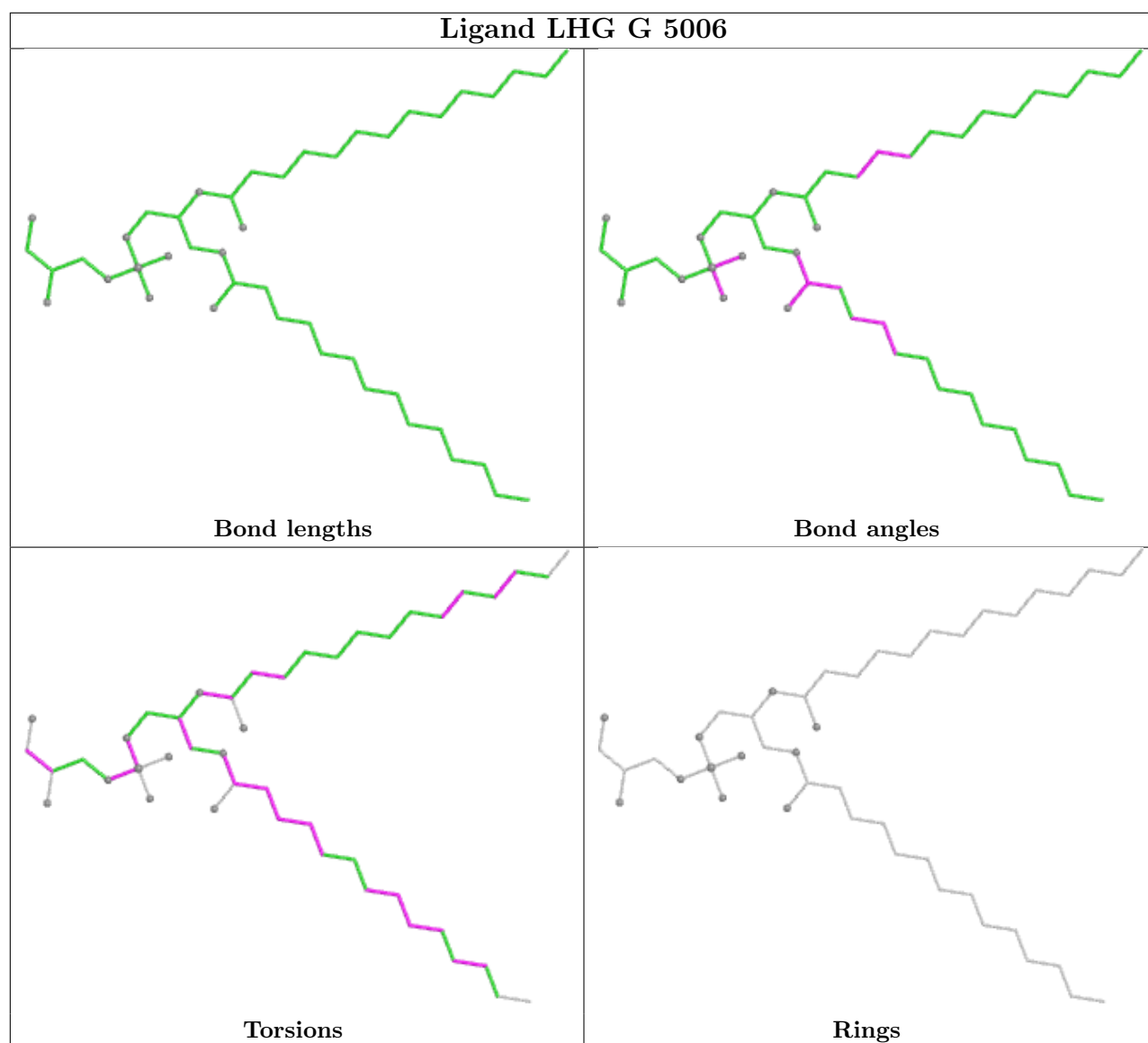


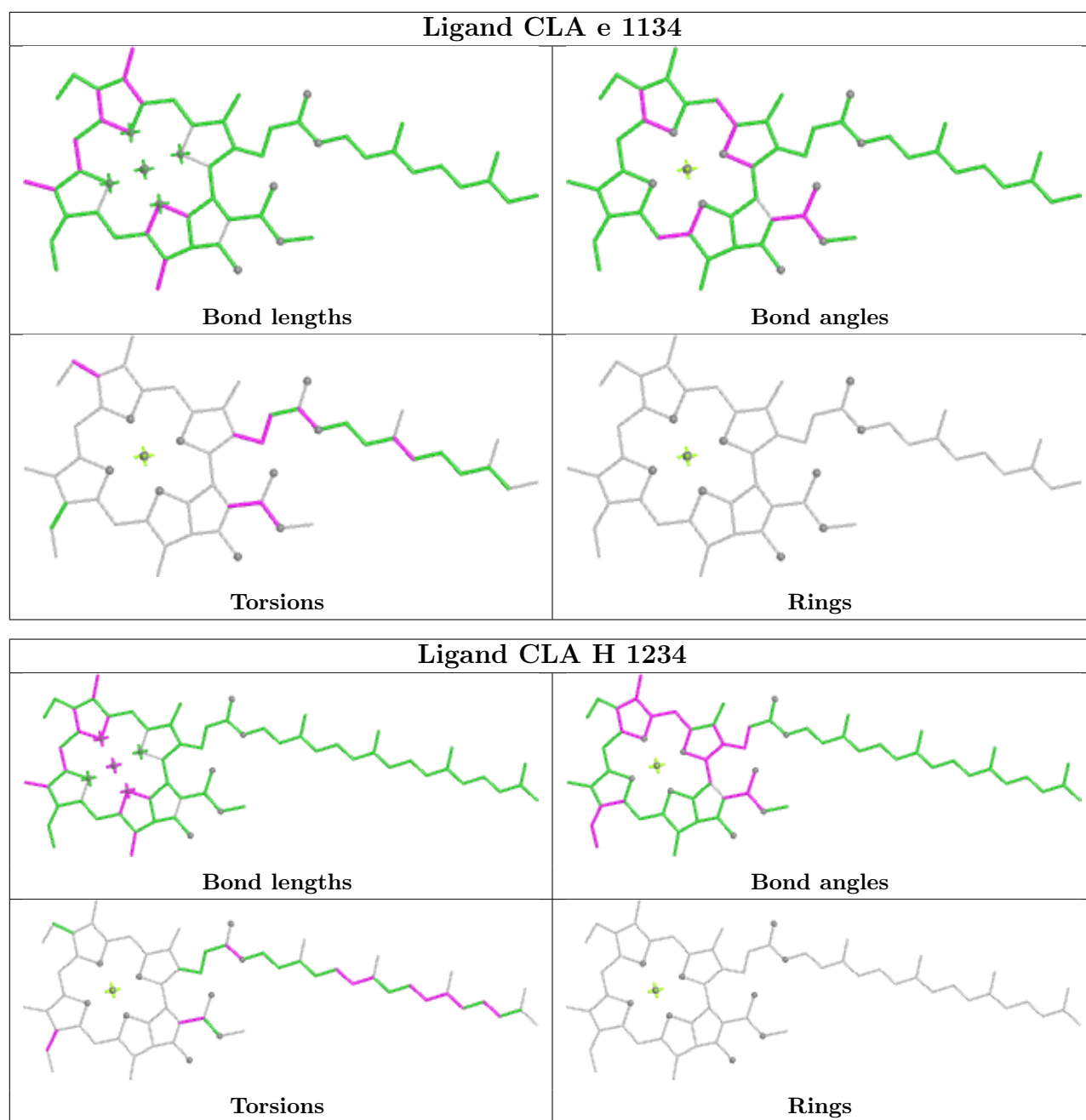




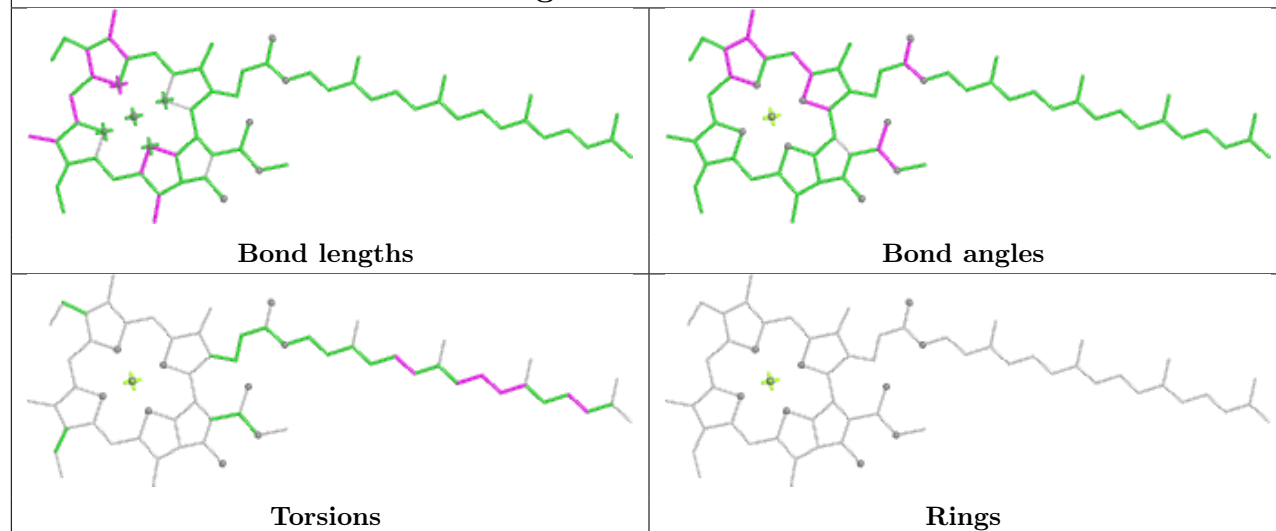




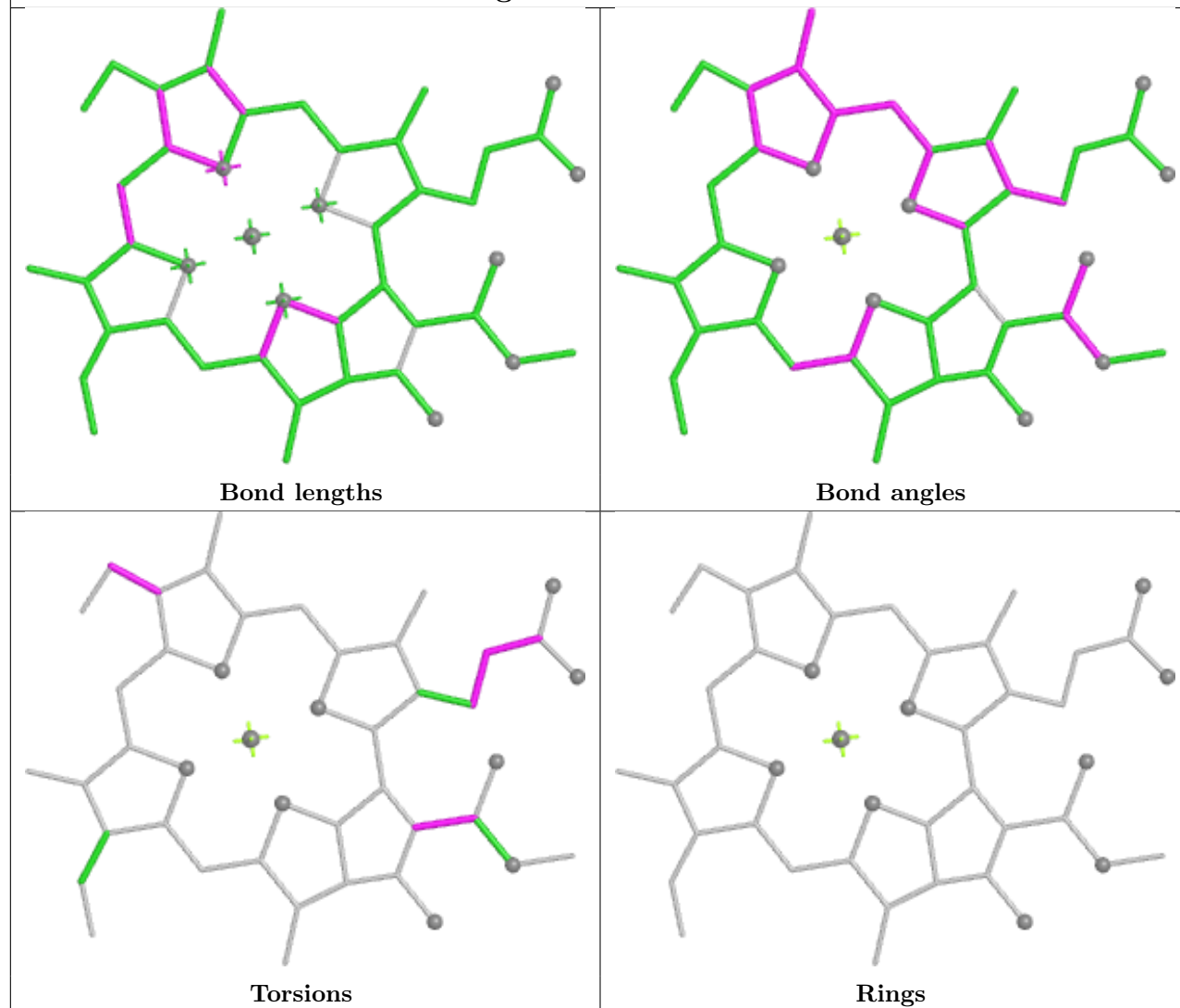


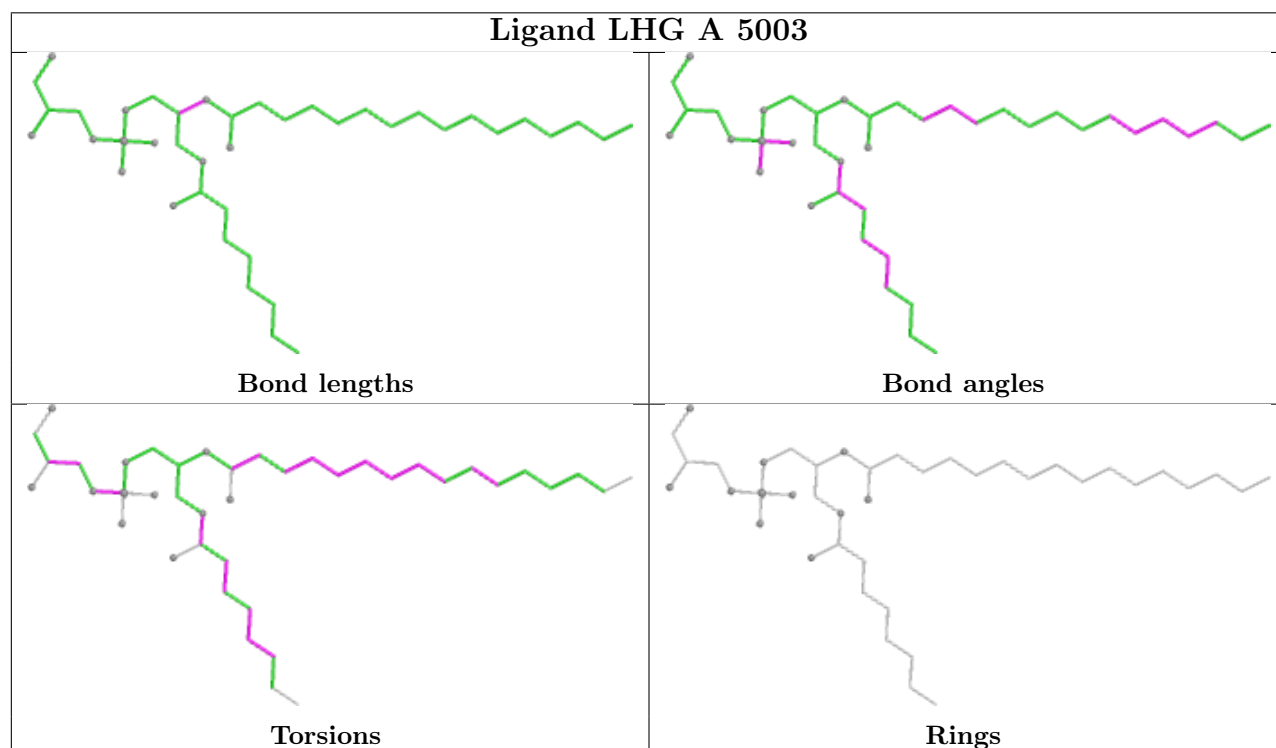
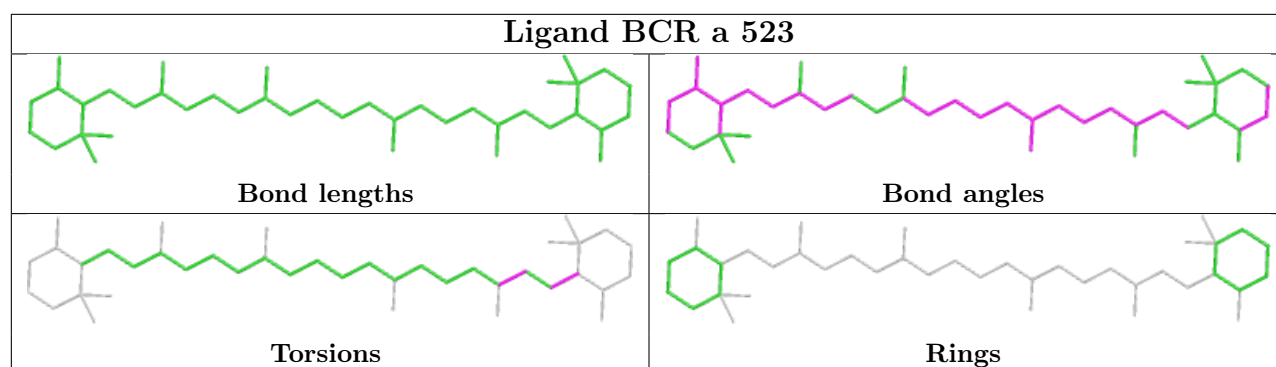


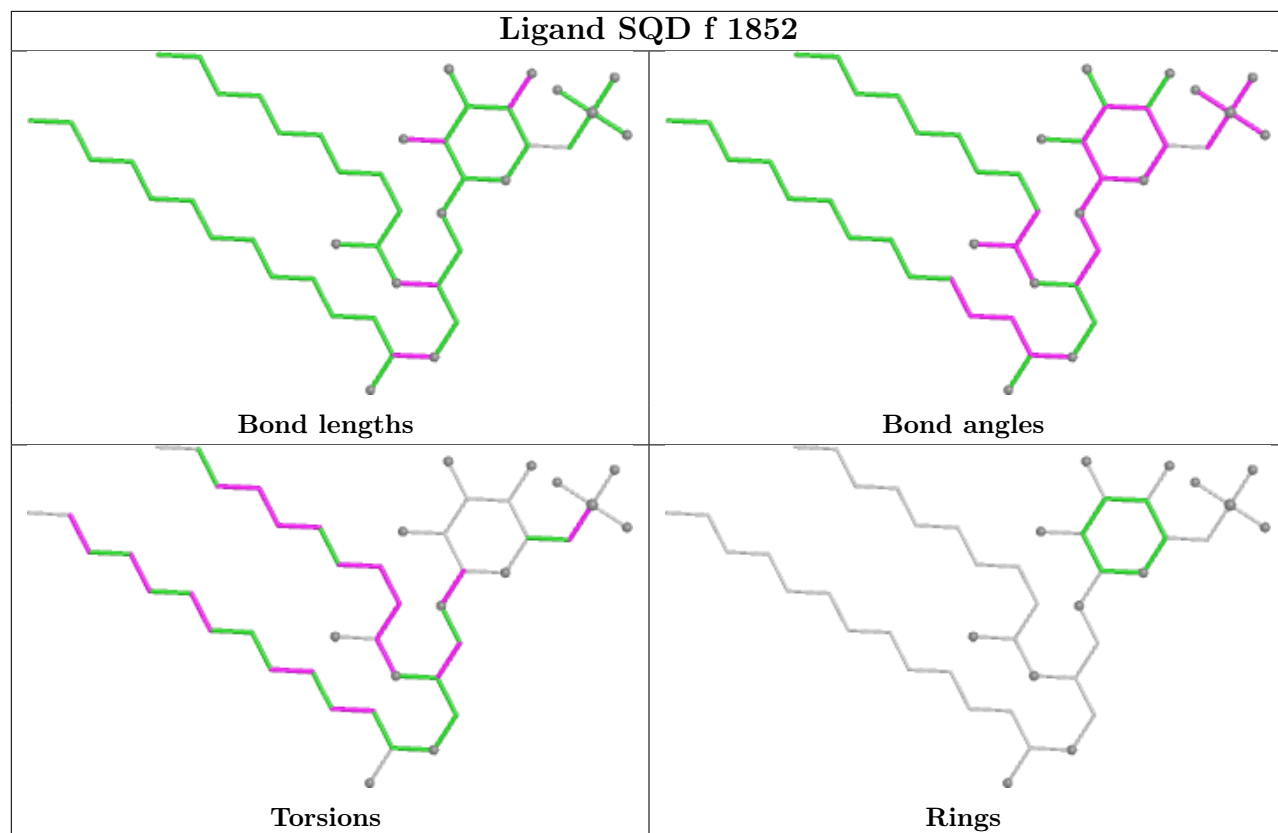
Ligand CLA 1 509



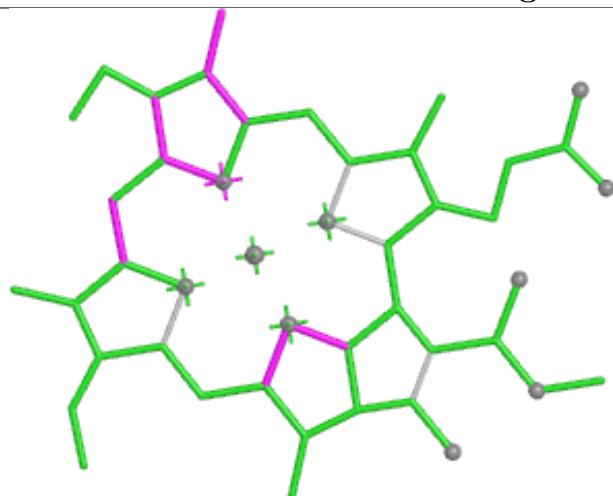
Ligand CLA 6 504



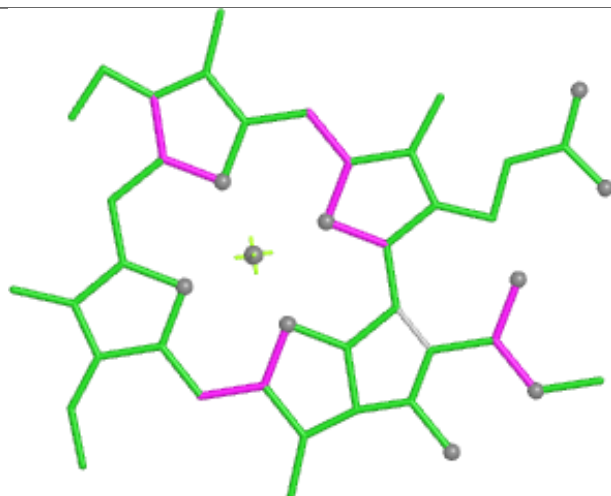




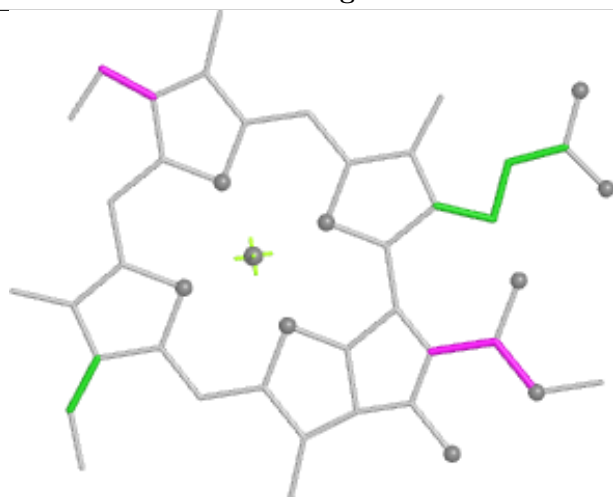
Ligand CLA c 504



Bond lengths



Bond angles

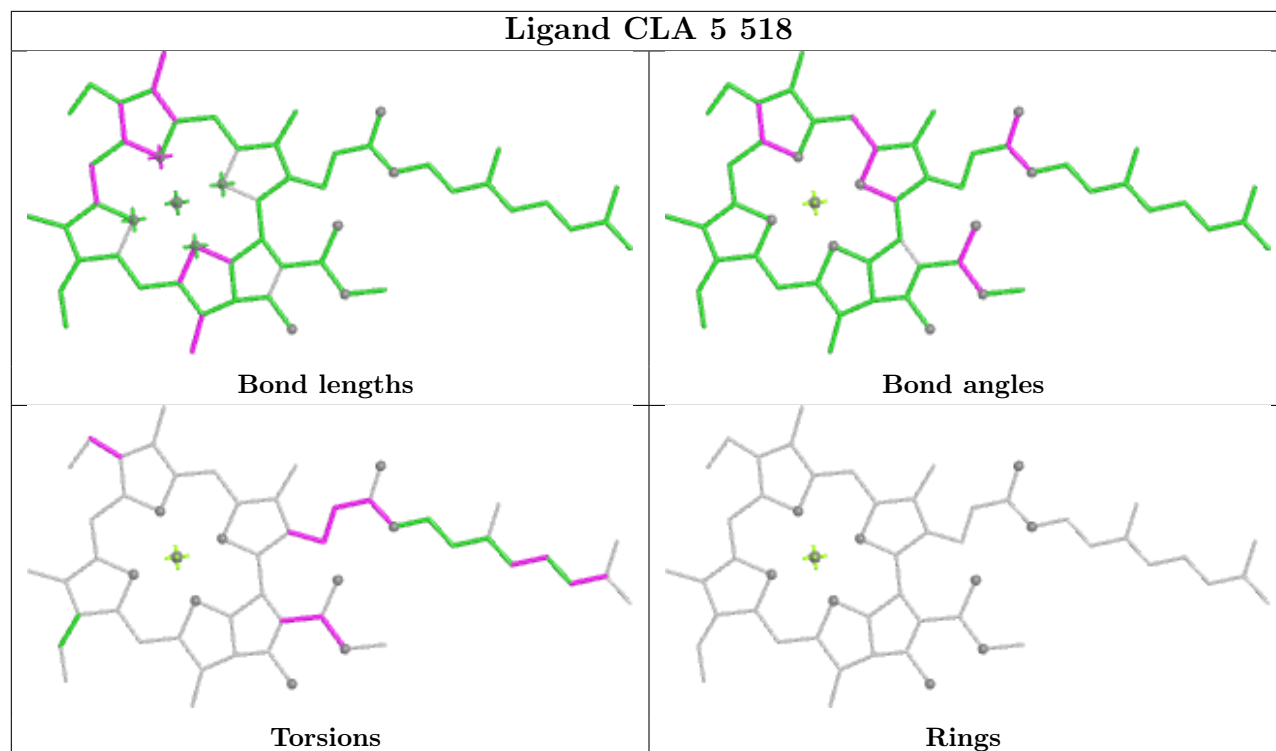


Torsions

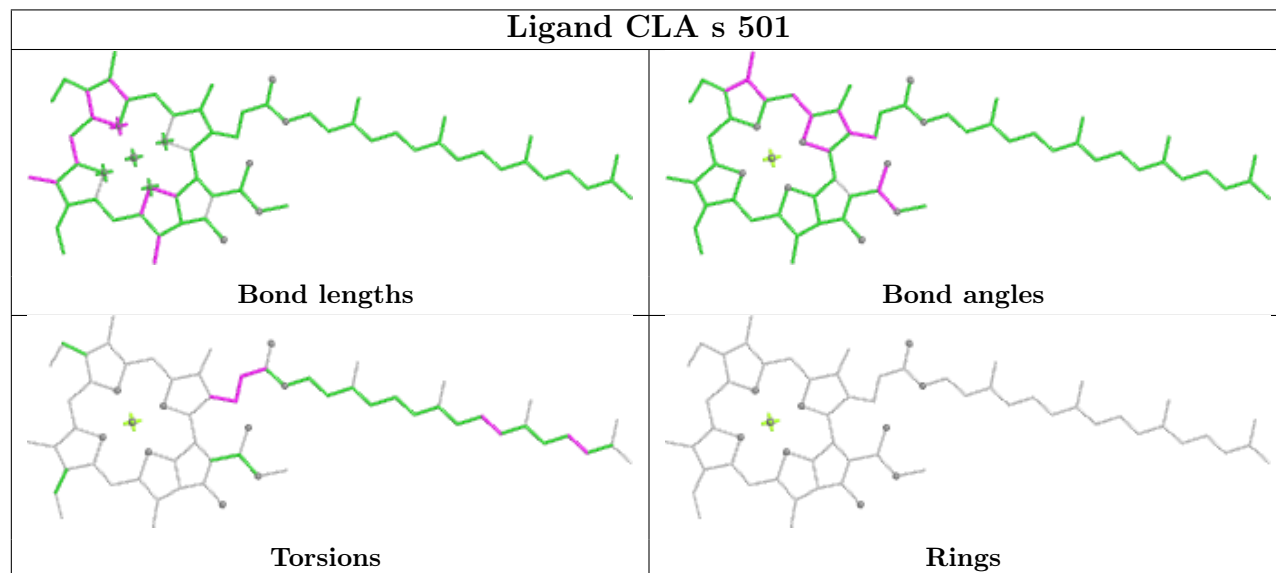


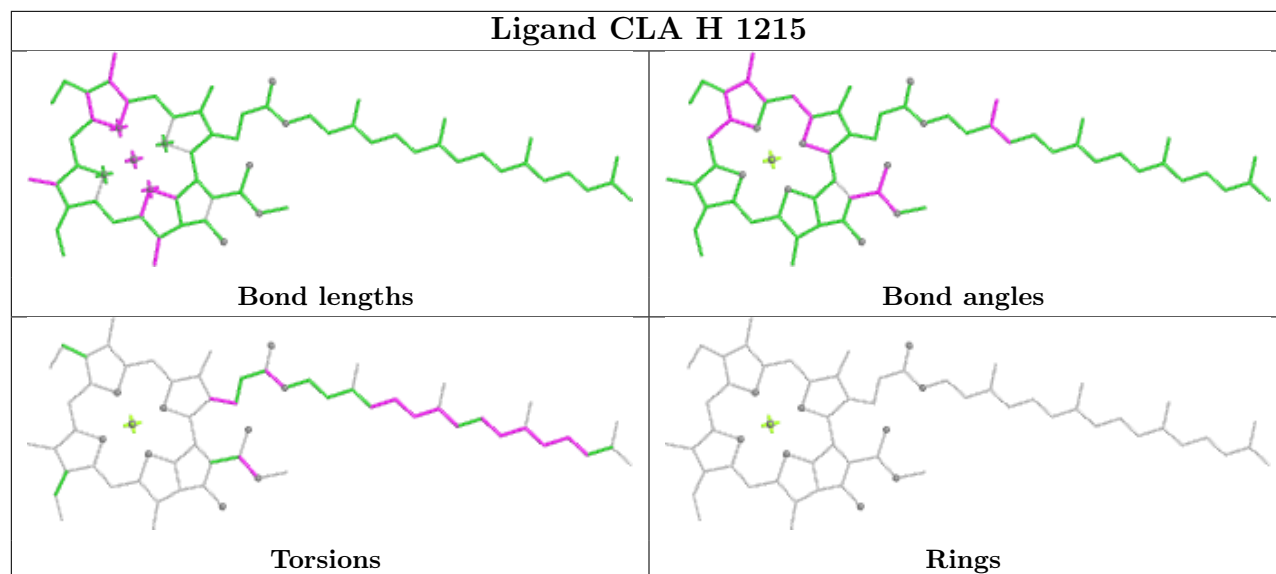
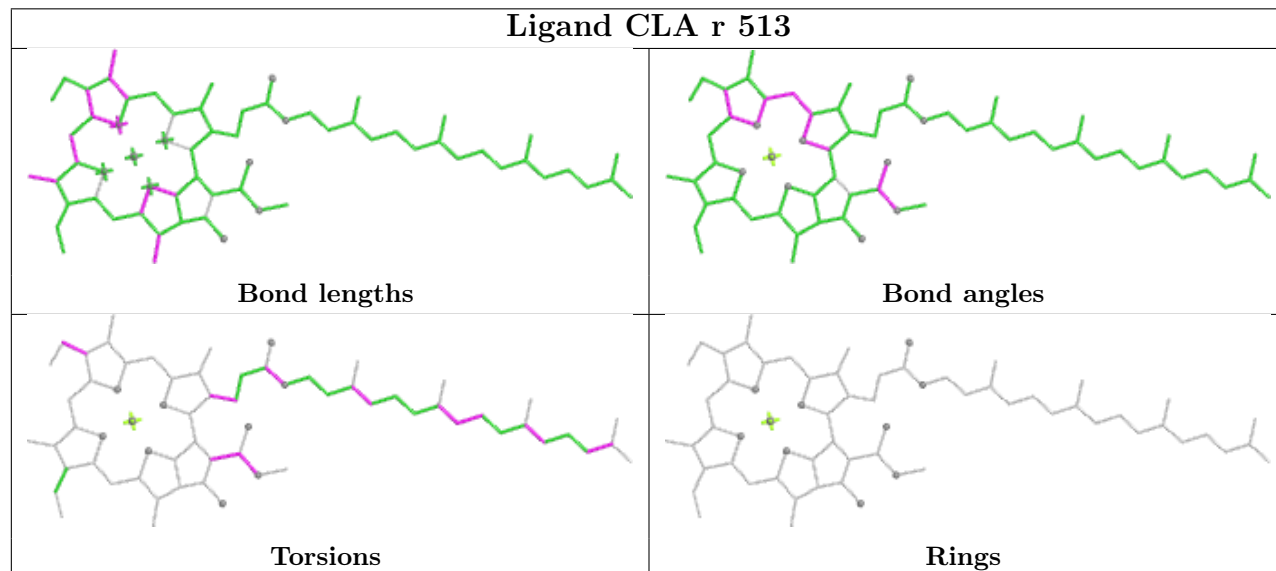
Rings

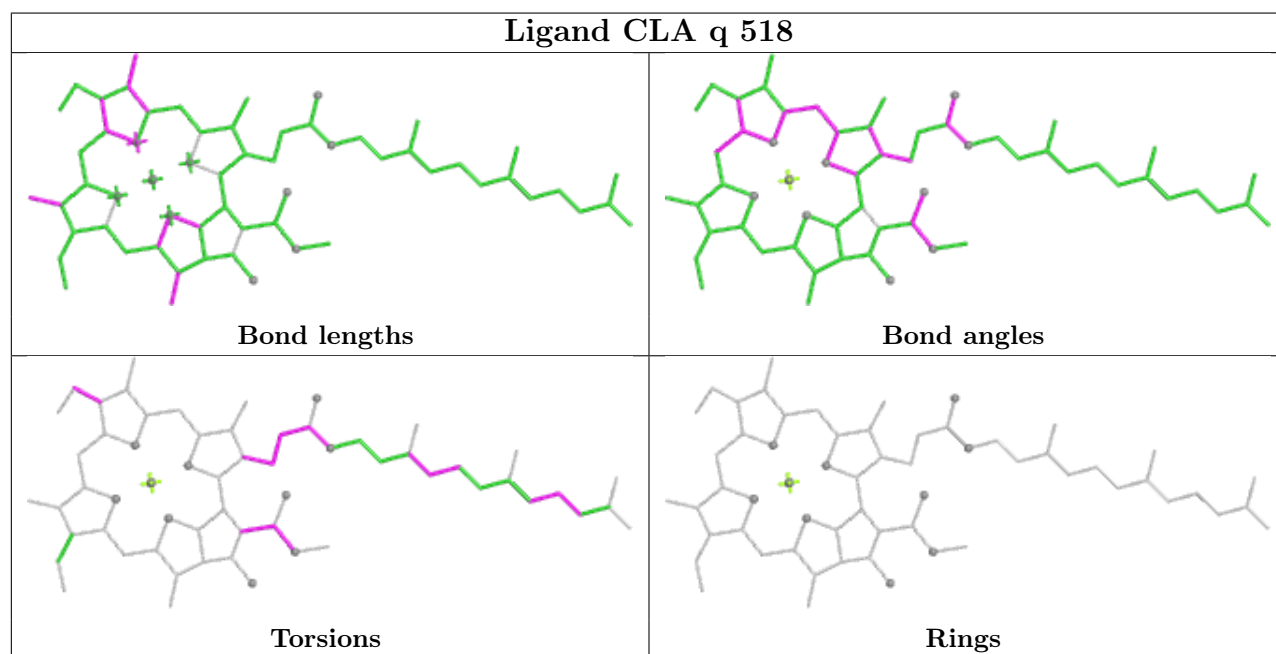
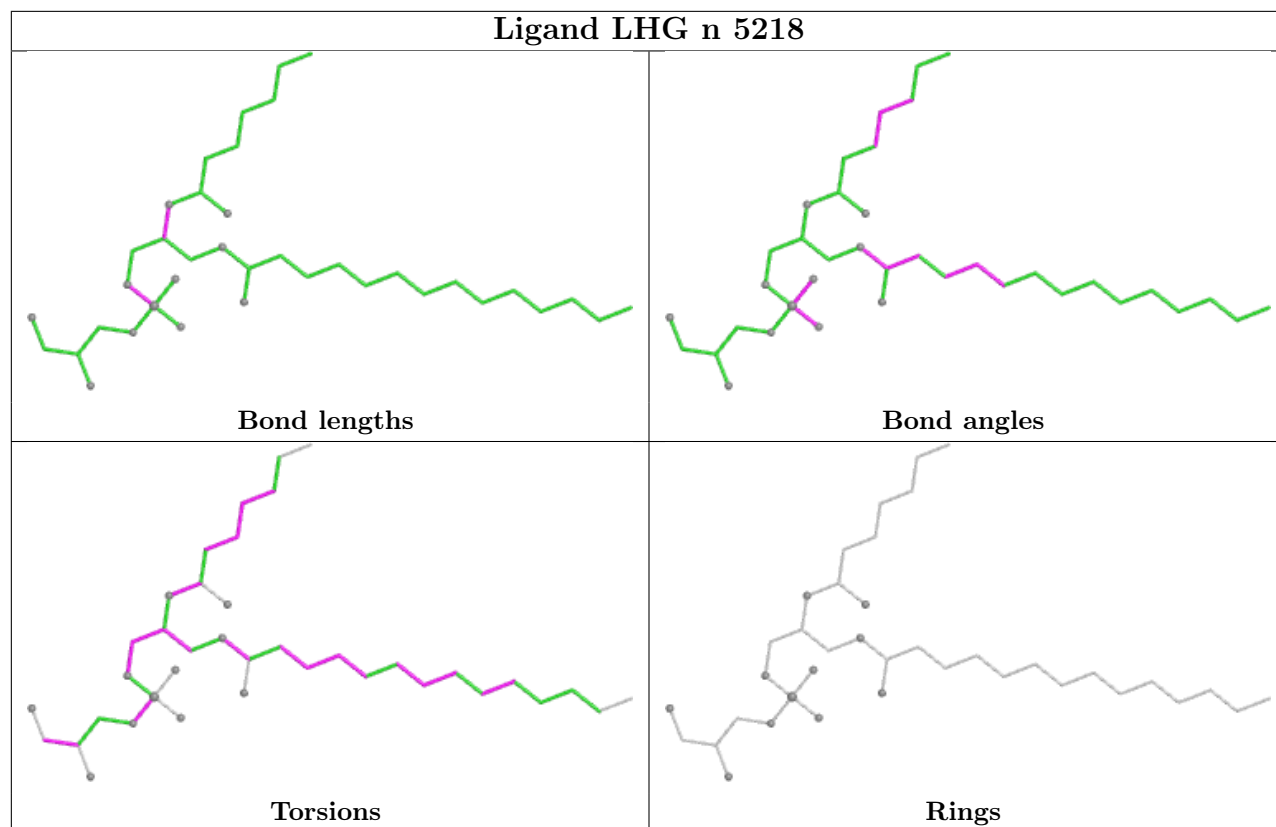
Ligand CLA 5 518

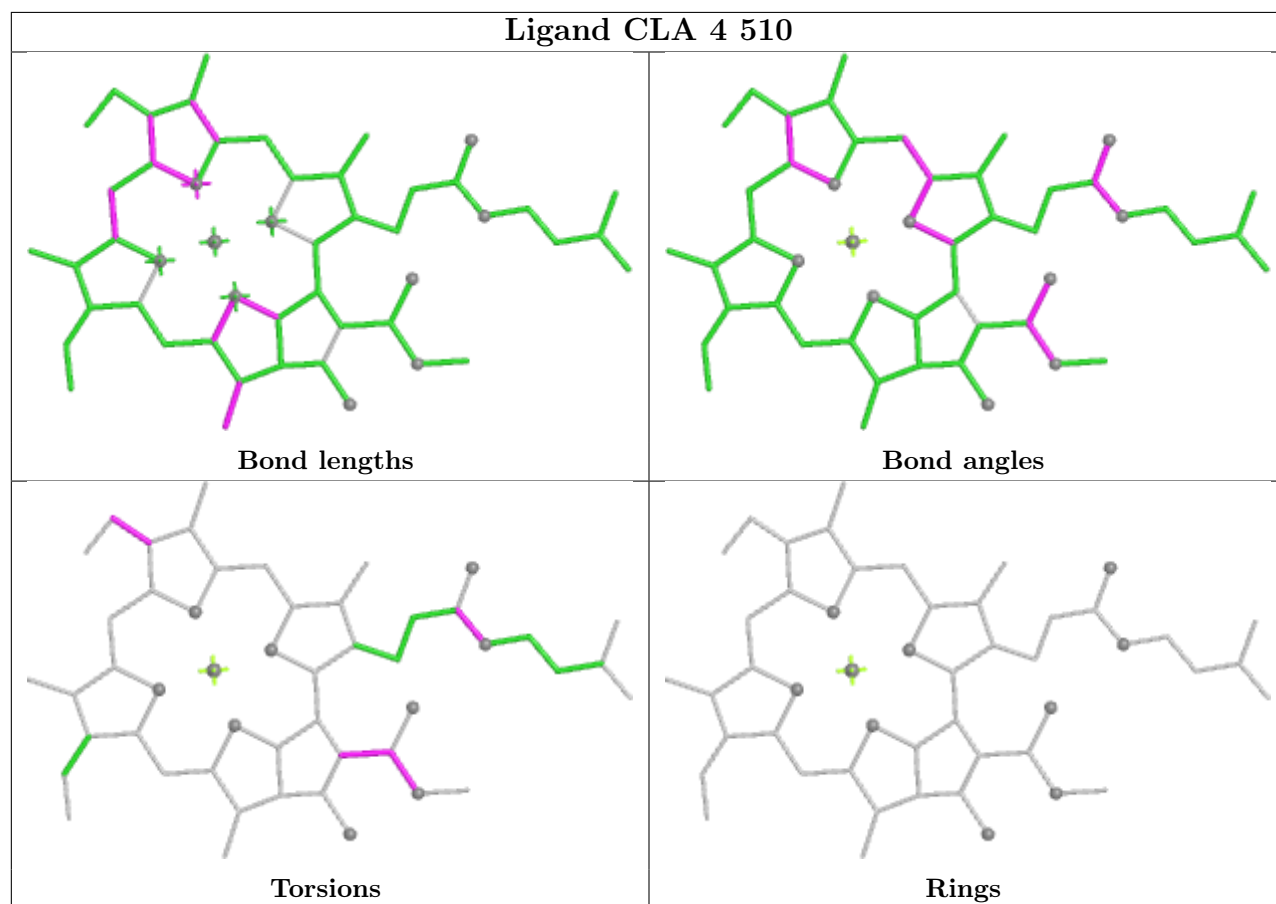
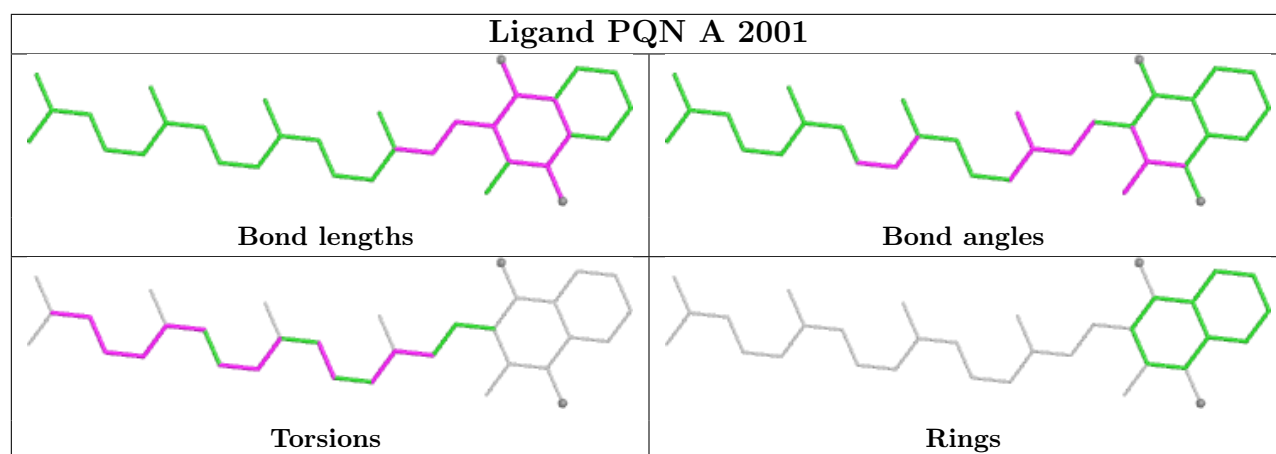


Ligand CLA s 501

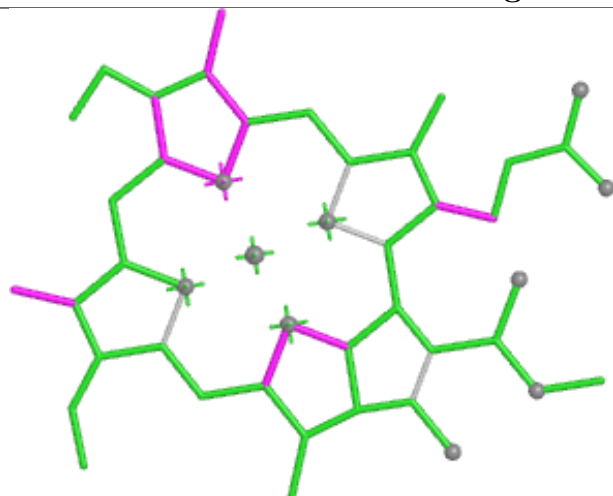


Ligand CLA H 1215**Ligand CLA r 513**

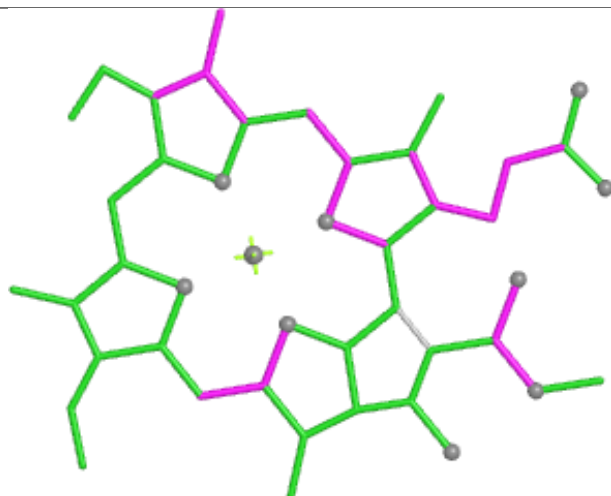




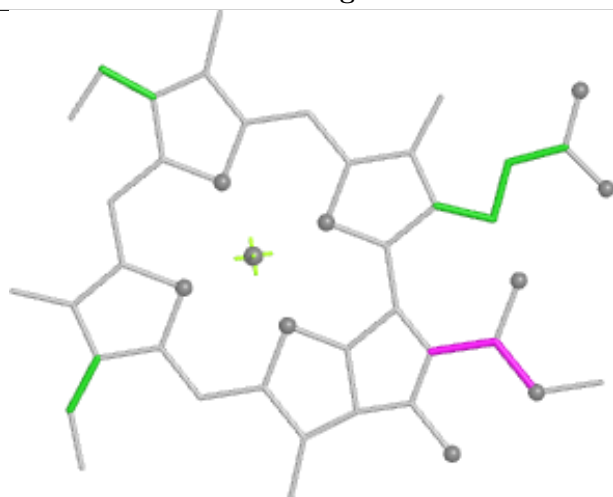
Ligand CLA G 1801



Bond lengths



Bond angles

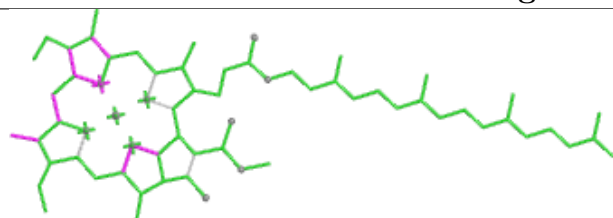


Torsions

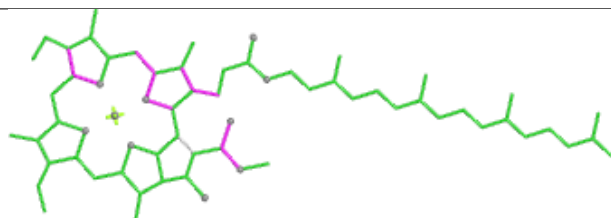


Rings

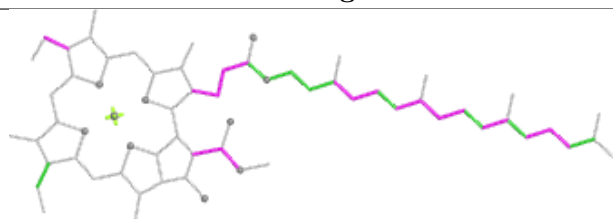
Ligand CLA 5 501



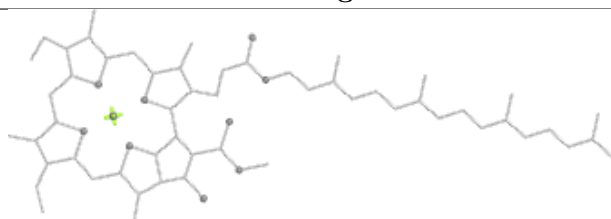
Bond lengths



Bond angles

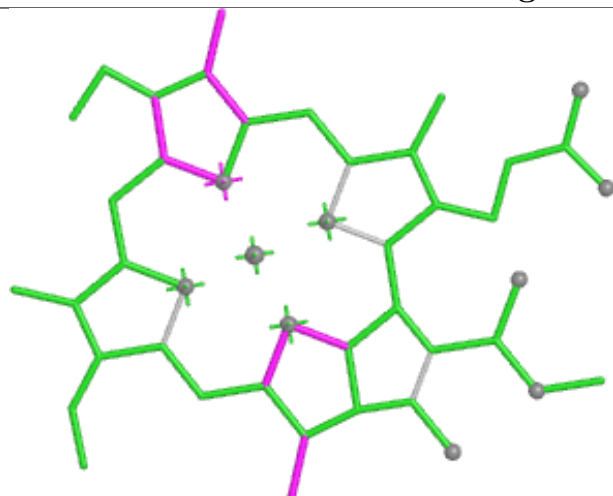


Torsions

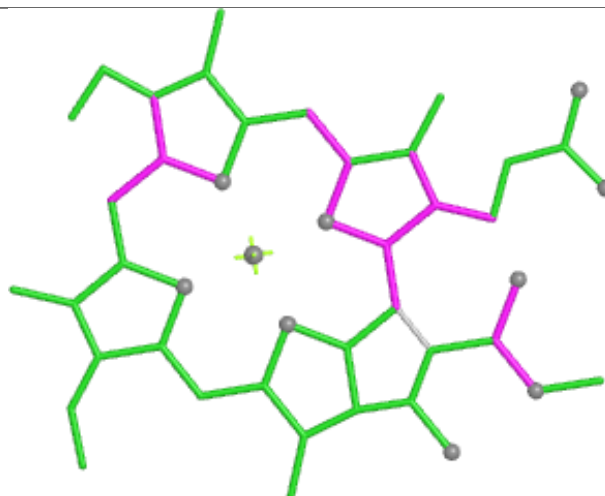


Rings

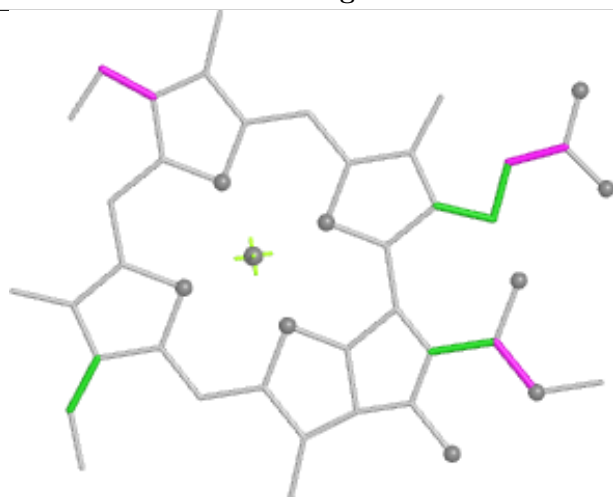
Ligand CLA 6 507



Bond lengths



Bond angles

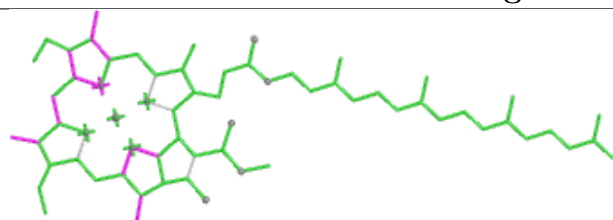


Torsions

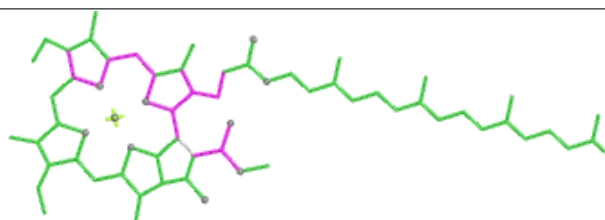


Rings

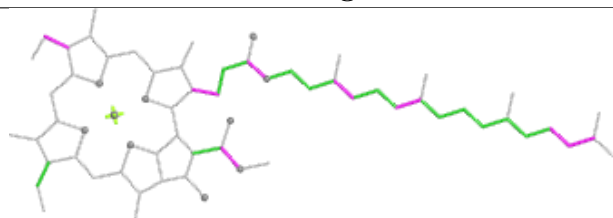
Ligand CLA G 1140



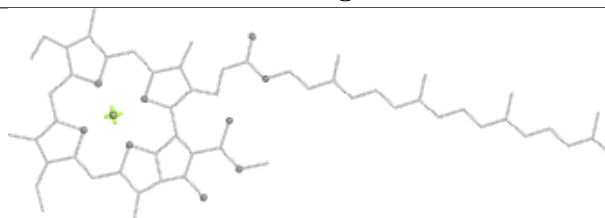
Bond lengths



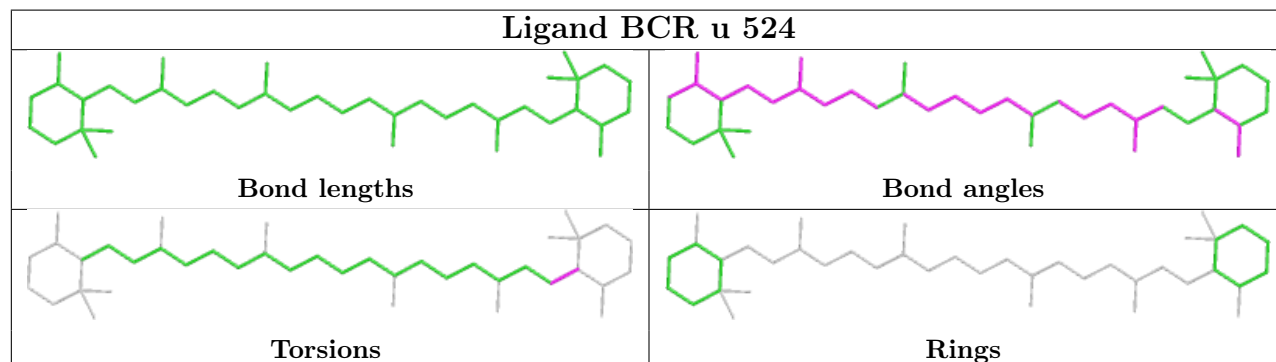
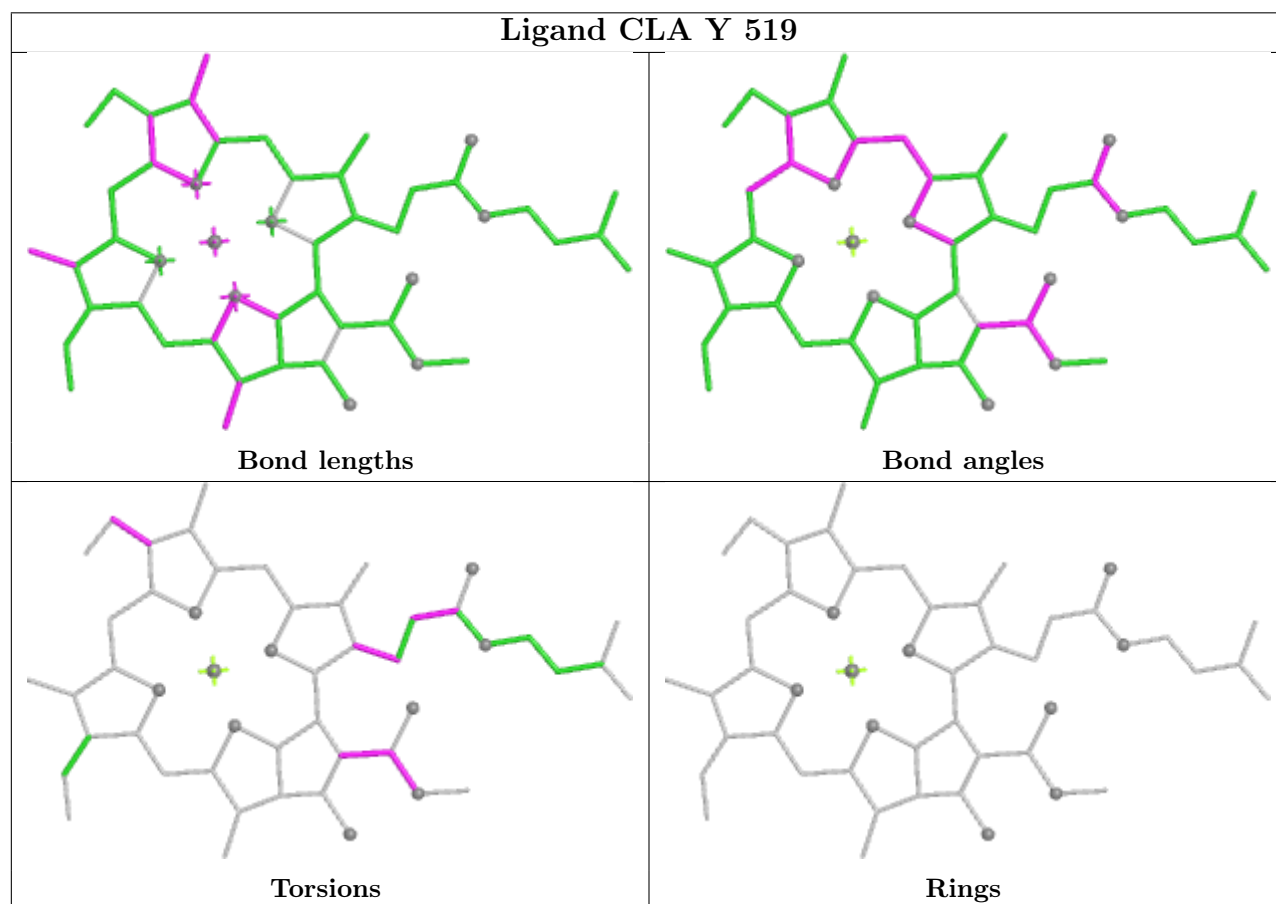
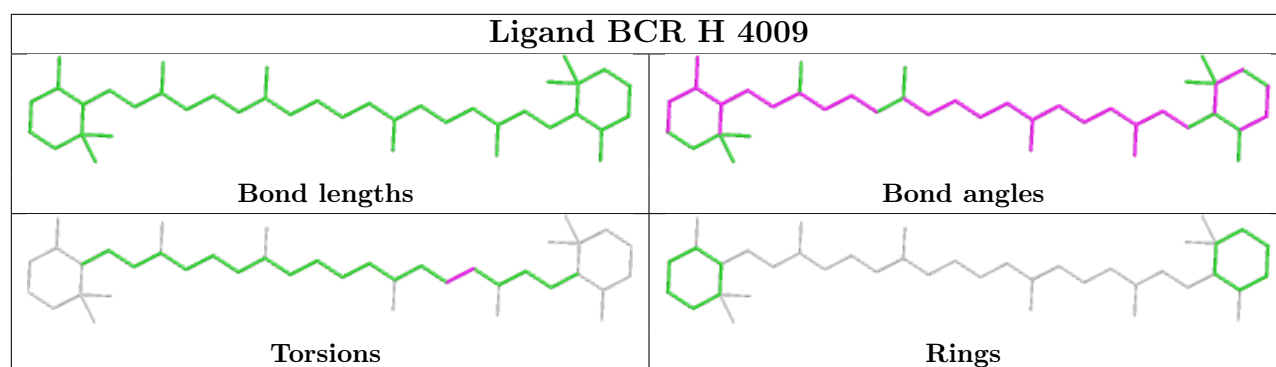
Bond angles

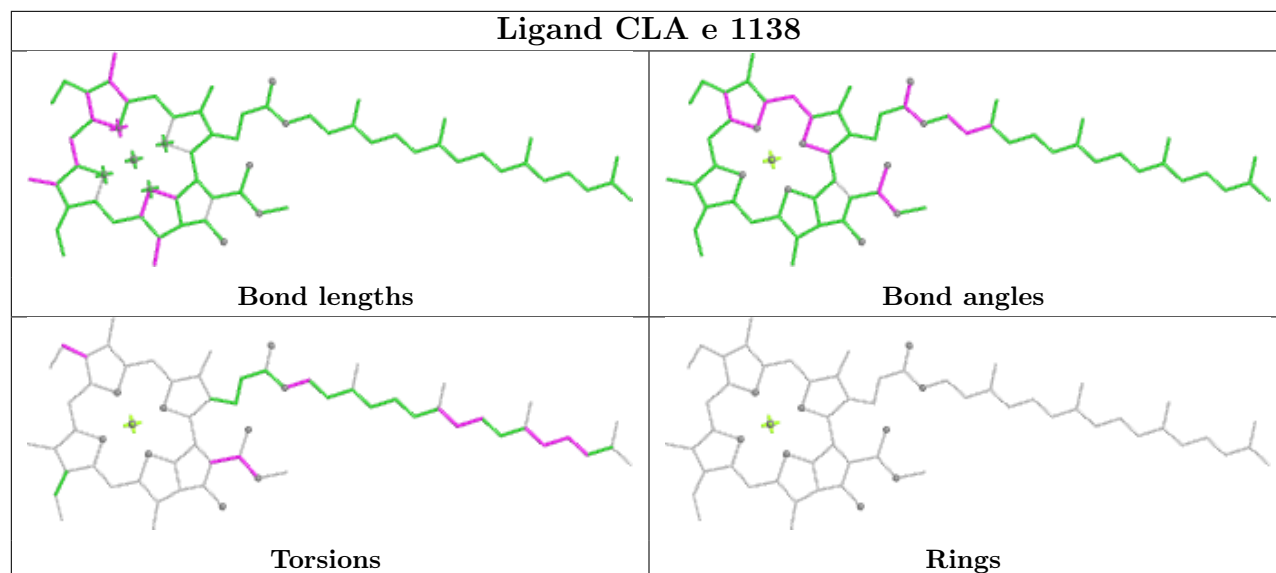
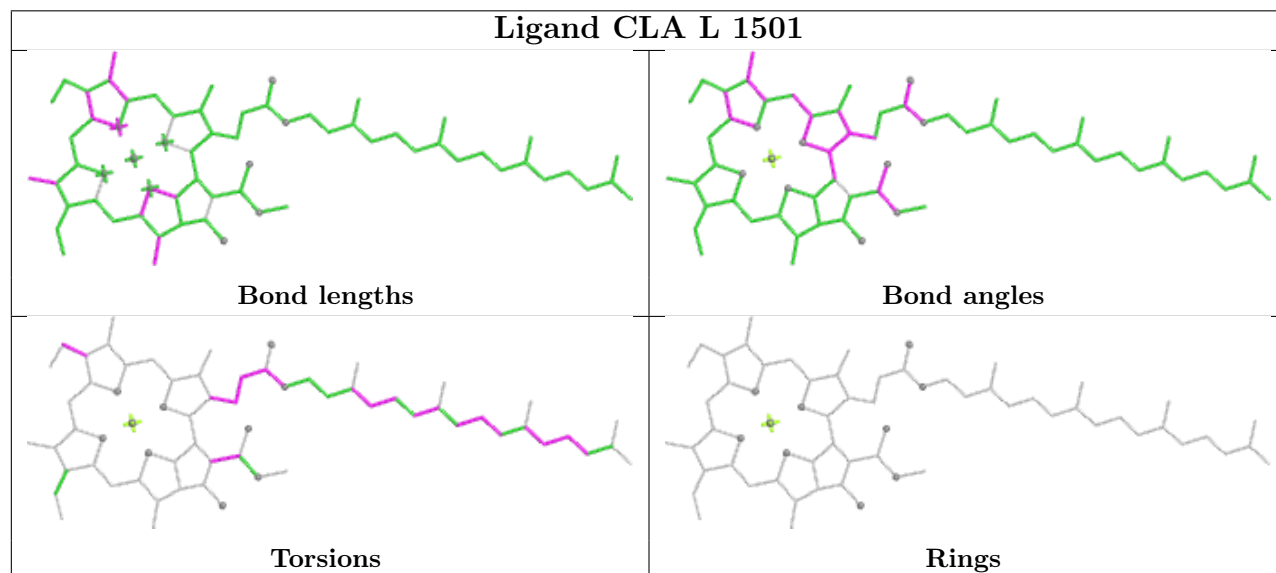
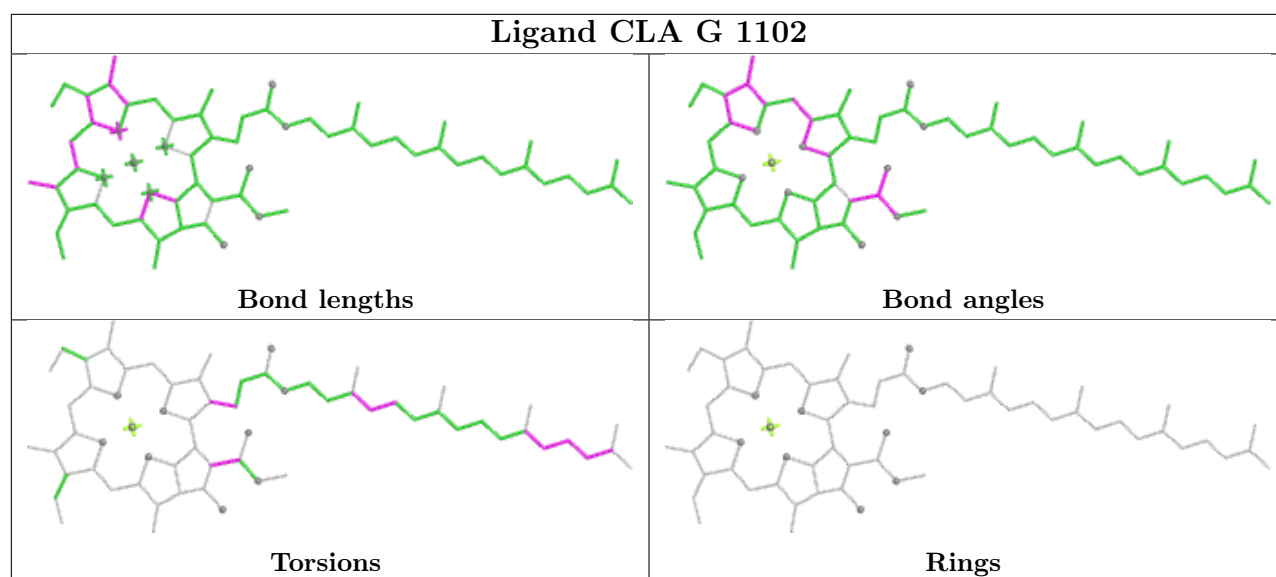


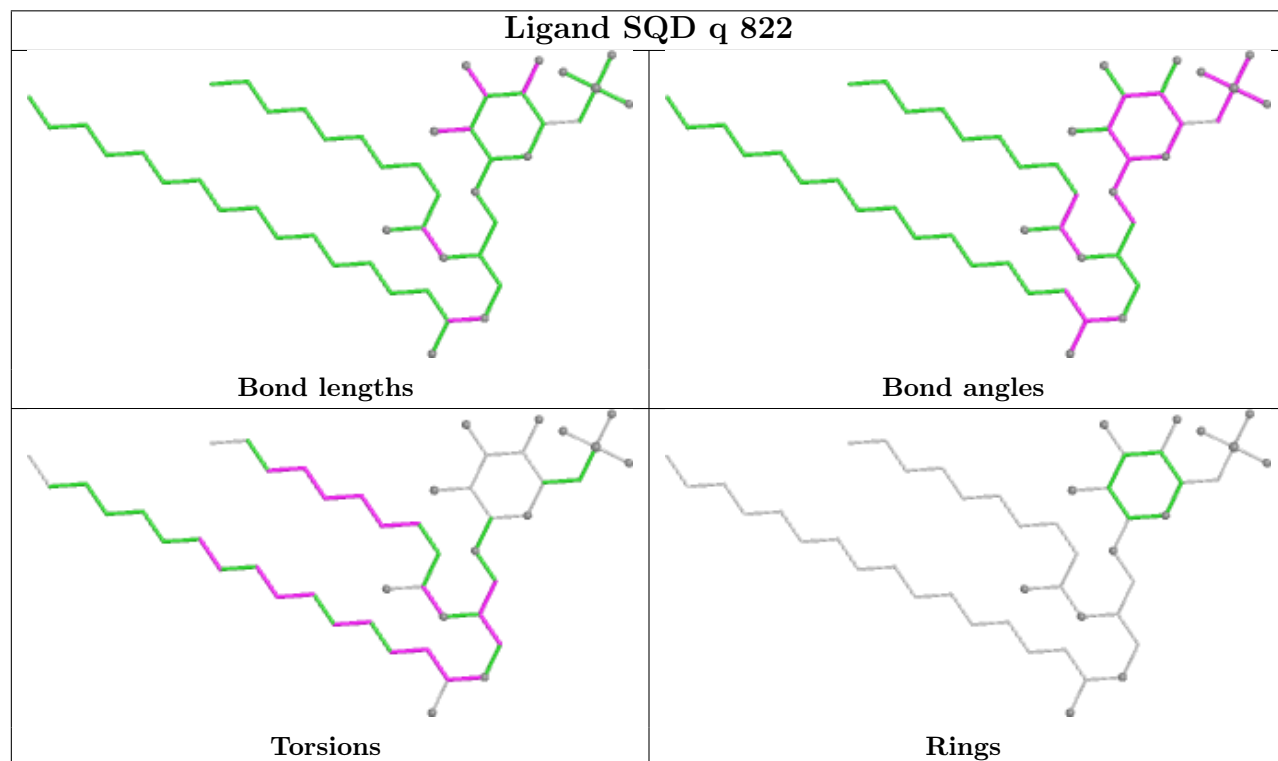
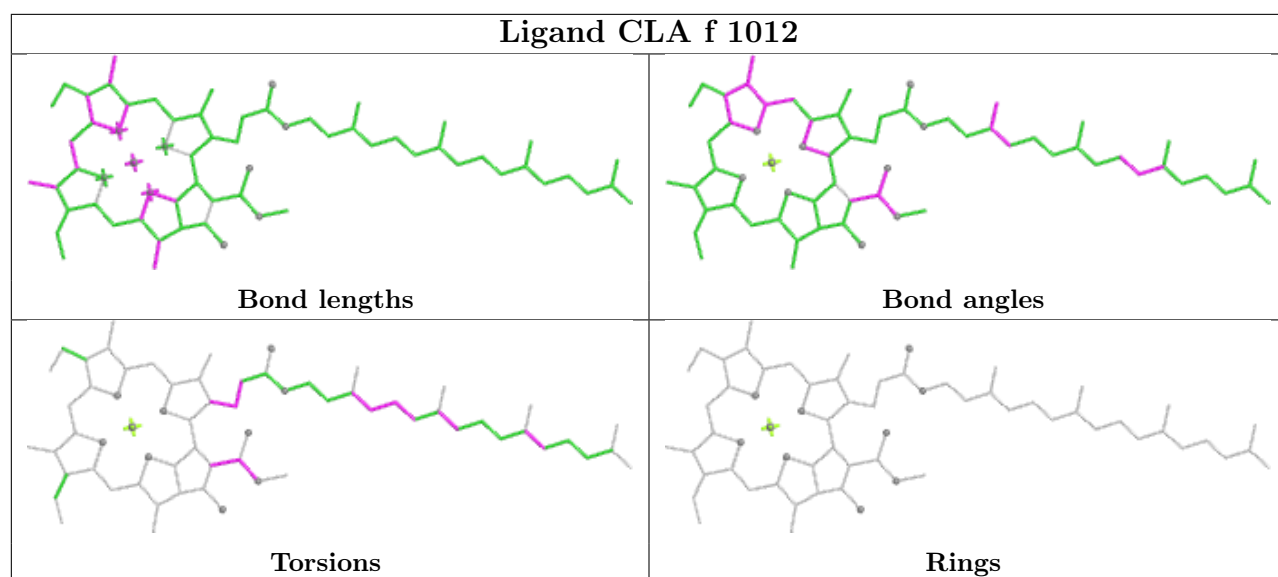
Torsions

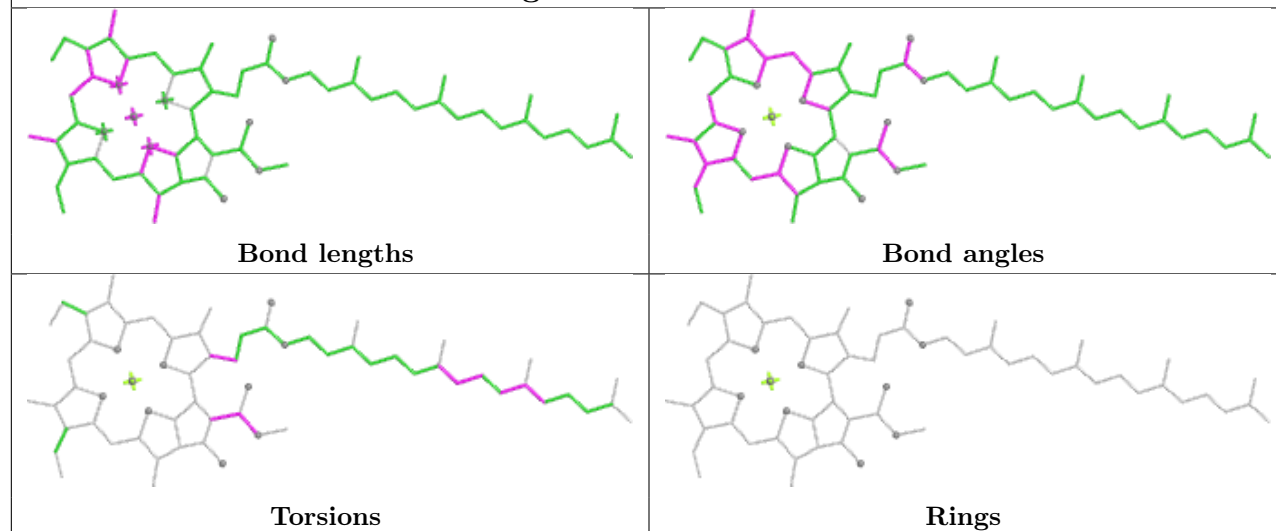
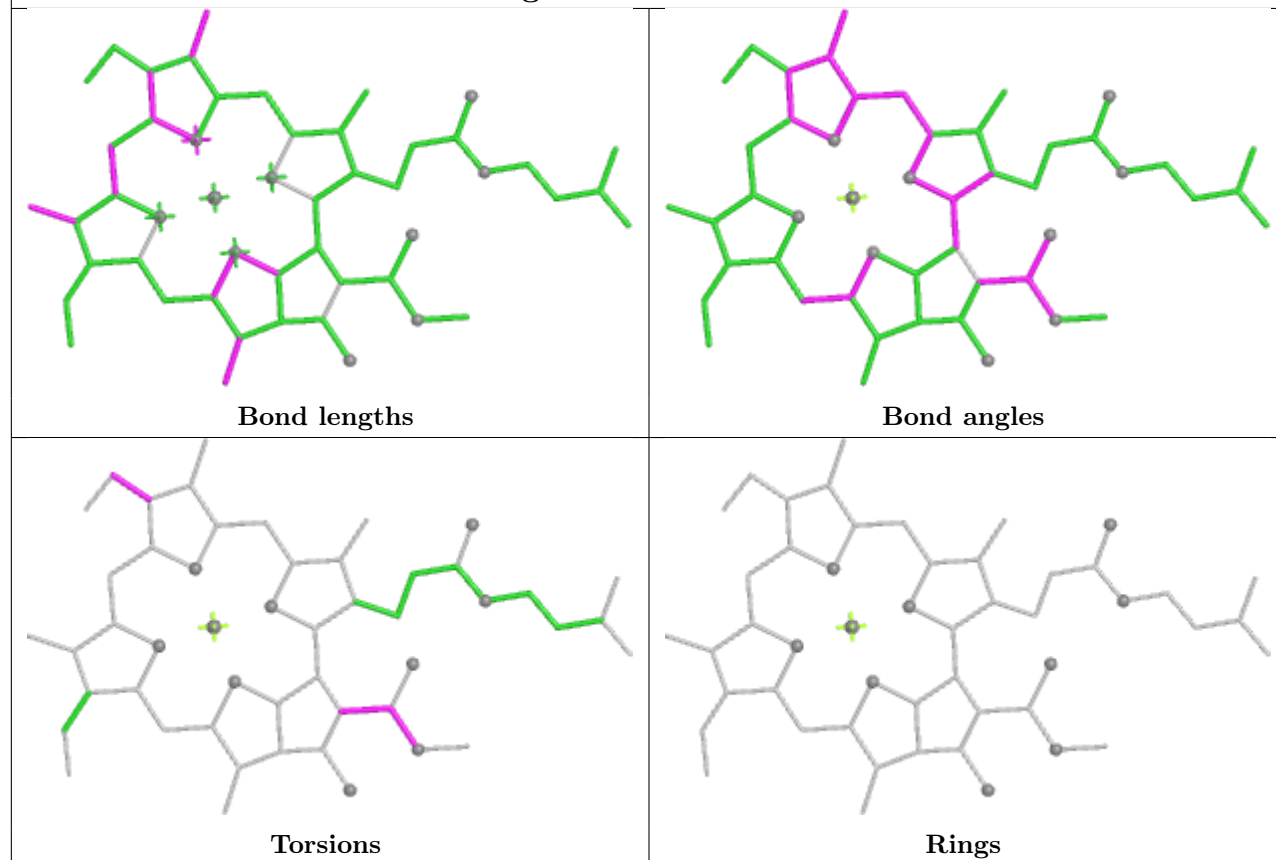


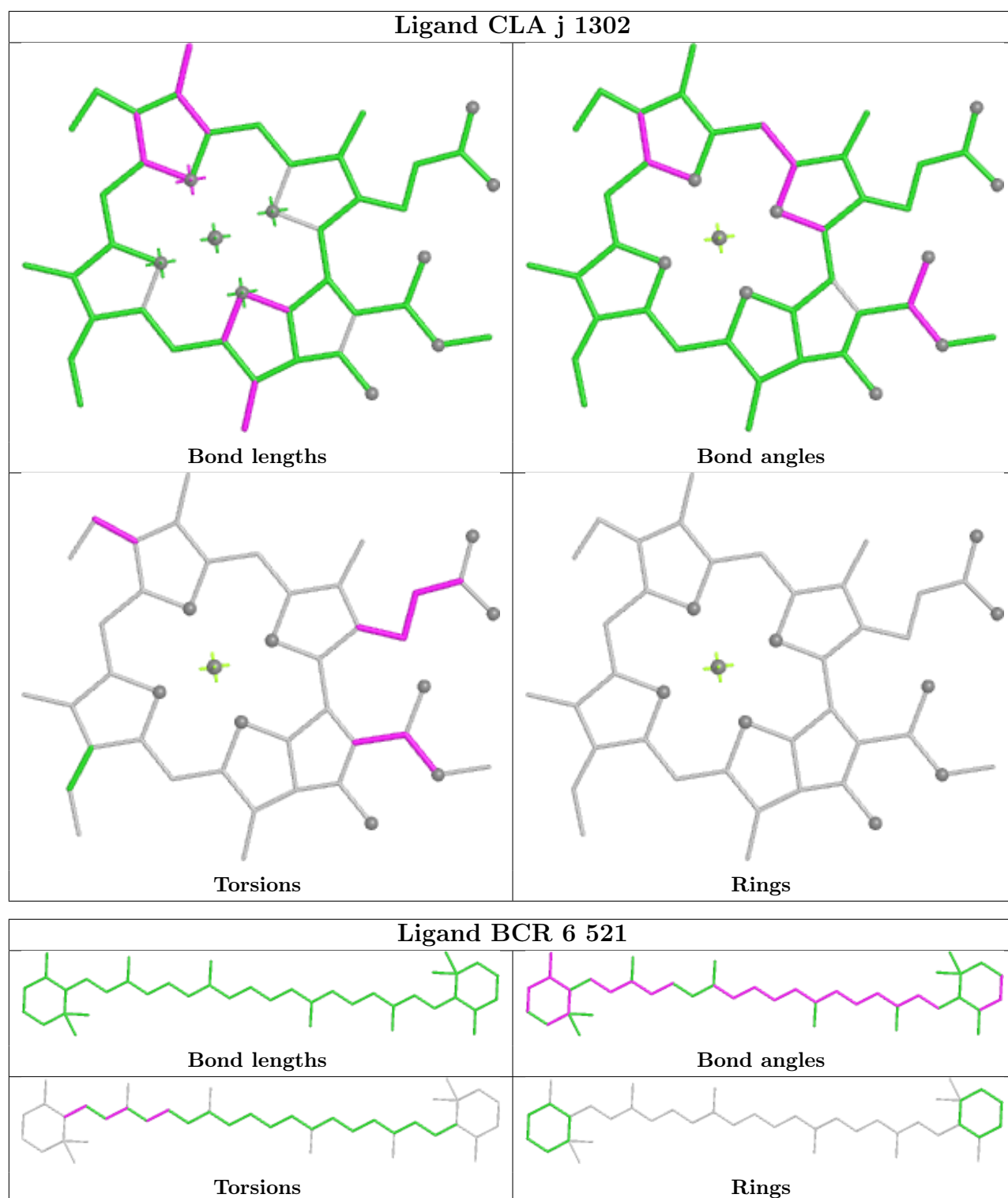
Rings

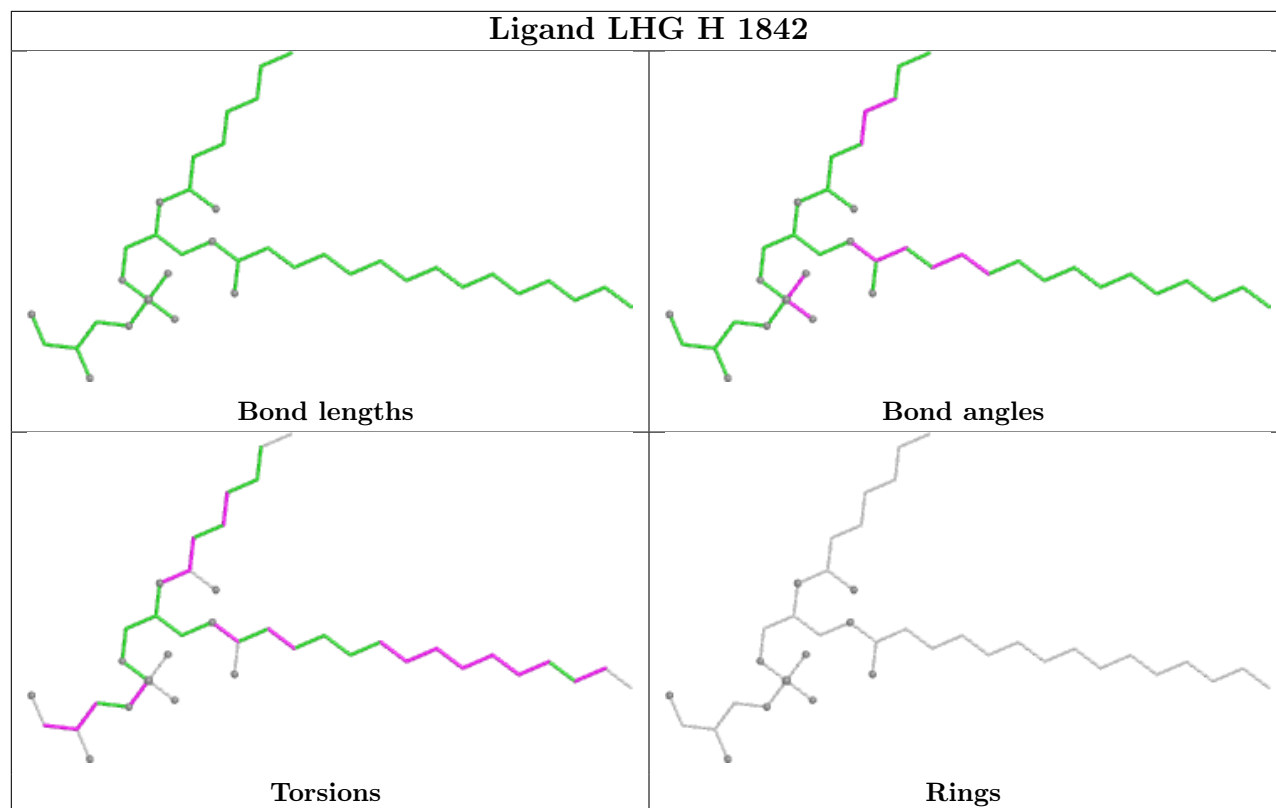




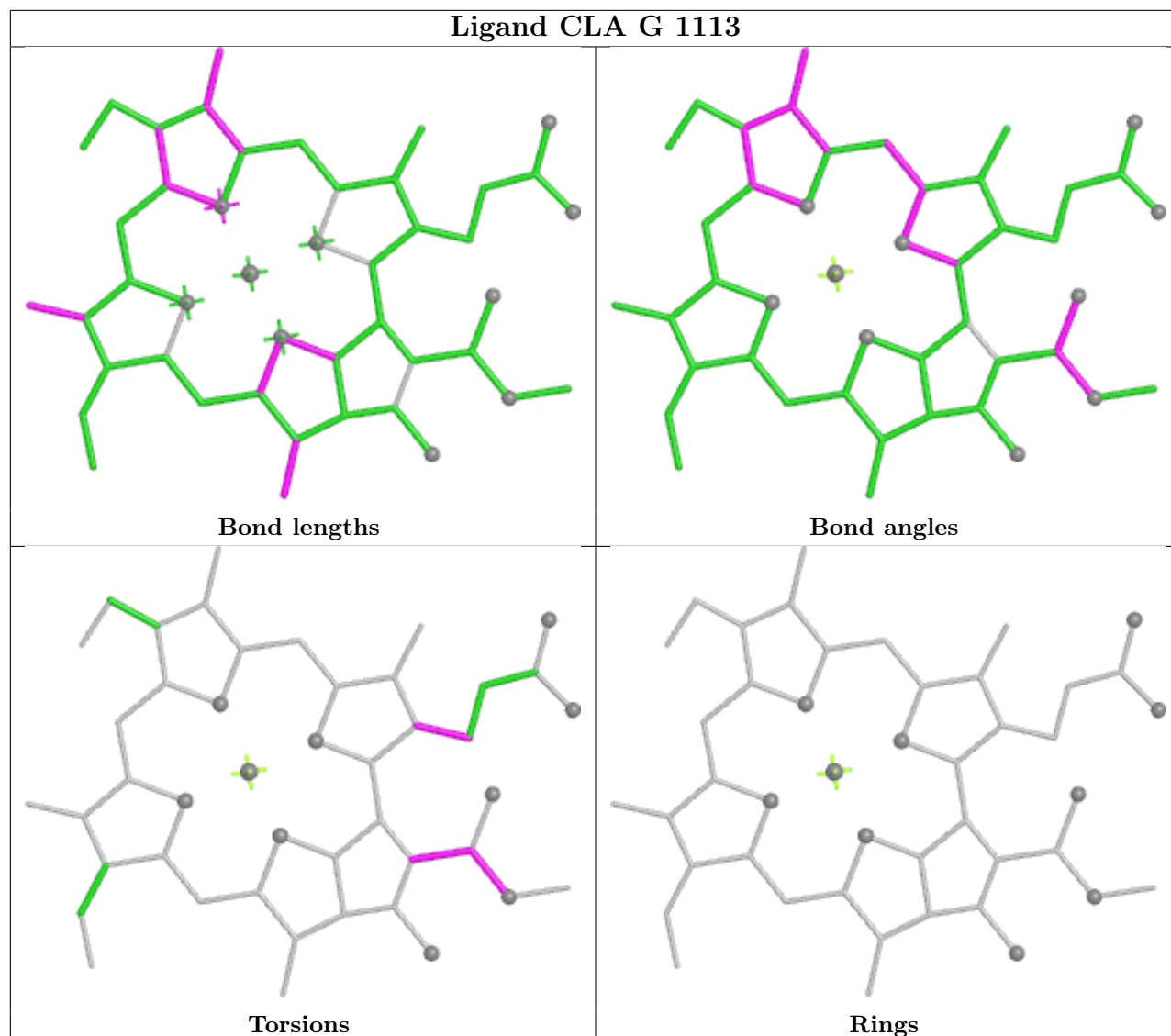


Ligand CLA H 1226**Ligand CLA G 1112**

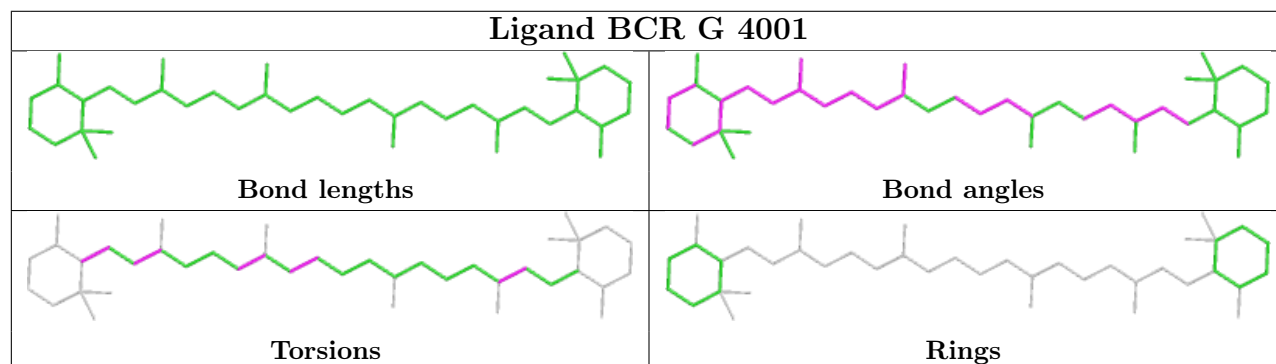


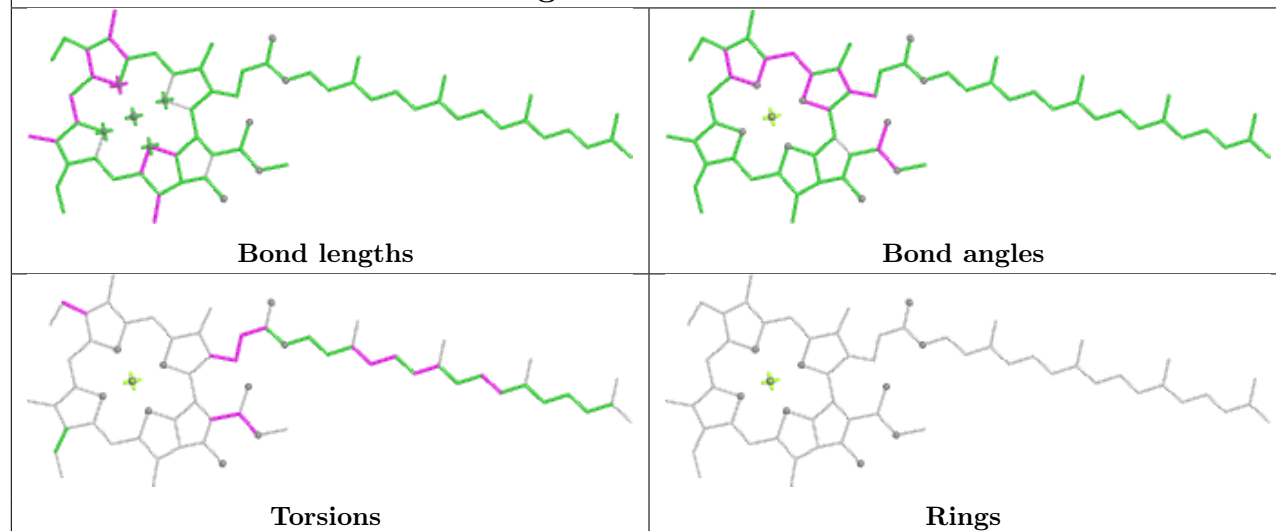
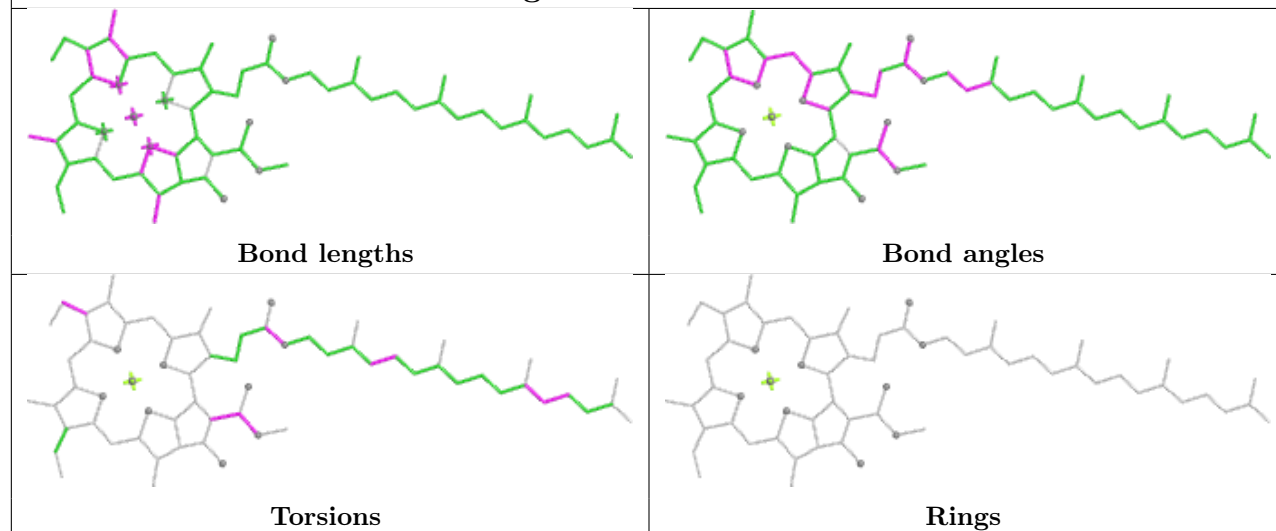
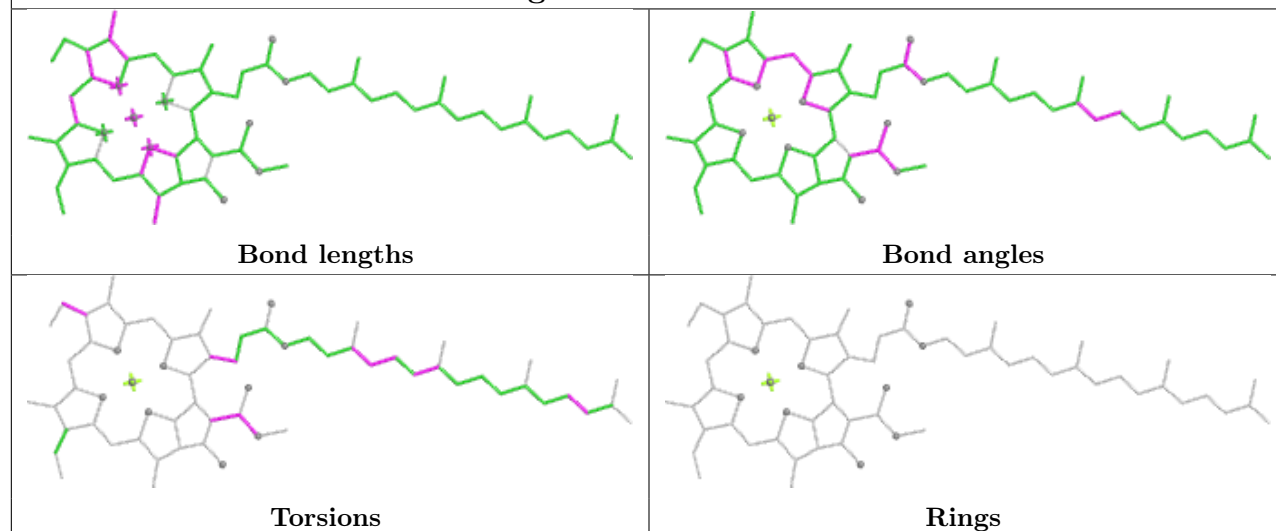


Ligand CLA G 1113

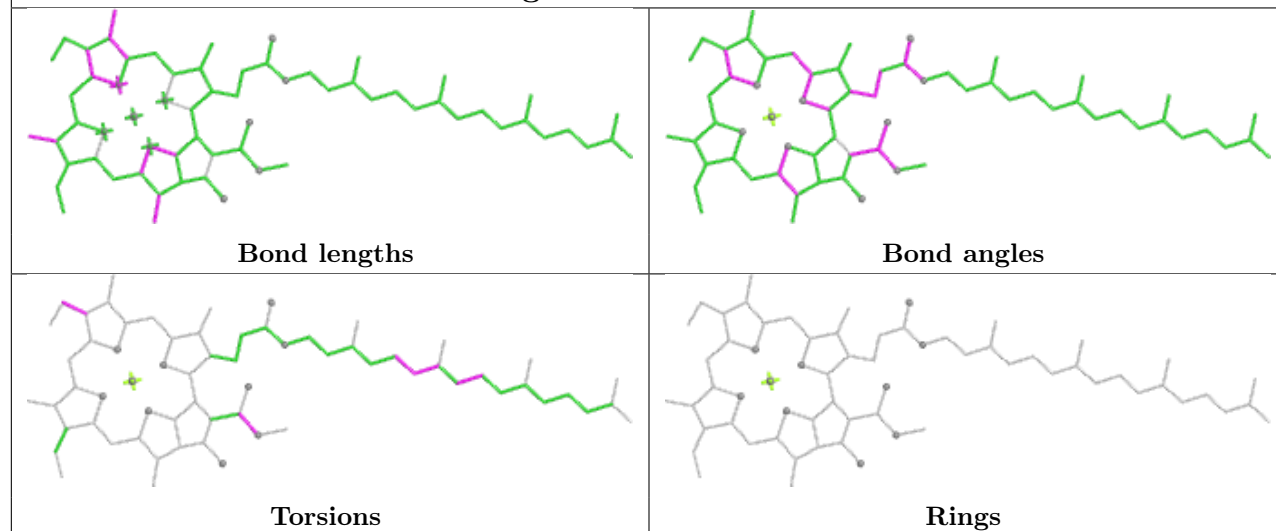


Ligand BCR G 4001

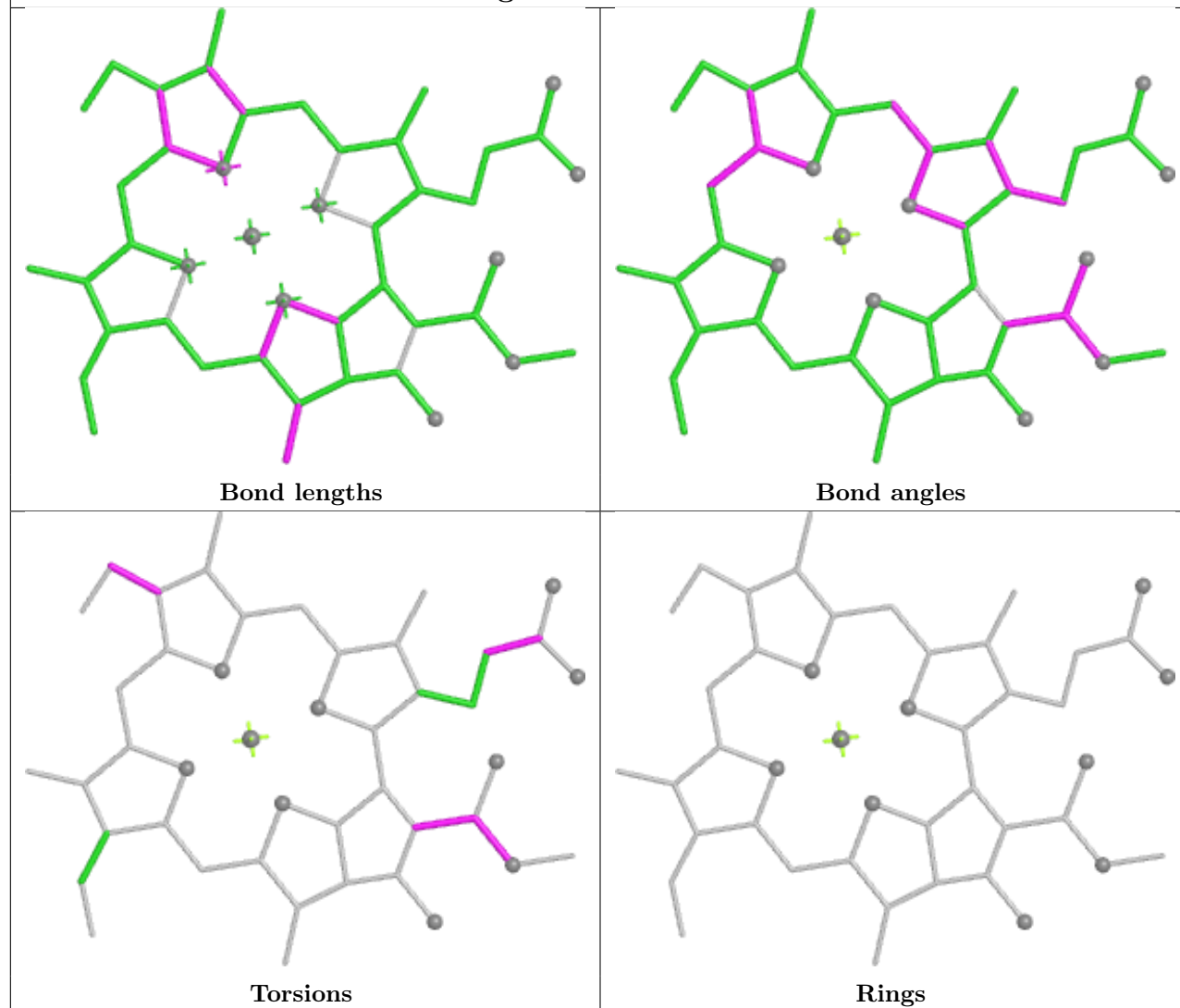


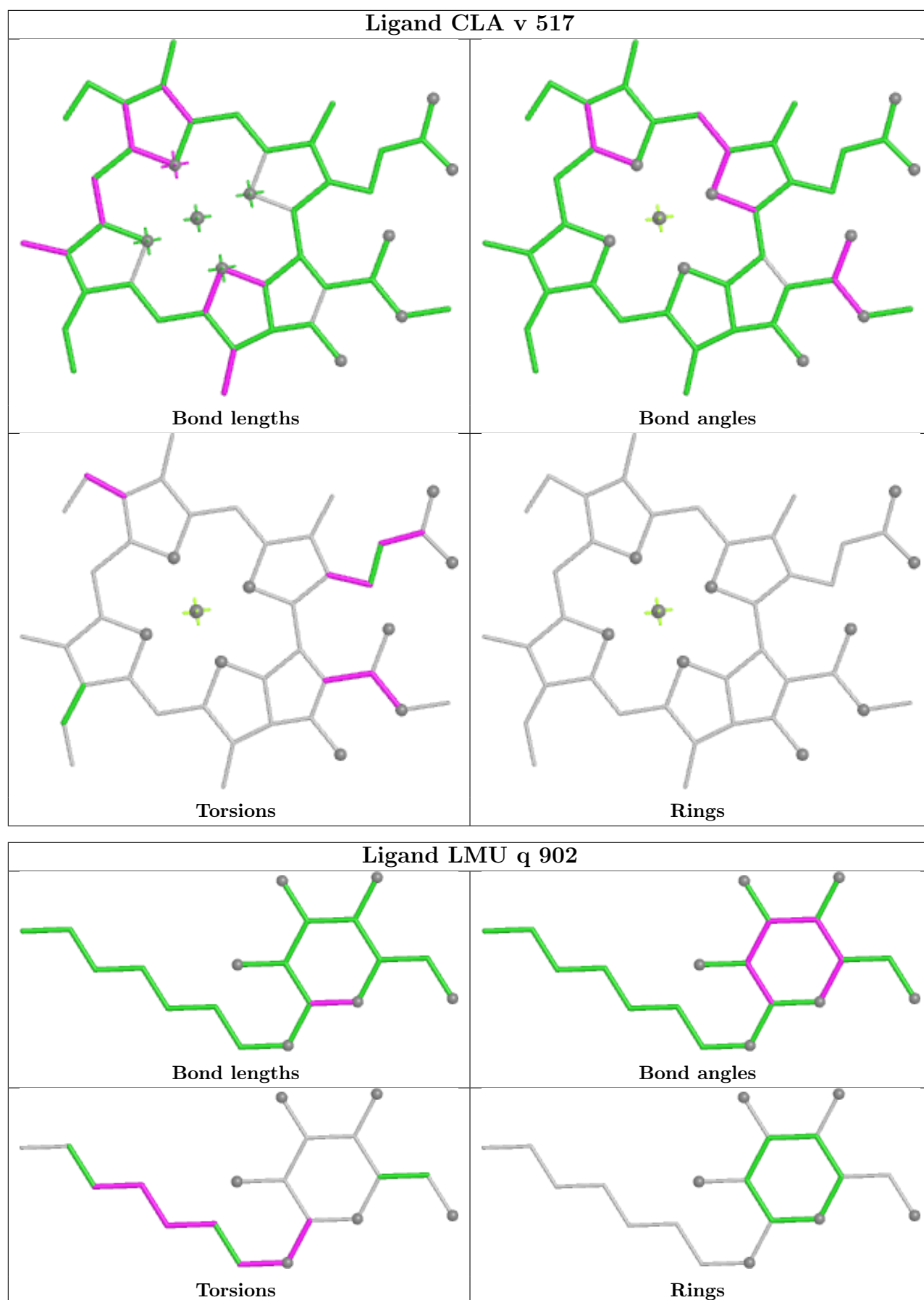
Ligand CLA r 501**Ligand CLA B 1205****Ligand CLA e 1139**

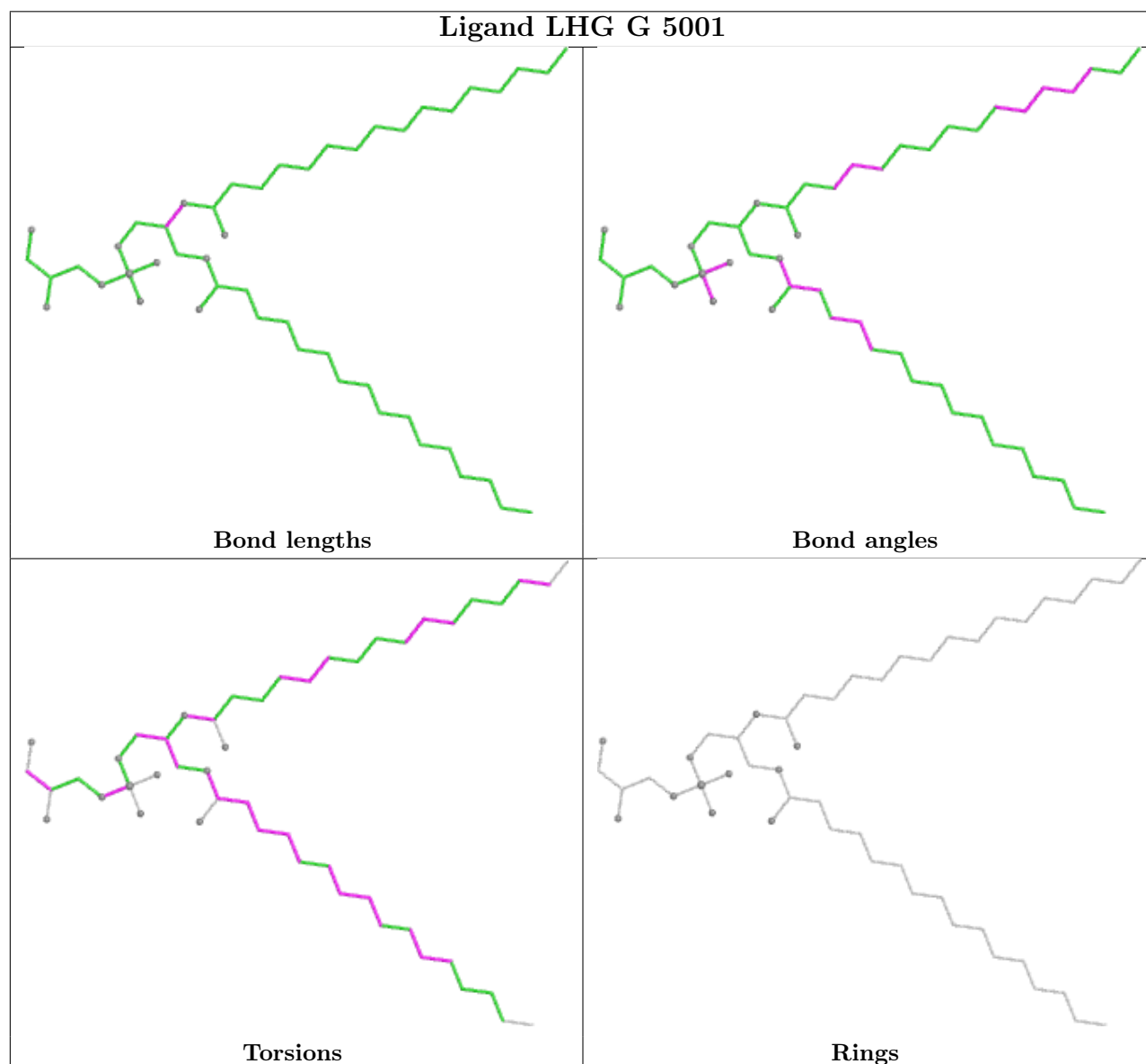
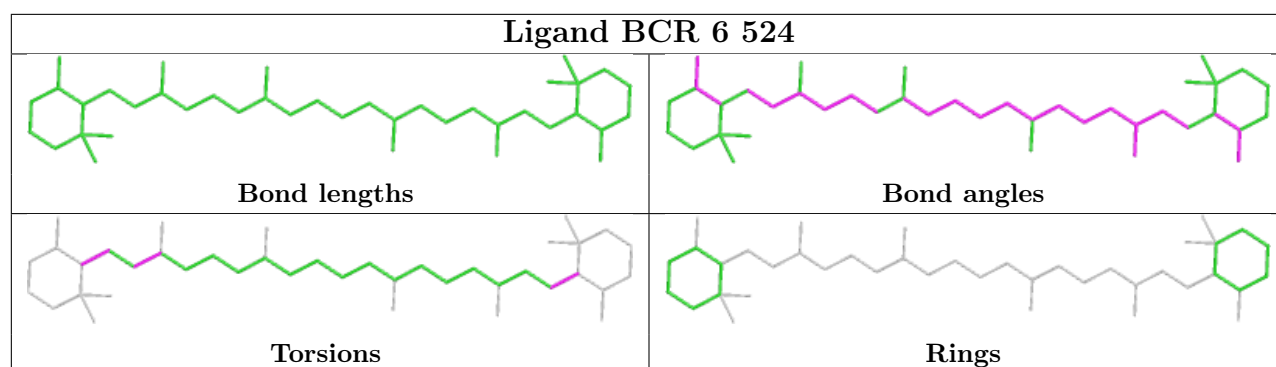
Ligand CLA H 1235

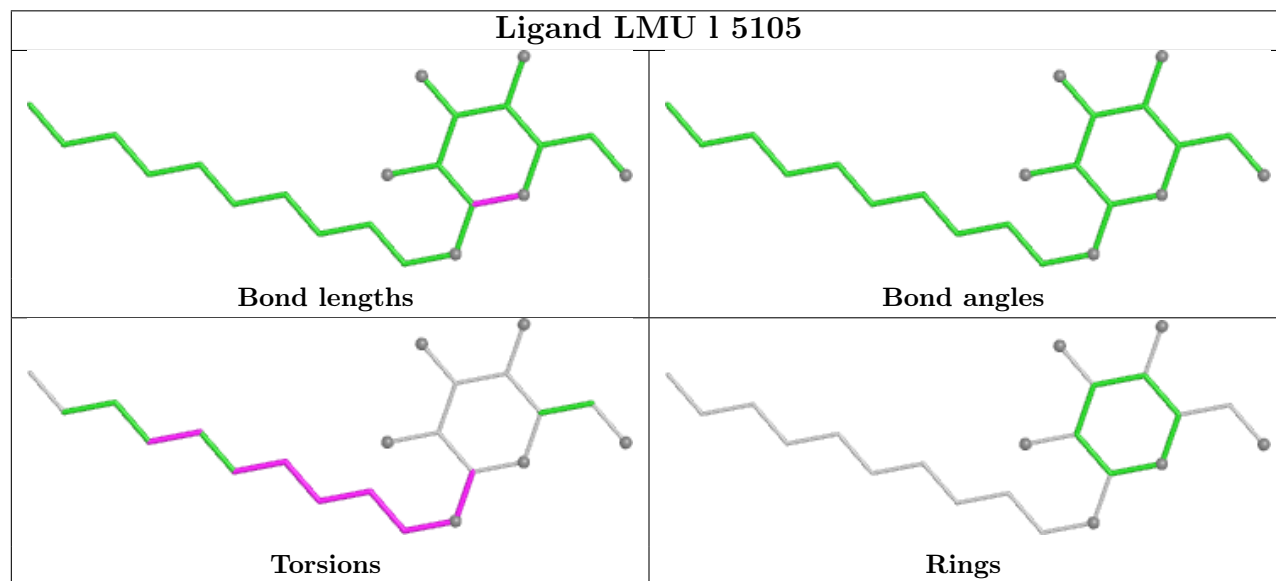
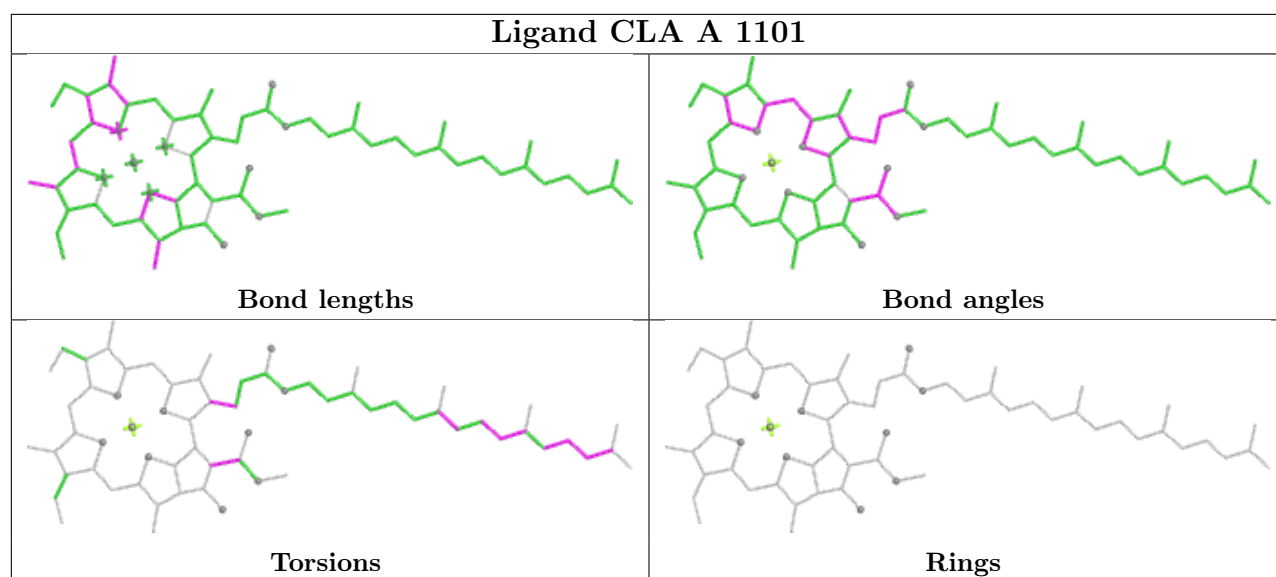


Ligand CLA t 507

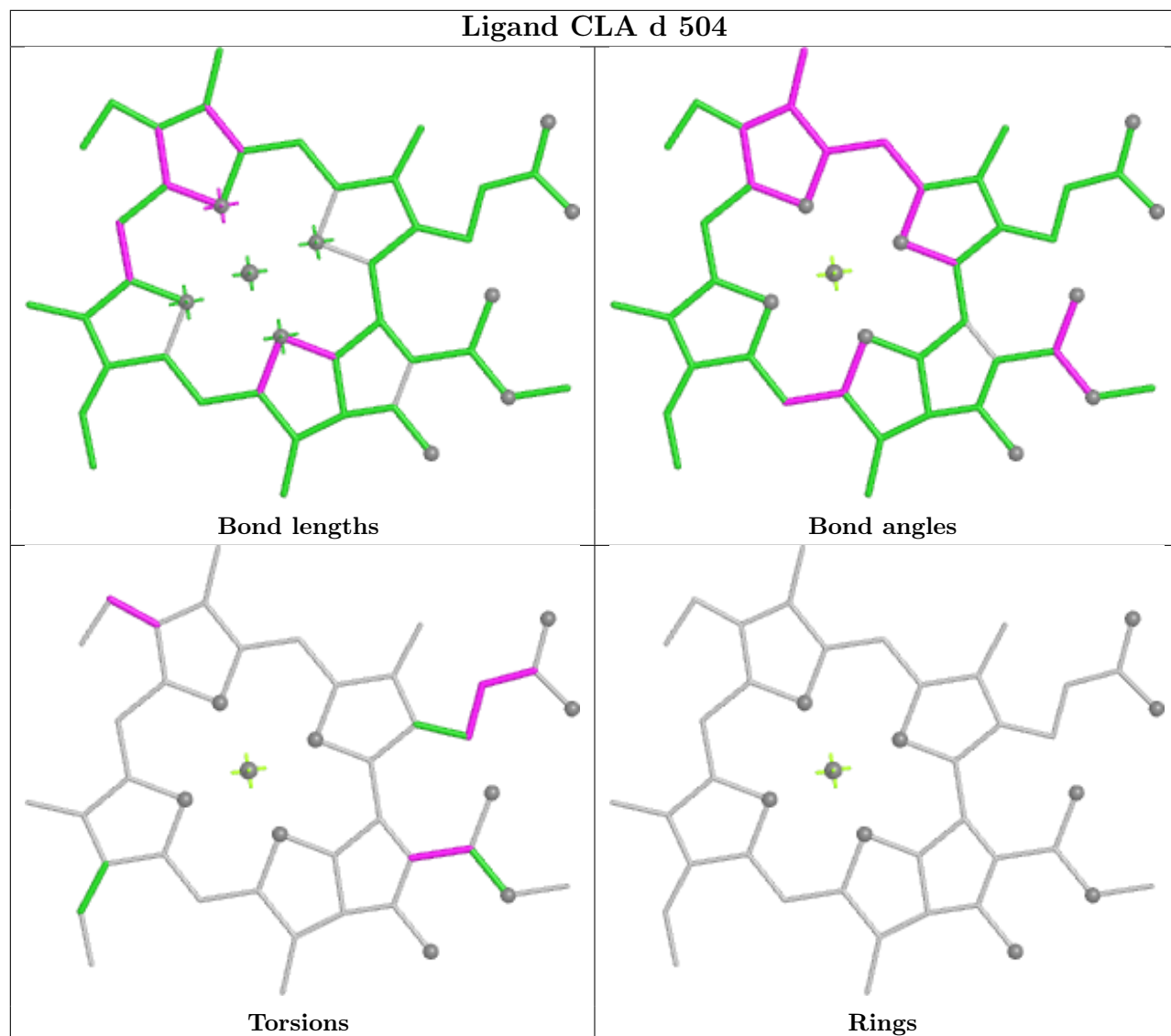




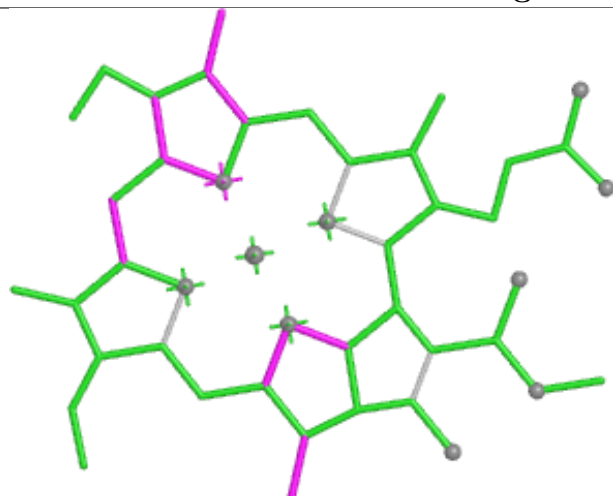




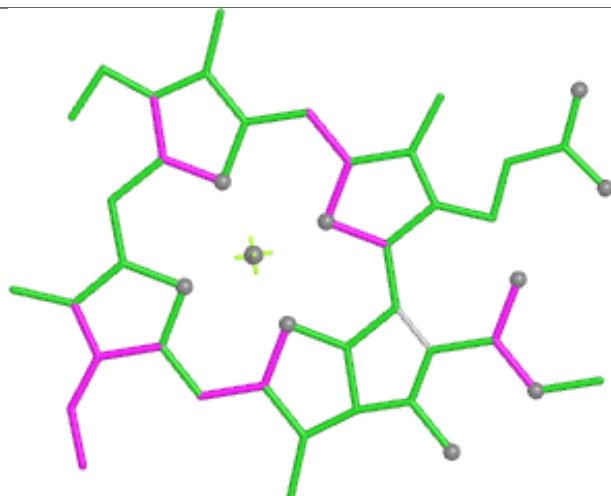
Ligand CLA d 504



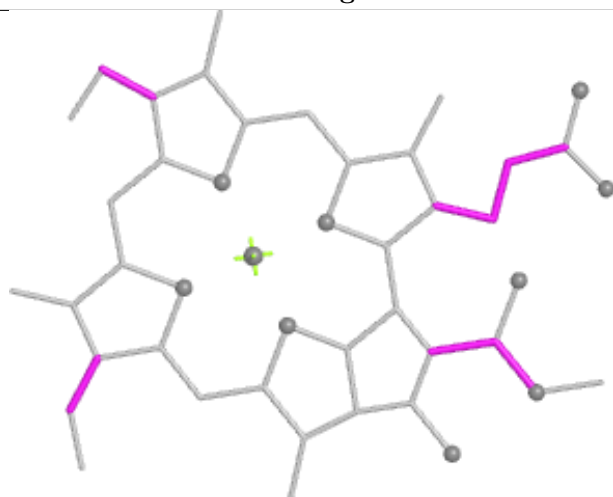
Ligand CLA Y 516



Bond lengths



Bond angles

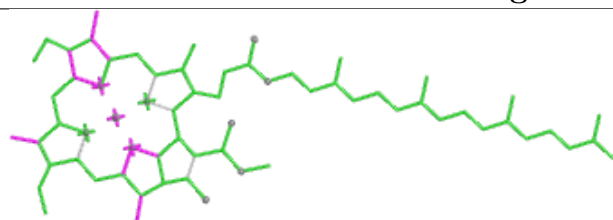


Torsions

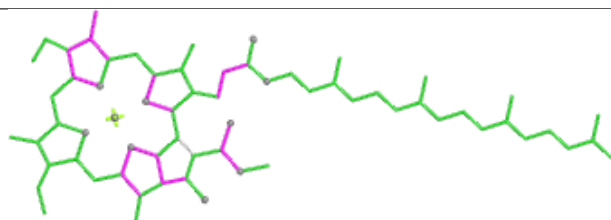


Rings

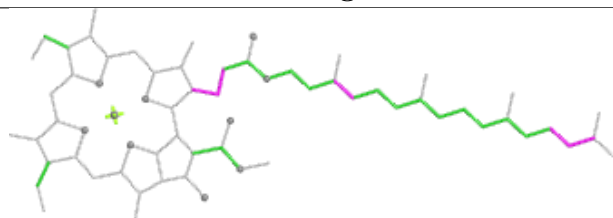
Ligand CLA e 1022



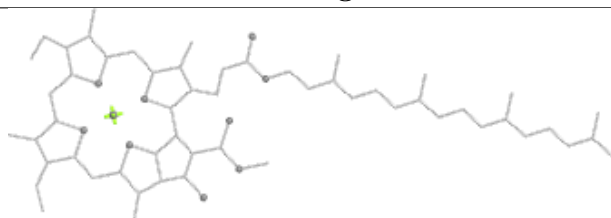
Bond lengths



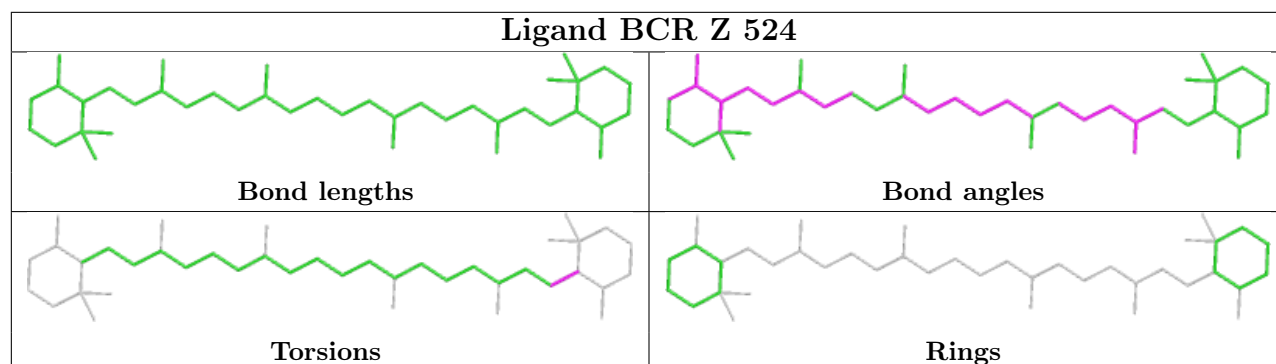
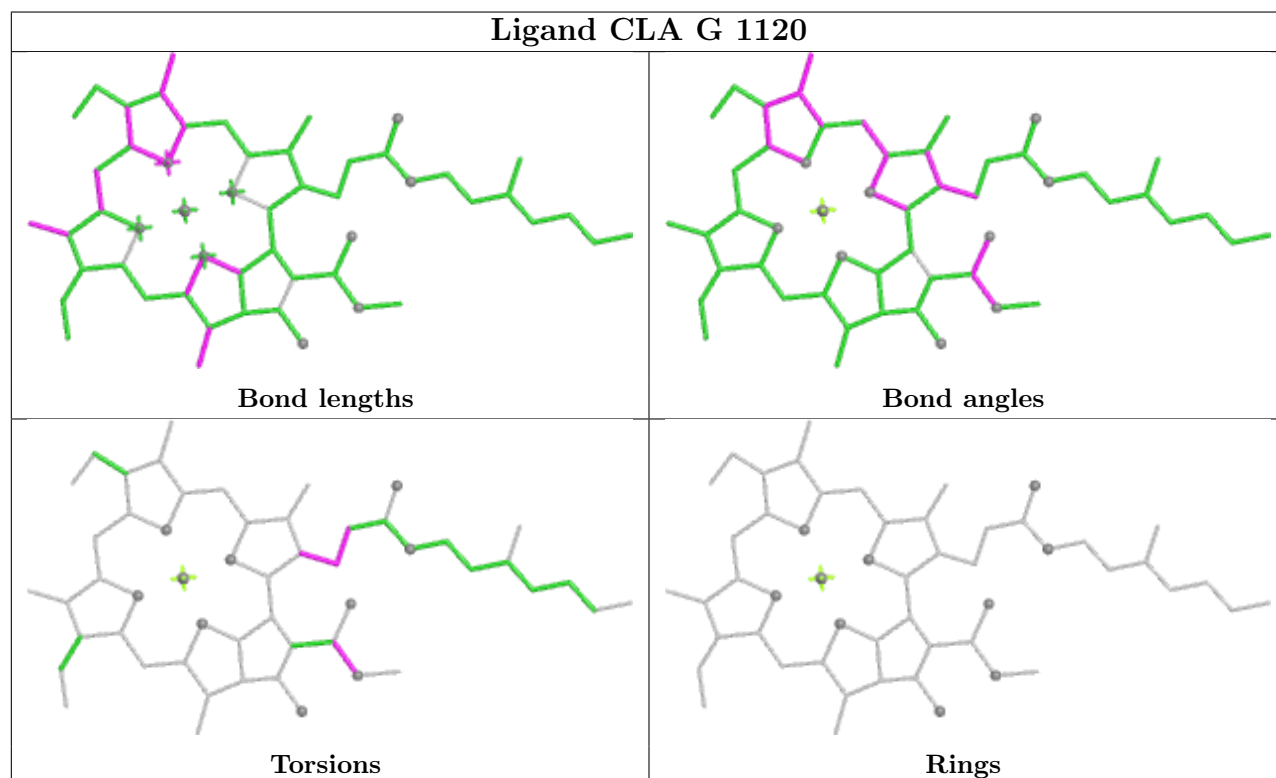
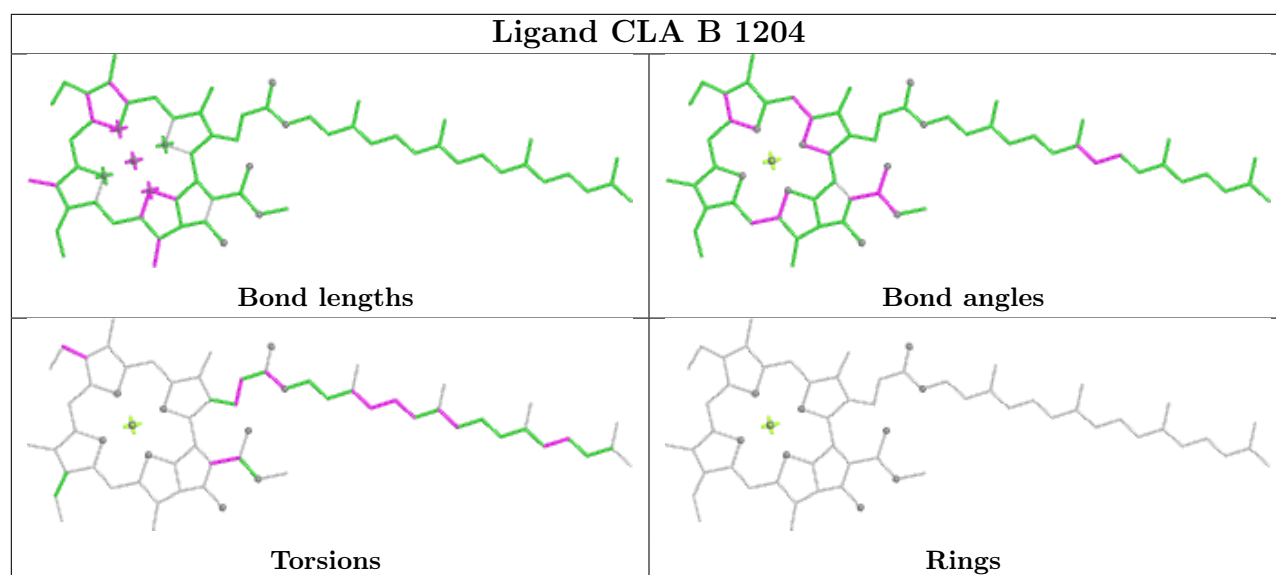
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

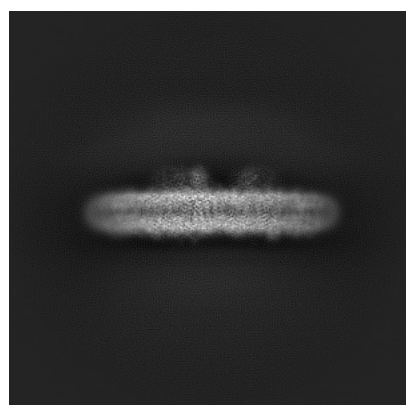
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9995. These allow visual inspection of the internal detail of the map and identification of artifacts.

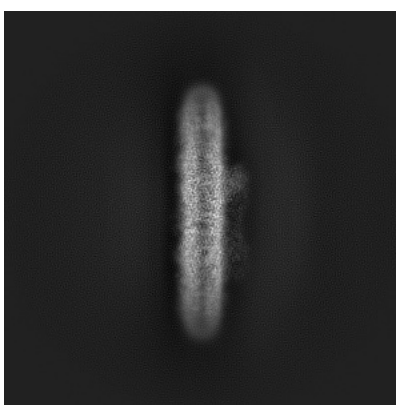
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

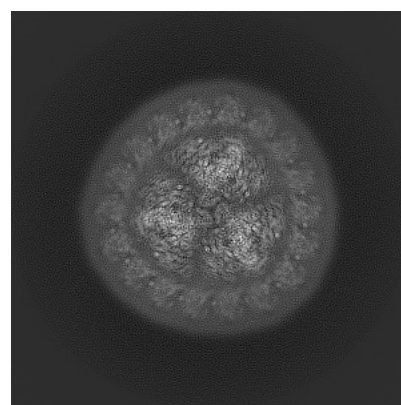
6.1.1 Primary map



X



Y

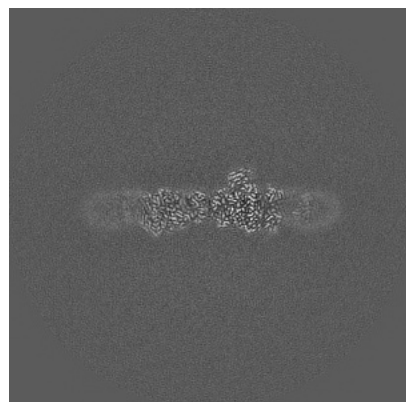


Z

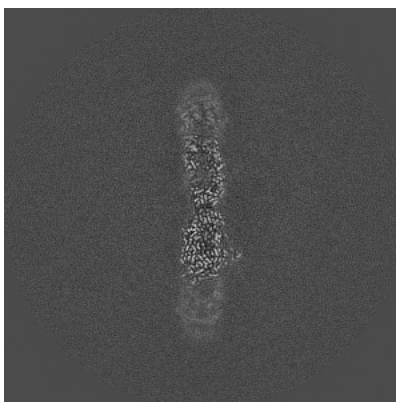
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

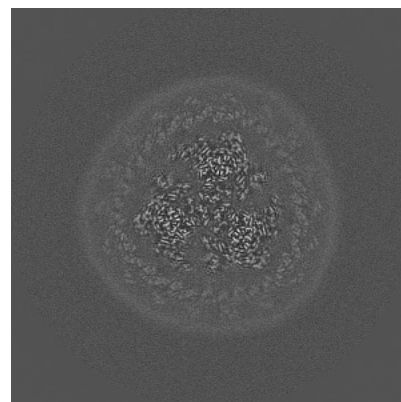
6.2.1 Primary map



X Index: 240



Y Index: 240

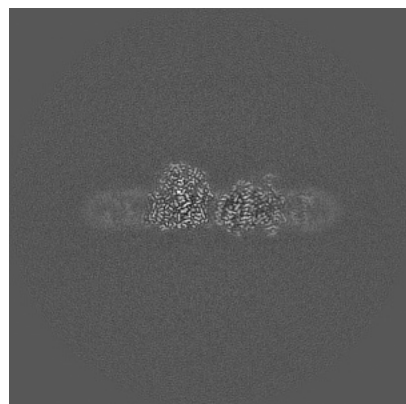


Z Index: 240

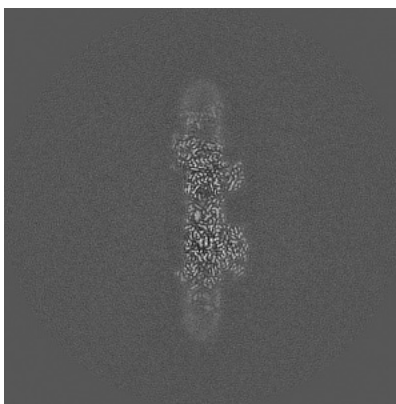
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

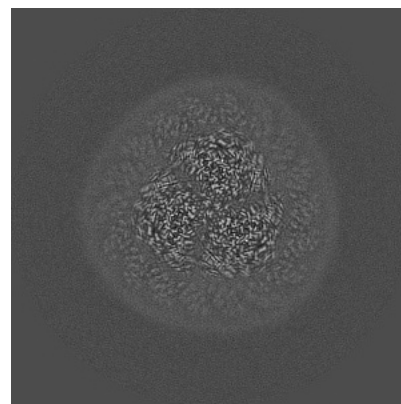
6.3.1 Primary map



X Index: 276



Y Index: 224

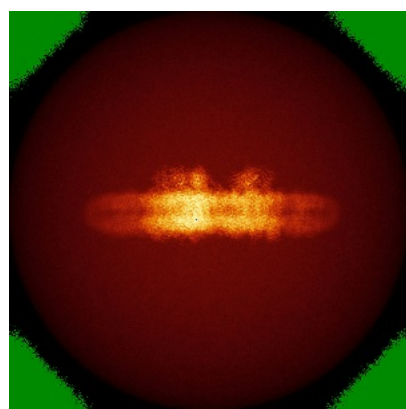


Z Index: 229

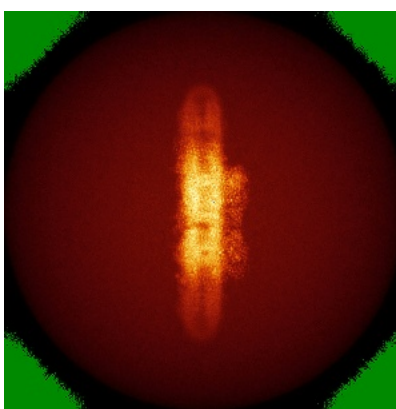
The images above show the largest variance slices of the map in three orthogonal directions.

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

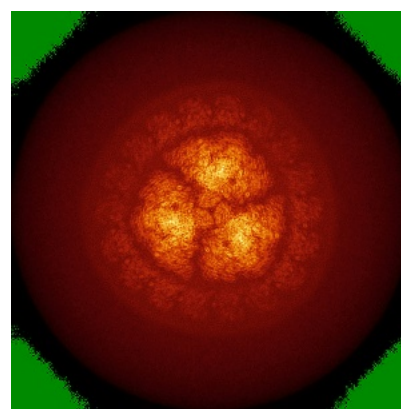
6.4.1 Primary map



X



Y

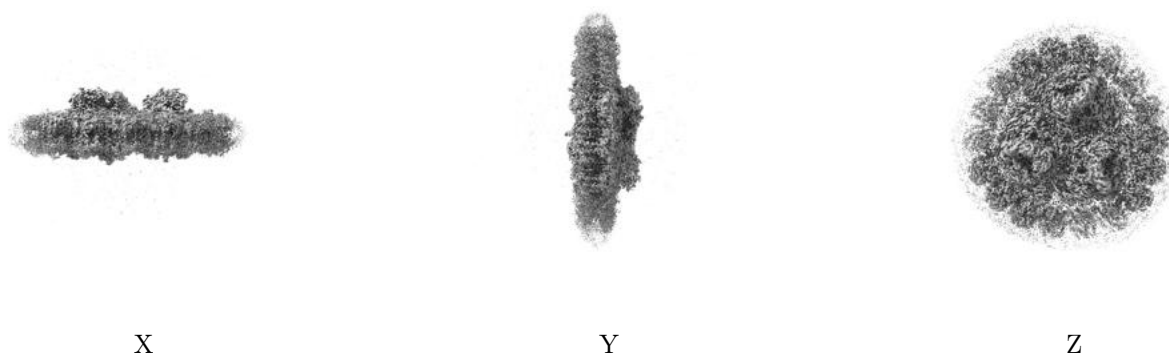


Z

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 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

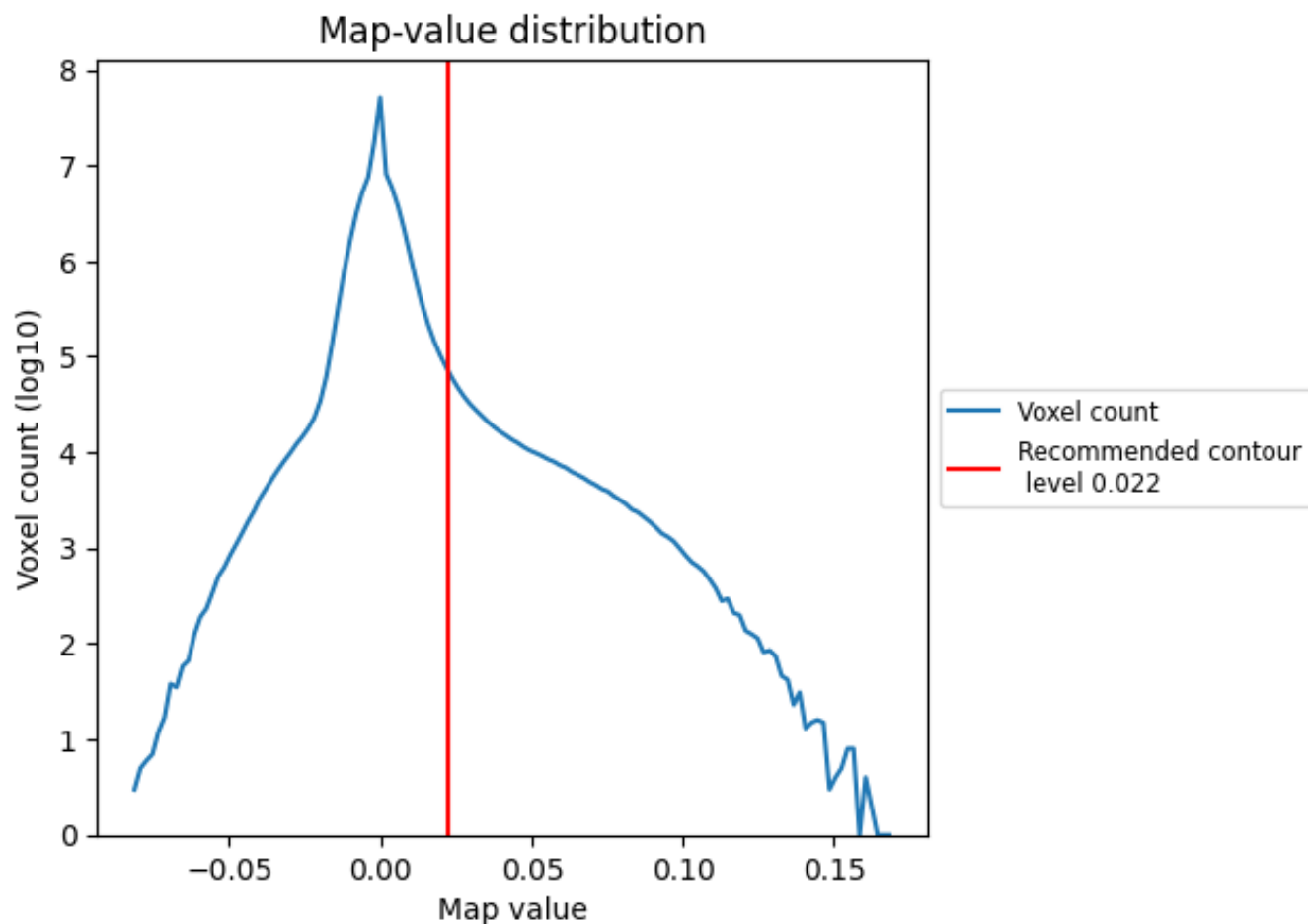
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

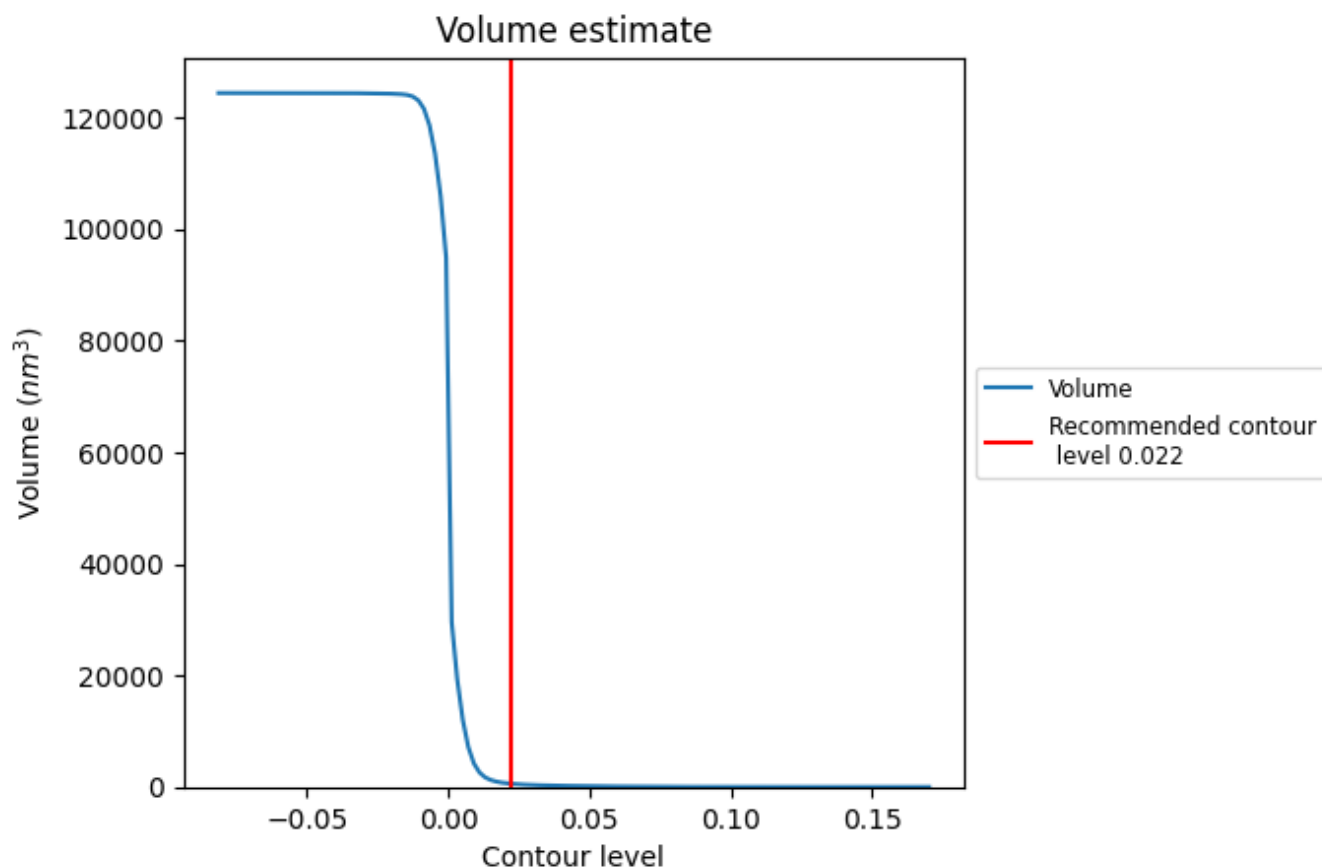
This section contains the results of statistical analysis of the map.

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.

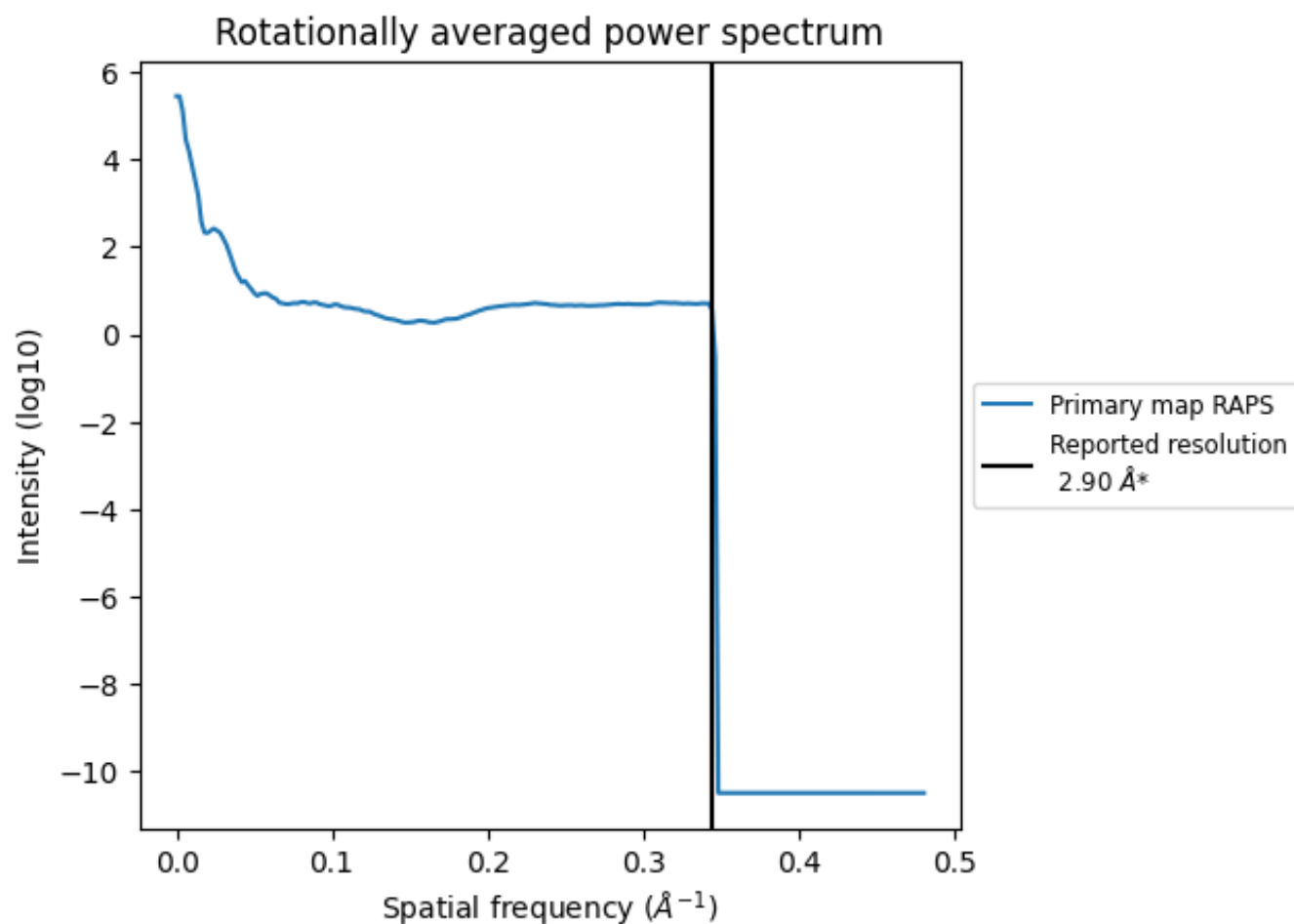
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 595 nm³; this corresponds to an approximate mass of 538 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 0.345 Å⁻¹

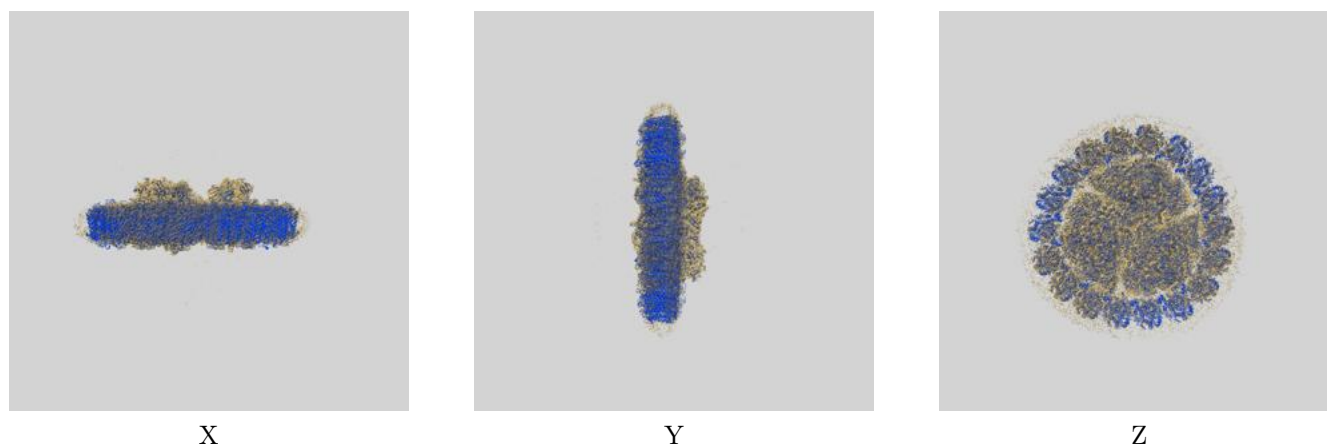
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

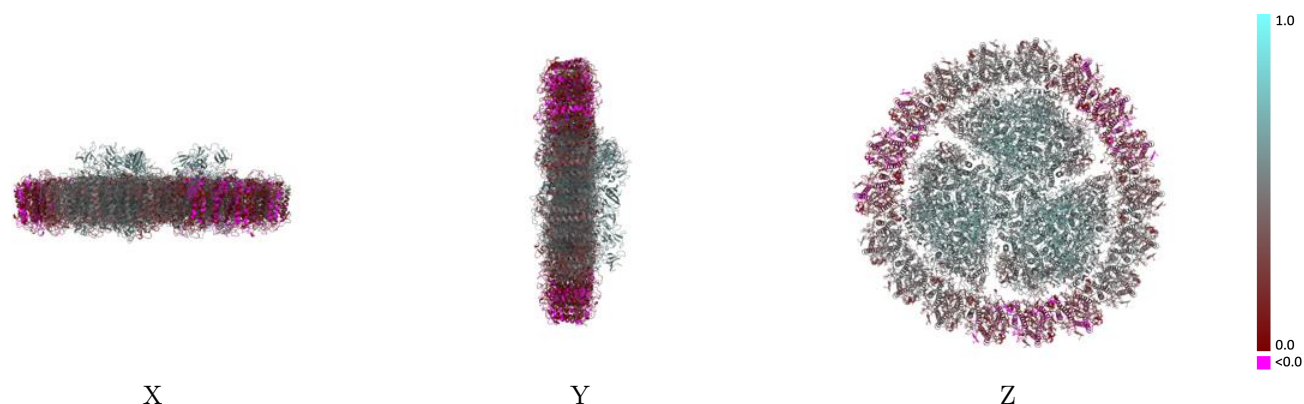
This section contains information regarding the fit between EMDB map EMD-9995 and PDB model 6KIG. Per-residue inclusion information can be found in section [3](#) on page [56](#).

9.1 Map-model overlay [i](#)



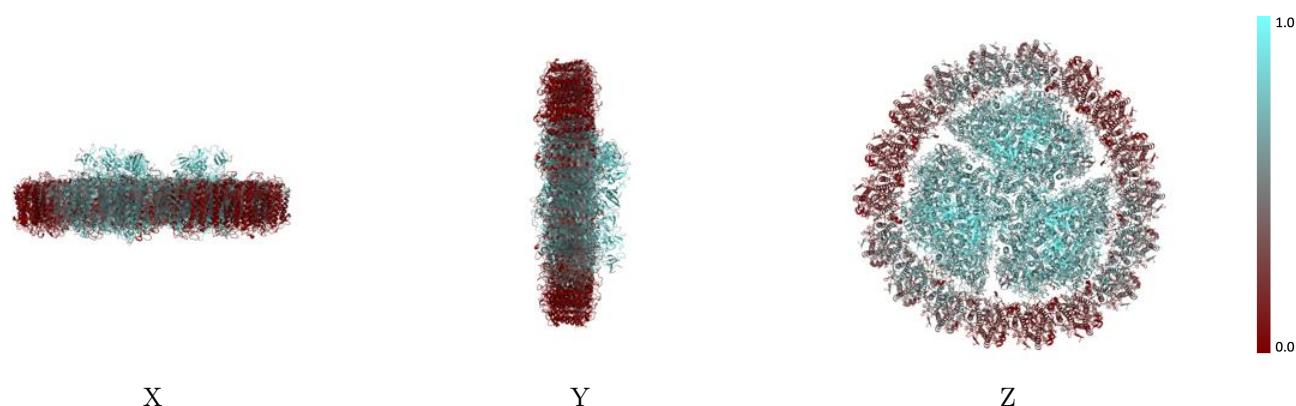
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



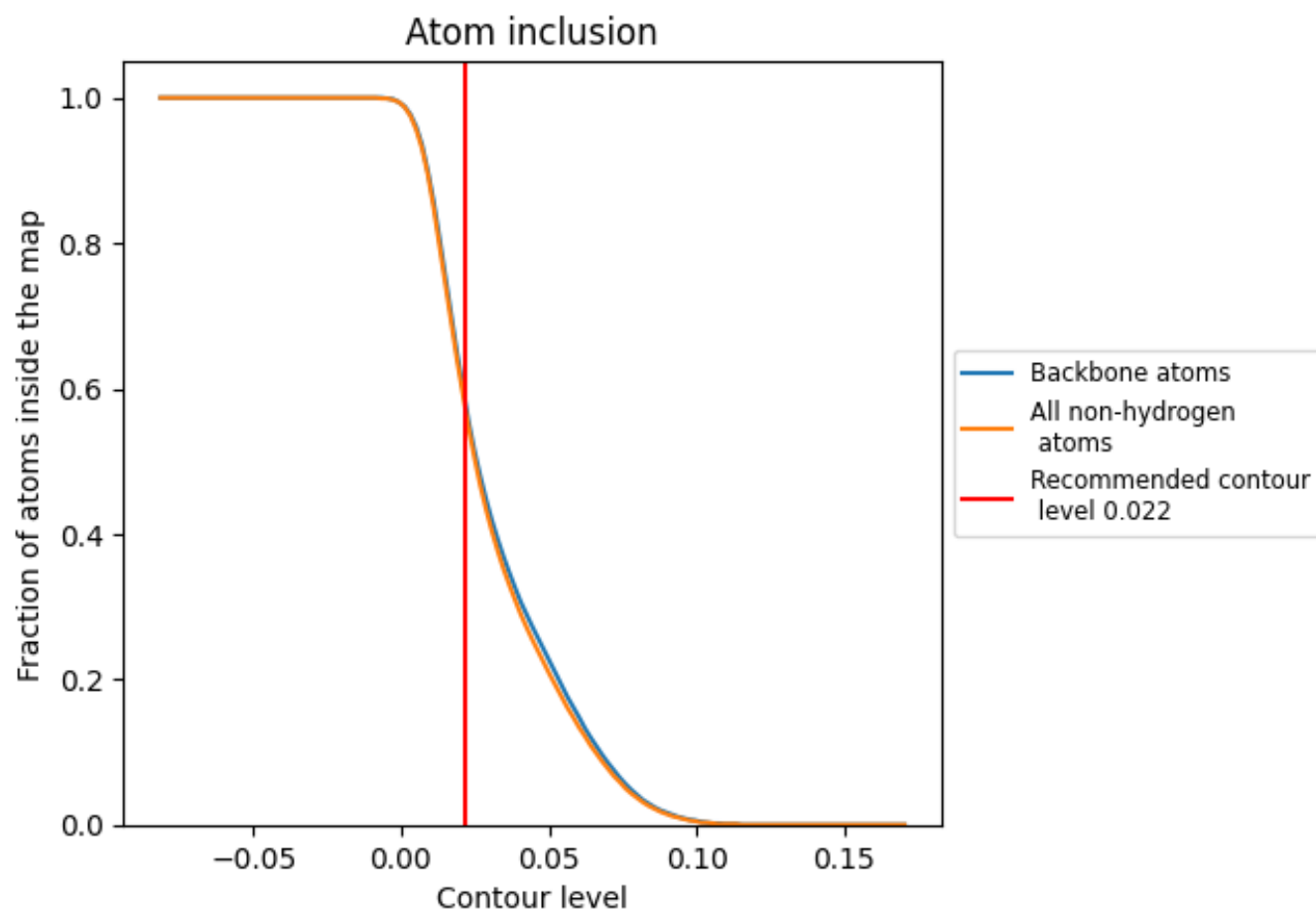
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 56% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5650	 0.4190
1	 0.4070	 0.3640
2	 0.4700	 0.4180
3	 0.3900	 0.3830
4	 0.1070	 0.1410
5	 0.0560	 0.0860
6	 0.1520	 0.1850
A	 0.8490	 0.5780
B	 0.8270	 0.5450
C	 0.9420	 0.6070
D	 0.8580	 0.5770
E	 0.7870	 0.5410
F	 0.7470	 0.5290
G	 0.8450	 0.5770
H	 0.8160	 0.5370
I	 0.8330	 0.5720
J	 0.7550	 0.5460
K	 0.5870	 0.3890
L	 0.8650	 0.5930
M	 0.7980	 0.5290
N	 0.9450	 0.6070
O	 0.8590	 0.5780
Q	 0.7810	 0.5500
R	 0.7440	 0.5230
S	 0.8250	 0.5780
T	 0.7360	 0.5460
U	 0.5810	 0.3860
V	 0.8690	 0.5940
W	 0.7790	 0.5320
Y	 0.4060	 0.3660
Z	 0.4670	 0.4160
a	 0.3870	 0.3780
b	 0.1040	 0.1380
c	 0.0530	 0.0780
d	 0.1450	 0.1710



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Chain	Atom inclusion	Q-score
e	 0.8420	 0.5750
f	 0.8210	 0.5420
g	 0.9420	 0.6070
h	 0.8690	 0.5800
i	 0.7950	 0.5480
j	 0.7500	 0.5280
k	 0.8410	 0.5750
l	 0.7470	 0.5450
m	 0.5790	 0.3770
n	 0.8670	 0.5940
o	 0.7820	 0.5290
q	 0.3920	 0.3580
r	 0.4580	 0.4140
s	 0.3910	 0.3860
t	 0.1100	 0.1390
u	 0.0560	 0.0810
v	 0.1540	 0.1840