



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 05:08 AM JST

PDB ID : 6KIF / pdb_00006kif
EMDB ID : EMD-9994
Title : Structure of cyanobacterial photosystem I-IsiA-flavodoxin 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 : 3.30 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:

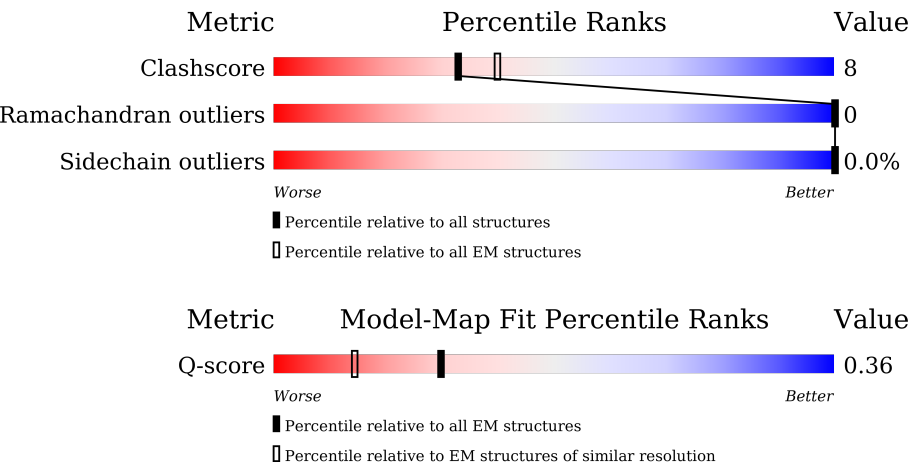
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

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

The reported resolution of this entry is 3.30 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.



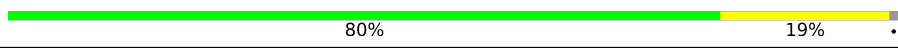
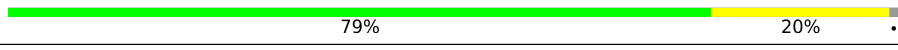
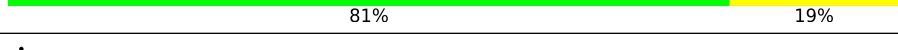
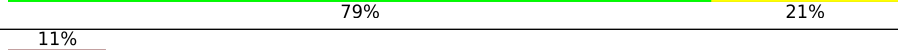
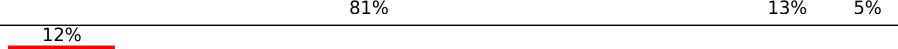
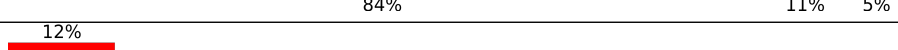
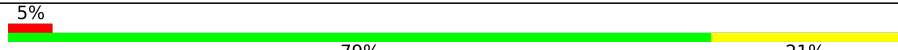
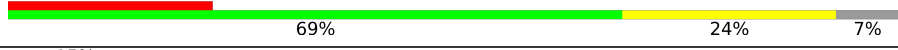
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	

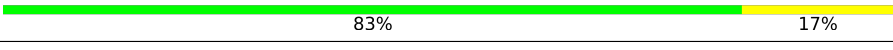
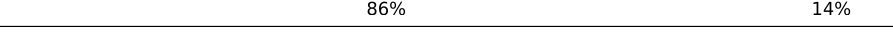
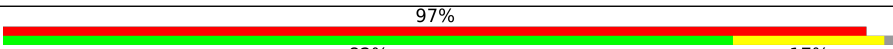
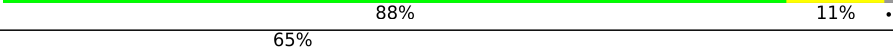
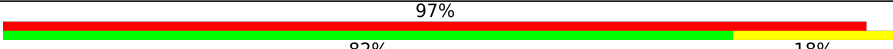
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Mol	Chain	Length	Quality of chain
2	H	734	
2	f	734	
3	C	81	
3	N	81	
3	g	81	
4	D	141	
4	O	141	
4	h	141	
5	E	75	
5	Q	75	
5	i	75	
6	F	159	
6	R	159	
6	j	159	
7	I	38	
7	S	38	
7	k	38	
8	J	41	
8	T	41	
8	l	41	
9	K	84	
9	U	84	
9	m	84	
10	L	166	
10	V	166	

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Mol	Chain	Length	Quality of chain
10	n	166	
11	M	29	
11	W	29	
11	o	29	
12	P	172	
12	X	172	
12	p	172	
13	1	342	
13	2	342	
13	3	342	
13	4	342	
13	5	342	
13	6	342	
13	Y	342	
13	Z	342	
13	a	342	
13	b	342	
13	c	342	
13	d	342	
13	q	342	
13	r	342	
13	s	342	
13	t	342	
13	u	342	
13	v	342	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 144312 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 Flavodoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	169	Total	C	N	O	S	0	0
			1318	831	210	275	2		
12	X	169	Total	C	N	O	S	0	0
			1318	831	210	275	2		
12	p	169	Total	C	N	O	S	0	0
			1318	831	210	275	2		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-2	GLY	-	expression tag	UNP P10340
P	-1	SER	-	expression tag	UNP P10340
P	0	HIS	-	expression tag	UNP P10340
X	-2	GLY	-	expression tag	UNP P10340
X	-1	SER	-	expression tag	UNP P10340
X	0	HIS	-	expression tag	UNP P10340
p	-2	GLY	-	expression tag	UNP P10340
p	-1	SER	-	expression tag	UNP P10340
p	0	HIS	-	expression tag	UNP P10340

- Molecule 13 is a protein called Iron stress-induced chlorophyll-binding protein.

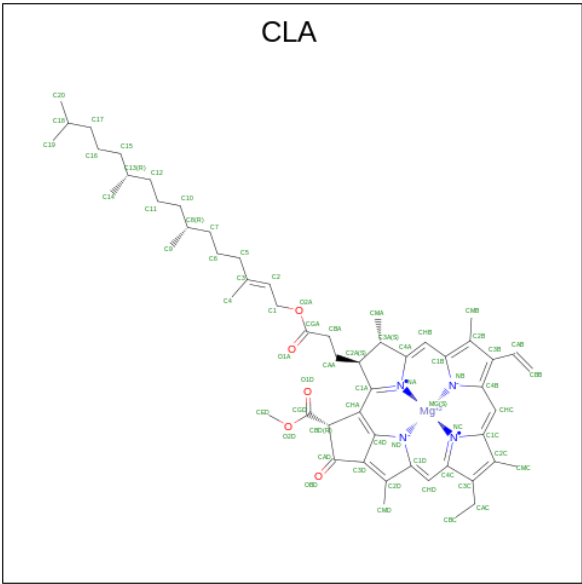
Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	2	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	3	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	4	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	5	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	6	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	Y	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	Z	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	a	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	b	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	c	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	d	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	q	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	r	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	s	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	t	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	u	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
13	v	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	B	1	Total 63	C 53	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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[illegible]

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Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	H	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	H	1	Total 61	C 51	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	H	1	Total 63	C 53	Mg 1	N 4	O 5	0
14	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	H	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	H	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	T	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	U	1	Total 48	C 38	Mg 1	N 4	O 5	0
14	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	V	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	V	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	e	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	e	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	e	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	f	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	f	1	Total 61	C 51	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	f	1	Total 63	C 53	Mg 1	N 4	O 5	0
14	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	f	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	f	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	l	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	l	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	m	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	m	1	Total 48	C 38	Mg 1	N 4	O 5	0
14	m	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	n	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	r	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0

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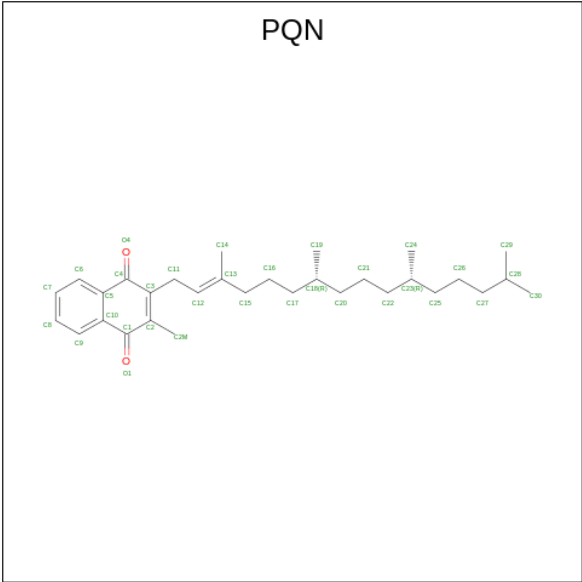
Mol	Chain	Residues	Atoms					AltConf
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	u	1	Total 45	C 35	Mg 1	N 4	O 5	0

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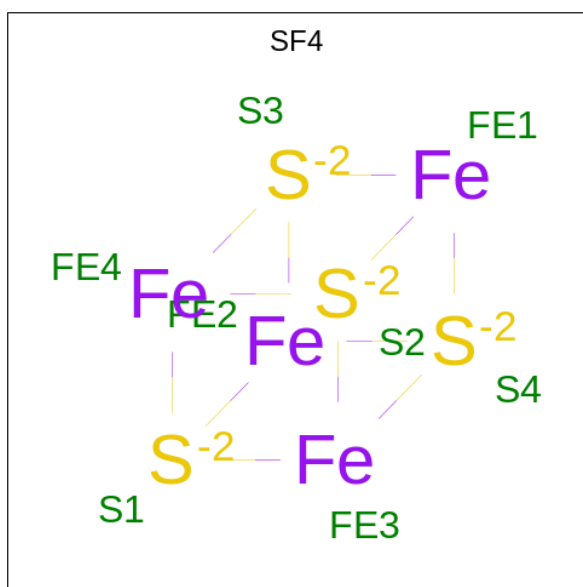
Mol	Chain	Residues	Atoms					AltConf
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



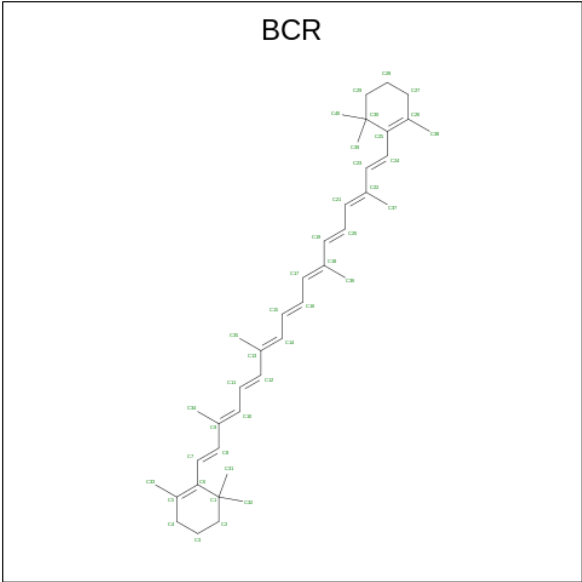
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			33	31	2	
15	B	1	Total	C	O	0
			33	31	2	
15	G	1	Total	C	O	0
			33	31	2	
15	H	1	Total	C	O	0
			33	31	2	
15	e	1	Total	C	O	0
			33	31	2	
15	f	1	Total	C	O	0
			33	31	2	

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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Mol	Chain	Residues	Atoms	AltConf
17	I	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	M	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	3	1	Total C 40 40	0
17	3	1	Total C 40 40	0
17	3	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	3	1	Total C 40 40	0
17	4	1	Total C 40 40	0
17	4	1	Total C 40 40	0
17	4	1	Total C 40 40	0
17	4	1	Total C 40 40	0
17	5	1	Total C 40 40	0
17	5	1	Total C 40 40	0
17	5	1	Total C 40 40	0
17	5	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	H	1	Total C 40 40	0
17	H	1	Total C 40 40	0

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

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

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

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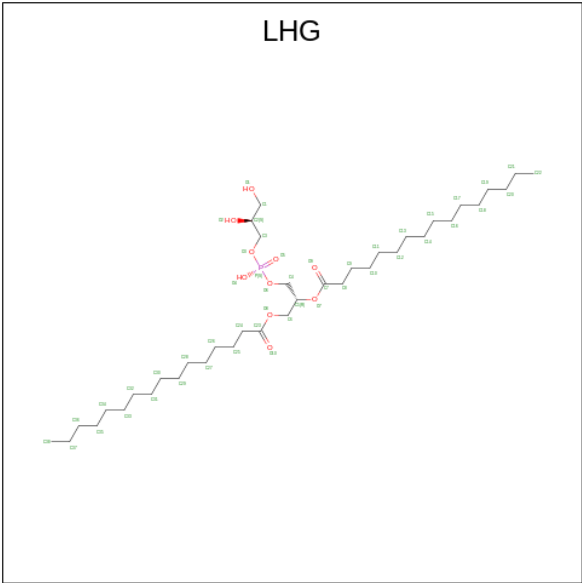
Mol	Chain	Residues	Atoms	AltConf
17	o	1	Total C 40 40	0
17	q	1	Total C 40 40	0
17	q	1	Total C 40 40	0
17	q	1	Total C 40 40	0
17	q	1	Total C 40 40	0
17	r	1	Total C 40 40	0
17	r	1	Total C 40 40	0
17	r	1	Total C 40 40	0
17	r	1	Total C 40 40	0
17	s	1	Total C 40 40	0
17	s	1	Total C 40 40	0
17	s	1	Total C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

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

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			43	32	10	1	
18	A	1	Total	C	O	P	0
			35	24	10	1	
18	A	1	Total	C	O	P	0
			43	32	10	1	
18	A	1	Total	C	O	P	0
			40	29	10	1	
18	A	1	Total	C	O	P	0
			47	36	10	1	
18	A	1	Total	C	O	P	0
			35	24	10	1	
18	A	1	Total	C	O	P	0
			42	31	10	1	

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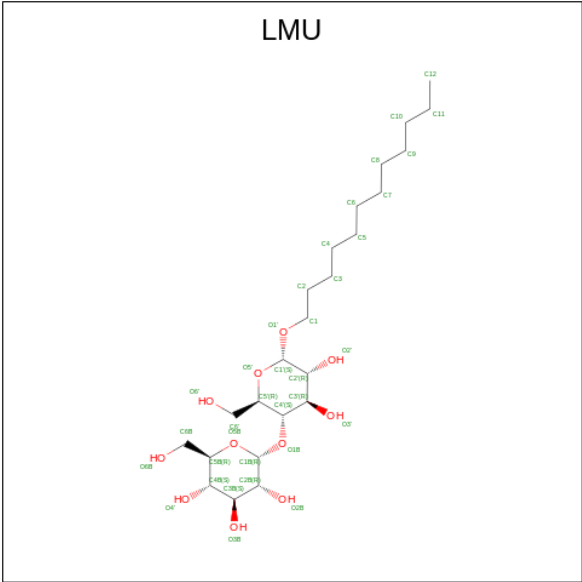
Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total 49	C 38	O 10	P 1	0
18	A	1	Total 40	C 29	O 10	P 1	0
18	B	1	Total 37	C 26	O 10	P 1	0
18	B	1	Total 41	C 30	O 10	P 1	0
18	I	1	Total 48	C 37	O 10	P 1	0
18	L	1	Total 37	C 26	O 10	P 1	0
18	L	1	Total 41	C 30	O 10	P 1	0
18	L	1	Total 49	C 38	O 10	P 1	0
18	G	1	Total 43	C 32	O 10	P 1	0
18	G	1	Total 35	C 24	O 10	P 1	0
18	G	1	Total 43	C 32	O 10	P 1	0
18	G	1	Total 40	C 29	O 10	P 1	0
18	G	1	Total 47	C 36	O 10	P 1	0
18	G	1	Total 35	C 24	O 10	P 1	0
18	G	1	Total 42	C 31	O 10	P 1	0
18	G	1	Total 49	C 38	O 10	P 1	0
18	G	1	Total 40	C 29	O 10	P 1	0
18	H	1	Total 37	C 26	O 10	P 1	0
18	H	1	Total 41	C 30	O 10	P 1	0
18	S	1	Total 48	C 37	O 10	P 1	0
18	V	1	Total 37	C 26	O 10	P 1	0

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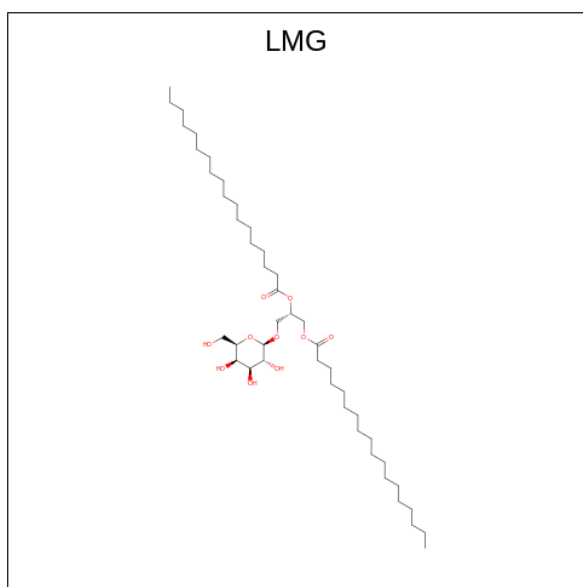
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			41	30	10	1	
18	V	1	Total	C	O	P	0
			49	38	10	1	
18	e	1	Total	C	O	P	0
			43	32	10	1	
18	e	1	Total	C	O	P	0
			35	24	10	1	
18	e	1	Total	C	O	P	0
			43	32	10	1	
18	e	1	Total	C	O	P	0
			40	29	10	1	
18	e	1	Total	C	O	P	0
			47	36	10	1	
18	e	1	Total	C	O	P	0
			35	24	10	1	
18	e	1	Total	C	O	P	0
			42	31	10	1	
18	e	1	Total	C	O	P	0
			49	38	10	1	
18	e	1	Total	C	O	P	0
			40	29	10	1	
18	f	1	Total	C	O	P	0
			37	26	10	1	
18	f	1	Total	C	O	P	0
			41	30	10	1	
18	k	1	Total	C	O	P	0
			48	37	10	1	
18	n	1	Total	C	O	P	0
			37	26	10	1	
18	n	1	Total	C	O	P	0
			41	30	10	1	
18	n	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 19 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



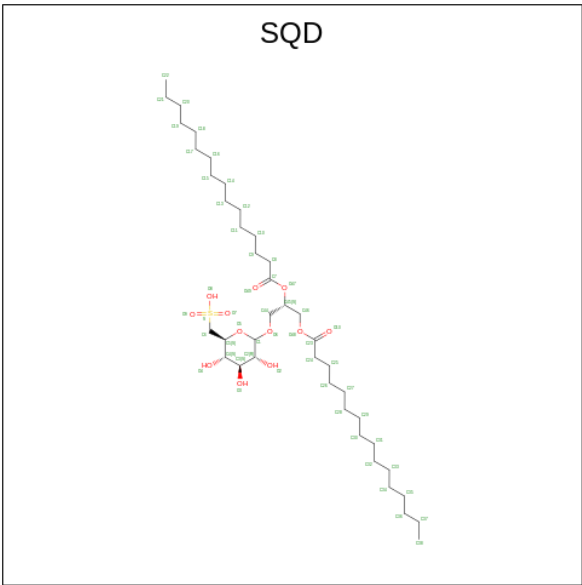
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			35	24	11	
19	A	1	Total	C	O	0
			23	17	6	
19	B	1	Total	C	O	0
			35	24	11	
19	J	1	Total	C	O	0
			22	16	6	
19	G	1	Total	C	O	0
			35	24	11	
19	G	1	Total	C	O	0
			23	17	6	
19	H	1	Total	C	O	0
			35	24	11	
19	T	1	Total	C	O	0
			22	16	6	
19	e	1	Total	C	O	0
			35	24	11	
19	e	1	Total	C	O	0
			23	17	6	
19	f	1	Total	C	O	0
			35	24	11	
19	l	1	Total	C	O	0
			22	16	6	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
20	B	1	Total	C	O	0
			53	43	10	
20	J	1	Total	C	O	0
			32	22	10	
20	H	1	Total	C	O	0
			53	43	10	
20	T	1	Total	C	O	0
			32	22	10	
20	f	1	Total	C	O	0
			53	43	10	
20	l	1	Total	C	O	0
			32	22	10	

- Molecule 21 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				AltConf
21	B	1	Total	C	O	S	0
			40	27	12	1	
21	L	1	Total	C	O	S	0
			46	33	12	1	
21	1	1	Total	C	O	S	0
			32	19	12	1	
21	2	1	Total	C	O	S	0
			28	15	12	1	
21	3	1	Total	C	O	S	0
			28	15	12	1	
21	4	1	Total	C	O	S	0
			26	13	12	1	
21	5	1	Total	C	O	S	0
			26	13	12	1	
21	6	1	Total	C	O	S	0
			26	13	12	1	
21	H	1	Total	C	O	S	0
			40	27	12	1	
21	V	1	Total	C	O	S	0
			46	33	12	1	
21	Y	1	Total	C	O	S	0
			32	19	12	1	
21	Z	1	Total	C	O	S	0
			28	15	12	1	
21	a	1	Total	C	O	S	0
			28	15	12	1	
21	b	1	Total	C	O	S	0
			26	13	12	1	

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Mol	Chain	Residues	Atoms				AltConf
21	c	1	Total 26	C 13	O 12	S 1	0
21	d	1	Total 26	C 13	O 12	S 1	0
21	f	1	Total 40	C 27	O 12	S 1	0
21	n	1	Total 46	C 33	O 12	S 1	0
21	q	1	Total 32	C 19	O 12	S 1	0
21	r	1	Total 28	C 15	O 12	S 1	0
21	s	1	Total 28	C 15	O 12	S 1	0
21	t	1	Total 26	C 13	O 12	S 1	0
21	u	1	Total 26	C 13	O 12	S 1	0
21	v	1	Total 26	C 13	O 12	S 1	0

-
- The chemical structure of FMN (Flavin Mononucleotide) is shown. It consists of an isoalloxazine ring system (a fused bicyclic system with two nitrogen atoms) and a ribityl chain. The ribityl chain is attached to the ring at the N10 position. The ribityl chain is a three-carbon chain with hydroxyl groups at the C2' and C3' positions. The C4' position is attached to a phosphate group (O3P). The phosphate group is shown as a phosphorus atom (P) bonded to four oxygen atoms: one double-bonded oxygen (O1P) and three single-bonded oxygens (O2P, O3P, O4P). The ribityl chain is shown with stereochemistry: the C2' hydroxyl group is on a wedge, the C3' hydroxyl group is on a dash, and the C4' phosphate group is on a wedge.

Mol	Chain	Residues	Atoms					AltConf
22	P	1	Total 31	C 17	N 4	O 9	P 1	0



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Mol	Chain	Residues	Atoms					AltConf
22	X	1	Total	C	N	O	P	0
			31	17	4	9	1	
22	p	1	Total	C	N	O	P	0
			31	17	4	9	1	

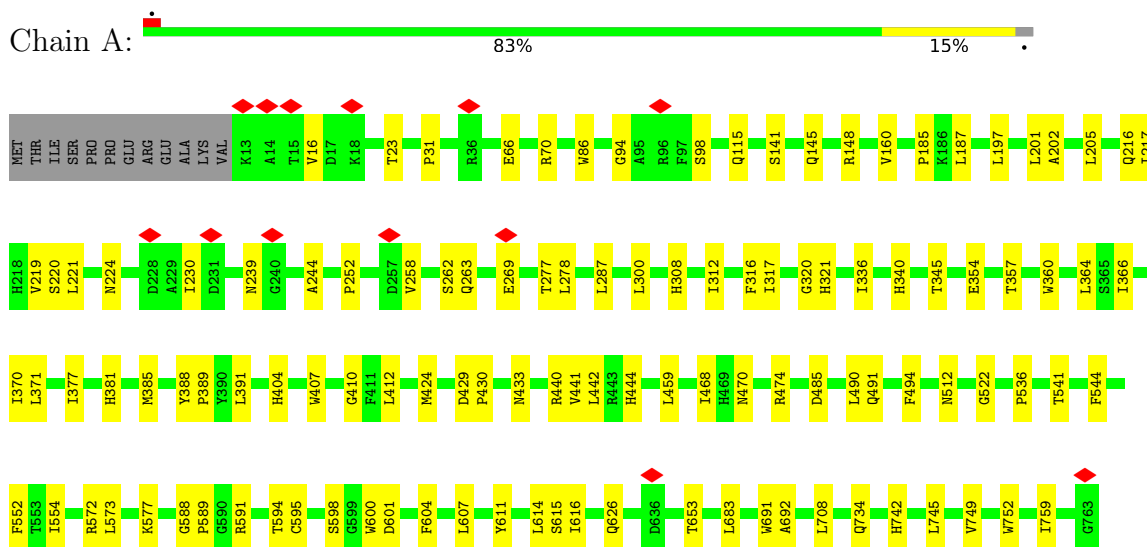
- Molecule 23 is water.

Mol	Chain	Residues	Atoms		AltConf
23	A	9	Total	O	0
			9	9	
23	B	7	Total	O	0
			7	7	
23	F	1	Total	O	0
			1	1	
23	L	1	Total	O	0
			1	1	
23	G	9	Total	O	0
			9	9	
23	H	7	Total	O	0
			7	7	
23	R	1	Total	O	0
			1	1	
23	V	1	Total	O	0
			1	1	
23	e	9	Total	O	0
			9	9	
23	f	7	Total	O	0
			7	7	
23	j	1	Total	O	0
			1	1	
23	n	1	Total	O	0
			1	1	

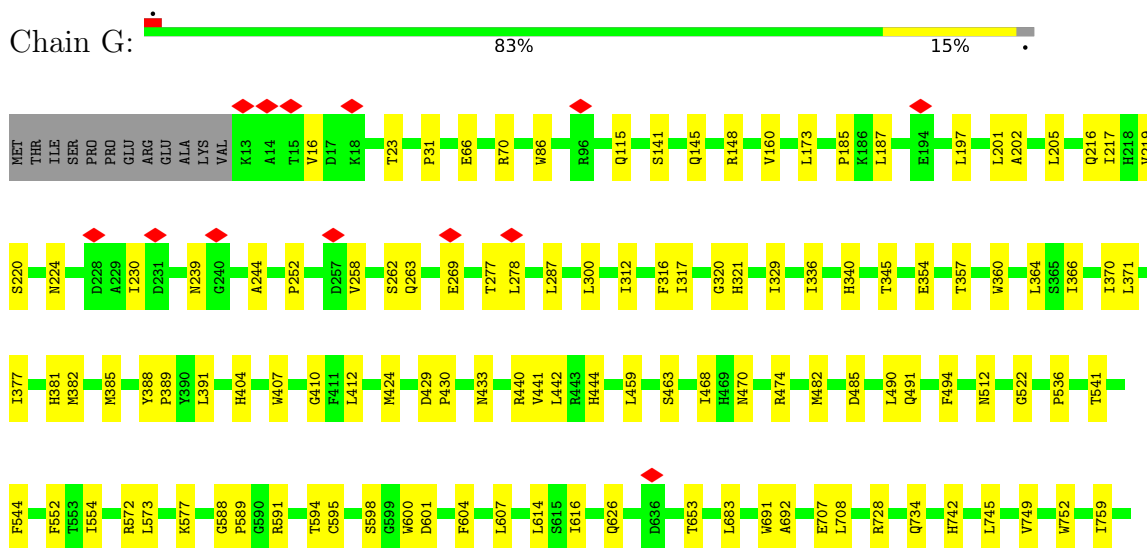
3 Residue-property plots

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

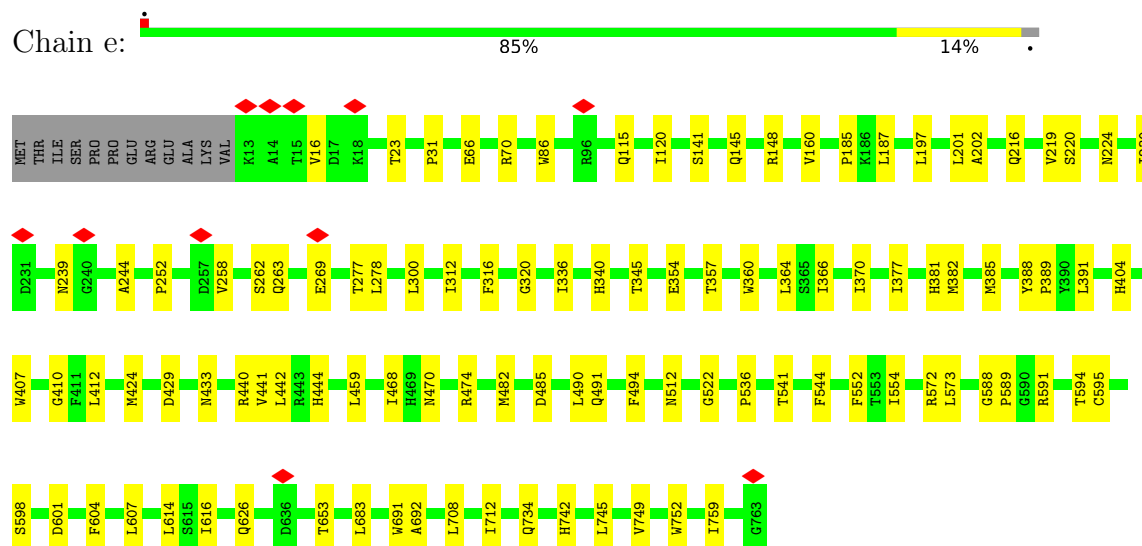


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

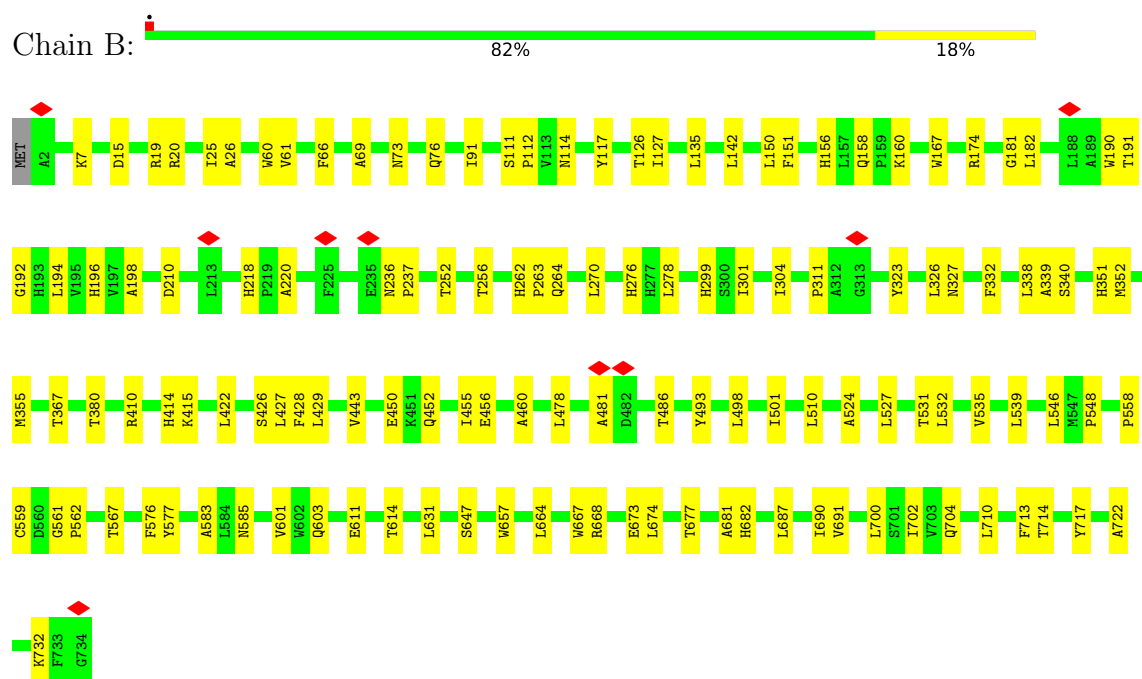




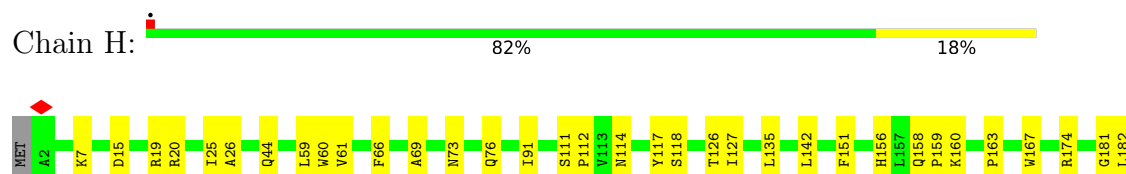
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

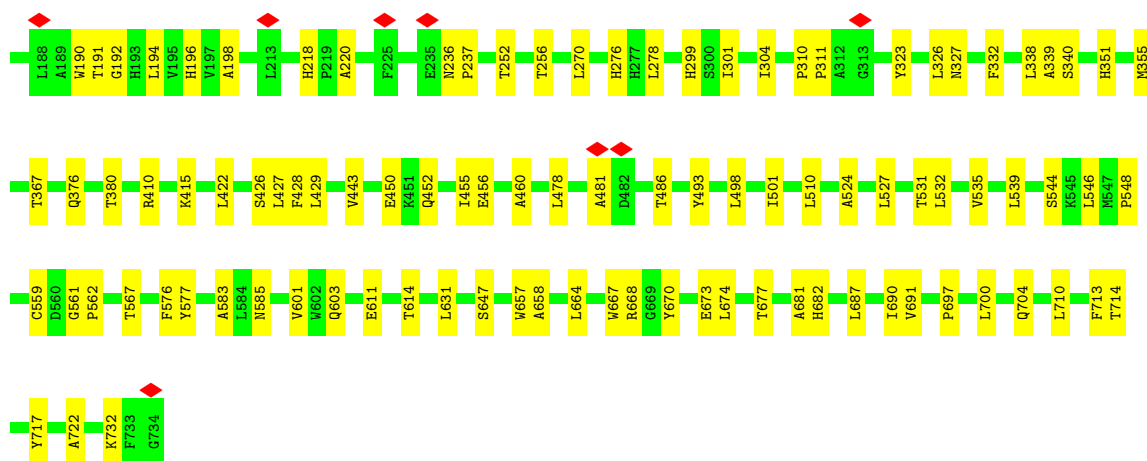


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

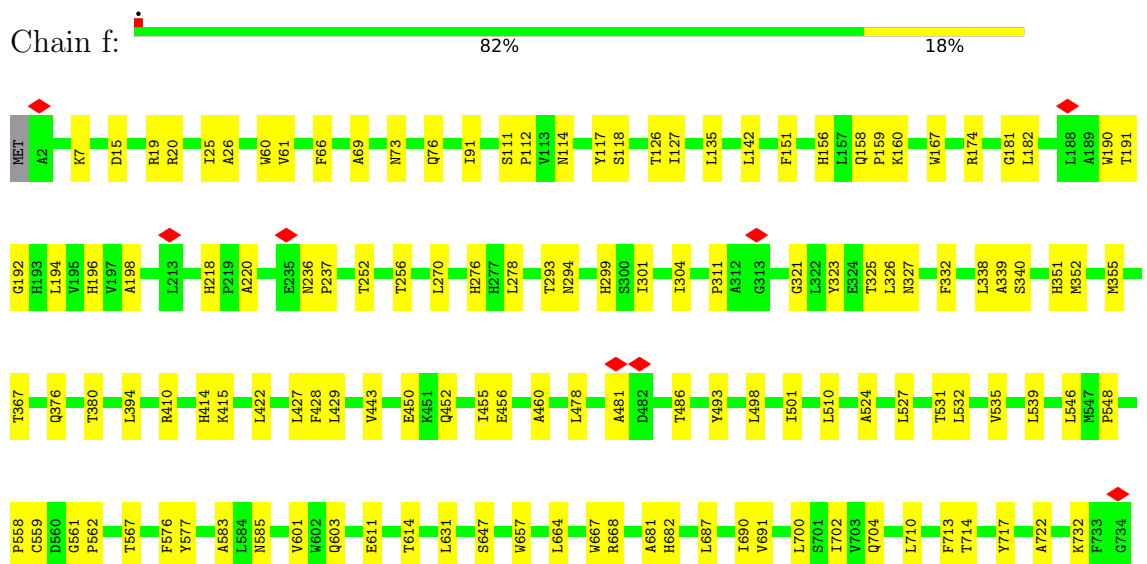


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

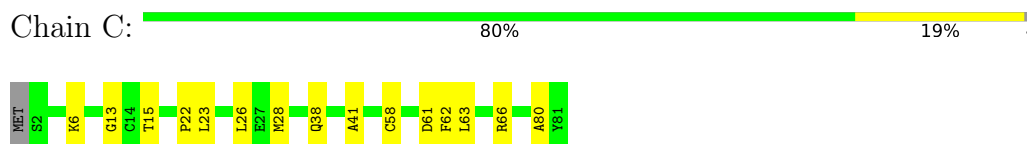




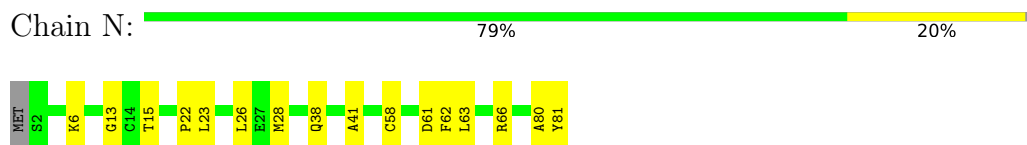
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



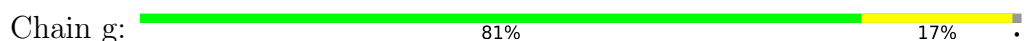
- Molecule 3: Photosystem I iron-sulfur center



- Molecule 3: Photosystem I iron-sulfur center

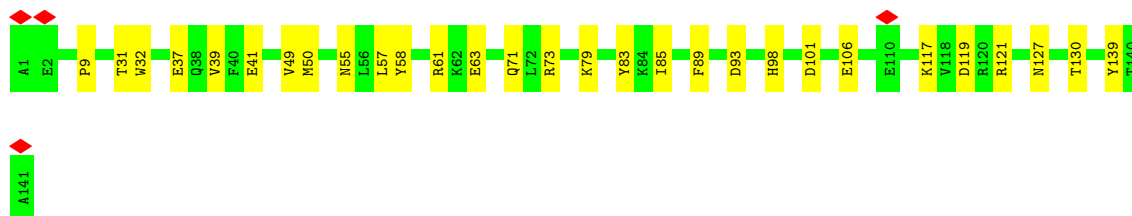
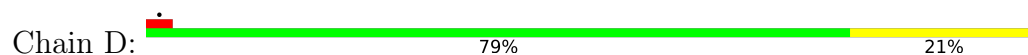


- Molecule 3: Photosystem I iron-sulfur center

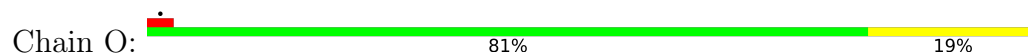




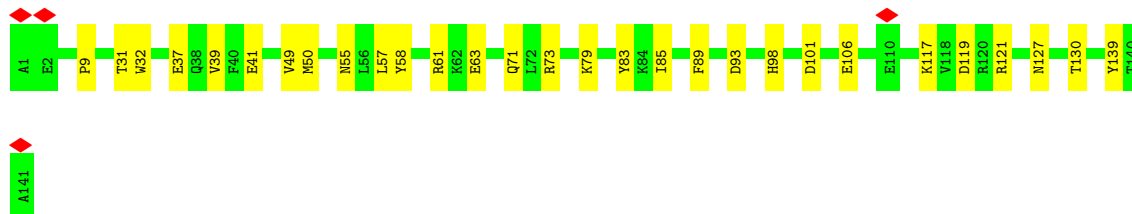
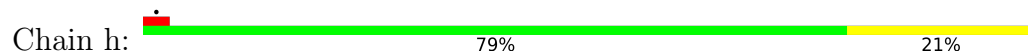
- Molecule 4: Photosystem I reaction center subunit II



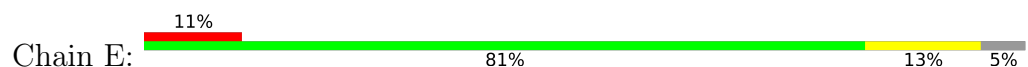
- Molecule 4: Photosystem I reaction center subunit II



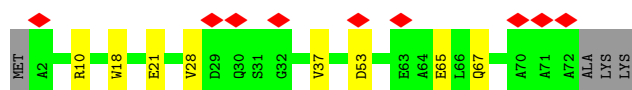
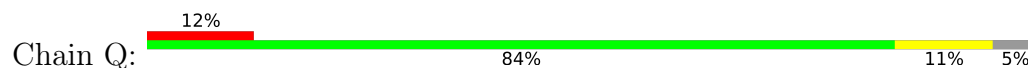
- Molecule 4: Photosystem I reaction center subunit II



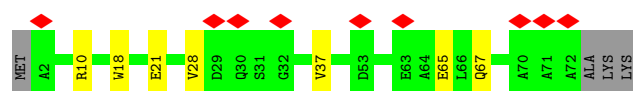
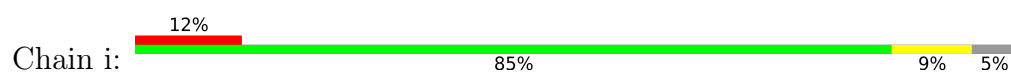
- Molecule 5: Photosystem I reaction center subunit IV



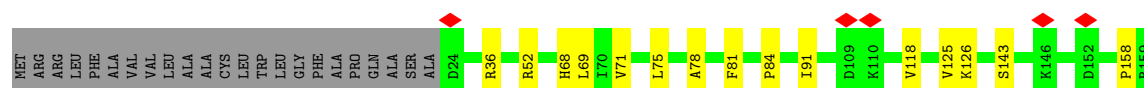
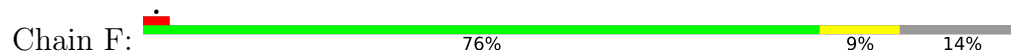
- Molecule 5: Photosystem I reaction center subunit IV



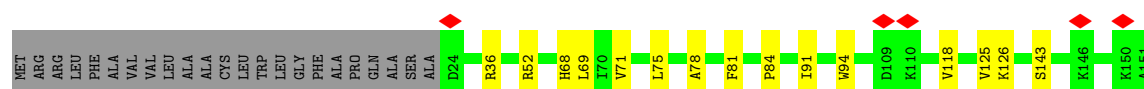
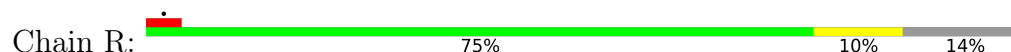
- Molecule 5: Photosystem I reaction center subunit IV



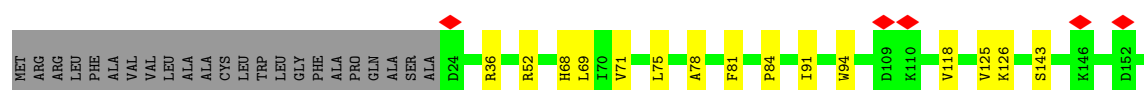
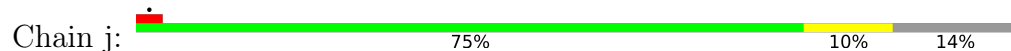
- Molecule 6: Photosystem I reaction center subunit III



- Molecule 6: Photosystem I reaction center subunit III



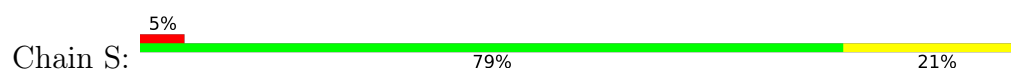
- Molecule 6: Photosystem I reaction center subunit III



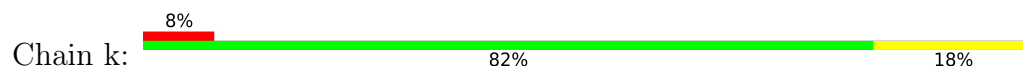
- Molecule 7: Photosystem I PsaI protein



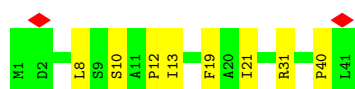
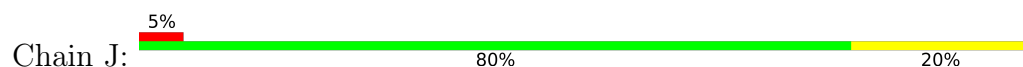
- Molecule 7: Photosystem I PsaI protein



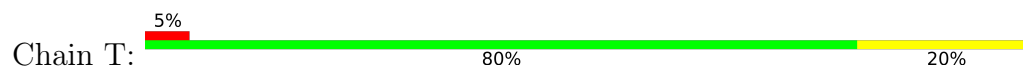
- Molecule 7: Photosystem I PsaI protein



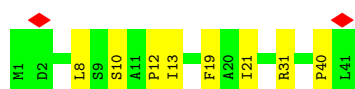
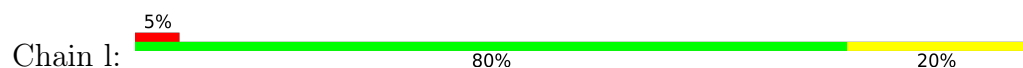
- Molecule 8: Photosystem I reaction center subunit IX



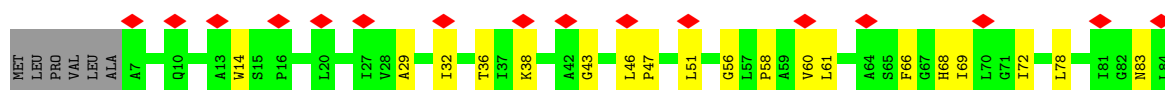
- Molecule 8: Photosystem I reaction center subunit IX



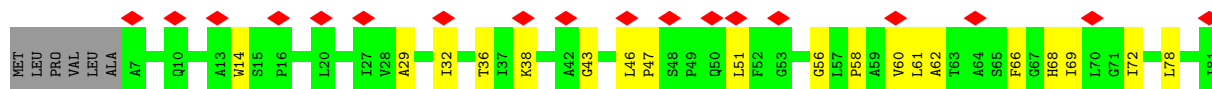
- Molecule 8: Photosystem I reaction center subunit IX



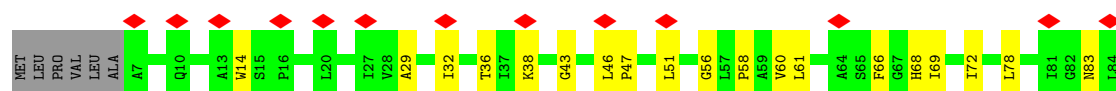
- Molecule 9: Photosystem I reaction center subunit PsaK



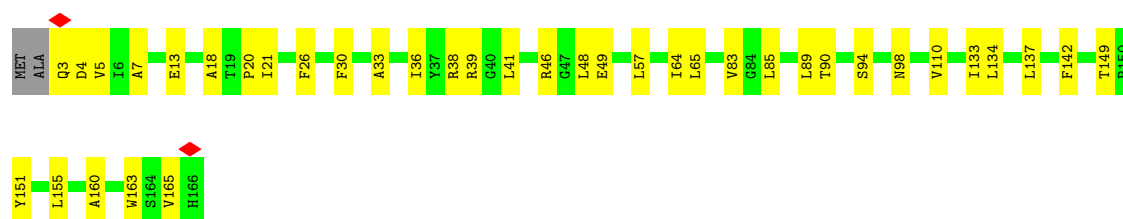
- Molecule 9: Photosystem I reaction center subunit PsaK



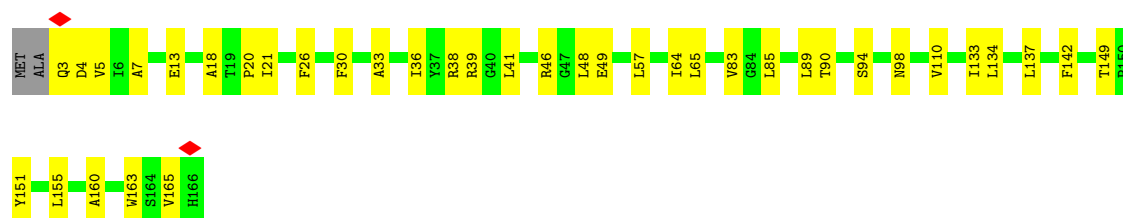
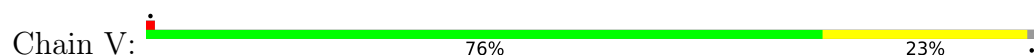
- Molecule 9: Photosystem I reaction center subunit PsaK



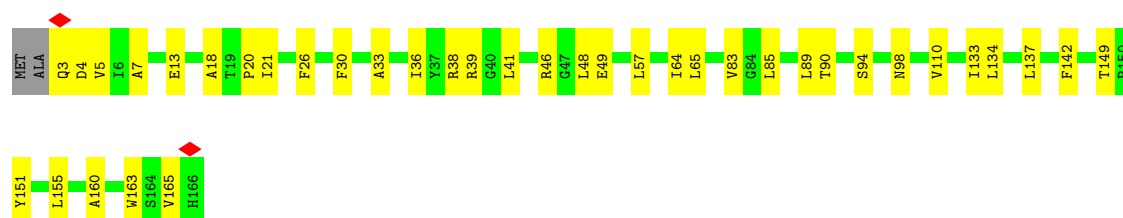
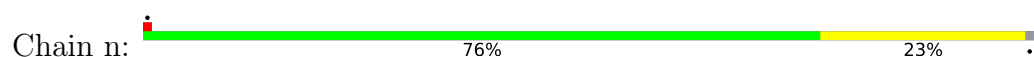
• Molecule 10: Photosystem I reaction center subunit XI



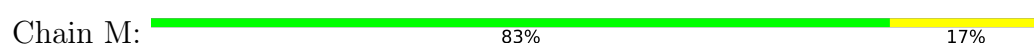
• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 11: Psam

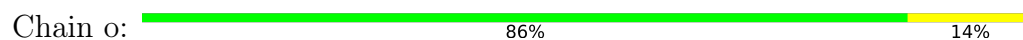


• Molecule 11: Psam

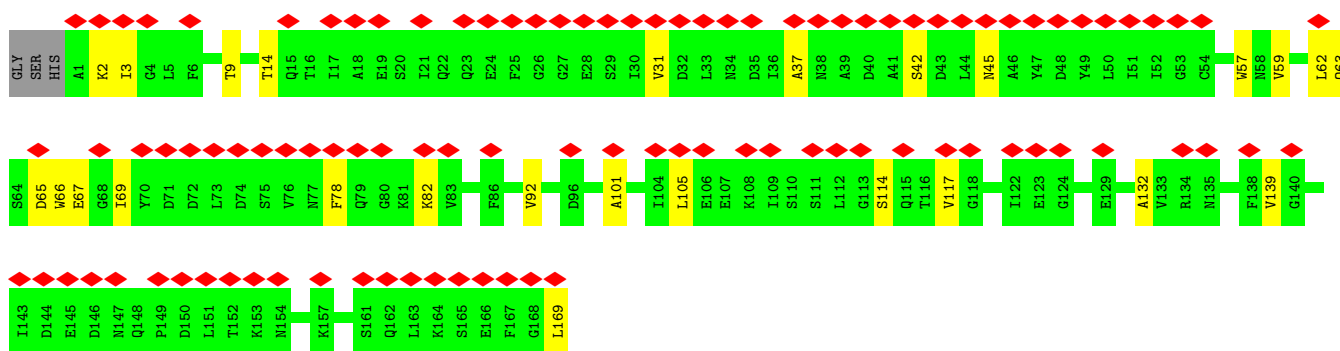
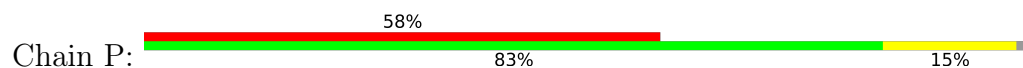




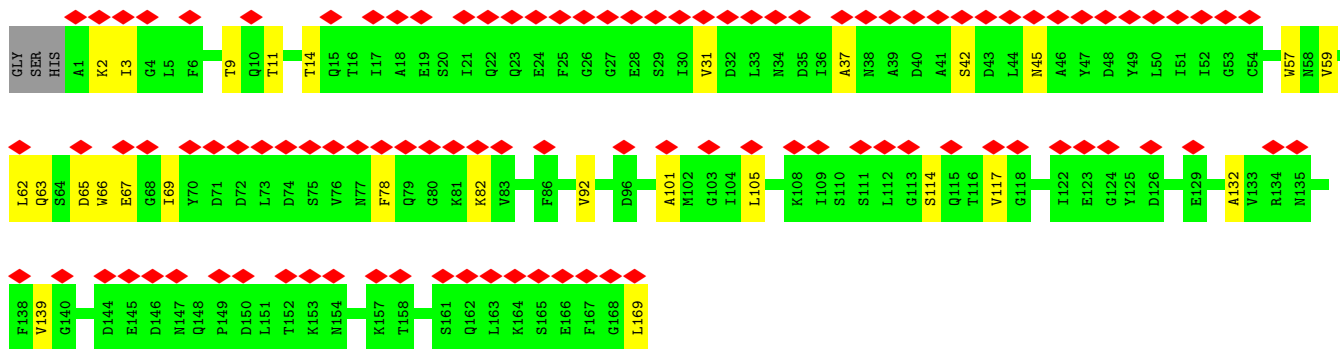
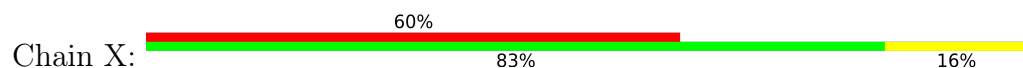
- Molecule 11: PsaM



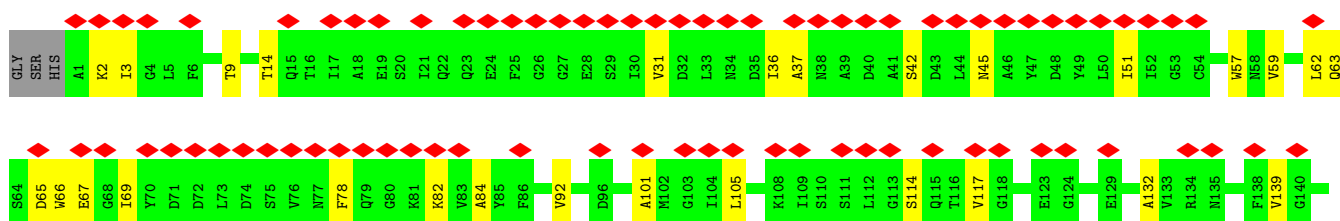
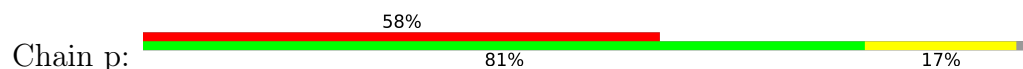
- Molecule 12: Flavodoxin

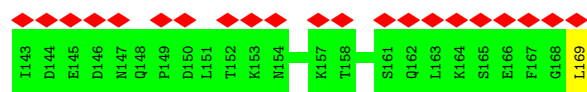


- Molecule 12: Flavodoxin

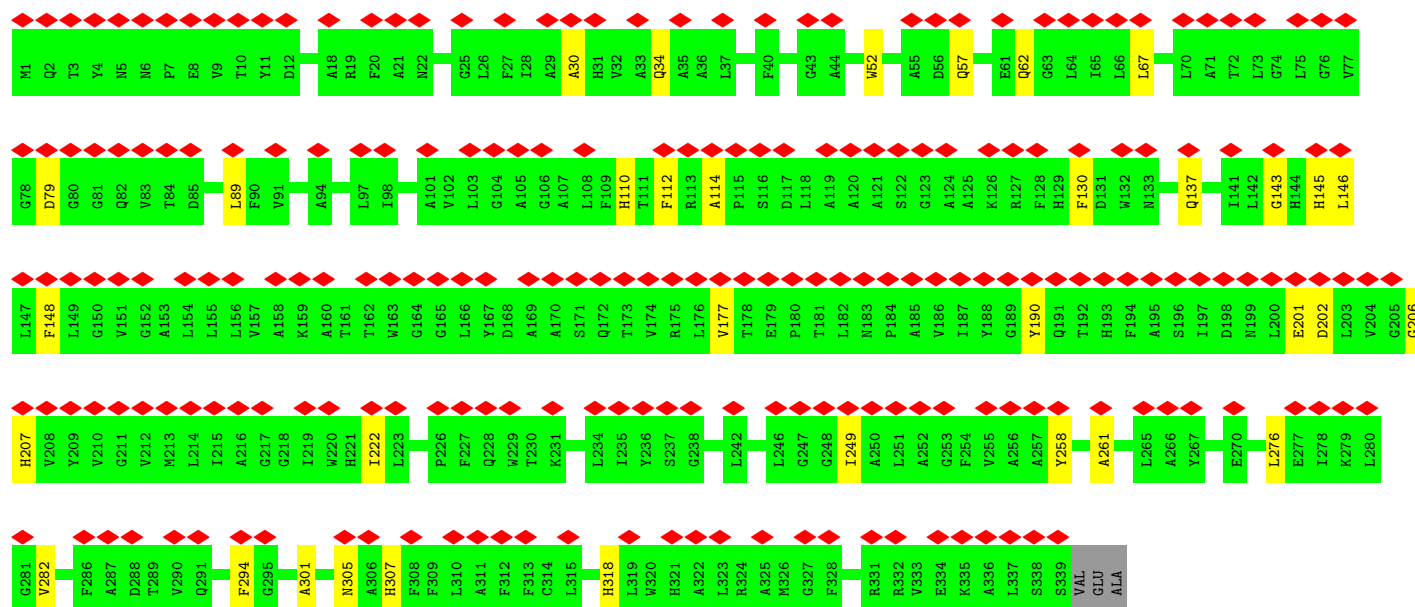
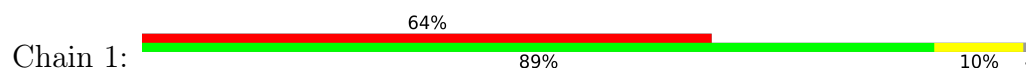


- Molecule 12: Flavodoxin

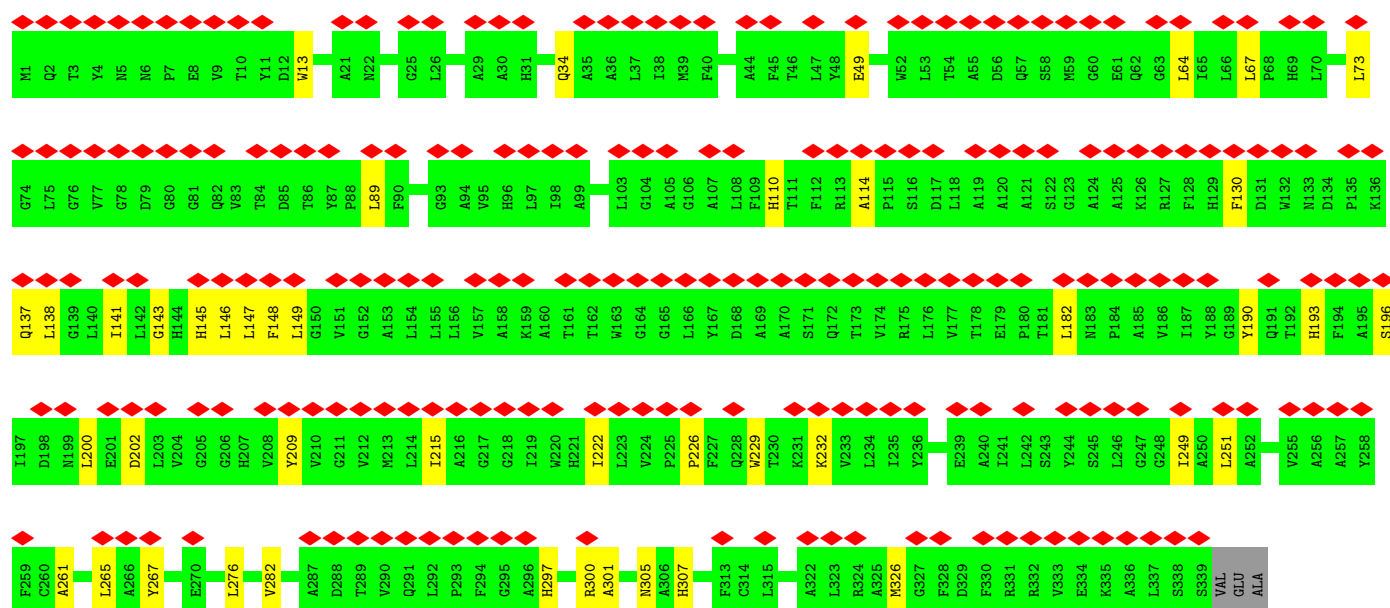
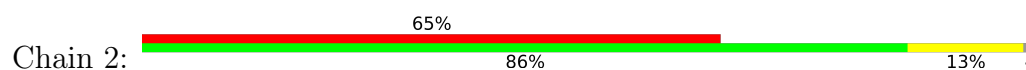




• Molecule 13: Iron stress-induced chlorophyll-binding protein

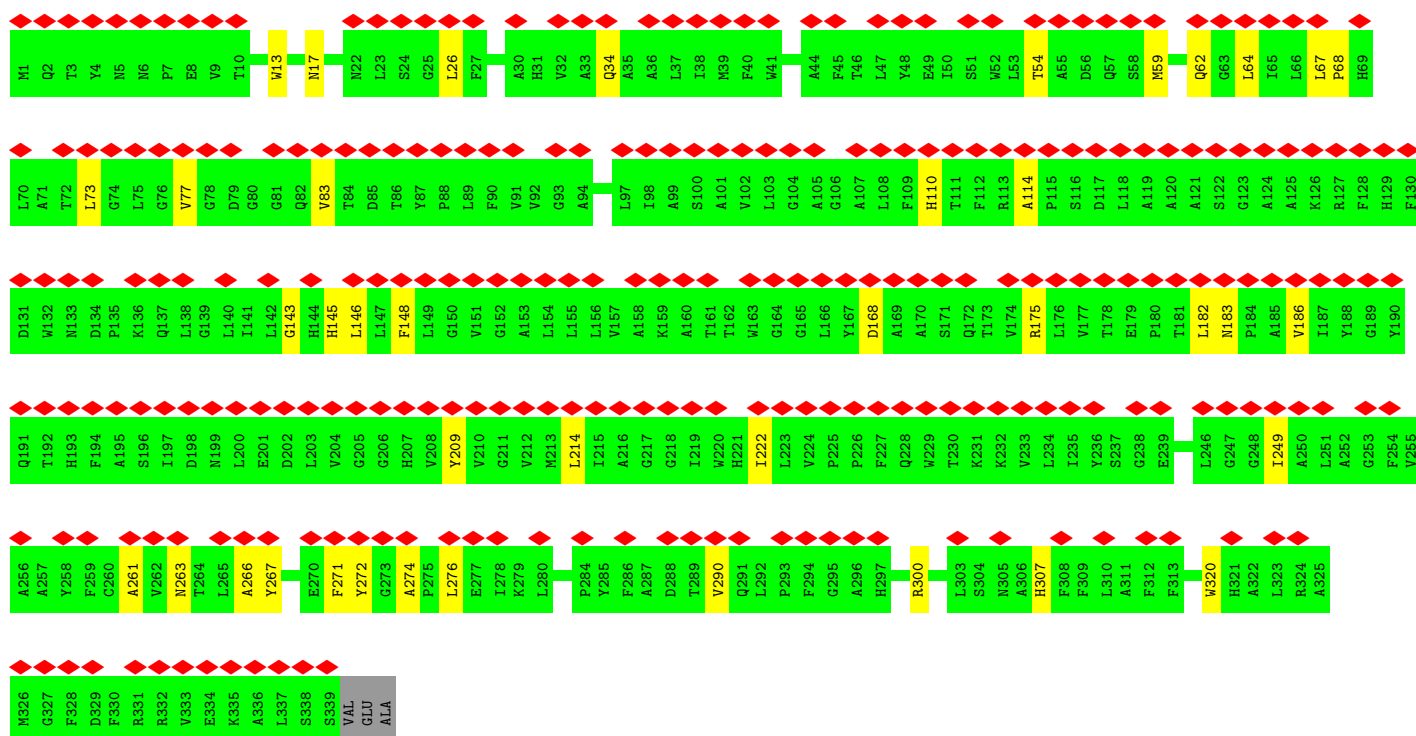


• Molecule 13: Iron stress-induced chlorophyll-binding protein

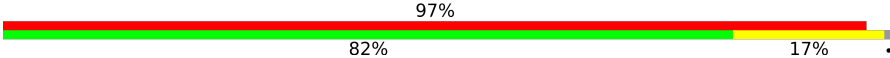


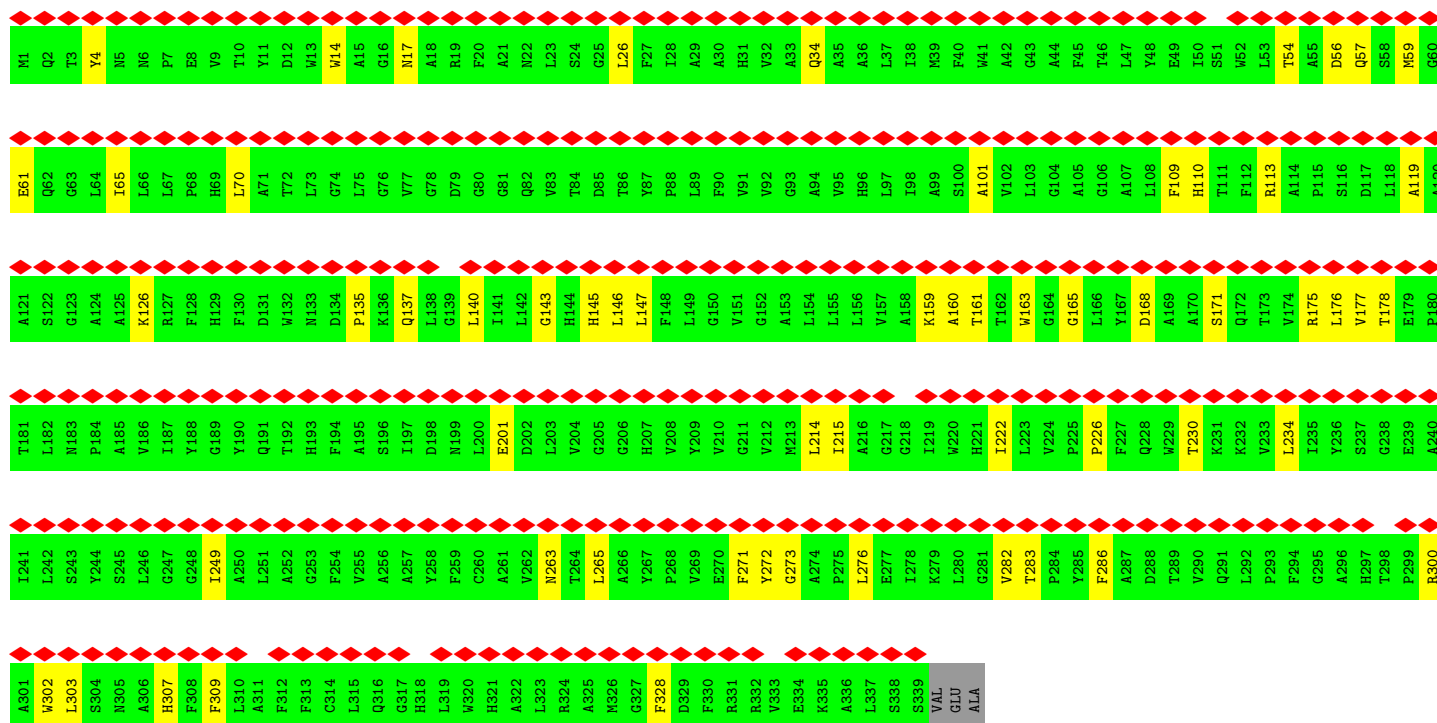
• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain 3: 

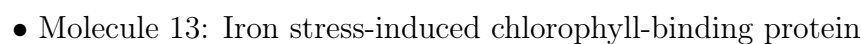
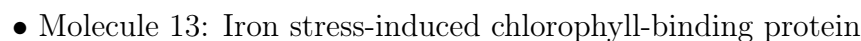


- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain 4: 



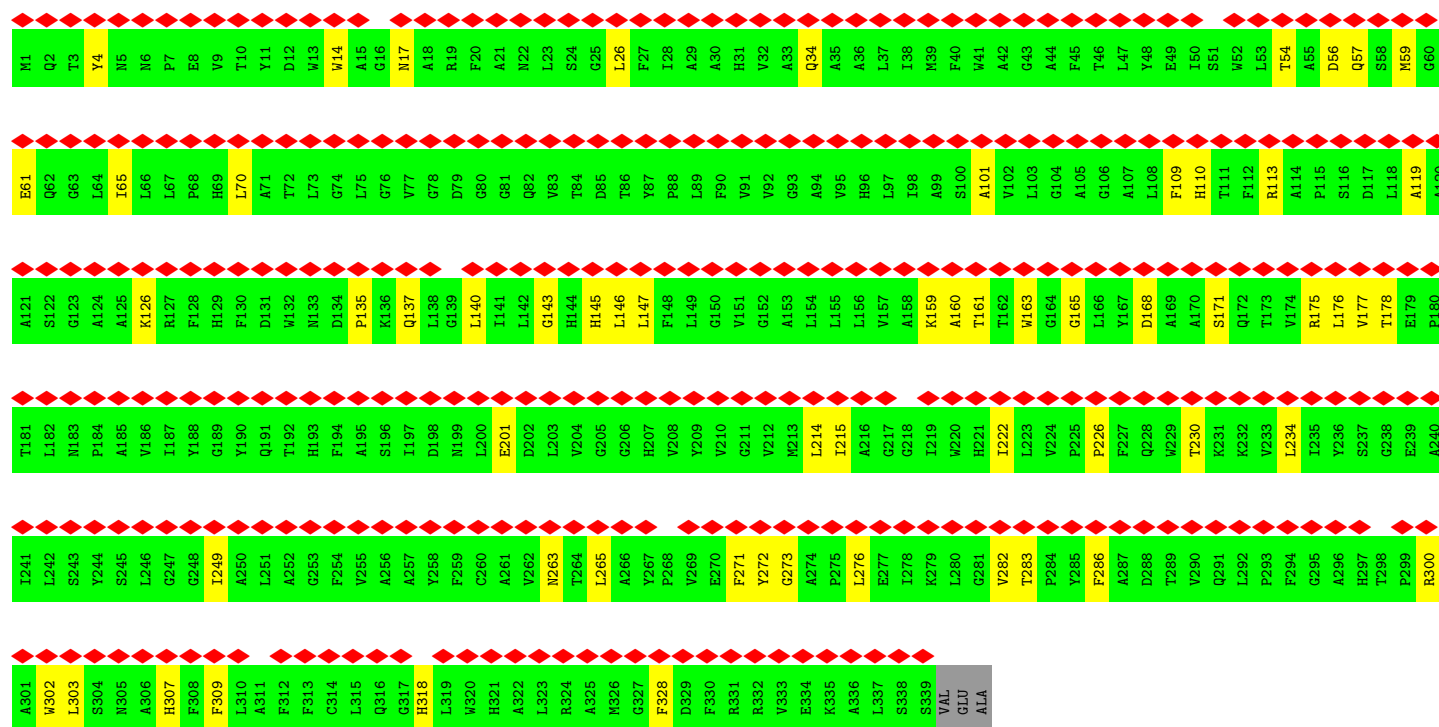
- Molecule 13: Iron stress-induced chlorophyll-binding protein





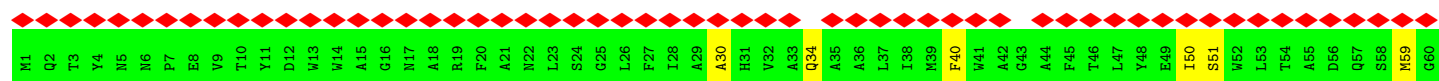
• Molecule 13: Iron stress-induced chlorophyll-binding protein

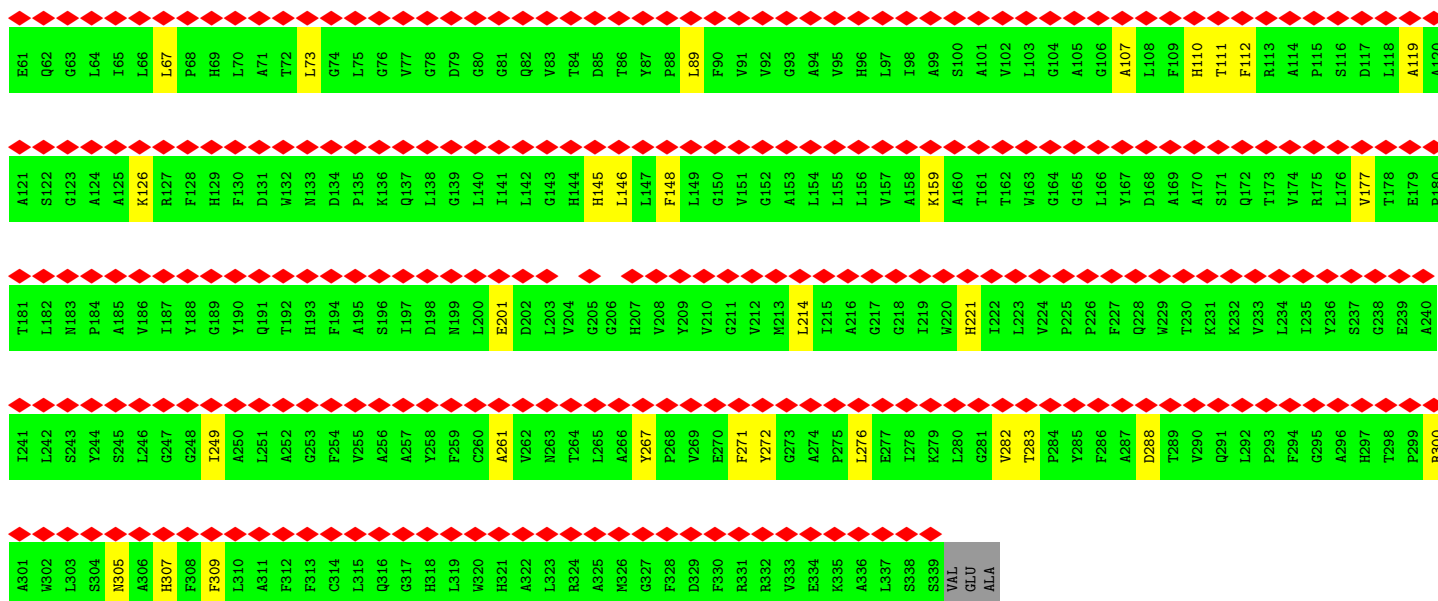
Chain b: 97% 82% 18%

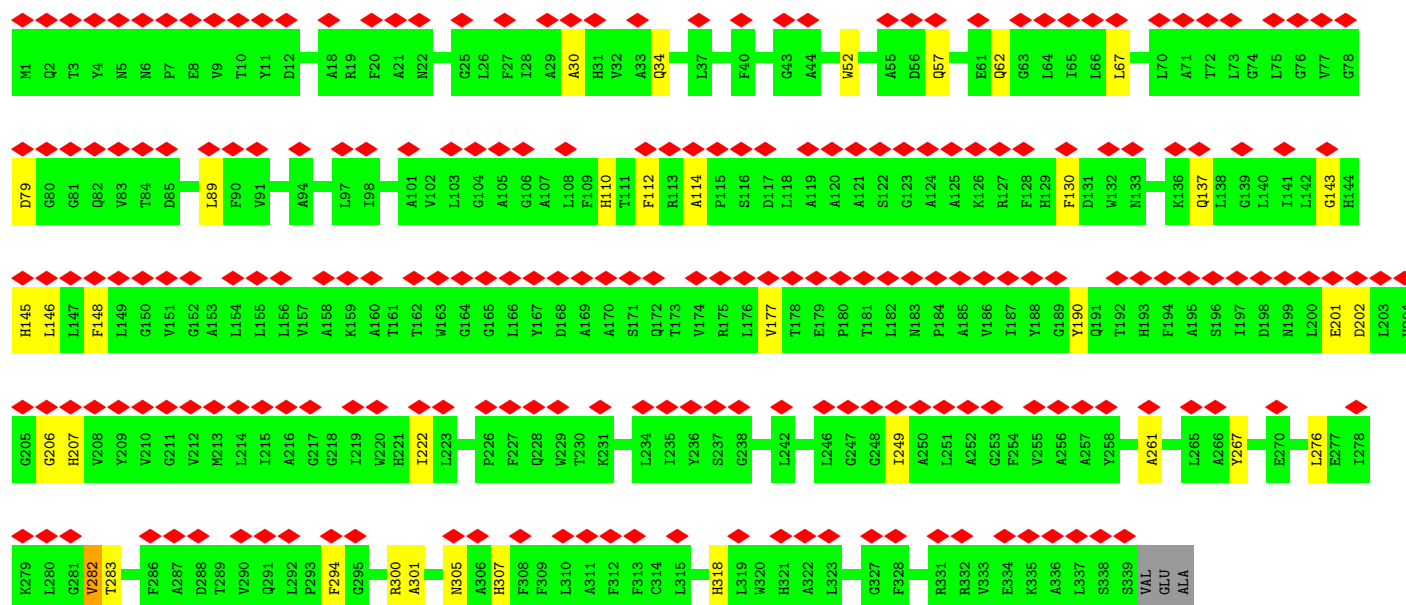


• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain c: 98% 89% 11%

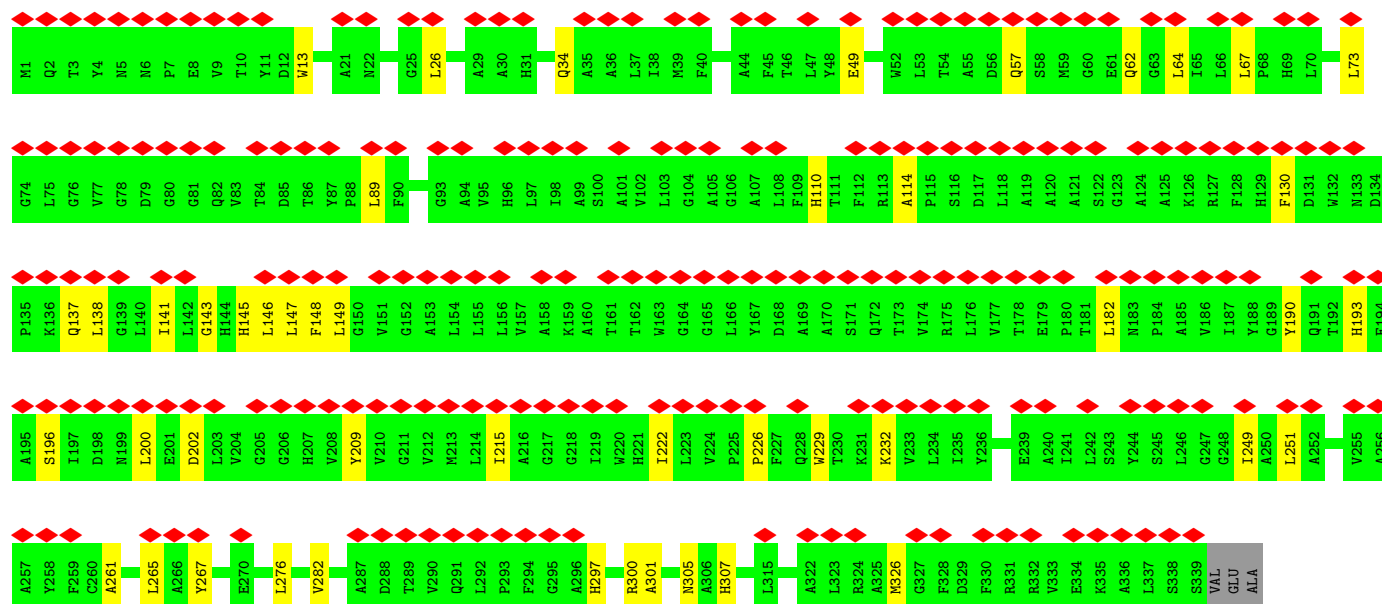






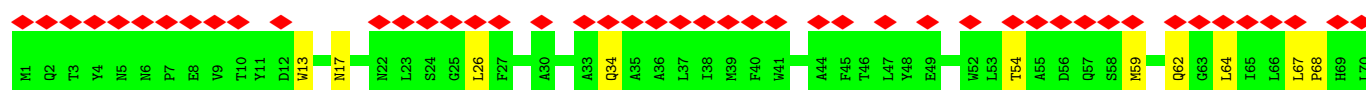
• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain r: 65% 85% 14%



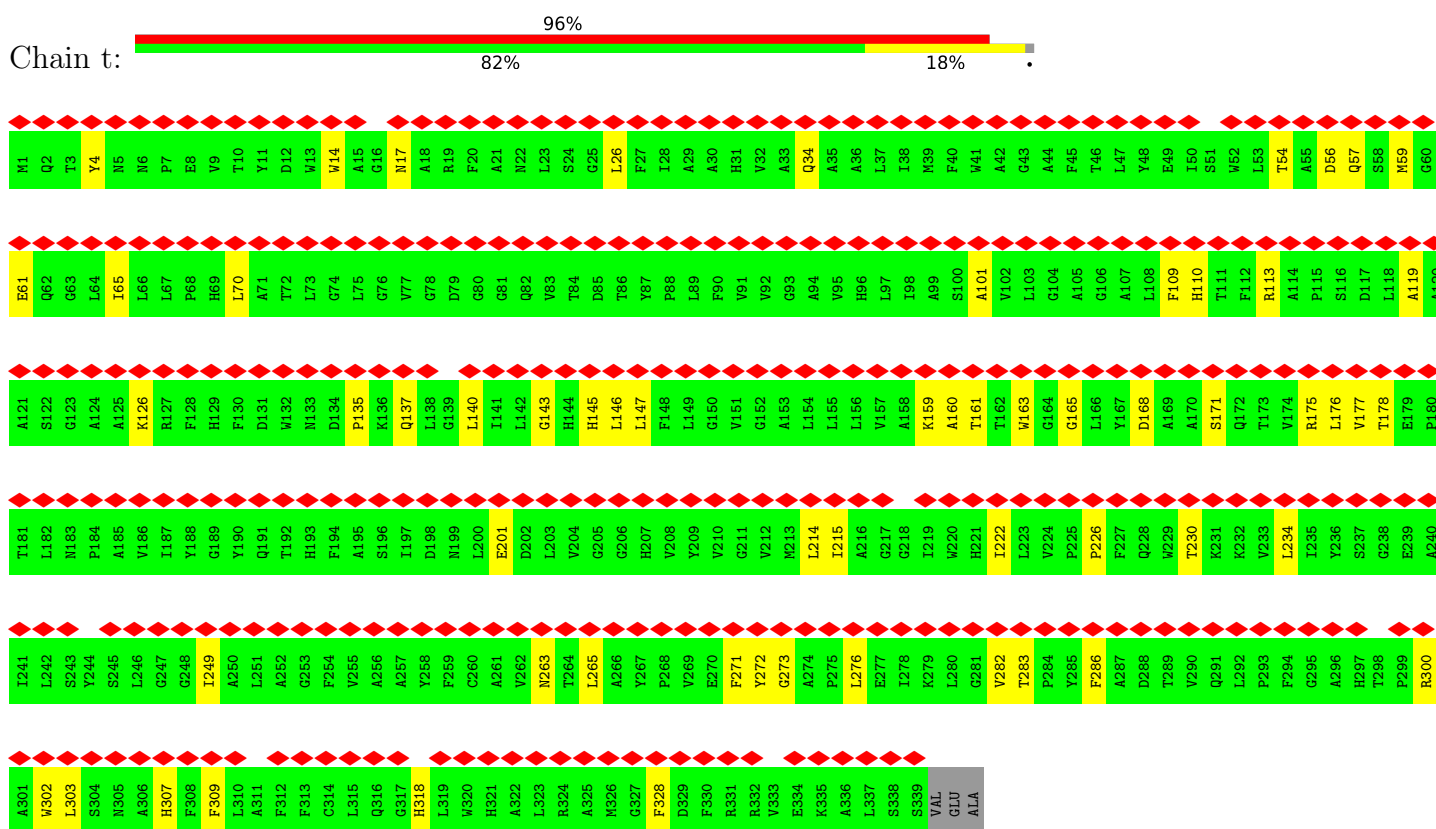
• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain s: 75% 87% 12%

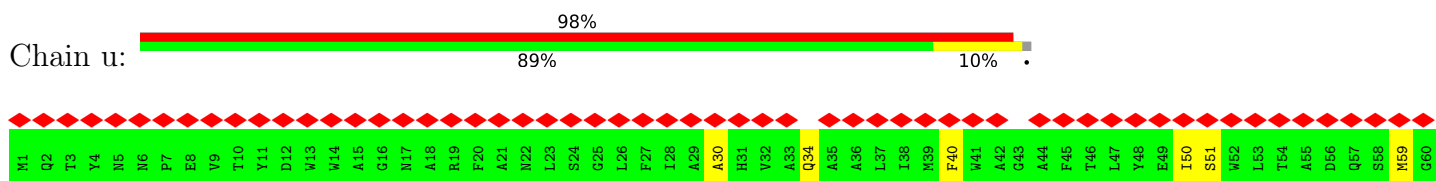


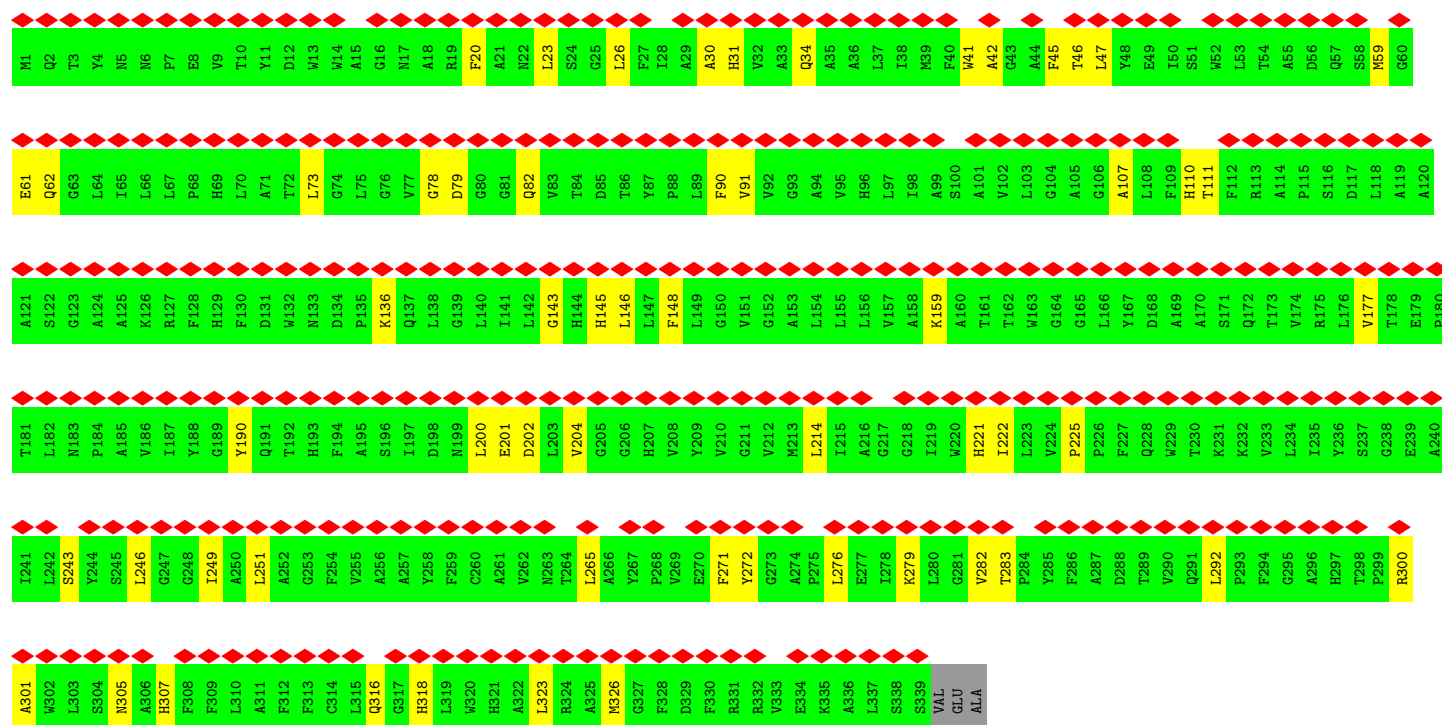


• Molecule 13: Iron stress-induced chlorophyll-binding protein



• Molecule 13: 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	29295	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	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	0.118	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.50	0/6064	0.54	0/8274
1	G	0.50	0/6064	0.54	0/8274
1	e	0.50	0/6064	0.54	0/8274
2	B	0.42	0/5999	0.54	1/8199 (0.0%)
2	H	0.42	0/5999	0.54	1/8199 (0.0%)
2	f	0.42	0/5999	0.54	1/8199 (0.0%)
3	C	0.43	0/608	0.61	0/823
3	N	0.43	0/608	0.61	0/823
3	g	0.43	0/608	0.61	0/823
4	D	0.43	0/1124	0.56	0/1516
4	O	0.43	0/1124	0.56	0/1516
4	h	0.43	0/1124	0.56	0/1516
5	E	0.36	0/553	0.54	0/750
5	Q	0.36	0/553	0.54	0/750
5	i	0.36	0/553	0.54	0/750
6	F	0.39	0/1062	0.56	0/1442
6	R	0.39	0/1062	0.56	0/1442
6	j	0.39	0/1062	0.56	0/1442
7	I	0.45	0/289	0.66	0/393
7	S	0.45	0/289	0.66	0/393
7	k	0.45	0/289	0.66	0/393
8	J	0.35	0/346	0.50	0/469
8	T	0.35	0/346	0.50	0/469
8	l	0.35	0/346	0.50	0/469
9	K	0.30	0/560	0.57	0/765
9	U	0.31	0/560	0.57	0/765
9	m	0.31	0/560	0.57	0/765
10	L	0.36	0/1242	0.58	1/1696 (0.1%)
10	V	0.36	0/1242	0.58	1/1696 (0.1%)
10	n	0.36	0/1242	0.58	1/1696 (0.1%)
11	M	0.42	0/231	0.61	0/314
11	W	0.42	0/231	0.61	0/314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	o	0.42	0/231	0.61	0/314
12	P	0.24	0/1344	0.45	0/1822
12	X	0.24	0/1344	0.45	0/1822
12	p	0.24	0/1344	0.45	0/1822
13	1	0.22	0/2689	0.45	1/3678 (0.0%)
13	2	0.21	0/2689	0.44	0/3678
13	3	0.19	0/2689	0.42	0/3678
13	4	0.19	0/2689	0.44	0/3678
13	5	0.19	0/2689	0.44	2/3678 (0.1%)
13	6	0.19	0/2689	0.43	0/3678
13	Y	0.22	0/2689	0.45	1/3678 (0.0%)
13	Z	0.22	0/2689	0.44	0/3678
13	a	0.19	0/2689	0.42	0/3678
13	b	0.19	0/2689	0.44	0/3678
13	c	0.19	0/2689	0.44	2/3678 (0.1%)
13	d	0.19	0/2689	0.43	0/3678
13	q	0.22	0/2689	0.45	1/3678 (0.0%)
13	r	0.22	0/2689	0.44	0/3678
13	s	0.19	0/2689	0.42	0/3678
13	t	0.19	0/2689	0.44	0/3678
13	u	0.19	0/2689	0.44	2/3678 (0.1%)
13	v	0.19	0/2689	0.43	0/3678
All	All	0.34	0/106668	0.50	15/145593 (0.0%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	5	VAL	N-CA-C	7.05	117.84	110.72
10	V	5	VAL	N-CA-C	7.05	117.84	110.72
10	n	5	VAL	N-CA-C	7.05	117.84	110.72
13	1	282	VAL	N-CA-C	-5.65	107.37	112.12
13	Y	282	VAL	N-CA-C	-5.63	107.39	112.12

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	94	0
1	G	5865	0	5744	98	0
1	e	5865	0	5744	85	0
2	B	5789	0	5575	106	0
2	H	5789	0	5575	110	0
2	f	5789	0	5575	104	0
3	C	598	0	579	9	0
3	N	598	0	579	10	0
3	g	598	0	579	9	0
4	D	1098	0	1099	21	0
4	O	1098	0	1099	20	0
4	h	1098	0	1099	20	0
5	E	543	0	525	7	0
5	Q	543	0	525	6	0
5	i	543	0	525	5	0
6	F	1036	0	1031	15	0
6	R	1036	0	1031	16	0
6	j	1036	0	1031	16	0
7	I	282	0	291	9	0
7	S	282	0	291	9	0
7	k	282	0	291	7	0
8	J	335	0	344	8	0
8	T	335	0	344	8	0
8	l	335	0	344	7	0
9	K	549	0	597	15	0
9	U	549	0	597	16	0
9	m	549	0	597	16	0
10	L	1210	0	1206	42	0
10	V	1210	0	1206	40	0
10	n	1210	0	1206	43	0
11	M	228	0	246	5	0
11	W	228	0	246	4	0
11	o	228	0	246	4	0
12	P	1318	0	1233	17	0
12	X	1318	0	1233	18	0
12	p	1318	0	1233	19	0
13	1	2605	0	2564	35	0
13	2	2605	0	2564	38	0
13	3	2605	0	2564	33	0
13	4	2605	0	2564	41	0
13	5	2605	0	2564	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	6	2605	0	2564	44	0
13	Y	2605	0	2564	38	0
13	Z	2605	0	2564	41	0
13	a	2605	0	2564	32	0
13	b	2605	0	2564	41	0
13	c	2605	0	2564	30	0
13	d	2605	0	2564	41	0
13	q	2605	0	2564	35	0
13	r	2605	0	2564	40	0
13	s	2605	0	2564	33	0
13	t	2605	0	2564	41	0
13	u	2605	0	2564	29	0
13	v	2605	0	2564	44	0
14	1	765	0	561	22	0
14	2	850	0	720	27	0
14	3	785	0	593	16	0
14	4	765	0	561	19	0
14	5	785	0	600	17	0
14	6	785	0	600	21	0
14	A	2712	0	2766	112	0
14	B	2515	0	2595	113	0
14	F	90	0	66	4	0
14	G	2712	0	2766	117	0
14	H	2515	0	2595	113	0
14	J	100	0	82	1	0
14	K	148	0	118	2	0
14	L	185	0	190	10	0
14	R	90	0	66	4	0
14	T	100	0	82	1	0
14	U	148	0	118	2	0
14	V	185	0	190	12	0
14	Y	765	0	561	24	0
14	Z	850	0	720	29	0
14	a	785	0	593	15	0
14	b	765	0	561	19	0
14	c	785	0	600	16	0
14	d	785	0	600	21	0
14	e	2712	0	2766	114	0
14	f	2515	0	2595	107	0
14	j	90	0	66	4	0
14	l	100	0	82	1	0
14	m	148	0	118	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	n	185	0	190	12	0
14	q	765	0	561	22	0
14	r	850	0	720	26	0
14	s	785	0	593	13	0
14	t	765	0	561	20	0
14	u	785	0	600	17	0
14	v	785	0	600	21	0
15	A	33	0	46	3	0
15	B	33	0	46	4	0
15	G	33	0	46	2	0
15	H	33	0	46	4	0
15	e	33	0	46	2	0
15	f	33	0	46	5	0
16	A	8	0	0	0	0
16	C	16	0	0	0	0
16	G	8	0	0	0	0
16	N	16	0	0	0	0
16	e	8	0	0	0	0
16	g	16	0	0	0	0
17	1	160	0	224	15	0
17	2	160	0	224	17	0
17	3	160	0	224	5	0
17	4	160	0	224	8	0
17	5	160	0	224	7	0
17	6	160	0	224	11	0
17	A	240	0	336	20	0
17	B	280	0	392	29	0
17	F	40	0	56	6	0
17	G	240	0	336	18	0
17	H	280	0	392	27	0
17	I	40	0	56	4	0
17	J	120	0	168	13	0
17	K	40	0	56	3	0
17	L	160	0	224	20	0
17	M	40	0	56	2	0
17	R	40	0	56	6	0
17	S	40	0	56	3	0
17	T	120	0	168	12	0
17	U	40	0	56	3	0
17	V	160	0	224	21	0
17	W	40	0	56	3	0
17	Y	160	0	224	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Z	160	0	224	17	0
17	a	160	0	224	4	0
17	b	160	0	224	5	0
17	c	160	0	224	7	0
17	d	160	0	224	12	0
17	e	240	0	336	17	0
17	f	280	0	392	27	0
17	j	40	0	56	6	0
17	k	40	0	56	5	0
17	l	120	0	168	13	0
17	m	40	0	56	3	0
17	n	160	0	224	25	0
17	o	40	0	56	1	0
17	q	160	0	224	12	0
17	r	160	0	224	15	0
17	s	160	0	224	5	0
17	t	160	0	224	7	0
17	u	160	0	224	11	0
17	v	160	0	224	10	0
18	A	374	0	493	30	0
18	B	78	0	96	5	0
18	G	374	0	493	30	0
18	H	78	0	96	5	0
18	I	48	0	69	2	0
18	L	127	0	170	12	0
18	S	48	0	69	2	0
18	V	127	0	170	14	0
18	e	374	0	493	30	0
18	f	78	0	96	5	0
18	k	48	0	69	2	0
18	n	127	0	170	12	0
19	A	58	0	76	3	0
19	B	35	0	46	1	0
19	G	58	0	76	3	0
19	H	35	0	46	1	0
19	J	22	0	28	0	0
19	T	22	0	28	0	0
19	e	58	0	76	3	0
19	f	35	0	46	1	0
19	l	22	0	28	0	0
20	B	53	0	76	5	0
20	H	53	0	76	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	J	32	0	34	0	0
20	T	32	0	34	1	0
20	f	53	0	76	6	0
20	l	32	0	34	0	0
21	1	32	0	28	1	0
21	2	28	0	20	0	0
21	3	28	0	20	2	0
21	4	26	0	16	0	0
21	5	26	0	16	0	0
21	6	26	0	16	0	0
21	B	40	0	42	8	0
21	H	40	0	42	9	0
21	L	46	0	58	6	0
21	V	46	0	58	6	0
21	Y	32	0	28	1	0
21	Z	28	0	20	0	0
21	a	28	0	20	2	0
21	b	26	0	16	0	0
21	c	26	0	16	0	0
21	d	26	0	16	0	0
21	f	40	0	42	9	0
21	n	46	0	58	6	0
21	q	32	0	28	1	0
21	r	28	0	20	0	0
21	s	28	0	20	2	0
21	t	26	0	16	0	0
21	u	26	0	16	0	0
21	v	26	0	16	0	0
22	P	31	0	19	1	0
22	X	31	0	19	2	0
22	p	31	0	19	1	0
23	A	9	0	0	1	0
23	B	7	0	0	0	0
23	F	1	0	0	0	0
23	G	9	0	0	1	0
23	H	7	0	0	0	0
23	L	1	0	0	0	0
23	R	1	0	0	0	0
23	V	1	0	0	0	0
23	e	9	0	0	1	0
23	f	7	0	0	0	0
23	j	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	n	1	0	0	0	0
All	All	144312	0	142227	2417	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 2417 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)
10:n:3:GLN:HG2	10:n:4:ASP:H	0.93	1.09
10:L:3:GLN:HG2	10:L:4:ASP:H	0.93	1.06
10:V:3:GLN:HG2	10:V:4:ASP:H	0.93	1.05
10:L:3:GLN:HG2	10:L:4:ASP:N	1.75	1.00
10:V:3:GLN:HG2	10:V:4:ASP:N	1.75	0.98

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%)	724 (97%)	25 (3%)	0	100	100
1	G	749/763 (98%)	724 (97%)	25 (3%)	0	100	100
1	e	749/763 (98%)	724 (97%)	25 (3%)	0	100	100
2	B	731/734 (100%)	710 (97%)	21 (3%)	0	100	100
2	H	731/734 (100%)	710 (97%)	21 (3%)	0	100	100
2	f	731/734 (100%)	710 (97%)	21 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	g	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
4	O	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
4	h	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
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%)	35 (97%)	1 (3%)	0	100	100
7	S	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	k	36/38 (95%)	35 (97%)	1 (3%)	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%)	158 (98%)	4 (2%)	0	100	100
10	V	162/166 (98%)	158 (98%)	4 (2%)	0	100	100
10	n	162/166 (98%)	158 (98%)	4 (2%)	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	P	167/172 (97%)	159 (95%)	8 (5%)	0	100	100
12	X	167/172 (97%)	159 (95%)	8 (5%)	0	100	100
12	p	167/172 (97%)	159 (95%)	8 (5%)	0	100	100
13	1	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	2	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	3	337/342 (98%)	330 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	4	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	5	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	6	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	Y	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	Z	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	a	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	b	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	c	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	d	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	q	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	r	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	s	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	t	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	u	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	v	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
All	All	13287/13605 (98%)	12906 (97%)	381 (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	88
2	H	583/584 (100%)	582 (100%)	1 (0%)	87	88
2	f	583/584 (100%)	582 (100%)	1 (0%)	87	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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	P	140/142 (99%)	140 (100%)	0	100	100
12	X	140/142 (99%)	140 (100%)	0	100	100
12	p	140/142 (99%)	140 (100%)	0	100	100
13	l	257/259 (99%)	257 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	2	257/259 (99%)	257 (100%)	0	100	100
13	3	257/259 (99%)	257 (100%)	0	100	100
13	4	257/259 (99%)	257 (100%)	0	100	100
13	5	257/259 (99%)	257 (100%)	0	100	100
13	6	257/259 (99%)	257 (100%)	0	100	100
13	Y	257/259 (99%)	257 (100%)	0	100	100
13	Z	257/259 (99%)	257 (100%)	0	100	100
13	a	257/259 (99%)	257 (100%)	0	100	100
13	b	257/259 (99%)	257 (100%)	0	100	100
13	c	257/259 (99%)	257 (100%)	0	100	100
13	d	257/259 (99%)	257 (100%)	0	100	100
13	q	257/259 (99%)	257 (100%)	0	100	100
13	r	257/259 (99%)	257 (100%)	0	100	100
13	s	257/259 (99%)	257 (100%)	0	100	100
13	t	257/259 (99%)	257 (100%)	0	100	100
13	u	257/259 (99%)	257 (100%)	0	100	100
13	v	257/259 (99%)	257 (100%)	0	100	100
All	All	10437/10593 (98%)	10434 (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 119 such sidechains are listed below:

Mol	Chain	Res	Type
6	R	55	ASN
13	r	291	GLN
13	a	263	ASN
13	r	263	ASN
13	v	133	ASN

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 ⓘ

843 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	$\# Z > 2$
17	BCR	W	4021	-	41,41,41	0.77	0	56,56,56	1.91	15 (26%)
14	CLA	B	1212	2	55,59,73	1.37	9 (16%)	66,96,113	1.49	6 (9%)
14	CLA	V	1501	10	64,68,73	1.33	11 (17%)	77,107,113	1.42	9 (11%)
17	BCR	J	4012	-	41,41,41	0.72	0	56,56,56	1.75	12 (21%)
14	CLA	s	507	-	49,53,73	1.47	7 (14%)	59,89,113	1.51	6 (10%)
17	BCR	r	522	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
14	CLA	s	516	13	49,53,73	1.47	7 (14%)	59,89,113	1.71	9 (15%)
14	CLA	m	1401	-	59,63,73	1.35	10 (16%)	71,101,113	1.49	10 (14%)
14	CLA	f	1012	23	69,73,73	1.28	11 (15%)	83,113,113	1.42	10 (12%)
17	BCR	d	521	-	41,41,41	0.67	0	56,56,56	1.79	12 (21%)
20	LMG	l	5104	-	32,32,55	0.96	2 (6%)	40,40,63	1.26	4 (10%)
14	CLA	Z	509	13	69,73,73	1.26	10 (14%)	83,113,113	1.39	8 (9%)
18	LHG	G	5009	-	41,41,48	0.67	0	44,47,54	1.22	4 (9%)
17	BCR	n	4022	-	41,41,41	0.79	0	56,56,56	1.82	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	V	4019	-	41,41,41	0.76	0	56,56,56	1.95	15 (26%)
14	CLA	G	1131	1	69,73,73	1.25	9 (13%)	83,113,113	1.36	8 (9%)
18	LHG	B	1855	-	40,40,48	0.69	1 (2%)	43,46,54	1.24	5 (11%)
20	LMG	T	5104	-	32,32,55	0.96	2 (6%)	40,40,63	1.26	4 (10%)
14	CLA	e	1114	23	49,53,73	1.51	9 (18%)	59,89,113	1.56	9 (15%)
18	LHG	e	5008	-	34,34,48	0.71	1 (2%)	37,40,54	1.25	4 (10%)
14	CLA	B	1228	2	59,63,73	1.31	10 (16%)	71,101,113	1.51	7 (9%)
14	CLA	A	1127	1	69,73,73	1.25	10 (14%)	83,113,113	1.40	11 (13%)
17	BCR	H	4009	-	41,41,41	0.78	0	56,56,56	1.90	20 (35%)
14	CLA	q	503	13	49,53,73	1.48	8 (16%)	59,89,113	1.52	5 (8%)
19	LMU	G	1849	-	23,23,36	1.18	1 (4%)	28,28,47	1.39	4 (14%)
14	CLA	A	1137	1	64,68,73	1.31	8 (12%)	77,107,113	1.46	9 (11%)
14	CLA	5	511	13	49,53,73	1.49	7 (14%)	59,89,113	1.54	8 (13%)
14	CLA	4	512	13	49,53,73	1.47	8 (16%)	59,89,113	1.48	5 (8%)
14	CLA	6	516	13	49,53,73	1.48	9 (18%)	59,89,113	1.46	8 (13%)
17	BCR	b	524	-	41,41,41	0.69	0	56,56,56	1.85	14 (25%)
17	BCR	a	524	-	41,41,41	0.78	0	56,56,56	1.93	18 (32%)
14	CLA	U	1105	9	49,53,73	1.47	8 (16%)	59,89,113	1.68	8 (13%)
14	CLA	5	507	-	49,53,73	1.45	8 (16%)	59,89,113	1.55	7 (11%)
14	CLA	m	1105	9	49,53,73	1.48	8 (16%)	59,89,113	1.67	8 (13%)
14	CLA	H	1226	2	59,63,73	1.49	11 (18%)	71,101,113	1.83	18 (25%)
14	CLA	A	1115	1	64,68,73	1.29	11 (17%)	77,107,113	1.49	8 (10%)
14	CLA	f	1216	23	64,68,73	1.33	10 (15%)	77,107,113	1.51	10 (12%)
14	CLA	H	1238	23	69,73,73	1.24	10 (14%)	83,113,113	1.49	12 (14%)
14	CLA	Y	519	13	49,53,73	1.50	10 (20%)	59,89,113	1.42	6 (10%)
14	CLA	f	1236	2	54,58,73	1.40	9 (16%)	65,95,113	1.43	9 (13%)
14	CLA	f	1232	23	59,63,73	1.34	10 (16%)	71,101,113	1.50	8 (11%)
14	CLA	f	1205	2	69,73,73	1.25	11 (15%)	83,113,113	1.50	10 (12%)
14	CLA	G	1137	1	64,68,73	1.31	8 (12%)	77,107,113	1.46	9 (11%)
17	BCR	G	4008	-	41,41,41	0.95	2 (4%)	56,56,56	2.17	16 (28%)
17	BCR	f	4017	-	41,41,41	0.97	3 (7%)	56,56,56	1.82	12 (21%)
14	CLA	A	1013	-	69,73,73	1.28	11 (15%)	83,113,113	1.69	14 (16%)
14	CLA	c	502	13	49,53,73	1.49	8 (16%)	59,89,113	1.57	6 (10%)
14	CLA	H	1206	2	69,73,73	1.29	12 (17%)	83,113,113	1.48	11 (13%)
14	CLA	B	1208	2	69,73,73	1.23	9 (13%)	83,113,113	1.28	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	1101	1	69,73,73	1.27	10 (14%)	83,113,113	1.54	12 (14%)
14	CLA	J	1302	8	59,63,73	1.31	9 (15%)	71,101,113	1.47	7 (9%)
14	CLA	1	503	13	49,53,73	1.48	8 (16%)	59,89,113	1.52	5 (8%)
14	CLA	A	1124	23	64,68,73	1.33	11 (17%)	77,107,113	1.46	10 (12%)
14	CLA	3	501	13	49,53,73	1.48	10 (20%)	59,89,113	1.50	8 (13%)
14	CLA	f	1207	2	69,73,73	1.25	9 (13%)	83,113,113	1.32	4 (4%)
14	CLA	d	518	13	49,53,73	1.46	8 (16%)	59,89,113	1.49	4 (6%)
14	CLA	f	1206	2	69,73,73	1.28	12 (17%)	83,113,113	1.49	11 (13%)
14	CLA	e	1125	1	69,73,73	1.26	11 (15%)	83,113,113	1.47	9 (10%)
14	CLA	b	502	13	49,53,73	1.49	9 (18%)	59,89,113	1.55	6 (10%)
14	CLA	G	1134	1	60,64,73	1.31	9 (15%)	72,102,113	1.51	9 (12%)
18	LHG	n	5220	-	40,40,48	0.70	1 (2%)	43,46,54	1.30	5 (11%)
14	CLA	A	1138	1	69,73,73	1.23	9 (13%)	83,113,113	1.45	6 (7%)
14	CLA	e	1011	1	69,73,73	1.27	8 (11%)	83,113,113	1.66	14 (16%)
14	CLA	Z	507	-	49,53,73	1.46	9 (18%)	59,89,113	1.53	8 (13%)
17	BCR	A	4008	-	41,41,41	0.95	2 (4%)	56,56,56	2.17	16 (28%)
14	CLA	t	512	13	49,53,73	1.47	8 (16%)	59,89,113	1.48	5 (8%)
17	BCR	t	522	-	41,41,41	0.74	0	56,56,56	1.91	19 (33%)
14	CLA	e	1237	23	69,73,73	1.27	13 (18%)	83,113,113	1.54	10 (12%)
14	CLA	H	1208	2	69,73,73	1.23	10 (14%)	83,113,113	1.28	7 (8%)
14	CLA	s	509	13	49,53,73	1.48	11 (22%)	59,89,113	1.57	8 (13%)
14	CLA	F	1302	6	49,53,73	1.48	9 (18%)	59,89,113	1.48	7 (11%)
14	CLA	A	1801	18	49,53,73	1.44	11 (22%)	59,89,113	1.51	7 (11%)
14	CLA	B	1235	2	69,73,73	1.27	11 (15%)	83,113,113	1.41	7 (8%)
14	CLA	G	1111	1	69,73,73	1.25	11 (15%)	83,113,113	1.40	7 (8%)
14	CLA	H	1225	2	69,73,73	1.27	10 (14%)	83,113,113	1.36	11 (13%)
14	CLA	v	509	13	49,53,73	1.48	10 (20%)	59,89,113	1.50	6 (10%)
17	BCR	A	4003	-	41,41,41	0.88	1 (2%)	56,56,56	1.78	14 (25%)
17	BCR	n	4219	-	41,41,41	1.09	5 (12%)	56,56,56	2.26	23 (41%)
18	LHG	e	5003	14	39,39,48	0.86	1 (2%)	42,45,54	1.38	6 (14%)
14	CLA	A	1134	1	60,64,73	1.32	9 (15%)	72,102,113	1.50	9 (12%)
14	CLA	4	504	-	49,53,73	1.49	9 (18%)	59,89,113	1.49	5 (8%)
14	CLA	q	513	13	49,53,73	1.47	10 (20%)	59,89,113	1.47	6 (10%)
14	CLA	Z	513	13	49,53,73	1.48	10 (20%)	59,89,113	1.43	5 (8%)
14	CLA	u	502	13	49,53,73	1.50	8 (16%)	59,89,113	1.57	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	4	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.58	7 (11%)
17	BCR	H	4017	-	41,41,41	0.97	4 (9%)	56,56,56	1.82	12 (21%)
17	BCR	a	522	-	41,41,41	0.70	0	56,56,56	2.03	17 (30%)
14	CLA	G	1113	1	49,53,73	1.45	10 (20%)	59,89,113	1.59	8 (13%)
14	CLA	R	1302	6	49,53,73	1.48	9 (18%)	59,89,113	1.49	7 (11%)
14	CLA	B	1221	23	66,70,73	1.32	11 (16%)	79,109,113	1.54	12 (15%)
14	CLA	a	513	13	49,53,73	1.48	8 (16%)	59,89,113	1.48	5 (8%)
14	CLA	1	510	13	49,53,73	1.48	10 (20%)	59,89,113	1.46	4 (6%)
14	CLA	f	1240	18	69,73,73	1.26	9 (13%)	83,113,113	1.35	8 (9%)
14	CLA	T	1303	8	49,53,73	1.47	10 (20%)	59,89,113	1.60	8 (13%)
14	CLA	G	1104	1	69,73,73	1.26	13 (18%)	83,113,113	1.47	13 (15%)
14	CLA	G	1138	1	69,73,73	1.23	9 (13%)	83,113,113	1.46	6 (7%)
14	CLA	r	510	13	49,53,73	1.46	10 (20%)	59,89,113	1.46	6 (10%)
17	BCR	3	522	-	41,41,41	0.69	0	56,56,56	2.04	18 (32%)
14	CLA	e	1121	1	59,63,73	1.36	11 (18%)	71,101,113	1.55	10 (14%)
14	CLA	G	1139	23	69,73,73	1.27	11 (15%)	83,113,113	1.28	6 (7%)
14	CLA	F	1301	23	49,53,73	1.49	11 (22%)	59,89,113	1.47	5 (8%)
14	CLA	t	511	13	49,53,73	1.50	9 (18%)	59,89,113	1.51	9 (15%)
14	CLA	H	1229	2	69,73,73	1.24	10 (14%)	83,113,113	1.45	10 (12%)
14	CLA	2	513	13	49,53,73	1.48	10 (20%)	59,89,113	1.42	5 (8%)
14	CLA	f	1229	2	69,73,73	1.23	10 (14%)	83,113,113	1.45	9 (10%)
20	LMG	B	5002	-	53,53,55	0.85	3 (5%)	61,61,63	1.51	12 (19%)
17	BCR	A	4011	-	41,41,41	0.82	0	56,56,56	1.79	12 (21%)
18	LHG	A	5006	-	39,39,48	0.67	1 (2%)	42,45,54	1.22	5 (11%)
14	CLA	t	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.58	7 (11%)
14	CLA	Y	516	13	49,53,73	1.46	10 (20%)	59,89,113	1.48	6 (10%)
14	CLA	B	1205	2	69,73,73	1.26	11 (15%)	83,113,113	1.50	10 (12%)
17	BCR	6	524	-	41,41,41	0.78	0	56,56,56	1.85	15 (26%)
14	CLA	v	512	13	49,53,73	1.47	9 (18%)	59,89,113	1.48	6 (10%)
14	CLA	G	1118	1	64,68,73	1.28	11 (17%)	77,107,113	1.46	7 (9%)
15	PQN	B	2002	-	34,34,34	2.84	11 (32%)	42,45,45	2.31	6 (14%)
14	CLA	A	1132	1	69,73,73	1.25	11 (15%)	83,113,113	1.45	9 (10%)
14	CLA	H	1215	2	69,73,73	1.26	10 (14%)	83,113,113	1.55	11 (13%)
17	BCR	J	4013	-	41,41,41	0.77	0	56,56,56	1.93	16 (28%)
17	BCR	B	4006	-	41,41,41	0.78	0	56,56,56	2.09	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	H	1204	2	69,73,73	1.22	10 (14%)	83,113,113	1.33	7 (8%)
17	BCR	s	524	-	41,41,41	0.77	0	56,56,56	1.93	18 (32%)
14	CLA	H	1228	2	59,63,73	1.30	10 (16%)	71,101,113	1.51	7 (9%)
14	CLA	f	1215	2	69,73,73	1.26	10 (14%)	83,113,113	1.56	11 (13%)
14	CLA	u	513	13	49,53,73	1.47	10 (20%)	59,89,113	1.42	5 (8%)
17	BCR	q	522	-	41,41,41	0.74	0	56,56,56	1.91	20 (35%)
14	CLA	v	510	13	49,53,73	1.49	10 (20%)	59,89,113	1.48	4 (6%)
14	CLA	s	505	13	59,63,73	1.33	8 (13%)	71,101,113	1.36	4 (5%)
17	BCR	Y	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)
14	CLA	e	1013	-	69,73,73	1.28	11 (15%)	83,113,113	1.69	14 (16%)
17	BCR	Z	523	-	41,41,41	0.72	0	56,56,56	1.76	17 (30%)
21	SQD	6	822	-	25,26,54	1.31	4 (16%)	34,37,65	2.00	10 (29%)
14	CLA	A	1118	1	64,68,73	1.28	11 (17%)	77,107,113	1.46	7 (9%)
18	LHG	L	5218	-	36,36,48	0.76	2 (5%)	39,42,54	1.20	4 (10%)
14	CLA	A	1133	1	69,73,73	1.23	10 (14%)	83,113,113	1.39	7 (8%)
14	CLA	q	505	13	49,53,73	1.46	8 (16%)	59,89,113	1.48	4 (6%)
17	BCR	L	4019	-	41,41,41	0.76	0	56,56,56	1.95	15 (26%)
14	CLA	5	502	13	49,53,73	1.49	8 (16%)	59,89,113	1.58	6 (10%)
14	CLA	G	1140	1	69,73,73	1.26	10 (14%)	83,113,113	1.46	9 (10%)
17	BCR	v	524	-	41,41,41	0.78	0	56,56,56	1.84	15 (26%)
14	CLA	d	511	13	49,53,73	1.49	8 (16%)	59,89,113	1.55	5 (8%)
14	CLA	f	1231	23	69,73,73	1.22	9 (13%)	83,113,113	1.36	9 (10%)
14	CLA	e	1132	1	69,73,73	1.25	11 (15%)	83,113,113	1.45	9 (10%)
14	CLA	a	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.44	4 (6%)
14	CLA	c	518	13	49,53,73	1.47	9 (18%)	59,89,113	1.43	6 (10%)
18	LHG	G	5004	-	34,34,48	0.67	0	37,40,54	1.28	4 (10%)
18	LHG	e	5009	-	41,41,48	0.67	0	44,47,54	1.22	4 (9%)
17	BCR	B	4010	-	41,41,41	0.91	1 (2%)	56,56,56	2.30	21 (37%)
14	CLA	e	1131	1	69,73,73	1.25	9 (13%)	83,113,113	1.36	8 (9%)
14	CLA	A	1114	23	49,53,73	1.50	9 (18%)	59,89,113	1.57	9 (15%)
18	LHG	A	5002	-	42,42,48	0.76	1 (2%)	45,48,54	1.22	4 (8%)
17	BCR	2	522	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
14	CLA	6	503	13	49,53,73	1.48	8 (16%)	59,89,113	1.55	5 (8%)
14	CLA	6	512	13	49,53,73	1.47	9 (18%)	59,89,113	1.48	6 (10%)
14	CLA	v	504	-	49,53,73	1.47	9 (18%)	59,89,113	1.52	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	1230	2	64,68,73	1.30	10 (15%)	77,107,113	1.40	7 (9%)
14	CLA	r	516	13	49,53,73	1.46	8 (16%)	59,89,113	1.50	6 (10%)
17	BCR	f	4014	-	41,41,41	0.83	1 (2%)	56,56,56	1.90	23 (41%)
14	CLA	B	1204	2	69,73,73	1.23	10 (14%)	83,113,113	1.33	7 (8%)
14	CLA	b	519	13	49,53,73	1.49	10 (20%)	59,89,113	1.50	6 (10%)
14	CLA	s	518	13	59,63,73	1.35	10 (16%)	71,101,113	1.37	5 (7%)
14	CLA	B	1224	2	64,68,73	1.28	9 (14%)	77,107,113	1.37	9 (11%)
14	CLA	K	1103	9	52,56,73	1.43	9 (17%)	62,92,113	1.51	6 (9%)
14	CLA	f	1214	2	69,73,73	1.26	9 (13%)	83,113,113	1.45	6 (7%)
17	BCR	b	523	-	41,41,41	0.73	0	56,56,56	1.77	14 (25%)
14	CLA	a	509	13	49,53,73	1.48	10 (20%)	59,89,113	1.57	8 (13%)
14	CLA	e	1140	1	69,73,73	1.25	10 (14%)	83,113,113	1.46	9 (10%)
21	SQD	b	822	-	25,26,54	1.32	4 (16%)	34,37,65	1.97	9 (26%)
17	BCR	f	4005	-	41,41,41	0.77	0	56,56,56	1.72	12 (21%)
14	CLA	4	518	13	49,53,73	1.48	9 (18%)	59,89,113	1.48	4 (6%)
14	CLA	G	1106	1	69,73,73	1.22	11 (15%)	83,113,113	1.42	9 (10%)
14	CLA	B	1234	2	69,73,73	1.29	11 (15%)	83,113,113	1.49	11 (13%)
14	CLA	u	503	13	49,53,73	1.48	9 (18%)	59,89,113	1.55	8 (13%)
18	LHG	A	5005	-	42,42,48	0.65	1 (2%)	45,48,54	1.21	4 (8%)
14	CLA	e	1102	1	59,63,73	1.35	12 (20%)	71,101,113	1.45	8 (11%)
17	BCR	J	4015	-	41,41,41	0.80	0	56,56,56	1.73	12 (21%)
17	BCR	T	4012	-	41,41,41	0.72	0	56,56,56	1.76	13 (23%)
21	SQD	l	822	-	31,32,54	1.20	5 (16%)	40,43,65	2.05	13 (32%)
14	CLA	q	501	13	49,53,73	1.47	10 (20%)	59,89,113	1.52	5 (8%)
14	CLA	d	516	13	49,53,73	1.48	9 (18%)	59,89,113	1.46	7 (11%)
18	LHG	G	5007	-	46,46,48	0.60	0	49,52,54	1.20	4 (8%)
14	CLA	d	506	13	49,53,73	1.48	10 (20%)	59,89,113	1.50	5 (8%)
14	CLA	B	1238	23	69,73,73	1.23	10 (14%)	83,113,113	1.48	11 (13%)
18	LHG	e	5001	-	48,48,48	0.80	1 (2%)	51,54,54	1.30	7 (13%)
14	CLA	v	516	13	49,53,73	1.48	9 (18%)	59,89,113	1.46	8 (13%)
18	LHG	G	5002	-	42,42,48	0.76	1 (2%)	45,48,54	1.23	4 (8%)
14	CLA	4	519	13	49,53,73	1.48	10 (20%)	59,89,113	1.51	6 (10%)
14	CLA	A	1106	1	69,73,73	1.23	11 (15%)	83,113,113	1.41	9 (10%)
14	CLA	e	1101	1	69,73,73	1.28	10 (14%)	83,113,113	1.55	12 (14%)
14	CLA	G	1119	23	69,73,73	1.32	10 (14%)	83,113,113	1.53	14 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	G	1105	1	59,63,73	1.31	9 (15%)	71,101,113	1.49	9 (12%)
14	CLA	H	1219	2	67,71,73	1.28	10 (14%)	80,110,113	1.34	10 (12%)
18	LHG	A	5007	-	46,46,48	0.60	0	49,52,54	1.20	4 (8%)
19	LMU	A	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.02	2 (4%)
14	CLA	H	1203	2	69,73,73	1.28	10 (14%)	83,113,113	1.41	10 (12%)
14	CLA	b	518	13	49,53,73	1.48	9 (18%)	59,89,113	1.49	4 (6%)
14	CLA	3	503	13	49,53,73	1.49	9 (18%)	59,89,113	1.51	7 (11%)
14	CLA	H	1221	23	66,70,73	1.32	11 (16%)	79,109,113	1.54	12 (15%)
17	BCR	4	522	-	41,41,41	0.73	0	56,56,56	1.91	19 (33%)
14	CLA	r	509	13	69,73,73	1.26	11 (15%)	83,113,113	1.38	8 (9%)
18	LHG	A	5008	-	34,34,48	0.70	1 (2%)	37,40,54	1.25	4 (10%)
14	CLA	d	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	6	519	13	49,53,73	1.48	10 (20%)	59,89,113	1.47	6 (10%)
14	CLA	B	1012	23	69,73,73	1.28	11 (15%)	83,113,113	1.42	10 (12%)
14	CLA	Z	508	13	49,53,73	1.49	11 (22%)	59,89,113	1.60	10 (16%)
14	CLA	f	1218	2	64,68,73	1.30	9 (14%)	77,107,113	1.35	5 (6%)
14	CLA	v	501	13	49,53,73	1.47	10 (20%)	59,89,113	1.56	5 (8%)
19	LMU	e	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.02	2 (4%)
21	SQD	Y	822	-	31,32,54	1.20	5 (16%)	40,43,65	2.05	13 (32%)
18	LHG	f	1842	14	36,36,48	0.81	1 (2%)	39,42,54	1.25	3 (7%)
14	CLA	u	508	13	49,53,73	1.51	10 (20%)	59,89,113	1.65	6 (10%)
17	BCR	a	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)
21	SQD	L	5216	-	45,46,54	1.01	5 (11%)	54,57,65	1.69	11 (20%)
14	CLA	A	1119	23	69,73,73	1.32	10 (14%)	83,113,113	1.54	14 (16%)
14	CLA	H	1214	2	69,73,73	1.26	9 (13%)	83,113,113	1.45	7 (8%)
14	CLA	c	503	13	49,53,73	1.48	9 (18%)	59,89,113	1.54	8 (13%)
14	CLA	s	519	13	49,53,73	1.47	8 (16%)	59,89,113	1.49	6 (10%)
14	CLA	l	513	13	49,53,73	1.47	10 (20%)	59,89,113	1.47	6 (10%)
17	BCR	d	523	-	41,41,41	0.72	0	56,56,56	1.72	14 (25%)
14	CLA	G	1116	1	64,68,73	1.30	11 (17%)	77,107,113	1.36	9 (11%)
14	CLA	f	1212	2	55,59,73	1.37	9 (16%)	66,96,113	1.49	6 (9%)
14	CLA	j	1301	23	49,53,73	1.49	11 (22%)	59,89,113	1.47	5 (8%)
14	CLA	r	501	13	64,68,73	1.28	9 (14%)	77,107,113	1.46	7 (9%)
14	CLA	t	502	13	49,53,73	1.49	9 (18%)	59,89,113	1.55	5 (8%)
14	CLA	e	1109	1	69,73,73	1.24	11 (15%)	83,113,113	1.46	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	e	1133	1	69,73,73	1.23	10 (14%)	83,113,113	1.40	7 (8%)
16	SF4	C	3002	3	0,12,12	-	-	-		
17	BCR	Z	524	-	41,41,41	0.74	0	56,56,56	1.75	12 (21%)
14	CLA	4	505	13	49,53,73	1.46	10 (20%)	59,89,113	1.43	4 (6%)
14	CLA	H	1213	2	65,69,73	1.26	11 (16%)	78,108,113	1.48	10 (12%)
14	CLA	e	1124	23	64,68,73	1.33	11 (17%)	77,107,113	1.46	11 (14%)
14	CLA	f	1210	2	69,73,73	1.27	12 (17%)	83,113,113	1.36	10 (12%)
14	CLA	b	503	13	49,53,73	1.50	9 (18%)	59,89,113	1.55	6 (10%)
17	BCR	Z	522	-	41,41,41	0.75	0	56,56,56	1.86	17 (30%)
14	CLA	6	506	13	49,53,73	1.48	10 (20%)	59,89,113	1.50	5 (8%)
14	CLA	c	504	-	49,53,73	1.48	9 (18%)	59,89,113	1.54	5 (8%)
17	BCR	u	524	-	41,41,41	0.71	0	56,56,56	1.74	11 (19%)
14	CLA	s	504	-	49,53,73	1.48	9 (18%)	59,89,113	1.57	9 (15%)
14	CLA	G	1133	1	69,73,73	1.23	11 (15%)	83,113,113	1.40	7 (8%)
14	CLA	e	1104	1	69,73,73	1.27	13 (18%)	83,113,113	1.47	13 (15%)
14	CLA	e	1120	1	54,58,73	1.37	12 (22%)	65,95,113	1.57	10 (15%)
14	CLA	a	503	13	49,53,73	1.49	8 (16%)	59,89,113	1.51	7 (11%)
17	BCR	n	4020	-	41,41,41	0.98	2 (4%)	56,56,56	1.67	14 (25%)
16	SF4	g	3002	3	0,12,12	-	-	-		
14	CLA	A	1116	1	64,68,73	1.30	11 (17%)	77,107,113	1.35	9 (11%)
14	CLA	e	1137	1	64,68,73	1.31	8 (12%)	77,107,113	1.46	9 (11%)
14	CLA	e	1117	1	69,73,73	1.26	10 (14%)	83,113,113	1.44	11 (13%)
17	BCR	A	4007	-	41,41,41	0.87	0	56,56,56	2.10	20 (35%)
17	BCR	e	4008	-	41,41,41	0.95	2 (4%)	56,56,56	2.17	16 (28%)
14	CLA	G	1120	1	54,58,73	1.37	12 (22%)	65,95,113	1.57	10 (15%)
14	CLA	u	504	-	49,53,73	1.48	10 (20%)	59,89,113	1.53	5 (8%)
22	FMN	P	170	-	33,33,33	1.13	2 (6%)	48,50,50	1.24	6 (12%)
14	CLA	K	1401	-	59,63,73	1.35	10 (16%)	71,101,113	1.49	10 (14%)
14	CLA	5	519	13	49,53,73	1.48	8 (16%)	59,89,113	1.49	6 (10%)
14	CLA	Y	512	13	49,53,73	1.47	10 (20%)	59,89,113	1.39	4 (6%)
14	CLA	2	510	13	49,53,73	1.46	10 (20%)	59,89,113	1.46	5 (8%)
21	SQD	f	1852	-	39,40,54	1.18	6 (15%)	48,51,65	1.84	12 (25%)
14	CLA	d	517	-	49,53,73	1.45	7 (14%)	59,89,113	1.47	6 (10%)
14	CLA	G	1022	23	69,73,73	1.32	10 (14%)	83,113,113	1.38	12 (14%)
14	CLA	L	1501	10	64,68,73	1.32	11 (17%)	77,107,113	1.41	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	Y	502	13	49,53,73	1.47	9 (18%)	59,89,113	1.53	7 (11%)
14	CLA	1	519	13	49,53,73	1.49	10 (20%)	59,89,113	1.43	5 (8%)
14	CLA	H	1217	2	64,68,73	1.29	9 (14%)	77,107,113	1.33	5 (6%)
17	BCR	3	524	-	41,41,41	0.78	0	56,56,56	1.93	18 (32%)
14	CLA	B	1209	2	57,61,73	1.38	11 (19%)	68,98,113	1.54	8 (11%)
14	CLA	e	1110	1	57,61,73	1.37	10 (17%)	68,98,113	1.45	7 (10%)
14	CLA	f	1220	2	59,63,73	1.36	10 (16%)	71,101,113	1.53	8 (11%)
14	CLA	f	1226	2	59,63,73	1.48	11 (18%)	71,101,113	1.81	17 (23%)
14	CLA	K	1105	9	49,53,73	1.48	8 (16%)	59,89,113	1.67	8 (13%)
17	BCR	b	521	-	41,41,41	0.68	0	56,56,56	1.78	11 (19%)
14	CLA	f	1217	2	64,68,73	1.28	9 (14%)	77,107,113	1.33	5 (6%)
19	LMU	e	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.39	4 (14%)
14	CLA	s	508	13	49,53,73	1.49	11 (22%)	59,89,113	1.59	7 (11%)
14	CLA	H	1209	2	57,61,73	1.38	11 (19%)	68,98,113	1.53	8 (11%)
14	CLA	A	1120	1	54,58,73	1.37	12 (22%)	65,95,113	1.57	10 (15%)
17	BCR	G	4002	-	41,41,41	0.88	1 (2%)	56,56,56	1.94	16 (28%)
17	BCR	G	4011	-	41,41,41	0.81	0	56,56,56	1.78	12 (21%)
14	CLA	e	1130	1	60,64,73	1.33	11 (18%)	72,102,113	1.54	11 (15%)
14	CLA	A	1022	23	69,73,73	1.32	10 (14%)	83,113,113	1.38	12 (14%)
14	CLA	H	1222	23	54,58,73	1.40	11 (20%)	65,95,113	1.55	10 (15%)
14	CLA	e	1129	1	57,61,73	1.41	10 (17%)	68,98,113	1.51	11 (16%)
19	LMU	l	5105	-	22,22,36	1.21	1 (4%)	27,27,47	1.43	5 (18%)
17	BCR	B	4014	-	41,41,41	0.83	1 (2%)	56,56,56	1.89	23 (41%)
14	CLA	f	1222	23	54,58,73	1.40	10 (18%)	65,95,113	1.54	10 (15%)
19	LMU	T	5105	-	22,22,36	1.21	1 (4%)	27,27,47	1.43	5 (18%)
14	CLA	v	508	13	49,53,73	1.48	9 (18%)	59,89,113	1.60	11 (18%)
14	CLA	v	519	13	49,53,73	1.48	10 (20%)	59,89,113	1.48	6 (10%)
14	CLA	q	510	13	49,53,73	1.49	10 (20%)	59,89,113	1.45	4 (6%)
17	BCR	G	4007	-	41,41,41	0.87	0	56,56,56	2.11	20 (35%)
17	BCR	a	523	-	41,41,41	0.69	0	56,56,56	1.82	15 (26%)
14	CLA	5	505	13	49,53,73	1.46	9 (18%)	59,89,113	1.45	4 (6%)
14	CLA	Z	501	13	64,68,73	1.28	10 (15%)	77,107,113	1.46	6 (7%)
14	CLA	a	502	13	49,53,73	1.48	9 (18%)	59,89,113	1.60	8 (13%)
14	CLA	3	509	13	49,53,73	1.49	10 (20%)	59,89,113	1.57	8 (13%)
17	BCR	A	4002	-	41,41,41	0.88	1 (2%)	56,56,56	1.94	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	508	13	49,53,73	1.49	11 (22%)	59,89,113	1.59	7 (11%)
14	CLA	3	508	13	49,53,73	1.49	11 (22%)	59,89,113	1.59	8 (13%)
19	LMU	A	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.39	4 (14%)
14	CLA	q	502	13	49,53,73	1.48	9 (18%)	59,89,113	1.54	7 (11%)
14	CLA	2	517	-	49,53,73	1.47	9 (18%)	59,89,113	1.50	6 (10%)
17	BCR	n	4019	-	41,41,41	0.76	0	56,56,56	1.95	15 (26%)
14	CLA	H	1201	2	64,68,73	1.26	9 (14%)	77,107,113	1.50	10 (12%)
17	BCR	e	4011	-	41,41,41	0.83	0	56,56,56	1.78	12 (21%)
14	CLA	v	503	13	49,53,73	1.47	8 (16%)	59,89,113	1.55	5 (8%)
17	BCR	S	4018	-	41,41,41	0.93	2 (4%)	56,56,56	1.93	16 (28%)
14	CLA	u	505	13	49,53,73	1.46	9 (18%)	59,89,113	1.44	4 (6%)
14	CLA	B	1202	2	69,73,73	1.22	10 (14%)	83,113,113	1.42	8 (9%)
14	CLA	l	509	13	49,53,73	1.48	9 (18%)	59,89,113	1.51	8 (13%)
14	CLA	v	506	13	49,53,73	1.48	10 (20%)	59,89,113	1.49	5 (8%)
17	BCR	T	4015	-	41,41,41	0.80	0	56,56,56	1.73	12 (21%)
14	CLA	4	510	13	49,53,73	1.47	9 (18%)	59,89,113	1.50	4 (6%)
14	CLA	Y	503	13	49,53,73	1.49	8 (16%)	59,89,113	1.53	5 (8%)
14	CLA	A	1108	1	58,62,73	1.34	10 (17%)	69,99,113	1.45	7 (10%)
14	CLA	r	507	-	49,53,73	1.46	10 (20%)	59,89,113	1.53	8 (13%)
14	CLA	4	516	13	49,53,73	1.48	9 (18%)	59,89,113	1.48	5 (8%)
14	CLA	6	518	13	49,53,73	1.46	8 (16%)	59,89,113	1.48	4 (6%)
18	LHG	I	5001	-	47,47,48	0.62	0	50,53,54	1.24	5 (10%)
14	CLA	q	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	e	1111	1	69,73,73	1.24	11 (15%)	83,113,113	1.40	8 (9%)
14	CLA	f	1239	2	69,73,73	1.26	9 (13%)	83,113,113	1.65	13 (15%)
17	BCR	s	521	-	41,41,41	0.66	0	56,56,56	1.83	11 (19%)
14	CLA	v	502	13	49,53,73	1.49	8 (16%)	59,89,113	1.54	6 (10%)
14	CLA	2	509	13	69,73,73	1.26	10 (14%)	83,113,113	1.38	8 (9%)
21	SQD	3	822	-	27,28,54	1.29	5 (18%)	36,39,65	1.80	11 (30%)
14	CLA	f	1227	2	64,68,73	1.29	10 (15%)	77,107,113	1.45	7 (9%)
14	CLA	Z	519	13	49,53,73	1.47	9 (18%)	59,89,113	1.51	7 (11%)
17	BCR	u	522	-	41,41,41	0.75	0	56,56,56	1.94	21 (37%)
16	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	Z	510	13	49,53,73	1.46	10 (20%)	59,89,113	1.45	5 (8%)
14	CLA	2	507	-	49,53,73	1.46	10 (20%)	59,89,113	1.53	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	5	516	13	49,53,73	1.47	9 (18%)	59,89,113	1.42	4 (6%)
14	CLA	r	502	13	49,53,73	1.46	8 (16%)	59,89,113	1.58	8 (13%)
14	CLA	f	1211	2	59,63,73	1.34	11 (18%)	71,101,113	1.50	8 (11%)
14	CLA	G	1128	1	69,73,73	1.36	11 (15%)	83,113,113	1.60	12 (14%)
14	CLA	Y	511	13	49,53,73	1.49	8 (16%)	59,89,113	1.54	8 (13%)
19	LMU	H	1843	-	36,36,36	1.17	2 (5%)	47,47,47	1.06	3 (6%)
14	CLA	f	1203	2	69,73,73	1.28	10 (14%)	83,113,113	1.41	10 (12%)
14	CLA	l	516	13	49,53,73	1.46	10 (20%)	59,89,113	1.47	5 (8%)
14	CLA	G	1130	1	60,64,73	1.33	11 (18%)	72,102,113	1.55	11 (15%)
14	CLA	t	519	13	49,53,73	1.48	10 (20%)	59,89,113	1.51	6 (10%)
14	CLA	a	512	13	49,53,73	1.49	10 (20%)	59,89,113	1.40	5 (8%)
14	CLA	b	510	13	49,53,73	1.46	9 (18%)	59,89,113	1.50	4 (6%)
14	CLA	e	1122	1	64,68,73	1.31	11 (17%)	77,107,113	1.44	8 (10%)
17	BCR	K	4104	-	41,41,41	0.78	0	56,56,56	1.88	16 (28%)
18	LHG	L	5220	-	40,40,48	0.70	1 (2%)	43,46,54	1.30	5 (11%)
18	LHG	V	5221	-	48,48,48	0.62	0	51,54,54	1.28	7 (13%)
14	CLA	l	501	13	49,53,73	1.47	8 (16%)	59,89,113	1.53	4 (6%)
17	BCR	B	4017	-	41,41,41	0.97	3 (7%)	56,56,56	1.82	12 (21%)
14	CLA	B	1201	2	64,68,73	1.27	9 (14%)	77,107,113	1.50	10 (12%)
14	CLA	f	1223	2	69,73,73	1.26	10 (14%)	83,113,113	1.47	7 (8%)
14	CLA	u	506	13	49,53,73	1.47	10 (20%)	59,89,113	1.47	5 (8%)
14	CLA	A	1128	1	69,73,73	1.36	11 (15%)	83,113,113	1.60	12 (14%)
14	CLA	G	1801	18	49,53,73	1.44	11 (22%)	59,89,113	1.52	6 (10%)
18	LHG	n	5221	-	48,48,48	0.62	0	51,54,54	1.28	7 (13%)
17	BCR	Y	523	-	41,41,41	0.74	0	56,56,56	1.69	14 (25%)
14	CLA	t	510	13	49,53,73	1.47	9 (18%)	59,89,113	1.51	4 (6%)
17	BCR	l	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)
14	CLA	V	1502	10	69,73,73	1.25	11 (15%)	83,113,113	1.42	9 (10%)
14	CLA	B	1231	23	69,73,73	1.22	9 (13%)	83,113,113	1.36	9 (10%)
14	CLA	H	1212	2	55,59,73	1.37	9 (16%)	66,96,113	1.50	6 (9%)
14	CLA	Y	508	13	49,53,73	1.51	11 (22%)	59,89,113	1.71	8 (13%)
16	SF4	N	3003	3	0,12,12	-	-	-	-	-
14	CLA	e	1118	1	64,68,73	1.28	11 (17%)	77,107,113	1.46	7 (9%)
14	CLA	t	501	13	49,53,73	1.48	9 (18%)	59,89,113	1.50	6 (10%)
14	CLA	A	1136	1	69,73,73	1.28	10 (14%)	83,113,113	1.47	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	1229	2	69,73,73	1.24	10 (14%)	83,113,113	1.45	9 (10%)
14	CLA	e	1103	1	69,73,73	1.28	12 (17%)	83,113,113	1.58	10 (12%)
14	CLA	t	505	13	49,53,73	1.47	10 (20%)	59,89,113	1.43	4 (6%)
18	LHG	B	1842	14	36,36,48	0.81	1 (2%)	39,42,54	1.26	3 (7%)
14	CLA	3	505	13	59,63,73	1.33	9 (15%)	71,101,113	1.35	4 (5%)
17	BCR	2	523	-	41,41,41	0.72	0	56,56,56	1.75	17 (30%)
14	CLA	b	512	13	49,53,73	1.46	8 (16%)	59,89,113	1.47	5 (8%)
17	BCR	b	522	-	41,41,41	0.73	0	56,56,56	1.91	19 (33%)
18	LHG	A	5004	-	34,34,48	0.67	0	37,40,54	1.28	4 (10%)
14	CLA	s	506	13	49,53,73	1.49	9 (18%)	59,89,113	1.50	7 (11%)
22	FMN	p	170	-	33,33,33	1.12	2 (6%)	48,50,50	1.24	6 (12%)
14	CLA	H	1205	2	69,73,73	1.26	11 (15%)	83,113,113	1.50	10 (12%)
14	CLA	r	503	13	69,73,73	1.25	7 (10%)	83,113,113	1.35	7 (8%)
14	CLA	H	1211	2	59,63,73	1.34	11 (18%)	71,101,113	1.50	8 (11%)
14	CLA	Y	517	-	49,53,73	1.47	9 (18%)	59,89,113	1.46	5 (8%)
14	CLA	H	1223	2	69,73,73	1.25	9 (13%)	83,113,113	1.47	7 (8%)
20	LMG	J	5104	-	32,32,55	0.96	2 (6%)	40,40,63	1.26	4 (10%)
17	BCR	f	4006	-	41,41,41	0.77	0	56,56,56	2.09	18 (32%)
14	CLA	V	1503	23	64,68,73	1.28	10 (15%)	77,107,113	1.42	5 (6%)
14	CLA	Z	516	13	49,53,73	1.47	8 (16%)	59,89,113	1.52	6 (10%)
14	CLA	Z	502	13	49,53,73	1.47	9 (18%)	59,89,113	1.59	8 (13%)
14	CLA	G	1115	1	64,68,73	1.29	11 (17%)	77,107,113	1.48	8 (10%)
17	BCR	6	523	-	41,41,41	0.72	0	56,56,56	1.72	14 (25%)
14	CLA	G	1136	1	69,73,73	1.27	9 (13%)	83,113,113	1.46	9 (10%)
14	CLA	r	504	-	49,53,73	1.48	8 (16%)	59,89,113	1.50	6 (10%)
14	CLA	a	519	13	49,53,73	1.47	8 (16%)	59,89,113	1.49	6 (10%)
14	CLA	d	513	13	49,53,73	1.47	9 (18%)	59,89,113	1.45	5 (8%)
14	CLA	2	504	-	49,53,73	1.48	8 (16%)	59,89,113	1.49	6 (10%)
14	CLA	A	1131	1	69,73,73	1.25	9 (13%)	83,113,113	1.37	8 (9%)
14	CLA	q	519	13	49,53,73	1.49	10 (20%)	59,89,113	1.44	6 (10%)
14	CLA	b	511	13	49,53,73	1.50	10 (20%)	59,89,113	1.51	9 (15%)
14	CLA	e	1105	1	59,63,73	1.32	10 (16%)	71,101,113	1.49	9 (12%)
14	CLA	e	1112	1	54,58,73	1.39	12 (22%)	65,95,113	1.54	7 (10%)
14	CLA	1	508	13	49,53,73	1.51	11 (22%)	59,89,113	1.71	7 (11%)
16	SF4	C	3003	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	B	4004	-	41,41,41	0.73	0	56,56,56	1.85	14 (25%)
14	CLA	b	517	-	49,53,73	1.48	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	f	1238	23	69,73,73	1.24	10 (14%)	83,113,113	1.48	11 (13%)
14	CLA	G	1108	1	58,62,73	1.34	10 (17%)	69,99,113	1.45	8 (11%)
14	CLA	t	516	13	49,53,73	1.48	9 (18%)	59,89,113	1.48	5 (8%)
14	CLA	f	1201	2	64,68,73	1.27	10 (15%)	77,107,113	1.50	10 (12%)
14	CLA	H	1232	23	59,63,73	1.34	11 (18%)	71,101,113	1.50	8 (11%)
14	CLA	T	1302	8	59,63,73	1.30	9 (15%)	71,101,113	1.46	7 (9%)
21	SQD	v	822	-	25,26,54	1.31	4 (16%)	34,37,65	2.00	10 (29%)
14	CLA	a	511	13	49,53,73	1.48	9 (18%)	59,89,113	1.53	8 (13%)
14	CLA	b	504	-	49,53,73	1.48	7 (14%)	59,89,113	1.48	5 (8%)
14	CLA	3	506	13	49,53,73	1.49	10 (20%)	59,89,113	1.51	7 (11%)
14	CLA	c	509	13	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
16	SF4	g	3003	3	0,12,12	-	-	-	-	-
17	BCR	Y	522	-	41,41,41	0.74	0	56,56,56	1.91	20 (35%)
18	LHG	L	5221	-	48,48,48	0.62	0	51,54,54	1.28	7 (13%)
14	CLA	e	1113	1	49,53,73	1.45	11 (22%)	59,89,113	1.59	8 (13%)
17	BCR	H	4010	-	41,41,41	0.91	1 (2%)	56,56,56	2.31	21 (37%)
14	CLA	q	508	13	49,53,73	1.51	11 (22%)	59,89,113	1.72	8 (13%)
17	BCR	T	4013	-	41,41,41	0.78	0	56,56,56	1.93	16 (28%)
14	CLA	d	508	13	49,53,73	1.49	9 (18%)	59,89,113	1.59	11 (18%)
14	CLA	f	1202	2	69,73,73	1.23	11 (15%)	83,113,113	1.42	8 (9%)
14	CLA	a	507	-	49,53,73	1.47	8 (16%)	59,89,113	1.52	6 (10%)
14	CLA	B	1222	23	54,58,73	1.40	10 (18%)	65,95,113	1.54	10 (15%)
14	CLA	Y	501	13	49,53,73	1.47	9 (18%)	59,89,113	1.53	4 (6%)
17	BCR	L	4219	-	41,41,41	1.09	5 (12%)	56,56,56	2.26	23 (41%)
17	BCR	f	4010	-	41,41,41	0.91	1 (2%)	56,56,56	2.30	21 (37%)
21	SQD	5	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.95	11 (32%)
14	CLA	b	509	13	49,53,73	1.48	10 (20%)	59,89,113	1.58	8 (13%)
14	CLA	A	1105	1	59,63,73	1.31	10 (16%)	71,101,113	1.49	9 (12%)
17	BCR	5	524	-	41,41,41	0.71	0	56,56,56	1.74	12 (21%)
14	CLA	u	512	13	49,53,73	1.47	9 (18%)	59,89,113	1.45	6 (10%)
14	CLA	H	1012	23	69,73,73	1.28	11 (15%)	83,113,113	1.42	10 (12%)
17	BCR	r	524	-	41,41,41	0.74	0	56,56,56	1.76	13 (23%)
14	CLA	5	513	13	49,53,73	1.48	10 (20%)	59,89,113	1.42	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	s	512	13	49,53,73	1.50	10 (20%)	59,89,113	1.39	5 (8%)
14	CLA	r	519	13	49,53,73	1.48	9 (18%)	59,89,113	1.50	7 (11%)
17	BCR	2	524	-	41,41,41	0.73	0	56,56,56	1.76	12 (21%)
18	LHG	e	5002	-	42,42,48	0.76	1 (2%)	45,48,54	1.23	4 (8%)
17	BCR	q	524	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
14	CLA	4	513	13	49,53,73	1.49	9 (18%)	59,89,113	1.50	4 (6%)
14	CLA	2	502	13	49,53,73	1.47	9 (18%)	59,89,113	1.58	8 (13%)
14	CLA	f	1234	2	69,73,73	1.28	11 (15%)	83,113,113	1.49	11 (13%)
14	CLA	s	502	13	49,53,73	1.48	9 (18%)	59,89,113	1.60	8 (13%)
14	CLA	4	517	-	49,53,73	1.49	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	f	1209	2	57,61,73	1.38	11 (19%)	68,98,113	1.54	8 (11%)
14	CLA	f	1225	2	69,73,73	1.27	10 (14%)	83,113,113	1.36	11 (13%)
17	BCR	f	4009	-	41,41,41	0.78	0	56,56,56	1.89	18 (32%)
14	CLA	b	506	13	49,53,73	1.48	10 (20%)	59,89,113	1.51	5 (8%)
14	CLA	u	519	13	49,53,73	1.47	8 (16%)	59,89,113	1.48	6 (10%)
14	CLA	3	510	13	49,53,73	1.47	10 (20%)	59,89,113	1.50	5 (8%)
14	CLA	6	511	13	49,53,73	1.50	8 (16%)	59,89,113	1.54	5 (8%)
14	CLA	2	501	13	64,68,73	1.28	9 (14%)	77,107,113	1.46	7 (9%)
14	CLA	B	1021	2	69,73,73	1.27	10 (14%)	83,113,113	1.39	8 (9%)
21	SQD	a	822	-	27,28,54	1.30	5 (18%)	36,39,65	1.79	10 (27%)
14	CLA	B	1207	2	69,73,73	1.25	9 (13%)	83,113,113	1.31	4 (4%)
21	SQD	V	5216	-	45,46,54	1.01	5 (11%)	54,57,65	1.69	11 (20%)
17	BCR	o	4021	-	41,41,41	0.77	0	56,56,56	1.91	15 (26%)
21	SQD	q	822	-	31,32,54	1.20	5 (16%)	40,43,65	2.05	13 (32%)
17	BCR	v	523	-	41,41,41	0.72	0	56,56,56	1.72	15 (26%)
14	CLA	B	1226	2	59,63,73	1.49	11 (18%)	71,101,113	1.81	17 (23%)
14	CLA	e	1119	23	69,73,73	1.32	10 (14%)	83,113,113	1.54	14 (16%)
14	CLA	q	516	13	49,53,73	1.46	10 (20%)	59,89,113	1.48	6 (10%)
14	CLA	d	501	13	49,53,73	1.47	10 (20%)	59,89,113	1.56	5 (8%)
14	CLA	G	1101	1	69,73,73	1.27	10 (14%)	83,113,113	1.55	12 (14%)
14	CLA	B	1223	2	69,73,73	1.25	11 (15%)	83,113,113	1.47	7 (8%)
14	CLA	r	508	13	49,53,73	1.49	11 (22%)	59,89,113	1.59	10 (16%)
14	CLA	B	1219	2	67,71,73	1.28	9 (13%)	80,110,113	1.35	10 (12%)
14	CLA	G	1135	1	59,63,73	1.36	8 (13%)	71,101,113	1.61	13 (18%)
14	CLA	6	504	-	49,53,73	1.47	9 (18%)	59,89,113	1.53	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	d	505	13	69,73,73	1.24	9 (13%)	83,113,113	1.33	6 (7%)
14	CLA	e	1135	1	59,63,73	1.37	9 (15%)	71,101,113	1.60	13 (18%)
21	SQD	n	5216	-	45,46,54	1.02	5 (11%)	54,57,65	1.68	11 (20%)
14	CLA	e	1116	1	64,68,73	1.31	11 (17%)	77,107,113	1.35	9 (11%)
14	CLA	l	512	13	49,53,73	1.47	11 (22%)	59,89,113	1.39	4 (6%)
14	CLA	J	1303	8	49,53,73	1.46	10 (20%)	59,89,113	1.60	8 (13%)
14	CLA	A	1237	23	69,73,73	1.27	13 (18%)	83,113,113	1.53	10 (12%)
17	BCR	l	522	-	41,41,41	0.74	0	56,56,56	1.91	20 (35%)
18	LHG	e	5006	-	39,39,48	0.67	1 (2%)	42,45,54	1.22	5 (11%)
16	SF4	e	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	v	511	13	49,53,73	1.50	7 (14%)	59,89,113	1.54	5 (8%)
14	CLA	e	1107	1	69,73,73	1.31	10 (14%)	83,113,113	1.40	10 (12%)
14	CLA	5	510	13	49,53,73	1.46	10 (20%)	59,89,113	1.49	5 (8%)
14	CLA	H	1207	2	69,73,73	1.25	9 (13%)	83,113,113	1.32	4 (4%)
17	BCR	H	4014	-	41,41,41	0.83	0	56,56,56	1.89	23 (41%)
14	CLA	B	1211	2	59,63,73	1.33	11 (18%)	71,101,113	1.49	8 (11%)
14	CLA	H	1234	2	69,73,73	1.28	11 (15%)	83,113,113	1.49	11 (13%)
17	BCR	e	4003	-	41,41,41	0.87	1 (2%)	56,56,56	1.78	14 (25%)
14	CLA	e	1127	1	69,73,73	1.26	11 (15%)	83,113,113	1.40	11 (13%)
14	CLA	H	1230	2	64,68,73	1.31	10 (15%)	77,107,113	1.39	6 (7%)
17	BCR	6	521	-	41,41,41	0.67	0	56,56,56	1.79	12 (21%)
14	CLA	A	1135	1	59,63,73	1.36	9 (15%)	71,101,113	1.61	13 (18%)
17	BCR	L	4020	-	41,41,41	0.98	2 (4%)	56,56,56	1.67	15 (26%)
17	BCR	4	524	-	41,41,41	0.70	0	56,56,56	1.85	14 (25%)
17	BCR	G	4003	-	41,41,41	0.87	1 (2%)	56,56,56	1.78	14 (25%)
14	CLA	a	518	13	59,63,73	1.35	9 (15%)	71,101,113	1.38	5 (7%)
14	CLA	B	1213	2	65,69,73	1.26	10 (15%)	78,108,113	1.48	10 (12%)
14	CLA	s	503	13	49,53,73	1.49	8 (16%)	59,89,113	1.50	7 (11%)
17	BCR	q	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)
14	CLA	5	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.41	4 (6%)
17	BCR	v	521	-	41,41,41	0.68	0	56,56,56	1.79	12 (21%)
19	LMU	G	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.02	2 (4%)
14	CLA	Y	505	13	49,53,73	1.46	8 (16%)	59,89,113	1.49	4 (6%)
14	CLA	3	519	13	49,53,73	1.48	8 (16%)	59,89,113	1.49	6 (10%)
14	CLA	f	1208	2	69,73,73	1.23	9 (13%)	83,113,113	1.28	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	e	1022	23	69,73,73	1.32	10 (14%)	83,113,113	1.38	12 (14%)
14	CLA	f	1228	2	59,63,73	1.31	10 (16%)	71,101,113	1.51	7 (9%)
14	CLA	d	519	13	49,53,73	1.47	10 (20%)	59,89,113	1.47	5 (8%)
14	CLA	B	1240	18	69,73,73	1.26	9 (13%)	83,113,113	1.35	8 (9%)
17	BCR	M	4021	-	41,41,41	0.76	0	56,56,56	1.91	15 (26%)
21	SQD	Z	822	-	27,28,54	1.22	4 (14%)	36,39,65	1.86	10 (27%)
14	CLA	A	1110	1	57,61,73	1.37	10 (17%)	68,98,113	1.45	7 (10%)
14	CLA	A	1102	1	59,63,73	1.35	12 (20%)	71,101,113	1.45	8 (11%)
14	CLA	5	504	-	49,53,73	1.47	9 (18%)	59,89,113	1.54	5 (8%)
14	CLA	r	505	13	69,73,73	1.23	8 (11%)	83,113,113	1.32	7 (8%)
14	CLA	a	510	13	49,53,73	1.47	9 (18%)	59,89,113	1.50	6 (10%)
14	CLA	G	1102	1	59,63,73	1.35	11 (18%)	71,101,113	1.45	8 (11%)
14	CLA	t	503	13	49,53,73	1.51	9 (18%)	59,89,113	1.55	6 (10%)
17	BCR	u	523	-	41,41,41	0.78	0	56,56,56	1.79	15 (26%)
21	SQD	u	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.95	11 (32%)
14	CLA	A	1109	1	69,73,73	1.25	11 (15%)	83,113,113	1.47	8 (9%)
15	PQN	A	2001	-	34,34,34	2.81	11 (32%)	42,45,45	2.19	6 (14%)
14	CLA	1	504	-	49,53,73	1.49	9 (18%)	59,89,113	1.64	7 (11%)
17	BCR	4	523	-	41,41,41	0.74	0	56,56,56	1.77	14 (25%)
21	SQD	t	822	-	25,26,54	1.32	4 (16%)	34,37,65	1.97	9 (26%)
15	PQN	f	2002	-	34,34,34	2.84	11 (32%)	42,45,45	2.30	6 (14%)
14	CLA	b	505	13	49,53,73	1.46	9 (18%)	59,89,113	1.42	4 (6%)
14	CLA	c	501	13	49,53,73	1.47	10 (20%)	59,89,113	1.55	6 (10%)
14	CLA	H	1235	2	69,73,73	1.27	11 (15%)	83,113,113	1.41	7 (8%)
14	CLA	c	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.55	7 (11%)
14	CLA	1	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	2	508	13	49,53,73	1.49	11 (22%)	59,89,113	1.59	10 (16%)
14	CLA	j	1302	6	49,53,73	1.48	9 (18%)	59,89,113	1.48	7 (11%)
14	CLA	q	511	13	49,53,73	1.49	9 (18%)	59,89,113	1.52	9 (15%)
14	CLA	m	1103	9	52,56,73	1.43	10 (19%)	62,92,113	1.50	6 (9%)
14	CLA	s	511	13	49,53,73	1.48	9 (18%)	59,89,113	1.54	8 (13%)
17	BCR	t	524	-	41,41,41	0.70	0	56,56,56	1.85	14 (25%)
14	CLA	1	517	-	49,53,73	1.46	9 (18%)	59,89,113	1.45	5 (8%)
14	CLA	H	1240	18	69,73,73	1.26	9 (13%)	83,113,113	1.35	8 (9%)
14	CLA	Z	512	13	49,53,73	1.49	10 (20%)	59,89,113	1.39	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	c	521	-	41,41,41	0.71	0	56,56,56	1.97	18 (32%)
14	CLA	c	512	13	49,53,73	1.47	9 (18%)	59,89,113	1.45	6 (10%)
17	BCR	e	4007	-	41,41,41	0.87	0	56,56,56	2.10	19 (33%)
14	CLA	H	1236	2	54,58,73	1.41	9 (16%)	65,95,113	1.43	9 (13%)
14	CLA	c	519	13	49,53,73	1.48	8 (16%)	59,89,113	1.50	6 (10%)
14	CLA	e	1128	1	69,73,73	1.36	11 (15%)	83,113,113	1.60	12 (14%)
14	CLA	R	1301	23	49,53,73	1.48	11 (22%)	59,89,113	1.47	5 (8%)
17	BCR	r	521	-	41,41,41	0.70	0	56,56,56	1.90	13 (23%)
14	CLA	e	1108	1	58,62,73	1.34	8 (13%)	69,99,113	1.45	7 (10%)
14	CLA	a	501	13	49,53,73	1.48	10 (20%)	59,89,113	1.51	8 (13%)
14	CLA	q	504	-	49,53,73	1.49	9 (18%)	59,89,113	1.65	10 (16%)
14	CLA	u	509	13	69,73,73	1.24	10 (14%)	83,113,113	1.35	7 (8%)
17	BCR	l	523	-	41,41,41	0.75	0	56,56,56	1.69	13 (23%)
14	CLA	6	509	13	49,53,73	1.48	10 (20%)	59,89,113	1.50	6 (10%)
14	CLA	2	503	13	69,73,73	1.25	8 (11%)	83,113,113	1.35	6 (7%)
17	BCR	s	523	-	41,41,41	0.69	0	56,56,56	1.82	15 (26%)
14	CLA	v	505	13	69,73,73	1.24	9 (13%)	83,113,113	1.32	6 (7%)
18	LHG	G	5005	-	42,42,48	0.65	1 (2%)	45,48,54	1.21	4 (8%)
14	CLA	c	513	13	49,53,73	1.47	10 (20%)	59,89,113	1.43	5 (8%)
14	CLA	q	518	13	49,53,73	1.48	8 (16%)	59,89,113	1.50	6 (10%)
14	CLA	B	1214	2	69,73,73	1.26	9 (13%)	83,113,113	1.45	6 (7%)
14	CLA	G	1110	1	57,61,73	1.37	10 (17%)	68,98,113	1.45	7 (10%)
17	BCR	u	521	-	41,41,41	0.71	0	56,56,56	1.97	18 (32%)
14	CLA	v	507	-	49,53,73	1.47	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	d	510	13	49,53,73	1.48	10 (20%)	59,89,113	1.47	4 (6%)
18	LHG	G	5006	-	39,39,48	0.67	1 (2%)	42,45,54	1.22	5 (11%)
17	BCR	H	4005	-	41,41,41	0.76	0	56,56,56	1.73	12 (21%)
14	CLA	d	503	13	49,53,73	1.47	8 (16%)	59,89,113	1.54	5 (8%)
15	PQN	G	2001	-	34,34,34	2.82	11 (32%)	42,45,45	2.20	6 (14%)
14	CLA	G	1127	1	69,73,73	1.25	10 (14%)	83,113,113	1.39	11 (13%)
14	CLA	B	1210	2	69,73,73	1.26	12 (17%)	83,113,113	1.36	10 (12%)
14	CLA	r	506	13	49,53,73	1.46	9 (18%)	59,89,113	1.49	7 (11%)
14	CLA	c	511	13	49,53,73	1.49	7 (14%)	59,89,113	1.54	9 (15%)
14	CLA	l	511	13	49,53,73	1.49	8 (16%)	59,89,113	1.53	8 (13%)
21	SQD	s	822	-	27,28,54	1.29	5 (18%)	36,39,65	1.80	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	1215	2	69,73,73	1.26	10 (14%)	83,113,113	1.55	11 (13%)
14	CLA	5	508	13	49,53,73	1.51	10 (20%)	59,89,113	1.65	7 (11%)
14	CLA	2	516	13	49,53,73	1.46	8 (16%)	59,89,113	1.51	6 (10%)
14	CLA	f	1021	2	69,73,73	1.27	10 (14%)	83,113,113	1.39	8 (9%)
14	CLA	q	506	13	49,53,73	1.47	8 (16%)	59,89,113	1.45	6 (10%)
17	BCR	A	4001	-	41,41,41	0.79	0	56,56,56	1.69	11 (19%)
14	CLA	A	1113	1	49,53,73	1.45	10 (20%)	59,89,113	1.59	8 (13%)
14	CLA	f	1204	2	69,73,73	1.23	10 (14%)	83,113,113	1.33	7 (8%)
14	CLA	s	513	13	49,53,73	1.48	8 (16%)	59,89,113	1.47	5 (8%)
17	BCR	U	4104	-	41,41,41	0.78	0	56,56,56	1.88	16 (28%)
14	CLA	3	507	-	49,53,73	1.47	8 (16%)	59,89,113	1.52	6 (10%)
14	CLA	f	1224	2	64,68,73	1.28	9 (14%)	77,107,113	1.37	9 (11%)
14	CLA	6	513	13	49,53,73	1.47	8 (16%)	59,89,113	1.46	5 (8%)
14	CLA	H	1216	23	64,68,73	1.34	11 (17%)	77,107,113	1.52	10 (12%)
14	CLA	B	1236	2	54,58,73	1.41	9 (16%)	65,95,113	1.43	9 (13%)
17	BCR	5	523	-	41,41,41	0.78	1 (2%)	56,56,56	1.78	15 (26%)
15	PQN	H	2002	-	34,34,34	2.84	11 (32%)	42,45,45	2.30	6 (14%)
14	CLA	G	1123	23	69,73,73	1.26	11 (15%)	83,113,113	1.38	9 (10%)
14	CLA	s	517	-	49,53,73	1.49	10 (20%)	59,89,113	1.45	4 (6%)
14	CLA	4	503	13	49,53,73	1.50	9 (18%)	59,89,113	1.55	6 (10%)
17	BCR	4	521	-	41,41,41	0.67	0	56,56,56	1.79	11 (19%)
14	CLA	G	1114	23	49,53,73	1.51	9 (18%)	59,89,113	1.57	9 (15%)
17	BCR	H	4004	-	41,41,41	0.73	0	56,56,56	1.85	14 (25%)
14	CLA	5	509	13	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
14	CLA	A	1125	1	69,73,73	1.26	11 (15%)	83,113,113	1.46	8 (9%)
14	CLA	Y	510	13	49,53,73	1.48	10 (20%)	59,89,113	1.46	4 (6%)
17	BCR	l	4013	-	41,41,41	0.77	0	56,56,56	1.93	16 (28%)
18	LHG	V	5218	-	36,36,48	0.76	2 (5%)	39,42,54	1.20	4 (10%)
14	CLA	3	516	13	49,53,73	1.48	7 (14%)	59,89,113	1.71	9 (15%)
18	LHG	V	5220	-	40,40,48	0.70	1 (2%)	43,46,54	1.30	5 (11%)
14	CLA	H	1231	23	69,73,73	1.23	9 (13%)	83,113,113	1.36	9 (10%)
17	BCR	F	4016	-	41,41,41	0.82	0	56,56,56	1.91	11 (19%)
17	BCR	G	4001	-	41,41,41	0.79	0	56,56,56	1.68	11 (19%)
14	CLA	Z	504	-	49,53,73	1.48	8 (16%)	59,89,113	1.50	6 (10%)
14	CLA	t	513	13	49,53,73	1.49	8 (16%)	59,89,113	1.49	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	3	502	13	49,53,73	1.48	8 (16%)	59,89,113	1.60	8 (13%)
17	BCR	B	4005	-	41,41,41	0.76	0	56,56,56	1.72	12 (21%)
14	CLA	3	513	13	49,53,73	1.48	8 (16%)	59,89,113	1.48	5 (8%)
14	CLA	c	508	13	49,53,73	1.51	10 (20%)	59,89,113	1.64	8 (13%)
14	CLA	e	1134	1	60,64,73	1.32	9 (15%)	72,102,113	1.50	9 (12%)
14	CLA	Z	518	13	59,63,73	1.33	9 (15%)	71,101,113	1.41	5 (7%)
20	LMG	f	5002	-	53,53,55	0.85	2 (3%)	61,61,63	1.51	12 (19%)
14	CLA	A	1126	1	69,73,73	1.23	12 (17%)	83,113,113	1.38	7 (8%)
17	BCR	V	4022	-	41,41,41	0.78	0	56,56,56	1.81	10 (17%)
14	CLA	4	501	13	49,53,73	1.47	8 (16%)	59,89,113	1.50	5 (8%)
14	CLA	u	518	13	49,53,73	1.48	9 (18%)	59,89,113	1.44	6 (10%)
14	CLA	A	1123	23	69,73,73	1.25	11 (15%)	83,113,113	1.38	9 (10%)
18	LHG	n	5218	-	36,36,48	0.76	2 (5%)	39,42,54	1.20	4 (10%)
14	CLA	t	504	-	49,53,73	1.49	8 (16%)	59,89,113	1.48	5 (8%)
14	CLA	u	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.55	7 (11%)
14	CLA	H	1227	2	64,68,73	1.30	11 (17%)	77,107,113	1.44	7 (9%)
14	CLA	f	1219	2	67,71,73	1.27	10 (14%)	80,110,113	1.35	10 (12%)
14	CLA	B	1239	2	69,73,73	1.26	9 (13%)	83,113,113	1.65	14 (16%)
21	SQD	c	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.95	11 (32%)
17	BCR	c	523	-	41,41,41	0.78	1 (2%)	56,56,56	1.78	15 (26%)
14	CLA	e	1115	1	64,68,73	1.29	11 (17%)	77,107,113	1.48	8 (10%)
14	CLA	G	1117	1	69,73,73	1.27	10 (14%)	83,113,113	1.44	11 (13%)
14	CLA	e	1136	1	69,73,73	1.27	9 (13%)	83,113,113	1.46	9 (10%)
14	CLA	4	511	13	49,53,73	1.50	10 (20%)	59,89,113	1.51	9 (15%)
14	CLA	e	1801	18	49,53,73	1.44	11 (22%)	59,89,113	1.51	7 (11%)
17	BCR	Z	521	-	41,41,41	0.70	0	56,56,56	1.90	13 (23%)
18	LHG	S	5001	-	47,47,48	0.62	0	50,53,54	1.24	5 (10%)
17	BCR	B	4009	-	41,41,41	0.77	0	56,56,56	1.90	18 (32%)
17	BCR	1	524	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
14	CLA	B	1227	2	64,68,73	1.30	11 (17%)	77,107,113	1.45	7 (9%)
14	CLA	B	1225	2	69,73,73	1.27	10 (14%)	83,113,113	1.36	10 (12%)
14	CLA	G	1129	1	57,61,73	1.41	10 (17%)	68,98,113	1.52	11 (16%)
14	CLA	d	502	13	49,53,73	1.49	8 (16%)	59,89,113	1.55	7 (11%)
18	LHG	e	5004	-	34,34,48	0.67	0	37,40,54	1.28	4 (10%)
14	CLA	n	1501	10	64,68,73	1.33	10 (15%)	77,107,113	1.41	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	1130	1	60,64,73	1.33	11 (18%)	72,102,113	1.54	11 (15%)
14	CLA	U	1401	-	59,63,73	1.35	10 (16%)	71,101,113	1.49	10 (14%)
14	CLA	b	513	13	49,53,73	1.49	9 (18%)	59,89,113	1.49	4 (6%)
14	CLA	l	1303	8	49,53,73	1.47	10 (20%)	59,89,113	1.61	8 (13%)
14	CLA	n	1502	10	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
14	CLA	Z	503	13	69,73,73	1.26	8 (11%)	83,113,113	1.35	6 (7%)
14	CLA	G	1125	1	69,73,73	1.26	11 (15%)	83,113,113	1.46	8 (9%)
14	CLA	e	1126	1	69,73,73	1.23	12 (17%)	83,113,113	1.38	7 (8%)
14	CLA	l	1302	8	59,63,73	1.30	9 (15%)	71,101,113	1.46	7 (9%)
14	CLA	A	1117	1	69,73,73	1.26	10 (14%)	83,113,113	1.44	11 (13%)
14	CLA	B	1220	2	59,63,73	1.35	10 (16%)	71,101,113	1.54	8 (11%)
14	CLA	A	1139	23	69,73,73	1.27	11 (15%)	83,113,113	1.29	7 (8%)
14	CLA	e	1123	23	69,73,73	1.25	11 (15%)	83,113,113	1.38	9 (10%)
14	CLA	s	501	13	49,53,73	1.48	10 (20%)	59,89,113	1.51	7 (11%)
14	CLA	3	518	13	59,63,73	1.35	9 (15%)	71,101,113	1.38	5 (7%)
14	CLA	B	1216	23	64,68,73	1.33	10 (15%)	77,107,113	1.51	10 (12%)
17	BCR	V	4219	-	41,41,41	1.08	5 (12%)	56,56,56	2.26	23 (41%)
17	BCR	d	524	-	41,41,41	0.79	0	56,56,56	1.84	15 (26%)
14	CLA	v	513	13	49,53,73	1.48	9 (18%)	59,89,113	1.45	5 (8%)
14	CLA	b	501	13	49,53,73	1.47	9 (18%)	59,89,113	1.49	5 (8%)
14	CLA	Y	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	Z	511	13	49,53,73	1.48	9 (18%)	59,89,113	1.55	7 (11%)
18	LHG	f	1855	-	40,40,48	0.69	1 (2%)	43,46,54	1.24	5 (11%)
14	CLA	6	505	13	69,73,73	1.24	9 (13%)	83,113,113	1.33	6 (7%)
14	CLA	6	517	-	49,53,73	1.46	8 (16%)	59,89,113	1.47	6 (10%)
14	CLA	n	1503	23	64,68,73	1.28	10 (15%)	77,107,113	1.42	5 (6%)
17	BCR	5	521	-	41,41,41	0.71	0	56,56,56	1.97	18 (32%)
14	CLA	A	1111	1	69,73,73	1.25	11 (15%)	83,113,113	1.40	9 (10%)
14	CLA	B	1218	2	64,68,73	1.30	9 (14%)	77,107,113	1.34	5 (6%)
14	CLA	e	1139	23	69,73,73	1.27	11 (15%)	83,113,113	1.28	7 (8%)
14	CLA	A	1122	1	64,68,73	1.30	11 (17%)	77,107,113	1.44	8 (10%)
14	CLA	G	1237	23	69,73,73	1.27	13 (18%)	83,113,113	1.53	10 (12%)
18	LHG	G	5008	-	34,34,48	0.71	1 (2%)	37,40,54	1.25	3 (8%)
14	CLA	B	1206	2	69,73,73	1.29	12 (17%)	83,113,113	1.48	11 (13%)
14	CLA	Y	509	13	49,53,73	1.49	9 (18%)	59,89,113	1.52	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	2	521	-	41,41,41	0.70	0	56,56,56	1.90	13 (23%)
18	LHG	G	5003	14	39,39,48	0.86	1 (2%)	42,45,54	1.38	6 (14%)
14	CLA	2	518	13	59,63,73	1.33	8 (13%)	71,101,113	1.41	5 (7%)
14	CLA	H	1220	2	59,63,73	1.35	10 (16%)	71,101,113	1.54	8 (11%)
18	LHG	H	1842	14	36,36,48	0.81	1 (2%)	39,42,54	1.26	3 (7%)
17	BCR	R	4016	-	41,41,41	0.81	0	56,56,56	1.91	12 (21%)
14	CLA	A	1011	1	69,73,73	1.27	8 (11%)	83,113,113	1.66	14 (16%)
16	SF4	N	3002	3	0,12,12	-	-	-		
14	CLA	t	508	13	49,53,73	1.51	11 (22%)	59,89,113	1.63	9 (15%)
14	CLA	5	501	13	49,53,73	1.48	10 (20%)	59,89,113	1.56	6 (10%)
14	CLA	5	503	13	49,53,73	1.48	9 (18%)	59,89,113	1.54	8 (13%)
17	BCR	c	522	-	41,41,41	0.76	0	56,56,56	1.94	20 (35%)
14	CLA	5	506	13	49,53,73	1.47	10 (20%)	59,89,113	1.46	5 (8%)
14	CLA	a	504	-	49,53,73	1.47	10 (20%)	59,89,113	1.56	9 (15%)
14	CLA	G	1103	1	69,73,73	1.28	12 (17%)	83,113,113	1.58	11 (13%)
14	CLA	v	518	13	49,53,73	1.46	8 (16%)	59,89,113	1.48	4 (6%)
17	BCR	t	523	-	41,41,41	0.73	0	56,56,56	1.77	14 (25%)
18	LHG	A	5003	14	39,39,48	0.86	1 (2%)	42,45,54	1.38	6 (14%)
14	CLA	L	1502	10	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
17	BCR	V	4020	-	41,41,41	0.99	2 (4%)	56,56,56	1.67	15 (26%)
14	CLA	G	1121	1	59,63,73	1.36	11 (18%)	71,101,113	1.55	10 (14%)
19	LMU	J	5105	-	22,22,36	1.21	1 (4%)	27,27,47	1.43	5 (18%)
14	CLA	2	505	13	69,73,73	1.23	9 (13%)	83,113,113	1.33	7 (8%)
18	LHG	H	1855	-	40,40,48	0.69	1 (2%)	43,46,54	1.24	5 (11%)
14	CLA	f	1213	2	65,69,73	1.26	11 (16%)	78,108,113	1.48	9 (11%)
14	CLA	G	1011	1	69,73,73	1.27	8 (11%)	83,113,113	1.66	14 (16%)
14	CLA	f	1230	2	64,68,73	1.30	10 (15%)	77,107,113	1.39	6 (7%)
17	BCR	s	522	-	41,41,41	0.70	0	56,56,56	2.04	18 (32%)
14	CLA	c	505	13	49,53,73	1.46	9 (18%)	59,89,113	1.46	4 (6%)
17	BCR	v	522	-	41,41,41	0.71	0	56,56,56	1.89	19 (33%)
17	BCR	H	4006	-	41,41,41	0.78	0	56,56,56	2.09	18 (32%)
14	CLA	A	1103	1	69,73,73	1.28	12 (17%)	83,113,113	1.58	11 (13%)
17	BCR	6	522	-	41,41,41	0.72	0	56,56,56	1.89	19 (33%)
14	CLA	5	518	13	49,53,73	1.48	9 (18%)	59,89,113	1.43	6 (10%)
14	CLA	4	509	13	49,53,73	1.48	11 (22%)	59,89,113	1.59	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	1	502	13	49,53,73	1.48	9 (18%)	59,89,113	1.54	7 (11%)
14	CLA	H	1021	2	69,73,73	1.26	10 (14%)	83,113,113	1.39	8 (9%)
14	CLA	a	506	13	49,53,73	1.48	9 (18%)	59,89,113	1.51	7 (11%)
14	CLA	f	1235	2	69,73,73	1.27	12 (17%)	83,113,113	1.42	7 (8%)
14	CLA	B	1232	23	59,63,73	1.34	11 (18%)	71,101,113	1.50	8 (11%)
14	CLA	A	1121	1	59,63,73	1.36	11 (18%)	71,101,113	1.55	10 (14%)
21	SQD	B	1852	-	39,40,54	1.18	6 (15%)	48,51,65	1.84	12 (25%)
14	CLA	L	1503	23	64,68,73	1.28	10 (15%)	77,107,113	1.42	5 (6%)
14	CLA	t	517	-	49,53,73	1.48	7 (14%)	59,89,113	1.53	6 (10%)
14	CLA	a	505	13	59,63,73	1.34	9 (15%)	71,101,113	1.35	5 (7%)
14	CLA	b	508	13	49,53,73	1.51	10 (20%)	59,89,113	1.63	9 (15%)
16	SF4	G	3001	2,1	0,12,12	-	-	-	-	-
21	SQD	H	1852	-	39,40,54	1.18	6 (15%)	48,51,65	1.84	12 (25%)
14	CLA	B	1217	2	64,68,73	1.29	9 (14%)	77,107,113	1.33	5 (6%)
14	CLA	r	512	13	49,53,73	1.48	10 (20%)	59,89,113	1.40	5 (8%)
20	LMG	H	5002	-	53,53,55	0.86	3 (5%)	61,61,63	1.51	12 (19%)
15	PQN	e	2001	-	34,34,34	2.81	11 (32%)	42,45,45	2.19	6 (14%)
14	CLA	4	502	13	49,53,73	1.49	9 (18%)	59,89,113	1.55	5 (8%)
14	CLA	H	1239	2	69,73,73	1.27	10 (14%)	83,113,113	1.65	13 (15%)
18	LHG	k	5001	-	47,47,48	0.62	0	50,53,54	1.24	5 (10%)
14	CLA	G	1124	23	64,68,73	1.33	11 (17%)	77,107,113	1.46	10 (12%)
14	CLA	6	510	13	49,53,73	1.48	10 (20%)	59,89,113	1.47	4 (6%)
14	CLA	A	1104	1	69,73,73	1.26	13 (18%)	83,113,113	1.47	13 (15%)
17	BCR	l	4012	-	41,41,41	0.73	0	56,56,56	1.75	12 (21%)
14	CLA	e	1106	1	69,73,73	1.23	11 (15%)	83,113,113	1.41	8 (9%)
14	CLA	t	509	13	49,53,73	1.48	11 (22%)	59,89,113	1.58	9 (15%)
14	CLA	v	517	-	49,53,73	1.47	9 (18%)	59,89,113	1.47	6 (10%)
14	CLA	4	506	13	49,53,73	1.48	9 (18%)	59,89,113	1.51	5 (8%)
14	CLA	b	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.58	7 (11%)
19	LMU	f	1843	-	36,36,36	1.16	2 (5%)	47,47,47	1.06	3 (6%)
14	CLA	2	506	13	49,53,73	1.47	9 (18%)	59,89,113	1.48	6 (10%)
14	CLA	G	1132	1	69,73,73	1.25	11 (15%)	83,113,113	1.45	9 (10%)
14	CLA	c	516	13	49,53,73	1.47	9 (18%)	59,89,113	1.41	4 (6%)
17	BCR	r	523	-	41,41,41	0.72	0	56,56,56	1.75	17 (30%)
17	BCR	t	521	-	41,41,41	0.67	0	56,56,56	1.79	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	SQD	r	822	-	27,28,54	1.22	4 (14%)	36,39,65	1.86	10 (27%)
14	CLA	c	506	13	49,53,73	1.47	10 (20%)	59,89,113	1.46	5 (8%)
14	CLA	A	1129	1	57,61,73	1.41	10 (17%)	68,98,113	1.52	11 (16%)
14	CLA	1	506	13	49,53,73	1.47	9 (18%)	59,89,113	1.46	7 (11%)
14	CLA	3	512	13	49,53,73	1.49	10 (20%)	59,89,113	1.39	5 (8%)
17	BCR	q	523	-	41,41,41	0.75	0	56,56,56	1.68	13 (23%)
14	CLA	H	1224	2	64,68,73	1.28	9 (14%)	77,107,113	1.36	9 (11%)
17	BCR	c	524	-	41,41,41	0.72	0	56,56,56	1.74	12 (21%)
14	CLA	f	1023	-	69,73,73	1.25	11 (15%)	83,113,113	1.74	12 (14%)
18	LHG	A	5001	-	48,48,48	0.80	1 (2%)	51,54,54	1.30	7 (13%)
14	CLA	d	512	13	49,53,73	1.47	10 (20%)	59,89,113	1.48	6 (10%)
17	BCR	d	522	-	41,41,41	0.71	0	56,56,56	1.89	19 (33%)
17	BCR	k	4018	-	41,41,41	0.93	2 (4%)	56,56,56	1.93	16 (28%)
14	CLA	b	516	13	49,53,73	1.48	9 (18%)	59,89,113	1.48	5 (8%)
14	CLA	u	510	13	49,53,73	1.47	9 (18%)	59,89,113	1.49	5 (8%)
17	BCR	I	4018	-	41,41,41	0.93	2 (4%)	56,56,56	1.93	17 (30%)
14	CLA	u	516	13	49,53,73	1.47	9 (18%)	59,89,113	1.41	4 (6%)
14	CLA	6	501	13	49,53,73	1.47	10 (20%)	59,89,113	1.56	5 (8%)
14	CLA	Y	518	13	49,53,73	1.48	7 (14%)	59,89,113	1.52	6 (10%)
14	CLA	a	516	13	49,53,73	1.48	7 (14%)	59,89,113	1.71	9 (15%)
14	CLA	e	1138	1	69,73,73	1.23	9 (13%)	83,113,113	1.44	6 (7%)
21	SQD	2	822	-	27,28,54	1.22	4 (14%)	36,39,65	1.86	10 (27%)
14	CLA	G	1112	1	54,58,73	1.39	12 (22%)	65,95,113	1.53	7 (10%)
14	CLA	6	508	13	49,53,73	1.49	9 (18%)	59,89,113	1.60	11 (18%)
14	CLA	Z	505	13	69,73,73	1.23	7 (10%)	83,113,113	1.33	7 (8%)
14	CLA	G	1013	-	69,73,73	1.28	11 (15%)	83,113,113	1.69	14 (16%)
14	CLA	f	1221	23	66,70,73	1.32	11 (16%)	79,109,113	1.53	12 (15%)
14	CLA	r	517	-	49,53,73	1.48	9 (18%)	59,89,113	1.50	6 (10%)
14	CLA	c	510	13	49,53,73	1.47	10 (20%)	59,89,113	1.49	5 (8%)
14	CLA	u	511	13	49,53,73	1.49	7 (14%)	59,89,113	1.54	9 (15%)
14	CLA	5	512	13	49,53,73	1.47	9 (18%)	59,89,113	1.45	6 (10%)
17	BCR	5	522	-	41,41,41	0.76	0	56,56,56	1.94	20 (35%)
17	BCR	j	4016	-	41,41,41	0.82	0	56,56,56	1.91	11 (19%)
14	CLA	Y	506	13	49,53,73	1.47	9 (18%)	59,89,113	1.45	7 (11%)
14	CLA	q	517	-	49,53,73	1.46	9 (18%)	59,89,113	1.45	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	Y	524	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
14	CLA	H	1218	2	64,68,73	1.30	9 (14%)	77,107,113	1.36	5 (6%)
14	CLA	A	1140	1	69,73,73	1.26	10 (14%)	83,113,113	1.47	9 (10%)
14	CLA	B	1023	-	69,73,73	1.25	11 (15%)	83,113,113	1.74	12 (14%)
22	FMN	X	170	-	33,33,33	1.12	2 (6%)	48,50,50	1.24	6 (12%)
14	CLA	2	519	13	49,53,73	1.48	9 (18%)	59,89,113	1.50	7 (11%)
14	CLA	H	1210	2	69,73,73	1.27	11 (15%)	83,113,113	1.36	10 (12%)
14	CLA	q	512	13	49,53,73	1.47	10 (20%)	59,89,113	1.38	4 (6%)
14	CLA	Y	513	13	49,53,73	1.47	10 (20%)	59,89,113	1.47	6 (10%)
14	CLA	A	1112	1	54,58,73	1.39	12 (22%)	65,95,113	1.54	7 (10%)
18	LHG	G	5001	-	48,48,48	0.80	1 (2%)	51,54,54	1.30	7 (13%)
14	CLA	6	507	-	49,53,73	1.46	8 (16%)	59,89,113	1.53	6 (10%)
14	CLA	d	504	-	49,53,73	1.47	9 (18%)	59,89,113	1.52	7 (11%)
14	CLA	t	518	13	49,53,73	1.48	9 (18%)	59,89,113	1.48	4 (6%)
14	CLA	r	513	13	49,53,73	1.48	10 (20%)	59,89,113	1.42	5 (8%)
14	CLA	s	510	13	49,53,73	1.47	10 (20%)	59,89,113	1.49	5 (8%)
17	BCR	L	4022	-	41,41,41	0.79	0	56,56,56	1.82	10 (17%)
21	SQD	4	822	-	25,26,54	1.32	4 (16%)	34,37,65	1.97	9 (26%)
14	CLA	Y	504	-	49,53,73	1.49	9 (18%)	59,89,113	1.64	8 (13%)
14	CLA	A	1107	1	69,73,73	1.31	10 (14%)	83,113,113	1.40	10 (12%)
17	BCR	l	4015	-	41,41,41	0.80	0	56,56,56	1.73	12 (21%)
14	CLA	3	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.44	4 (6%)
14	CLA	q	509	13	49,53,73	1.49	10 (20%)	59,89,113	1.51	8 (13%)
18	LHG	e	5007	-	46,46,48	0.61	0	49,52,54	1.20	4 (8%)
14	CLA	3	504	-	49,53,73	1.47	10 (20%)	59,89,113	1.56	9 (15%)
14	CLA	H	1023	-	69,73,73	1.25	11 (15%)	83,113,113	1.75	12 (14%)
14	CLA	r	511	13	49,53,73	1.49	9 (18%)	59,89,113	1.55	8 (13%)
17	BCR	3	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)
14	CLA	4	508	13	49,53,73	1.51	10 (20%)	59,89,113	1.63	9 (15%)
18	LHG	A	5009	-	41,41,48	0.67	0	44,47,54	1.22	5 (11%)
14	CLA	2	511	13	49,53,73	1.48	9 (18%)	59,89,113	1.55	7 (11%)
14	CLA	6	502	13	49,53,73	1.49	8 (16%)	59,89,113	1.55	6 (10%)
21	SQD	d	822	-	25,26,54	1.31	4 (16%)	34,37,65	2.00	10 (29%)
14	CLA	1	505	13	49,53,73	1.46	8 (16%)	59,89,113	1.48	4 (6%)
17	BCR	m	4104	-	41,41,41	0.79	0	56,56,56	1.88	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	c	517	-	49,53,73	1.48	10 (20%)	59,89,113	1.41	4 (6%)
14	CLA	1	518	13	49,53,73	1.48	8 (16%)	59,89,113	1.51	6 (10%)
17	BCR	3	523	-	41,41,41	0.69	0	56,56,56	1.82	15 (26%)
19	LMU	B	1843	-	36,36,36	1.16	2 (5%)	47,47,47	1.06	3 (6%)
14	CLA	Z	506	13	49,53,73	1.47	9 (18%)	59,89,113	1.47	6 (10%)
17	BCR	e	4001	-	41,41,41	0.79	0	56,56,56	1.69	11 (19%)
14	CLA	G	1122	1	64,68,73	1.31	11 (17%)	77,107,113	1.43	8 (10%)
14	CLA	u	501	13	49,53,73	1.48	10 (20%)	59,89,113	1.56	6 (10%)
18	LHG	e	5005	-	42,42,48	0.65	1 (2%)	45,48,54	1.21	4 (8%)
14	CLA	G	1126	1	69,73,73	1.24	12 (17%)	83,113,113	1.38	7 (8%)
14	CLA	G	1107	1	69,73,73	1.31	10 (14%)	83,113,113	1.41	10 (12%)
14	CLA	G	1109	1	69,73,73	1.25	11 (15%)	83,113,113	1.47	8 (9%)
14	CLA	B	1203	2	69,73,73	1.28	10 (14%)	83,113,113	1.41	10 (12%)
14	CLA	Z	517	-	49,53,73	1.47	9 (18%)	59,89,113	1.50	6 (10%)
14	CLA	t	506	13	49,53,73	1.48	10 (20%)	59,89,113	1.50	5 (8%)
14	CLA	r	518	13	59,63,73	1.33	9 (15%)	71,101,113	1.41	6 (8%)
14	CLA	2	512	13	49,53,73	1.49	10 (20%)	59,89,113	1.39	5 (8%)
14	CLA	u	517	-	49,53,73	1.49	10 (20%)	59,89,113	1.42	4 (6%)
14	CLA	3	511	13	49,53,73	1.48	9 (18%)	59,89,113	1.54	8 (13%)
17	BCR	e	4002	-	41,41,41	0.87	1 (2%)	56,56,56	1.94	16 (28%)
14	CLA	U	1103	9	52,56,73	1.44	10 (19%)	62,92,113	1.51	6 (9%)
14	CLA	d	509	13	49,53,73	1.48	10 (20%)	59,89,113	1.51	6 (10%)
14	CLA	H	1202	2	69,73,73	1.22	11 (15%)	83,113,113	1.42	8 (9%)
17	BCR	f	4004	-	41,41,41	0.74	0	56,56,56	1.85	14 (25%)

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
17	BCR	W	4021	-	-	6/29/63/63	0/2/2/2
14	CLA	B	1212	2	-	8/23/99/115	-
14	CLA	V	1501	10	-	11/33/109/115	-
17	BCR	J	4012	-	-	9/29/63/63	0/2/2/2
14	CLA	s	507	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	r	522	-	-	6/29/63/63	0/2/2/2
14	CLA	s	516	13	-	9/15/91/115	-
14	CLA	m	1401	-	-	10/27/103/115	-
14	CLA	f	1012	23	-	15/39/115/115	-
17	BCR	d	521	-	-	5/29/63/63	0/2/2/2
20	LMG	l	5104	-	-	13/27/47/70	0/1/1/1
14	CLA	Z	509	13	-	3/39/115/115	-
18	LHG	G	5009	-	-	28/46/46/53	-
17	BCR	n	4022	-	-	3/29/63/63	0/2/2/2
17	BCR	V	4019	-	-	6/29/63/63	0/2/2/2
14	CLA	G	1131	1	-	8/39/115/115	-
18	LHG	B	1855	-	-	24/45/45/53	-
20	LMG	T	5104	-	-	13/27/47/70	0/1/1/1
14	CLA	e	1114	23	-	3/15/91/115	-
18	LHG	e	5008	-	-	18/39/39/53	-
14	CLA	B	1228	2	-	6/27/103/115	-
14	CLA	A	1127	1	-	12/39/115/115	-
17	BCR	H	4009	-	-	1/29/63/63	0/2/2/2
14	CLA	q	503	13	-	9/15/91/115	-
19	LMU	G	1849	-	-	6/14/34/61	0/1/1/2
14	CLA	A	1137	1	-	20/33/109/115	-
14	CLA	5	511	13	-	3/15/91/115	-
14	CLA	4	512	13	-	5/15/91/115	-
14	CLA	6	516	13	-	11/15/91/115	-
17	BCR	b	524	-	-	4/29/63/63	0/2/2/2
17	BCR	a	524	-	-	5/29/63/63	0/2/2/2
14	CLA	U	1105	9	-	10/15/91/115	-
14	CLA	5	507	-	-	9/15/91/115	-
14	CLA	m	1105	9	-	10/15/91/115	-
14	CLA	H	1226	2	-	7/27/103/115	-
14	CLA	A	1115	1	-	13/33/109/115	-
14	CLA	f	1216	23	-	13/33/109/115	-
14	CLA	H	1238	23	-	4/39/115/115	-
14	CLA	Y	519	13	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	f	1236	2	-	5/21/97/115	-
14	CLA	f	1232	23	-	6/27/103/115	-
14	CLA	f	1205	2	-	10/39/115/115	-
14	CLA	G	1137	1	-	20/33/109/115	-
17	BCR	G	4008	-	-	7/29/63/63	0/2/2/2
17	BCR	f	4017	-	-	2/29/63/63	0/2/2/2
14	CLA	A	1013	-	-	13/39/115/115	-
14	CLA	c	502	13	-	7/15/91/115	-
14	CLA	H	1206	2	-	15/39/115/115	-
14	CLA	B	1208	2	-	17/39/115/115	-
14	CLA	A	1101	1	-	18/39/115/115	-
14	CLA	J	1302	8	-	14/27/103/115	-
14	CLA	l	503	13	-	9/15/91/115	-
14	CLA	A	1124	23	-	13/33/109/115	-
14	CLA	3	501	13	-	6/15/91/115	-
14	CLA	f	1207	2	-	18/39/115/115	-
14	CLA	d	518	13	-	9/15/91/115	-
14	CLA	f	1206	2	-	15/39/115/115	-
14	CLA	e	1125	1	-	12/39/115/115	-
14	CLA	b	502	13	-	5/15/91/115	-
14	CLA	G	1134	1	-	11/29/105/115	-
18	LHG	n	5220	-	-	28/45/45/53	-
14	CLA	A	1138	1	-	14/39/115/115	-
14	CLA	e	1011	1	-	12/39/115/115	-
14	CLA	Z	507	-	-	10/15/91/115	-
17	BCR	A	4008	-	-	7/29/63/63	0/2/2/2
14	CLA	t	512	13	-	5/15/91/115	-
17	BCR	t	522	-	-	4/29/63/63	0/2/2/2
14	CLA	e	1237	23	-	25/39/115/115	-
14	CLA	H	1208	2	-	17/39/115/115	-
14	CLA	s	509	13	-	2/15/91/115	-
14	CLA	F	1302	6	-	9/15/91/115	-
14	CLA	A	1801	18	-	7/15/91/115	-
14	CLA	B	1235	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1111	1	-	20/39/115/115	-
14	CLA	H	1225	2	-	7/39/115/115	-
14	CLA	v	509	13	-	4/15/91/115	-
17	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
17	BCR	n	4219	-	-	2/29/63/63	0/2/2/2
18	LHG	e	5003	14	-	17/44/44/53	-
14	CLA	A	1134	1	-	11/29/105/115	-
14	CLA	4	504	-	-	6/15/91/115	-
14	CLA	q	513	13	-	6/15/91/115	-
14	CLA	Z	513	13	-	4/15/91/115	-
14	CLA	u	502	13	-	7/15/91/115	-
14	CLA	4	507	-	-	8/15/91/115	-
17	BCR	H	4017	-	-	2/29/63/63	0/2/2/2
17	BCR	a	522	-	-	5/29/63/63	0/2/2/2
14	CLA	G	1113	1	-	6/15/91/115	-
14	CLA	R	1302	6	-	9/15/91/115	-
14	CLA	B	1221	23	-	14/36/112/115	-
14	CLA	a	513	13	-	5/15/91/115	-
14	CLA	l	510	13	-	6/15/91/115	-
14	CLA	f	1240	18	-	15/39/115/115	-
14	CLA	T	1303	8	-	6/15/91/115	-
14	CLA	G	1104	1	-	10/39/115/115	-
14	CLA	G	1138	1	-	14/39/115/115	-
14	CLA	r	510	13	-	7/15/91/115	-
17	BCR	3	522	-	-	5/29/63/63	0/2/2/2
14	CLA	e	1121	1	-	10/27/103/115	-
14	CLA	G	1139	23	-	20/39/115/115	-
14	CLA	F	1301	23	-	3/15/91/115	-
14	CLA	t	511	13	-	5/15/91/115	-
14	CLA	H	1229	2	-	12/39/115/115	-
14	CLA	2	513	13	-	4/15/91/115	-
14	CLA	f	1229	2	-	12/39/115/115	-
20	LMG	B	5002	-	-	24/48/68/70	0/1/1/1
17	BCR	A	4011	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LHG	A	5006	-	-	26/44/44/53	-
14	CLA	t	507	-	-	8/15/91/115	-
14	CLA	Y	516	13	-	14/15/91/115	-
14	CLA	B	1205	2	-	10/39/115/115	-
17	BCR	6	524	-	-	5/29/63/63	0/2/2/2
14	CLA	v	512	13	-	9/15/91/115	-
14	CLA	G	1118	1	-	10/33/109/115	-
15	PQN	B	2002	-	-	6/23/43/43	0/2/2/2
14	CLA	A	1132	1	-	18/39/115/115	-
14	CLA	H	1215	2	-	19/39/115/115	-
17	BCR	J	4013	-	-	4/29/63/63	0/2/2/2
17	BCR	B	4006	-	-	4/29/63/63	0/2/2/2
14	CLA	H	1204	2	-	13/39/115/115	-
17	BCR	s	524	-	-	5/29/63/63	0/2/2/2
14	CLA	H	1228	2	-	6/27/103/115	-
14	CLA	f	1215	2	-	19/39/115/115	-
14	CLA	u	513	13	-	7/15/91/115	-
17	BCR	q	522	-	-	6/29/63/63	0/2/2/2
14	CLA	v	510	13	-	10/15/91/115	-
14	CLA	s	505	13	-	11/27/103/115	-
17	BCR	Y	521	-	-	7/29/63/63	0/2/2/2
14	CLA	e	1013	-	-	13/39/115/115	-
17	BCR	Z	523	-	-	6/29/63/63	0/2/2/2
21	SQD	6	822	-	-	7/19/39/69	0/1/1/1
14	CLA	A	1118	1	-	10/33/109/115	-
18	LHG	L	5218	-	-	19/41/41/53	-
14	CLA	A	1133	1	-	17/39/115/115	-
14	CLA	q	505	13	-	6/15/91/115	-
17	BCR	L	4019	-	-	6/29/63/63	0/2/2/2
14	CLA	5	502	13	-	7/15/91/115	-
14	CLA	G	1140	1	-	14/39/115/115	-
17	BCR	v	524	-	-	5/29/63/63	0/2/2/2
14	CLA	d	511	13	-	8/15/91/115	-
14	CLA	f	1231	23	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	e	1132	1	-	18/39/115/115	-
14	CLA	a	517	-	-	9/15/91/115	-
14	CLA	c	518	13	-	5/15/91/115	-
18	LHG	G	5004	-	-	18/39/39/53	-
18	LHG	e	5009	-	-	28/46/46/53	-
17	BCR	B	4010	-	-	7/29/63/63	0/2/2/2
14	CLA	e	1131	1	-	8/39/115/115	-
14	CLA	A	1114	23	-	3/15/91/115	-
18	LHG	A	5002	-	-	22/47/47/53	-
17	BCR	2	522	-	-	6/29/63/63	0/2/2/2
14	CLA	6	503	13	-	8/15/91/115	-
14	CLA	6	512	13	-	9/15/91/115	-
14	CLA	v	504	-	-	6/15/91/115	-
14	CLA	B	1230	2	-	12/33/109/115	-
14	CLA	r	516	13	-	8/15/91/115	-
17	BCR	f	4014	-	-	7/29/63/63	0/2/2/2
14	CLA	B	1204	2	-	13/39/115/115	-
14	CLA	b	519	13	-	10/15/91/115	-
14	CLA	s	518	13	-	11/27/103/115	-
14	CLA	B	1224	2	-	7/33/109/115	-
14	CLA	K	1103	9	-	10/19/95/115	-
14	CLA	f	1214	2	-	14/39/115/115	-
17	BCR	b	523	-	-	5/29/63/63	0/2/2/2
14	CLA	a	509	13	-	2/15/91/115	-
14	CLA	e	1140	1	-	14/39/115/115	-
21	SQD	b	822	-	-	10/19/39/69	0/1/1/1
17	BCR	f	4005	-	-	6/29/63/63	0/2/2/2
14	CLA	4	518	13	-	6/15/91/115	-
14	CLA	G	1106	1	-	23/39/115/115	-
14	CLA	B	1234	2	-	15/39/115/115	-
14	CLA	u	503	13	-	9/15/91/115	-
18	LHG	A	5005	-	-	28/47/47/53	-
14	CLA	e	1102	1	-	7/27/103/115	-
17	BCR	J	4015	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	T	4012	-	-	9/29/63/63	0/2/2/2
21	SQD	1	822	-	-	10/27/47/69	0/1/1/1
14	CLA	q	501	13	-	11/15/91/115	-
14	CLA	d	516	13	-	11/15/91/115	-
18	LHG	G	5007	-	-	23/51/51/53	-
14	CLA	d	506	13	-	8/15/91/115	-
14	CLA	B	1238	23	-	4/39/115/115	-
18	LHG	e	5001	-	-	23/53/53/53	-
14	CLA	v	516	13	-	11/15/91/115	-
18	LHG	G	5002	-	-	22/47/47/53	-
14	CLA	4	519	13	-	10/15/91/115	-
14	CLA	A	1106	1	-	23/39/115/115	-
14	CLA	e	1101	1	-	18/39/115/115	-
14	CLA	G	1119	23	-	14/39/115/115	-
14	CLA	G	1105	1	-	8/27/103/115	-
14	CLA	H	1219	2	-	20/37/113/115	-
18	LHG	A	5007	-	-	23/51/51/53	-
19	LMU	A	1848	-	-	7/21/61/61	0/2/2/2
14	CLA	H	1203	2	-	16/39/115/115	-
14	CLA	b	518	13	-	6/15/91/115	-
14	CLA	3	503	13	-	9/15/91/115	-
14	CLA	H	1221	23	-	14/36/112/115	-
17	BCR	4	522	-	-	4/29/63/63	0/2/2/2
14	CLA	r	509	13	-	4/39/115/115	-
18	LHG	A	5008	-	-	18/39/39/53	-
14	CLA	d	507	-	-	7/15/91/115	-
14	CLA	6	519	13	-	8/15/91/115	-
14	CLA	B	1012	23	-	15/39/115/115	-
14	CLA	Z	508	13	-	4/15/91/115	-
14	CLA	f	1218	2	-	9/33/109/115	-
14	CLA	v	501	13	-	9/15/91/115	-
19	LMU	e	1848	-	-	7/21/61/61	0/2/2/2
21	SQD	Y	822	-	-	10/27/47/69	0/1/1/1
18	LHG	f	1842	14	-	19/41/41/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	u	508	13	-	6/15/91/115	-
17	BCR	a	521	-	-	7/29/63/63	0/2/2/2
21	SQD	L	5216	-	-	17/41/61/69	0/1/1/1
14	CLA	A	1119	23	-	15/39/115/115	-
14	CLA	H	1214	2	-	14/39/115/115	-
14	CLA	c	503	13	-	9/15/91/115	-
14	CLA	s	519	13	-	7/15/91/115	-
14	CLA	l	513	13	-	6/15/91/115	-
17	BCR	d	523	-	-	4/29/63/63	0/2/2/2
14	CLA	G	1116	1	-	9/33/109/115	-
14	CLA	f	1212	2	-	8/23/99/115	-
14	CLA	j	1301	23	-	3/15/91/115	-
14	CLA	r	501	13	-	13/33/109/115	-
14	CLA	t	502	13	-	5/15/91/115	-
14	CLA	e	1109	1	-	16/39/115/115	-
14	CLA	e	1133	1	-	17/39/115/115	-
17	BCR	Z	524	-	-	3/29/63/63	0/2/2/2
16	SF4	C	3002	3	-	-	0/6/5/5
14	CLA	4	505	13	-	5/15/91/115	-
14	CLA	H	1213	2	-	11/35/111/115	-
14	CLA	e	1124	23	-	13/33/109/115	-
14	CLA	f	1210	2	-	22/39/115/115	-
14	CLA	b	503	13	-	4/15/91/115	-
17	BCR	Z	522	-	-	6/29/63/63	0/2/2/2
14	CLA	6	506	13	-	8/15/91/115	-
14	CLA	c	504	-	-	5/15/91/115	-
17	BCR	u	524	-	-	2/29/63/63	0/2/2/2
14	CLA	s	504	-	-	7/15/91/115	-
14	CLA	G	1133	1	-	17/39/115/115	-
14	CLA	e	1104	1	-	10/39/115/115	-
14	CLA	e	1120	1	-	11/21/97/115	-
14	CLA	a	503	13	-	9/15/91/115	-
17	BCR	n	4020	-	-	4/29/63/63	0/2/2/2
16	SF4	g	3002	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1116	1	-	9/33/109/115	-
14	CLA	e	1137	1	-	20/33/109/115	-
14	CLA	e	1117	1	-	13/39/115/115	-
17	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
17	BCR	e	4008	-	-	7/29/63/63	0/2/2/2
14	CLA	G	1120	1	-	11/21/97/115	-
14	CLA	u	504	-	-	5/15/91/115	-
22	FMN	P	170	-	-	0/18/18/18	0/3/3/3
14	CLA	K	1401	-	-	10/27/103/115	-
14	CLA	5	519	13	-	8/15/91/115	-
14	CLA	Y	512	13	-	7/15/91/115	-
14	CLA	2	510	13	-	7/15/91/115	-
21	SQD	f	1852	-	-	18/35/55/69	0/1/1/1
14	CLA	d	517	-	-	12/15/91/115	-
14	CLA	G	1022	23	-	9/39/115/115	-
14	CLA	L	1501	10	-	11/33/109/115	-
14	CLA	Y	502	13	-	4/15/91/115	-
14	CLA	1	519	13	-	8/15/91/115	-
14	CLA	H	1217	2	-	14/33/109/115	-
17	BCR	3	524	-	-	5/29/63/63	0/2/2/2
14	CLA	B	1209	2	-	11/25/101/115	-
14	CLA	e	1110	1	-	12/25/101/115	-
14	CLA	f	1220	2	-	11/27/103/115	-
14	CLA	f	1226	2	-	7/27/103/115	-
14	CLA	K	1105	9	-	10/15/91/115	-
17	BCR	b	521	-	-	10/29/63/63	0/2/2/2
14	CLA	f	1217	2	-	14/33/109/115	-
19	LMU	e	1849	-	-	6/14/34/61	0/1/1/2
14	CLA	s	508	13	-	4/15/91/115	-
14	CLA	H	1209	2	-	11/25/101/115	-
14	CLA	A	1120	1	-	11/21/97/115	-
17	BCR	G	4002	-	-	0/29/63/63	0/2/2/2
17	BCR	G	4011	-	-	13/29/63/63	0/2/2/2
14	CLA	e	1130	1	-	7/29/105/115	-
14	CLA	A	1022	23	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1222	23	-	2/21/97/115	-
14	CLA	e	1129	1	-	10/25/101/115	-
19	LMU	l	5105	-	-	9/13/33/61	0/1/1/2
17	BCR	B	4014	-	-	7/29/63/63	0/2/2/2
14	CLA	f	1222	23	-	2/21/97/115	-
19	LMU	T	5105	-	-	9/13/33/61	0/1/1/2
14	CLA	v	508	13	-	6/15/91/115	-
14	CLA	v	519	13	-	8/15/91/115	-
14	CLA	q	510	13	-	6/15/91/115	-
17	BCR	G	4007	-	-	0/29/63/63	0/2/2/2
17	BCR	a	523	-	-	4/29/63/63	0/2/2/2
14	CLA	5	505	13	-	5/15/91/115	-
14	CLA	Z	501	13	-	13/33/109/115	-
14	CLA	a	502	13	-	3/15/91/115	-
14	CLA	3	509	13	-	2/15/91/115	-
17	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
14	CLA	a	508	13	-	4/15/91/115	-
14	CLA	3	508	13	-	4/15/91/115	-
19	LMU	A	1849	-	-	6/14/34/61	0/1/1/2
14	CLA	q	502	13	-	4/15/91/115	-
14	CLA	2	517	-	-	9/15/91/115	-
17	BCR	n	4019	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1201	2	-	8/33/109/115	-
17	BCR	e	4011	-	-	13/29/63/63	0/2/2/2
14	CLA	v	503	13	-	8/15/91/115	-
17	BCR	S	4018	-	-	0/29/63/63	0/2/2/2
14	CLA	u	505	13	-	5/15/91/115	-
14	CLA	B	1202	2	-	12/39/115/115	-
14	CLA	1	509	13	-	5/15/91/115	-
14	CLA	v	506	13	-	8/15/91/115	-
17	BCR	T	4015	-	-	5/29/63/63	0/2/2/2
14	CLA	4	510	13	-	7/15/91/115	-
14	CLA	Y	503	13	-	9/15/91/115	-
14	CLA	A	1108	1	-	16/26/102/115	-
14	CLA	r	507	-	-	10/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	4	516	13	-	9/15/91/115	-
14	CLA	6	518	13	-	9/15/91/115	-
18	LHG	I	5001	-	-	25/52/52/53	-
14	CLA	q	507	-	-	8/15/91/115	-
14	CLA	e	1111	1	-	20/39/115/115	-
14	CLA	f	1239	2	-	16/39/115/115	-
17	BCR	s	521	-	-	7/29/63/63	0/2/2/2
14	CLA	v	502	13	-	3/15/91/115	-
14	CLA	2	509	13	-	3/39/115/115	-
21	SQD	3	822	-	-	9/23/43/69	0/1/1/1
14	CLA	f	1227	2	-	13/33/109/115	-
14	CLA	Z	519	13	-	7/15/91/115	-
17	BCR	u	522	-	-	5/29/63/63	0/2/2/2
16	SF4	A	3001	2,1	-	-	0/6/5/5
14	CLA	Z	510	13	-	7/15/91/115	-
14	CLA	2	507	-	-	10/15/91/115	-
14	CLA	5	516	13	-	7/15/91/115	-
14	CLA	r	502	13	-	3/15/91/115	-
14	CLA	f	1211	2	-	8/27/103/115	-
14	CLA	G	1128	1	-	10/39/115/115	-
14	CLA	Y	511	13	-	4/15/91/115	-
19	LMU	H	1843	-	-	12/21/61/61	0/2/2/2
14	CLA	f	1203	2	-	16/39/115/115	-
14	CLA	1	516	13	-	14/15/91/115	-
14	CLA	G	1130	1	-	7/29/105/115	-
14	CLA	t	519	13	-	10/15/91/115	-
14	CLA	a	512	13	-	3/15/91/115	-
14	CLA	b	510	13	-	7/15/91/115	-
14	CLA	e	1122	1	-	14/33/109/115	-
17	BCR	K	4104	-	-	2/29/63/63	0/2/2/2
18	LHG	L	5220	-	-	28/45/45/53	-
18	LHG	V	5221	-	-	31/53/53/53	-
14	CLA	1	501	13	-	11/15/91/115	-
17	BCR	B	4017	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	1201	2	-	8/33/109/115	-
14	CLA	f	1223	2	-	10/39/115/115	-
14	CLA	u	506	13	-	8/15/91/115	-
14	CLA	A	1128	1	-	10/39/115/115	-
14	CLA	G	1801	18	-	7/15/91/115	-
18	LHG	n	5221	-	-	31/53/53/53	-
17	BCR	Y	523	-	-	6/29/63/63	0/2/2/2
14	CLA	t	510	13	-	7/15/91/115	-
17	BCR	l	521	-	-	7/29/63/63	0/2/2/2
14	CLA	V	1502	10	-	10/39/115/115	-
14	CLA	B	1231	23	-	8/39/115/115	-
14	CLA	H	1212	2	-	8/23/99/115	-
14	CLA	Y	508	13	-	5/15/91/115	-
16	SF4	N	3003	3	-	-	0/6/5/5
14	CLA	e	1118	1	-	10/33/109/115	-
14	CLA	t	501	13	-	8/15/91/115	-
14	CLA	A	1136	1	-	10/39/115/115	-
14	CLA	B	1229	2	-	13/39/115/115	-
14	CLA	e	1103	1	-	21/39/115/115	-
14	CLA	t	505	13	-	5/15/91/115	-
18	LHG	B	1842	14	-	19/41/41/53	-
14	CLA	3	505	13	-	11/27/103/115	-
17	BCR	2	523	-	-	6/29/63/63	0/2/2/2
14	CLA	b	512	13	-	5/15/91/115	-
17	BCR	b	522	-	-	4/29/63/63	0/2/2/2
18	LHG	A	5004	-	-	18/39/39/53	-
14	CLA	s	506	13	-	8/15/91/115	-
22	FMN	p	170	-	-	0/18/18/18	0/3/3/3
14	CLA	H	1205	2	-	10/39/115/115	-
14	CLA	r	503	13	-	10/39/115/115	-
14	CLA	H	1211	2	-	8/27/103/115	-
14	CLA	Y	517	-	-	9/15/91/115	-
14	CLA	H	1223	2	-	9/39/115/115	-
20	LMG	J	5104	-	-	13/27/47/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	f	4006	-	-	4/29/63/63	0/2/2/2
14	CLA	V	1503	23	-	10/33/109/115	-
14	CLA	Z	516	13	-	8/15/91/115	-
14	CLA	Z	502	13	-	3/15/91/115	-
14	CLA	G	1115	1	-	13/33/109/115	-
17	BCR	6	523	-	-	4/29/63/63	0/2/2/2
14	CLA	G	1136	1	-	10/39/115/115	-
14	CLA	r	504	-	-	9/15/91/115	-
14	CLA	a	519	13	-	7/15/91/115	-
14	CLA	d	513	13	-	5/15/91/115	-
14	CLA	2	504	-	-	9/15/91/115	-
14	CLA	A	1131	1	-	8/39/115/115	-
14	CLA	q	519	13	-	8/15/91/115	-
14	CLA	b	511	13	-	5/15/91/115	-
14	CLA	e	1105	1	-	7/27/103/115	-
14	CLA	e	1112	1	-	4/21/97/115	-
14	CLA	1	508	13	-	5/15/91/115	-
17	BCR	B	4004	-	-	8/29/63/63	0/2/2/2
16	SF4	C	3003	3	-	-	0/6/5/5
14	CLA	b	517	-	-	7/15/91/115	-
14	CLA	f	1238	23	-	4/39/115/115	-
14	CLA	G	1108	1	-	16/26/102/115	-
14	CLA	t	516	13	-	9/15/91/115	-
14	CLA	f	1201	2	-	8/33/109/115	-
14	CLA	H	1232	23	-	6/27/103/115	-
14	CLA	T	1302	8	-	14/27/103/115	-
21	SQD	v	822	-	-	7/19/39/69	0/1/1/1
14	CLA	a	511	13	-	2/15/91/115	-
14	CLA	b	504	-	-	6/15/91/115	-
14	CLA	3	506	13	-	8/15/91/115	-
14	CLA	c	509	13	-	13/39/115/115	-
16	SF4	g	3003	3	-	-	0/6/5/5
17	BCR	Y	522	-	-	6/29/63/63	0/2/2/2
18	LHG	L	5221	-	-	31/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	e	1113	1	-	6/15/91/115	-
17	BCR	H	4010	-	-	7/29/63/63	0/2/2/2
14	CLA	q	508	13	-	5/15/91/115	-
17	BCR	T	4013	-	-	4/29/63/63	0/2/2/2
14	CLA	d	508	13	-	6/15/91/115	-
14	CLA	f	1202	2	-	12/39/115/115	-
14	CLA	a	507	-	-	7/15/91/115	-
14	CLA	B	1222	23	-	2/21/97/115	-
14	CLA	Y	501	13	-	11/15/91/115	-
17	BCR	L	4219	-	-	2/29/63/63	0/2/2/2
17	BCR	f	4010	-	-	7/29/63/63	0/2/2/2
21	SQD	5	822	-	-	3/19/39/69	0/1/1/1
14	CLA	b	509	13	-	6/15/91/115	-
14	CLA	A	1105	1	-	7/27/103/115	-
17	BCR	5	524	-	-	2/29/63/63	0/2/2/2
14	CLA	u	512	13	-	7/15/91/115	-
14	CLA	H	1012	23	-	15/39/115/115	-
17	BCR	r	524	-	-	3/29/63/63	0/2/2/2
14	CLA	5	513	13	-	7/15/91/115	-
14	CLA	s	512	13	-	3/15/91/115	-
14	CLA	r	519	13	-	7/15/91/115	-
17	BCR	2	524	-	-	3/29/63/63	0/2/2/2
18	LHG	e	5002	-	-	22/47/47/53	-
17	BCR	q	524	-	-	2/29/63/63	0/2/2/2
14	CLA	4	513	13	-	7/15/91/115	-
14	CLA	2	502	13	-	3/15/91/115	-
14	CLA	f	1234	2	-	15/39/115/115	-
14	CLA	s	502	13	-	3/15/91/115	-
14	CLA	4	517	-	-	7/15/91/115	-
14	CLA	f	1209	2	-	11/25/101/115	-
14	CLA	f	1225	2	-	7/39/115/115	-
17	BCR	f	4009	-	-	1/29/63/63	0/2/2/2
14	CLA	b	506	13	-	6/15/91/115	-
14	CLA	u	519	13	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	3	510	13	-	8/15/91/115	-
14	CLA	6	511	13	-	7/15/91/115	-
14	CLA	2	501	13	-	13/33/109/115	-
14	CLA	B	1021	2	-	11/39/115/115	-
21	SQD	a	822	-	-	9/23/43/69	0/1/1/1
14	CLA	B	1207	2	-	18/39/115/115	-
21	SQD	V	5216	-	-	17/41/61/69	0/1/1/1
17	BCR	o	4021	-	-	6/29/63/63	0/2/2/2
21	SQD	q	822	-	-	10/27/47/69	0/1/1/1
17	BCR	v	523	-	-	4/29/63/63	0/2/2/2
14	CLA	B	1226	2	-	7/27/103/115	-
14	CLA	e	1119	23	-	15/39/115/115	-
14	CLA	q	516	13	-	14/15/91/115	-
14	CLA	d	501	13	-	9/15/91/115	-
14	CLA	G	1101	1	-	18/39/115/115	-
14	CLA	B	1223	2	-	9/39/115/115	-
14	CLA	r	508	13	-	4/15/91/115	-
14	CLA	B	1219	2	-	20/37/113/115	-
14	CLA	G	1135	1	-	10/27/103/115	-
14	CLA	6	504	-	-	6/15/91/115	-
14	CLA	d	505	13	-	15/39/115/115	-
14	CLA	e	1135	1	-	10/27/103/115	-
21	SQD	n	5216	-	-	17/41/61/69	0/1/1/1
14	CLA	e	1116	1	-	9/33/109/115	-
14	CLA	1	512	13	-	7/15/91/115	-
14	CLA	J	1303	8	-	6/15/91/115	-
14	CLA	A	1237	23	-	24/39/115/115	-
17	BCR	1	522	-	-	6/29/63/63	0/2/2/2
18	LHG	e	5006	-	-	26/44/44/53	-
16	SF4	e	3001	2,1	-	-	0/6/5/5
14	CLA	v	511	13	-	7/15/91/115	-
14	CLA	e	1107	1	-	16/39/115/115	-
14	CLA	5	510	13	-	9/15/91/115	-
14	CLA	H	1207	2	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	H	4014	-	-	7/29/63/63	0/2/2/2
14	CLA	B	1211	2	-	8/27/103/115	-
14	CLA	H	1234	2	-	15/39/115/115	-
17	BCR	e	4003	-	-	0/29/63/63	0/2/2/2
14	CLA	e	1127	1	-	12/39/115/115	-
14	CLA	H	1230	2	-	12/33/109/115	-
17	BCR	6	521	-	-	5/29/63/63	0/2/2/2
14	CLA	A	1135	1	-	10/27/103/115	-
17	BCR	L	4020	-	-	4/29/63/63	0/2/2/2
17	BCR	4	524	-	-	4/29/63/63	0/2/2/2
17	BCR	G	4003	-	-	0/29/63/63	0/2/2/2
14	CLA	a	518	13	-	11/27/103/115	-
14	CLA	B	1213	2	-	11/35/111/115	-
14	CLA	s	503	13	-	9/15/91/115	-
17	BCR	q	521	-	-	7/29/63/63	0/2/2/2
14	CLA	5	517	-	-	12/15/91/115	-
17	BCR	v	521	-	-	5/29/63/63	0/2/2/2
19	LMU	G	1848	-	-	7/21/61/61	0/2/2/2
14	CLA	Y	505	13	-	6/15/91/115	-
14	CLA	3	519	13	-	7/15/91/115	-
14	CLA	f	1208	2	-	17/39/115/115	-
14	CLA	e	1022	23	-	9/39/115/115	-
14	CLA	f	1228	2	-	6/27/103/115	-
14	CLA	d	519	13	-	8/15/91/115	-
14	CLA	B	1240	18	-	15/39/115/115	-
17	BCR	M	4021	-	-	6/29/63/63	0/2/2/2
21	SQD	Z	822	-	-	7/22/42/69	0/1/1/1
14	CLA	A	1110	1	-	12/25/101/115	-
14	CLA	A	1102	1	-	7/27/103/115	-
14	CLA	5	504	-	-	5/15/91/115	-
14	CLA	r	505	13	-	14/39/115/115	-
14	CLA	a	510	13	-	8/15/91/115	-
14	CLA	G	1102	1	-	7/27/103/115	-
14	CLA	t	503	13	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	u	523	-	-	4/29/63/63	0/2/2/2
21	SQD	u	822	-	-	3/19/39/69	0/1/1/1
14	CLA	A	1109	1	-	16/39/115/115	-
15	PQN	A	2001	-	-	14/23/43/43	0/2/2/2
14	CLA	1	504	-	-	7/15/91/115	-
17	BCR	4	523	-	-	5/29/63/63	0/2/2/2
21	SQD	t	822	-	-	10/19/39/69	0/1/1/1
15	PQN	f	2002	-	-	6/23/43/43	0/2/2/2
14	CLA	b	505	13	-	5/15/91/115	-
14	CLA	c	501	13	-	8/15/91/115	-
14	CLA	H	1235	2	-	9/39/115/115	-
14	CLA	c	507	-	-	9/15/91/115	-
14	CLA	1	507	-	-	8/15/91/115	-
14	CLA	2	508	13	-	4/15/91/115	-
14	CLA	j	1302	6	-	9/15/91/115	-
14	CLA	q	511	13	-	4/15/91/115	-
14	CLA	m	1103	9	-	10/19/95/115	-
14	CLA	s	511	13	-	2/15/91/115	-
17	BCR	t	524	-	-	4/29/63/63	0/2/2/2
14	CLA	1	517	-	-	9/15/91/115	-
14	CLA	H	1240	18	-	15/39/115/115	-
14	CLA	Z	512	13	-	5/15/91/115	-
17	BCR	c	521	-	-	7/29/63/63	0/2/2/2
14	CLA	c	512	13	-	7/15/91/115	-
17	BCR	e	4007	-	-	0/29/63/63	0/2/2/2
14	CLA	H	1236	2	-	5/21/97/115	-
14	CLA	c	519	13	-	8/15/91/115	-
14	CLA	e	1128	1	-	10/39/115/115	-
14	CLA	R	1301	23	-	3/15/91/115	-
17	BCR	r	521	-	-	4/29/63/63	0/2/2/2
14	CLA	e	1108	1	-	16/26/102/115	-
14	CLA	a	501	13	-	6/15/91/115	-
14	CLA	q	504	-	-	7/15/91/115	-
14	CLA	u	509	13	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	1	523	-	-	6/29/63/63	0/2/2/2
14	CLA	6	509	13	-	4/15/91/115	-
14	CLA	2	503	13	-	10/39/115/115	-
17	BCR	s	523	-	-	4/29/63/63	0/2/2/2
14	CLA	v	505	13	-	15/39/115/115	-
18	LHG	G	5005	-	-	28/47/47/53	-
14	CLA	c	513	13	-	7/15/91/115	-
14	CLA	q	518	13	-	8/15/91/115	-
14	CLA	B	1214	2	-	14/39/115/115	-
14	CLA	G	1110	1	-	12/25/101/115	-
17	BCR	u	521	-	-	7/29/63/63	0/2/2/2
14	CLA	v	507	-	-	7/15/91/115	-
14	CLA	d	510	13	-	10/15/91/115	-
18	LHG	G	5006	-	-	26/44/44/53	-
17	BCR	H	4005	-	-	6/29/63/63	0/2/2/2
14	CLA	d	503	13	-	8/15/91/115	-
15	PQN	G	2001	-	-	14/23/43/43	0/2/2/2
14	CLA	G	1127	1	-	12/39/115/115	-
14	CLA	B	1210	2	-	22/39/115/115	-
14	CLA	r	506	13	-	7/15/91/115	-
14	CLA	c	511	13	-	3/15/91/115	-
14	CLA	1	511	13	-	4/15/91/115	-
21	SQD	s	822	-	-	9/23/43/69	0/1/1/1
14	CLA	B	1215	2	-	19/39/115/115	-
14	CLA	5	508	13	-	6/15/91/115	-
14	CLA	2	516	13	-	8/15/91/115	-
14	CLA	f	1021	2	-	11/39/115/115	-
14	CLA	q	506	13	-	5/15/91/115	-
17	BCR	A	4001	-	-	8/29/63/63	0/2/2/2
14	CLA	A	1113	1	-	6/15/91/115	-
14	CLA	f	1204	2	-	13/39/115/115	-
14	CLA	s	513	13	-	5/15/91/115	-
17	BCR	U	4104	-	-	2/29/63/63	0/2/2/2
14	CLA	3	507	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	f	1224	2	-	7/33/109/115	-
14	CLA	6	513	13	-	5/15/91/115	-
14	CLA	H	1216	23	-	13/33/109/115	-
14	CLA	B	1236	2	-	5/21/97/115	-
17	BCR	5	523	-	-	4/29/63/63	0/2/2/2
15	PQN	H	2002	-	-	6/23/43/43	0/2/2/2
14	CLA	G	1123	23	-	11/39/115/115	-
14	CLA	s	517	-	-	9/15/91/115	-
14	CLA	4	503	13	-	4/15/91/115	-
17	BCR	4	521	-	-	10/29/63/63	0/2/2/2
14	CLA	G	1114	23	-	3/15/91/115	-
17	BCR	H	4004	-	-	8/29/63/63	0/2/2/2
14	CLA	5	509	13	-	13/39/115/115	-
14	CLA	A	1125	1	-	12/39/115/115	-
14	CLA	Y	510	13	-	6/15/91/115	-
17	BCR	l	4013	-	-	4/29/63/63	0/2/2/2
18	LHG	V	5218	-	-	19/41/41/53	-
14	CLA	3	516	13	-	9/15/91/115	-
18	LHG	V	5220	-	-	28/45/45/53	-
14	CLA	H	1231	23	-	8/39/115/115	-
17	BCR	F	4016	-	-	2/29/63/63	0/2/2/2
17	BCR	G	4001	-	-	8/29/63/63	0/2/2/2
14	CLA	Z	504	-	-	9/15/91/115	-
14	CLA	t	513	13	-	7/15/91/115	-
14	CLA	3	502	13	-	3/15/91/115	-
17	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
14	CLA	3	513	13	-	5/15/91/115	-
14	CLA	c	508	13	-	6/15/91/115	-
14	CLA	e	1134	1	-	11/29/105/115	-
14	CLA	Z	518	13	-	16/27/103/115	-
20	LMG	f	5002	-	-	24/48/68/70	0/1/1/1
14	CLA	A	1126	1	-	18/39/115/115	-
17	BCR	V	4022	-	-	3/29/63/63	0/2/2/2
14	CLA	4	501	13	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	u	518	13	-	5/15/91/115	-
14	CLA	A	1123	23	-	11/39/115/115	-
18	LHG	n	5218	-	-	19/41/41/53	-
14	CLA	t	504	-	-	6/15/91/115	-
14	CLA	u	507	-	-	9/15/91/115	-
14	CLA	H	1227	2	-	13/33/109/115	-
14	CLA	f	1219	2	-	20/37/113/115	-
14	CLA	B	1239	2	-	16/39/115/115	-
21	SQD	c	822	-	-	3/19/39/69	0/1/1/1
17	BCR	c	523	-	-	4/29/63/63	0/2/2/2
14	CLA	e	1115	1	-	12/33/109/115	-
14	CLA	G	1117	1	-	13/39/115/115	-
14	CLA	e	1136	1	-	10/39/115/115	-
14	CLA	4	511	13	-	5/15/91/115	-
14	CLA	e	1801	18	-	7/15/91/115	-
17	BCR	Z	521	-	-	4/29/63/63	0/2/2/2
18	LHG	S	5001	-	-	25/52/52/53	-
17	BCR	B	4009	-	-	1/29/63/63	0/2/2/2
17	BCR	l	524	-	-	2/29/63/63	0/2/2/2
14	CLA	B	1227	2	-	13/33/109/115	-
14	CLA	B	1225	2	-	7/39/115/115	-
14	CLA	G	1129	1	-	10/25/101/115	-
14	CLA	d	502	13	-	3/15/91/115	-
18	LHG	e	5004	-	-	18/39/39/53	-
14	CLA	n	1501	10	-	11/33/109/115	-
14	CLA	A	1130	1	-	7/29/105/115	-
14	CLA	U	1401	-	-	10/27/103/115	-
14	CLA	b	513	13	-	7/15/91/115	-
14	CLA	l	1303	8	-	6/15/91/115	-
14	CLA	n	1502	10	-	10/39/115/115	-
14	CLA	Z	503	13	-	10/39/115/115	-
14	CLA	G	1125	1	-	12/39/115/115	-
14	CLA	e	1126	1	-	18/39/115/115	-
14	CLA	l	1302	8	-	14/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1117	1	-	13/39/115/115	-
14	CLA	B	1220	2	-	11/27/103/115	-
14	CLA	A	1139	23	-	20/39/115/115	-
14	CLA	e	1123	23	-	11/39/115/115	-
14	CLA	s	501	13	-	6/15/91/115	-
14	CLA	3	518	13	-	11/27/103/115	-
14	CLA	B	1216	23	-	13/33/109/115	-
17	BCR	V	4219	-	-	2/29/63/63	0/2/2/2
17	BCR	d	524	-	-	5/29/63/63	0/2/2/2
14	CLA	v	513	13	-	5/15/91/115	-
14	CLA	b	501	13	-	8/15/91/115	-
14	CLA	Y	507	-	-	8/15/91/115	-
14	CLA	Z	511	13	-	5/15/91/115	-
18	LHG	f	1855	-	-	24/45/45/53	-
14	CLA	6	505	13	-	15/39/115/115	-
14	CLA	6	517	-	-	12/15/91/115	-
14	CLA	n	1503	23	-	10/33/109/115	-
17	BCR	5	521	-	-	7/29/63/63	0/2/2/2
14	CLA	A	1111	1	-	20/39/115/115	-
14	CLA	B	1218	2	-	9/33/109/115	-
14	CLA	e	1139	23	-	20/39/115/115	-
14	CLA	A	1122	1	-	14/33/109/115	-
14	CLA	G	1237	23	-	25/39/115/115	-
18	LHG	G	5008	-	-	18/39/39/53	-
14	CLA	B	1206	2	-	15/39/115/115	-
14	CLA	Y	509	13	-	5/15/91/115	-
17	BCR	2	521	-	-	4/29/63/63	0/2/2/2
18	LHG	G	5003	14	-	17/44/44/53	-
14	CLA	2	518	13	-	16/27/103/115	-
14	CLA	H	1220	2	-	11/27/103/115	-
18	LHG	H	1842	14	-	19/41/41/53	-
17	BCR	R	4016	-	-	2/29/63/63	0/2/2/2
14	CLA	A	1011	1	-	12/39/115/115	-
16	SF4	N	3002	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	t	508	13	-	6/15/91/115	-
14	CLA	5	501	13	-	8/15/91/115	-
14	CLA	5	503	13	-	9/15/91/115	-
17	BCR	c	522	-	-	5/29/63/63	0/2/2/2
14	CLA	5	506	13	-	8/15/91/115	-
14	CLA	a	504	-	-	7/15/91/115	-
14	CLA	G	1103	1	-	21/39/115/115	-
14	CLA	v	518	13	-	9/15/91/115	-
17	BCR	t	523	-	-	5/29/63/63	0/2/2/2
18	LHG	A	5003	14	-	17/44/44/53	-
14	CLA	L	1502	10	-	10/39/115/115	-
17	BCR	V	4020	-	-	4/29/63/63	0/2/2/2
14	CLA	G	1121	1	-	10/27/103/115	-
19	LMU	J	5105	-	-	9/13/33/61	0/1/1/2
14	CLA	2	505	13	-	14/39/115/115	-
18	LHG	H	1855	-	-	24/45/45/53	-
14	CLA	f	1213	2	-	11/35/111/115	-
14	CLA	G	1011	1	-	12/39/115/115	-
14	CLA	f	1230	2	-	12/33/109/115	-
17	BCR	s	522	-	-	5/29/63/63	0/2/2/2
14	CLA	c	505	13	-	5/15/91/115	-
17	BCR	v	522	-	-	5/29/63/63	0/2/2/2
17	BCR	H	4006	-	-	4/29/63/63	0/2/2/2
14	CLA	A	1103	1	-	21/39/115/115	-
17	BCR	6	522	-	-	5/29/63/63	0/2/2/2
14	CLA	5	518	13	-	5/15/91/115	-
14	CLA	4	509	13	-	6/15/91/115	-
14	CLA	1	502	13	-	4/15/91/115	-
14	CLA	H	1021	2	-	11/39/115/115	-
14	CLA	a	506	13	-	8/15/91/115	-
14	CLA	f	1235	2	-	9/39/115/115	-
14	CLA	B	1232	23	-	6/27/103/115	-
14	CLA	A	1121	1	-	10/27/103/115	-
21	SQD	B	1852	-	-	18/35/55/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	L	1503	23	-	10/33/109/115	-
14	CLA	t	517	-	-	7/15/91/115	-
14	CLA	a	505	13	-	11/27/103/115	-
14	CLA	b	508	13	-	6/15/91/115	-
21	SQD	H	1852	-	-	18/35/55/69	0/1/1/1
16	SF4	G	3001	2,1	-	-	0/6/5/5
14	CLA	B	1217	2	-	14/33/109/115	-
14	CLA	r	512	13	-	5/15/91/115	-
20	LMG	H	5002	-	-	24/48/68/70	0/1/1/1
15	PQN	e	2001	-	-	14/23/43/43	0/2/2/2
14	CLA	4	502	13	-	5/15/91/115	-
14	CLA	H	1239	2	-	16/39/115/115	-
18	LHG	k	5001	-	-	25/52/52/53	-
14	CLA	G	1124	23	-	13/33/109/115	-
14	CLA	6	510	13	-	10/15/91/115	-
14	CLA	A	1104	1	-	10/39/115/115	-
17	BCR	l	4012	-	-	9/29/63/63	0/2/2/2
14	CLA	e	1106	1	-	23/39/115/115	-
14	CLA	t	509	13	-	6/15/91/115	-
14	CLA	v	517	-	-	12/15/91/115	-
14	CLA	4	506	13	-	6/15/91/115	-
14	CLA	b	507	-	-	8/15/91/115	-
19	LMU	f	1843	-	-	12/21/61/61	0/2/2/2
14	CLA	2	506	13	-	7/15/91/115	-
14	CLA	G	1132	1	-	18/39/115/115	-
14	CLA	c	516	13	-	7/15/91/115	-
17	BCR	r	523	-	-	6/29/63/63	0/2/2/2
17	BCR	t	521	-	-	10/29/63/63	0/2/2/2
21	SQD	r	822	-	-	7/22/42/69	0/1/1/1
14	CLA	c	506	13	-	8/15/91/115	-
14	CLA	A	1129	1	-	10/25/101/115	-
14	CLA	1	506	13	-	5/15/91/115	-
14	CLA	3	512	13	-	3/15/91/115	-
17	BCR	q	523	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1224	2	-	7/33/109/115	-
17	BCR	c	524	-	-	2/29/63/63	0/2/2/2
14	CLA	f	1023	-	-	10/39/115/115	-
18	LHG	A	5001	-	-	23/53/53/53	-
14	CLA	d	512	13	-	9/15/91/115	-
17	BCR	d	522	-	-	5/29/63/63	0/2/2/2
17	BCR	k	4018	-	-	0/29/63/63	0/2/2/2
14	CLA	b	516	13	-	9/15/91/115	-
14	CLA	u	510	13	-	9/15/91/115	-
17	BCR	I	4018	-	-	0/29/63/63	0/2/2/2
14	CLA	u	516	13	-	7/15/91/115	-
14	CLA	6	501	13	-	9/15/91/115	-
14	CLA	Y	518	13	-	8/15/91/115	-
14	CLA	a	516	13	-	9/15/91/115	-
14	CLA	e	1138	1	-	14/39/115/115	-
21	SQD	2	822	-	-	7/22/42/69	0/1/1/1
14	CLA	G	1112	1	-	4/21/97/115	-
14	CLA	6	508	13	-	6/15/91/115	-
14	CLA	Z	505	13	-	14/39/115/115	-
14	CLA	G	1013	-	-	14/39/115/115	-
14	CLA	f	1221	23	-	14/36/112/115	-
14	CLA	r	517	-	-	9/15/91/115	-
14	CLA	c	510	13	-	9/15/91/115	-
14	CLA	u	511	13	-	3/15/91/115	-
14	CLA	5	512	13	-	7/15/91/115	-
17	BCR	5	522	-	-	5/29/63/63	0/2/2/2
17	BCR	j	4016	-	-	2/29/63/63	0/2/2/2
14	CLA	Y	506	13	-	5/15/91/115	-
14	CLA	q	517	-	-	9/15/91/115	-
17	BCR	Y	524	-	-	2/29/63/63	0/2/2/2
14	CLA	H	1218	2	-	9/33/109/115	-
14	CLA	A	1140	1	-	14/39/115/115	-
14	CLA	B	1023	-	-	10/39/115/115	-
22	FMN	X	170	-	-	0/18/18/18	0/3/3/3
14	CLA	2	519	13	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1210	2	-	22/39/115/115	-
14	CLA	q	512	13	-	7/15/91/115	-
14	CLA	Y	513	13	-	6/15/91/115	-
14	CLA	A	1112	1	-	4/21/97/115	-
18	LHG	G	5001	-	-	23/53/53/53	-
14	CLA	6	507	-	-	7/15/91/115	-
14	CLA	d	504	-	-	6/15/91/115	-
14	CLA	t	518	13	-	6/15/91/115	-
14	CLA	r	513	13	-	4/15/91/115	-
14	CLA	s	510	13	-	8/15/91/115	-
17	BCR	L	4022	-	-	3/29/63/63	0/2/2/2
21	SQD	4	822	-	-	10/19/39/69	0/1/1/1
14	CLA	Y	504	-	-	7/15/91/115	-
14	CLA	A	1107	1	-	16/39/115/115	-
17	BCR	l	4015	-	-	5/29/63/63	0/2/2/2
14	CLA	3	517	-	-	9/15/91/115	-
14	CLA	q	509	13	-	5/15/91/115	-
18	LHG	e	5007	-	-	23/51/51/53	-
14	CLA	3	504	-	-	7/15/91/115	-
14	CLA	H	1023	-	-	10/39/115/115	-
14	CLA	r	511	13	-	4/15/91/115	-
17	BCR	3	521	-	-	7/29/63/63	0/2/2/2
14	CLA	4	508	13	-	6/15/91/115	-
18	LHG	A	5009	-	-	28/46/46/53	-
14	CLA	2	511	13	-	4/15/91/115	-
14	CLA	6	502	13	-	3/15/91/115	-
21	SQD	d	822	-	-	7/19/39/69	0/1/1/1
14	CLA	1	505	13	-	6/15/91/115	-
17	BCR	m	4104	-	-	2/29/63/63	0/2/2/2
14	CLA	c	517	-	-	12/15/91/115	-
14	CLA	1	518	13	-	8/15/91/115	-
17	BCR	3	523	-	-	4/29/63/63	0/2/2/2
19	LMU	B	1843	-	-	12/21/61/61	0/2/2/2
14	CLA	Z	506	13	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	e	4001	-	-	8/29/63/63	0/2/2/2
14	CLA	G	1122	1	-	14/33/109/115	-
14	CLA	u	501	13	-	8/15/91/115	-
18	LHG	e	5005	-	-	28/47/47/53	-
14	CLA	G	1126	1	-	18/39/115/115	-
14	CLA	G	1107	1	-	16/39/115/115	-
14	CLA	G	1109	1	-	16/39/115/115	-
14	CLA	B	1203	2	-	16/39/115/115	-
14	CLA	Z	517	-	-	9/15/91/115	-
14	CLA	t	506	13	-	6/15/91/115	-
14	CLA	r	518	13	-	16/27/103/115	-
14	CLA	2	512	13	-	5/15/91/115	-
14	CLA	u	517	-	-	12/15/91/115	-
14	CLA	3	511	13	-	2/15/91/115	-
17	BCR	e	4002	-	-	0/29/63/63	0/2/2/2
14	CLA	U	1103	9	-	10/19/95/115	-
14	CLA	d	509	13	-	4/15/91/115	-
14	CLA	H	1202	2	-	12/39/115/115	-
17	BCR	f	4004	-	-	8/29/63/63	0/2/2/2

The worst 5 of 6040 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	2001	PQN	C12-C13	8.46	1.53	1.33
15	A	2001	PQN	C12-C13	8.44	1.53	1.33
15	e	2001	PQN	C12-C13	8.44	1.53	1.33
15	B	2002	PQN	C12-C13	8.38	1.53	1.33
15	H	2002	PQN	C12-C13	8.38	1.53	1.33

The worst 5 of 7290 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1023	CLA	C4A-NA-C1A	9.67	111.06	106.71
14	B	1023	CLA	C4A-NA-C1A	9.59	111.02	106.71
14	f	1023	CLA	C4A-NA-C1A	9.53	110.99	106.71
15	G	2001	PQN	C11-C12-C13	-9.51	110.96	126.79
15	A	2001	PQN	C11-C12-C13	-9.50	110.98	126.79

There are no chirality outliers.

5 of 7891 torsion outliers are listed below:

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

There are no ring outliers.

661 monomers are involved in 1532 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	W	4021	BCR	3	0
14	B	1212	CLA	1	0
14	V	1501	CLA	8	0
17	J	4012	BCR	3	0
17	r	522	BCR	1	0
14	f	1012	CLA	4	0
17	d	521	BCR	2	0
14	Z	509	CLA	2	0
18	G	5009	LHG	3	0
17	n	4022	BCR	9	0
17	V	4019	BCR	3	0
14	G	1131	CLA	2	0
18	B	1855	LHG	3	0
20	T	5104	LMG	1	0
14	e	1114	CLA	1	0
18	e	5008	LHG	7	0
14	B	1228	CLA	4	0
14	A	1127	CLA	1	0
17	H	4009	BCR	2	0
19	G	1849	LMU	1	0
14	A	1137	CLA	5	0
14	5	511	CLA	1	0
14	4	512	CLA	2	0
17	b	524	BCR	3	0
17	a	524	BCR	1	0
14	U	1105	CLA	2	0
14	5	507	CLA	1	0
14	m	1105	CLA	2	0
14	H	1226	CLA	5	0
14	A	1115	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	f	1216	CLA	4	0
14	H	1238	CLA	1	0
14	f	1236	CLA	3	0
14	f	1205	CLA	2	0
14	G	1137	CLA	5	0
17	G	4008	BCR	3	0
17	f	4017	BCR	5	0
14	A	1013	CLA	8	0
14	c	502	CLA	2	0
14	H	1206	CLA	5	0
14	B	1208	CLA	5	0
14	A	1101	CLA	5	0
14	J	1302	CLA	1	0
14	A	1124	CLA	3	0
14	f	1207	CLA	8	0
14	d	518	CLA	1	0
14	f	1206	CLA	5	0
14	e	1125	CLA	5	0
14	b	502	CLA	3	0
14	G	1134	CLA	1	0
18	n	5220	LHG	4	0
14	A	1138	CLA	1	0
14	e	1011	CLA	2	0
17	A	4008	BCR	5	0
14	t	512	CLA	3	0
17	t	522	BCR	1	0
14	e	1237	CLA	6	0
14	H	1208	CLA	4	0
14	F	1302	CLA	3	0
14	A	1801	CLA	3	0
14	B	1235	CLA	4	0
14	H	1225	CLA	4	0
14	v	509	CLA	1	0
17	A	4003	BCR	1	0
17	n	4219	BCR	10	0
18	e	5003	LHG	2	0
14	A	1134	CLA	2	0
14	4	504	CLA	1	0
14	q	513	CLA	2	0
14	Z	513	CLA	2	0
14	u	502	CLA	2	0
14	4	507	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	4017	BCR	3	0
17	a	522	BCR	1	0
14	R	1302	CLA	3	0
14	B	1221	CLA	9	0
14	a	513	CLA	2	0
14	1	510	CLA	1	0
14	G	1104	CLA	6	0
14	G	1138	CLA	1	0
14	r	510	CLA	1	0
17	3	522	BCR	1	0
14	e	1121	CLA	3	0
14	F	1301	CLA	1	0
14	t	511	CLA	2	0
14	H	1229	CLA	5	0
14	2	513	CLA	2	0
14	f	1229	CLA	6	0
20	B	5002	LMG	5	0
17	A	4011	BCR	3	0
18	A	5006	LHG	3	0
14	t	507	CLA	1	0
14	Y	516	CLA	6	0
14	B	1205	CLA	2	0
17	6	524	BCR	4	0
14	v	512	CLA	3	0
14	G	1118	CLA	2	0
15	B	2002	PQN	4	0
14	H	1215	CLA	4	0
17	J	4013	BCR	6	0
17	B	4006	BCR	4	0
14	H	1204	CLA	2	0
14	H	1228	CLA	3	0
14	f	1215	CLA	3	0
14	u	513	CLA	2	0
17	q	522	BCR	2	0
14	v	510	CLA	1	0
17	Y	521	BCR	6	0
14	e	1013	CLA	7	0
17	Z	523	BCR	2	0
14	A	1118	CLA	2	0
18	L	5218	LHG	2	0
14	A	1133	CLA	2	0
14	q	505	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	L	4019	BCR	3	0
14	5	502	CLA	2	0
14	G	1140	CLA	3	0
17	v	524	BCR	3	0
14	d	511	CLA	2	0
14	f	1231	CLA	3	0
14	a	517	CLA	1	0
18	G	5004	LHG	2	0
18	e	5009	LHG	4	0
17	B	4010	BCR	6	0
14	e	1131	CLA	2	0
14	A	1114	CLA	1	0
17	2	522	BCR	2	0
14	6	512	CLA	4	0
17	f	4014	BCR	3	0
14	B	1204	CLA	3	0
14	B	1224	CLA	3	0
14	f	1214	CLA	2	0
17	b	523	BCR	1	0
14	e	1140	CLA	3	0
17	f	4005	BCR	4	0
14	G	1106	CLA	4	0
14	B	1234	CLA	5	0
18	A	5005	LHG	7	0
17	J	4015	BCR	5	0
17	T	4012	BCR	3	0
21	1	822	SQD	1	0
18	G	5007	LHG	2	0
14	d	506	CLA	2	0
14	B	1238	CLA	1	0
18	e	5001	LHG	4	0
14	A	1106	CLA	4	0
14	e	1101	CLA	5	0
14	G	1119	CLA	7	0
14	G	1105	CLA	2	0
14	H	1219	CLA	2	0
18	A	5007	LHG	2	0
19	A	1848	LMU	2	0
14	H	1203	CLA	2	0
14	3	503	CLA	1	0
14	H	1221	CLA	9	0
17	4	522	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	r	509	CLA	2	0
18	A	5008	LHG	7	0
14	6	519	CLA	1	0
14	B	1012	CLA	5	0
14	f	1218	CLA	2	0
19	e	1848	LMU	2	0
21	Y	822	SQD	1	0
18	f	1842	LHG	2	0
17	a	521	BCR	1	0
21	L	5216	SQD	6	0
14	A	1119	CLA	5	0
14	H	1214	CLA	2	0
14	l	513	CLA	2	0
17	d	523	BCR	4	0
14	G	1116	CLA	6	0
14	f	1212	CLA	1	0
14	j	1301	CLA	1	0
14	r	501	CLA	2	0
14	t	502	CLA	3	0
14	e	1109	CLA	2	0
17	Z	524	BCR	6	0
14	e	1124	CLA	2	0
14	f	1210	CLA	7	0
14	b	503	CLA	1	0
17	Z	522	BCR	2	0
14	6	506	CLA	2	0
17	u	524	BCR	2	0
14	G	1133	CLA	2	0
14	e	1104	CLA	5	0
14	e	1120	CLA	2	0
14	a	503	CLA	1	0
17	n	4020	BCR	2	0
14	A	1116	CLA	4	0
14	e	1137	CLA	6	0
14	e	1117	CLA	4	0
17	A	4007	BCR	2	0
17	e	4008	BCR	5	0
14	G	1120	CLA	2	0
22	P	170	FMN	1	0
14	Y	512	CLA	4	0
14	2	510	CLA	1	0
21	f	1852	SQD	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	d	517	CLA	2	0
14	G	1022	CLA	2	0
14	L	1501	CLA	7	0
14	Y	502	CLA	2	0
14	H	1217	CLA	1	0
17	3	524	BCR	1	0
14	B	1209	CLA	2	0
14	e	1110	CLA	2	0
14	f	1220	CLA	2	0
14	f	1226	CLA	5	0
14	K	1105	CLA	2	0
17	b	521	BCR	1	0
14	f	1217	CLA	2	0
19	e	1849	LMU	1	0
14	H	1209	CLA	2	0
14	A	1120	CLA	2	0
17	G	4002	BCR	2	0
17	G	4011	BCR	4	0
14	e	1130	CLA	4	0
14	A	1022	CLA	2	0
14	H	1222	CLA	2	0
14	e	1129	CLA	5	0
17	B	4014	BCR	5	0
14	f	1222	CLA	1	0
14	v	519	CLA	2	0
14	q	510	CLA	1	0
17	G	4007	BCR	3	0
17	a	523	BCR	1	0
14	5	505	CLA	1	0
14	Z	501	CLA	3	0
14	a	502	CLA	3	0
17	A	4002	BCR	5	0
19	A	1849	LMU	1	0
14	q	502	CLA	2	0
14	2	517	CLA	1	0
17	n	4019	BCR	4	0
14	H	1201	CLA	2	0
17	e	4011	BCR	3	0
17	S	4018	BCR	3	0
14	u	505	CLA	1	0
14	B	1202	CLA	2	0
14	1	509	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	v	506	CLA	2	0
17	T	4015	BCR	4	0
14	4	510	CLA	2	0
14	A	1108	CLA	1	0
14	4	516	CLA	2	0
14	6	518	CLA	1	0
18	I	5001	LHG	2	0
14	q	507	CLA	1	0
14	f	1239	CLA	4	0
17	s	521	BCR	1	0
14	v	502	CLA	2	0
14	2	509	CLA	2	0
21	3	822	SQD	2	0
14	f	1227	CLA	2	0
14	Z	519	CLA	1	0
17	u	522	BCR	1	0
14	Z	510	CLA	1	0
14	r	502	CLA	3	0
14	G	1128	CLA	7	0
14	Y	511	CLA	1	0
19	H	1843	LMU	1	0
14	f	1203	CLA	2	0
14	1	516	CLA	6	0
14	G	1130	CLA	4	0
14	a	512	CLA	5	0
14	b	510	CLA	2	0
14	e	1122	CLA	3	0
17	K	4104	BCR	3	0
18	L	5220	LHG	4	0
18	V	5221	LHG	8	0
17	B	4017	BCR	4	0
14	B	1201	CLA	2	0
14	f	1223	CLA	4	0
14	u	506	CLA	2	0
14	A	1128	CLA	7	0
14	G	1801	CLA	3	0
18	n	5221	LHG	6	0
17	Y	523	BCR	1	0
14	t	510	CLA	1	0
17	1	521	BCR	6	0
14	V	1502	CLA	3	0
14	B	1231	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	1212	CLA	1	0
14	e	1118	CLA	2	0
14	t	501	CLA	1	0
14	A	1136	CLA	1	0
14	B	1229	CLA	7	0
14	e	1103	CLA	4	0
14	t	505	CLA	1	0
18	B	1842	LHG	2	0
14	3	505	CLA	1	0
17	2	523	BCR	2	0
14	b	512	CLA	2	0
18	A	5004	LHG	3	0
22	p	170	FMN	1	0
14	H	1205	CLA	2	0
14	r	503	CLA	3	0
14	H	1223	CLA	4	0
17	f	4006	BCR	4	0
14	V	1503	CLA	2	0
14	Z	502	CLA	3	0
14	G	1115	CLA	3	0
17	6	523	BCR	3	0
14	G	1136	CLA	2	0
14	d	513	CLA	2	0
14	A	1131	CLA	2	0
14	b	511	CLA	2	0
14	e	1105	CLA	2	0
14	e	1112	CLA	1	0
17	B	4004	BCR	3	0
14	b	517	CLA	1	0
14	f	1238	CLA	1	0
14	G	1108	CLA	1	0
14	t	516	CLA	2	0
14	f	1201	CLA	4	0
14	T	1302	CLA	1	0
14	a	511	CLA	1	0
14	b	504	CLA	1	0
14	c	509	CLA	1	0
18	L	5221	LHG	6	0
17	H	4010	BCR	7	0
17	T	4013	BCR	6	0
14	f	1202	CLA	3	0
14	B	1222	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	L	4219	BCR	7	0
17	f	4010	BCR	6	0
14	b	509	CLA	2	0
14	A	1105	CLA	2	0
14	u	512	CLA	5	0
14	H	1012	CLA	4	0
17	r	524	BCR	5	0
14	5	513	CLA	2	0
14	s	512	CLA	5	0
14	r	519	CLA	1	0
17	2	524	BCR	6	0
18	e	5002	LHG	1	0
17	q	524	BCR	4	0
14	4	513	CLA	2	0
14	2	502	CLA	3	0
14	f	1234	CLA	4	0
14	s	502	CLA	2	0
14	4	517	CLA	1	0
14	f	1209	CLA	2	0
14	f	1225	CLA	4	0
17	f	4009	BCR	3	0
14	3	510	CLA	2	0
14	6	511	CLA	2	0
14	2	501	CLA	3	0
14	B	1021	CLA	1	0
21	a	822	SQD	2	0
14	B	1207	CLA	10	0
21	V	5216	SQD	6	0
17	o	4021	BCR	1	0
21	q	822	SQD	1	0
17	v	523	BCR	3	0
14	B	1226	CLA	5	0
14	e	1119	CLA	7	0
14	q	516	CLA	6	0
14	G	1101	CLA	5	0
14	B	1223	CLA	4	0
14	B	1219	CLA	2	0
14	G	1135	CLA	3	0
14	d	505	CLA	4	0
14	e	1135	CLA	3	0
21	n	5216	SQD	6	0
14	e	1116	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1	512	CLA	4	0
14	A	1237	CLA	6	0
17	1	522	BCR	2	0
18	e	5006	LHG	3	0
14	v	511	CLA	2	0
14	e	1107	CLA	1	0
14	5	510	CLA	1	0
14	H	1207	CLA	8	0
17	H	4014	BCR	3	0
14	B	1211	CLA	1	0
14	H	1234	CLA	6	0
17	e	4003	BCR	3	0
14	H	1230	CLA	1	0
14	A	1135	CLA	3	0
17	L	4020	BCR	2	0
17	4	524	BCR	3	0
17	G	4003	BCR	3	0
14	s	503	CLA	1	0
17	q	521	BCR	5	0
17	v	521	BCR	2	0
19	G	1848	LMU	2	0
14	Y	505	CLA	4	0
14	f	1208	CLA	4	0
14	e	1022	CLA	2	0
14	f	1228	CLA	4	0
14	d	519	CLA	2	0
14	B	1240	CLA	1	0
17	M	4021	BCR	2	0
14	A	1110	CLA	2	0
14	A	1102	CLA	1	0
14	r	505	CLA	3	0
14	a	510	CLA	2	0
14	t	503	CLA	1	0
17	u	523	BCR	2	0
14	A	1109	CLA	1	0
15	A	2001	PQN	3	0
14	1	504	CLA	1	0
17	4	523	BCR	2	0
15	f	2002	PQN	5	0
14	b	505	CLA	1	0
14	H	1235	CLA	4	0
14	c	507	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	l	507	CLA	1	0
14	j	1302	CLA	3	0
14	q	511	CLA	1	0
14	s	511	CLA	1	0
17	t	524	BCR	3	0
14	Z	512	CLA	6	0
17	c	521	BCR	4	0
14	c	512	CLA	4	0
17	e	4007	BCR	2	0
14	H	1236	CLA	3	0
14	e	1128	CLA	5	0
14	R	1301	CLA	1	0
17	r	521	BCR	8	0
14	e	1108	CLA	1	0
14	q	504	CLA	1	0
14	u	509	CLA	3	0
17	l	523	BCR	2	0
14	6	509	CLA	1	0
14	2	503	CLA	3	0
17	s	523	BCR	2	0
14	v	505	CLA	4	0
18	G	5005	LHG	6	0
14	c	513	CLA	2	0
14	q	518	CLA	1	0
14	B	1214	CLA	2	0
14	G	1110	CLA	1	0
17	u	521	BCR	6	0
14	d	510	CLA	1	0
18	G	5006	LHG	3	0
17	H	4005	BCR	3	0
15	G	2001	PQN	2	0
14	G	1127	CLA	1	0
14	B	1210	CLA	7	0
14	r	506	CLA	2	0
14	c	511	CLA	1	0
14	l	511	CLA	1	0
21	s	822	SQD	2	0
14	B	1215	CLA	3	0
14	f	1021	CLA	2	0
17	A	4001	BCR	4	0
14	f	1204	CLA	2	0
14	s	513	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	U	4104	BCR	3	0
14	f	1224	CLA	4	0
14	6	513	CLA	2	0
14	H	1216	CLA	5	0
14	B	1236	CLA	3	0
17	5	523	BCR	2	0
15	H	2002	PQN	4	0
14	G	1123	CLA	3	0
14	4	503	CLA	1	0
17	4	521	BCR	2	0
14	G	1114	CLA	1	0
17	H	4004	BCR	5	0
14	5	509	CLA	2	0
14	A	1125	CLA	3	0
14	Y	510	CLA	1	0
17	l	4013	BCR	5	0
18	V	5218	LHG	2	0
18	V	5220	LHG	4	0
14	H	1231	CLA	3	0
17	F	4016	BCR	6	0
17	G	4001	BCR	3	0
14	t	513	CLA	2	0
14	3	502	CLA	3	0
17	B	4005	BCR	4	0
14	3	513	CLA	2	0
14	e	1134	CLA	2	0
14	Z	518	CLA	2	0
20	f	5002	LMG	6	0
14	A	1126	CLA	9	0
17	V	4022	BCR	8	0
14	4	501	CLA	1	0
14	A	1123	CLA	1	0
18	n	5218	LHG	2	0
14	t	504	CLA	1	0
14	u	507	CLA	1	0
14	H	1227	CLA	2	0
14	f	1219	CLA	1	0
14	B	1239	CLA	4	0
17	c	523	BCR	2	0
14	e	1115	CLA	2	0
14	G	1117	CLA	4	0
14	e	1136	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	4	511	CLA	2	0
14	e	1801	CLA	3	0
17	Z	521	BCR	7	0
18	S	5001	LHG	2	0
17	B	4009	BCR	3	0
17	1	524	BCR	5	0
14	B	1227	CLA	2	0
14	B	1225	CLA	4	0
14	G	1129	CLA	5	0
14	d	502	CLA	2	0
18	e	5004	LHG	2	0
14	n	1501	CLA	7	0
14	A	1130	CLA	3	0
14	b	513	CLA	2	0
14	n	1502	CLA	3	0
14	Z	503	CLA	3	0
14	G	1125	CLA	3	0
14	e	1126	CLA	8	0
14	l	1302	CLA	1	0
14	A	1117	CLA	5	0
14	B	1220	CLA	3	0
14	A	1139	CLA	2	0
14	e	1123	CLA	2	0
14	B	1216	CLA	4	0
17	V	4219	BCR	8	0
17	d	524	BCR	4	0
14	v	513	CLA	2	0
14	b	501	CLA	1	0
14	Y	507	CLA	1	0
14	Z	511	CLA	1	0
18	f	1855	LHG	3	0
14	6	505	CLA	4	0
14	6	517	CLA	2	0
14	n	1503	CLA	3	0
17	5	521	BCR	3	0
14	B	1218	CLA	2	0
14	e	1139	CLA	2	0
14	A	1122	CLA	2	0
14	G	1237	CLA	6	0
18	G	5008	LHG	8	0
14	B	1206	CLA	4	0
14	Y	509	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	2	521	BCR	7	0
18	G	5003	LHG	2	0
14	2	518	CLA	2	0
14	H	1220	CLA	3	0
18	H	1842	LHG	2	0
17	R	4016	BCR	6	0
14	A	1011	CLA	2	0
14	t	508	CLA	1	0
17	c	522	BCR	1	0
14	5	506	CLA	3	0
14	G	1103	CLA	4	0
14	v	518	CLA	1	0
17	t	523	BCR	1	0
18	A	5003	LHG	2	0
14	L	1502	CLA	3	0
17	V	4020	BCR	2	0
14	G	1121	CLA	3	0
14	2	505	CLA	4	0
18	H	1855	LHG	3	0
14	G	1011	CLA	3	0
17	s	522	BCR	2	0
14	c	505	CLA	1	0
17	v	522	BCR	2	0
17	H	4006	BCR	4	0
14	A	1103	CLA	3	0
17	6	522	BCR	4	0
14	4	509	CLA	3	0
14	1	502	CLA	2	0
14	H	1021	CLA	2	0
14	f	1235	CLA	4	0
14	A	1121	CLA	3	0
21	B	1852	SQD	8	0
14	L	1503	CLA	1	0
14	t	517	CLA	2	0
14	b	508	CLA	1	0
21	H	1852	SQD	9	0
14	B	1217	CLA	2	0
14	r	512	CLA	5	0
20	H	5002	LMG	6	0
15	e	2001	PQN	2	0
14	4	502	CLA	3	0
14	H	1239	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	k	5001	LHG	2	0
14	G	1124	CLA	3	0
14	6	510	CLA	1	0
14	A	1104	CLA	6	0
17	l	4012	BCR	3	0
14	e	1106	CLA	5	0
14	t	509	CLA	1	0
14	v	517	CLA	2	0
14	b	507	CLA	1	0
19	f	1843	LMU	1	0
14	2	506	CLA	2	0
17	r	523	BCR	1	0
17	t	521	BCR	2	0
14	c	506	CLA	3	0
14	A	1129	CLA	5	0
14	3	512	CLA	5	0
17	q	523	BCR	1	0
14	H	1224	CLA	3	0
14	f	1023	CLA	2	0
18	A	5001	LHG	5	0
14	d	512	CLA	3	0
17	d	522	BCR	2	0
17	k	4018	BCR	5	0
14	b	516	CLA	2	0
14	u	510	CLA	1	0
17	I	4018	BCR	4	0
14	Y	518	CLA	1	0
14	e	1138	CLA	3	0
14	G	1112	CLA	1	0
14	Z	505	CLA	4	0
14	G	1013	CLA	7	0
14	f	1221	CLA	7	0
14	r	517	CLA	1	0
14	c	510	CLA	1	0
14	u	511	CLA	1	0
14	5	512	CLA	4	0
17	5	522	BCR	2	0
17	j	4016	BCR	6	0
17	Y	524	BCR	5	0
14	H	1218	CLA	2	0
14	A	1140	CLA	3	0
14	B	1023	CLA	2	0

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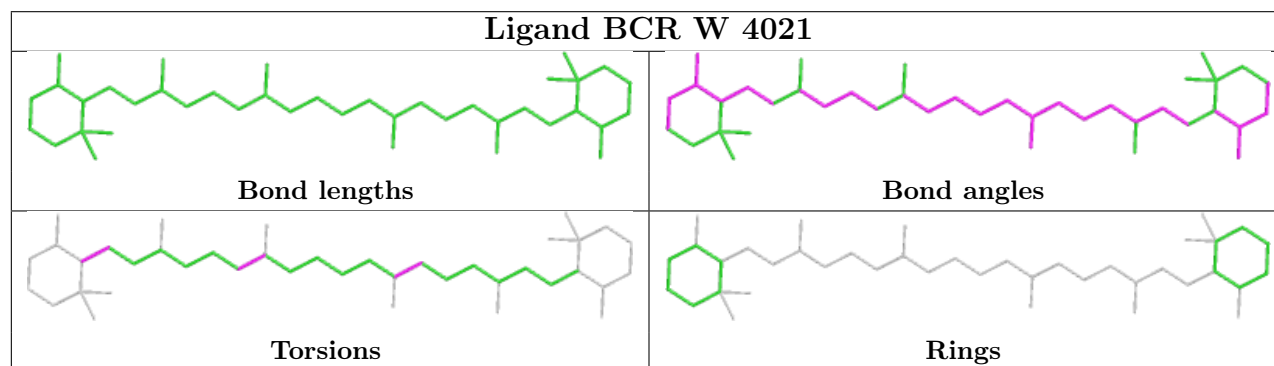
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	X	170	FMN	2	0
14	2	519	CLA	1	0
14	H	1210	CLA	7	0
14	q	512	CLA	4	0
14	Y	513	CLA	2	0
14	A	1112	CLA	1	0
18	G	5001	LHG	5	0
14	r	513	CLA	2	0
14	s	510	CLA	2	0
17	L	4022	BCR	8	0
14	Y	504	CLA	1	0
14	A	1107	CLA	1	0
17	l	4015	BCR	6	0
14	3	517	CLA	1	0
14	q	509	CLA	1	0
18	e	5007	LHG	2	0
14	H	1023	CLA	5	0
14	r	511	CLA	1	0
17	3	521	BCR	1	0
14	4	508	CLA	1	0
18	A	5009	LHG	3	0
14	6	502	CLA	2	0
14	1	505	CLA	2	0
17	m	4104	BCR	3	0
14	1	518	CLA	1	0
17	3	523	BCR	2	0
19	B	1843	LMU	1	0
14	Z	506	CLA	2	0
17	e	4001	BCR	3	0
14	G	1122	CLA	3	0
18	e	5005	LHG	6	0
14	G	1126	CLA	10	0
14	G	1107	CLA	1	0
14	G	1109	CLA	1	0
14	B	1203	CLA	2	0
14	Z	517	CLA	1	0
14	r	518	CLA	2	0
14	2	512	CLA	5	0
14	3	511	CLA	1	0
17	e	4002	BCR	1	0
14	d	509	CLA	1	0
14	H	1202	CLA	3	0

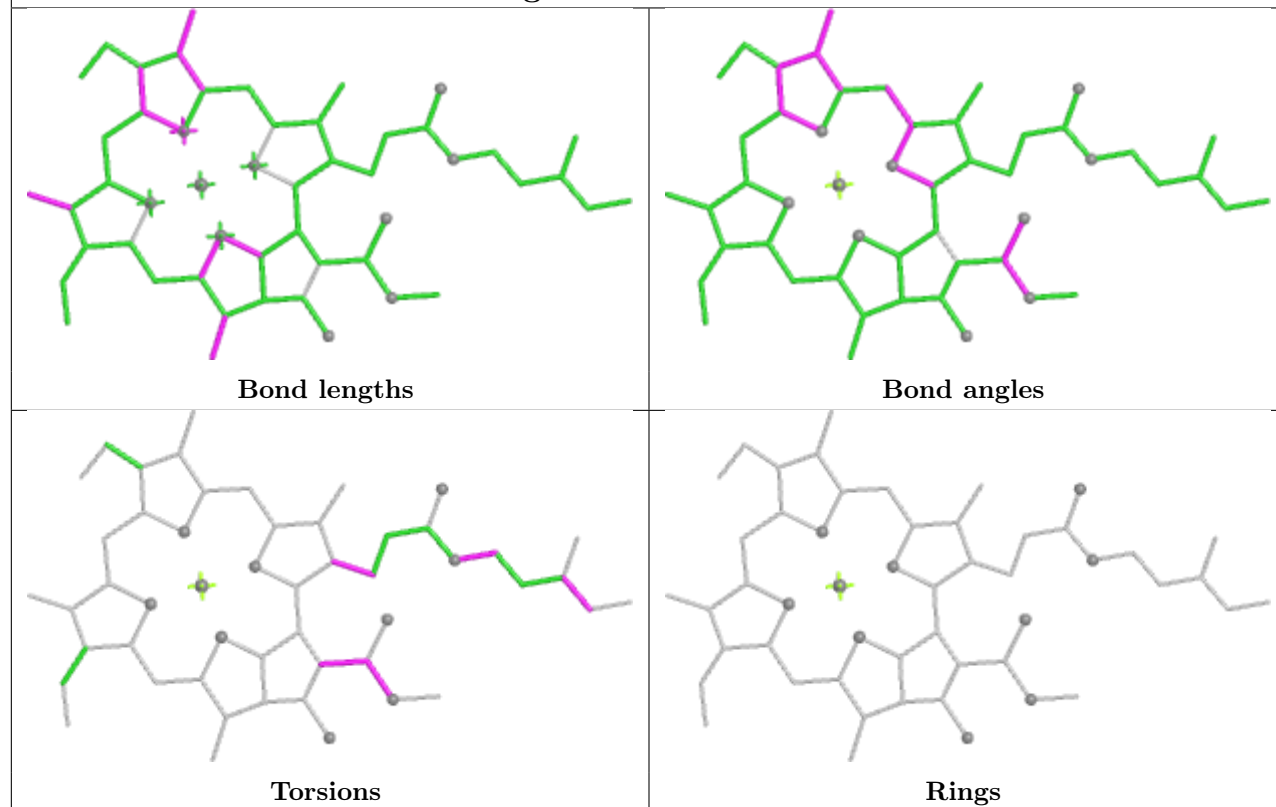
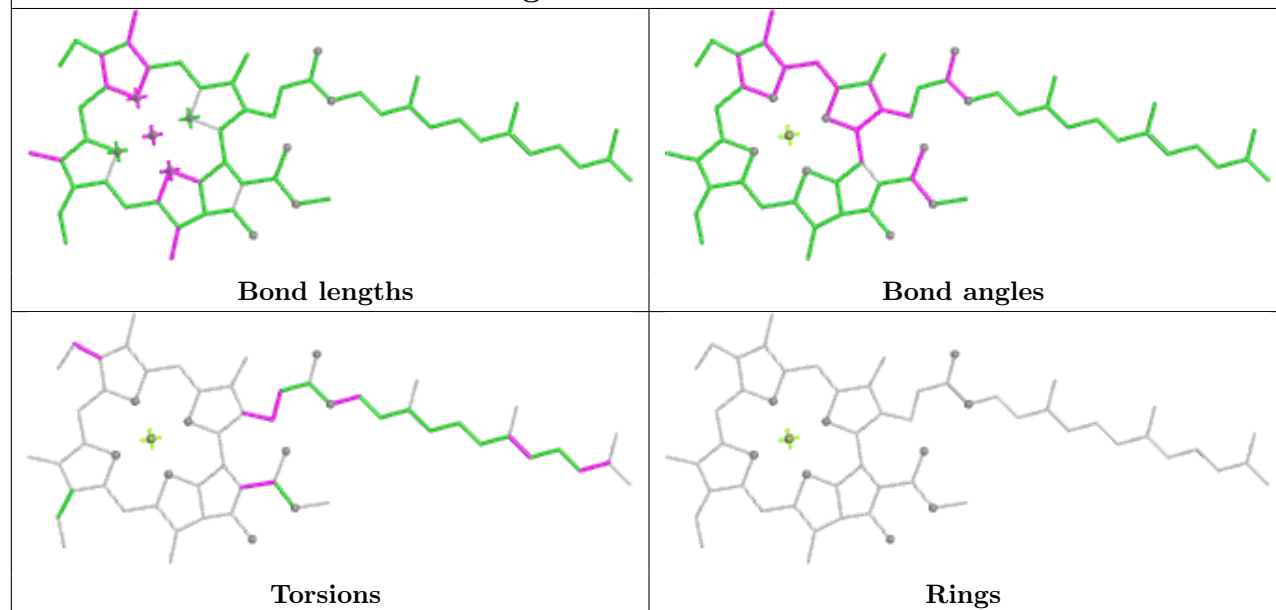
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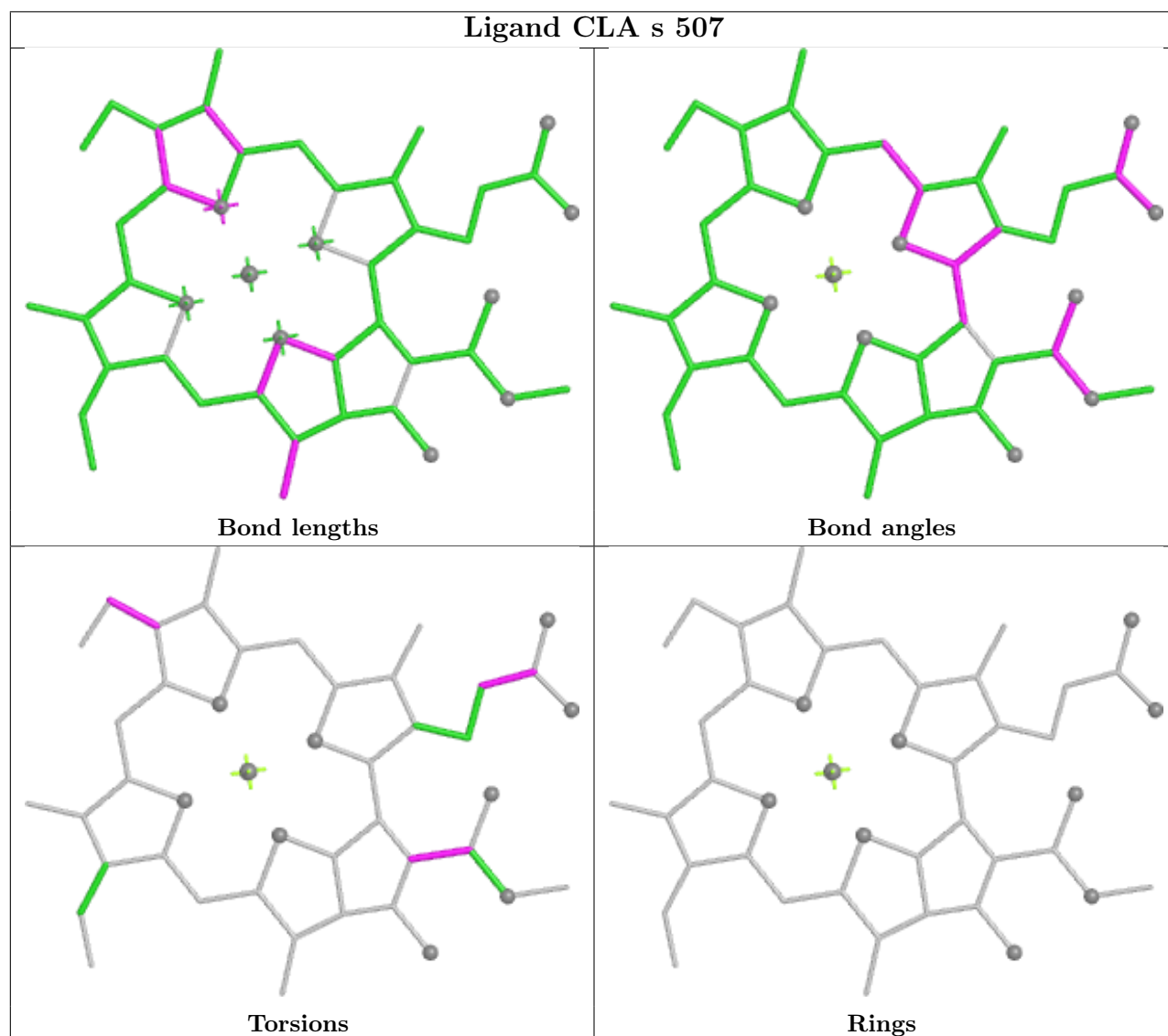
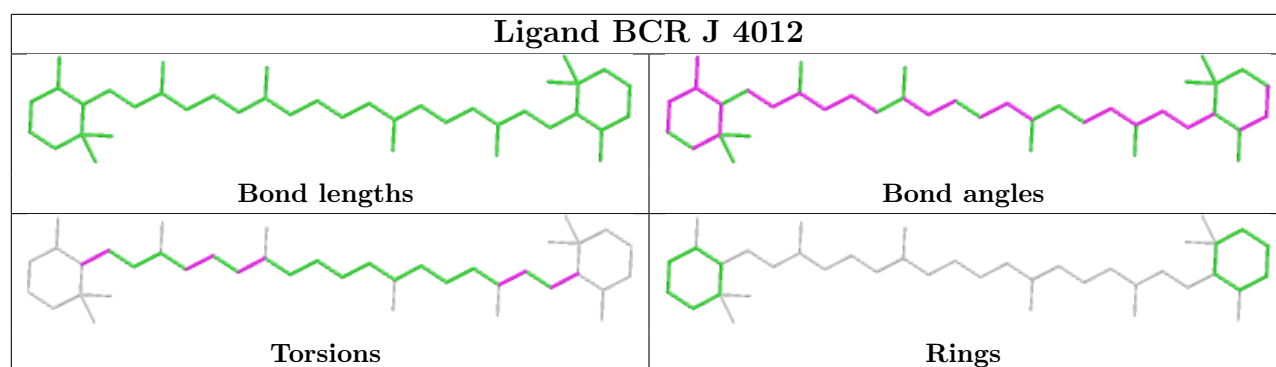
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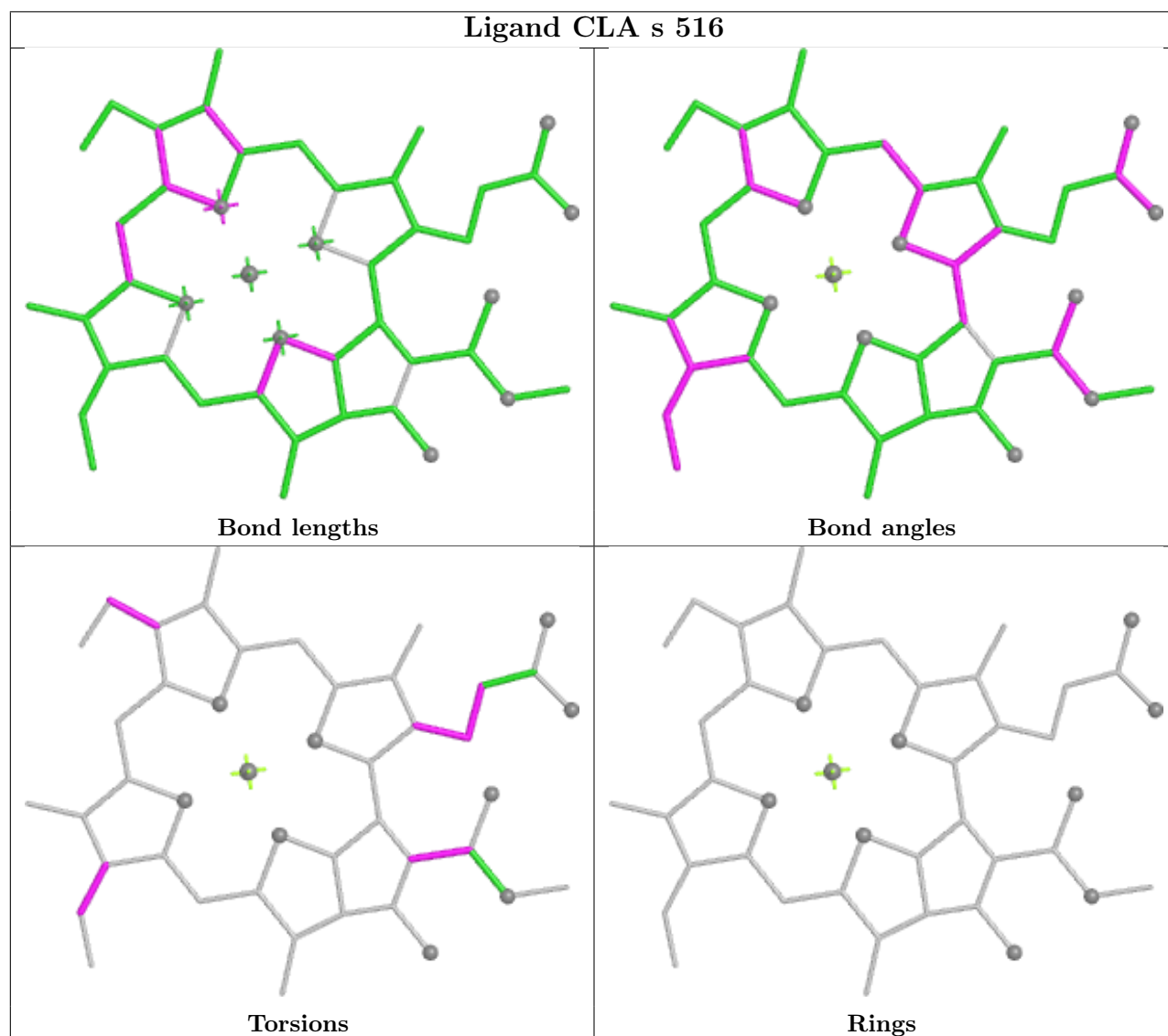
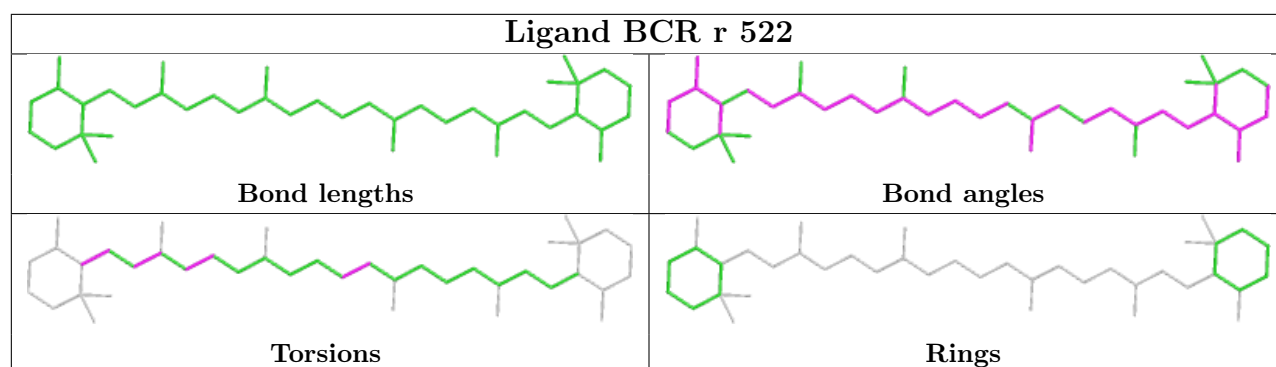
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	f	4004	BCR	2	0

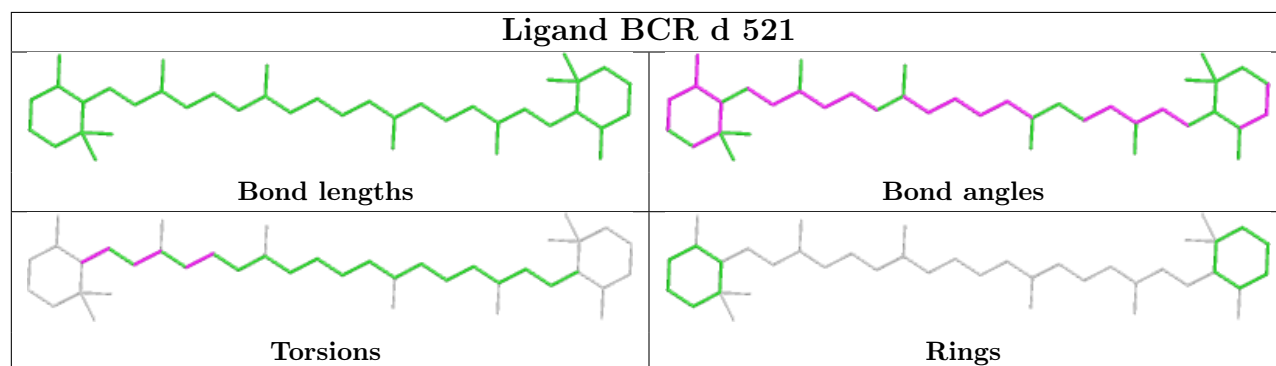
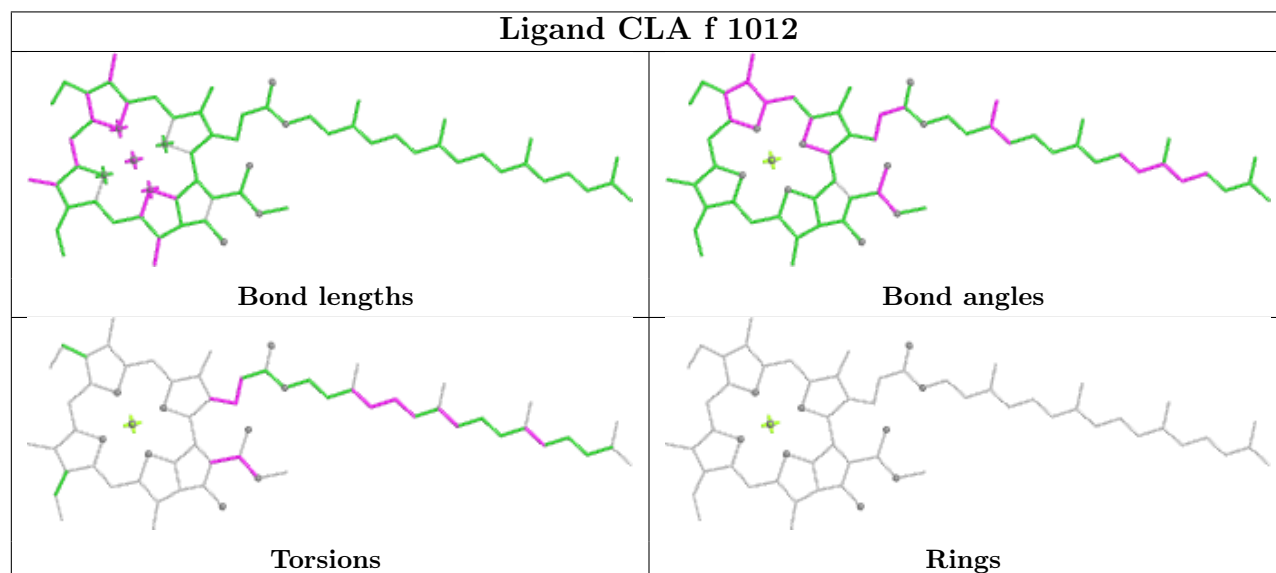
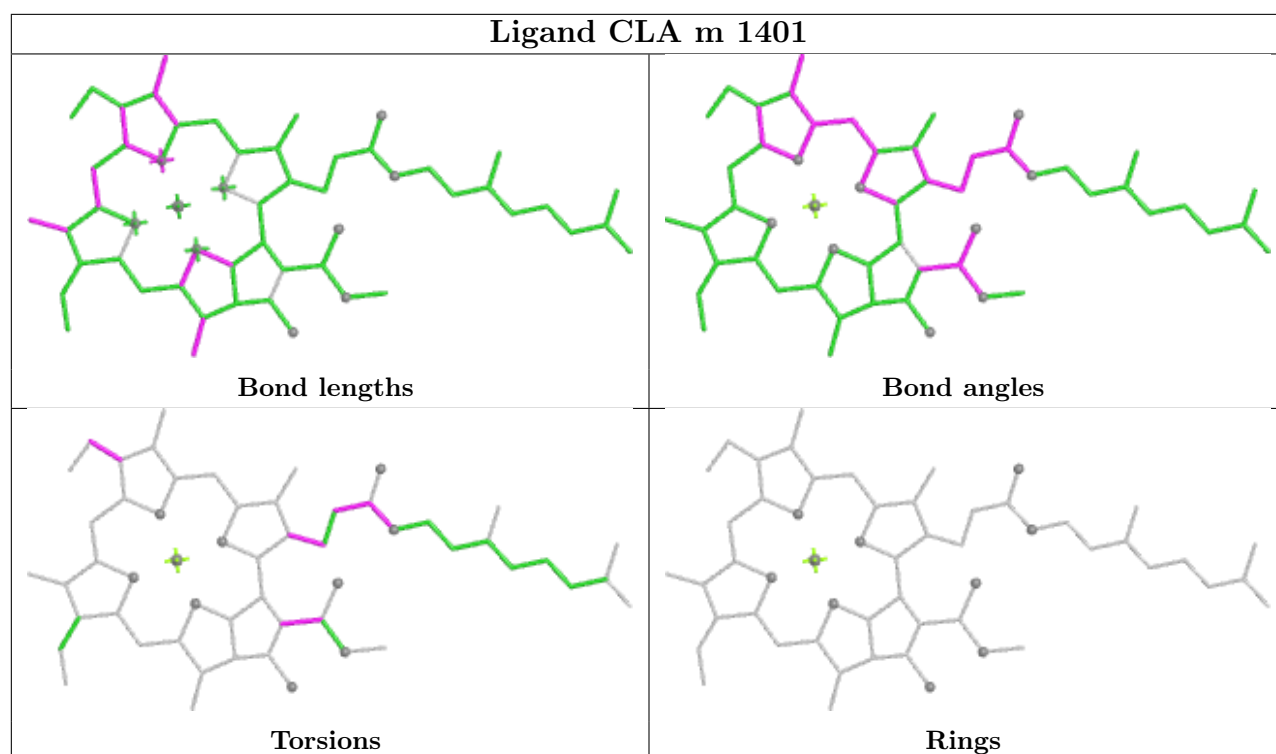
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

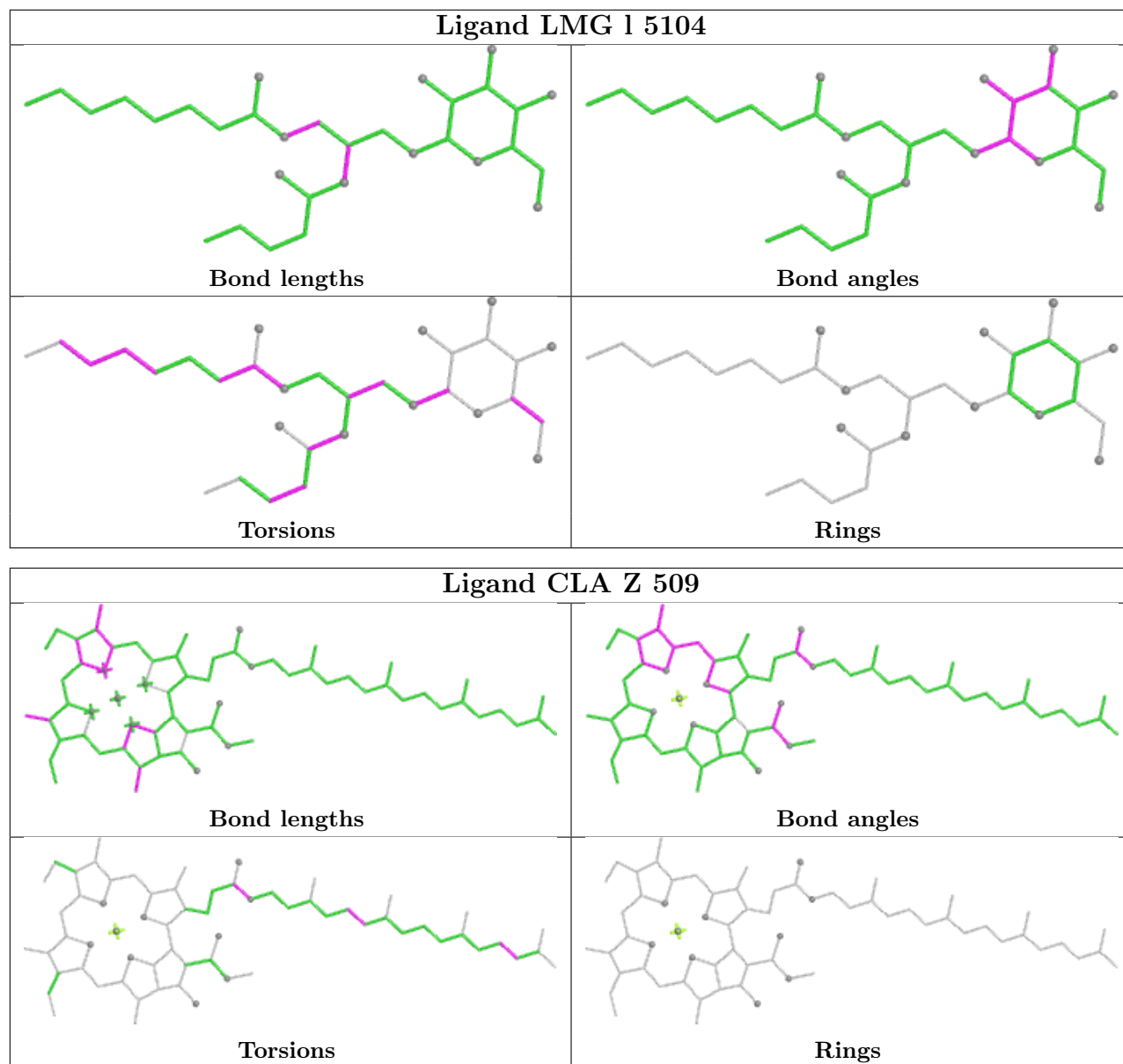


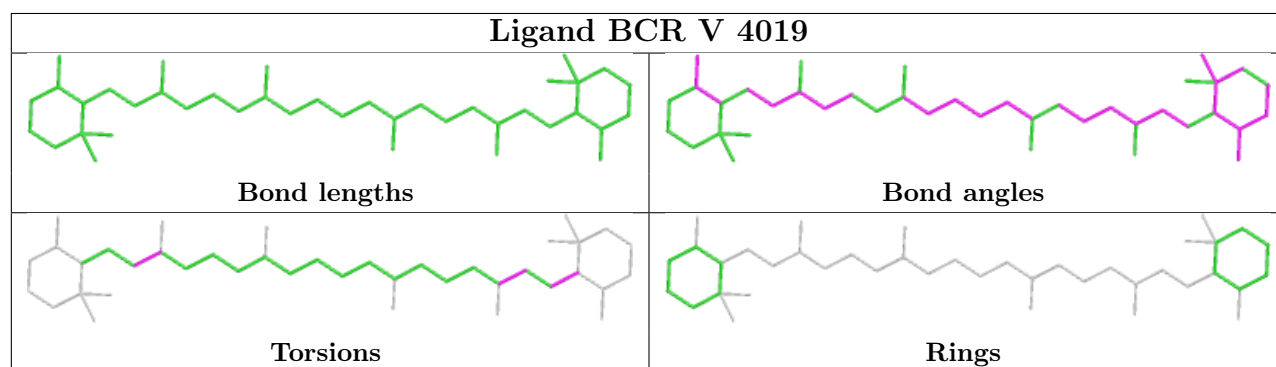
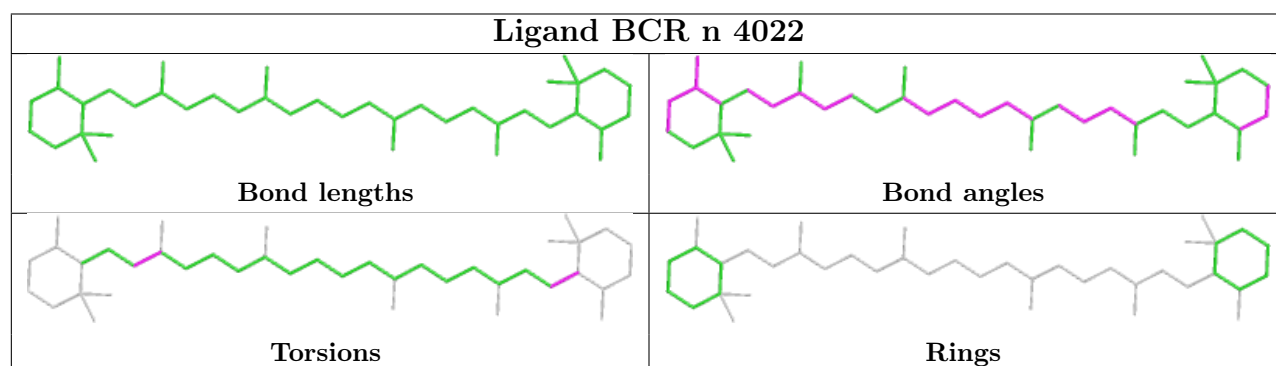
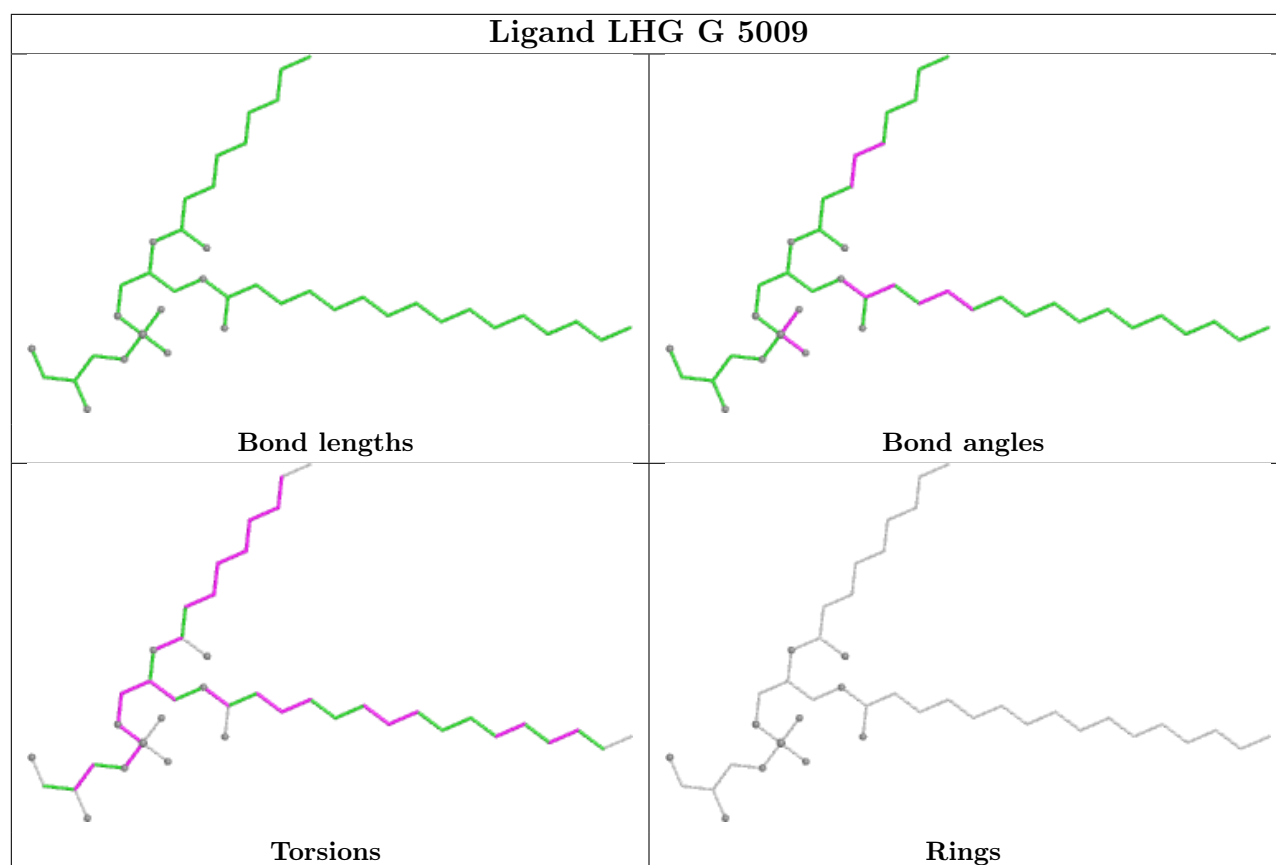
Ligand CLA B 1212**Ligand CLA V 1501**

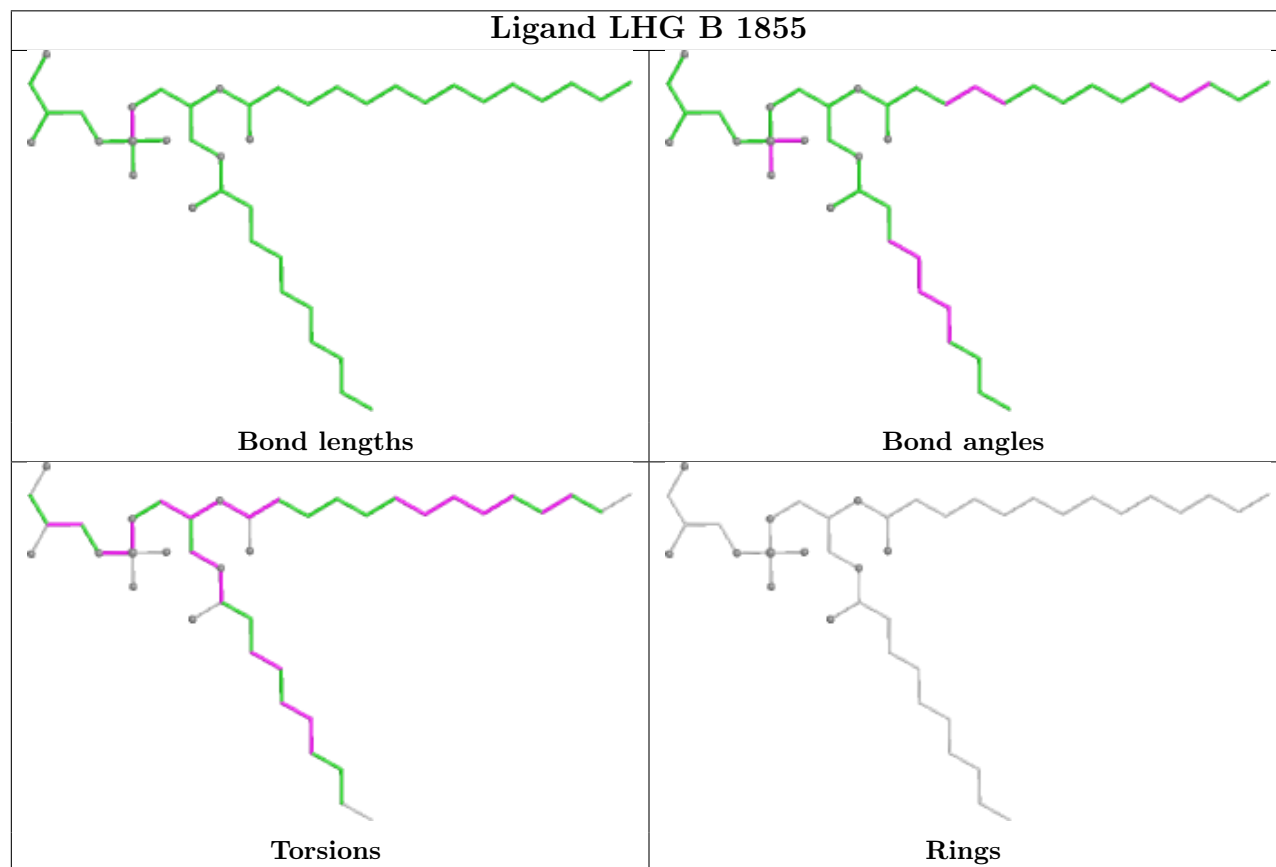
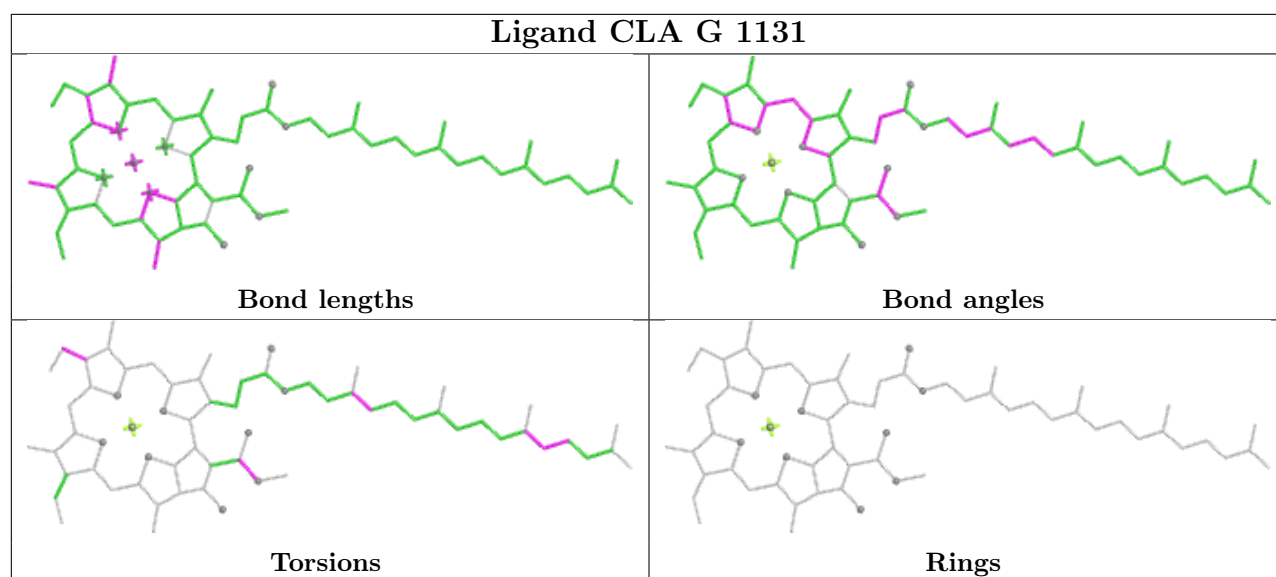


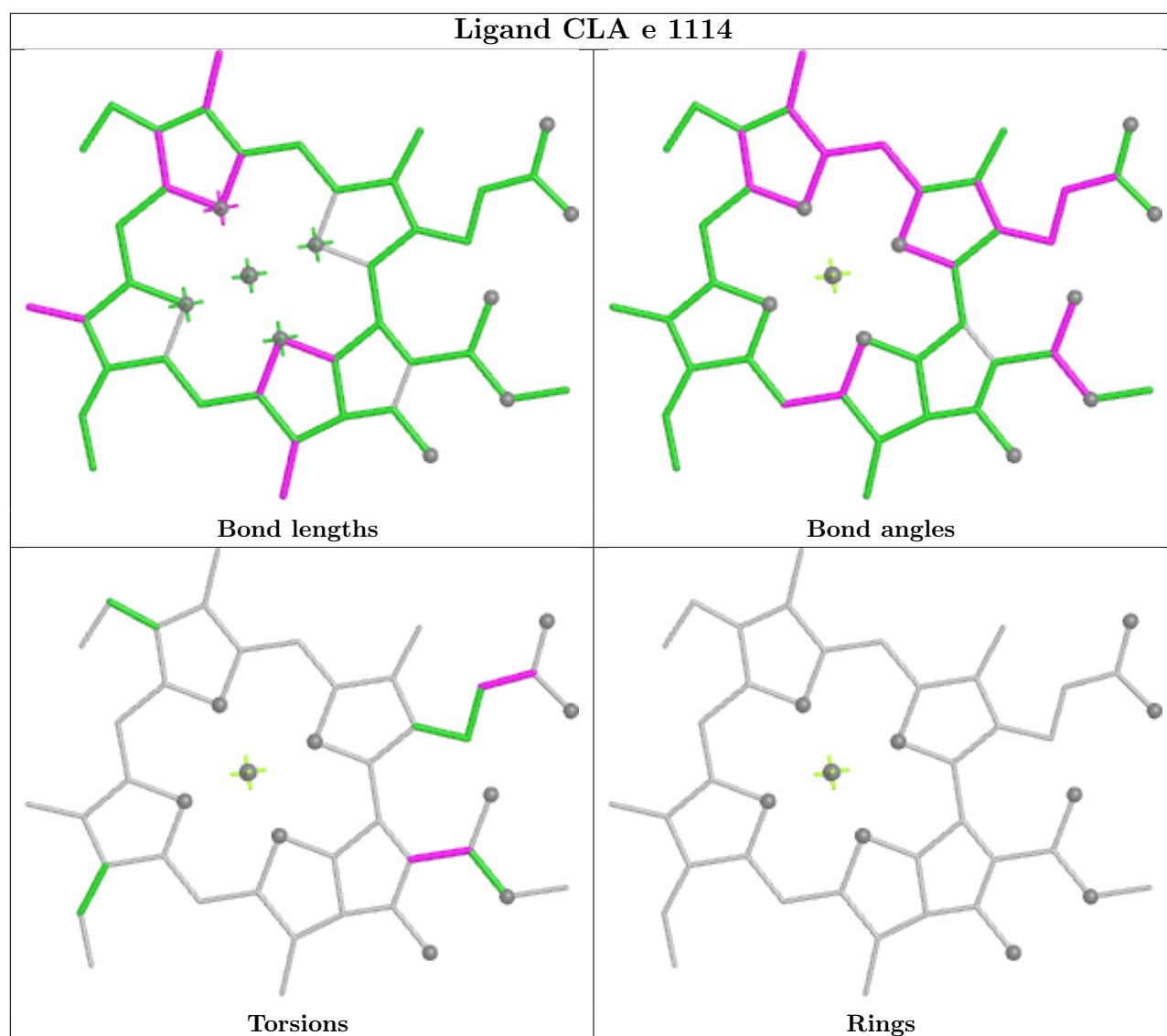
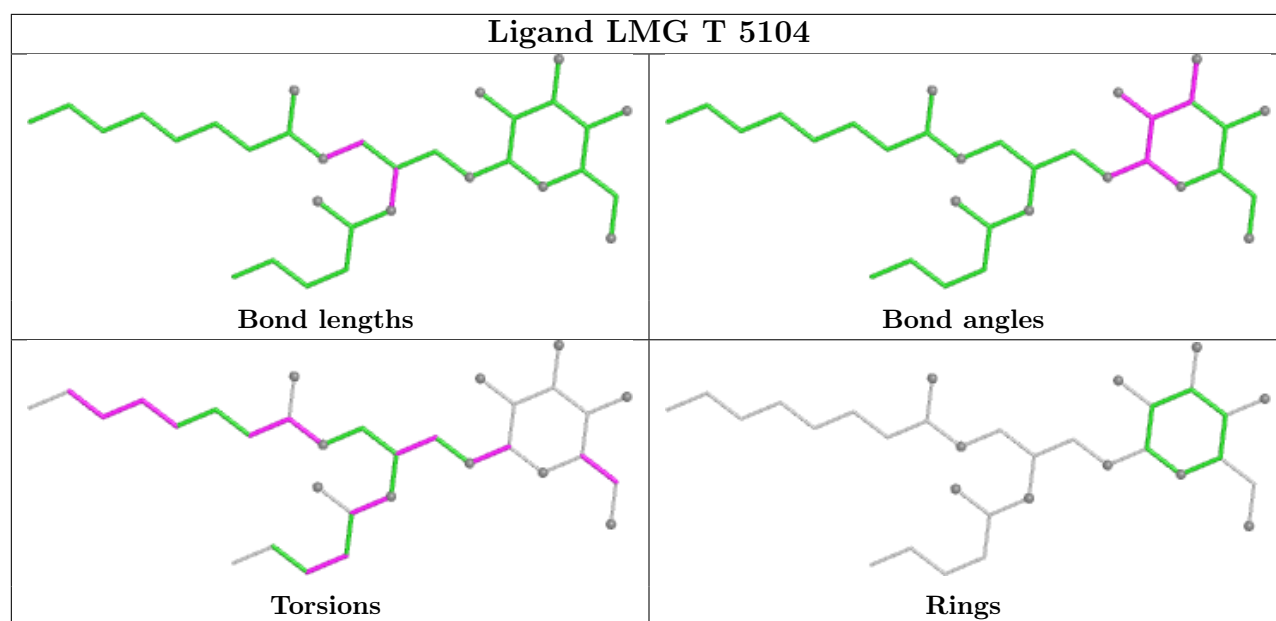


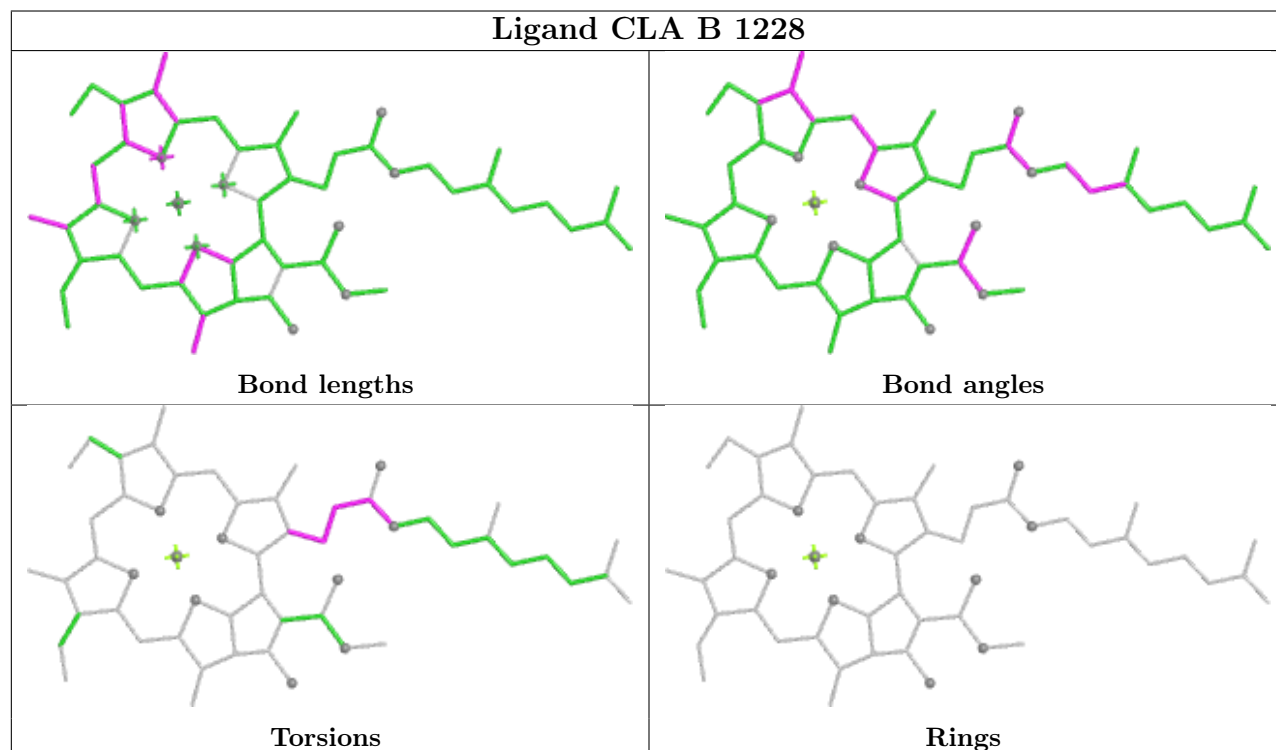
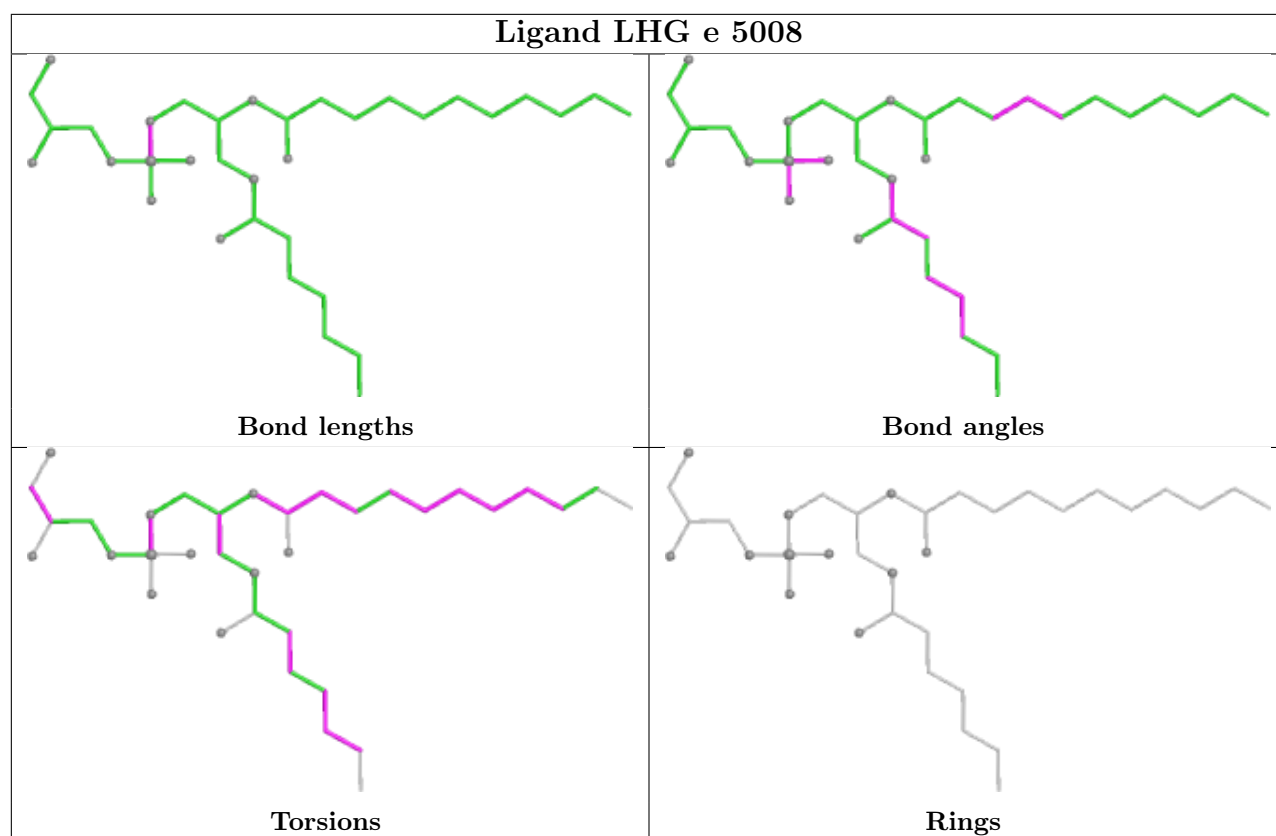


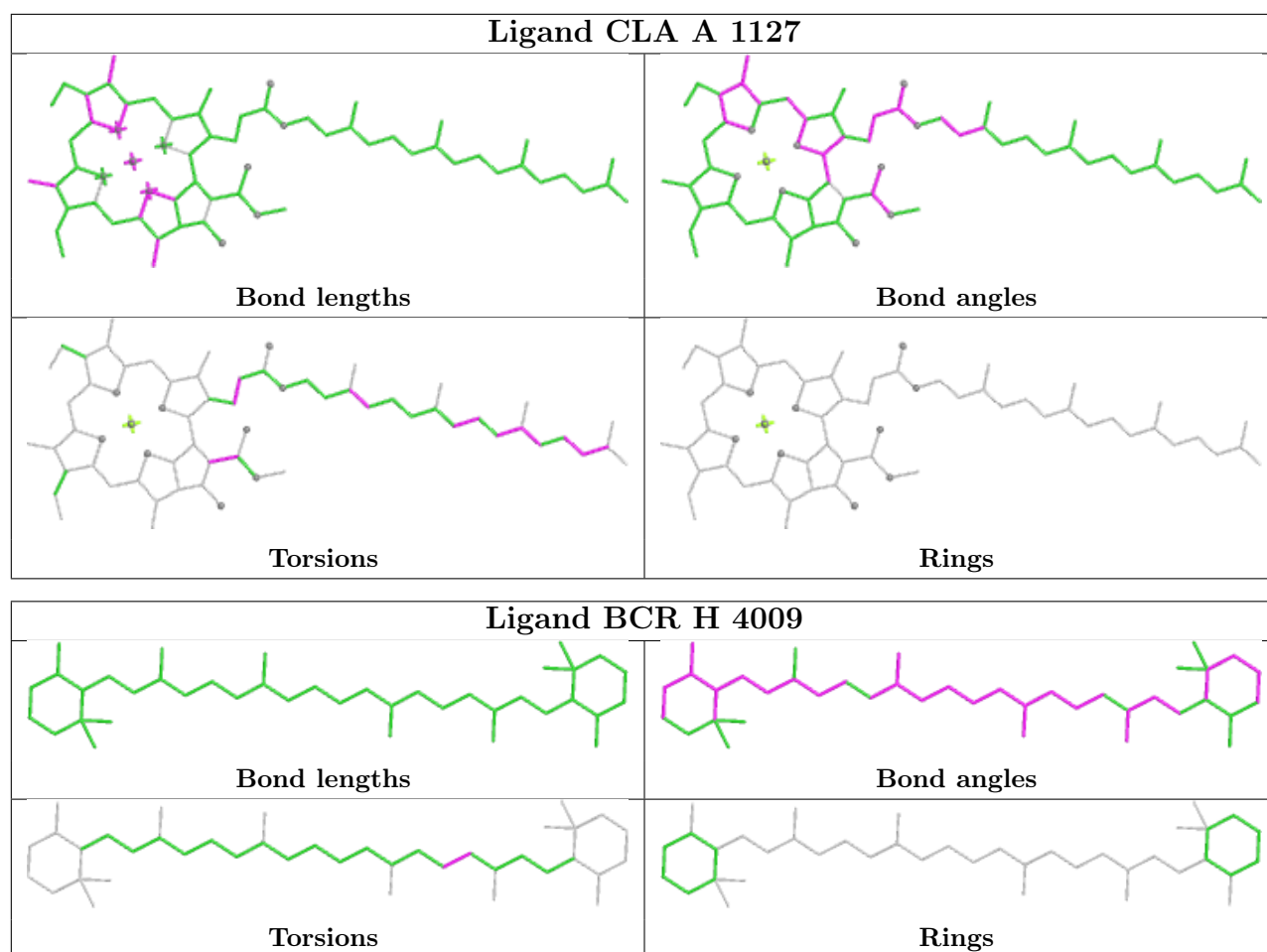




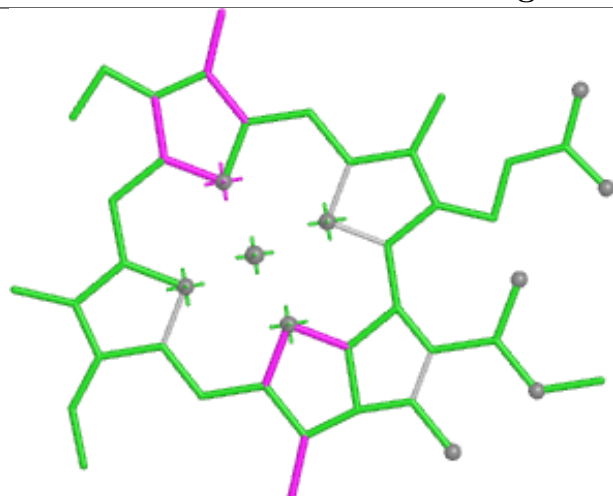




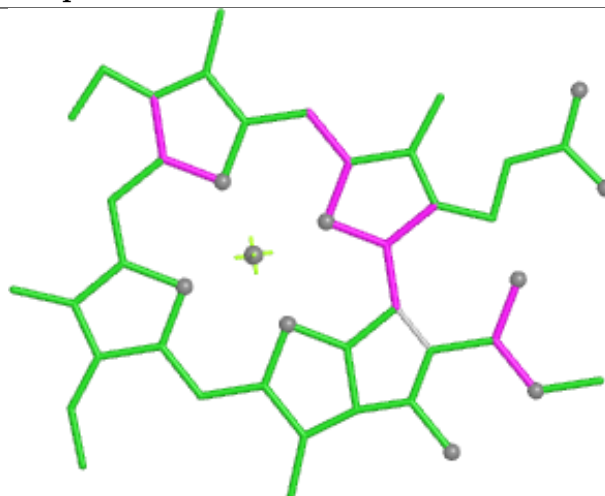




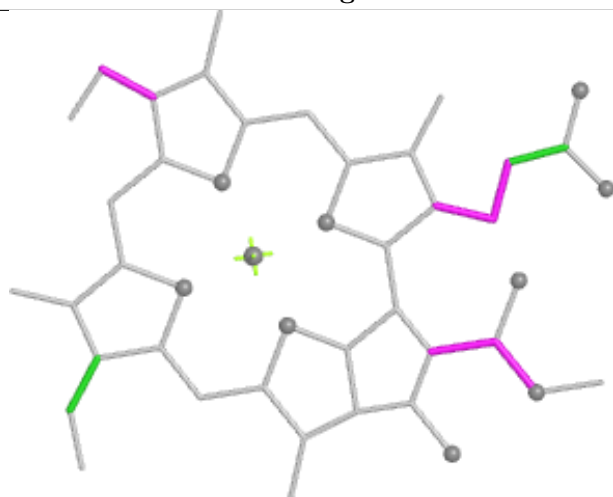
Ligand CLA q 503



Bond lengths



Bond angles

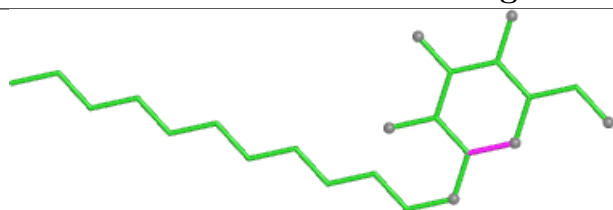


Torsions

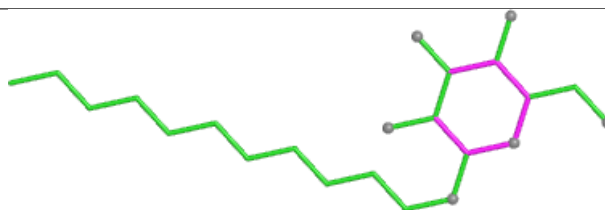


Rings

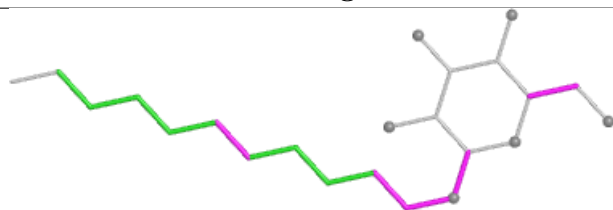
Ligand LMU G 1849



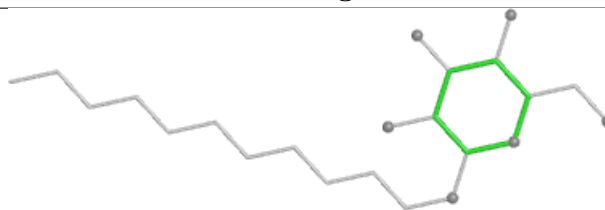
Bond lengths



Bond angles

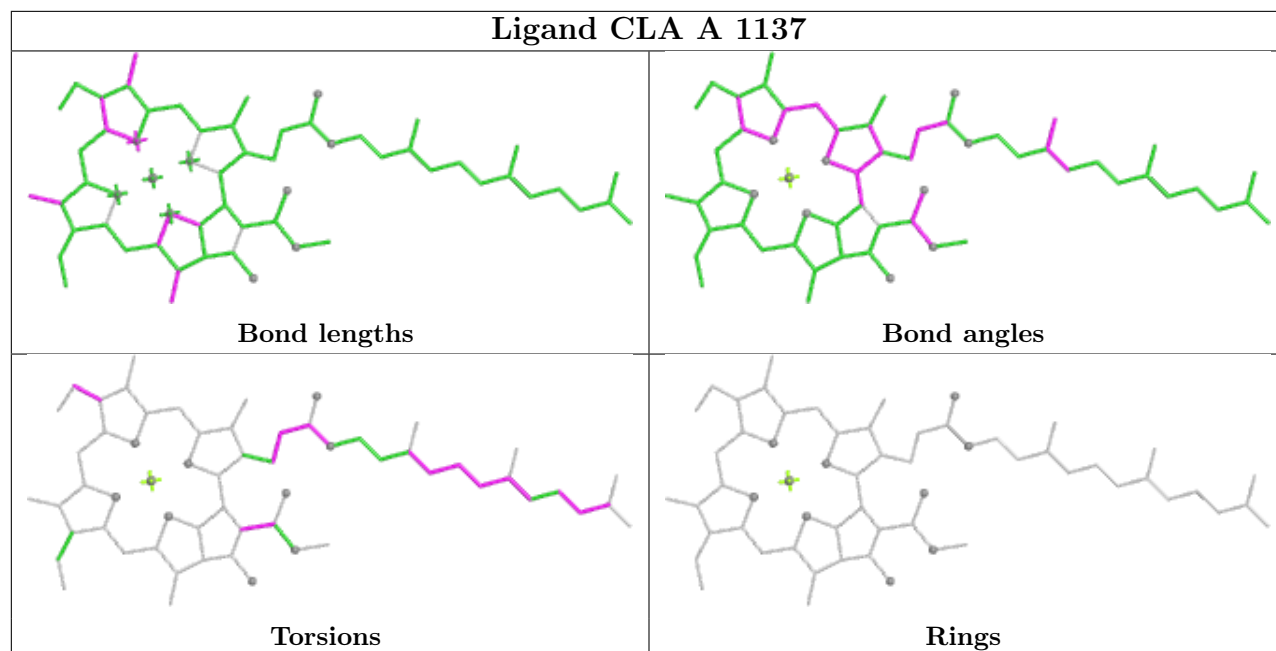


Torsions

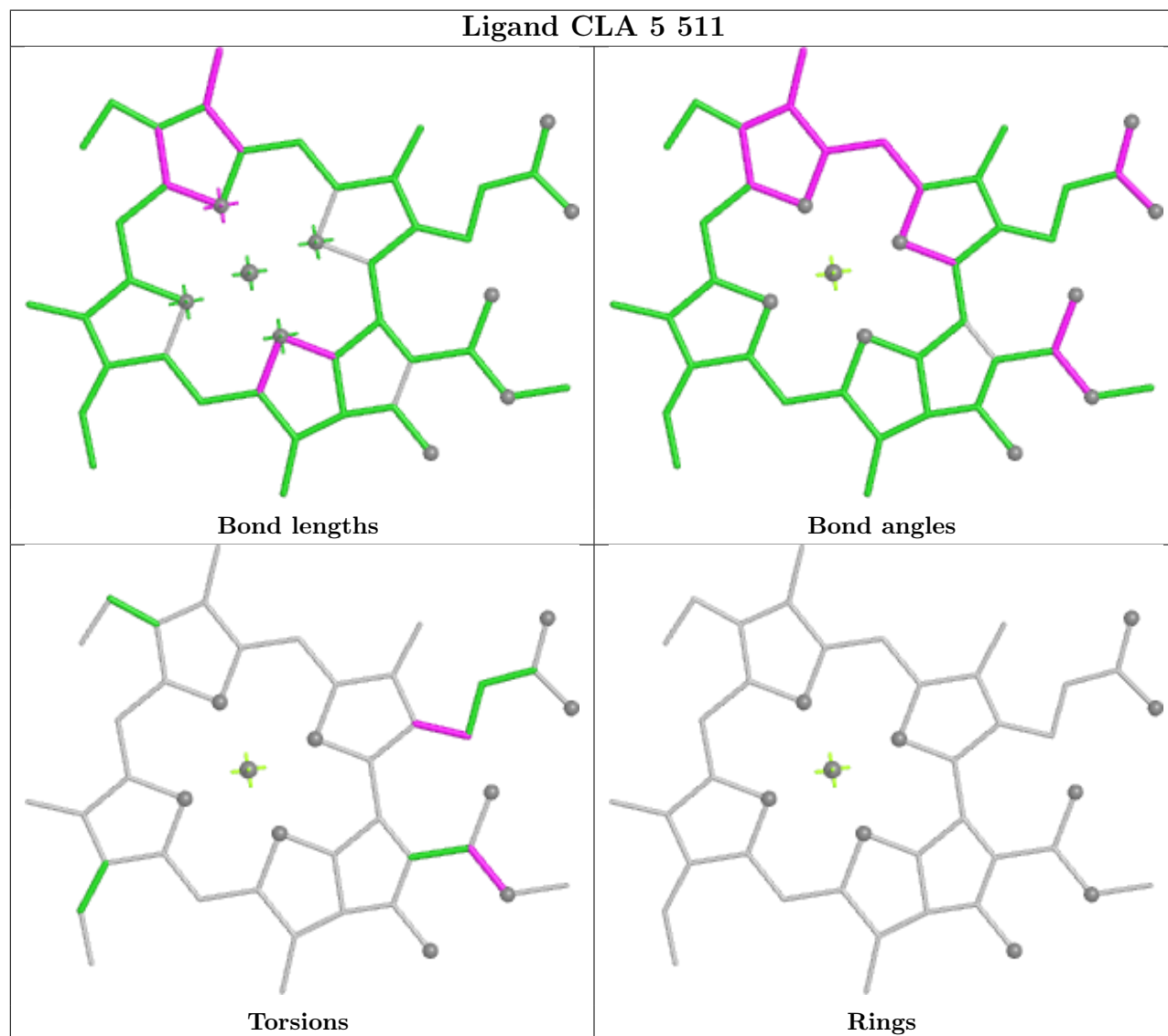


Rings

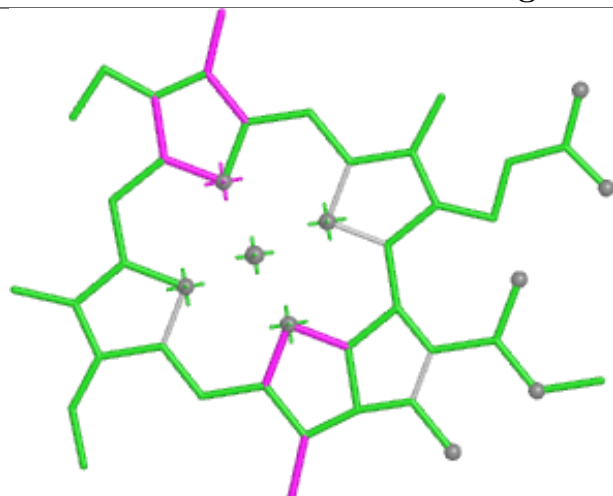
Ligand CLA A 1137



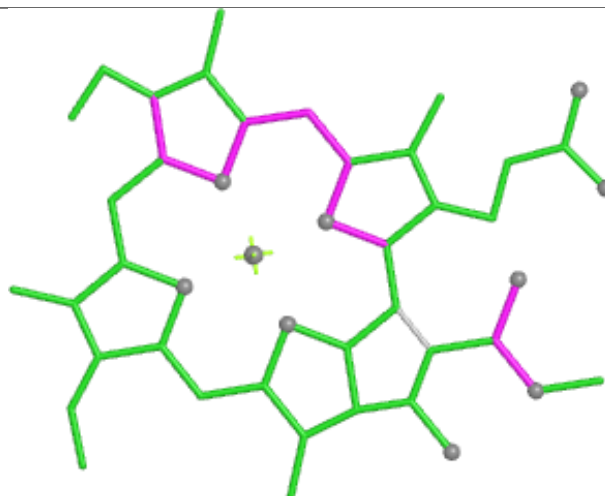
Ligand CLA 5 511



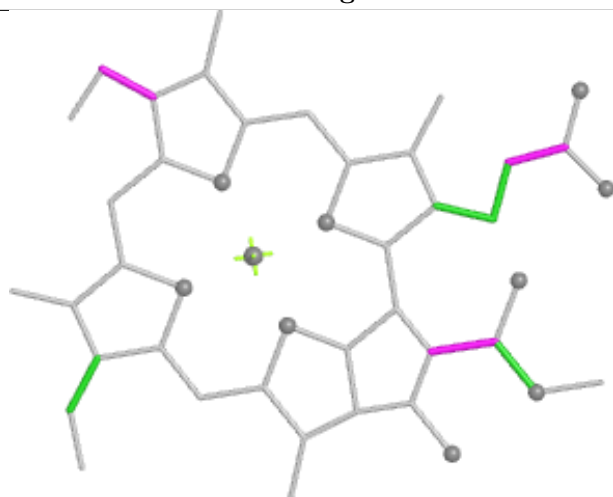
Ligand CLA 4 512



Bond lengths



Bond angles

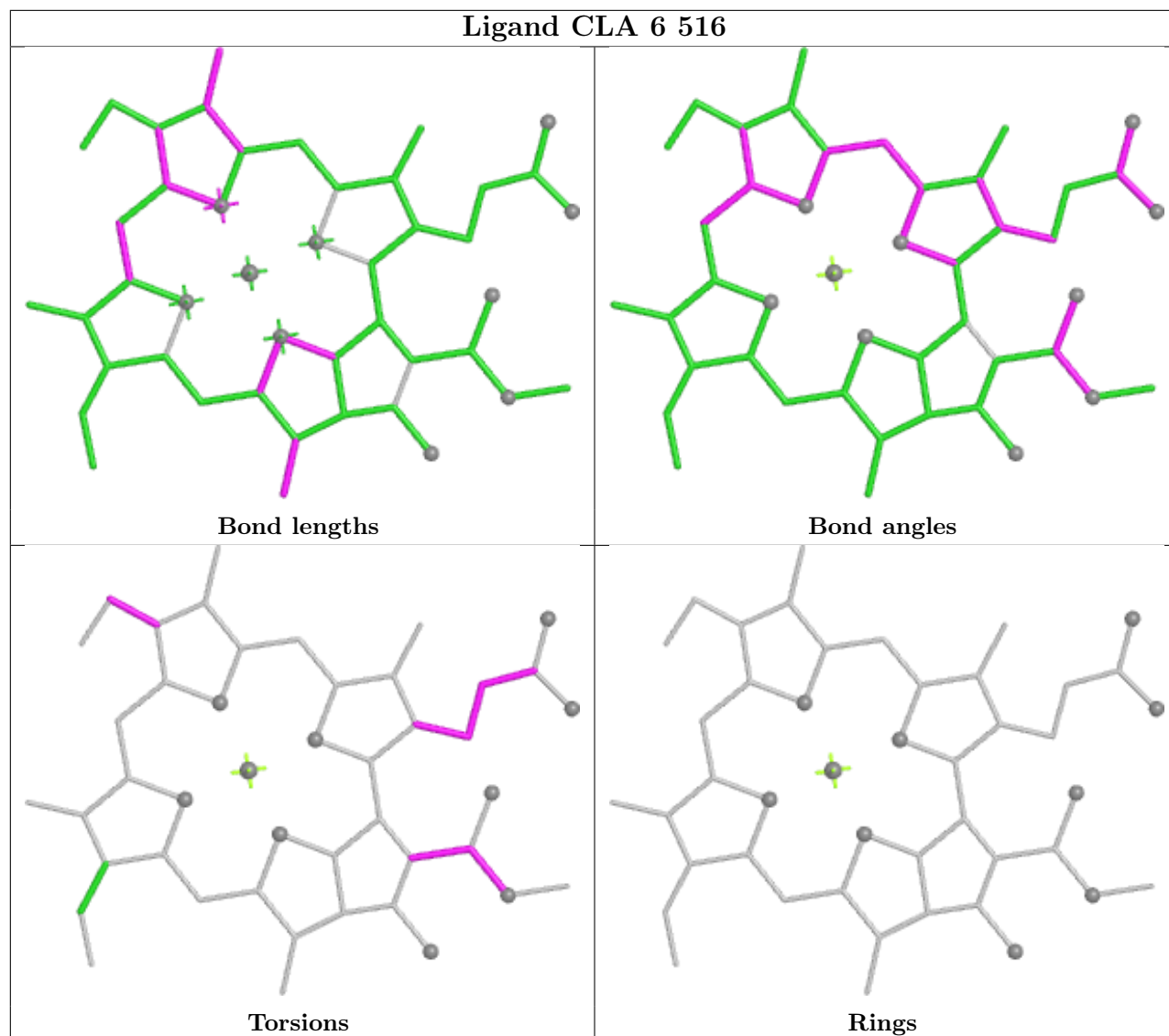


Torsions

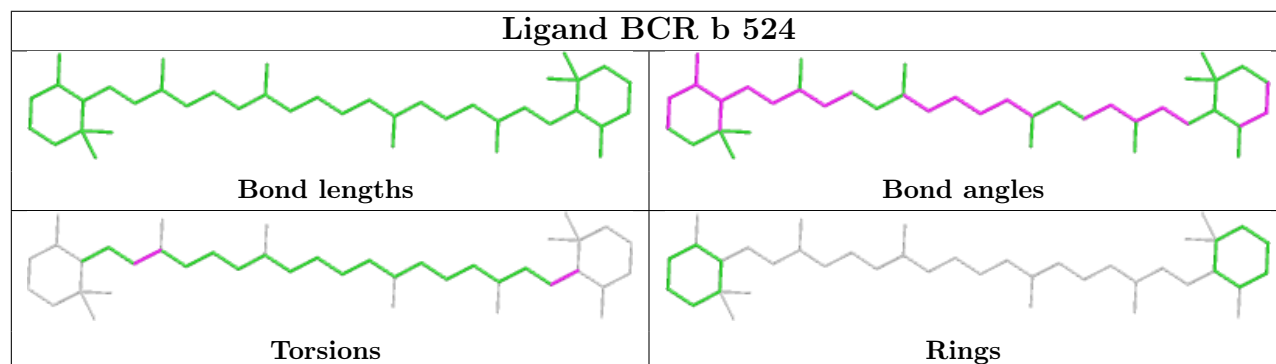


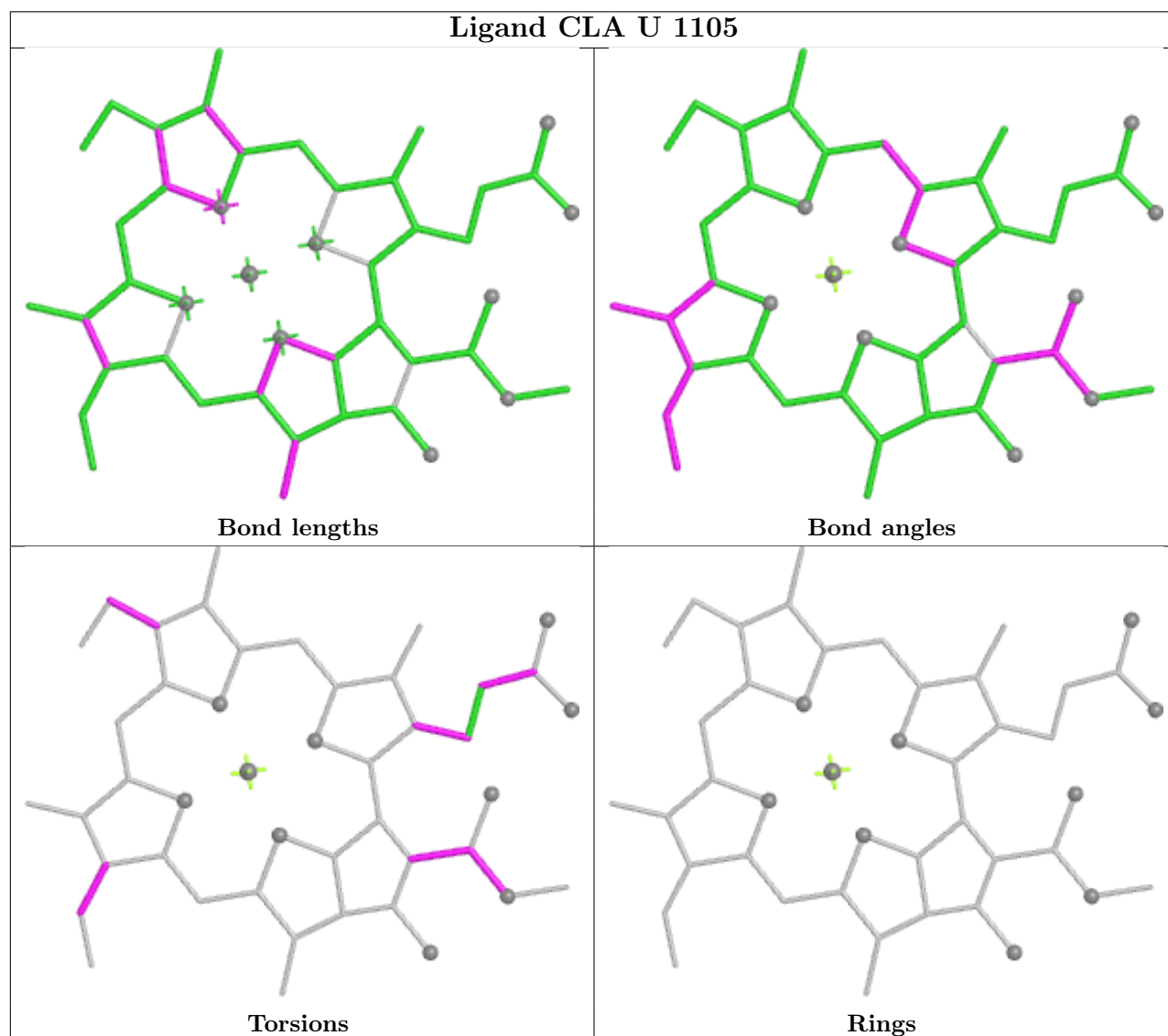
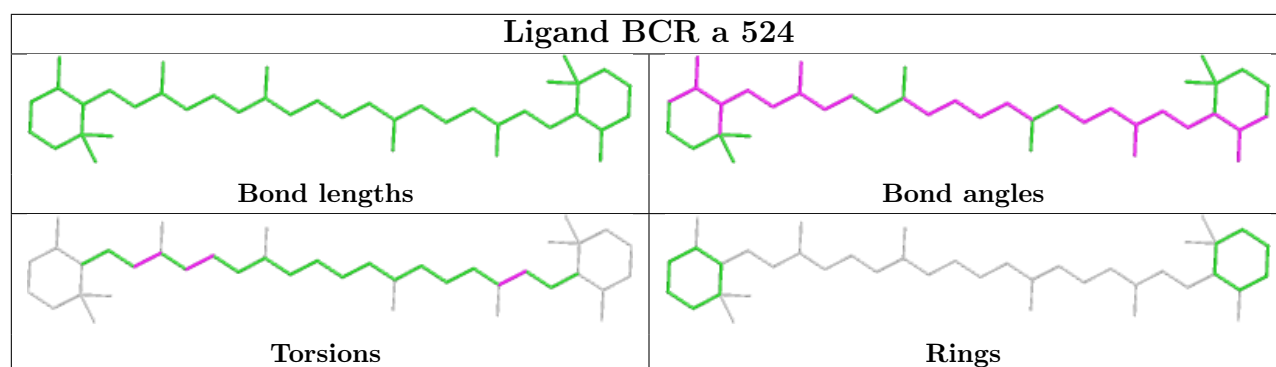
Rings

Ligand CLA 6 516

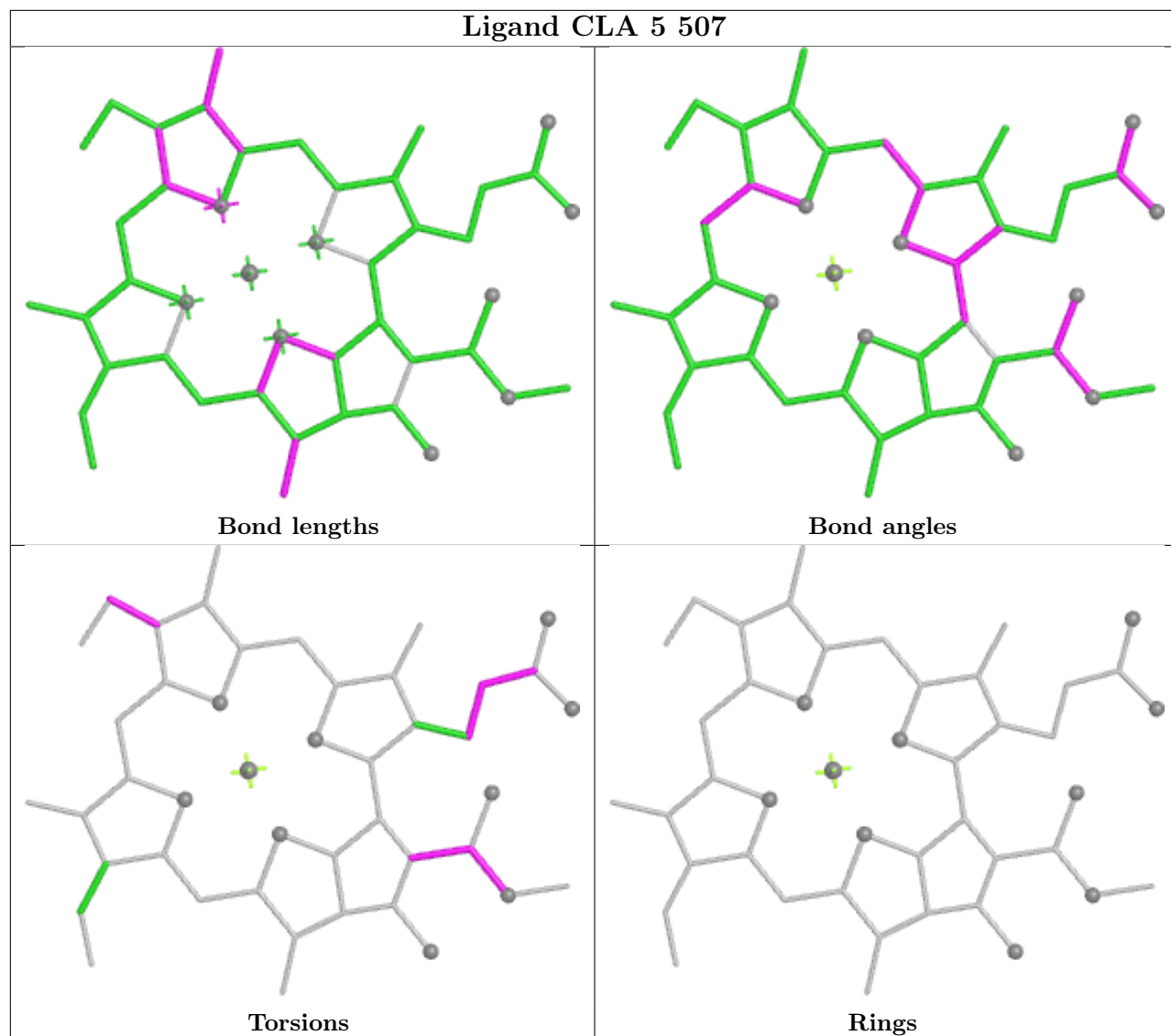


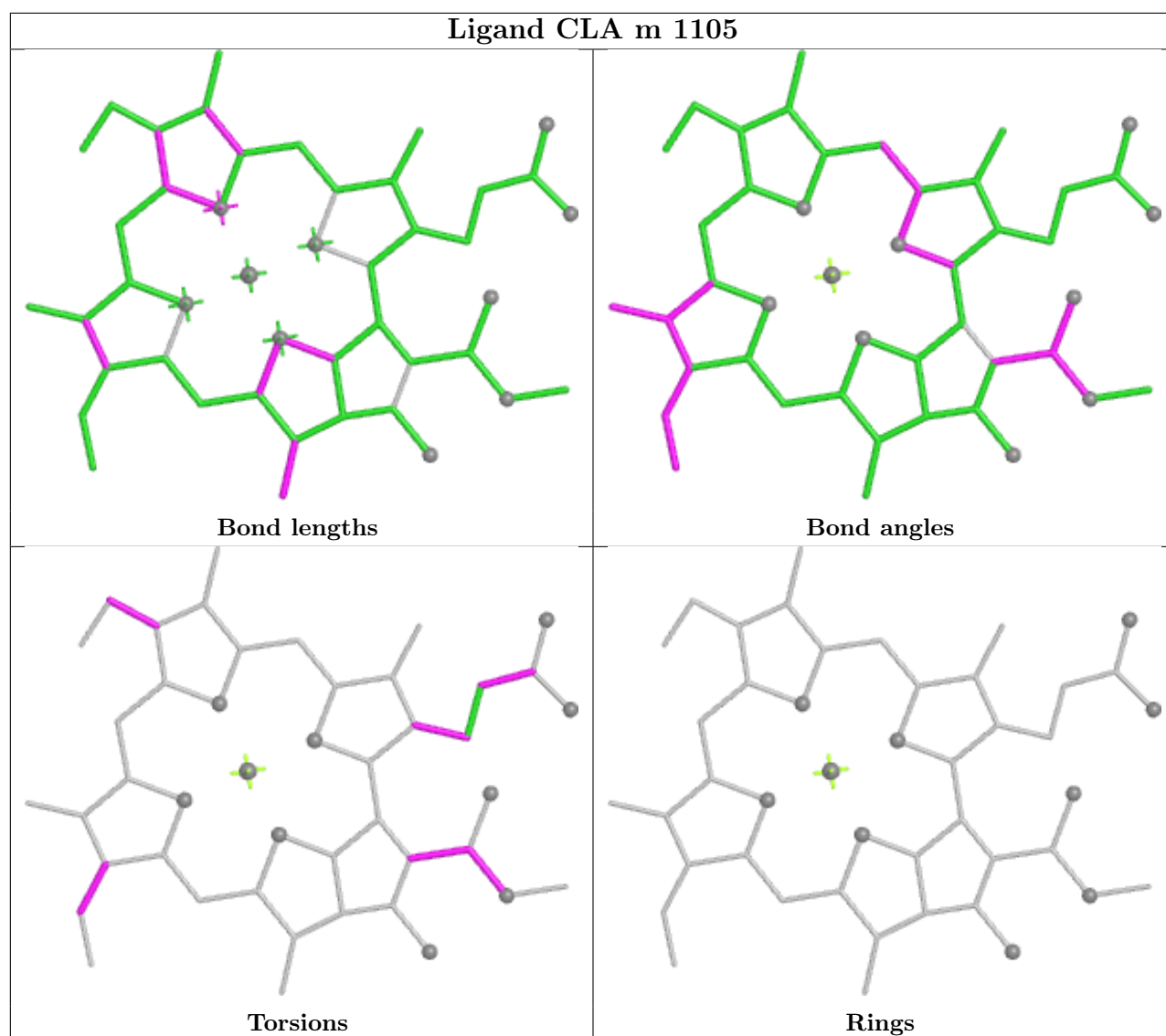
Ligand BCR b 524

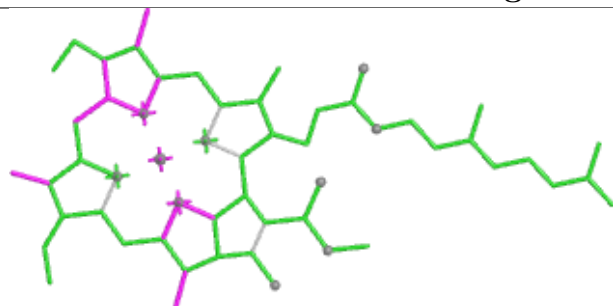




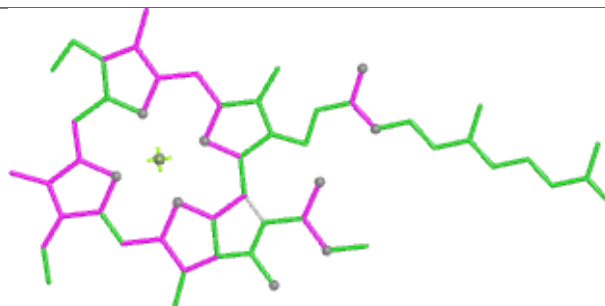
Ligand CLA 5 507



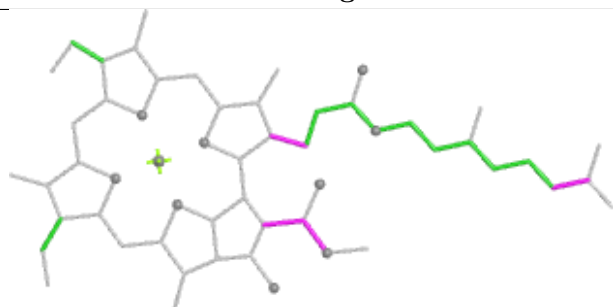


Ligand CLA H 1226

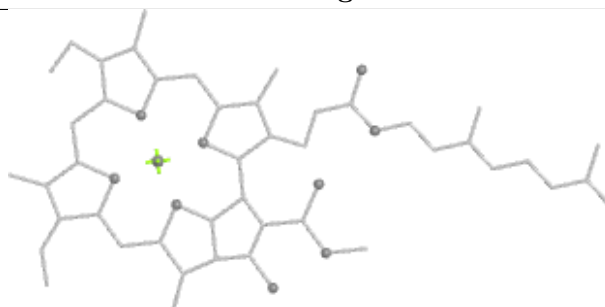
Bond lengths



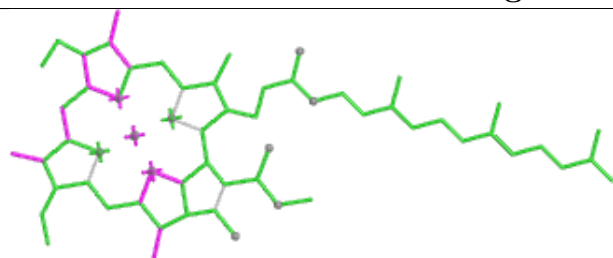
Bond angles



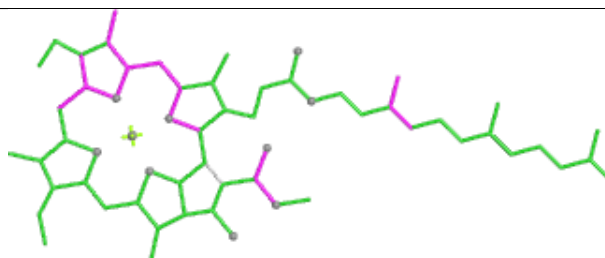
Torsions



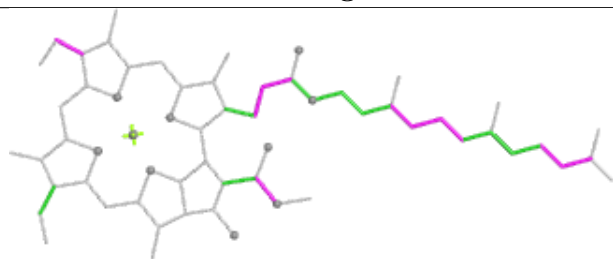
Rings

Ligand CLA A 1115

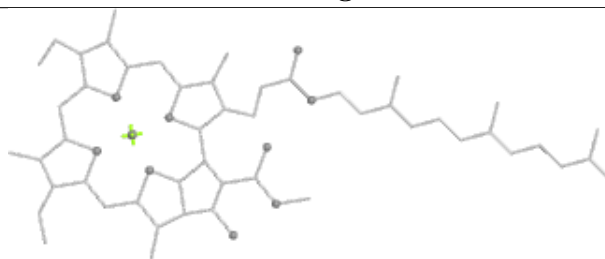
Bond lengths



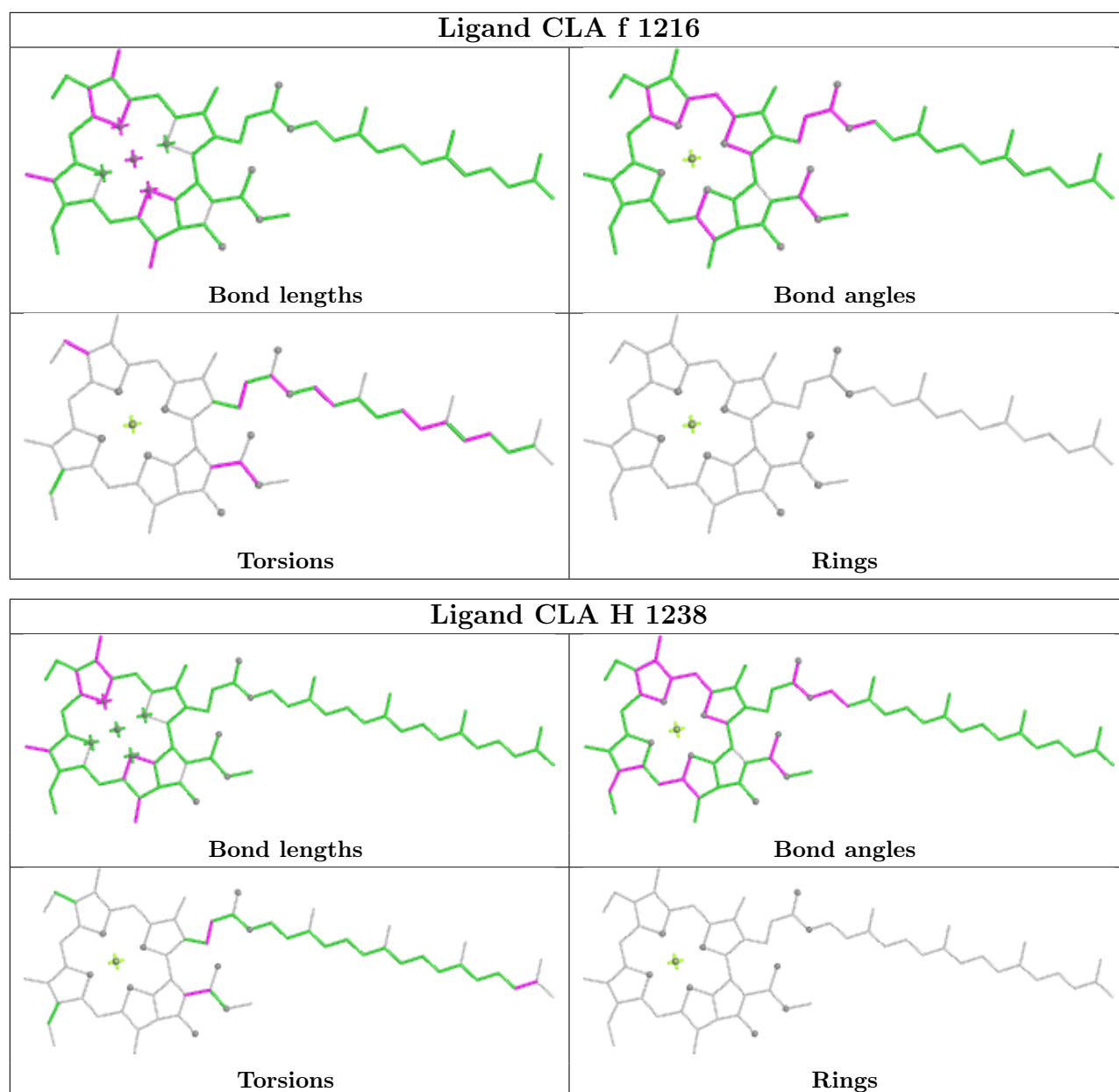
Bond angles



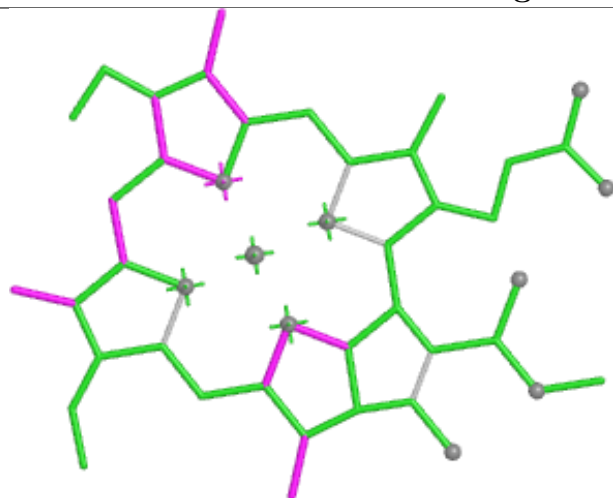
Torsions



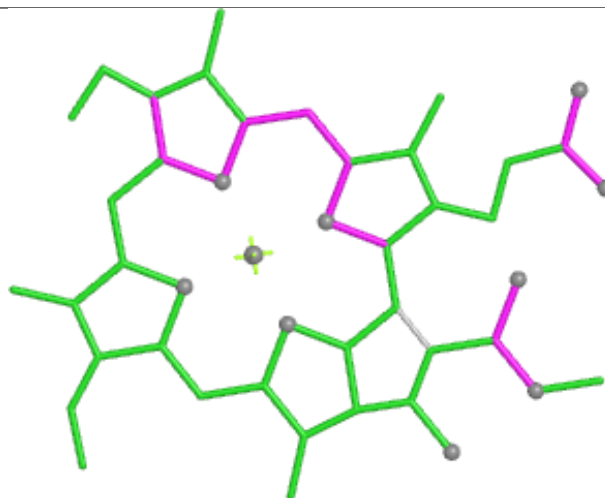
Rings



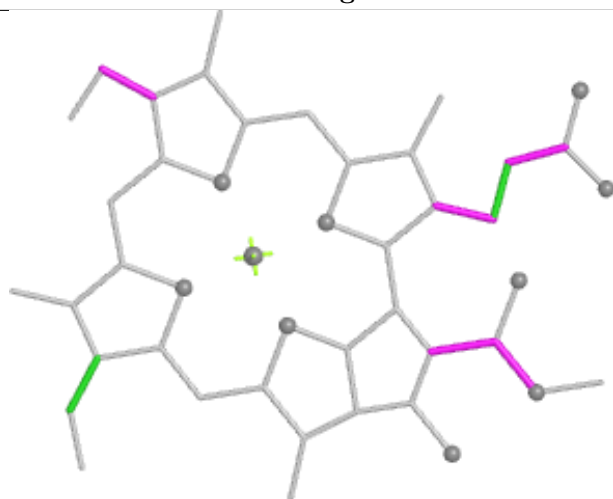
Ligand CLA Y 519



Bond lengths



Bond angles

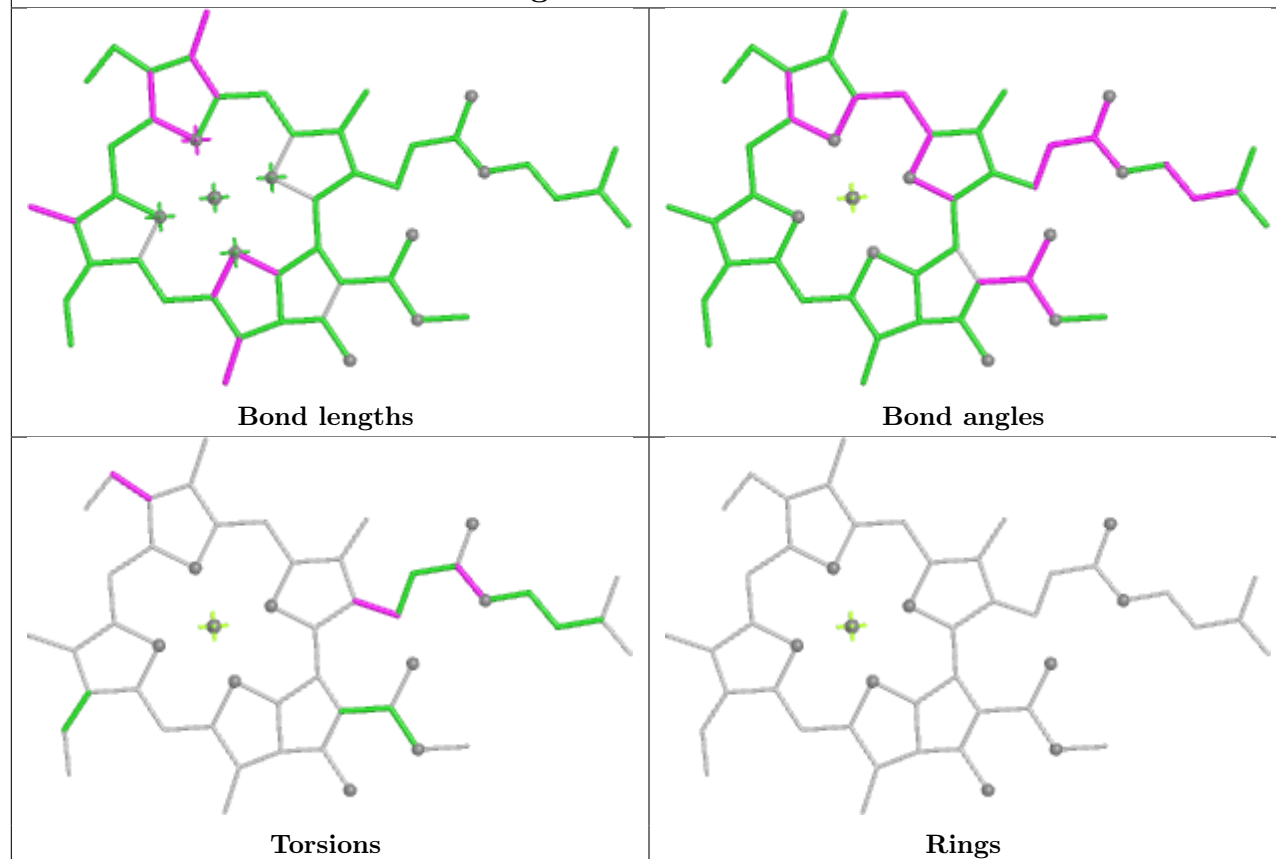


Torsions

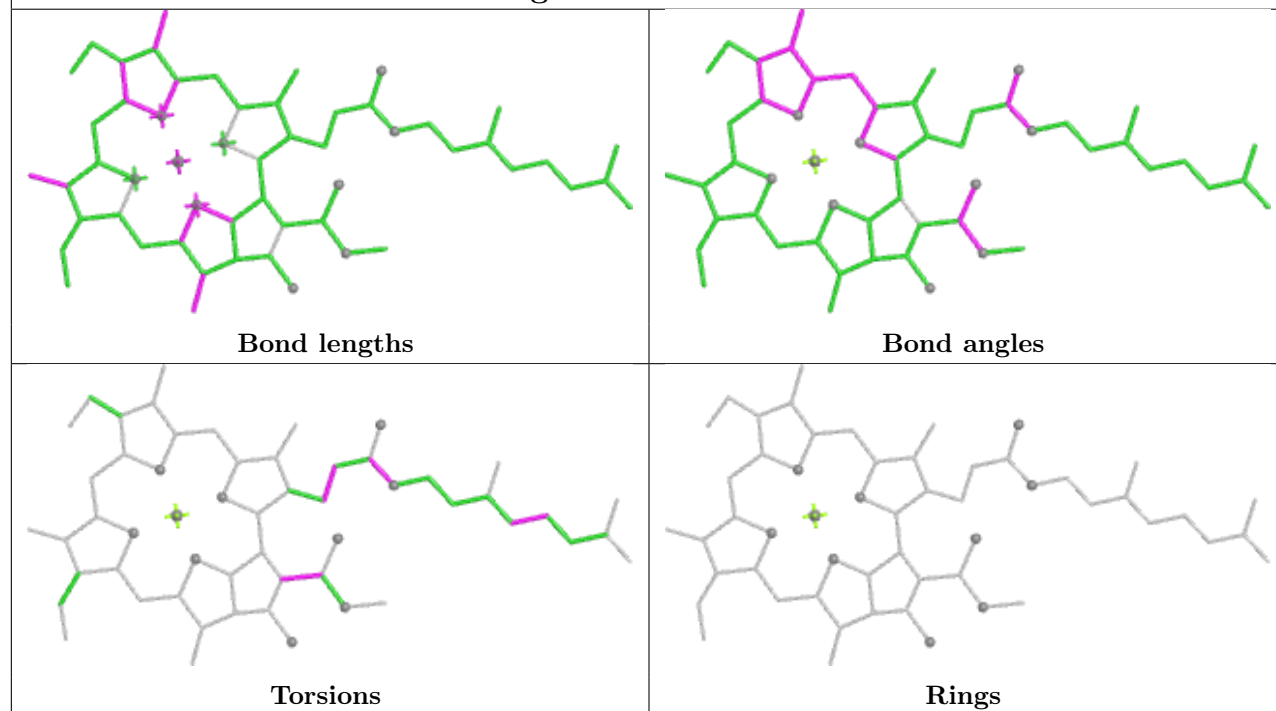


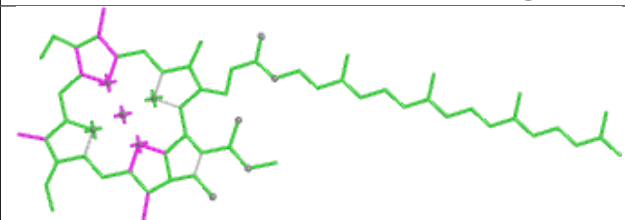
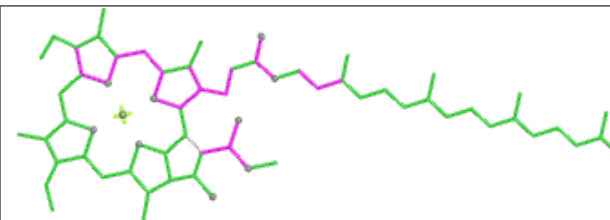
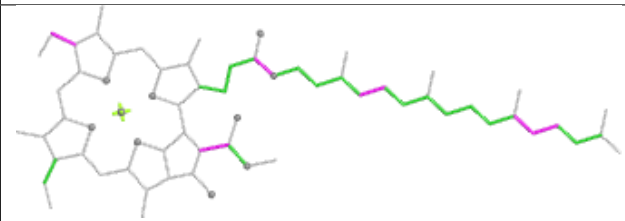
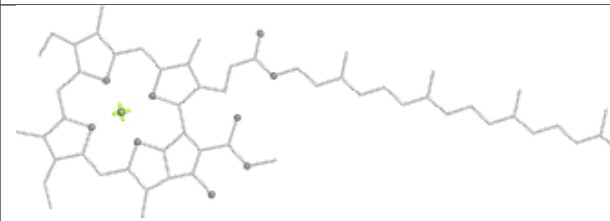
Rings

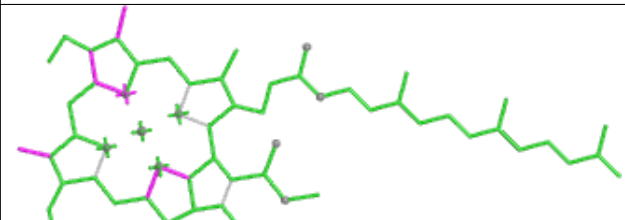
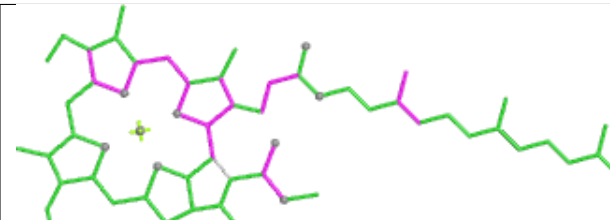
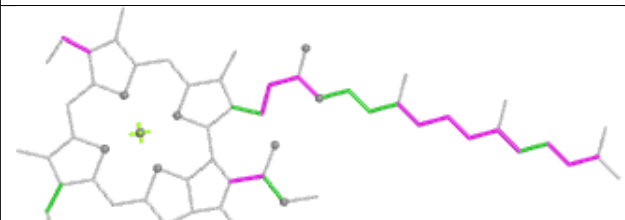
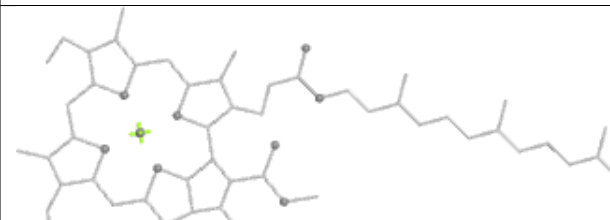
Ligand CLA f 1236

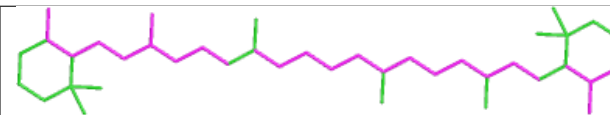
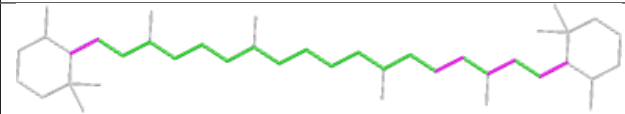
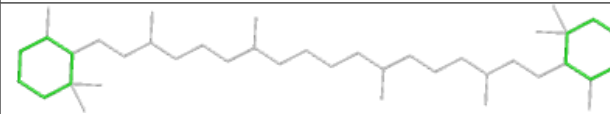


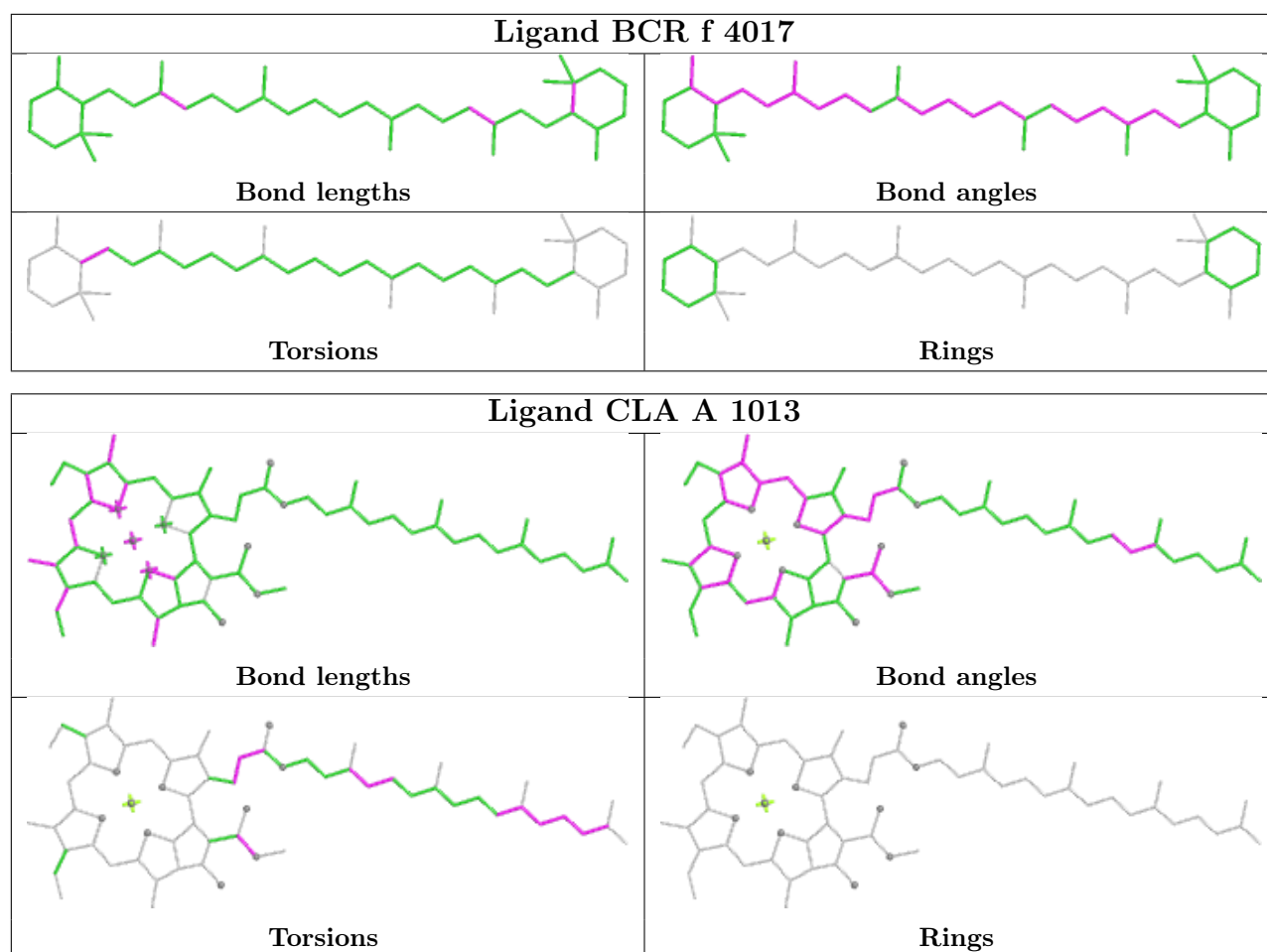
Ligand CLA f 1232



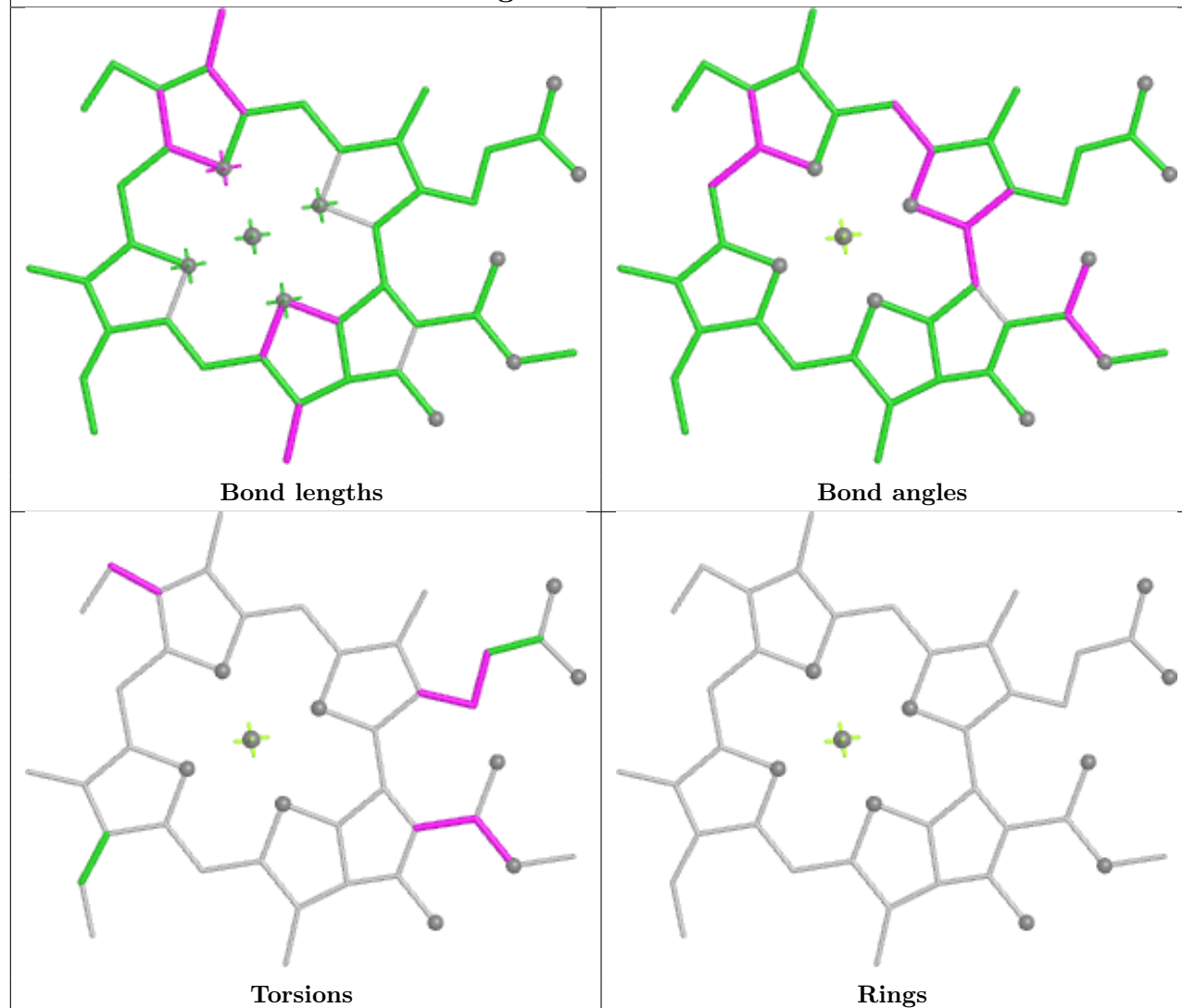
Ligand CLA f 1205	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1137	
	
Bond lengths	Bond angles
	
Torsions	Rings

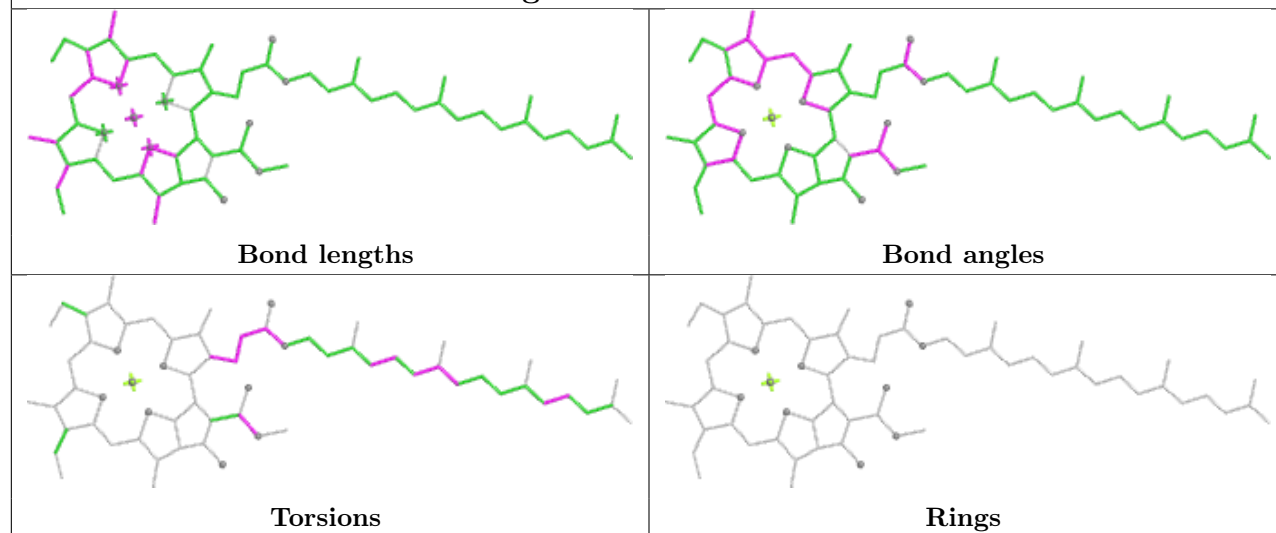
Ligand BCR G 4008	
	
Bond lengths	Bond angles
	
Torsions	Rings

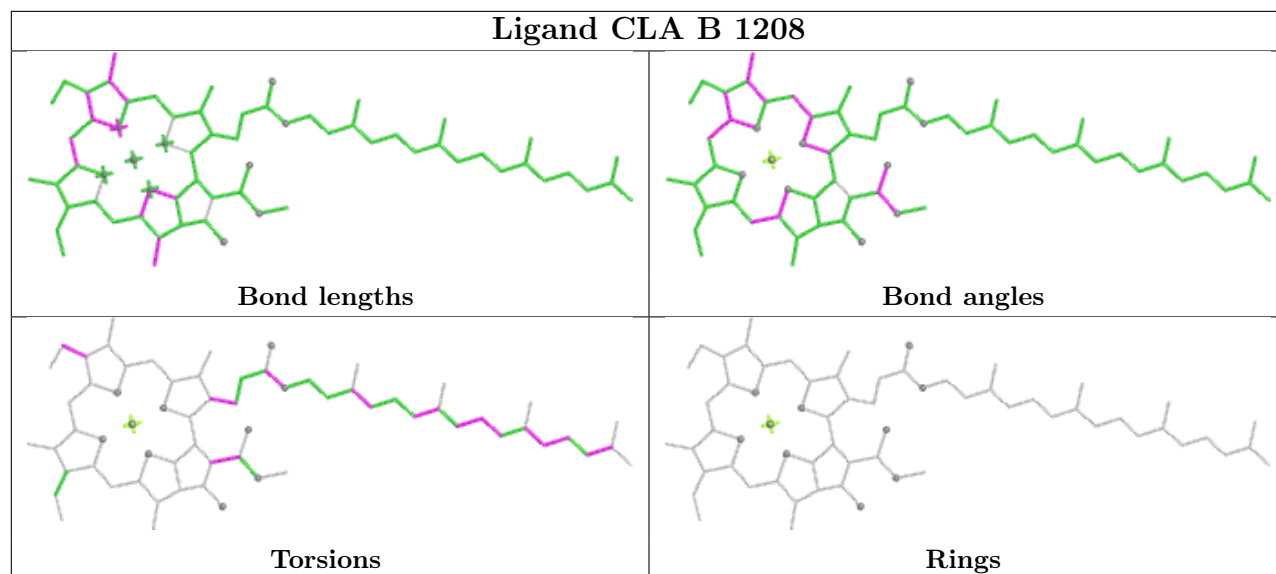
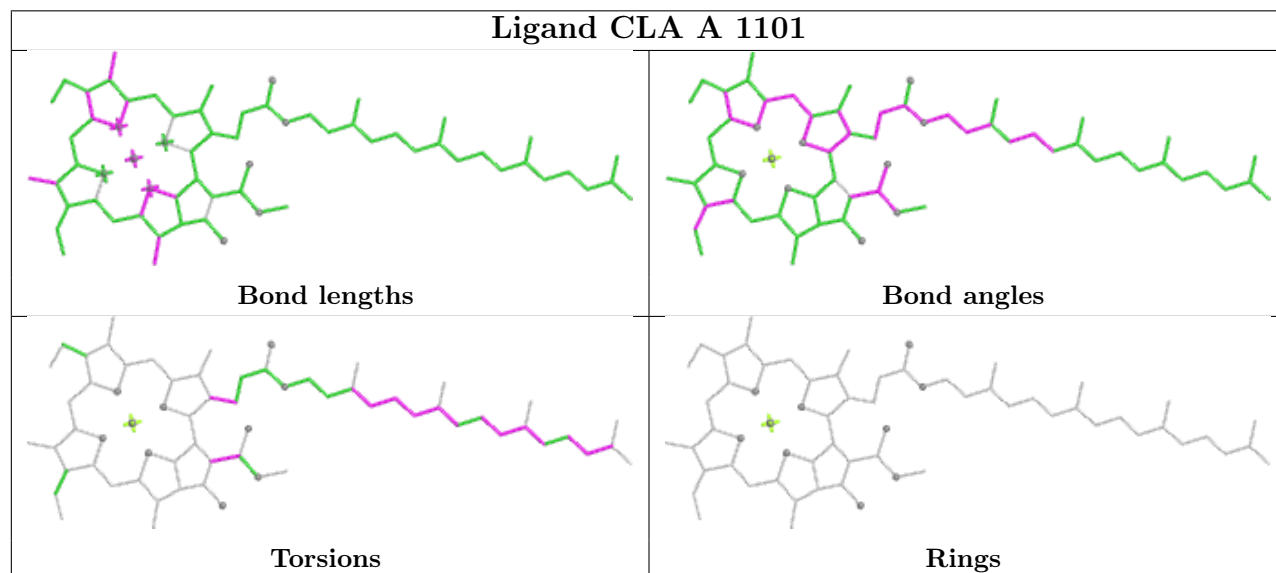


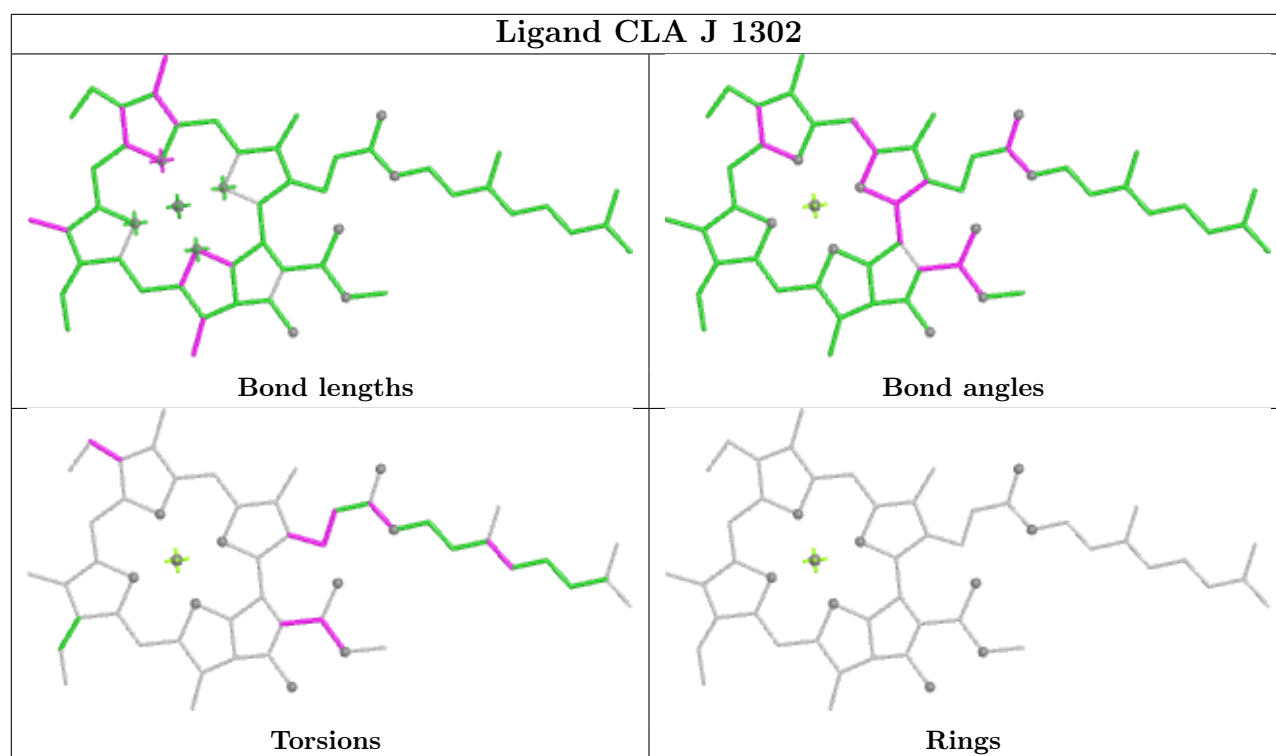
Ligand CLA c 502



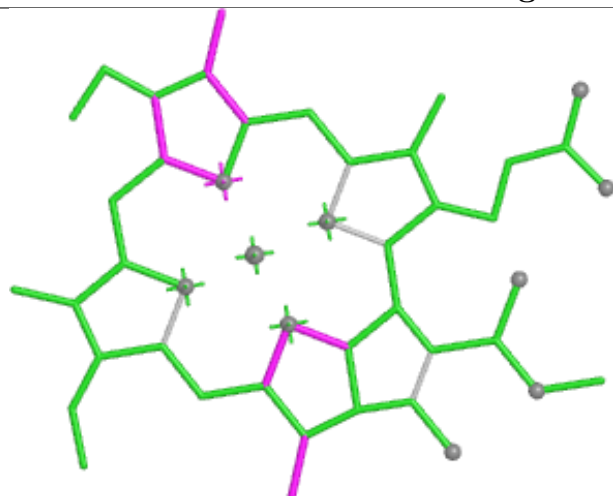
Ligand CLA H 1206



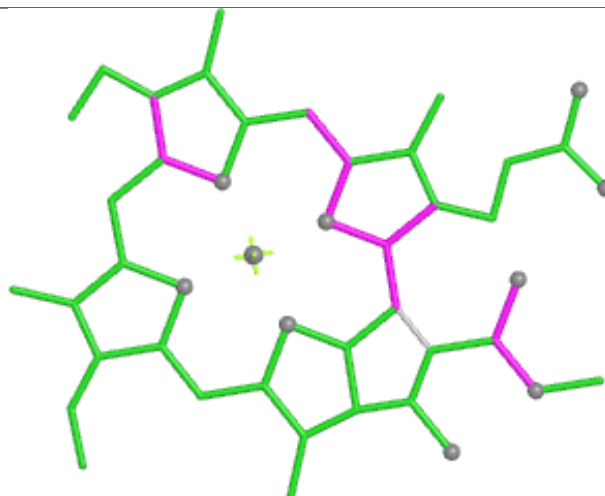
Ligand CLA B 1208**Ligand CLA A 1101**



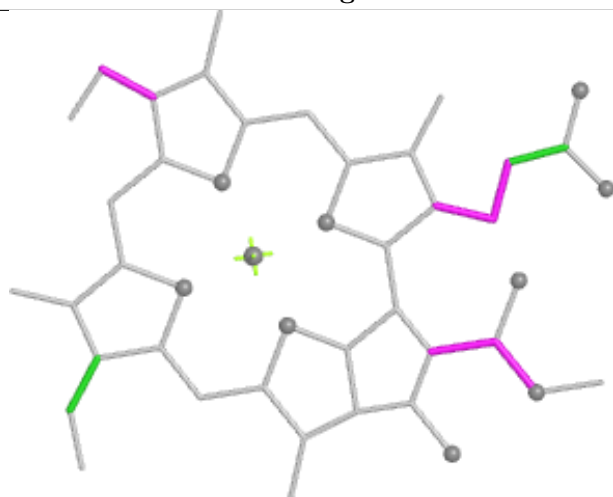
Ligand CLA 1 503



Bond lengths



Bond angles

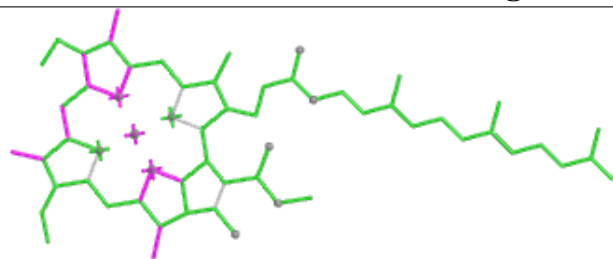


Torsions

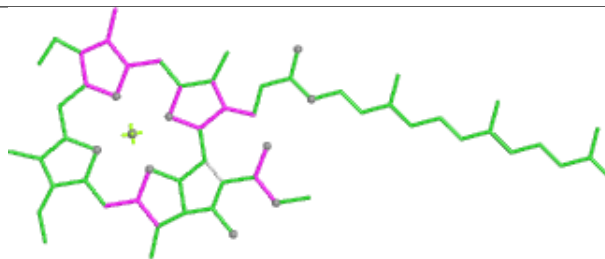


Rings

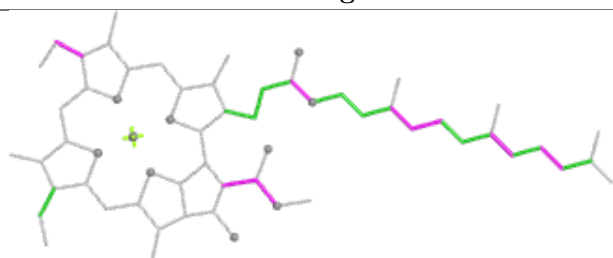
Ligand CLA A 1124



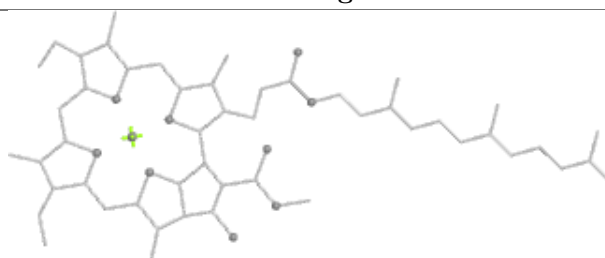
Bond lengths



Bond angles

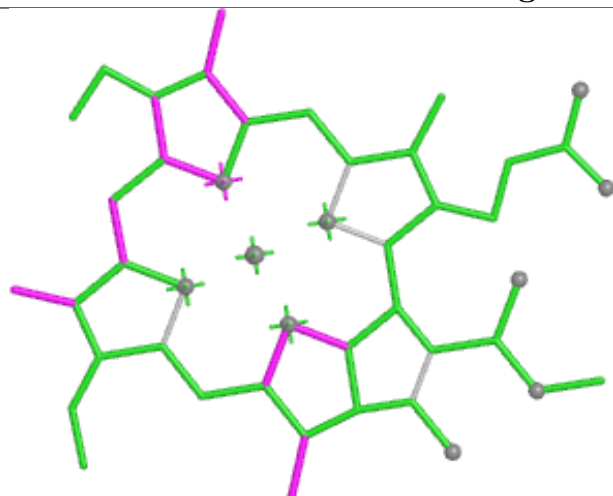


Torsions

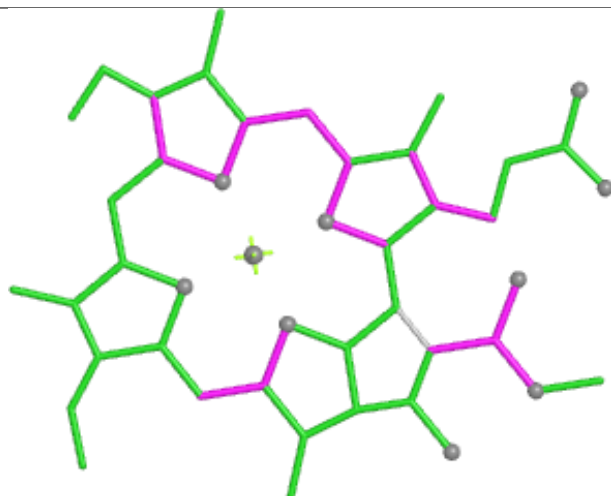


Rings

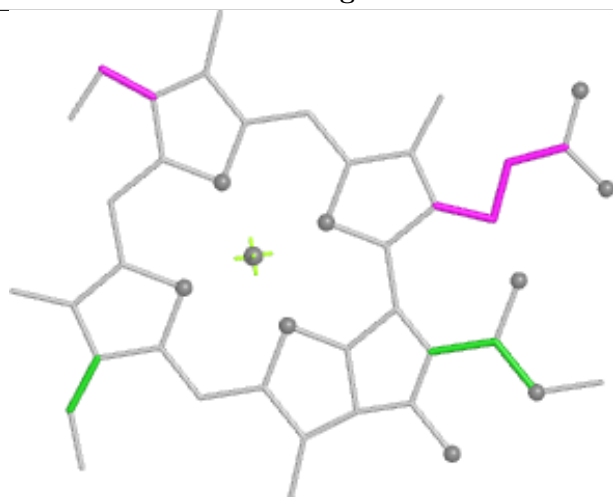
Ligand CLA 3 501



Bond lengths



Bond angles

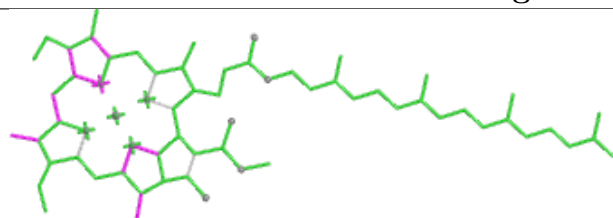


Torsions

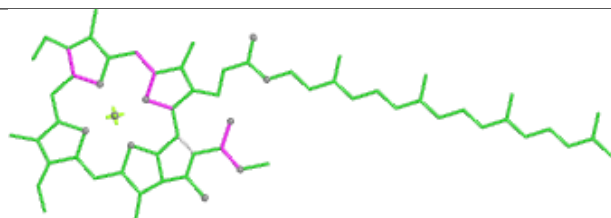


Rings

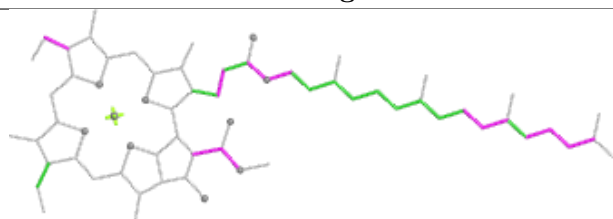
Ligand CLA f 1207



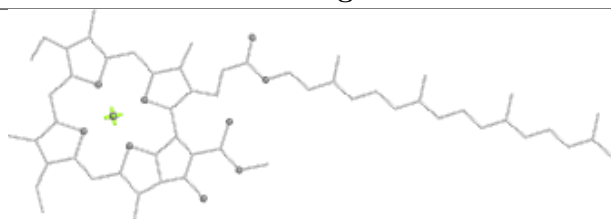
Bond lengths



Bond angles

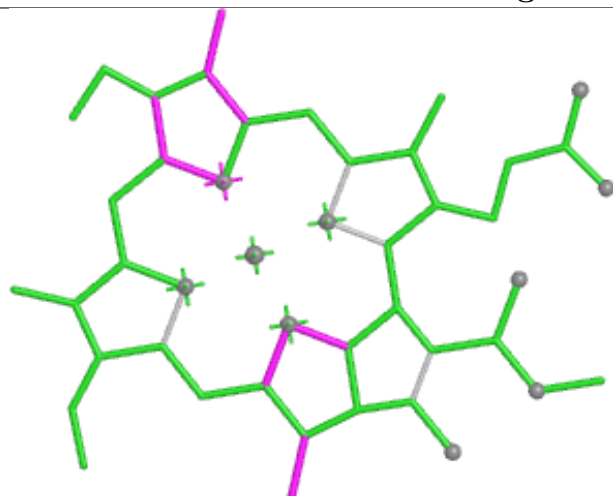


Torsions

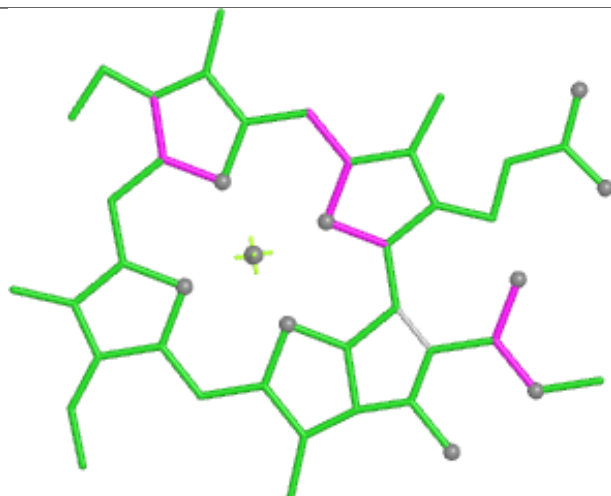


Rings

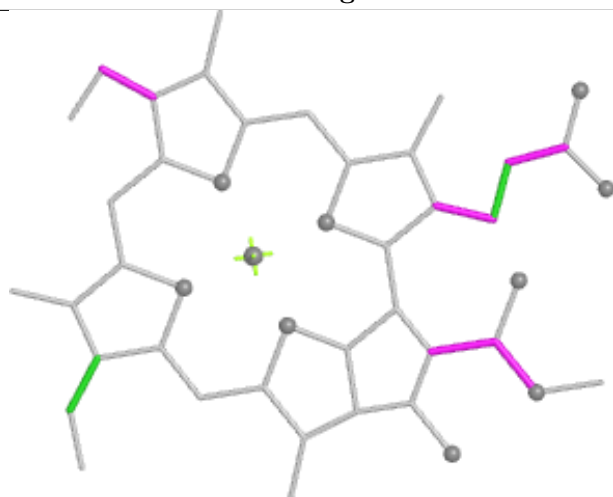
Ligand CLA d 518



Bond lengths



Bond angles

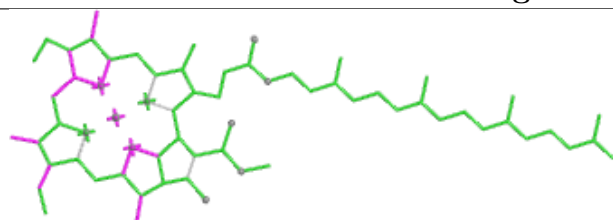


Torsions

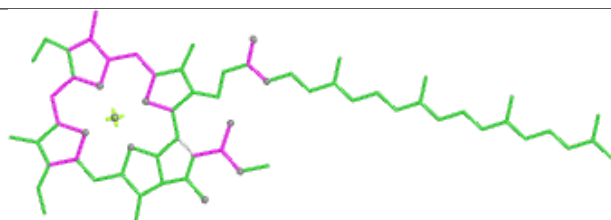


Rings

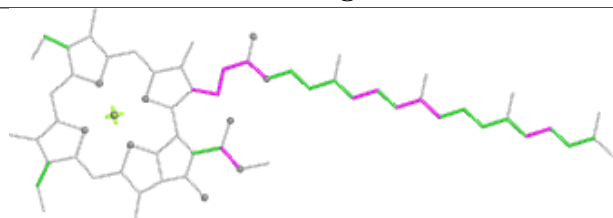
Ligand CLA f 1206



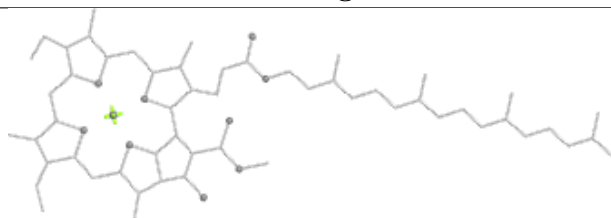
Bond lengths



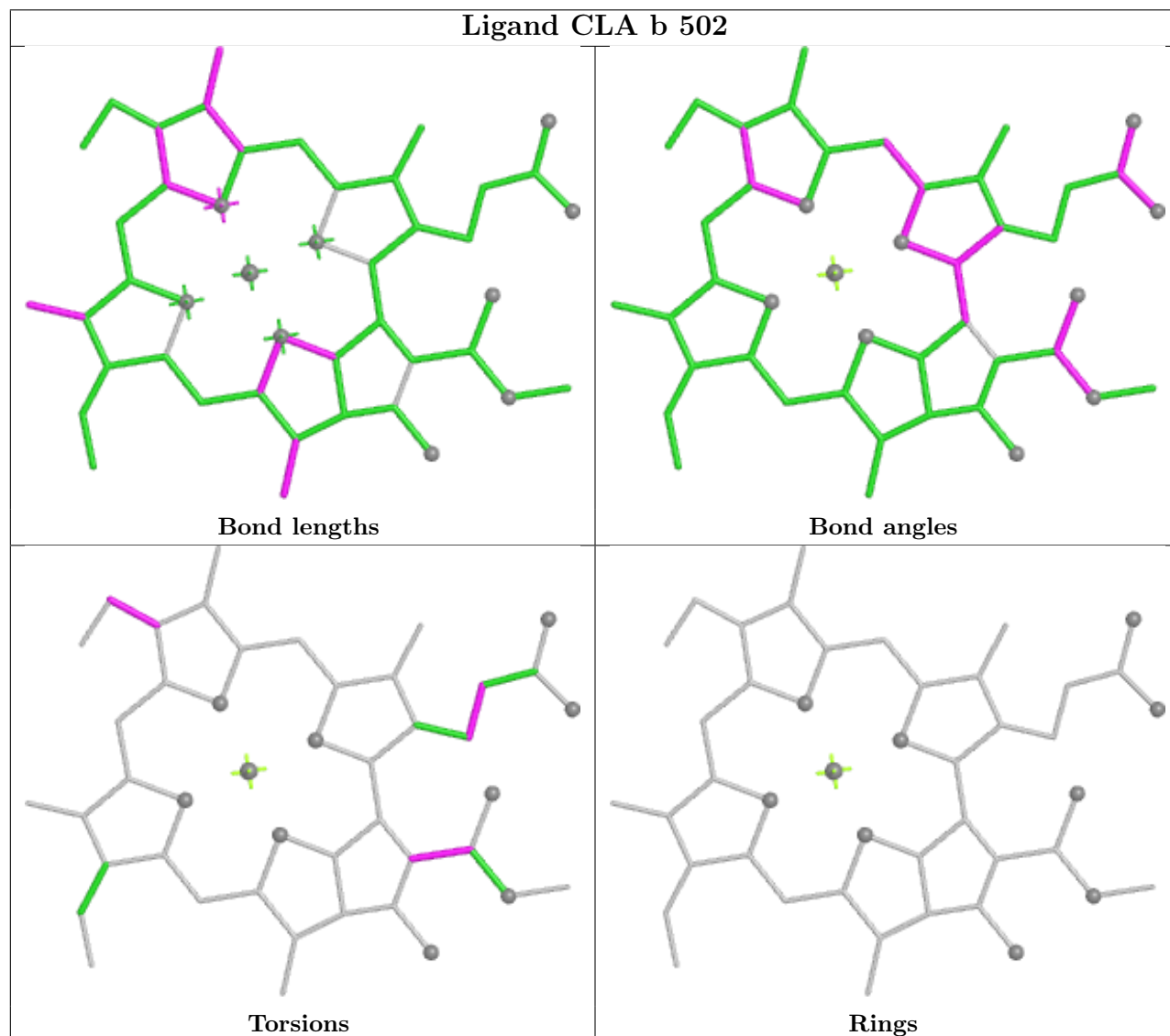
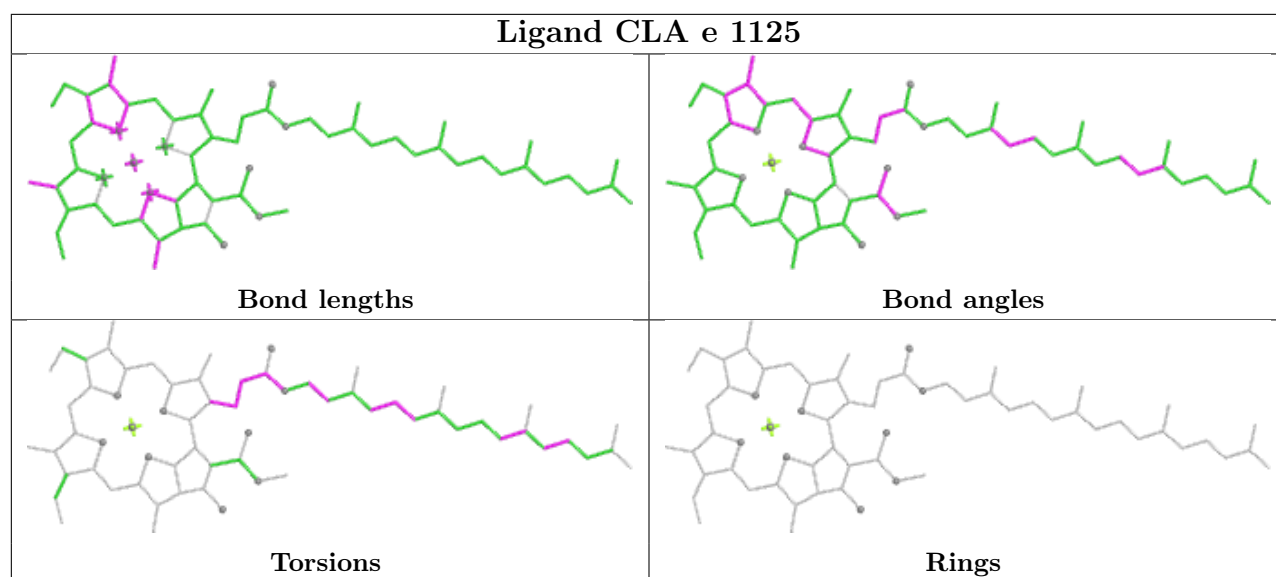
Bond angles

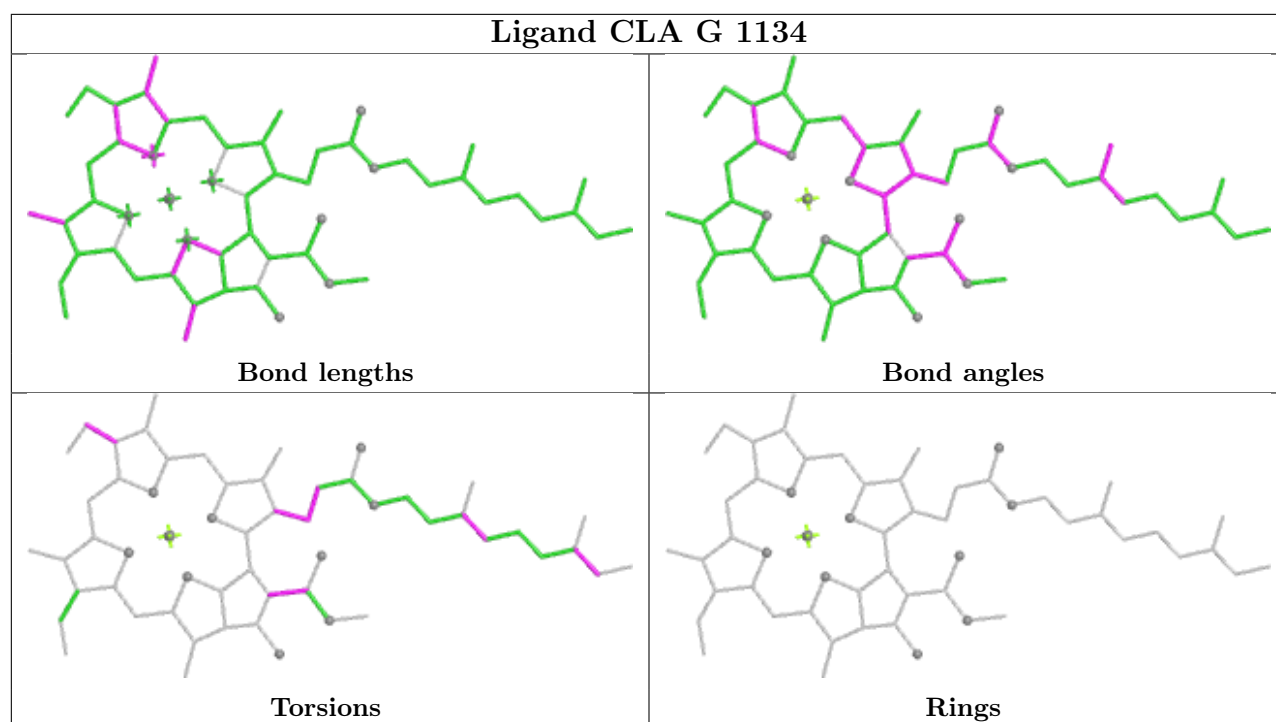


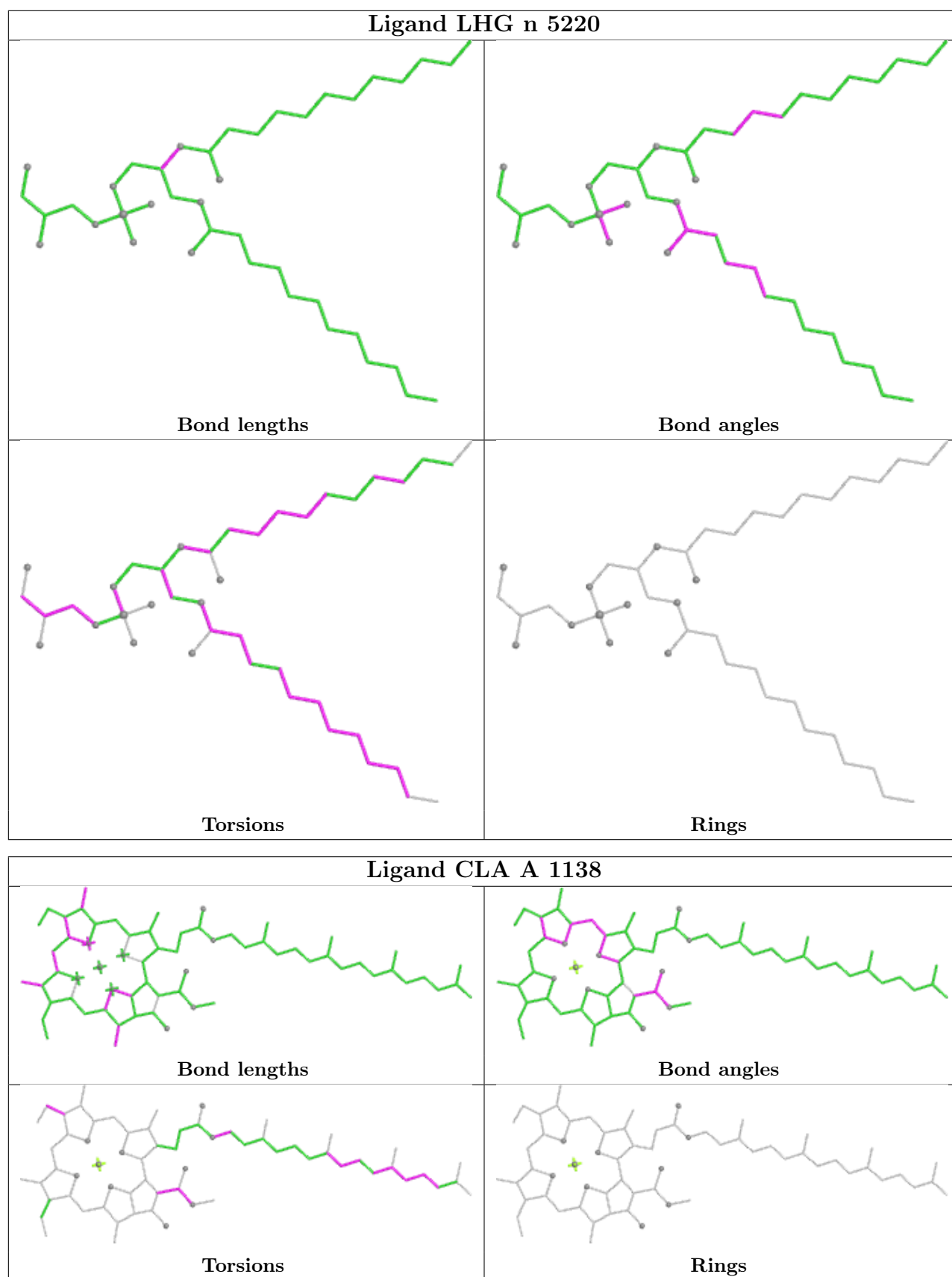
Torsions

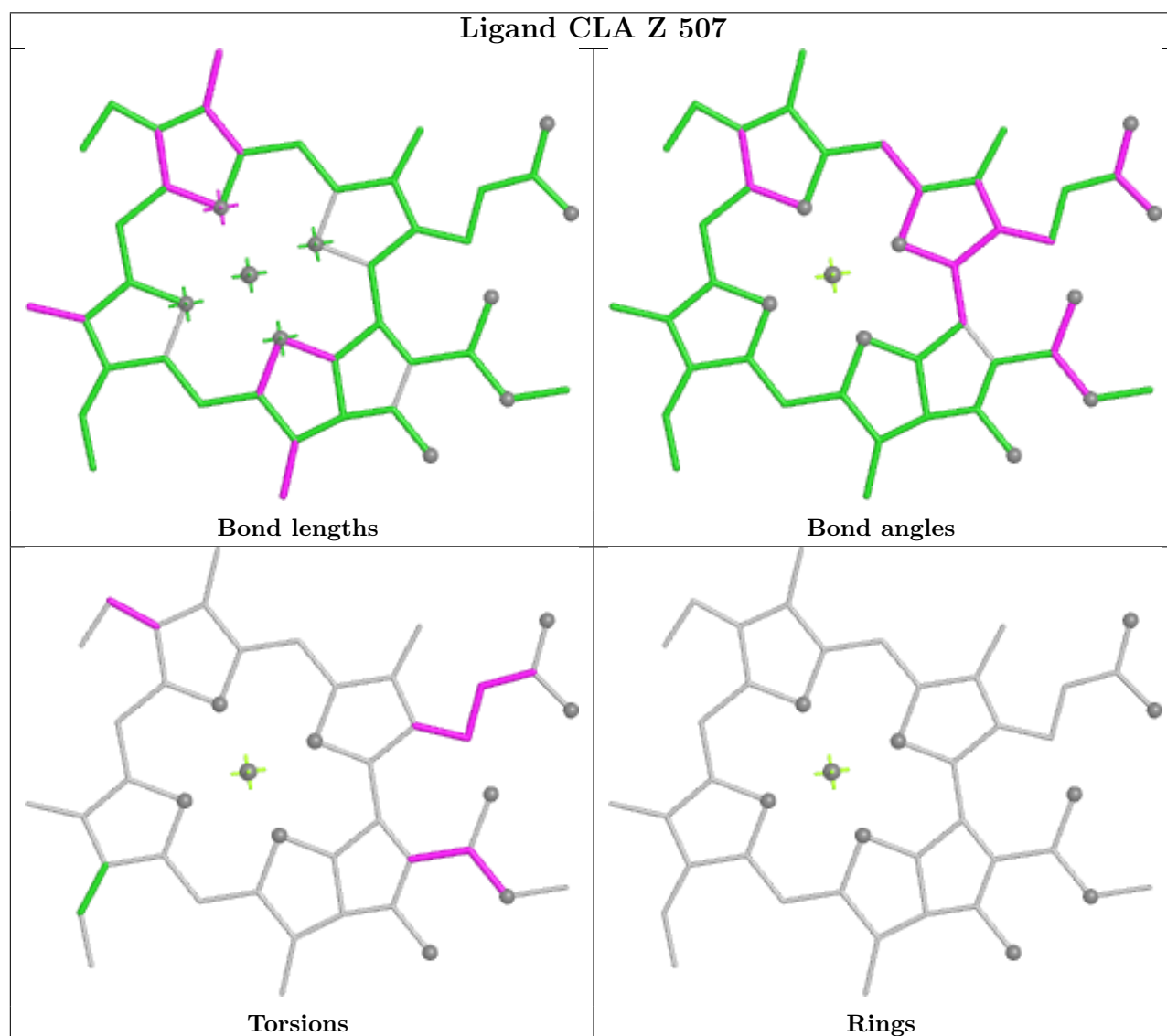
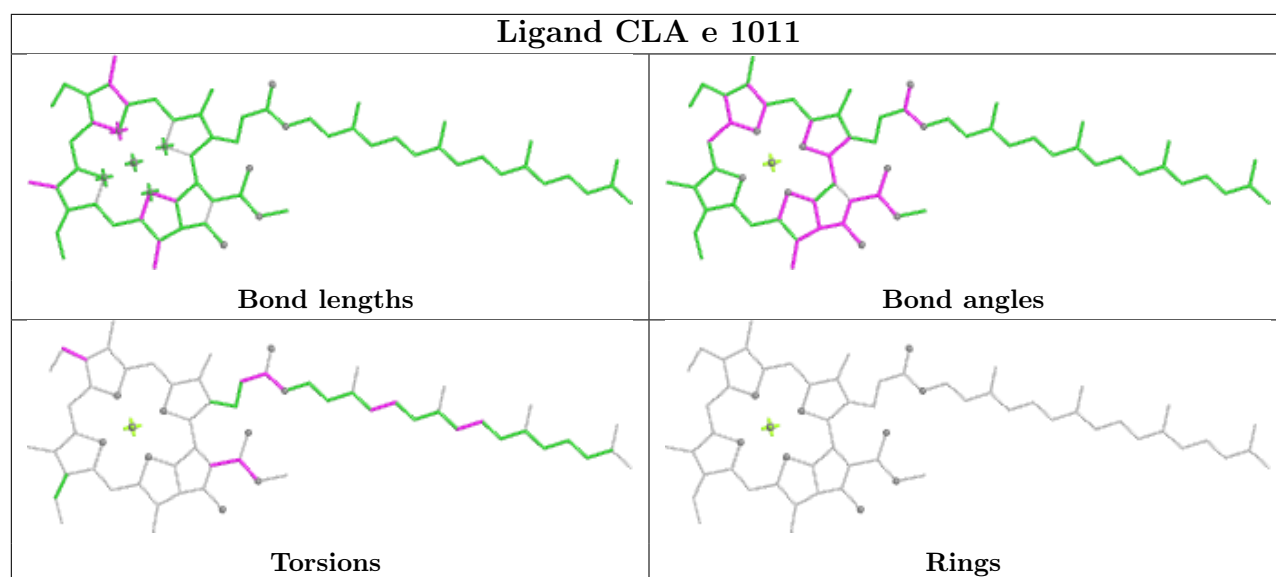


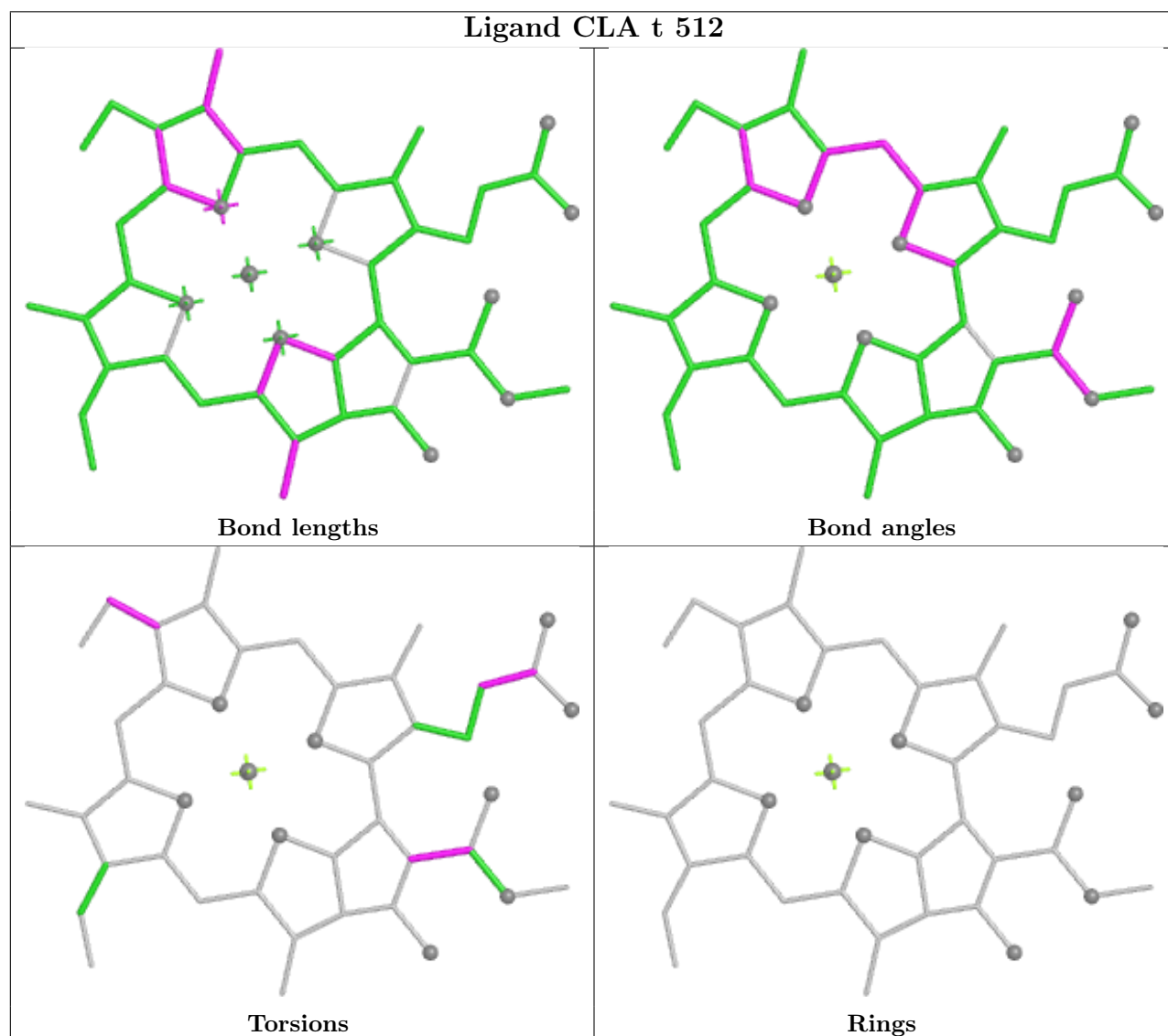
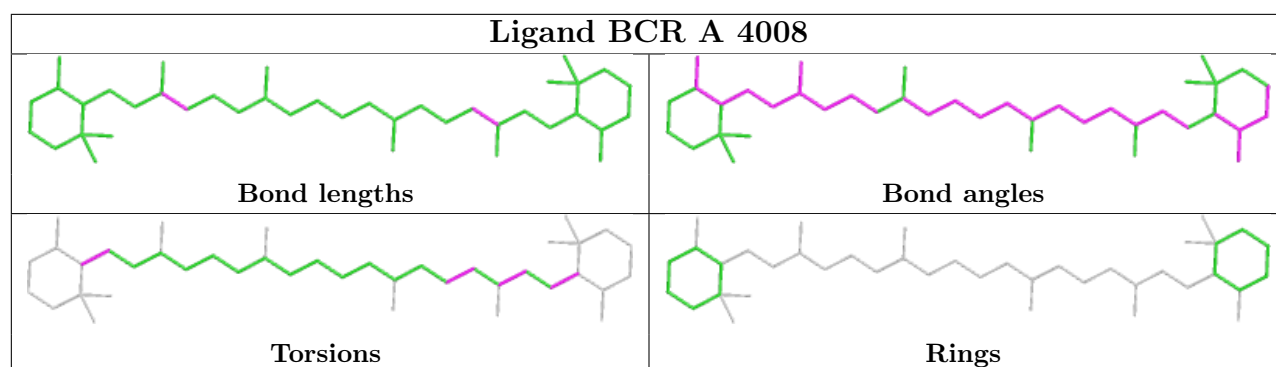
Rings

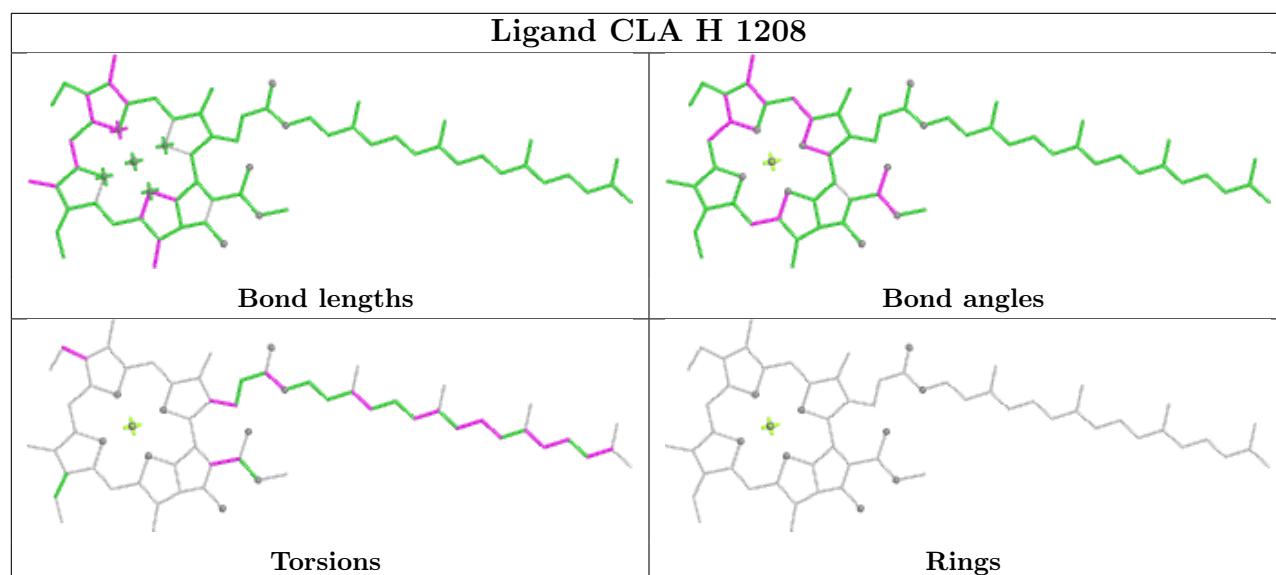
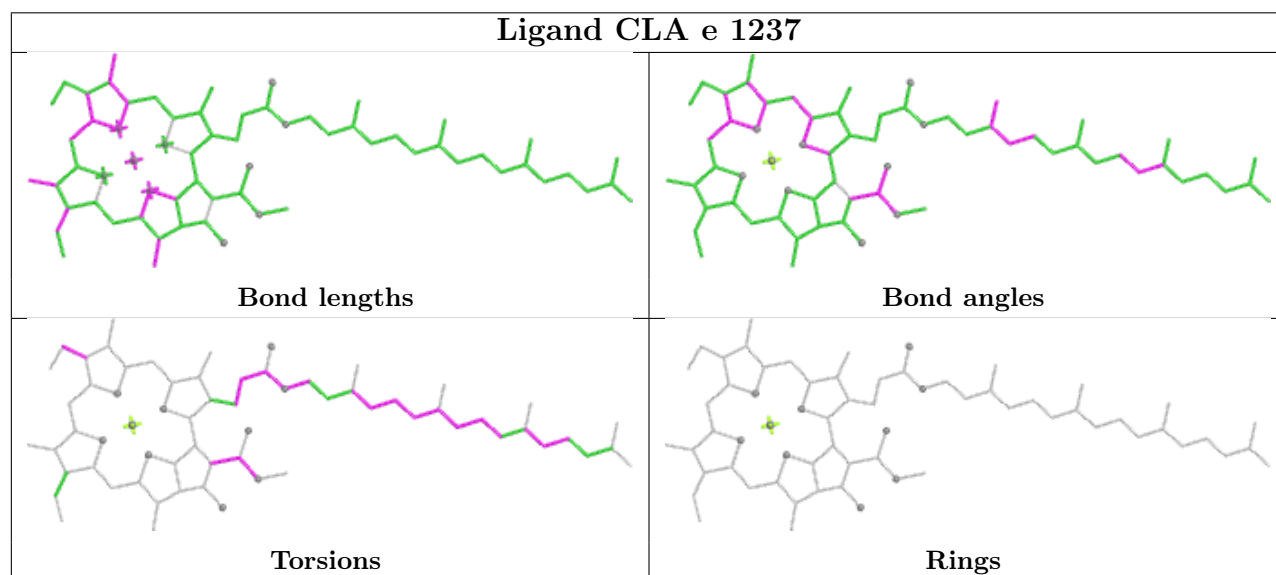
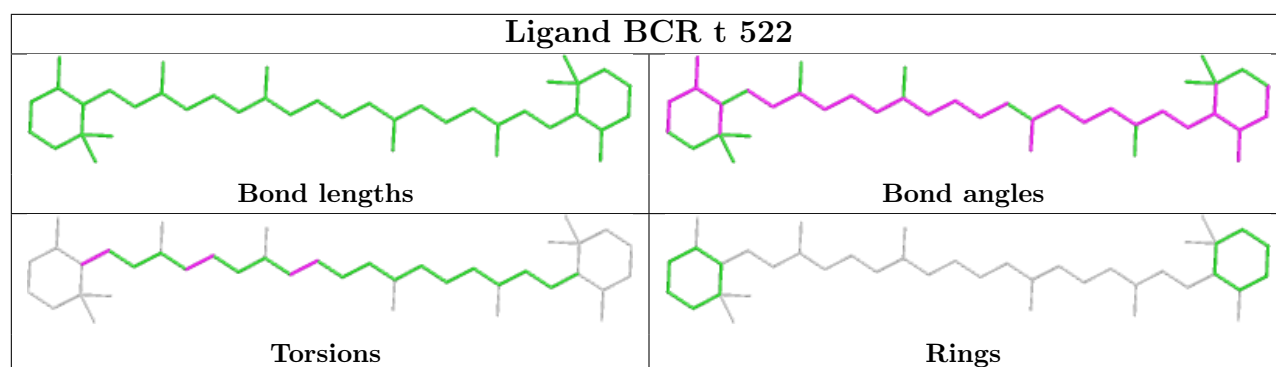




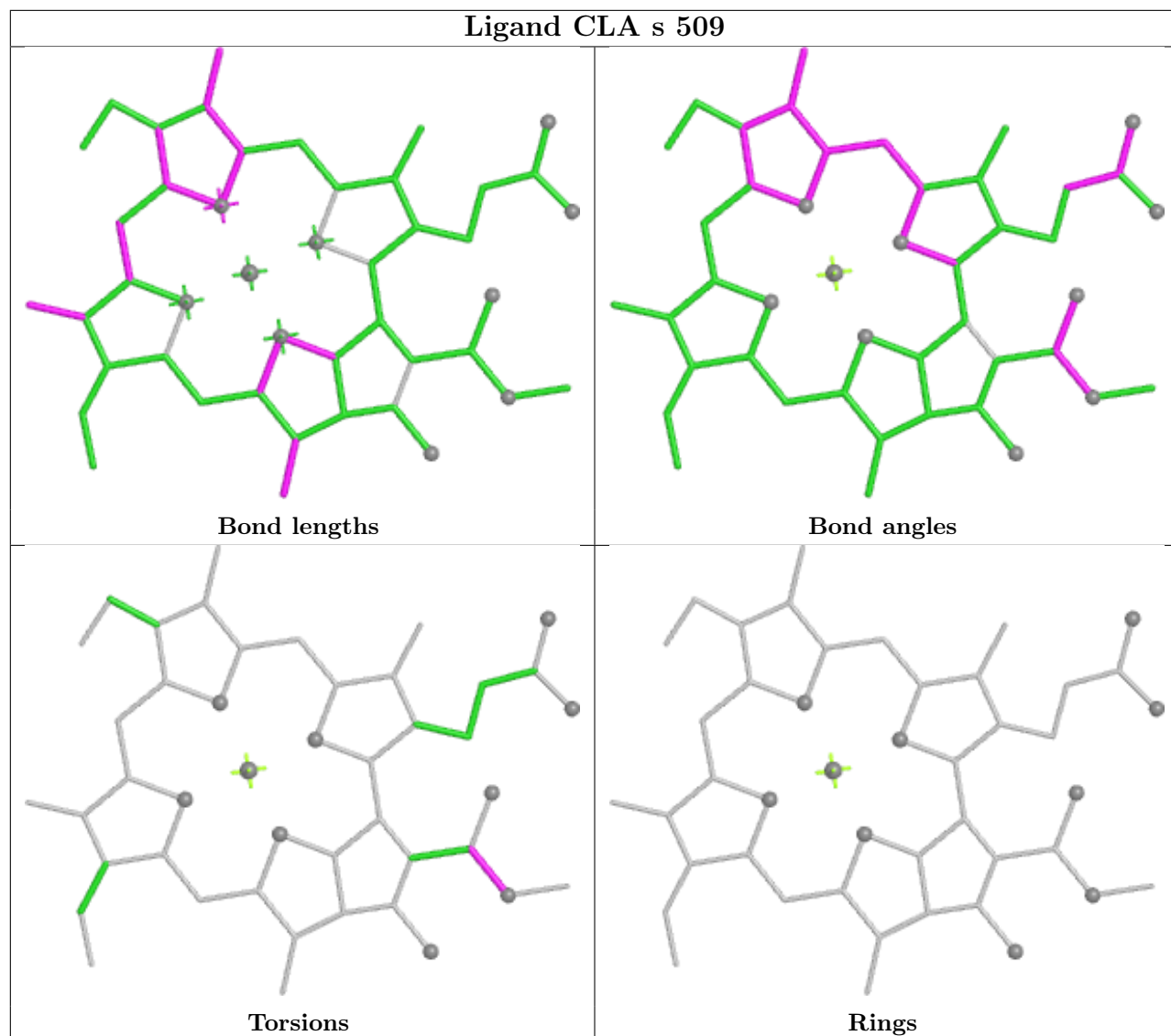


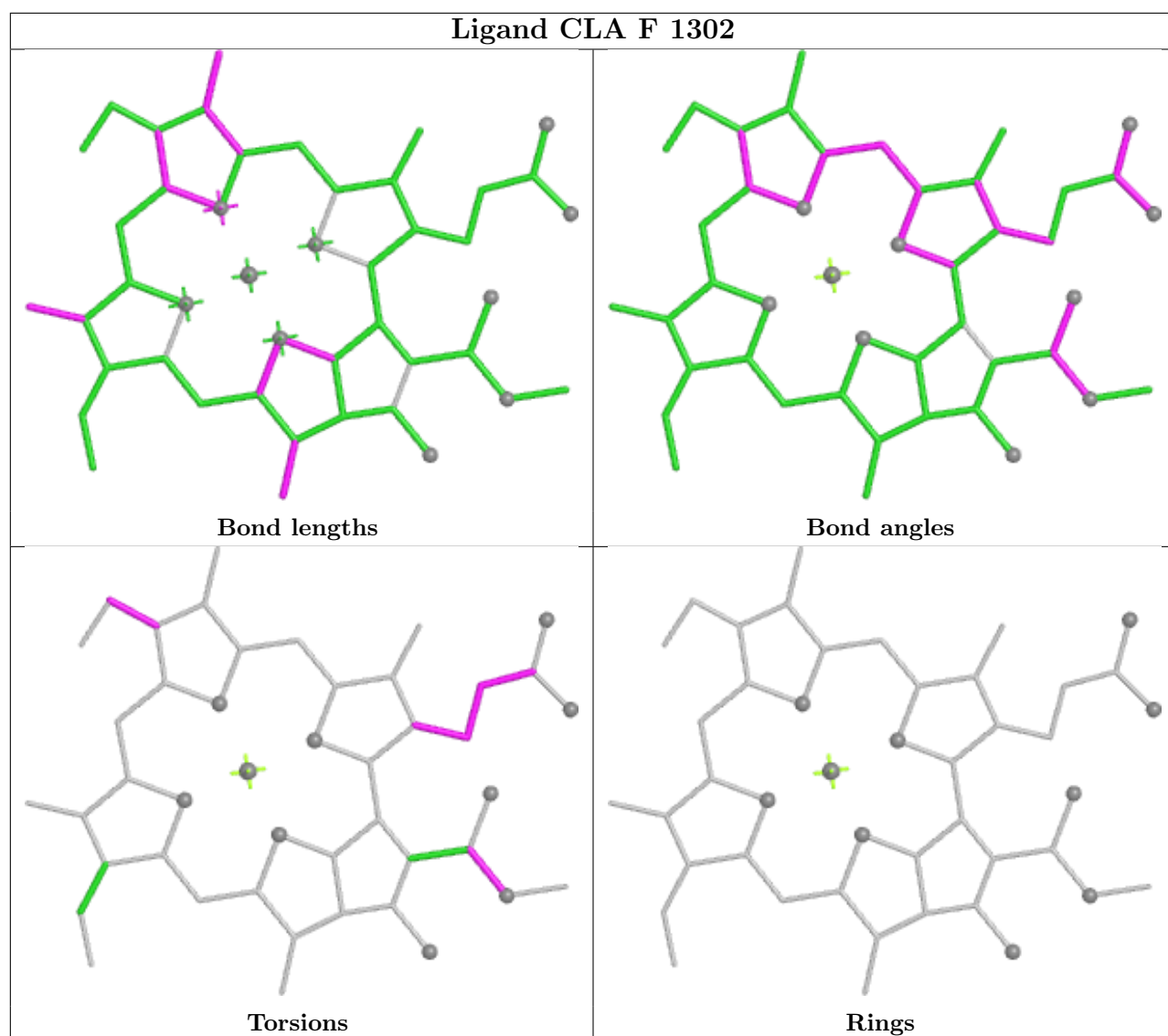




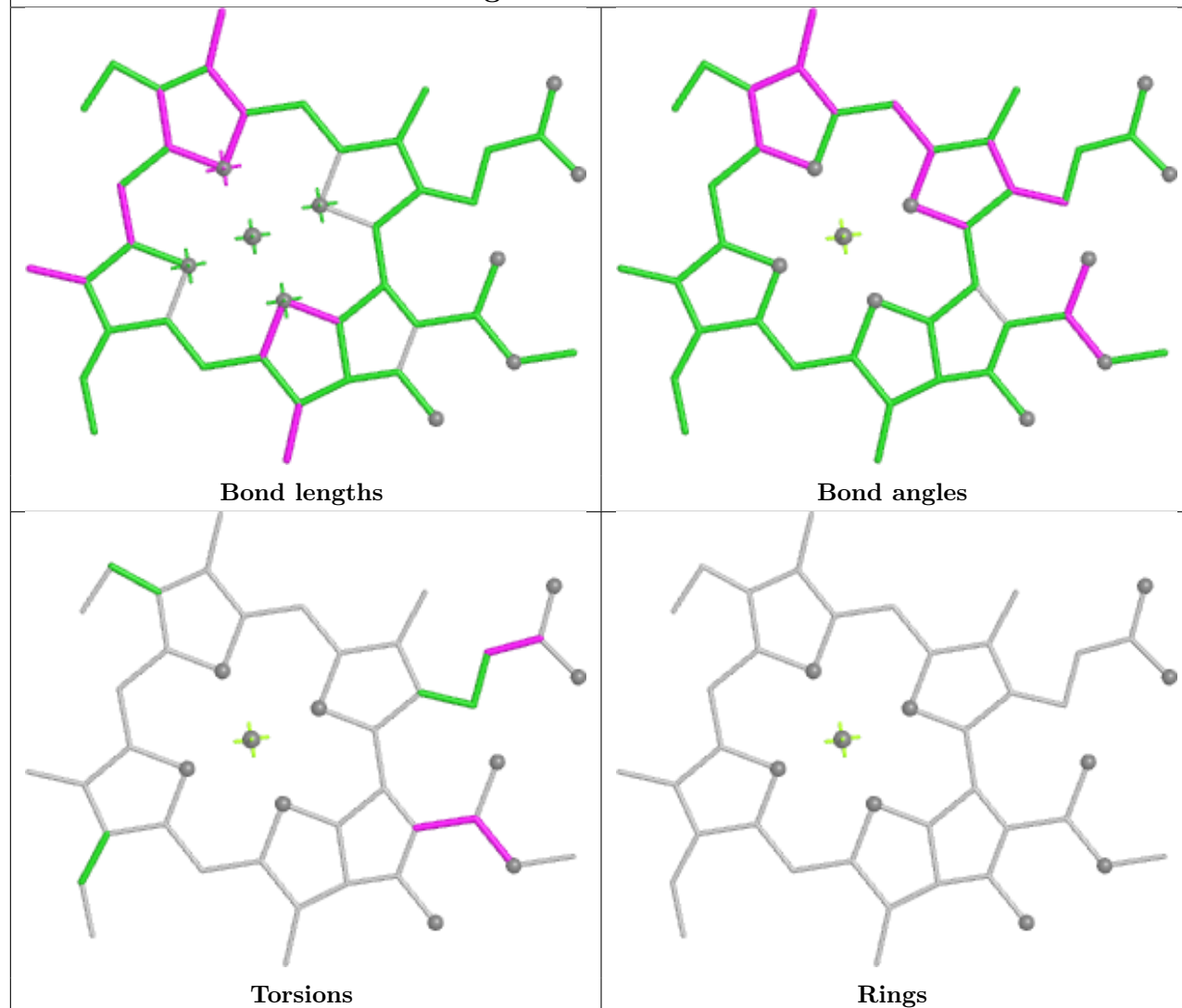


Ligand CLA s 509

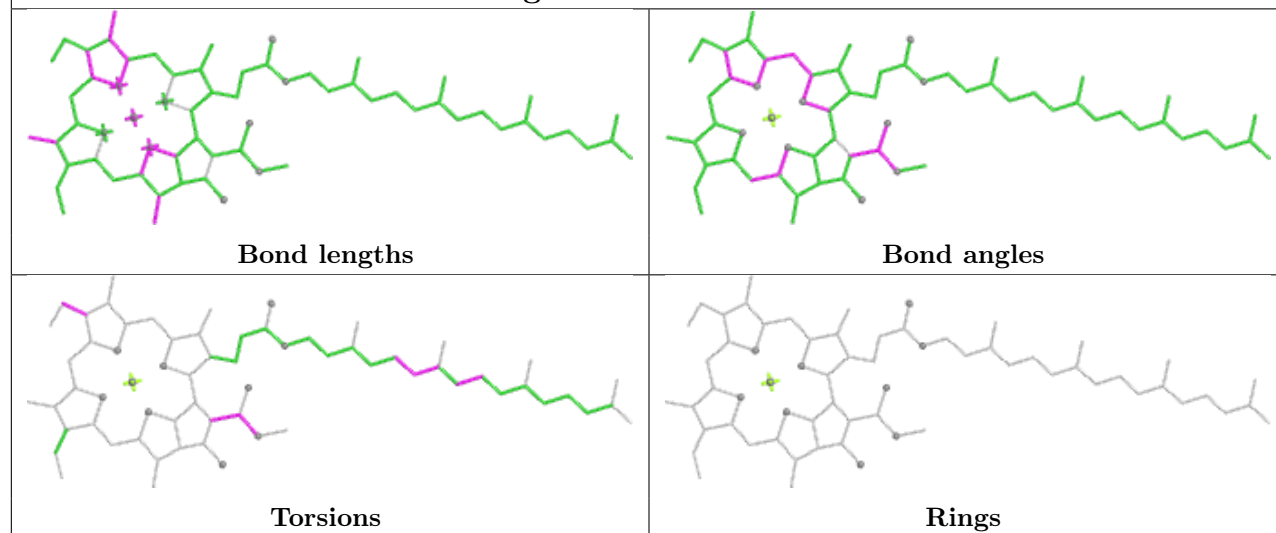


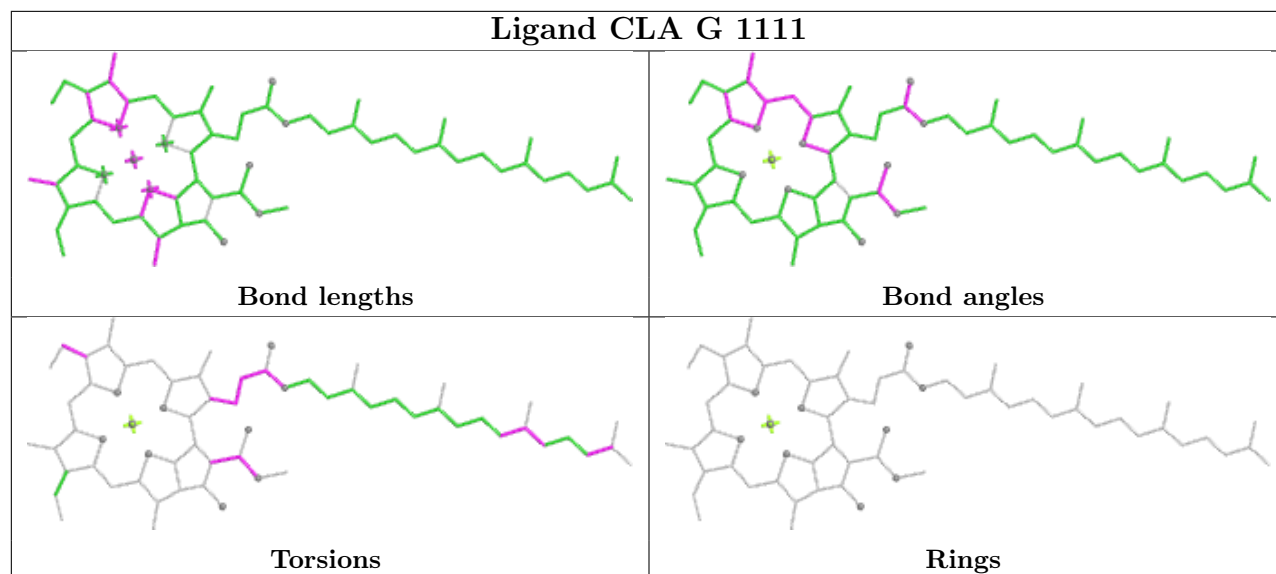
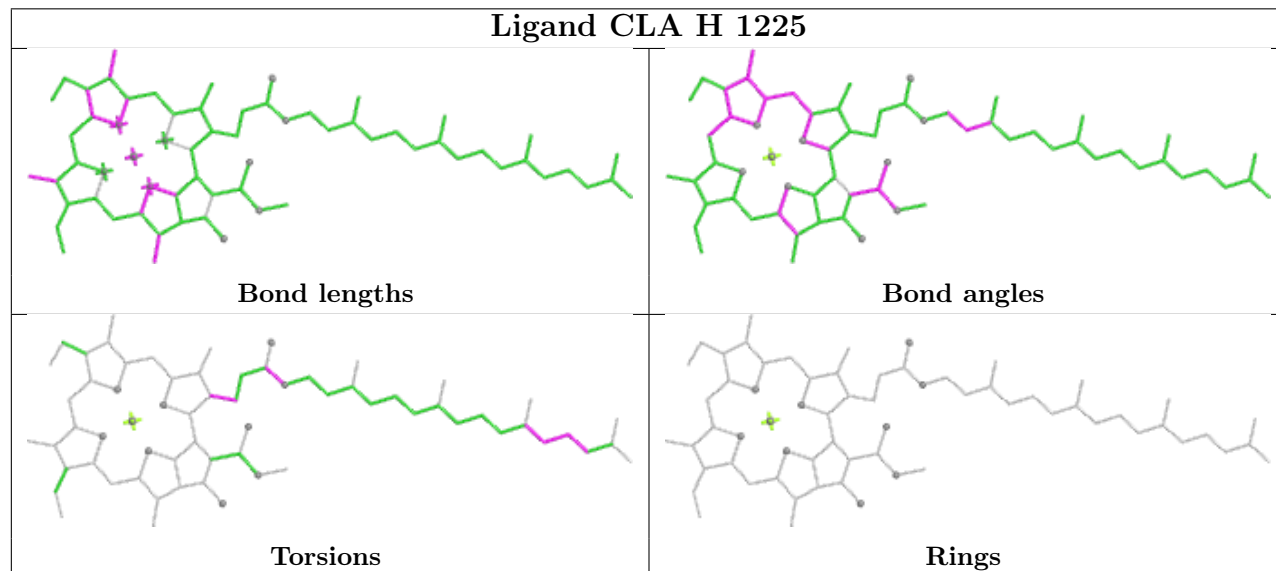


Ligand CLA A 1801

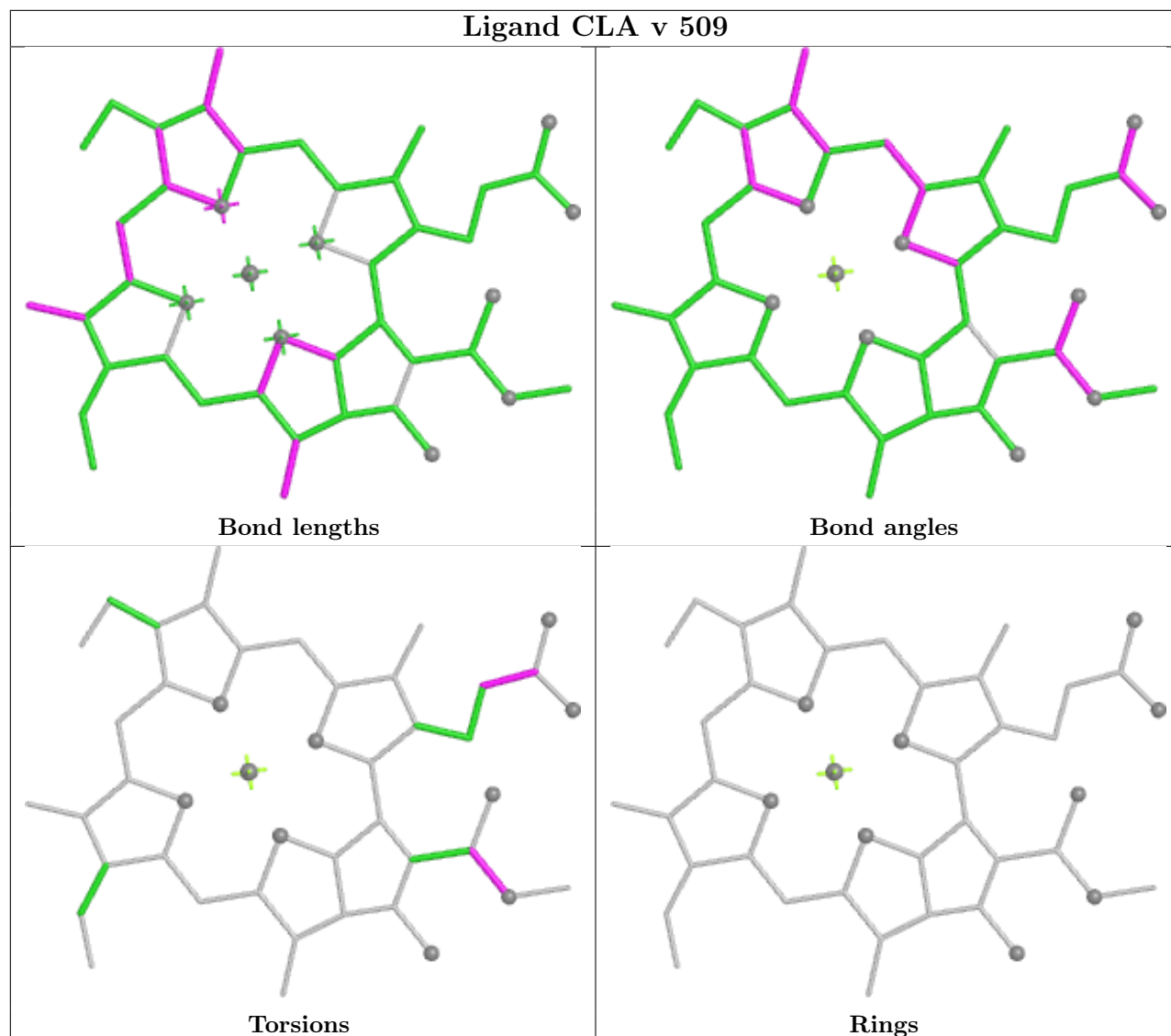


Ligand CLA B 1235

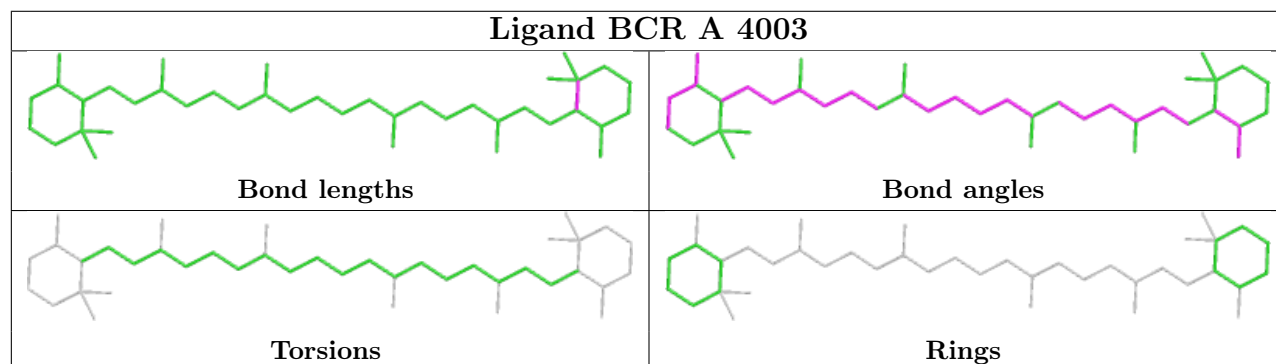


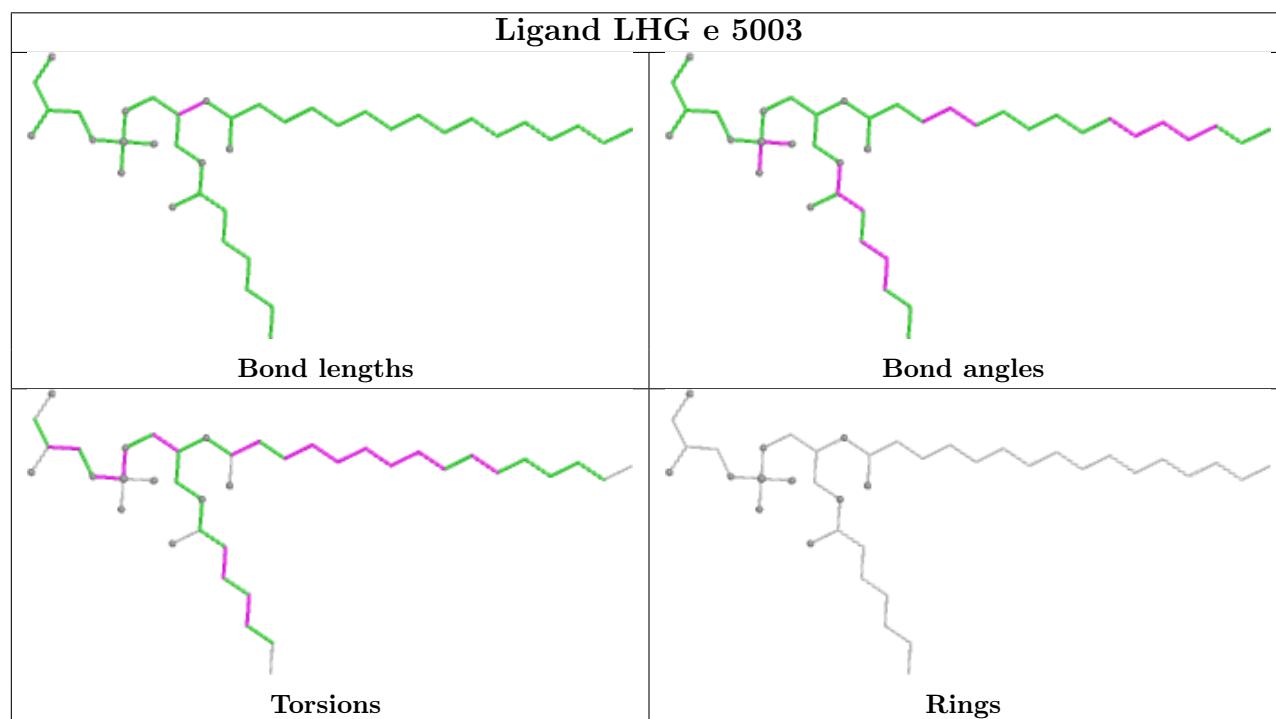
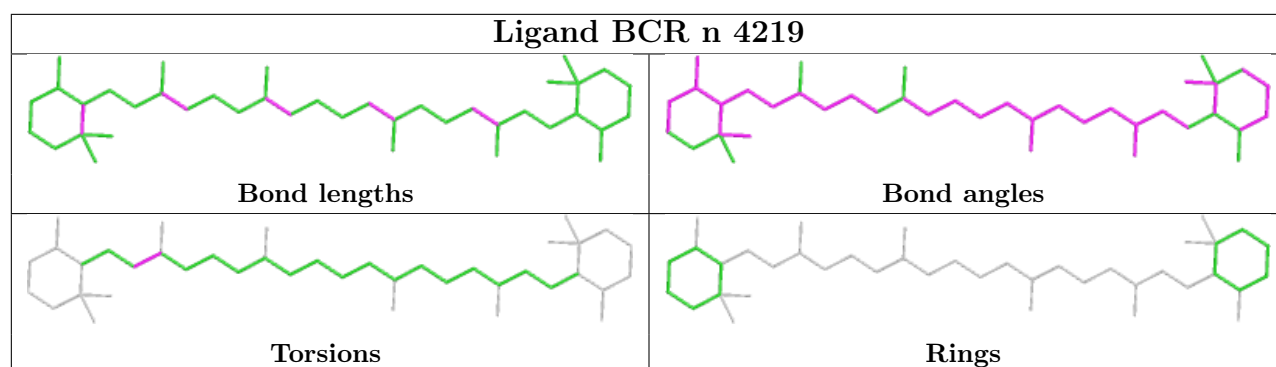
Ligand CLA G 1111**Ligand CLA H 1225**

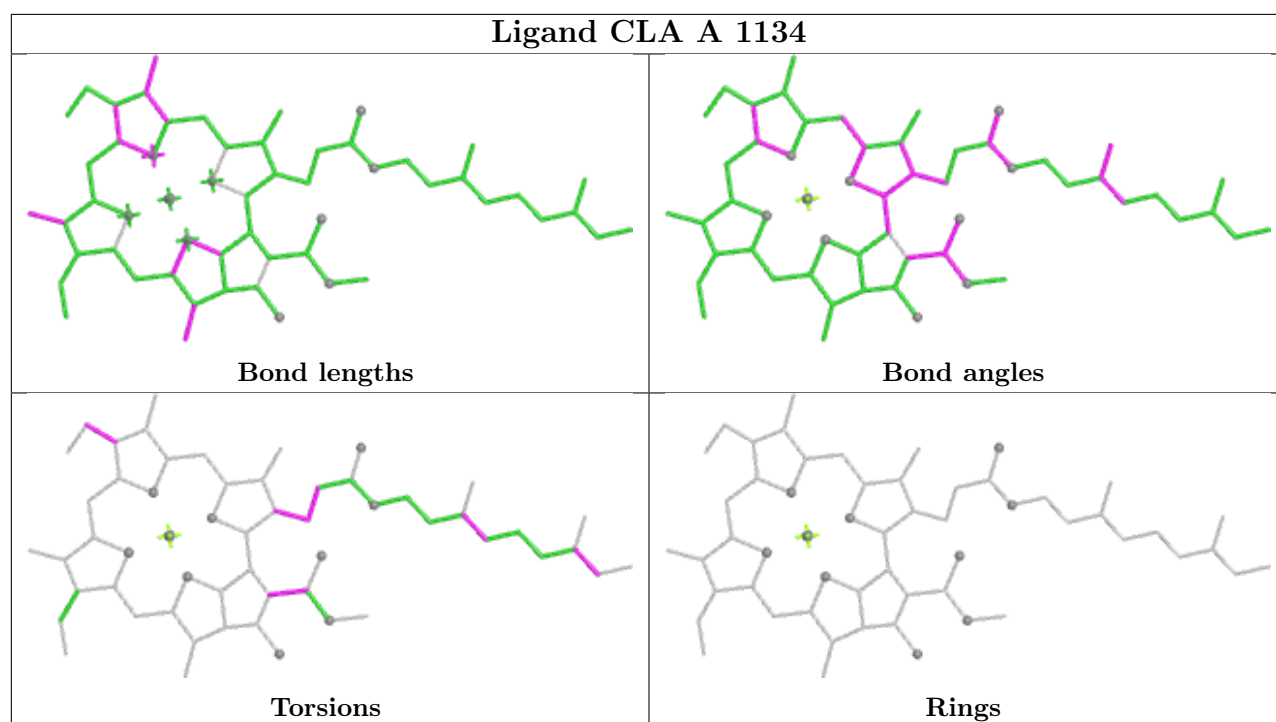
Ligand CLA v 509



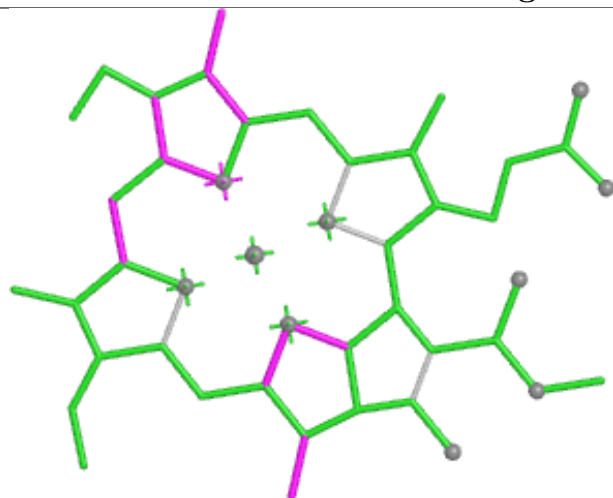
Ligand BCR A 4003



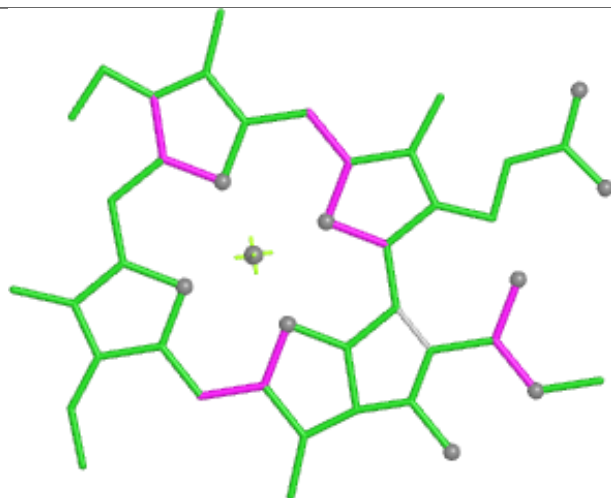




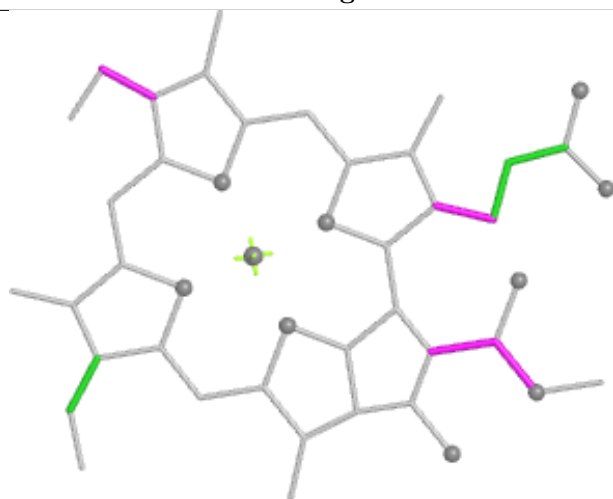
Ligand CLA 4 504



Bond lengths



Bond angles

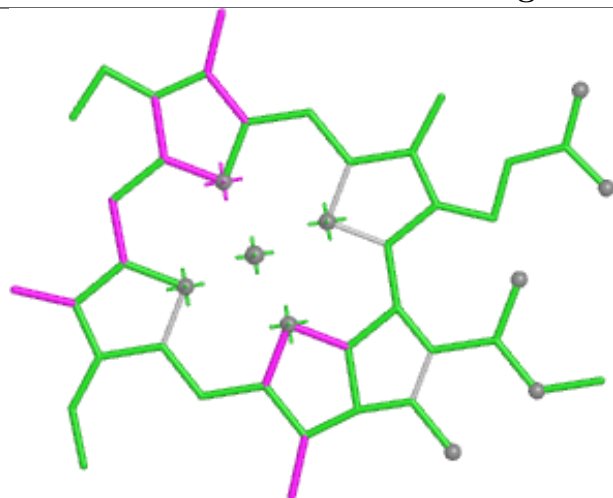


Torsions

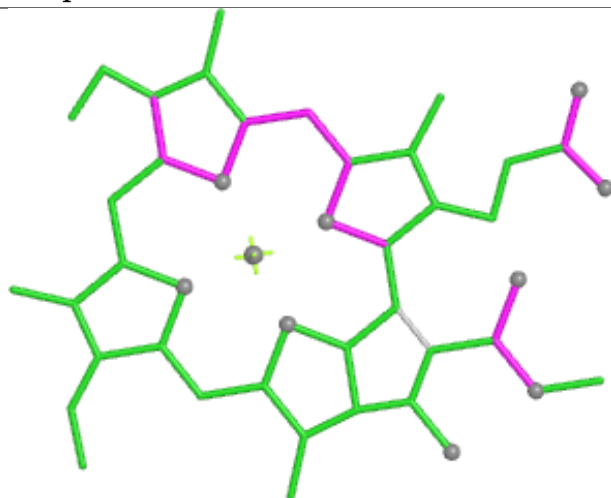


Rings

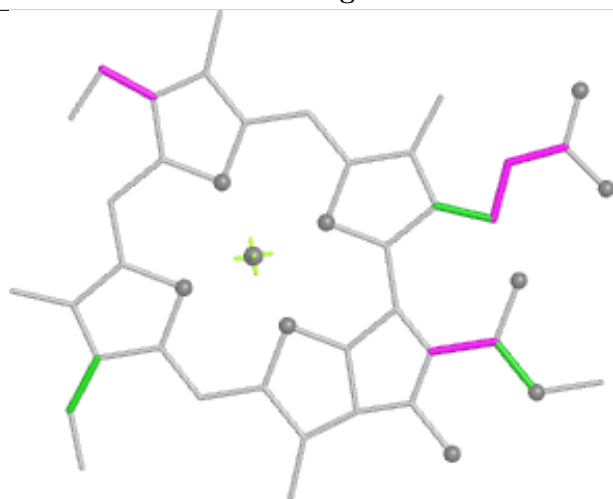
Ligand CLA q 513



Bond lengths



Bond angles

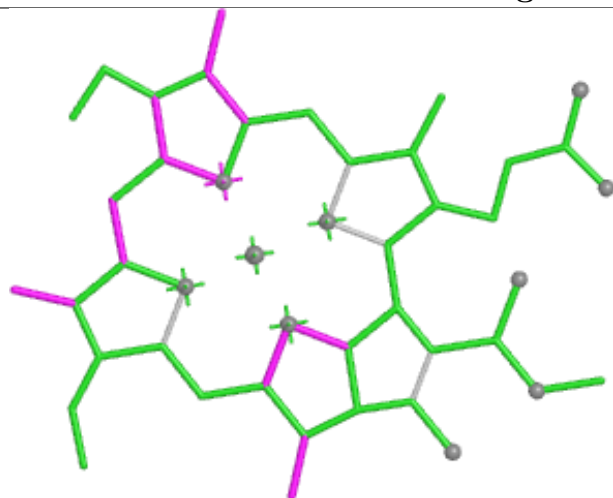


Torsions

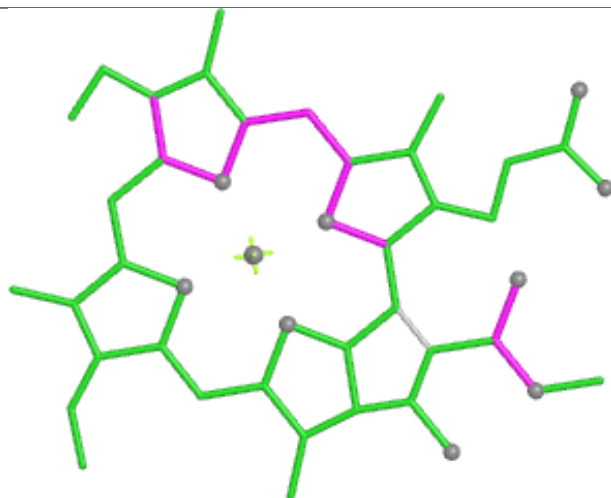


Rings

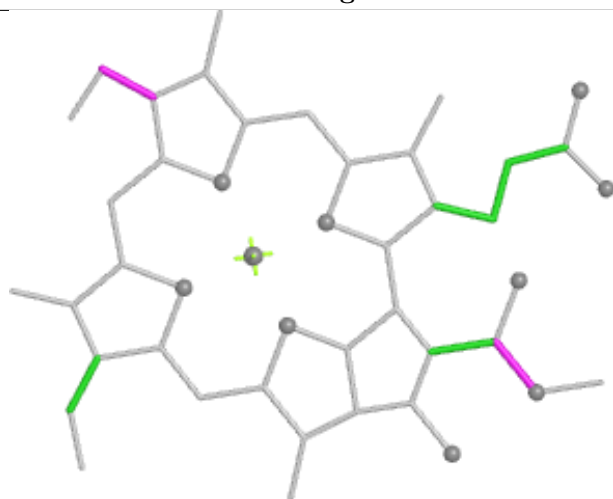
Ligand CLA Z 513



Bond lengths



Bond angles

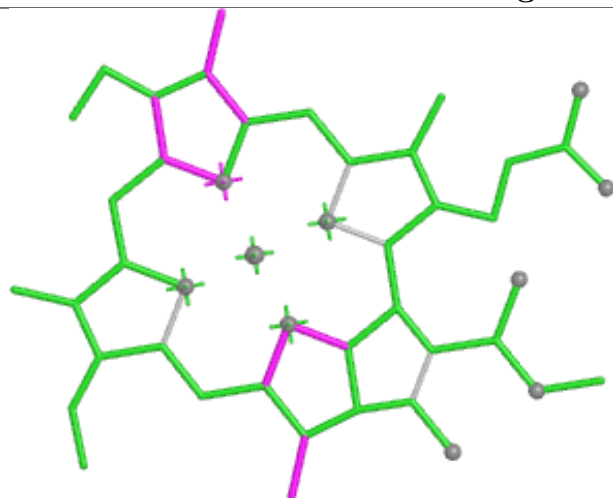


Torsions

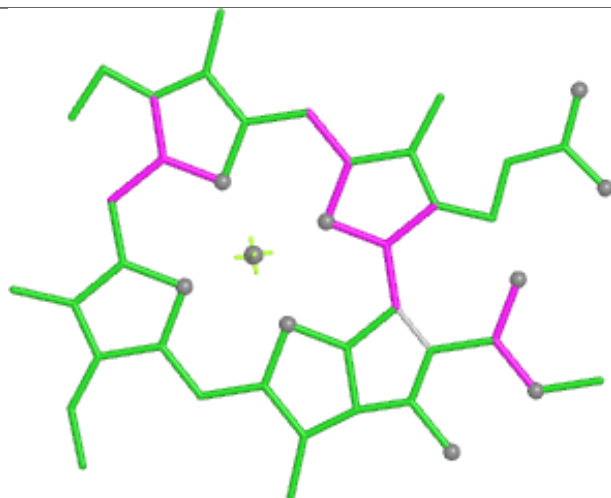


Rings

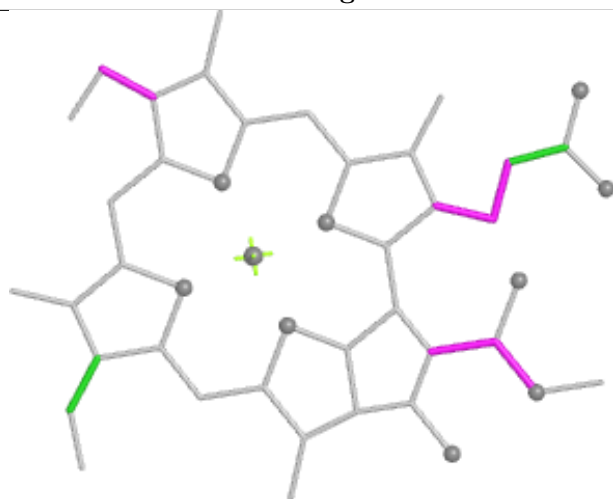
Ligand CLA u 502



Bond lengths



Bond angles

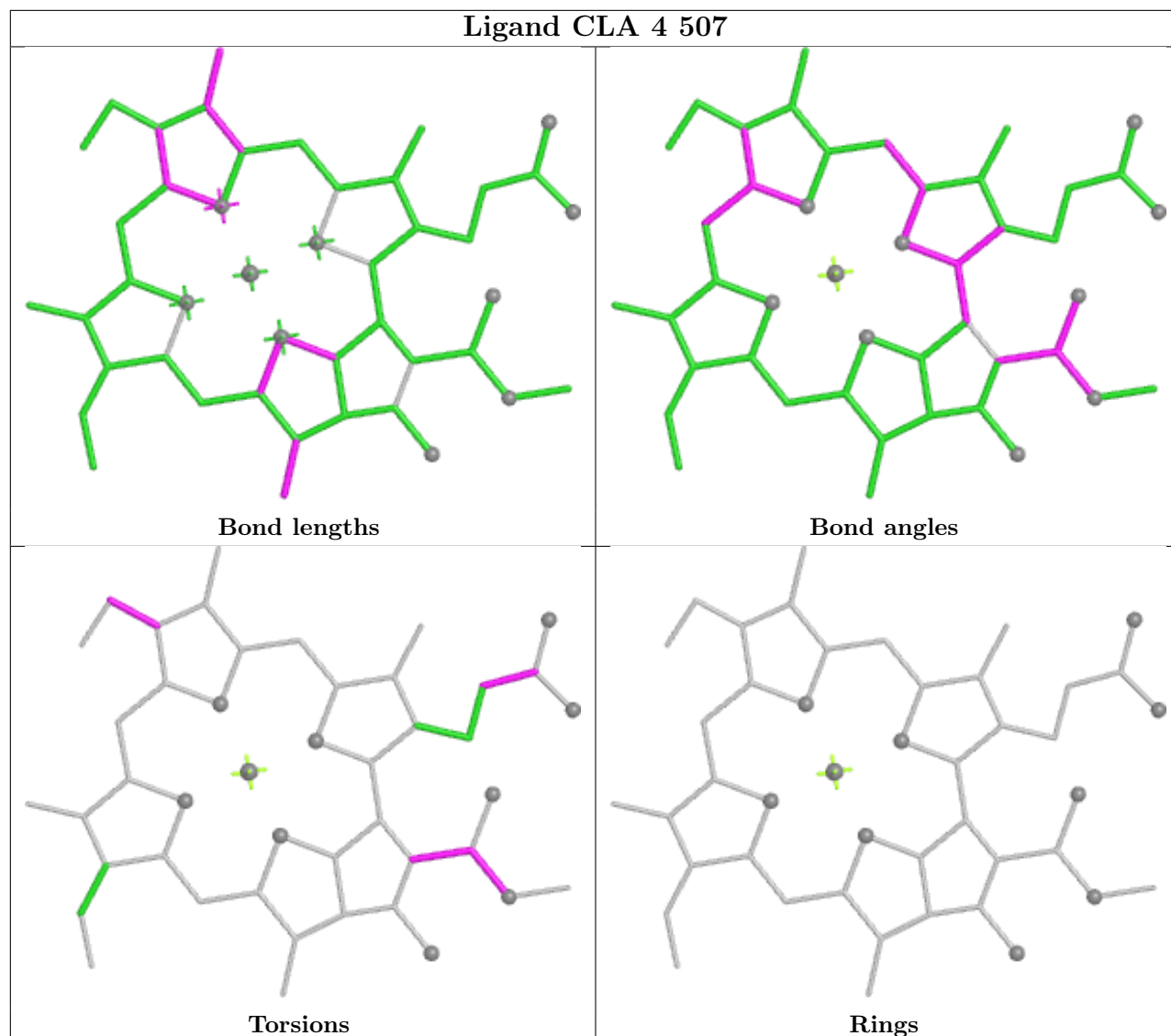


Torsions

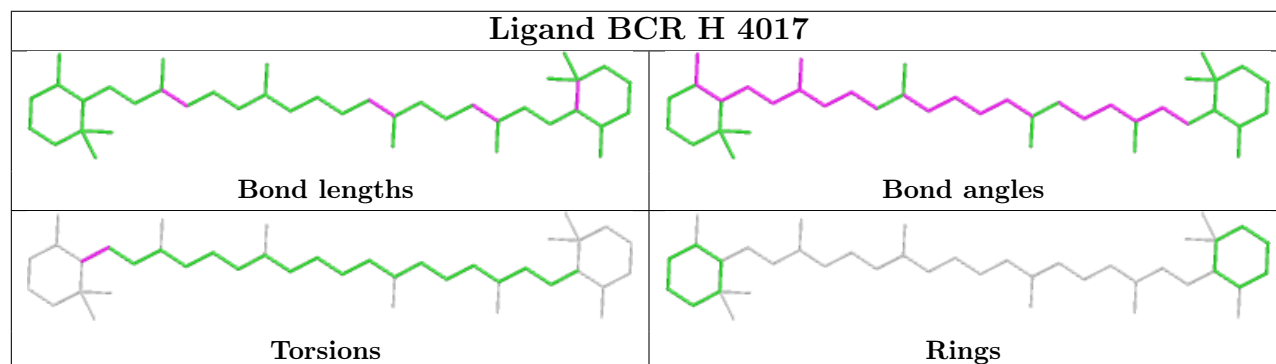


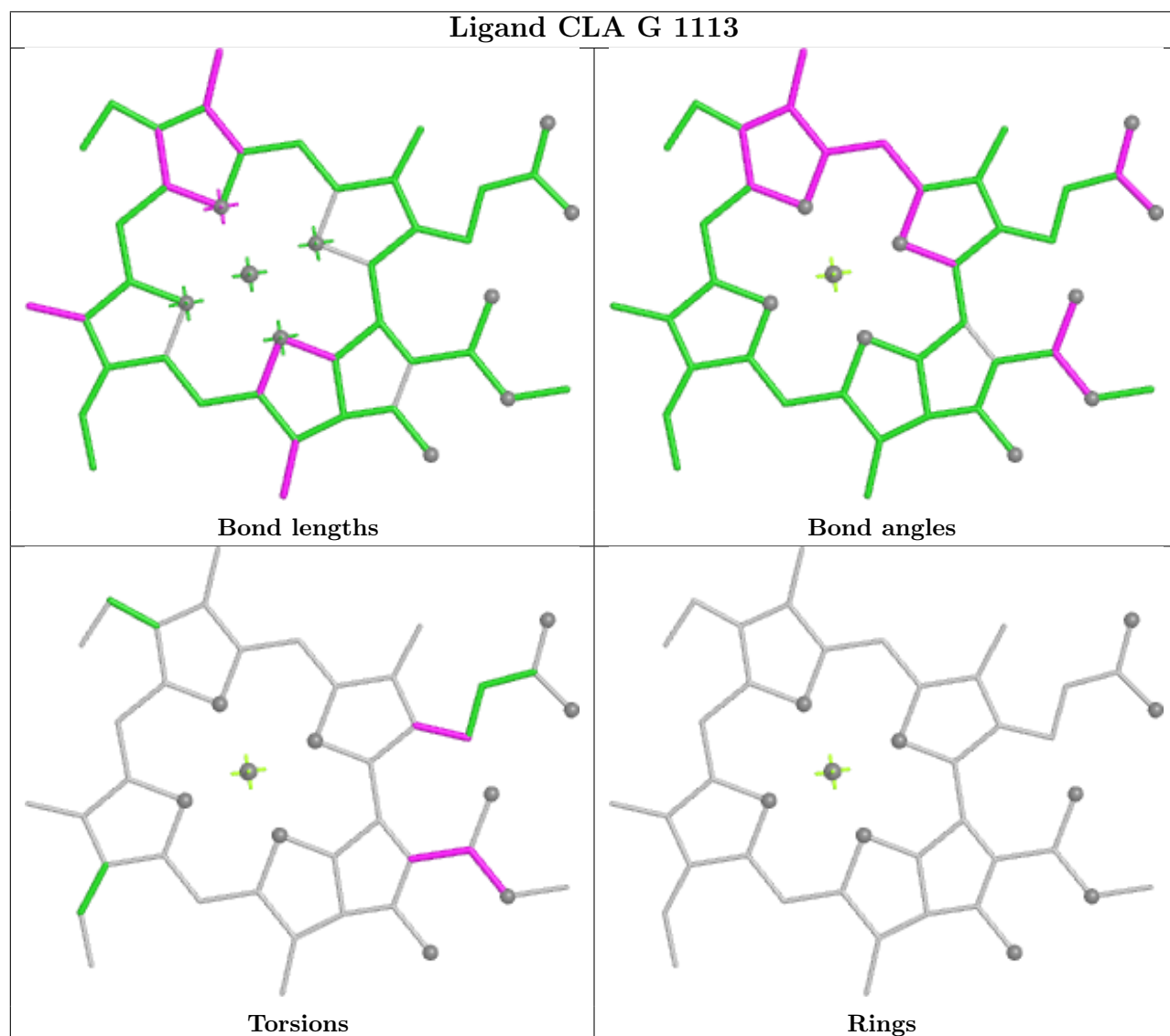
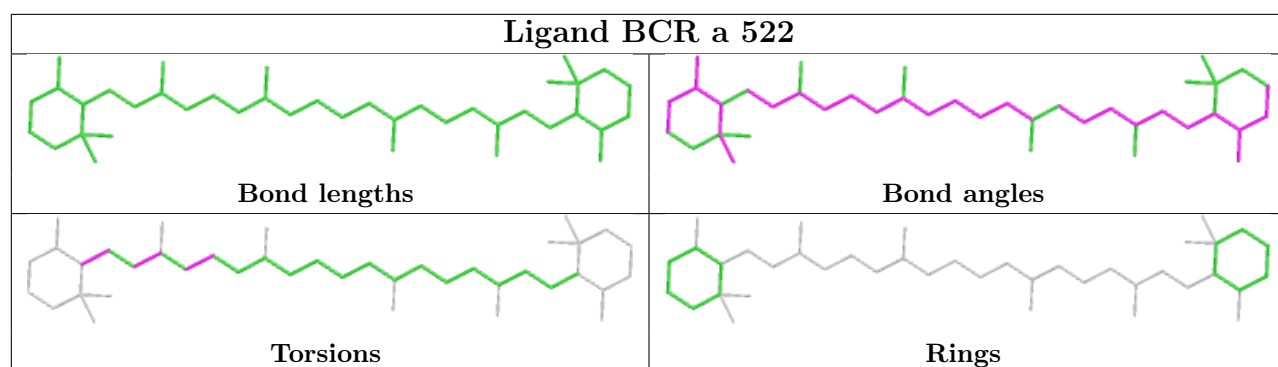
Rings

Ligand CLA 4 507

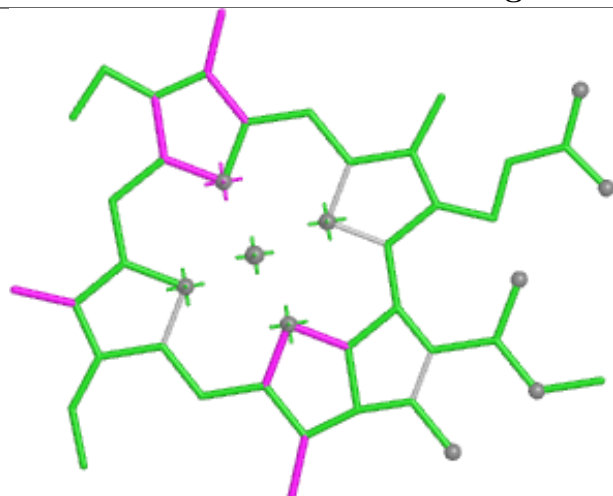


Ligand BCR H 4017

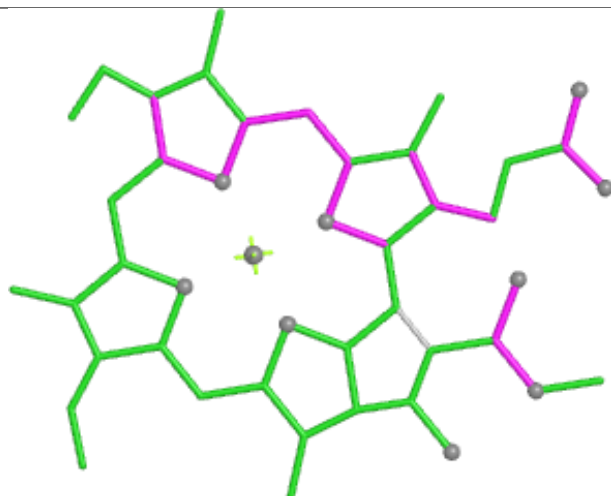




Ligand CLA R 1302



Bond lengths



Bond angles

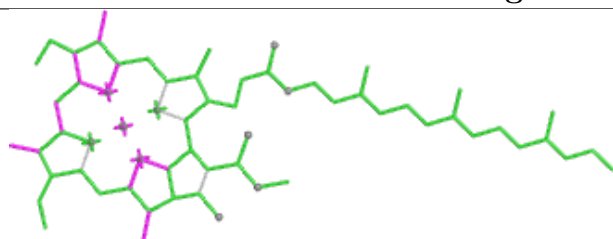


Torsions

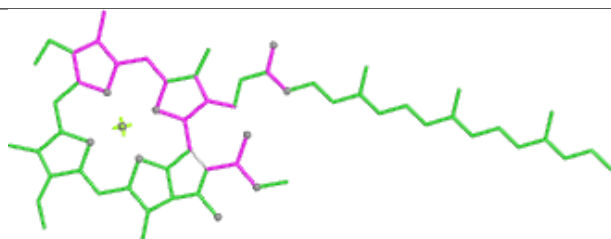


Rings

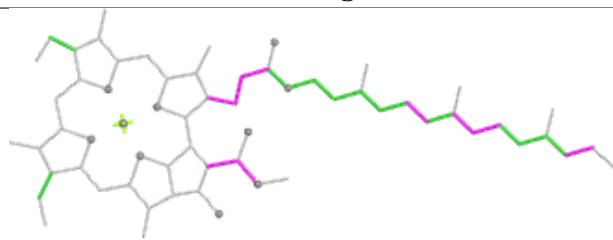
Ligand CLA B 1221



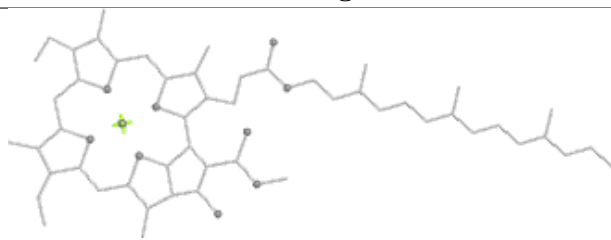
Bond lengths



Bond angles

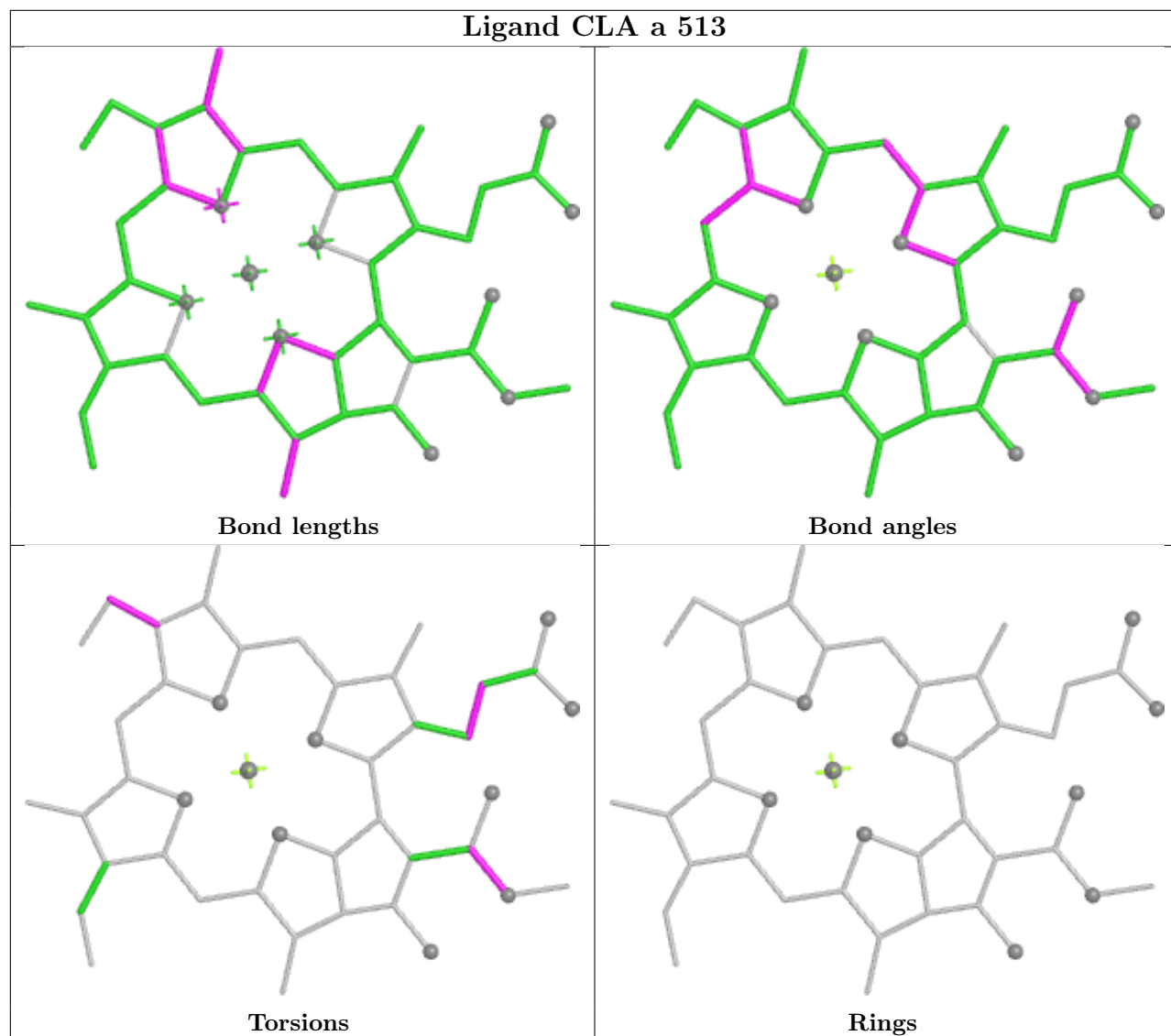


Torsions

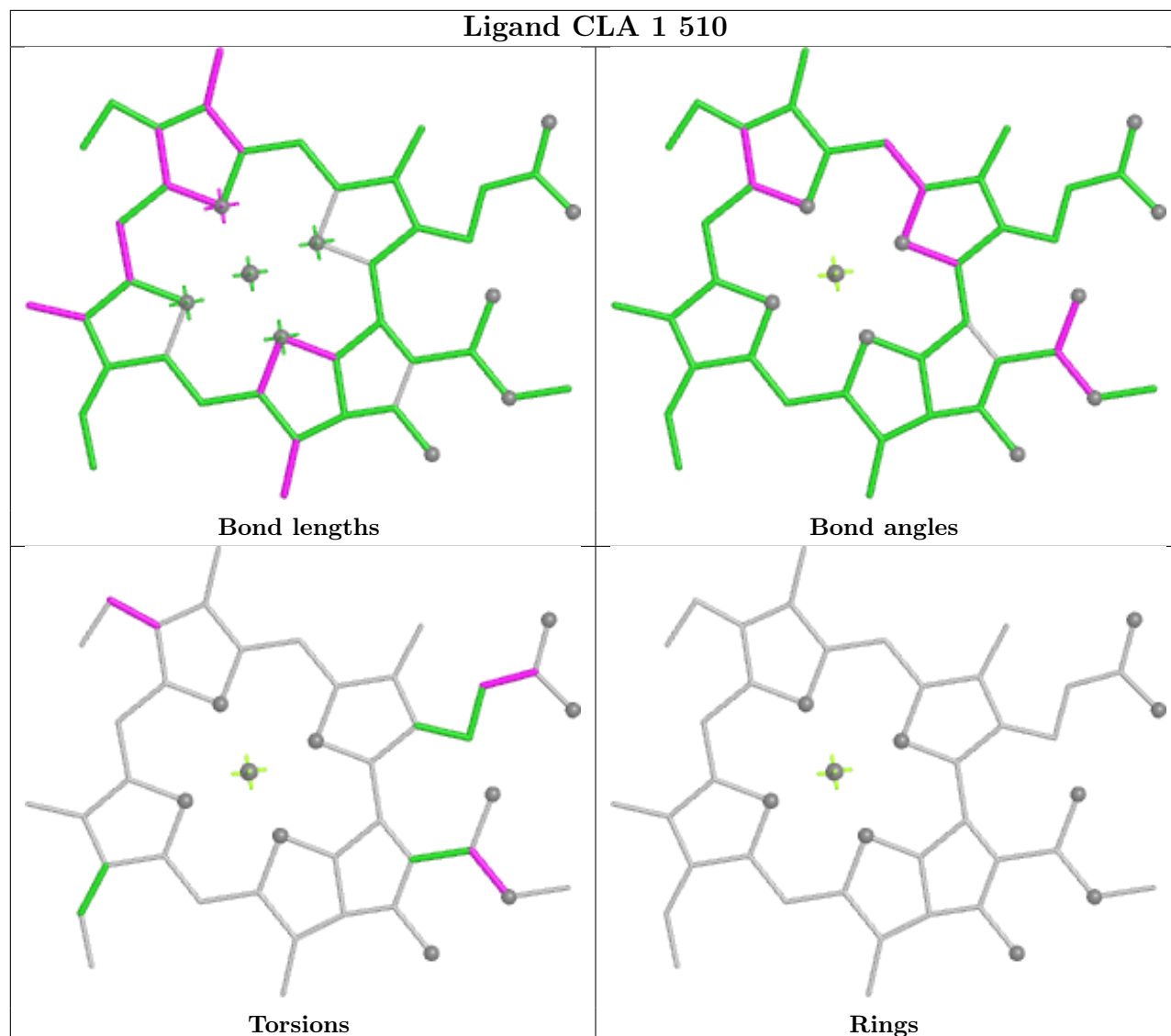


Rings

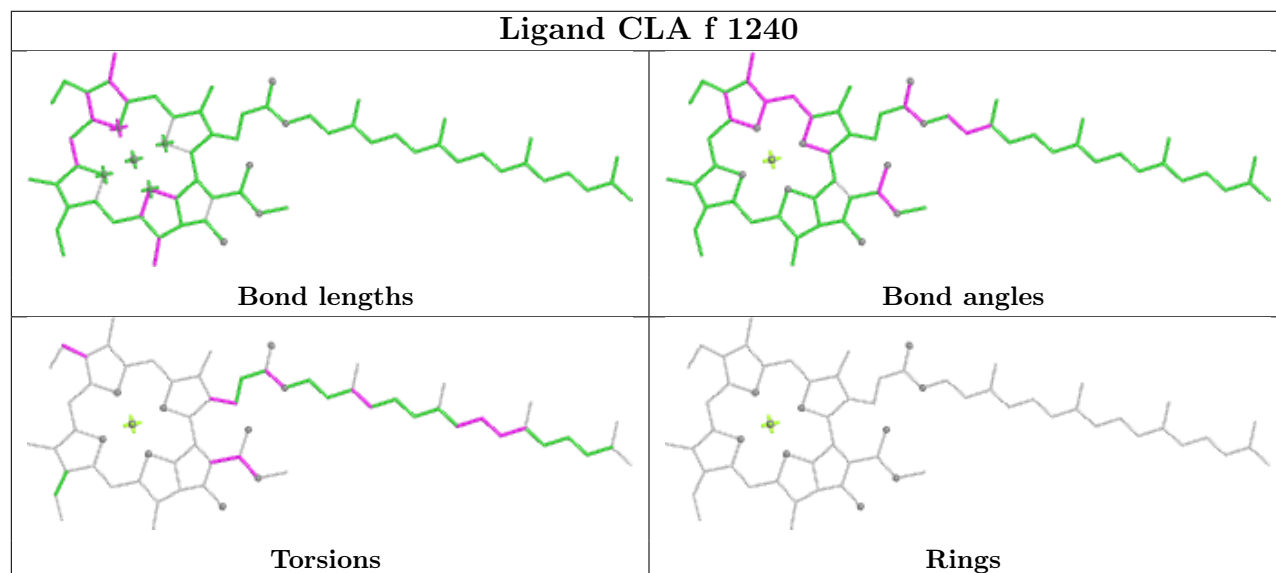
Ligand CLA a 513



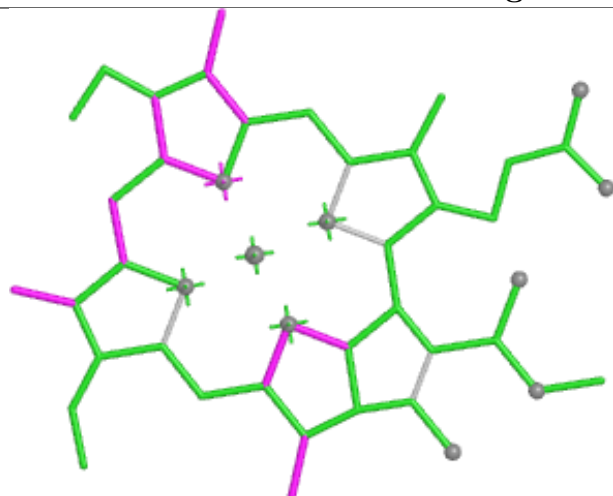
Ligand CLA 1 510



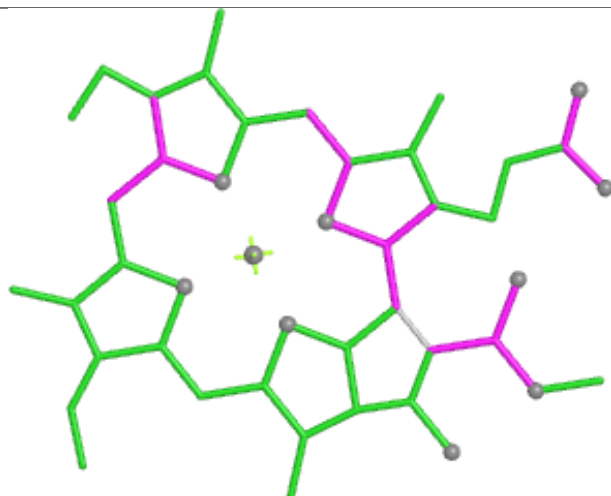
Ligand CLA f 1240



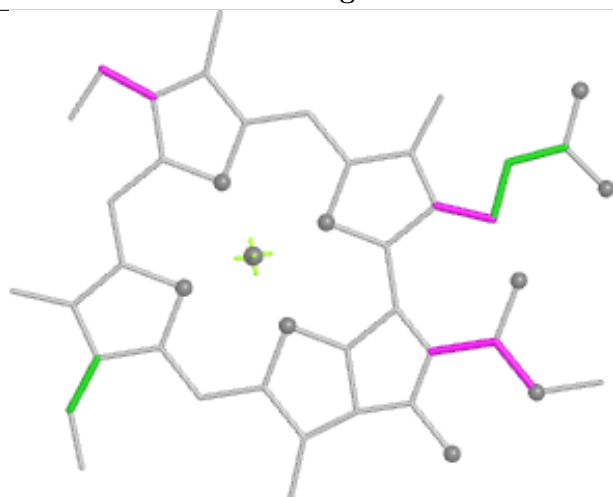
Ligand CLA T 1303



Bond lengths



Bond angles

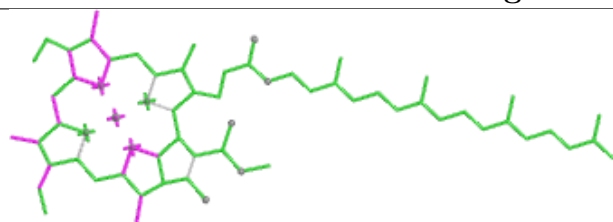


Torsions

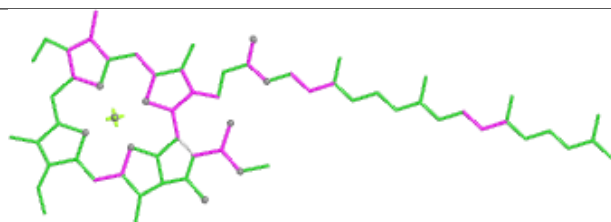


Rings

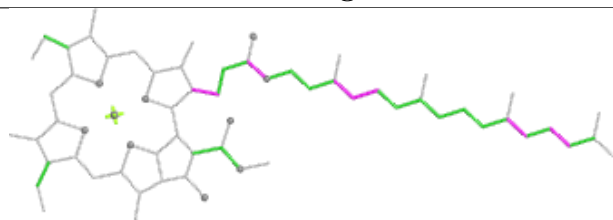
Ligand CLA G 1104



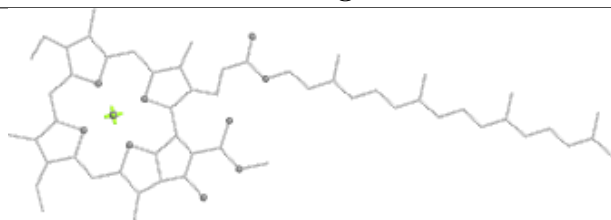
Bond lengths



Bond angles

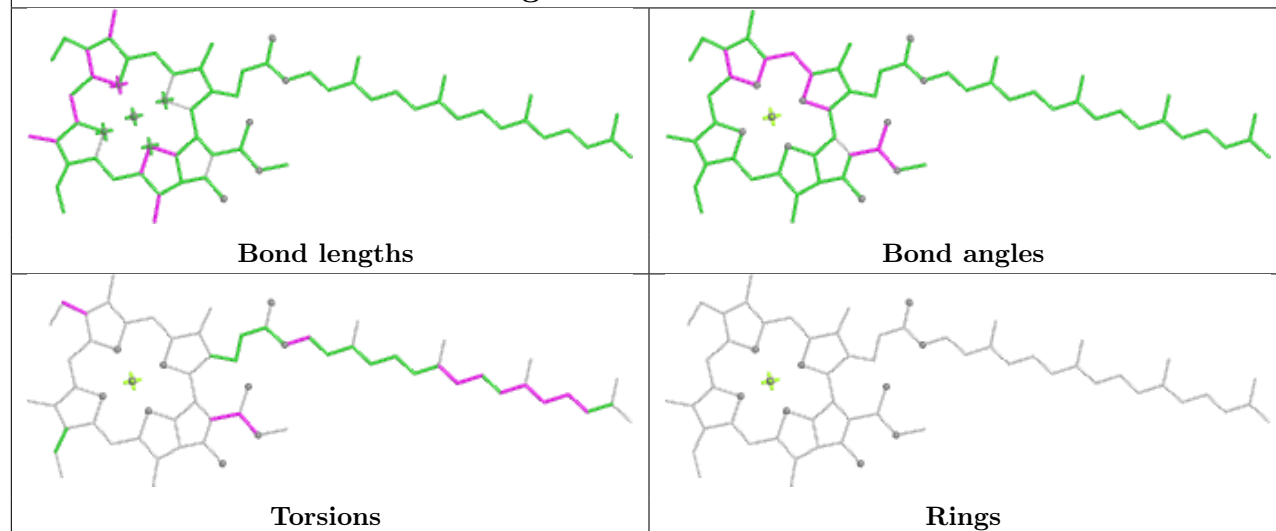


Torsions

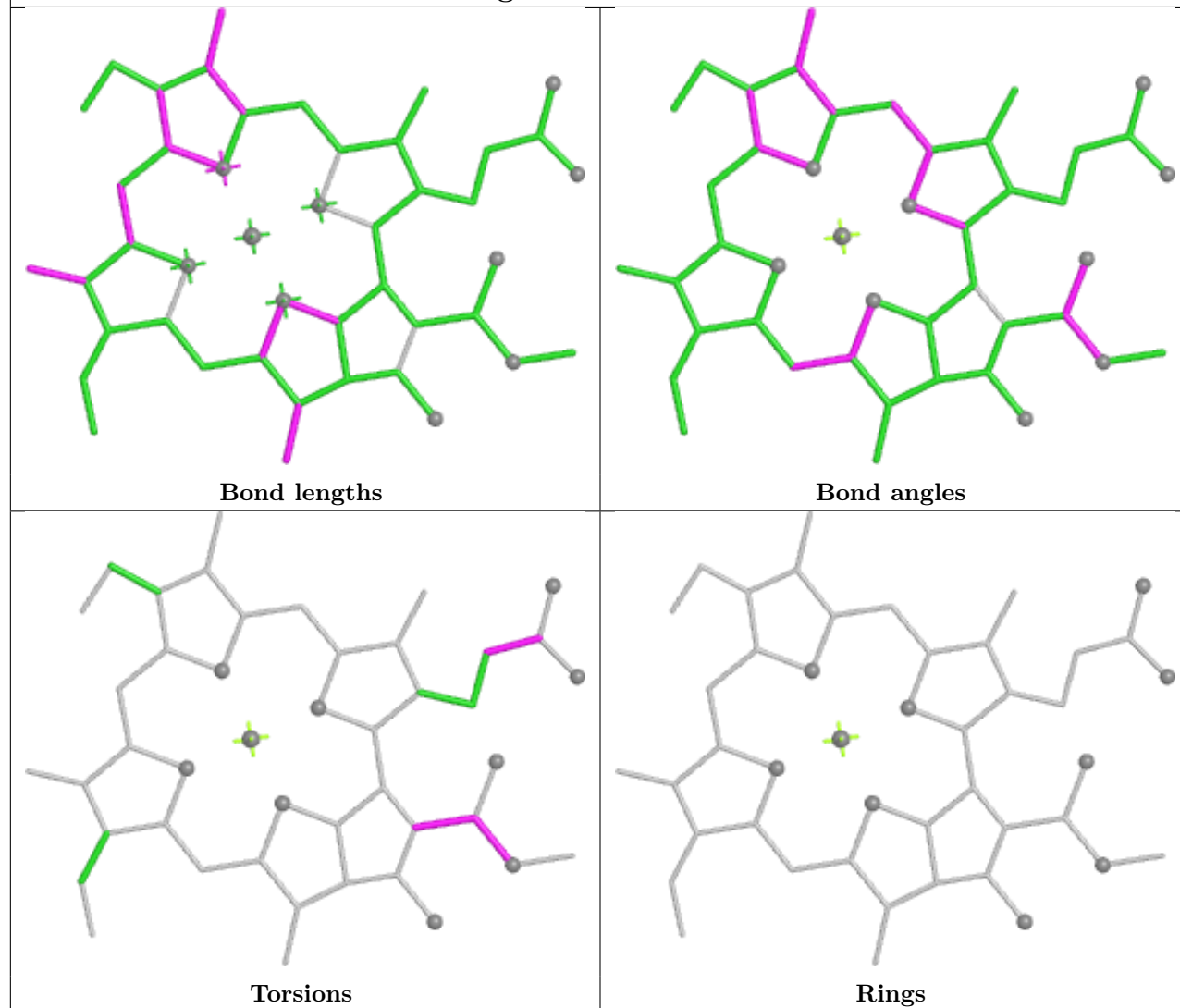


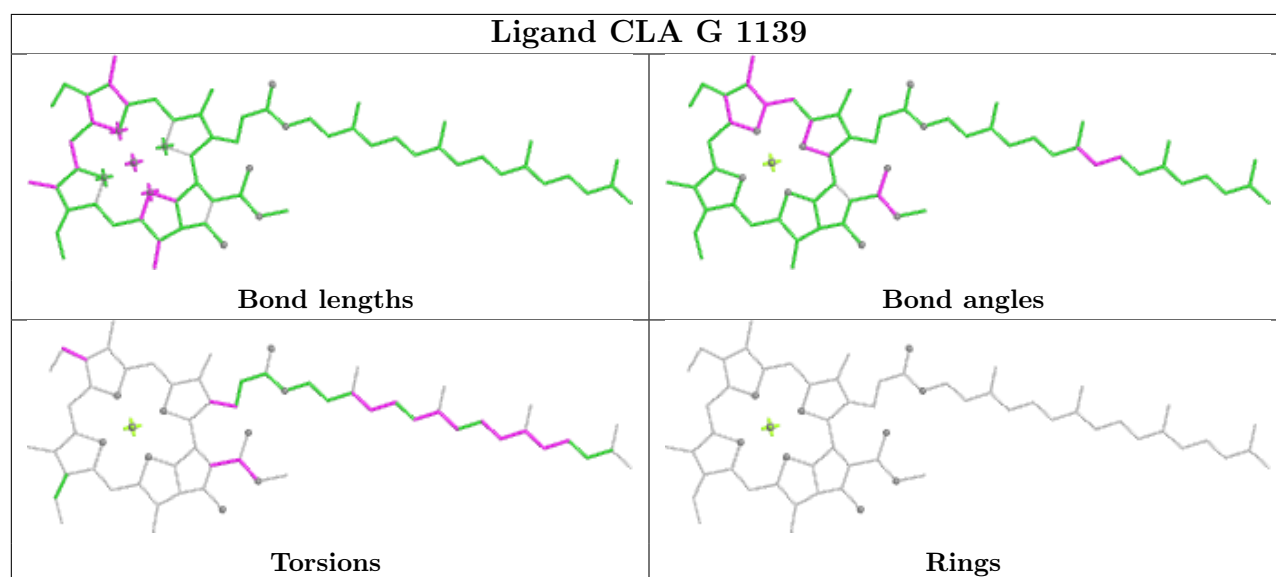
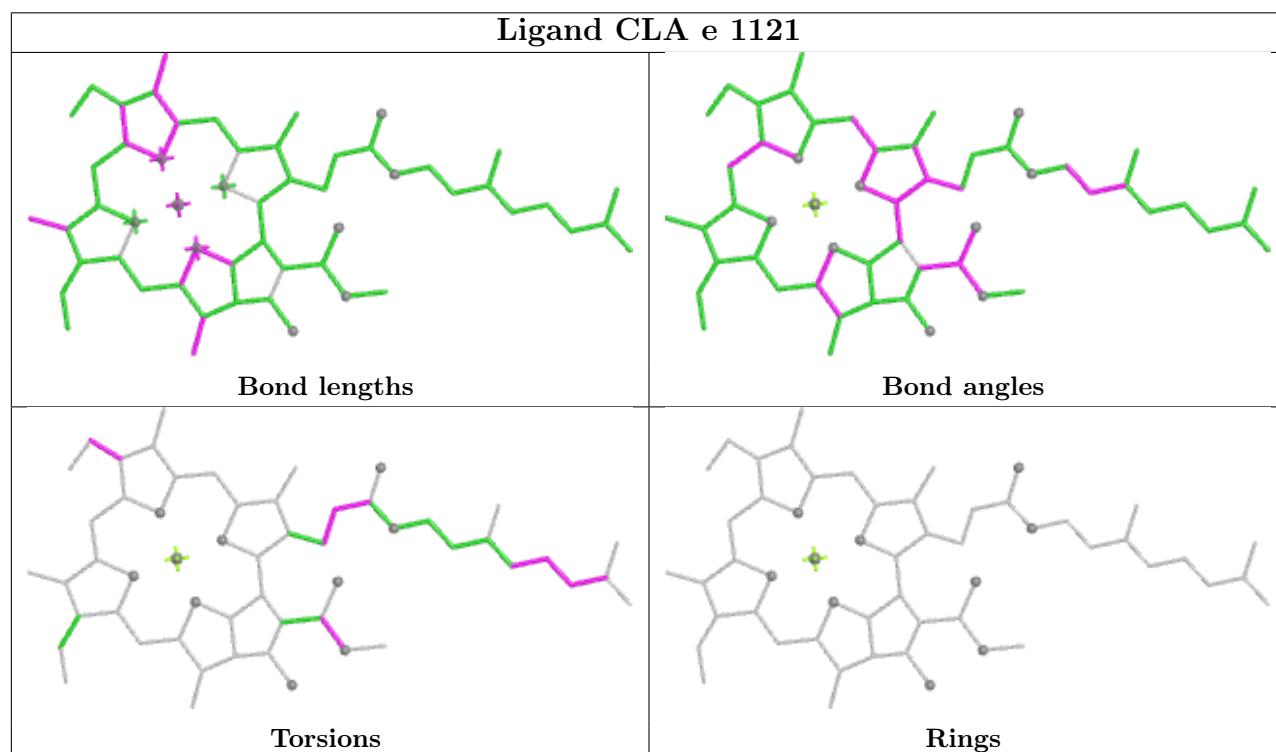
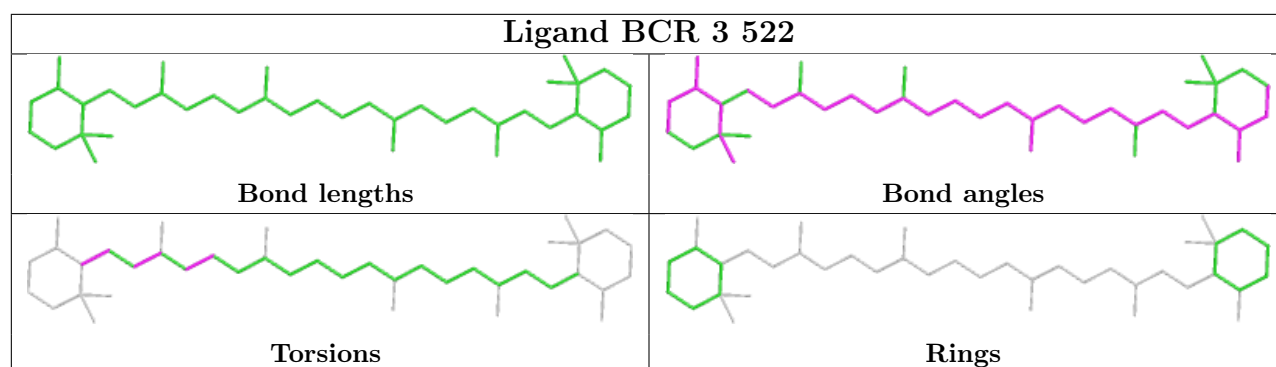
Rings

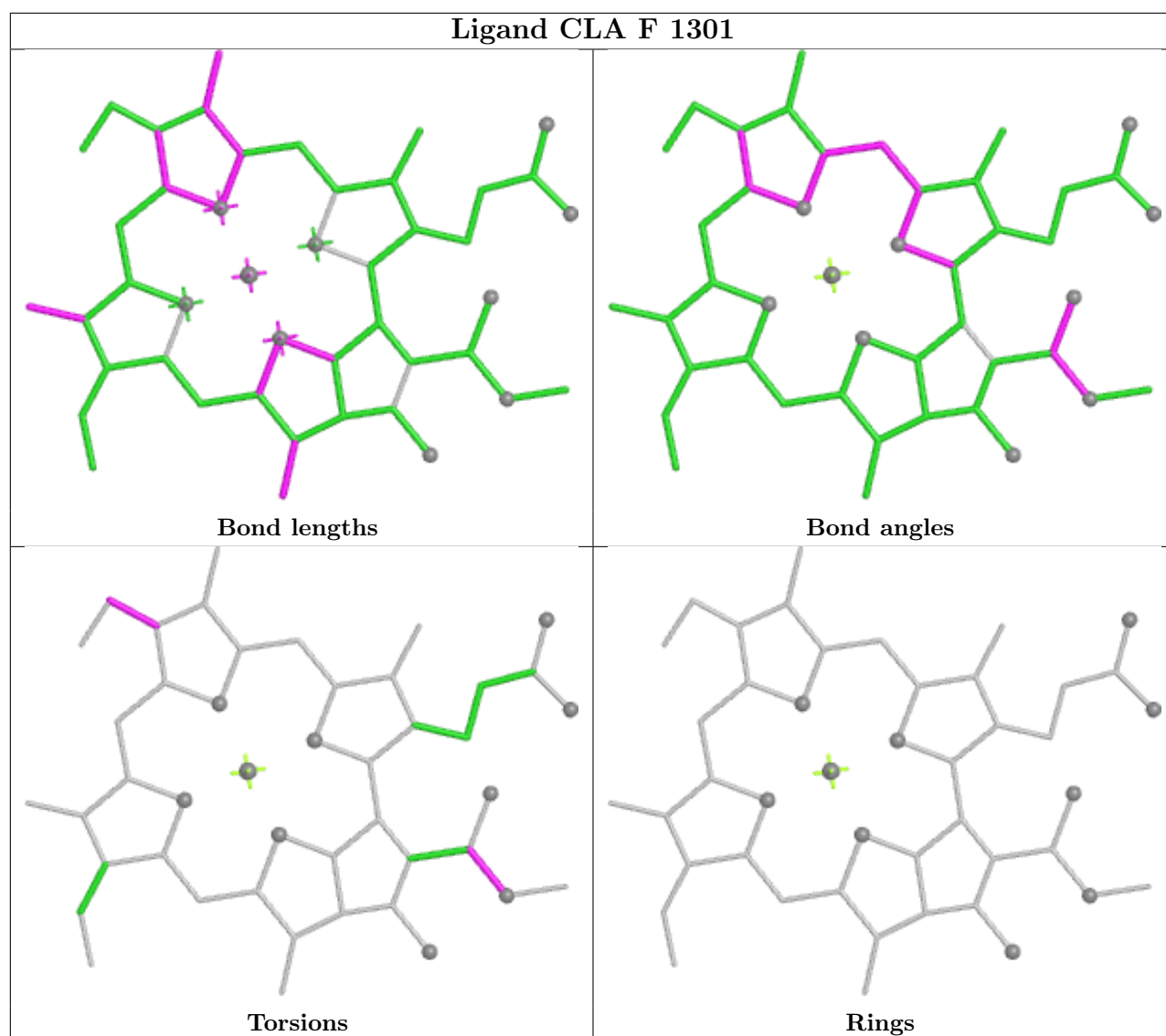
Ligand CLA G 1138



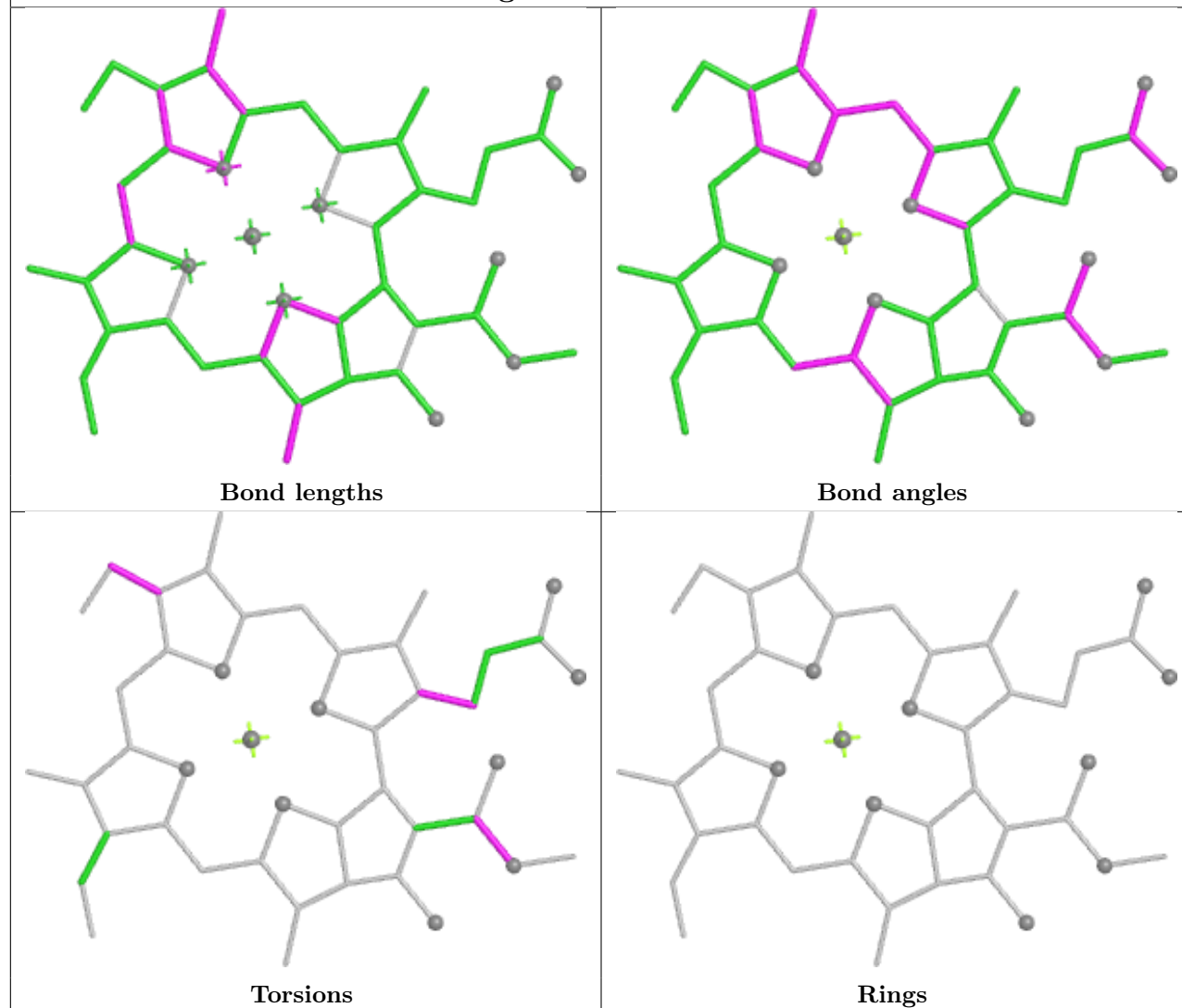
Ligand CLA r 510



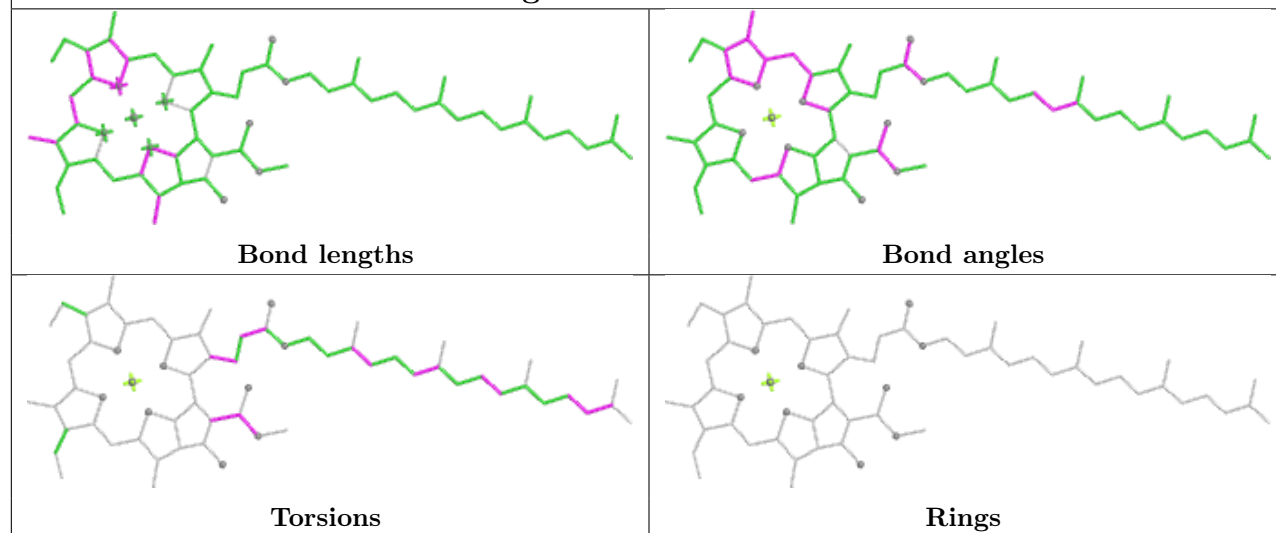




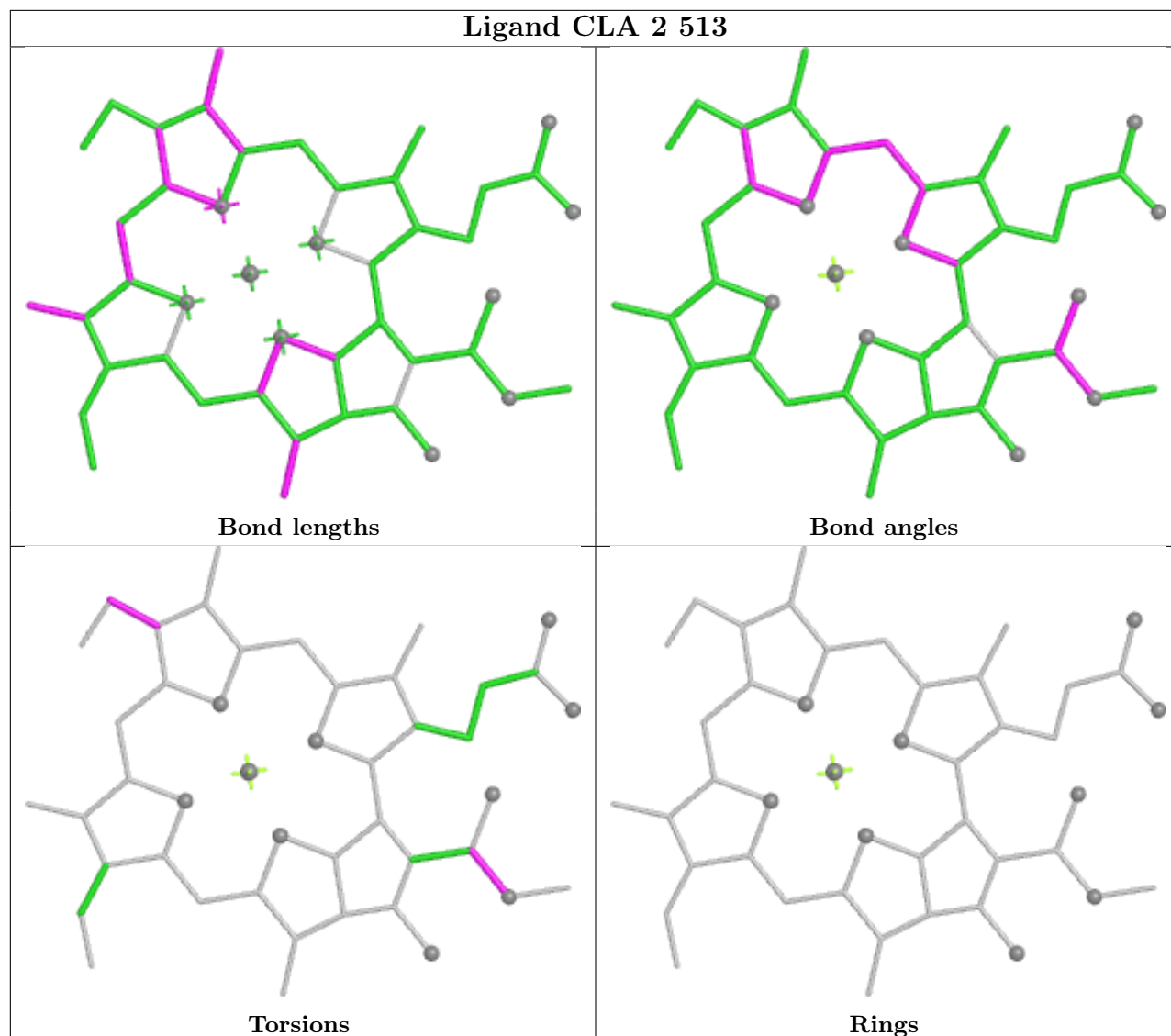
Ligand CLA t 511



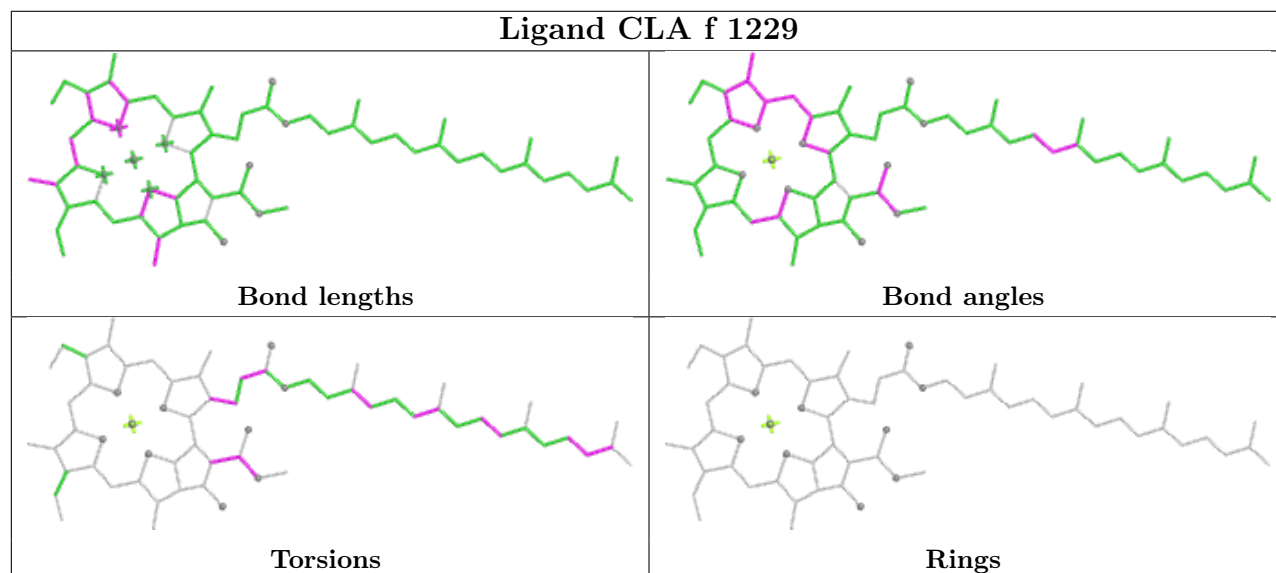
Ligand CLA H 1229

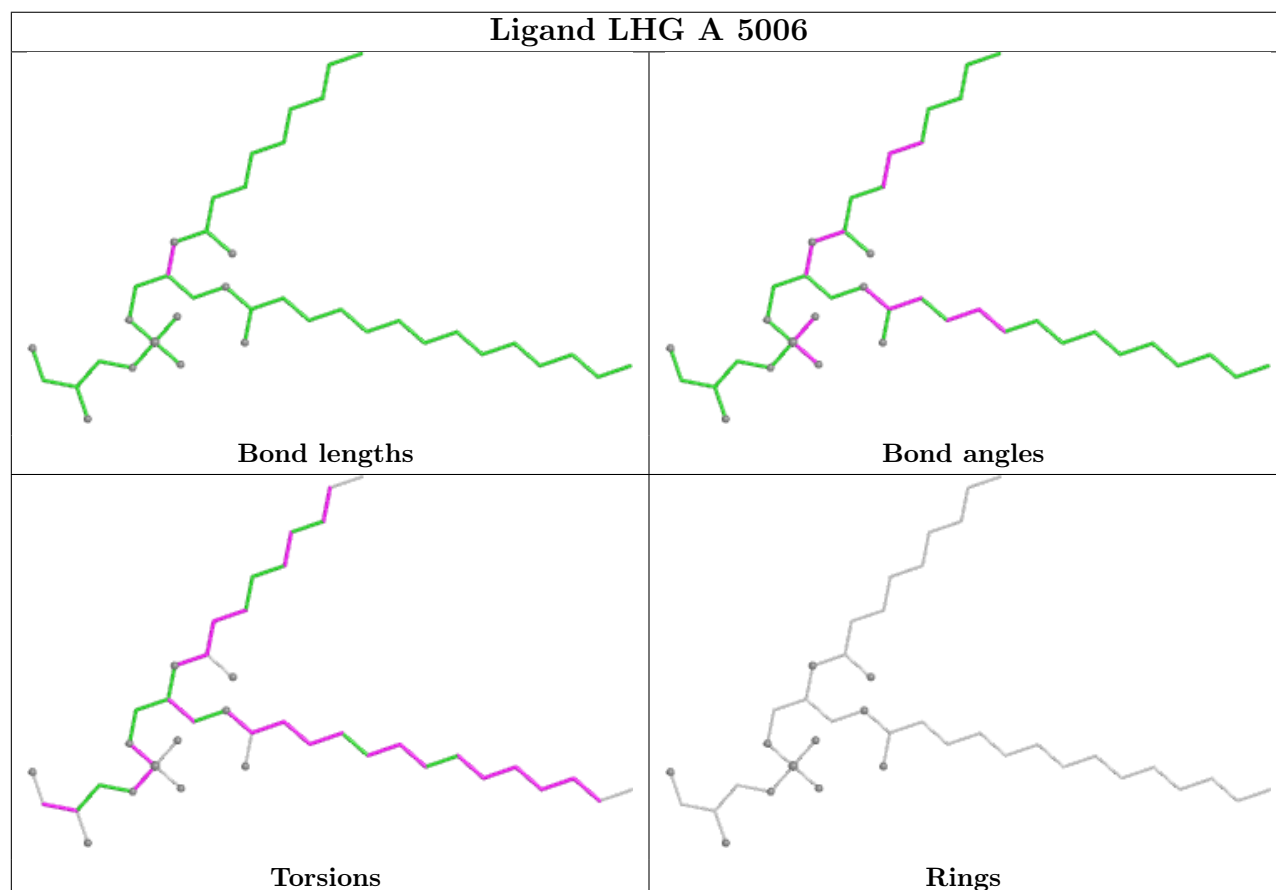
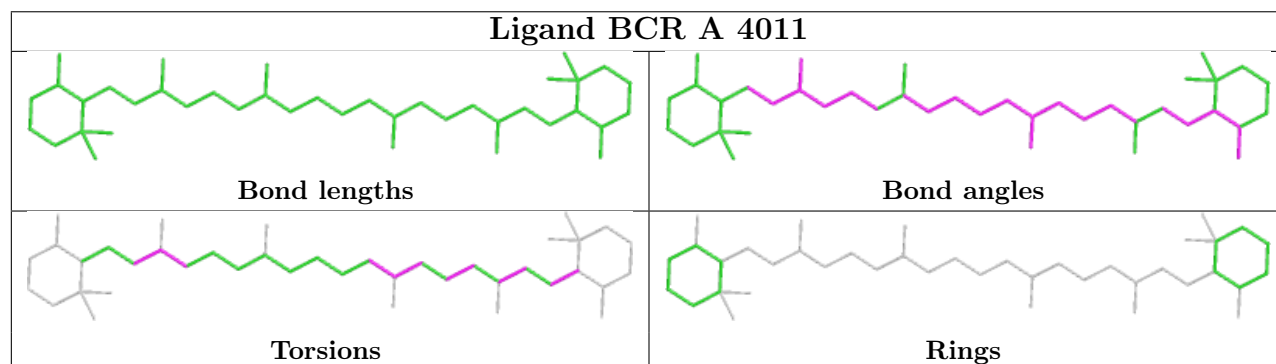
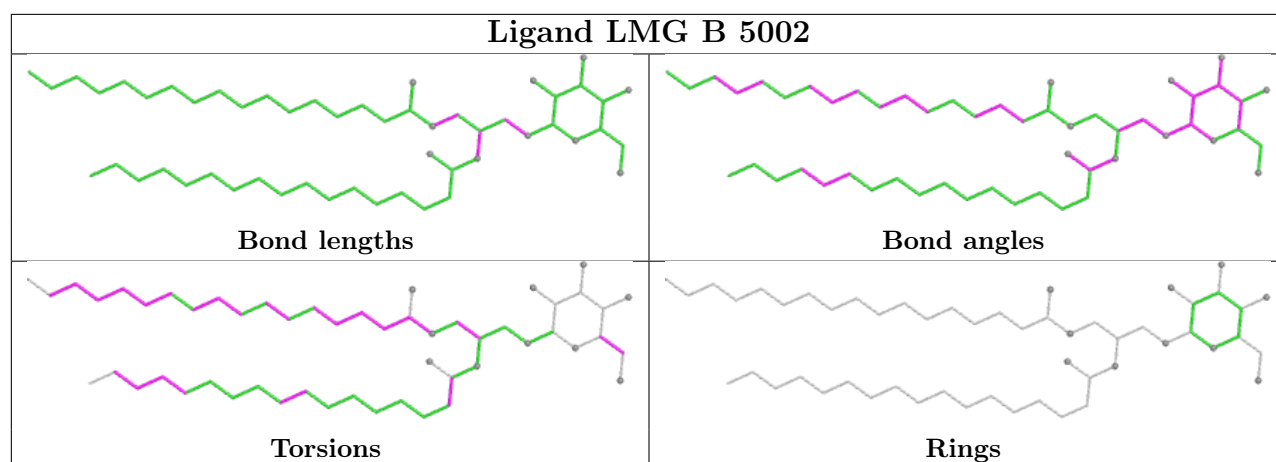


Ligand CLA 2 513

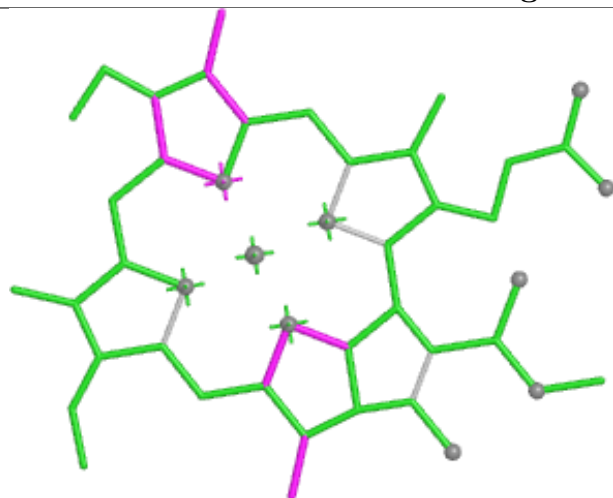


Ligand CLA f 1229

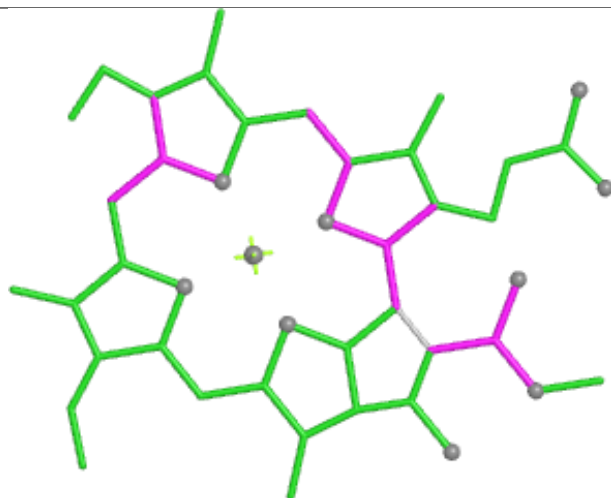




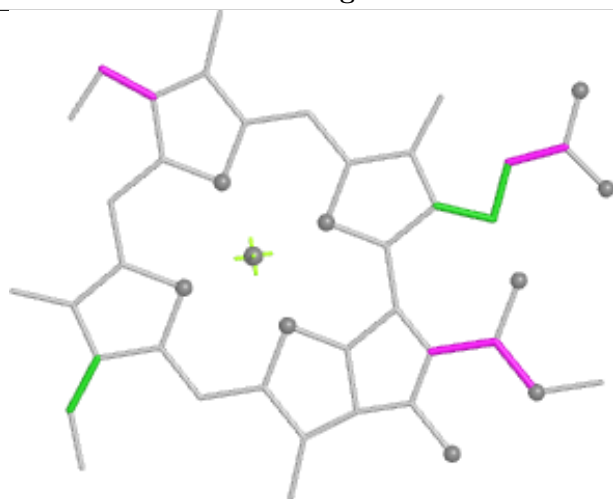
Ligand CLA t 507



Bond lengths



Bond angles

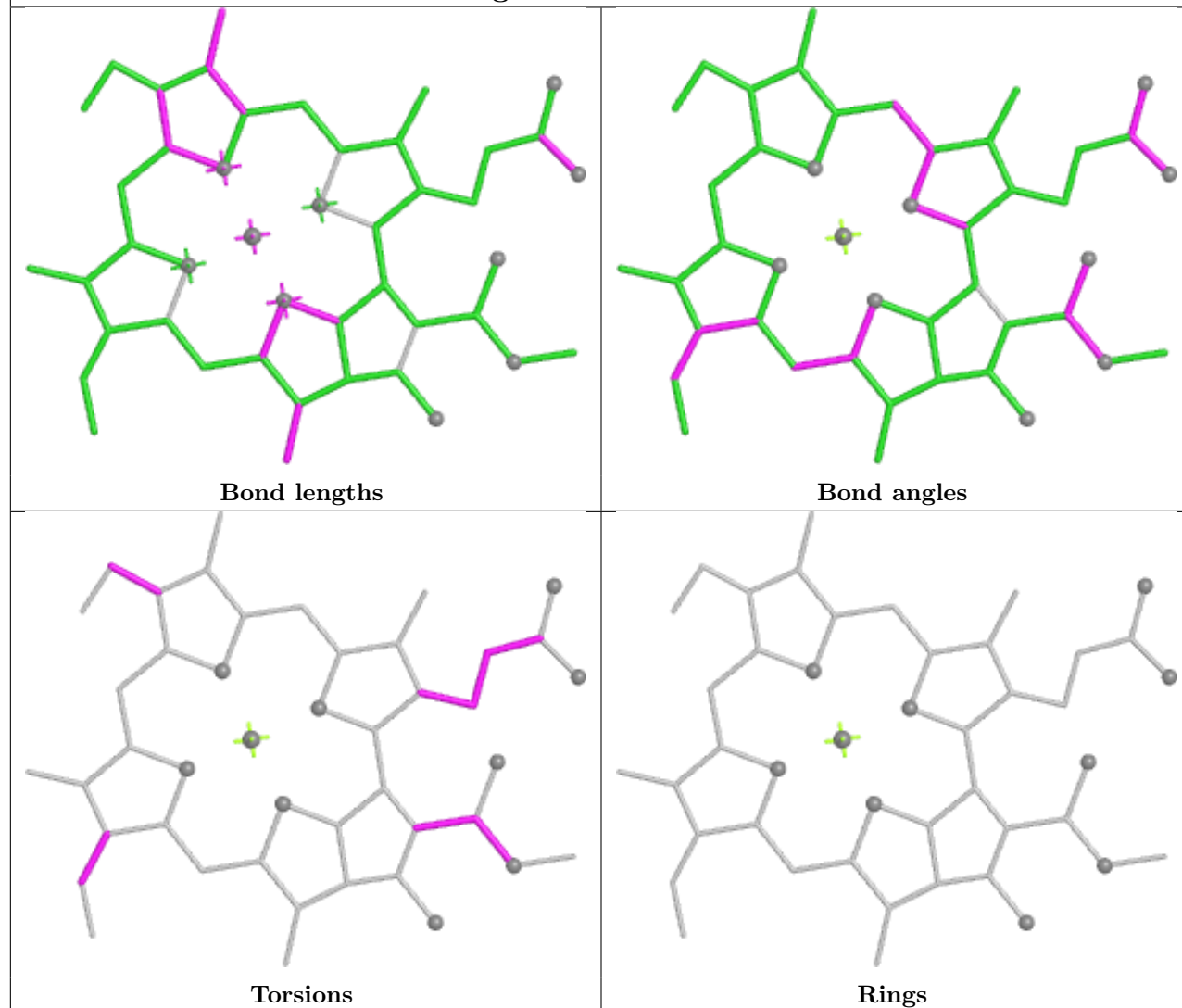


Torsions

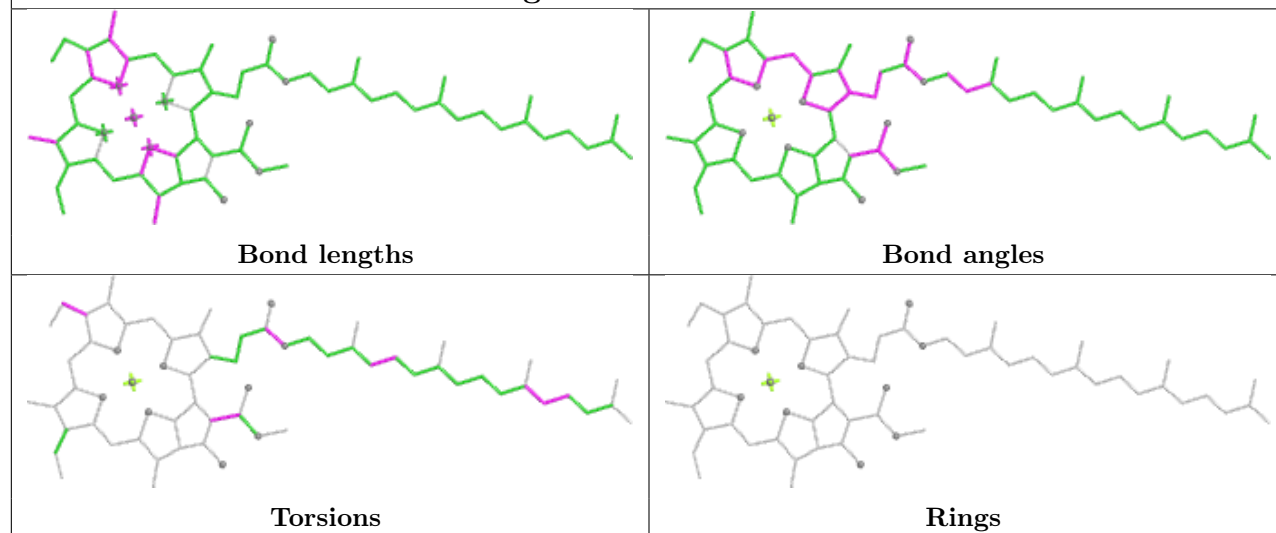


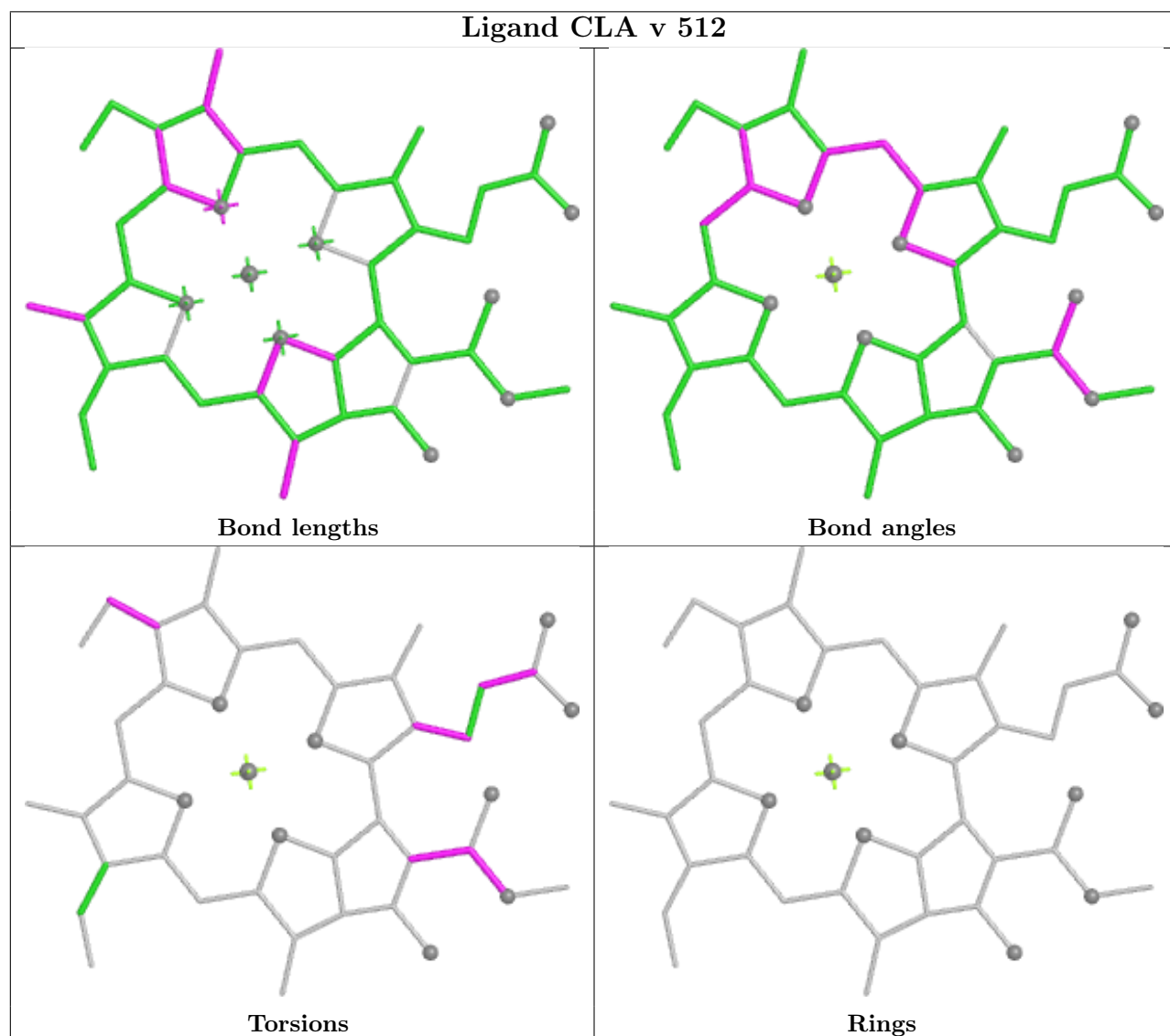
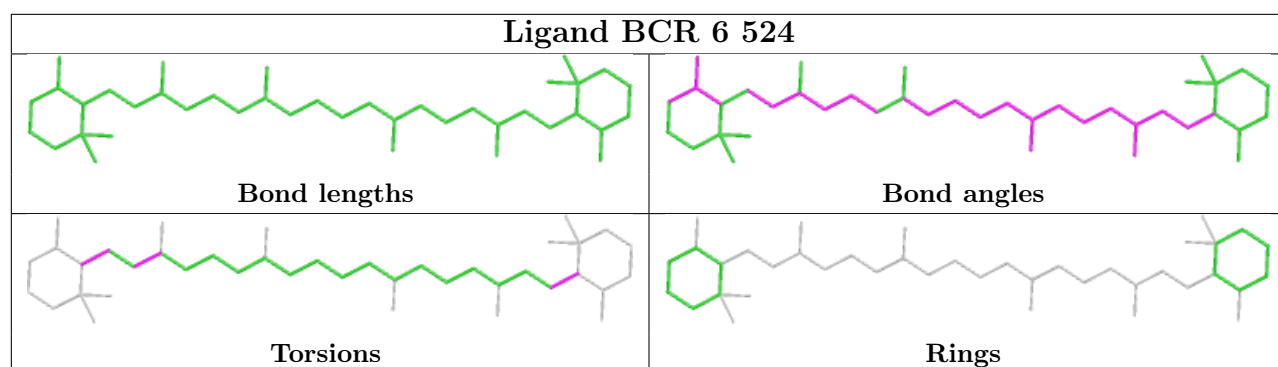
Rings

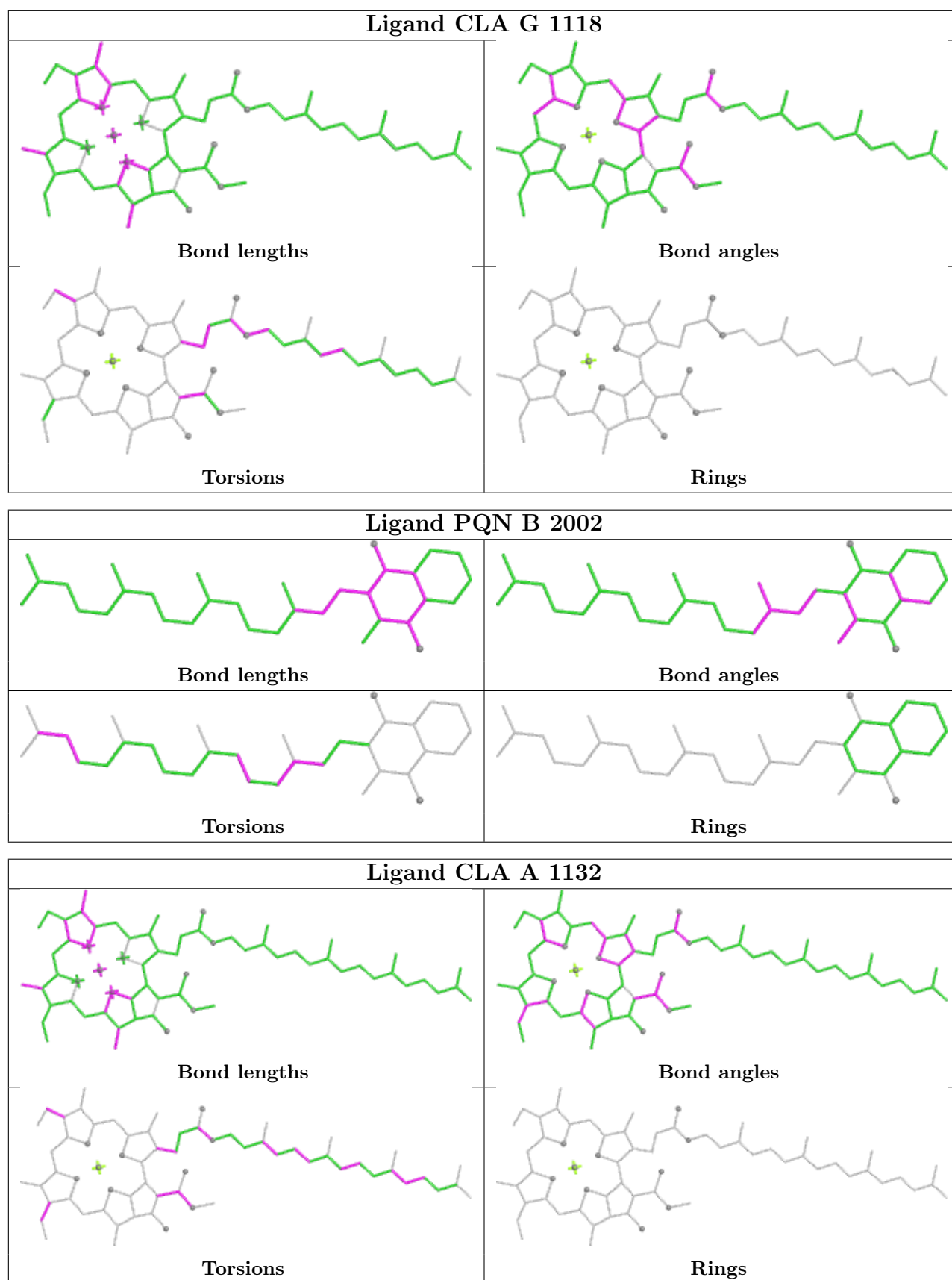
Ligand CLA Y 516

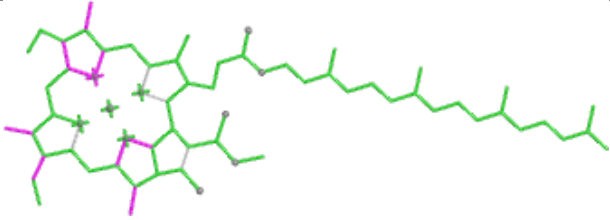
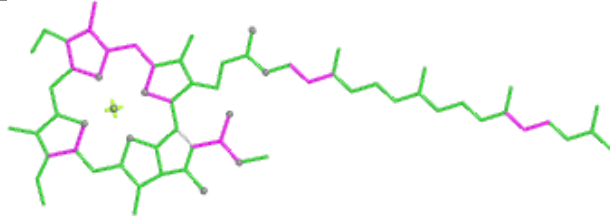
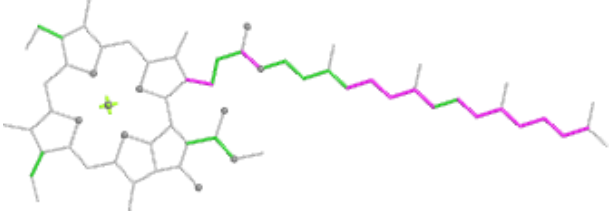
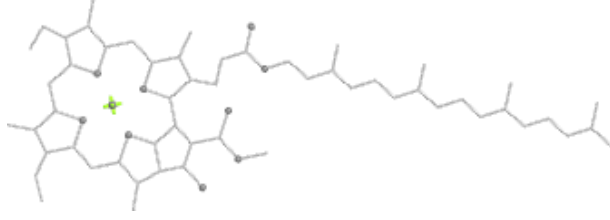
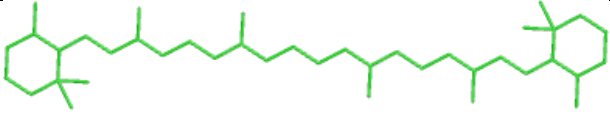
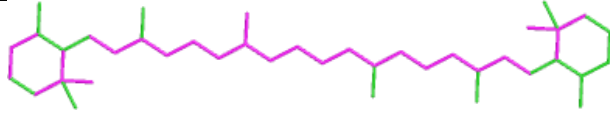
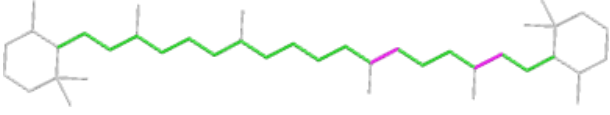
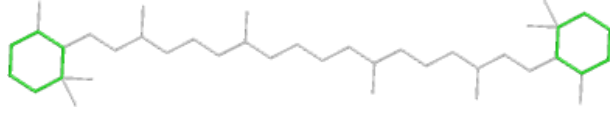
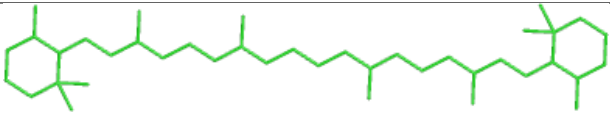
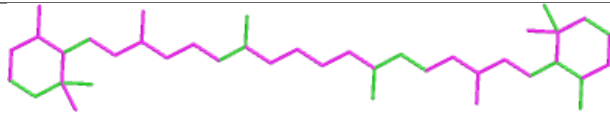
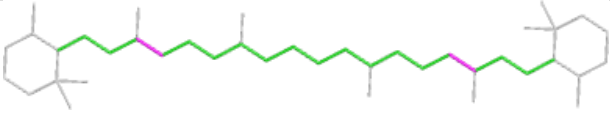
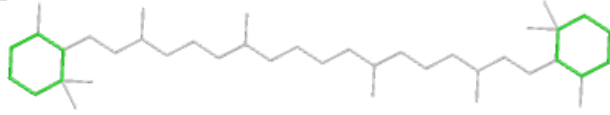


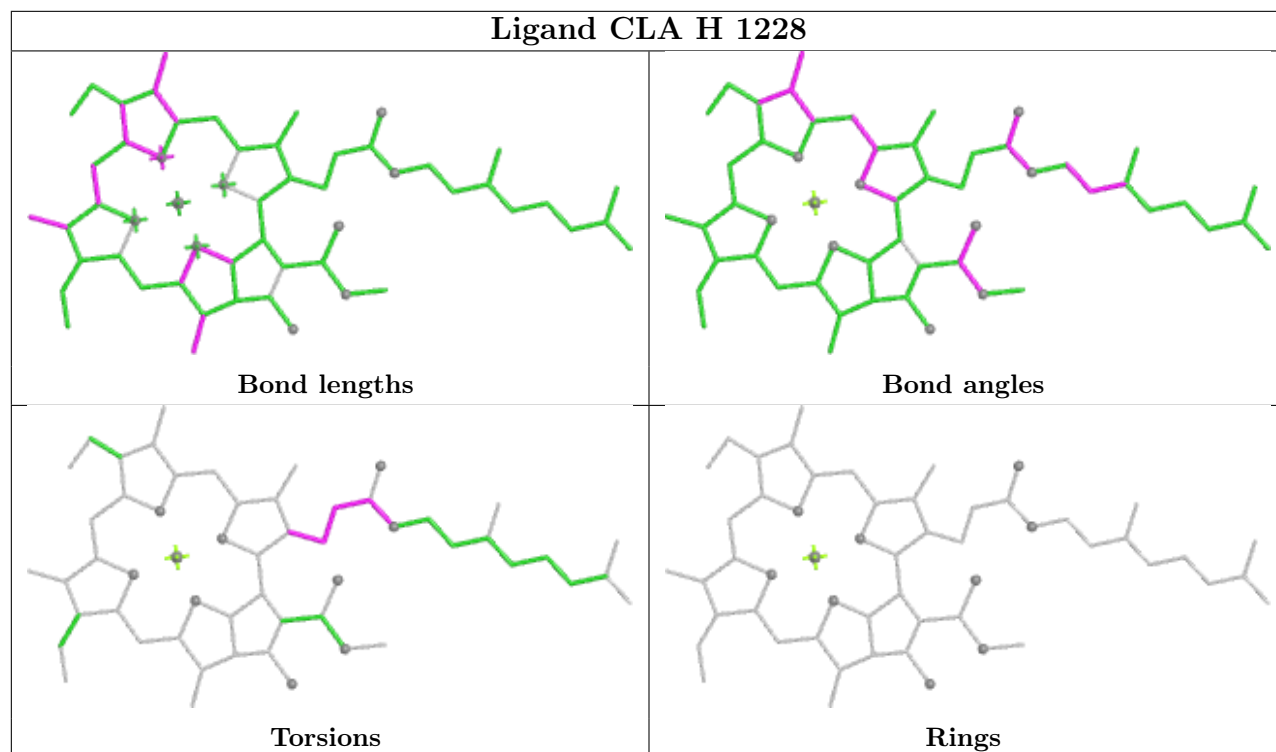
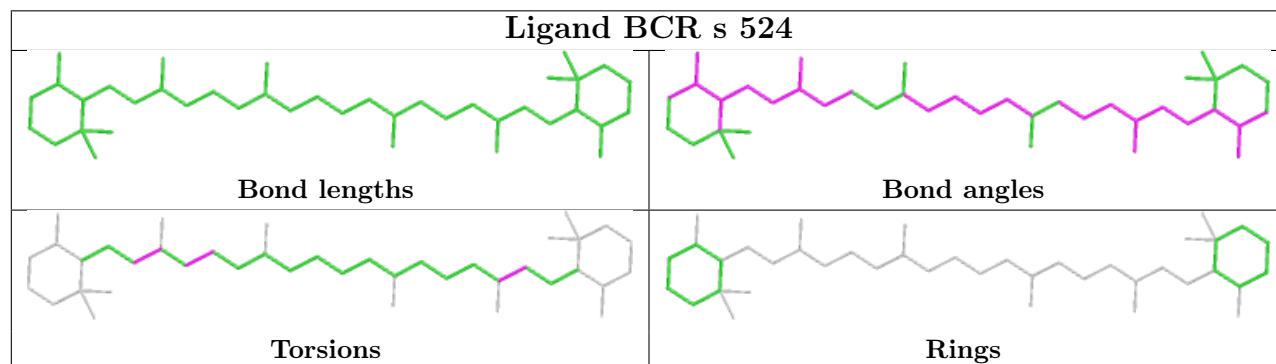
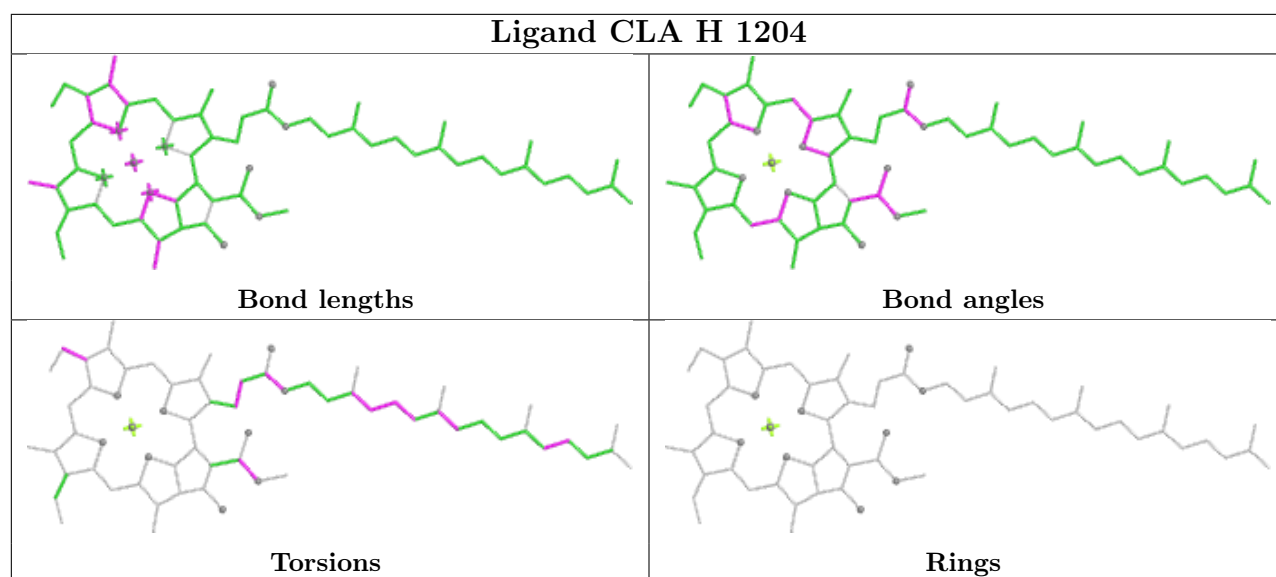
Ligand CLA B 1205



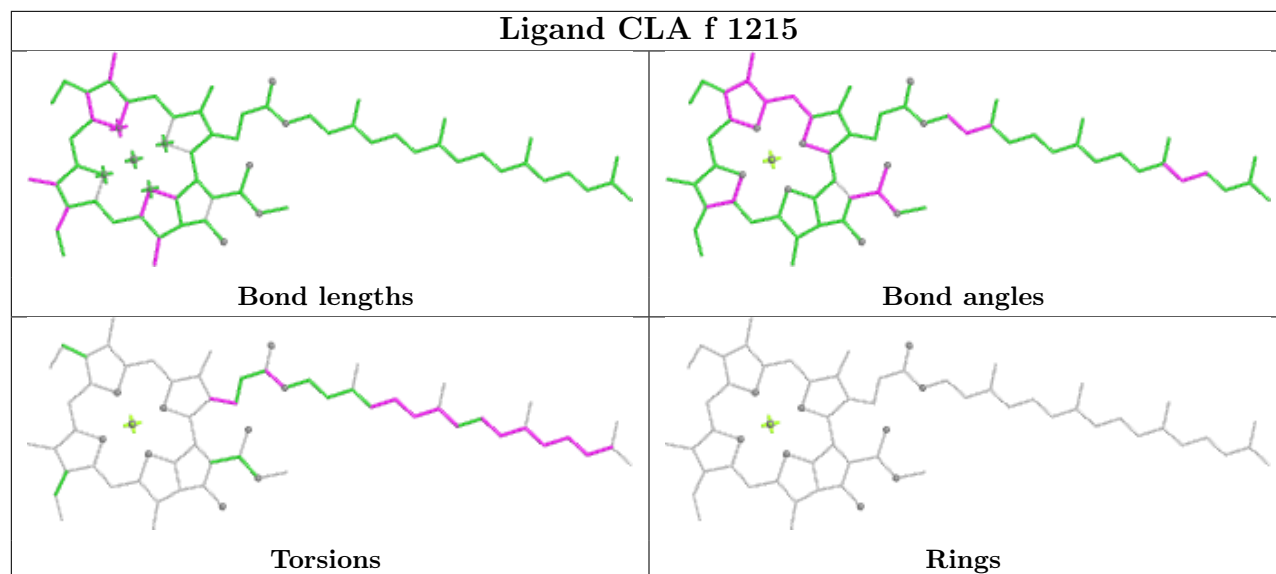




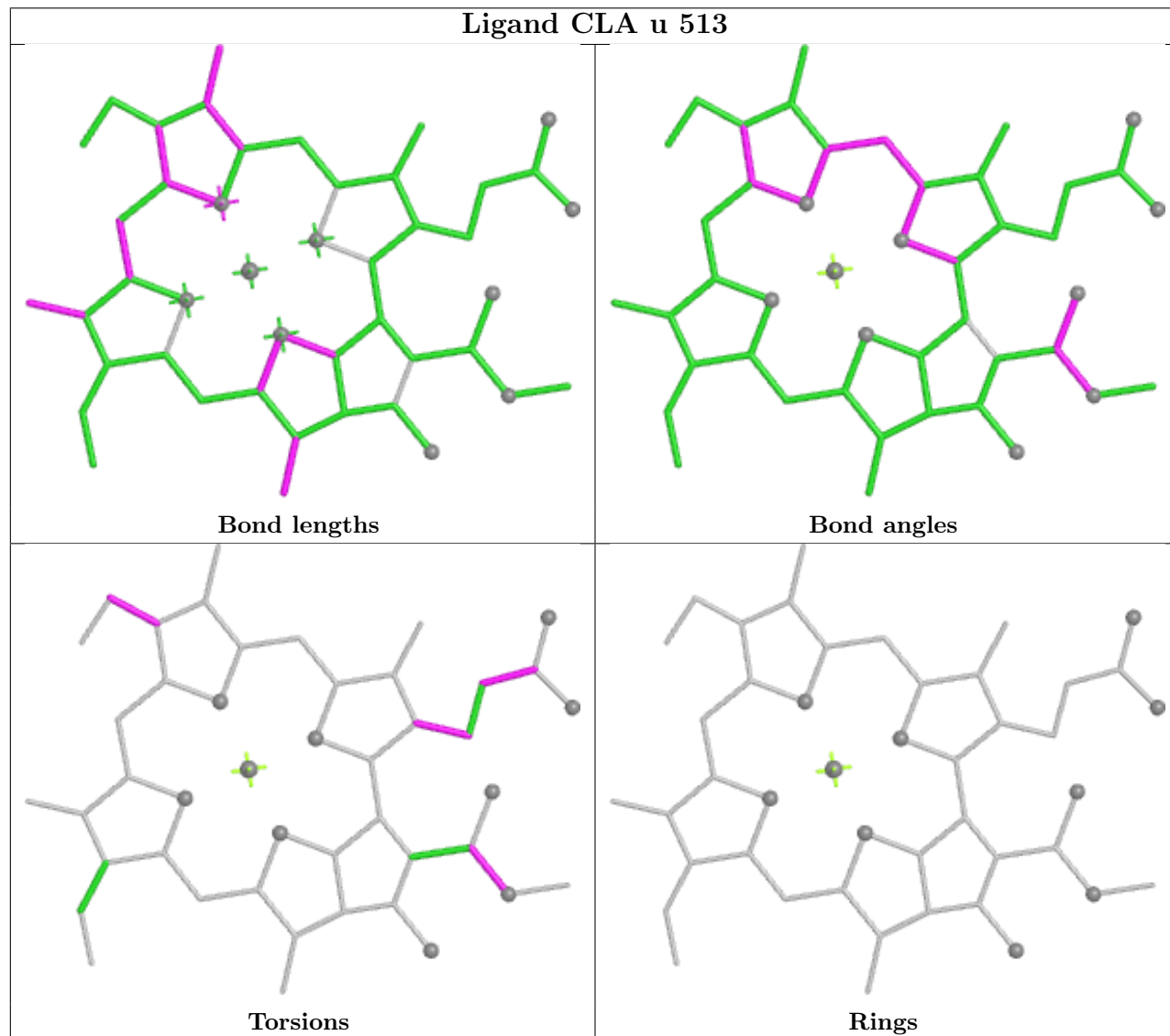
Ligand CLA H 1215	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR J 4013	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 4006	
 Bond lengths	 Bond angles
 Torsions	 Rings

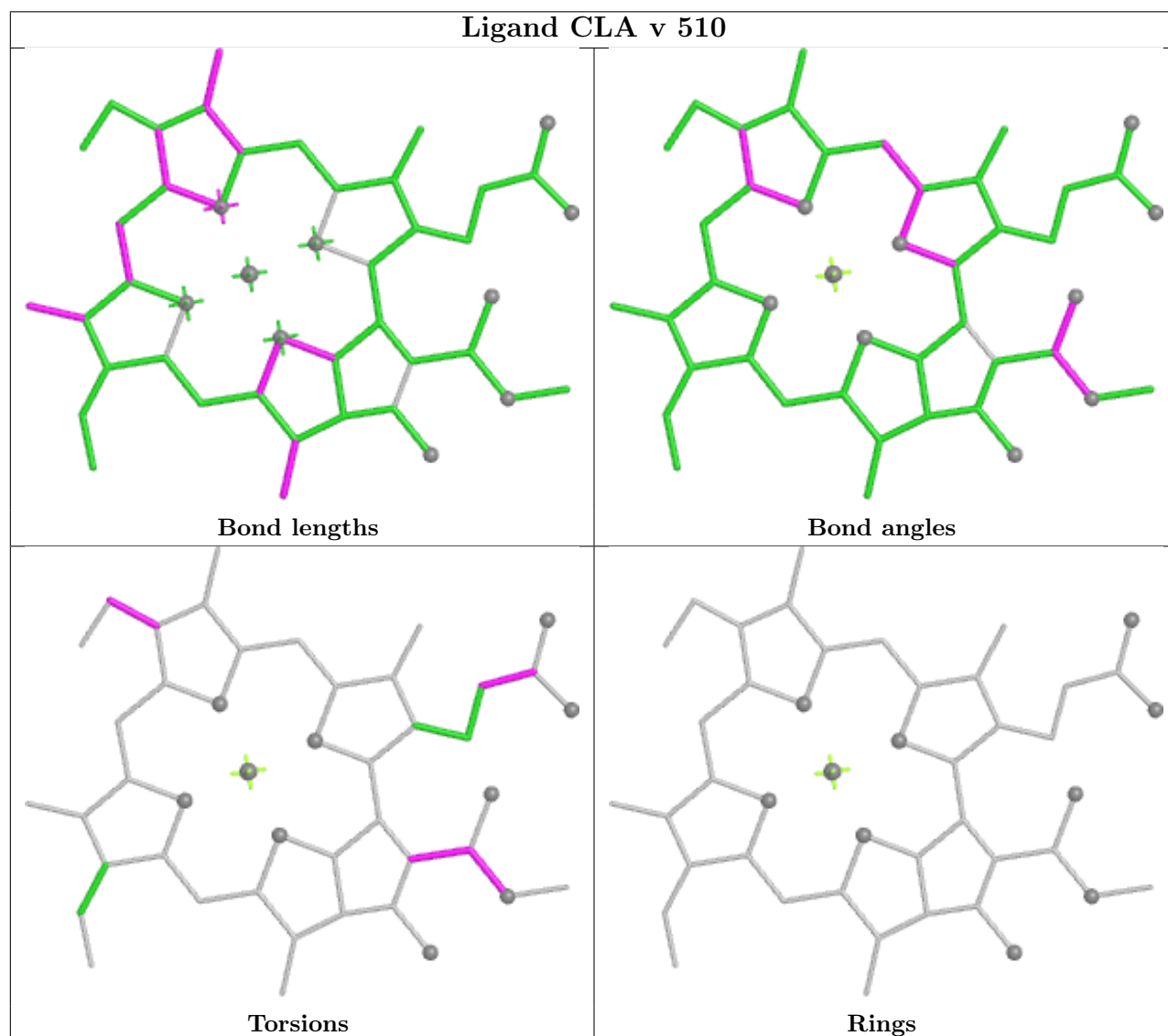
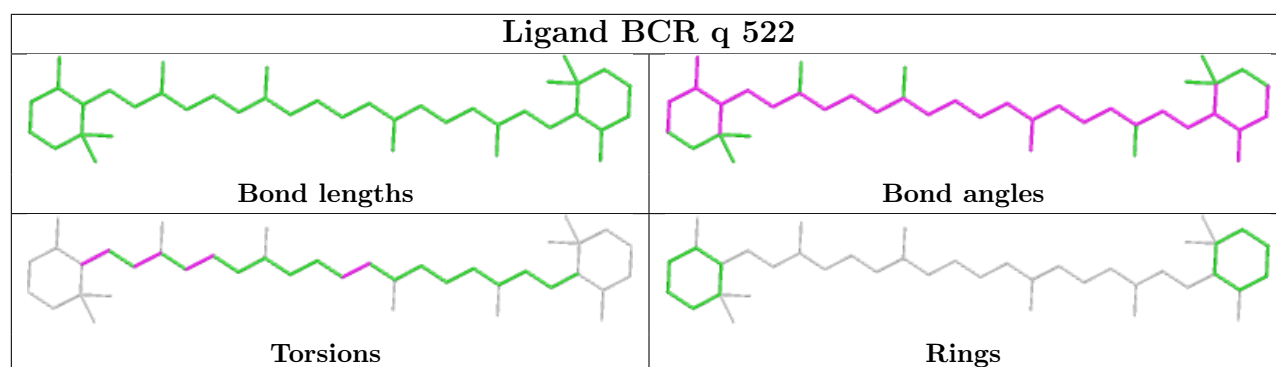


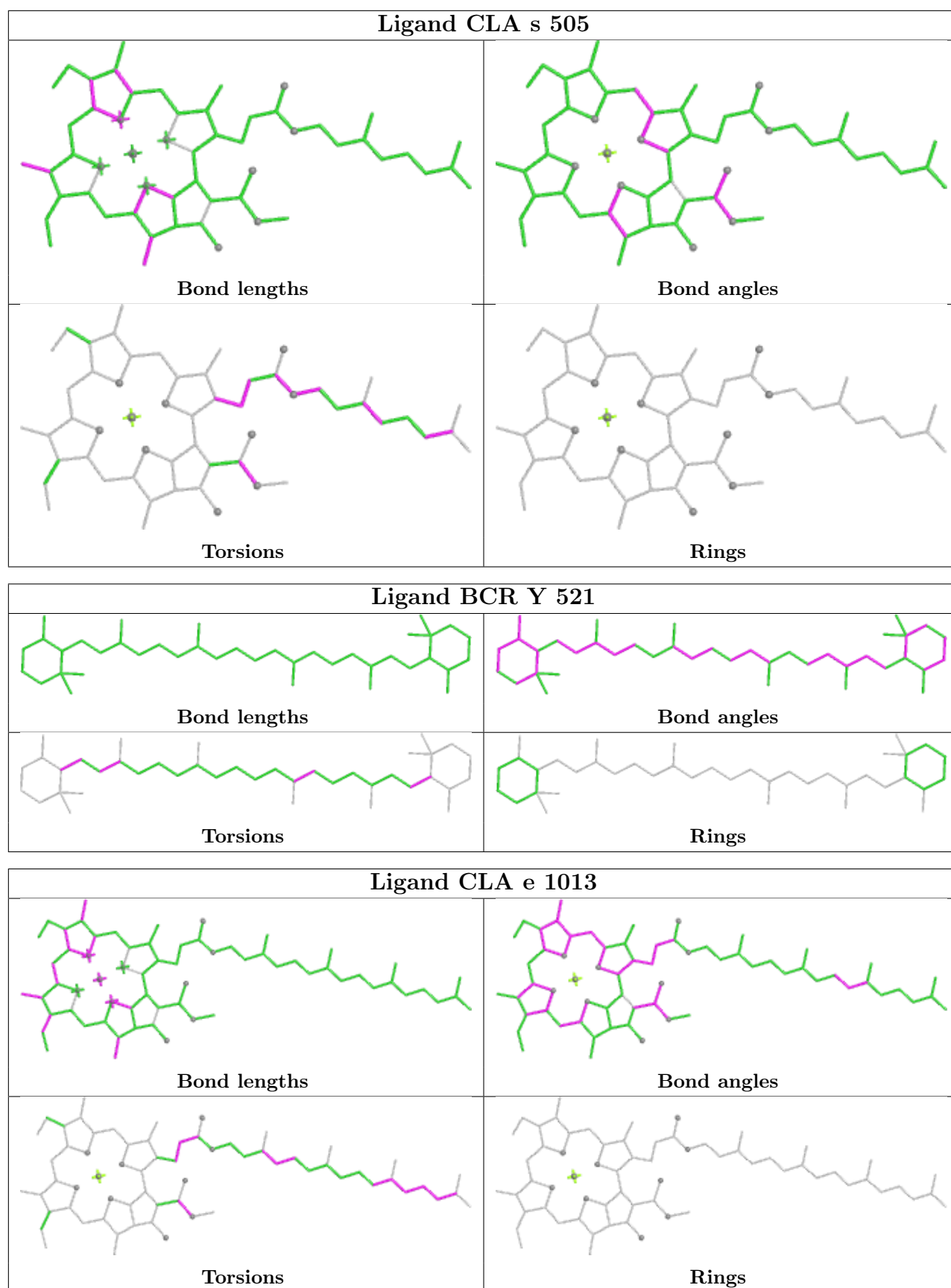
Ligand CLA f 1215

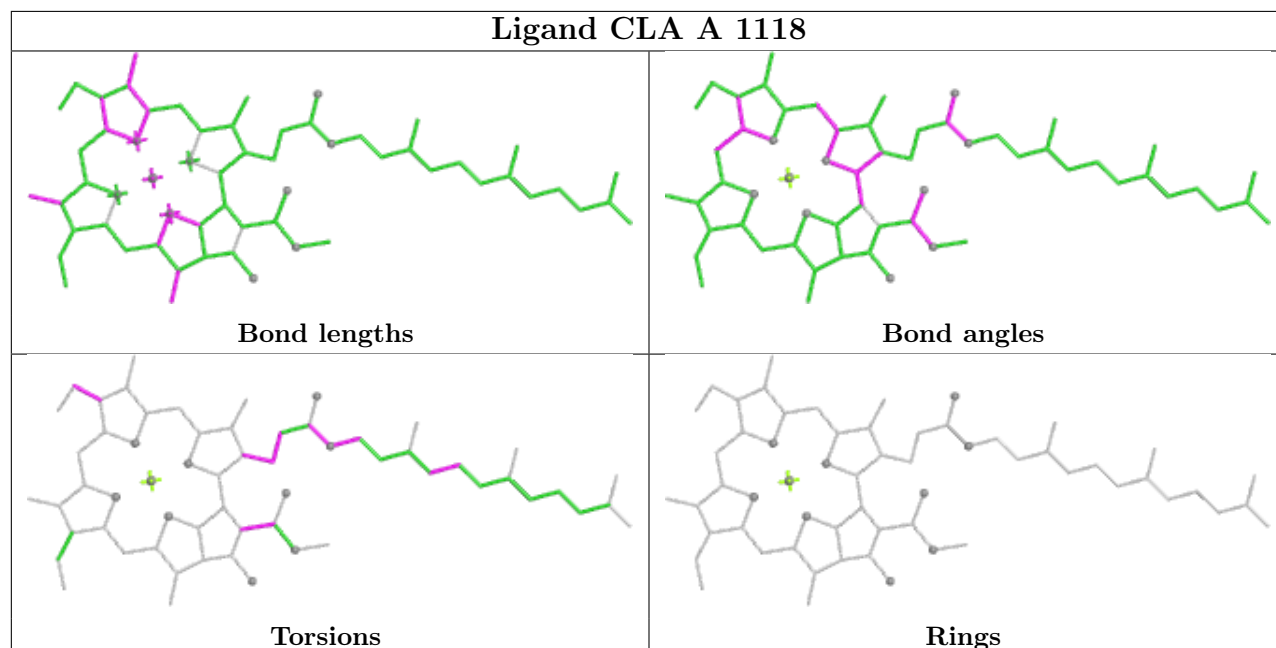
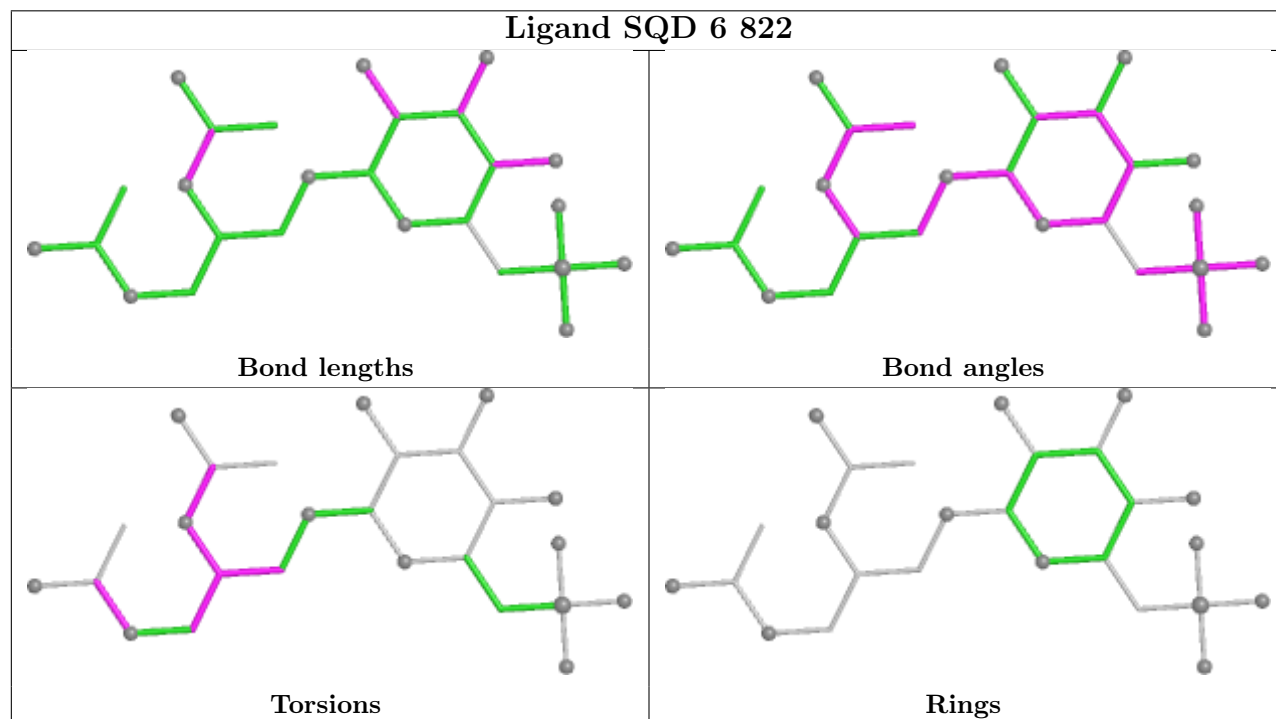
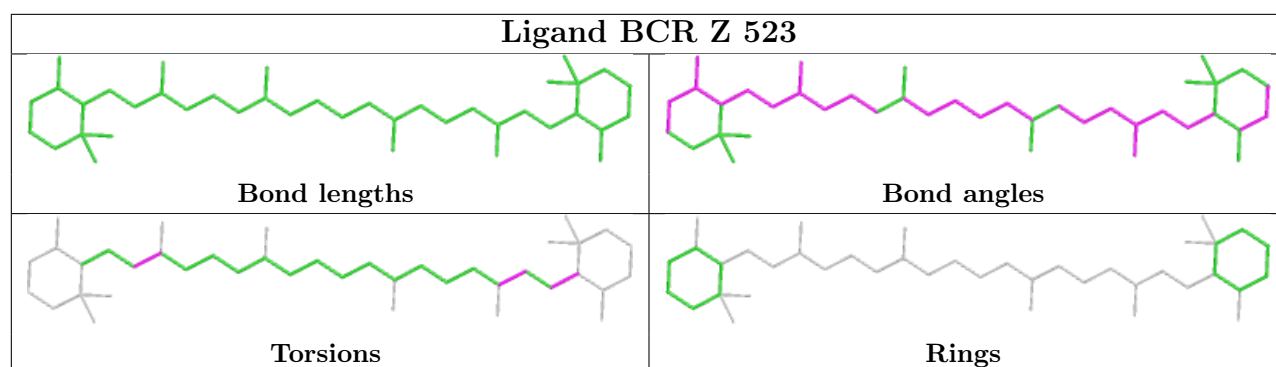


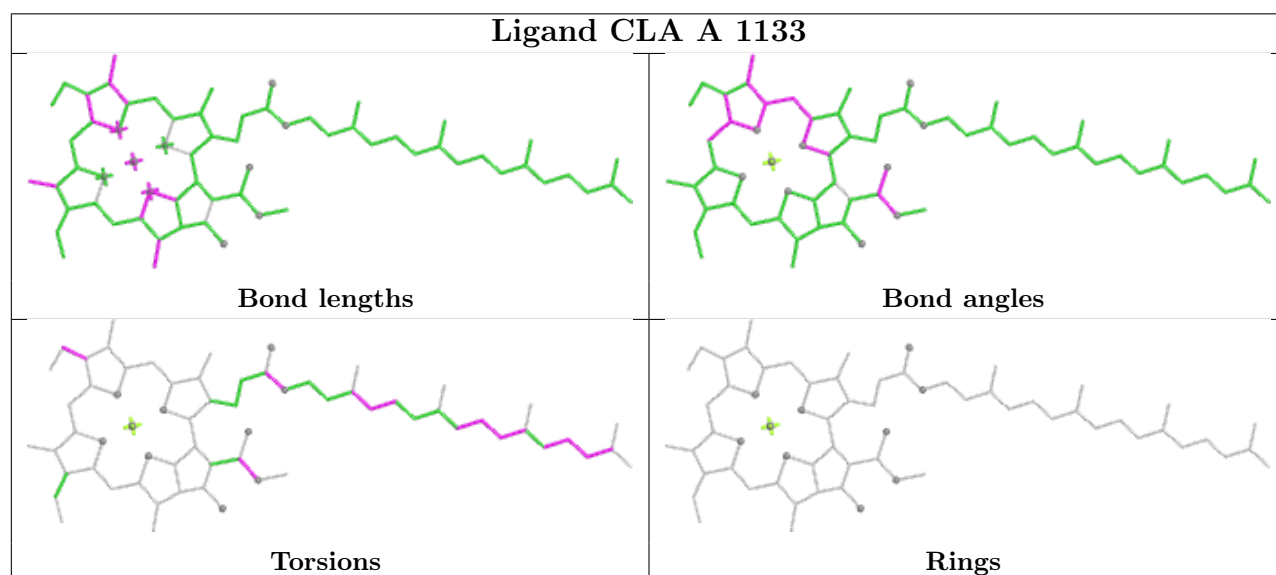
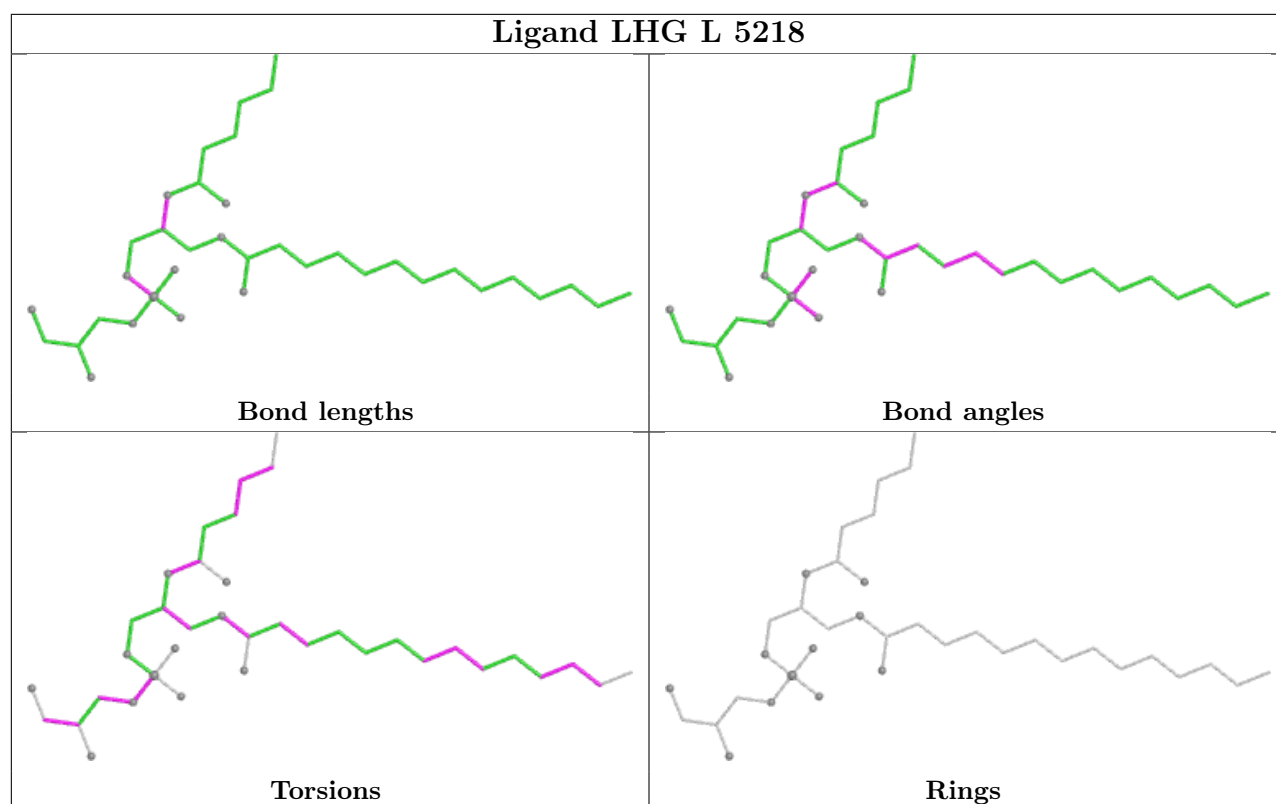
Ligand CLA u 513



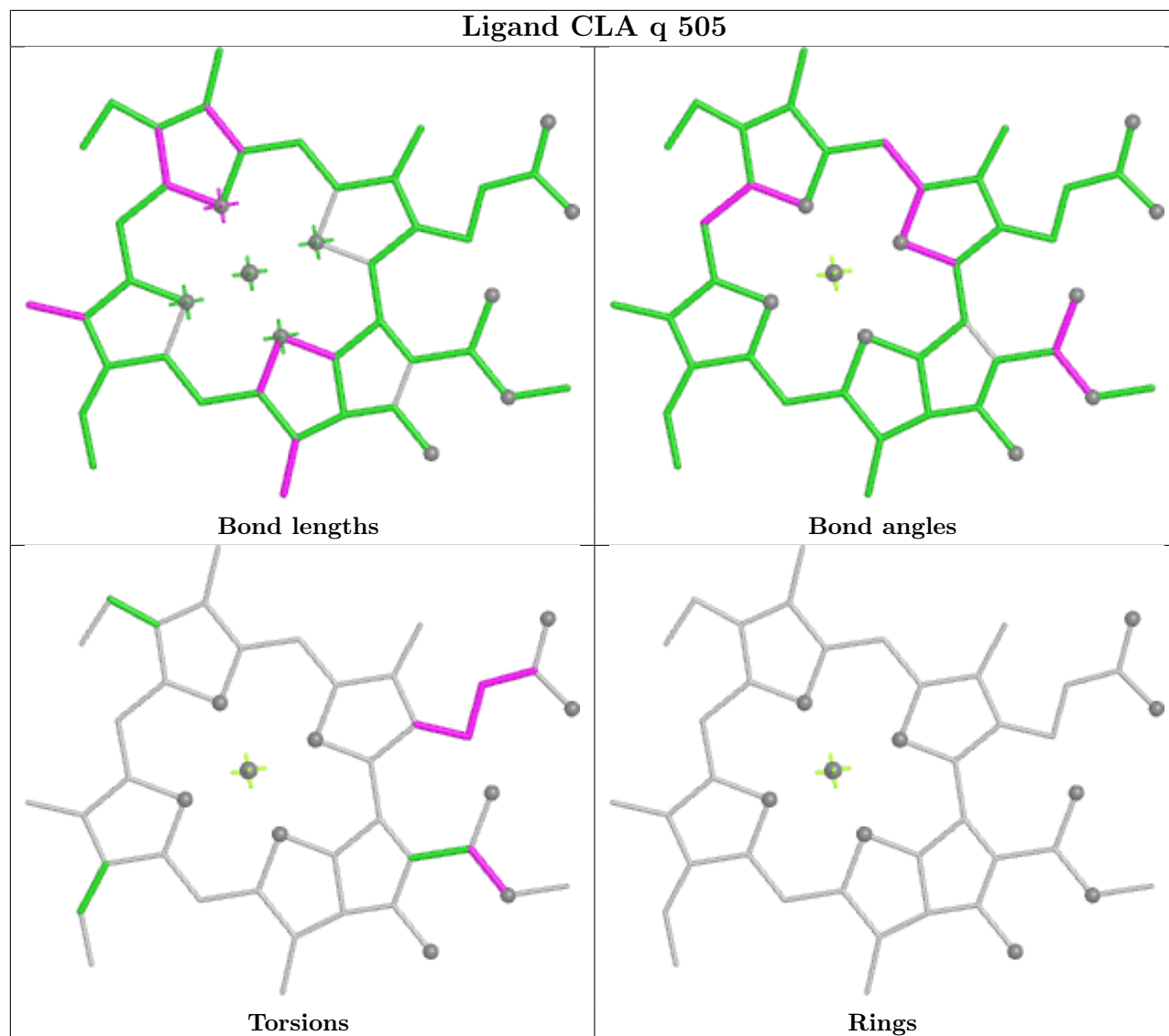




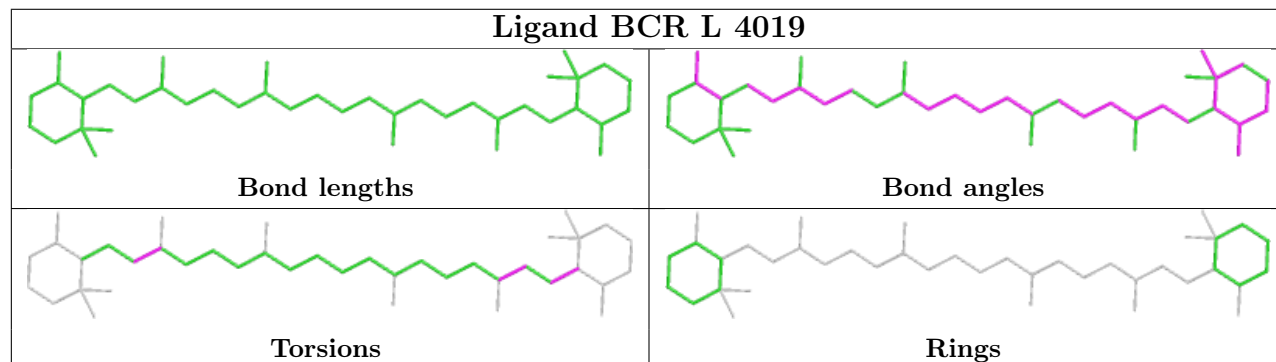




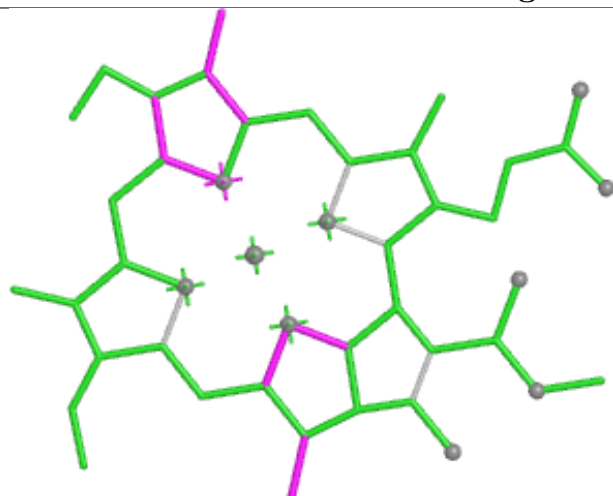
Ligand CLA q 505



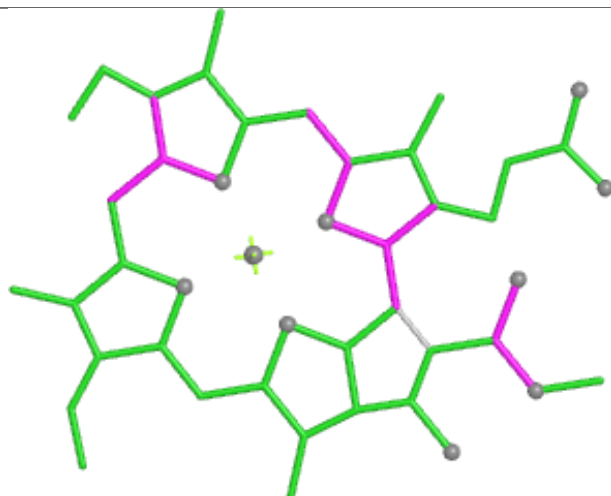
Ligand BCR L 4019



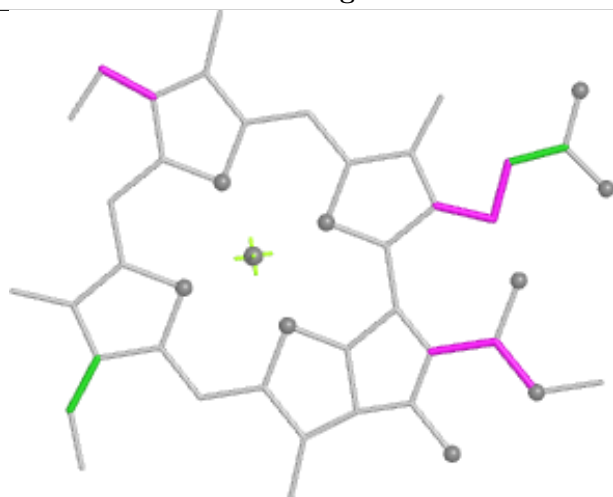
Ligand CLA 5 502



Bond lengths



Bond angles

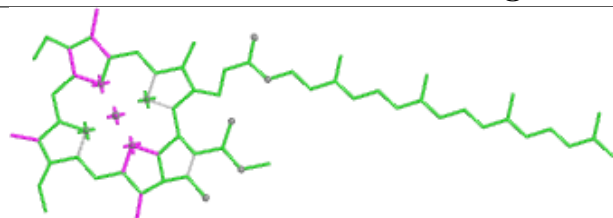


Torsions

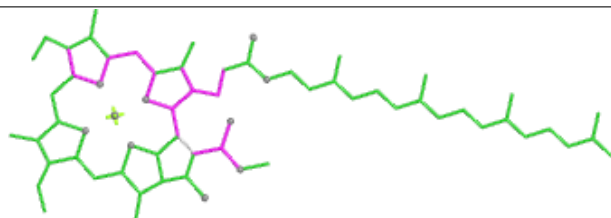


Rings

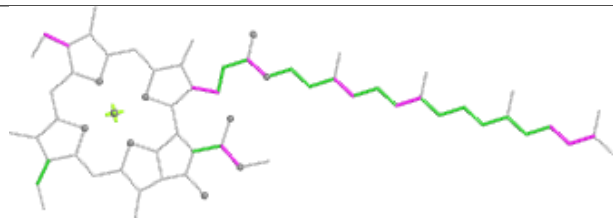
Ligand CLA G 1140



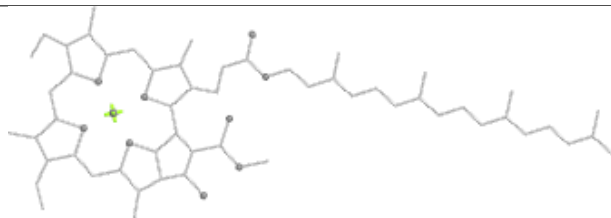
Bond lengths



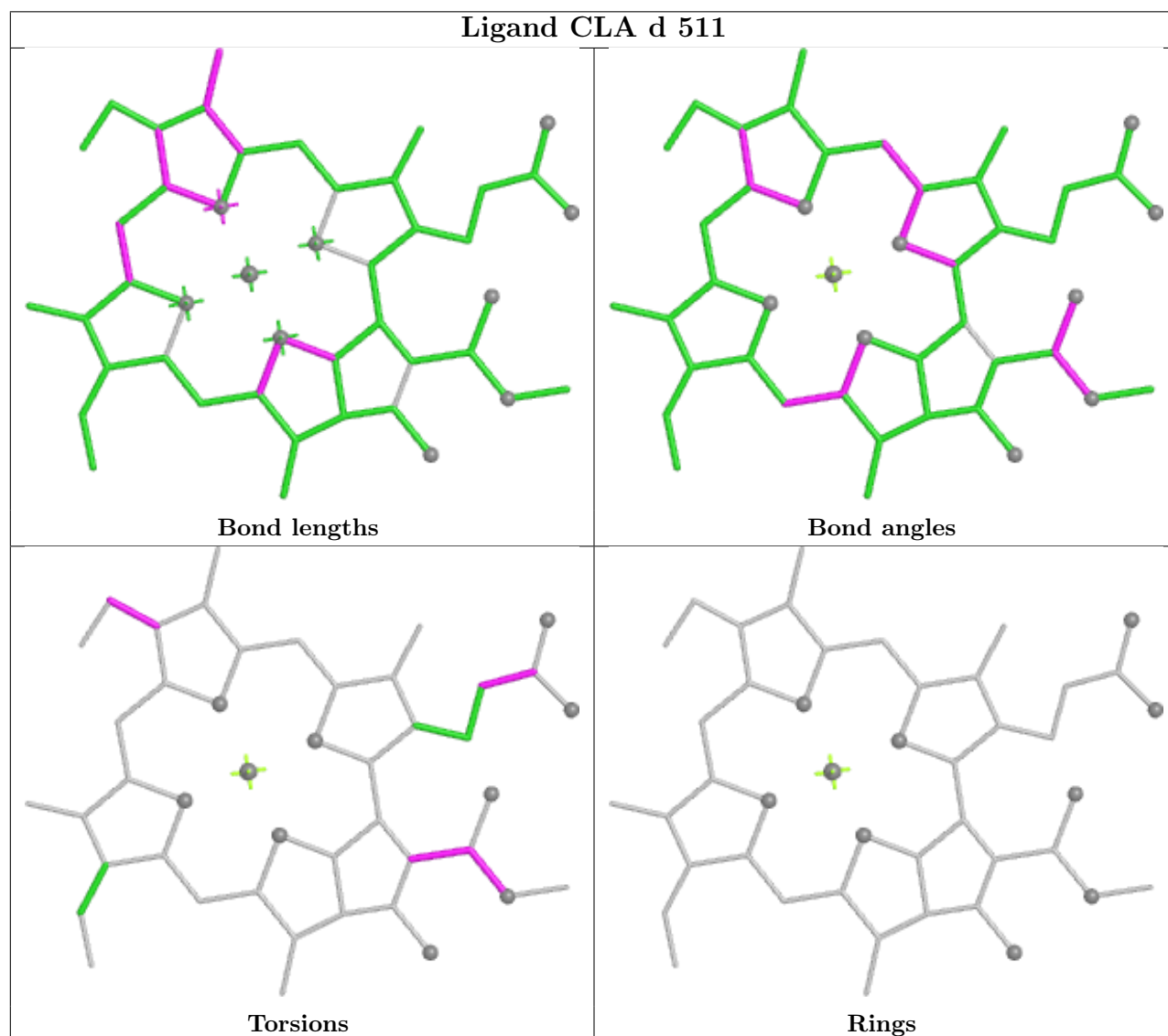
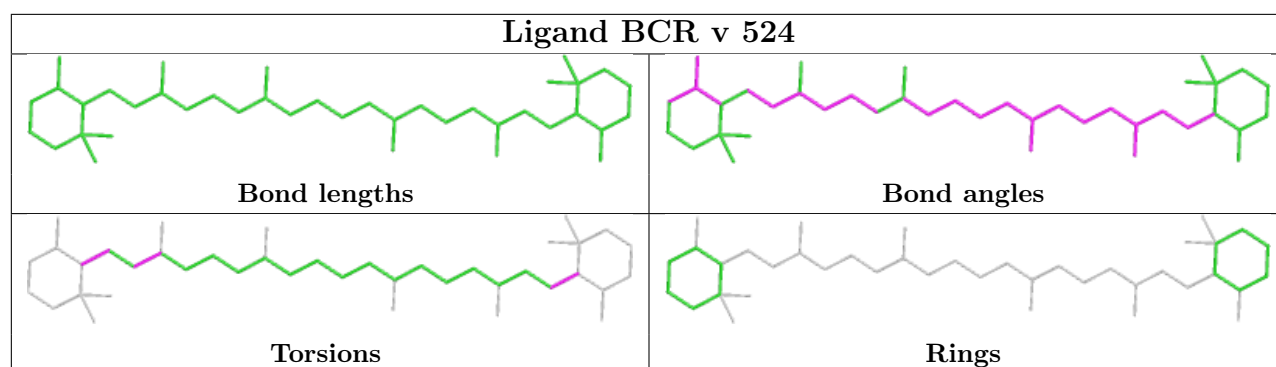
Bond angles

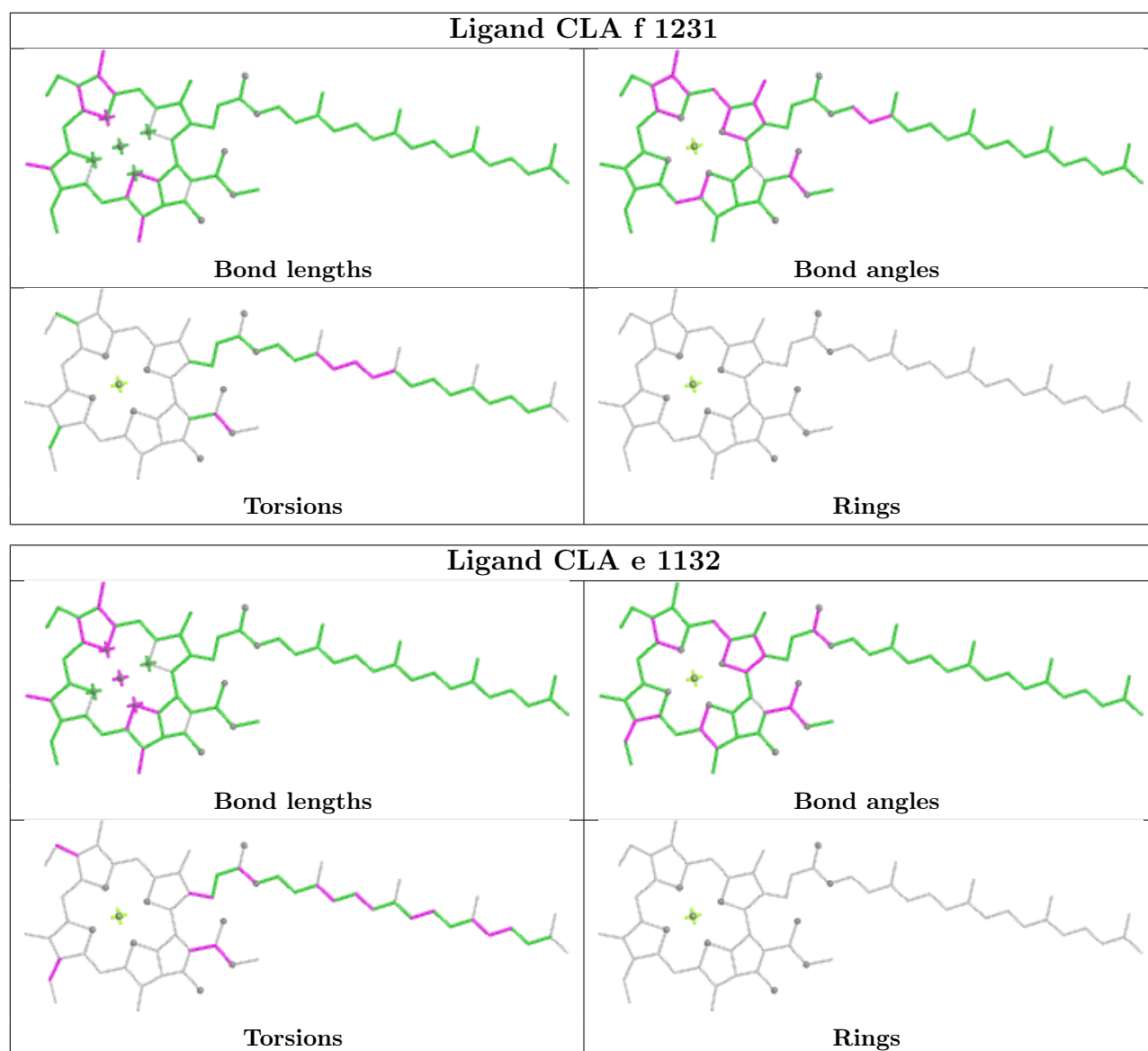


Torsions

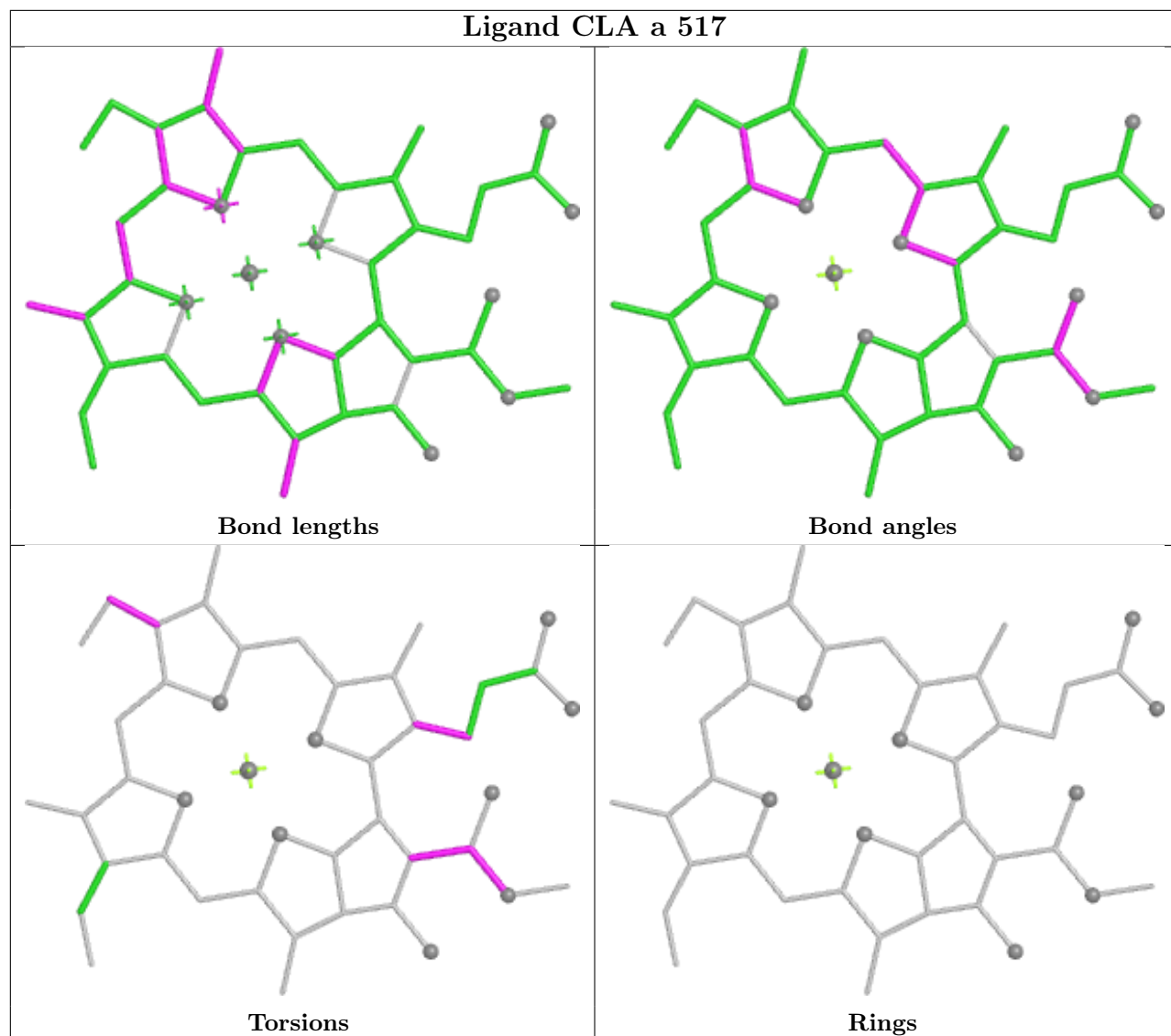


Rings

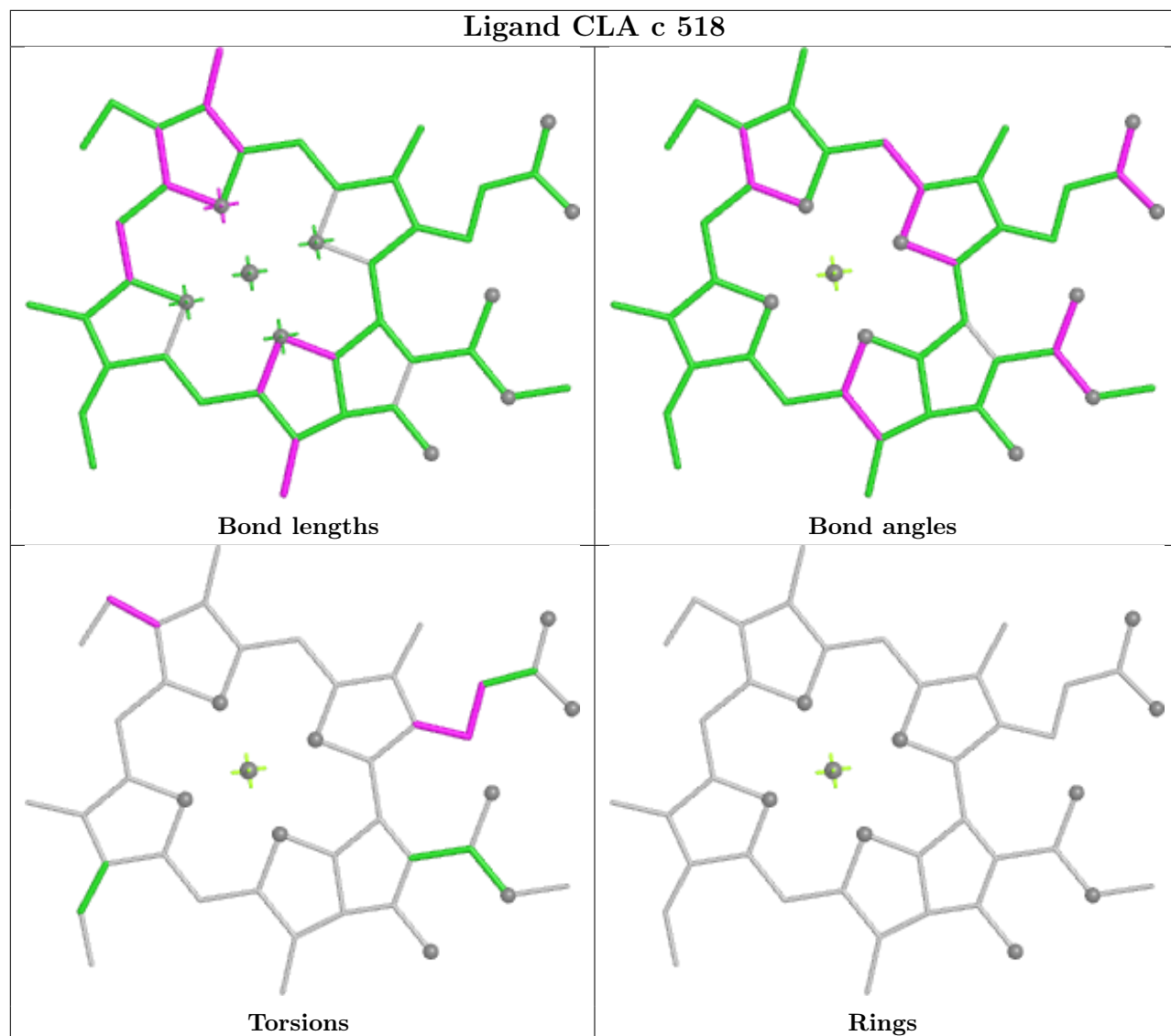


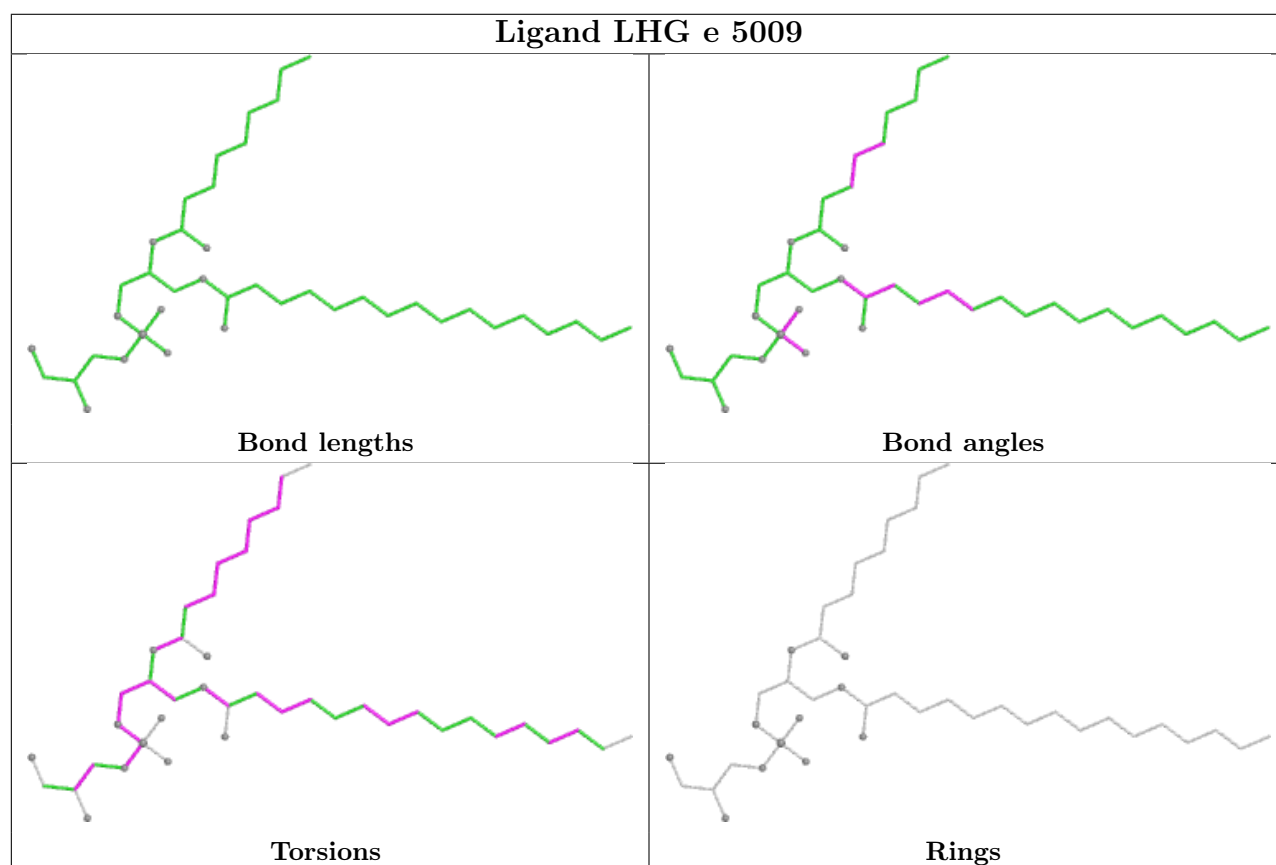
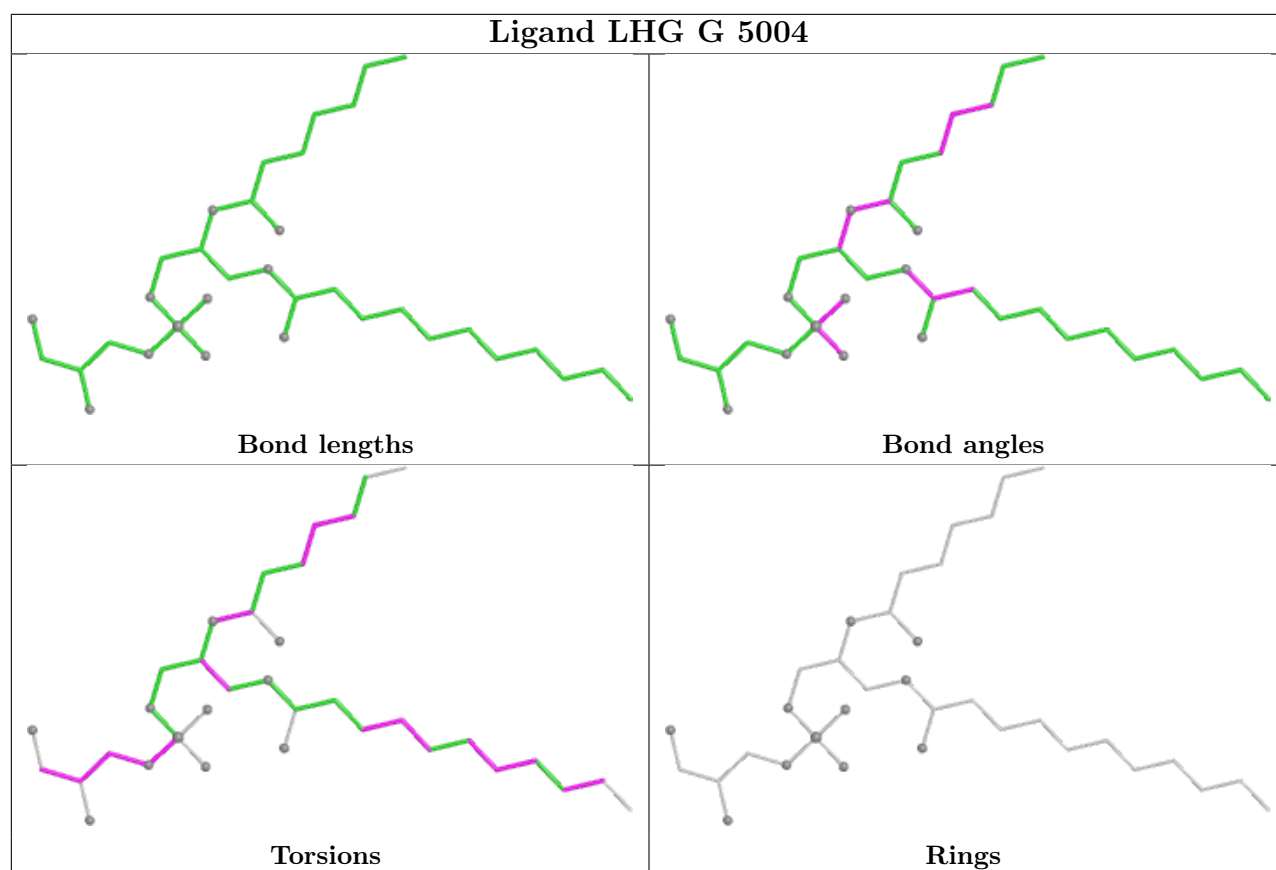


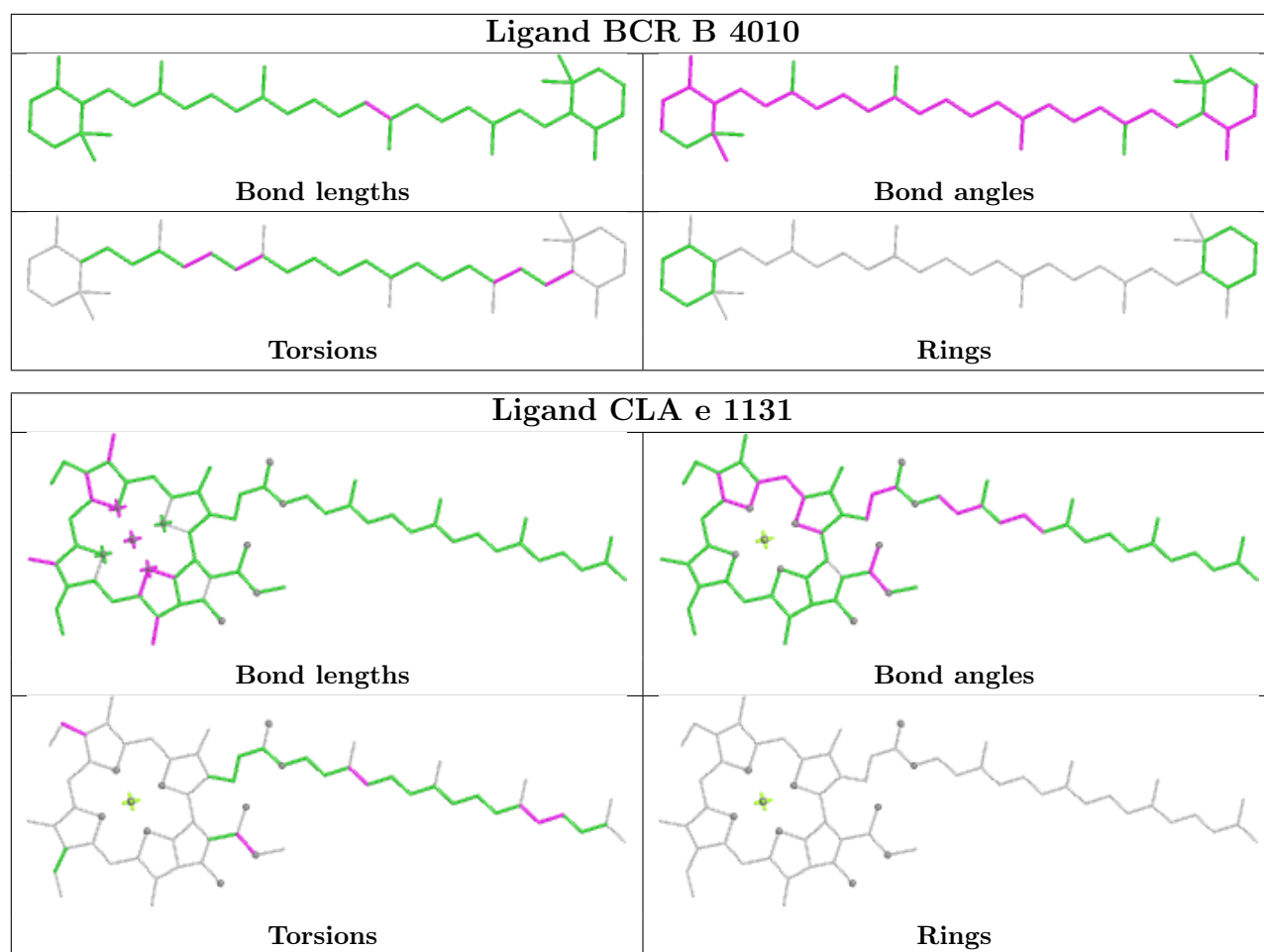
Ligand CLA a 517



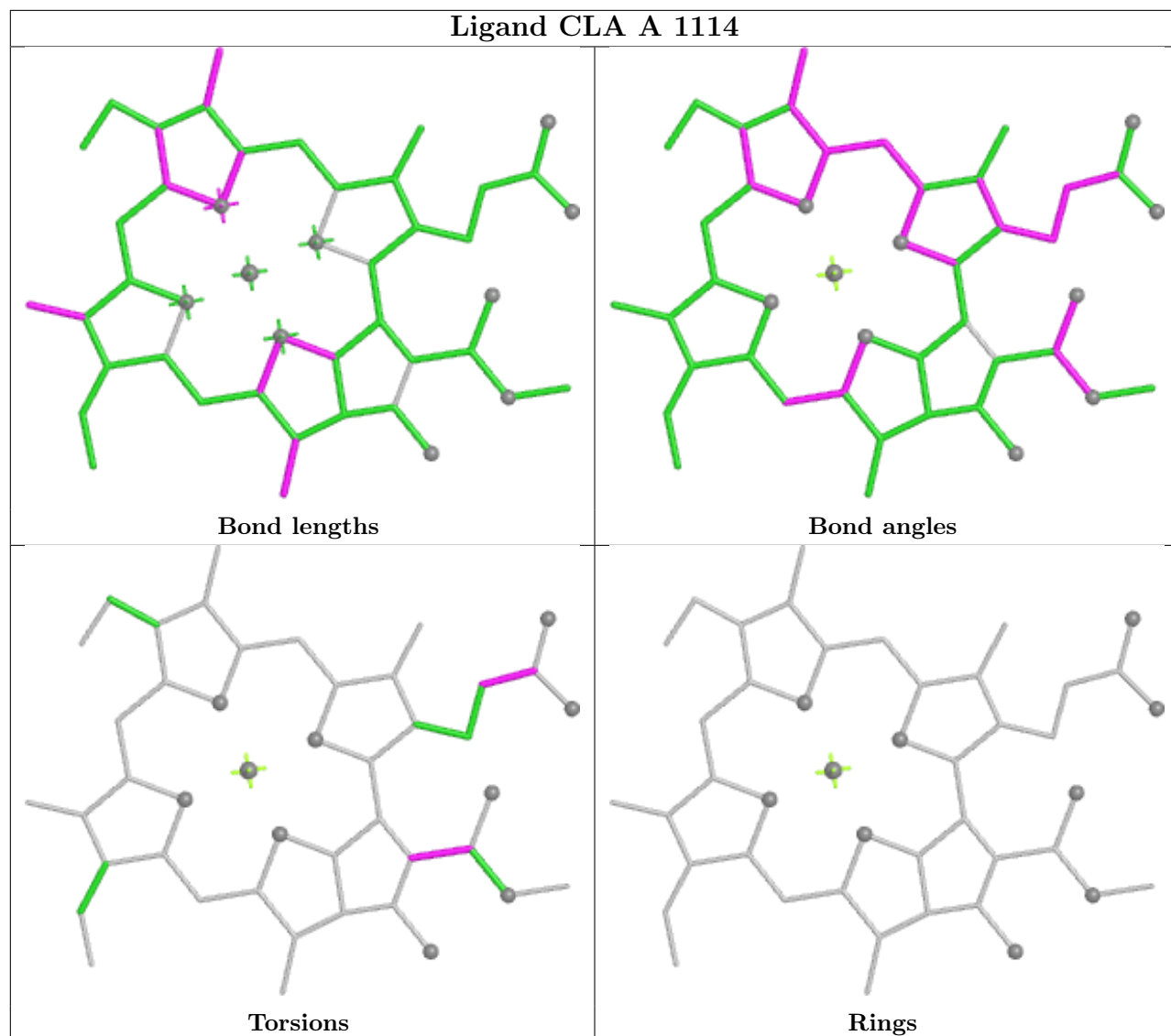
Ligand CLA c 518

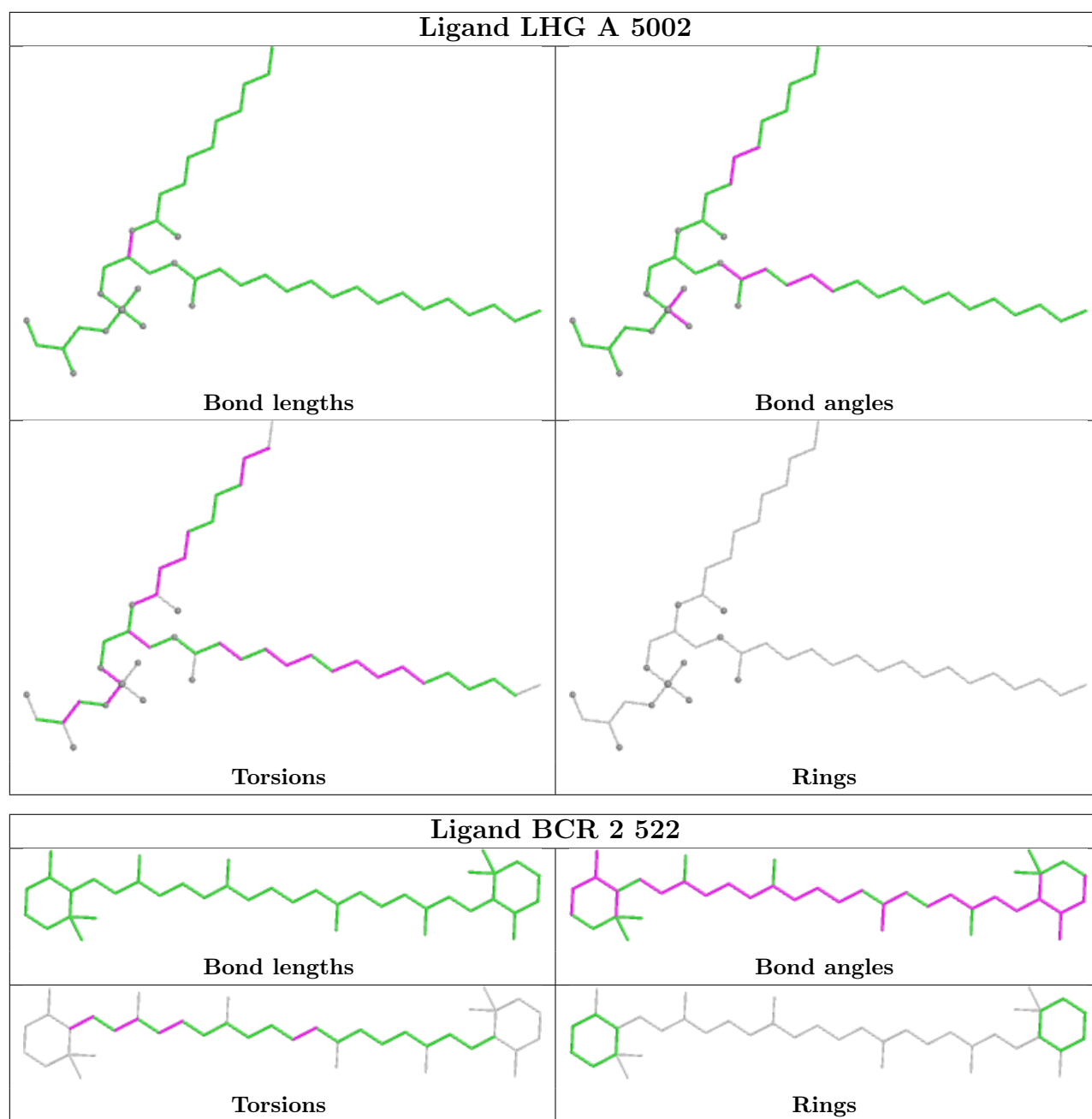




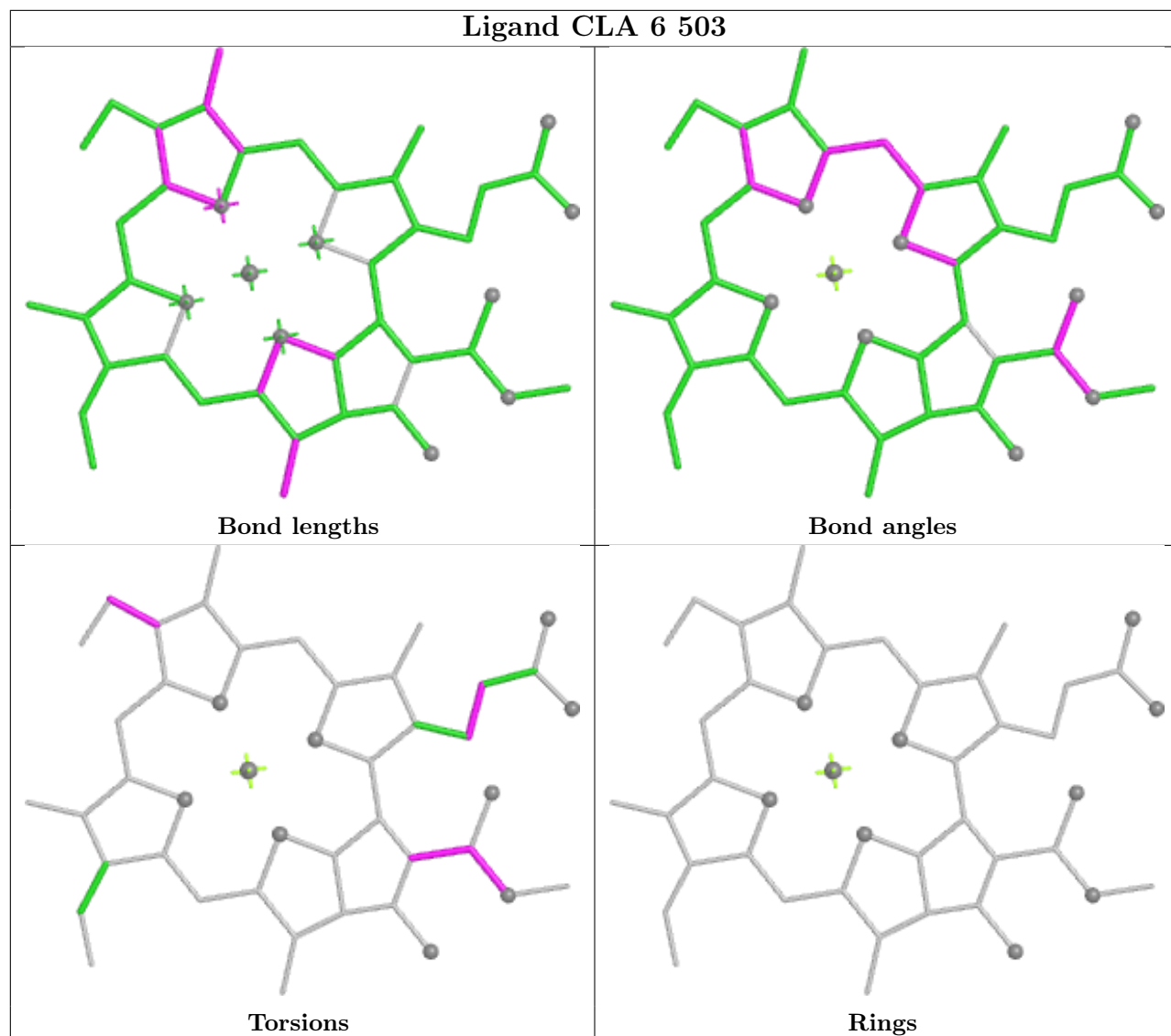


Ligand CLA A 1114

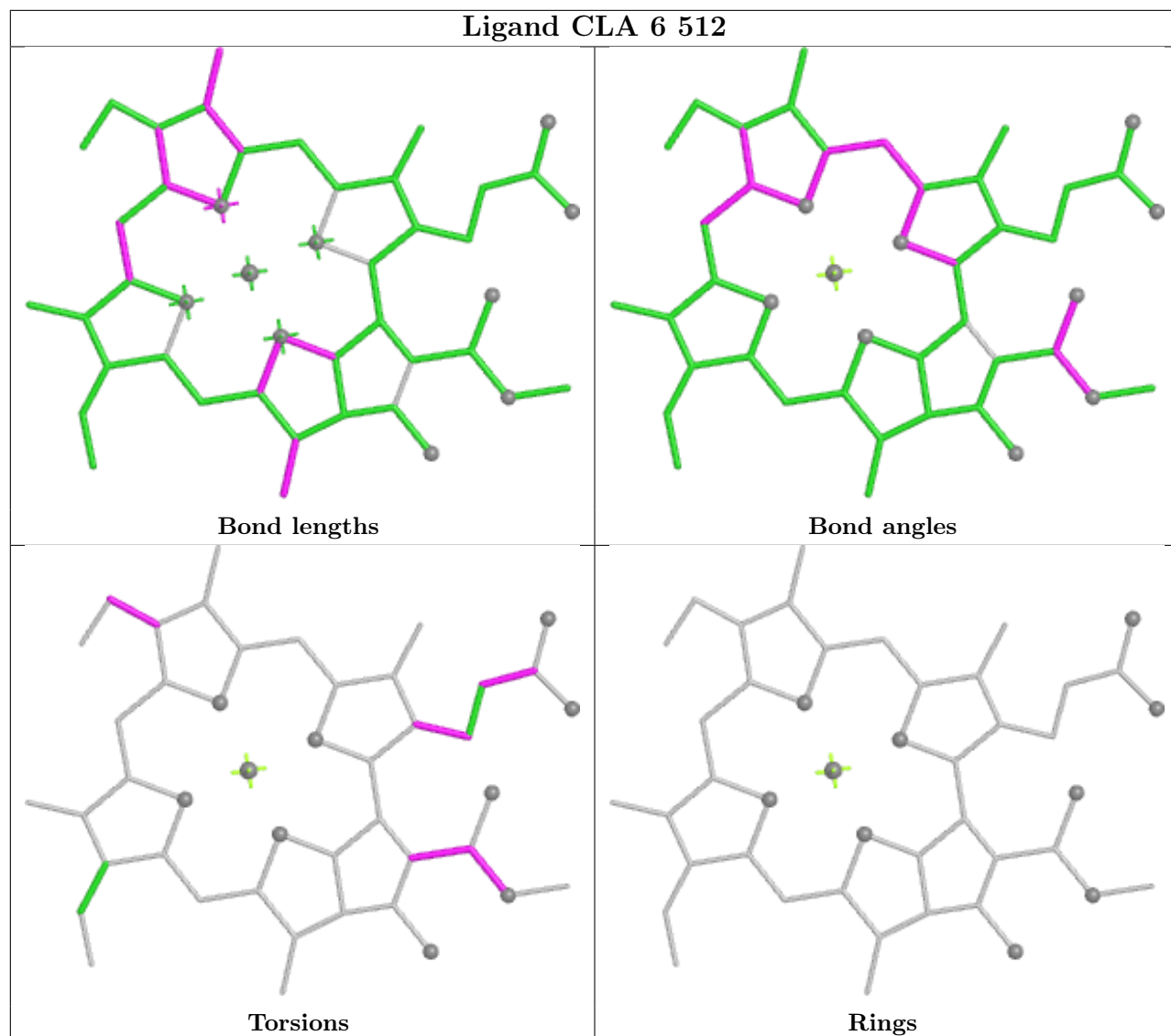




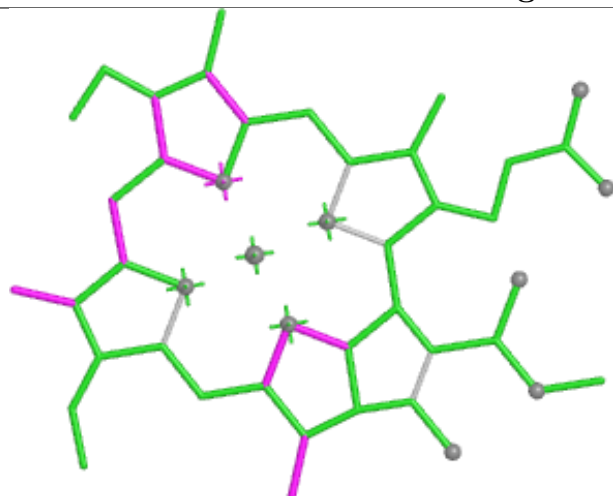
Ligand CLA 6 503



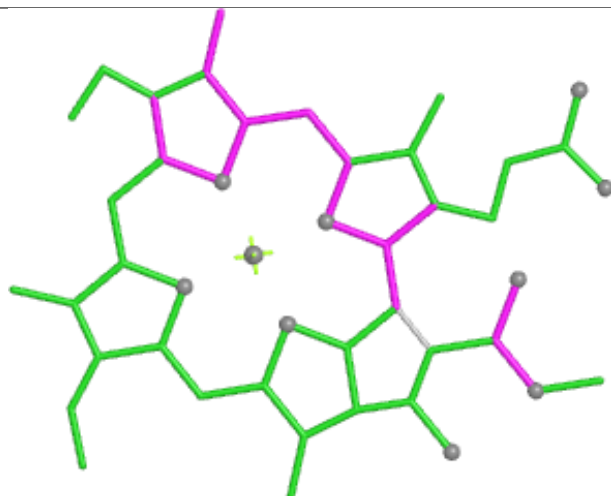
Ligand CLA 6 512



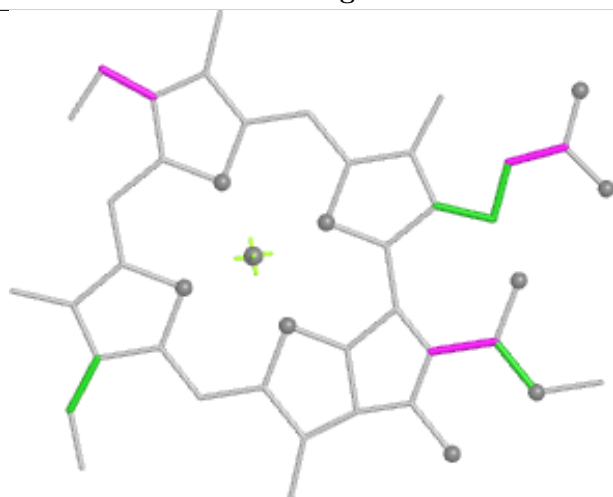
Ligand CLA v 504



Bond lengths



Bond angles

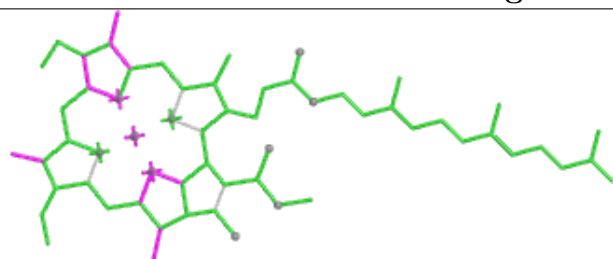


Torsions

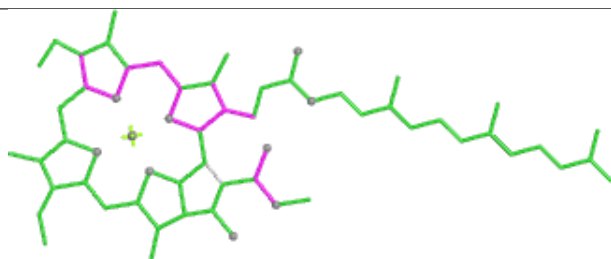


Rings

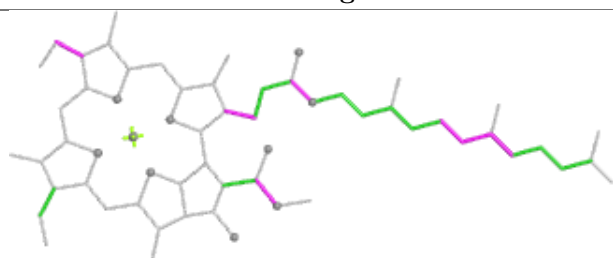
Ligand CLA B 1230



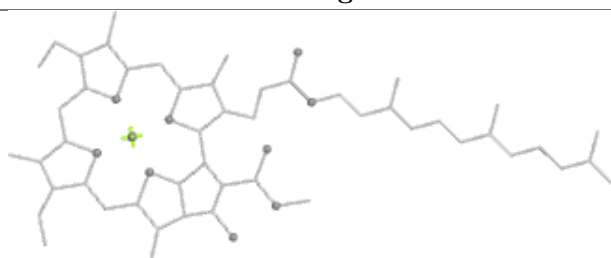
Bond lengths



Bond angles

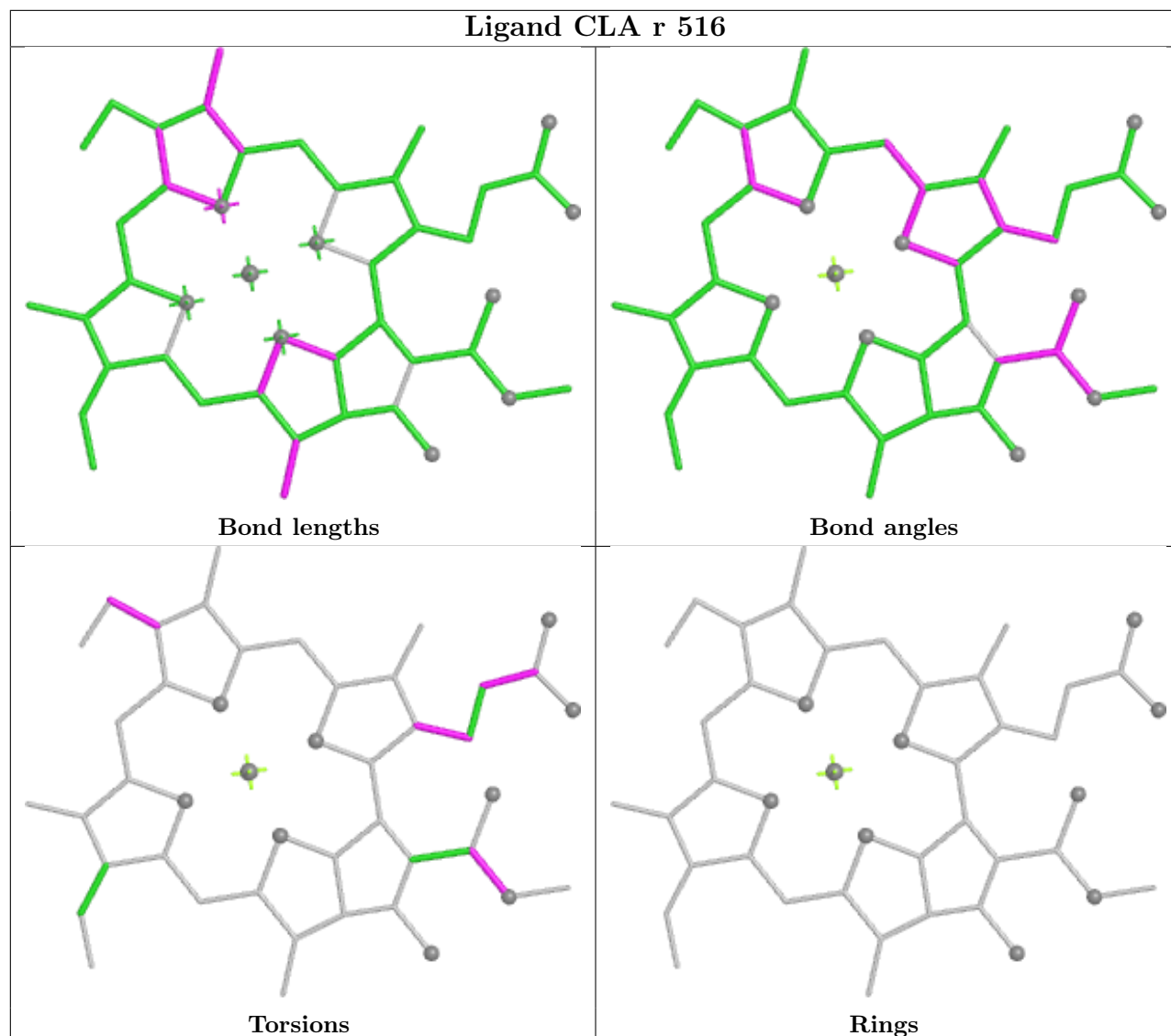


Torsions

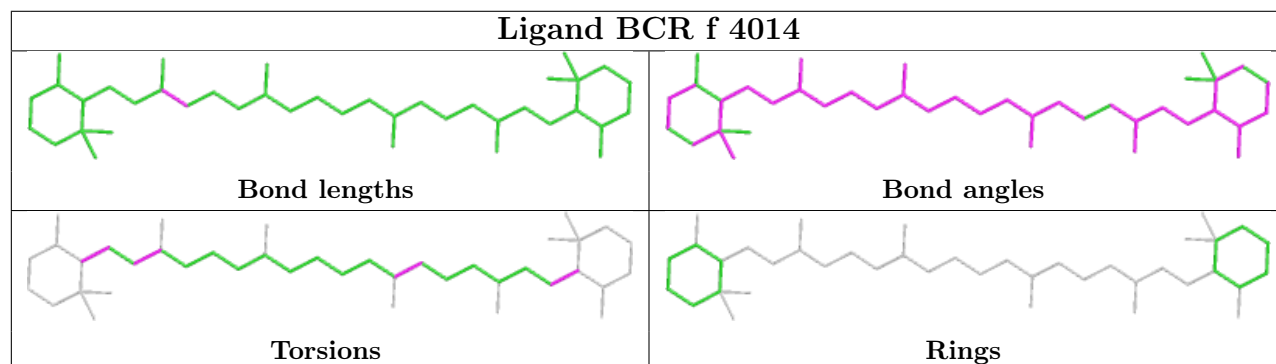


Rings

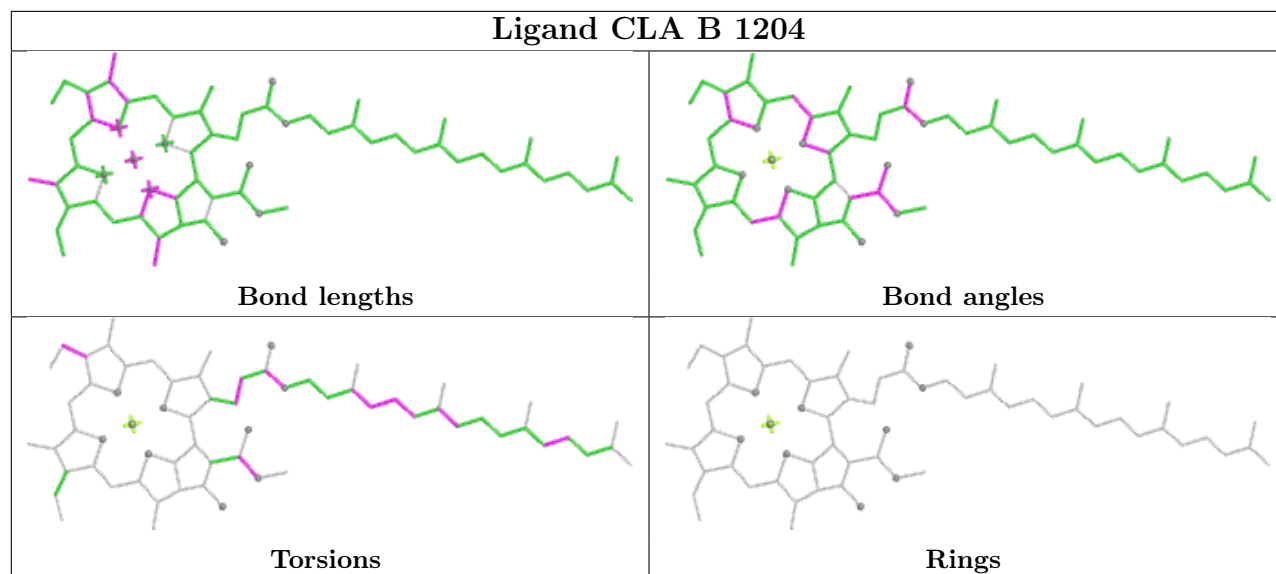
Ligand CLA r 516



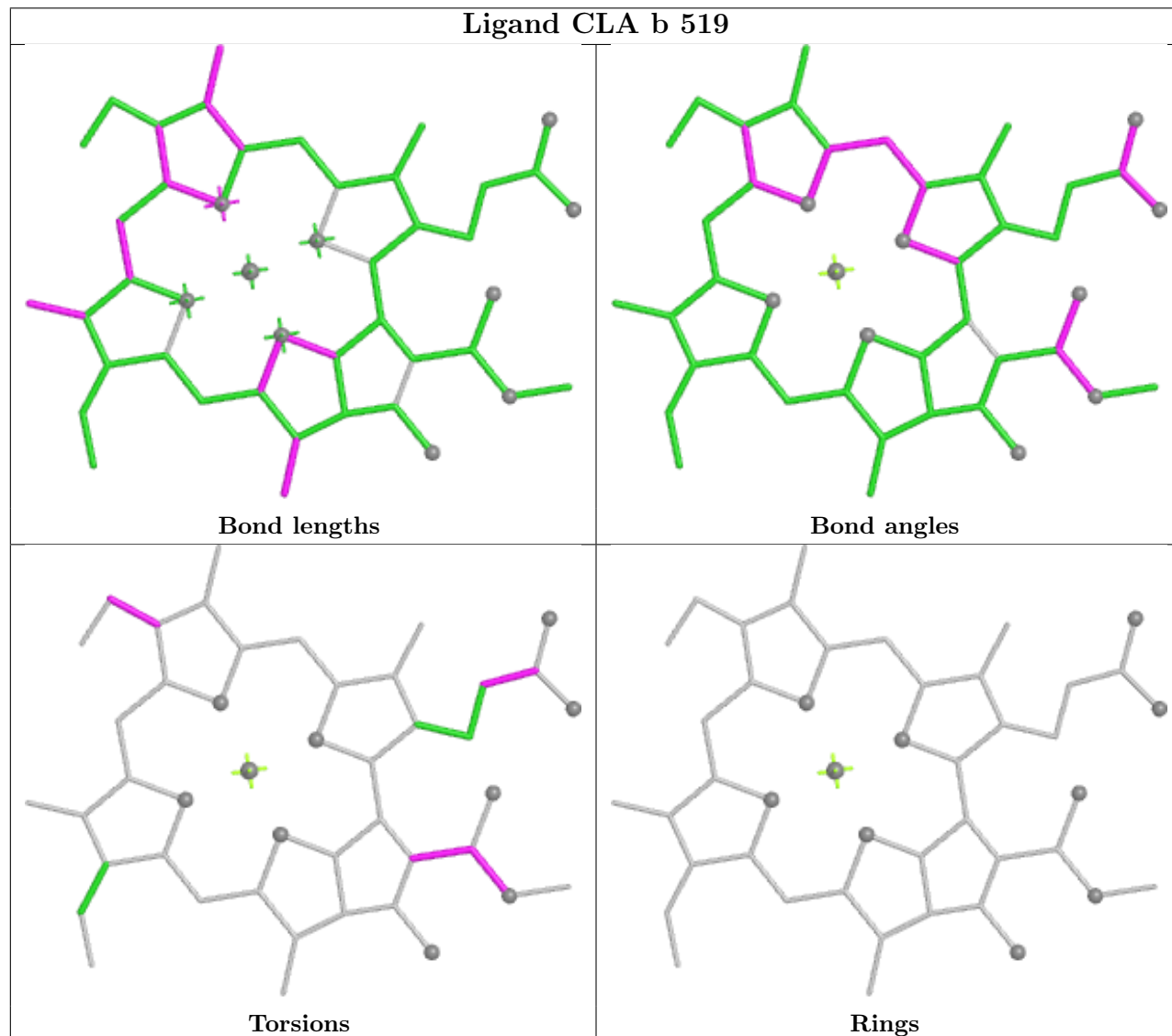
Ligand BCR f 4014



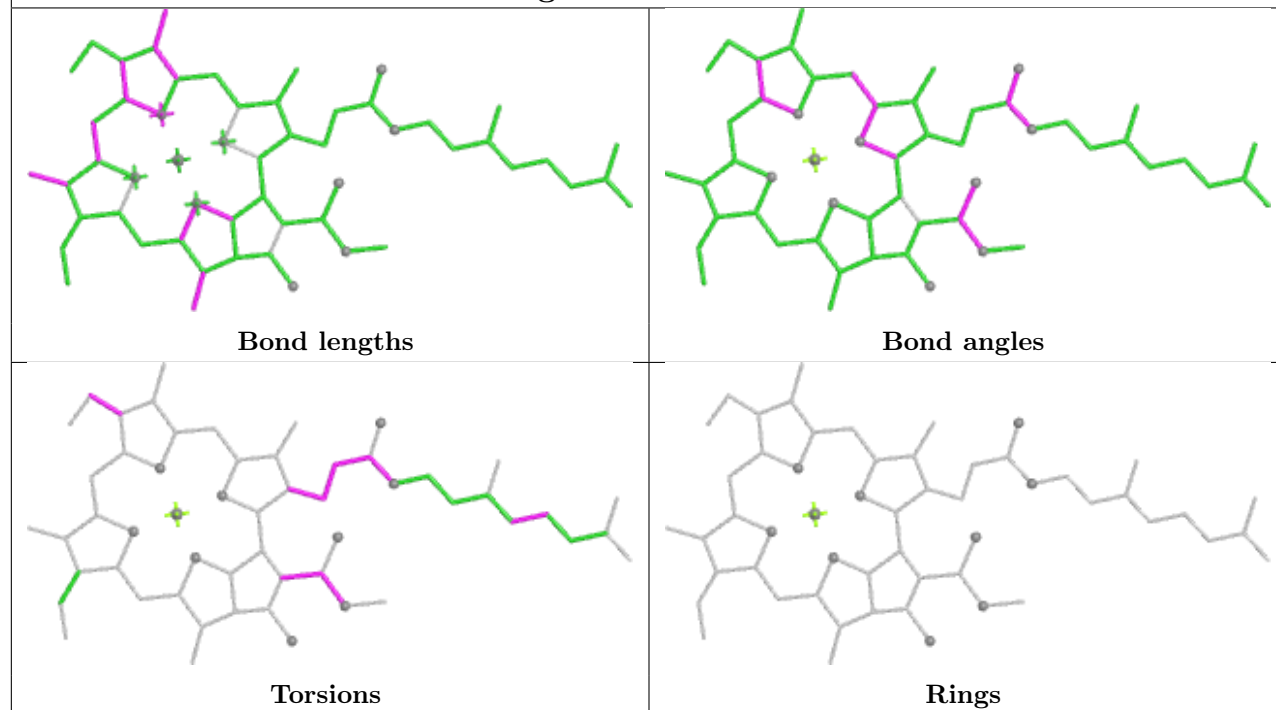
Ligand CLA B 1204



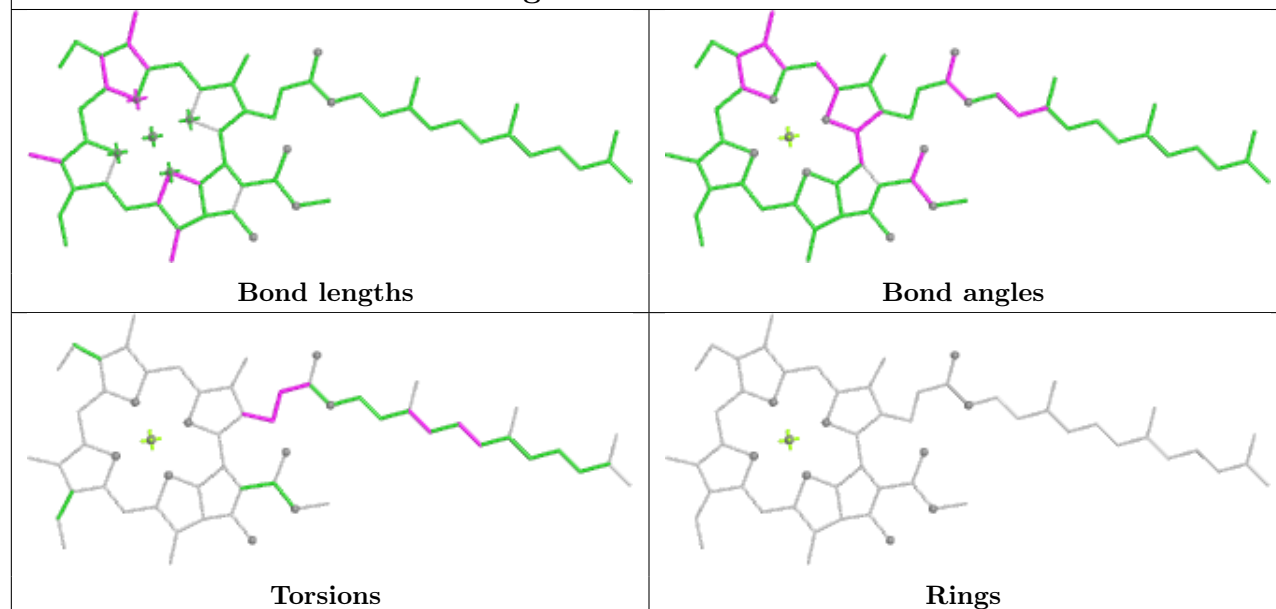
Ligand CLA b 519



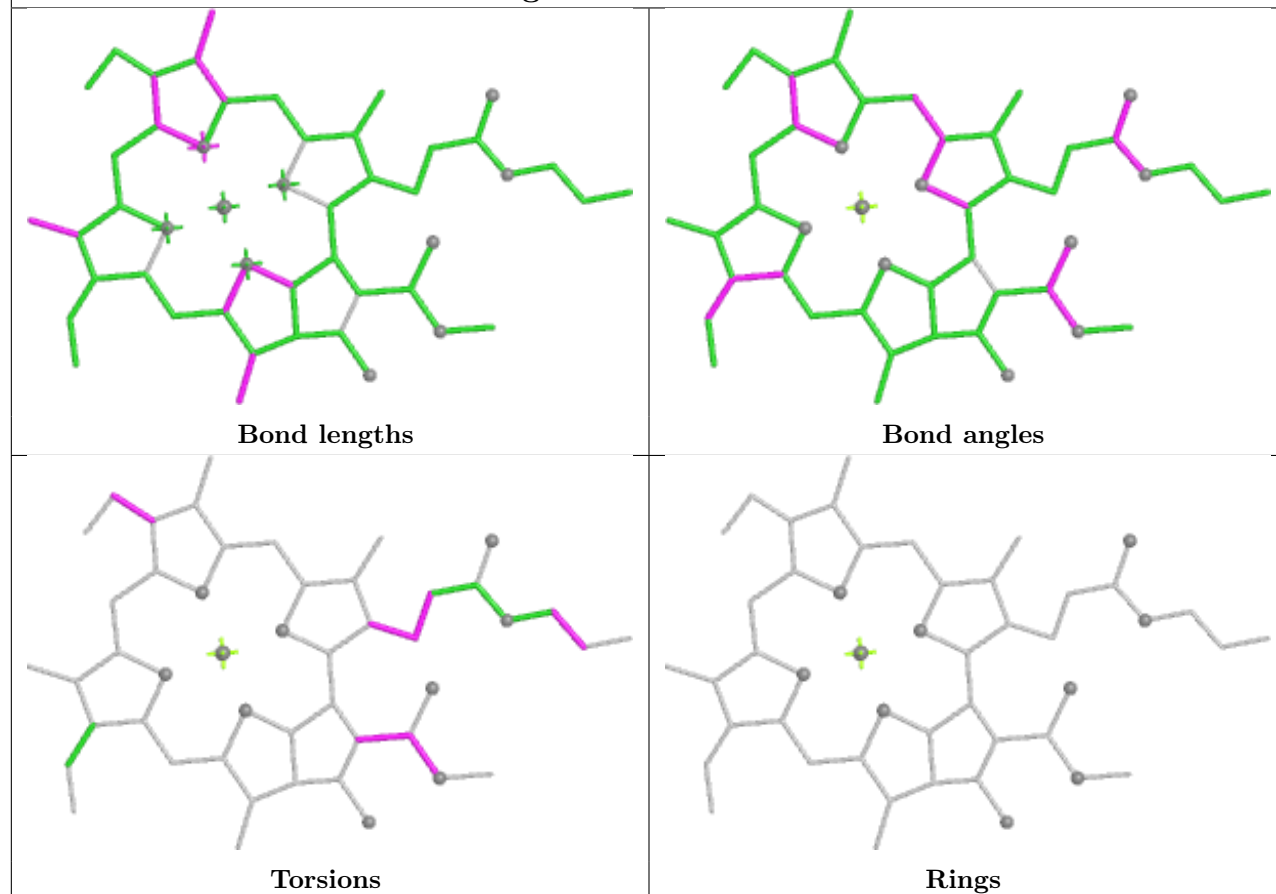
Ligand CLA s 518



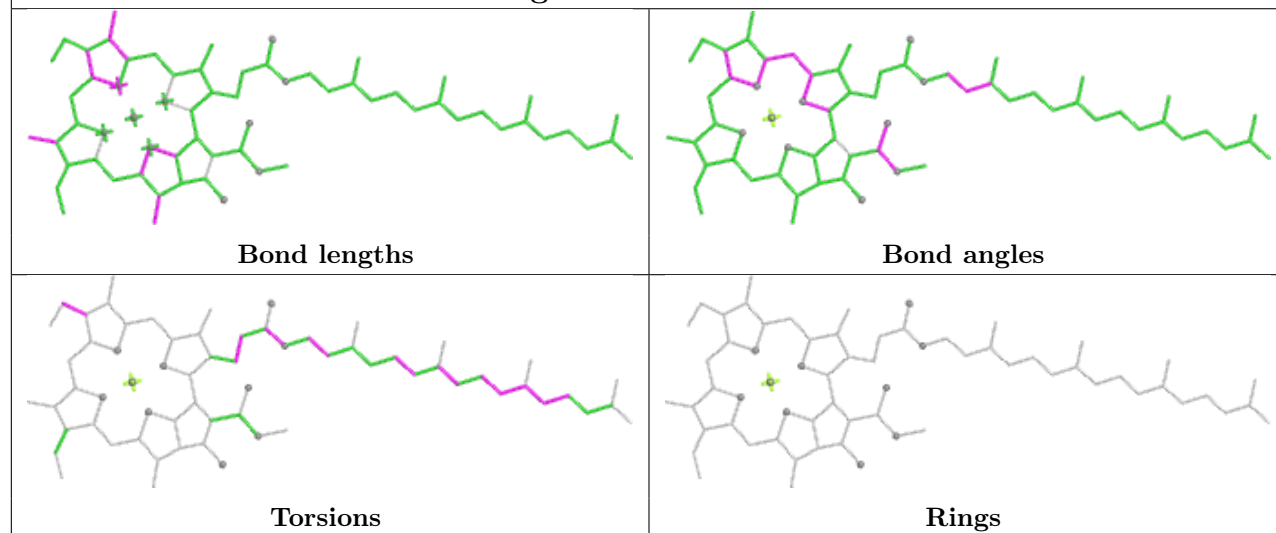
Ligand CLA B 1224

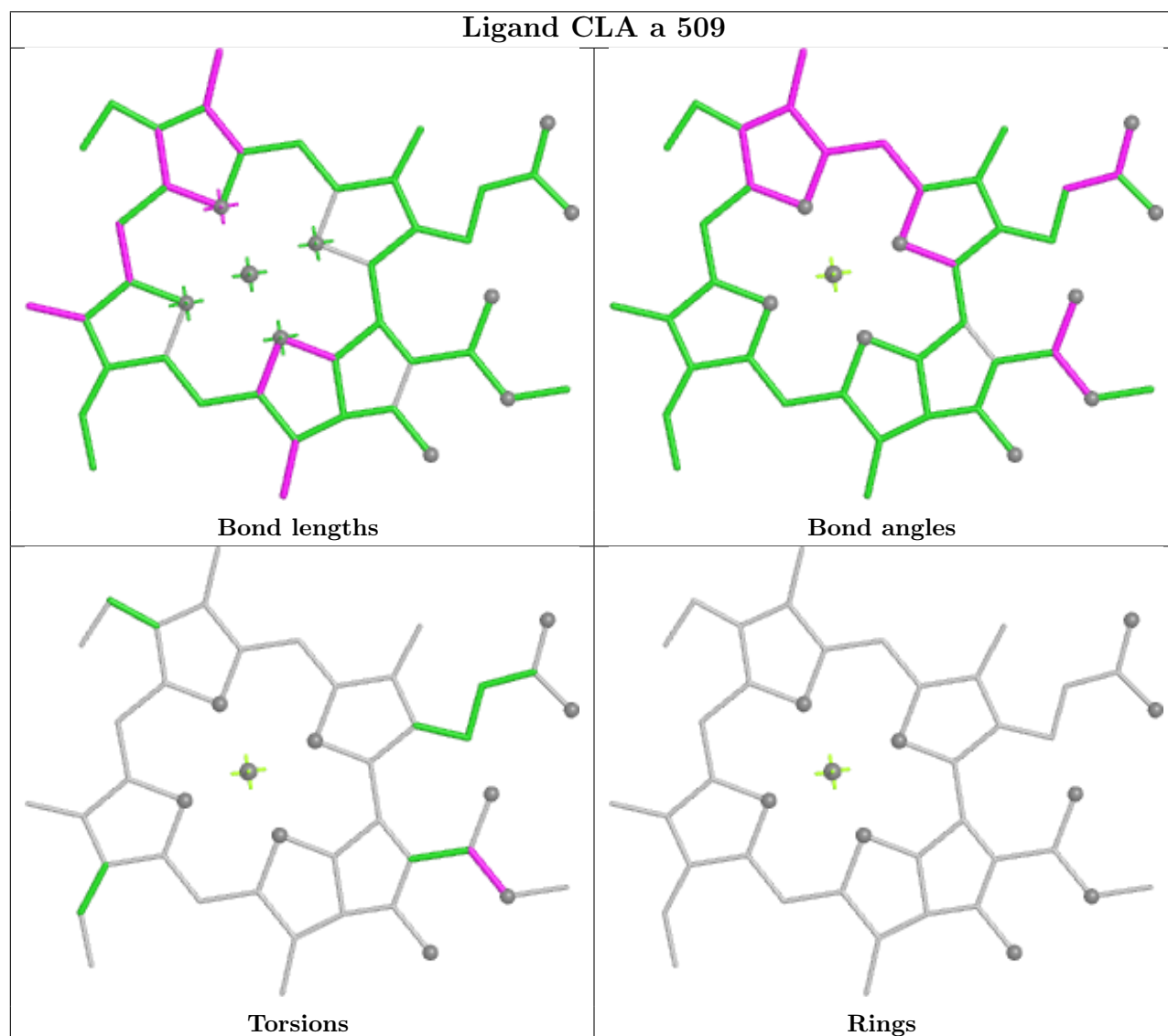
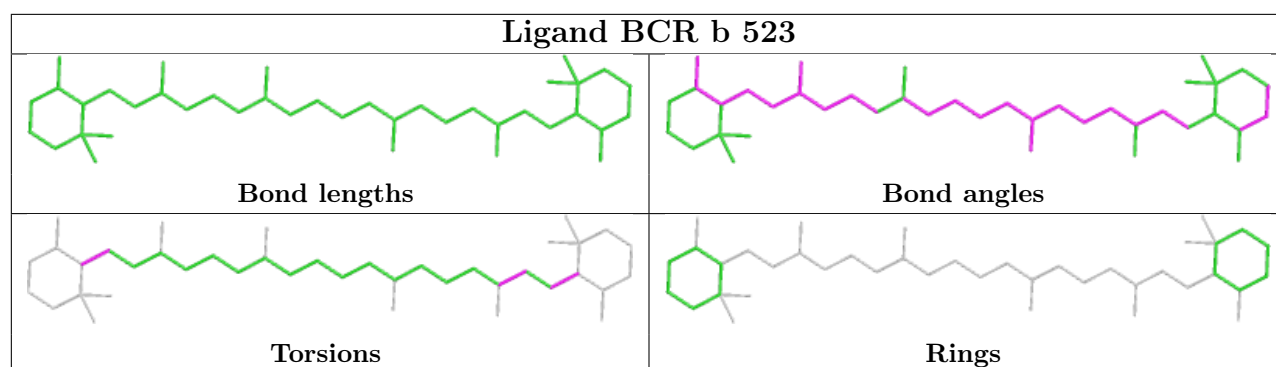


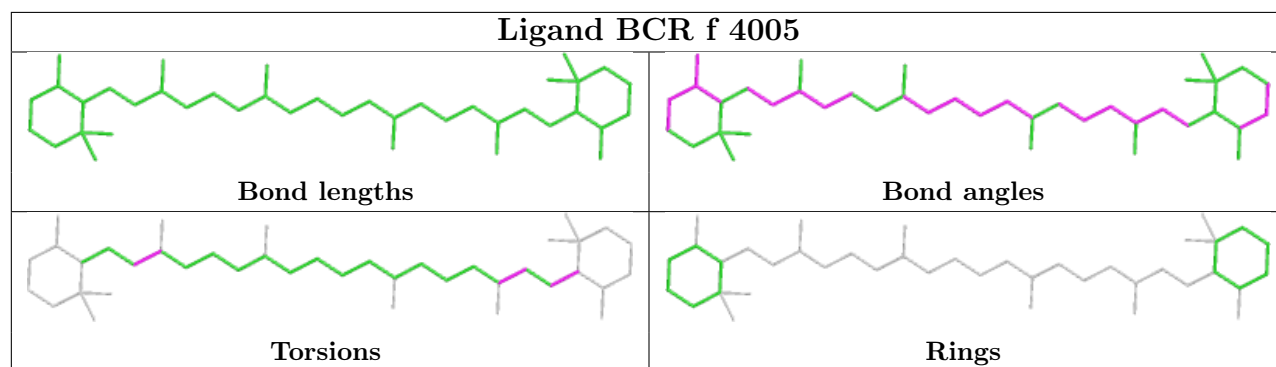
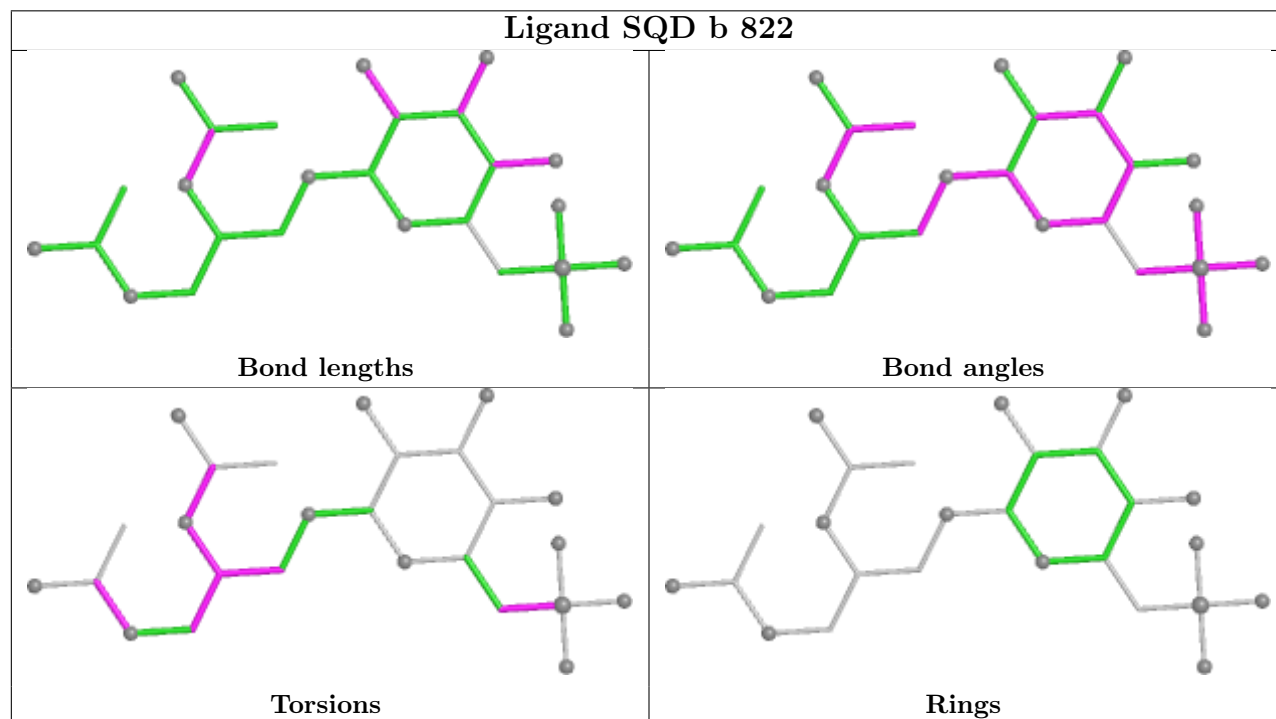
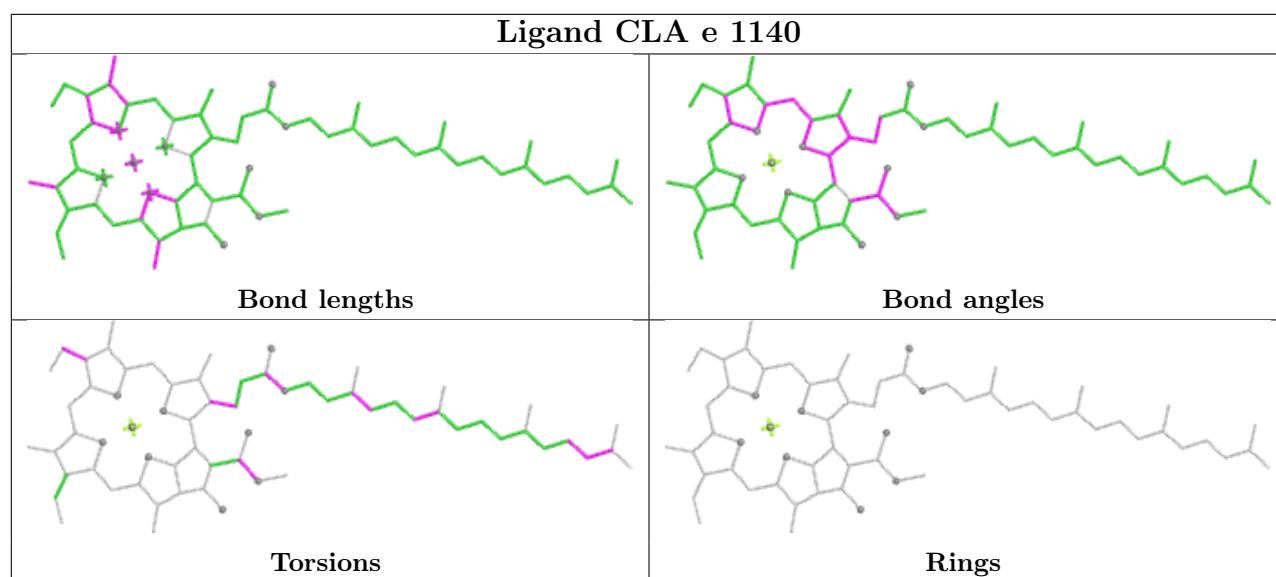
Ligand CLA K 1103



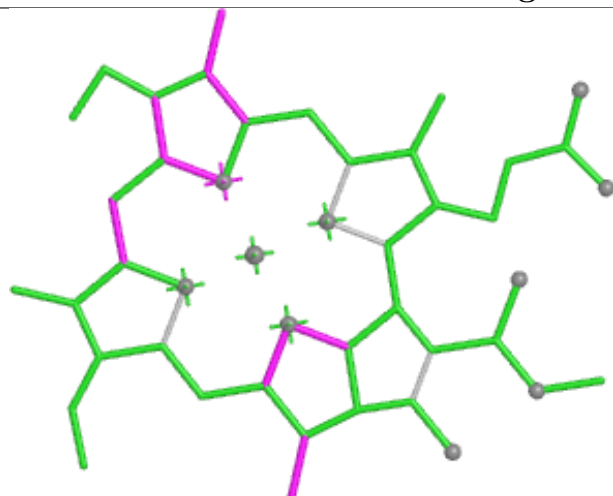
Ligand CLA f 1214



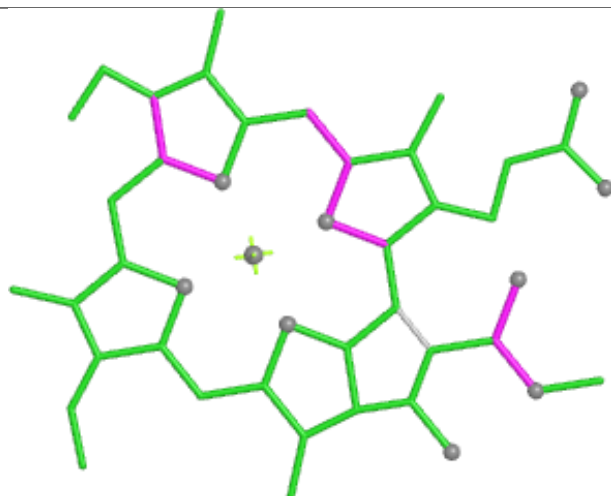




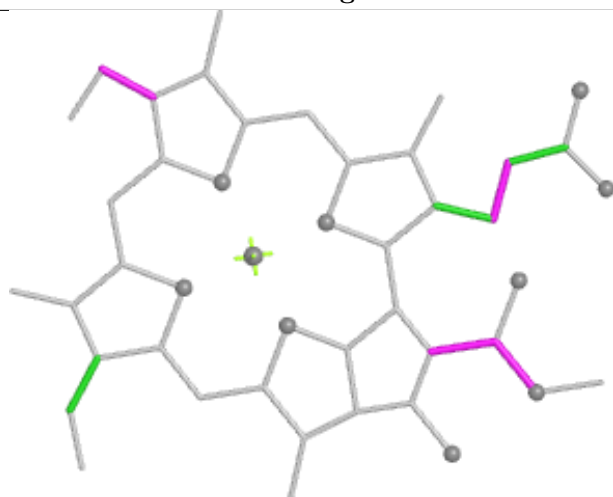
Ligand CLA 4 518



Bond lengths



Bond angles

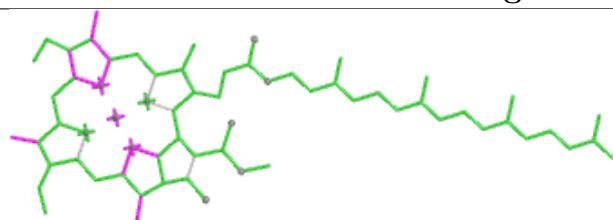


Torsions

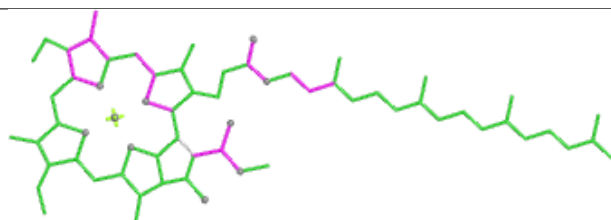


Rings

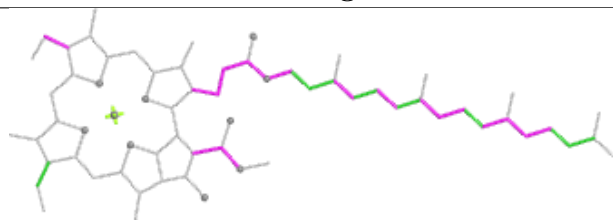
Ligand CLA G 1106



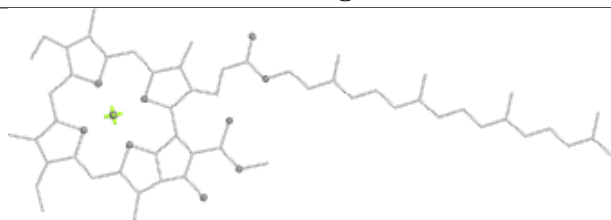
Bond lengths



Bond angles

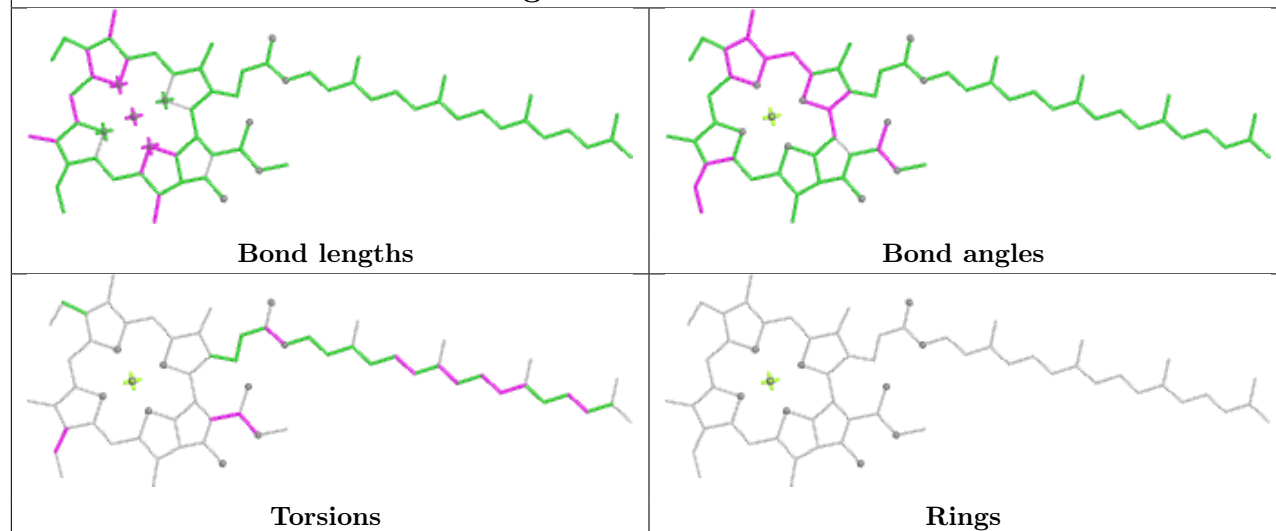


Torsions

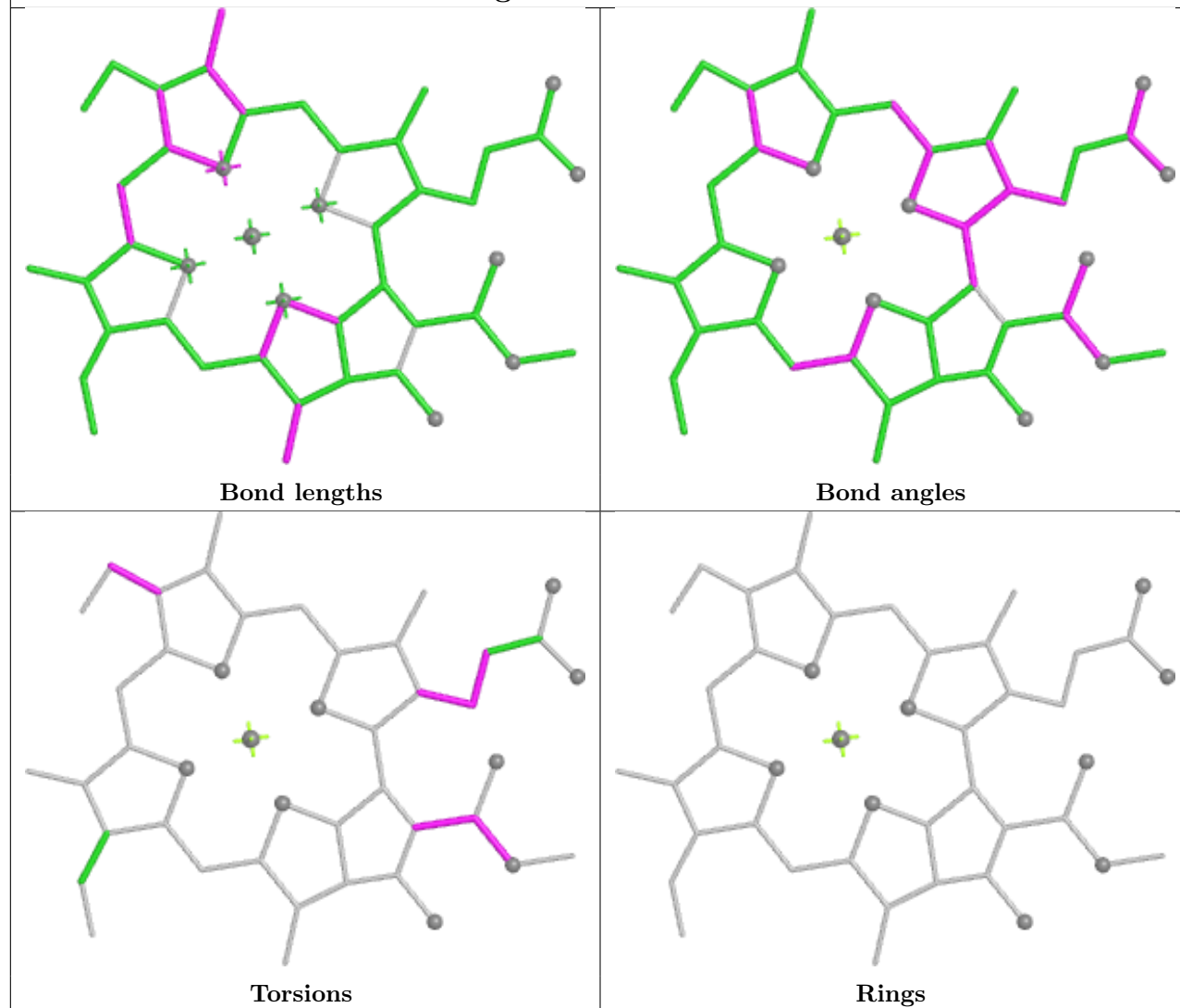


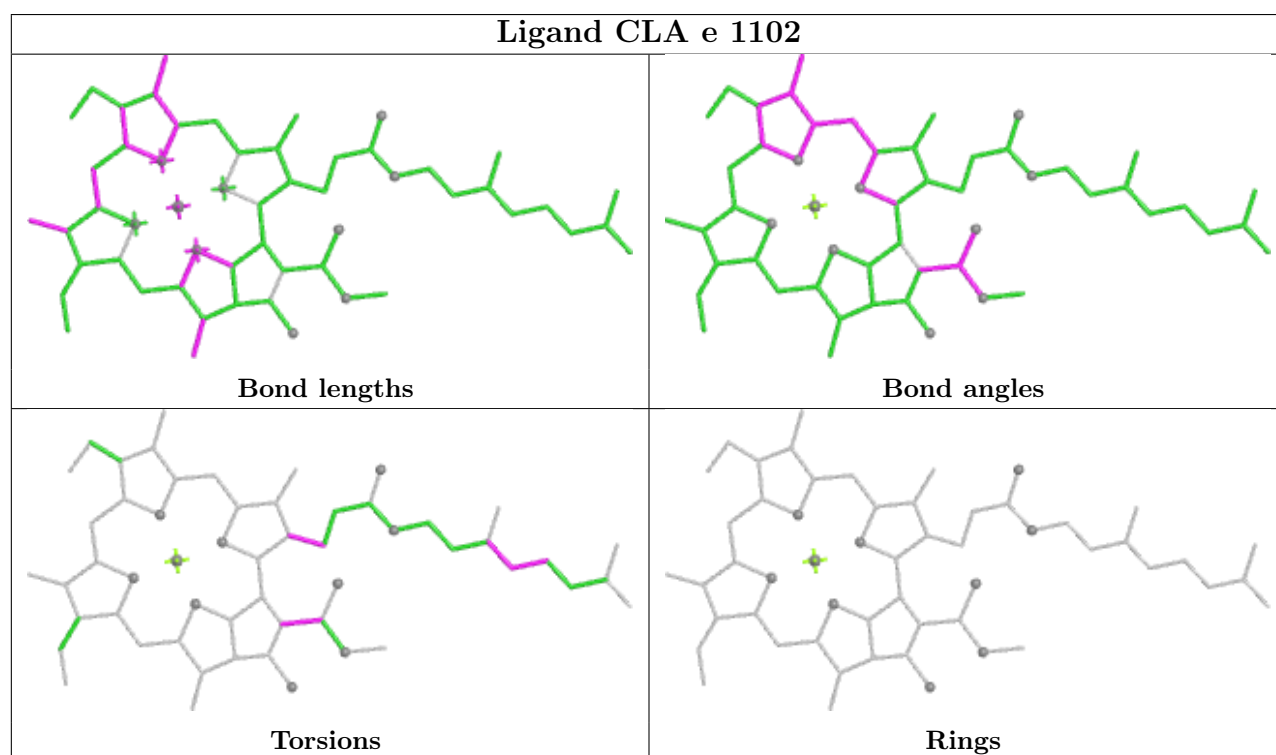
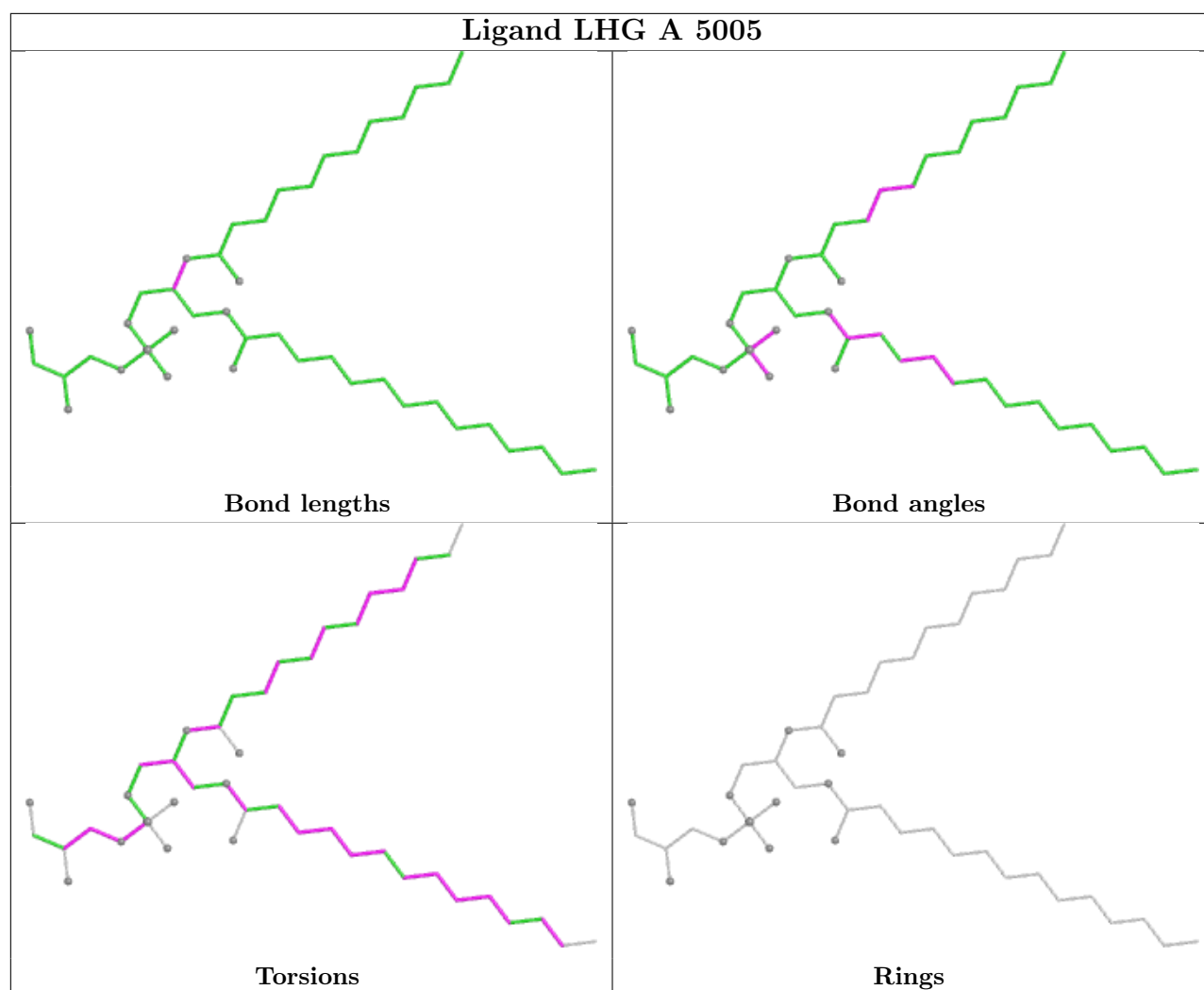
Rings

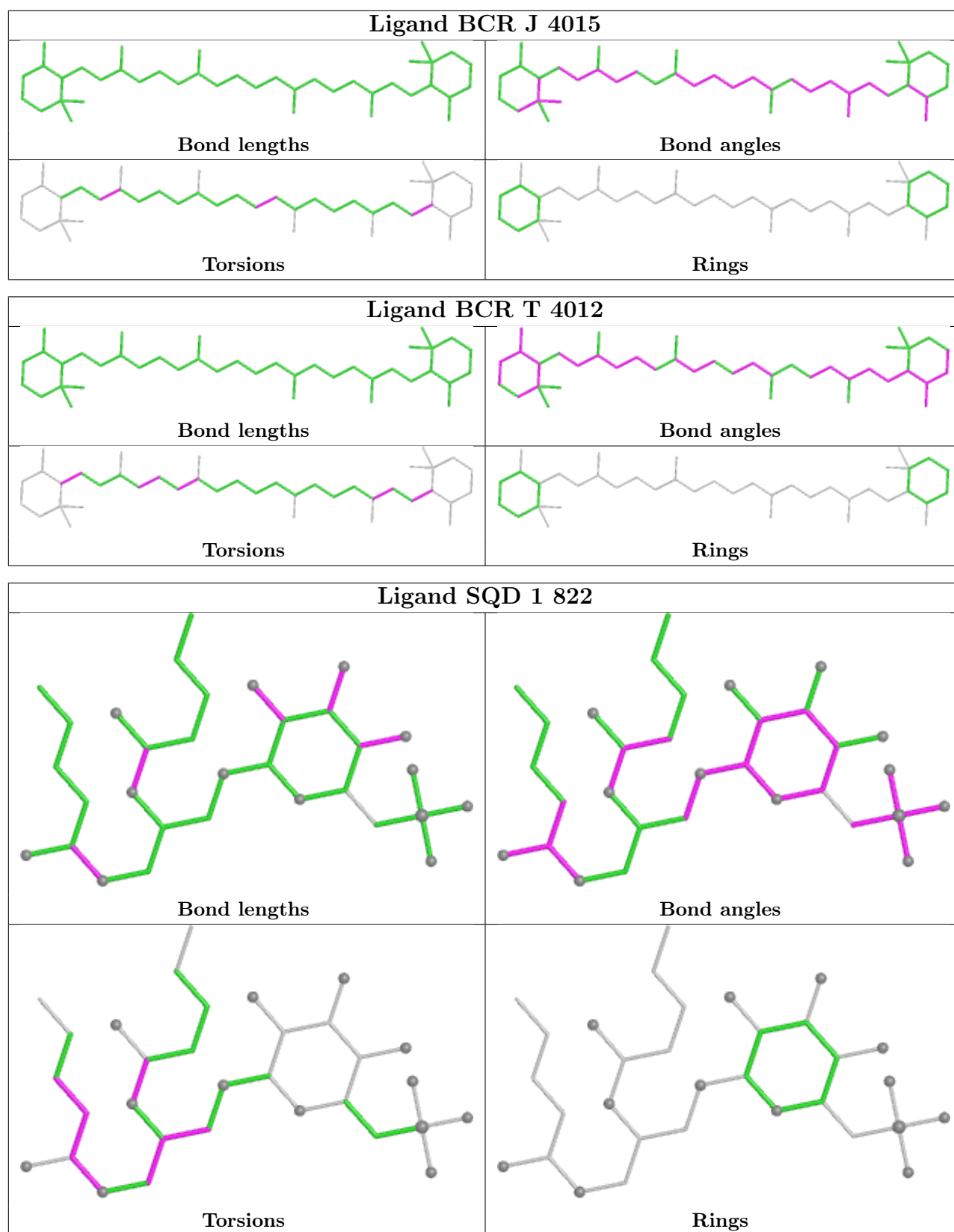
Ligand CLA B 1234



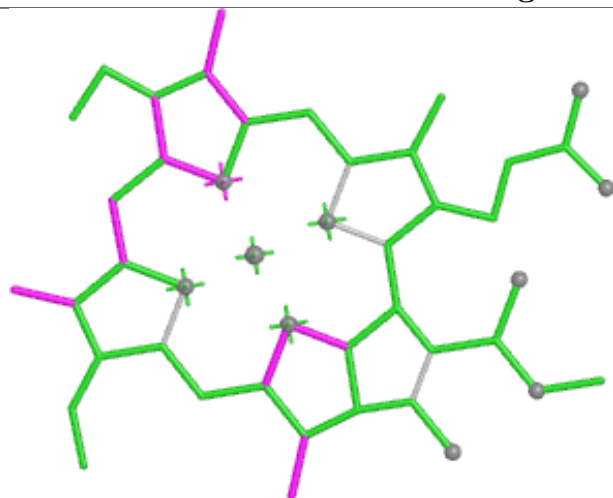
Ligand CLA u 503



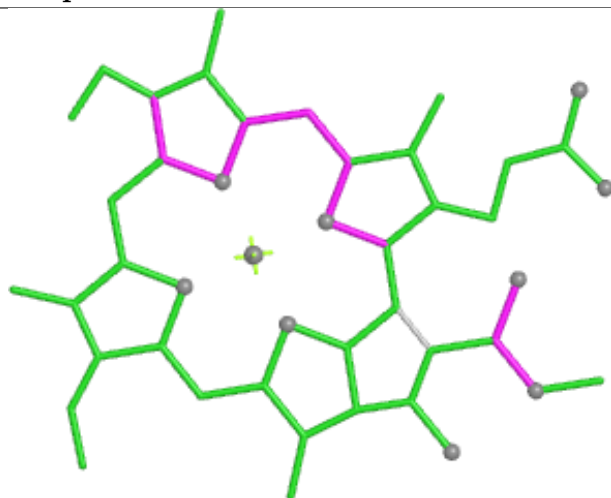




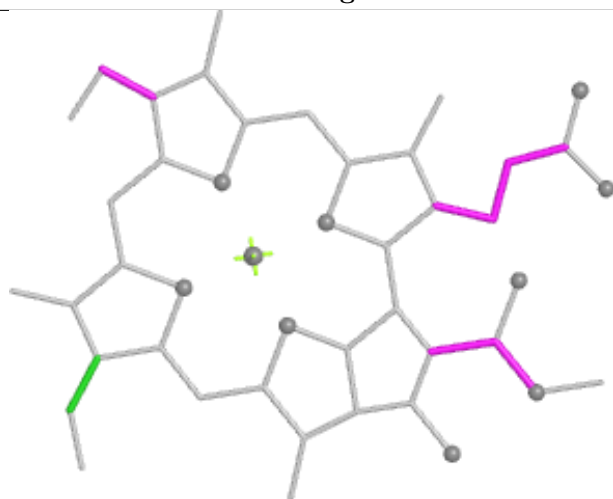
Ligand CLA q 501



Bond lengths



Bond angles

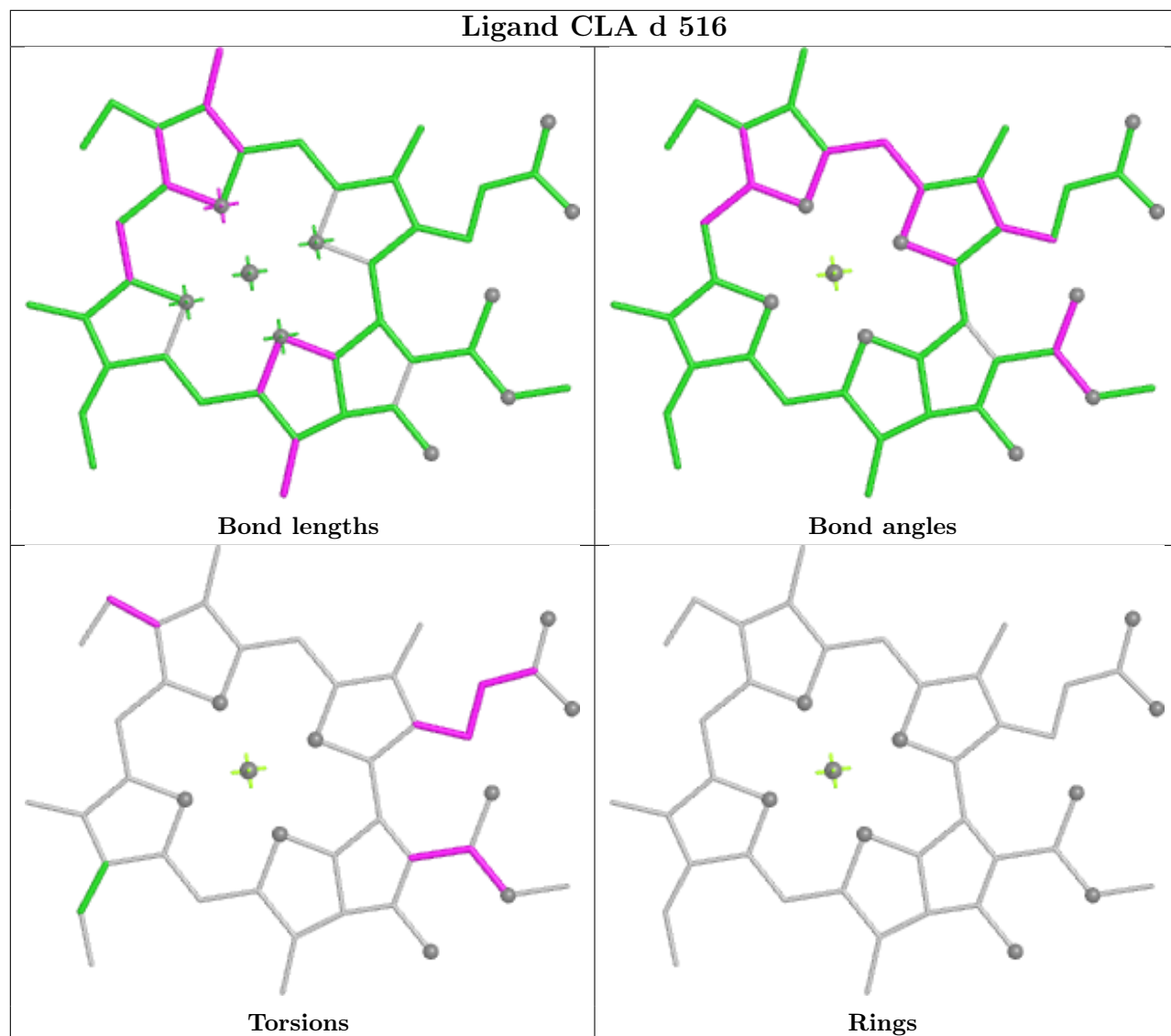


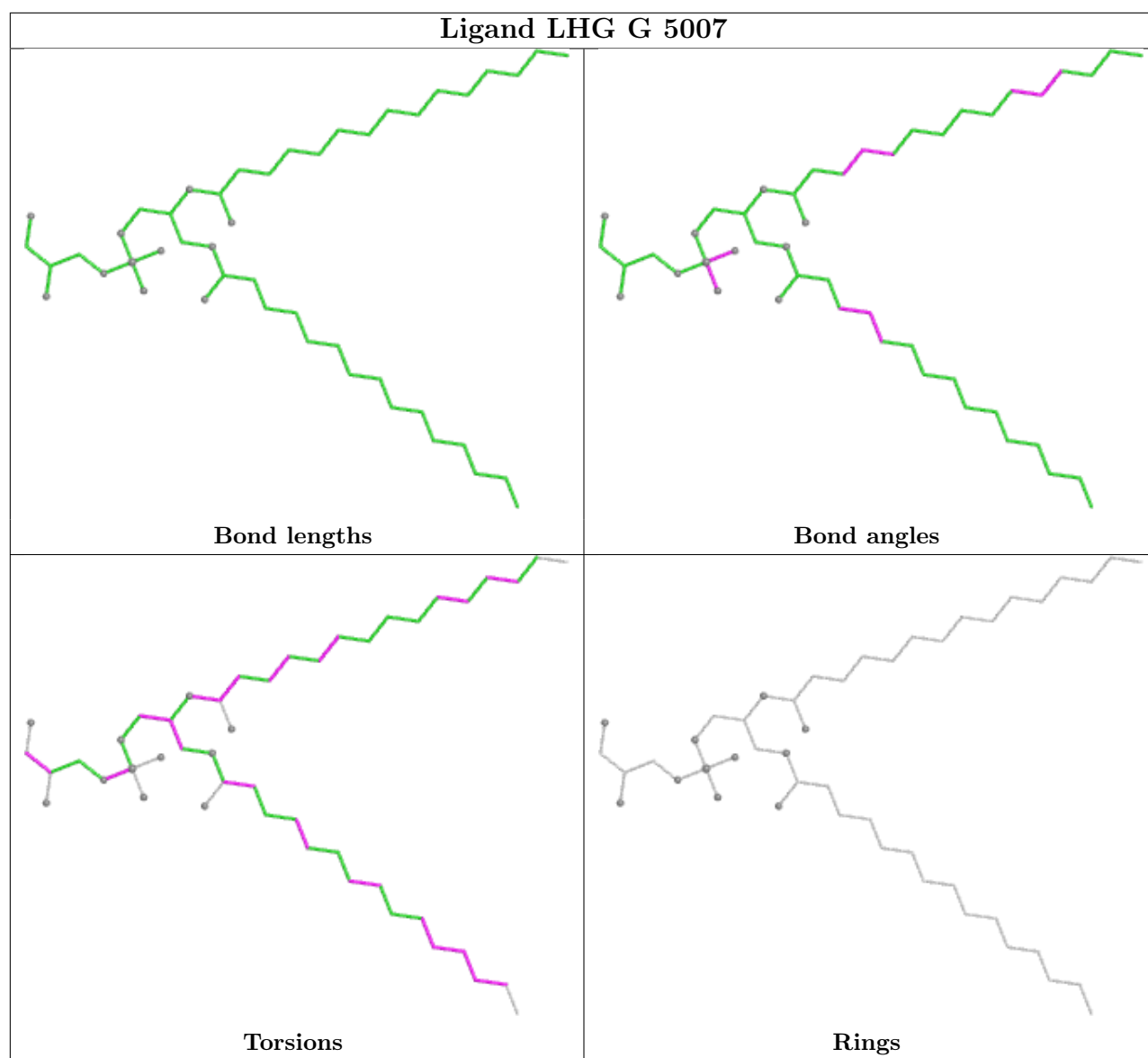
Torsions



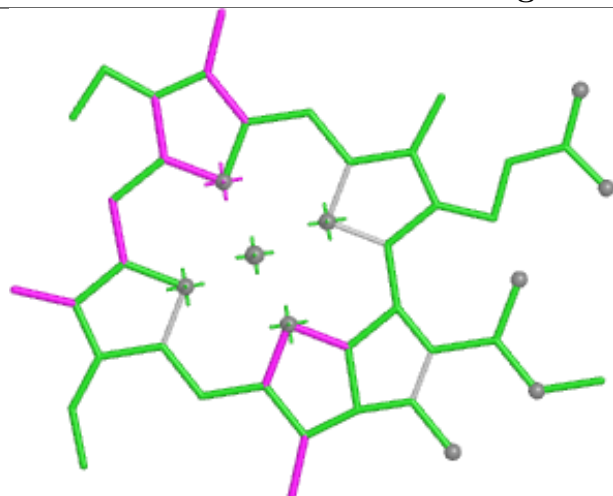
Rings

Ligand CLA d 516

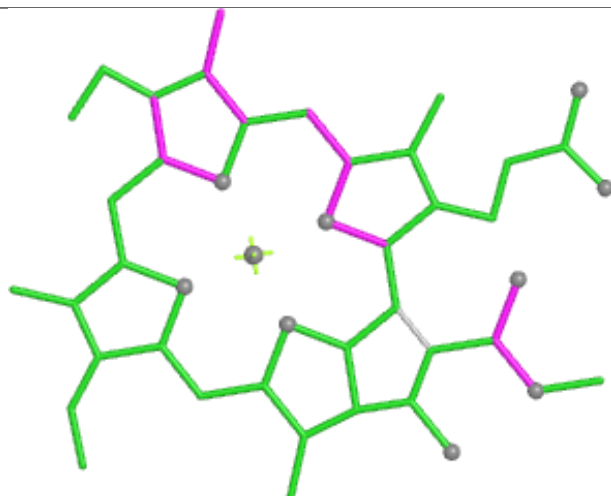




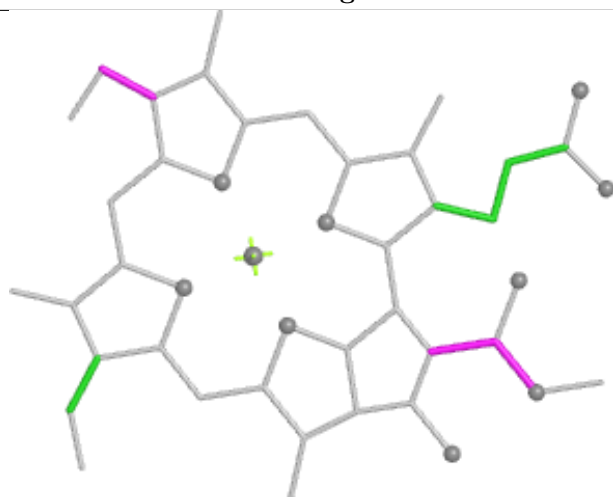
Ligand CLA d 506



Bond lengths



Bond angles

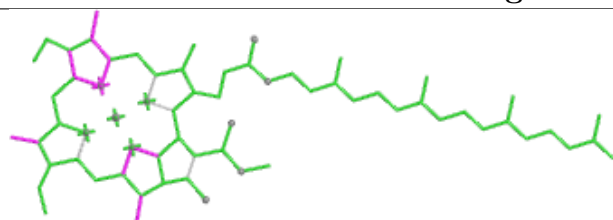


Torsions

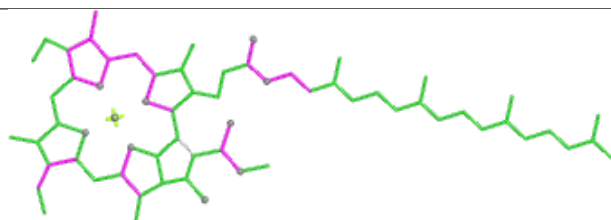


Rings

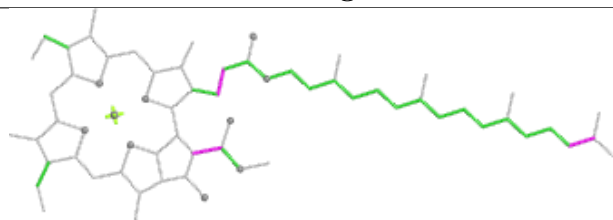
Ligand CLA B 1238



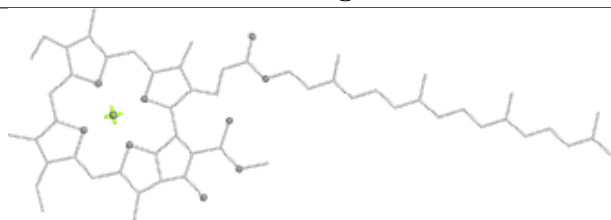
Bond lengths



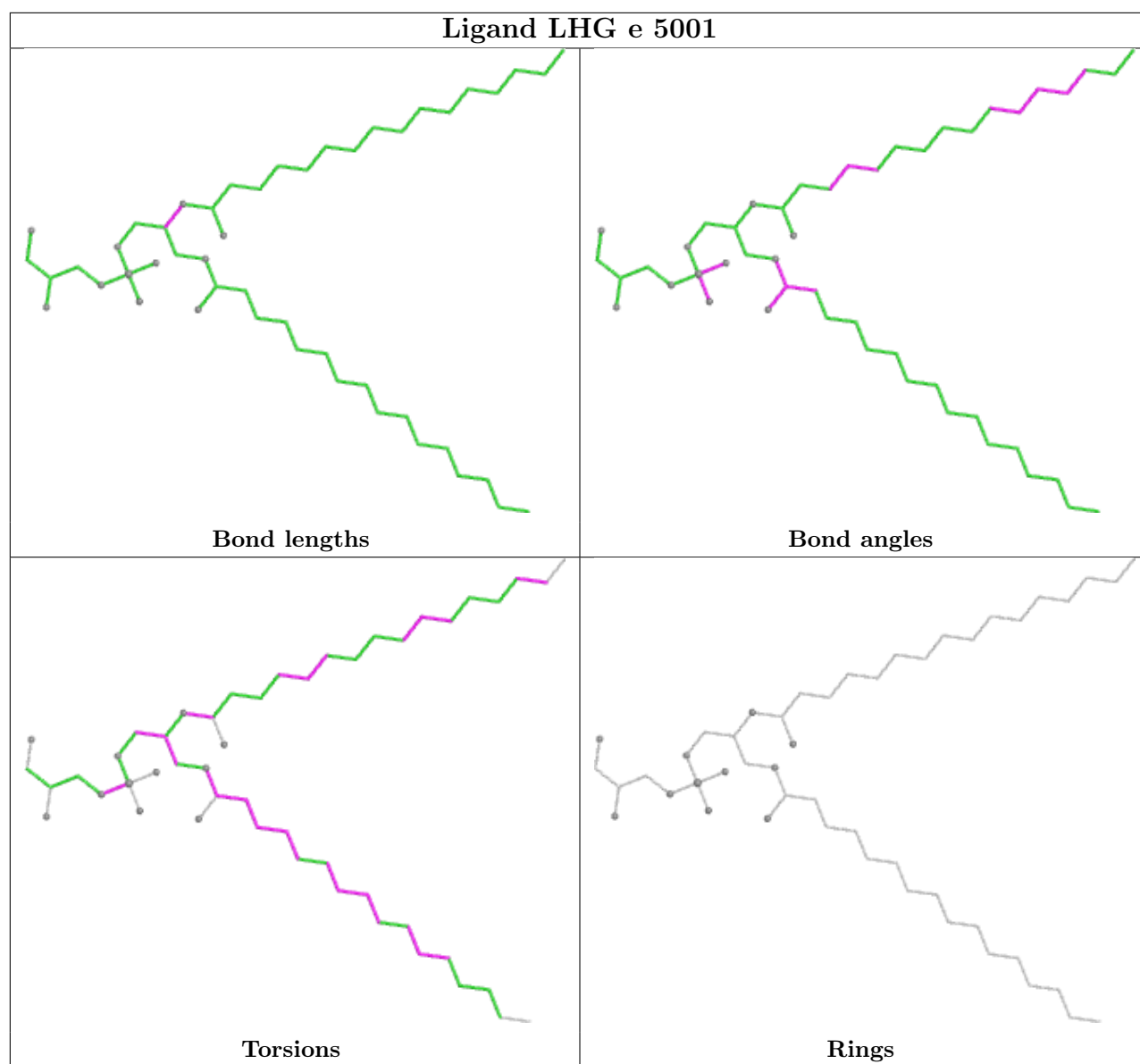
Bond angles



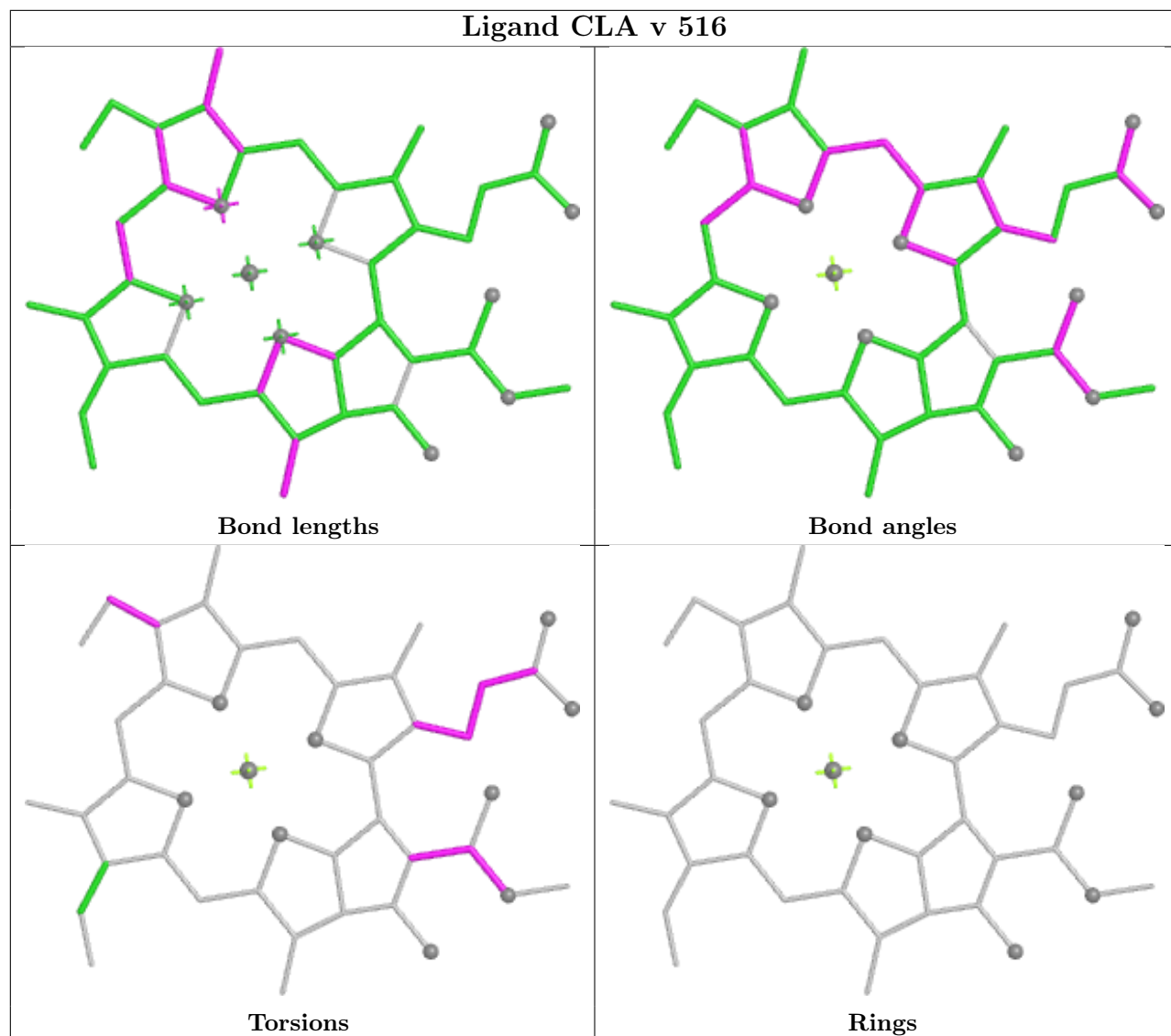
Torsions

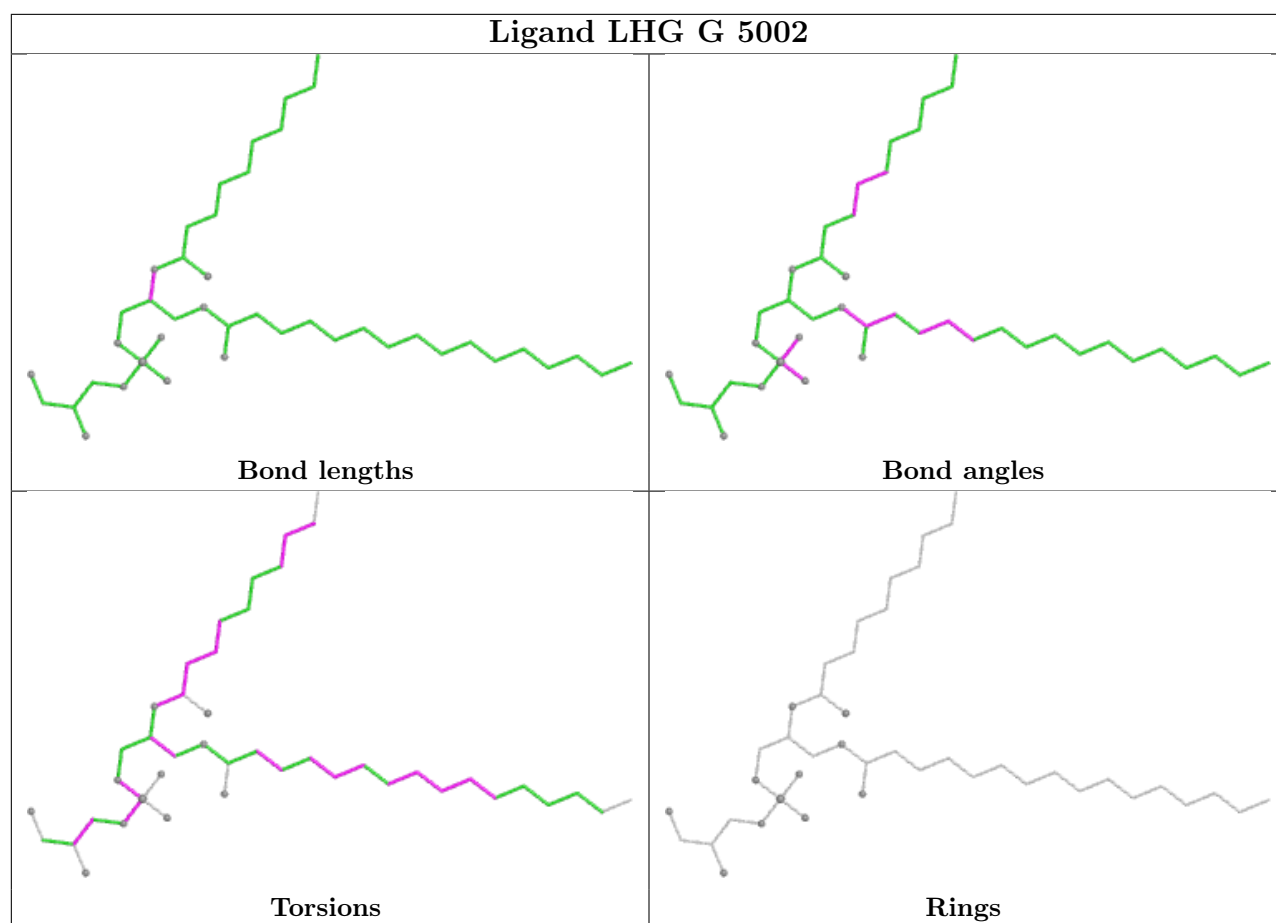


Rings

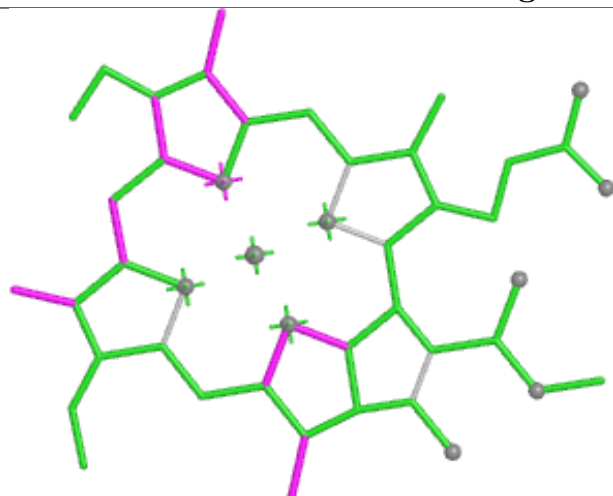


Ligand CLA v 516

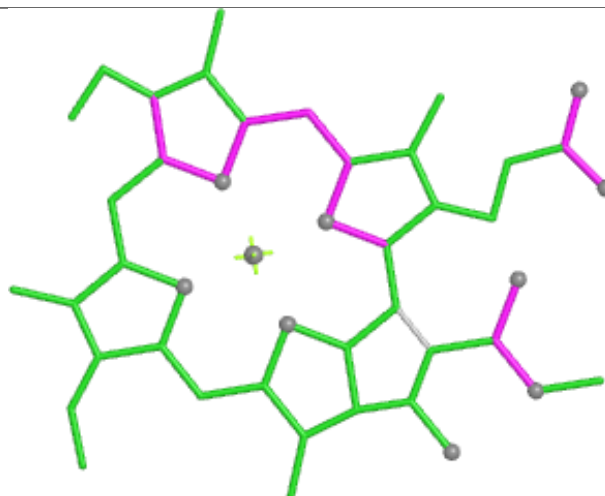




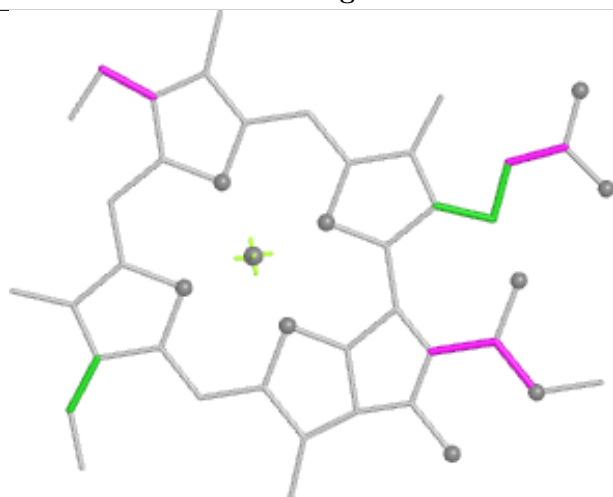
Ligand CLA 4 519



Bond lengths



Bond angles

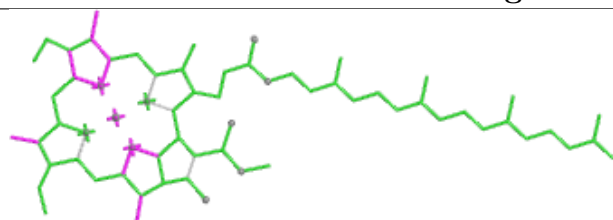


Torsions

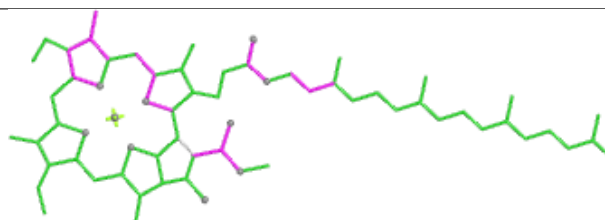


Rings

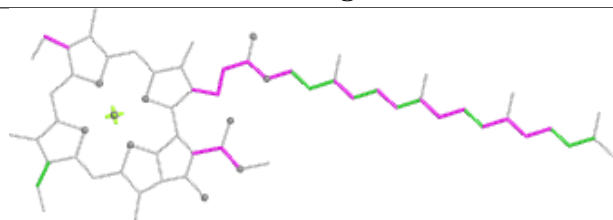
Ligand CLA A 1106



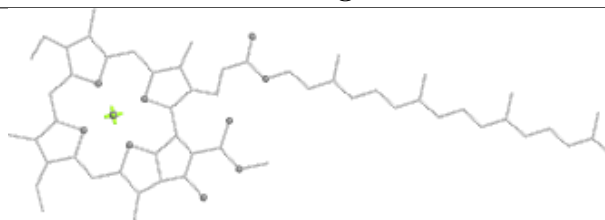
Bond lengths



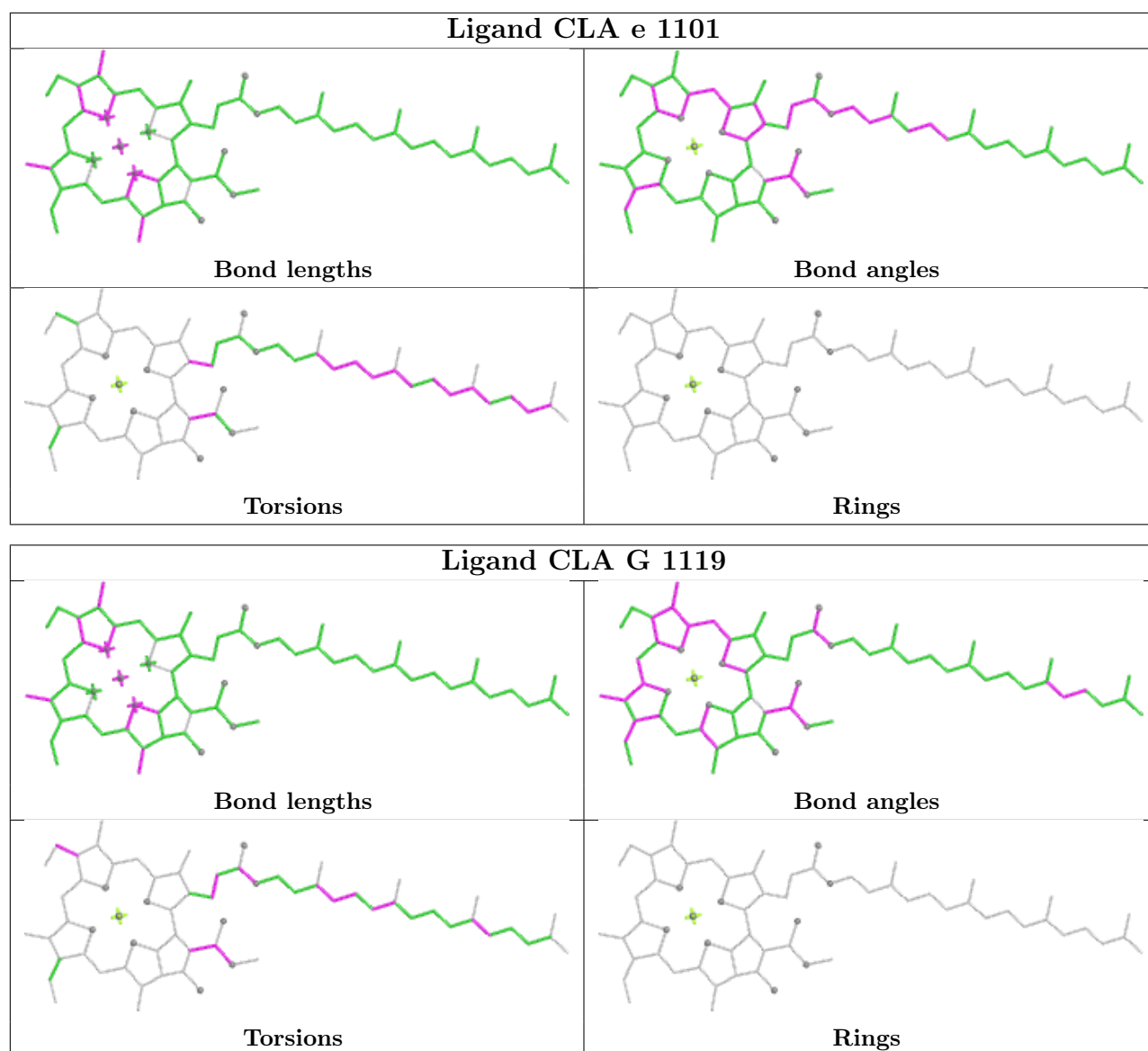
Bond angles

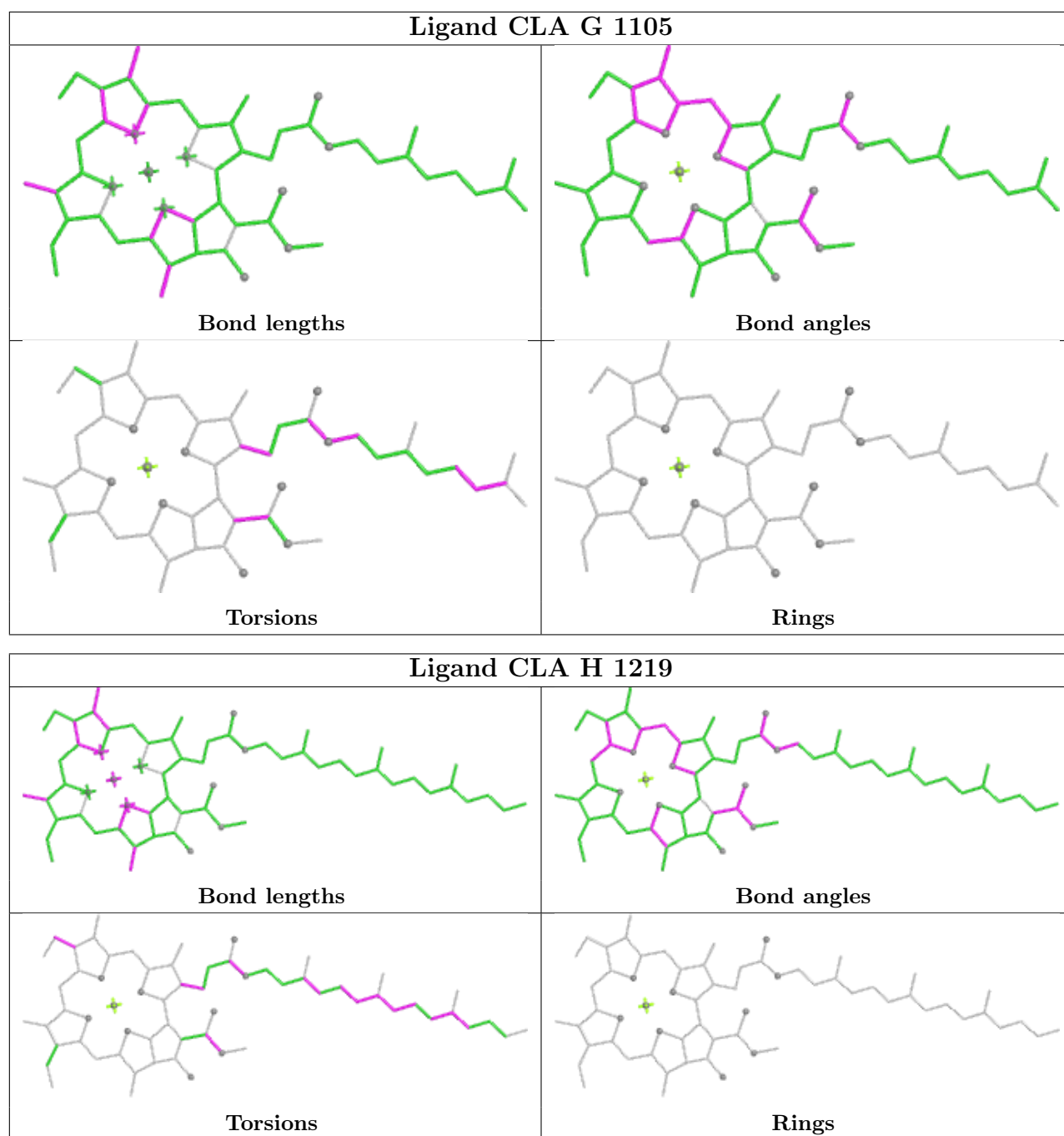


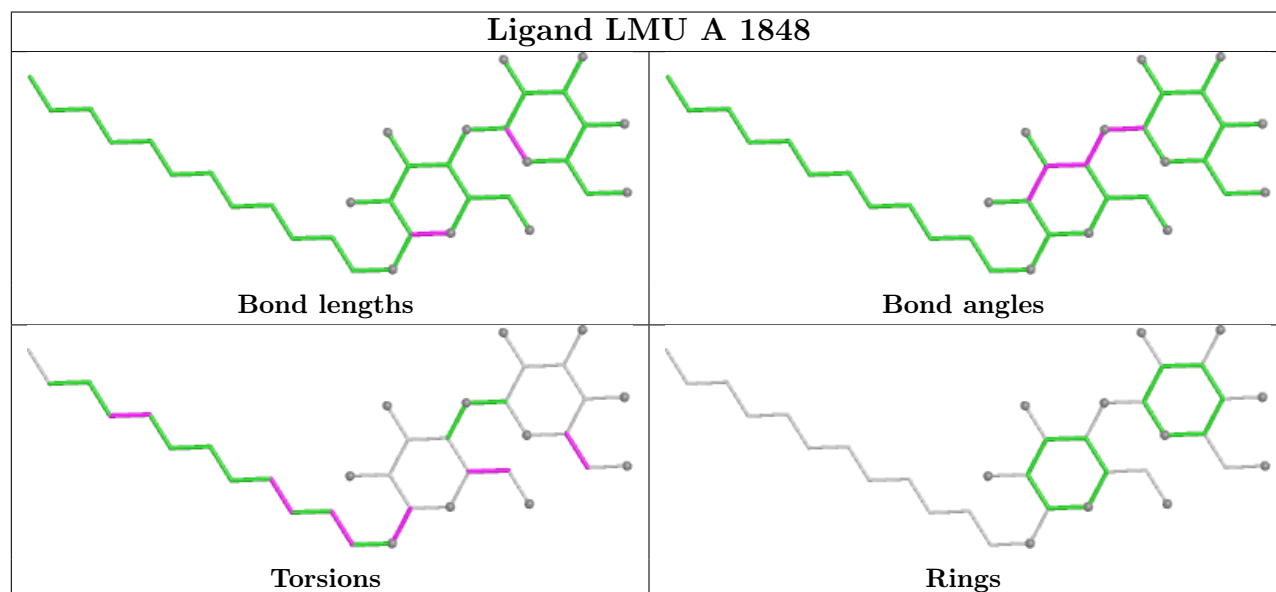
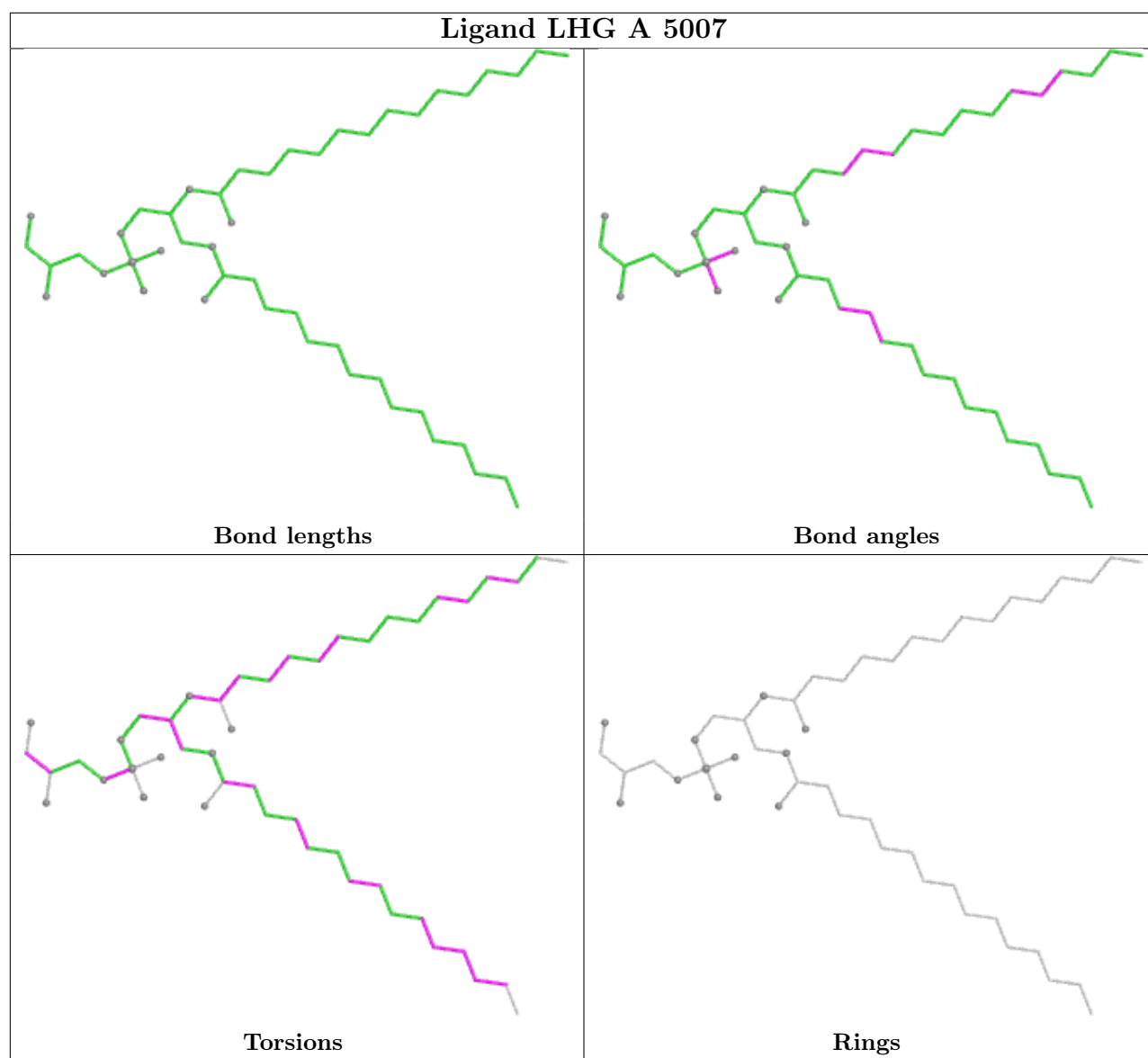
Torsions



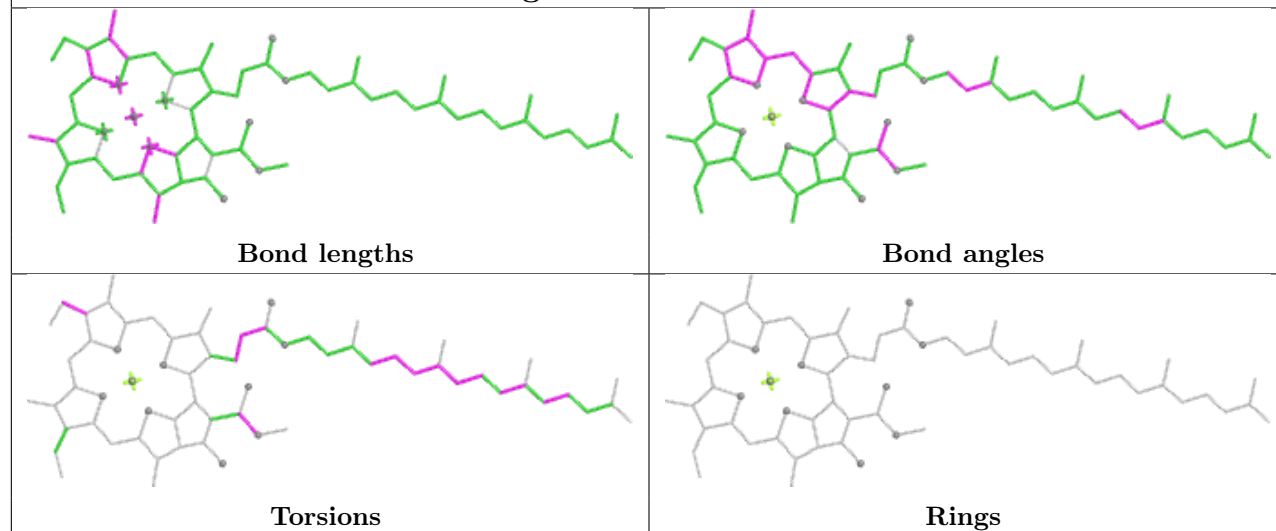
Rings



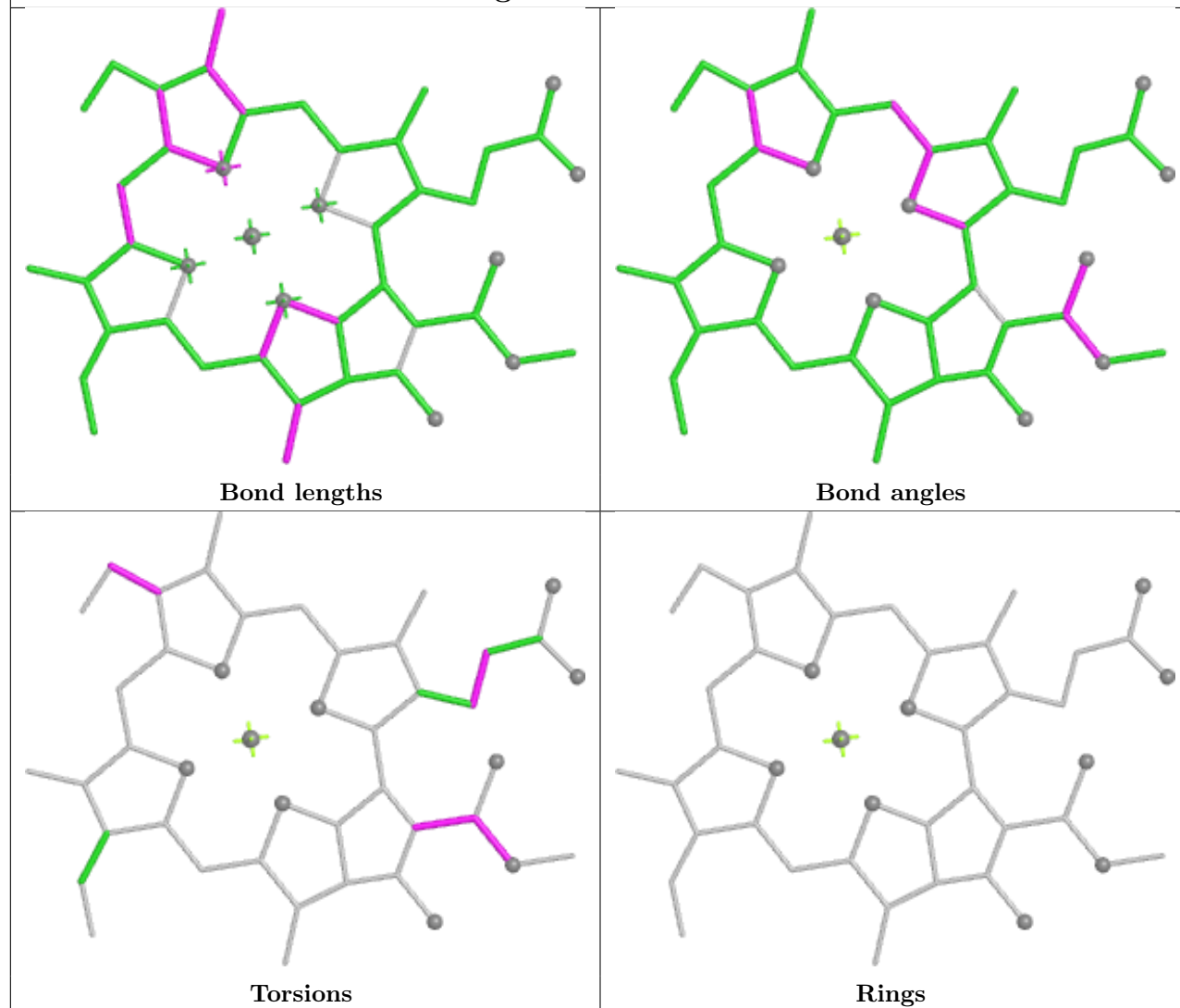




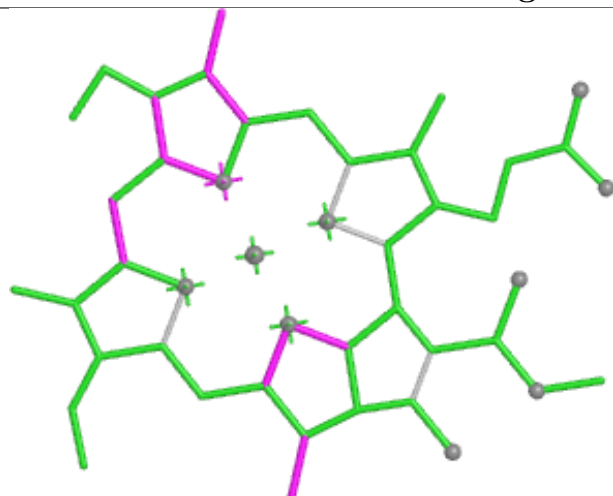
Ligand CLA H 1203



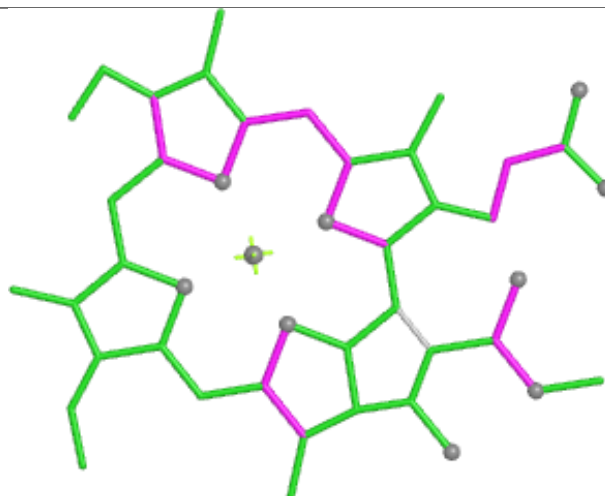
Ligand CLA b 518



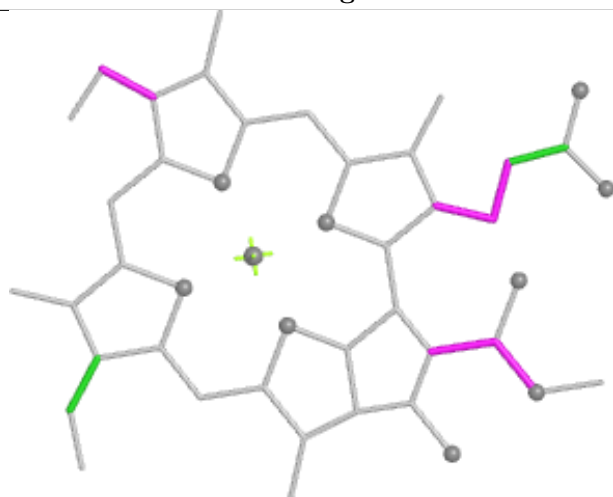
Ligand CLA 3 503



Bond lengths



Bond angles

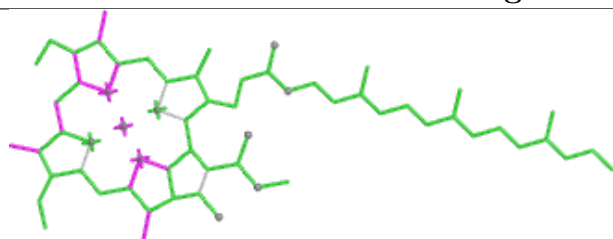


Torsions

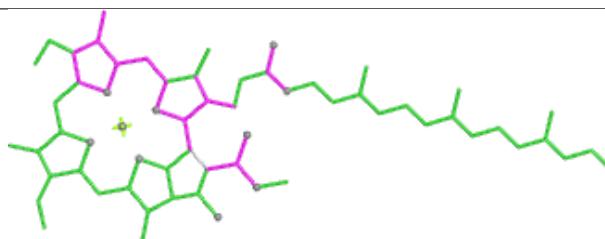


Rings

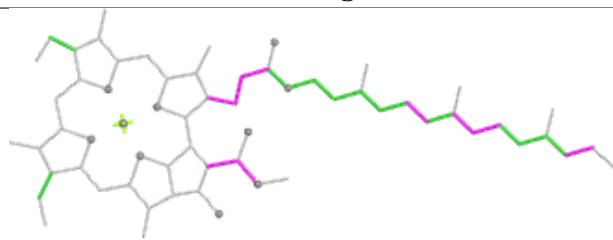
Ligand CLA H 1221



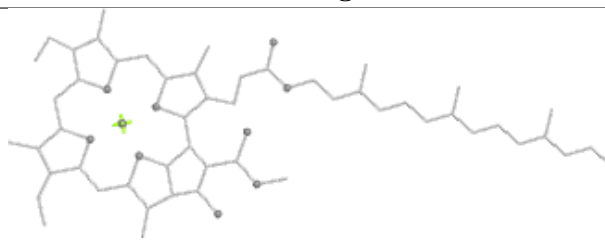
Bond lengths



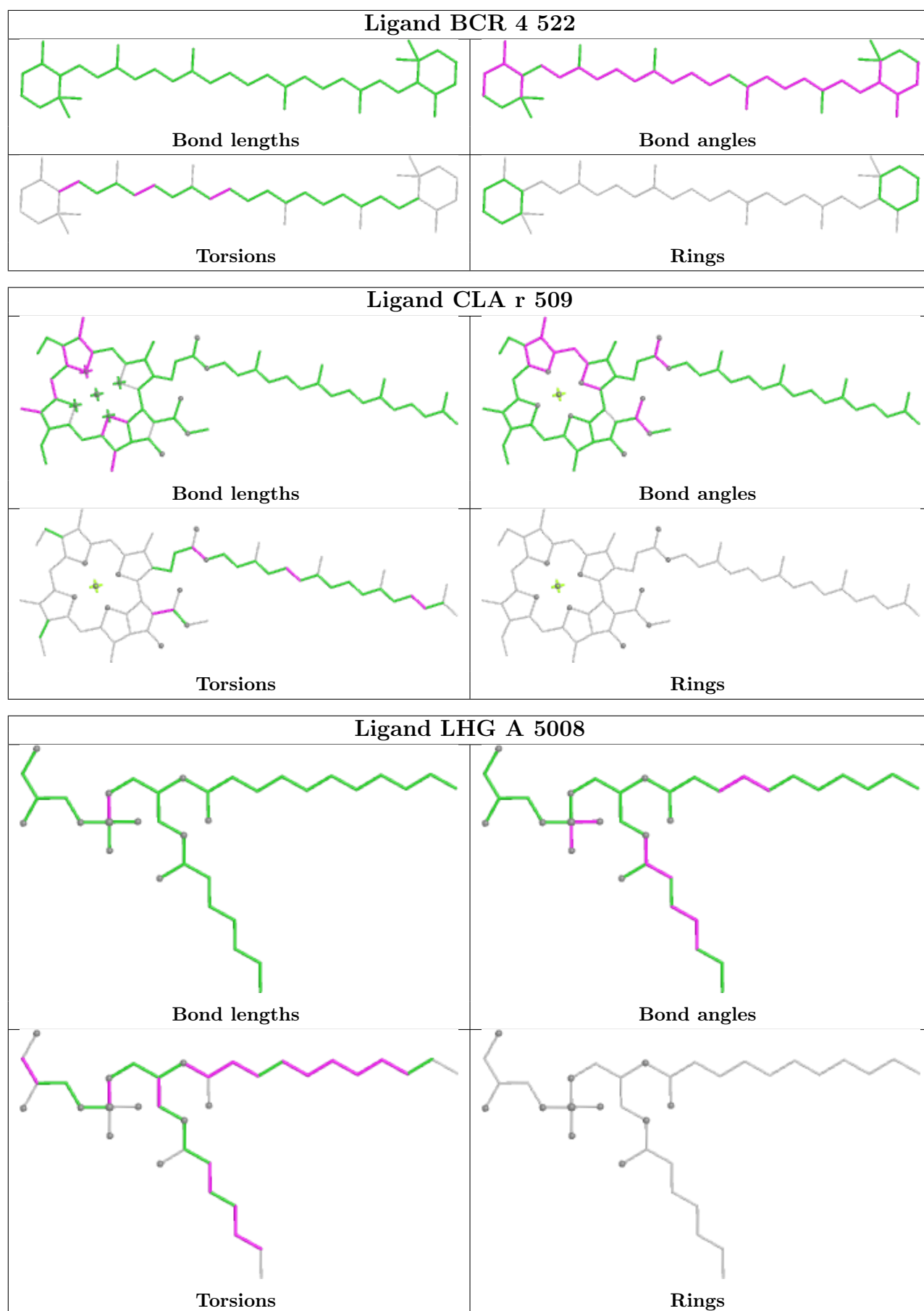
Bond angles



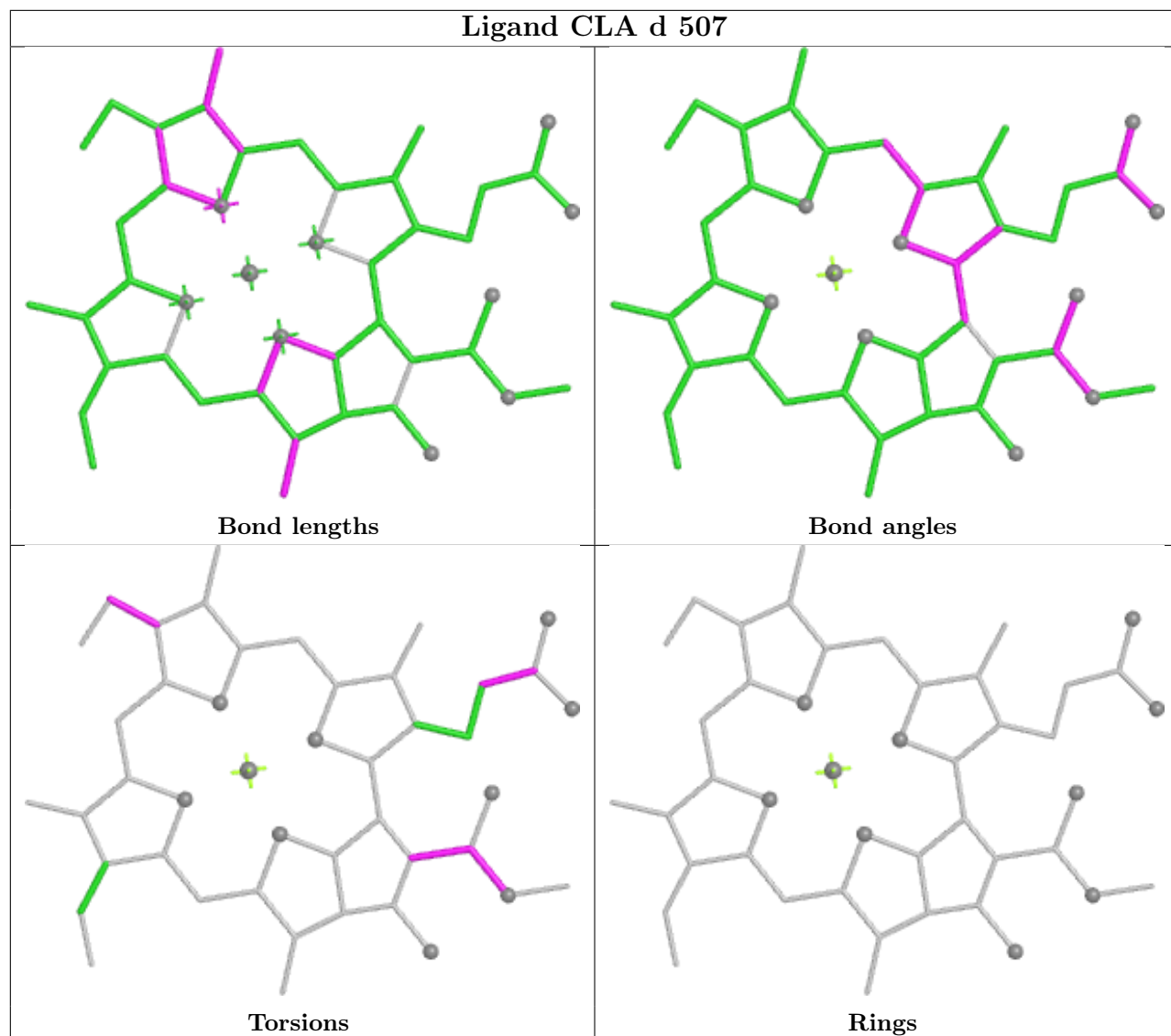
Torsions



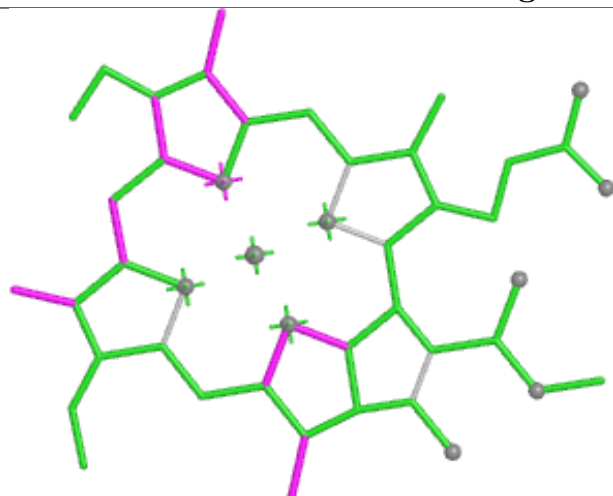
Rings



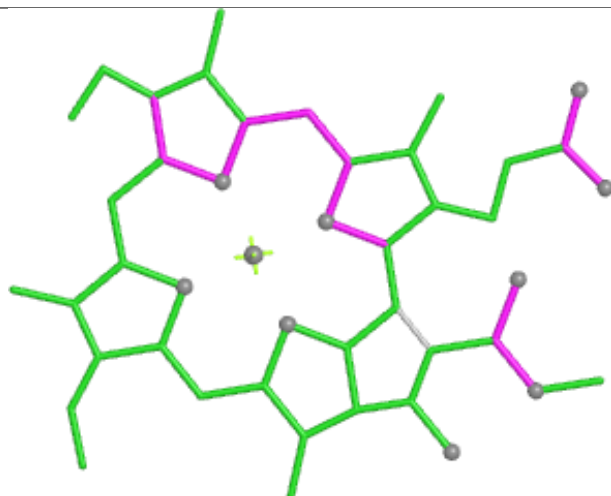
Ligand CLA d 507



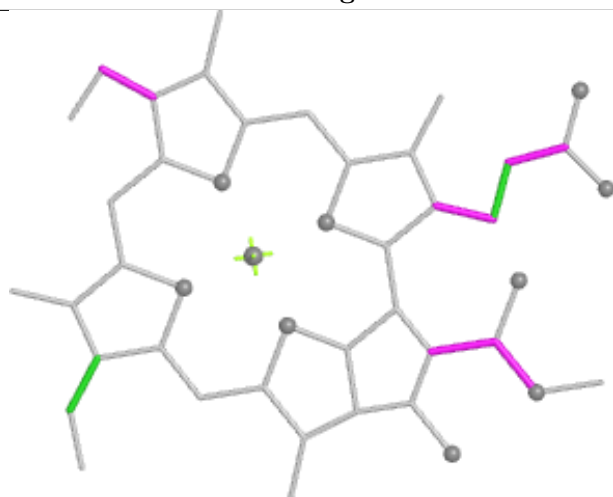
Ligand CLA 6 519



Bond lengths



Bond angles

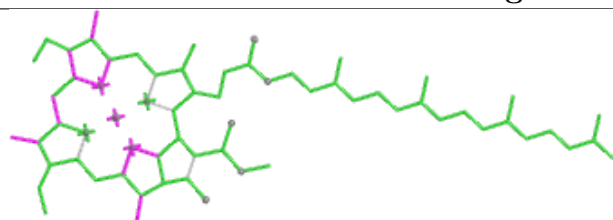


Torsions

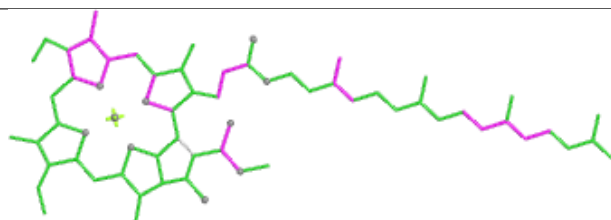


Rings

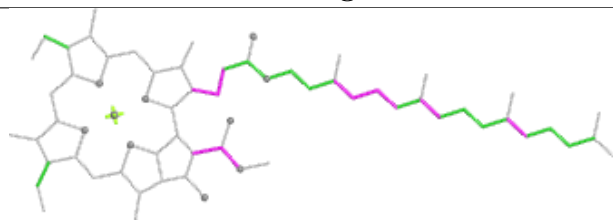
Ligand CLA B 1012



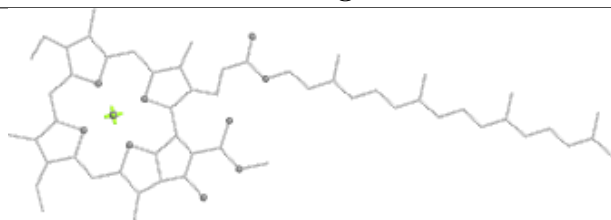
Bond lengths



Bond angles

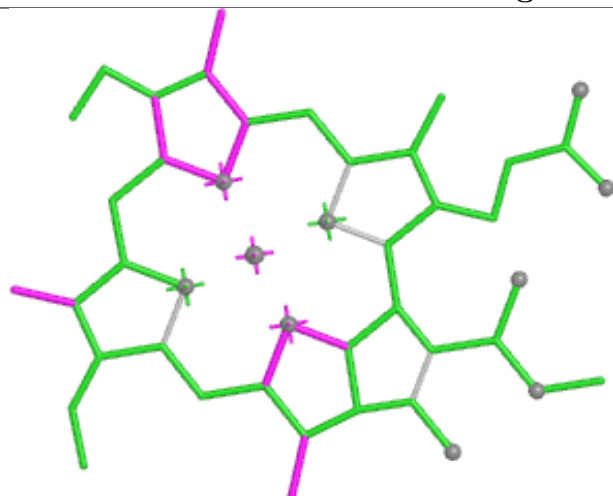


Torsions

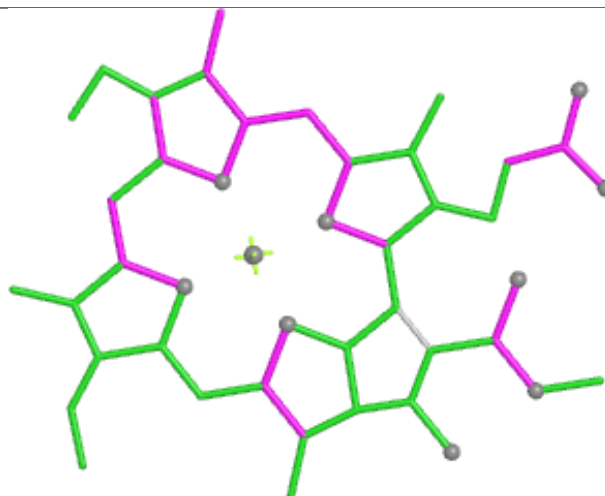


Rings

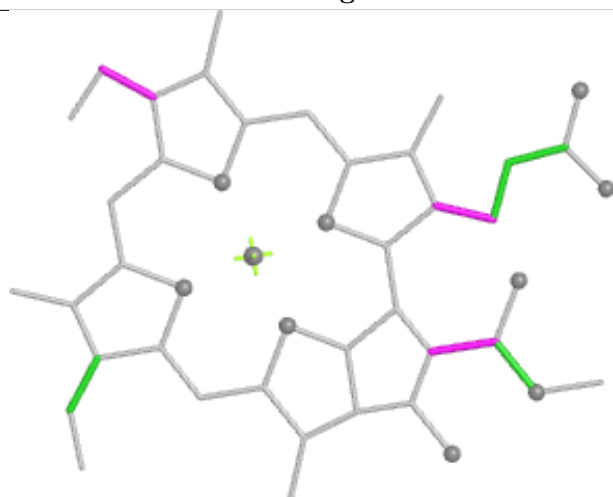
Ligand CLA Z 508



Bond lengths



Bond angles

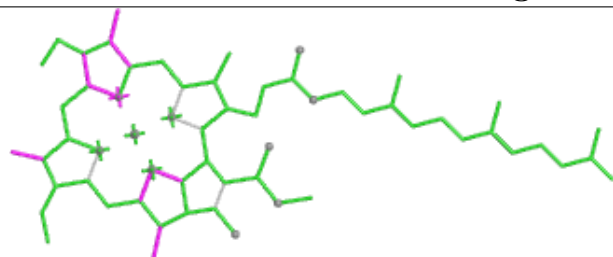


Torsions

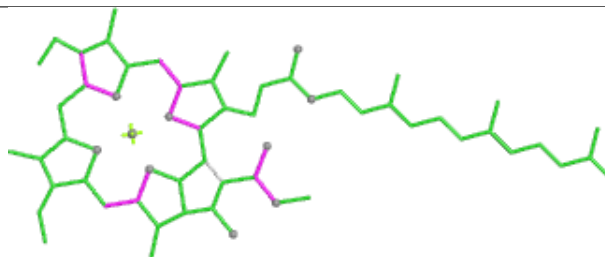


Rings

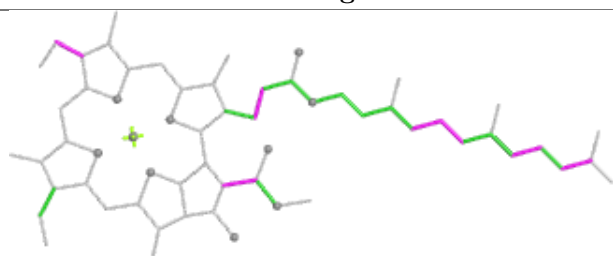
Ligand CLA f 1218



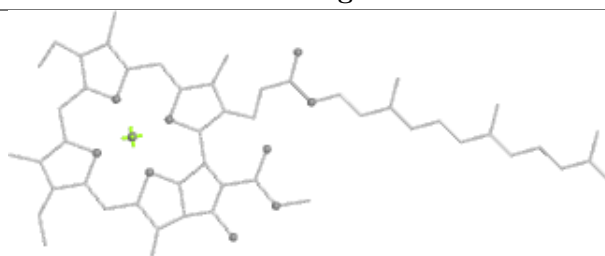
Bond lengths



Bond angles

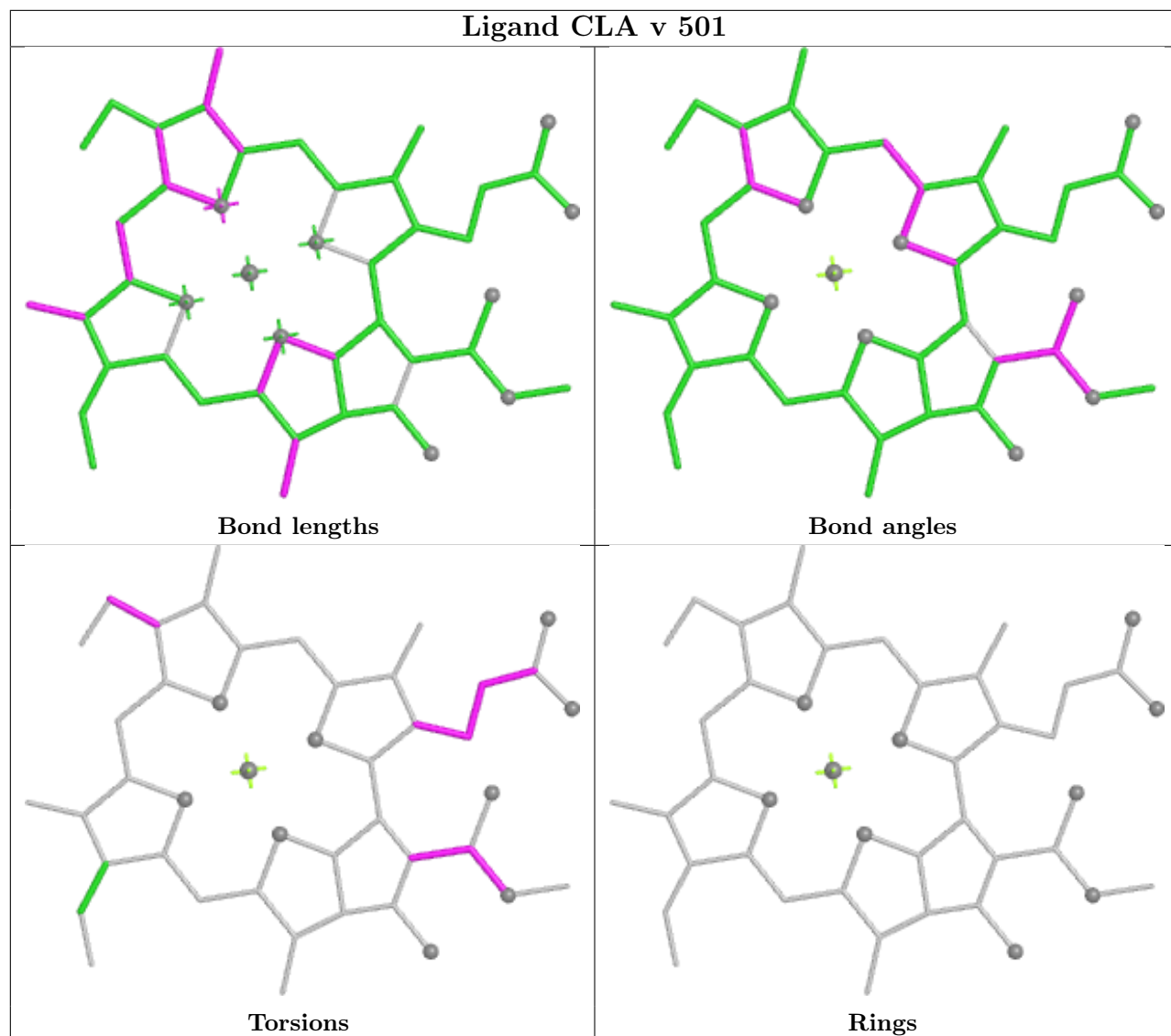


Torsions

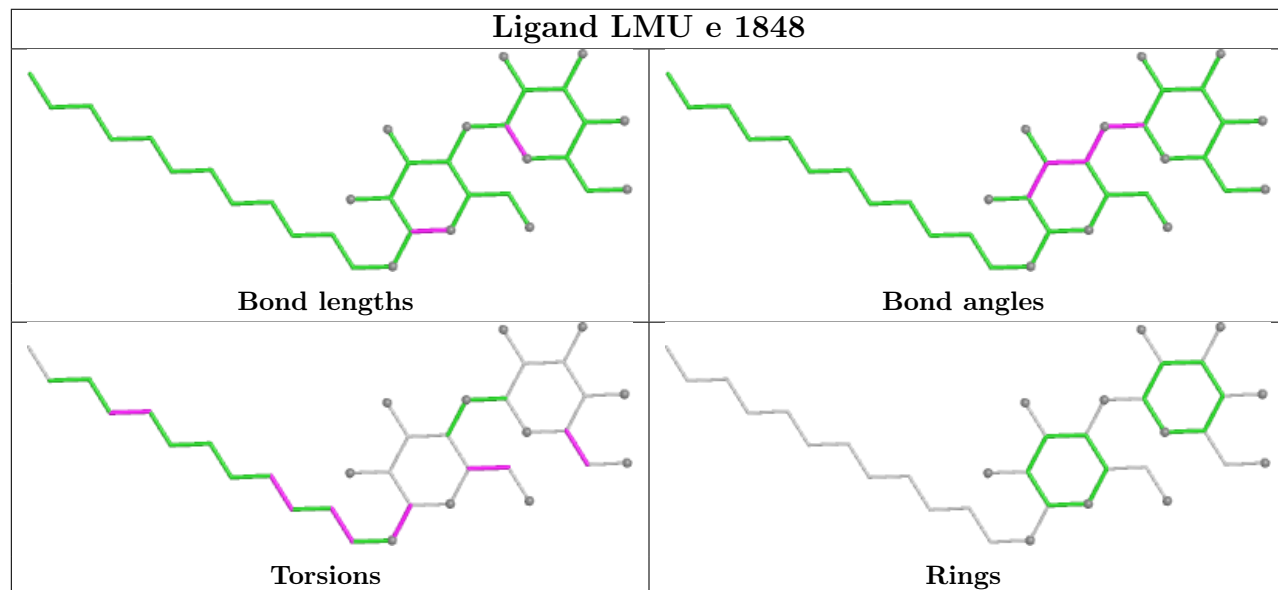


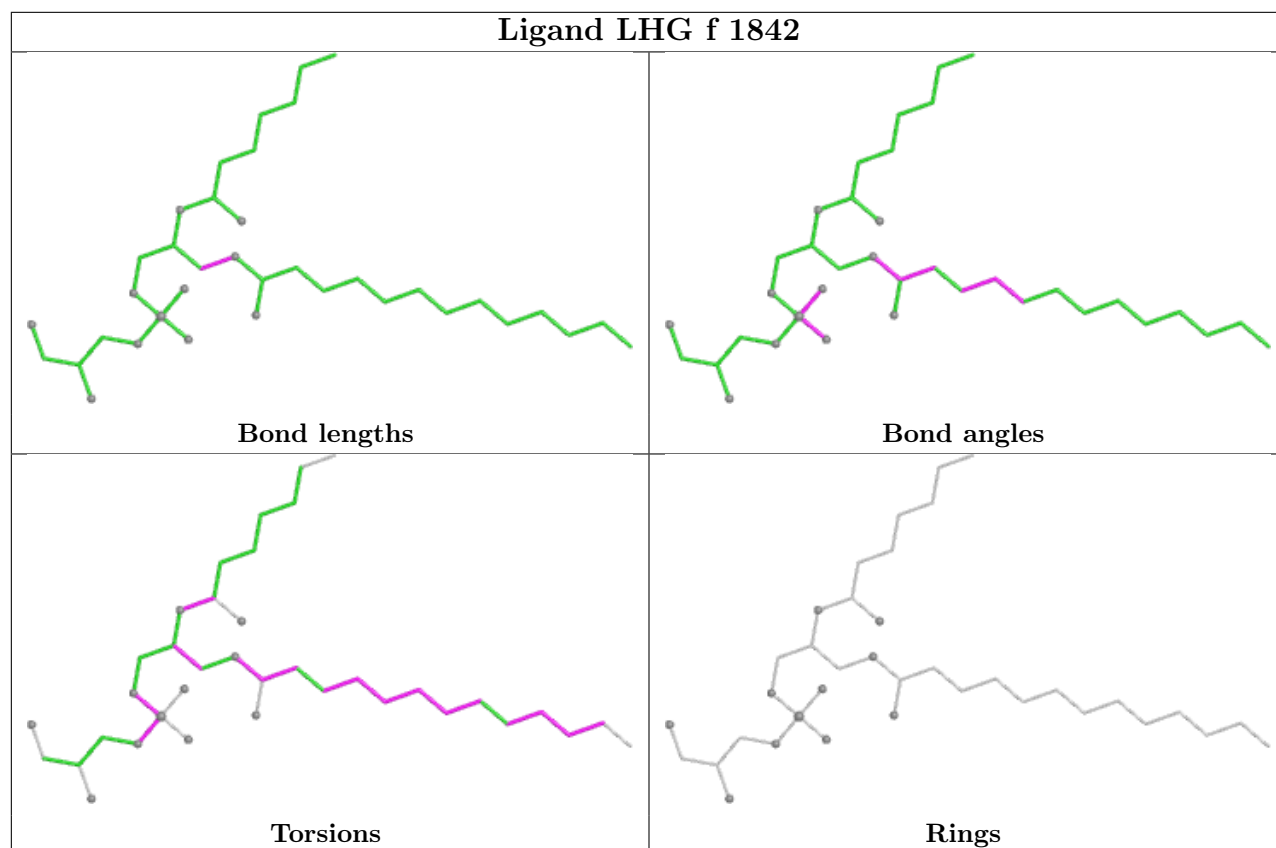
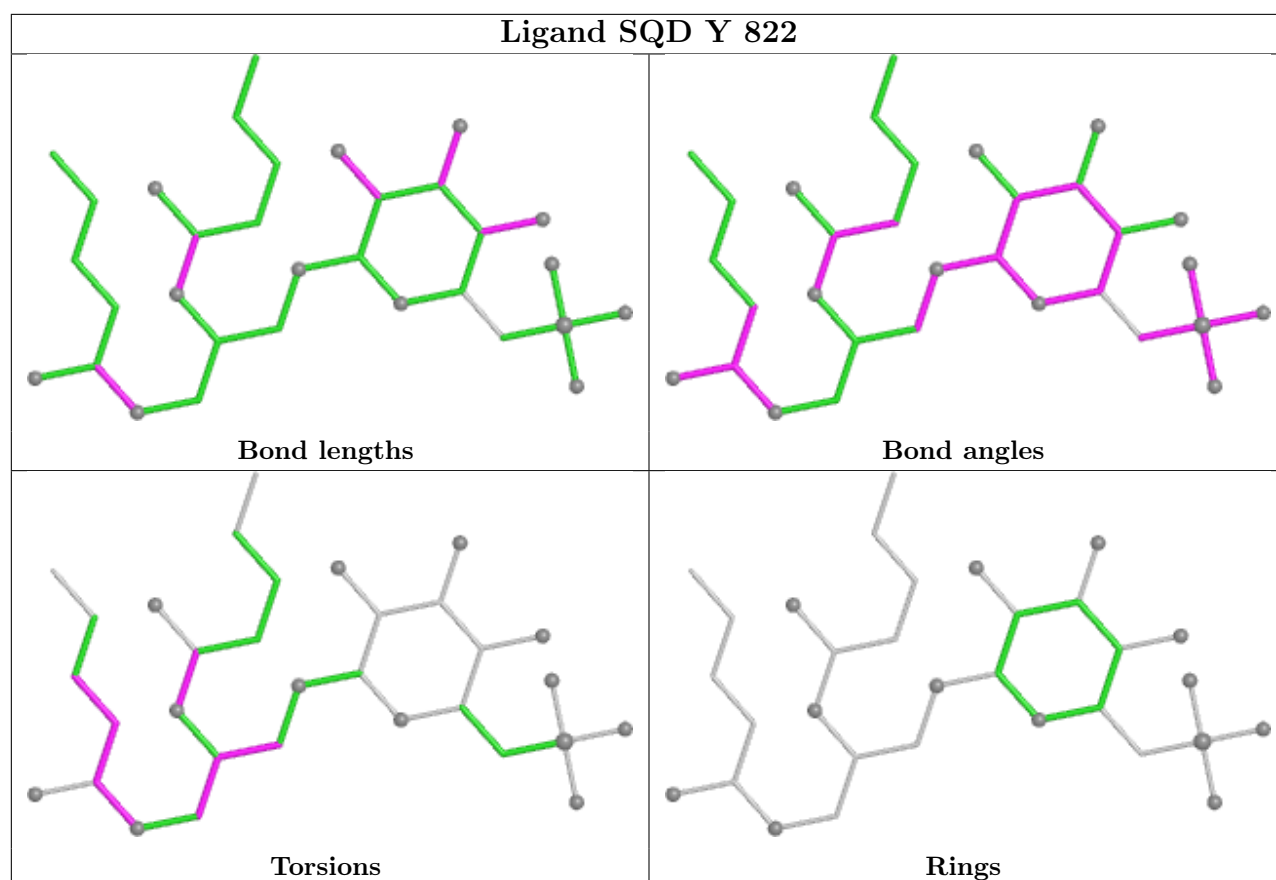
Rings

Ligand CLA v 501

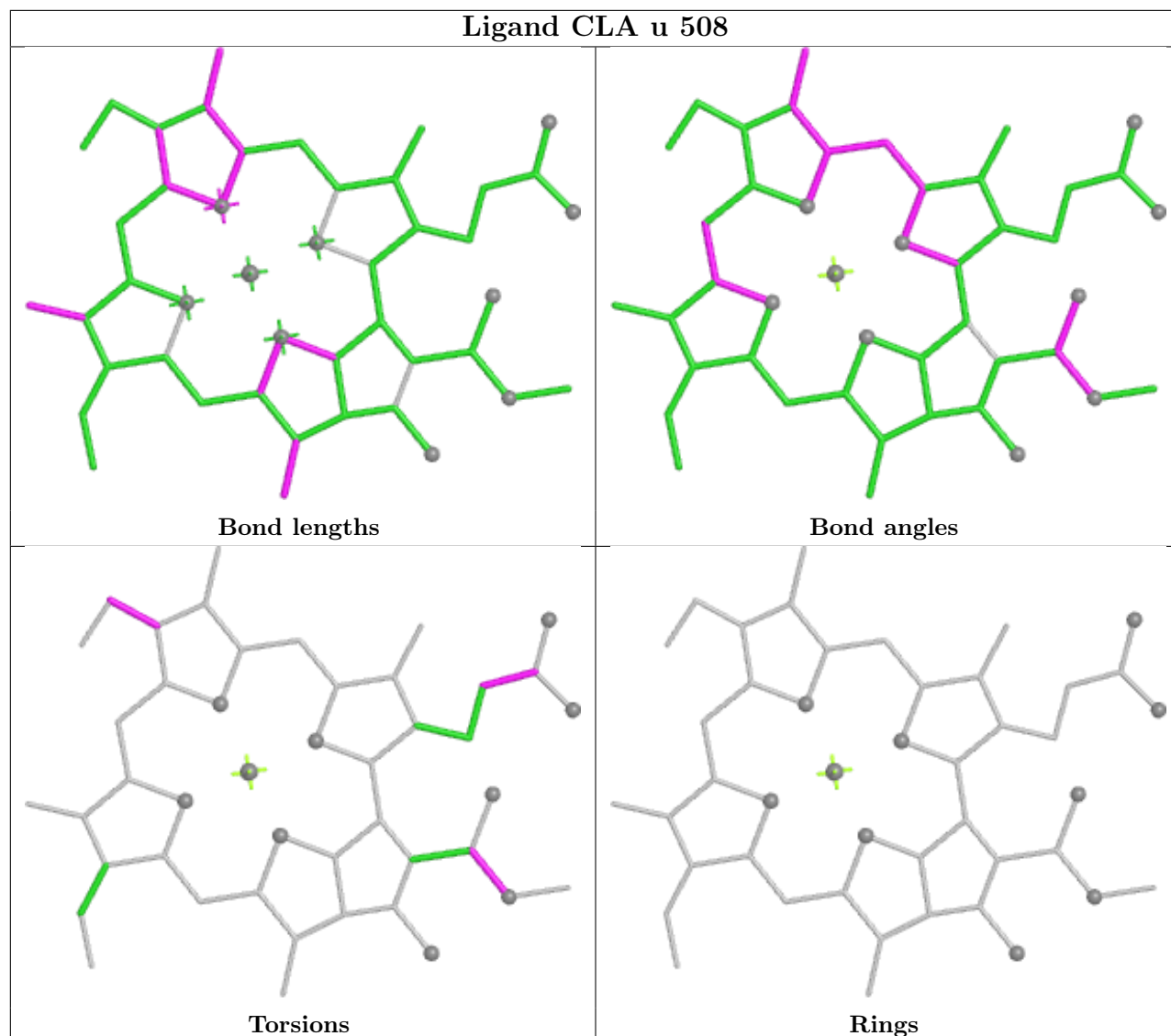


Ligand LMU e 1848

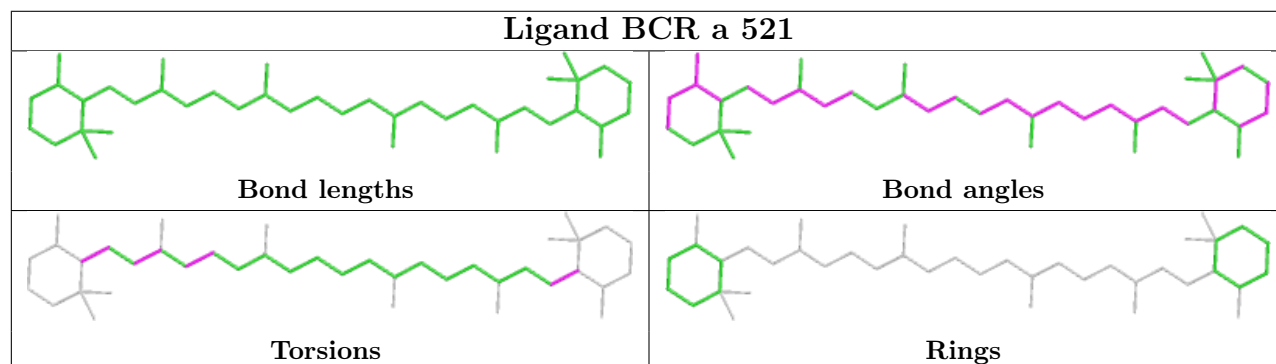


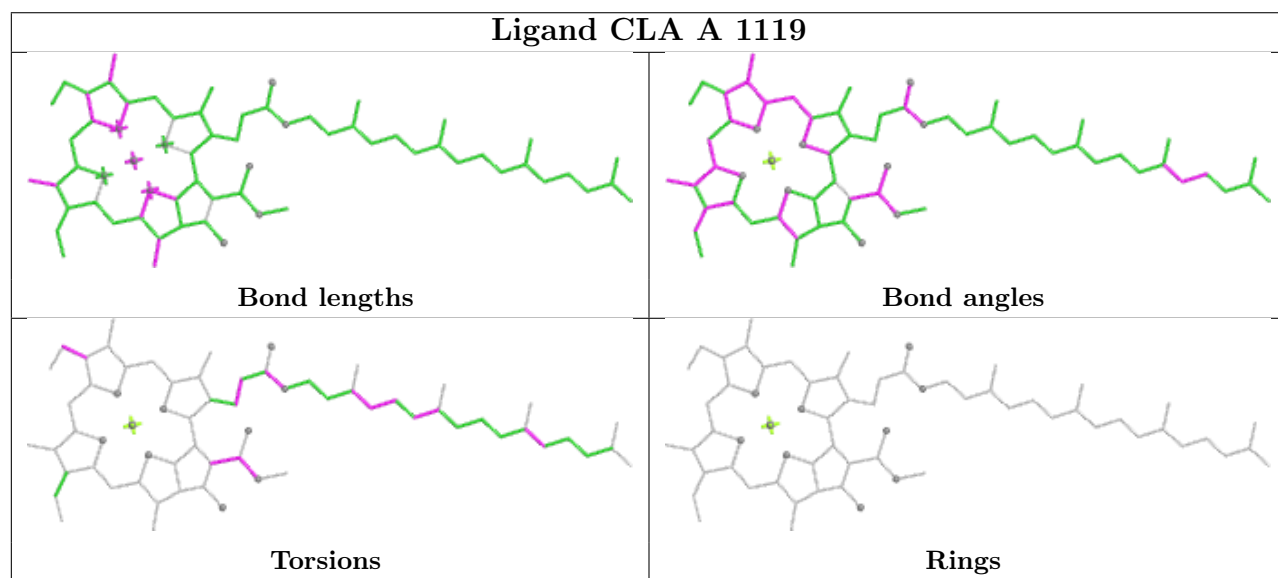
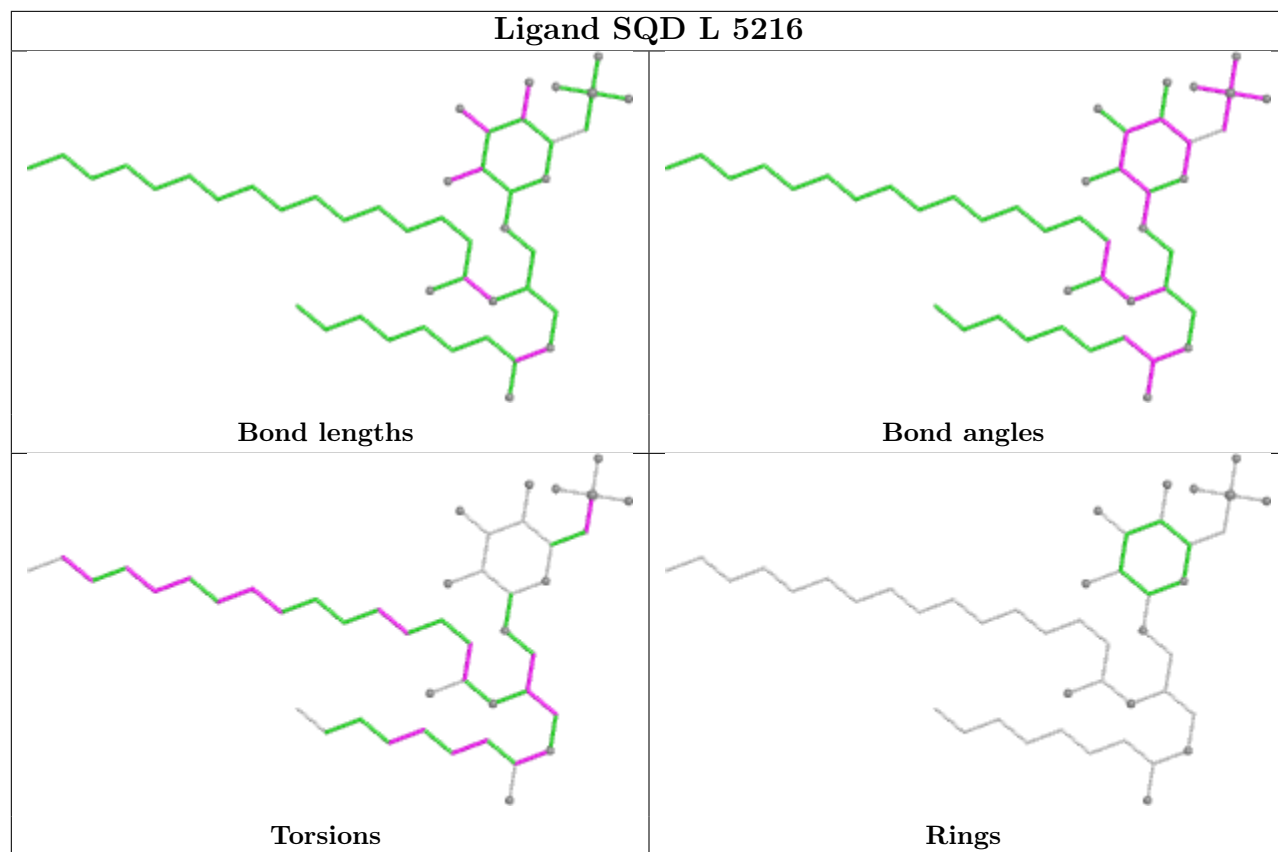


Ligand CLA u 508

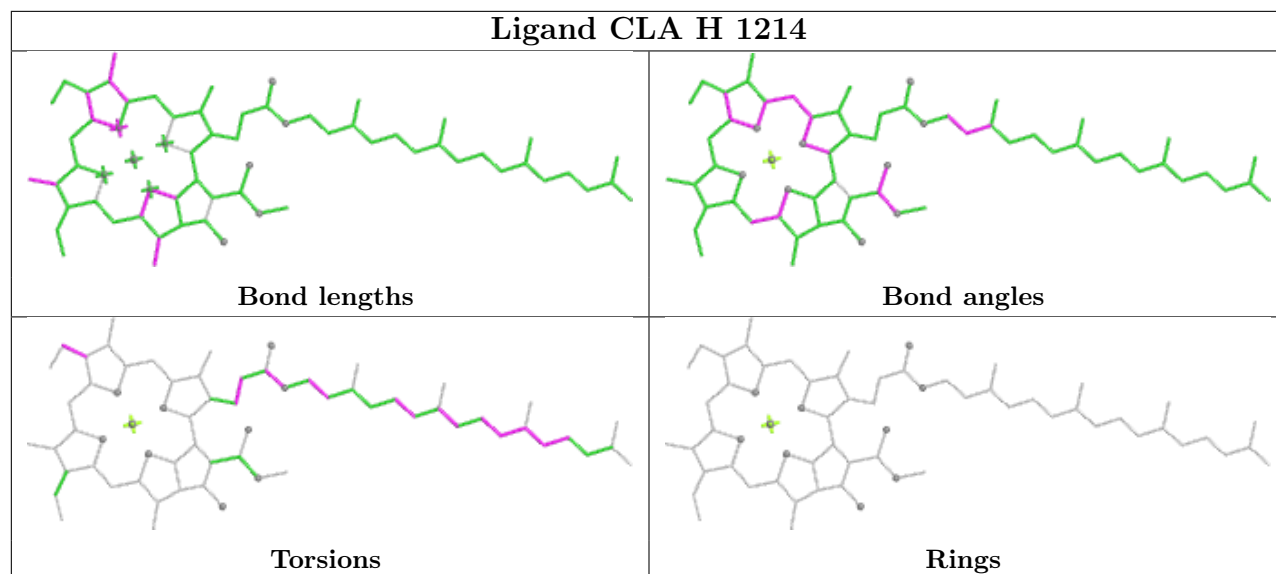


Ligand BCR a 521

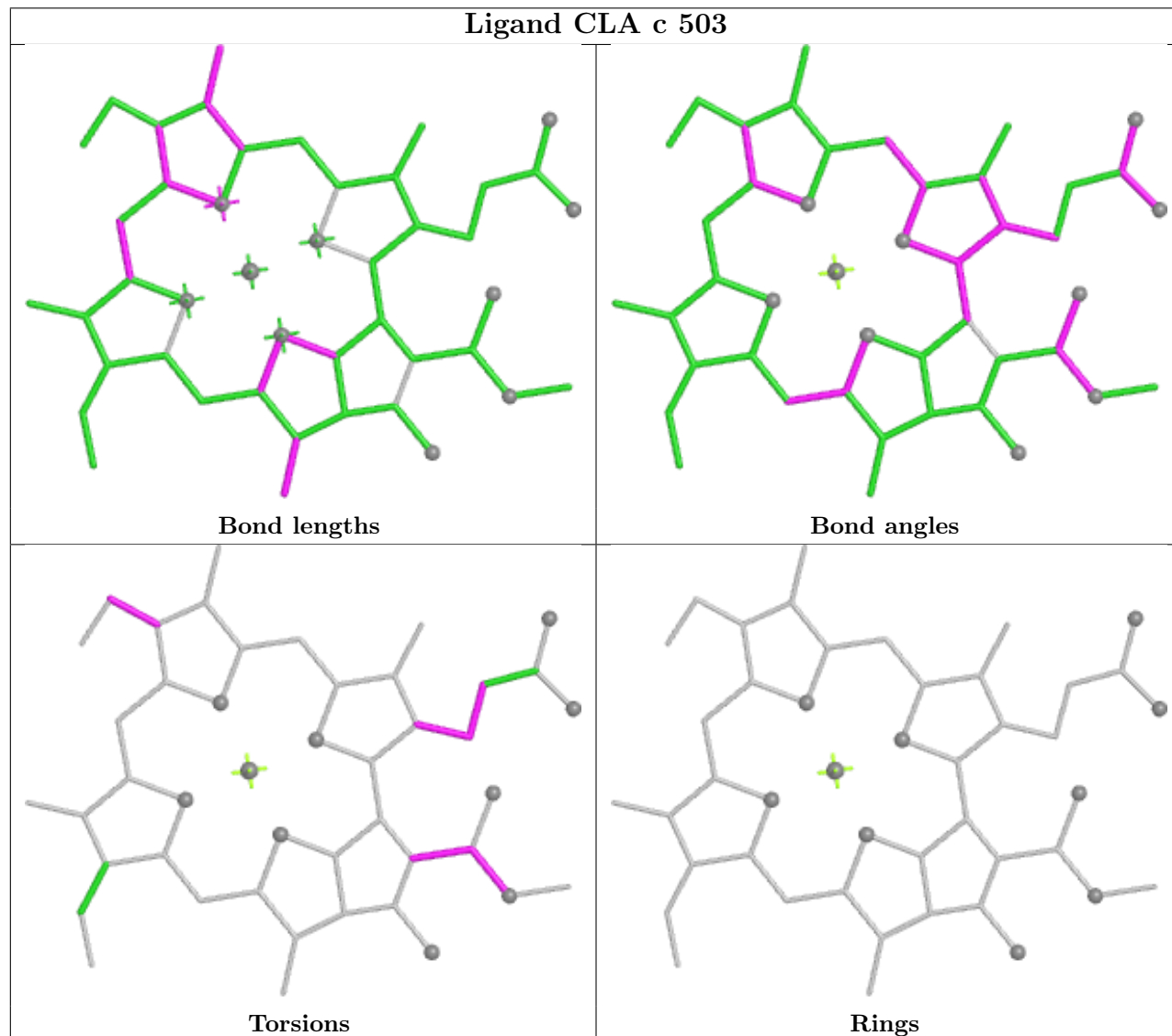




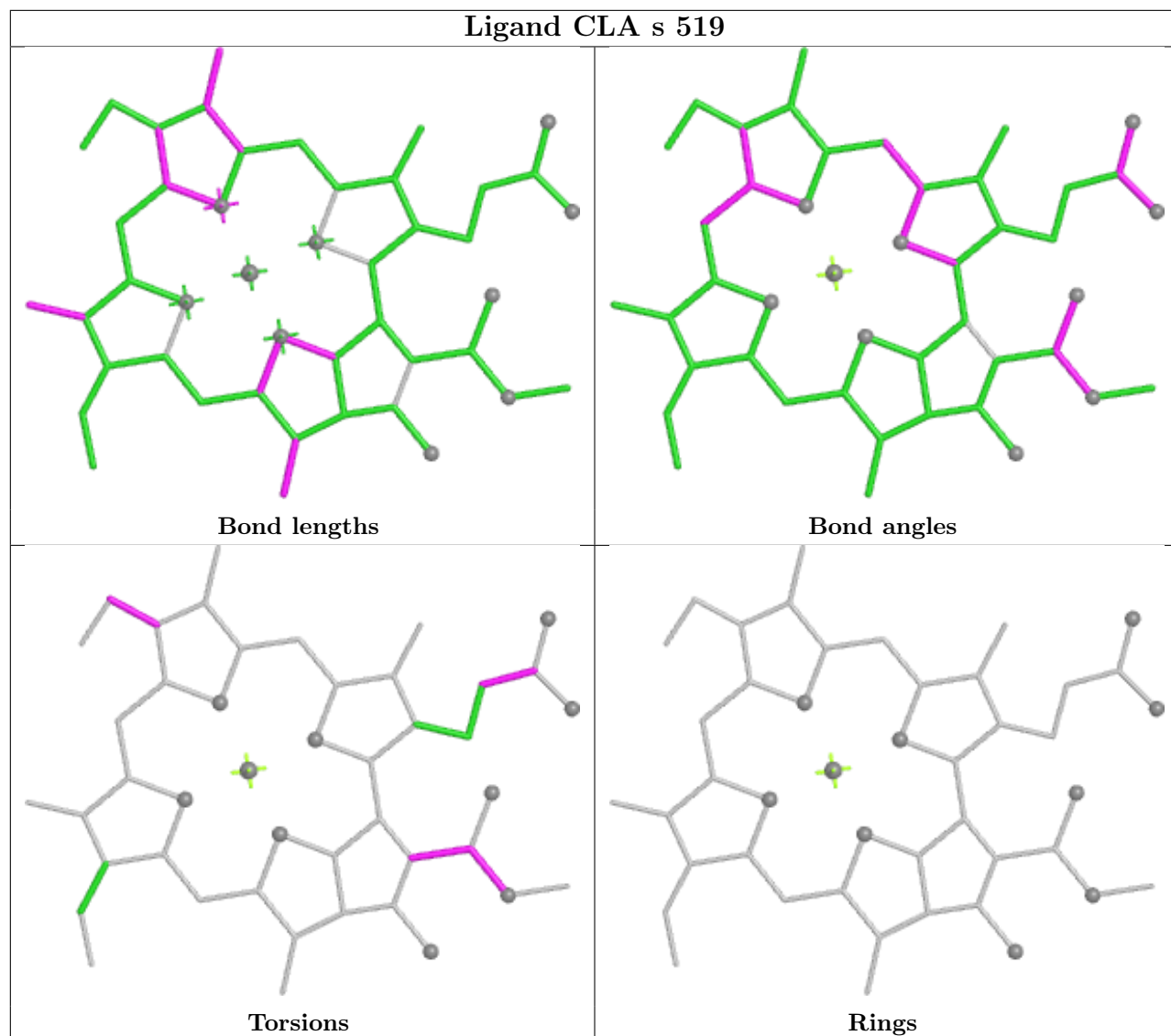
Ligand CLA H 1214



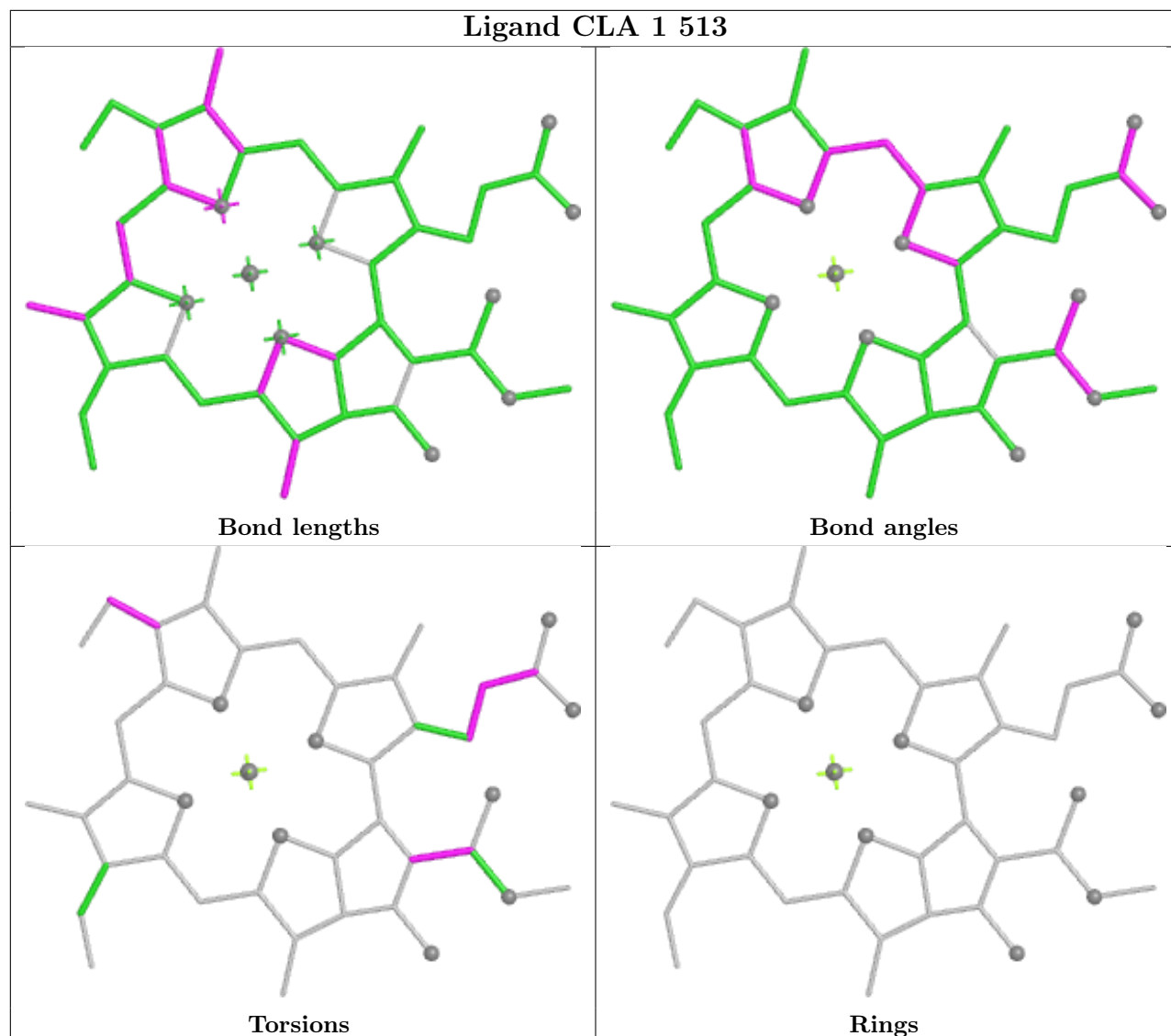
Ligand CLA c 503



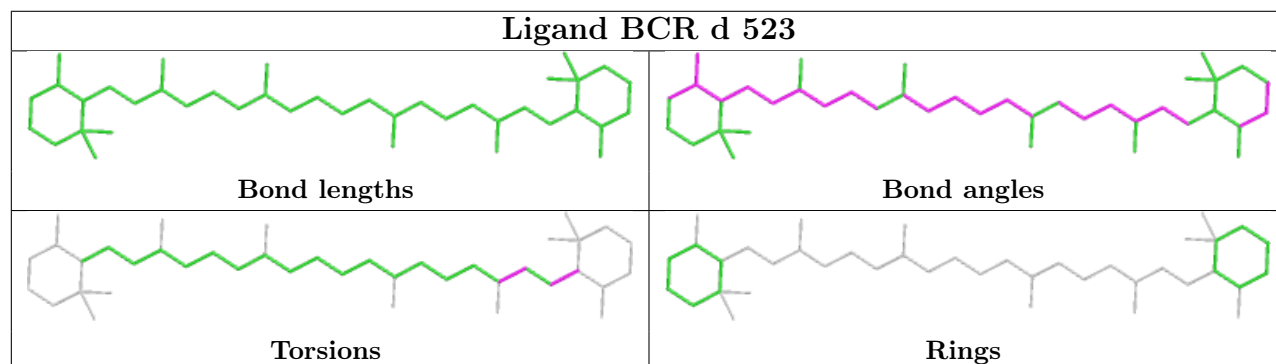
Ligand CLA s 519



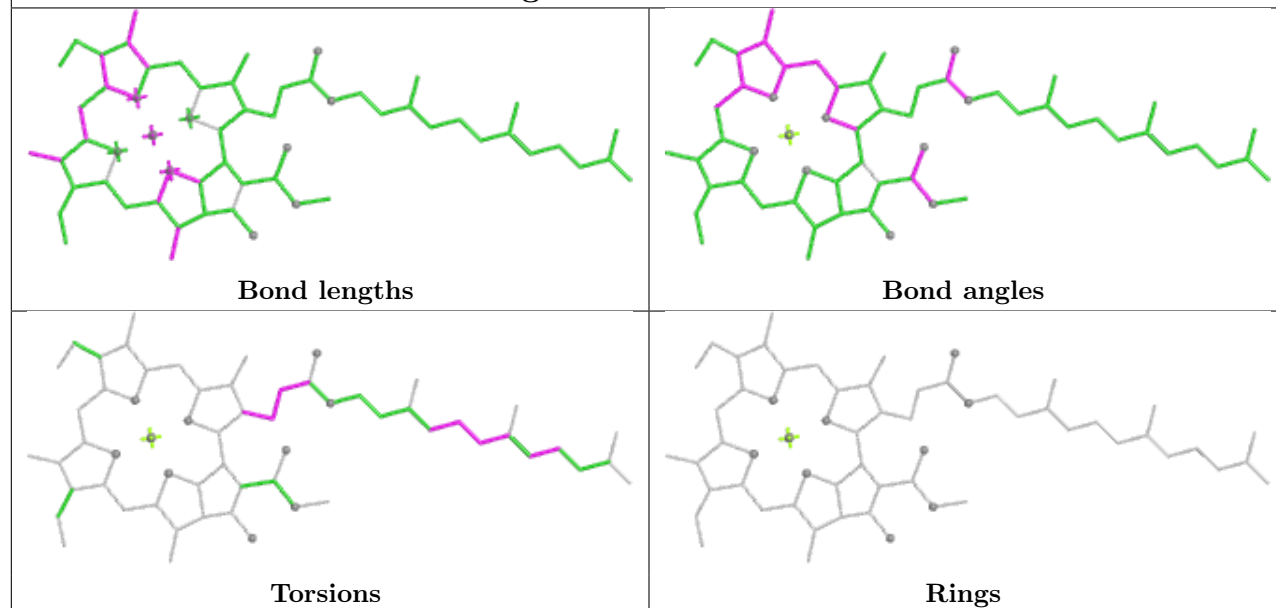
Ligand CLA 1 513



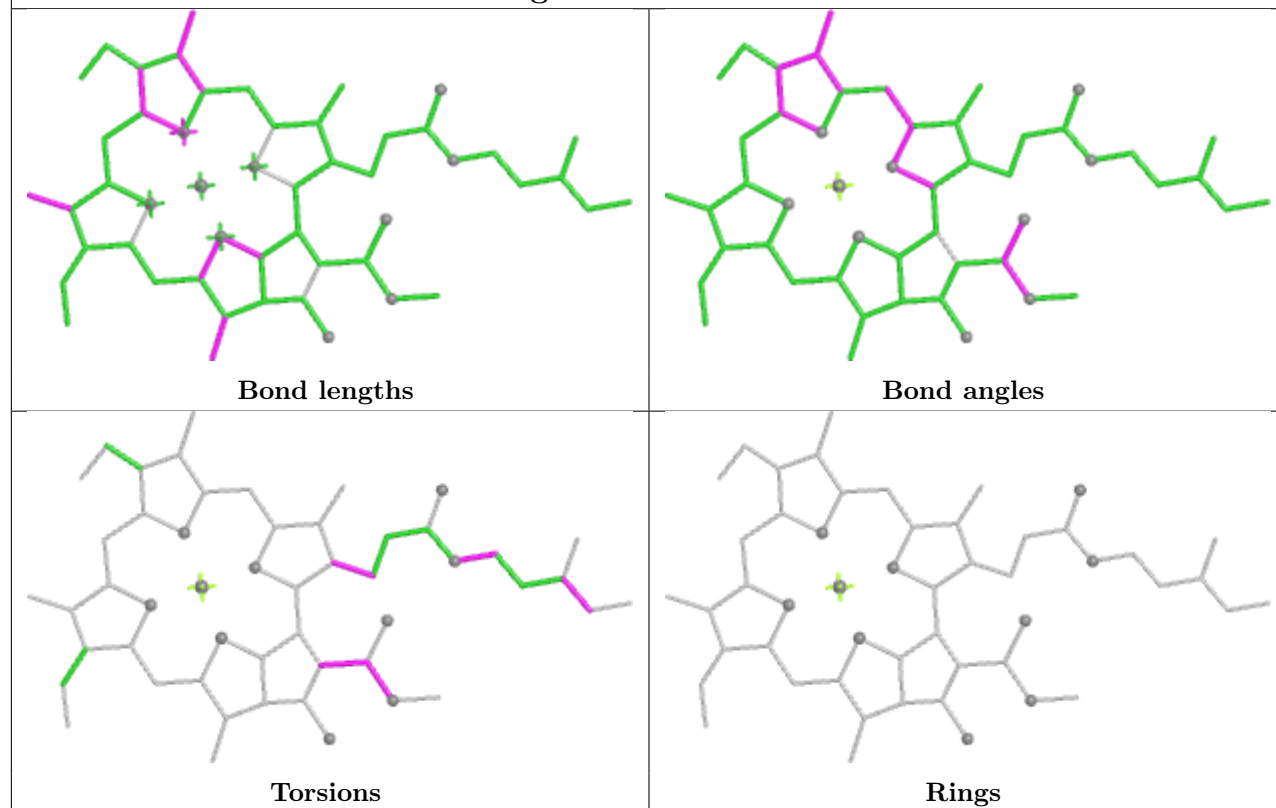
Ligand BCR d 523



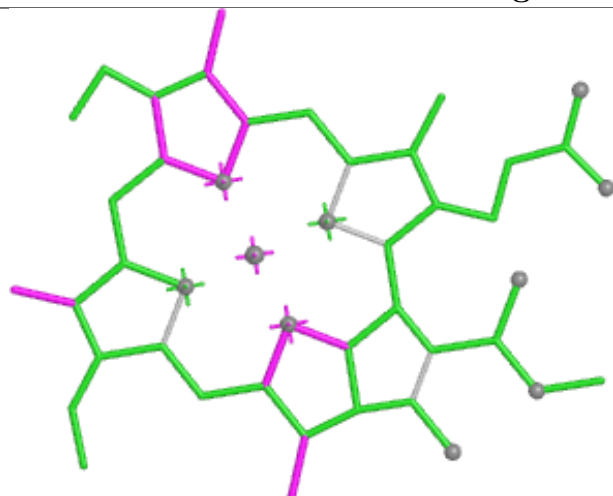
Ligand CLA G 1116



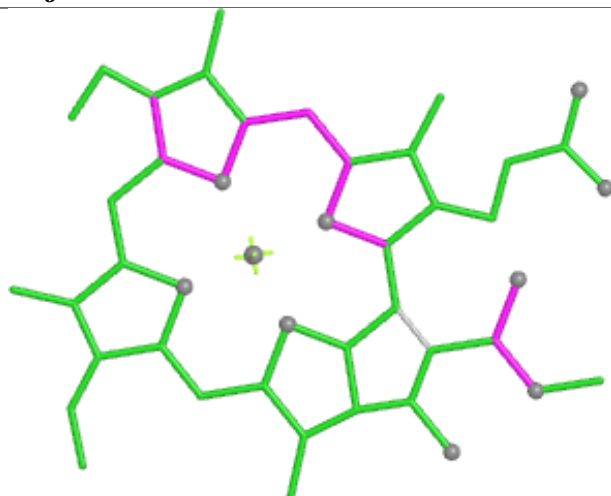
Ligand CLA f 1212



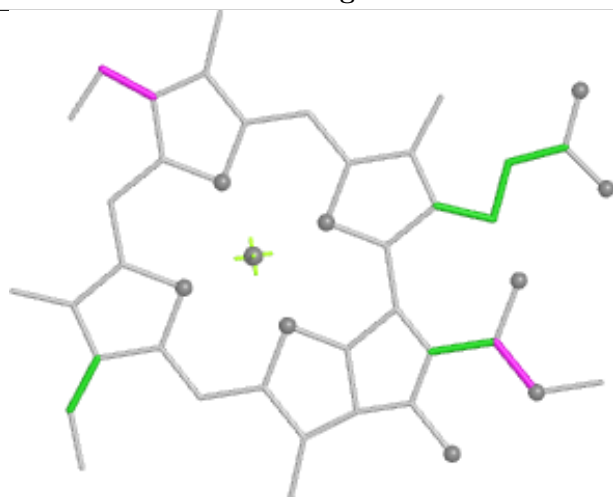
Ligand CLA j 1301



Bond lengths



Bond angles

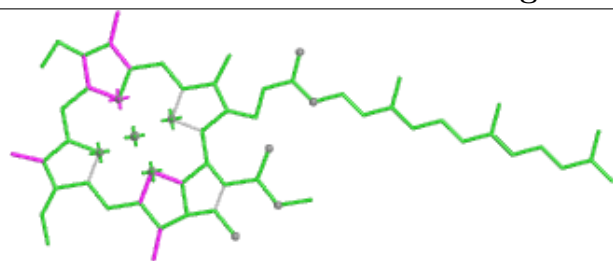


Torsions

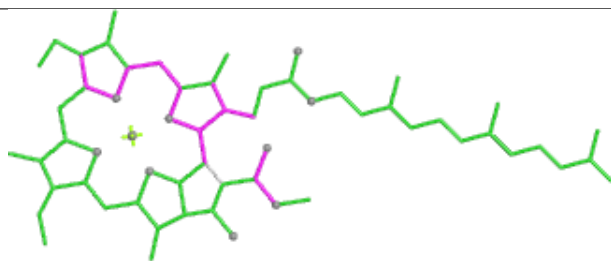


Rings

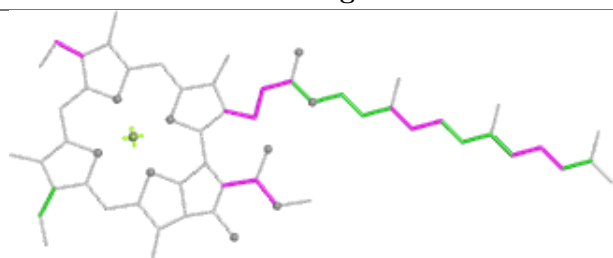
Ligand CLA r 501



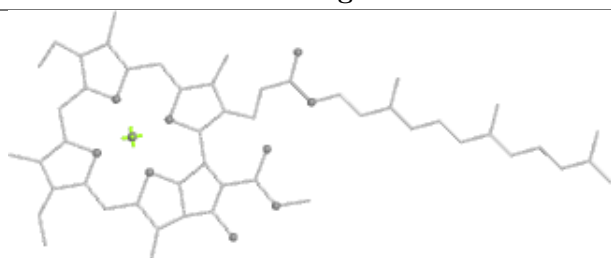
Bond lengths



Bond angles

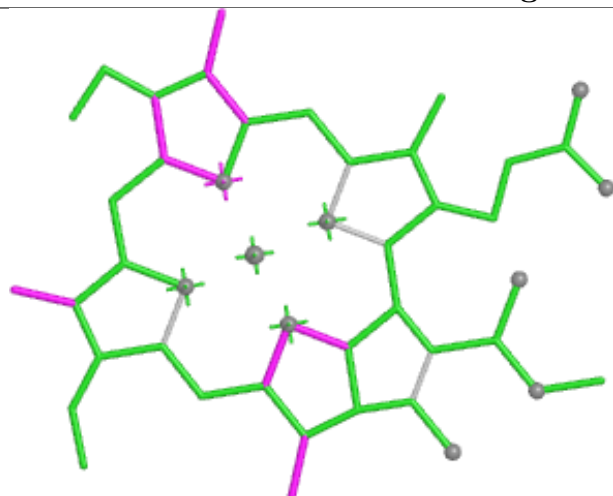


Torsions

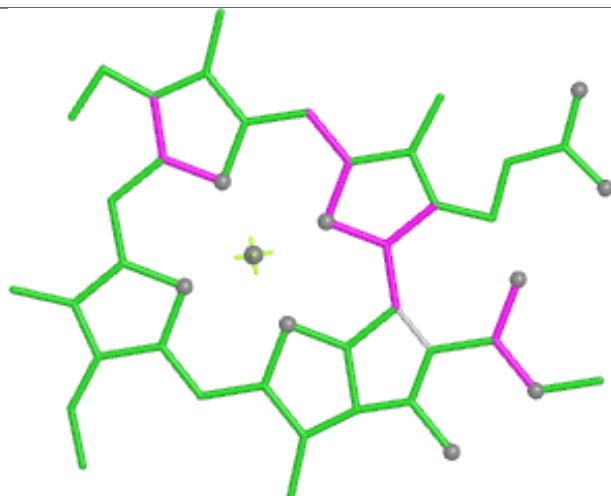


Rings

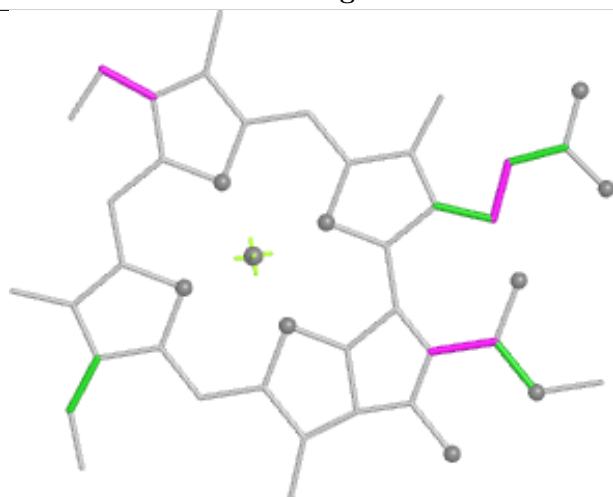
Ligand CLA t 502



Bond lengths



Bond angles

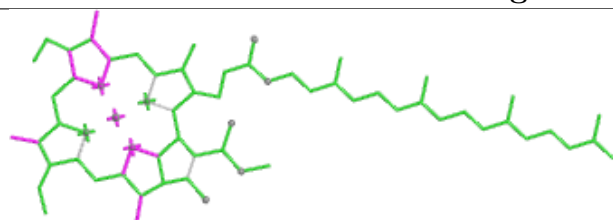


Torsions

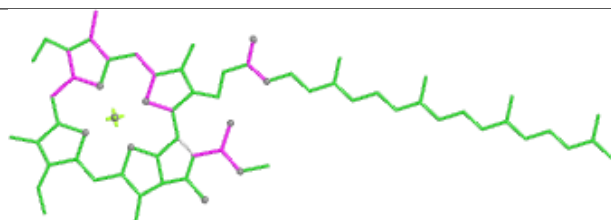


Rings

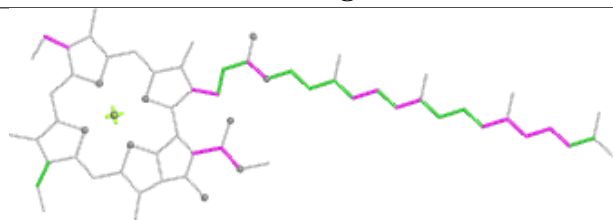
Ligand CLA e 1109



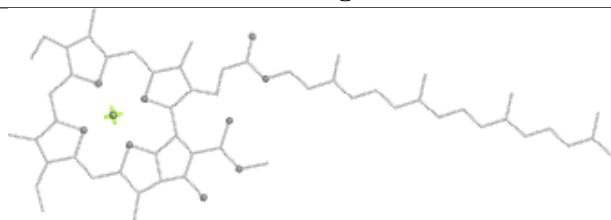
Bond lengths



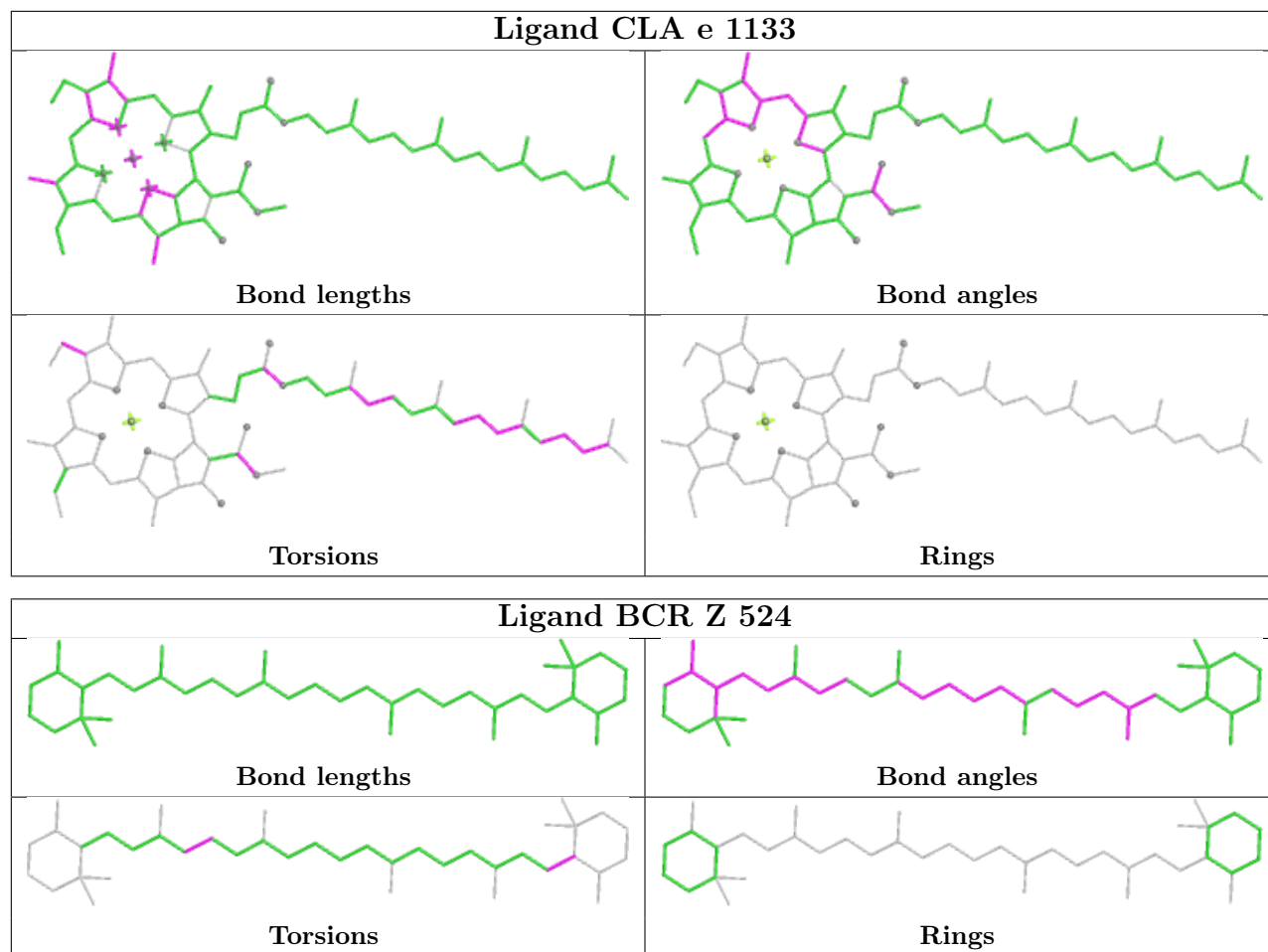
Bond angles



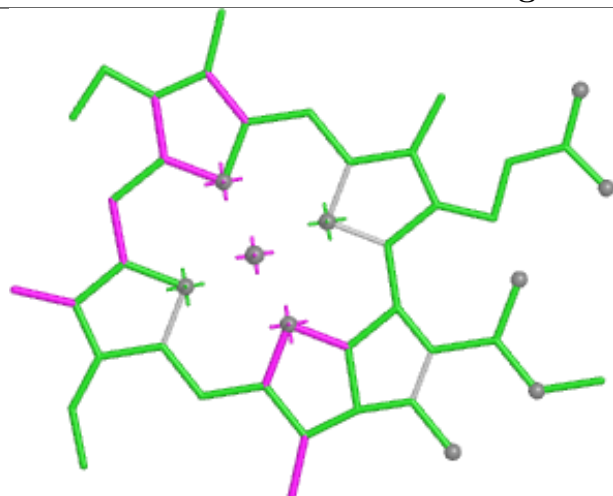
Torsions



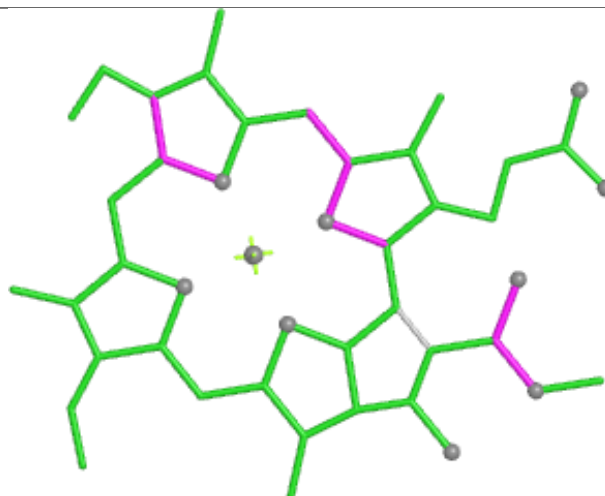
Rings



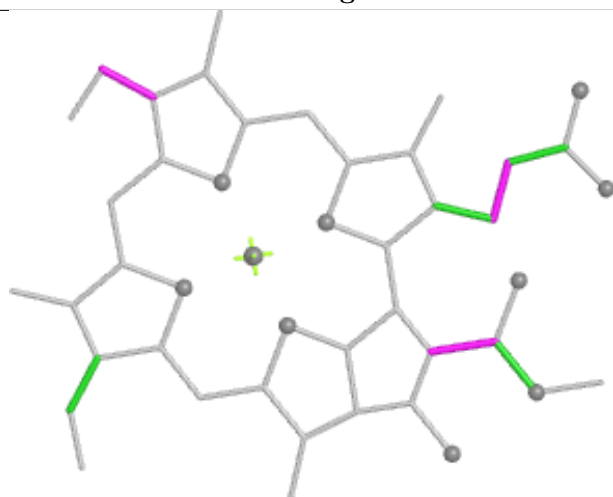
Ligand CLA 4 505



Bond lengths



Bond angles

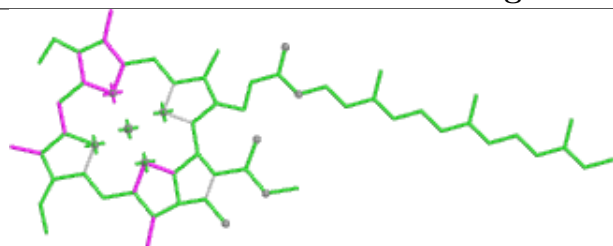


Torsions

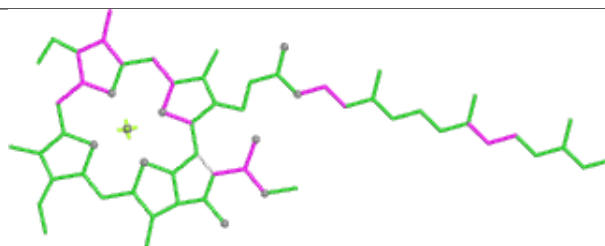


Rings

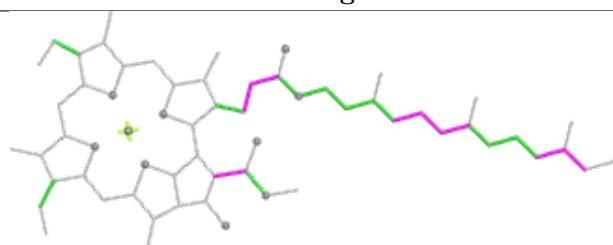
Ligand CLA H 1213



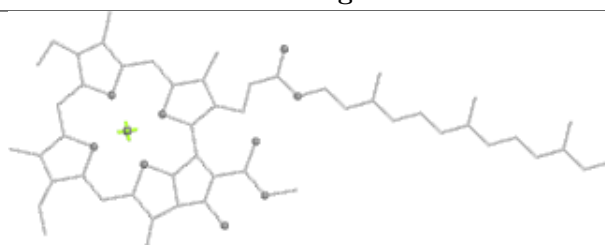
Bond lengths



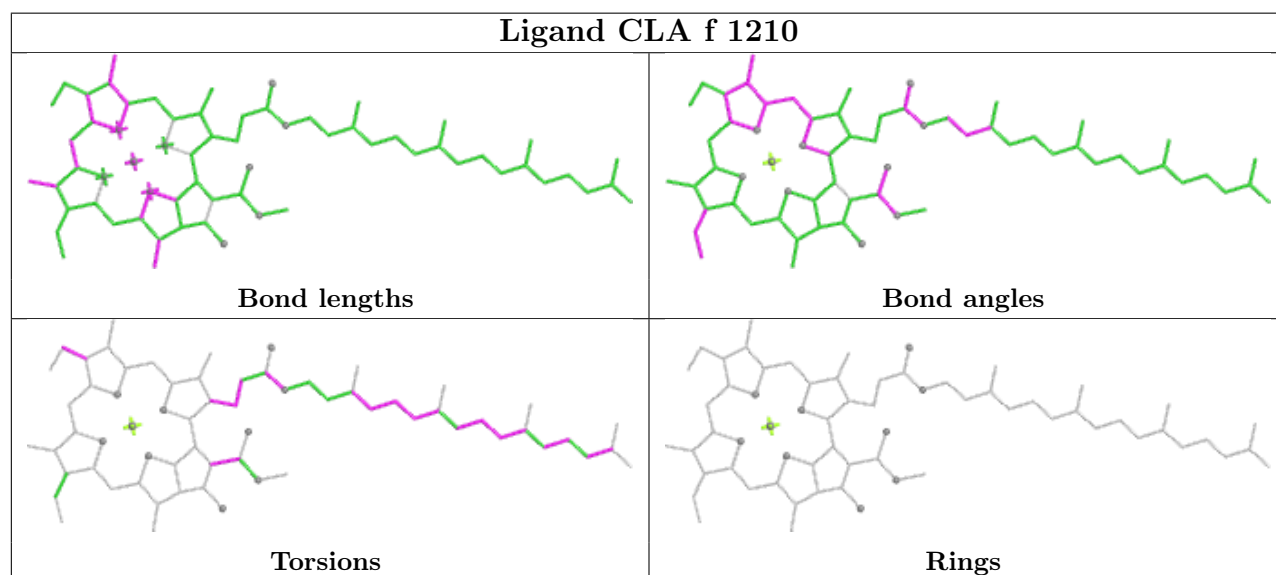
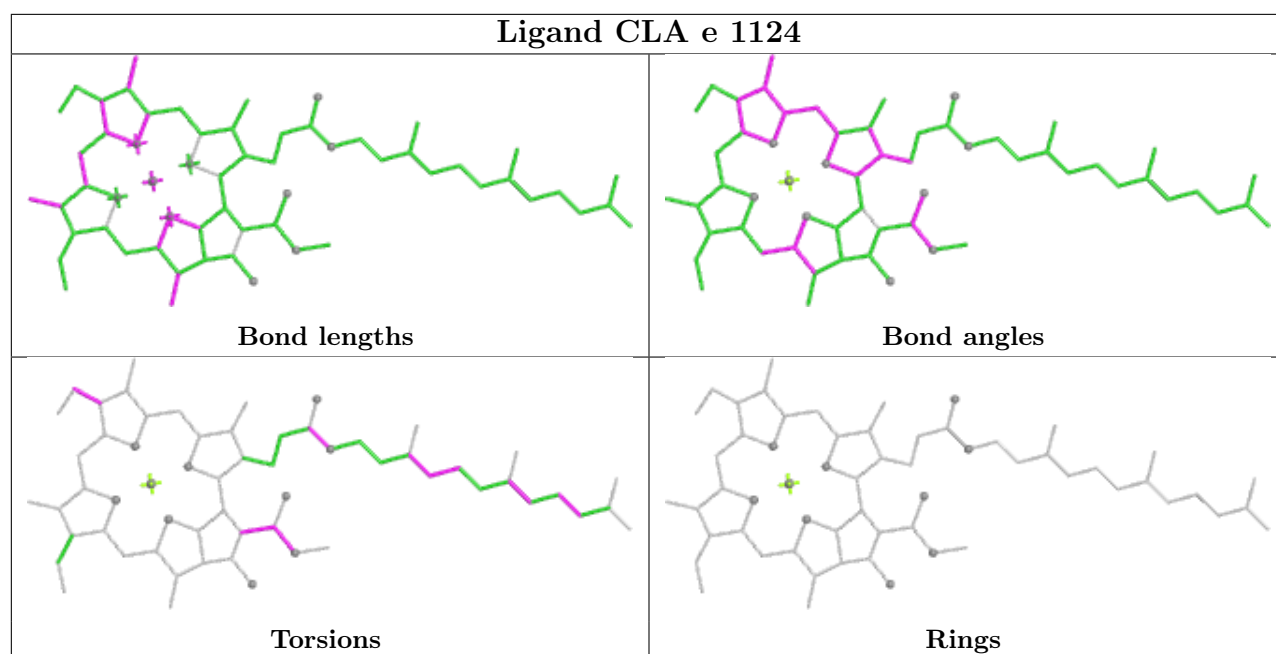
Bond angles



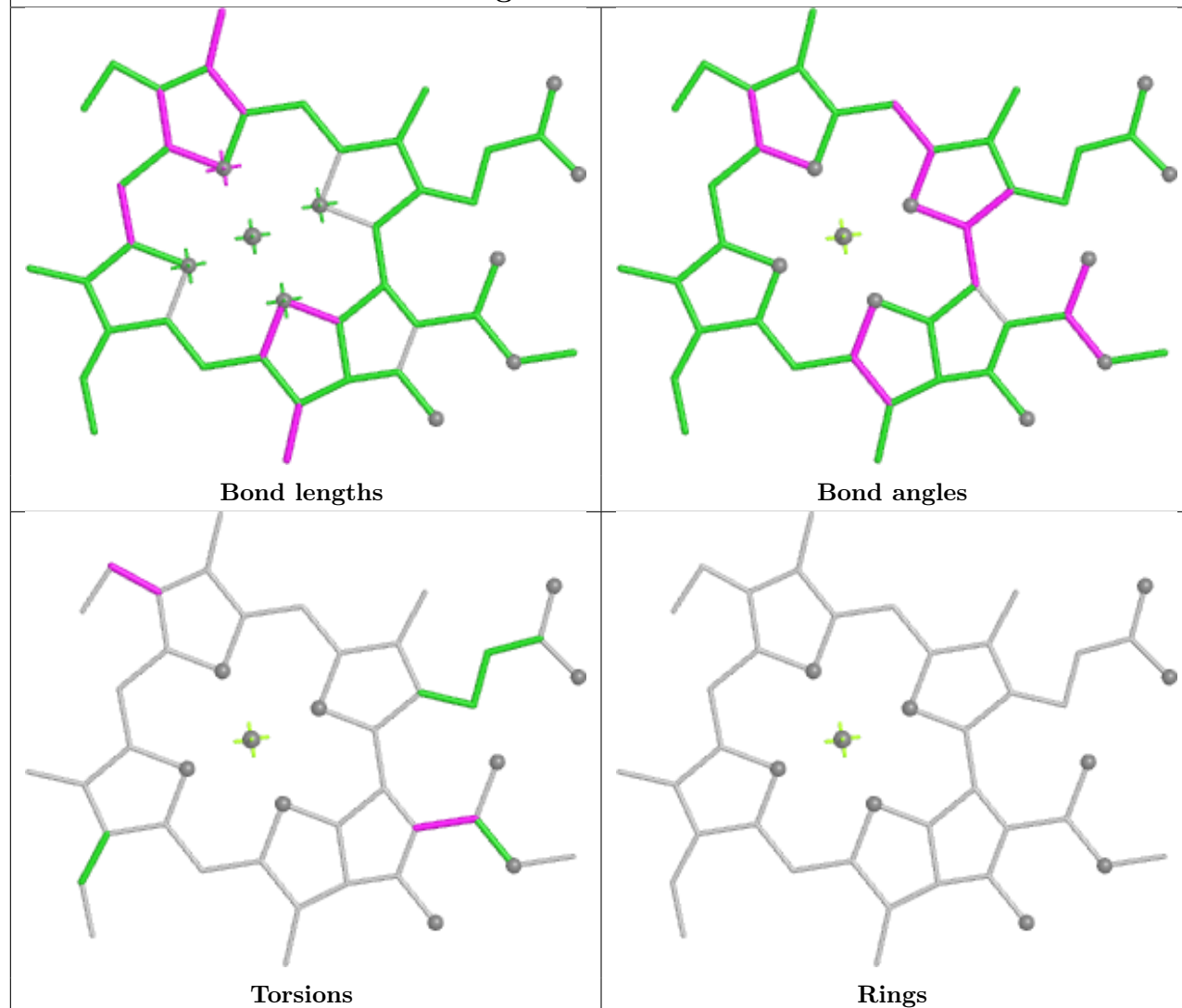
Torsions



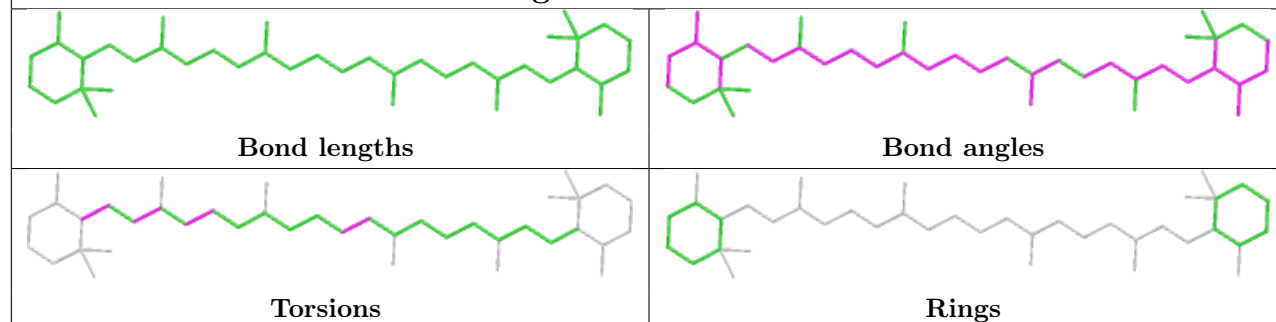
Rings



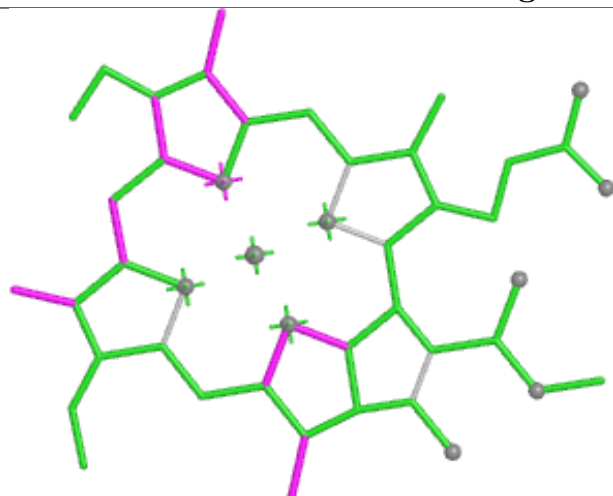
Ligand CLA b 503



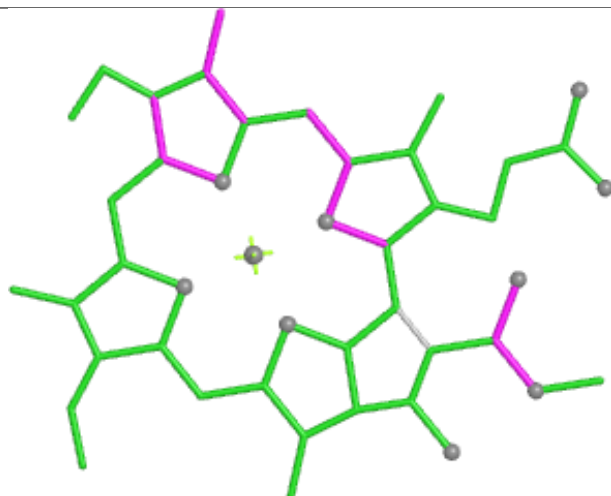
Ligand BCR Z 522



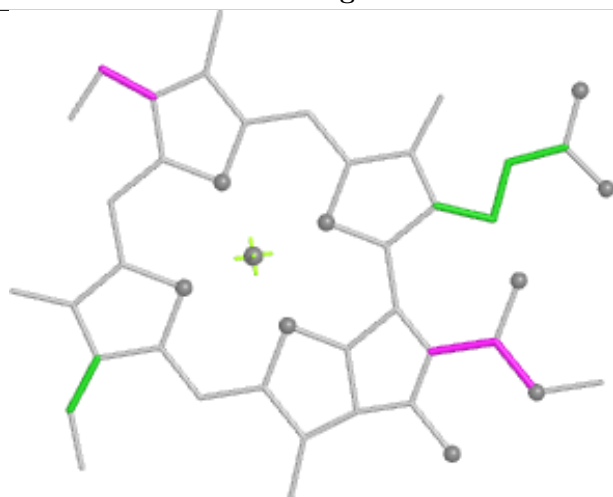
Ligand CLA 6 506



Bond lengths



Bond angles

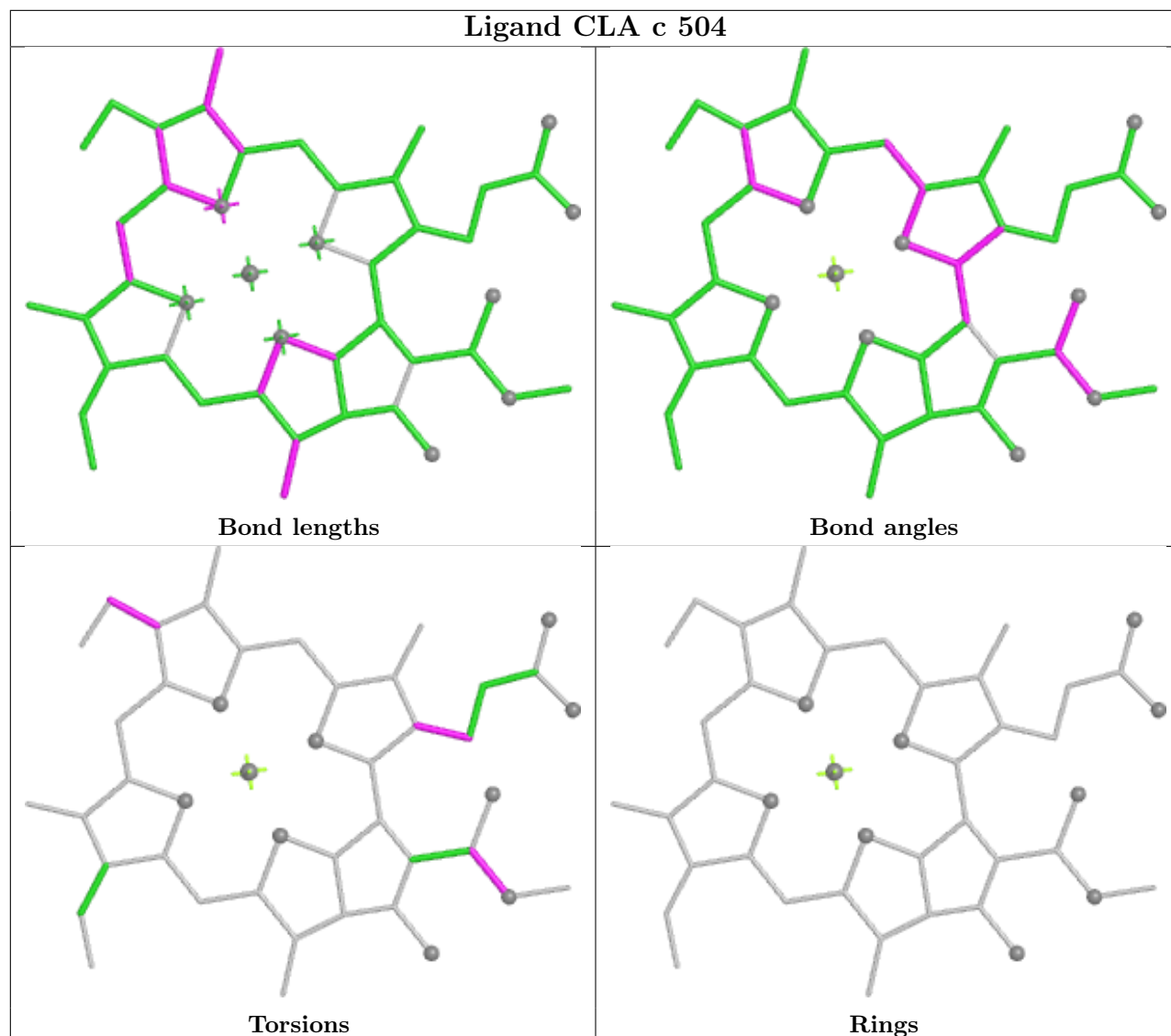


Torsions

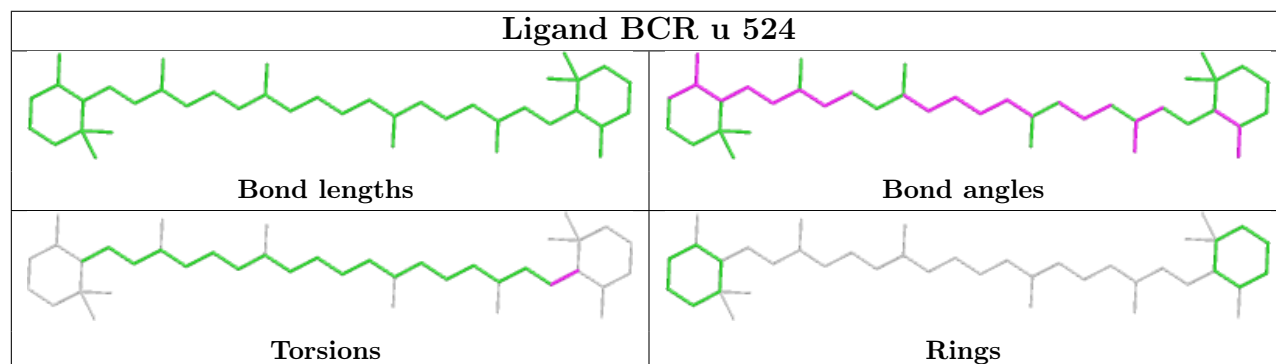


Rings

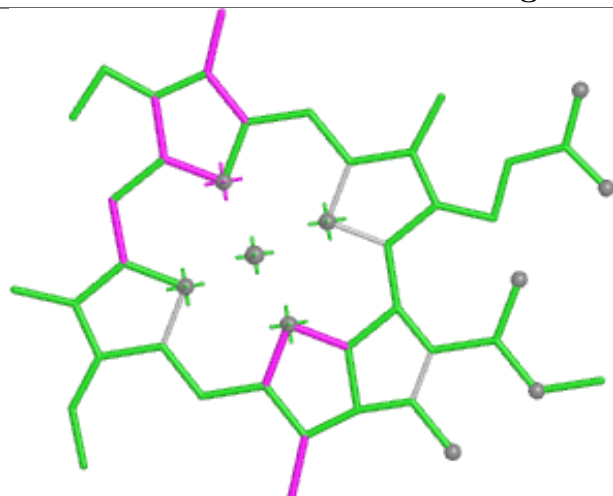
Ligand CLA c 504



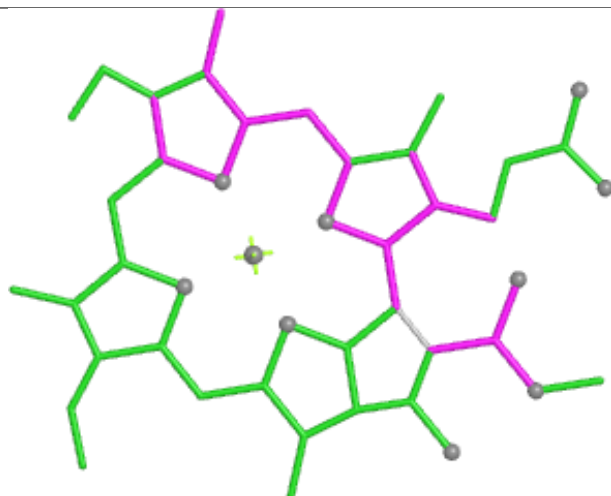
Ligand BCR u 524



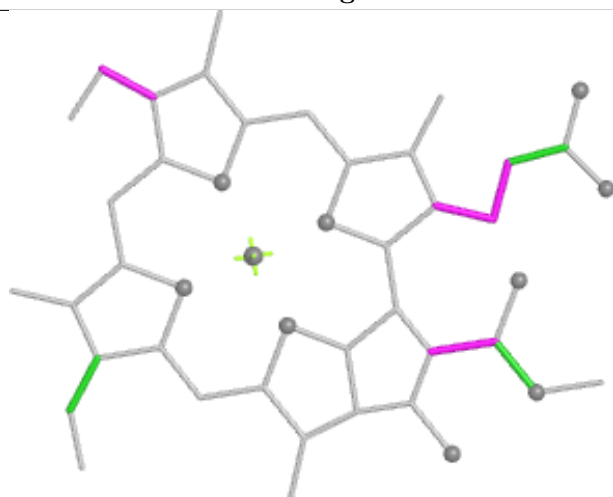
Ligand CLA s 504



Bond lengths



Bond angles

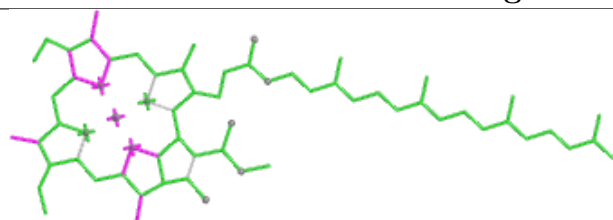


Torsions

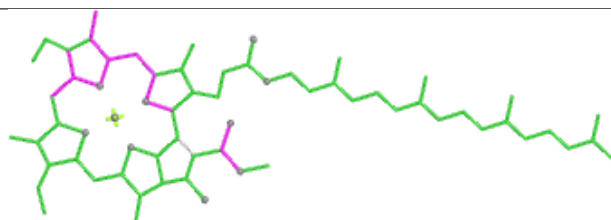


Rings

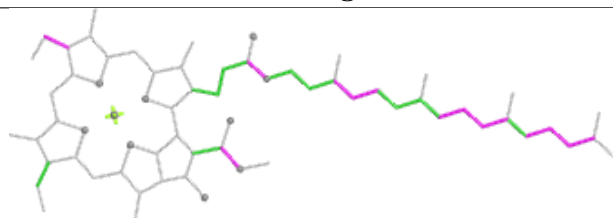
Ligand CLA G 1133



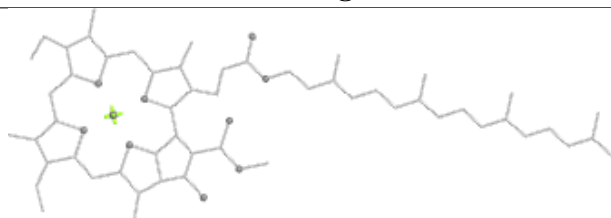
Bond lengths



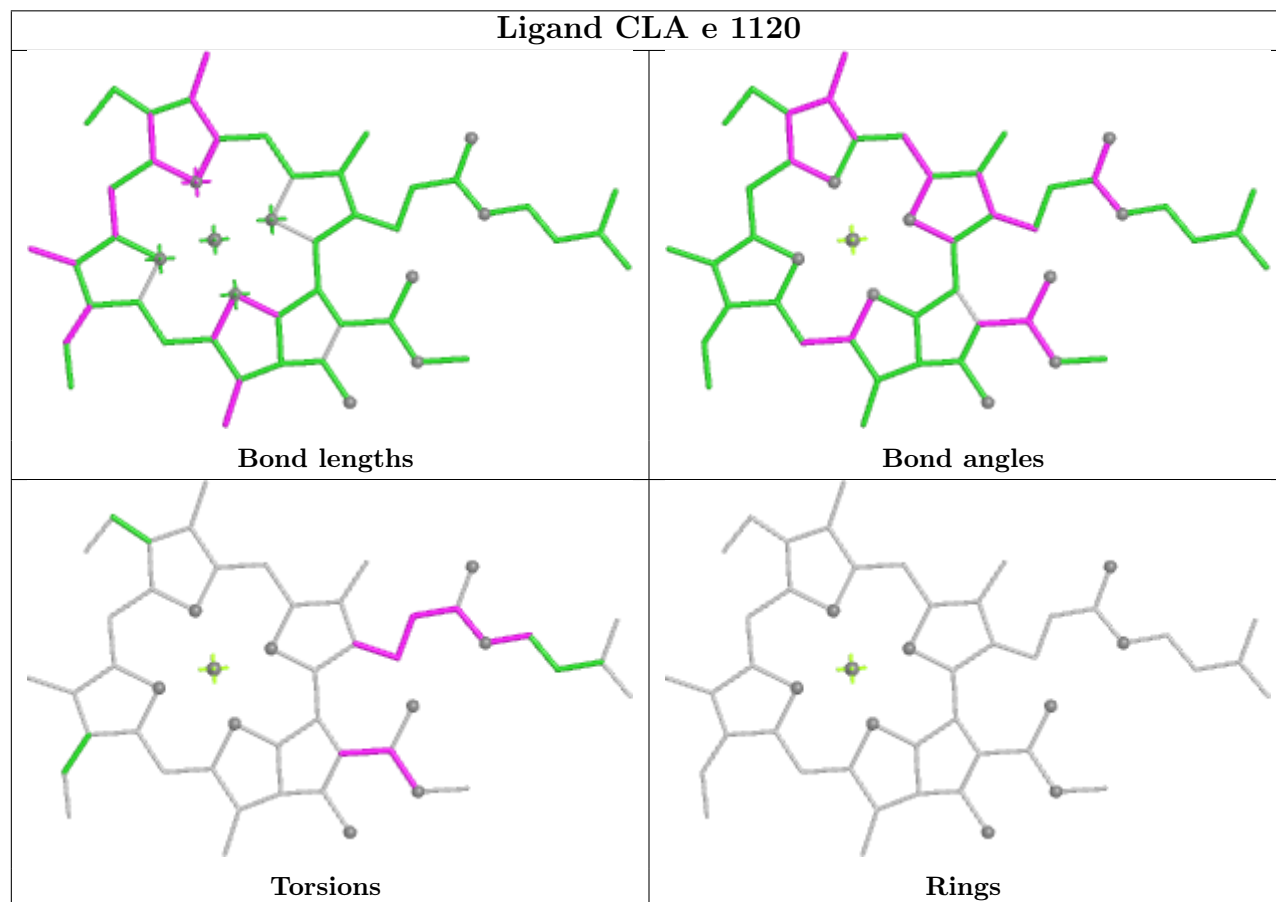
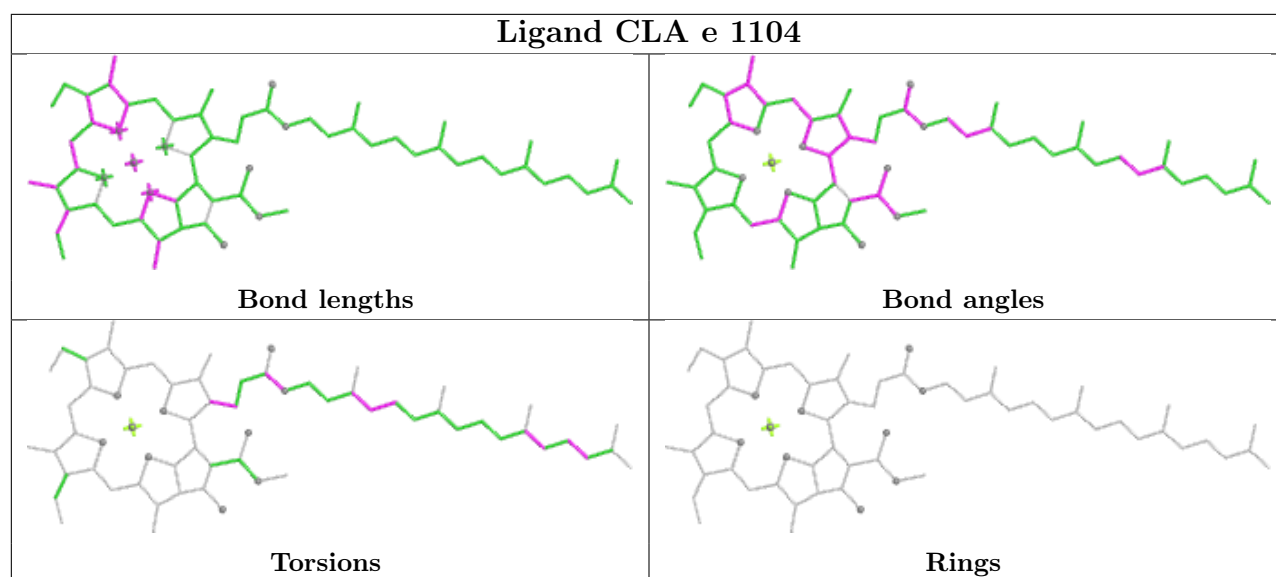
Bond angles



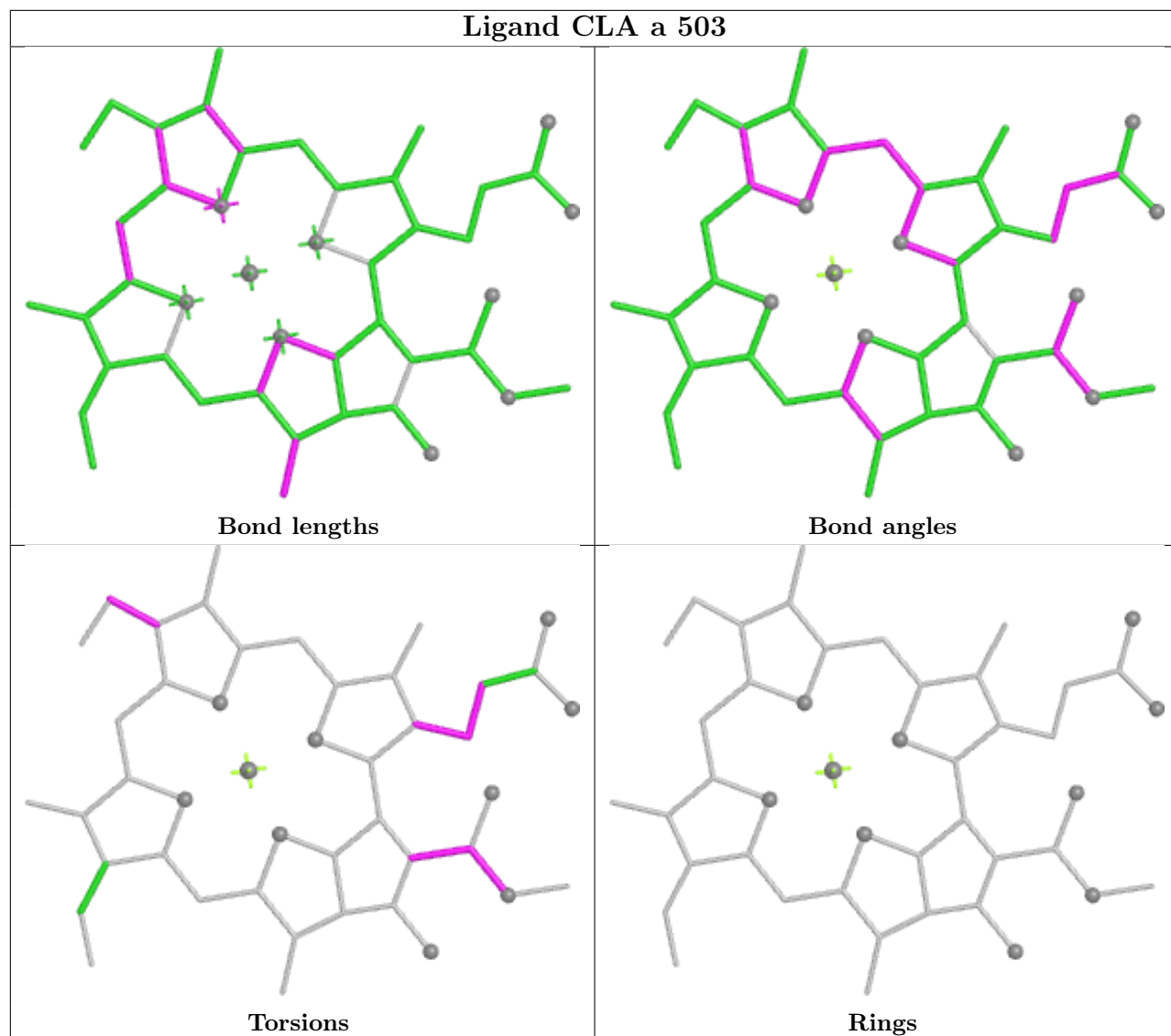
Torsions



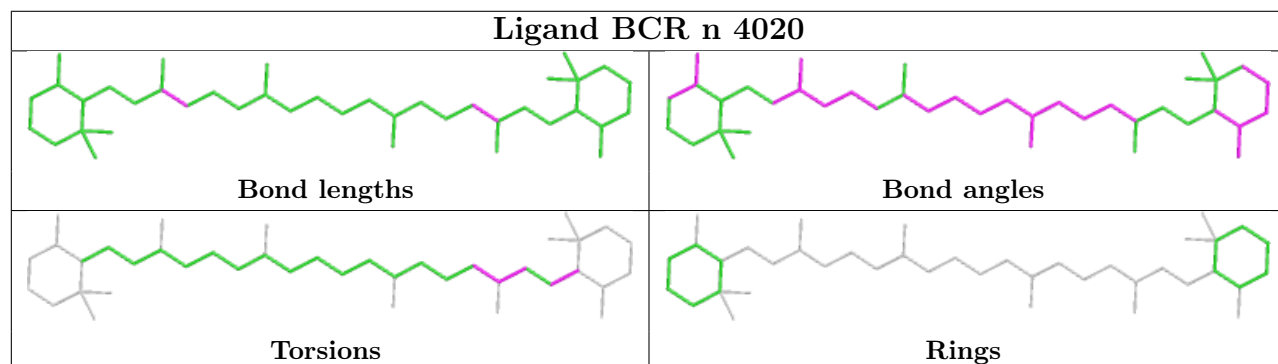
Rings

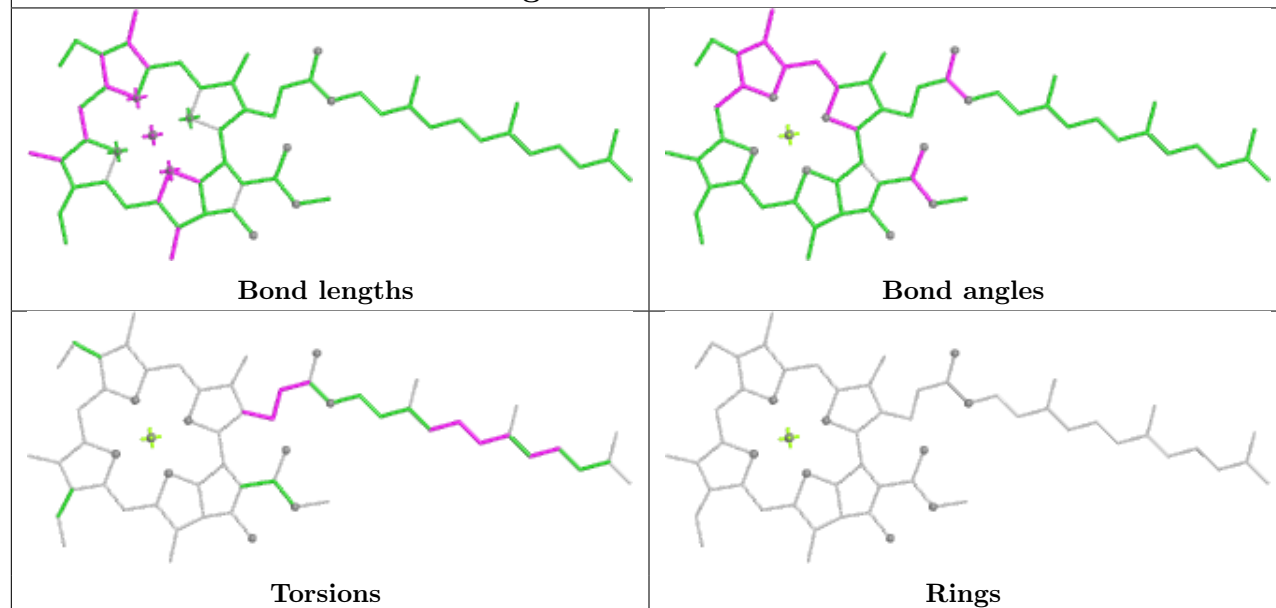
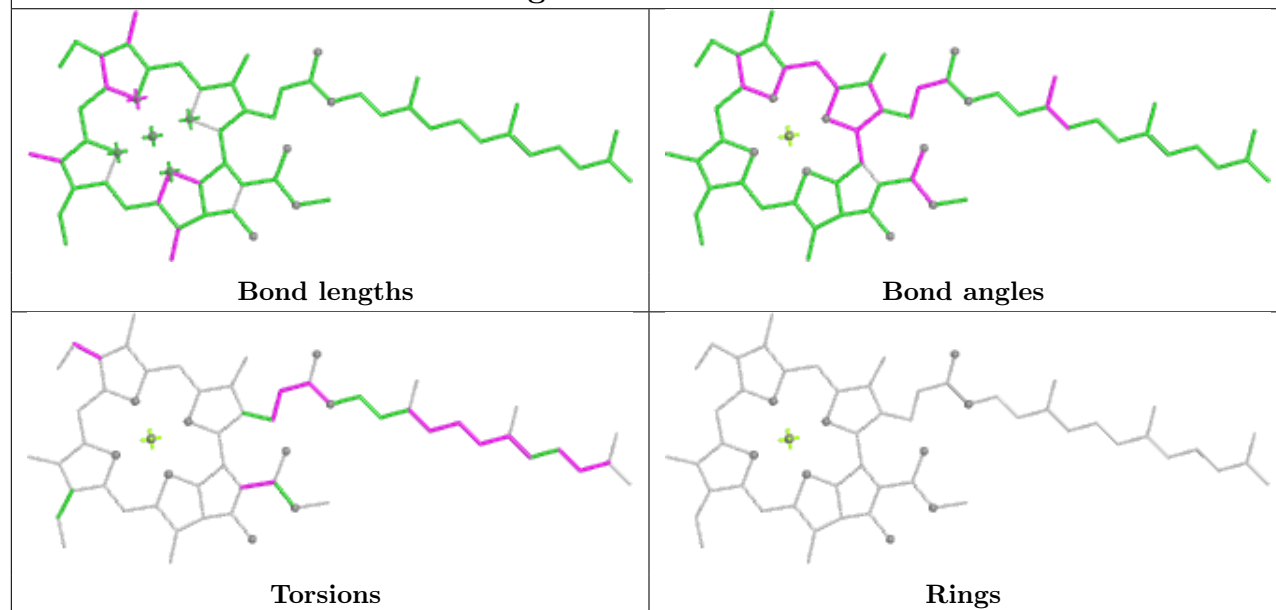


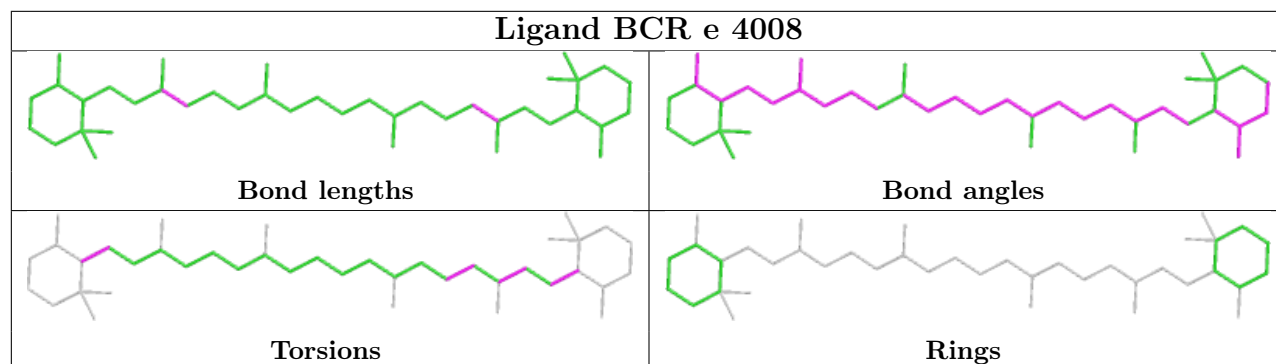
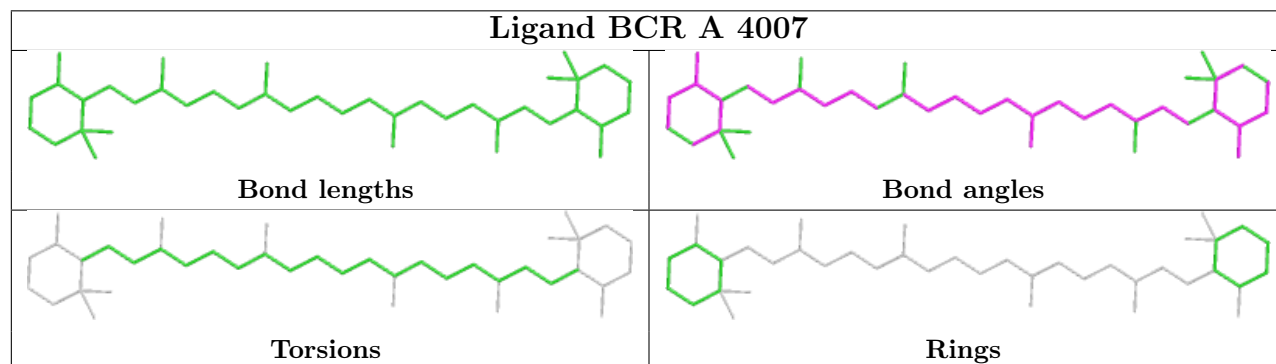
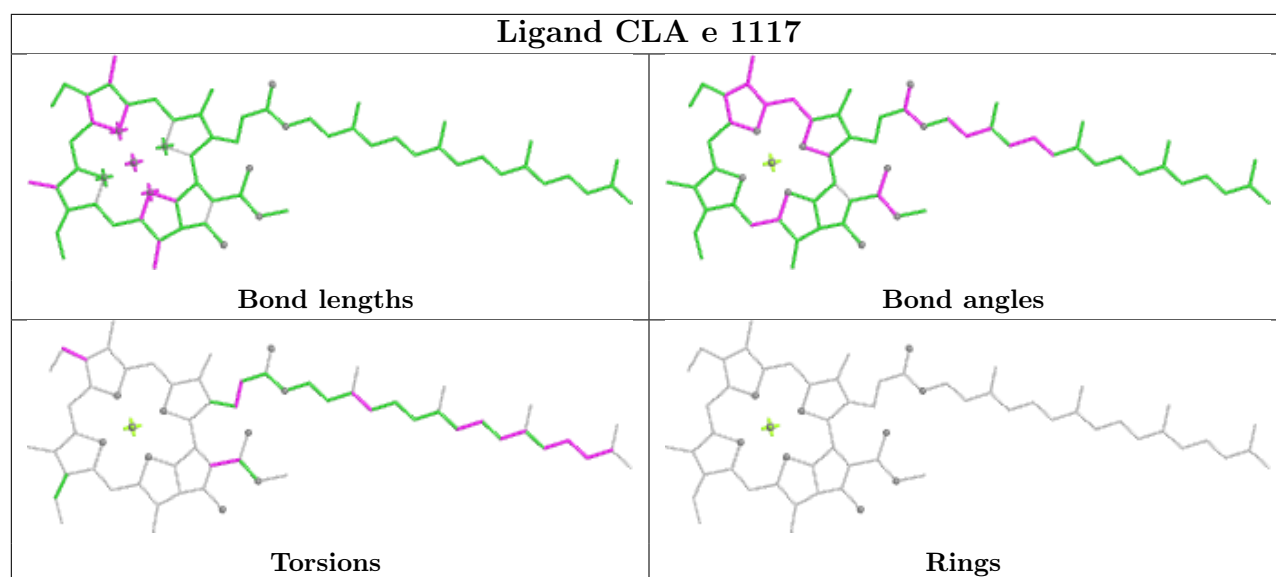
Ligand CLA a 503

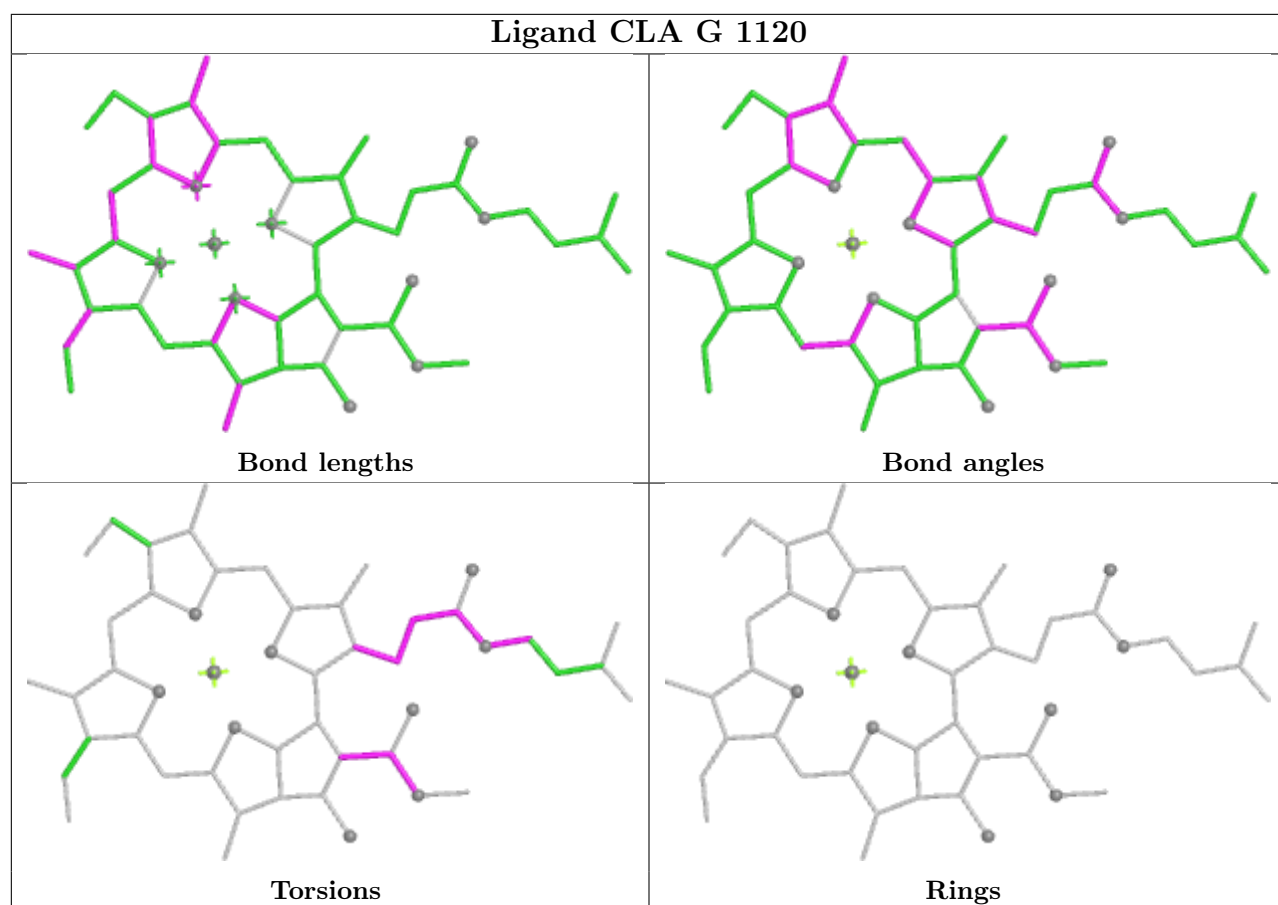


Ligand BCR n 4020

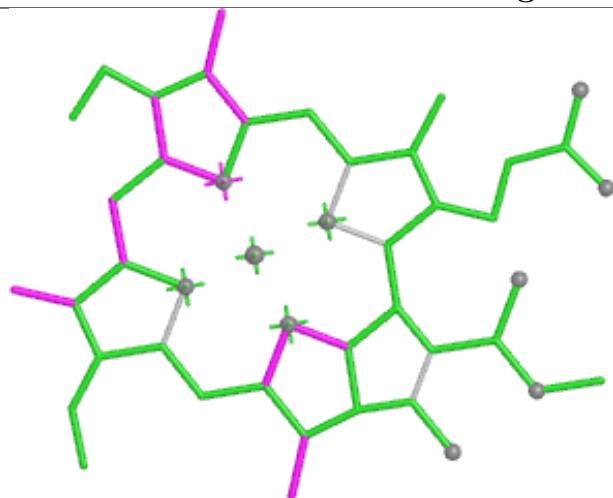


Ligand CLA A 1116**Ligand CLA e 1137**

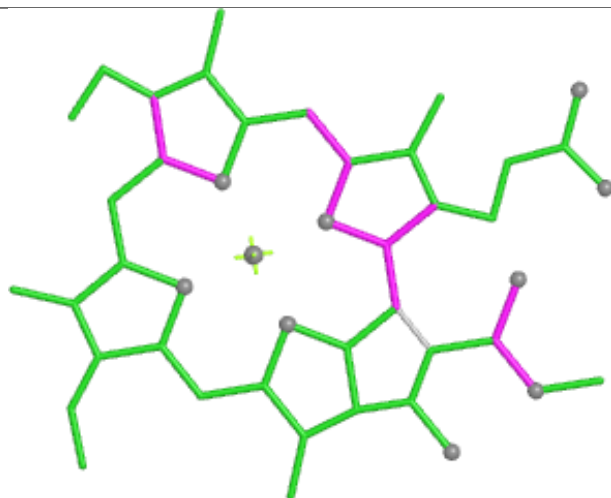




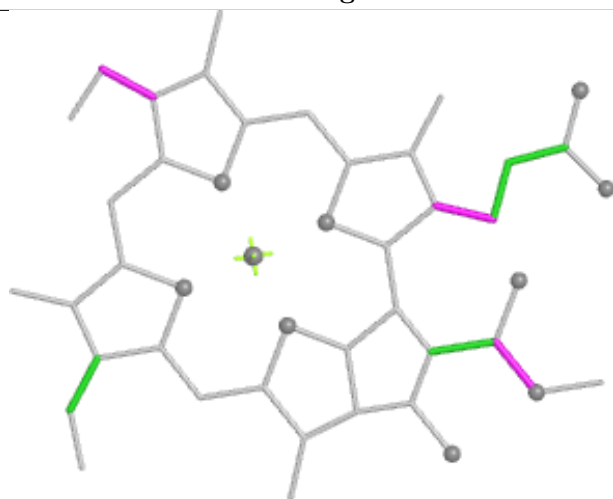
Ligand CLA u 504



Bond lengths



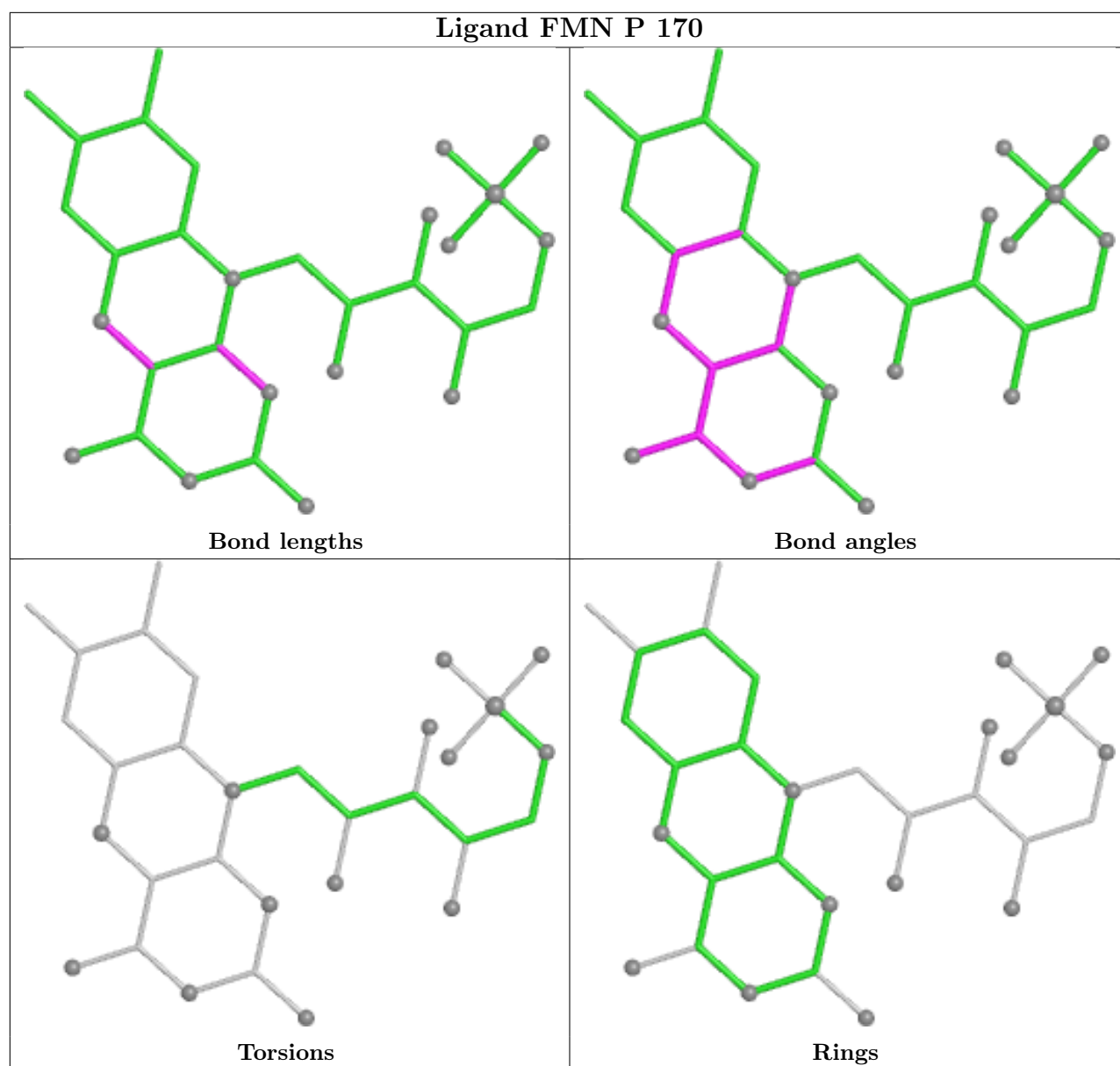
Bond angles

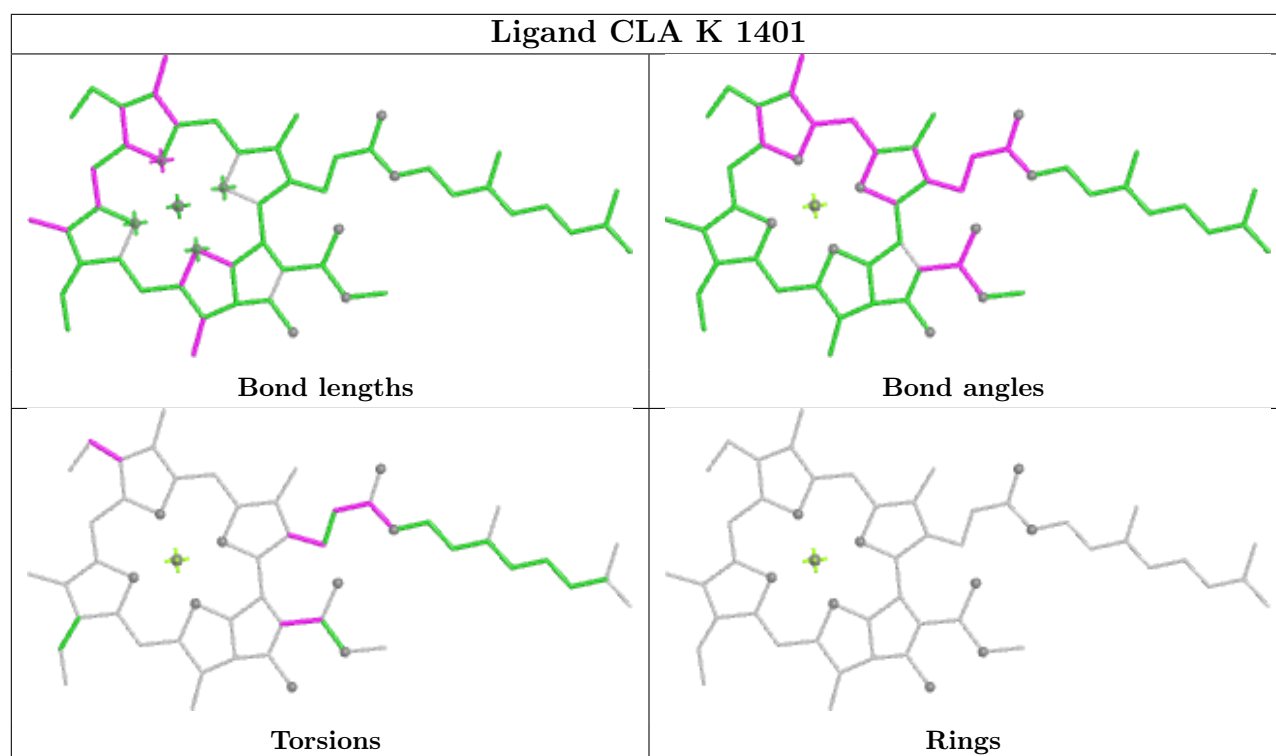


Torsions

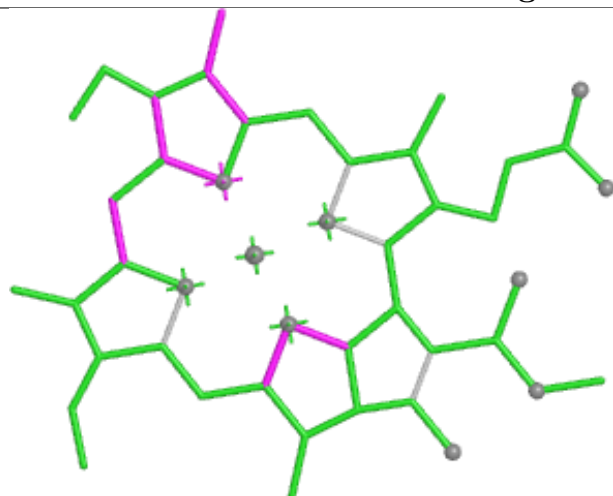


Rings

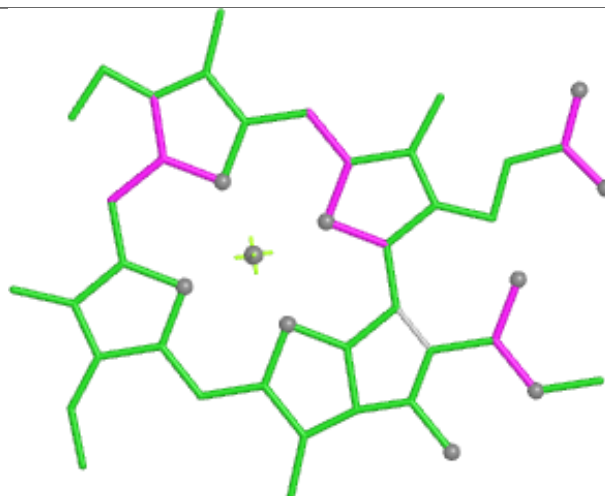




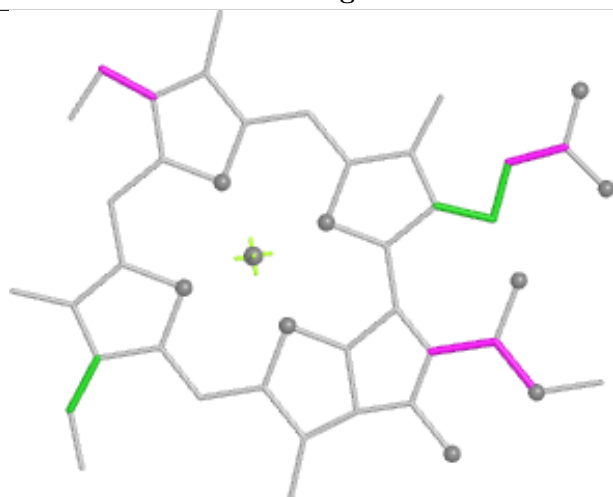
Ligand CLA 5 519



Bond lengths



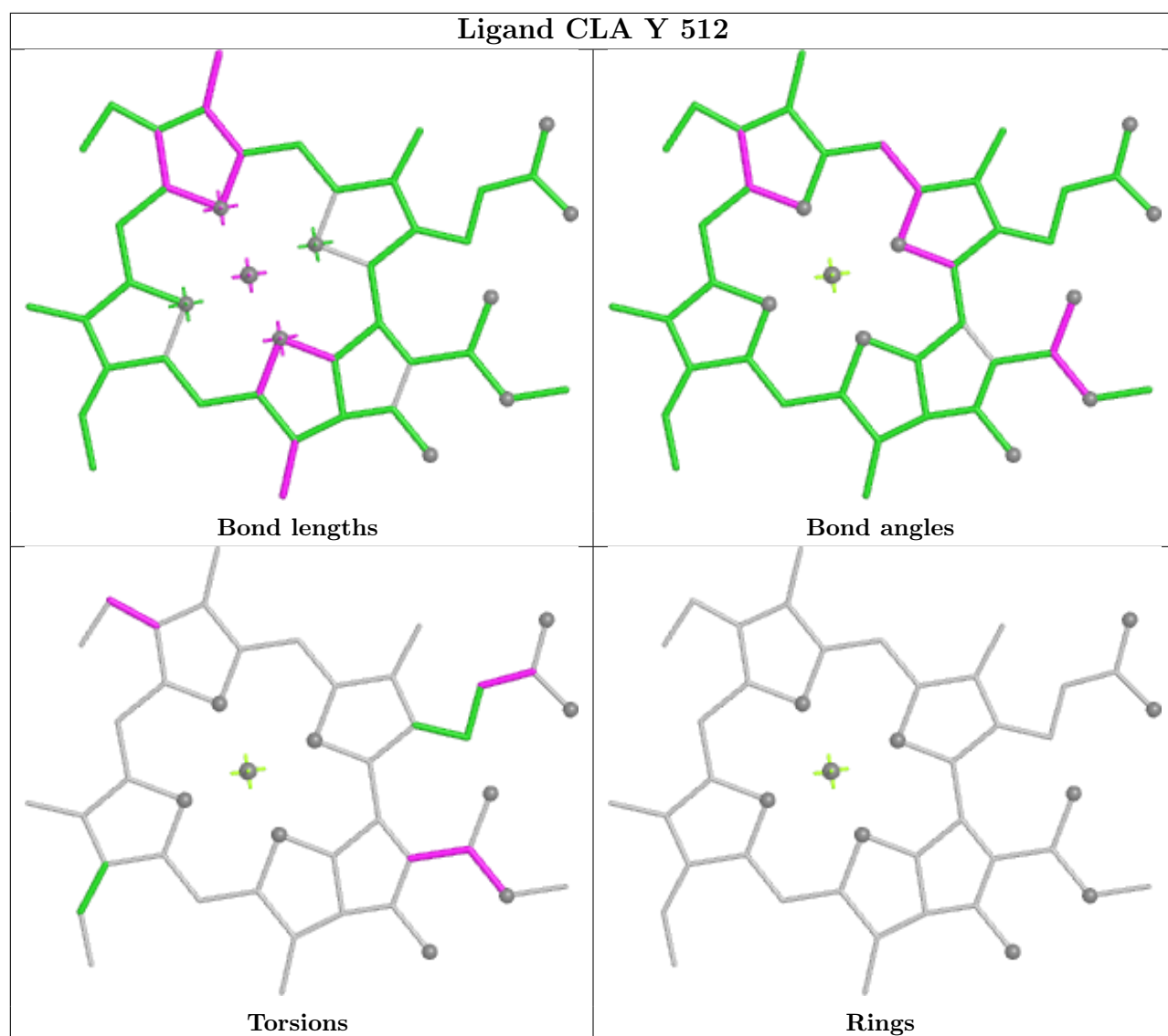
Bond angles



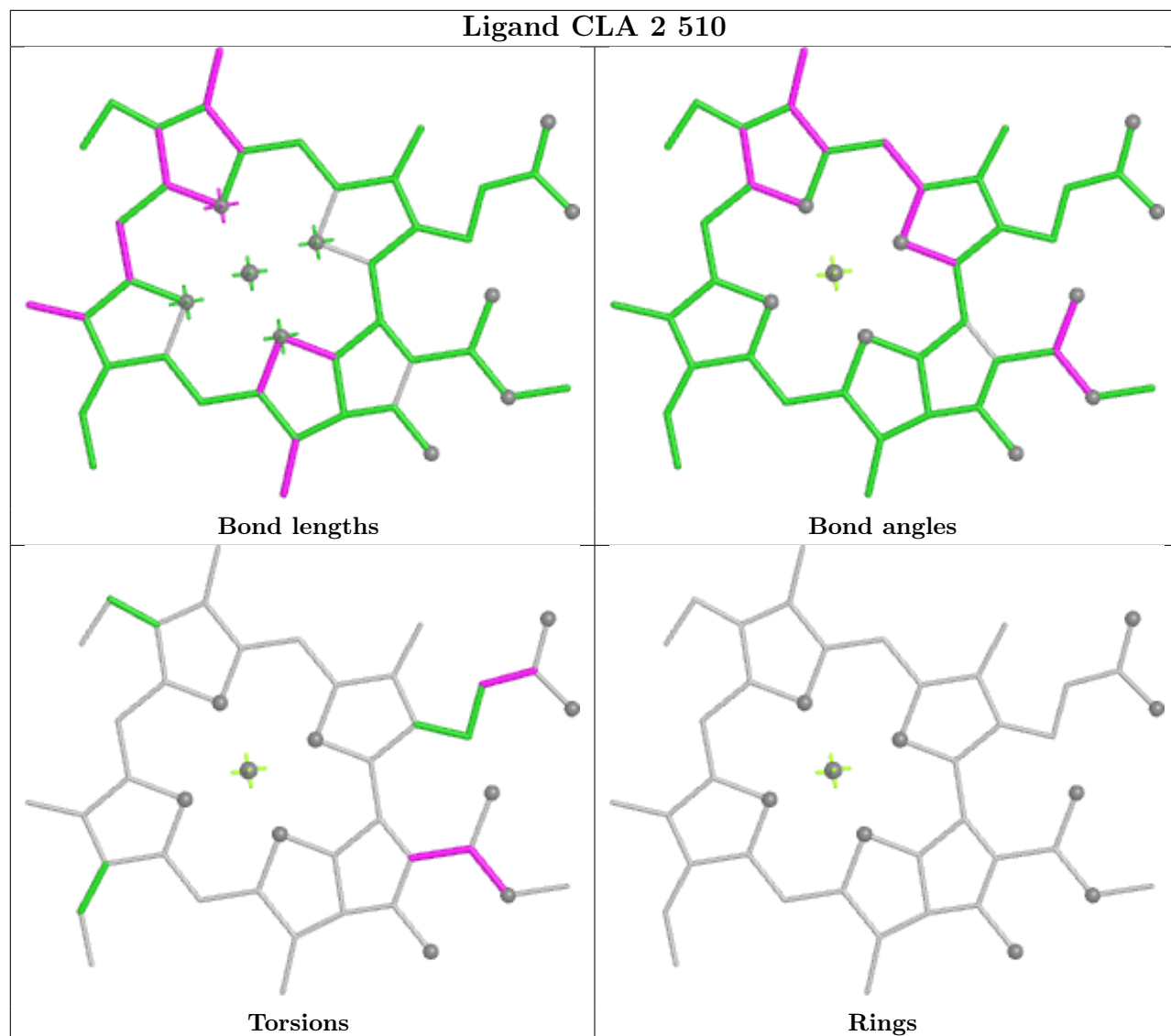
Torsions

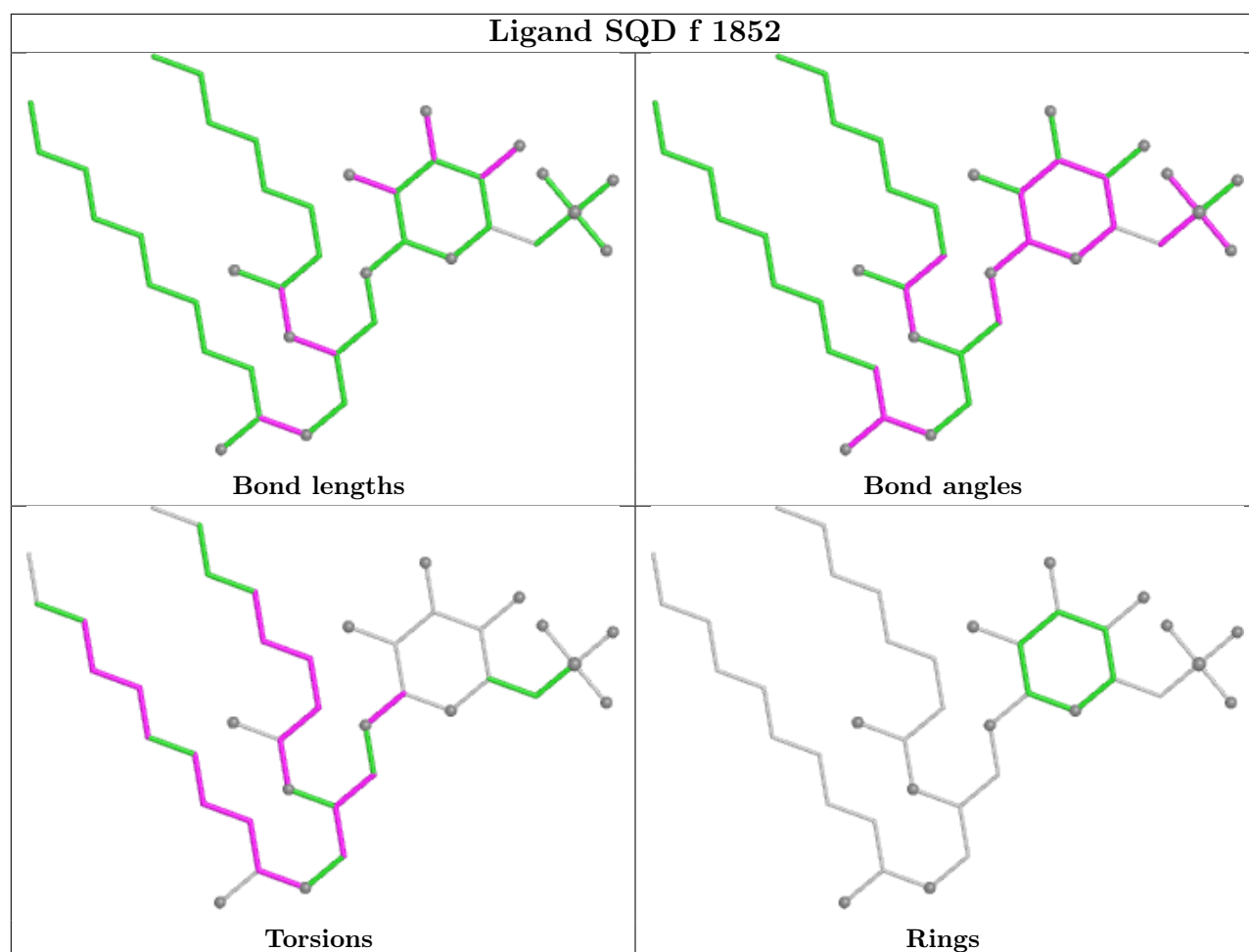


Rings

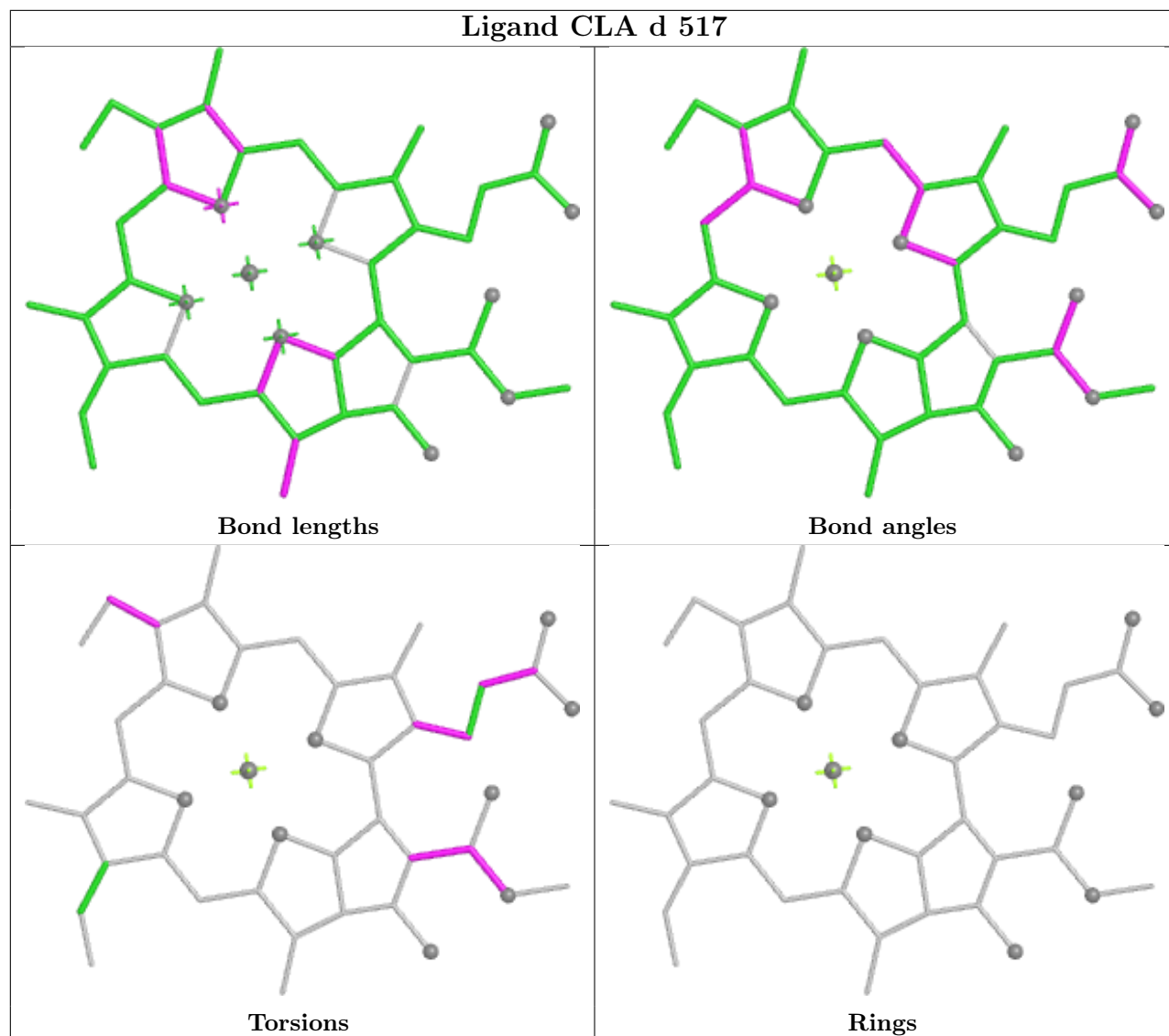


Ligand CLA 2 510

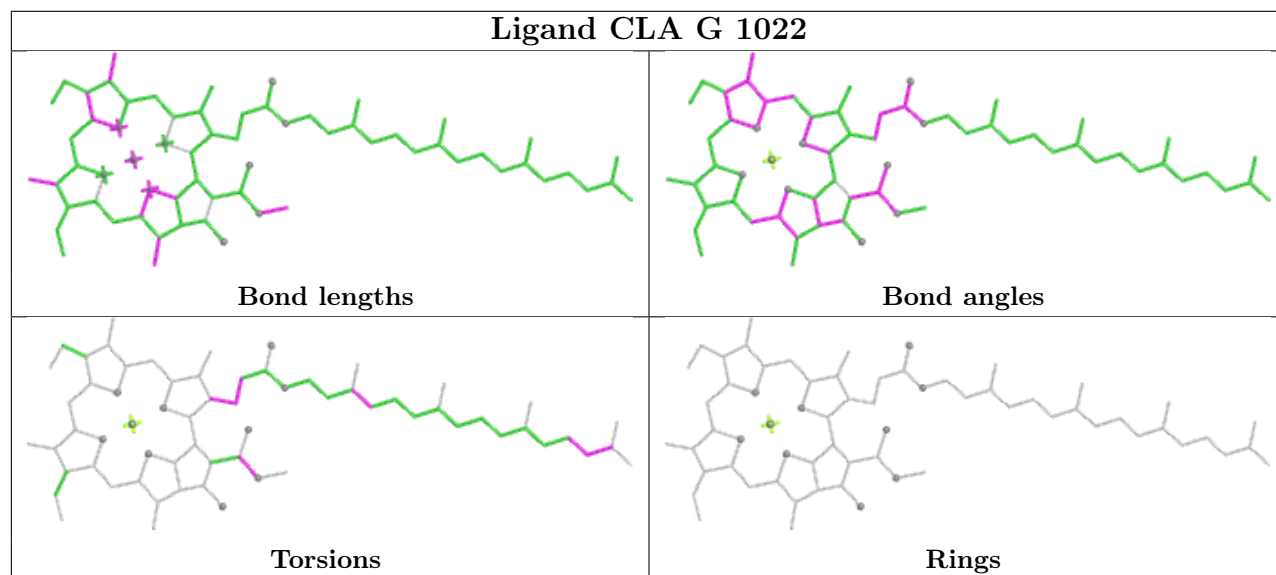


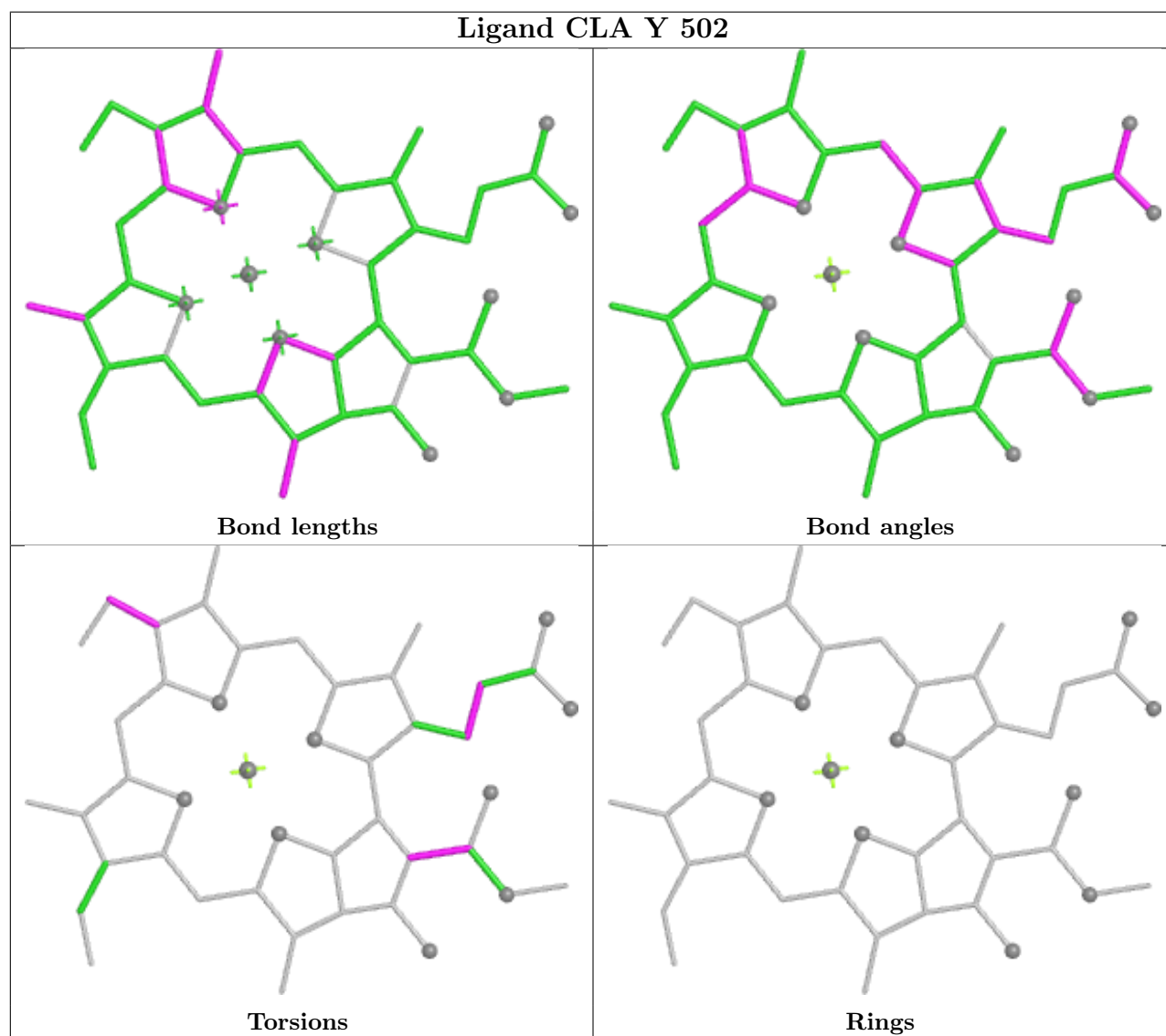
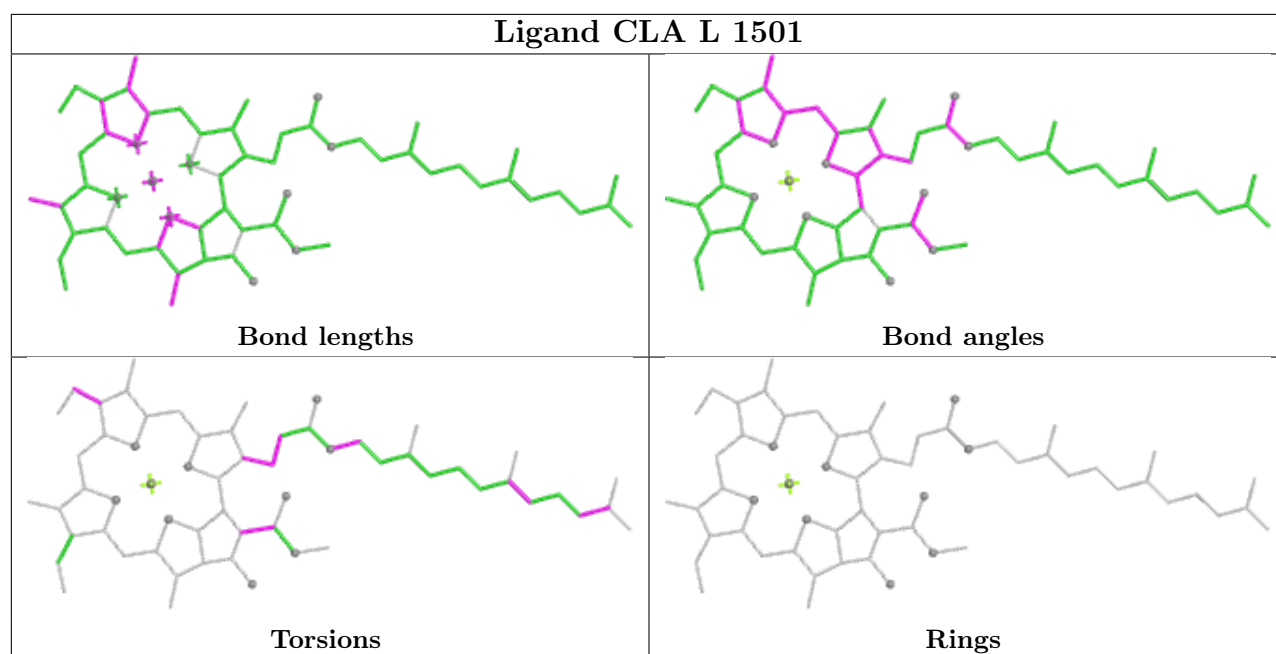


Ligand CLA d 517

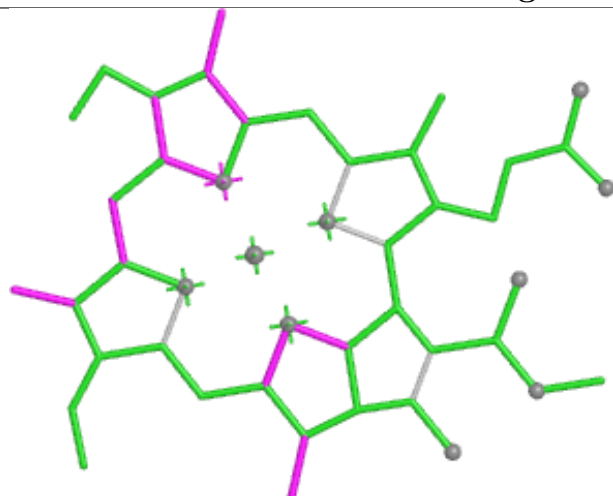


Ligand CLA G 1022

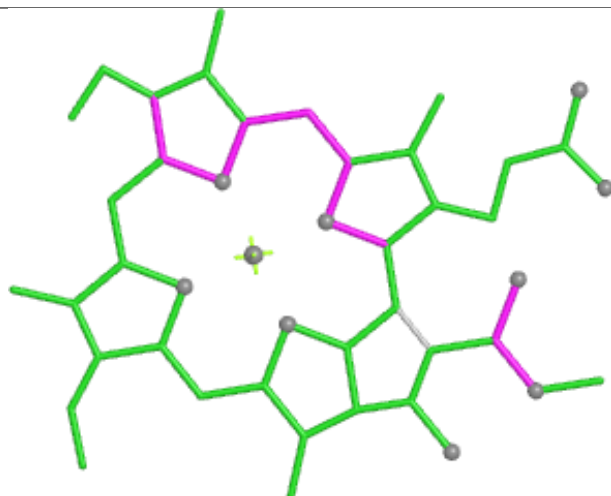




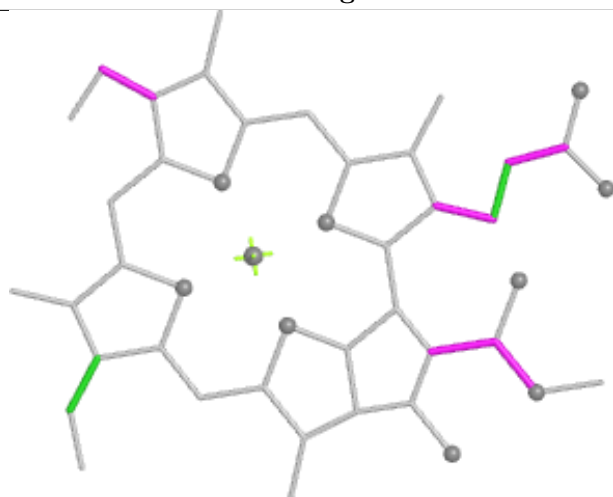
Ligand CLA 1 519



Bond lengths



Bond angles

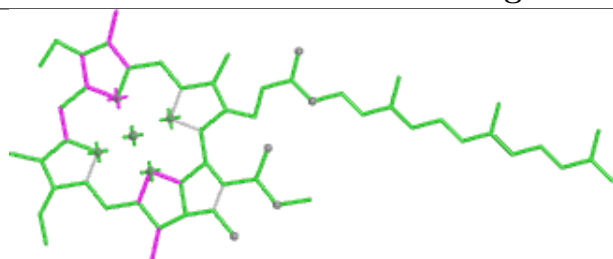


Torsions

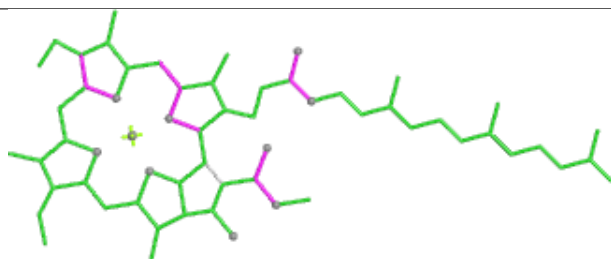


Rings

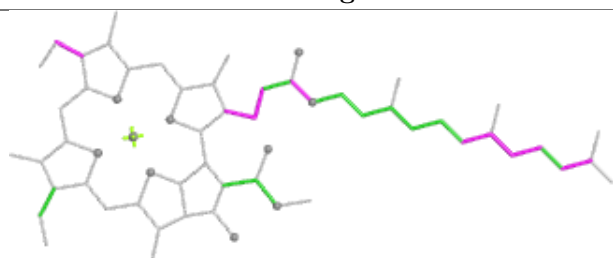
Ligand CLA H 1217



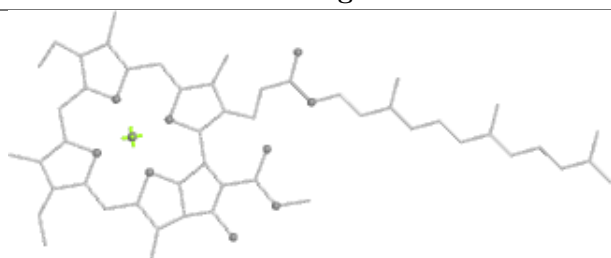
Bond lengths



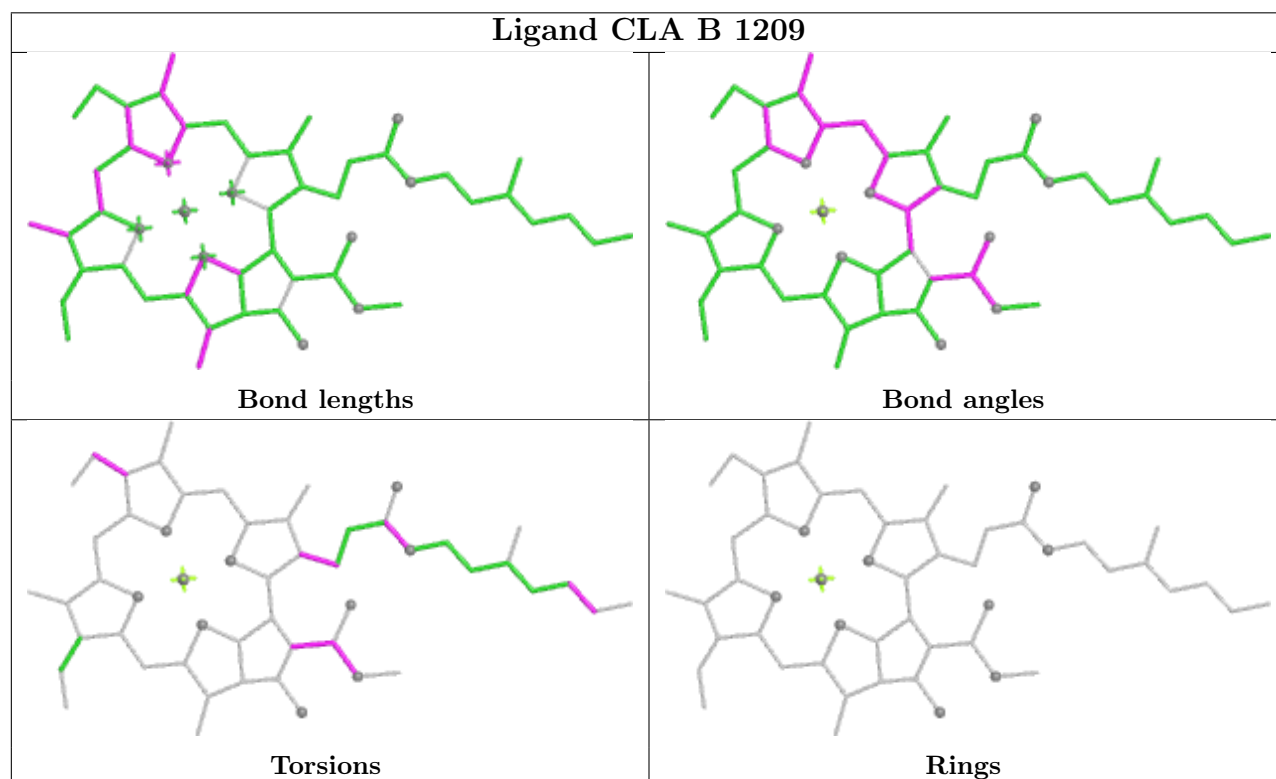
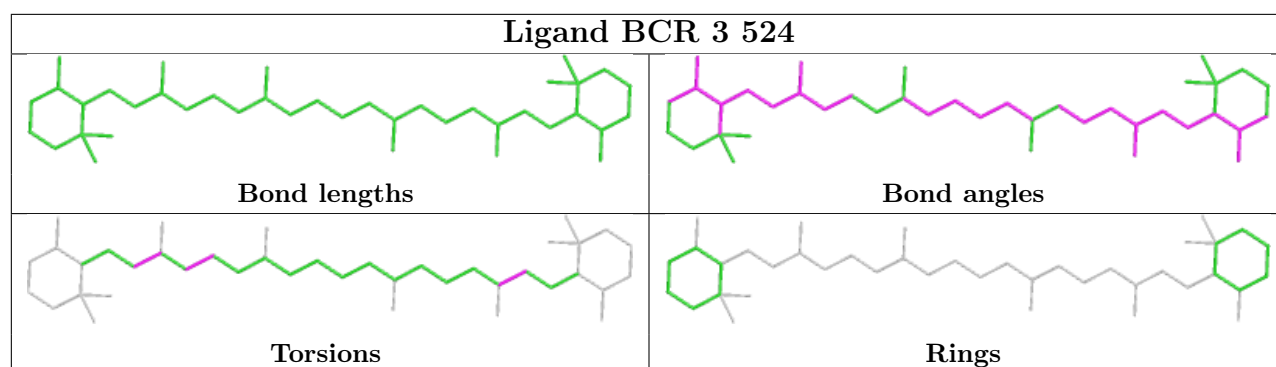
Bond angles

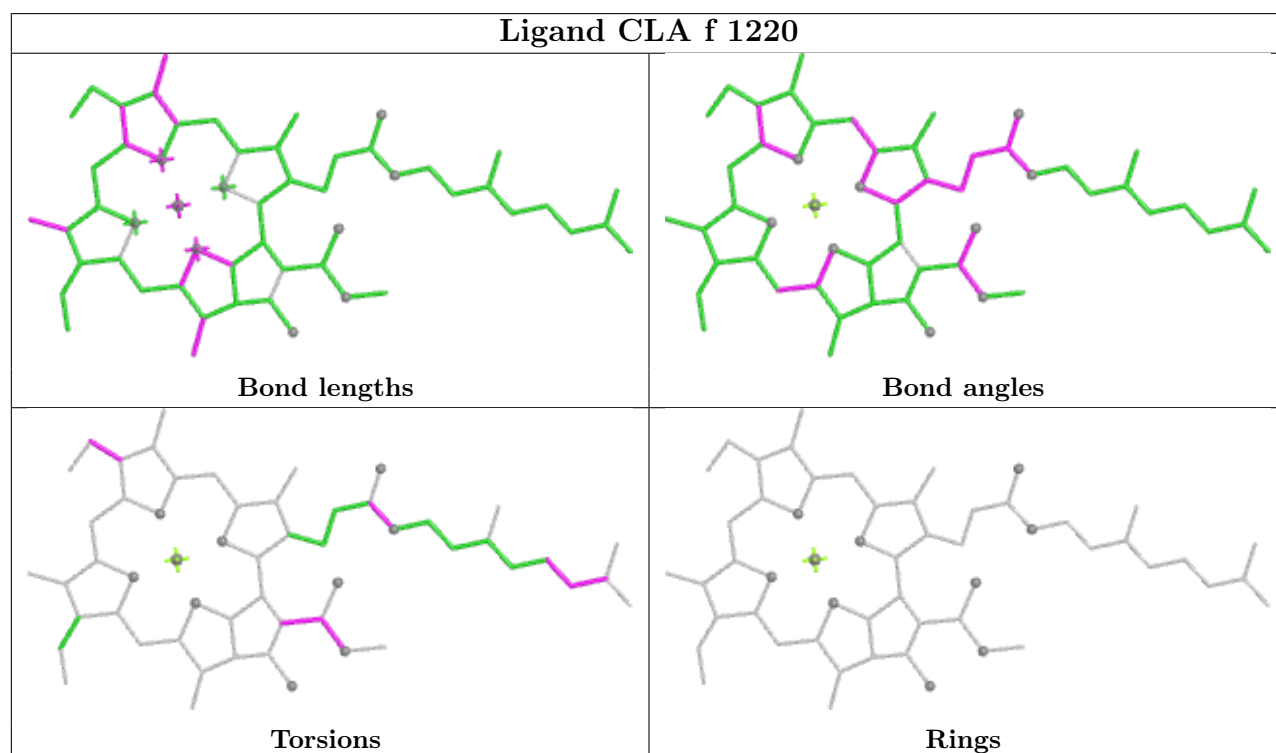
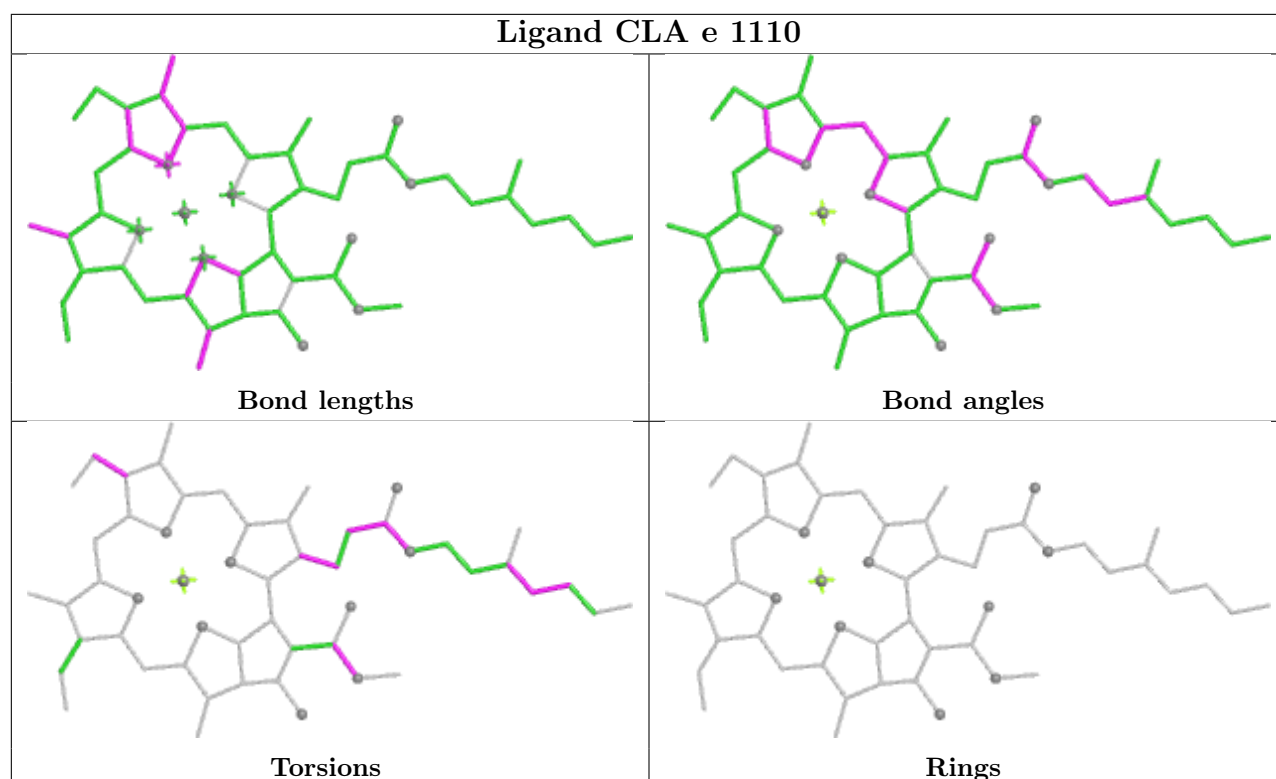


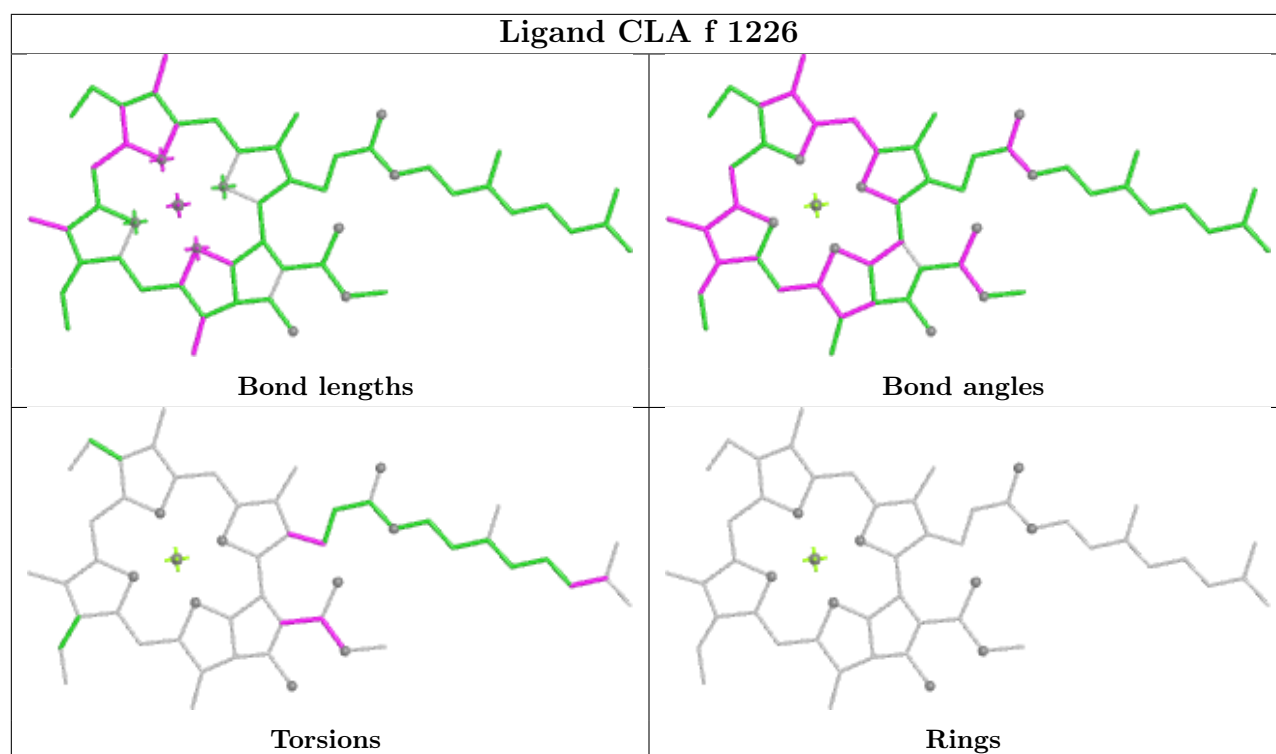
Torsions



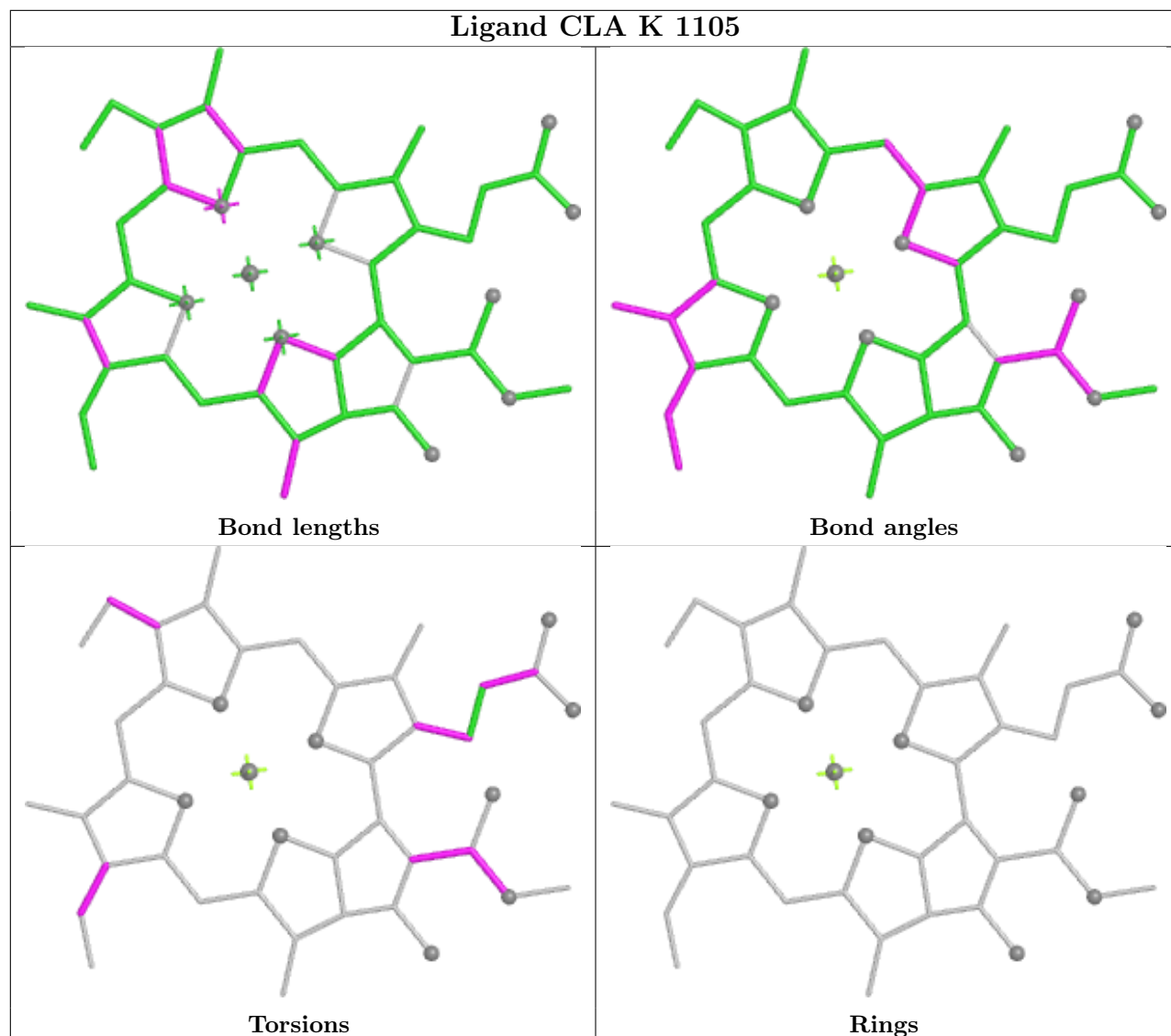
Rings



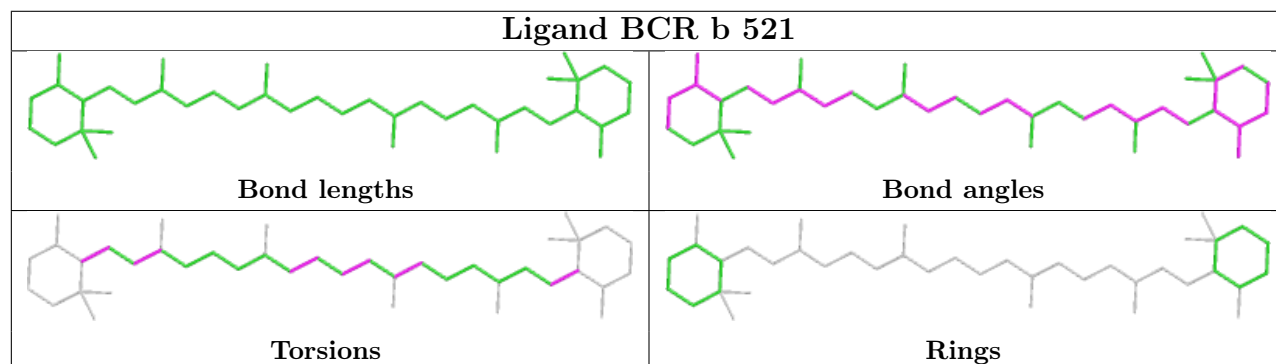


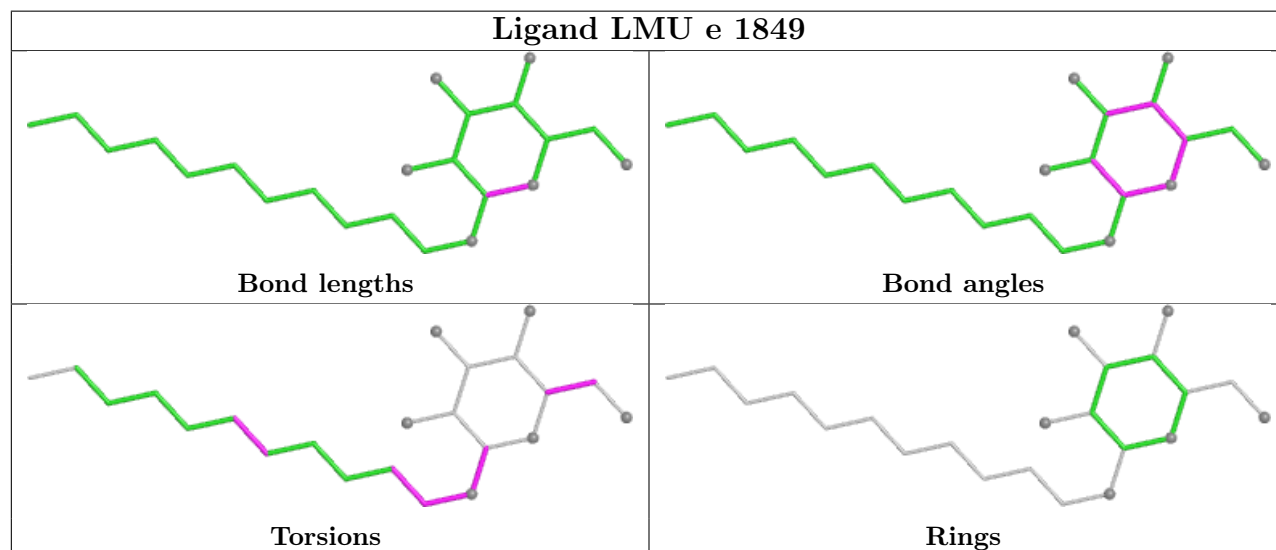
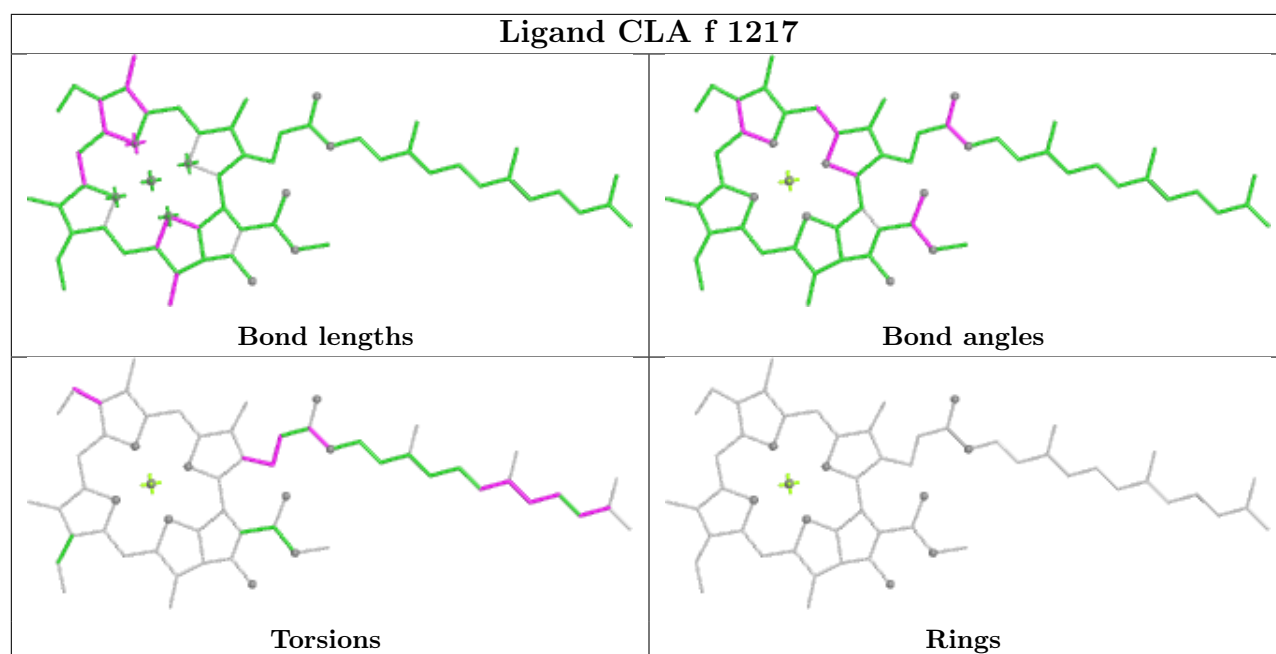


Ligand CLA K 1105

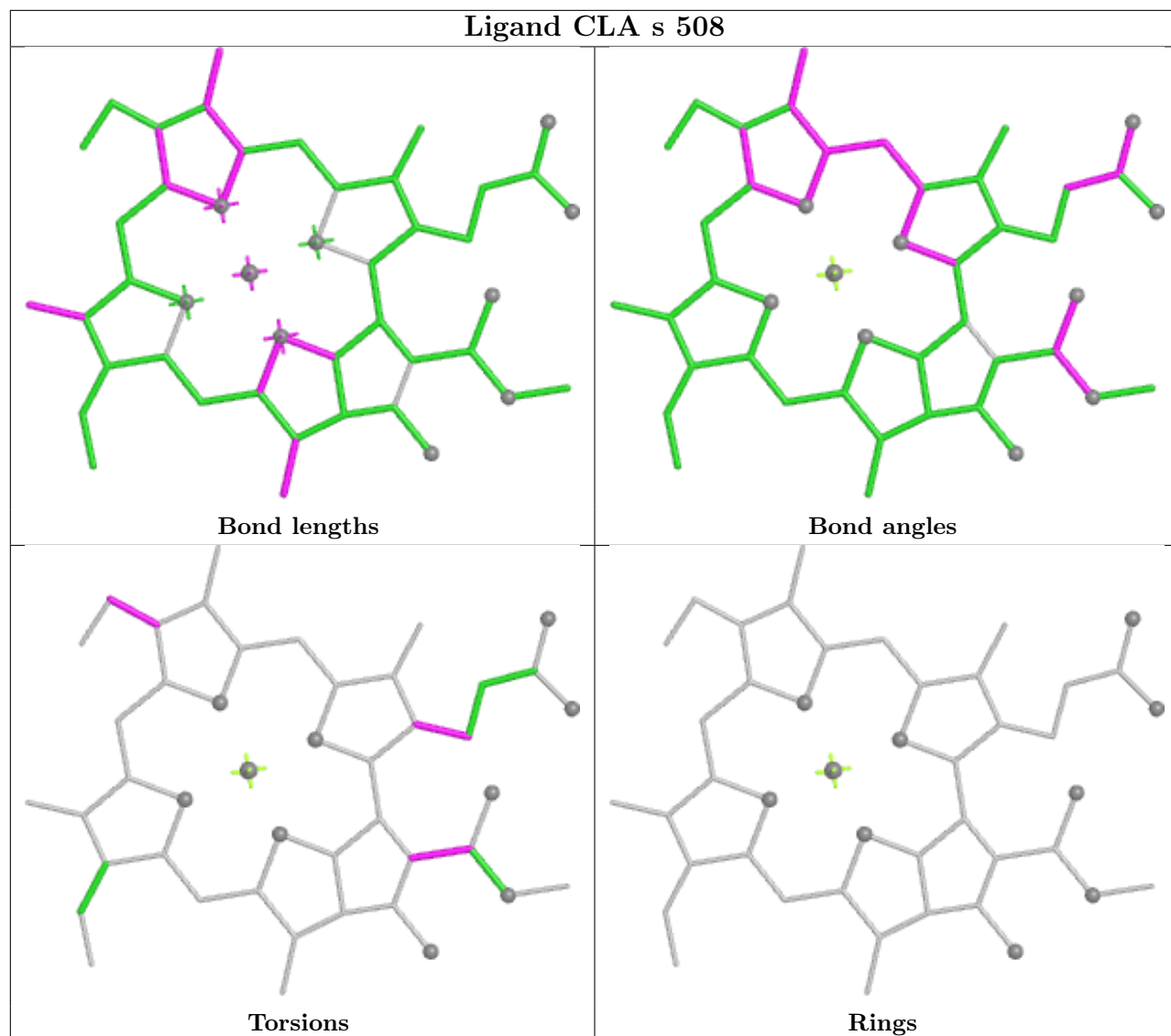


Ligand BCR b 521

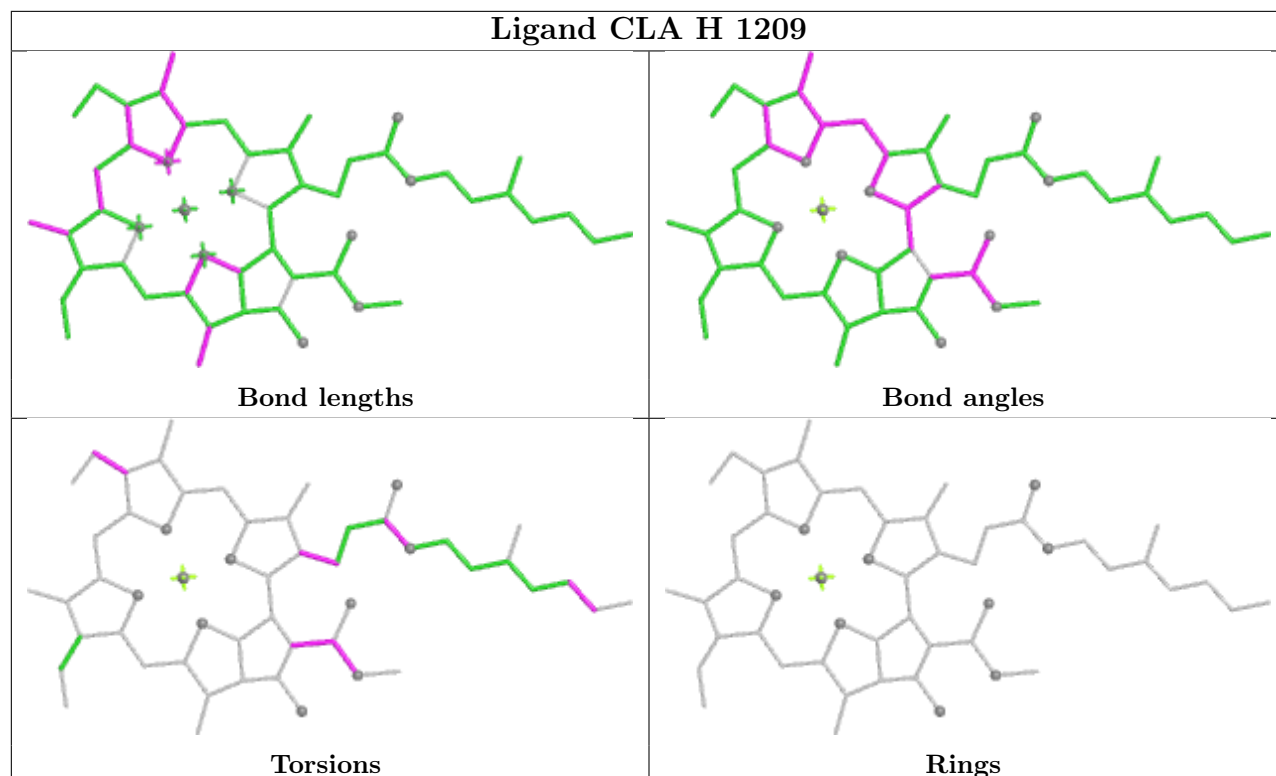




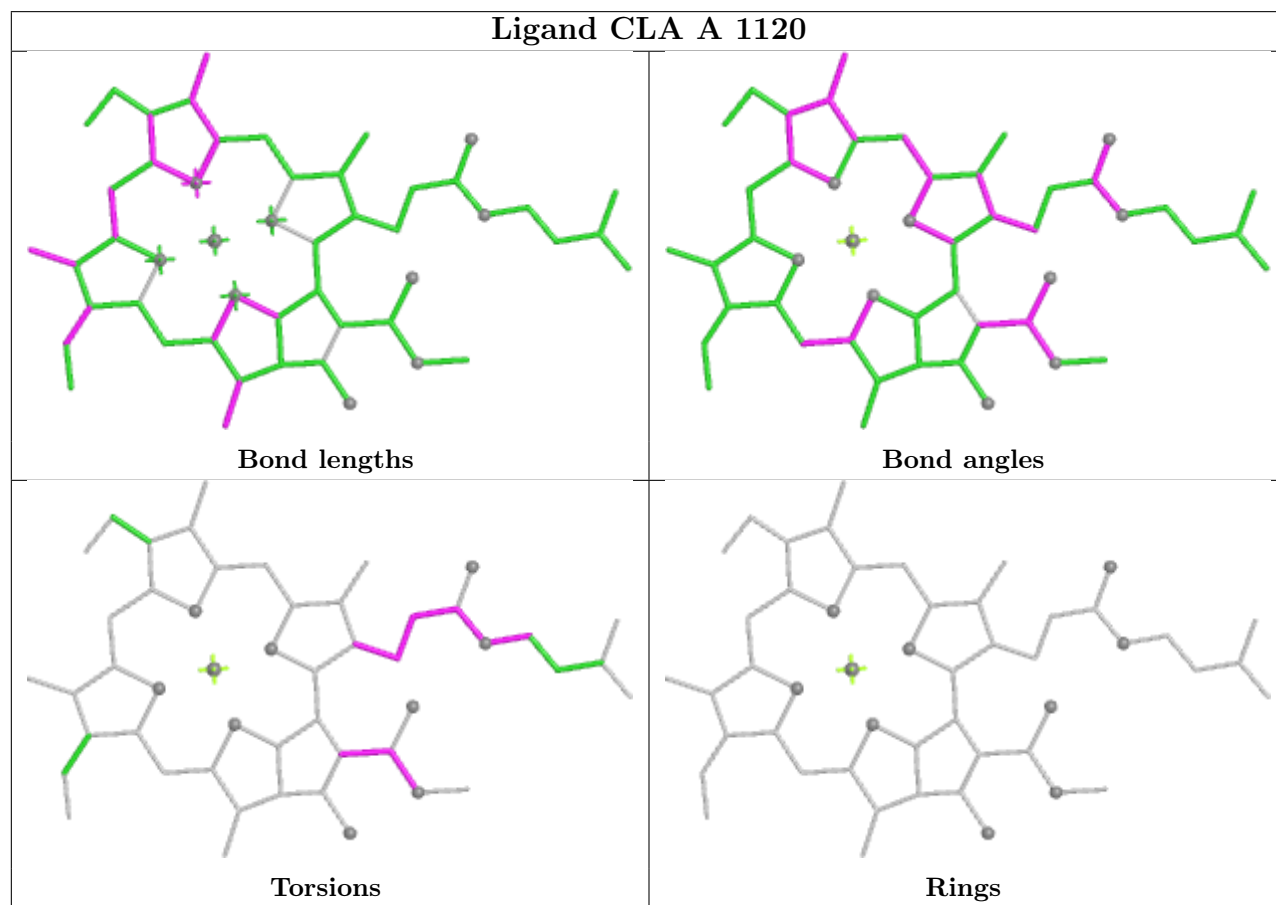
Ligand CLA s 508

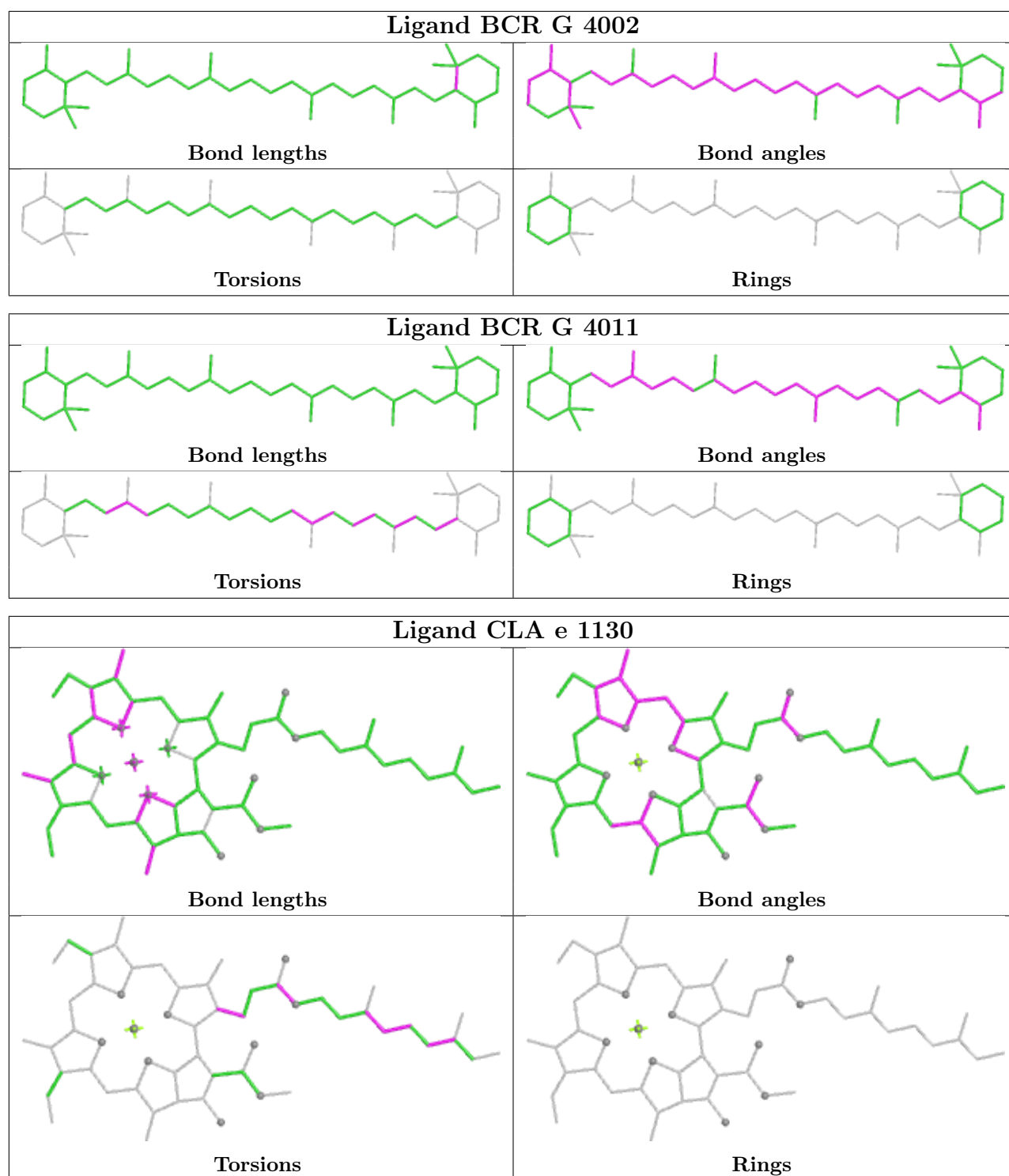


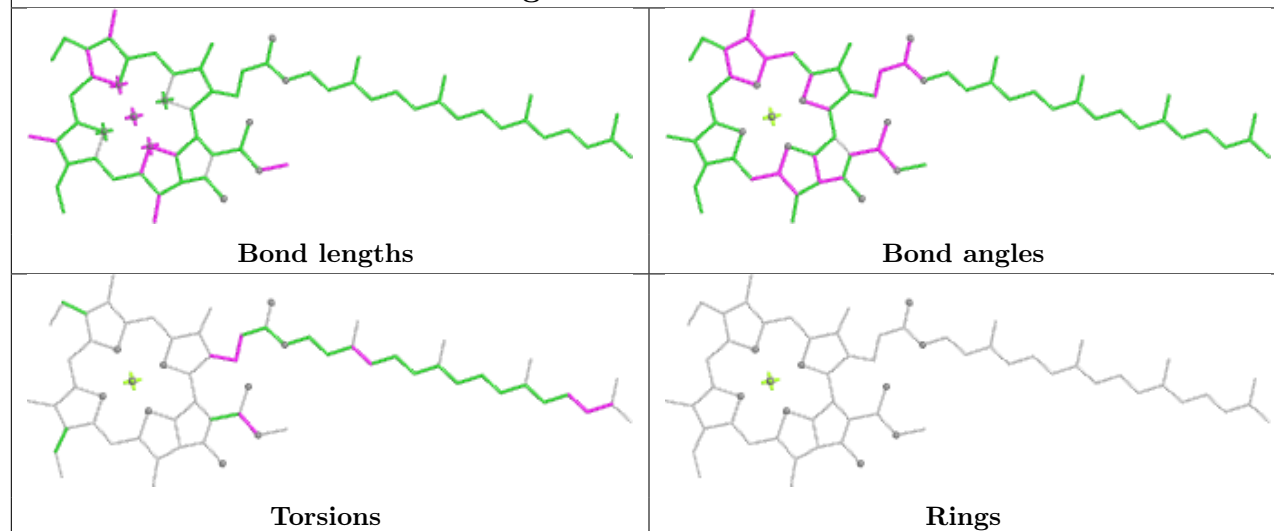
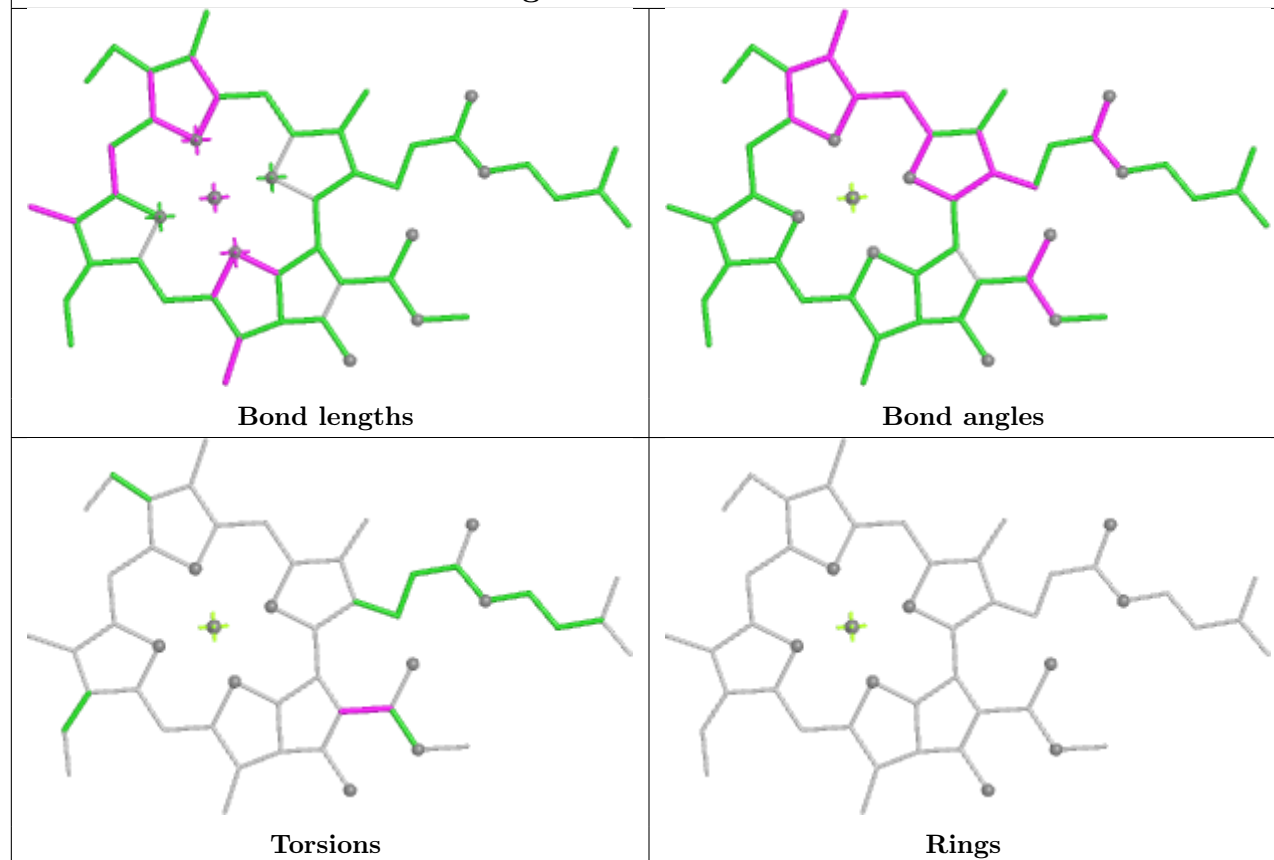
Ligand CLA H 1209

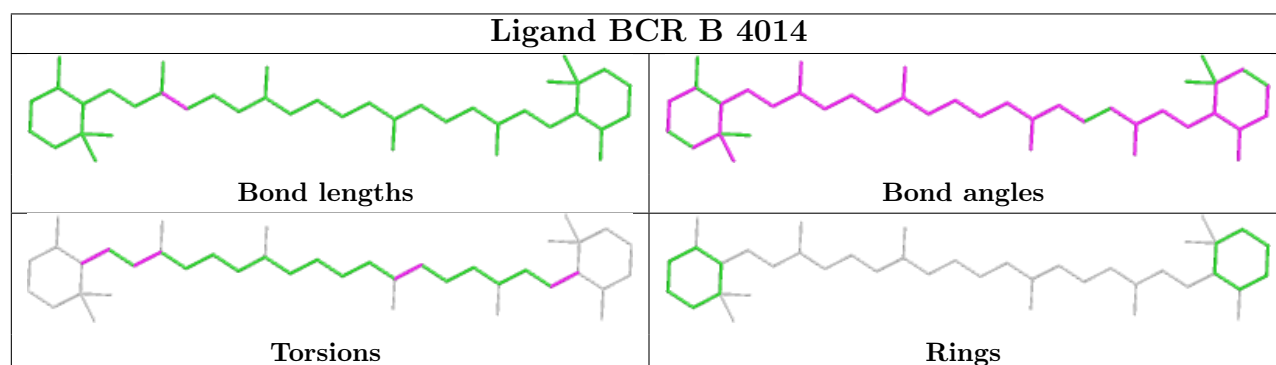
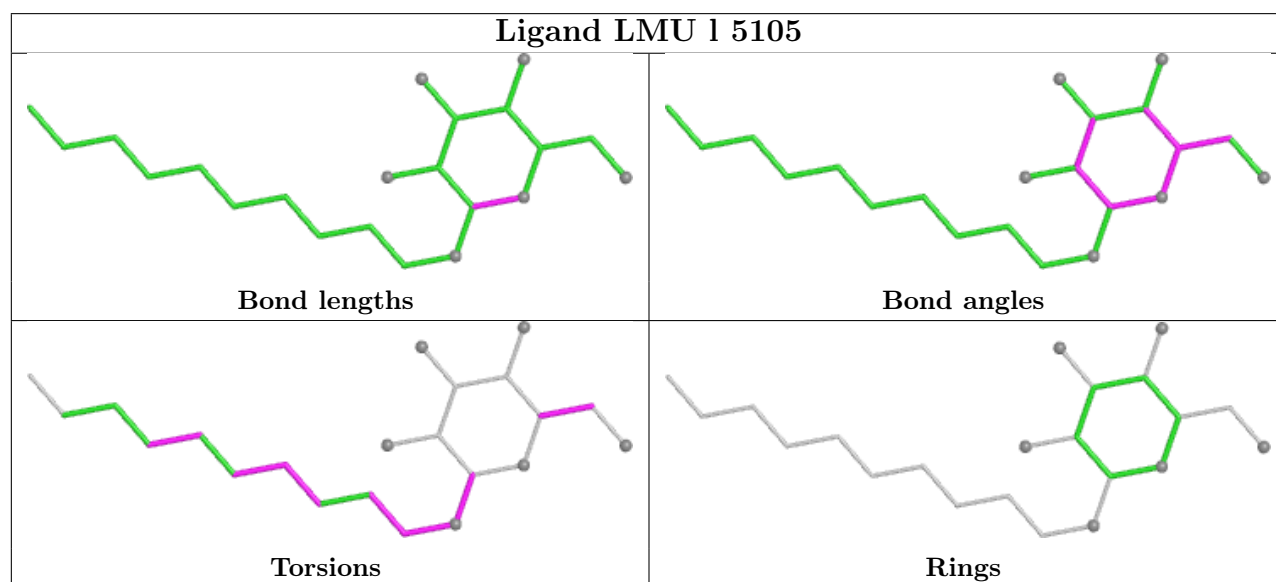
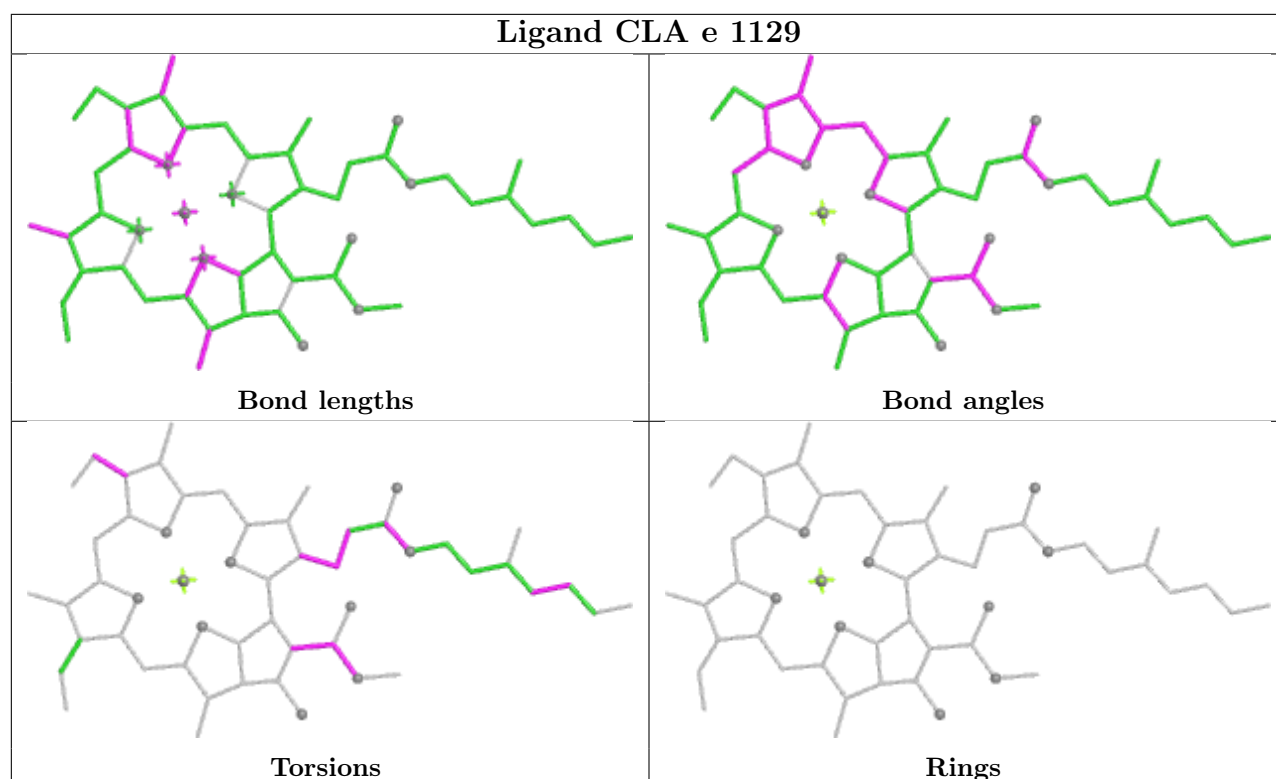


Ligand CLA A 1120

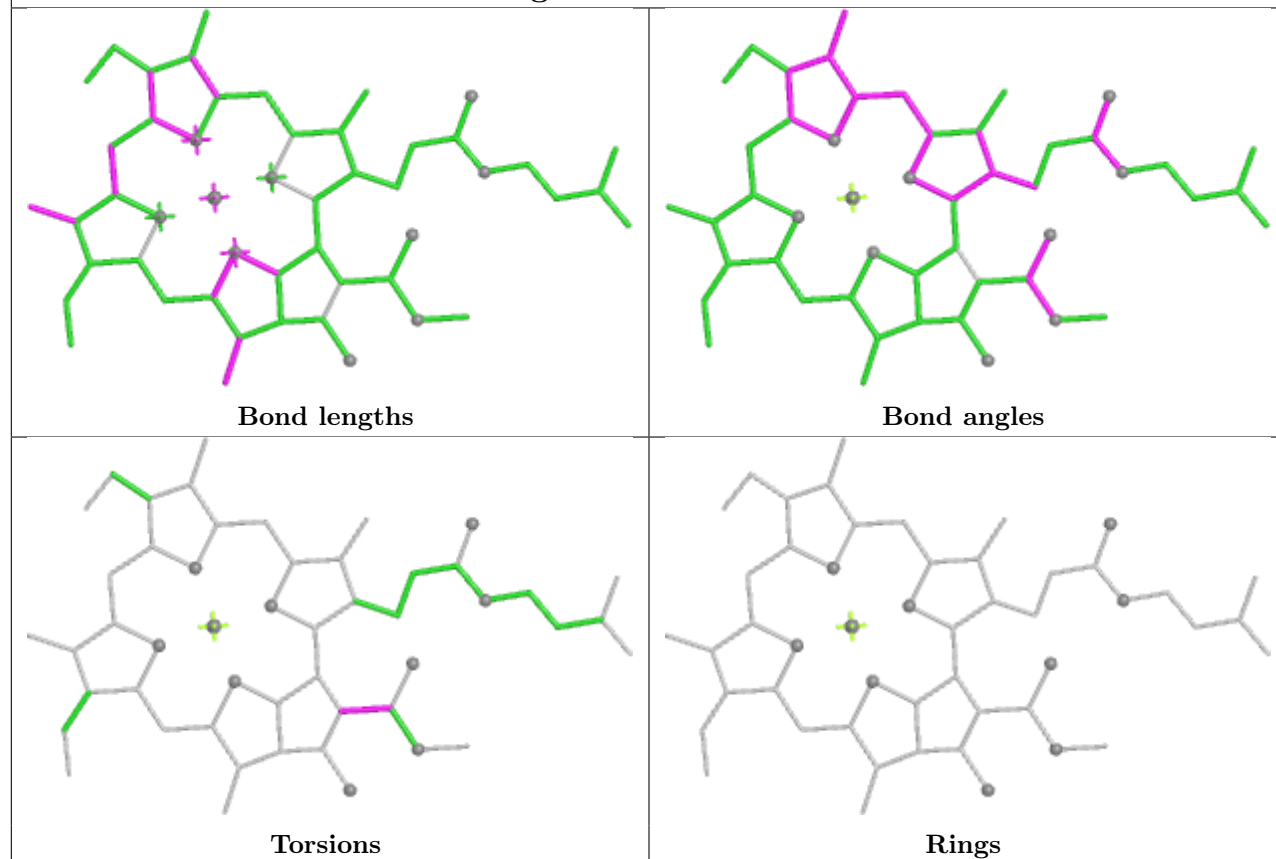




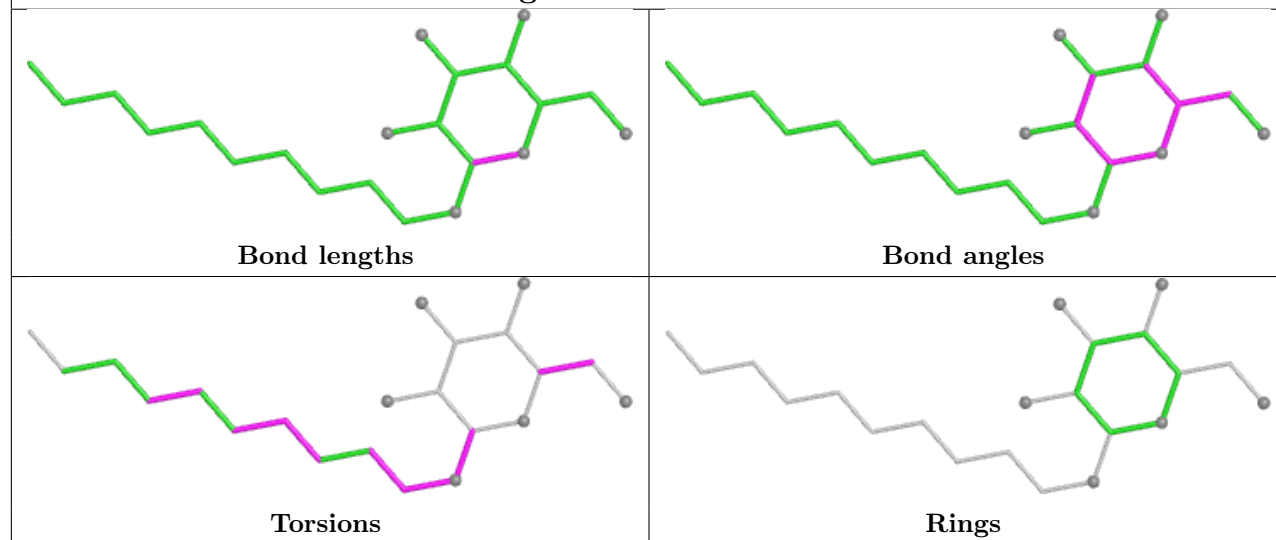
Ligand CLA A 1022**Ligand CLA H 1222**



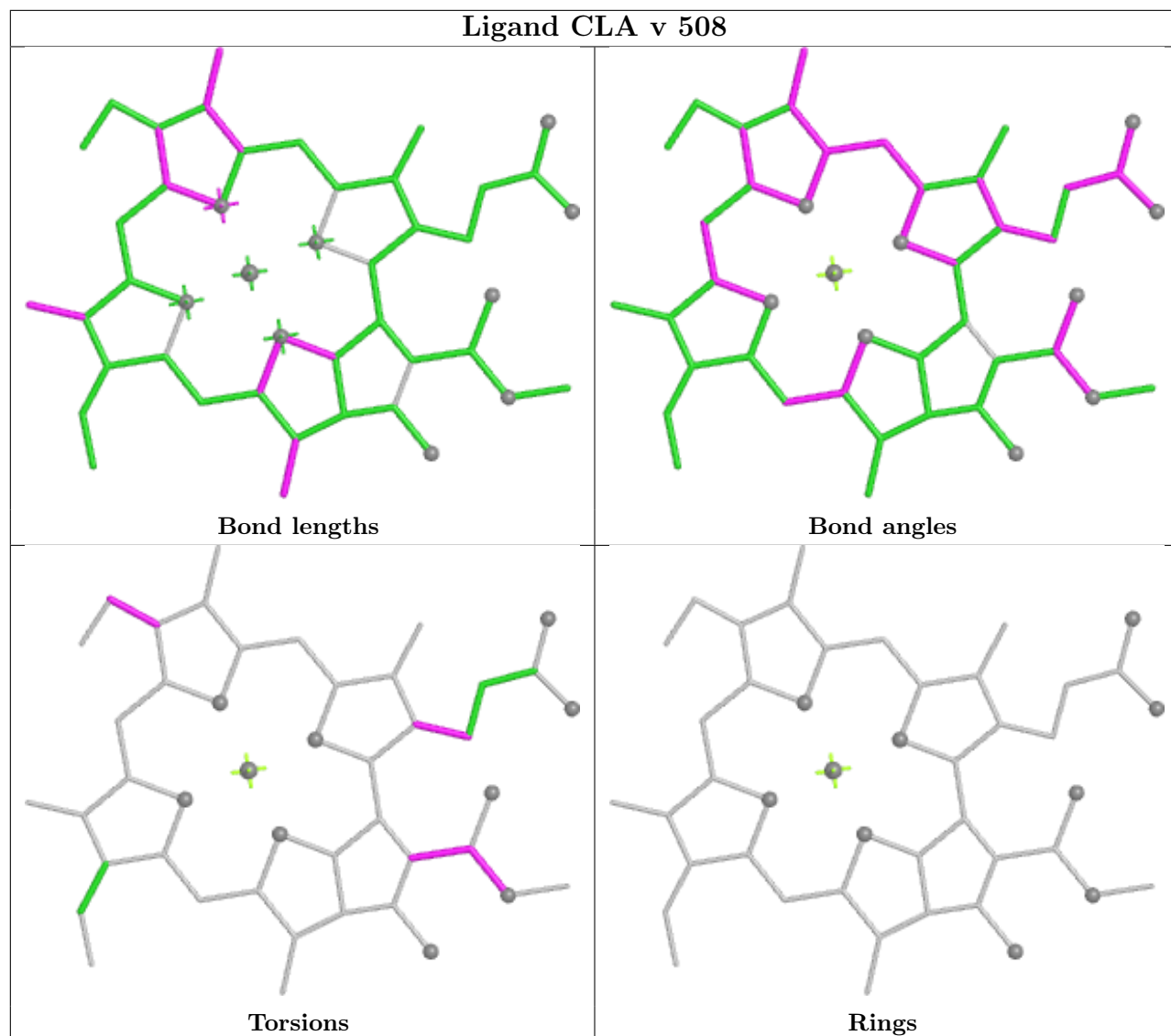
Ligand CLA f 1222



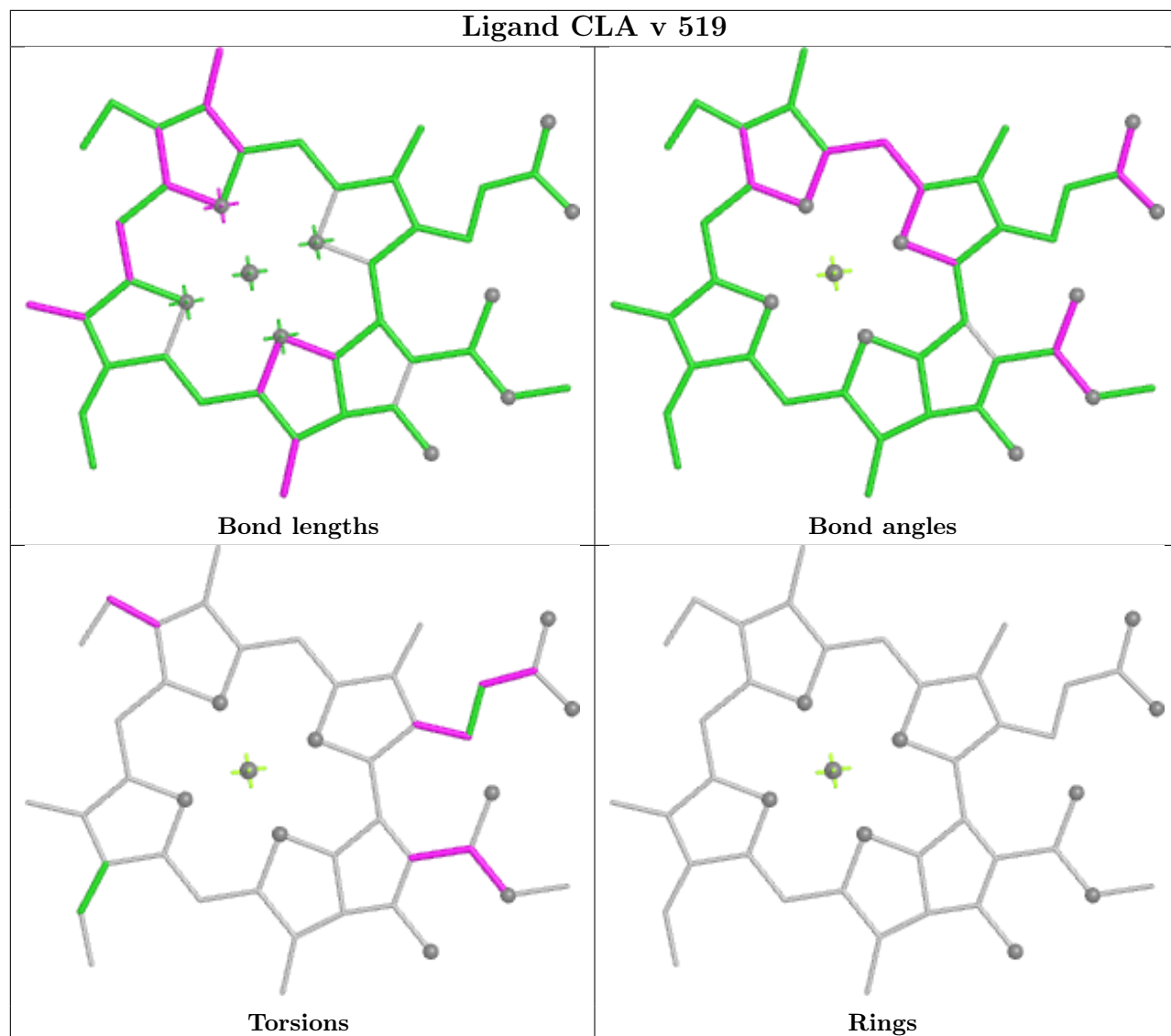
Ligand LMU T 5105

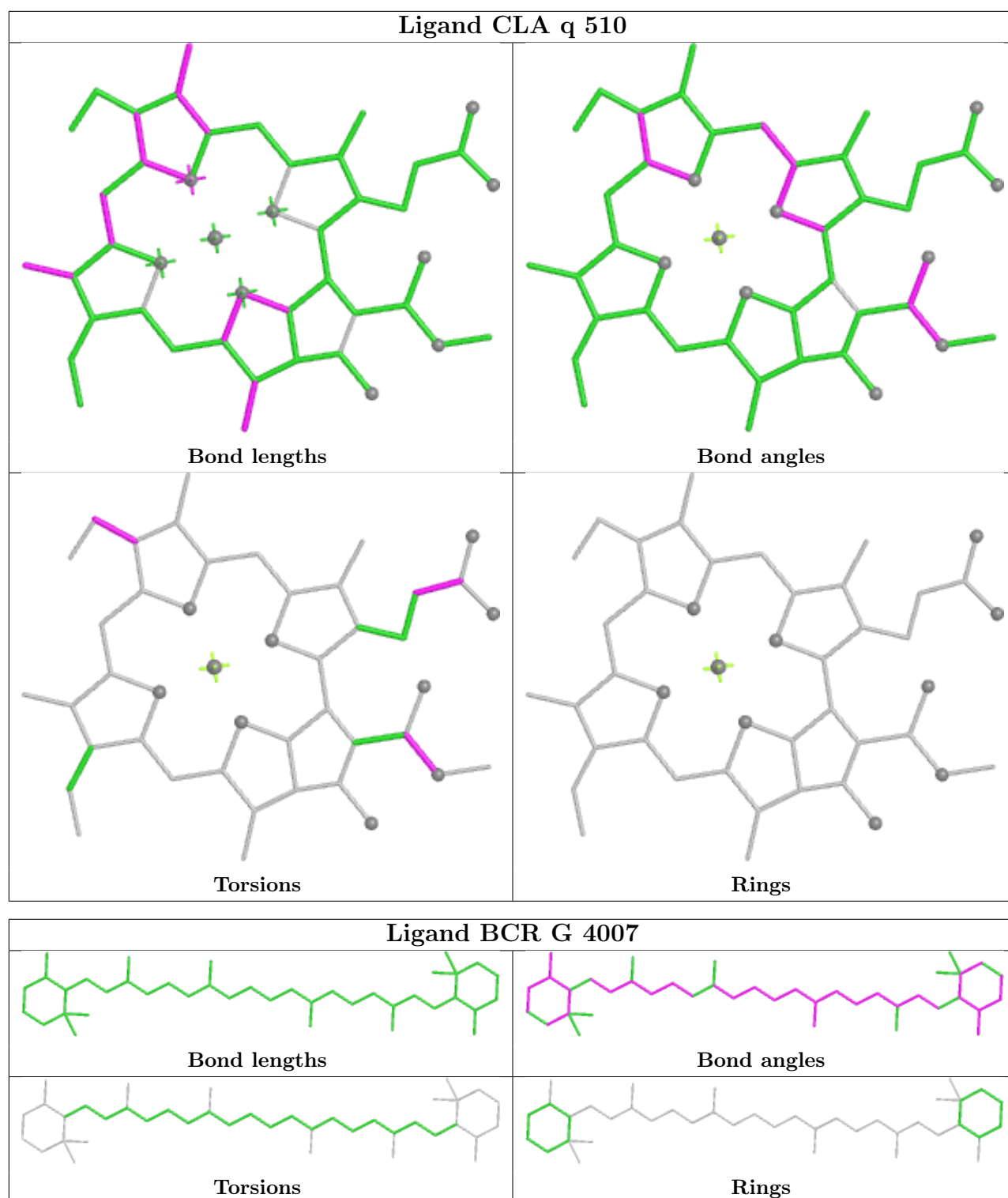


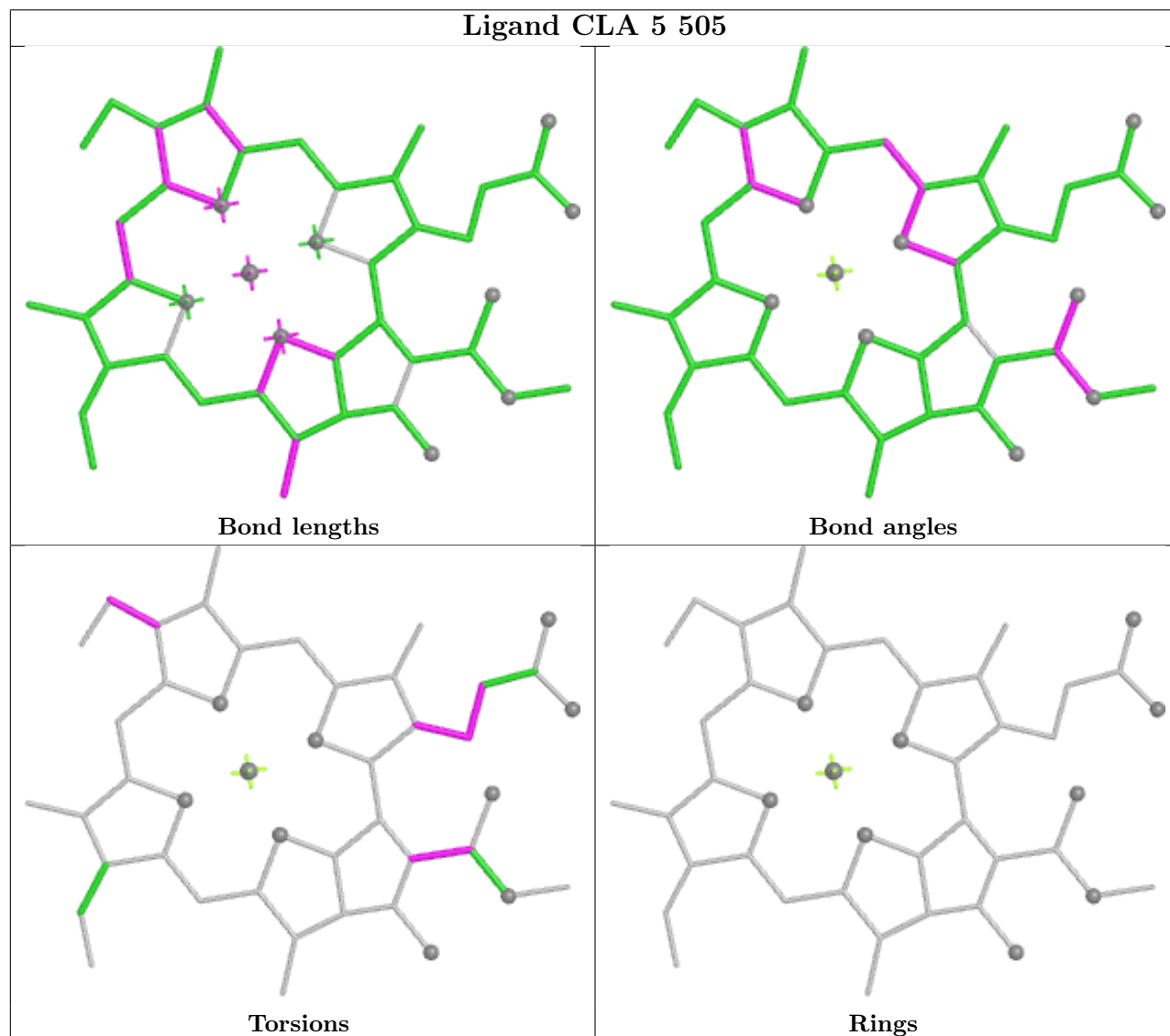
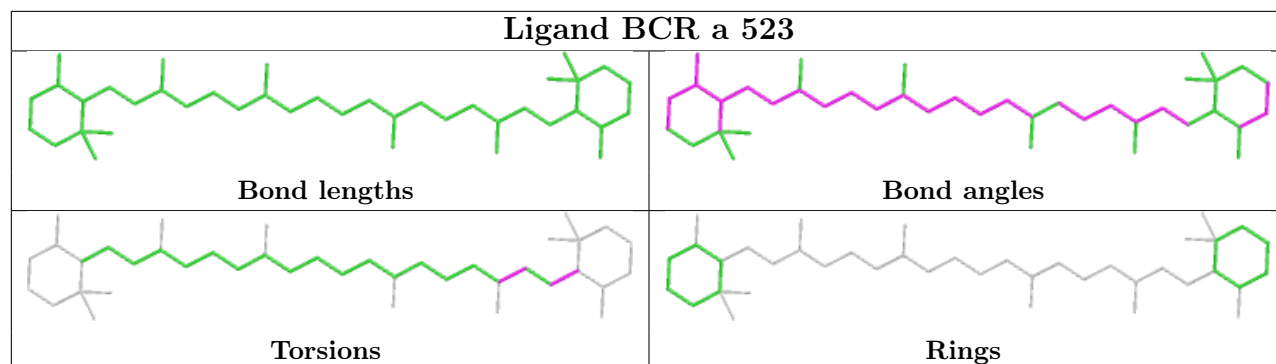
Ligand CLA v 508



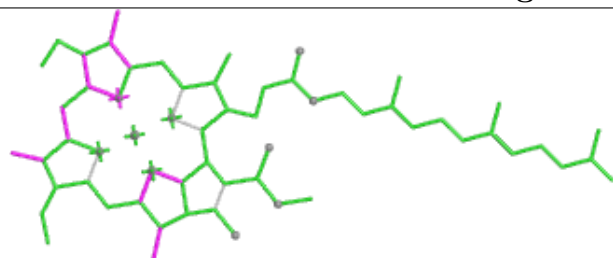
Ligand CLA v 519



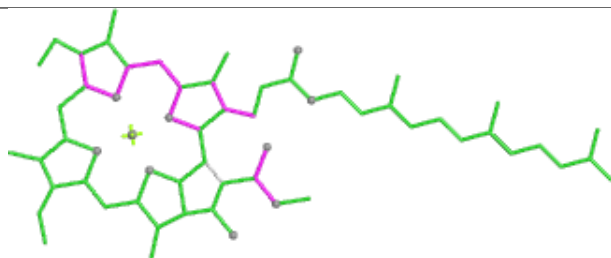




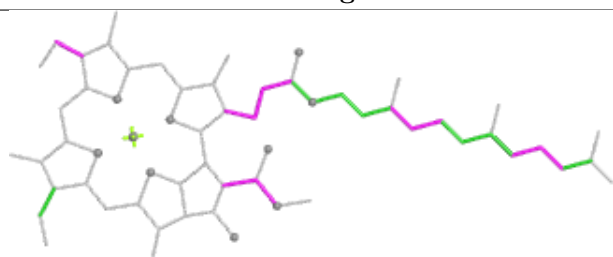
Ligand CLA Z 501



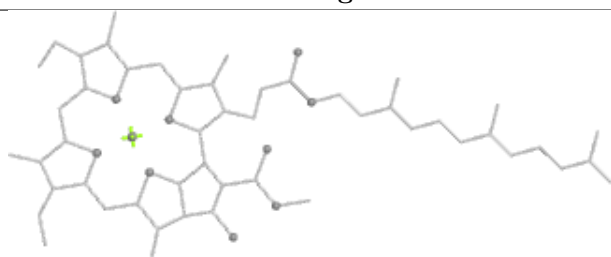
Bond lengths



Bond angles

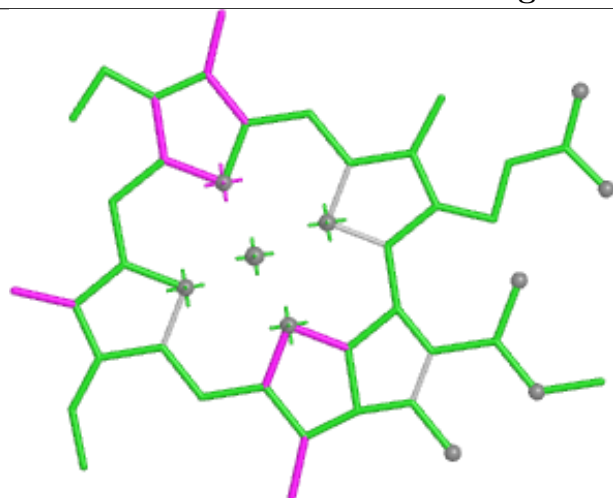


Torsions

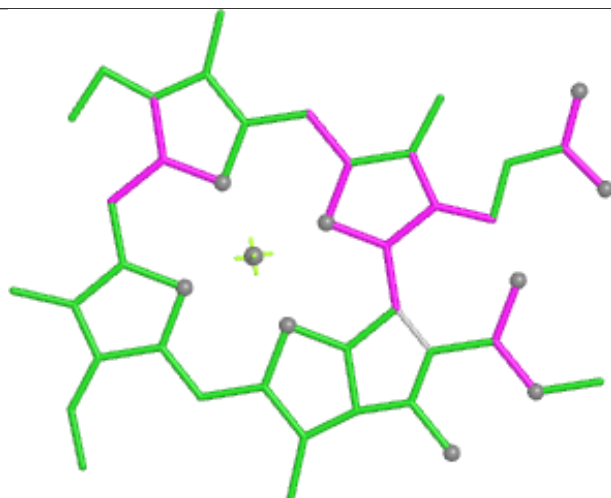


Rings

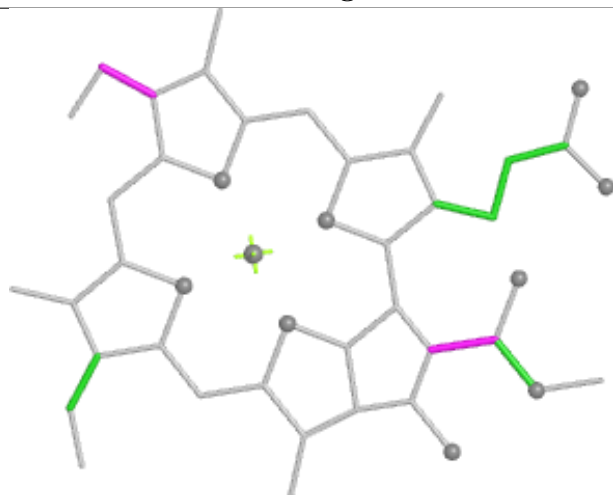
Ligand CLA a 502



Bond lengths



Bond angles

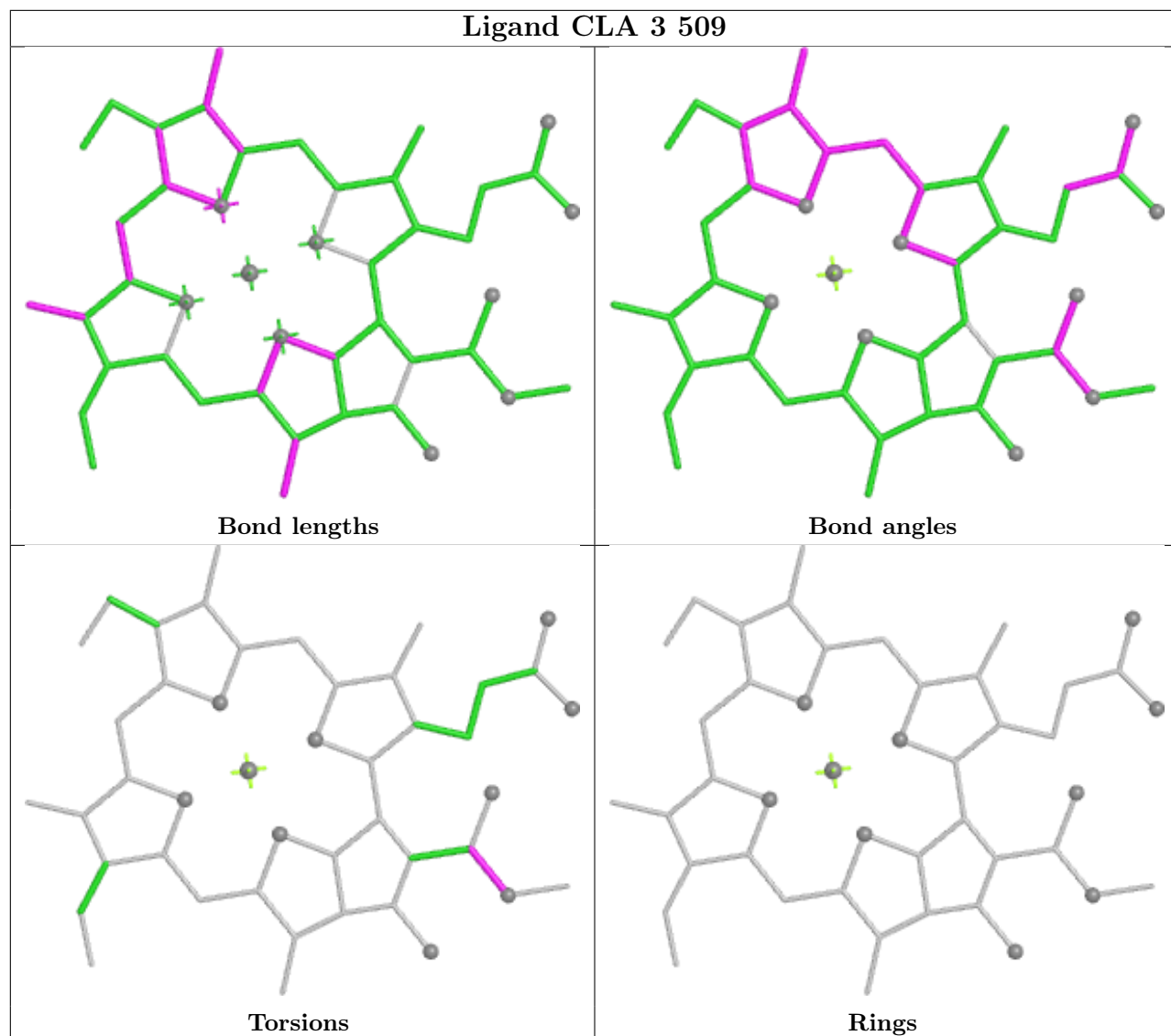


Torsions

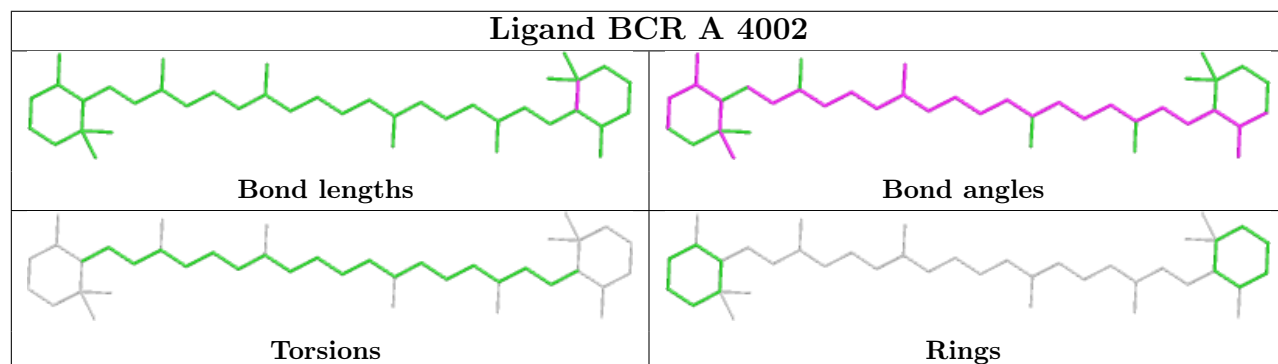


Rings

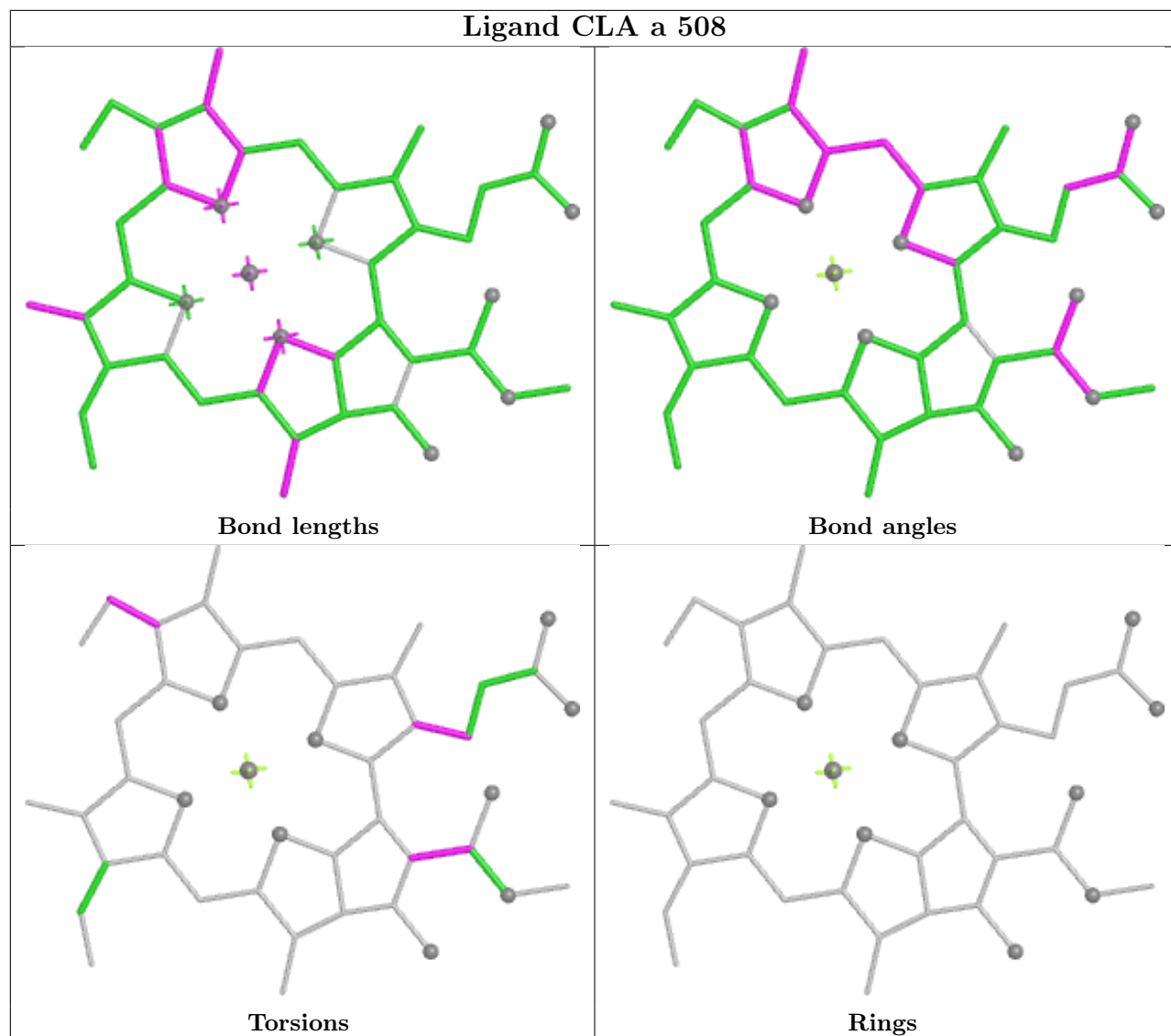
Ligand CLA 3 509



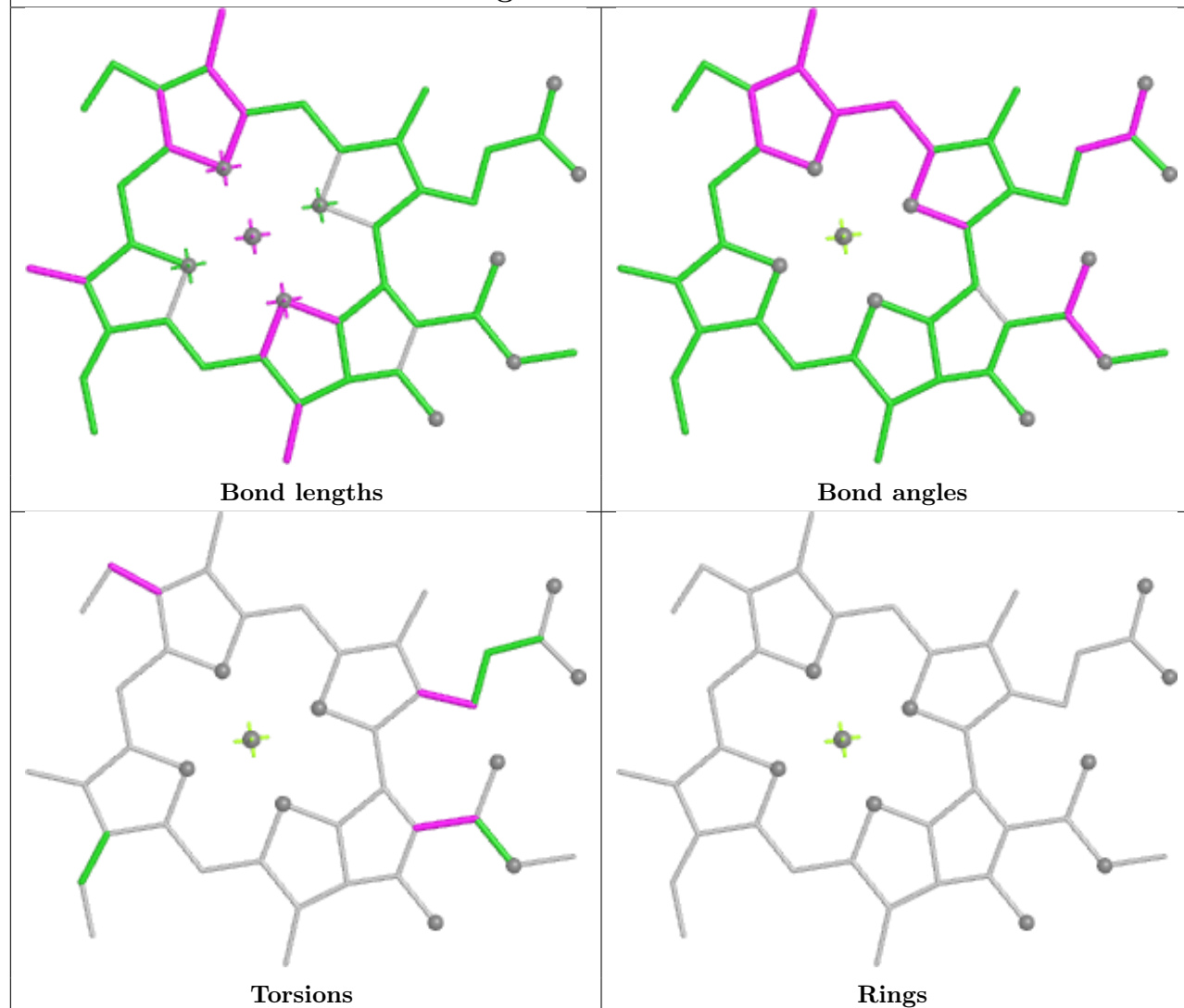
Ligand BCR A 4002



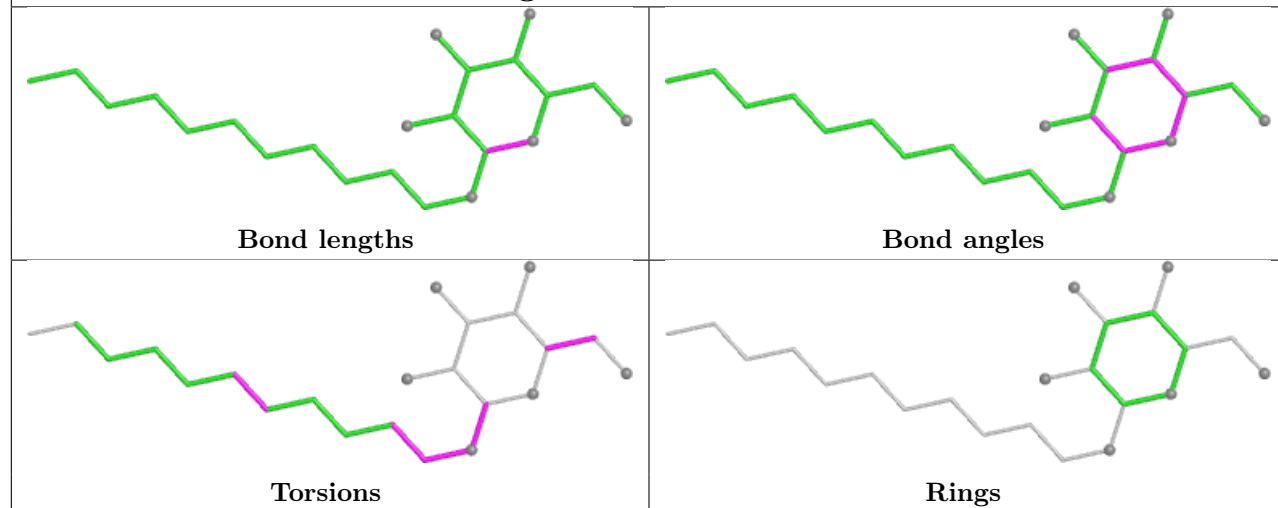
Ligand CLA a 508



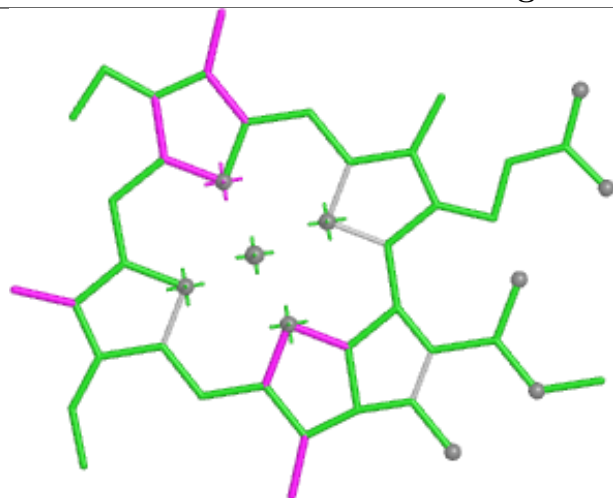
Ligand CLA 3 508



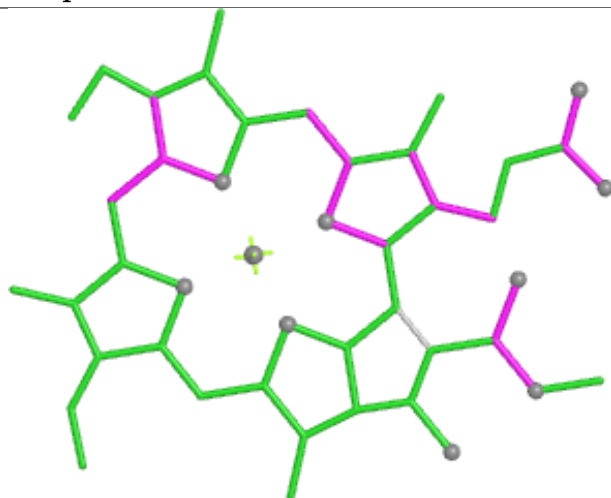
Ligand LMU A 1849



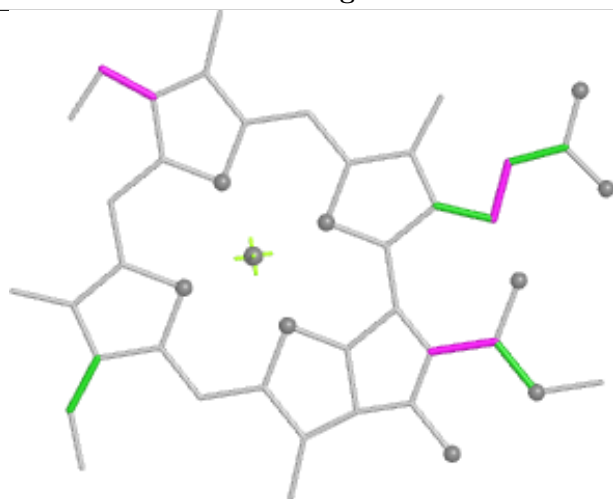
Ligand CLA q 502



Bond lengths



Bond angles

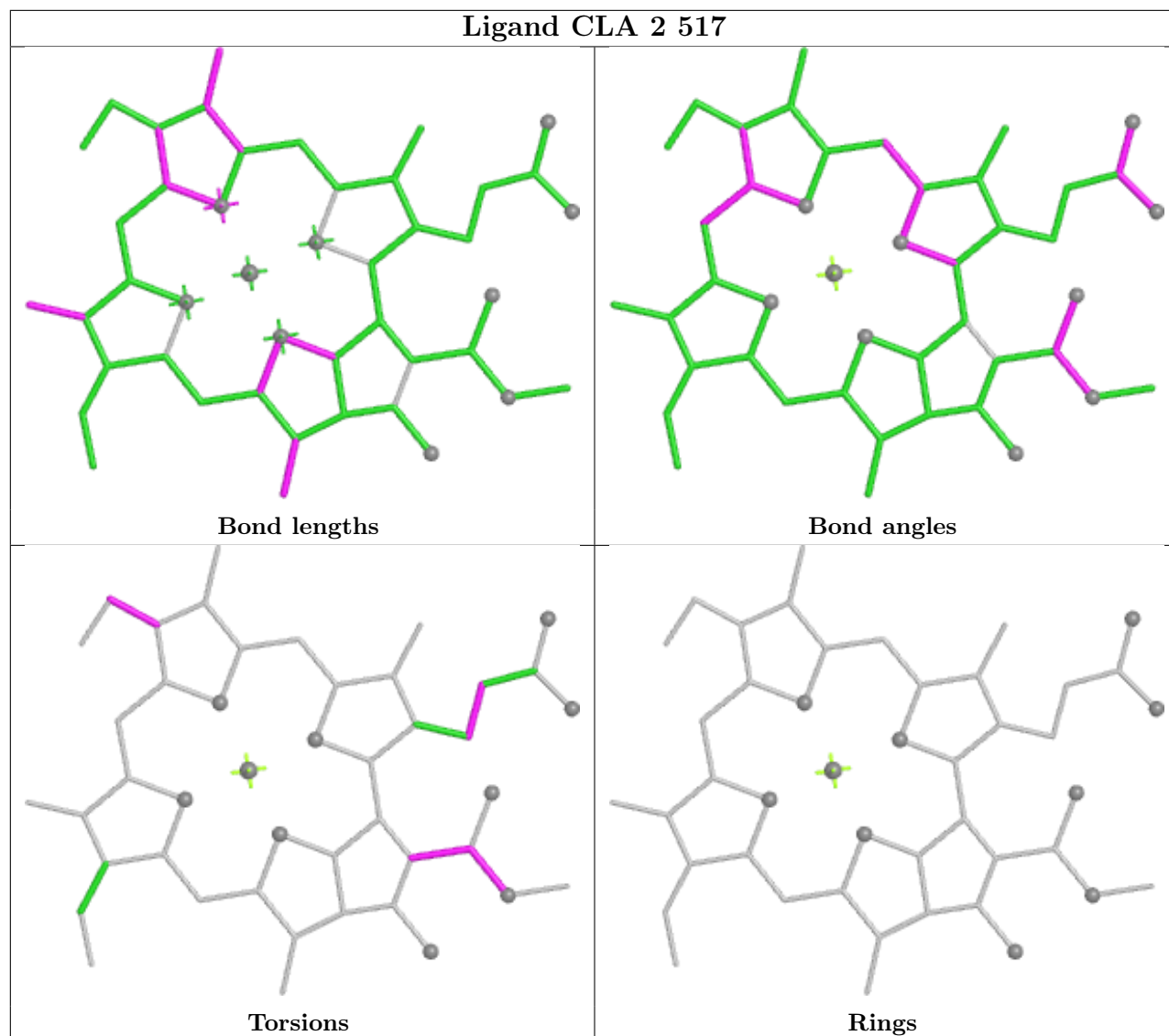


Torsions

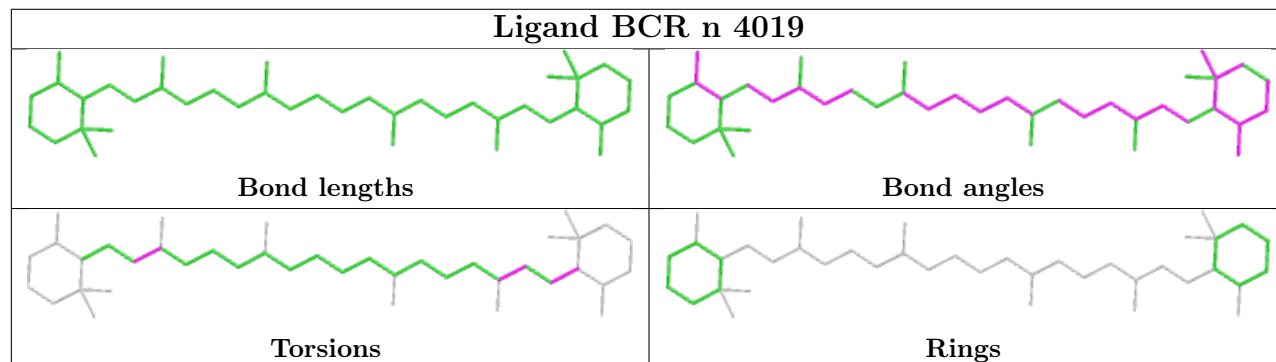


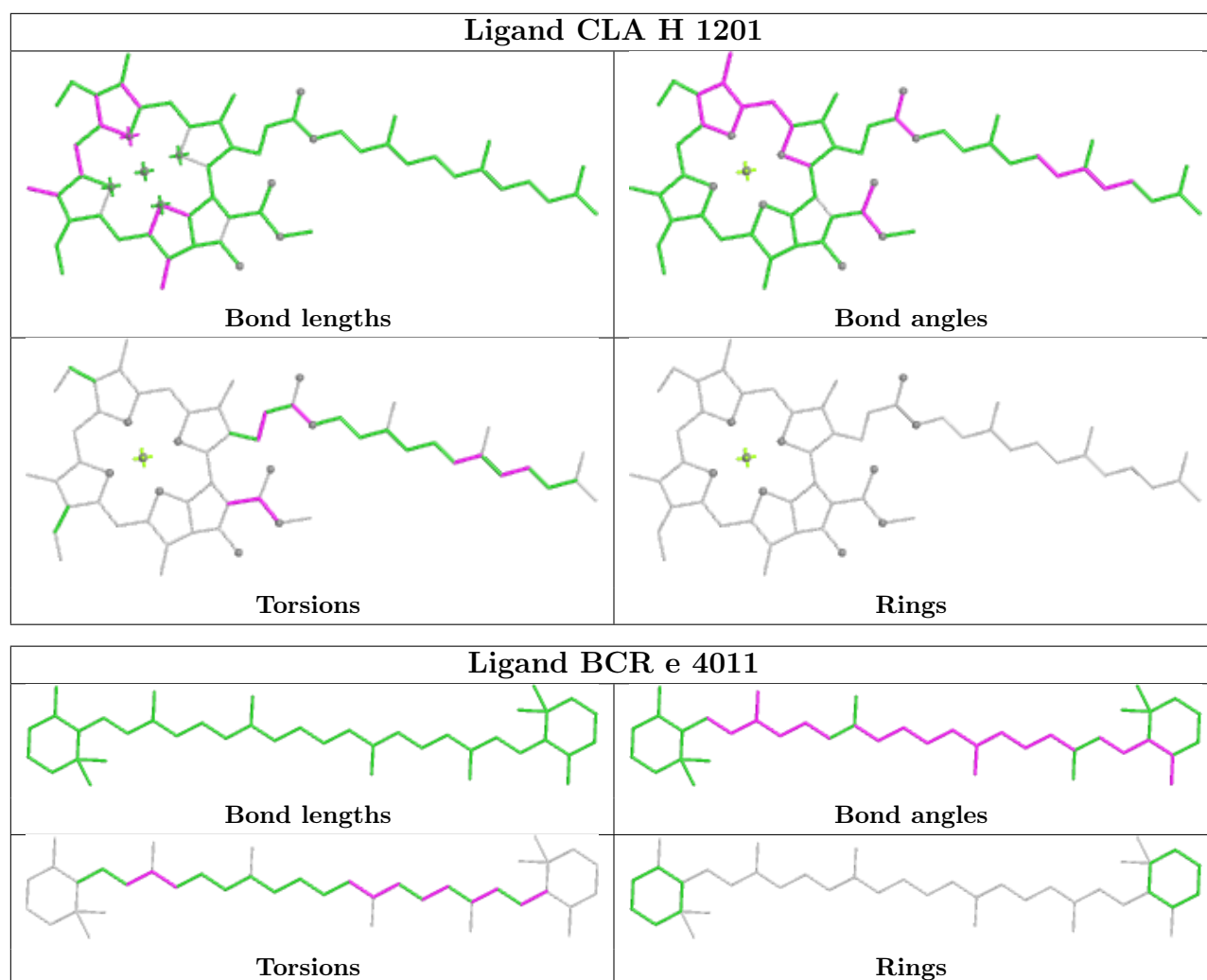
Rings

Ligand CLA 2 517

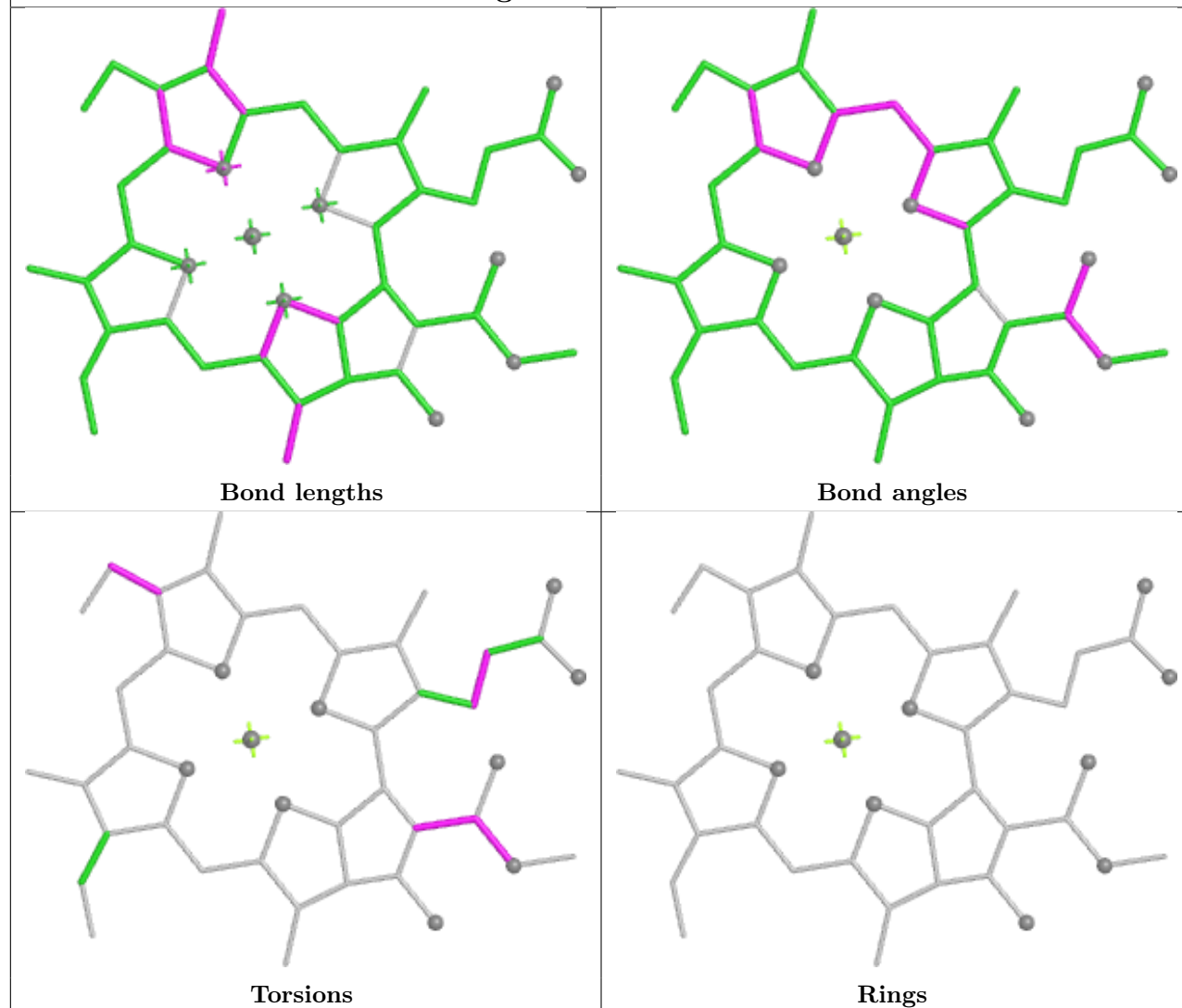


Ligand BCR n 4019

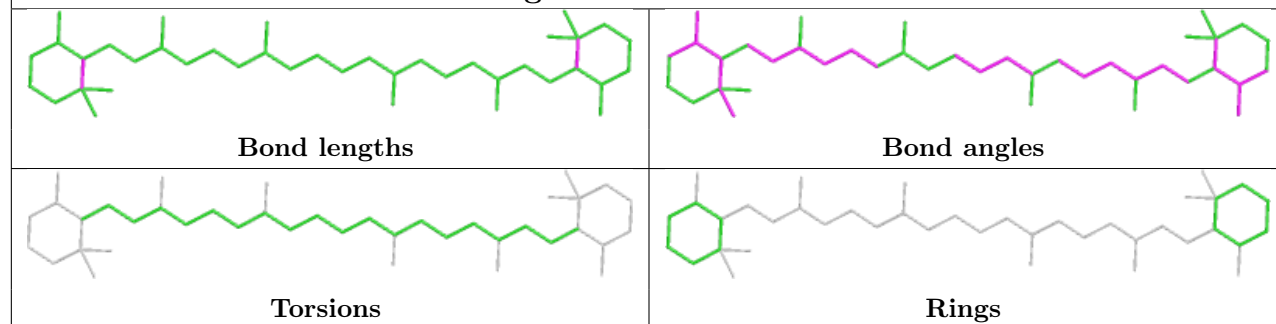




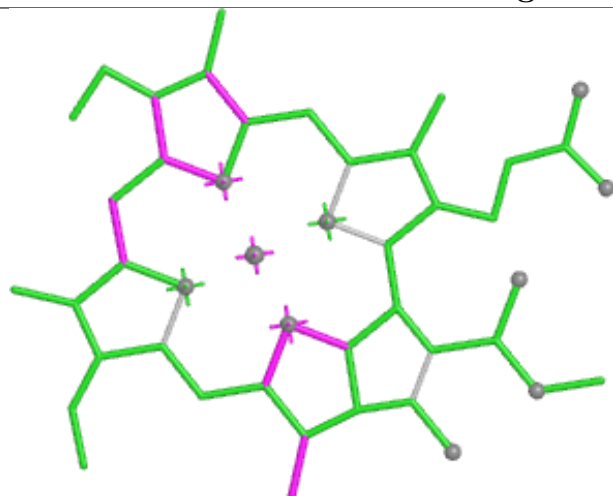
Ligand CLA v 503



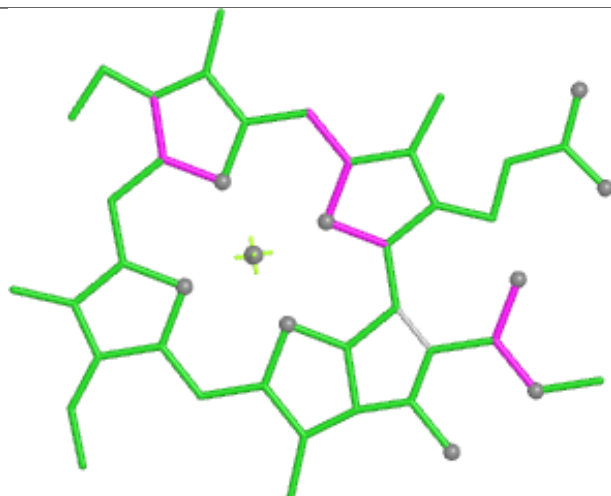
Ligand BCR S 4018



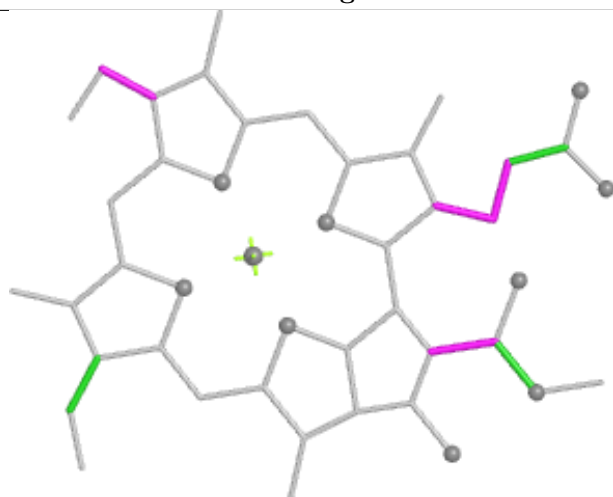
Ligand CLA u 505



Bond lengths



Bond angles

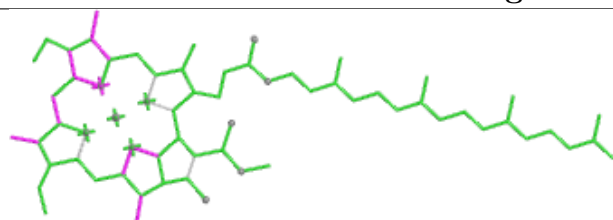


Torsions

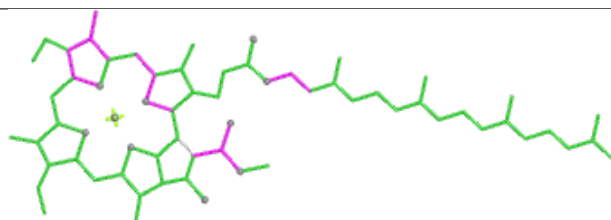


Rings

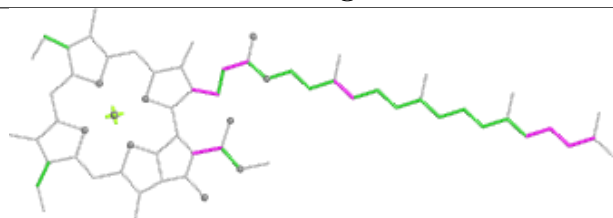
Ligand CLA B 1202



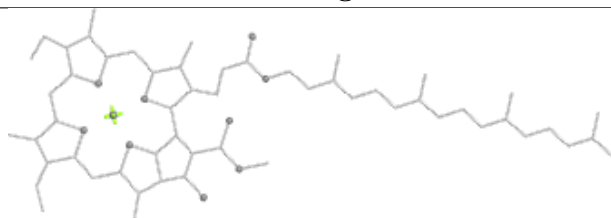
Bond lengths



Bond angles

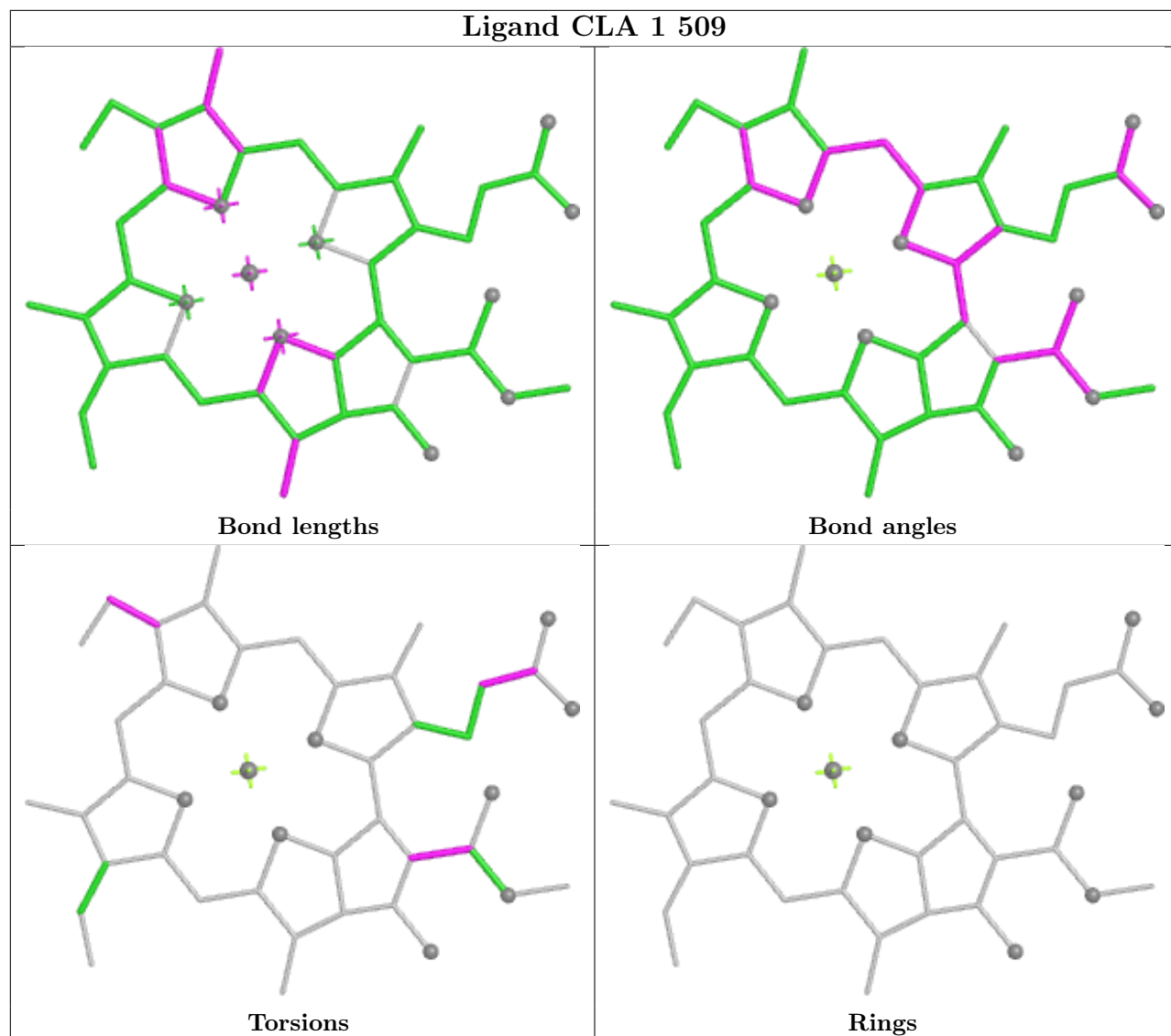


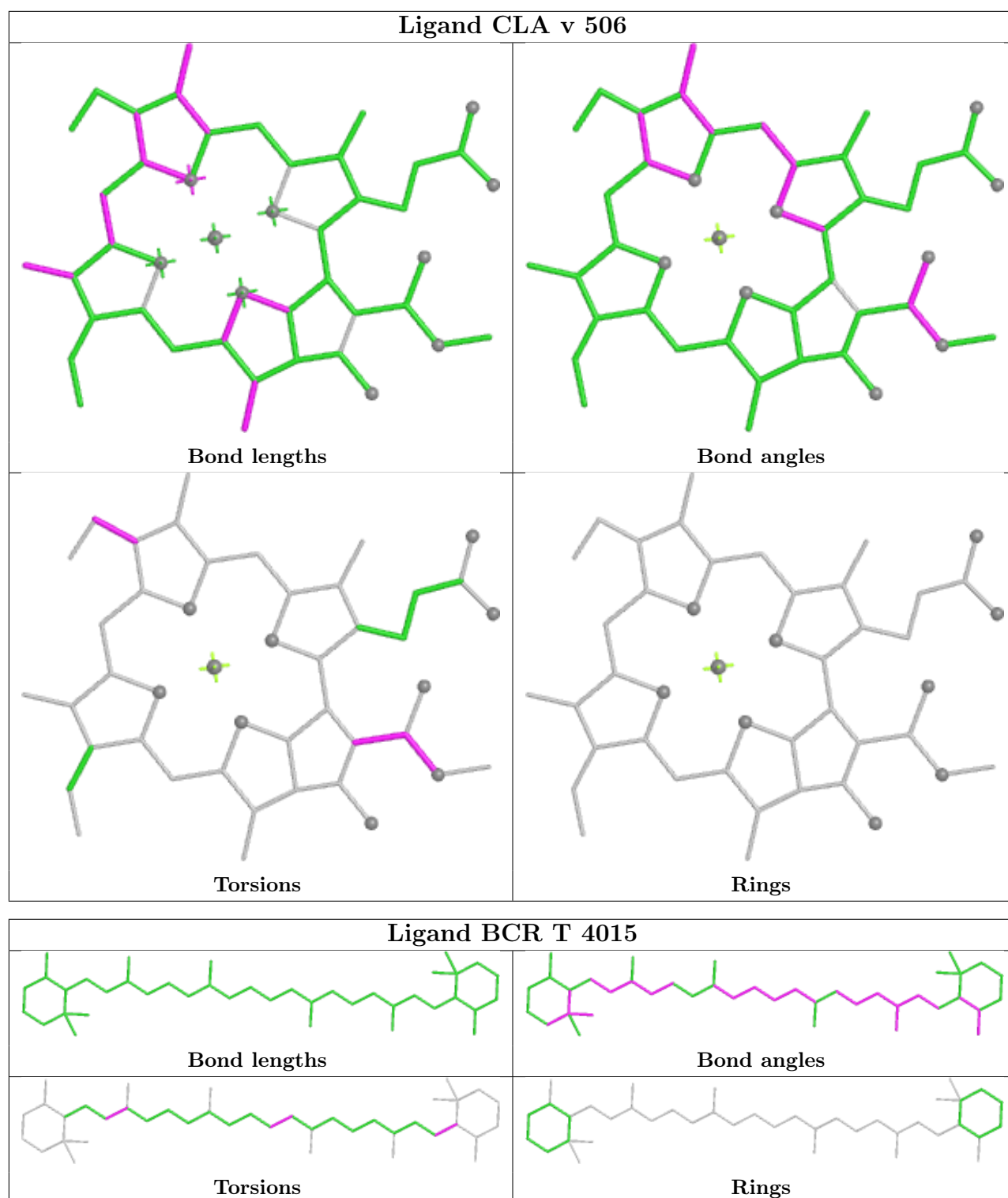
Torsions



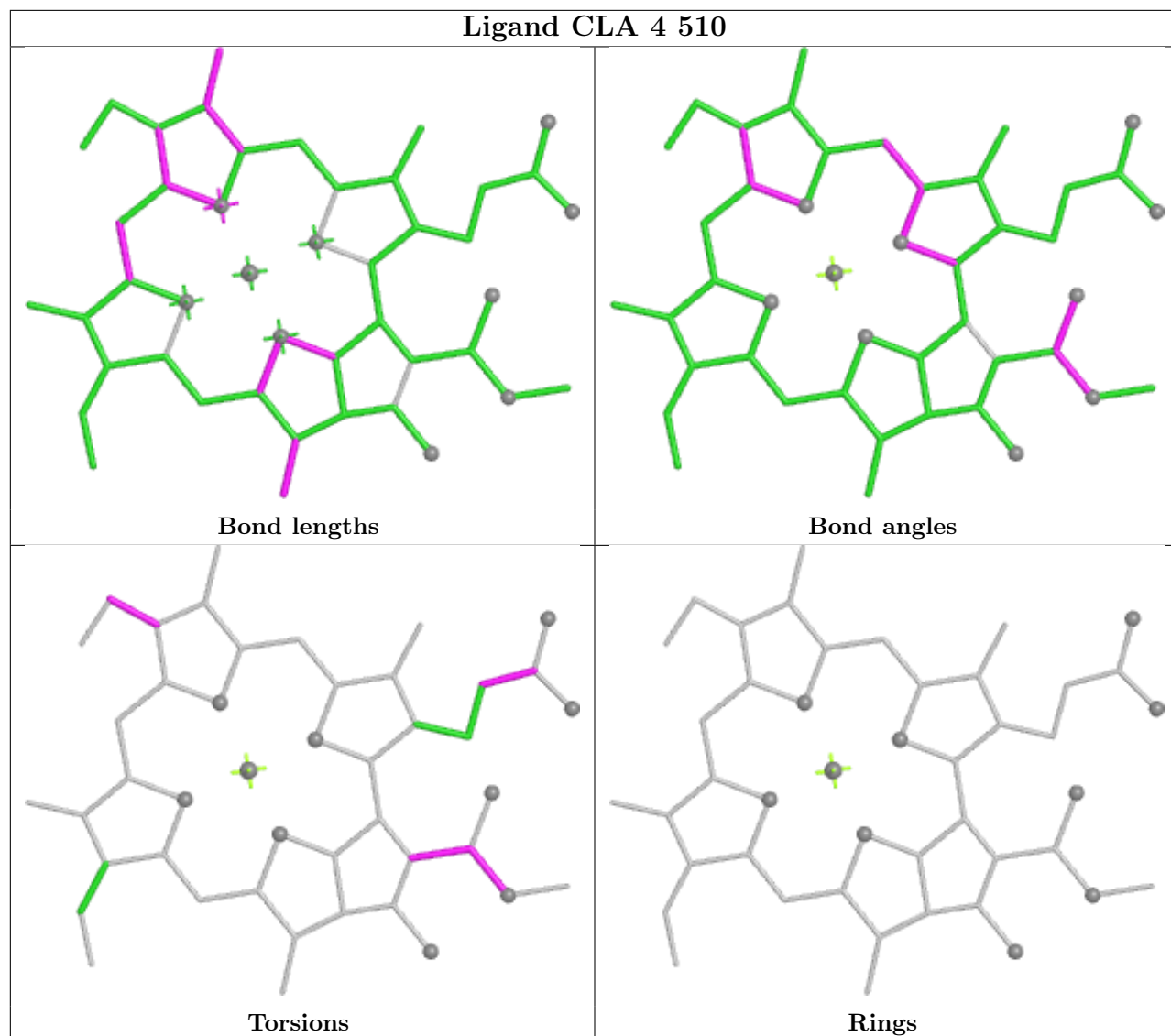
Rings

Ligand CLA 1 509

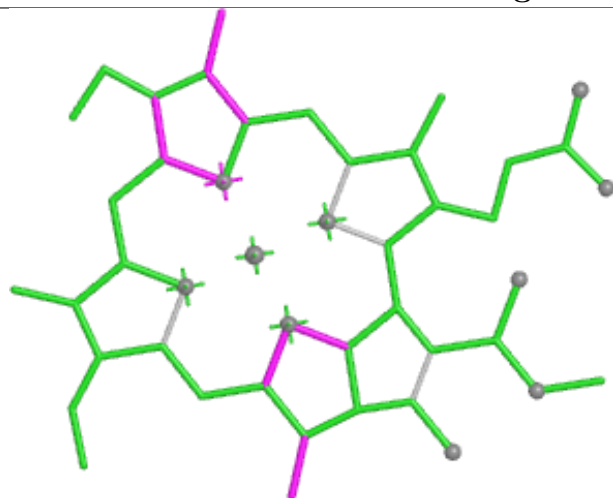




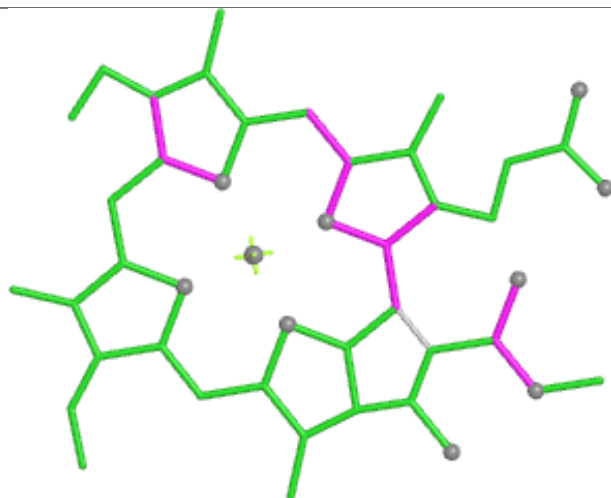
Ligand CLA 4 510



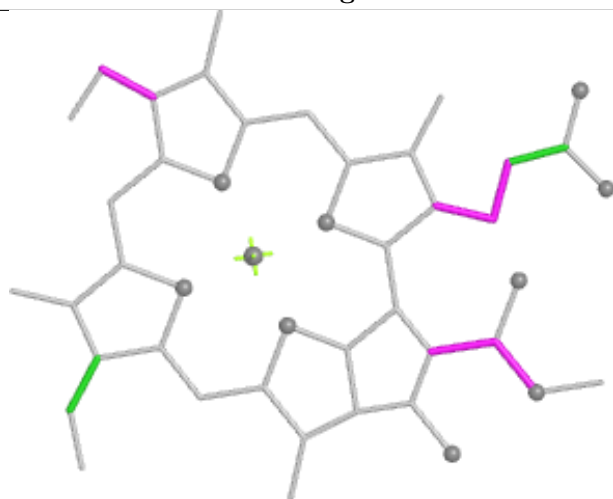
Ligand CLA Y 503



Bond lengths



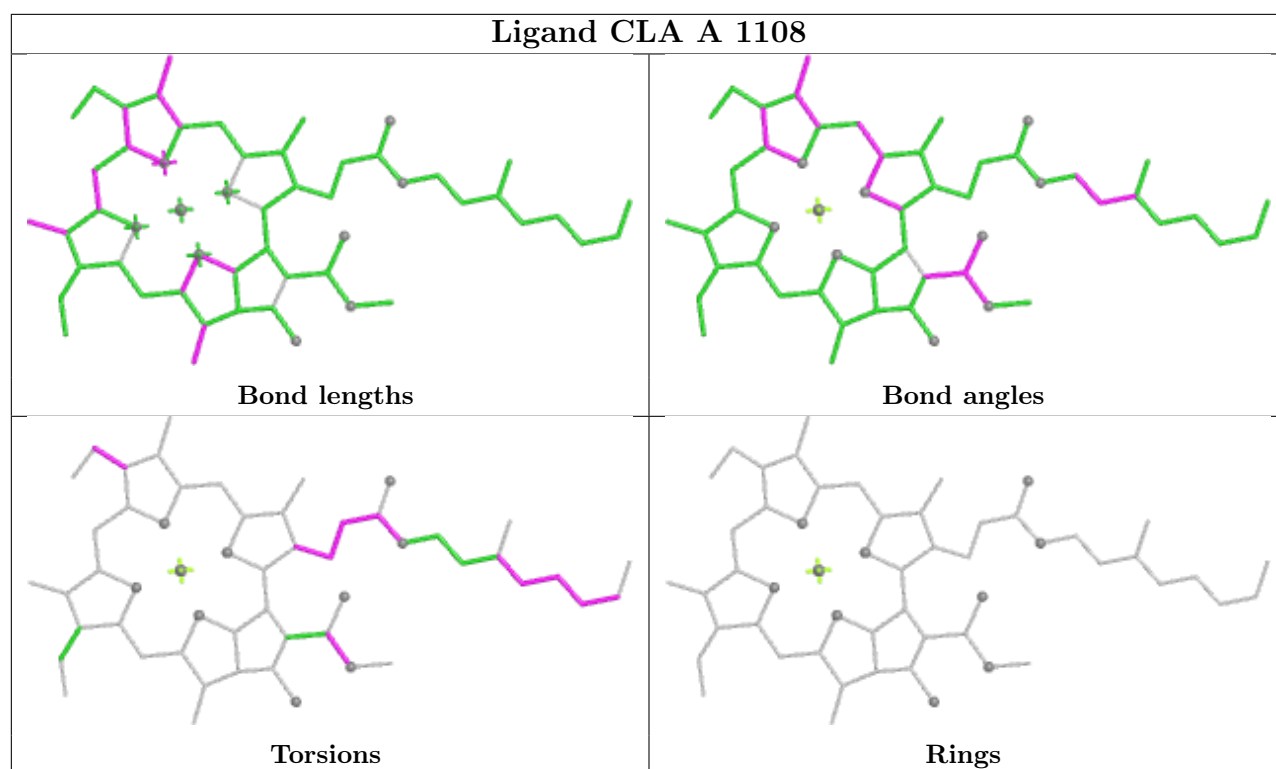
Bond angles



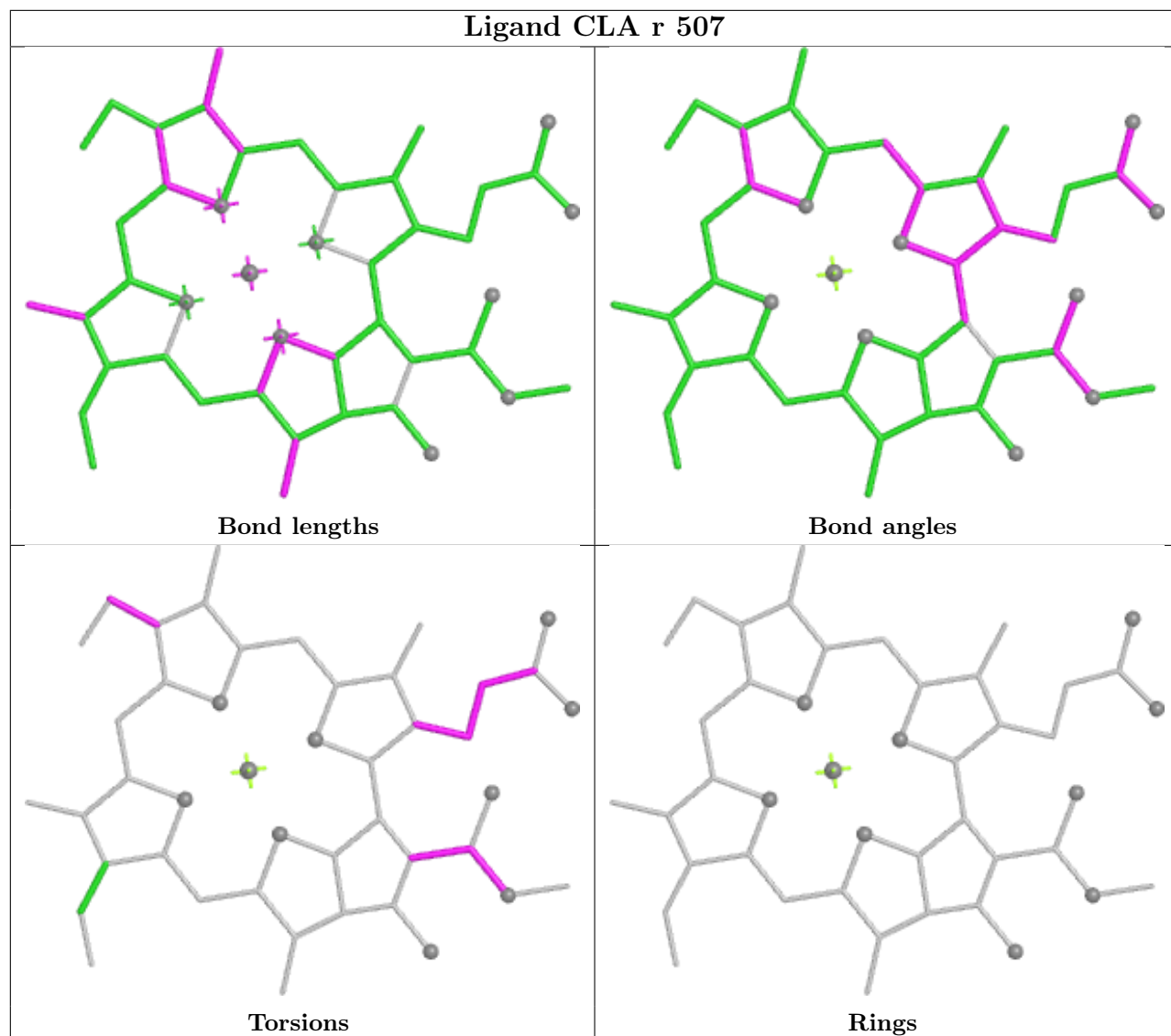
Torsions



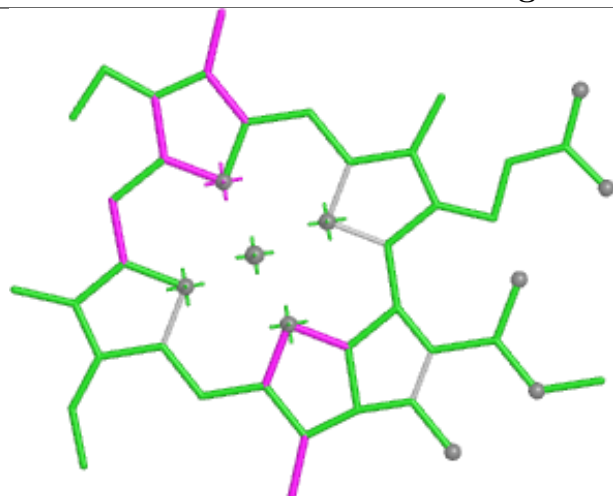
Rings



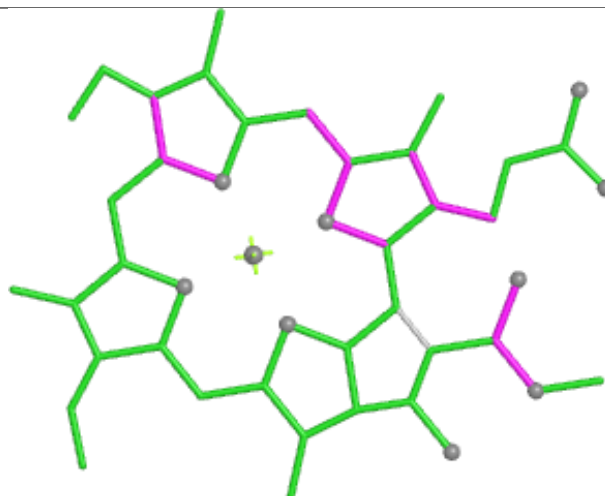
Ligand CLA r 507



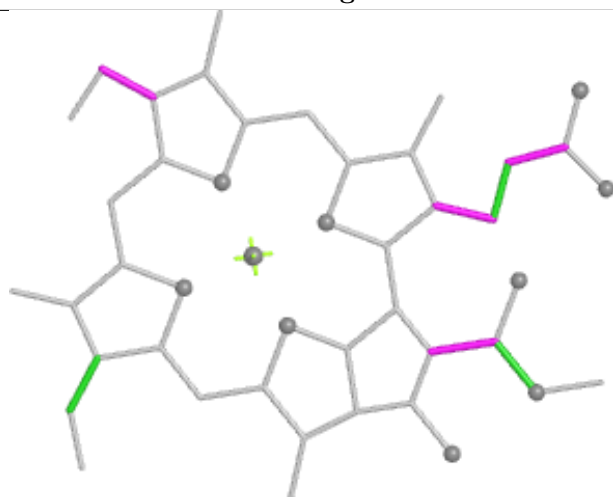
Ligand CLA 4 516



Bond lengths



Bond angles

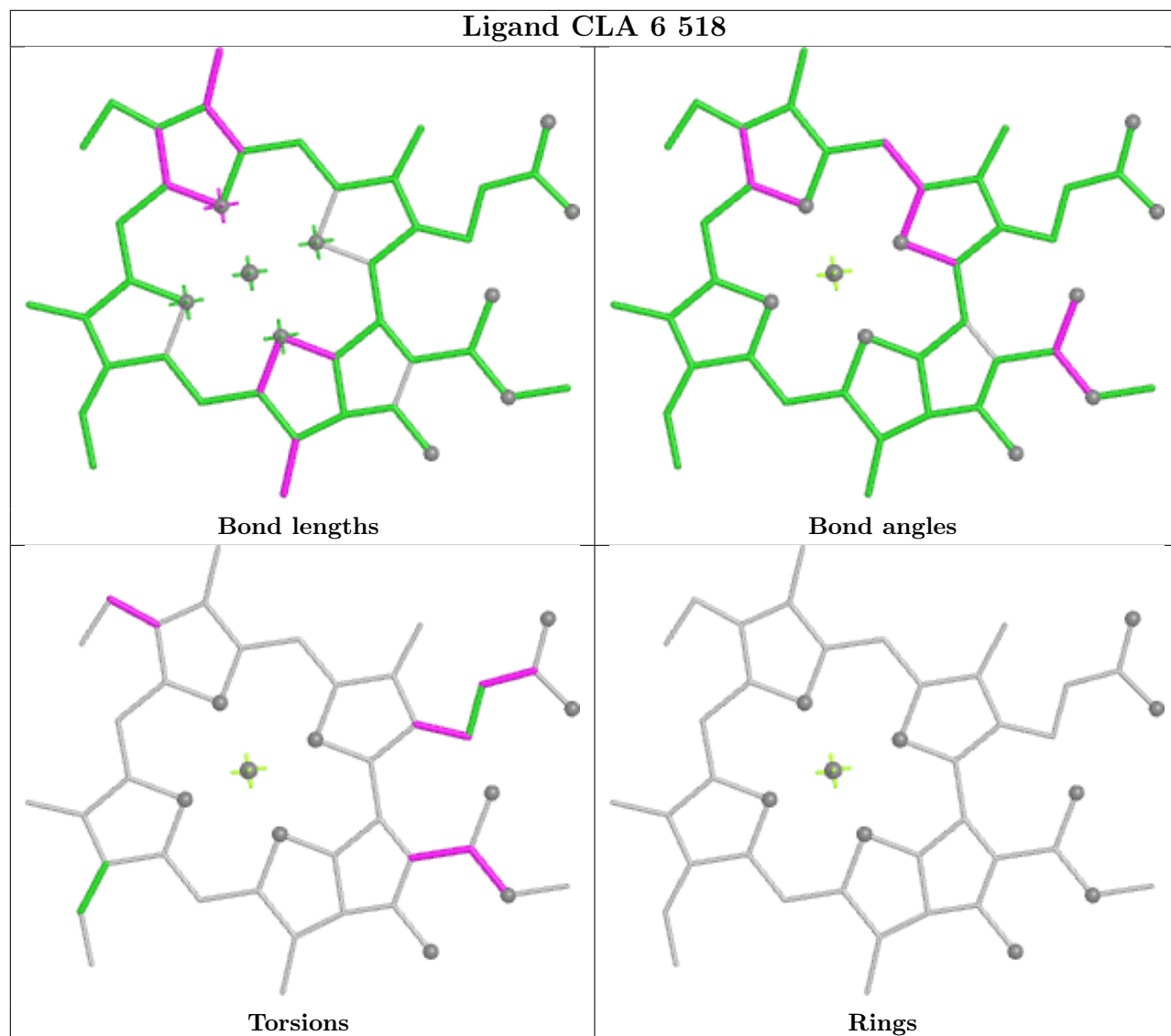


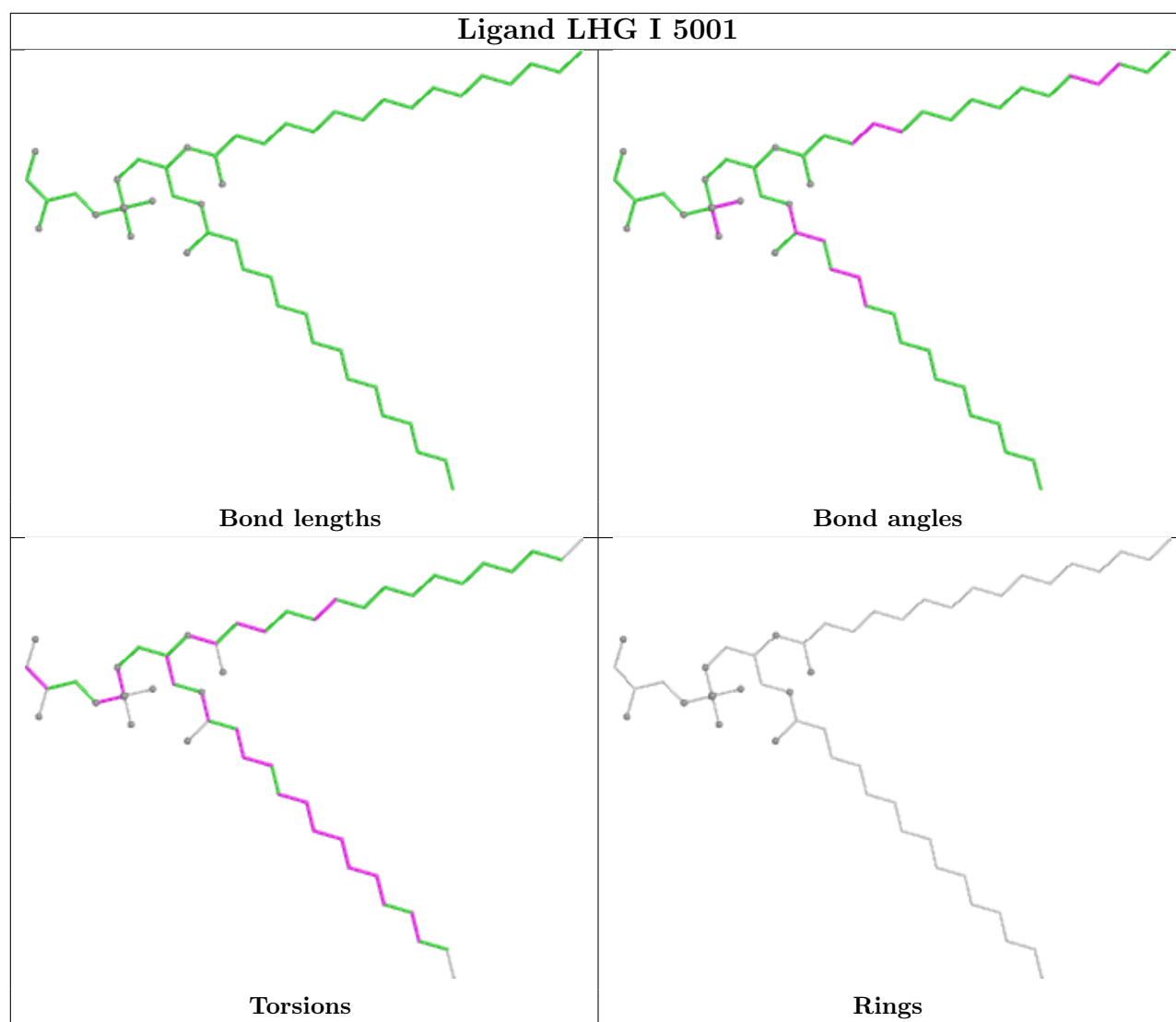
Torsions



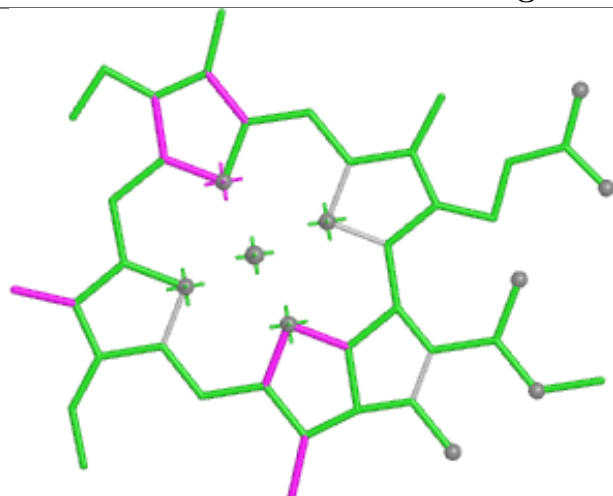
Rings

Ligand CLA 6 518

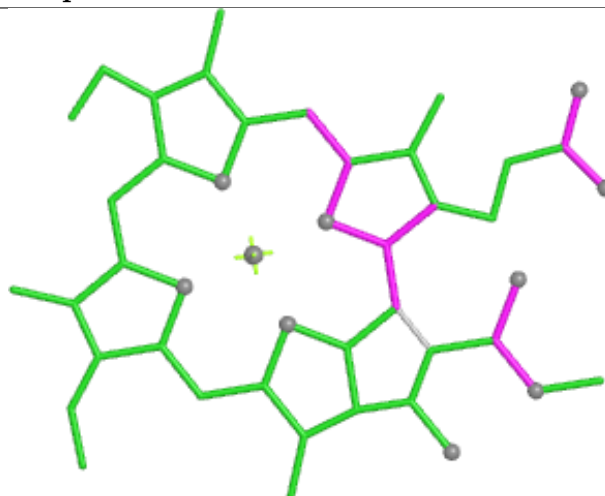




Ligand CLA q 507



Bond lengths



Bond angles

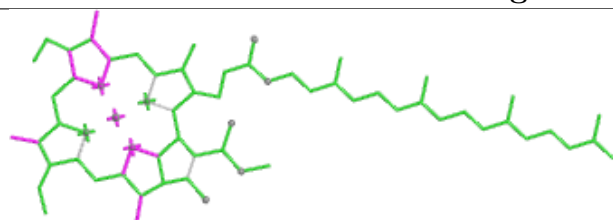


Torsions

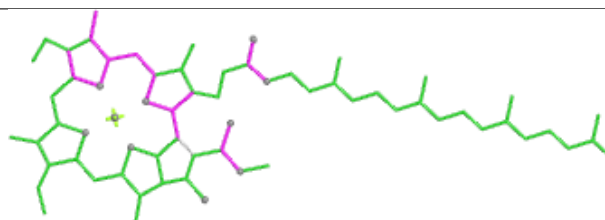


Rings

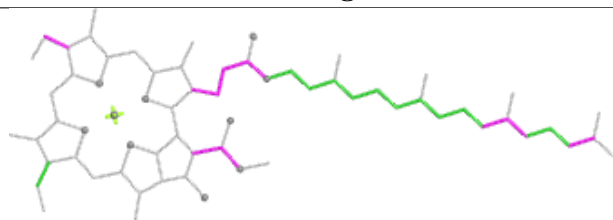
Ligand CLA e 1111



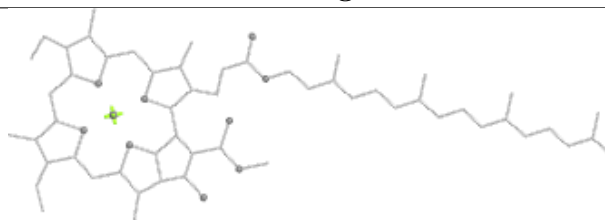
Bond lengths



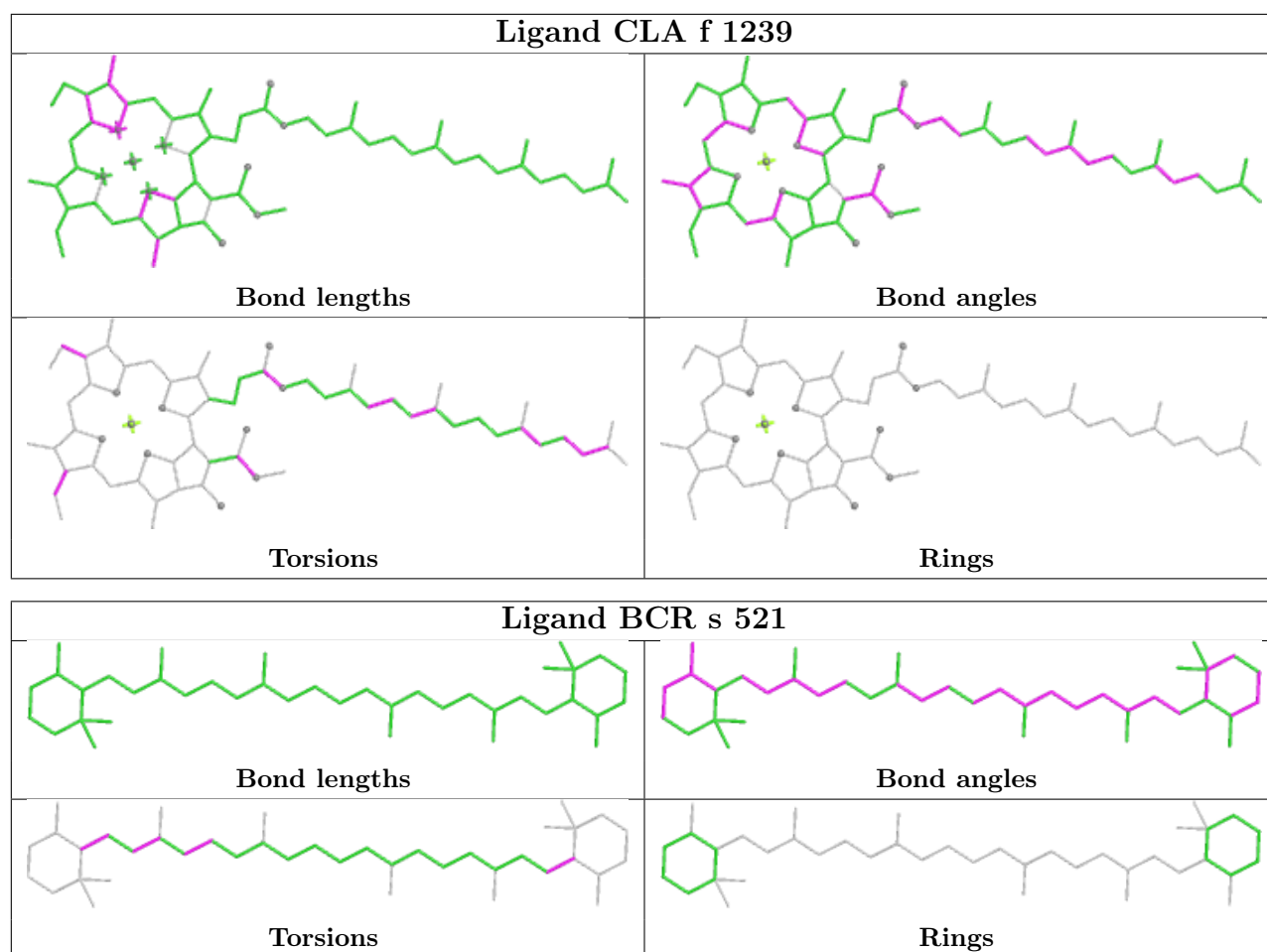
Bond angles



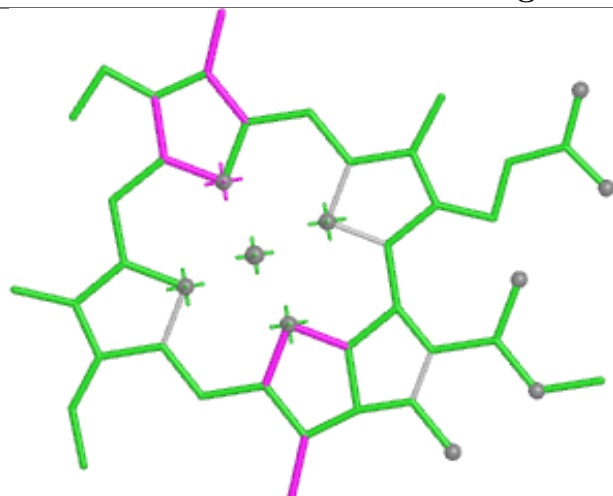
Torsions



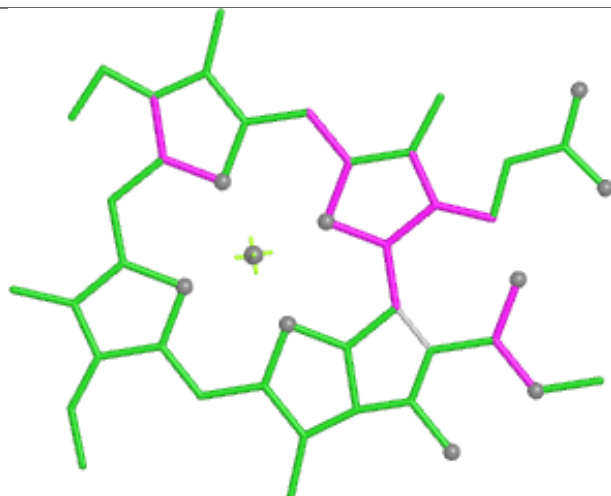
Rings



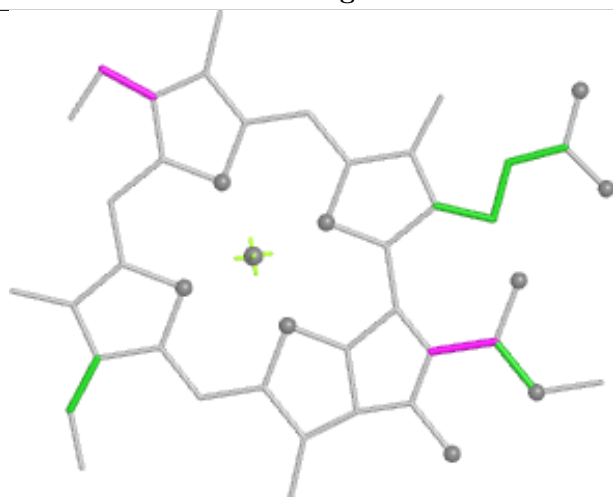
Ligand CLA v 502



Bond lengths



Bond angles

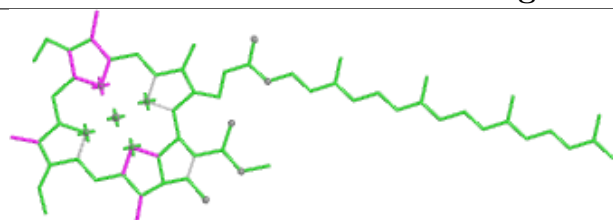


Torsions

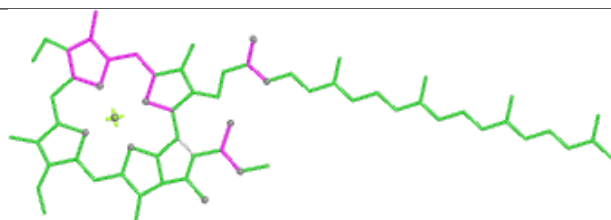


Rings

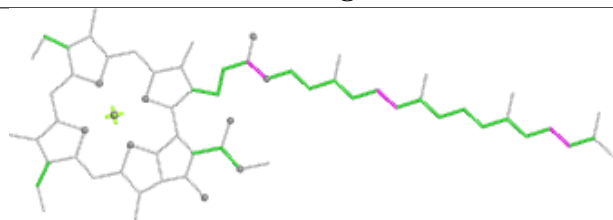
Ligand CLA 2 509



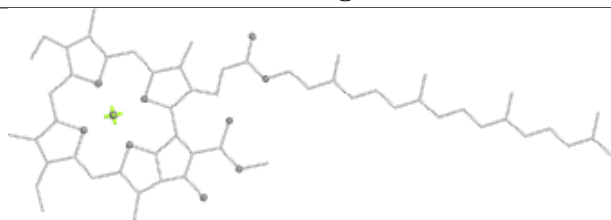
Bond lengths



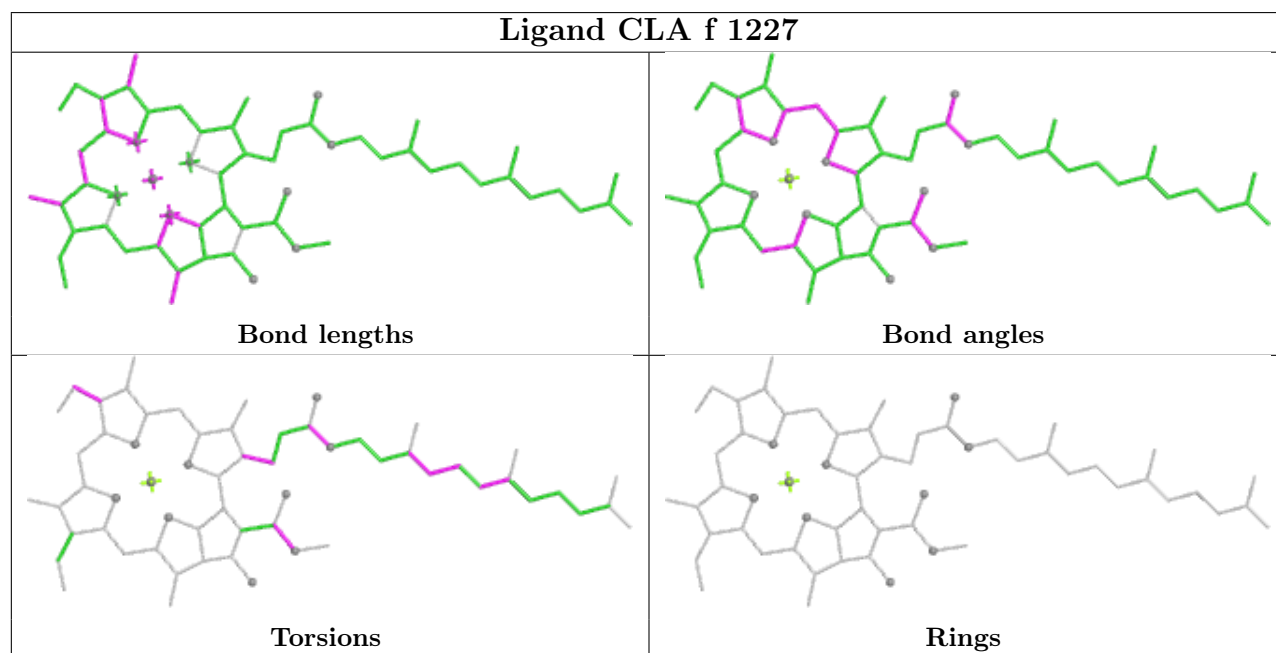
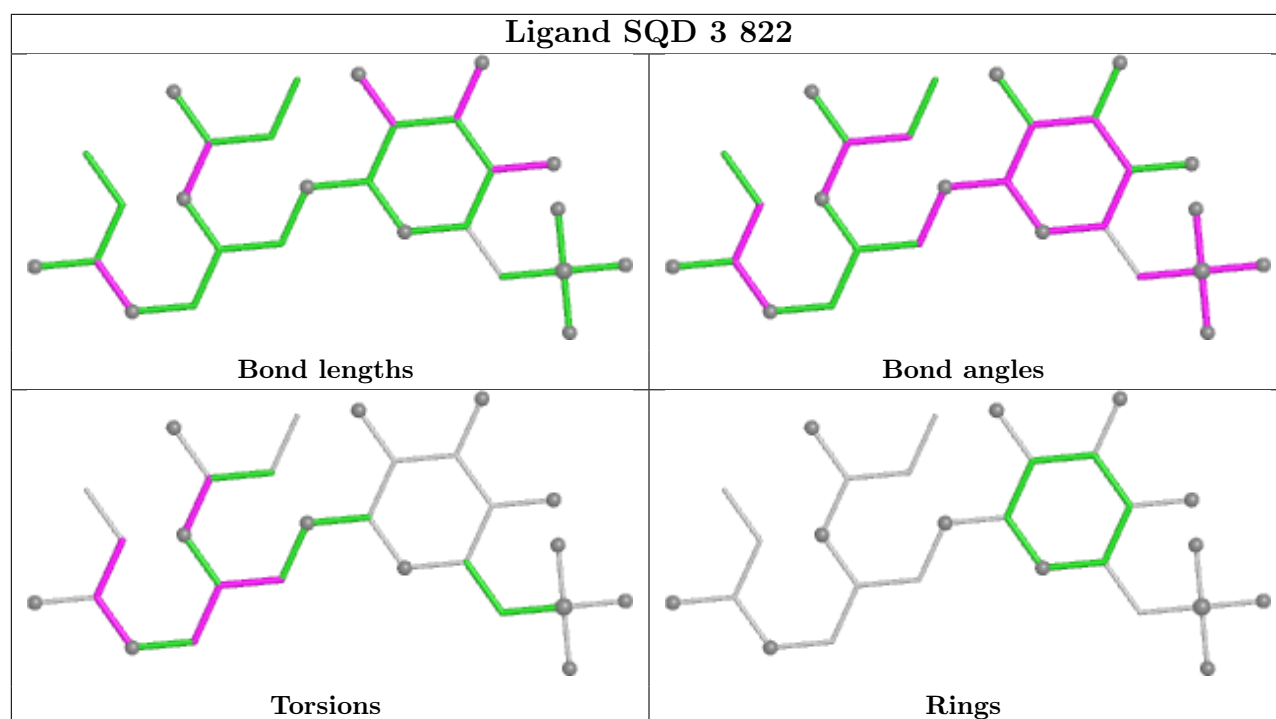
Bond angles



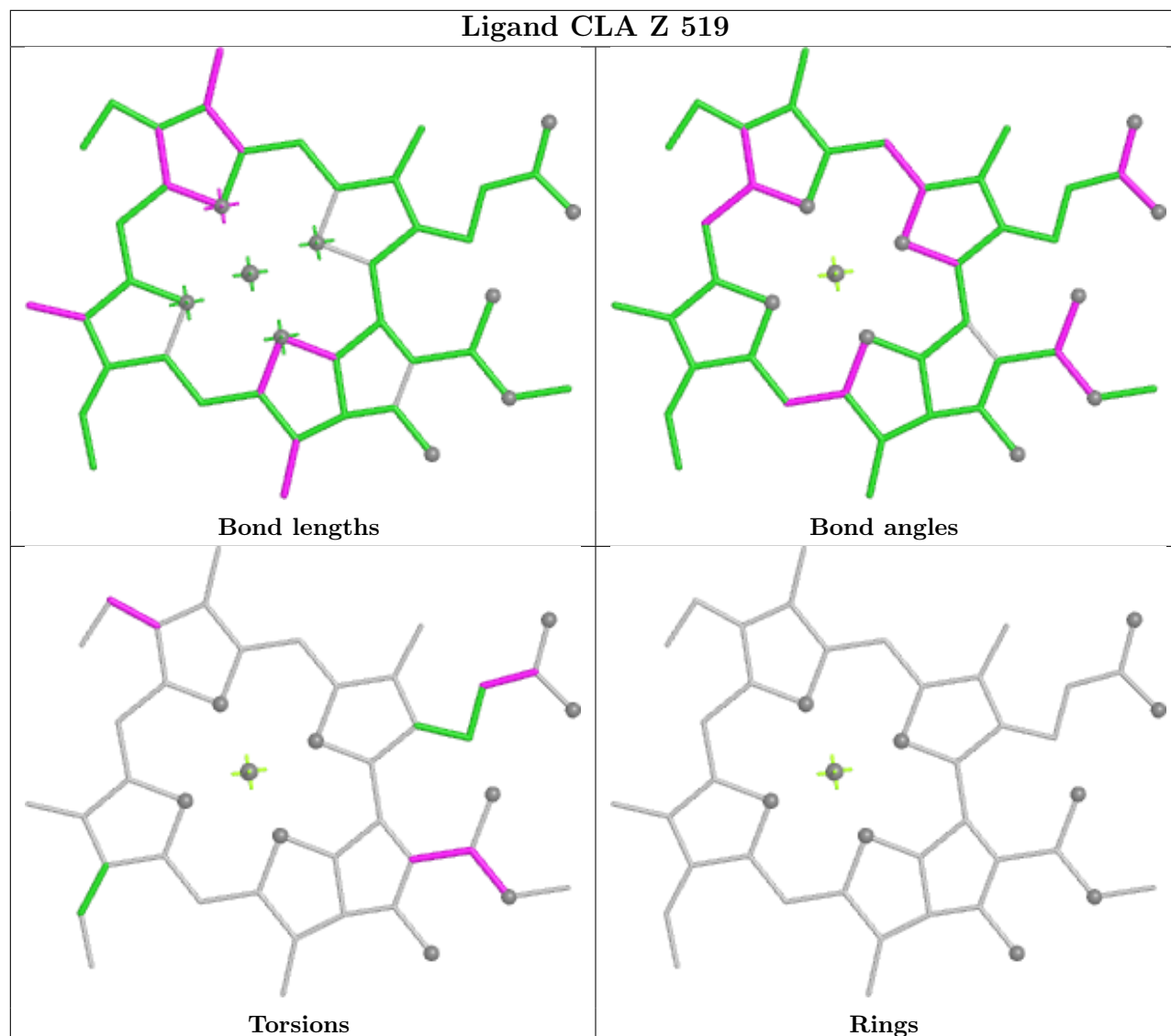
Torsions



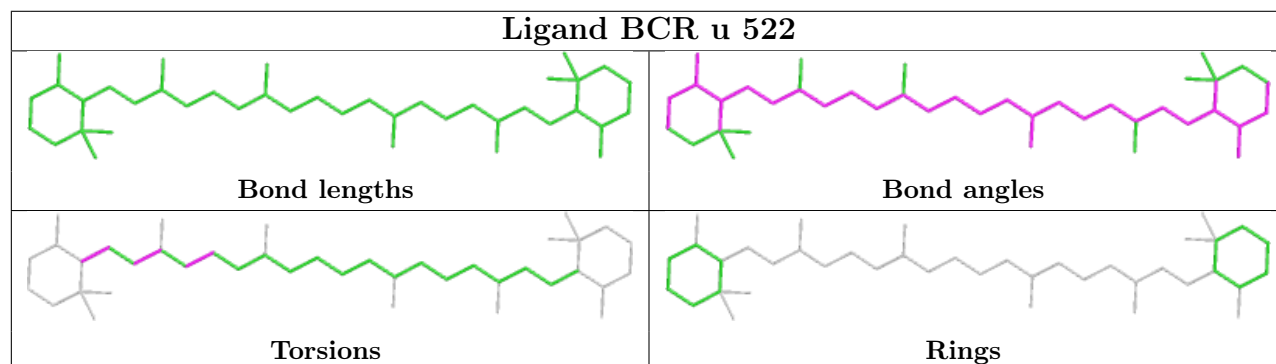
Rings



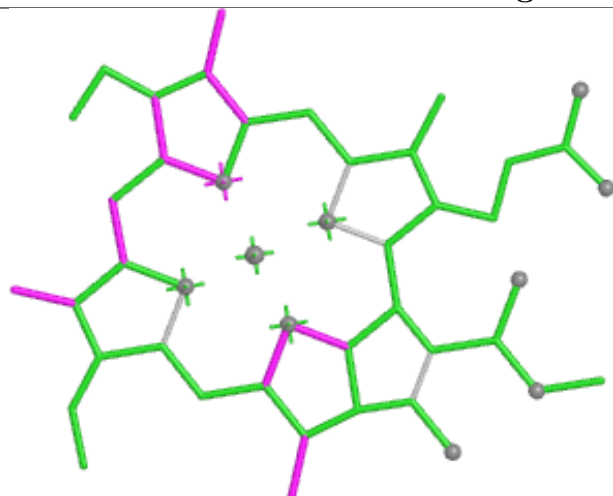
Ligand CLA Z 519



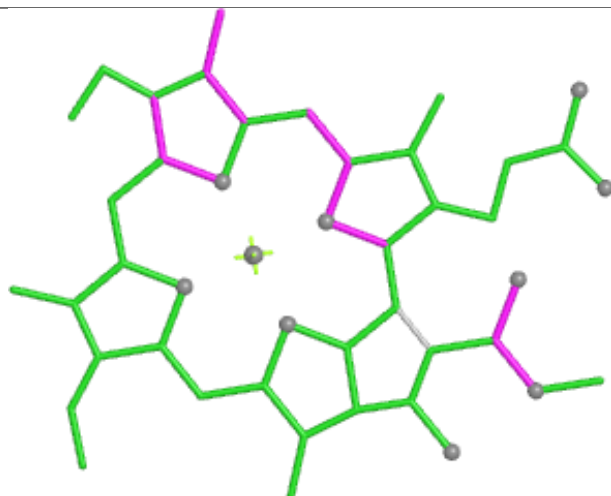
Ligand BCR u 522



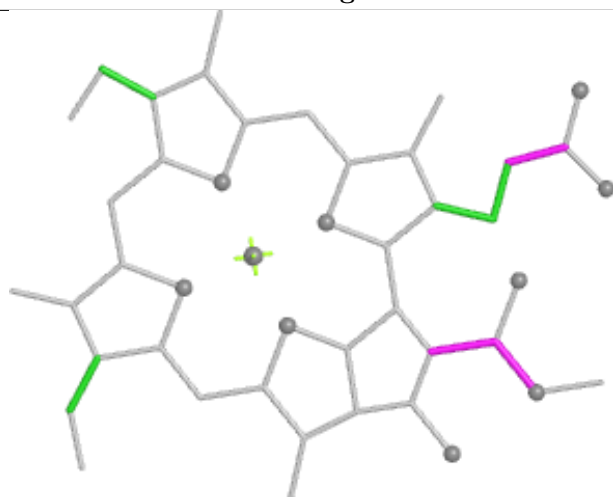
Ligand CLA Z 510



Bond lengths



Bond angles

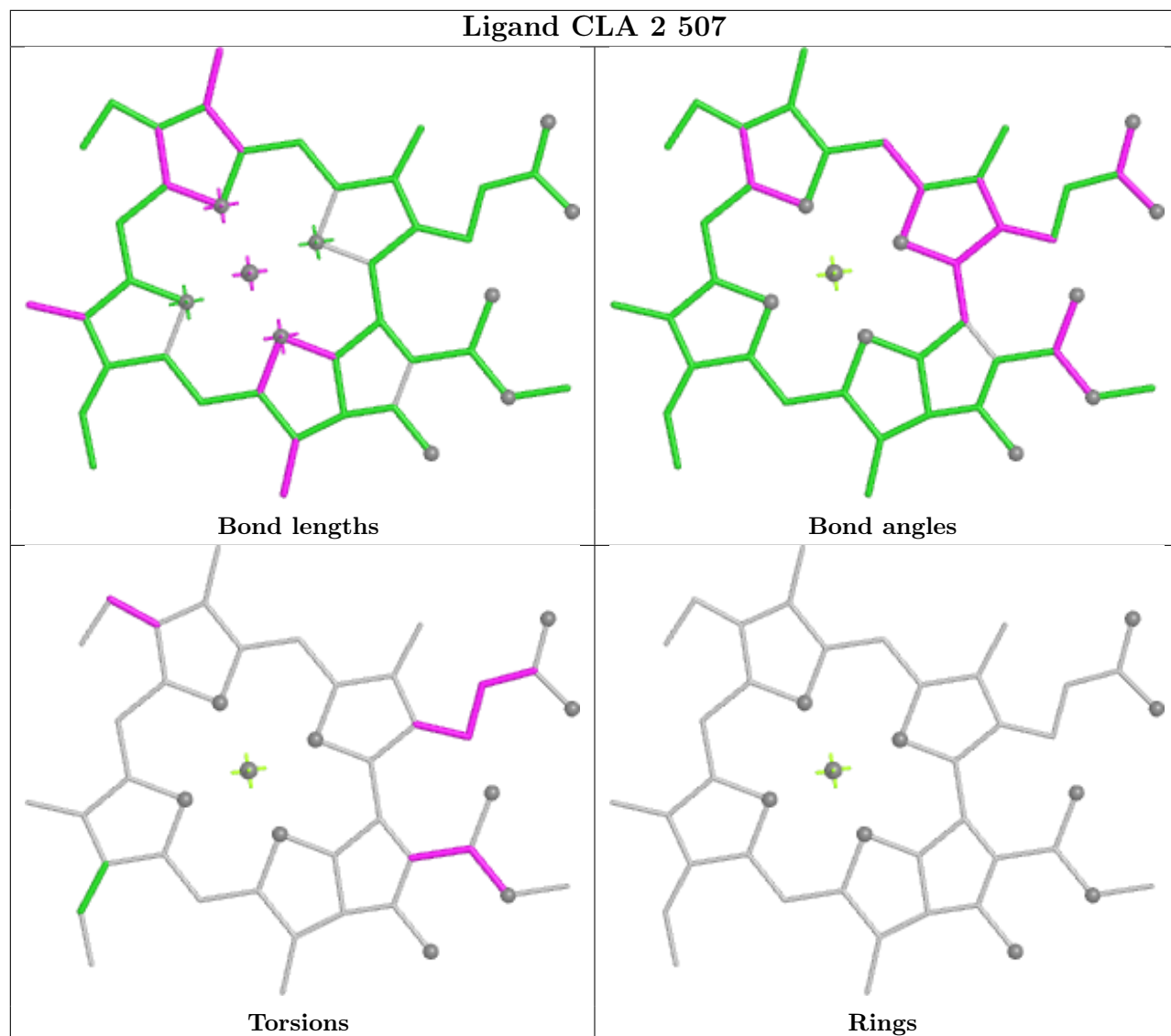


Torsions

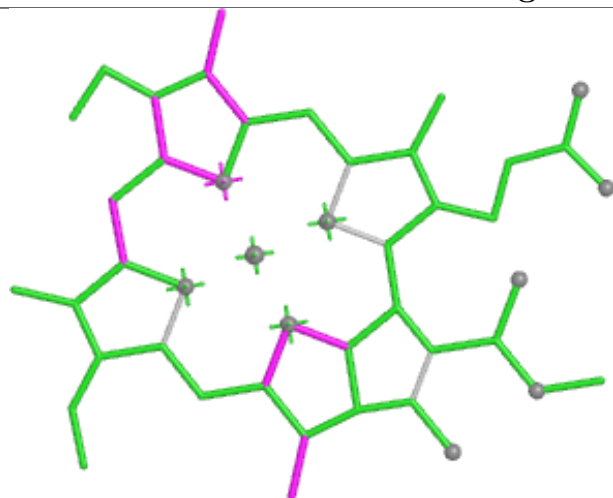


Rings

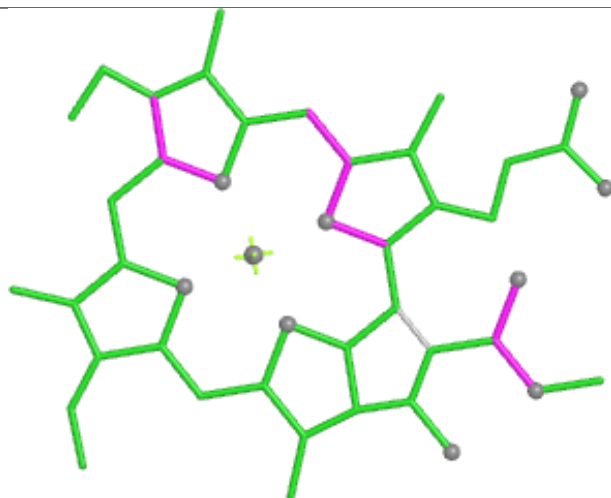
Ligand CLA 2 507



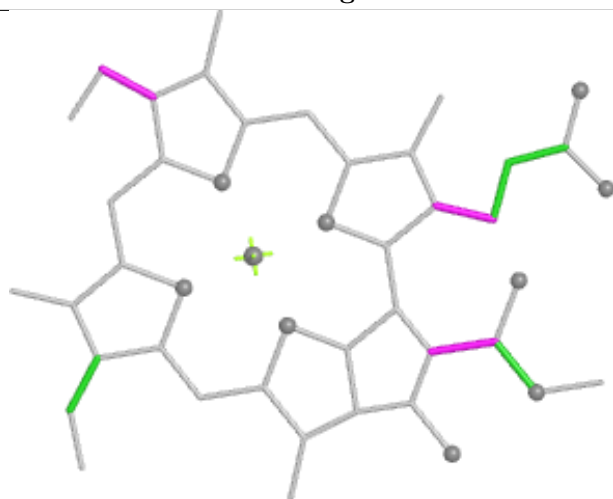
Ligand CLA 5 516



Bond lengths



Bond angles

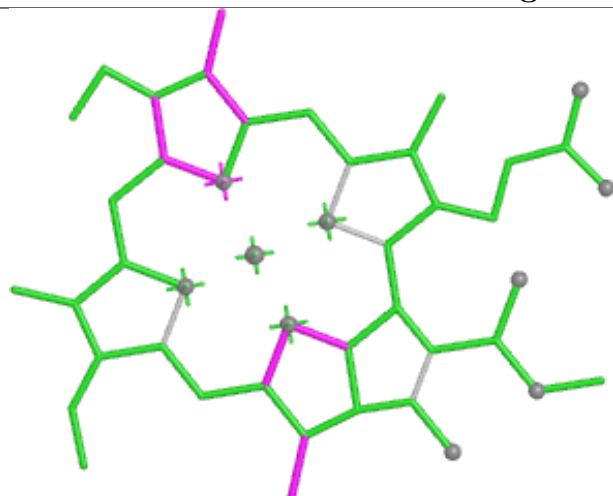


Torsions

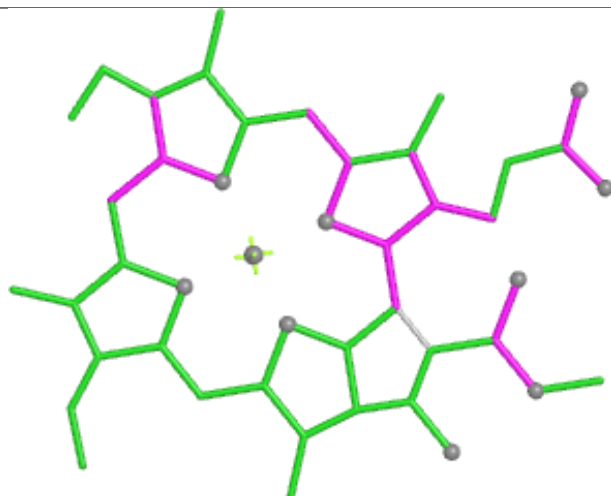


Rings

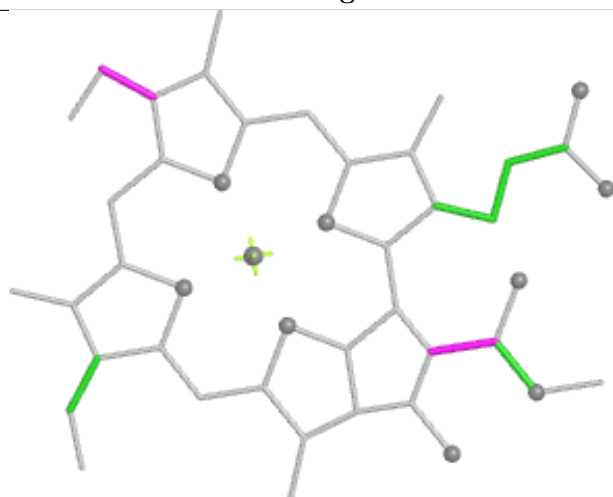
Ligand CLA r 502



Bond lengths



Bond angles

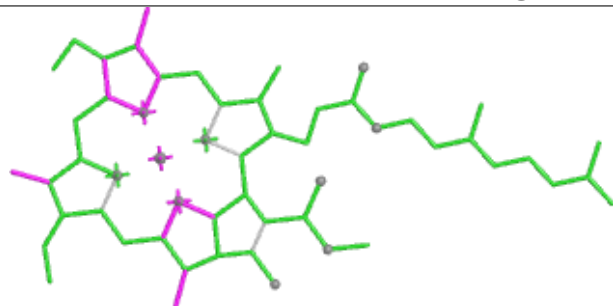


Torsions

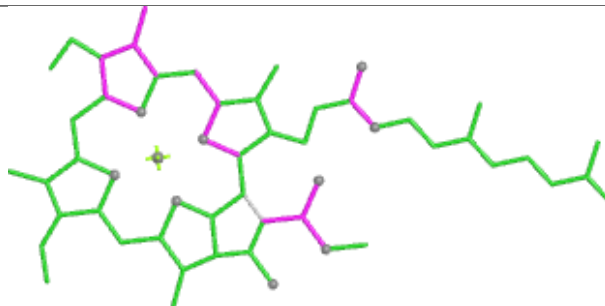


Rings

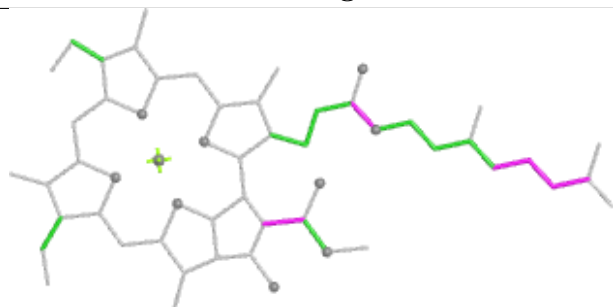
Ligand CLA f 1211



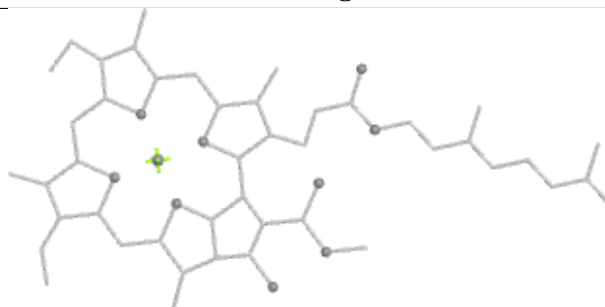
Bond lengths



Bond angles

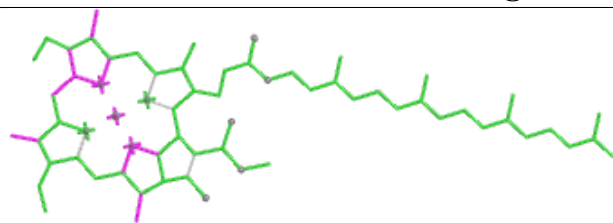


Torsions

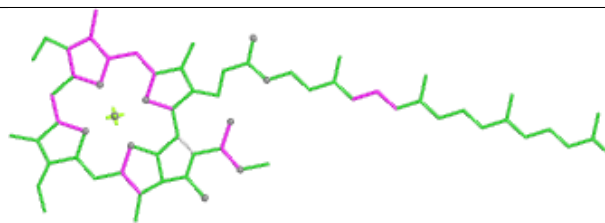


Rings

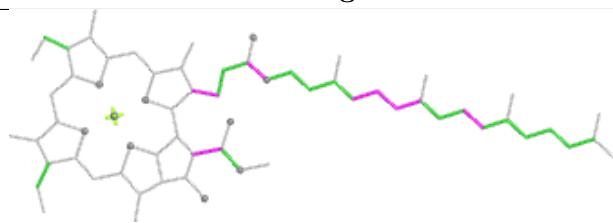
Ligand CLA G 1128



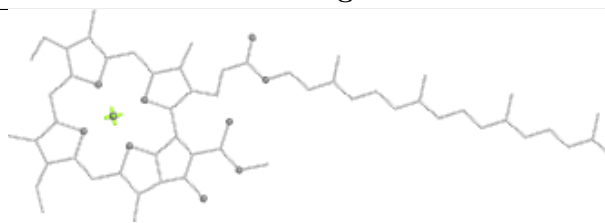
Bond lengths



Bond angles

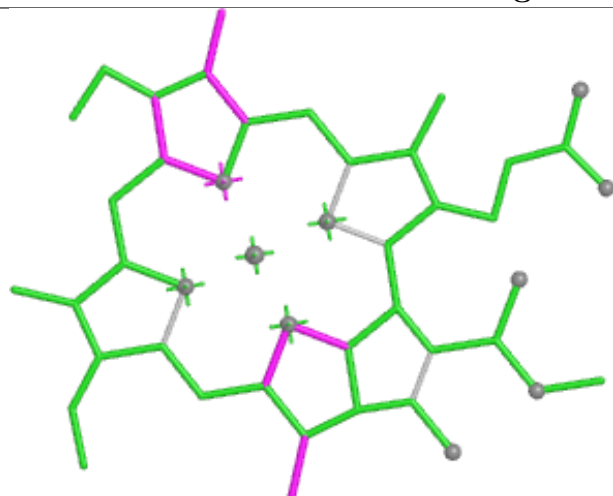


Torsions

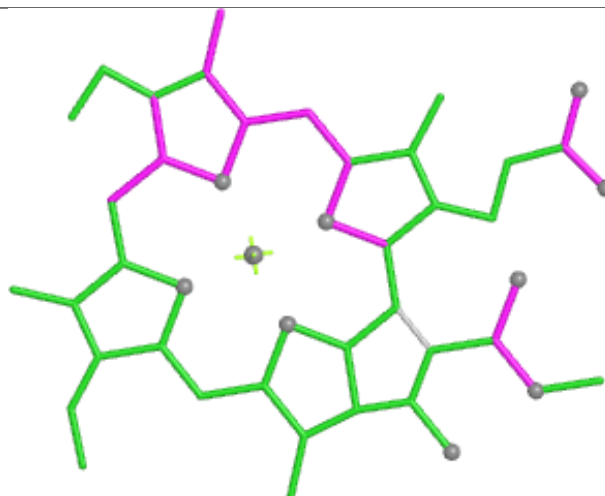


Rings

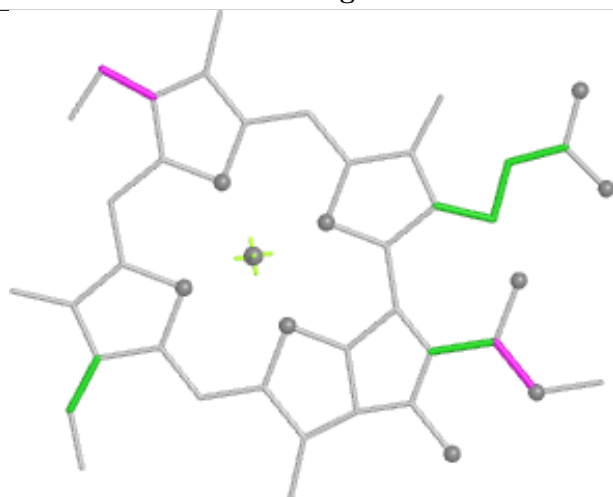
Ligand CLA Y 511



Bond lengths



Bond angles

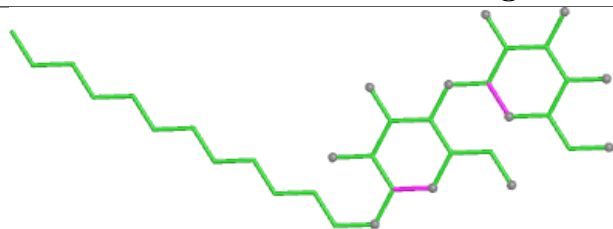


Torsions

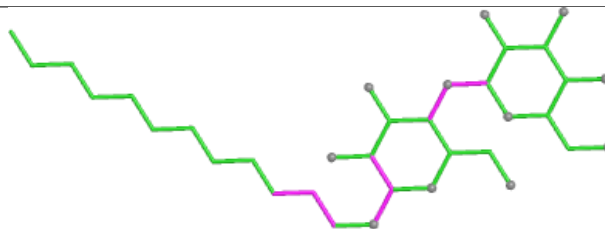


Rings

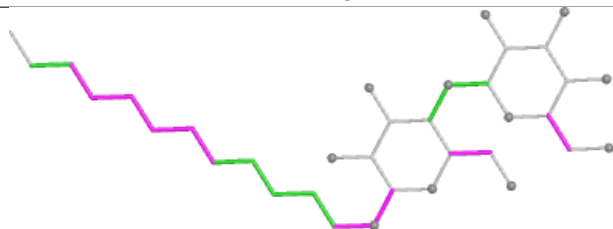
Ligand LMU H 1843



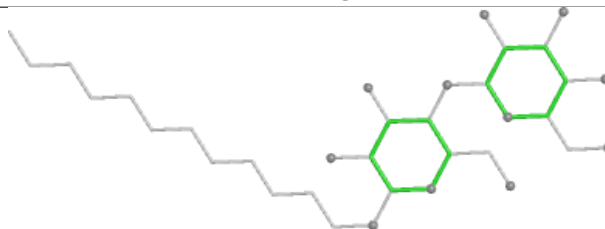
Bond lengths



Bond angles

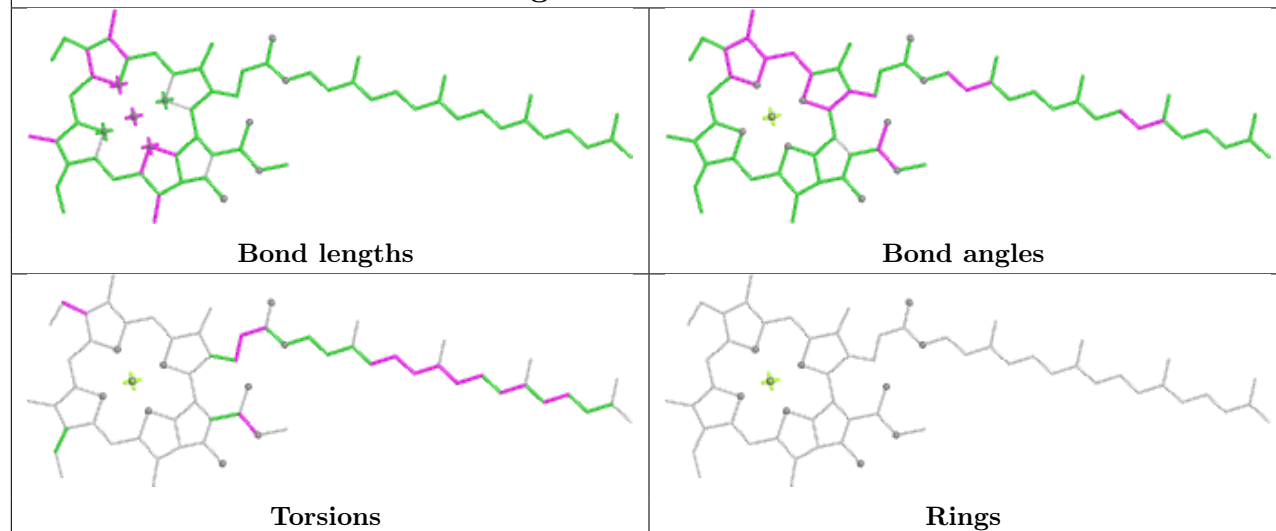


Torsions

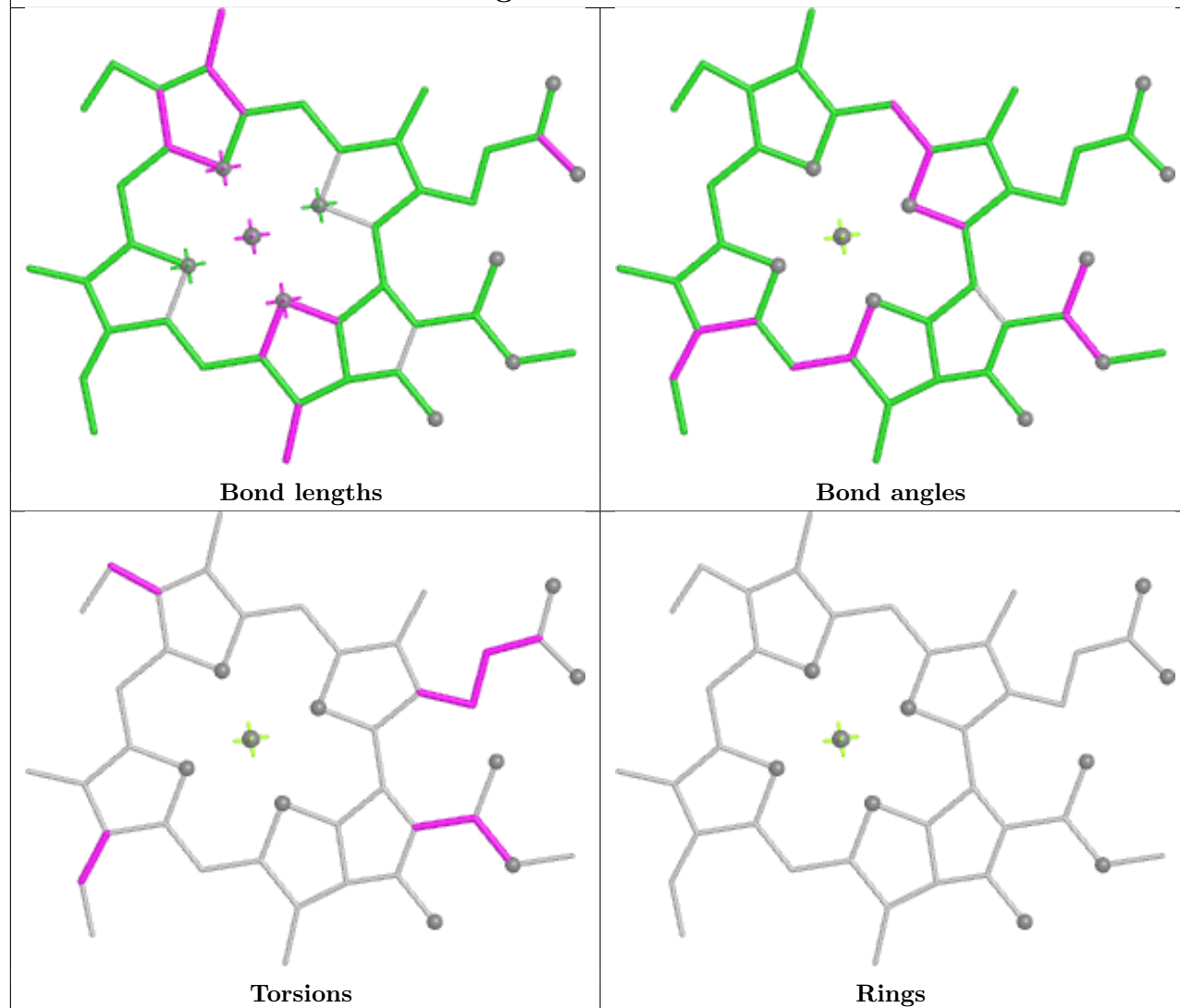


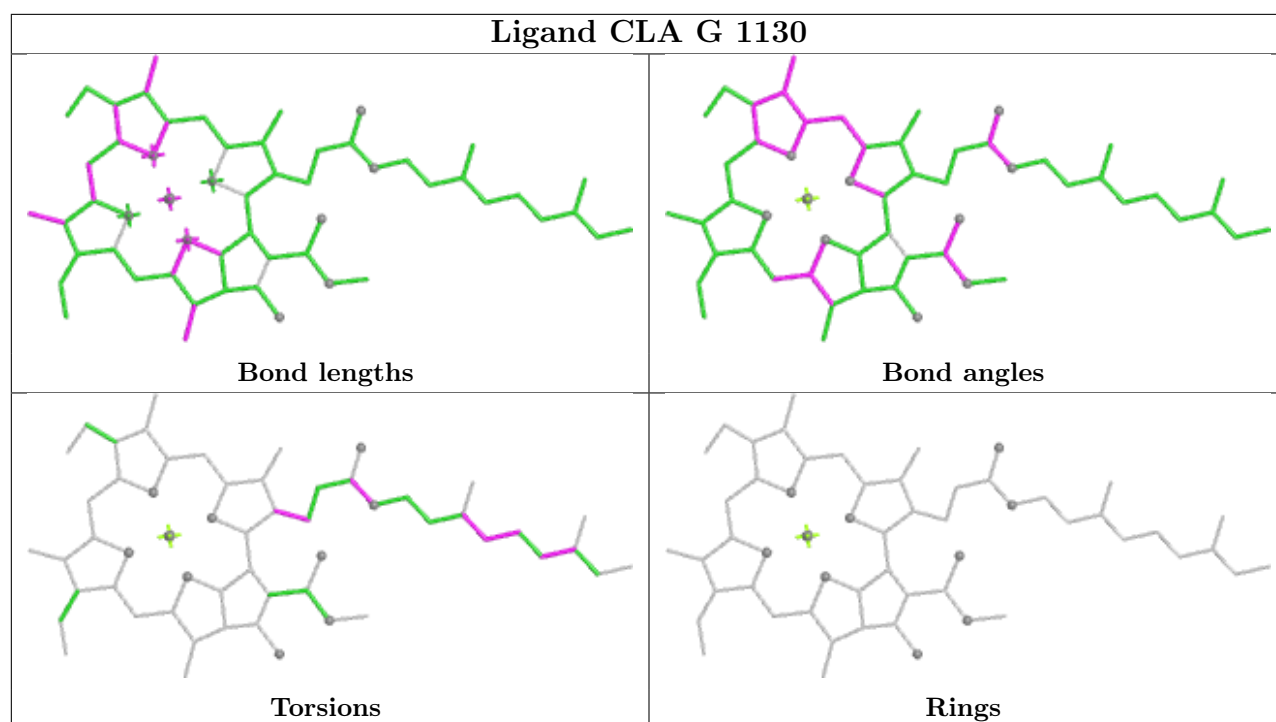
Rings

Ligand CLA f 1203

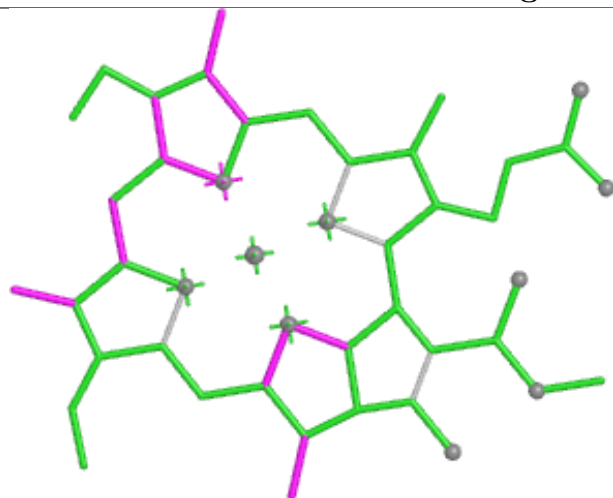


Ligand CLA 1 516

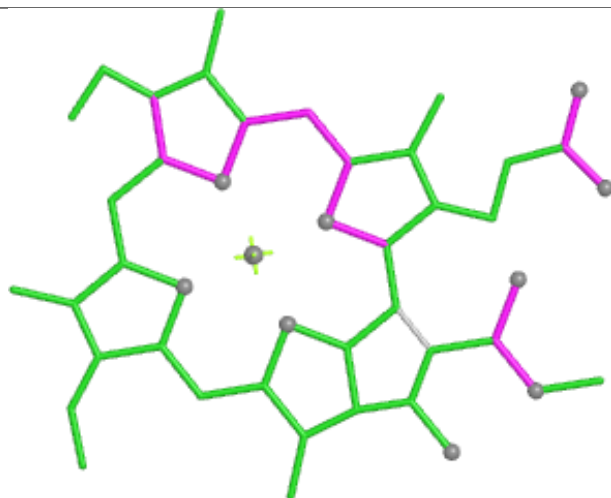




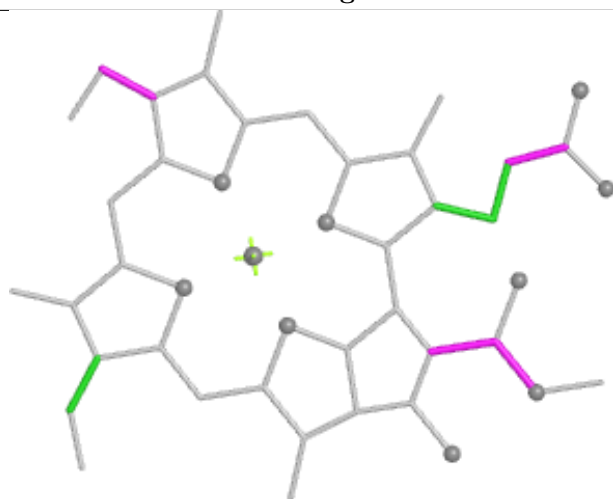
Ligand CLA t 519



Bond lengths



Bond angles

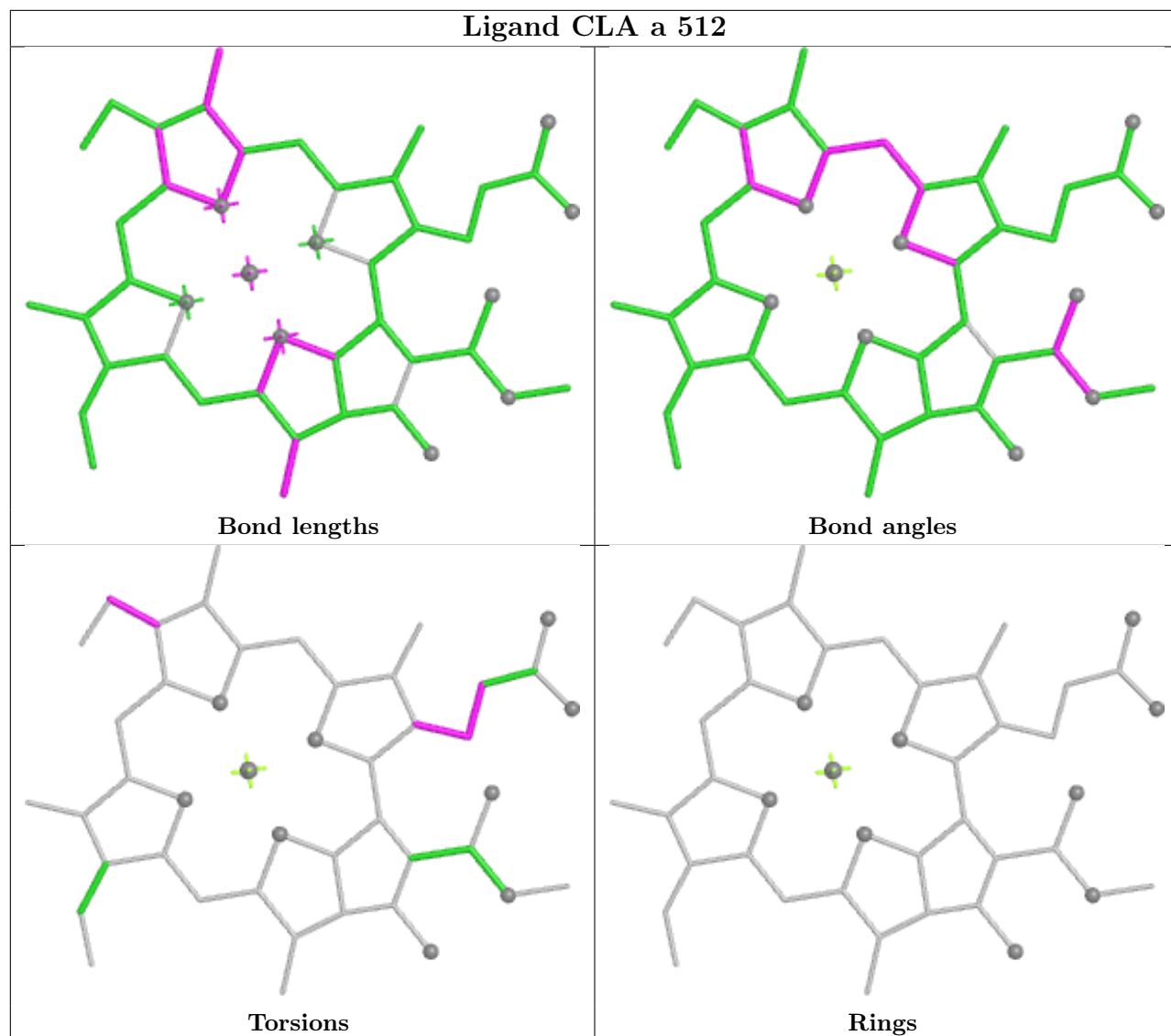


Torsions

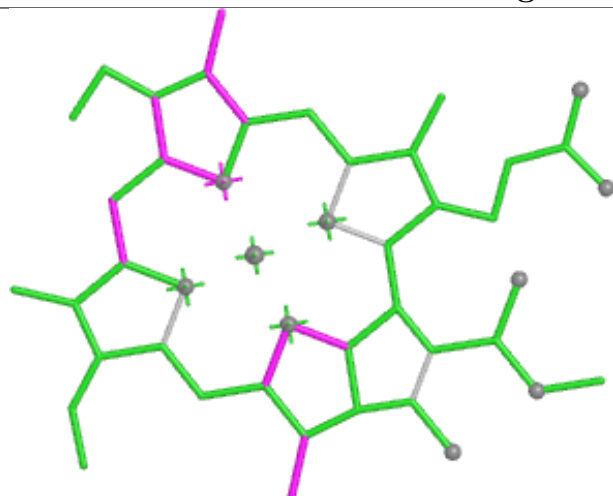


Rings

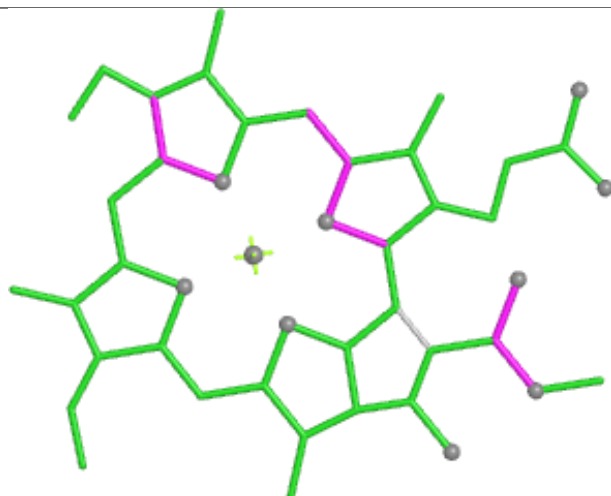
Ligand CLA a 512



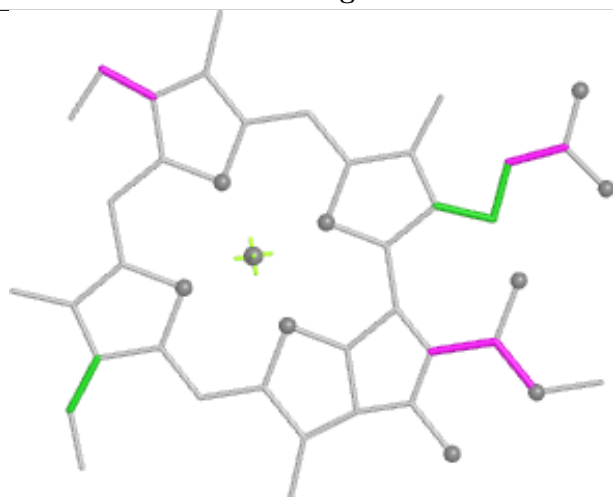
Ligand CLA b 510



Bond lengths



Bond angles

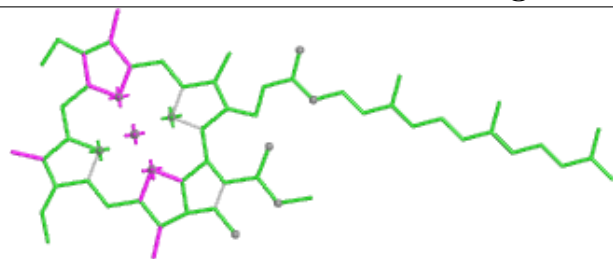


Torsions

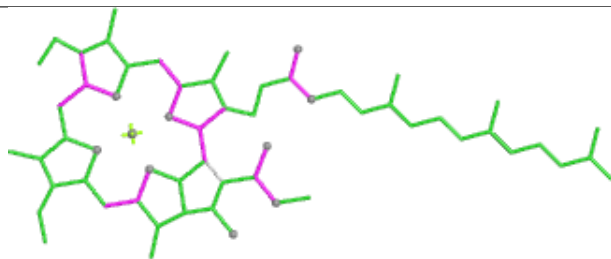


Rings

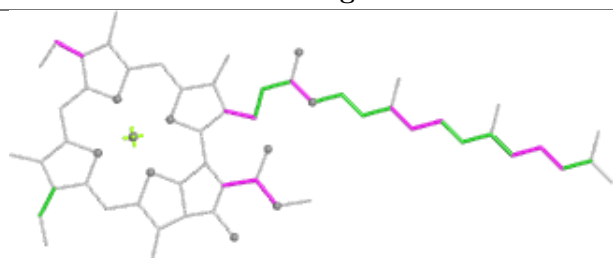
Ligand CLA e 1122



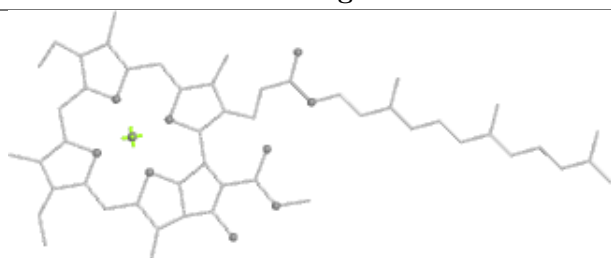
Bond lengths



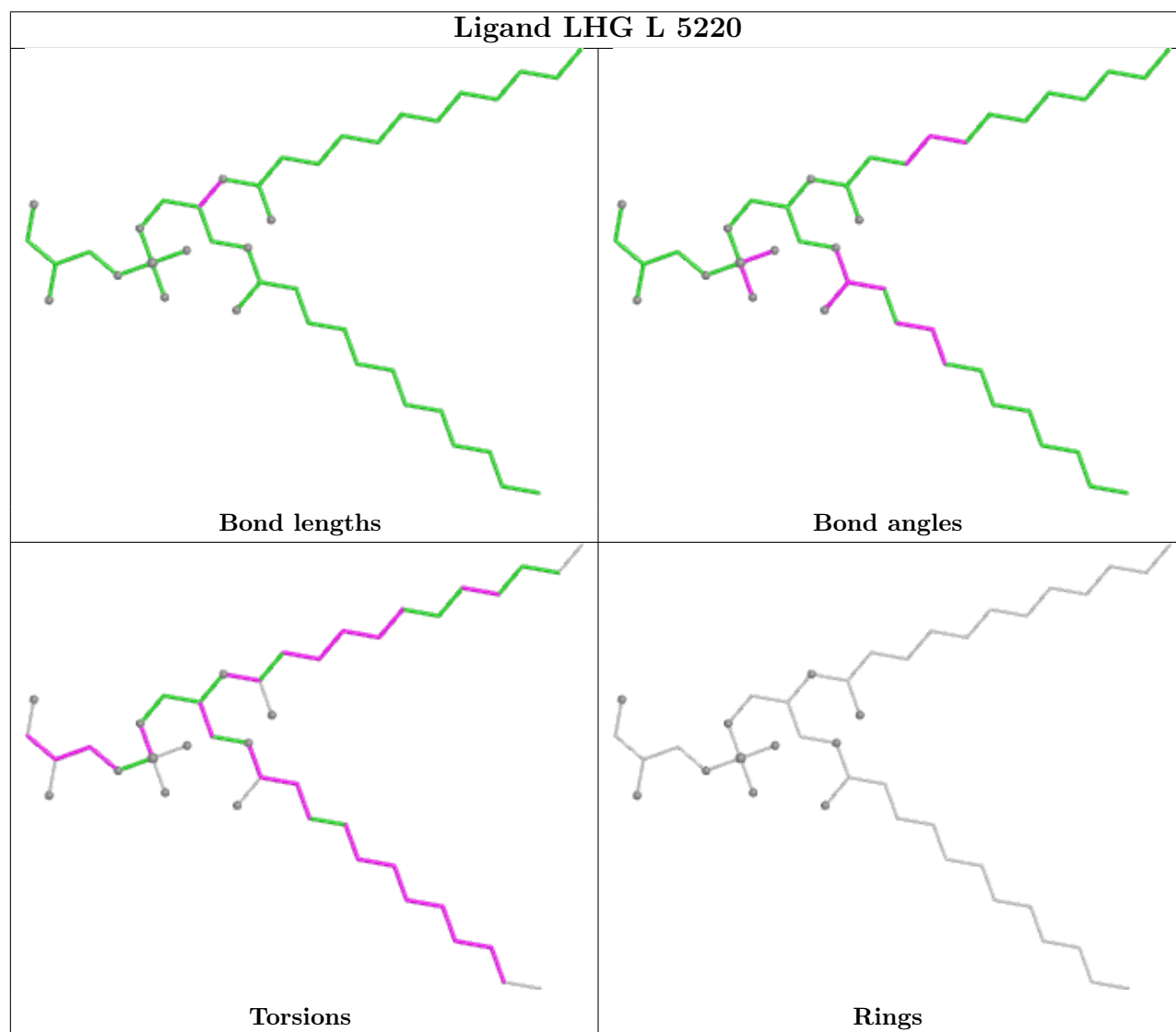
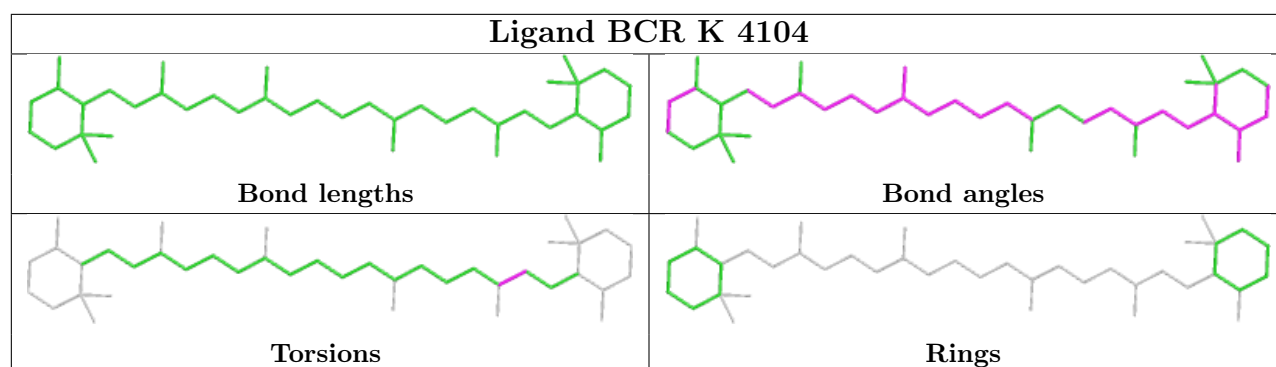
Bond angles

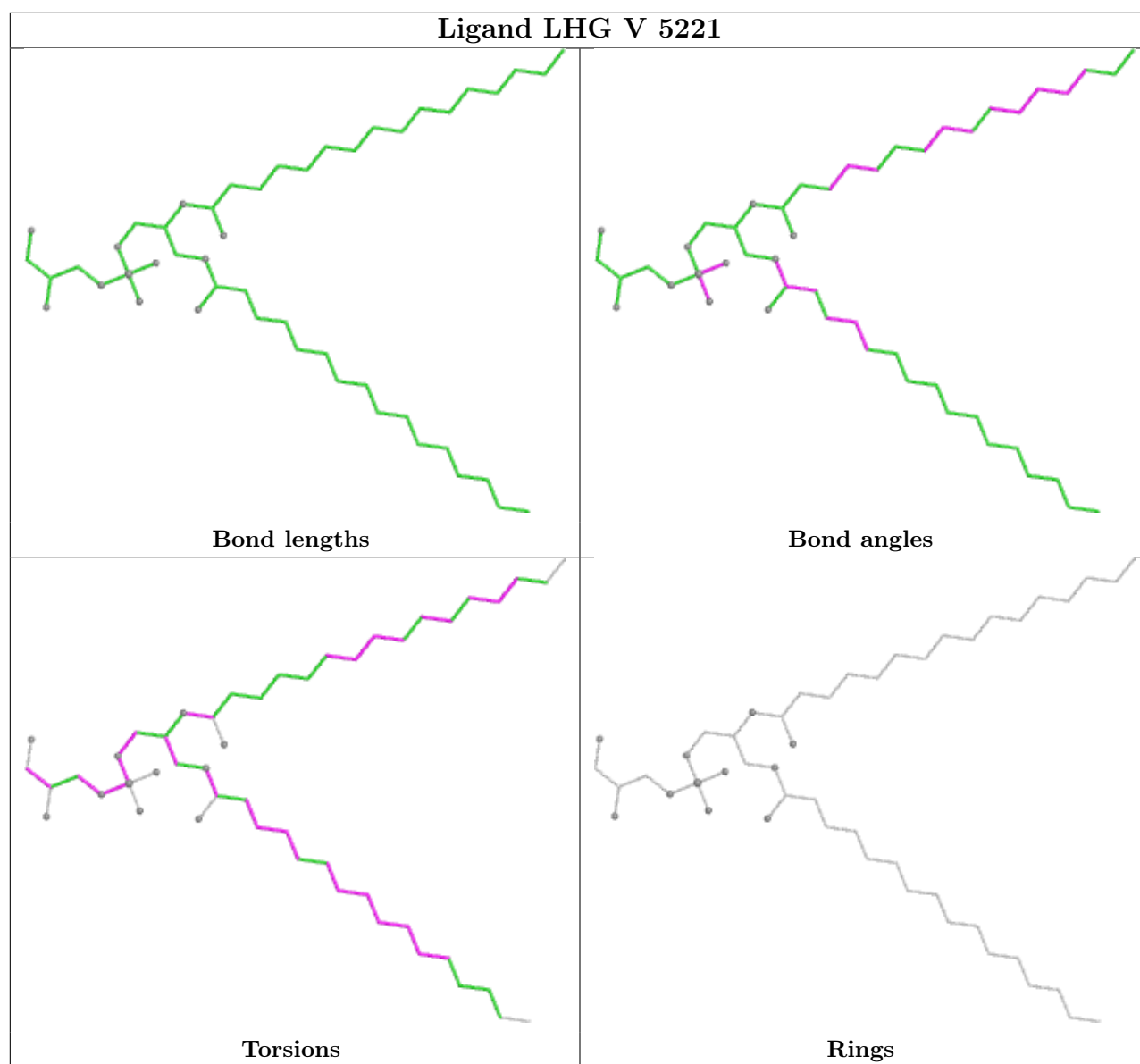


Torsions

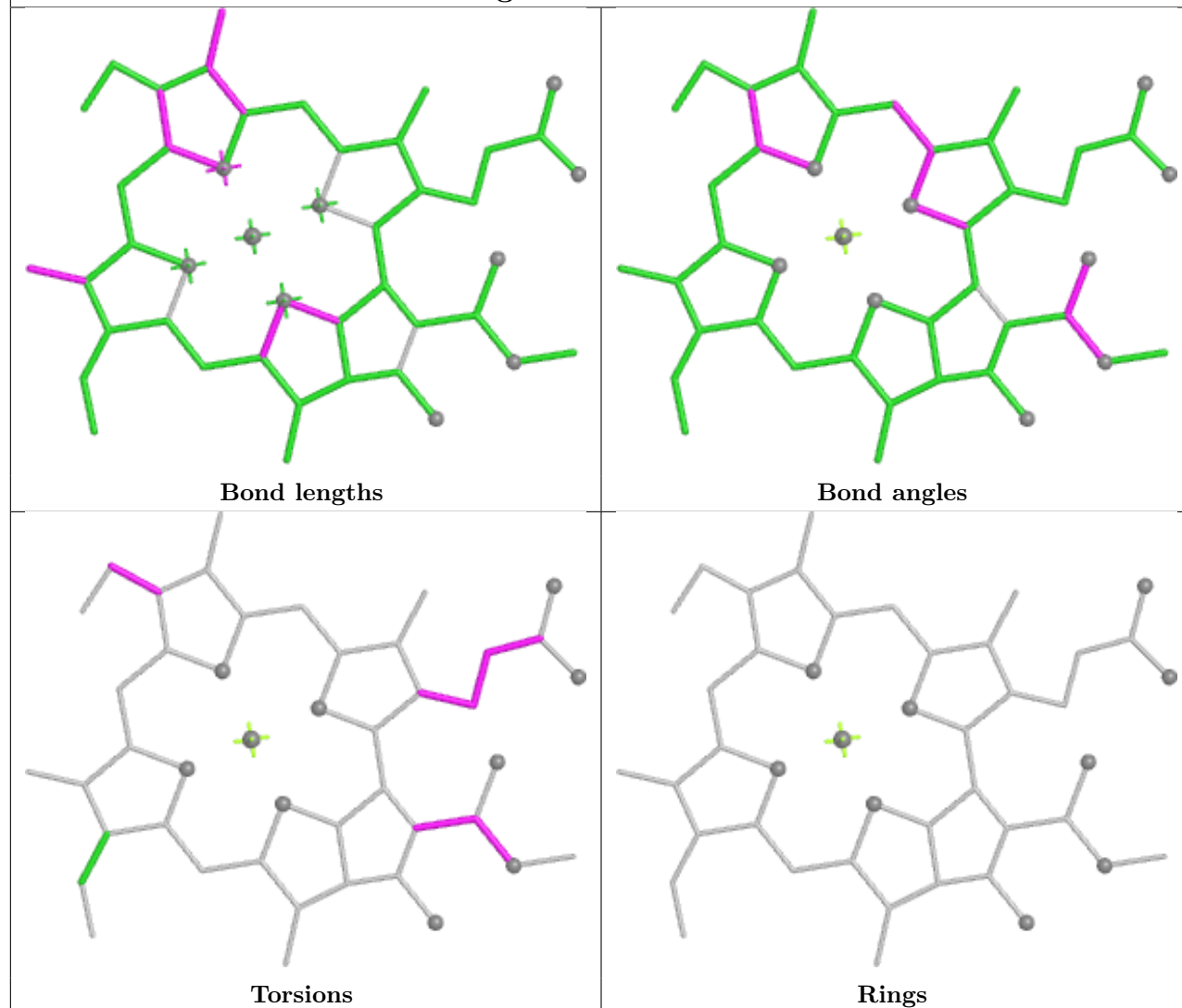


Rings

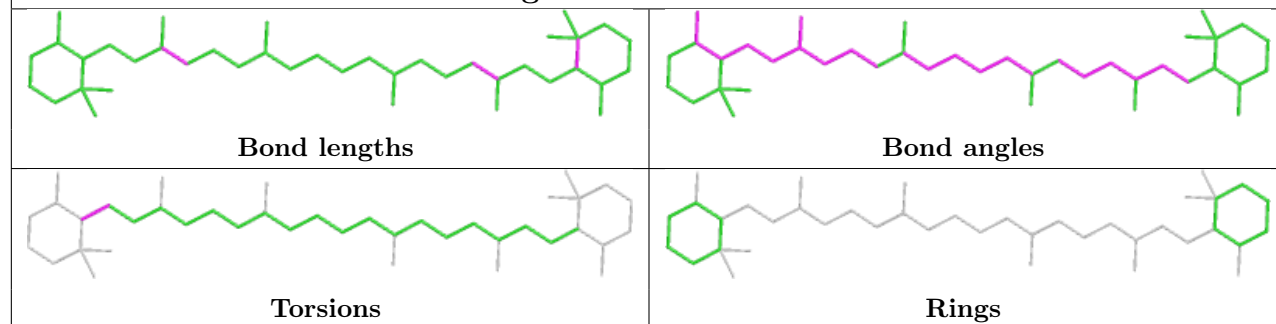


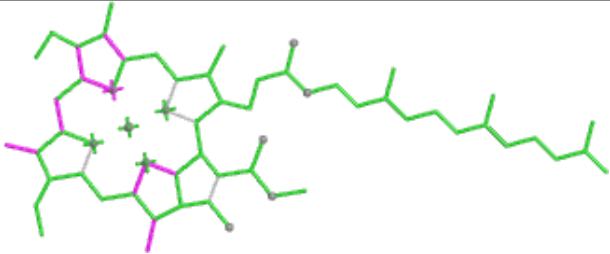
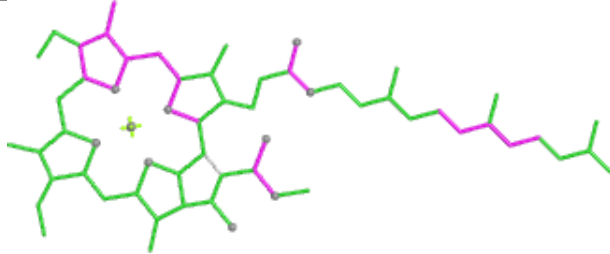
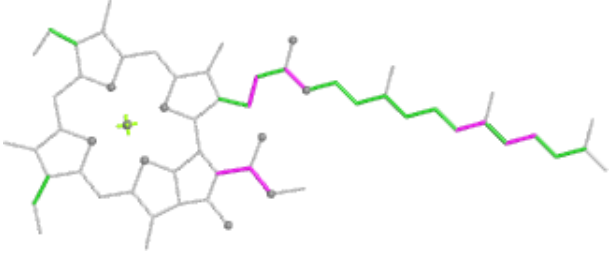
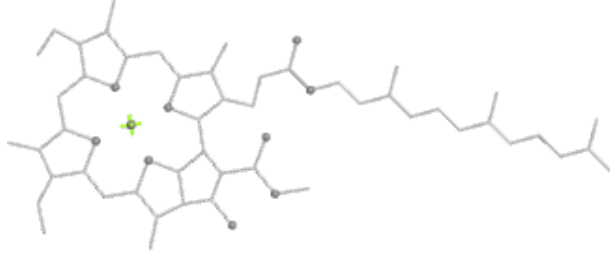
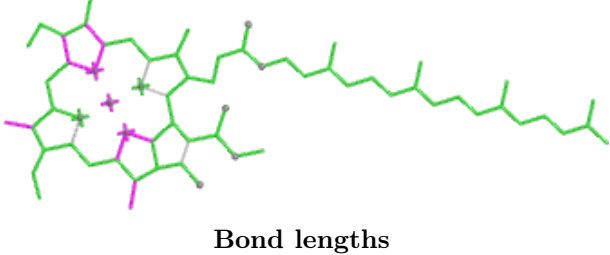
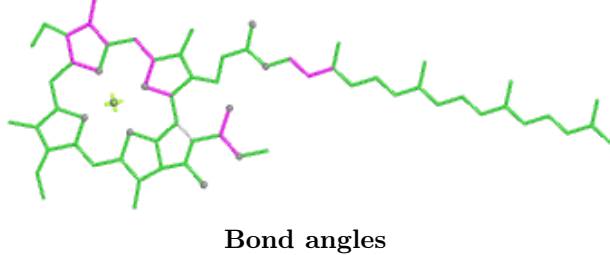
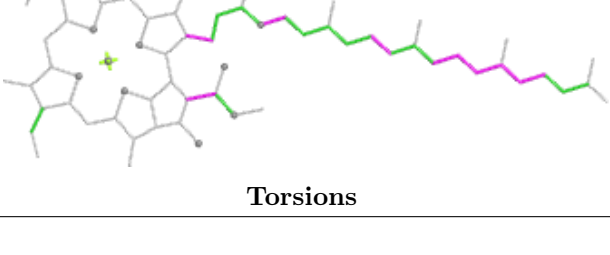
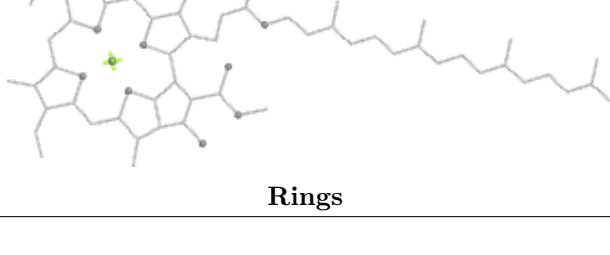


Ligand CLA 1 501

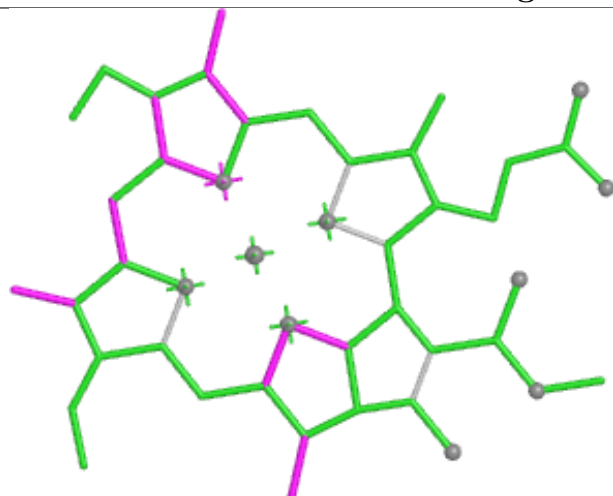


Ligand BCR B 4017

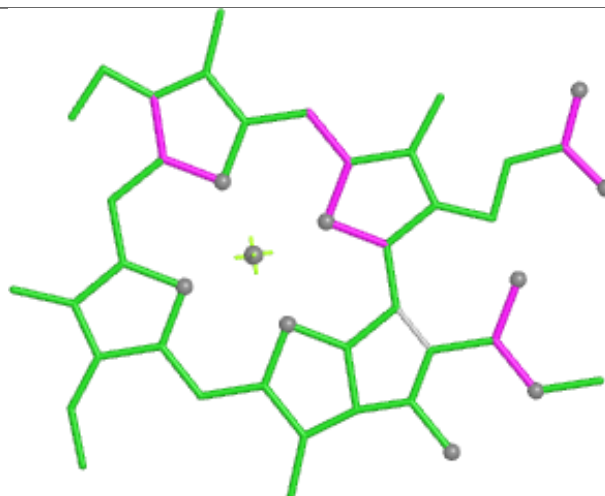


Ligand CLA B 1201	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA f 1223	
 Bond lengths	 Bond angles
 Torsions	 Rings

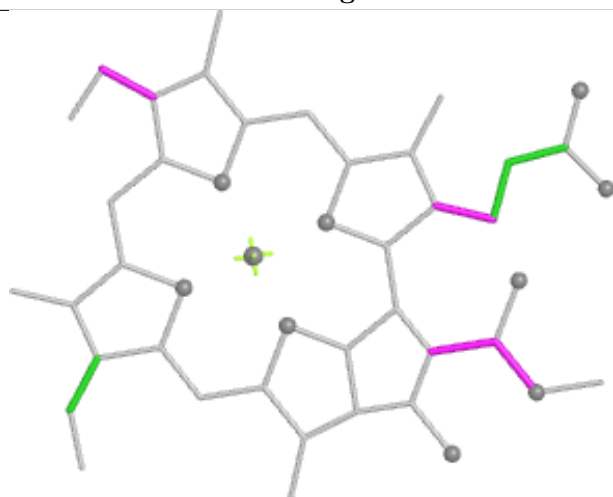
Ligand CLA u 506



Bond lengths



Bond angles

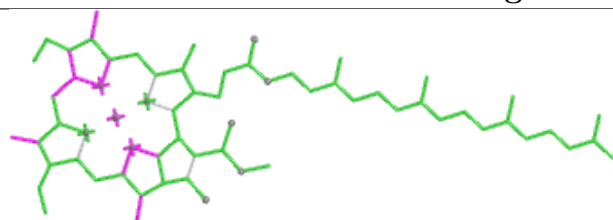


Torsions

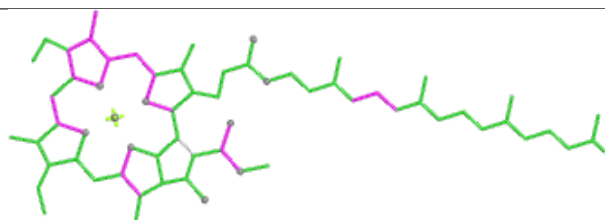


Rings

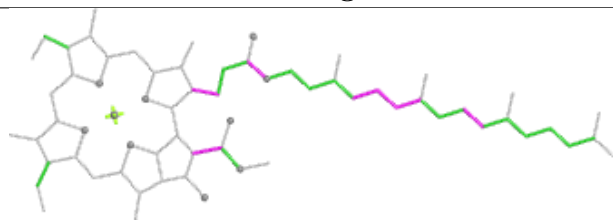
Ligand CLA A 1128



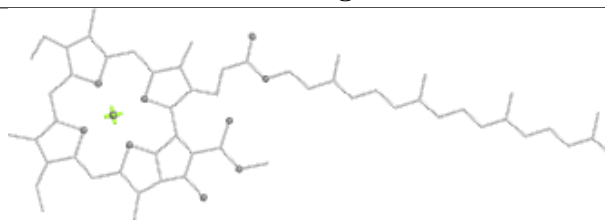
Bond lengths



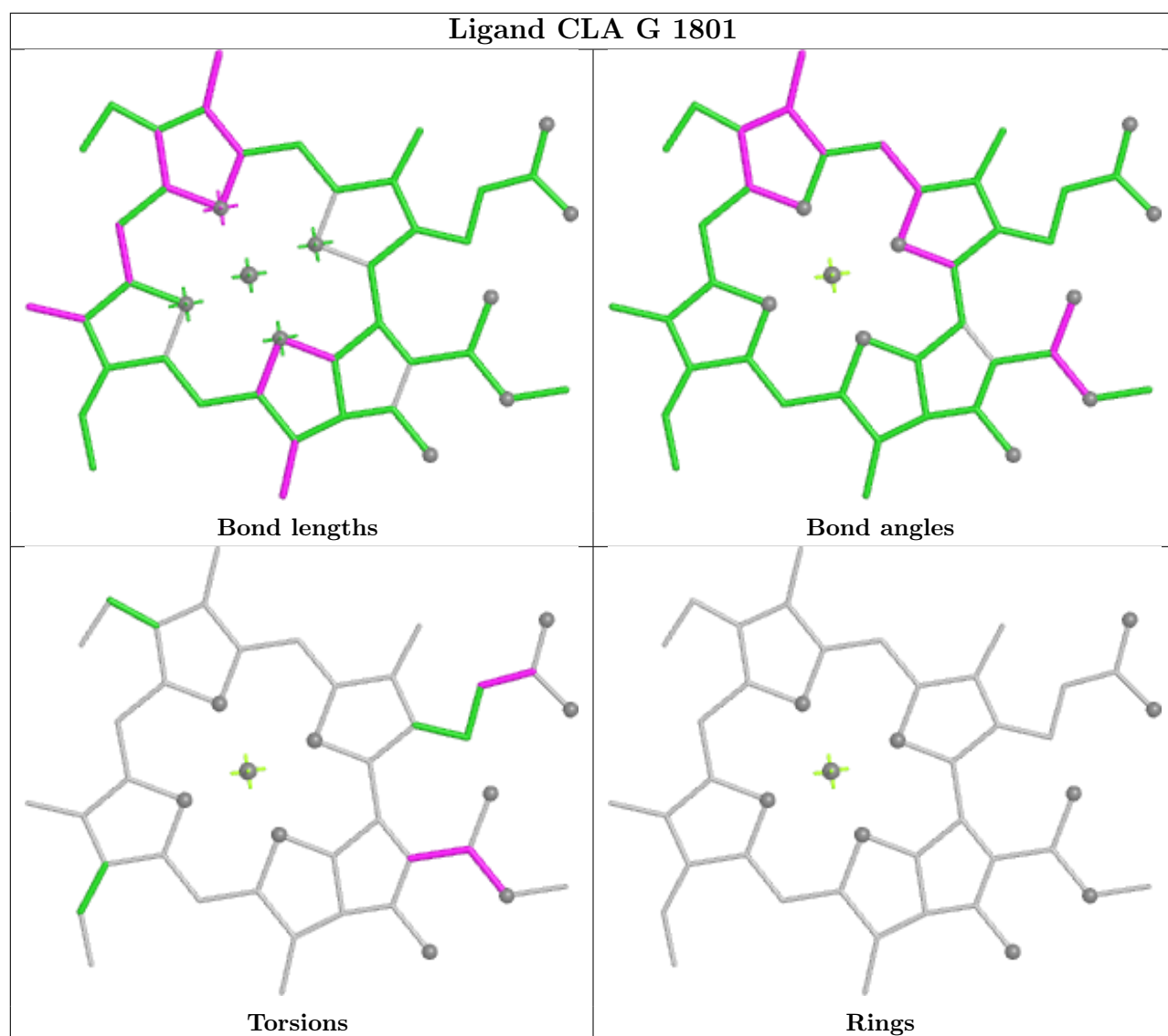
Bond angles

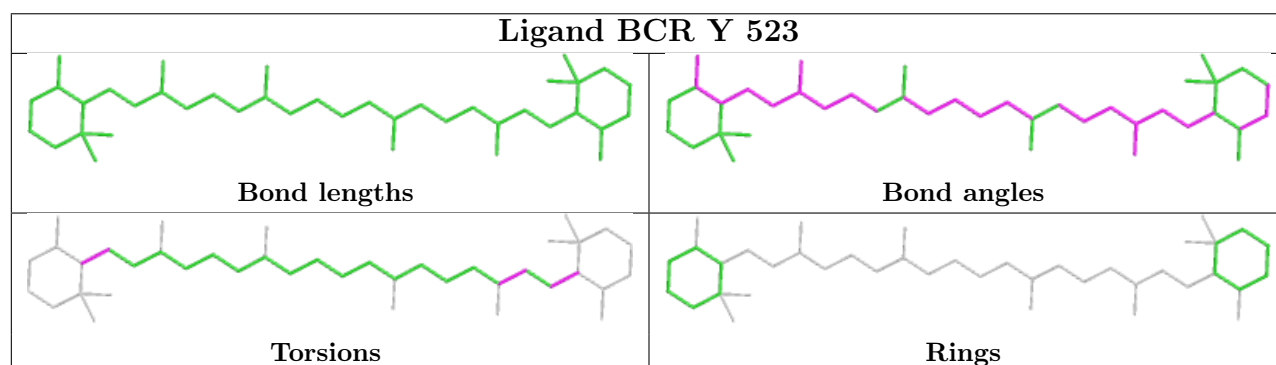
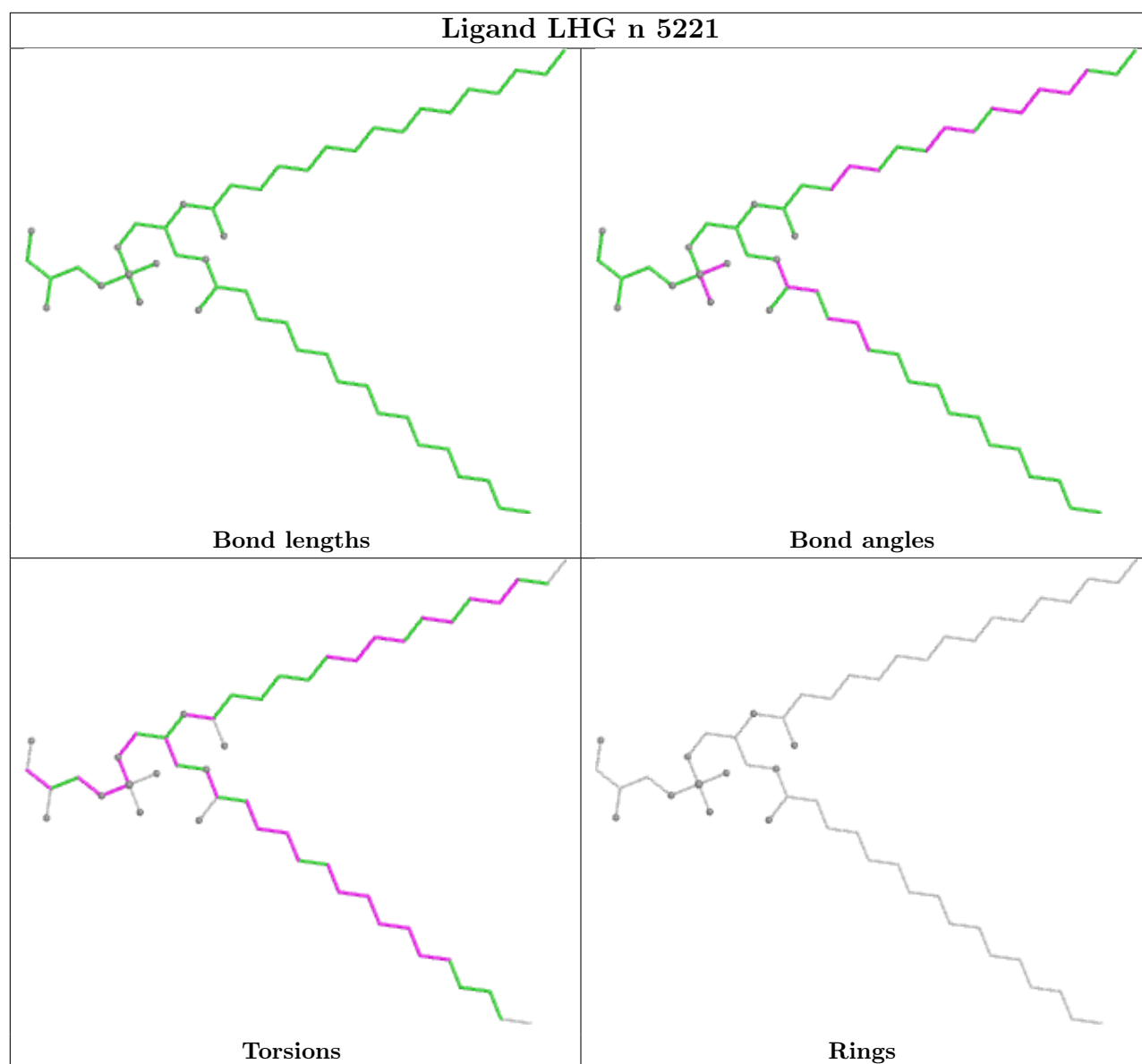


Torsions

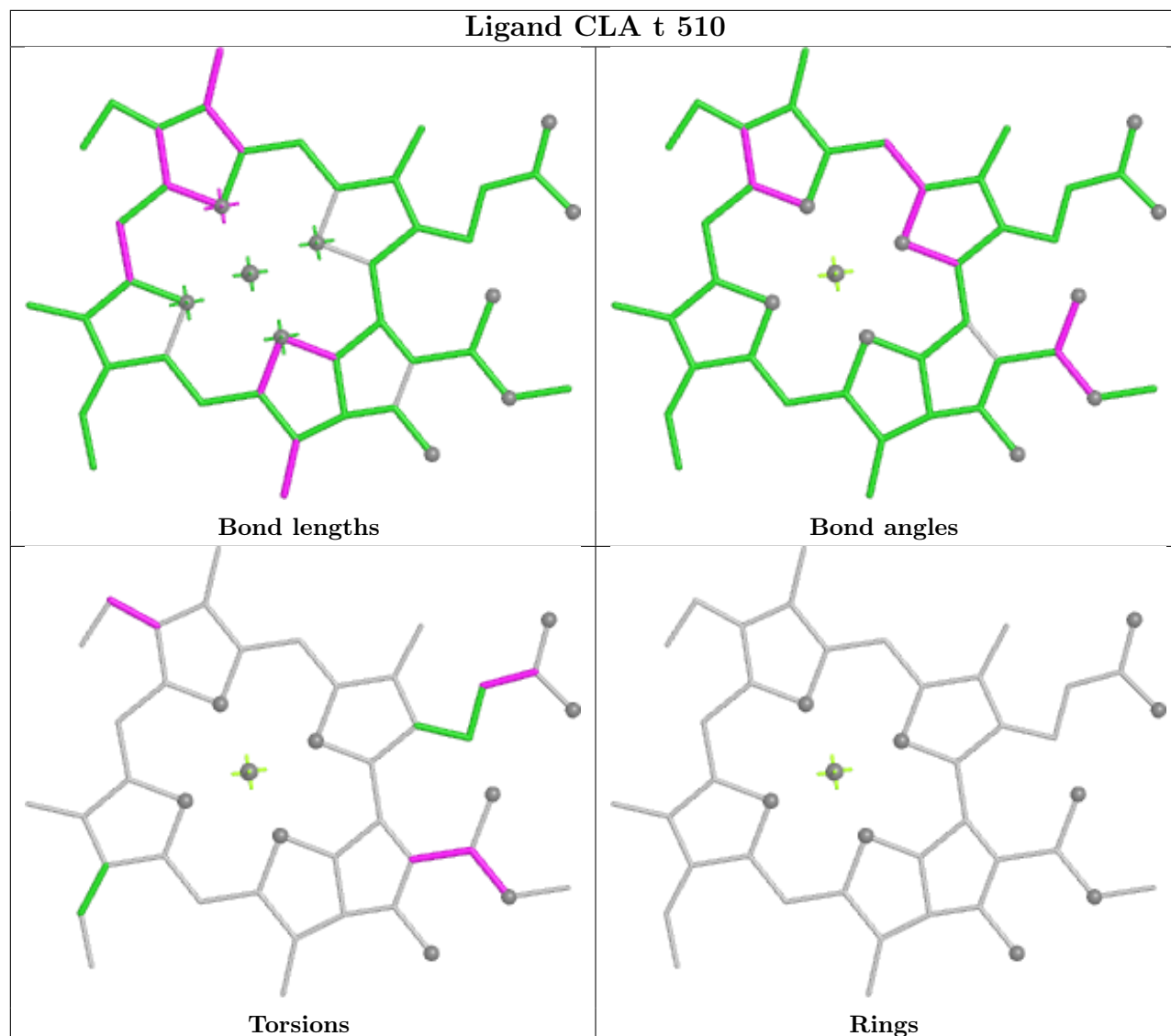


Rings

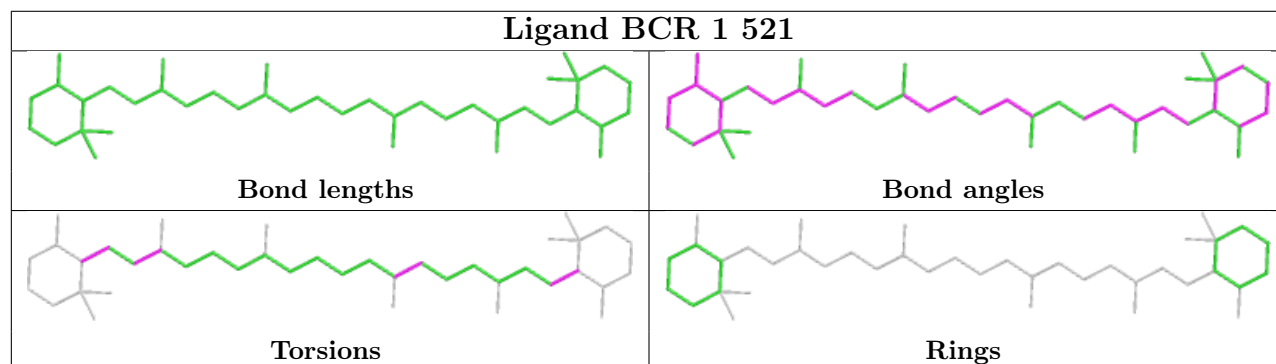


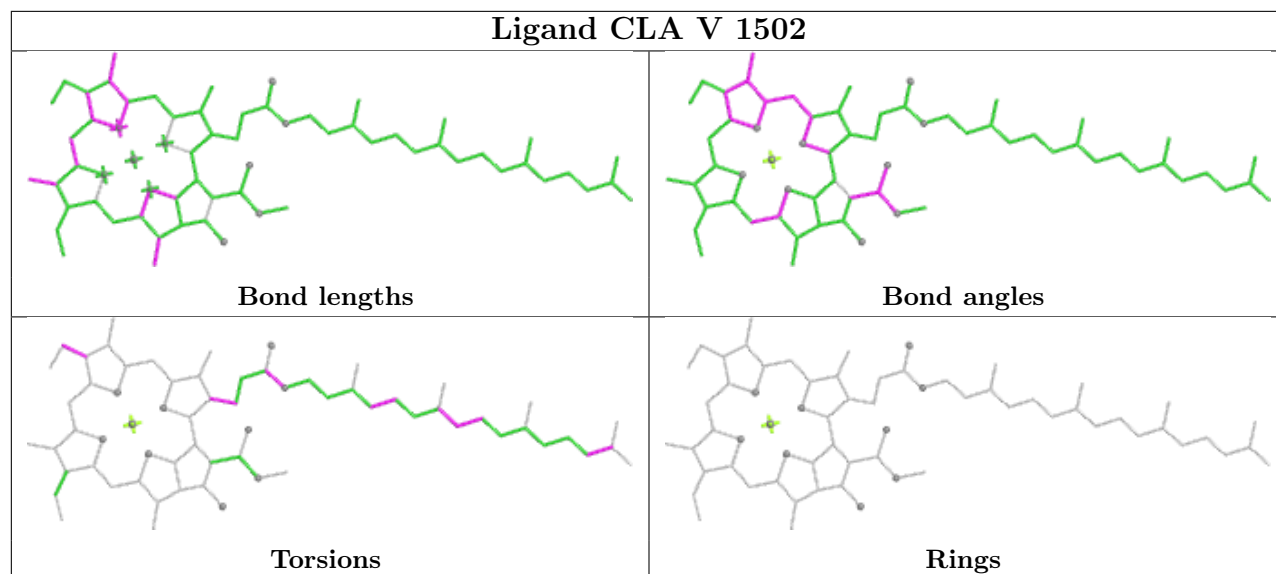
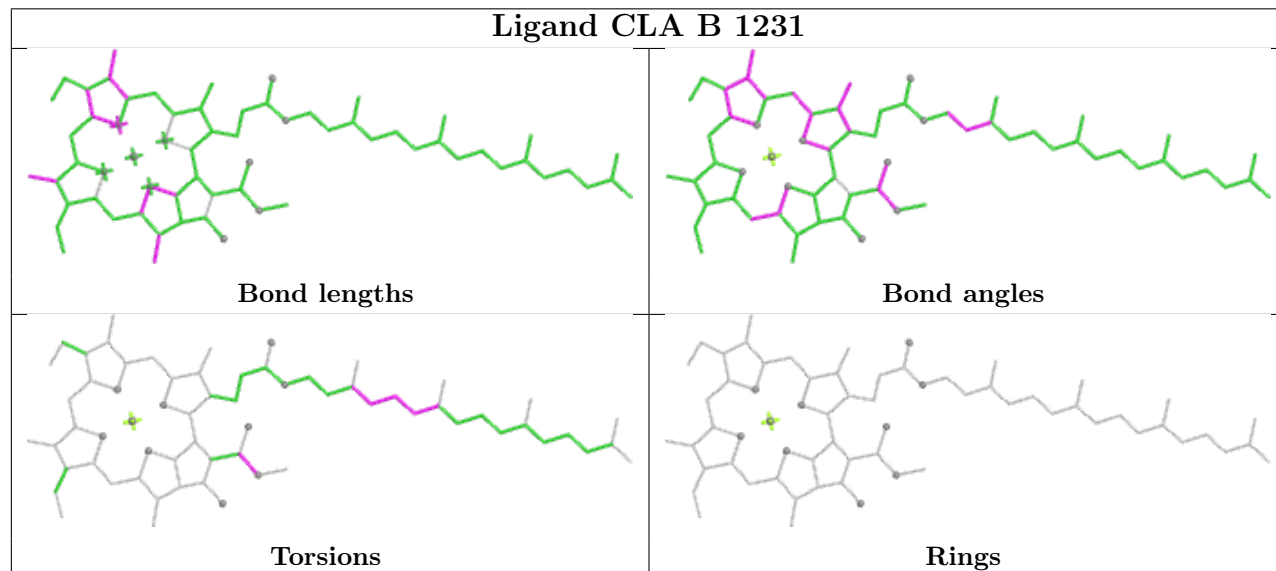


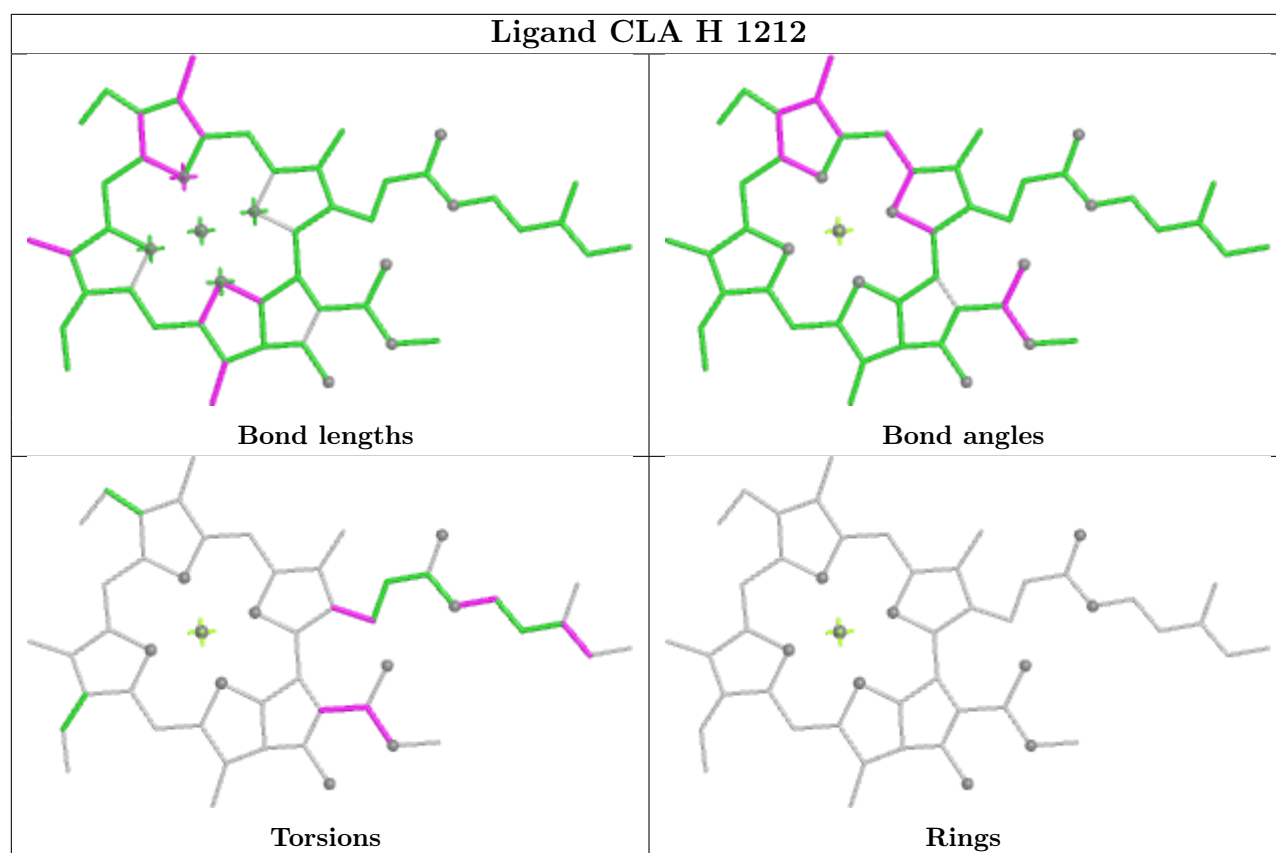
Ligand CLA t 510



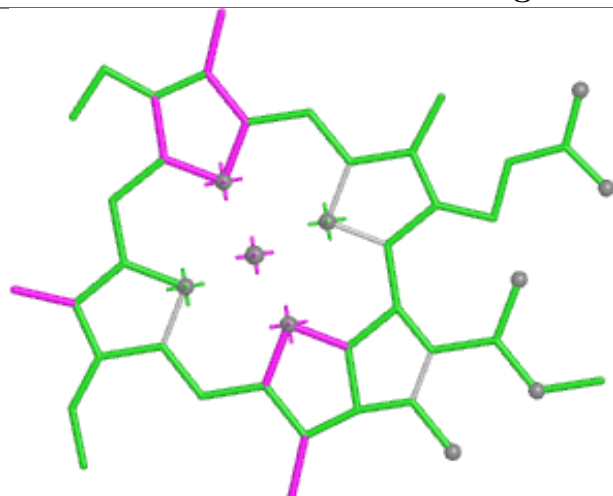
Ligand BCR 1 521



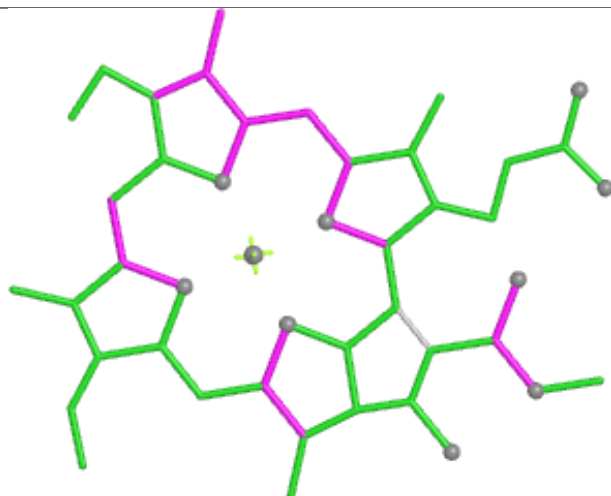
Ligand CLA V 1502**Ligand CLA B 1231**



Ligand CLA Y 508



Bond lengths



Bond angles

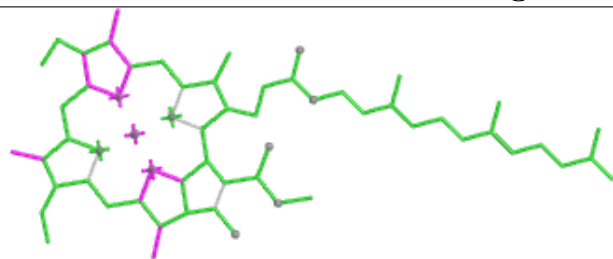


Torsions

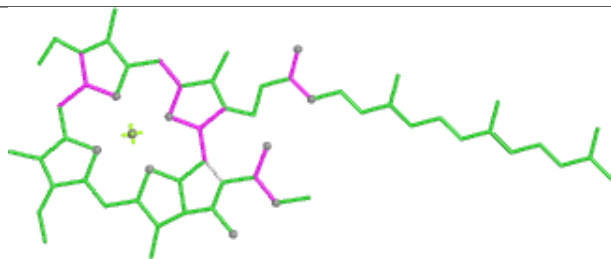


Rings

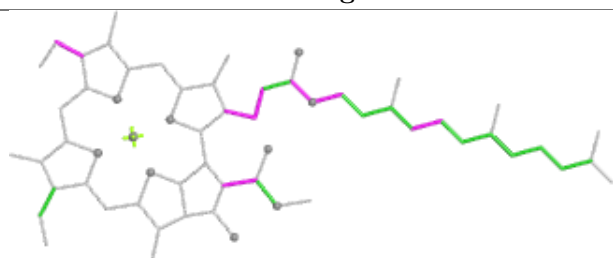
Ligand CLA e 1118



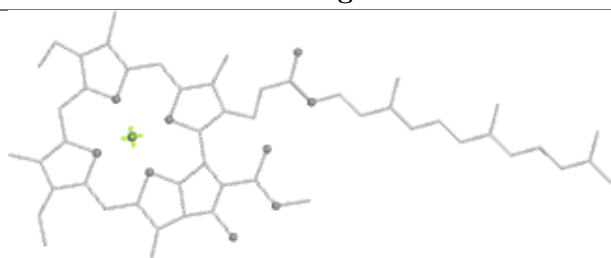
Bond lengths



Bond angles

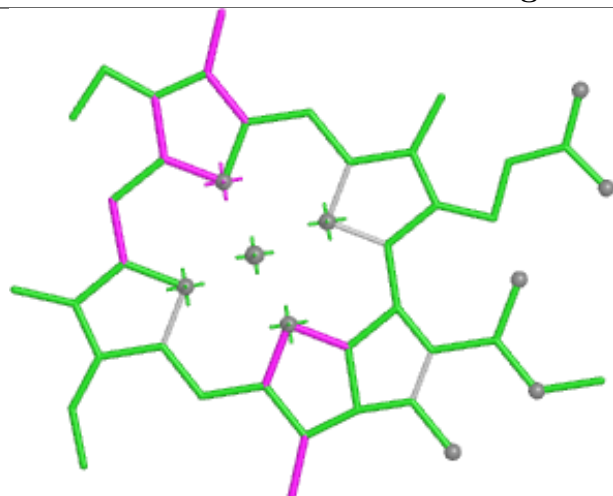


Torsions

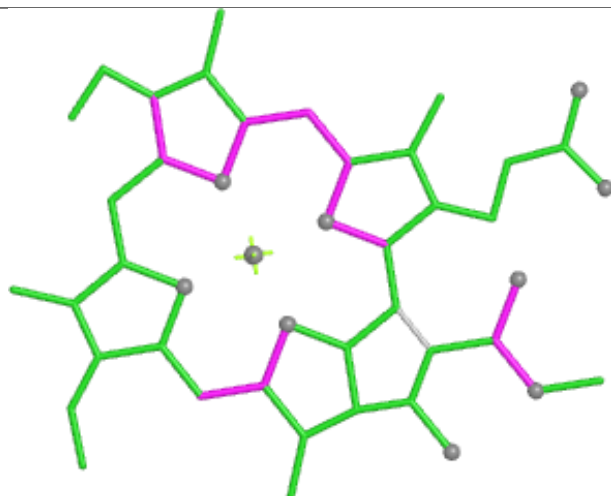


Rings

Ligand CLA t 501



Bond lengths



Bond angles

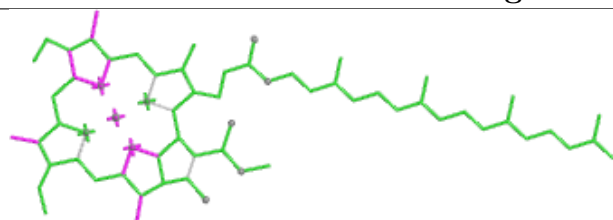


Torsions

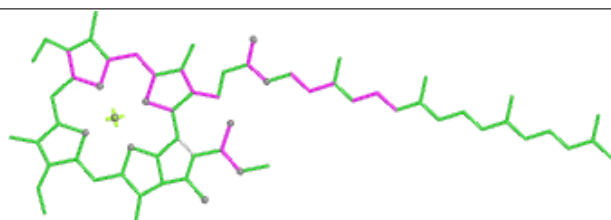


Rings

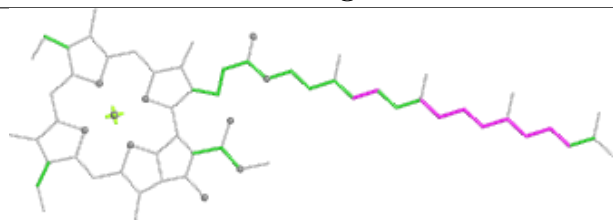
Ligand CLA A 1136



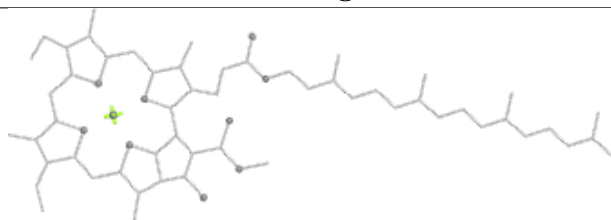
Bond lengths



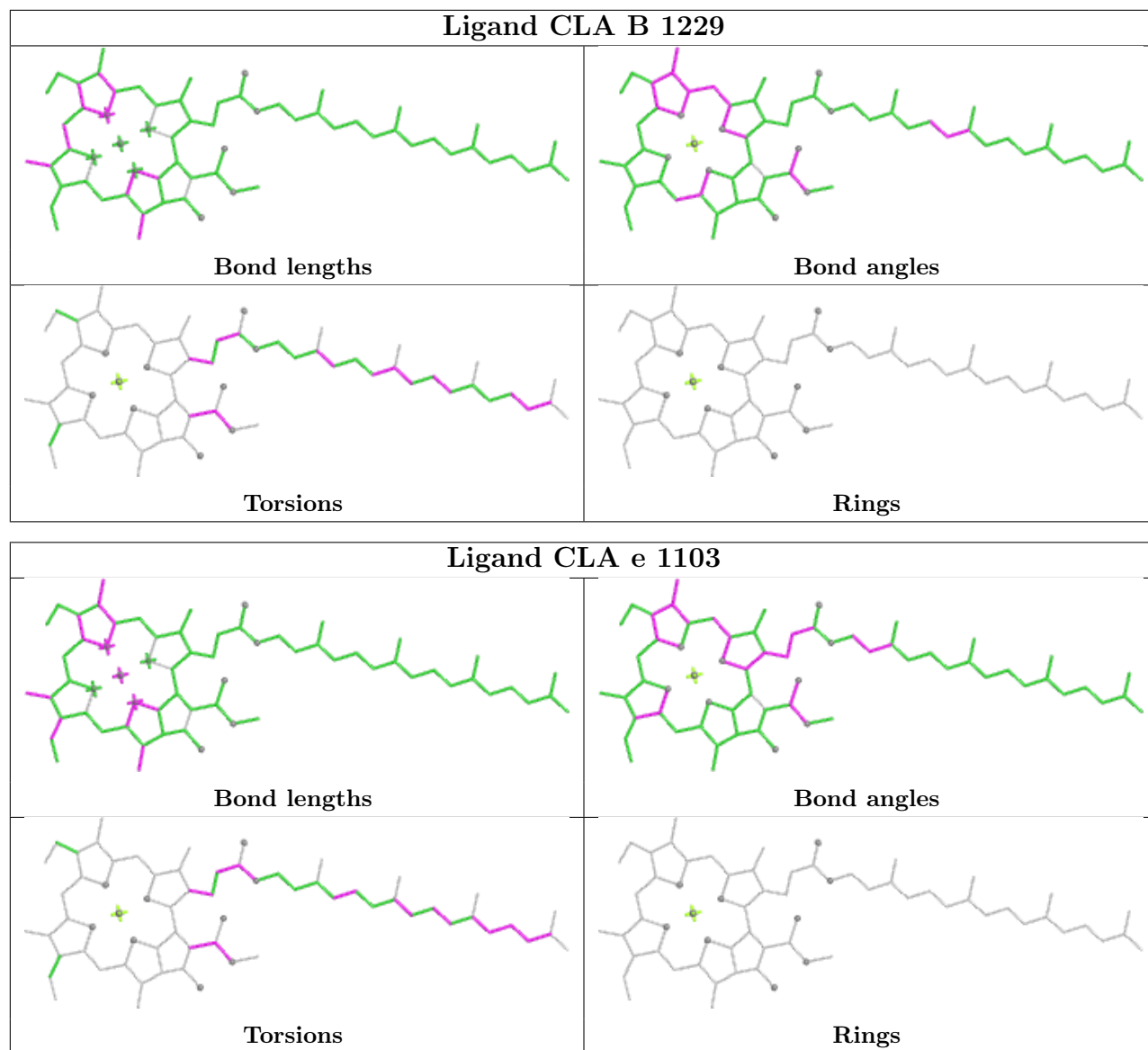
Bond angles



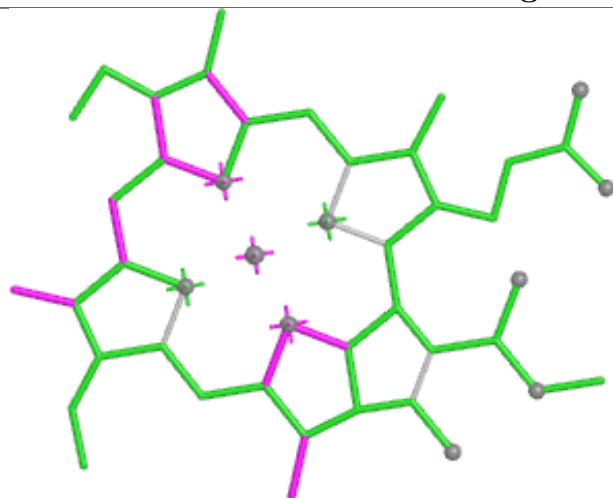
Torsions



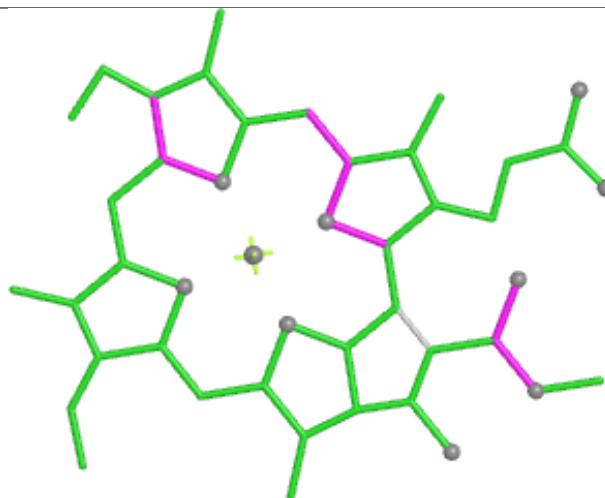
Rings



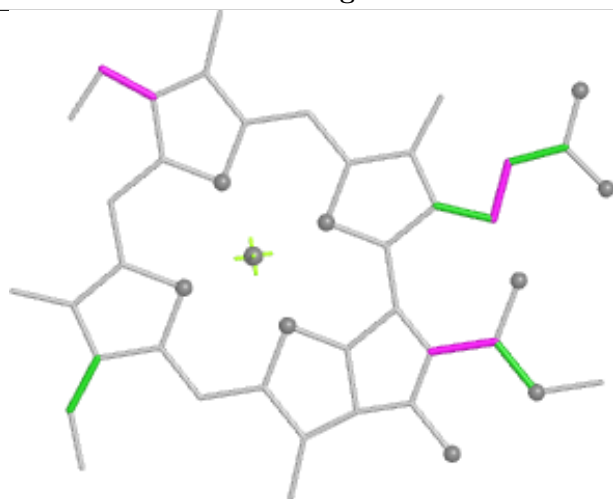
Ligand CLA t 505



Bond lengths



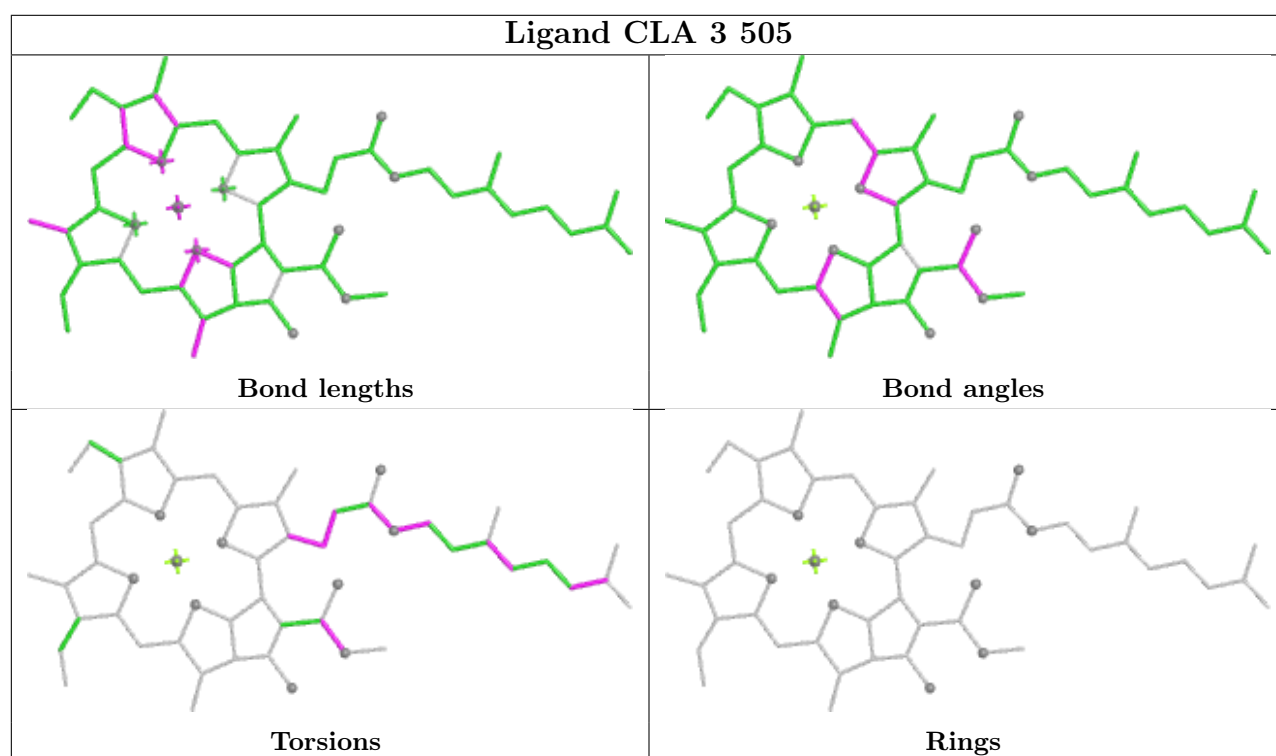
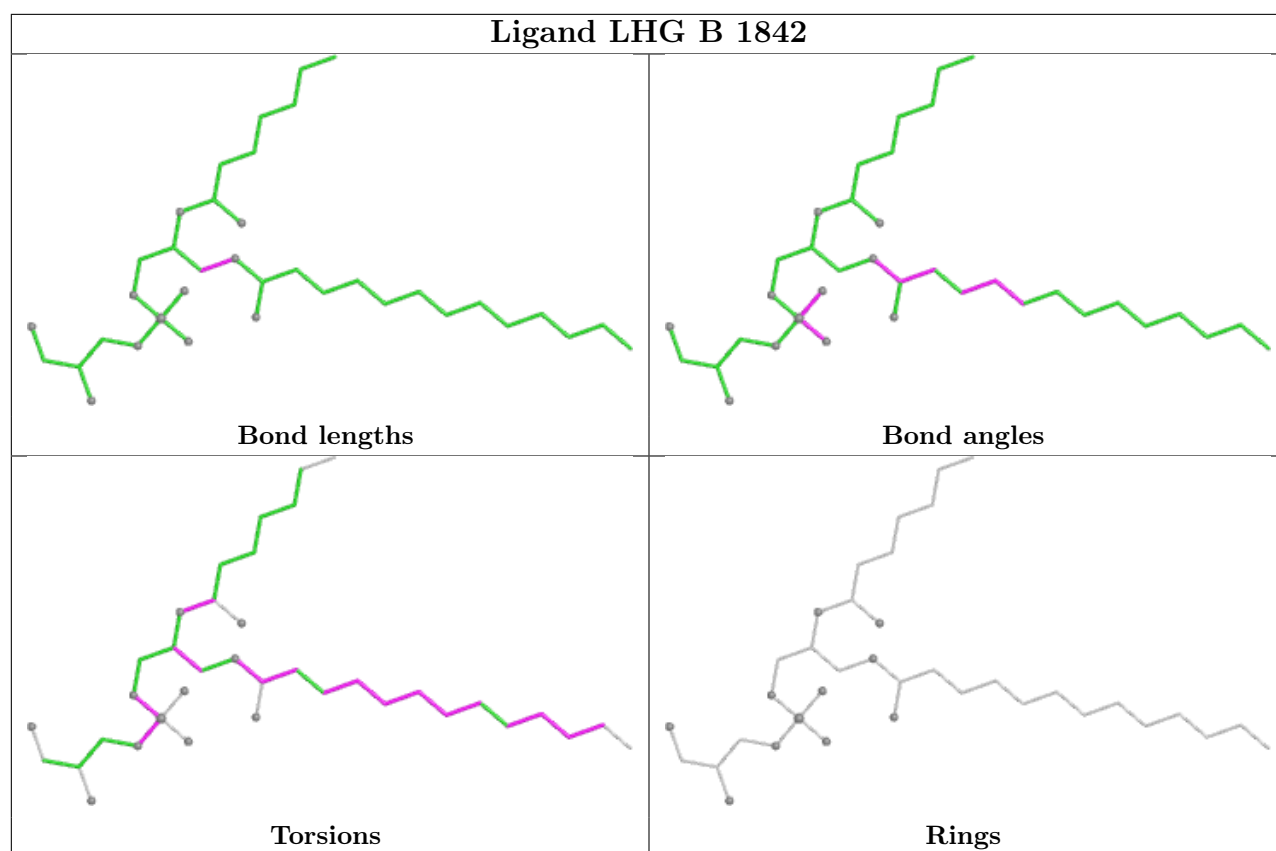
Bond angles

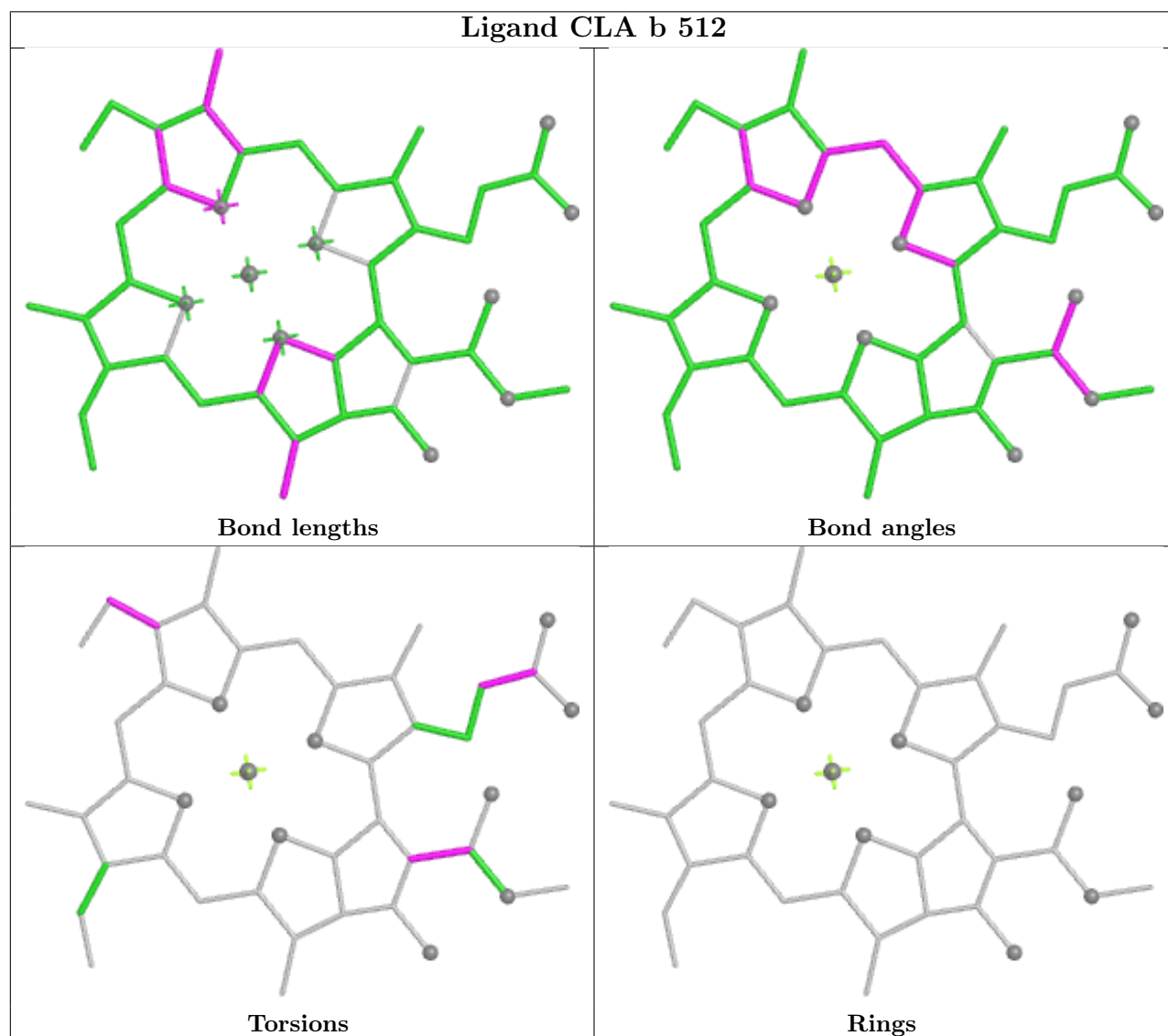
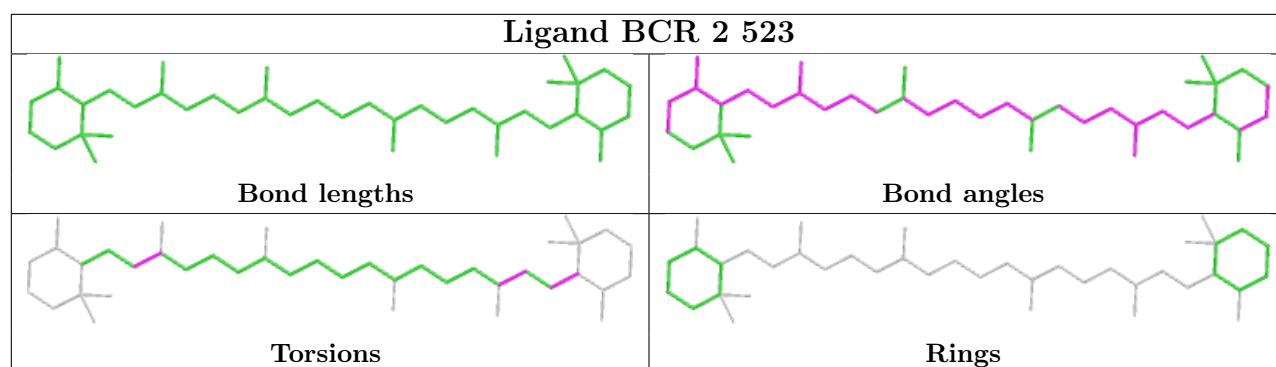


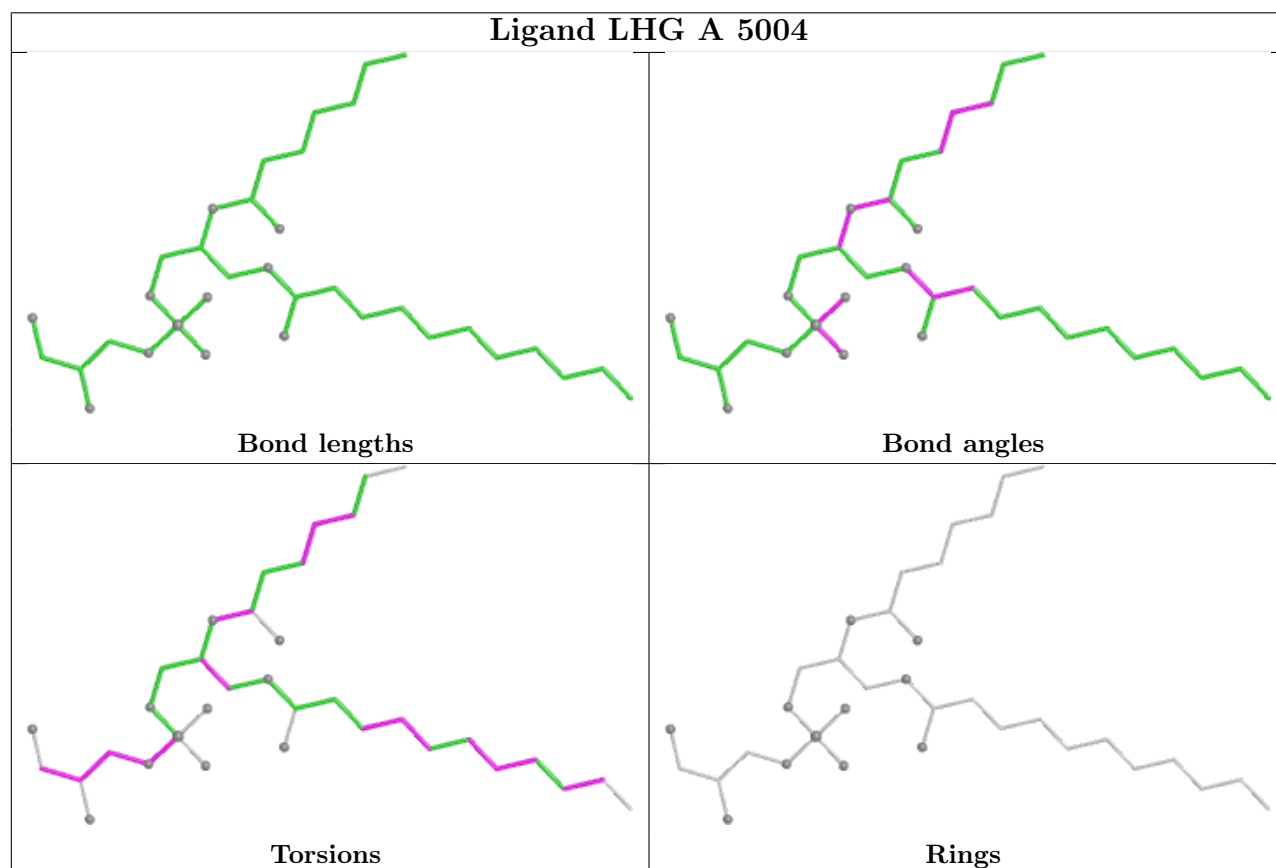
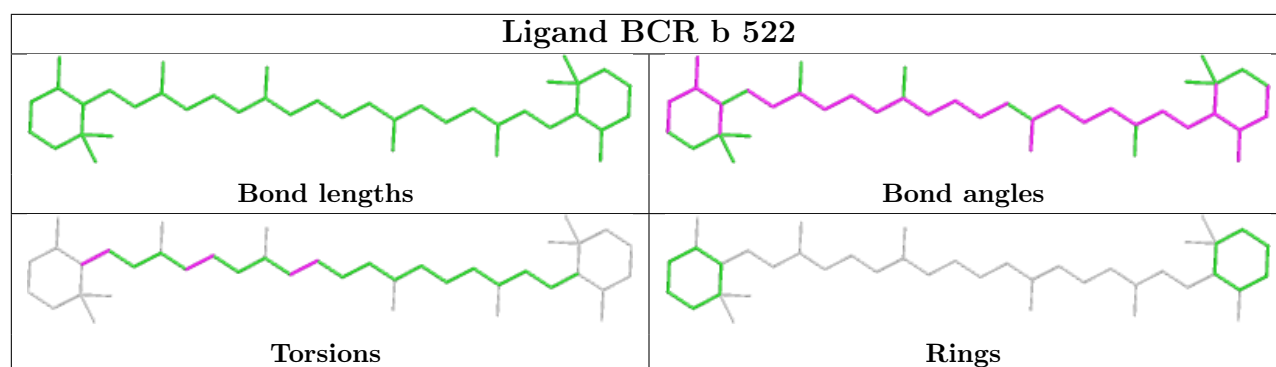
Torsions



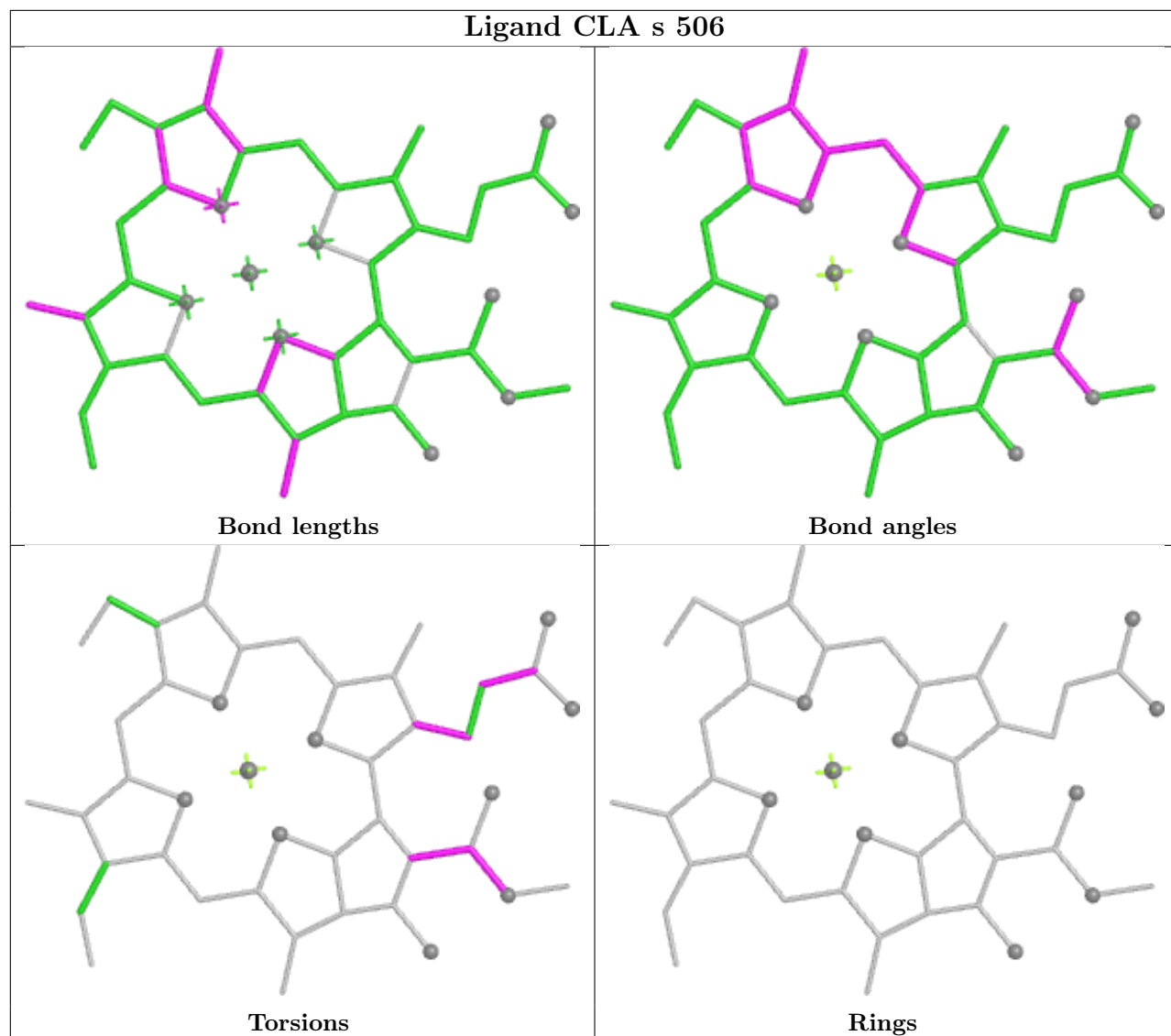
Rings

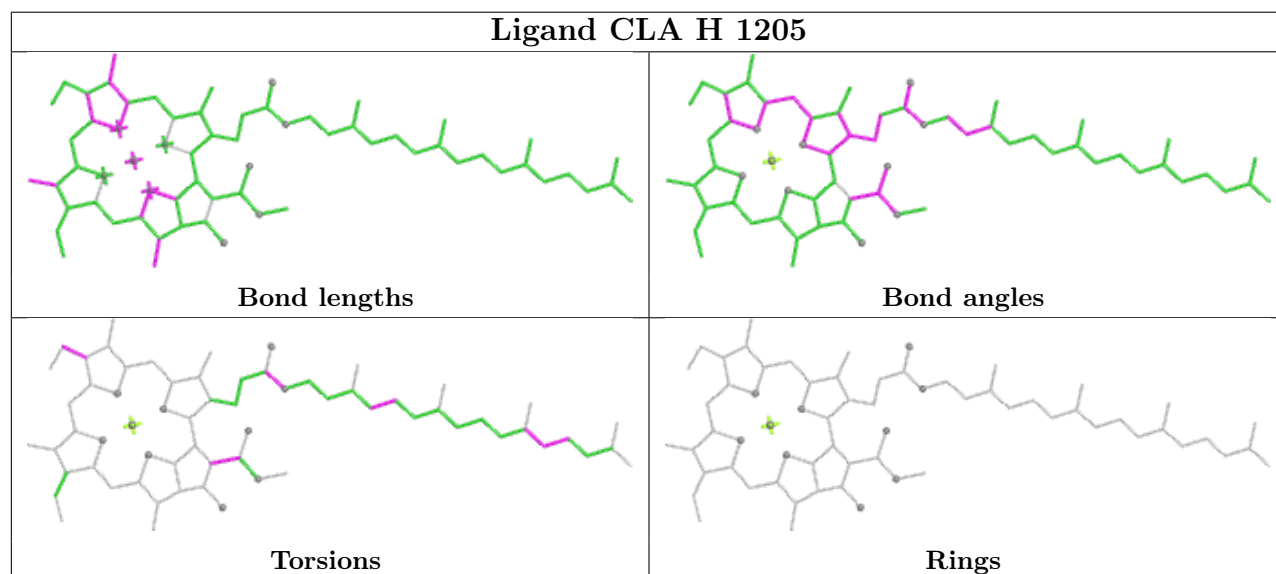
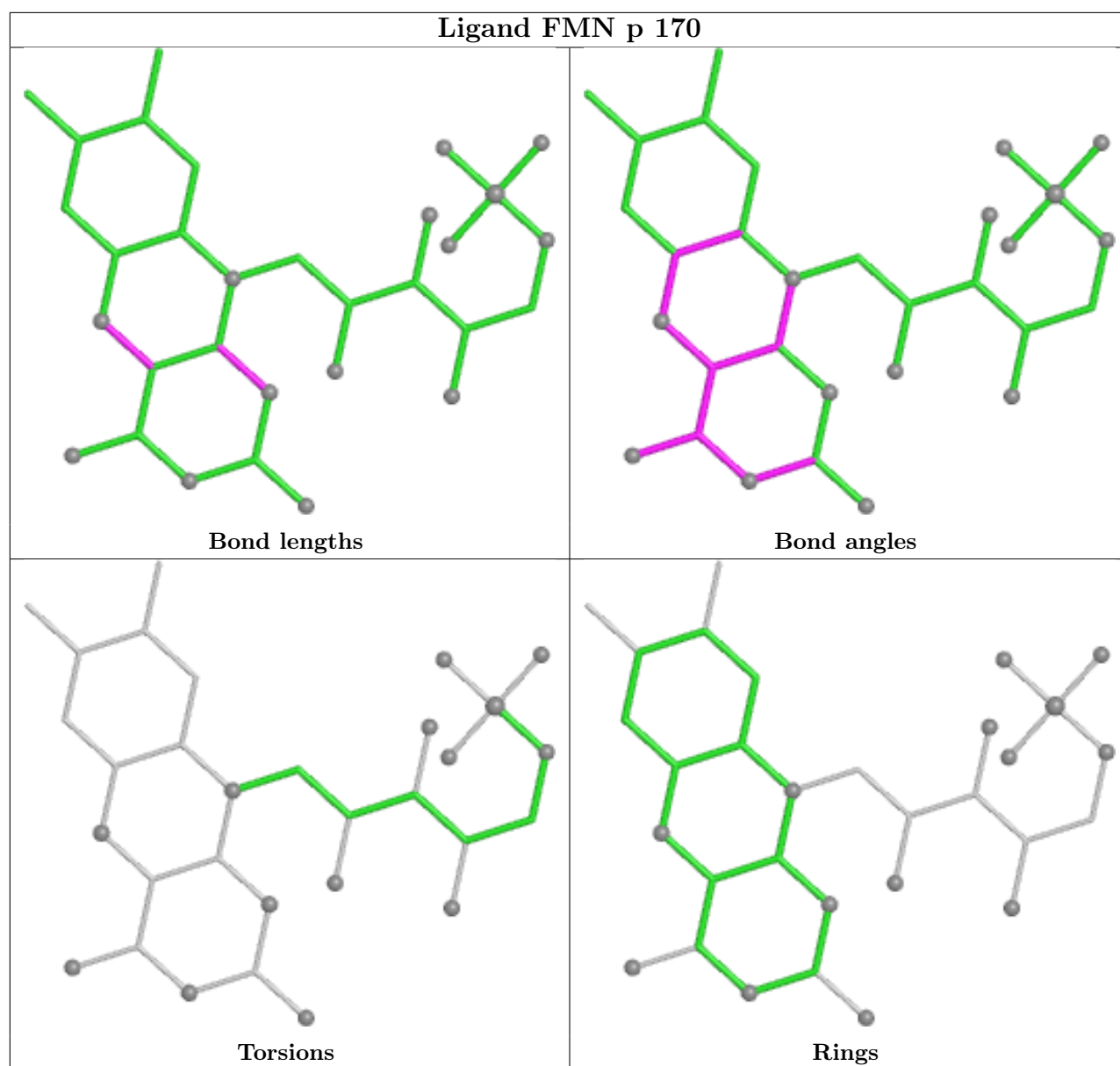




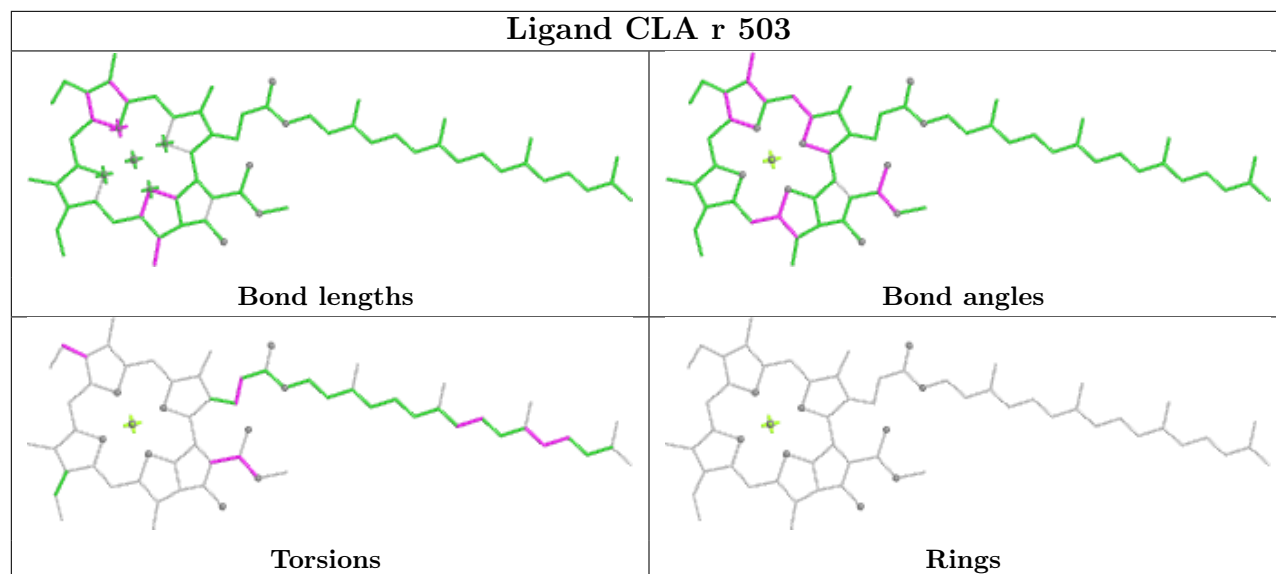


Ligand CLA s 506

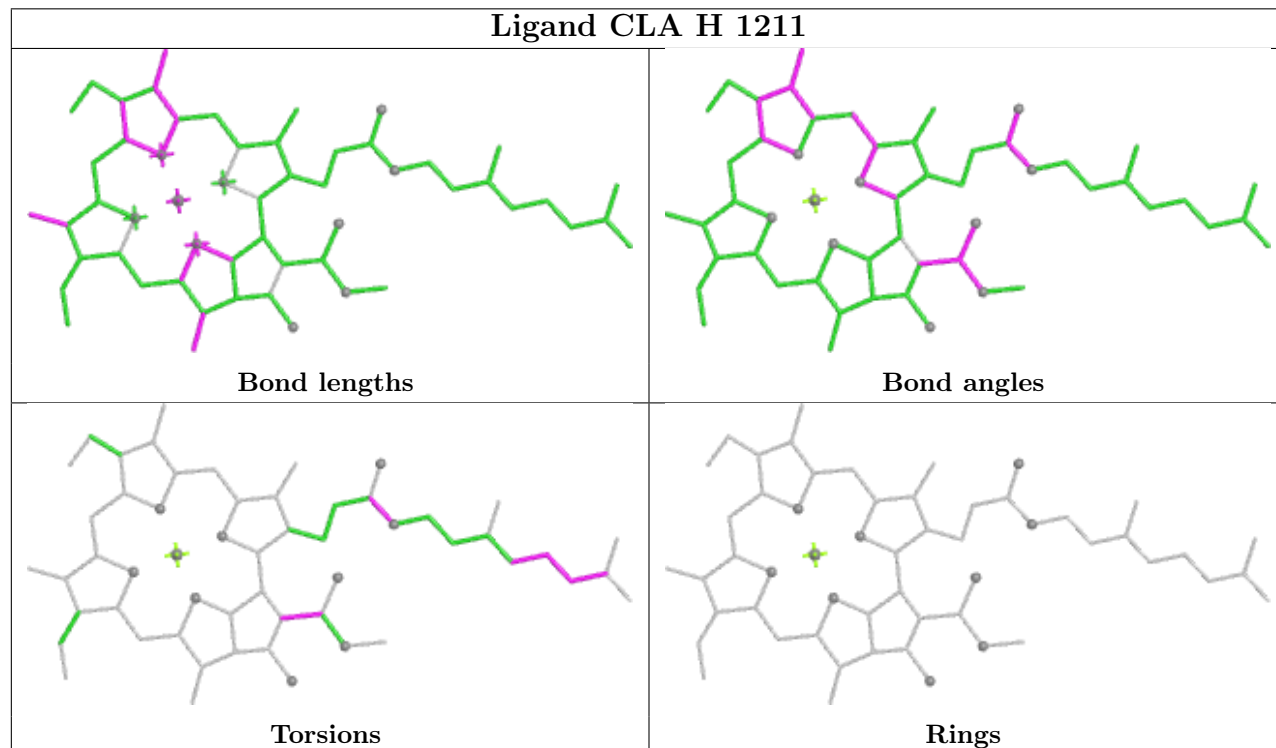




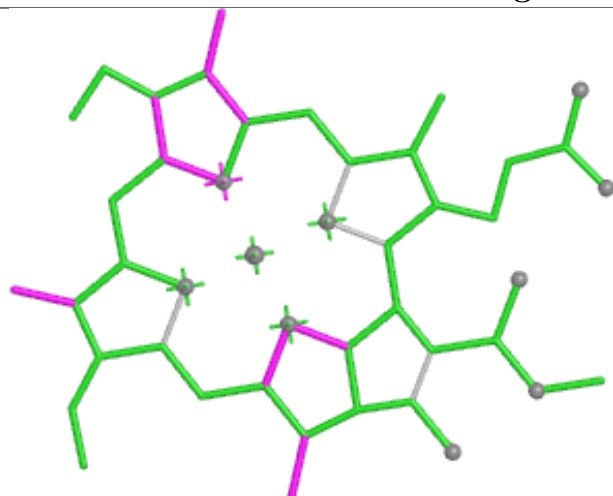
Ligand CLA r 503



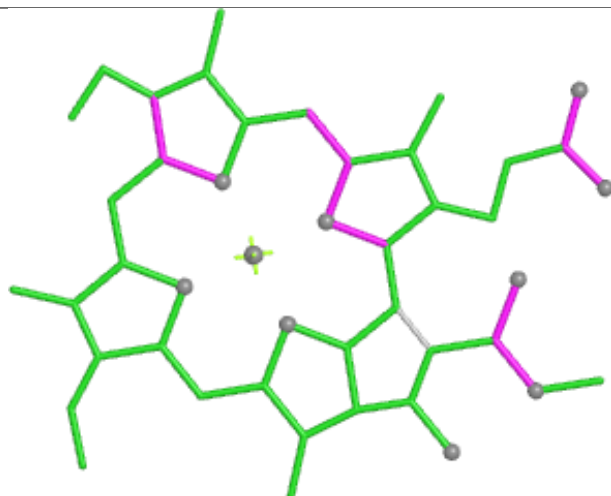
Ligand CLA H 1211



Ligand CLA Y 517



Bond lengths



Bond angles

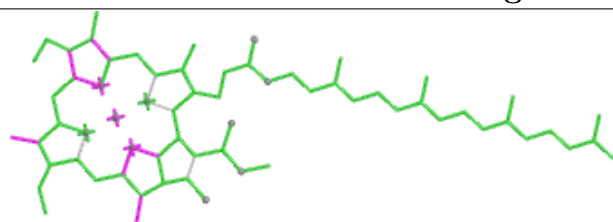


Torsions

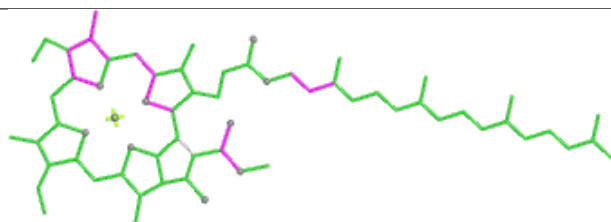


Rings

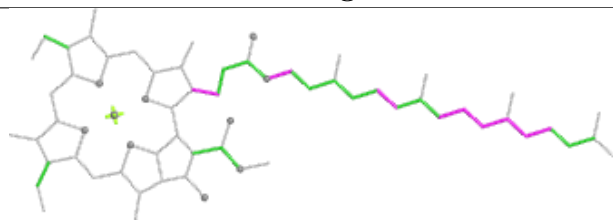
Ligand CLA H 1223



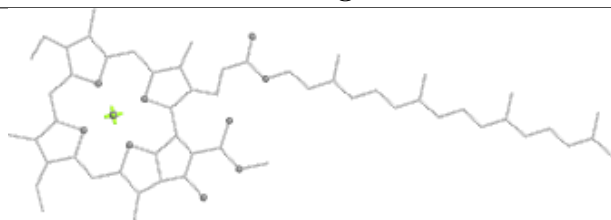
Bond lengths



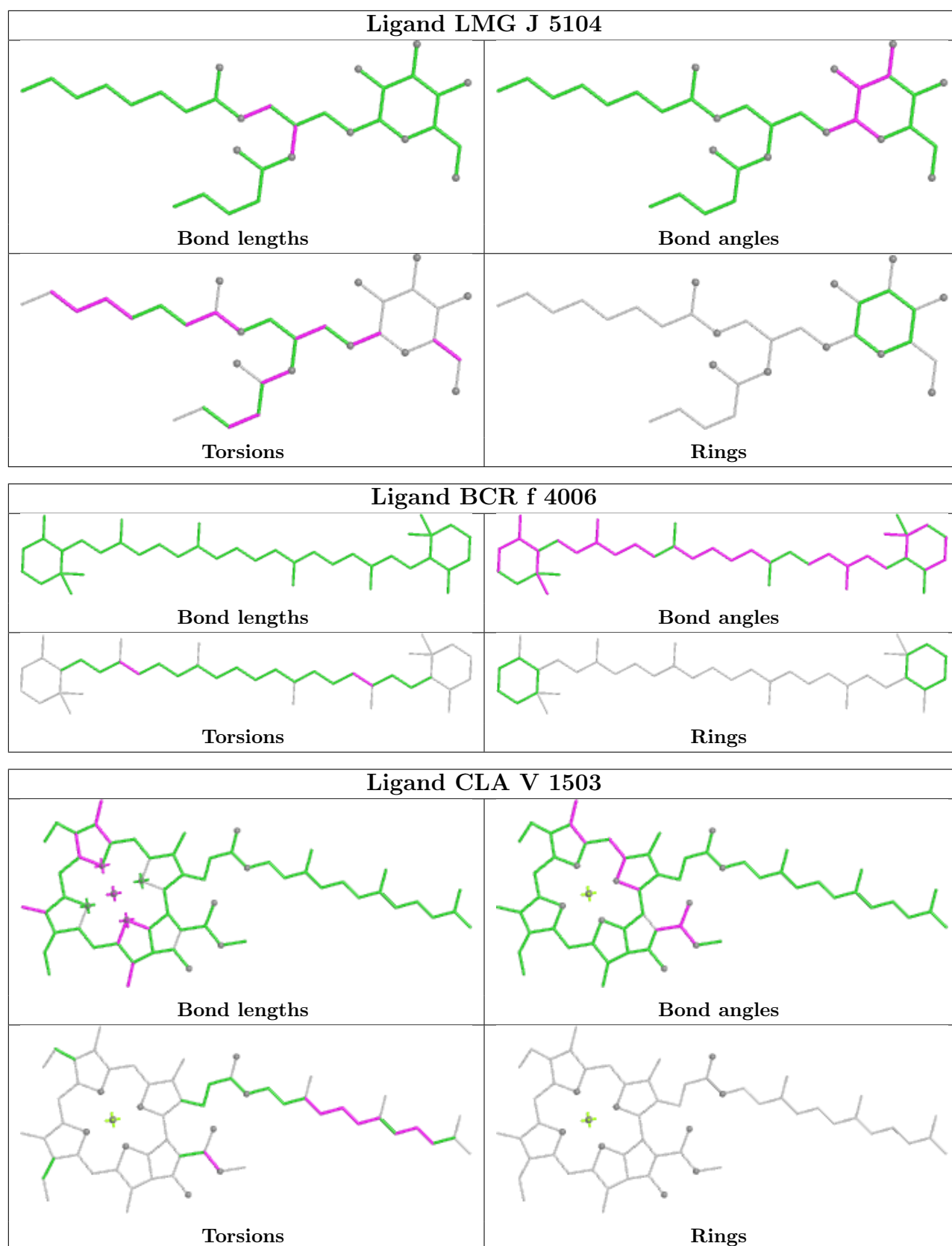
Bond angles



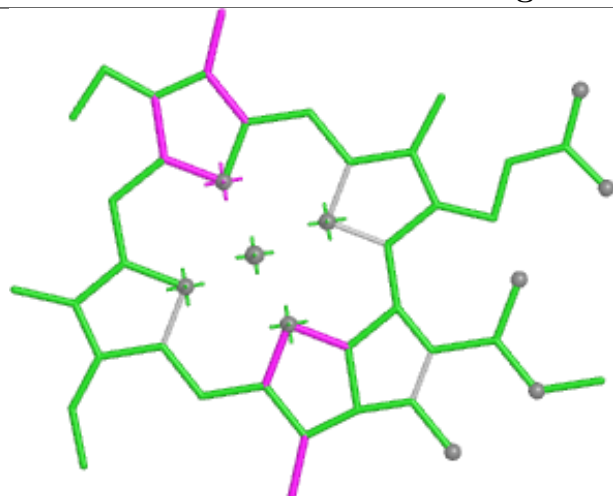
Torsions



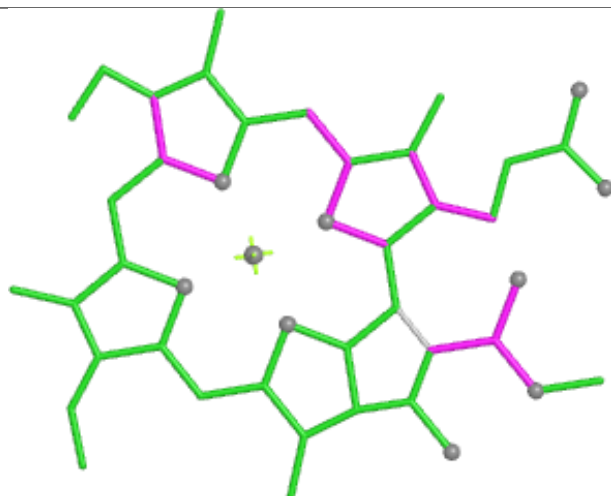
Rings



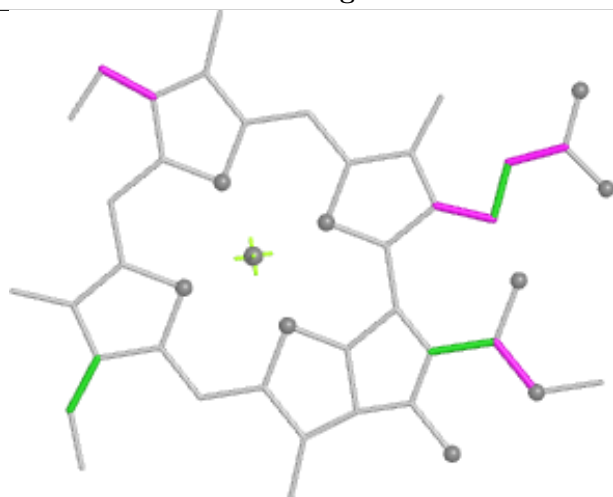
Ligand CLA Z 516



Bond lengths



Bond angles

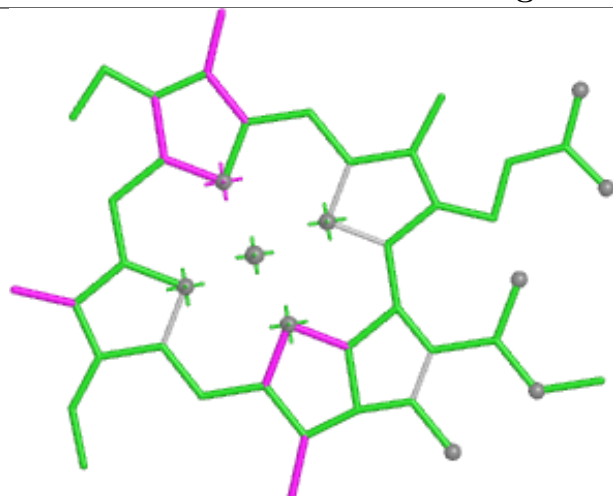


Torsions

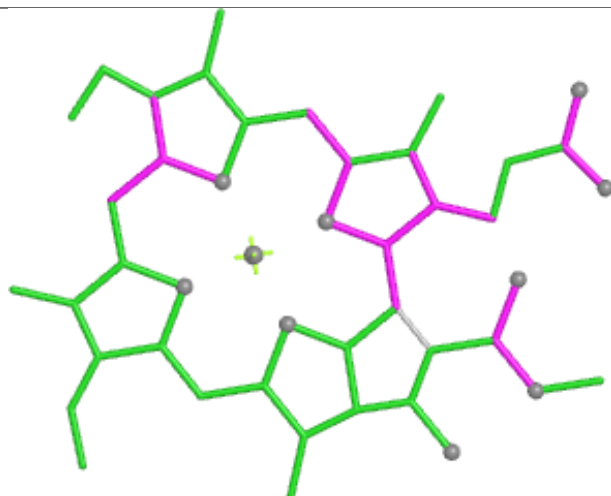


Rings

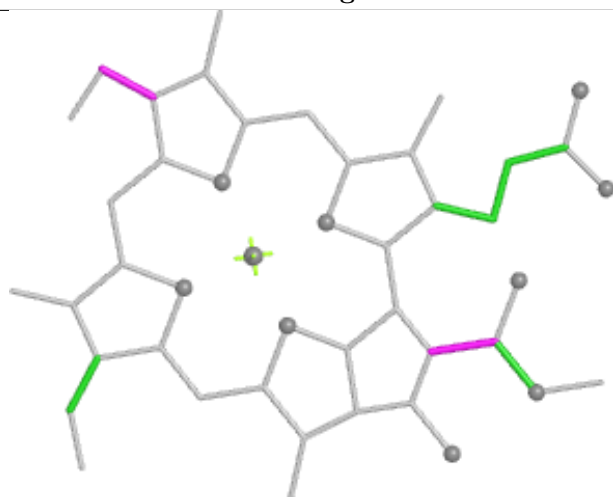
Ligand CLA Z 502



Bond lengths



Bond angles

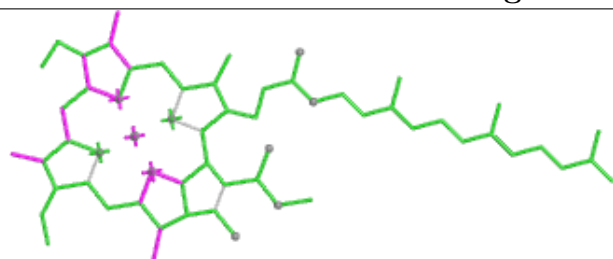


Torsions

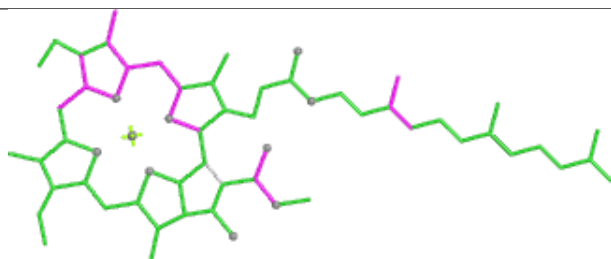


Rings

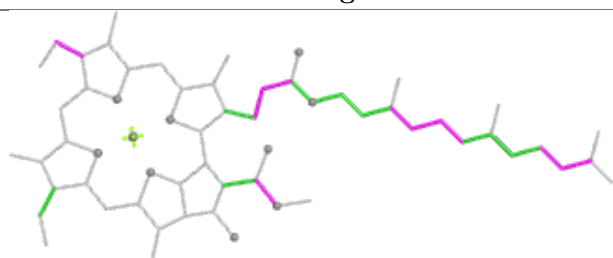
Ligand CLA G 1115



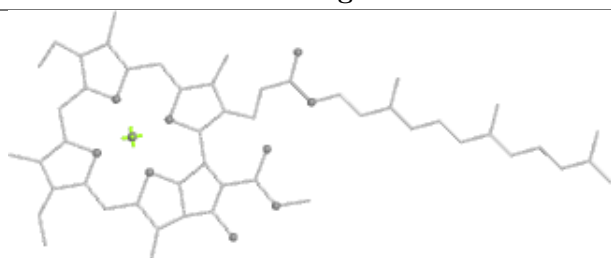
Bond lengths



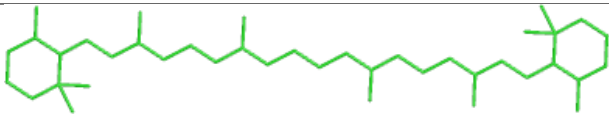
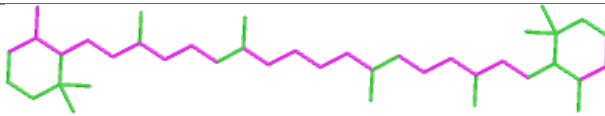
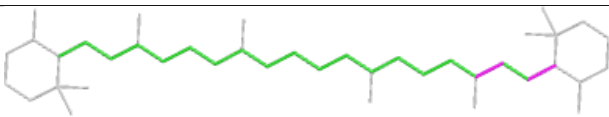
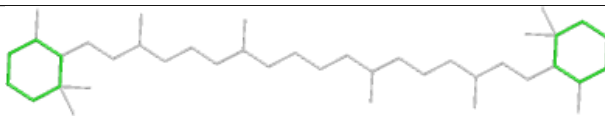
Bond angles

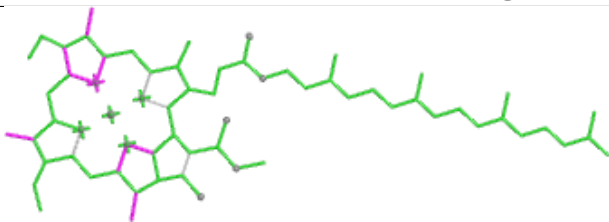
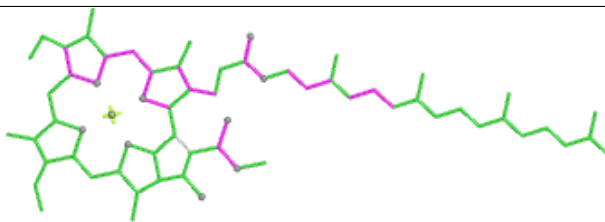
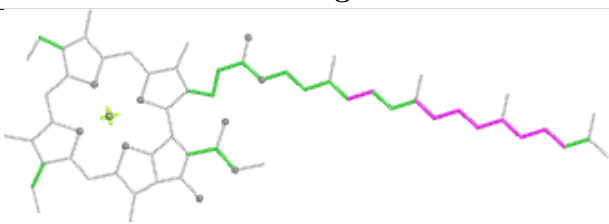
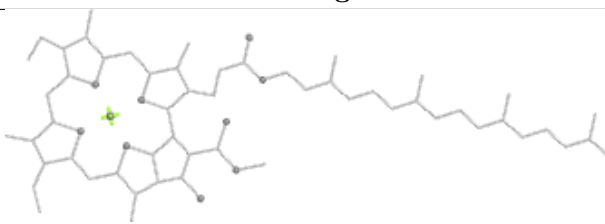


Torsions

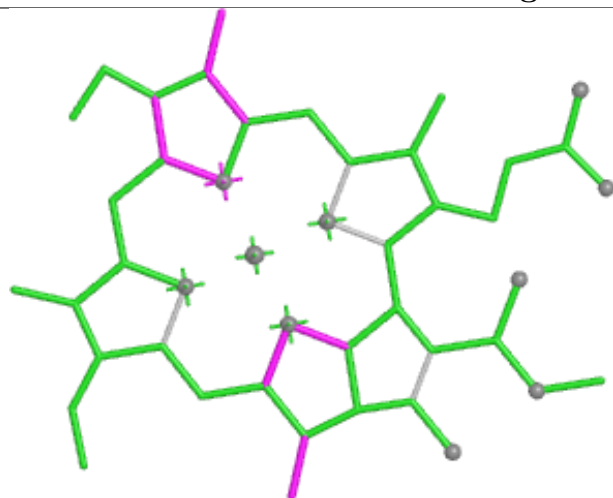


Rings

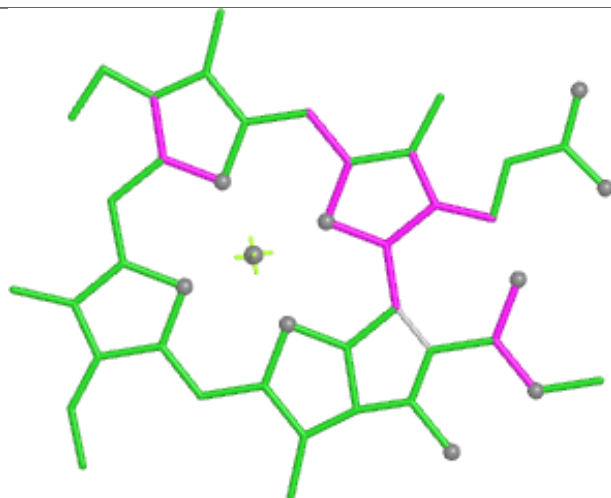
Ligand BCR 6 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1136	
	
Bond lengths	Bond angles
	
Torsions	Rings

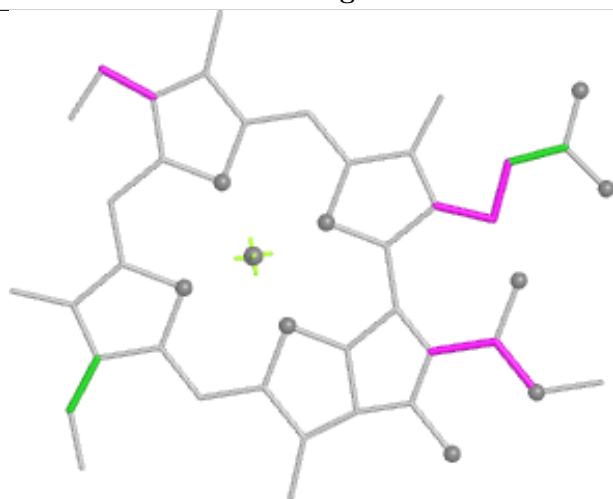
Ligand CLA r 504



Bond lengths



Bond angles

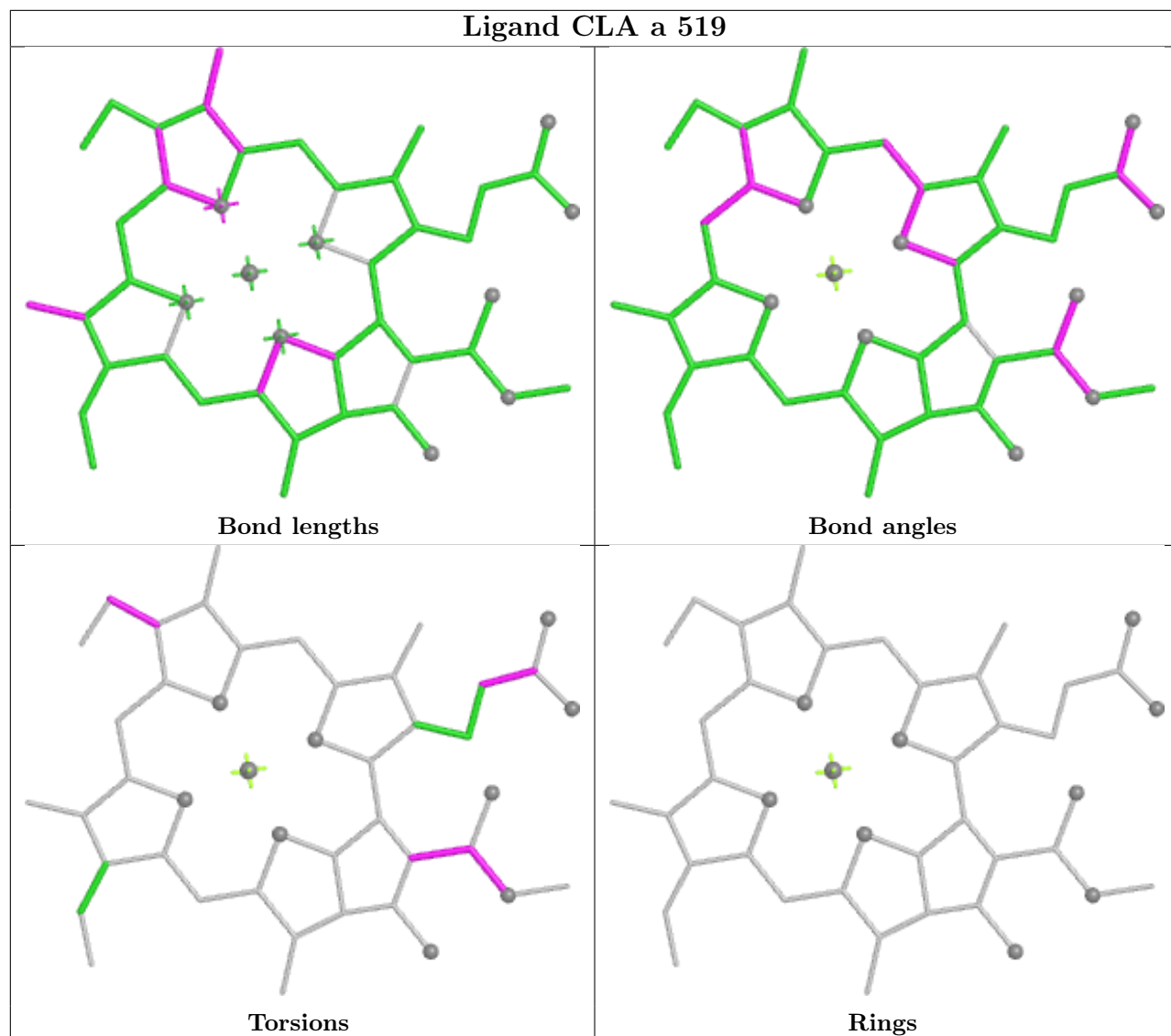


Torsions

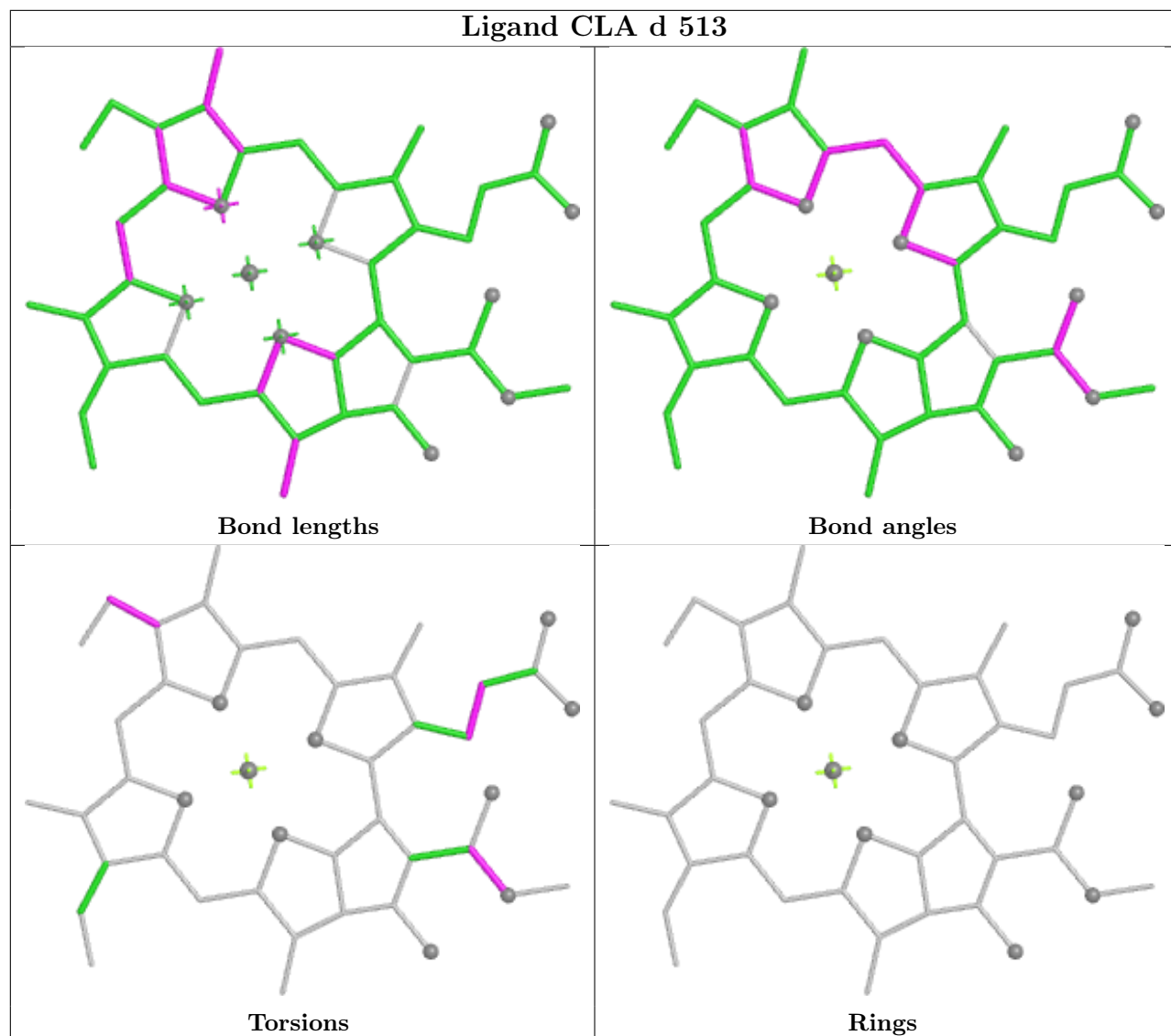


Rings

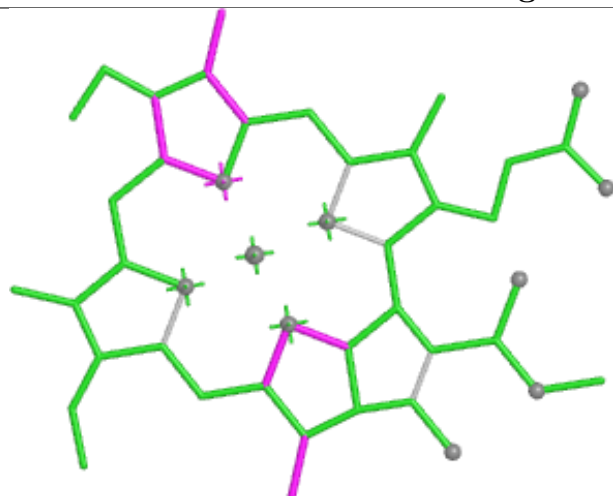
Ligand CLA a 519



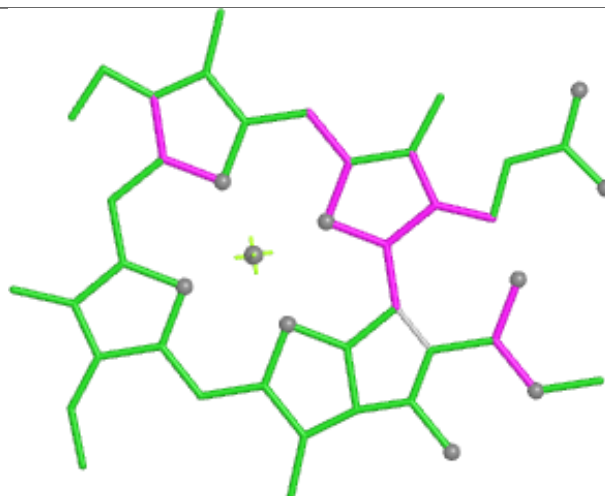
Ligand CLA d 513



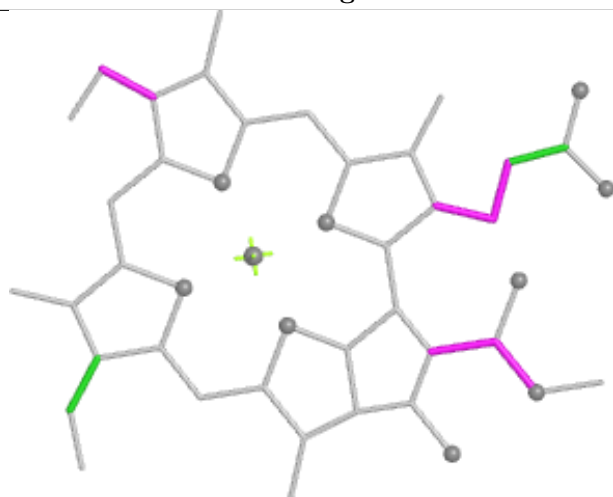
Ligand CLA 2 504



Bond lengths



Bond angles

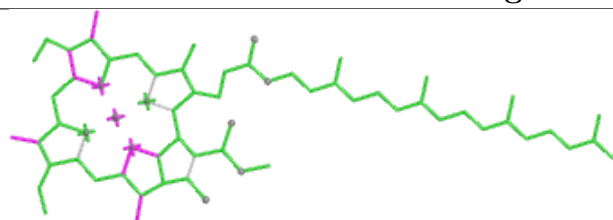


Torsions

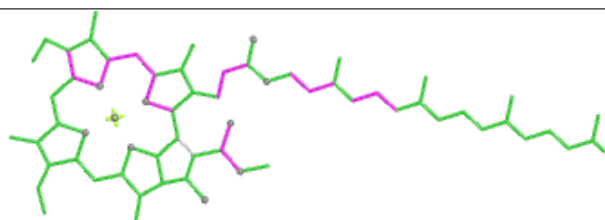


Rings

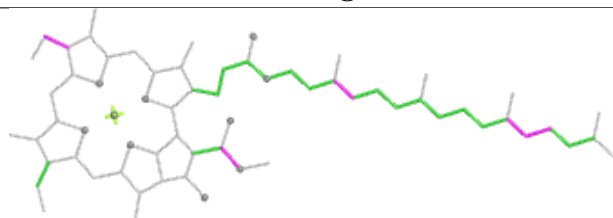
Ligand CLA A 1131



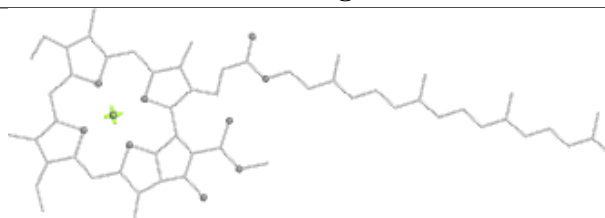
Bond lengths



Bond angles

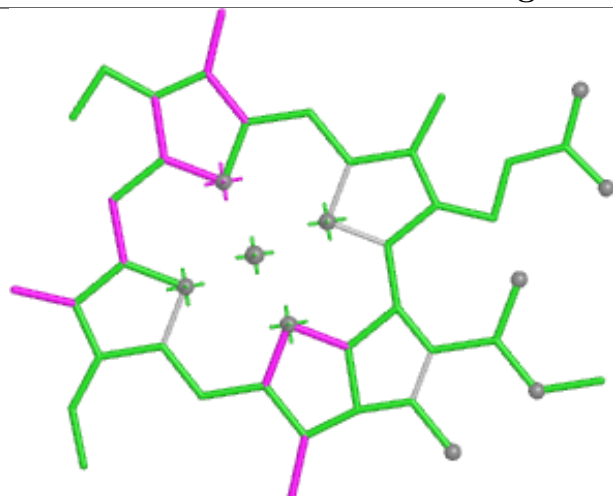


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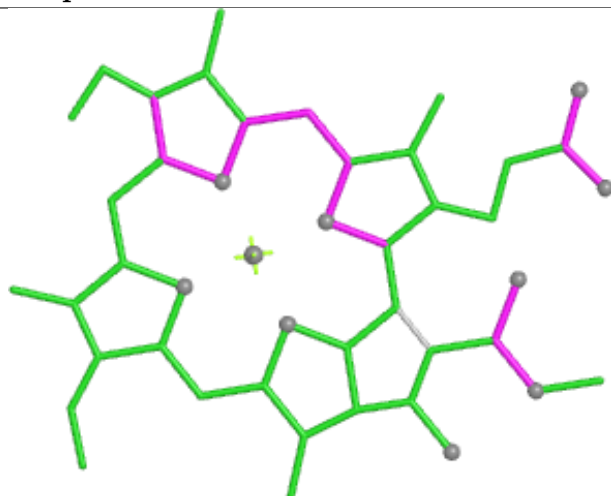


Rings

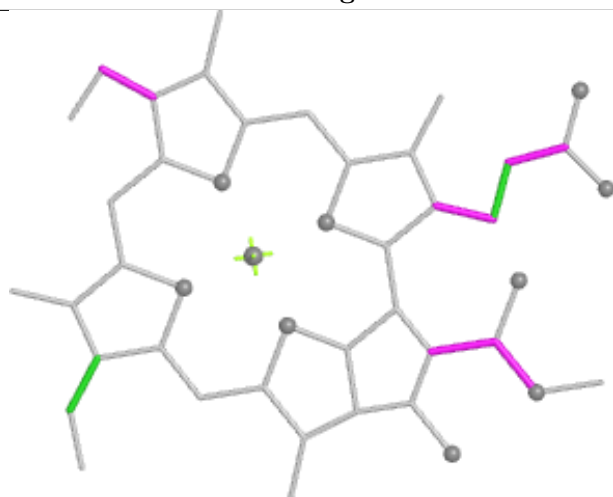
Ligand CLA q 519



Bond lengths



Bond angles

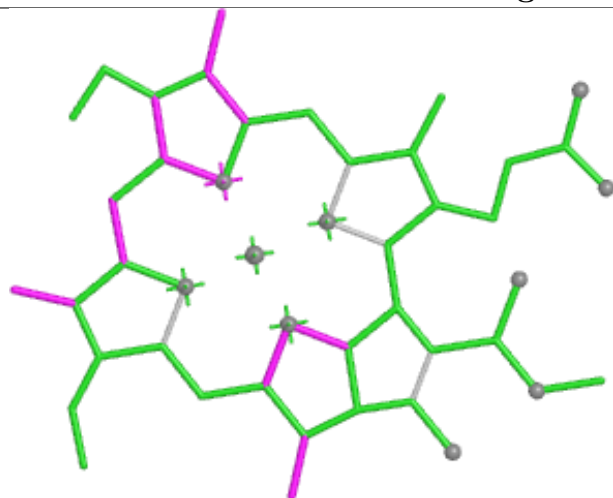


Torsions

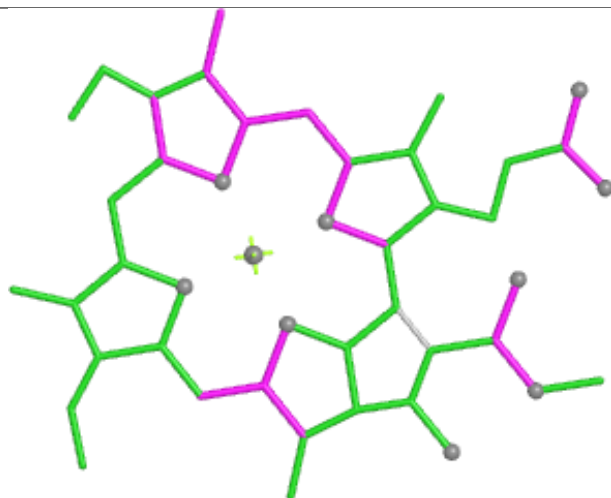


Rings

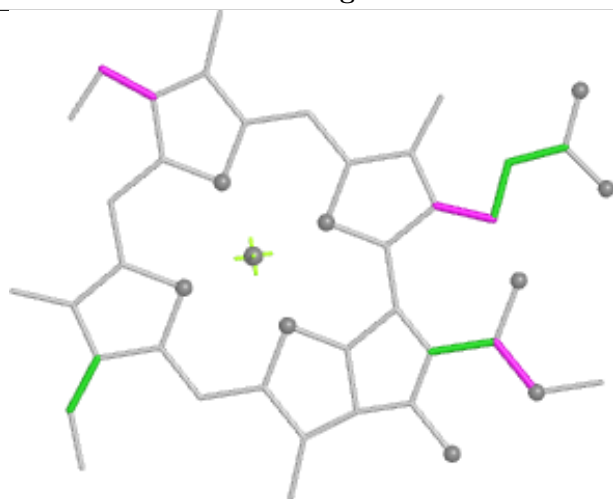
Ligand CLA b 511



Bond lengths



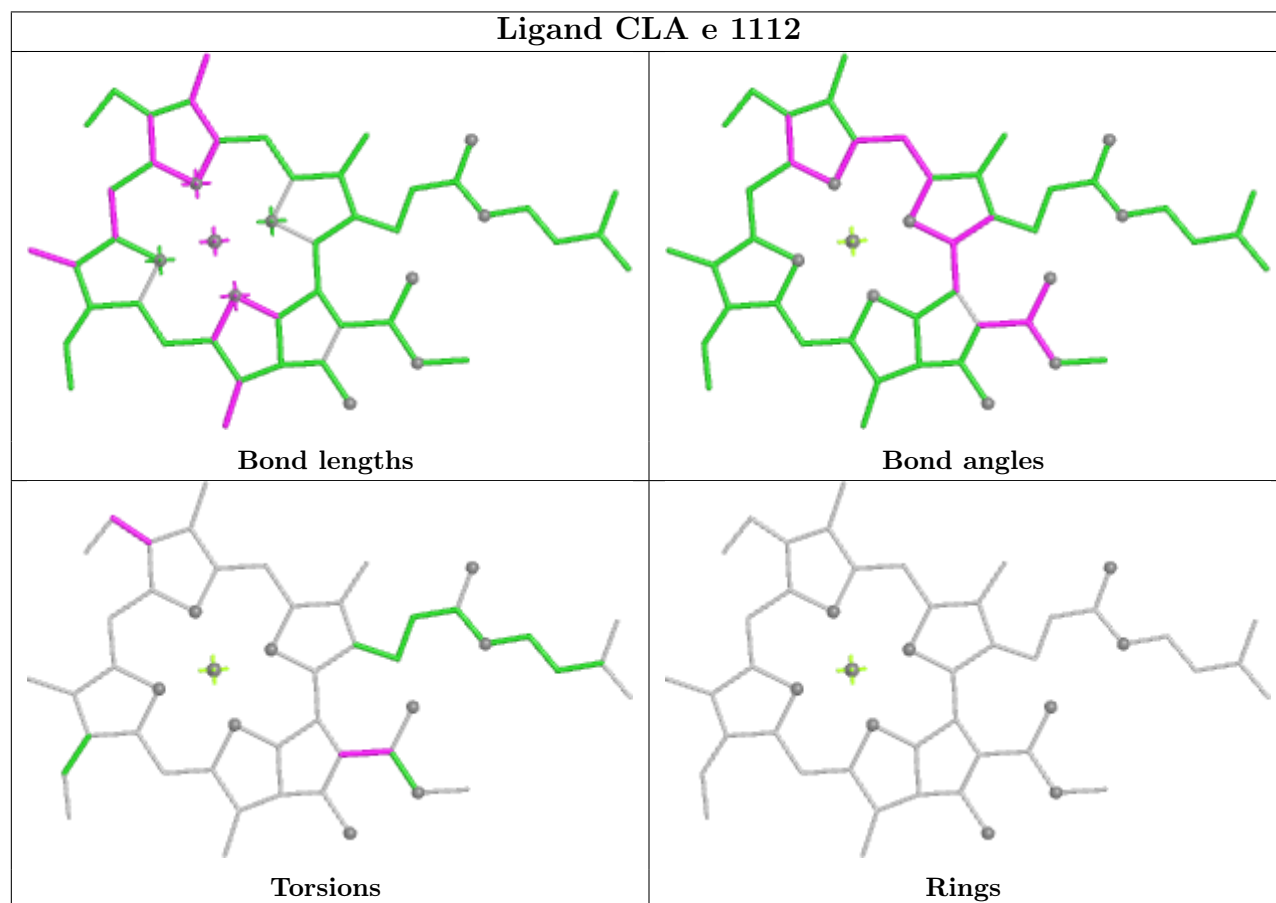
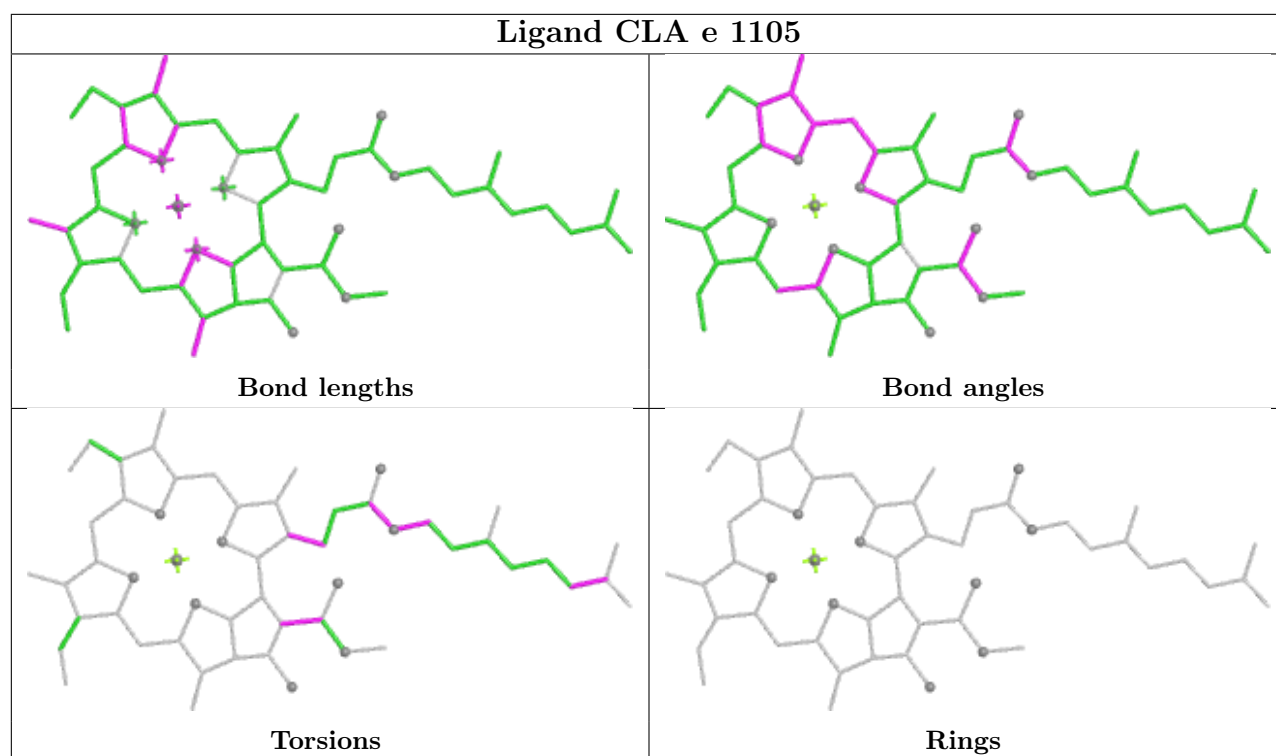
Bond angles



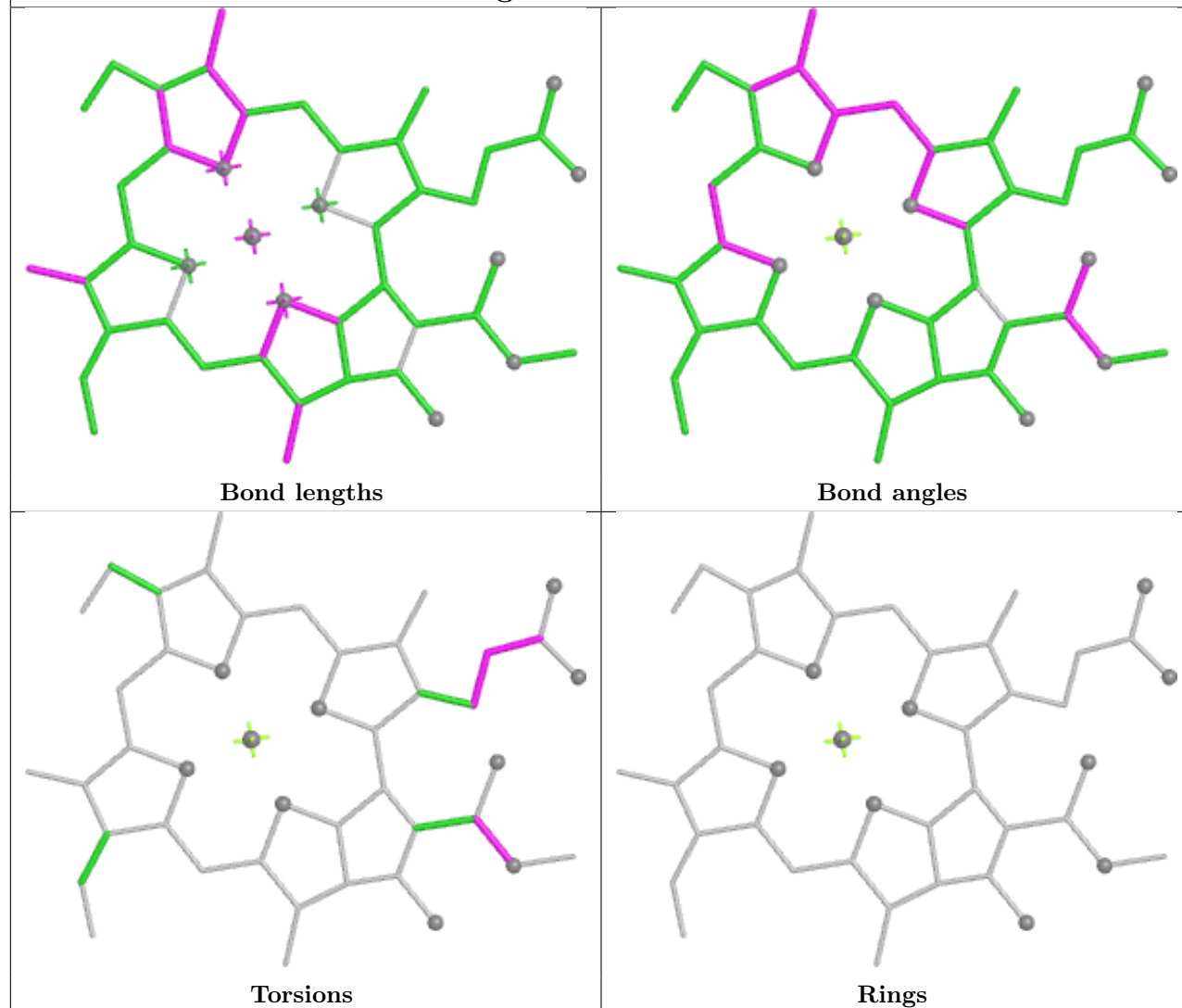
Torsions



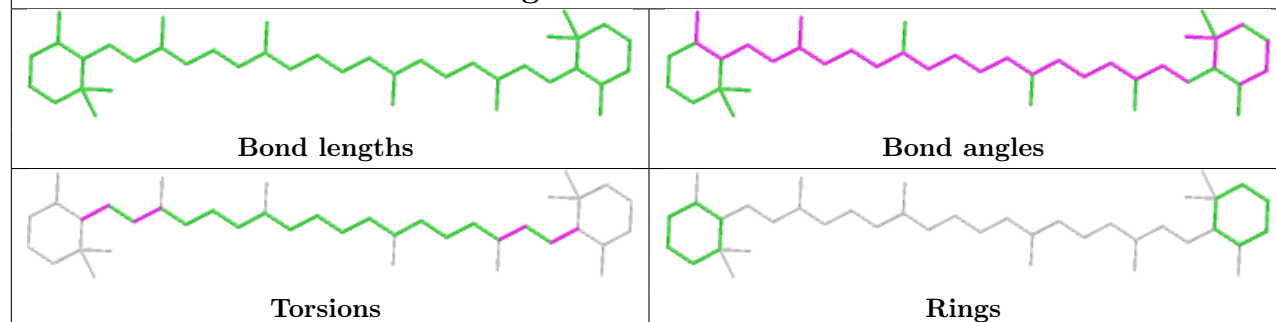
Rings



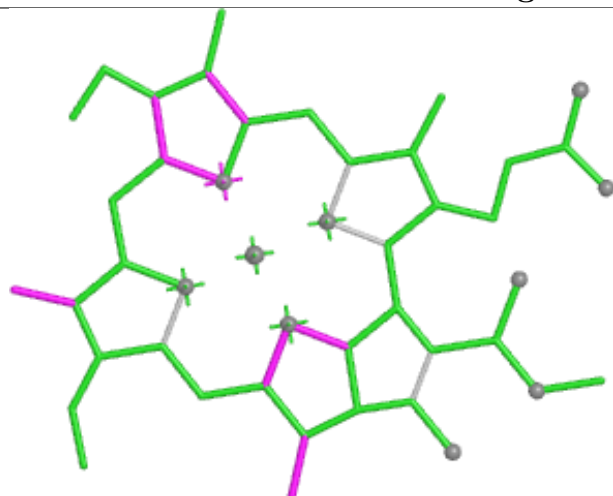
Ligand CLA 1 508



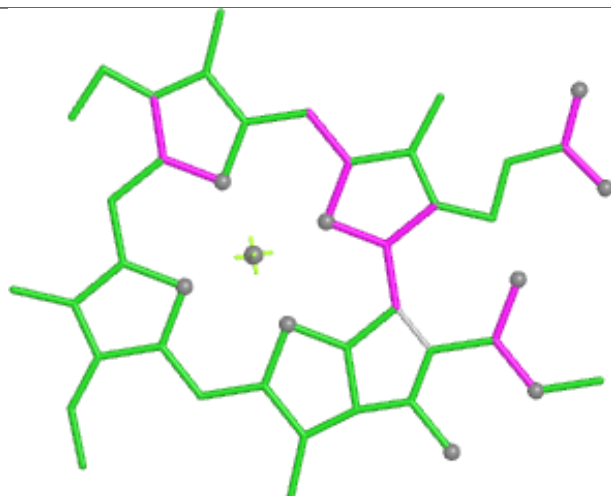
Ligand BCR B 4004



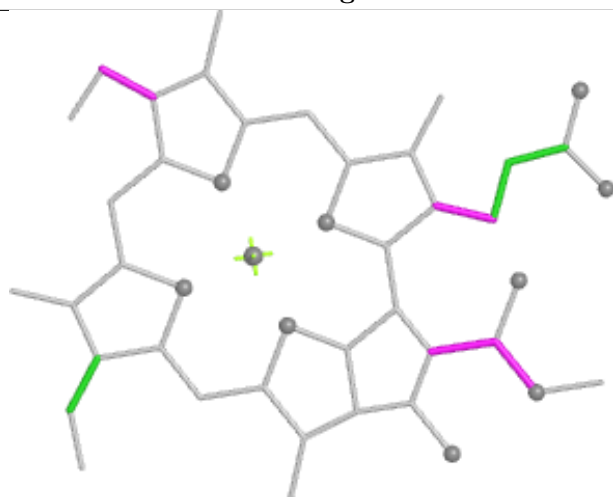
Ligand CLA b 517



Bond lengths



Bond angles

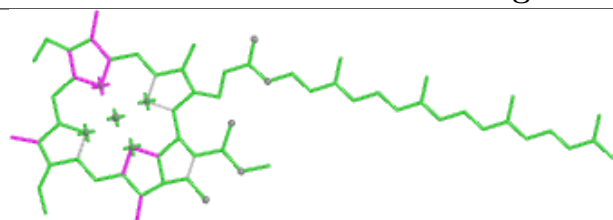


Torsions

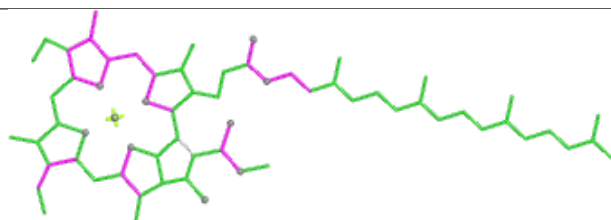


Rings

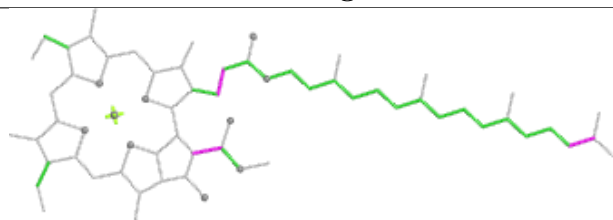
Ligand CLA f 1238



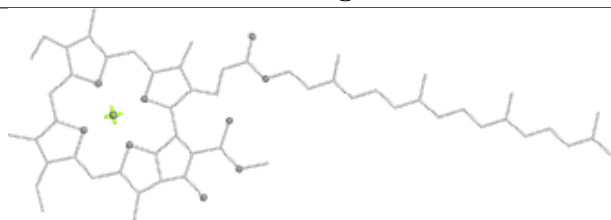
Bond lengths



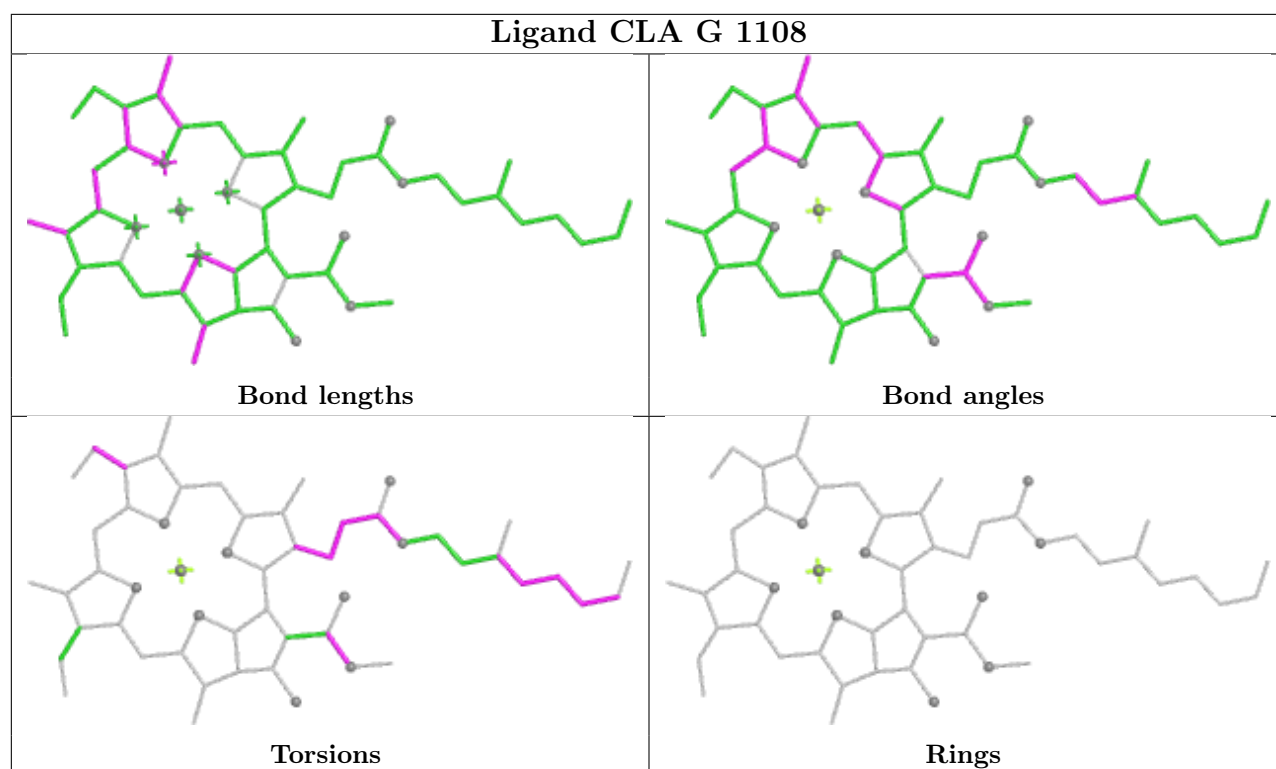
Bond angles



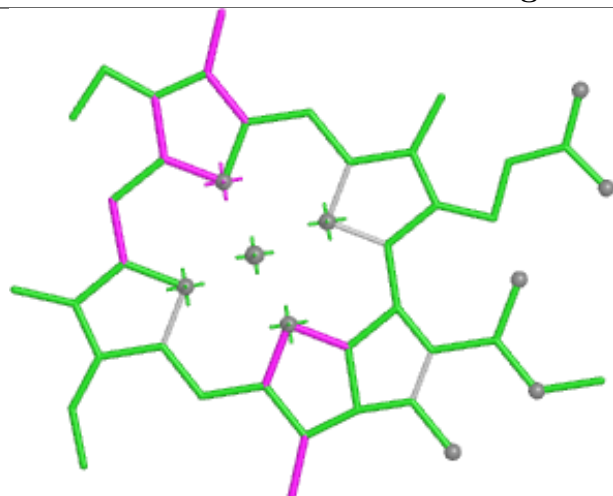
Torsions



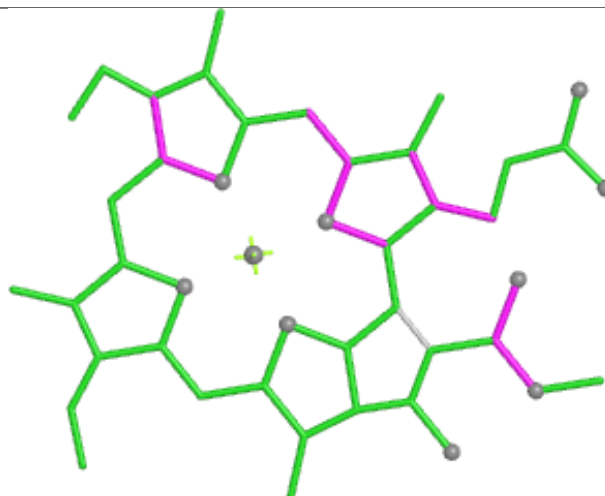
Rings



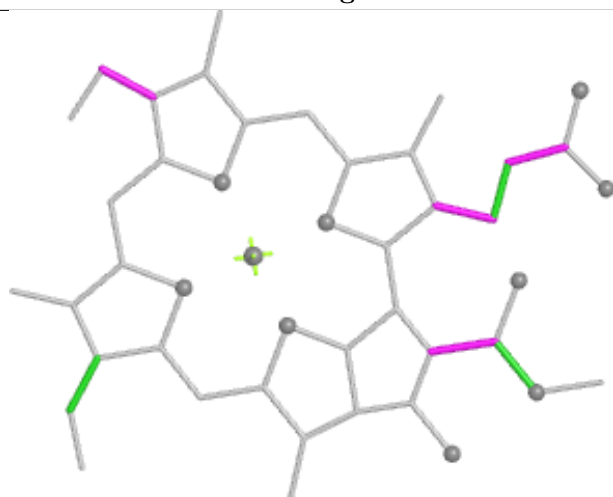
Ligand CLA t 516



Bond lengths



Bond angles

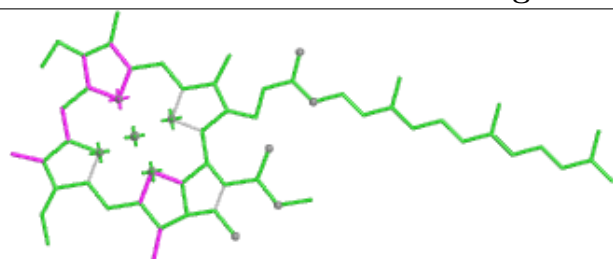


Torsions

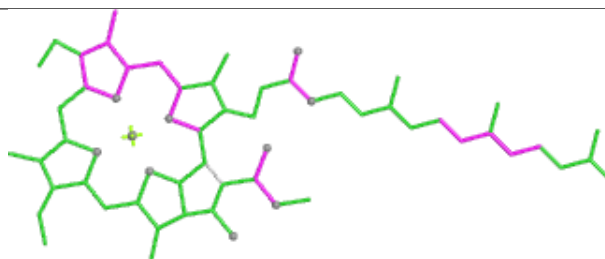


Rings

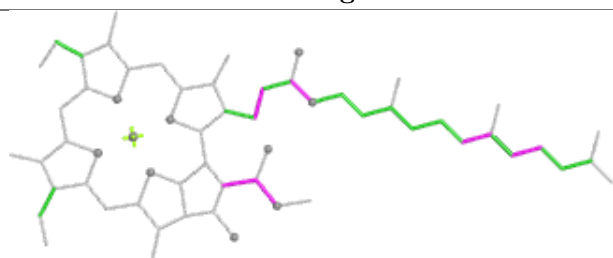
Ligand CLA f 1201



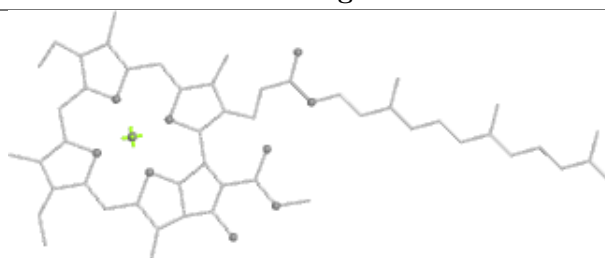
Bond lengths



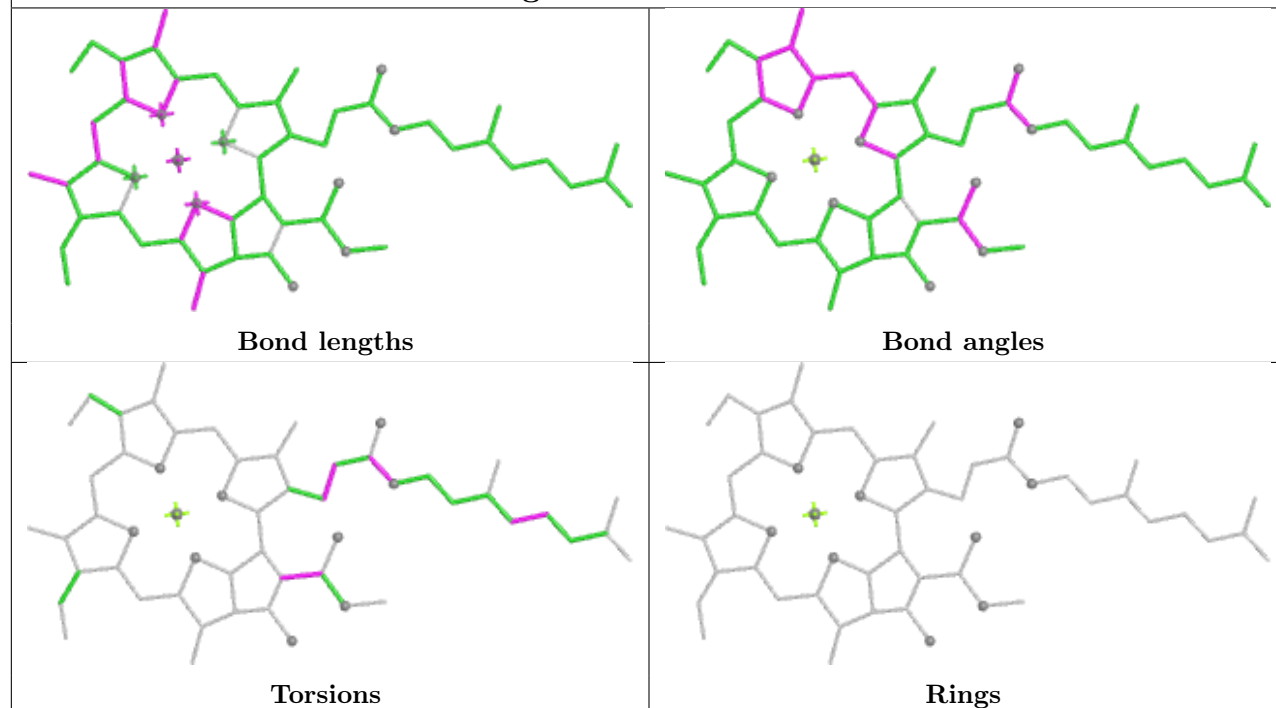
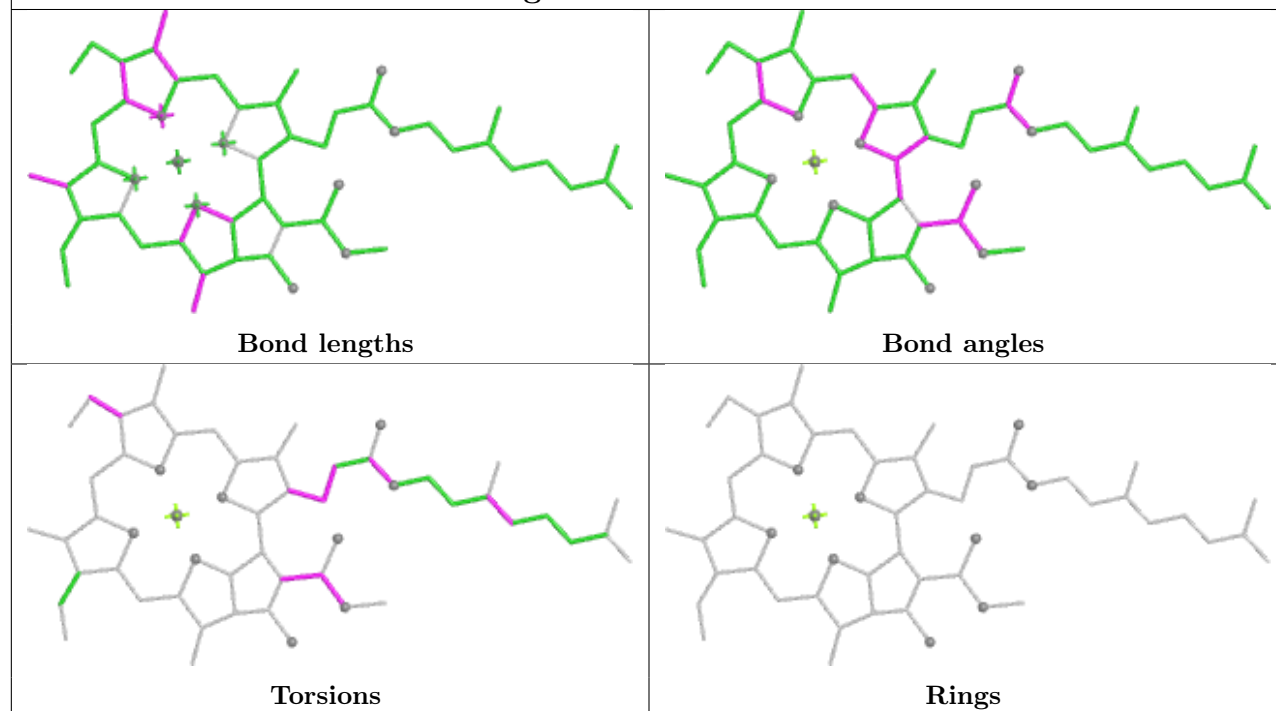
Bond angles

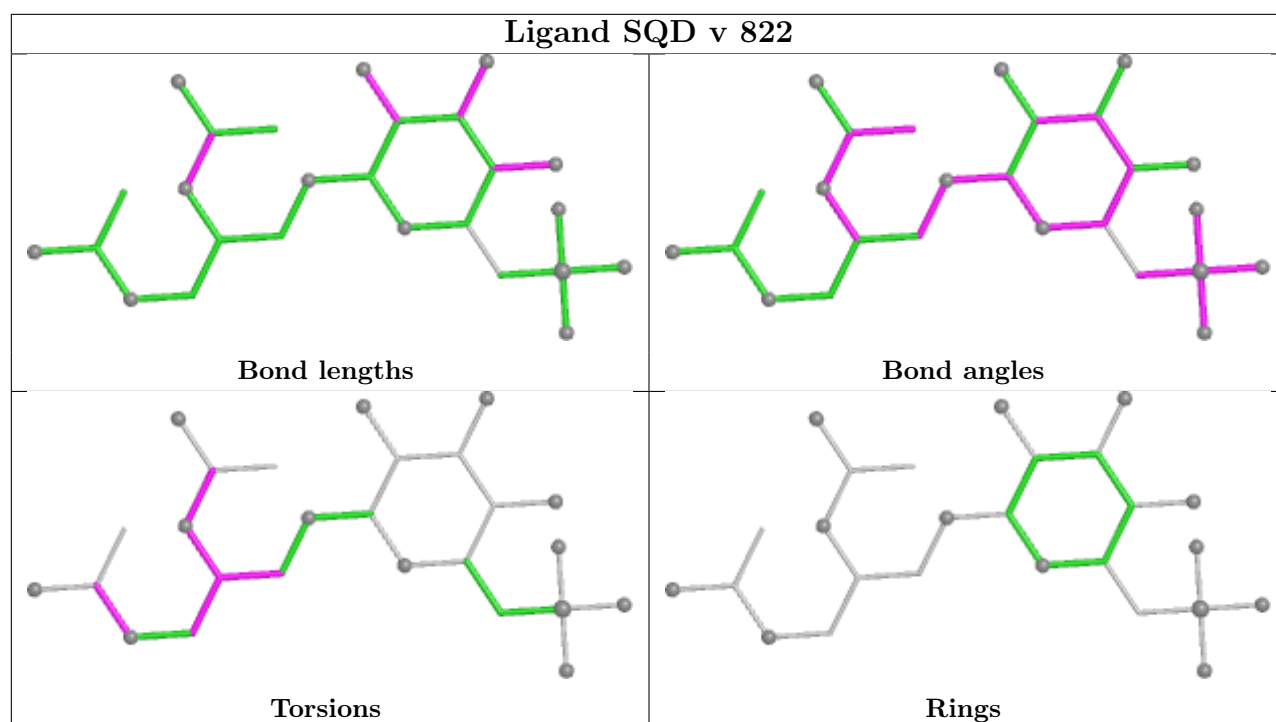


Torsions

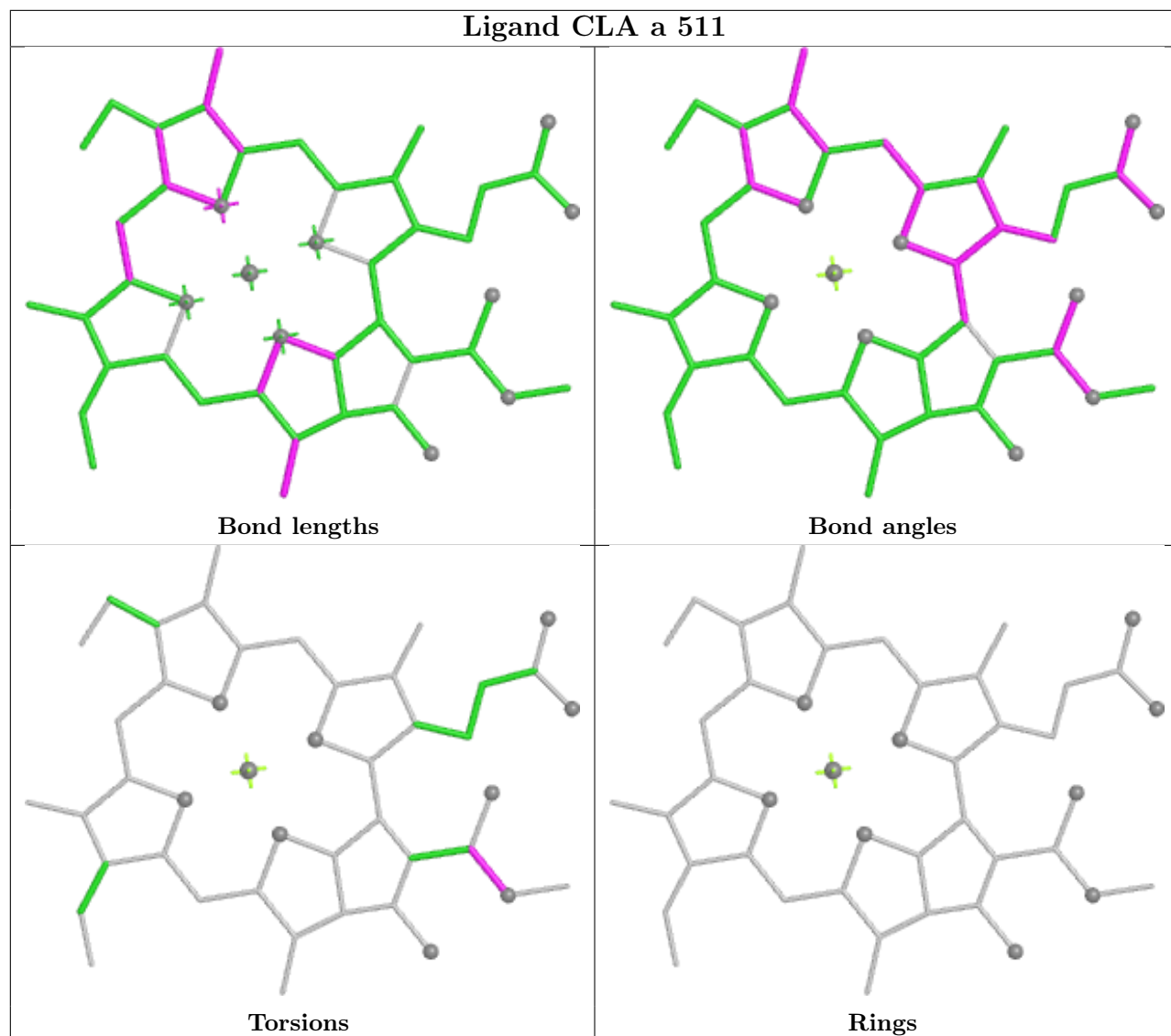


Rings

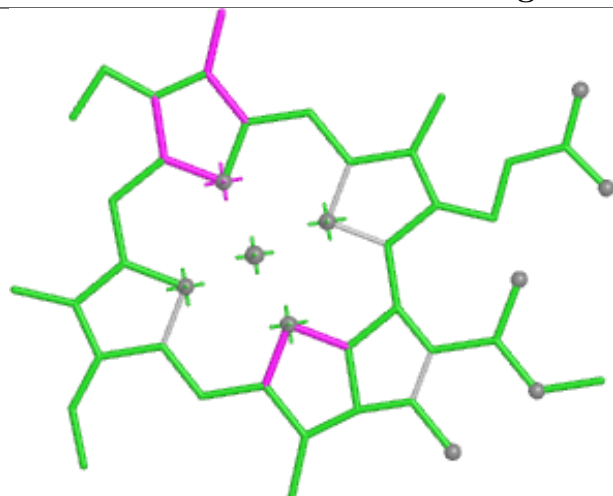
Ligand CLA H 1232**Ligand CLA T 1302**



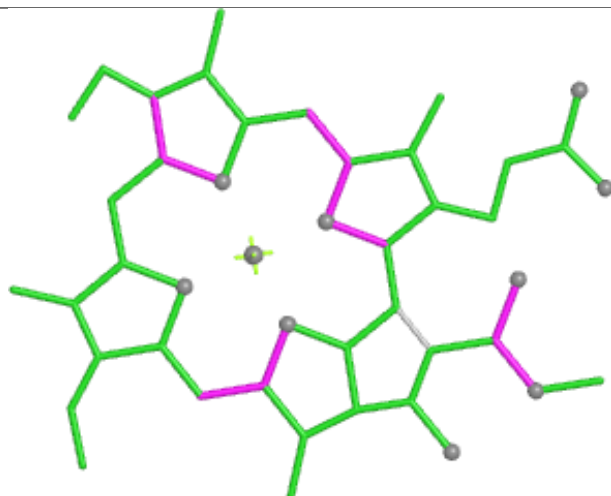
Ligand CLA a 511



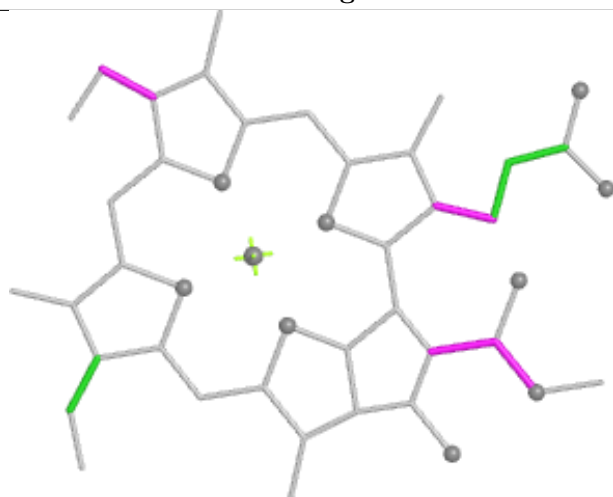
Ligand CLA b 504



Bond lengths



Bond angles

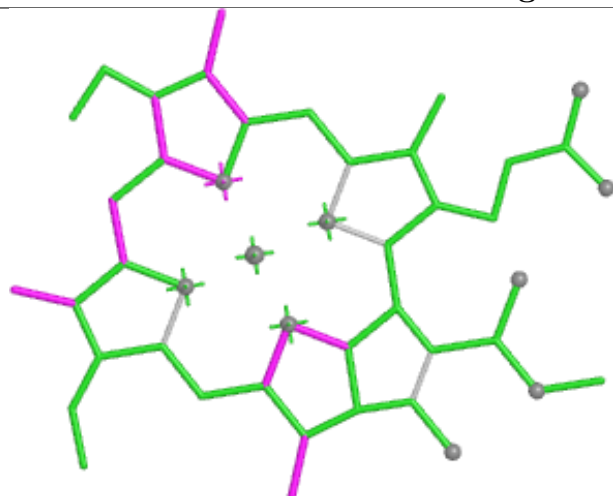


Torsions

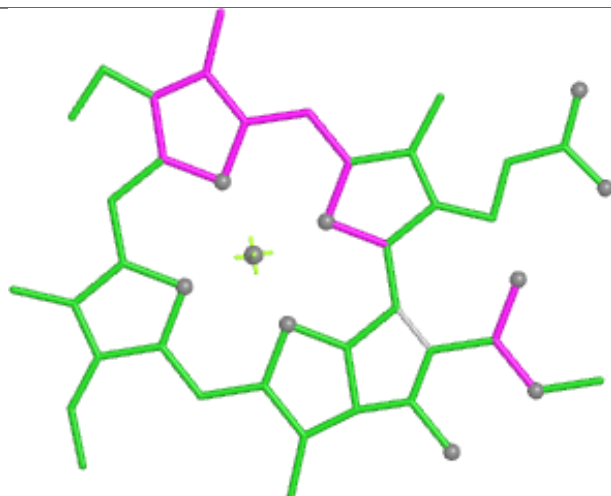


Rings

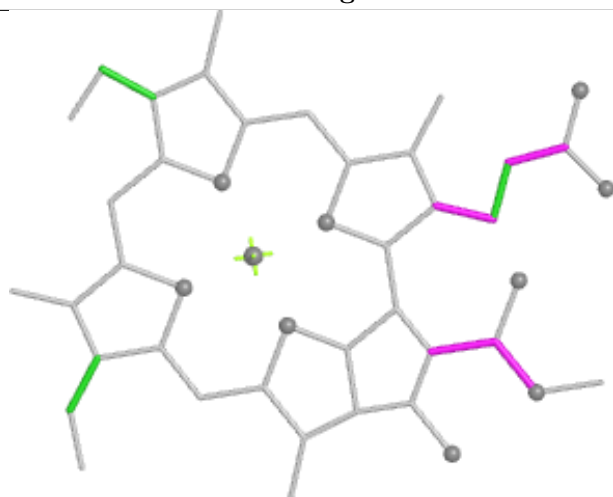
Ligand CLA 3 506



Bond lengths



Bond angles

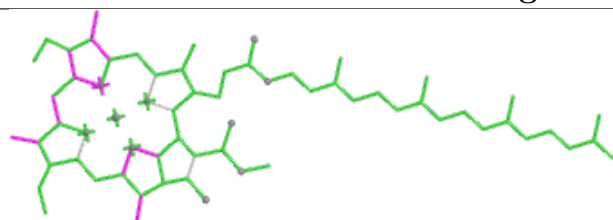


Torsions

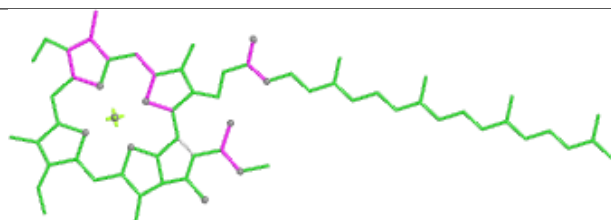


Rings

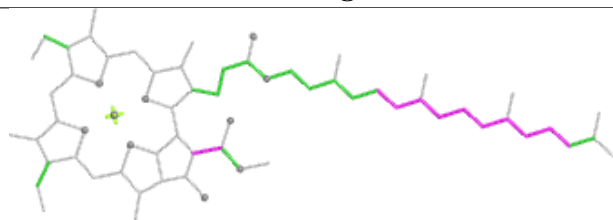
Ligand CLA c 509



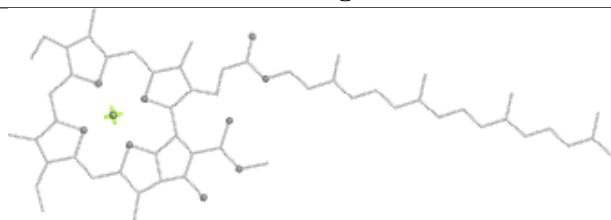
Bond lengths



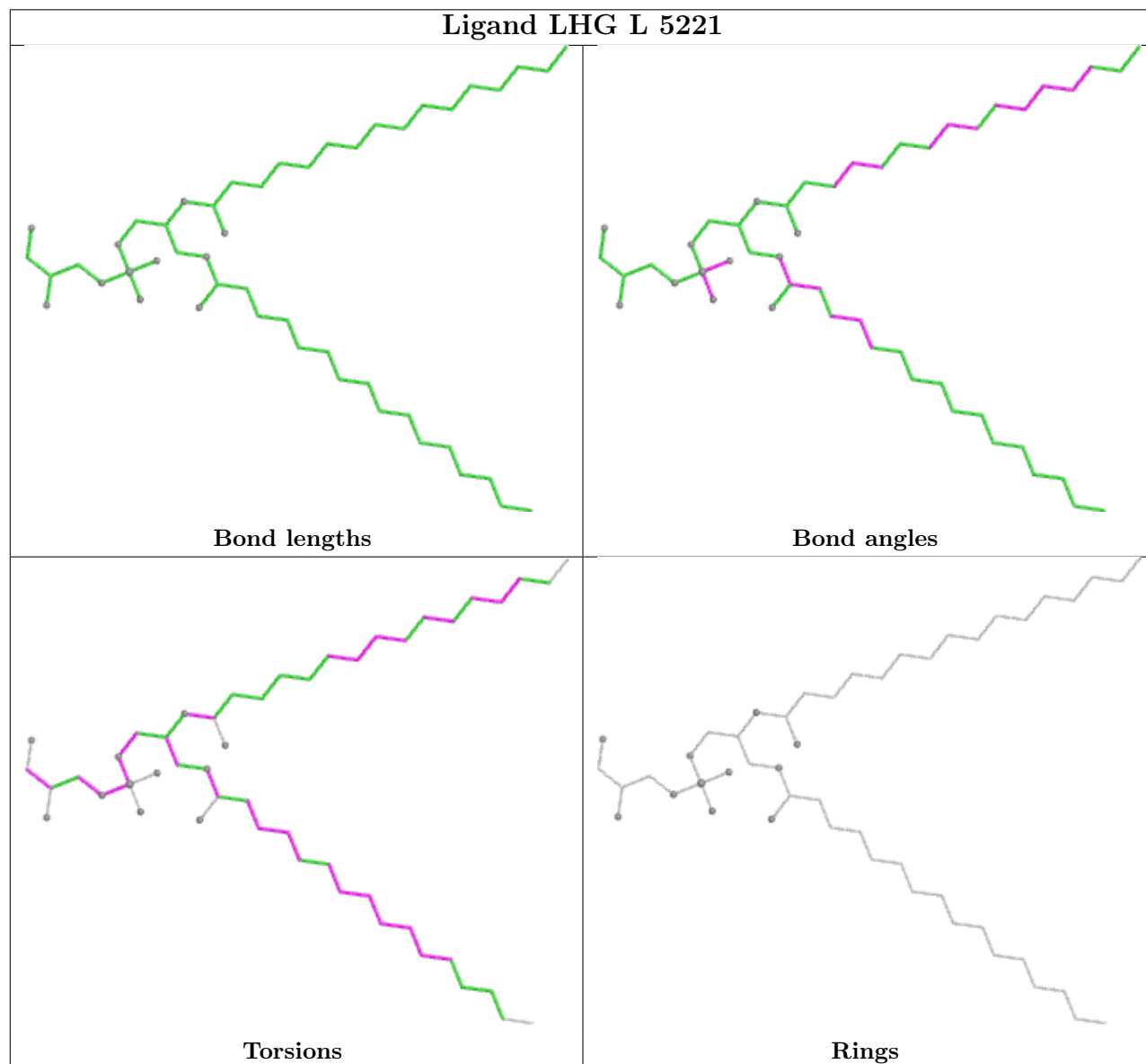
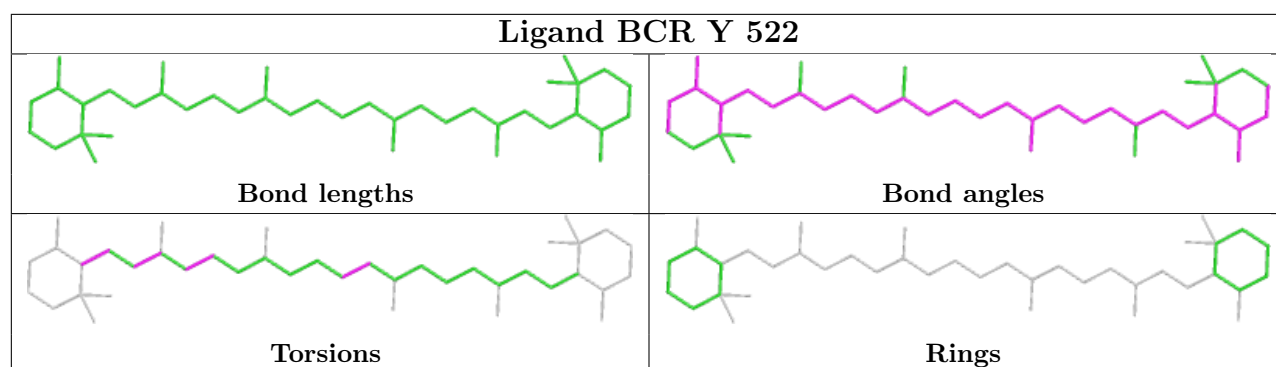
Bond angles

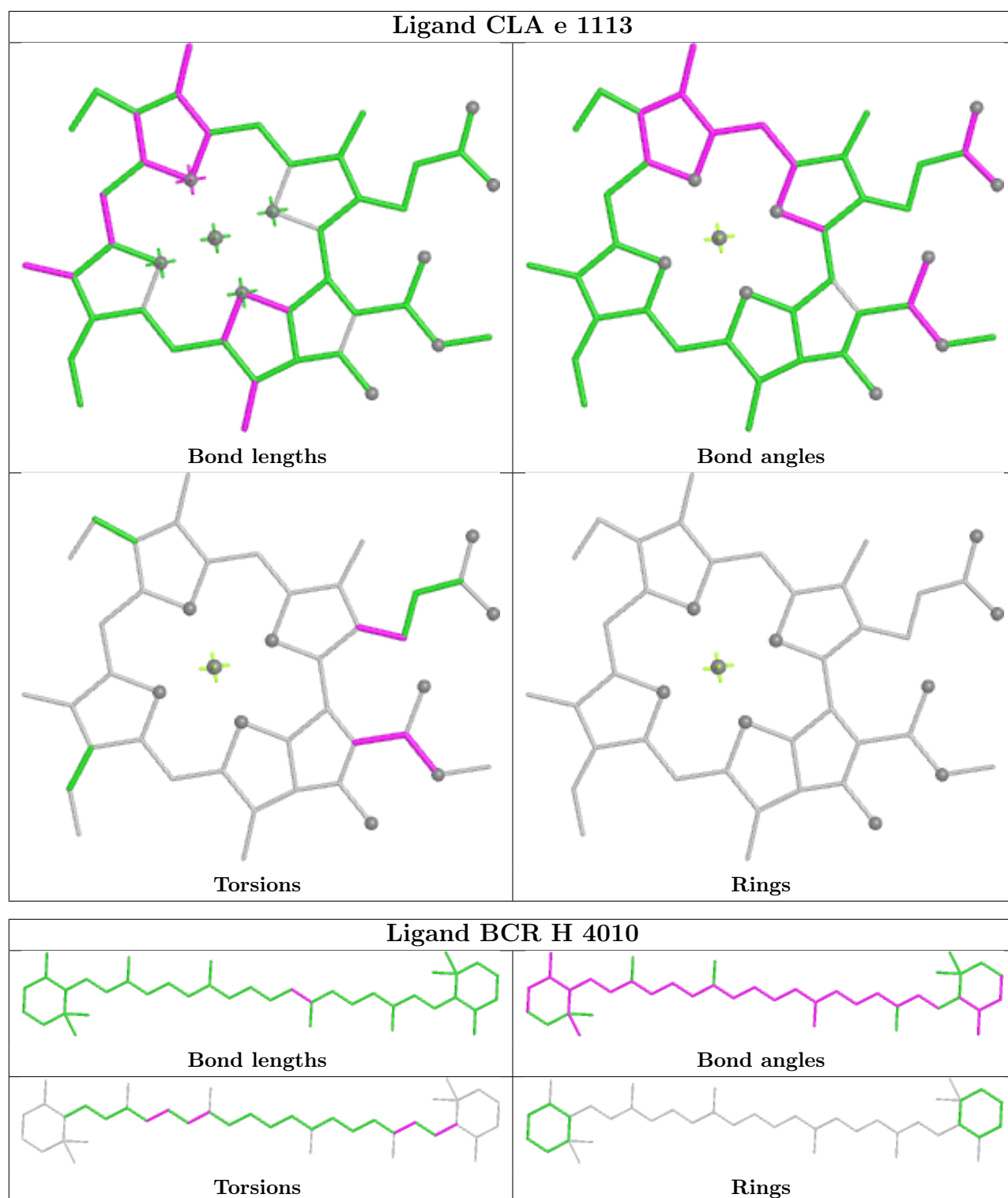


Torsions

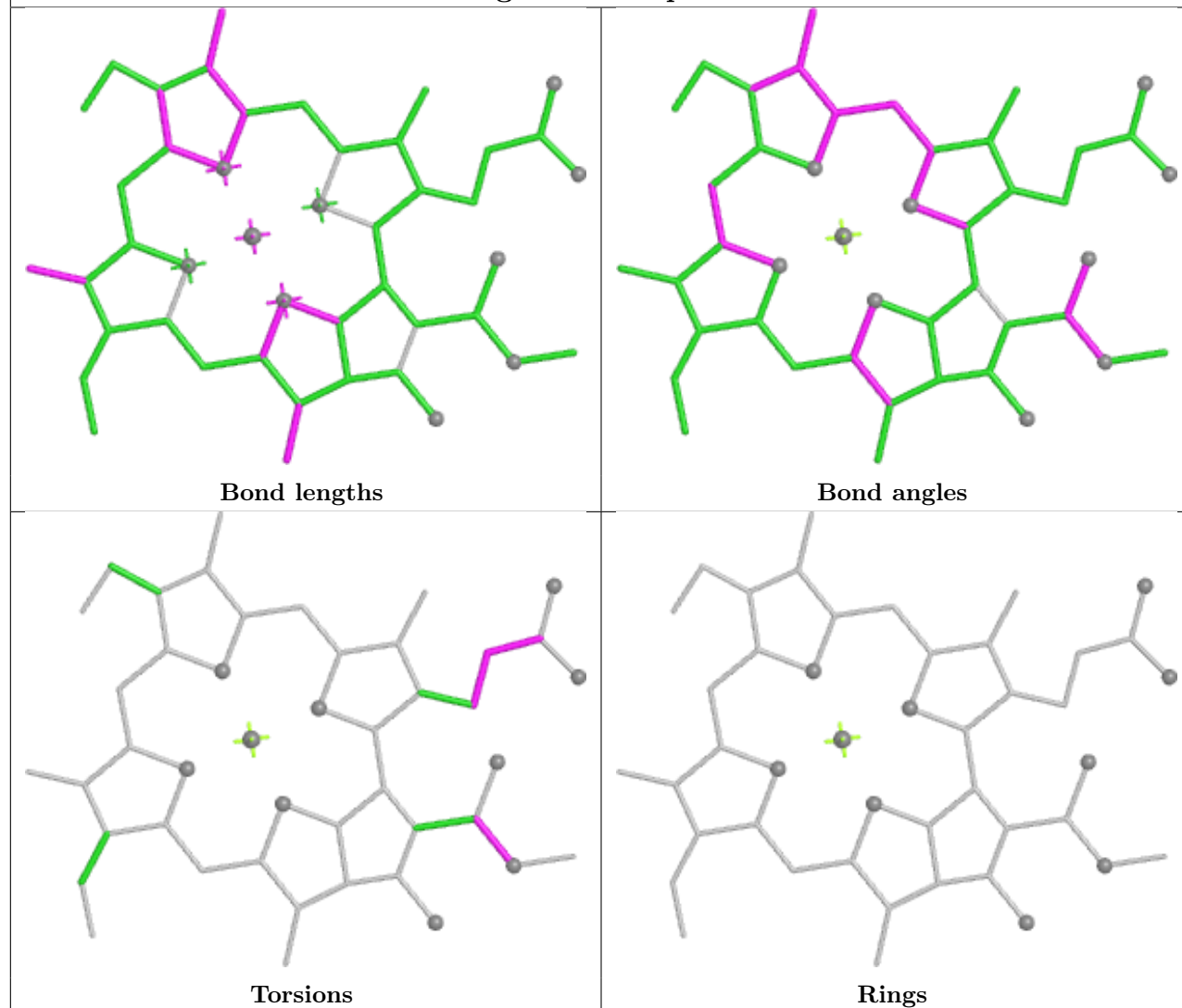


Rings

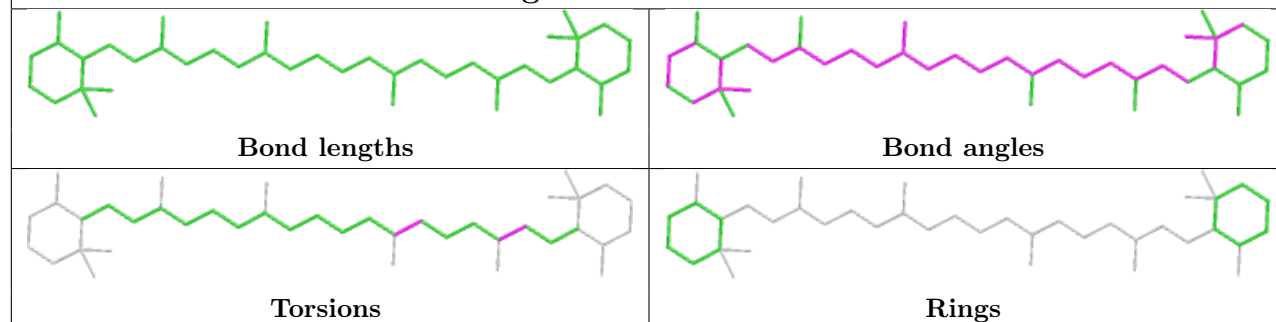




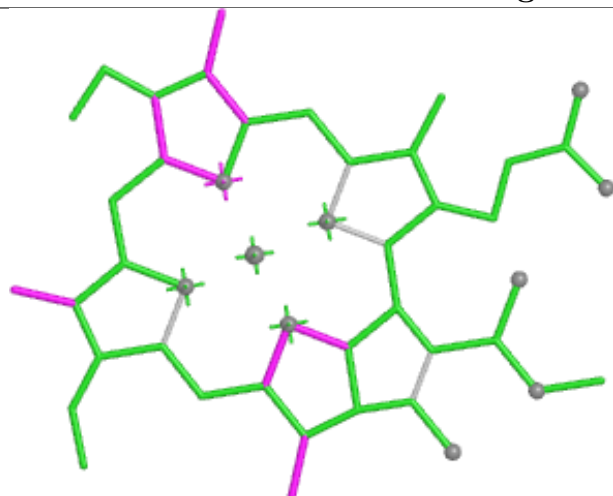
Ligand CLA q 508



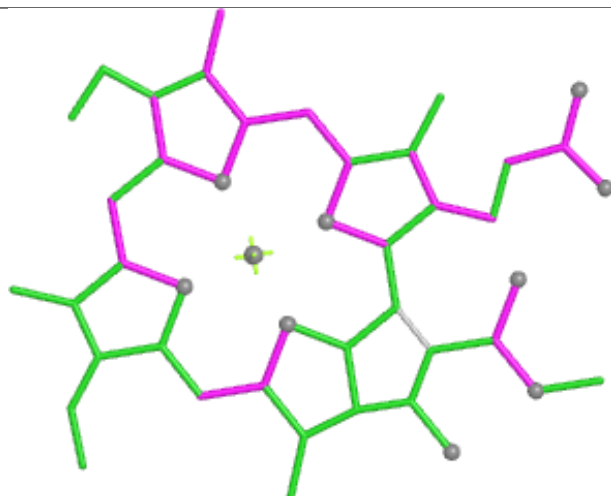
Ligand BCR T 4013



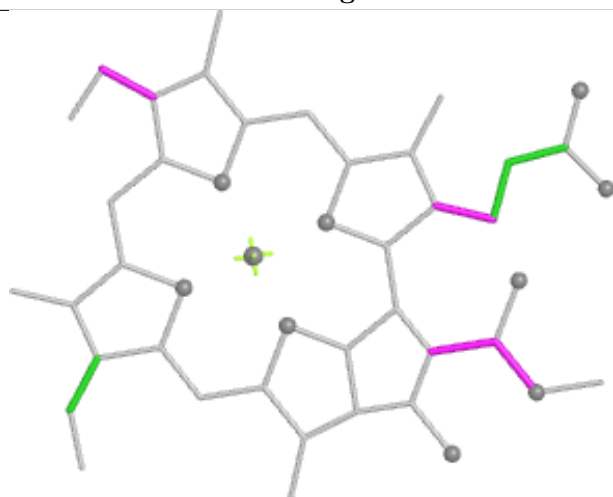
Ligand CLA d 508



Bond lengths



Bond angles

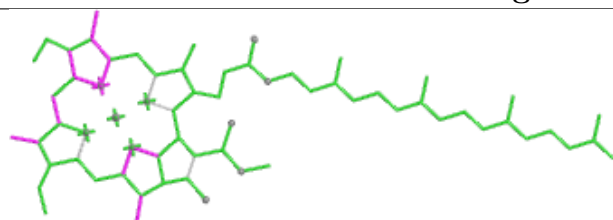


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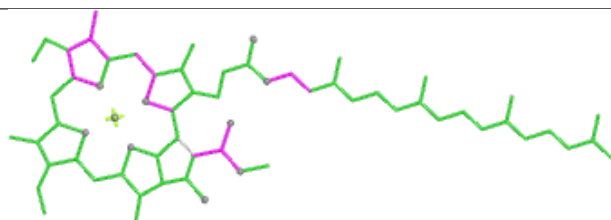


Rings

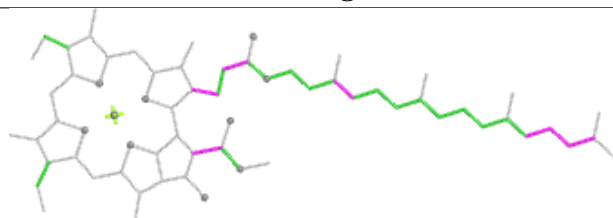
Ligand CLA f 1202



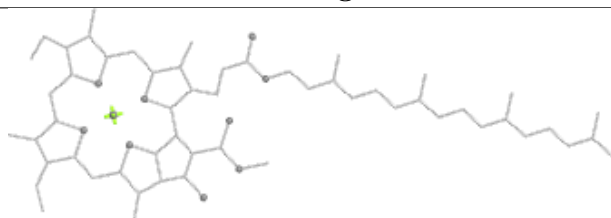
Bond lengths



Bond angles

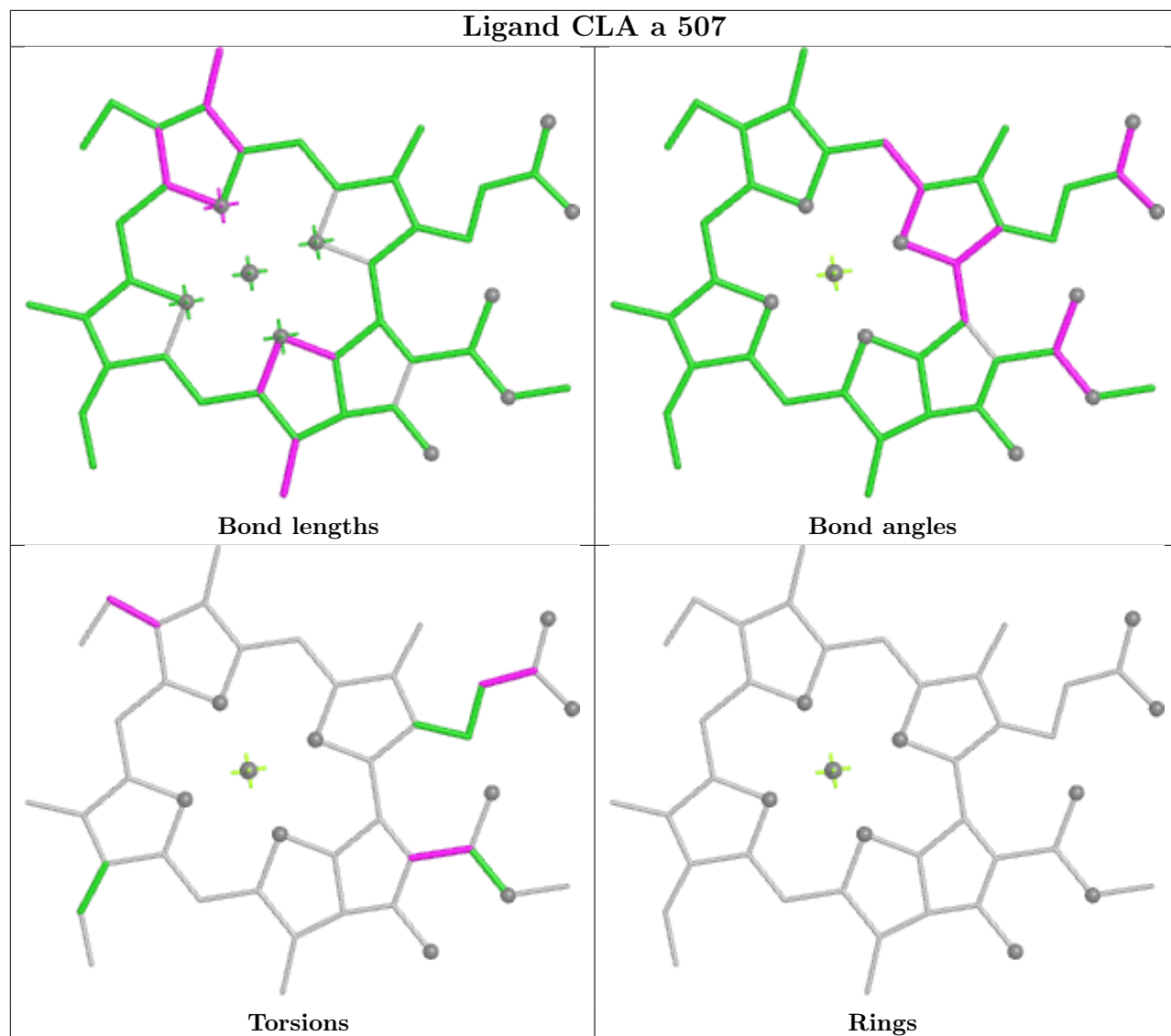


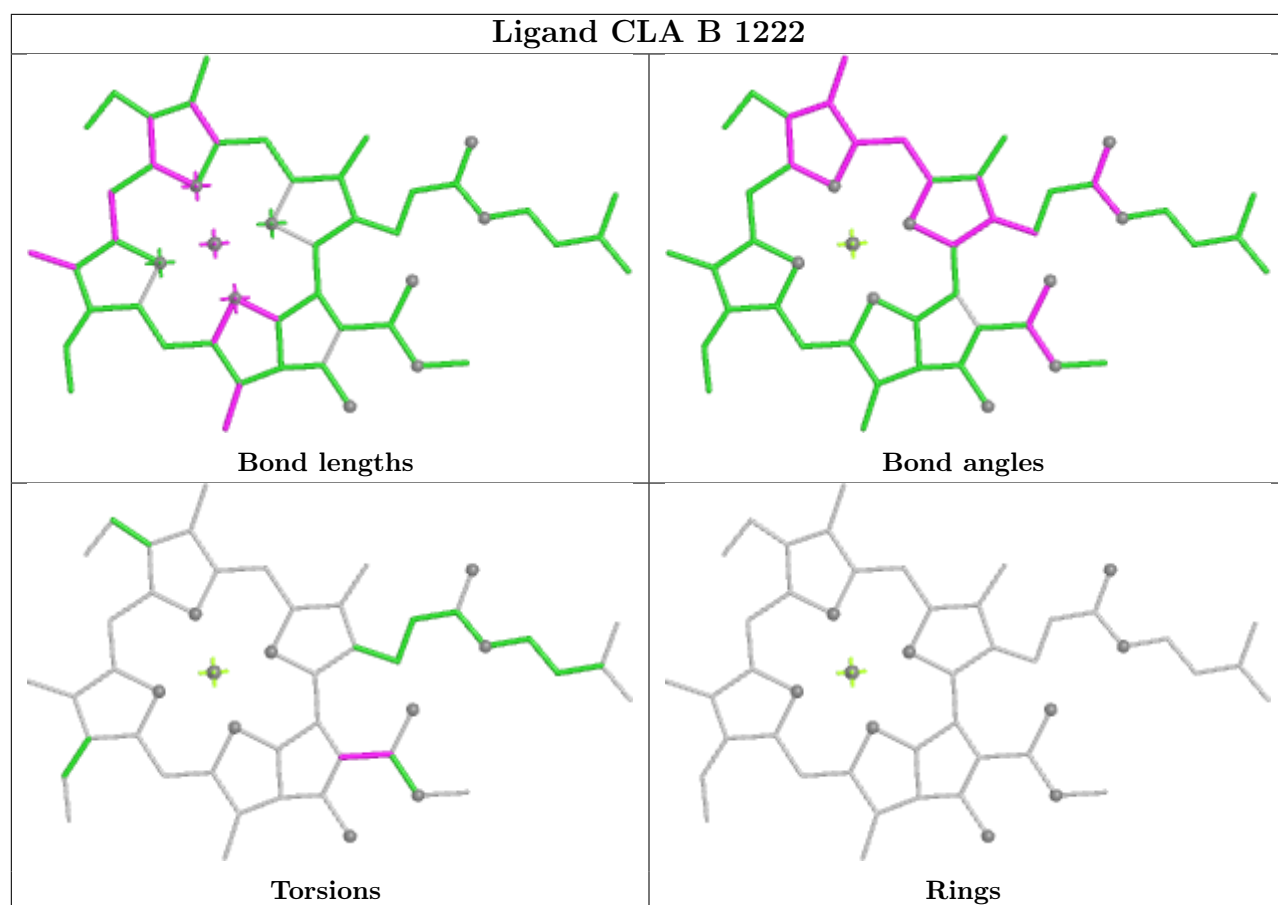
Torsions



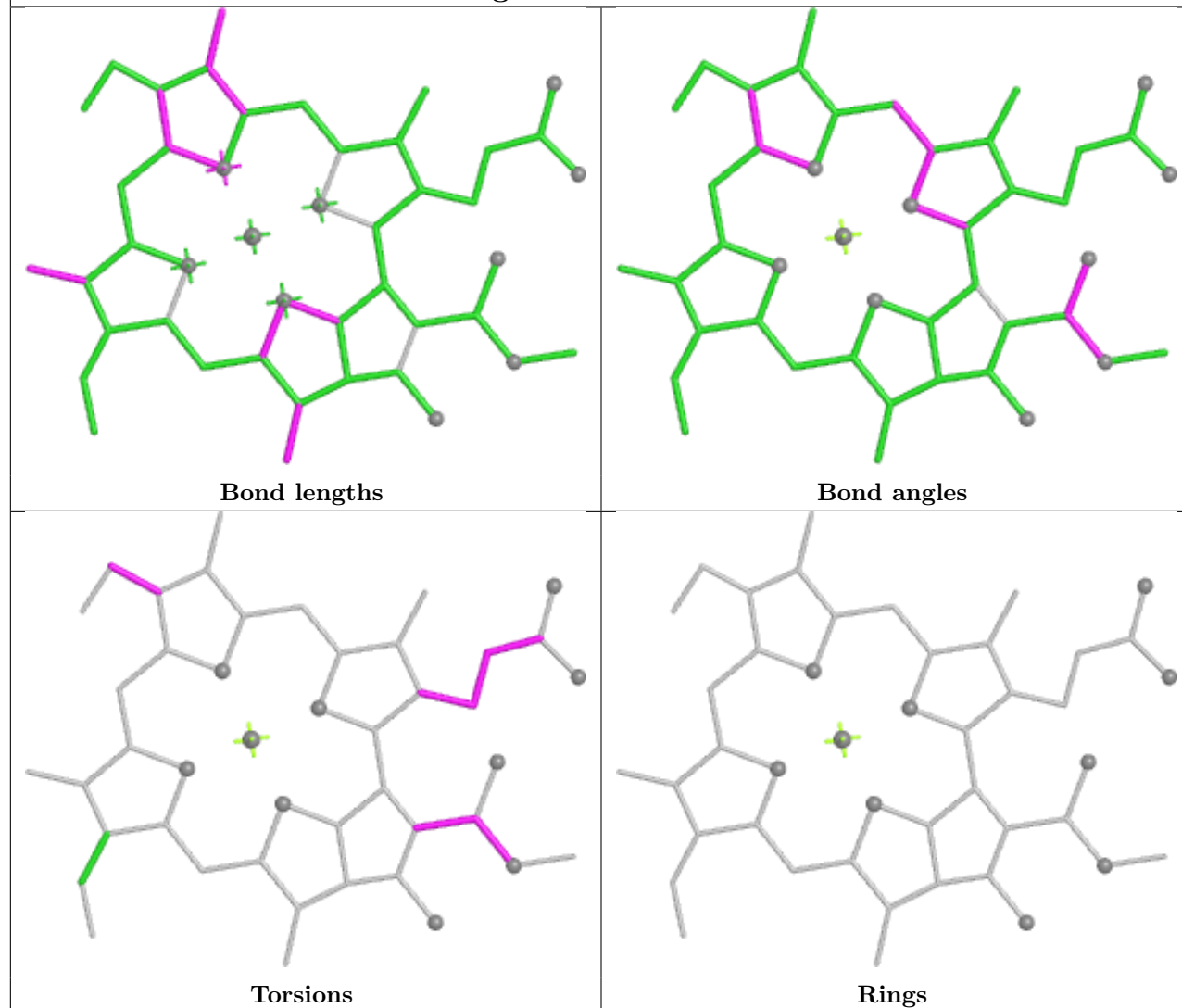
Rings

Ligand CLA a 507

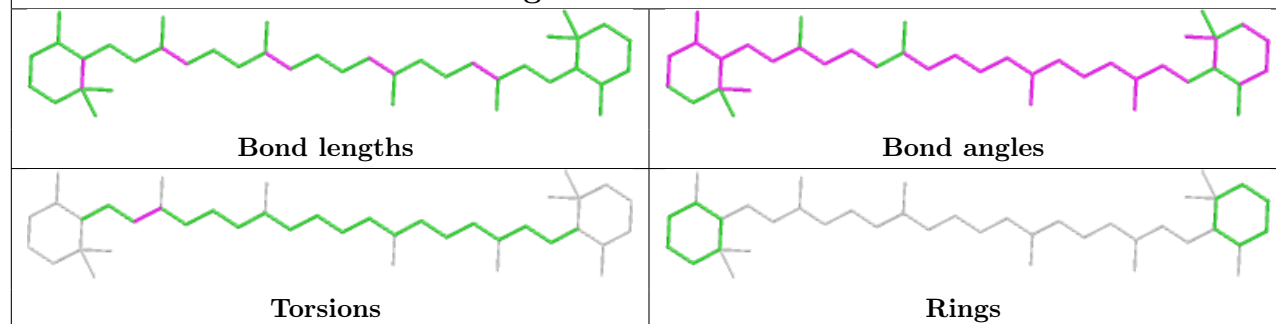


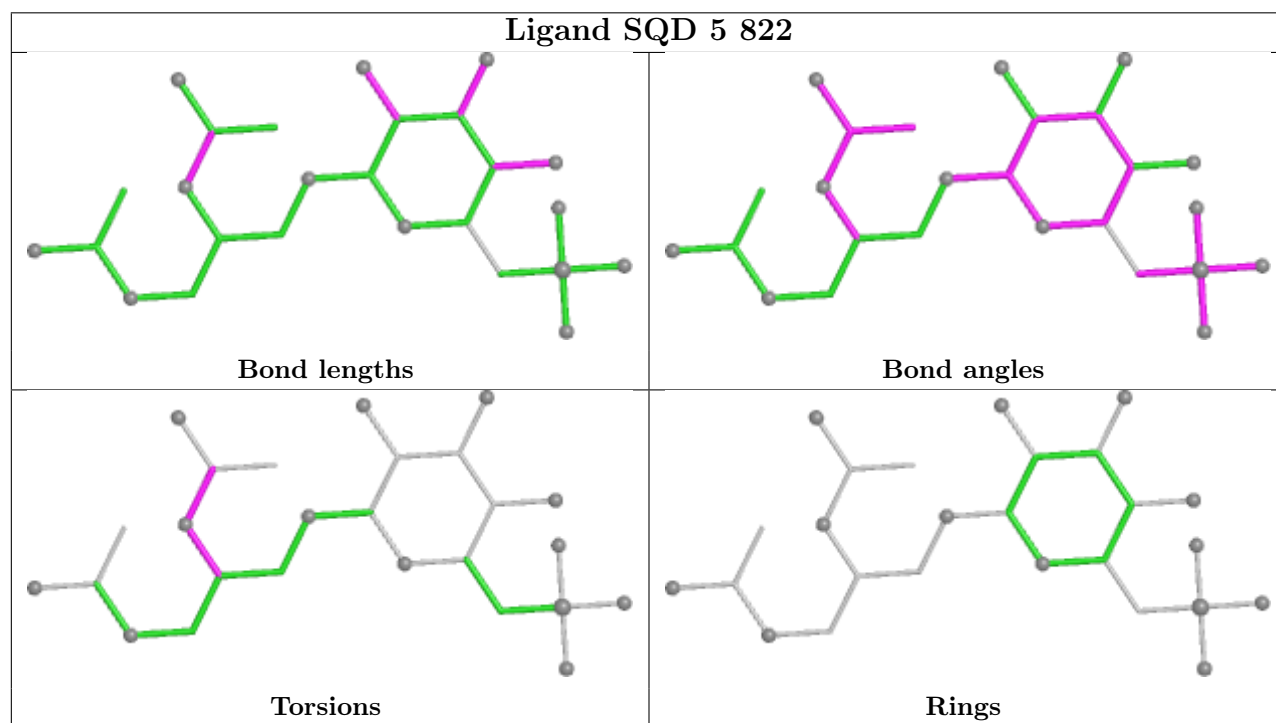
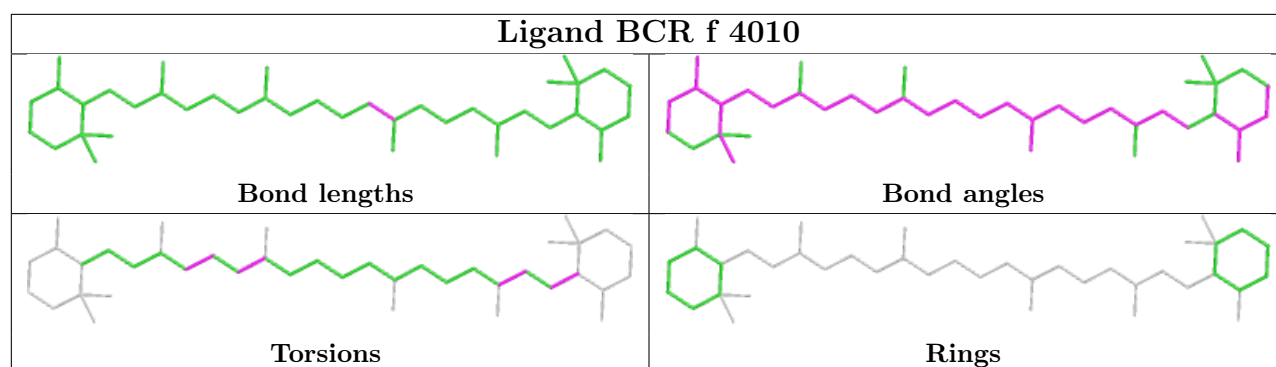


Ligand CLA Y 501

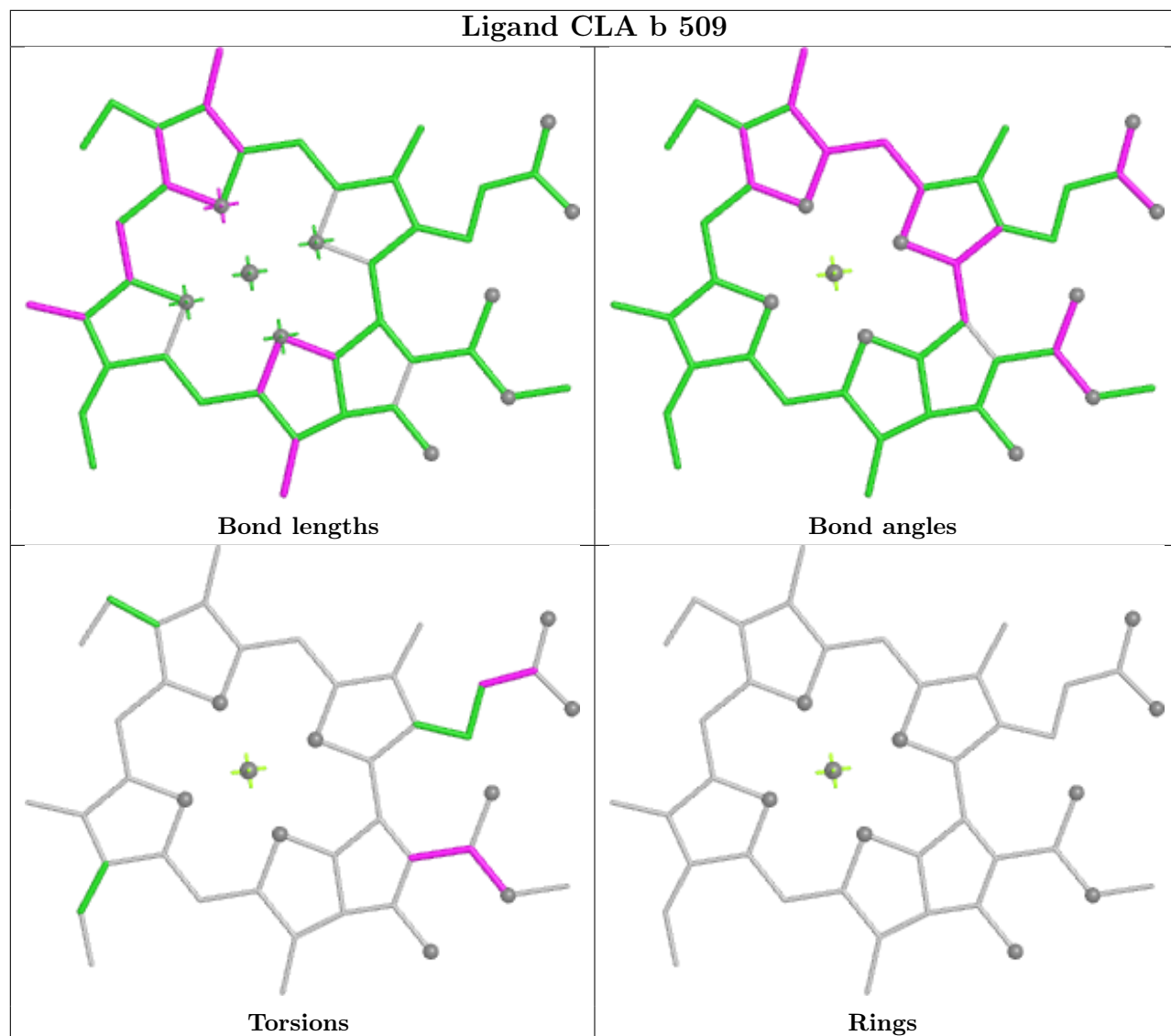


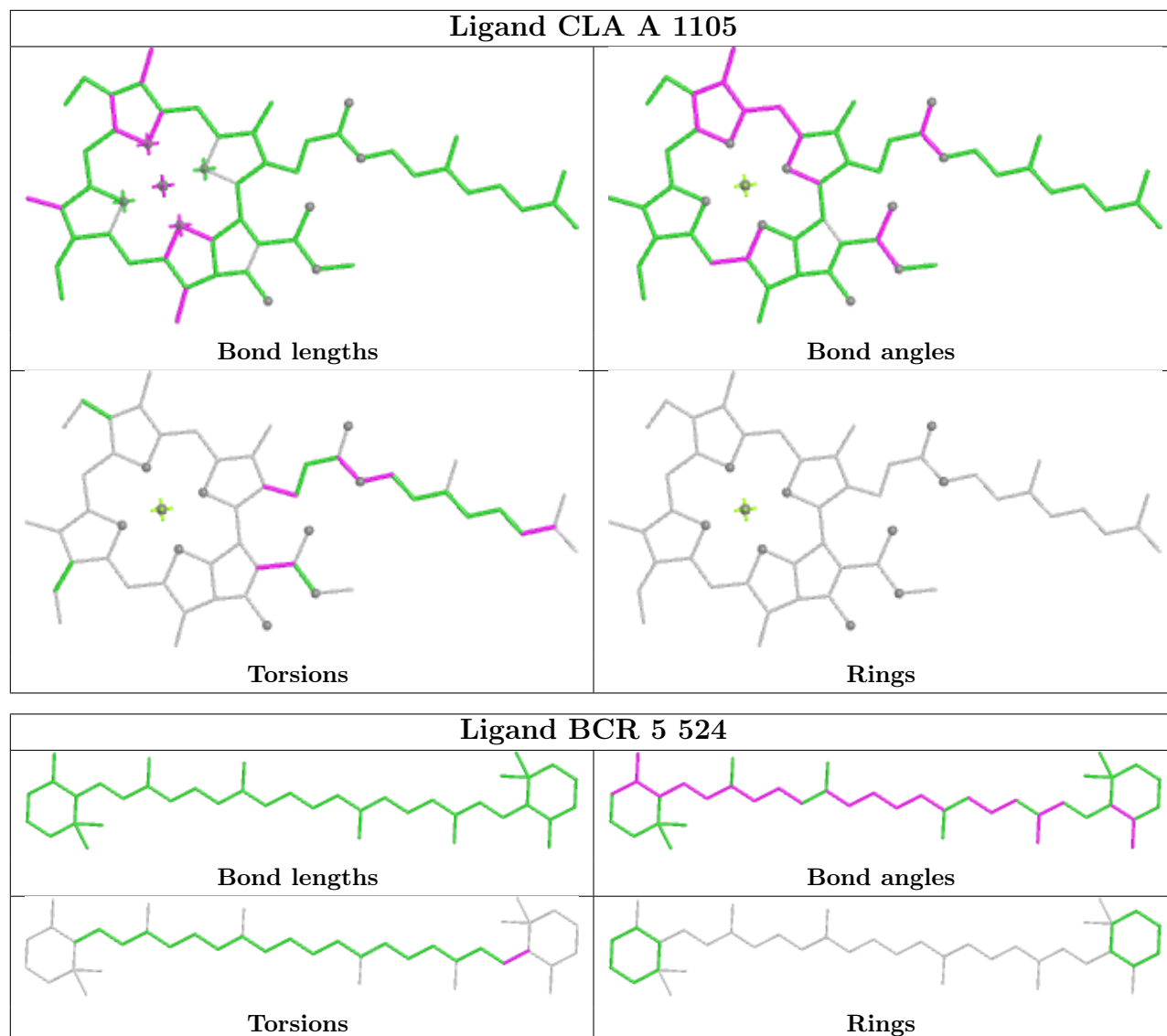
Ligand BCR L 4219



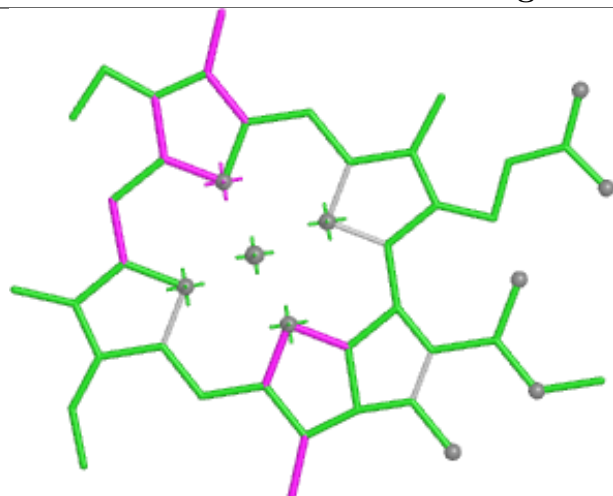


Ligand CLA b 509

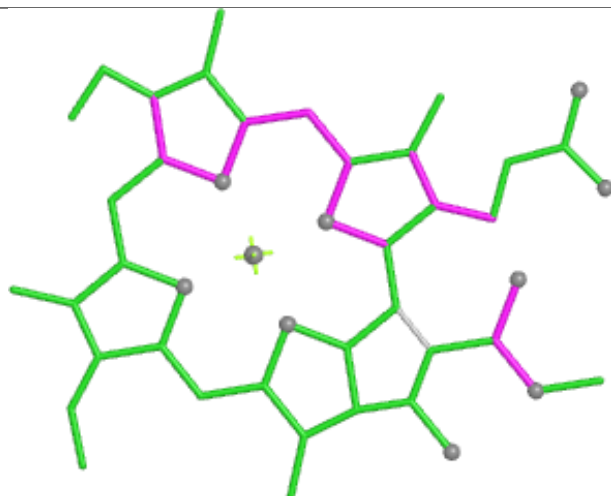




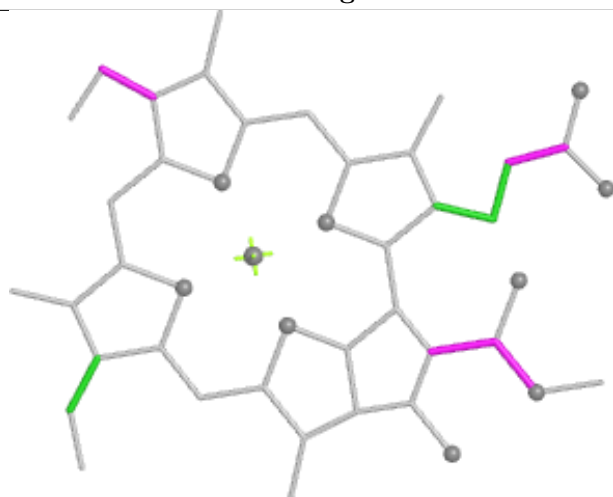
Ligand CLA u 512



Bond lengths



Bond angles

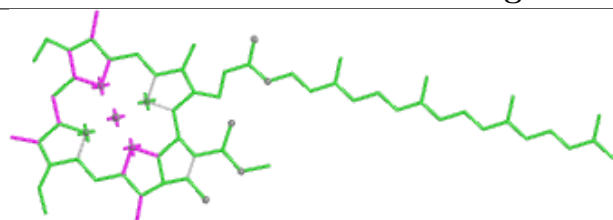


Torsions

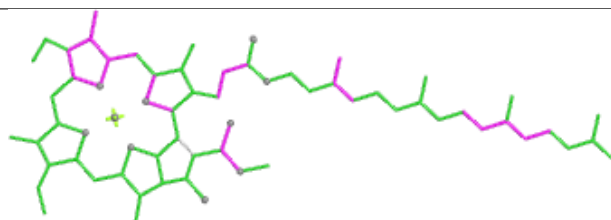


Rings

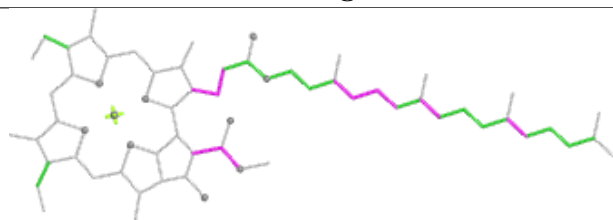
Ligand CLA H 1012



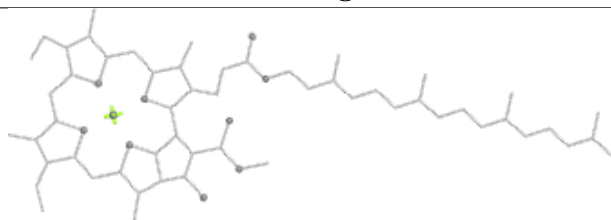
Bond lengths



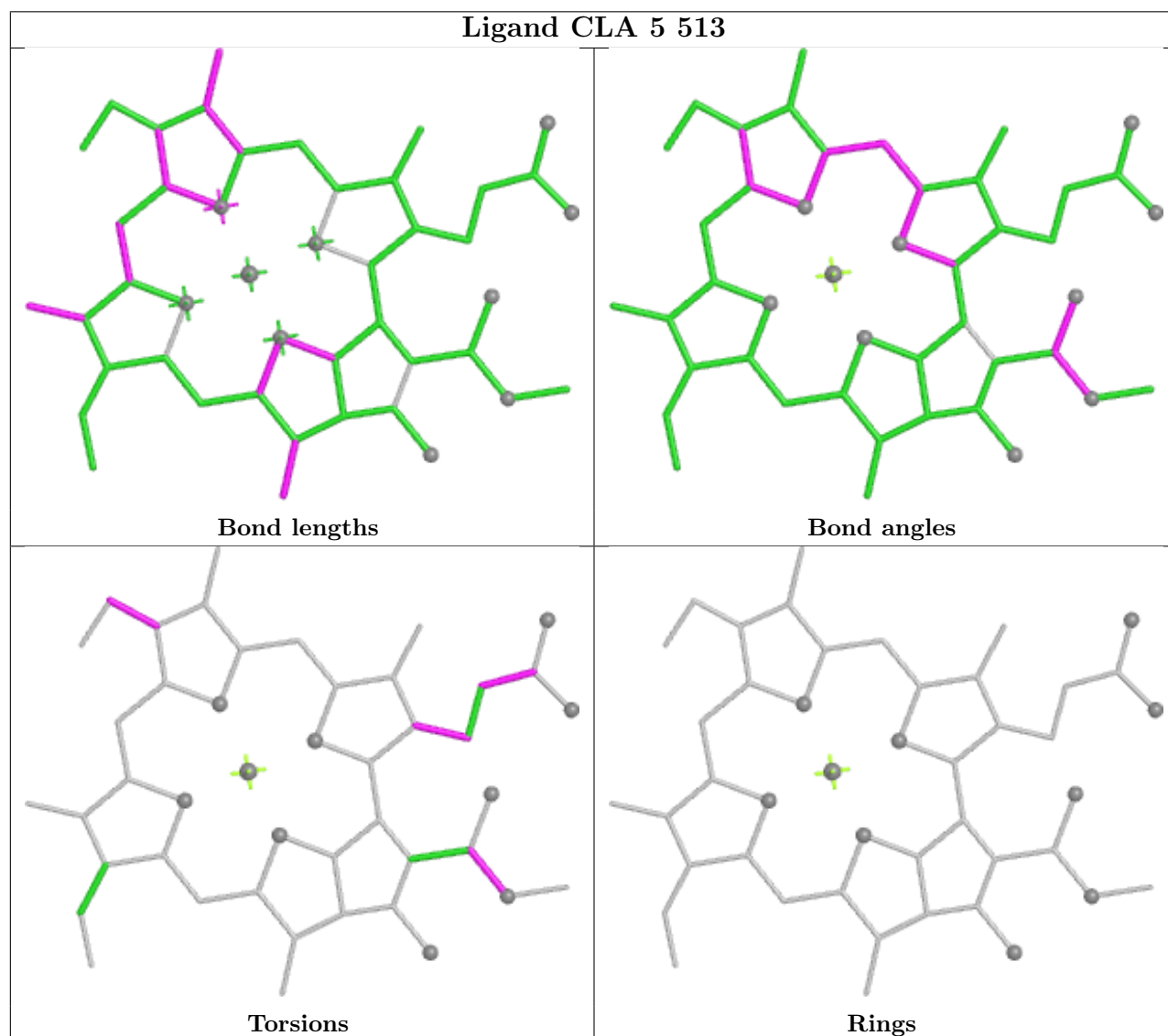
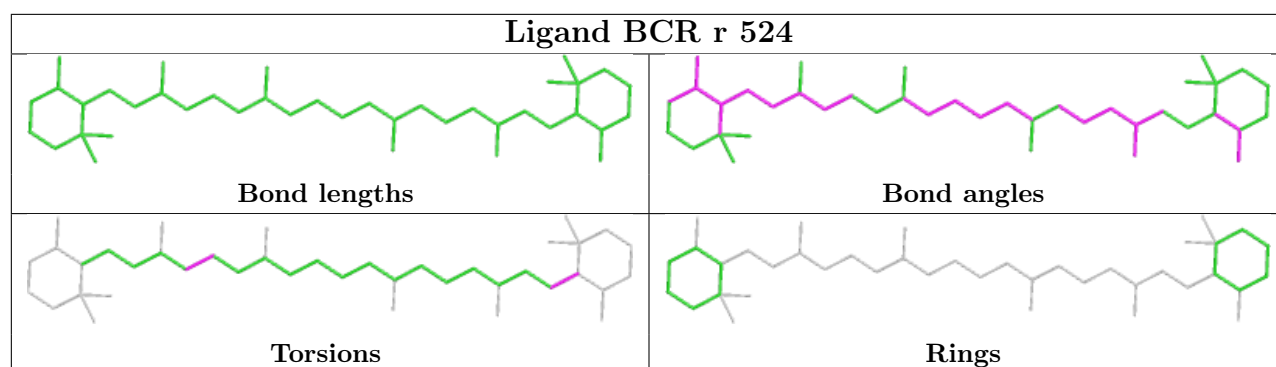
Bond angles



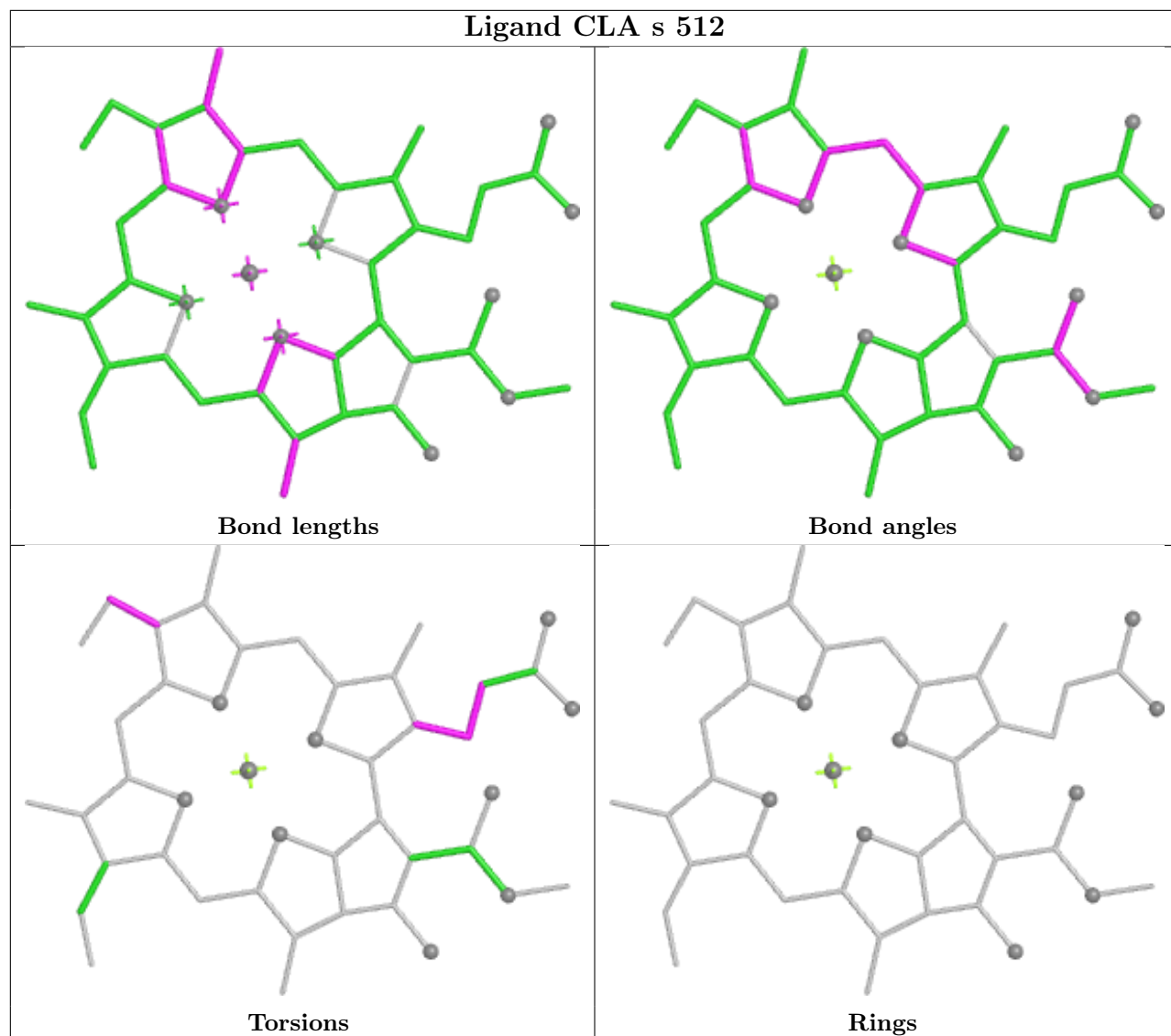
Torsions



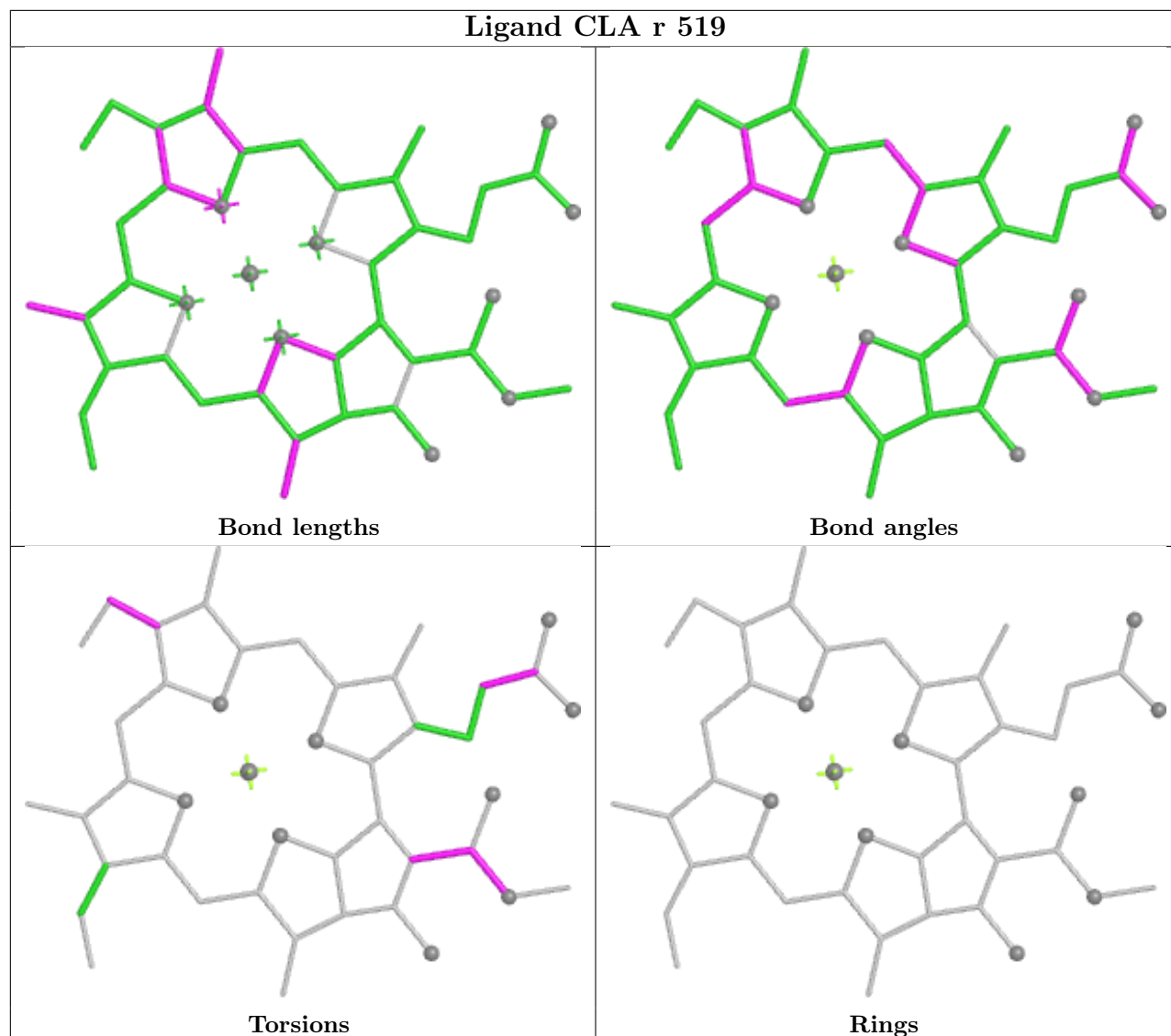
Rings



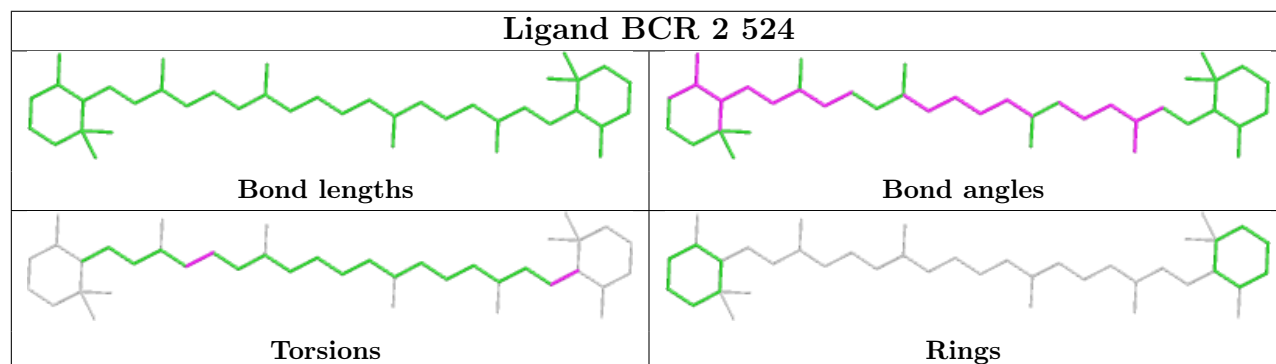
Ligand CLA s 512

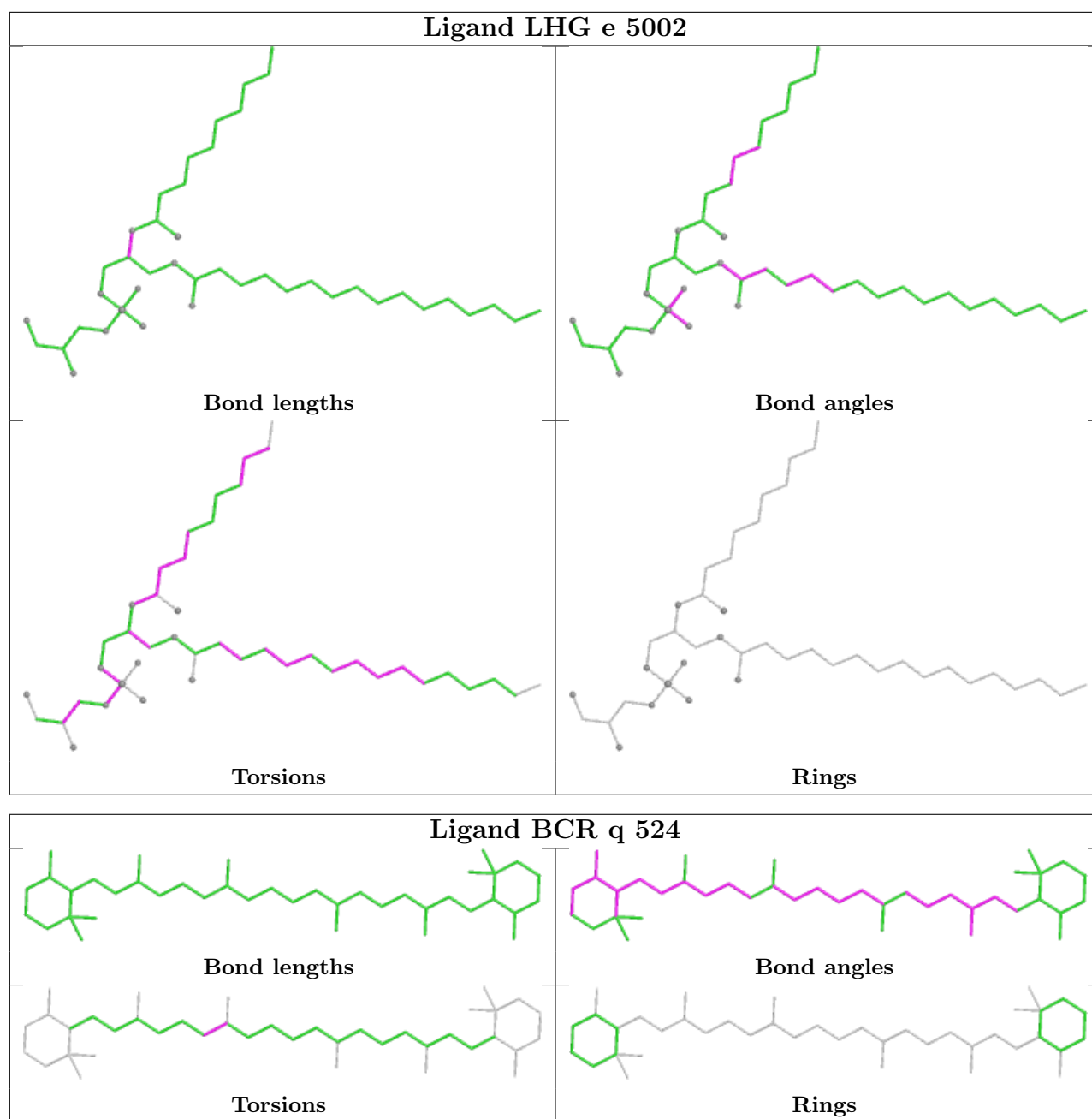


Ligand CLA r 519

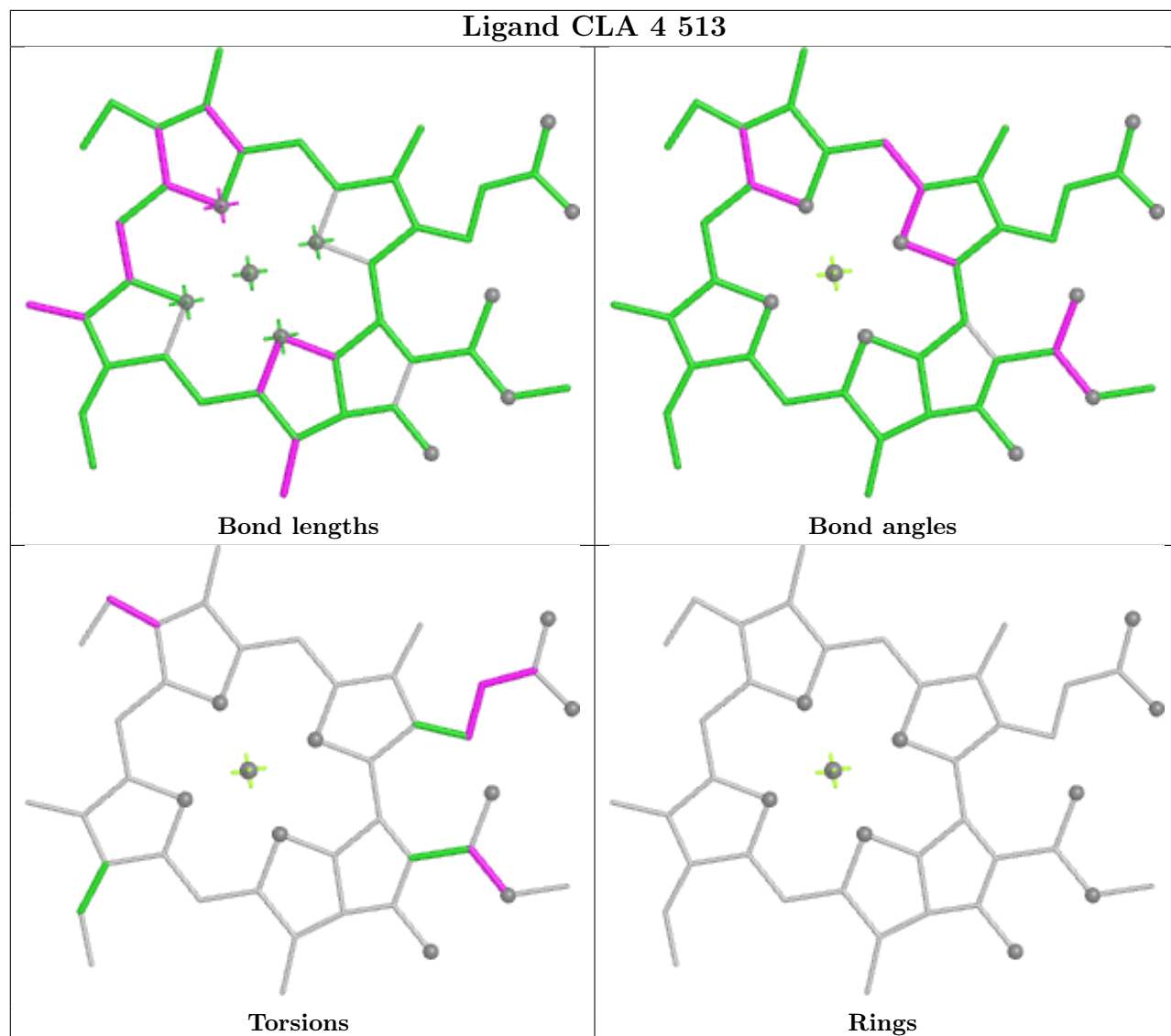


Ligand BCR 2 524

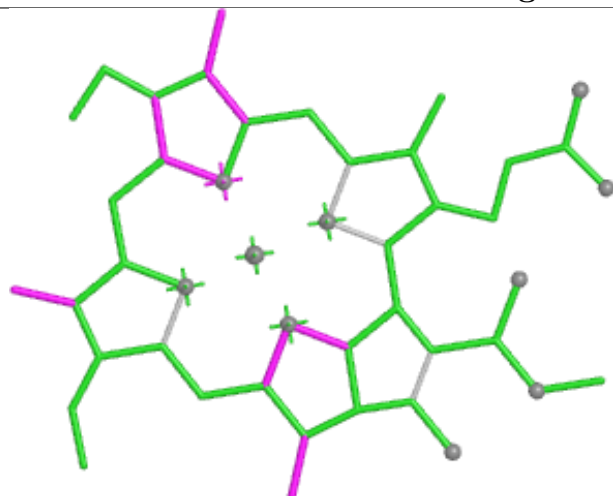




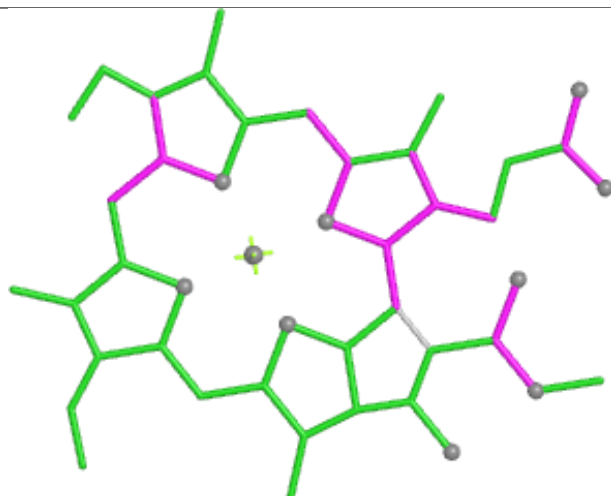
Ligand CLA 4 513



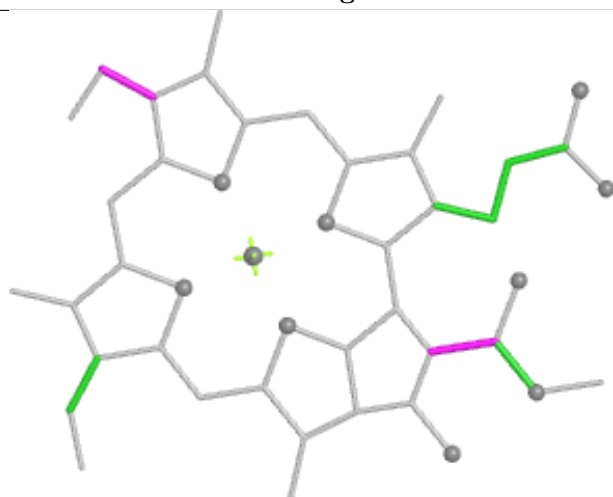
Ligand CLA 2 502



Bond lengths



Bond angles

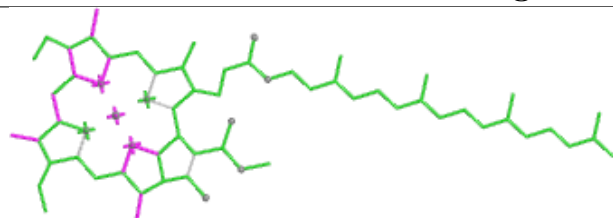


Torsions

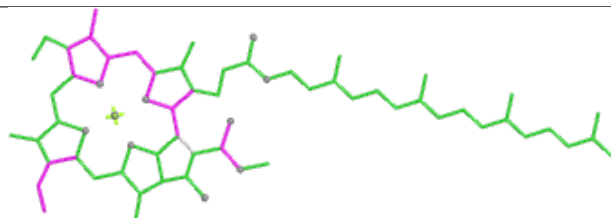


Rings

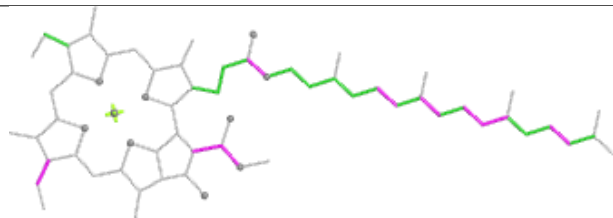
Ligand CLA f 1234



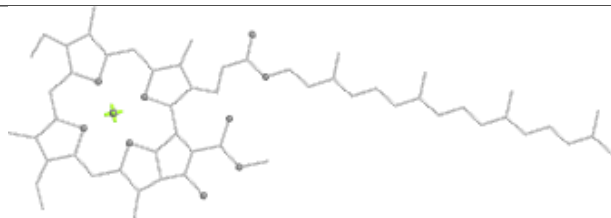
Bond lengths



Bond angles

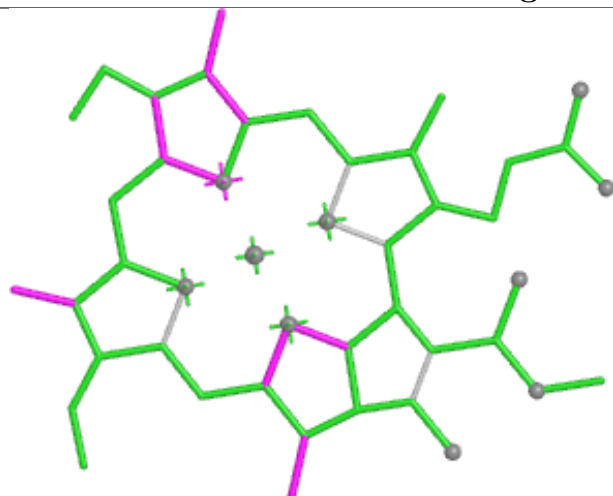


Torsions

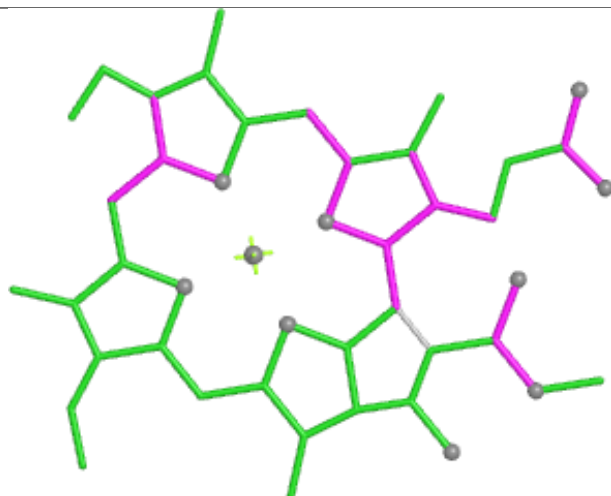


Rings

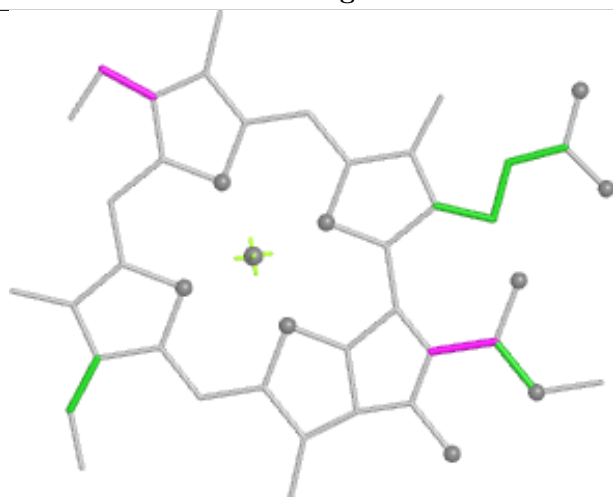
Ligand CLA s 502



Bond lengths



Bond angles

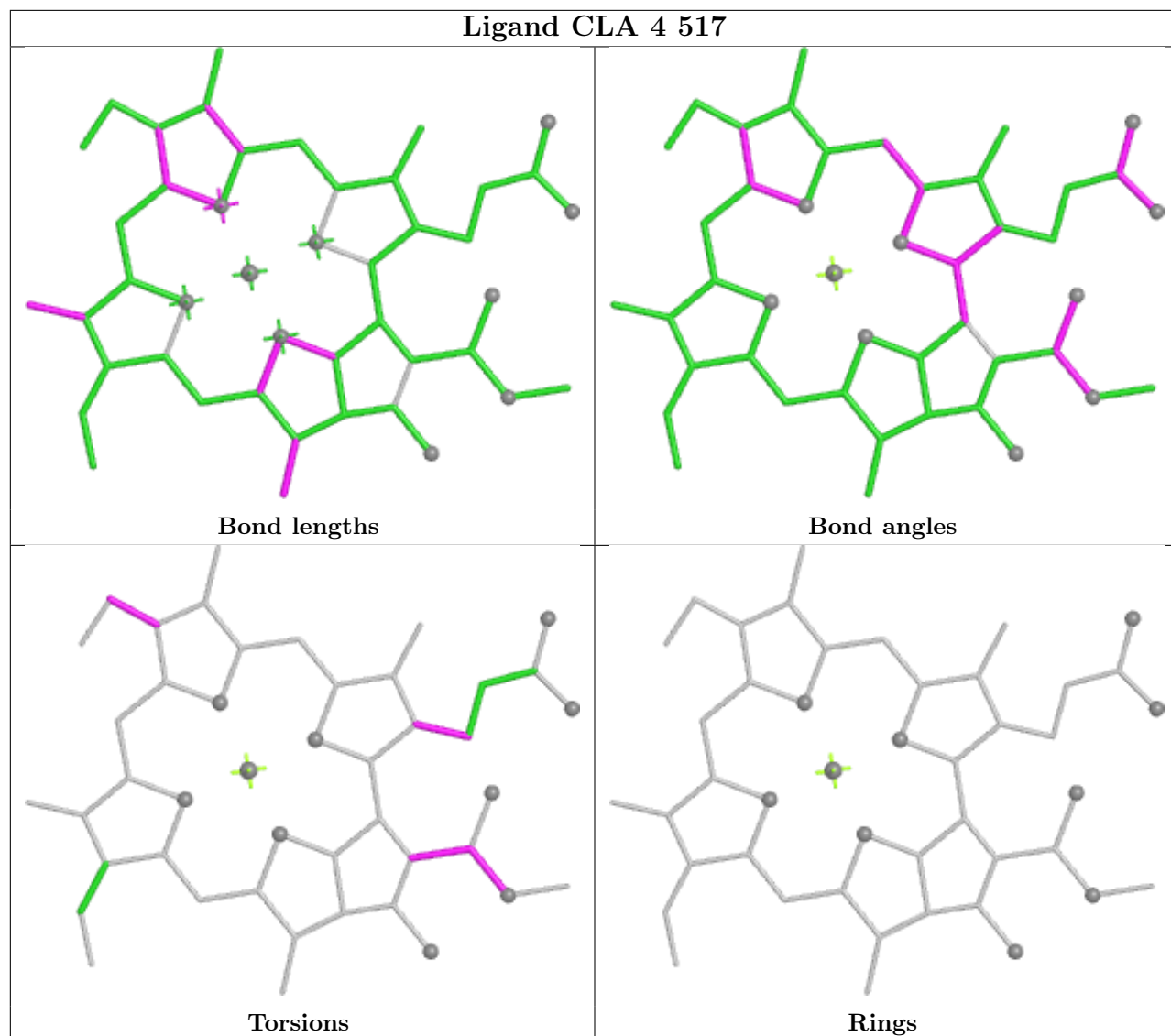


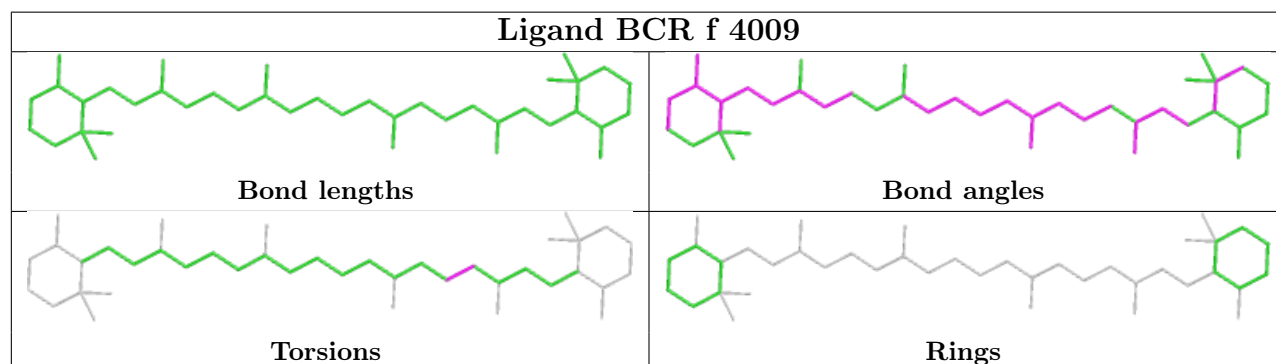
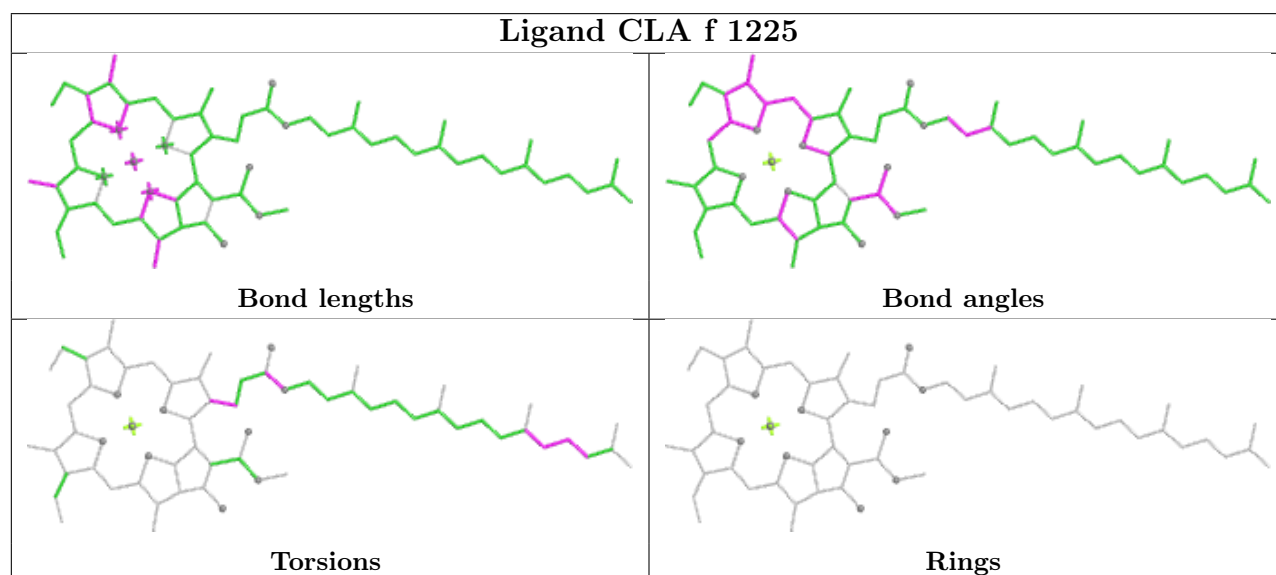
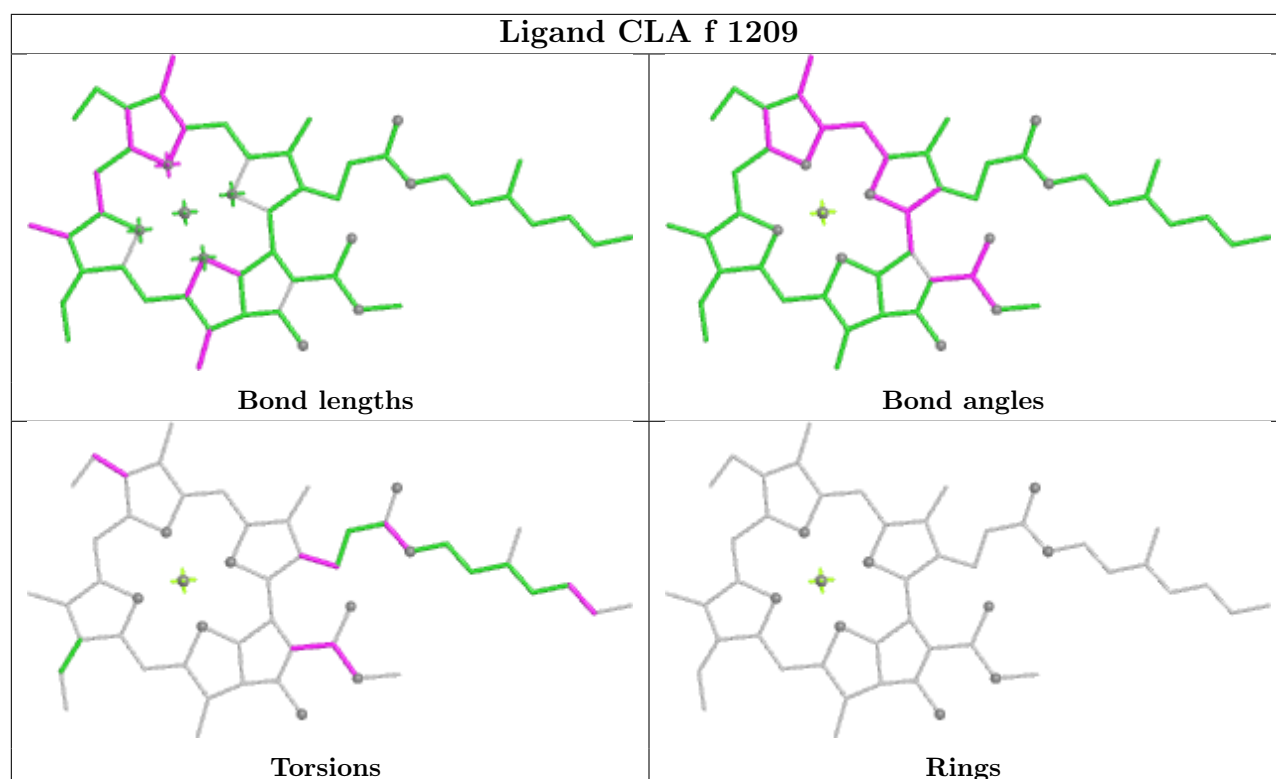
Torsions



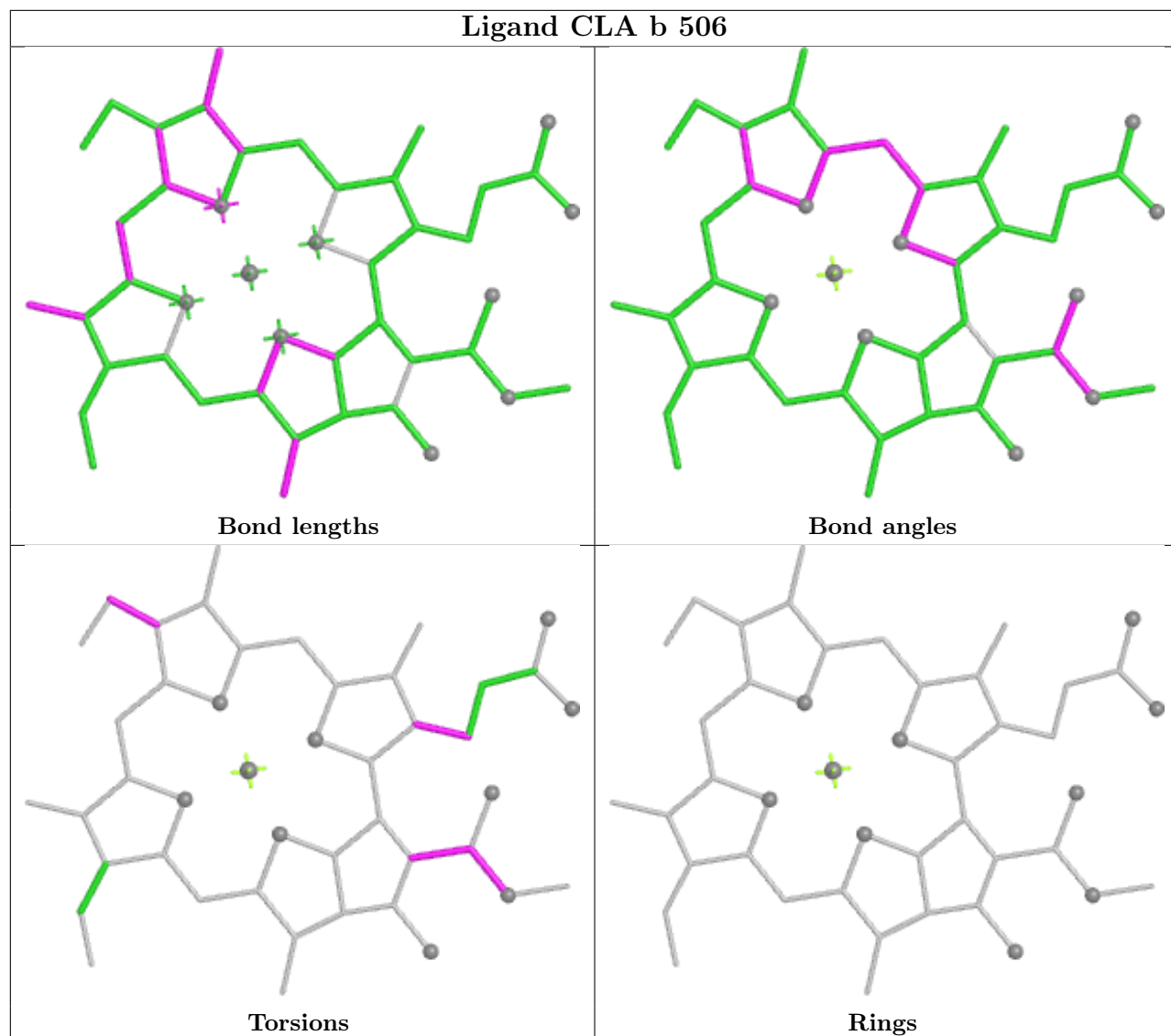
Rings

Ligand CLA 4 517

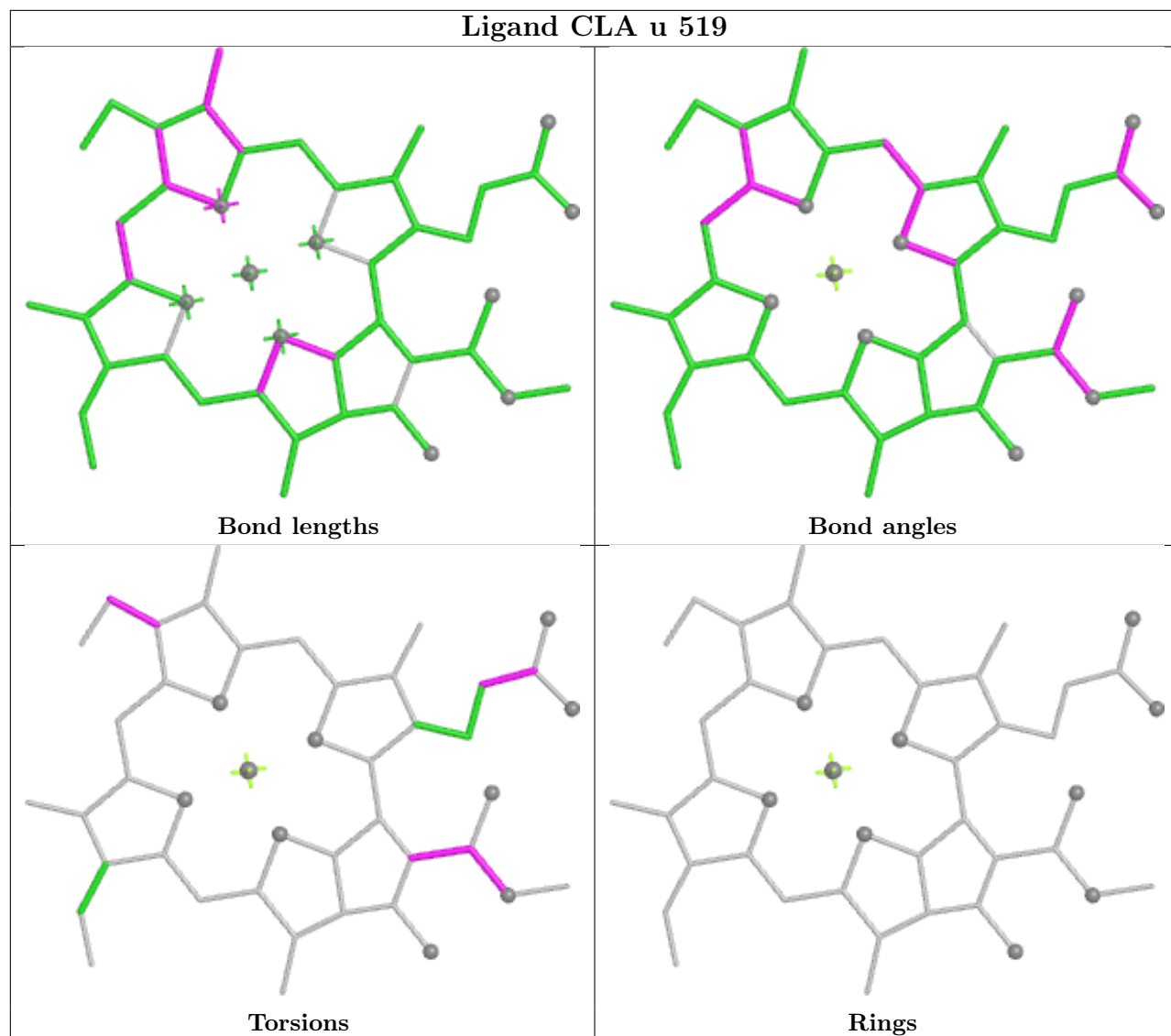




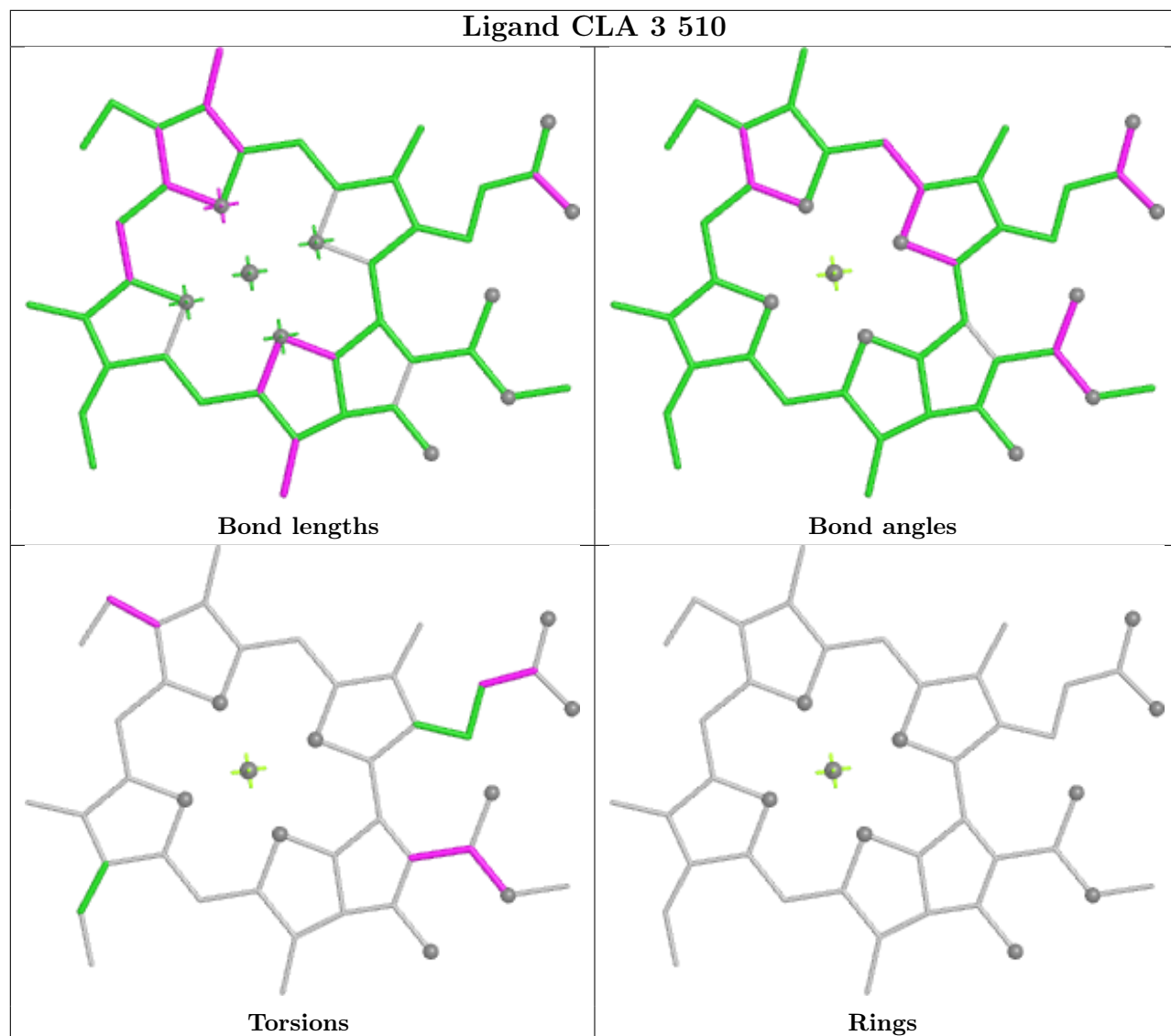
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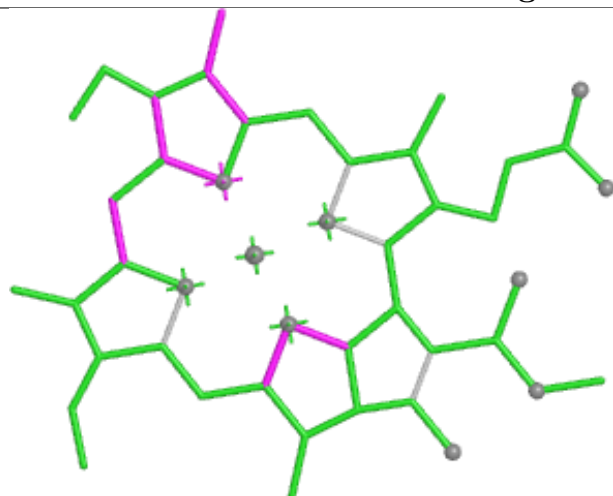
Ligand CLA u 519



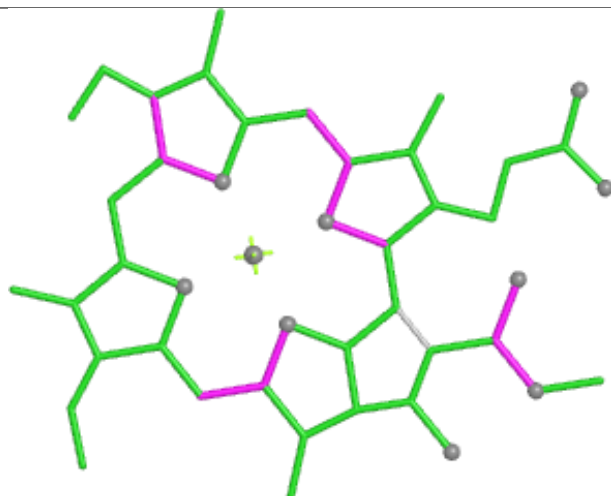
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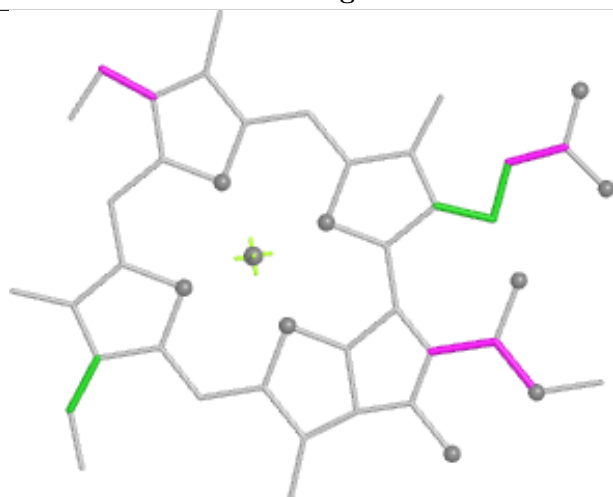
Ligand CLA 6 511



Bond lengths



Bond angles

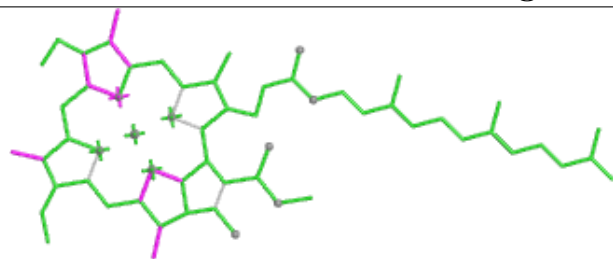


Torsions

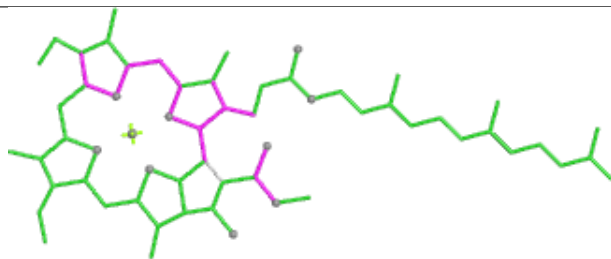


Rings

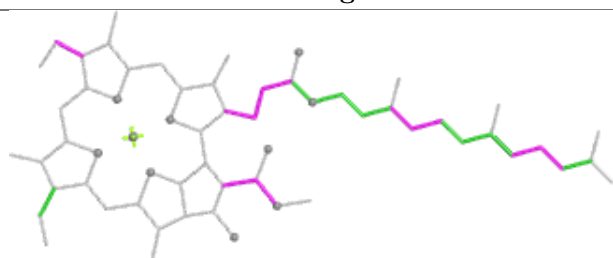
Ligand CLA 2 501



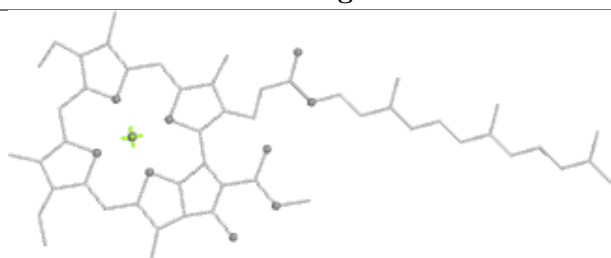
Bond lengths



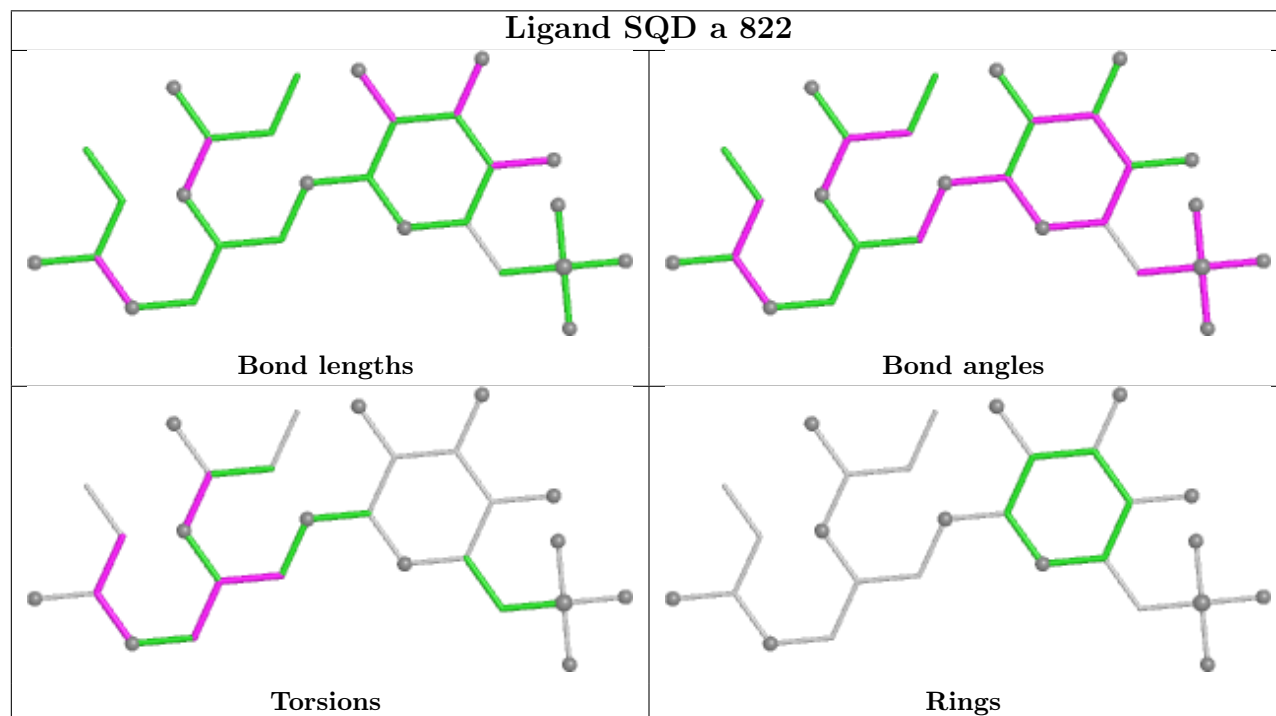
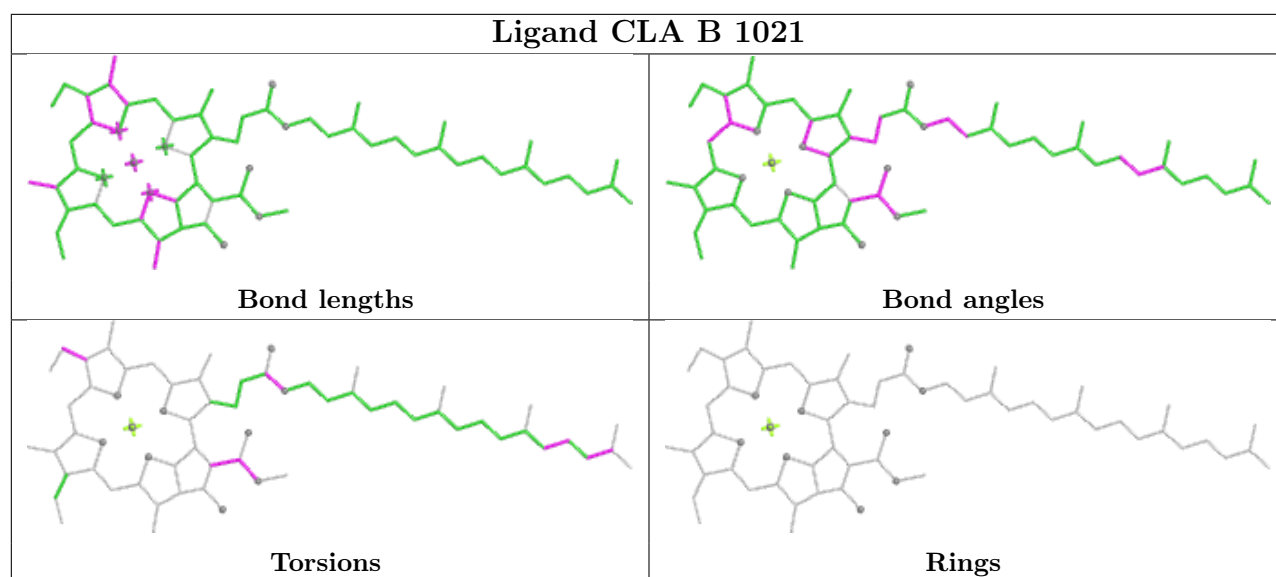
Bond angles

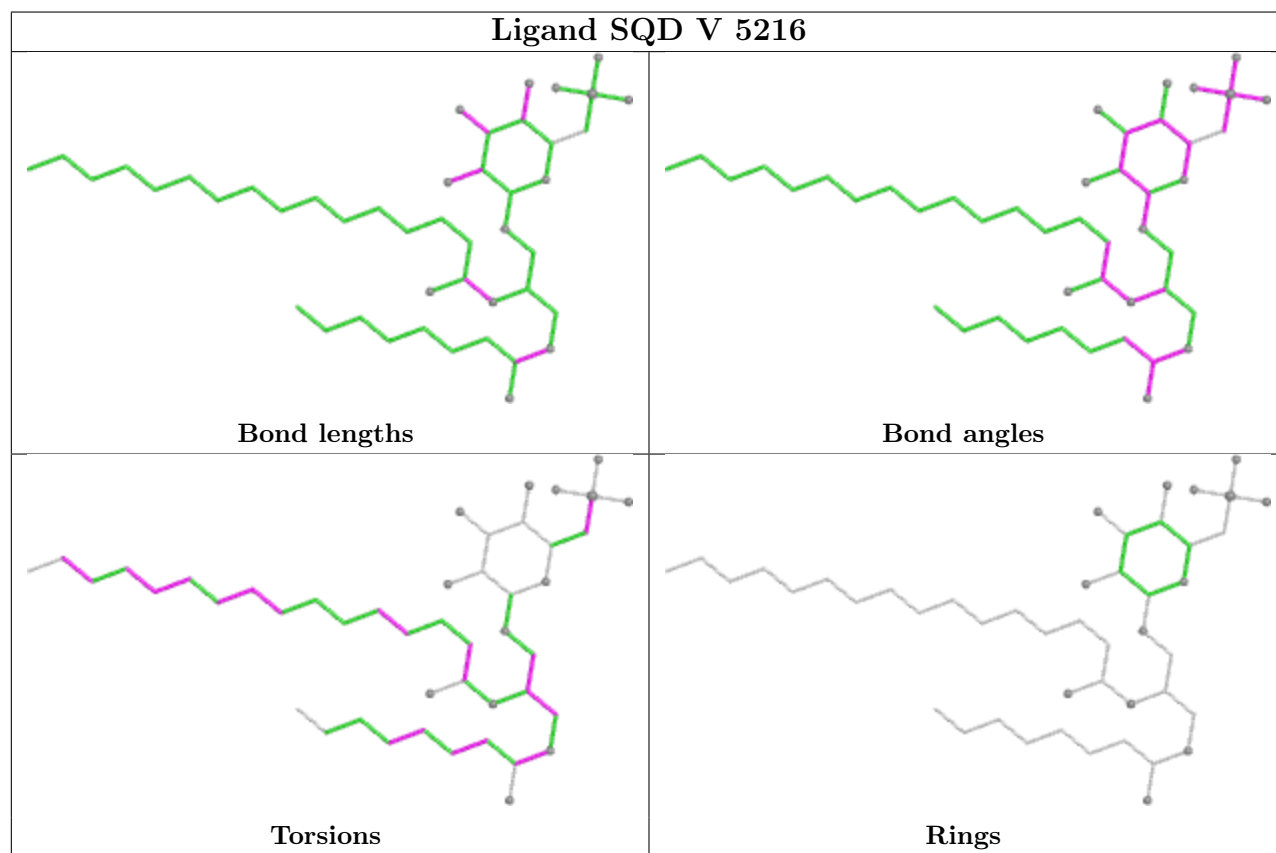
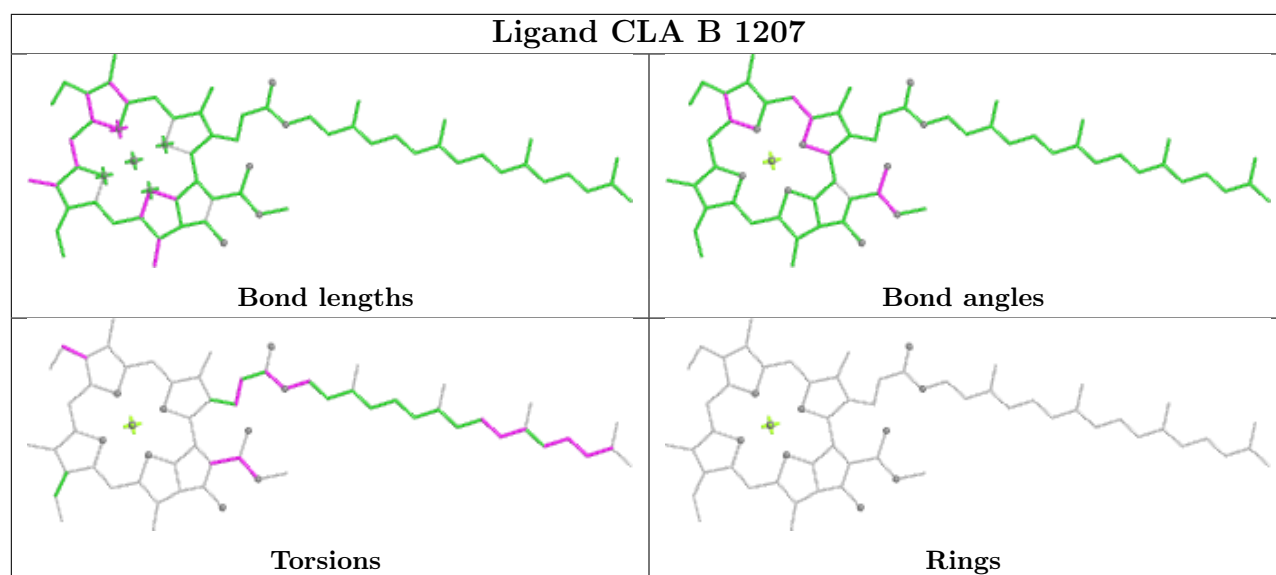


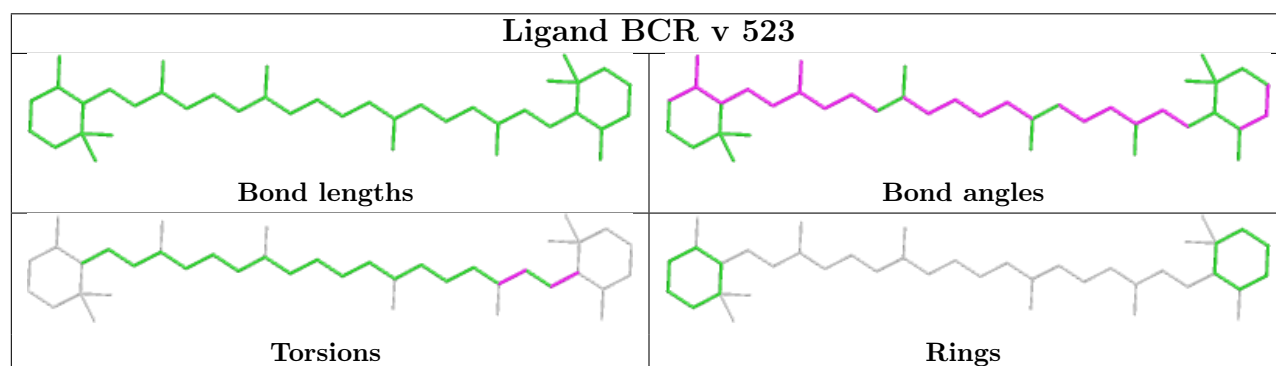
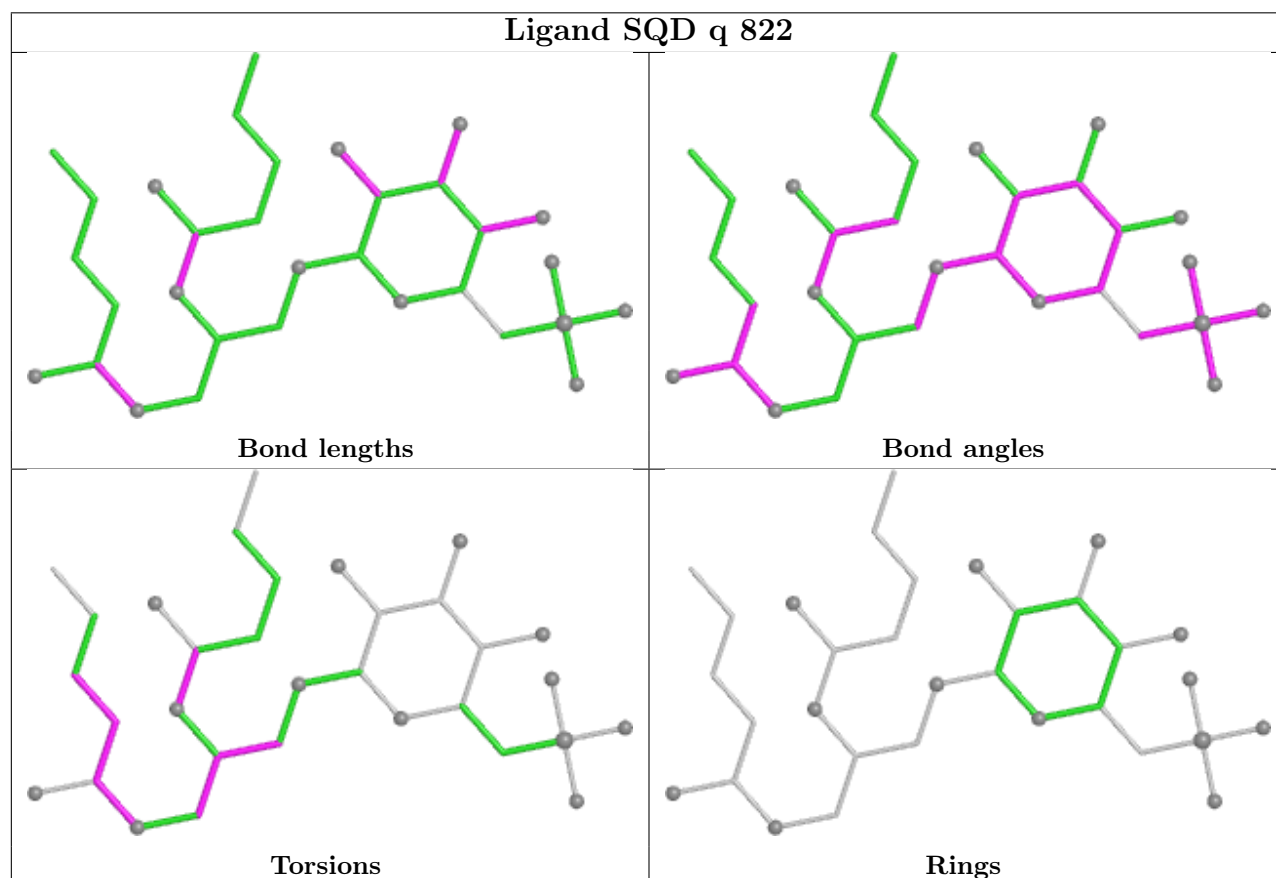
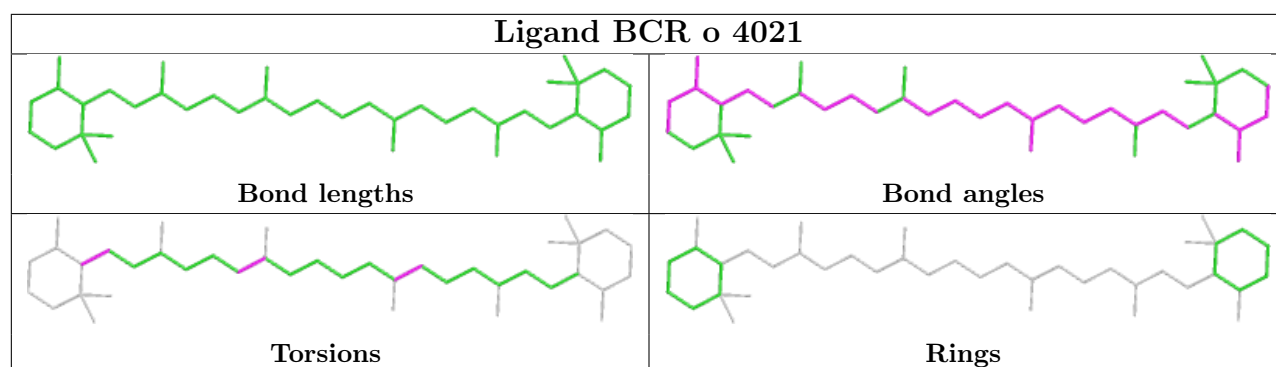
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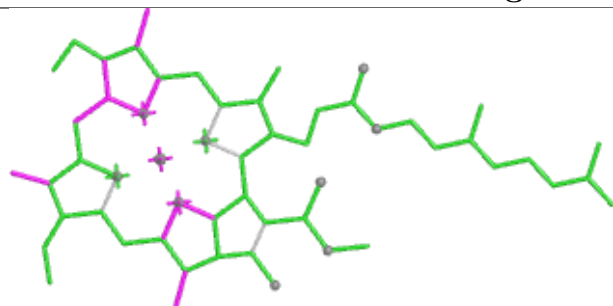


Rings

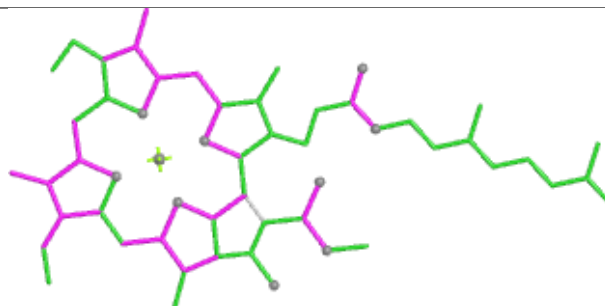




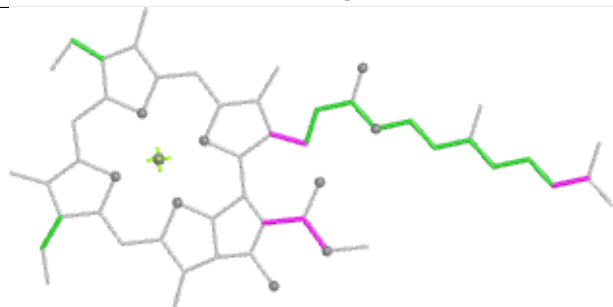


Ligand CLA B 1226

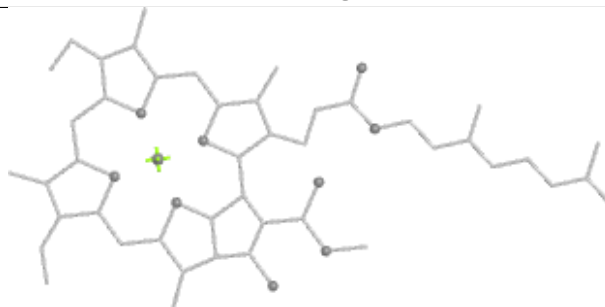
Bond lengths



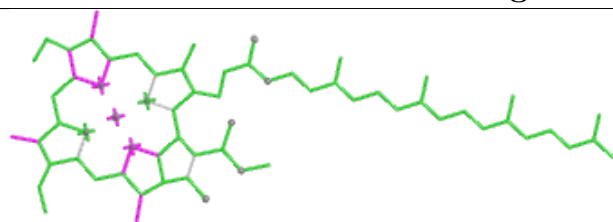
Bond angles



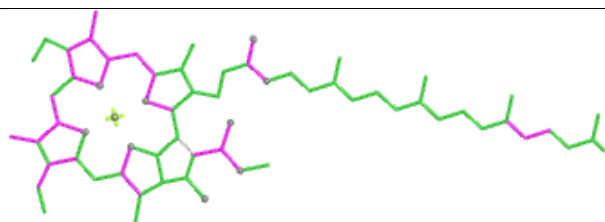
Torsions



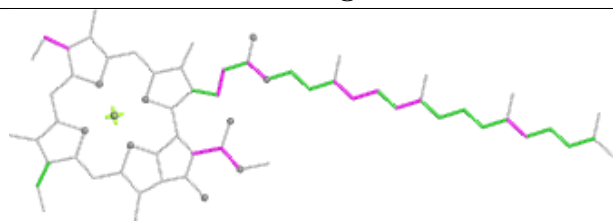
Rings

Ligand CLA e 1119

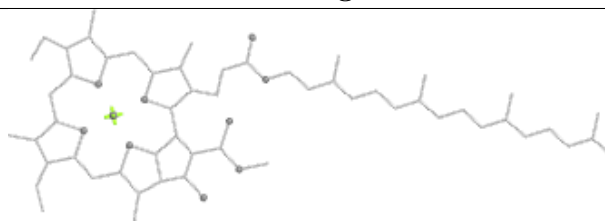
Bond lengths



Bond angles

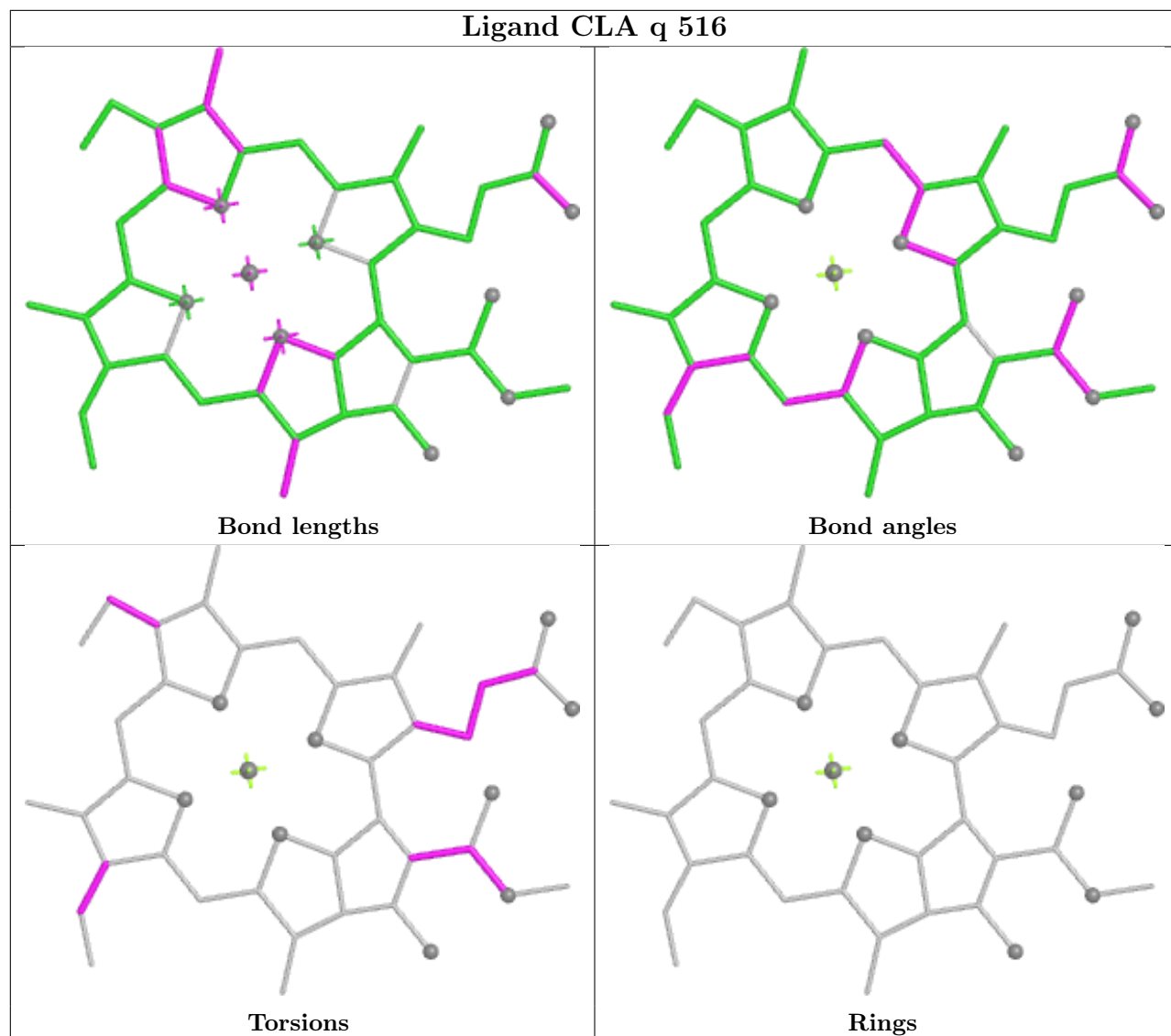


Torsions

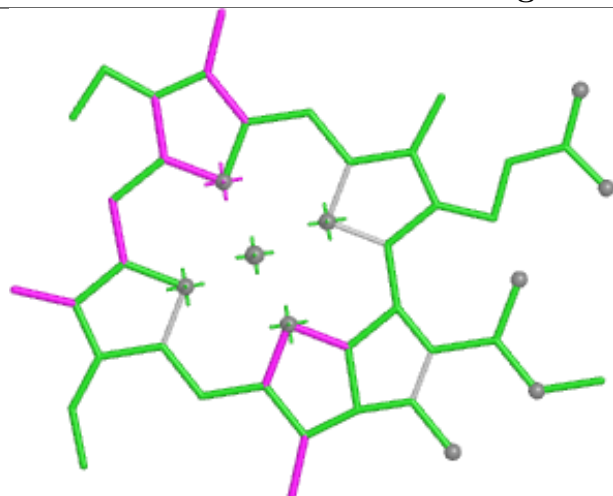


Rings

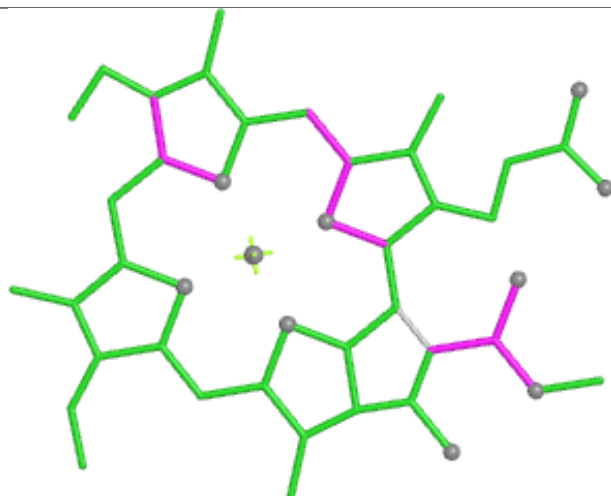
Ligand CLA q 516



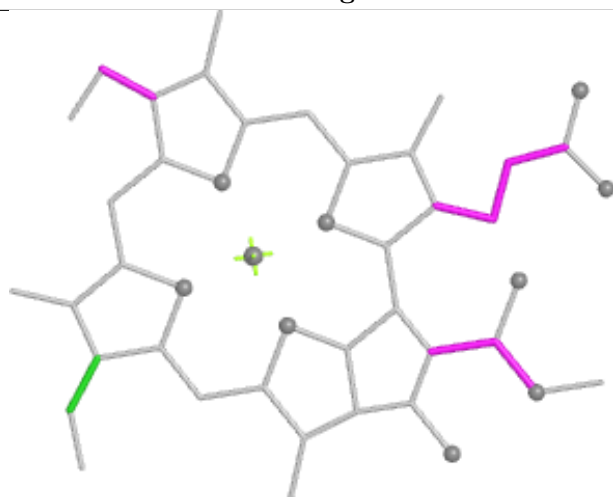
Ligand CLA d 501



Bond lengths



Bond angles

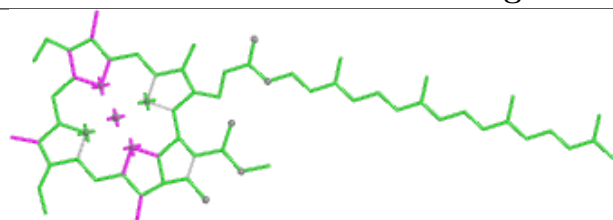


Torsions

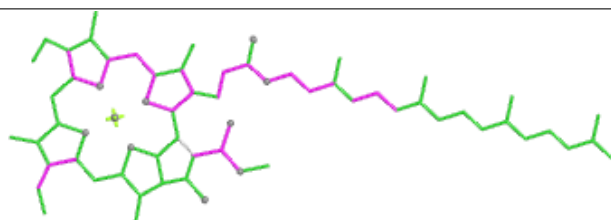


Rings

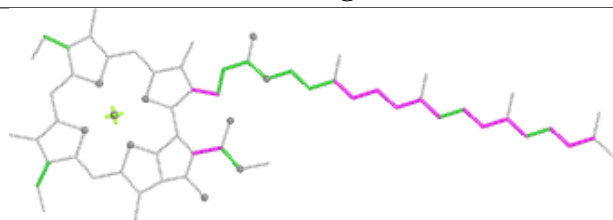
Ligand CLA G 1101



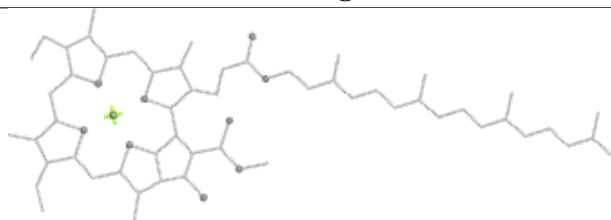
Bond lengths



Bond angles

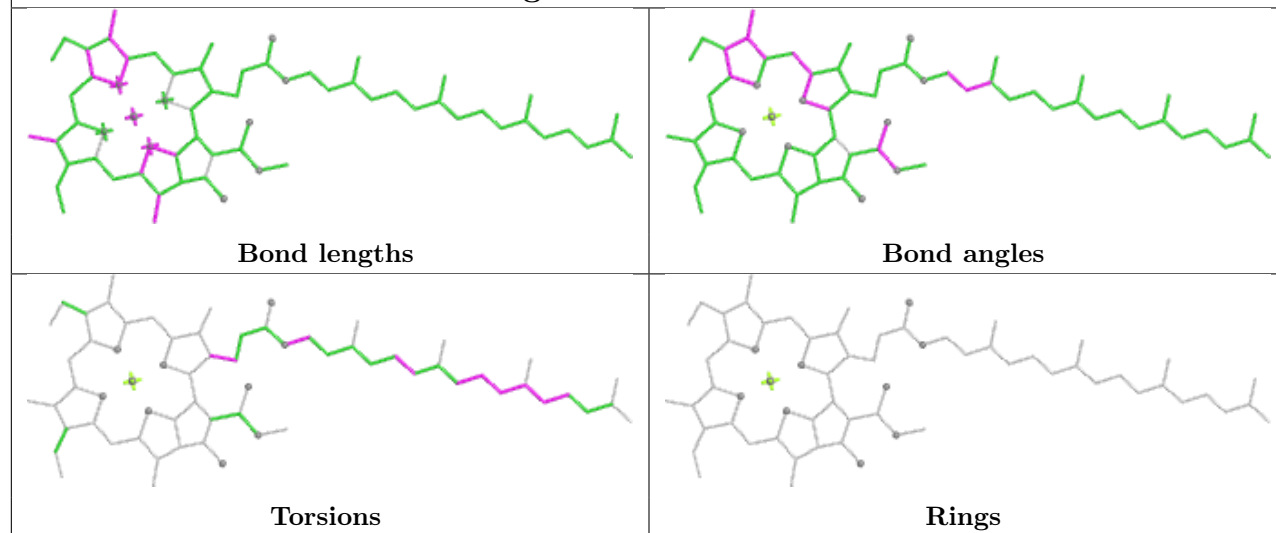


Torsions

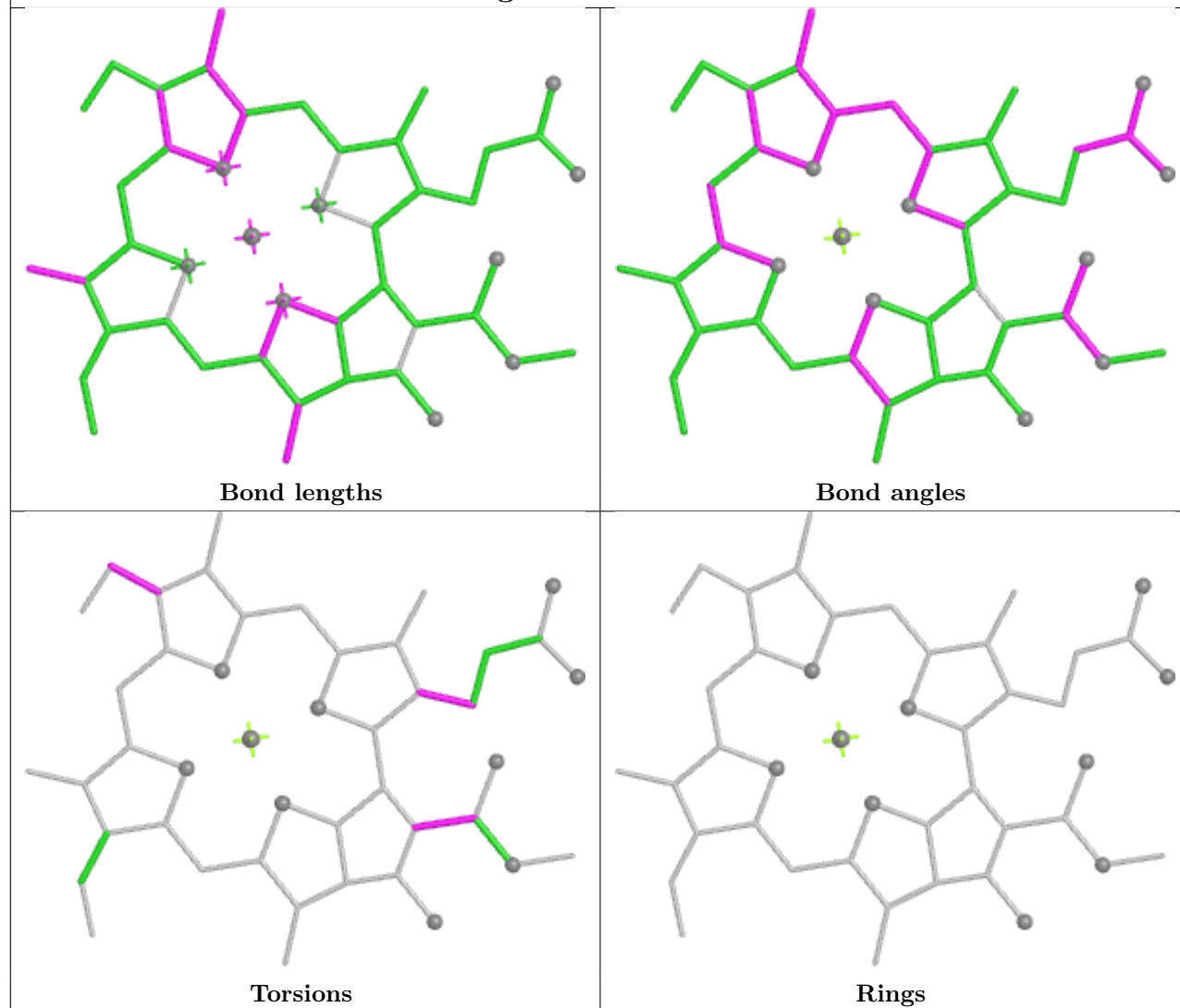


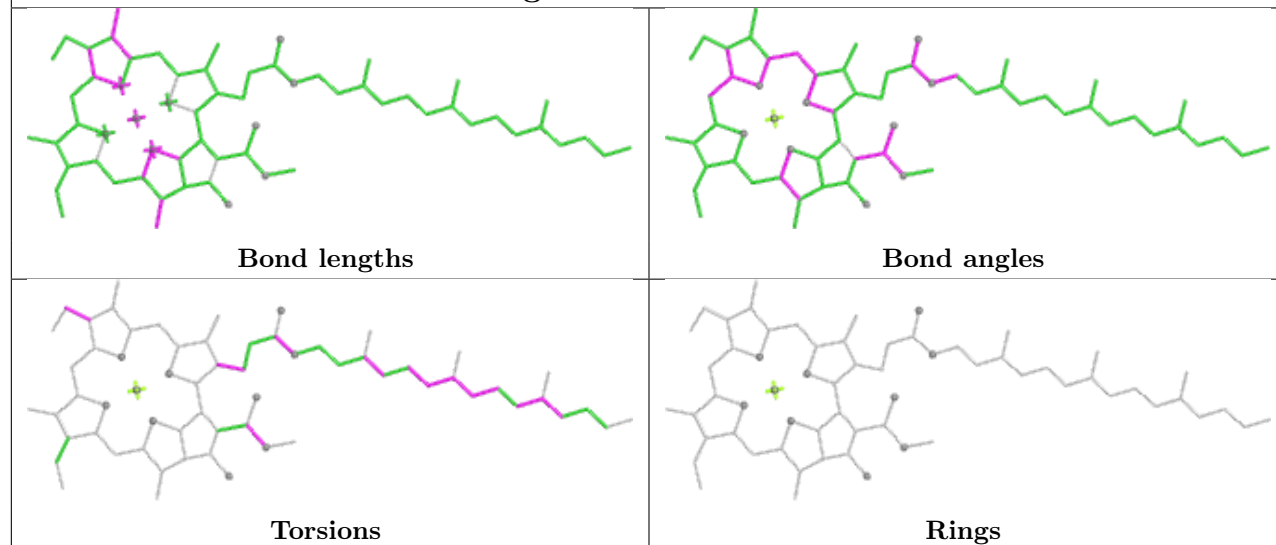
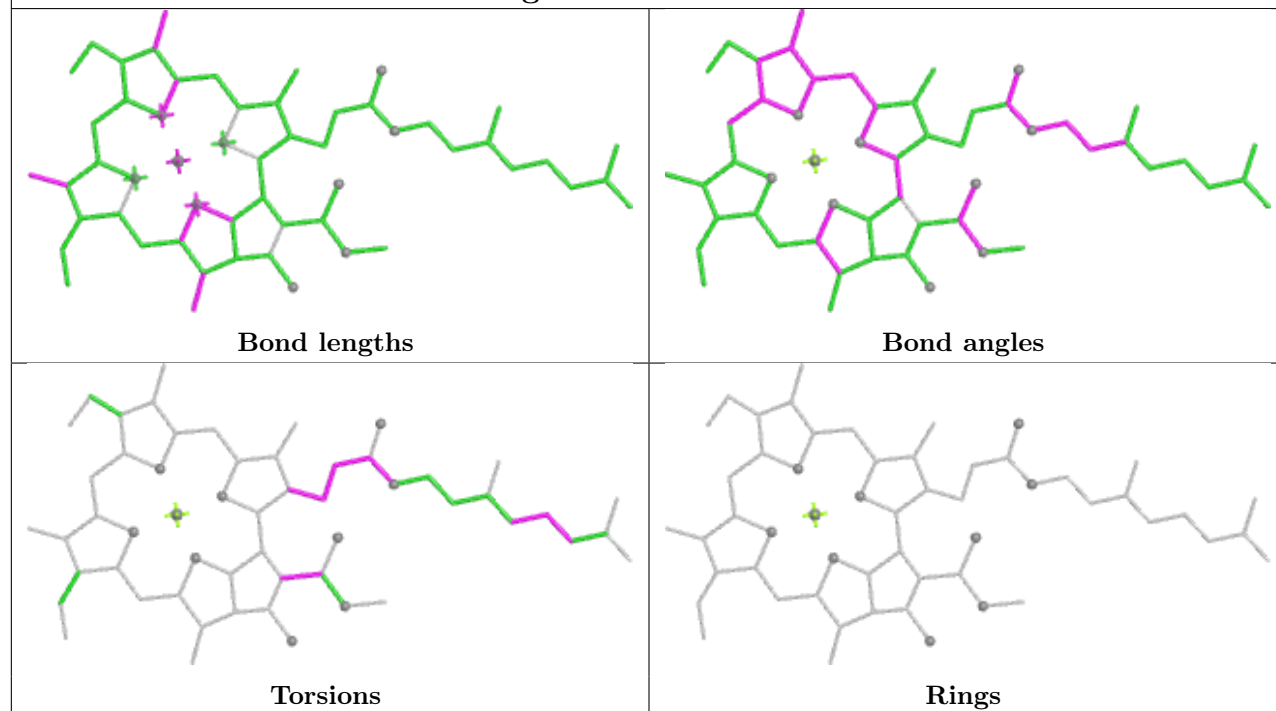
Rings

Ligand CLA B 1223

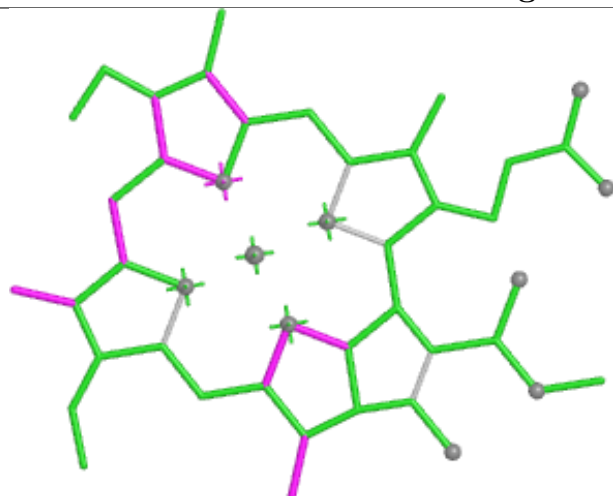


Ligand CLA r 508

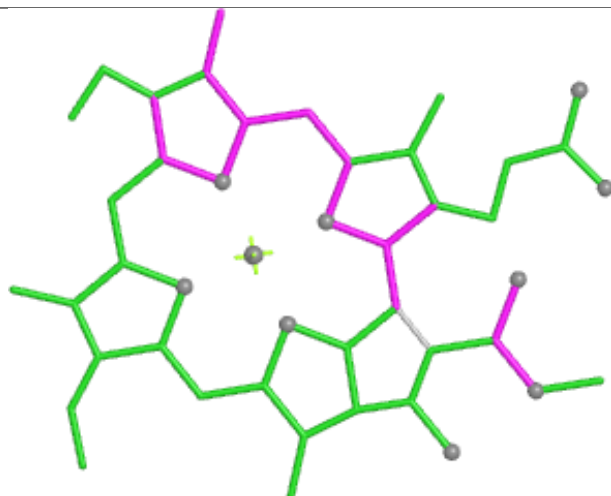


Ligand CLA B 1219**Ligand CLA G 1135**

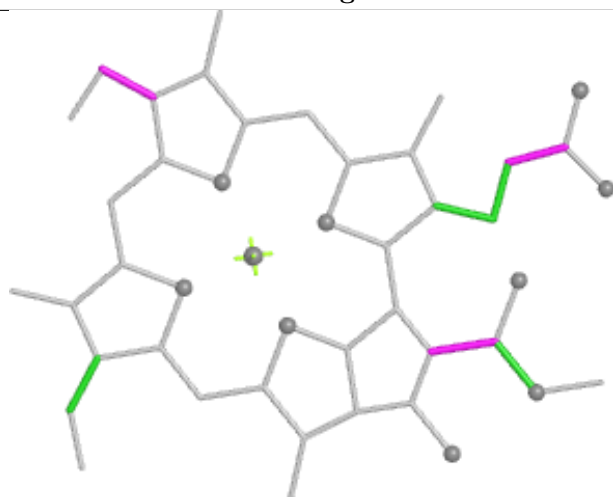
Ligand CLA 6 504



Bond lengths



Bond angles

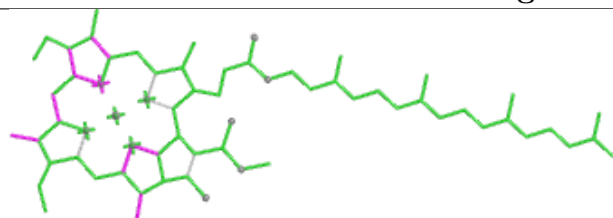


Torsions

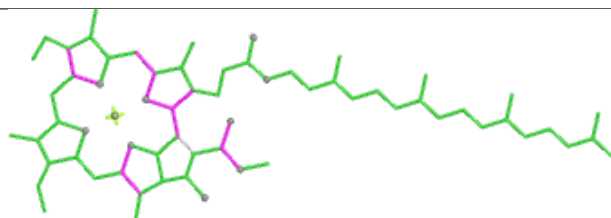


Rings

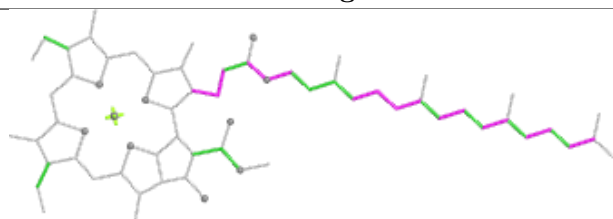
Ligand CLA d 505



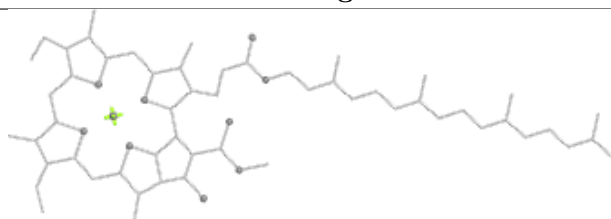
Bond lengths



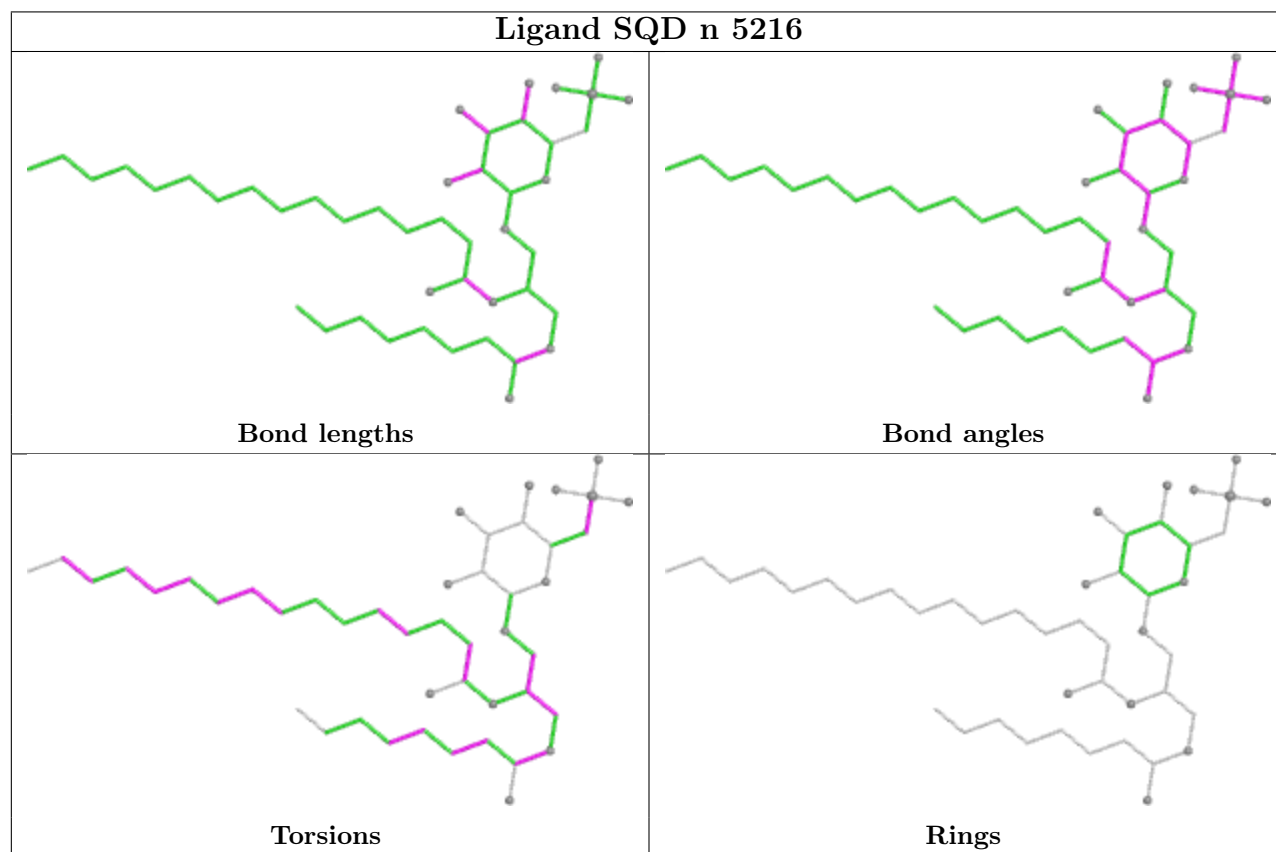
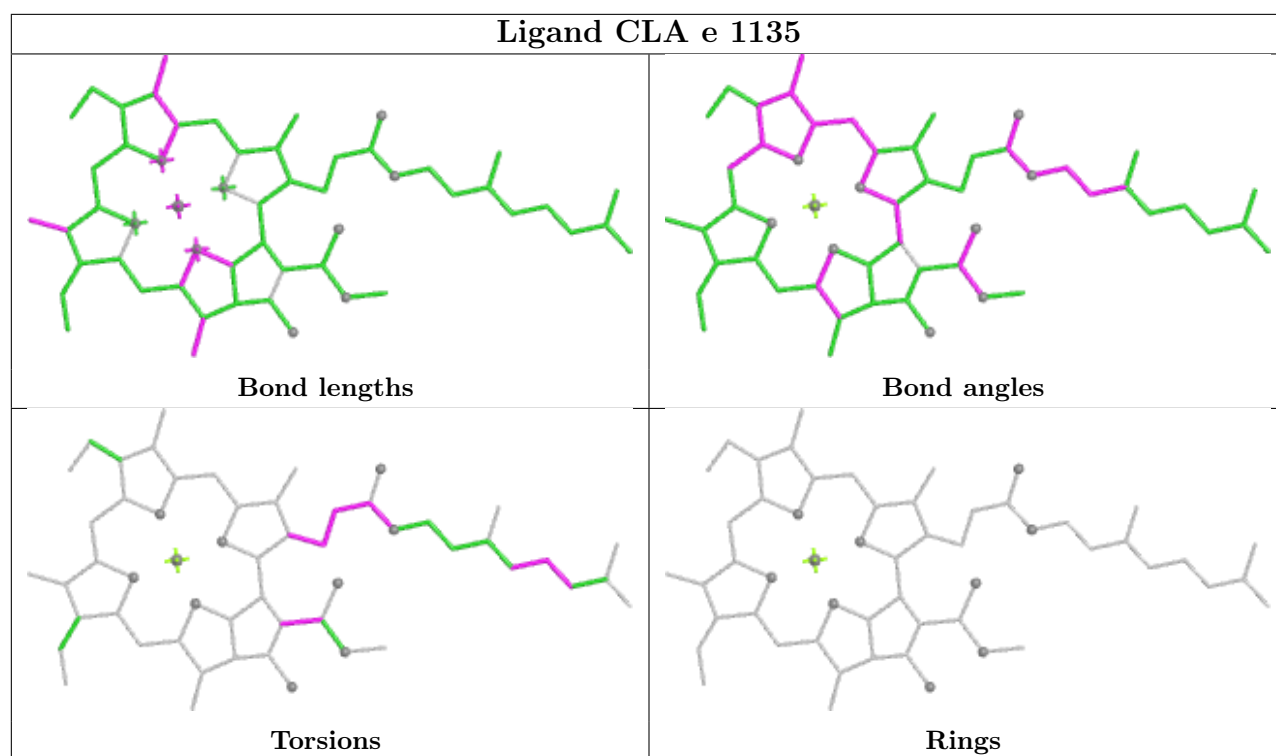
Bond angles

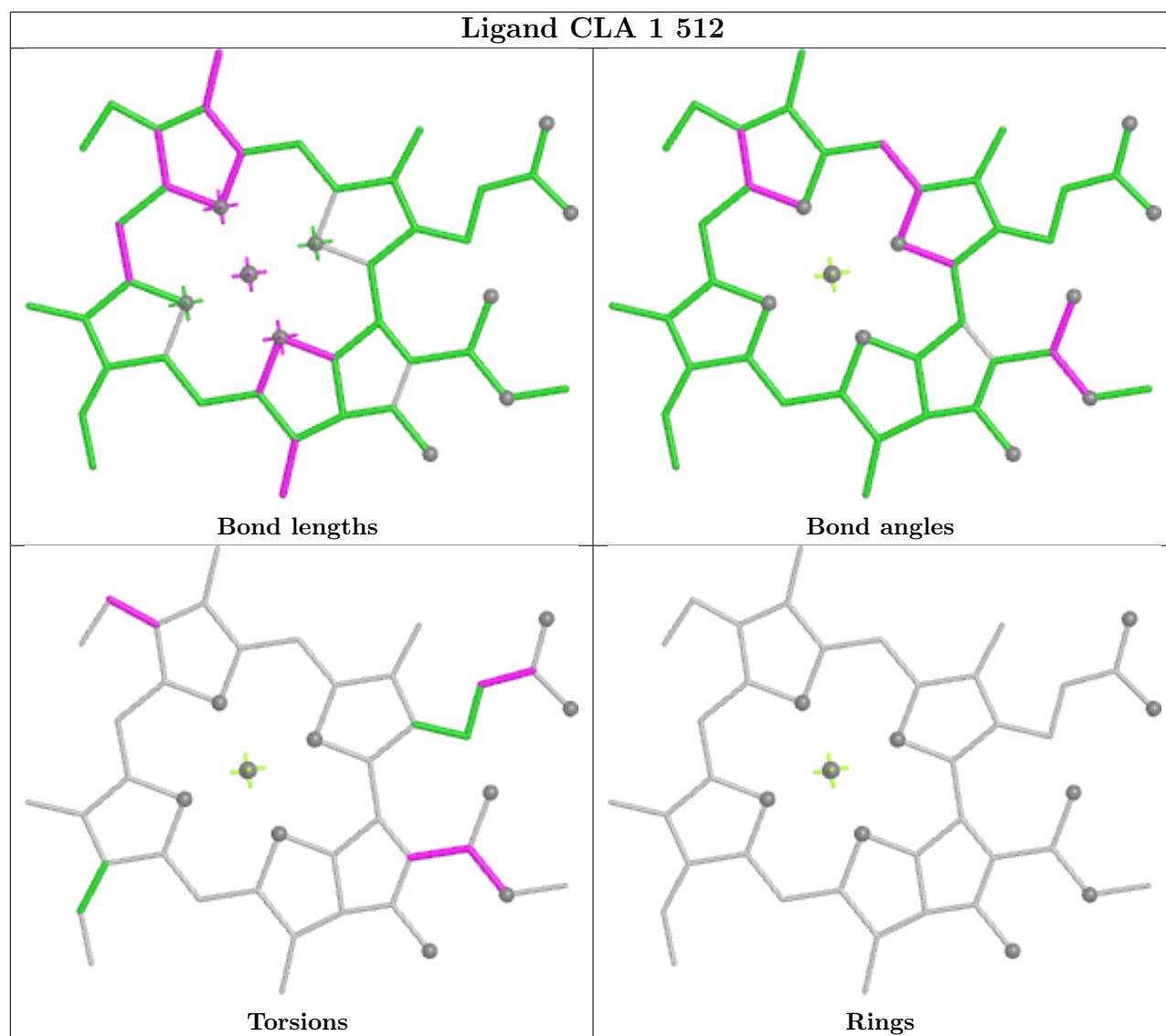
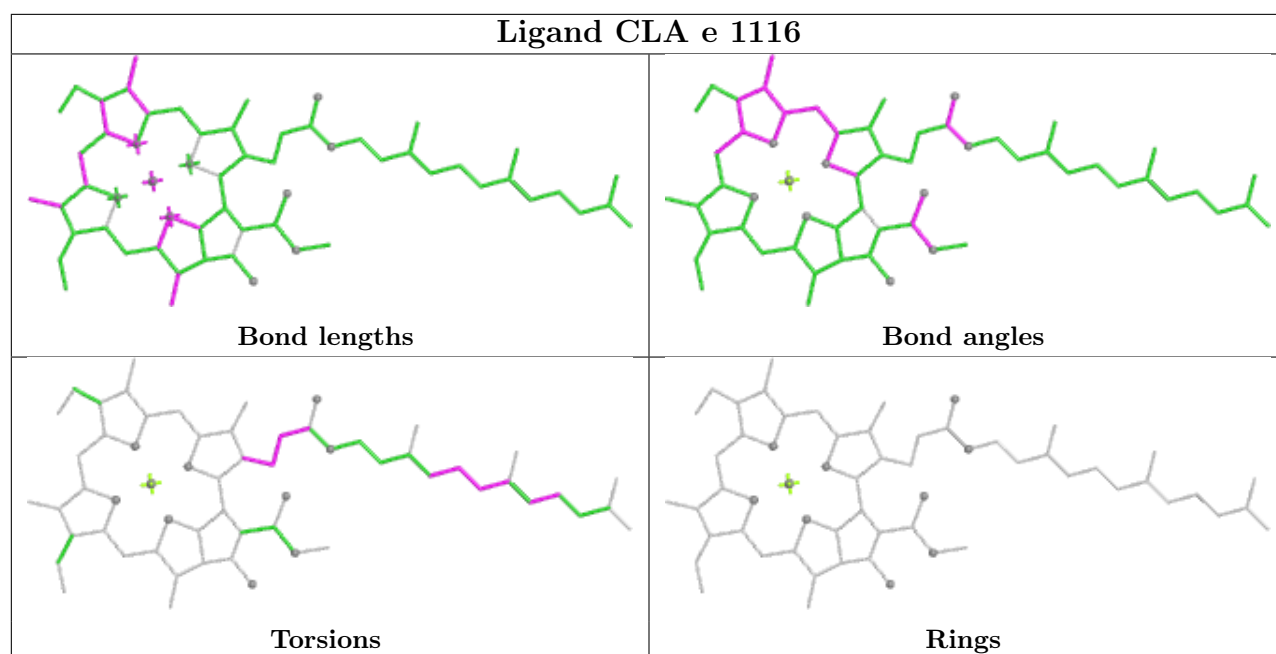


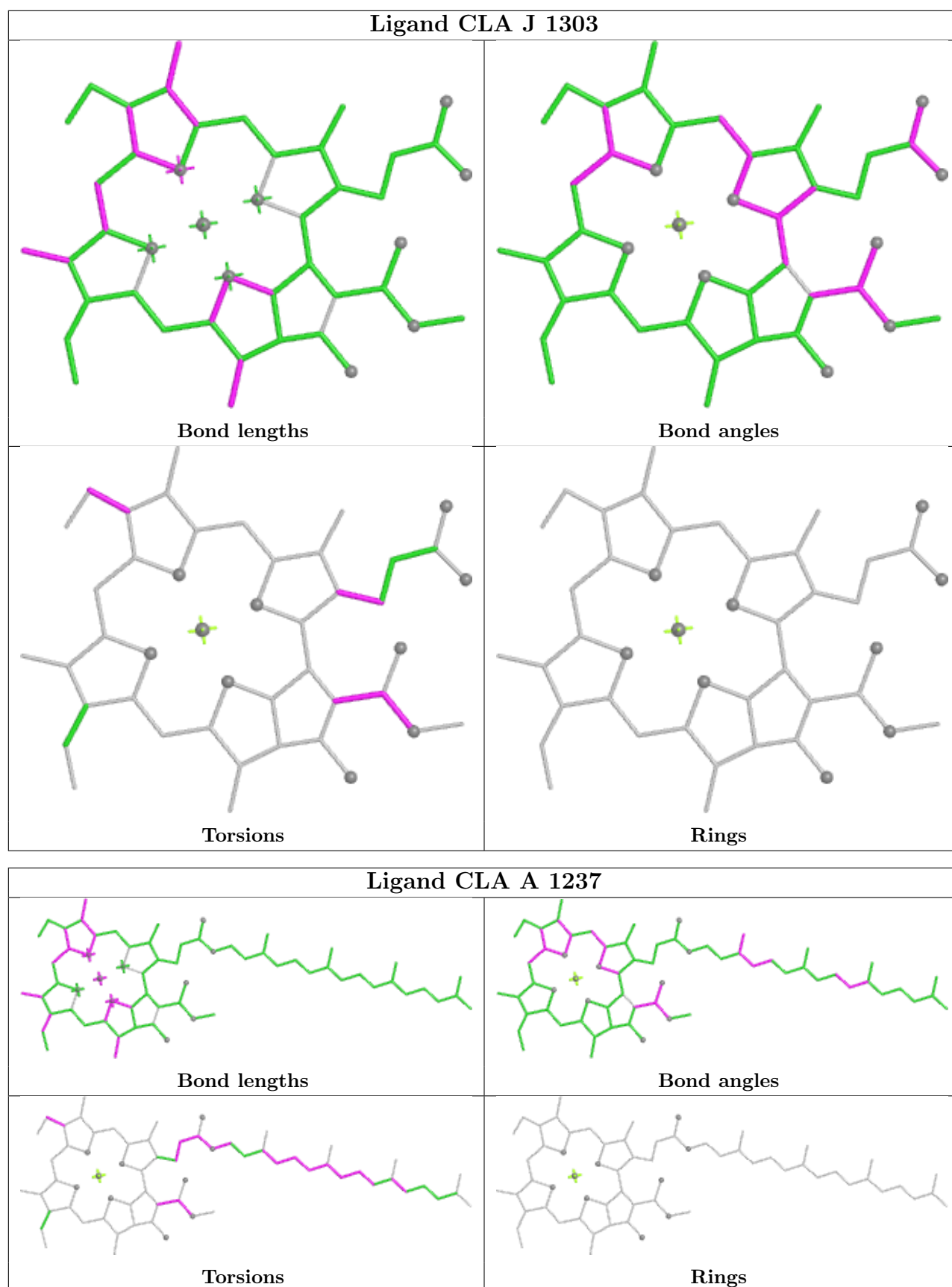
Torsions

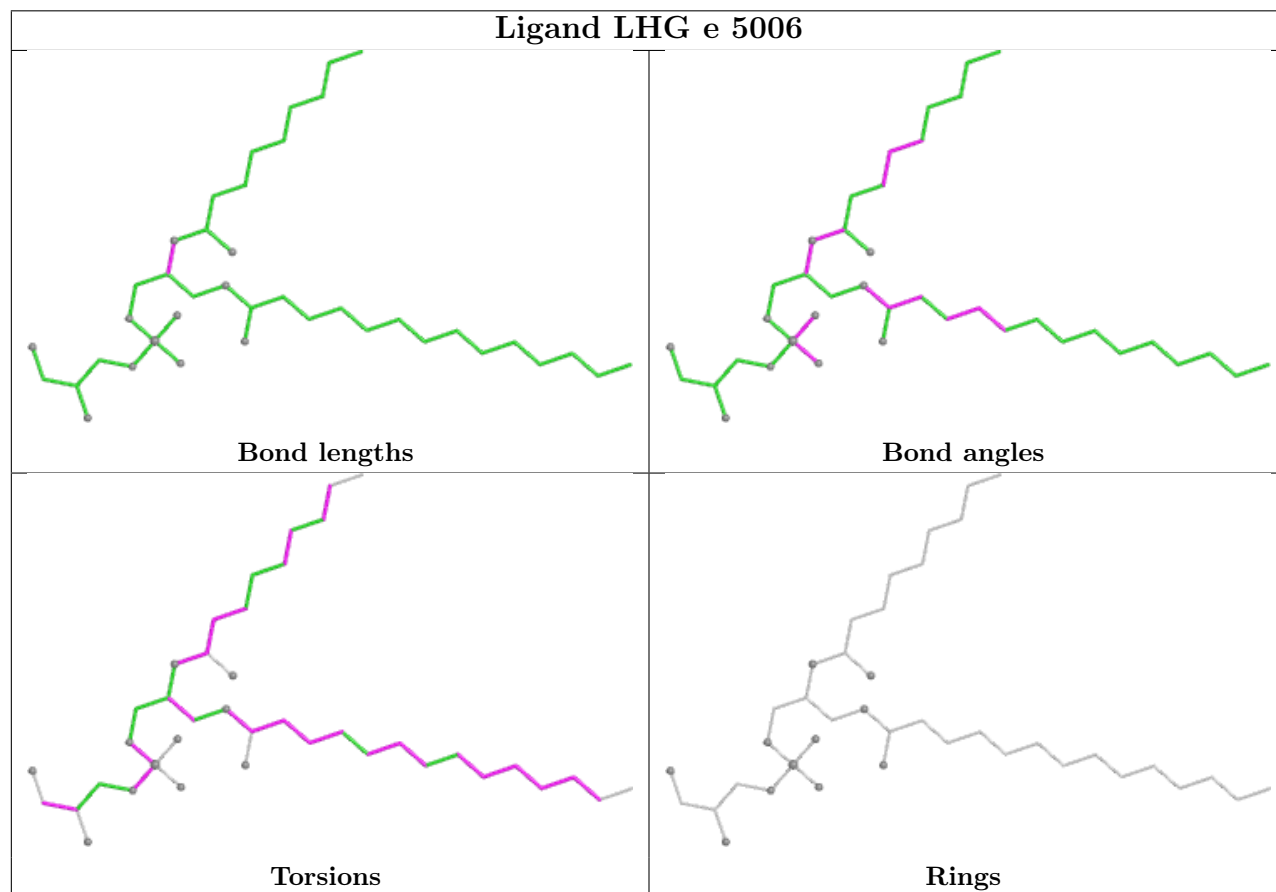
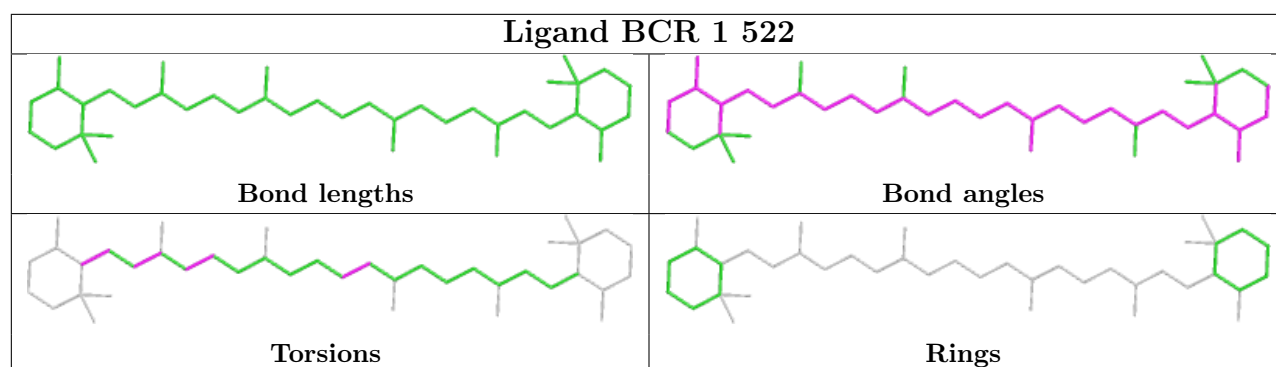


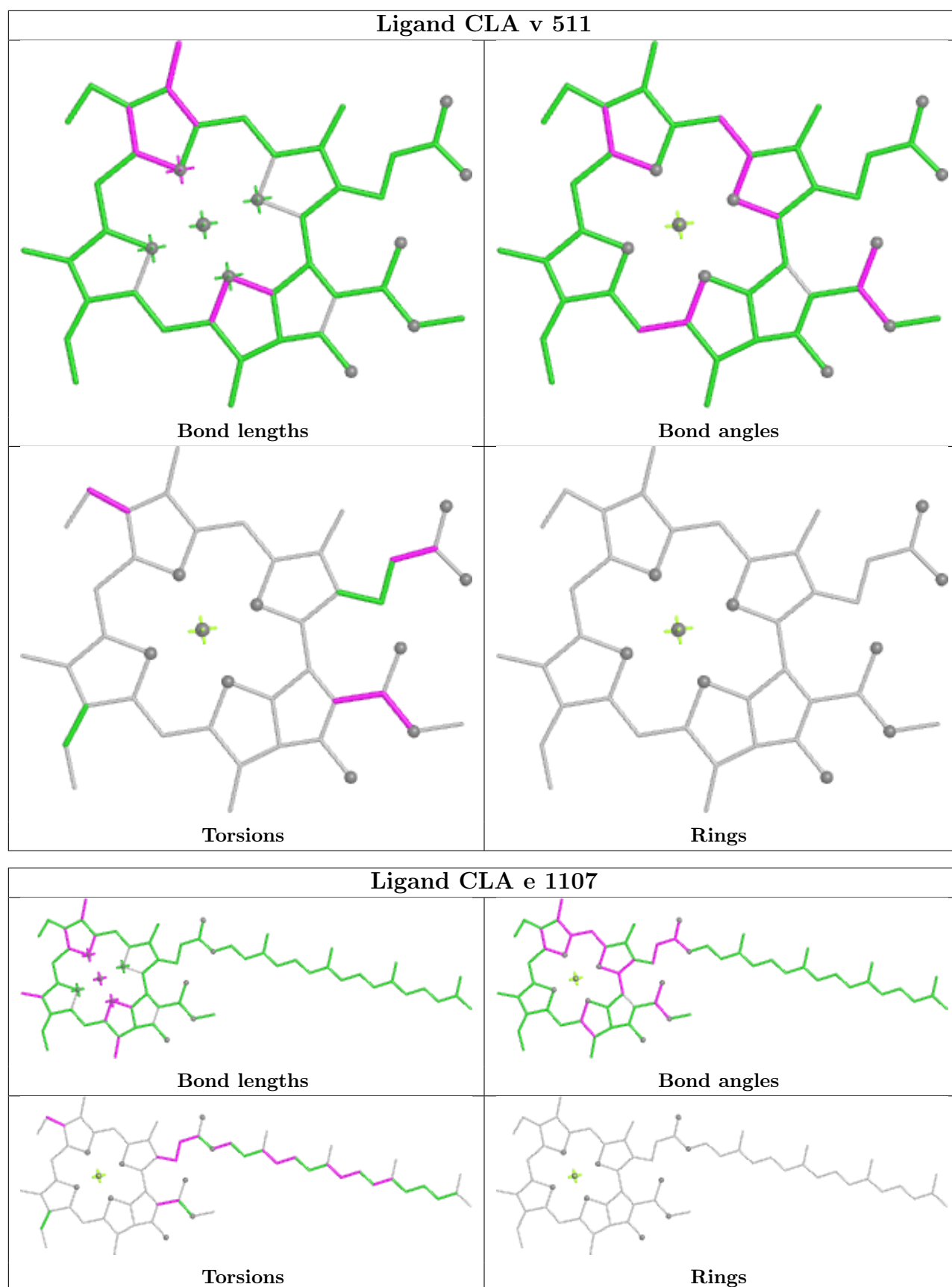
Rings



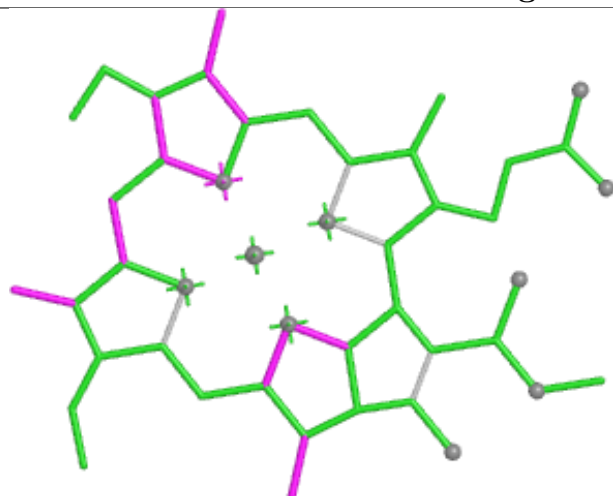




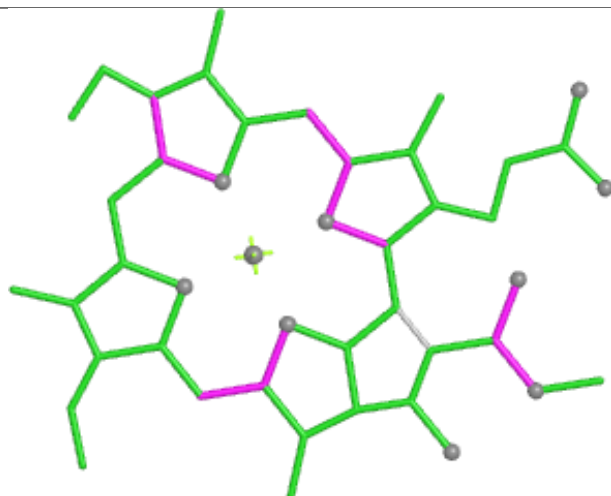




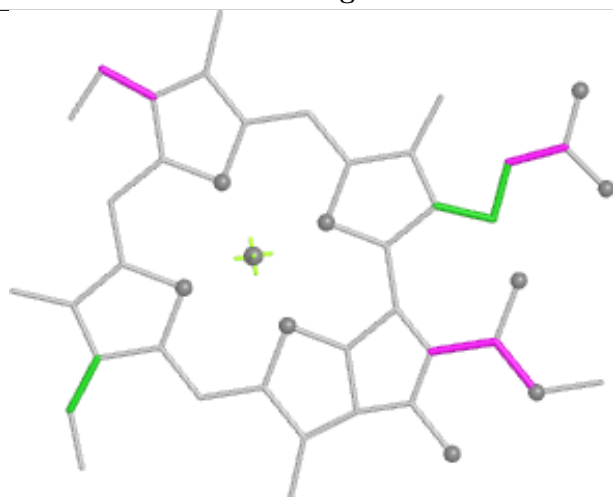
Ligand CLA 5 510



Bond lengths



Bond angles

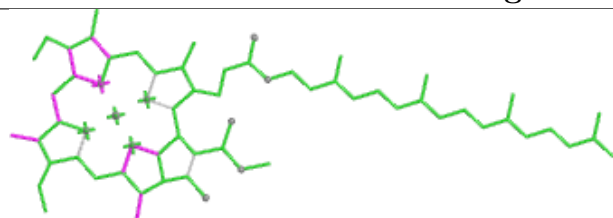


Torsions

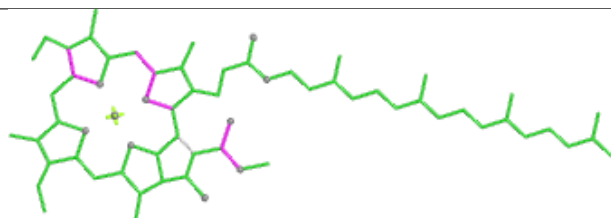


Rings

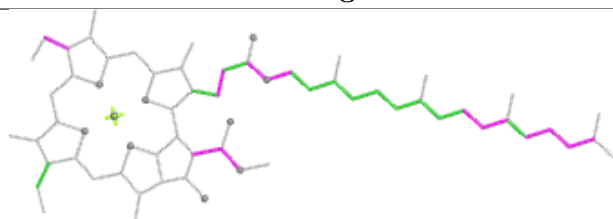
Ligand CLA H 1207



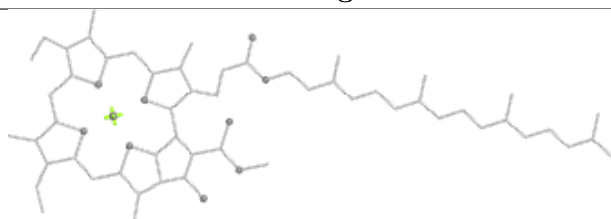
Bond lengths



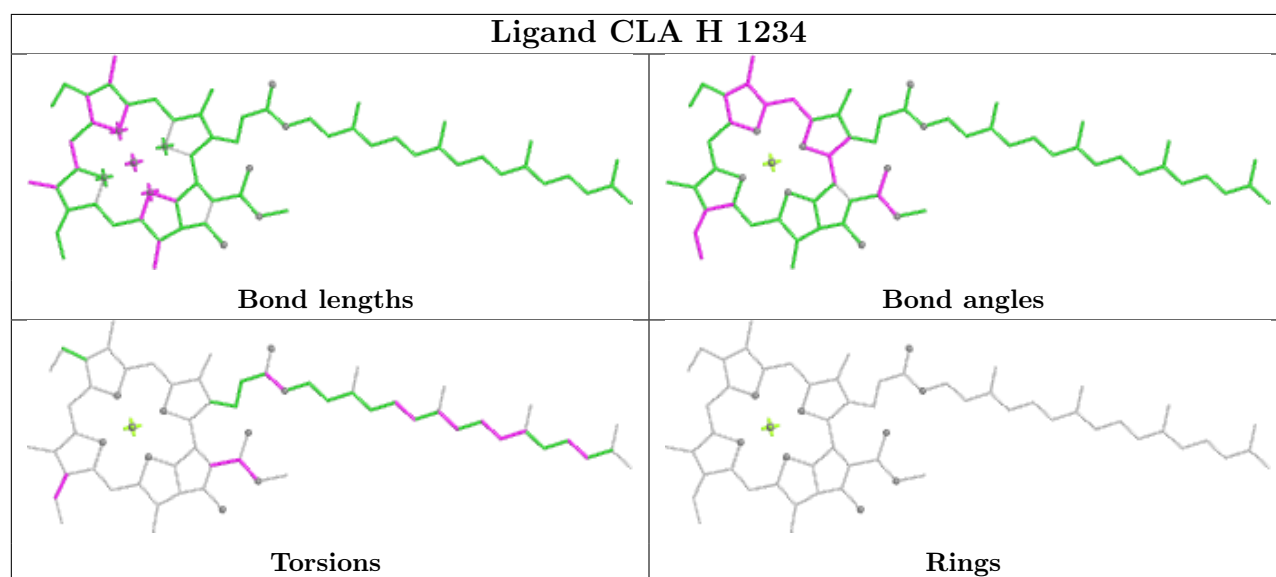
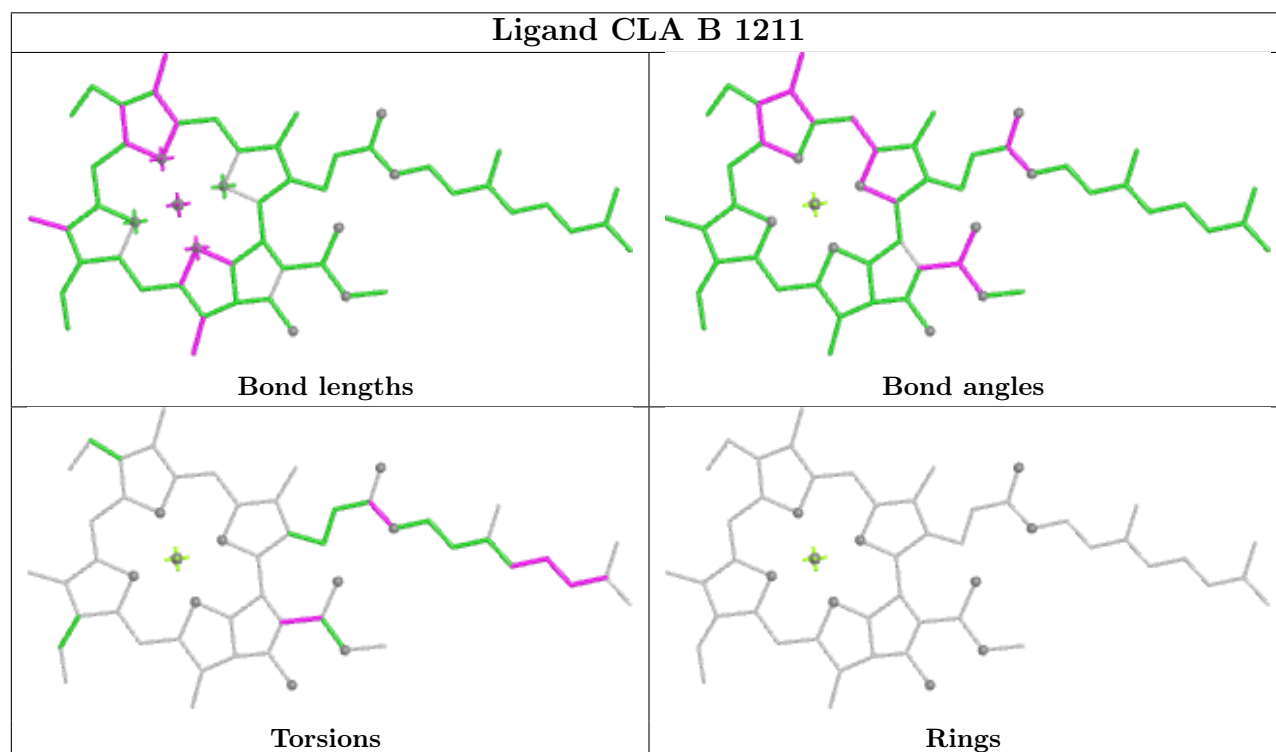
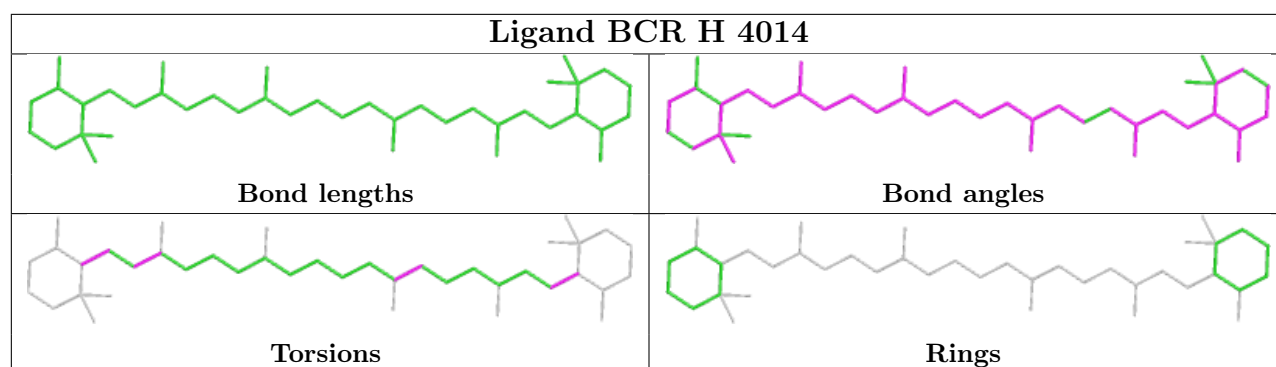
Bond angles

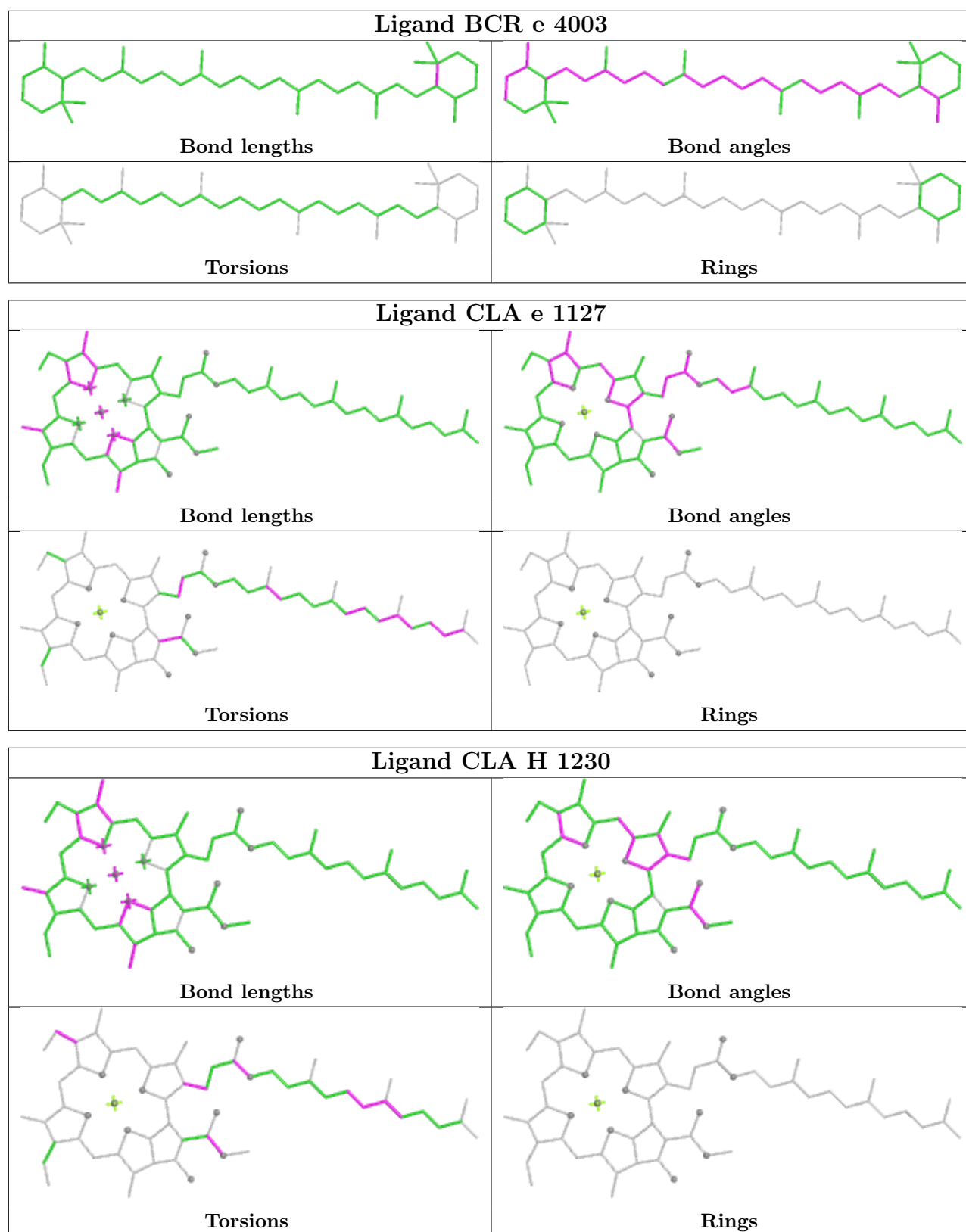


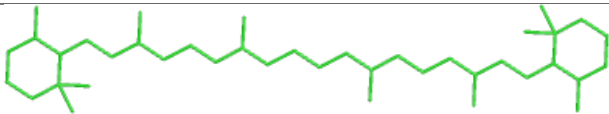
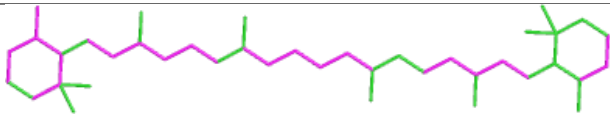
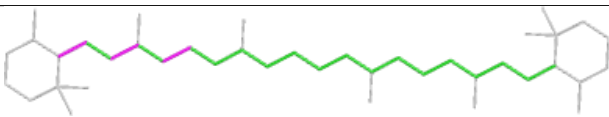
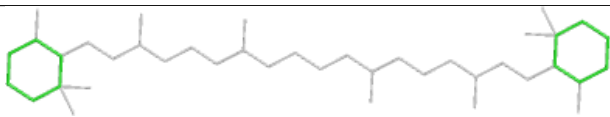
Torsions

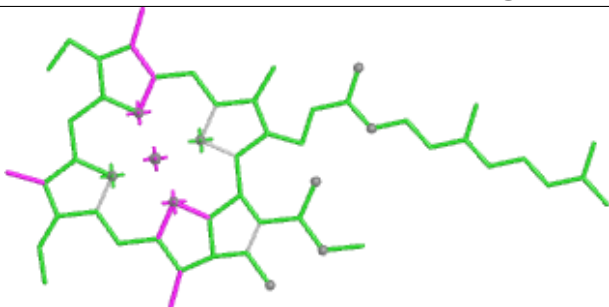
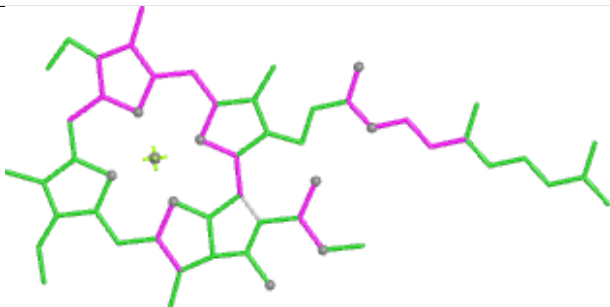
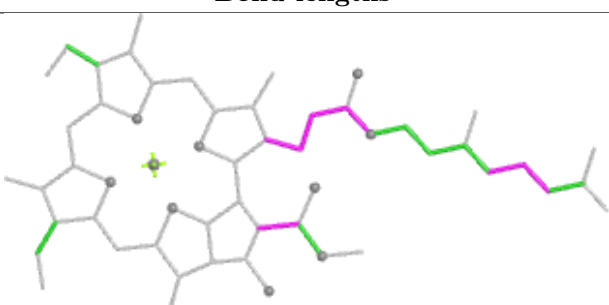
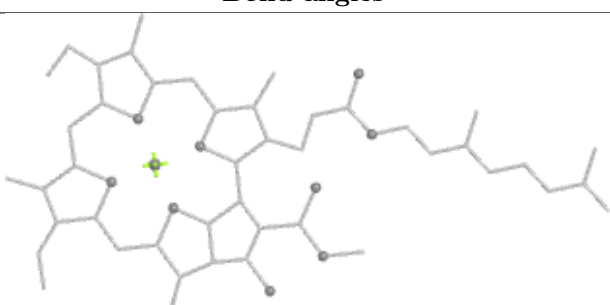


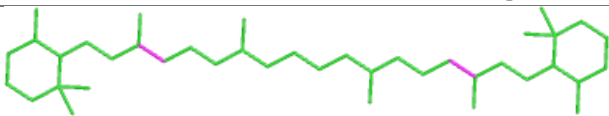
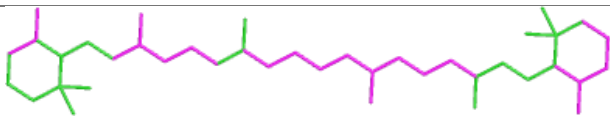
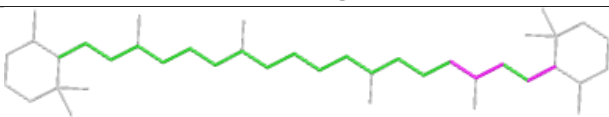
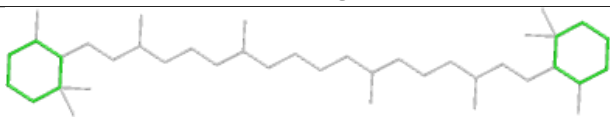
Rings

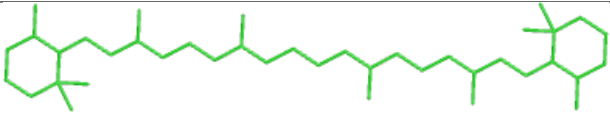
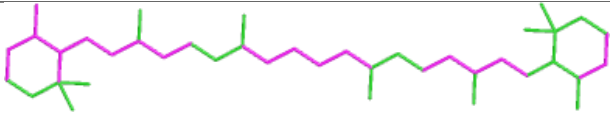
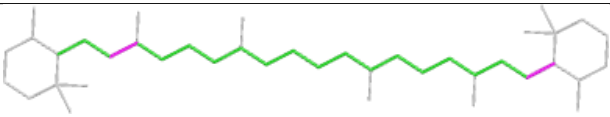
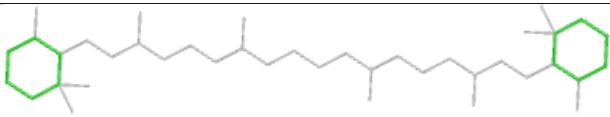
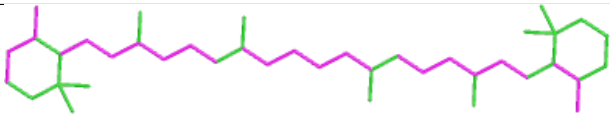
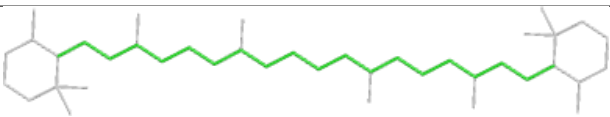
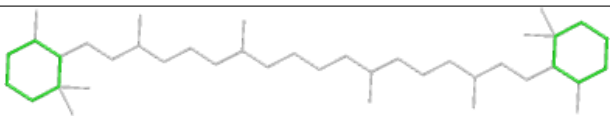
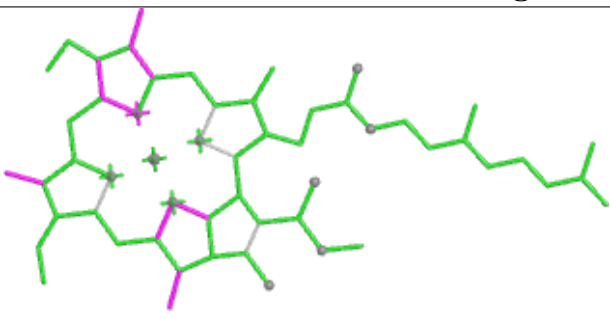
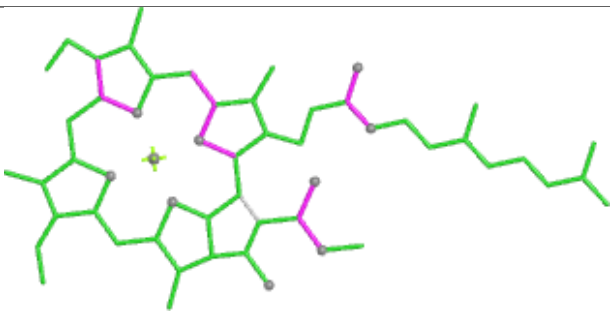
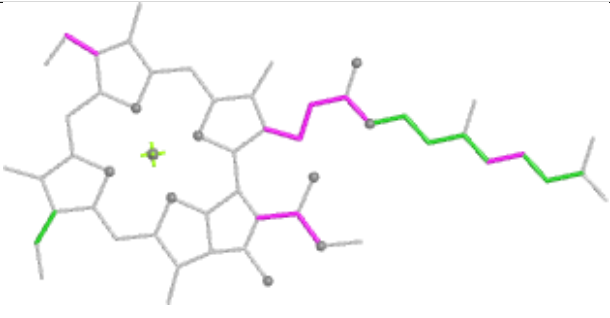
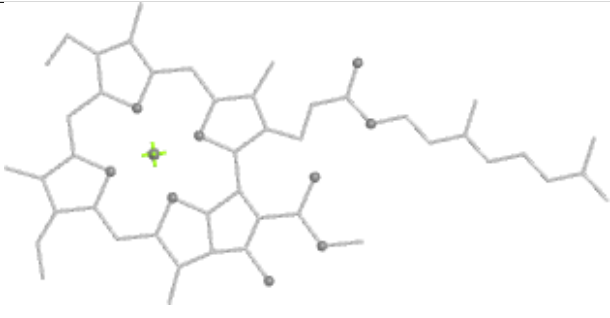


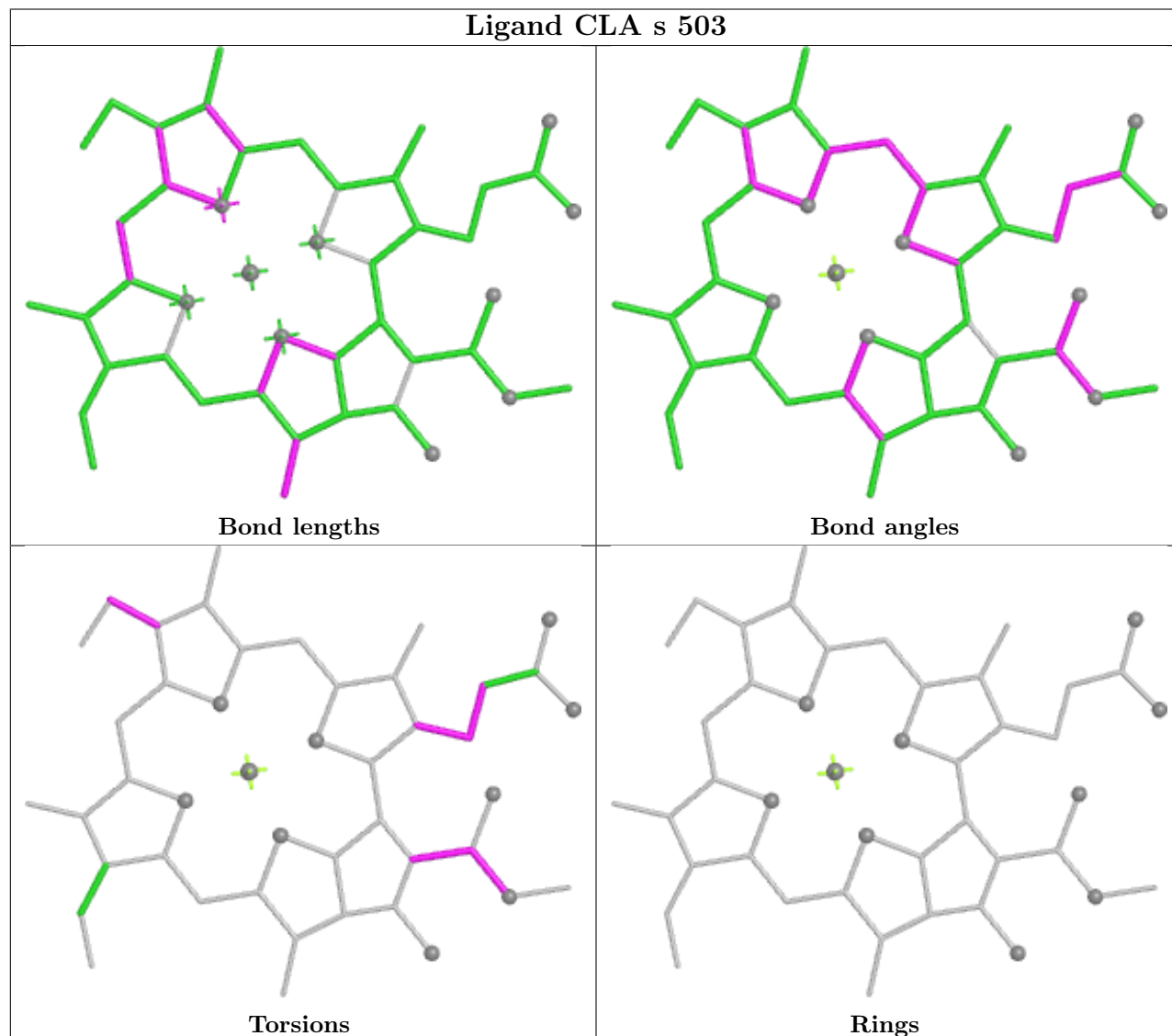
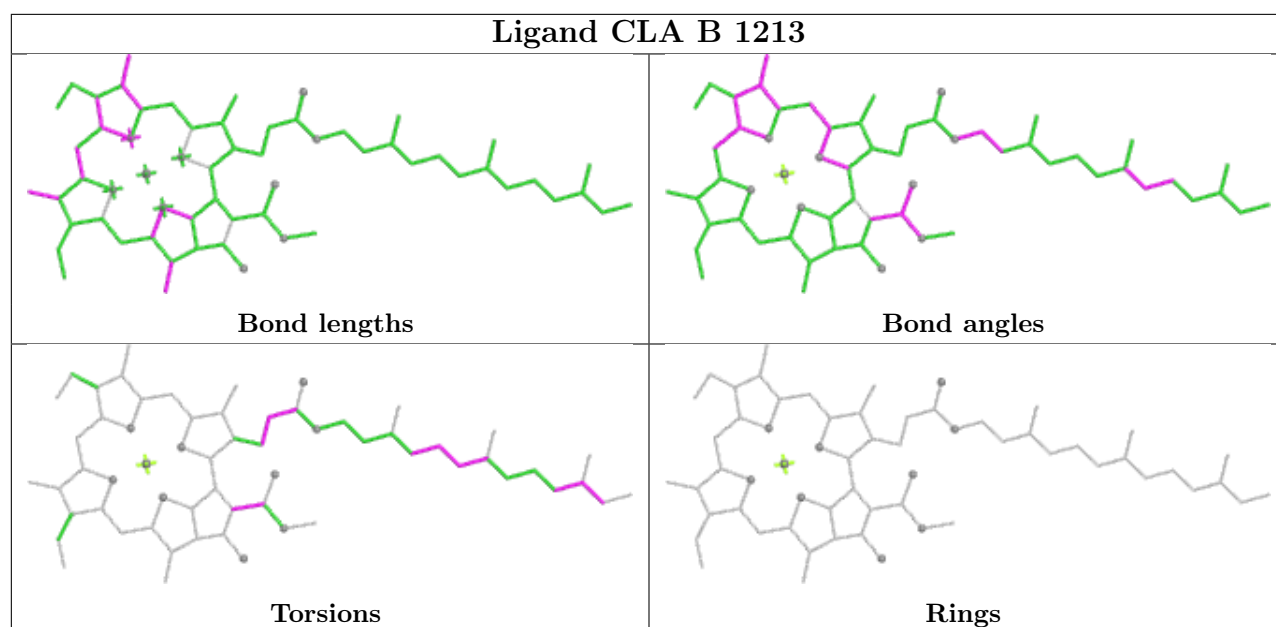


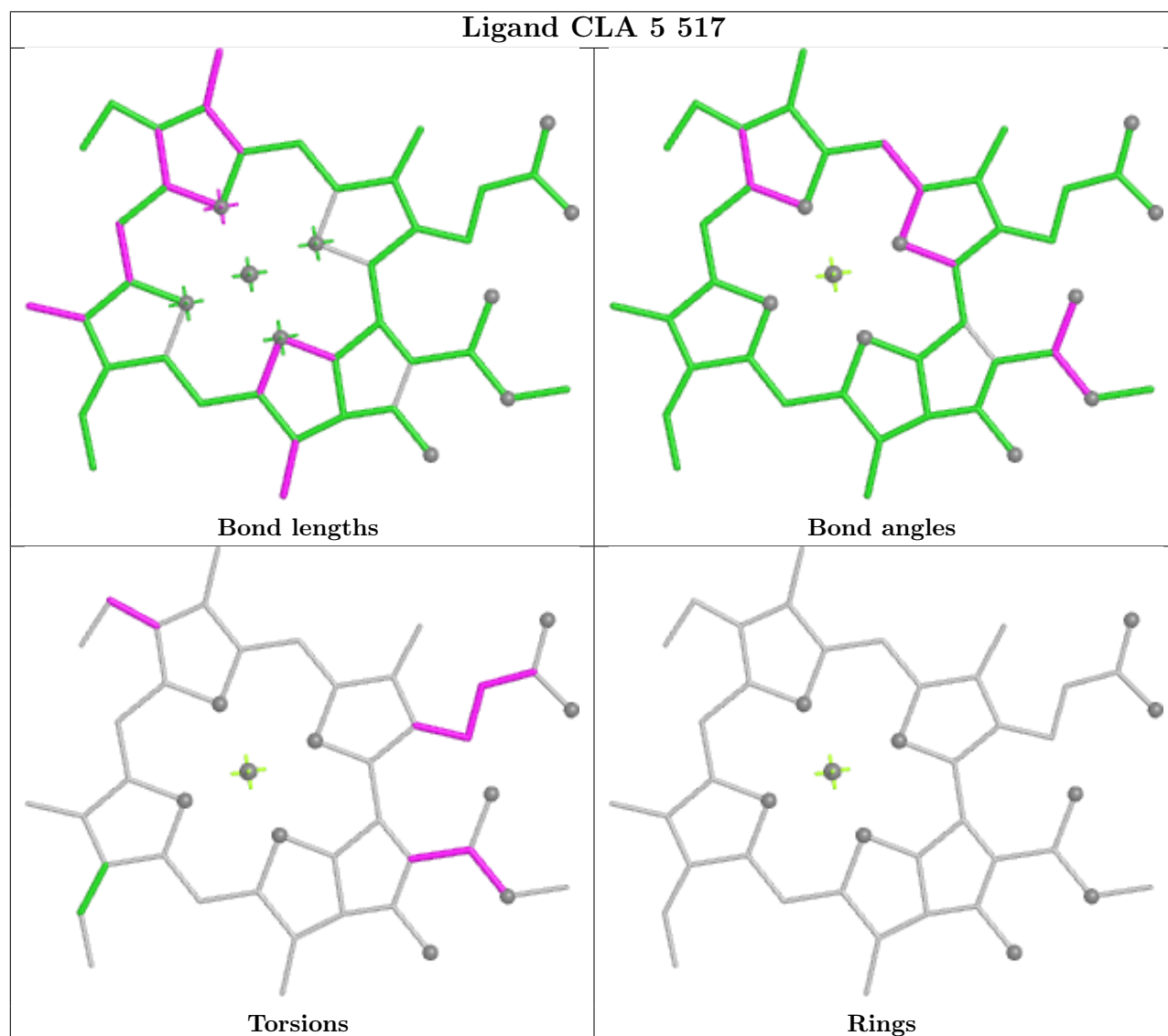
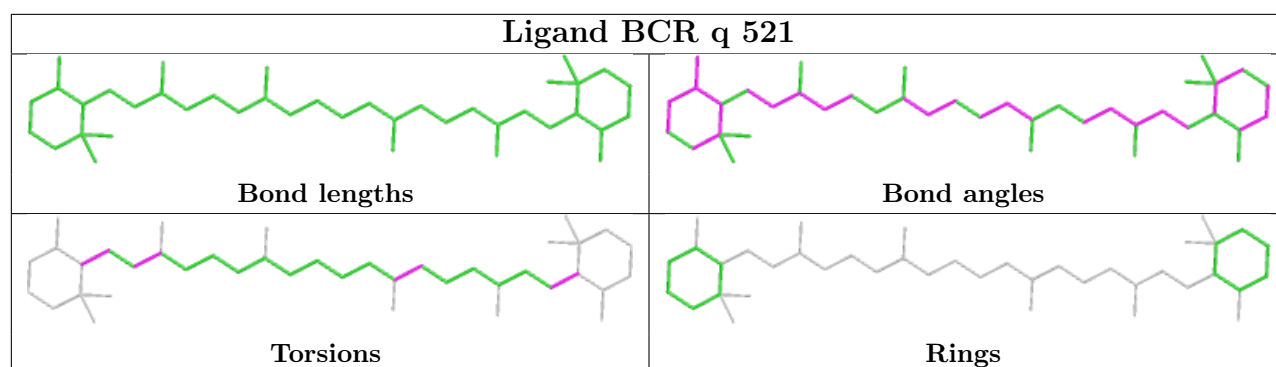
Ligand BCR 6 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

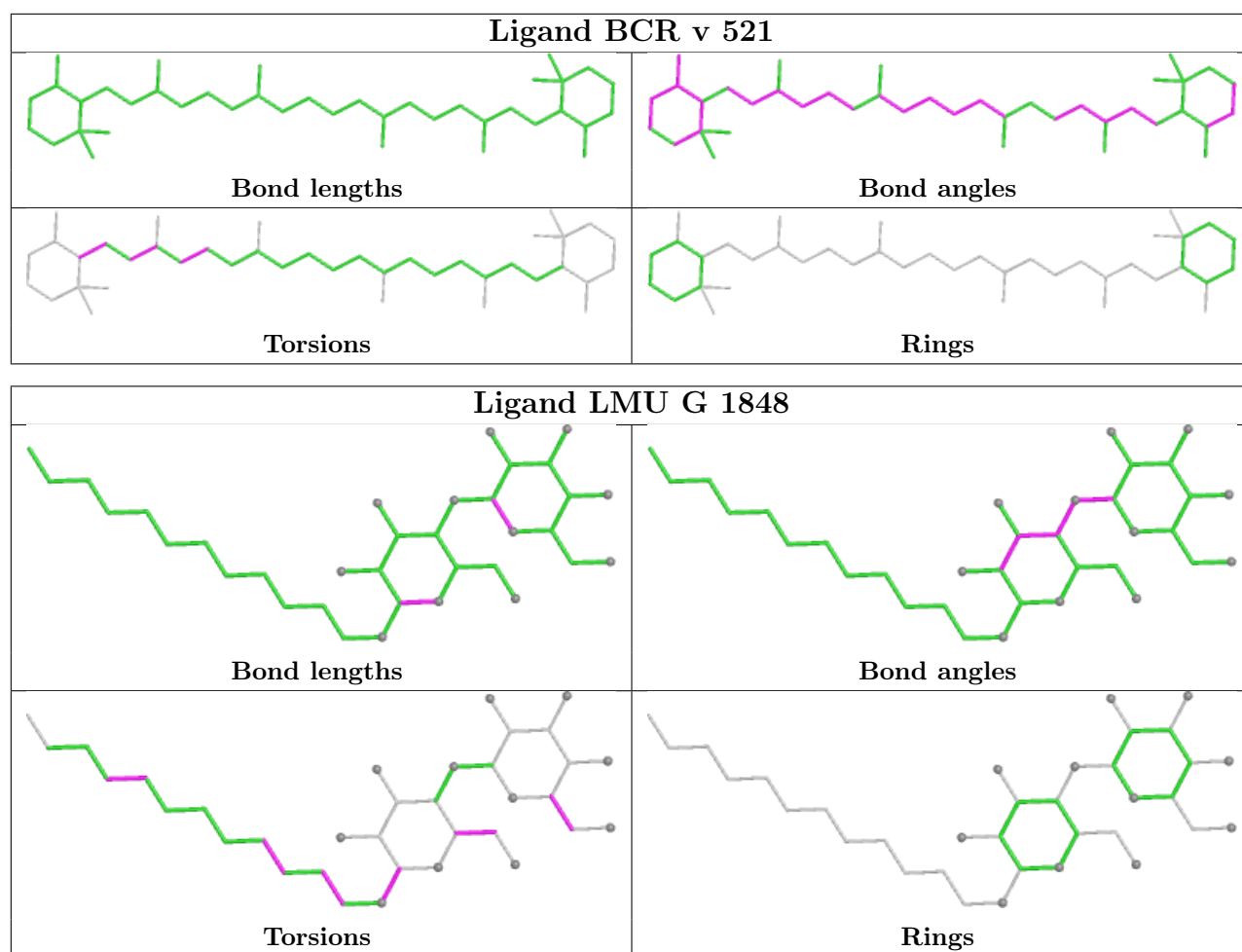
Ligand CLA A 1135	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR L 4020	
	
Bond lengths	Bond angles
	
Torsions	Rings

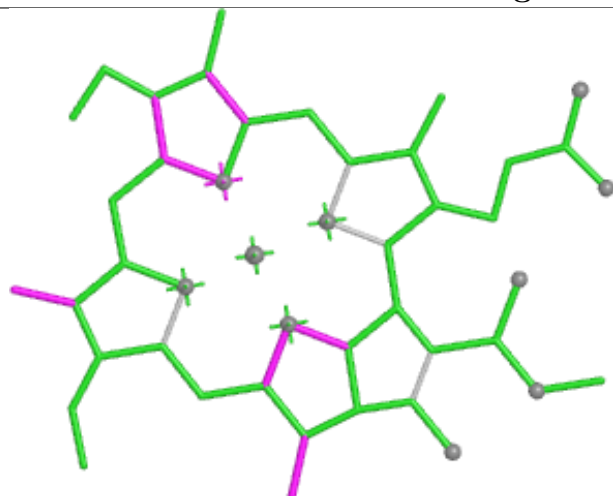
Ligand BCR 4 524	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR G 4003	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA a 518	
 Bond lengths	 Bond angles
 Torsions	 Rings



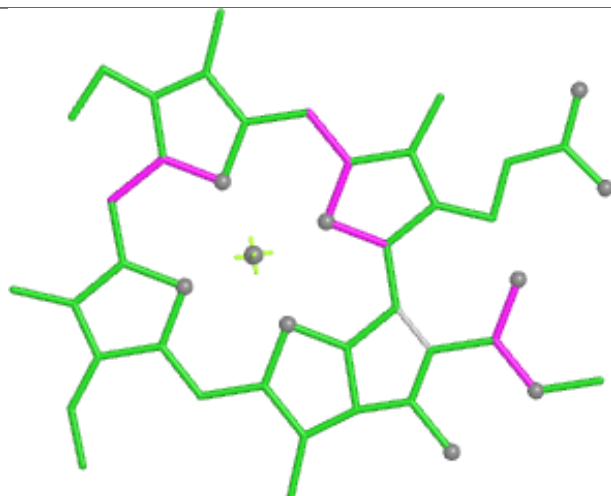




Ligand CLA Y 505



Bond lengths



Bond angles

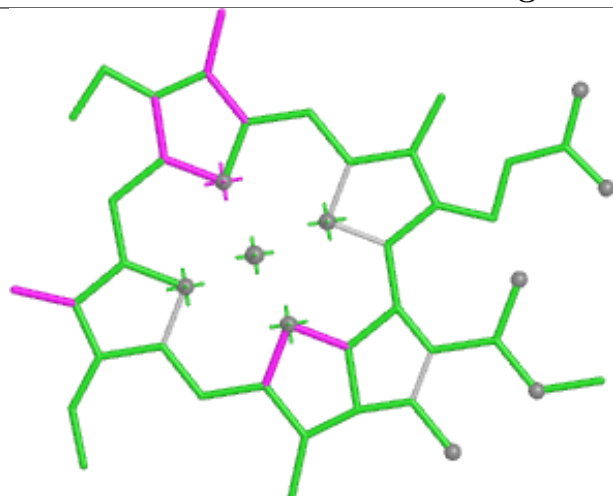


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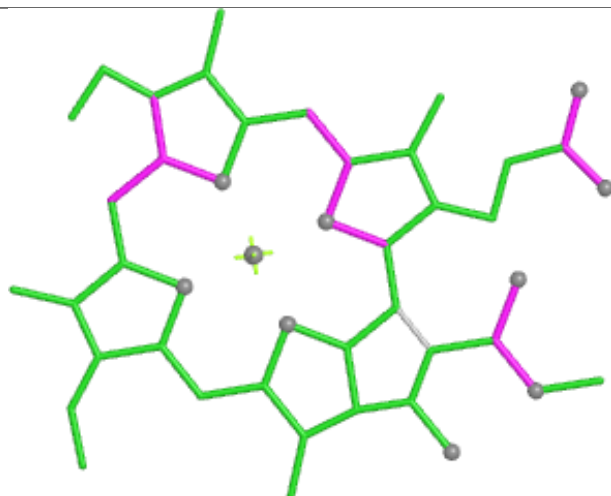


Rings

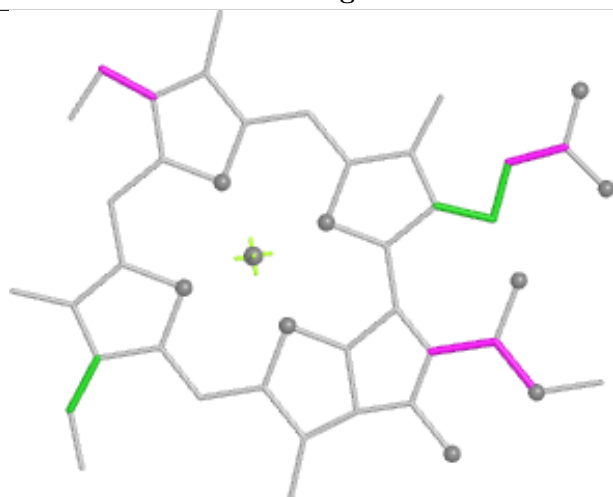
Ligand CLA 3 519



Bond lengths



Bond angles

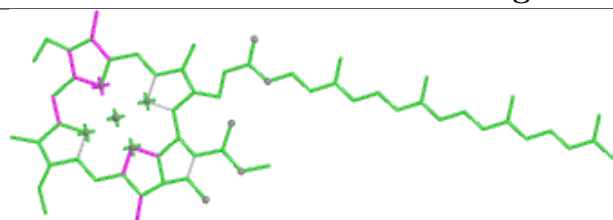


Torsions

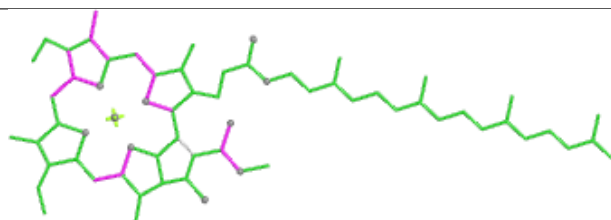


Rings

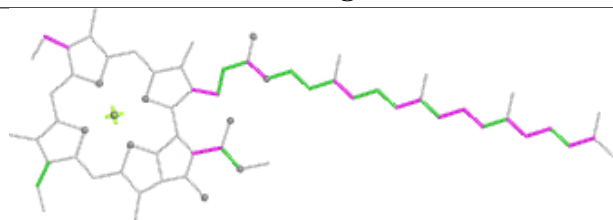
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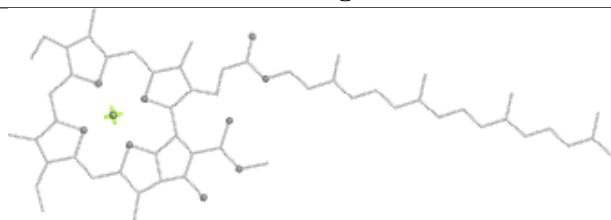
Bond lengths



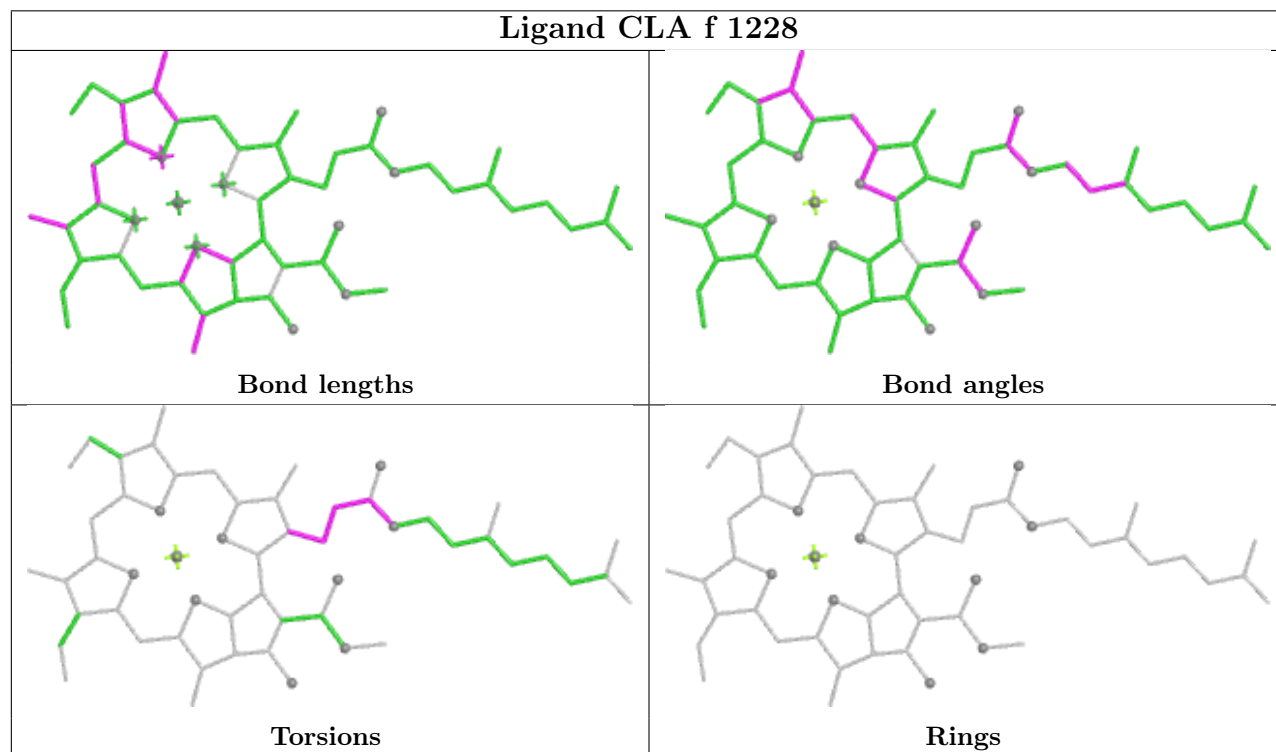
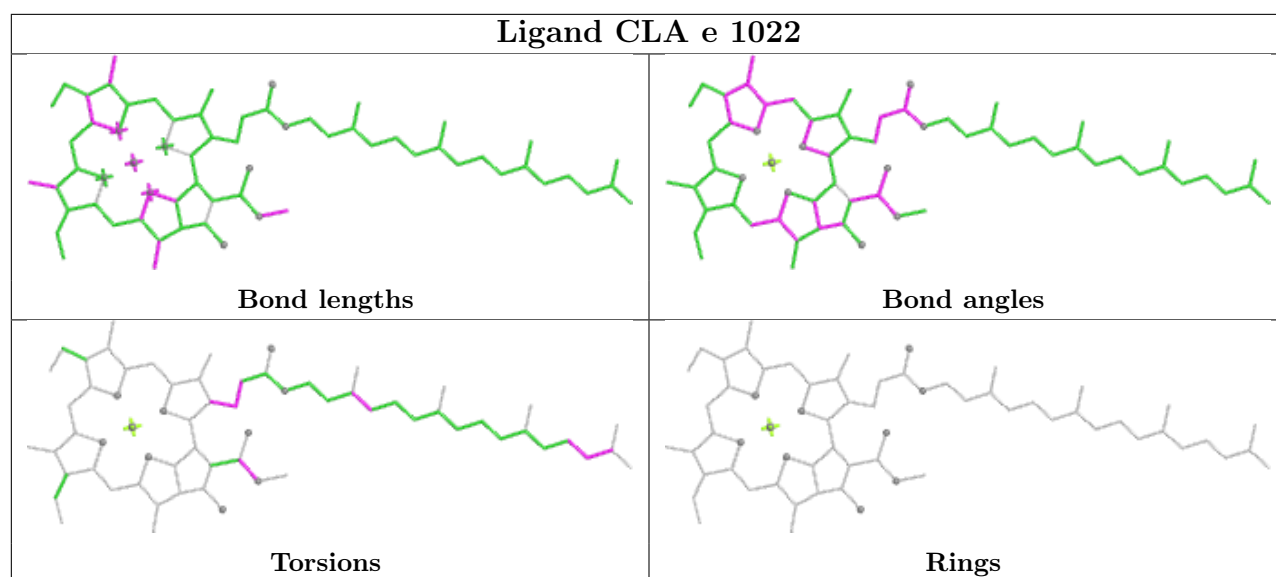
Bond angles



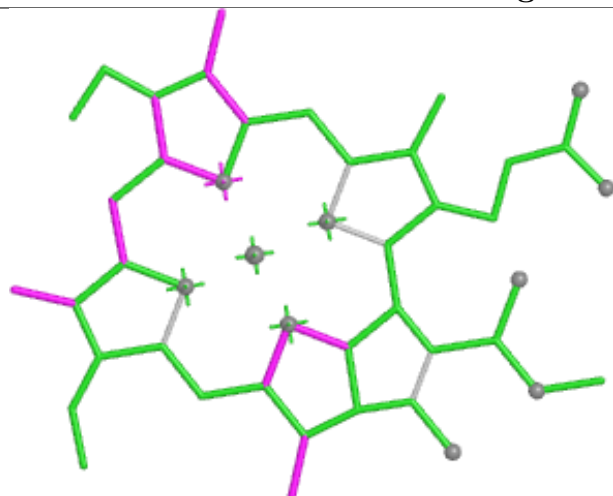
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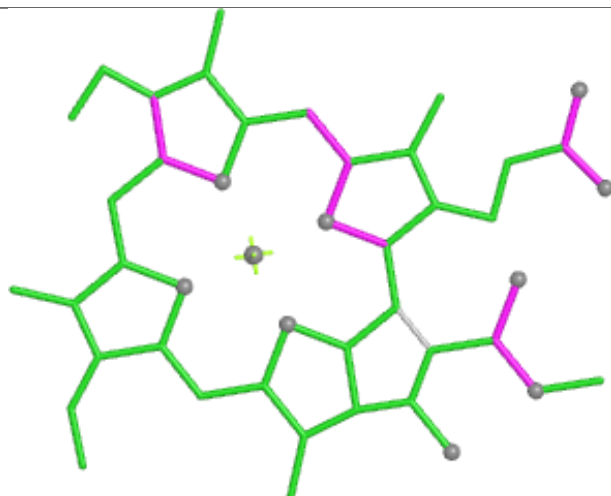
Rings



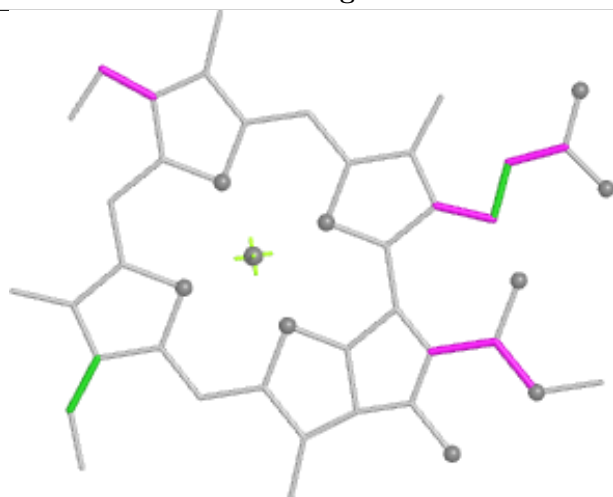
Ligand CLA d 519



Bond lengths



Bond angles

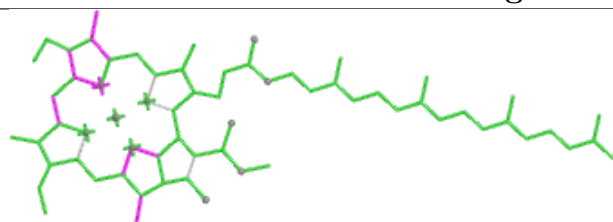


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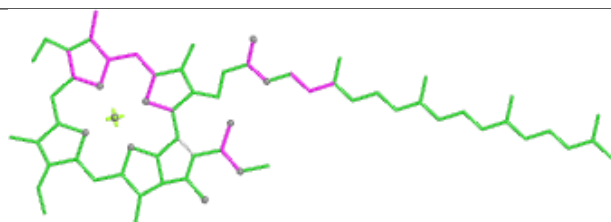


Rings

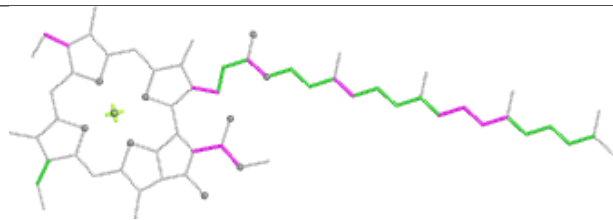
Ligand CLA B 1240



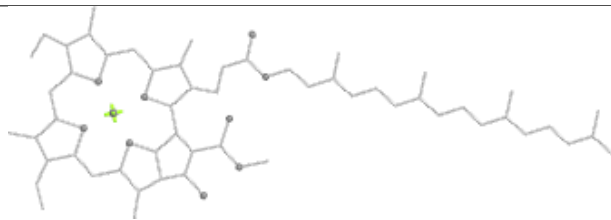
Bond lengths



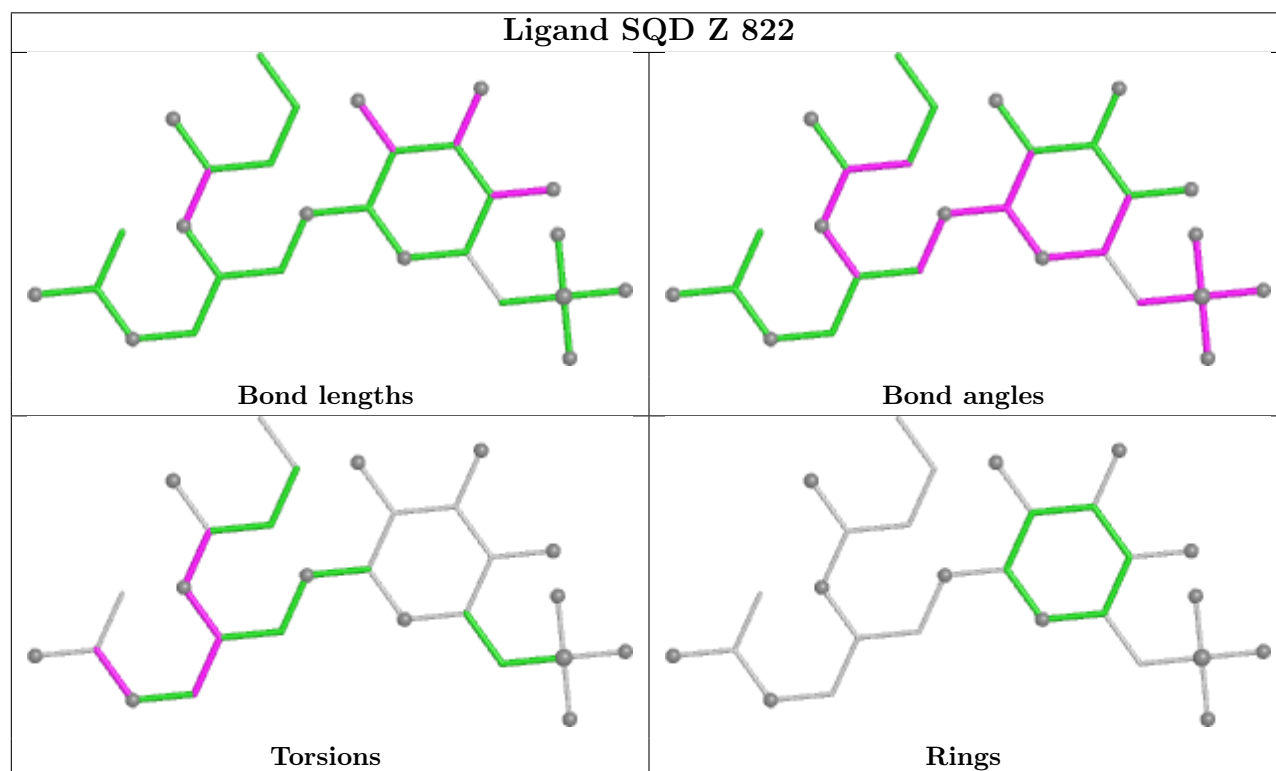
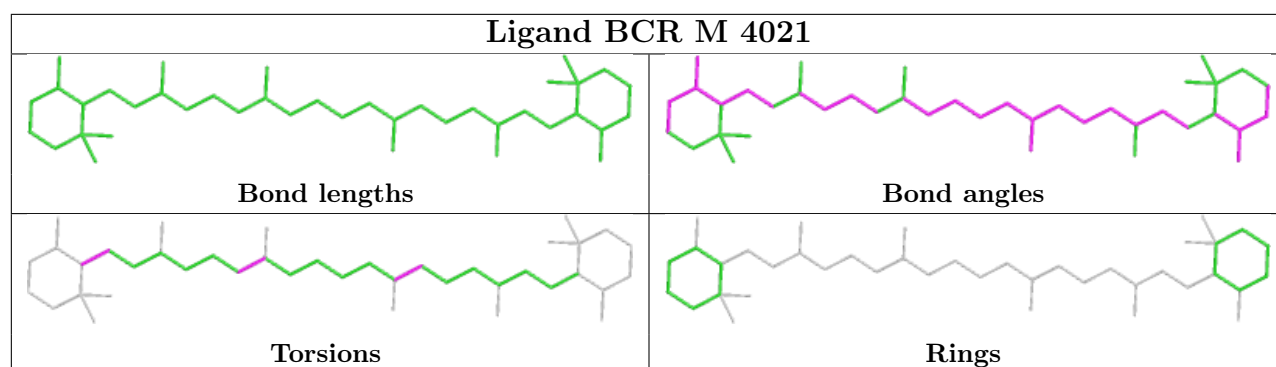
Bond angles

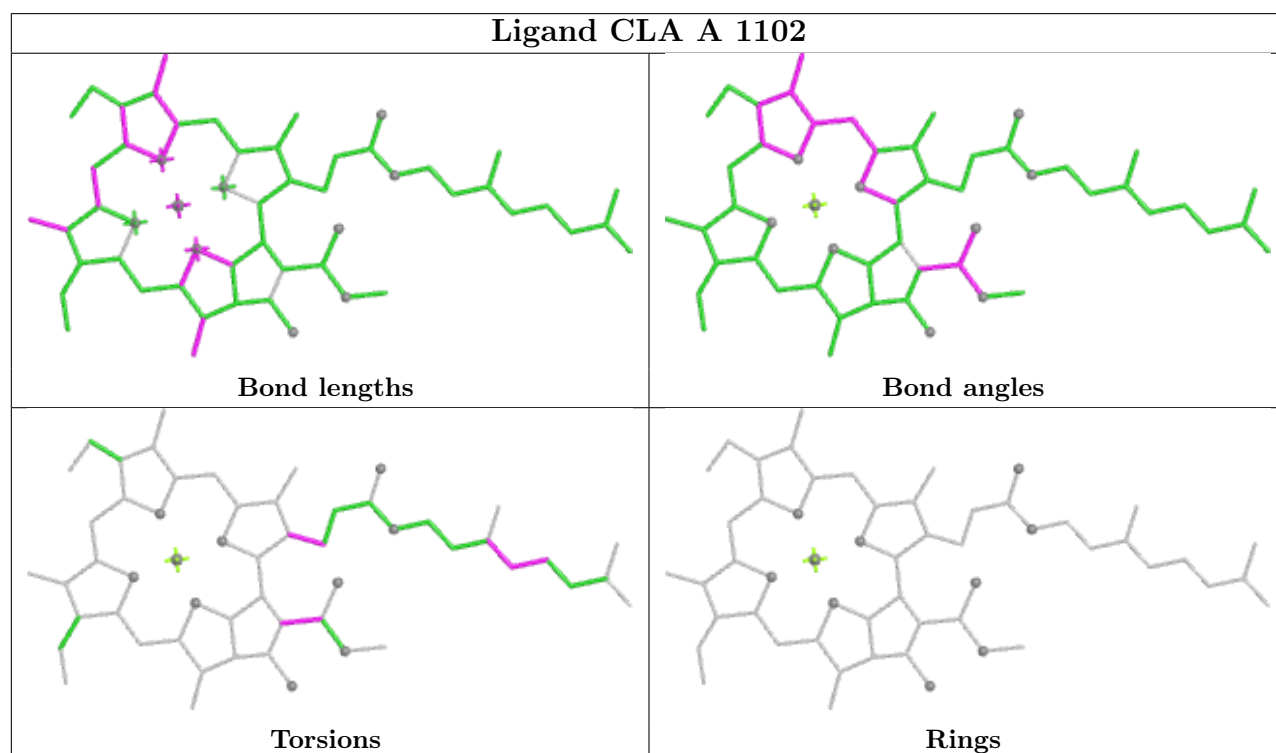
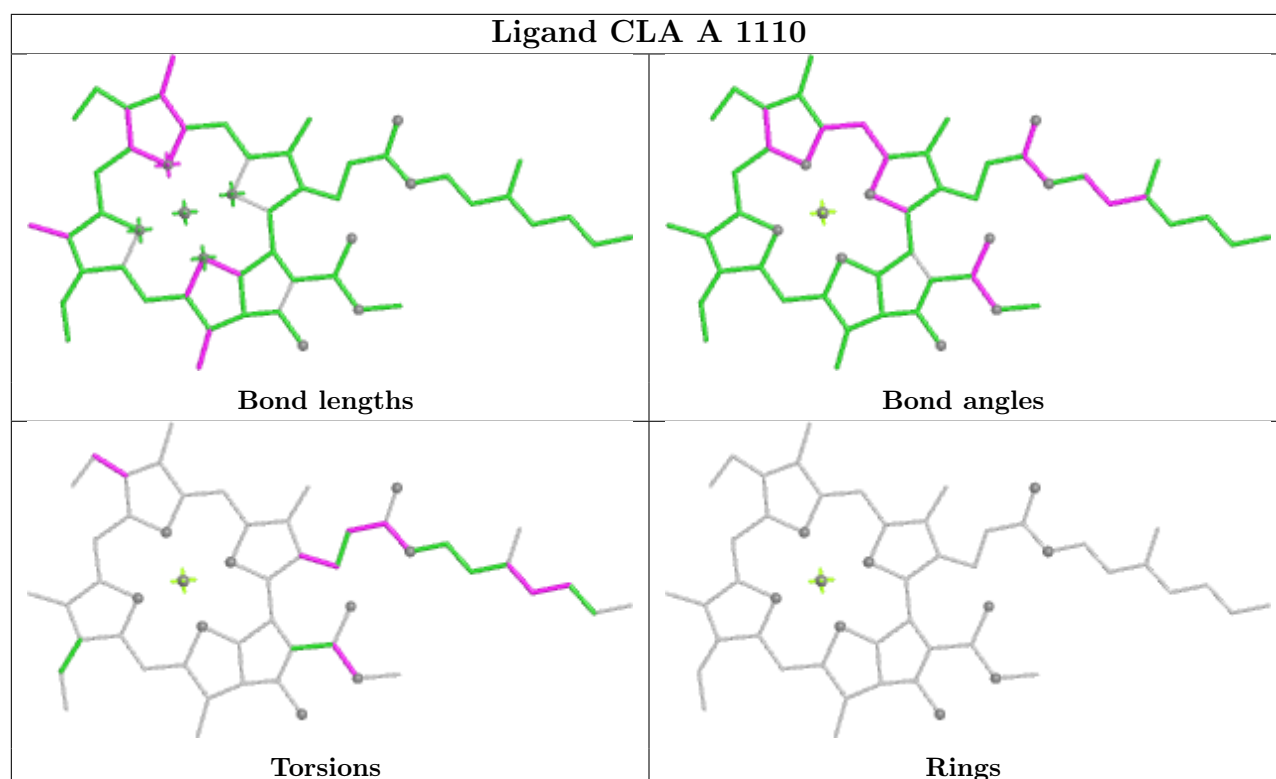


Torsions

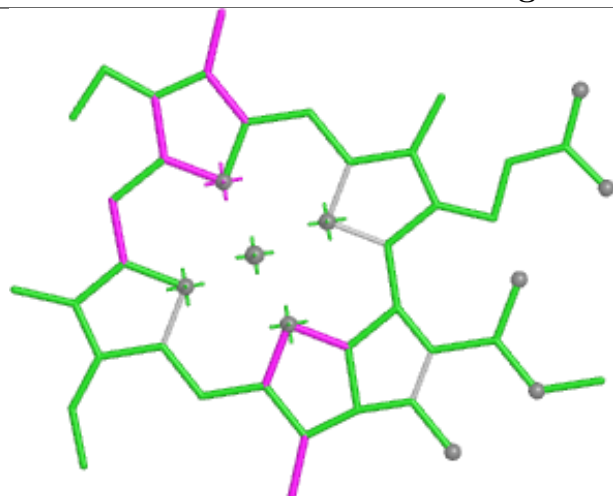


Rings

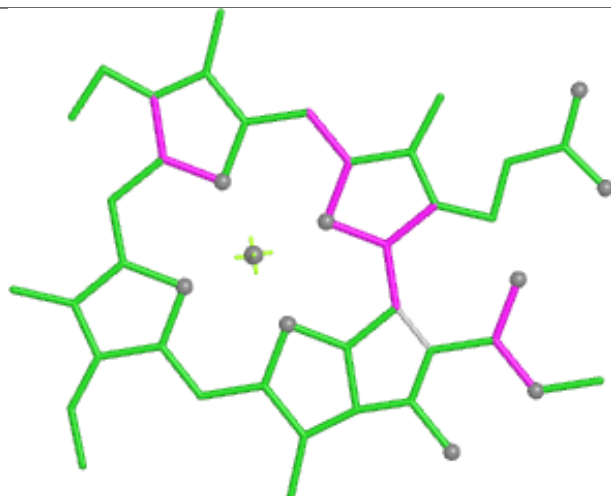




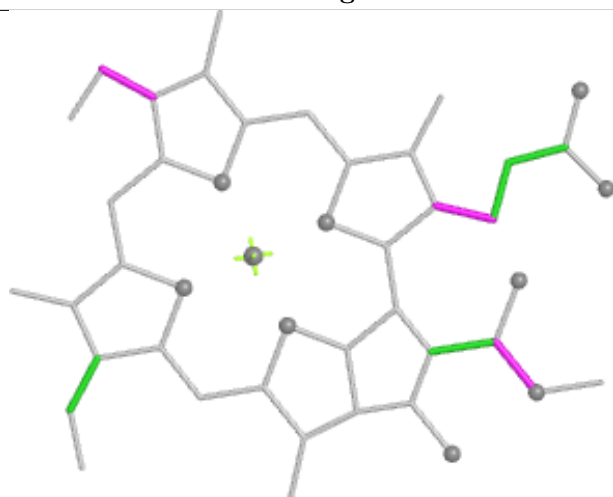
Ligand CLA 5 504



Bond lengths



Bond angles

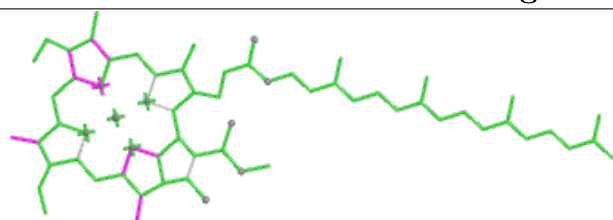


Torsions

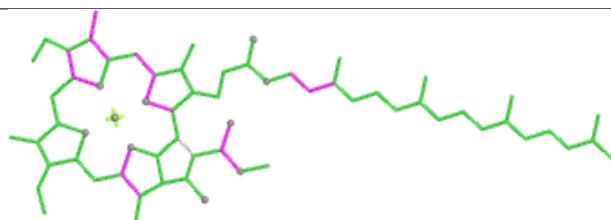


Rings

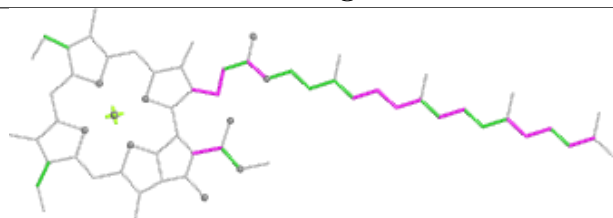
Ligand CLA r 505



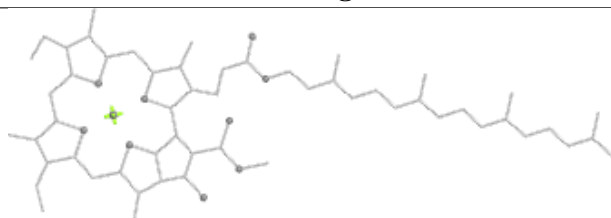
Bond lengths



Bond angles

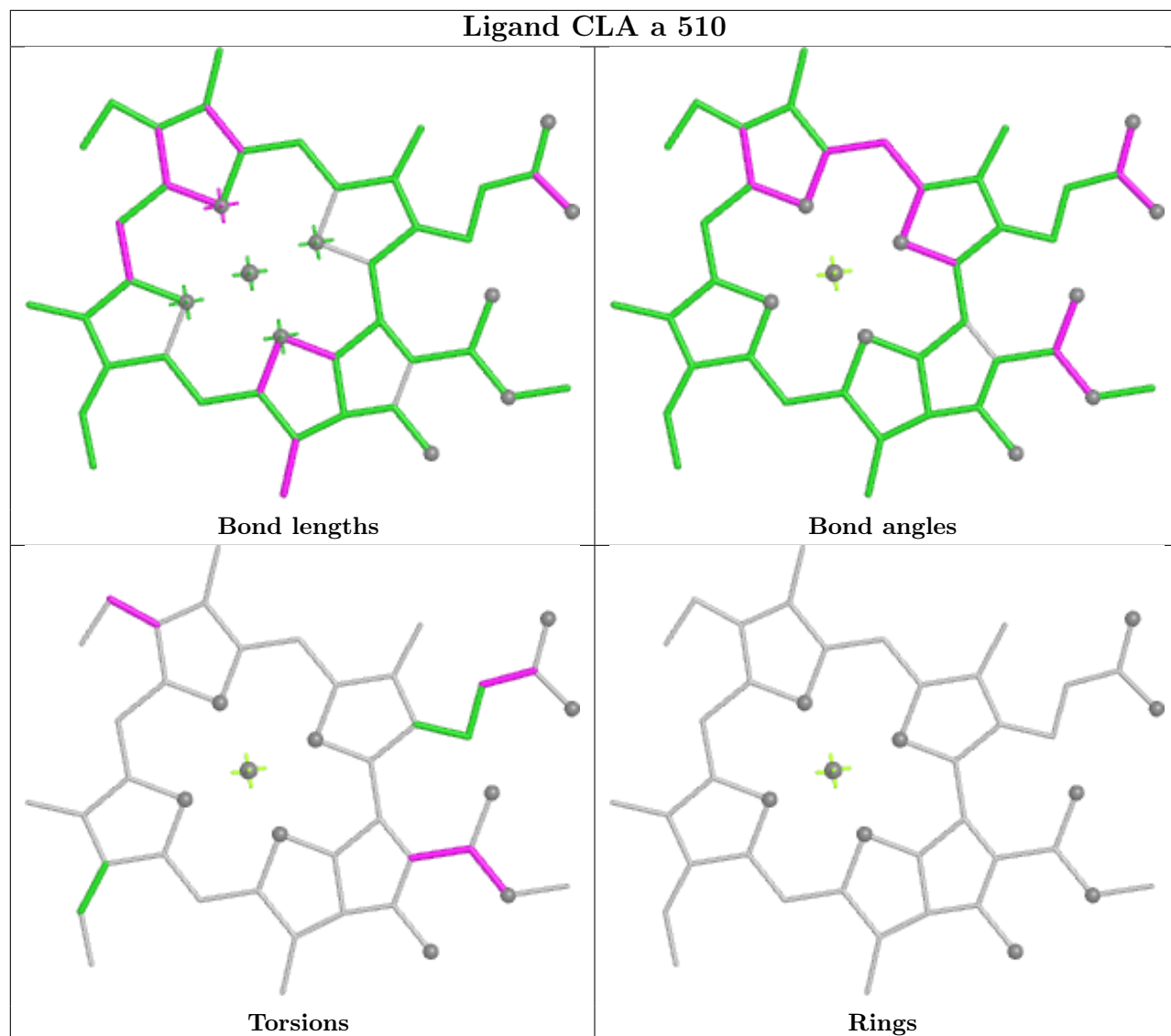


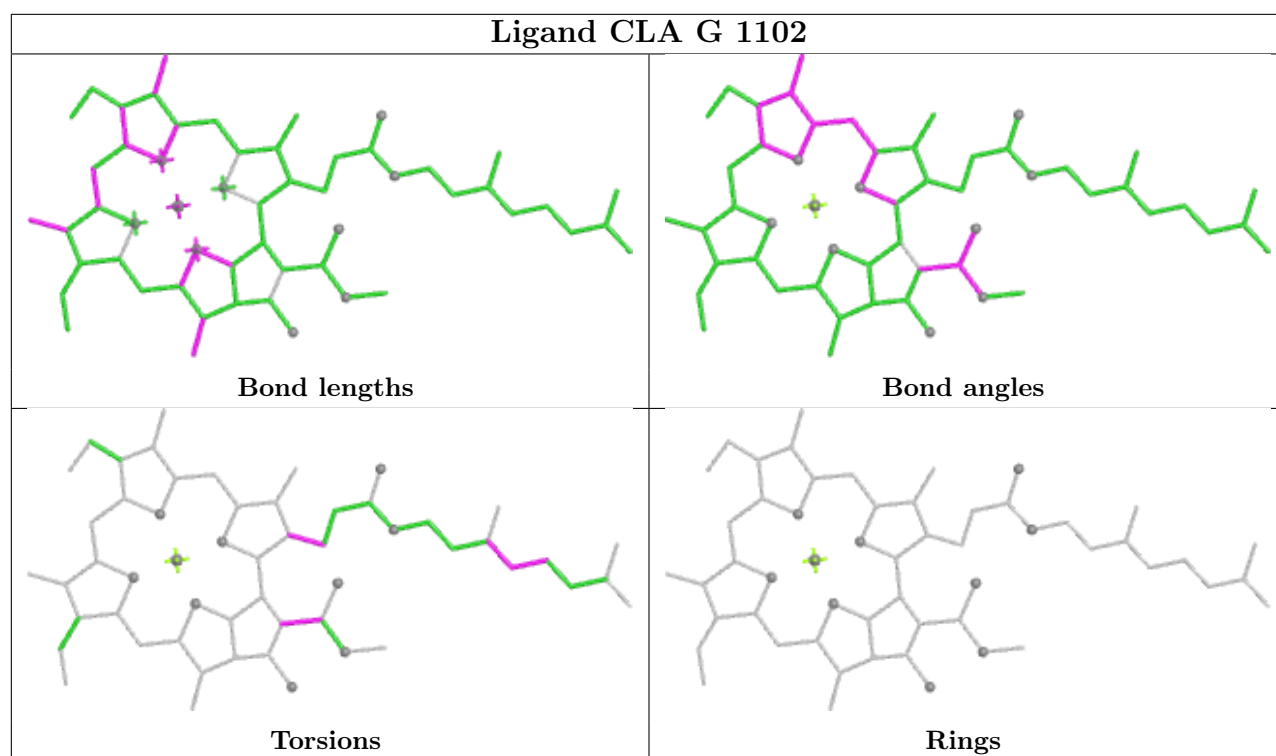
Torsions



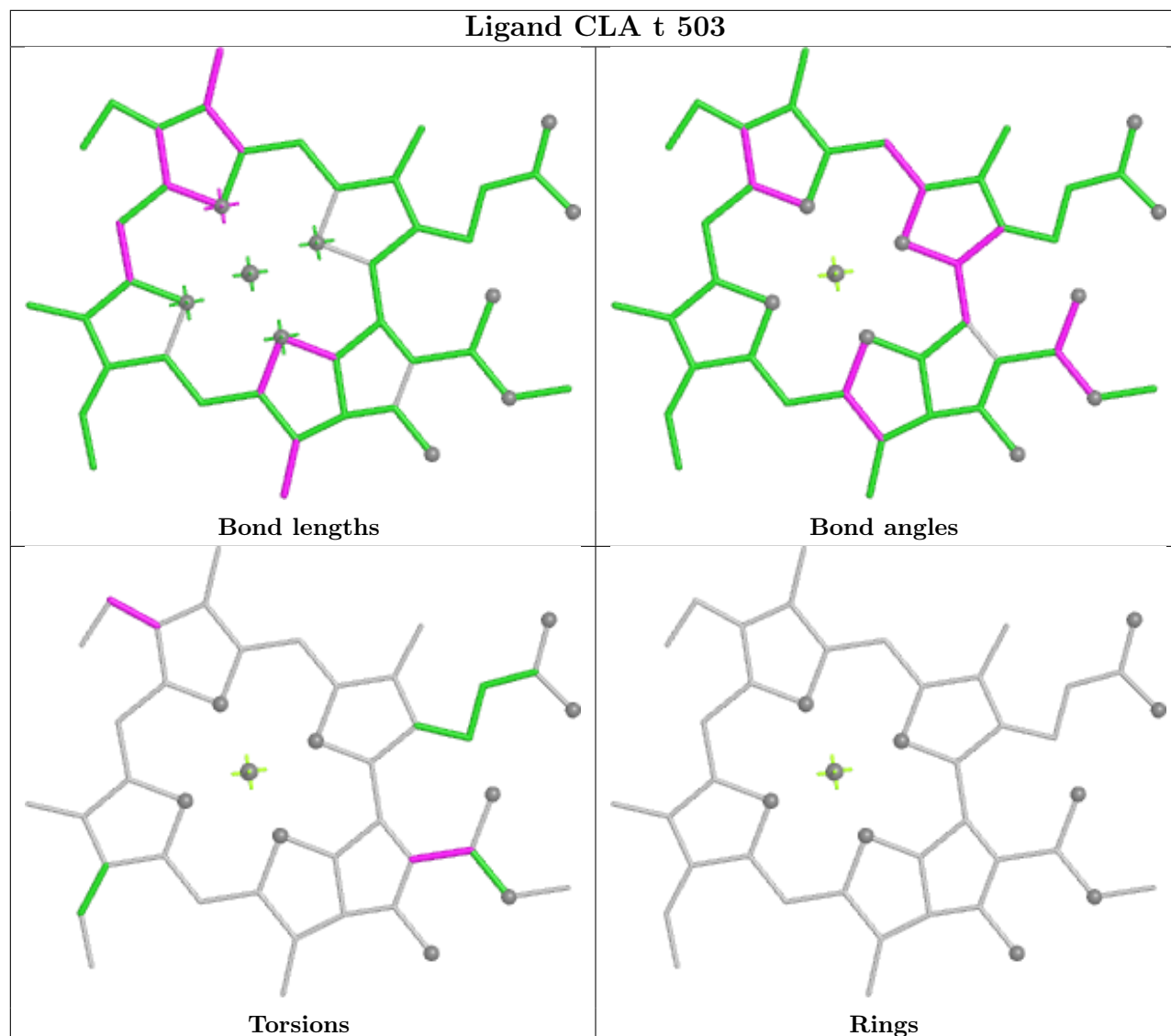
Rings

Ligand CLA a 510

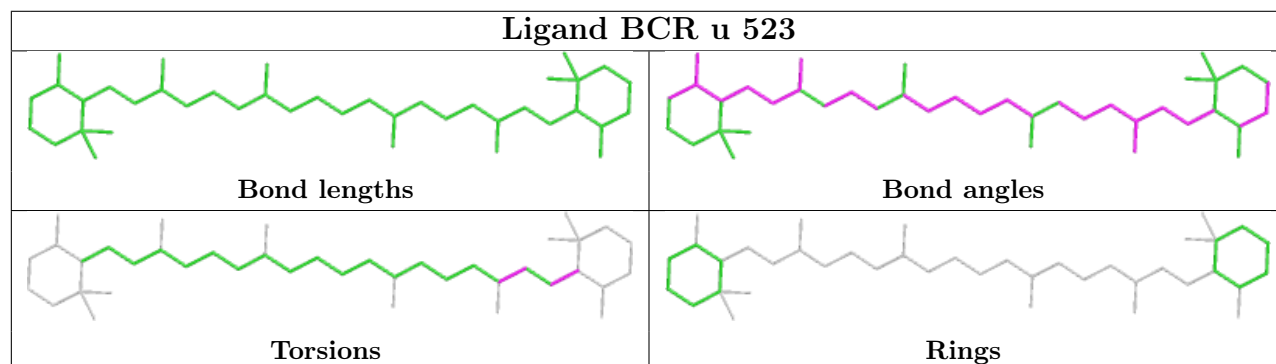


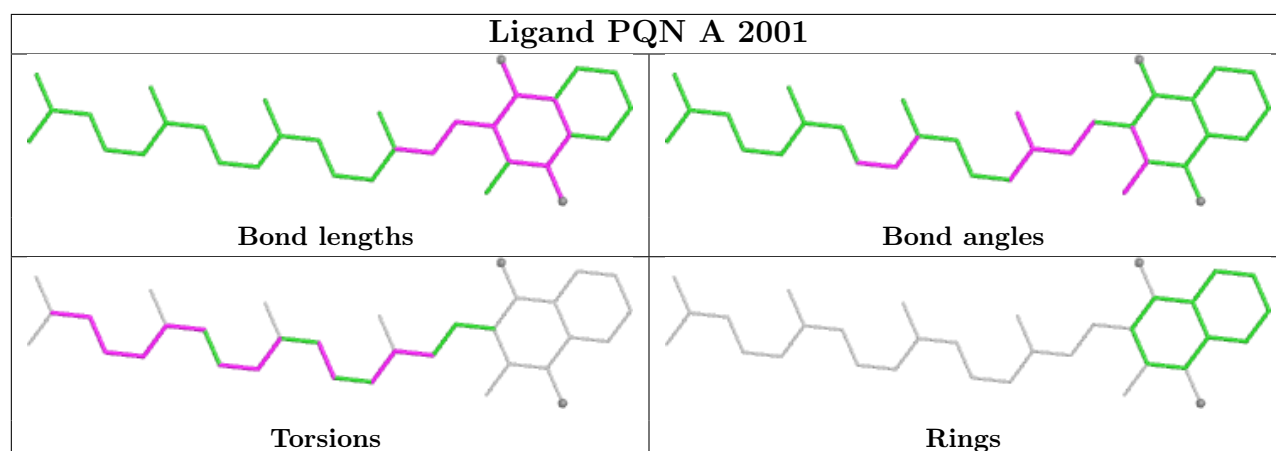
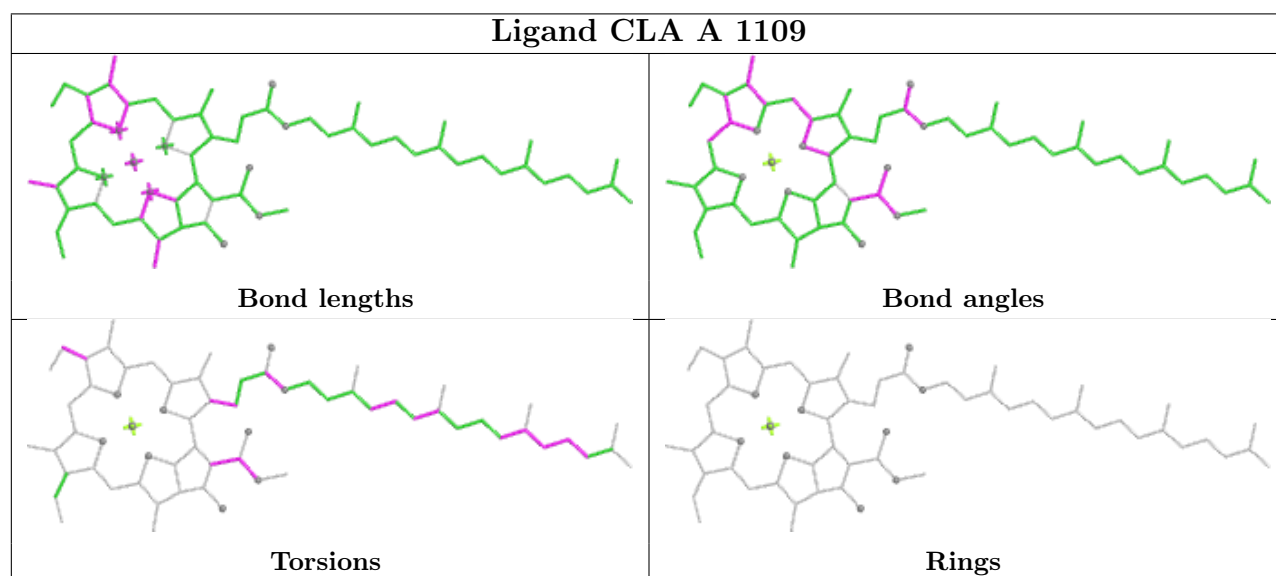
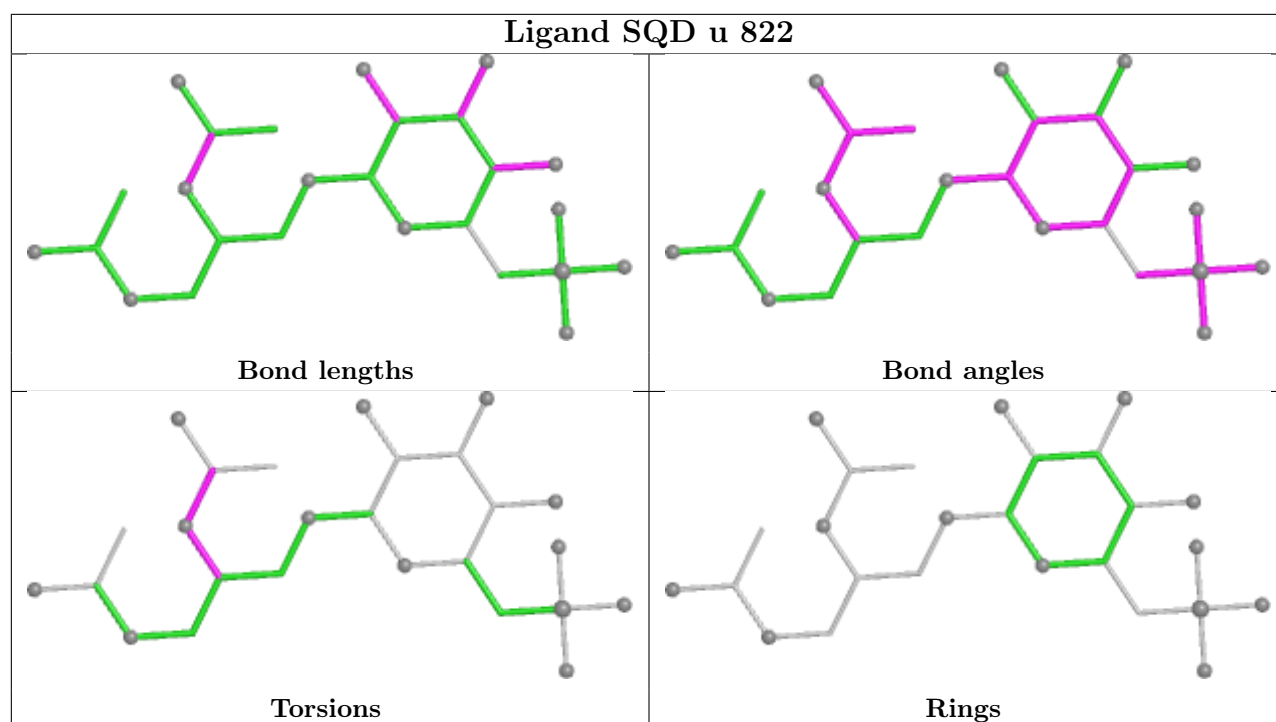


Ligand CLA t 503

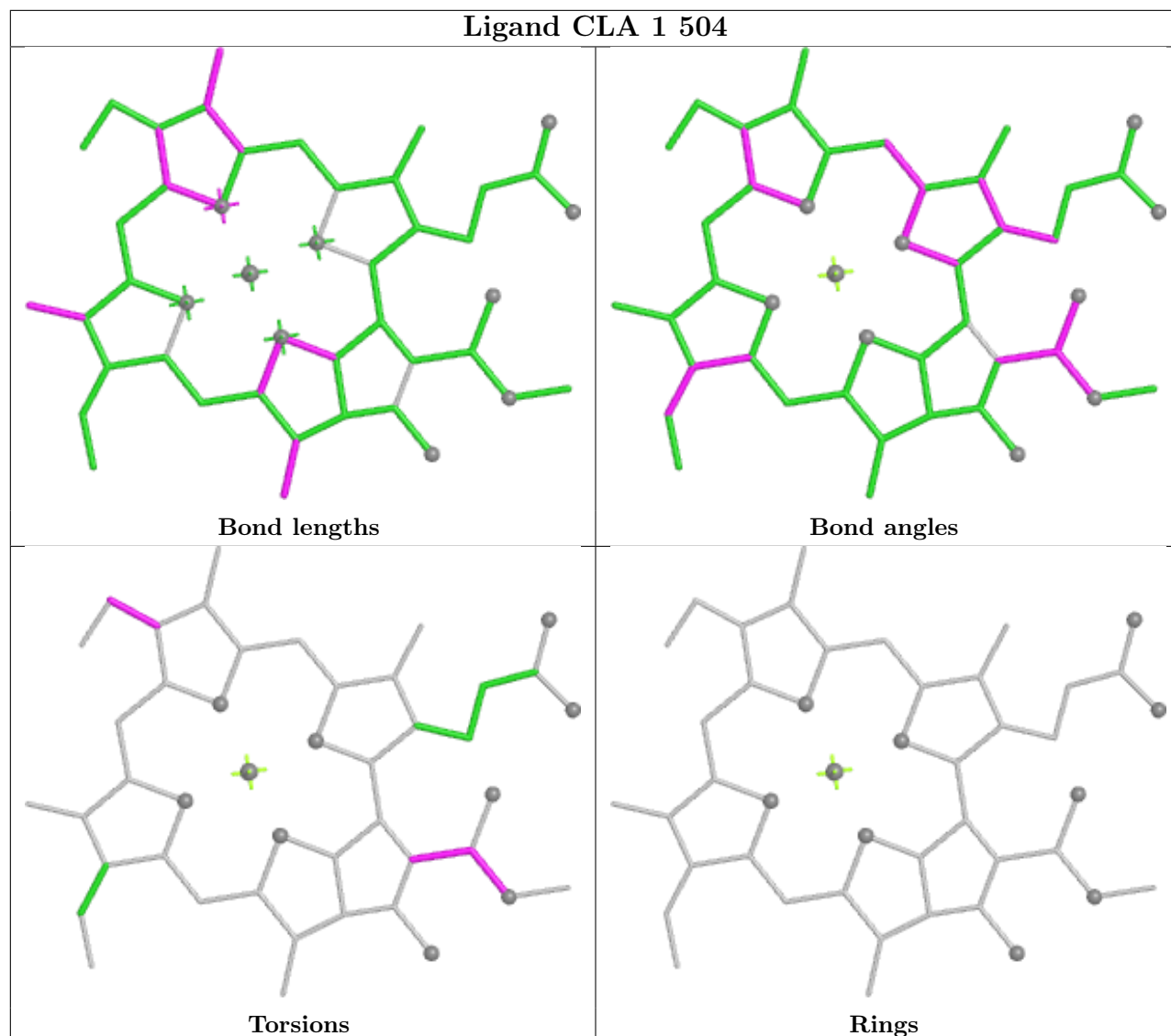


Ligand BCR u 523

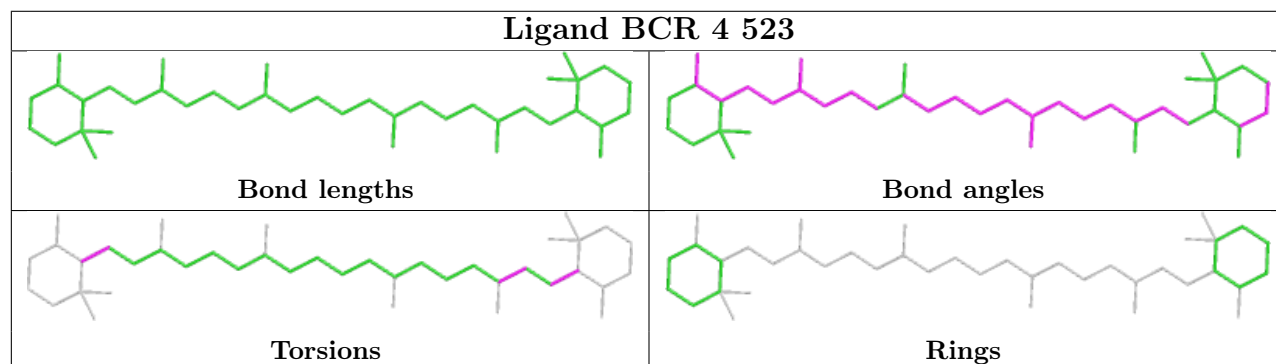


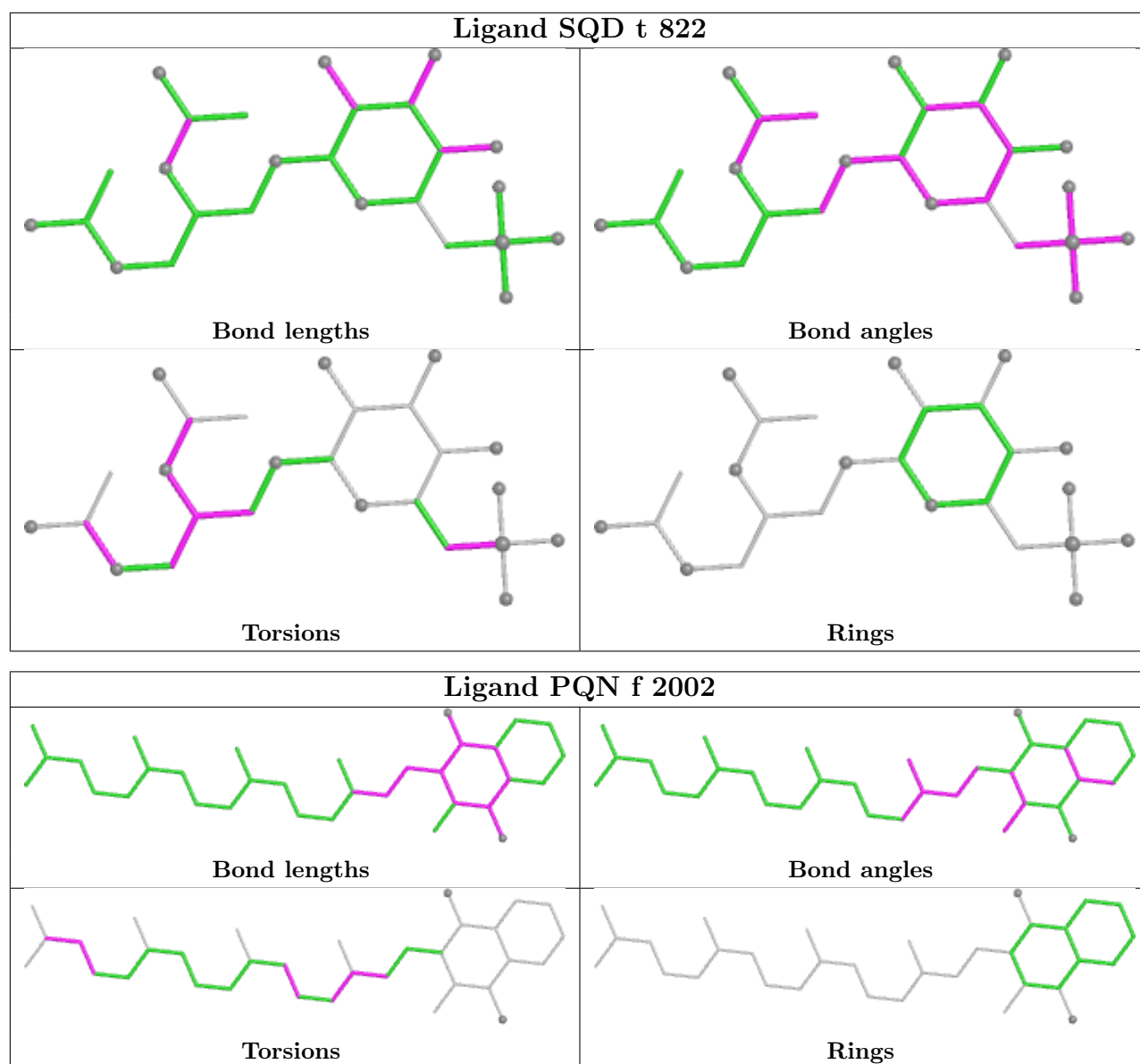


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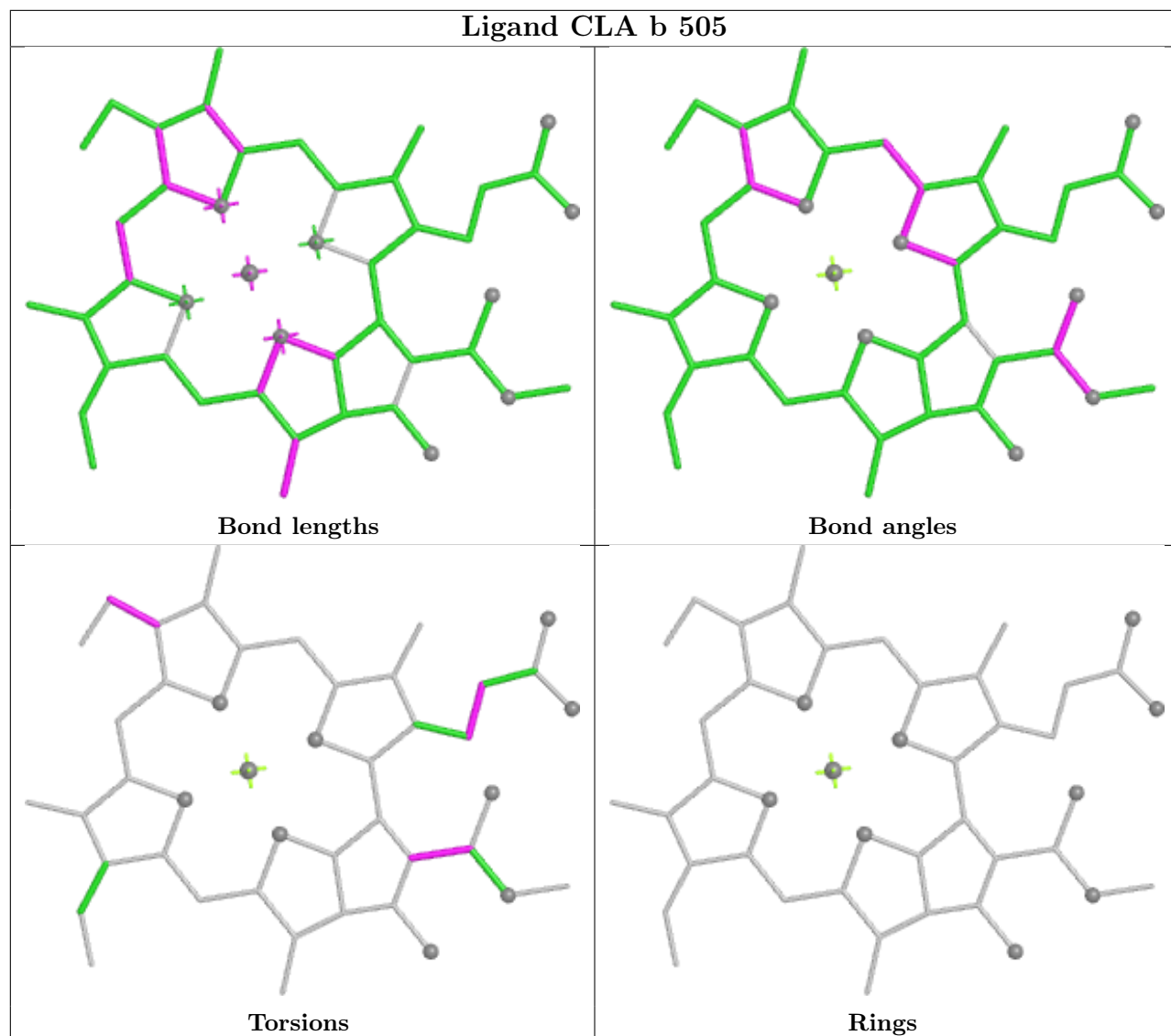


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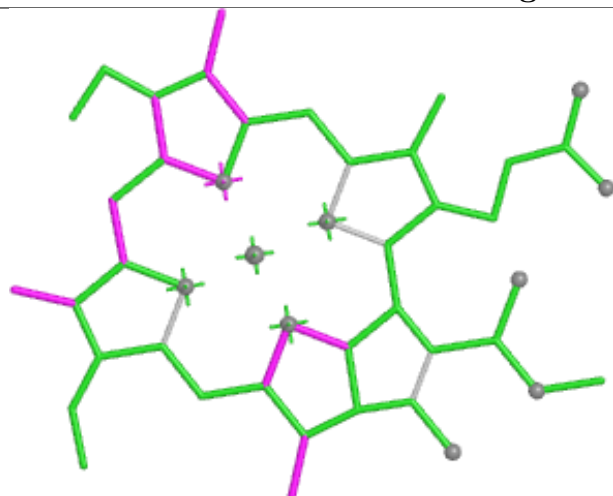




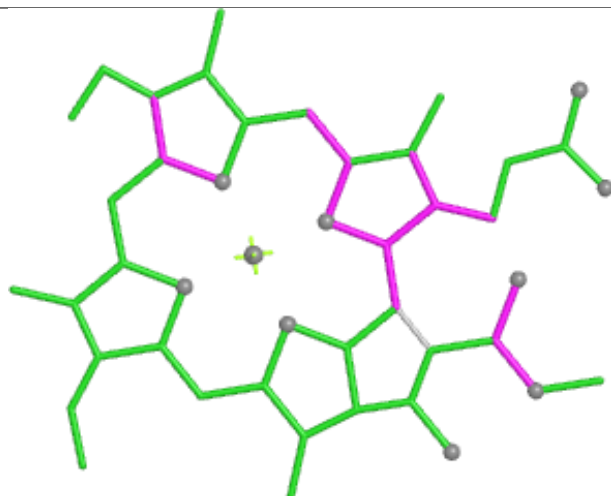
Ligand CLA b 505



Ligand CLA c 501



Bond lengths



Bond angles

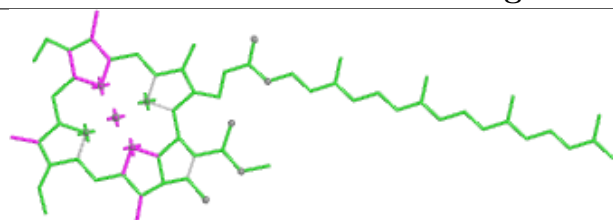


Torsions

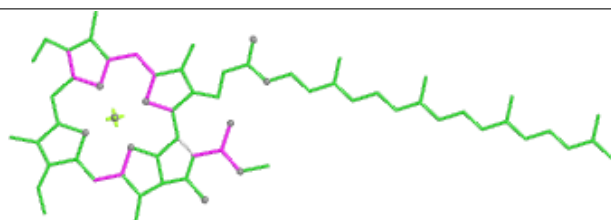


Rings

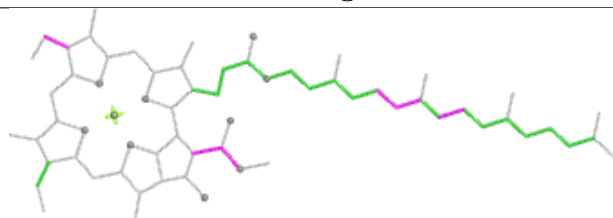
Ligand CLA H 1235



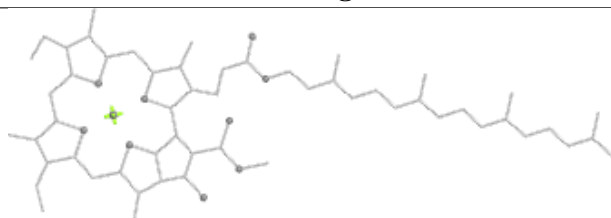
Bond lengths



Bond angles

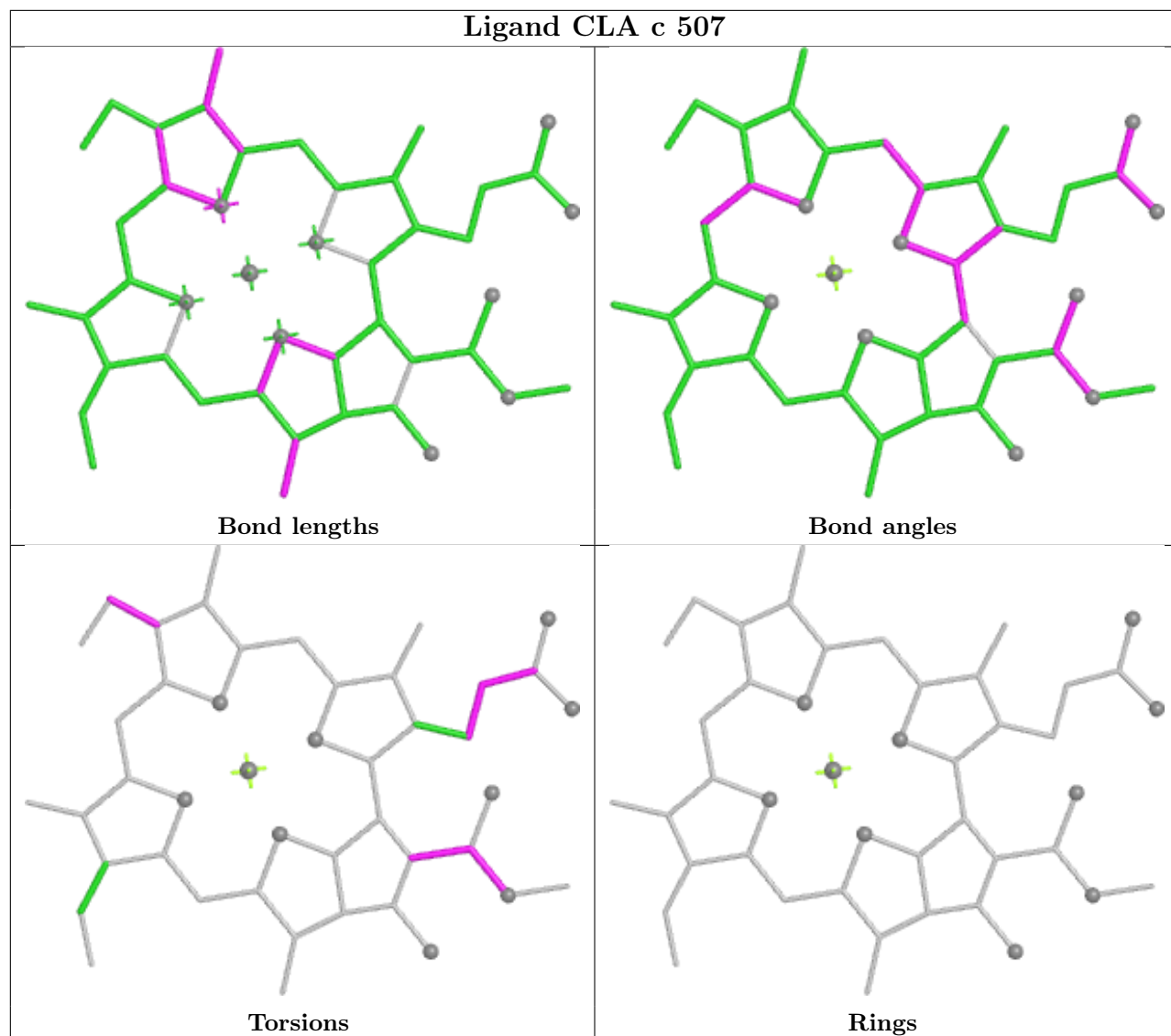


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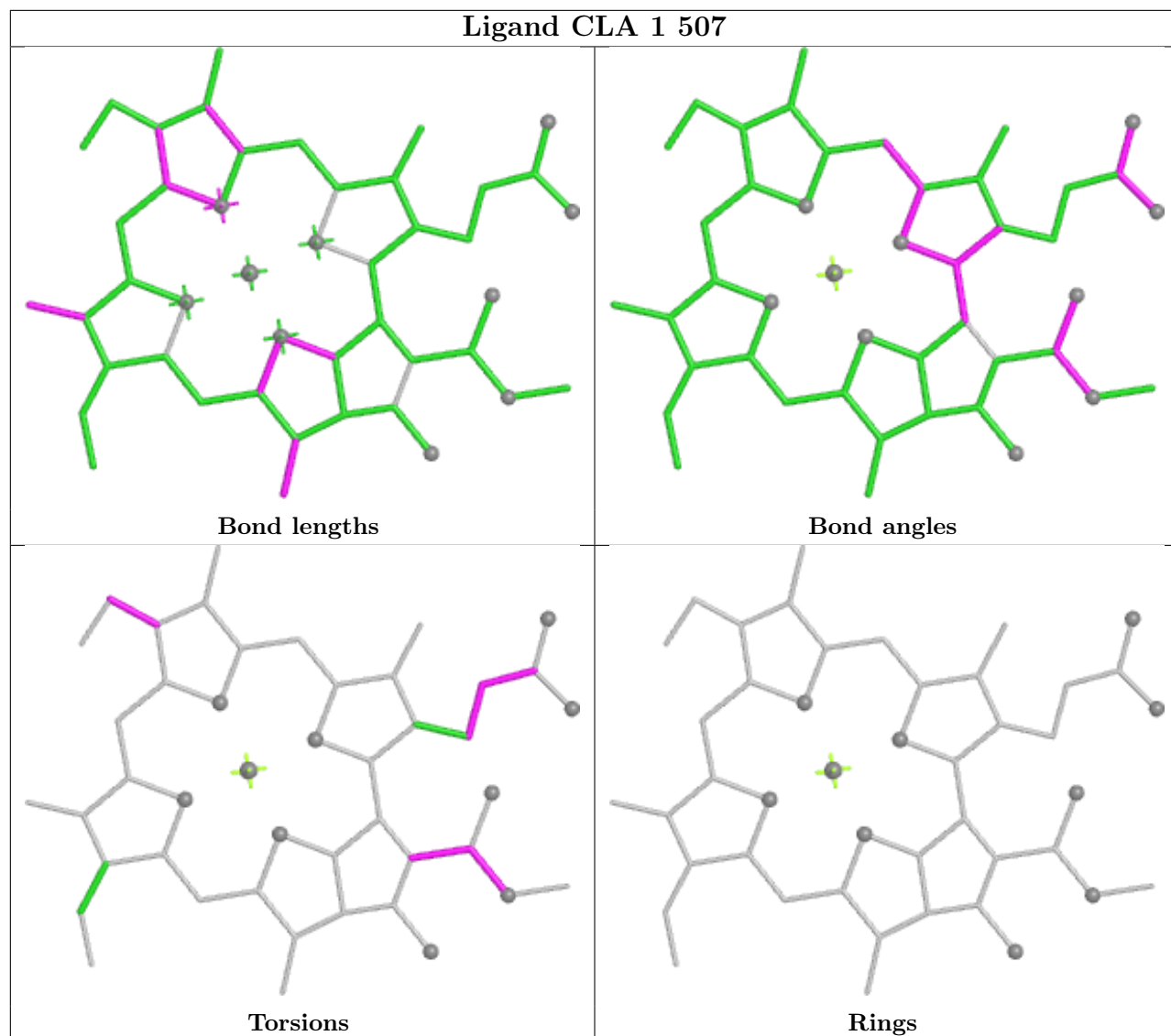


Rings

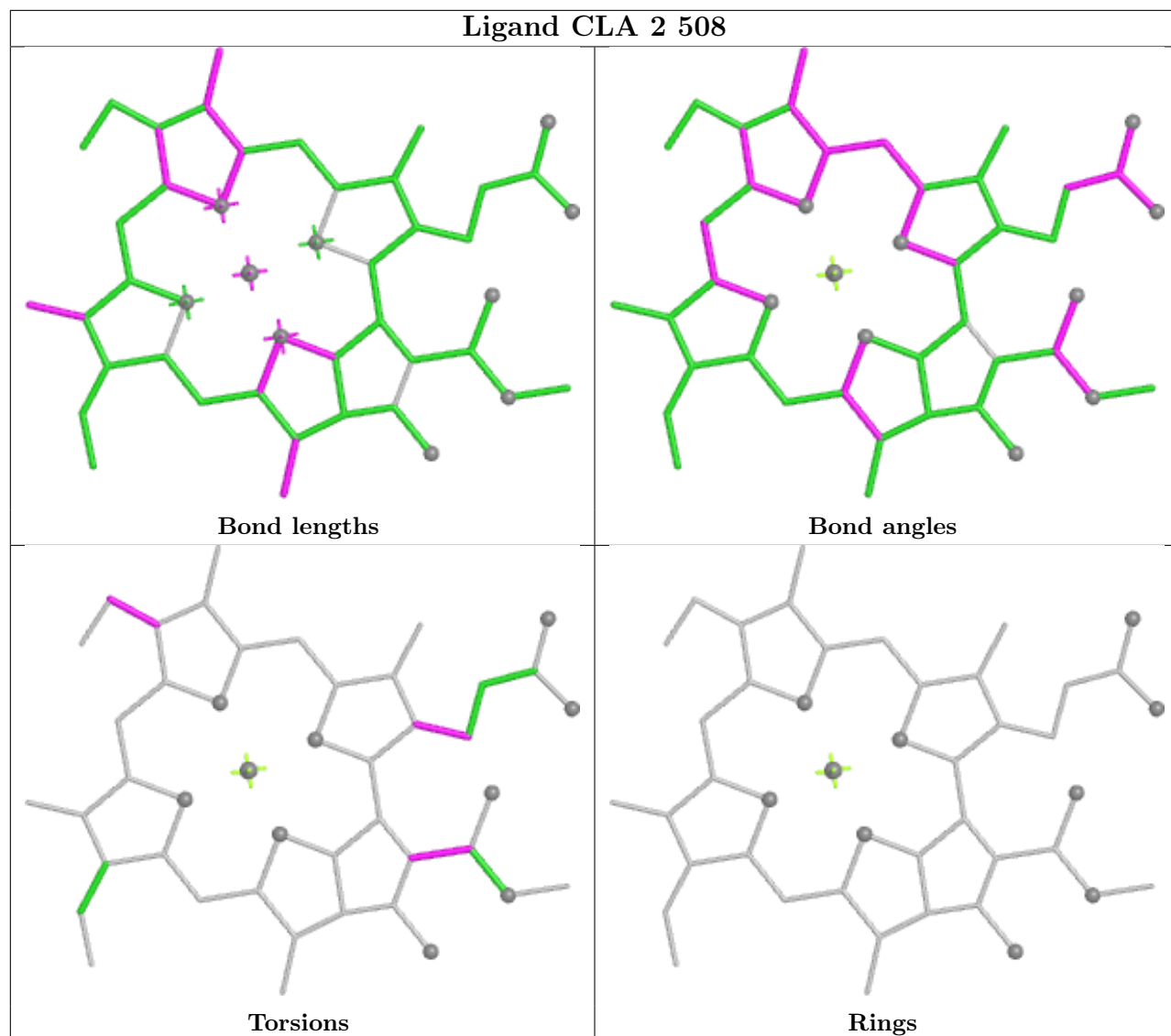
Ligand CLA c 507

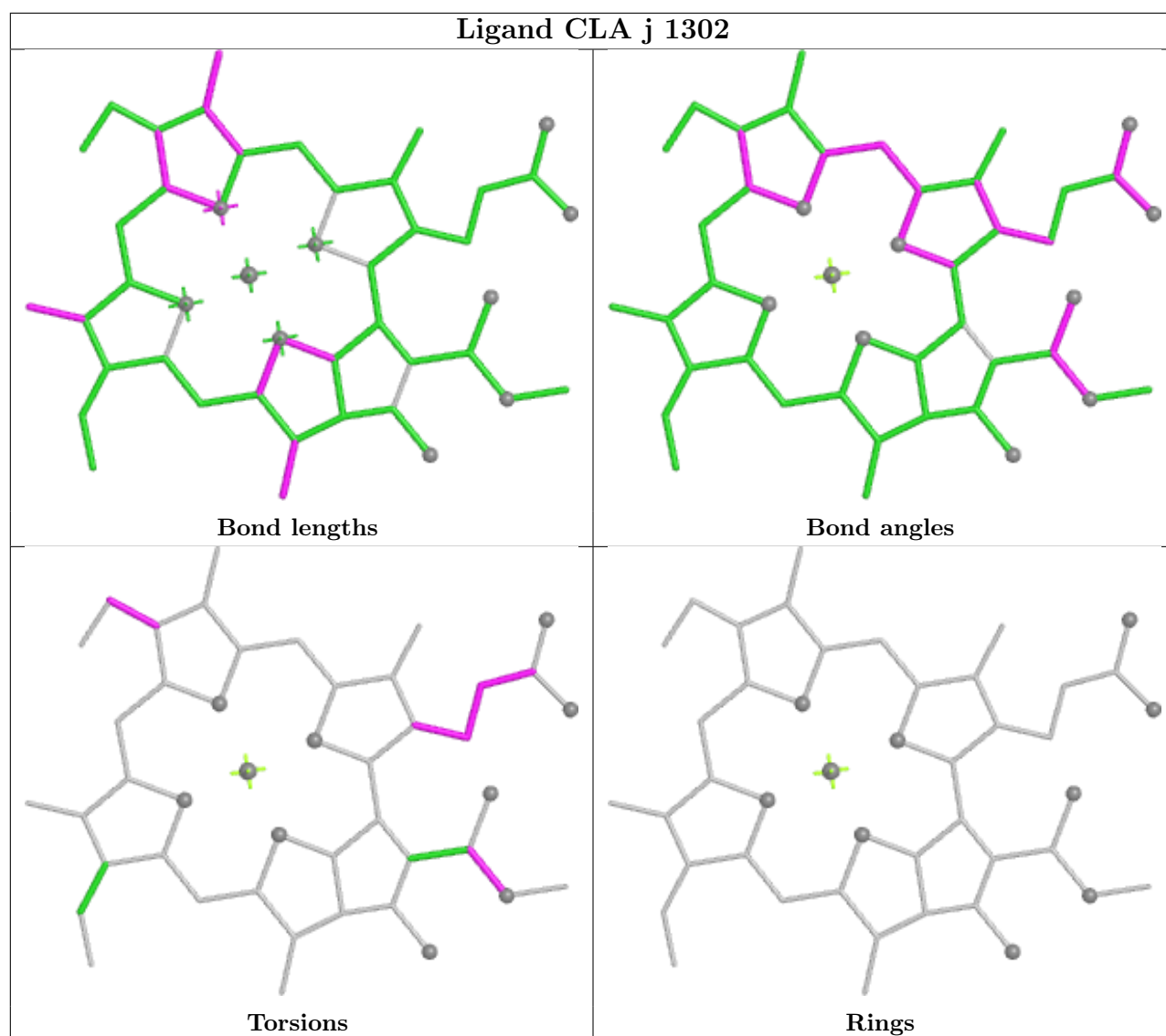


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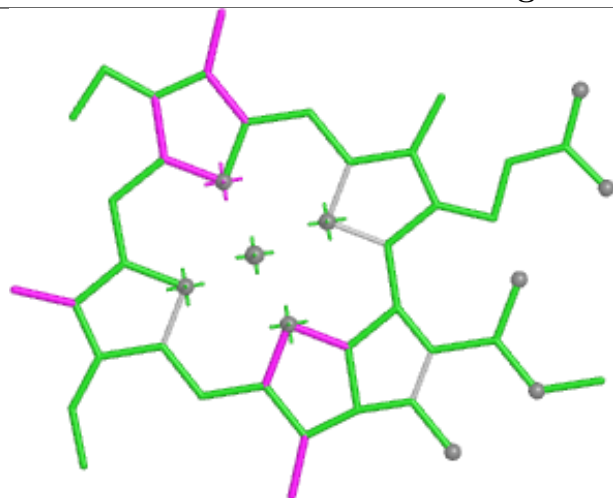


Ligand CLA 2 508

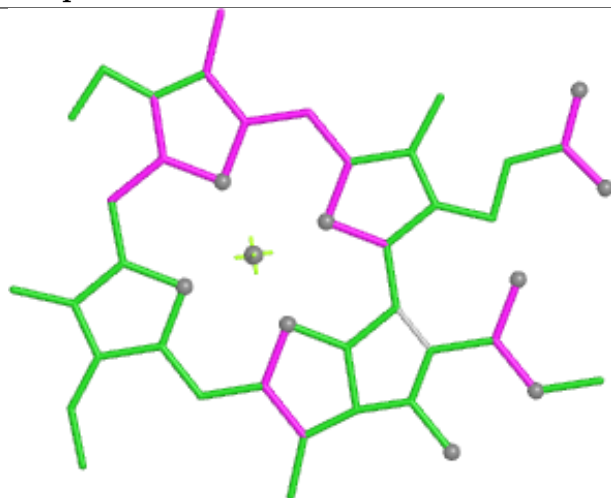




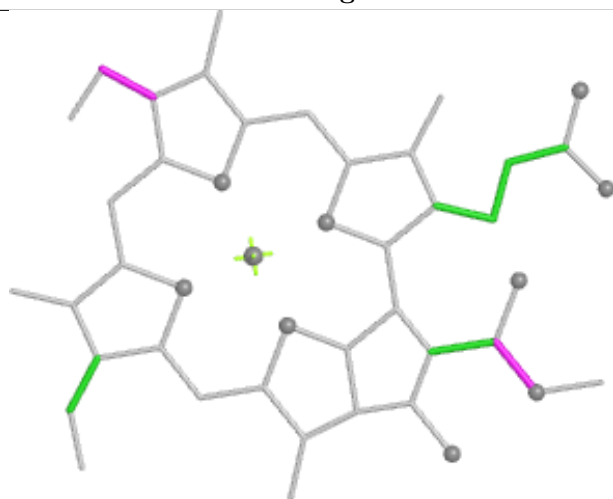
Ligand CLA q 511



Bond lengths



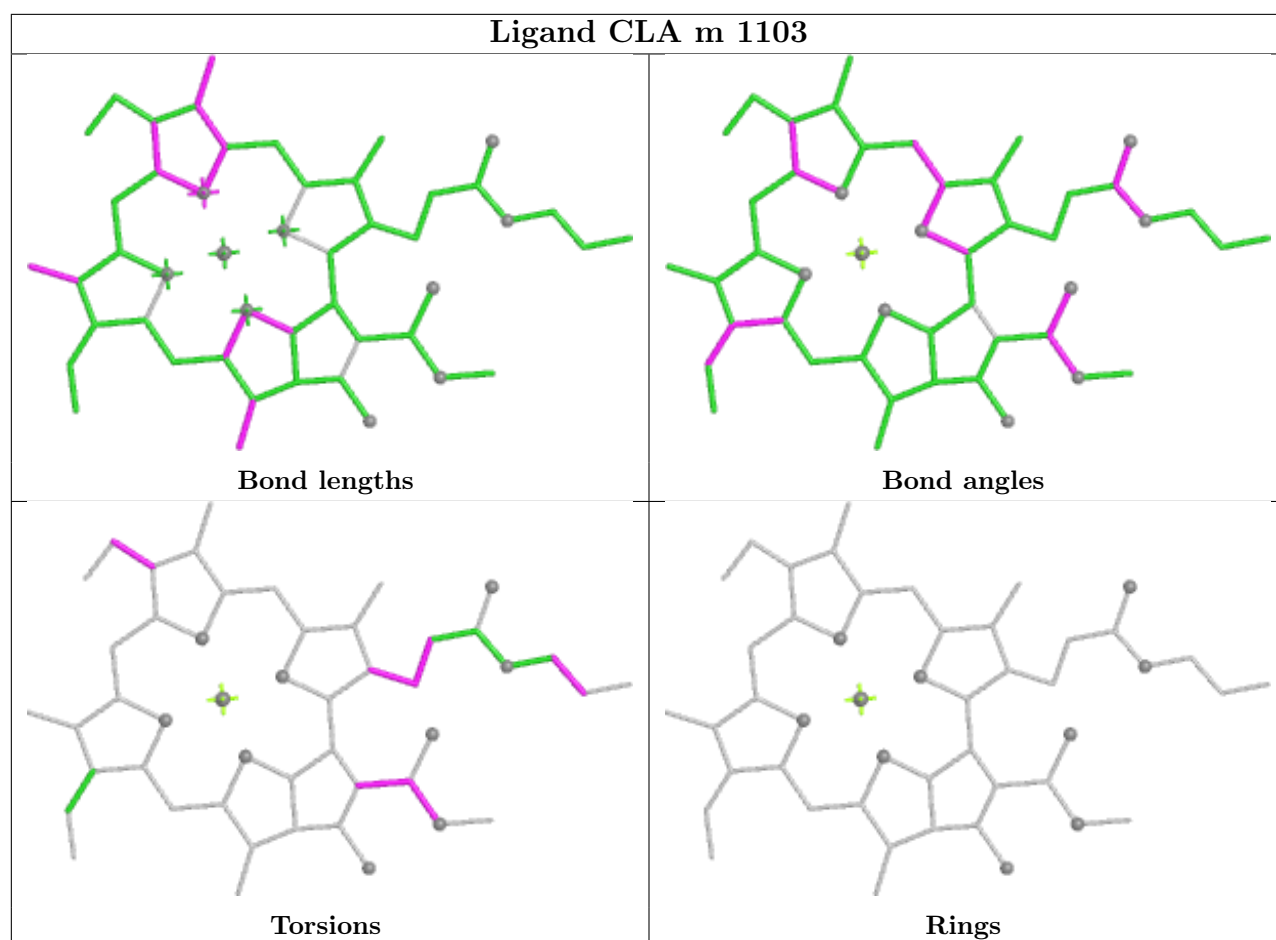
Bond angles



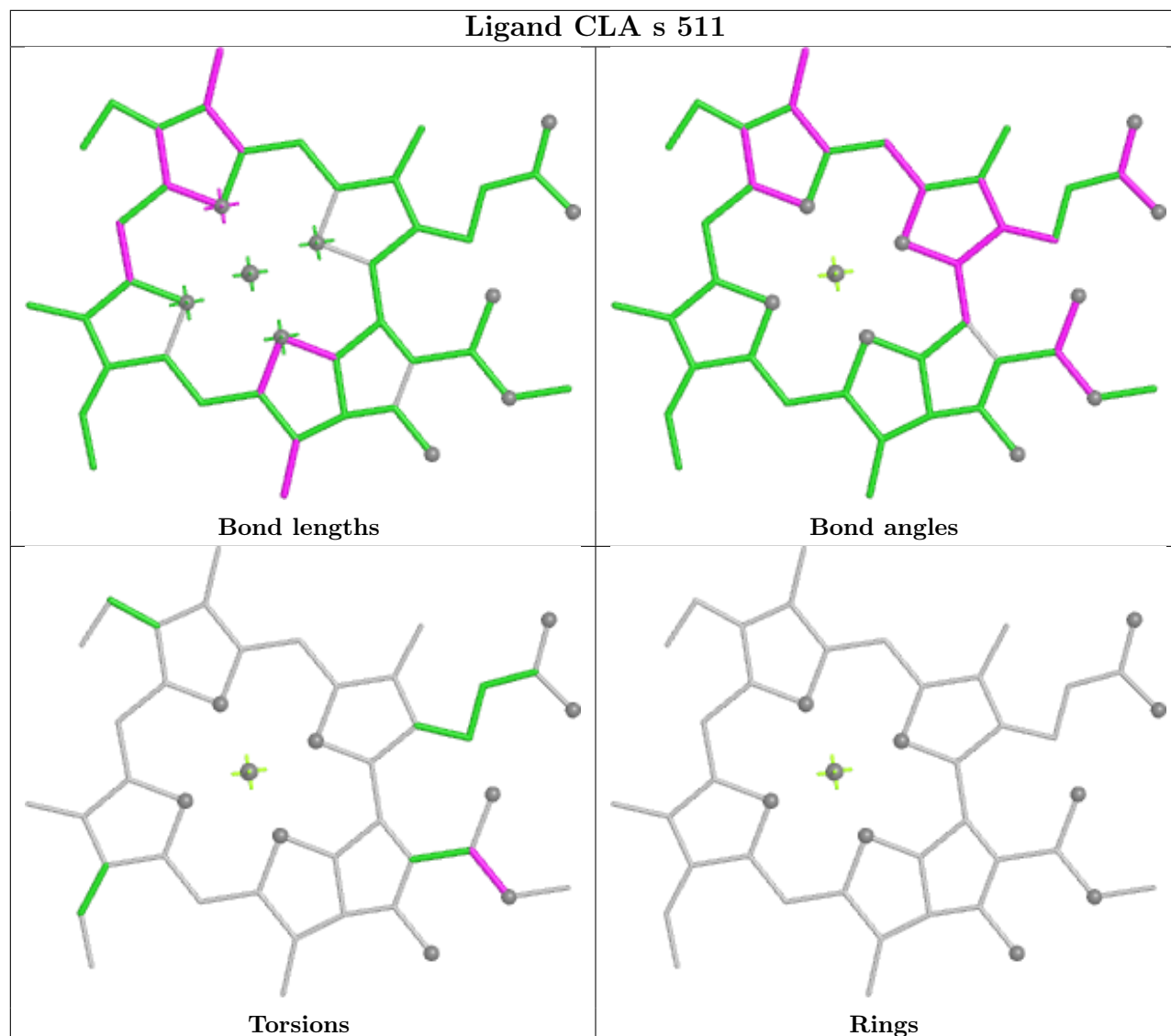
Torsions



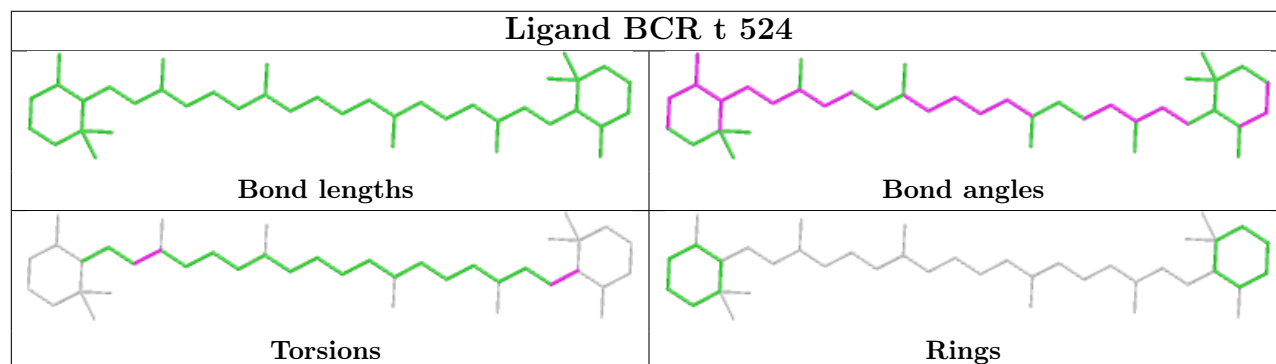
Rings



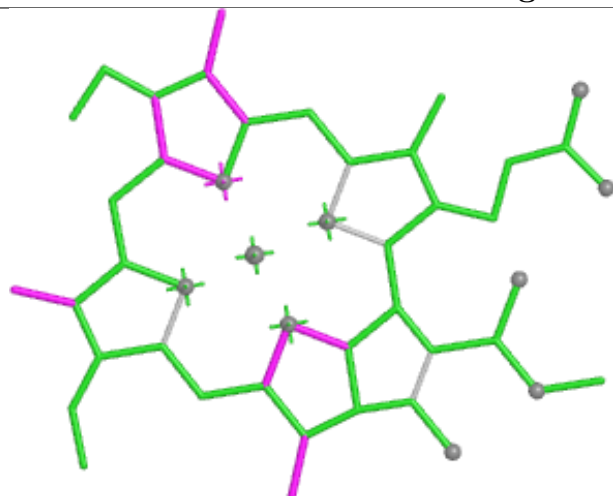
Ligand CLA s 511



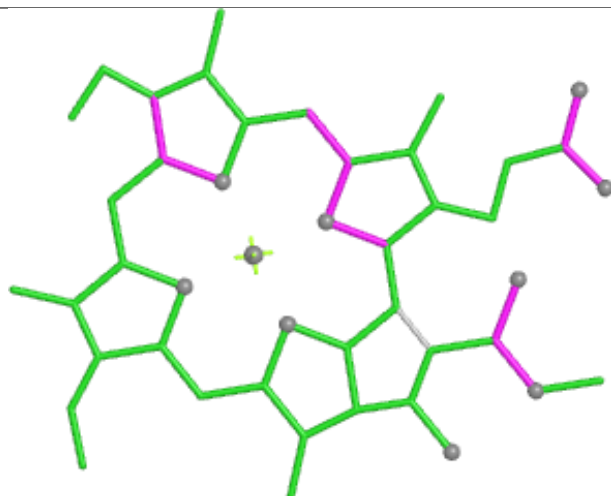
Ligand BCR t 524



Ligand CLA 1 517



Bond lengths



Bond angles

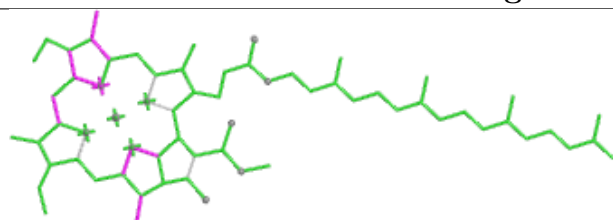


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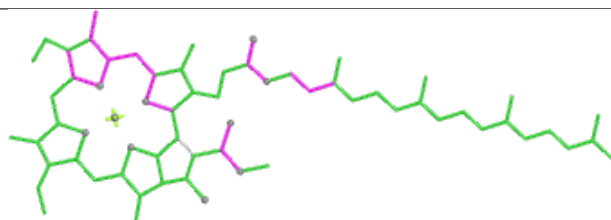


Rings

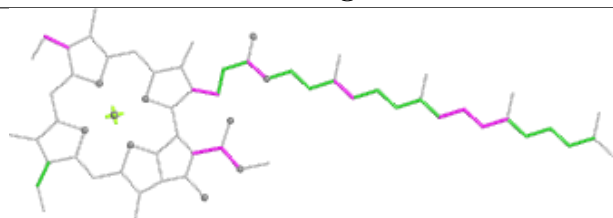
Ligand CLA H 1240



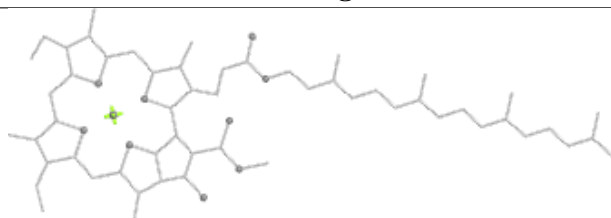
Bond lengths



Bond angles

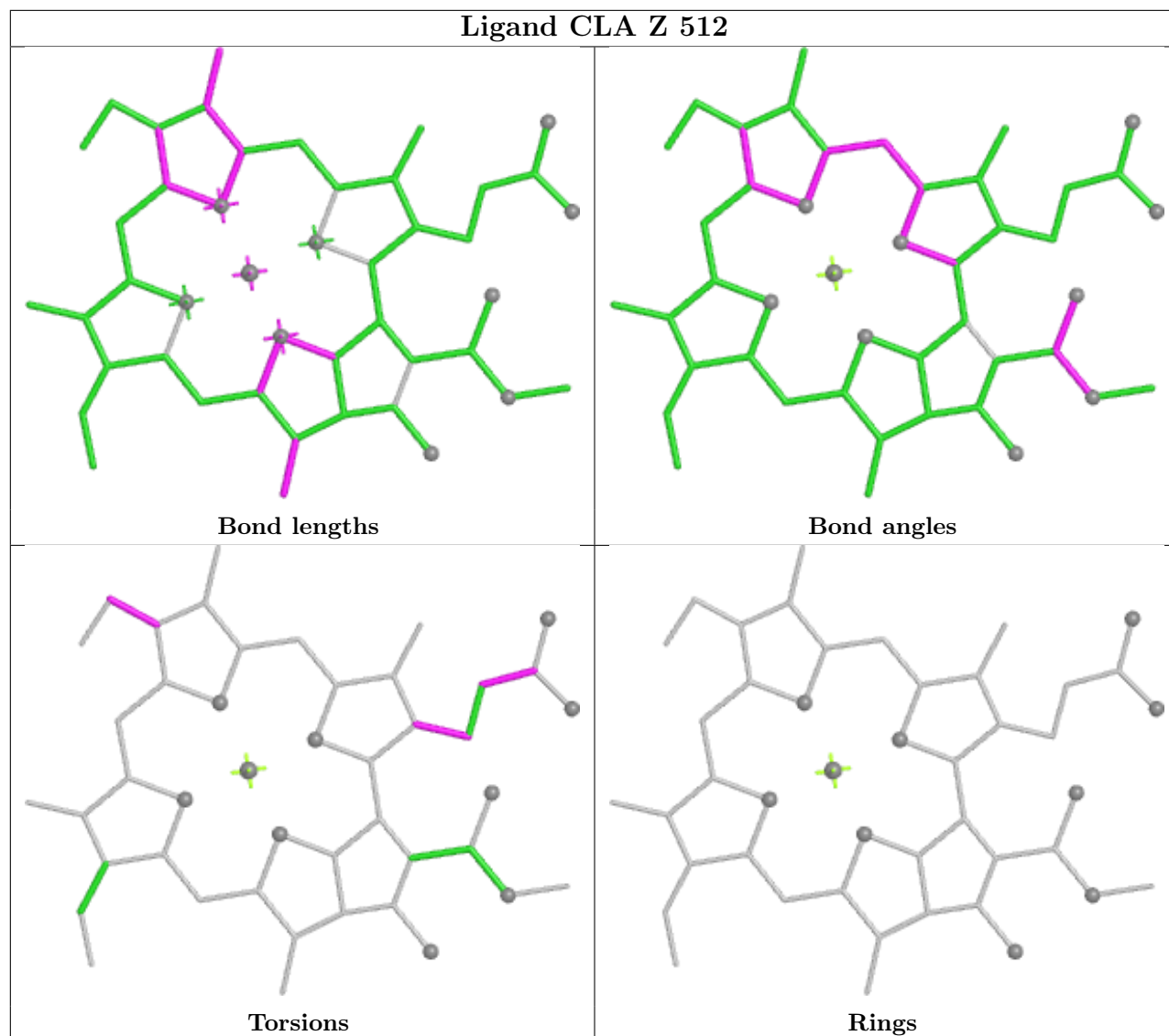


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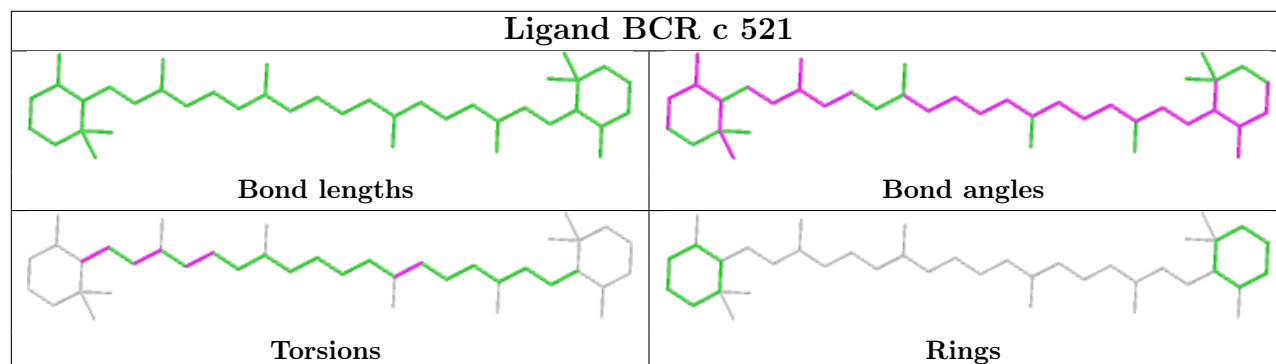


Rings

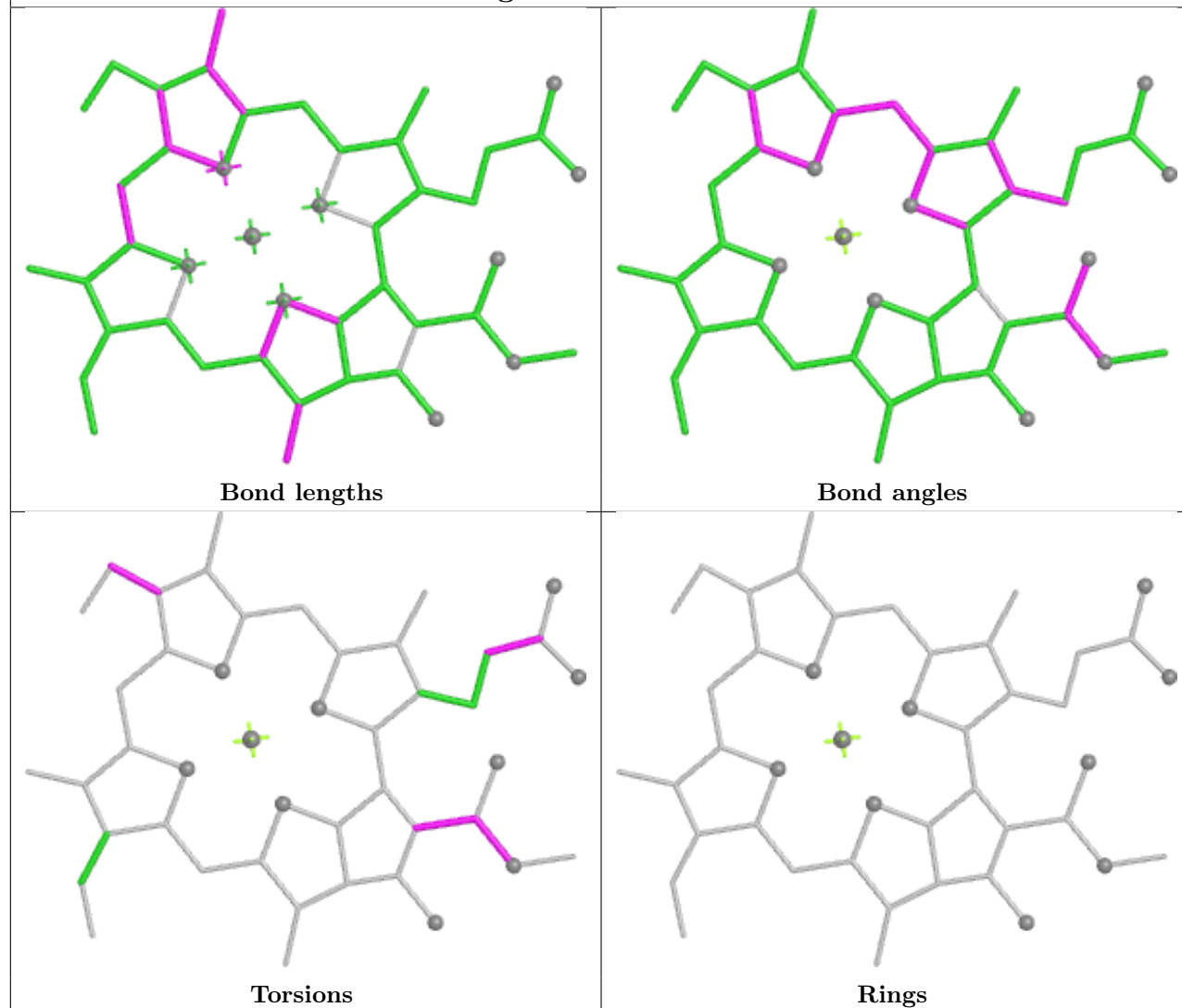
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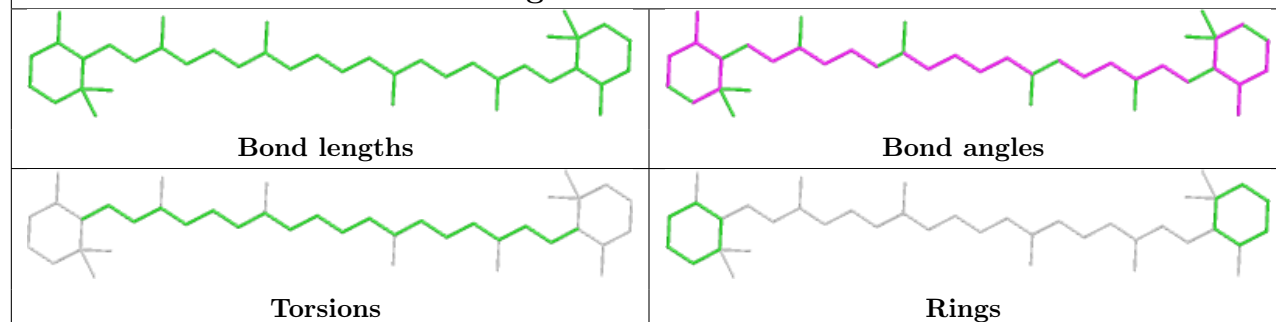
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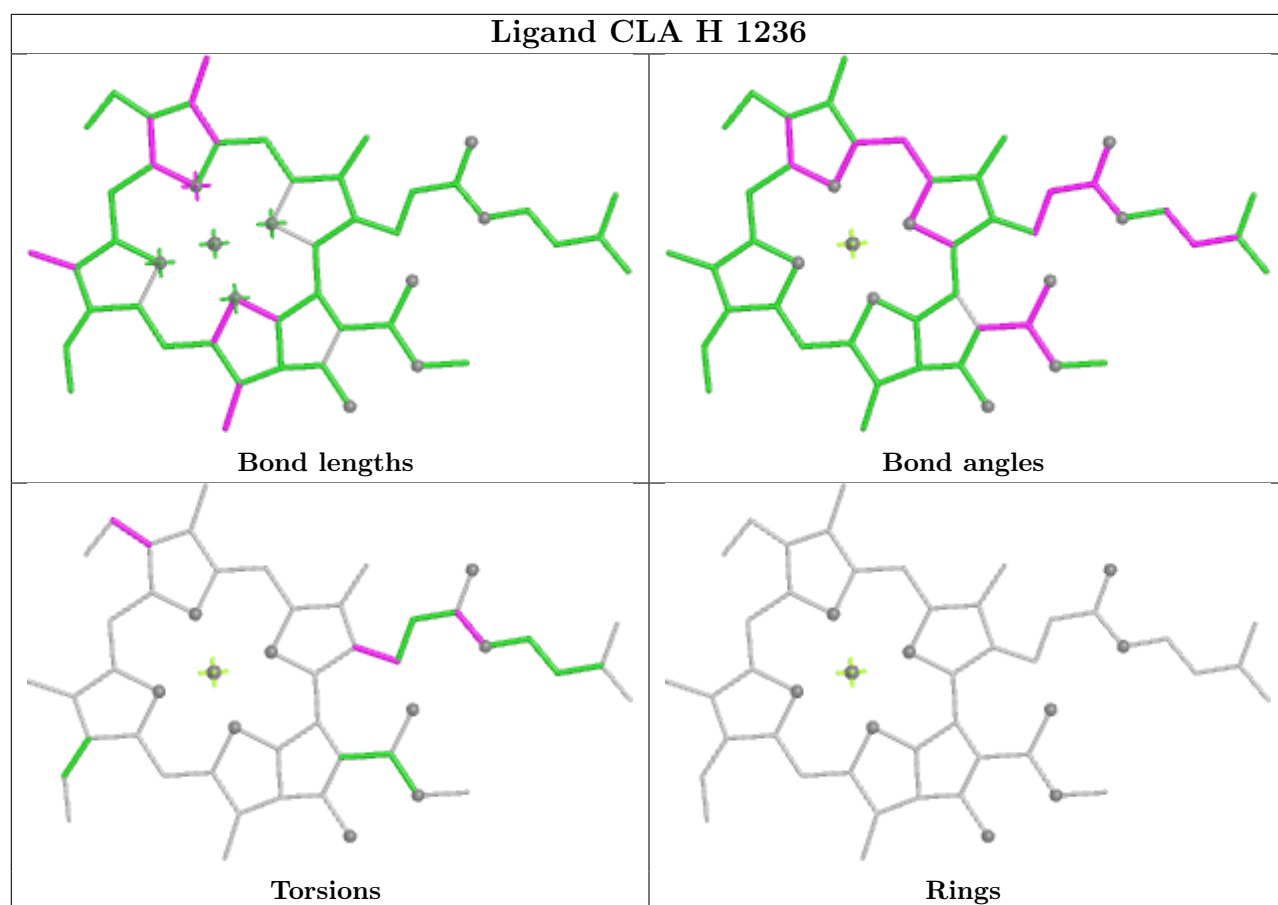


Ligand CLA c 512

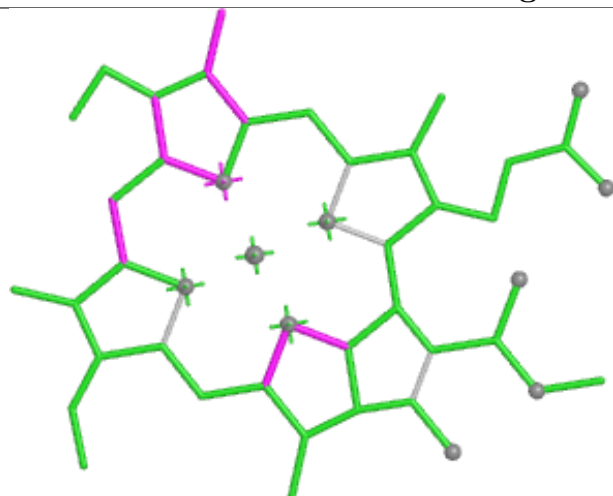


Ligand BCR e 4007

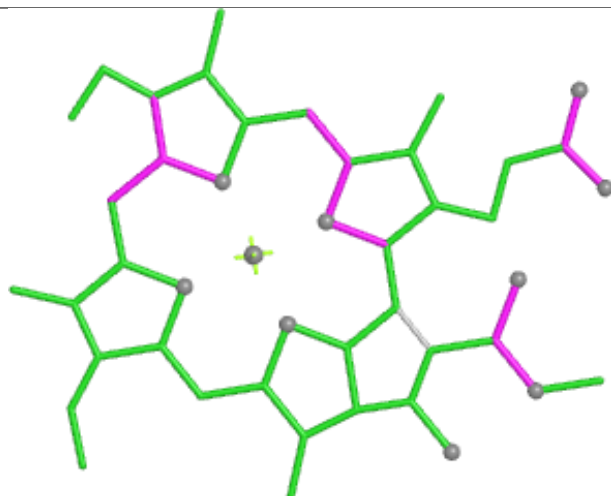




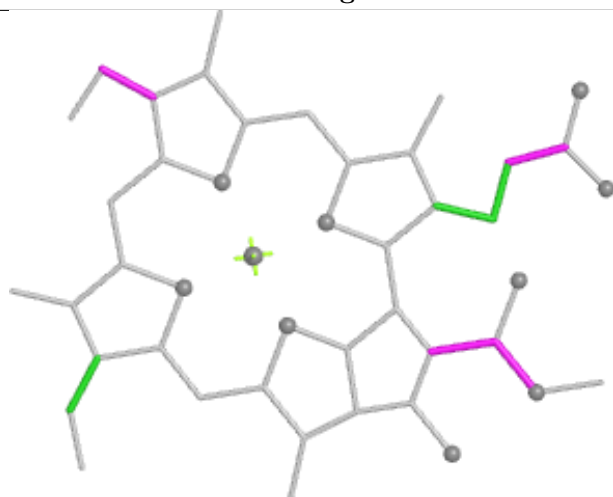
Ligand CLA c 519



Bond lengths



Bond angles

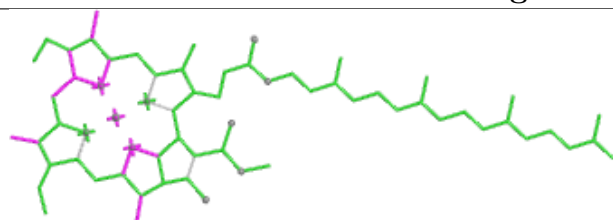


Torsions

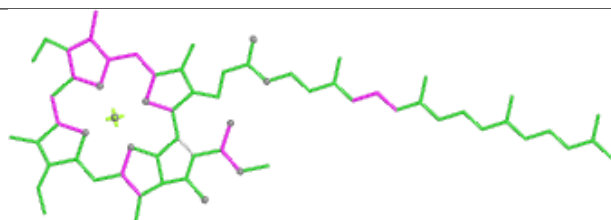


Rings

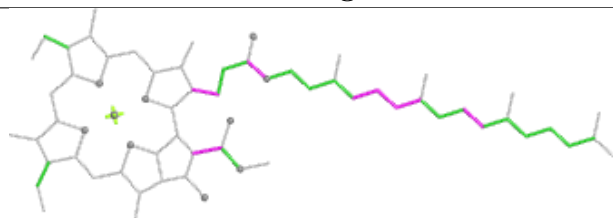
Ligand CLA e 1128



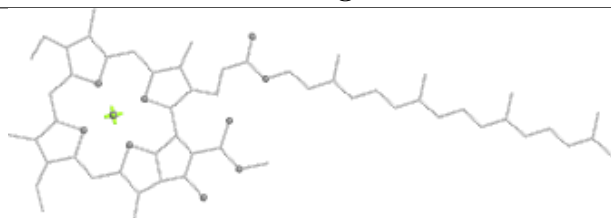
Bond lengths



Bond angles

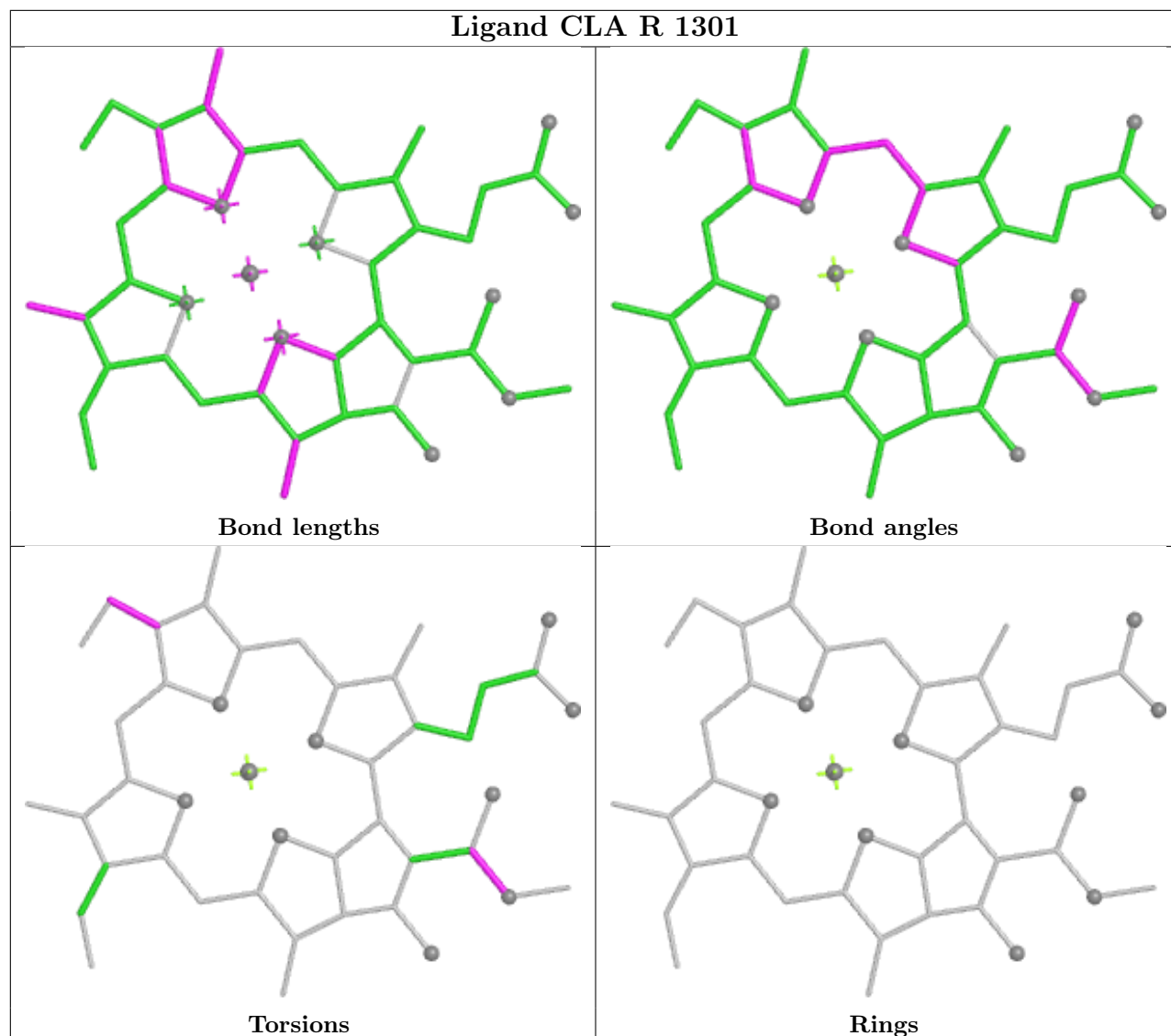


Torsions

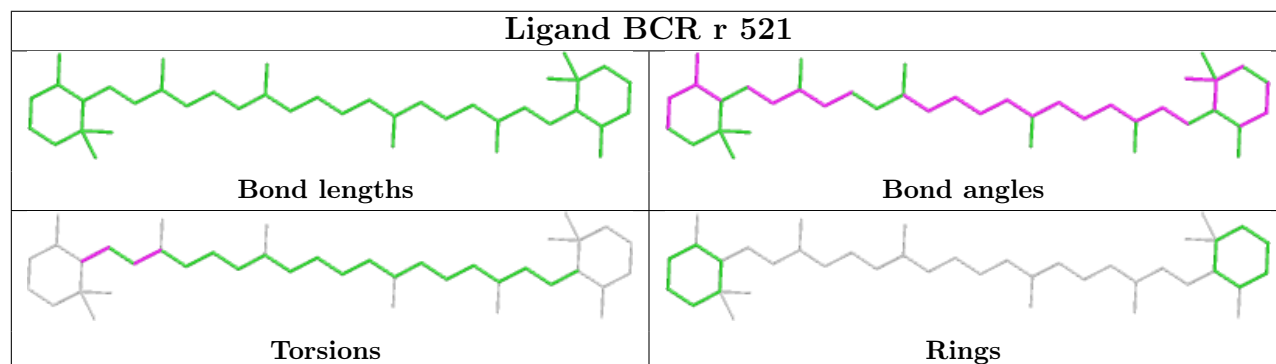


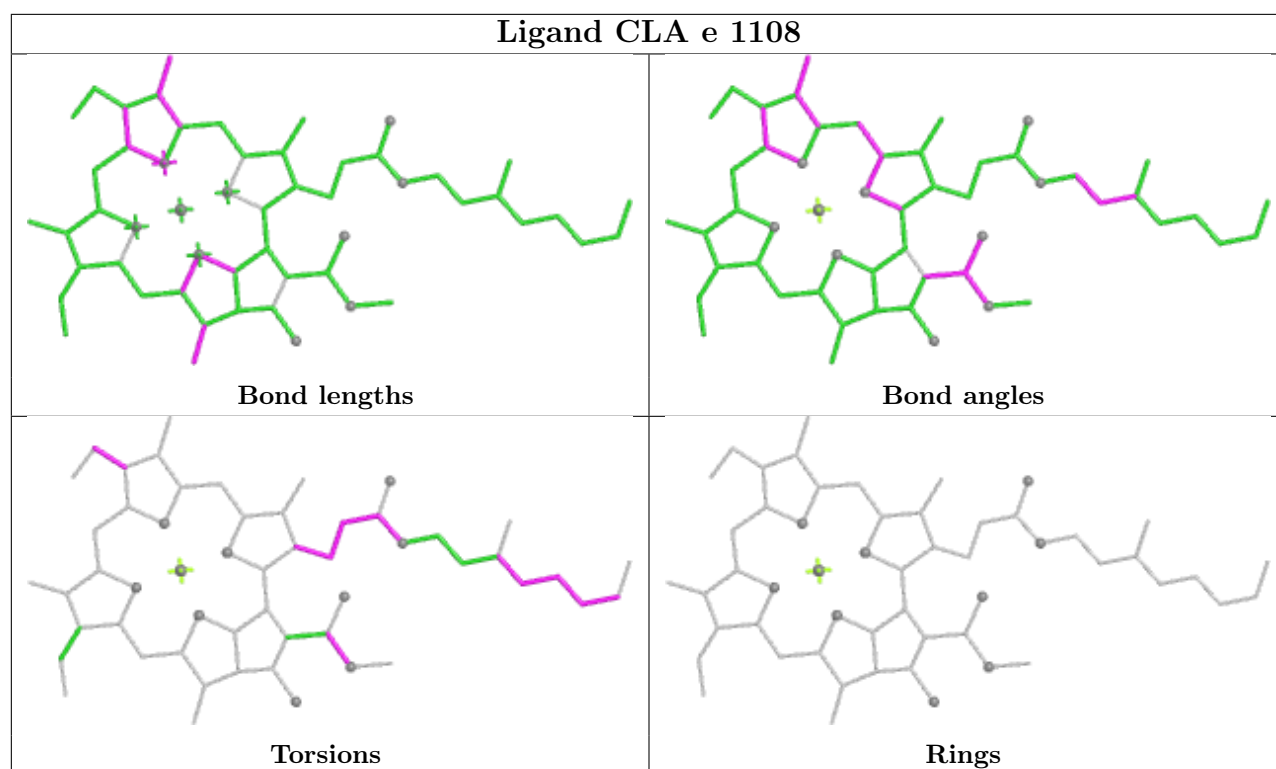
Rings

Ligand CLA R 1301

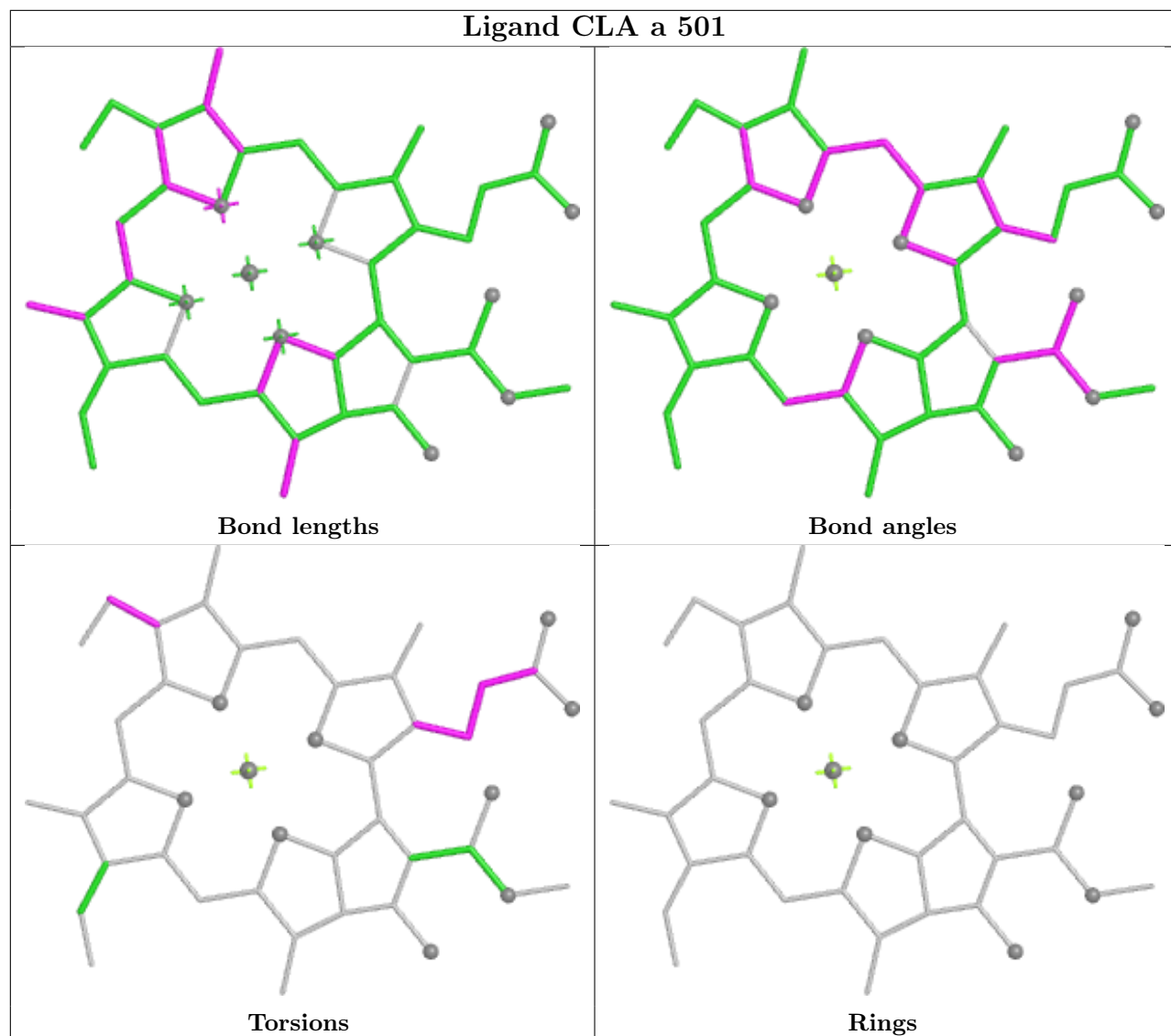


Ligand BCR r 521

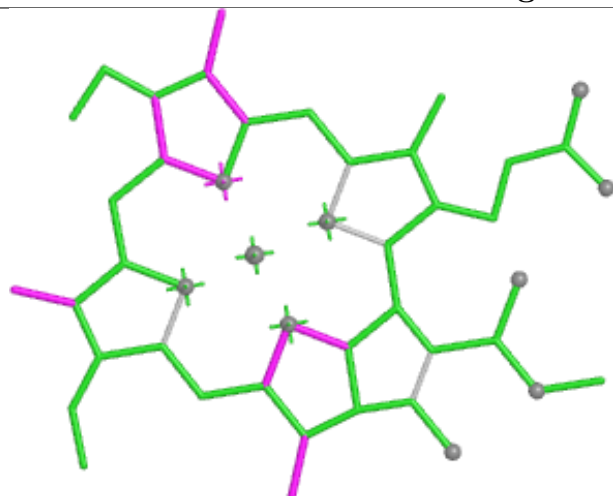




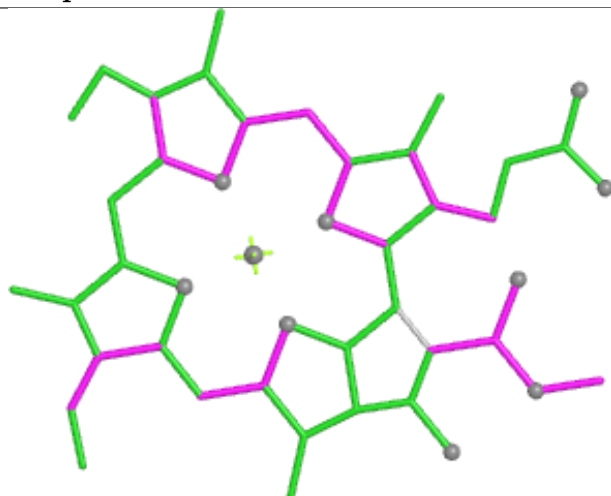
Ligand CLA a 501



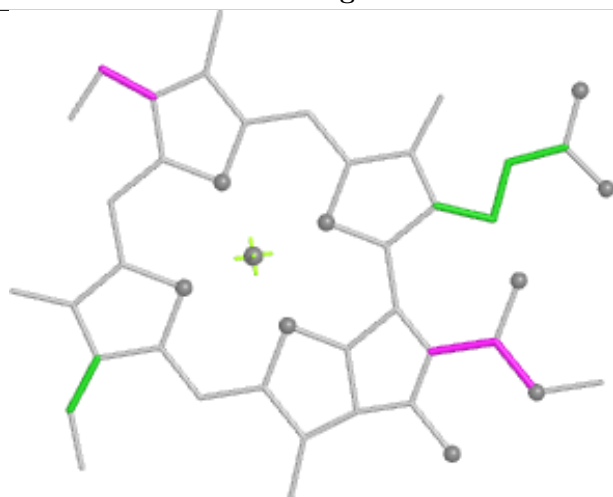
Ligand CLA q 504



Bond lengths



Bond angles

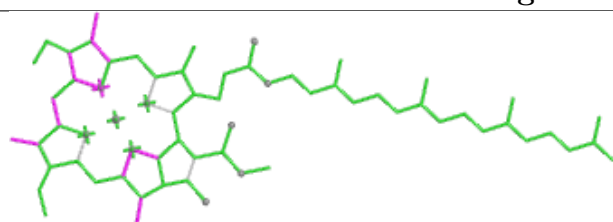


Torsions

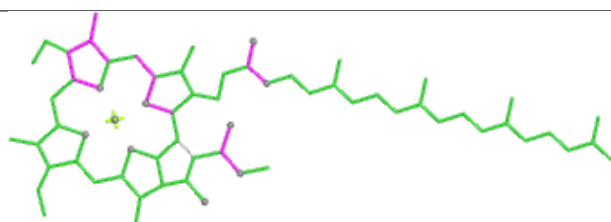


Rings

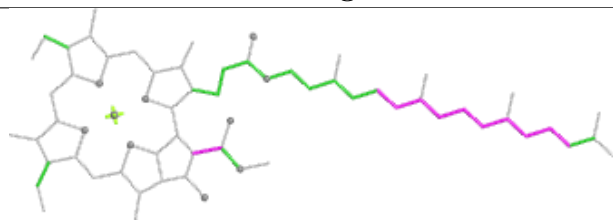
Ligand CLA u 509



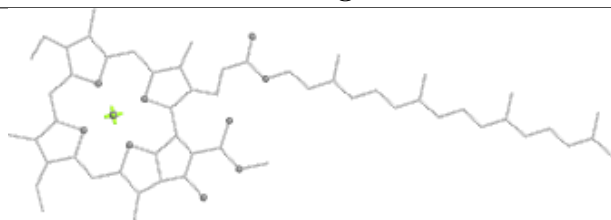
Bond lengths



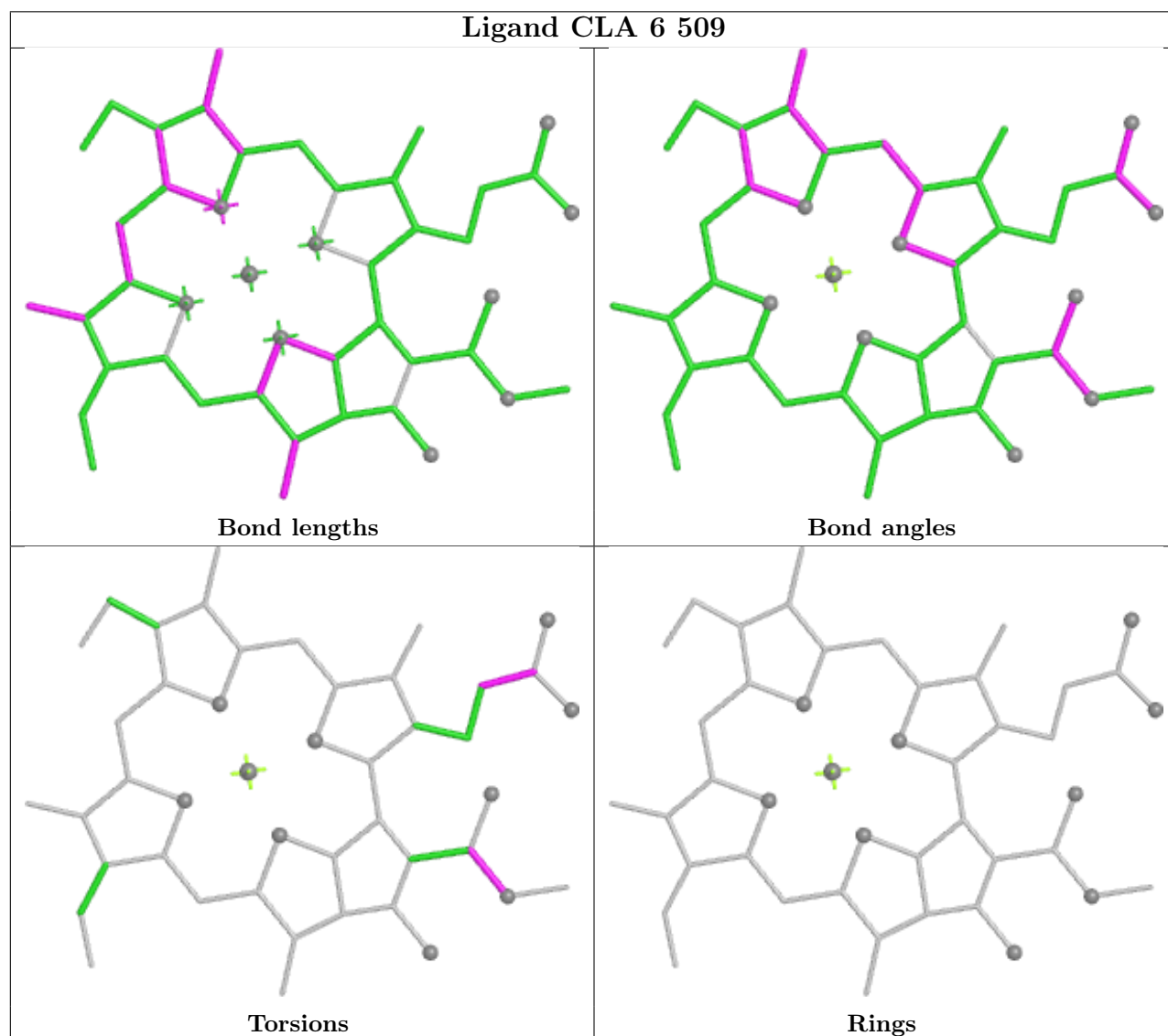
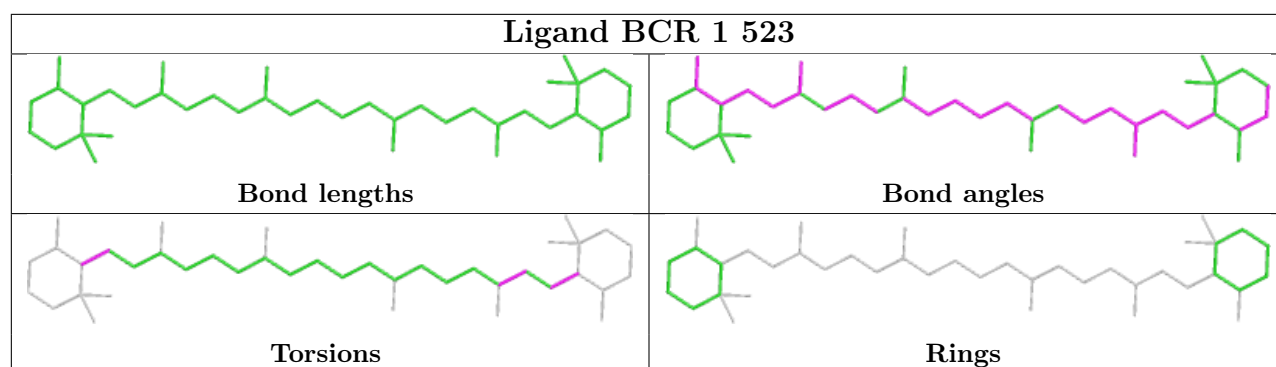
Bond angles

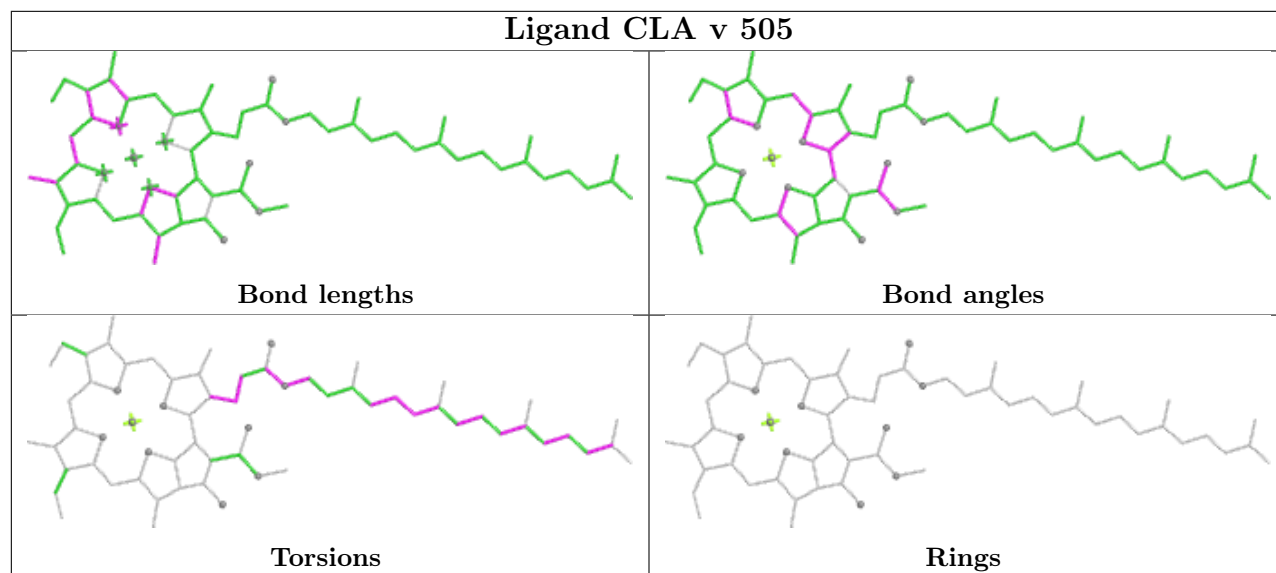
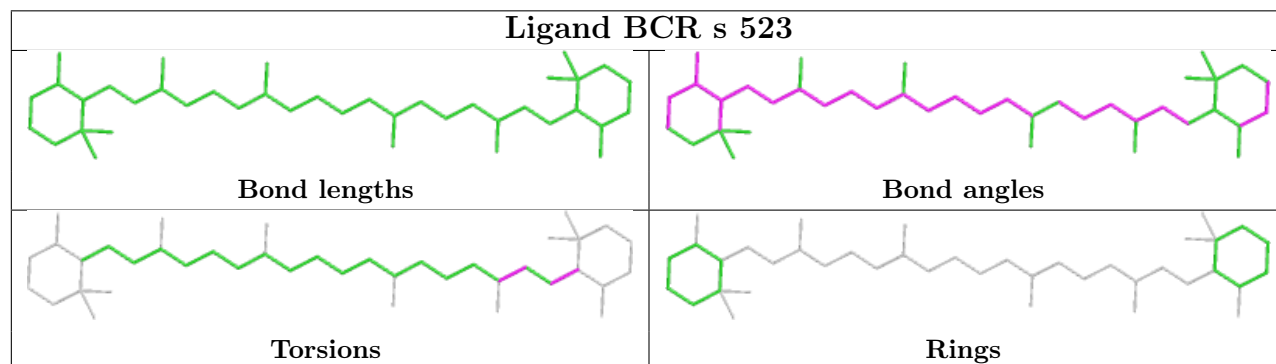
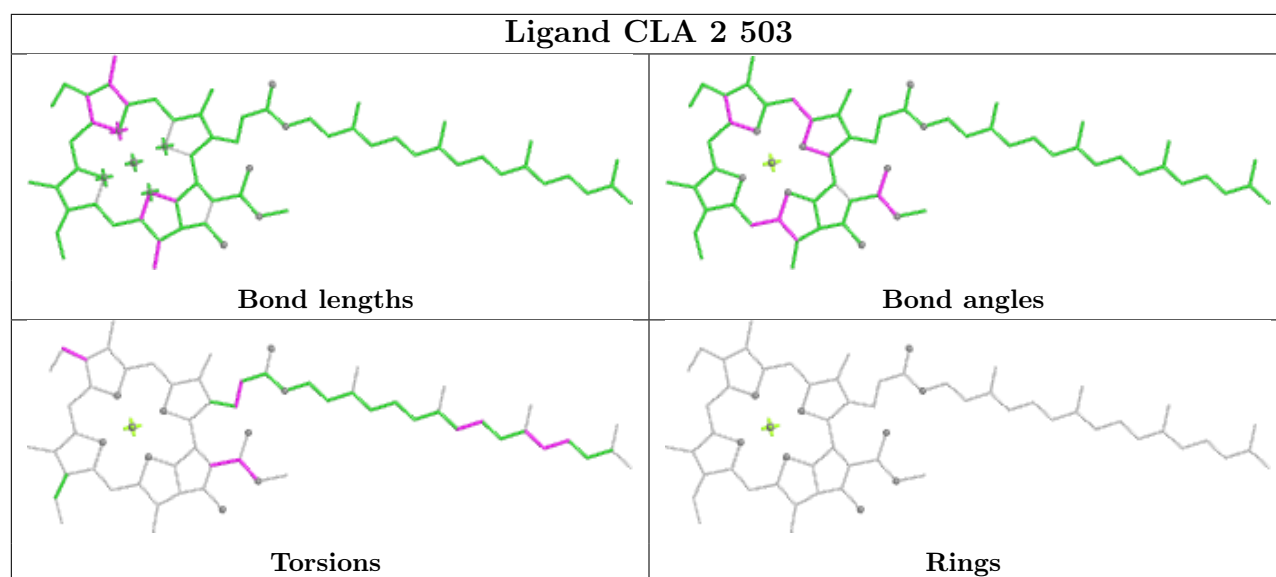


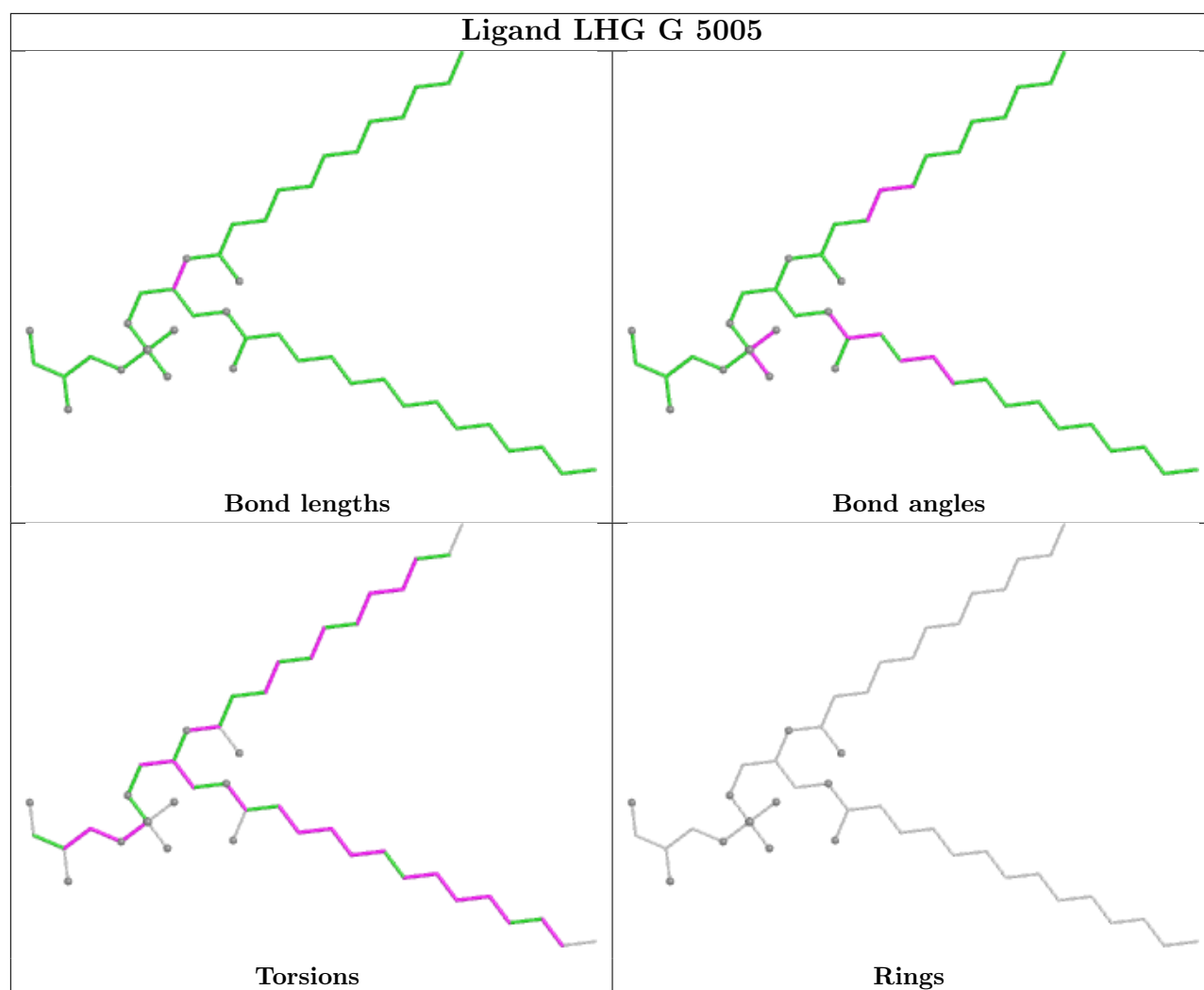
Torsions



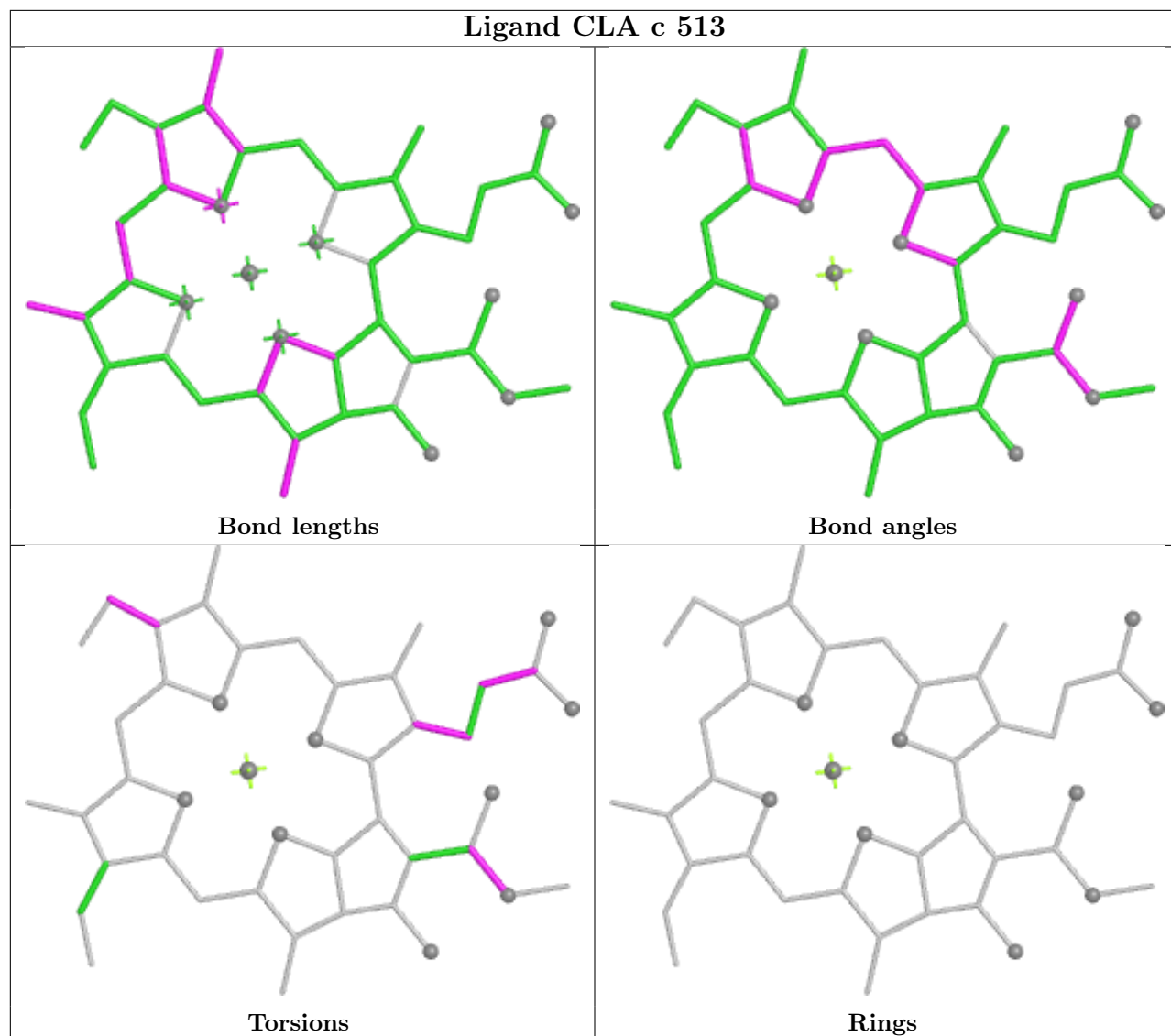
Rings



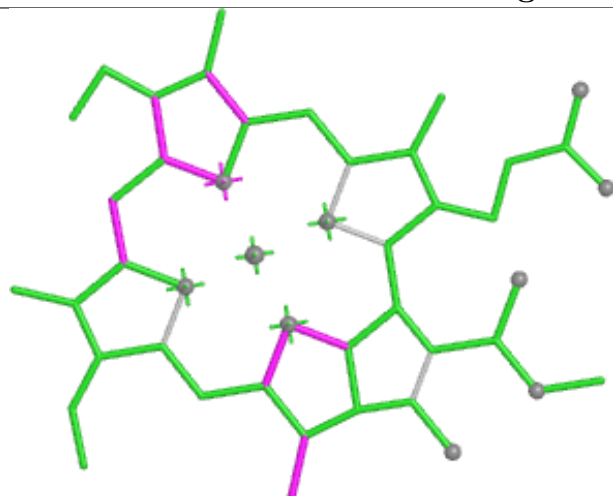




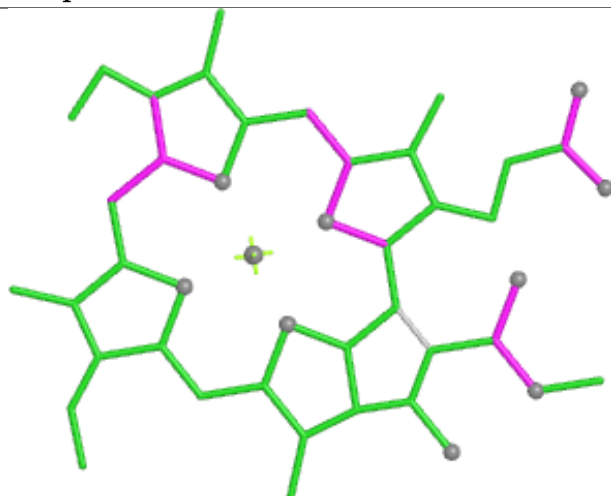
Ligand CLA c 513



Ligand CLA q 518



Bond lengths



Bond angles

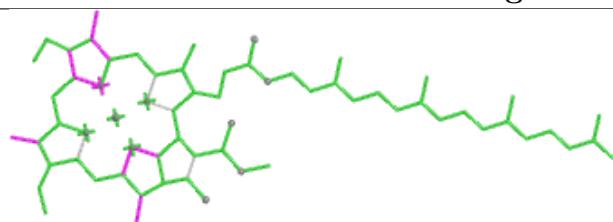


Torsions

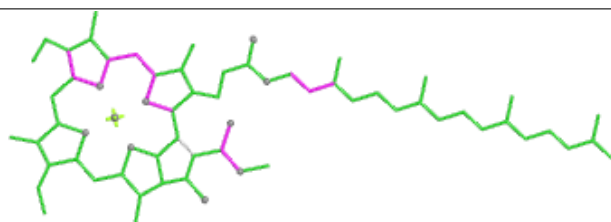


Rings

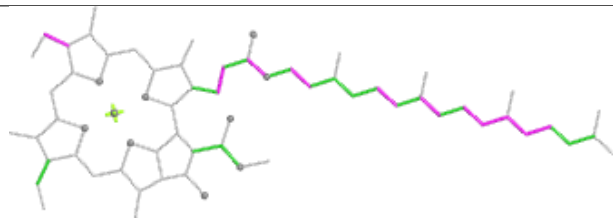
Ligand CLA B 1214



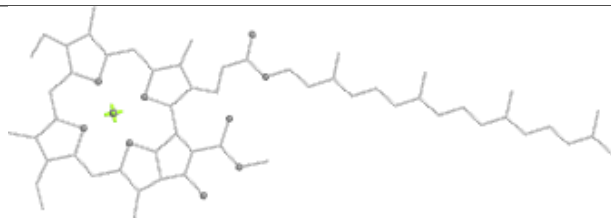
Bond lengths



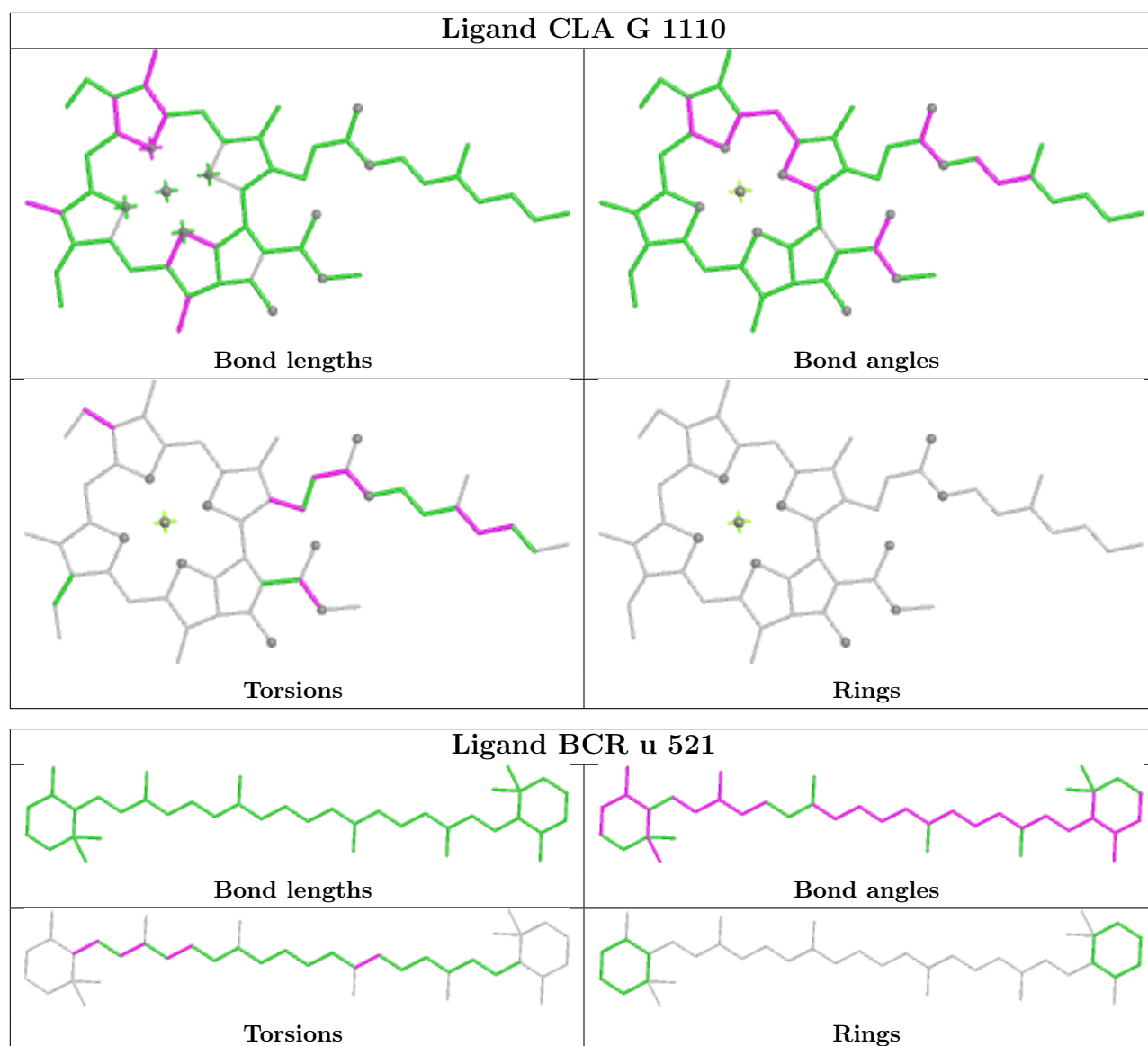
Bond angles



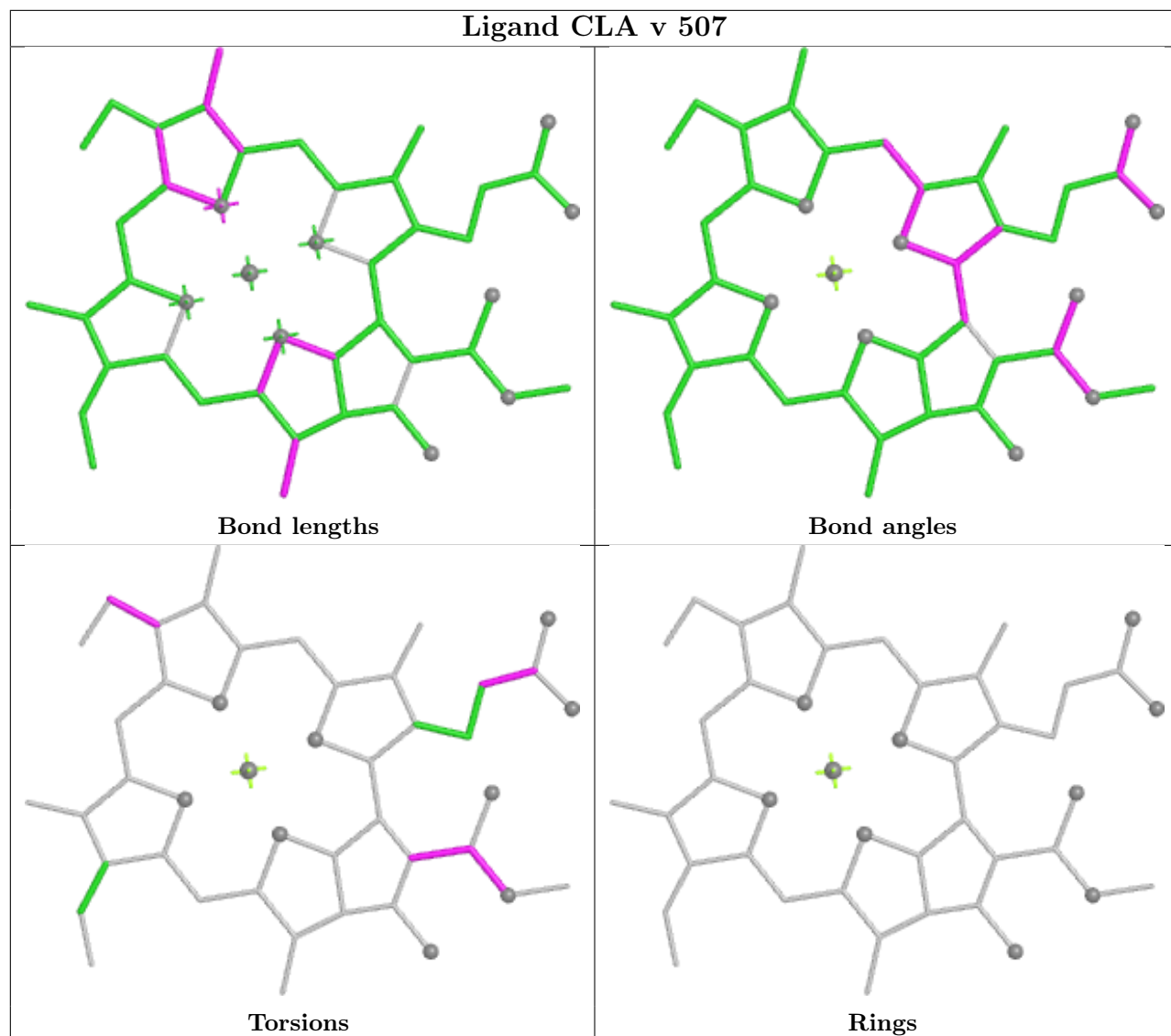
Torsions



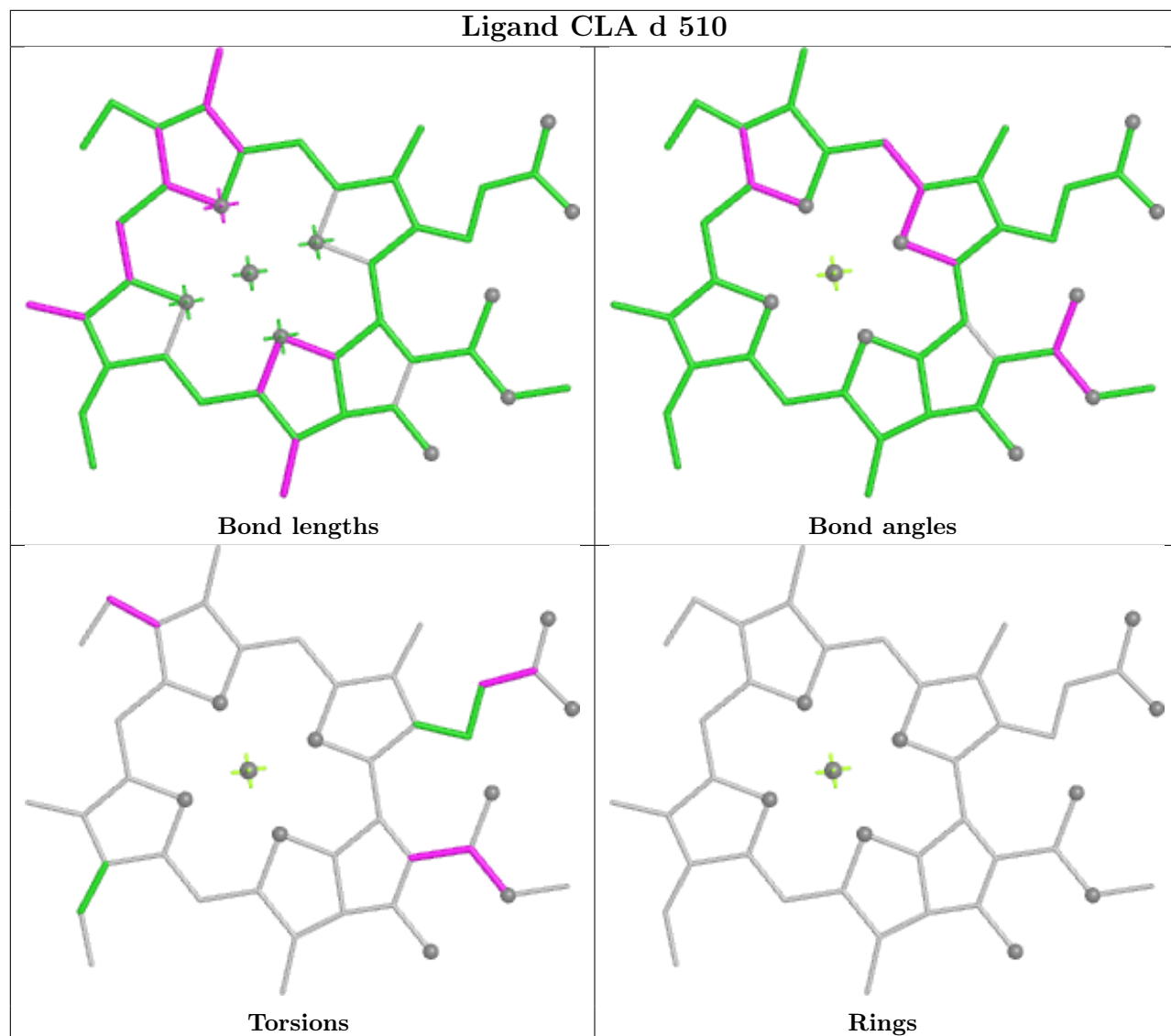
Rings

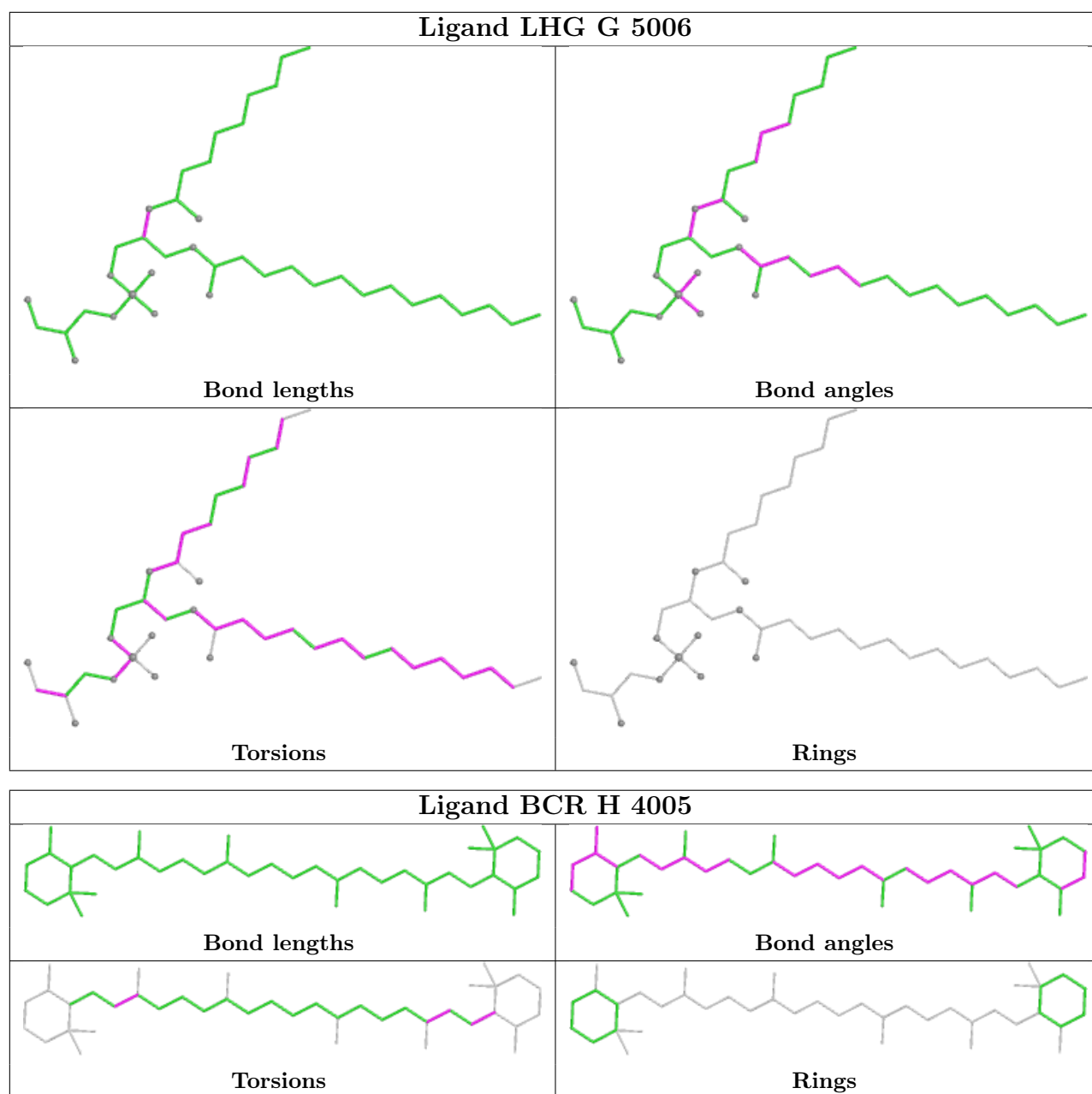


Ligand CLA v 507

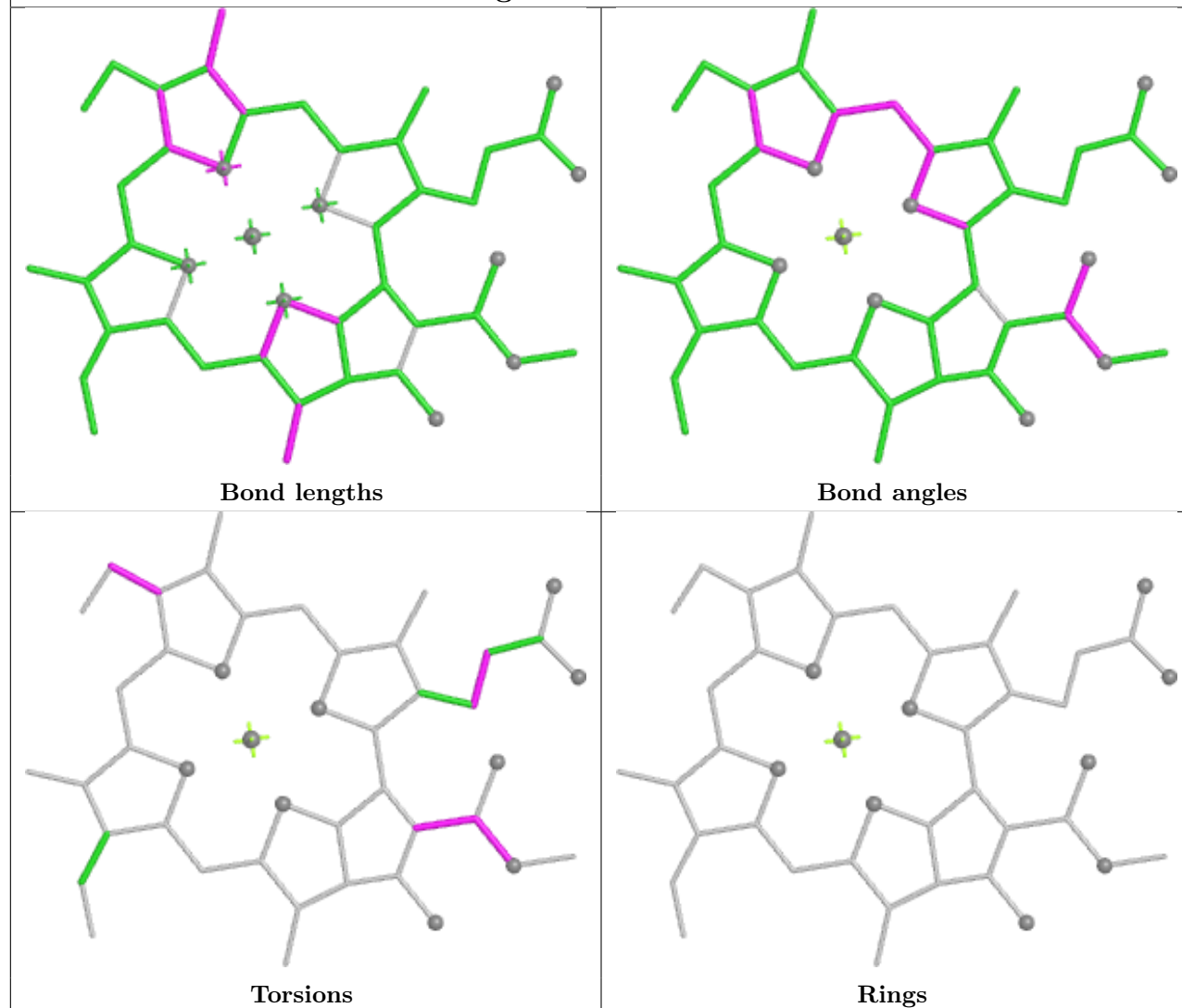


Ligand CLA d 510

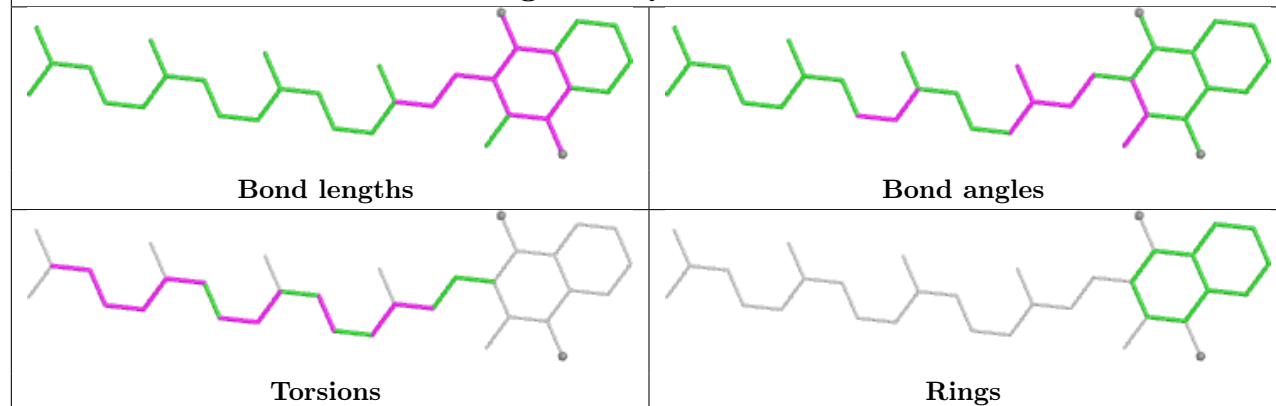


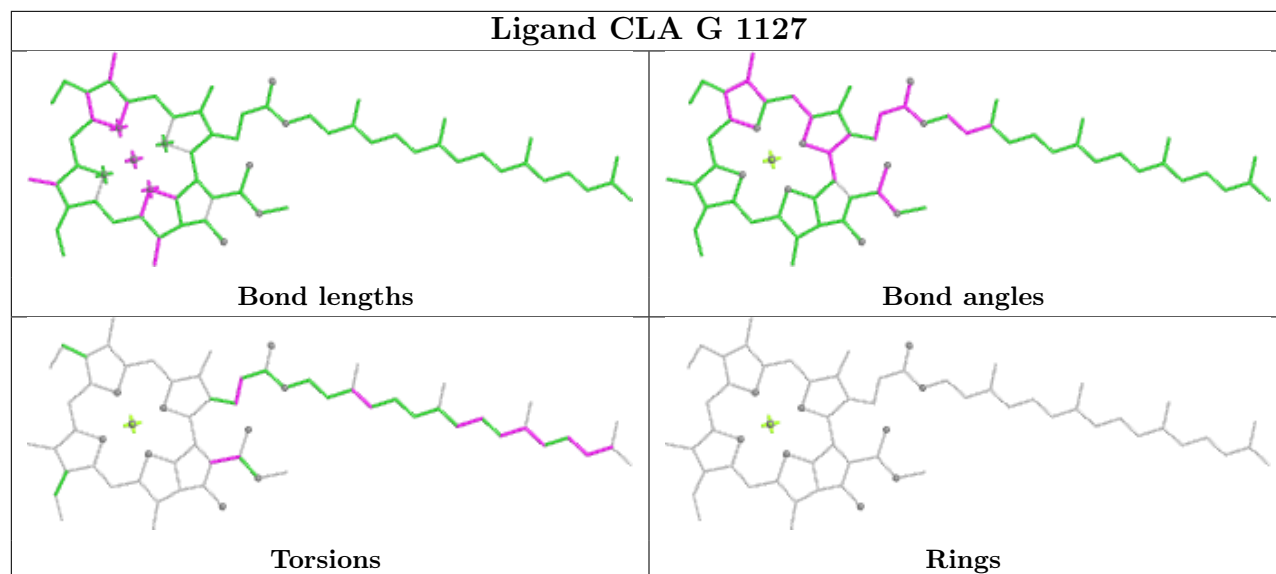
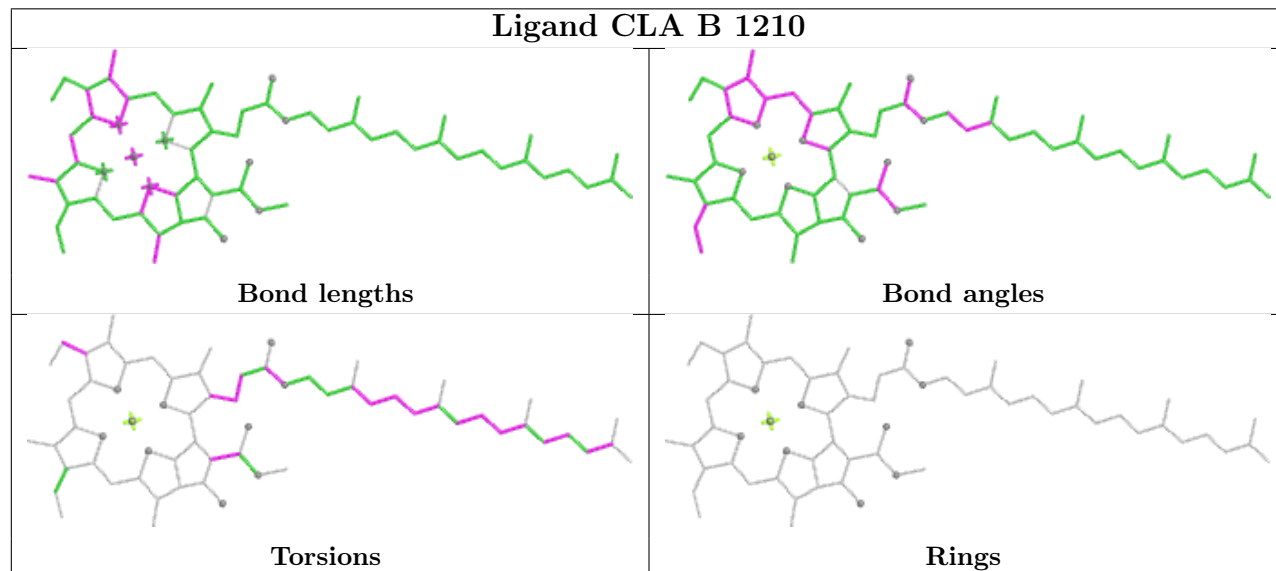


Ligand CLA d 503

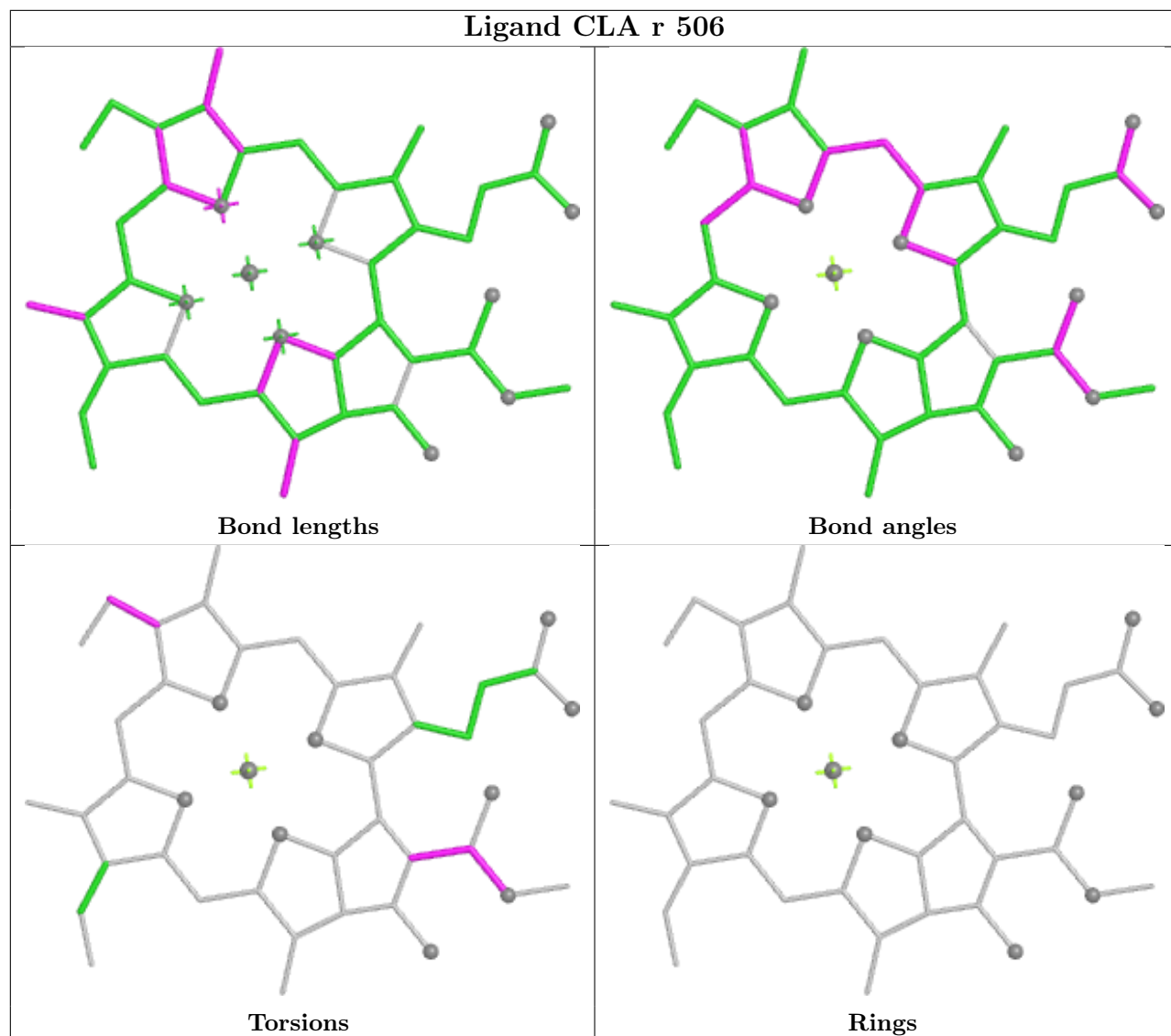


Ligand PQN G 2001

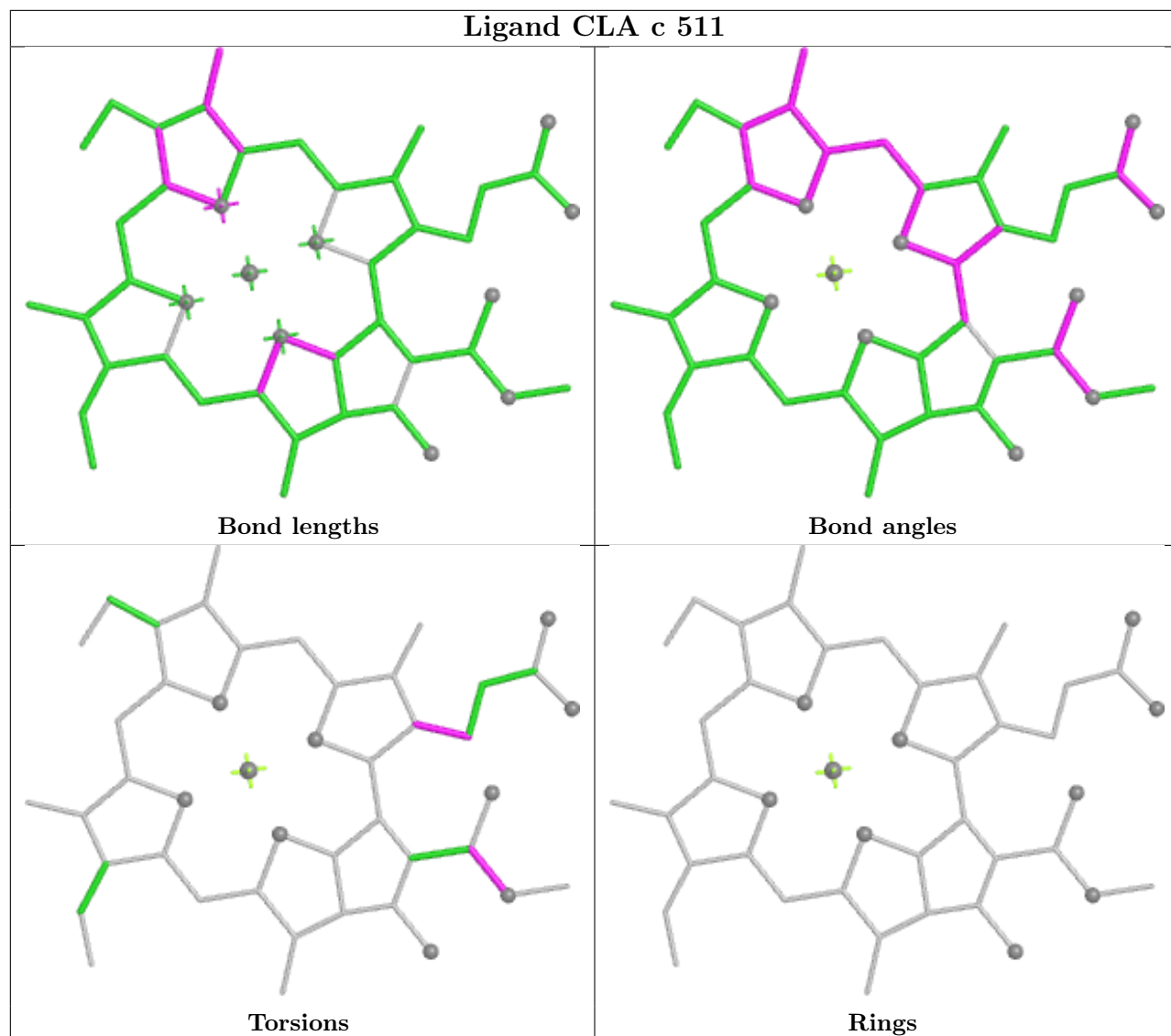


Ligand CLA G 1127**Ligand CLA B 1210**

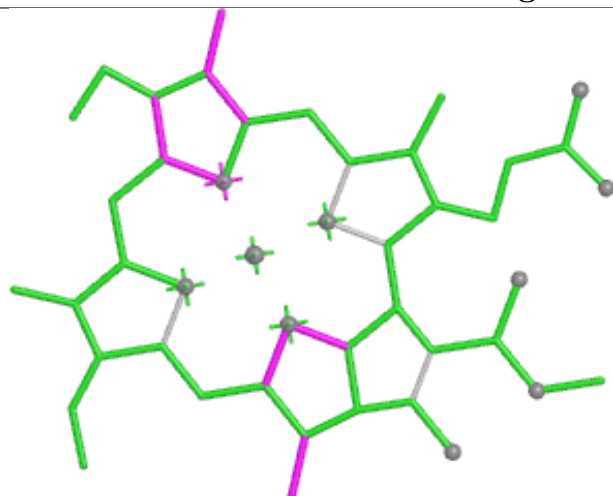
Ligand CLA r 506



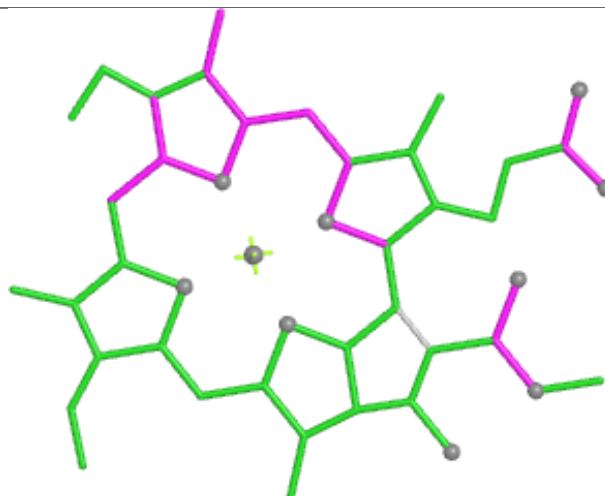
Ligand CLA c 511



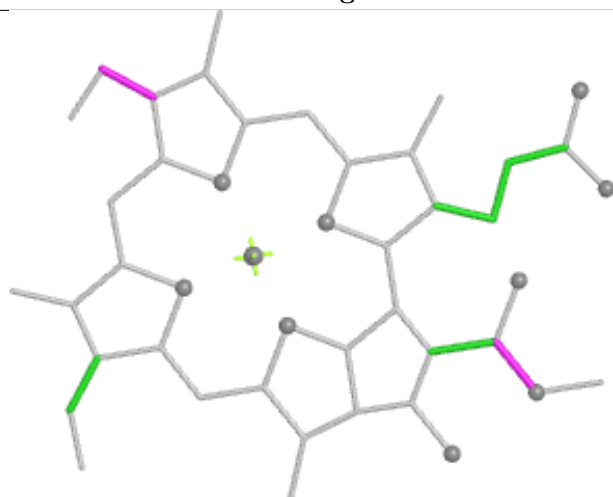
Ligand CLA 1 511



Bond lengths



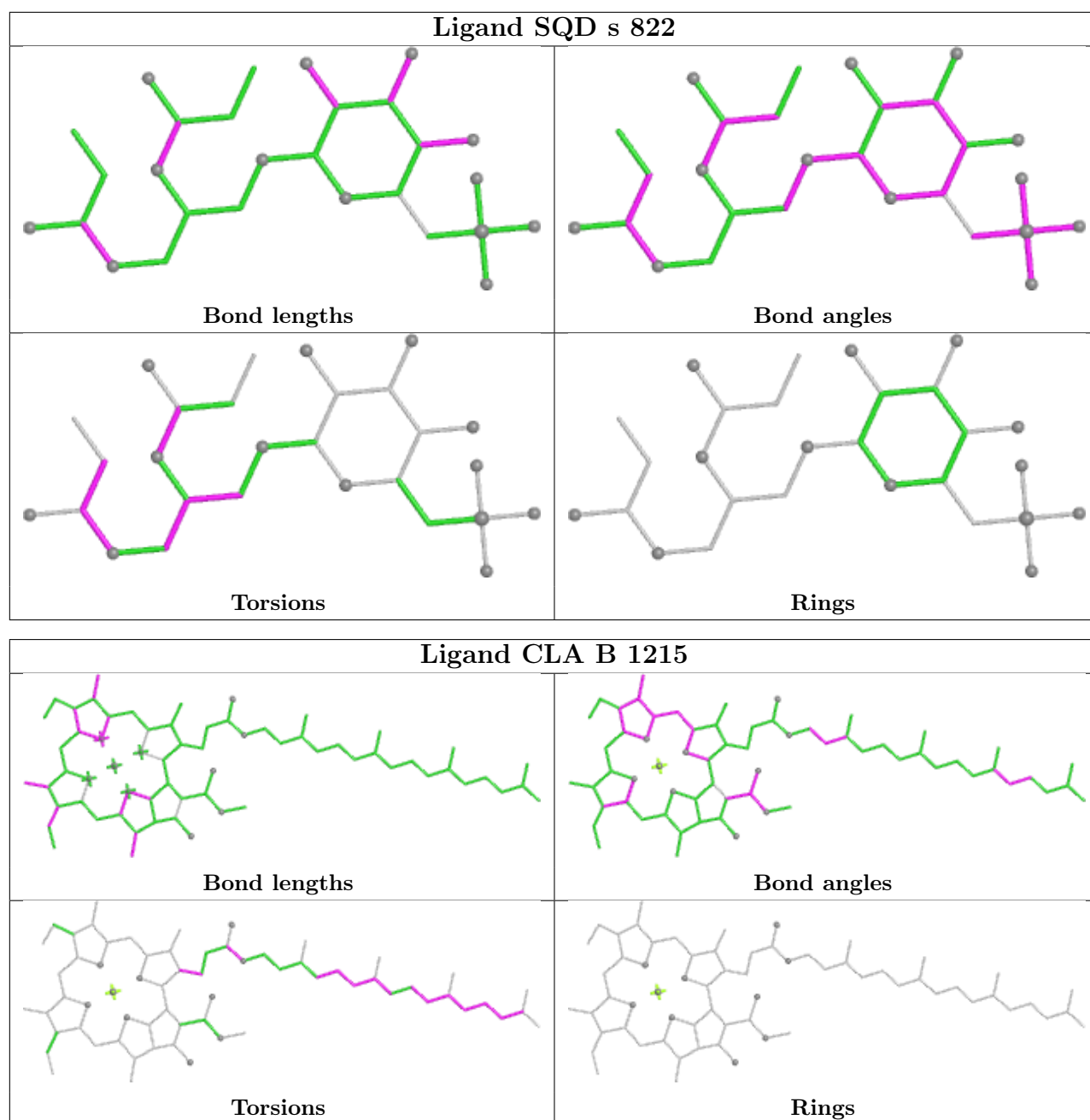
Bond angles



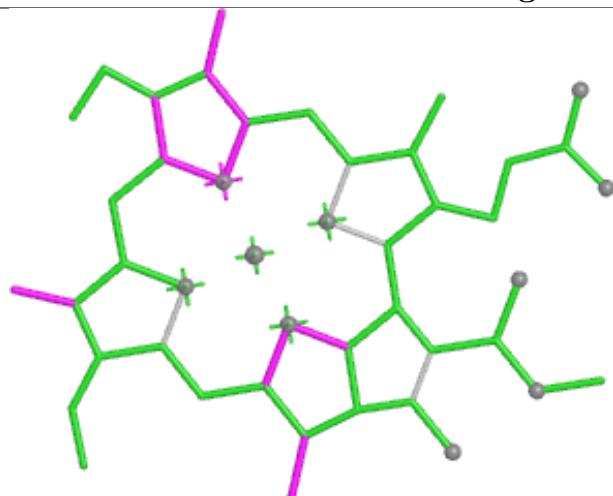
Torsions



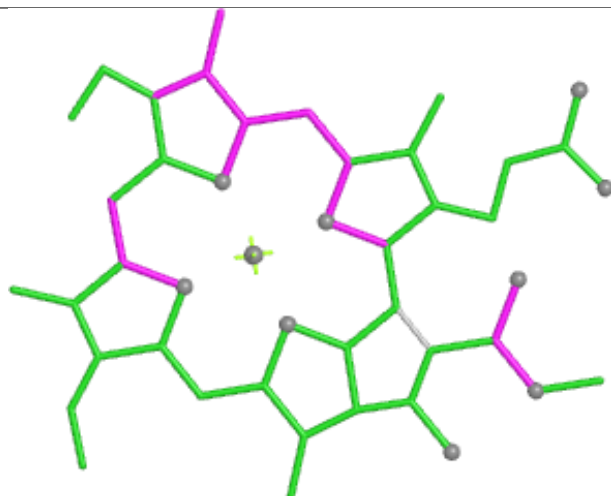
Rings



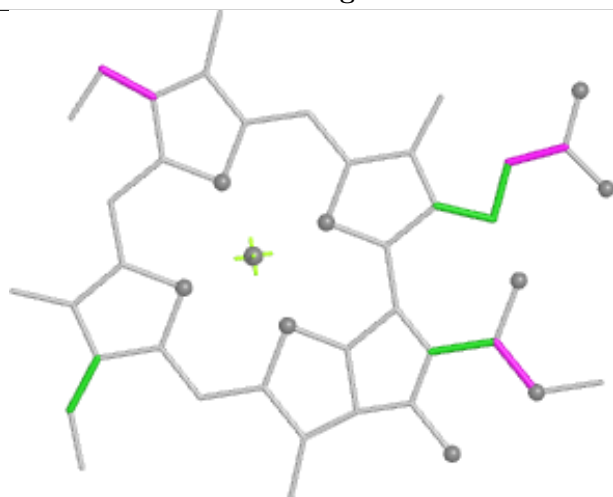
Ligand CLA 5 508



Bond lengths



Bond angles

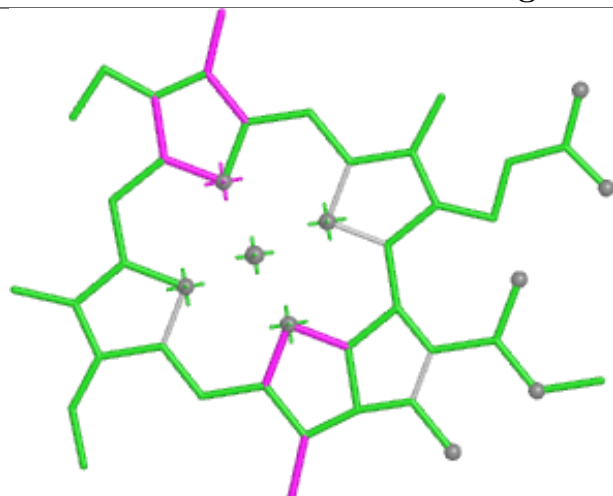


Torsions

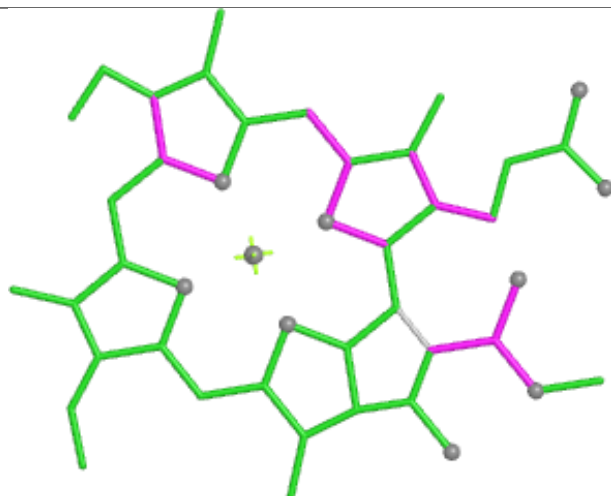


Rings

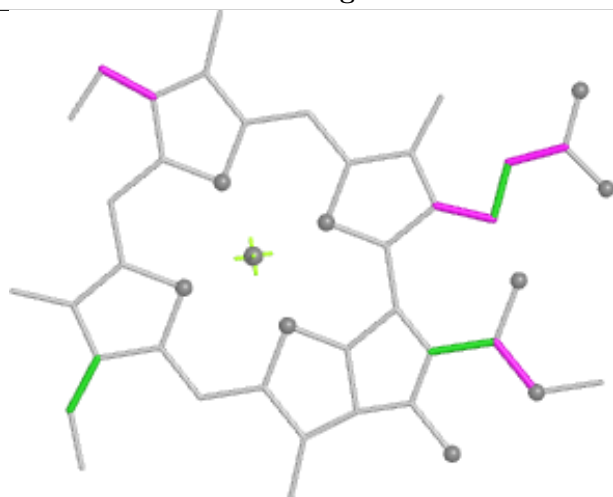
Ligand CLA 2 516



Bond lengths



Bond angles

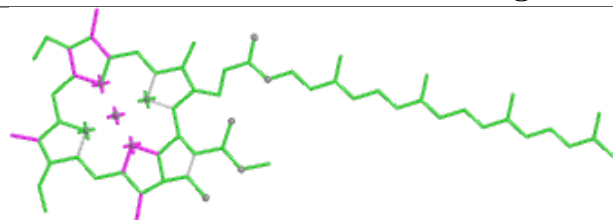


Torsions

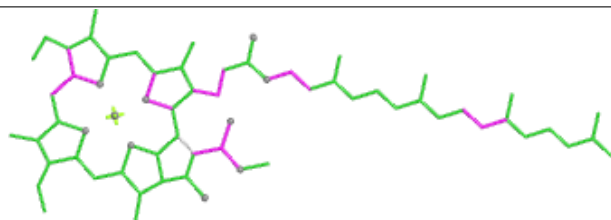


Rings

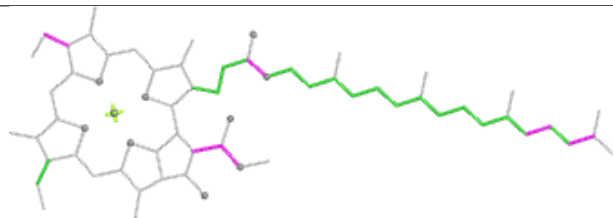
Ligand CLA f 1021



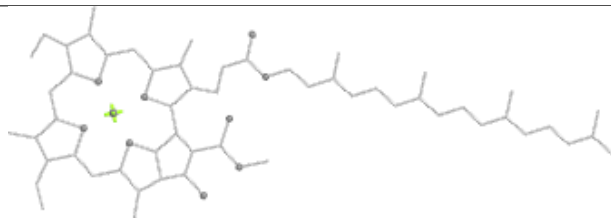
Bond lengths



Bond angles

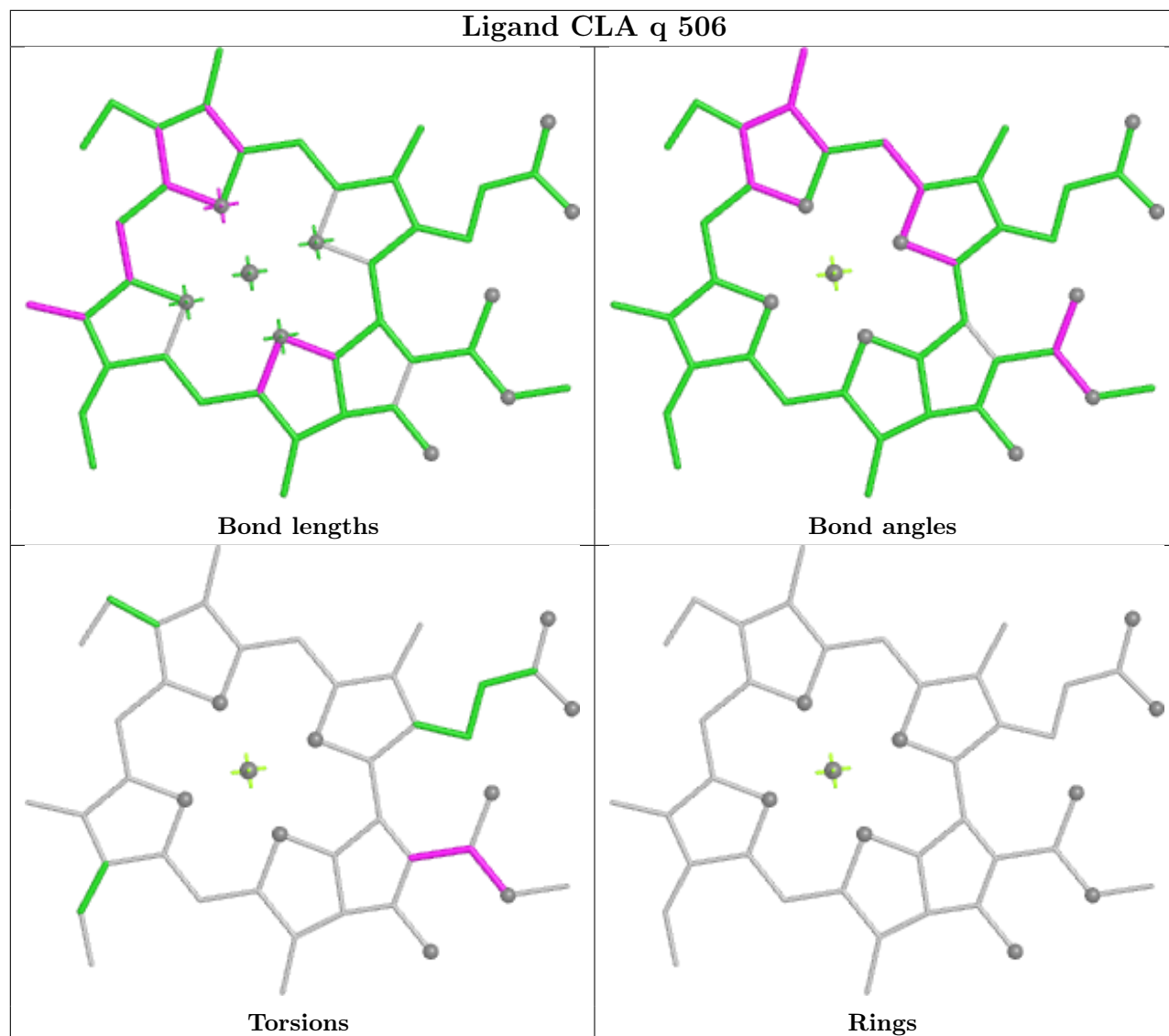


Torsions

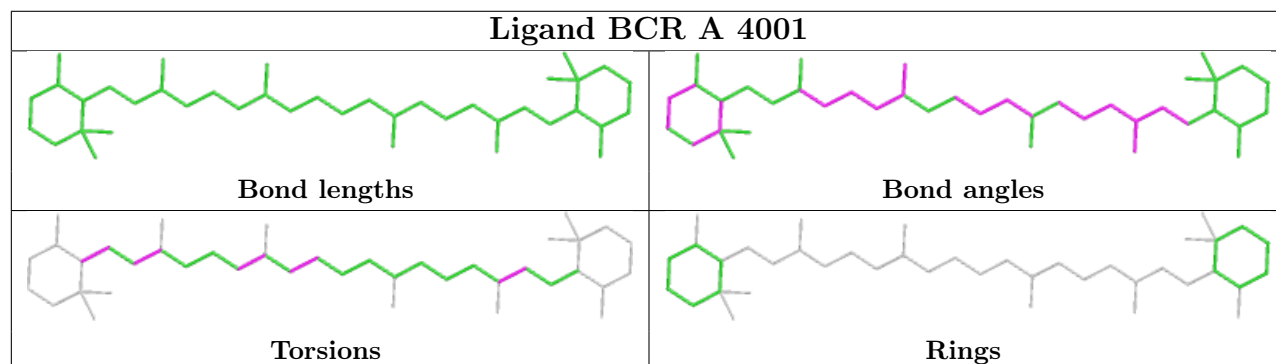


Rings

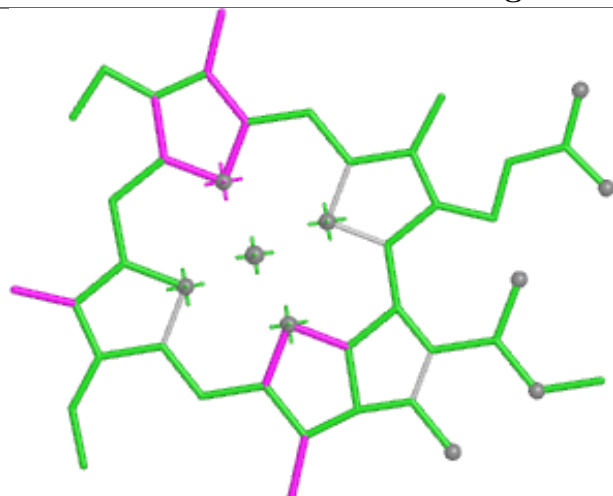
Ligand CLA q 506



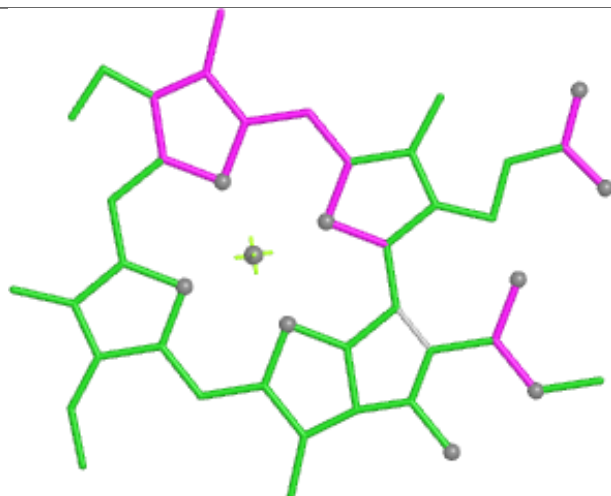
Ligand BCR A 4001



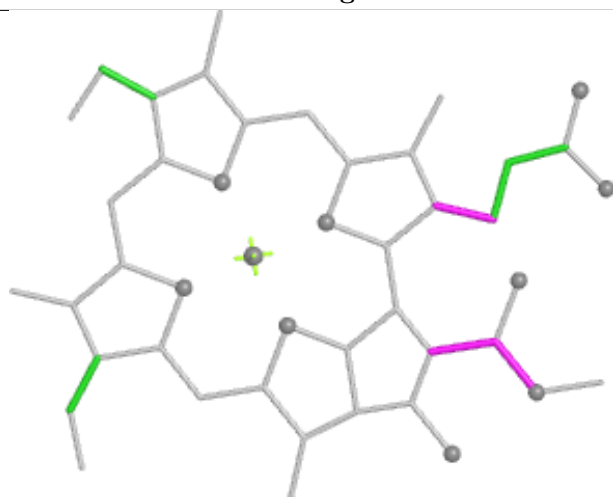
Ligand CLA A 1113



Bond lengths



Bond angles

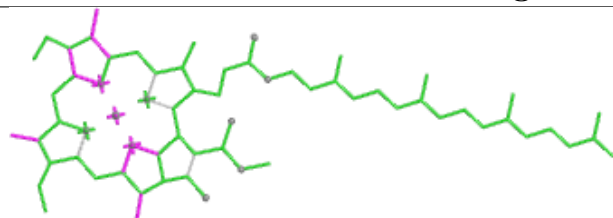


Torsions

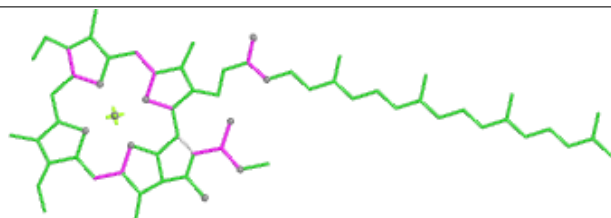


Rings

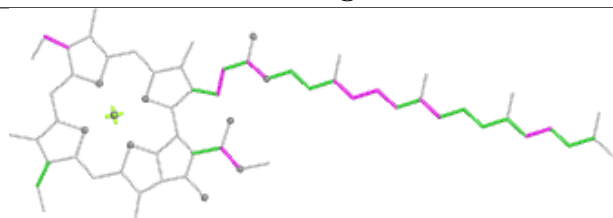
Ligand CLA f 1204



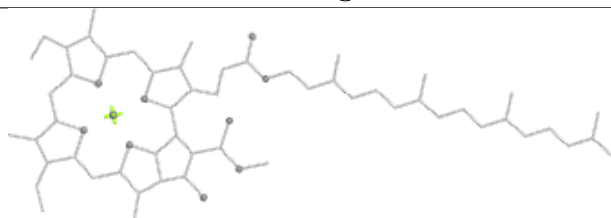
Bond lengths



Bond angles

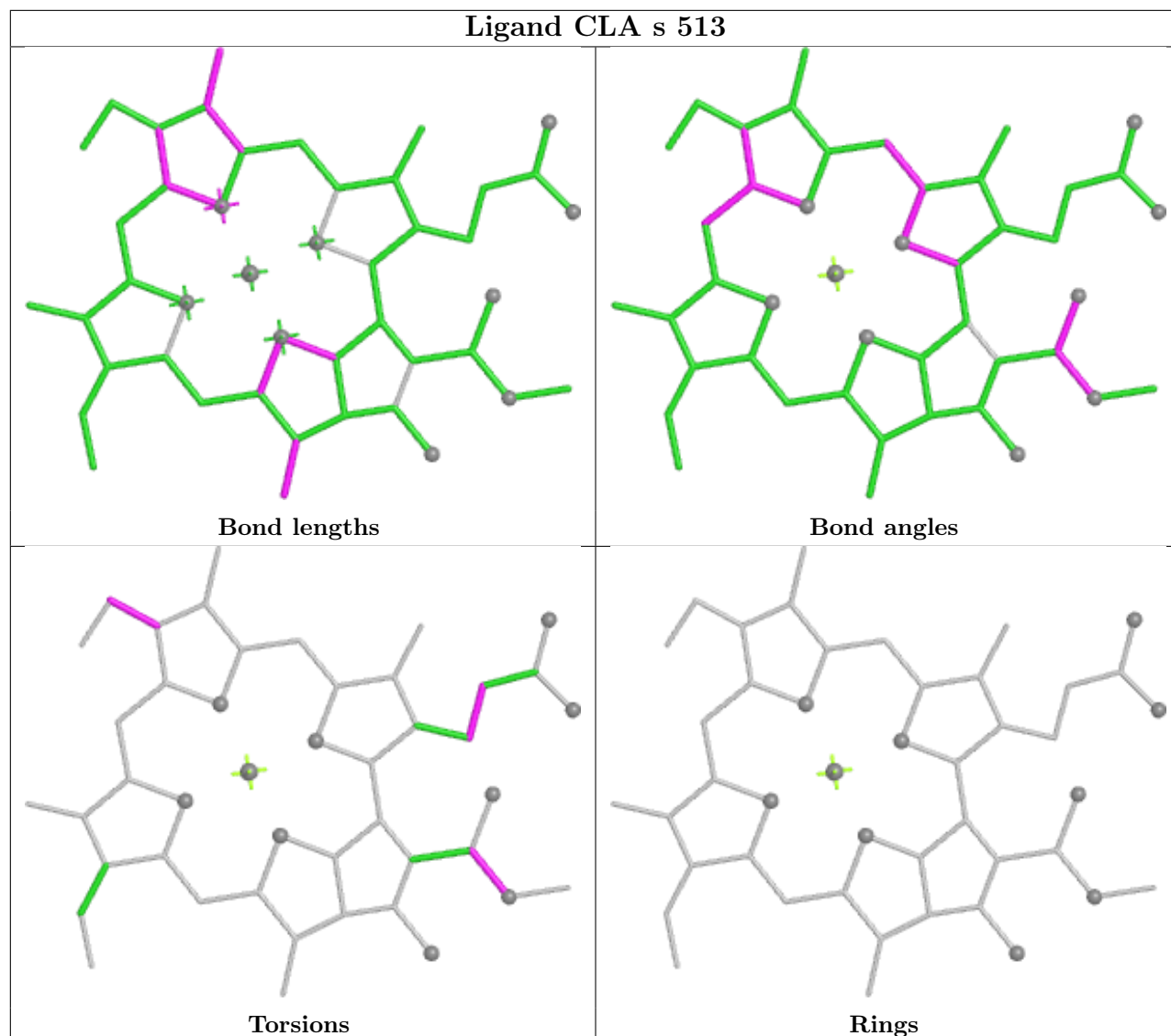


Torsions

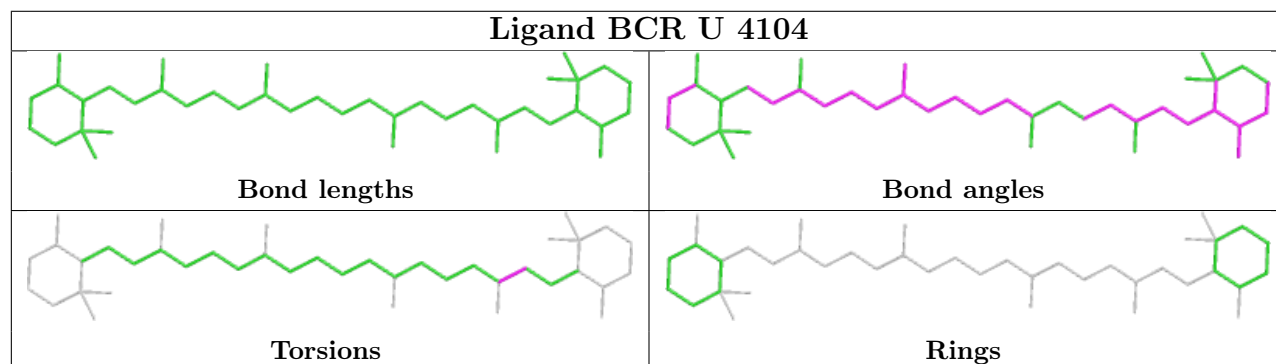


Rings

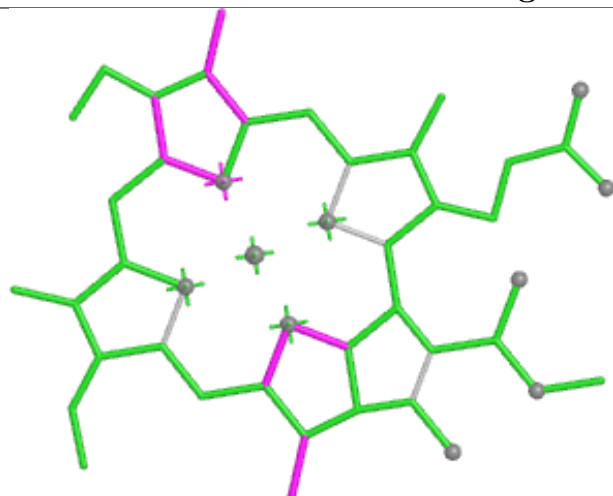
Ligand CLA s 513



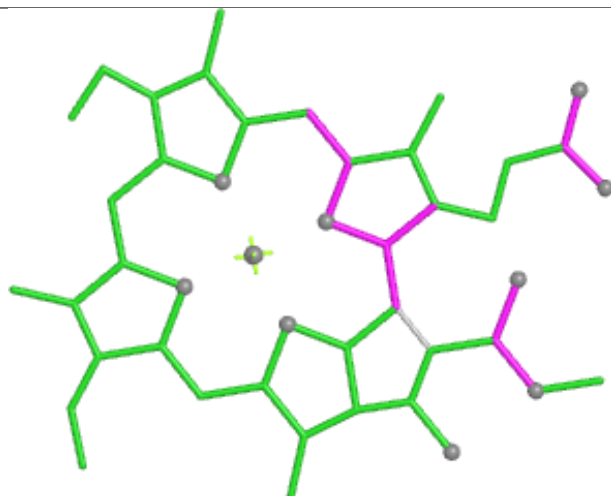
Ligand BCR U 4104



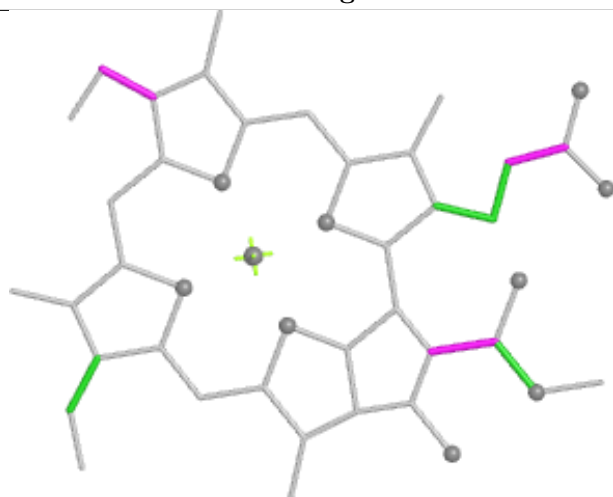
Ligand CLA 3 507



Bond lengths



Bond angles

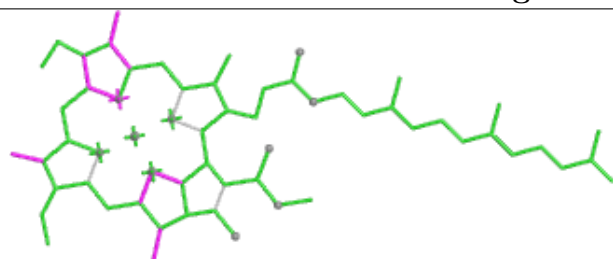


Torsions

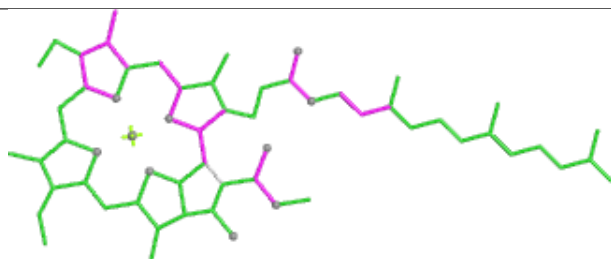


Rings

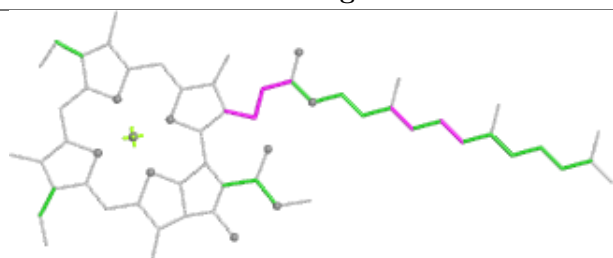
Ligand CLA f 1224



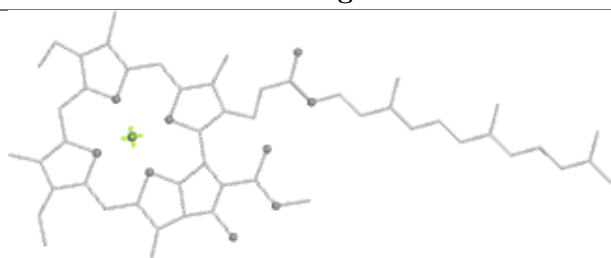
Bond lengths



Bond angles

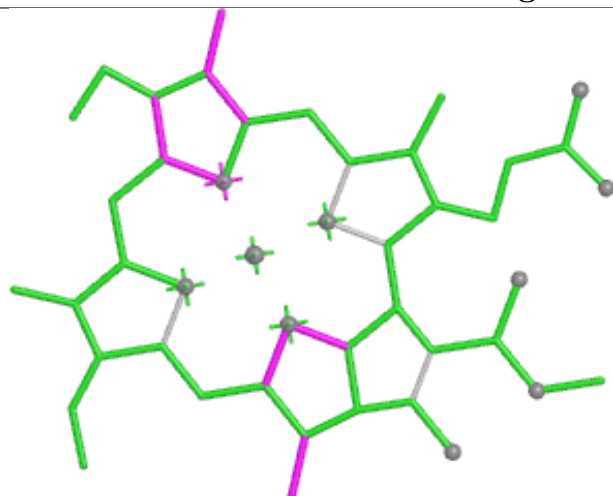


Torsions

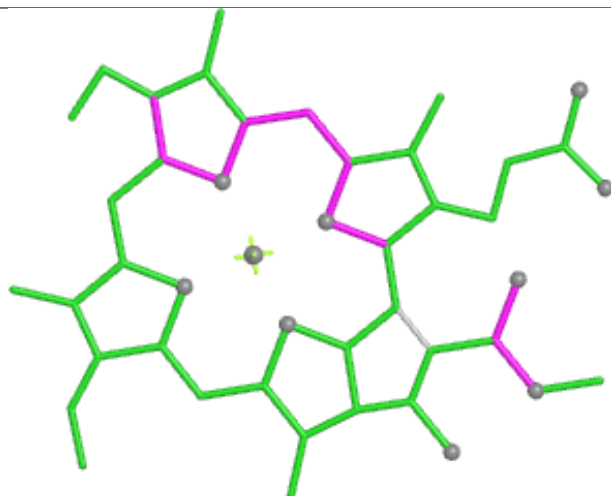


Rings

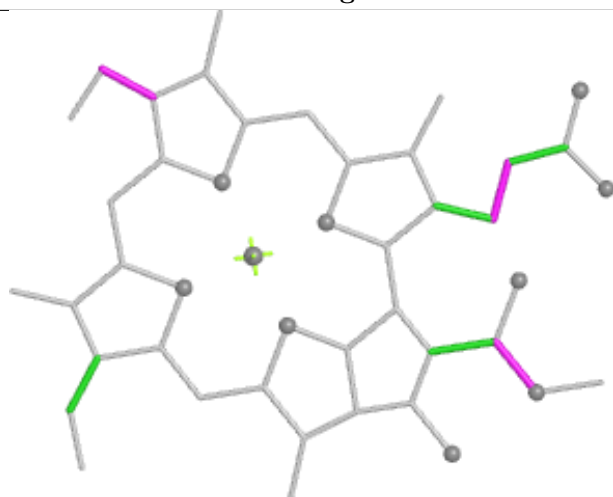
Ligand CLA 6 513



Bond lengths



Bond angles

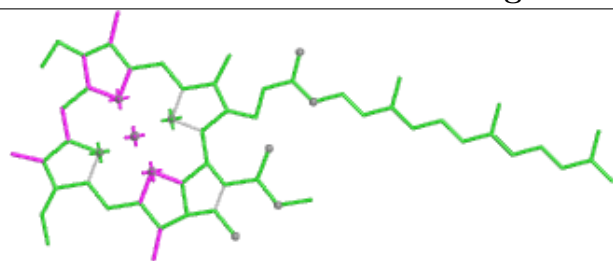


Torsions

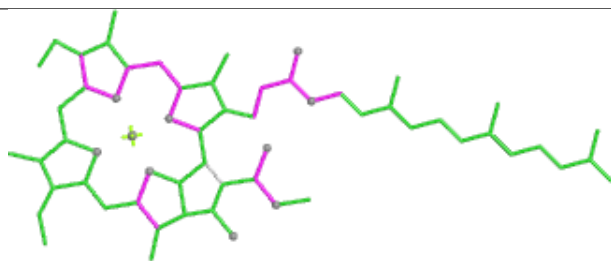


Rings

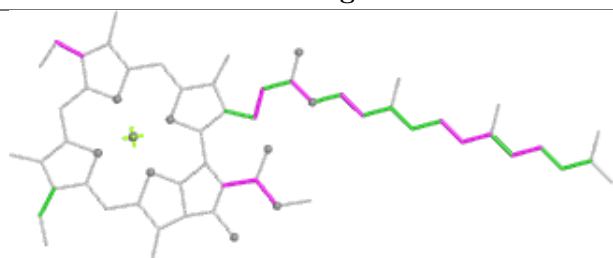
Ligand CLA H 1216



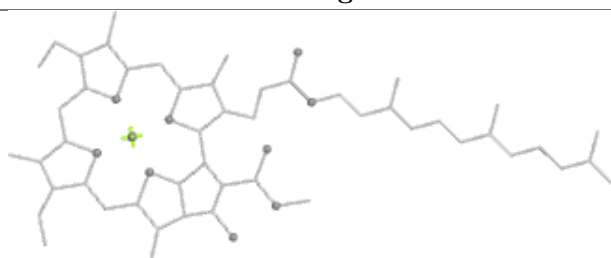
Bond lengths



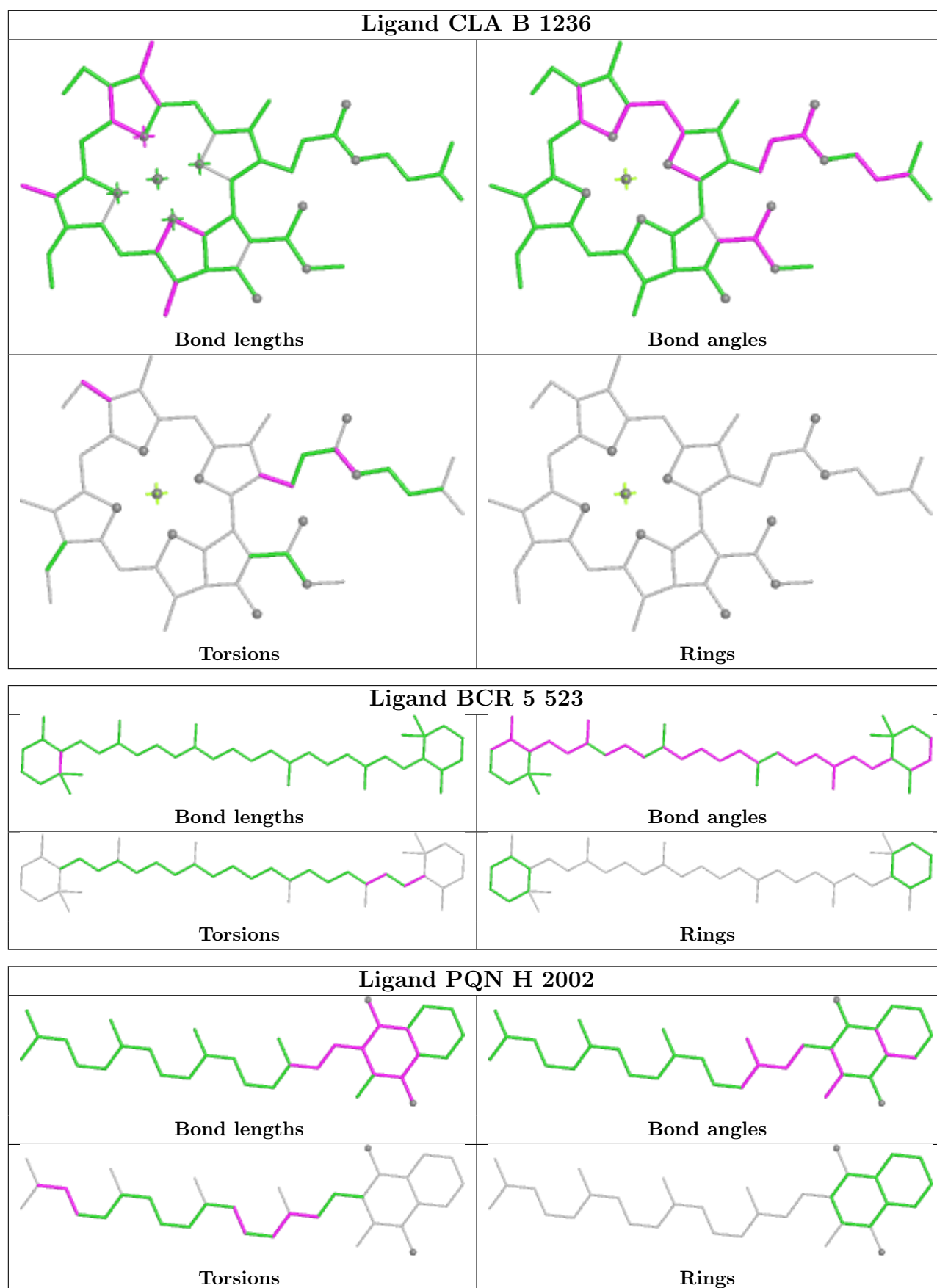
Bond angles



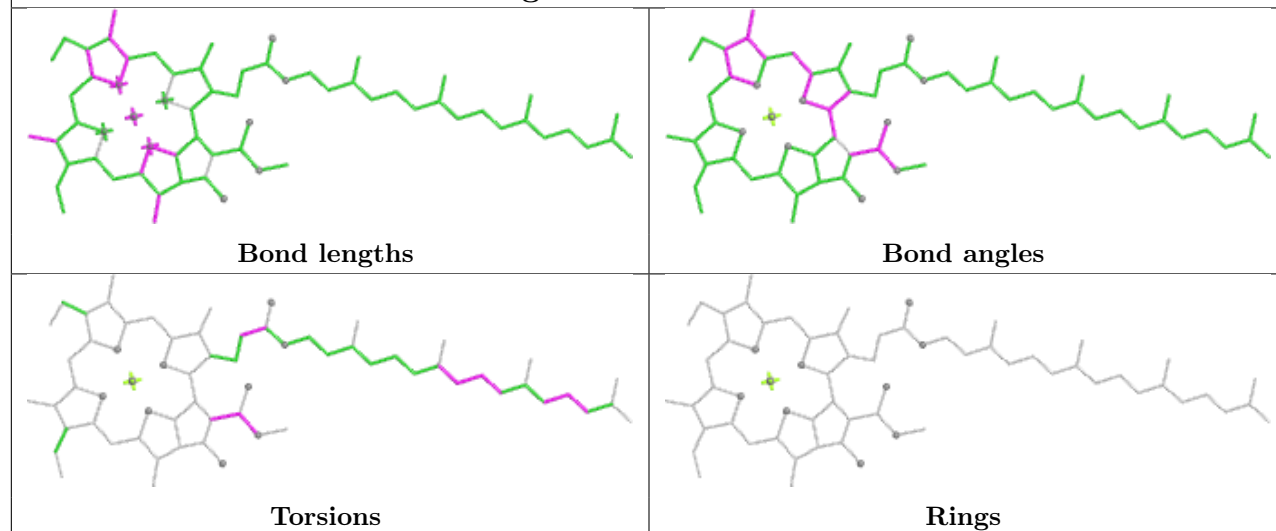
Torsions



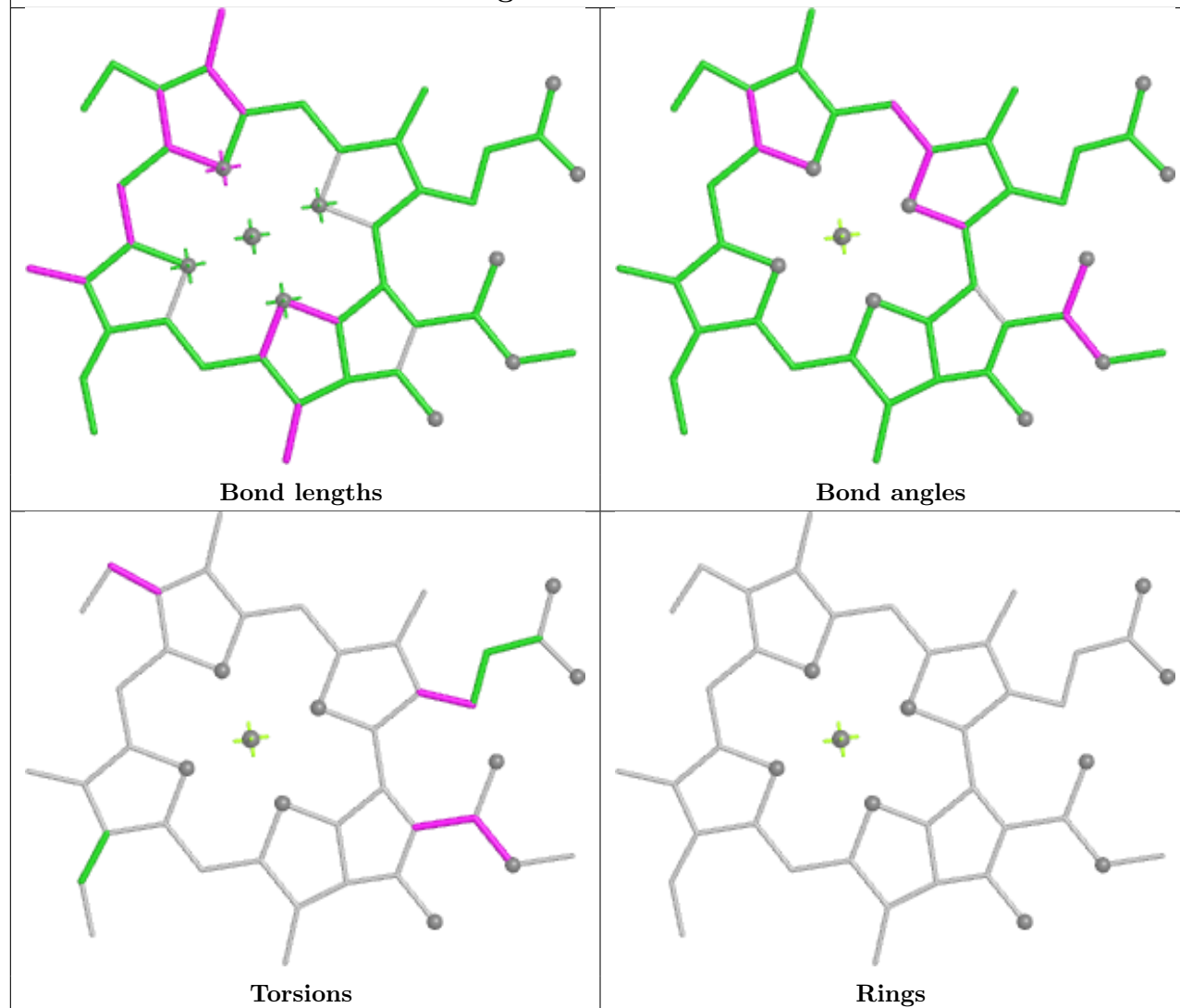
Rings



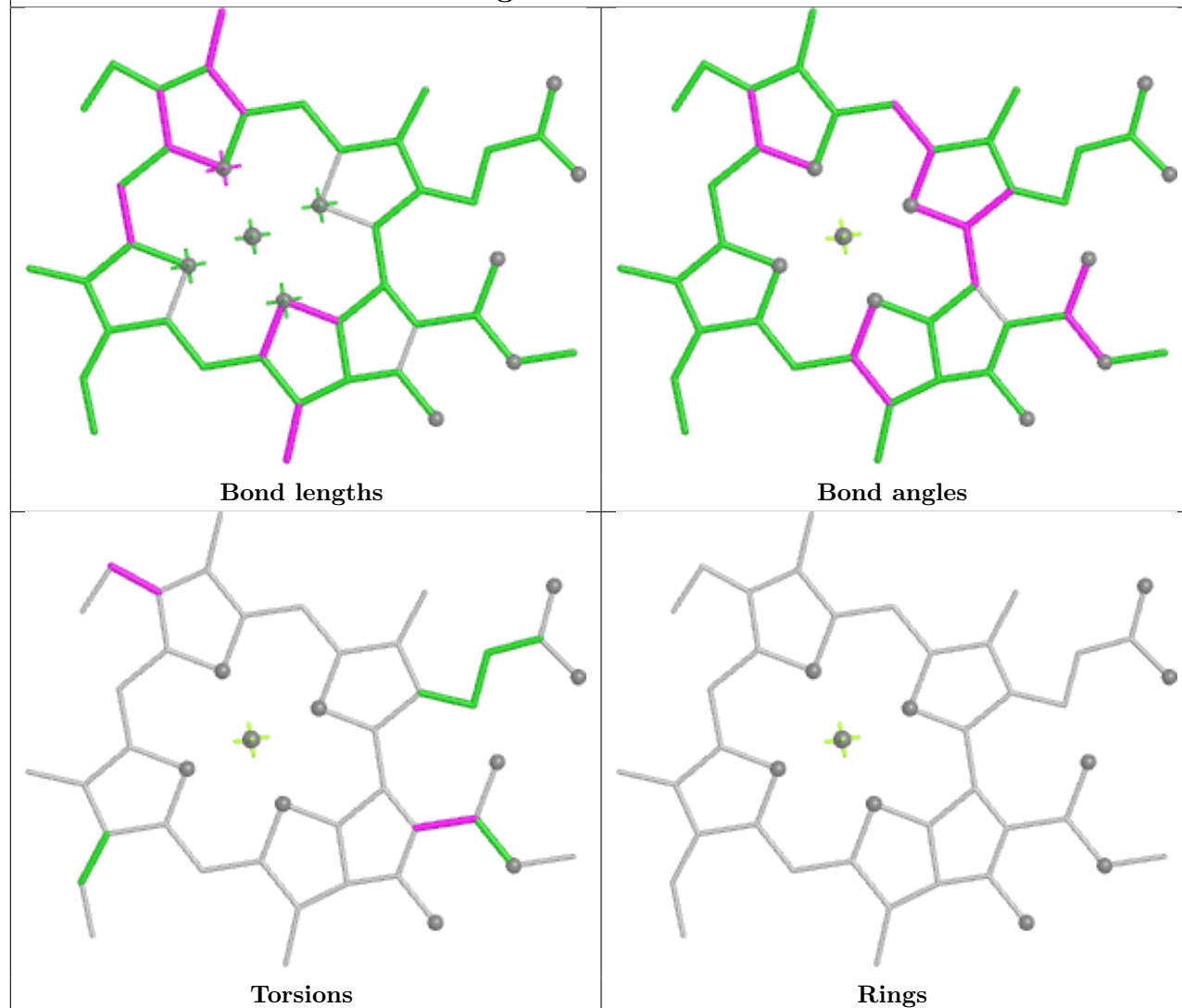
Ligand CLA G 1123



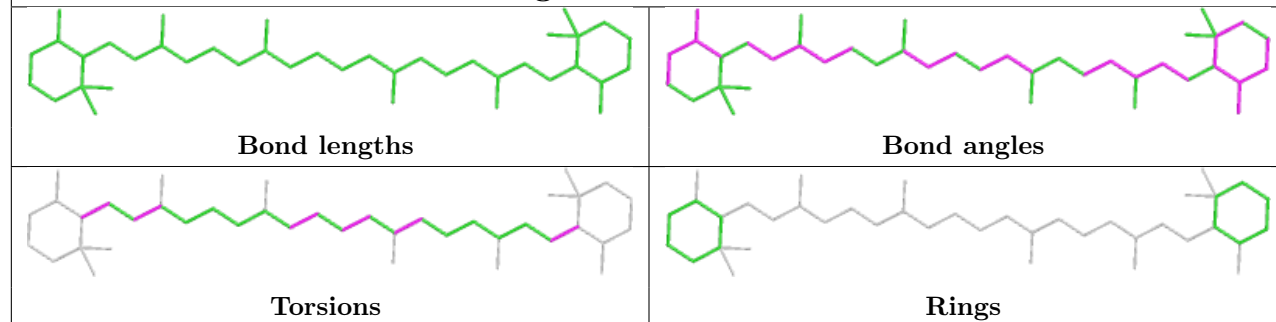
Ligand CLA s 517



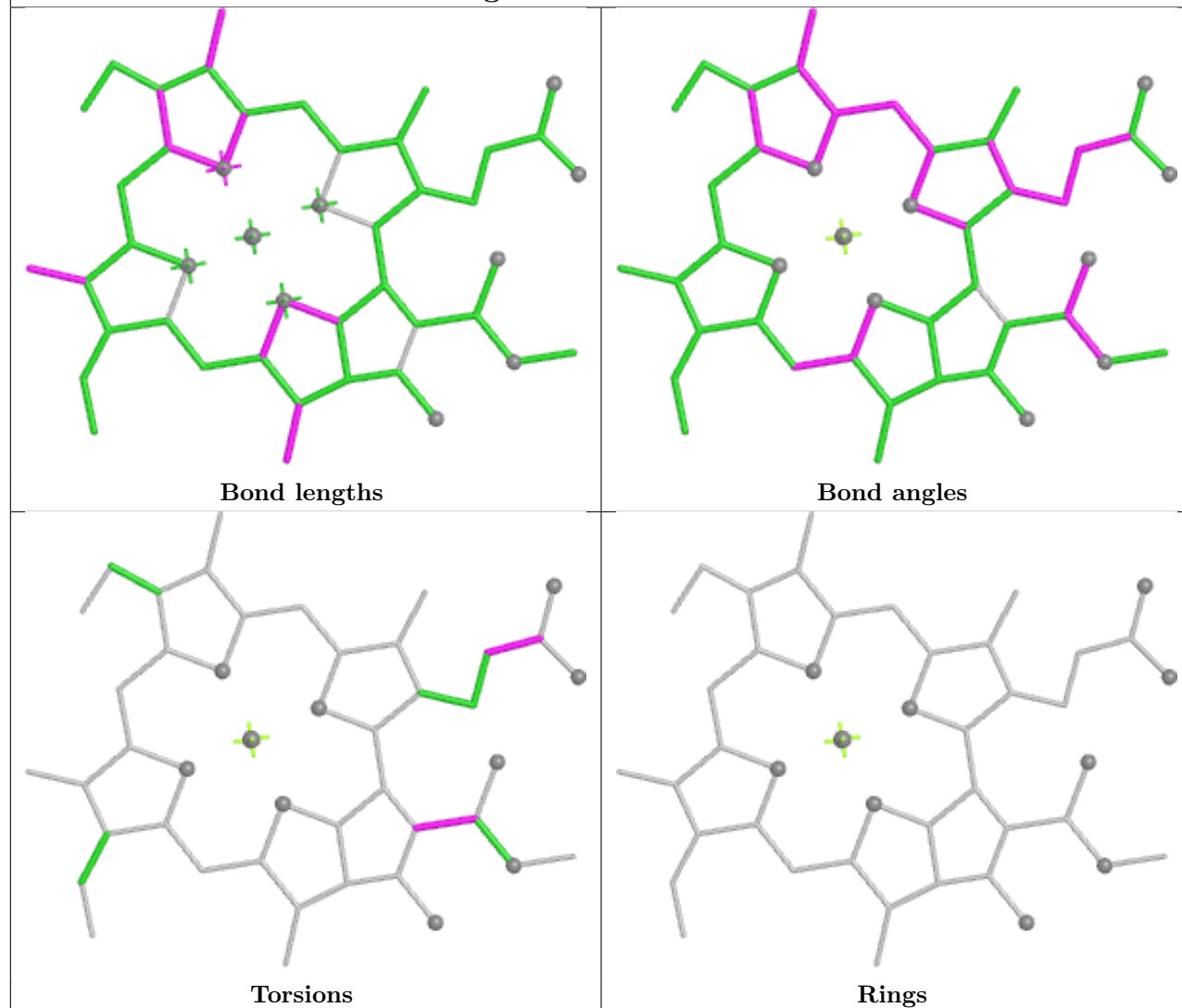
Ligand CLA 4 503



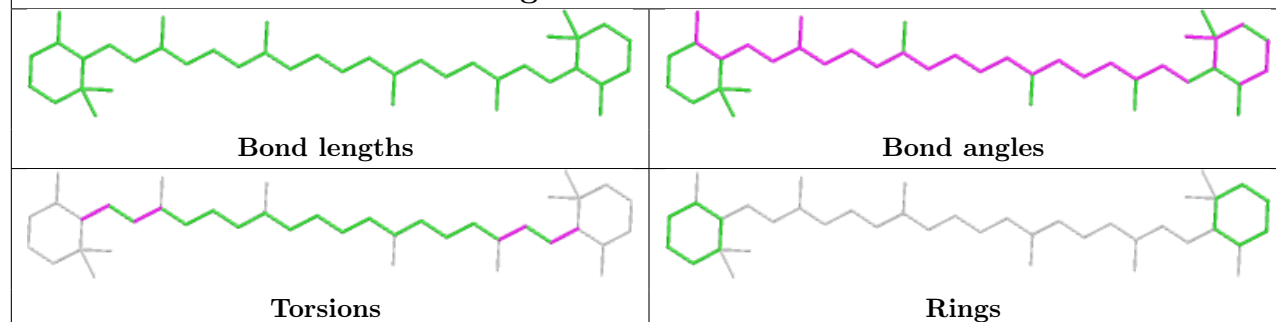
Ligand BCR 4 521

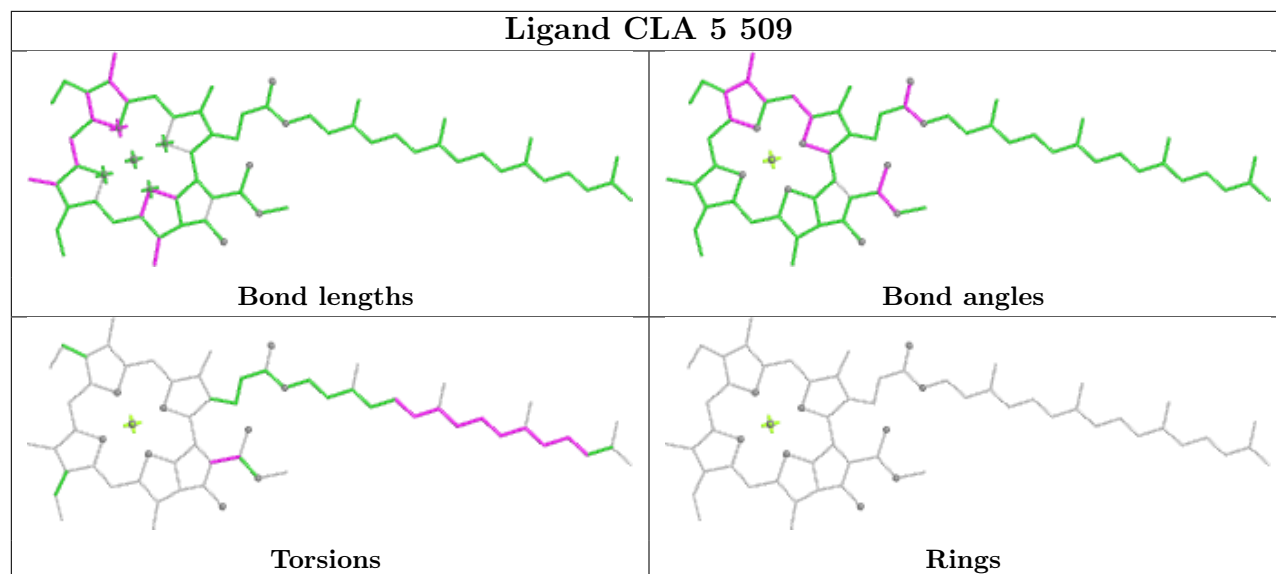
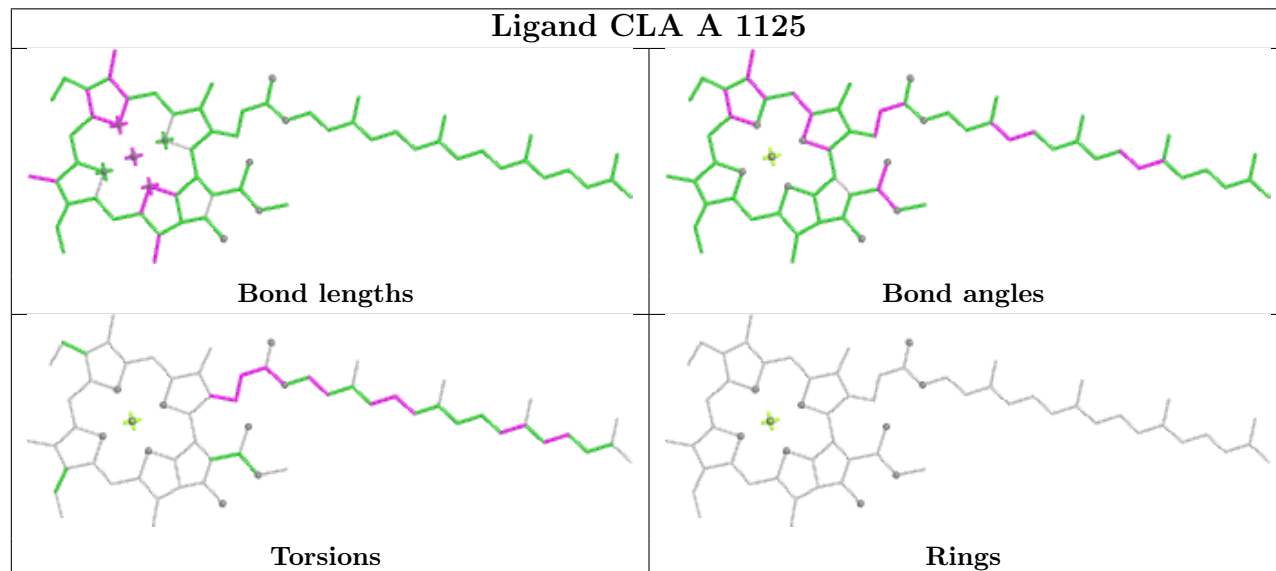


Ligand CLA G 1114

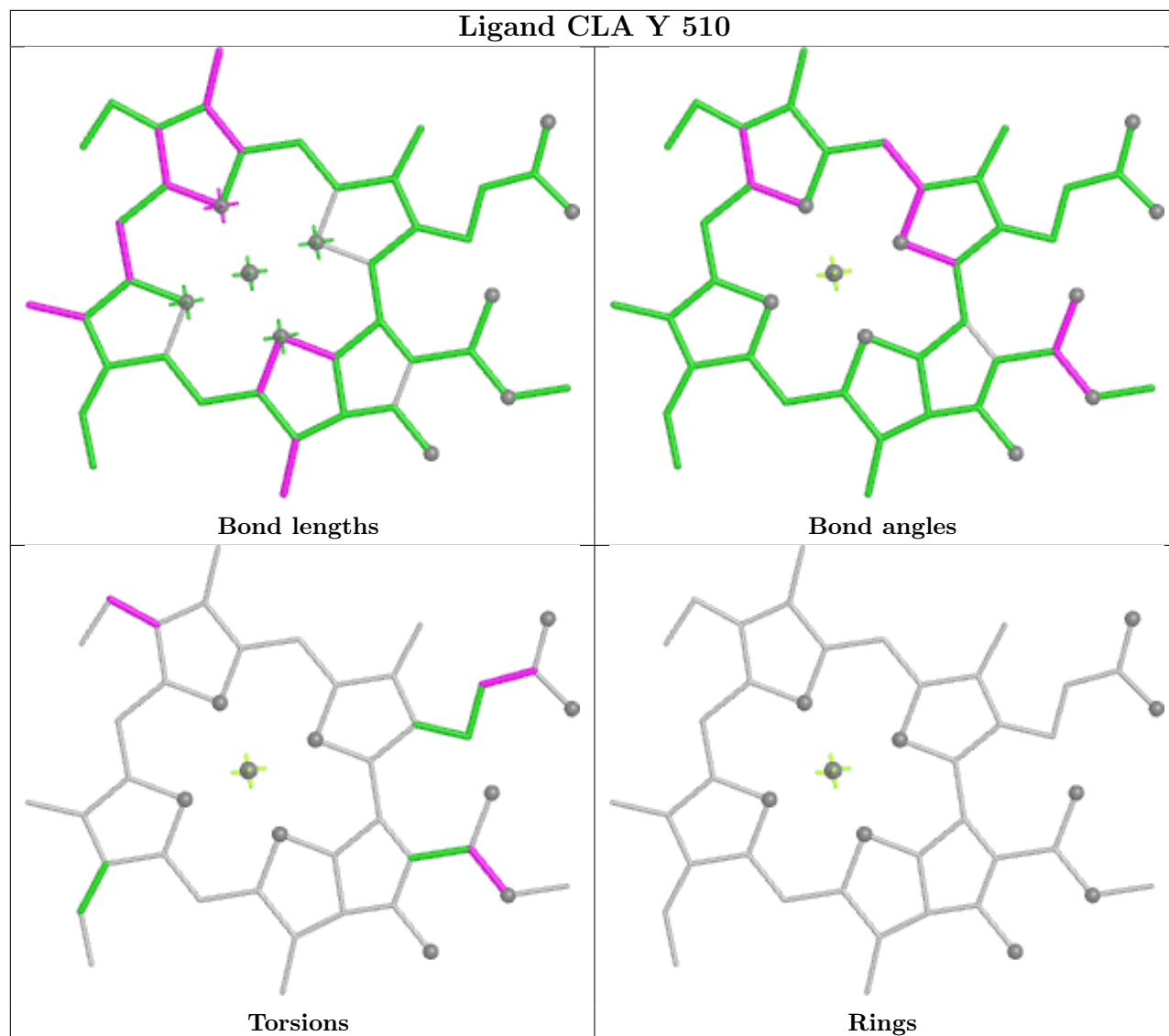


Ligand BCR H 4004

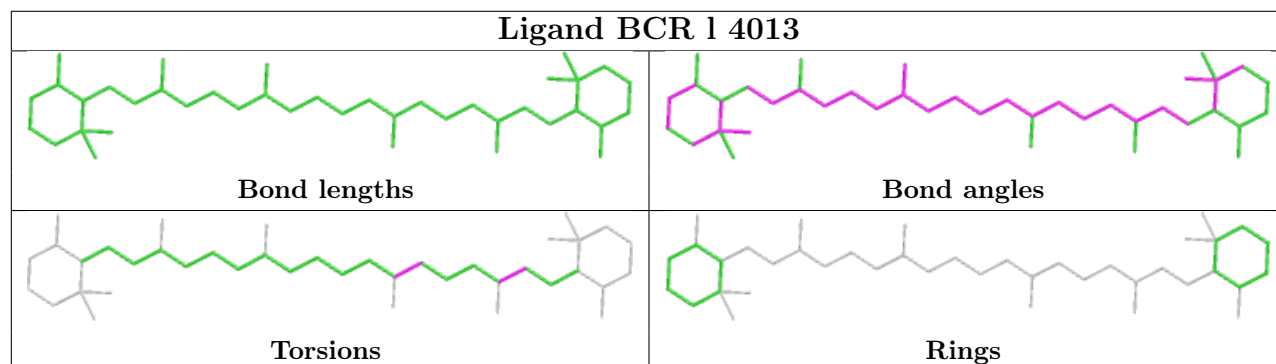


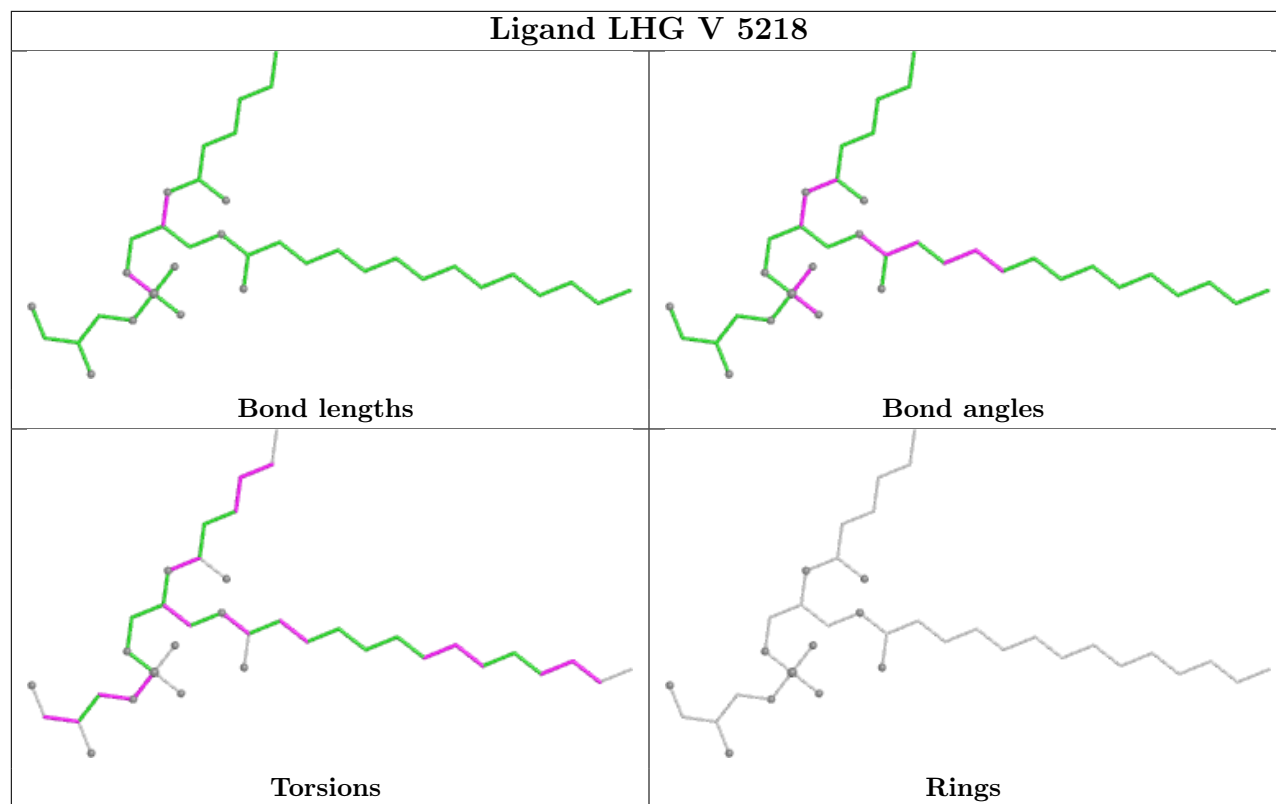
Ligand CLA 5 509**Ligand CLA A 1125**

Ligand CLA Y 510

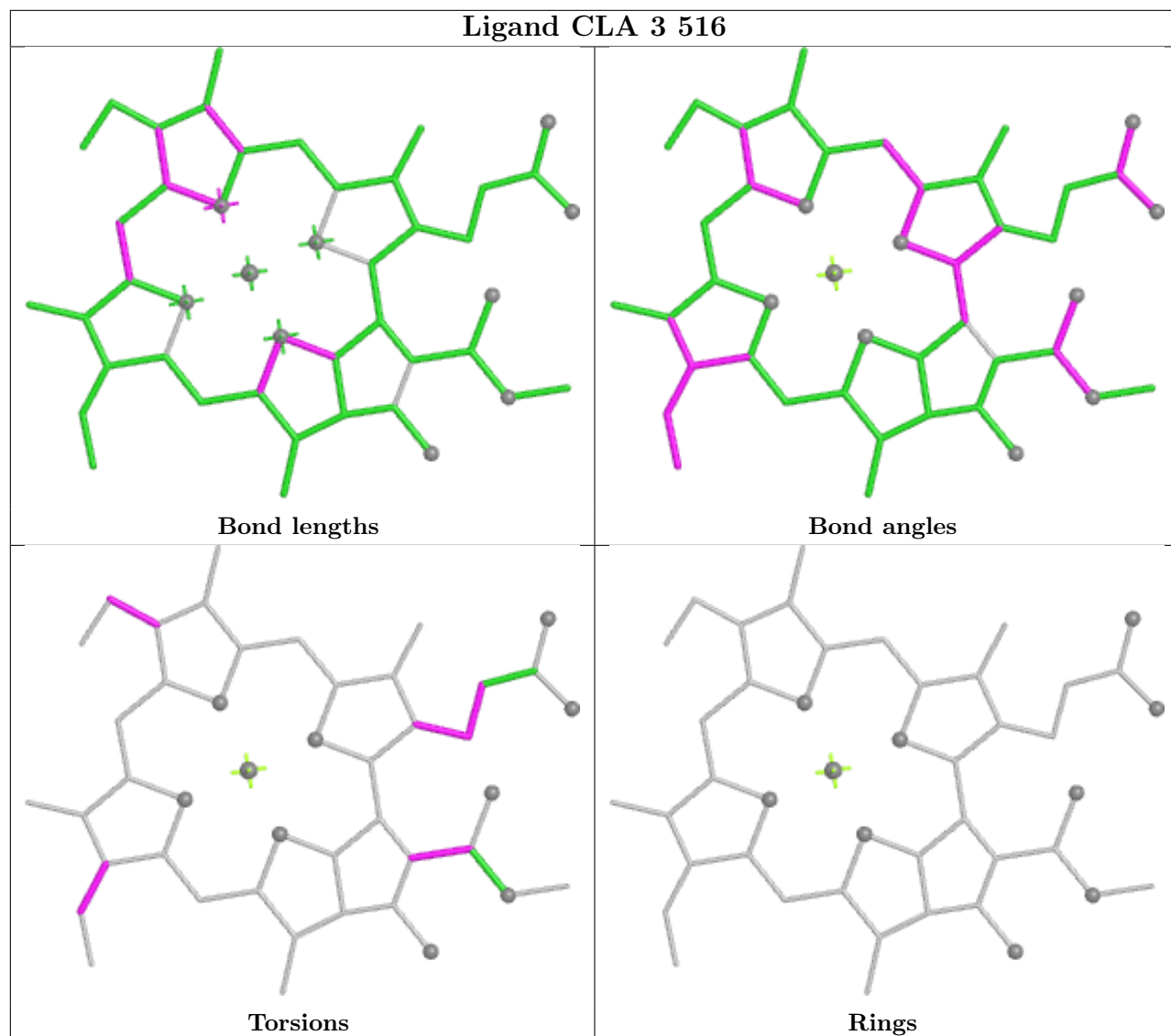


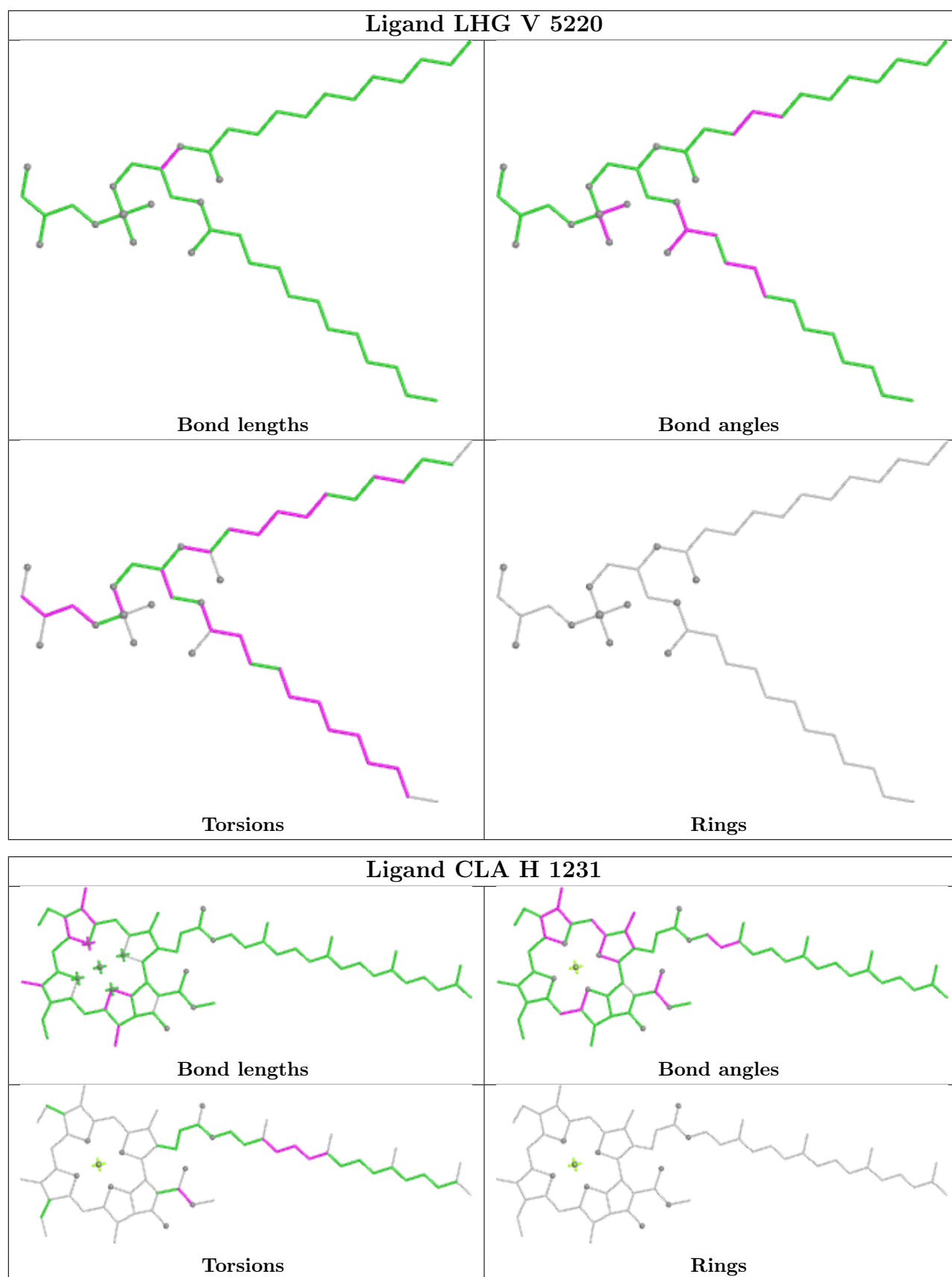
Ligand BCR 1 4013

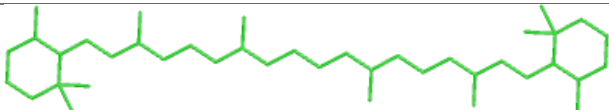
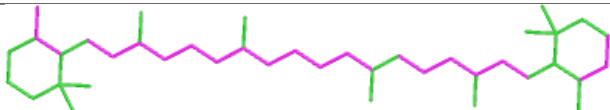
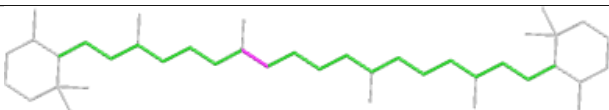
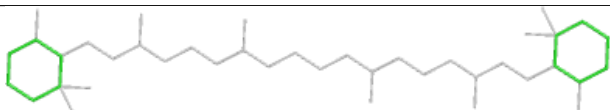


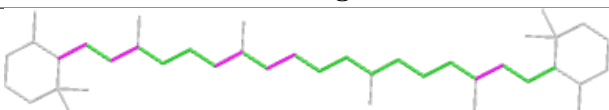
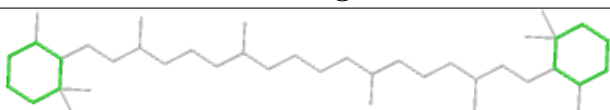


Ligand CLA 3 516

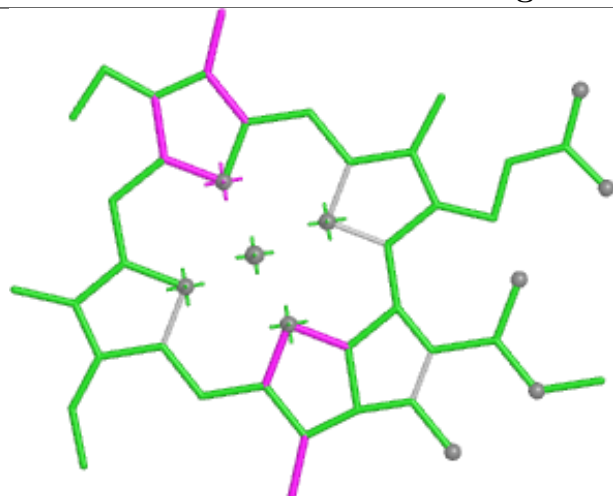




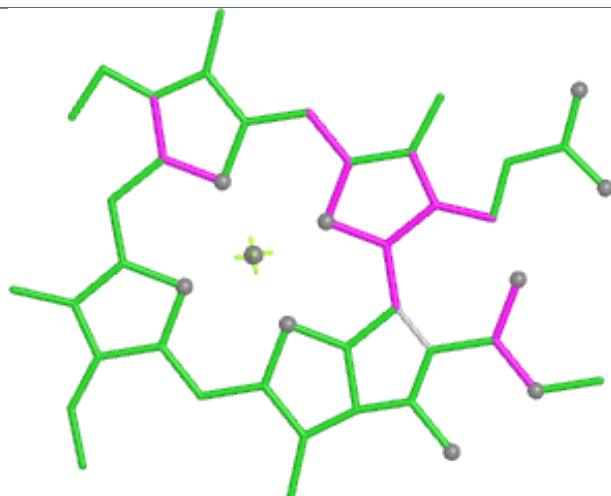
Ligand BCR F 4016	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR G 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

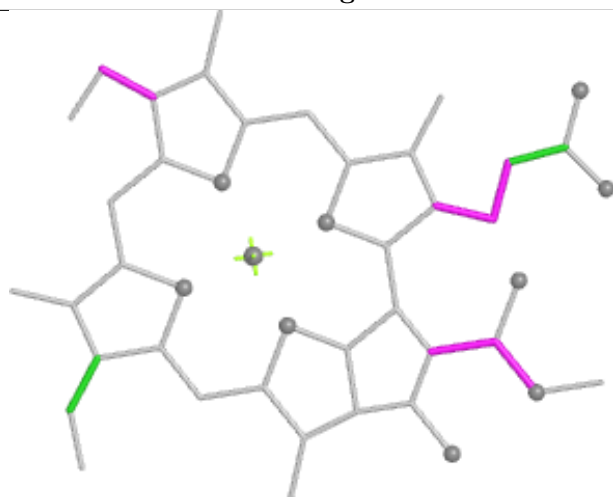
Ligand CLA Z 504



Bond lengths



Bond angles

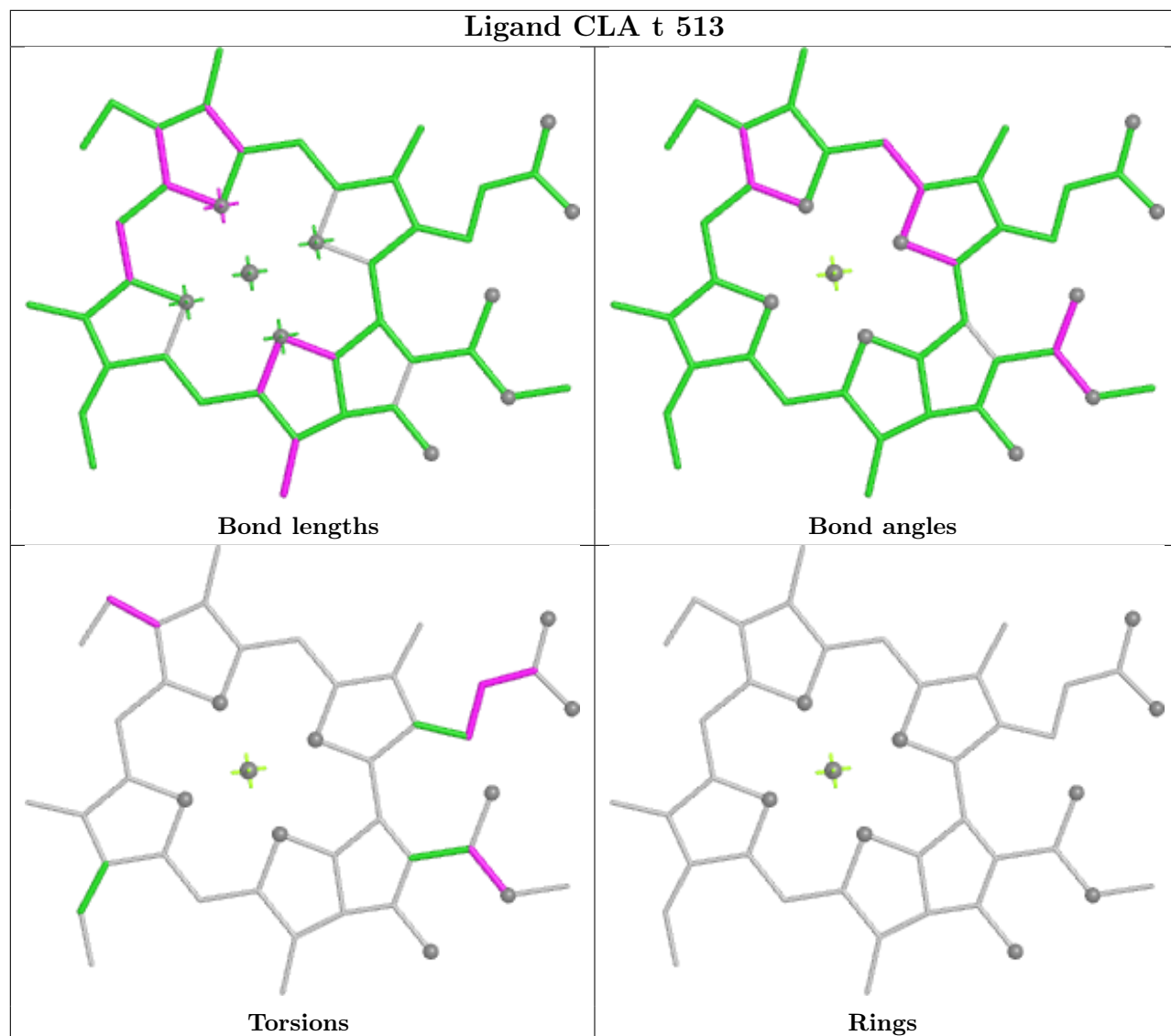


Torsions

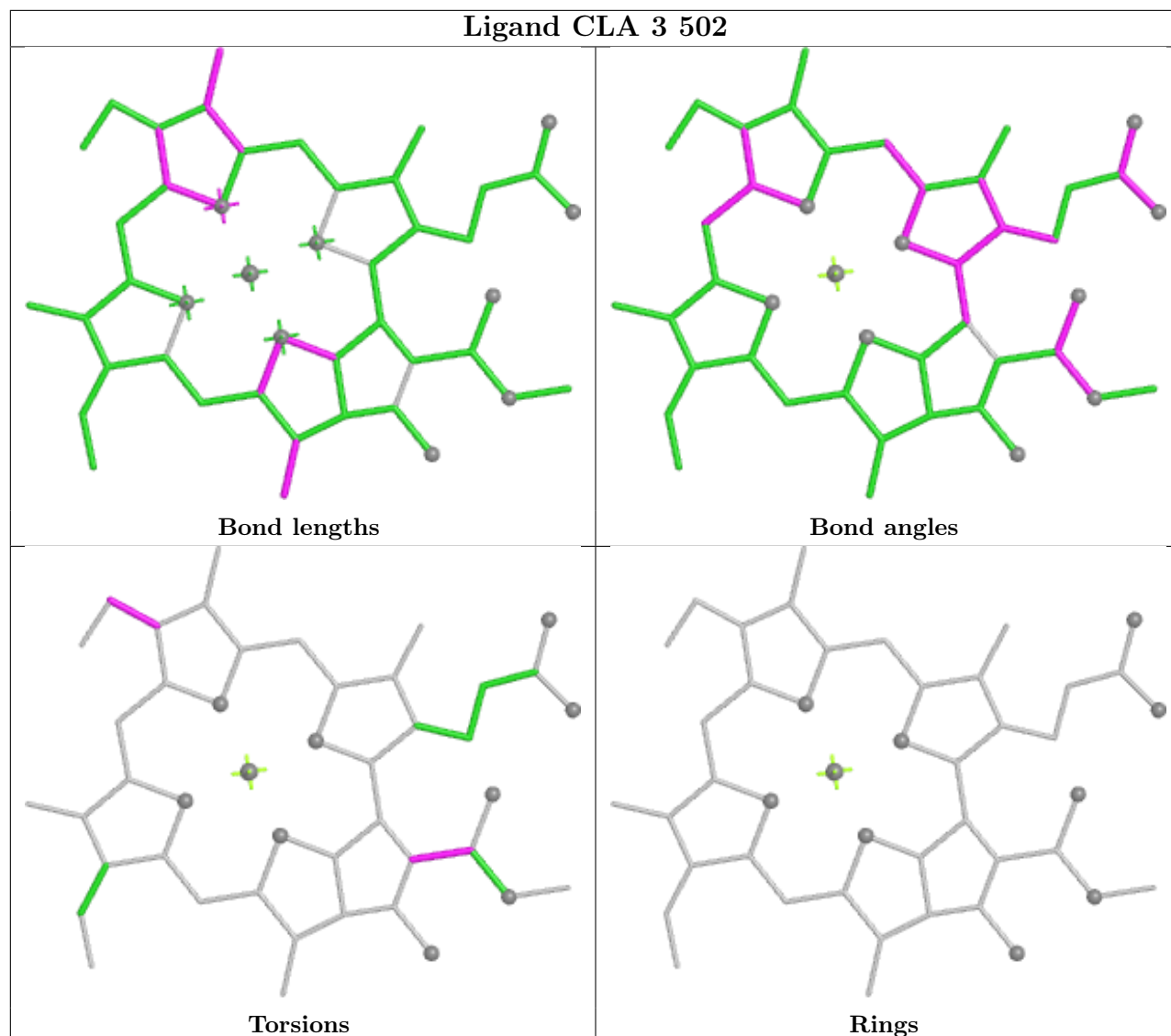


Rings

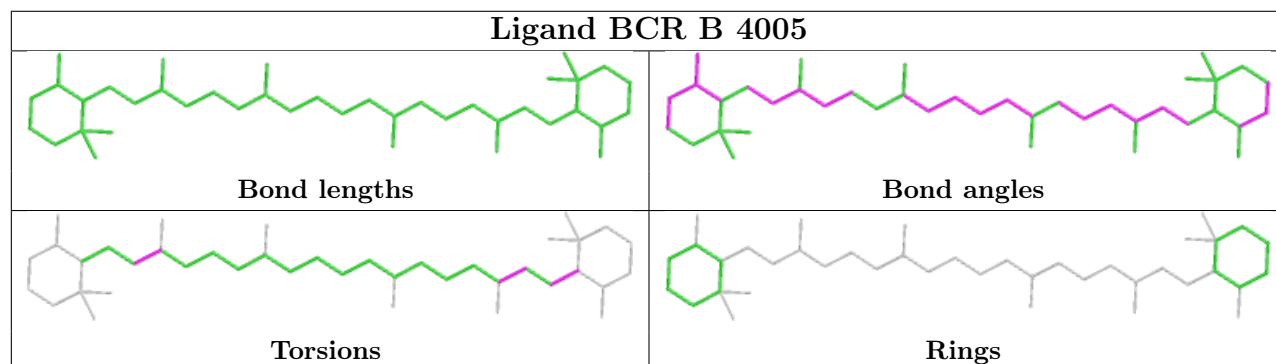
Ligand CLA t 513



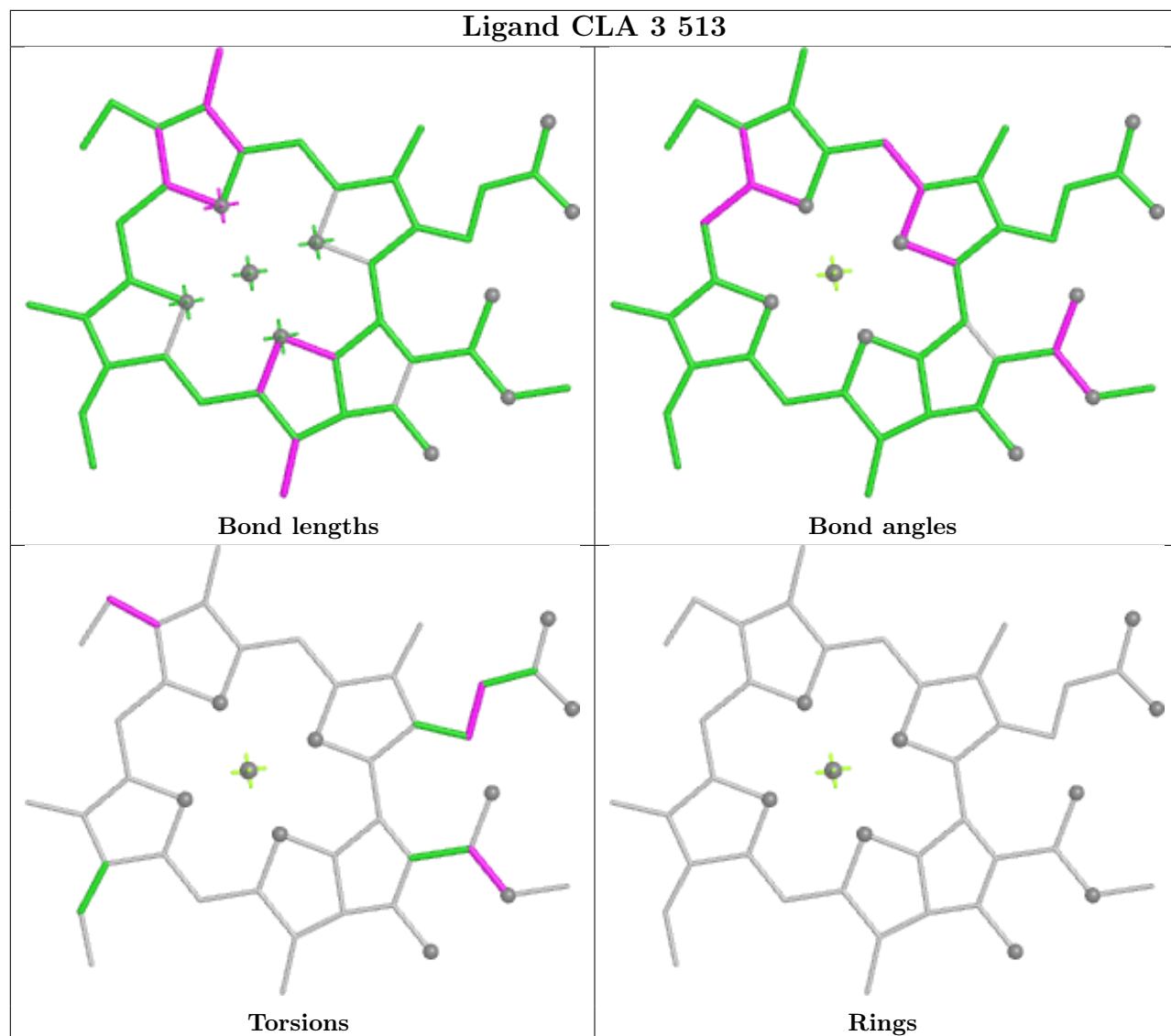
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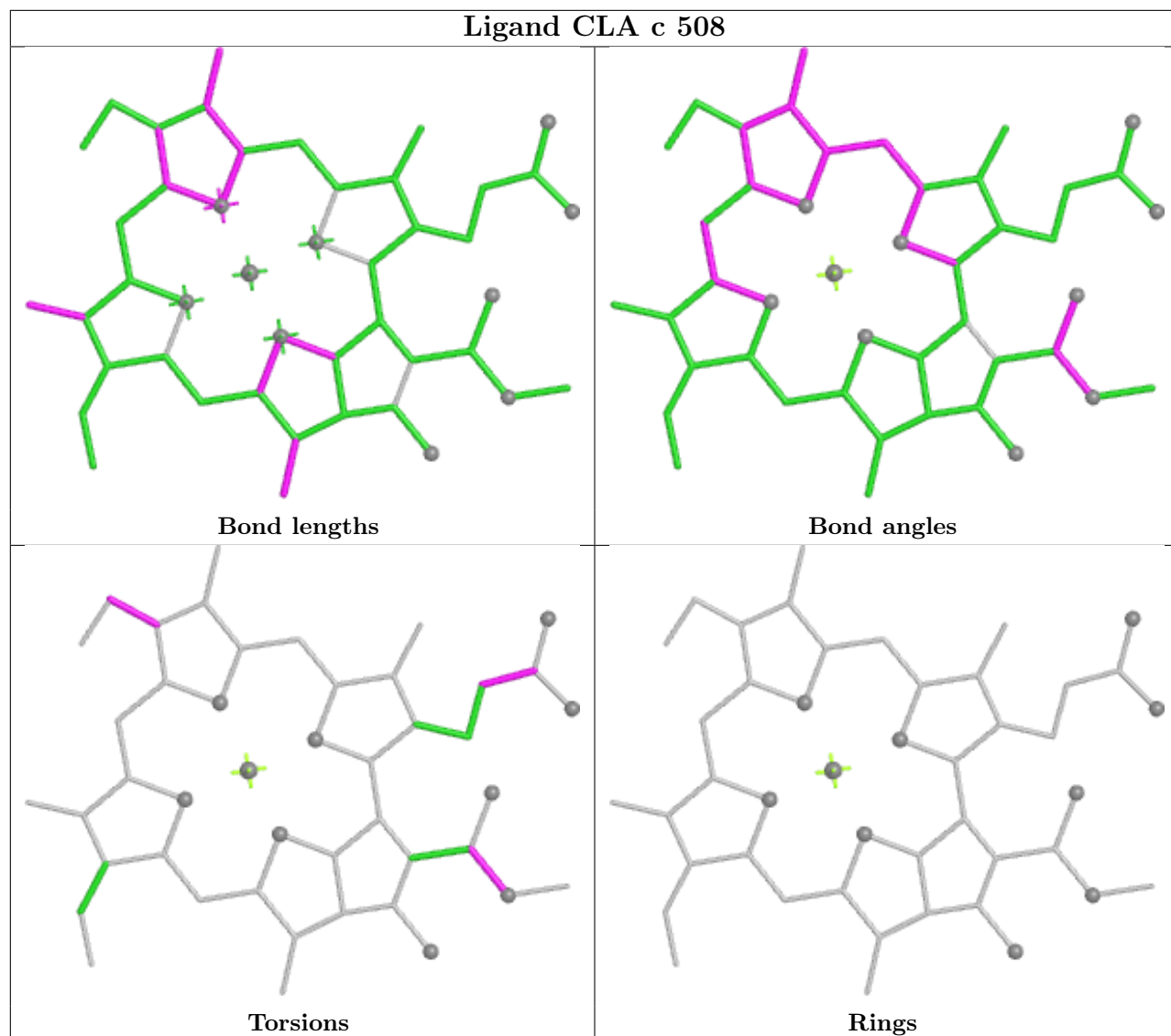
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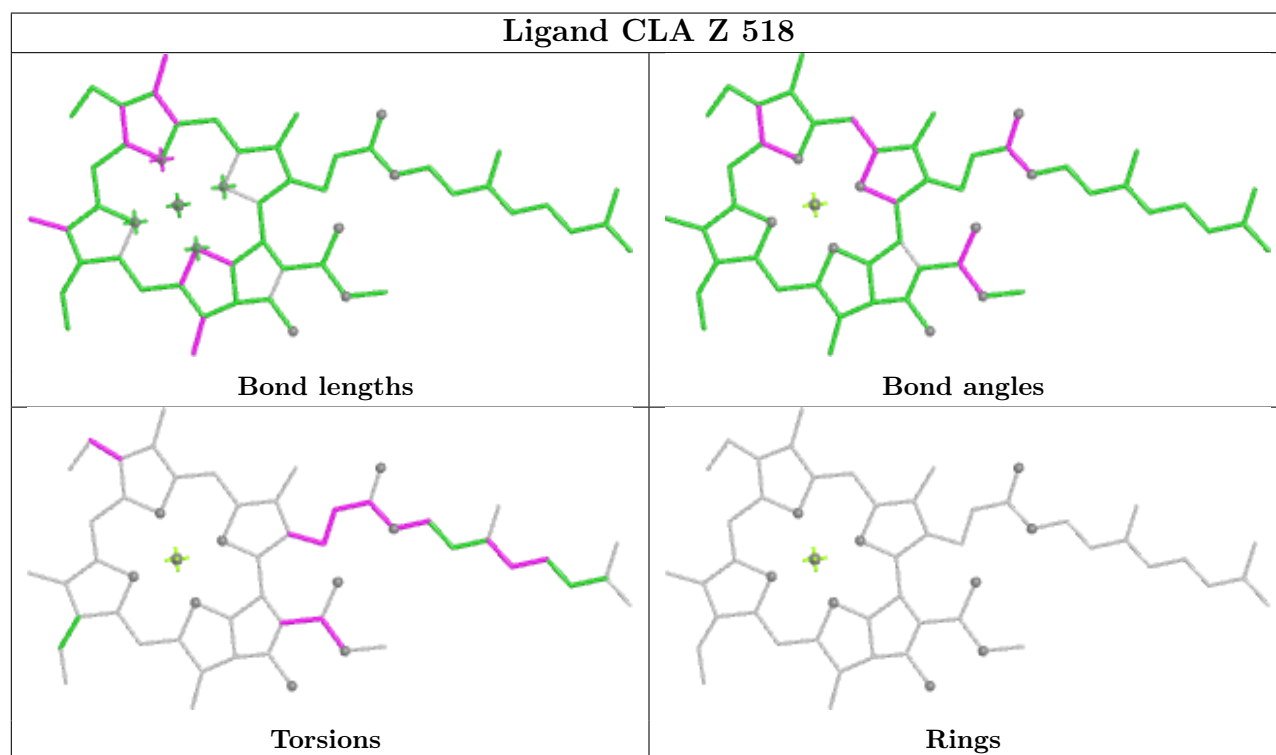
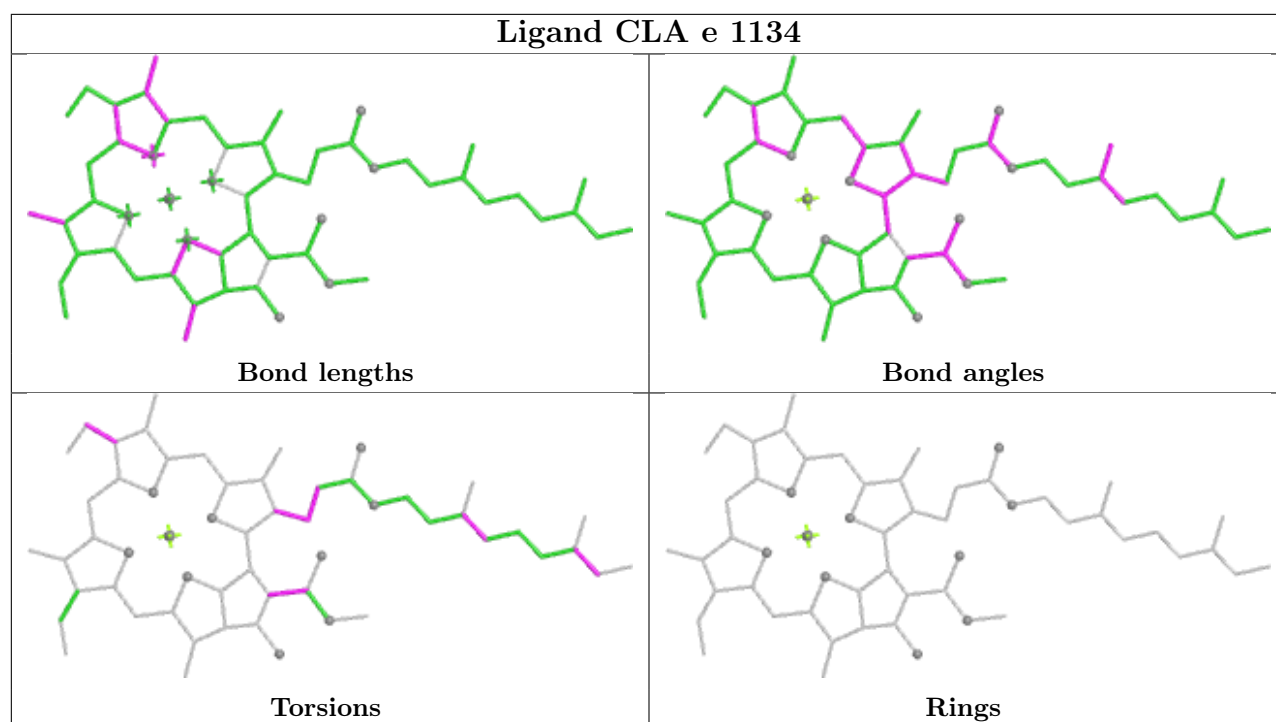


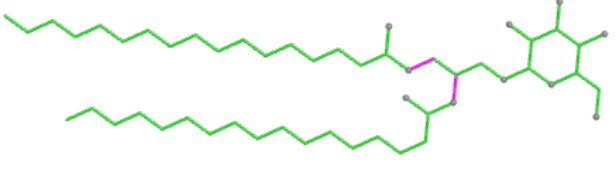
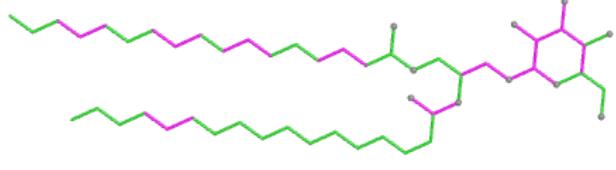
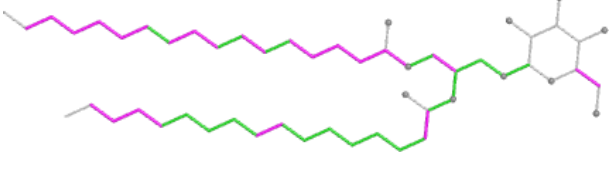
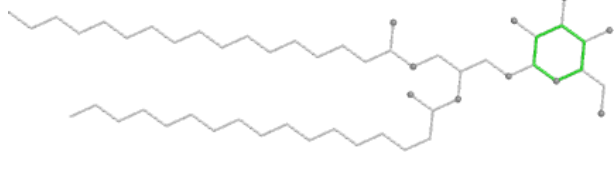
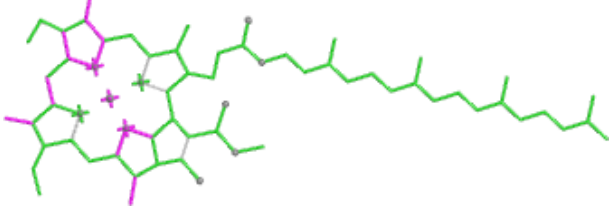
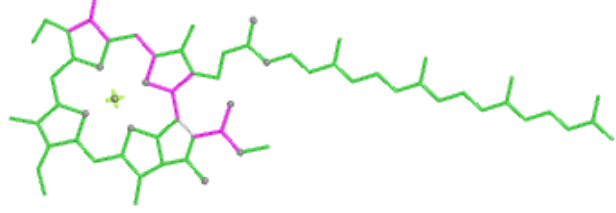
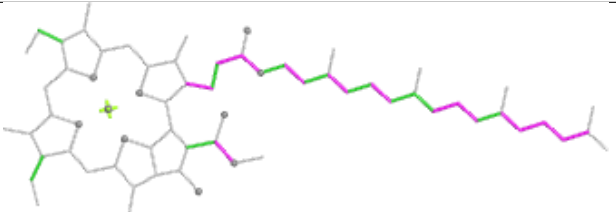
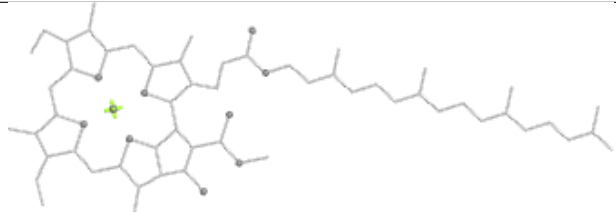
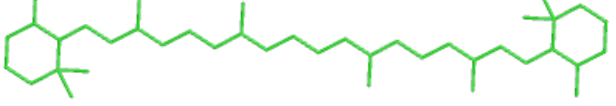
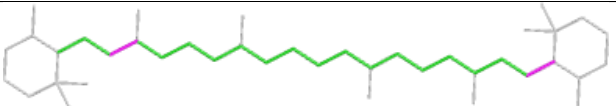
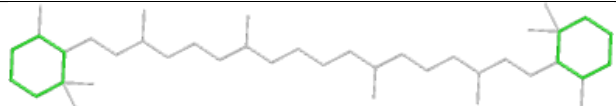
Ligand CLA 3 513



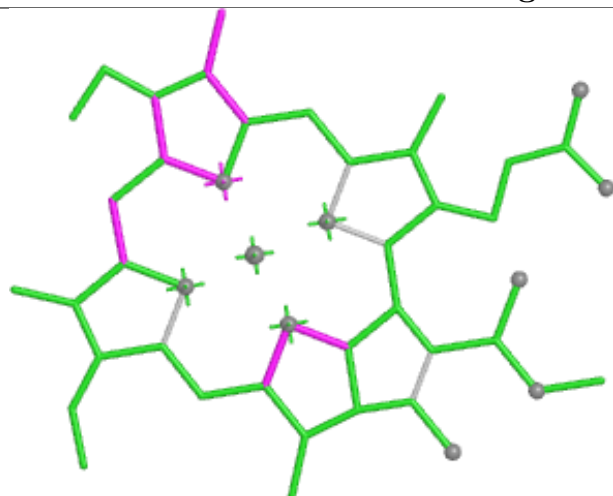
Ligand CLA c 508



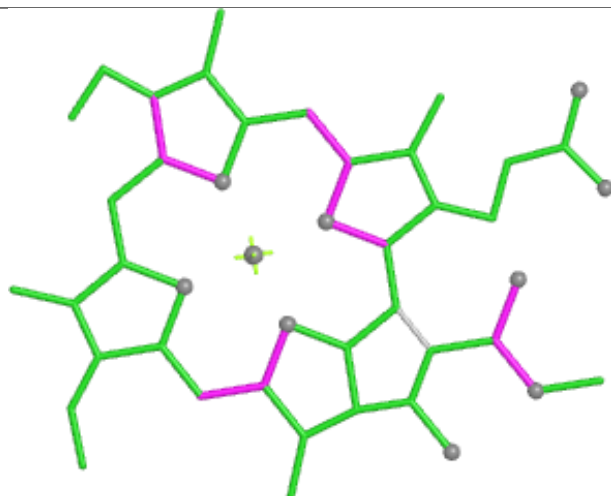


Ligand LMG f 5002	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 1126	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR V 4022	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 501



Bond lengths



Bond angles

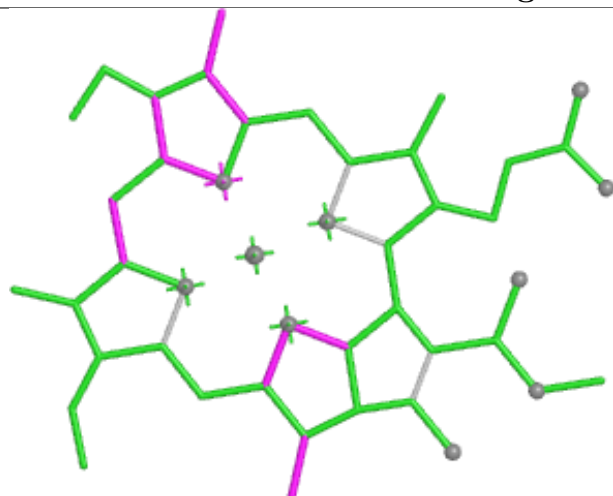


Torsions

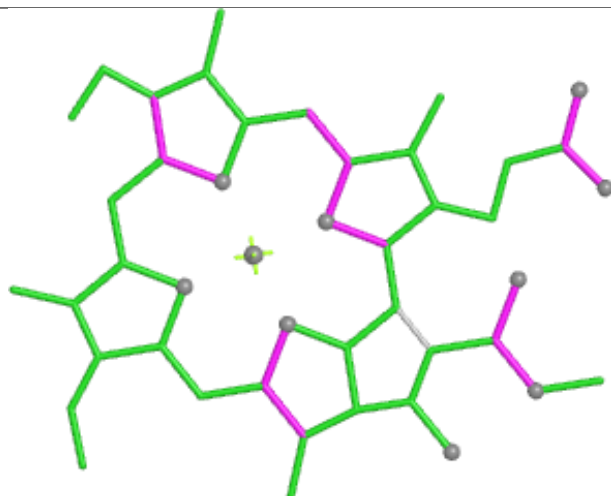


Rings

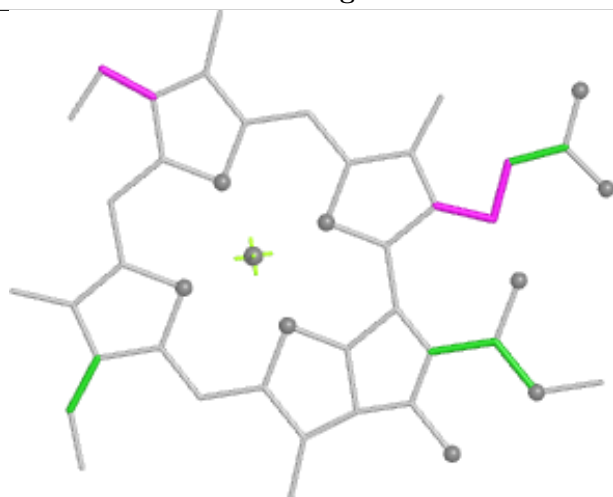
Ligand CLA u 518



Bond lengths



Bond angles

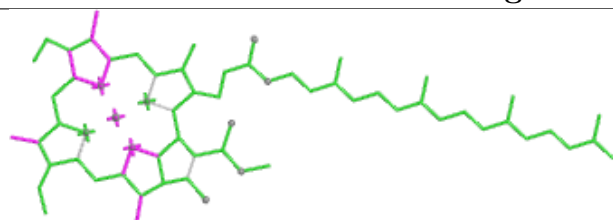


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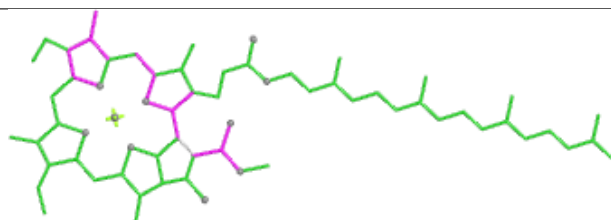


Rings

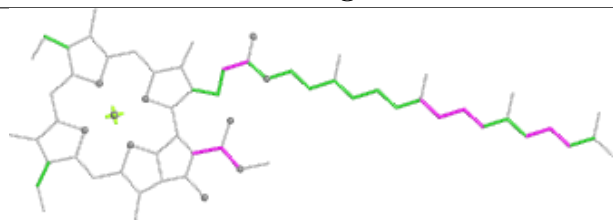
Ligand CLA A 1123



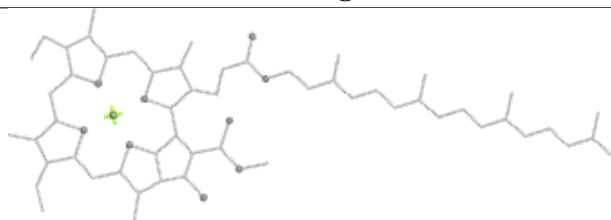
Bond lengths



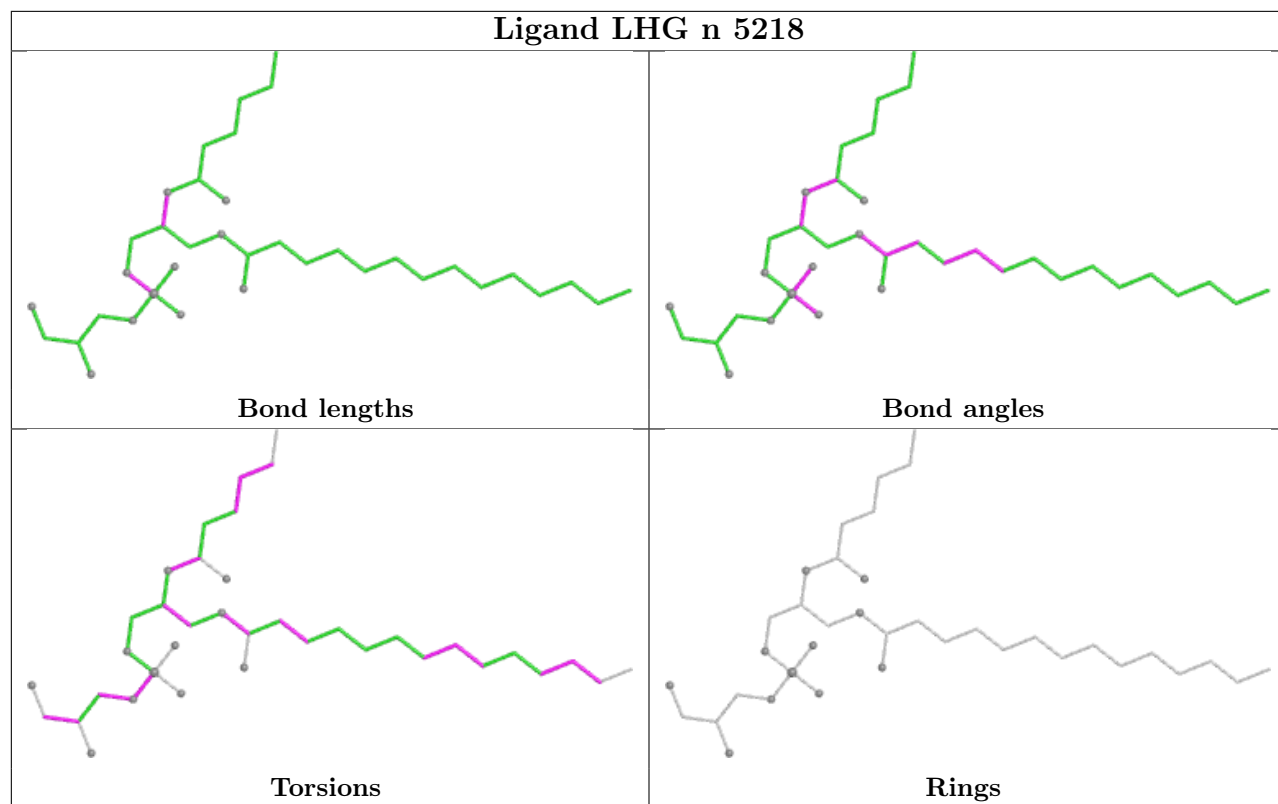
Bond angles



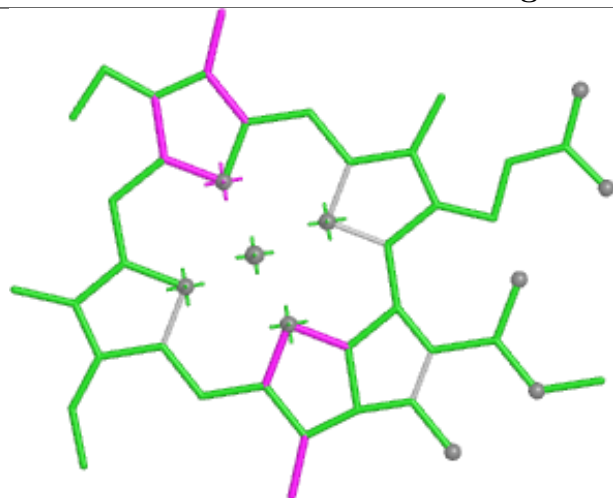
Torsions



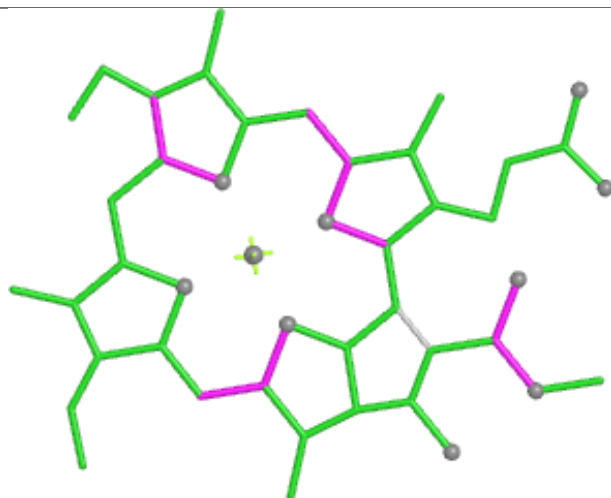
Rings



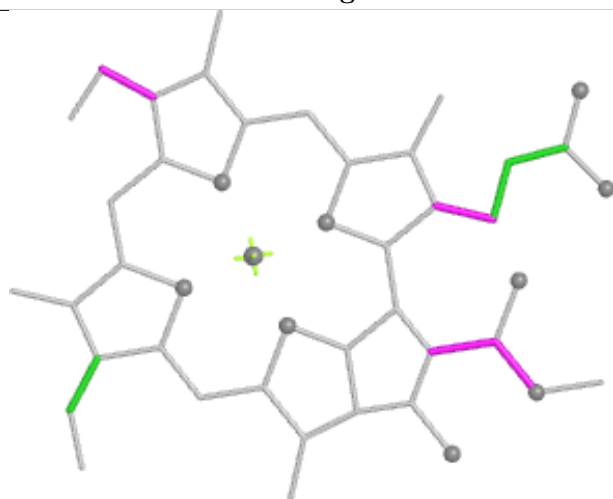
Ligand CLA t 504



Bond lengths



Bond angles

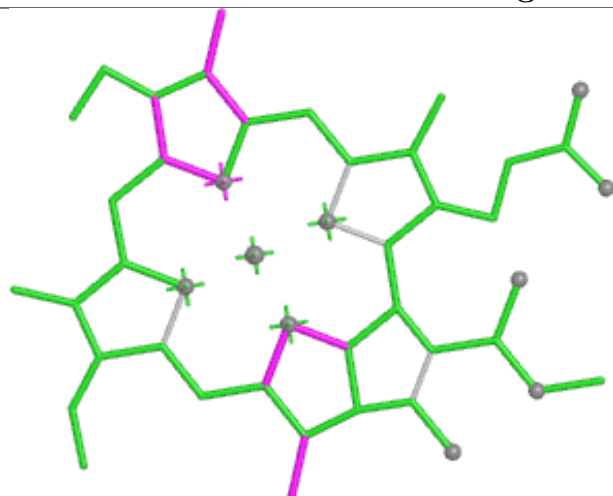


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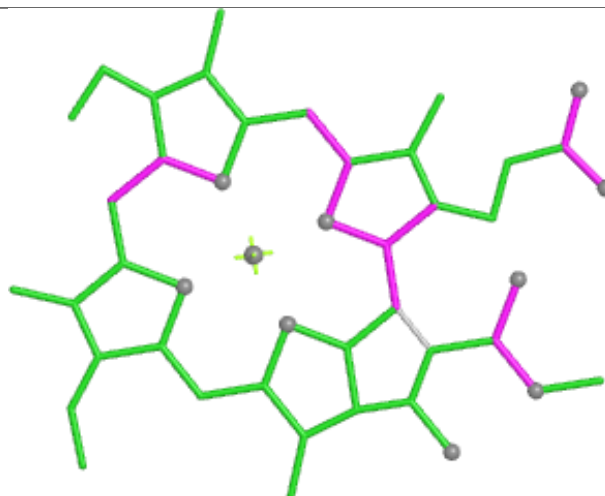


Rings

Ligand CLA u 507



Bond lengths



Bond angles

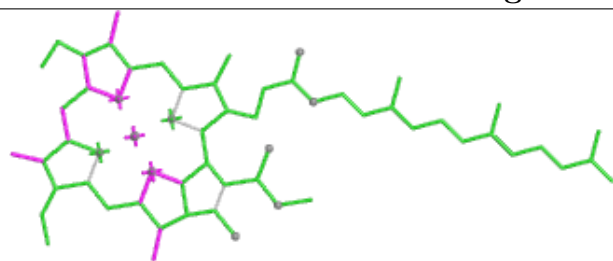


Torsions

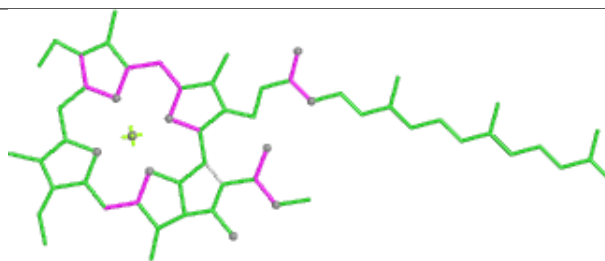


Rings

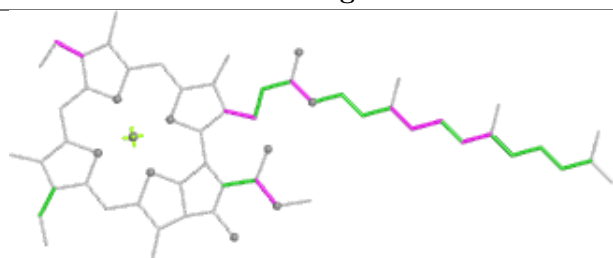
Ligand CLA H 1227



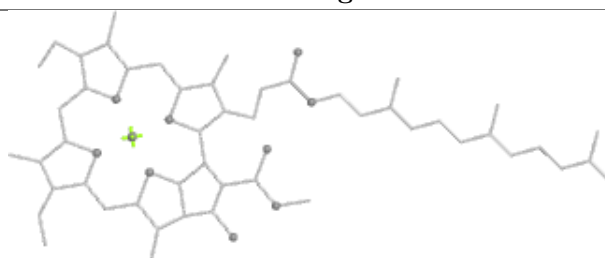
Bond lengths



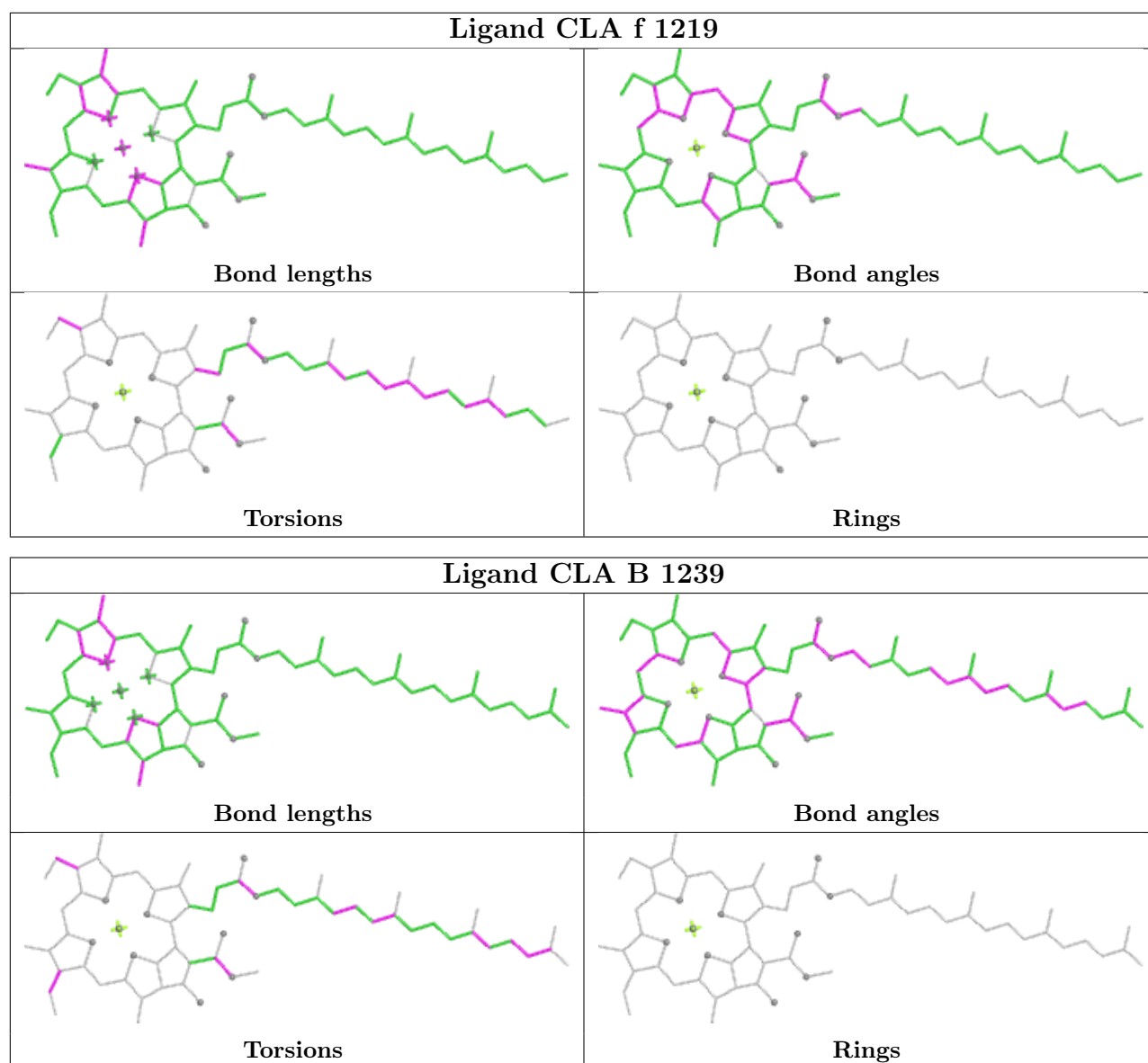
Bond angles

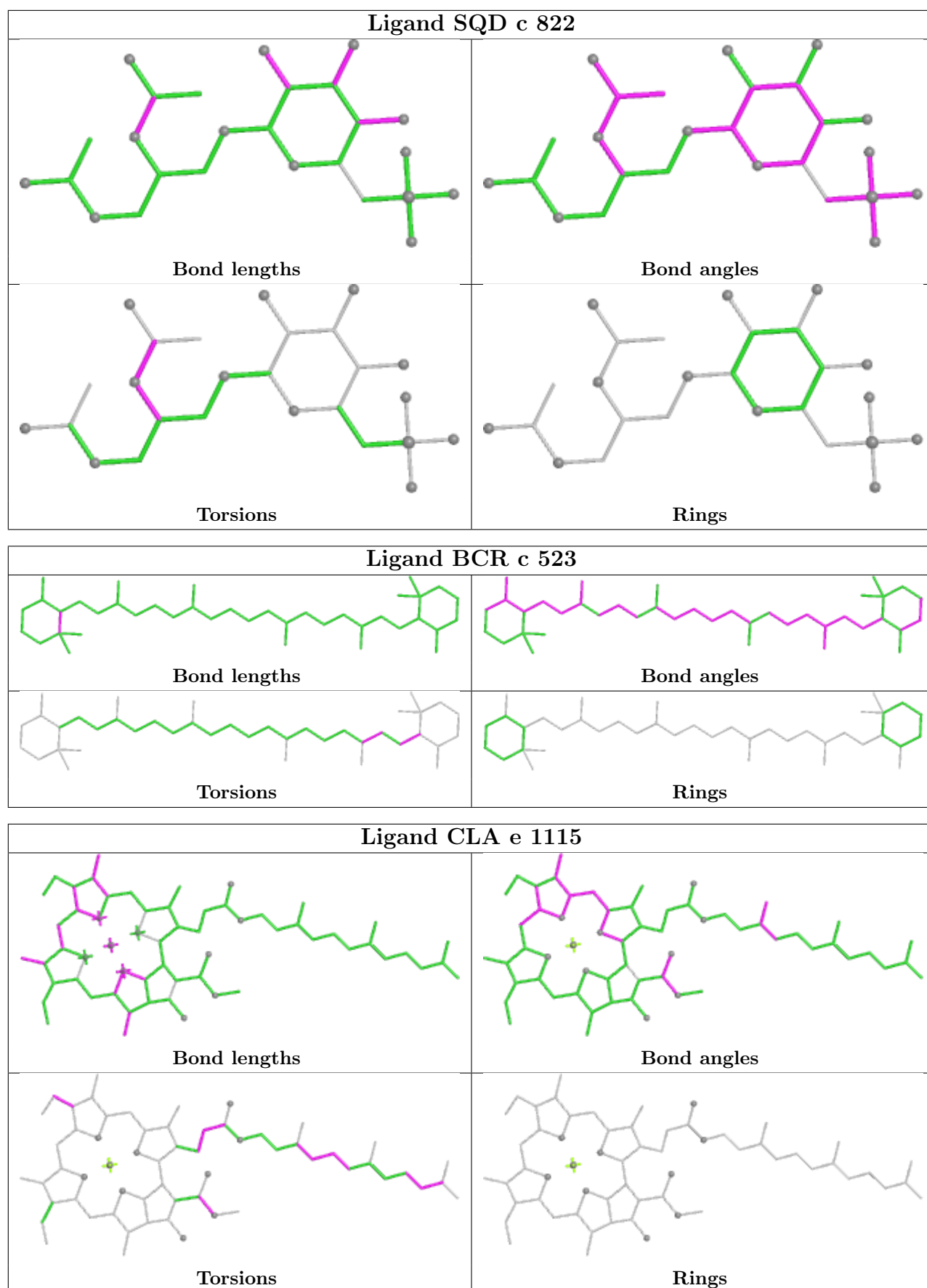


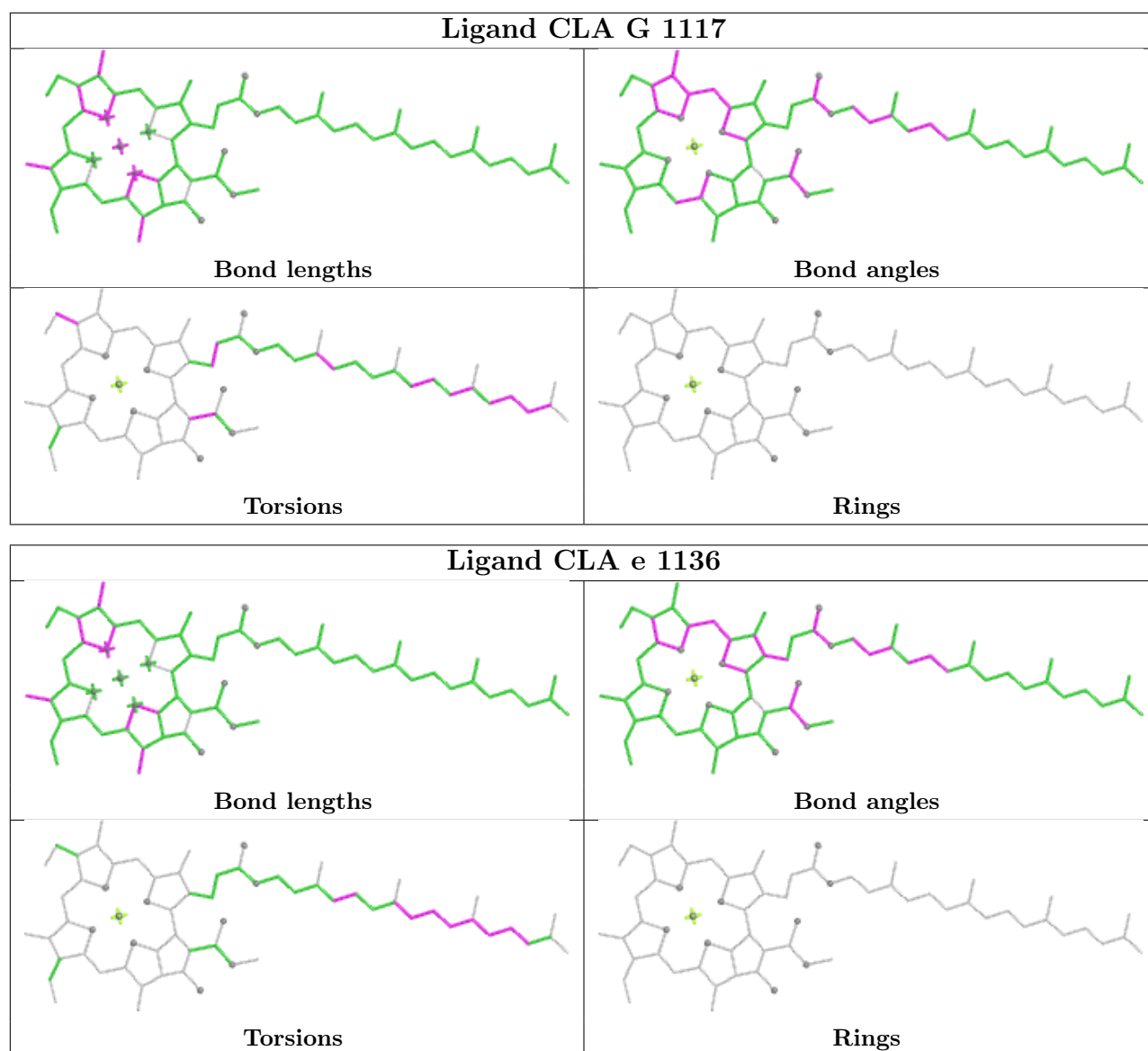
Torsions



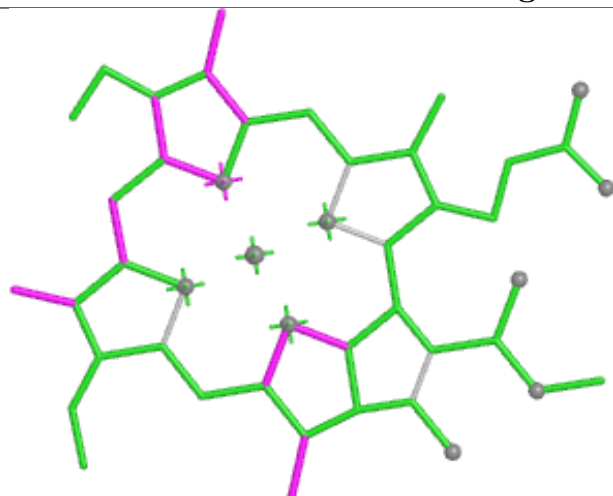
Rings



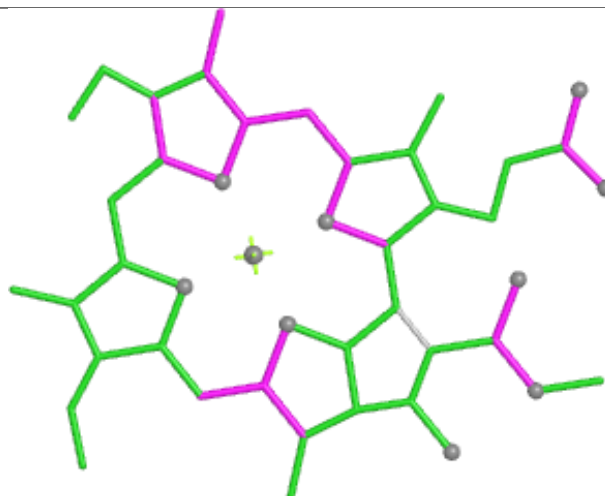




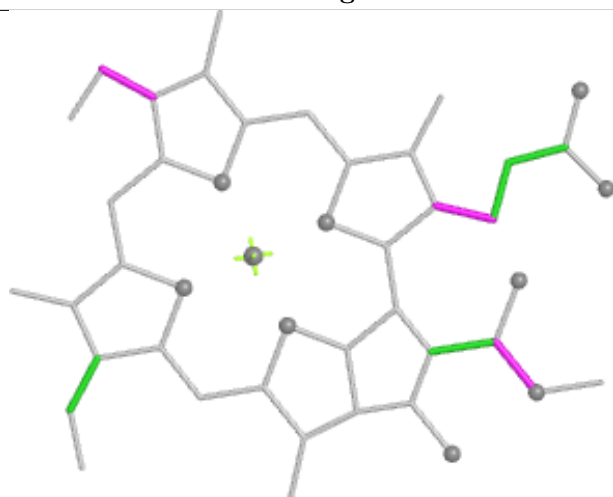
Ligand CLA 4 511



Bond lengths



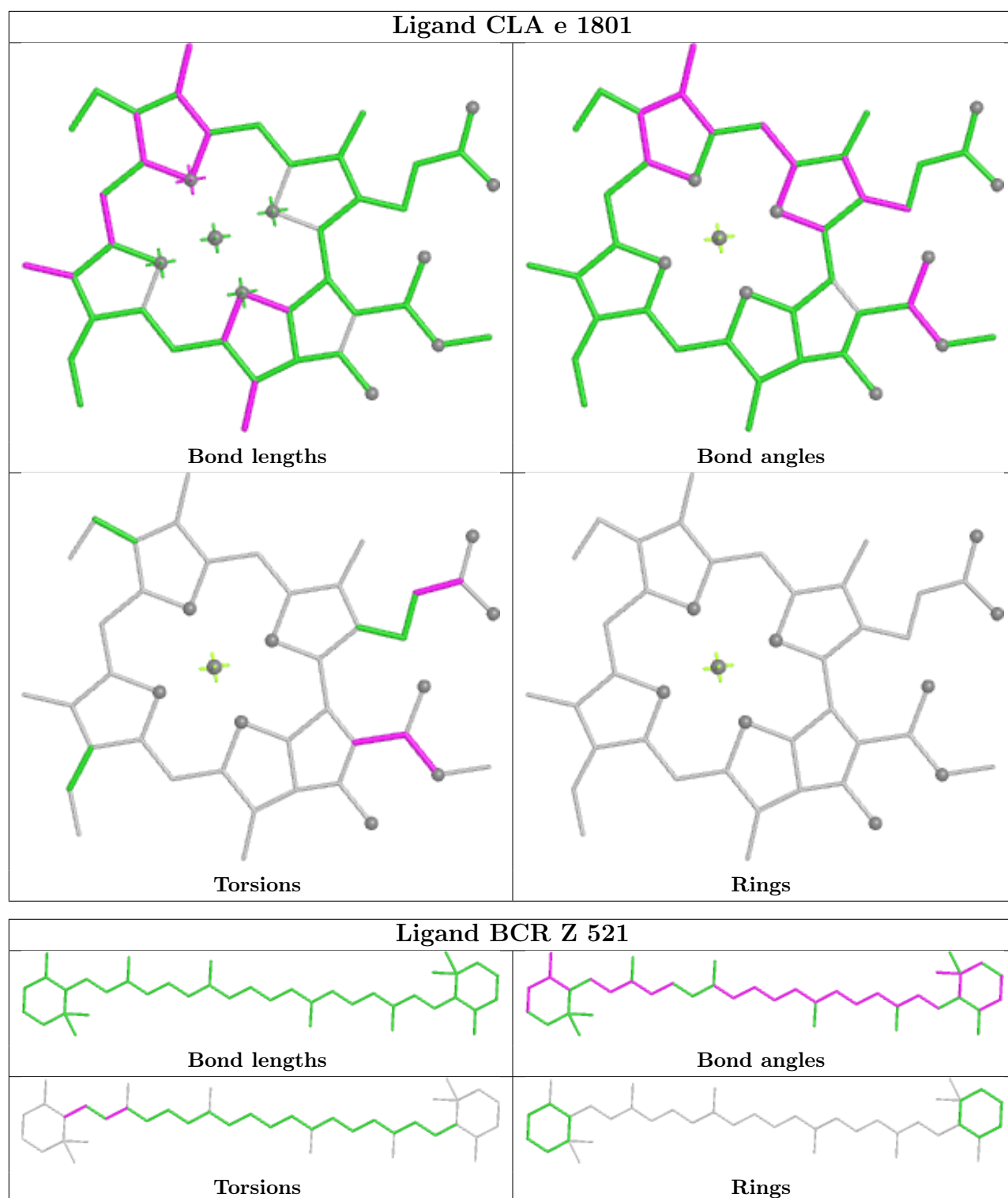
Bond angles

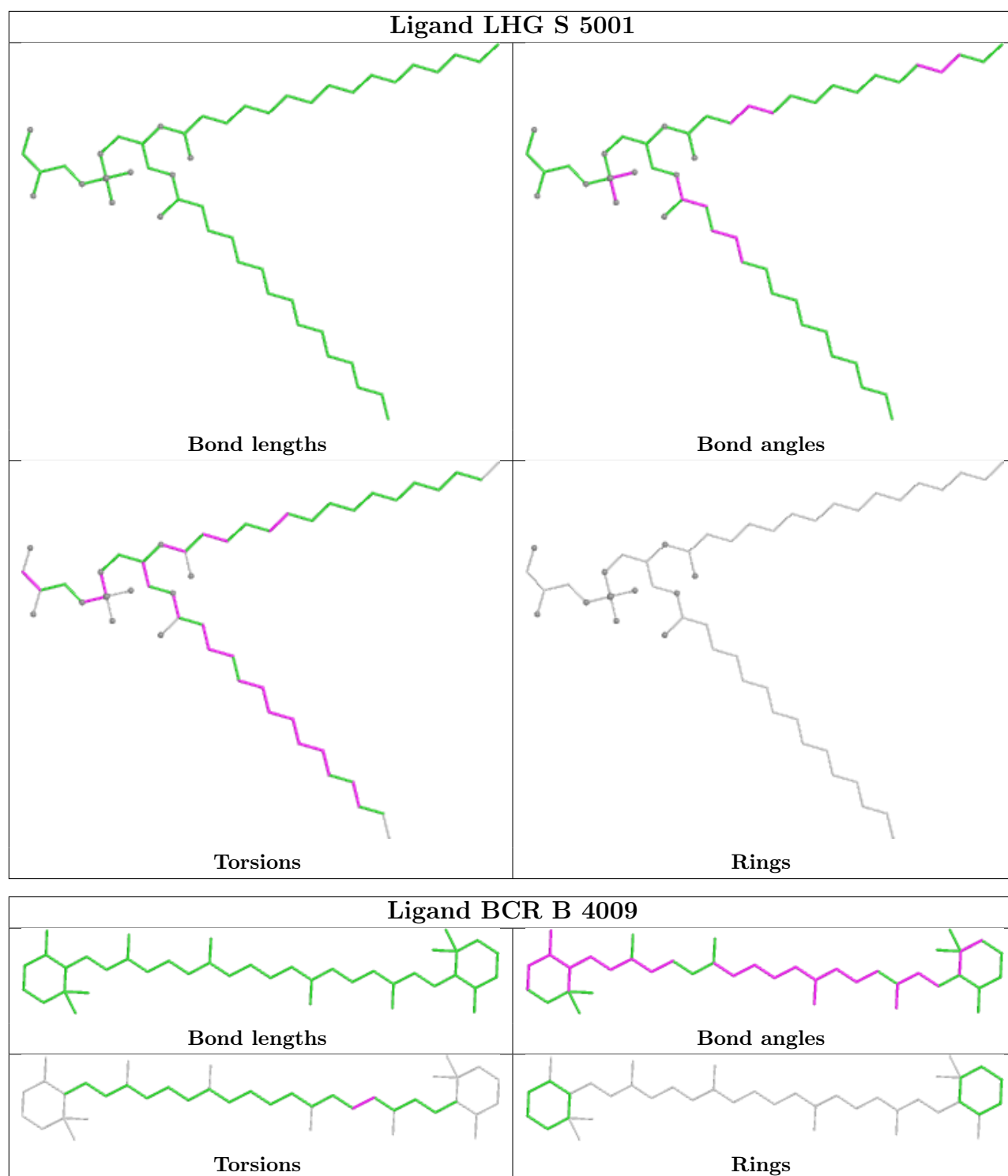


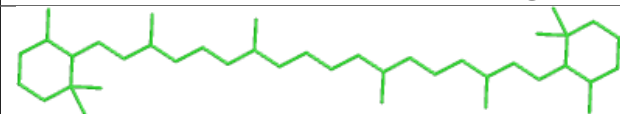
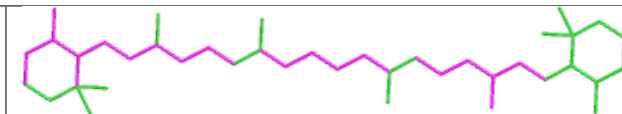
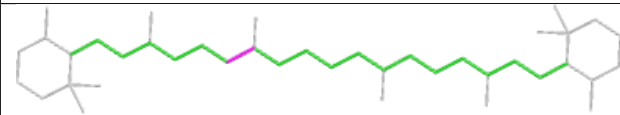
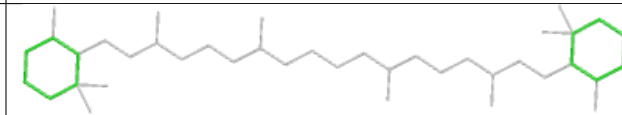
Torsions

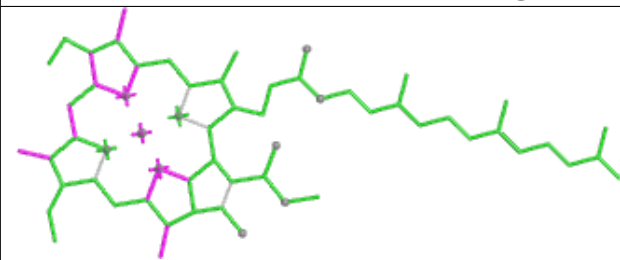
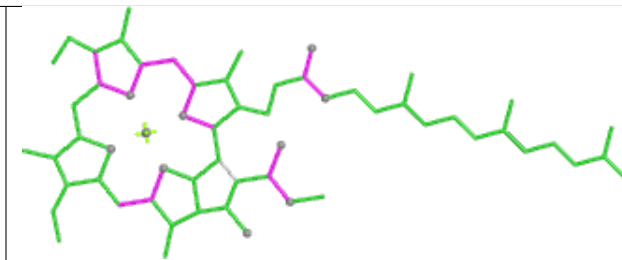
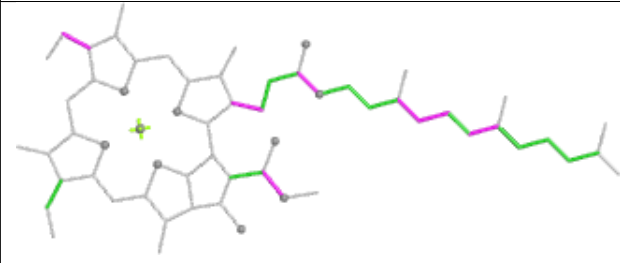
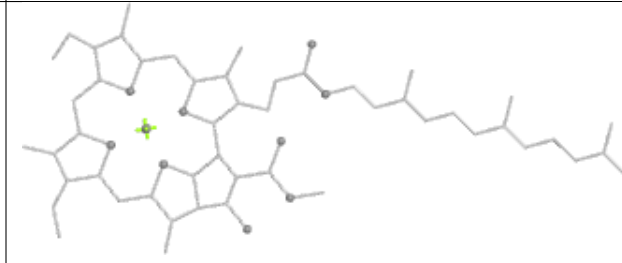


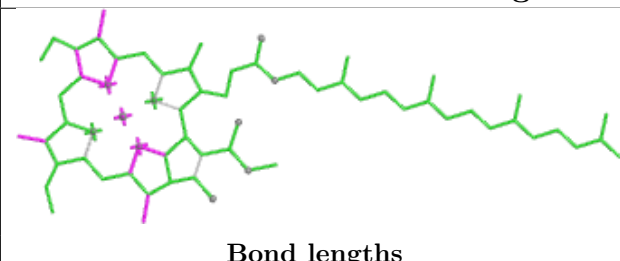
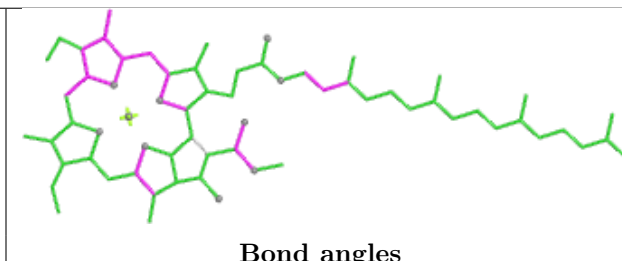
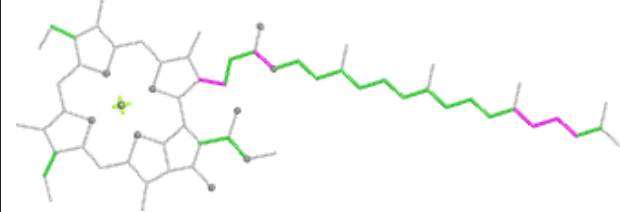
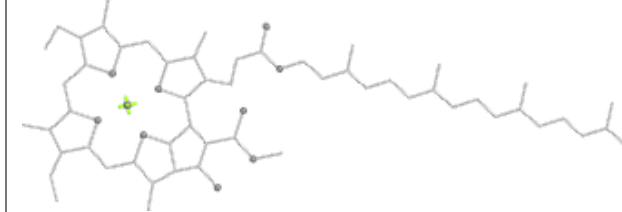
Rings

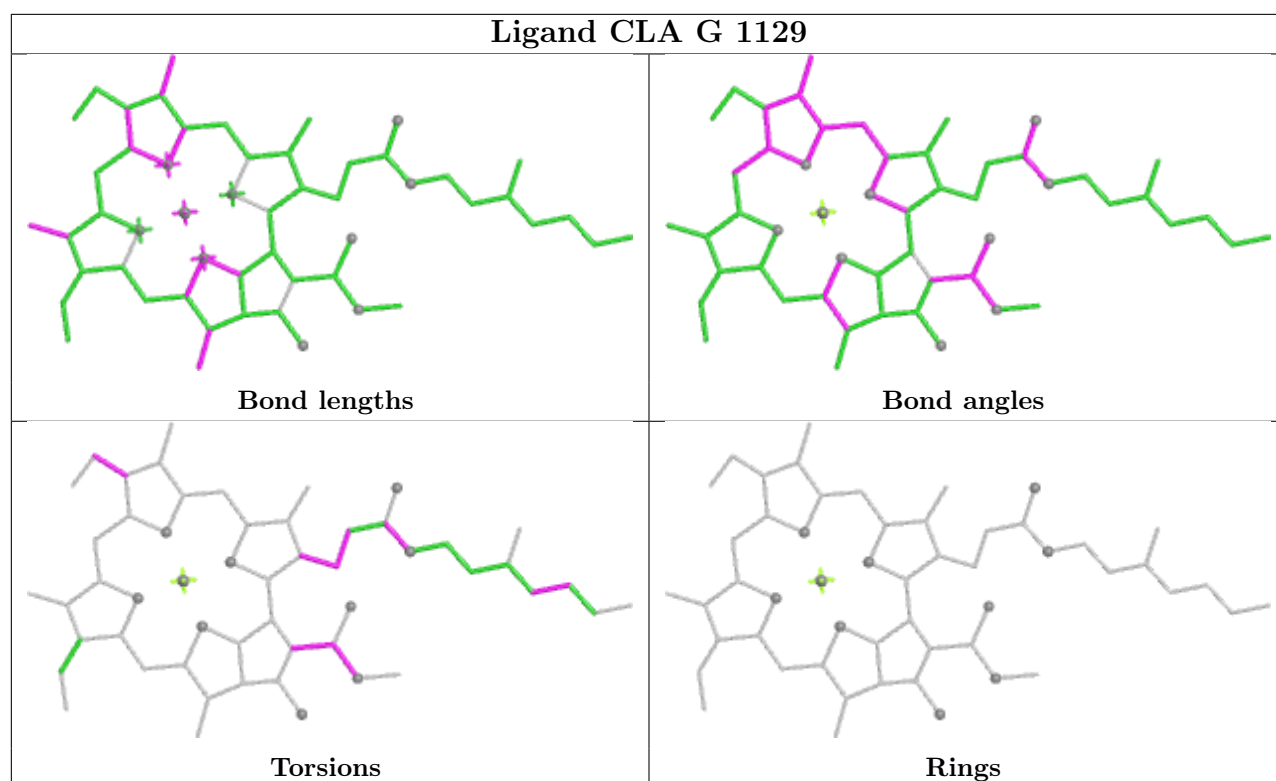




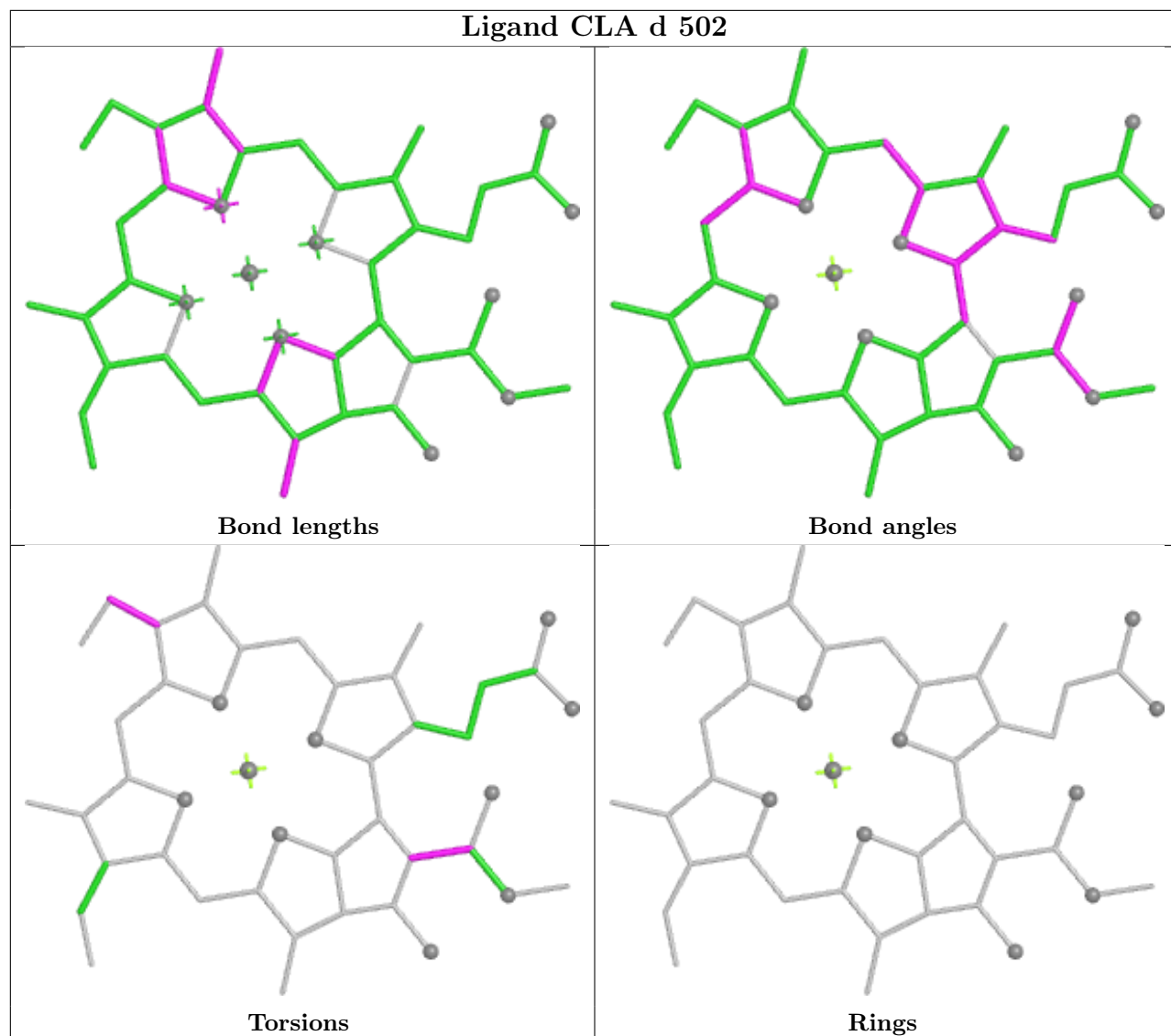
Ligand BCR 1 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

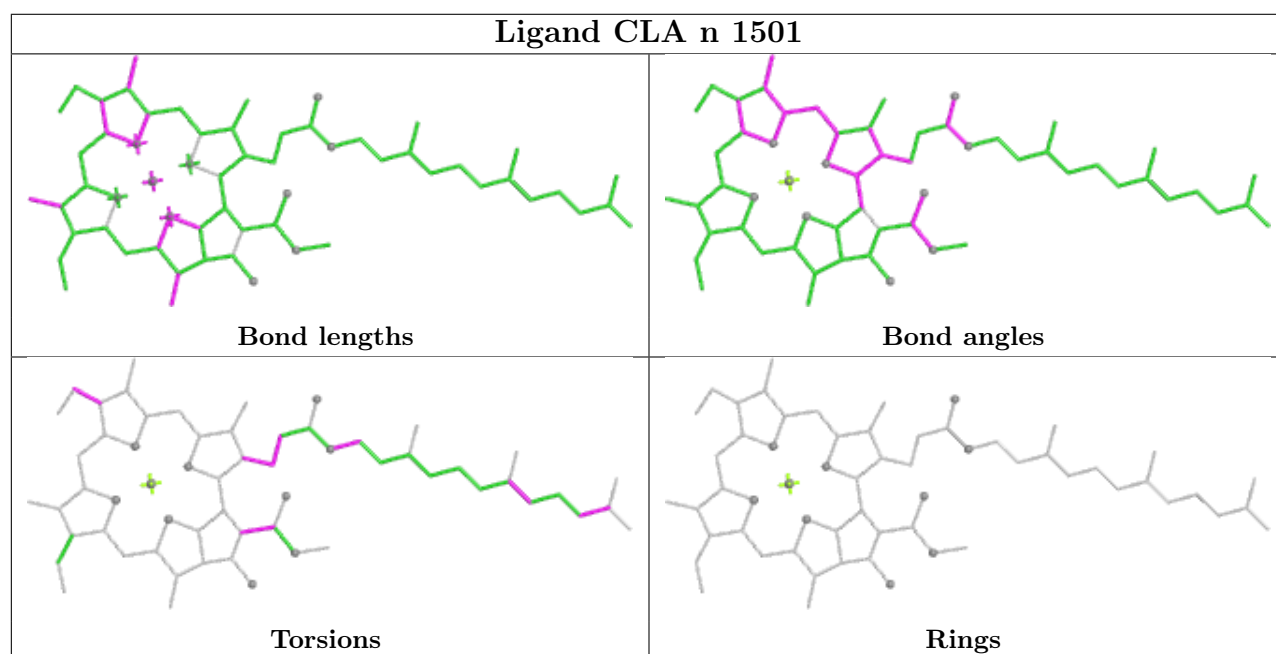
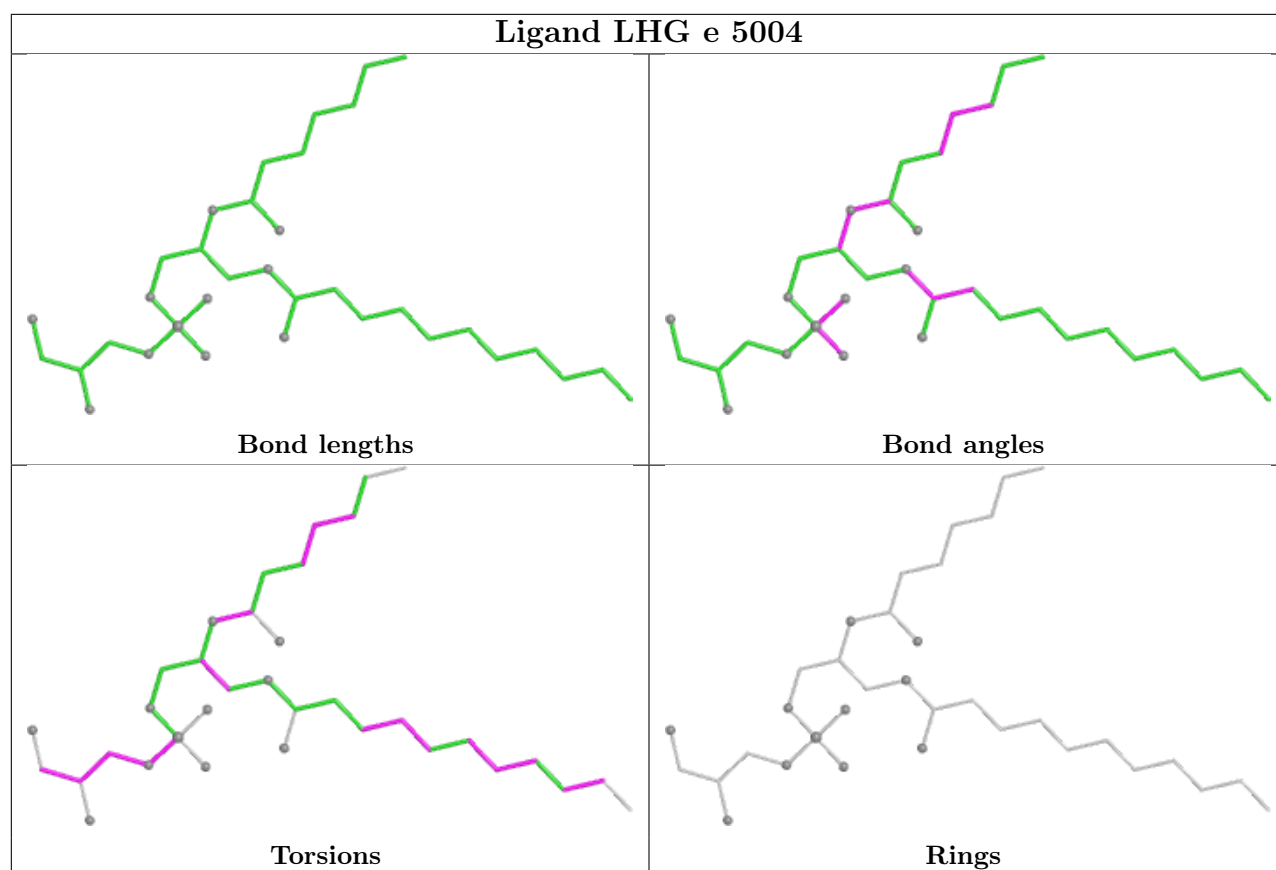
Ligand CLA B 1227	
	
Bond lengths	Bond angles
	
Torsions	Rings

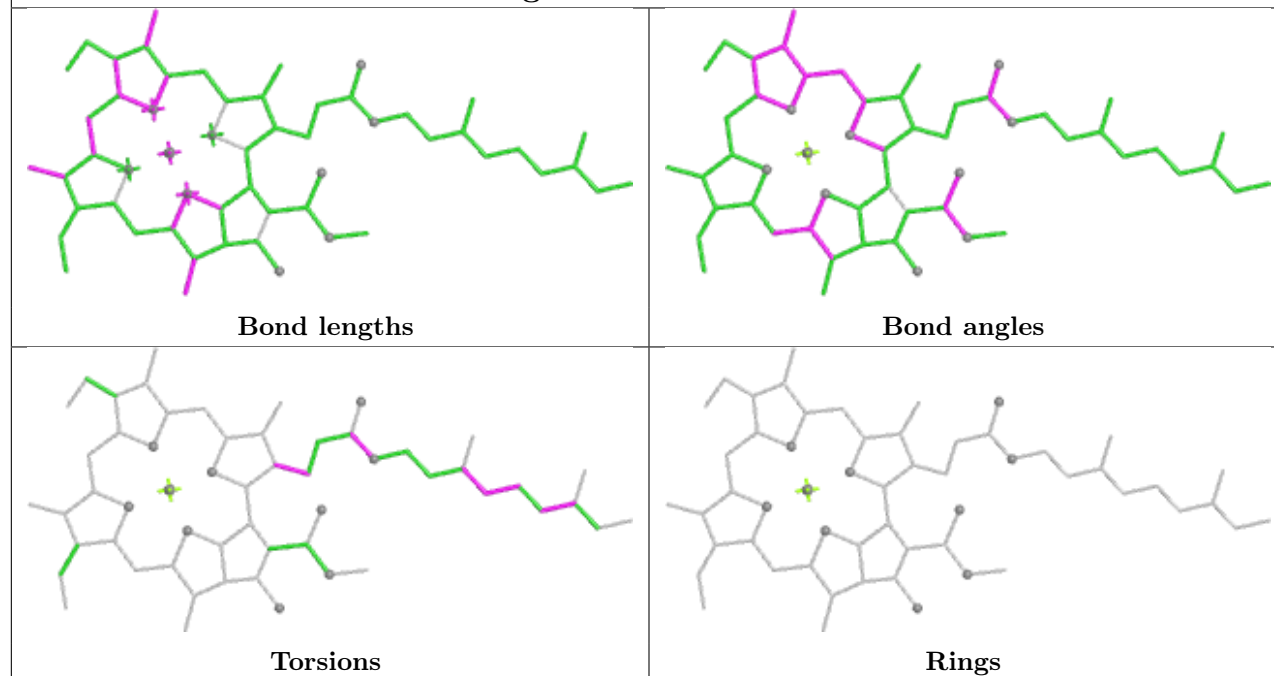
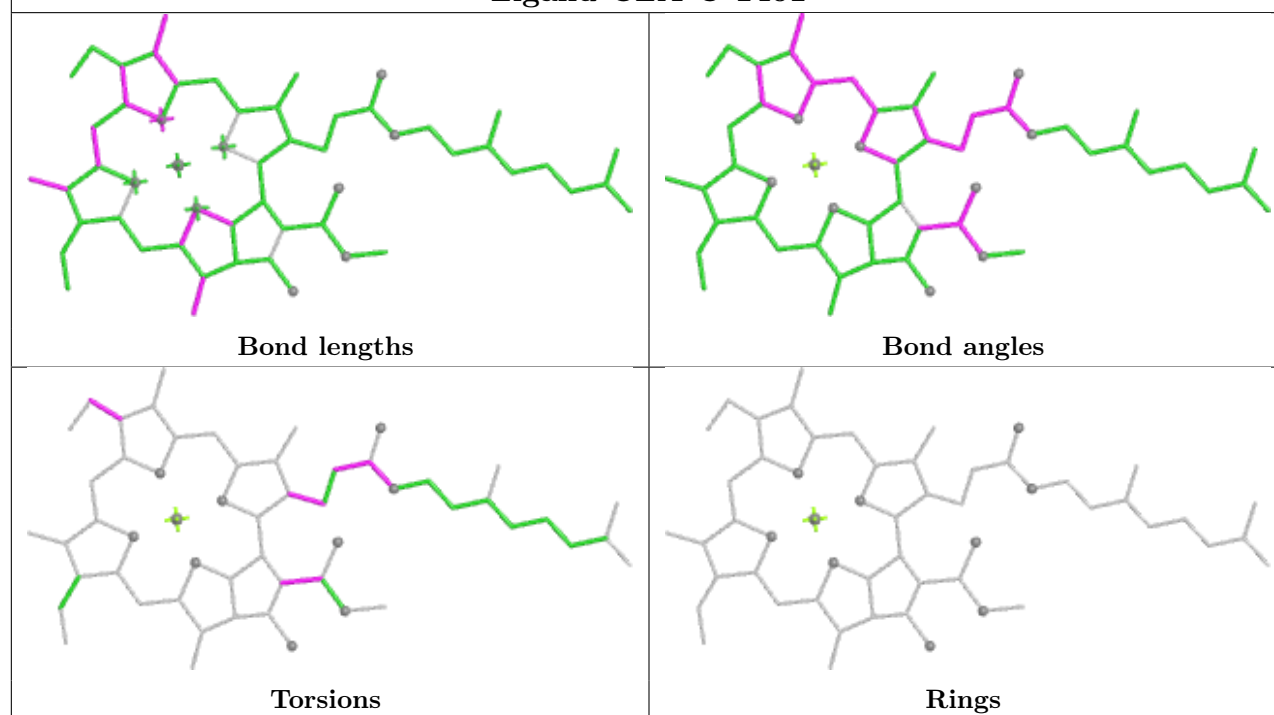
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Bond lengths	Bond angles
	
Torsions	Rings



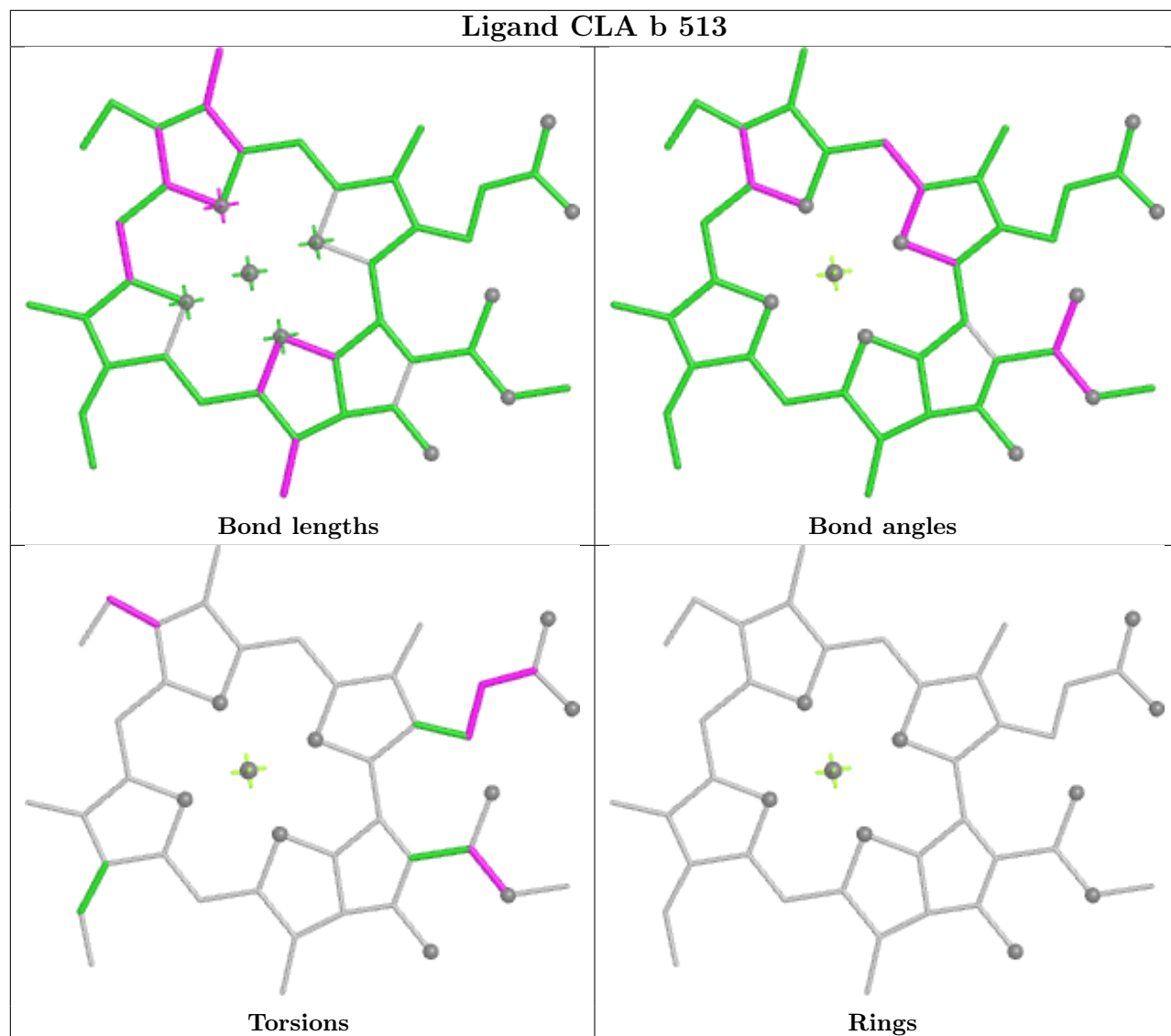
Ligand CLA d 502

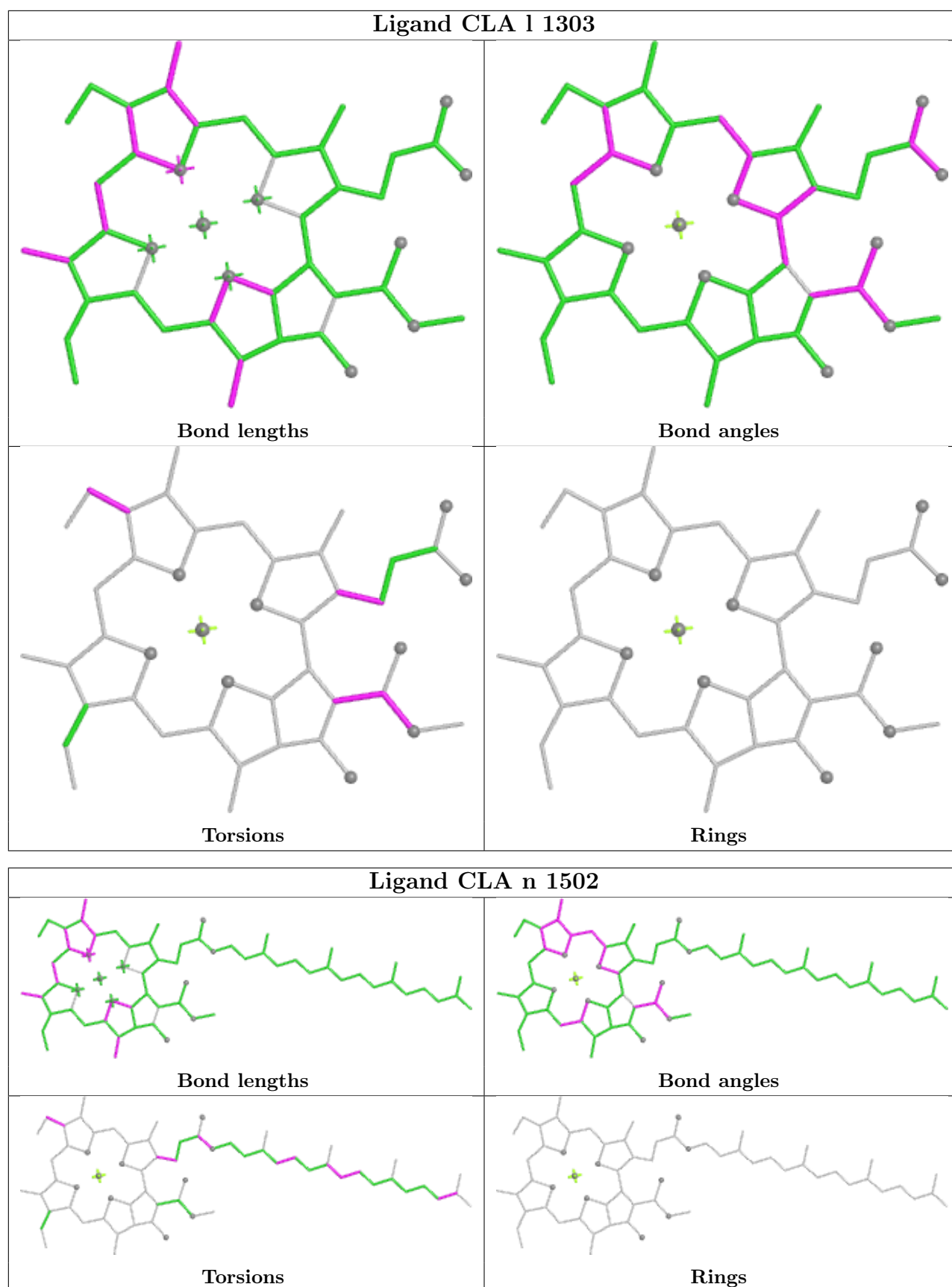


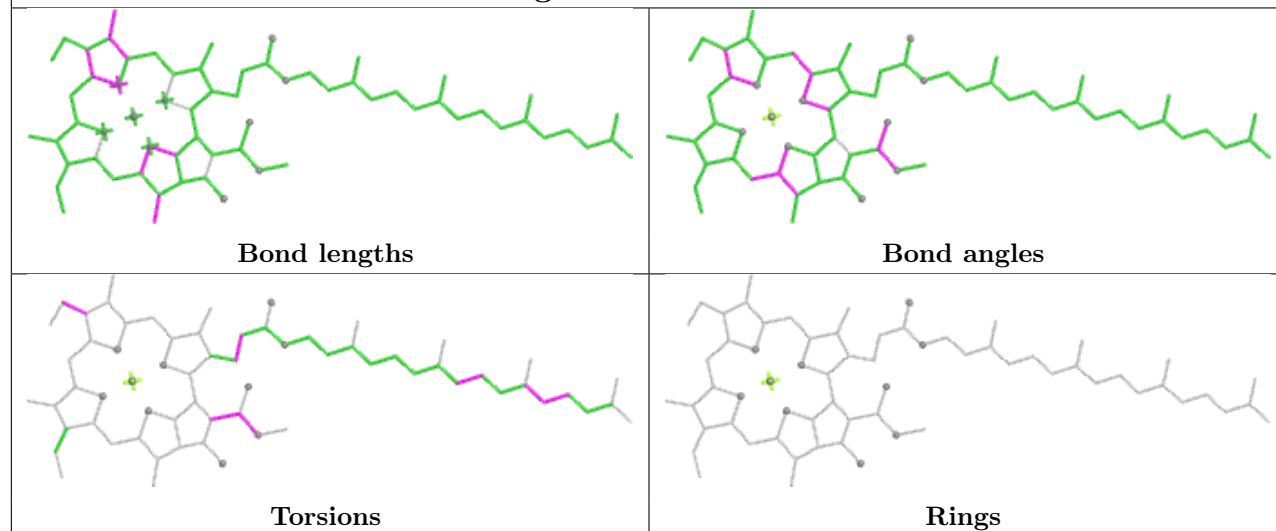
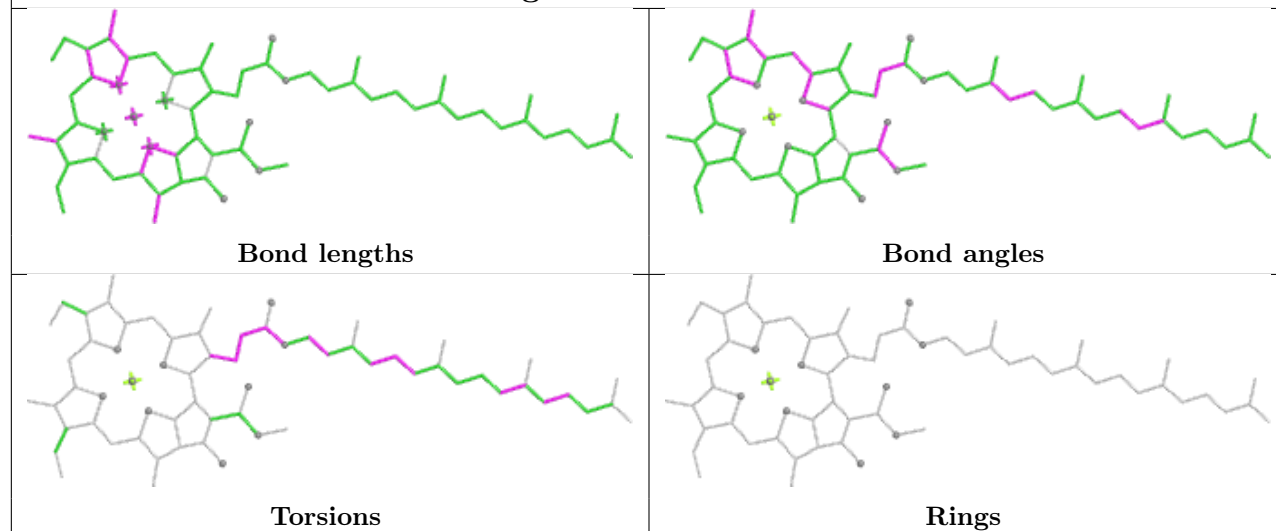
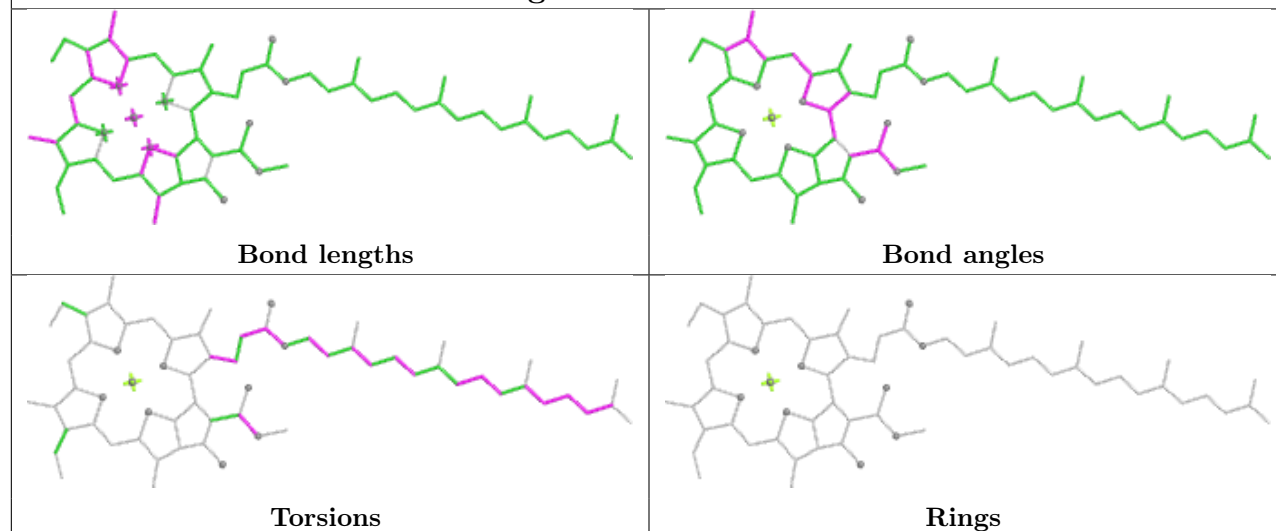


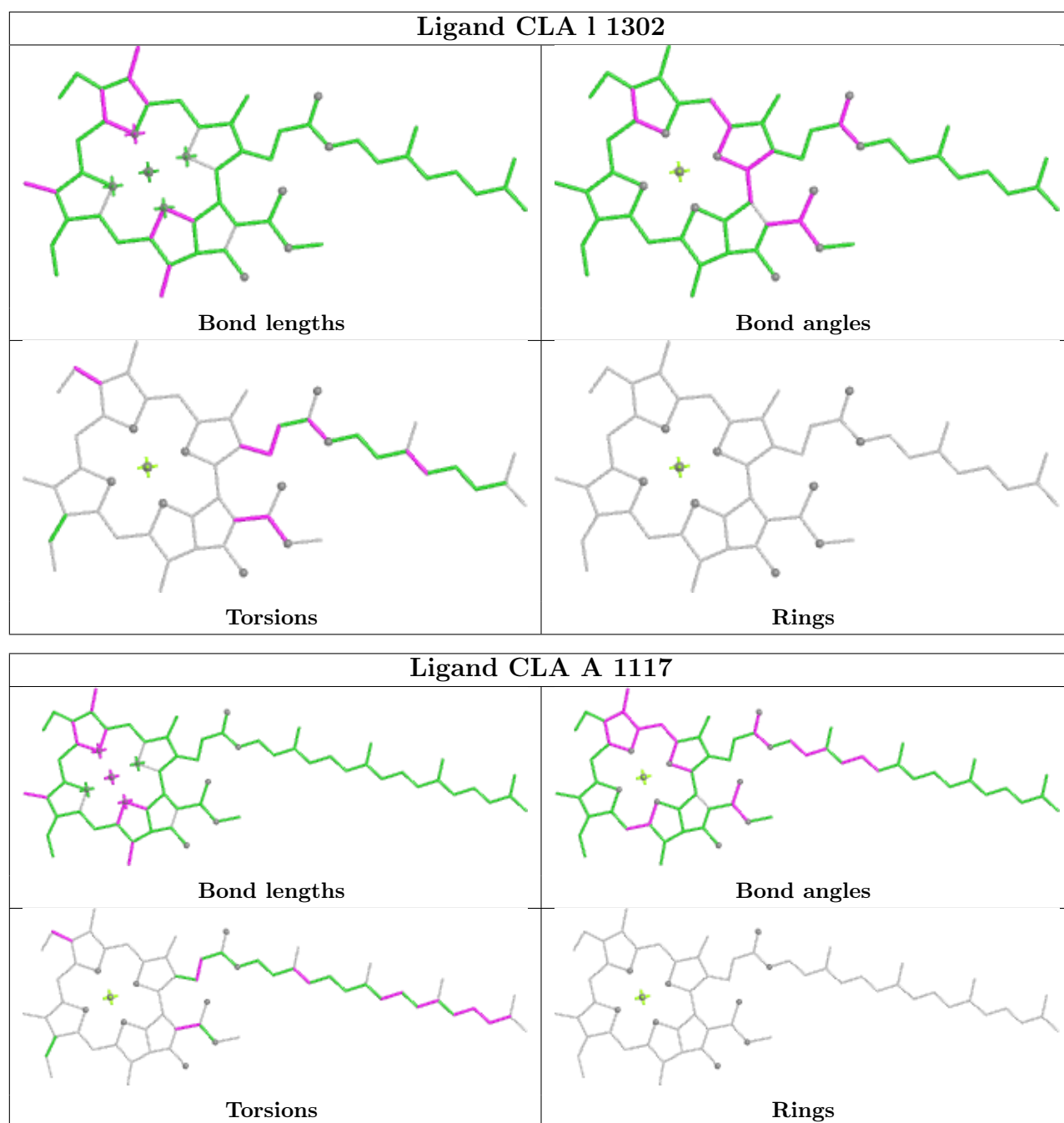
Ligand CLA A 1130**Ligand CLA U 1401**

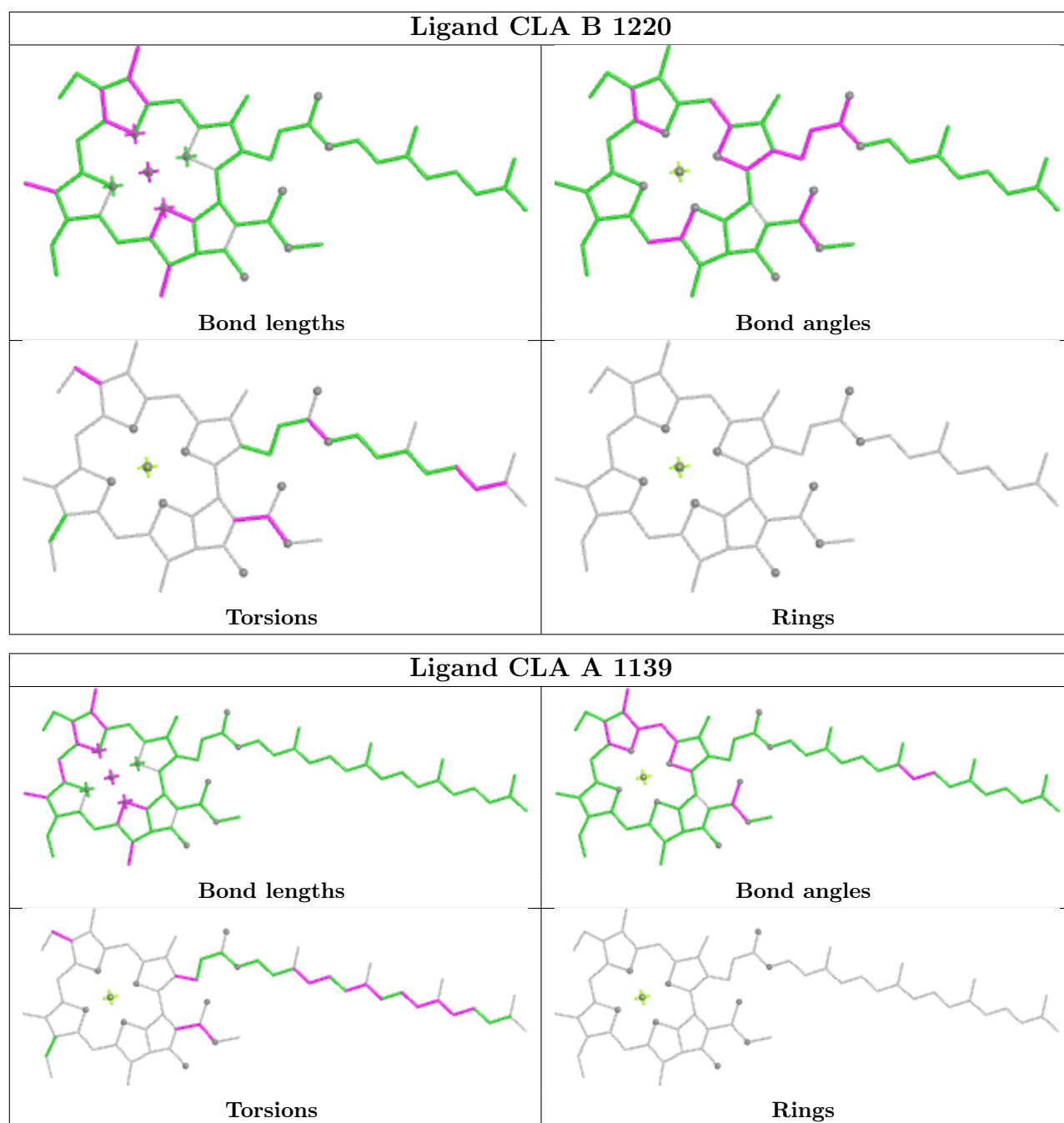
Ligand CLA b 513

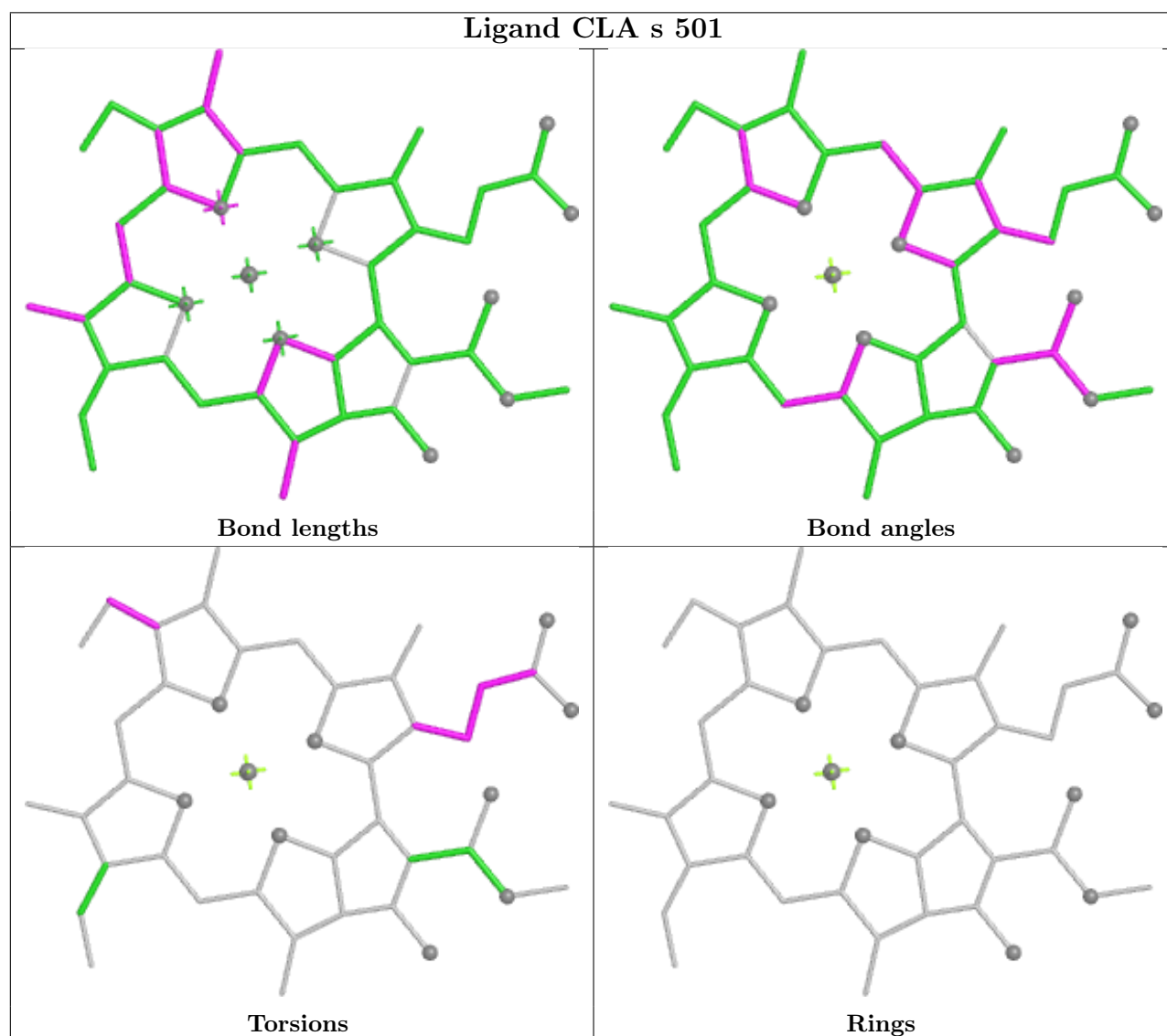
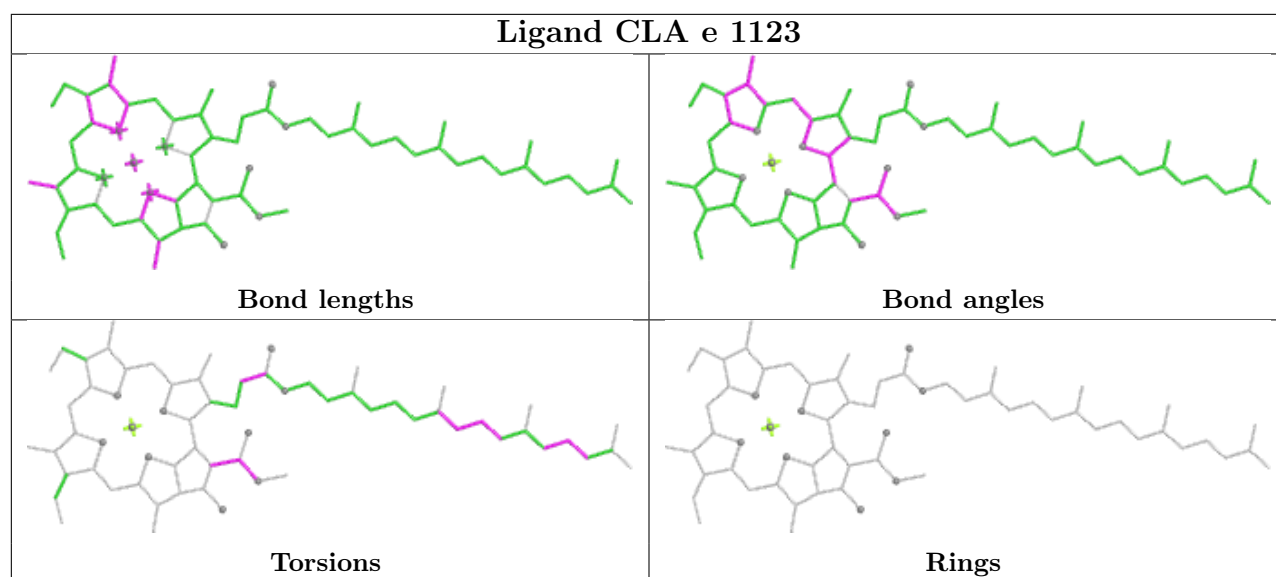


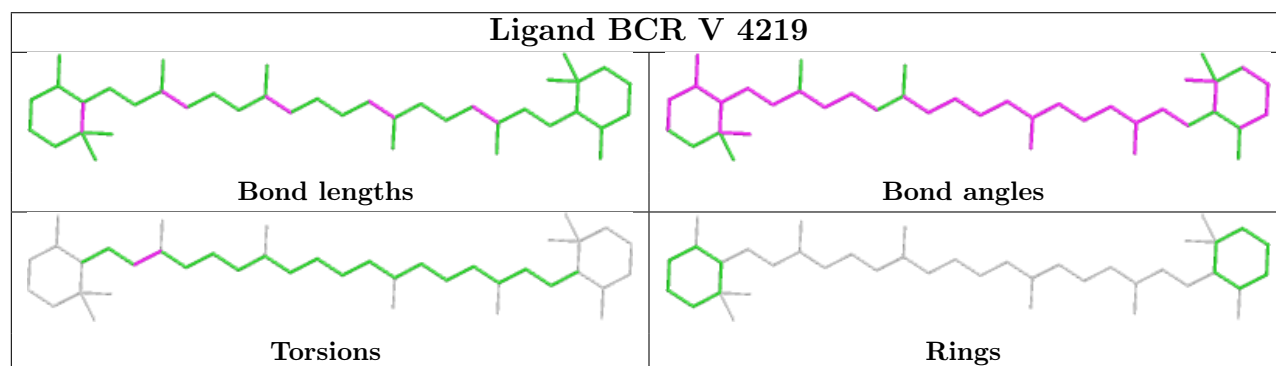
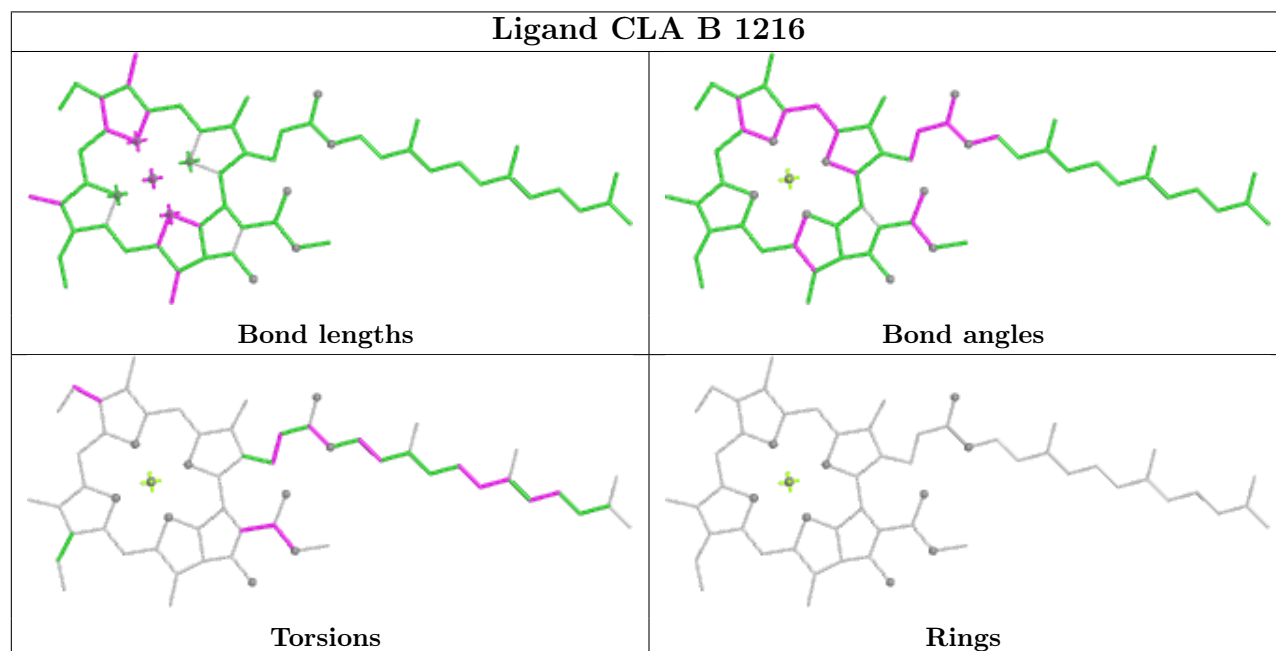
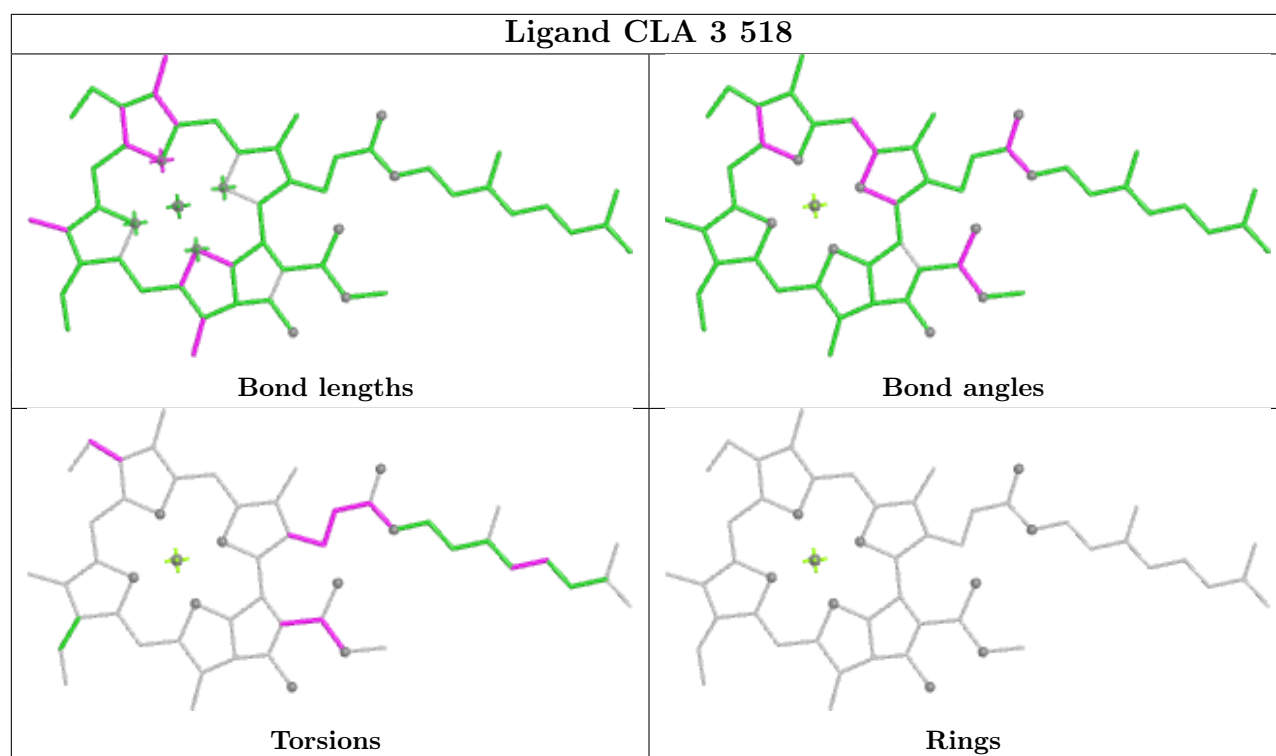


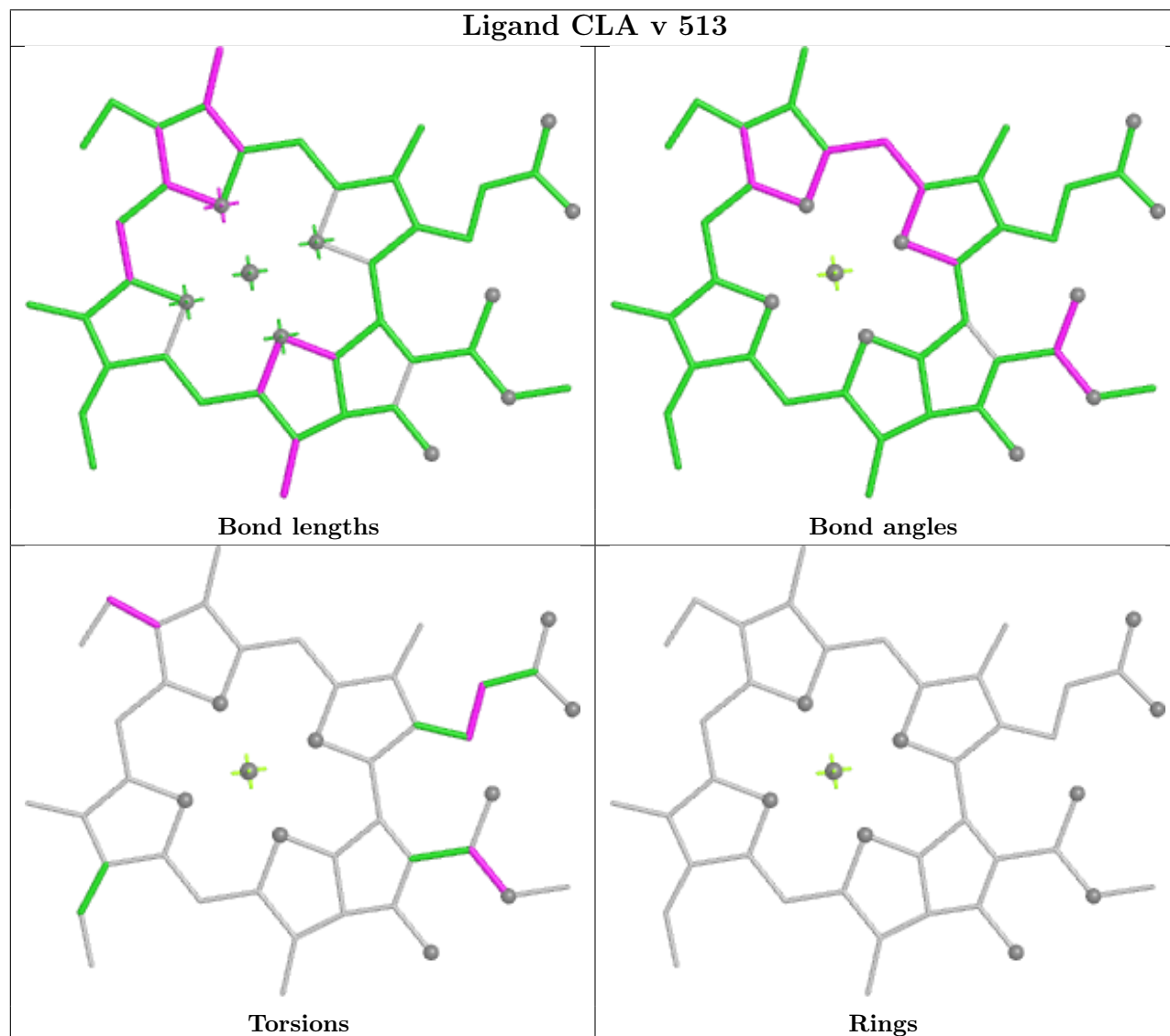
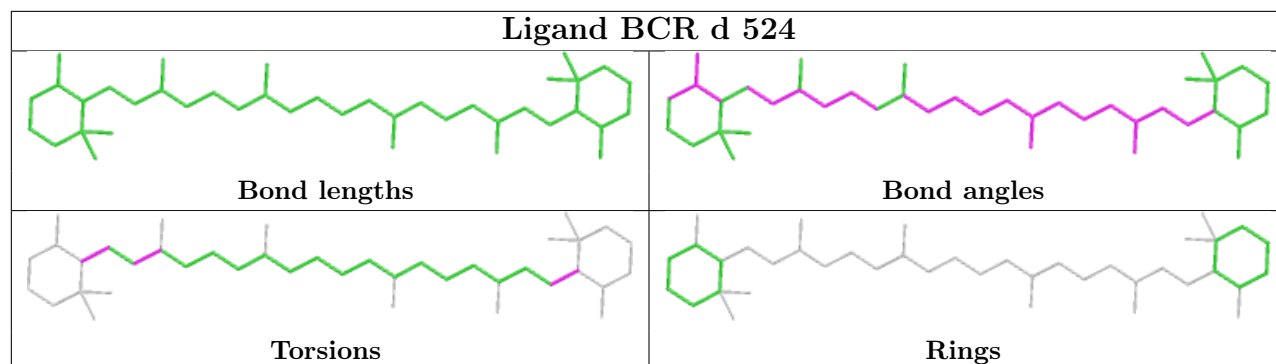
Ligand CLA Z 503**Ligand CLA G 1125****Ligand CLA e 1126**



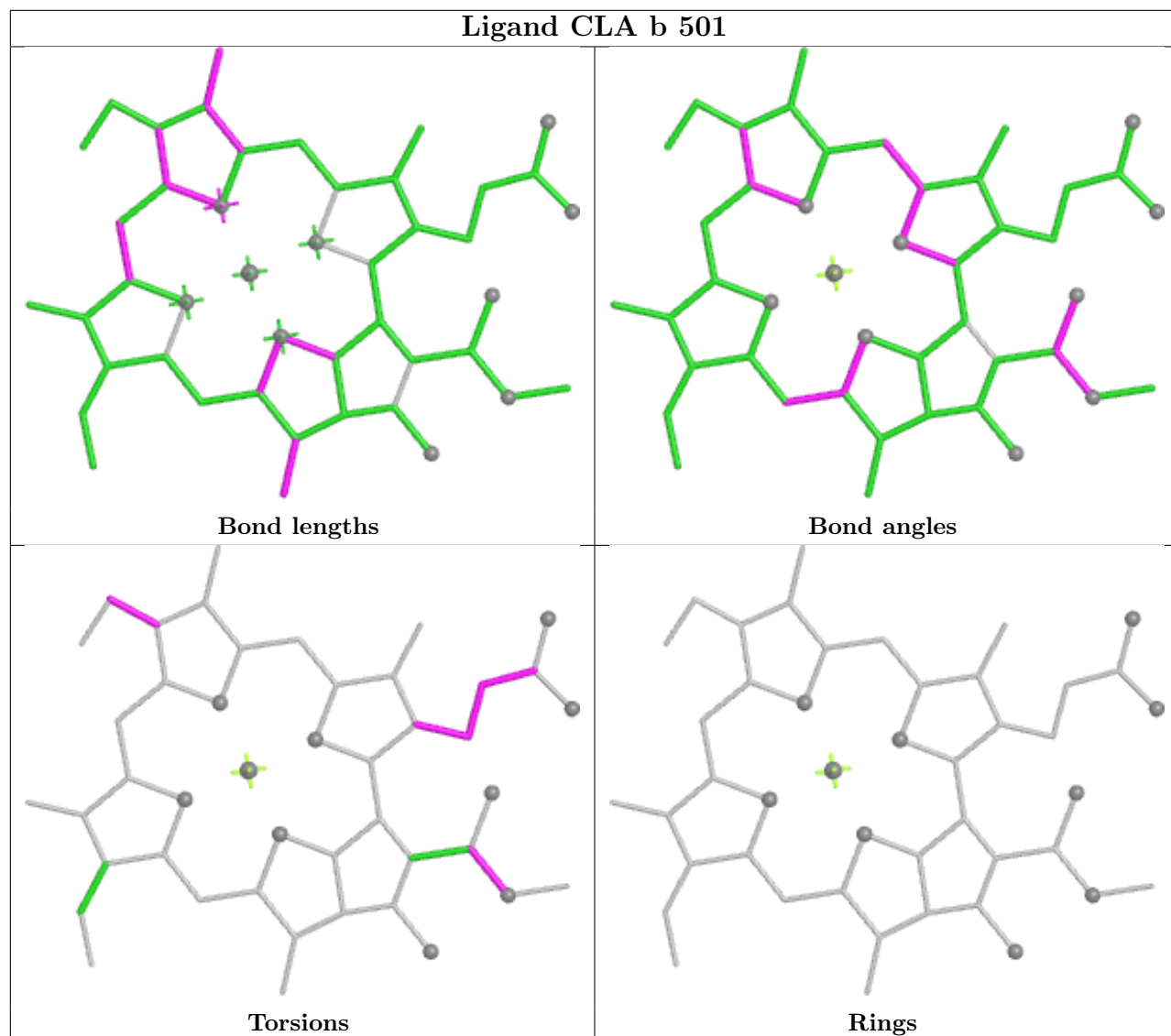




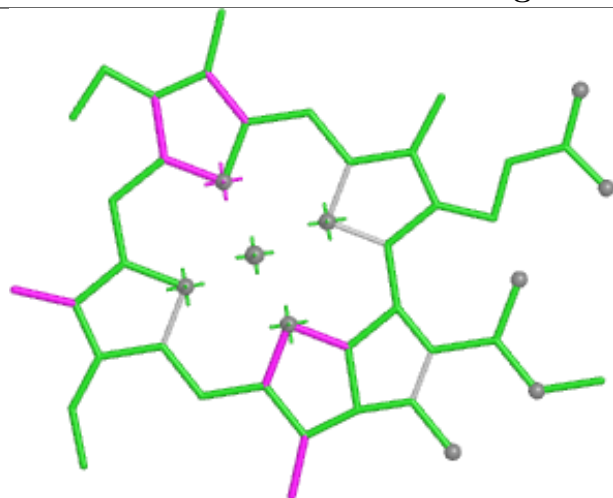




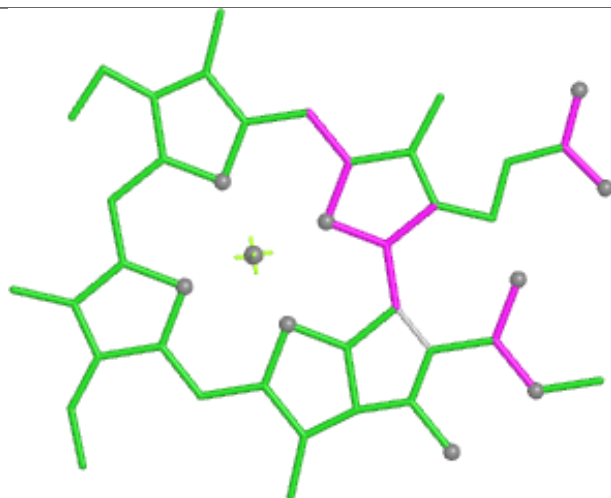
Ligand CLA b 501



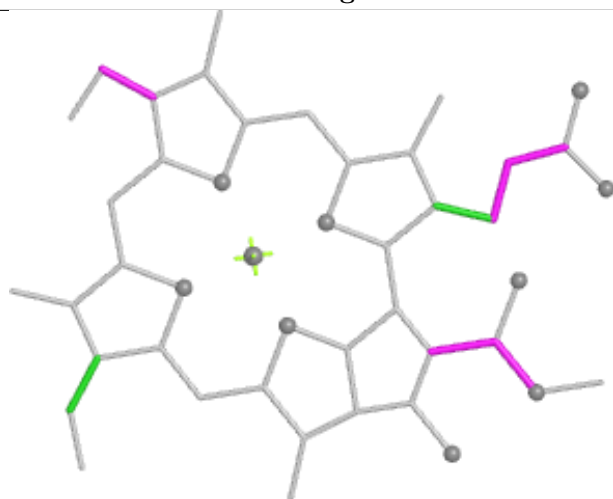
Ligand CLA Y 507



Bond lengths



Bond angles

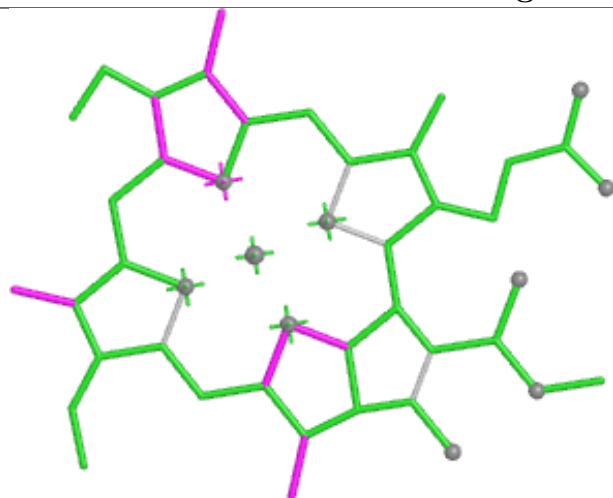


Torsions

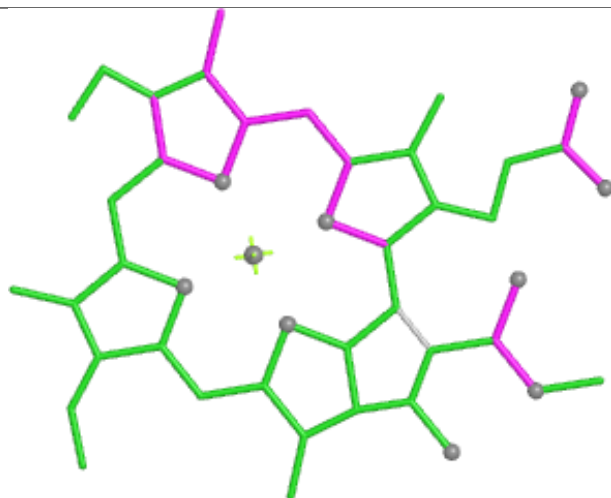


Rings

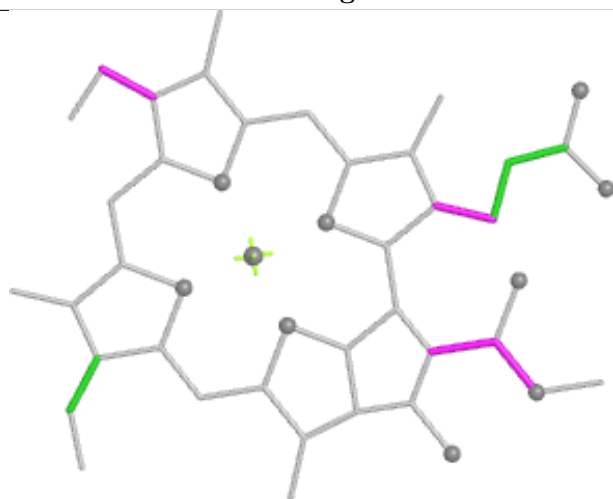
Ligand CLA Z 511



Bond lengths



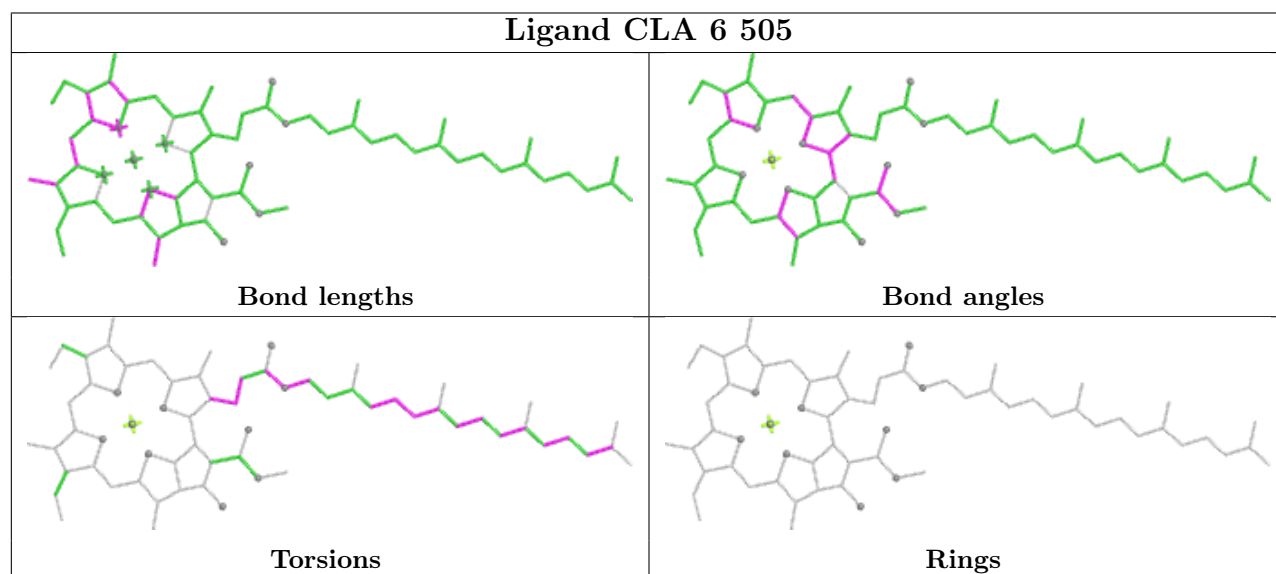
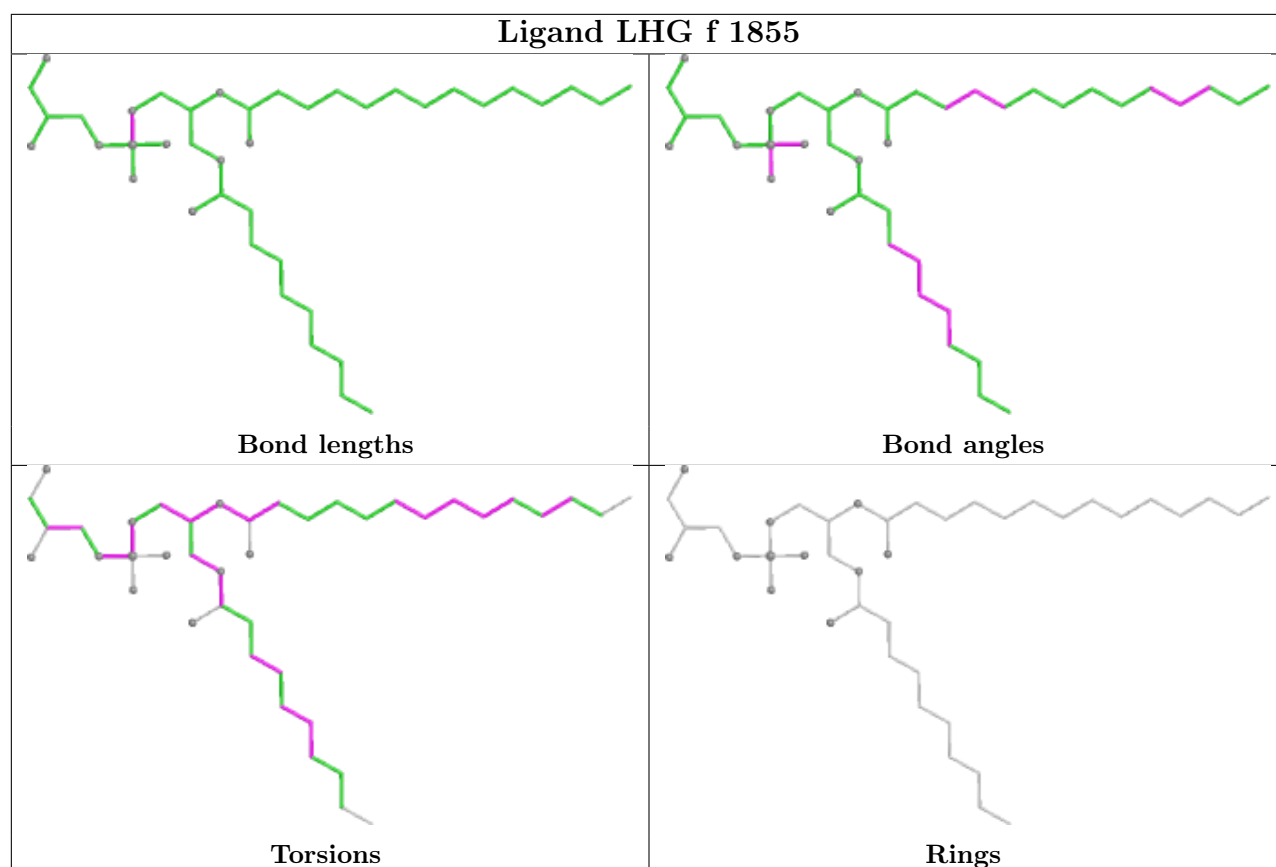
Bond angles



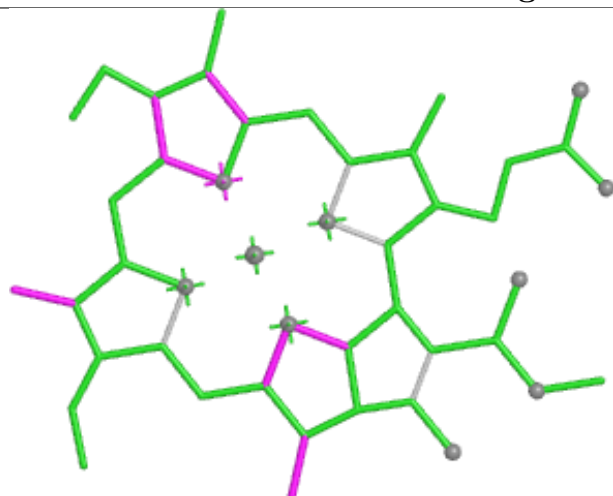
Torsions



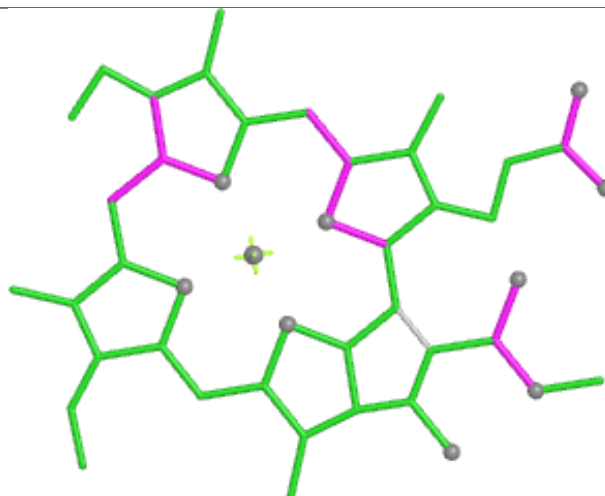
Rings



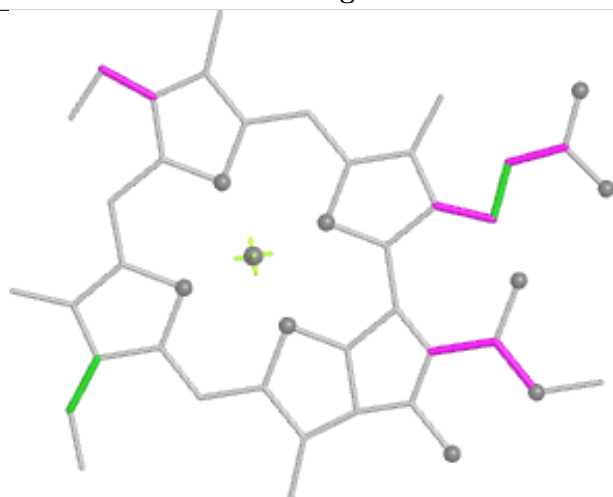
Ligand CLA 6 517



Bond lengths



Bond angles

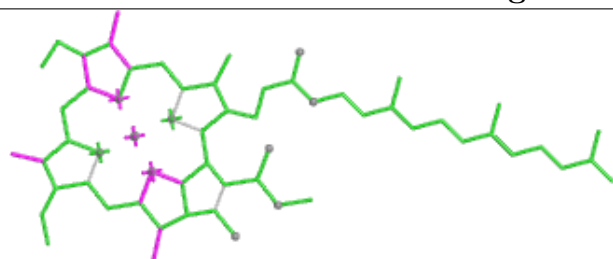


Torsions

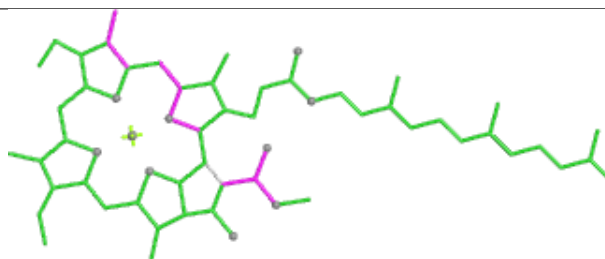


Rings

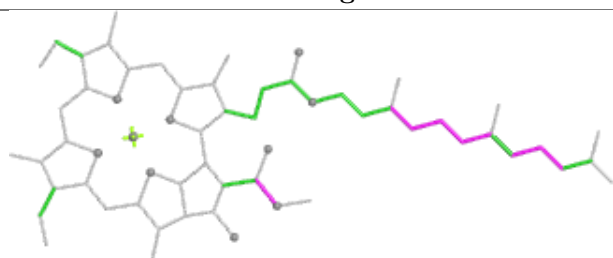
Ligand CLA n 1503



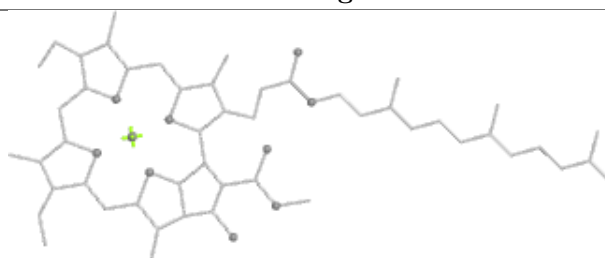
Bond lengths



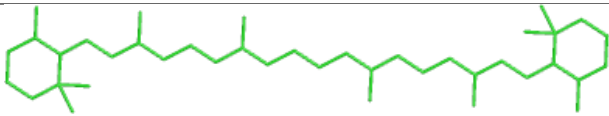
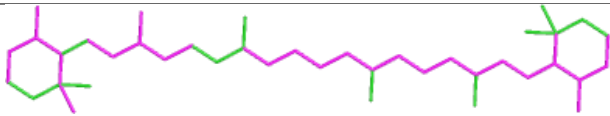
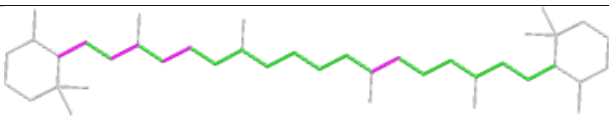
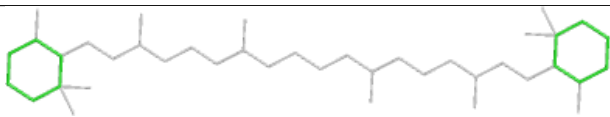
Bond angles

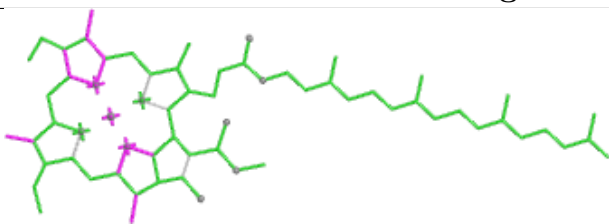
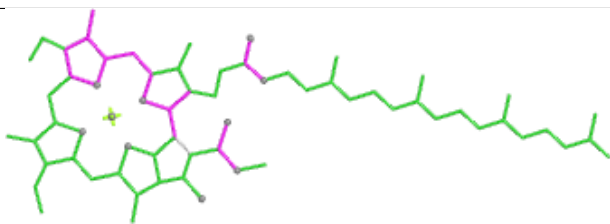
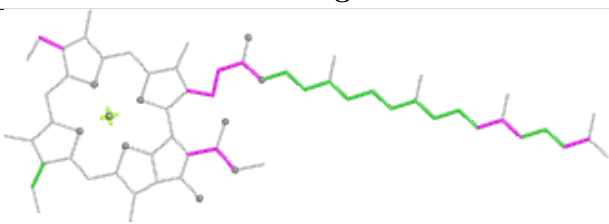
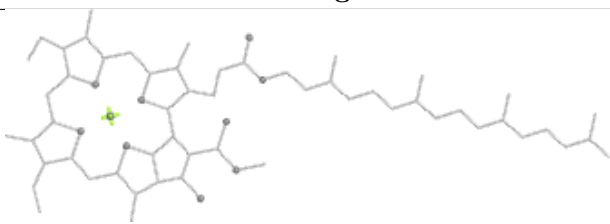


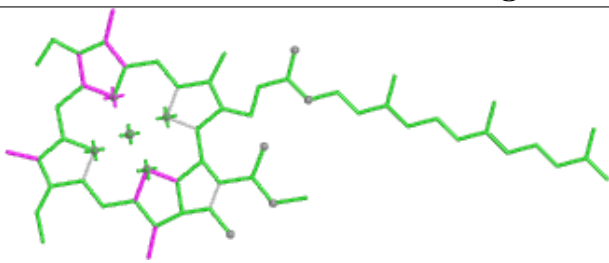
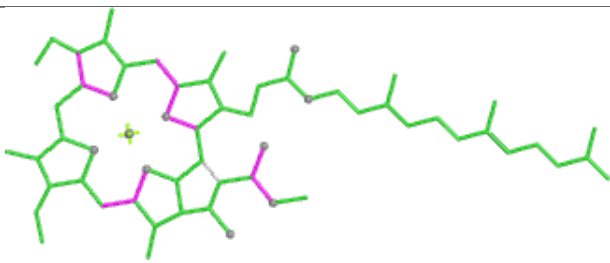
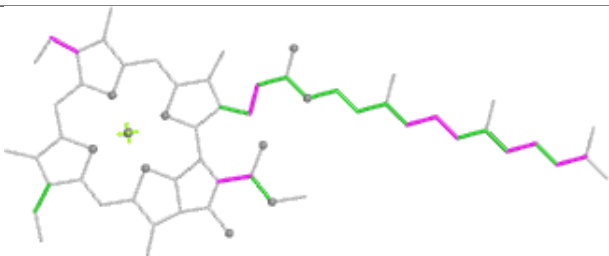
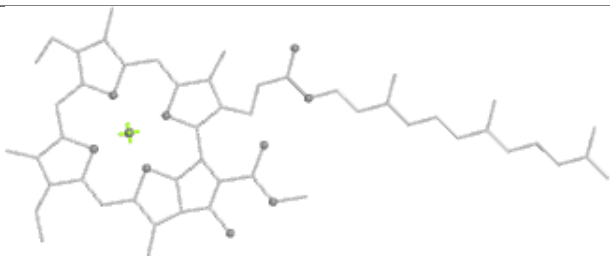
Torsions

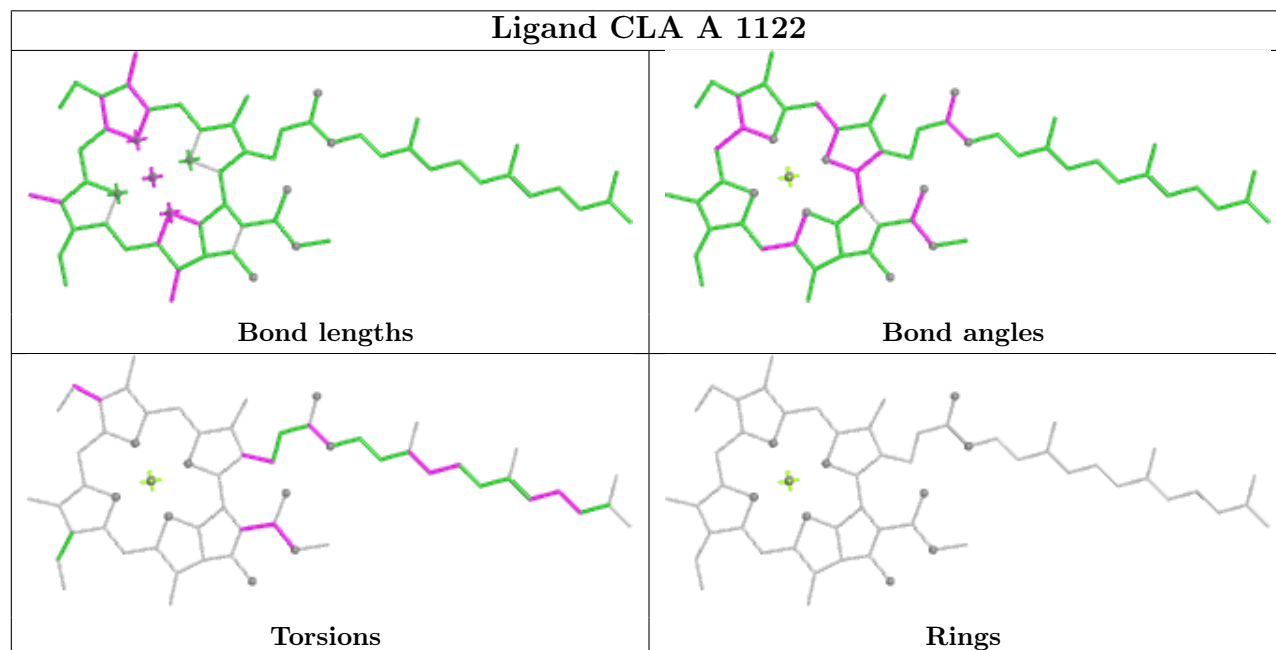
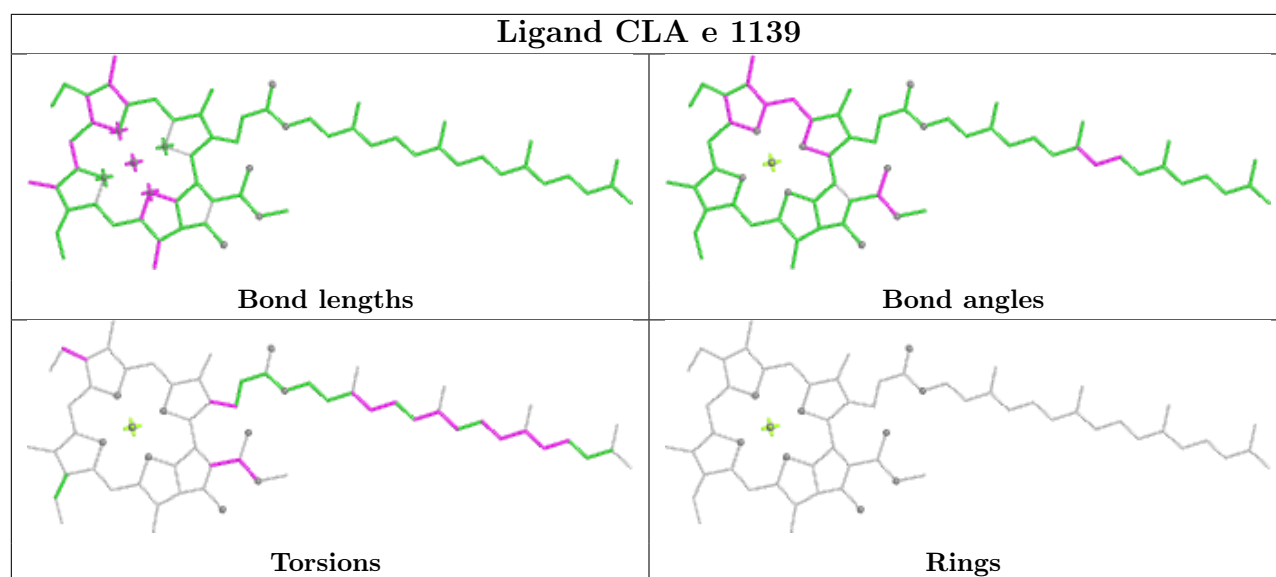


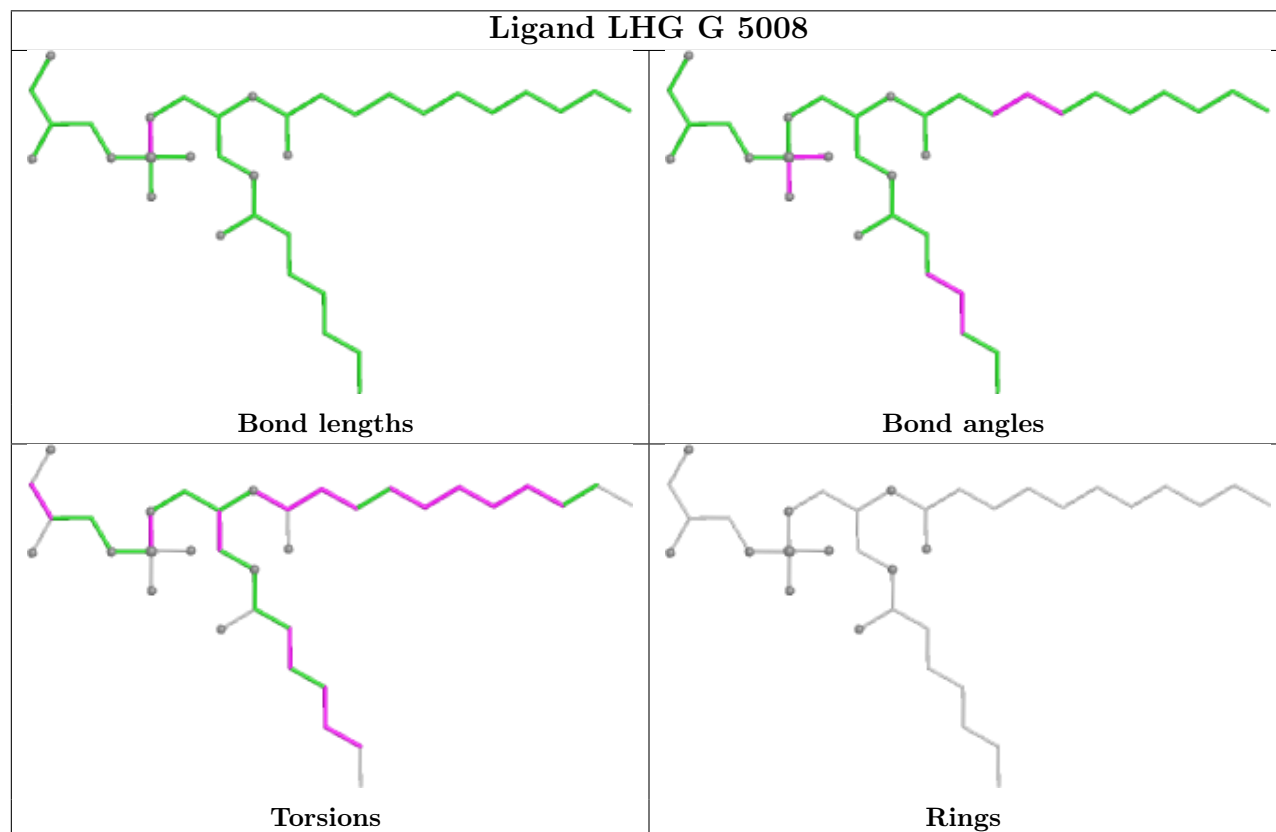
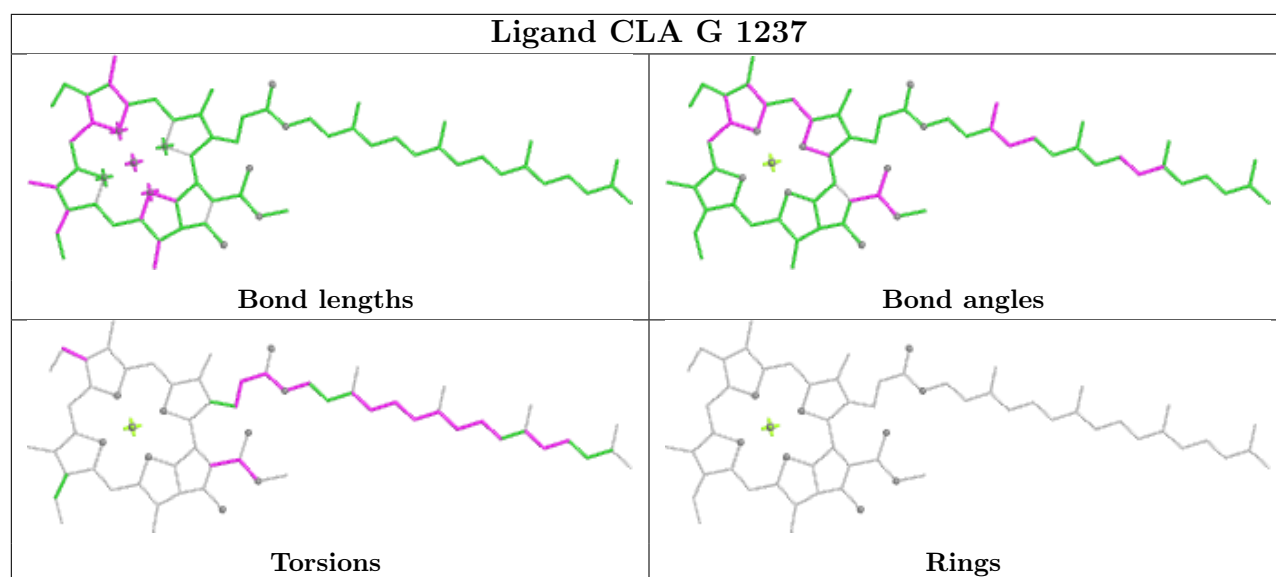
Rings

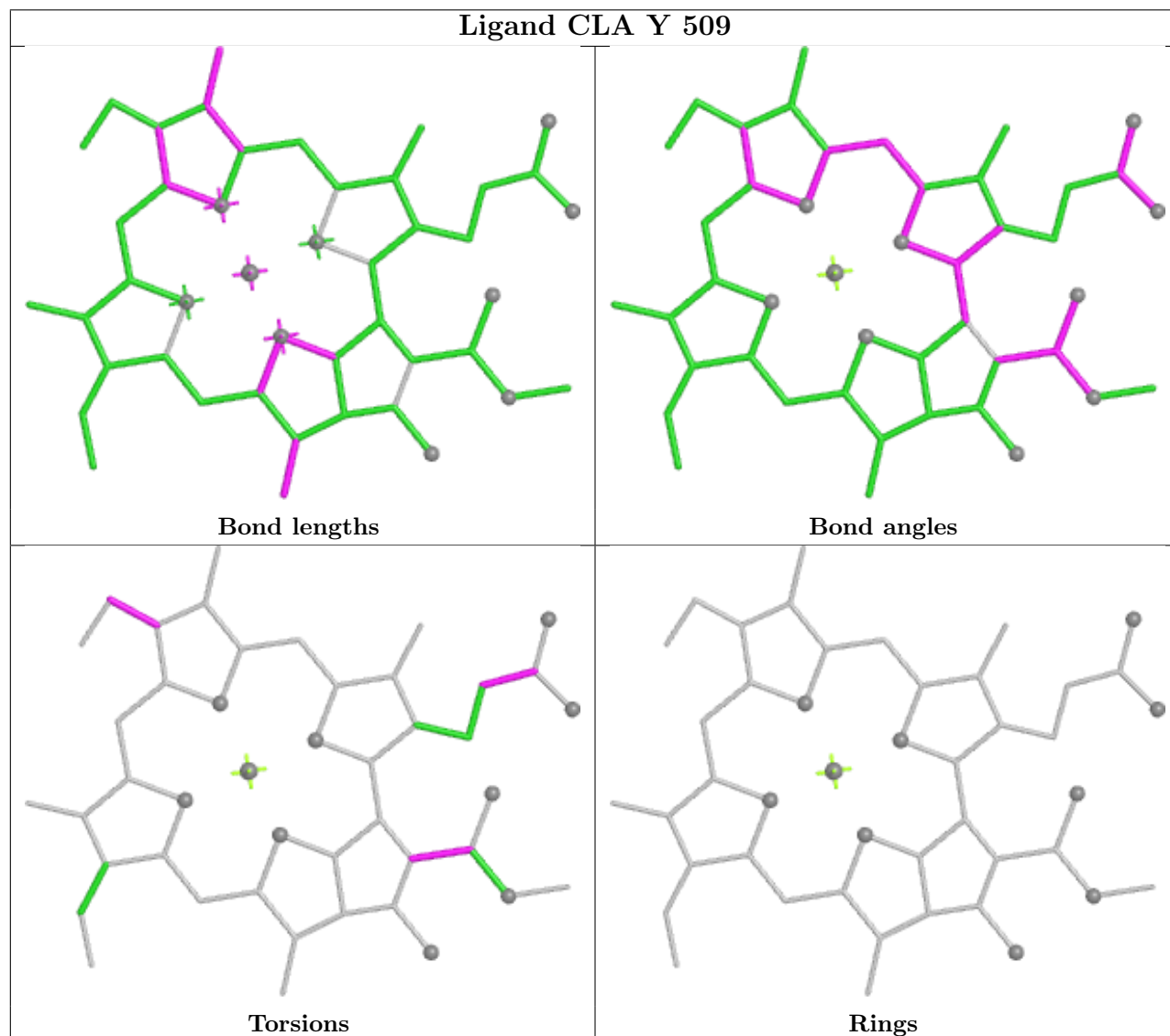
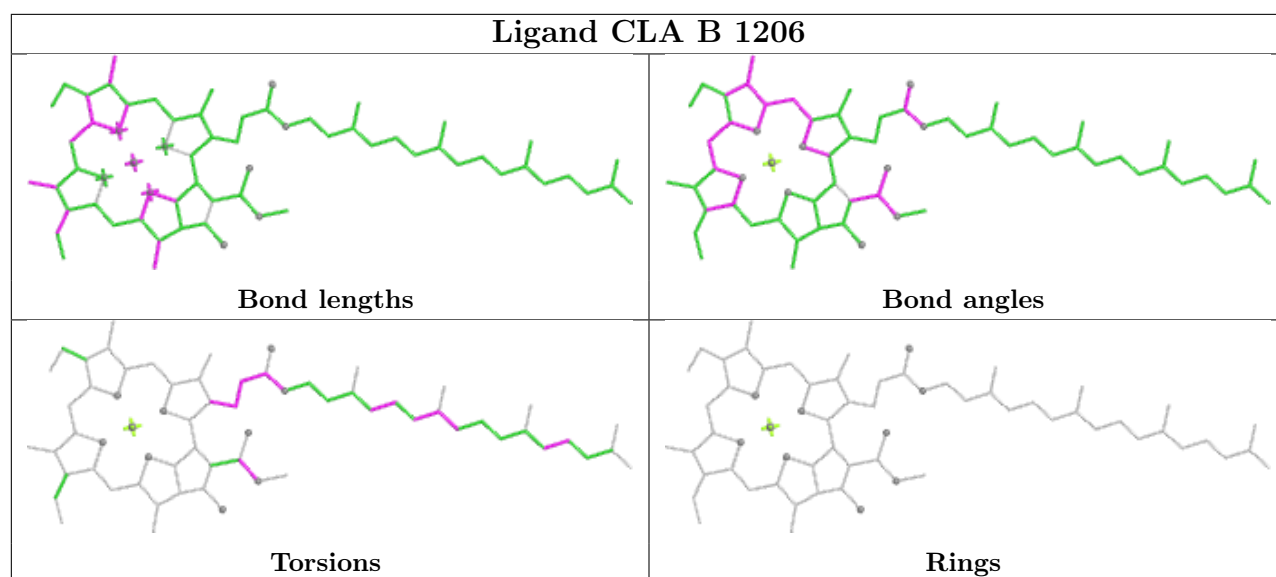
Ligand BCR 5 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

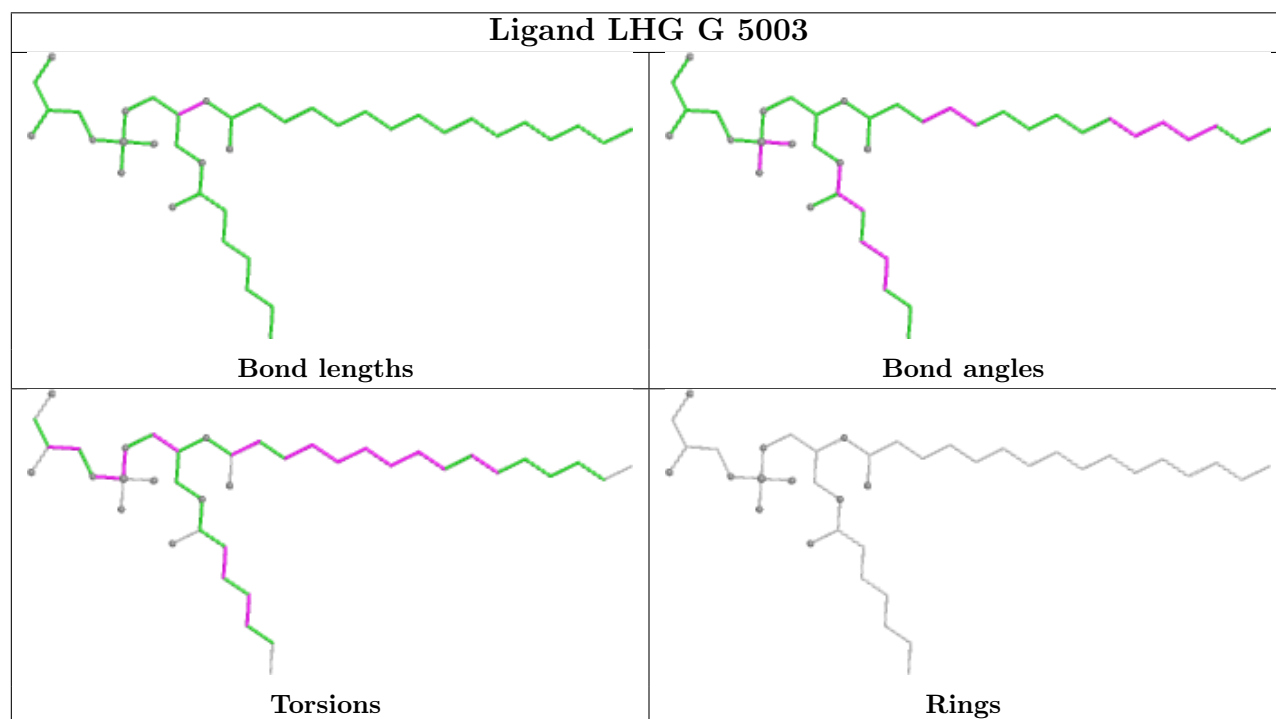
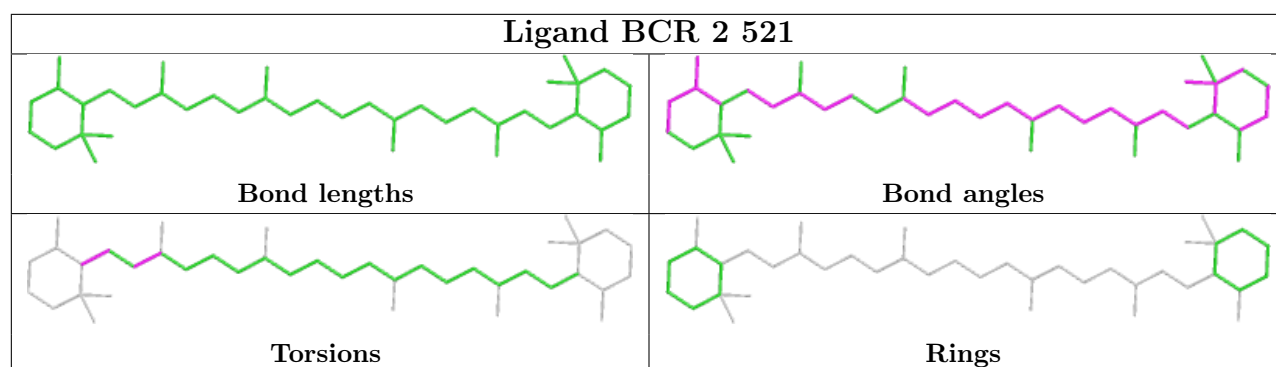
Ligand CLA A 1111	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1218	
	
Bond lengths	Bond angles
	
Torsions	Rings

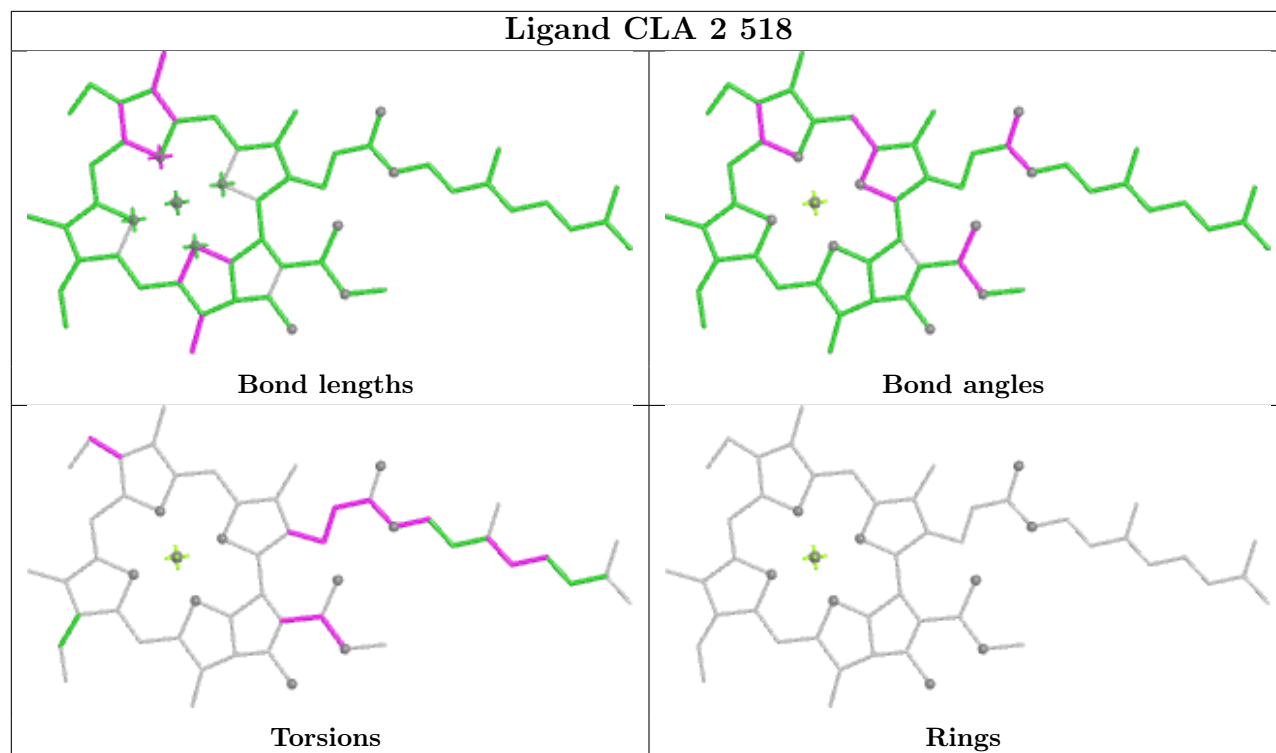




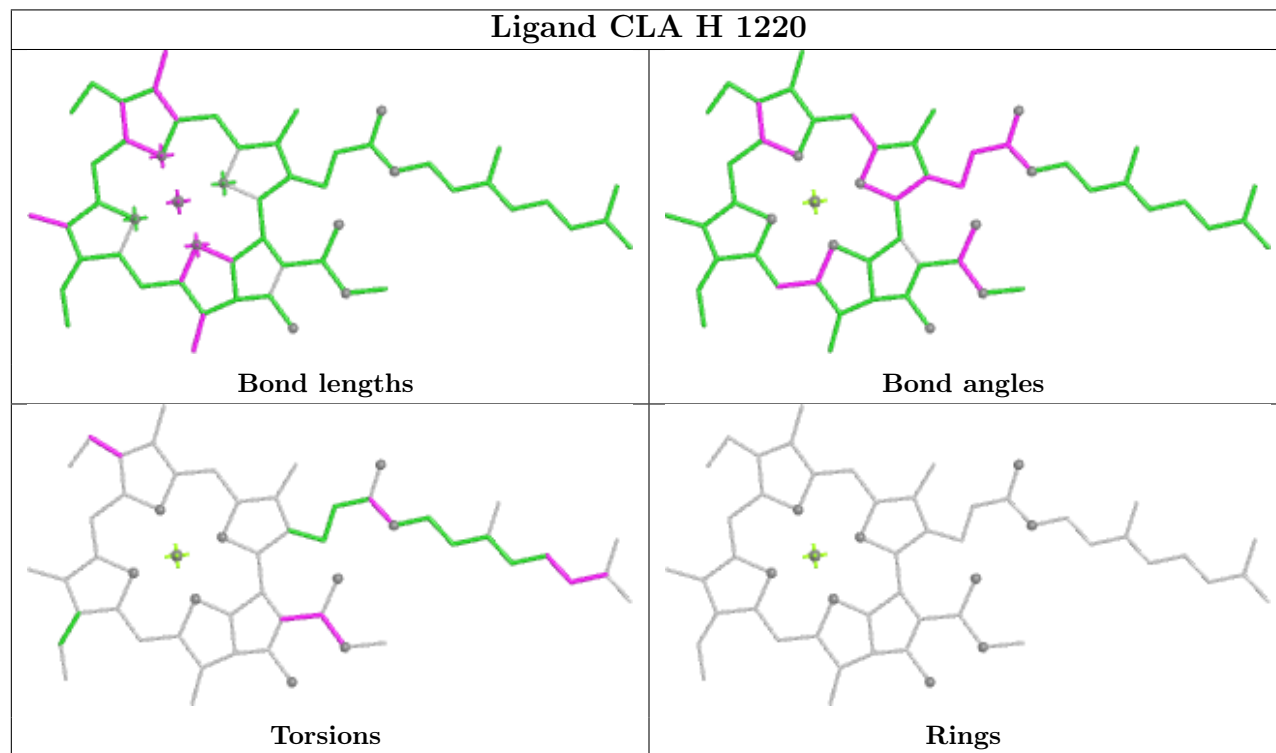


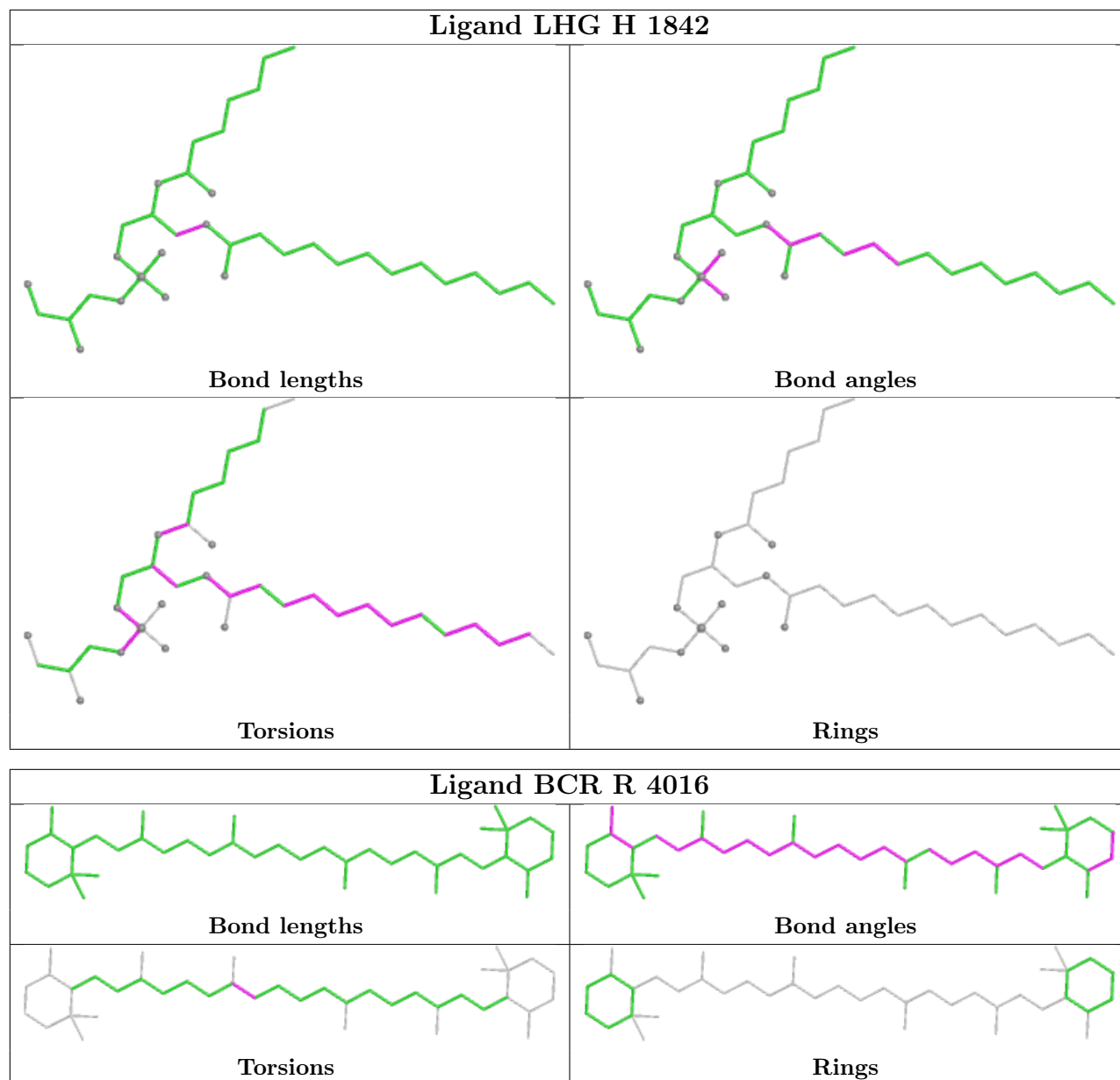


Ligand CLA 2 518

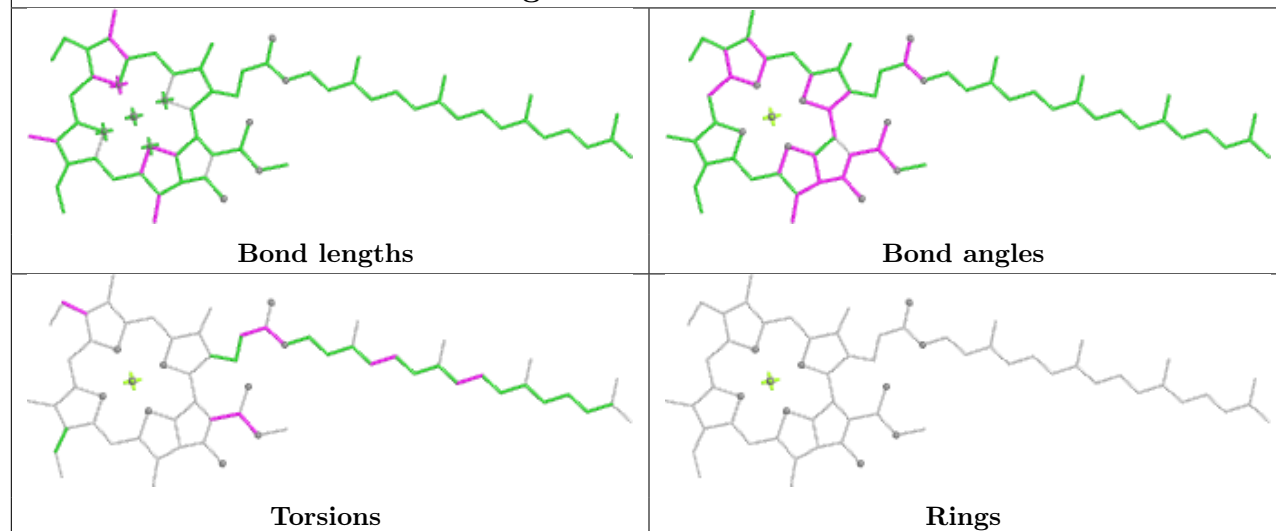


Ligand CLA H 1220

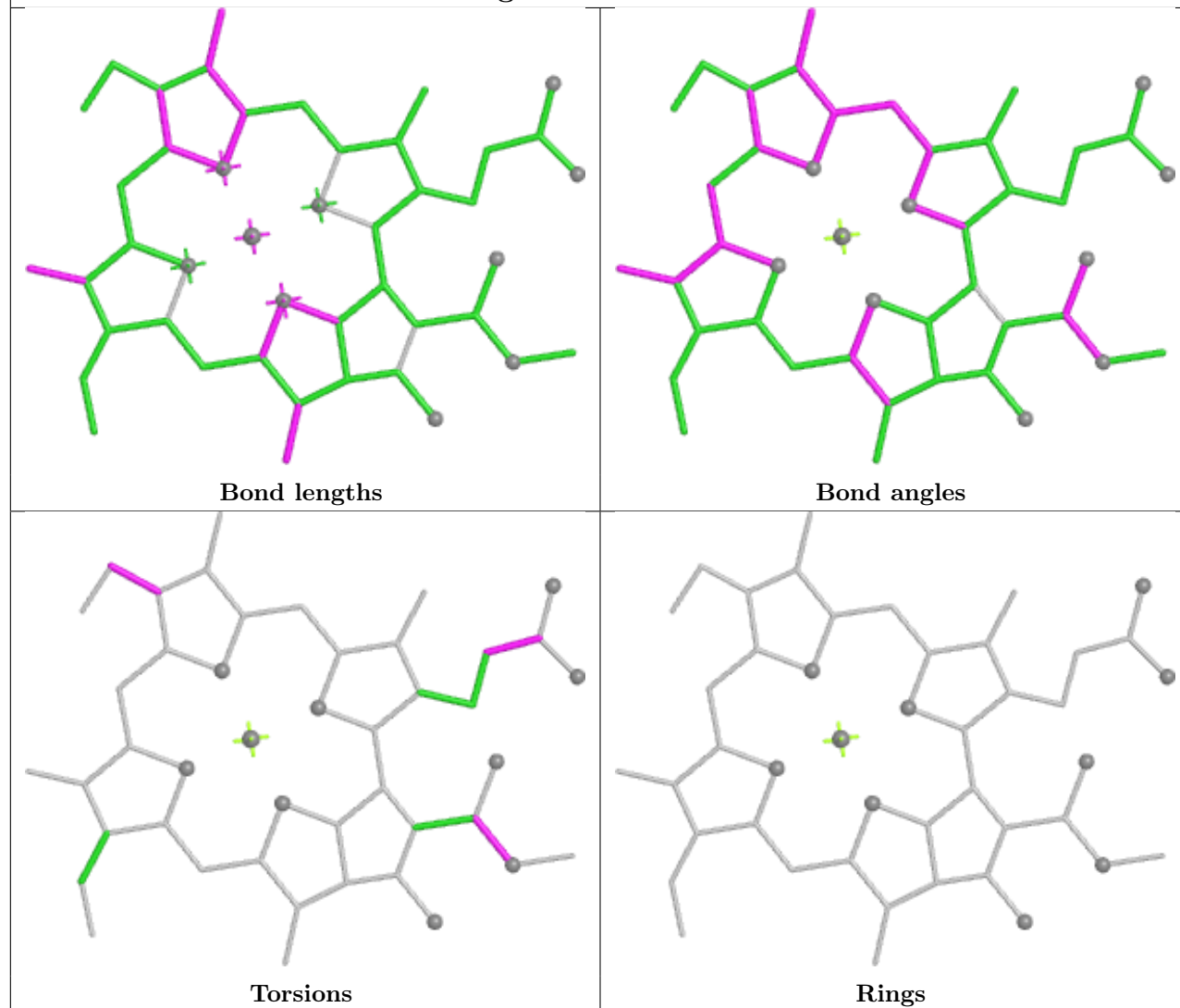




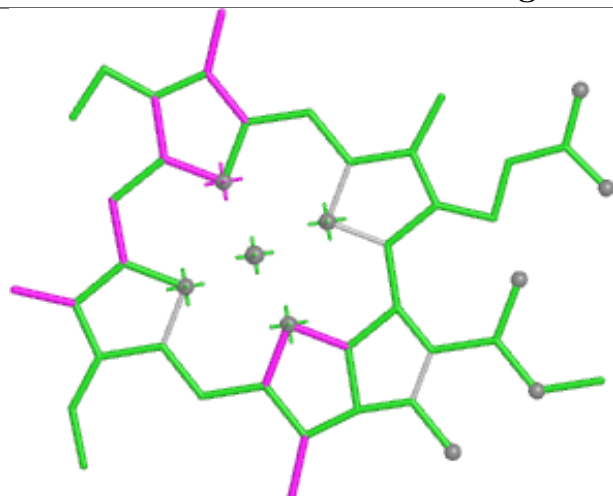
Ligand CLA A 1011



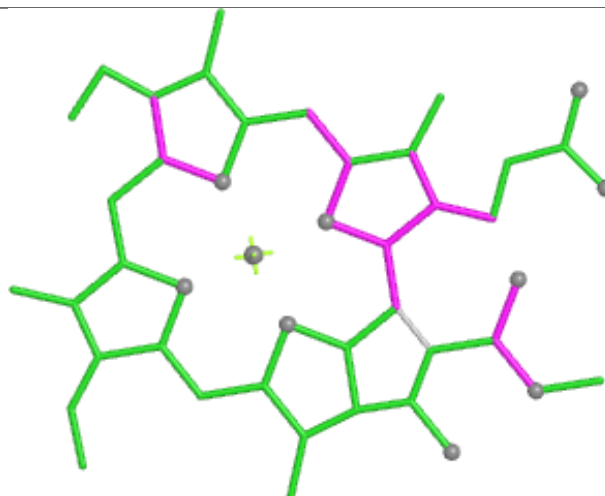
Ligand CLA t 508



Ligand CLA 5 501



Bond lengths



Bond angles

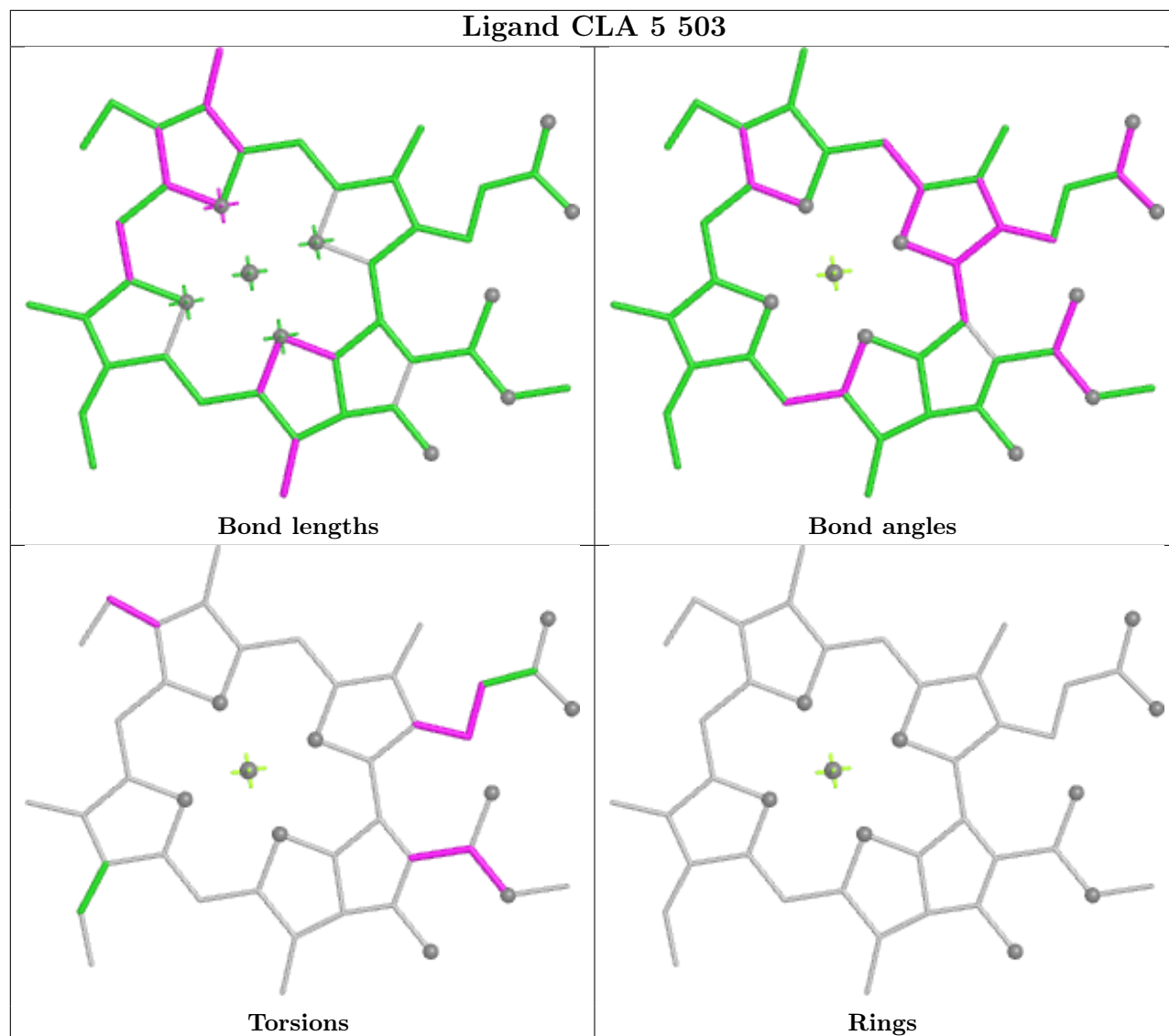


Torsions

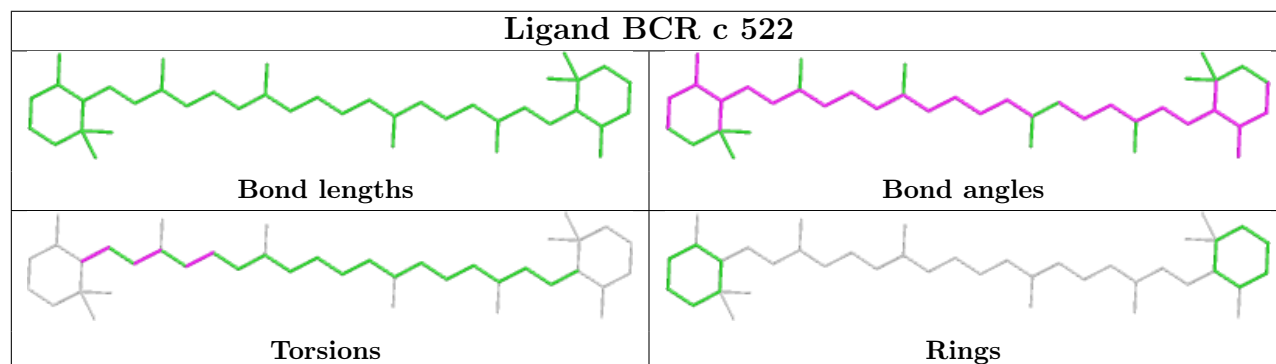


Rings

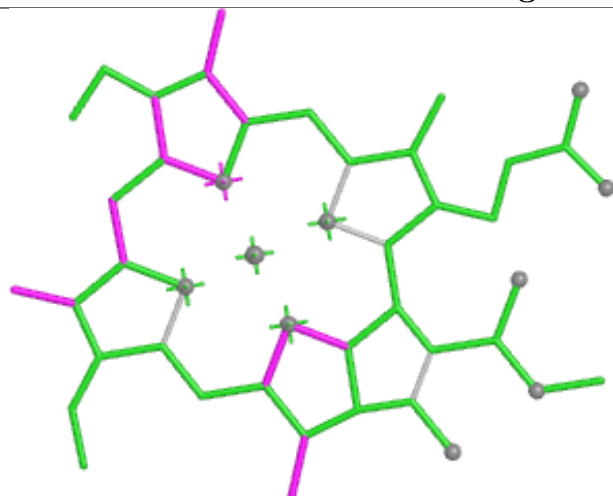
Ligand CLA 5 503



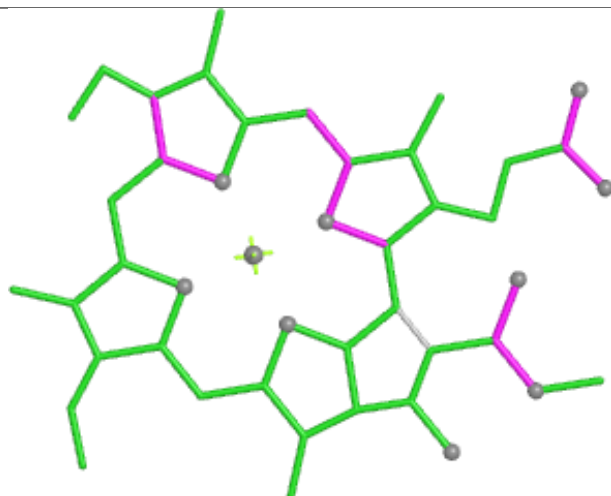
Ligand BCR c 522



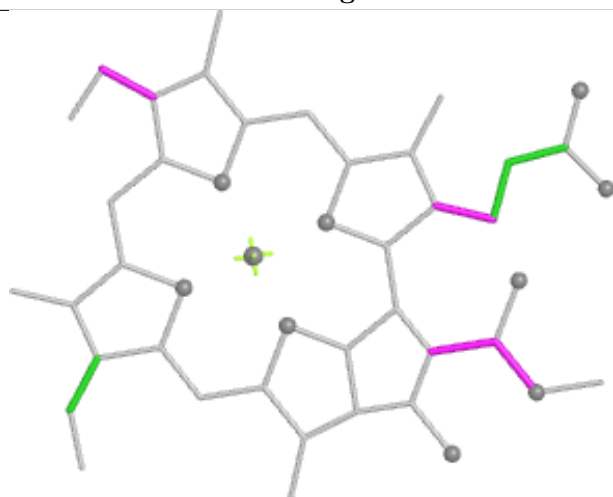
Ligand CLA 5 506



Bond lengths



Bond angles

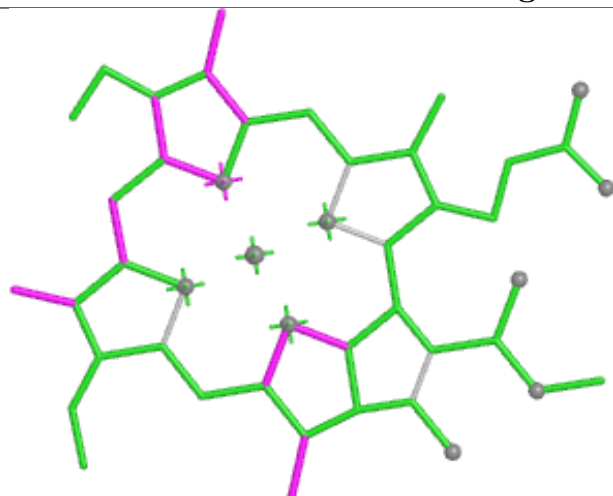


Torsions

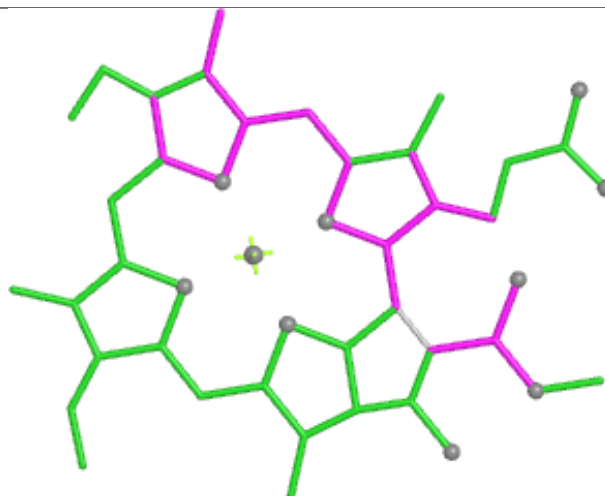


Rings

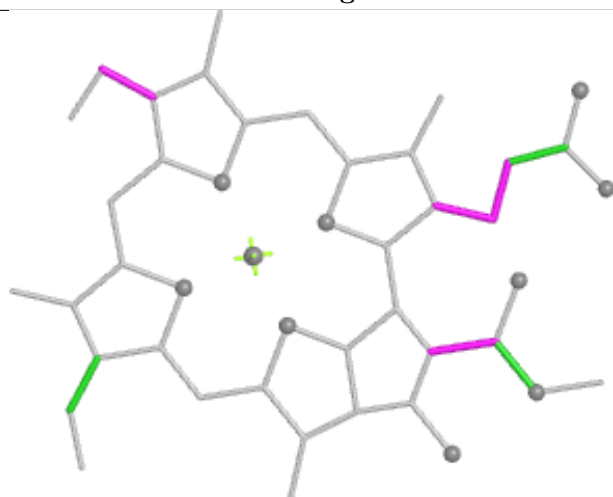
Ligand CLA a 504



Bond lengths



Bond angles

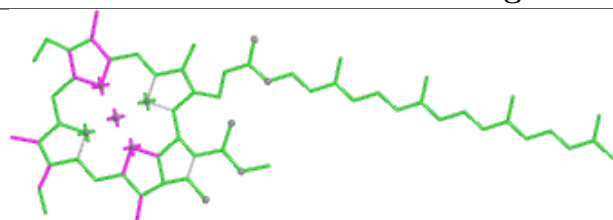


Torsions

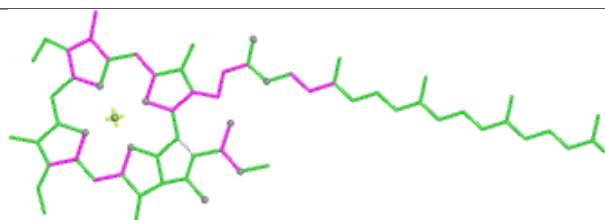


Rings

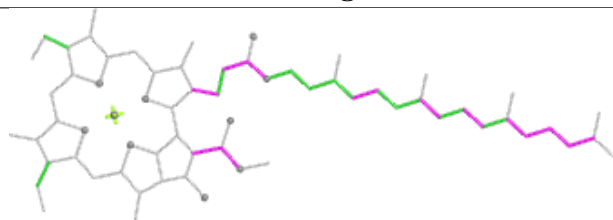
Ligand CLA G 1103



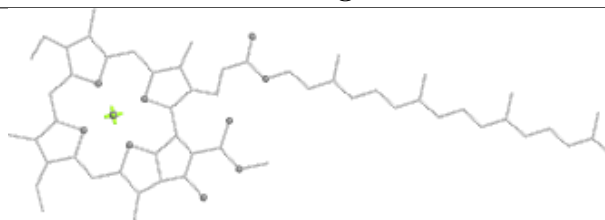
Bond lengths



Bond angles

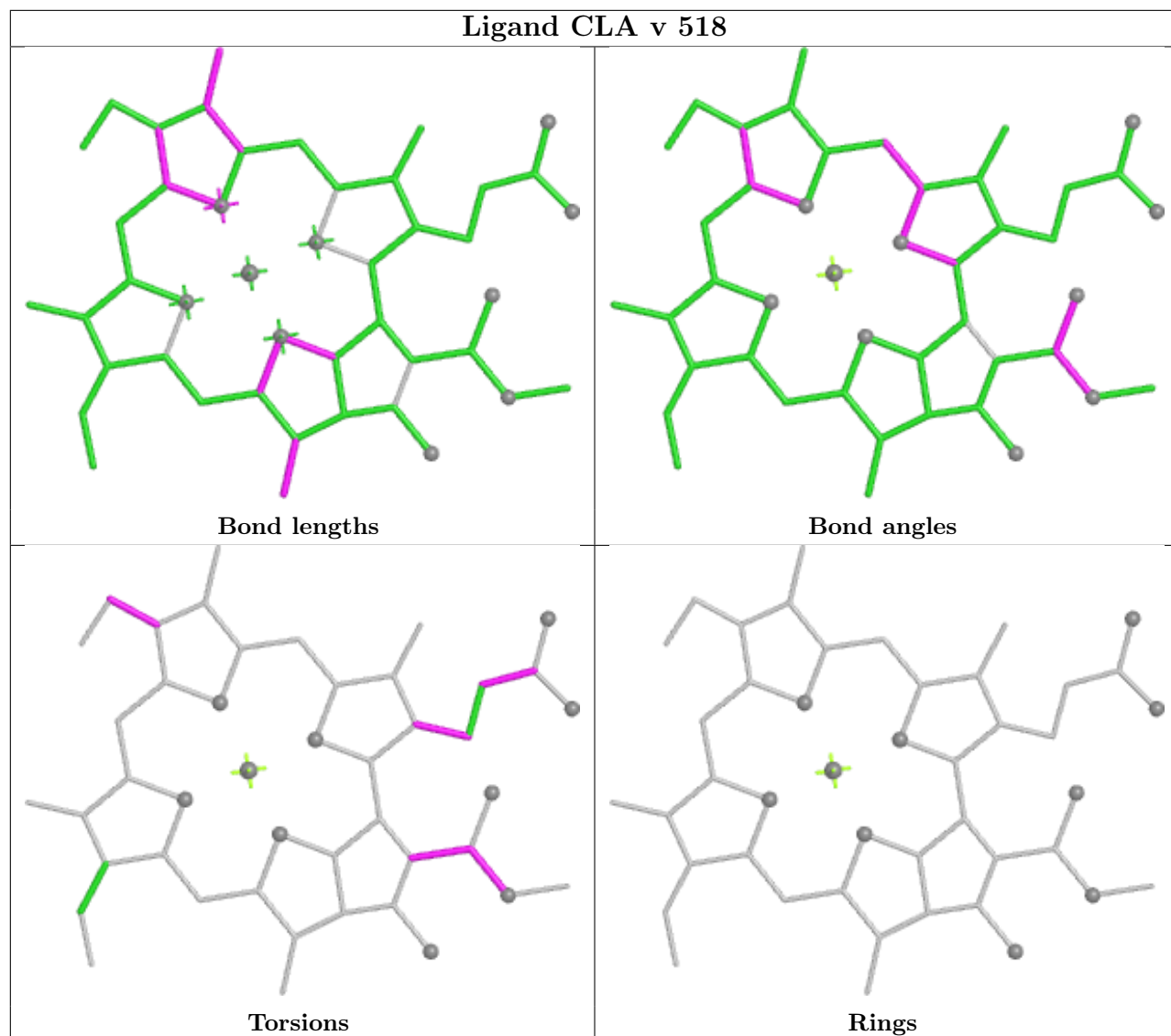


Torsions

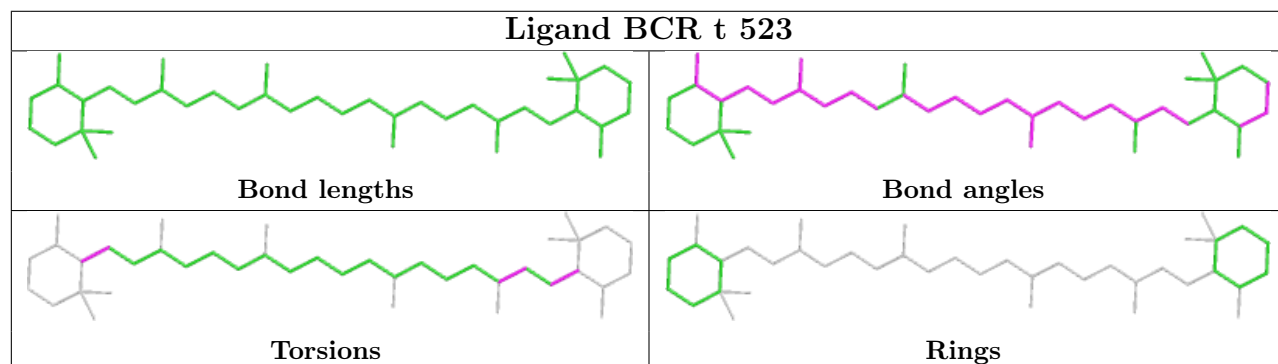


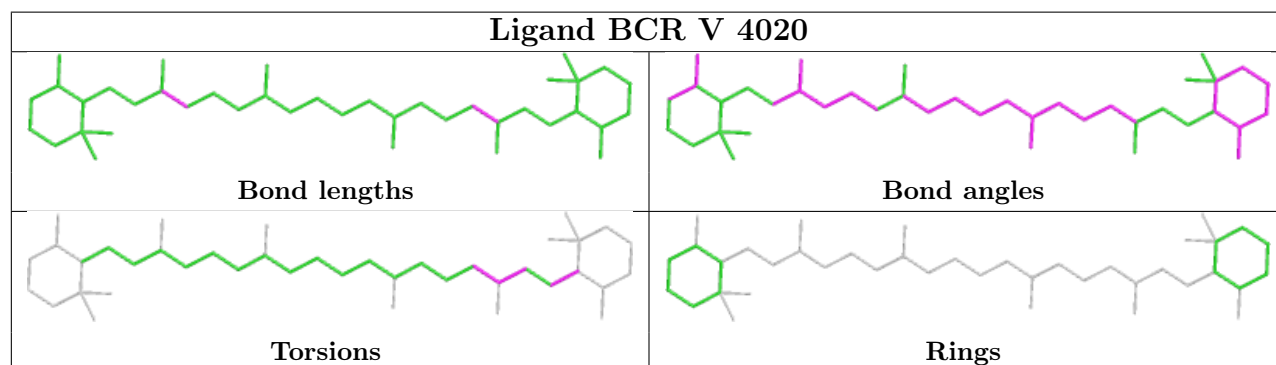
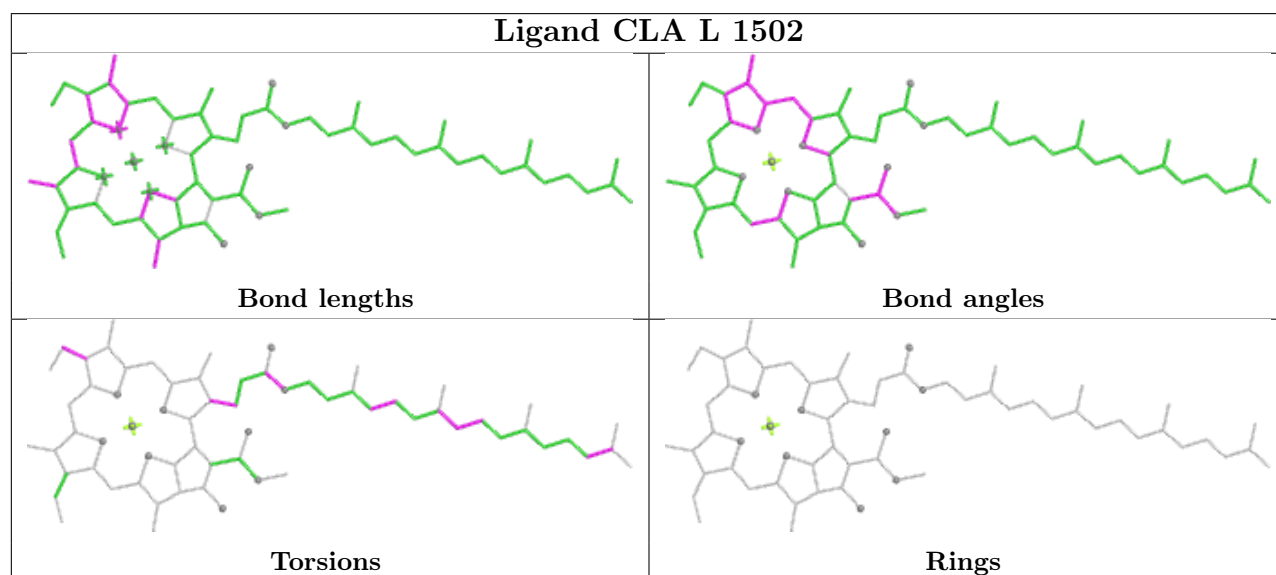
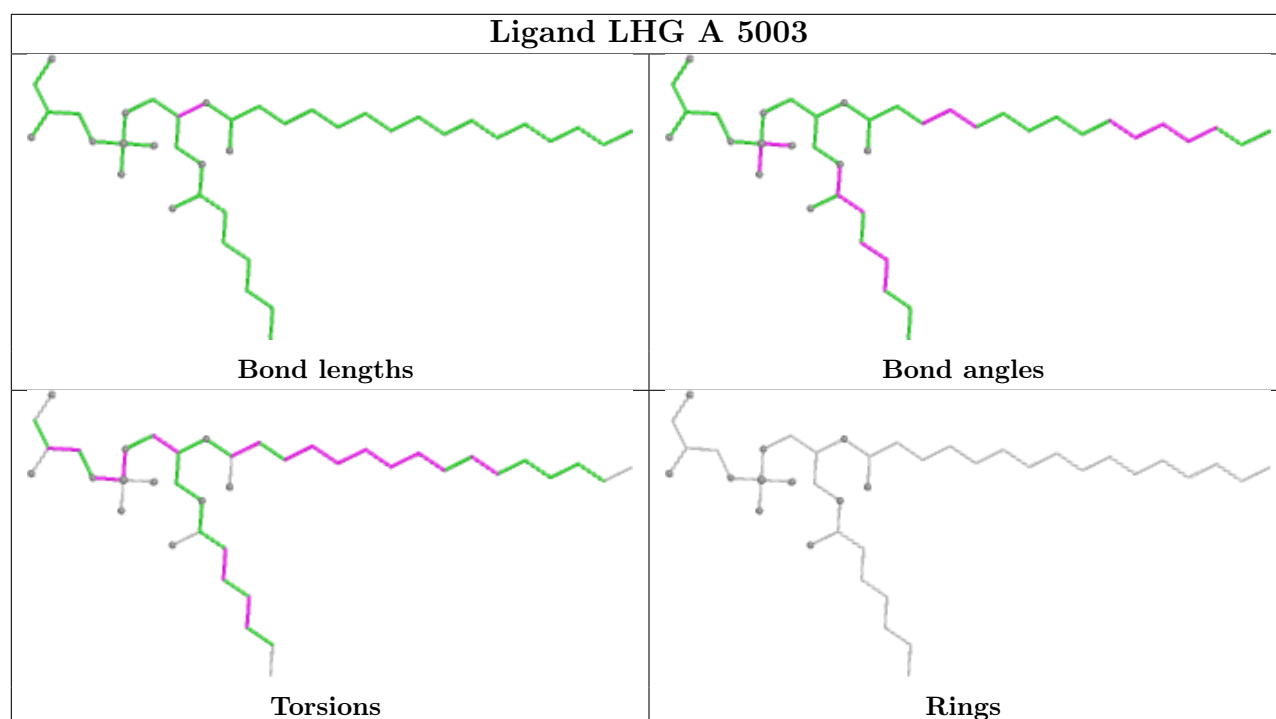
Rings

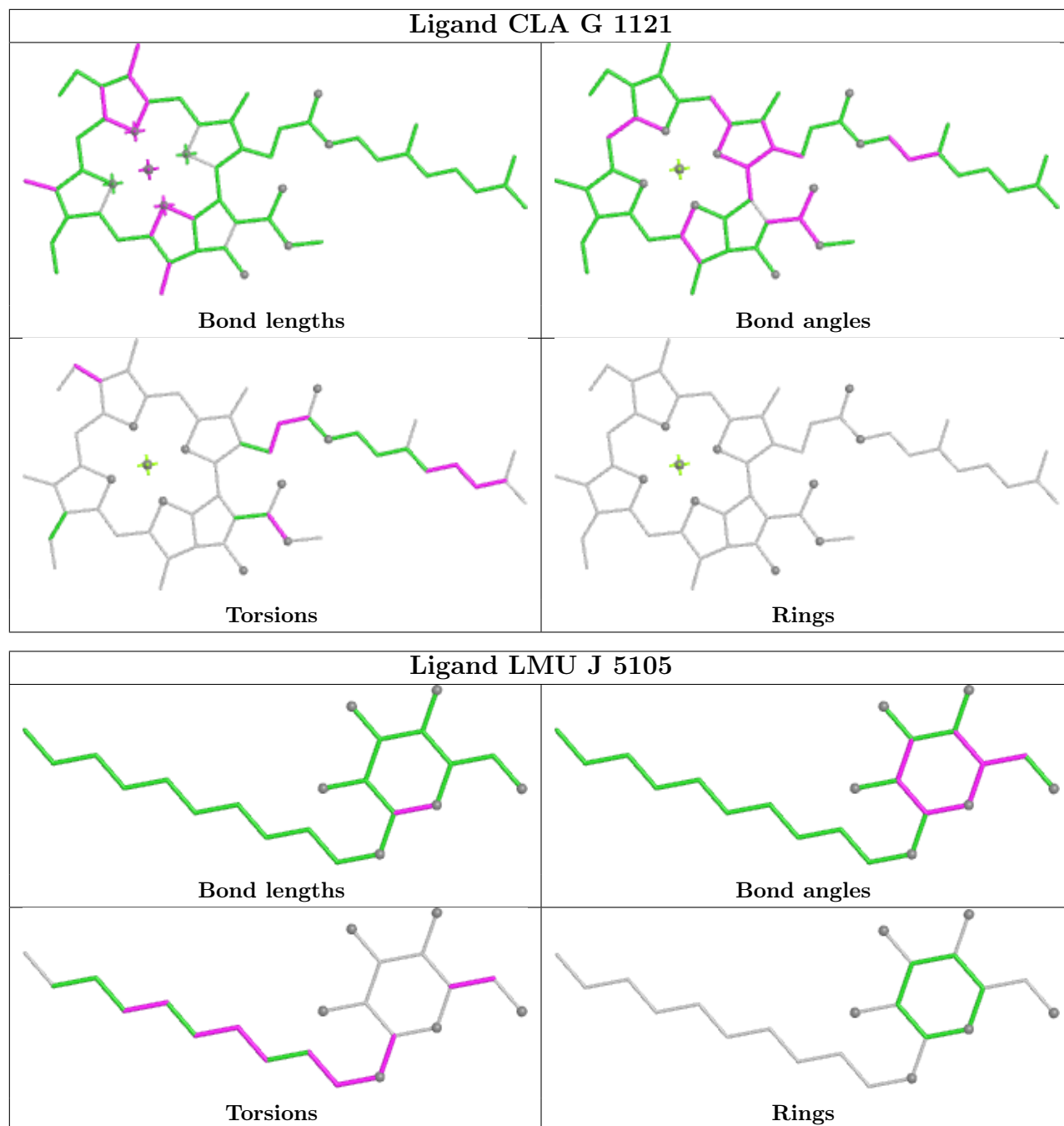
Ligand CLA v 518

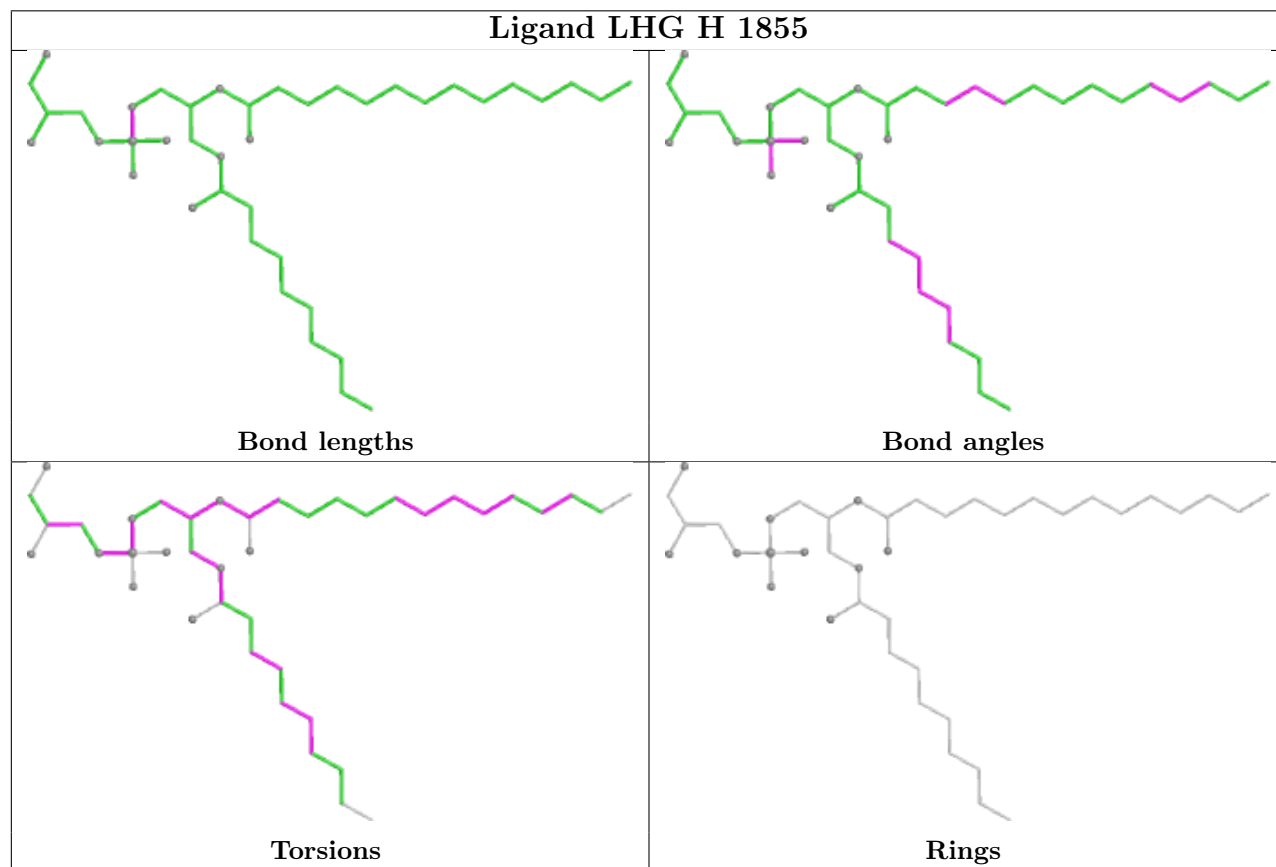
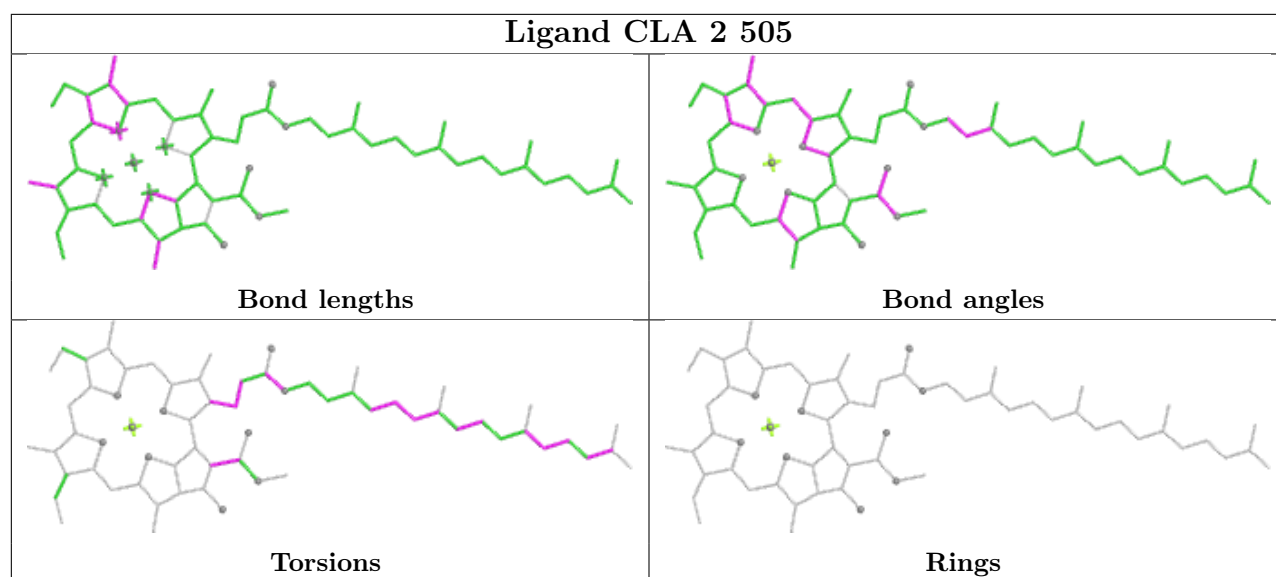


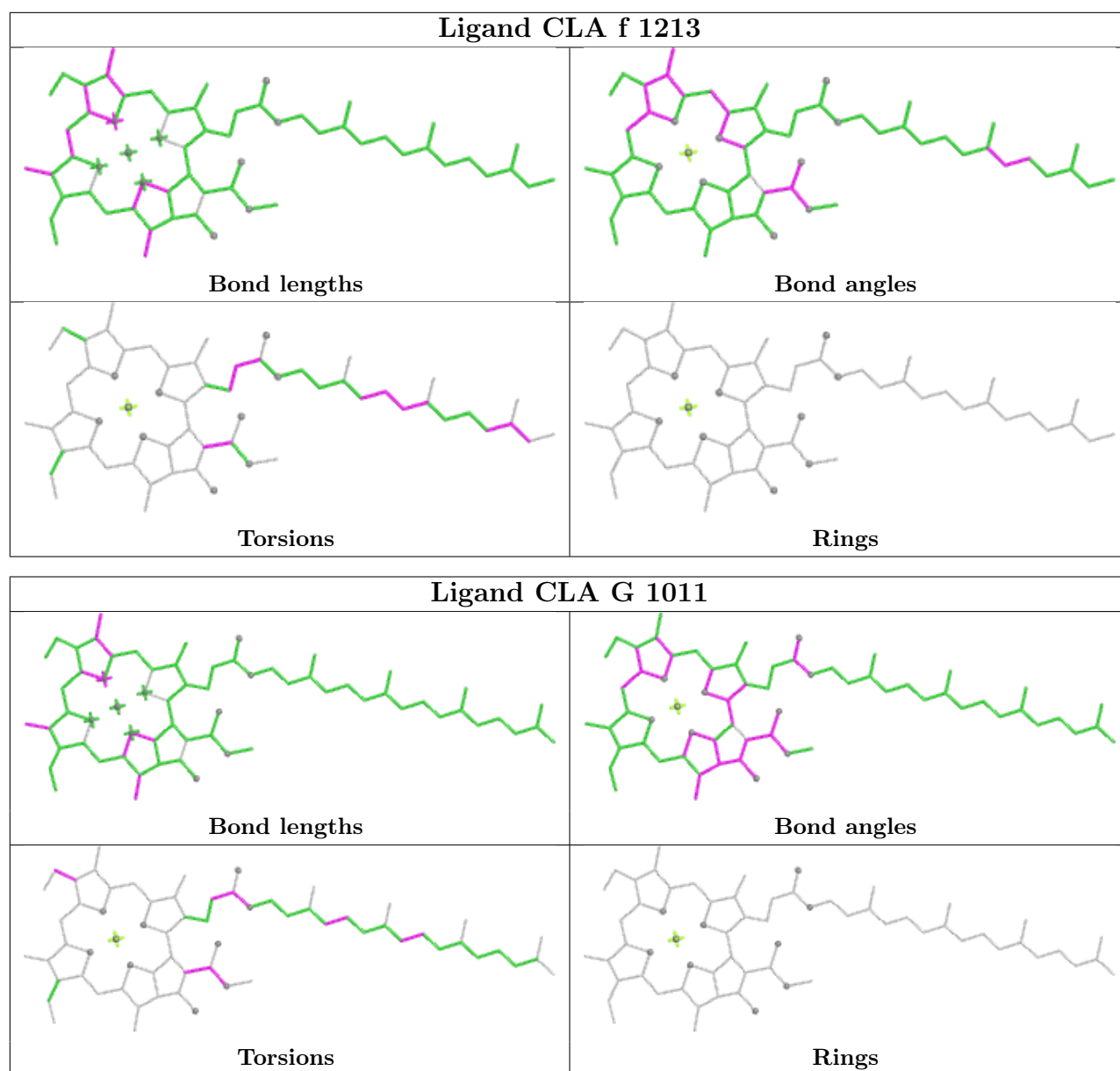
Ligand BCR t 523

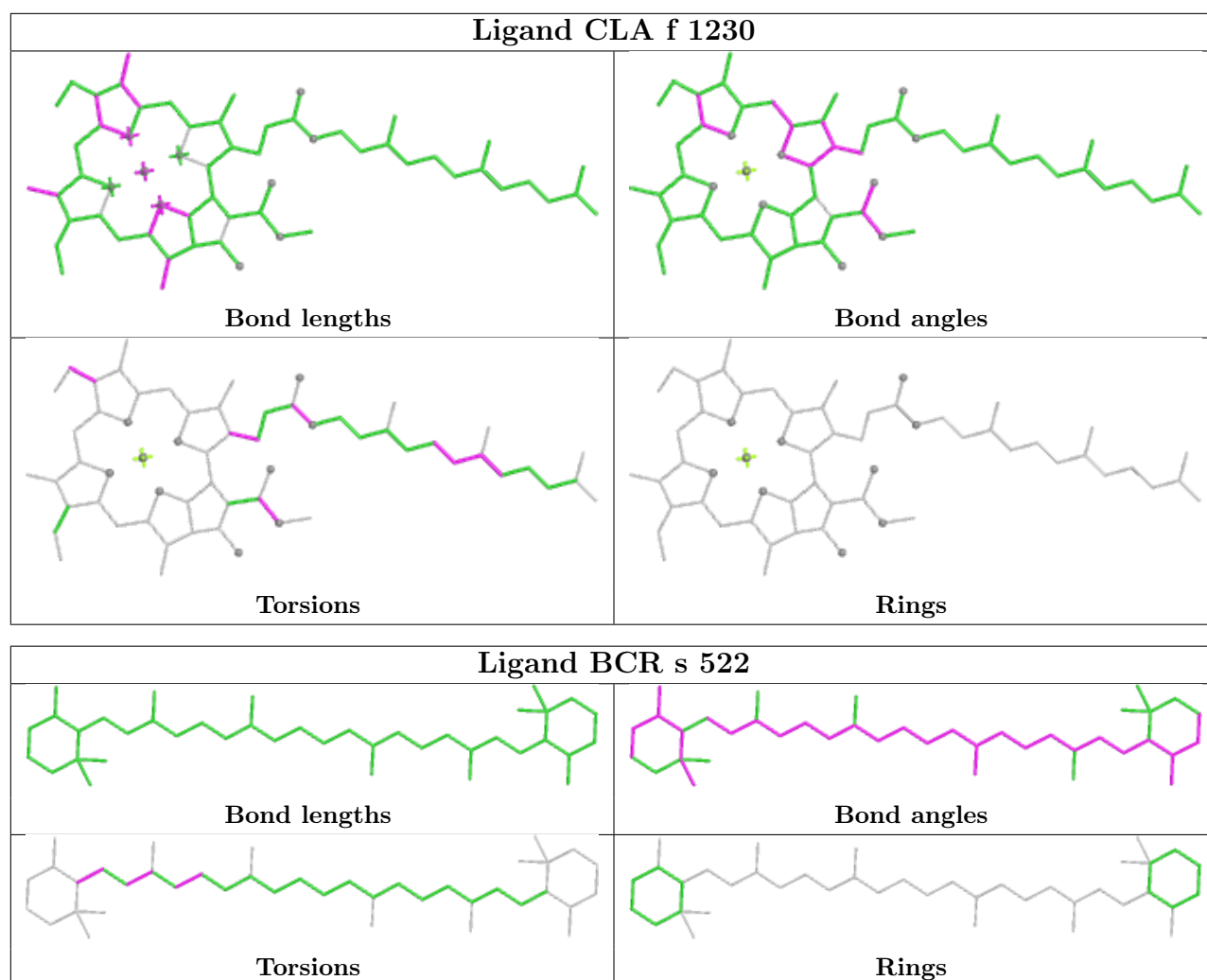




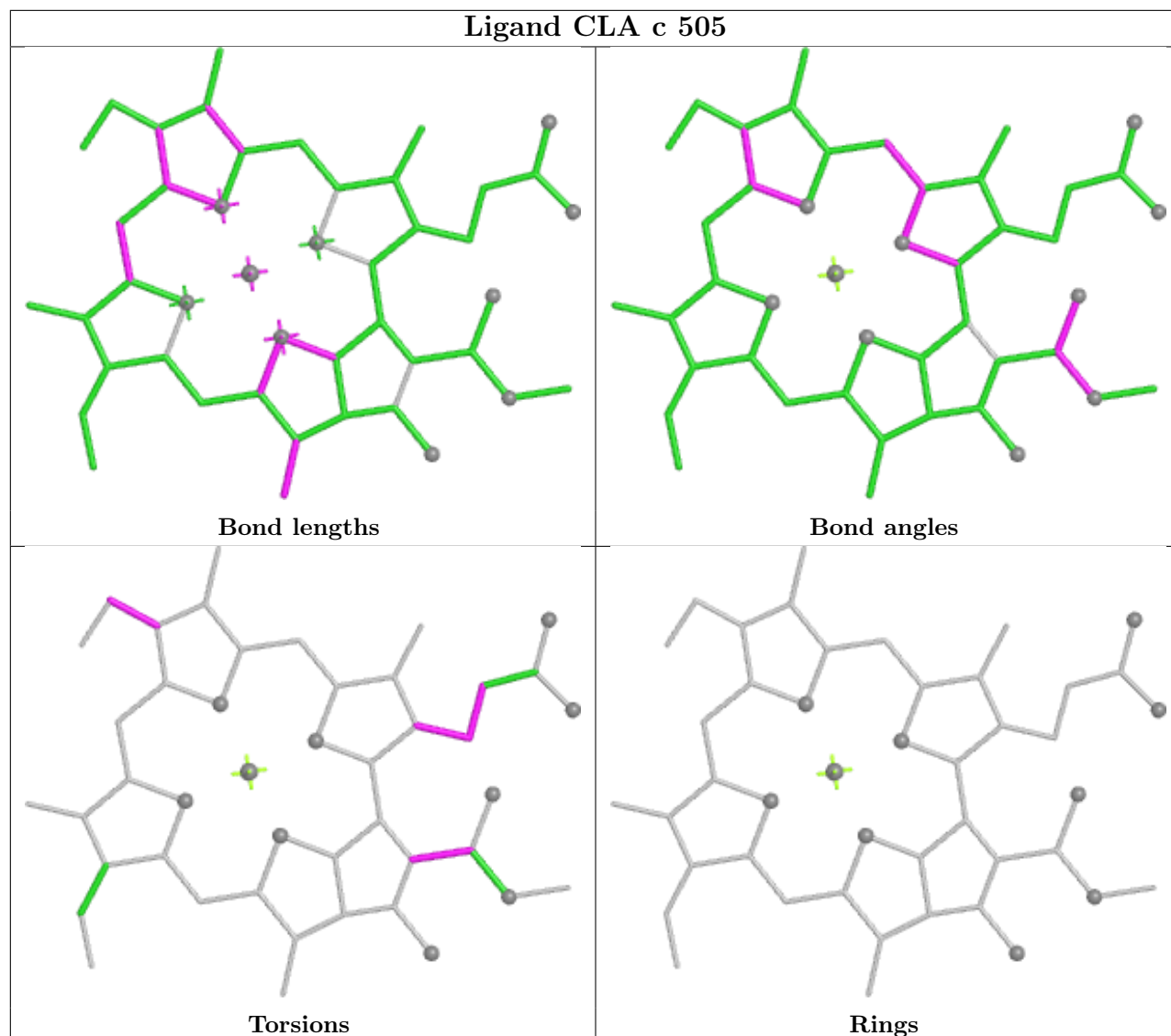




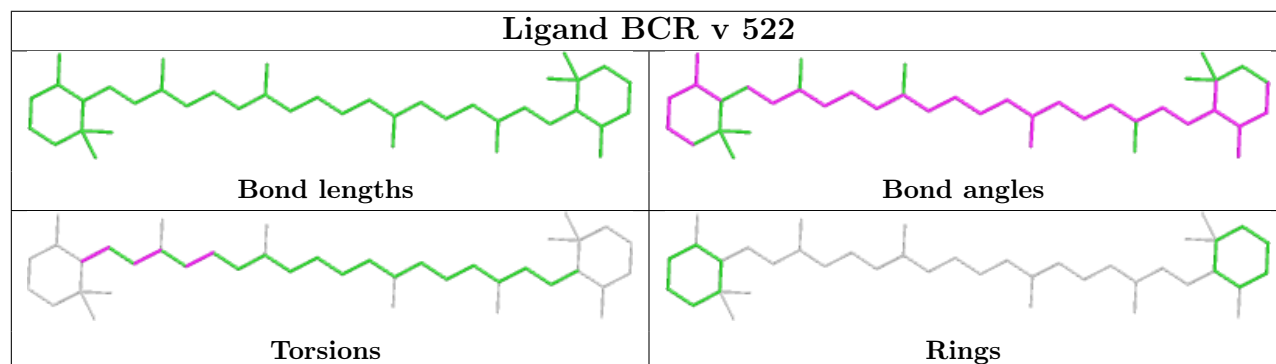


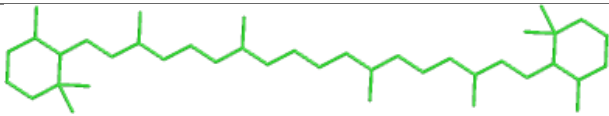
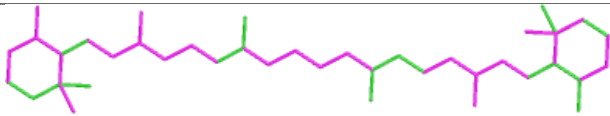
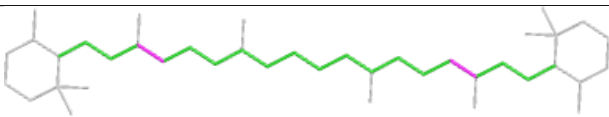
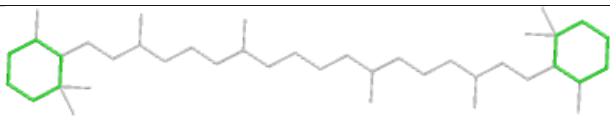


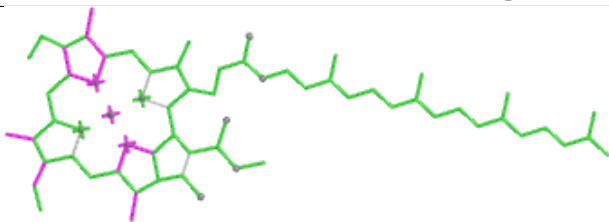
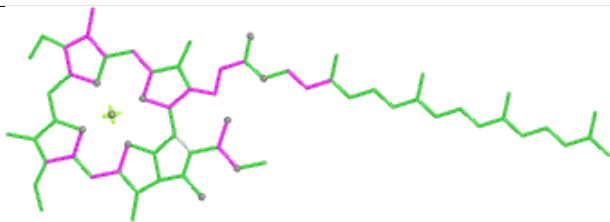
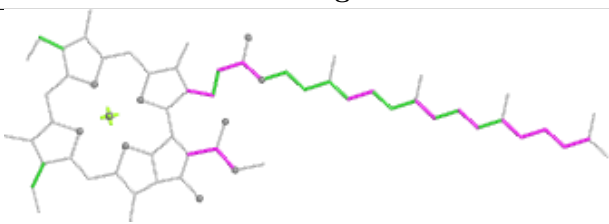
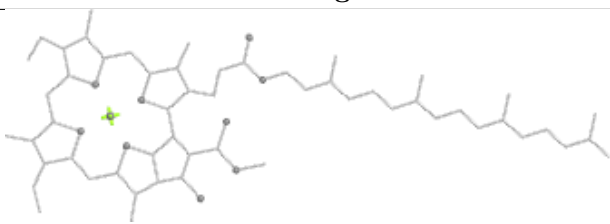
Ligand CLA c 505

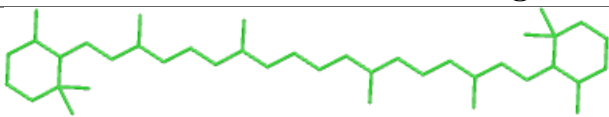
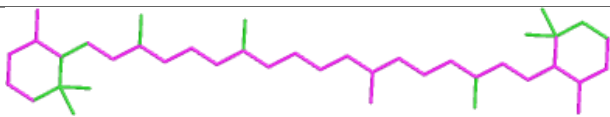
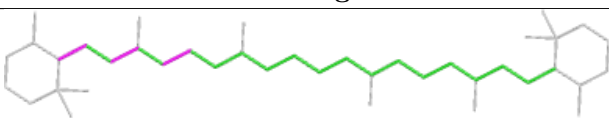
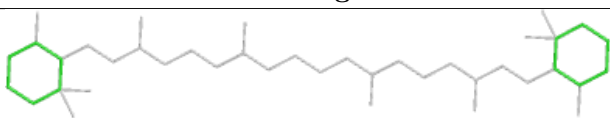


Ligand BCR v 522

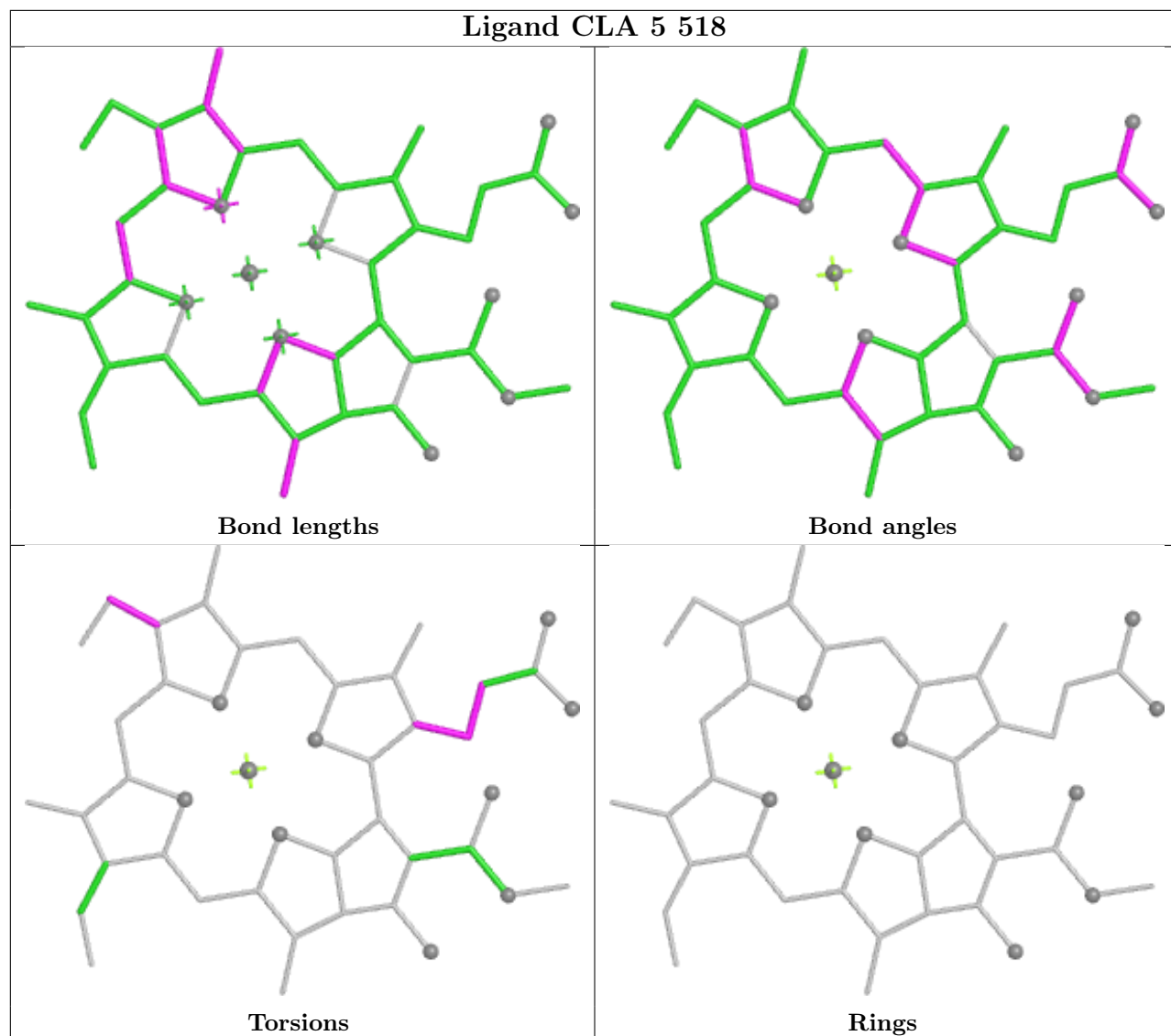


Ligand BCR H 4006	
	
Bond lengths	Bond angles
	
Torsions	Rings

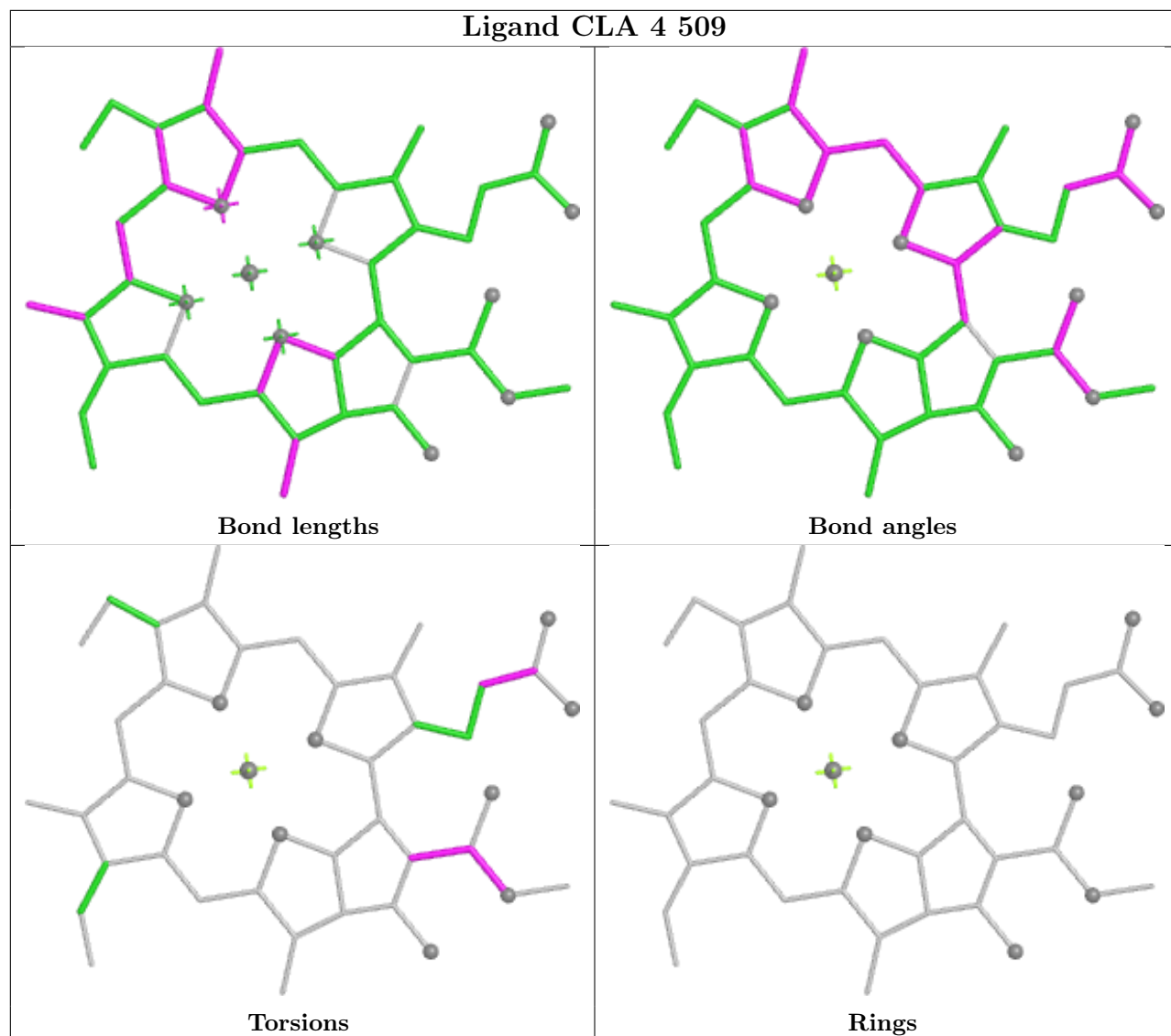
Ligand CLA A 1103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 6 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

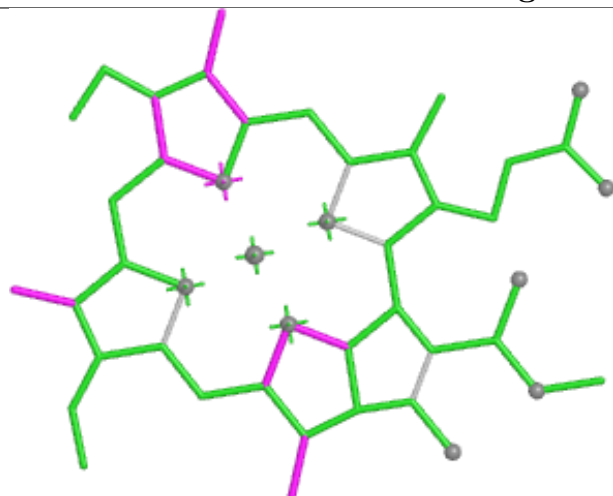
Ligand CLA 5 518



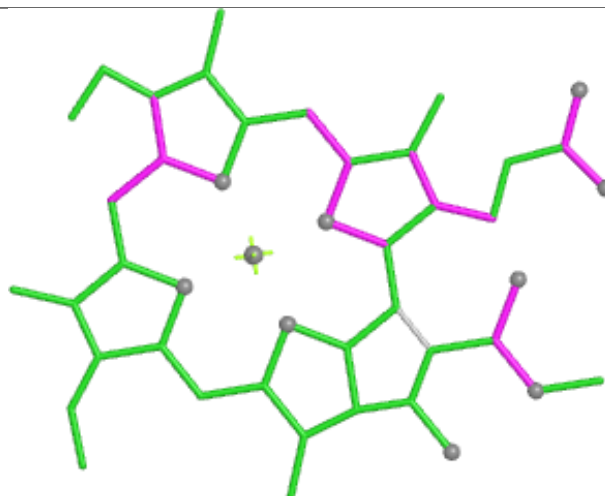
Ligand CLA 4 509



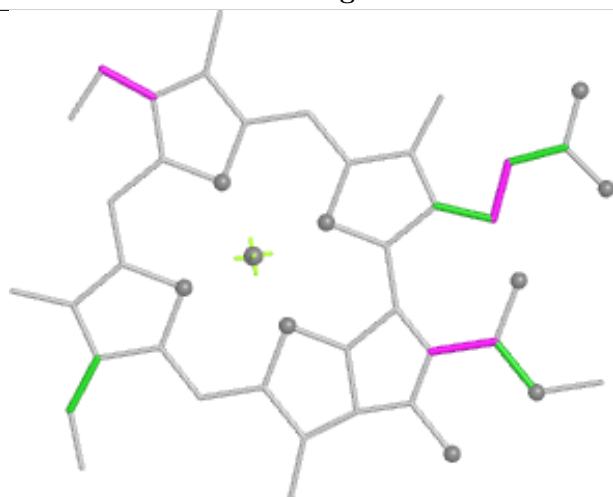
Ligand CLA 1 502



Bond lengths



Bond angles

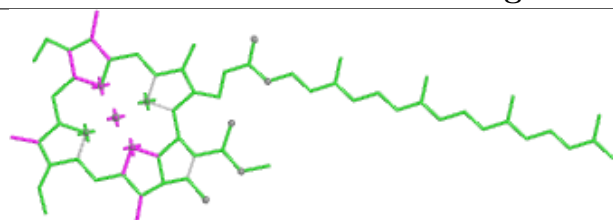


Torsions

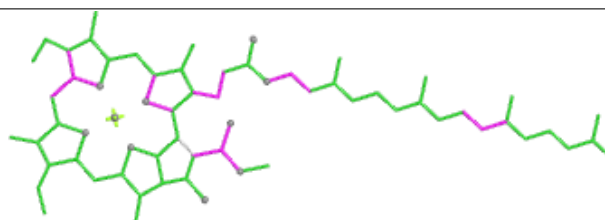


Rings

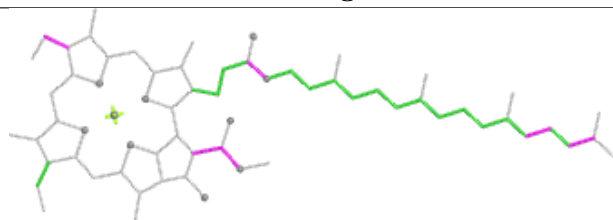
Ligand CLA H 1021



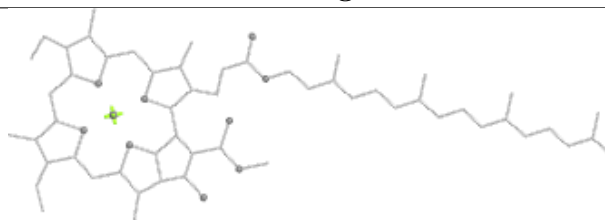
Bond lengths



Bond angles

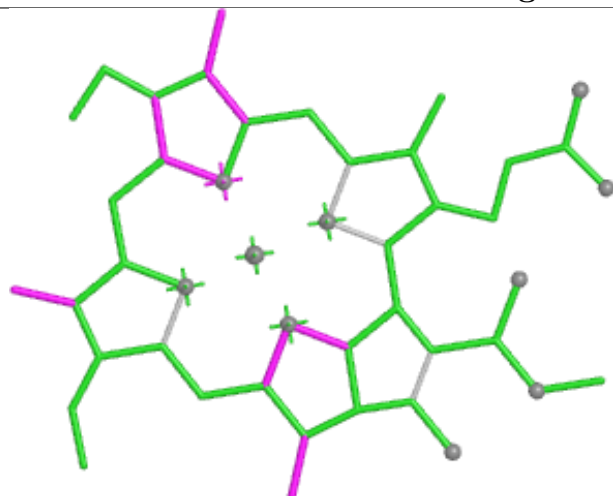


Torsions

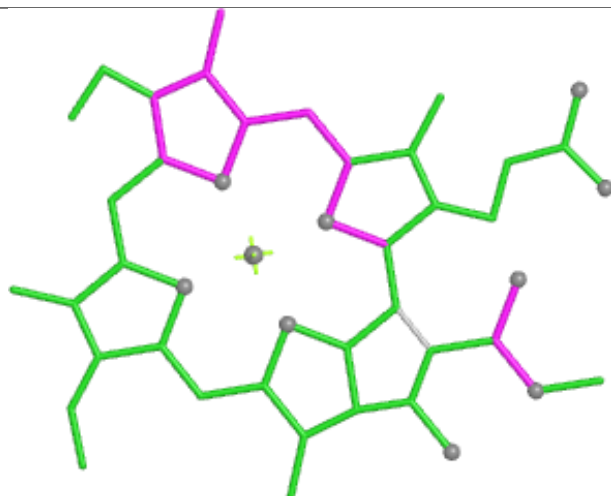


Rings

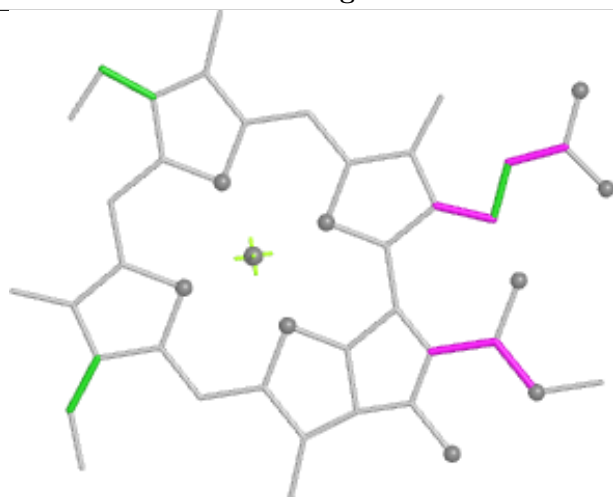
Ligand CLA a 506



Bond lengths



Bond angles

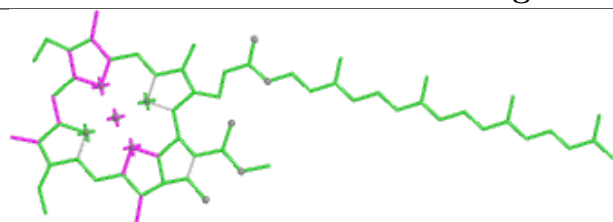


Torsions

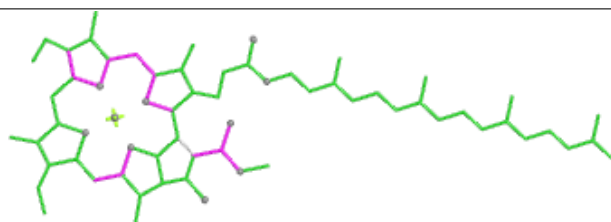


Rings

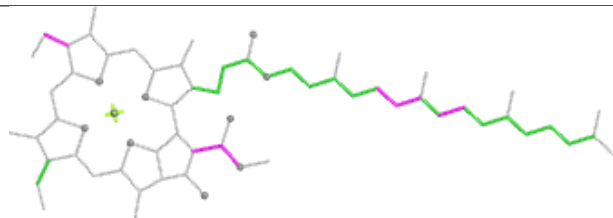
Ligand CLA f 1235



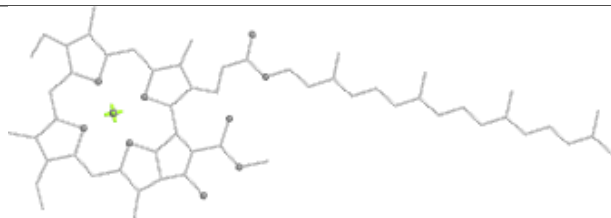
Bond lengths



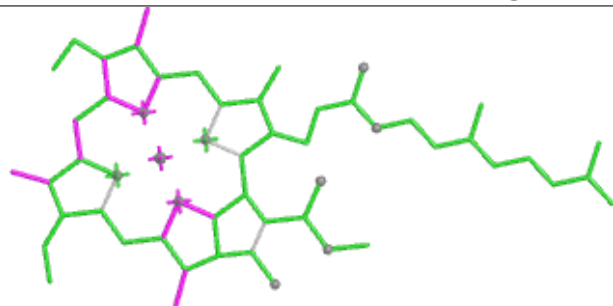
Bond angles



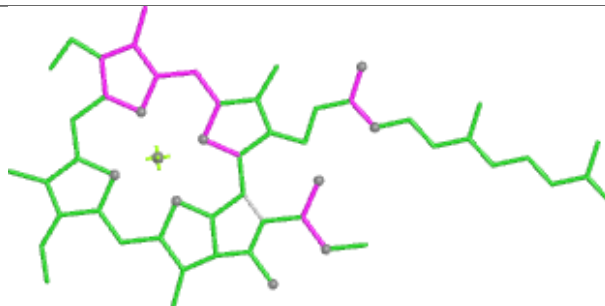
Torsions



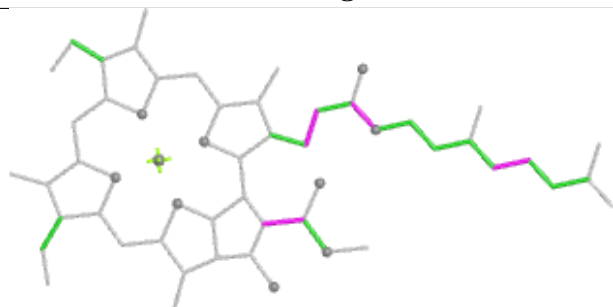
Rings

Ligand CLA B 1232

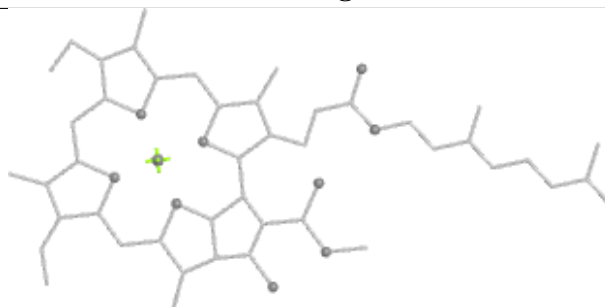
Bond lengths



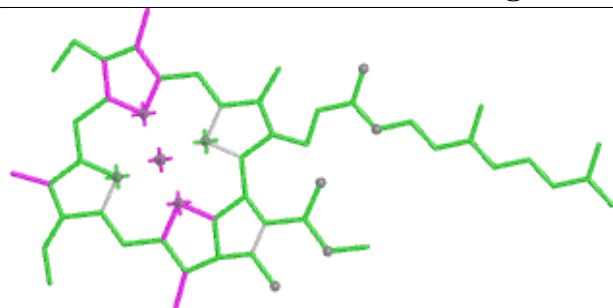
Bond angles



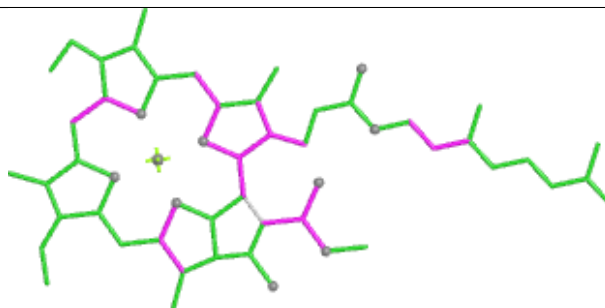
Torsions



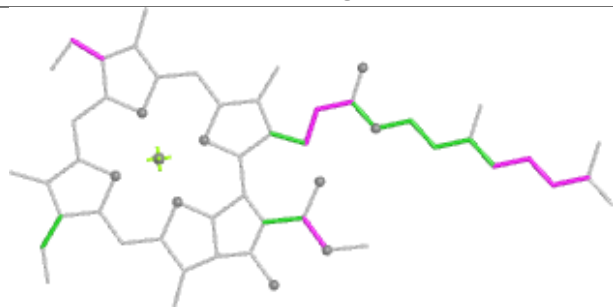
Rings

Ligand CLA A 1121

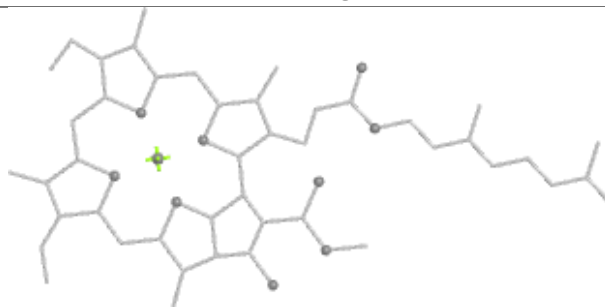
Bond lengths



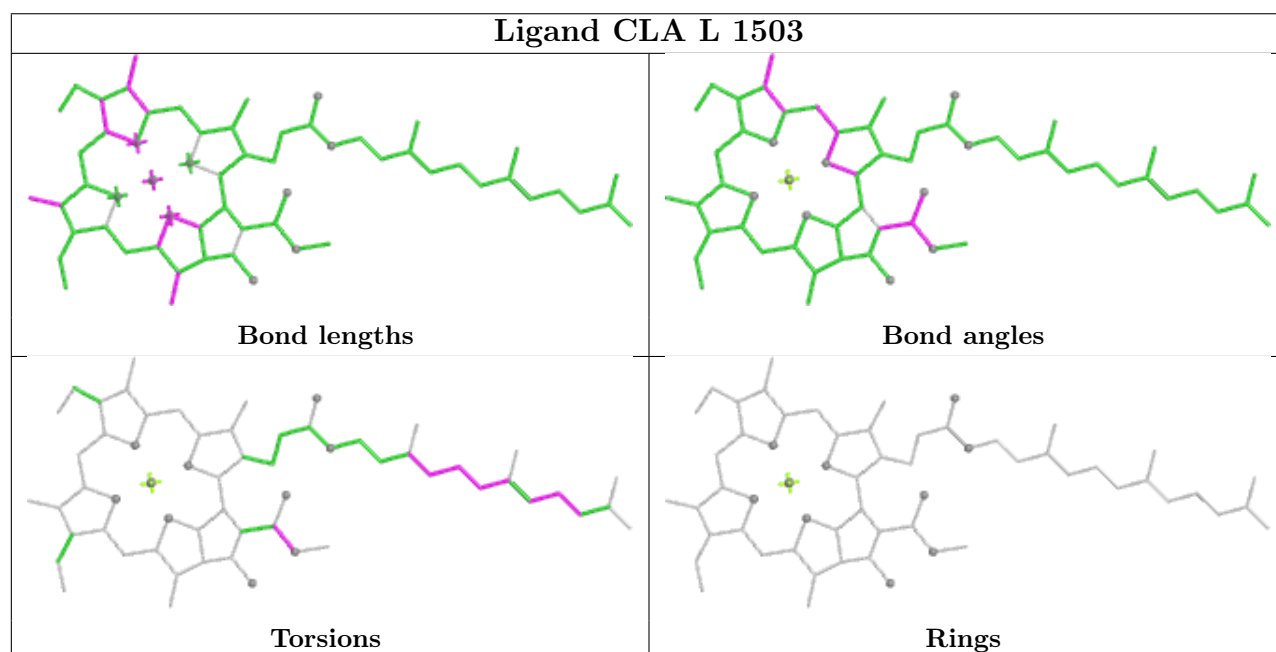
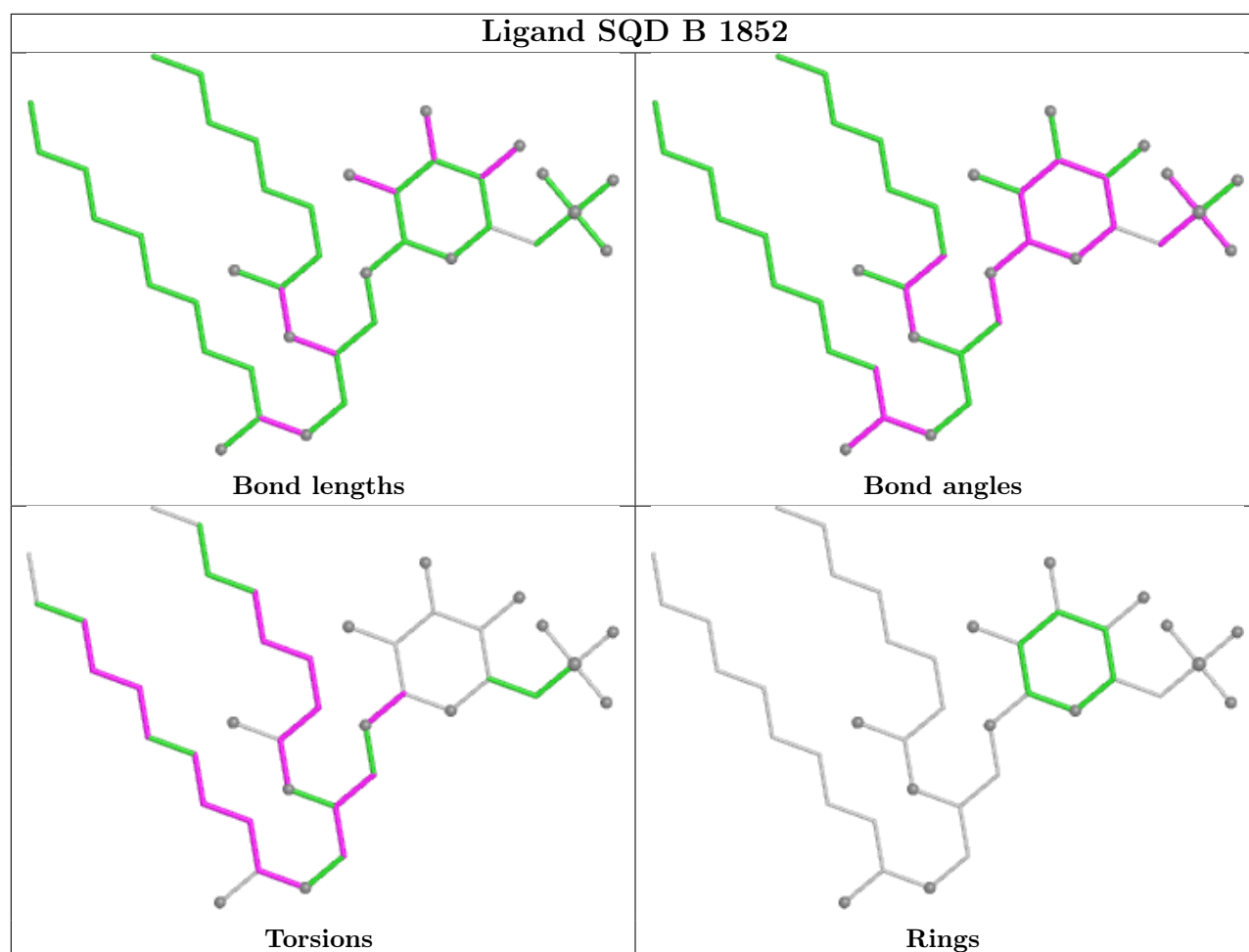
Bond angles



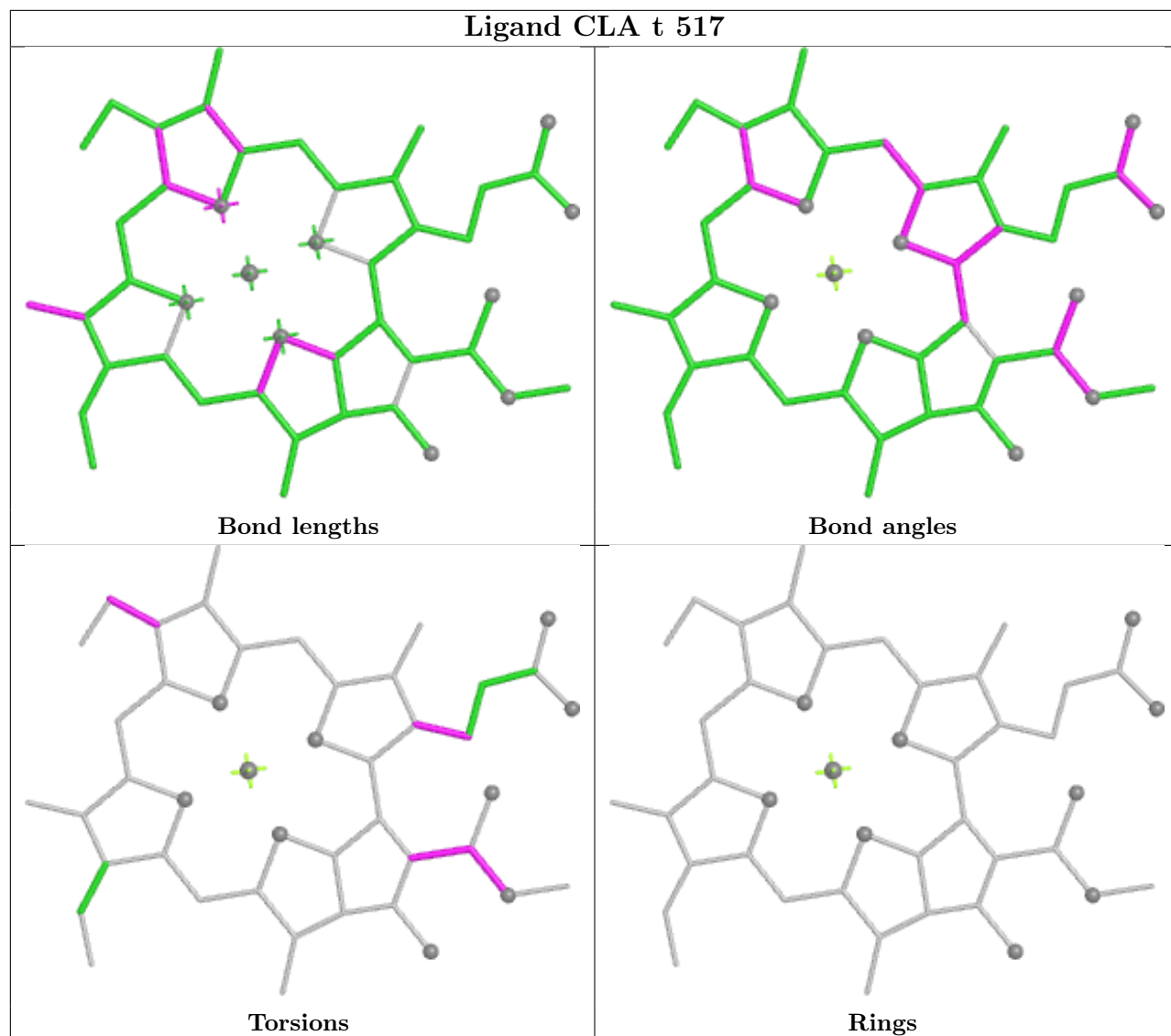
Torsions

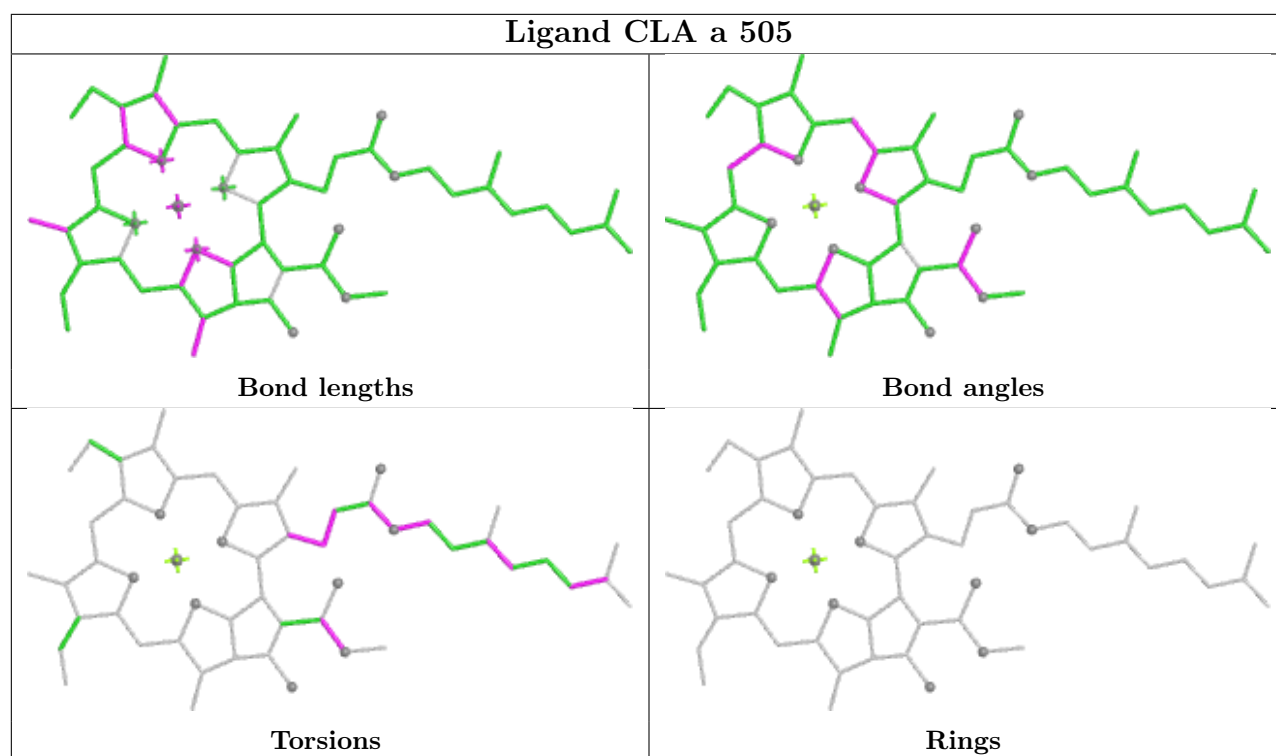


Rings

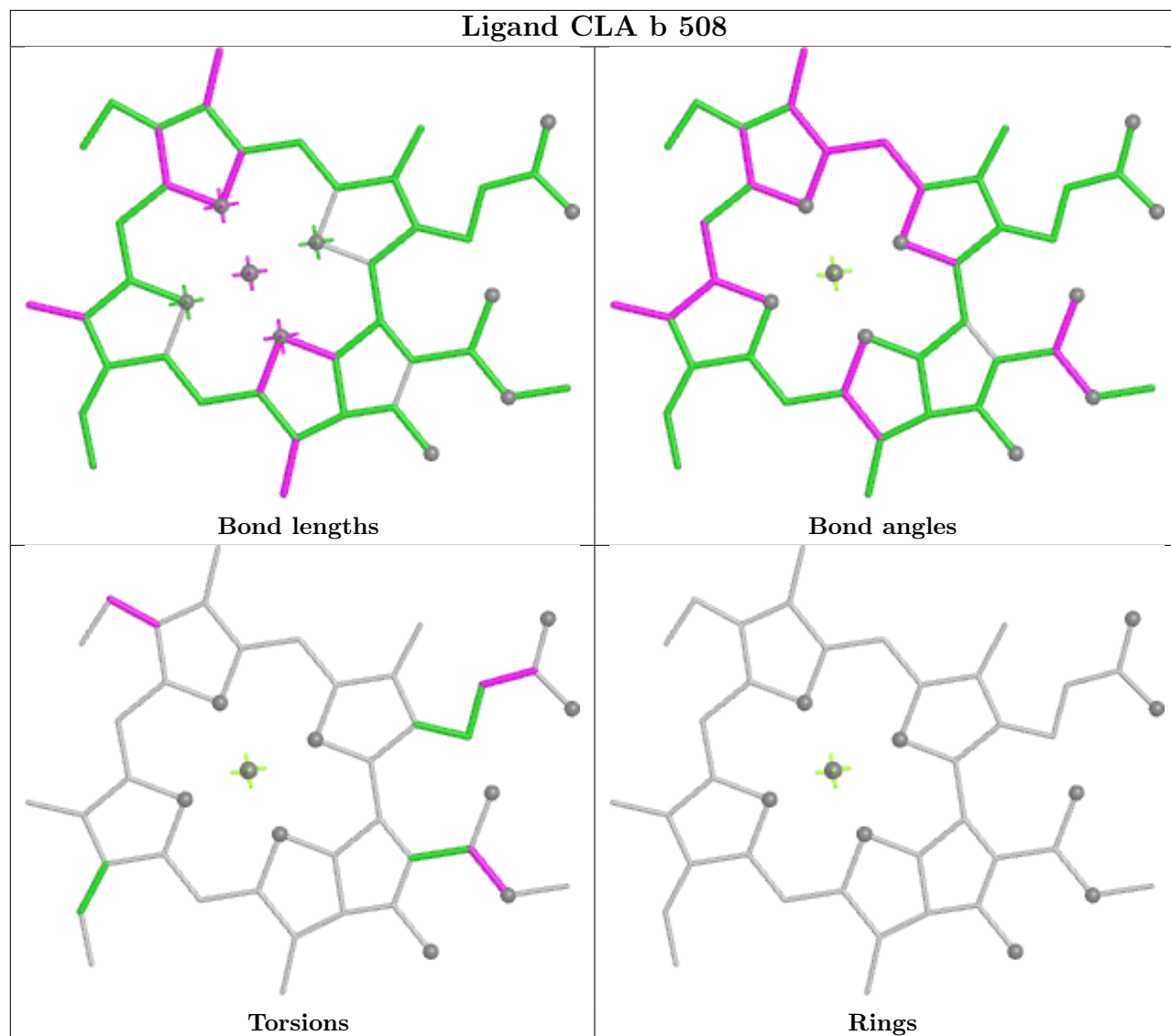


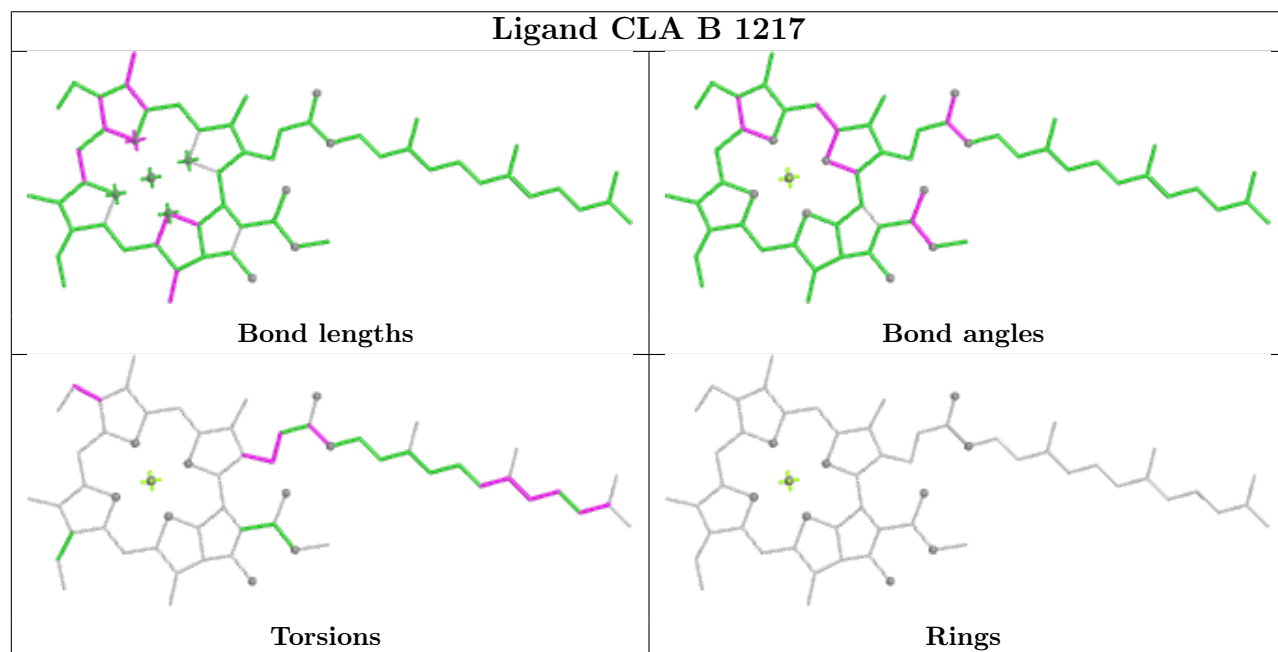
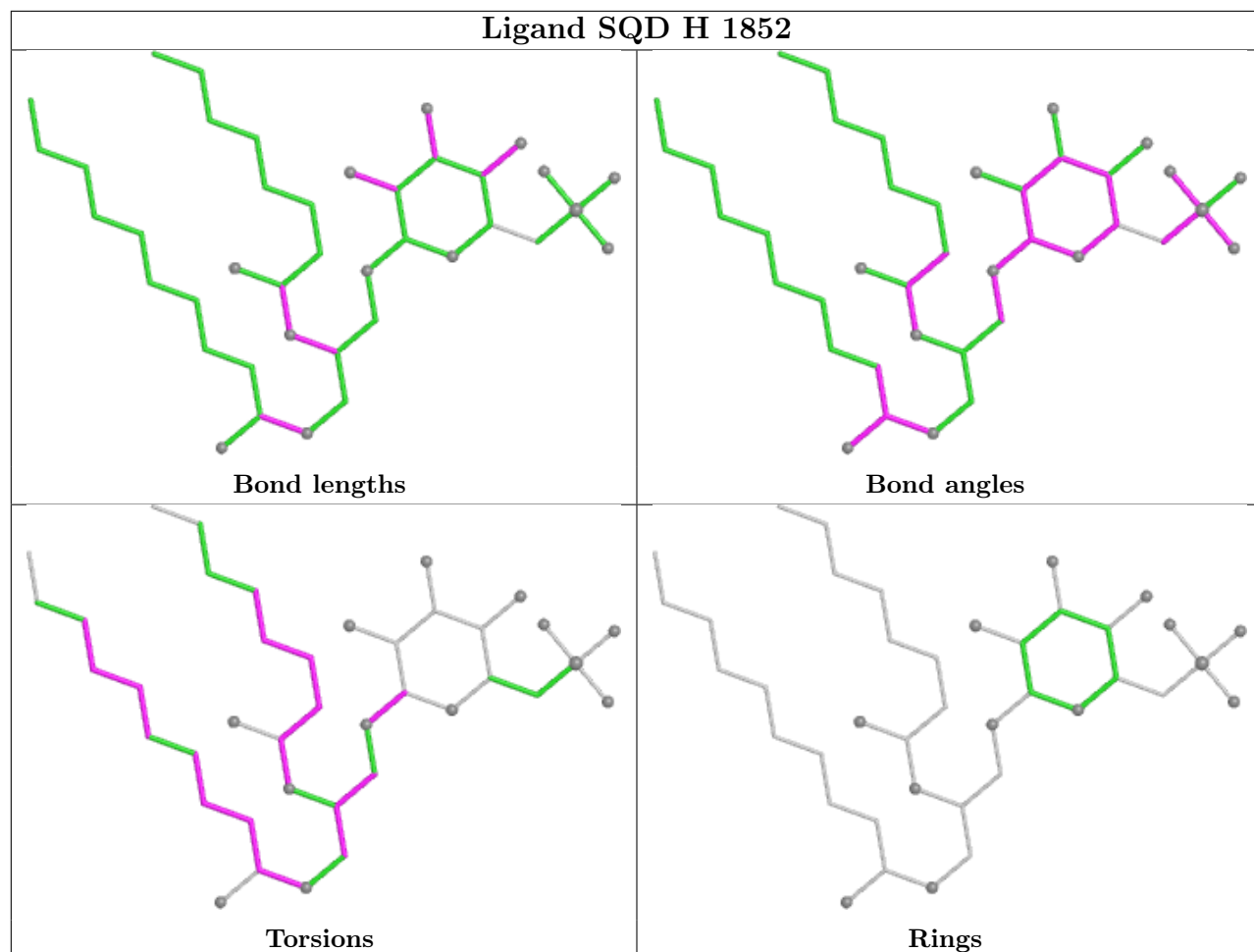
Ligand CLA t 517



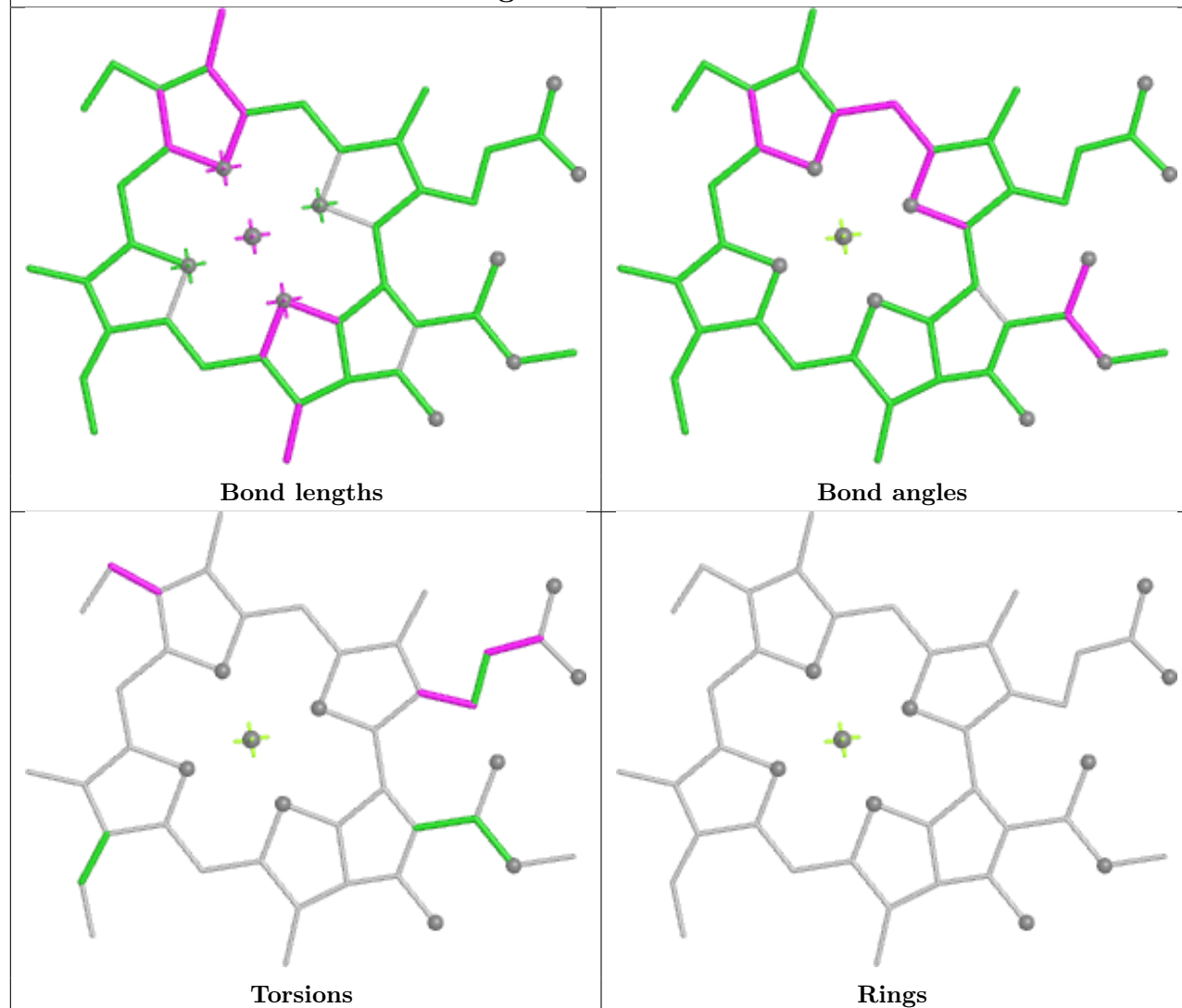


Ligand CLA b 508

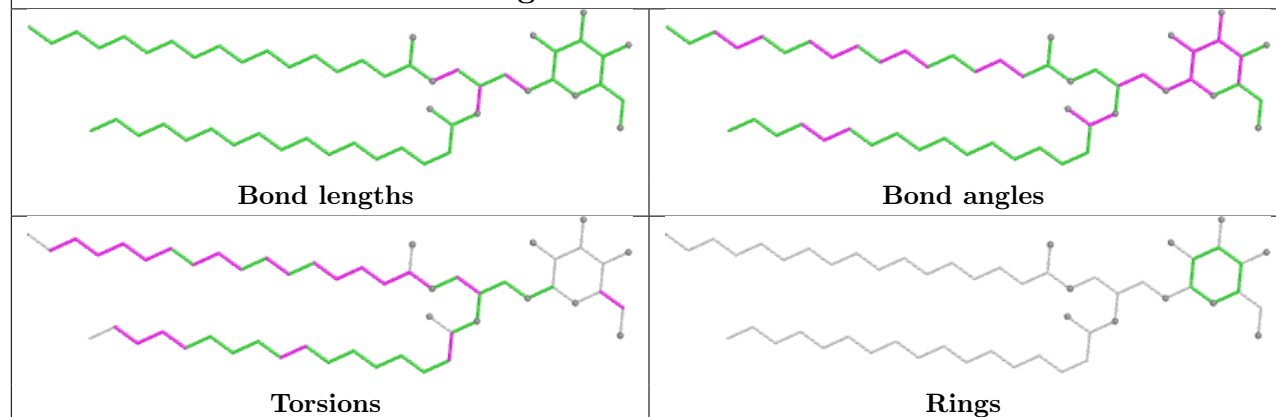


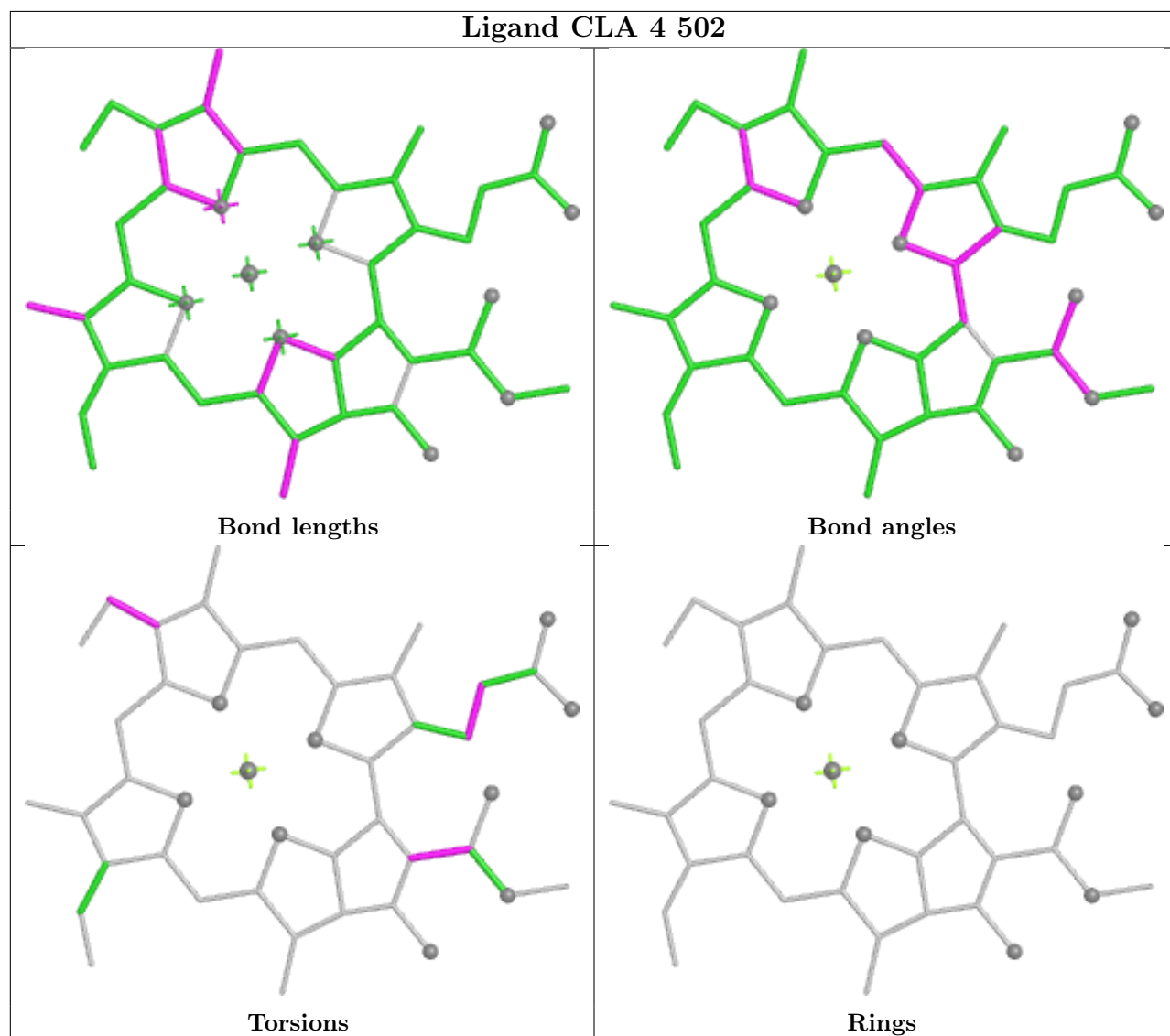
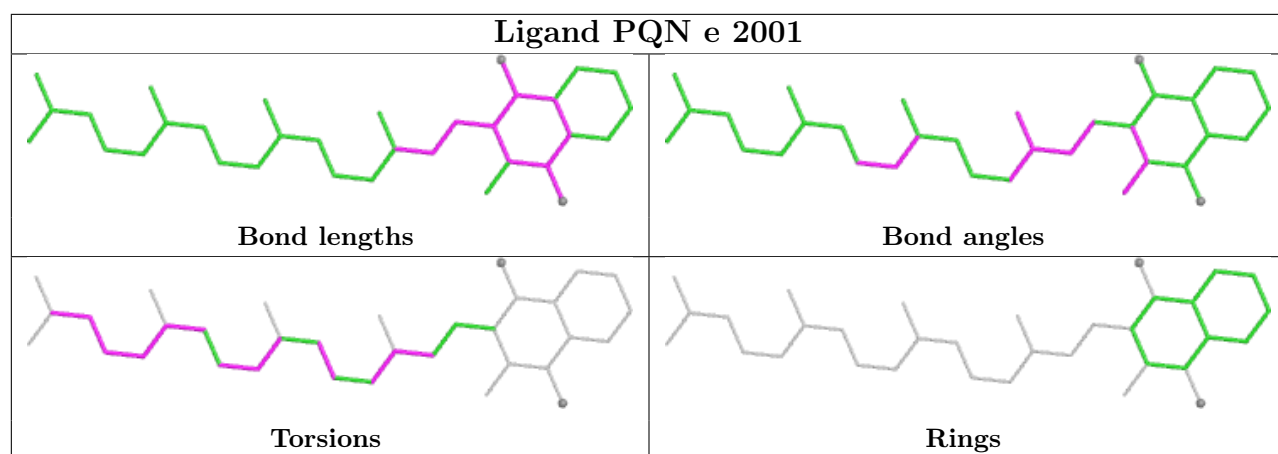


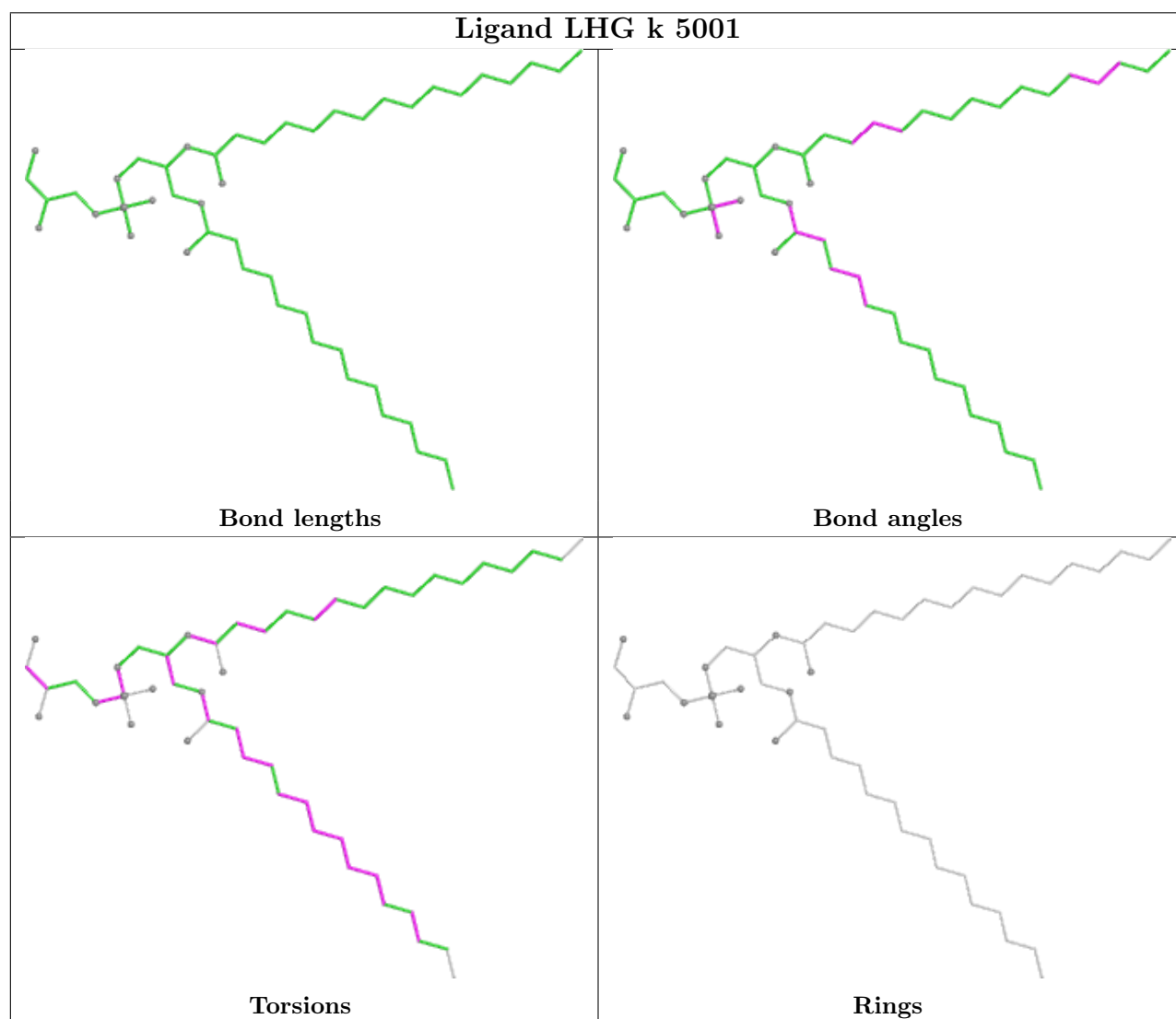
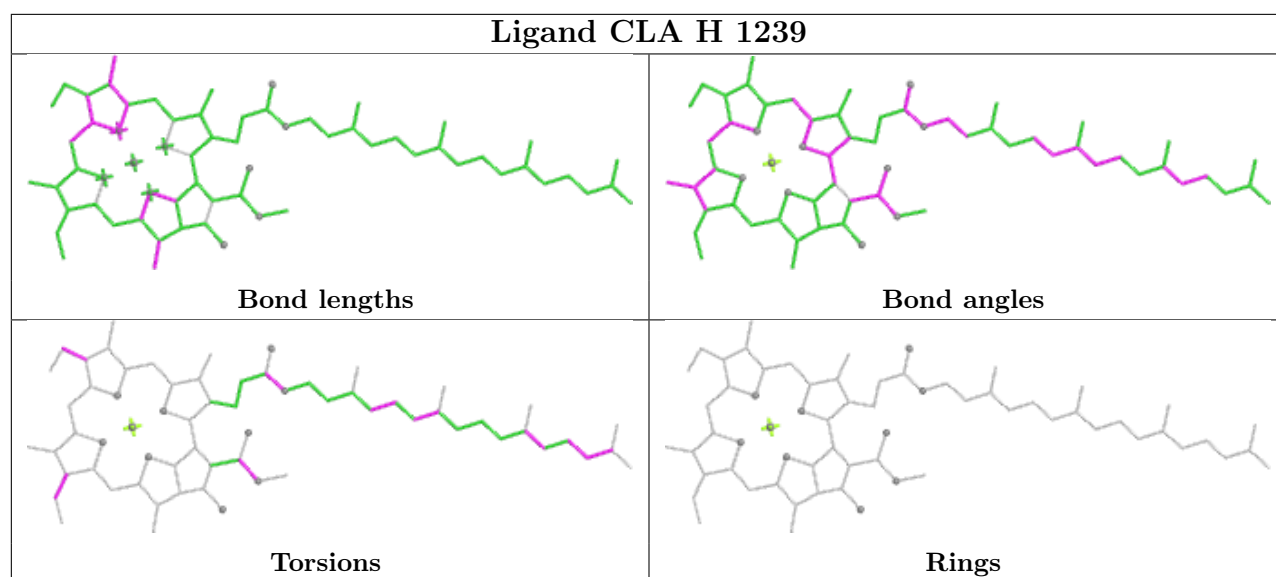
Ligand CLA r 512



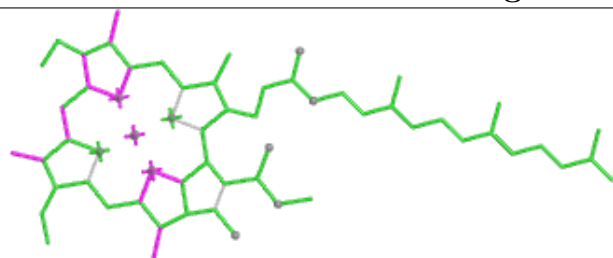
Ligand LMG H 5002



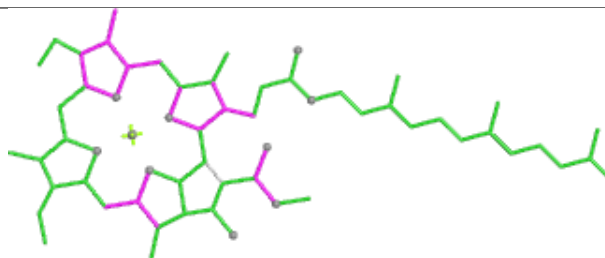




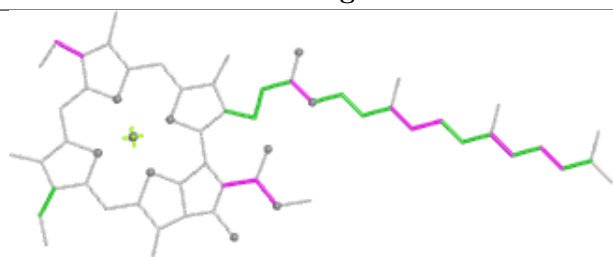
Ligand CLA G 1124



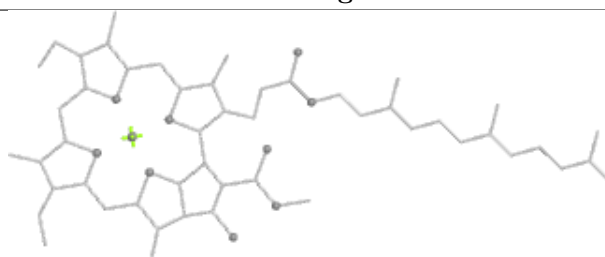
Bond lengths



Bond angles

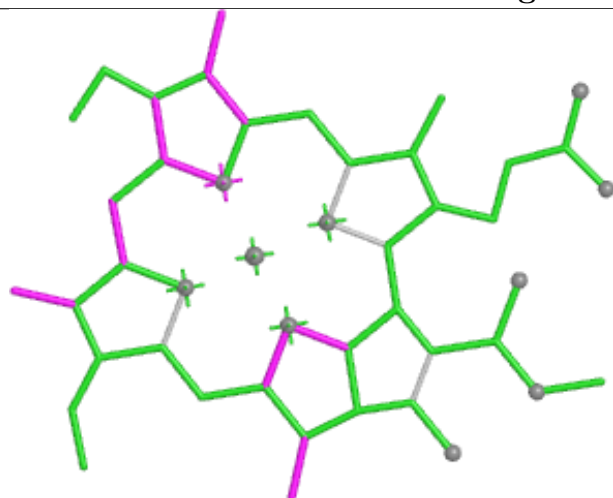


Torsions

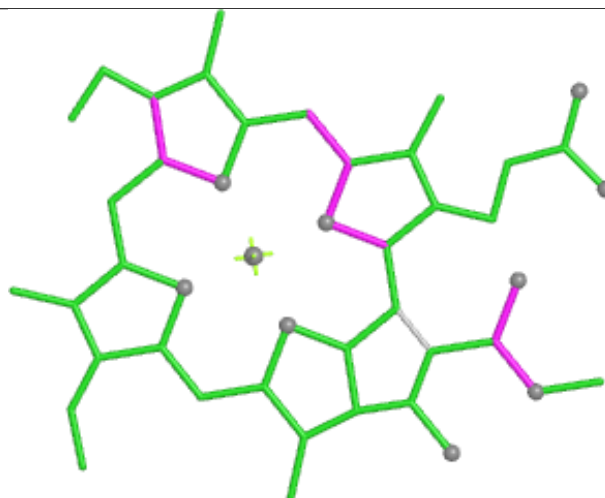


Rings

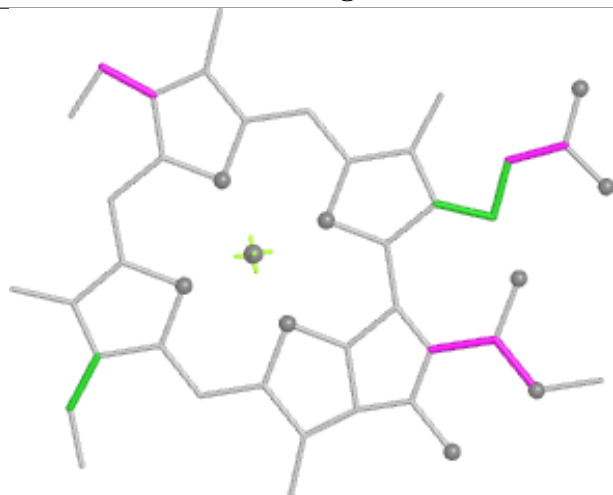
Ligand CLA 6 510



Bond lengths



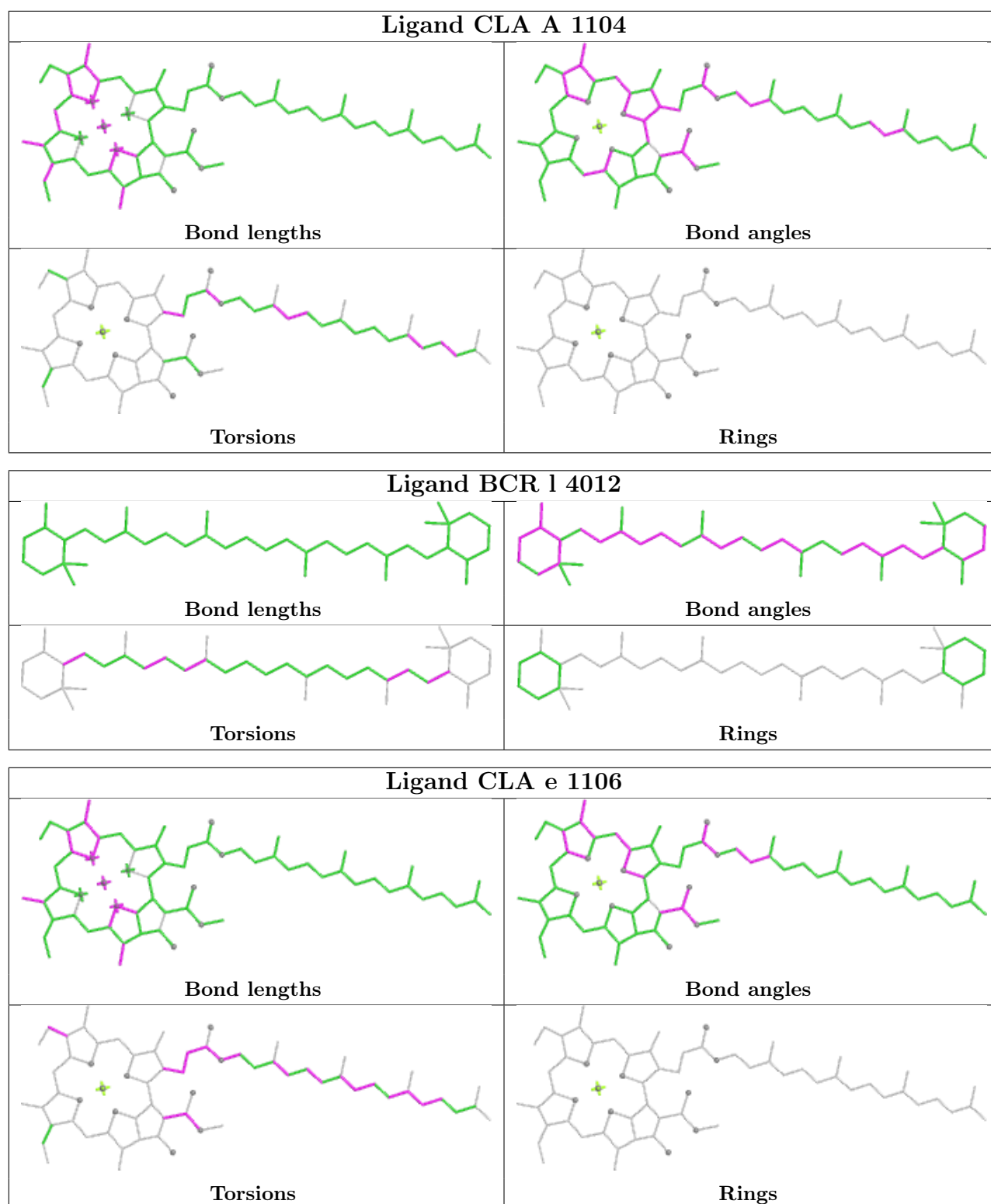
Bond angles



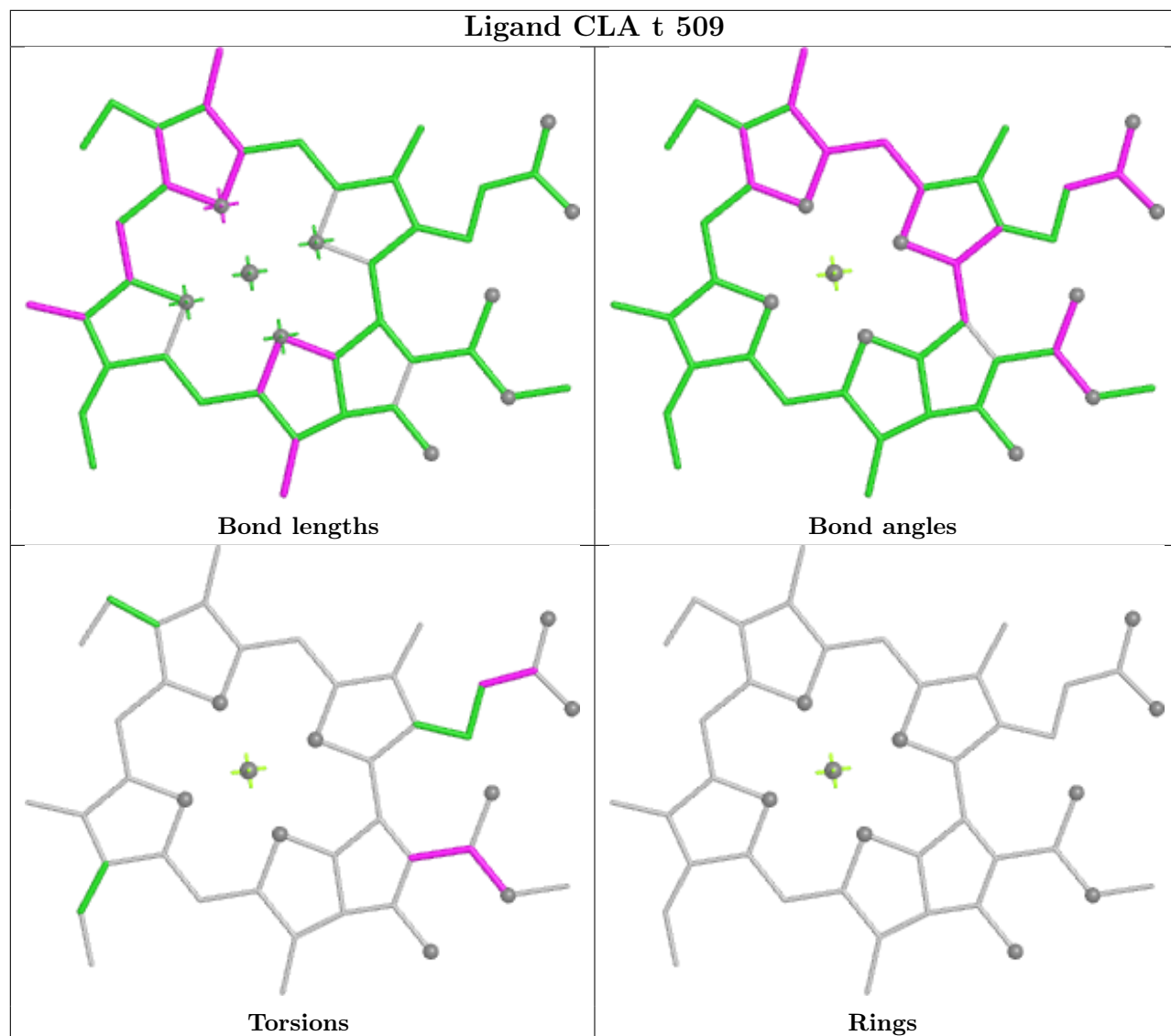
Torsions



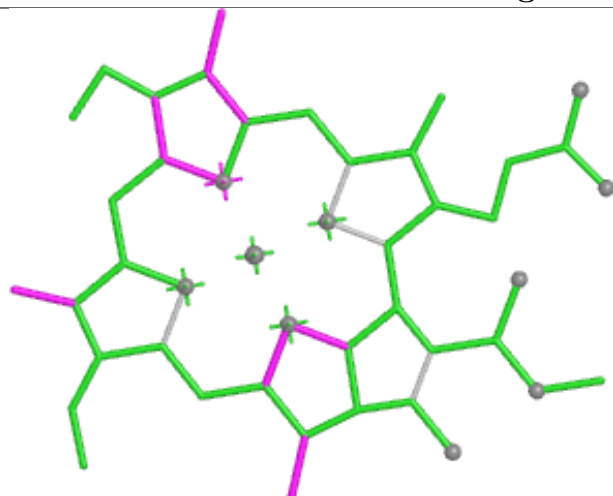
Rings



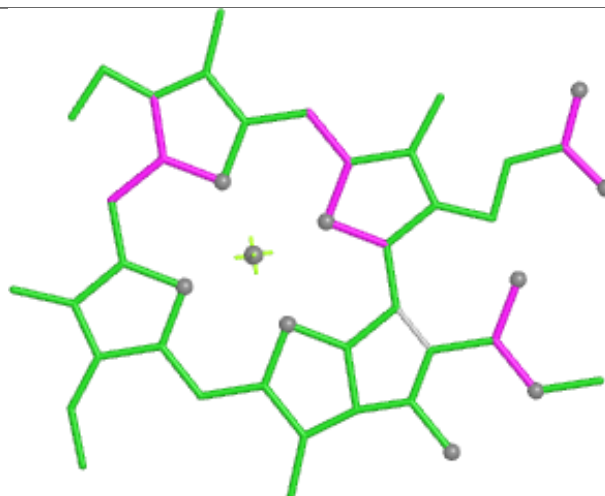
Ligand CLA t 509



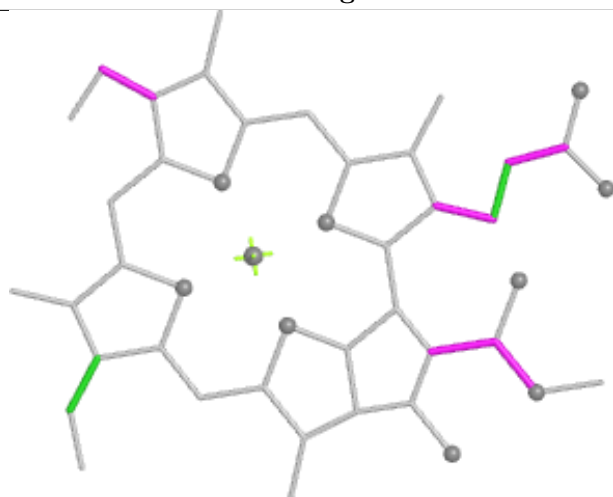
Ligand CLA v 517



Bond lengths



Bond angles

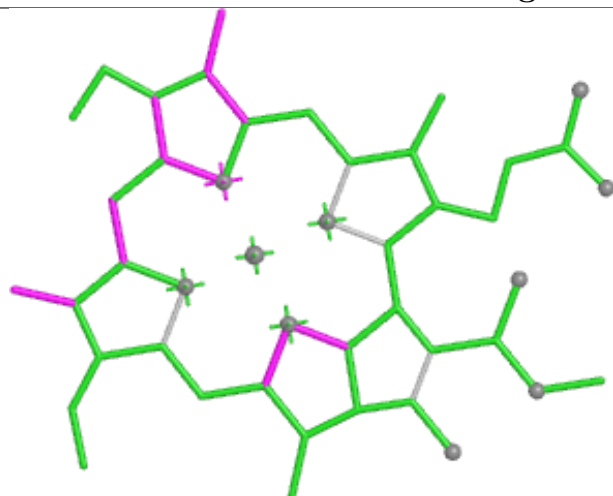


Torsions

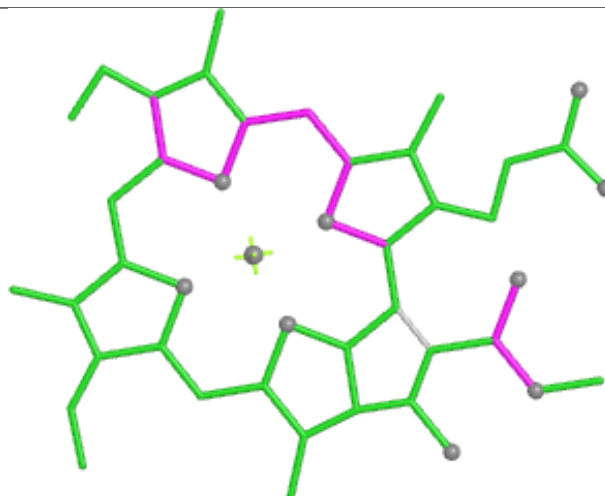


Rings

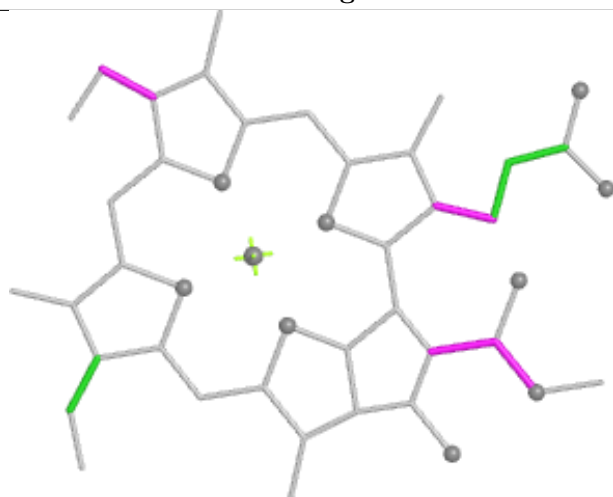
Ligand CLA 4 506



Bond lengths



Bond angles

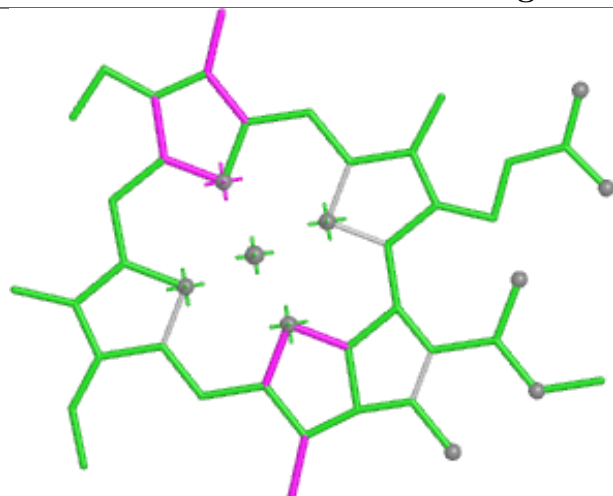


Torsions

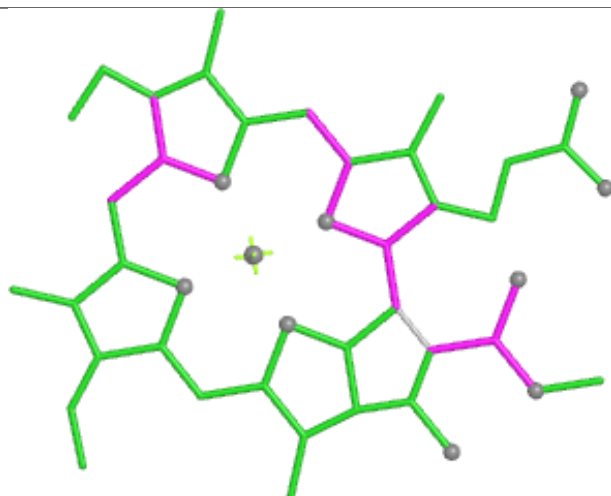


Rings

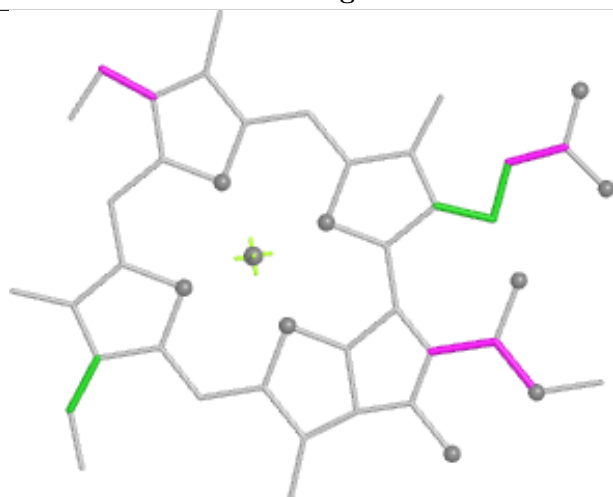
Ligand CLA b 507



Bond lengths



Bond angles

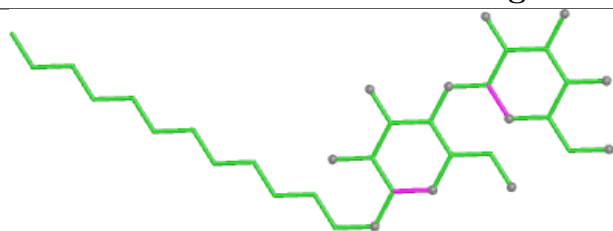


Torsions

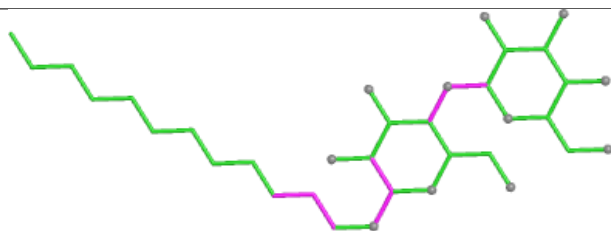


Rings

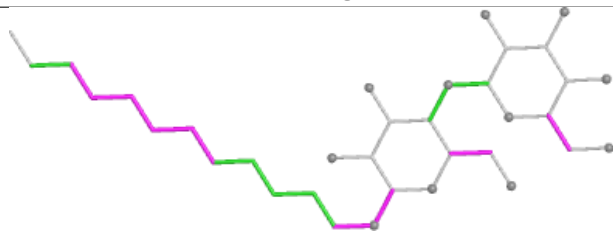
Ligand LMU f 1843



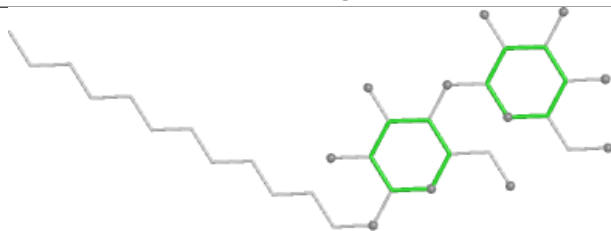
Bond lengths



Bond angles

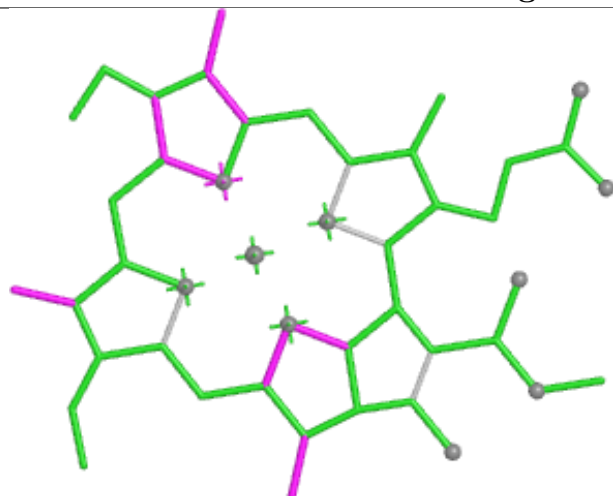


Torsions

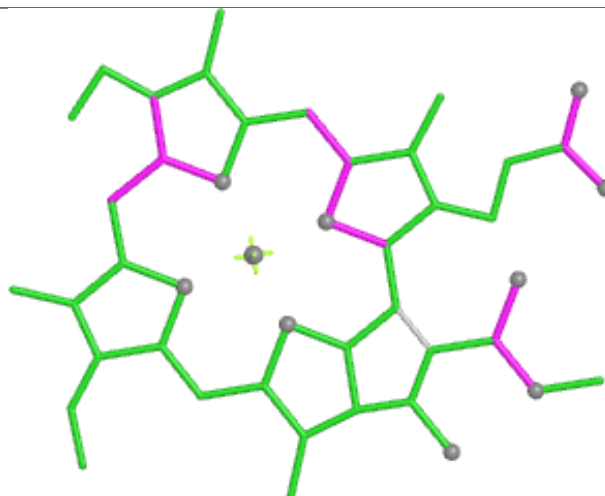


Rings

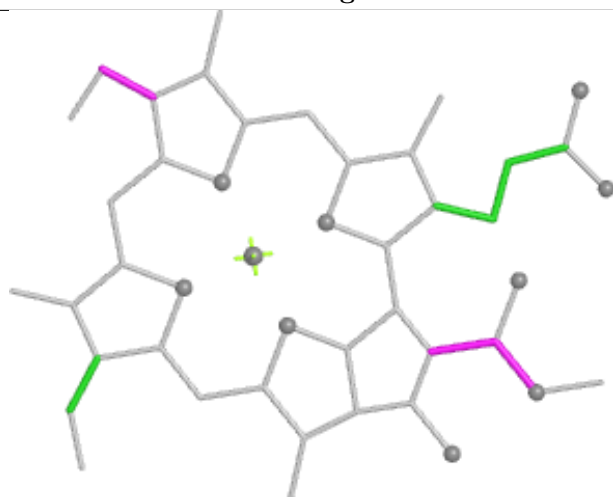
Ligand CLA 2 506



Bond lengths



Bond angles

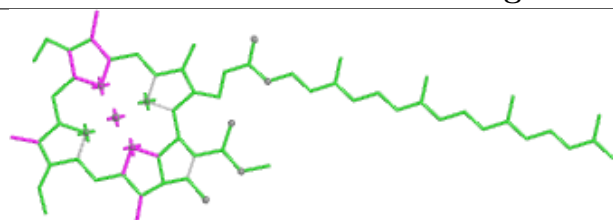


Torsions

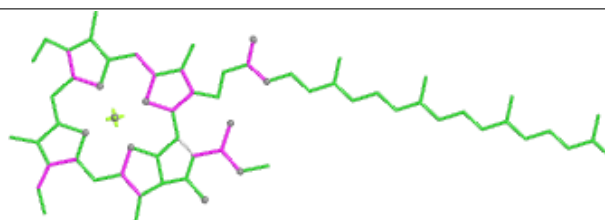


Rings

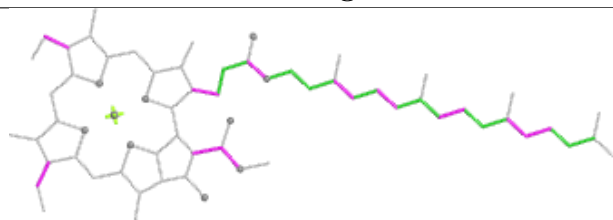
Ligand CLA G 1132



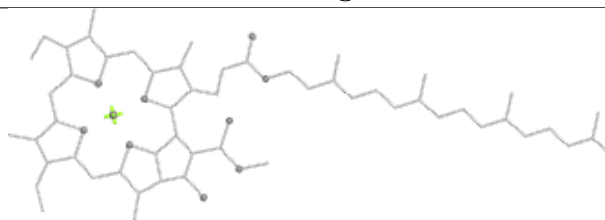
Bond lengths



Bond angles

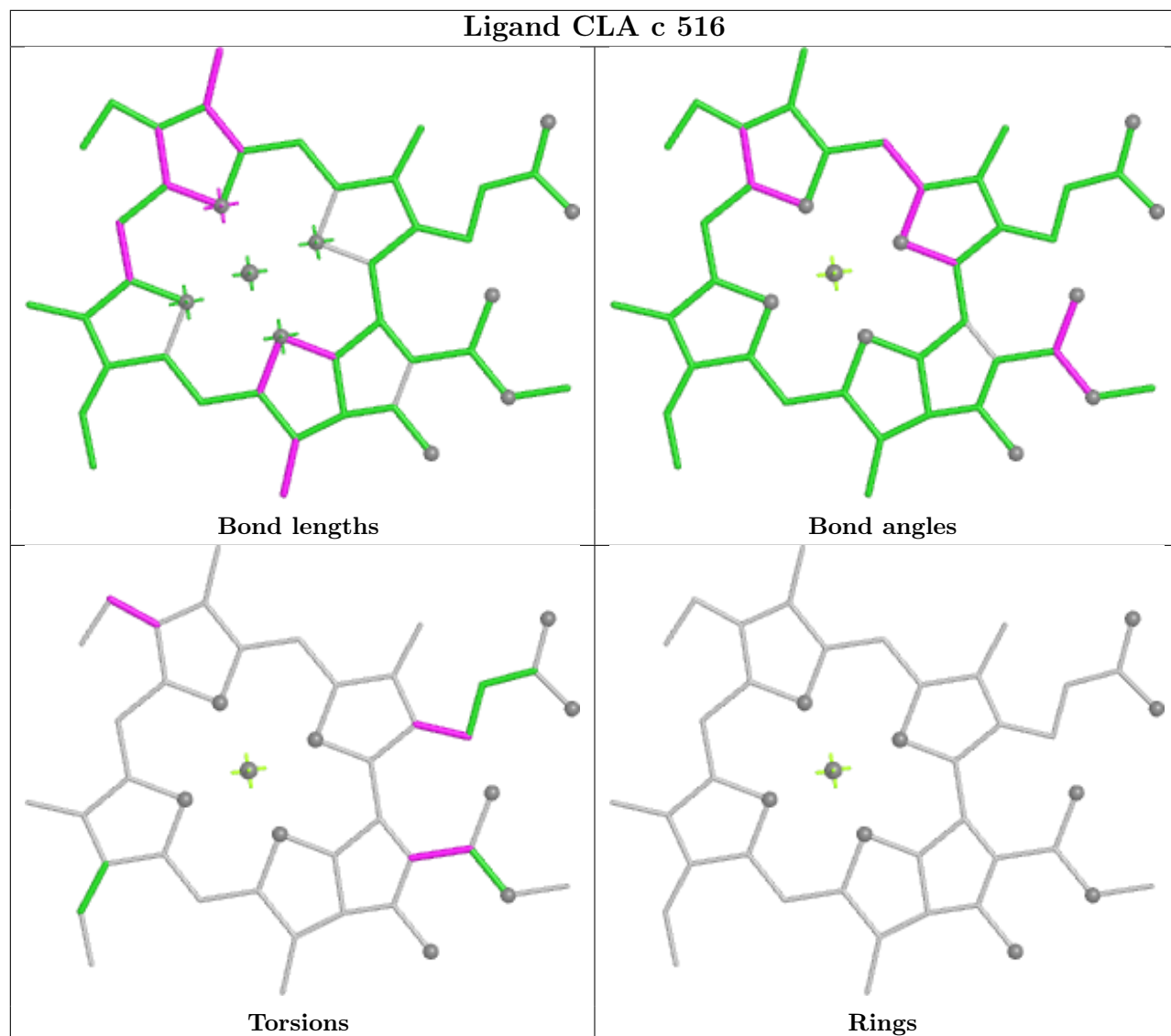


Torsions

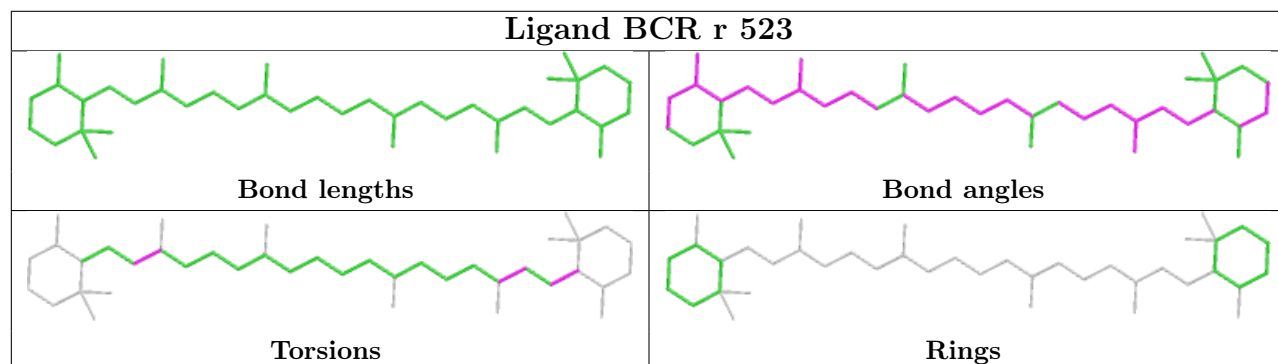


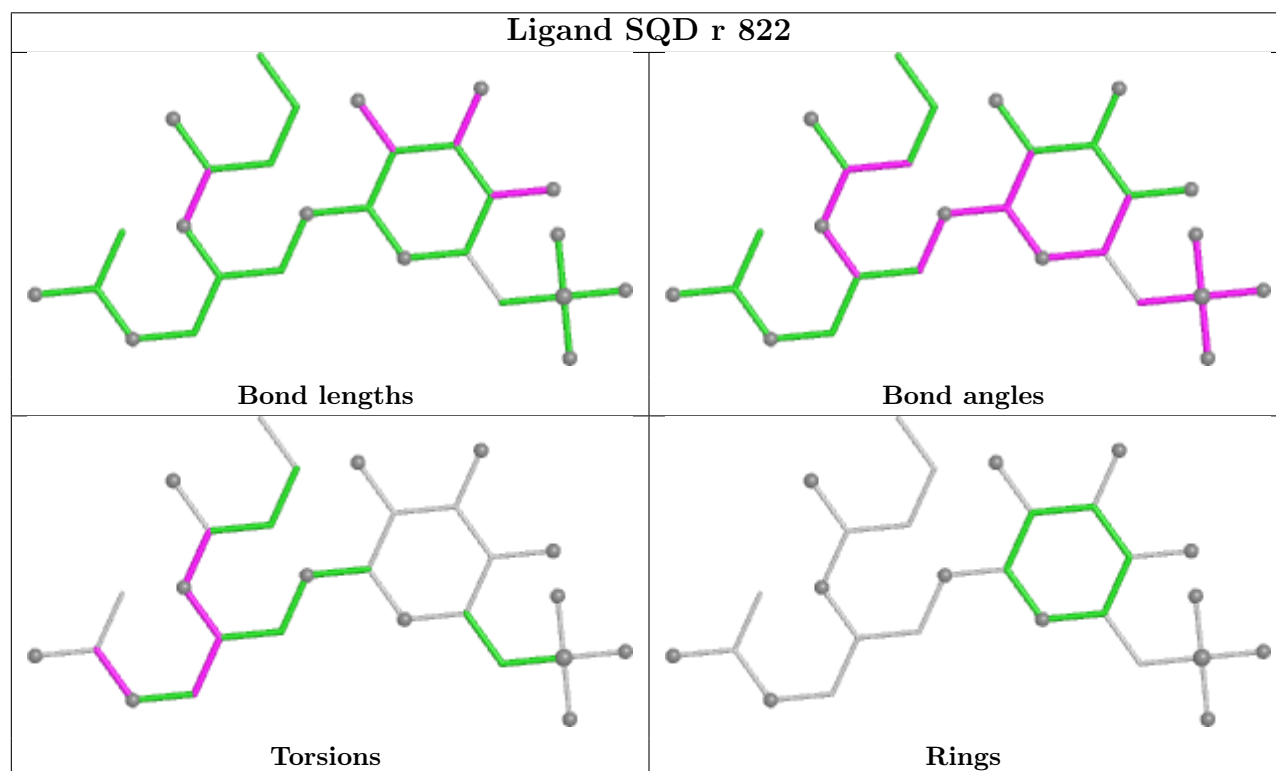
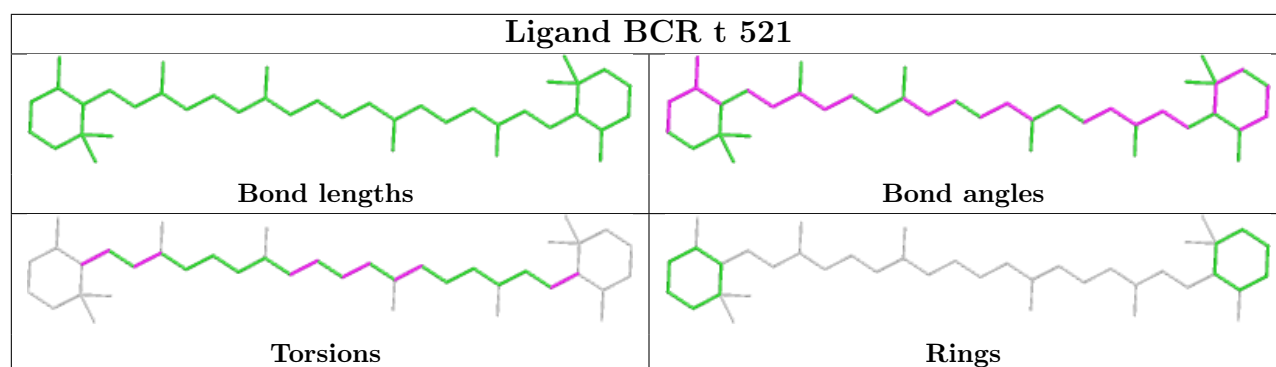
Rings

Ligand CLA c 516

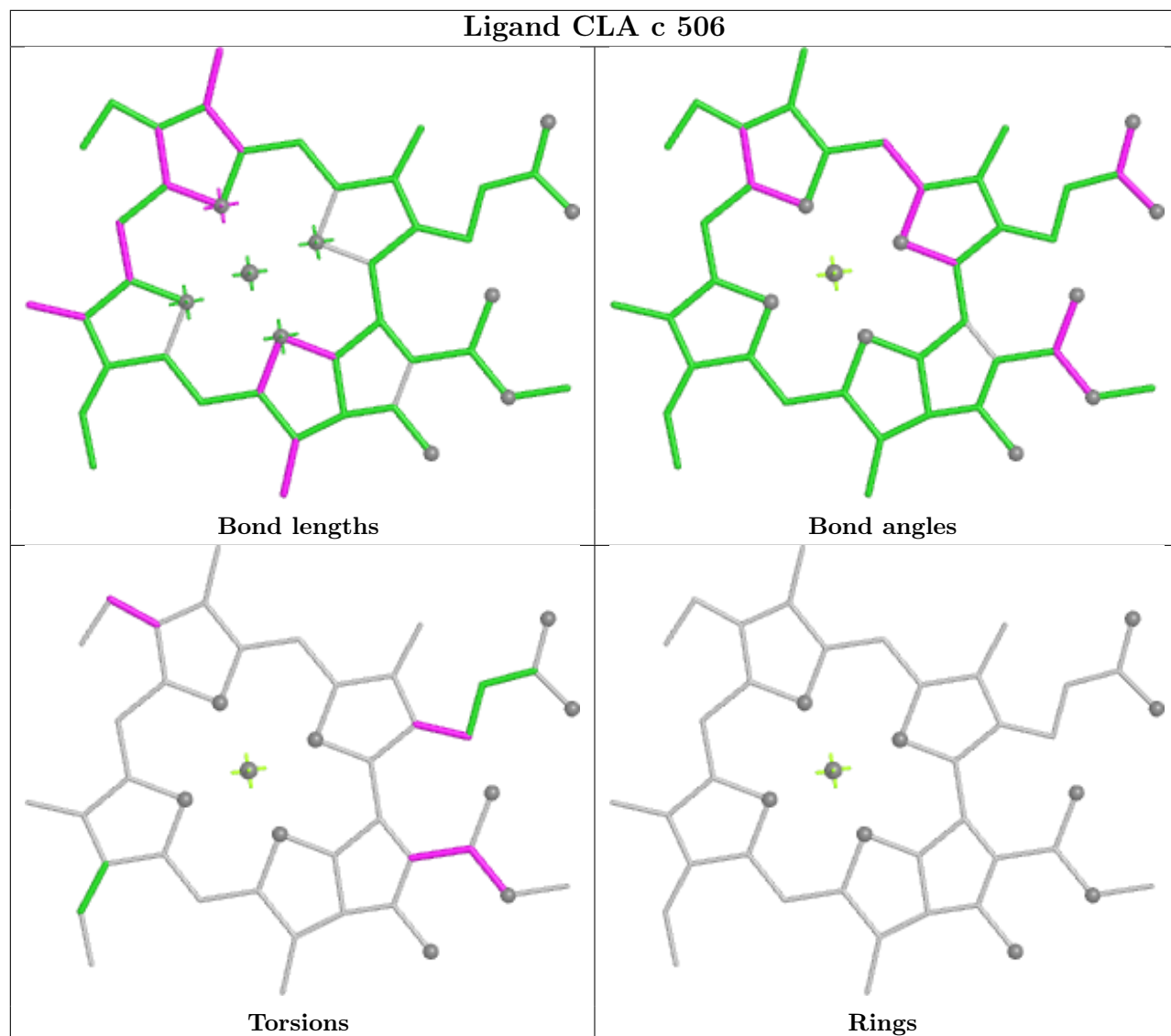


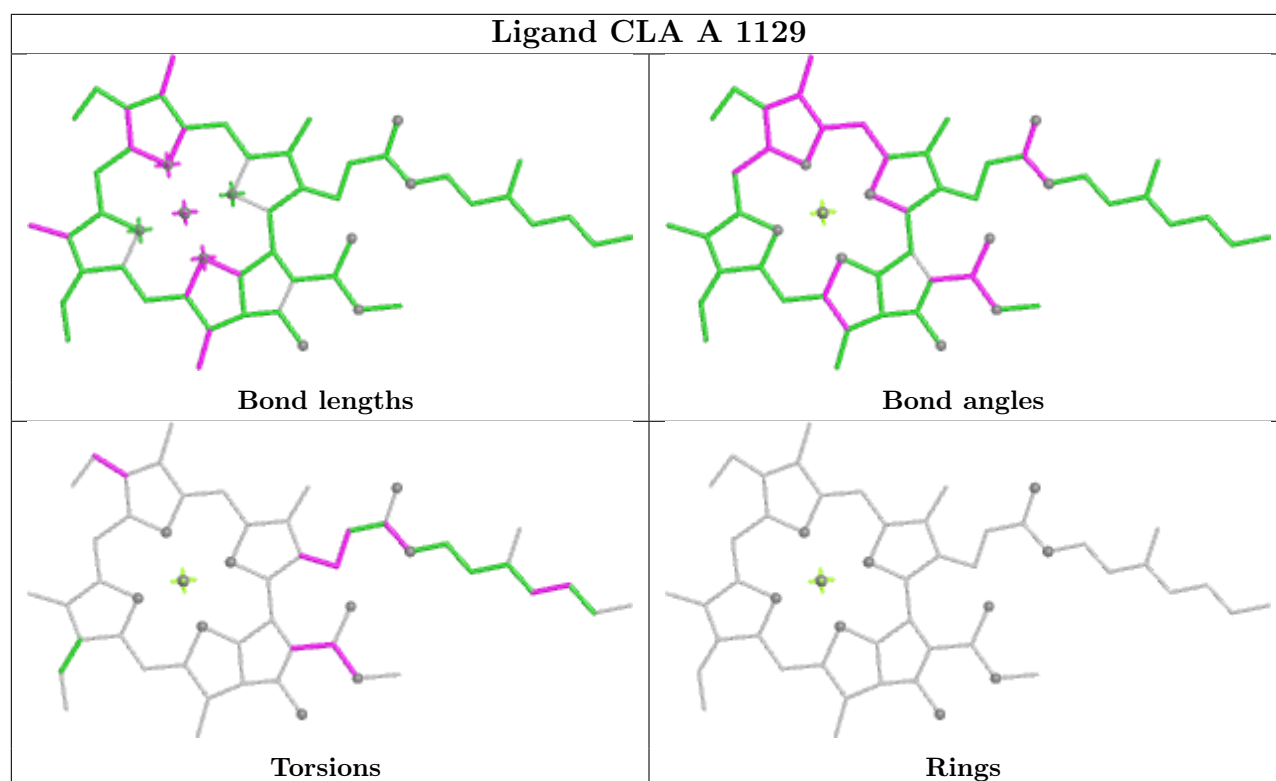
Ligand BCR r 523



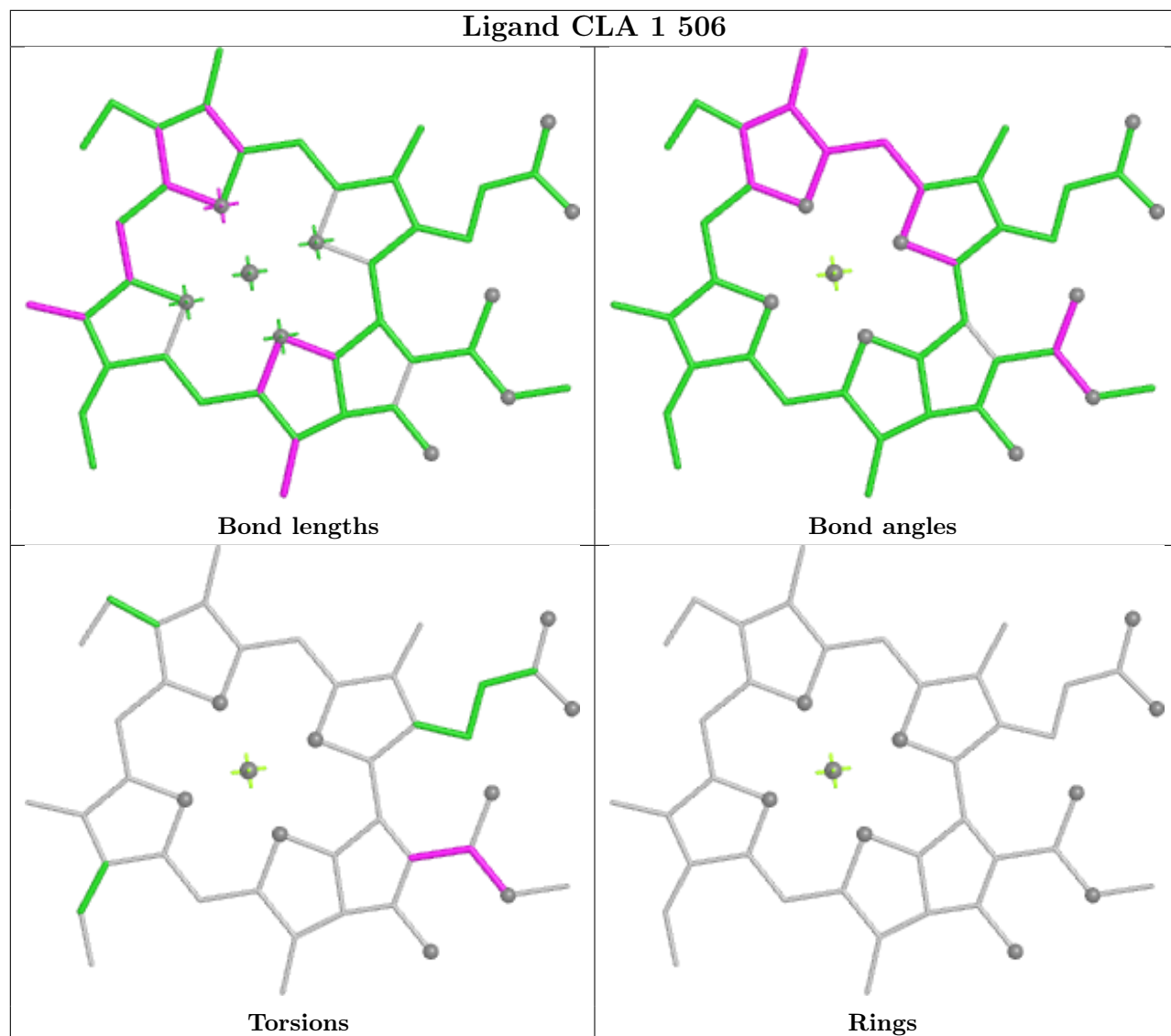


Ligand CLA c 506

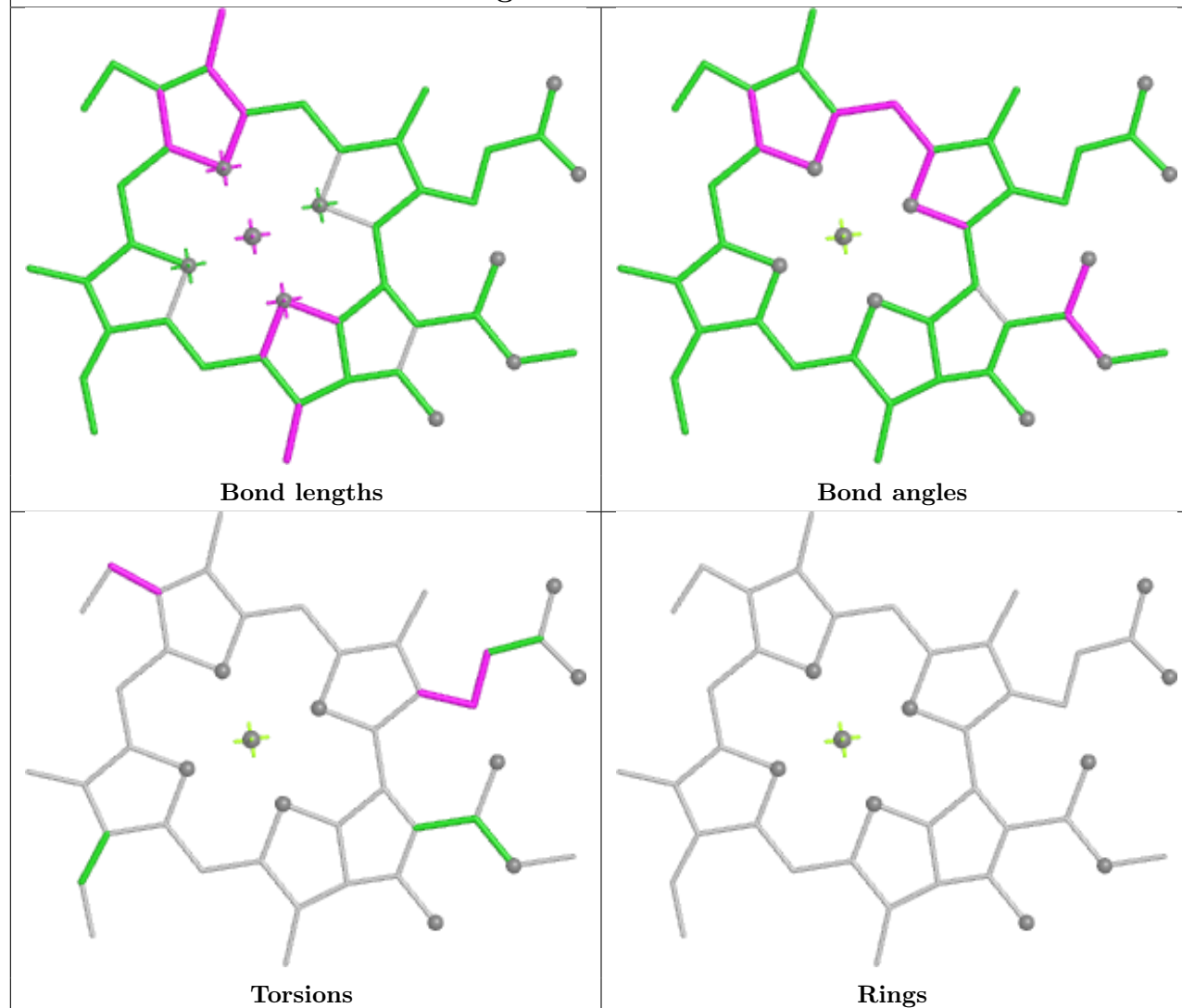




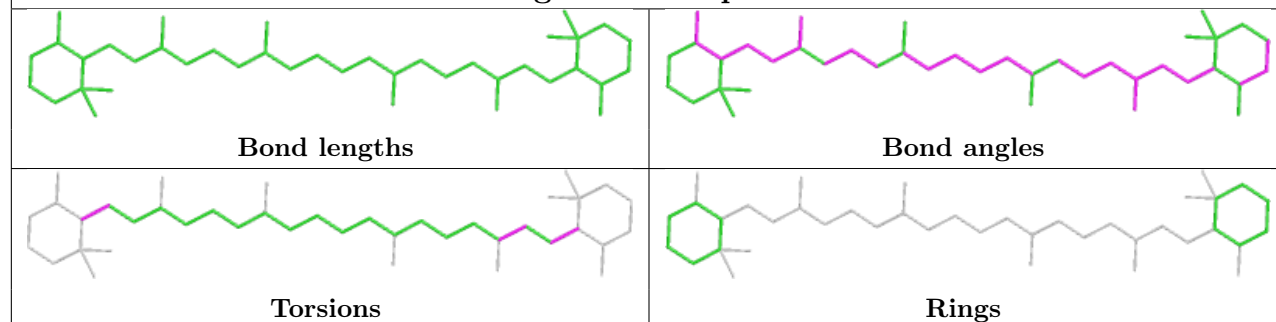
Ligand CLA 1 506



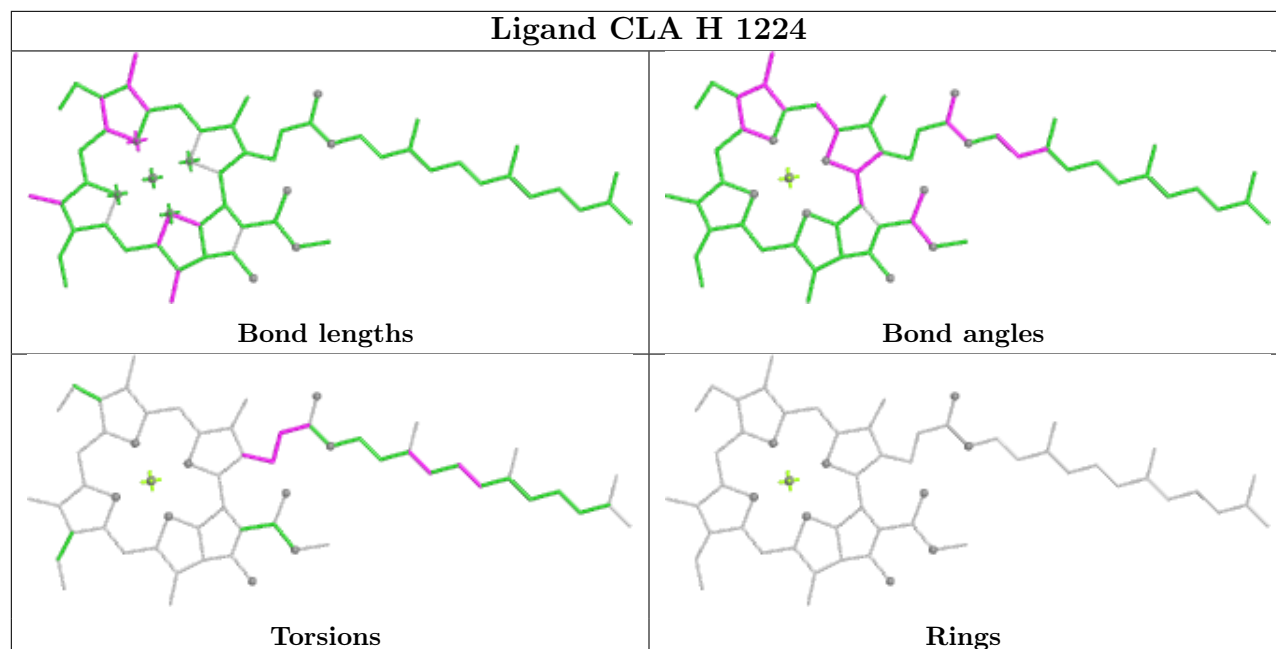
Ligand CLA 3 512



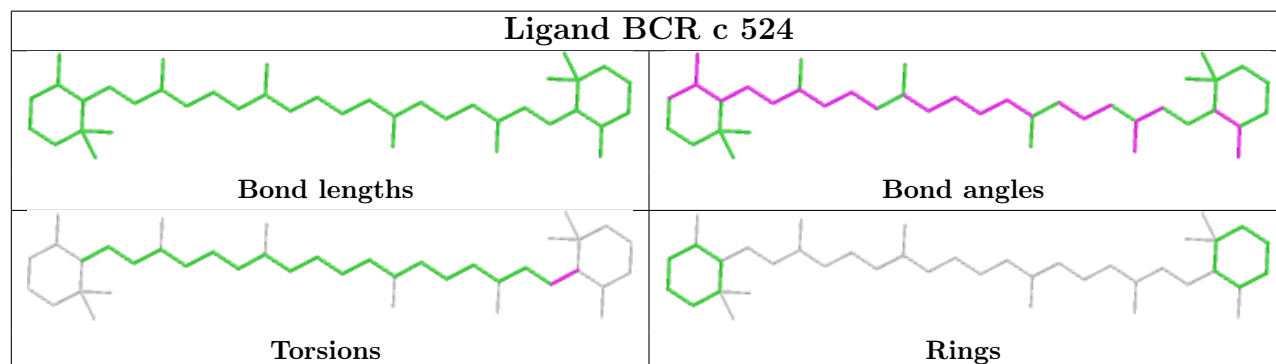
Ligand BCR q 523



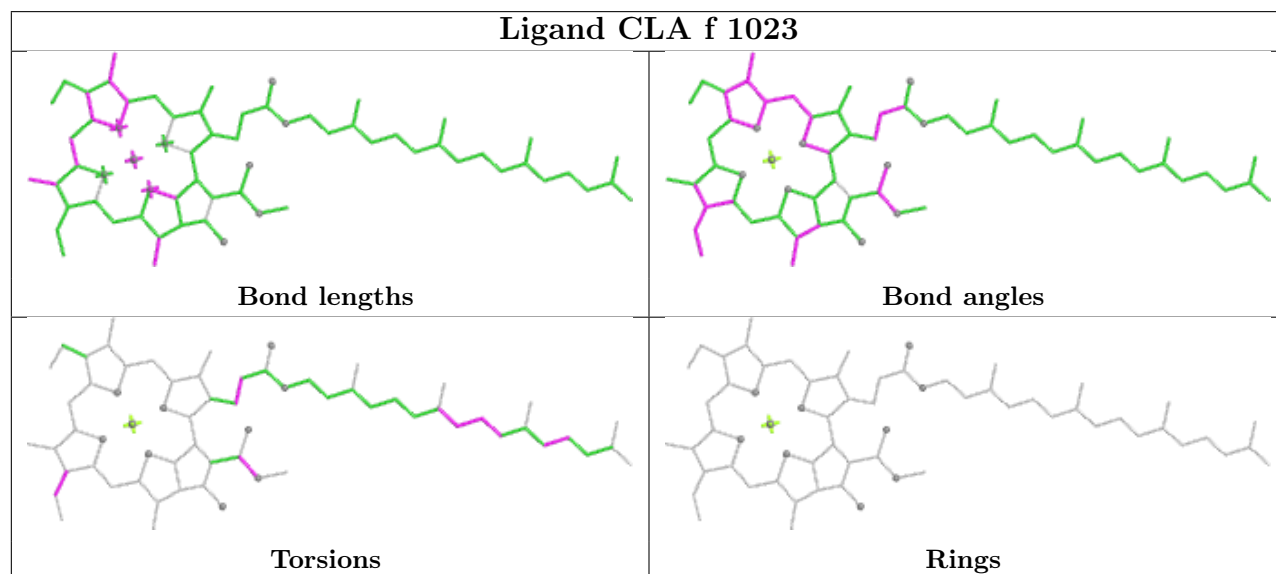
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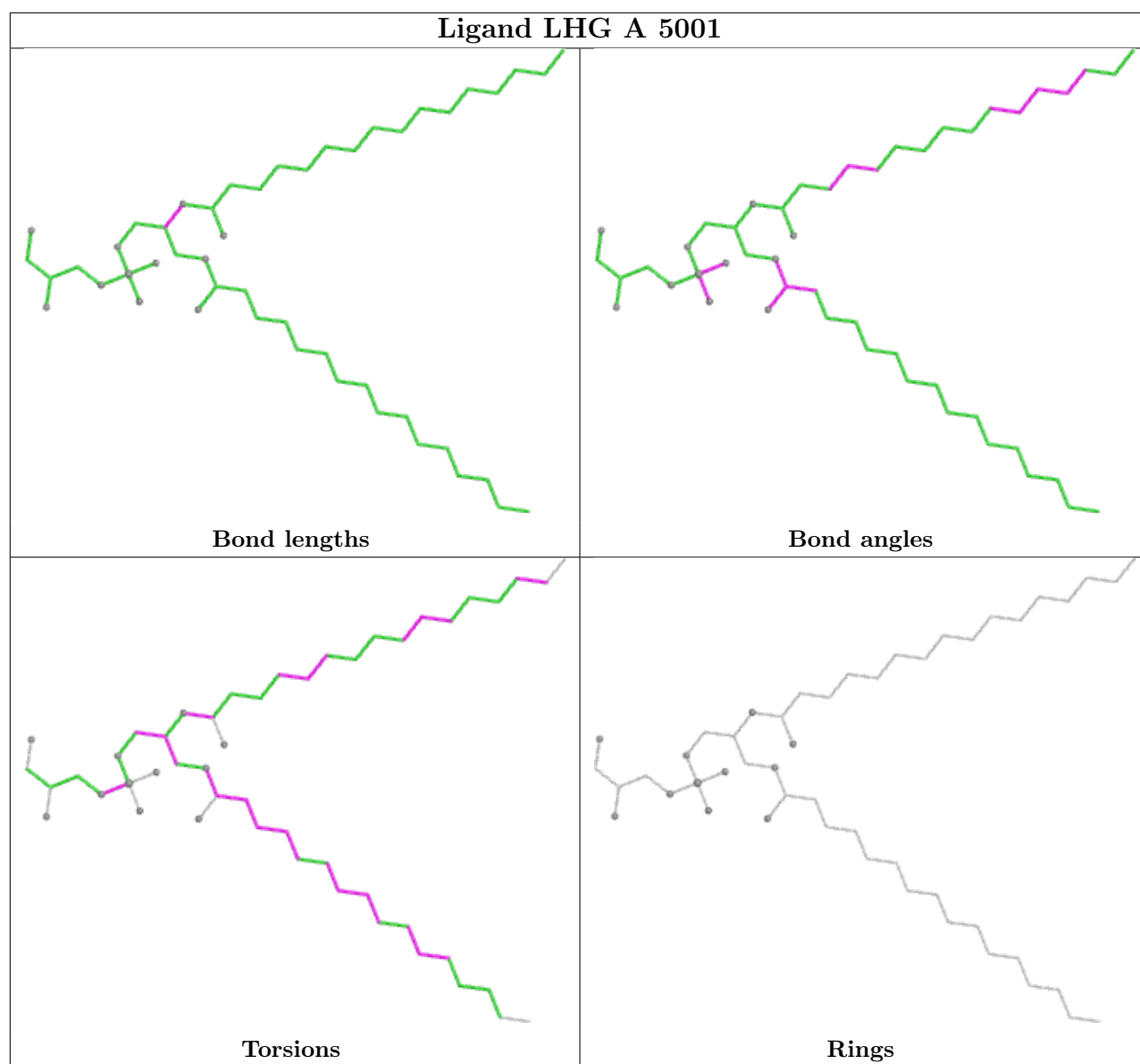


Ligand BCR c 524

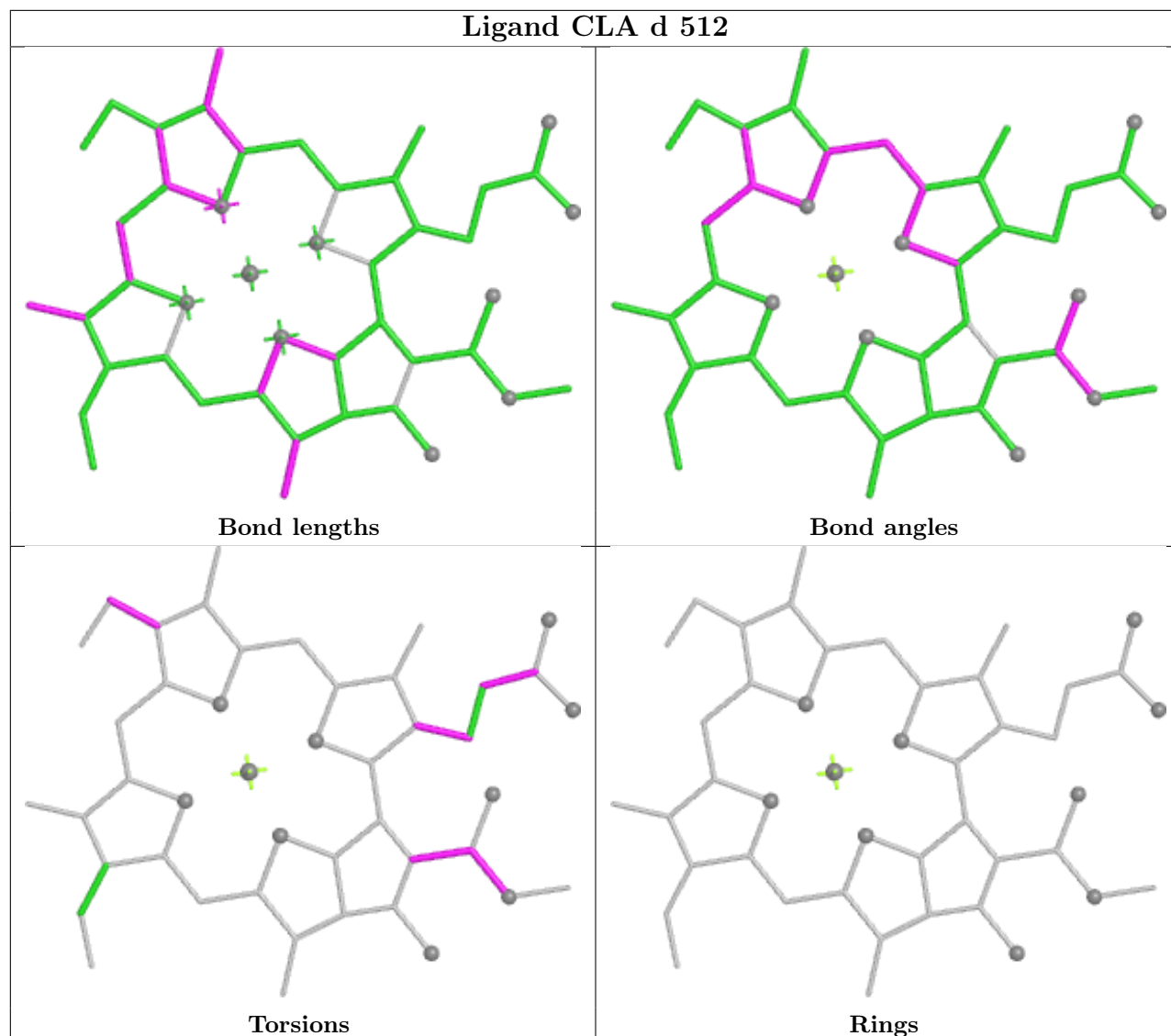


Ligand CLA f 1023

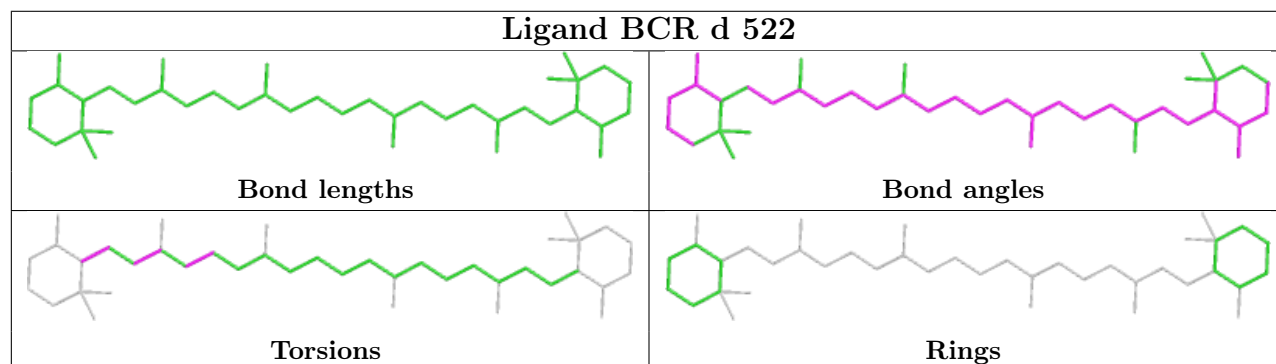


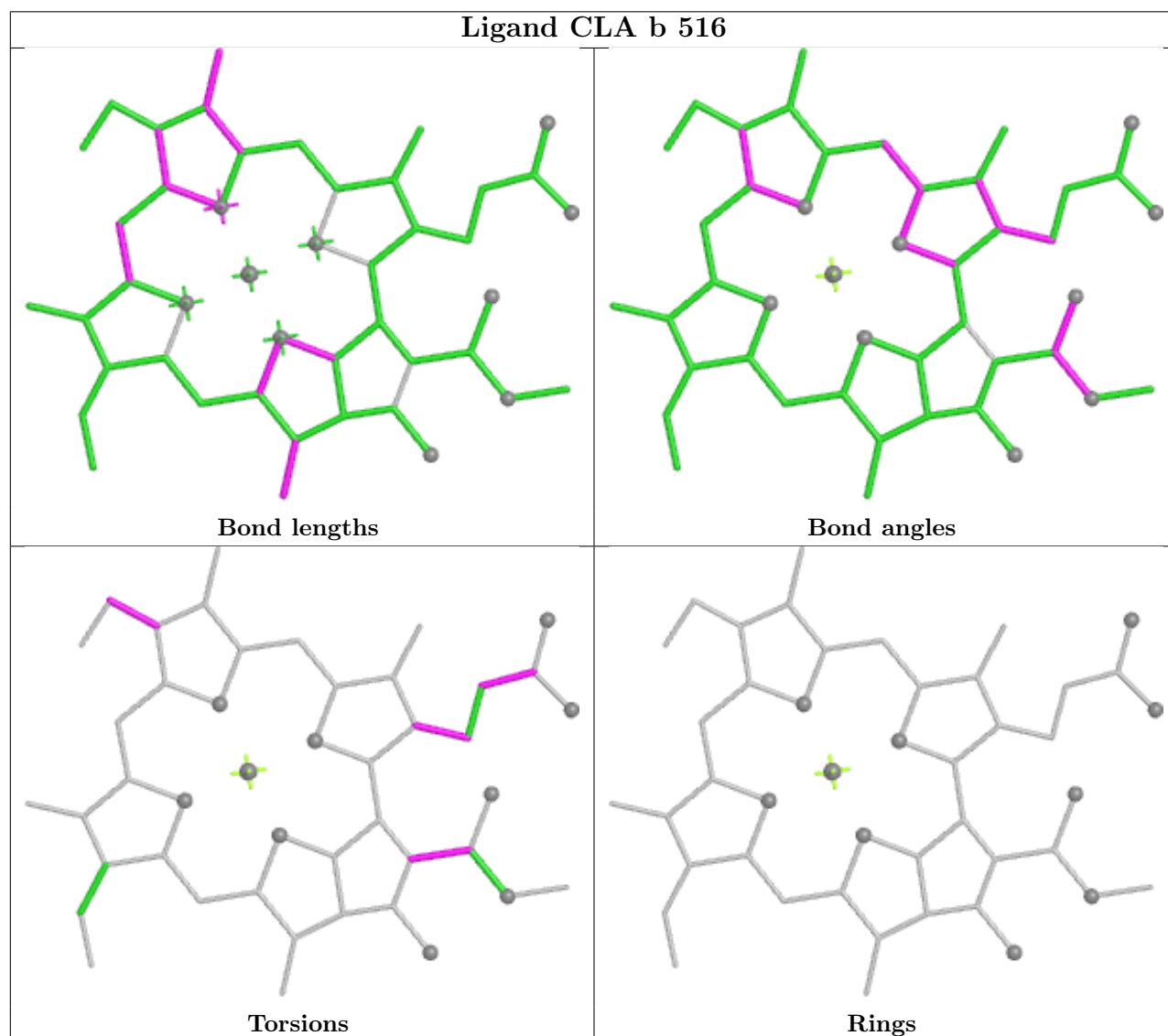
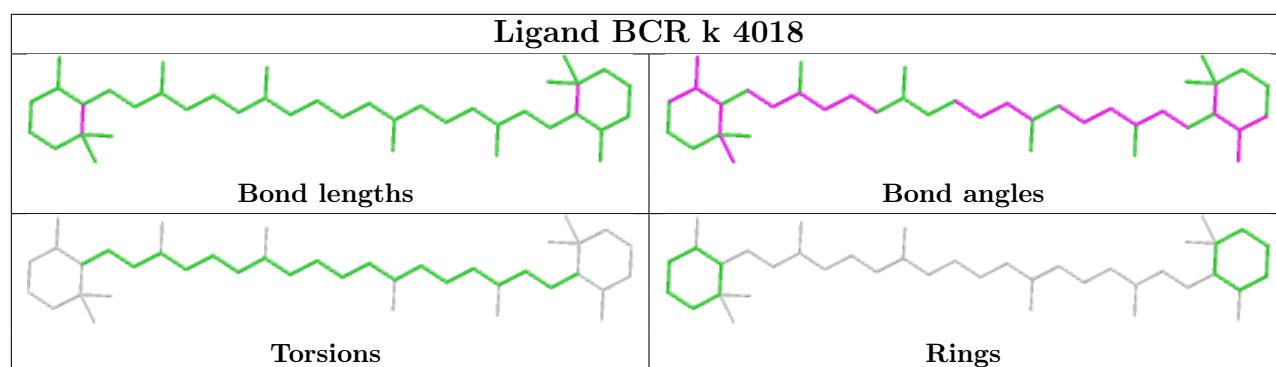


Ligand CLA d 512

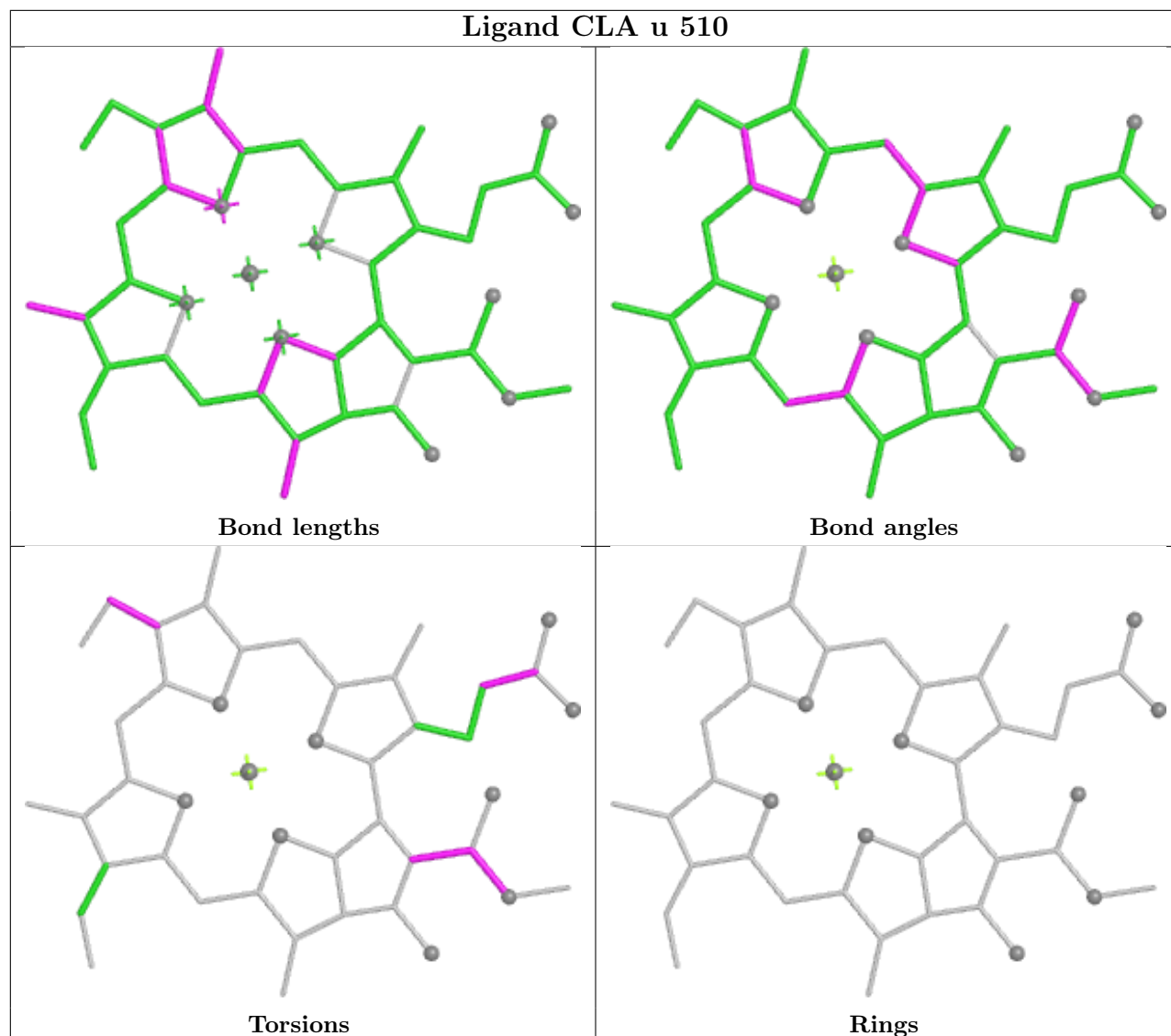


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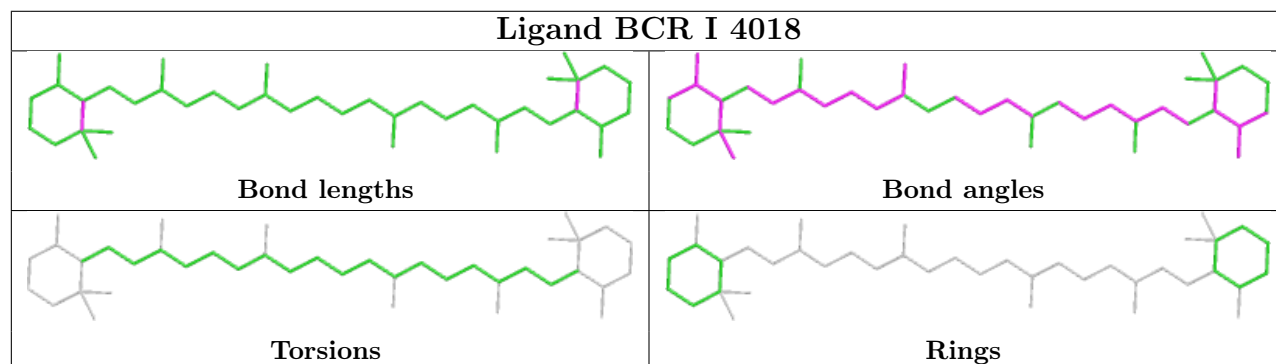




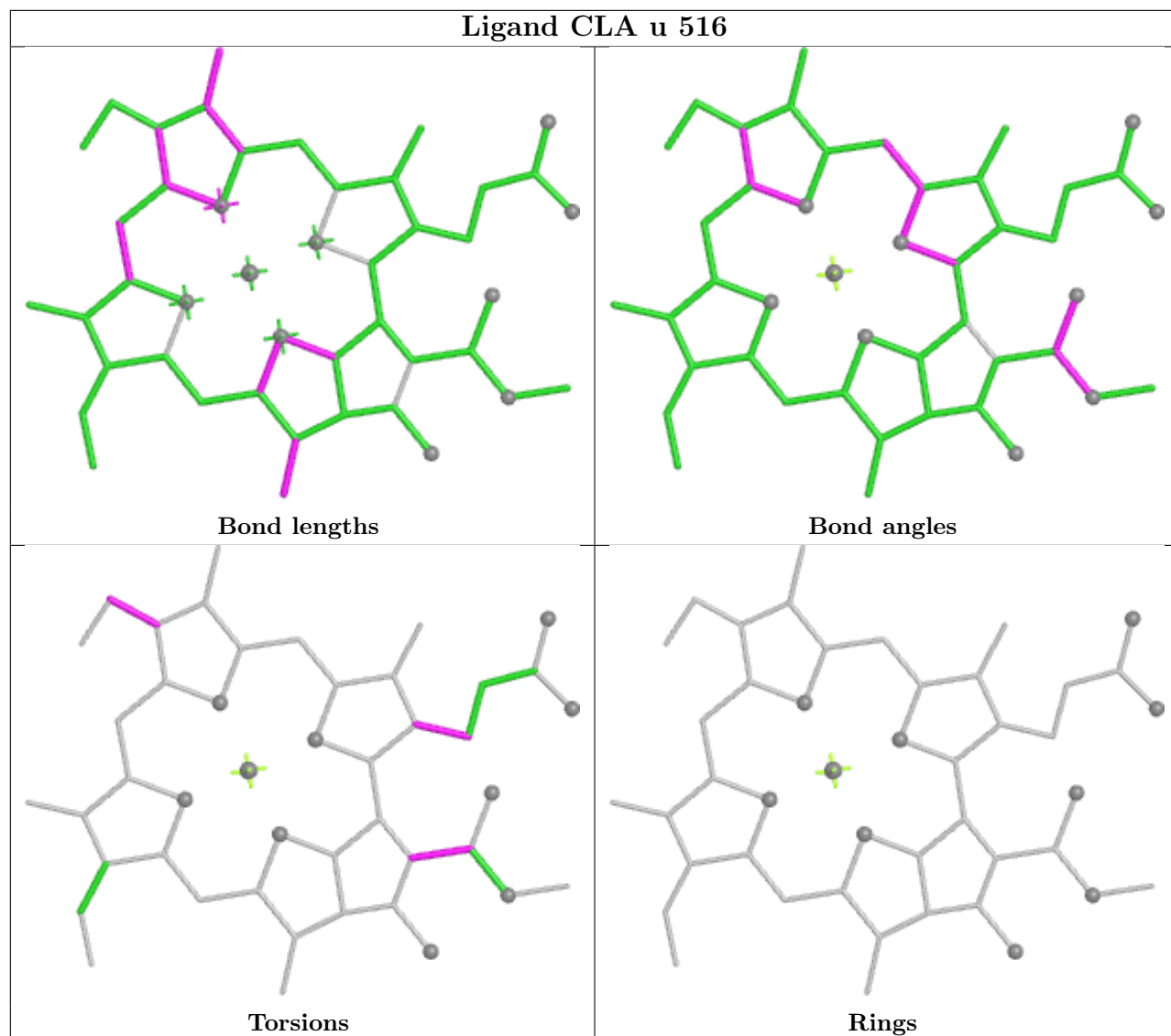
Ligand CLA u 510



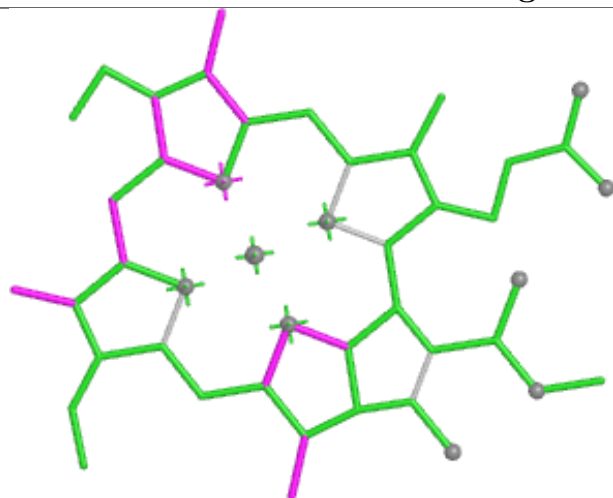
Ligand BCR I 4018



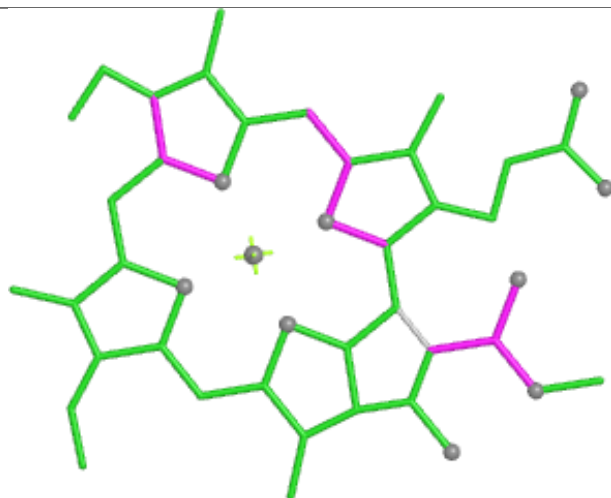
Ligand CLA u 516



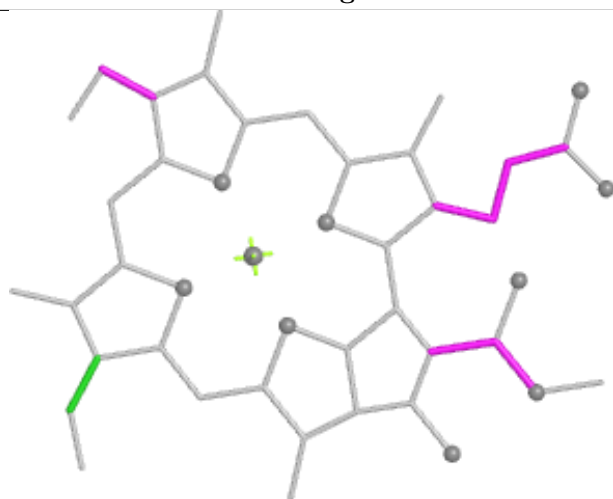
Ligand CLA 6 501



Bond lengths



Bond angles

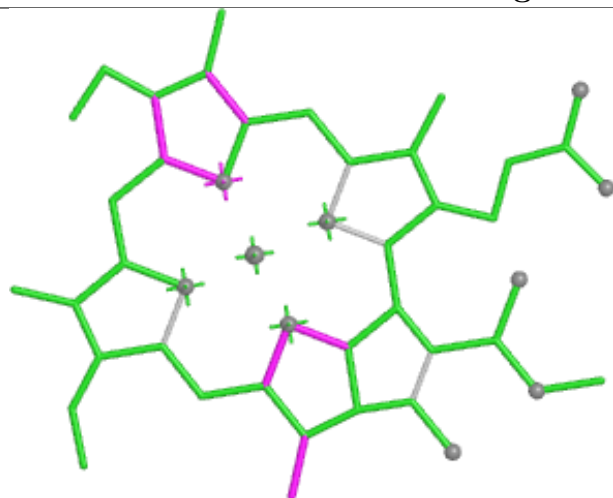


Torsions

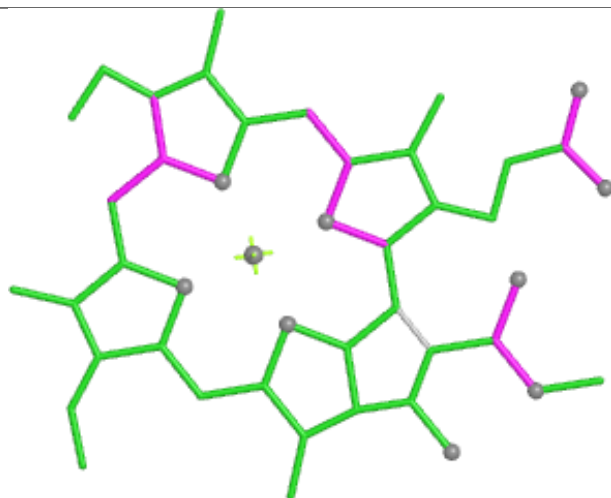


Rings

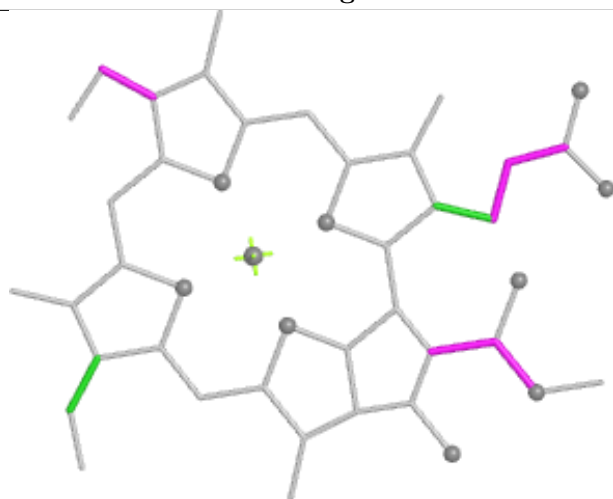
Ligand CLA Y 518



Bond lengths



Bond angles

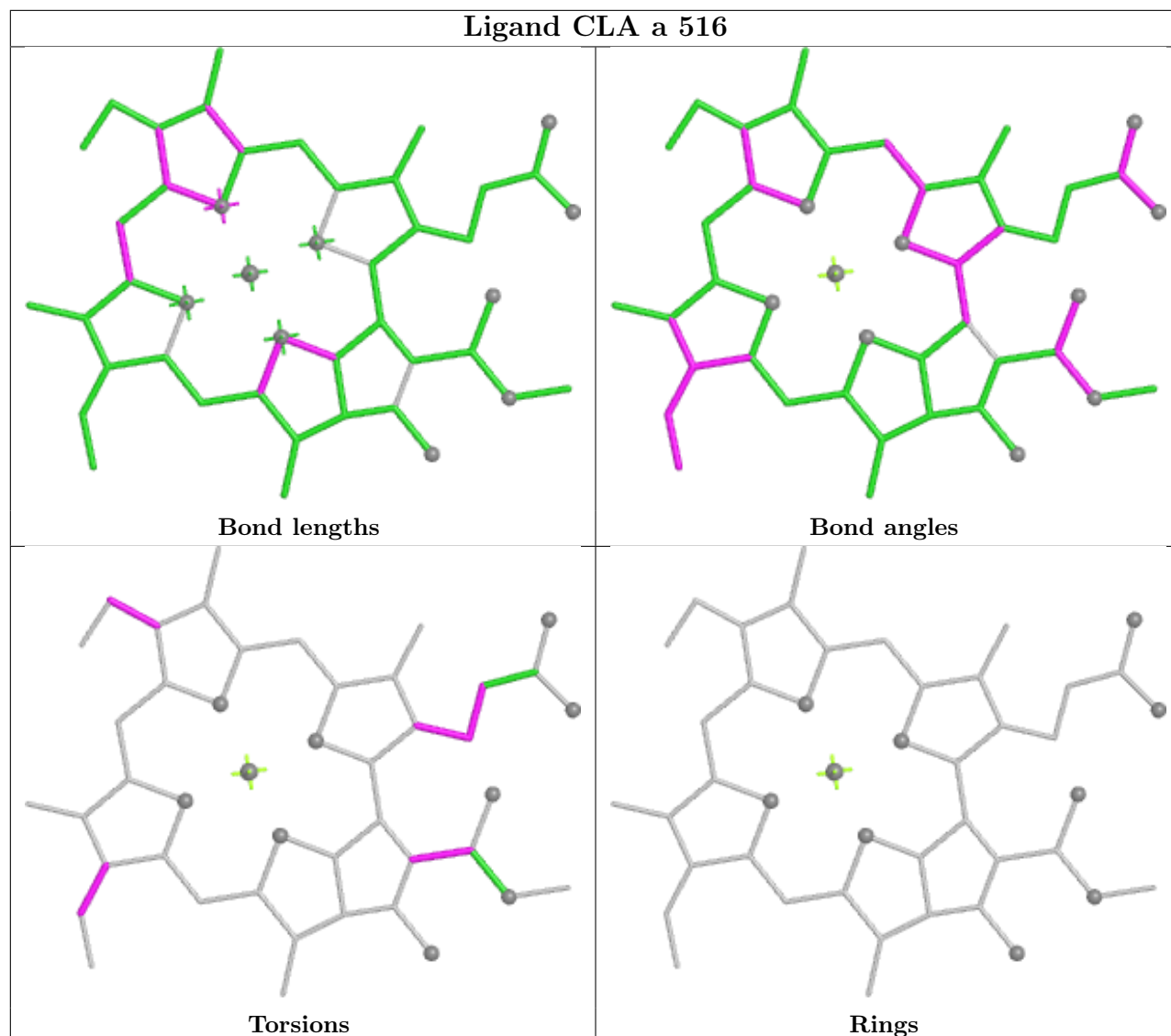


Torsions

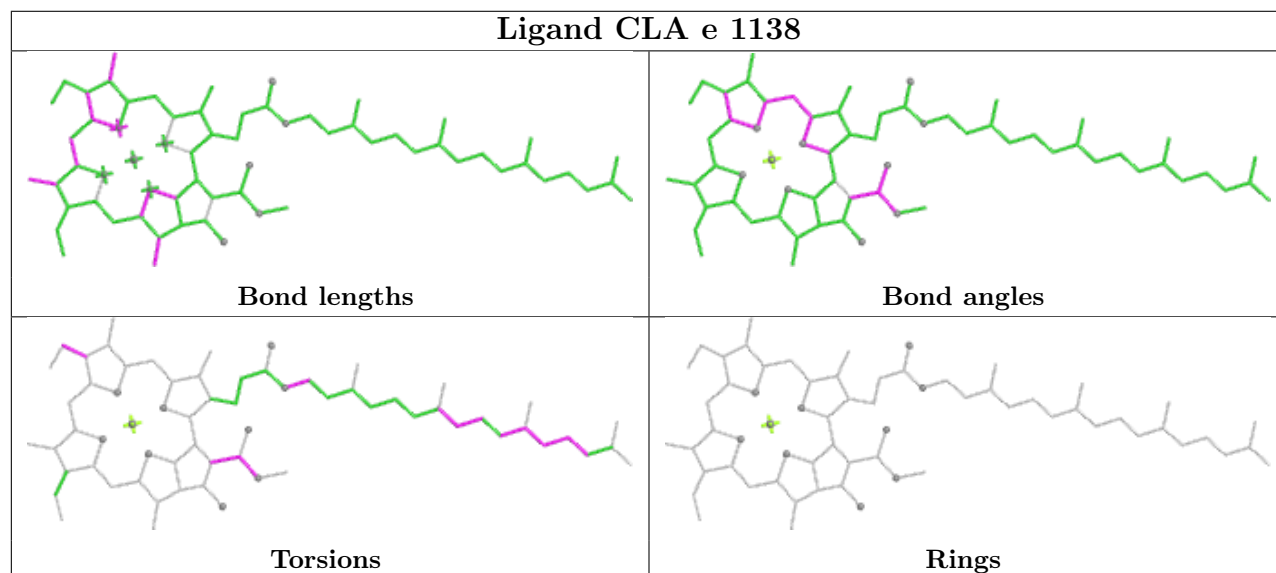


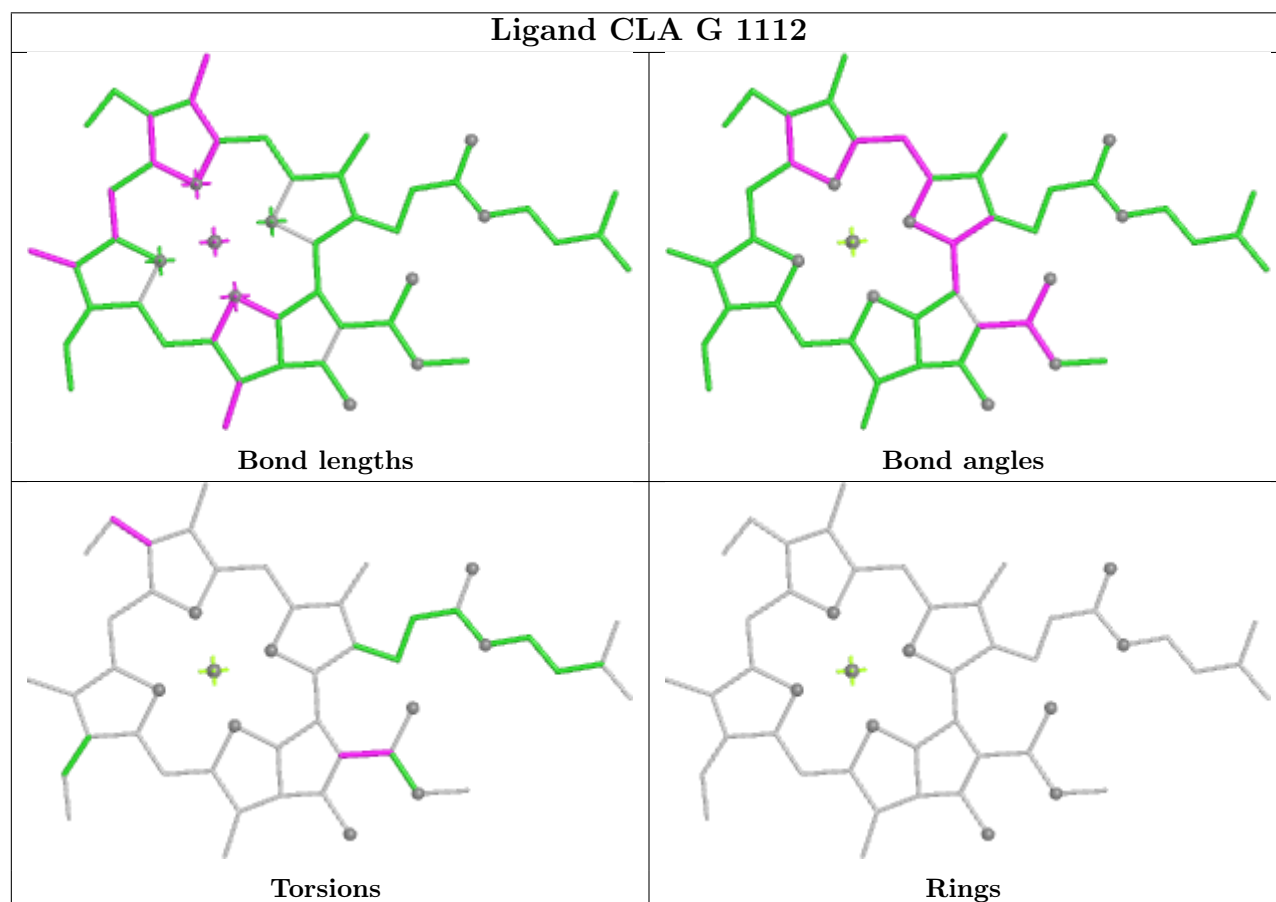
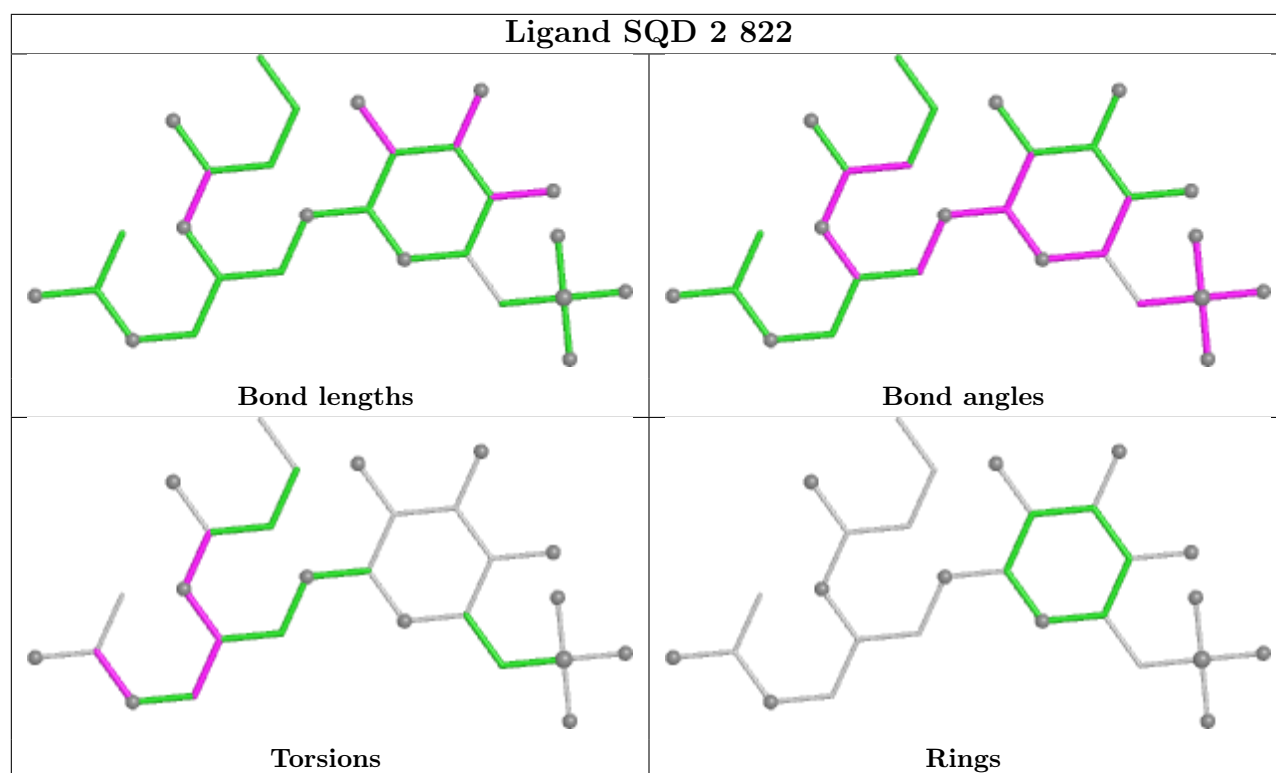
Rings

Ligand CLA a 516

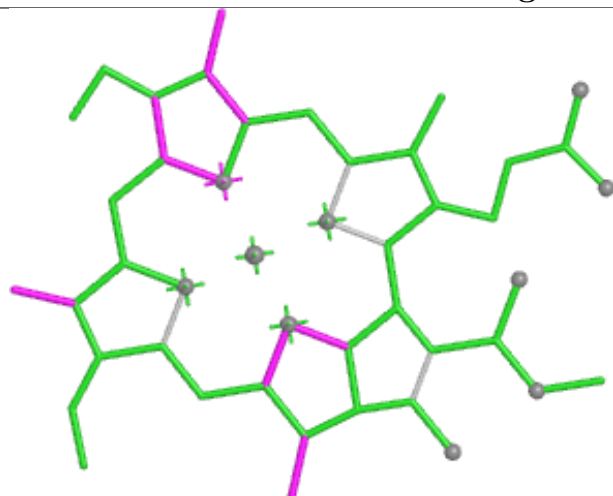


Ligand CLA e 1138

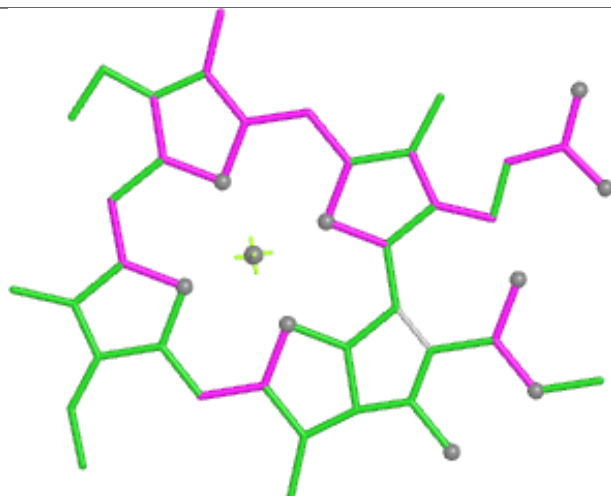




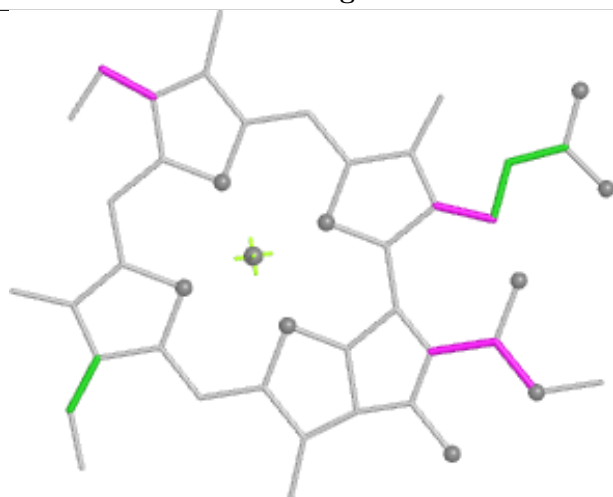
Ligand CLA 6 508



Bond lengths



Bond angles

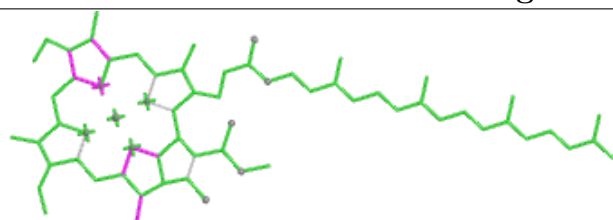


Torsions

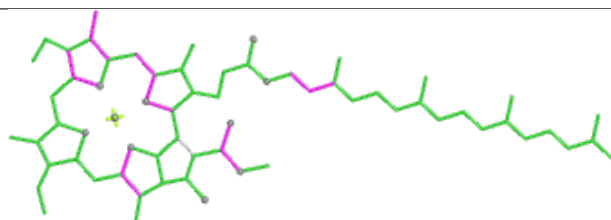


Rings

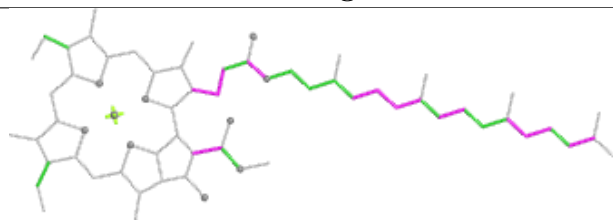
Ligand CLA Z 505



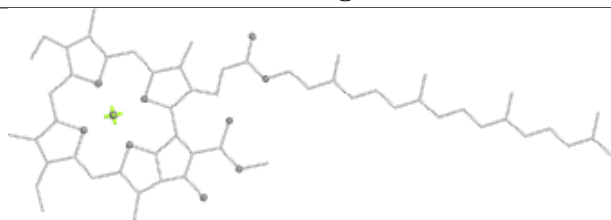
Bond lengths



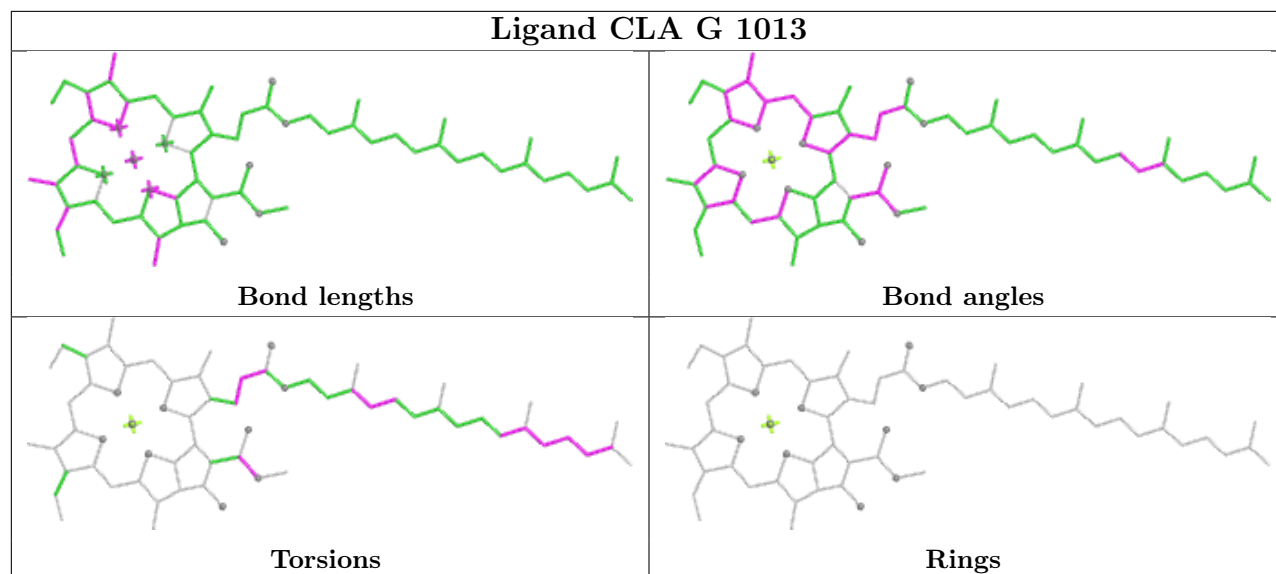
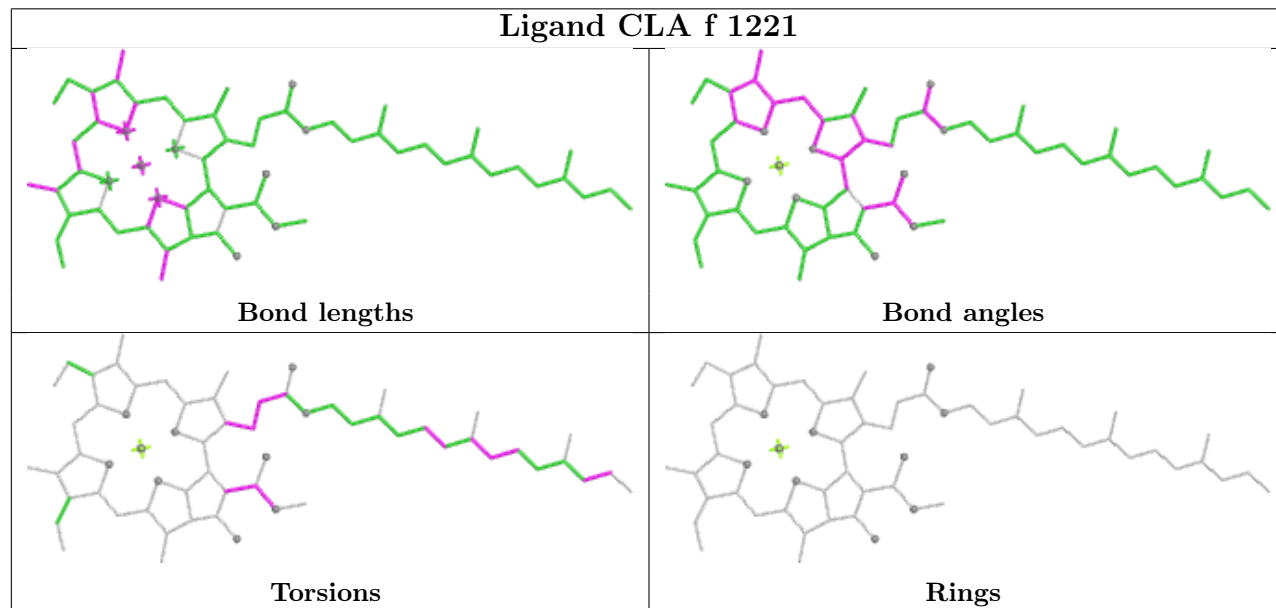
Bond angles



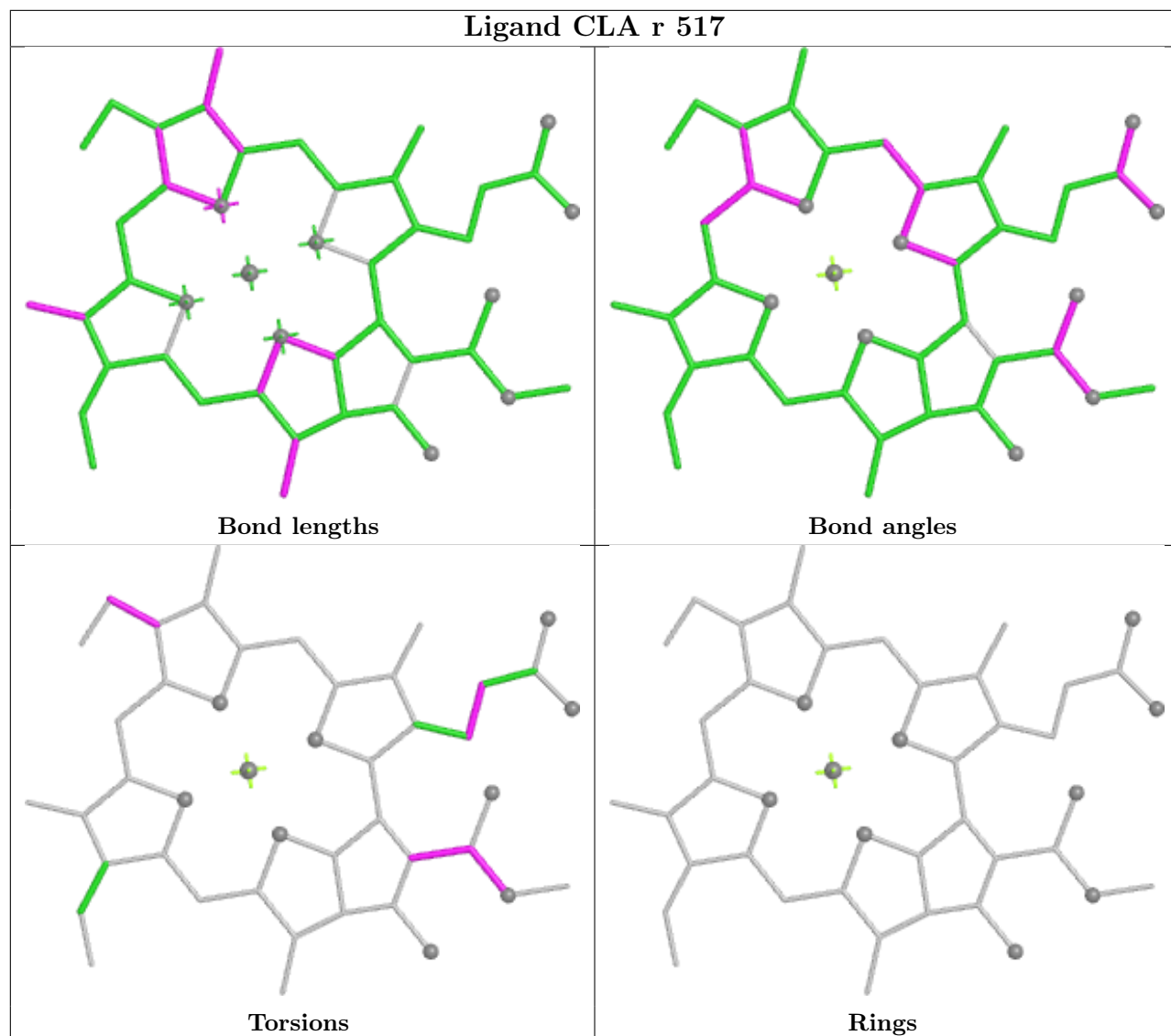
Torsions



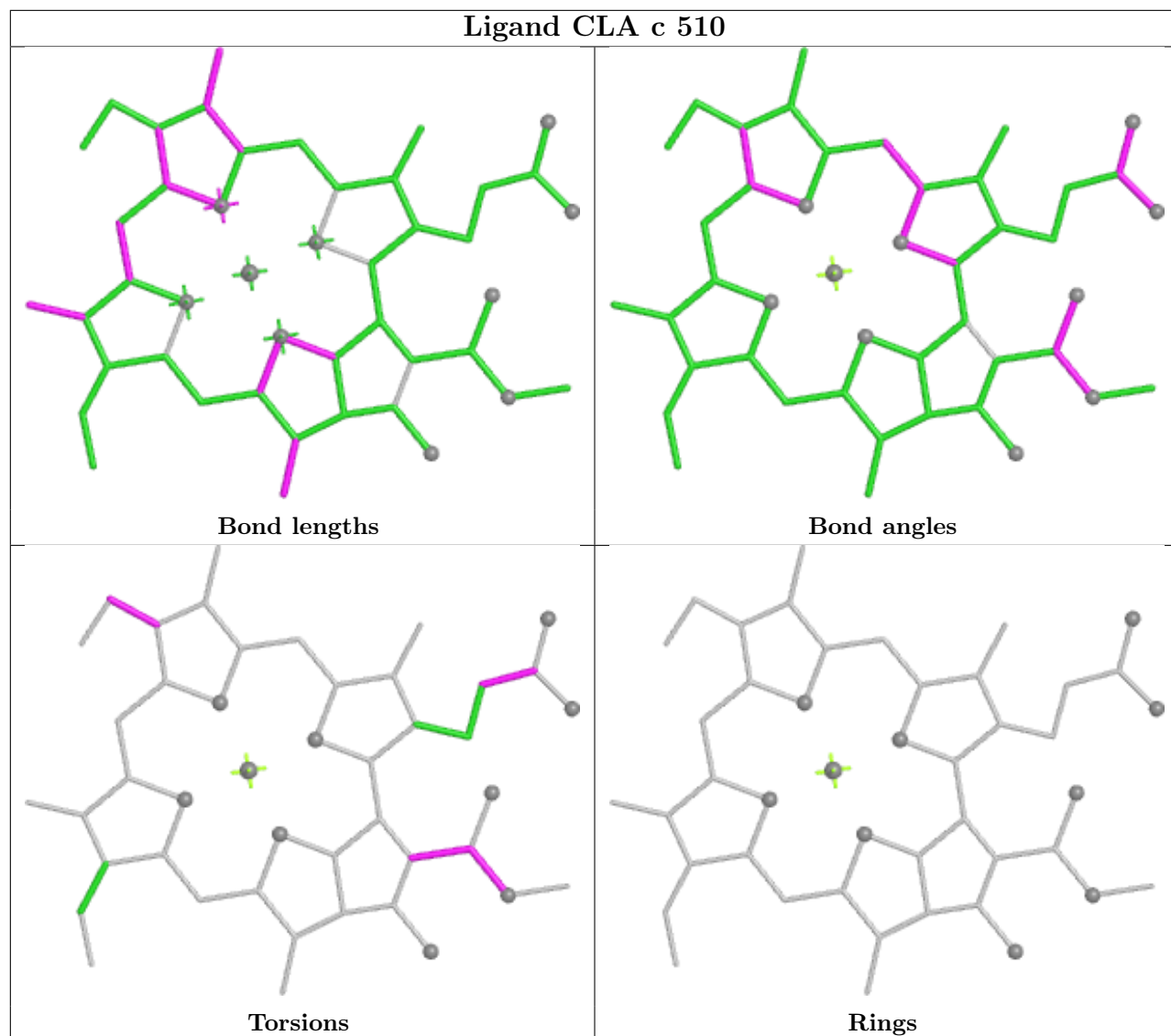
Rings

Ligand CLA G 1013**Ligand CLA f 1221**

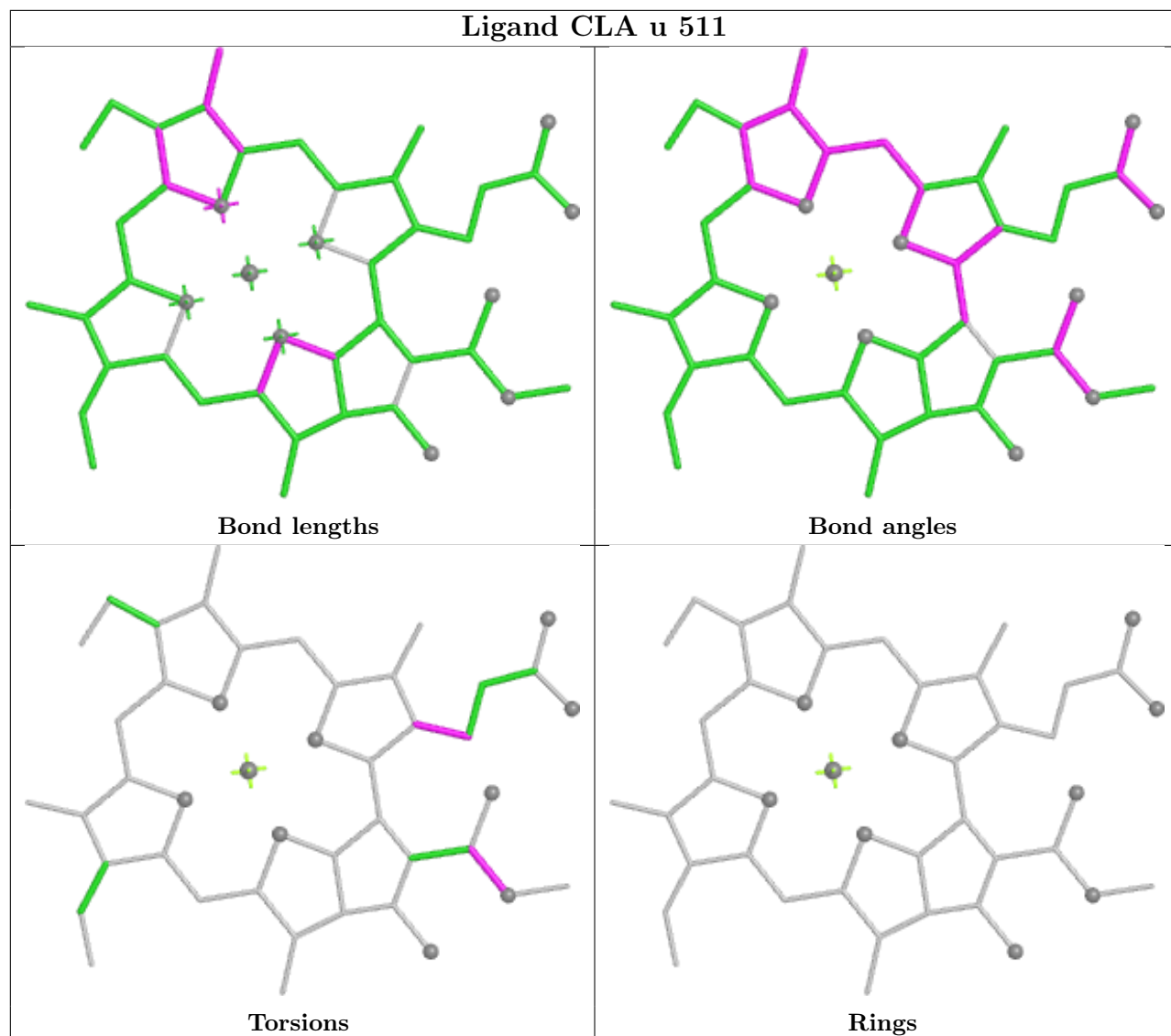
Ligand CLA r 517



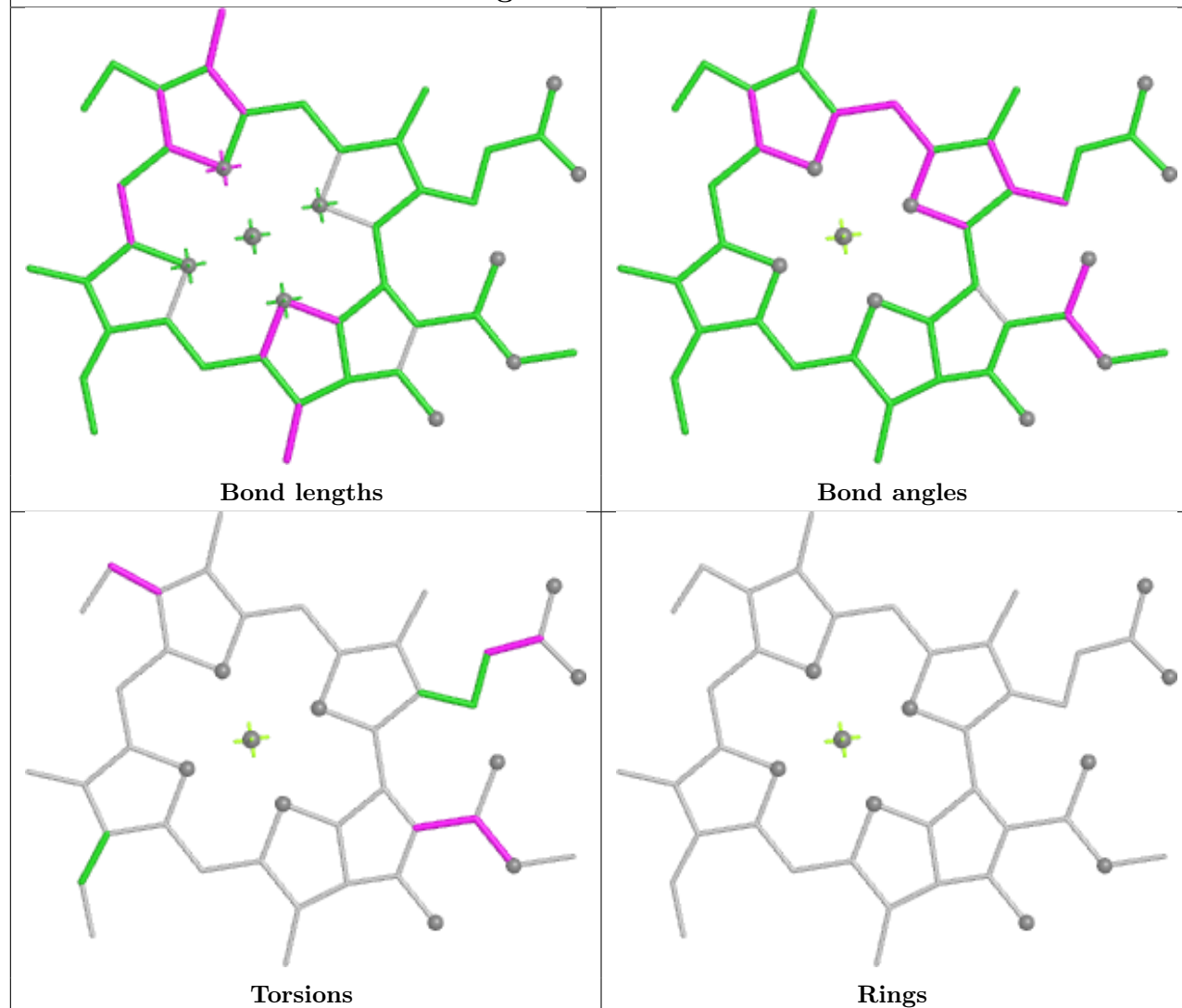
Ligand CLA c 510



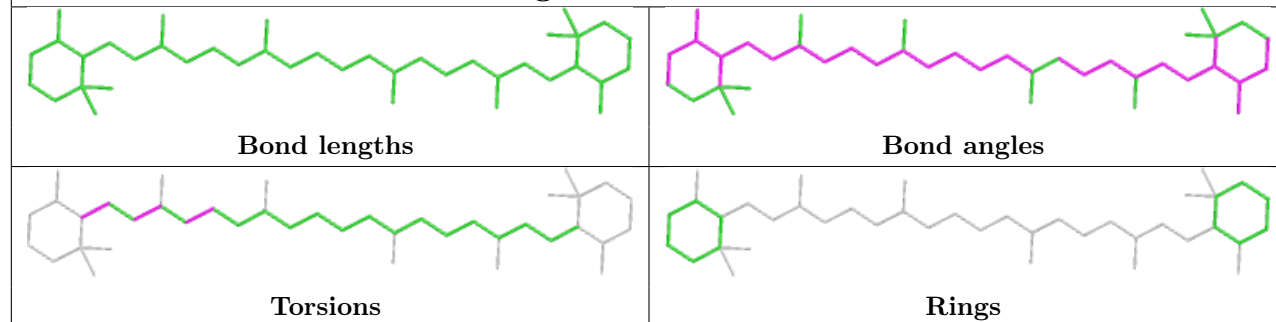
Ligand CLA u 511

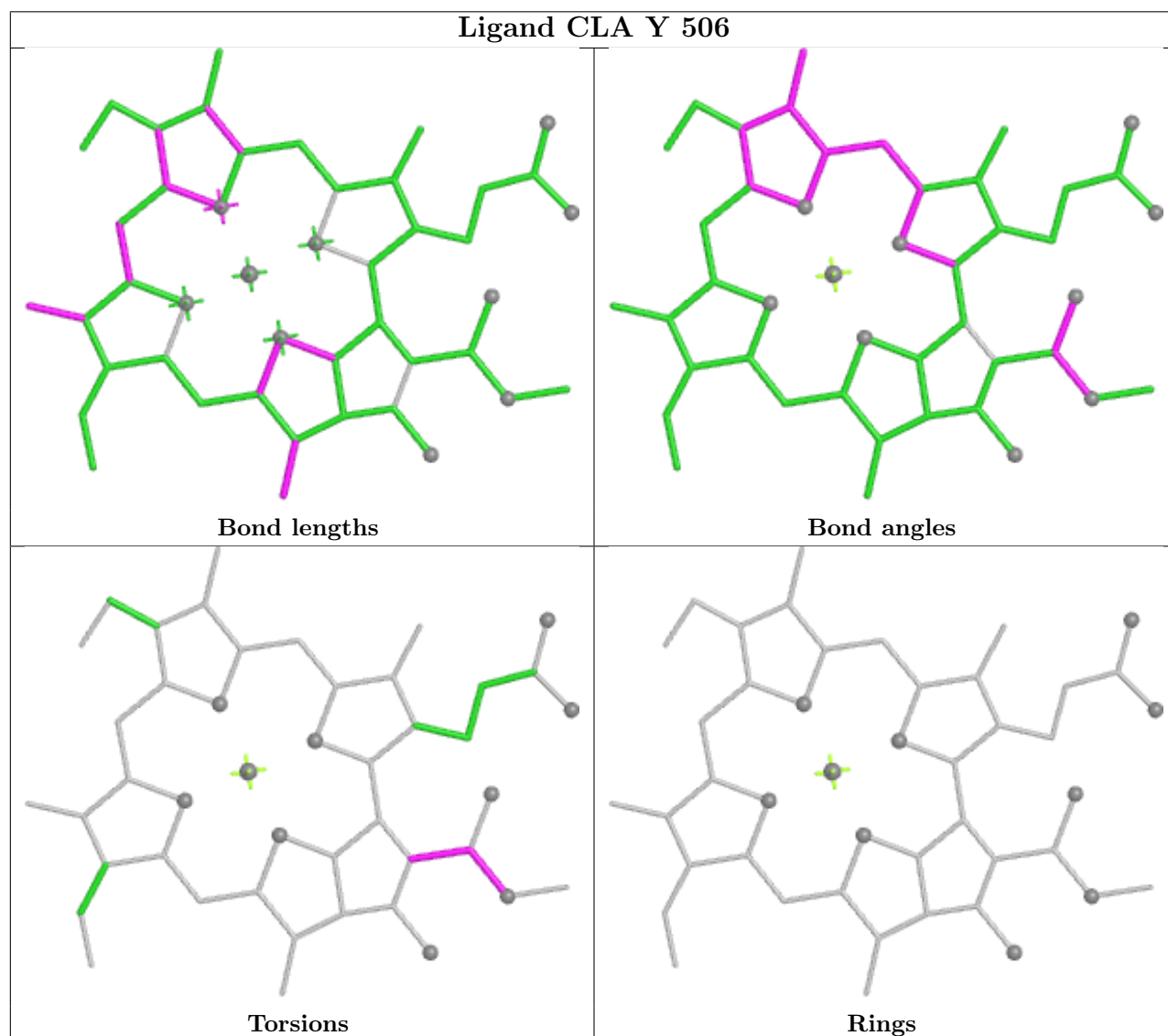
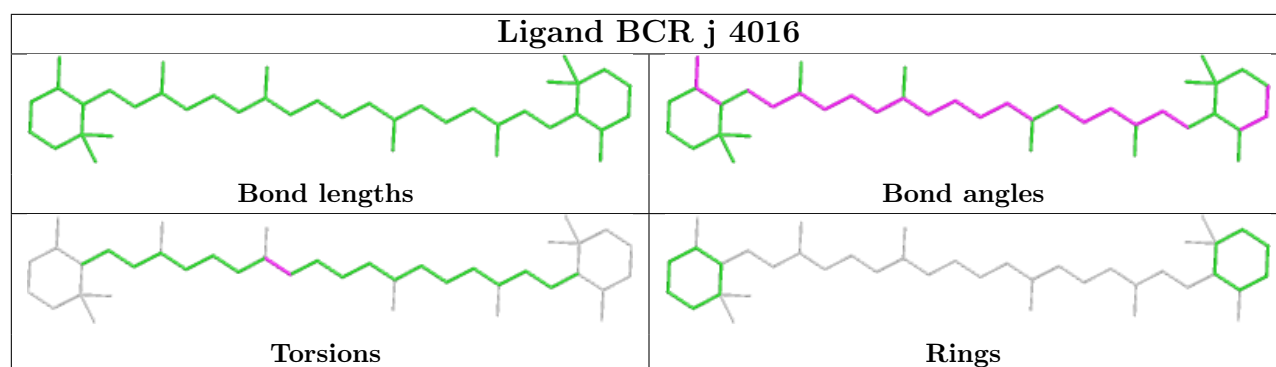


Ligand CLA 5 512

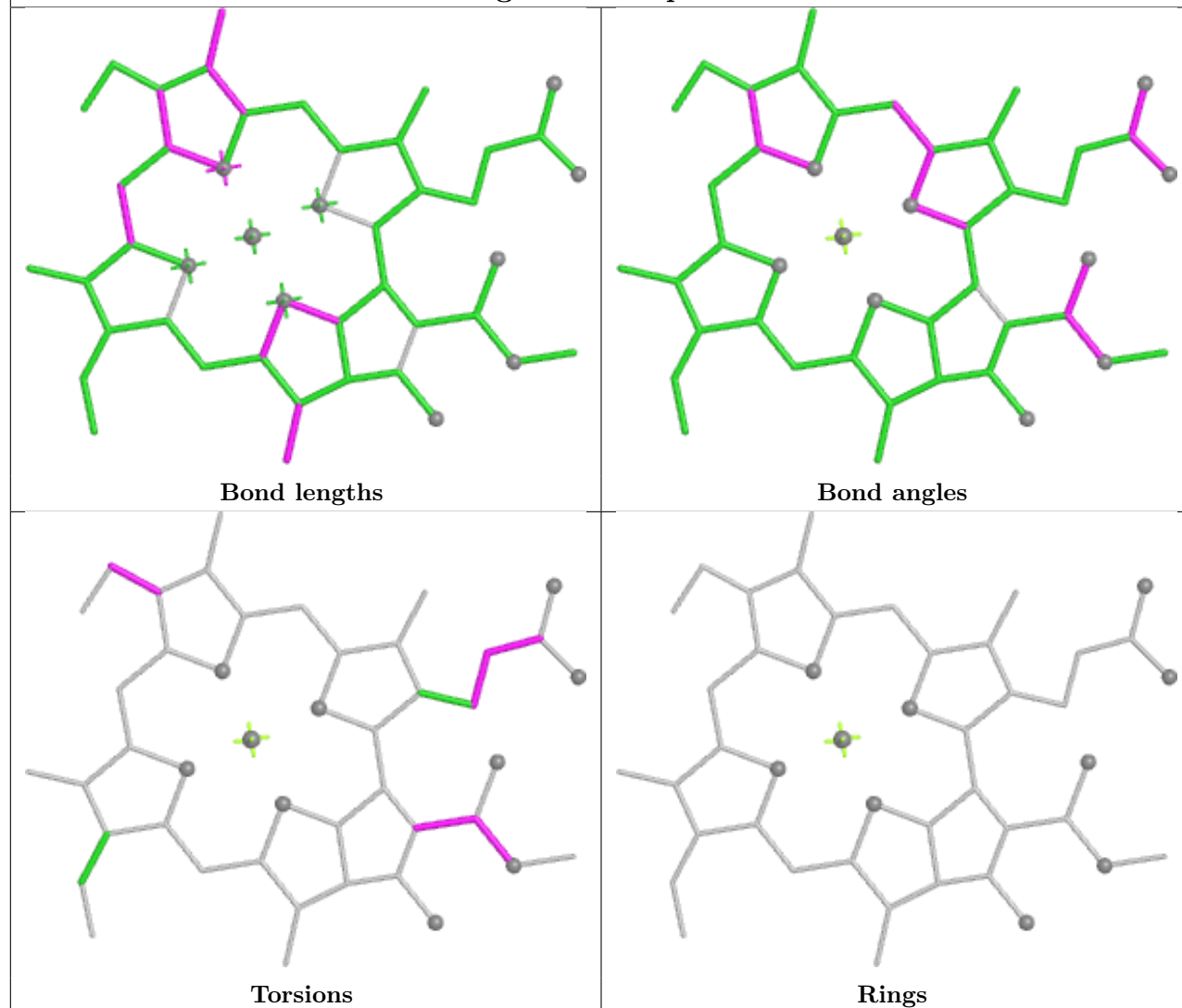


Ligand BCR 5 522

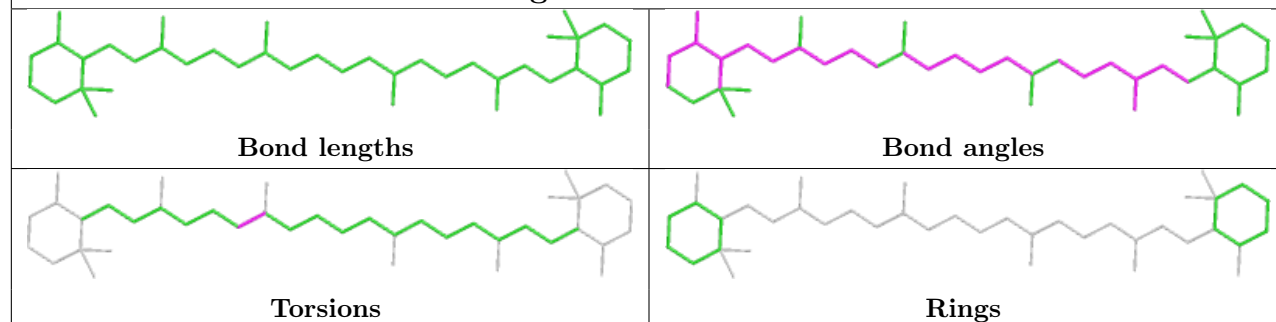


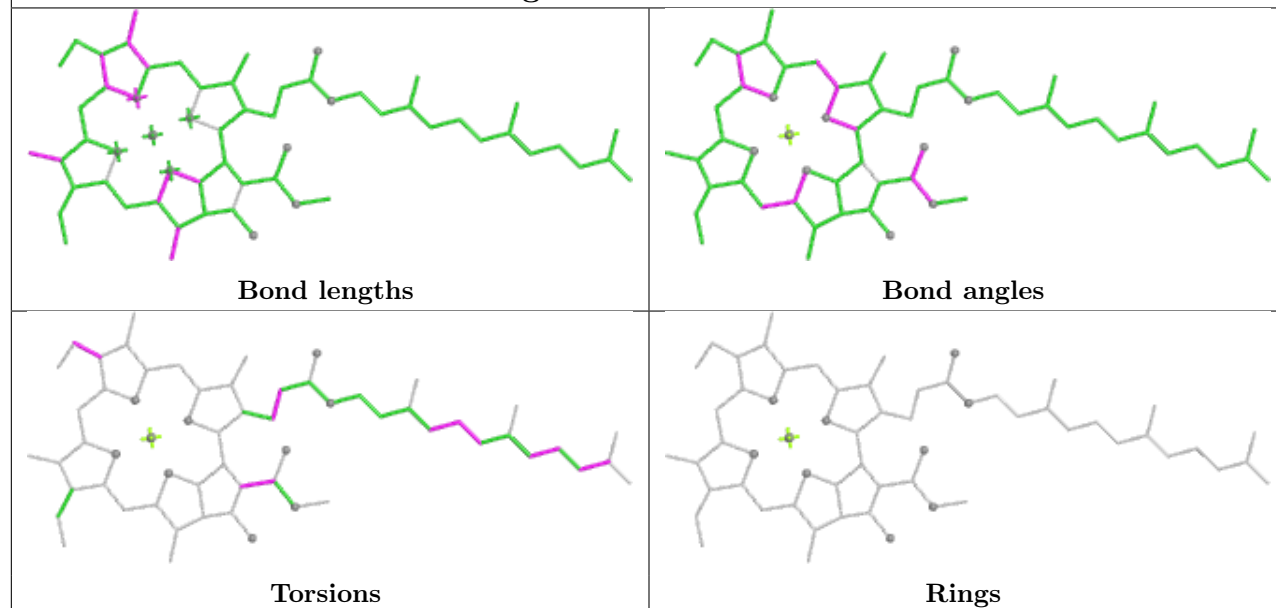
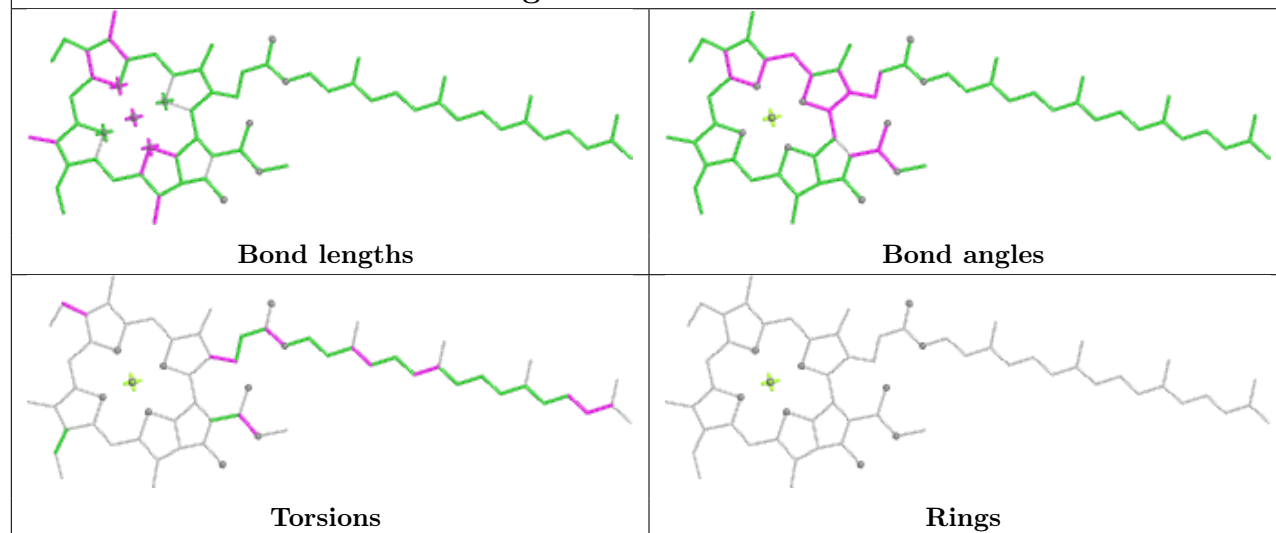


Ligand CLA q 517

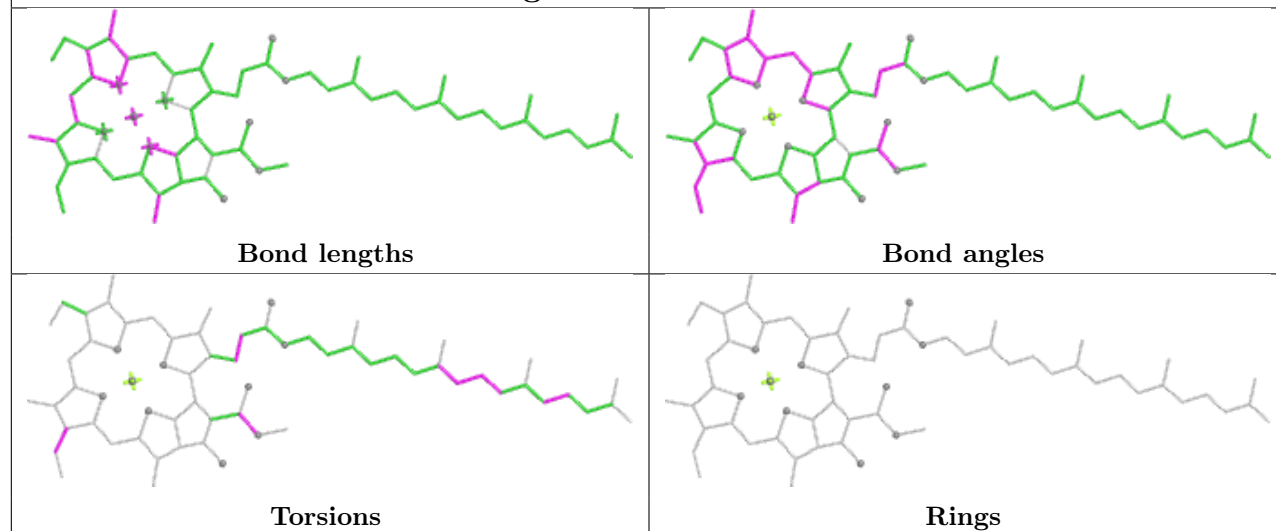


Ligand BCR Y 524

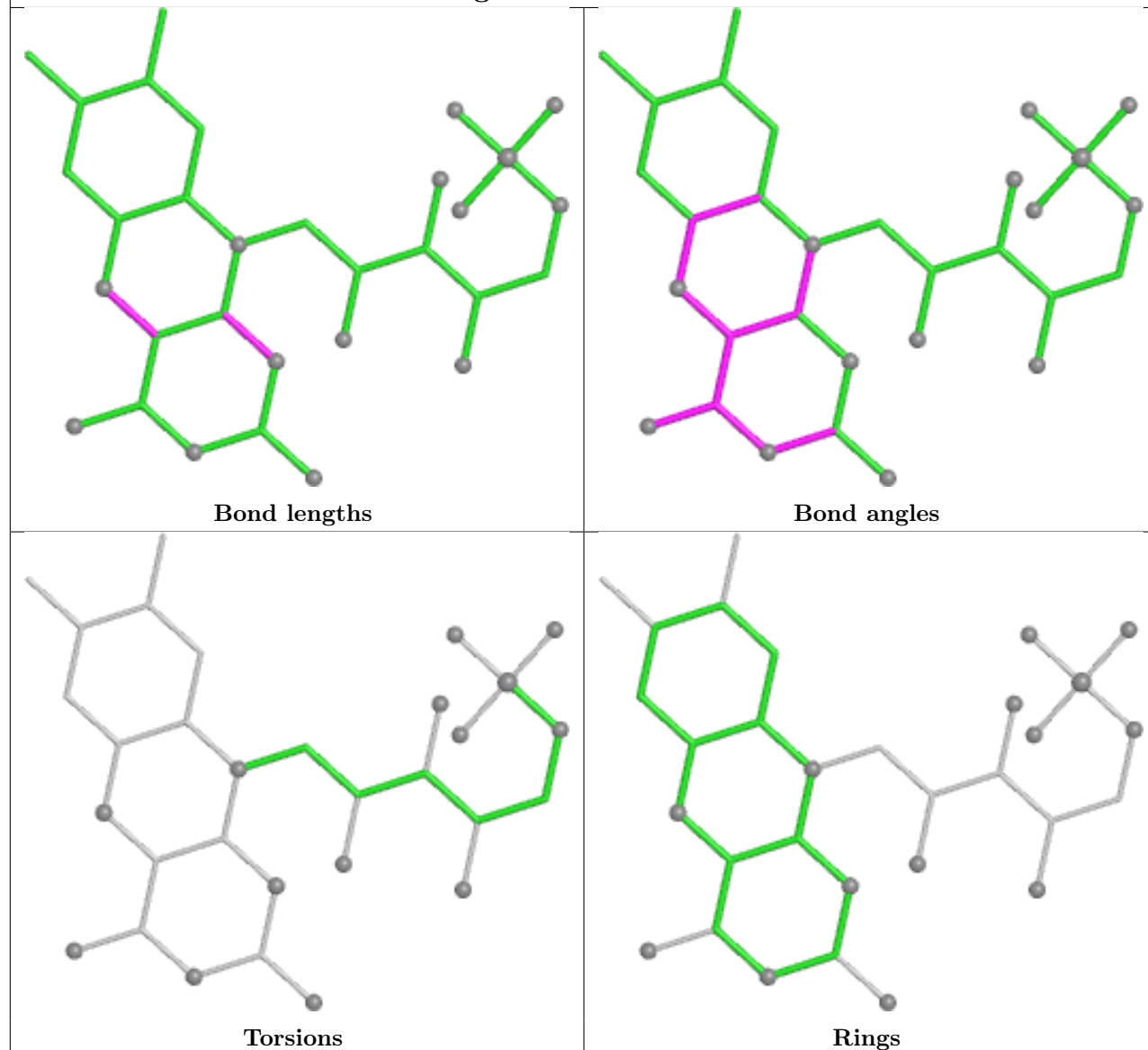


Ligand CLA H 1218**Ligand CLA A 1140**

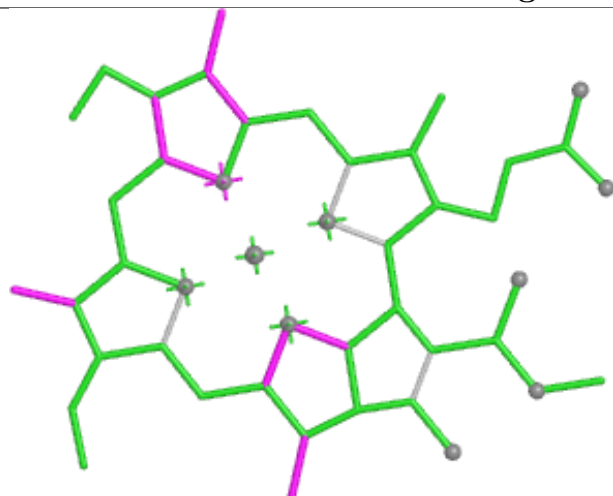
Ligand CLA B 1023



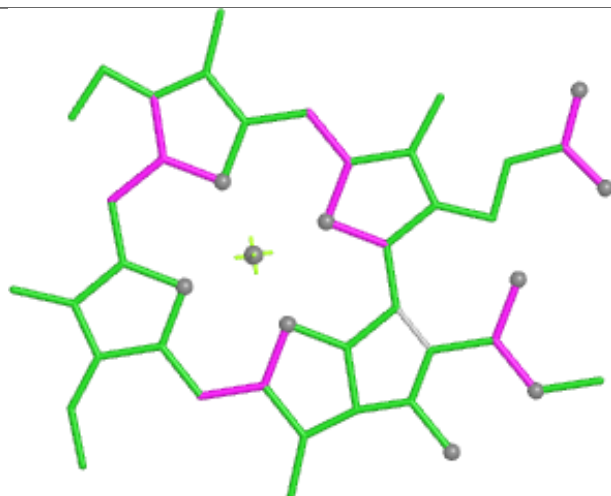
Ligand FMN X 170



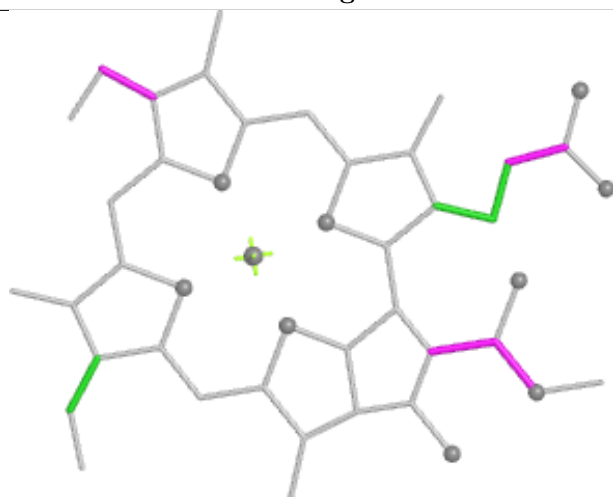
Ligand CLA 2 519



Bond lengths



Bond angles

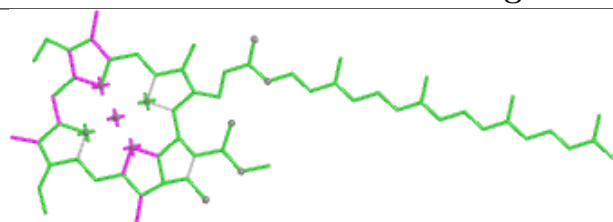


Torsions

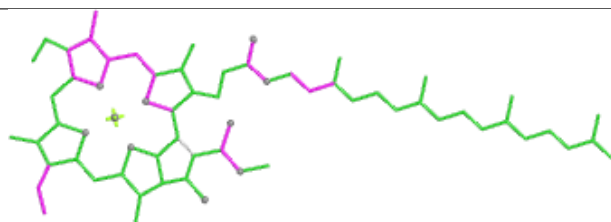


Rings

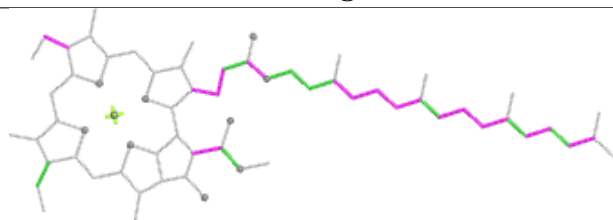
Ligand CLA H 1210



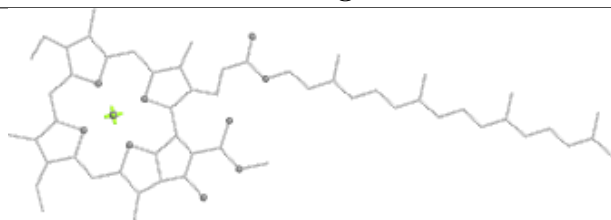
Bond lengths



Bond angles

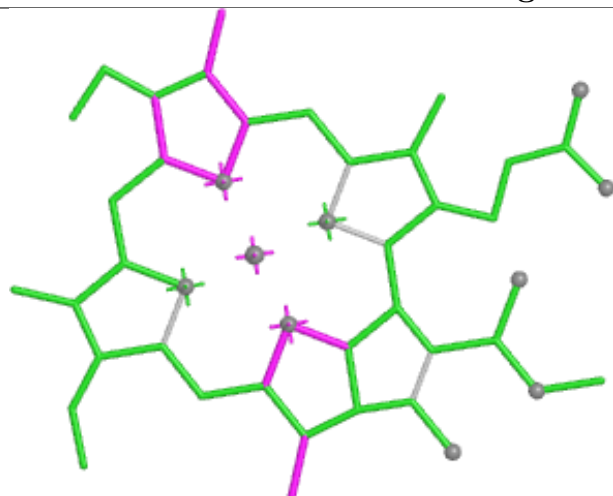


Torsions

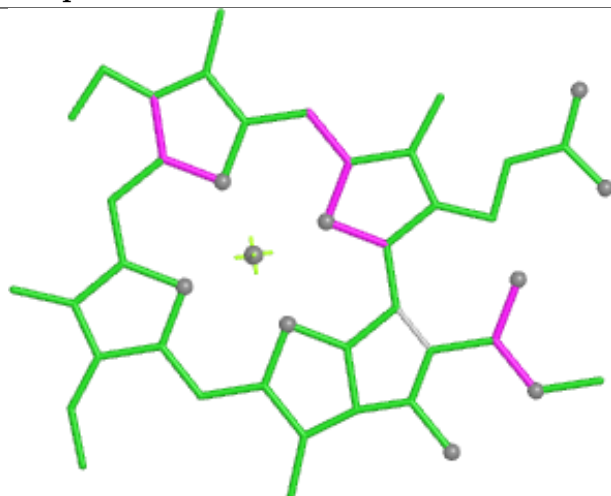


Rings

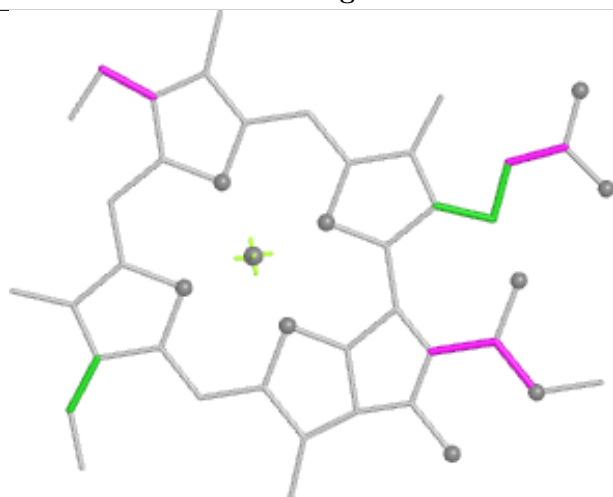
Ligand CLA q 512



Bond lengths



Bond angles

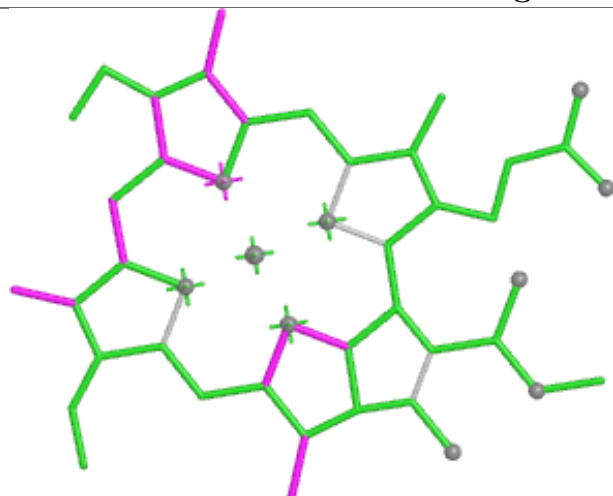


Torsions

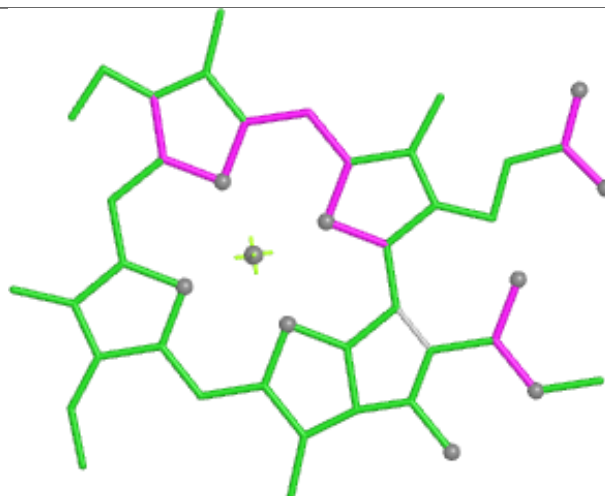


Rings

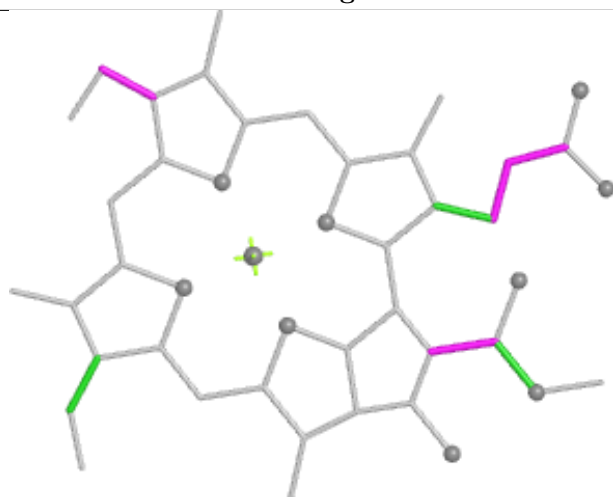
Ligand CLA Y 513



Bond lengths



Bond angles

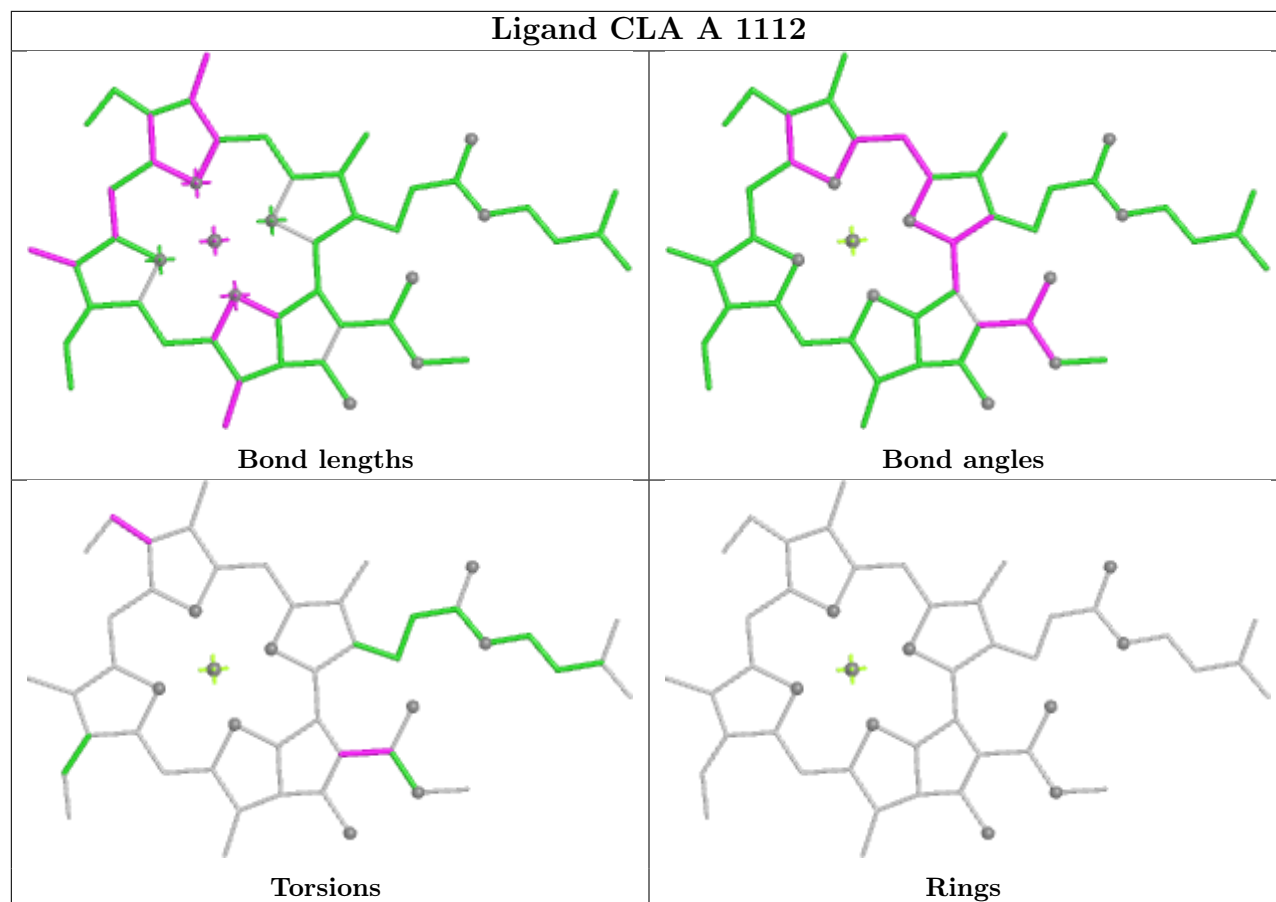


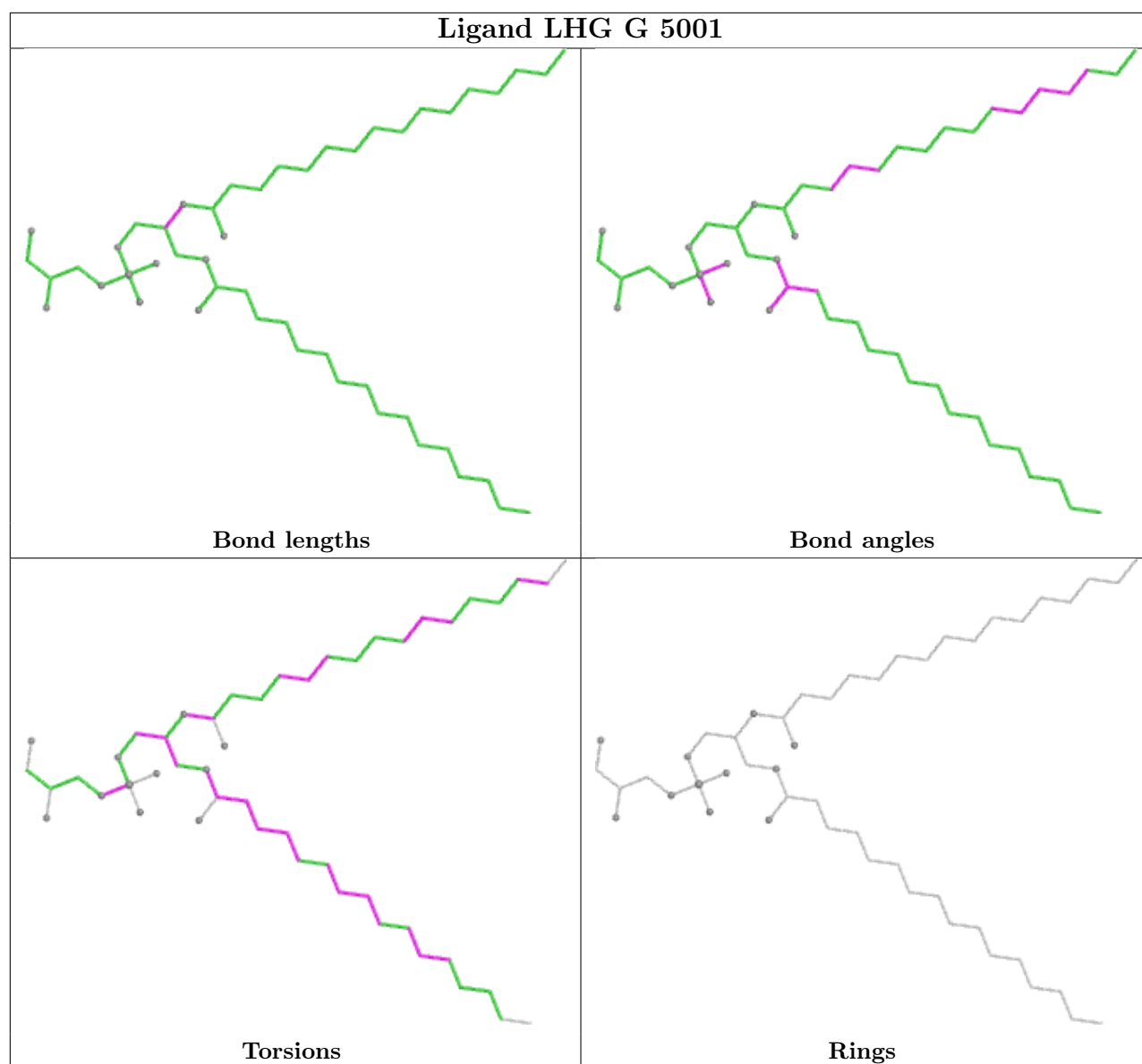
Torsions



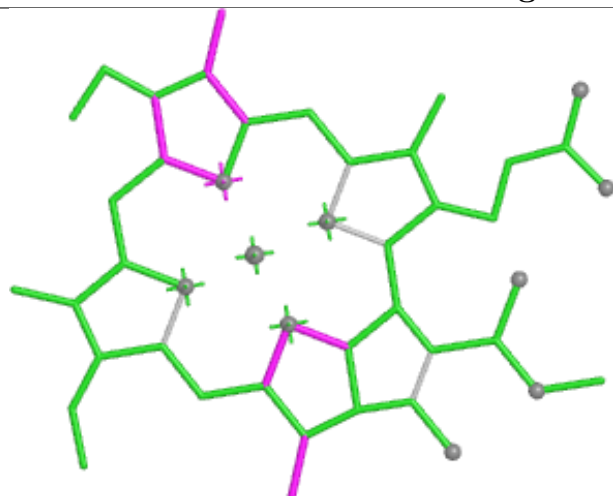
Rings

Ligand CLA A 1112

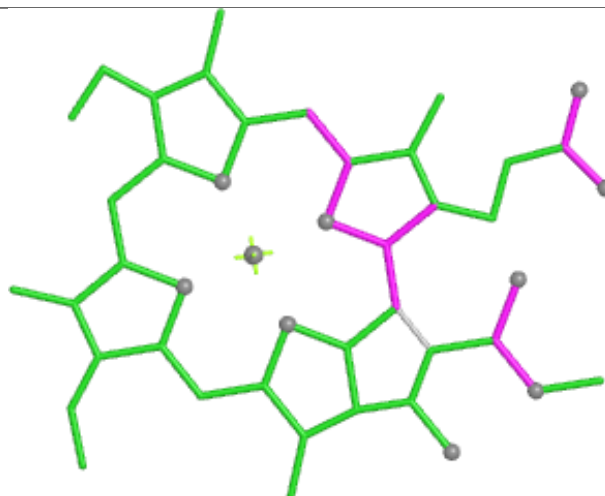




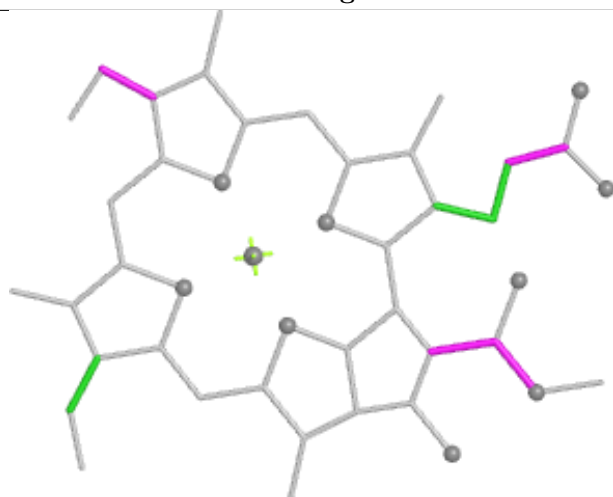
Ligand CLA 6 507



Bond lengths



Bond angles

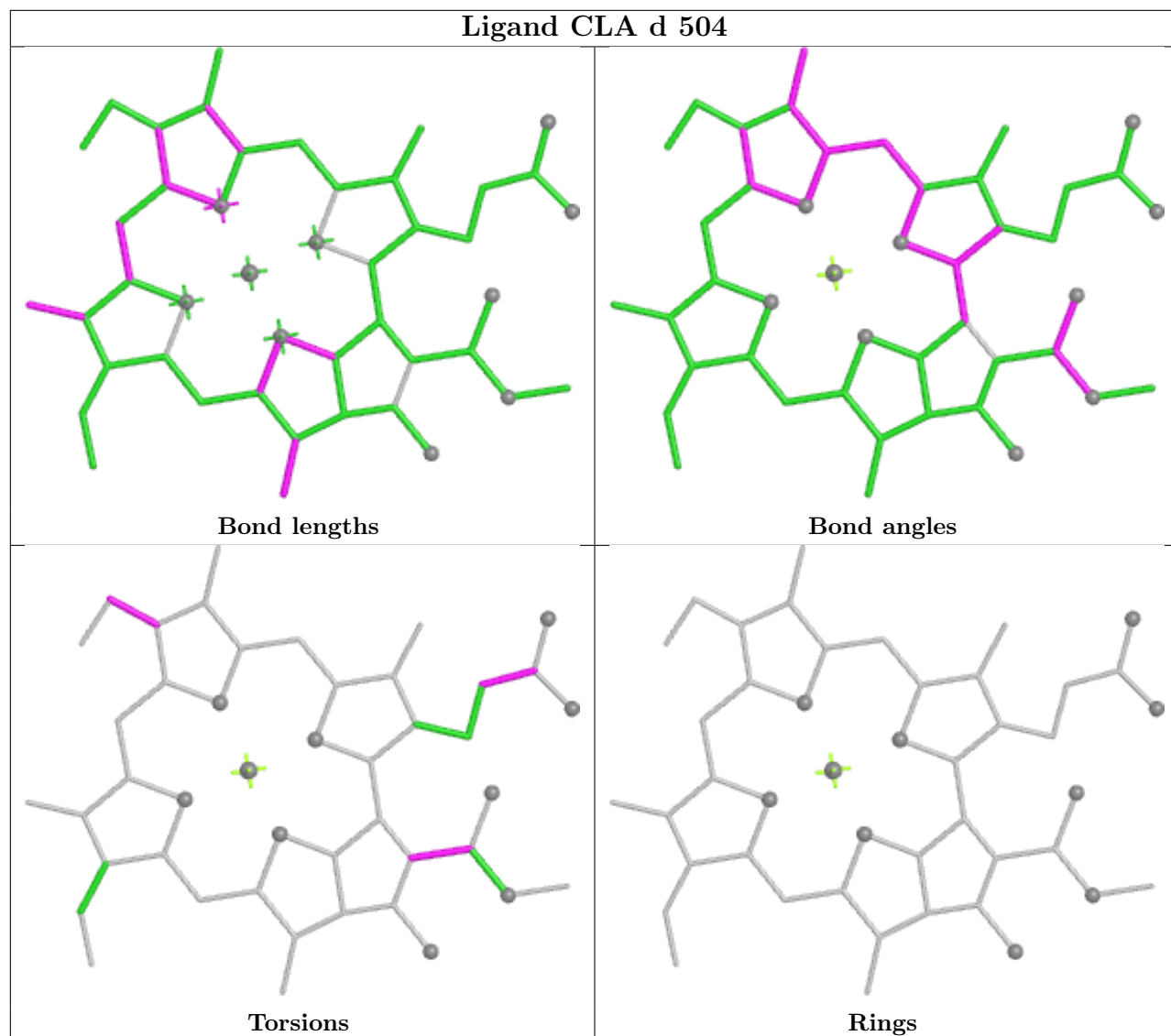


Torsions

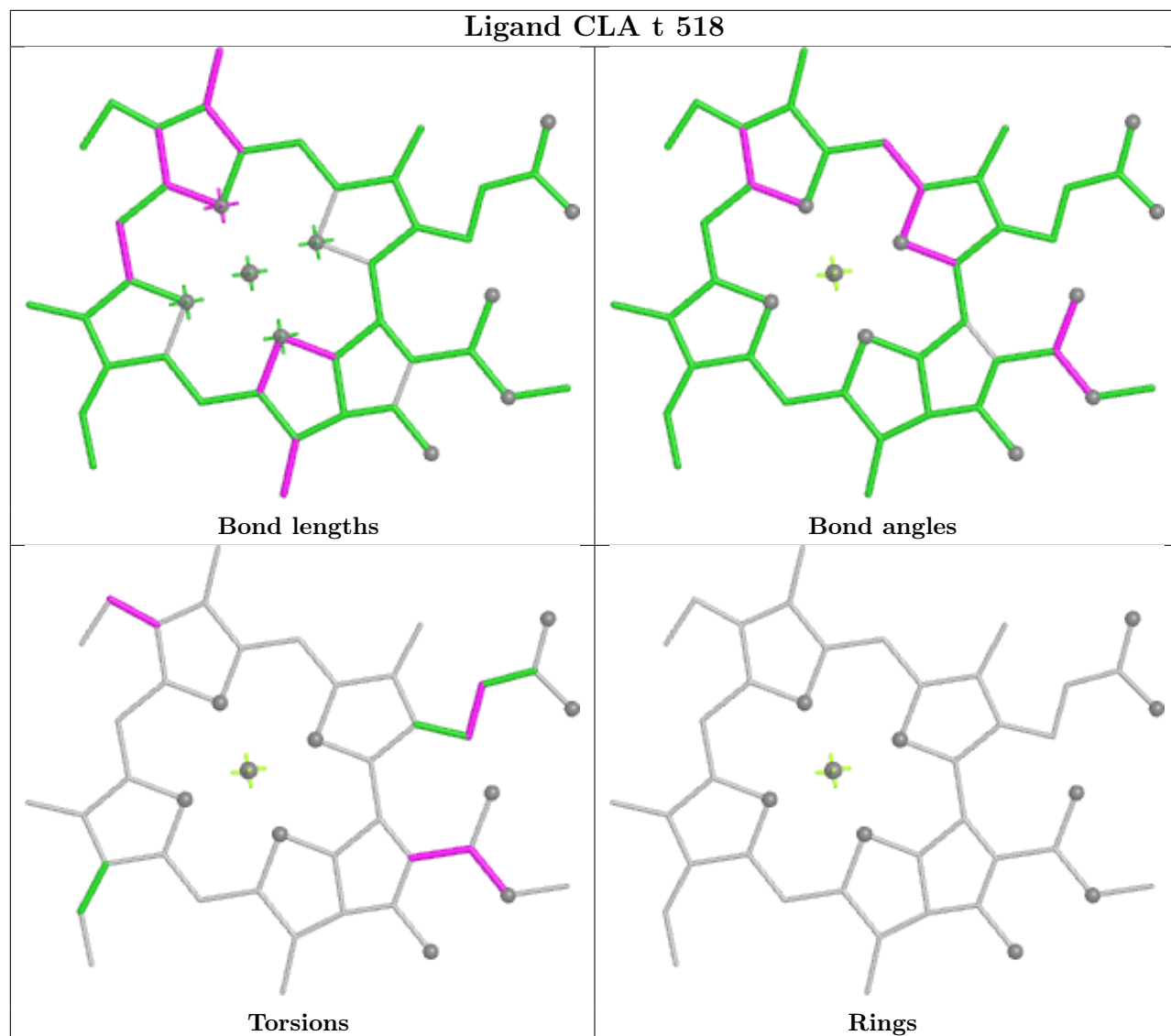


Rings

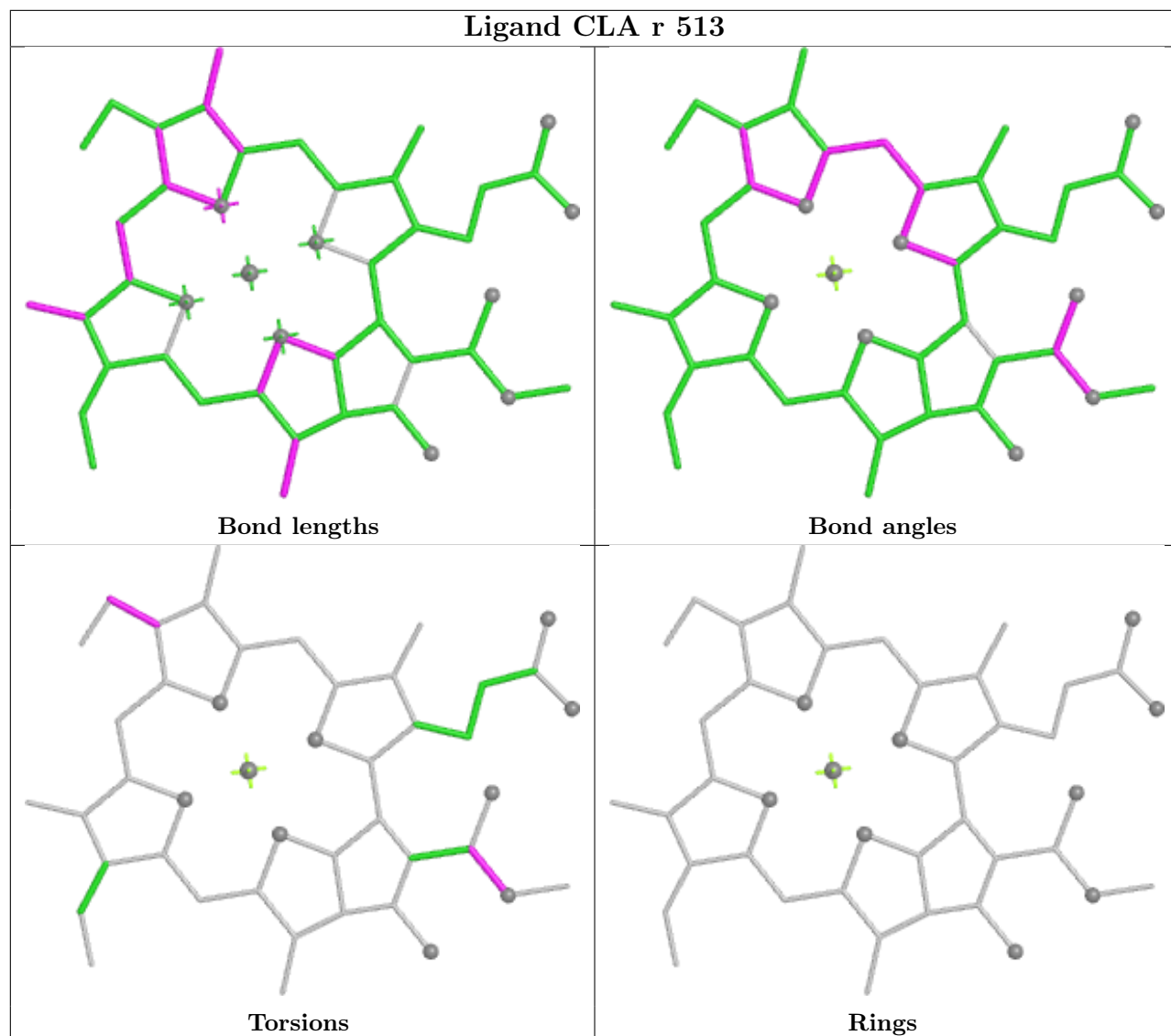
Ligand CLA d 504



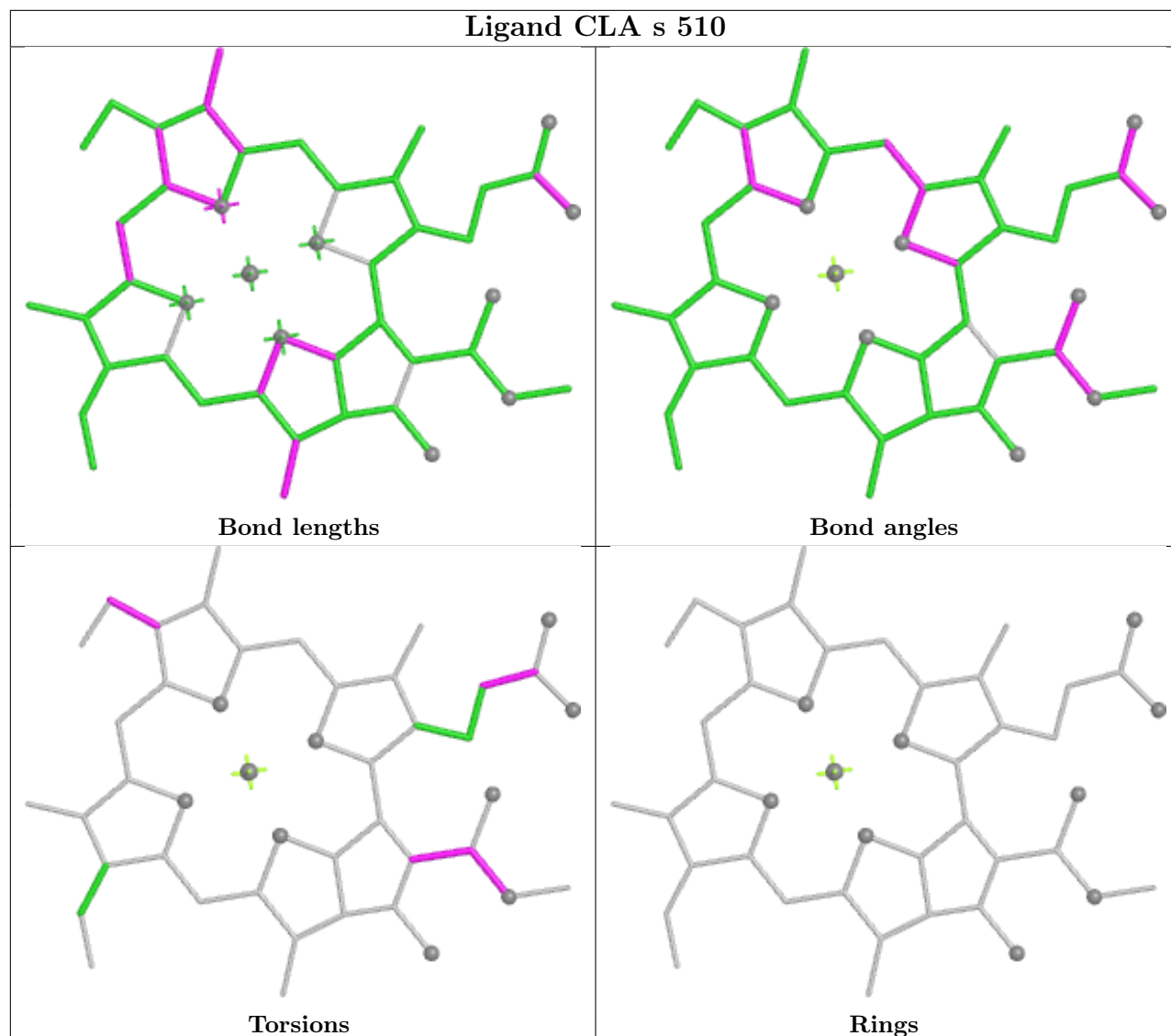
Ligand CLA t 518



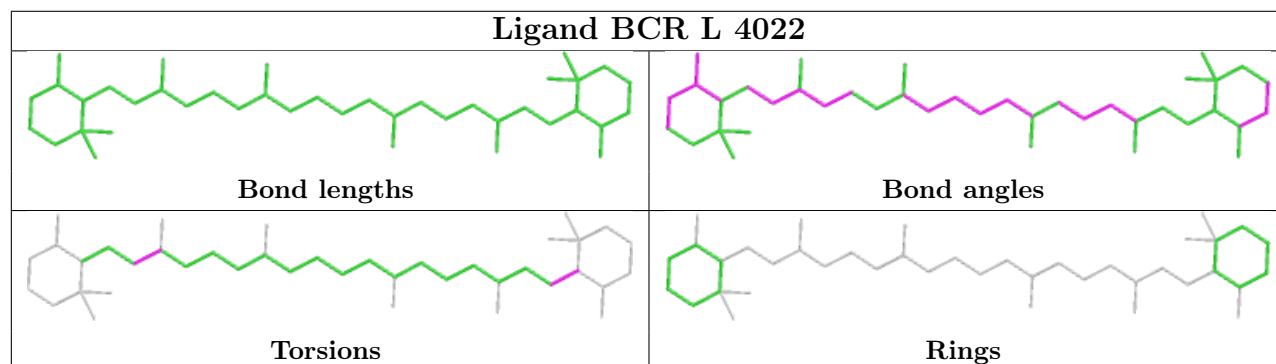
Ligand CLA r 513

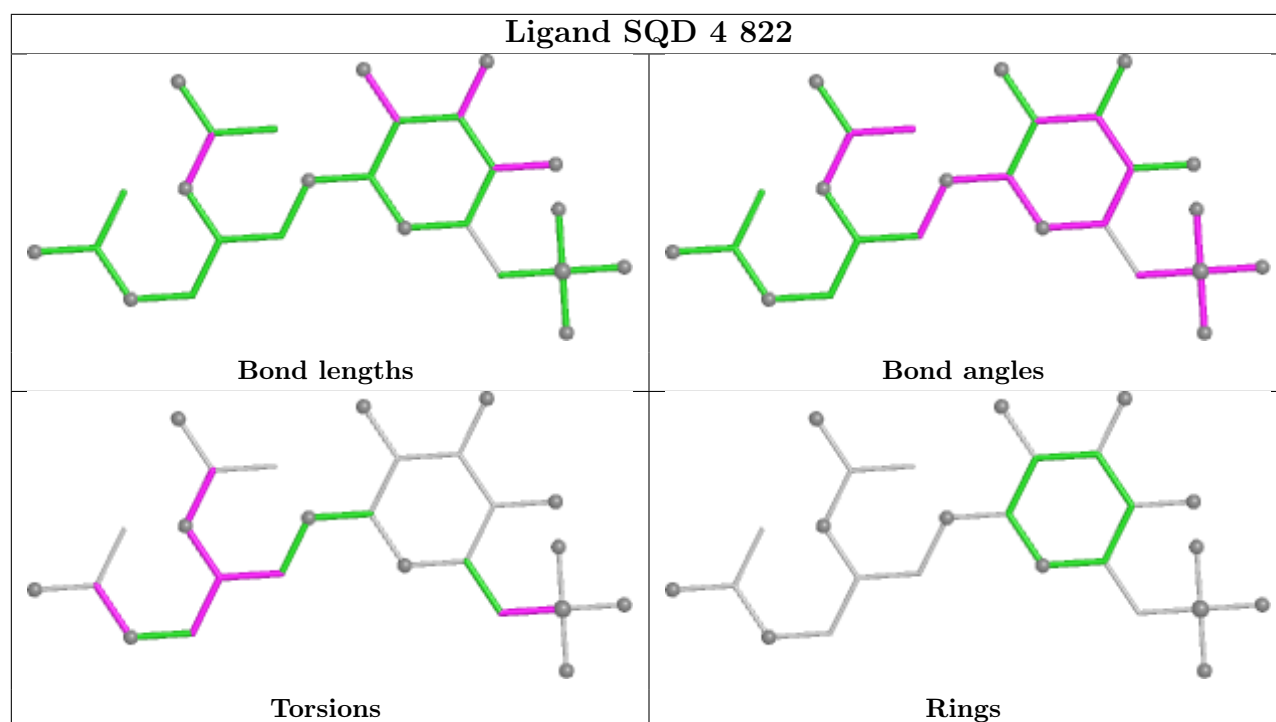


Ligand CLA s 510

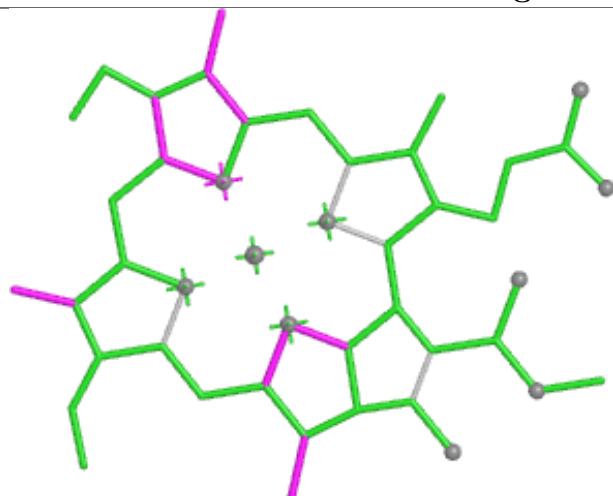


Ligand BCR L 4022

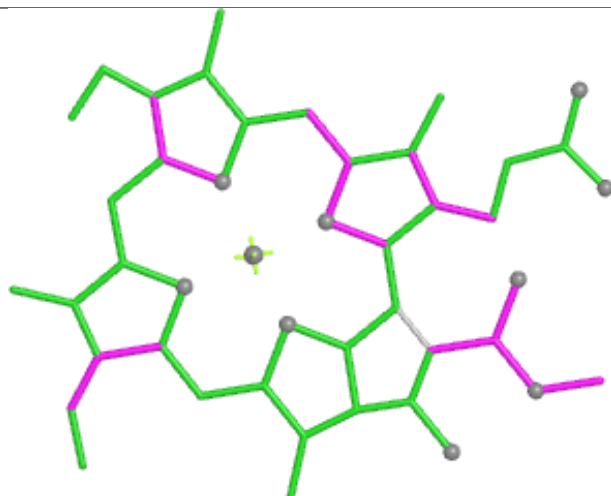




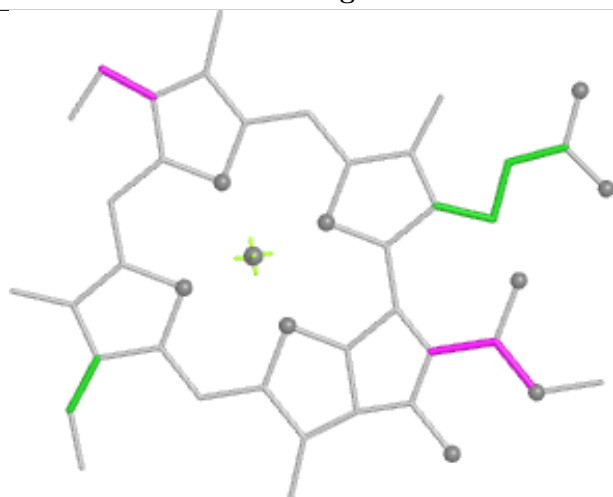
Ligand CLA Y 504



Bond lengths



Bond angles

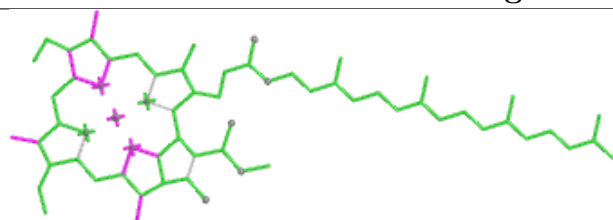


Torsions

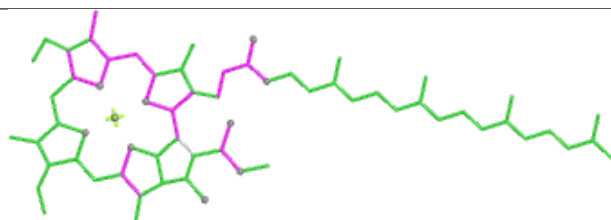


Rings

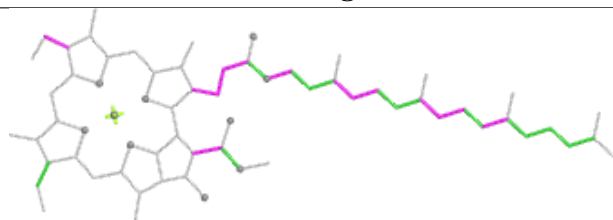
Ligand CLA A 1107



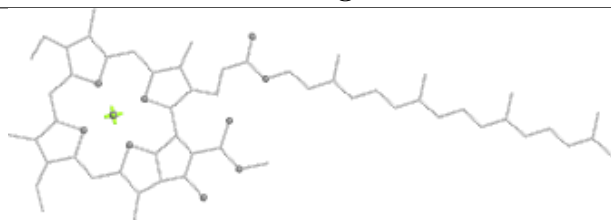
Bond lengths



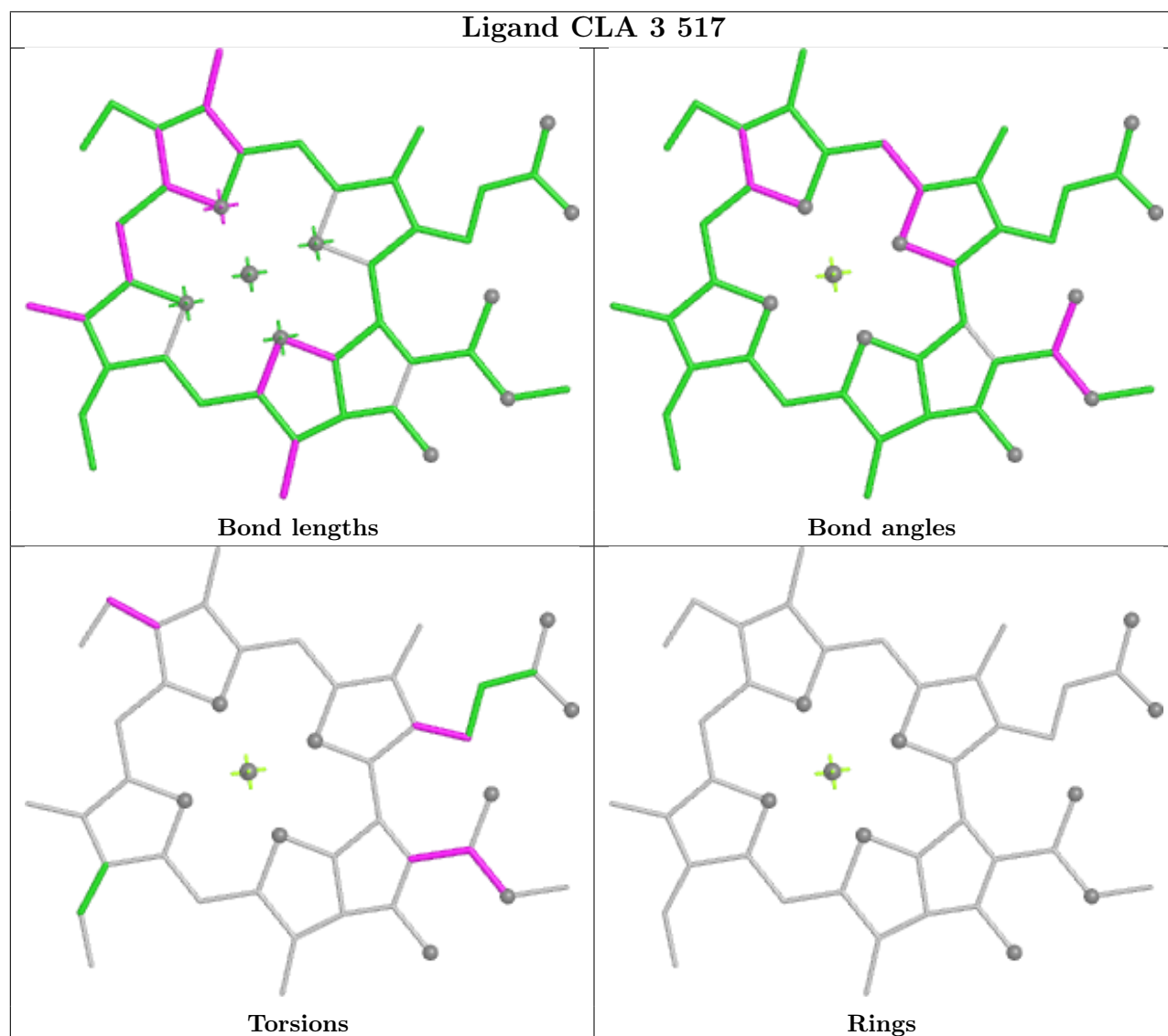
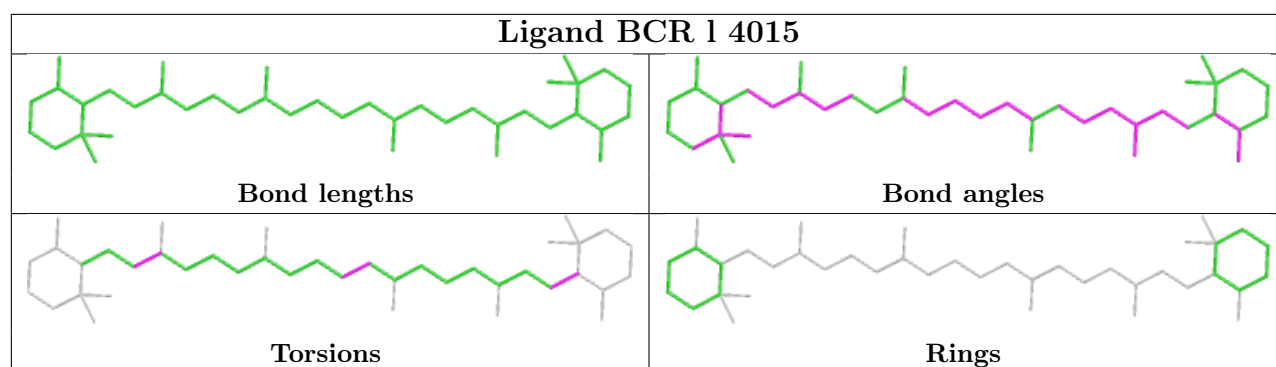
Bond angles



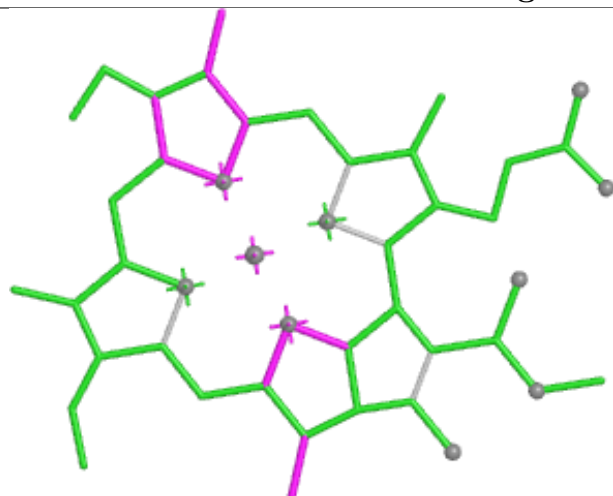
Torsions



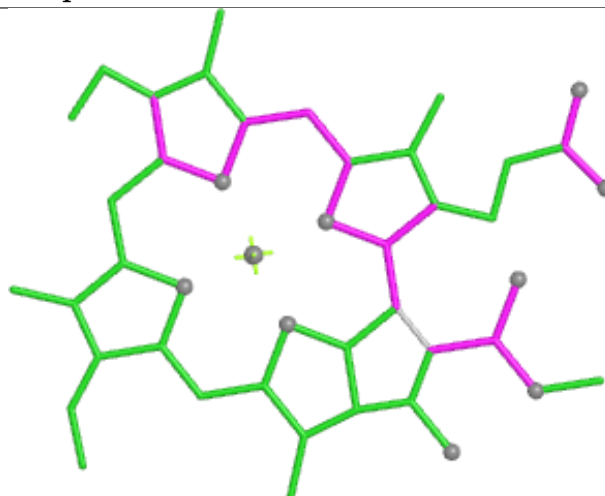
Rings



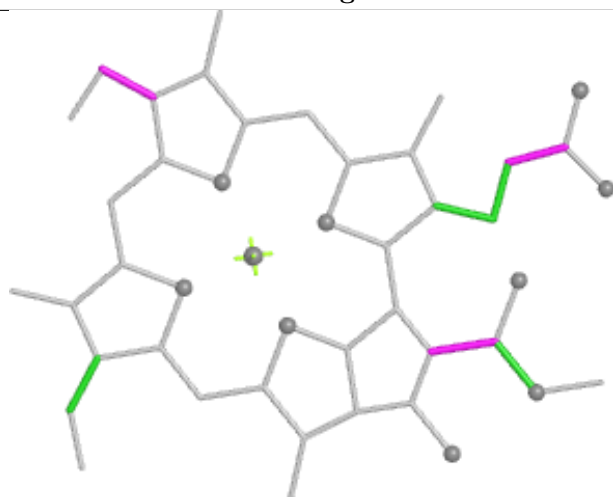
Ligand CLA q 509



Bond lengths



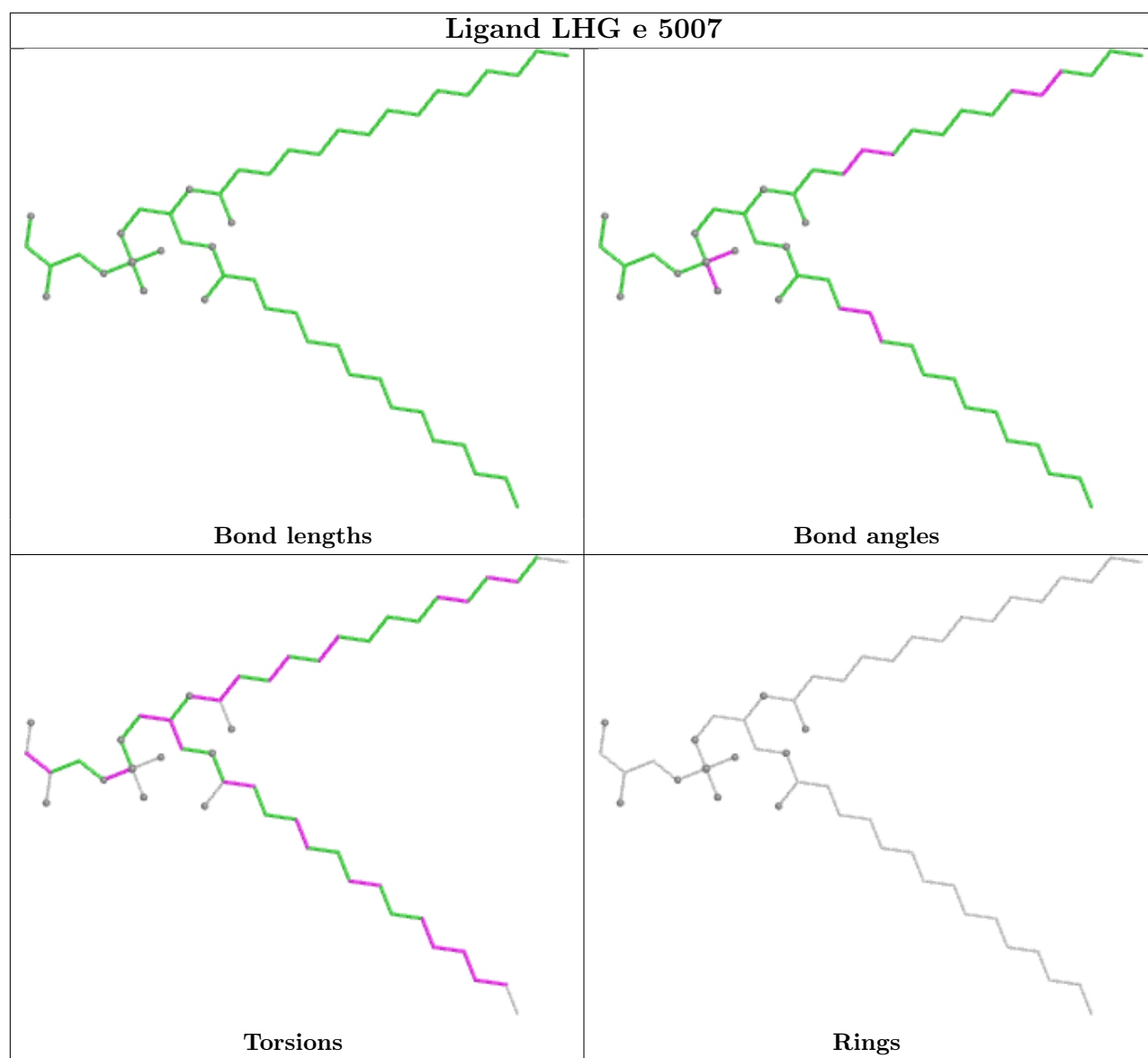
Bond angles



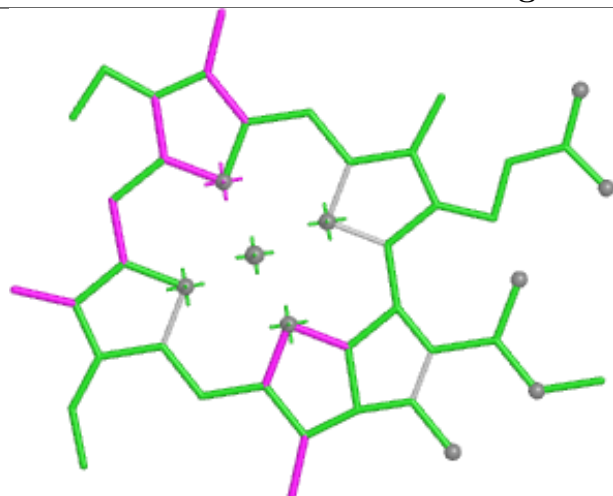
Torsions



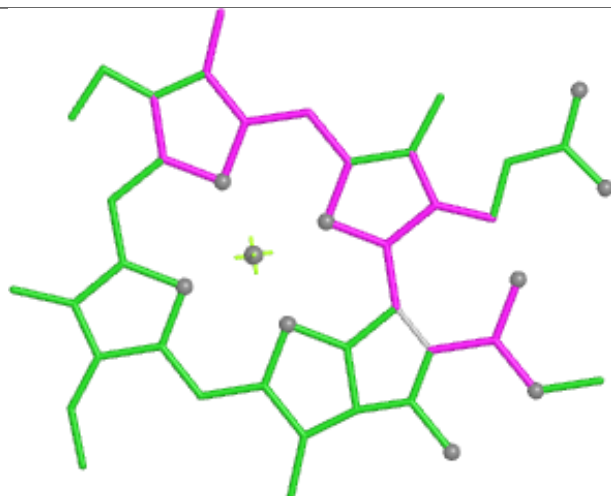
Rings



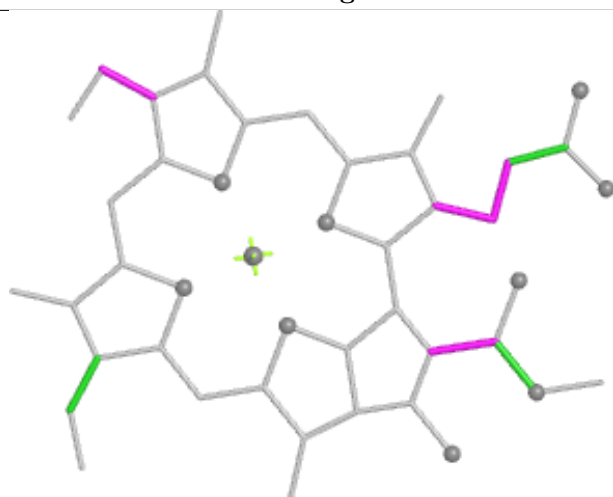
Ligand CLA 3 504



Bond lengths



Bond angles

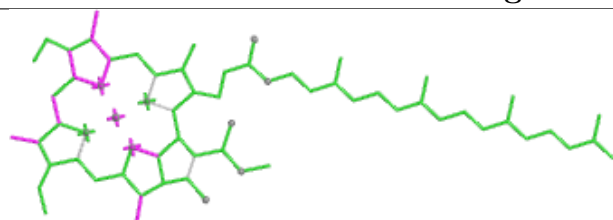


Torsions

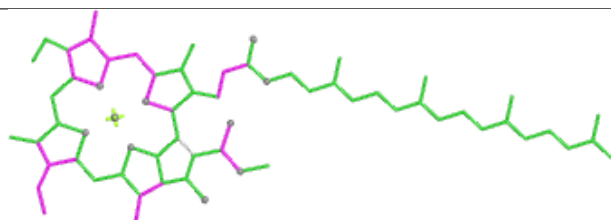


Rings

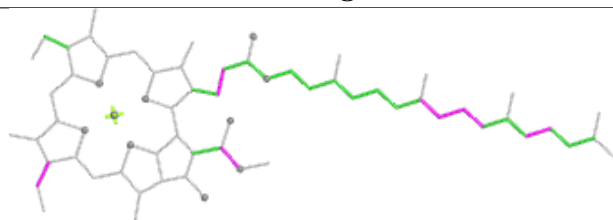
Ligand CLA H 1023



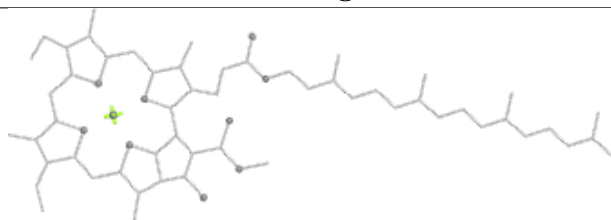
Bond lengths



Bond angles

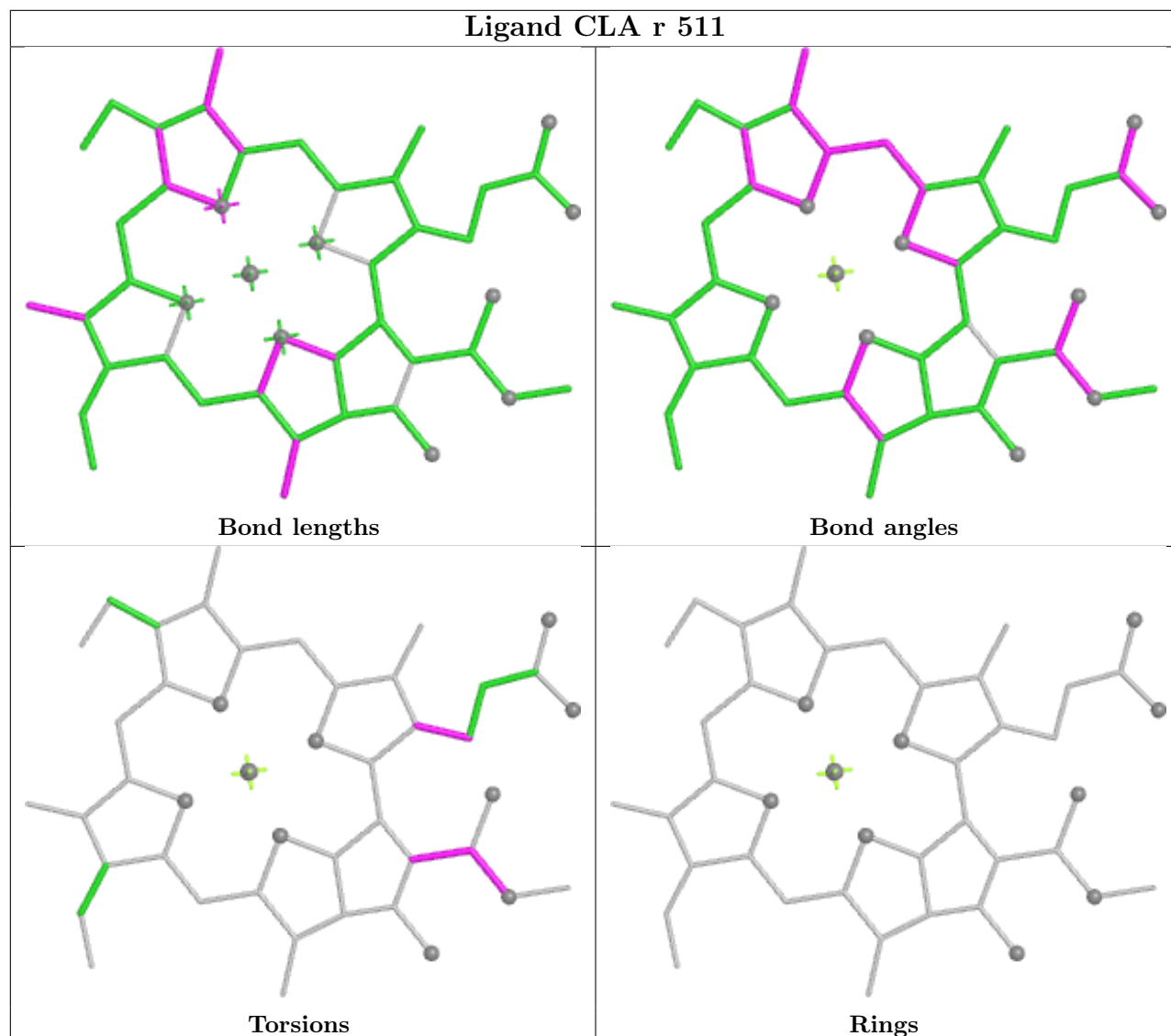


Torsions

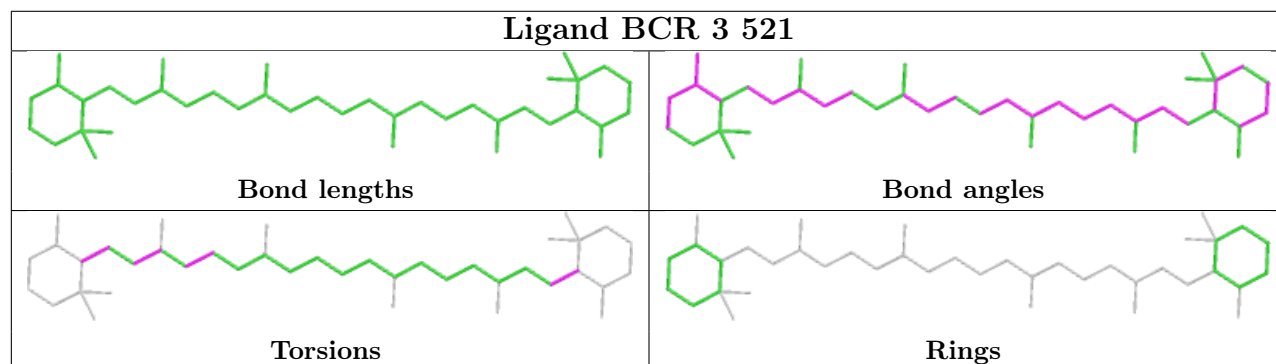


Rings

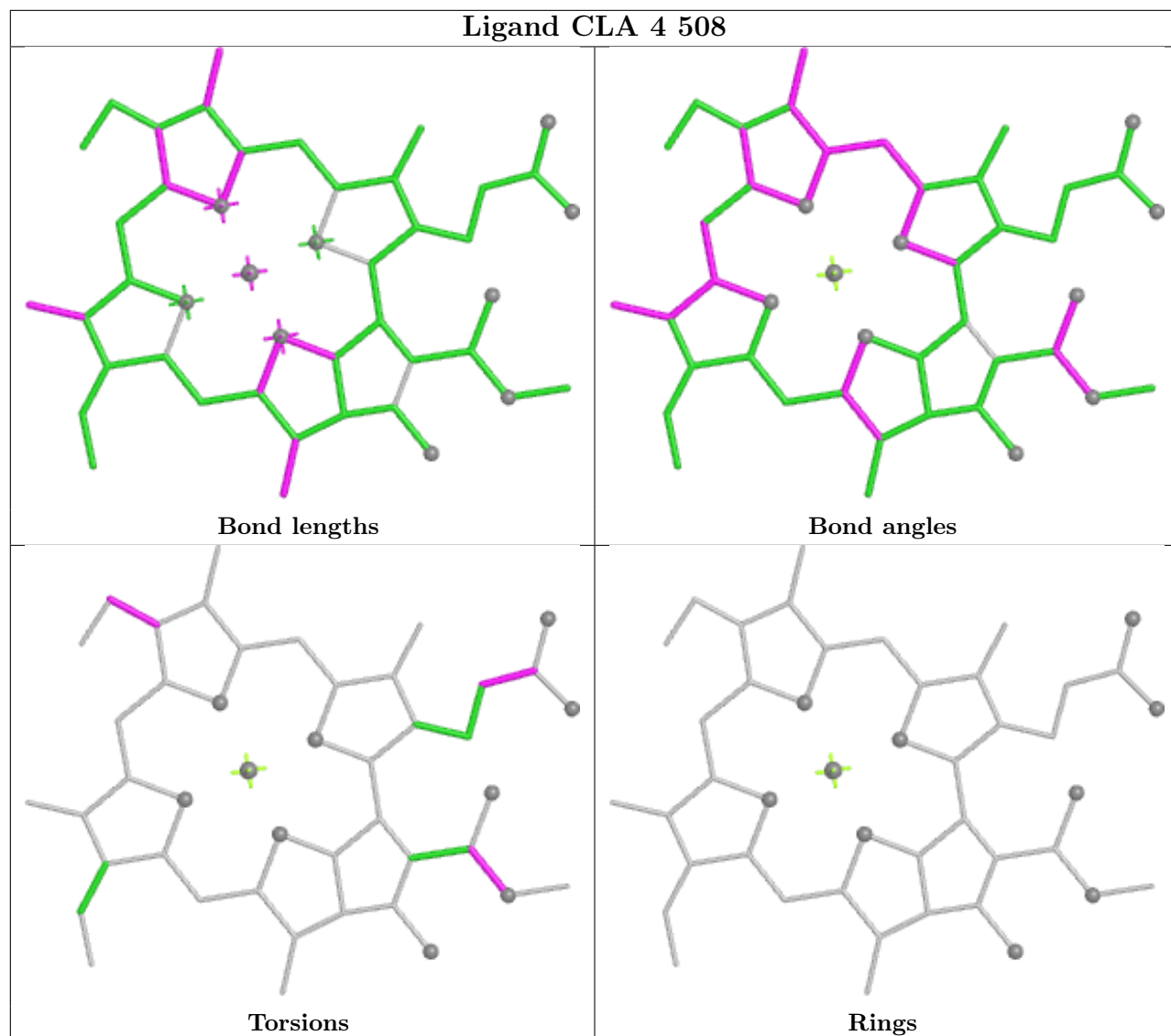
Ligand CLA r 511

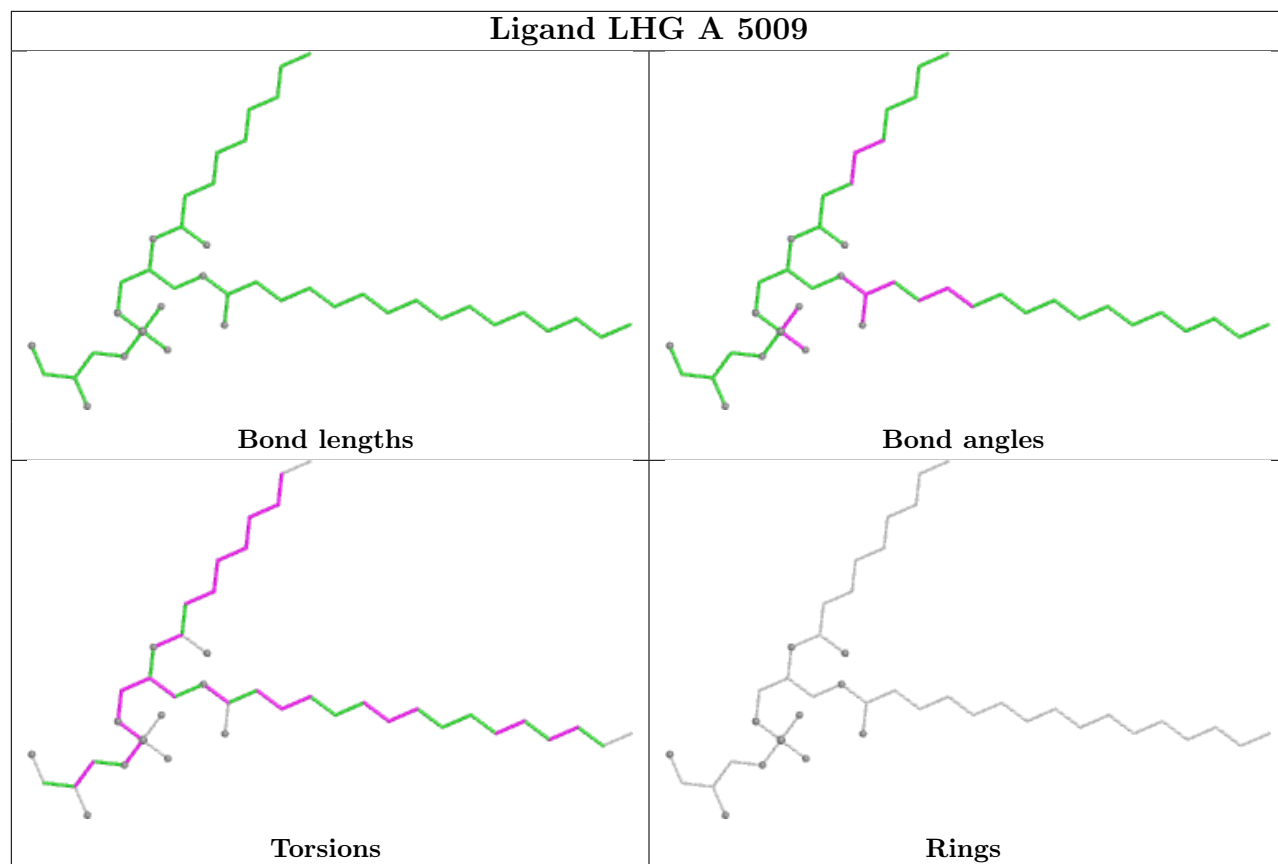


Ligand BCR 3 521

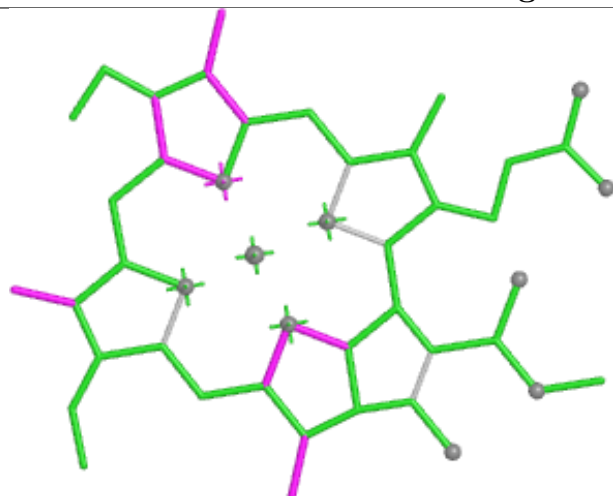


Ligand CLA 4 508

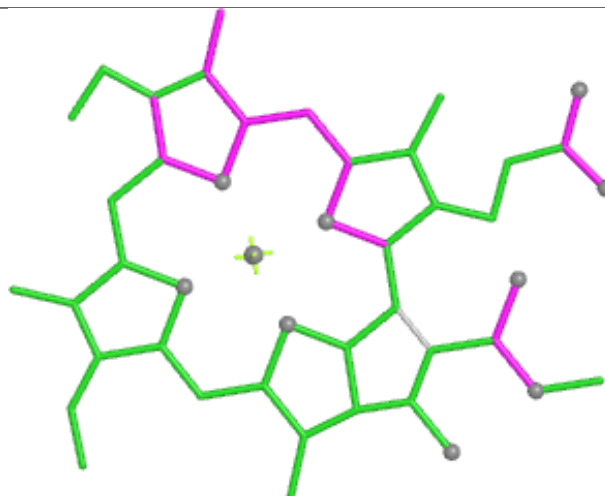




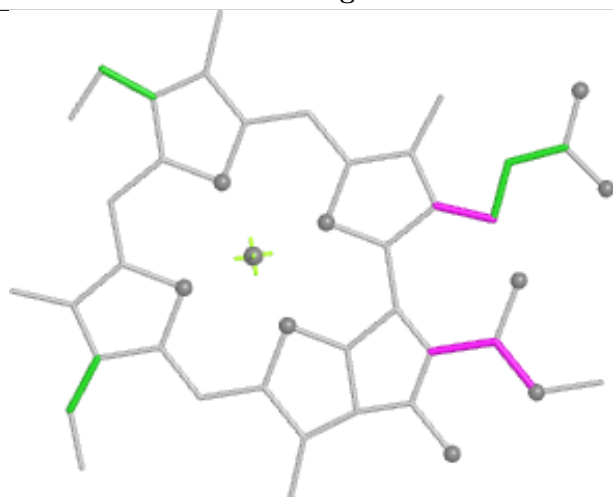
Ligand CLA 2 511



Bond lengths



Bond angles

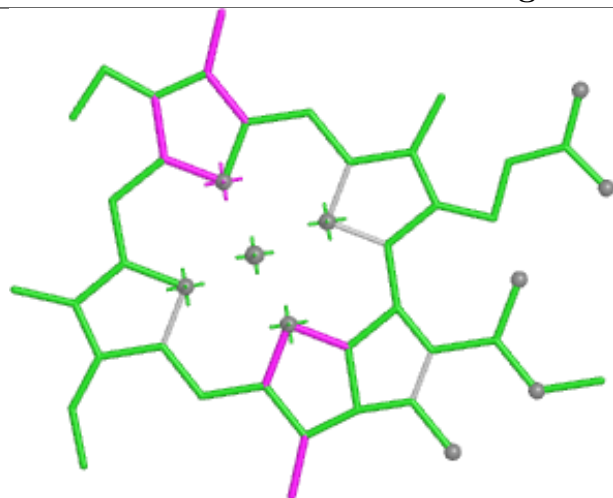


Torsions

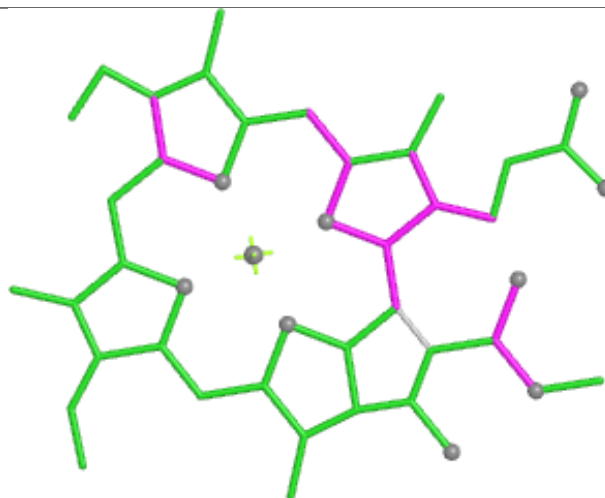


Rings

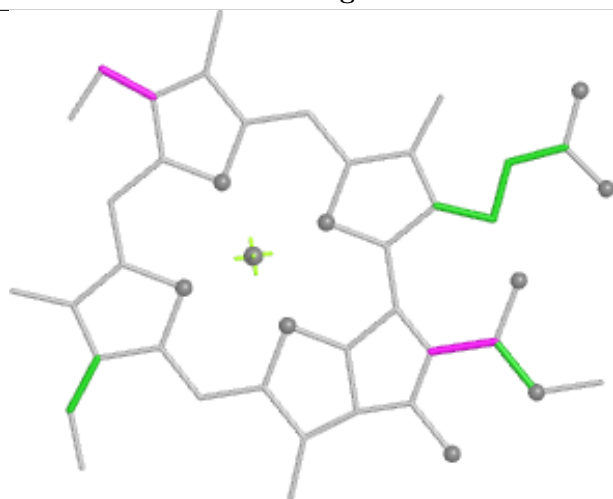
Ligand CLA 6 502



Bond lengths



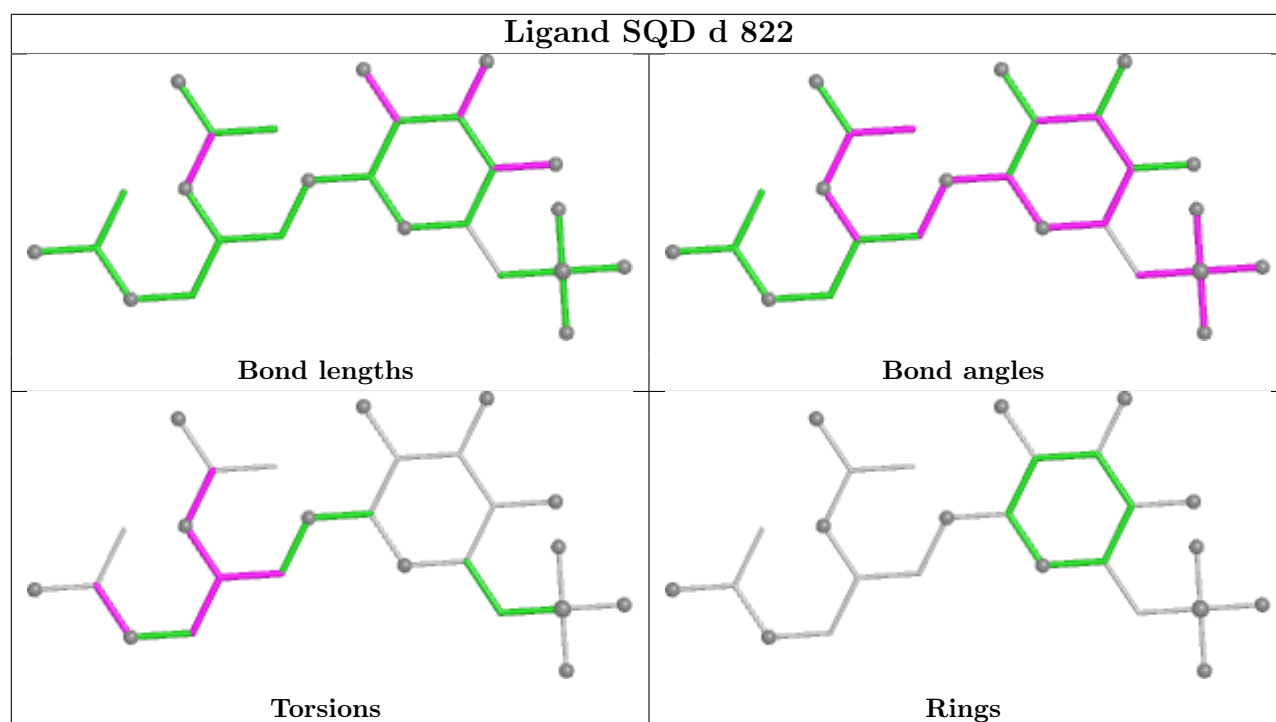
Bond angles



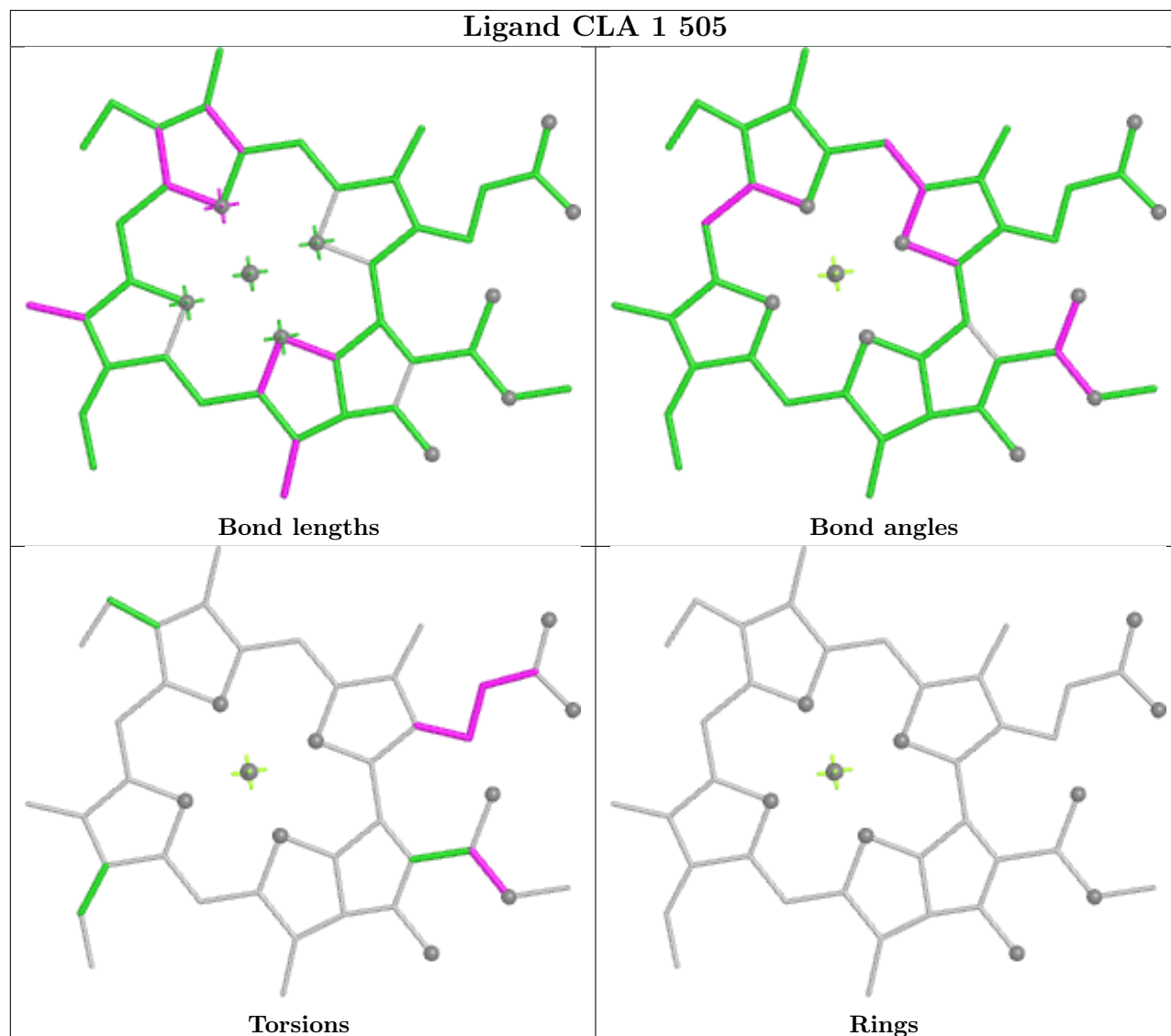
Torsions



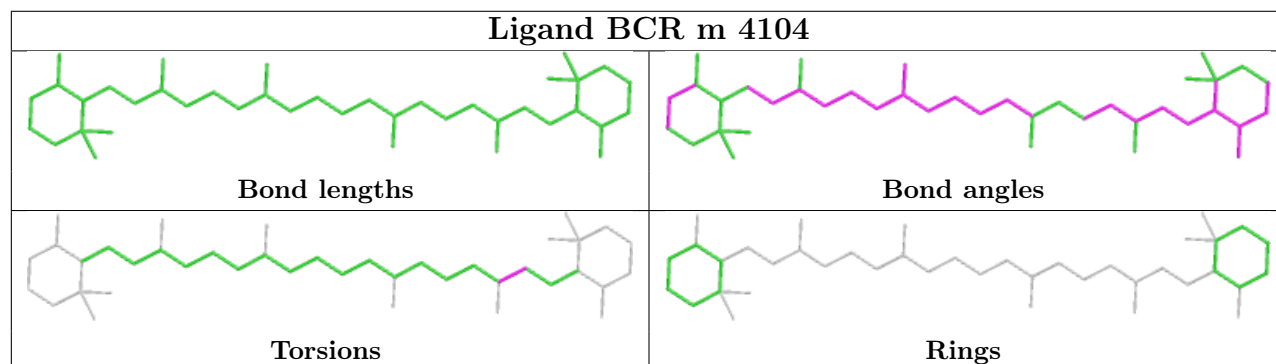
Rings



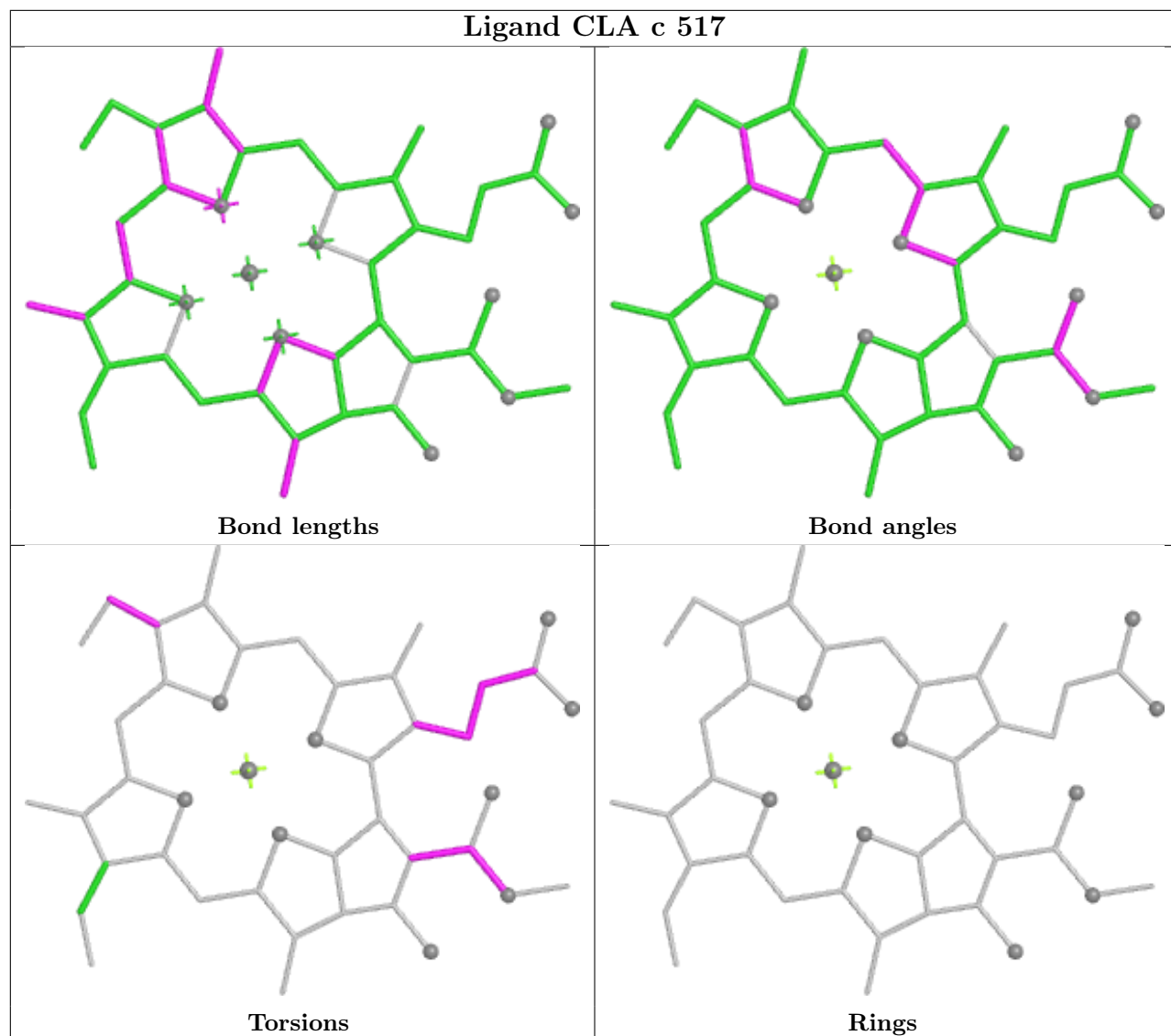
Ligand CLA 1 505



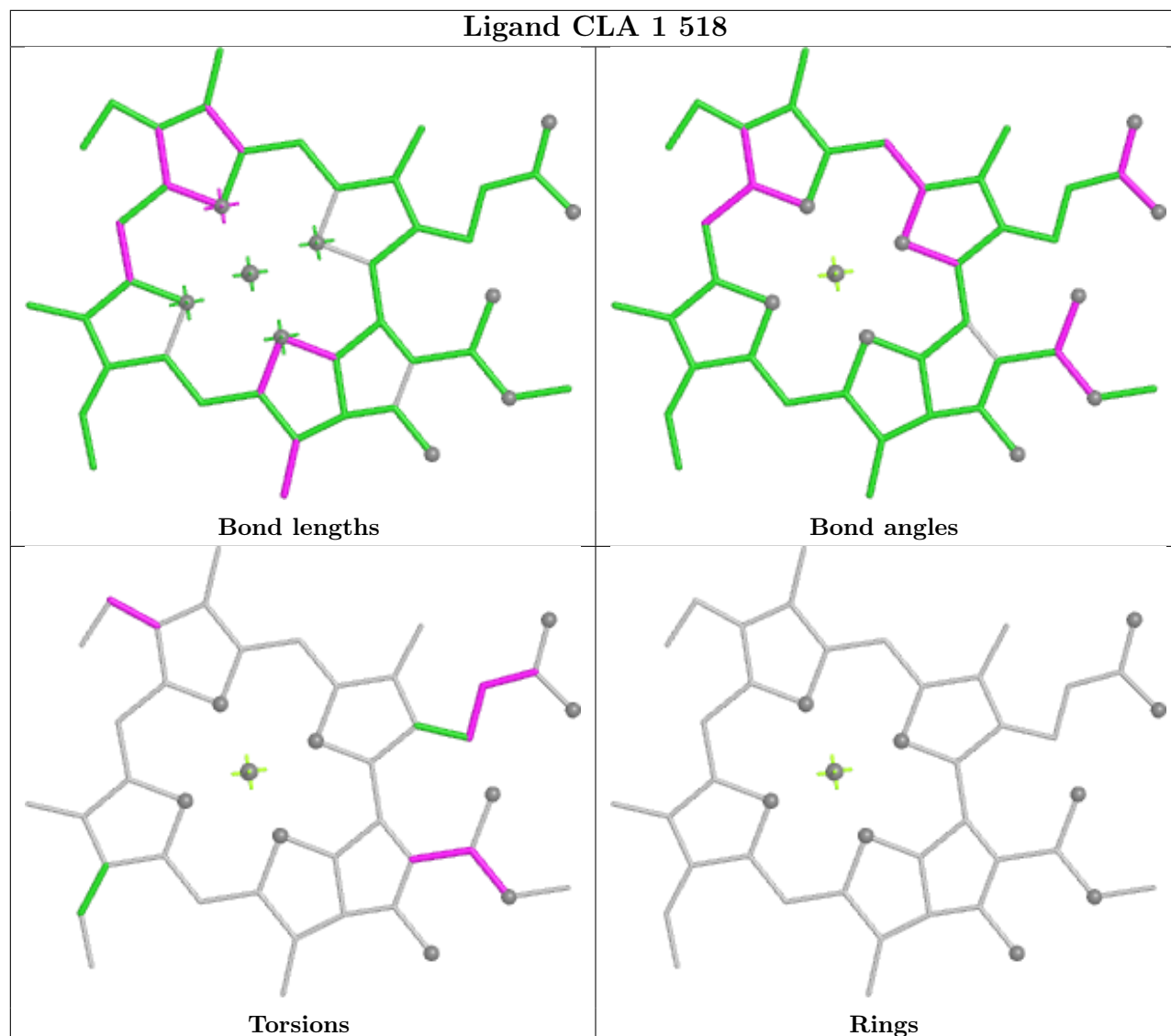
Ligand BCR m 4104



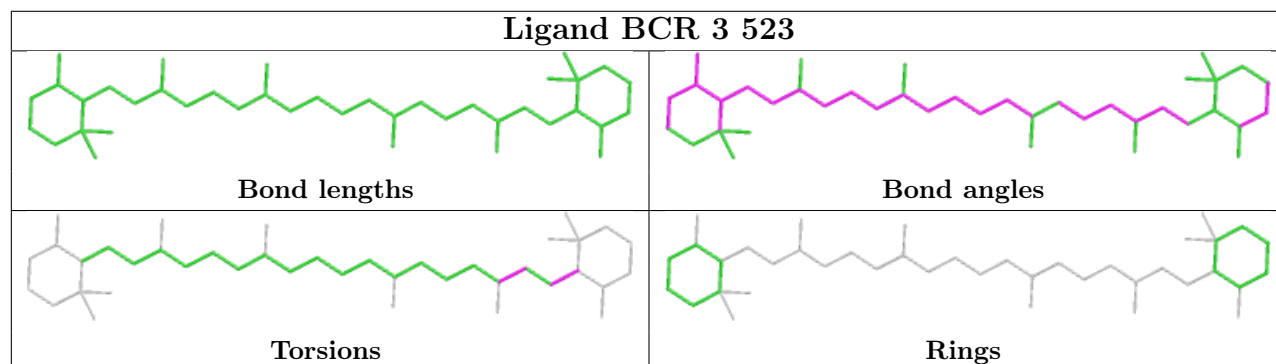
Ligand CLA c 517

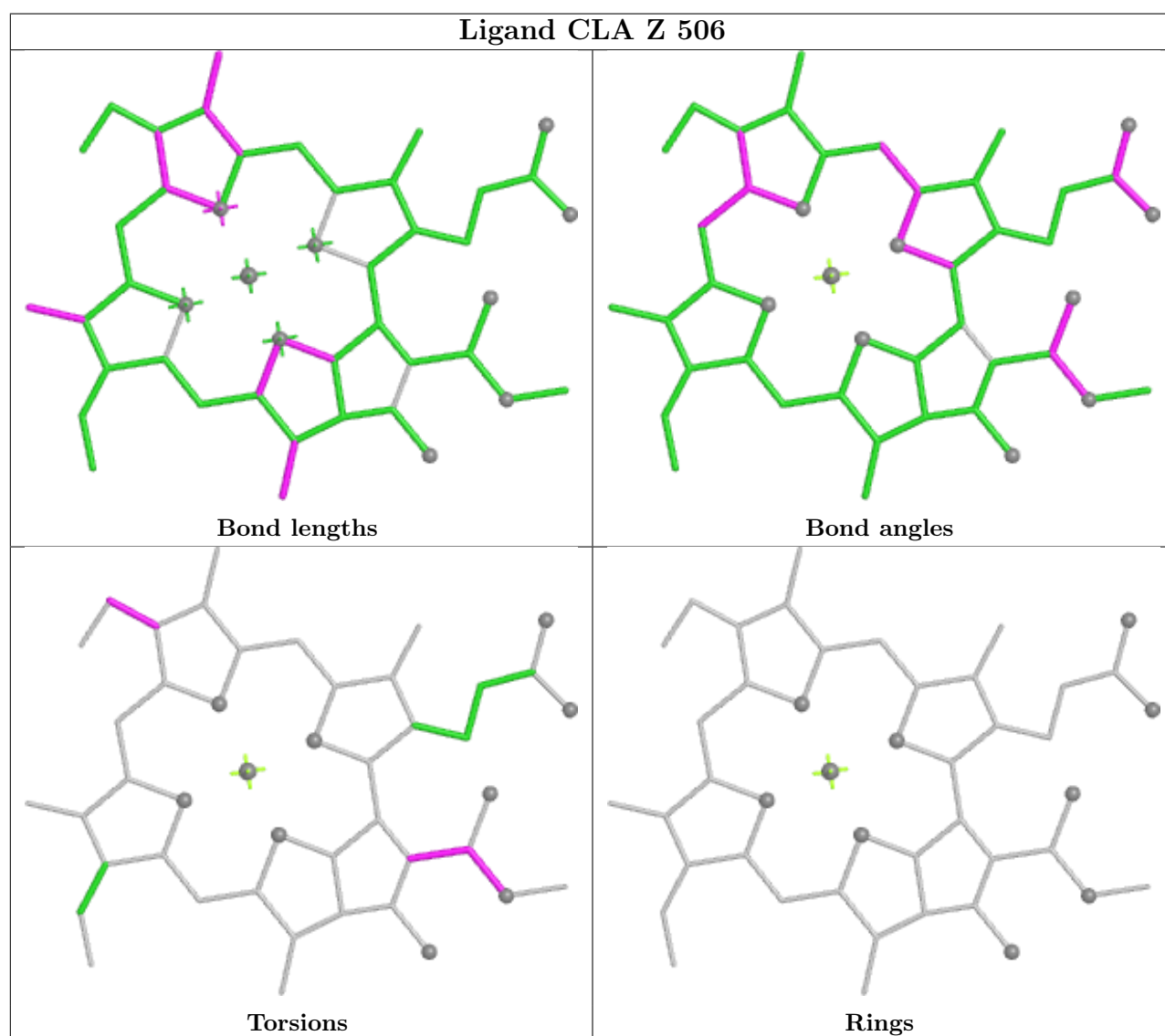
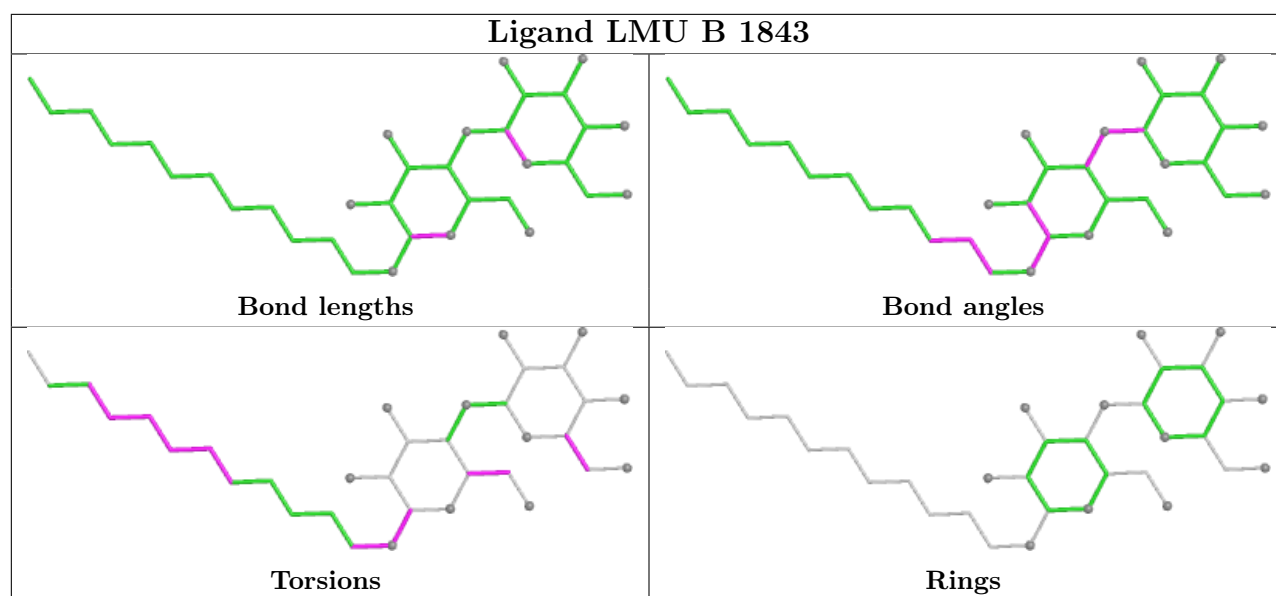


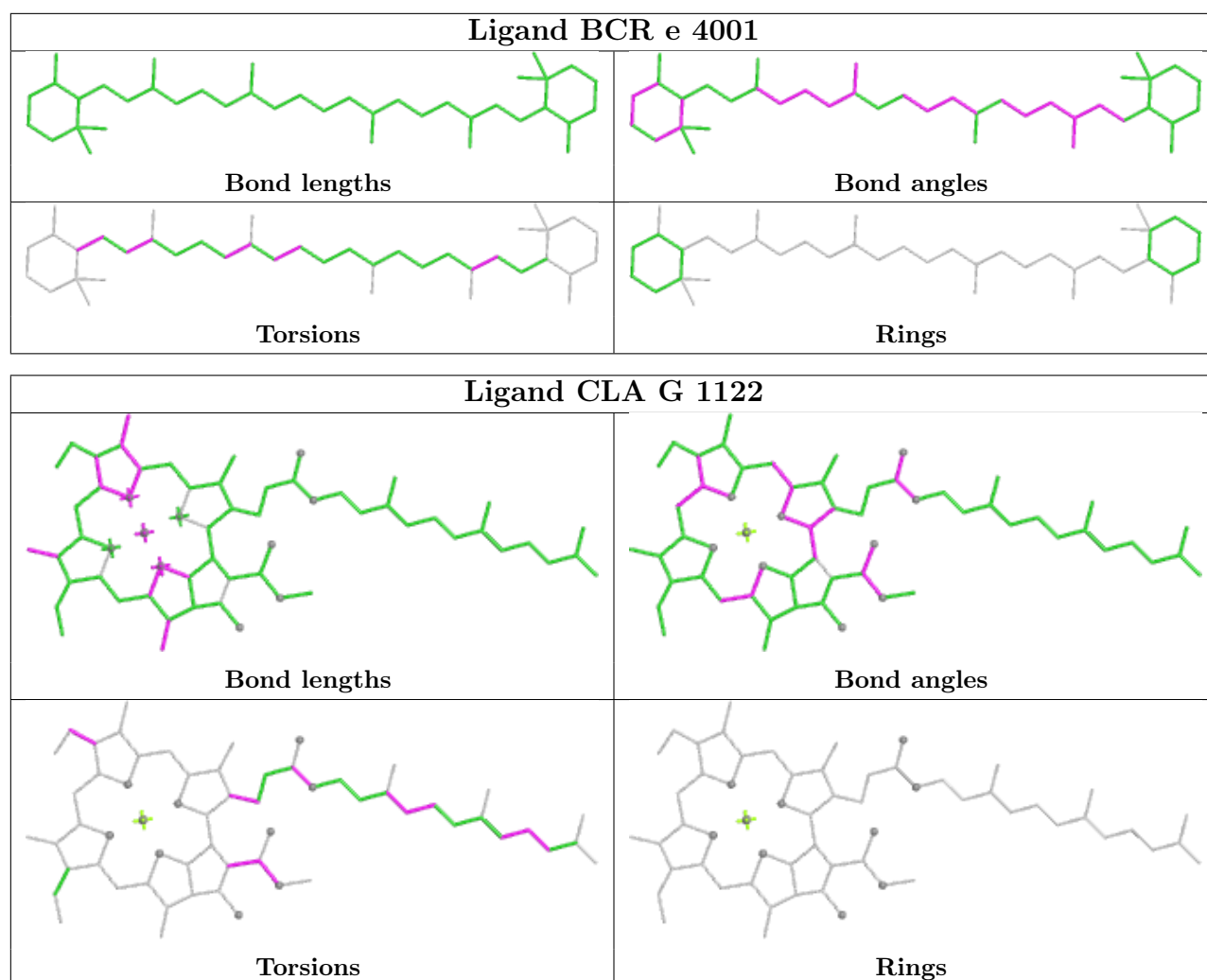
Ligand CLA 1 518



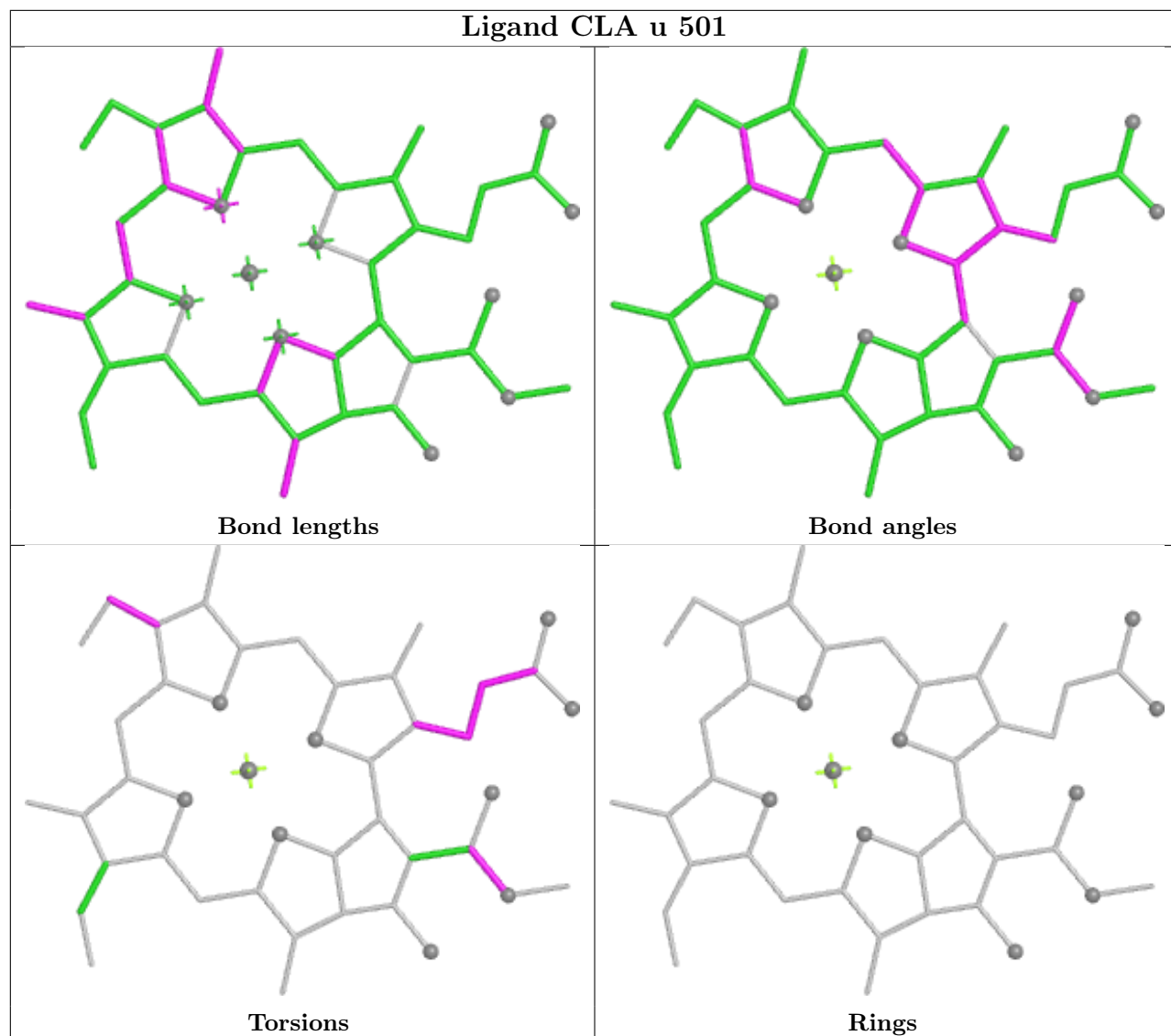
Ligand BCR 3 523

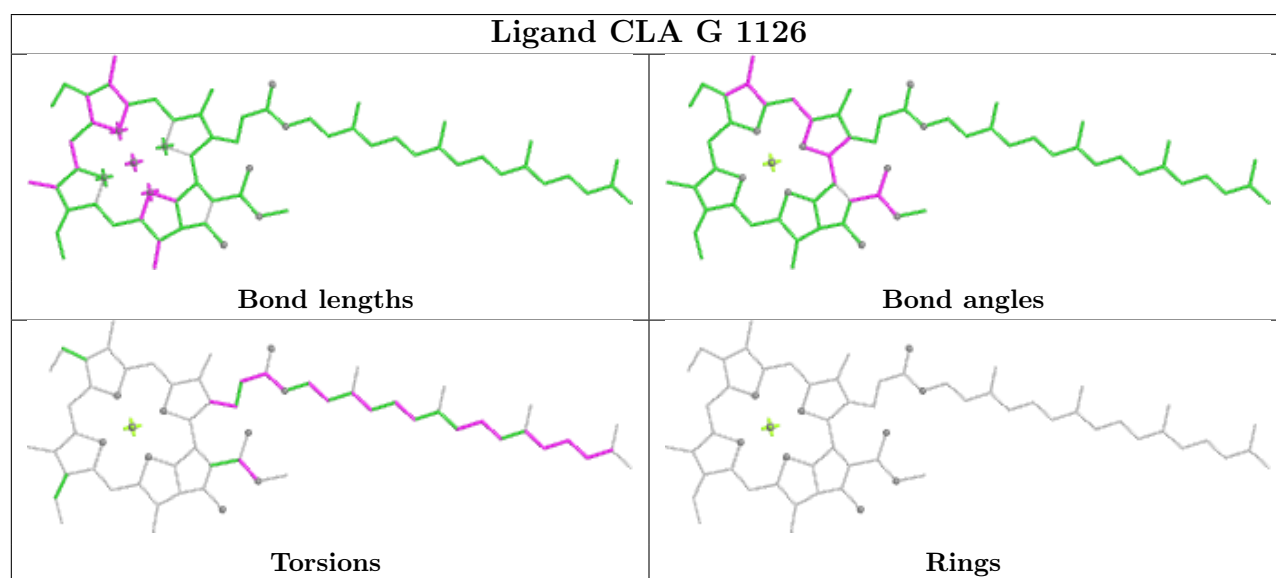
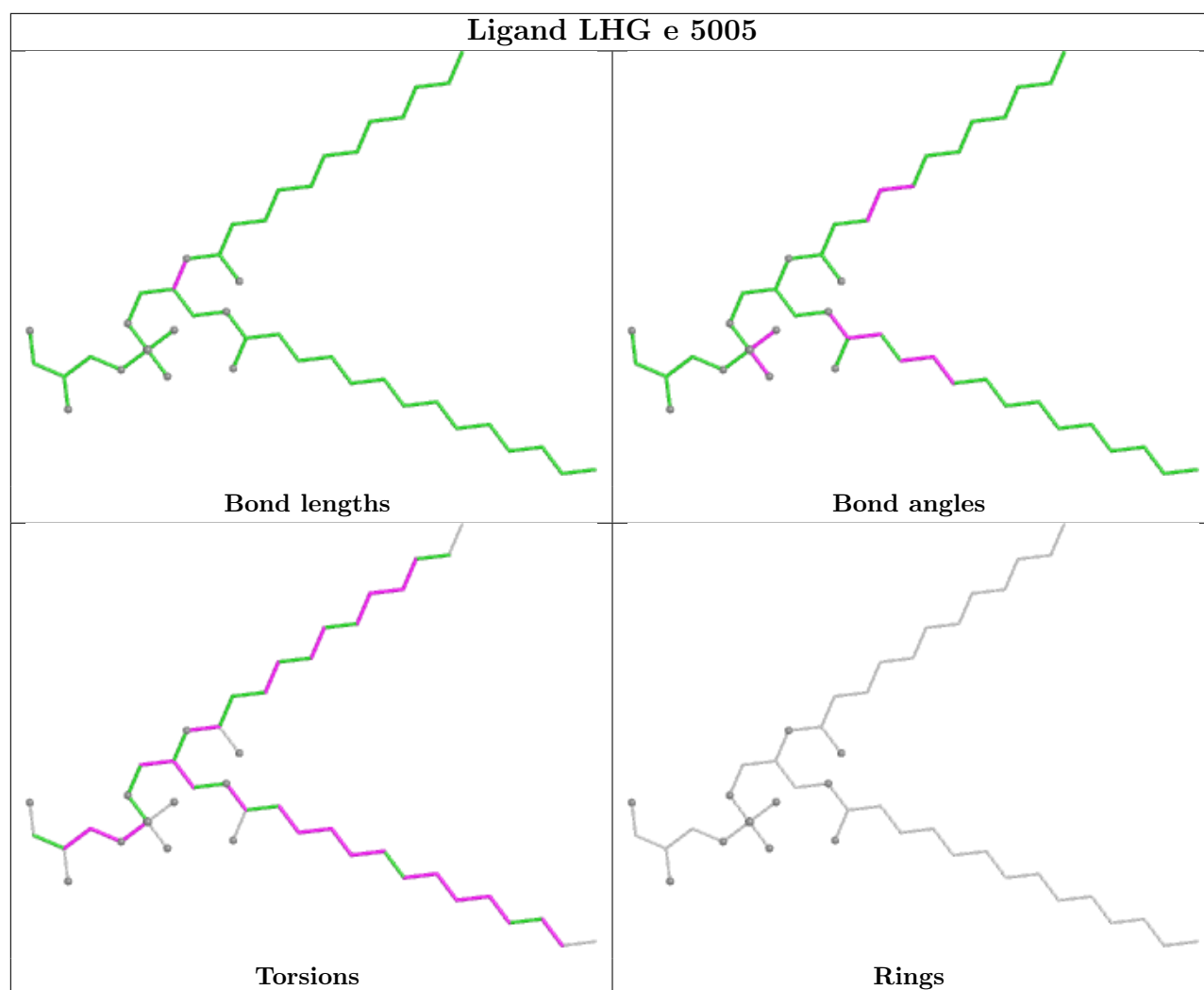


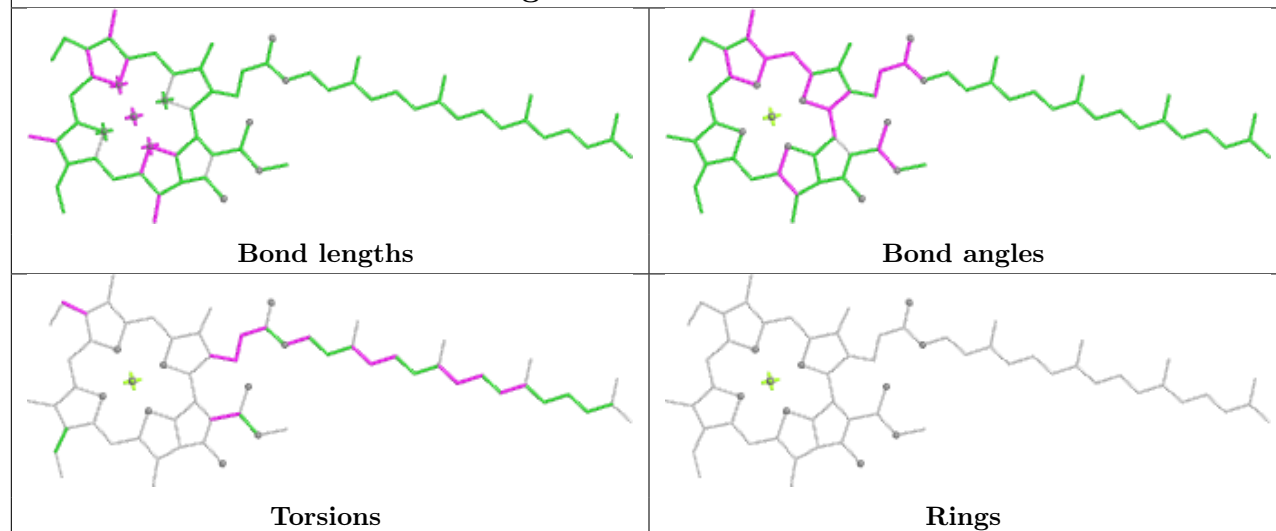
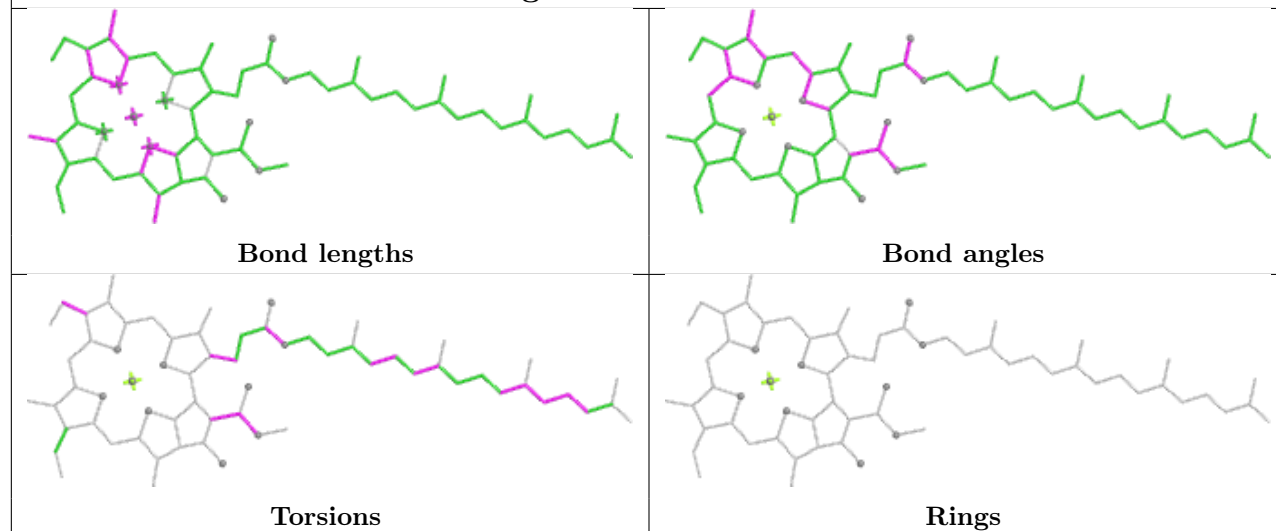
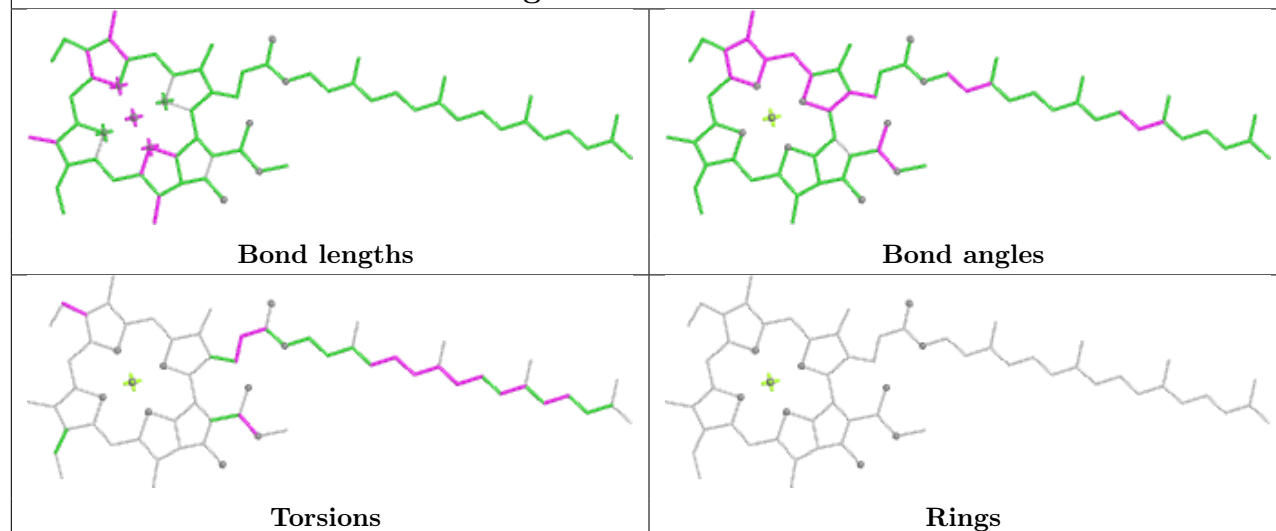




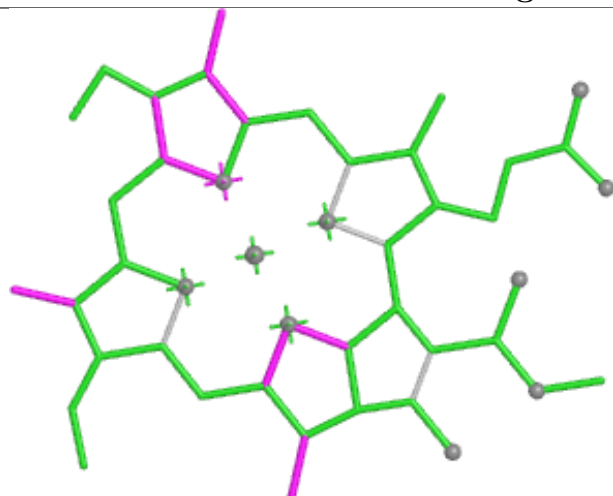
Ligand CLA u 501



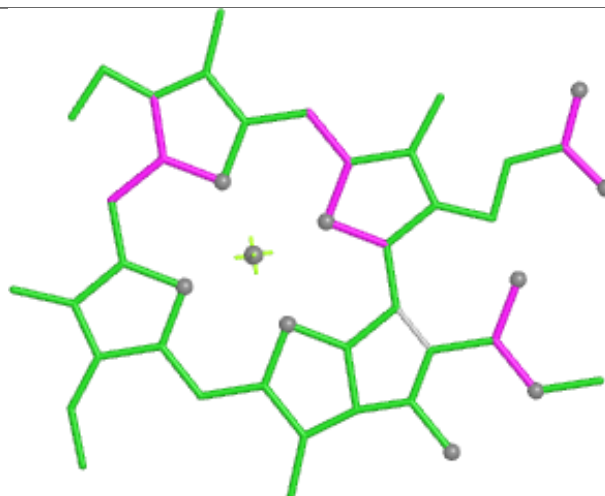


Ligand CLA G 1107**Ligand CLA G 1109****Ligand CLA B 1203**

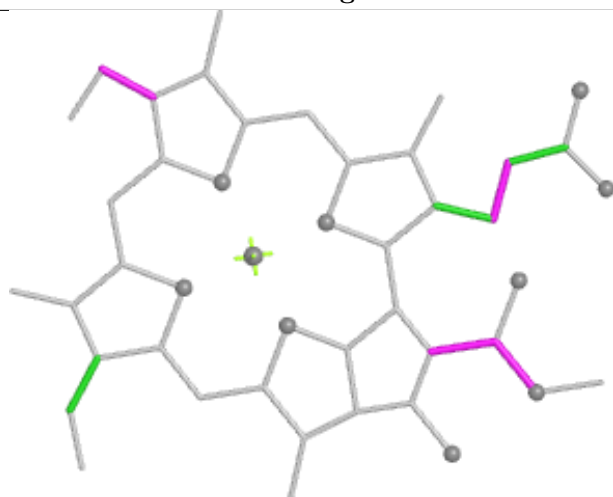
Ligand CLA Z 517



Bond lengths



Bond angles

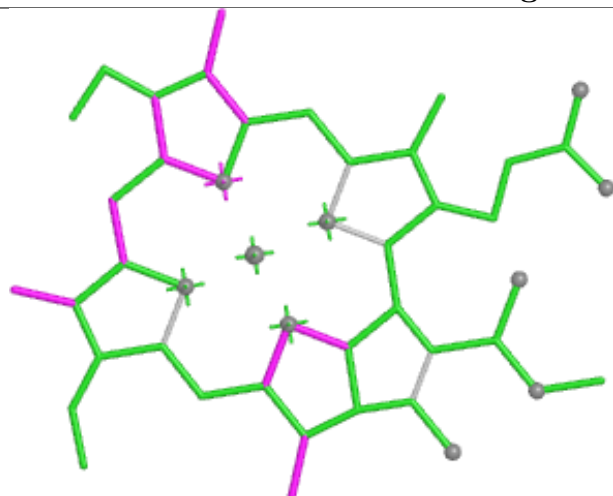


Torsions

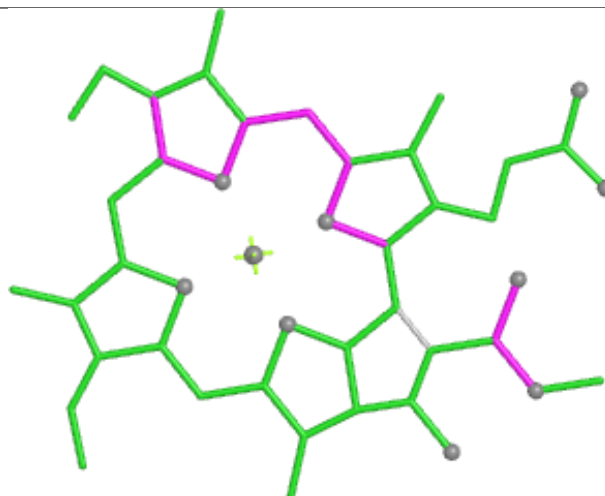


Rings

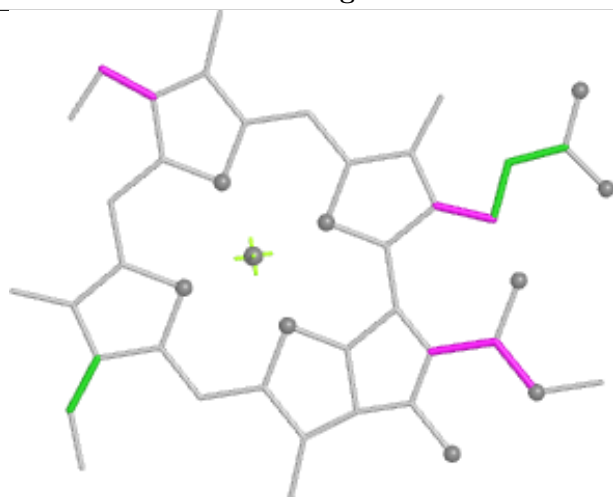
Ligand CLA t 506



Bond lengths



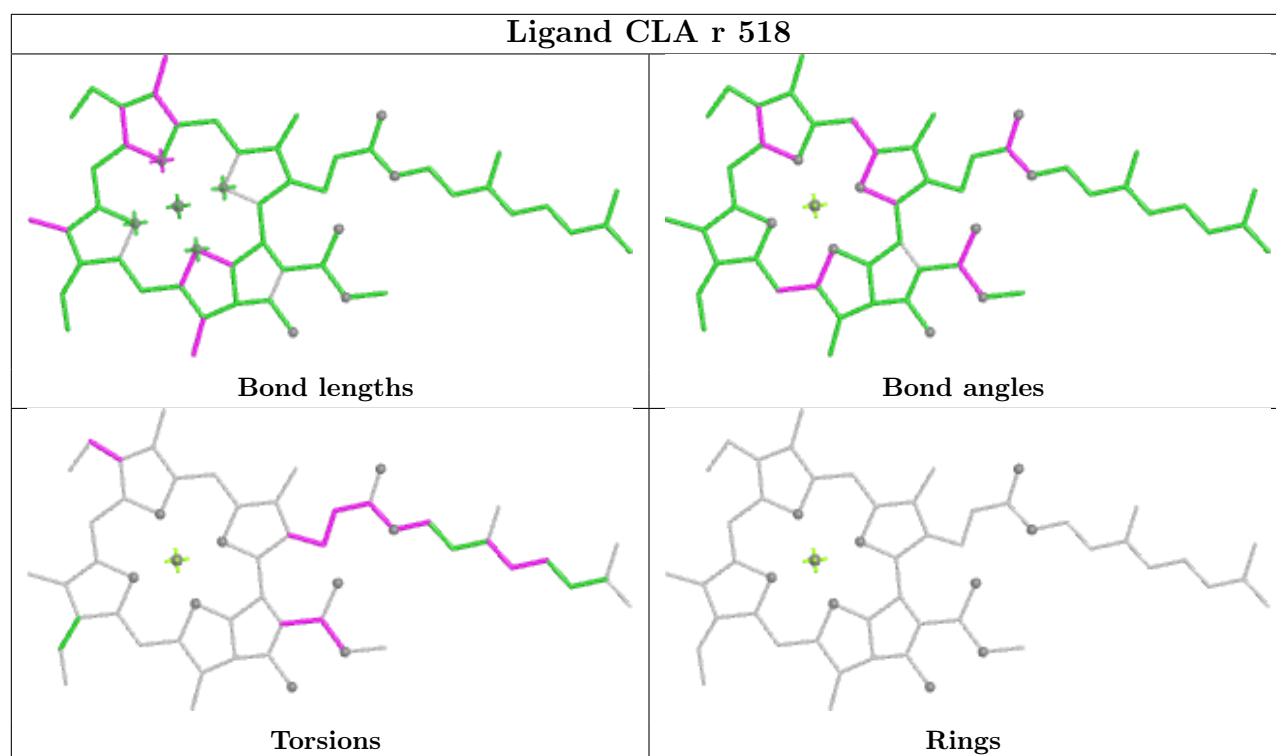
Bond angles



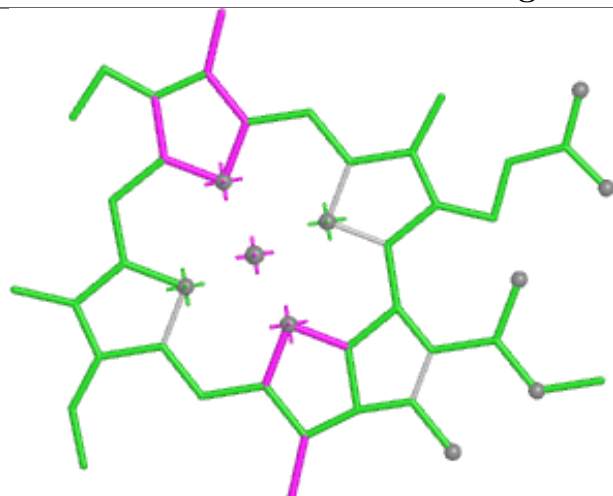
Torsions



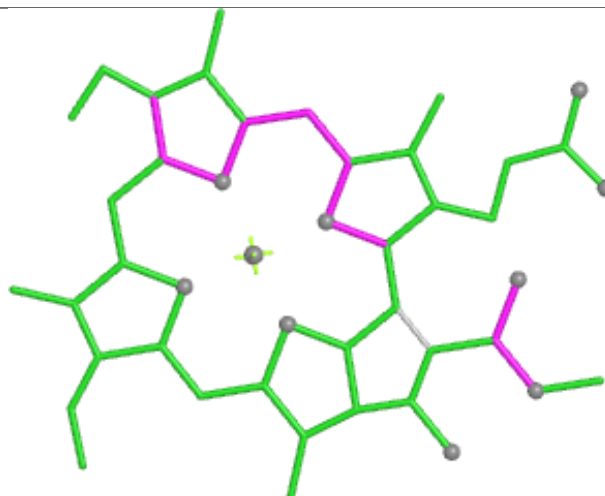
Rings



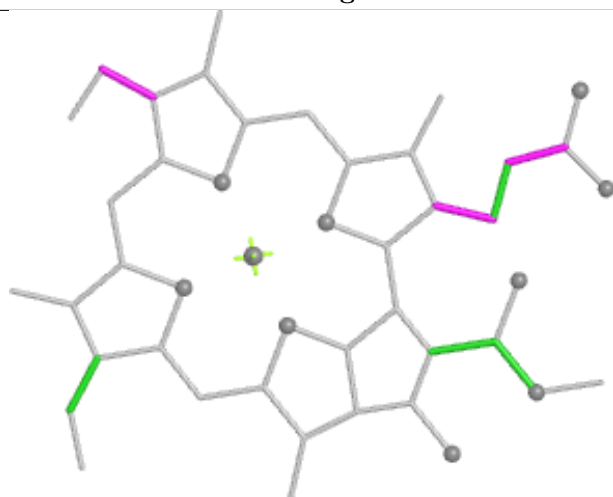
Ligand CLA 2 512



Bond lengths



Bond angles

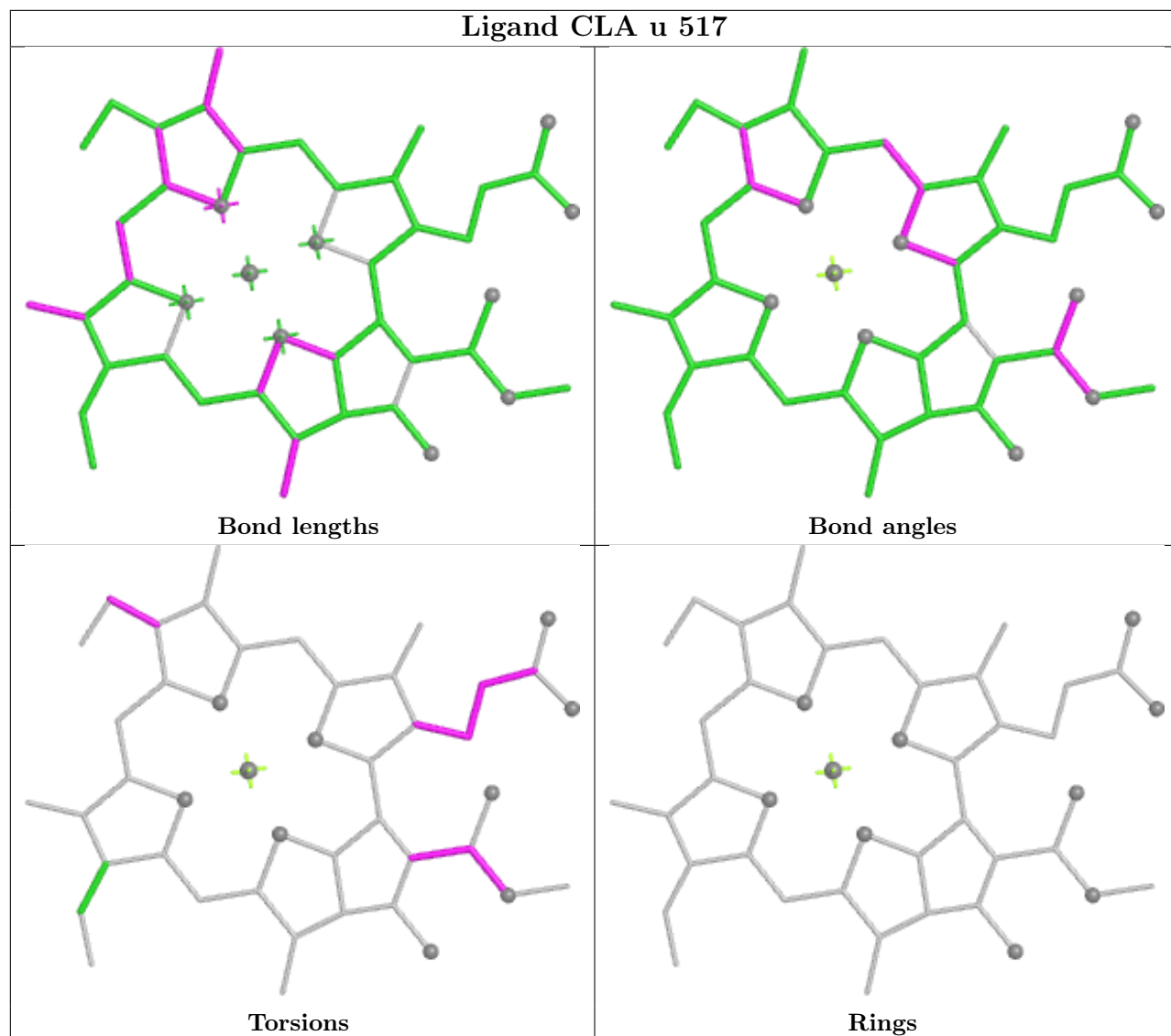


Torsions

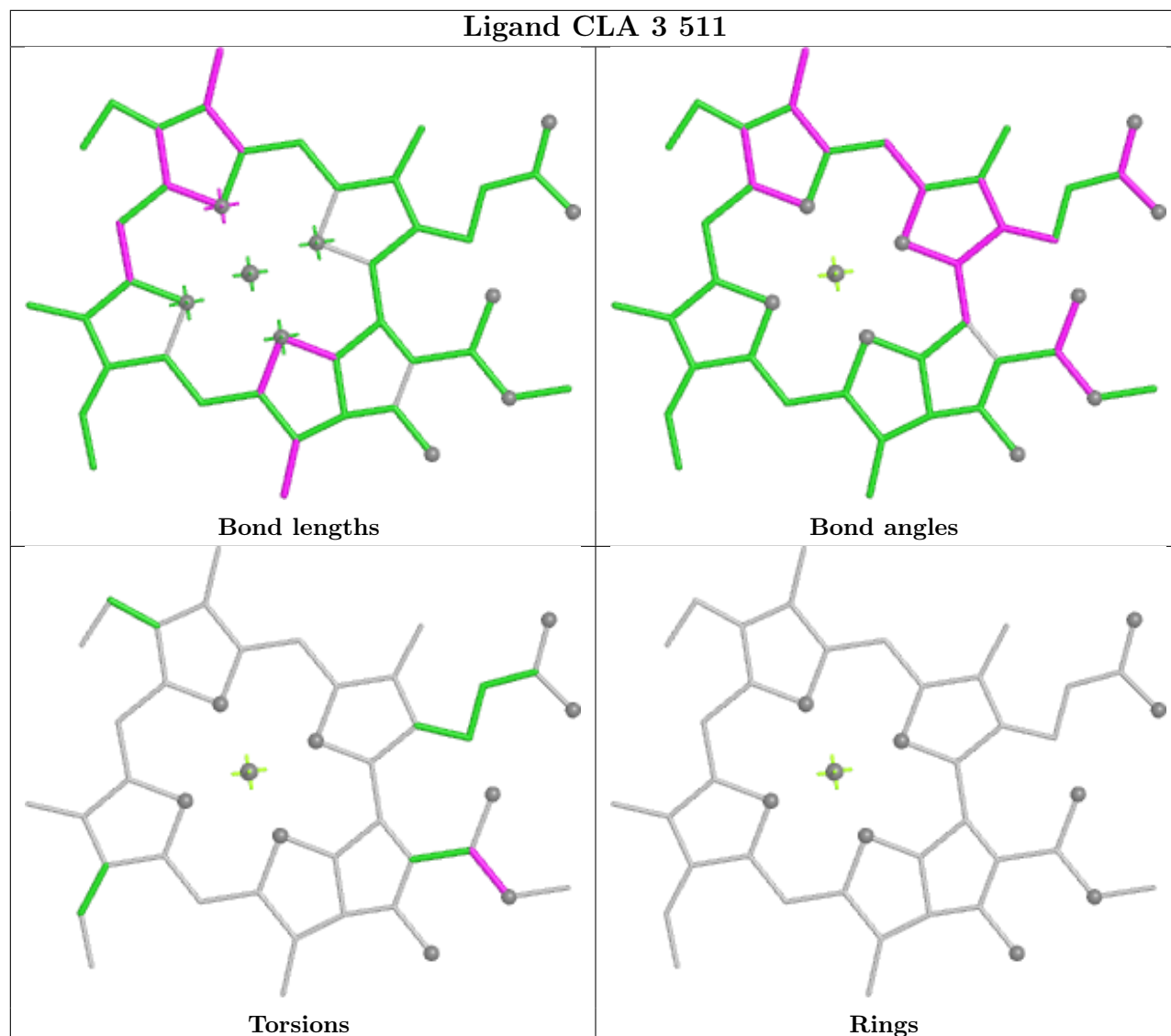


Rings

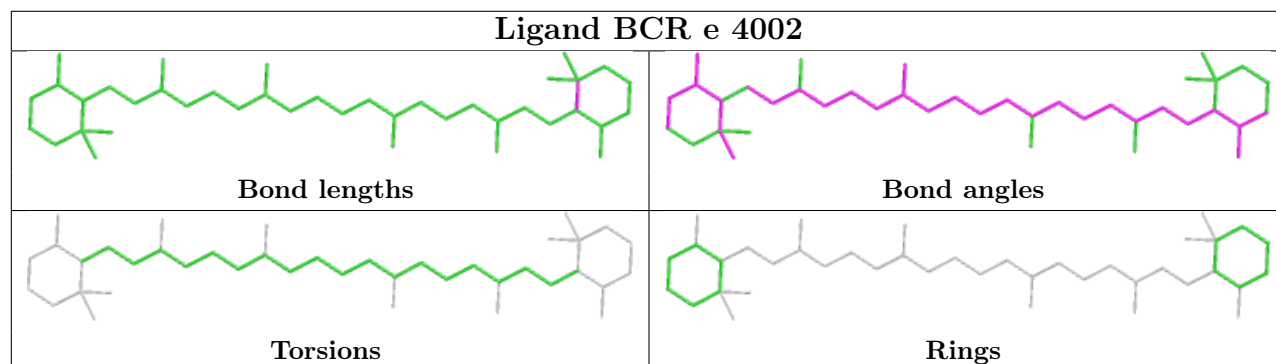
Ligand CLA u 517

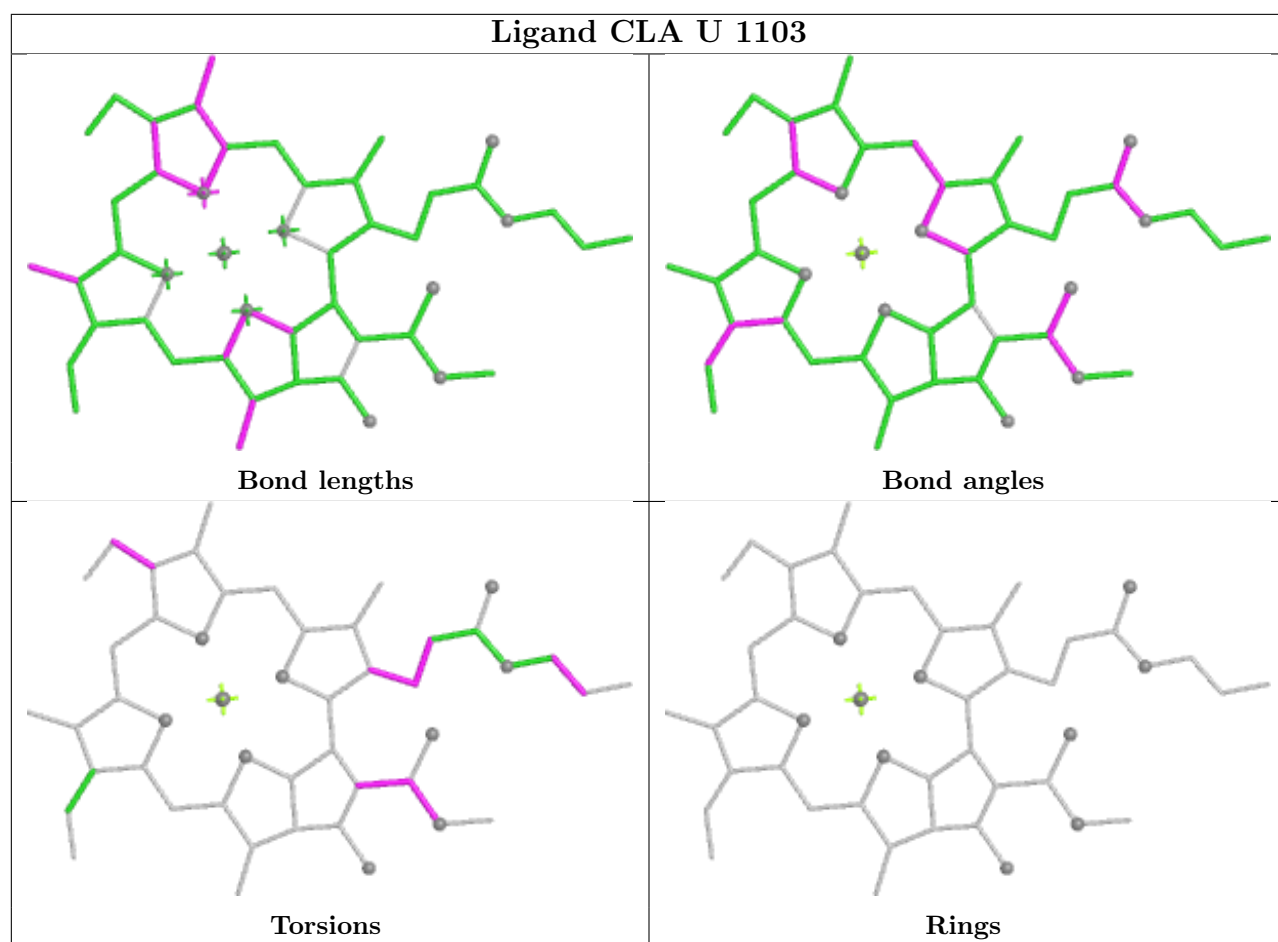


Ligand CLA 3 511

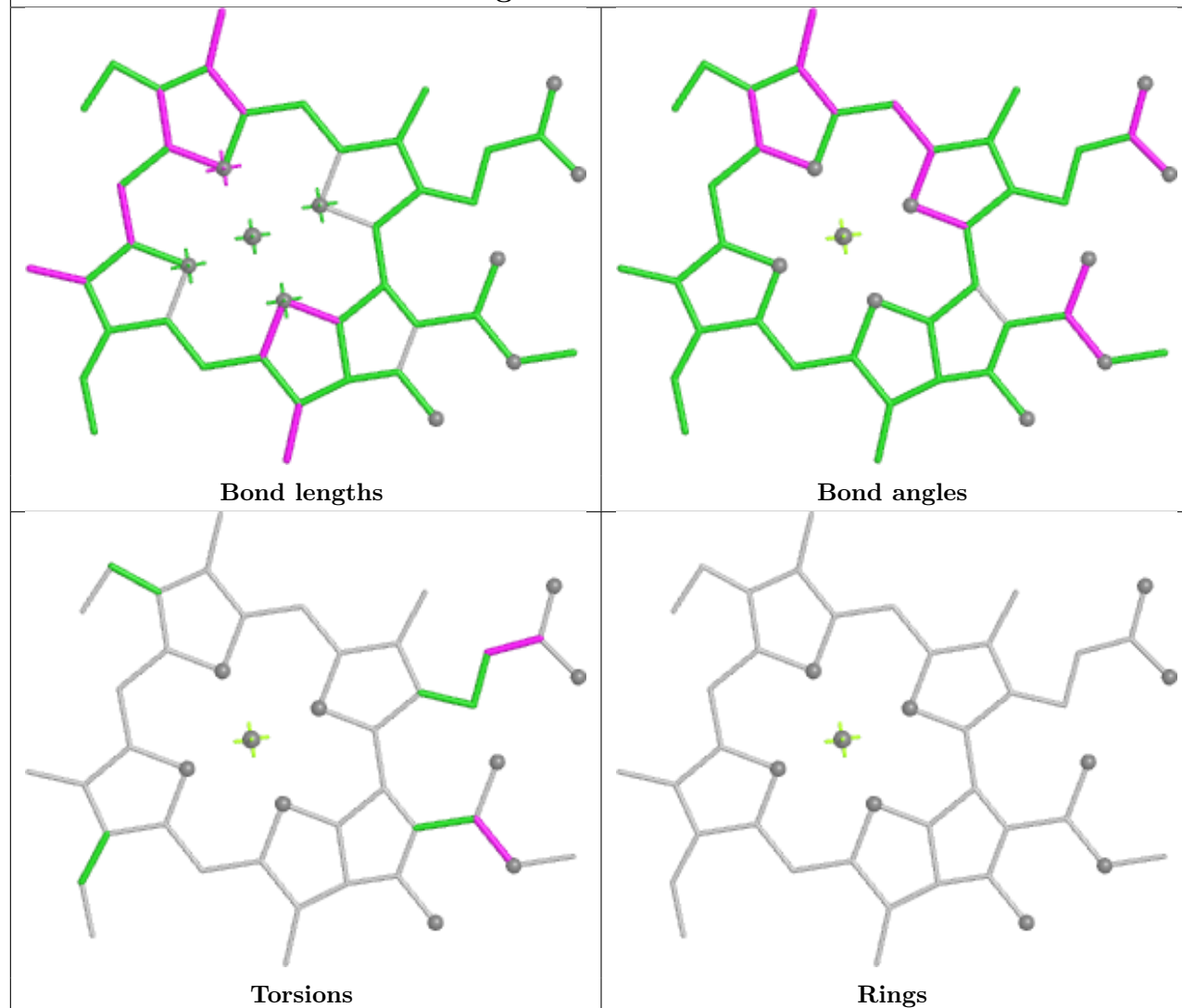


Ligand BCR e 4002

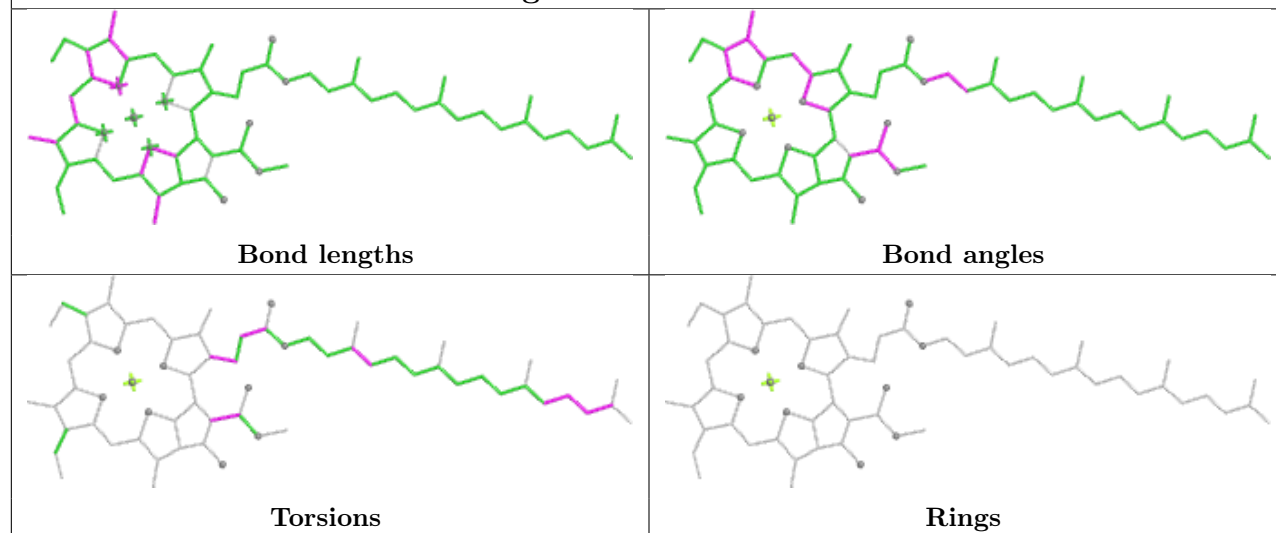


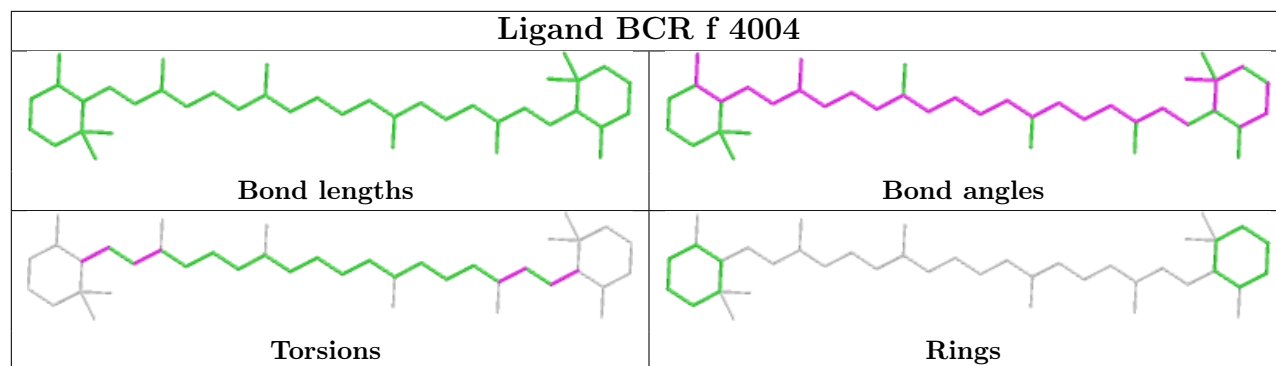


Ligand CLA d 509



Ligand CLA H 1202





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.

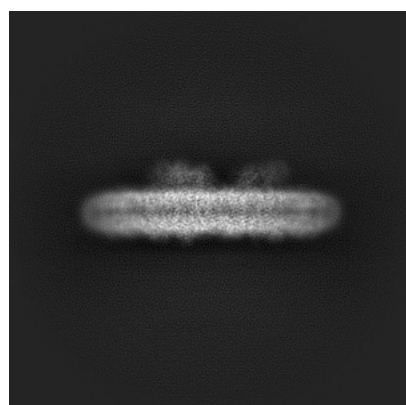
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9994. These allow visual inspection of the internal detail of the map and identification of artifacts.

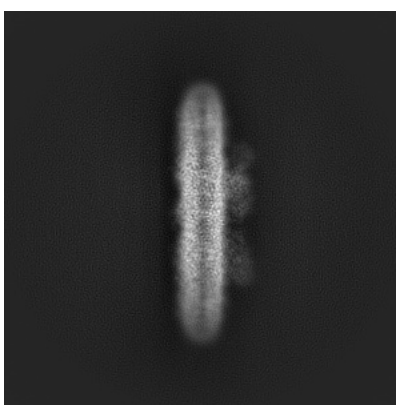
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

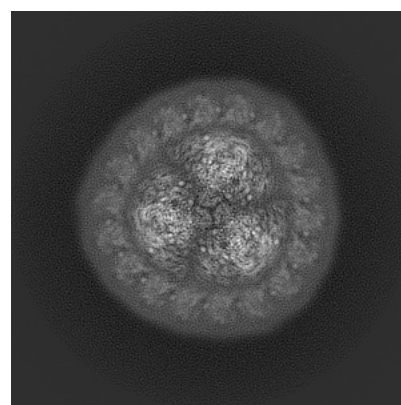
6.1.1 Primary map



X



Y

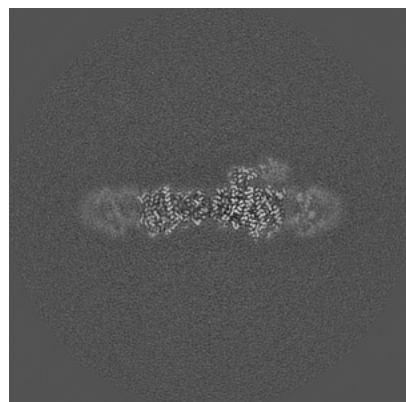


Z

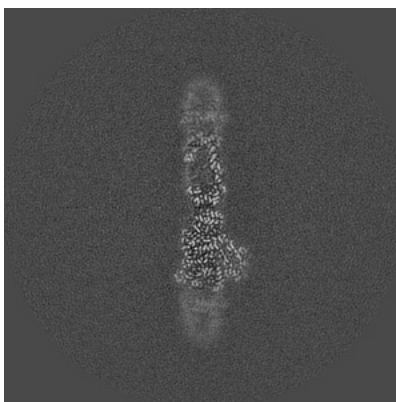
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

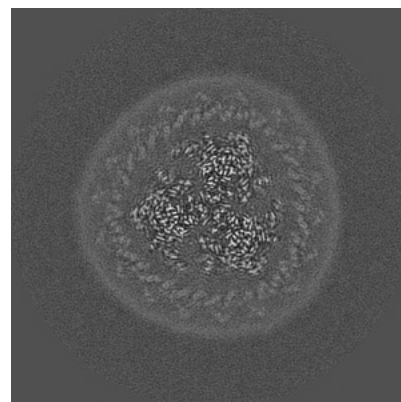
6.2.1 Primary map



X Index: 240



Y Index: 240

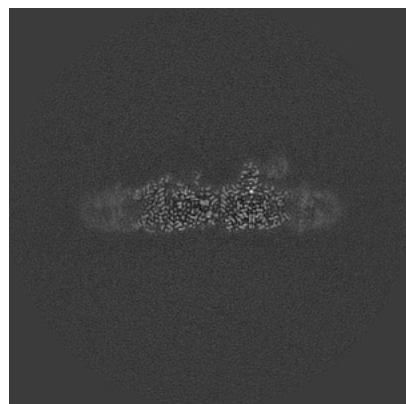


Z Index: 240

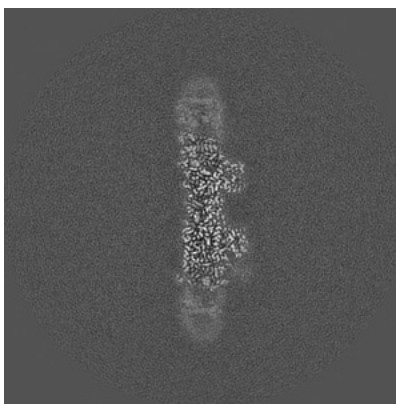
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

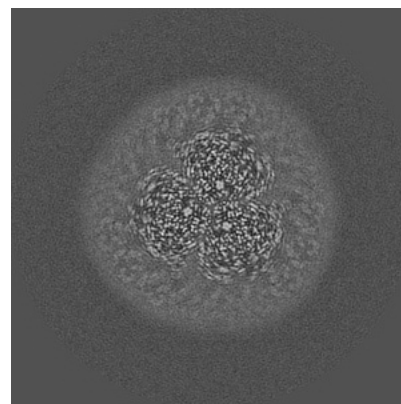
6.3.1 Primary map



X Index: 259



Y Index: 225

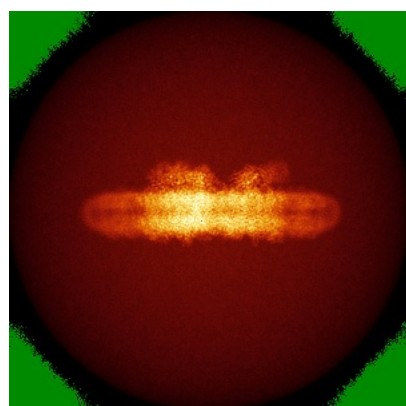


Z Index: 253

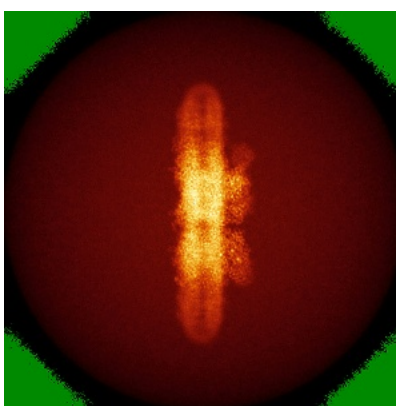
The images above show the largest variance slices of the map in three orthogonal directions.

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

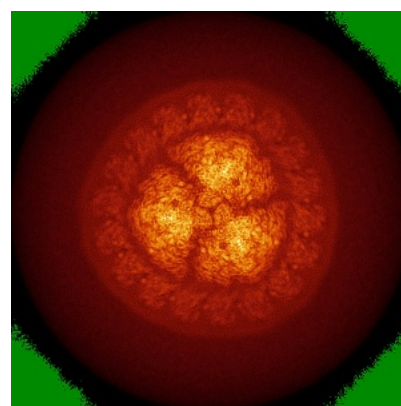
6.4.1 Primary map



X



Y

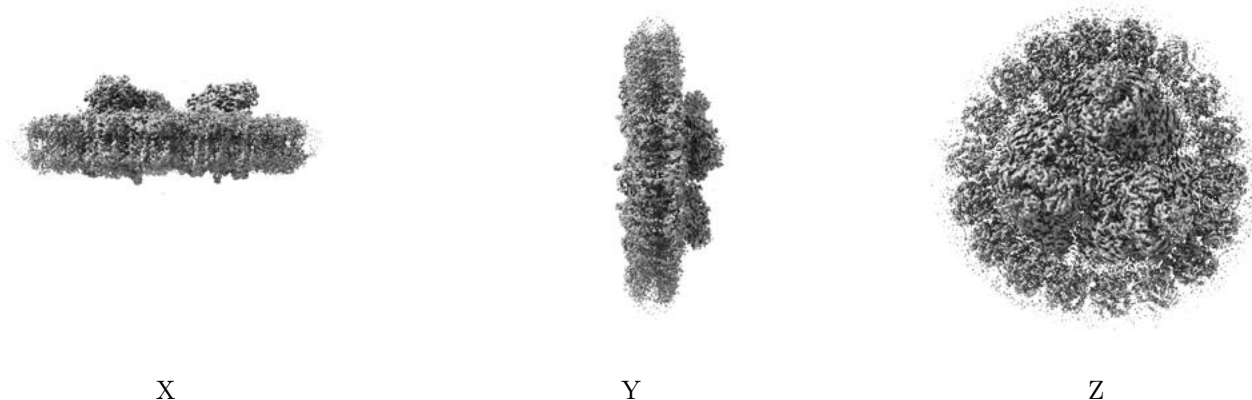


Z

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

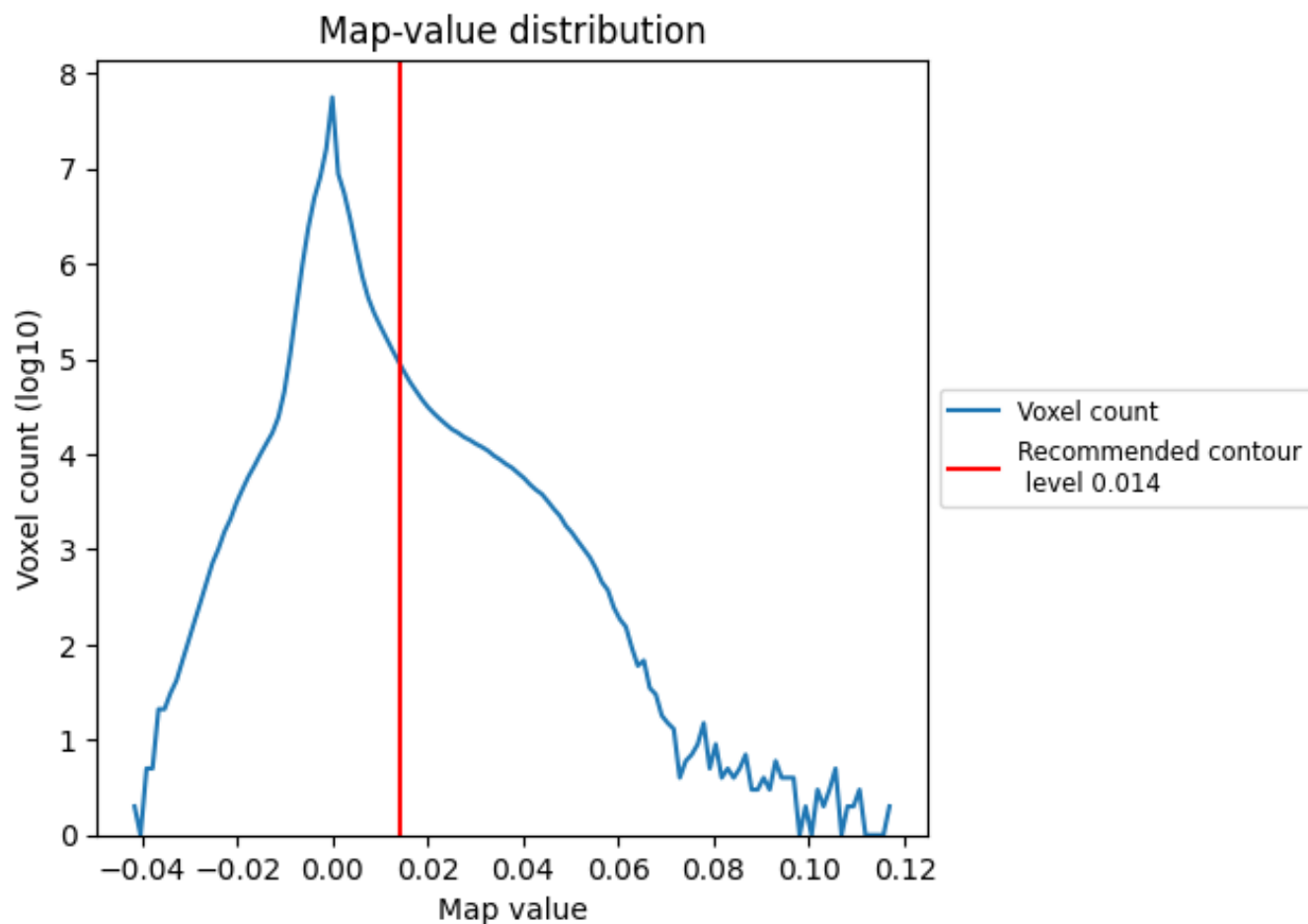
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

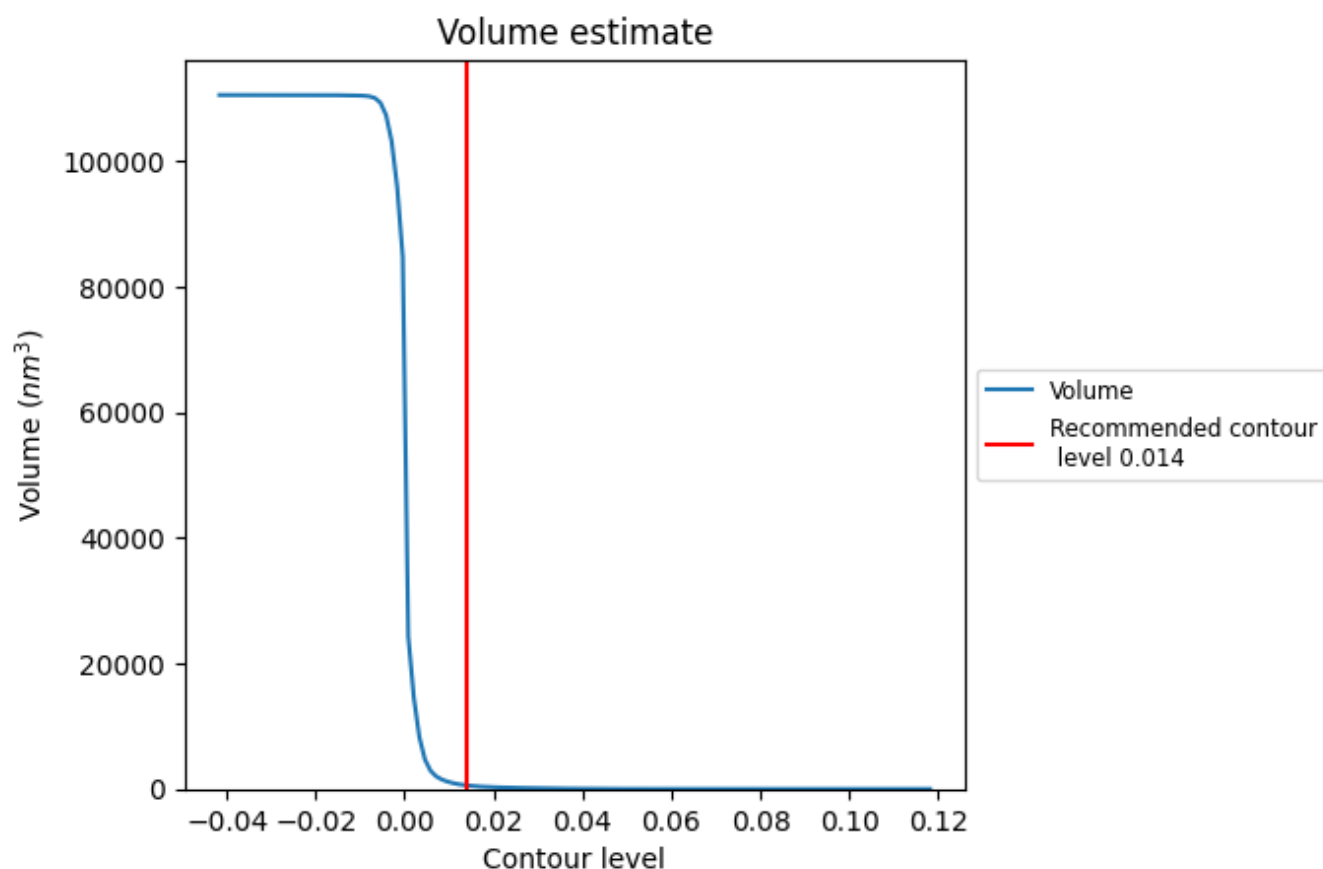
This section contains the results of statistical analysis of the map.

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.

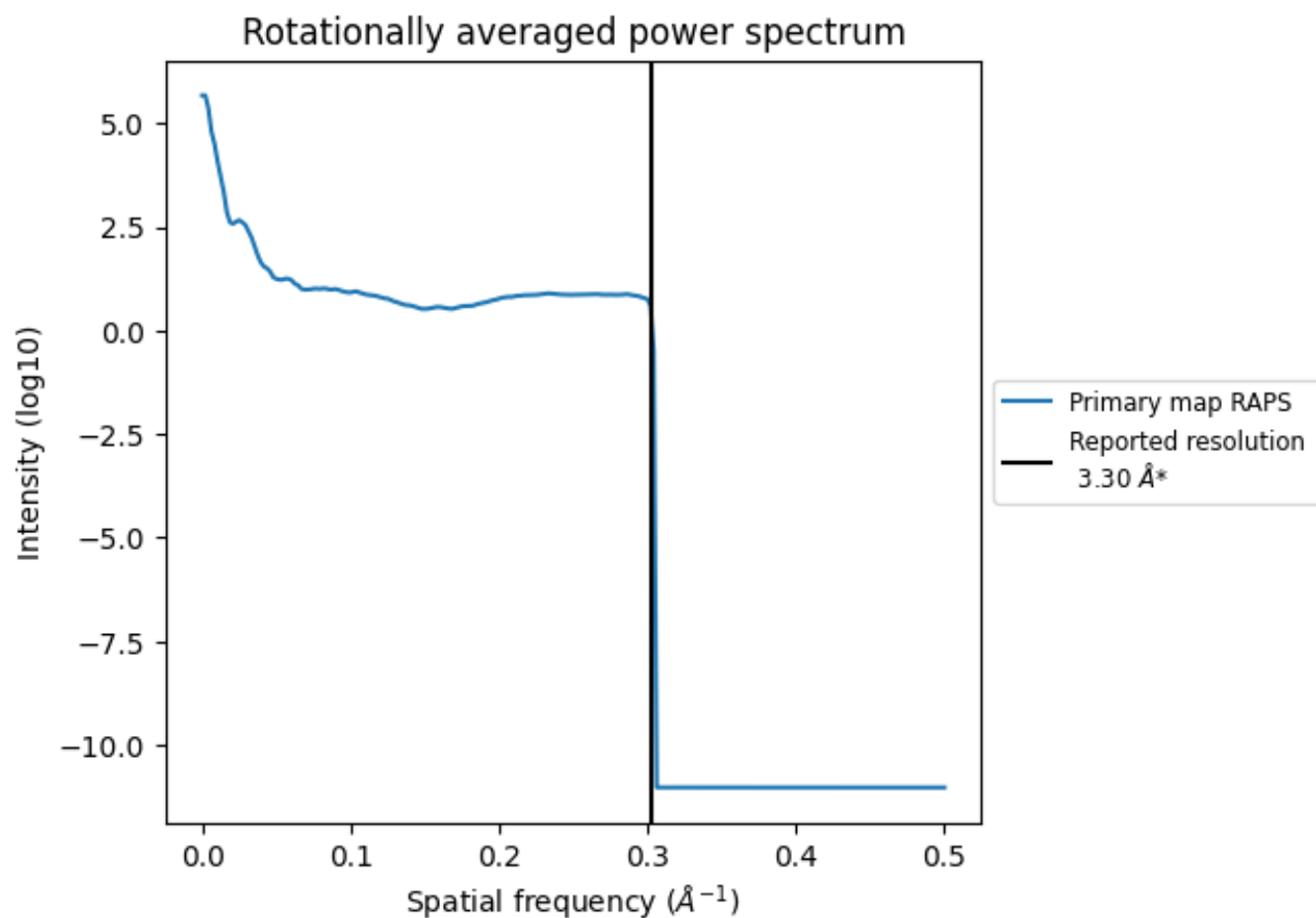
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 567 nm^3 ; this corresponds to an approximate mass of 512 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 0.303 $\text{\AA}^{-1}$

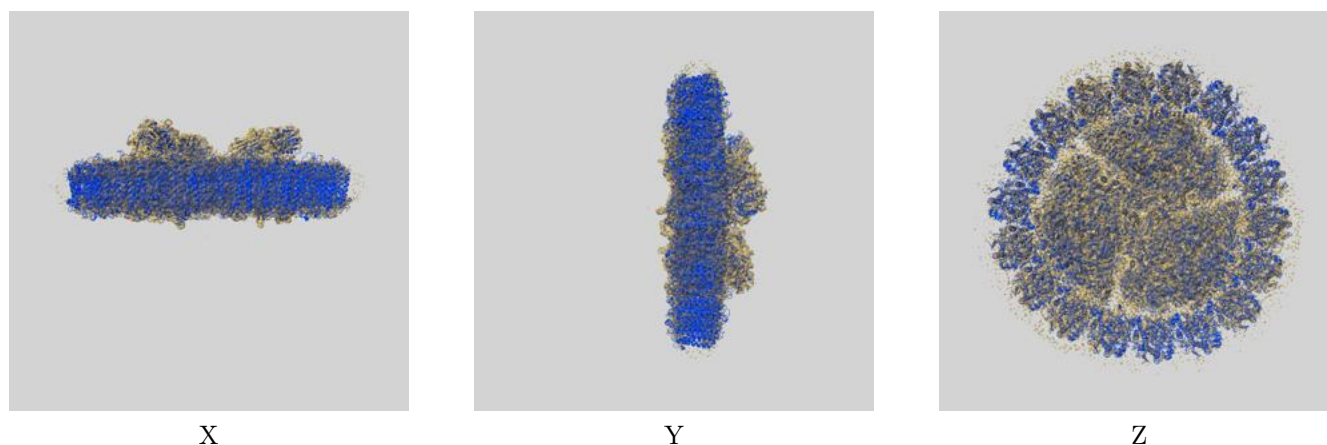
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

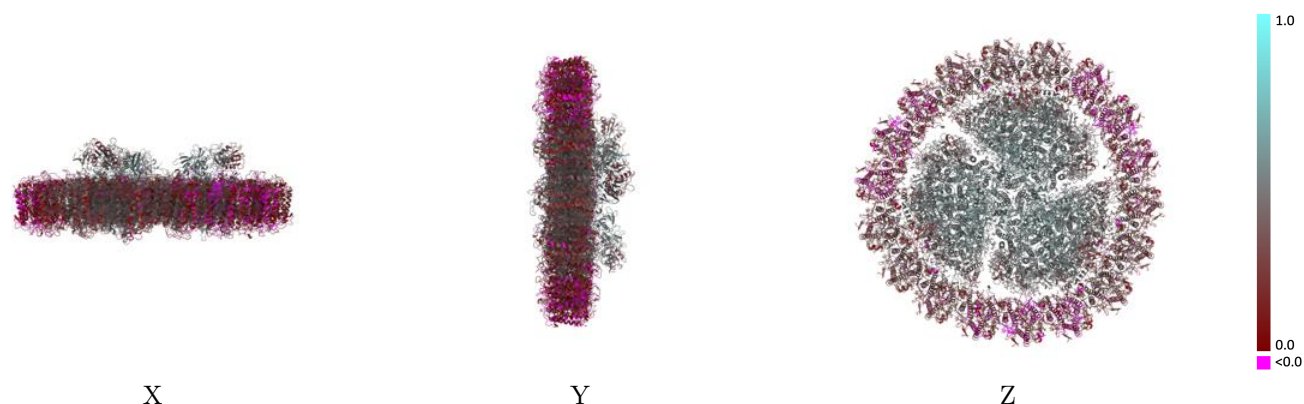
This section contains information regarding the fit between EMDB map EMD-9994 and PDB model 6KIF. Per-residue inclusion information can be found in [section 3](#) on [page 55](#).

9.1 Map-model overlay [i](#)



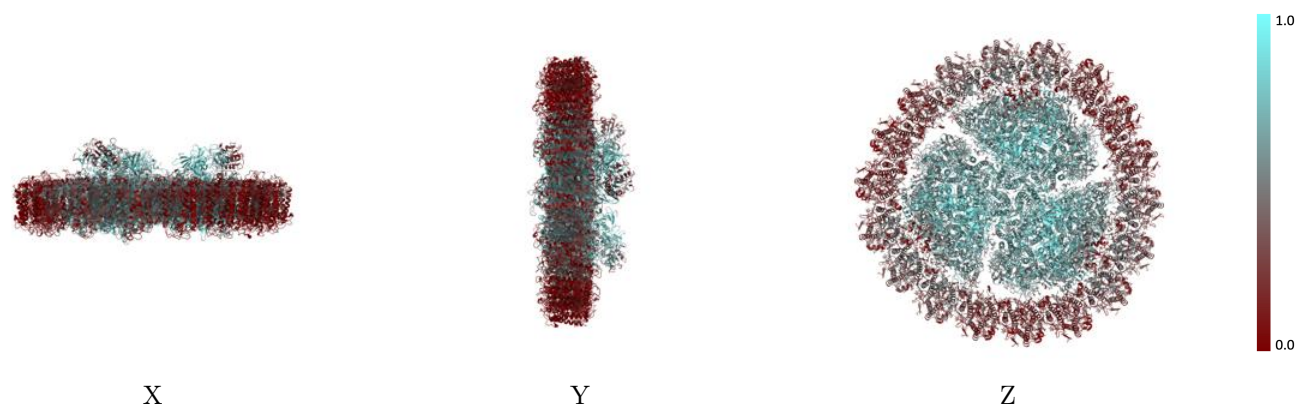
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



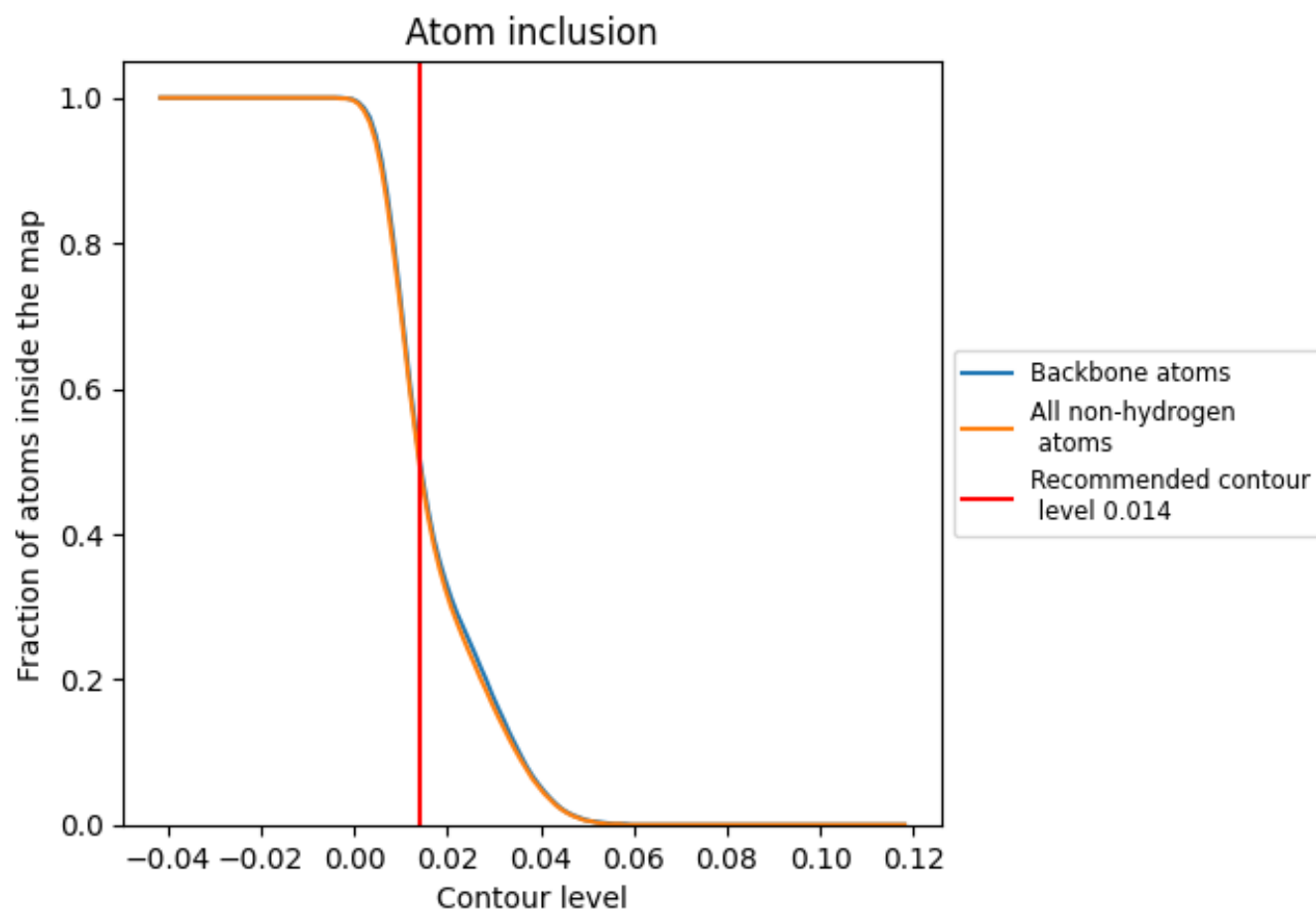
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion ⓘ



At the recommended contour level, 50% of all backbone atoms, 50% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4950	 0.3600
1	 0.3260	 0.2570
2	 0.3300	 0.2860
3	 0.2650	 0.2560
4	 0.0820	 0.0950
5	 0.0790	 0.1060
6	 0.1420	 0.1610
A	 0.7560	 0.5190
B	 0.7500	 0.5000
C	 0.8750	 0.5350
D	 0.7920	 0.5270
E	 0.7270	 0.4830
F	 0.6900	 0.4570
G	 0.7550	 0.5150
H	 0.7500	 0.5000
I	 0.7510	 0.5410
J	 0.6790	 0.4920
K	 0.5300	 0.3470
L	 0.7810	 0.5400
M	 0.7060	 0.5080
N	 0.8720	 0.5370
O	 0.7930	 0.5260
P	 0.3710	 0.3350
Q	 0.7210	 0.4810
R	 0.6900	 0.4570
S	 0.7590	 0.5440
T	 0.6690	 0.4930
U	 0.5180	 0.3330
V	 0.7830	 0.5400
W	 0.6990	 0.5040
X	 0.3680	 0.3320
Y	 0.3180	 0.2520
Z	 0.3280	 0.2790
a	 0.2610	 0.2510
b	 0.0830	 0.0900



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Chain	Atom inclusion	Q-score
c	 0.0760	 0.1030
d	 0.1460	 0.1570
e	 0.7560	 0.5190
f	 0.7500	 0.4990
g	 0.8680	 0.5350
h	 0.7920	 0.5260
i	 0.7180	 0.4760
j	 0.6890	 0.4540
k	 0.7530	 0.5370
l	 0.6690	 0.4910
m	 0.5360	 0.3490
n	 0.7850	 0.5390
o	 0.7020	 0.5050
p	 0.3780	 0.3340
q	 0.3240	 0.2590
r	 0.3350	 0.2880
s	 0.2640	 0.2580
t	 0.0810	 0.0950
u	 0.0770	 0.1070
v	 0.1480	 0.1590