



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 07:03 AM EDT

PDB ID : 6PNJ / pdb_00006pnj
EMDB ID : EMD-20397
Title : Structure of Photosystem I Acclimated to Far-red Light
Authors : Gisriel, C.J.; Shen, G.; Kurashov, V.; Ho, M.; Zhang, S.; Williams, D.; Golbeck, J.H.; Fromme, P.; Bryant, D.A.
Deposited on : 2019-07-02
Resolution : 3.19 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:

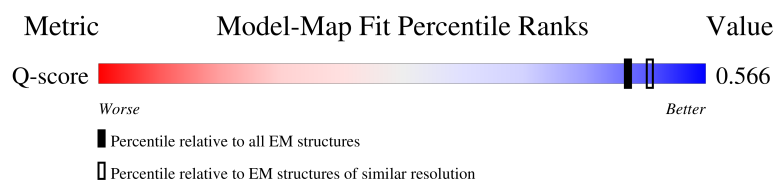
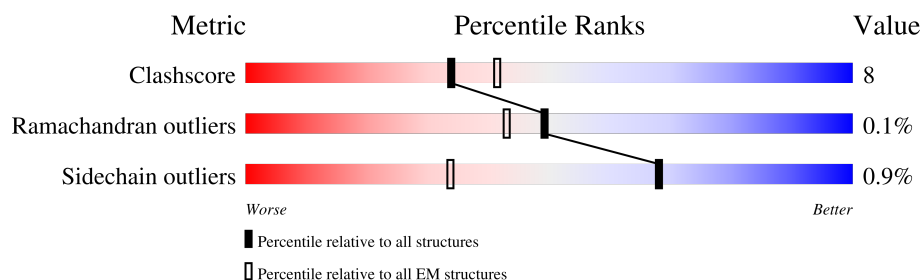
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.19 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	14455 (2.69 - 3.69)

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	788	 7% 79% 15% 5%
1	G	788	 7% 79% 16% 5%
1	a	788	 7% 79% 16% 5%
2	B	741	 5% 83% 17%

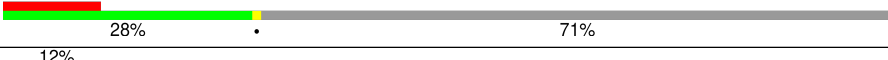
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Mol	Chain	Length	Quality of chain
2	H	741	
2	b	741	
3	C	81	
3	N	81	
3	c	81	
4	D	159	
4	O	159	
4	d	159	
5	E	72	
5	P	72	
5	e	72	
6	F	159	
6	Q	159	
6	f	159	
7	I	67	
7	R	67	
7	i	67	
8	J	48	
8	S	48	
8	j	48	
9	K	39	
9	T	39	
9	k	39	
10	L	174	
10	U	174	

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Mol	Chain	Length	Quality of chain
10	l	174	
11	M	31	
11	V	31	
11	m	31	
12	W	101	
12	X	101	
12	x	101	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	F6C	A	1120	X	-	-	-
15	F6C	A	1121	X	-	-	-
15	F6C	B	1230	X	-	-	-
15	F6C	B	1237	X	-	-	-
15	F6C	G	1120	X	-	-	-
15	F6C	G	1121	X	-	-	-
15	F6C	H	1230	X	-	-	-
15	F6C	H	1237	X	-	-	-
15	F6C	a	1120	X	-	-	-
15	F6C	a	1121	X	-	-	-
15	F6C	b	1230	X	-	-	-
15	F6C	b	1237	X	-	-	-

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 71511 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	747	Total	C	N	O	S	0	0
			5906	3877	1008	988	33		
1	G	747	Total	C	N	O	S	0	0
			5906	3877	1008	988	33		
1	a	747	Total	C	N	O	S	0	0
			5906	3877	1008	988	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	738	Total	C	N	O	S	0	0
			5909	3894	996	1001	18		
2	H	738	Total	C	N	O	S	0	0
			5909	3894	996	1001	18		
2	b	738	Total	C	N	O	S	0	0
			5909	3894	996	1001	18		

- 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
			601	367	105	118	11		
3	N	80	Total	C	N	O	S	0	0
			601	367	105	118	11		
3	c	80	Total	C	N	O	S	0	0
			601	367	105	118	11		

- Molecule 4 is a protein called Photosystem I protein PsuD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1092	694	192	203	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	139	Total	C	N	O	S	0	0
			1092	694	192	203	3		
4	d	139	Total	C	N	O	S	0	0
			1092	694	192	203	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	62	Total	C	N	O	S	0	0
			497	313	88	96			
5	P	62	Total	C	N	O	S	0	0
			497	313	88	96			
5	e	62	Total	C	N	O	S	0	0
			497	313	88	96			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	135	Total	C	N	O	S	0	0
			1060	694	167	192	7		
6	Q	135	Total	C	N	O	S	0	0
			1060	694	167	192	7		
6	f	135	Total	C	N	O	S	0	0
			1060	694	167	192	7		

- Molecule 7 is a protein called photosystem I subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	42	Total	C	N	O	S	0	0
			350	246	48	54	2		
7	R	42	Total	C	N	O	S	0	0
			350	246	48	54	2		
7	i	42	Total	C	N	O	S	0	0
			350	246	48	54	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	MET	-	initiating methionine	UNP A0A2N6MR25
R	1	MET	-	initiating methionine	UNP A0A2N6MR25
i	1	MET	-	initiating methionine	UNP A0A2N6MR25

- Molecule 8 is a protein called Photosystem I reaction centre subunit IX / PsaJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	J	43	Total	C	N	O	0	0
			344	238	51	55		
8	S	43	Total	C	N	O	0	0
			344	238	51	55		
8	j	43	Total	C	N	O	0	0
			344	238	51	55		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	34	Total	C	N	O	S	0	0
			201	130	36	34	1		
9	T	34	Total	C	N	O	S	0	0
			201	130	36	34	1		
9	k	34	Total	C	N	O	S	0	0
			201	130	36	34	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	156	Total	C	N	O	S	0	0
			1172	760	198	209	5		
10	U	156	Total	C	N	O	S	0	0
			1172	760	198	209	5		
10	l	156	Total	C	N	O	S	0	0
			1172	760	198	209	5		

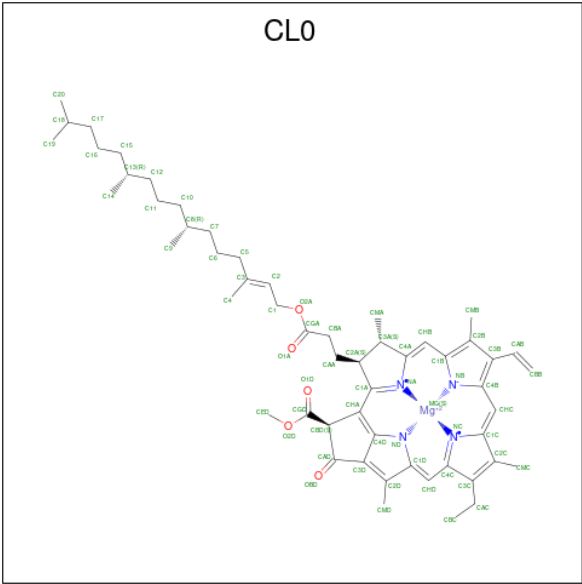
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			245	164	37	43	1		
11	V	31	Total	C	N	O	S	0	0
			245	164	37	43	1		
11	m	31	Total	C	N	O	S	0	0
			245	164	37	43	1		

- Molecule 12 is a protein called Photosystem one PsaX.

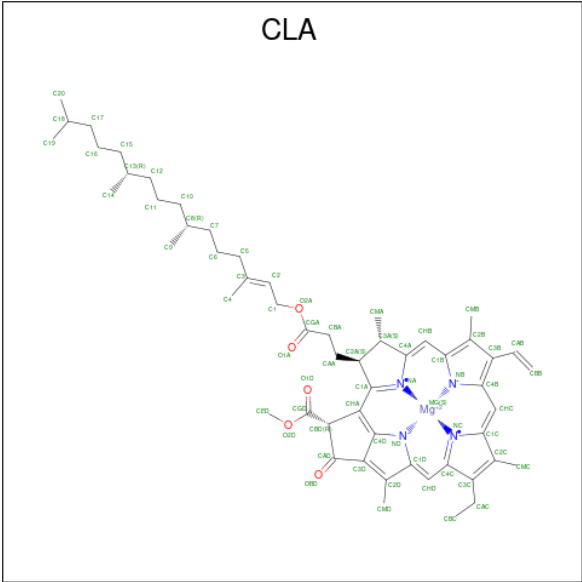
Mol	Chain	Residues	Atoms				AltConf	Trace
12	W	29	Total	C	N	O	0	0
			246	172	36	38		
12	X	29	Total	C	N	O	0	0
			246	172	36	38		
12	x	29	Total	C	N	O	0	0
			246	172	36	38		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- 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
			60	50	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
			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
			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
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
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 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 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 55	C 45	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 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 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 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 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 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	A	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 45	C 35	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 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	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 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 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 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 65	C 55	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 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 45	C 35	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

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

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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	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 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 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 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 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 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 45	C 35	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 55	C 45	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 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 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 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 60	C 50	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 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 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 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 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	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 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 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 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	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 45	C 35	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 45	C 35	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 45	C 35	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 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 55	C 45	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
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 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 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	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 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	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 45	C 35	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	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	L	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	L	1	Total 65	C 55	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 60	C 50	Mg 1	N 4	O 5	0
14	U	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	X	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 60	C 50	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 60	C 50	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 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 60	C 50	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 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 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 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 55	C 45	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 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 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 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 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 60	C 50	Mg 1	N 4	O 5	0
14	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	a	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total 45	C 35	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 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	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 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 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 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 65	C 55	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 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 45	C 35	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

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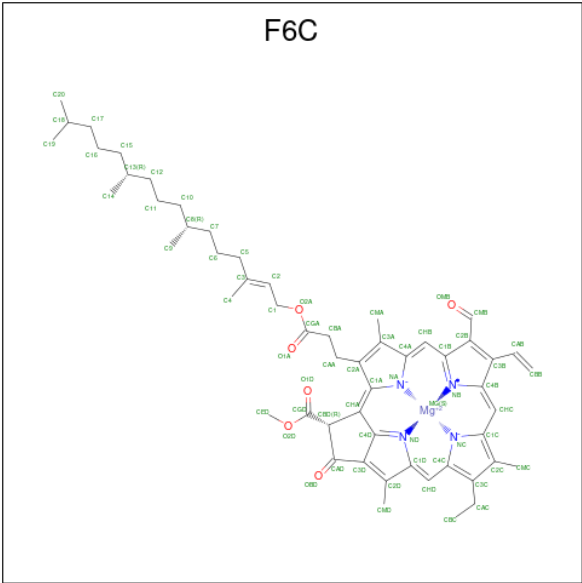
Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total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

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is Chlorophyll F (CCD ID: F6C) (formula: C₅₅H₆₈MgN₄O₆).



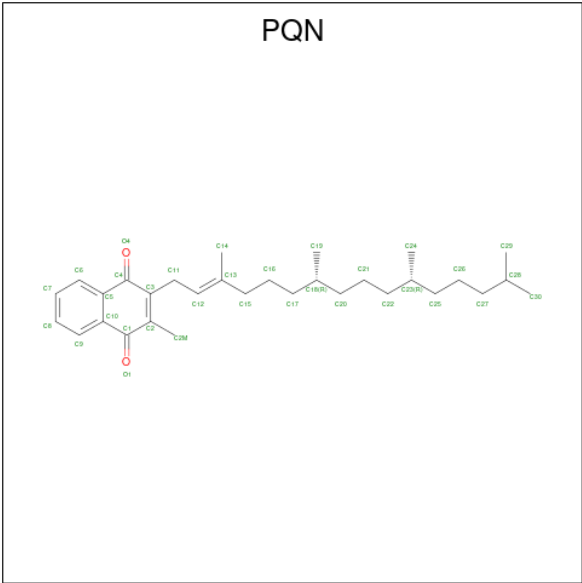
Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
15	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 16 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



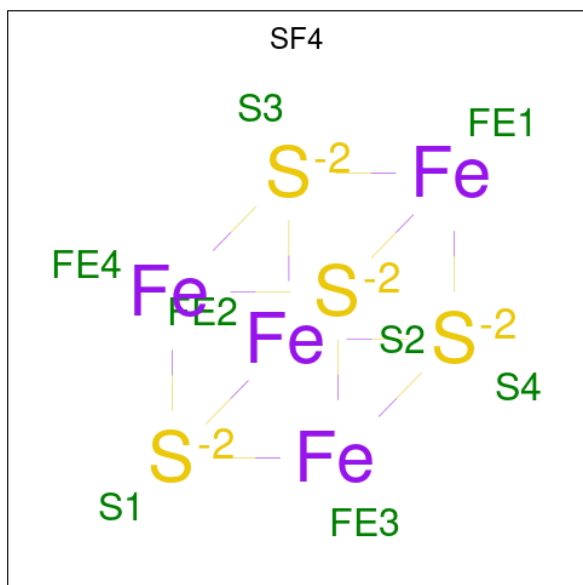
Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	C	O	0
			33	31	2	
16	B	1	Total	C	O	0
			33	31	2	
16	G	1	Total	C	O	0
			33	31	2	

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Mol	Chain	Residues	Atoms			AltConf
16	H	1	Total	C	O	0
			33	31	2	
16	a	1	Total	C	O	0
			33	31	2	
16	b	1	Total	C	O	0
			33	31	2	

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



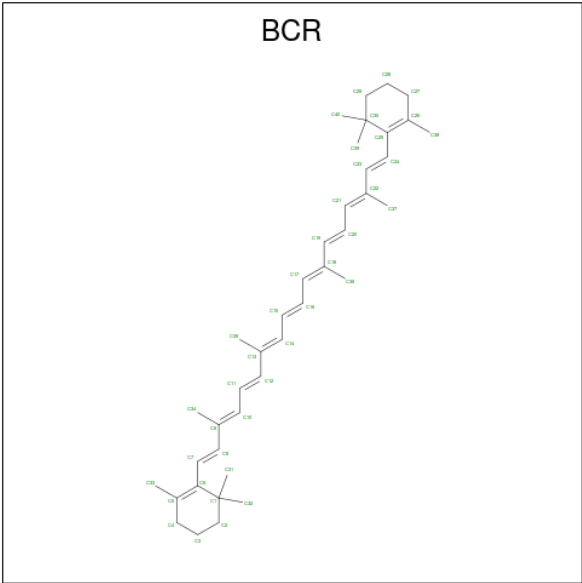
Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	Fe	S	0
			8	4	4	
17	C	1	Total	Fe	S	0
			8	4	4	
17	C	1	Total	Fe	S	0
			8	4	4	
17	G	1	Total	Fe	S	0
			8	4	4	
17	N	1	Total	Fe	S	0
			8	4	4	
17	N	1	Total	Fe	S	0
			8	4	4	
17	a	1	Total	Fe	S	0
			8	4	4	
17	c	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
17	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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Mol	Chain	Residues	Atoms	AltConf
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0

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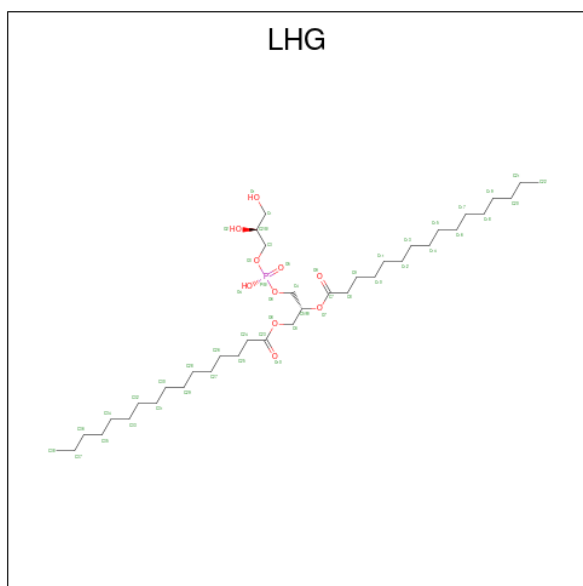
Mol	Chain	Residues	Atoms	AltConf
18	H	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	L	1	Total C 40 40	0
18	L	1	Total C 40 40	0
18	M	1	Total C 40 40	0
18	R	1	Total C 40 40	0
18	R	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	V	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0

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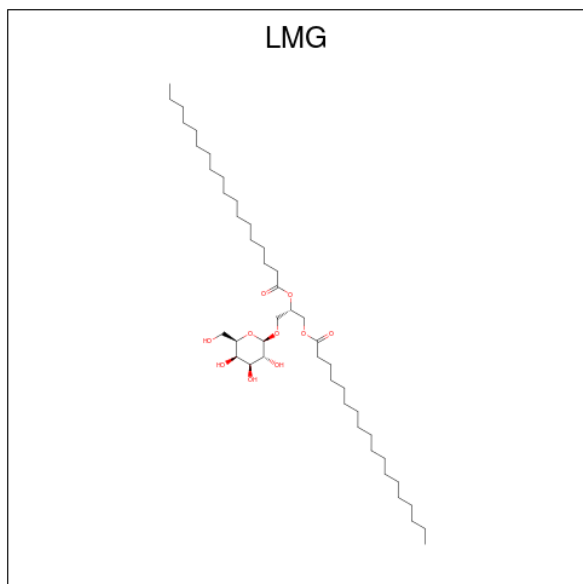
Mol	Chain	Residues	Atoms	AltConf
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	i	1	Total C 40 40	0
18	i	1	Total C 40 40	0
18	l	1	Total C 40 40	0
18	l	1	Total C 40 40	0
18	m	1	Total C 40 40	0

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			42	31	10	1	
19	B	1	Total	C	O	P	0
			44	33	10	1	
19	G	1	Total	C	O	P	0
			42	31	10	1	
19	H	1	Total	C	O	P	0
			44	33	10	1	
19	a	1	Total	C	O	P	0
			42	31	10	1	
19	b	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



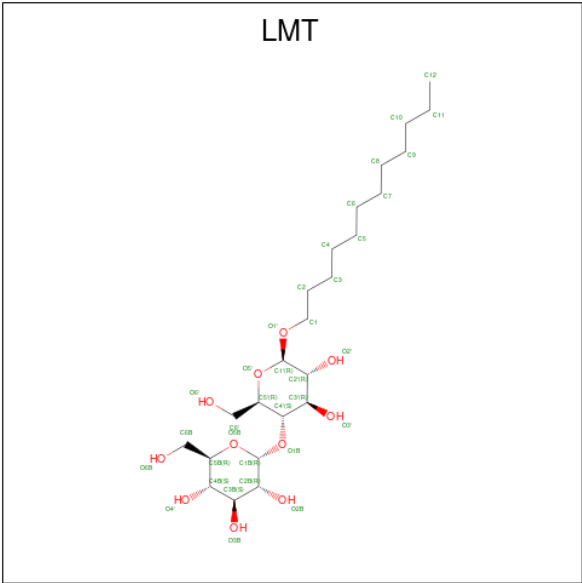
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			46	36	10	
20	B	1	Total	C	O	0
			46	36	10	
20	G	1	Total	C	O	0
			46	36	10	
20	H	1	Total	C	O	0
			46	36	10	
20	I	1	Total	C	O	0
			37	27	10	

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Mol	Chain	Residues	Atoms			AltConf
20	L	1	Total	C	O	0
			50	40	10	
20	R	1	Total	C	O	0
			37	27	10	
20	U	1	Total	C	O	0
			50	40	10	
20	a	1	Total	C	O	0
			46	36	10	
20	b	1	Total	C	O	0
			46	36	10	
20	i	1	Total	C	O	0
			37	27	10	
20	l	1	Total	C	O	0
			50	40	10	

- Molecule 21 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			31	20	11	
21	A	1	Total	C	O	0
			28	17	11	
21	G	1	Total	C	O	0
			31	20	11	
21	G	1	Total	C	O	0
			28	17	11	

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Mol	Chain	Residues	Atoms			AltConf
21	a	1	Total	C	O	0
			31	20	11	
21	a	1	Total	C	O	0
			28	17	11	

- Molecule 22 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
22	L	1	Total	Ca	0
			1	1	
22	U	1	Total	Ca	0
			1	1	
22	1	1	Total	Ca	0
			1	1	

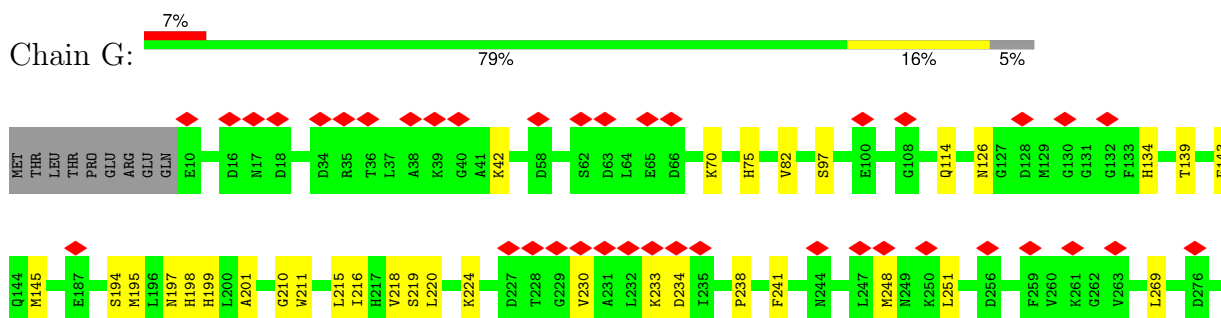
3 Residue-property plots

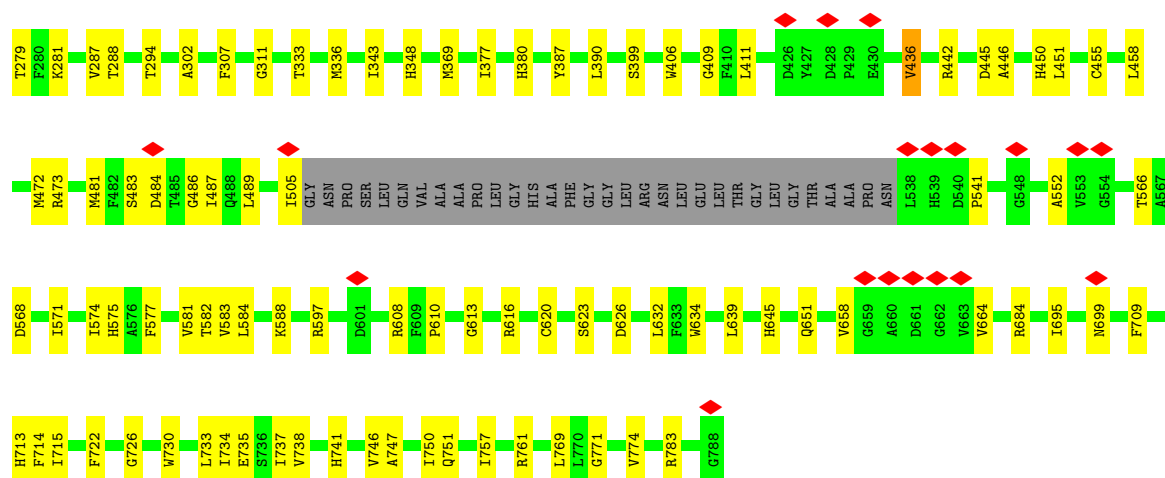
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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





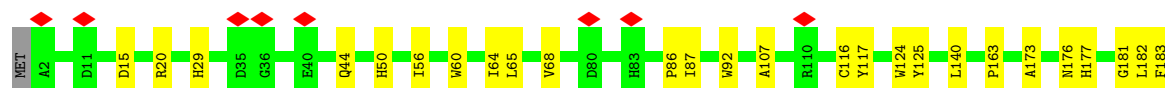
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

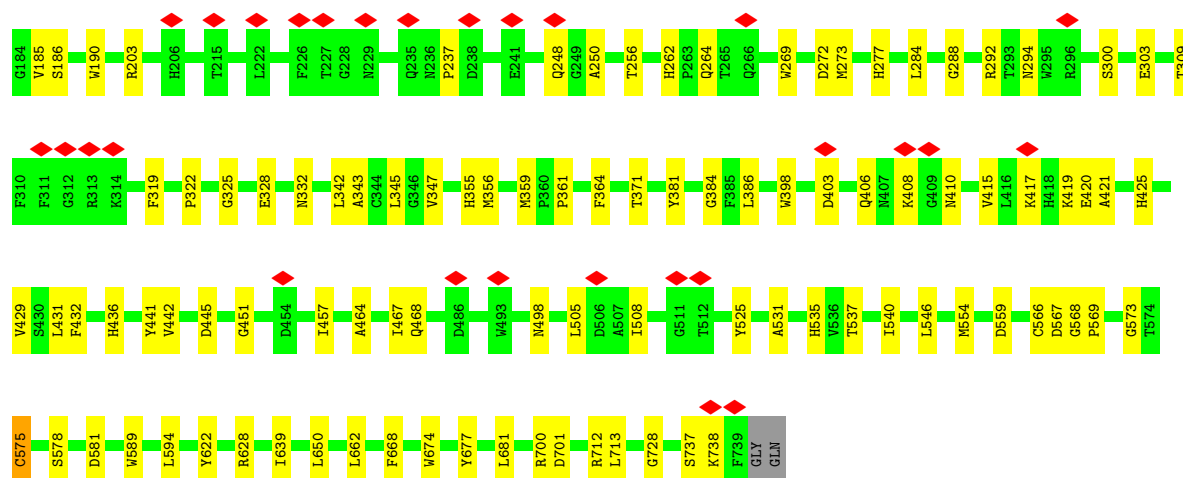
Chain a: 7% 79% 16% 5%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 5% 83% 17%

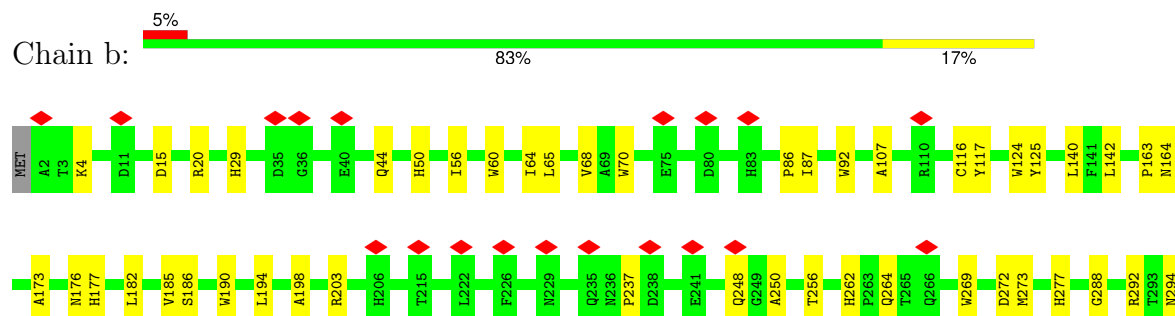


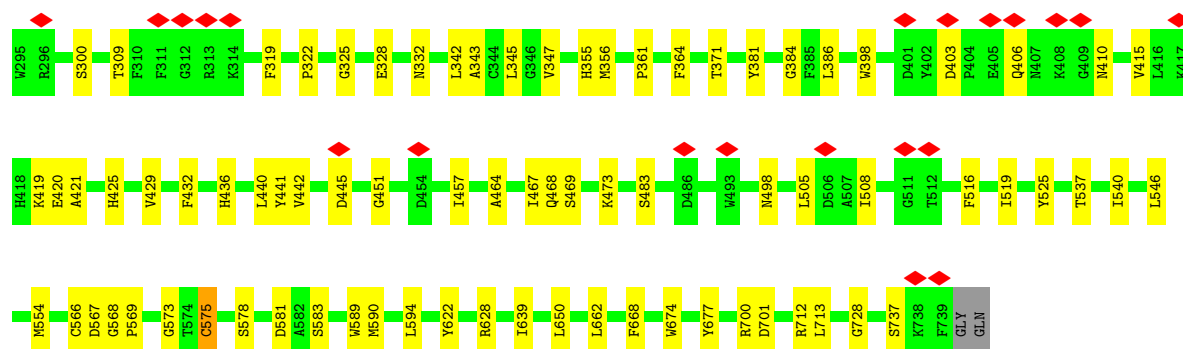


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

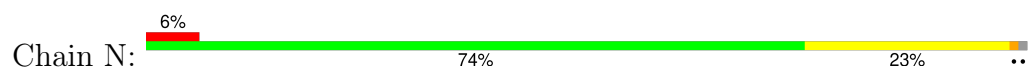




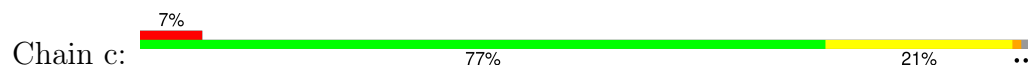
• Molecule 3: Photosystem I iron-sulfur center



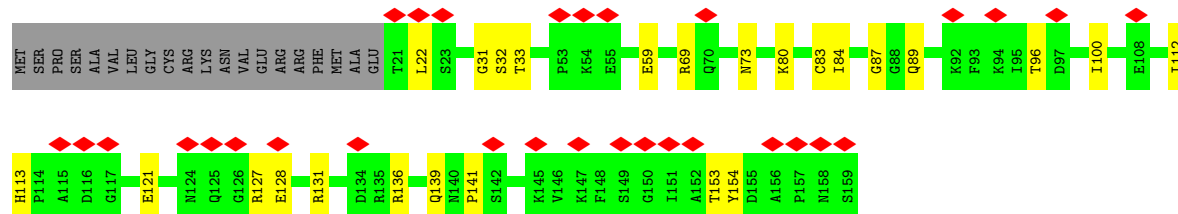
• Molecule 3: Photosystem I iron-sulfur center



• Molecule 3: Photosystem I iron-sulfur center

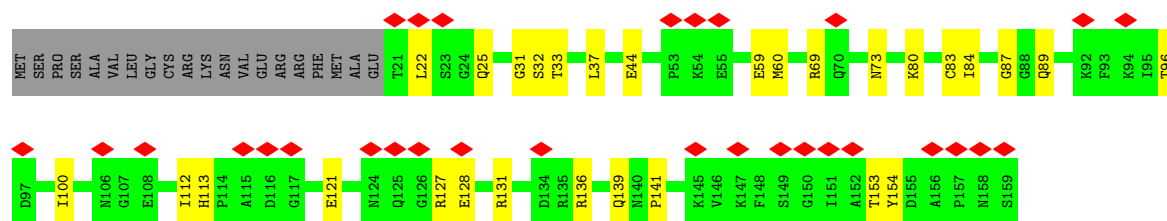


• Molecule 4: Photosystem I protein PsaD

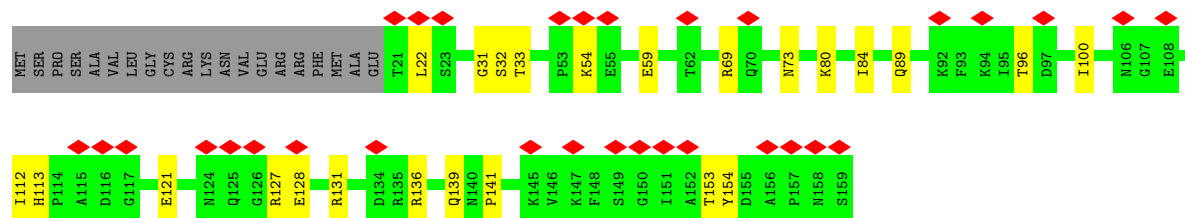


• Molecule 4: Photosystem I protein PsaD

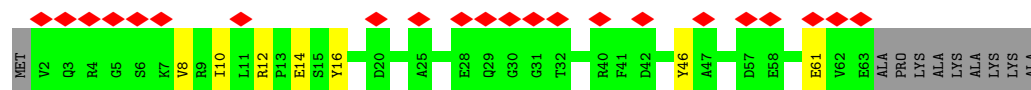
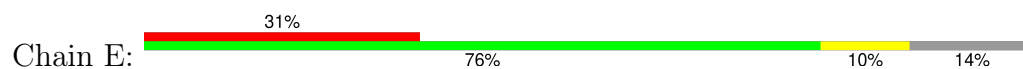




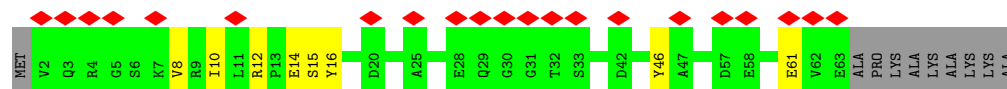
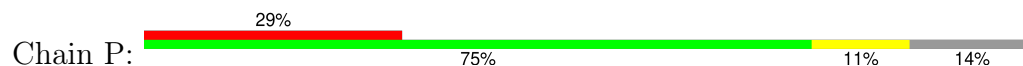
• Molecule 4: Photosystem I protein PsaD



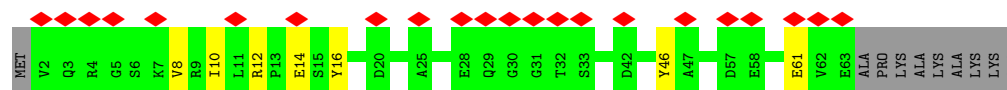
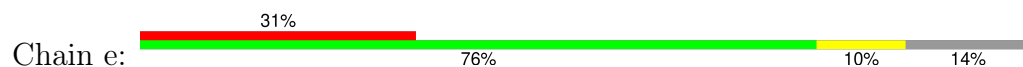
• Molecule 5: Photosystem I reaction center subunit IV



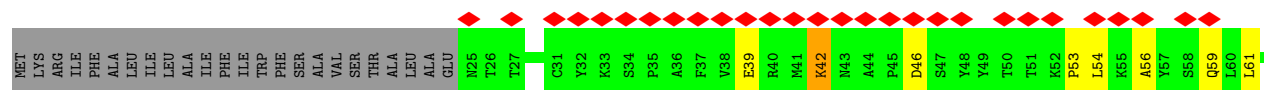
• Molecule 5: Photosystem I reaction center subunit IV

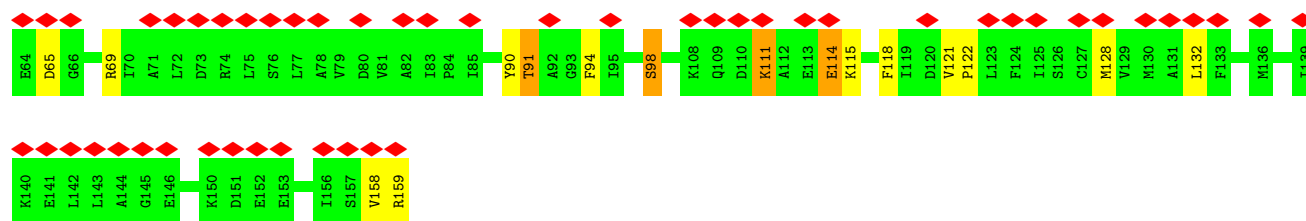


• Molecule 5: Photosystem I reaction center subunit IV

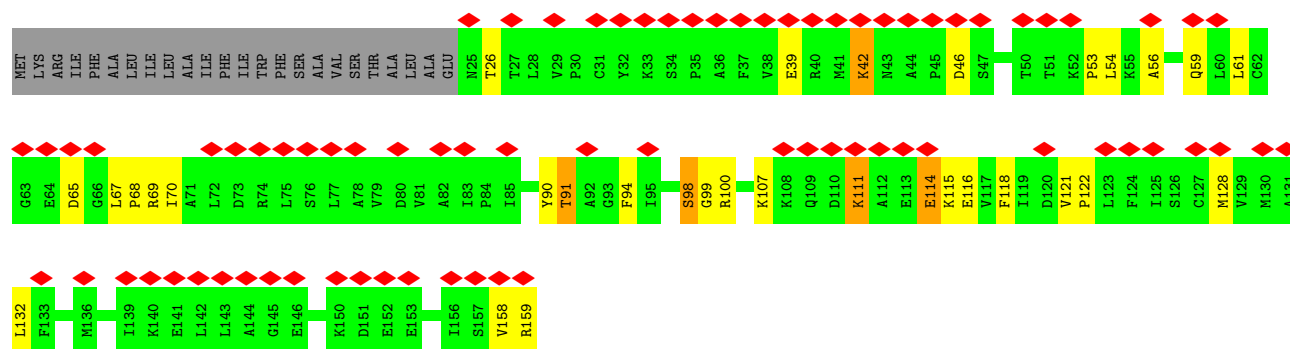


• Molecule 6: Photosystem I reaction center protein PsaF subunit III

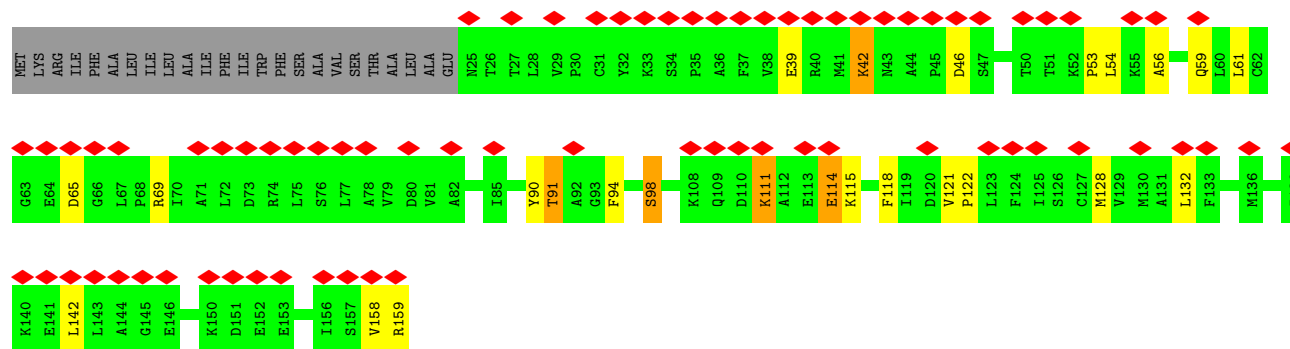




• Molecule 6: Photosystem I reaction center protein Psaf subunit III



• Molecule 6: Photosystem I reaction center protein Psaf subunit III

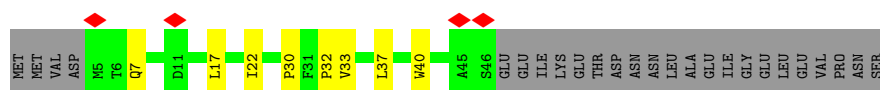


• Molecule 7: photosystem I subunit VIII

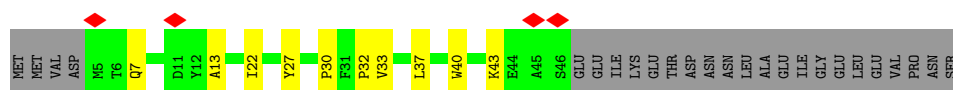


• Molecule 7: photosystem I subunit VIII

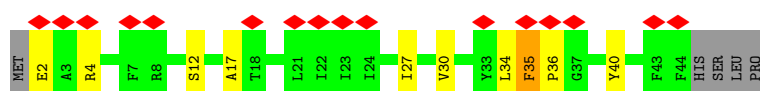




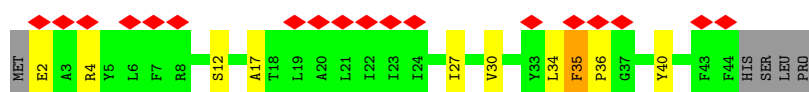
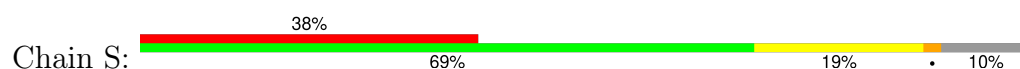
- Molecule 7: photosystem I subunit VIII



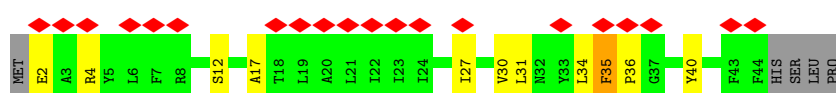
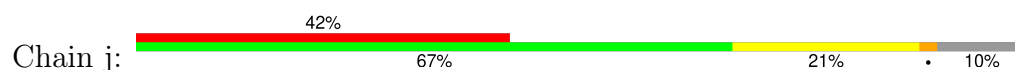
- Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



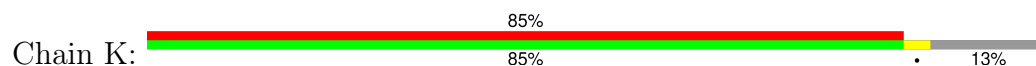
- Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



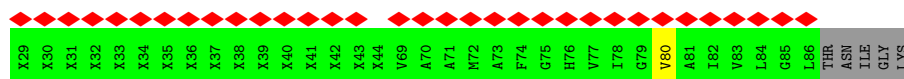
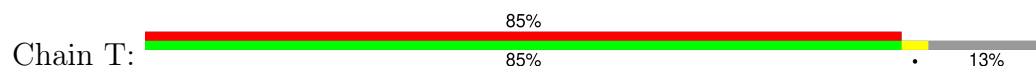
- Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



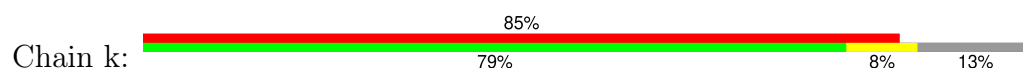
- Molecule 9: photosystem I reaction center subunit PsaK



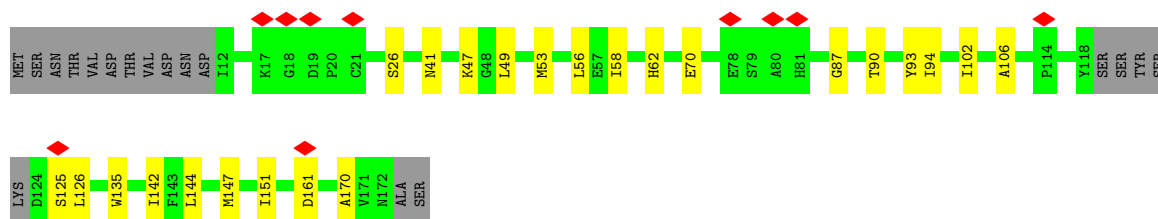
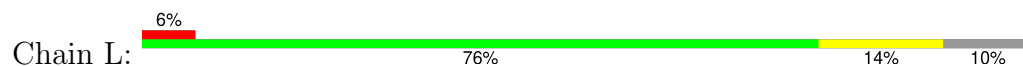
- Molecule 9: photosystem I reaction center subunit PsaK



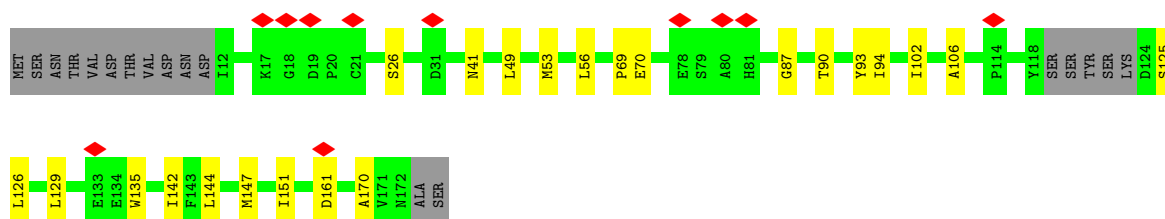
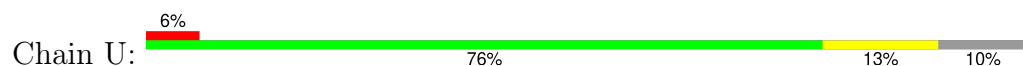
- Molecule 9: photosystem I reaction center subunit PsaK



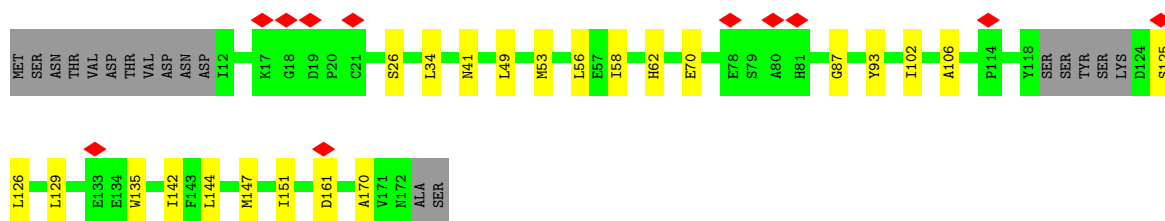
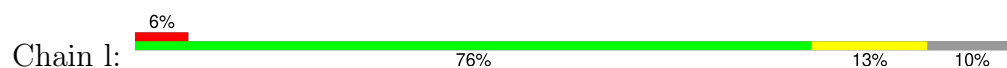
- Molecule 10: Photosystem I reaction center protein subunit XI



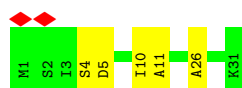
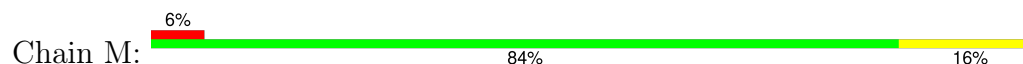
- Molecule 10: Photosystem I reaction center protein subunit XI



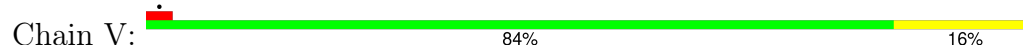
- Molecule 10: Photosystem I reaction center protein subunit XI

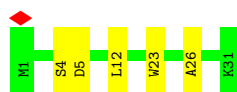


- Molecule 11: Photosystem I reaction center subunit XII

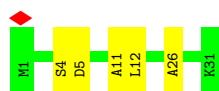
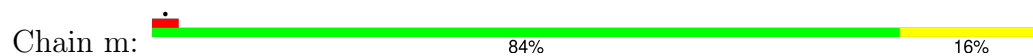


- Molecule 11: Photosystem I reaction center subunit XII

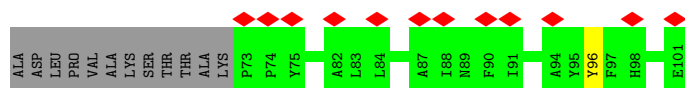
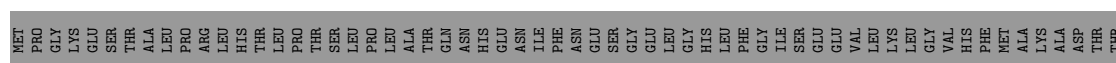




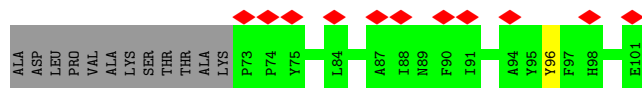
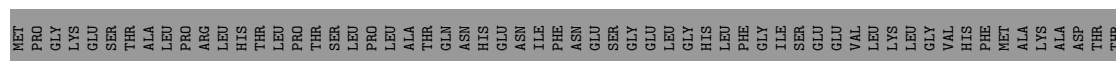
- Molecule 11: Photosystem I reaction center subunit XII



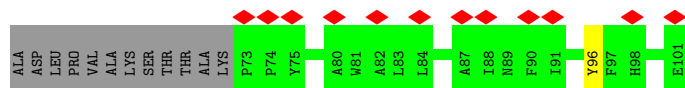
- Molecule 12: Photosystem one Psax



- Molecule 12: Photosystem one Psax



- Molecule 12: Photosystem one Psax



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	178666	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5252	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	0.251	Depositor
Minimum map value	-0.165	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0293	Depositor
Map size ($\text{\AA}$)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, LHG, CA, LMT, CL0, BCR, SF4, PQN, CLA, F6C

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	0.43	0/6112	0.50	0/8325
1	G	0.43	0/6112	0.50	0/8325
1	a	0.43	0/6112	0.50	0/8325
2	B	0.44	0/6131	0.51	0/8380
2	H	0.44	0/6131	0.51	0/8380
2	b	0.44	0/6131	0.51	0/8380
3	C	0.39	0/611	0.68	2/828 (0.2%)
3	N	0.39	0/611	0.69	2/828 (0.2%)
3	c	0.39	0/611	0.68	2/828 (0.2%)
4	D	0.30	0/1116	0.52	0/1505
4	O	0.30	0/1116	0.51	0/1505
4	d	0.30	0/1116	0.52	0/1505
5	E	0.25	0/506	0.50	0/686
5	P	0.25	0/506	0.50	0/686
5	e	0.25	0/506	0.50	0/686
6	F	0.26	0/1084	0.63	1/1470 (0.1%)
6	Q	0.26	0/1084	0.63	1/1470 (0.1%)
6	f	0.26	0/1084	0.63	1/1470 (0.1%)
7	I	0.41	0/365	0.64	0/502
7	R	0.41	0/365	0.63	0/502
7	i	0.41	0/365	0.63	0/502
8	J	0.30	0/353	0.74	0/482
8	S	0.30	0/353	0.75	0/482
8	j	0.30	0/353	0.74	0/482
9	K	0.21	0/122	0.46	0/165
9	T	0.21	0/122	0.46	0/165
9	k	0.21	0/122	0.46	0/165
10	L	0.41	0/1198	0.63	2/1624 (0.1%)
10	U	0.42	0/1198	0.62	2/1624 (0.1%)
10	l	0.42	0/1198	0.63	2/1624 (0.1%)
11	M	0.32	0/250	0.51	0/340
11	V	0.32	0/250	0.51	0/340

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	m	0.32	0/250	0.51	0/340
12	W	0.20	0/256	0.55	0/350
12	X	0.21	0/256	0.55	0/350
12	x	0.21	0/256	0.55	0/350
All	All	0.40	0/54312	0.54	15/73971 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
1	a	0	1
6	F	0	1
6	Q	0	1
6	f	0	1
8	J	0	1
8	S	0	1
8	j	0	1
All	All	0	9

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	U	26	SER	CA-C-N	6.40	139.15	120.97
10	U	26	SER	C-N-CA	6.40	139.15	120.97
10	l	26	SER	CA-C-N	6.38	139.10	120.97
10	l	26	SER	C-N-CA	6.38	139.10	120.97
10	L	26	SER	CA-C-N	6.38	139.09	120.97

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	THR	Peptide
6	F	46	ASP	Peptide
1	G	333	THR	Peptide
8	J	35	PHE	Peptide

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Mol	Chain	Res	Type	Group
6	Q	46	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5906	0	5753	91	0
1	G	5906	0	5753	92	0
1	a	5906	0	5753	91	0
2	B	5909	0	5668	96	0
2	H	5909	0	5668	95	0
2	b	5909	0	5668	99	0
3	C	601	0	585	15	0
3	N	601	0	585	18	0
3	c	601	0	585	16	0
4	D	1092	0	1098	14	0
4	O	1092	0	1098	18	0
4	d	1092	0	1098	14	0
5	E	497	0	482	5	0
5	P	497	0	482	6	0
5	e	497	0	482	5	0
6	F	1060	0	1091	15	0
6	Q	1060	0	1091	22	0
6	f	1060	0	1091	16	0
7	I	350	0	354	5	0
7	R	350	0	354	6	0
7	i	350	0	354	8	0
8	J	344	0	360	7	0
8	S	344	0	360	7	0
8	j	344	0	360	9	0
9	K	201	0	152	1	0
9	T	201	0	152	1	0
9	k	201	0	152	3	0
10	L	1172	0	1191	18	0
10	U	1172	0	1191	19	0
10	l	1172	0	1191	16	0
11	M	245	0	259	4	0
11	V	245	0	259	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	m	245	0	259	4	0
12	W	246	0	246	1	0
12	X	246	0	246	1	0
12	x	246	0	246	1	0
13	A	65	0	72	1	0
13	G	65	0	72	2	0
13	a	65	0	72	1	0
14	A	2140	0	1975	61	0
14	B	2280	0	2206	95	0
14	G	2140	0	1975	65	0
14	H	2280	0	2206	94	0
14	K	45	0	33	0	0
14	L	185	0	189	7	0
14	T	45	0	33	0	0
14	U	185	0	189	8	0
14	W	45	0	32	2	0
14	X	45	0	32	1	0
14	a	2140	0	1975	66	0
14	b	2280	0	2206	93	0
14	k	45	0	33	0	0
14	l	185	0	189	6	0
14	x	45	0	32	1	0
15	A	92	0	0	0	0
15	B	107	0	0	4	0
15	G	92	0	0	0	0
15	H	107	0	0	3	0
15	a	92	0	0	0	0
15	b	107	0	0	6	0
16	A	33	0	46	6	0
16	B	33	0	46	4	0
16	G	33	0	46	6	0
16	H	33	0	46	4	0
16	a	33	0	46	6	0
16	b	33	0	46	4	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
17	G	8	0	0	0	0
17	N	16	0	0	0	0
17	a	8	0	0	0	0
17	c	16	0	0	0	0
18	A	240	0	293	17	0
18	B	400	0	487	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	G	240	0	293	16	0
18	H	400	0	487	26	0
18	I	80	0	97	8	0
18	L	80	0	98	6	0
18	M	40	0	48	3	0
18	R	80	0	97	9	0
18	U	80	0	98	6	0
18	V	40	0	48	4	0
18	a	240	0	292	18	0
18	b	400	0	487	26	0
18	i	80	0	97	5	0
18	l	80	0	98	6	0
18	m	40	0	48	2	0
19	A	42	0	54	1	0
19	B	44	0	61	0	0
19	G	42	0	54	1	0
19	H	44	0	61	1	0
19	a	42	0	54	1	0
19	b	44	0	61	0	0
20	A	46	0	65	0	0
20	B	46	0	62	3	0
20	G	46	0	65	1	0
20	H	46	0	62	3	0
20	I	37	0	44	2	0
20	L	50	0	70	2	0
20	R	37	0	44	5	0
20	U	50	0	70	3	0
20	a	46	0	65	1	0
20	b	46	0	62	3	0
20	i	37	0	44	2	0
20	l	50	0	70	2	0
21	A	59	0	58	0	0
21	G	59	0	57	1	0
21	a	59	0	57	0	0
22	L	1	0	0	0	0
22	U	1	0	0	0	0
22	l	1	0	0	0	0
All	All	71511	0	69822	1161	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 1161 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)
15:b:1230:F6C:OMB	8:j:40:TYR:OH	1.85	0.92
3:N:2:SER:N	3:N:76:SER:HG	1.80	0.80
3:C:2:SER:N	3:C:76:SER:HG	1.79	0.79
14:b:1223:CLA:H2	18:b:4010:BCR:H14C	1.65	0.78
14:B:1223:CLA:H2	18:B:4010:BCR:H14C	1.66	0.77

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	743/788 (94%)	699 (94%)	44 (6%)	0	100	100
1	G	743/788 (94%)	700 (94%)	43 (6%)	0	100	100
1	a	743/788 (94%)	699 (94%)	44 (6%)	0	100	100
2	B	736/741 (99%)	706 (96%)	30 (4%)	0	100	100
2	H	736/741 (99%)	706 (96%)	30 (4%)	0	100	100
2	b	736/741 (99%)	706 (96%)	30 (4%)	0	100	100
3	C	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	40
3	N	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	40
3	c	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	40
4	D	137/159 (86%)	125 (91%)	12 (9%)	0	100	100
4	O	137/159 (86%)	125 (91%)	12 (9%)	0	100	100
4	d	137/159 (86%)	125 (91%)	12 (9%)	0	100	100
5	E	60/72 (83%)	54 (90%)	6 (10%)	0	100	100
5	P	60/72 (83%)	54 (90%)	6 (10%)	0	100	100
5	e	60/72 (83%)	54 (90%)	6 (10%)	0	100	100
6	F	133/159 (84%)	122 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Q	133/159 (84%)	122 (92%)	11 (8%)	0	100	100
6	f	133/159 (84%)	122 (92%)	11 (8%)	0	100	100
7	I	40/67 (60%)	33 (82%)	7 (18%)	0	100	100
7	R	40/67 (60%)	33 (82%)	7 (18%)	0	100	100
7	i	40/67 (60%)	33 (82%)	7 (18%)	0	100	100
8	J	41/48 (85%)	36 (88%)	4 (10%)	1 (2%)	4	28
8	S	41/48 (85%)	36 (88%)	4 (10%)	1 (2%)	4	28
8	j	41/48 (85%)	36 (88%)	4 (10%)	1 (2%)	4	28
9	K	16/39 (41%)	16 (100%)	0	0	100	100
9	T	16/39 (41%)	16 (100%)	0	0	100	100
9	k	16/39 (41%)	16 (100%)	0	0	100	100
10	L	152/174 (87%)	140 (92%)	12 (8%)	0	100	100
10	U	152/174 (87%)	140 (92%)	12 (8%)	0	100	100
10	l	152/174 (87%)	140 (92%)	12 (8%)	0	100	100
11	M	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	V	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	m	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
12	W	27/101 (27%)	25 (93%)	2 (7%)	0	100	100
12	X	27/101 (27%)	25 (93%)	2 (7%)	0	100	100
12	x	27/101 (27%)	25 (93%)	2 (7%)	0	100	100
All	All	6576/7380 (89%)	6166 (94%)	404 (6%)	6 (0%)	49	79

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	63	LEU
3	N	63	LEU
3	c	63	LEU
8	J	36	PRO
8	S	36	PRO

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	611/641 (95%)	608 (100%)	3 (0%)	81	85
1	G	611/641 (95%)	608 (100%)	3 (0%)	81	85
1	a	611/641 (95%)	608 (100%)	3 (0%)	81	85
2	B	595/597 (100%)	592 (100%)	3 (0%)	81	85
2	H	595/597 (100%)	592 (100%)	3 (0%)	81	85
2	b	595/597 (100%)	592 (100%)	3 (0%)	81	85
3	C	68/69 (99%)	68 (100%)	0	100	100
3	N	68/69 (99%)	68 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	D	115/132 (87%)	112 (97%)	3 (3%)	40	69
4	O	115/132 (87%)	112 (97%)	3 (3%)	40	69
4	d	115/132 (87%)	112 (97%)	3 (3%)	40	69
5	E	54/60 (90%)	54 (100%)	0	100	100
5	P	54/60 (90%)	54 (100%)	0	100	100
5	e	54/60 (90%)	54 (100%)	0	100	100
6	F	115/134 (86%)	108 (94%)	7 (6%)	17	49
6	Q	115/134 (86%)	108 (94%)	7 (6%)	17	49
6	f	115/134 (86%)	108 (94%)	7 (6%)	17	49
7	I	37/60 (62%)	37 (100%)	0	100	100
7	R	37/60 (62%)	37 (100%)	0	100	100
7	i	37/60 (62%)	37 (100%)	0	100	100
8	J	36/42 (86%)	36 (100%)	0	100	100
8	S	36/42 (86%)	36 (100%)	0	100	100
8	j	36/42 (86%)	36 (100%)	0	100	100
9	K	11/15 (73%)	11 (100%)	0	100	100
9	T	11/15 (73%)	11 (100%)	0	100	100
9	k	11/15 (73%)	11 (100%)	0	100	100
10	L	121/138 (88%)	120 (99%)	1 (1%)	73	82
10	U	121/138 (88%)	120 (99%)	1 (1%)	73	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	l	121/138 (88%)	120 (99%)	1 (1%)	73	82
11	M	26/26 (100%)	26 (100%)	0	100	100
11	V	26/26 (100%)	26 (100%)	0	100	100
11	m	26/26 (100%)	26 (100%)	0	100	100
12	W	24/84 (29%)	24 (100%)	0	100	100
12	X	24/84 (29%)	24 (100%)	0	100	100
12	x	24/84 (29%)	24 (100%)	0	100	100
All	All	5439/5994 (91%)	5388 (99%)	51 (1%)	68	81

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	Q	91	THR
1	a	436	VAL
6	f	158	VAL
6	Q	98	SER
6	Q	158	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	332	ASN
4	d	73	ASN
11	M	7	GLN
2	b	691	GLN
10	l	139	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 372 ligands modelled in this entry, 3 are monoatomic - leaving 369 for Mogul analysis.

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$
14	CLA	a	1130	-	59,63,73	2.39	19 (32%)	70,101,113	2.58	27 (38%)
14	CLA	b	1203	-	69,73,73	2.16	20 (28%)	82,113,113	2.55	28 (34%)
14	CLA	G	1133	-	64,68,73	2.29	21 (32%)	76,107,113	2.60	27 (35%)
14	CLA	A	1131	1	64,68,73	2.27	21 (32%)	76,107,113	2.59	25 (32%)
16	PQN	H	2002	-	34,34,34	1.52	2 (5%)	43,45,45	1.18	1 (2%)
14	CLA	A	1139	-	49,53,73	2.49	20 (40%)	58,89,113	2.70	22 (37%)
21	LMT	A	6002	-	29,29,36	1.35	5 (17%)	40,40,47	1.42	8 (20%)
14	CLA	A	1105	-	49,53,73	2.53	21 (42%)	58,89,113	2.76	22 (37%)
18	BCR	b	4013	-	41,41,41	2.63	6 (14%)	56,56,56	6.72	23 (41%)
14	CLA	H	1228	-	49,53,73	2.51	21 (42%)	58,89,113	2.75	26 (44%)
14	CLA	b	1202	-	64,68,73	2.26	20 (31%)	76,107,113	2.59	28 (36%)
20	LMG	G	5005	-	46,46,55	1.36	5 (10%)	54,54,63	1.16	3 (5%)
14	CLA	B	1224	-	69,73,73	2.21	20 (28%)	82,113,113	2.48	29 (35%)
14	CLA	H	1217	-	59,63,73	2.38	21 (35%)	70,101,113	2.64	25 (35%)
14	CLA	B	1213	-	59,63,73	2.40	21 (35%)	70,101,113	2.72	26 (37%)
18	BCR	L	4019	-	41,41,41	2.68	6 (14%)	56,56,56	6.70	24 (42%)
14	CLA	G	1112	-	49,53,73	2.50	22 (44%)	58,89,113	2.78	22 (37%)
14	CLA	H	1215	-	64,68,73	2.29	19 (29%)	76,107,113	2.52	30 (39%)
17	SF4	N	3003	-	0,12,12	-	-	-	-	-
14	CLA	B	1202	-	64,68,73	2.25	20 (31%)	76,107,113	2.59	28 (36%)
18	BCR	b	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.62	26 (46%)
14	CLA	b	1201	-	59,63,73	2.37	21 (35%)	70,101,113	2.83	27 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	1205	-	69,73,73	2.19	20 (28%)	82,113,113	2.64	29 (35%)
14	CLA	H	1224	-	69,73,73	2.21	20 (28%)	82,113,113	2.48	29 (35%)
14	CLA	G	1114	-	49,53,73	2.55	21 (42%)	58,89,113	2.74	24 (41%)
18	BCR	B	4014	-	41,41,41	2.75	6 (14%)	56,56,56	6.59	24 (42%)
14	CLA	H	1239	-	69,73,73	2.23	22 (31%)	82,113,113	2.63	30 (36%)
14	CLA	a	1135	-	54,58,73	2.52	21 (38%)	64,95,113	2.83	29 (45%)
18	BCR	I	4020	-	41,41,41	2.87	7 (17%)	56,56,56	6.44	24 (42%)
14	CLA	G	1138	-	64,68,73	2.29	22 (34%)	76,107,113	2.61	30 (39%)
19	LHG	H	5004	-	43,43,48	0.98	2 (4%)	46,49,54	1.21	3 (6%)
20	LMG	b	5002	-	46,46,55	1.35	5 (10%)	54,54,63	1.18	3 (5%)
18	BCR	a	4011	-	41,41,41	2.75	7 (17%)	56,56,56	6.68	25 (44%)
18	BCR	H	4016	-	41,41,41	2.67	6 (14%)	56,56,56	6.65	18 (32%)
14	CLA	H	1236	-	49,53,73	2.49	20 (40%)	58,89,113	2.80	23 (39%)
14	CLA	G	1116	-	59,63,73	2.39	20 (33%)	70,101,113	2.67	28 (40%)
18	BCR	B	4009	-	41,41,41	2.71	6 (14%)	56,56,56	6.72	25 (44%)
15	F6C	G	1120	-	52,54,74	3.10	26 (50%)	59,90,114	3.72	28 (47%)
14	CLA	B	1022	-	69,73,73	2.20	20 (28%)	82,113,113	2.48	29 (35%)
14	CLA	a	1110	-	49,53,73	2.49	20 (40%)	58,89,113	2.90	23 (39%)
14	CLA	G	1139	-	49,53,73	2.49	20 (40%)	58,89,113	2.70	22 (37%)
14	CLA	H	1220	-	59,63,73	2.38	20 (33%)	70,101,113	2.64	25 (35%)
20	LMG	B	5002	-	46,46,55	1.36	5 (10%)	54,54,63	1.18	3 (5%)
14	CLA	G	1129	-	49,53,73	2.51	18 (36%)	58,89,113	2.77	25 (43%)
14	CLA	A	1138	-	64,68,73	2.30	21 (32%)	76,107,113	2.61	30 (39%)
14	CLA	A	1118	-	59,63,73	2.37	20 (33%)	70,101,113	2.73	28 (40%)
14	CLA	A	1116	-	59,63,73	2.39	20 (33%)	70,101,113	2.66	28 (40%)
14	CLA	A	1125	-	69,73,73	2.18	20 (28%)	82,113,113	2.57	27 (32%)
14	CLA	G	1140	-	69,73,73	2.21	21 (30%)	82,113,113	2.41	27 (32%)
18	BCR	A	4011	-	41,41,41	2.75	7 (17%)	56,56,56	6.67	25 (44%)
14	CLA	B	1215	-	64,68,73	2.29	19 (29%)	76,107,113	2.53	30 (39%)
14	CLA	L	1503	-	69,73,73	2.19	20 (28%)	82,113,113	2.46	26 (31%)
14	CLA	B	1206	-	49,53,73	2.49	19 (38%)	58,89,113	2.62	22 (37%)
14	CLA	H	1238	-	69,73,73	2.26	19 (27%)	82,113,113	2.60	32 (39%)
14	CLA	a	1105	-	49,53,73	2.53	20 (40%)	58,89,113	2.76	22 (37%)
14	CLA	a	1108	-	49,53,73	2.52	21 (42%)	58,89,113	2.75	23 (39%)
14	CLA	B	1210	-	69,73,73	2.23	21 (30%)	82,113,113	2.56	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	1221	-	64,68,73	2.27	20 (31%)	76,107,113	2.49	27 (35%)
18	BCR	H	4010	-	41,41,41	2.75	6 (14%)	56,56,56	6.74	22 (39%)
14	CLA	H	1204	2	69,73,73	2.24	20 (28%)	82,113,113	2.49	27 (32%)
14	CLA	G	1115	-	59,63,73	2.39	21 (35%)	70,101,113	2.71	26 (37%)
18	BCR	H	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.62	25 (44%)
14	CLA	B	1236	-	49,53,73	2.49	20 (40%)	58,89,113	2.79	23 (39%)
18	BCR	B	4017	-	41,41,41	2.76	6 (14%)	56,56,56	6.76	18 (32%)
15	F6C	a	1121	-	52,54,74	3.05	27 (51%)	59,90,114	3.70	31 (52%)
20	LMG	H	5002	-	46,46,55	1.36	5 (10%)	54,54,63	1.18	3 (5%)
18	BCR	a	4003	-	41,41,41	2.70	6 (14%)	56,56,56	6.66	23 (41%)
15	F6C	B	1237	-	67,69,74	2.79	25 (37%)	77,108,114	3.21	36 (46%)
18	BCR	B	4005	-	41,41,41	2.66	7 (17%)	56,56,56	6.77	27 (48%)
14	CLA	B	1211	-	69,73,73	2.21	20 (28%)	82,113,113	2.40	26 (31%)
14	CLA	B	1229	-	64,68,73	2.30	21 (32%)	76,107,113	2.64	26 (34%)
18	BCR	i	4020	-	41,41,41	2.86	7 (17%)	56,56,56	6.44	24 (42%)
14	CLA	B	1204	2	69,73,73	2.24	20 (28%)	82,113,113	2.49	27 (32%)
14	CLA	G	1106	-	49,53,73	2.48	20 (40%)	58,89,113	2.91	25 (43%)
14	CLA	B	1222	-	69,73,73	2.23	20 (28%)	82,113,113	2.58	32 (39%)
14	CLA	b	1210	-	69,73,73	2.22	21 (30%)	82,113,113	2.56	32 (39%)
14	CLA	b	1023	-	69,73,73	2.20	22 (31%)	82,113,113	2.80	31 (37%)
18	BCR	V	4021	-	41,41,41	2.72	6 (14%)	56,56,56	6.70	23 (41%)
14	CLA	A	1113	-	49,53,73	2.49	19 (38%)	58,89,113	2.86	23 (39%)
14	CLA	B	1207	-	49,53,73	2.48	20 (40%)	58,89,113	2.83	24 (41%)
18	BCR	G	4008	-	41,41,41	2.89	7 (17%)	56,56,56	6.49	22 (39%)
14	CLA	H	1226	-	69,73,73	2.26	21 (30%)	82,113,113	2.39	27 (32%)
14	CLA	A	1133	-	64,68,73	2.29	21 (32%)	76,107,113	2.59	27 (35%)
14	CLA	X	1701	-	49,53,73	2.48	19 (38%)	58,89,113	2.75	23 (39%)
14	CLA	x	1701	-	49,53,73	2.48	19 (38%)	58,89,113	2.76	23 (39%)
14	CLA	H	1211	-	69,73,73	2.21	20 (28%)	82,113,113	2.39	26 (31%)
14	CLA	U	1501	-	64,68,73	2.28	21 (32%)	76,107,113	2.72	27 (35%)
18	BCR	R	4018	-	41,41,41	2.86	7 (17%)	56,56,56	6.84	25 (44%)
14	CLA	a	1119	-	69,73,73	2.22	20 (28%)	82,113,113	2.35	28 (34%)
14	CLA	H	1231	-	59,63,73	2.42	20 (33%)	70,101,113	2.66	26 (37%)
18	BCR	a	4002	-	41,41,41	2.70	6 (14%)	56,56,56	6.30	24 (42%)
14	CLA	B	1226	-	69,73,73	2.26	21 (30%)	82,113,113	2.39	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	1203	-	69,73,73	2.16	20 (28%)	82,113,113	2.55	28 (34%)
18	BCR	A	4002	-	41,41,41	2.70	6 (14%)	56,56,56	6.30	23 (41%)
14	CLA	A	1101	-	49,53,73	2.48	19 (38%)	58,89,113	2.80	25 (43%)
15	F6C	A	1120	-	52,54,74	3.10	25 (48%)	59,90,114	3.71	28 (47%)
18	BCR	G	4007	-	41,41,41	2.76	7 (17%)	56,56,56	6.81	24 (42%)
14	CLA	H	1222	-	69,73,73	2.23	20 (28%)	82,113,113	2.57	32 (39%)
14	CLA	A	1108	-	49,53,73	2.53	21 (42%)	58,89,113	2.76	23 (39%)
18	BCR	G	4001	-	41,41,41	2.74	6 (14%)	56,56,56	6.64	22 (39%)
14	CLA	H	1202	-	64,68,73	2.25	20 (31%)	76,107,113	2.59	27 (35%)
14	CLA	A	1115	-	59,63,73	2.39	21 (35%)	70,101,113	2.71	26 (37%)
14	CLA	A	1102	-	64,68,73	2.33	21 (32%)	76,107,113	2.60	27 (35%)
14	CLA	B	1225	-	69,73,73	2.25	20 (28%)	82,113,113	2.25	21 (25%)
14	CLA	a	1137	-	49,53,73	2.48	19 (38%)	58,89,113	2.95	25 (43%)
14	CLA	A	1122	-	59,63,73	2.37	21 (35%)	70,101,113	2.62	27 (38%)
14	CLA	b	1236	-	49,53,73	2.48	20 (40%)	58,89,113	2.79	23 (39%)
17	SF4	C	3002	-	0,12,12	-	-	-	-	-
14	CLA	B	1023	-	69,73,73	2.19	22 (31%)	82,113,113	2.81	31 (37%)
14	CLA	G	1102	-	64,68,73	2.33	20 (31%)	76,107,113	2.59	27 (35%)
14	CLA	H	1225	-	69,73,73	2.25	20 (28%)	82,113,113	2.25	21 (25%)
14	CLA	A	1136	-	59,63,73	2.35	21 (35%)	70,101,113	2.76	28 (40%)
14	CLA	G	1109	-	49,53,73	2.47	21 (42%)	58,89,113	2.85	23 (39%)
14	CLA	G	1126	-	64,68,73	2.33	20 (31%)	76,107,113	2.60	26 (34%)
18	BCR	A	4008	-	41,41,41	2.89	7 (17%)	56,56,56	6.49	22 (39%)
14	CLA	b	1232	-	49,53,73	2.51	22 (44%)	58,89,113	2.70	23 (39%)
18	BCR	A	4003	-	41,41,41	2.70	6 (14%)	56,56,56	6.65	23 (41%)
15	F6C	G	1121	-	52,54,74	3.05	27 (51%)	59,90,114	3.69	30 (50%)
14	CLA	A	1117	-	69,73,73	2.19	21 (30%)	82,113,113	2.41	28 (34%)
14	CLA	H	1208	-	69,73,73	2.22	22 (31%)	82,113,113	2.45	25 (30%)
14	CLA	a	1102	-	64,68,73	2.33	20 (31%)	76,107,113	2.60	28 (36%)
18	BCR	l	4022	-	41,41,41	2.82	6 (14%)	56,56,56	6.63	24 (42%)
14	CLA	a	1138	-	64,68,73	2.30	22 (34%)	76,107,113	2.61	30 (39%)
14	CLA	b	1214	-	64,68,73	2.33	20 (31%)	76,107,113	2.53	34 (44%)
14	CLA	b	1220	-	59,63,73	2.39	20 (33%)	70,101,113	2.64	25 (35%)
14	CLA	B	1231	-	59,63,73	2.42	20 (33%)	70,101,113	2.65	26 (37%)
18	BCR	I	4018	-	41,41,41	2.86	7 (17%)	56,56,56	6.84	25 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	G	1118	-	59,63,73	2.37	20 (33%)	70,101,113	2.74	29 (41%)
21	LMT	G	6002	-	29,29,36	1.35	5 (17%)	40,40,47	1.42	8 (20%)
14	CLA	b	1207	-	49,53,73	2.48	20 (40%)	58,89,113	2.84	23 (39%)
14	CLA	A	1112	-	49,53,73	2.50	22 (44%)	58,89,113	2.78	22 (37%)
14	CLA	B	1233	-	49,53,73	2.51	21 (42%)	58,89,113	2.77	24 (41%)
19	LHG	B	5004	-	43,43,48	0.98	2 (4%)	46,49,54	1.21	3 (6%)
21	LMT	G	6001	-	32,32,36	1.26	6 (18%)	43,43,47	1.04	4 (9%)
14	CLA	A	1135	-	54,58,73	2.53	21 (38%)	64,95,113	2.84	29 (45%)
14	CLA	B	1239	-	69,73,73	2.23	22 (31%)	82,113,113	2.62	30 (36%)
13	CL0	G	1011	-	69,73,73	2.24	22 (31%)	82,113,113	2.66	29 (35%)
20	LMG	l	5007	-	50,50,55	1.44	7 (14%)	58,58,63	1.10	2 (3%)
14	CLA	a	1129	1	49,53,73	2.51	18 (36%)	58,89,113	2.77	25 (43%)
14	CLA	G	1113	-	49,53,73	2.48	19 (38%)	58,89,113	2.85	23 (39%)
14	CLA	A	1123	-	64,68,73	2.30	20 (31%)	76,107,113	2.57	29 (38%)
14	CLA	a	1013	-	64,68,73	2.35	22 (34%)	76,107,113	2.67	30 (39%)
14	CLA	B	1228	-	49,53,73	2.51	21 (42%)	58,89,113	2.75	26 (44%)
14	CLA	H	1212	-	49,53,73	2.51	20 (40%)	58,89,113	2.81	23 (39%)
14	CLA	B	1201	-	59,63,73	2.37	21 (35%)	70,101,113	2.83	27 (38%)
14	CLA	G	1111	-	64,68,73	2.29	22 (34%)	76,107,113	2.62	29 (38%)
14	CLA	a	1117	-	69,73,73	2.19	21 (30%)	82,113,113	2.41	28 (34%)
14	CLA	b	1218	-	49,53,73	2.50	19 (38%)	58,89,113	2.83	21 (36%)
18	BCR	H	4009	-	41,41,41	2.71	6 (14%)	56,56,56	6.71	25 (44%)
20	LMG	i	5006	-	37,37,55	1.16	3 (8%)	45,45,63	1.22	4 (8%)
14	CLA	G	1131	1	64,68,73	2.27	21 (32%)	76,107,113	2.59	25 (32%)
14	CLA	a	1132	-	69,73,73	2.21	20 (28%)	82,113,113	2.57	28 (34%)
14	CLA	G	1137	-	49,53,73	2.48	19 (38%)	58,89,113	2.96	25 (43%)
17	SF4	a	3001	-	0,12,12	-	-	-	-	-
14	CLA	G	1117	-	69,73,73	2.19	22 (31%)	82,113,113	2.42	28 (34%)
14	CLA	U	1503	-	69,73,73	2.19	20 (28%)	82,113,113	2.46	26 (31%)
14	CLA	A	1110	-	49,53,73	2.49	20 (40%)	58,89,113	2.91	23 (39%)
14	CLA	G	1122	-	59,63,73	2.37	21 (35%)	70,101,113	2.62	27 (38%)
16	PQN	b	2002	-	34,34,34	1.52	2 (5%)	43,45,45	1.18	1 (2%)
18	BCR	H	4013	-	41,41,41	2.63	6 (14%)	56,56,56	6.72	23 (41%)
14	CLA	b	1217	-	59,63,73	2.38	21 (35%)	70,101,113	2.64	25 (35%)
14	CLA	A	1128	-	64,68,73	2.33	19 (29%)	76,107,113	2.48	30 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	A	4007	-	41,41,41	2.77	7 (17%)	56,56,56	6.82	24 (42%)
18	BCR	H	4012	-	41,41,41	2.59	6 (14%)	56,56,56	6.78	27 (48%)
18	BCR	m	4021	-	41,41,41	2.72	6 (14%)	56,56,56	6.70	23 (41%)
14	CLA	A	1107	-	49,53,73	2.48	19 (38%)	58,89,113	2.70	24 (41%)
14	CLA	a	1136	-	59,63,73	2.35	22 (37%)	70,101,113	2.76	28 (40%)
18	BCR	G	4003	-	41,41,41	2.70	6 (14%)	56,56,56	6.66	23 (41%)
14	CLA	B	1227	-	49,53,73	2.56	19 (38%)	58,89,113	2.64	24 (41%)
14	CLA	a	1140	-	69,73,73	2.20	21 (30%)	82,113,113	2.40	27 (32%)
18	BCR	L	4022	-	41,41,41	2.82	6 (14%)	56,56,56	6.63	25 (44%)
14	CLA	A	1109	-	49,53,73	2.47	21 (42%)	58,89,113	2.85	23 (39%)
18	BCR	M	4021	-	41,41,41	2.72	6 (14%)	56,56,56	6.71	23 (41%)
14	CLA	b	1224	-	69,73,73	2.21	19 (27%)	82,113,113	2.48	29 (35%)
18	BCR	B	4013	-	41,41,41	2.63	6 (14%)	56,56,56	6.72	23 (41%)
18	BCR	b	4012	-	41,41,41	2.59	6 (14%)	56,56,56	6.78	27 (48%)
14	CLA	b	1235	-	64,68,73	2.30	19 (29%)	76,107,113	2.65	27 (35%)
20	LMG	R	5006	-	37,37,55	1.16	3 (8%)	45,45,63	1.22	4 (8%)
19	LHG	b	5004	-	43,43,48	0.98	2 (4%)	46,49,54	1.21	3 (6%)
14	CLA	a	1115	-	59,63,73	2.39	21 (35%)	70,101,113	2.71	26 (37%)
14	CLA	H	1213	-	59,63,73	2.40	21 (35%)	70,101,113	2.72	26 (37%)
18	BCR	B	4006	-	41,41,41	2.65	6 (14%)	56,56,56	6.70	23 (41%)
14	CLA	H	1023	-	69,73,73	2.20	22 (31%)	82,113,113	2.80	32 (39%)
14	CLA	G	1136	-	59,63,73	2.34	21 (35%)	70,101,113	2.75	28 (40%)
14	CLA	H	1227	-	49,53,73	2.55	20 (40%)	58,89,113	2.65	24 (41%)
13	CL0	A	1011	-	69,73,73	2.24	22 (31%)	82,113,113	2.66	28 (34%)
16	PQN	A	2001	-	34,34,34	1.48	2 (5%)	43,45,45	1.12	2 (4%)
14	CLA	a	1104	-	69,73,73	2.16	20 (28%)	82,113,113	2.56	25 (30%)
14	CLA	a	1106	-	49,53,73	2.49	20 (40%)	58,89,113	2.91	25 (43%)
14	CLA	G	1012	-	69,73,73	2.21	20 (28%)	82,113,113	2.51	29 (35%)
21	LMT	A	6001	-	32,32,36	1.26	6 (18%)	43,43,47	1.04	4 (9%)
14	CLA	A	1137	-	49,53,73	2.48	19 (38%)	58,89,113	2.95	25 (43%)
14	CLA	H	1233	-	49,53,73	2.51	21 (42%)	58,89,113	2.78	24 (41%)
18	BCR	a	4001	-	41,41,41	2.74	6 (14%)	56,56,56	6.63	22 (39%)
14	CLA	b	1215	-	64,68,73	2.30	19 (29%)	76,107,113	2.52	30 (39%)
18	BCR	b	4014	-	41,41,41	2.75	6 (14%)	56,56,56	6.60	24 (42%)
14	CLA	G	1132	-	69,73,73	2.21	20 (28%)	82,113,113	2.56	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	H	4017	-	41,41,41	2.76	6 (14%)	56,56,56	6.76	18 (32%)
14	CLA	a	1122	-	59,63,73	2.37	21 (35%)	70,101,113	2.63	28 (40%)
21	LMT	a	6002	-	29,29,36	1.35	5 (17%)	40,40,47	1.42	8 (20%)
14	CLA	H	1214	-	64,68,73	2.33	20 (31%)	76,107,113	2.53	35 (46%)
14	CLA	b	1239	-	69,73,73	2.23	22 (31%)	82,113,113	2.63	30 (36%)
15	F6C	H	1237	-	67,69,74	2.78	25 (37%)	77,108,114	3.21	36 (46%)
14	CLA	L	1502	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	24 (31%)
14	CLA	H	1229	-	64,68,73	2.30	21 (32%)	76,107,113	2.65	26 (34%)
14	CLA	A	1130	-	59,63,73	2.39	19 (32%)	70,101,113	2.58	27 (38%)
14	CLA	H	1203	-	69,73,73	2.16	20 (28%)	82,113,113	2.55	28 (34%)
14	CLA	G	1110	-	49,53,73	2.48	20 (40%)	58,89,113	2.90	23 (39%)
14	CLA	b	1238	-	69,73,73	2.25	20 (28%)	82,113,113	2.60	32 (39%)
14	CLA	b	1223	-	69,73,73	2.20	21 (30%)	82,113,113	2.47	26 (31%)
18	BCR	a	4007	-	41,41,41	2.77	7 (17%)	56,56,56	6.81	24 (42%)
14	CLA	A	1129	1	49,53,73	2.50	18 (36%)	58,89,113	2.77	25 (43%)
14	CLA	a	1126	-	64,68,73	2.33	20 (31%)	76,107,113	2.60	27 (35%)
14	CLA	A	1111	-	64,68,73	2.29	22 (34%)	76,107,113	2.62	29 (38%)
18	BCR	G	4002	-	41,41,41	2.70	6 (14%)	56,56,56	6.30	24 (42%)
14	CLA	k	1401	-	49,53,73	2.55	22 (44%)	58,89,113	2.77	21 (36%)
18	BCR	a	4008	-	41,41,41	2.89	7 (17%)	56,56,56	6.48	22 (39%)
14	CLA	L	1501	-	64,68,73	2.28	21 (32%)	76,107,113	2.72	27 (35%)
18	BCR	b	4010	-	41,41,41	2.75	6 (14%)	56,56,56	6.73	21 (37%)
14	CLA	b	1234	-	59,63,73	2.34	20 (33%)	70,101,113	2.66	27 (38%)
14	CLA	H	1021	-	69,73,73	2.20	21 (30%)	82,113,113	2.56	30 (36%)
14	CLA	b	1219	-	49,53,73	2.51	20 (40%)	58,89,113	2.75	22 (37%)
17	SF4	A	3001	-	0,12,12	-	-	-	-	-
14	CLA	a	1103	-	64,68,73	2.22	20 (31%)	76,107,113	2.63	26 (34%)
14	CLA	G	1123	-	64,68,73	2.29	20 (31%)	76,107,113	2.56	29 (38%)
14	CLA	b	1212	-	49,53,73	2.51	20 (40%)	58,89,113	2.81	23 (39%)
16	PQN	a	2001	-	34,34,34	1.47	2 (5%)	43,45,45	1.12	2 (4%)
14	CLA	U	1502	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	24 (31%)
14	CLA	a	1125	-	69,73,73	2.18	20 (28%)	82,113,113	2.58	27 (32%)
14	CLA	a	1118	-	59,63,73	2.37	20 (33%)	70,101,113	2.73	29 (41%)
14	CLA	B	1208	-	69,73,73	2.22	22 (31%)	82,113,113	2.45	25 (30%)
14	CLA	H	1201	-	59,63,73	2.37	21 (35%)	70,101,113	2.83	27 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	1119	-	69,73,73	2.22	19 (27%)	82,113,113	2.36	27 (32%)
14	CLA	G	1107	-	49,53,73	2.48	19 (38%)	58,89,113	2.69	24 (41%)
14	CLA	A	1126	-	64,68,73	2.33	20 (31%)	76,107,113	2.60	26 (34%)
16	PQN	B	2002	-	34,34,34	1.52	2 (5%)	43,45,45	1.18	1 (2%)
18	BCR	H	4005	-	41,41,41	2.66	7 (17%)	56,56,56	6.76	28 (50%)
14	CLA	a	1112	-	49,53,73	2.51	22 (44%)	58,89,113	2.78	22 (37%)
14	CLA	A	1114	-	49,53,73	2.56	22 (44%)	58,89,113	2.74	24 (41%)
14	CLA	G	1127	-	69,73,73	2.23	21 (30%)	82,113,113	2.41	28 (34%)
14	CLA	B	1217	-	59,63,73	2.38	21 (35%)	70,101,113	2.64	25 (35%)
14	CLA	a	1133	-	64,68,73	2.29	21 (32%)	76,107,113	2.59	27 (35%)
14	CLA	H	1206	-	49,53,73	2.49	19 (38%)	58,89,113	2.62	23 (39%)
14	CLA	G	1119	-	69,73,73	2.22	19 (27%)	82,113,113	2.35	28 (34%)
13	CL0	a	1011	-	69,73,73	2.24	22 (31%)	82,113,113	2.66	28 (34%)
15	F6C	b	1230	-	52,54,74	3.07	27 (51%)	59,90,114	3.57	32 (54%)
18	BCR	b	4016	-	41,41,41	2.66	6 (14%)	56,56,56	6.65	18 (32%)
14	CLA	G	1103	-	64,68,73	2.22	20 (31%)	76,107,113	2.63	26 (34%)
14	CLA	G	1128	-	64,68,73	2.33	20 (31%)	76,107,113	2.48	29 (38%)
14	CLA	A	1132	-	69,73,73	2.21	20 (28%)	82,113,113	2.56	28 (34%)
14	CLA	l	1502	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	25 (32%)
15	F6C	a	1120	-	52,54,74	3.10	25 (48%)	59,90,114	3.72	27 (45%)
14	CLA	B	1209	-	49,53,73	2.50	21 (42%)	58,89,113	2.77	23 (39%)
18	BCR	l	4019	-	41,41,41	2.68	6 (14%)	56,56,56	6.70	24 (42%)
14	CLA	b	1206	-	49,53,73	2.49	19 (38%)	58,89,113	2.61	23 (39%)
14	CLA	b	1222	-	69,73,73	2.23	21 (30%)	82,113,113	2.58	32 (39%)
14	CLA	B	1216	-	59,63,73	2.40	22 (37%)	70,101,113	2.60	31 (44%)
21	LMT	a	6001	-	32,32,36	1.26	6 (18%)	43,43,47	1.04	4 (9%)
18	BCR	b	4006	-	41,41,41	2.65	6 (14%)	56,56,56	6.71	23 (41%)
19	LHG	A	5001	-	41,41,48	1.02	2 (4%)	44,47,54	1.12	4 (9%)
14	CLA	B	1021	-	69,73,73	2.19	21 (30%)	82,113,113	2.55	30 (36%)
14	CLA	G	1125	-	69,73,73	2.18	20 (28%)	82,113,113	2.57	27 (32%)
14	CLA	a	1124	-	59,63,73	2.37	20 (33%)	70,101,113	2.68	27 (38%)
14	CLA	H	1209	-	49,53,73	2.50	21 (42%)	58,89,113	2.77	23 (39%)
19	LHG	a	5001	-	41,41,48	1.02	2 (4%)	44,47,54	1.12	4 (9%)
14	CLA	a	1113	-	49,53,73	2.49	19 (38%)	58,89,113	2.86	23 (39%)
14	CLA	A	1103	-	64,68,73	2.23	20 (31%)	76,107,113	2.63	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	G	1130	-	59,63,73	2.39	19 (32%)	70,101,113	2.58	28 (40%)
14	CLA	G	1135	-	54,58,73	2.53	21 (38%)	64,95,113	2.84	28 (43%)
14	CLA	a	1116	-	59,63,73	2.40	20 (33%)	70,101,113	2.67	28 (40%)
14	CLA	H	1216	-	59,63,73	2.40	22 (37%)	70,101,113	2.60	30 (42%)
14	CLA	B	1220	-	59,63,73	2.39	20 (33%)	70,101,113	2.64	25 (35%)
18	BCR	A	4001	-	41,41,41	2.74	6 (14%)	56,56,56	6.63	22 (39%)
14	CLA	a	1111	-	64,68,73	2.29	22 (34%)	76,107,113	2.62	29 (38%)
14	CLA	B	1232	-	49,53,73	2.52	22 (44%)	58,89,113	2.70	23 (39%)
14	CLA	T	1401	-	49,53,73	2.55	22 (44%)	58,89,113	2.77	21 (36%)
18	BCR	b	4009	-	41,41,41	2.71	6 (14%)	56,56,56	6.72	25 (44%)
14	CLA	H	1221	-	64,68,73	2.27	20 (31%)	76,107,113	2.49	27 (35%)
14	CLA	a	1131	1	64,68,73	2.27	21 (32%)	76,107,113	2.58	25 (32%)
15	F6C	H	1230	-	52,54,74	3.08	27 (51%)	59,90,114	3.55	32 (54%)
14	CLA	a	1107	-	49,53,73	2.48	19 (38%)	58,89,113	2.69	24 (41%)
16	PQN	G	2001	-	34,34,34	1.48	2 (5%)	43,45,45	1.12	2 (4%)
14	CLA	l	1503	-	69,73,73	2.20	20 (28%)	82,113,113	2.46	27 (32%)
14	CLA	b	1021	-	69,73,73	2.18	21 (30%)	82,113,113	2.56	30 (36%)
18	BCR	i	4018	-	41,41,41	2.86	7 (17%)	56,56,56	6.85	25 (44%)
19	LHG	G	5001	-	41,41,48	1.02	2 (4%)	44,47,54	1.12	4 (9%)
14	CLA	b	1216	-	59,63,73	2.40	22 (37%)	70,101,113	2.61	29 (41%)
14	CLA	K	1401	-	49,53,73	2.55	22 (44%)	58,89,113	2.76	21 (36%)
17	SF4	G	3001	-	0,12,12	-	-	-	-	-
14	CLA	b	1229	-	64,68,73	2.29	21 (32%)	76,107,113	2.64	26 (34%)
14	CLA	b	1228	-	49,53,73	2.50	21 (42%)	58,89,113	2.75	26 (44%)
14	CLA	H	1219	-	49,53,73	2.51	20 (40%)	58,89,113	2.76	22 (37%)
14	CLA	H	1210	-	69,73,73	2.23	21 (30%)	82,113,113	2.57	32 (39%)
14	CLA	B	1238	-	69,73,73	2.25	19 (27%)	82,113,113	2.60	32 (39%)
15	F6C	b	1237	-	67,69,74	2.78	26 (38%)	77,108,114	3.21	36 (46%)
14	CLA	b	1211	-	69,73,73	2.21	20 (28%)	82,113,113	2.39	26 (31%)
14	CLA	a	1012	-	69,73,73	2.21	20 (28%)	82,113,113	2.51	29 (35%)
14	CLA	A	1106	-	49,53,73	2.49	20 (40%)	58,89,113	2.91	24 (41%)
18	BCR	U	4022	-	41,41,41	2.82	6 (14%)	56,56,56	6.62	24 (42%)
14	CLA	G	1013	-	64,68,73	2.36	22 (34%)	76,107,113	2.67	30 (39%)
18	BCR	H	4006	-	41,41,41	2.65	6 (14%)	56,56,56	6.71	22 (39%)
14	CLA	B	1234	-	59,63,73	2.34	20 (33%)	70,101,113	2.66	27 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	W	1701	-	49,53,73	2.48	19 (38%)	58,89,113	2.75	23 (39%)
14	CLA	b	1208	-	69,73,73	2.22	22 (31%)	82,113,113	2.45	25 (30%)
14	CLA	B	1219	-	49,53,73	2.51	20 (40%)	58,89,113	2.76	23 (39%)
18	BCR	G	4011	-	41,41,41	2.75	7 (17%)	56,56,56	6.68	26 (46%)
14	CLA	G	1105	-	49,53,73	2.53	20 (40%)	58,89,113	2.76	22 (37%)
20	LMG	I	5006	-	37,37,55	1.15	3 (8%)	45,45,63	1.22	4 (8%)
14	CLA	b	1231	-	59,63,73	2.42	20 (33%)	70,101,113	2.66	26 (37%)
14	CLA	A	1104	-	69,73,73	2.16	20 (28%)	82,113,113	2.55	25 (30%)
15	F6C	B	1230	-	52,54,74	3.08	27 (51%)	59,90,114	3.56	32 (54%)
18	BCR	B	4012	-	41,41,41	2.59	6 (14%)	56,56,56	6.78	27 (48%)
14	CLA	H	1234	-	59,63,73	2.33	20 (33%)	70,101,113	2.66	26 (37%)
17	SF4	C	3003	-	0,12,12	-	-	-	-	-
14	CLA	G	1124	-	59,63,73	2.37	21 (35%)	70,101,113	2.69	28 (40%)
14	CLA	b	1226	-	69,73,73	2.26	21 (30%)	82,113,113	2.39	27 (32%)
14	CLA	H	1205	-	69,73,73	2.19	21 (30%)	82,113,113	2.65	29 (35%)
20	LMG	U	5007	-	50,50,55	1.44	7 (14%)	58,58,63	1.10	2 (3%)
18	BCR	B	4016	-	41,41,41	2.67	6 (14%)	56,56,56	6.65	18 (32%)
14	CLA	B	1214	-	64,68,73	2.33	21 (32%)	76,107,113	2.53	34 (44%)
18	BCR	B	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.62	26 (46%)
14	CLA	B	1205	-	69,73,73	2.19	21 (30%)	82,113,113	2.64	29 (35%)
18	BCR	U	4019	-	41,41,41	2.68	6 (14%)	56,56,56	6.69	24 (42%)
20	LMG	a	5005	-	46,46,55	1.37	5 (10%)	54,54,63	1.16	3 (5%)
14	CLA	H	1223	-	69,73,73	2.20	21 (30%)	82,113,113	2.48	26 (31%)
18	BCR	R	4020	-	41,41,41	2.87	7 (17%)	56,56,56	6.44	24 (42%)
14	CLA	b	1022	-	69,73,73	2.20	20 (28%)	82,113,113	2.48	28 (34%)
14	CLA	B	1235	-	64,68,73	2.29	19 (29%)	76,107,113	2.65	27 (35%)
14	CLA	a	1109	-	49,53,73	2.46	21 (42%)	58,89,113	2.84	22 (37%)
14	CLA	A	1012	-	69,73,73	2.21	20 (28%)	82,113,113	2.52	29 (35%)
14	CLA	H	1207	-	49,53,73	2.49	20 (40%)	58,89,113	2.84	23 (39%)
14	CLA	H	1235	-	64,68,73	2.29	19 (29%)	76,107,113	2.65	27 (35%)
14	CLA	b	1209	-	49,53,73	2.50	21 (42%)	58,89,113	2.78	23 (39%)
14	CLA	a	1114	-	49,53,73	2.55	21 (42%)	58,89,113	2.74	24 (41%)
20	LMG	A	5005	-	46,46,55	1.36	5 (10%)	54,54,63	1.17	2 (3%)
15	F6C	A	1121	-	52,54,74	3.05	27 (51%)	59,90,114	3.69	30 (50%)
17	SF4	c	3003	-	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMG	L	5007	-	50,50,55	1.44	7 (14%)	58,58,63	1.10	2 (3%)
14	CLA	b	1225	-	69,73,73	2.25	20 (28%)	82,113,113	2.25	21 (25%)
14	CLA	G	1101	-	49,53,73	2.47	19 (38%)	58,89,113	2.79	25 (43%)
14	CLA	a	1128	-	64,68,73	2.33	20 (31%)	76,107,113	2.47	29 (38%)
14	CLA	b	1213	-	59,63,73	2.40	21 (35%)	70,101,113	2.72	26 (37%)
14	CLA	A	1124	-	59,63,73	2.37	20 (33%)	70,101,113	2.69	28 (40%)
14	CLA	a	1123	-	64,68,73	2.29	20 (31%)	76,107,113	2.56	29 (38%)
18	BCR	B	4010	-	41,41,41	2.75	6 (14%)	56,56,56	6.74	21 (37%)
14	CLA	b	1204	2	69,73,73	2.24	20 (28%)	82,113,113	2.50	27 (32%)
14	CLA	B	1218	-	49,53,73	2.50	19 (38%)	58,89,113	2.83	21 (36%)
14	CLA	G	1108	-	49,53,73	2.53	21 (42%)	58,89,113	2.75	23 (39%)
14	CLA	b	1227	-	49,53,73	2.55	19 (38%)	58,89,113	2.64	24 (41%)
14	CLA	B	1212	-	49,53,73	2.51	20 (40%)	58,89,113	2.82	23 (39%)
14	CLA	H	1012	-	69,73,73	2.20	20 (28%)	82,113,113	2.48	29 (35%)
14	CLA	H	1232	-	49,53,73	2.51	20 (40%)	58,89,113	2.70	23 (39%)
14	CLA	b	1233	-	49,53,73	2.52	21 (42%)	58,89,113	2.78	24 (41%)
18	BCR	H	4014	-	41,41,41	2.75	6 (14%)	56,56,56	6.60	23 (41%)
14	CLA	A	1127	-	69,73,73	2.24	21 (30%)	82,113,113	2.40	28 (34%)
14	CLA	a	1139	-	49,53,73	2.49	20 (40%)	58,89,113	2.70	22 (37%)
14	CLA	A	1013	-	64,68,73	2.35	22 (34%)	76,107,113	2.67	30 (39%)
17	SF4	N	3002	-	0,12,12	-	-	-	-	-
14	CLA	a	1127	-	69,73,73	2.24	20 (28%)	82,113,113	2.41	28 (34%)
17	SF4	c	3002	-	0,12,12	-	-	-	-	-
14	CLA	A	1140	-	69,73,73	2.21	21 (30%)	82,113,113	2.42	27 (32%)
14	CLA	H	1218	-	49,53,73	2.50	19 (38%)	58,89,113	2.83	21 (36%)
14	CLA	l	1501	-	64,68,73	2.28	21 (32%)	76,107,113	2.71	28 (36%)
18	BCR	b	4017	-	41,41,41	2.76	6 (14%)	56,56,56	6.75	18 (32%)
14	CLA	B	1221	-	64,68,73	2.27	20 (31%)	76,107,113	2.50	27 (35%)
14	CLA	B	1223	-	69,73,73	2.21	21 (30%)	82,113,113	2.47	26 (31%)
14	CLA	a	1101	-	49,53,73	2.47	19 (38%)	58,89,113	2.79	25 (43%)
14	CLA	G	1104	-	69,73,73	2.16	20 (28%)	82,113,113	2.55	25 (30%)
18	BCR	b	4005	-	41,41,41	2.67	7 (17%)	56,56,56	6.77	28 (50%)

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
14	CLA	a	1130	-	-	10/27/103/115	-
14	CLA	b	1203	-	-	18/39/115/115	-
14	CLA	G	1133	-	-	19/33/109/115	-
14	CLA	A	1131	1	-	17/33/109/115	-
16	PQN	H	2002	-	-	11/23/43/43	0/2/2/2
14	CLA	A	1139	-	-	4/15/91/115	-
21	LMT	A	6002	-	-	3/14/54/61	0/2/2/2
14	CLA	A	1105	-	-	7/15/91/115	-
18	BCR	b	4013	-	-	19/29/63/63	0/2/2/2
14	CLA	H	1228	-	-	6/15/91/115	-
14	CLA	b	1202	-	-	11/33/109/115	-
20	LMG	G	5005	-	-	17/41/61/70	0/1/1/1
14	CLA	B	1224	-	-	12/39/115/115	-
14	CLA	H	1217	-	-	10/27/103/115	-
14	CLA	B	1213	-	-	14/27/103/115	-
18	BCR	L	4019	-	-	8/29/63/63	0/2/2/2
14	CLA	G	1112	-	-	7/15/91/115	-
14	CLA	H	1215	-	-	14/33/109/115	-
17	SF4	N	3003	-	-	-	0/6/5/5
14	CLA	B	1202	-	-	11/33/109/115	-
18	BCR	b	4004	-	-	8/29/63/63	0/2/2/2
14	CLA	b	1201	-	-	12/27/103/115	-
14	CLA	b	1205	-	-	14/39/115/115	-
14	CLA	H	1224	-	-	12/39/115/115	-
14	CLA	G	1114	-	-	7/15/91/115	-
18	BCR	B	4014	-	-	11/29/63/63	0/2/2/2
14	CLA	H	1239	-	-	20/39/115/115	-
14	CLA	a	1135	-	-	6/21/97/115	-
18	BCR	I	4020	-	-	11/29/63/63	0/2/2/2
14	CLA	G	1138	-	-	14/33/109/115	-
19	LHG	H	5004	-	-	19/48/48/53	-
20	LMG	b	5002	-	-	17/41/61/70	0/1/1/1
18	BCR	a	4011	-	-	15/29/63/63	0/2/2/2
18	BCR	H	4016	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1236	-	-	5/15/91/115	-
14	CLA	G	1116	-	-	12/27/103/115	-
18	BCR	B	4009	-	-	4/29/63/63	0/2/2/2
15	F6C	G	1120	-	1/1/6/16	8/17/73/97	-
14	CLA	B	1022	-	-	17/39/115/115	-
14	CLA	a	1110	-	-	8/15/91/115	-
14	CLA	G	1139	-	-	4/15/91/115	-
14	CLA	H	1220	-	-	10/27/103/115	-
20	LMG	B	5002	-	-	17/41/61/70	0/1/1/1
14	CLA	G	1129	-	-	4/15/91/115	-
14	CLA	A	1138	-	-	14/33/109/115	-
14	CLA	A	1118	-	-	14/27/103/115	-
14	CLA	A	1116	-	-	12/27/103/115	-
14	CLA	A	1125	-	-	23/39/115/115	-
14	CLA	G	1140	-	-	19/39/115/115	-
18	BCR	A	4011	-	-	15/29/63/63	0/2/2/2
14	CLA	B	1215	-	-	14/33/109/115	-
14	CLA	L	1503	-	-	12/39/115/115	-
14	CLA	B	1206	-	-	5/15/91/115	-
14	CLA	H	1238	-	-	15/39/115/115	-
14	CLA	a	1105	-	-	7/15/91/115	-
14	CLA	a	1108	-	-	6/15/91/115	-
14	CLA	B	1210	-	-	9/39/115/115	-
14	CLA	b	1221	-	-	13/33/109/115	-
18	BCR	H	4010	-	-	9/29/63/63	0/2/2/2
14	CLA	H	1204	2	-	19/39/115/115	-
14	CLA	G	1115	-	-	9/27/103/115	-
18	BCR	H	4004	-	-	8/29/63/63	0/2/2/2
14	CLA	B	1236	-	-	5/15/91/115	-
18	BCR	B	4017	-	-	11/29/63/63	0/2/2/2
15	F6C	a	1121	-	1/1/6/16	8/17/73/97	-
20	LMG	H	5002	-	-	17/41/61/70	0/1/1/1
18	BCR	a	4003	-	-	14/29/63/63	0/2/2/2
15	F6C	B	1237	-	1/1/9/16	17/35/91/97	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	B	4005	-	-	4/29/63/63	0/2/2/2
14	CLA	B	1211	-	-	16/39/115/115	-
14	CLA	B	1229	-	-	15/33/109/115	-
18	BCR	i	4020	-	-	11/29/63/63	0/2/2/2
14	CLA	B	1204	2	-	19/39/115/115	-
14	CLA	G	1106	-	-	9/15/91/115	-
14	CLA	B	1222	-	-	16/39/115/115	-
14	CLA	b	1210	-	-	9/39/115/115	-
14	CLA	b	1023	-	-	15/39/115/115	-
18	BCR	V	4021	-	-	11/29/63/63	0/2/2/2
14	CLA	A	1113	-	-	6/15/91/115	-
14	CLA	B	1207	-	-	7/15/91/115	-
18	BCR	G	4008	-	-	10/29/63/63	0/2/2/2
14	CLA	H	1226	-	-	16/39/115/115	-
14	CLA	A	1133	-	-	19/33/109/115	-
14	CLA	X	1701	-	-	8/15/91/115	-
14	CLA	x	1701	-	-	8/15/91/115	-
14	CLA	H	1211	-	-	16/39/115/115	-
14	CLA	U	1501	-	-	12/33/109/115	-
18	BCR	R	4018	-	-	11/29/63/63	0/2/2/2
14	CLA	a	1119	-	-	15/39/115/115	-
14	CLA	H	1231	-	-	5/27/103/115	-
18	BCR	a	4002	-	-	7/29/63/63	0/2/2/2
14	CLA	B	1226	-	-	16/39/115/115	-
14	CLA	B	1203	-	-	18/39/115/115	-
18	BCR	A	4002	-	-	7/29/63/63	0/2/2/2
14	CLA	A	1101	-	-	8/15/91/115	-
15	F6C	A	1120	-	1/1/6/16	8/17/73/97	-
18	BCR	G	4007	-	-	13/29/63/63	0/2/2/2
14	CLA	H	1222	-	-	16/39/115/115	-
14	CLA	A	1108	-	-	6/15/91/115	-
18	BCR	G	4001	-	-	12/29/63/63	0/2/2/2
14	CLA	H	1202	-	-	11/33/109/115	-
14	CLA	A	1115	-	-	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1102	-	-	11/33/109/115	-
14	CLA	B	1225	-	-	14/39/115/115	-
14	CLA	a	1137	-	-	7/15/91/115	-
14	CLA	A	1122	-	-	9/27/103/115	-
14	CLA	b	1236	-	-	5/15/91/115	-
17	SF4	C	3002	-	-	-	0/6/5/5
14	CLA	B	1023	-	-	15/39/115/115	-
14	CLA	G	1102	-	-	11/33/109/115	-
14	CLA	H	1225	-	-	14/39/115/115	-
14	CLA	A	1136	-	-	15/27/103/115	-
14	CLA	G	1109	-	-	7/15/91/115	-
14	CLA	G	1126	-	-	24/33/109/115	-
18	BCR	A	4008	-	-	10/29/63/63	0/2/2/2
14	CLA	b	1232	-	-	4/15/91/115	-
18	BCR	A	4003	-	-	14/29/63/63	0/2/2/2
15	F6C	G	1121	-	1/1/6/16	8/17/73/97	-
14	CLA	A	1117	-	-	15/39/115/115	-
14	CLA	H	1208	-	-	10/39/115/115	-
14	CLA	a	1102	-	-	11/33/109/115	-
18	BCR	l	4022	-	-	7/29/63/63	0/2/2/2
14	CLA	a	1138	-	-	14/33/109/115	-
14	CLA	b	1214	-	-	17/33/109/115	-
14	CLA	b	1220	-	-	10/27/103/115	-
14	CLA	B	1231	-	-	5/27/103/115	-
18	BCR	I	4018	-	-	10/29/63/63	0/2/2/2
14	CLA	G	1118	-	-	14/27/103/115	-
21	LMT	G	6002	-	-	3/14/54/61	0/2/2/2
14	CLA	b	1207	-	-	7/15/91/115	-
14	CLA	A	1112	-	-	7/15/91/115	-
14	CLA	B	1233	-	-	9/15/91/115	-
19	LHG	B	5004	-	-	19/48/48/53	-
21	LMT	G	6001	-	-	9/17/57/61	0/2/2/2
14	CLA	A	1135	-	-	6/21/97/115	-
14	CLA	B	1239	-	-	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CL0	G	1011	-	-	9/39/115/115	-
20	LMG	l	5007	-	-	13/45/65/70	0/1/1/1
14	CLA	a	1129	1	-	4/15/91/115	-
14	CLA	G	1113	-	-	6/15/91/115	-
14	CLA	A	1123	-	-	7/33/109/115	-
14	CLA	a	1013	-	-	13/33/109/115	-
14	CLA	B	1228	-	-	6/15/91/115	-
14	CLA	H	1212	-	-	11/15/91/115	-
14	CLA	B	1201	-	-	12/27/103/115	-
14	CLA	G	1111	-	-	15/33/109/115	-
14	CLA	a	1117	-	-	15/39/115/115	-
14	CLA	b	1218	-	-	6/15/91/115	-
18	BCR	H	4009	-	-	4/29/63/63	0/2/2/2
20	LMG	i	5006	-	-	13/32/52/70	0/1/1/1
14	CLA	G	1131	1	-	17/33/109/115	-
14	CLA	a	1132	-	-	20/39/115/115	-
14	CLA	G	1137	-	-	7/15/91/115	-
17	SF4	a	3001	-	-	-	0/6/5/5
14	CLA	G	1117	-	-	15/39/115/115	-
14	CLA	U	1503	-	-	12/39/115/115	-
14	CLA	A	1110	-	-	8/15/91/115	-
14	CLA	G	1122	-	-	9/27/103/115	-
16	PQN	b	2002	-	-	11/23/43/43	0/2/2/2
18	BCR	H	4013	-	-	19/29/63/63	0/2/2/2
14	CLA	b	1217	-	-	10/27/103/115	-
14	CLA	A	1128	-	-	11/33/109/115	-
18	BCR	A	4007	-	-	12/29/63/63	0/2/2/2
18	BCR	H	4012	-	-	20/29/63/63	0/2/2/2
18	BCR	m	4021	-	-	11/29/63/63	0/2/2/2
14	CLA	A	1107	-	-	5/15/91/115	-
14	CLA	a	1136	-	-	15/27/103/115	-
18	BCR	G	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	B	1227	-	-	7/15/91/115	-
14	CLA	a	1140	-	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	L	4022	-	-	7/29/63/63	0/2/2/2
14	CLA	A	1109	-	-	7/15/91/115	-
18	BCR	M	4021	-	-	11/29/63/63	0/2/2/2
14	CLA	b	1224	-	-	12/39/115/115	-
18	BCR	B	4013	-	-	19/29/63/63	0/2/2/2
18	BCR	b	4012	-	-	20/29/63/63	0/2/2/2
14	CLA	b	1235	-	-	9/33/109/115	-
20	LMG	R	5006	-	-	13/32/52/70	0/1/1/1
19	LHG	b	5004	-	-	19/48/48/53	-
14	CLA	a	1115	-	-	9/27/103/115	-
14	CLA	H	1213	-	-	14/27/103/115	-
18	BCR	B	4006	-	-	10/29/63/63	0/2/2/2
14	CLA	H	1023	-	-	15/39/115/115	-
14	CLA	G	1136	-	-	15/27/103/115	-
14	CLA	H	1227	-	-	7/15/91/115	-
13	CL0	A	1011	-	-	9/39/115/115	-
16	PQN	A	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	a	1104	-	-	13/39/115/115	-
14	CLA	a	1106	-	-	9/15/91/115	-
14	CLA	G	1012	-	-	14/39/115/115	-
21	LMT	A	6001	-	-	9/17/57/61	0/2/2/2
14	CLA	A	1137	-	-	7/15/91/115	-
14	CLA	H	1233	-	-	9/15/91/115	-
18	BCR	a	4001	-	-	12/29/63/63	0/2/2/2
14	CLA	b	1215	-	-	14/33/109/115	-
18	BCR	b	4014	-	-	11/29/63/63	0/2/2/2
14	CLA	G	1132	-	-	20/39/115/115	-
18	BCR	H	4017	-	-	11/29/63/63	0/2/2/2
14	CLA	a	1122	-	-	9/27/103/115	-
21	LMT	a	6002	-	-	3/14/54/61	0/2/2/2
14	CLA	H	1214	-	-	17/33/109/115	-
14	CLA	b	1239	-	-	20/39/115/115	-
15	F6C	H	1237	-	1/1/9/16	17/35/91/97	-
14	CLA	L	1502	-	-	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1229	-	-	15/33/109/115	-
14	CLA	A	1130	-	-	10/27/103/115	-
14	CLA	H	1203	-	-	18/39/115/115	-
14	CLA	G	1110	-	-	8/15/91/115	-
14	CLA	b	1238	-	-	15/39/115/115	-
14	CLA	b	1223	-	-	11/39/115/115	-
18	BCR	a	4007	-	-	13/29/63/63	0/2/2/2
14	CLA	A	1129	1	-	4/15/91/115	-
14	CLA	a	1126	-	-	24/33/109/115	-
14	CLA	A	1111	-	-	15/33/109/115	-
18	BCR	G	4002	-	-	7/29/63/63	0/2/2/2
14	CLA	k	1401	-	-	6/15/91/115	-
18	BCR	a	4008	-	-	10/29/63/63	0/2/2/2
14	CLA	L	1501	-	-	12/33/109/115	-
18	BCR	b	4010	-	-	9/29/63/63	0/2/2/2
14	CLA	b	1234	-	-	9/27/103/115	-
14	CLA	H	1021	-	-	13/39/115/115	-
14	CLA	b	1219	-	-	7/15/91/115	-
17	SF4	A	3001	-	-	-	0/6/5/5
14	CLA	a	1103	-	-	17/33/109/115	-
14	CLA	G	1123	-	-	7/33/109/115	-
14	CLA	b	1212	-	-	11/15/91/115	-
16	PQN	a	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	U	1502	-	-	12/33/109/115	-
14	CLA	a	1125	-	-	23/39/115/115	-
14	CLA	a	1118	-	-	14/27/103/115	-
14	CLA	B	1208	-	-	10/39/115/115	-
14	CLA	H	1201	-	-	12/27/103/115	-
14	CLA	A	1119	-	-	15/39/115/115	-
14	CLA	G	1107	-	-	5/15/91/115	-
14	CLA	A	1126	-	-	24/33/109/115	-
16	PQN	B	2002	-	-	11/23/43/43	0/2/2/2
18	BCR	H	4005	-	-	4/29/63/63	0/2/2/2
14	CLA	a	1112	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1114	-	-	7/15/91/115	-
14	CLA	G	1127	-	-	15/39/115/115	-
14	CLA	B	1217	-	-	10/27/103/115	-
14	CLA	a	1133	-	-	19/33/109/115	-
14	CLA	H	1206	-	-	5/15/91/115	-
14	CLA	G	1119	-	-	15/39/115/115	-
13	CL0	a	1011	-	-	9/39/115/115	-
15	F6C	b	1230	-	1/1/6/16	3/17/73/97	-
18	BCR	b	4016	-	-	15/29/63/63	0/2/2/2
14	CLA	G	1103	-	-	17/33/109/115	-
14	CLA	G	1128	-	-	11/33/109/115	-
14	CLA	A	1132	-	-	20/39/115/115	-
14	CLA	l	1502	-	-	12/33/109/115	-
15	F6C	a	1120	-	1/1/6/16	8/17/73/97	-
14	CLA	B	1209	-	-	4/15/91/115	-
18	BCR	l	4019	-	-	8/29/63/63	0/2/2/2
14	CLA	b	1206	-	-	5/15/91/115	-
14	CLA	b	1222	-	-	16/39/115/115	-
14	CLA	B	1216	-	-	10/27/103/115	-
21	LMT	a	6001	-	-	9/17/57/61	0/2/2/2
18	BCR	b	4006	-	-	10/29/63/63	0/2/2/2
19	LHG	A	5001	-	-	20/46/46/53	-
14	CLA	B	1021	-	-	14/39/115/115	-
14	CLA	G	1125	-	-	23/39/115/115	-
14	CLA	a	1124	-	-	9/27/103/115	-
14	CLA	H	1209	-	-	4/15/91/115	-
19	LHG	a	5001	-	-	20/46/46/53	-
14	CLA	a	1113	-	-	6/15/91/115	-
14	CLA	A	1103	-	-	17/33/109/115	-
14	CLA	G	1130	-	-	10/27/103/115	-
14	CLA	G	1135	-	-	6/21/97/115	-
14	CLA	a	1116	-	-	12/27/103/115	-
14	CLA	H	1216	-	-	10/27/103/115	-
14	CLA	B	1220	-	-	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	A	4001	-	-	12/29/63/63	0/2/2/2
14	CLA	a	1111	-	-	15/33/109/115	-
14	CLA	B	1232	-	-	4/15/91/115	-
14	CLA	T	1401	-	-	6/15/91/115	-
18	BCR	b	4009	-	-	4/29/63/63	0/2/2/2
14	CLA	H	1221	-	-	13/33/109/115	-
14	CLA	a	1131	1	-	17/33/109/115	-
15	F6C	H	1230	-	1/1/6/16	5/17/73/97	-
14	CLA	a	1107	-	-	5/15/91/115	-
16	PQN	G	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	l	1503	-	-	12/39/115/115	-
14	CLA	b	1021	-	-	13/39/115/115	-
18	BCR	i	4018	-	-	11/29/63/63	0/2/2/2
19	LHG	G	5001	-	-	20/46/46/53	-
14	CLA	b	1216	-	-	10/27/103/115	-
14	CLA	K	1401	-	-	6/15/91/115	-
17	SF4	G	3001	-	-	-	0/6/5/5
14	CLA	b	1229	-	-	15/33/109/115	-
14	CLA	b	1228	-	-	6/15/91/115	-
14	CLA	H	1219	-	-	7/15/91/115	-
14	CLA	H	1210	-	-	9/39/115/115	-
14	CLA	B	1238	-	-	15/39/115/115	-
15	F6C	b	1237	-	1/1/9/16	17/35/91/97	-
14	CLA	b	1211	-	-	16/39/115/115	-
14	CLA	a	1012	-	-	14/39/115/115	-
14	CLA	A	1106	-	-	9/15/91/115	-
18	BCR	U	4022	-	-	7/29/63/63	0/2/2/2
14	CLA	G	1013	-	-	13/33/109/115	-
18	BCR	H	4006	-	-	10/29/63/63	0/2/2/2
14	CLA	B	1234	-	-	9/27/103/115	-
14	CLA	W	1701	-	-	8/15/91/115	-
14	CLA	b	1208	-	-	10/39/115/115	-
14	CLA	B	1219	-	-	7/15/91/115	-
18	BCR	G	4011	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1105	-	-	7/15/91/115	-
20	LMG	I	5006	-	-	13/32/52/70	0/1/1/1
14	CLA	b	1231	-	-	5/27/103/115	-
14	CLA	A	1104	-	-	13/39/115/115	-
15	F6C	B	1230	-	1/1/6/16	8/17/73/97	-
18	BCR	B	4012	-	-	20/29/63/63	0/2/2/2
14	CLA	H	1234	-	-	9/27/103/115	-
17	SF4	C	3003	-	-	-	0/6/5/5
14	CLA	G	1124	-	-	9/27/103/115	-
14	CLA	b	1226	-	-	16/39/115/115	-
14	CLA	H	1205	-	-	14/39/115/115	-
20	LMG	U	5007	-	-	13/45/65/70	0/1/1/1
18	BCR	B	4016	-	-	15/29/63/63	0/2/2/2
14	CLA	B	1214	-	-	17/33/109/115	-
18	BCR	B	4004	-	-	8/29/63/63	0/2/2/2
14	CLA	B	1205	-	-	14/39/115/115	-
18	BCR	U	4019	-	-	8/29/63/63	0/2/2/2
20	LMG	a	5005	-	-	17/41/61/70	0/1/1/1
14	CLA	H	1223	-	-	11/39/115/115	-
18	BCR	R	4020	-	-	11/29/63/63	0/2/2/2
14	CLA	b	1022	-	-	17/39/115/115	-
14	CLA	B	1235	-	-	9/33/109/115	-
14	CLA	a	1109	-	-	7/15/91/115	-
14	CLA	A	1012	-	-	14/39/115/115	-
14	CLA	H	1207	-	-	7/15/91/115	-
14	CLA	H	1235	-	-	9/33/109/115	-
14	CLA	b	1209	-	-	4/15/91/115	-
14	CLA	a	1114	-	-	7/15/91/115	-
20	LMG	A	5005	-	-	17/41/61/70	0/1/1/1
15	F6C	A	1121	-	1/1/6/16	8/17/73/97	-
17	SF4	c	3003	-	-	-	0/6/5/5
20	LMG	L	5007	-	-	13/45/65/70	0/1/1/1
14	CLA	b	1225	-	-	14/39/115/115	-
14	CLA	G	1101	-	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	1128	-	-	11/33/109/115	-
14	CLA	b	1213	-	-	14/27/103/115	-
14	CLA	A	1124	-	-	9/27/103/115	-
14	CLA	a	1123	-	-	7/33/109/115	-
18	BCR	B	4010	-	-	9/29/63/63	0/2/2/2
14	CLA	b	1204	2	-	19/39/115/115	-
14	CLA	B	1218	-	-	6/15/91/115	-
14	CLA	G	1108	-	-	6/15/91/115	-
14	CLA	b	1227	-	-	7/15/91/115	-
14	CLA	B	1212	-	-	11/15/91/115	-
14	CLA	H	1012	-	-	17/39/115/115	-
18	BCR	H	4014	-	-	11/29/63/63	0/2/2/2
14	CLA	H	1232	-	-	4/15/91/115	-
14	CLA	b	1233	-	-	9/15/91/115	-
14	CLA	A	1127	-	-	15/39/115/115	-
14	CLA	a	1139	-	-	4/15/91/115	-
14	CLA	A	1013	-	-	13/33/109/115	-
17	SF4	N	3002	-	-	-	0/6/5/5
14	CLA	a	1127	-	-	15/39/115/115	-
17	SF4	c	3002	-	-	-	0/6/5/5
14	CLA	A	1140	-	-	19/39/115/115	-
14	CLA	H	1218	-	-	6/15/91/115	-
14	CLA	l	1501	-	-	12/33/109/115	-
18	BCR	b	4017	-	-	11/29/63/63	0/2/2/2
14	CLA	B	1221	-	-	13/33/109/115	-
14	CLA	B	1223	-	-	11/39/115/115	-
14	CLA	a	1101	-	-	8/15/91/115	-
14	CLA	G	1104	-	-	13/39/115/115	-
18	BCR	b	4005	-	-	4/29/63/63	0/2/2/2

The worst 5 of 6030 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1237	F6C	C1A-CHA	9.88	1.51	1.35
15	b	1237	F6C	C1A-CHA	9.88	1.51	1.35
15	G	1120	F6C	C1A-CHA	9.87	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1120	F6C	C1A-CHA	9.86	1.51	1.35
15	a	1120	F6C	C1A-CHA	9.86	1.51	1.35

The worst 5 of 8685 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	H	4010	BCR	C16-C17-C18	25.54	163.10	127.28
18	B	4010	BCR	C16-C17-C18	25.53	163.08	127.28
18	b	4010	BCR	C16-C17-C18	25.51	163.05	127.28
18	B	4017	BCR	C20-C21-C22	23.94	160.85	127.28
18	b	4017	BCR	C20-C21-C22	23.91	160.81	127.28

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	A	1120	F6C	NA
15	A	1121	F6C	NA
15	B	1230	F6C	NA
15	B	1237	F6C	NA
15	G	1120	F6C	NA

5 of 4092 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1011	CL0	C2-C1-O2A-CGA
13	G	1011	CL0	C2-C1-O2A-CGA
13	a	1011	CL0	C2-C1-O2A-CGA
14	A	1012	CLA	C2B-C3B-CAB-CBB
14	A	1012	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

292 monomers are involved in 651 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a	1130	CLA	2	0
14	b	1203	CLA	3	0
14	G	1133	CLA	4	0
14	A	1131	CLA	1	0
16	H	2002	PQN	4	0
14	b	1202	CLA	6	0
20	G	5005	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	1224	CLA	5	0
14	H	1217	CLA	3	0
14	B	1213	CLA	1	0
18	L	4019	BCR	2	0
14	G	1112	CLA	1	0
14	H	1215	CLA	5	0
14	B	1202	CLA	4	0
18	b	4004	BCR	1	0
14	b	1201	CLA	1	0
14	b	1205	CLA	7	0
14	H	1224	CLA	6	0
18	B	4014	BCR	2	0
14	H	1239	CLA	3	0
18	I	4020	BCR	3	0
14	G	1138	CLA	2	0
19	H	5004	LHG	1	0
20	b	5002	LMG	3	0
18	a	4011	BCR	5	0
18	H	4016	BCR	1	0
14	H	1236	CLA	1	0
14	G	1116	CLA	3	0
18	B	4009	BCR	6	0
14	B	1022	CLA	5	0
14	a	1110	CLA	1	0
14	H	1220	CLA	1	0
20	B	5002	LMG	3	0
14	G	1129	CLA	1	0
14	A	1138	CLA	1	0
14	A	1118	CLA	1	0
14	A	1116	CLA	3	0
14	A	1125	CLA	2	0
14	G	1140	CLA	3	0
18	A	4011	BCR	6	0
14	B	1215	CLA	6	0
14	L	1503	CLA	3	0
14	B	1206	CLA	1	0
14	H	1238	CLA	7	0
14	B	1210	CLA	6	0
14	b	1221	CLA	1	0
18	H	4010	BCR	6	0
14	H	1204	CLA	5	0
18	H	4004	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	1236	CLA	1	0
18	B	4017	BCR	1	0
20	H	5002	LMG	3	0
18	a	4003	BCR	5	0
18	B	4005	BCR	4	0
14	B	1211	CLA	4	0
14	B	1229	CLA	2	0
18	i	4020	BCR	1	0
14	B	1204	CLA	4	0
14	G	1106	CLA	2	0
14	B	1222	CLA	4	0
14	b	1210	CLA	6	0
14	b	1023	CLA	4	0
18	V	4021	BCR	4	0
14	B	1207	CLA	1	0
18	G	4008	BCR	1	0
14	H	1226	CLA	4	0
14	A	1133	CLA	3	0
14	X	1701	CLA	1	0
14	x	1701	CLA	1	0
14	H	1211	CLA	4	0
14	U	1501	CLA	5	0
18	R	4018	BCR	5	0
14	a	1119	CLA	6	0
14	H	1231	CLA	1	0
18	a	4002	BCR	1	0
14	B	1226	CLA	3	0
14	B	1203	CLA	5	0
18	G	4007	BCR	2	0
14	H	1222	CLA	3	0
14	H	1202	CLA	7	0
14	A	1102	CLA	1	0
14	B	1225	CLA	3	0
14	A	1122	CLA	1	0
14	b	1236	CLA	1	0
14	B	1023	CLA	5	0
14	G	1102	CLA	1	0
14	H	1225	CLA	3	0
14	A	1136	CLA	2	0
14	G	1109	CLA	1	0
14	G	1126	CLA	3	0
18	A	4008	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	1232	CLA	1	0
18	A	4003	BCR	6	0
14	A	1117	CLA	2	0
14	H	1208	CLA	3	0
18	l	4022	BCR	5	0
14	a	1138	CLA	1	0
14	b	1214	CLA	4	0
14	b	1220	CLA	1	0
14	B	1231	CLA	1	0
18	I	4018	BCR	5	0
14	G	1118	CLA	1	0
14	b	1207	CLA	1	0
14	A	1112	CLA	1	0
21	G	6001	LMT	1	0
14	B	1239	CLA	4	0
13	G	1011	CL0	2	0
20	l	5007	LMG	2	0
14	A	1123	CLA	3	0
14	a	1013	CLA	3	0
14	H	1212	CLA	1	0
14	B	1201	CLA	1	0
14	G	1111	CLA	3	0
14	a	1117	CLA	2	0
18	H	4009	BCR	7	0
20	i	5006	LMG	2	0
14	G	1131	CLA	1	0
14	a	1132	CLA	2	0
14	G	1137	CLA	1	0
14	G	1117	CLA	3	0
14	U	1503	CLA	3	0
14	A	1110	CLA	1	0
14	G	1122	CLA	1	0
16	b	2002	PQN	4	0
14	b	1217	CLA	3	0
14	A	1128	CLA	1	0
18	A	4007	BCR	2	0
18	H	4012	BCR	4	0
18	m	4021	BCR	2	0
14	A	1107	CLA	1	0
14	a	1136	CLA	2	0
18	G	4003	BCR	6	0
14	B	1227	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a	1140	CLA	3	0
18	L	4022	BCR	4	0
14	A	1109	CLA	2	0
18	M	4021	BCR	3	0
14	b	1224	CLA	6	0
18	b	4012	BCR	5	0
14	b	1235	CLA	2	0
20	R	5006	LMG	5	0
14	a	1115	CLA	1	0
18	B	4006	BCR	4	0
14	H	1023	CLA	5	0
14	G	1136	CLA	2	0
14	H	1227	CLA	1	0
13	A	1011	CL0	1	0
16	A	2001	PQN	6	0
14	a	1104	CLA	2	0
14	a	1106	CLA	2	0
14	G	1012	CLA	4	0
18	a	4001	BCR	3	0
14	b	1215	CLA	6	0
18	b	4014	BCR	1	0
14	G	1132	CLA	2	0
18	H	4017	BCR	1	0
14	a	1122	CLA	1	0
14	H	1214	CLA	3	0
14	b	1239	CLA	4	0
14	L	1502	CLA	1	0
14	H	1229	CLA	2	0
14	A	1130	CLA	2	0
14	H	1203	CLA	3	0
14	G	1110	CLA	1	0
14	b	1238	CLA	7	0
14	b	1223	CLA	3	0
18	a	4007	BCR	3	0
14	a	1126	CLA	5	0
14	A	1111	CLA	2	0
18	G	4002	BCR	1	0
18	a	4008	BCR	1	0
14	L	1501	CLA	4	0
18	b	4010	BCR	6	0
14	b	1234	CLA	2	0
14	H	1021	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	1219	CLA	4	0
14	a	1103	CLA	3	0
14	G	1123	CLA	4	0
14	b	1212	CLA	1	0
16	a	2001	PQN	6	0
14	U	1502	CLA	1	0
14	a	1125	CLA	2	0
14	a	1118	CLA	1	0
14	B	1208	CLA	3	0
14	H	1201	CLA	1	0
14	A	1119	CLA	4	0
14	G	1107	CLA	1	0
14	A	1126	CLA	4	0
16	B	2002	PQN	4	0
18	H	4005	BCR	4	0
14	a	1112	CLA	1	0
14	G	1127	CLA	3	0
14	B	1217	CLA	3	0
14	a	1133	CLA	4	0
14	H	1206	CLA	1	0
14	G	1119	CLA	4	0
13	a	1011	CL0	1	0
15	b	1230	F6C	6	0
14	G	1103	CLA	5	0
14	G	1128	CLA	1	0
14	A	1132	CLA	3	0
14	l	1502	CLA	1	0
14	B	1209	CLA	1	0
18	l	4019	BCR	1	0
14	b	1206	CLA	1	0
14	b	1222	CLA	4	0
14	B	1216	CLA	2	0
18	b	4006	BCR	5	0
19	A	5001	LHG	1	0
14	B	1021	CLA	3	0
14	G	1125	CLA	2	0
14	a	1124	CLA	5	0
14	H	1209	CLA	1	0
19	a	5001	LHG	1	0
14	A	1103	CLA	4	0
14	G	1130	CLA	2	0
14	a	1116	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	1216	CLA	2	0
14	B	1220	CLA	1	0
18	A	4001	BCR	1	0
14	a	1111	CLA	2	0
14	B	1232	CLA	1	0
18	b	4009	BCR	6	0
14	H	1221	CLA	1	0
14	a	1131	CLA	3	0
15	H	1230	F6C	3	0
14	a	1107	CLA	1	0
16	G	2001	PQN	6	0
14	l	1503	CLA	3	0
14	b	1021	CLA	4	0
18	i	4018	BCR	4	0
19	G	5001	LHG	1	0
14	b	1216	CLA	2	0
14	b	1229	CLA	2	0
14	H	1219	CLA	4	0
14	H	1210	CLA	3	0
14	B	1238	CLA	7	0
14	b	1211	CLA	3	0
14	a	1012	CLA	4	0
14	A	1106	CLA	1	0
18	U	4022	BCR	5	0
14	G	1013	CLA	3	0
18	H	4006	BCR	4	0
14	B	1234	CLA	2	0
14	W	1701	CLA	2	0
14	b	1208	CLA	2	0
14	B	1219	CLA	4	0
18	G	4011	BCR	6	0
20	I	5006	LMG	2	0
14	A	1104	CLA	2	0
15	B	1230	F6C	4	0
18	B	4012	BCR	5	0
14	H	1234	CLA	2	0
14	G	1124	CLA	5	0
14	b	1226	CLA	3	0
14	H	1205	CLA	7	0
20	U	5007	LMG	3	0
14	B	1214	CLA	3	0
18	B	4004	BCR	1	0

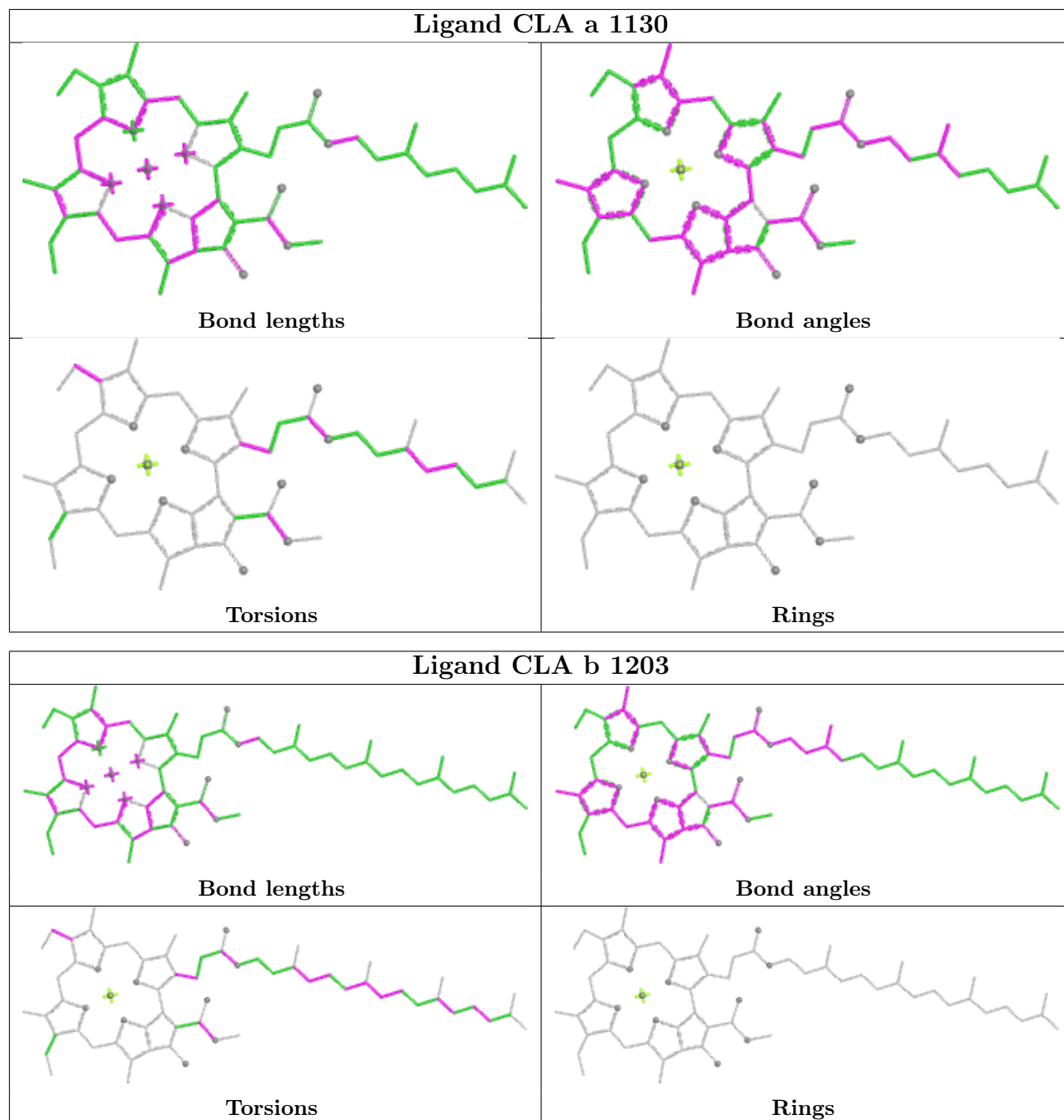
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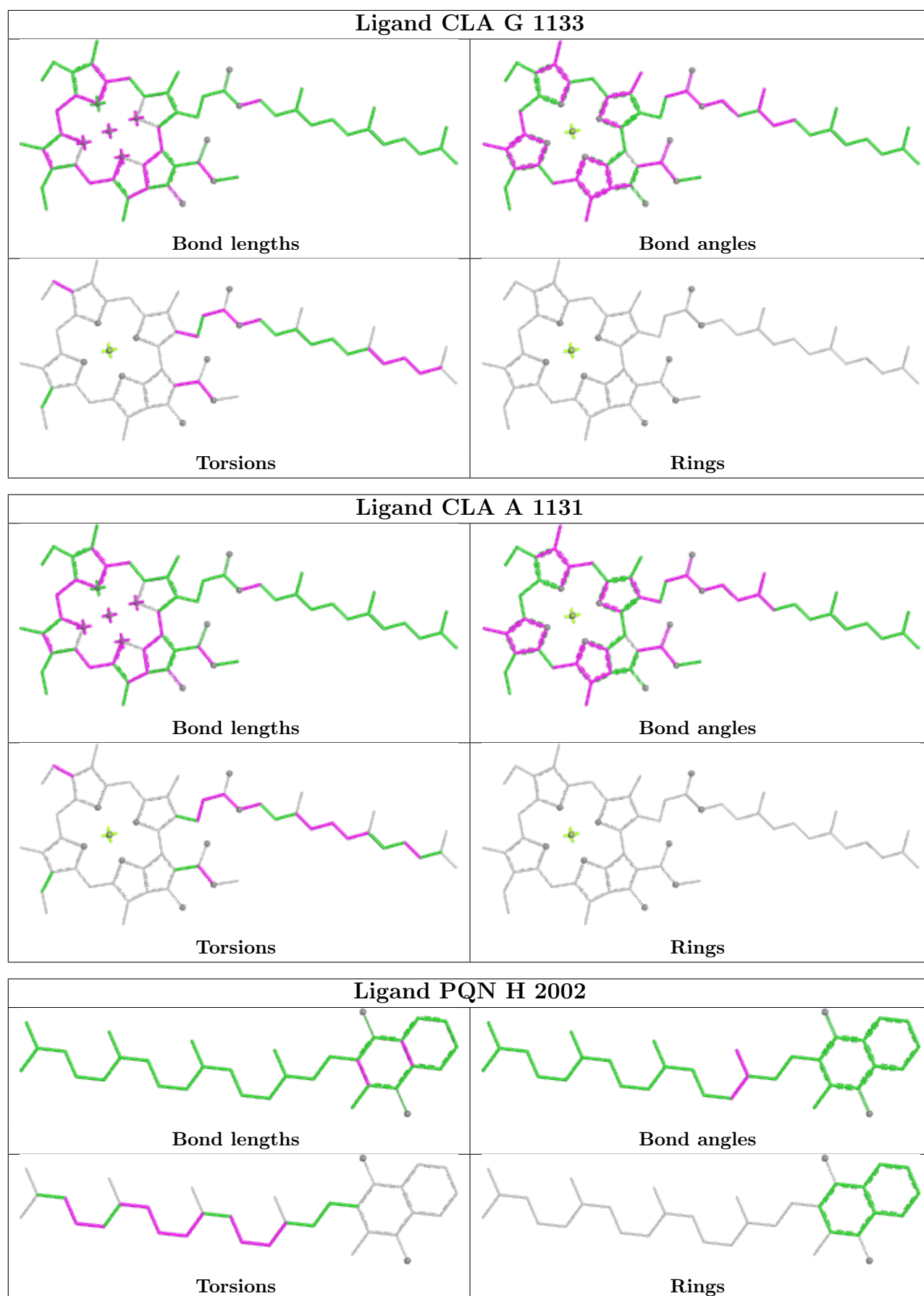
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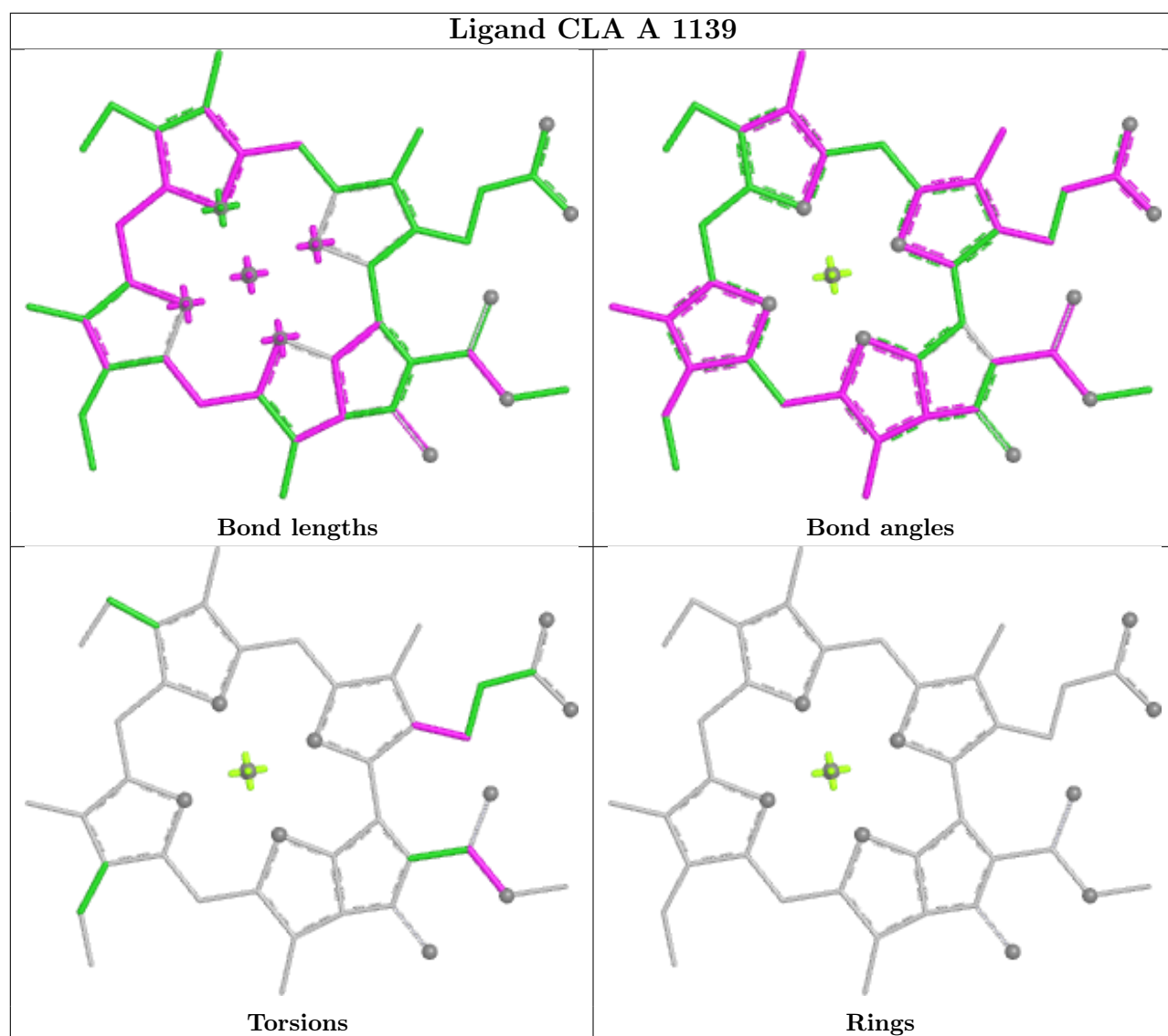
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	1205	CLA	7	0
18	U	4019	BCR	1	0
20	a	5005	LMG	1	0
14	H	1223	CLA	4	0
18	R	4020	BCR	4	0
14	b	1022	CLA	5	0
14	B	1235	CLA	2	0
14	a	1109	CLA	2	0
14	A	1012	CLA	3	0
14	H	1207	CLA	1	0
14	H	1235	CLA	3	0
14	b	1209	CLA	1	0
20	L	5007	LMG	2	0
14	b	1225	CLA	3	0
14	a	1128	CLA	1	0
14	A	1124	CLA	4	0
14	a	1123	CLA	4	0
18	B	4010	BCR	6	0
14	b	1204	CLA	5	0
14	b	1227	CLA	1	0
14	B	1212	CLA	1	0
14	H	1012	CLA	5	0
14	H	1232	CLA	1	0
14	A	1127	CLA	3	0
14	A	1013	CLA	5	0
14	a	1127	CLA	3	0
14	A	1140	CLA	3	0
14	l	1501	CLA	3	0
18	b	4017	BCR	1	0
14	B	1221	CLA	2	0
14	B	1223	CLA	3	0
14	G	1104	CLA	2	0
18	b	4005	BCR	3	0

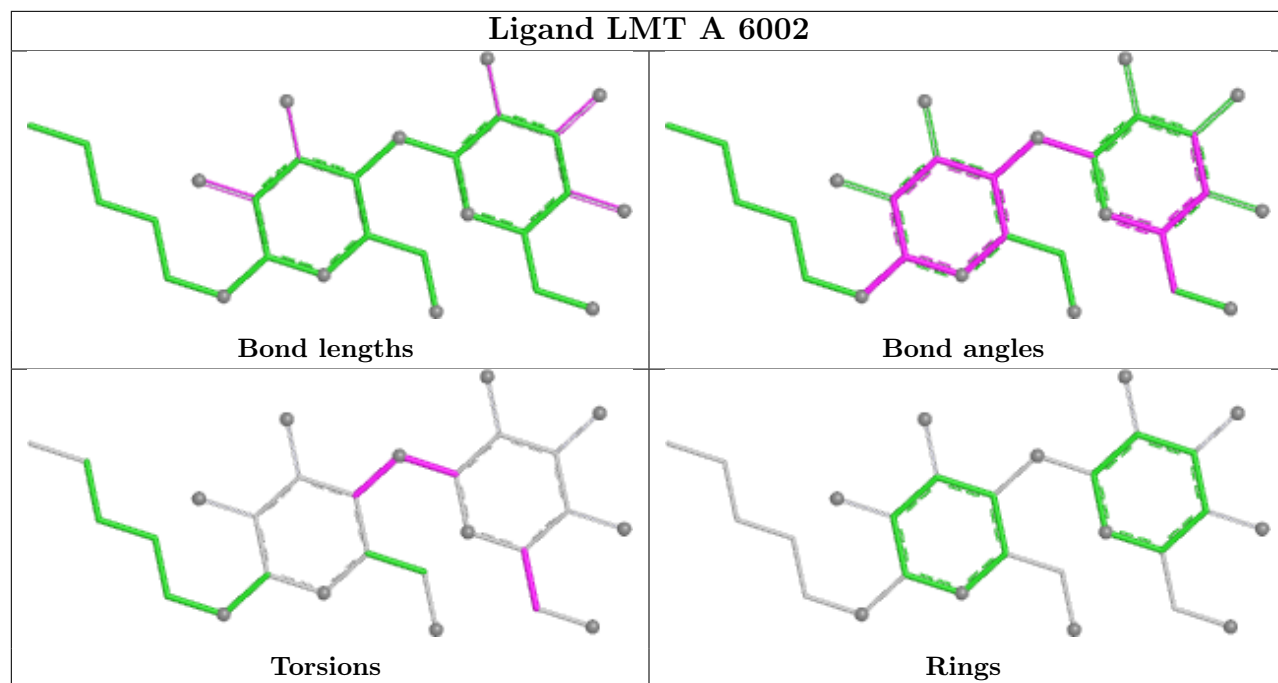
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

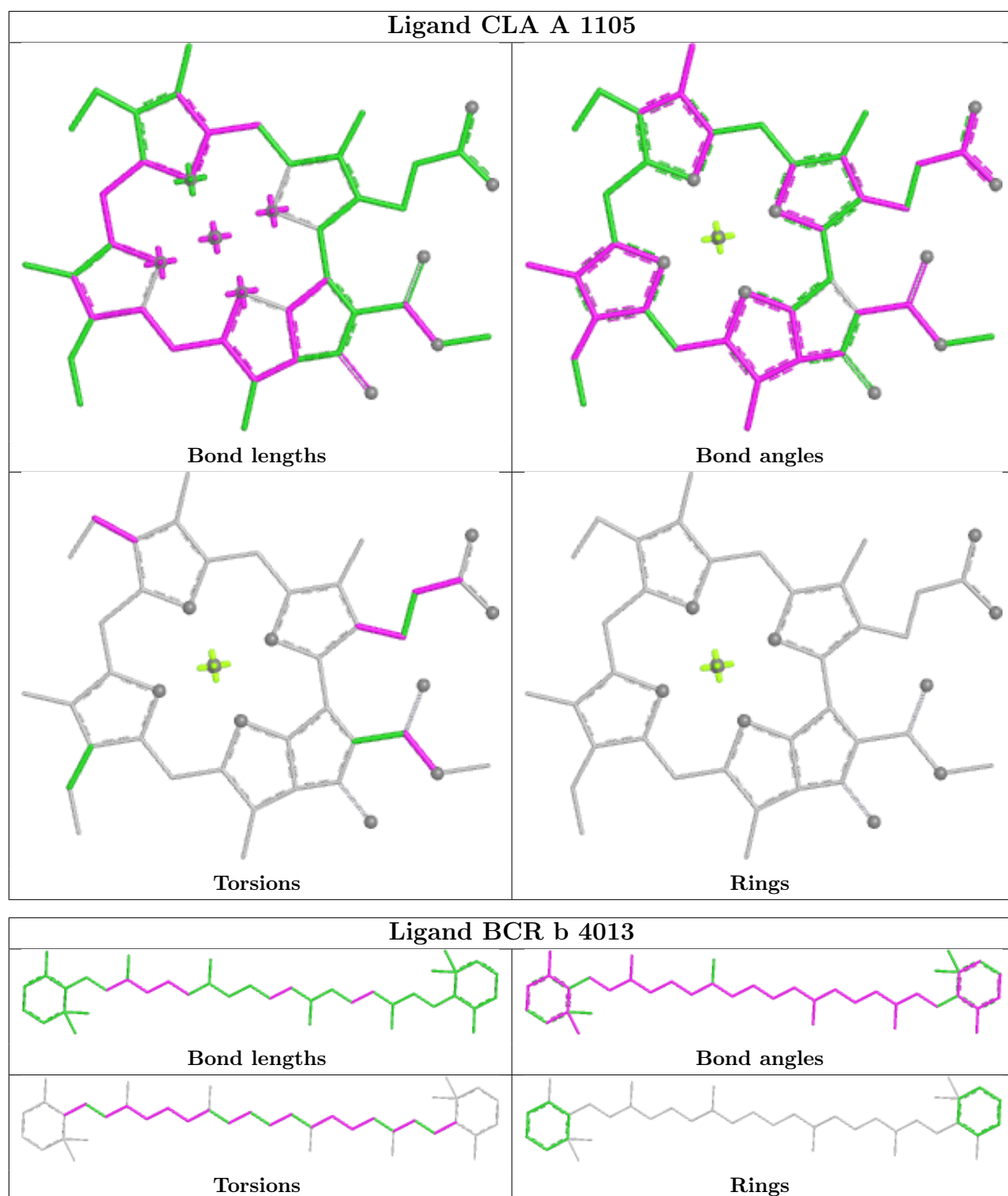
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



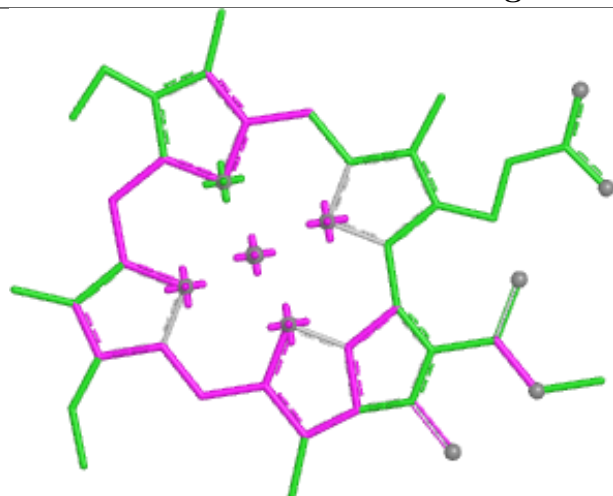




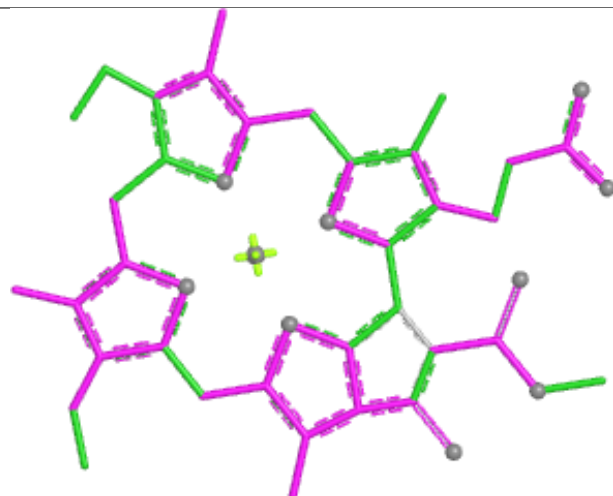




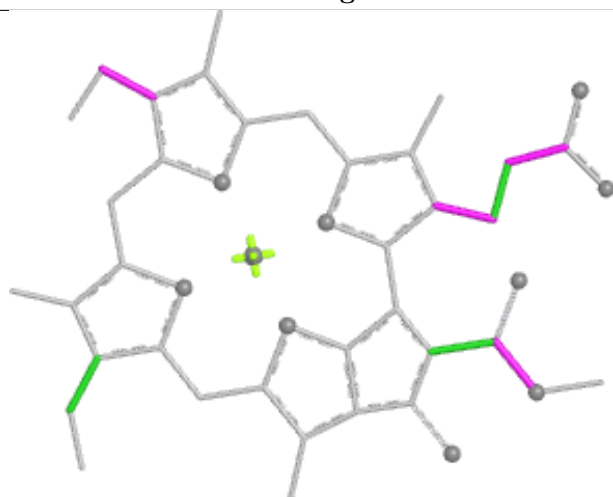
Ligand CLA H 1228



Bond lengths



Bond angles

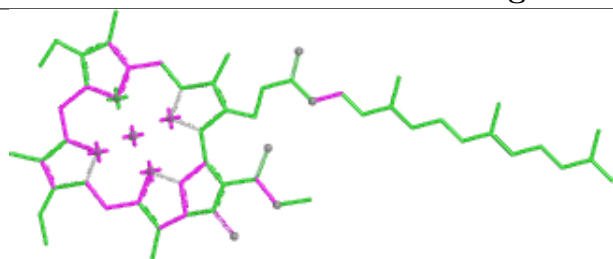


Torsions

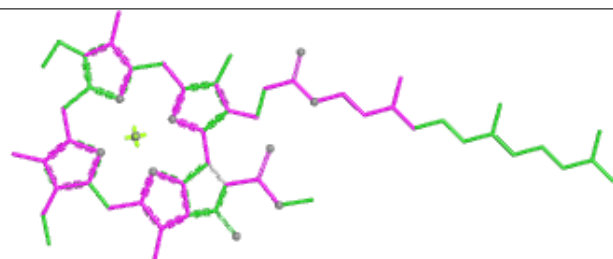


Rings

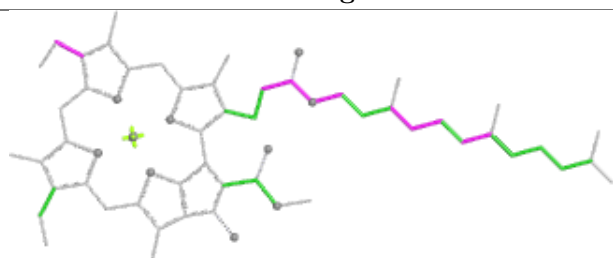
Ligand CLA b 1202



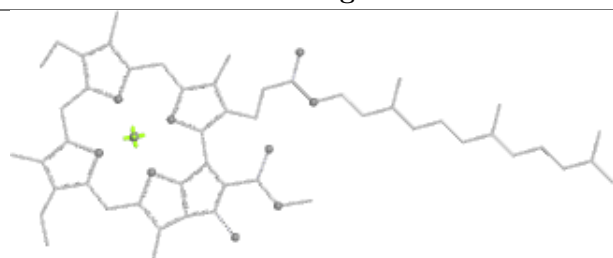
Bond lengths



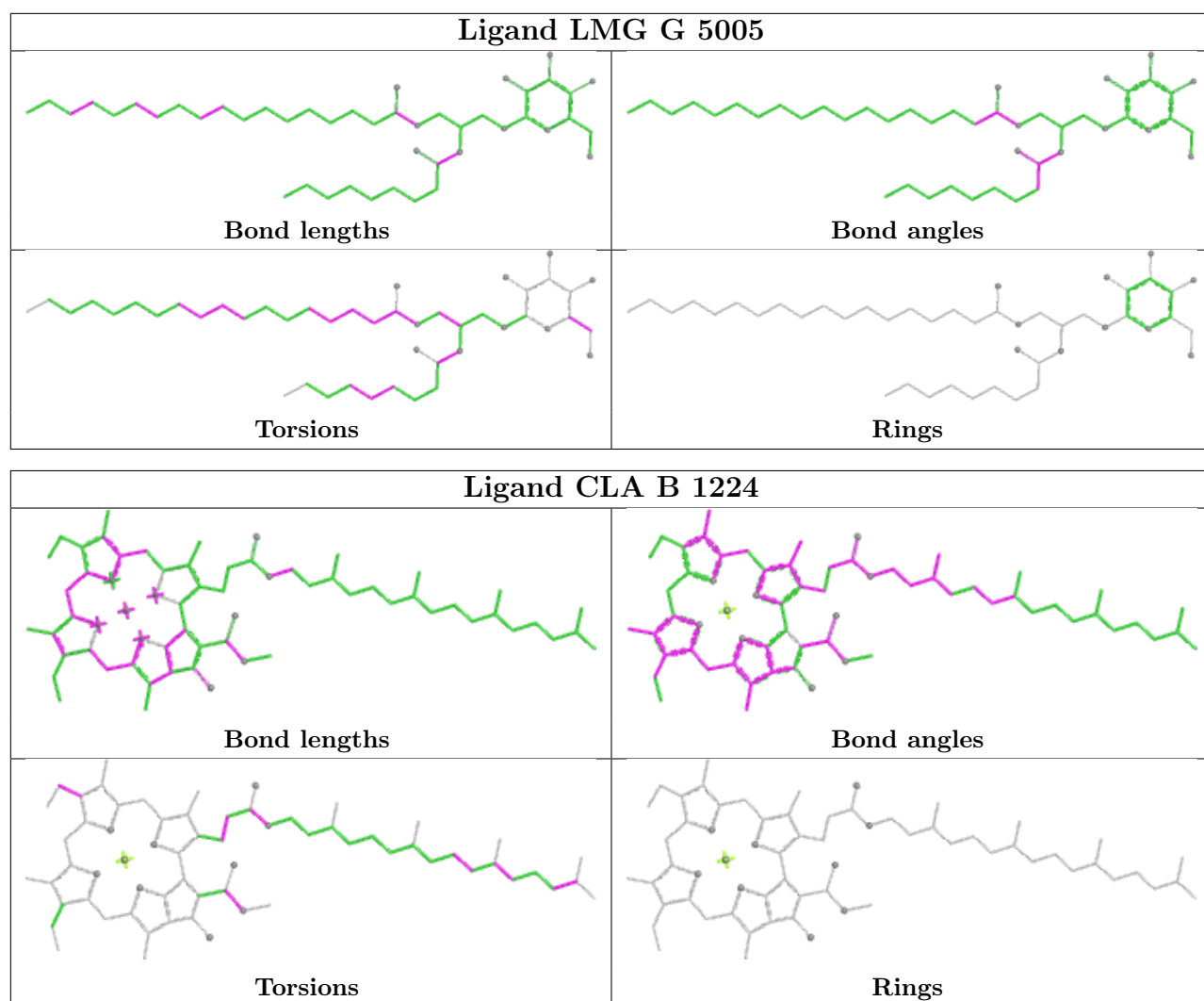
Bond angles



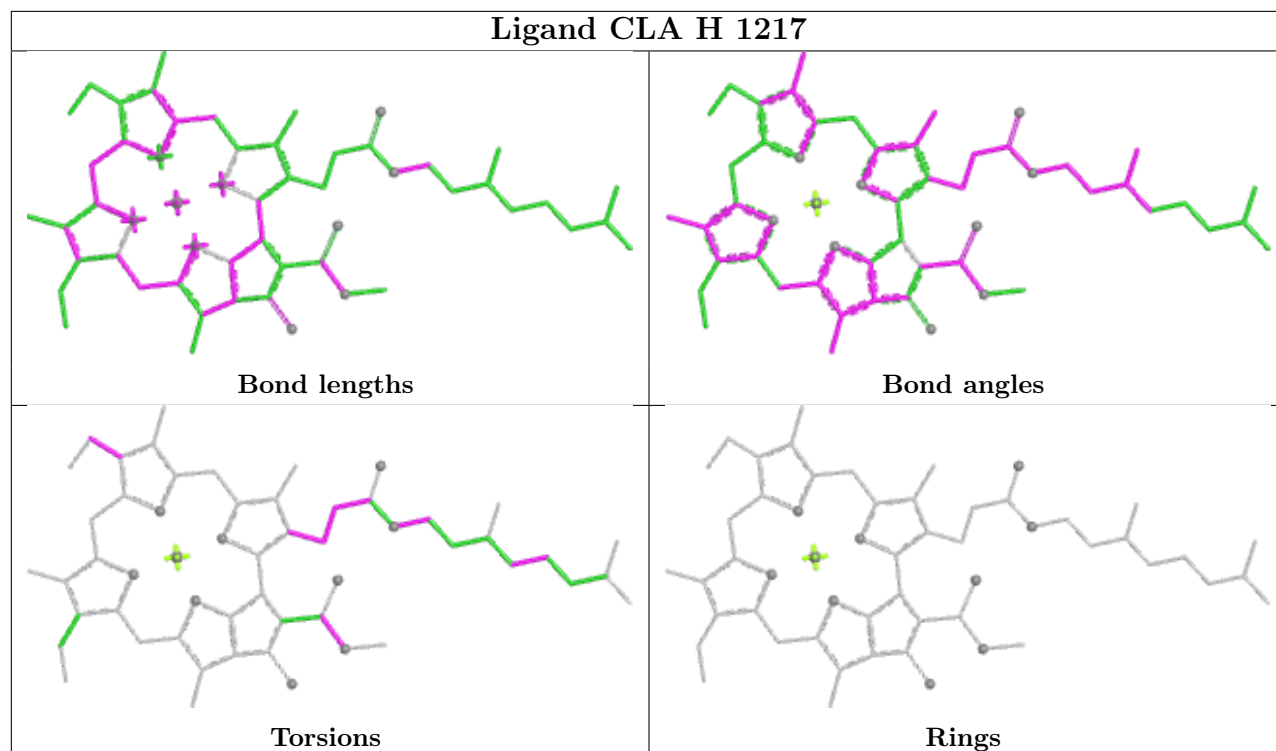
Torsions



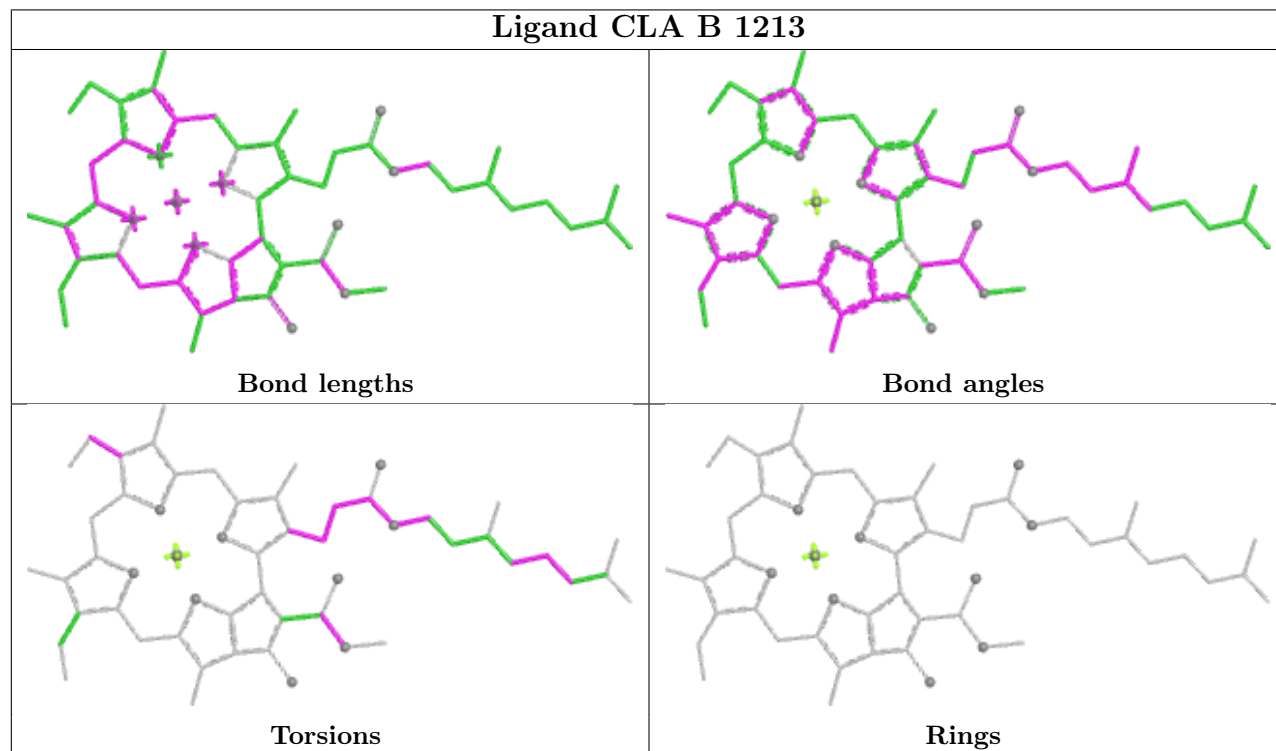
Rings

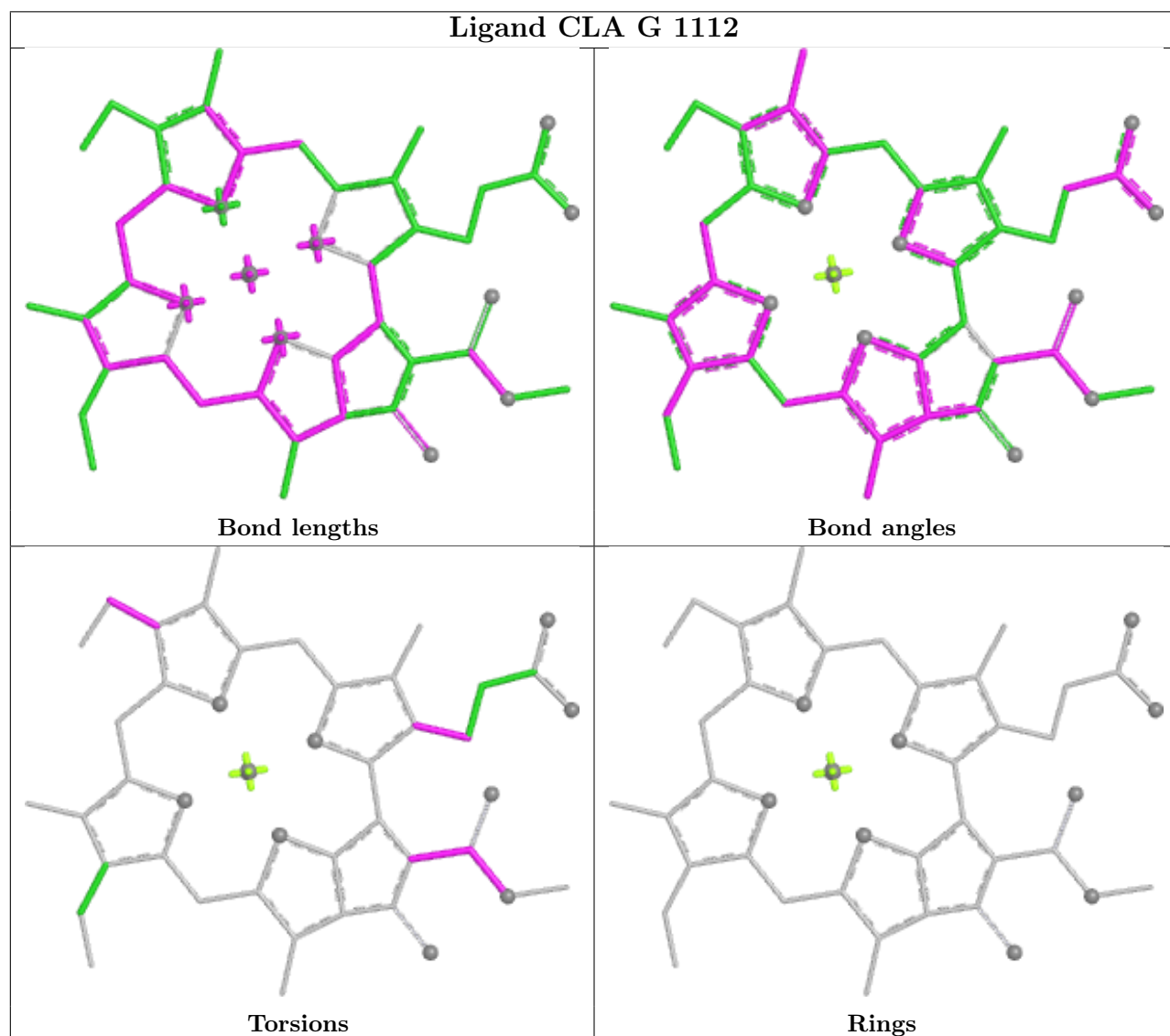
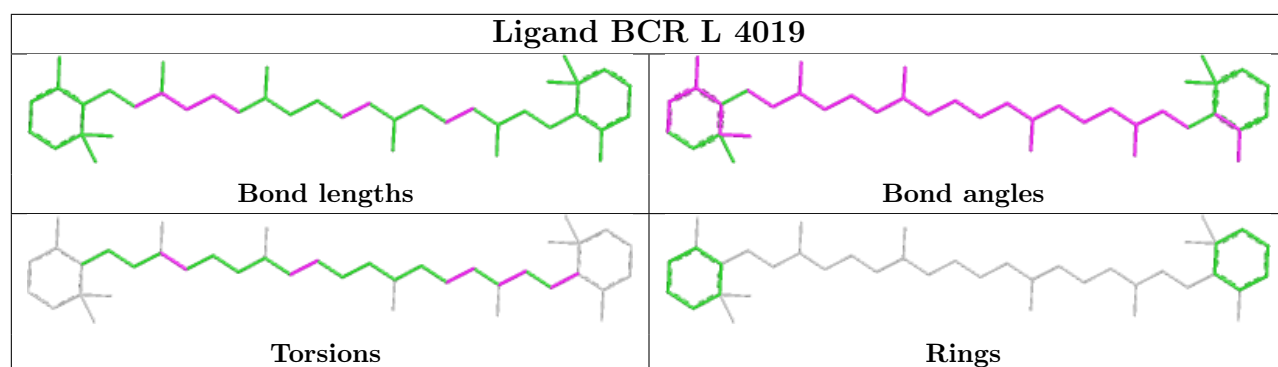


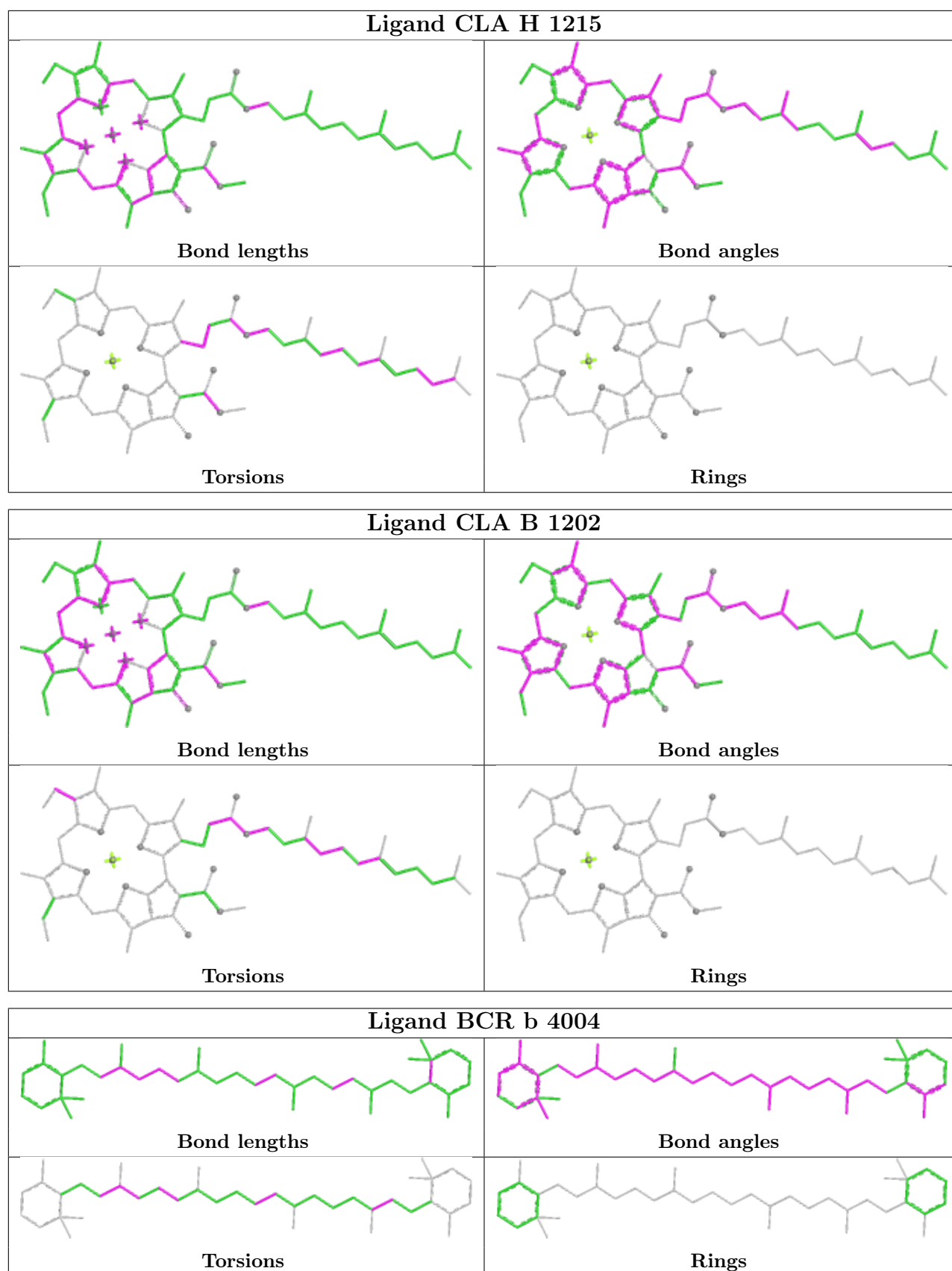
Ligand CLA H 1217

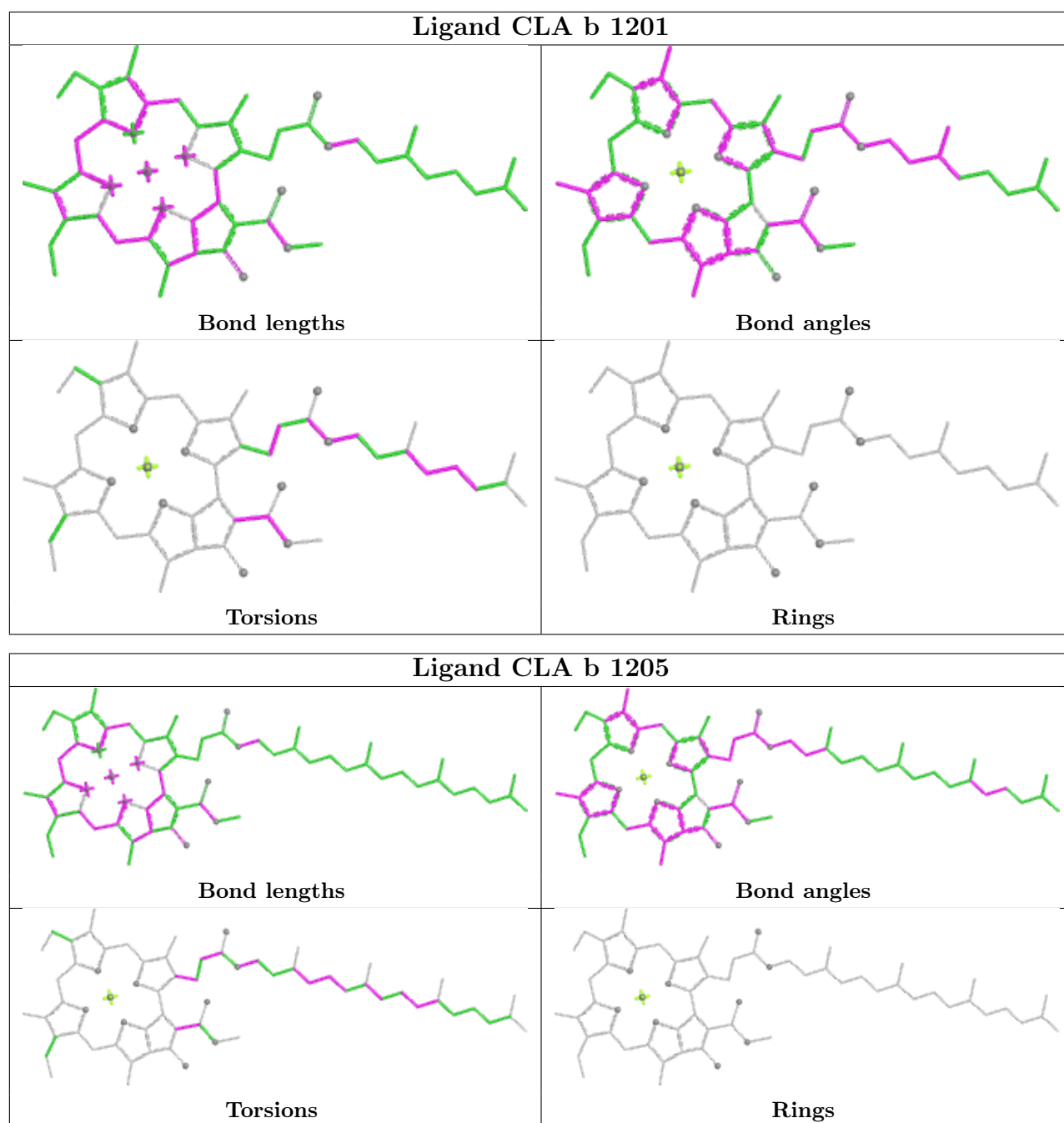


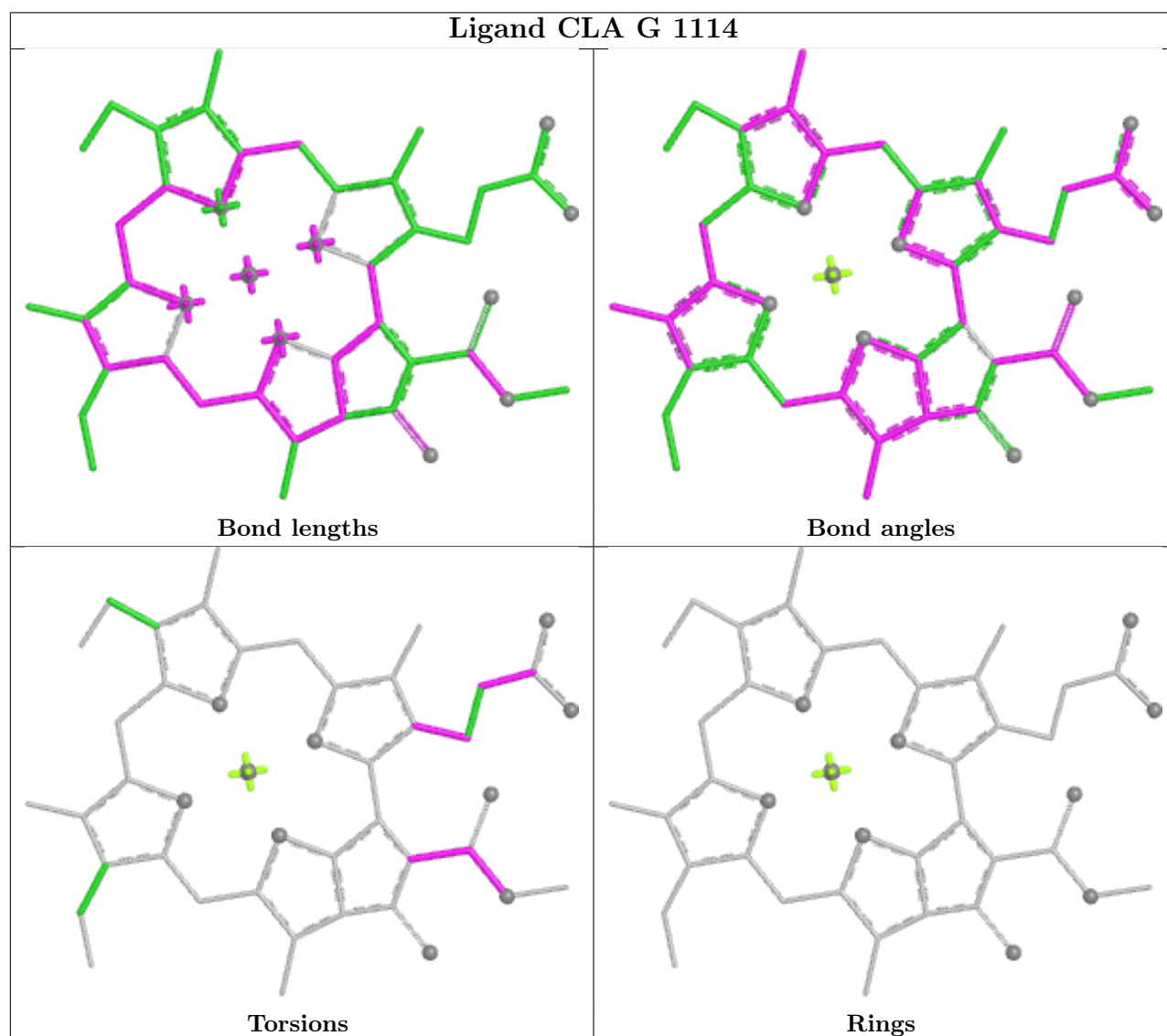
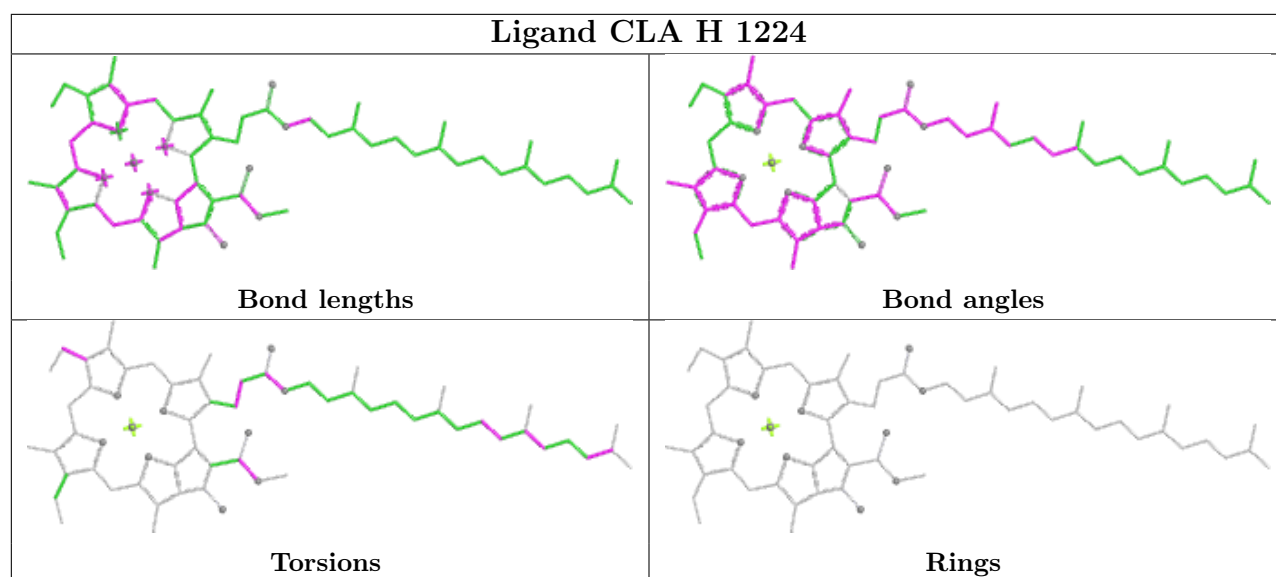
Ligand CLA B 1213

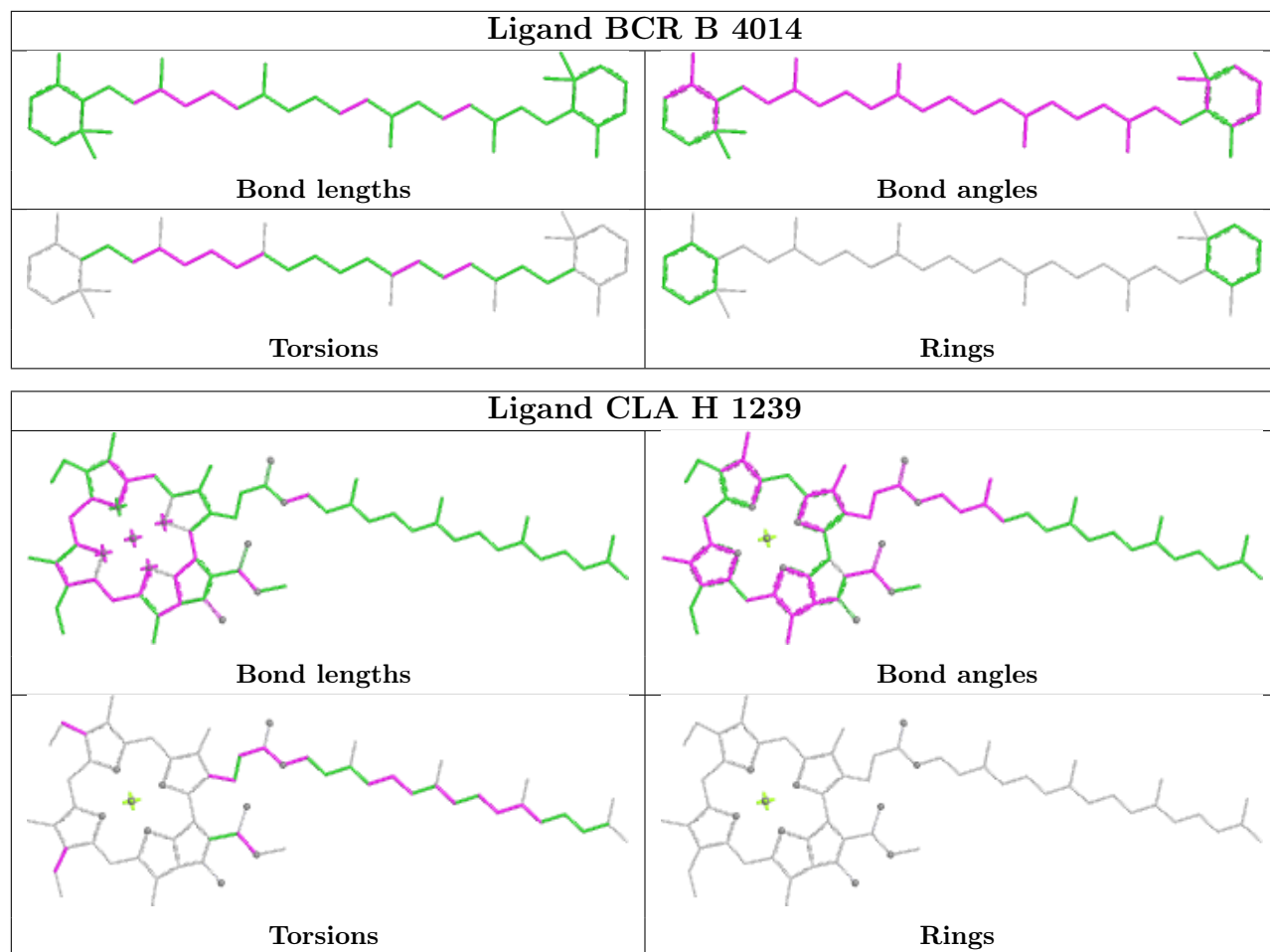


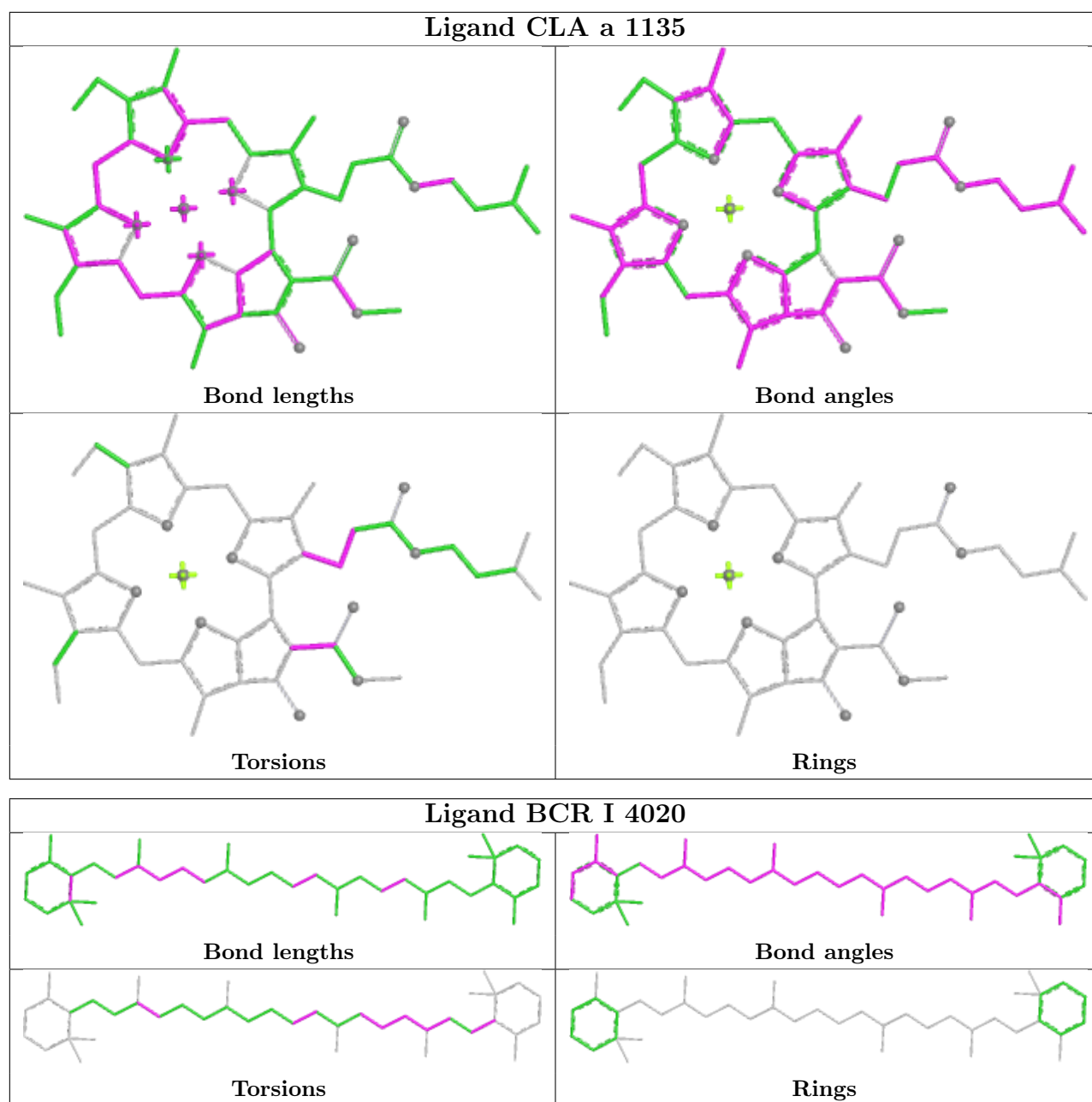


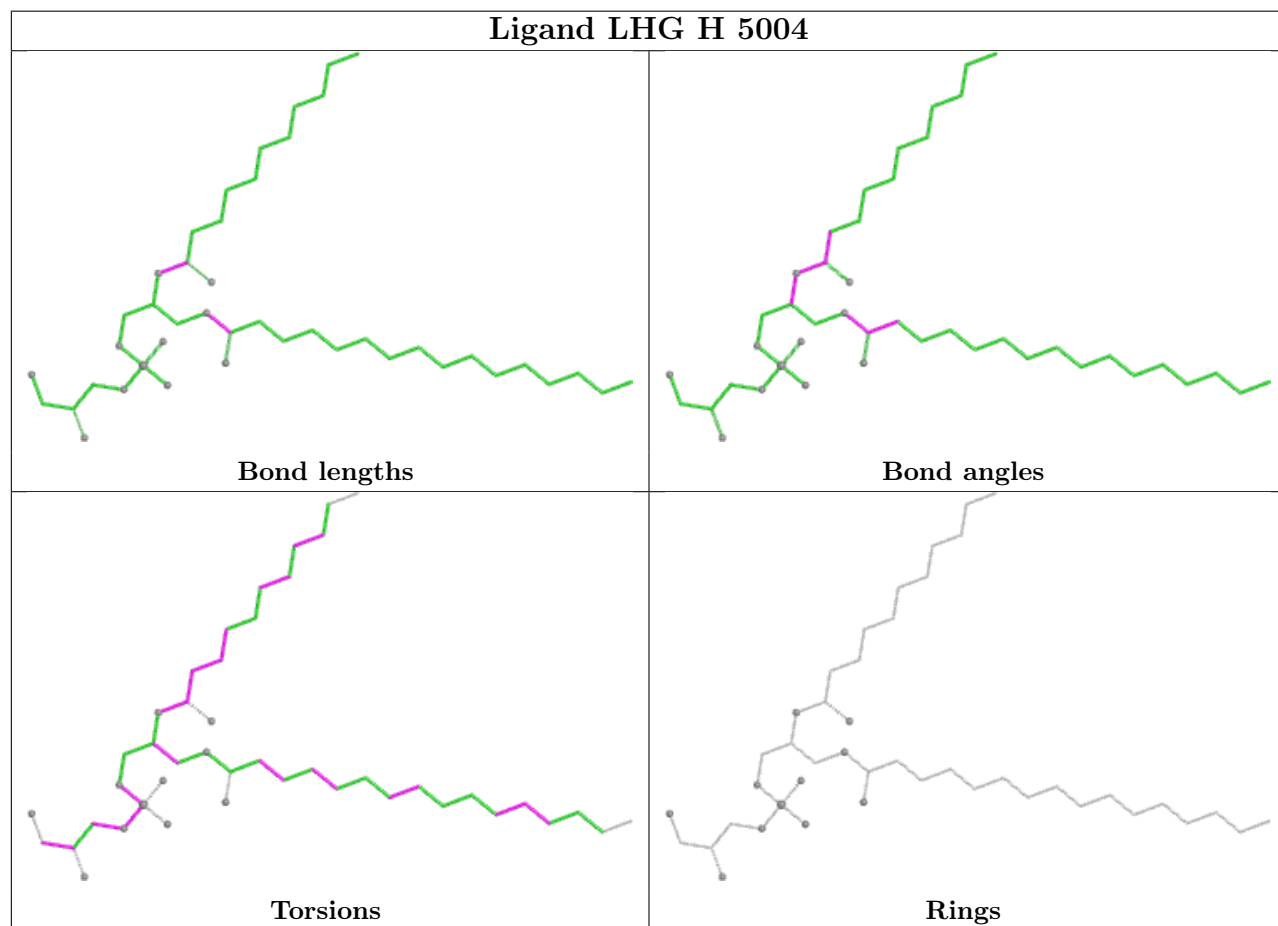
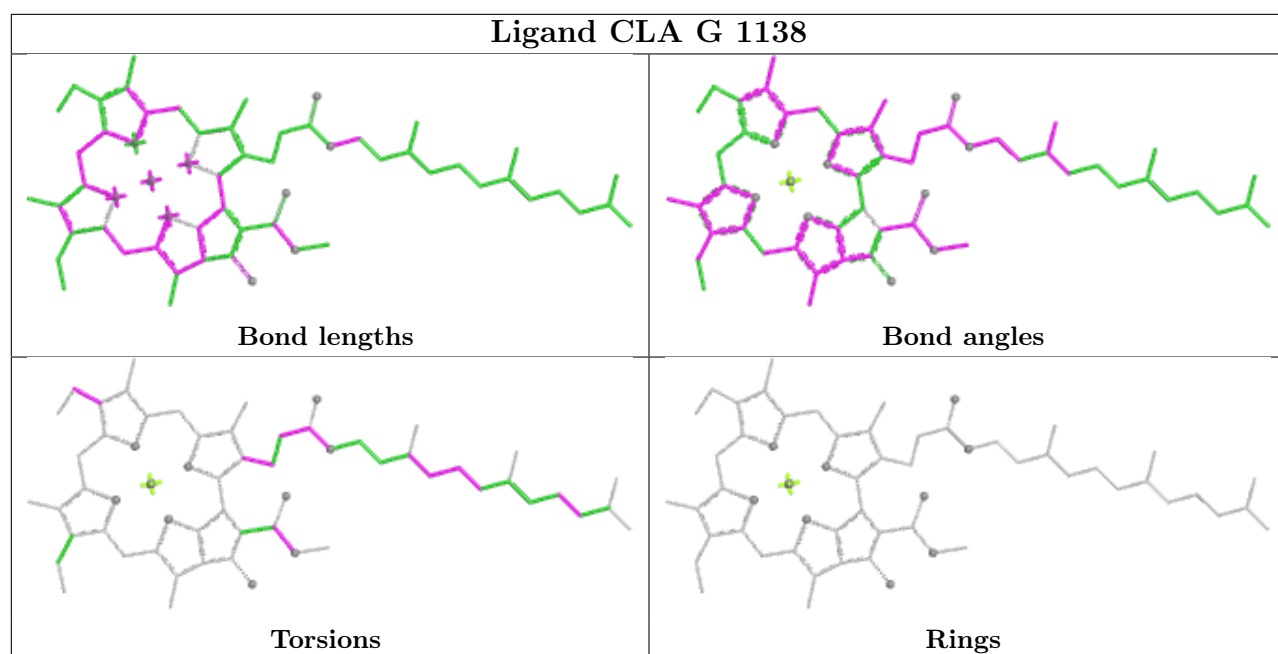


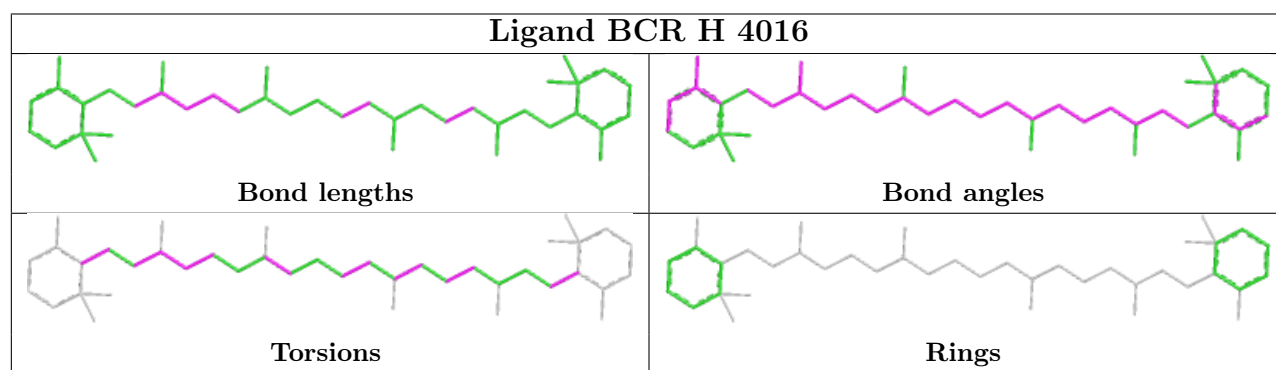
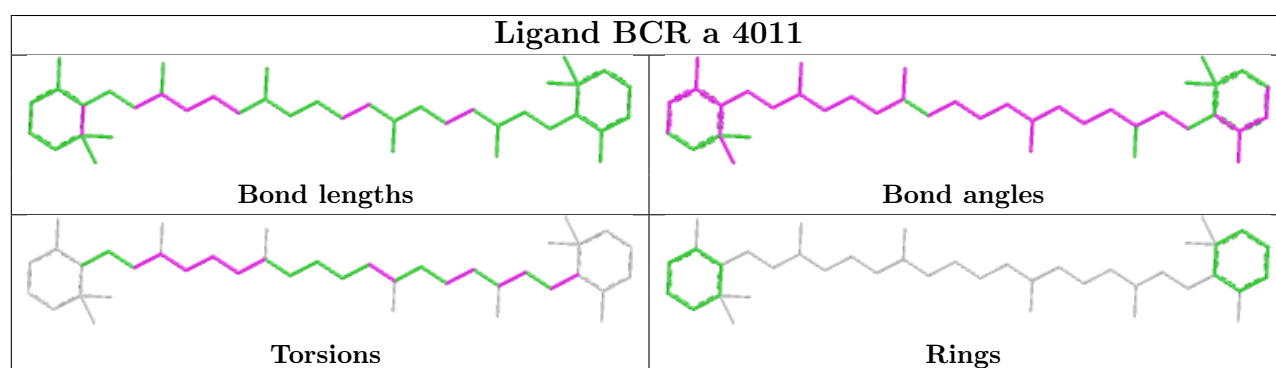
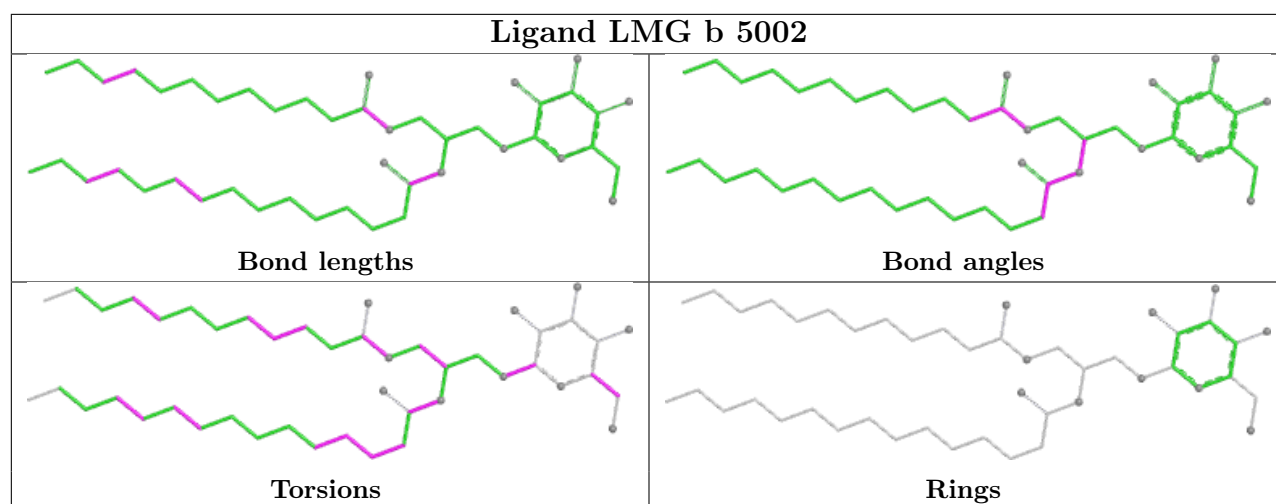


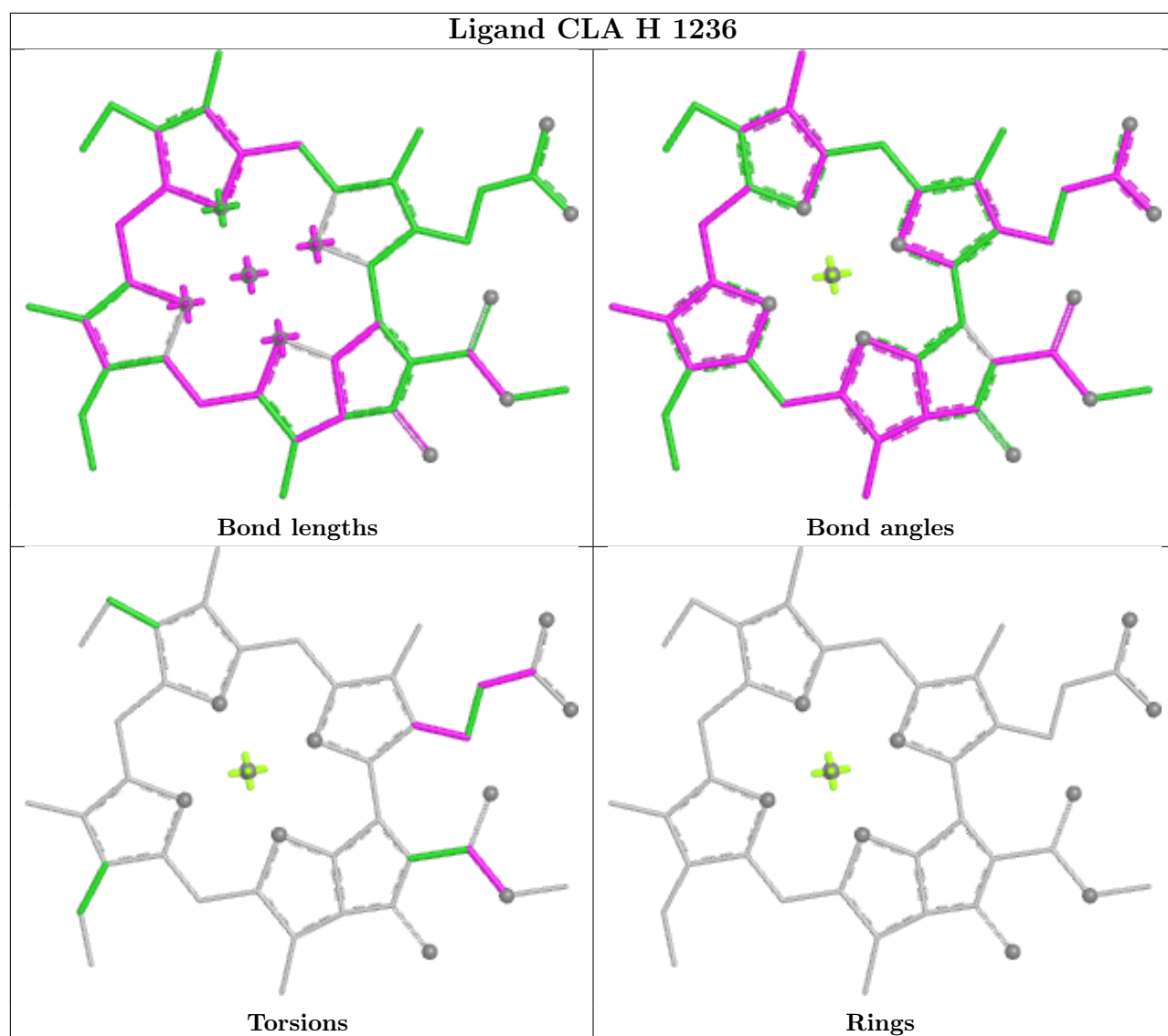


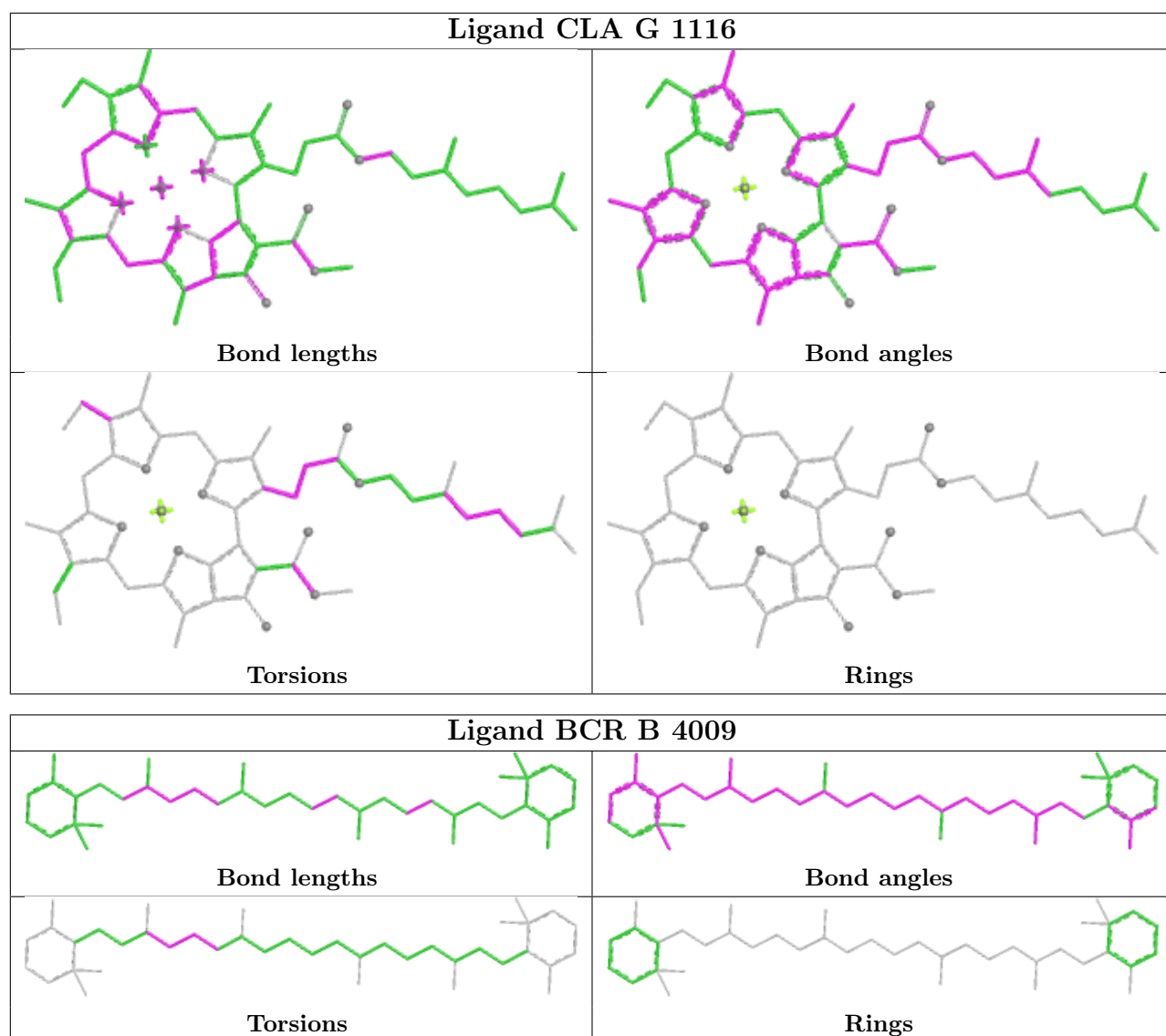


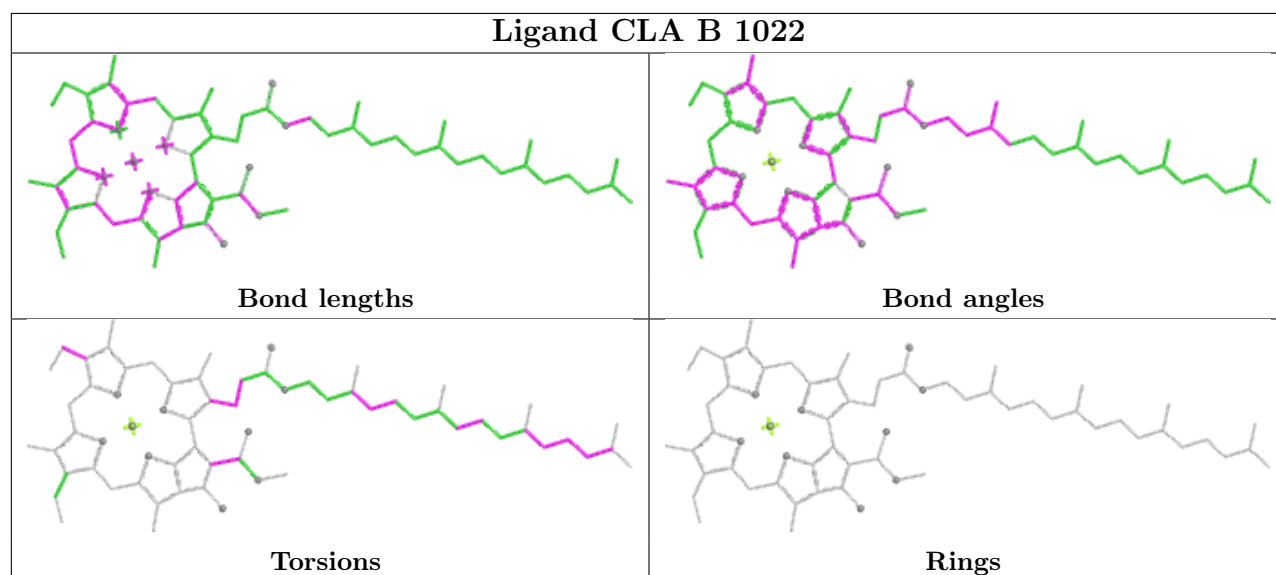
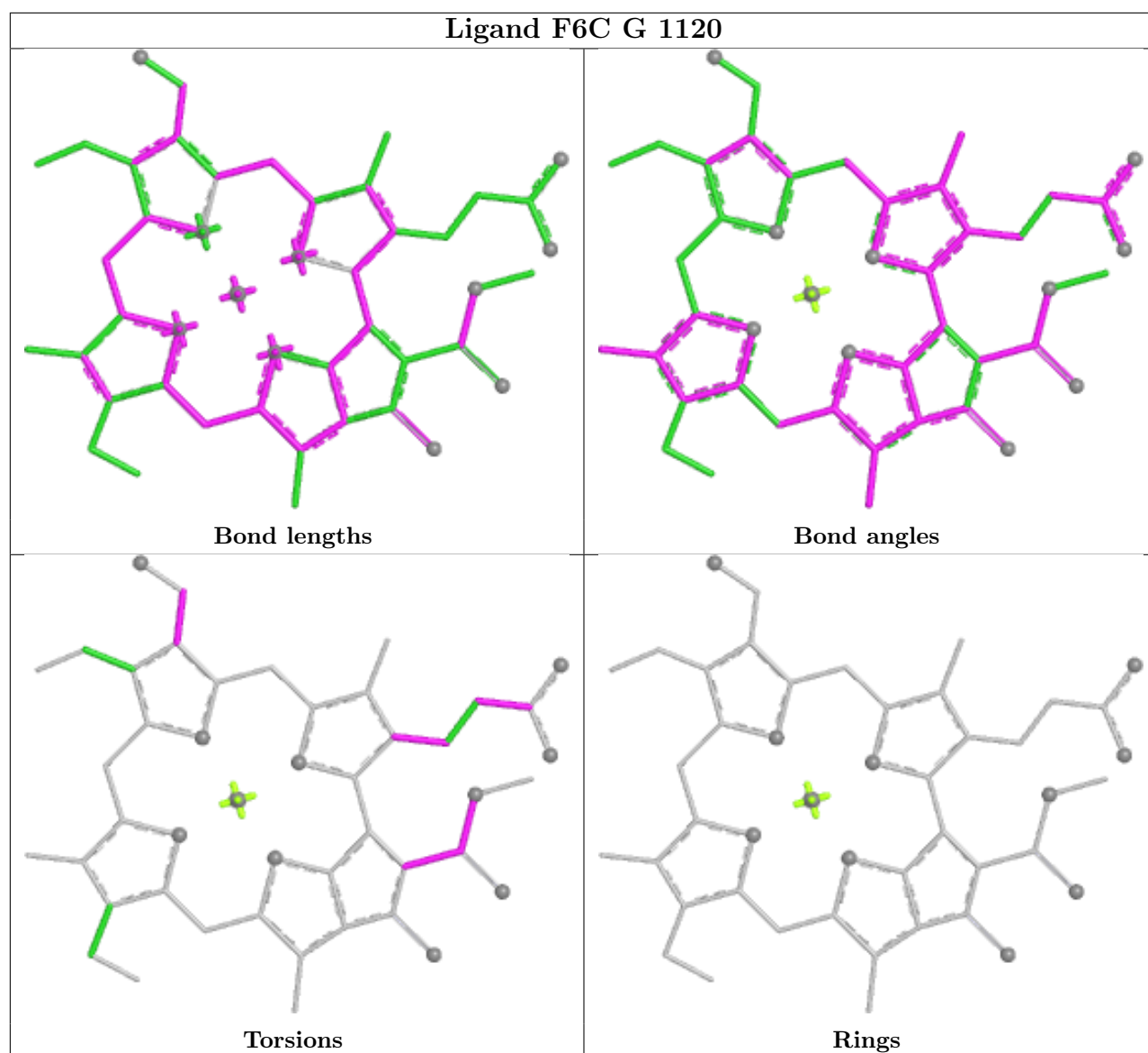


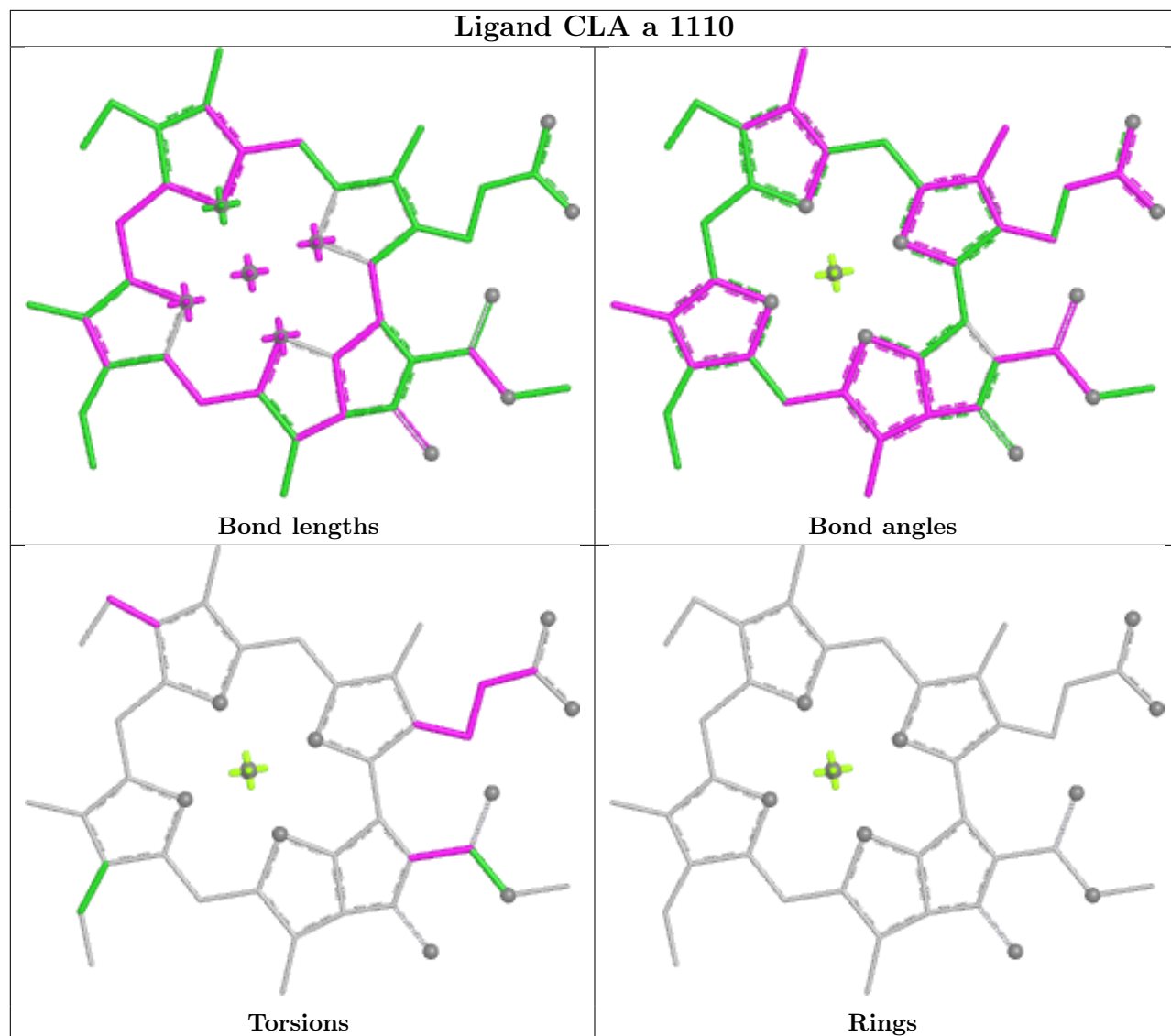




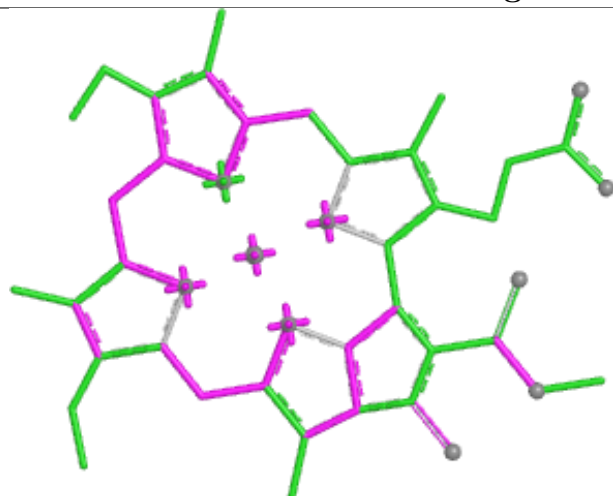




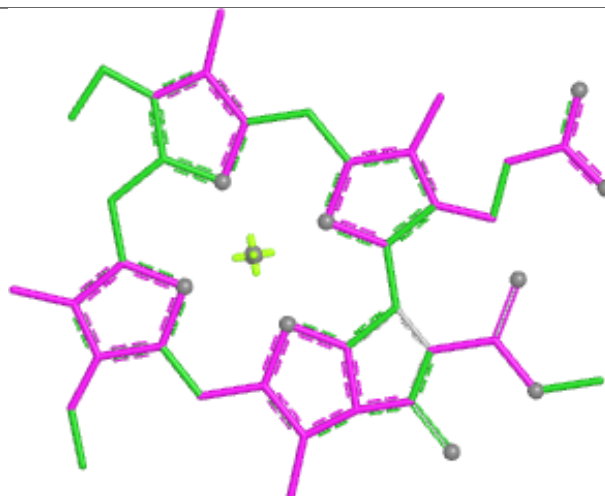




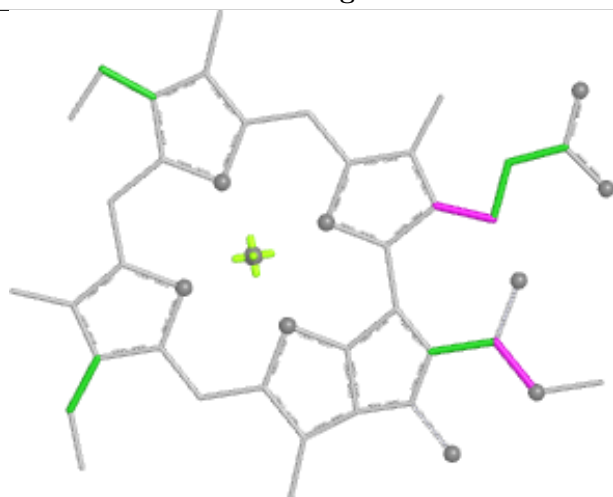
Ligand CLA G 1139



Bond lengths



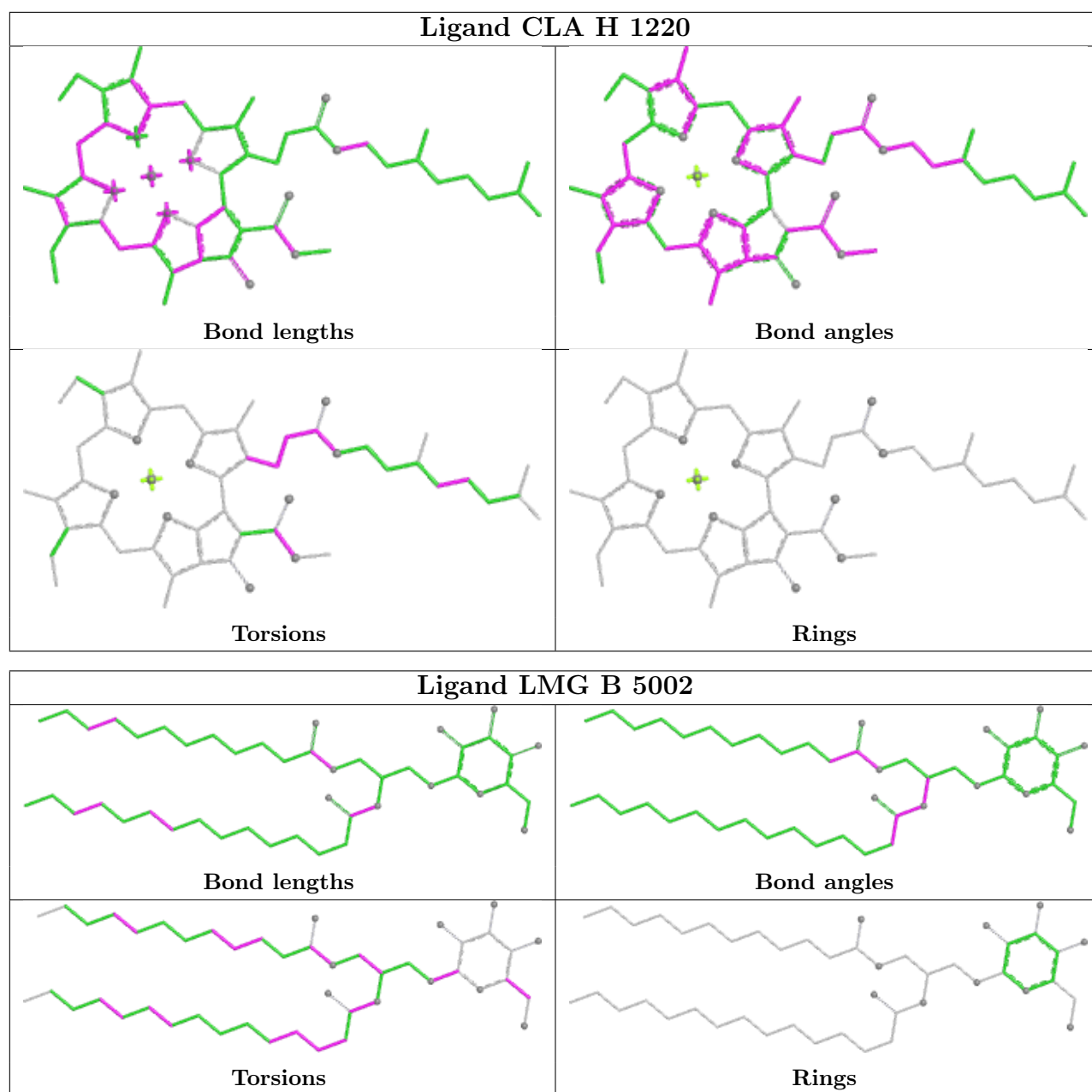
Bond angles



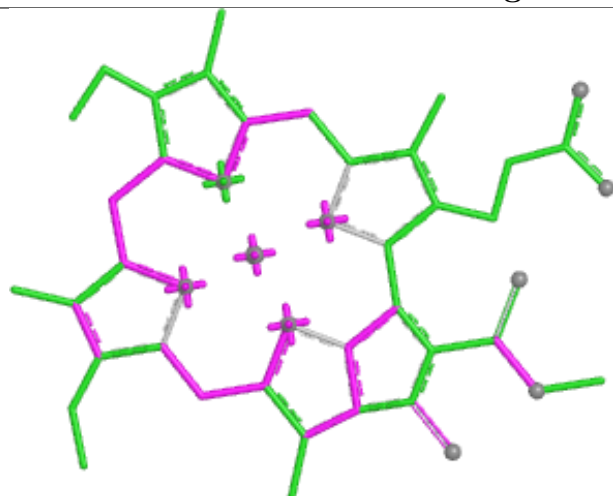
Torsions



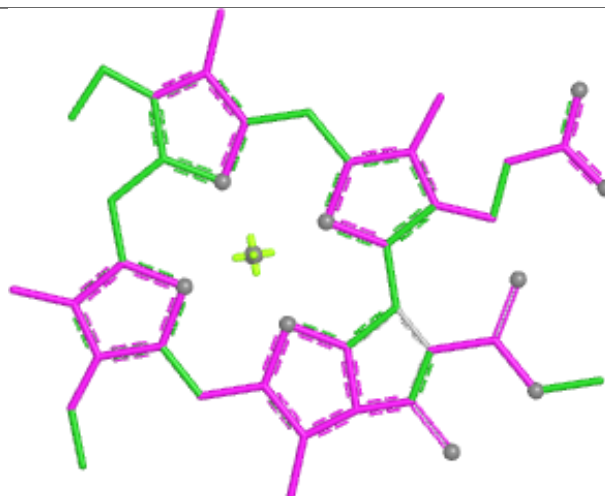
Rings



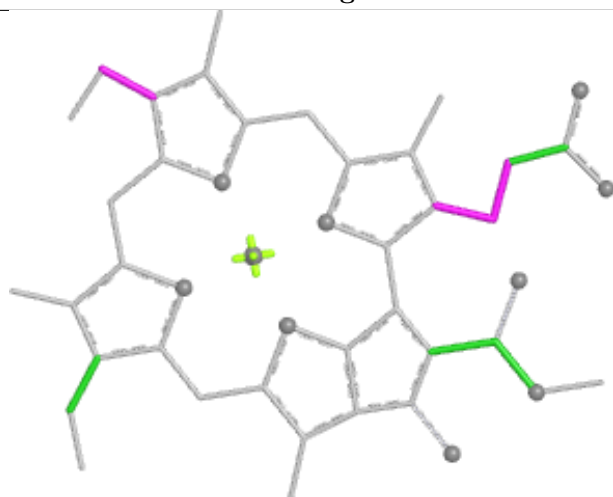
Ligand CLA G 1129



Bond lengths



Bond angles

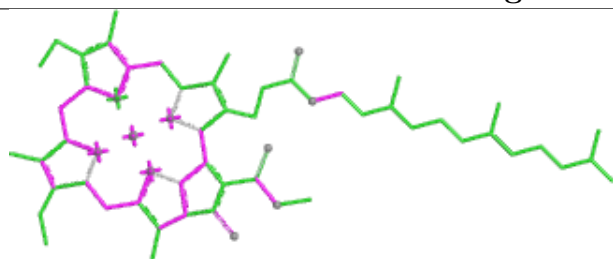


Torsions

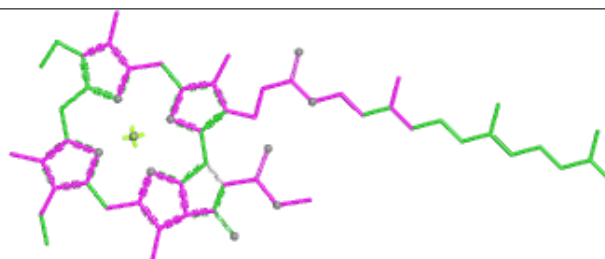


Rings

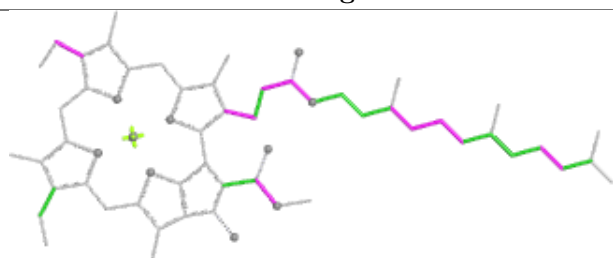
Ligand CLA A 1138



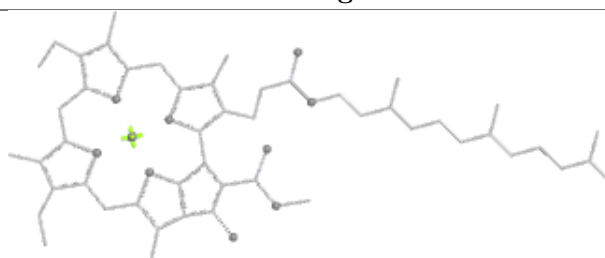
Bond lengths



Bond angles

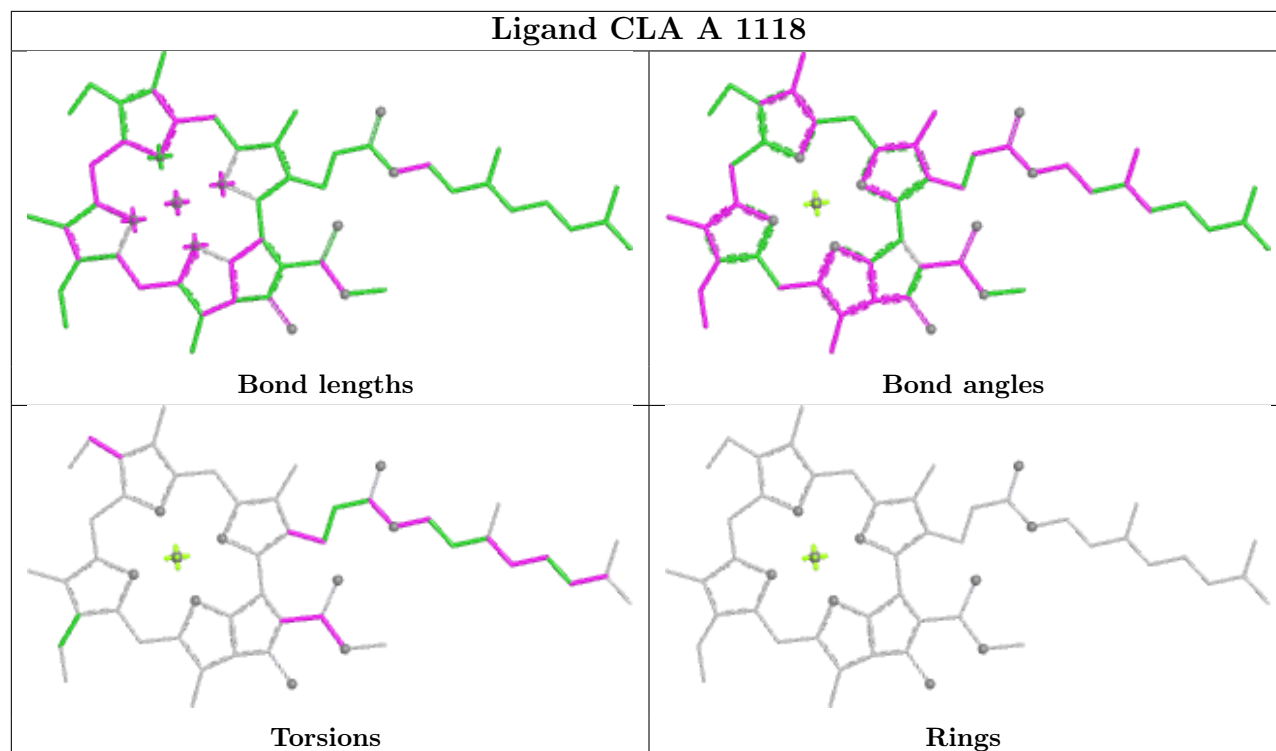


Torsions

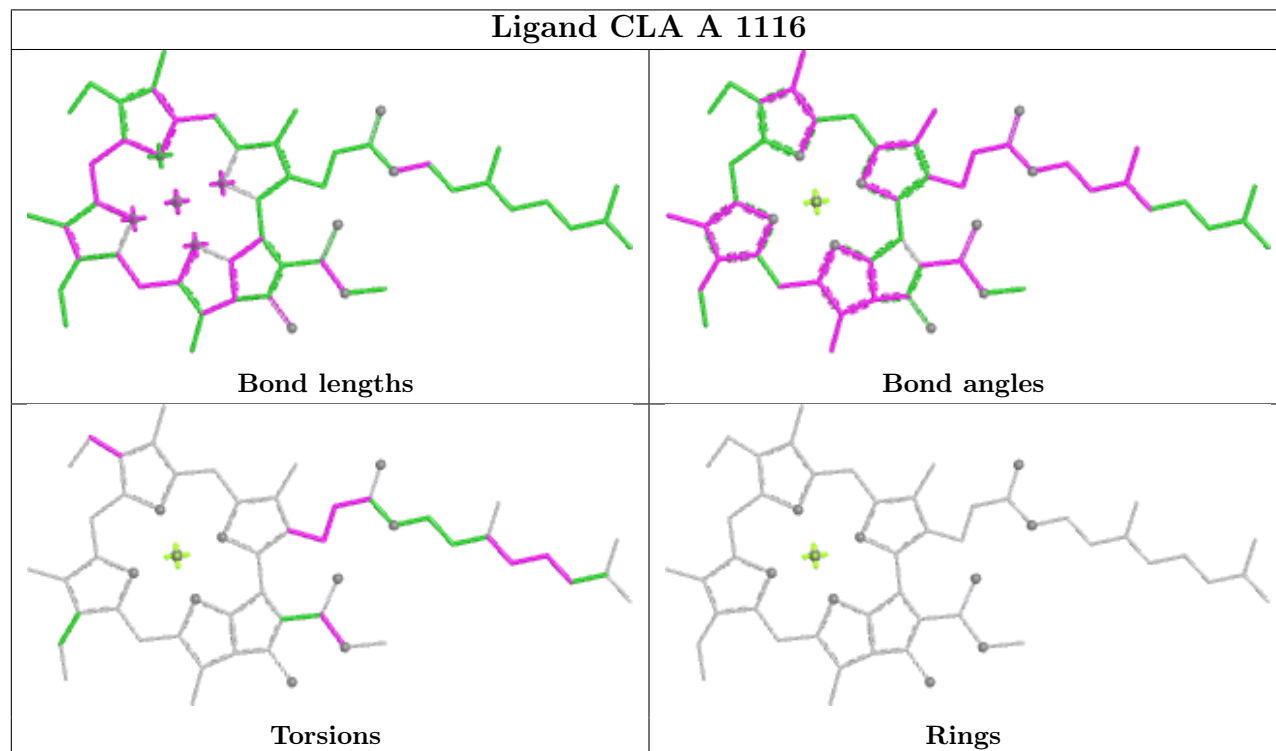


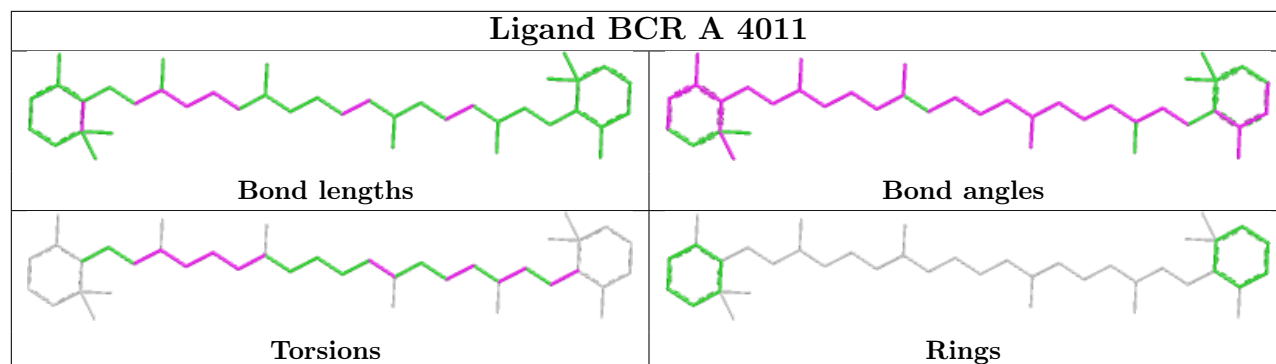
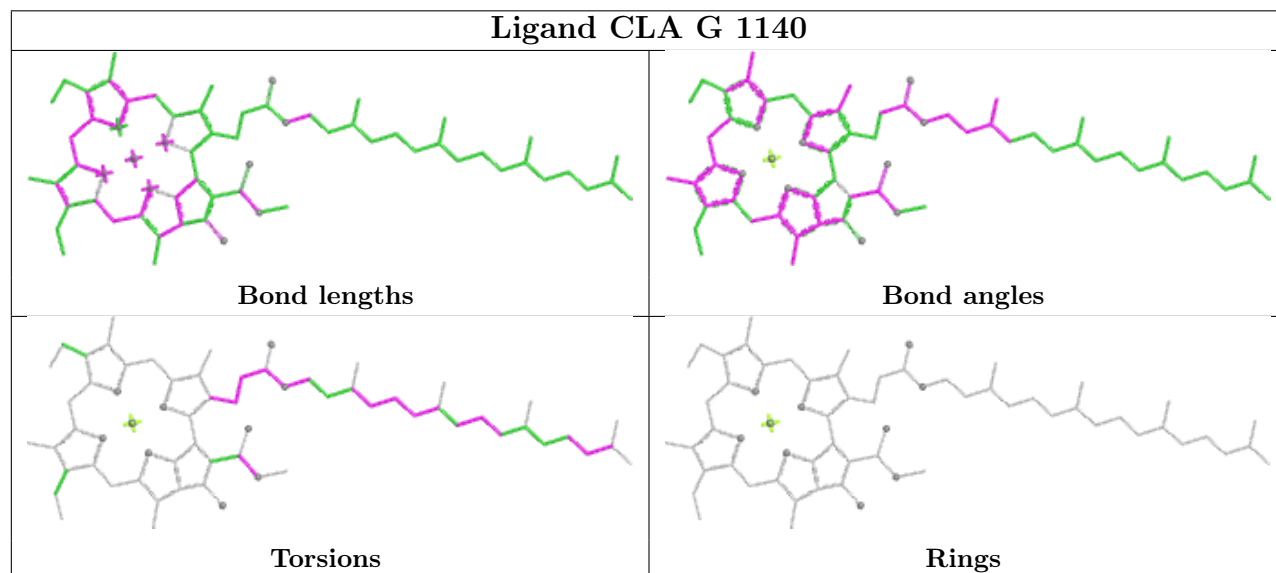
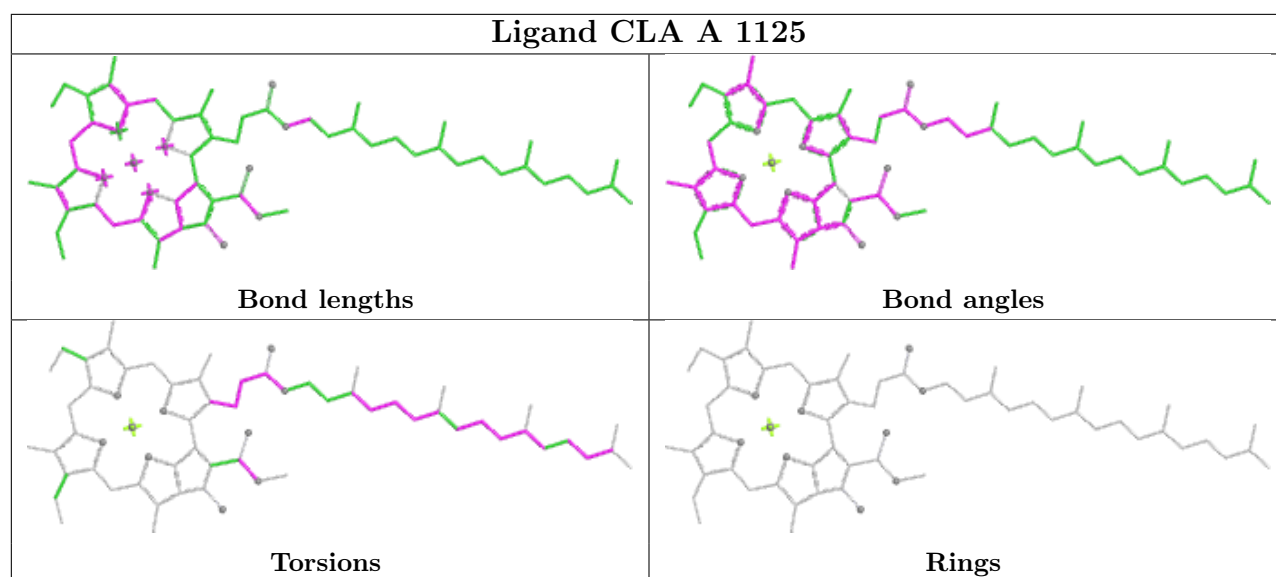
Rings

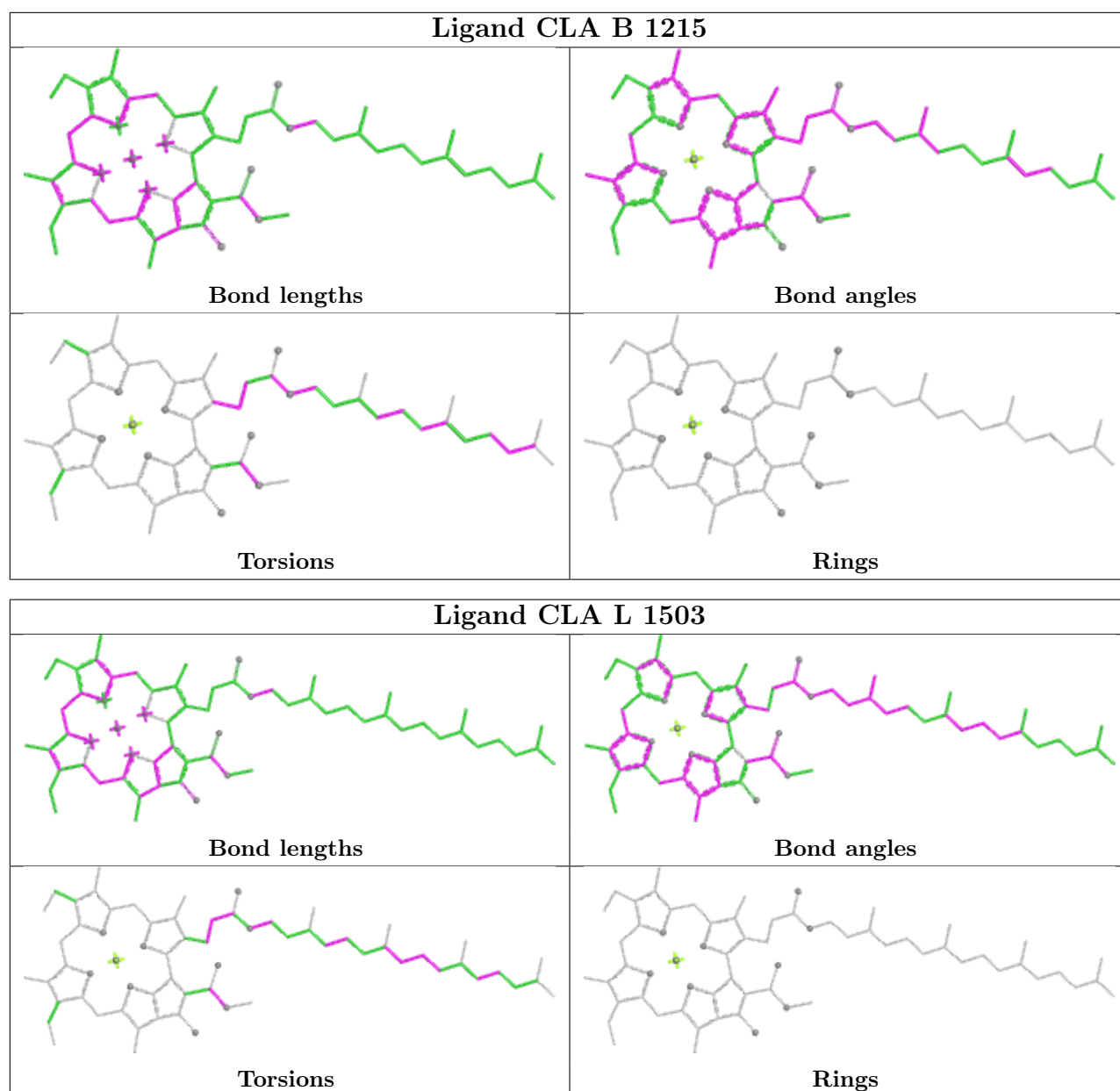
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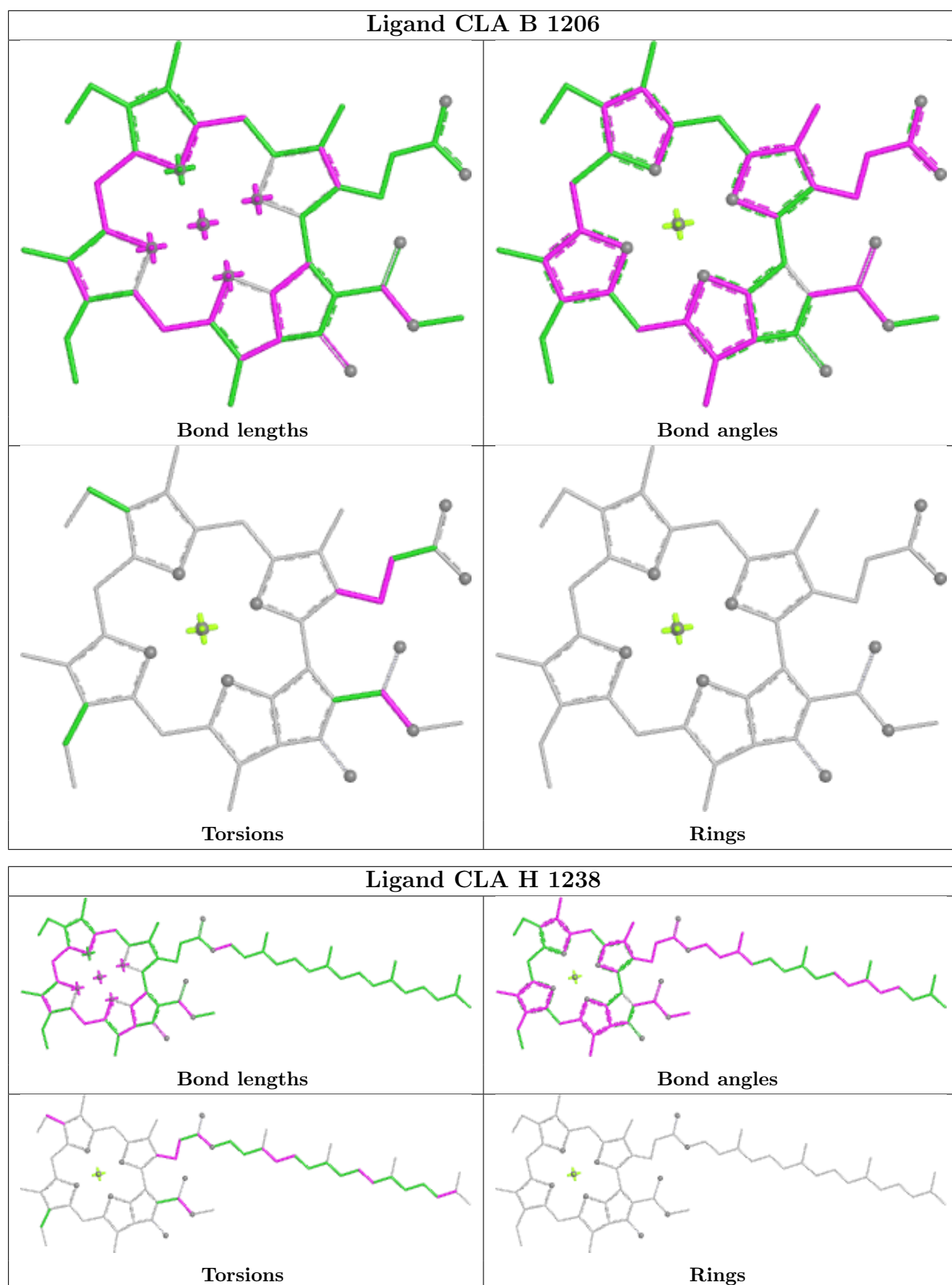


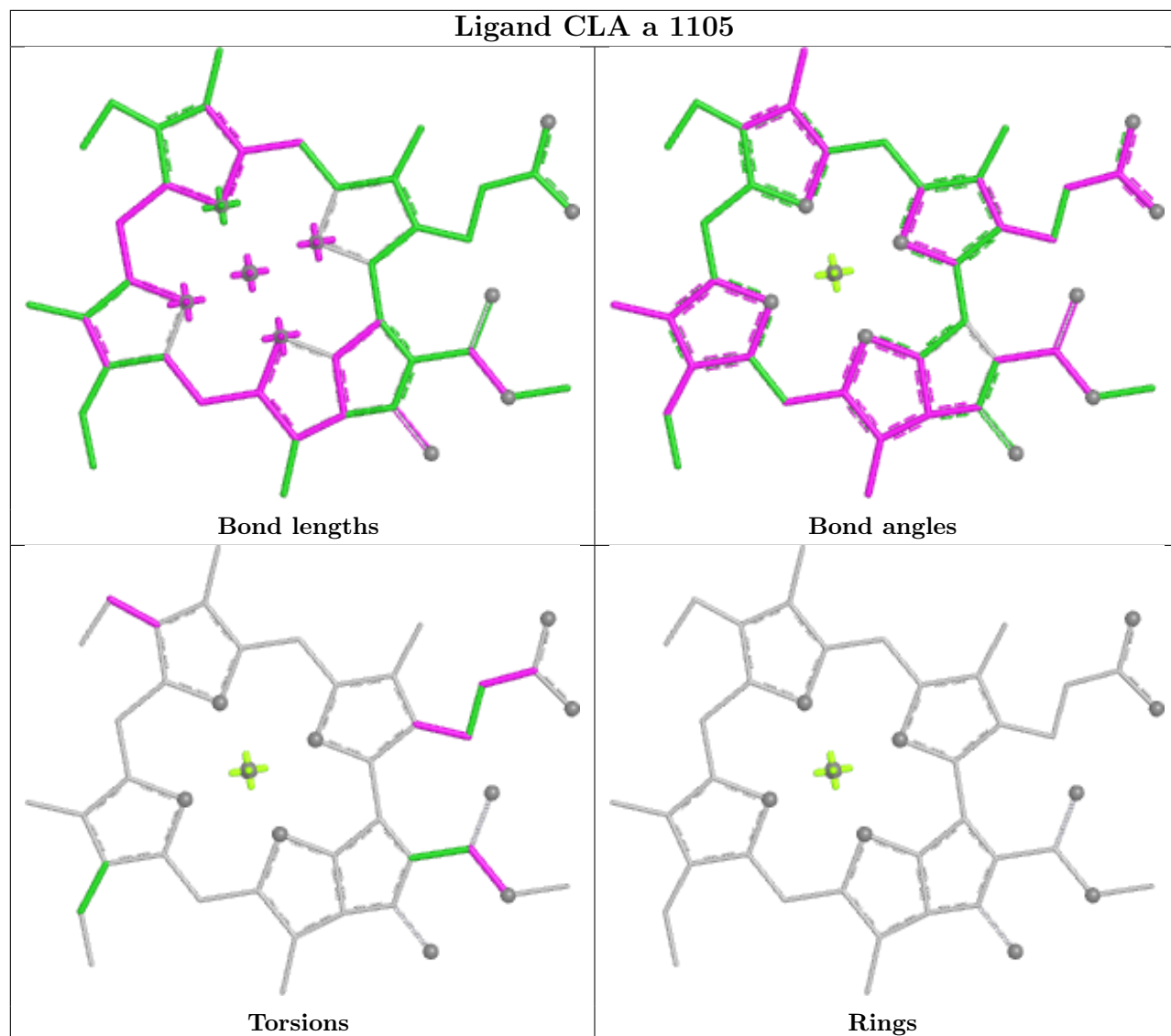
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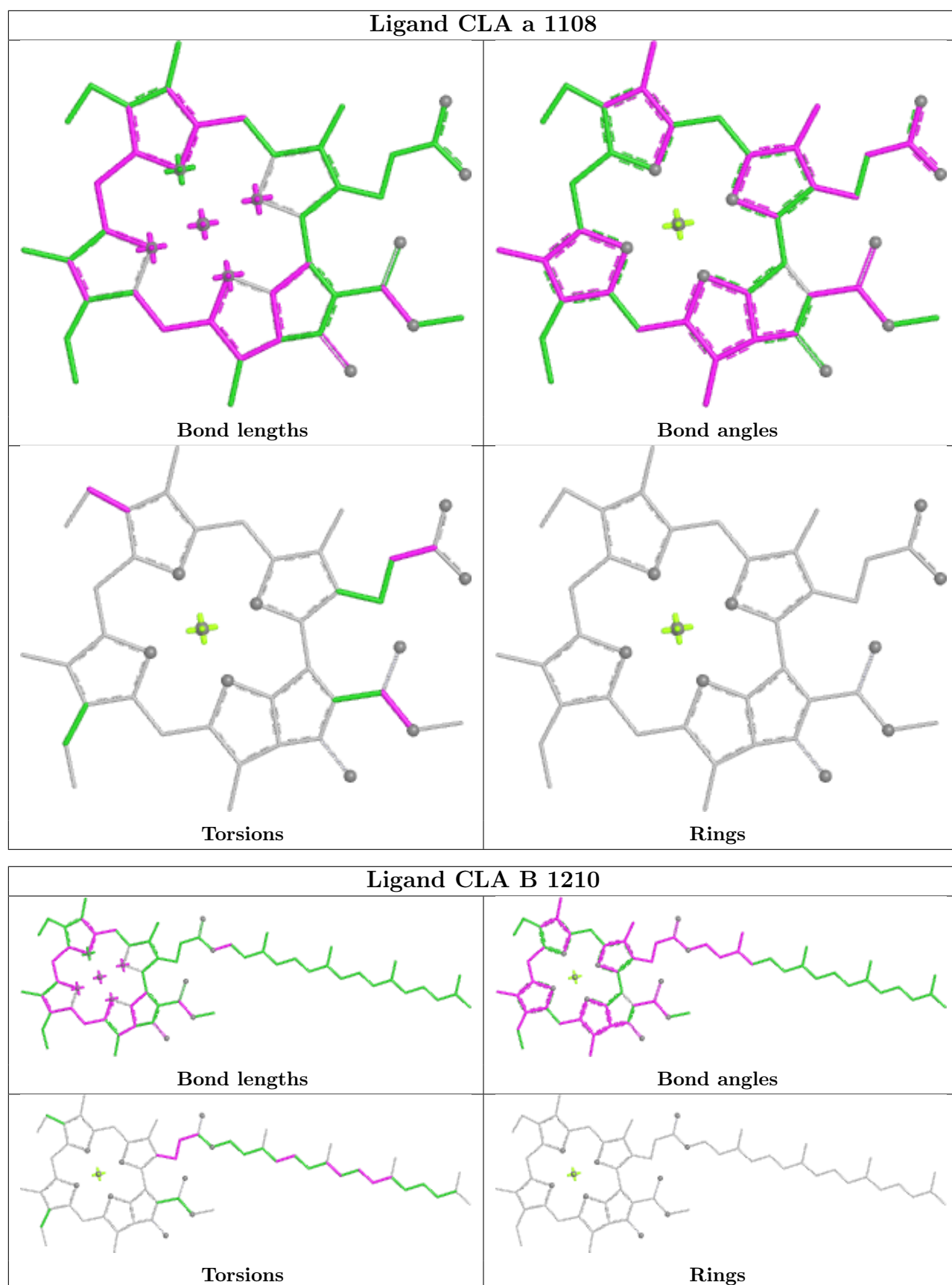


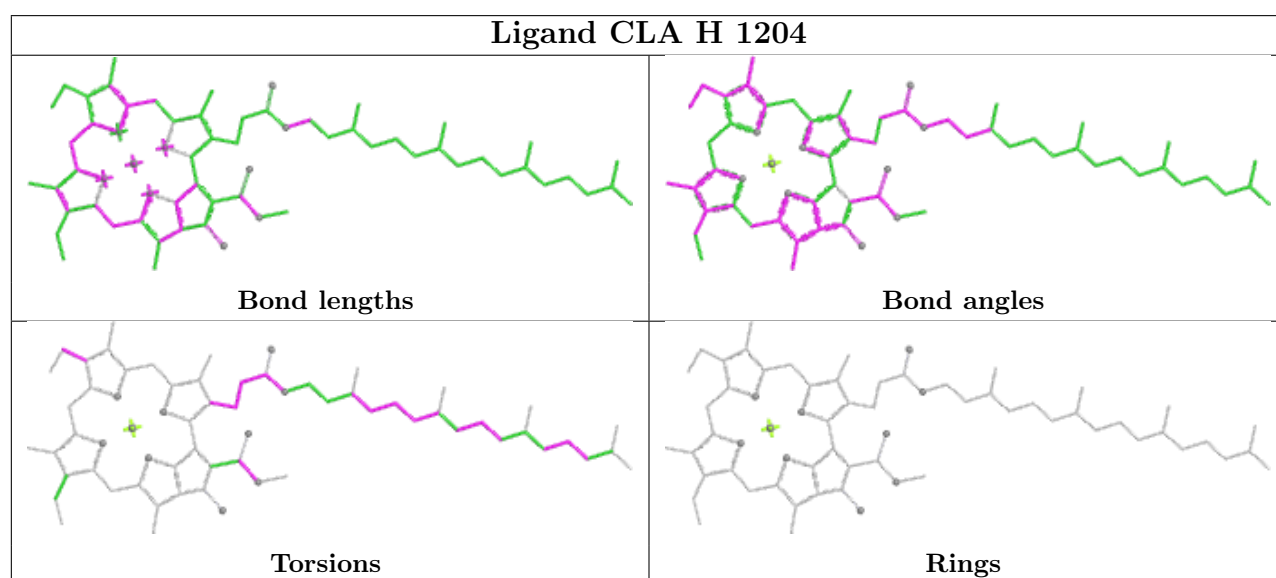
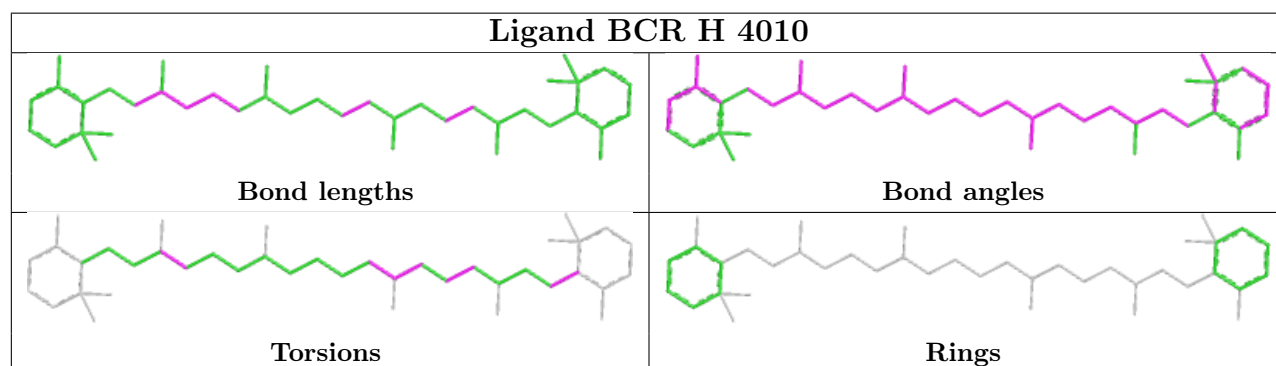
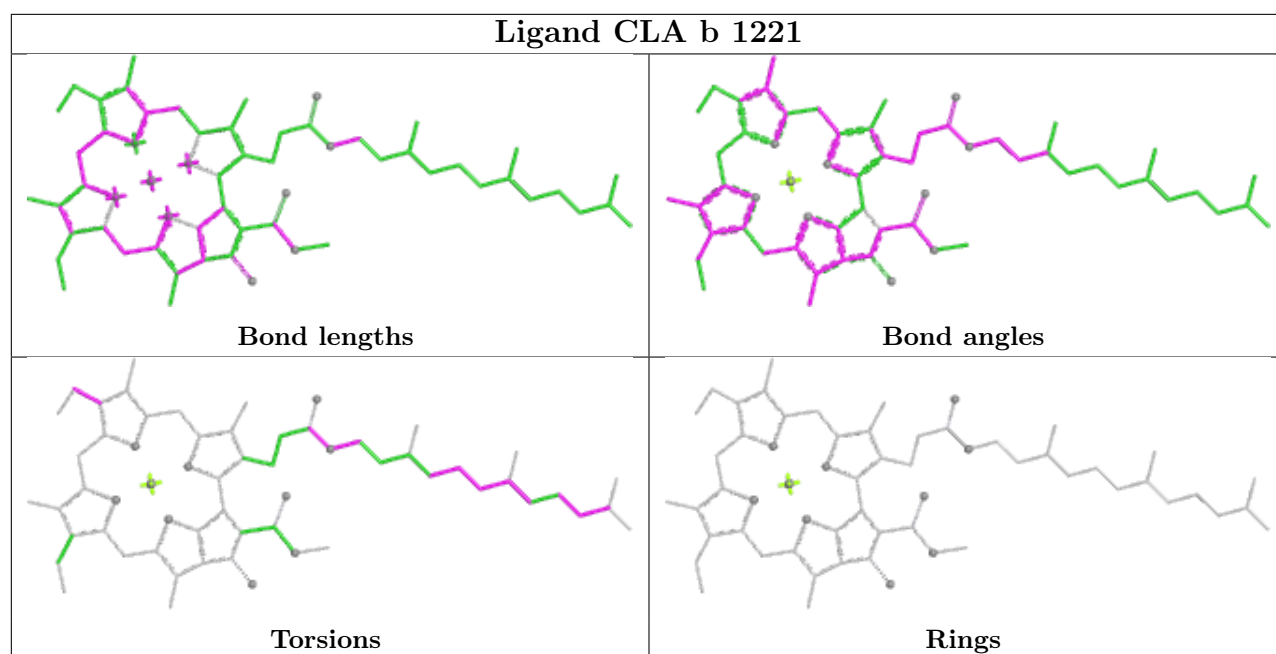


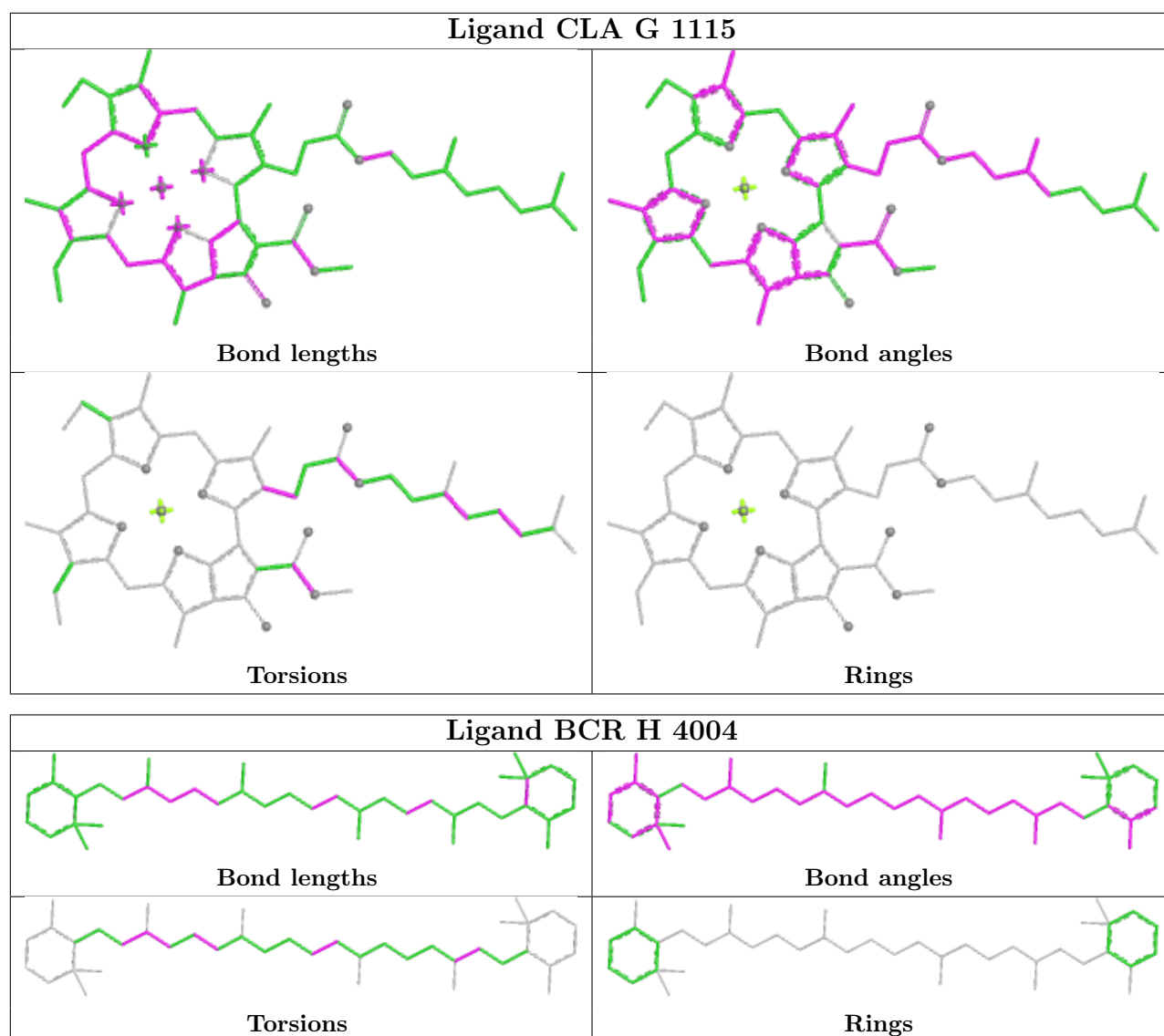


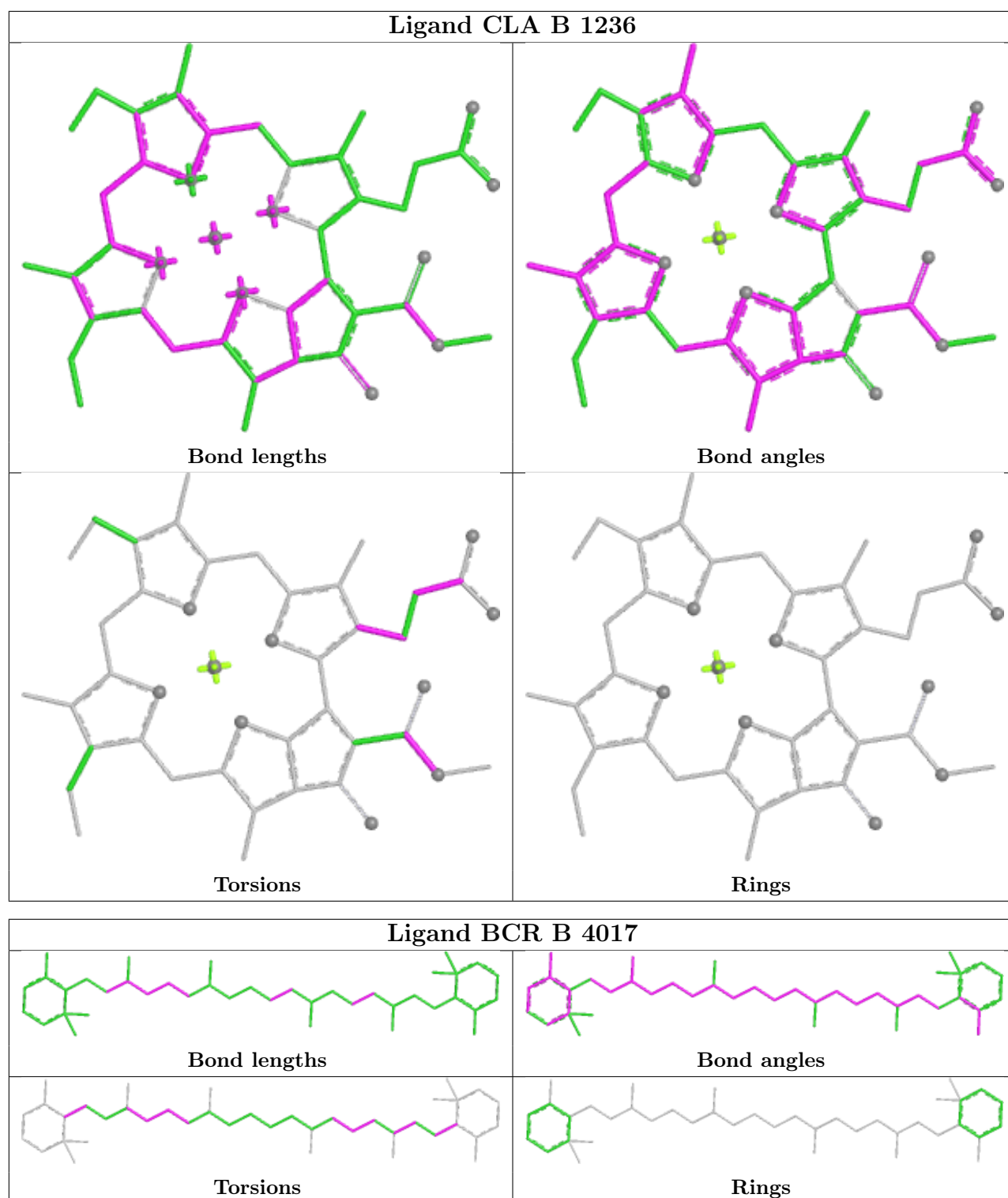


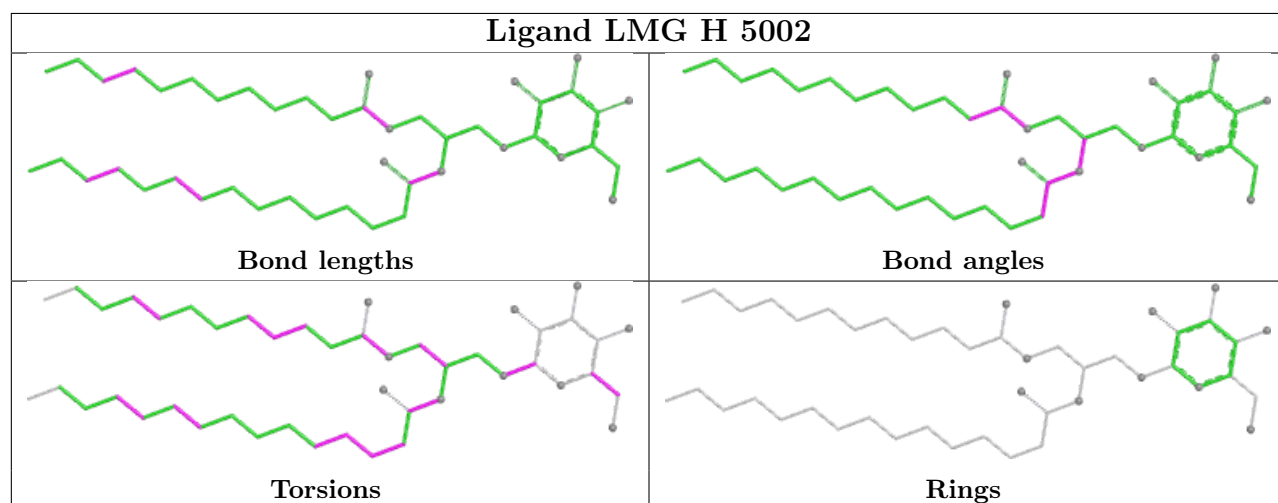
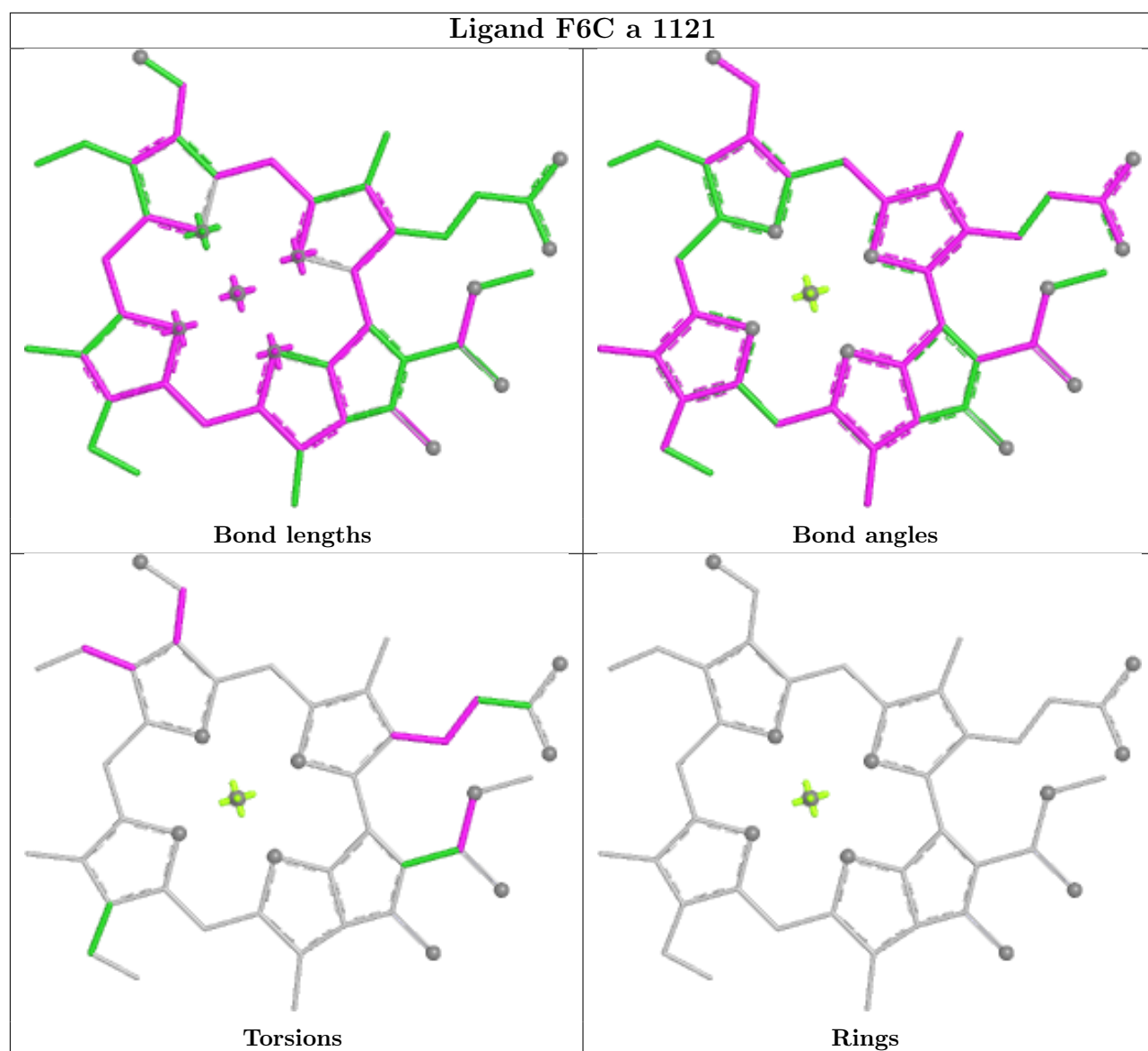


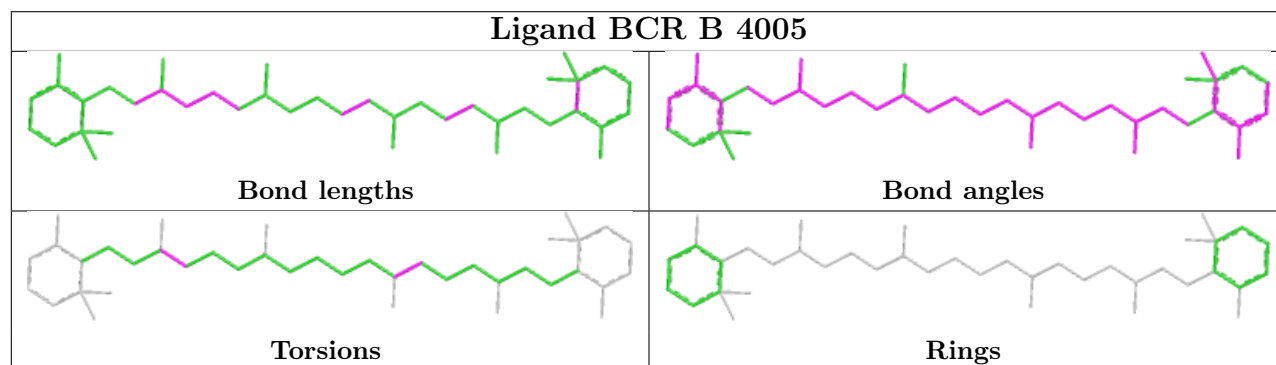
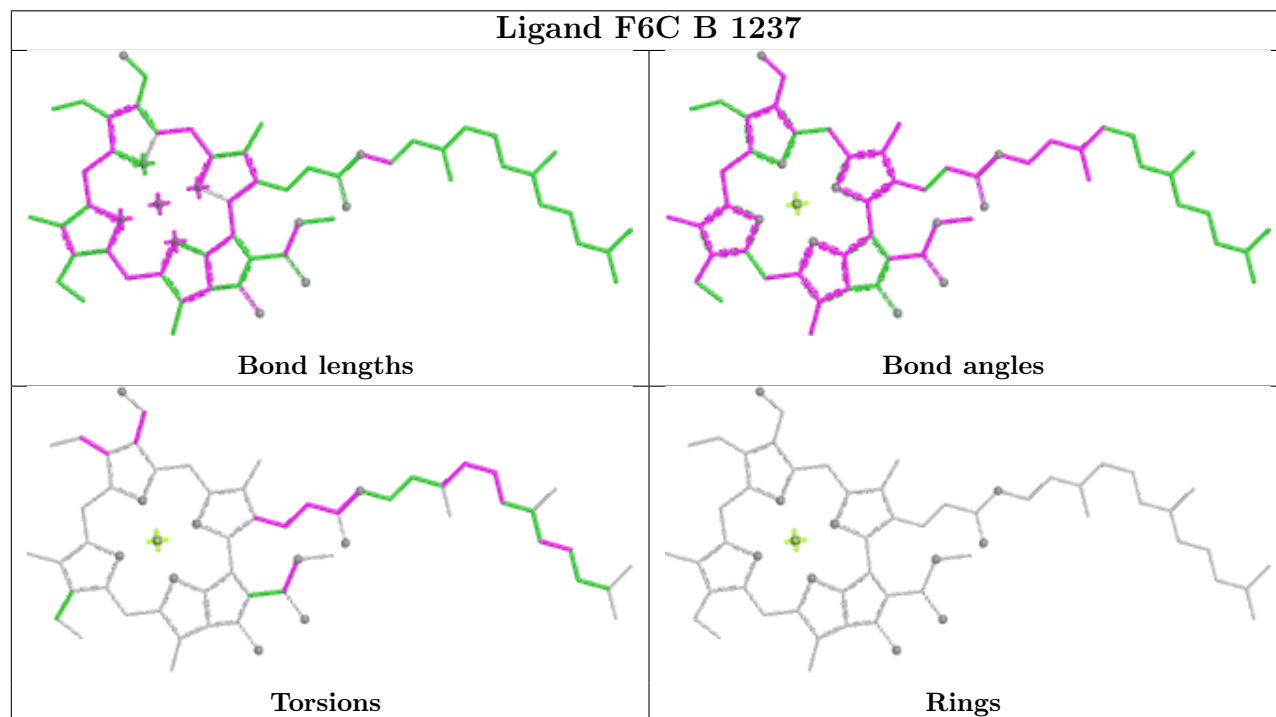
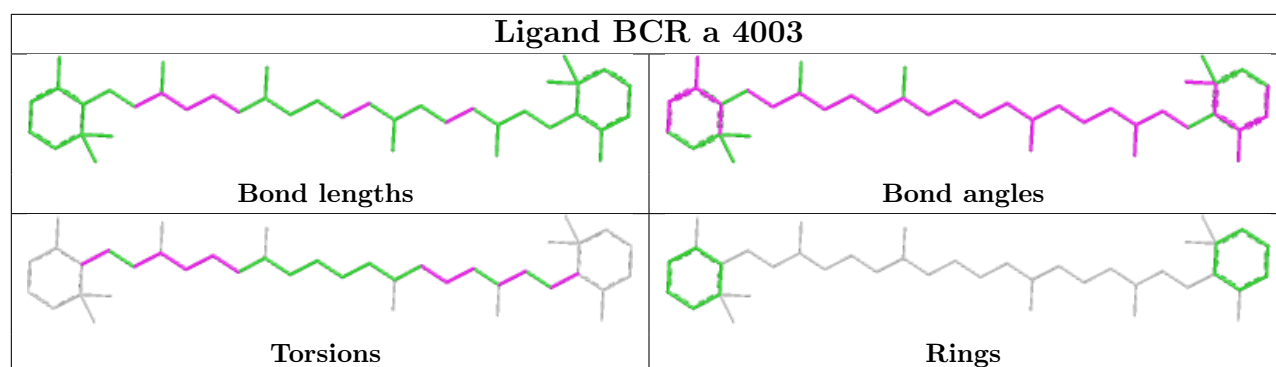


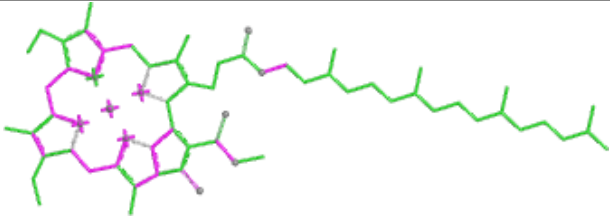
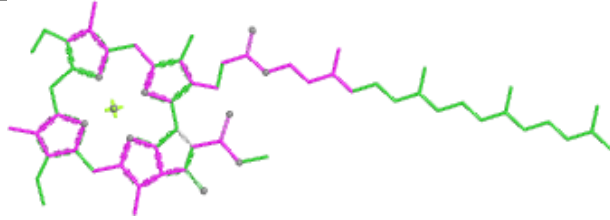
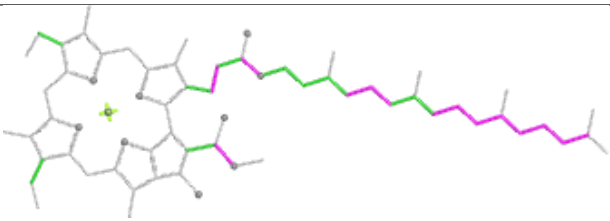
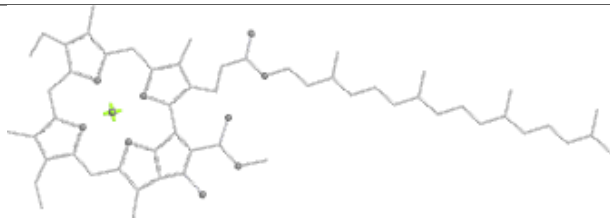
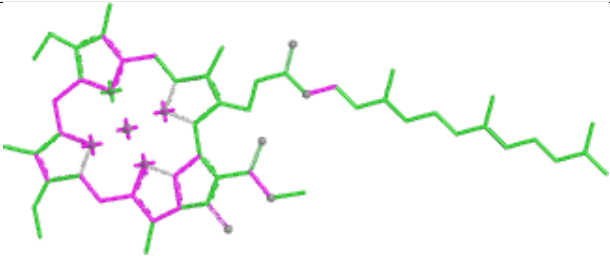
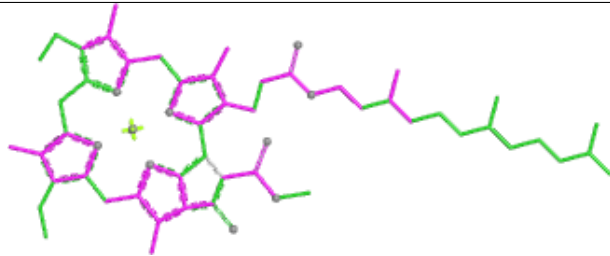
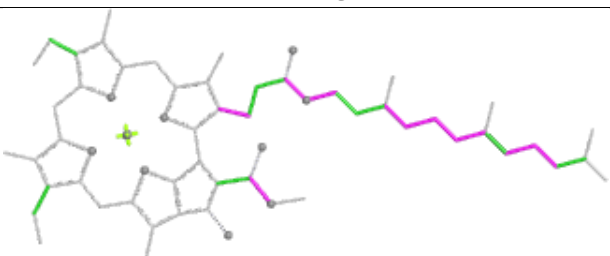
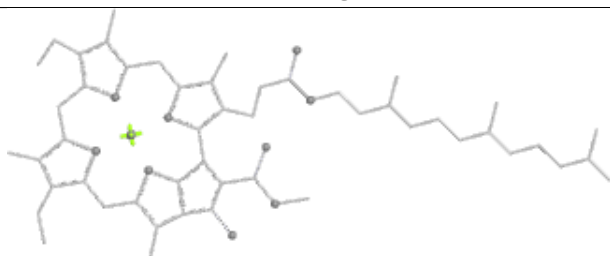
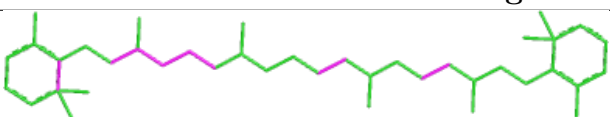
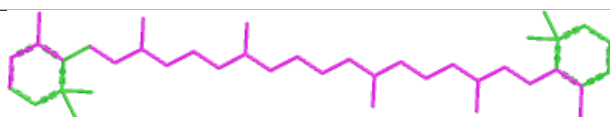
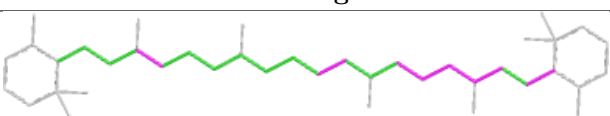
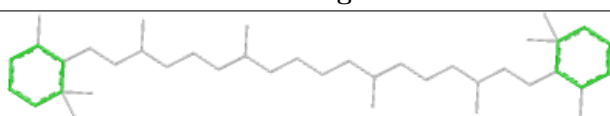


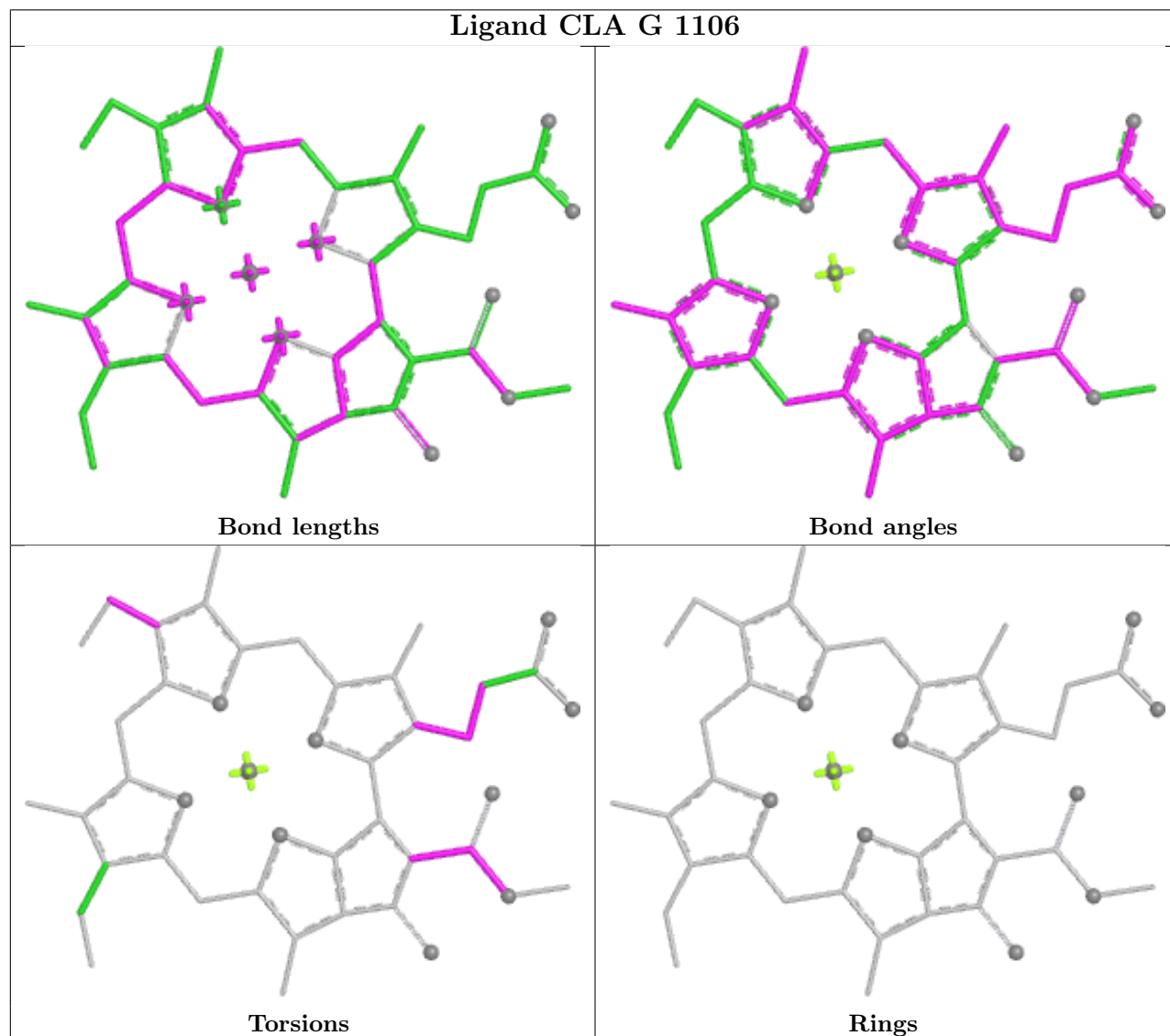
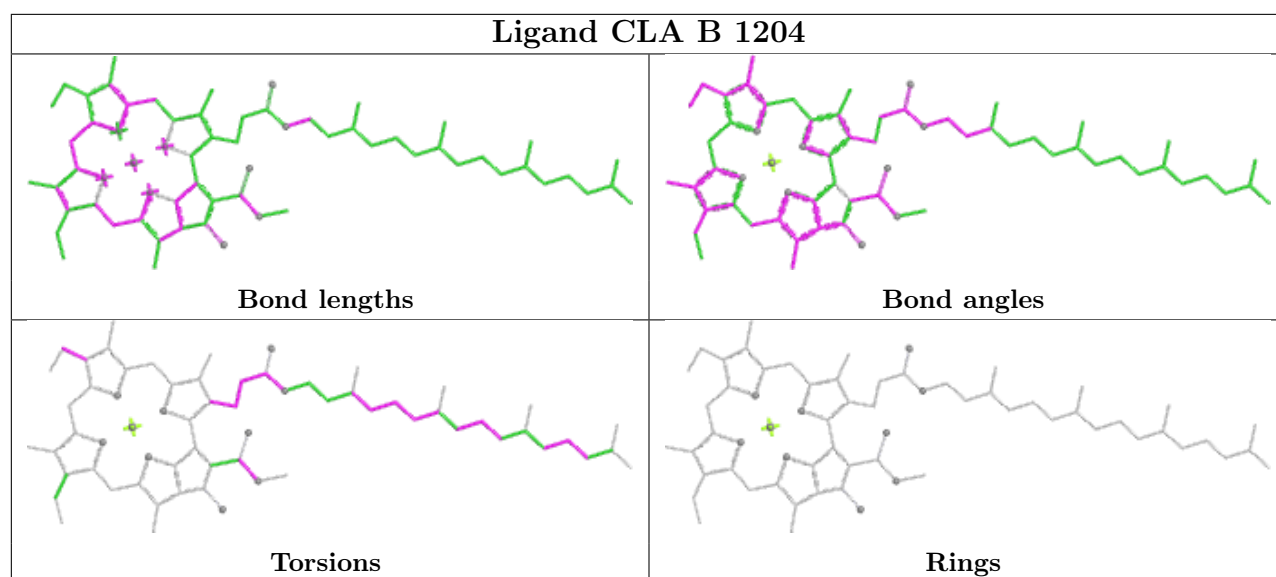


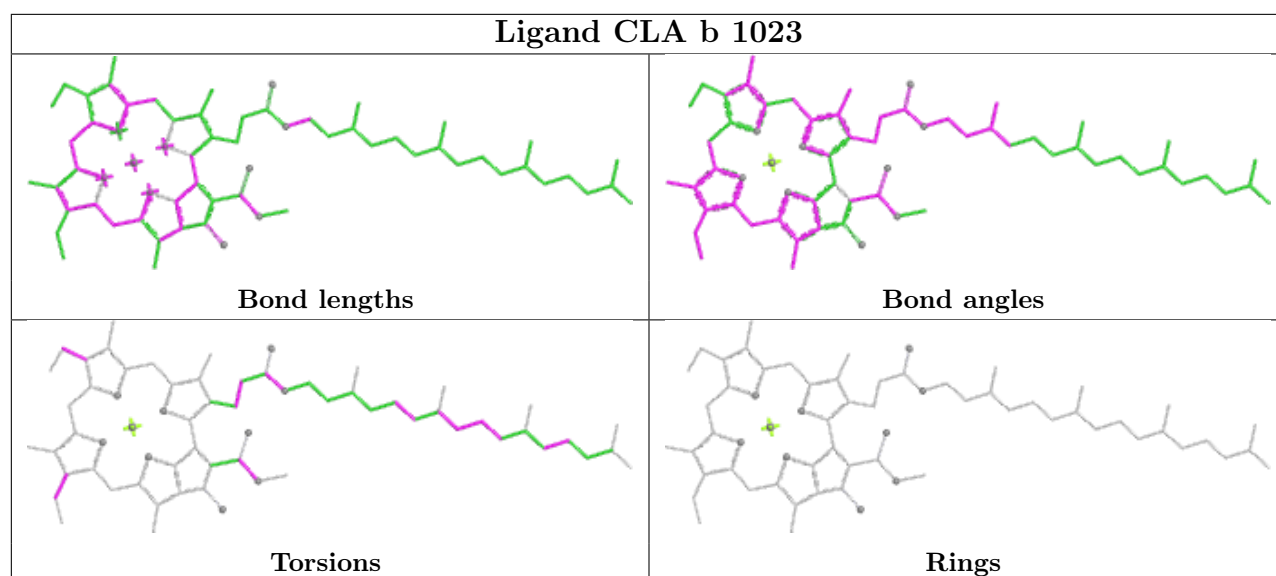
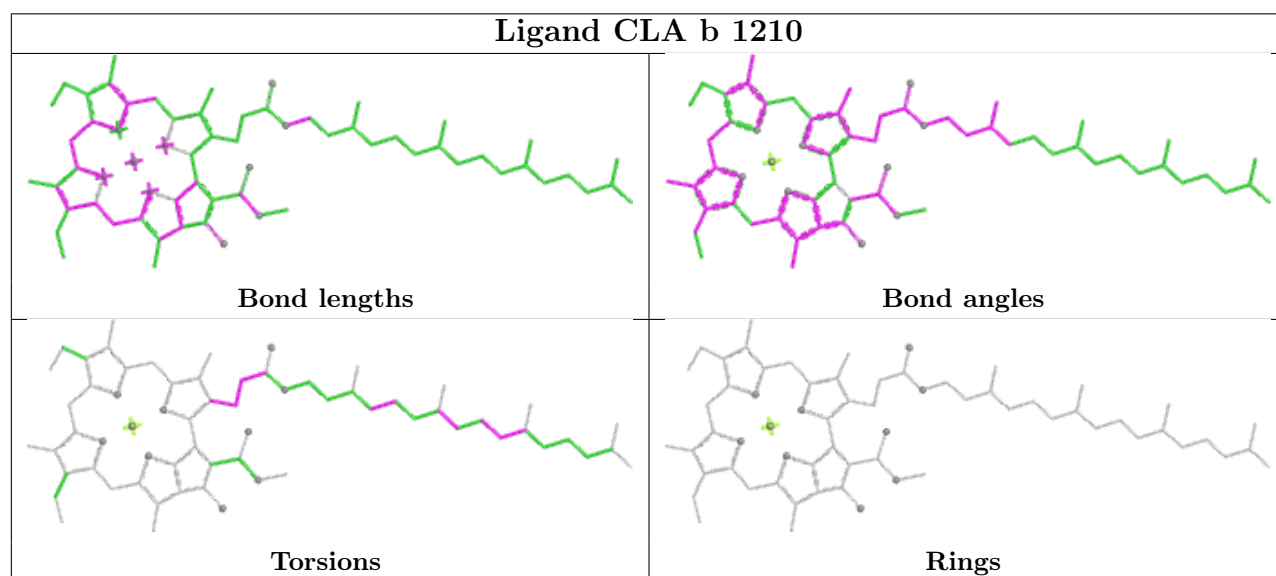
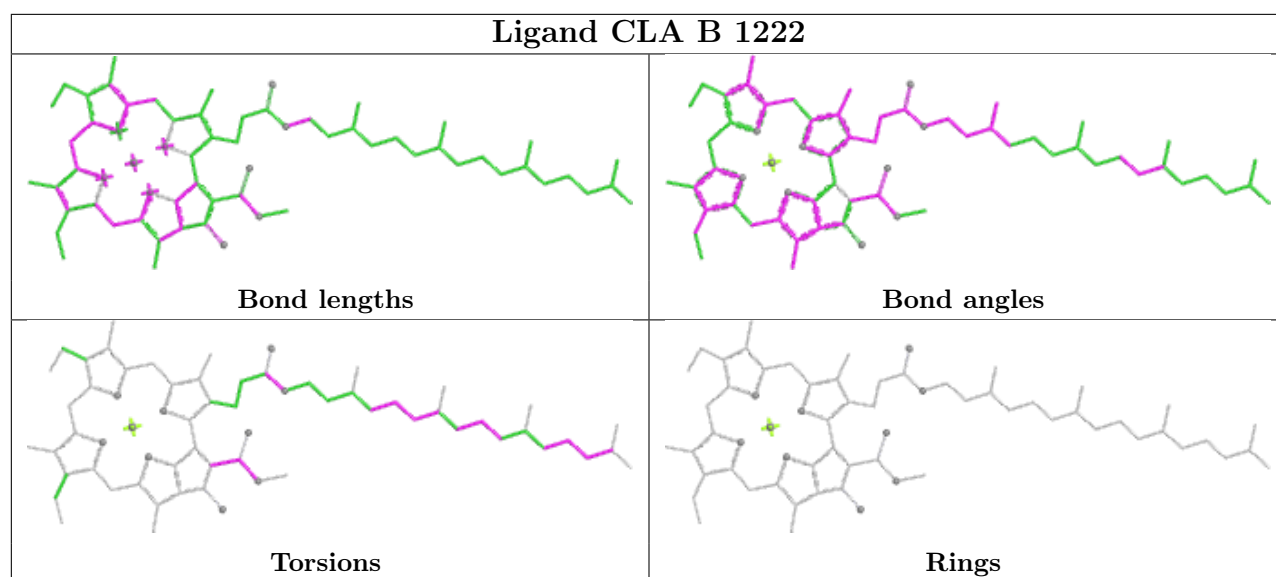


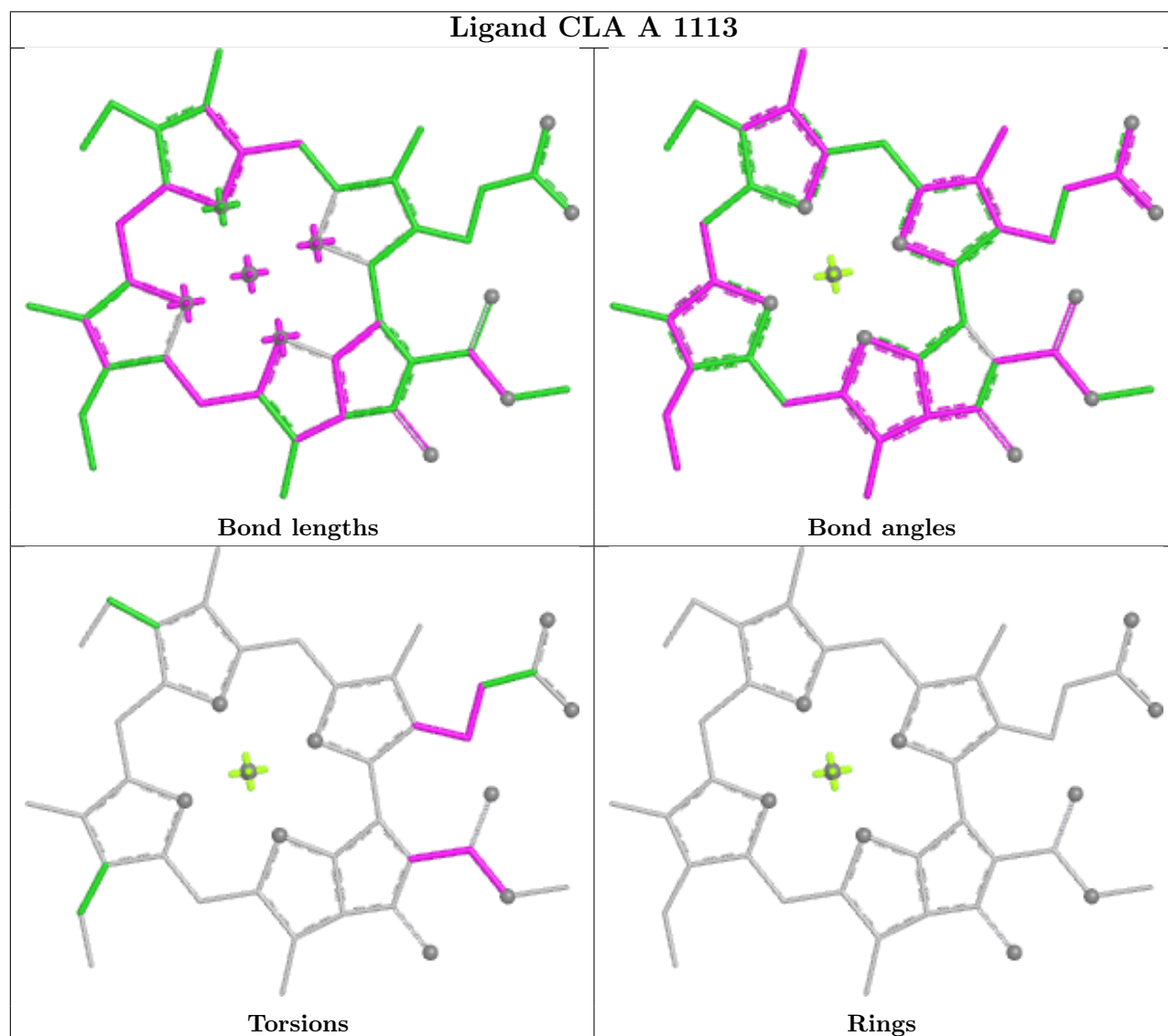
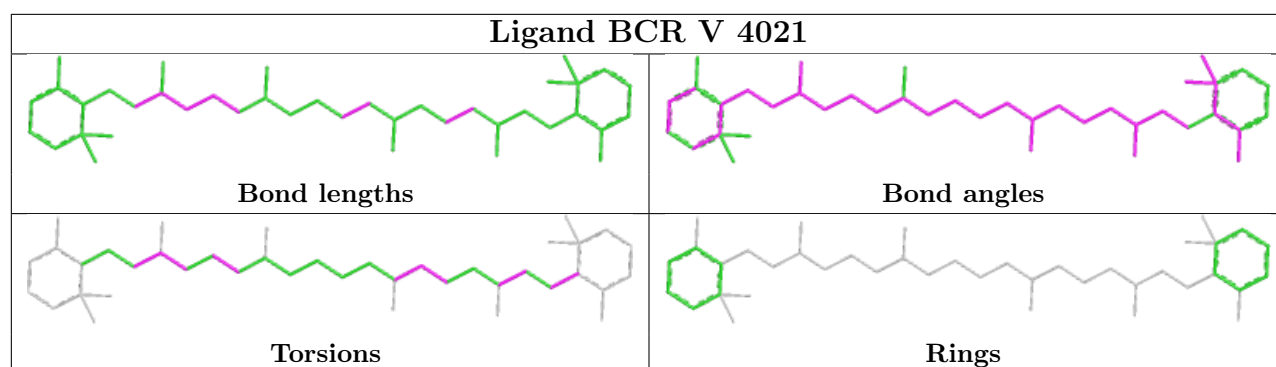


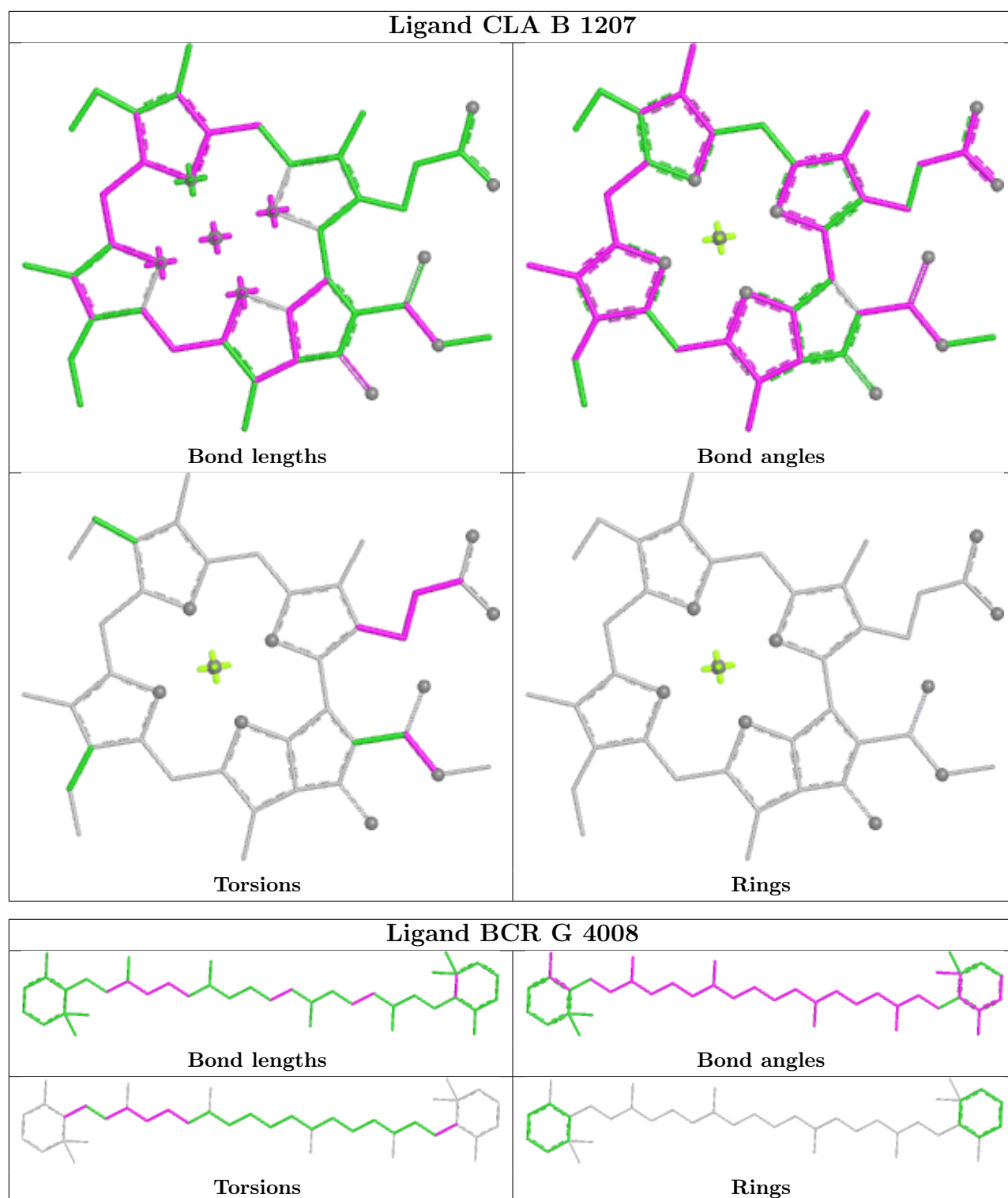


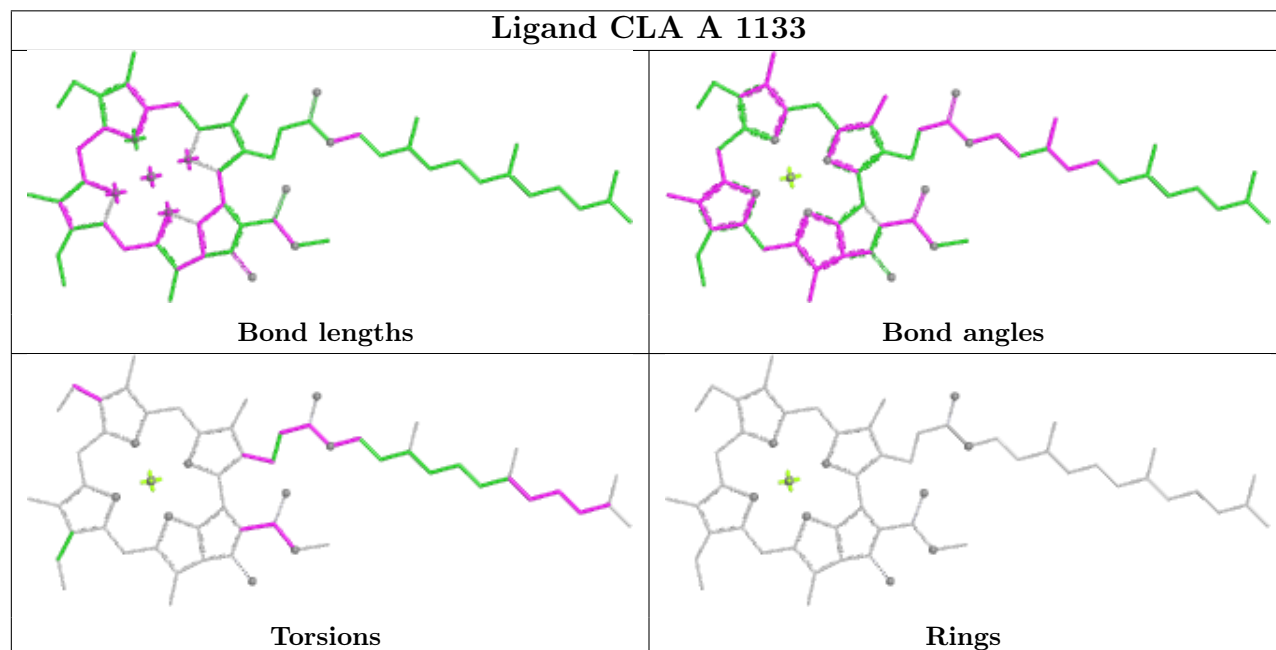
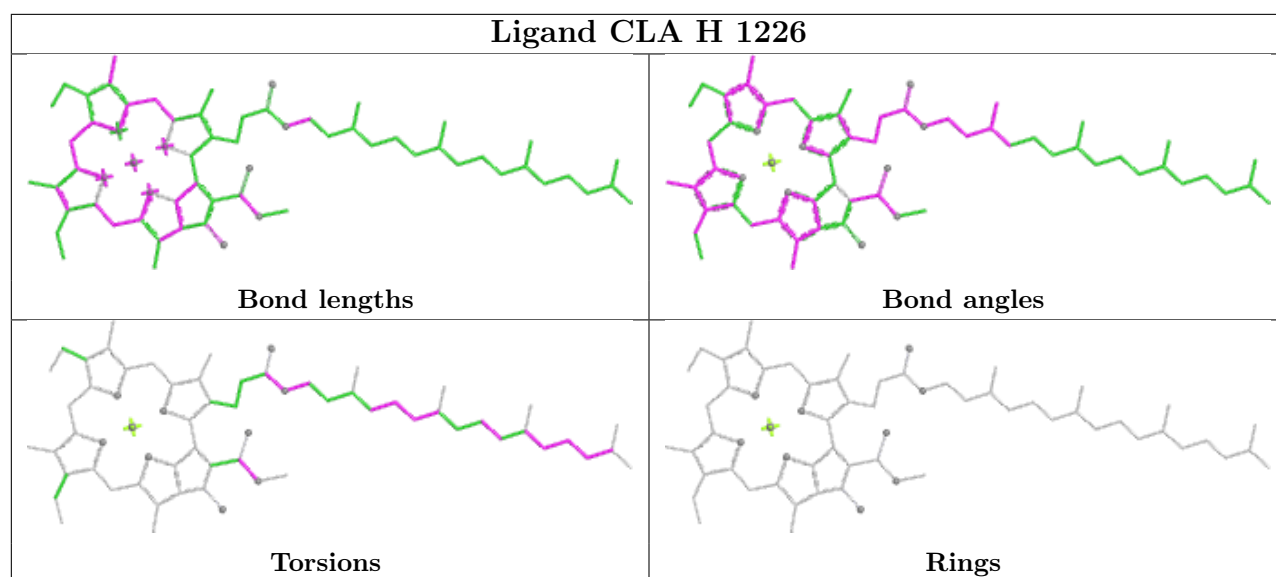
Ligand CLA B 1211	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 1229	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR i 4020	
 Bond lengths	 Bond angles
 Torsions	 Rings



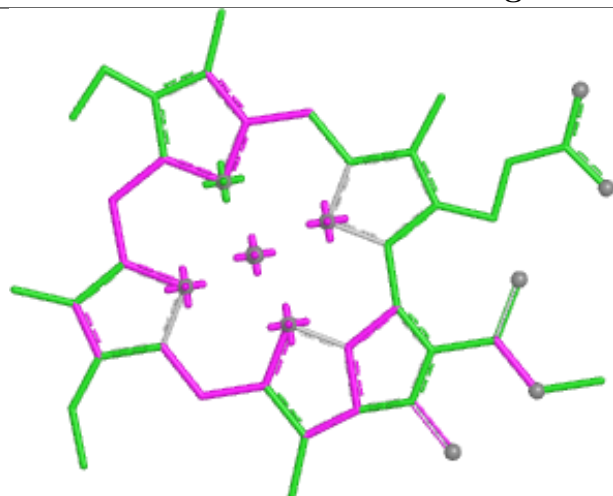




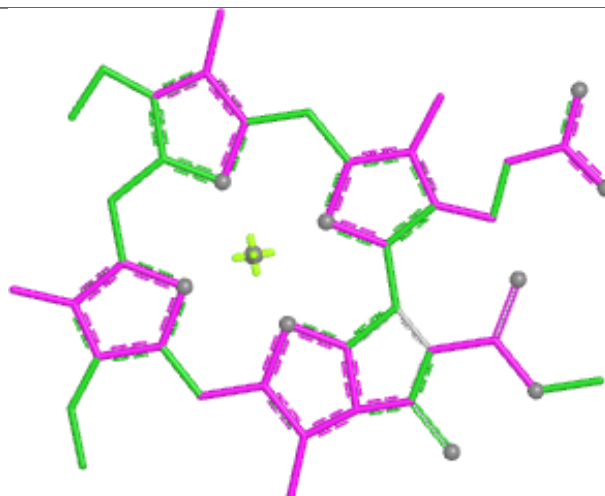




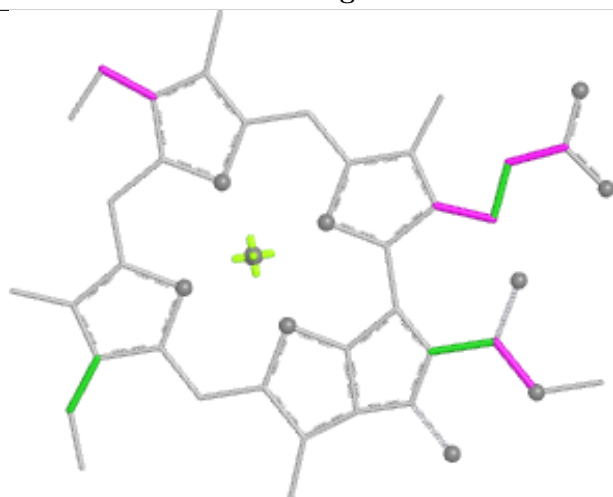
Ligand CLA X 1701



Bond lengths



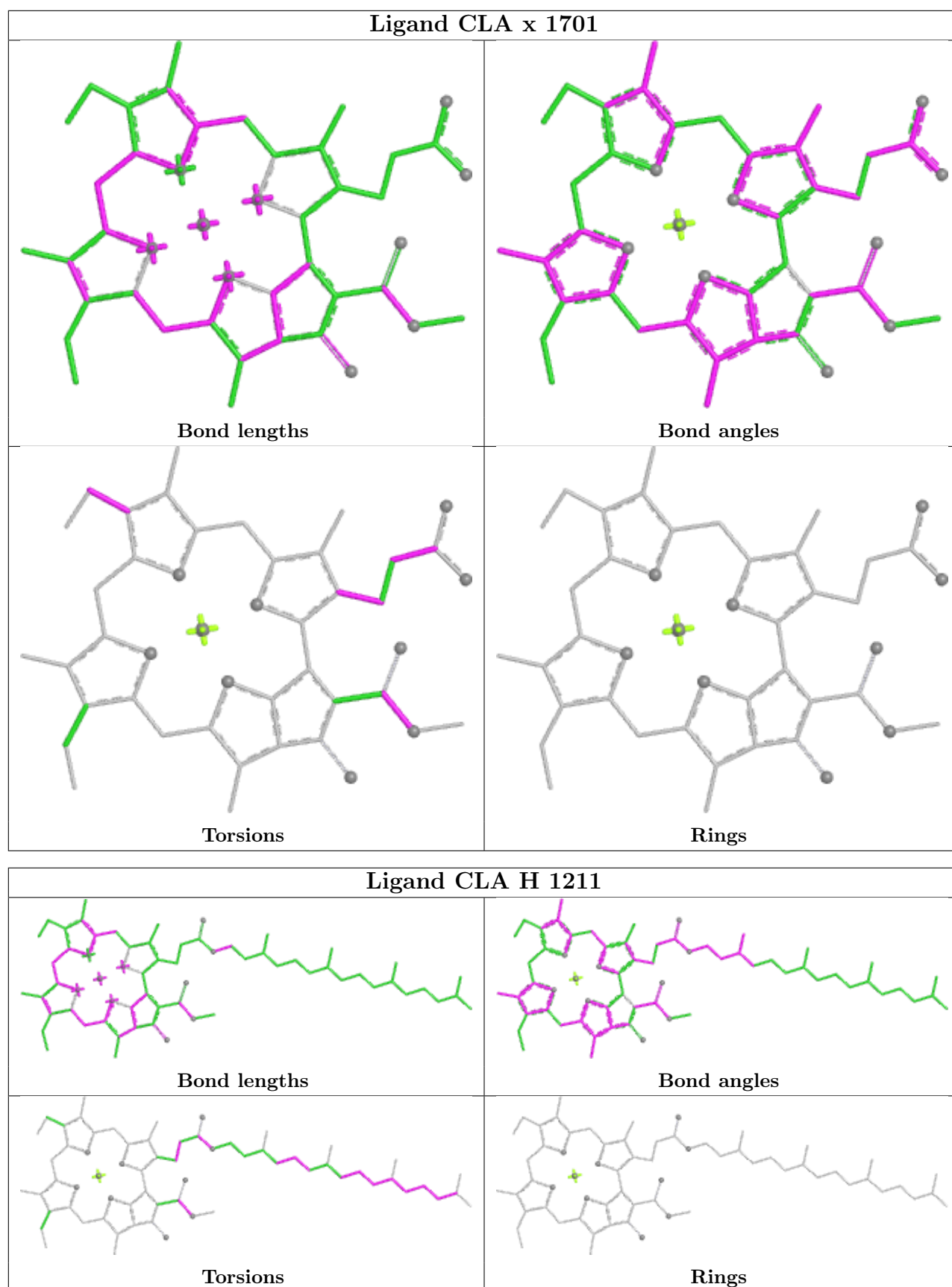
Bond angles

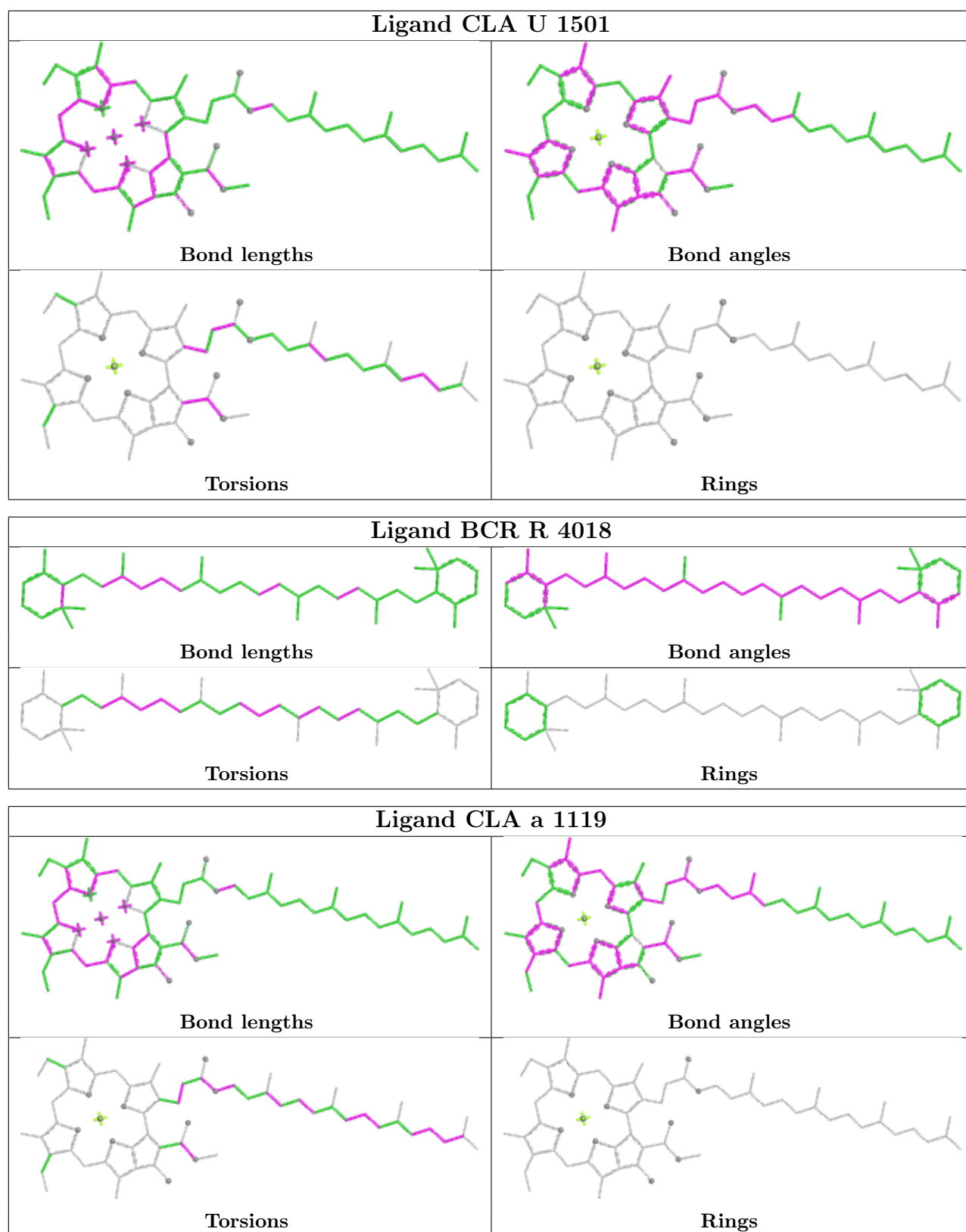


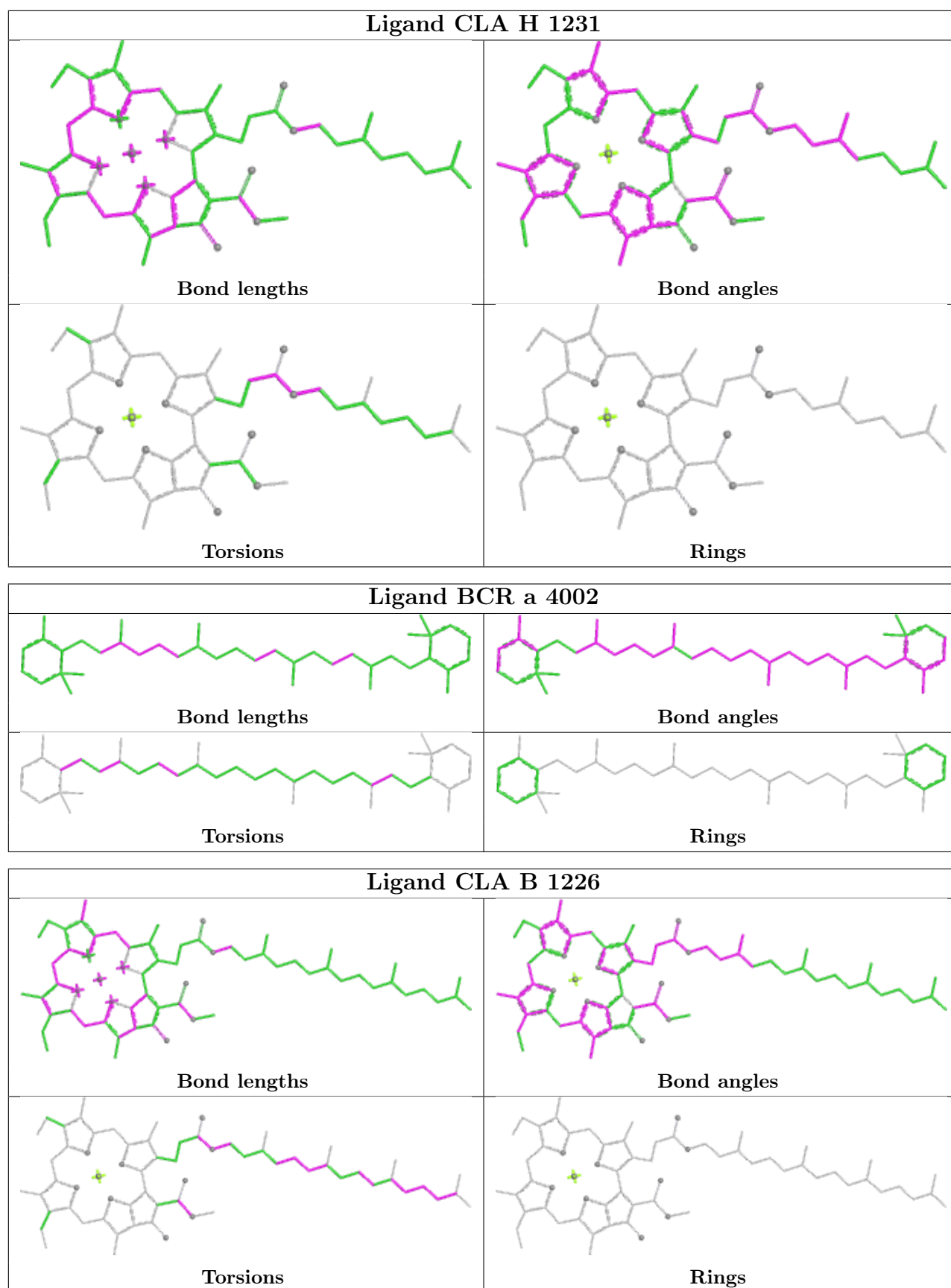
Torsions

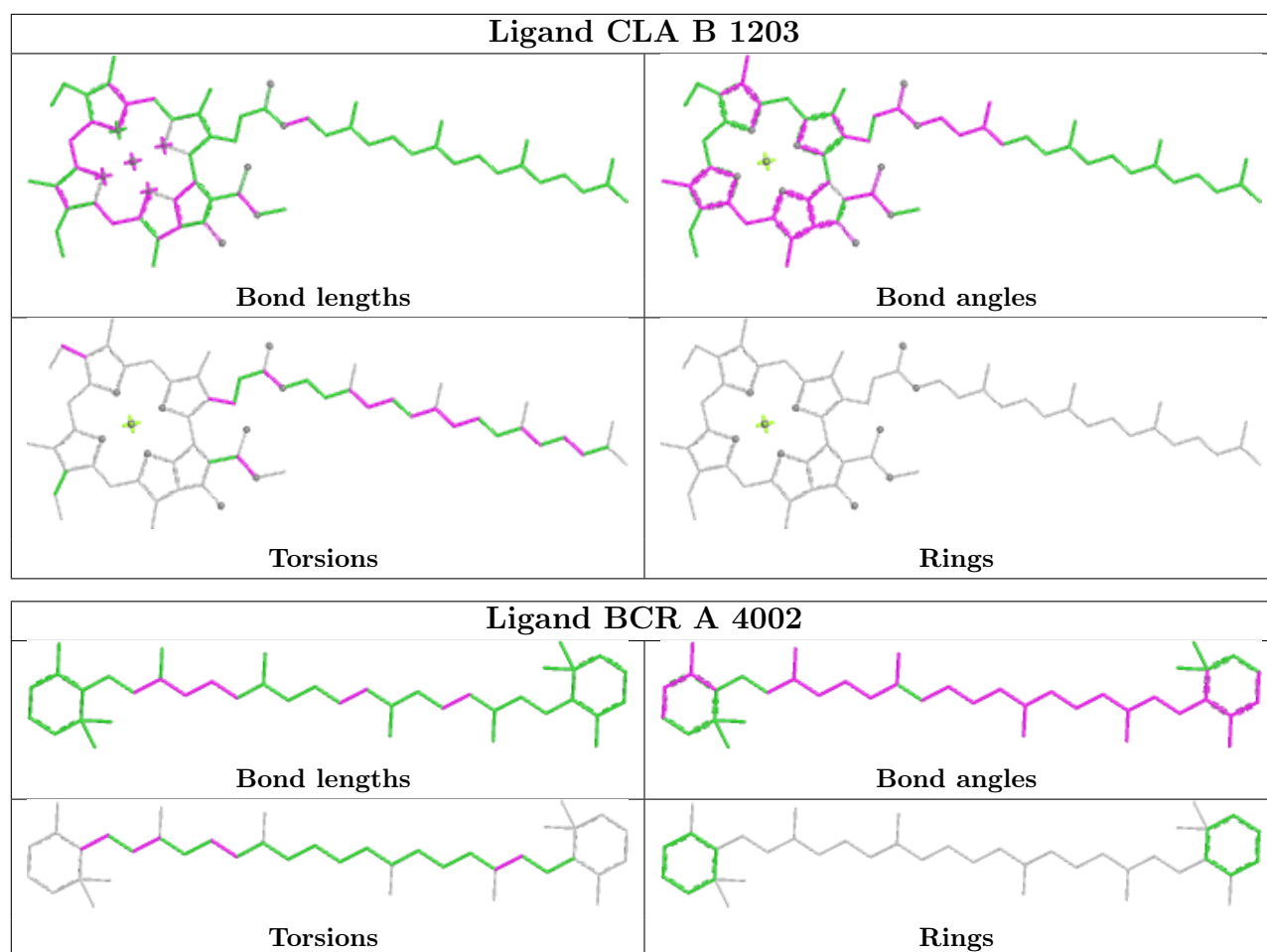


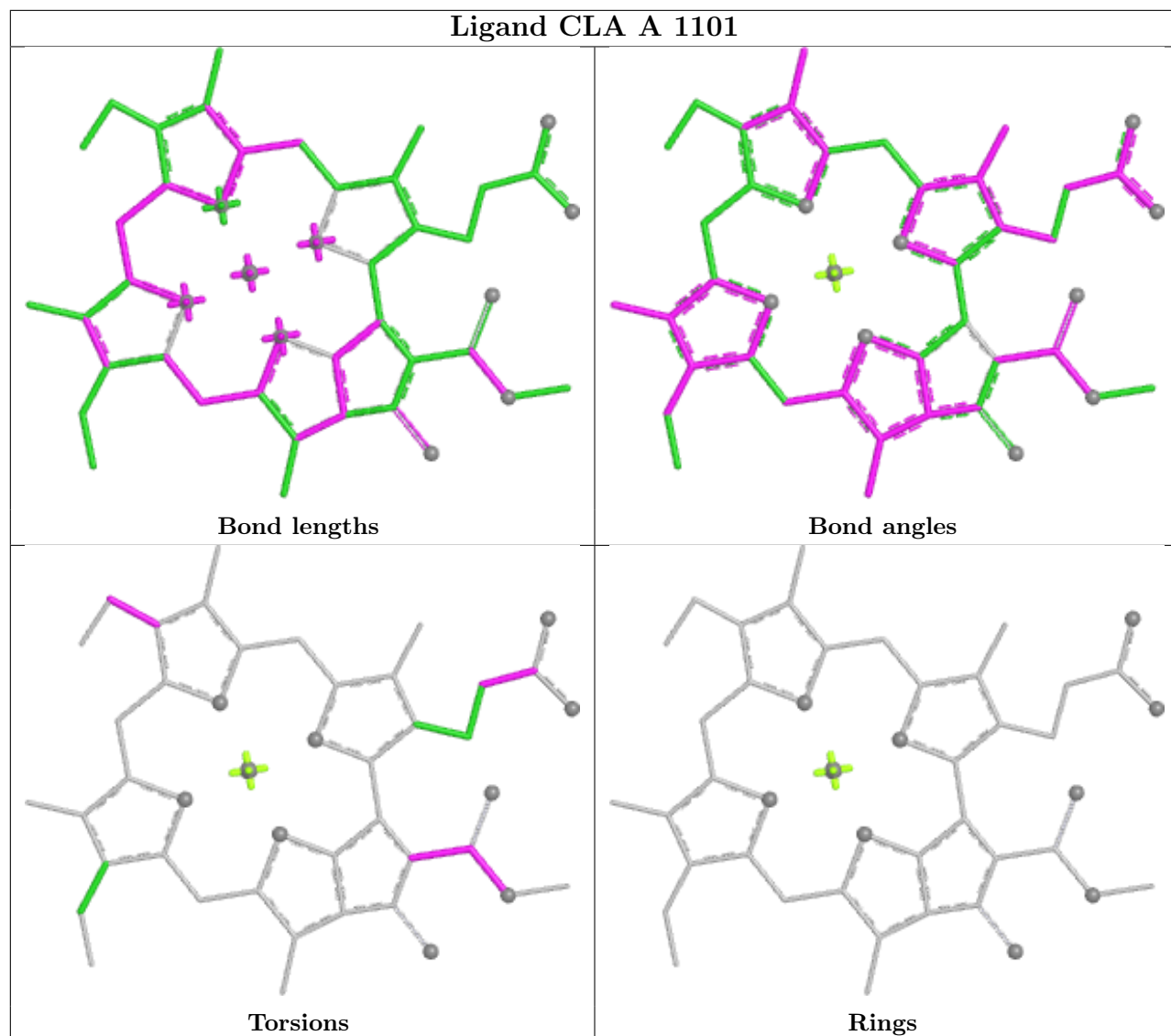
Rings

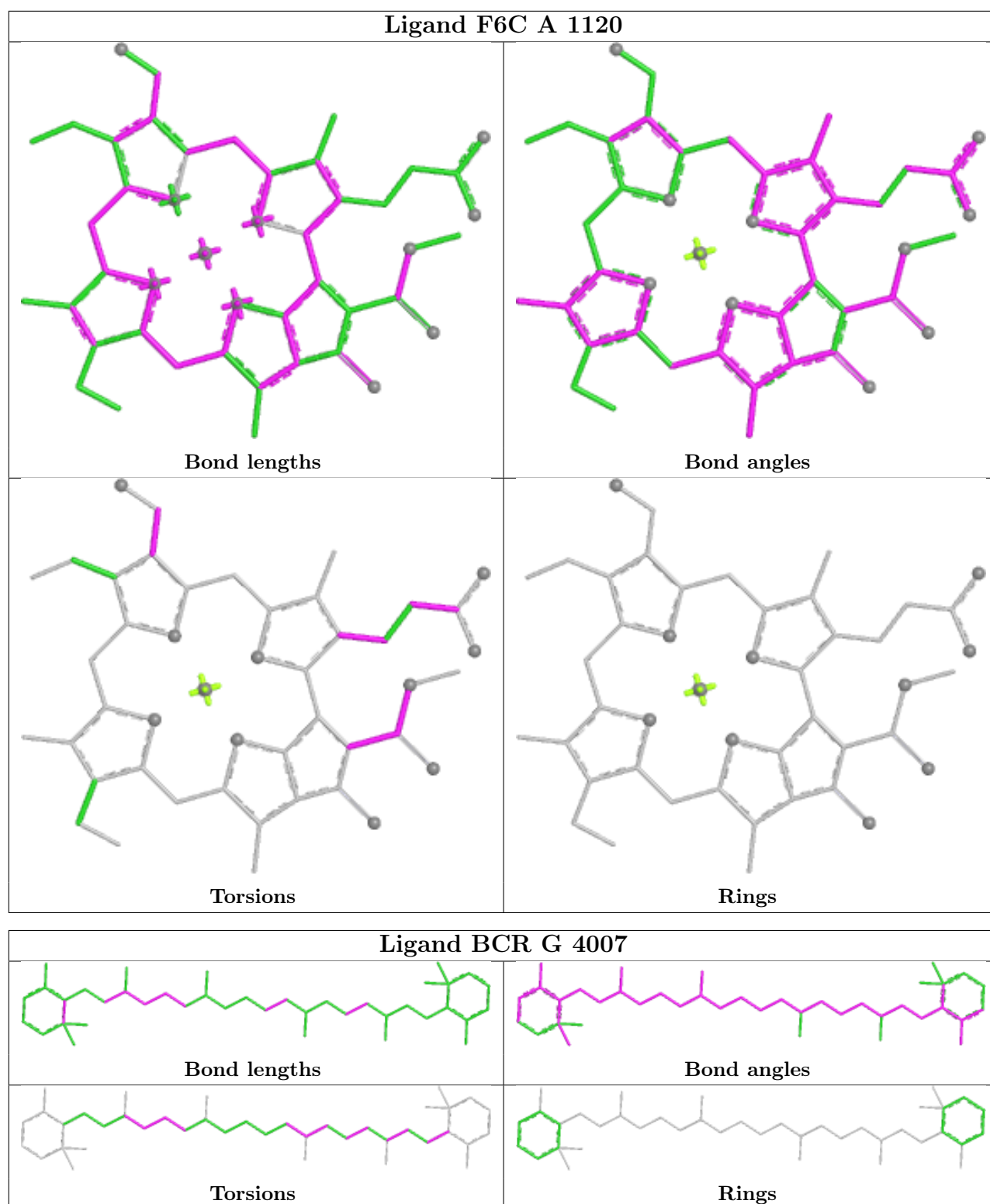


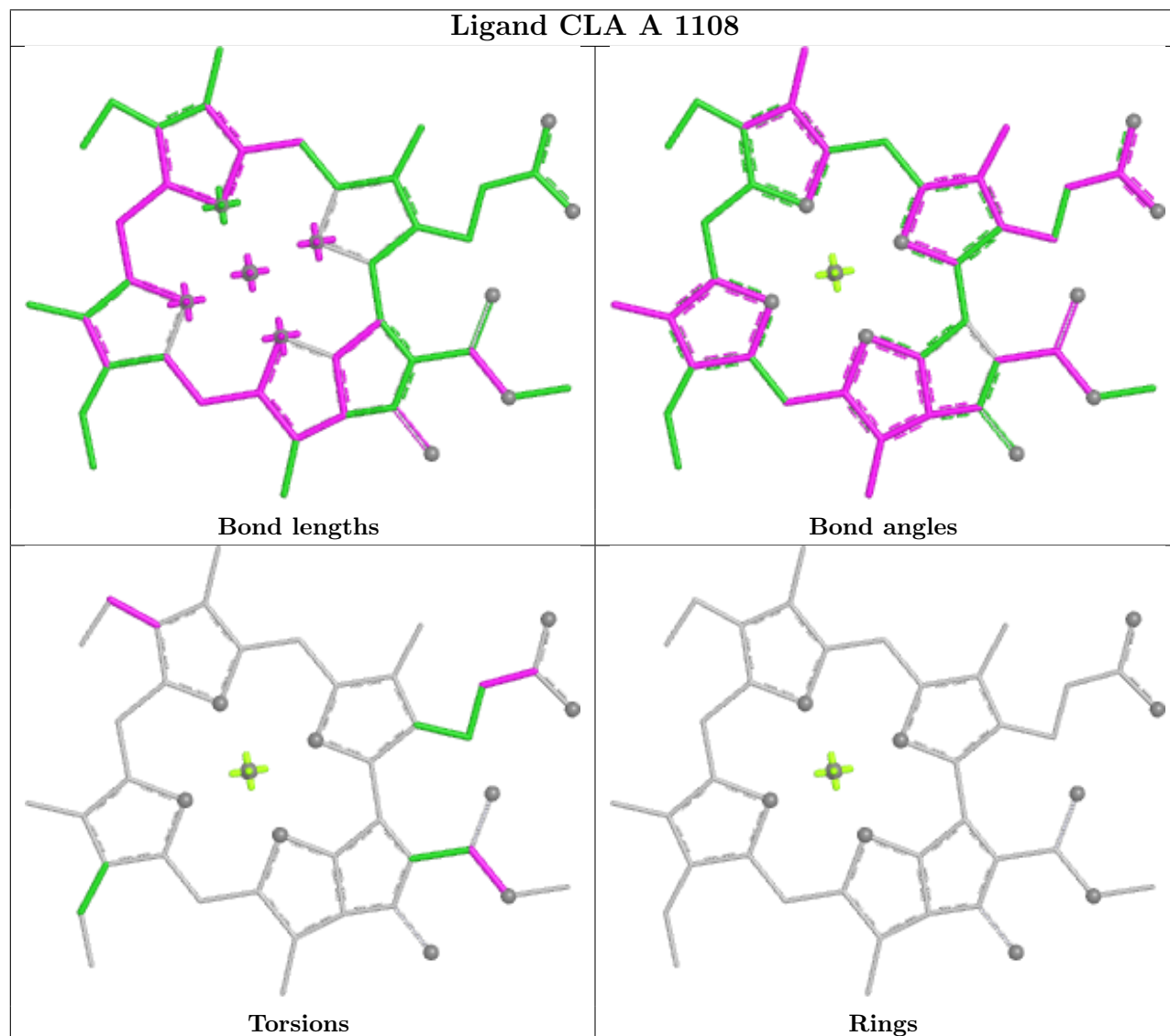
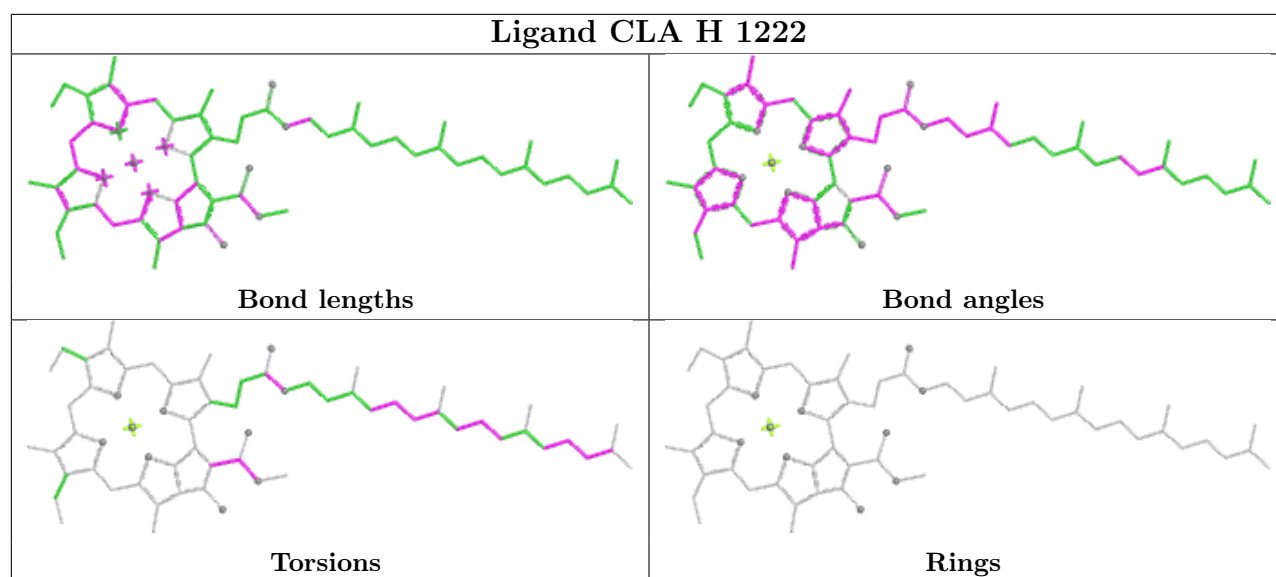


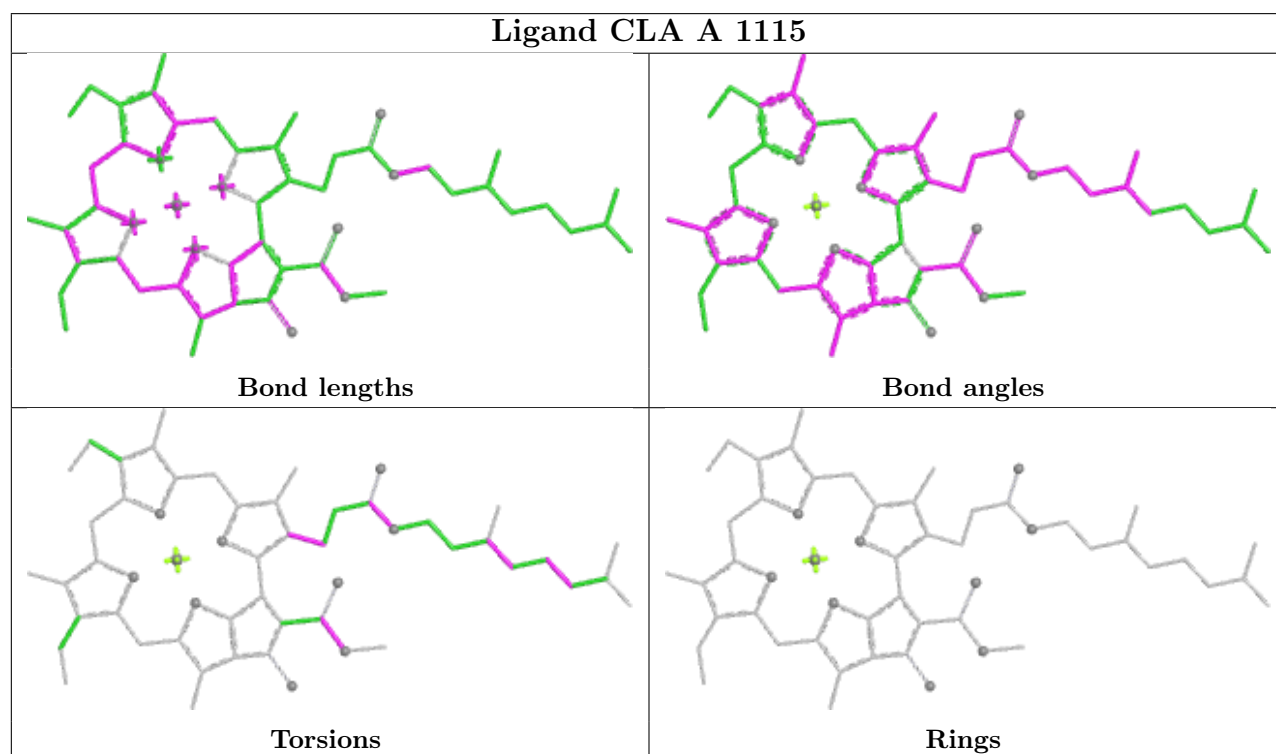
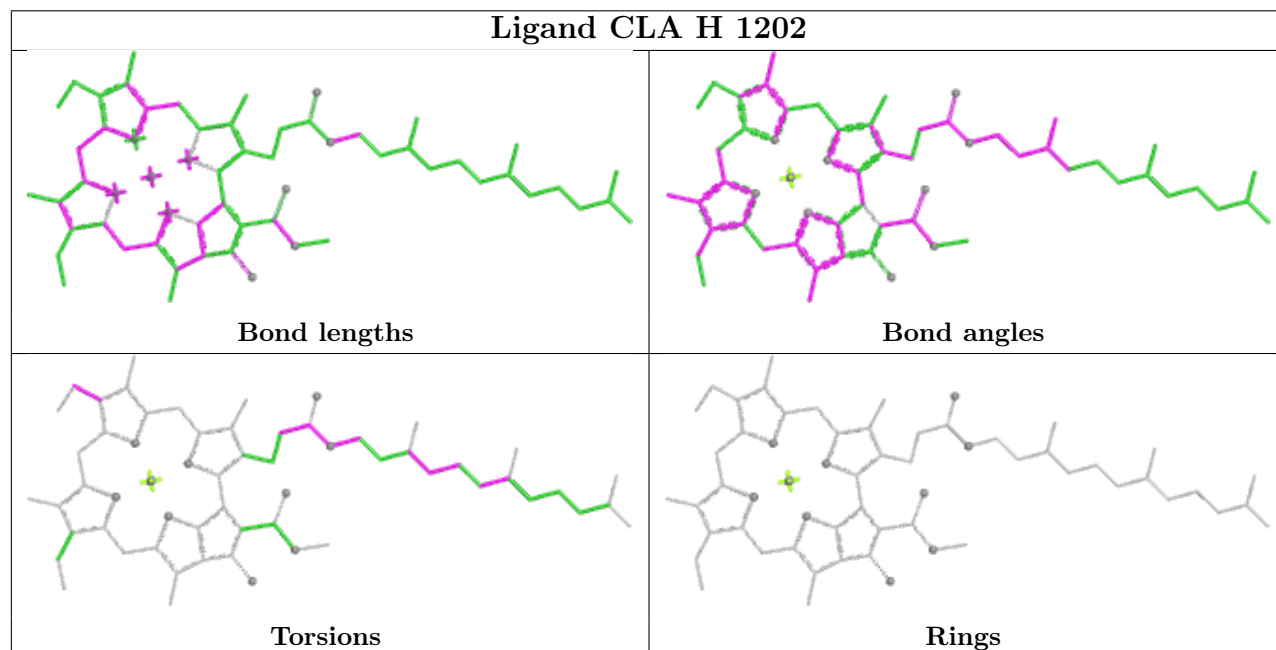
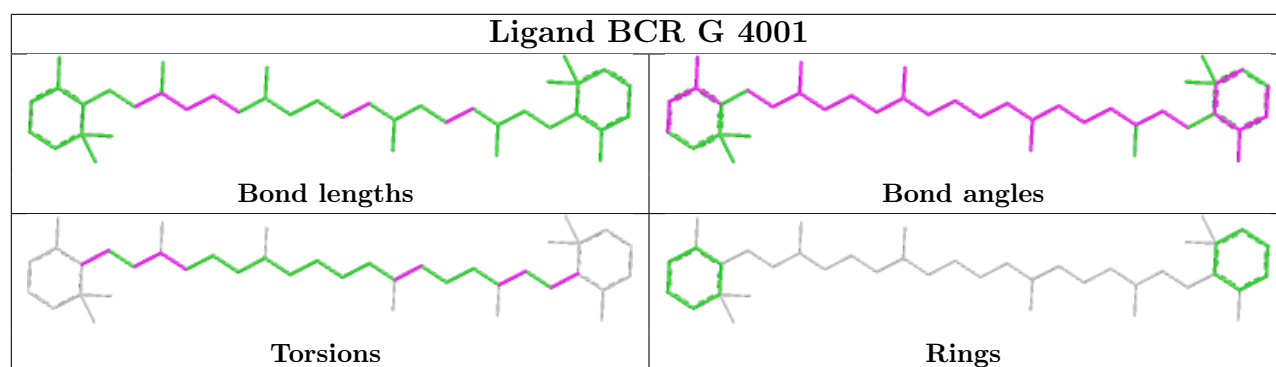


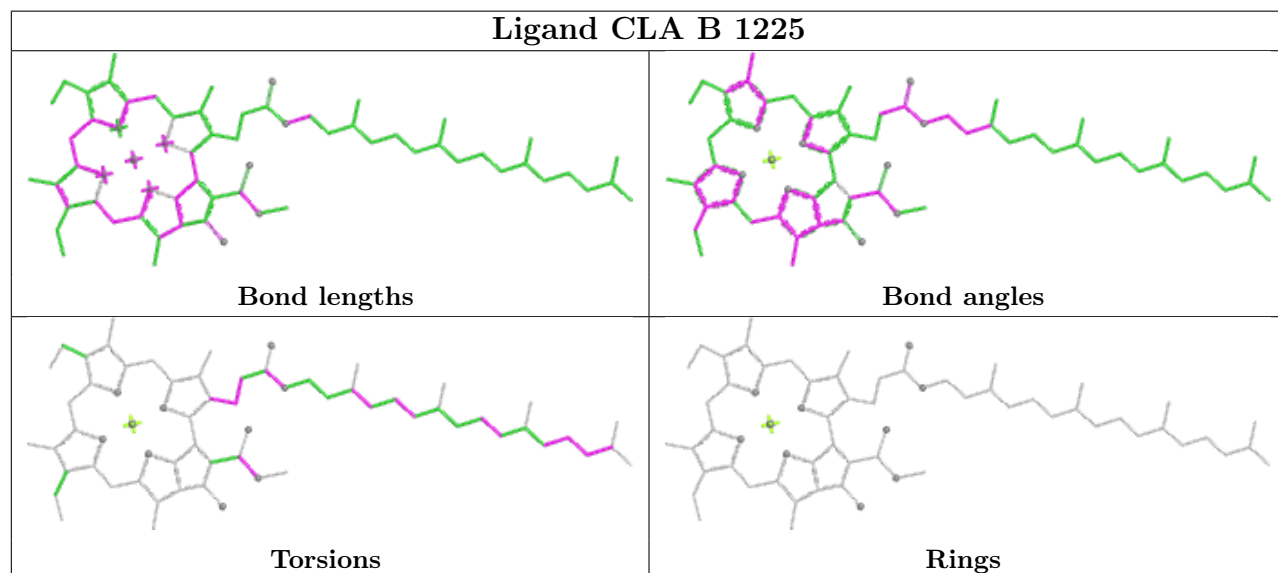
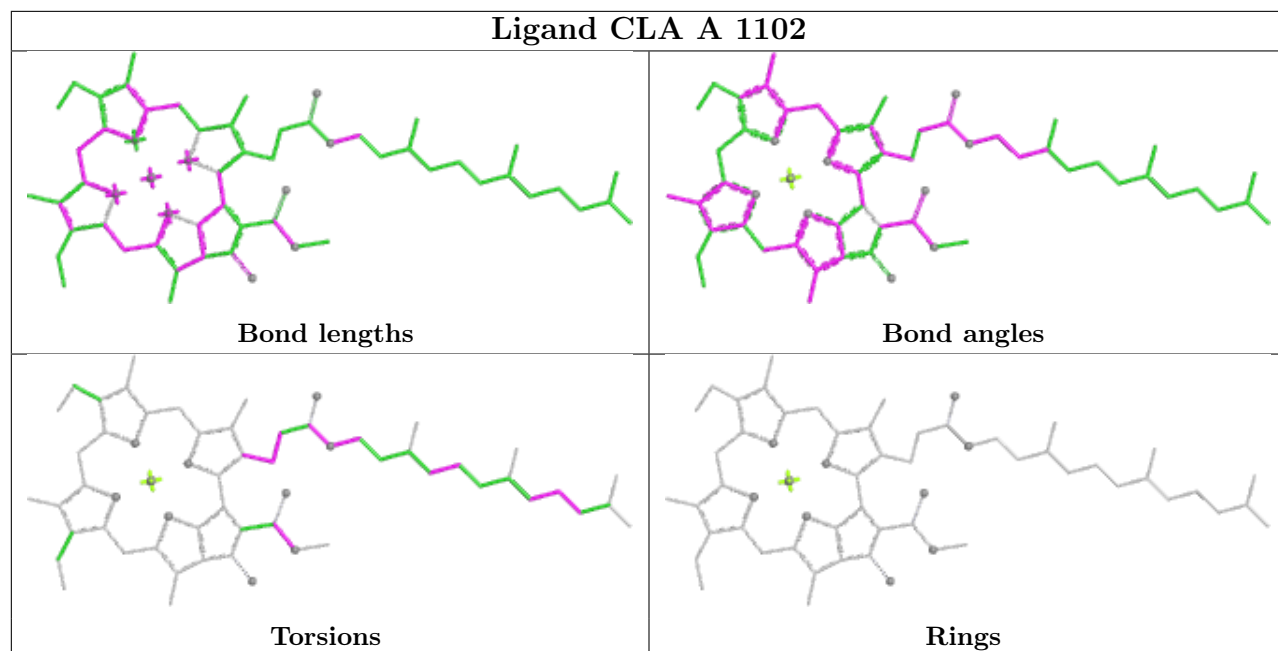


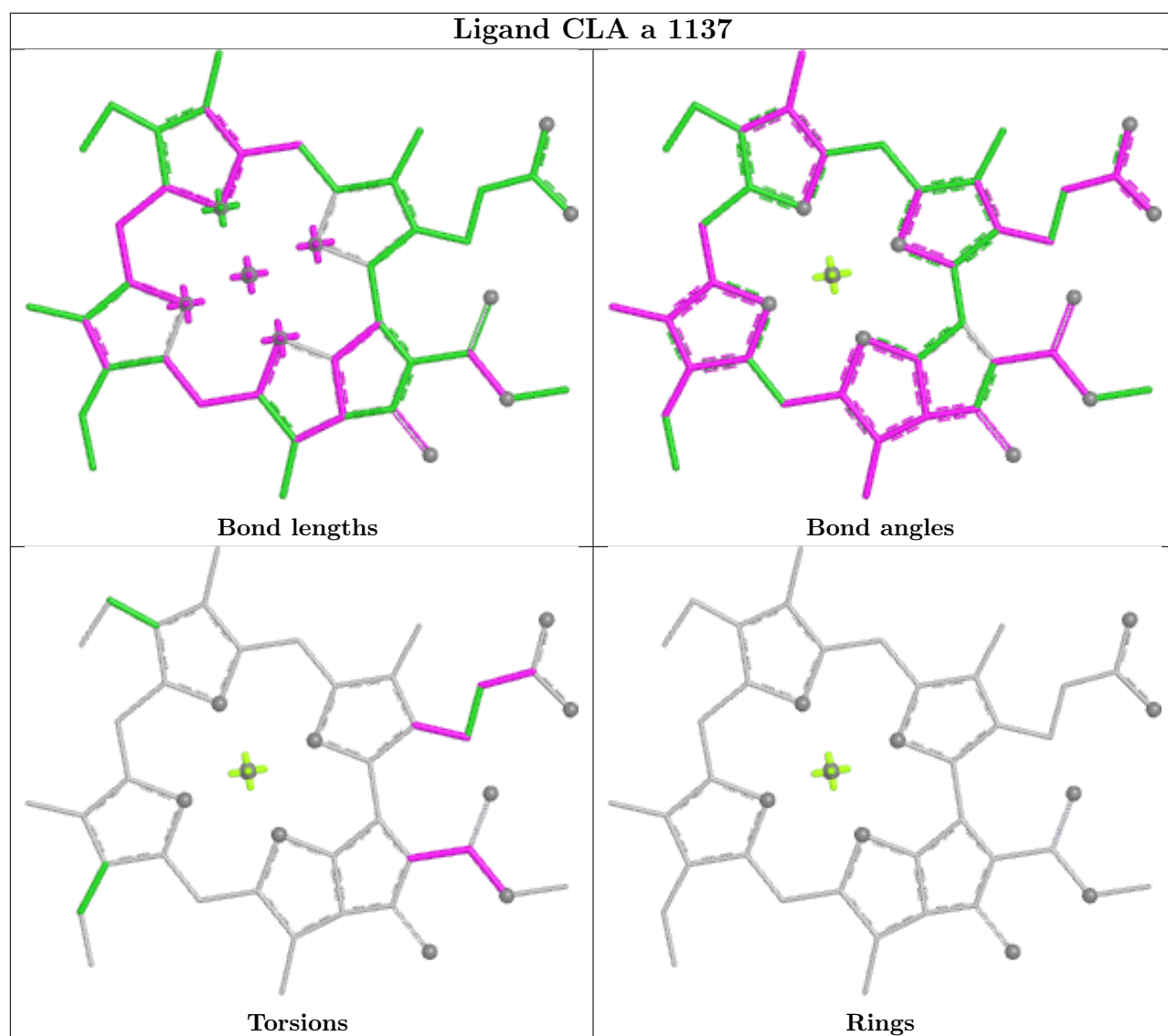


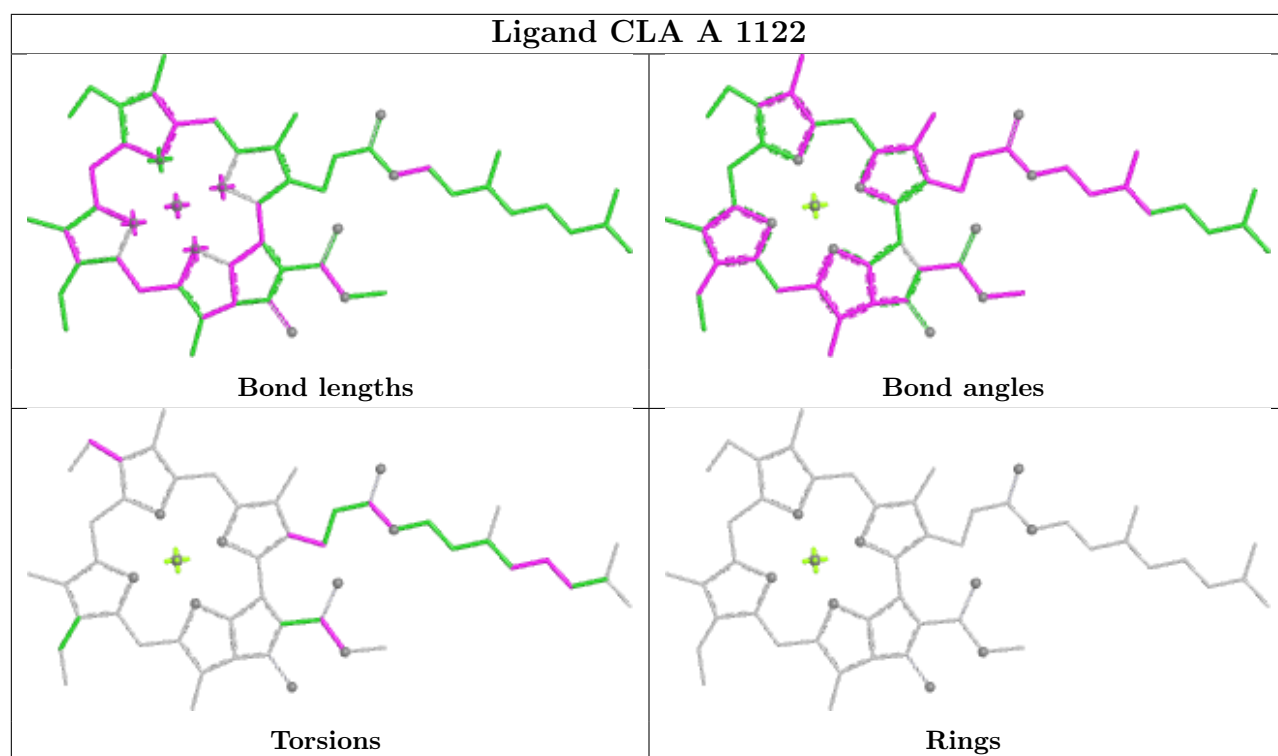


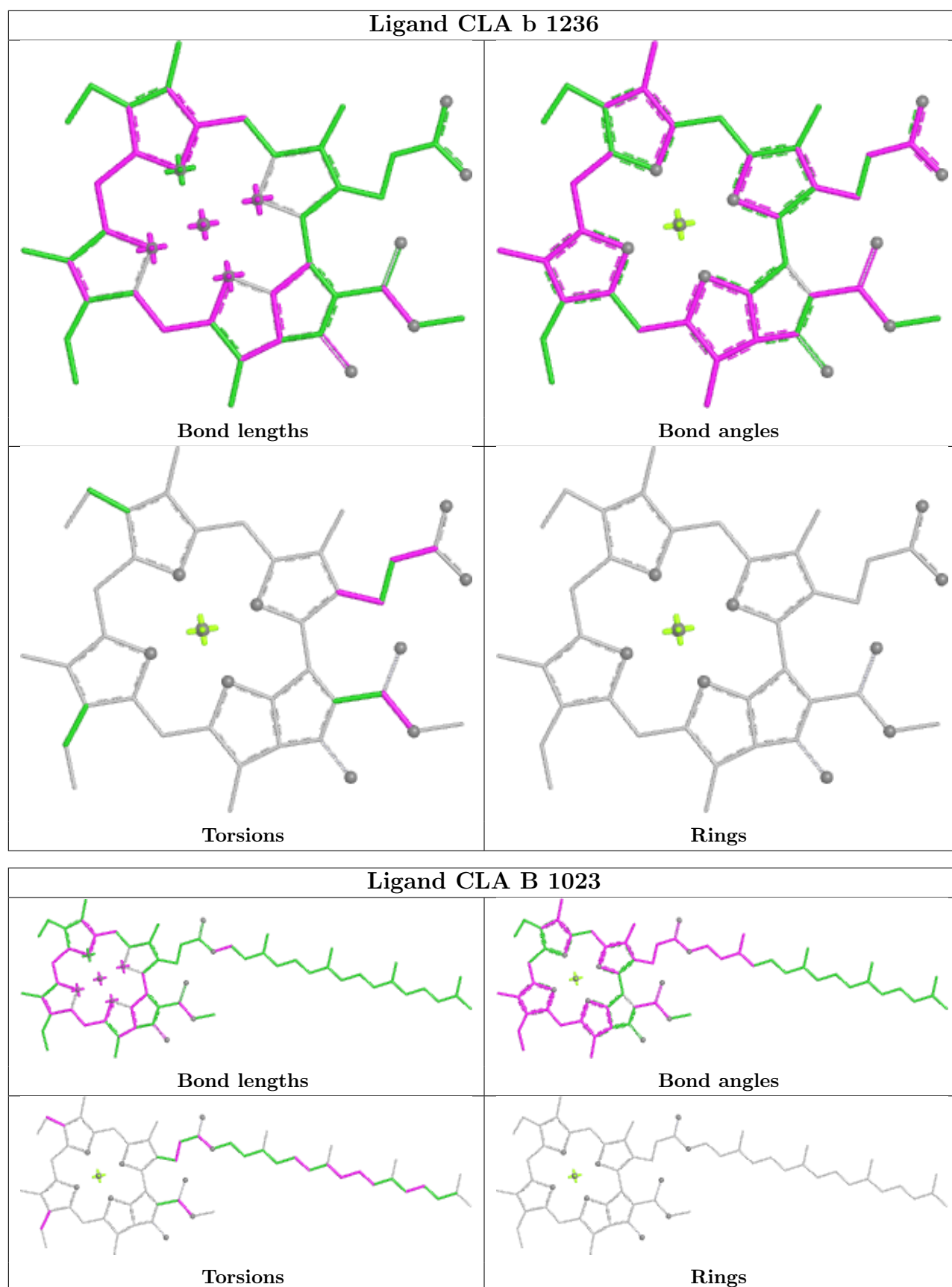


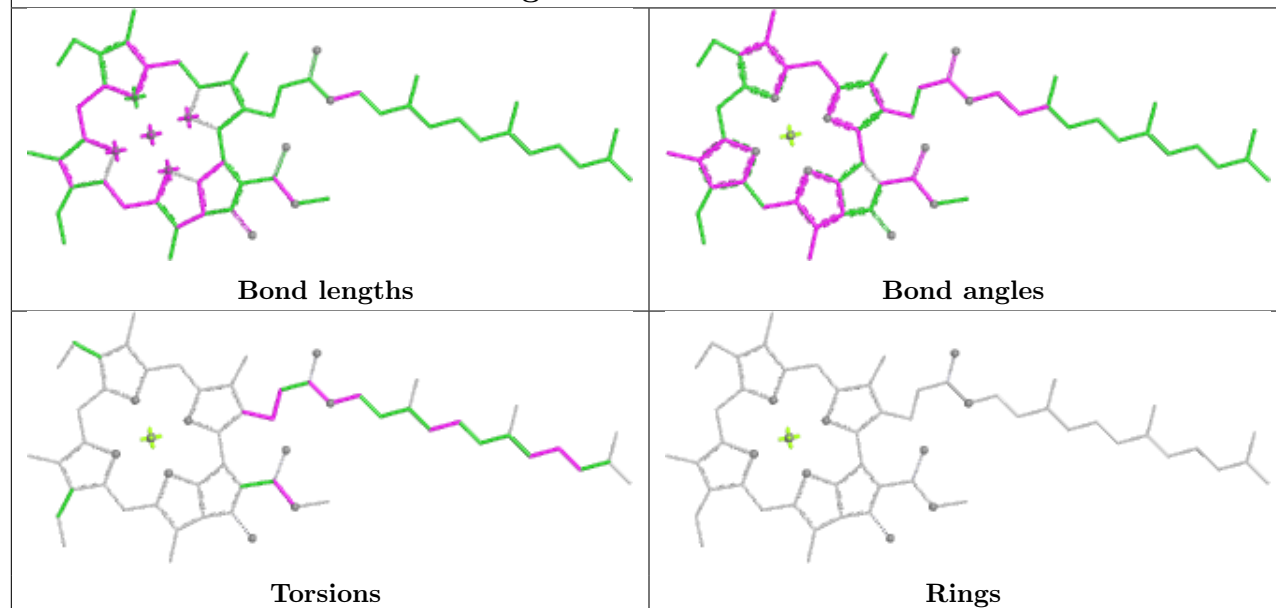
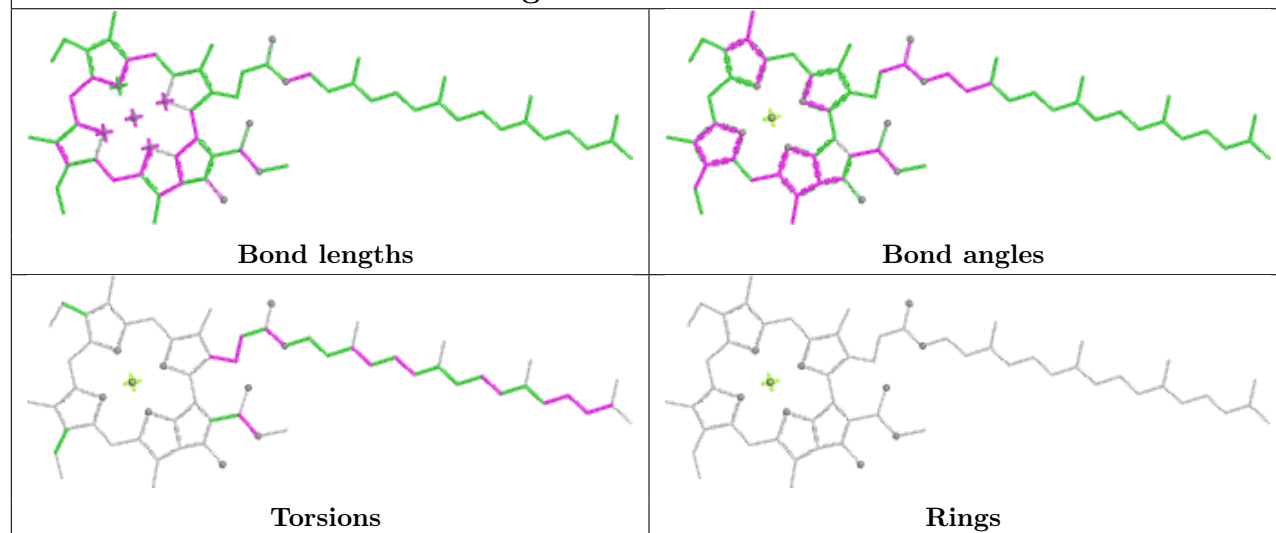


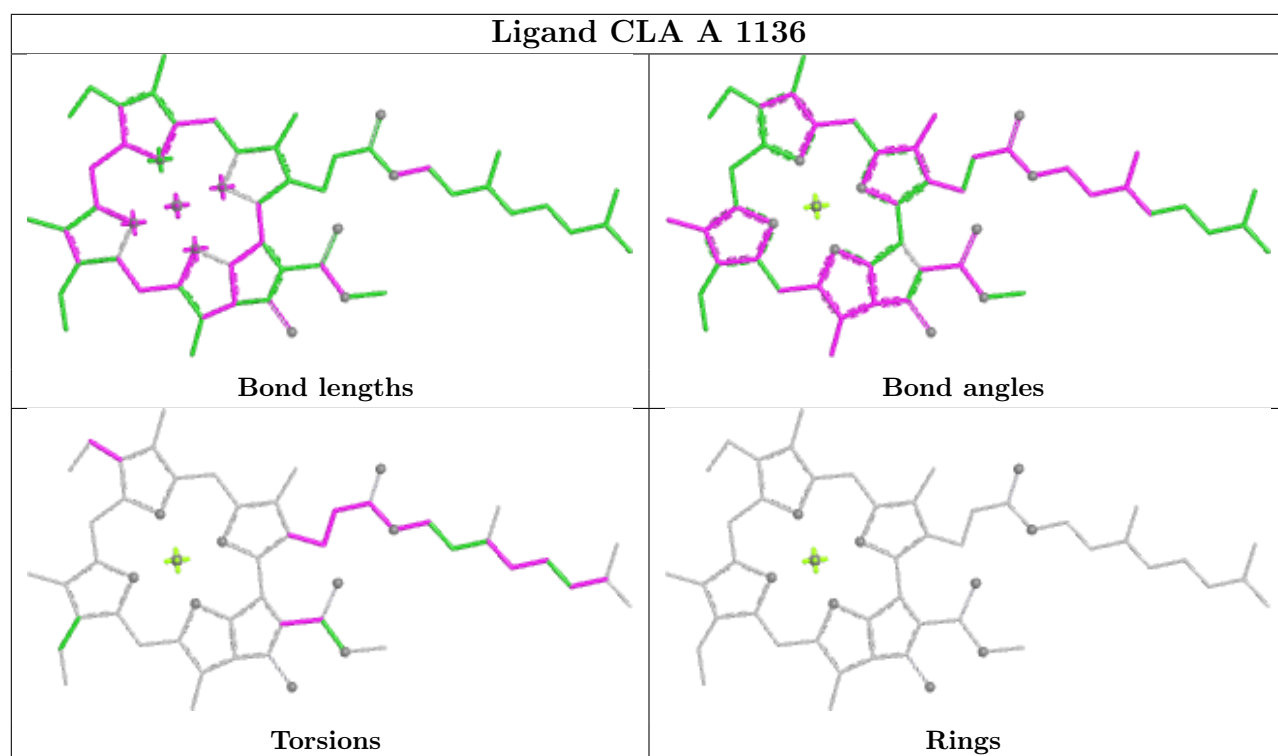




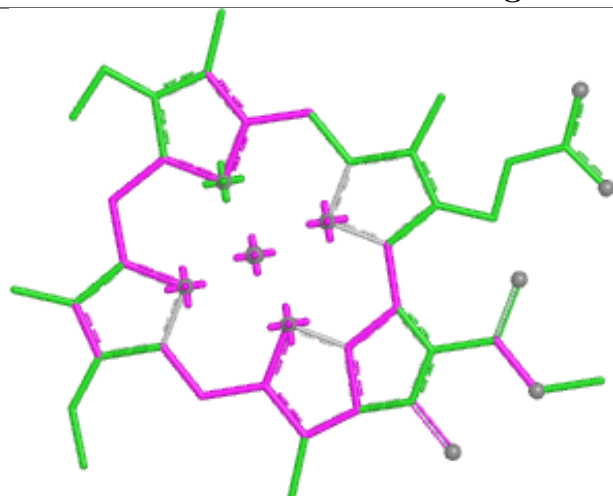




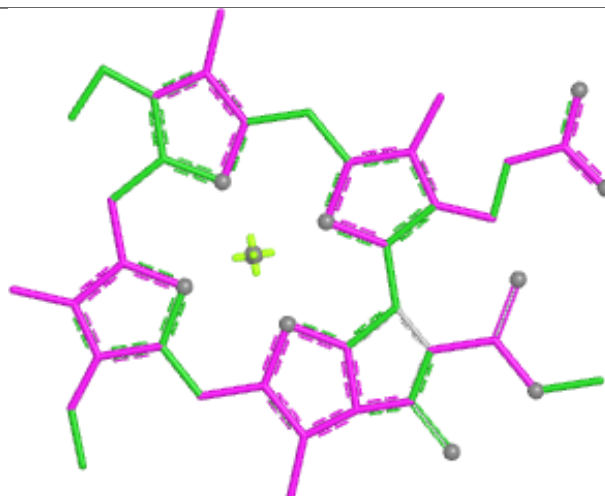
Ligand CLA G 1102**Ligand CLA H 1225**



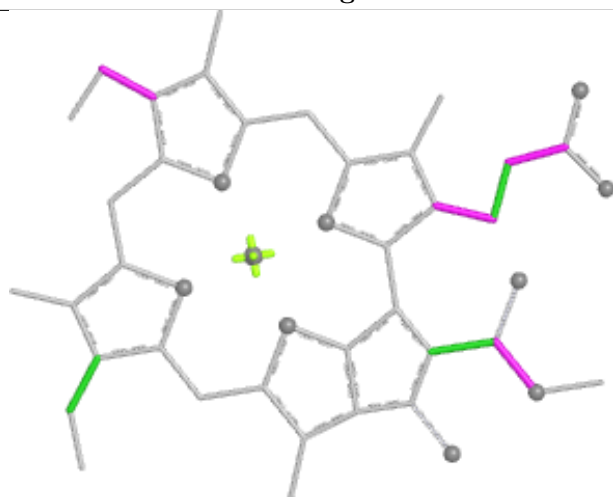
Ligand CLA G 1109



Bond lengths



Bond angles

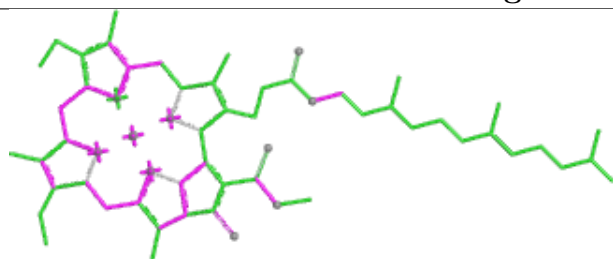


Torsions

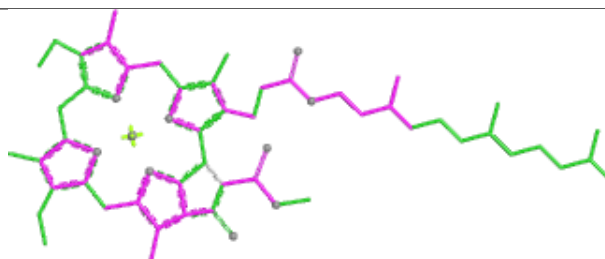


Rings

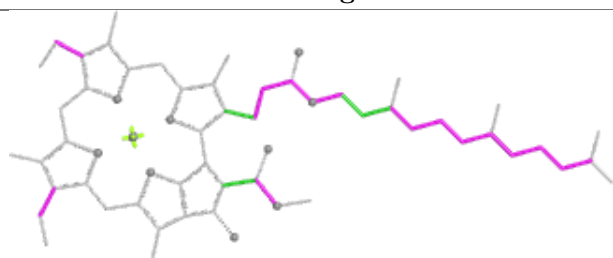
Ligand CLA G 1126



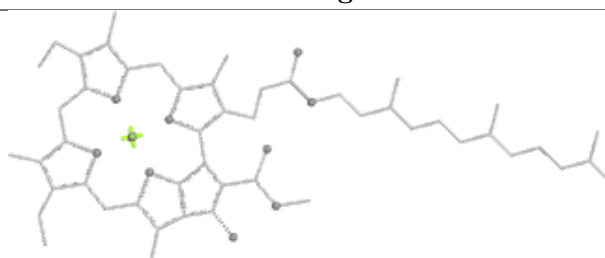
Bond lengths



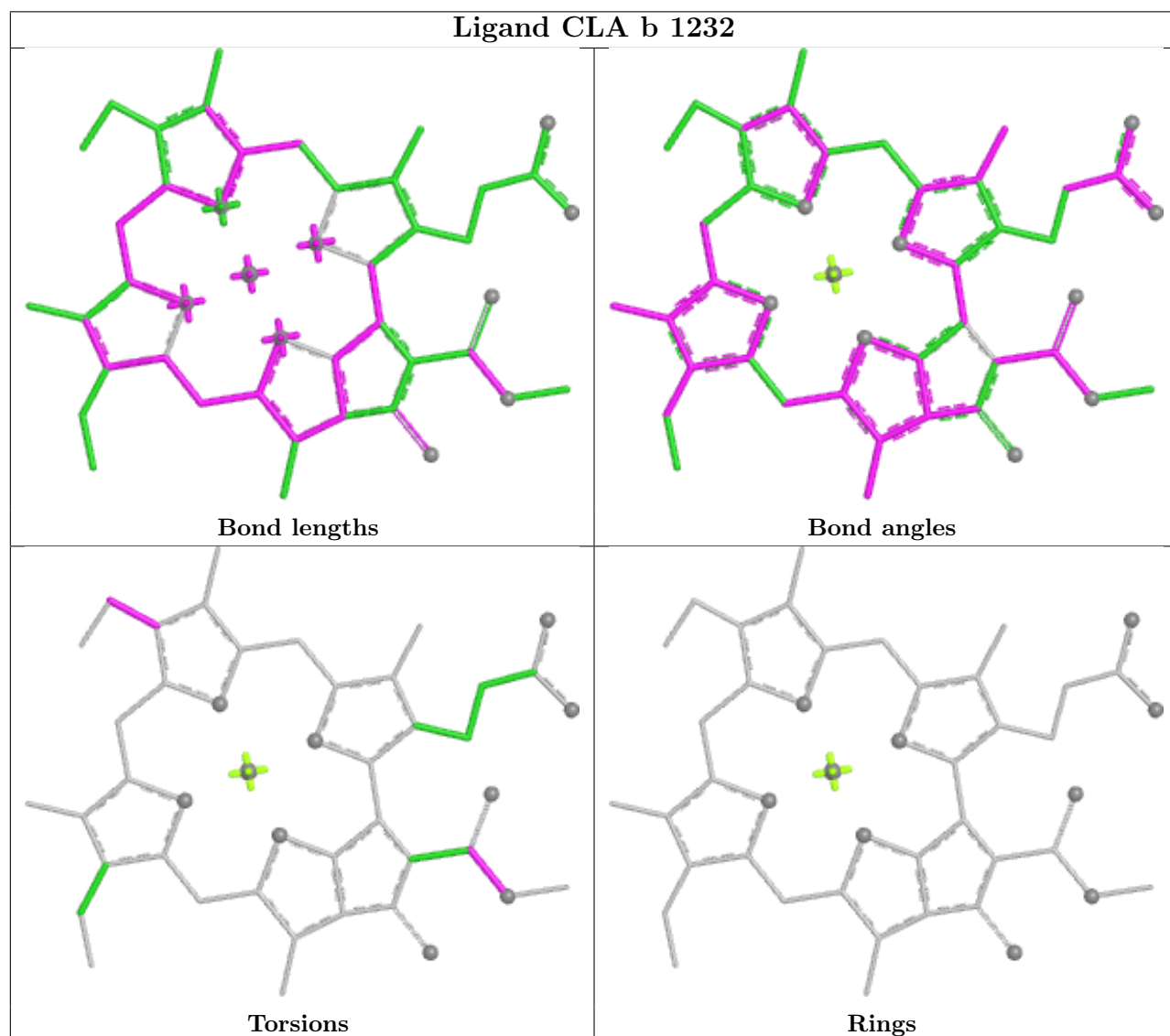
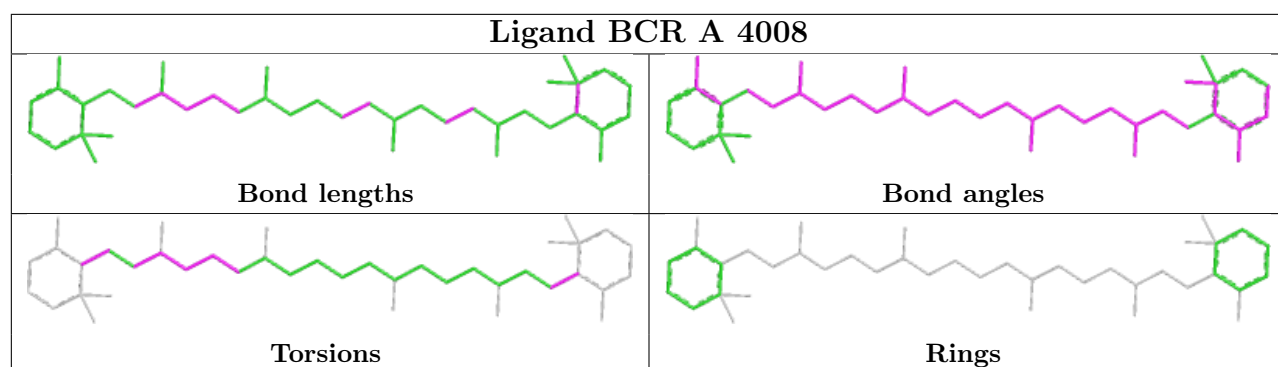
Bond angles

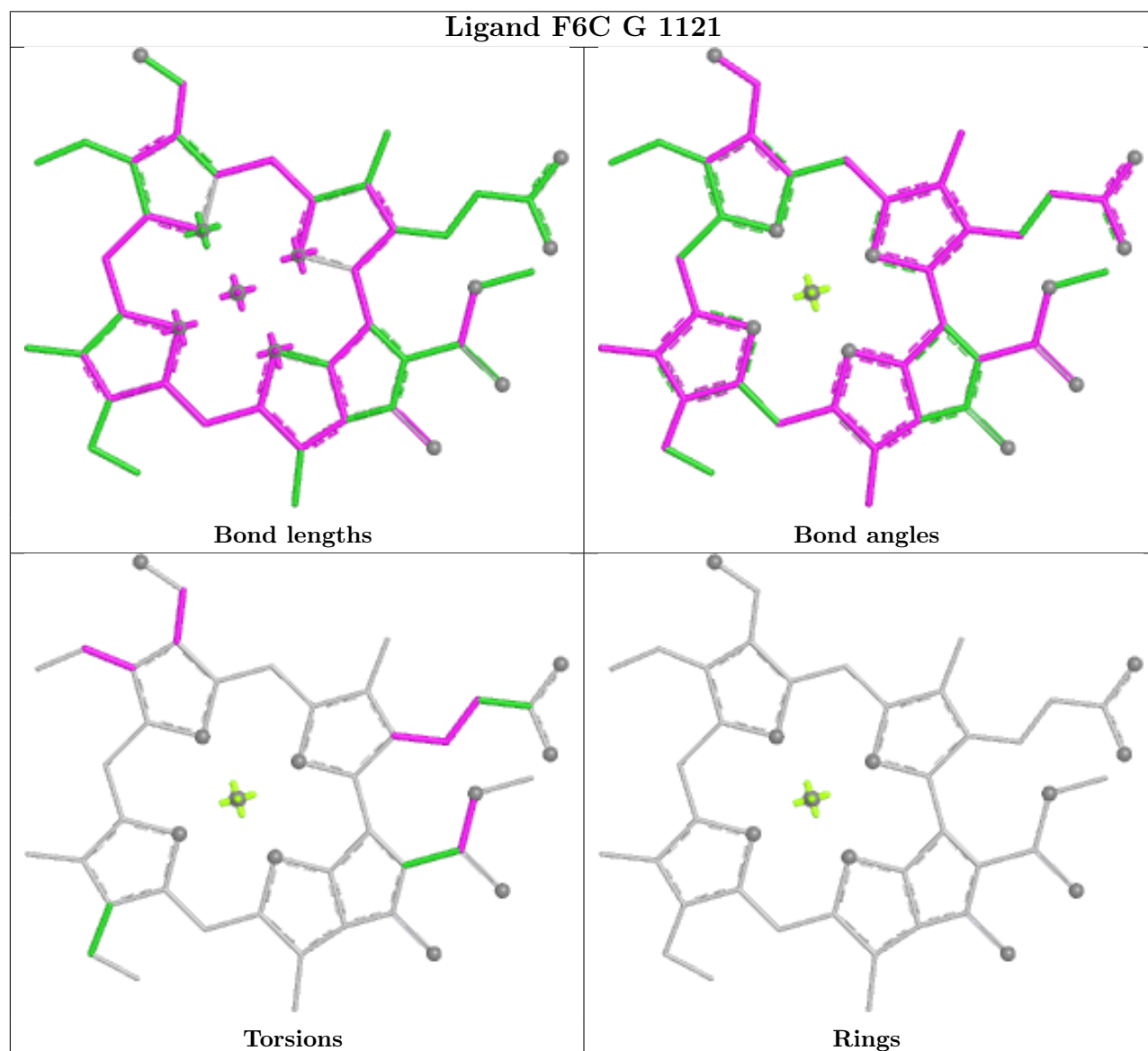
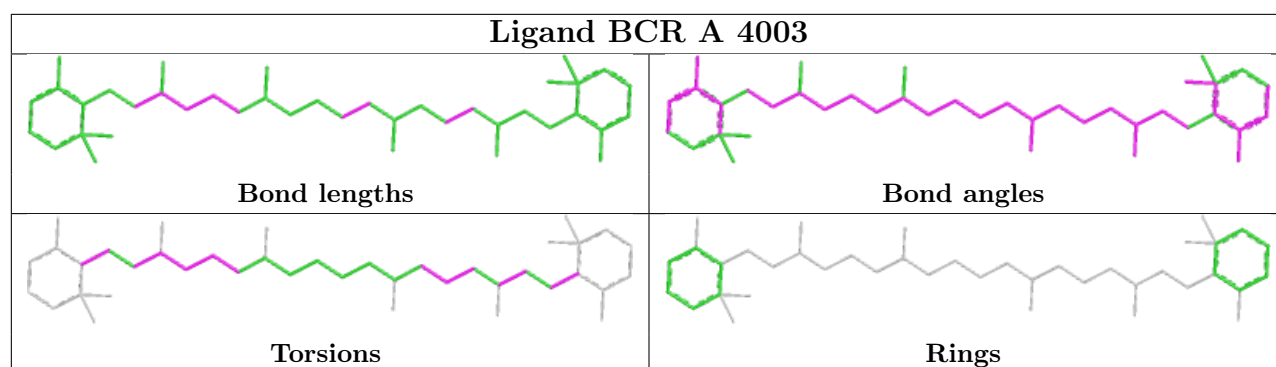


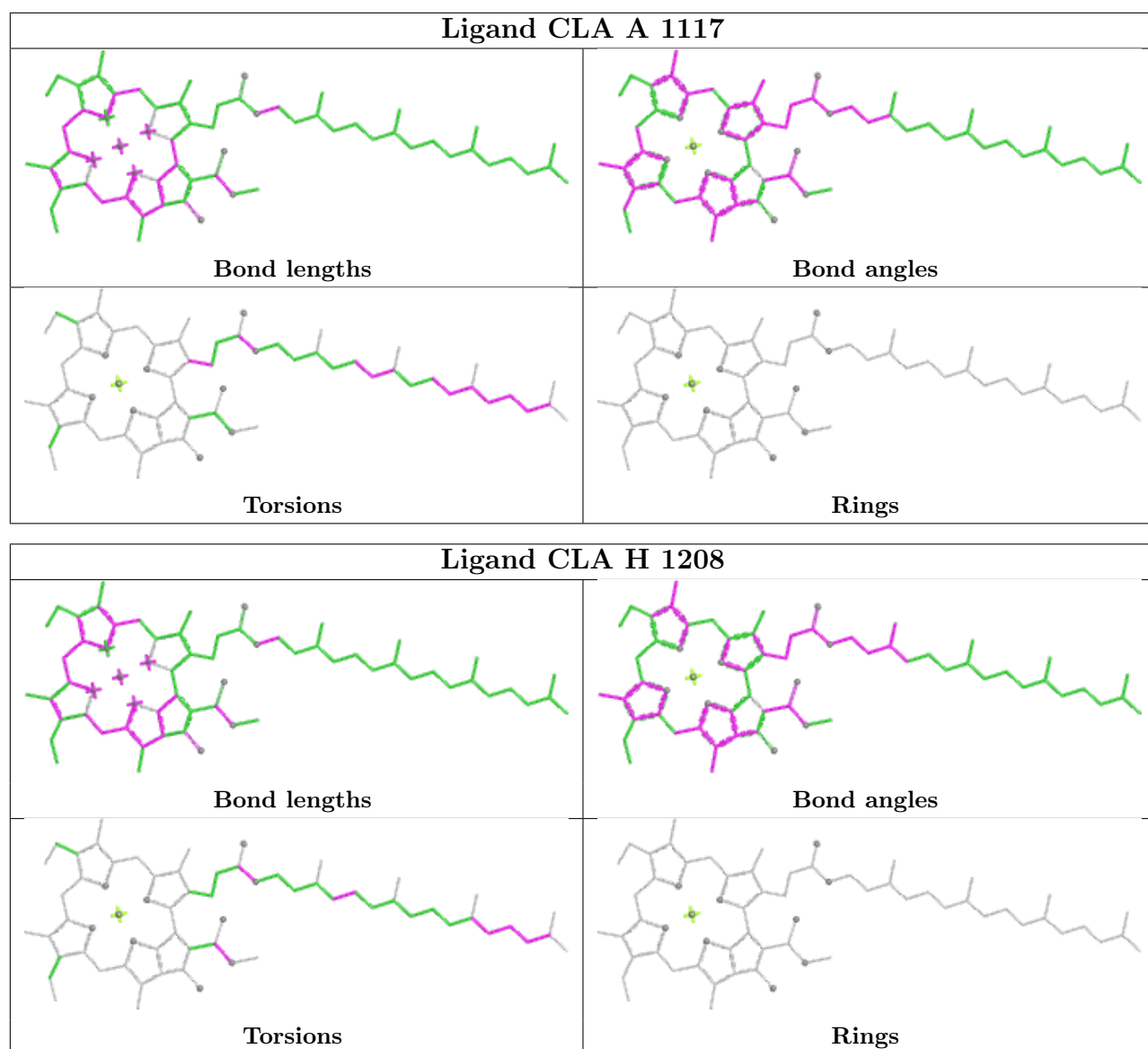
Torsions

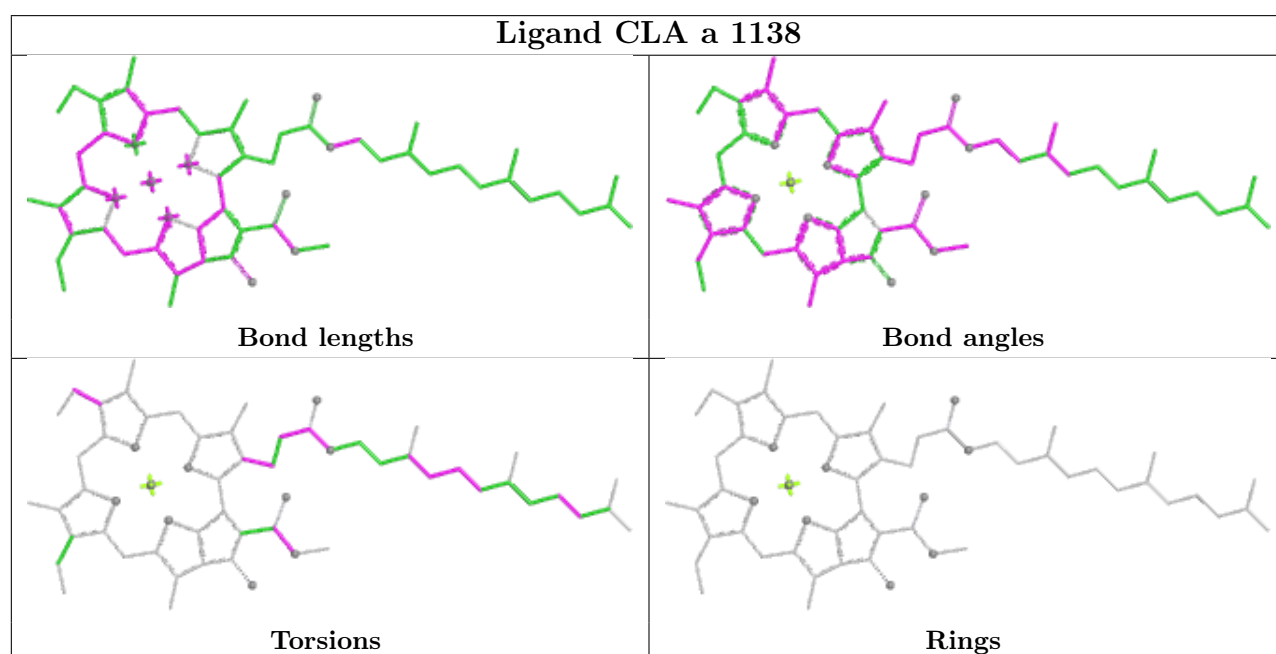
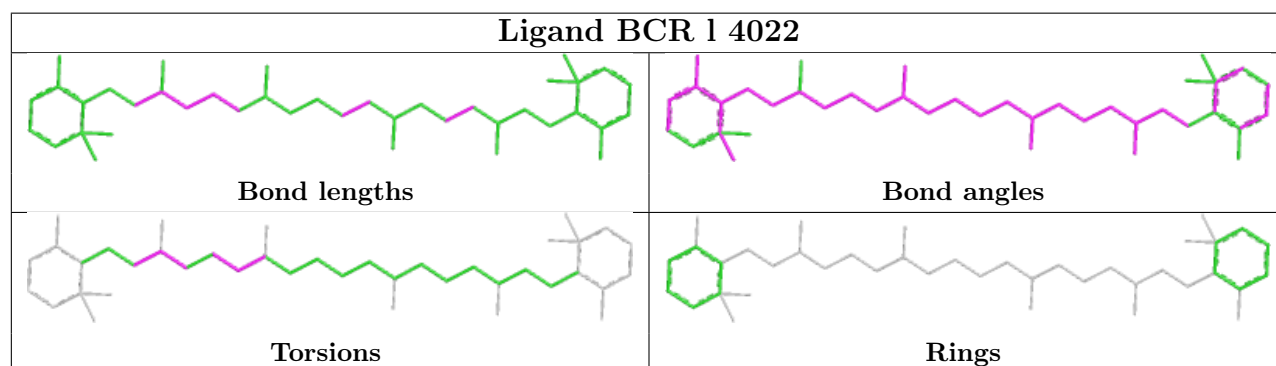
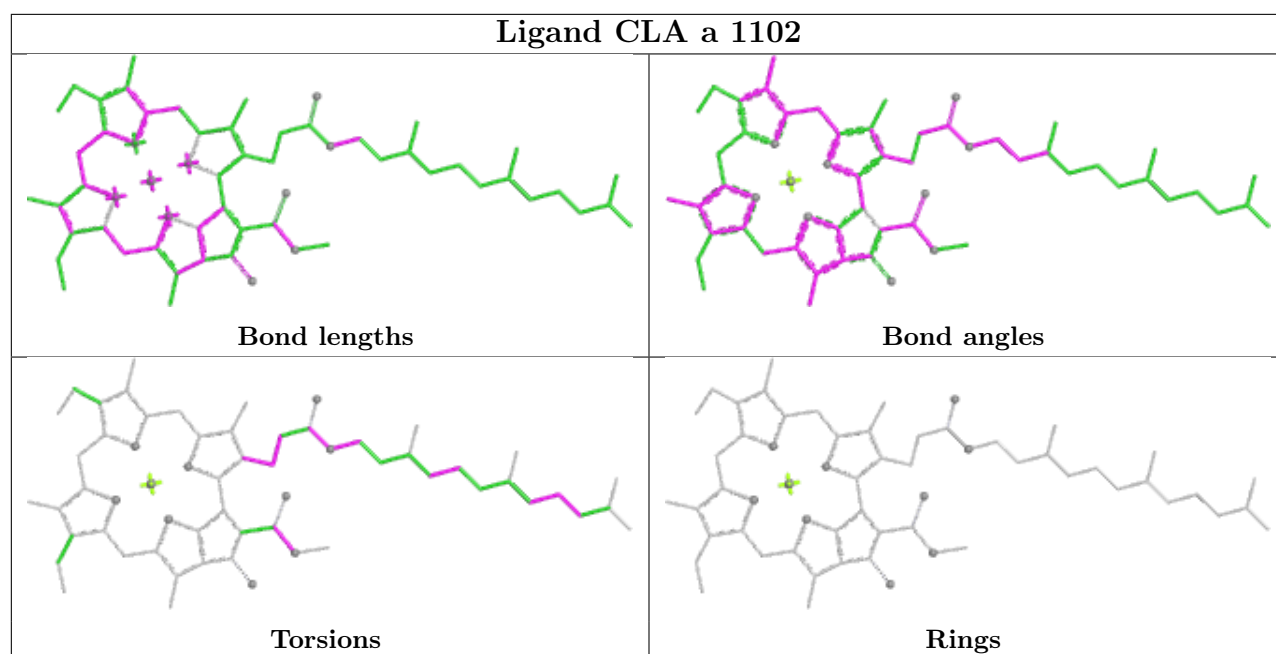


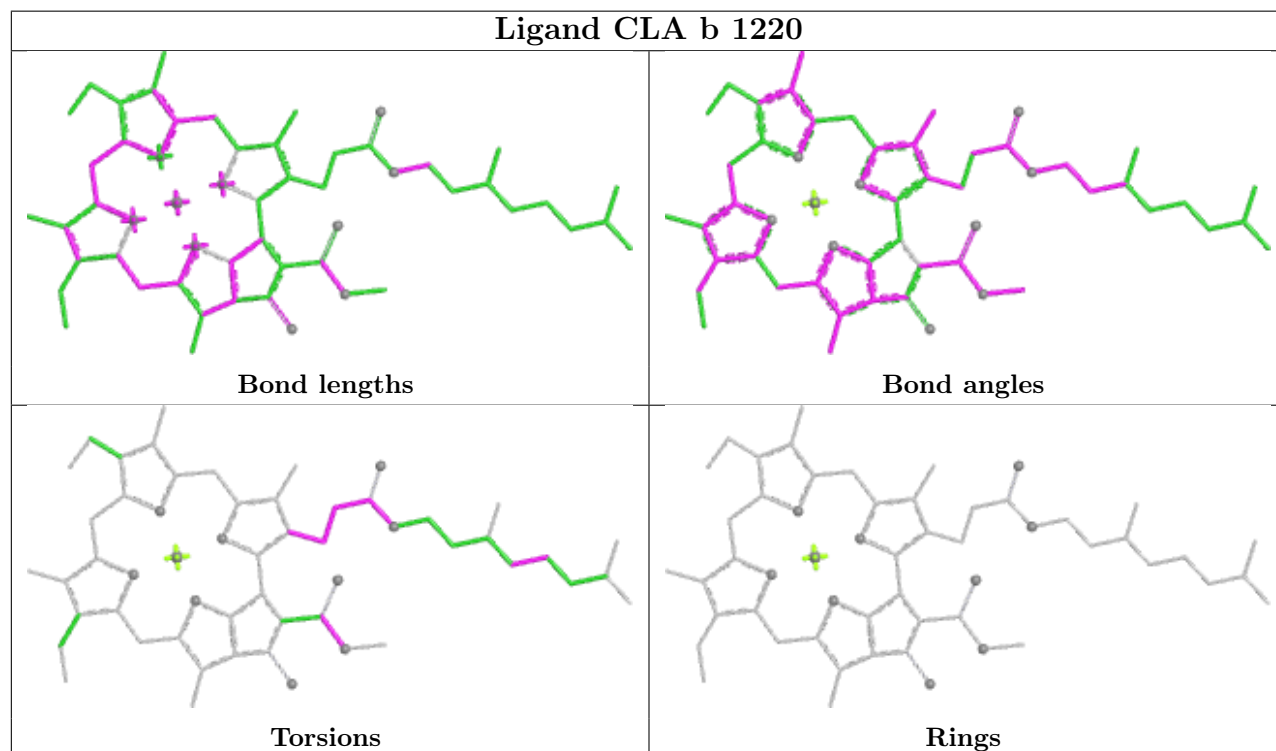
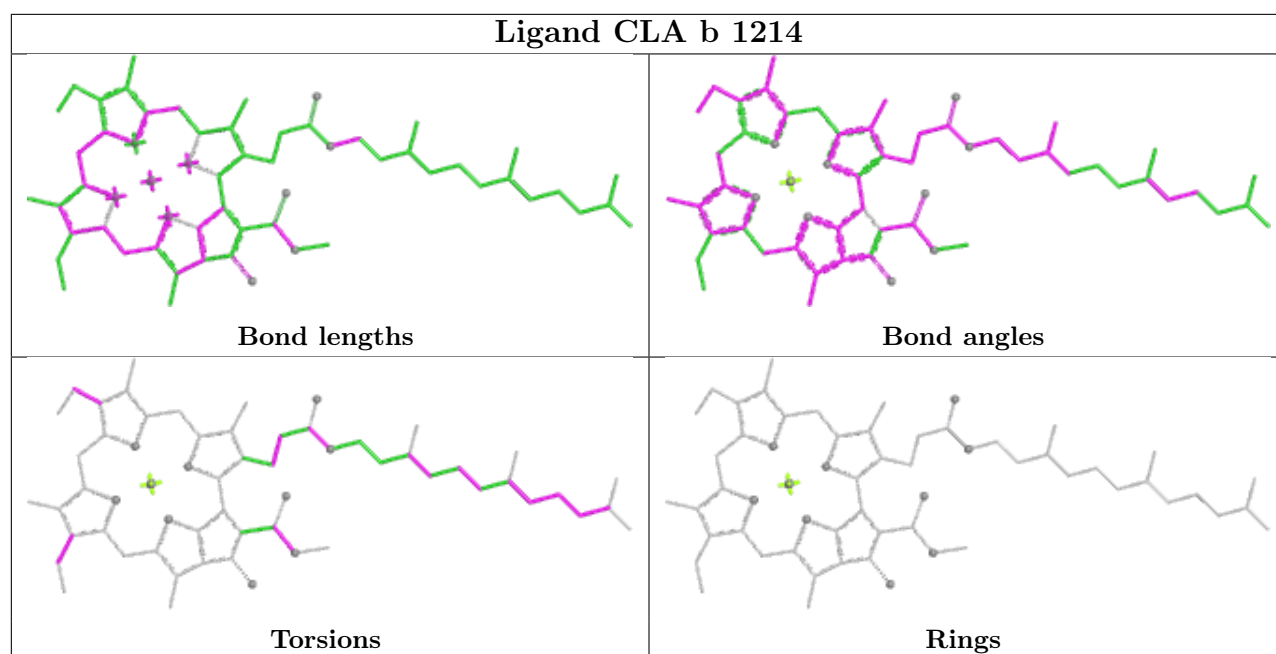
Rings

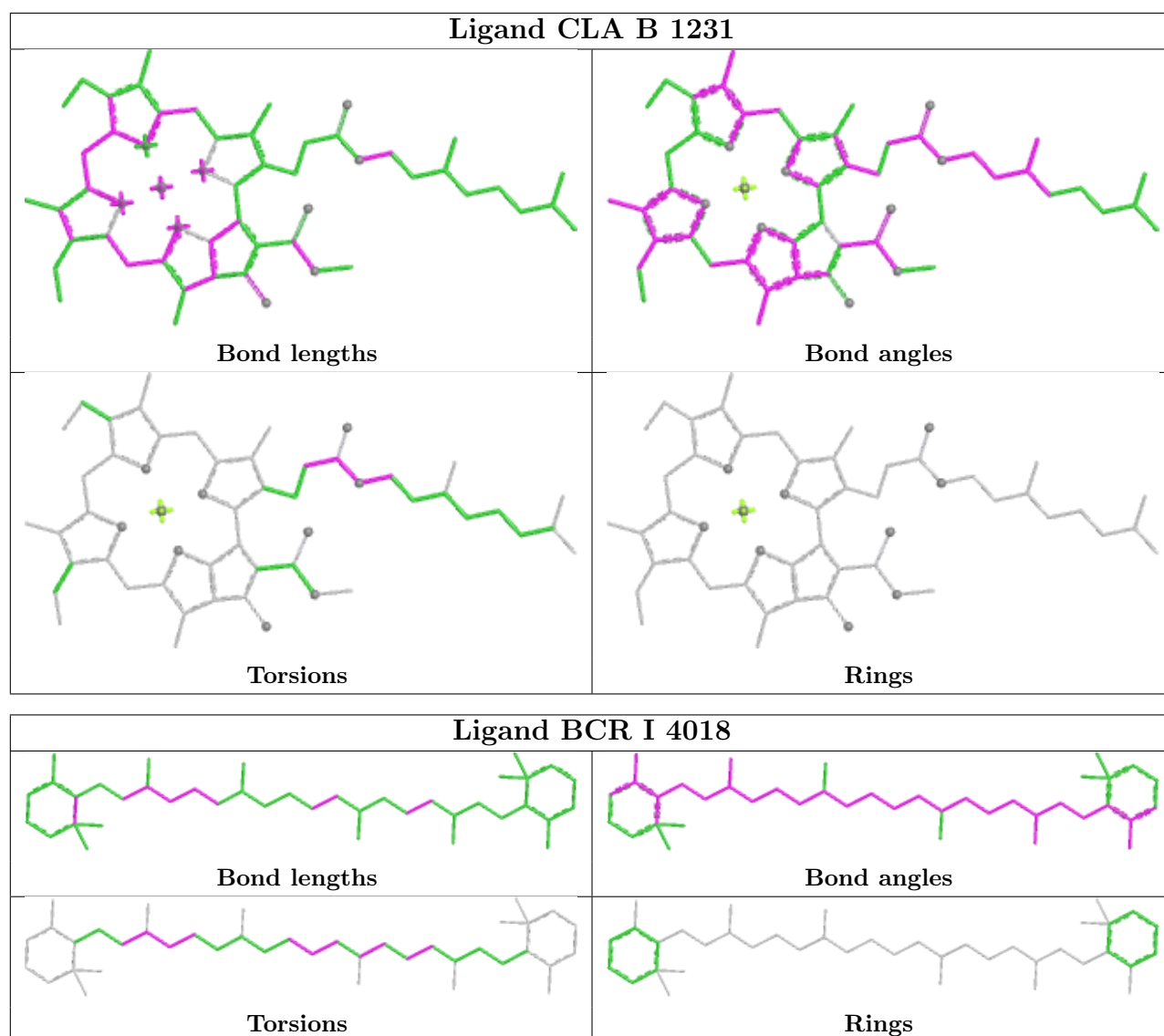


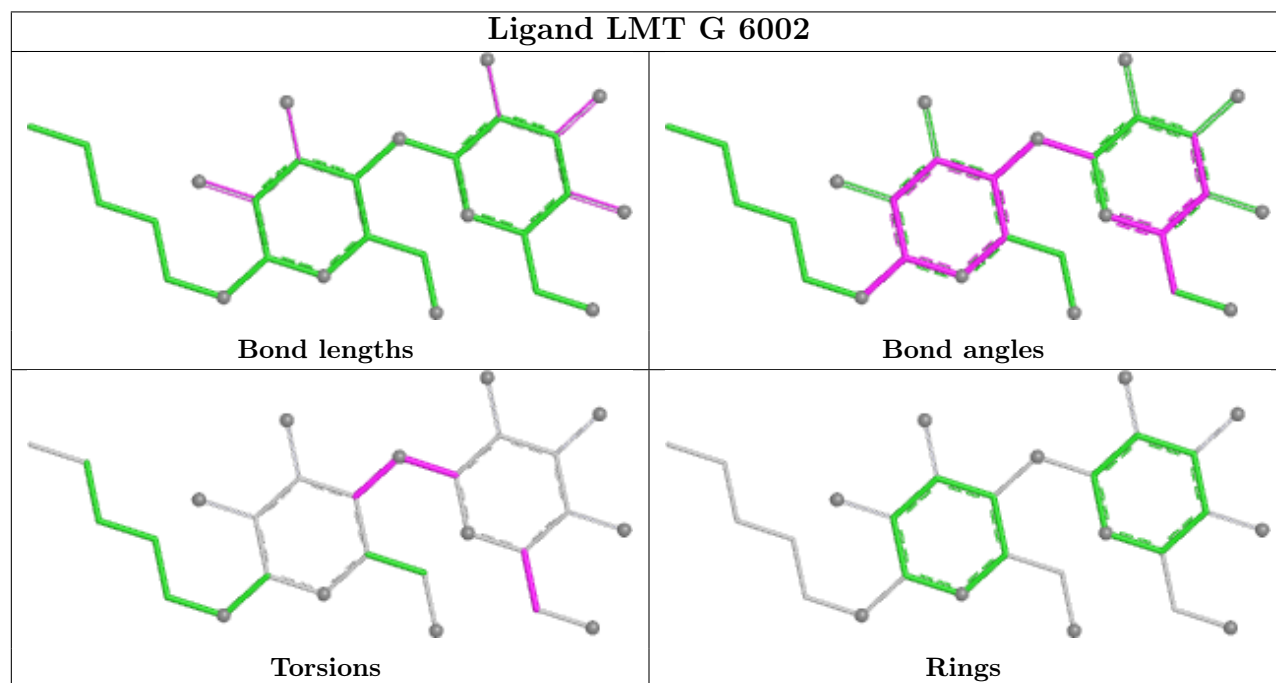
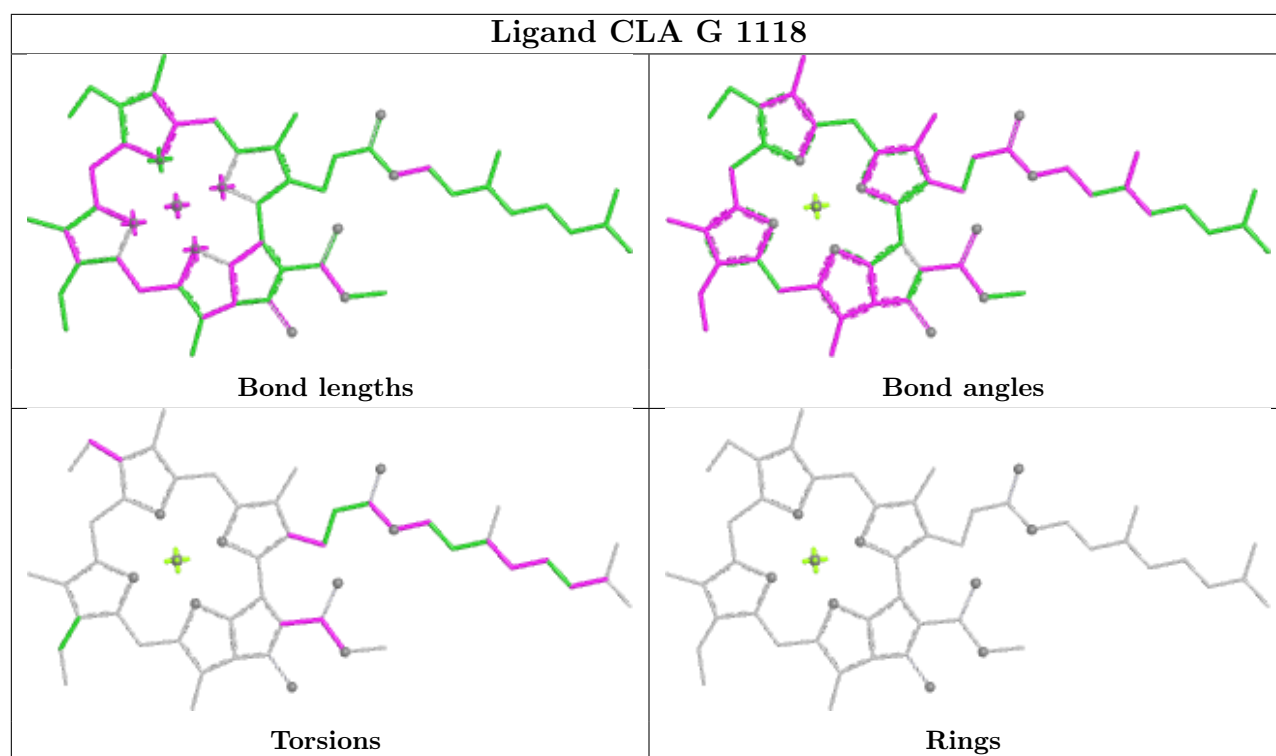


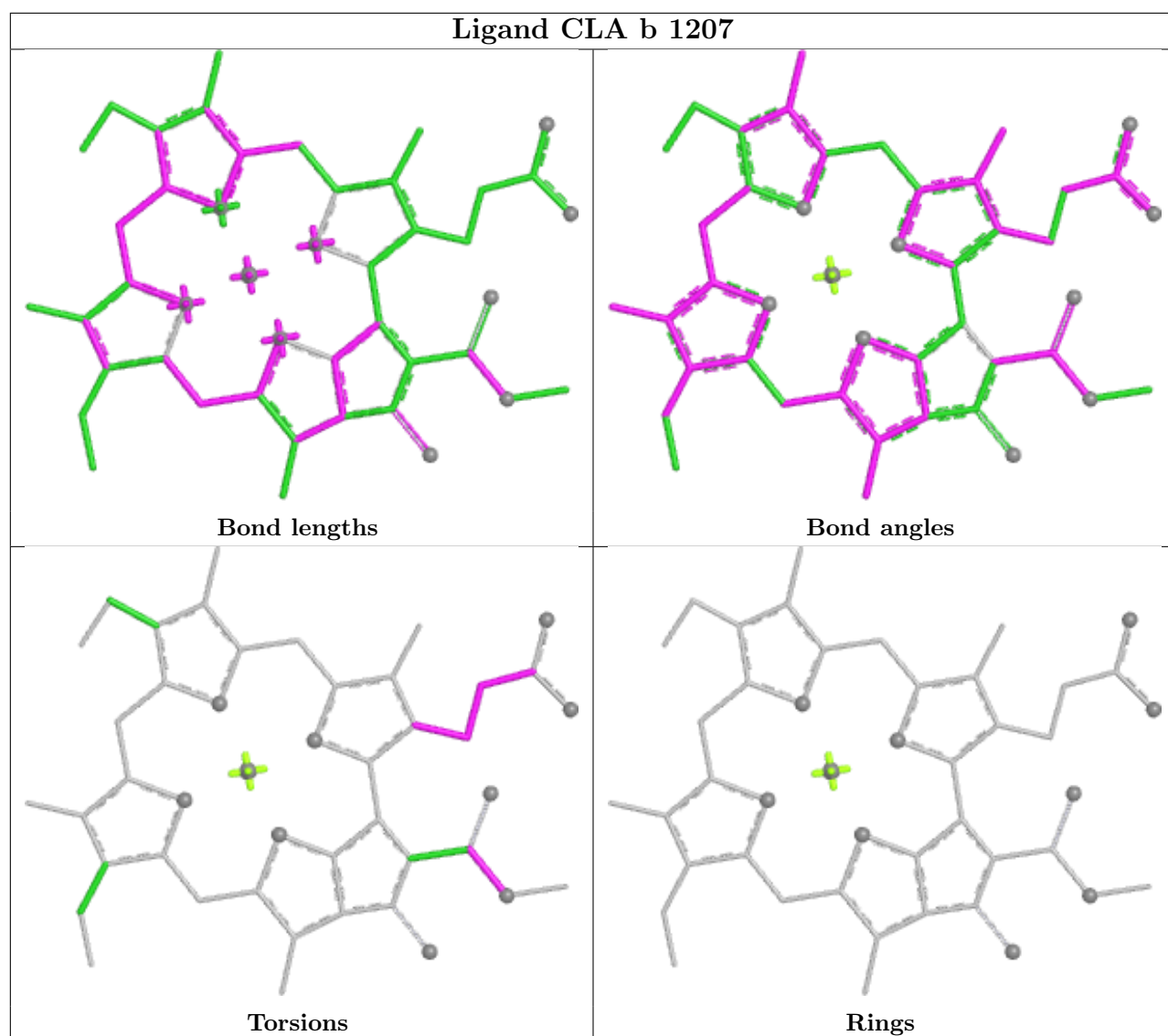




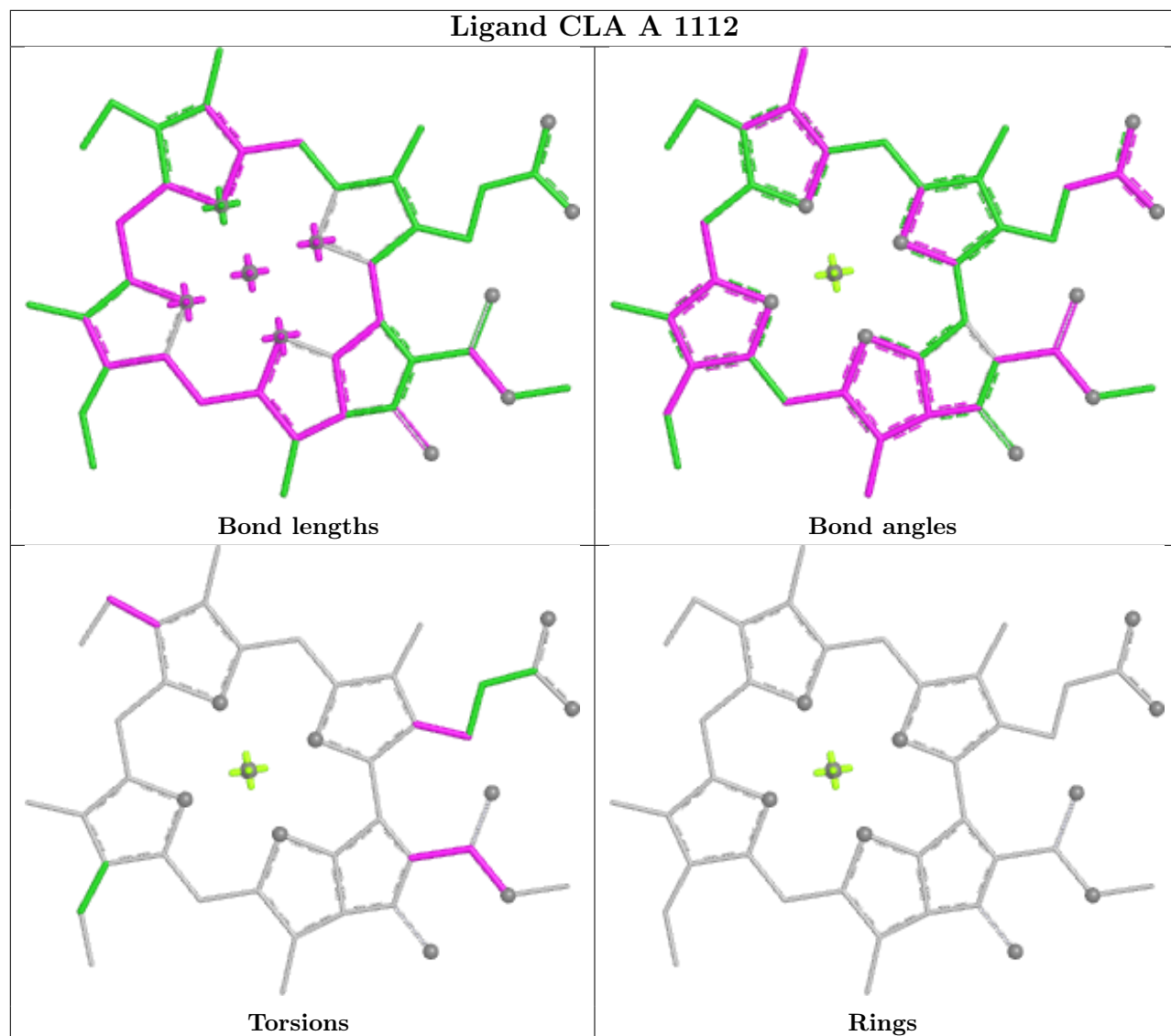


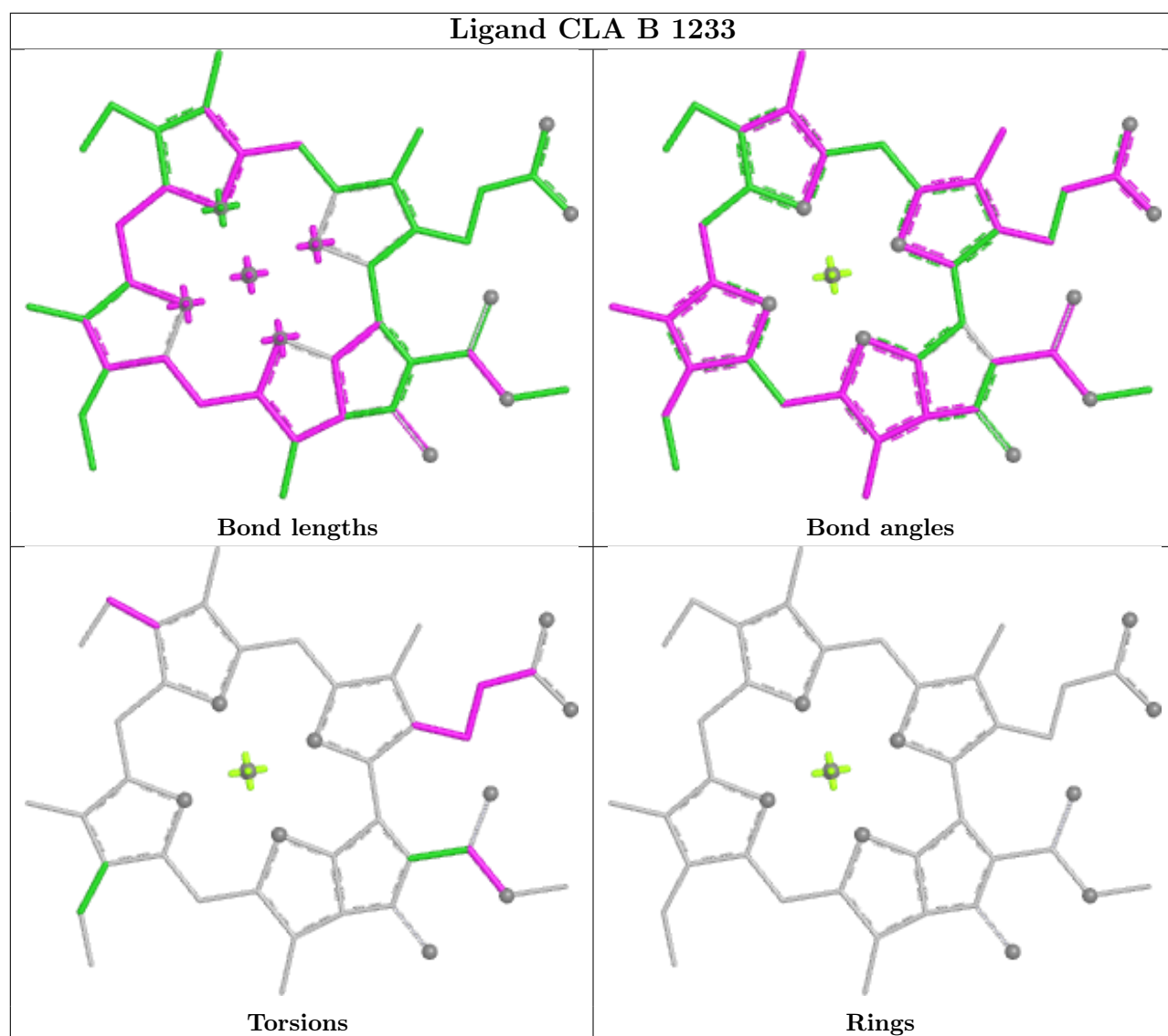


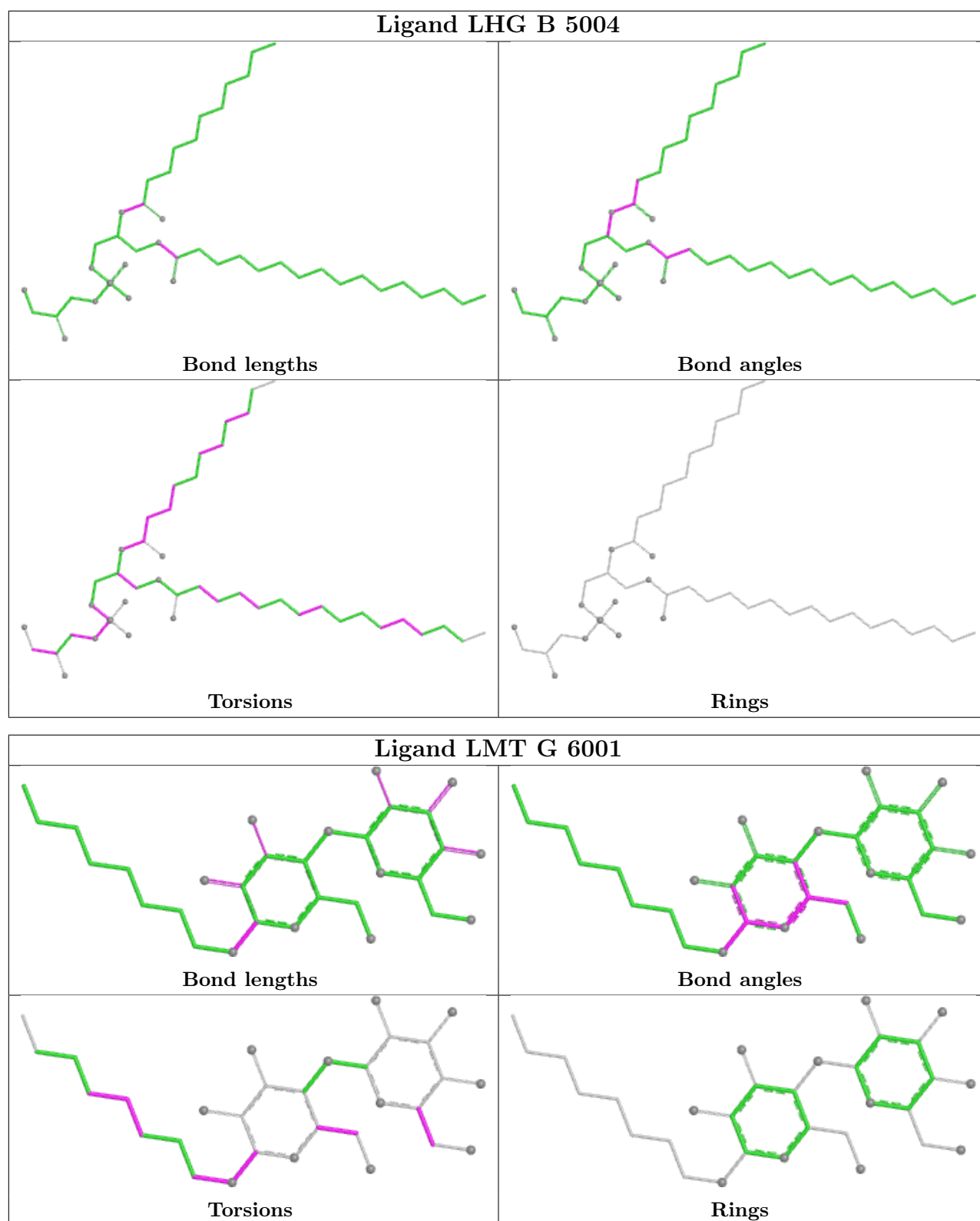




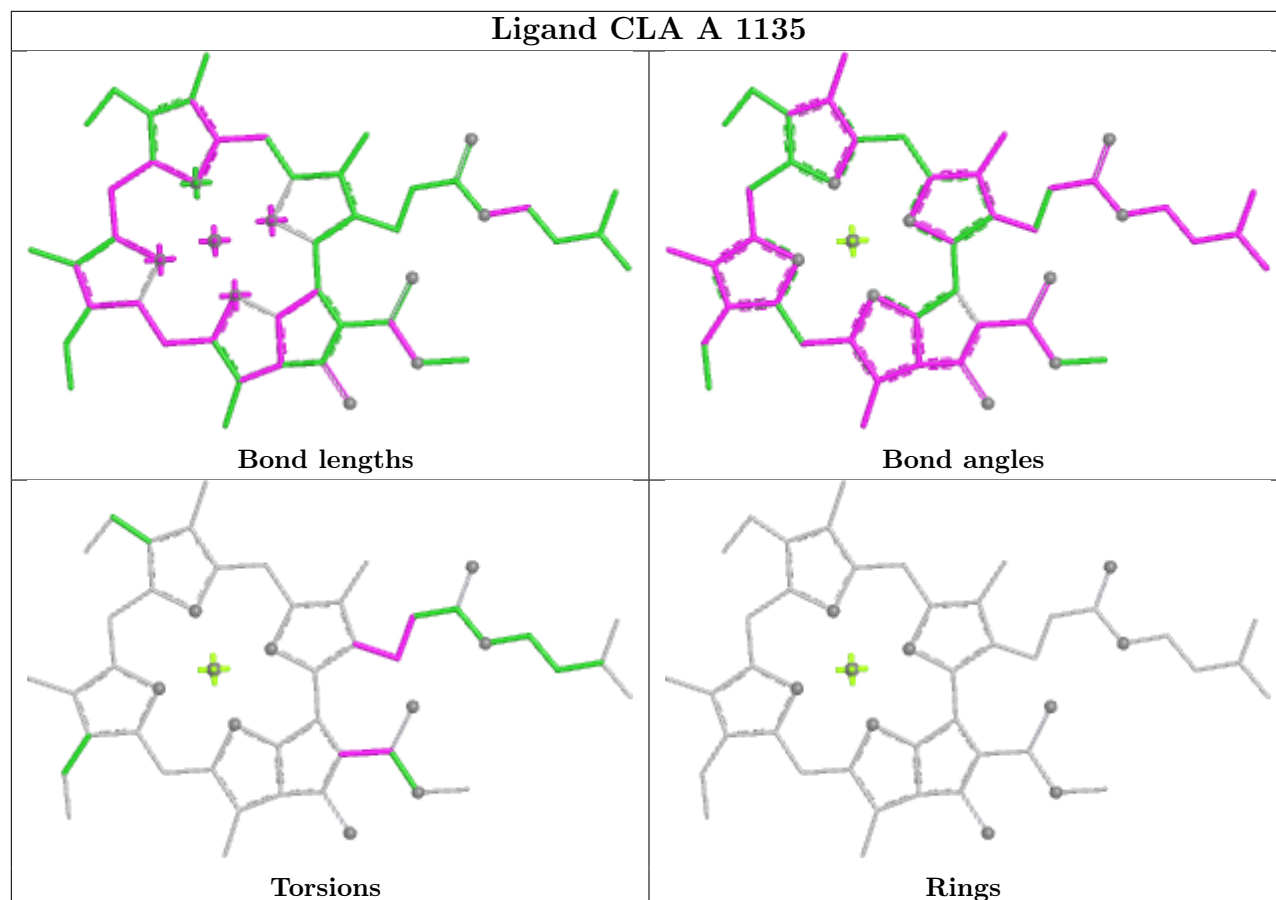
Ligand CLA A 1112



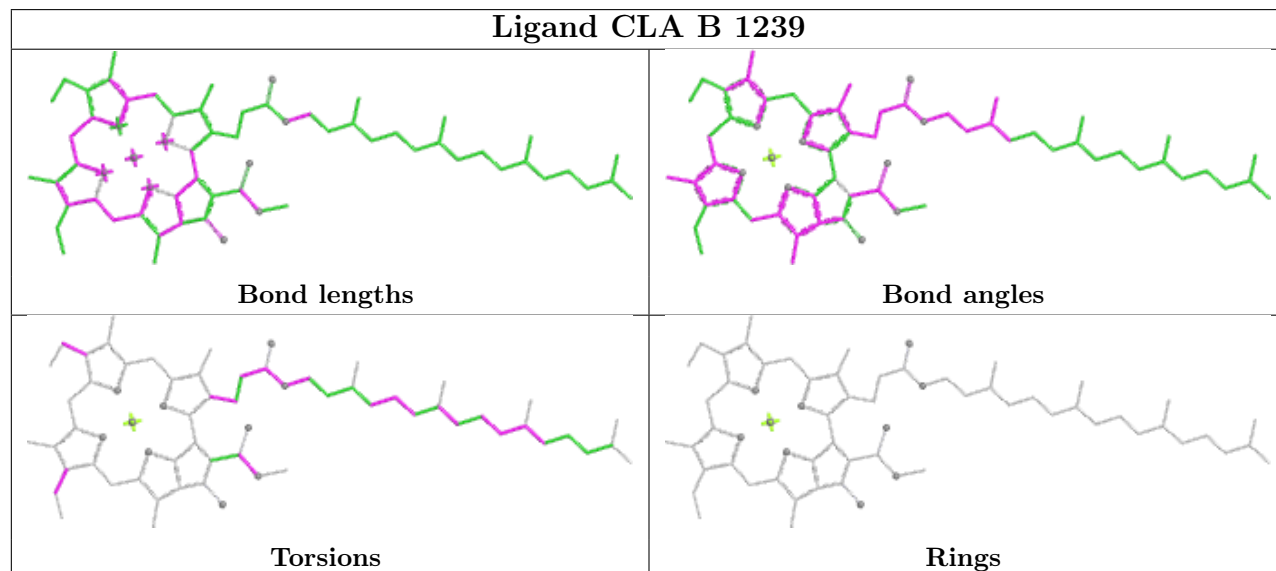


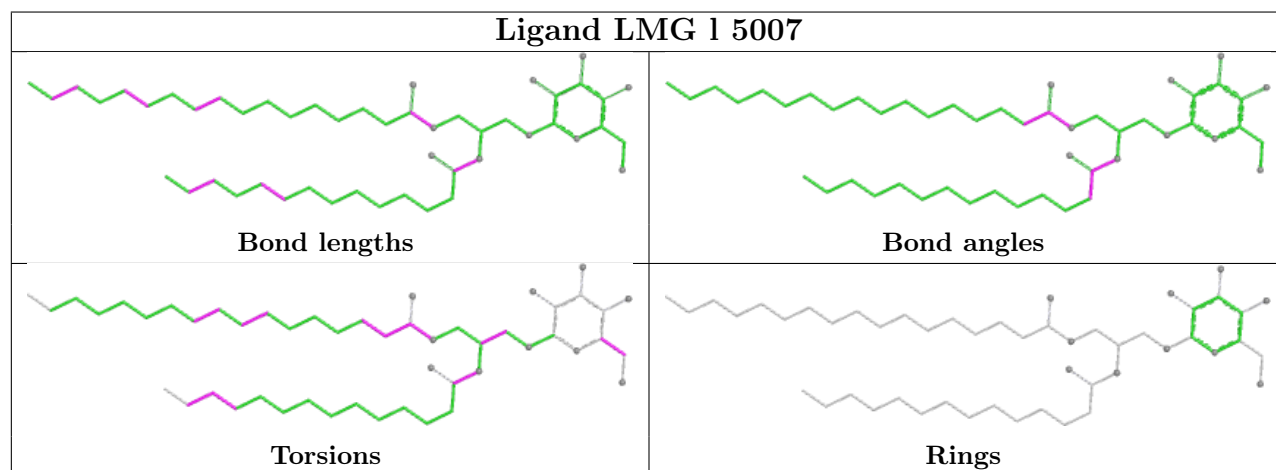
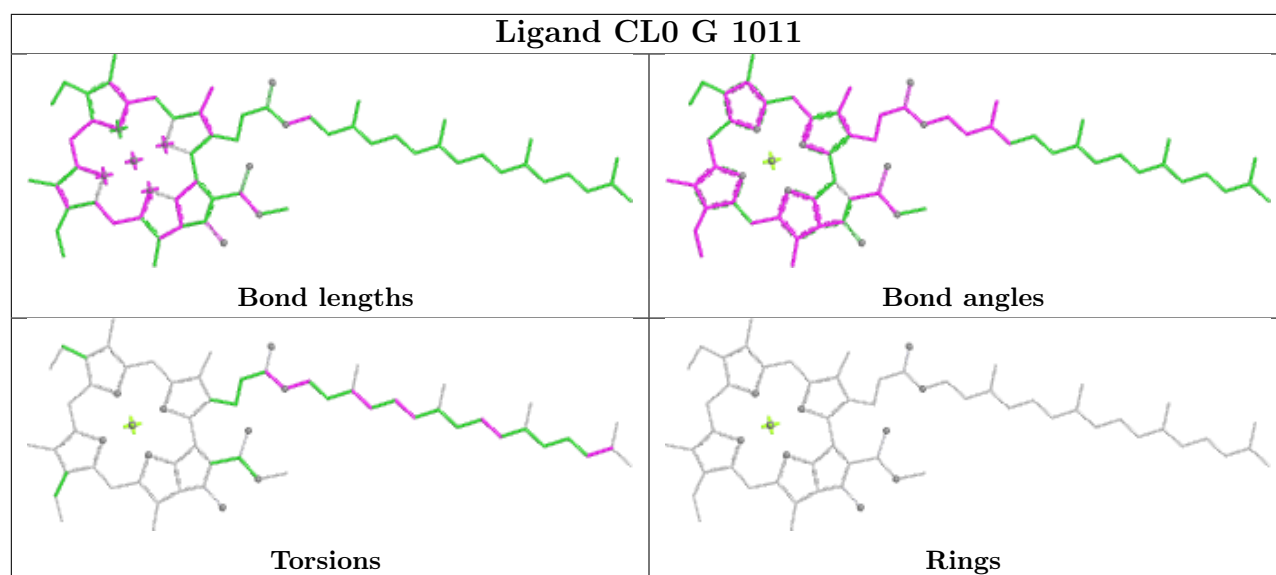


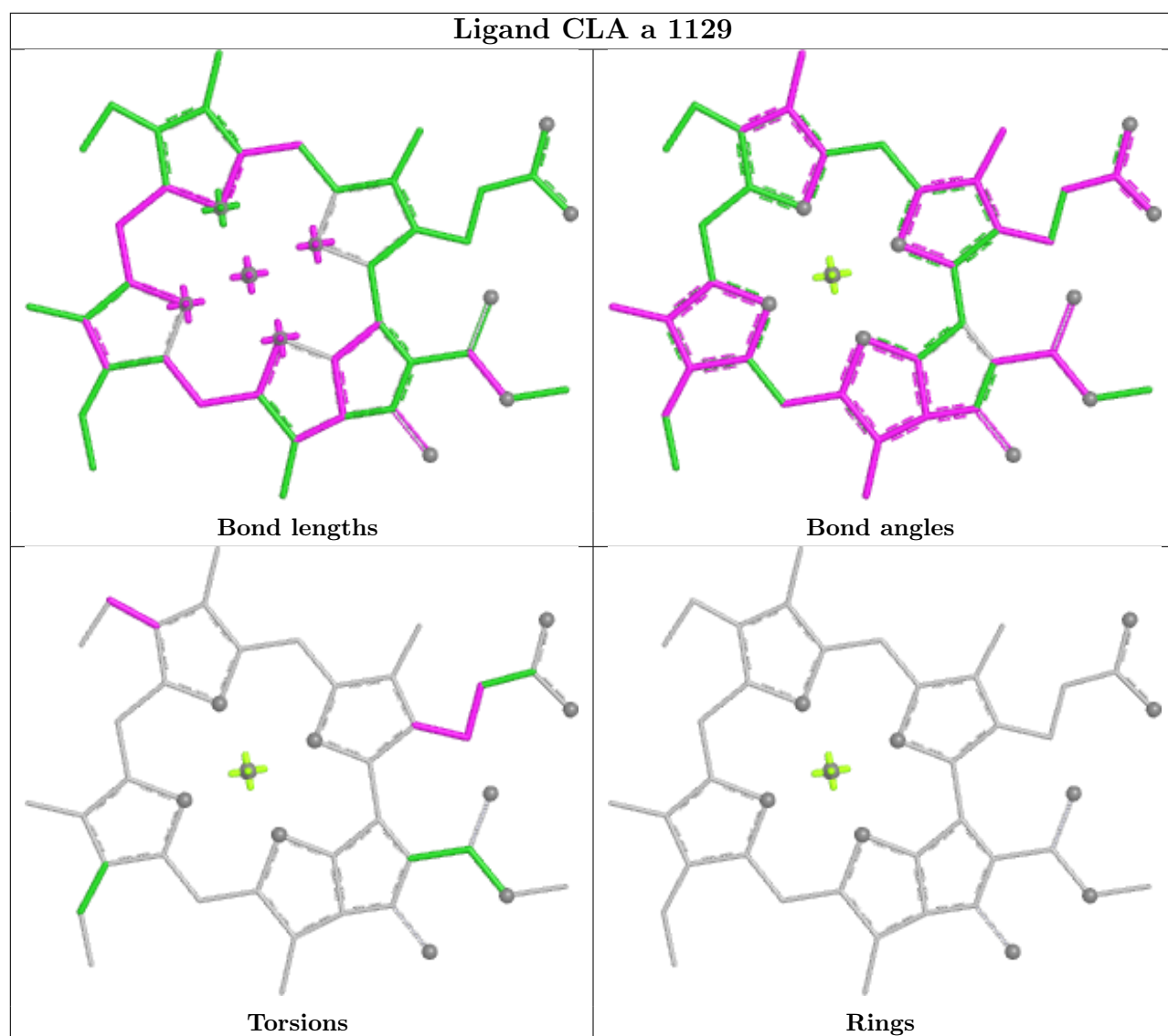
Ligand CLA A 1135



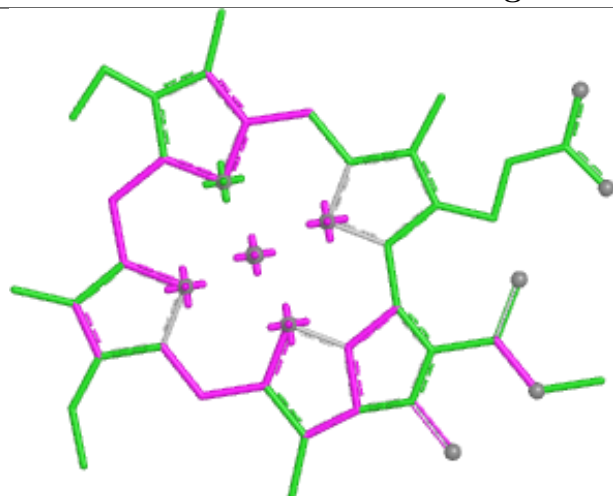
Ligand CLA B 1239



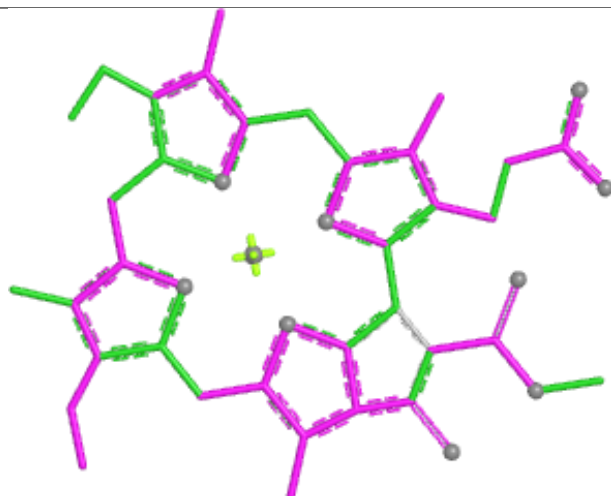




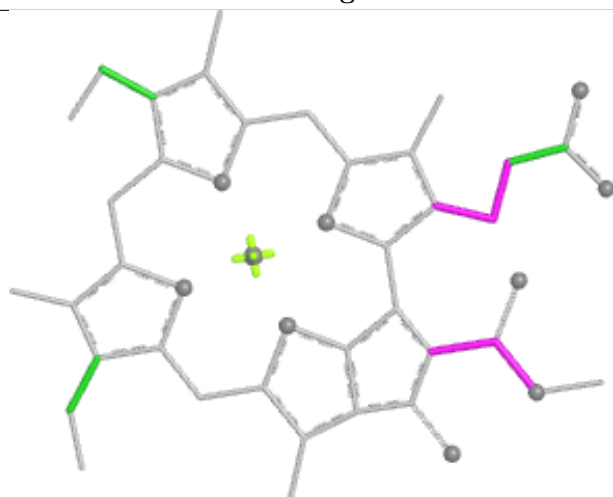
Ligand CLA G 1113



Bond lengths



Bond angles

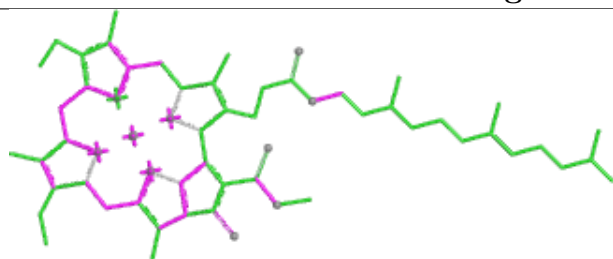


Torsions

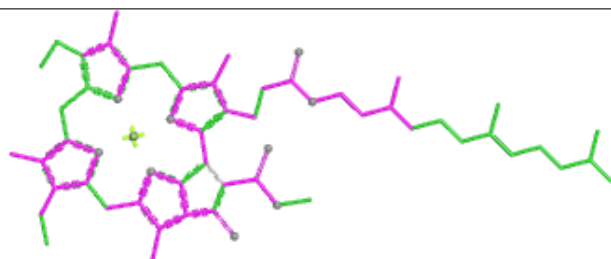


Rings

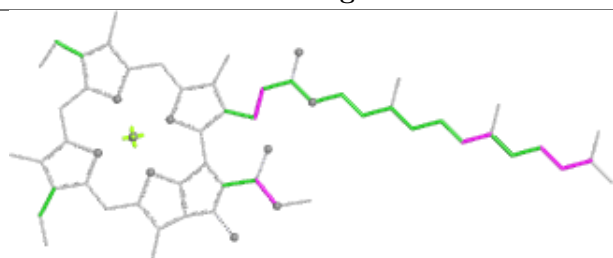
Ligand CLA A 1123



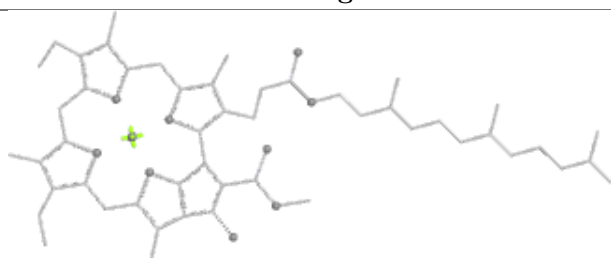
Bond lengths



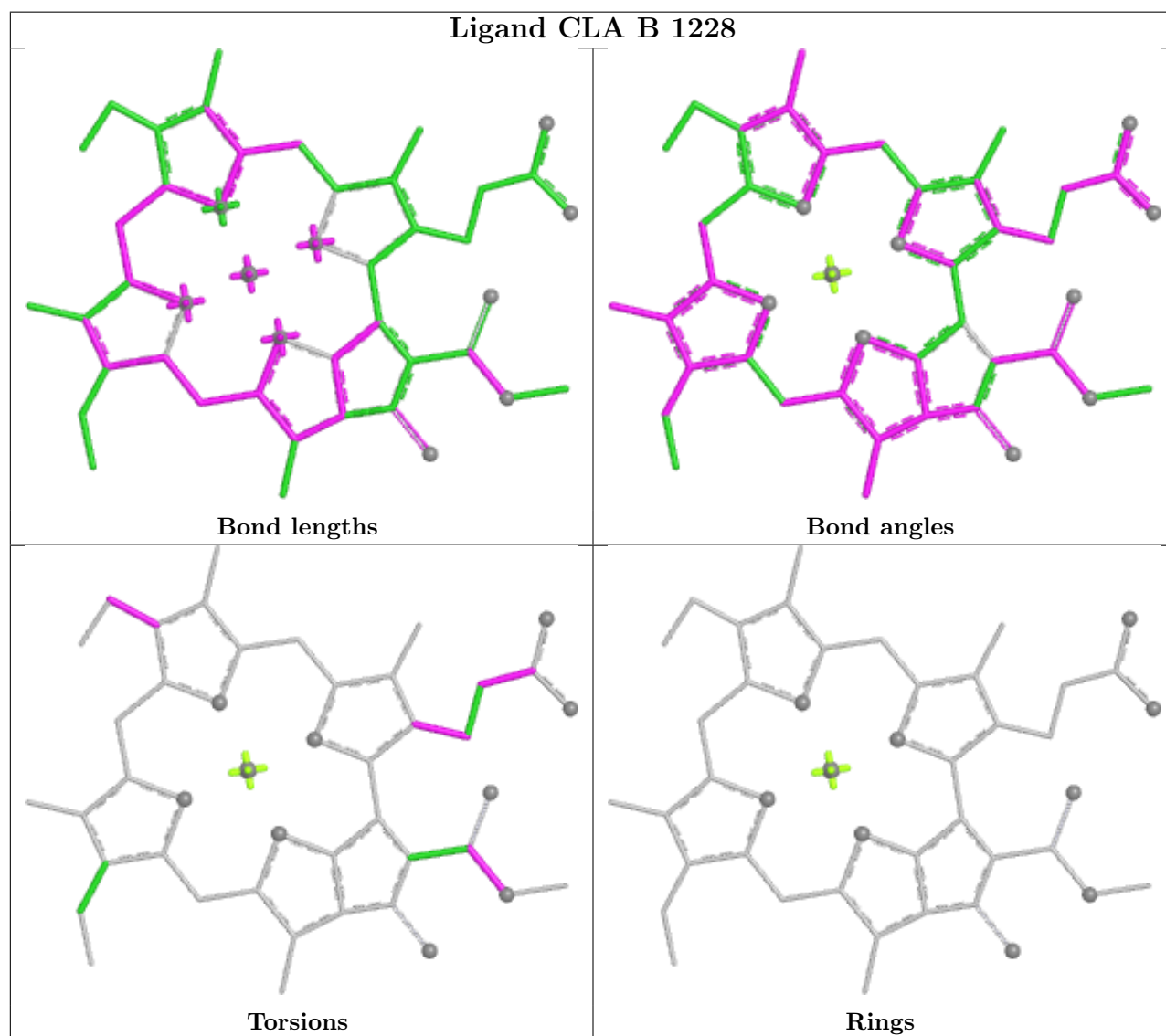
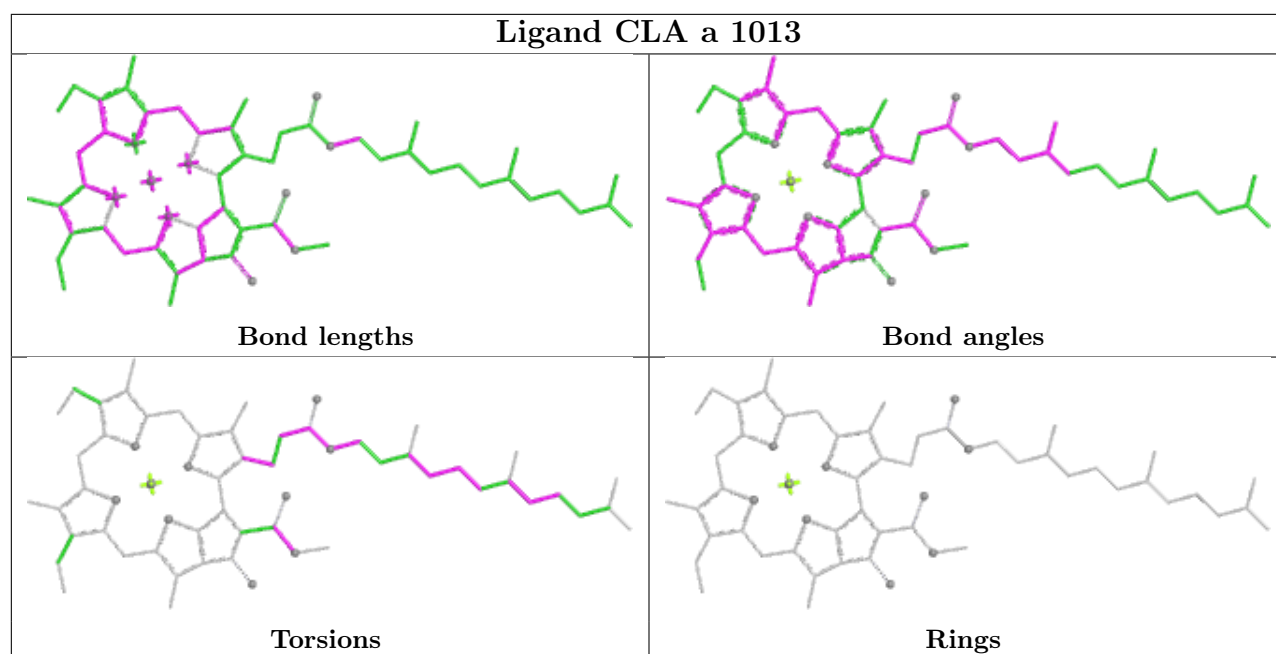
Bond angles

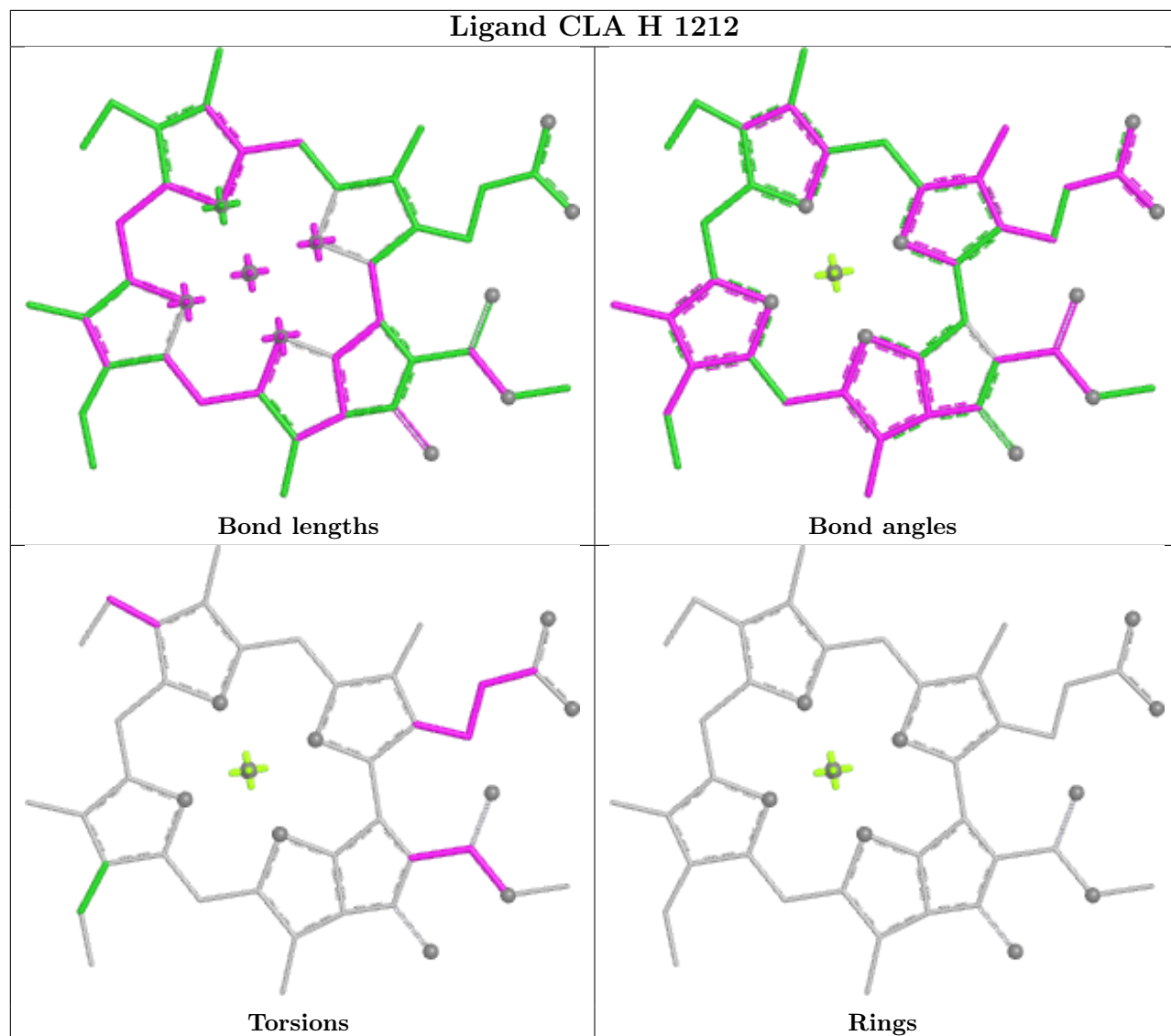


Torsions

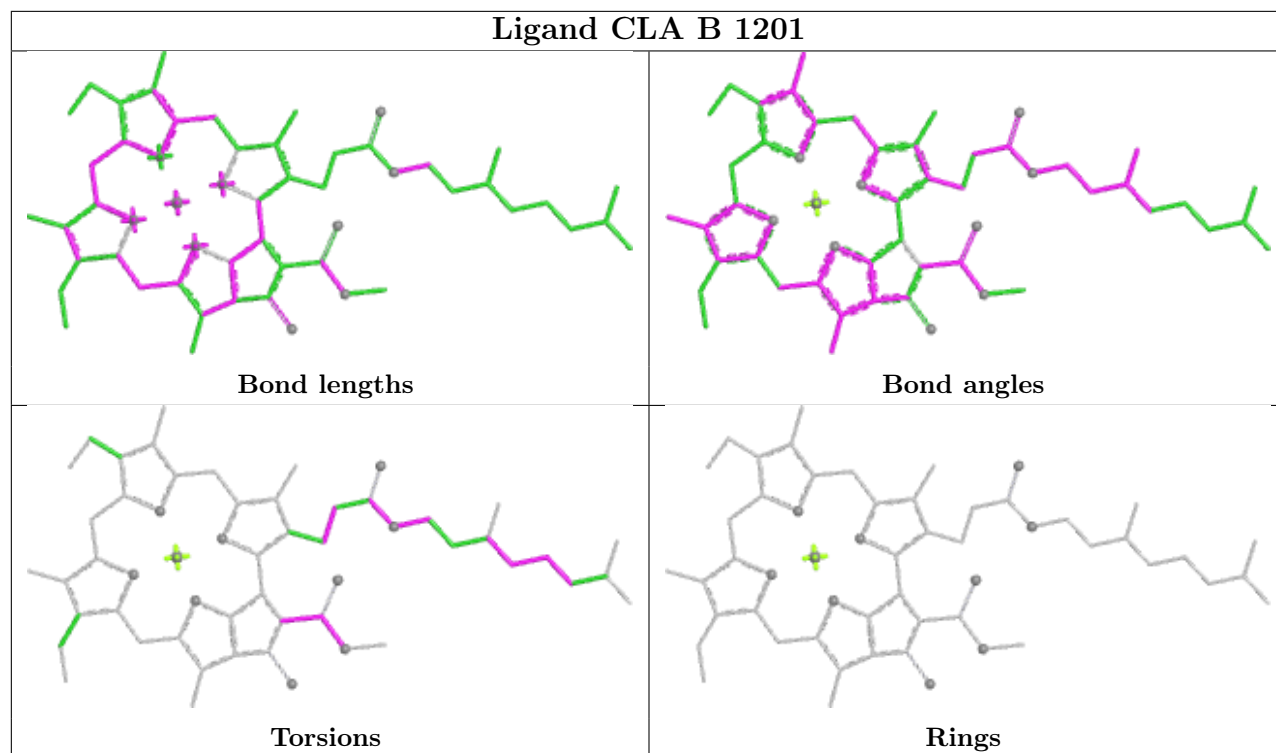


Rings

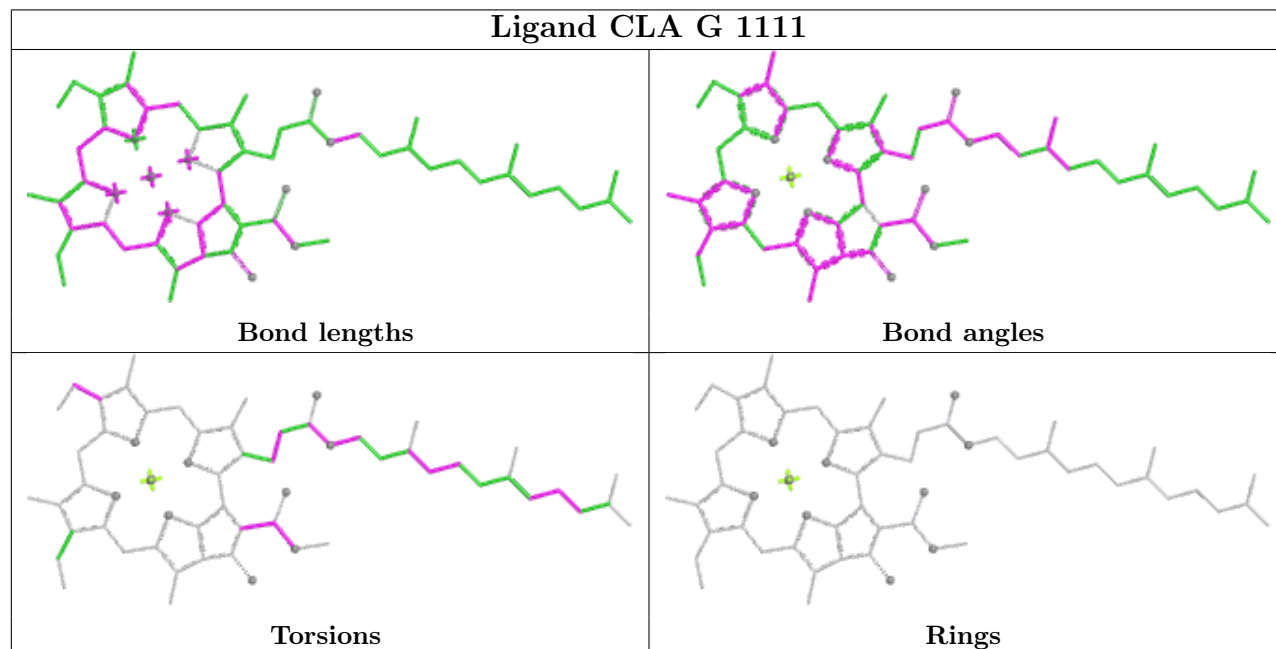


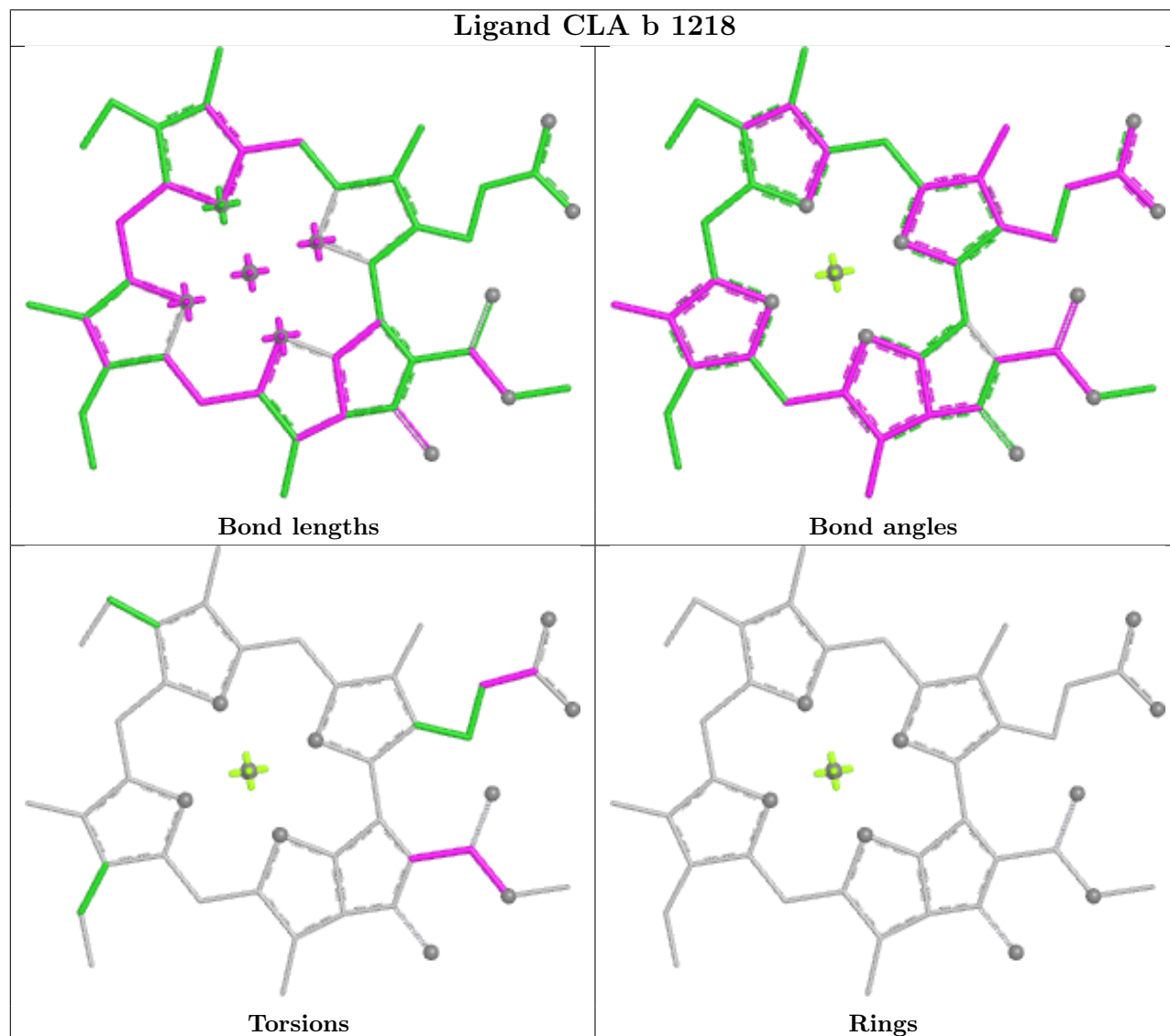
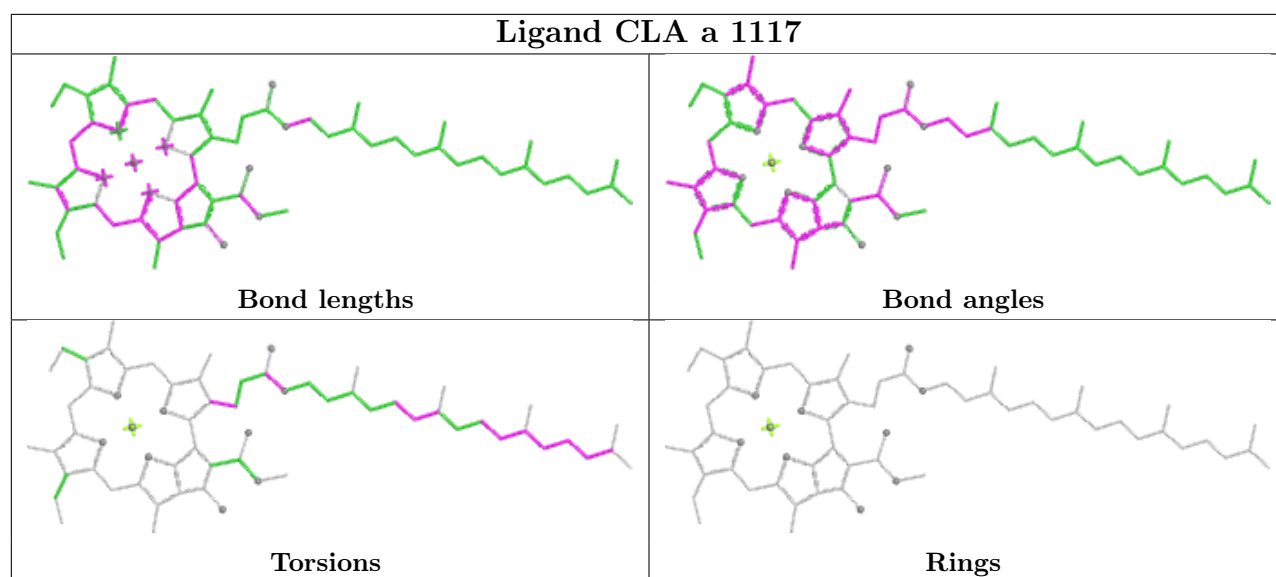


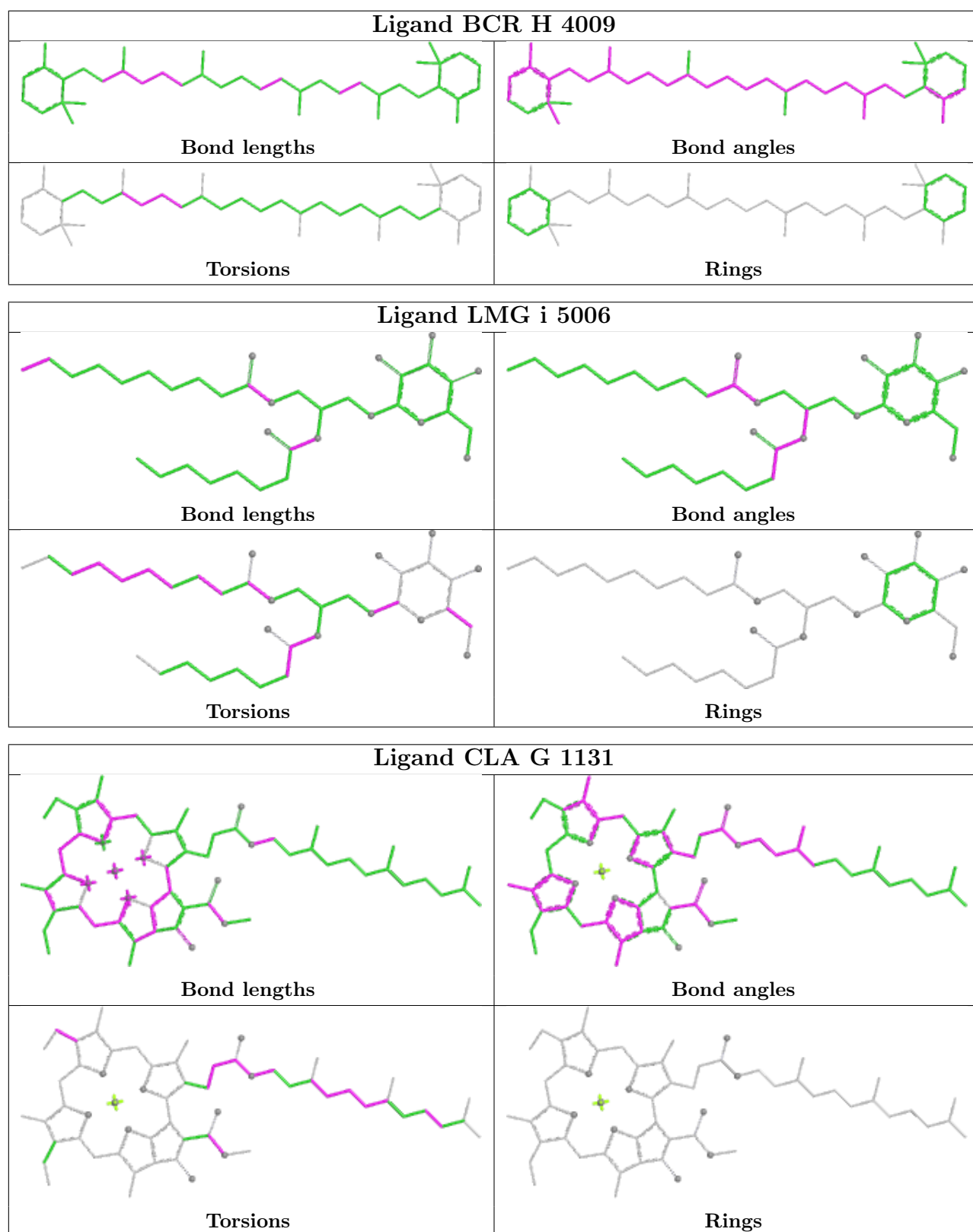
Ligand CLA B 1201

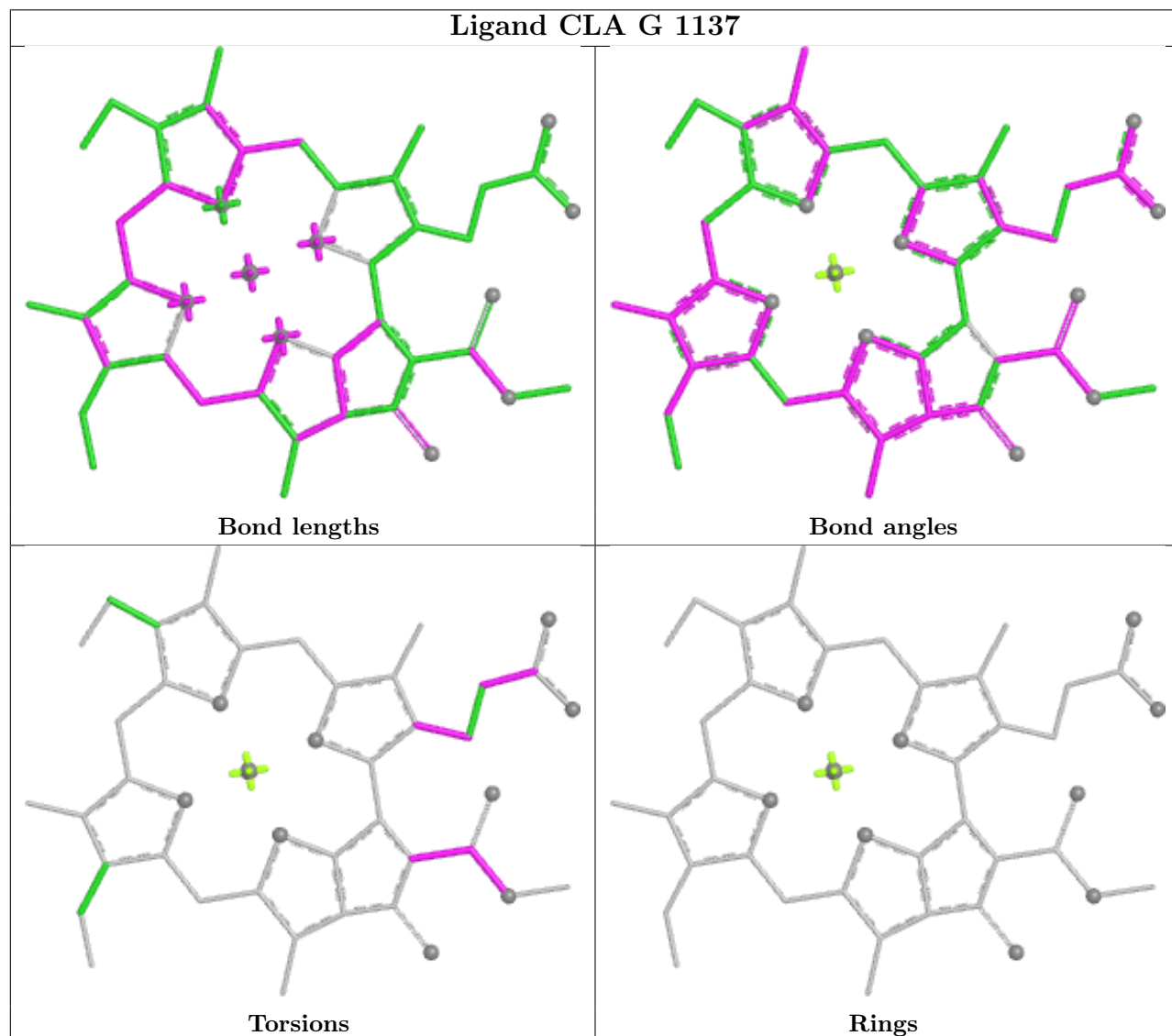
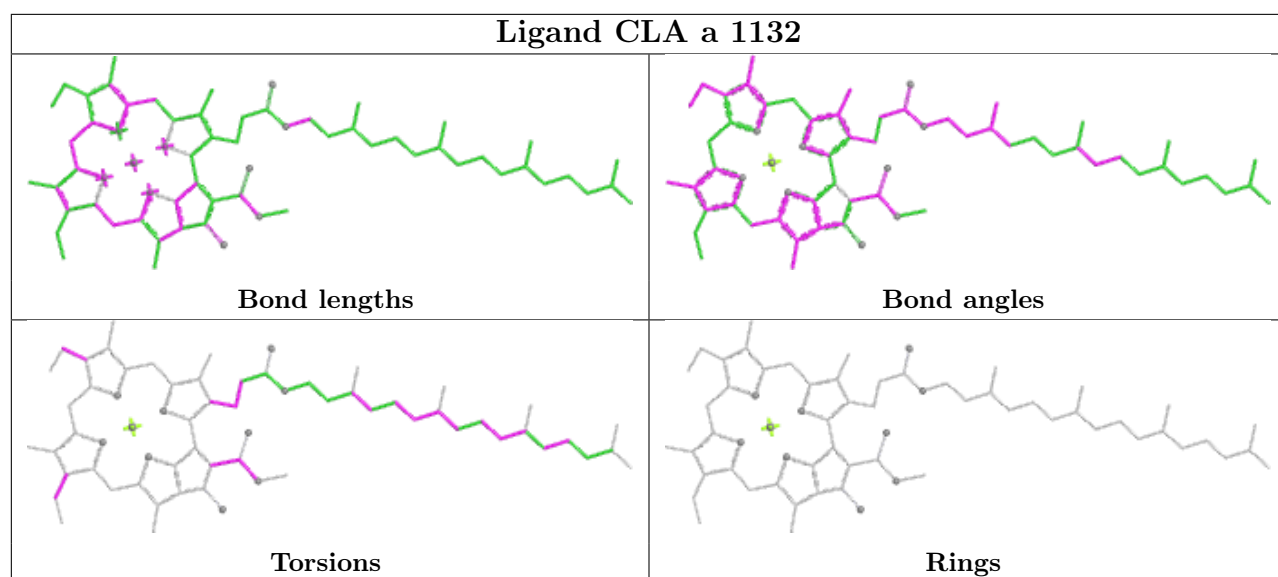


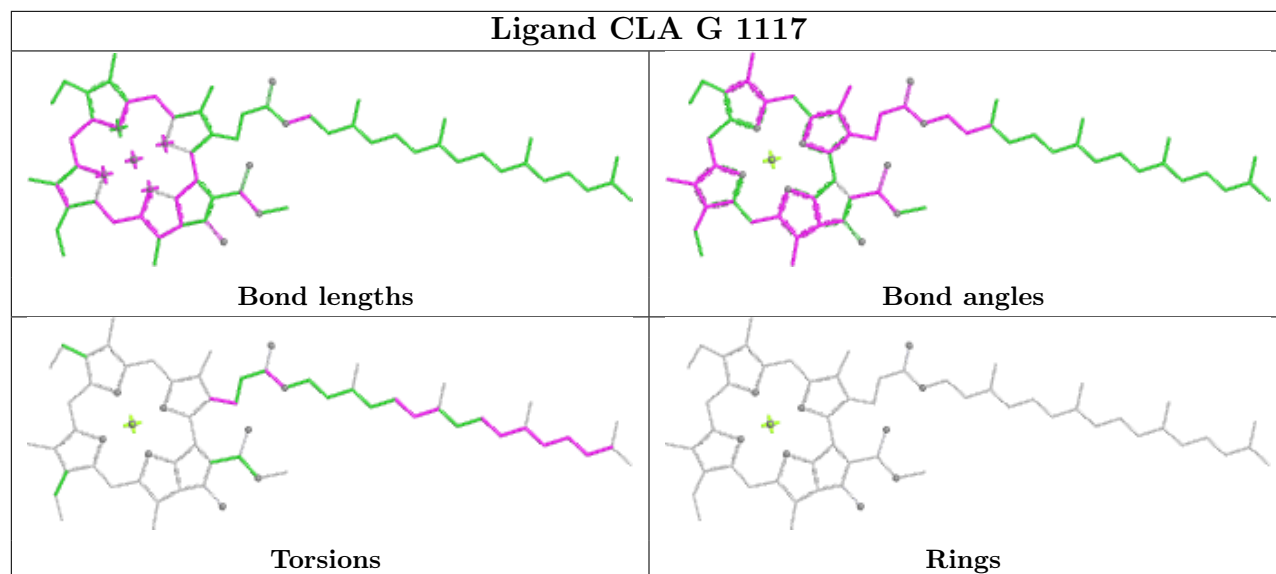
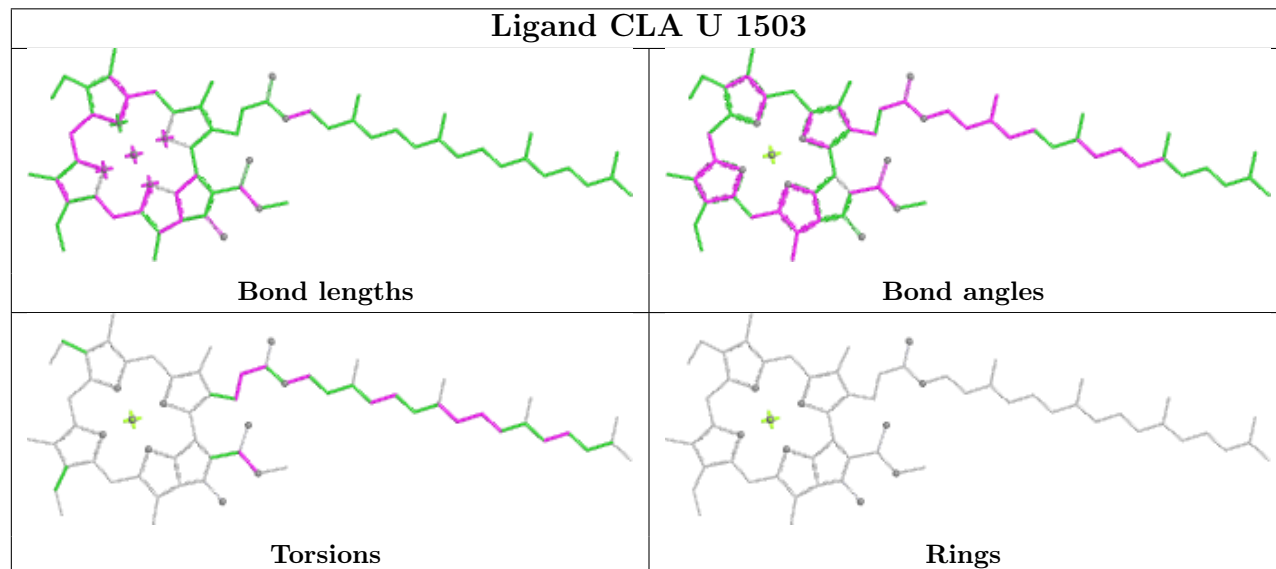
Ligand CLA G 1111



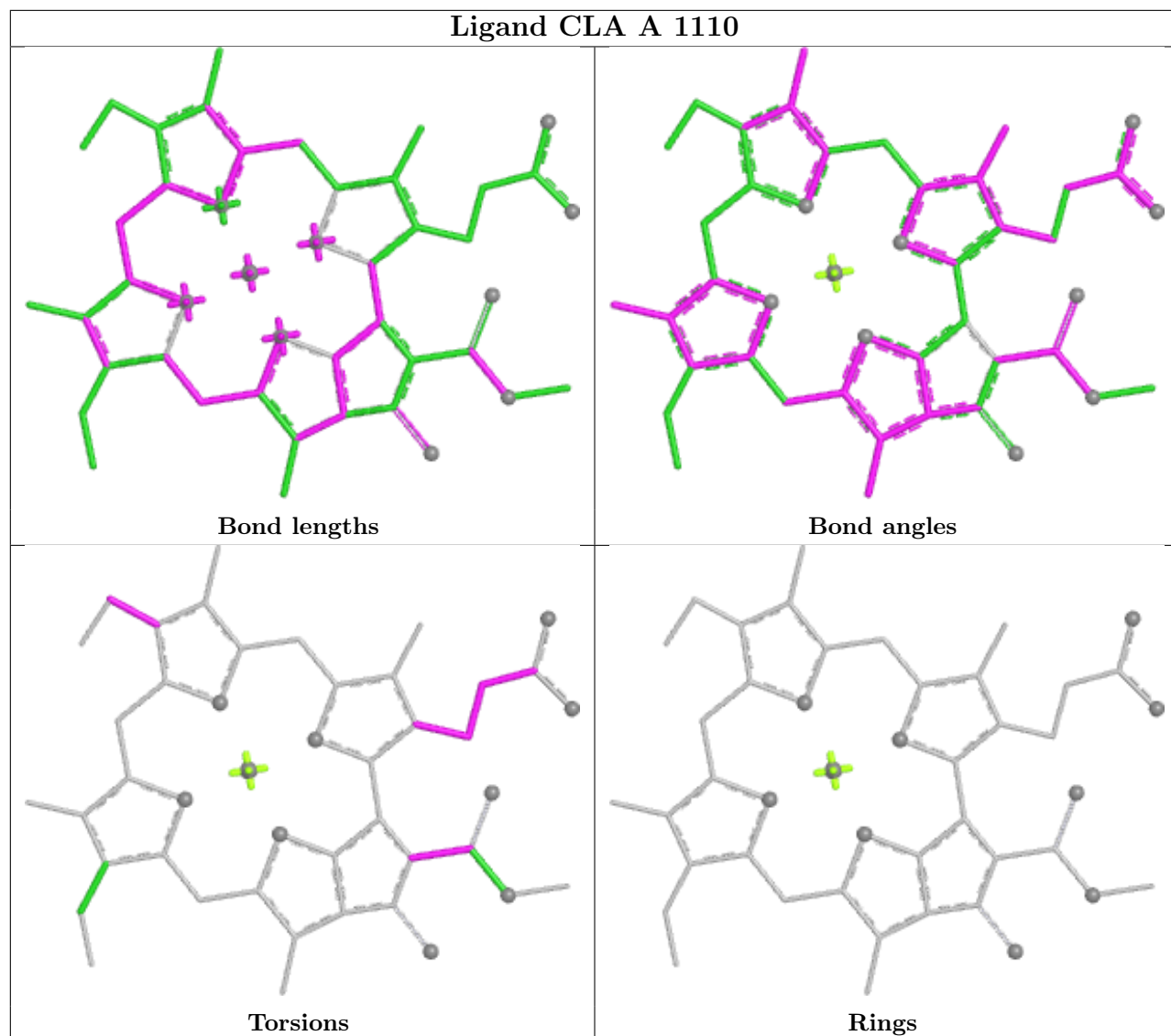


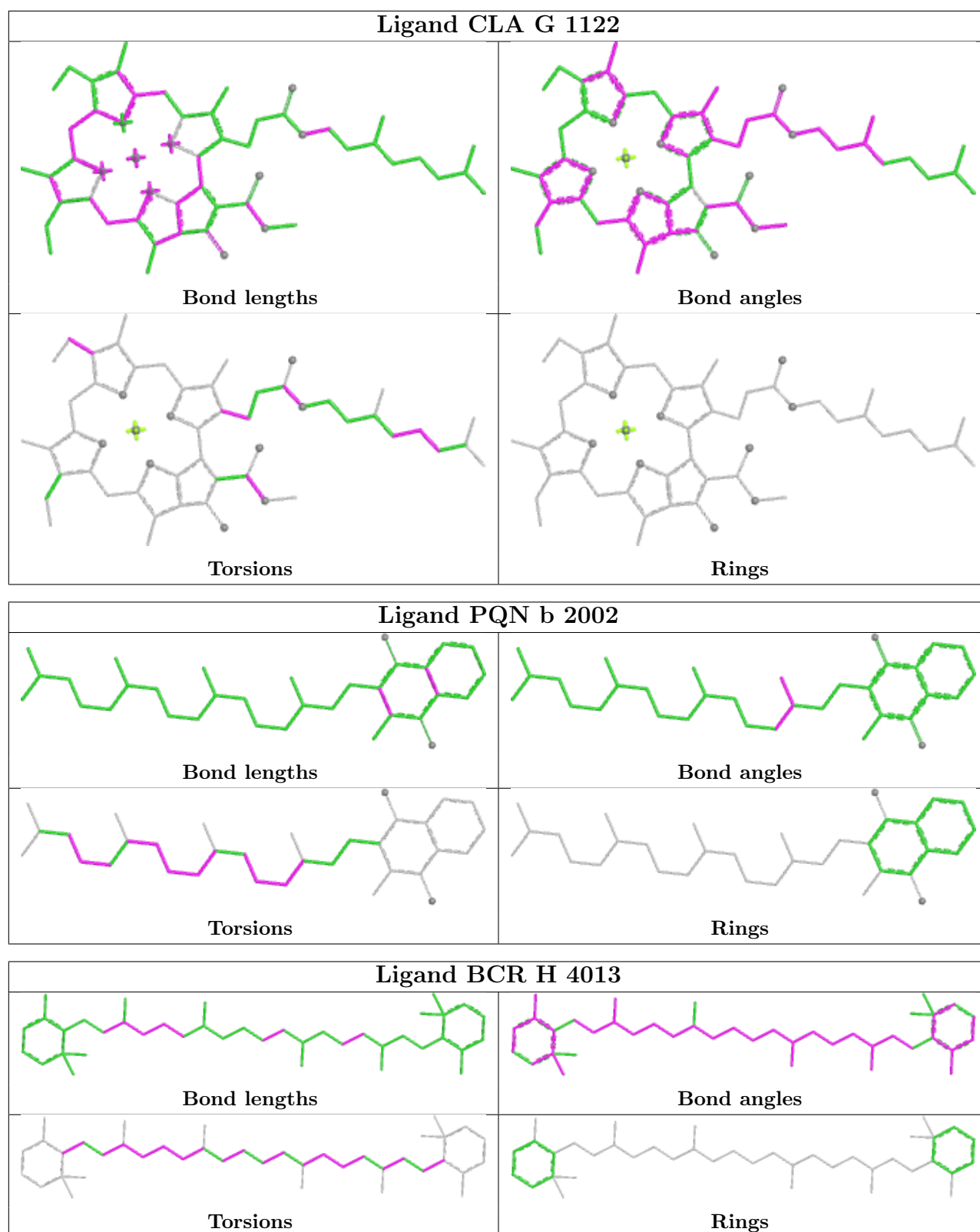


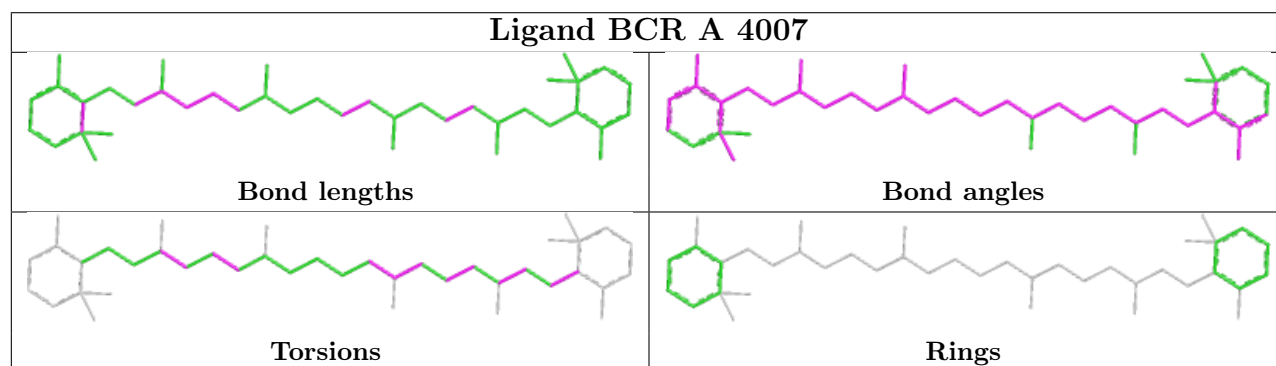
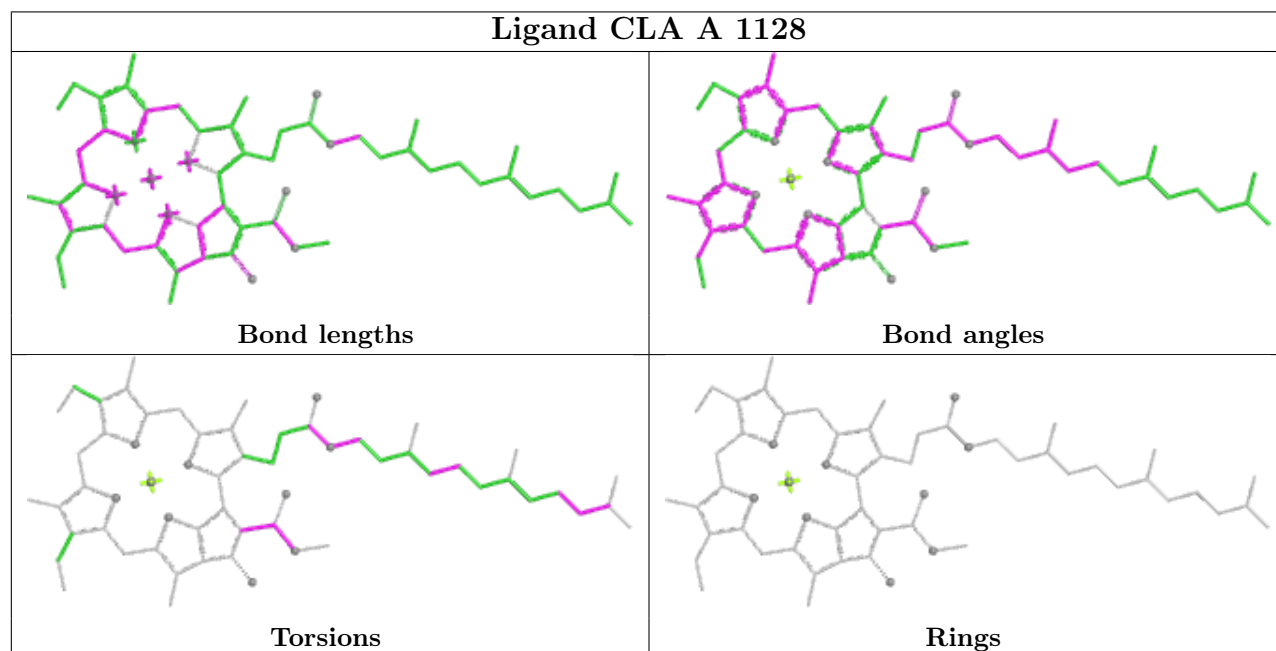
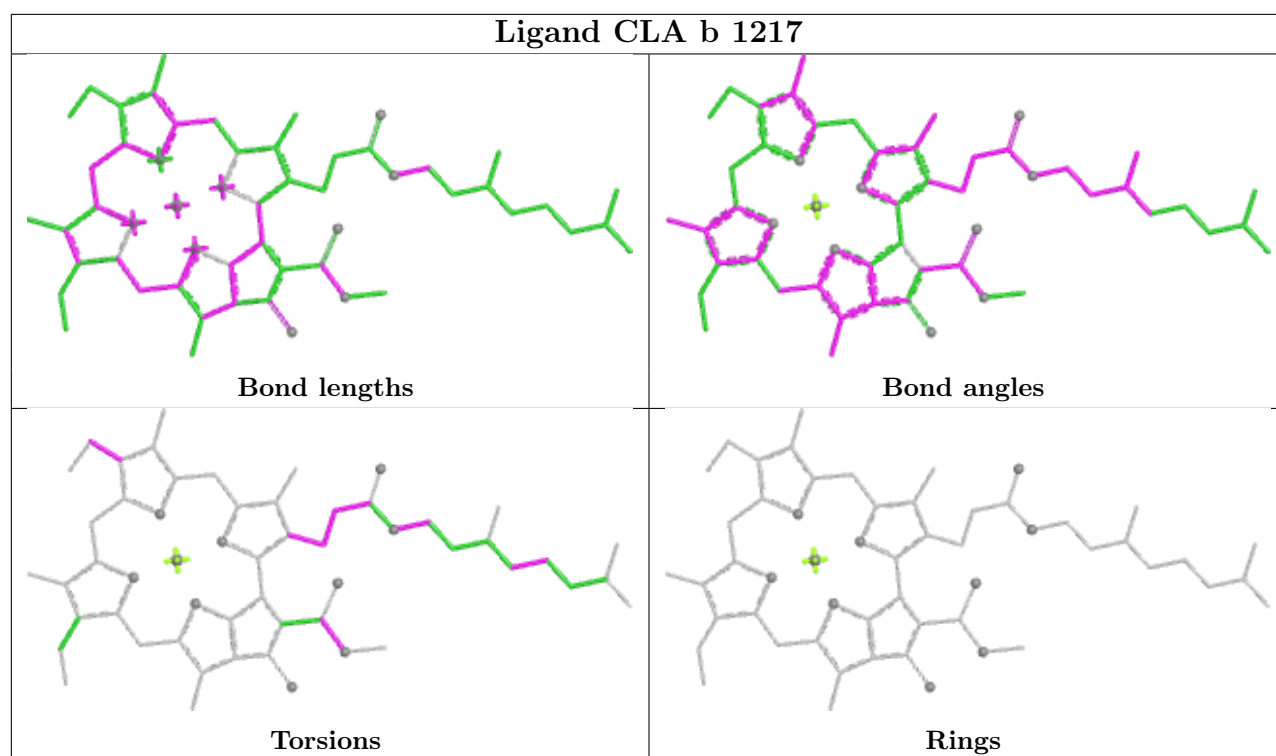


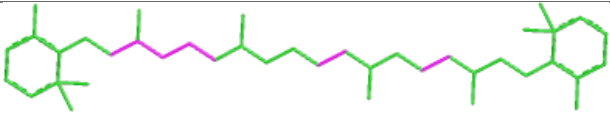
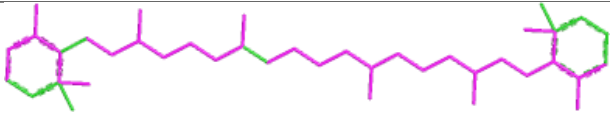
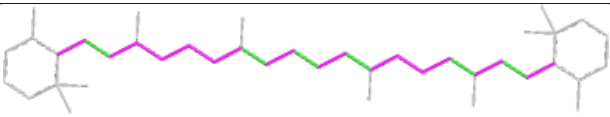
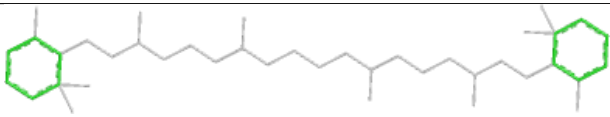
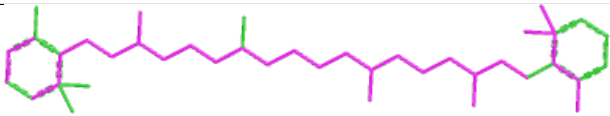
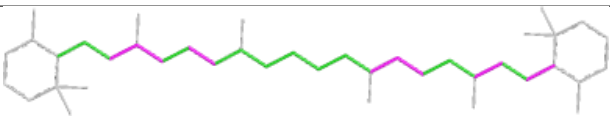
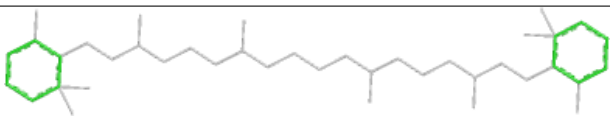
Ligand CLA G 1117**Ligand CLA U 1503**

Ligand CLA A 1110

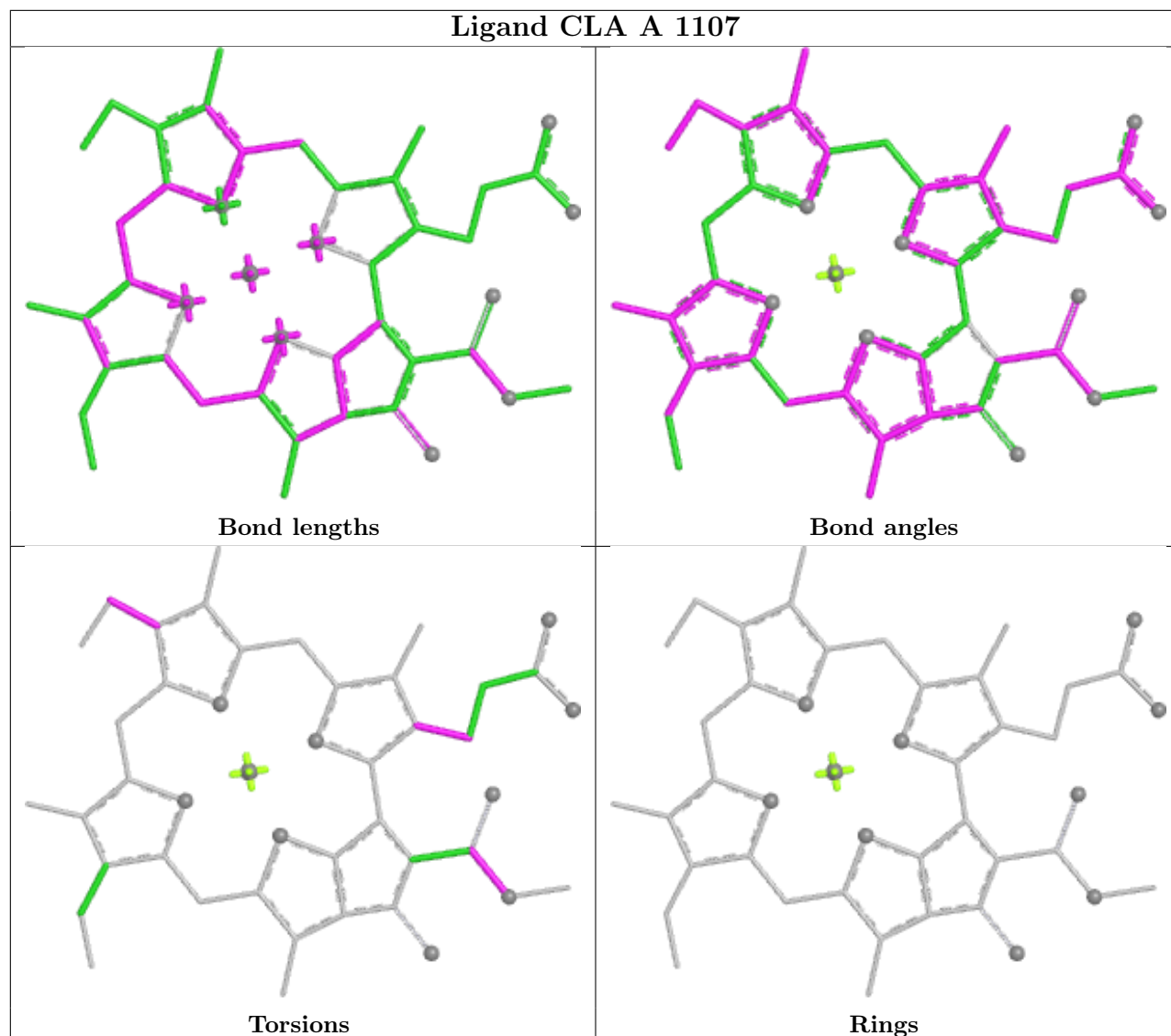


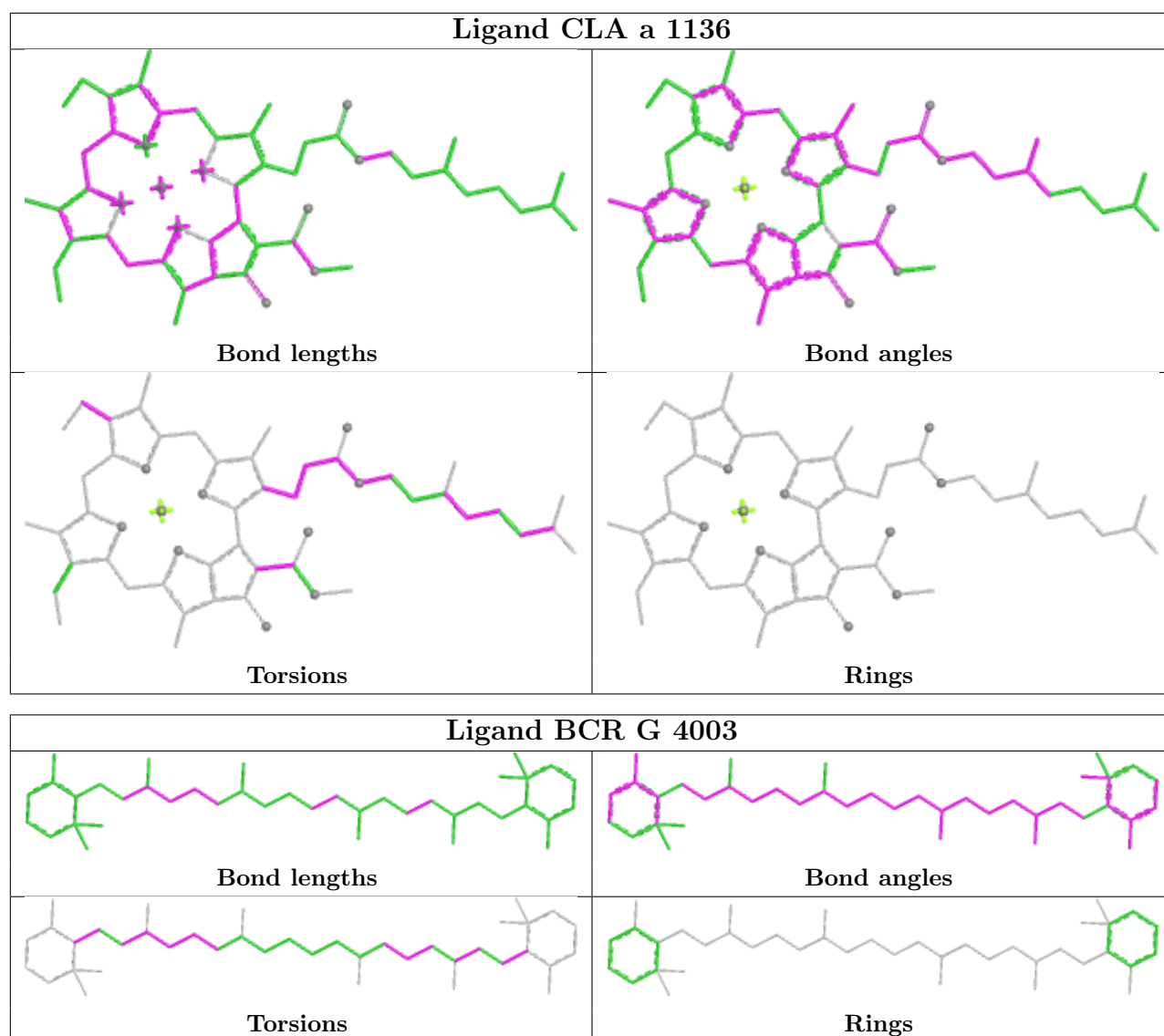




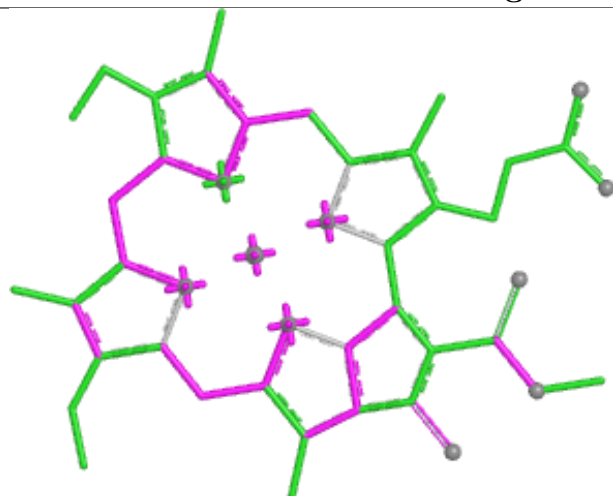
Ligand BCR H 4012	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR m 4021	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1107

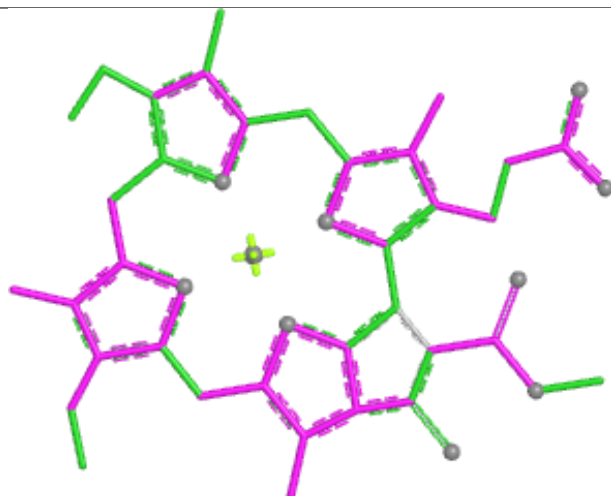




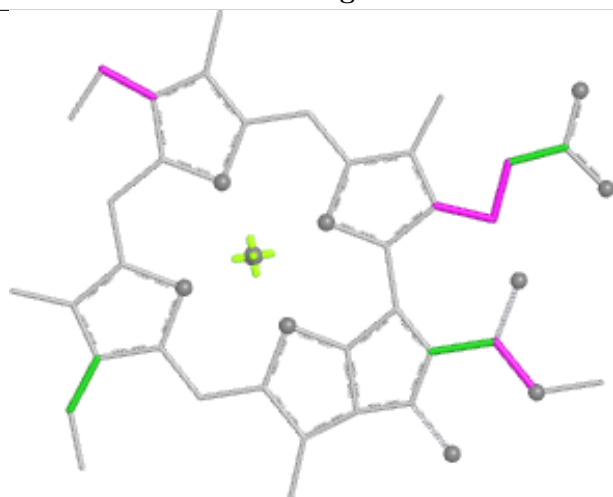
Ligand CLA B 1227



Bond lengths



Bond angles

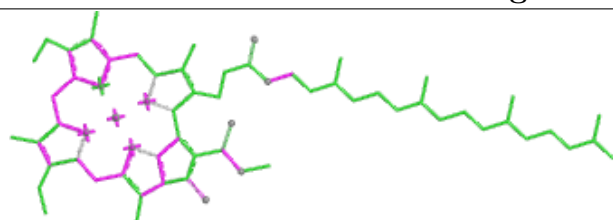


Torsions

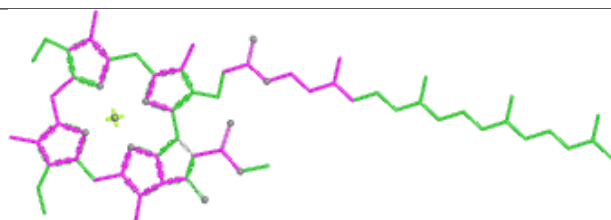


Rings

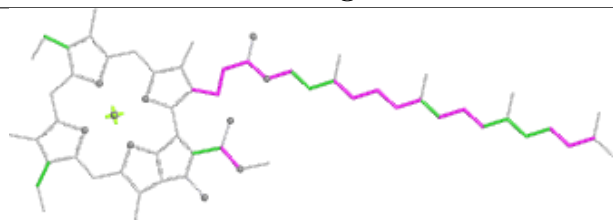
Ligand CLA a 1140



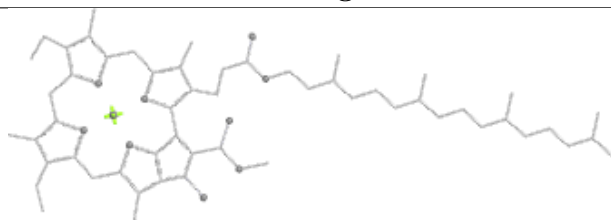
Bond lengths



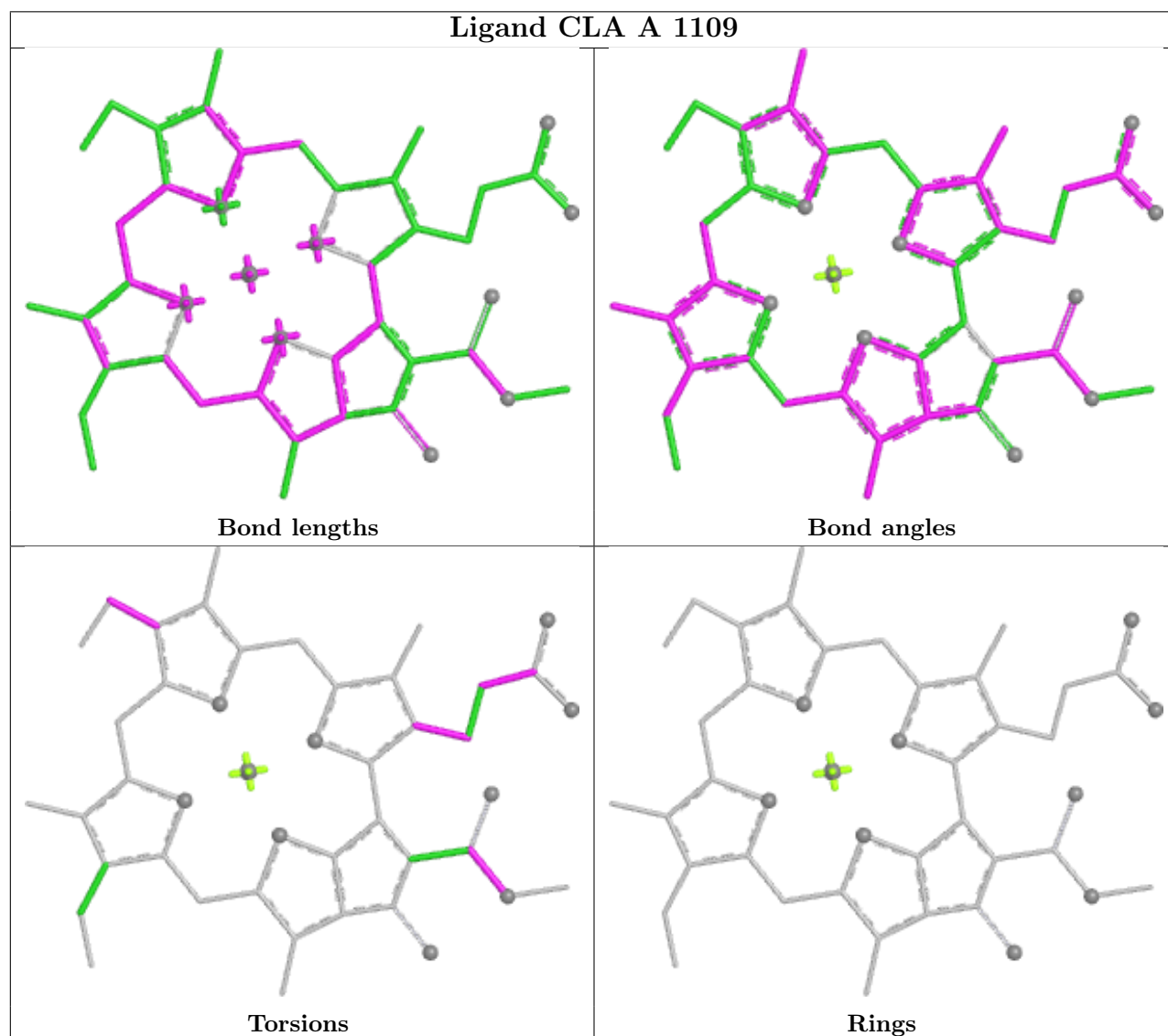
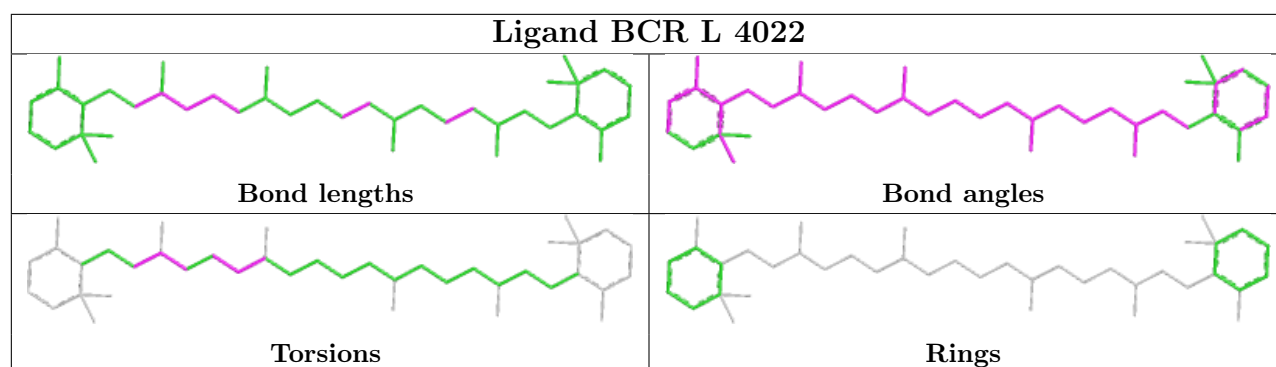
Bond angles

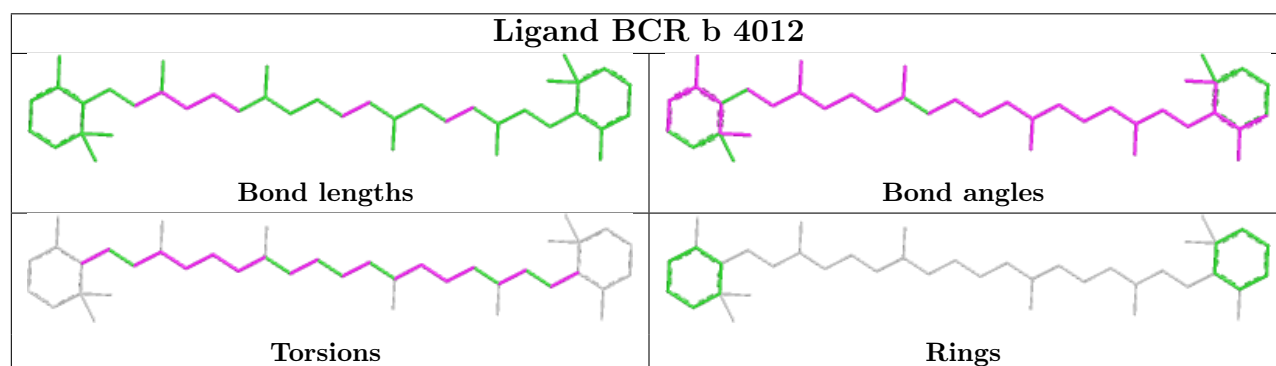
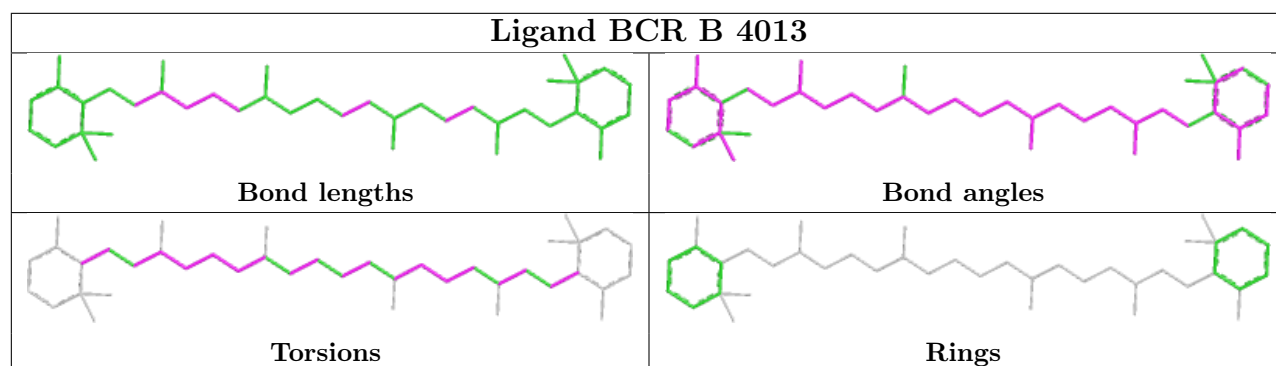
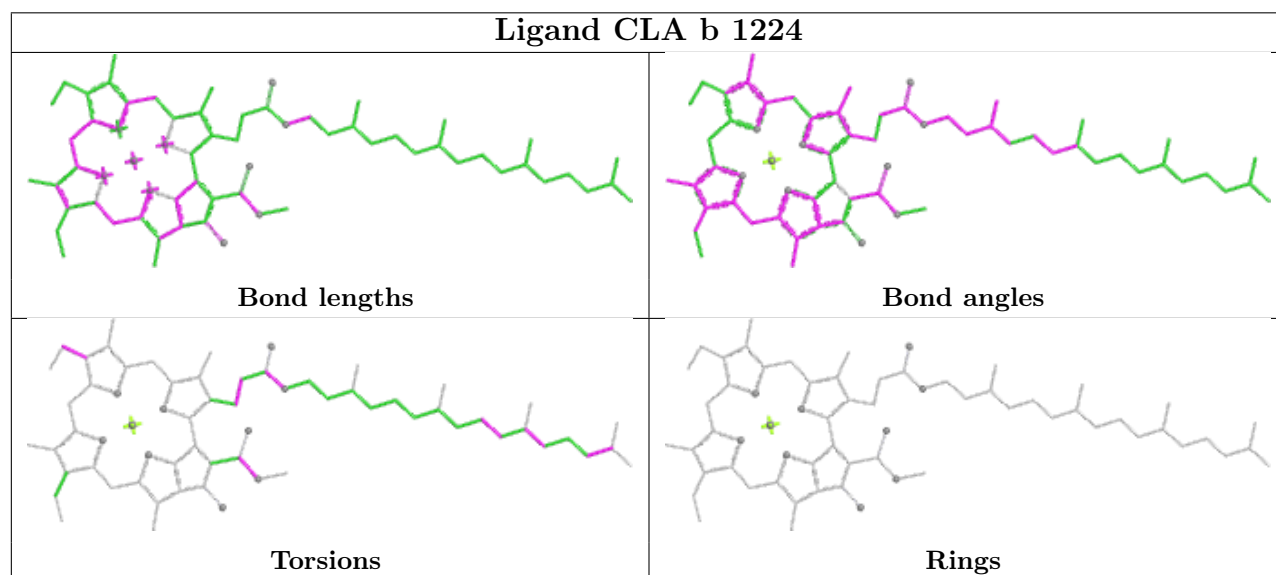
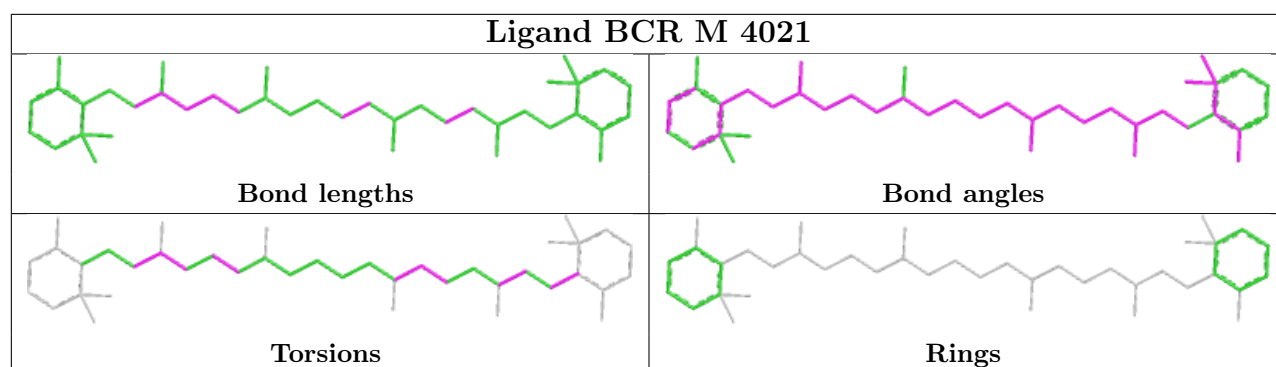


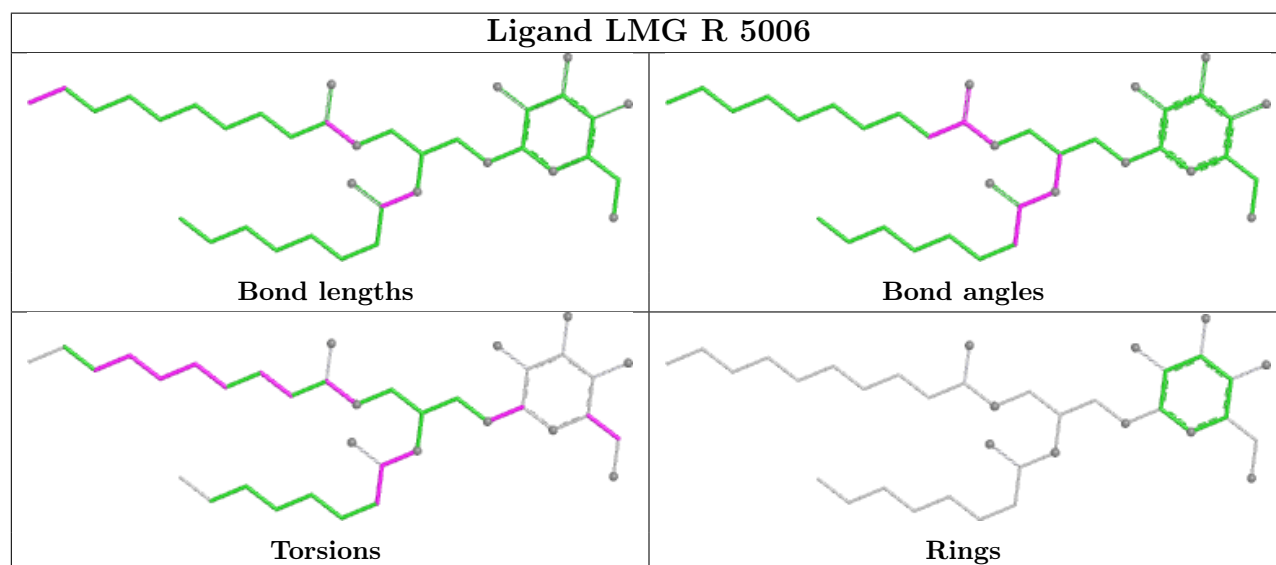
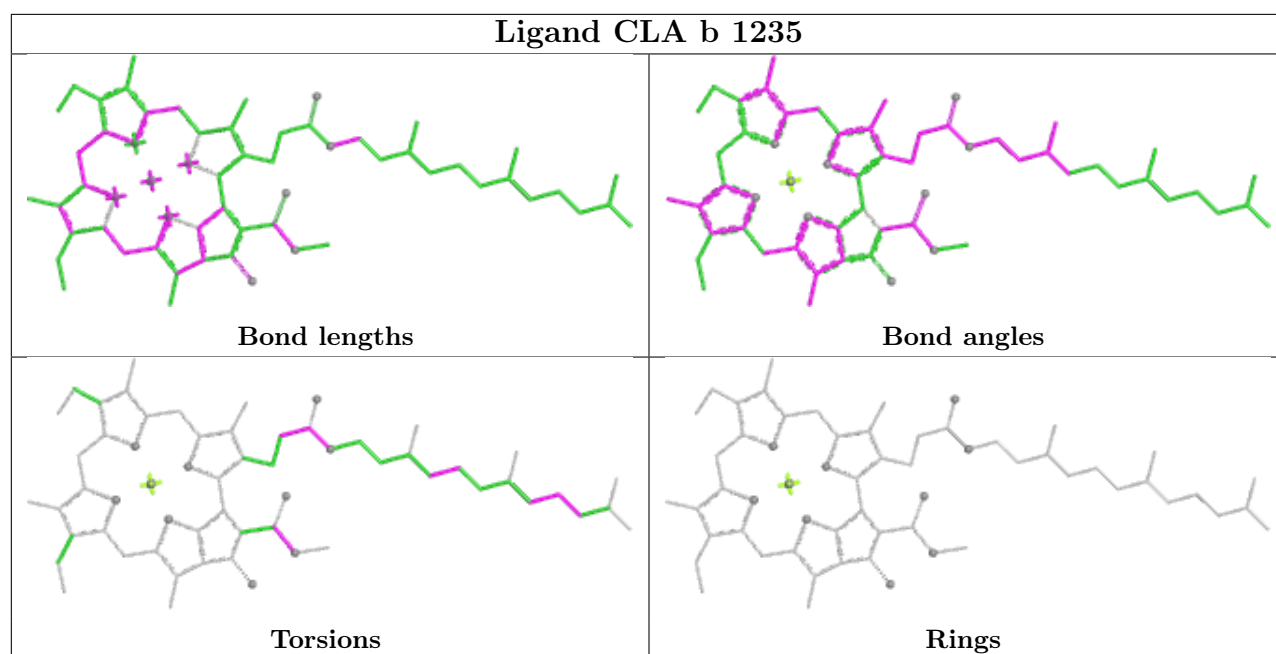
Torsions

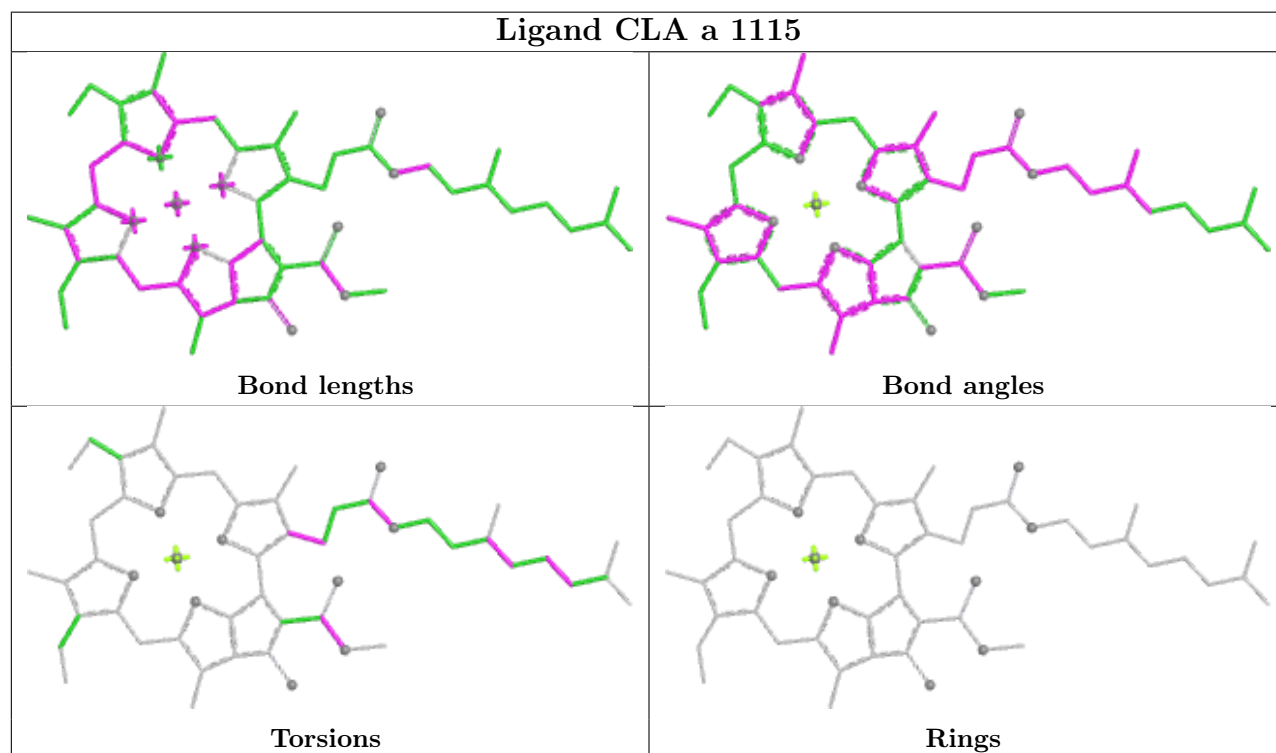
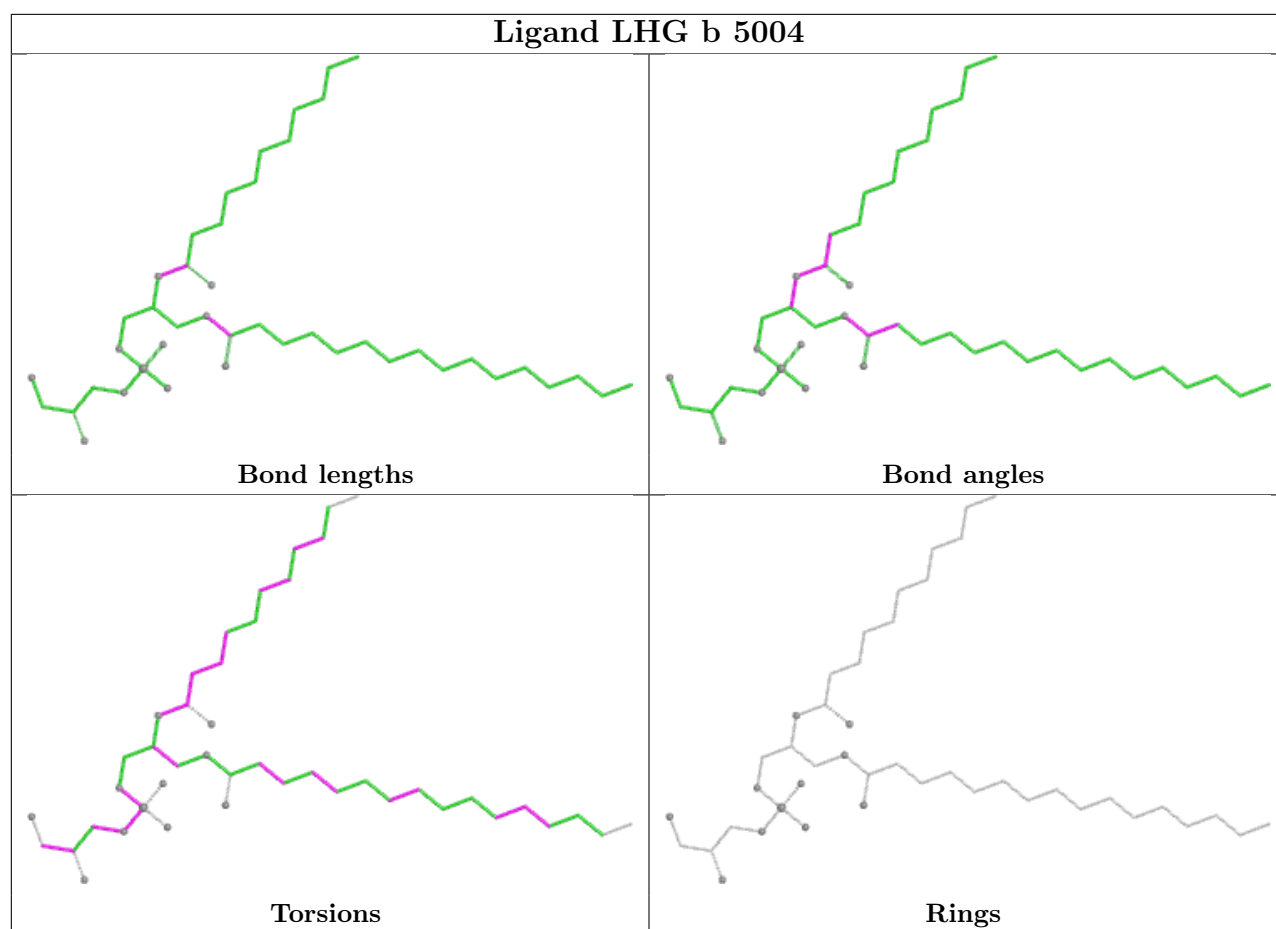


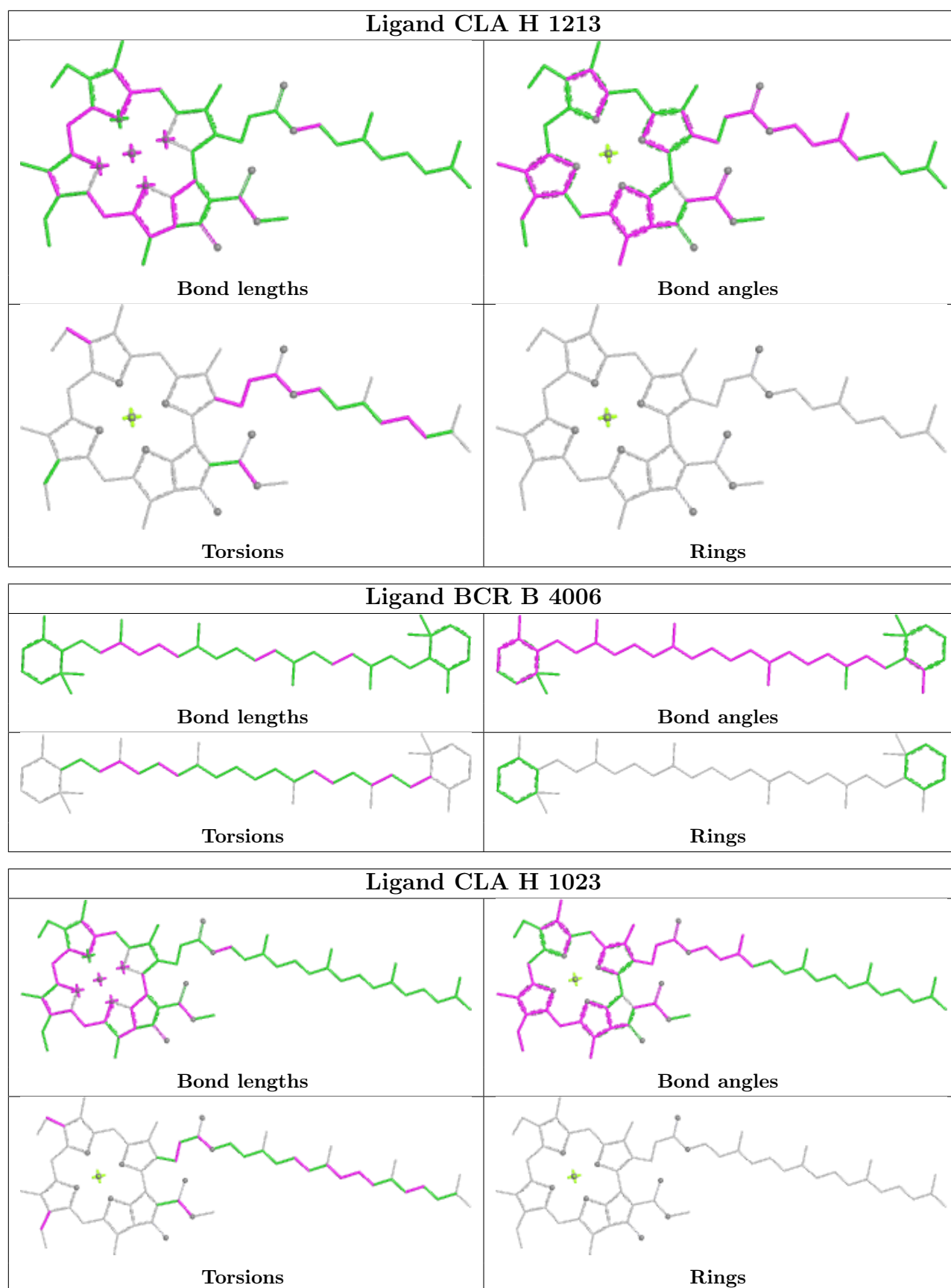
Rings

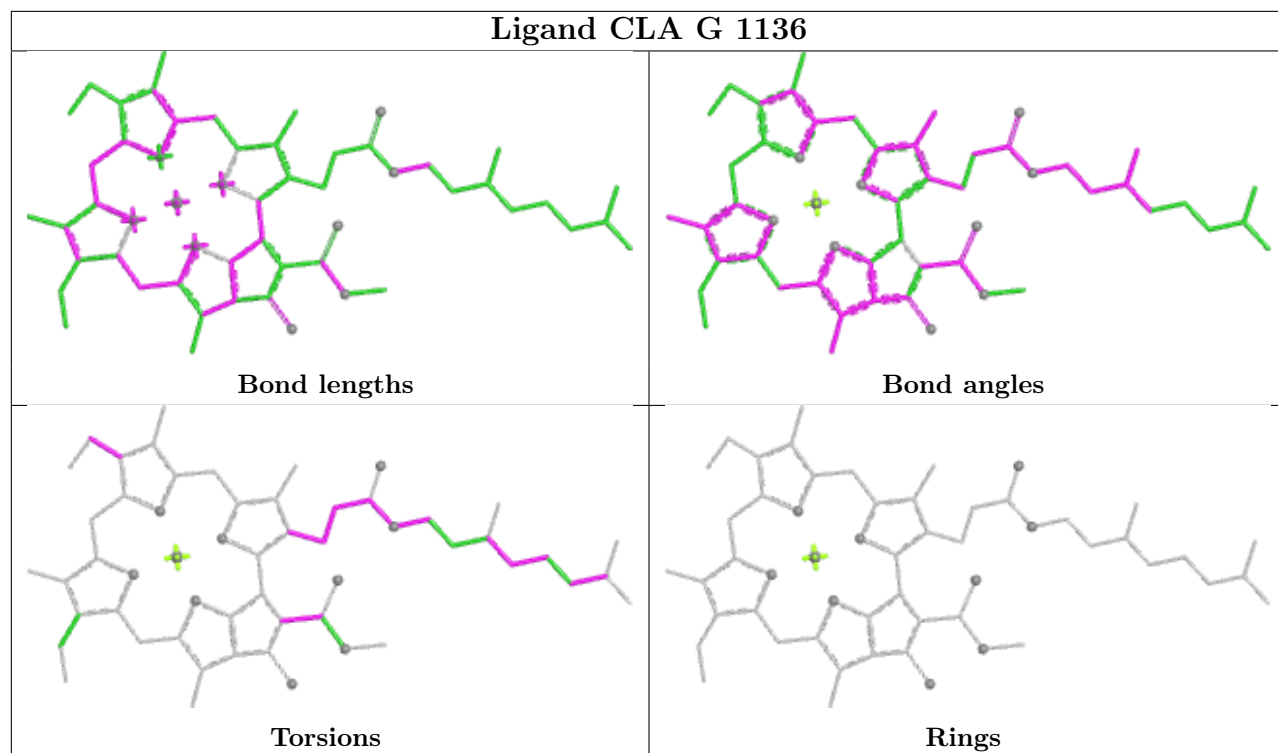




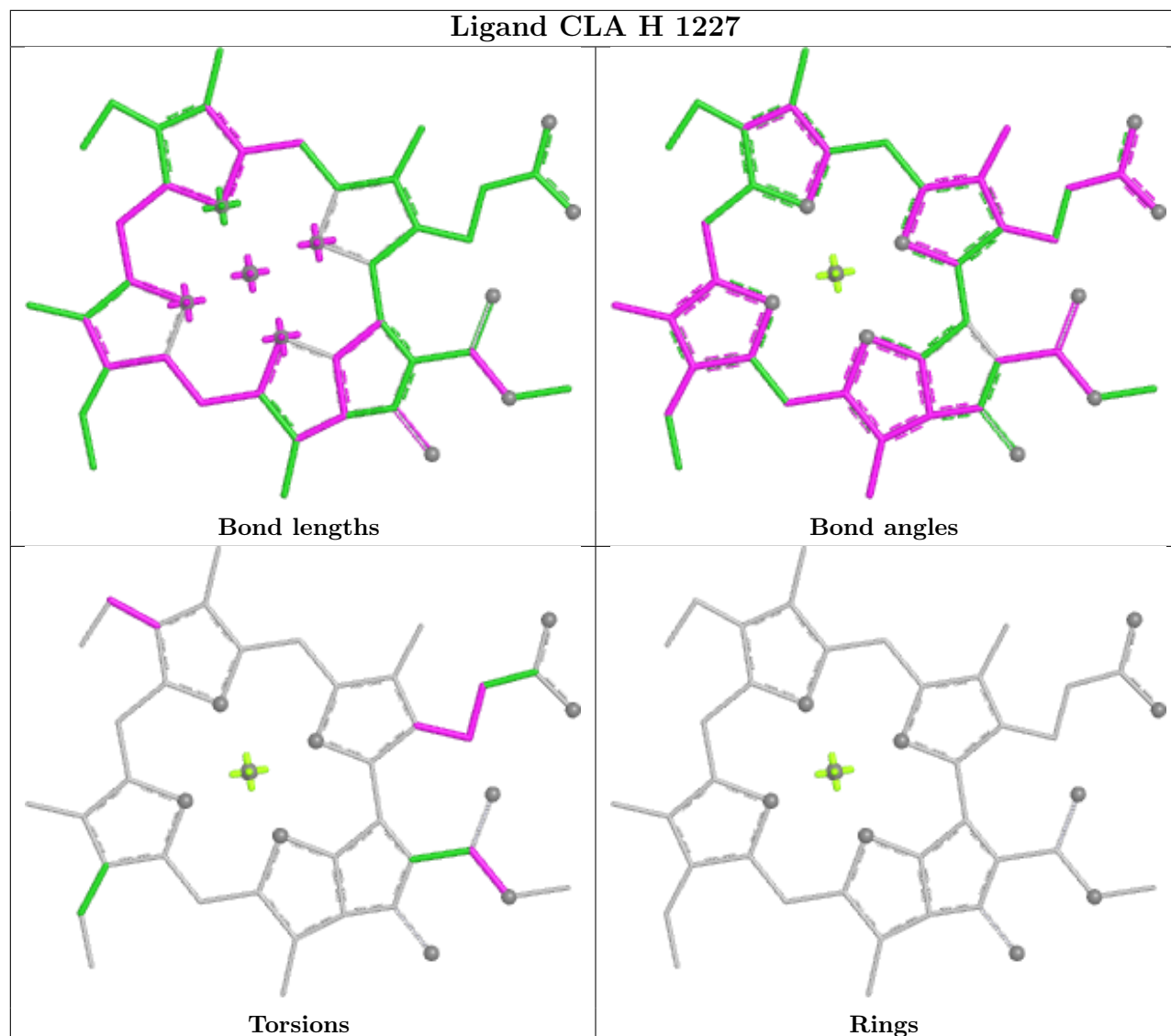




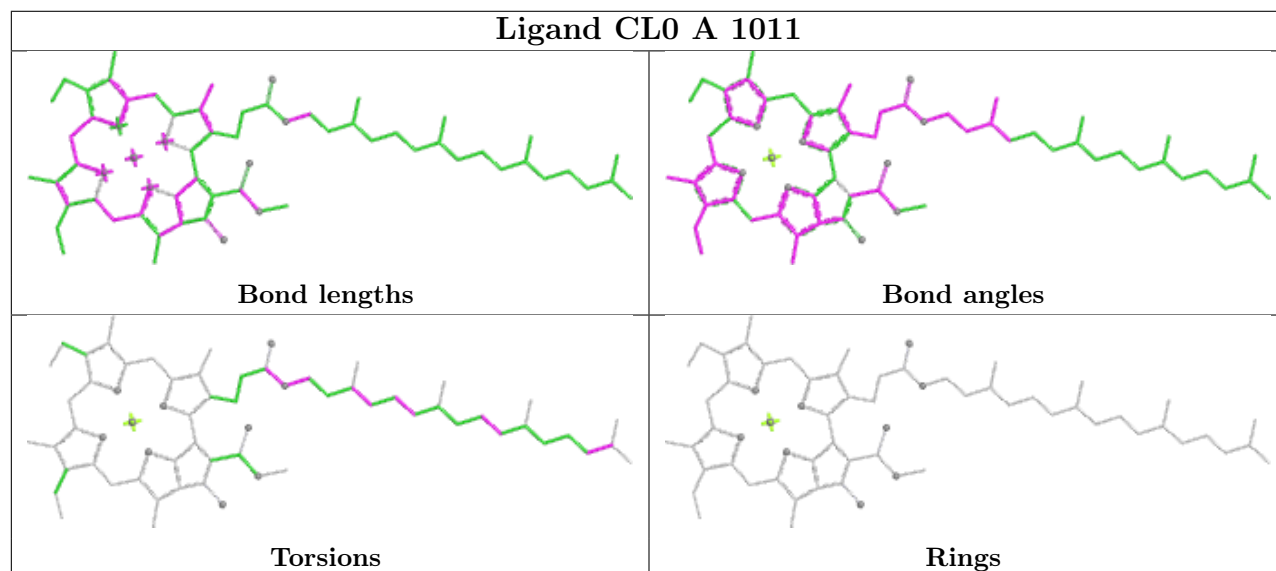


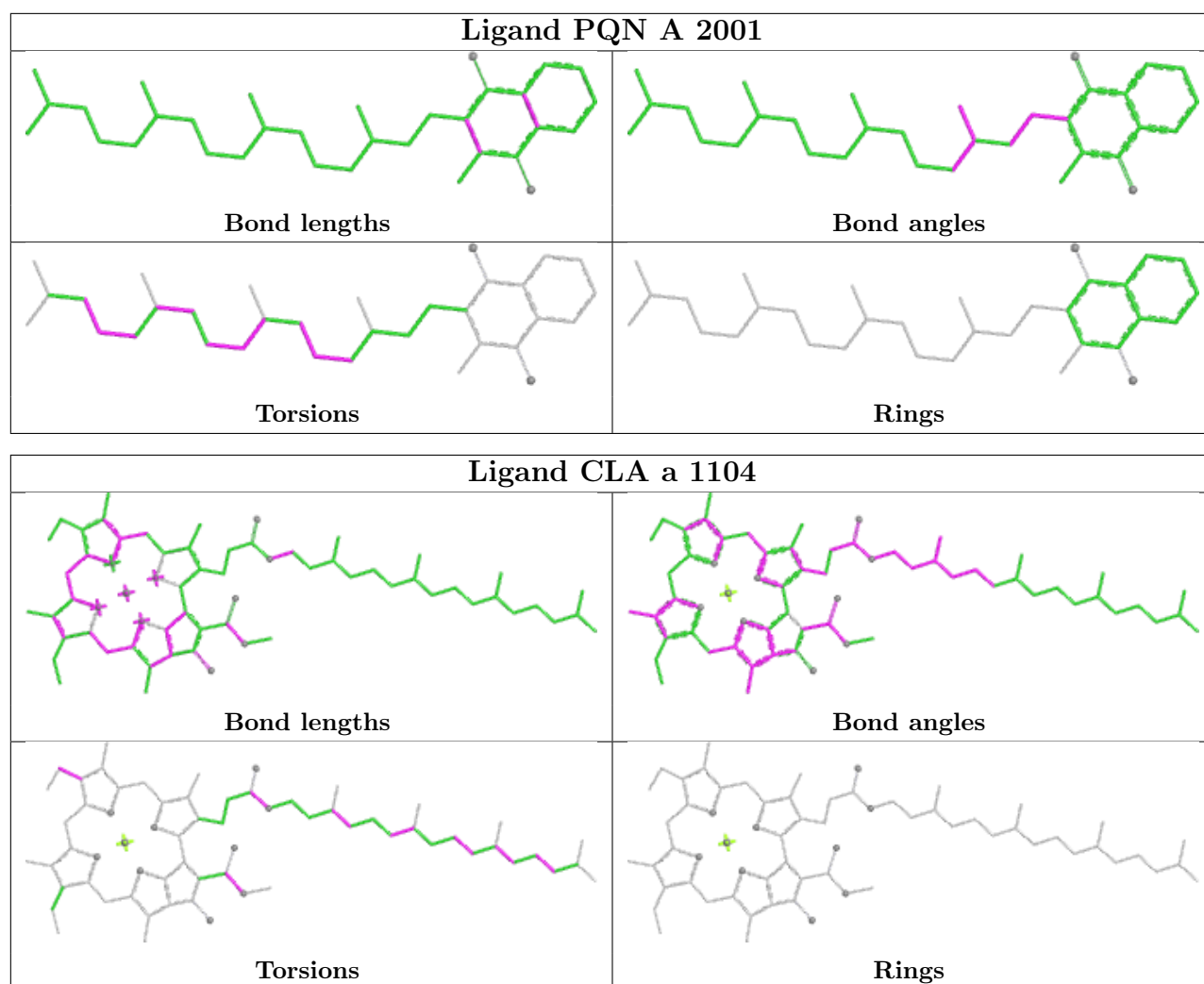


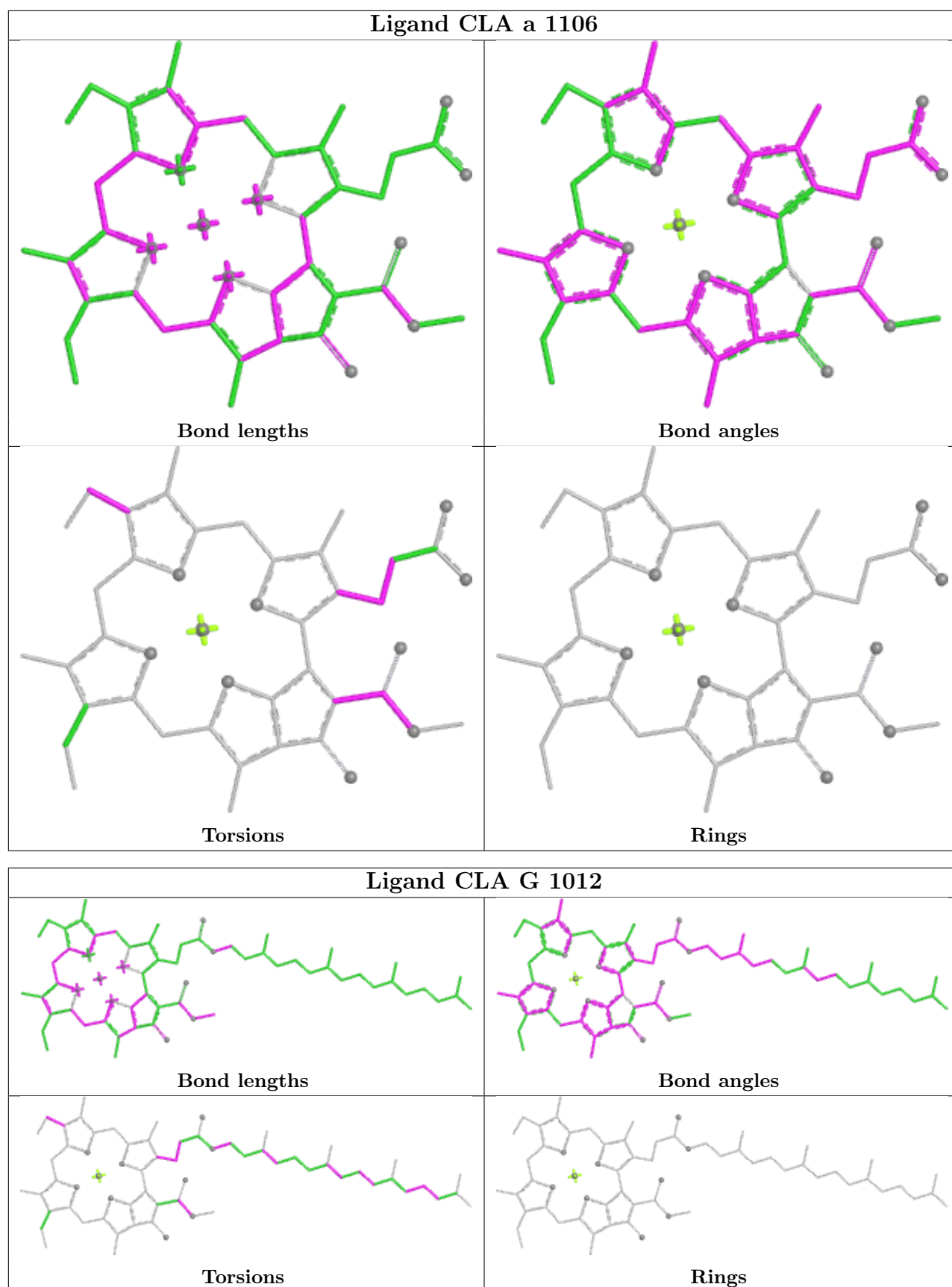
Ligand CLA H 1227

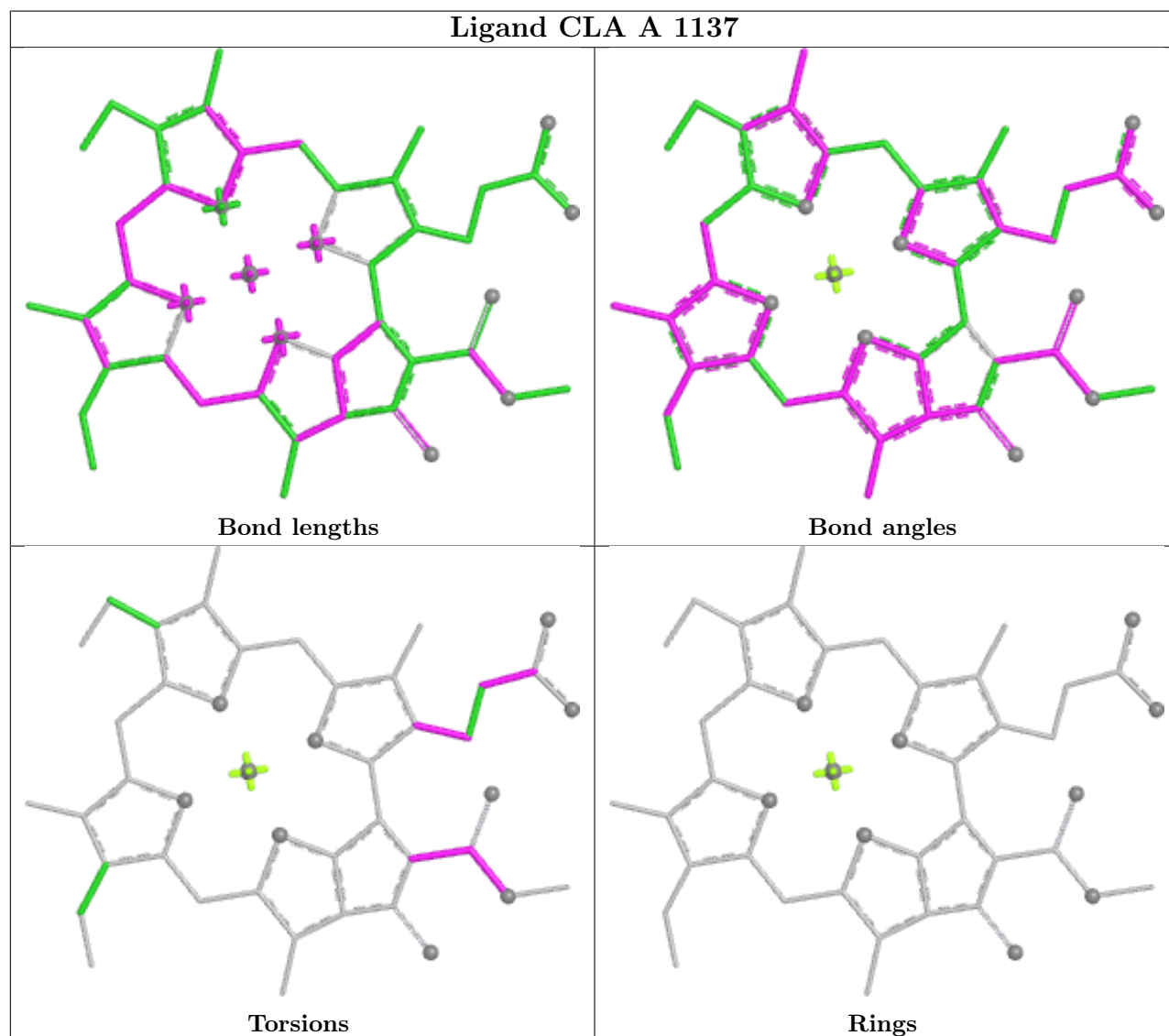
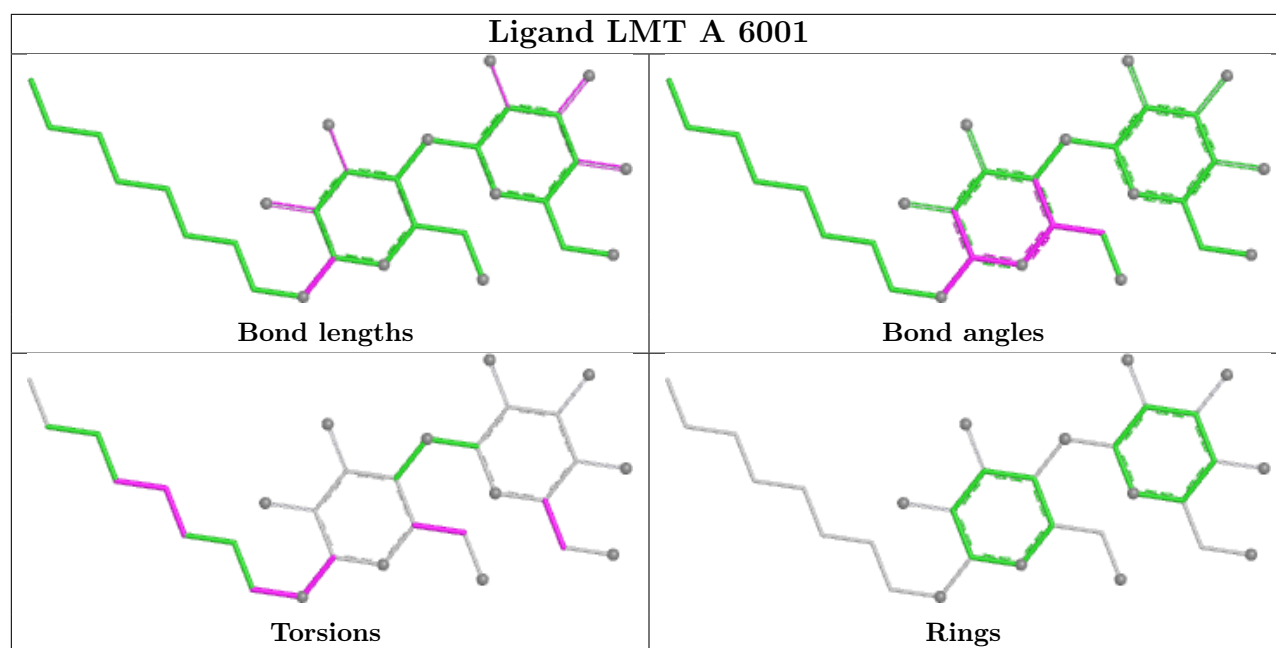


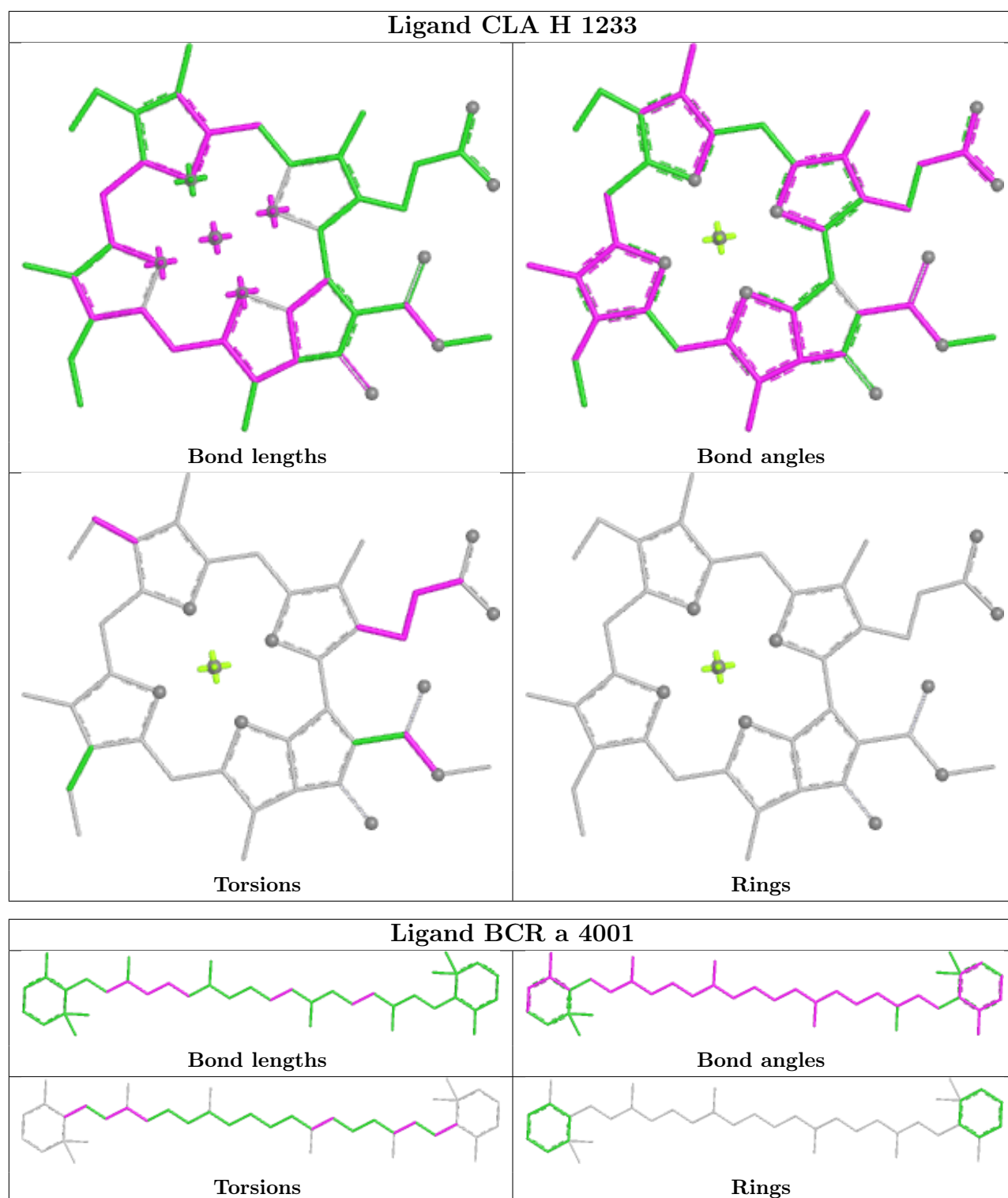
Ligand CL0 A 1011

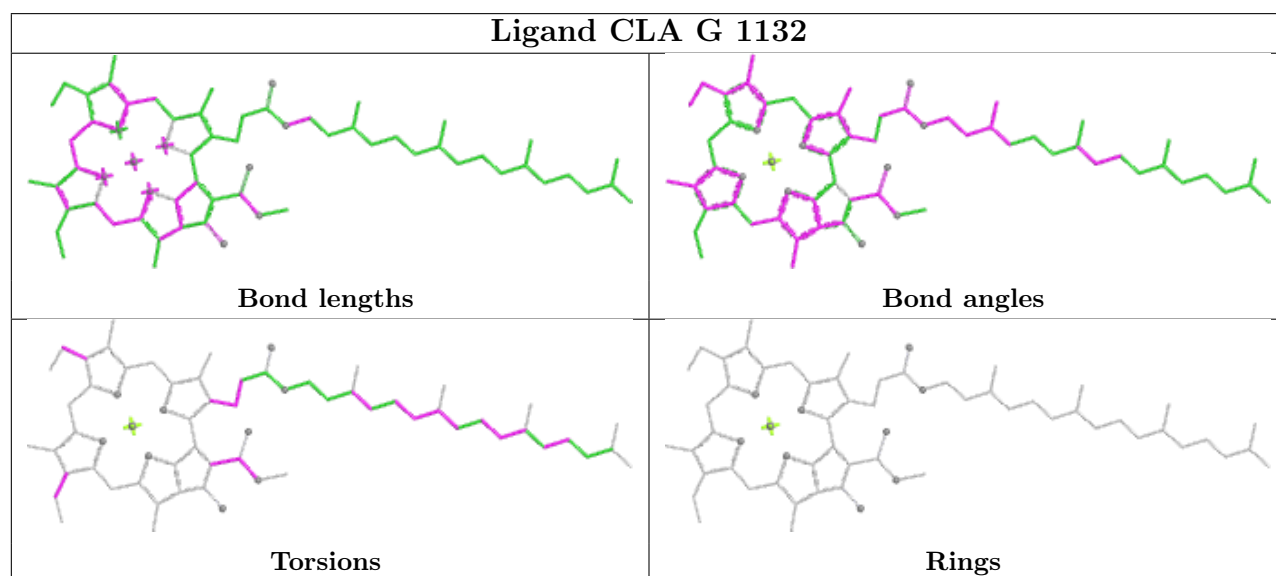
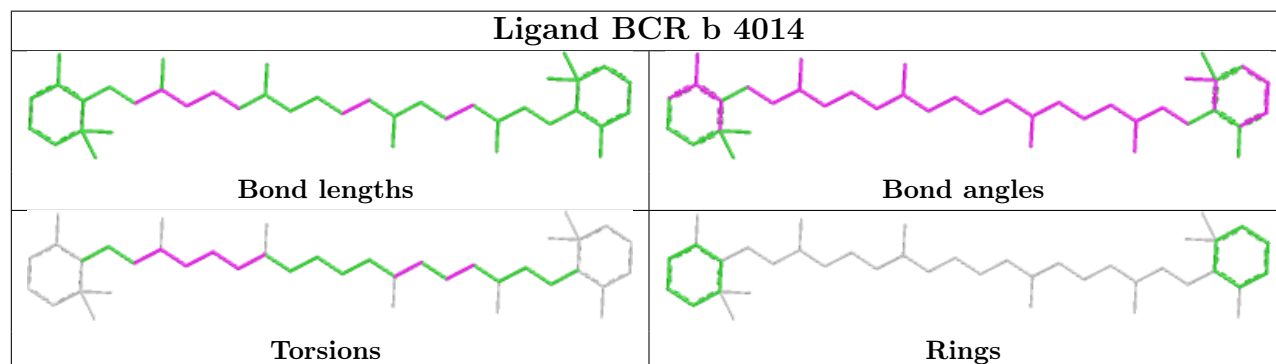
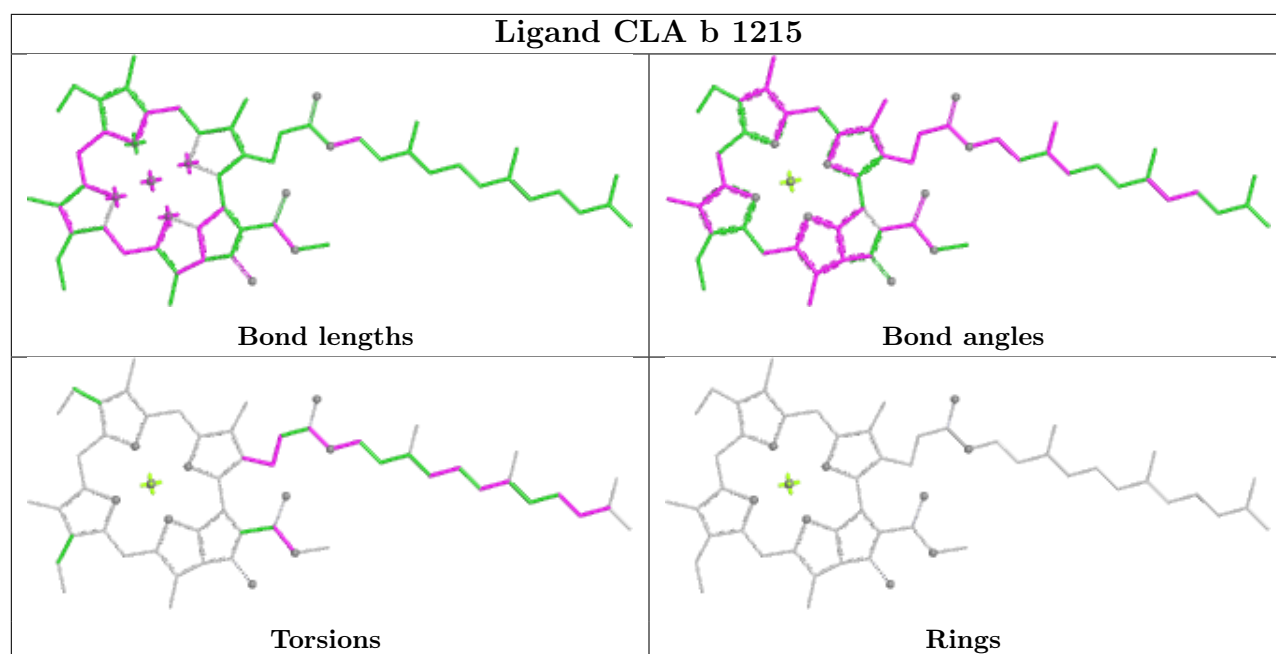


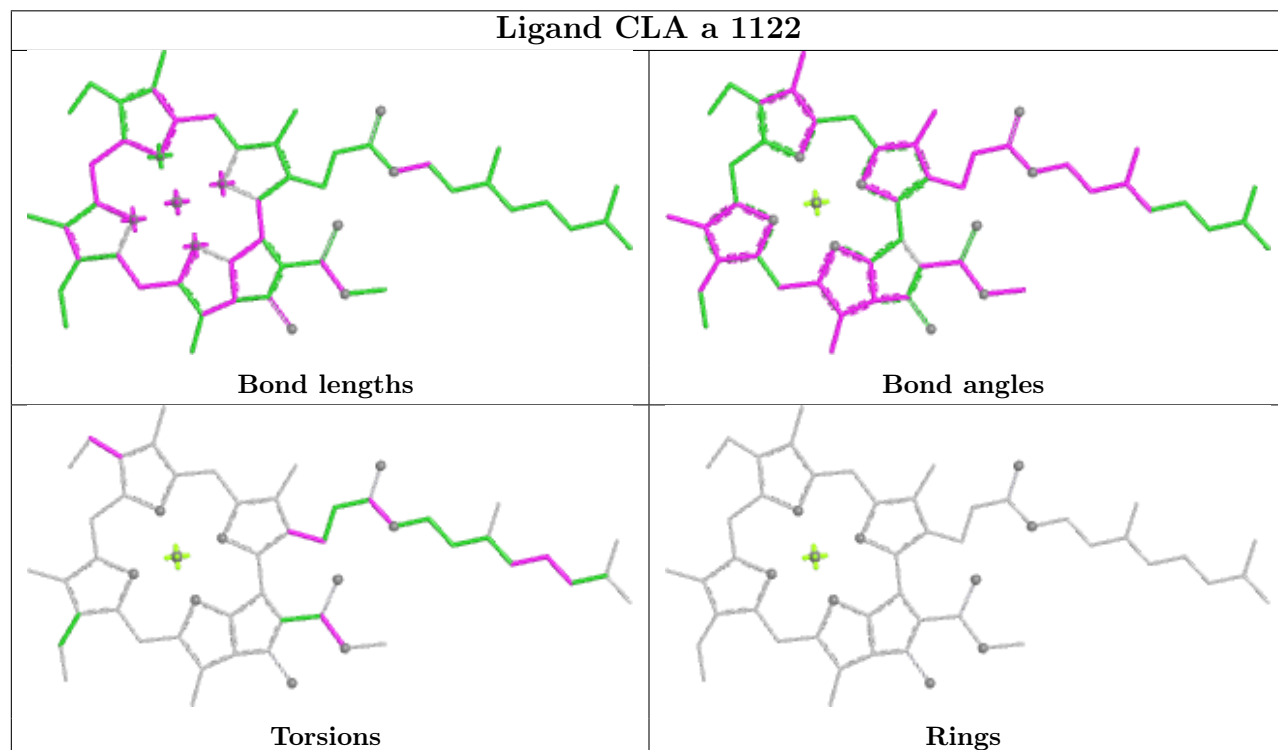
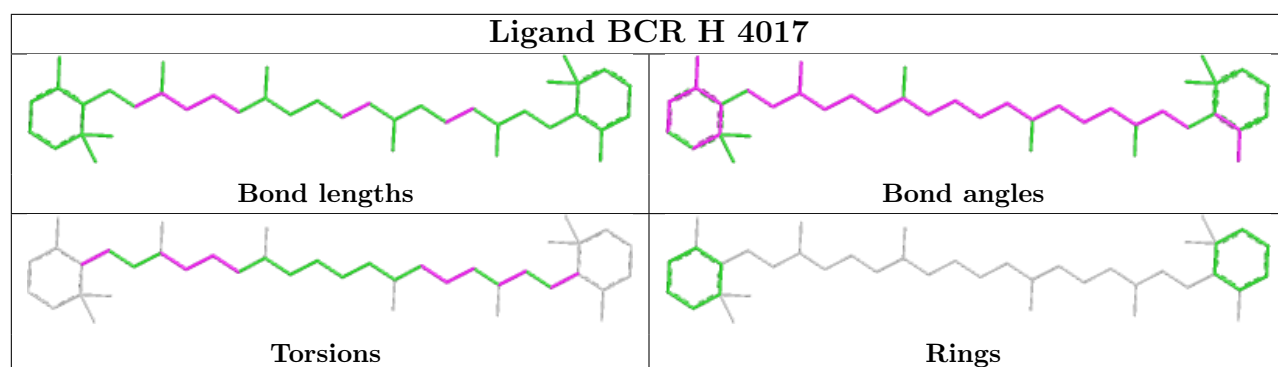


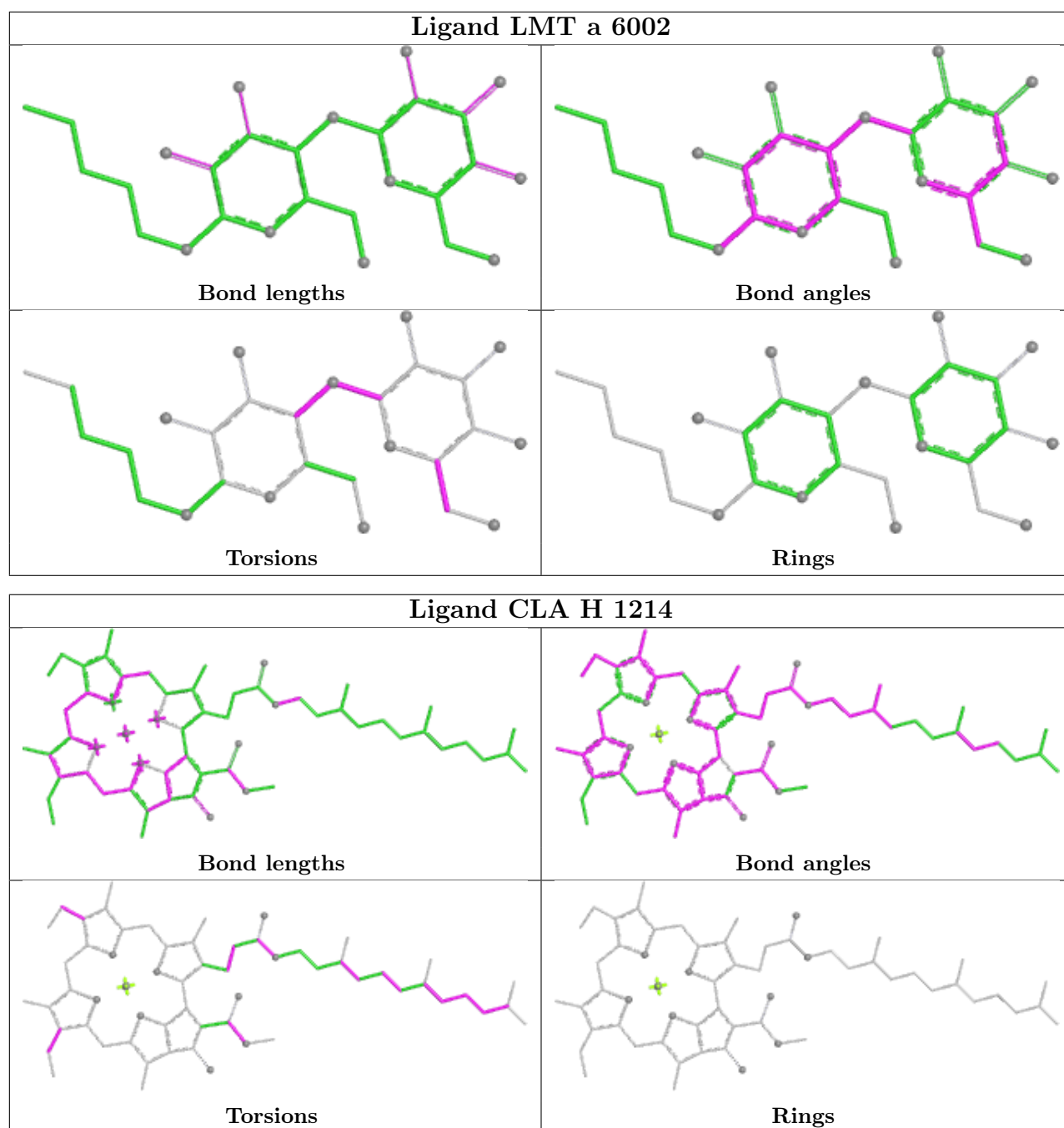


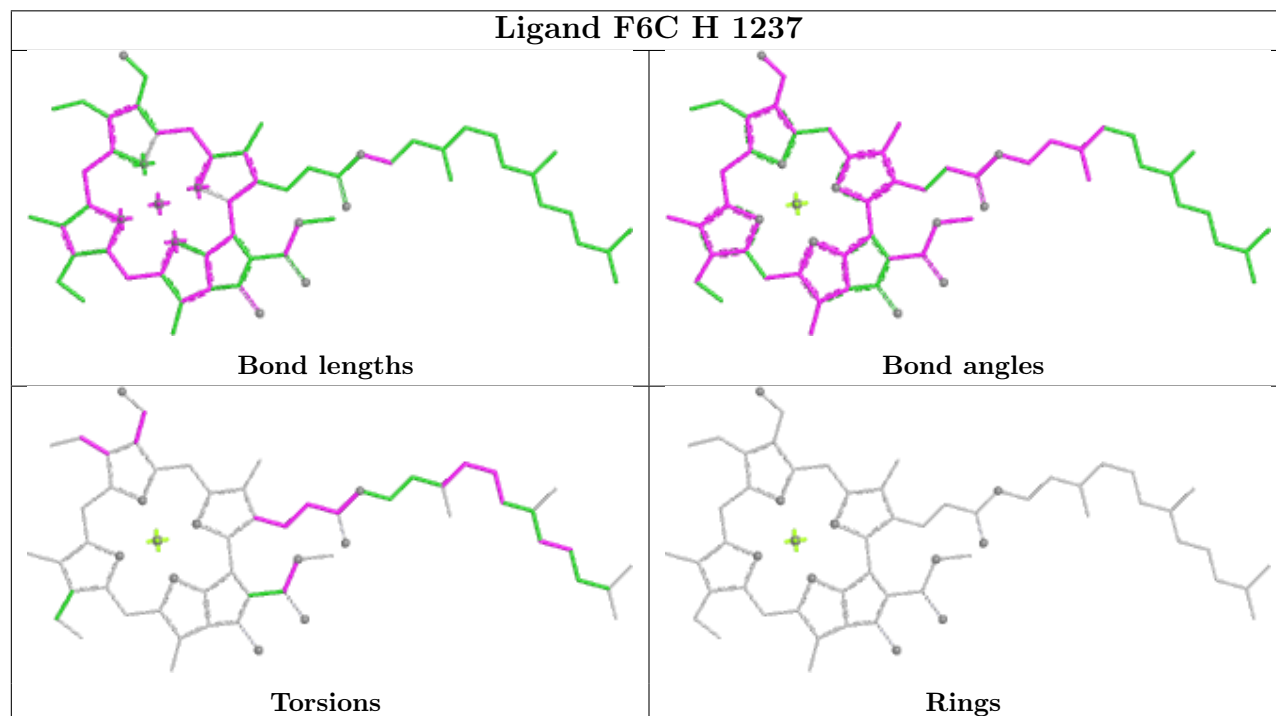
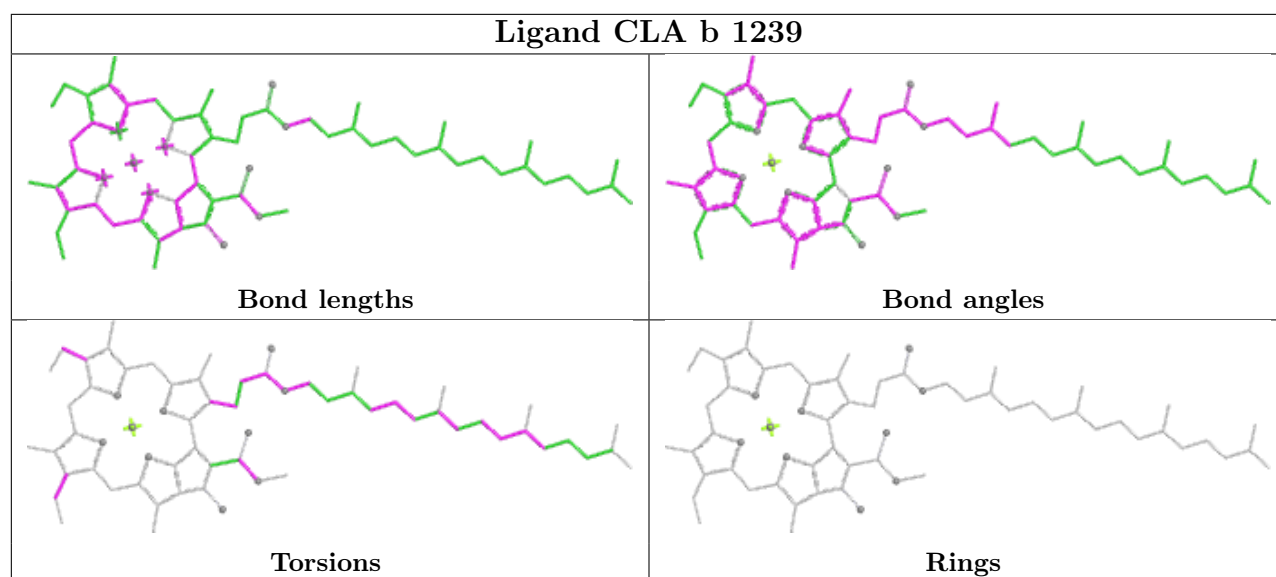


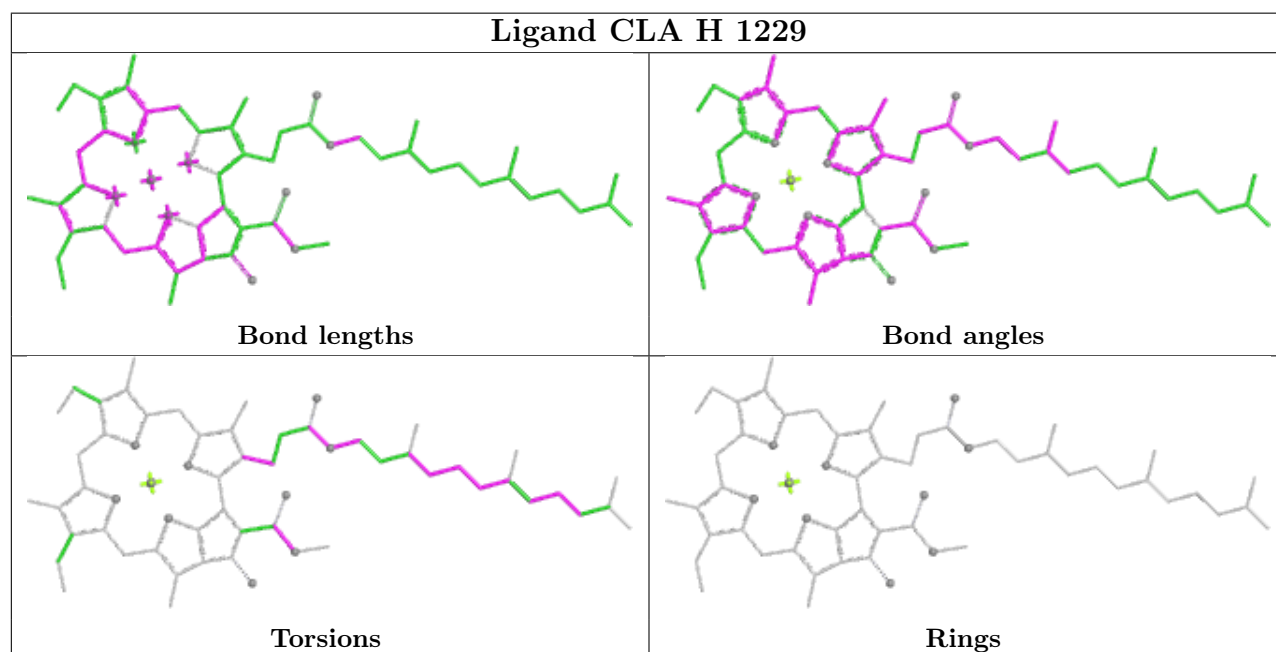
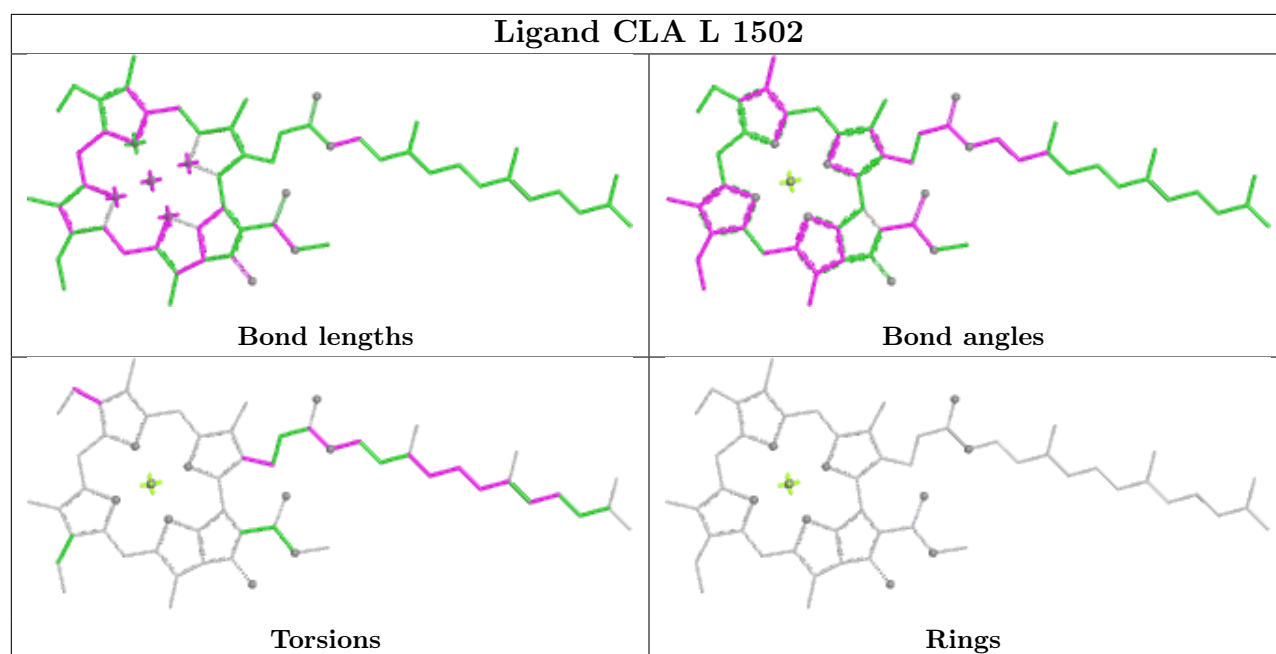


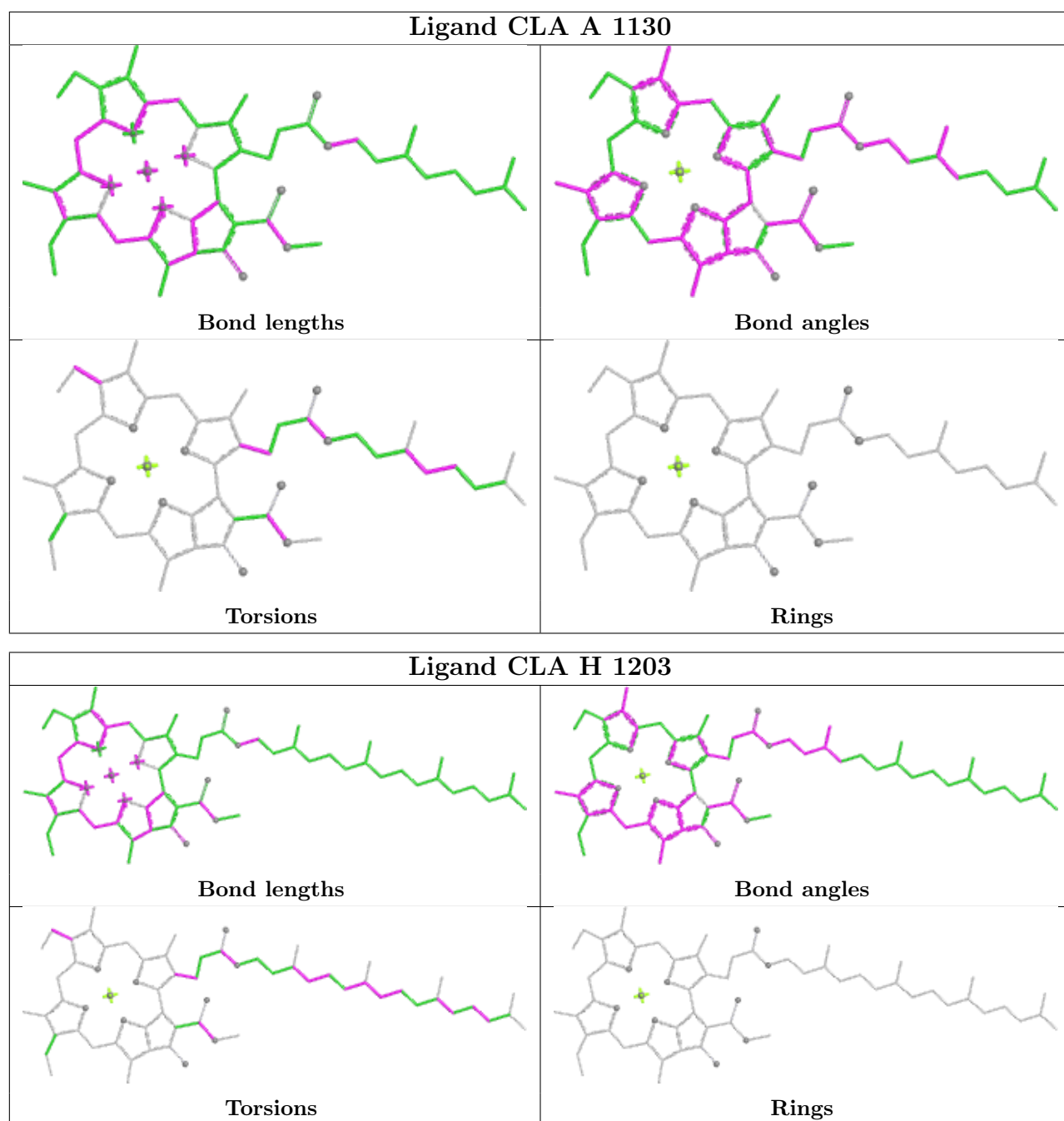


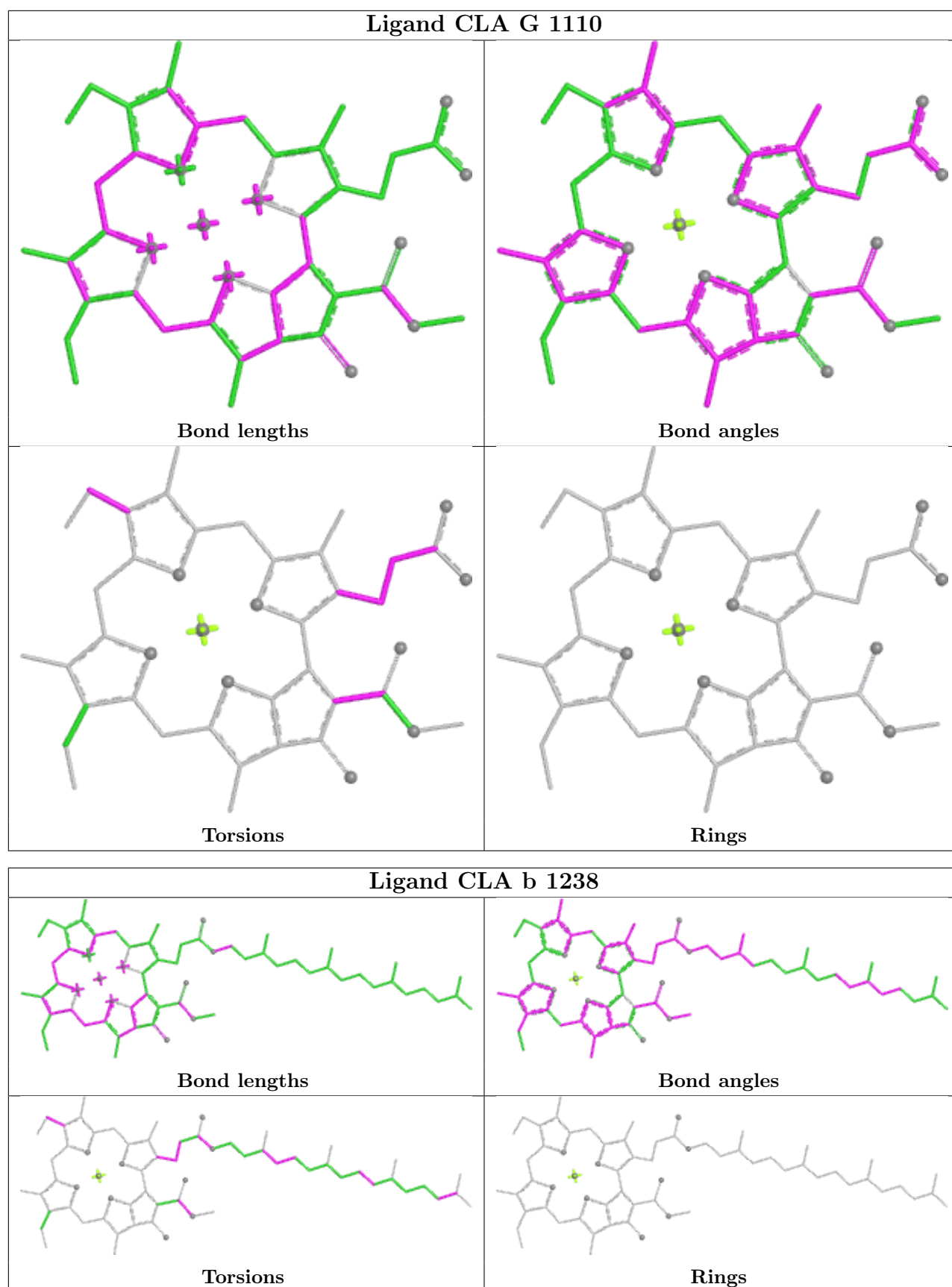


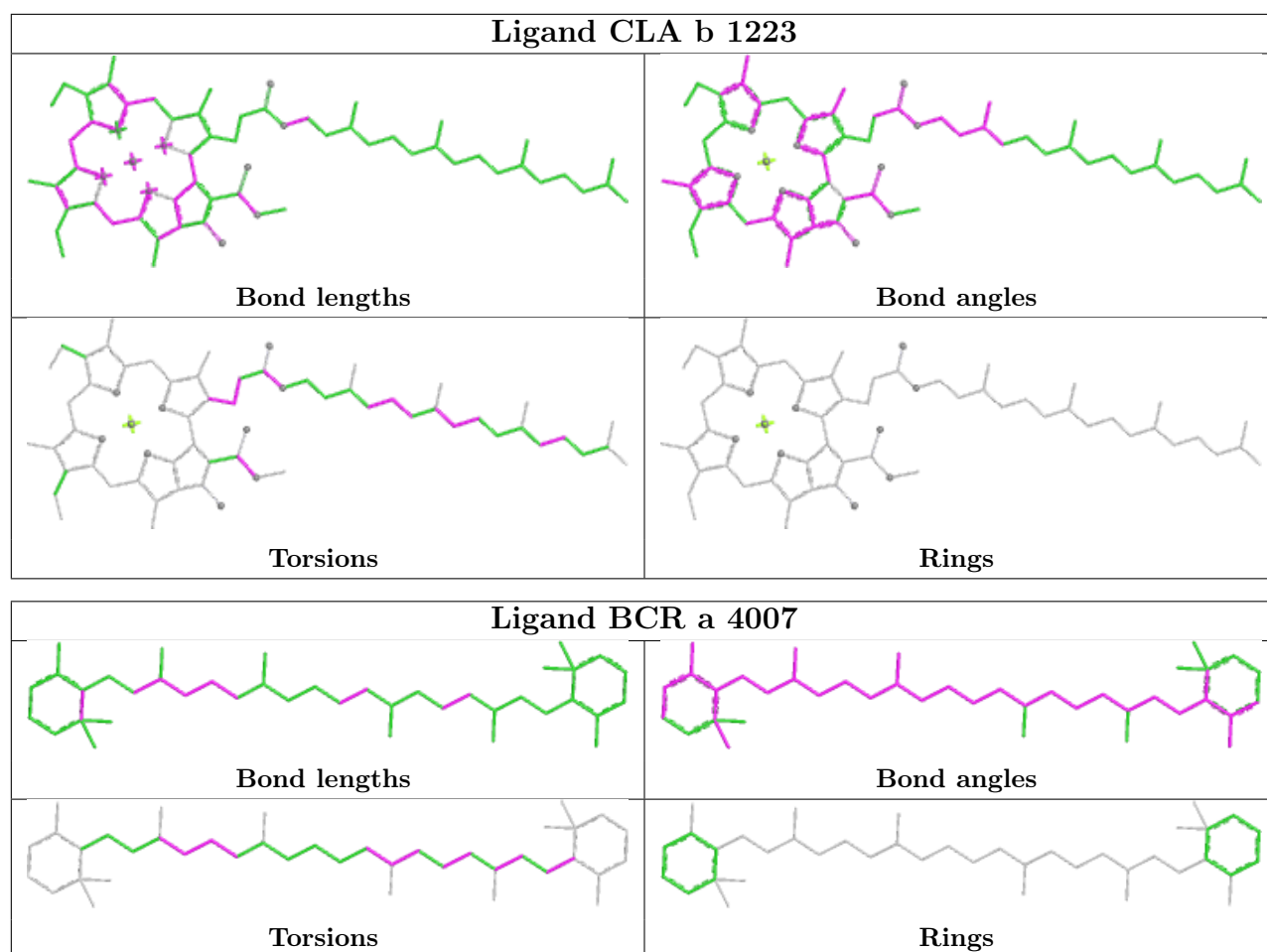




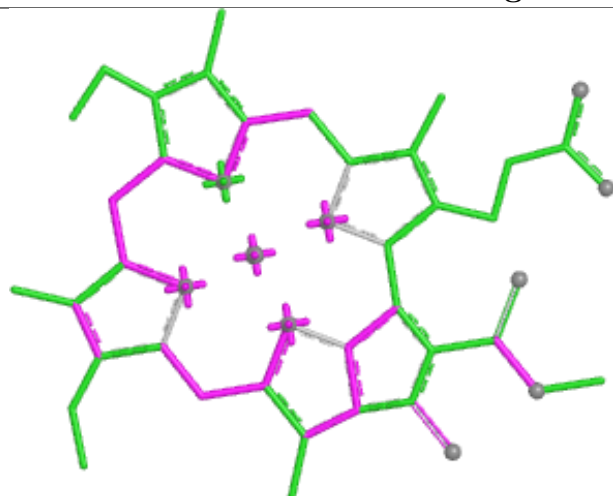




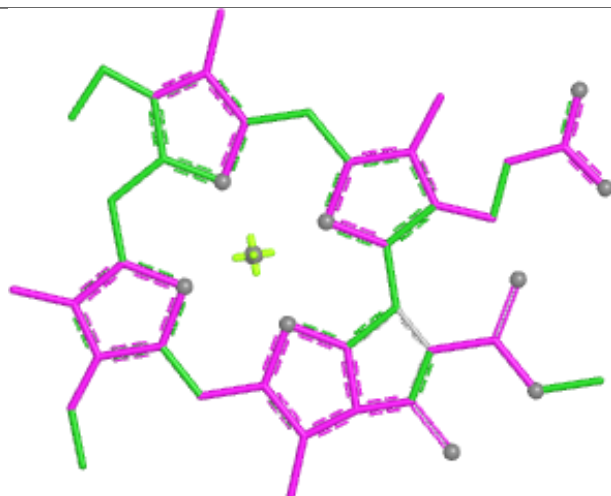




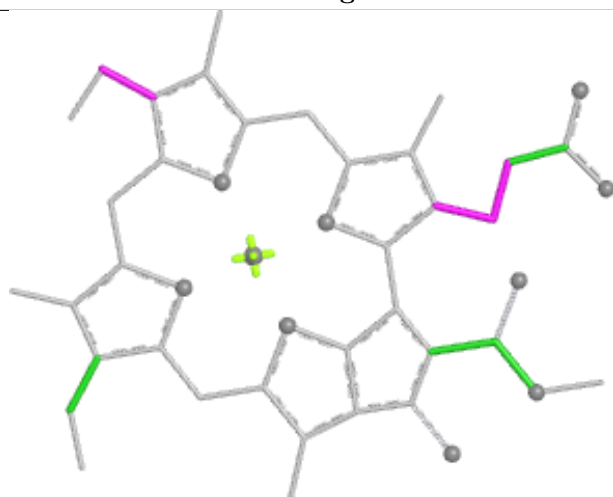
Ligand CLA A 1129



Bond lengths



Bond angles

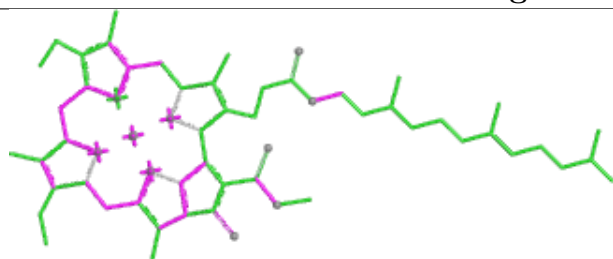


Torsions

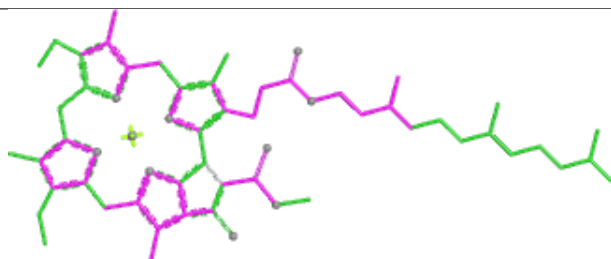


Rings

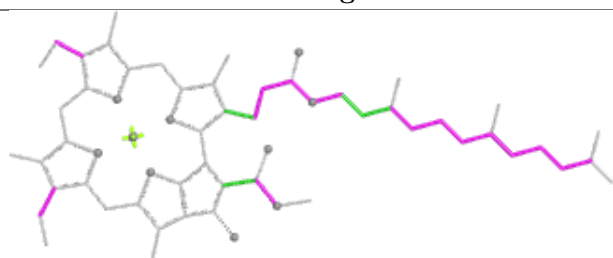
Ligand CLA a 1126



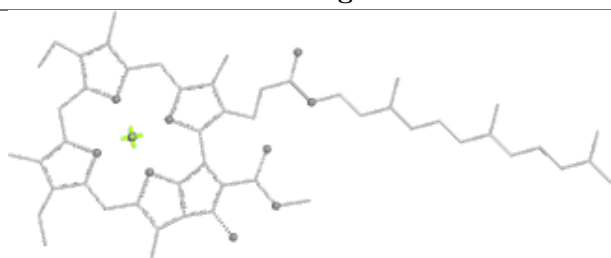
Bond lengths



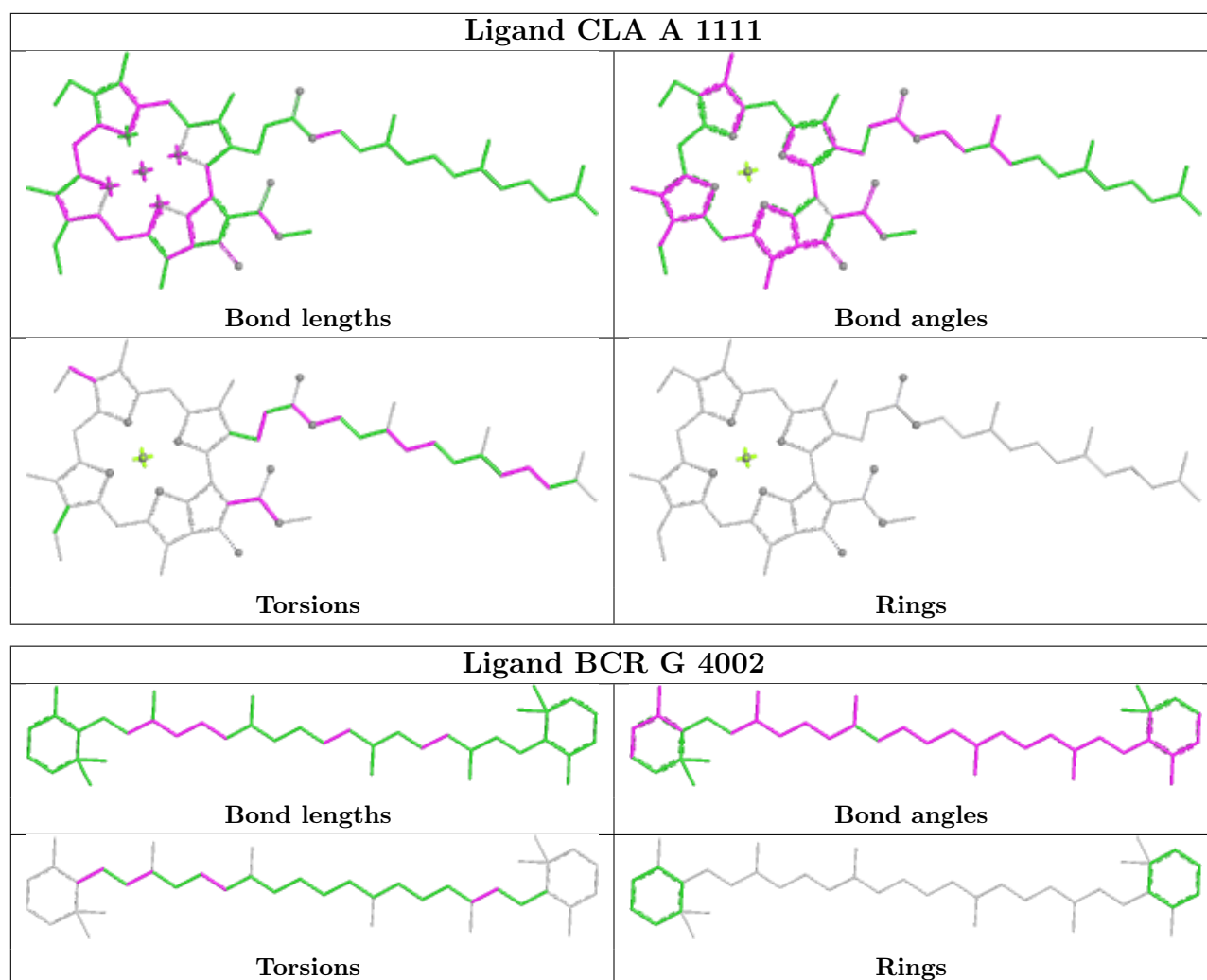
Bond angles

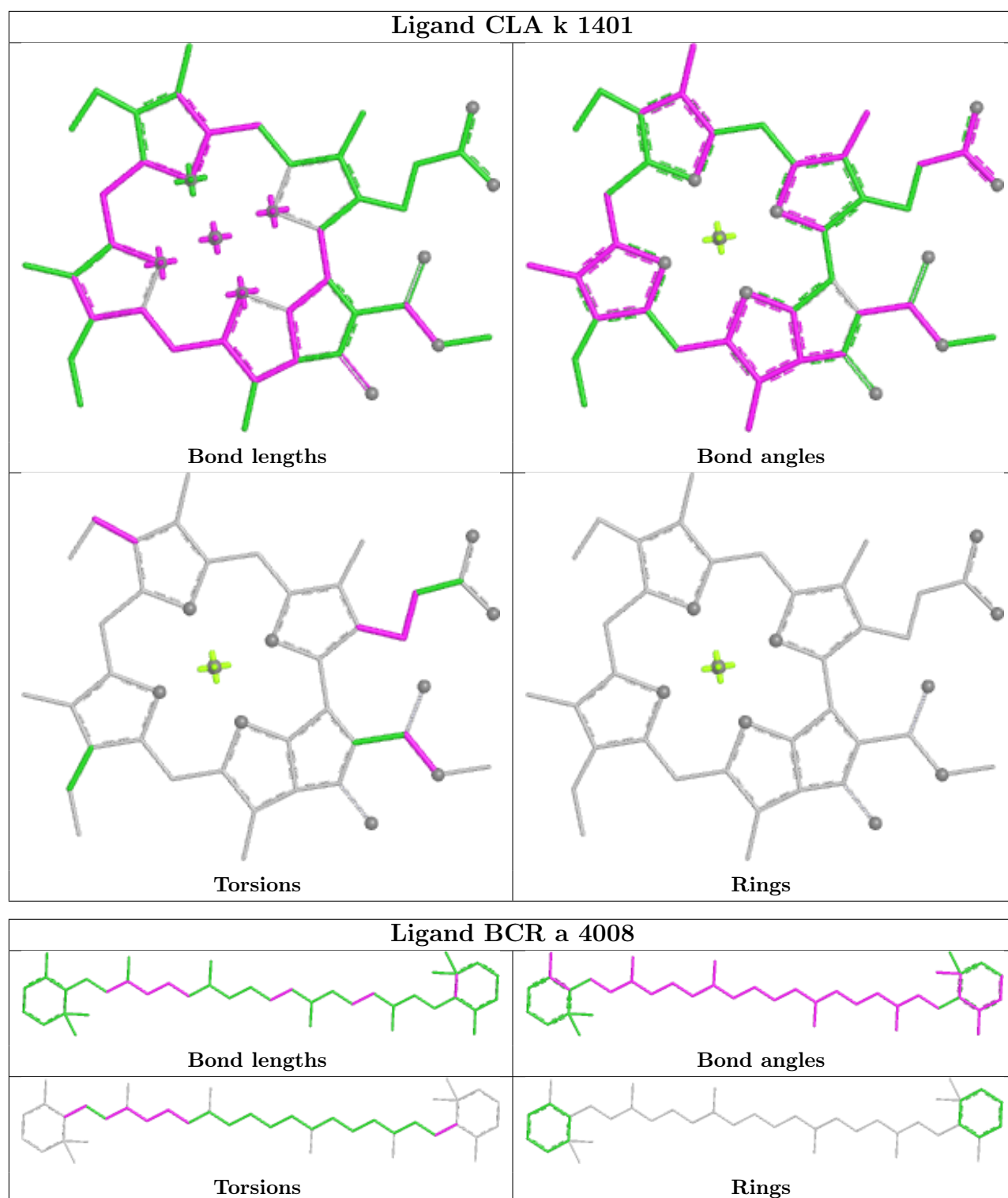


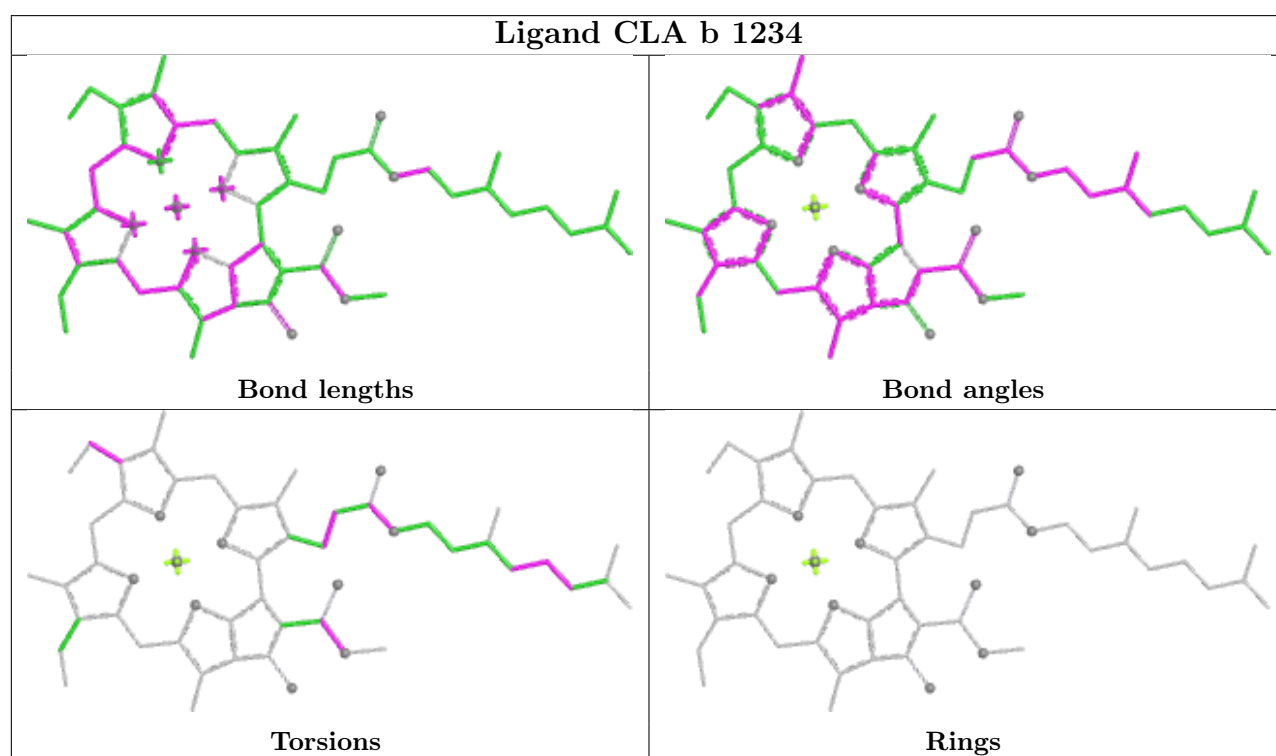
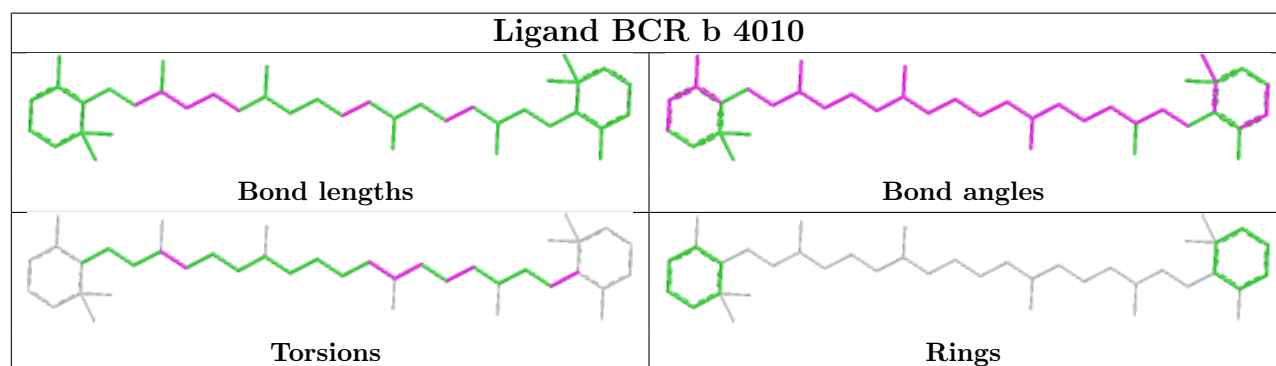
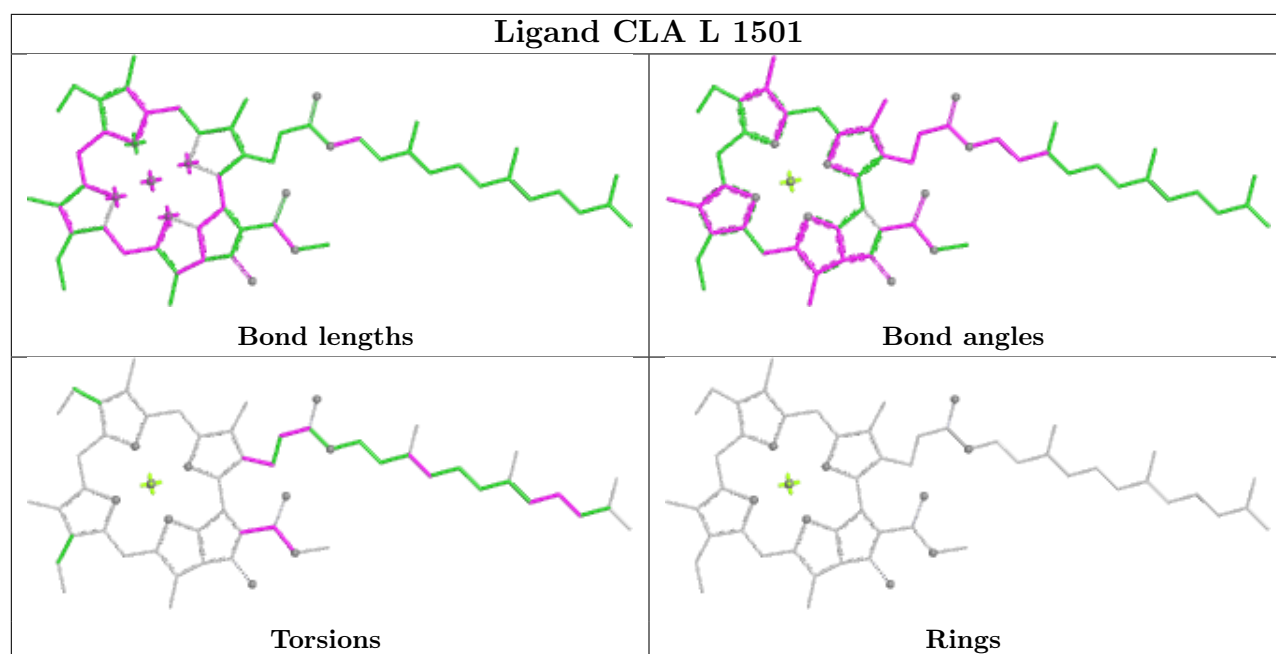
Torsions

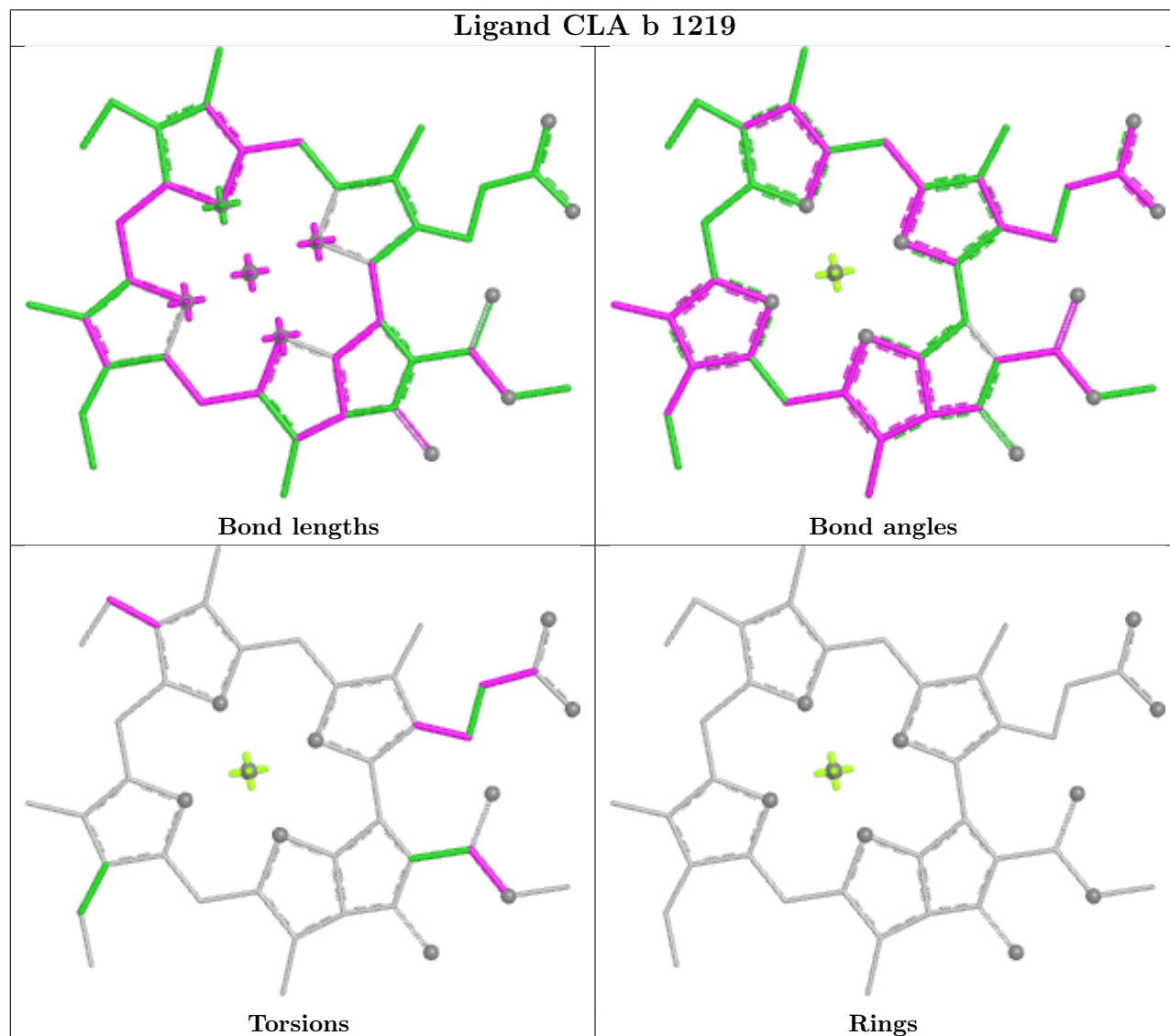
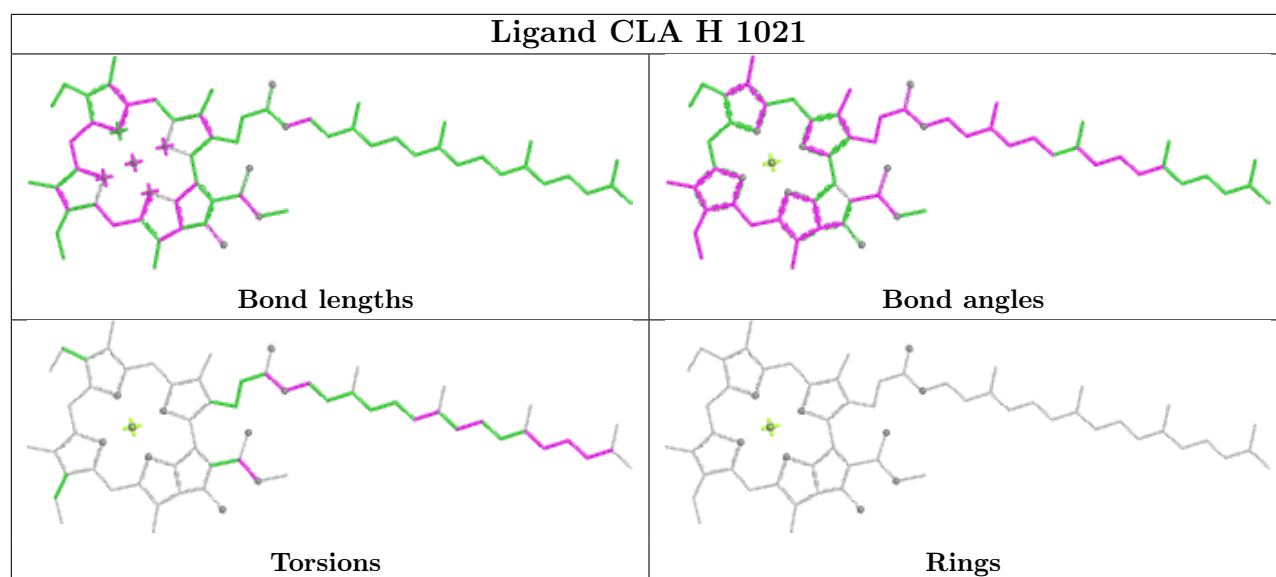


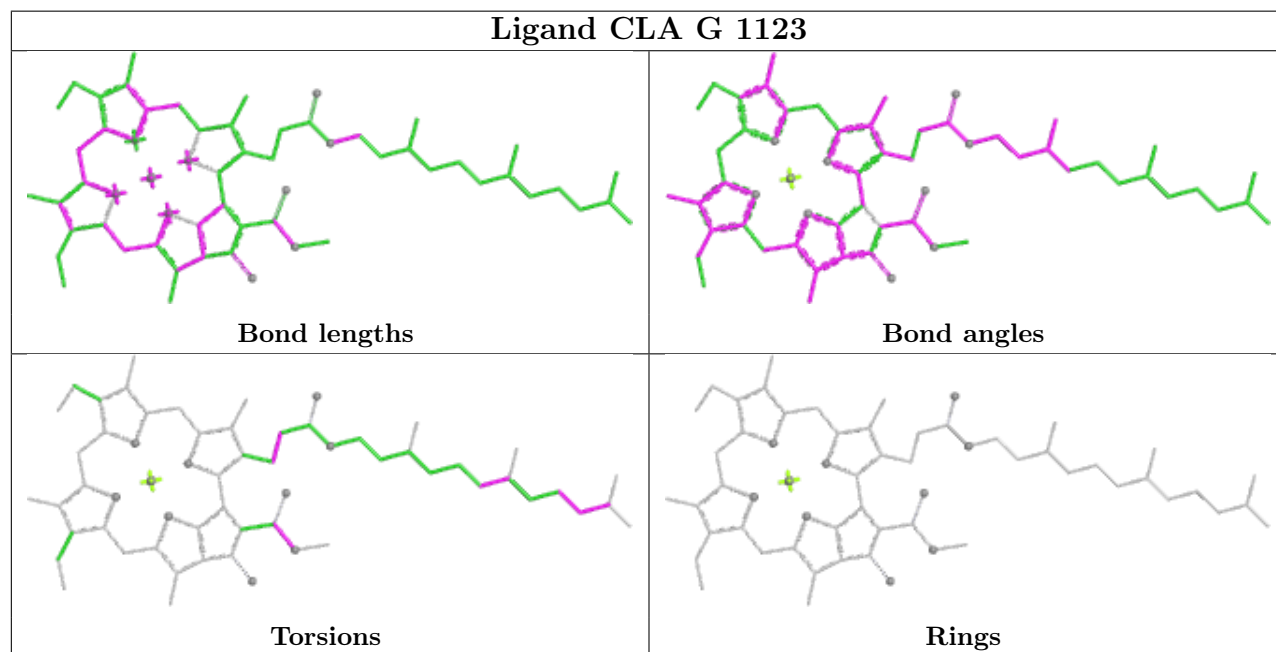
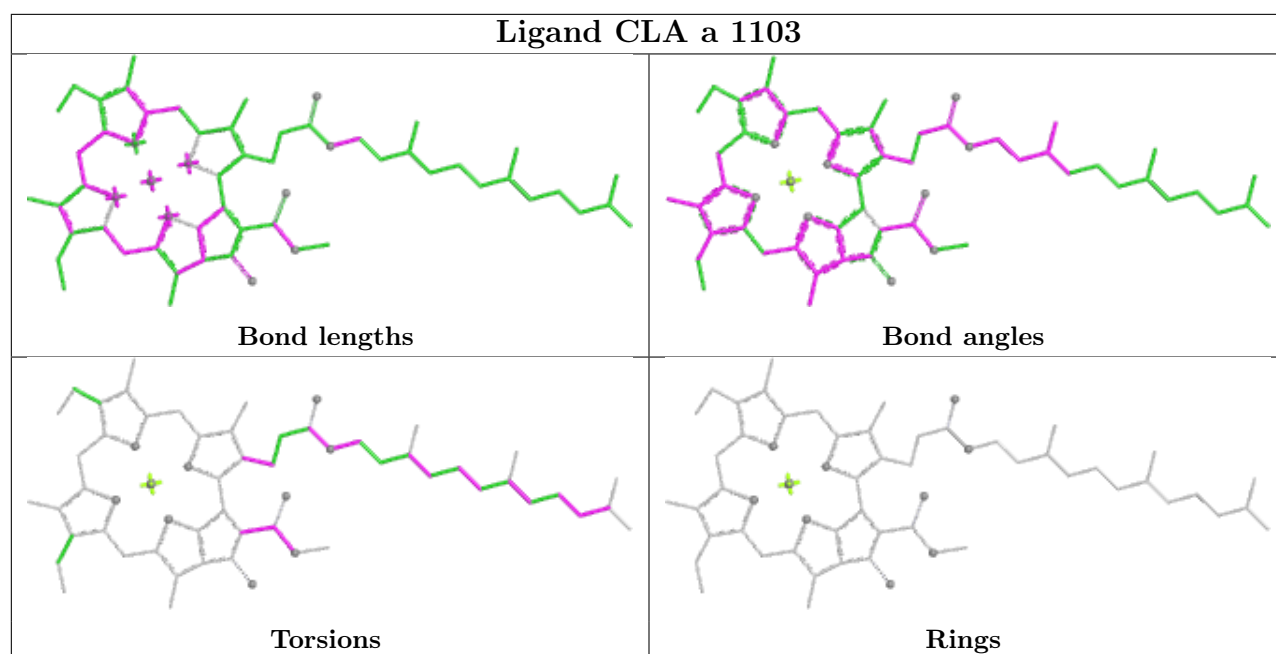
Rings

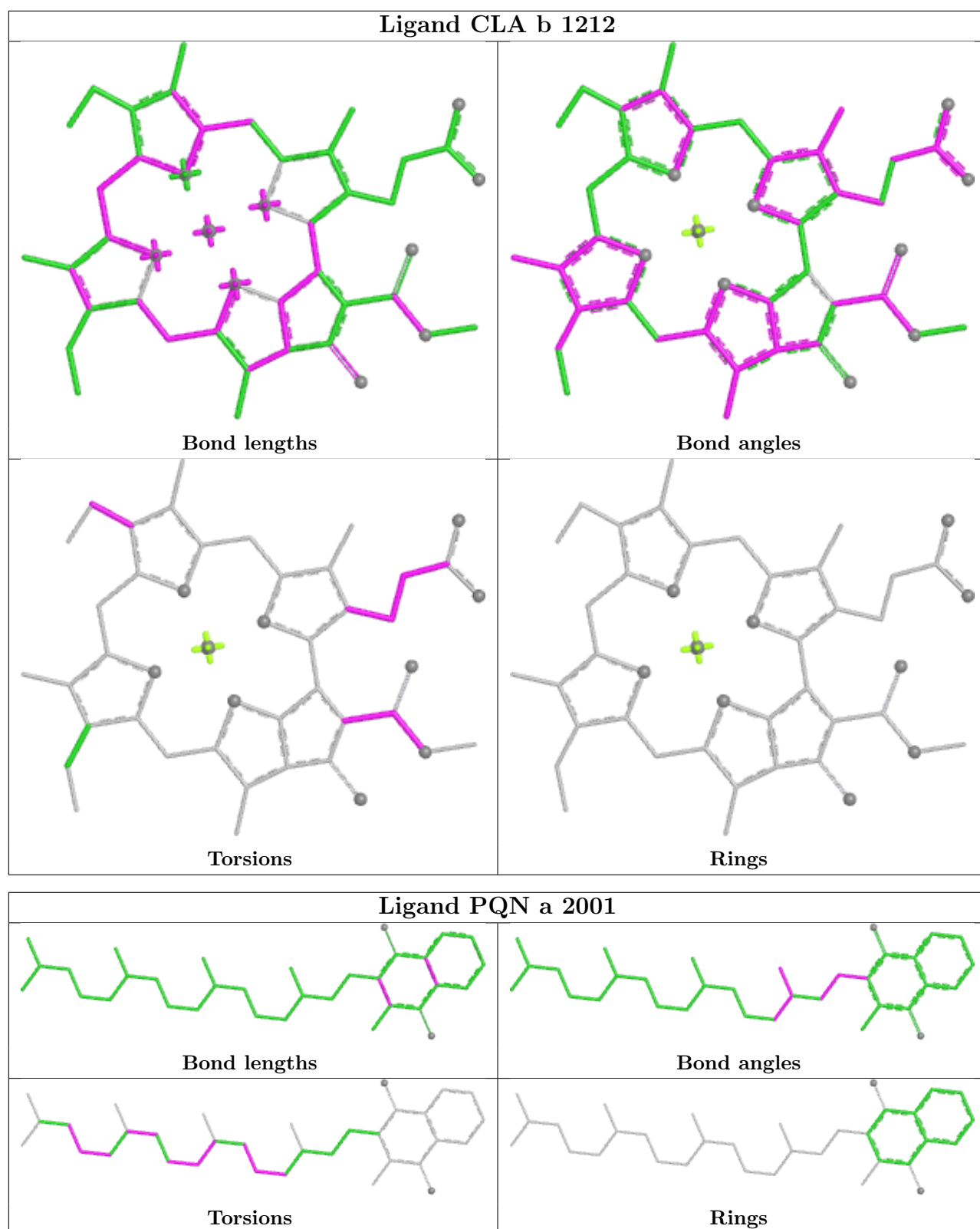


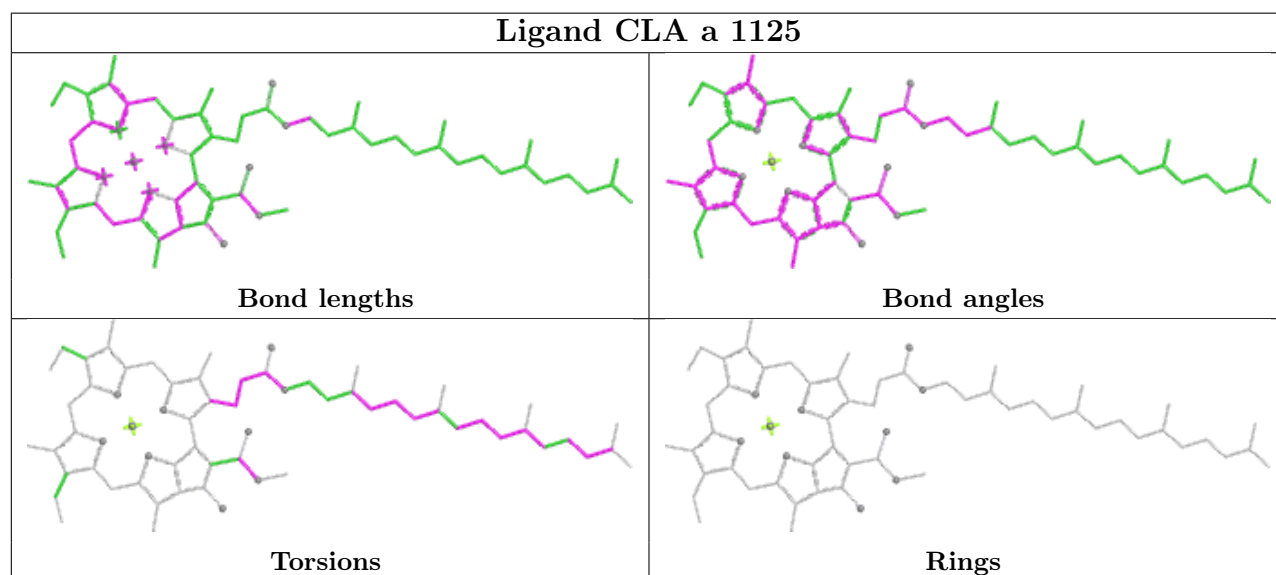
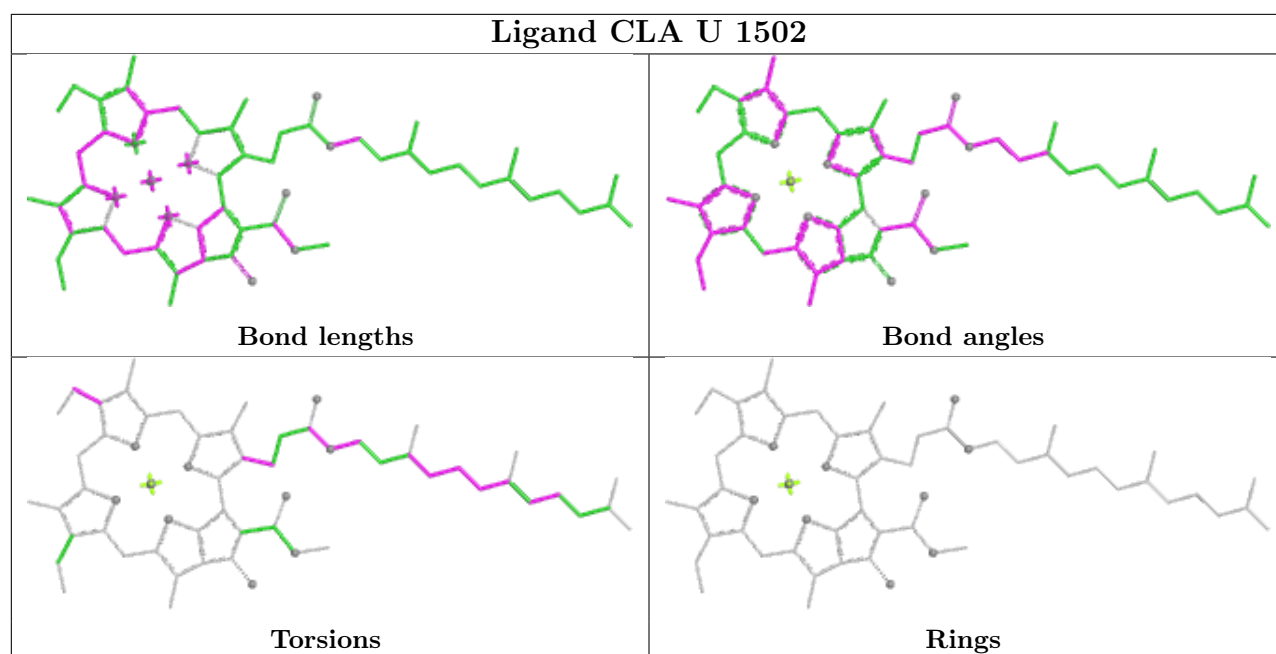


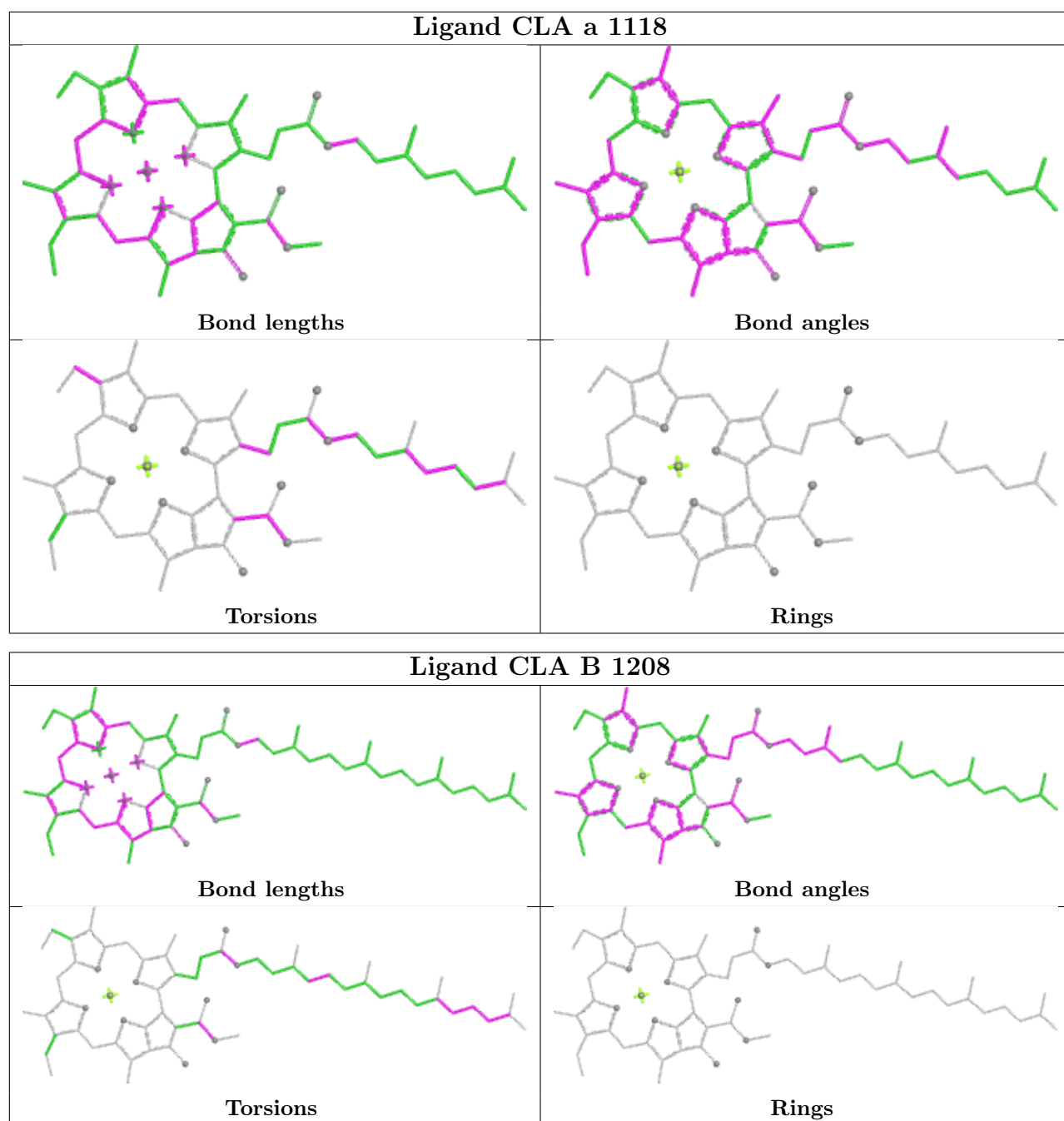


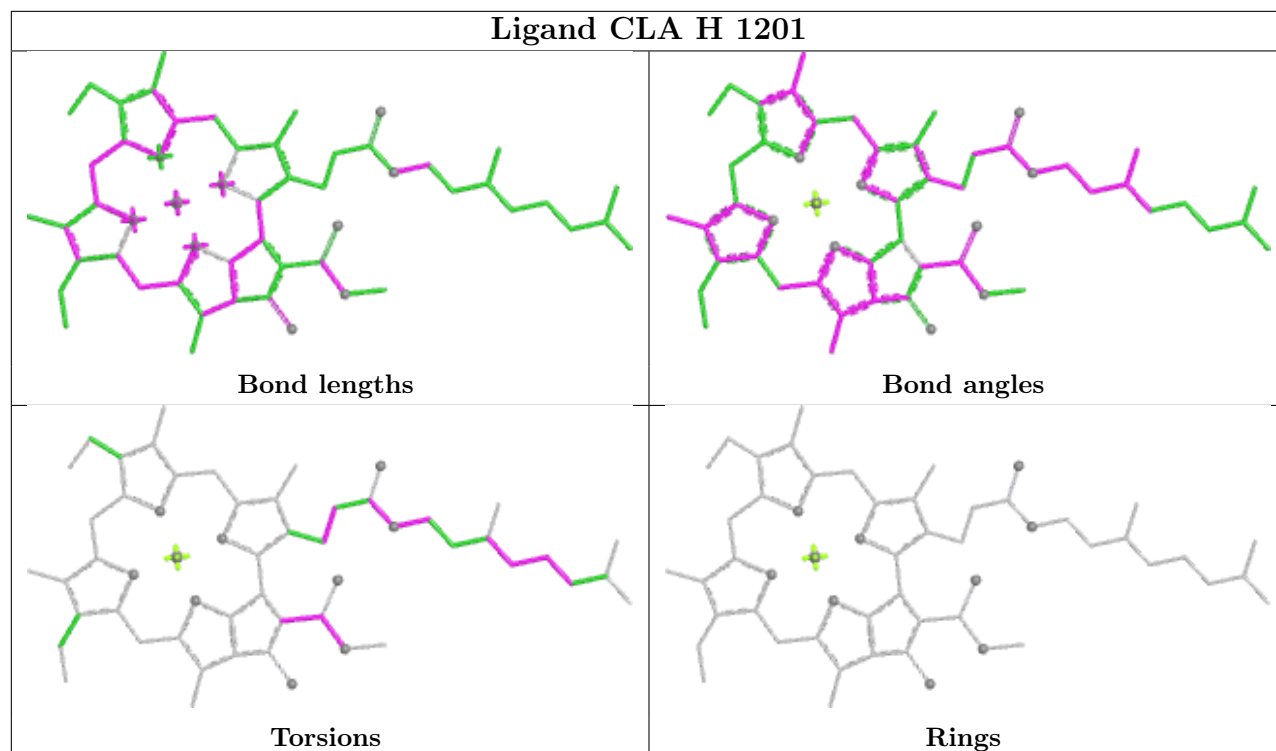
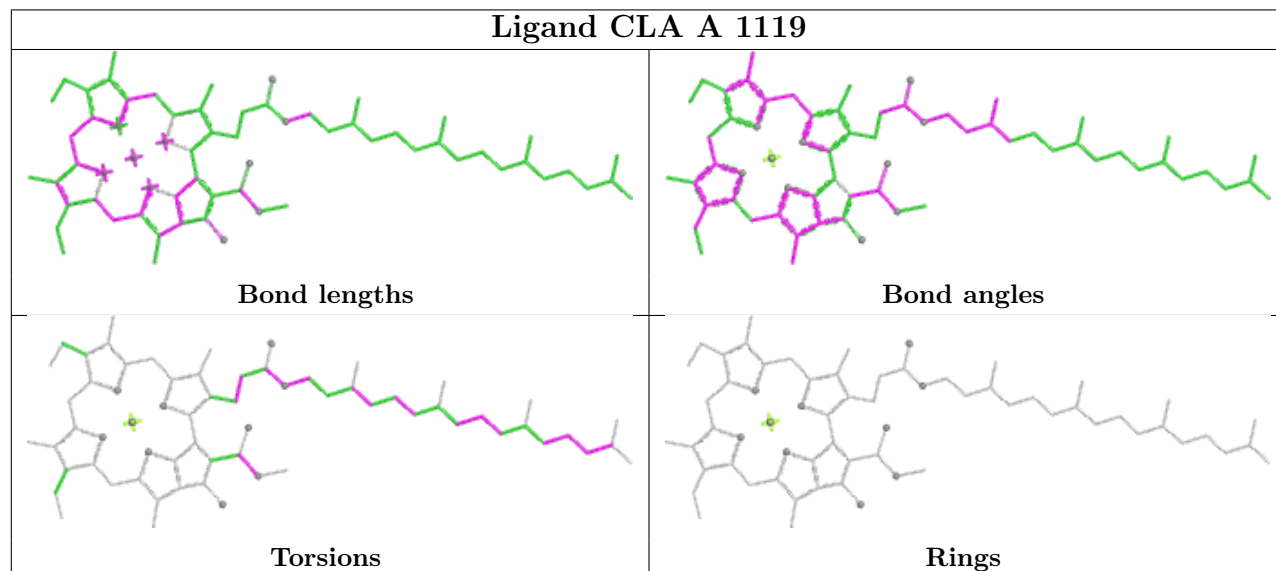




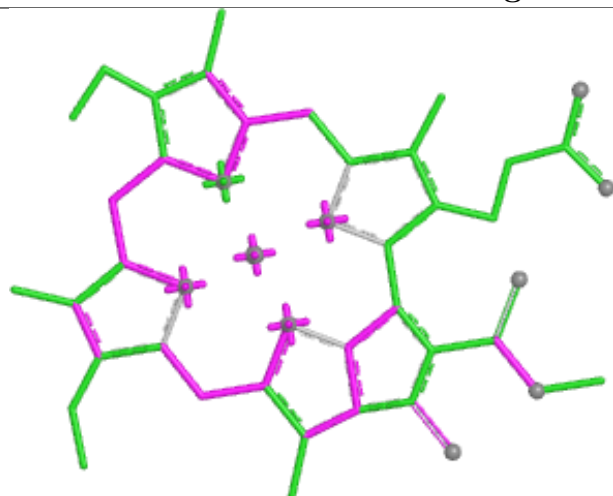




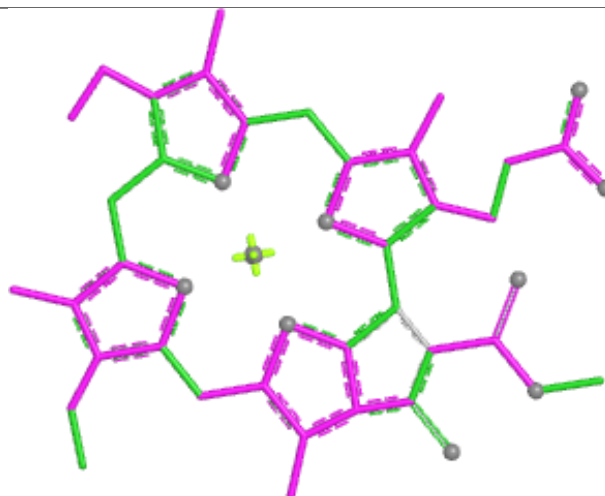


Ligand CLA H 1201**Ligand CLA A 1119**

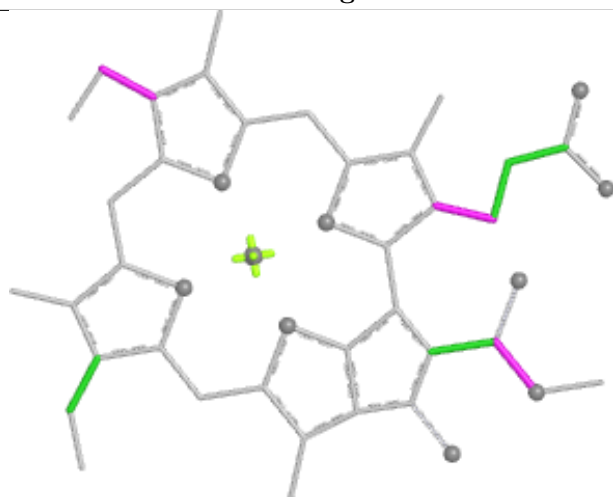
Ligand CLA G 1107



Bond lengths



Bond angles

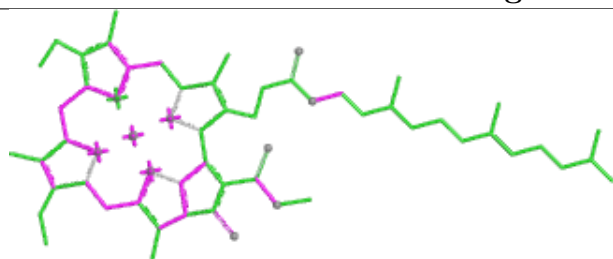


Torsions

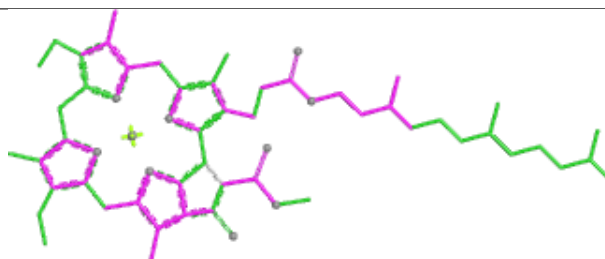


Rings

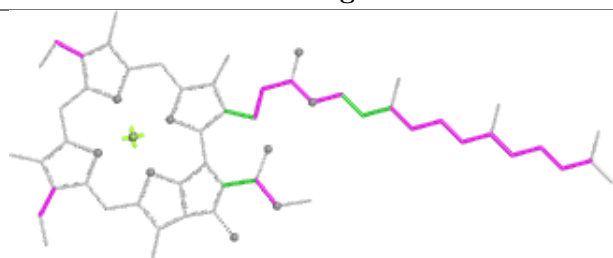
Ligand CLA A 1126



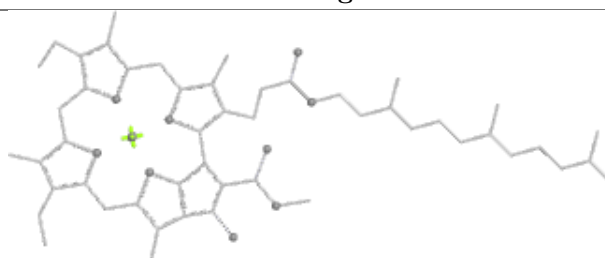
Bond lengths



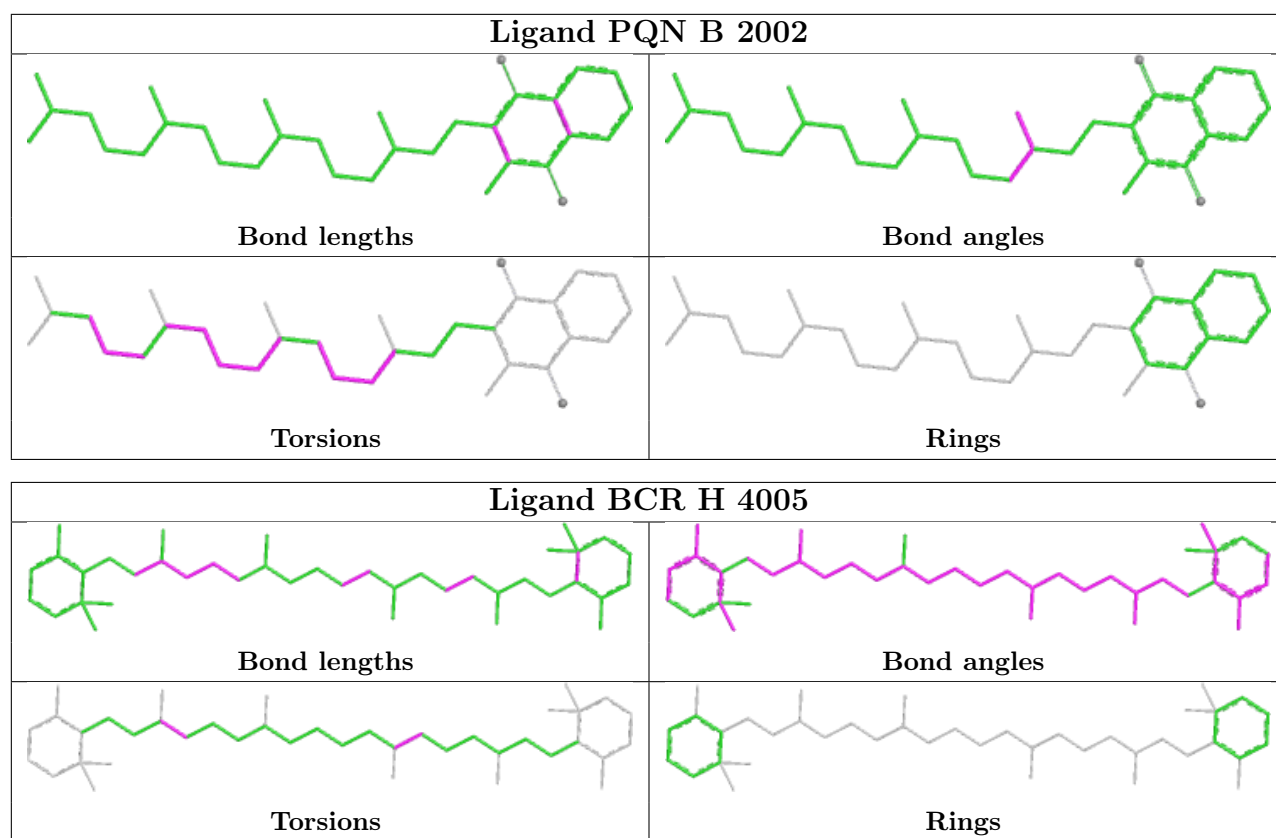
Bond angles

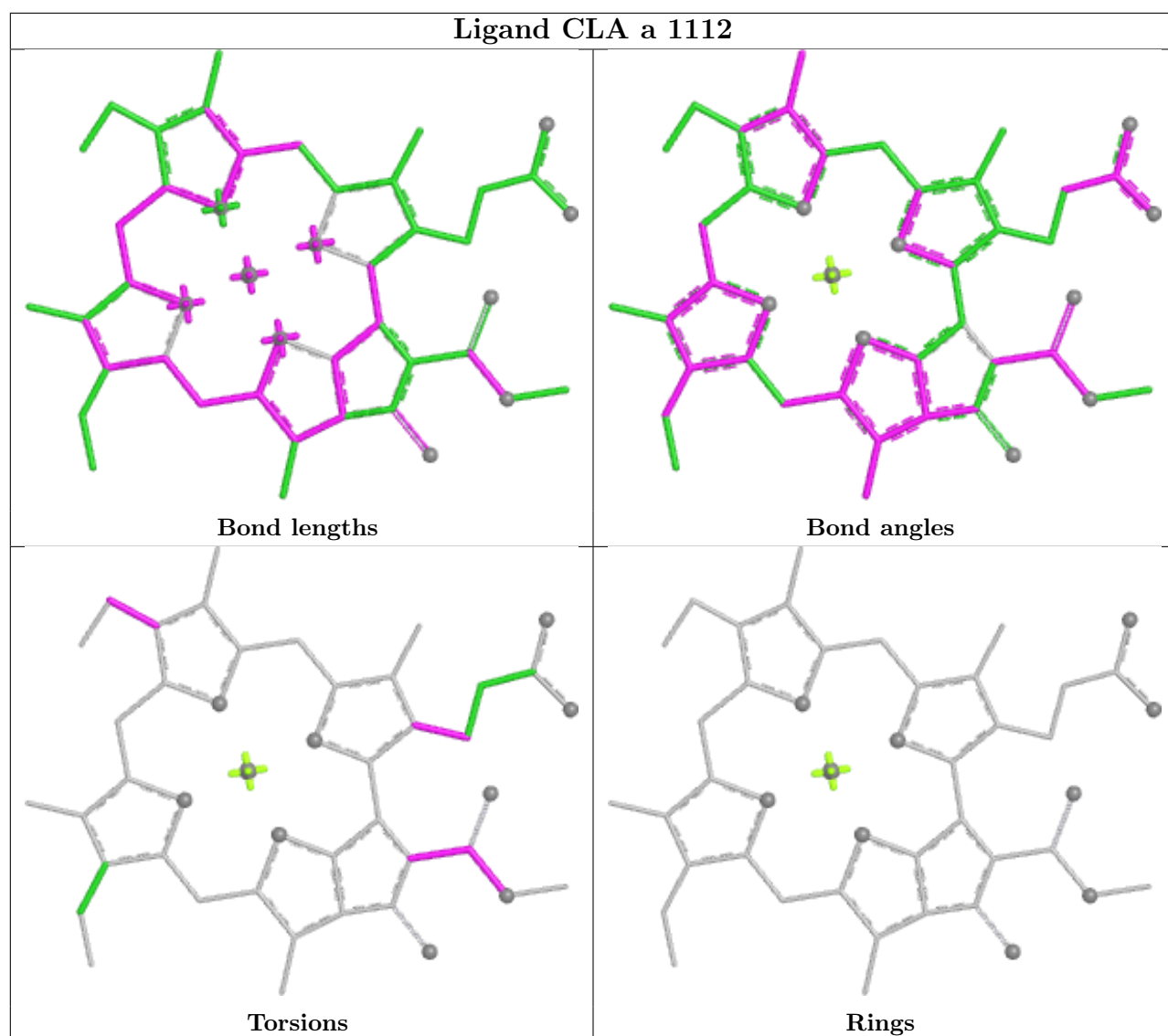


Torsions

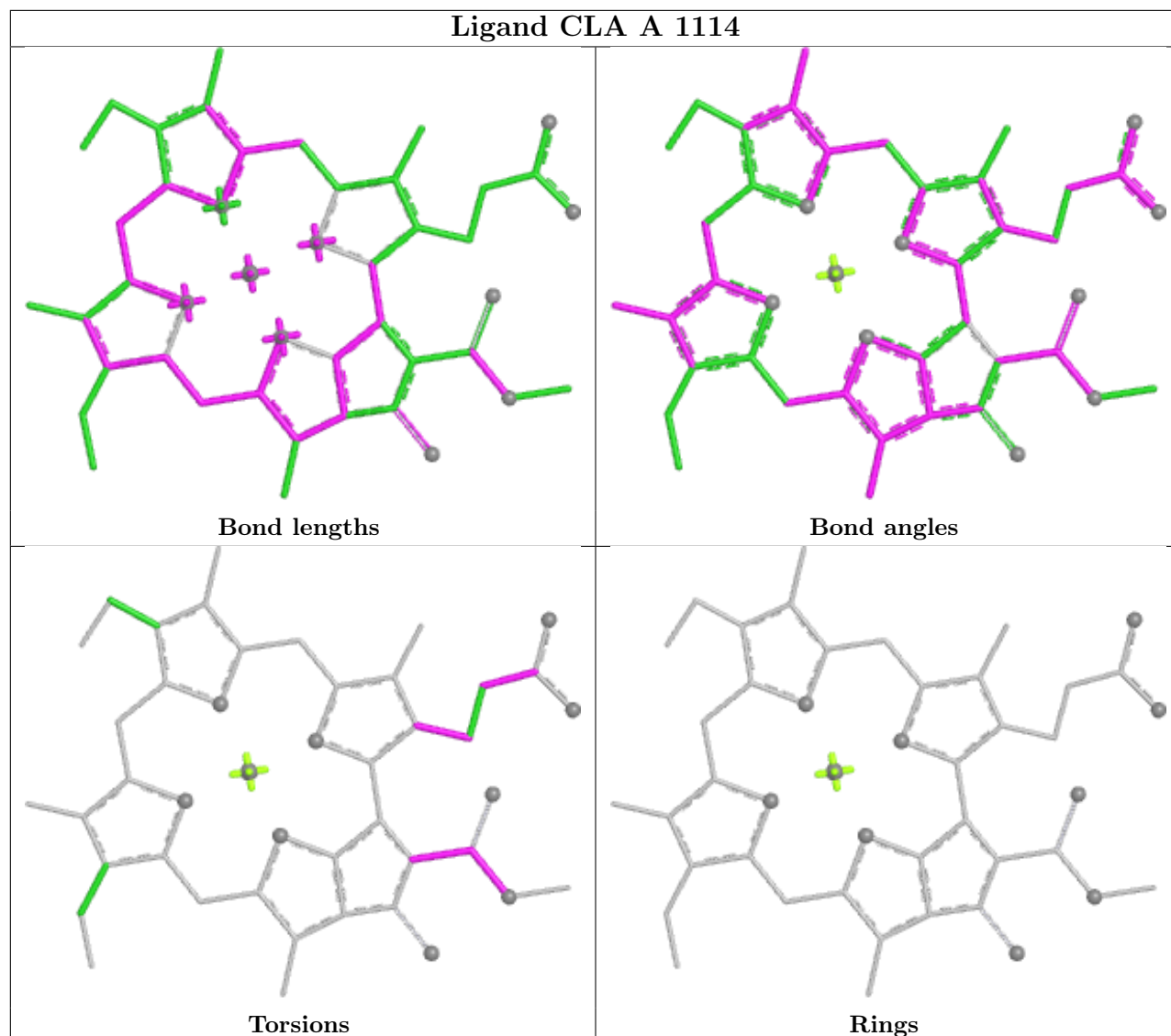


Rings

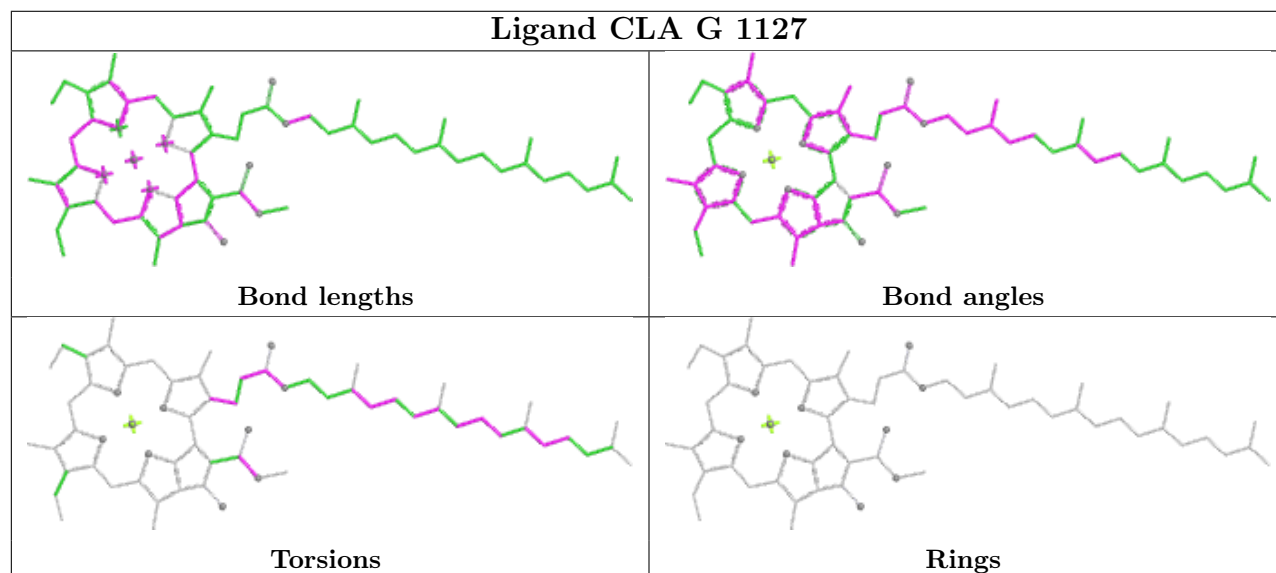




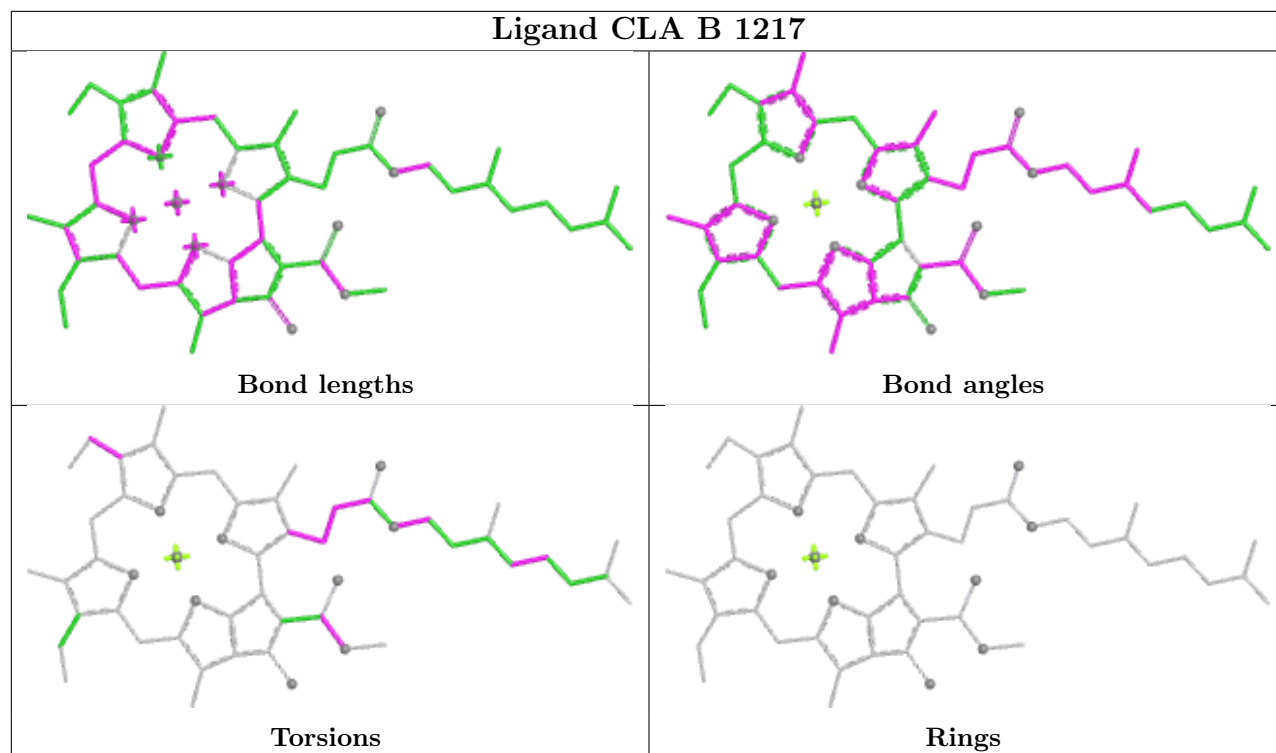
Ligand CLA A 1114



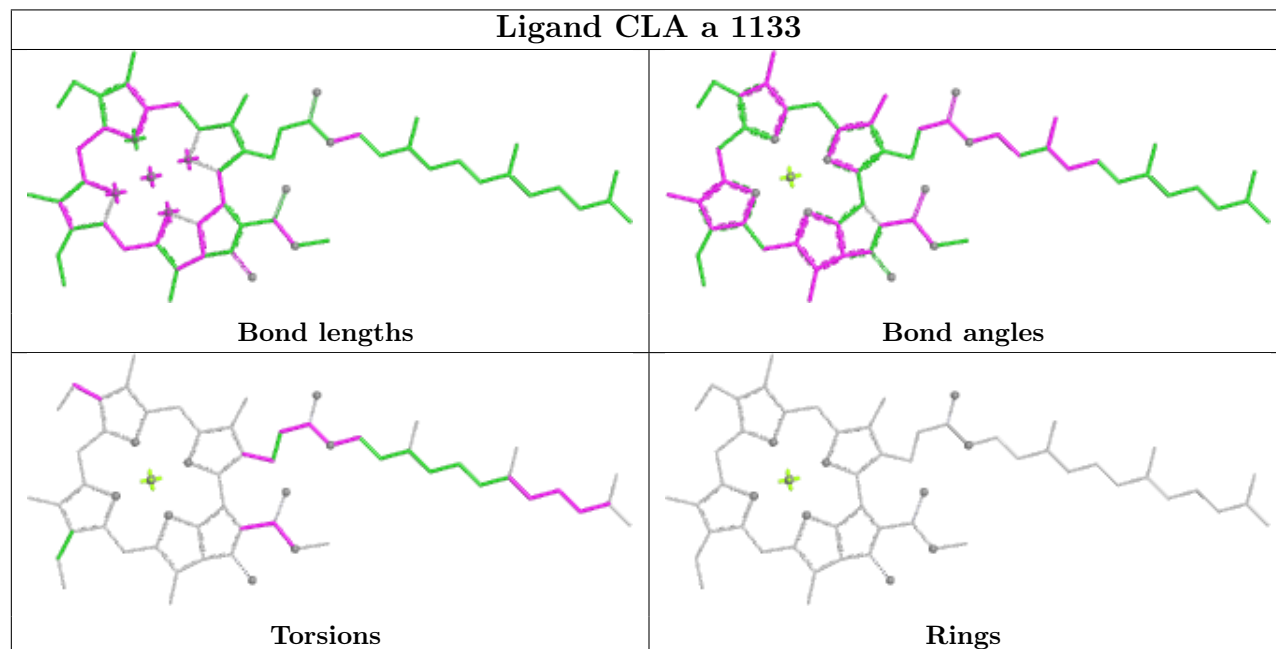
Ligand CLA G 1127



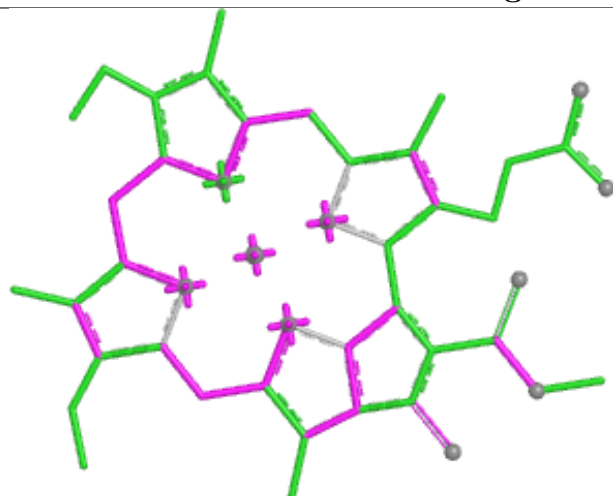
Ligand CLA B 1217



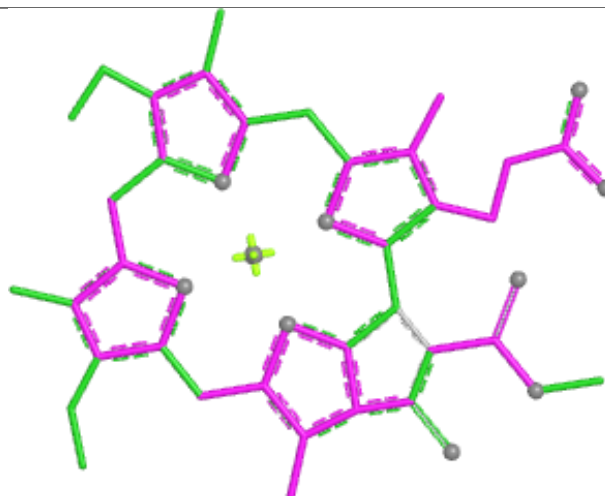
Ligand CLA a 1133



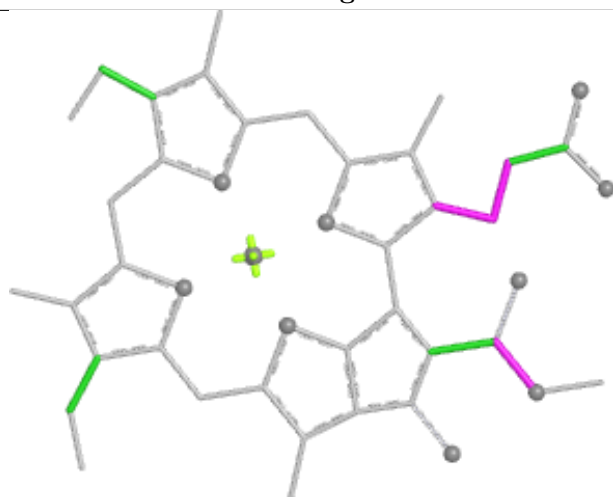
Ligand CLA H 1206



Bond lengths



Bond angles

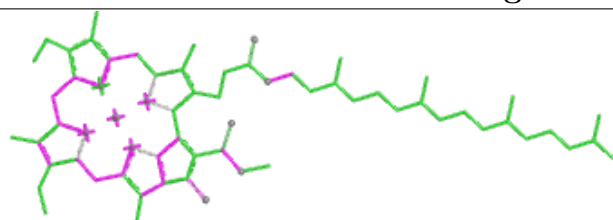


Torsions

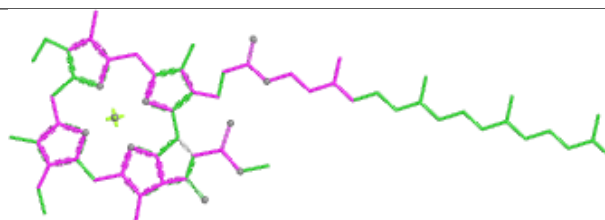


Rings

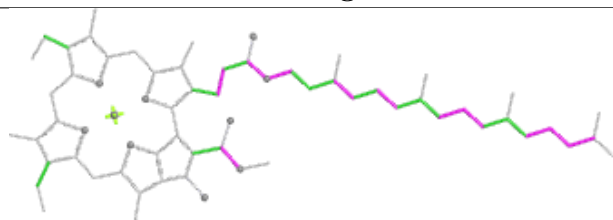
Ligand CLA G 1119



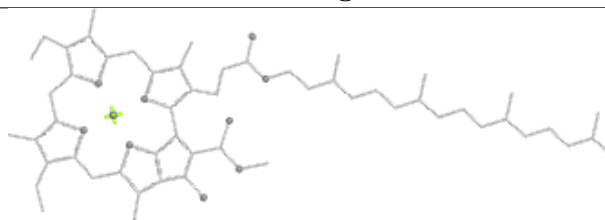
Bond lengths



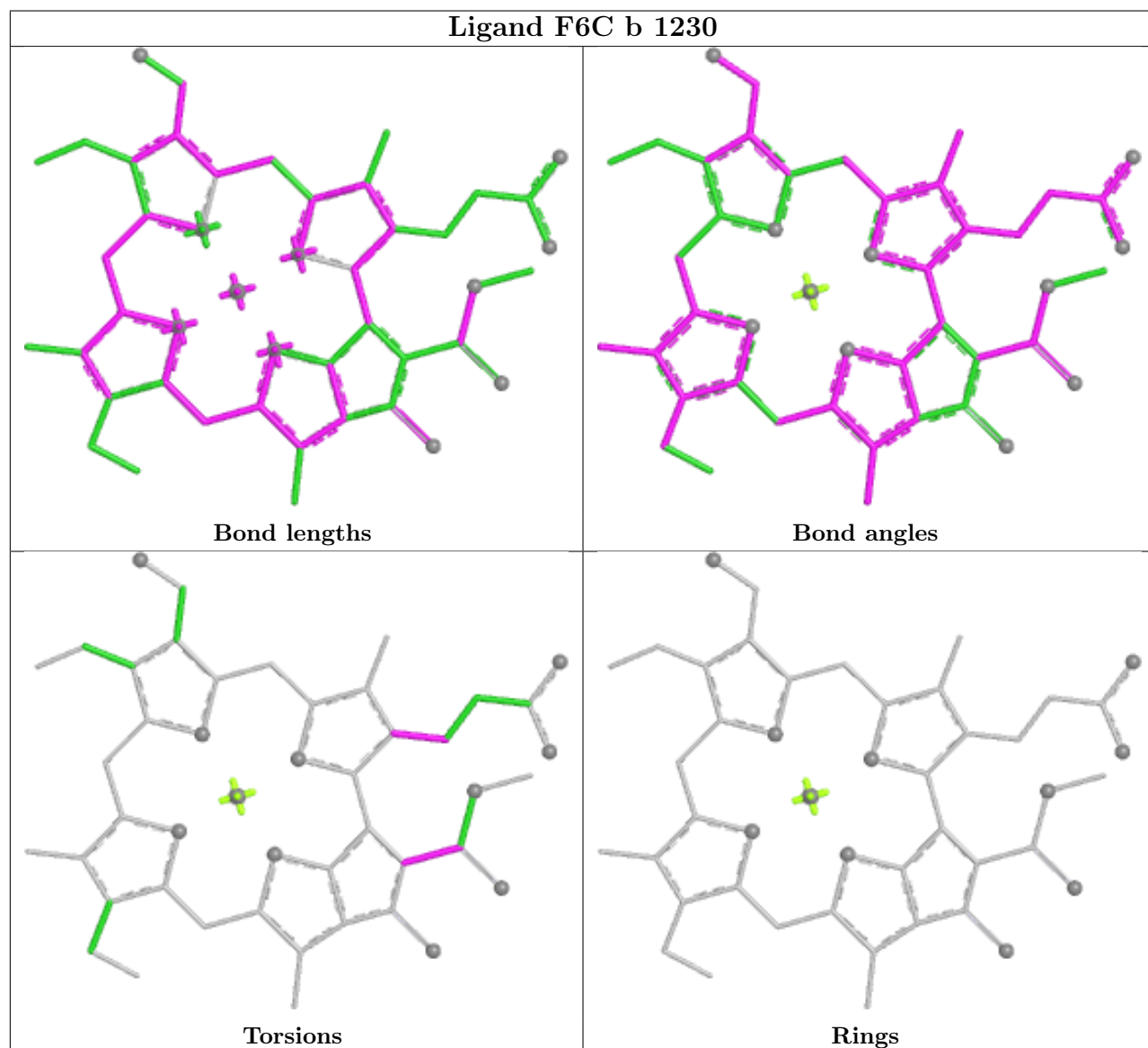
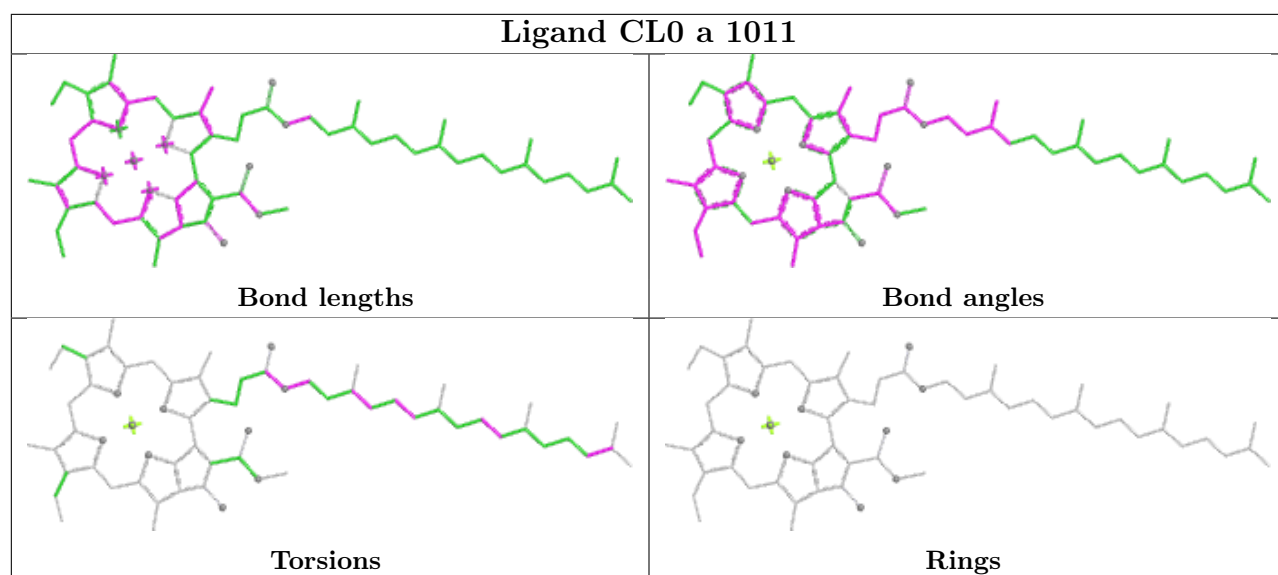
Bond angles

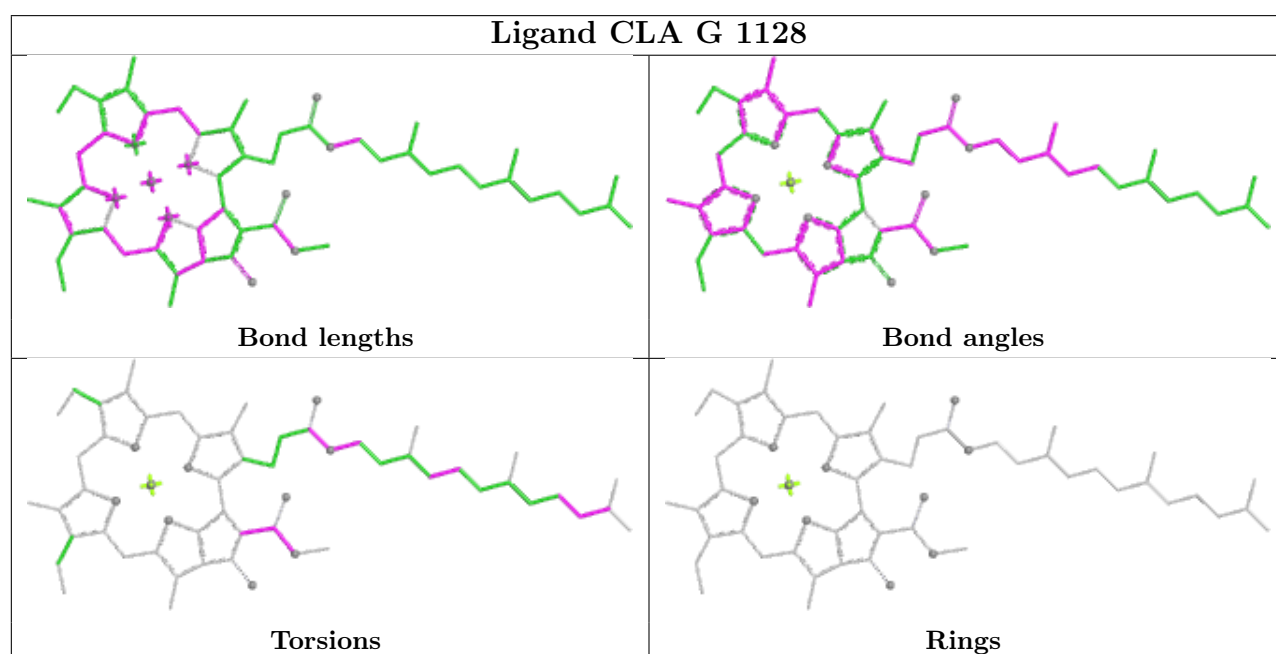
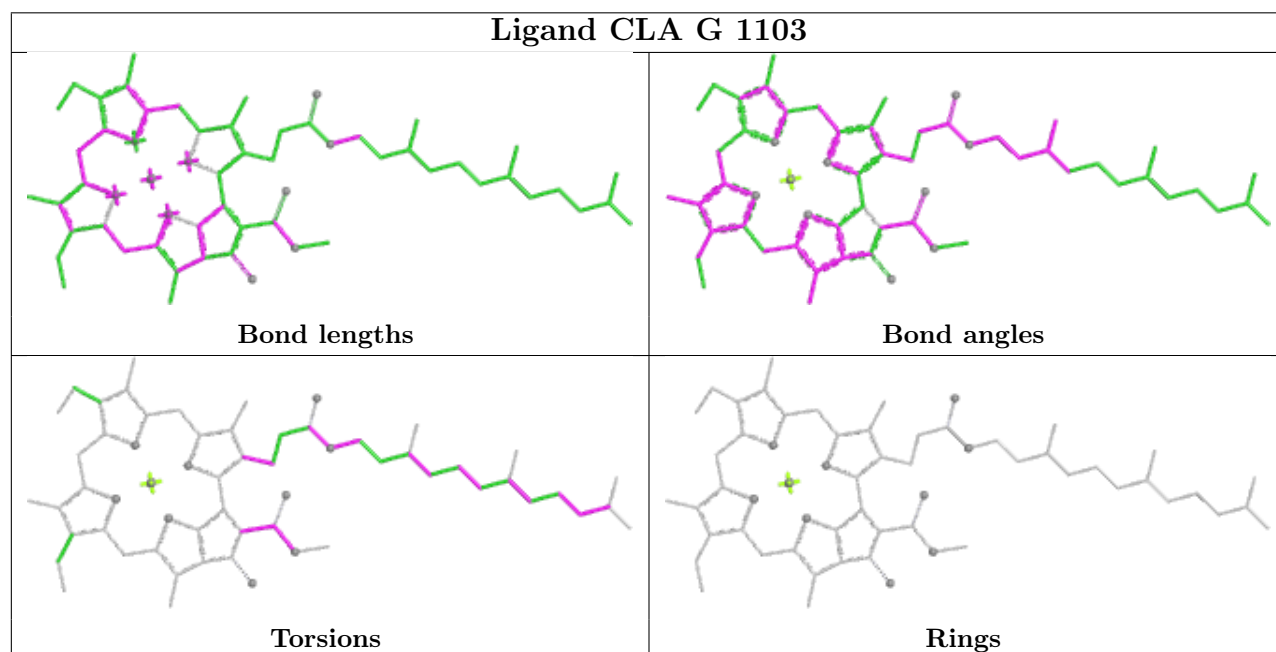
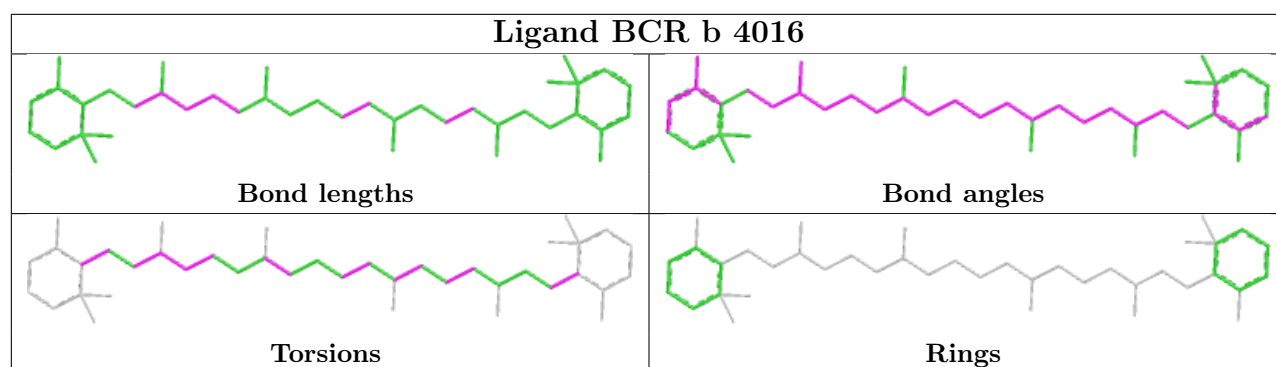


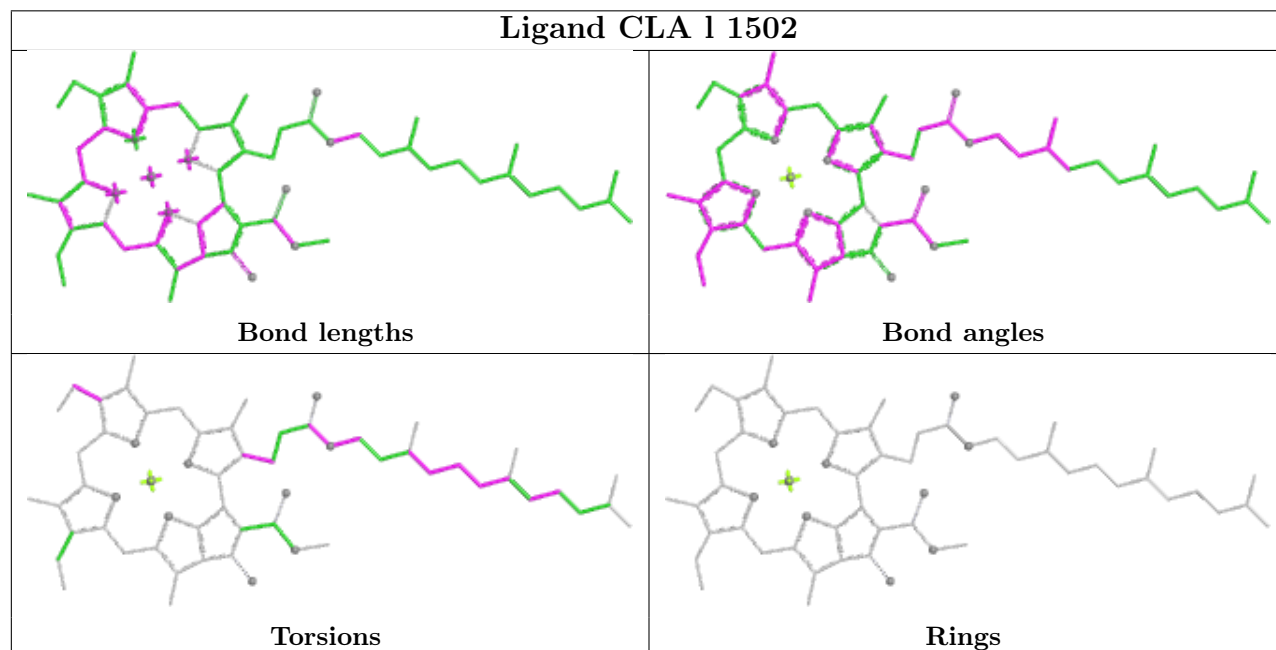
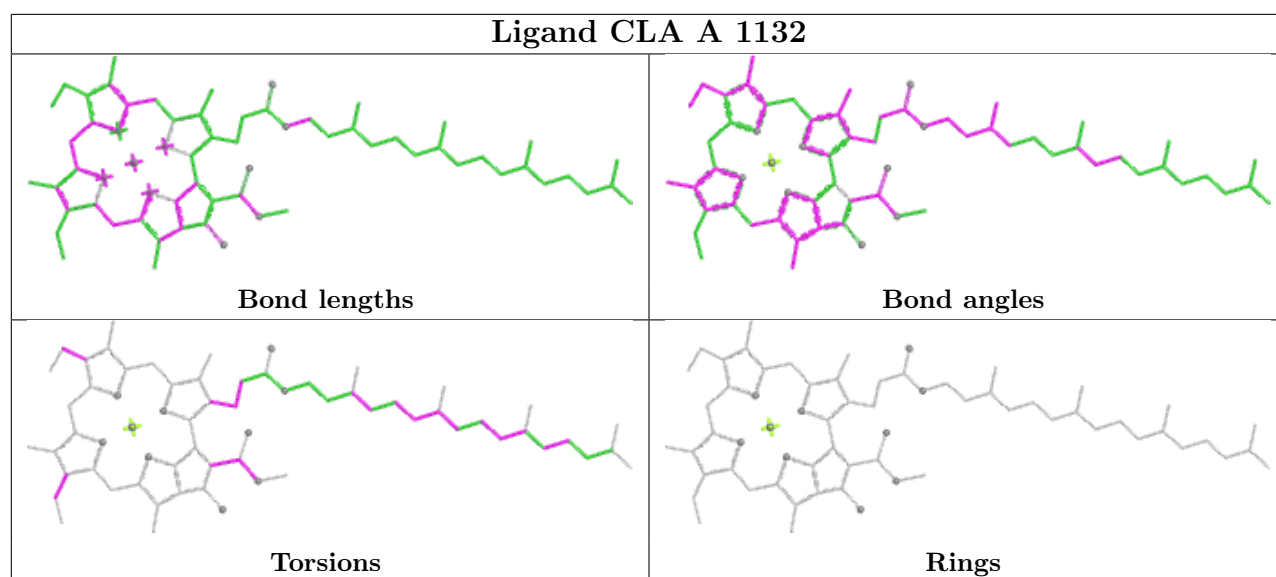
Torsions

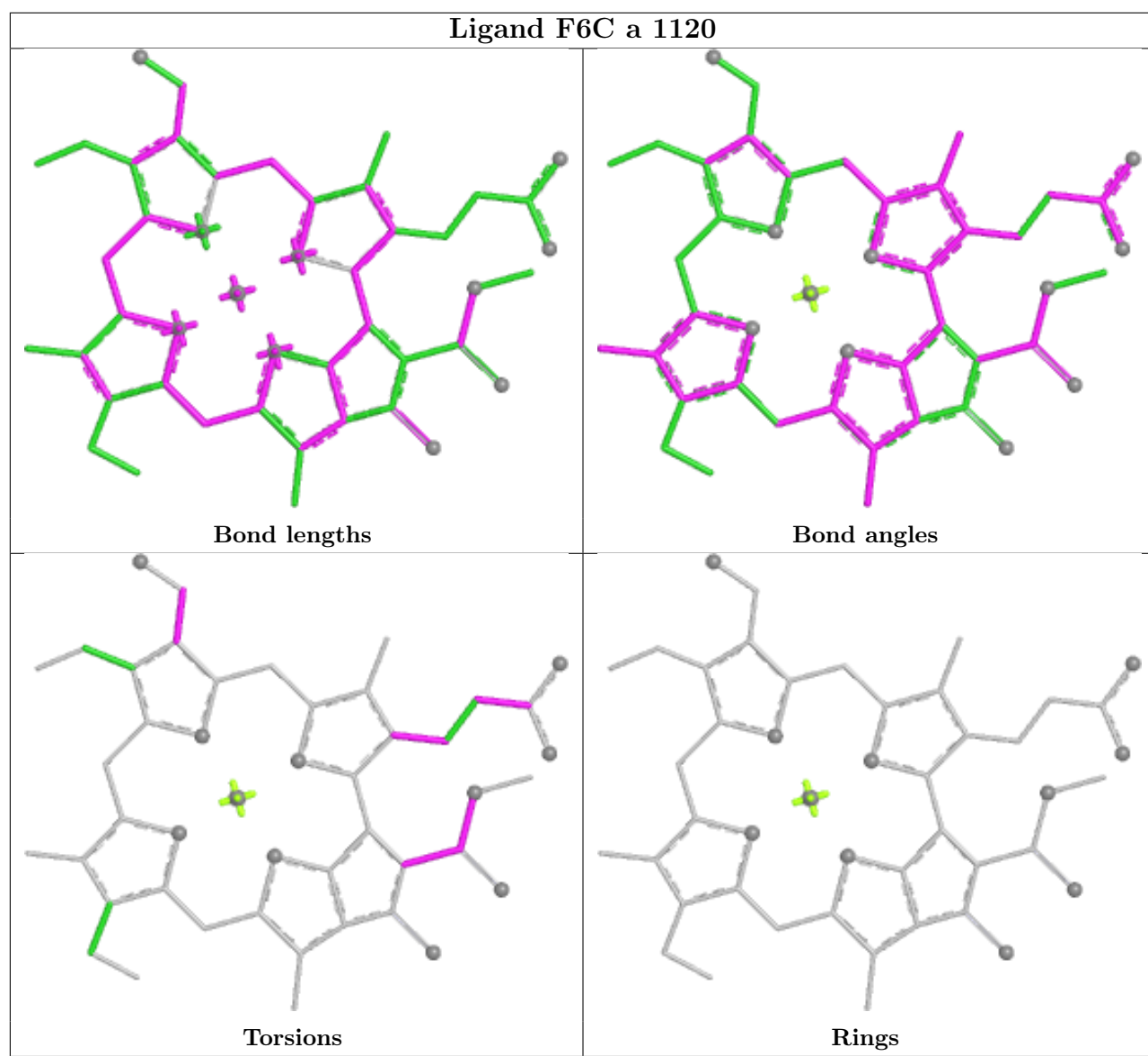


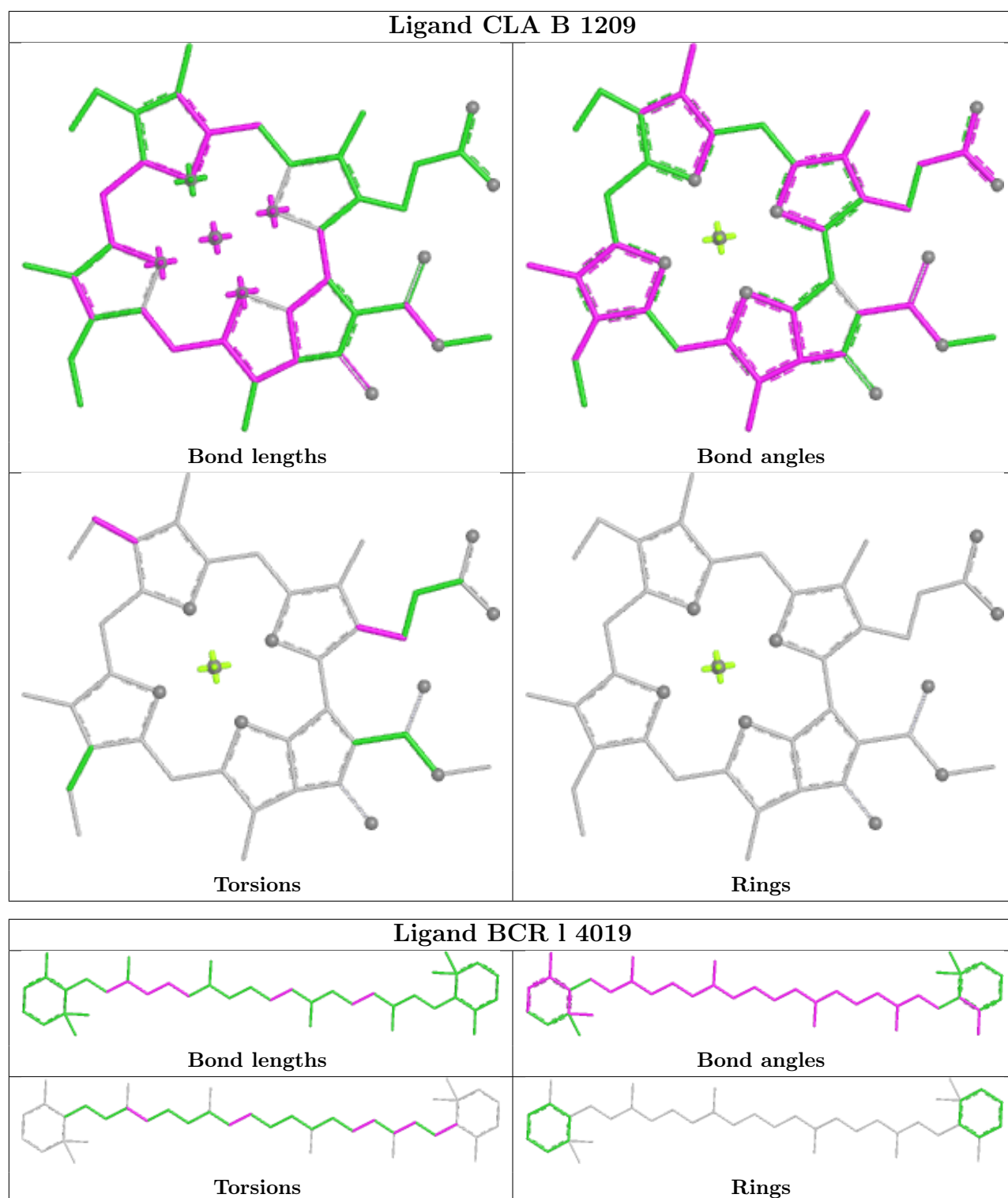
Rings

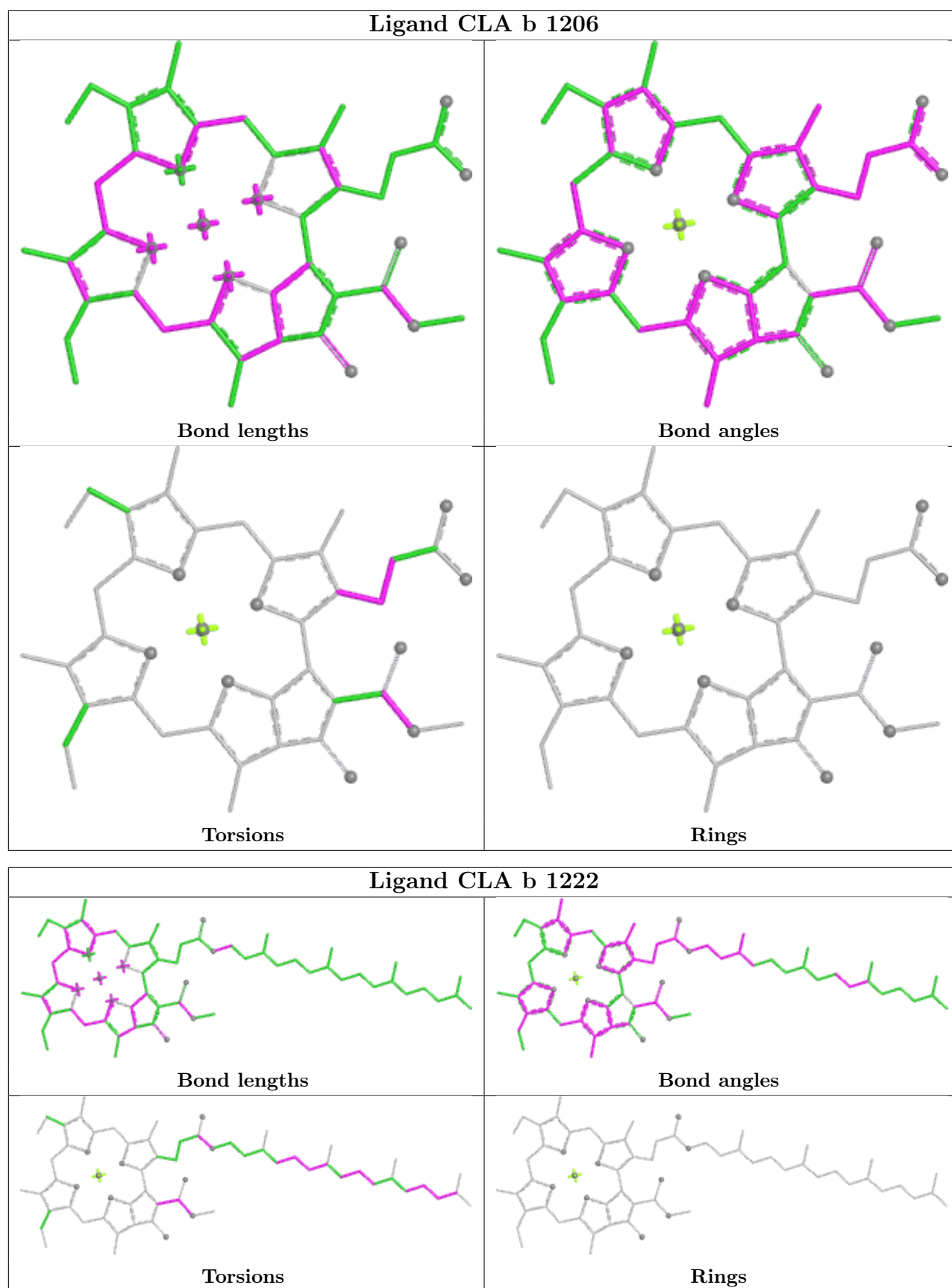


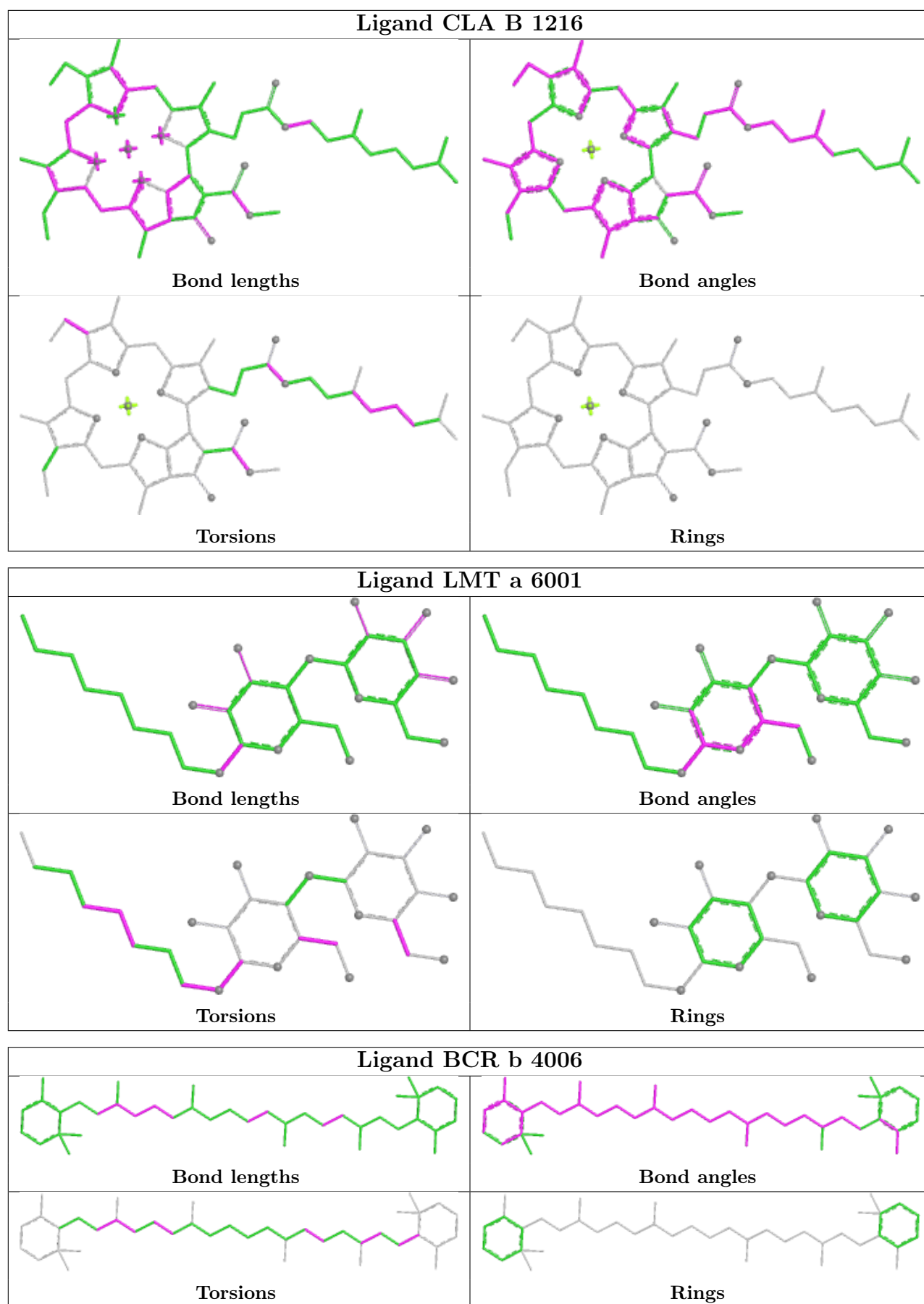


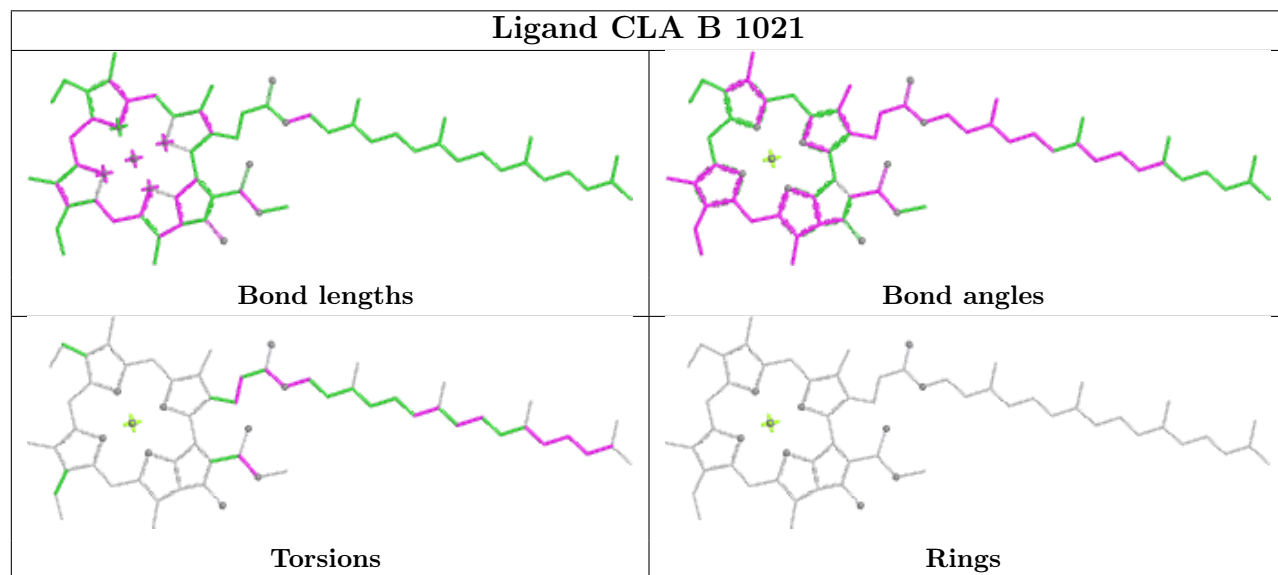
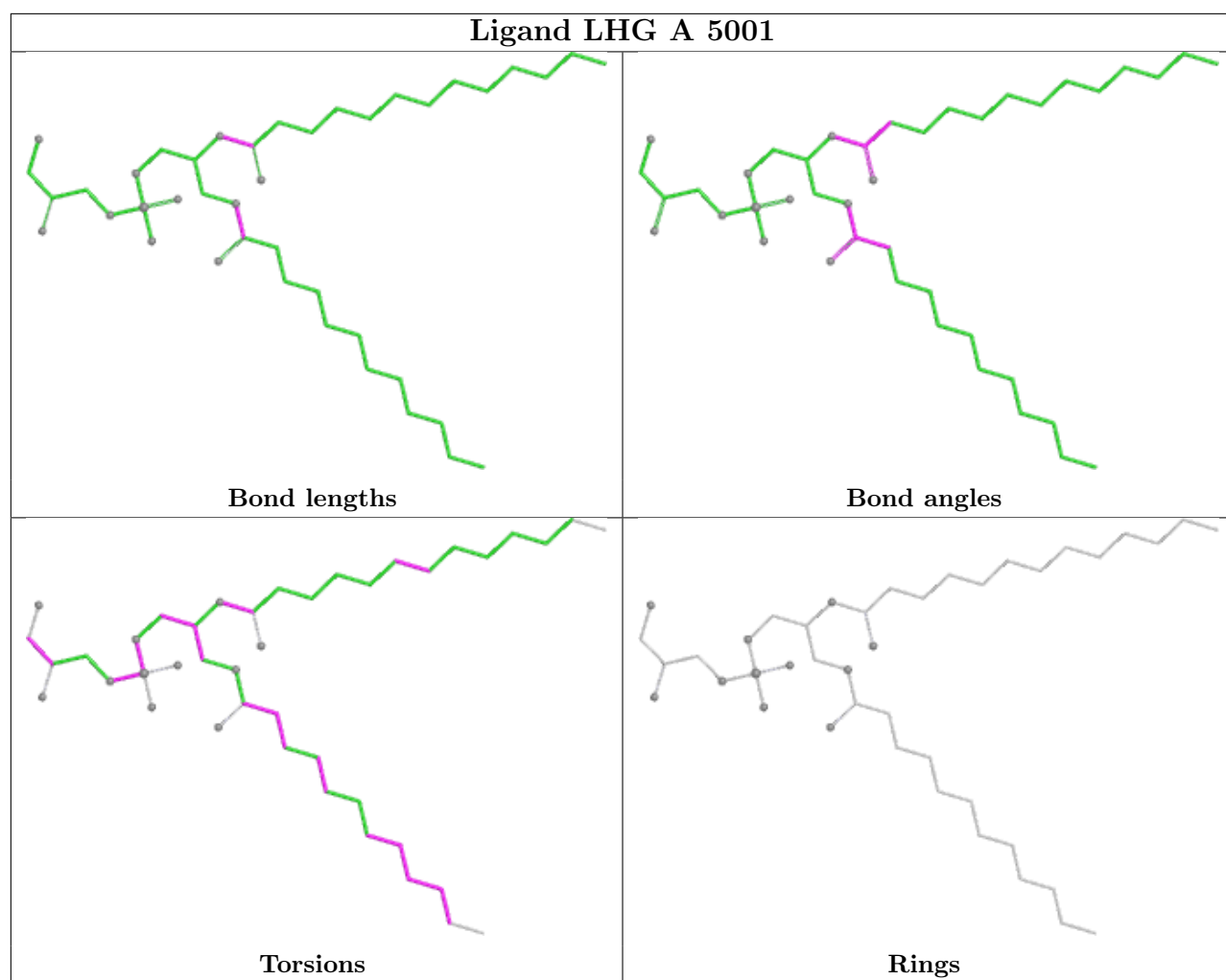


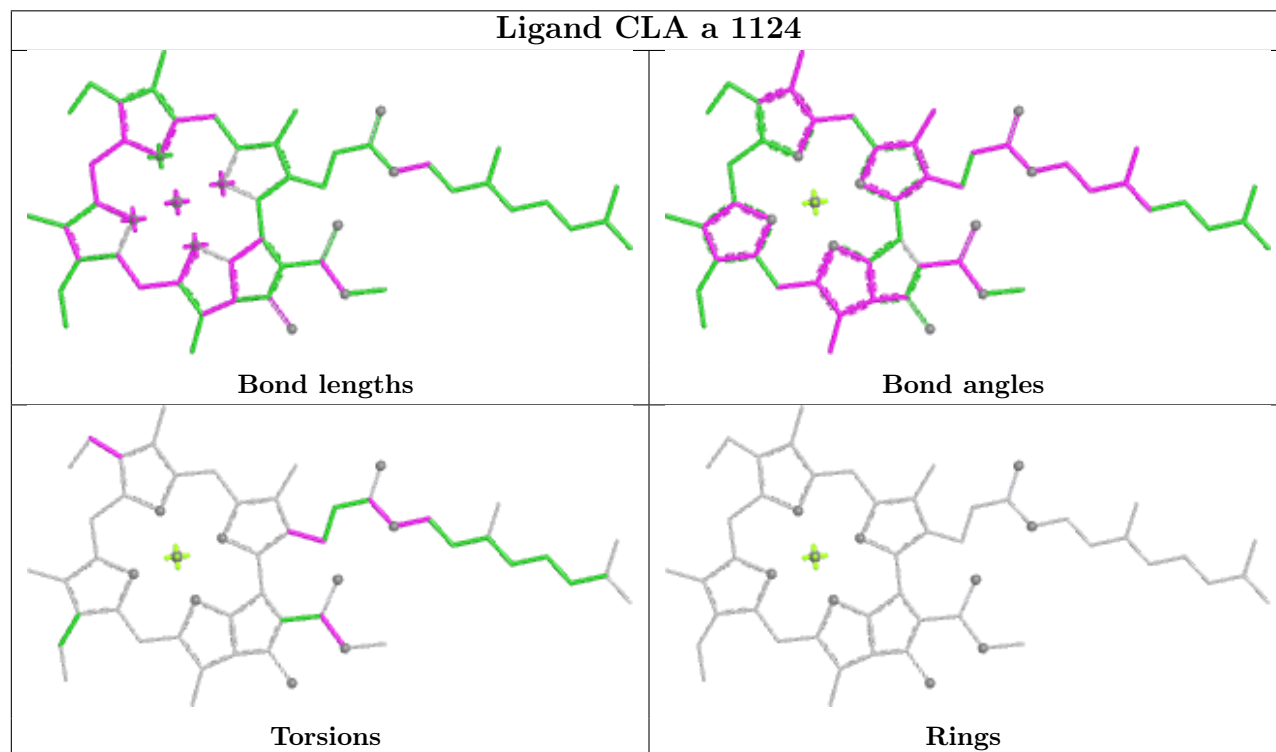
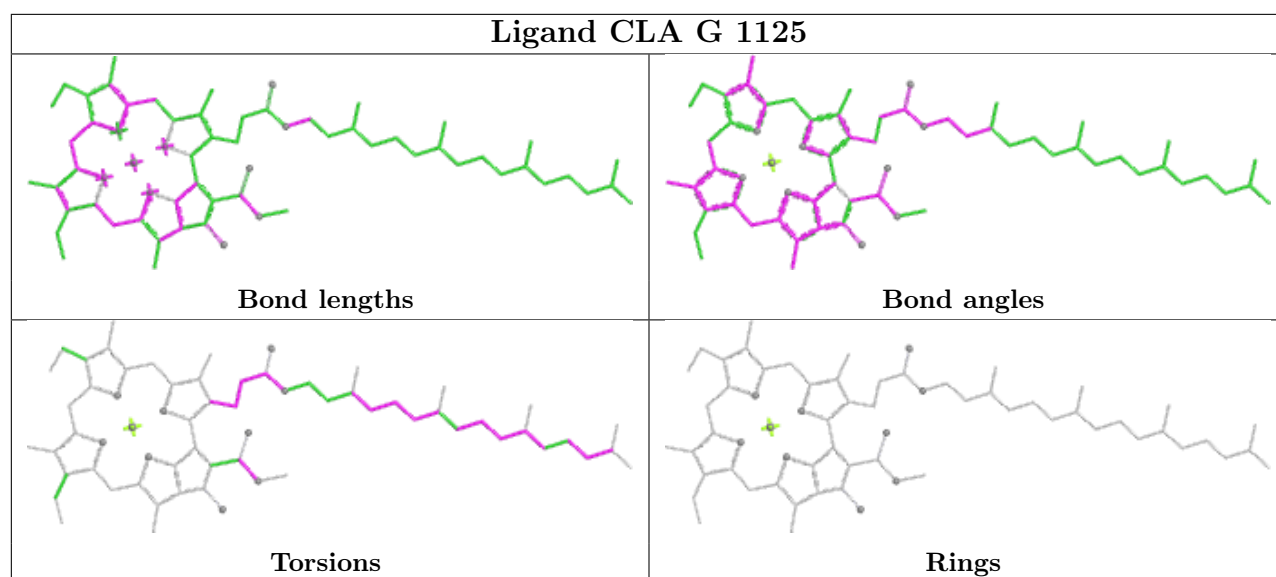




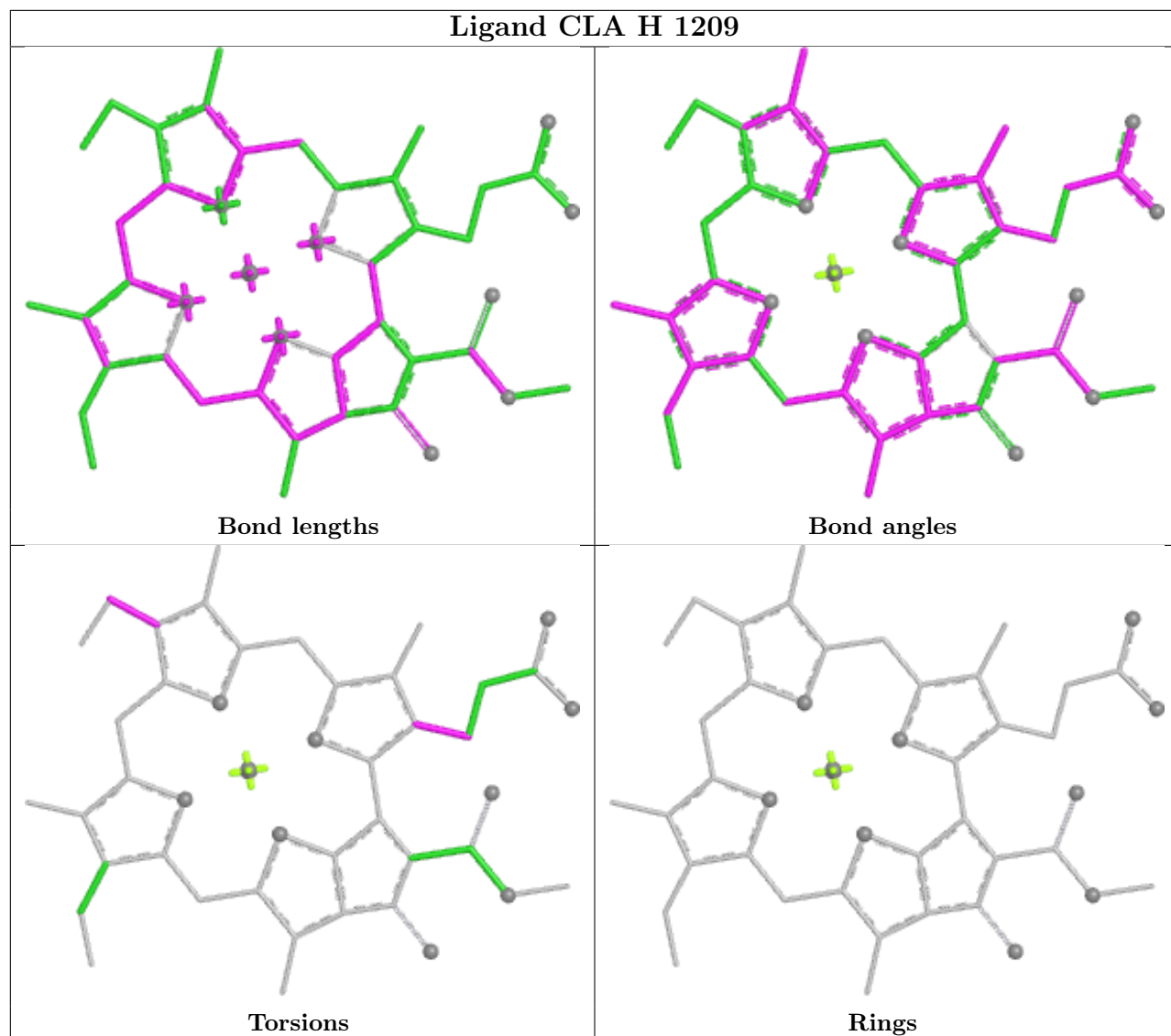


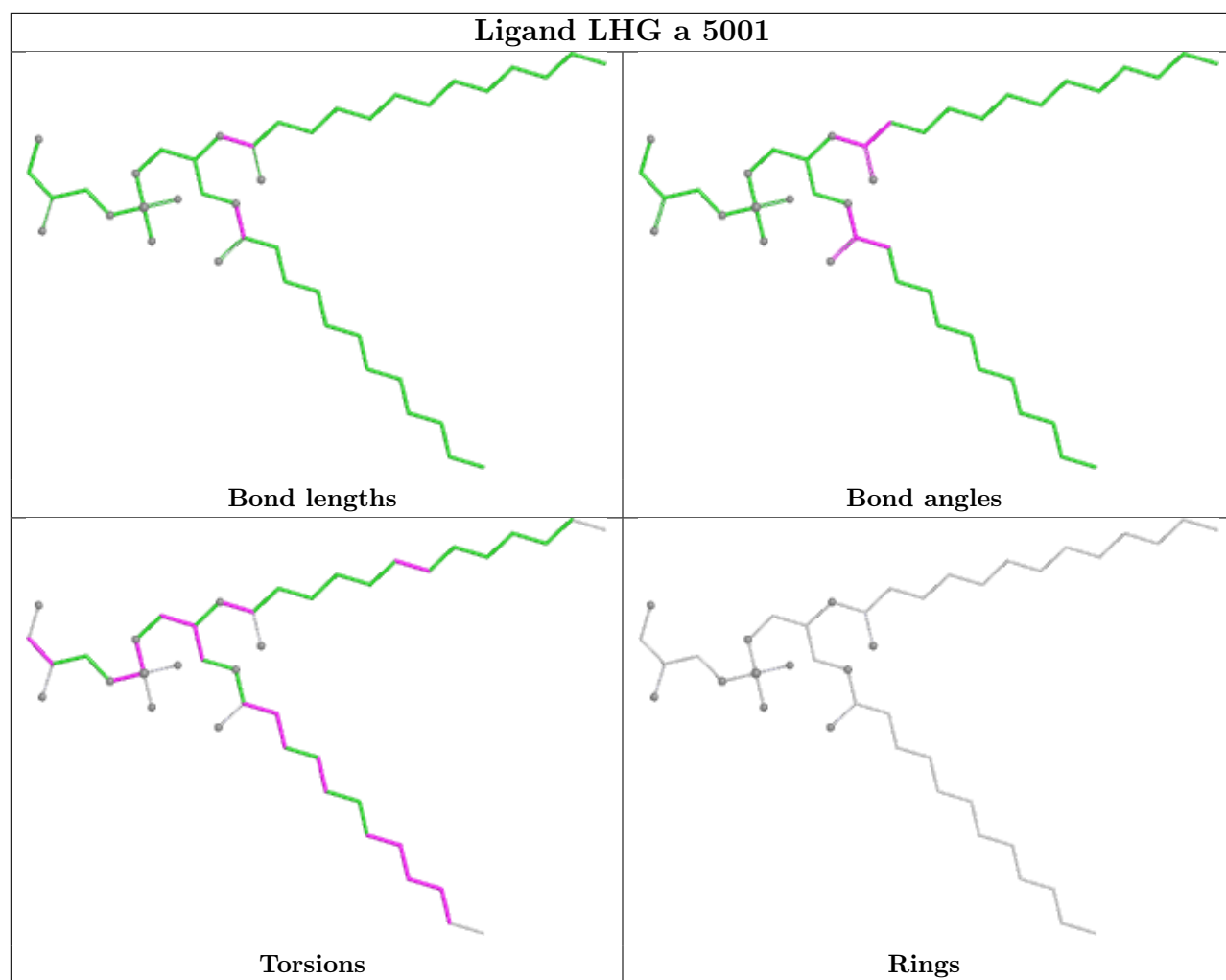


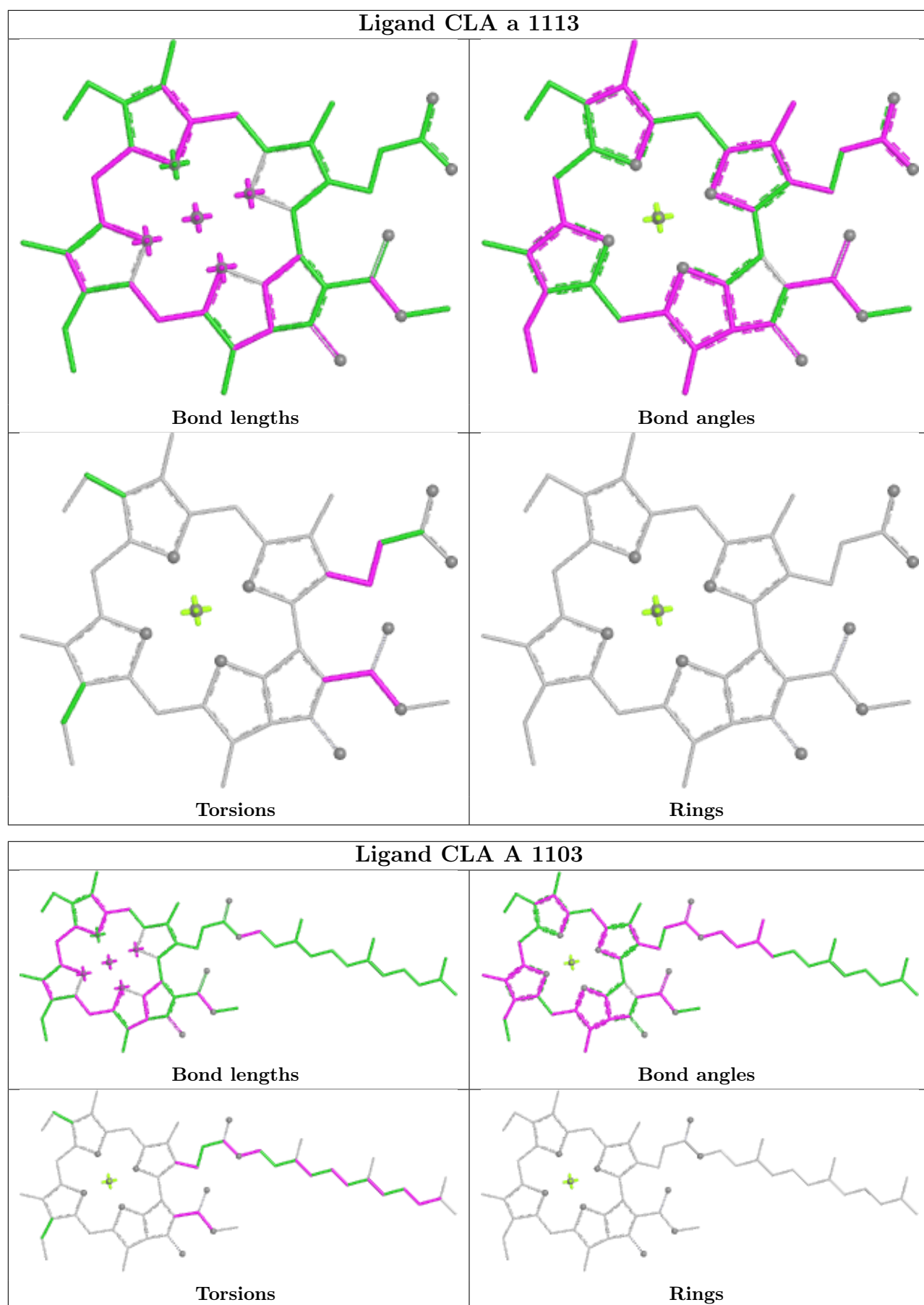


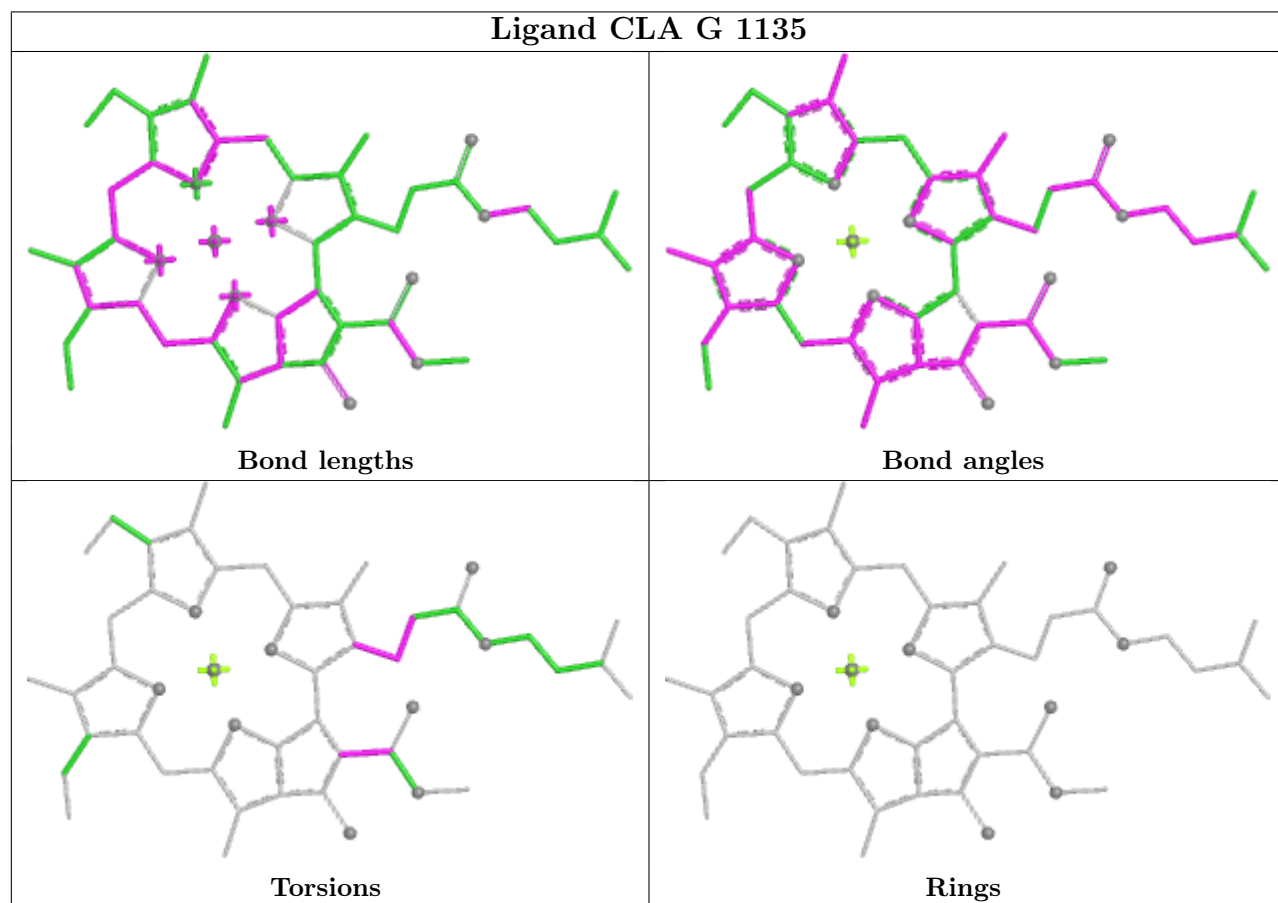
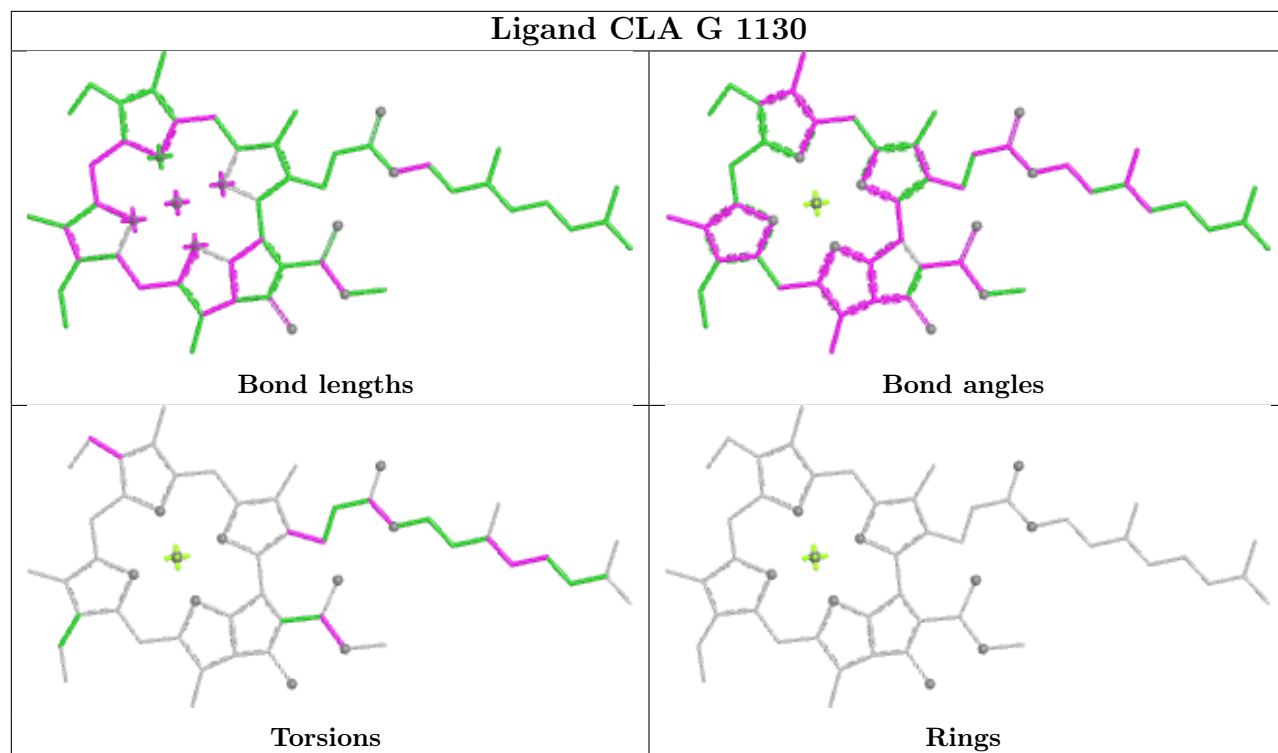


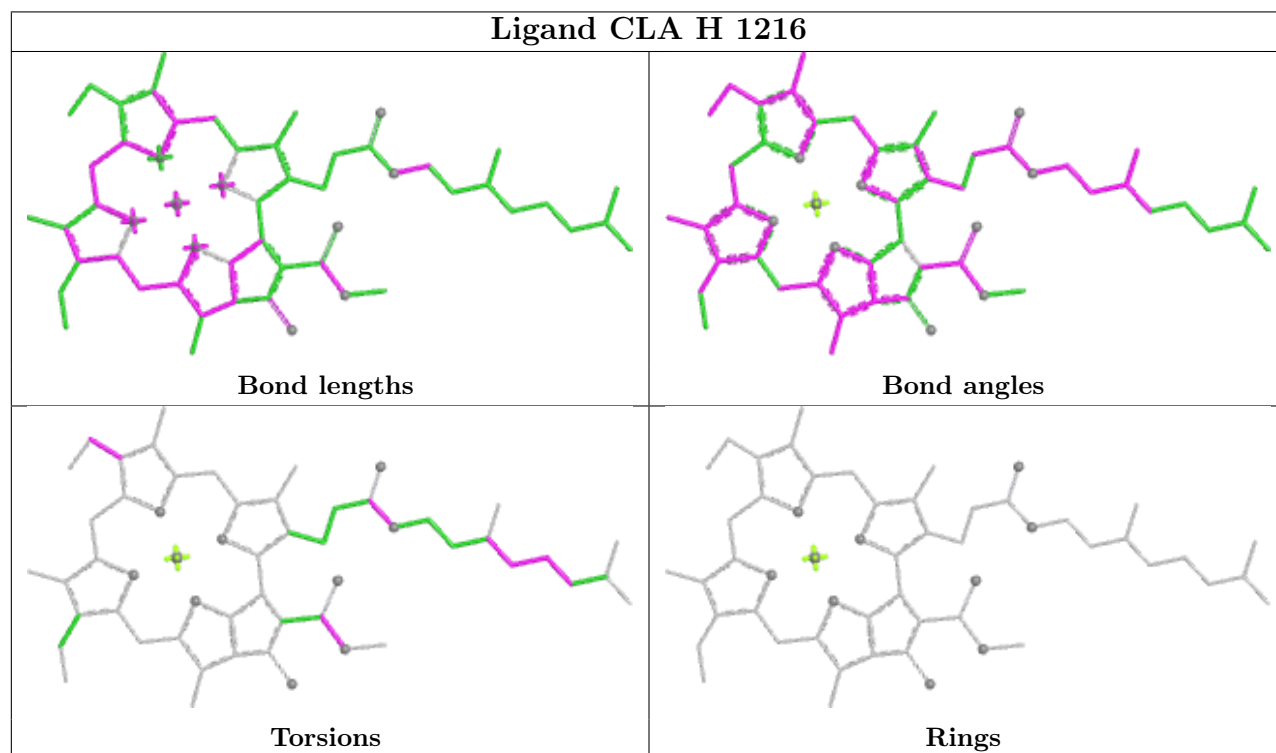
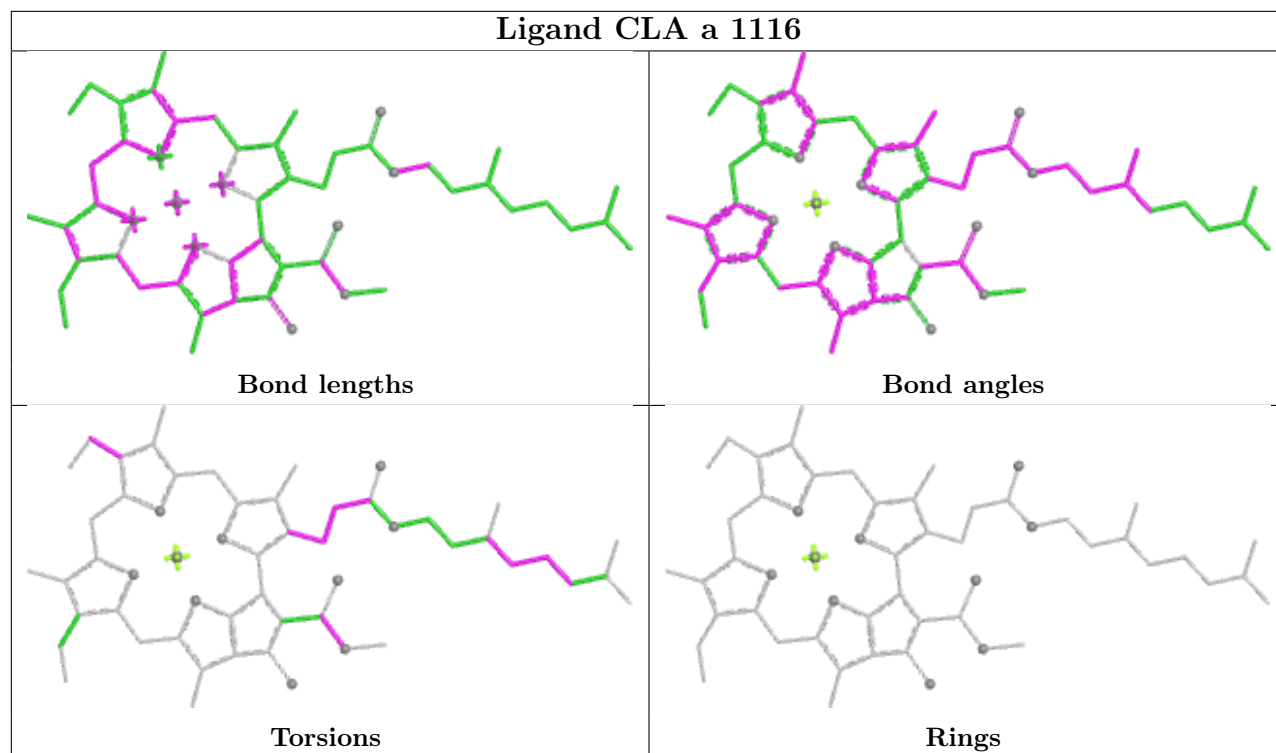
Ligand CLA H 1209

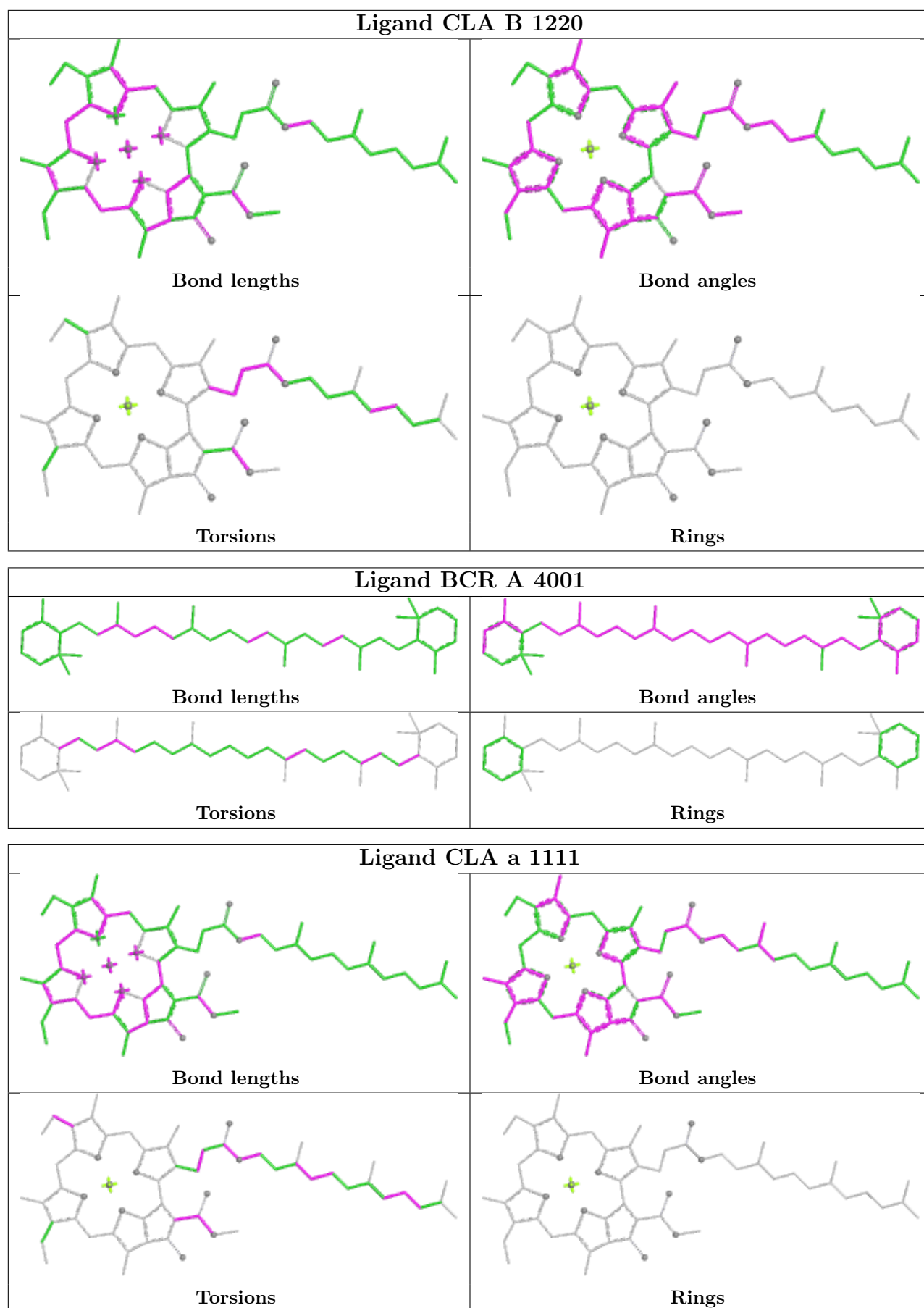


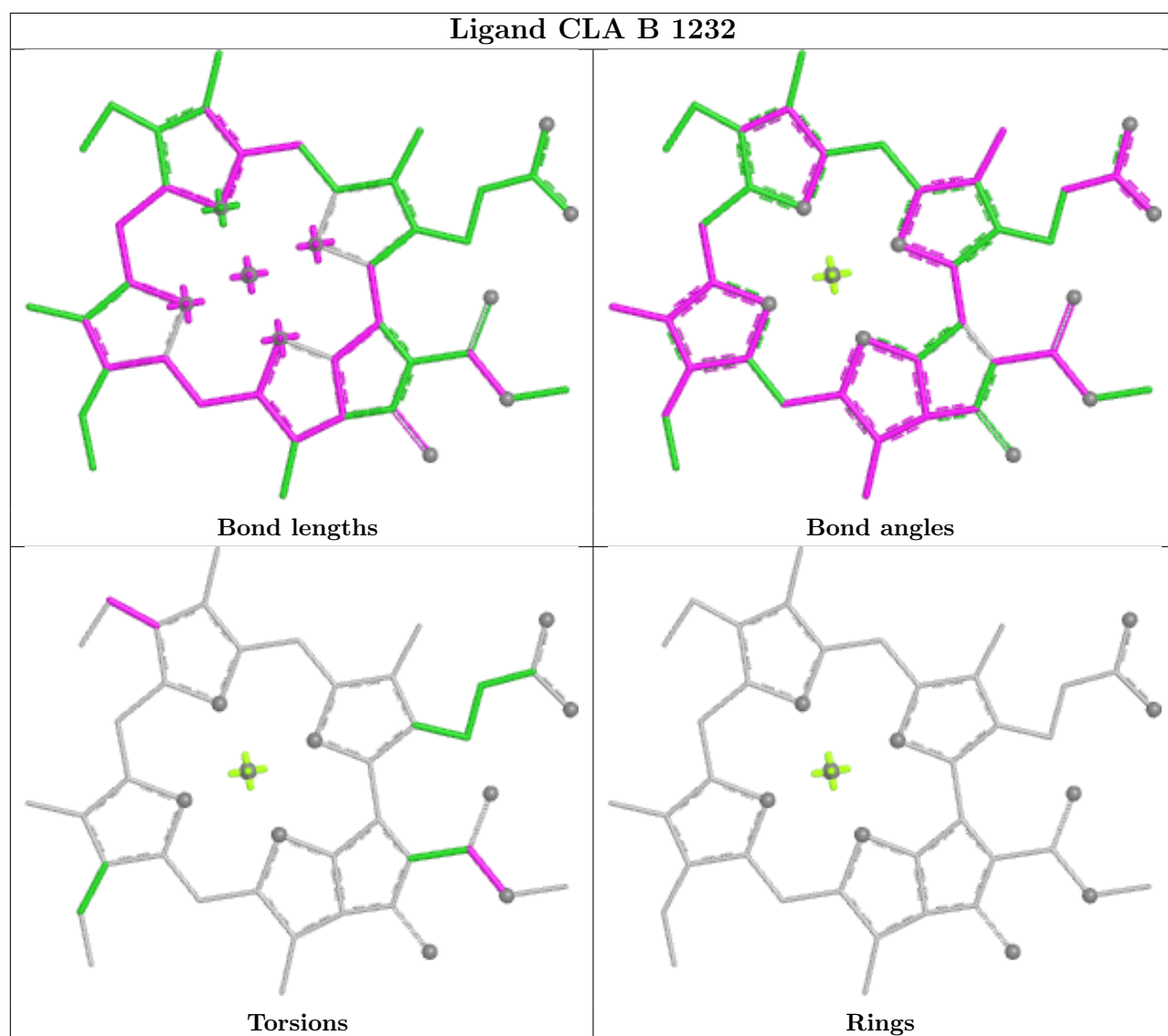


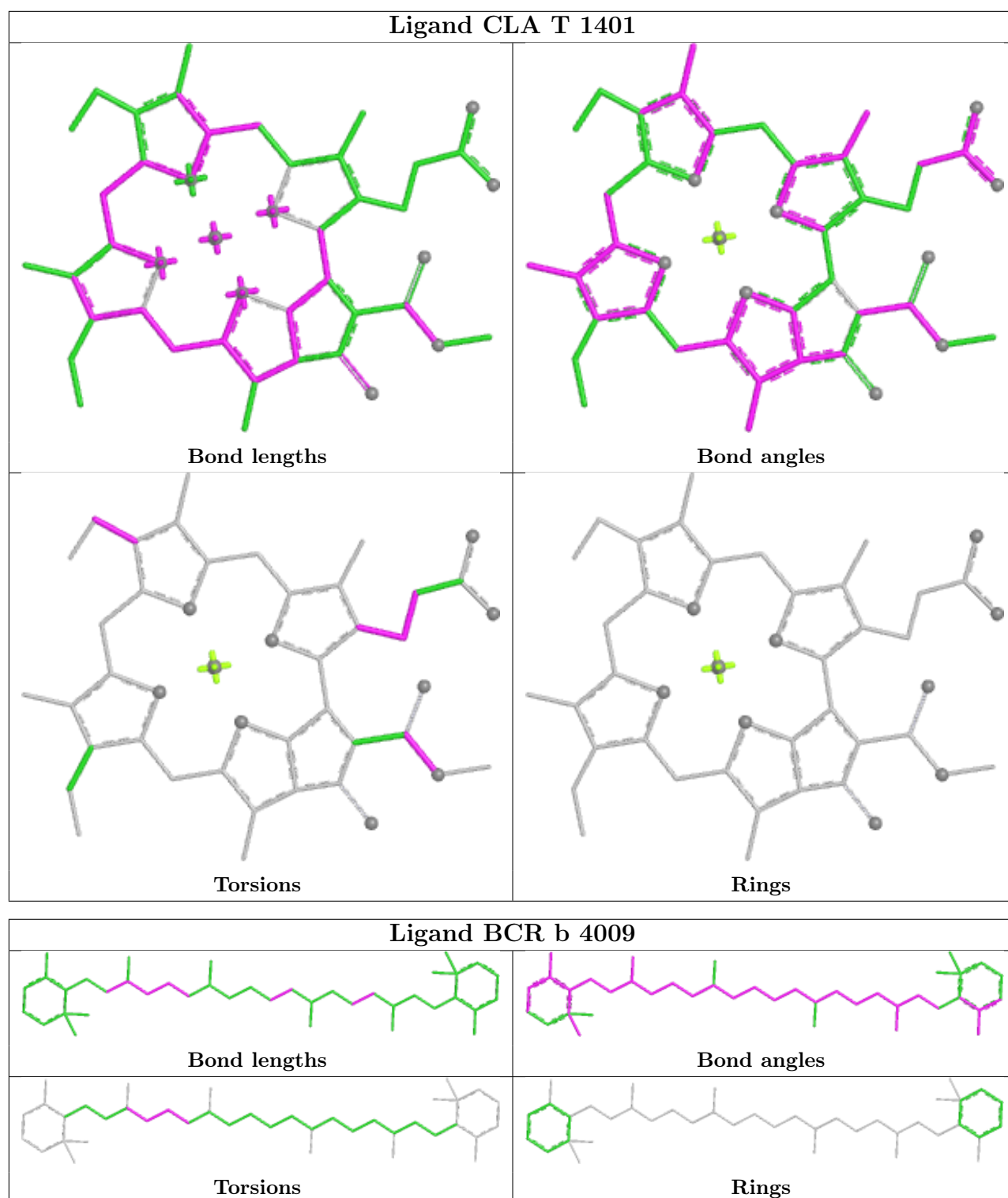


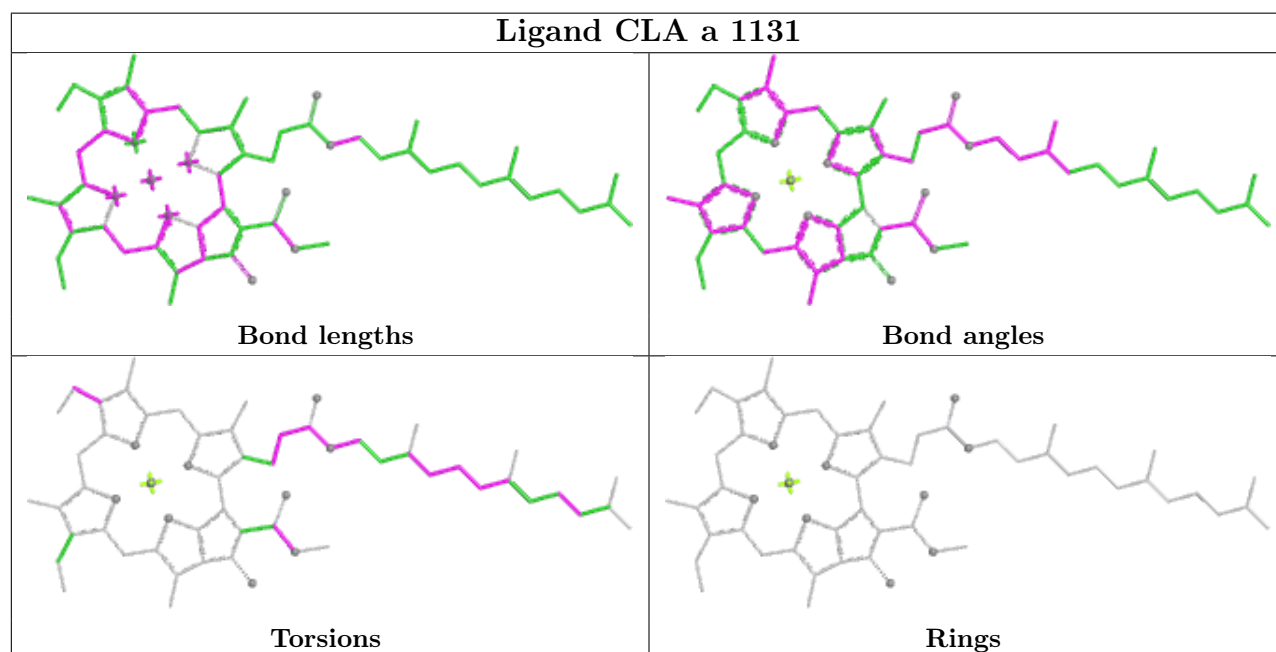
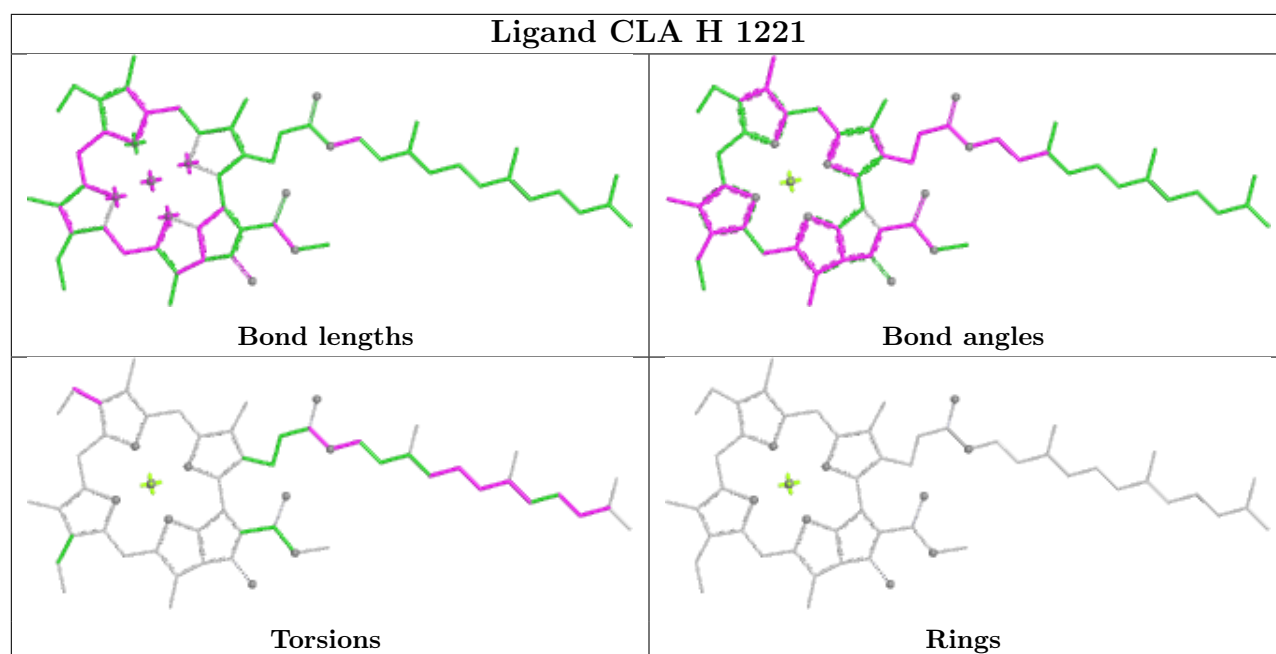


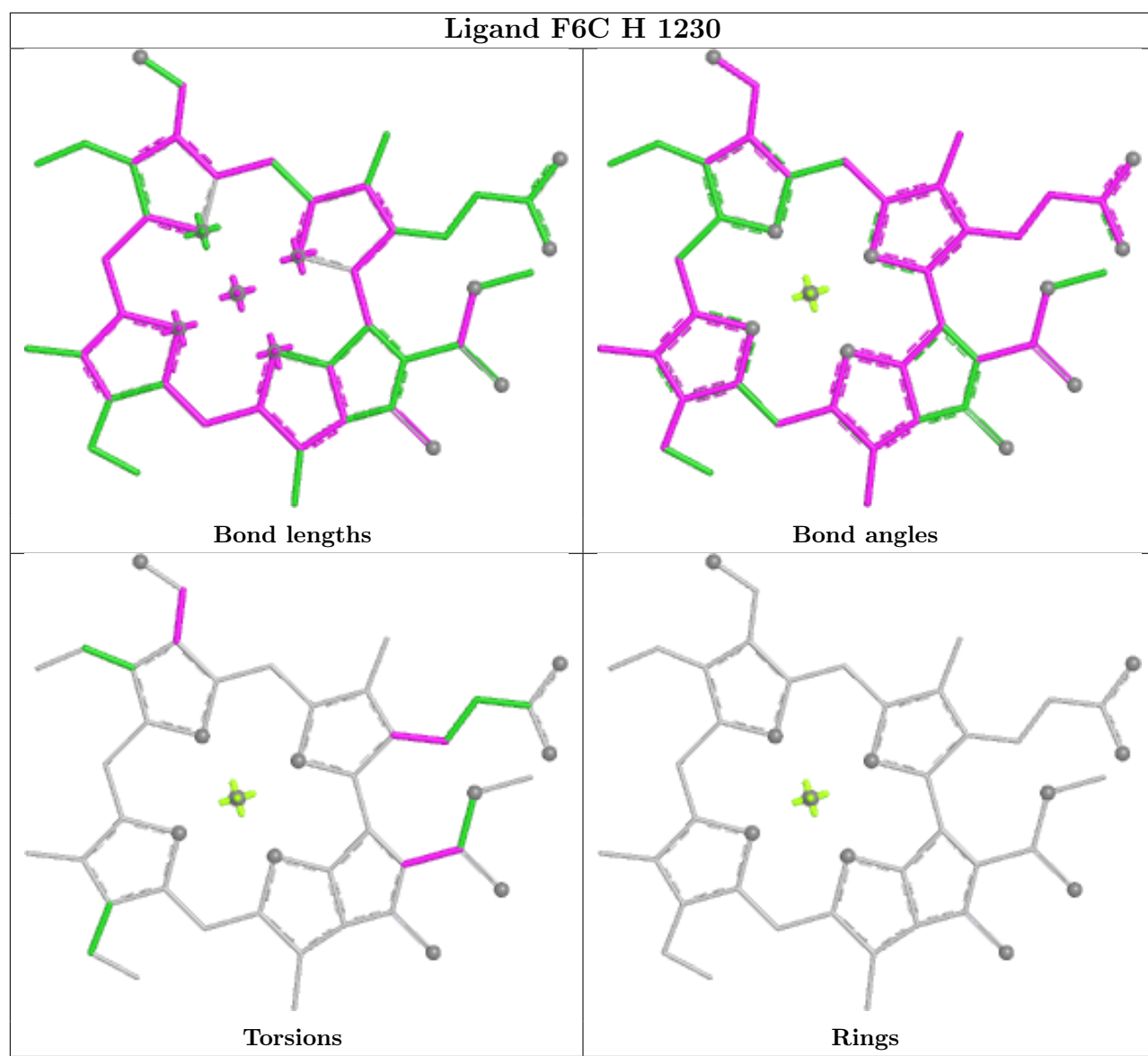


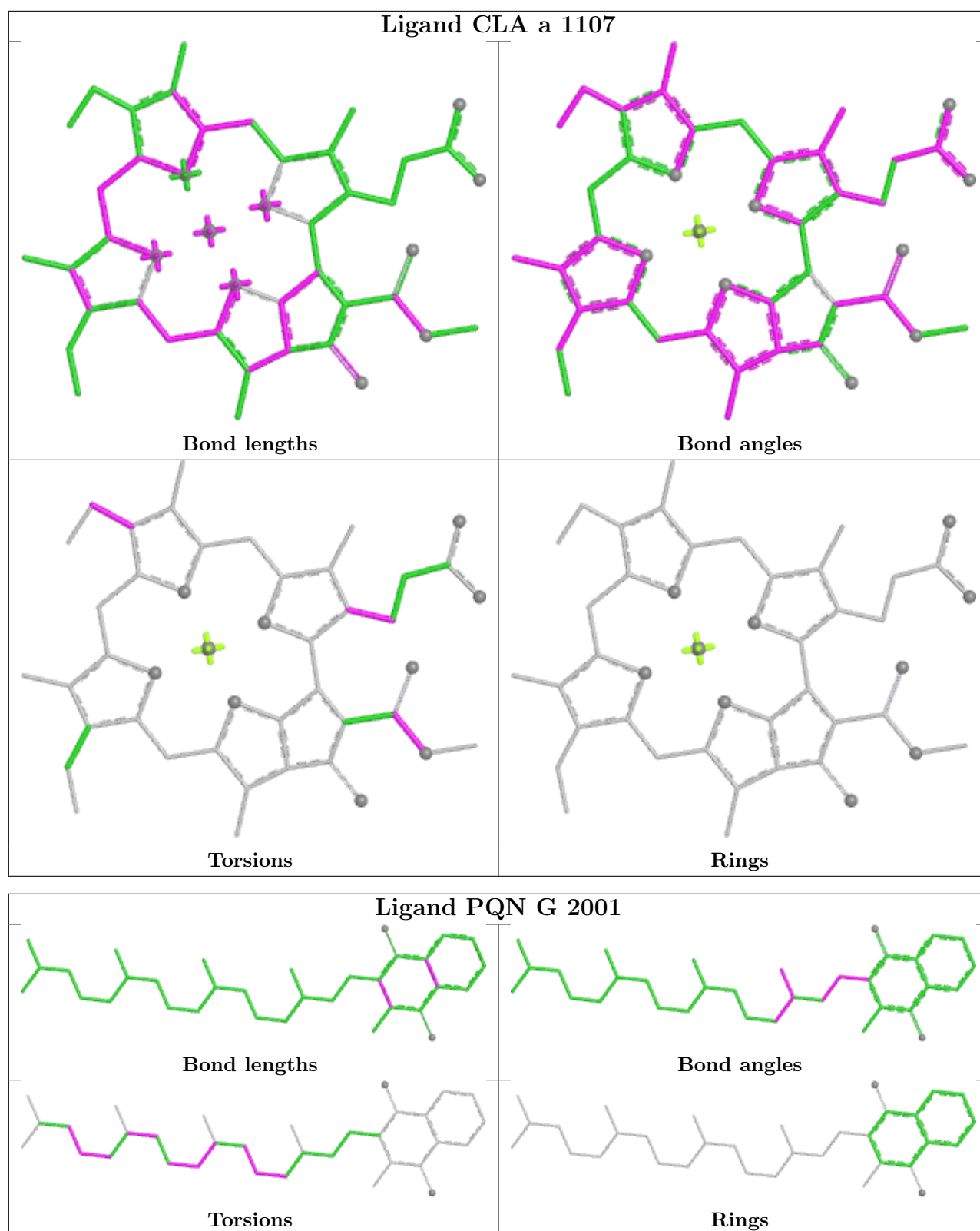


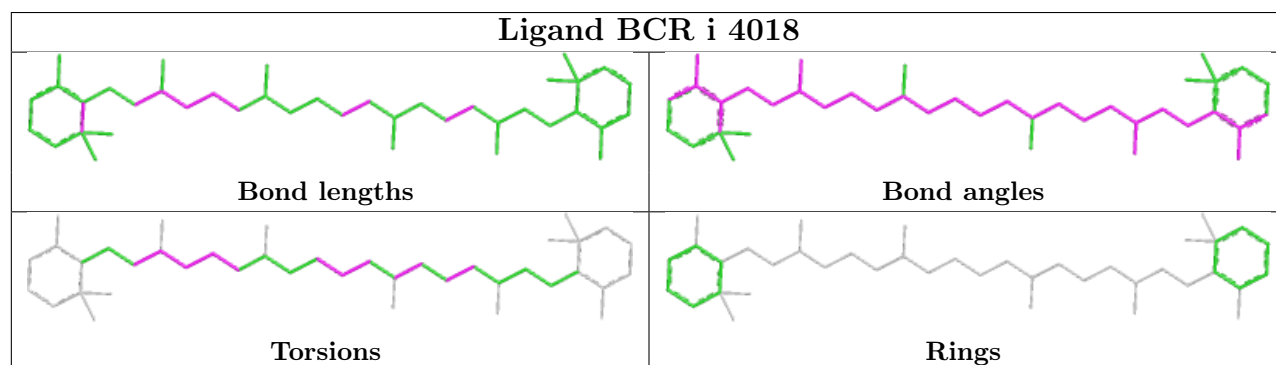
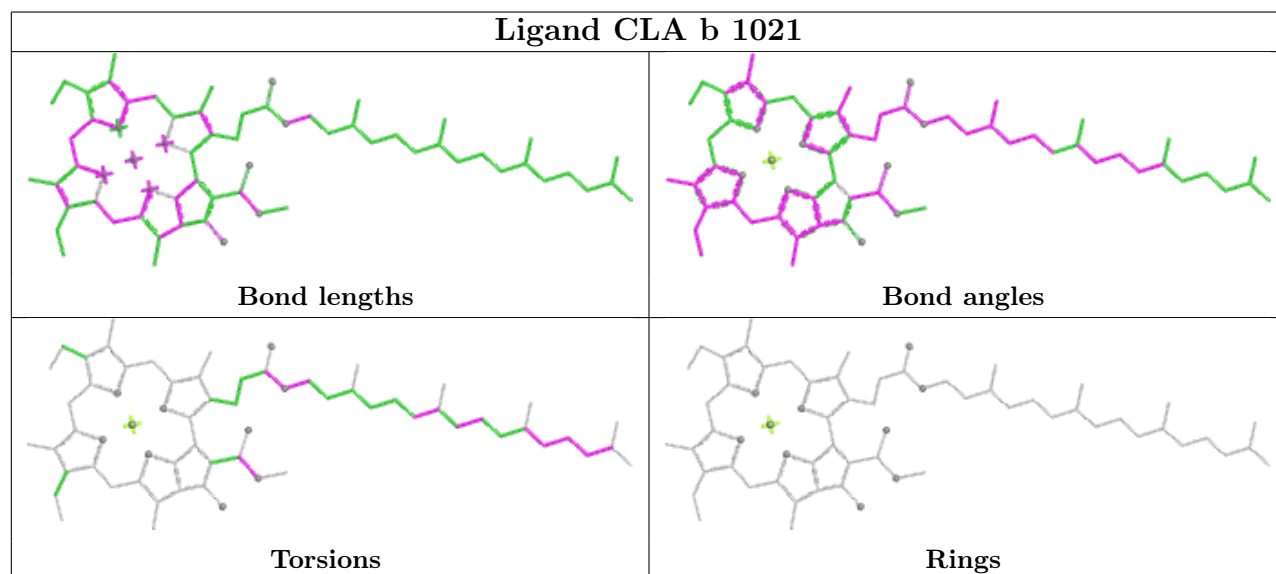
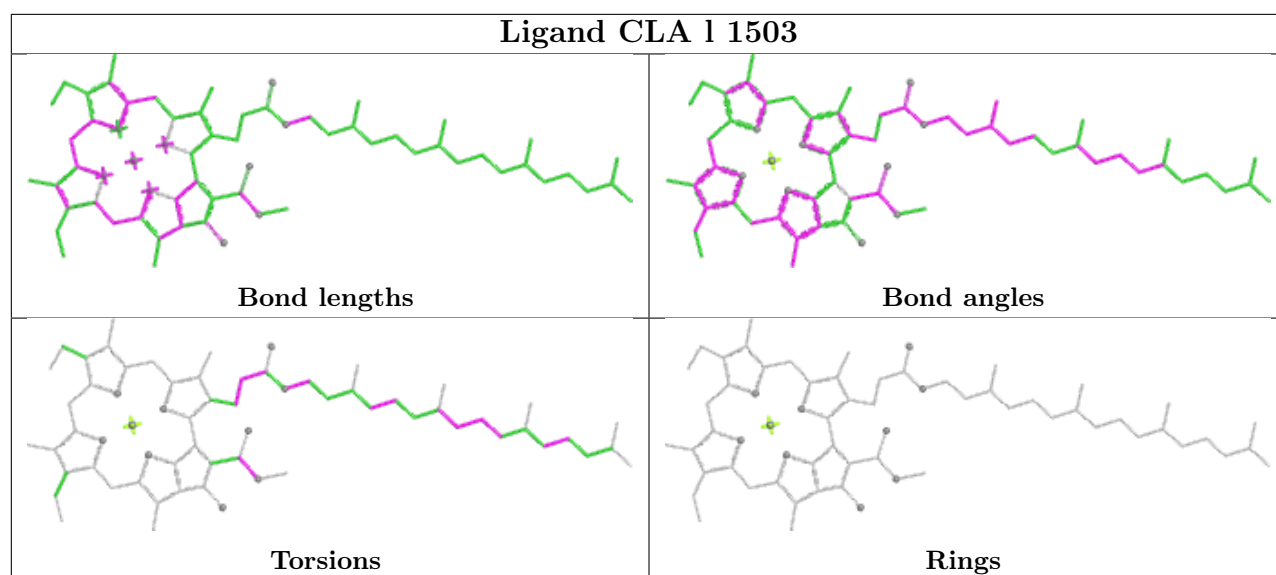


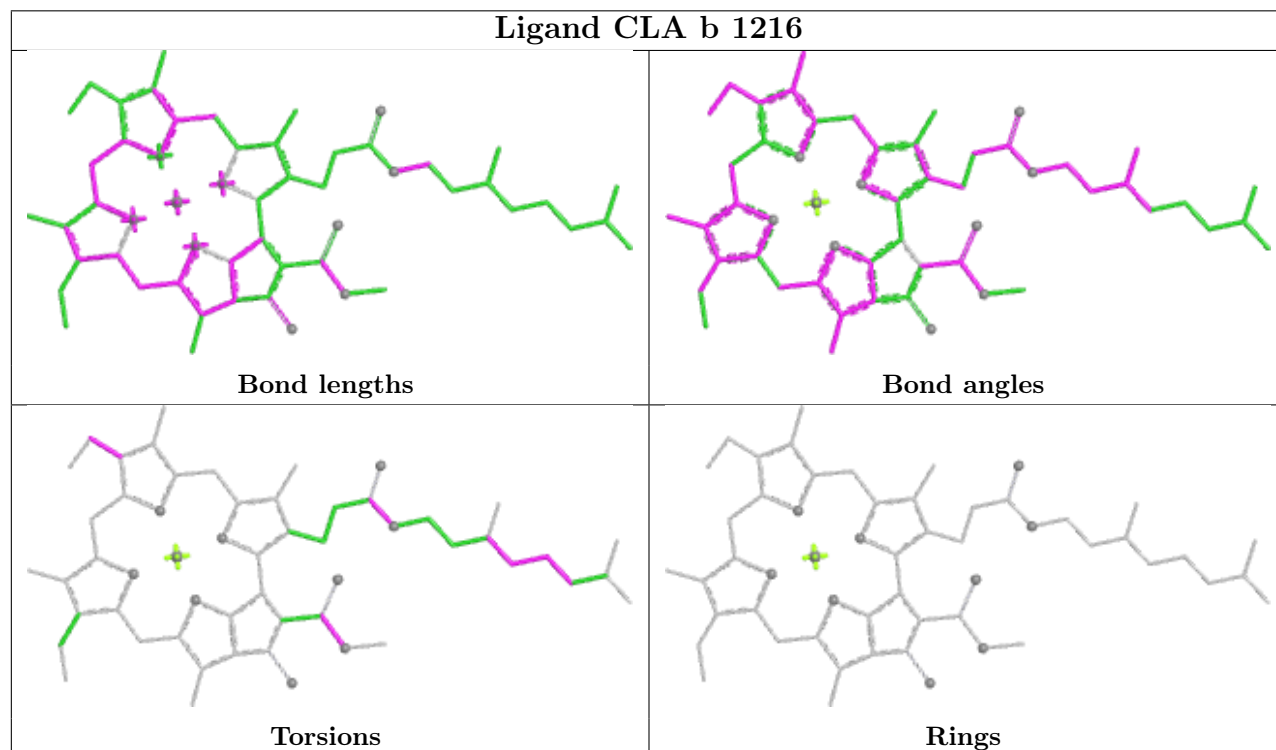
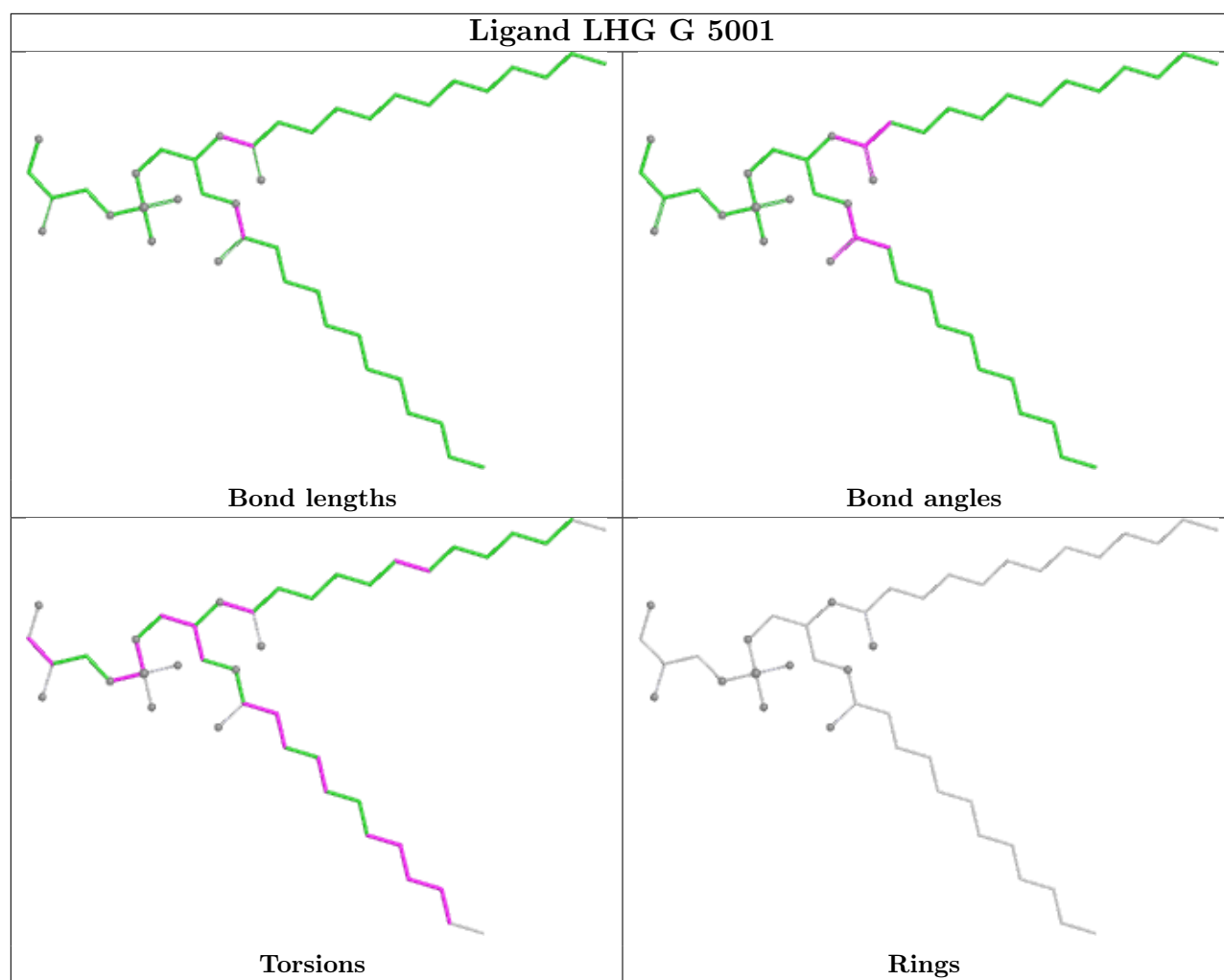




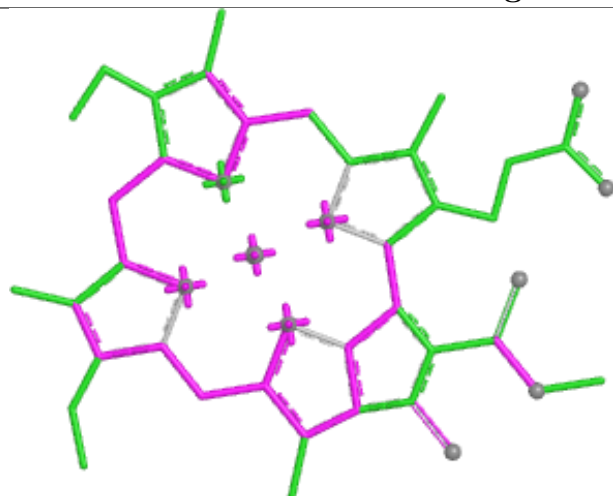




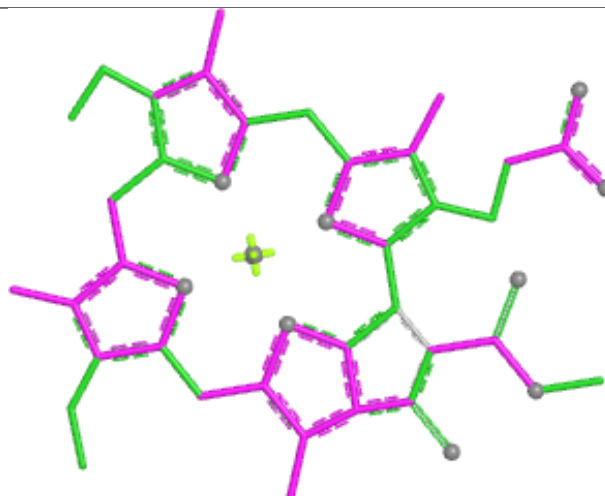




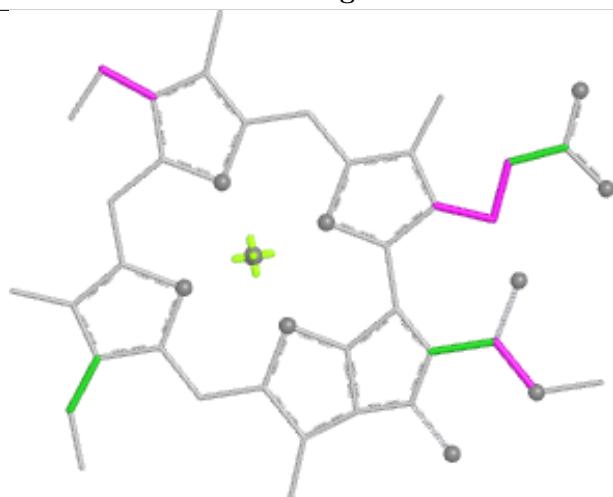
Ligand CLA K 1401



Bond lengths



Bond angles

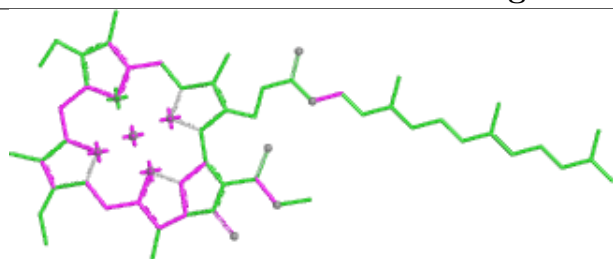


Torsions

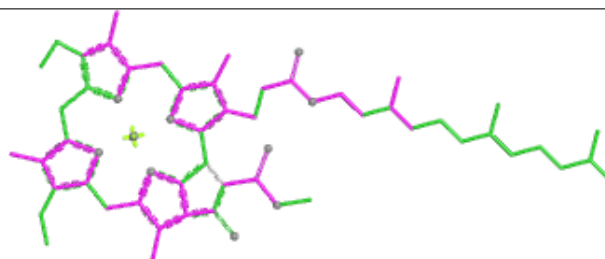


Rings

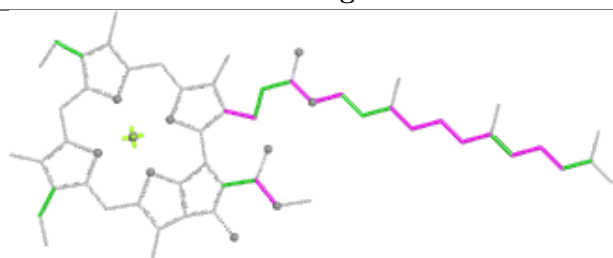
Ligand CLA b 1229



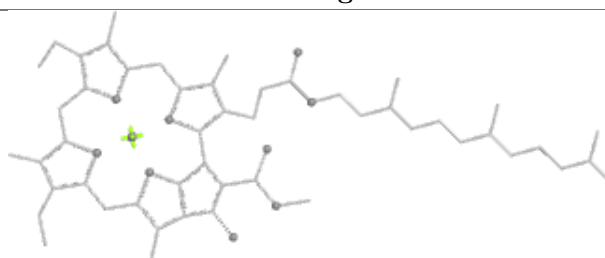
Bond lengths



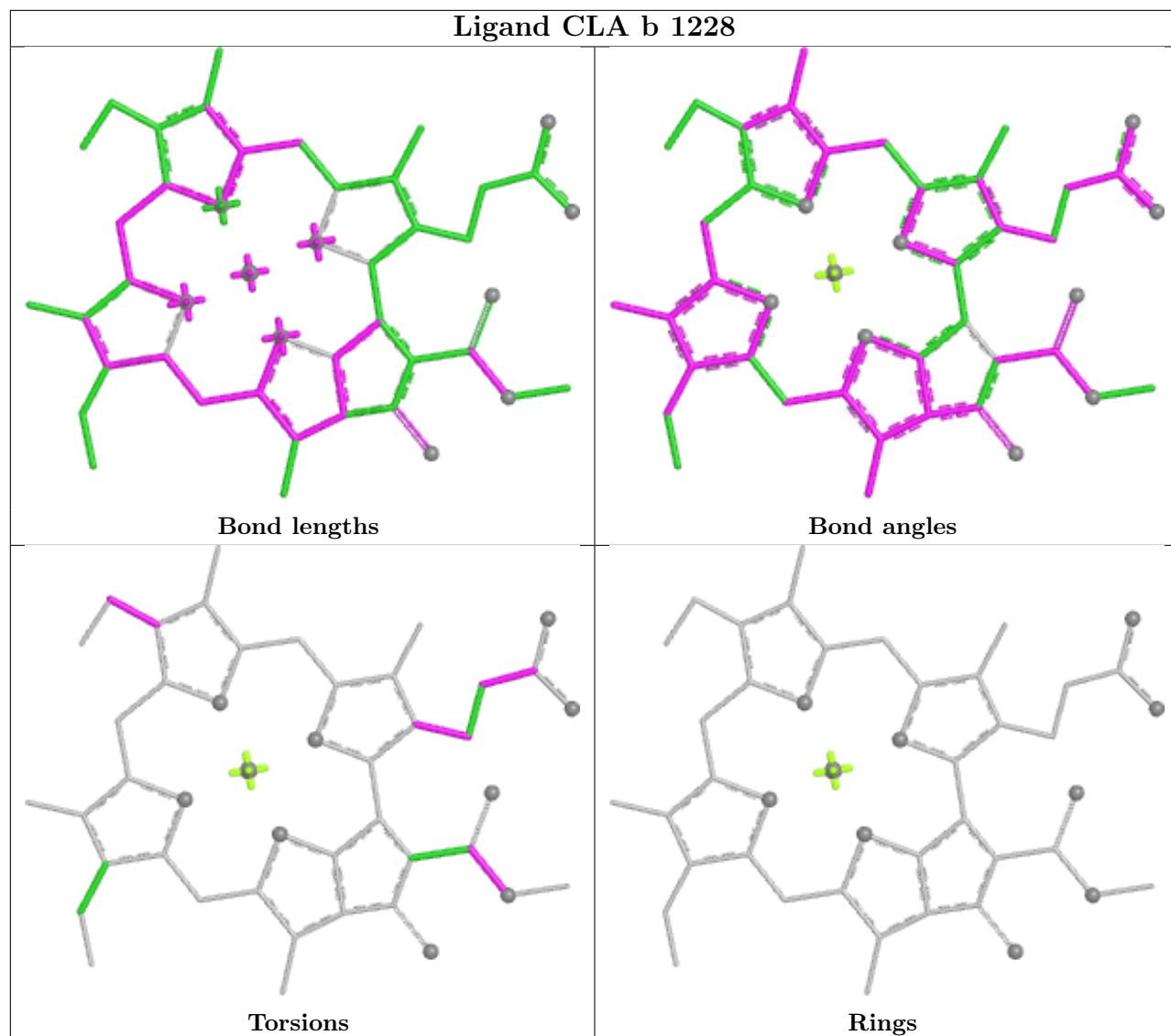
Bond angles



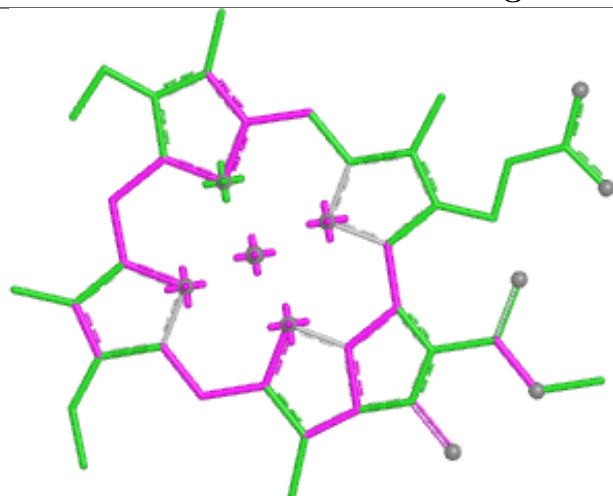
Torsions



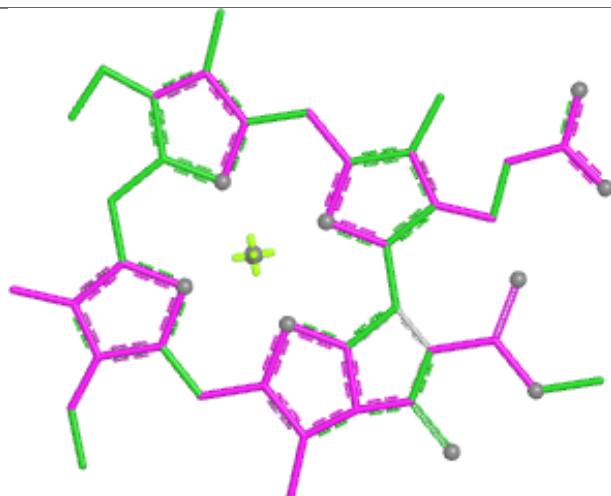
Rings



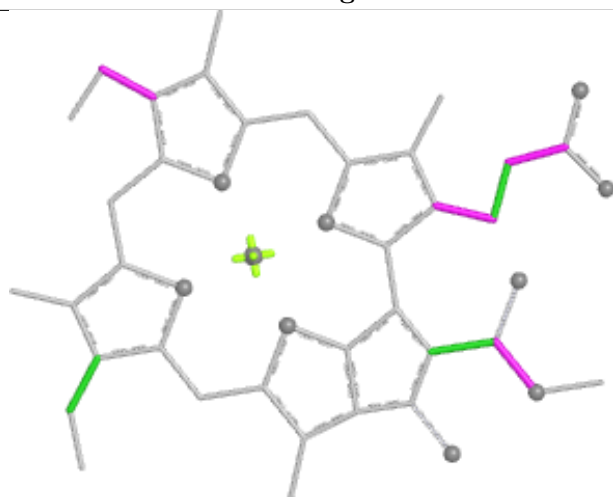
Ligand CLA H 1219



Bond lengths



Bond angles

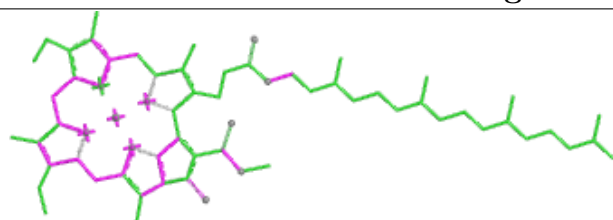


Torsions

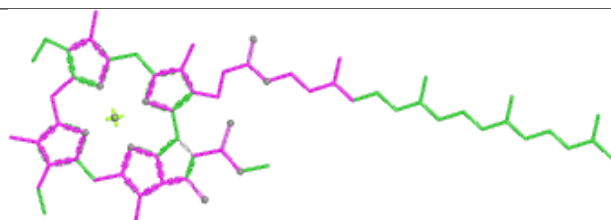


Rings

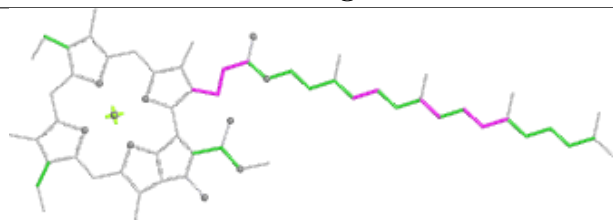
Ligand CLA H 1210



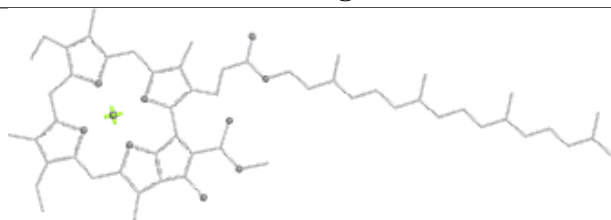
Bond lengths



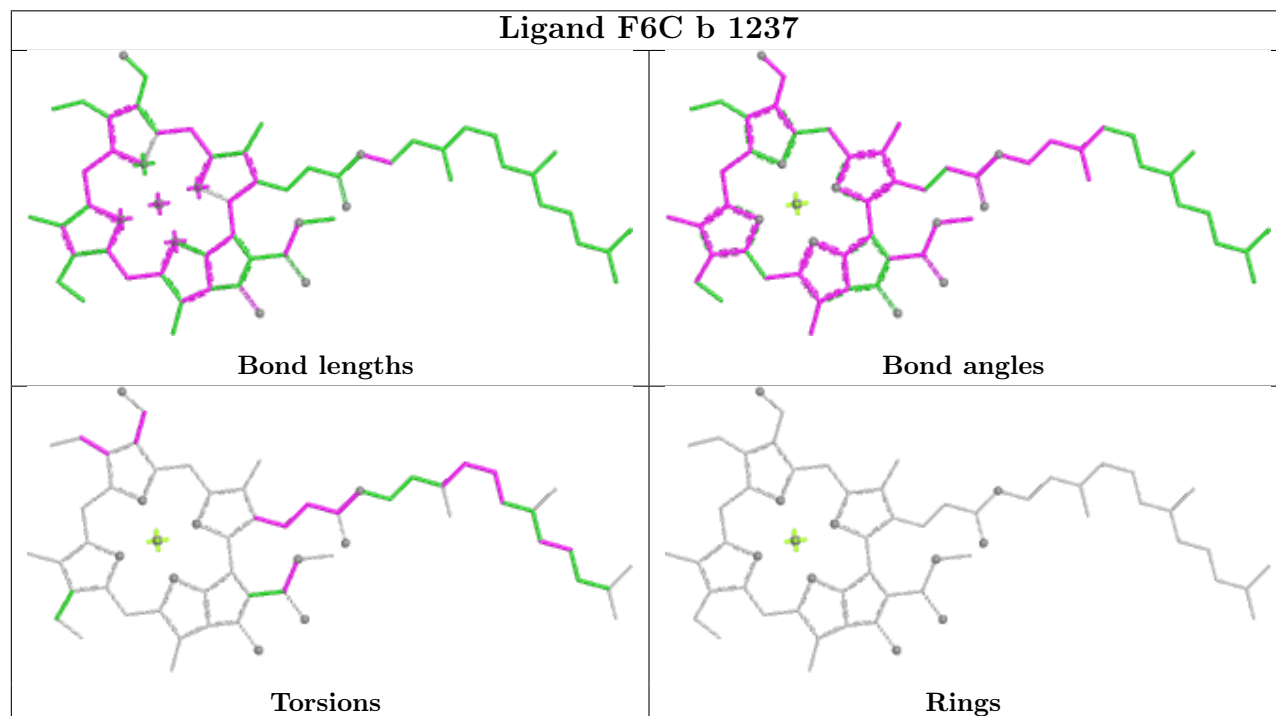
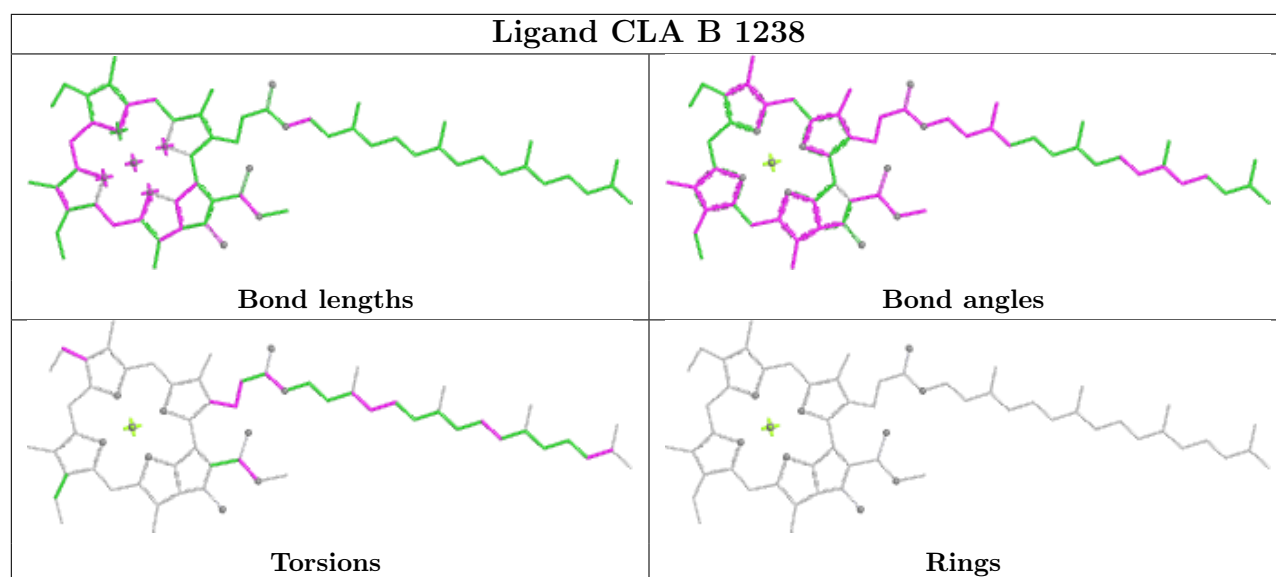
Bond angles

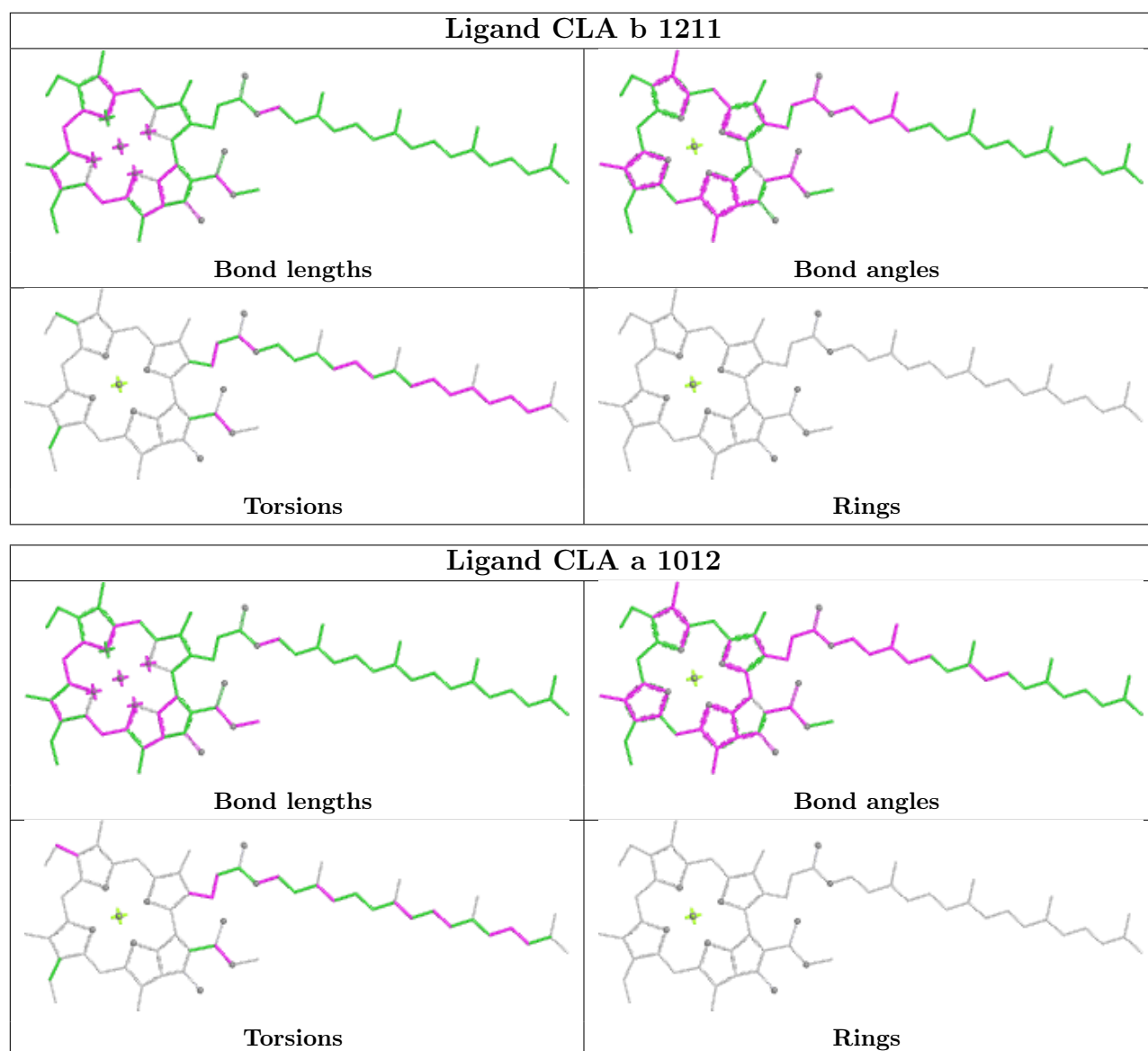


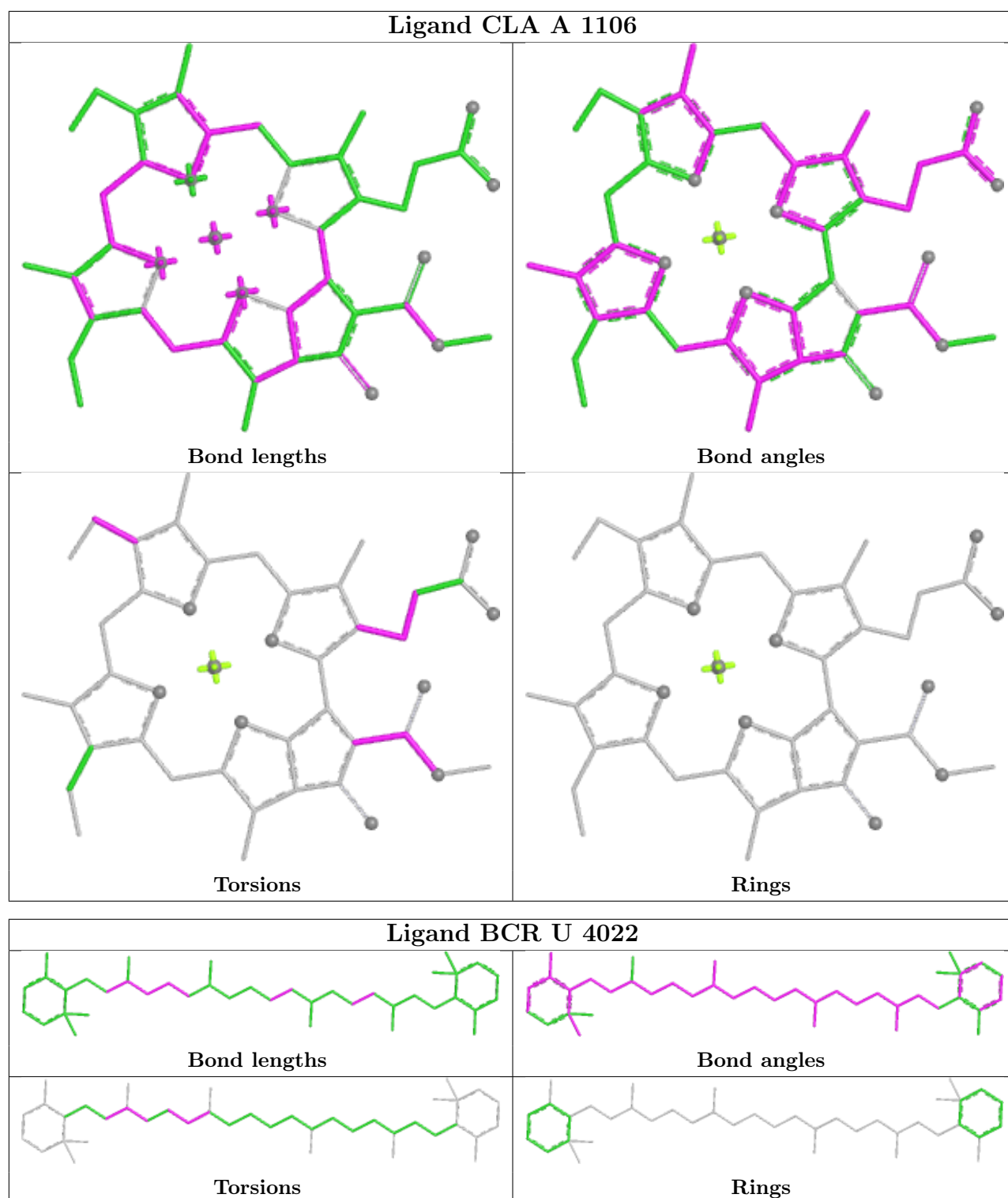
Torsions

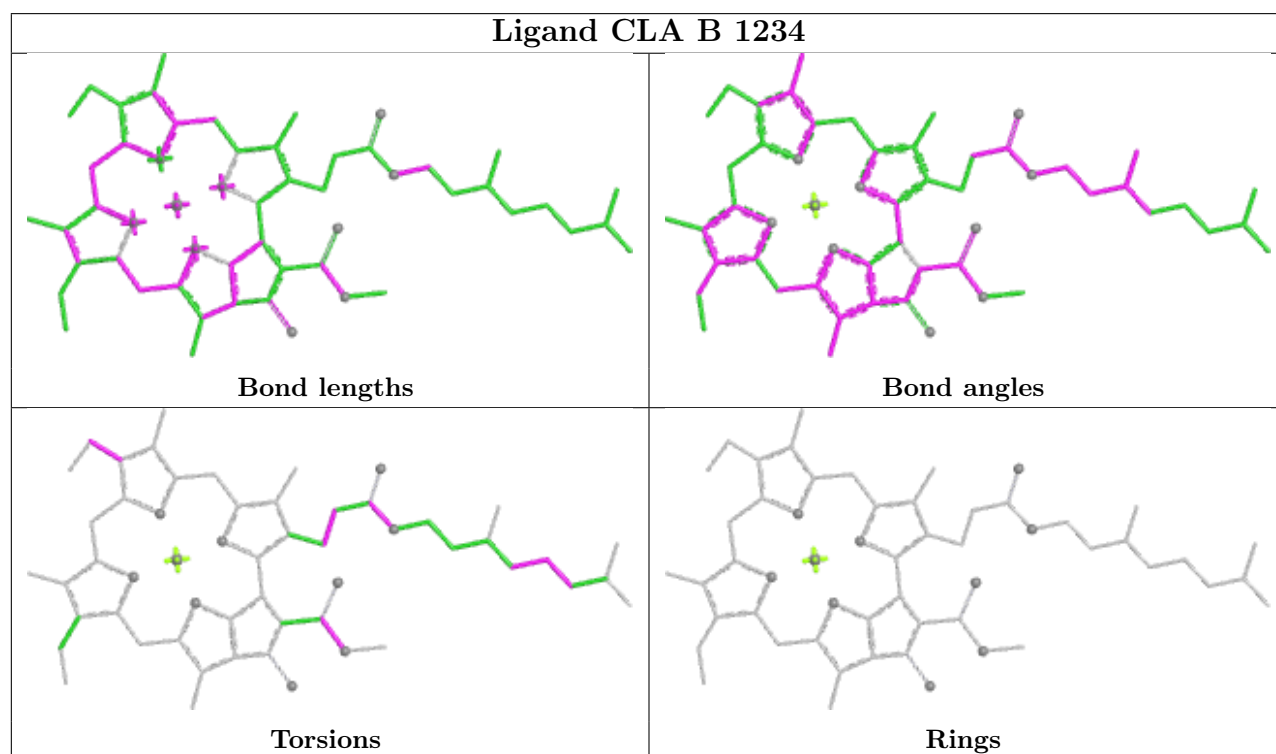
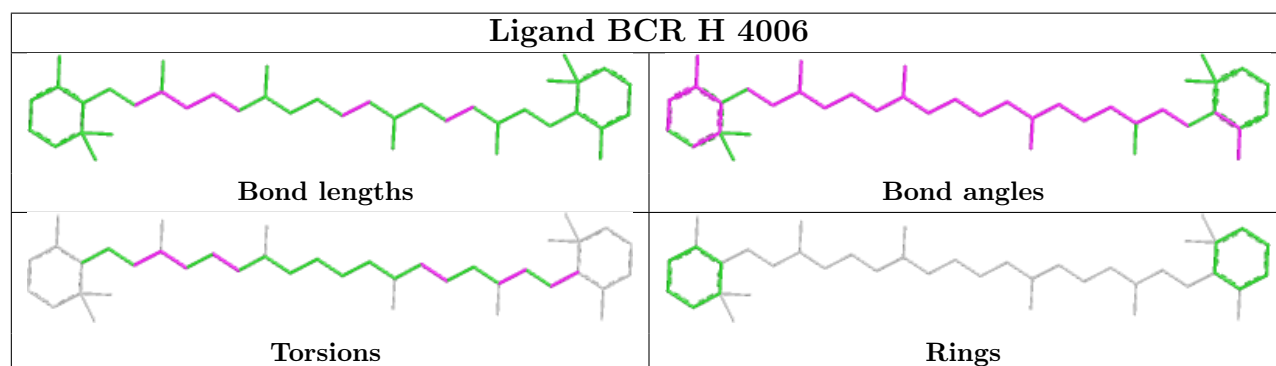
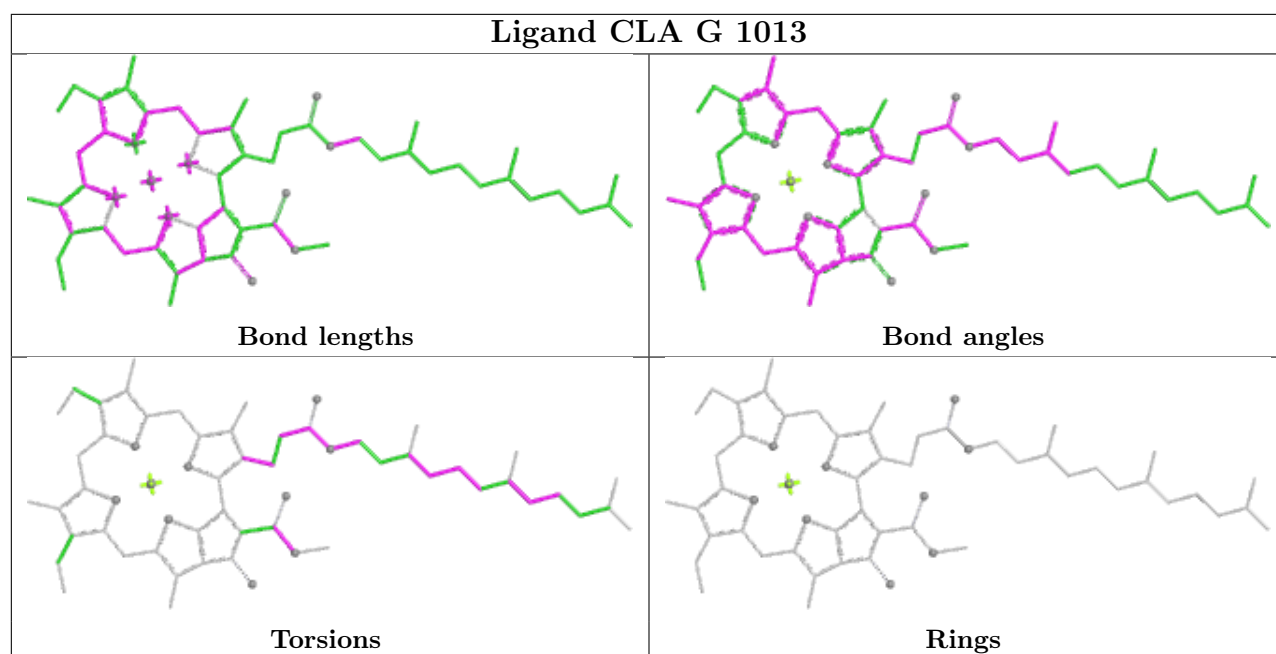


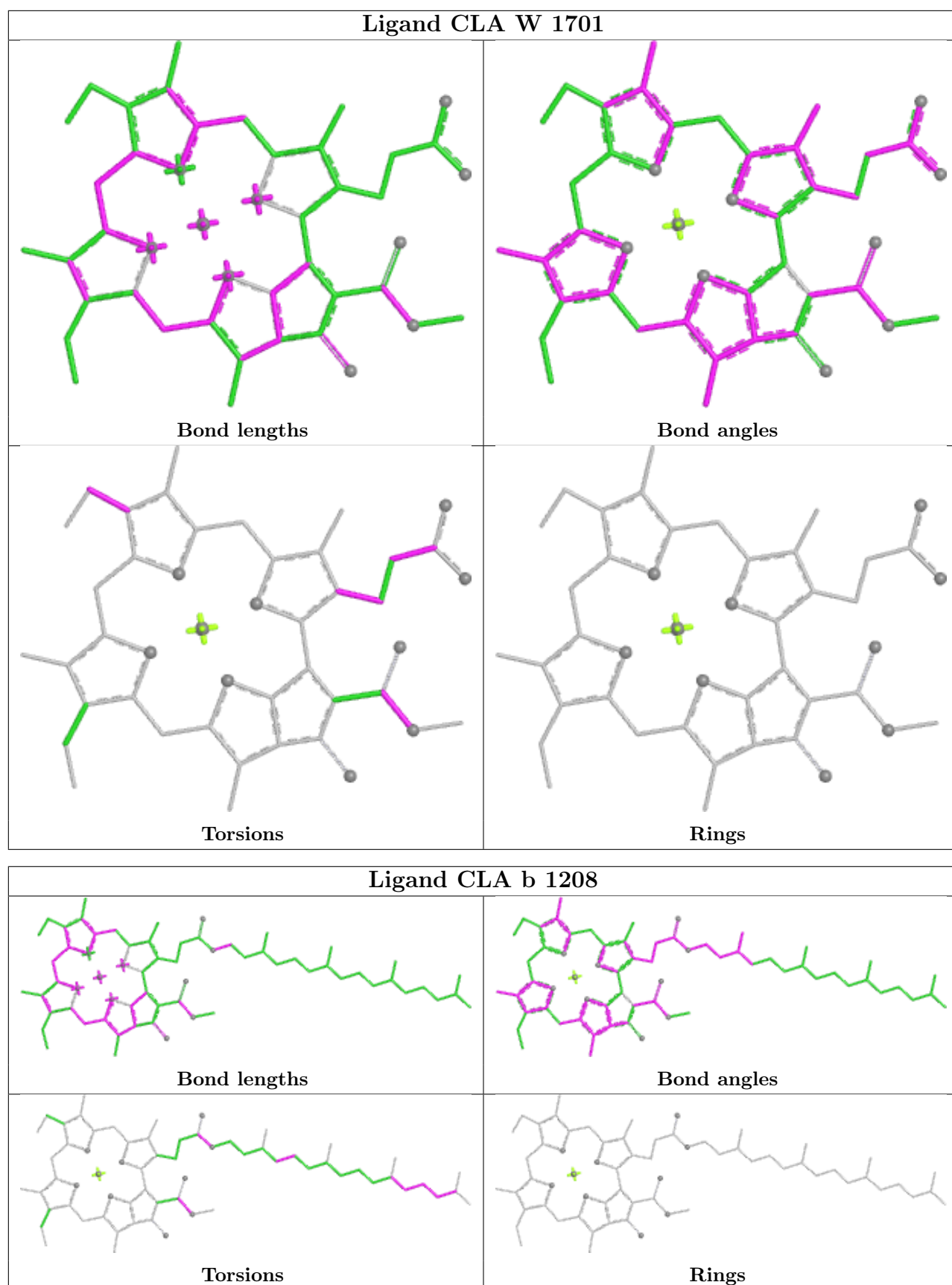
Rings

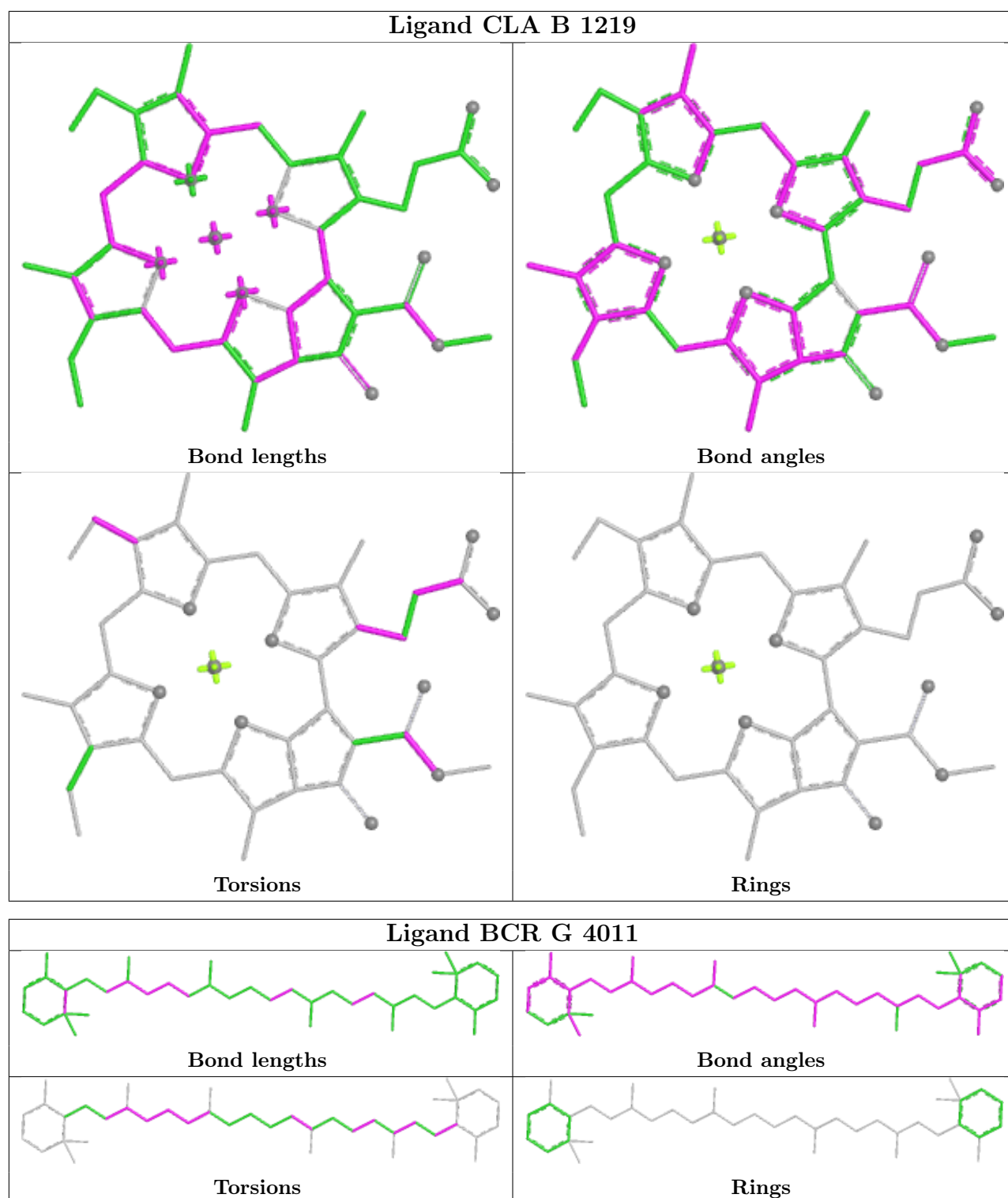


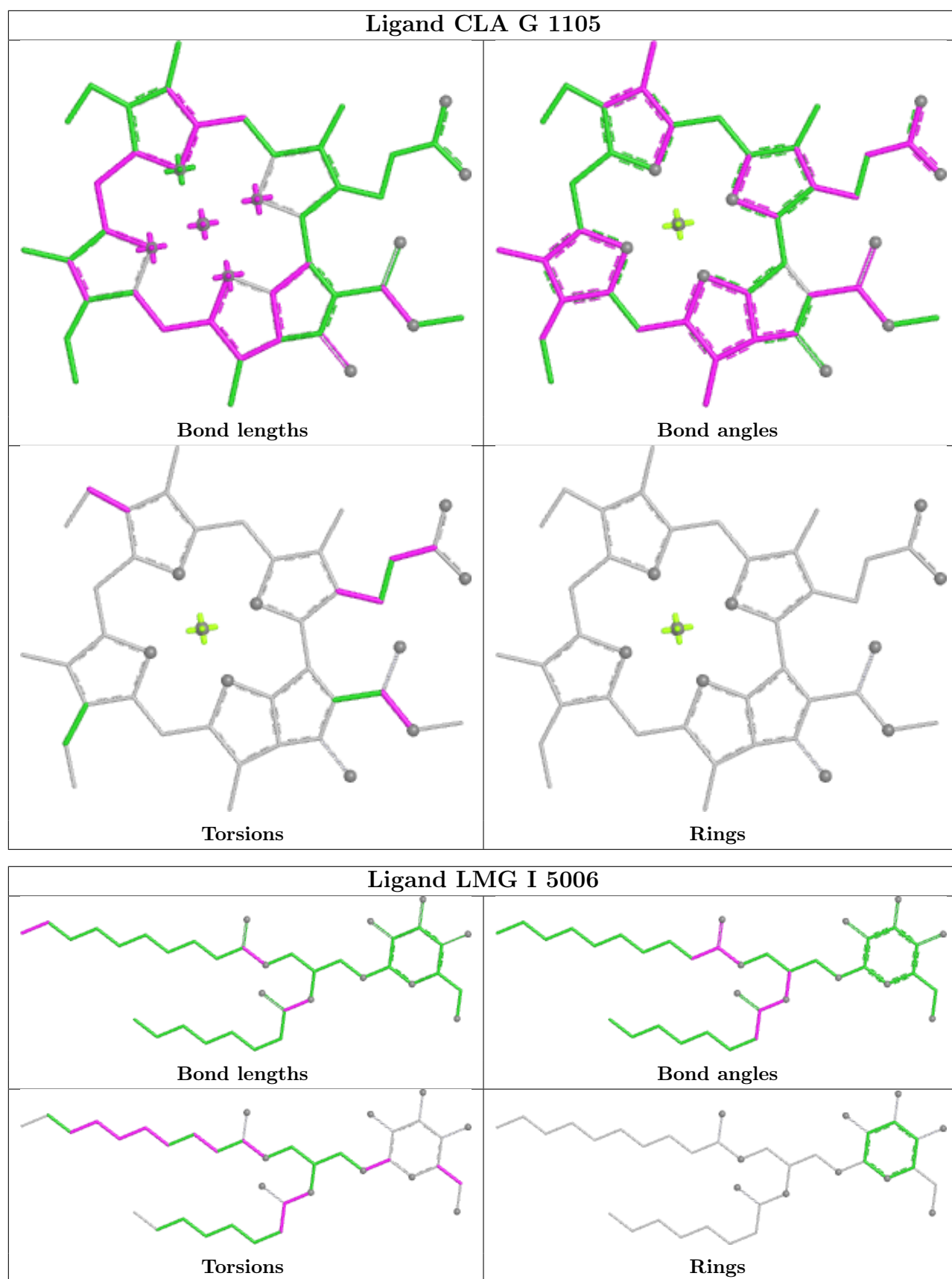


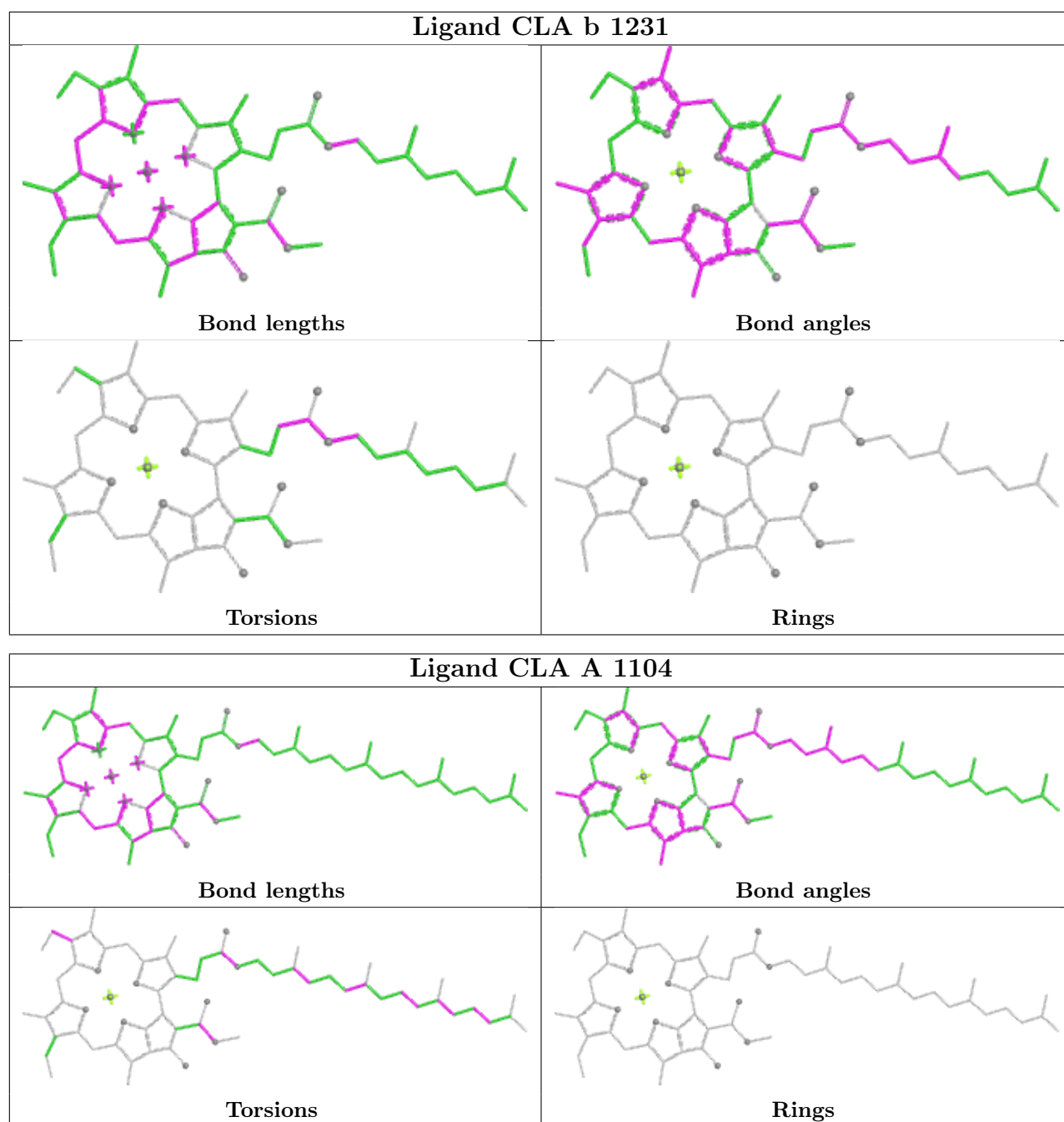


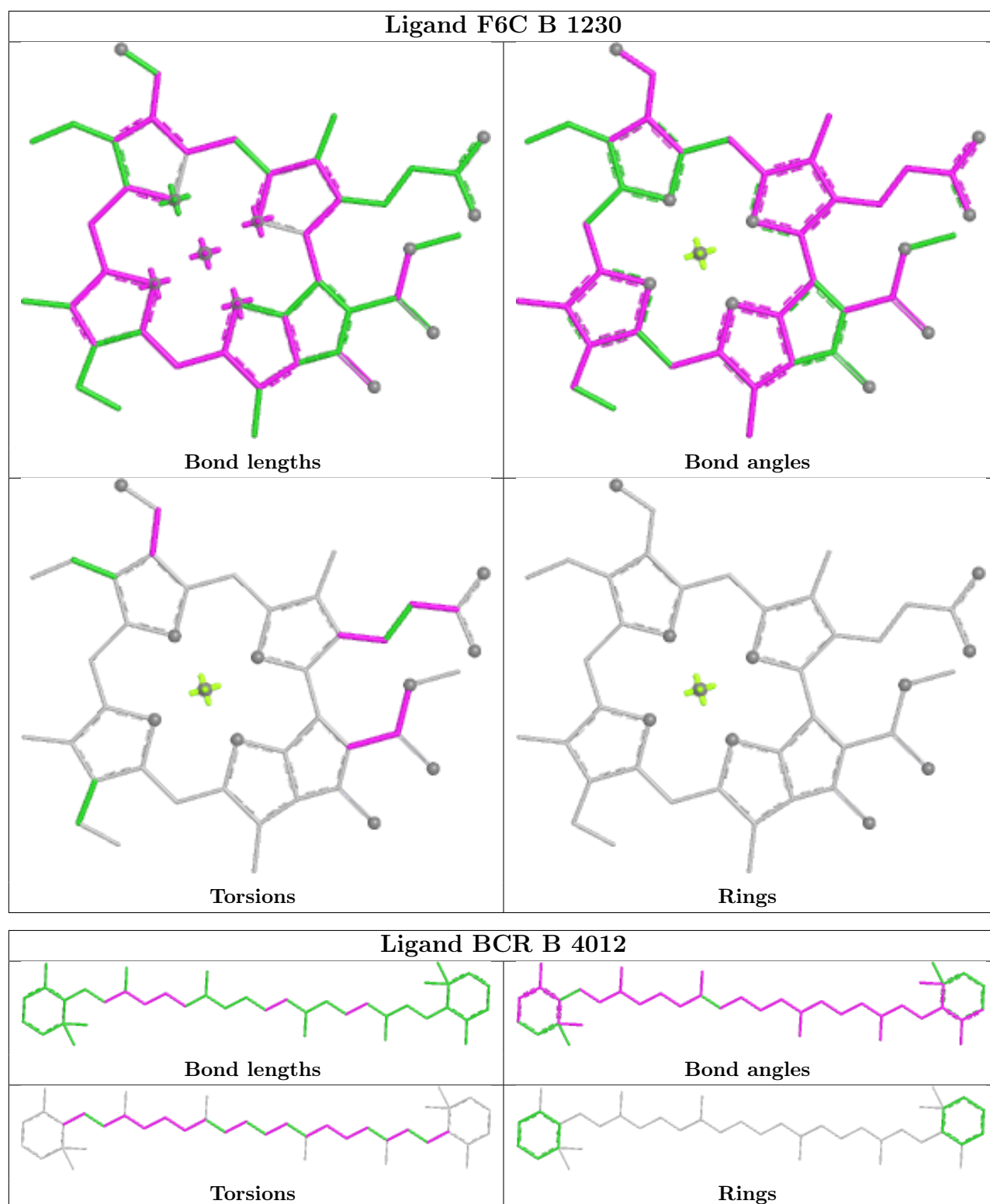




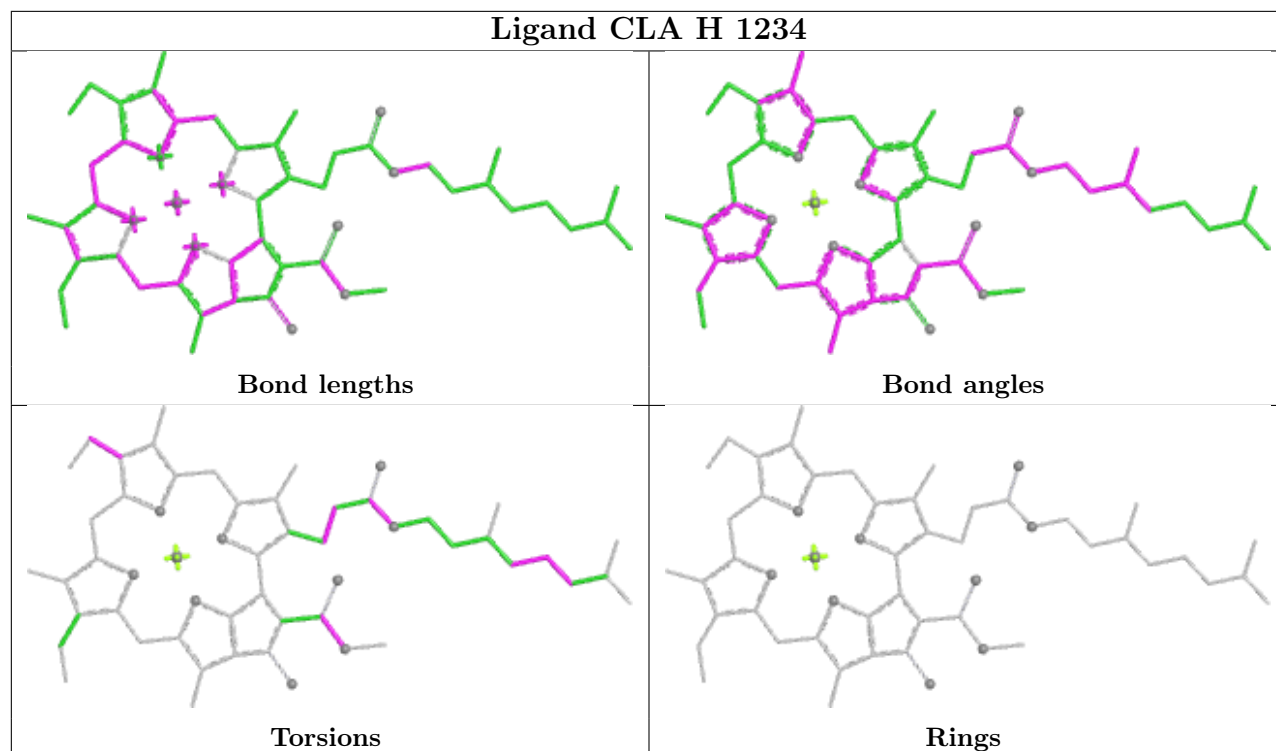




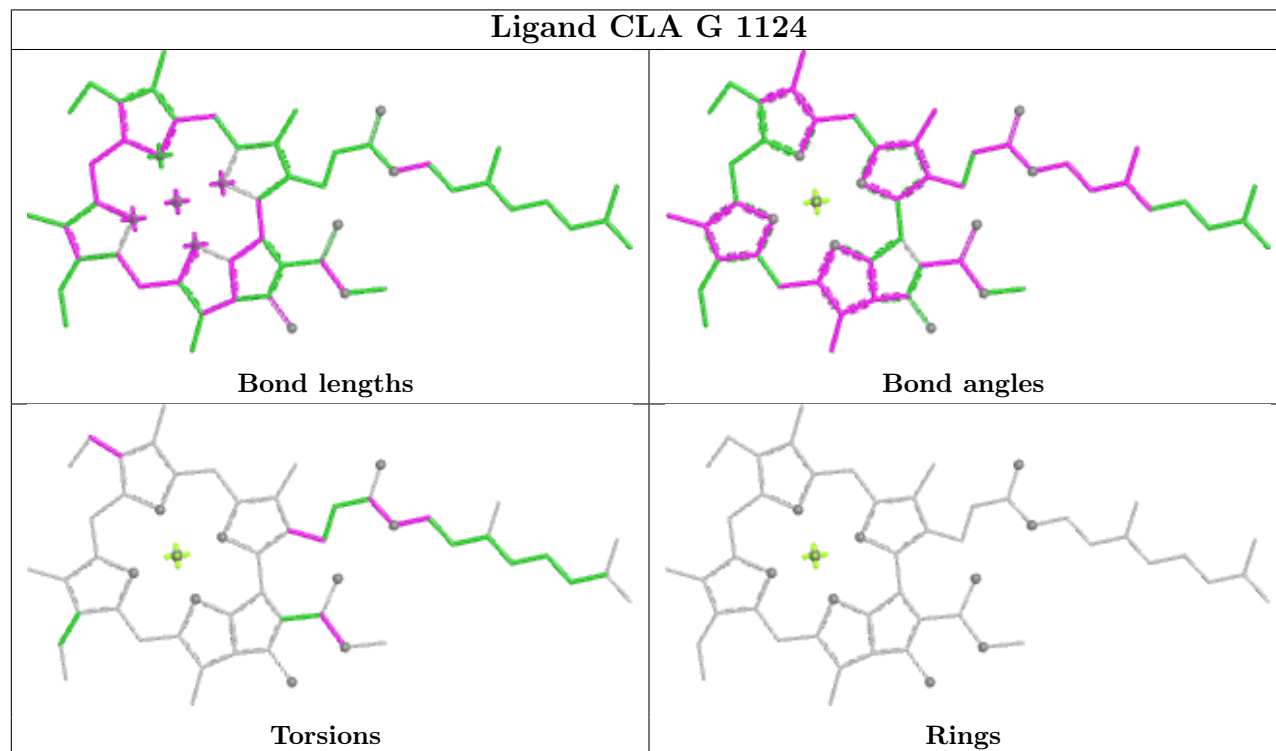


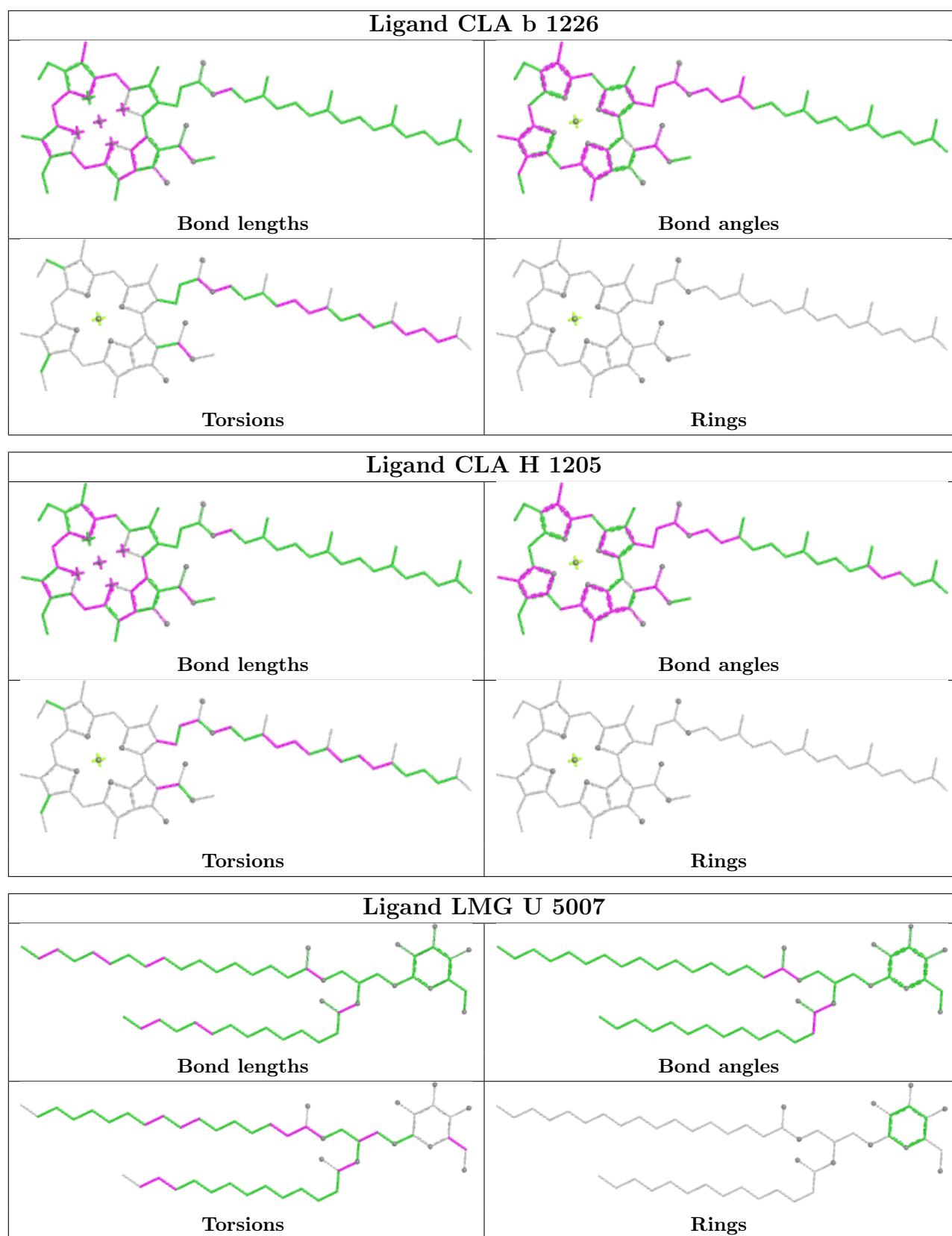


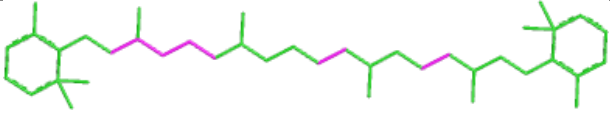
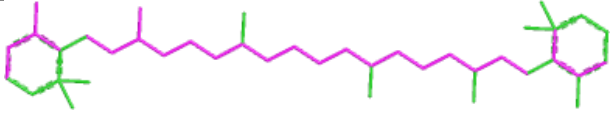
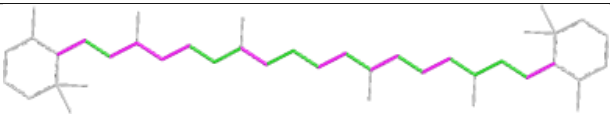
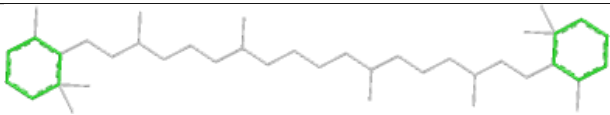
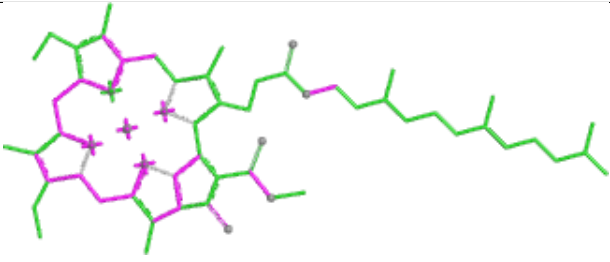
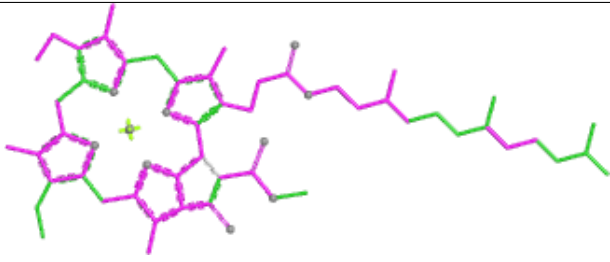
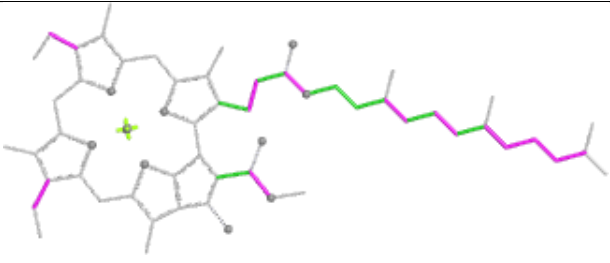
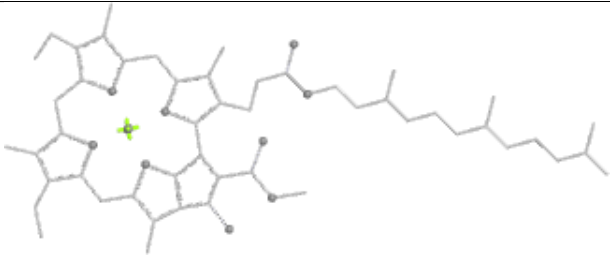
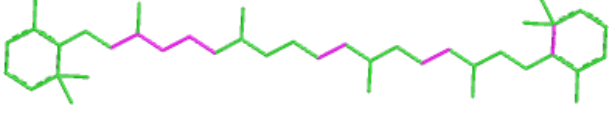
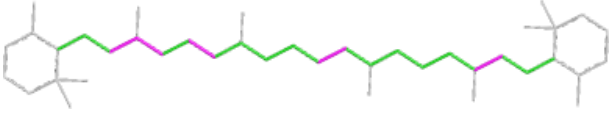
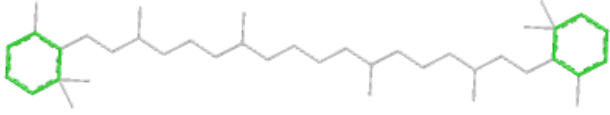
Ligand CLA H 1234

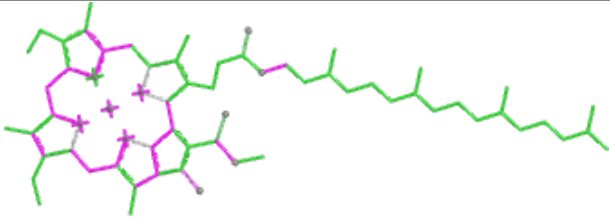
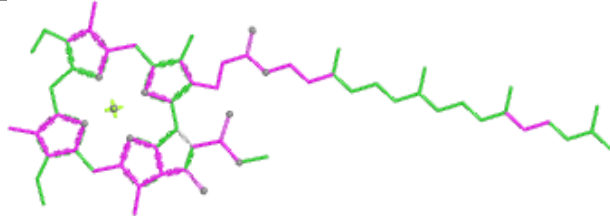
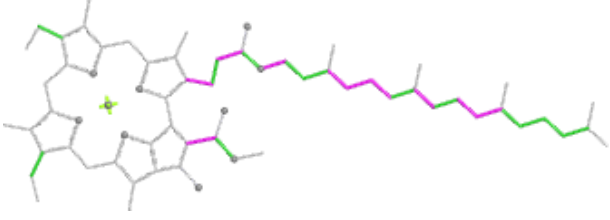
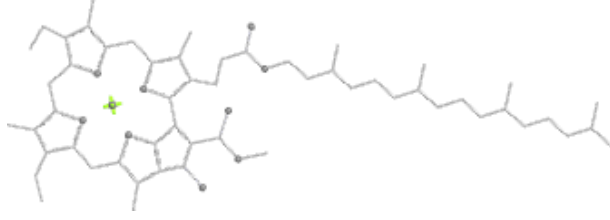
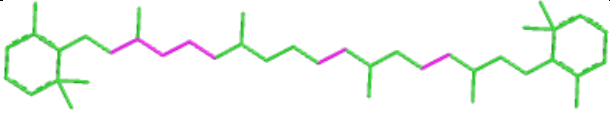
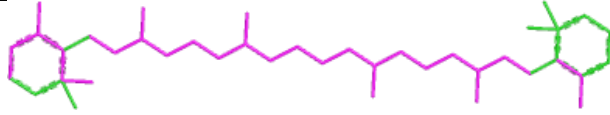
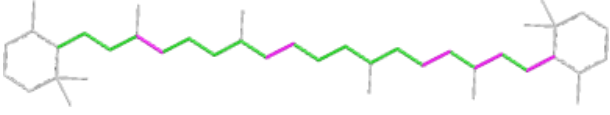
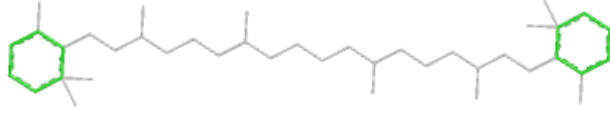
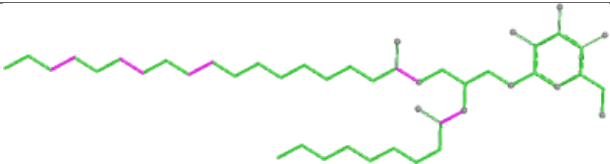
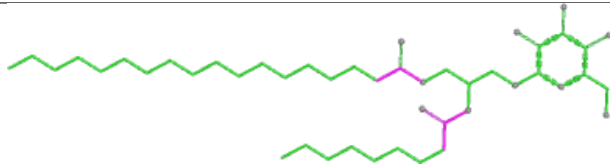
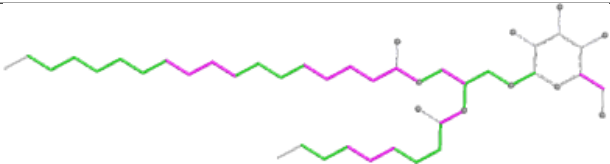
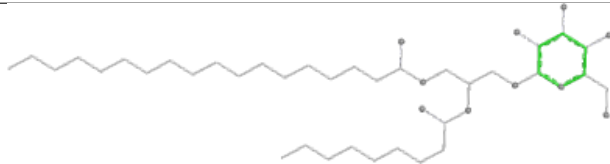


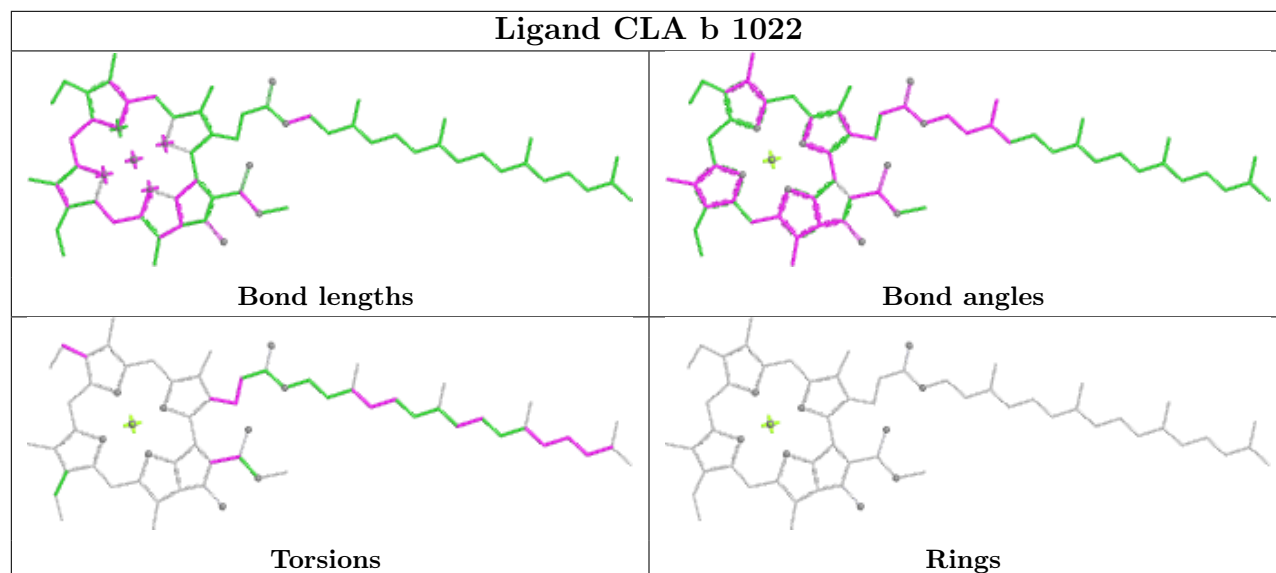
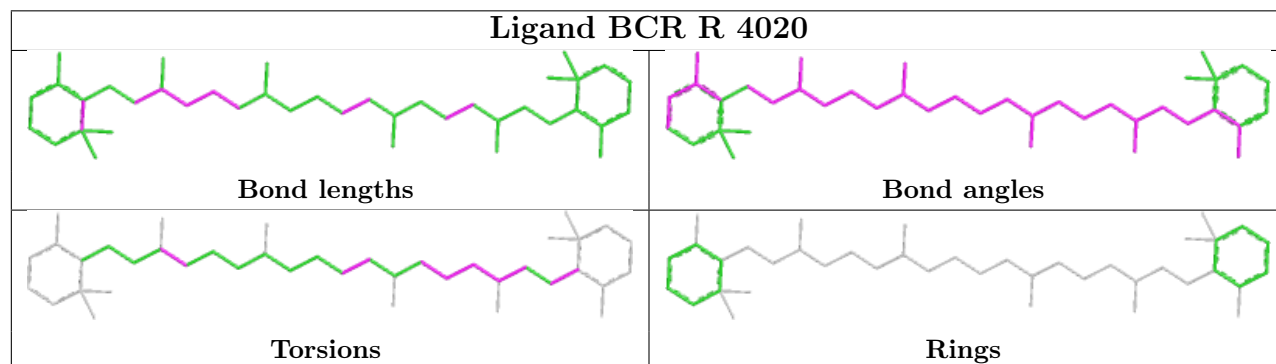
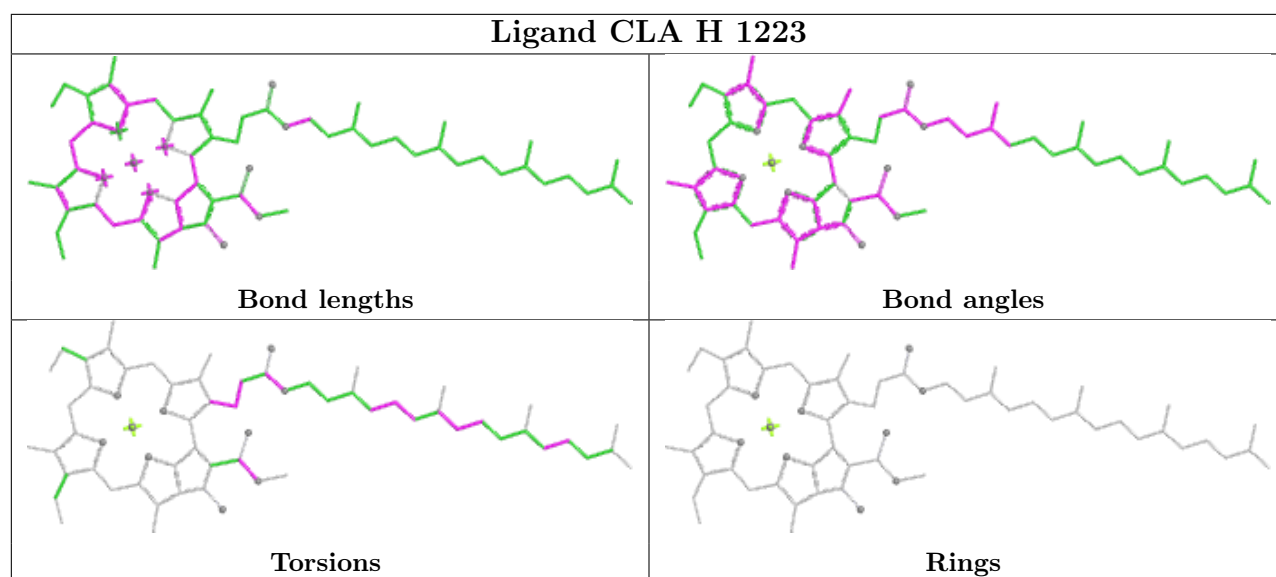
Ligand CLA G 1124



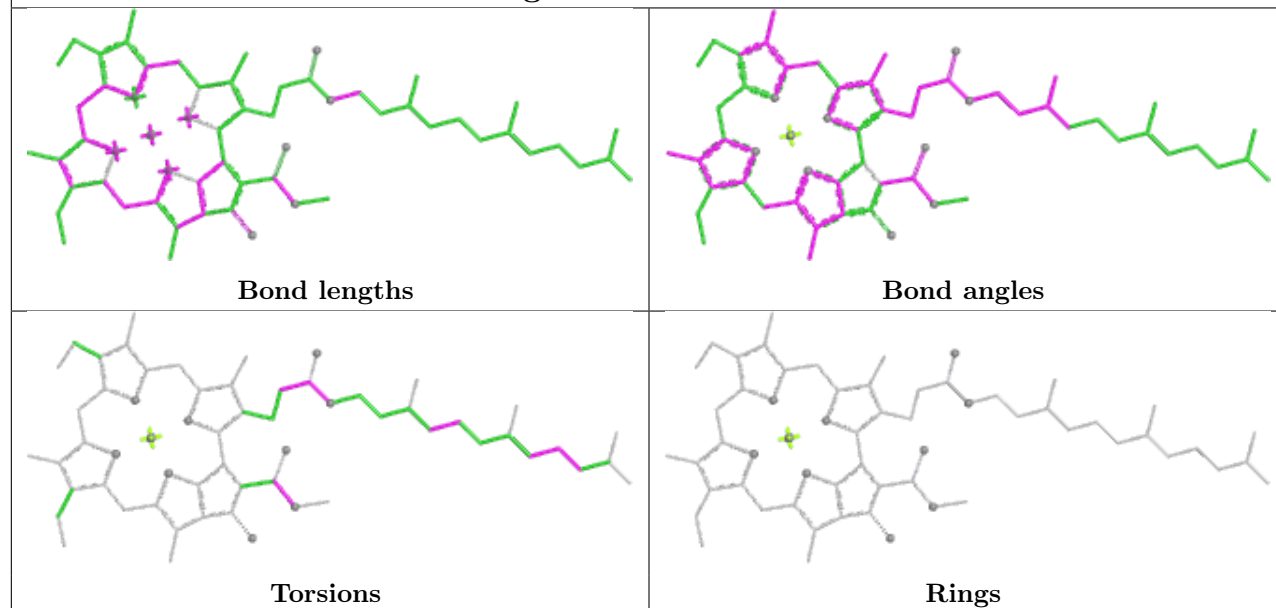


Ligand BCR B 4016	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 1214	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 4004	
 Bond lengths	 Bond angles
 Torsions	 Rings

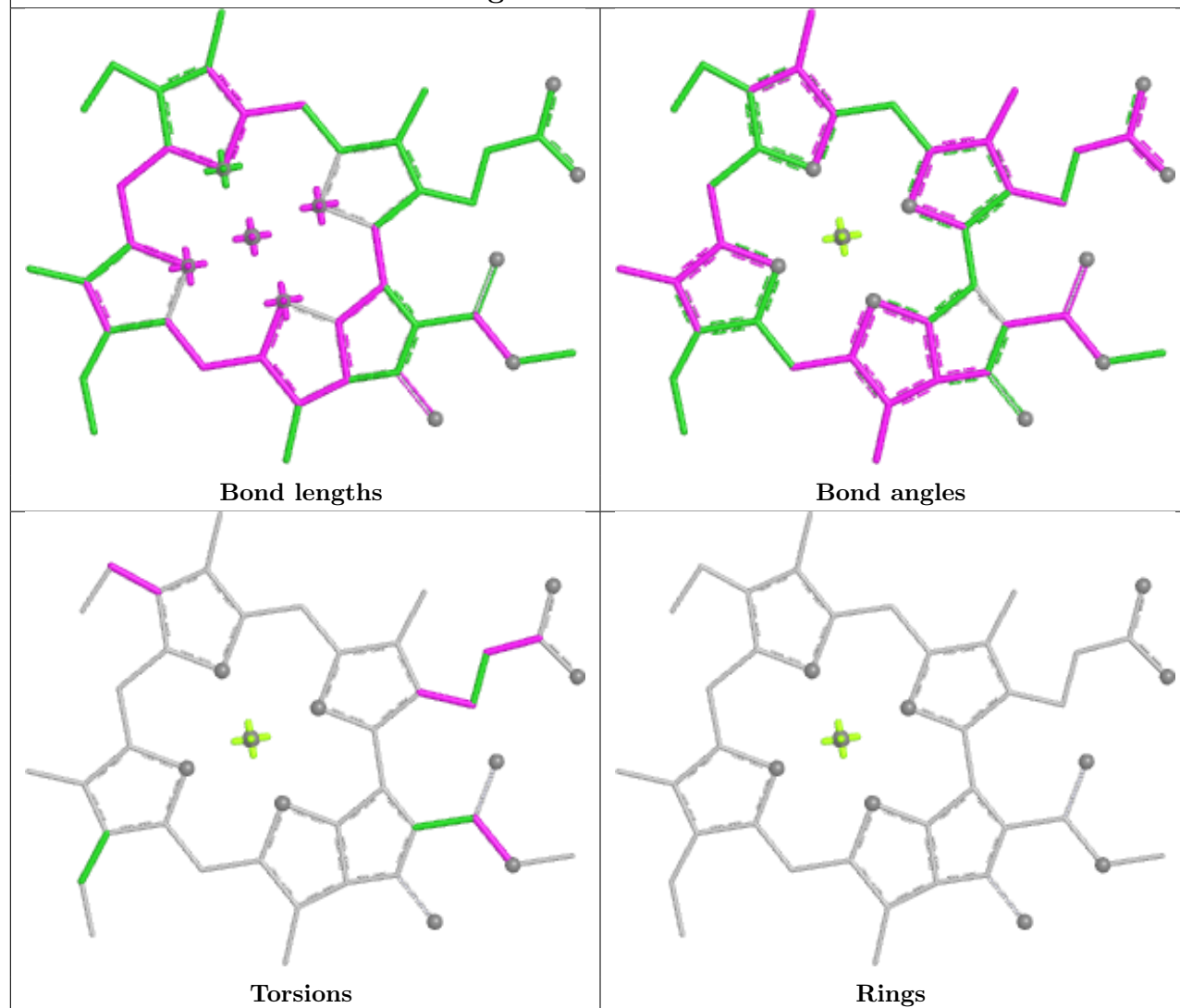
Ligand CLA B 1205	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR U 4019	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG a 5005	
 Bond lengths	 Bond angles
 Torsions	 Rings

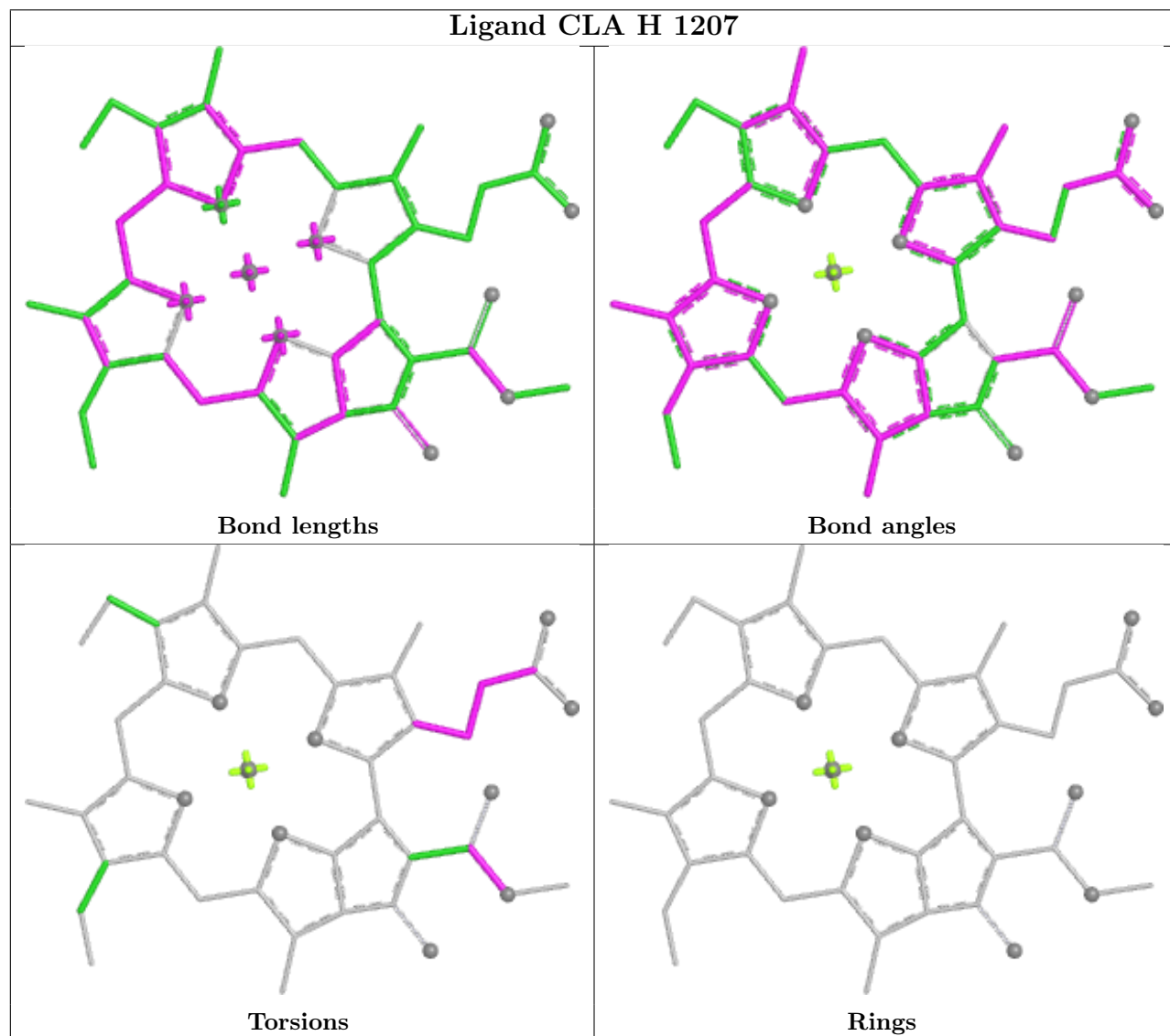
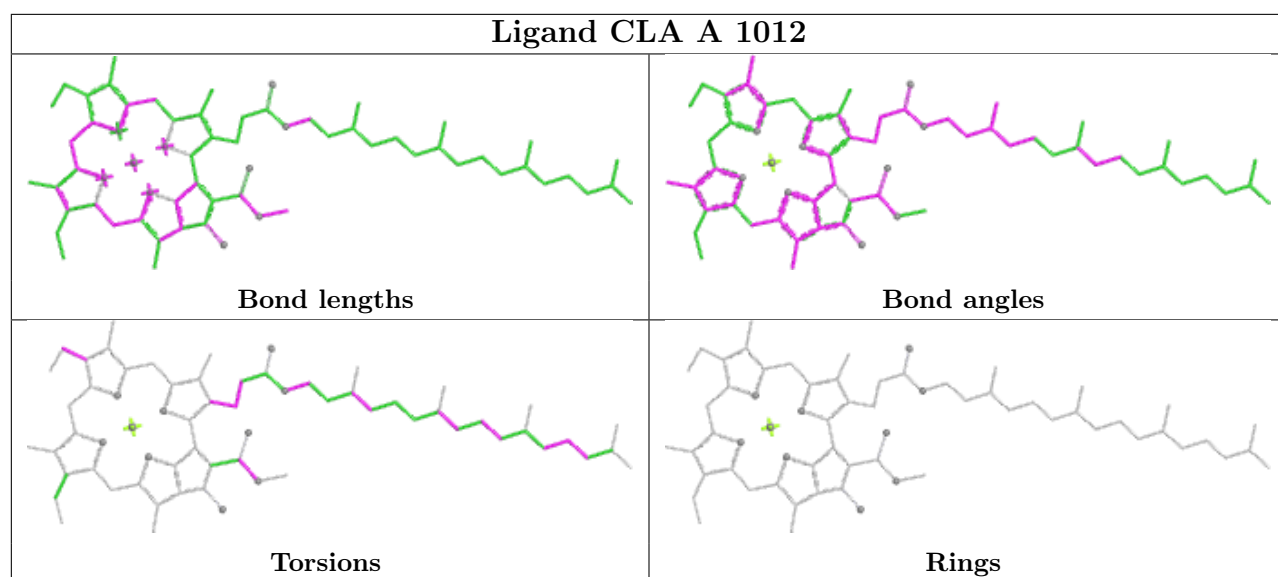


Ligand CLA B 1235

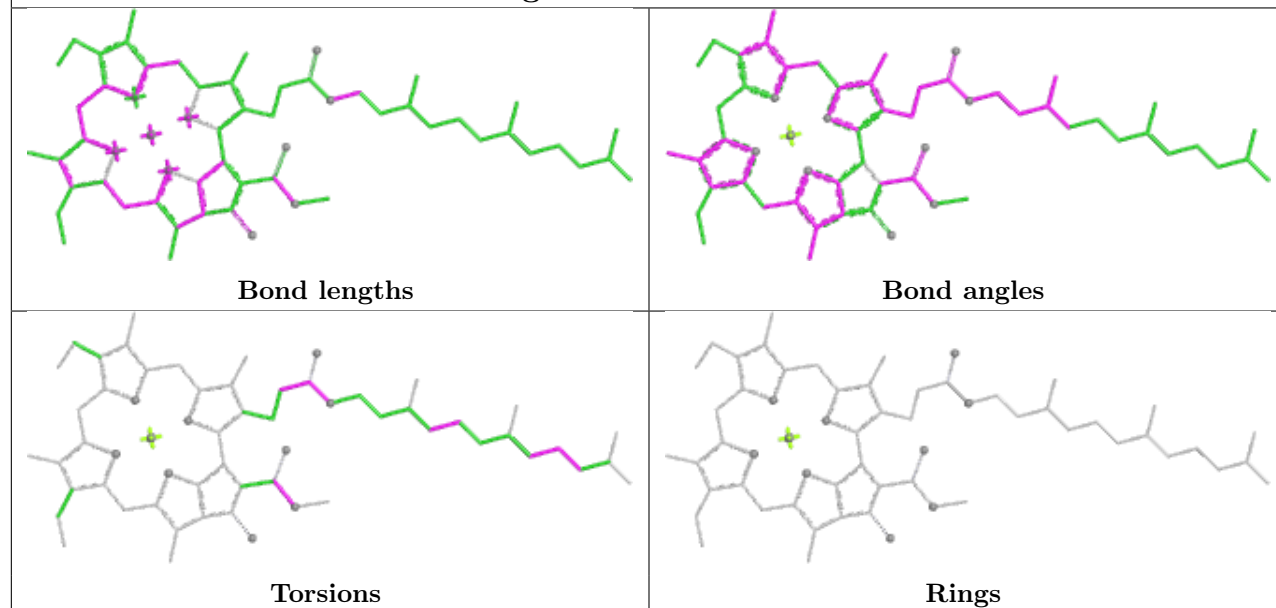


Ligand CLA a 1109

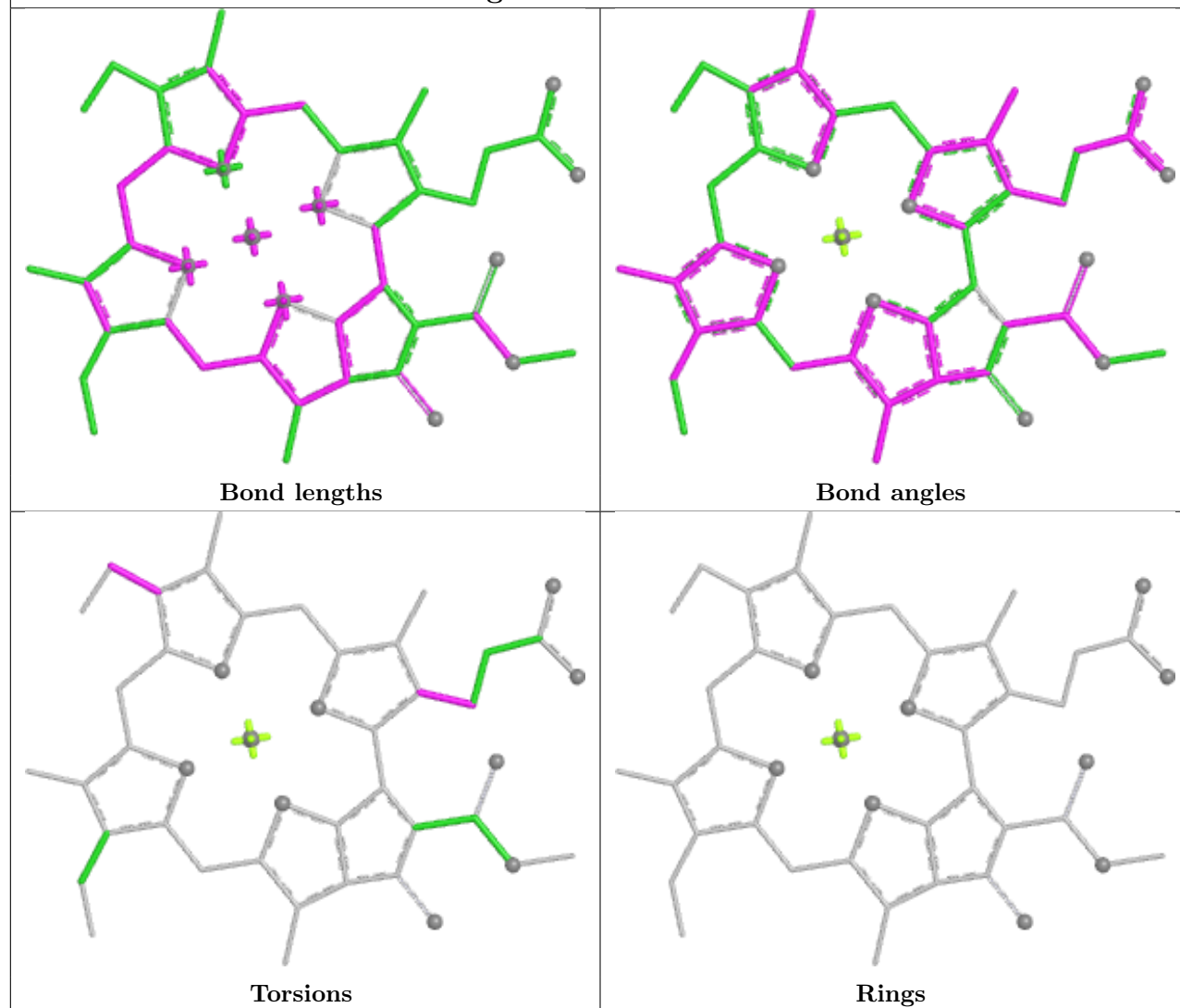


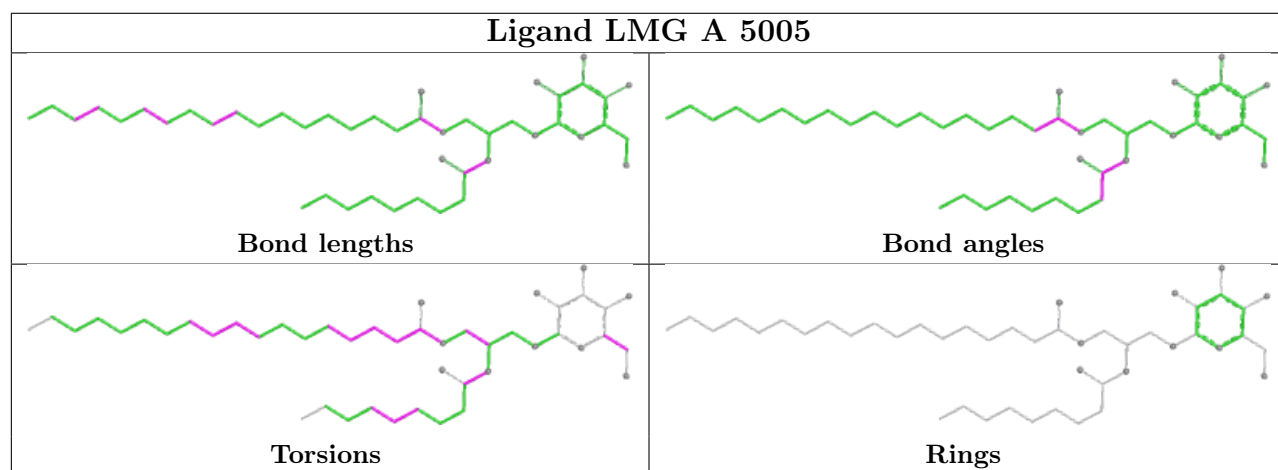
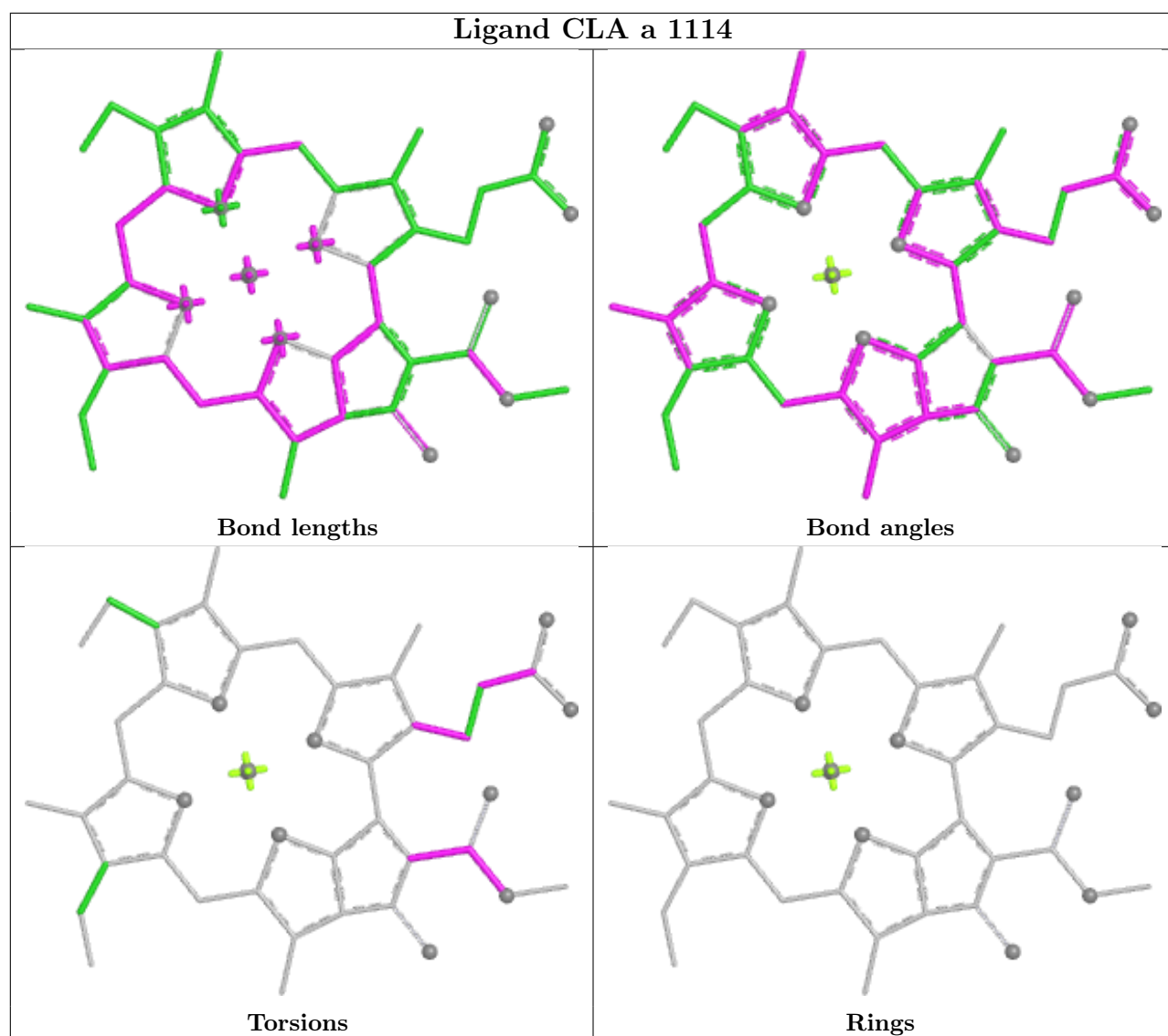


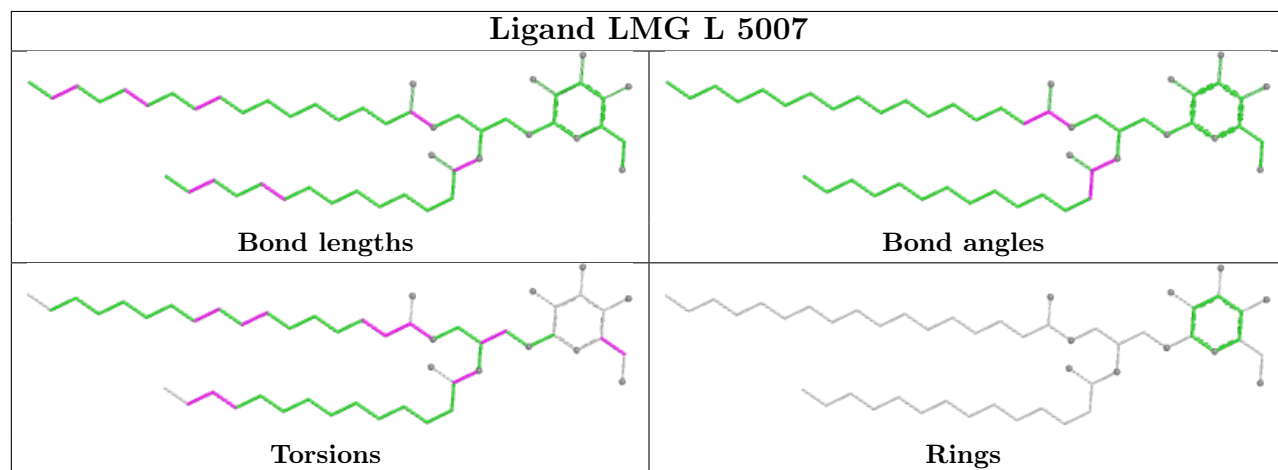
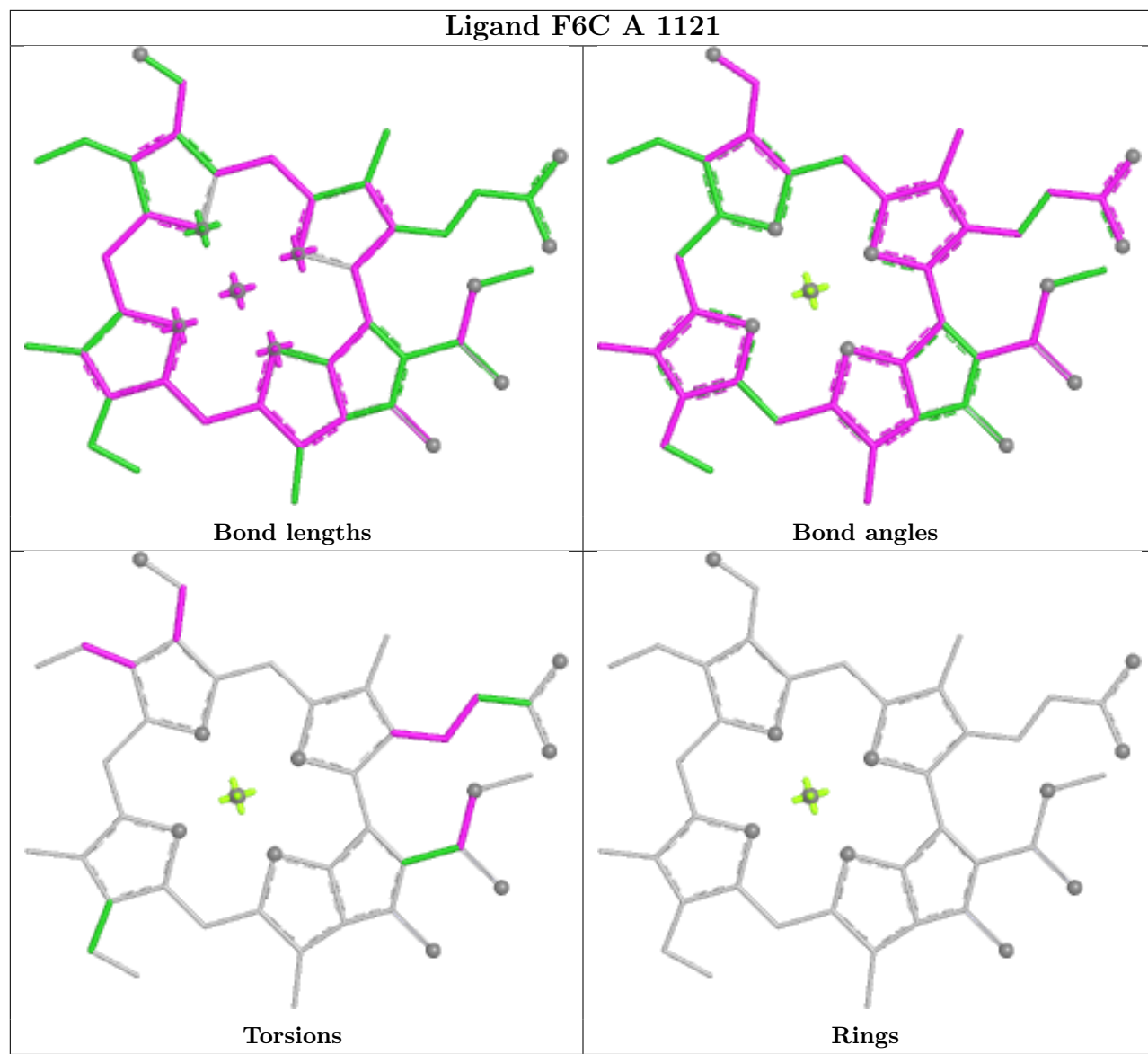
Ligand CLA H 1235

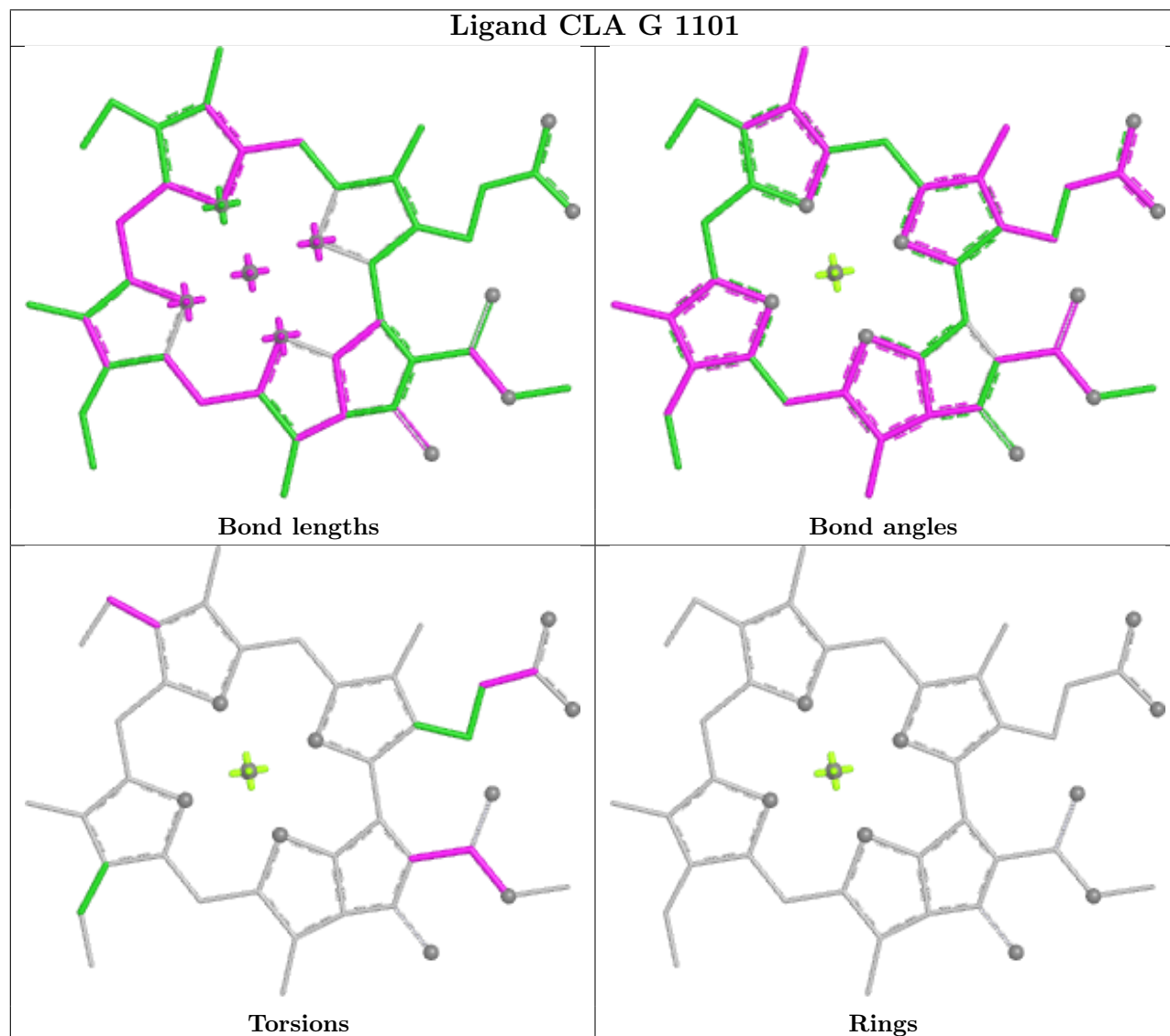
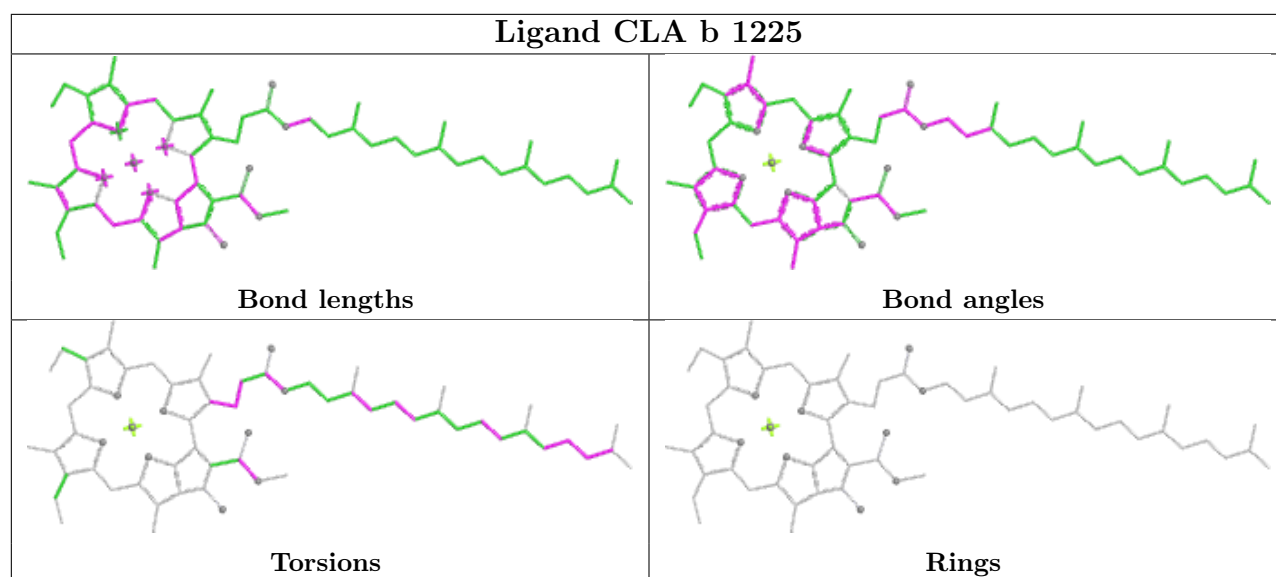


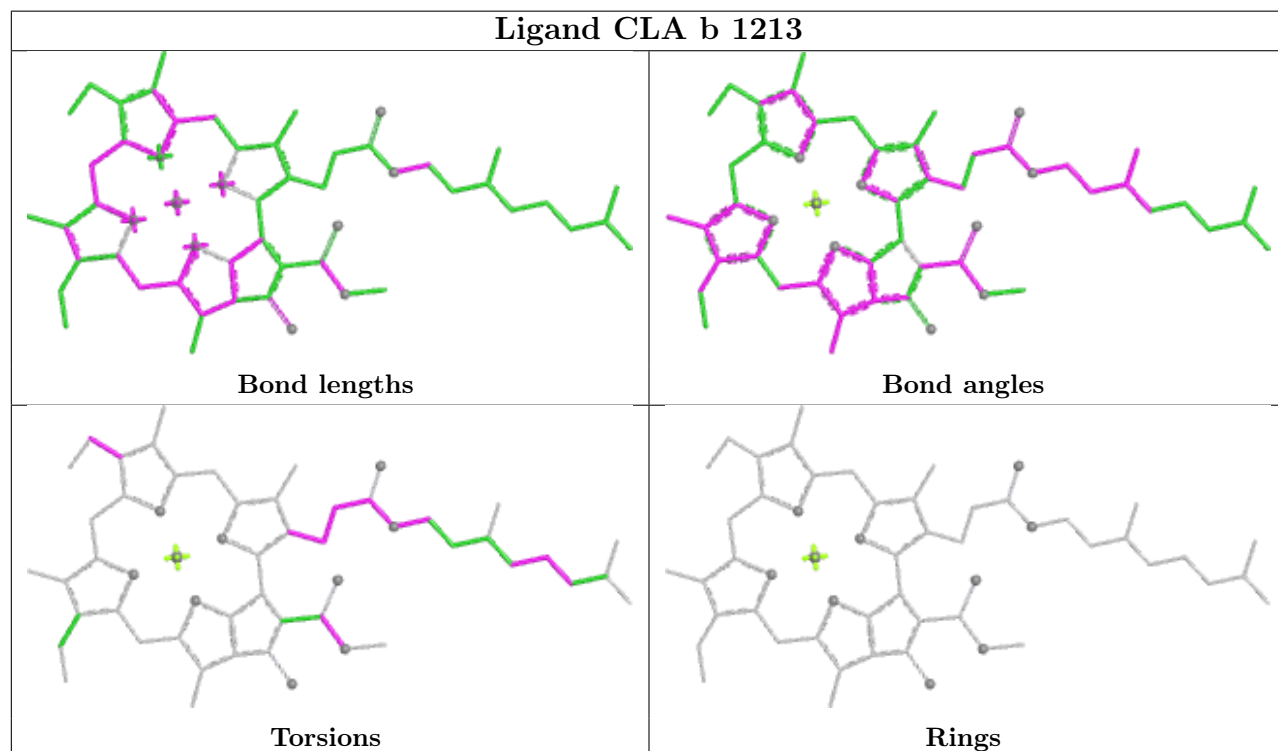
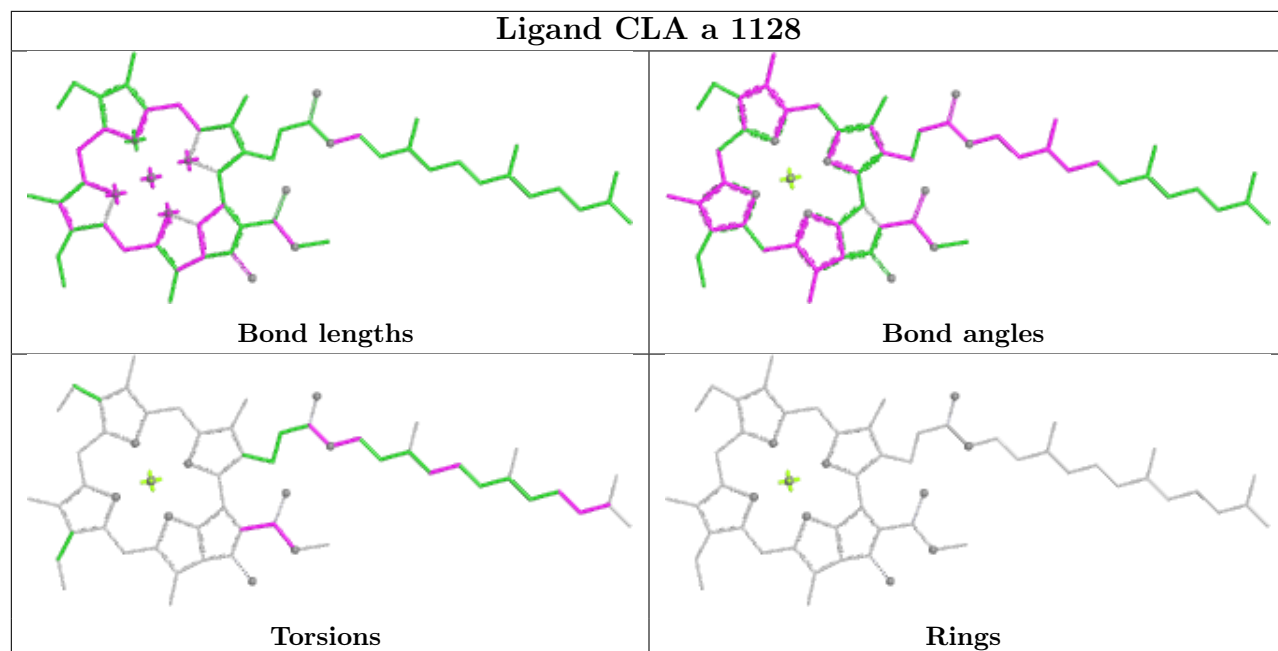
Ligand CLA b 1209

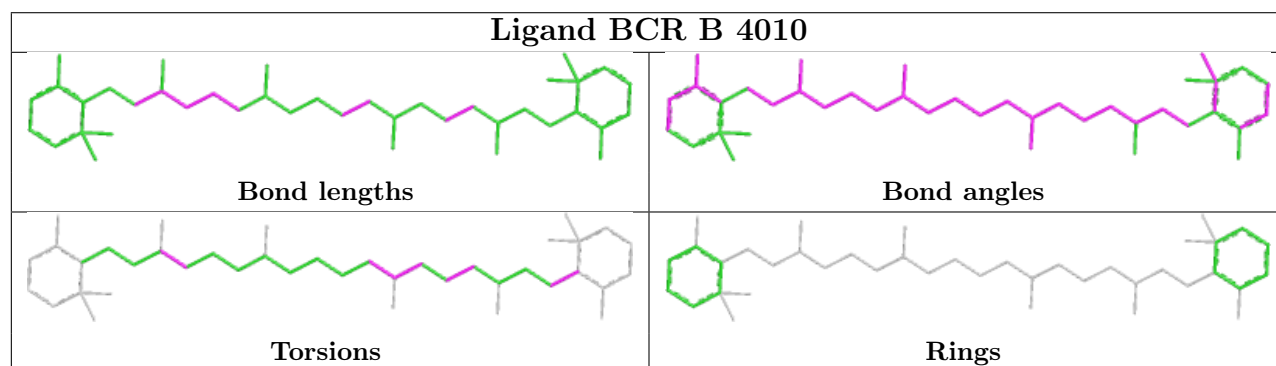
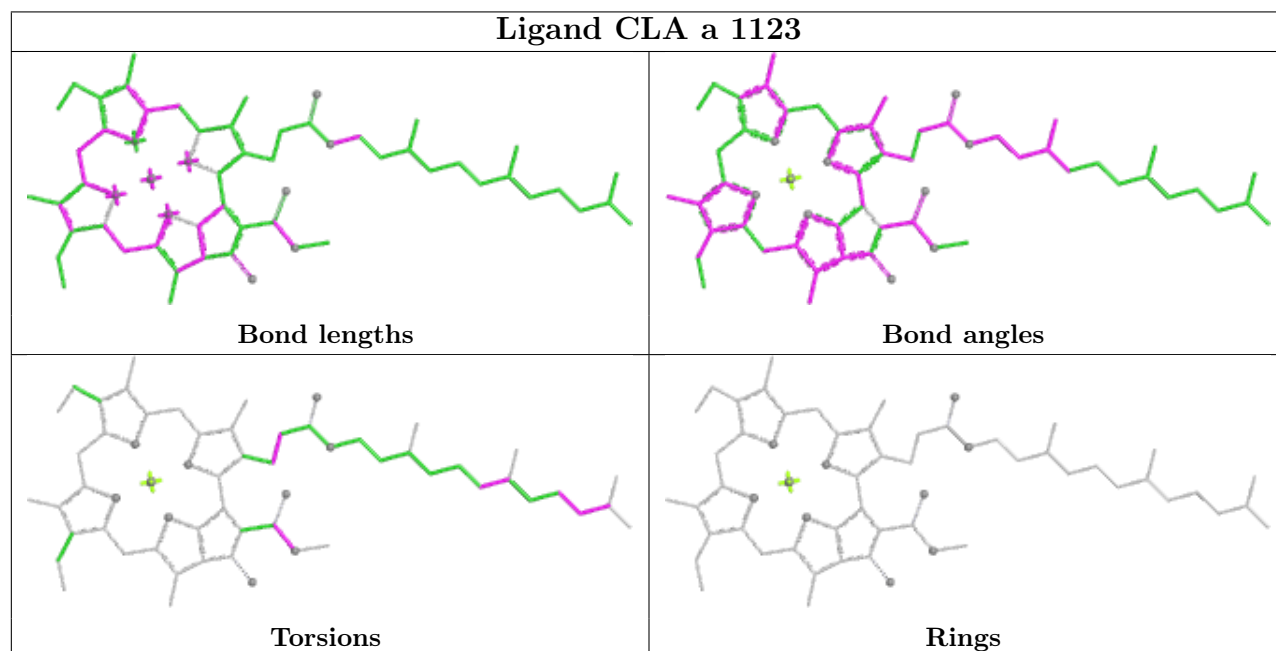
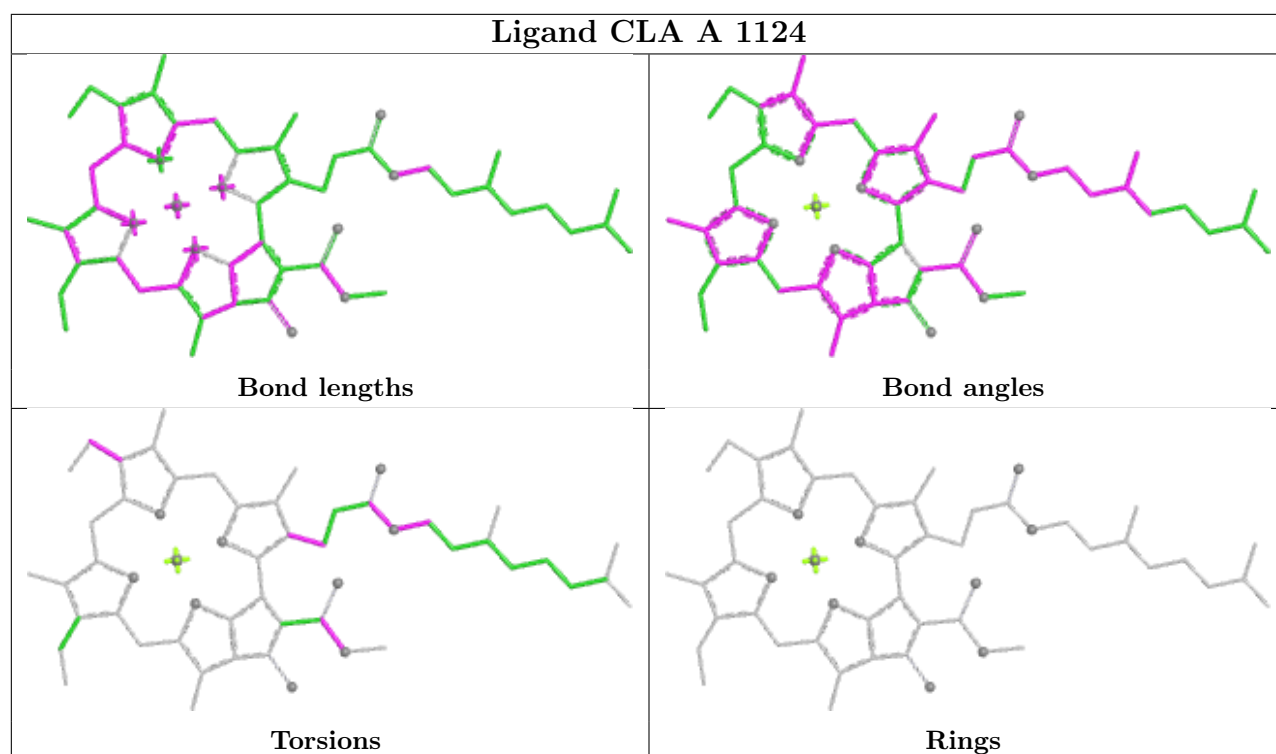


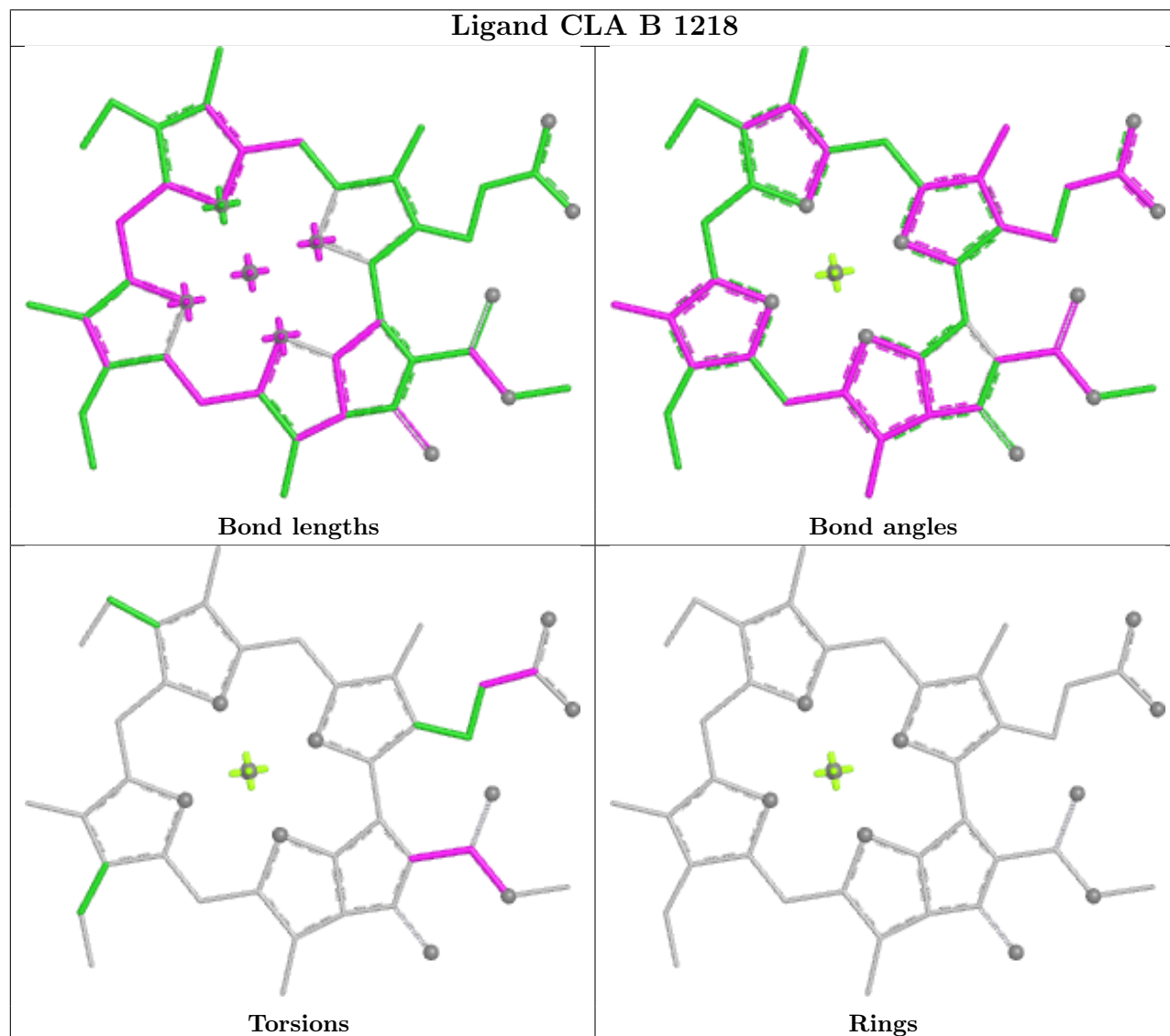
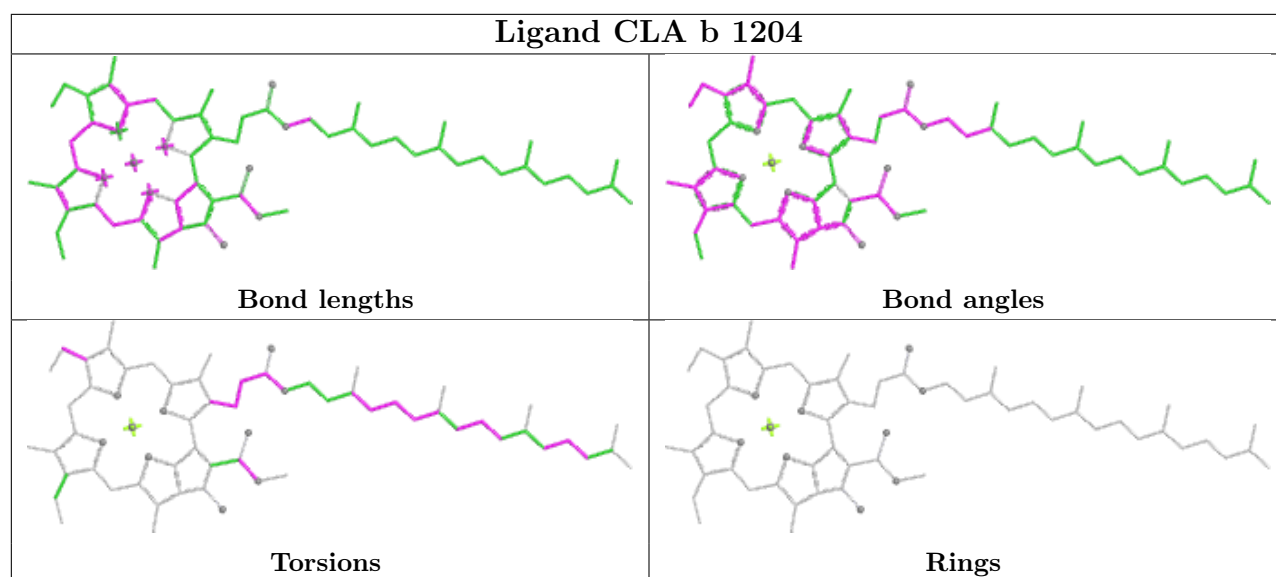


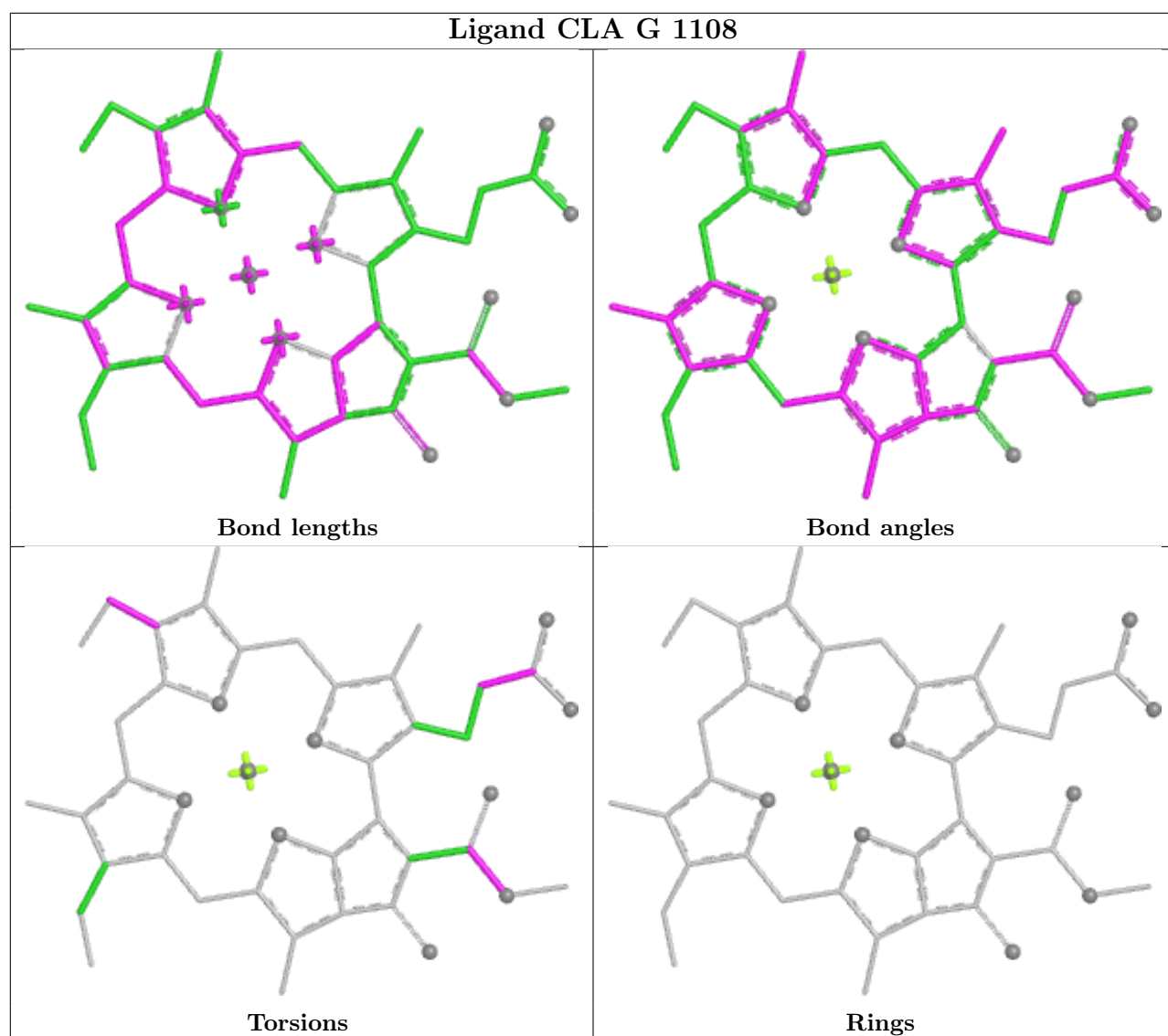


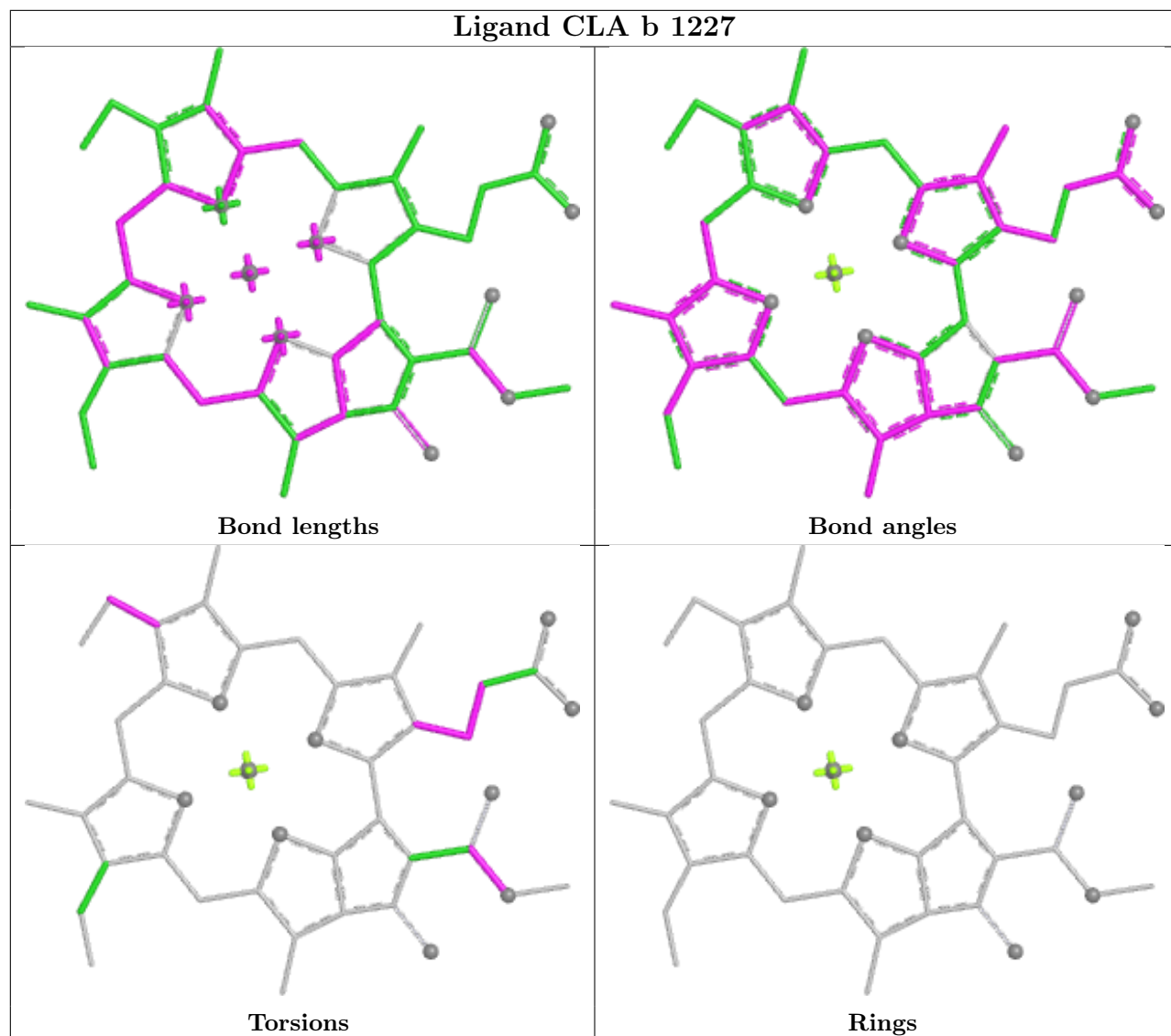


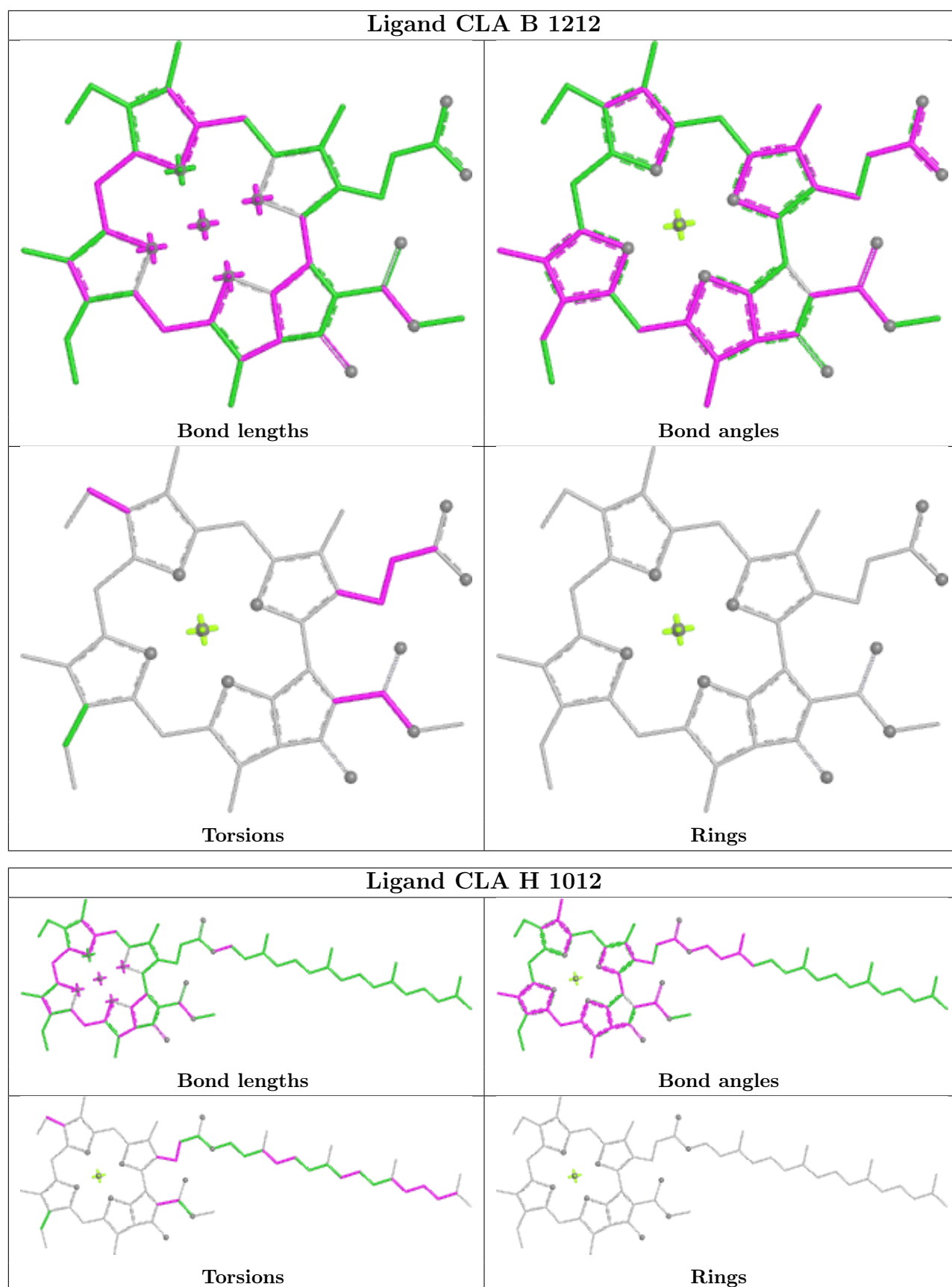




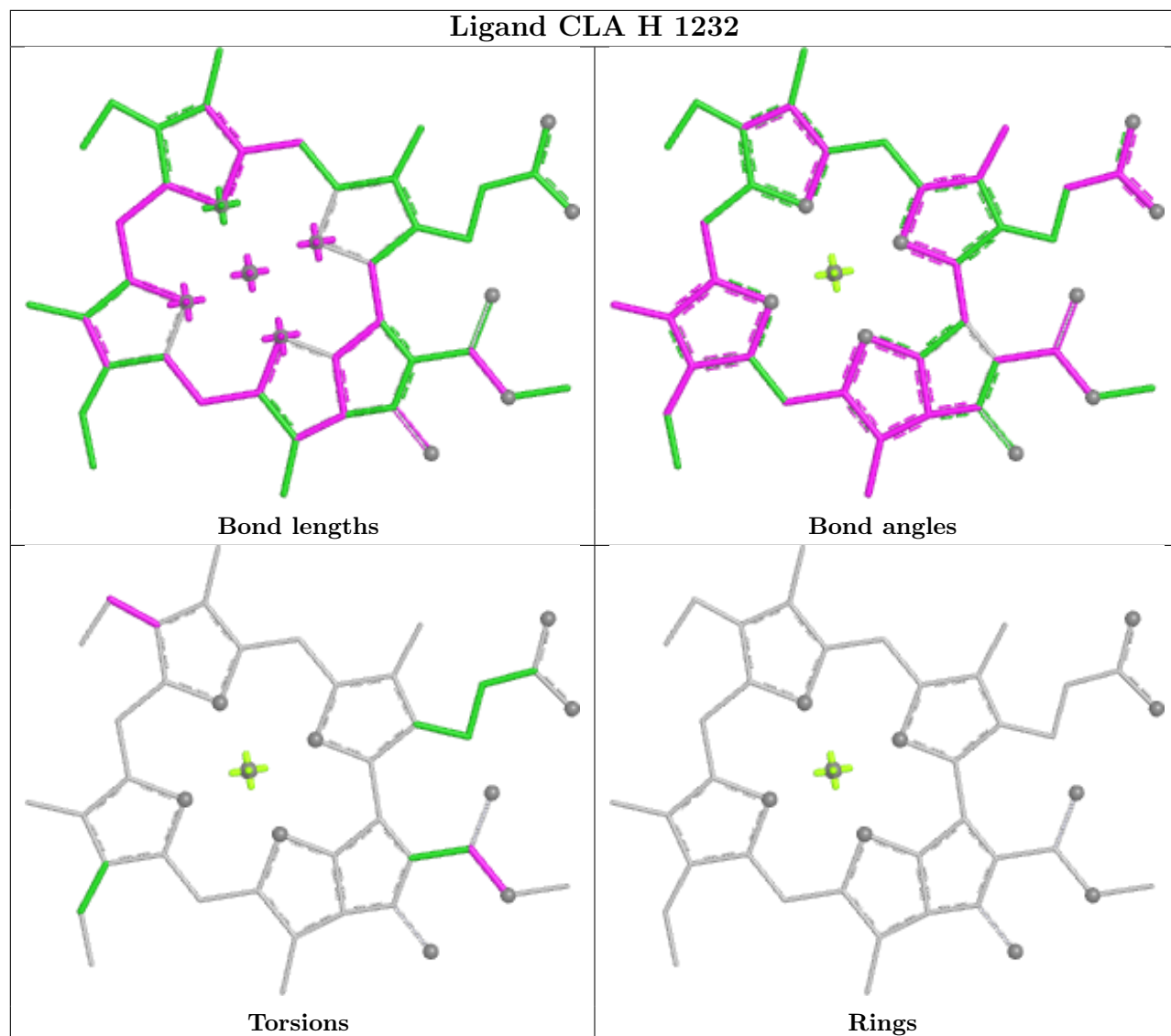


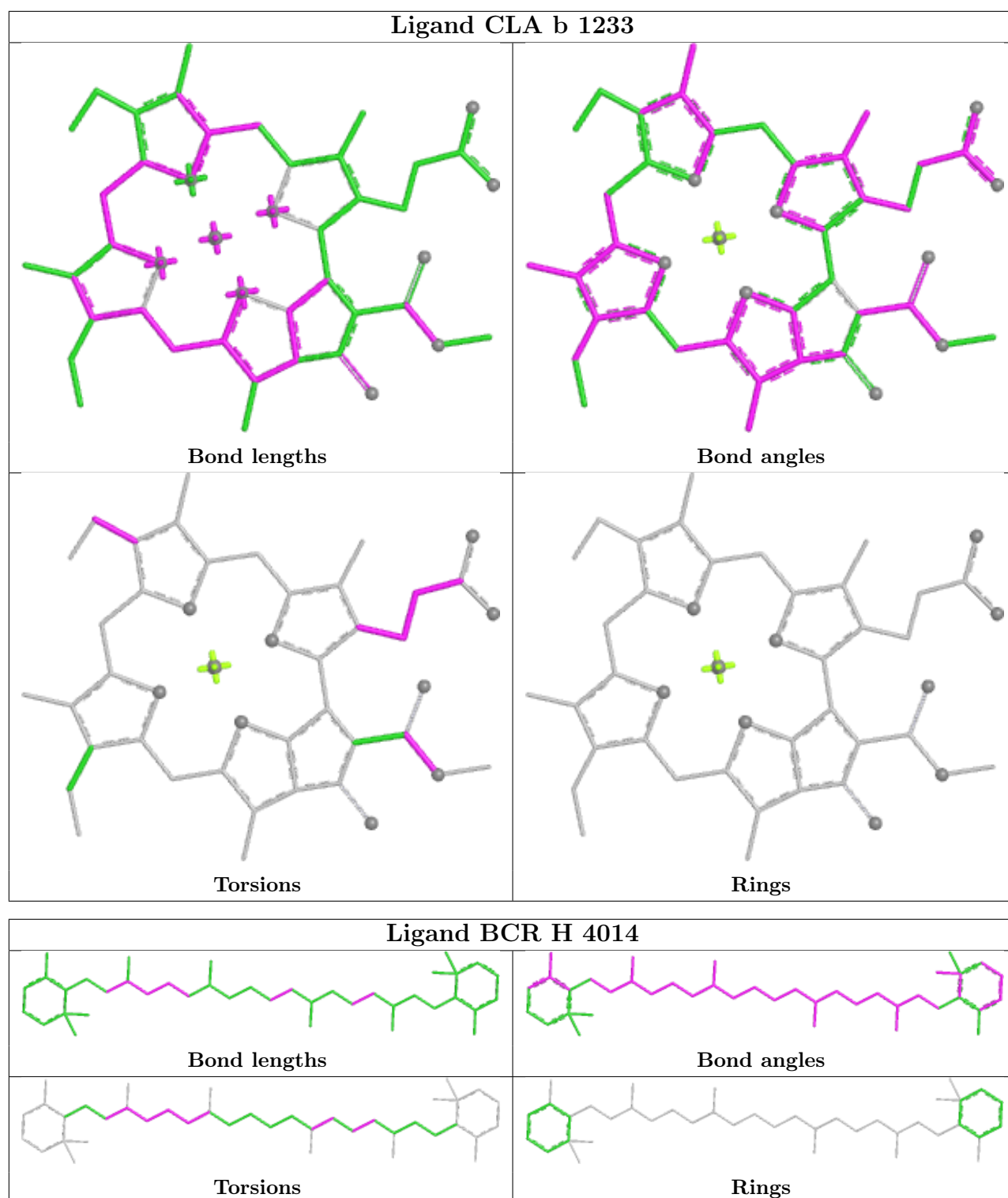




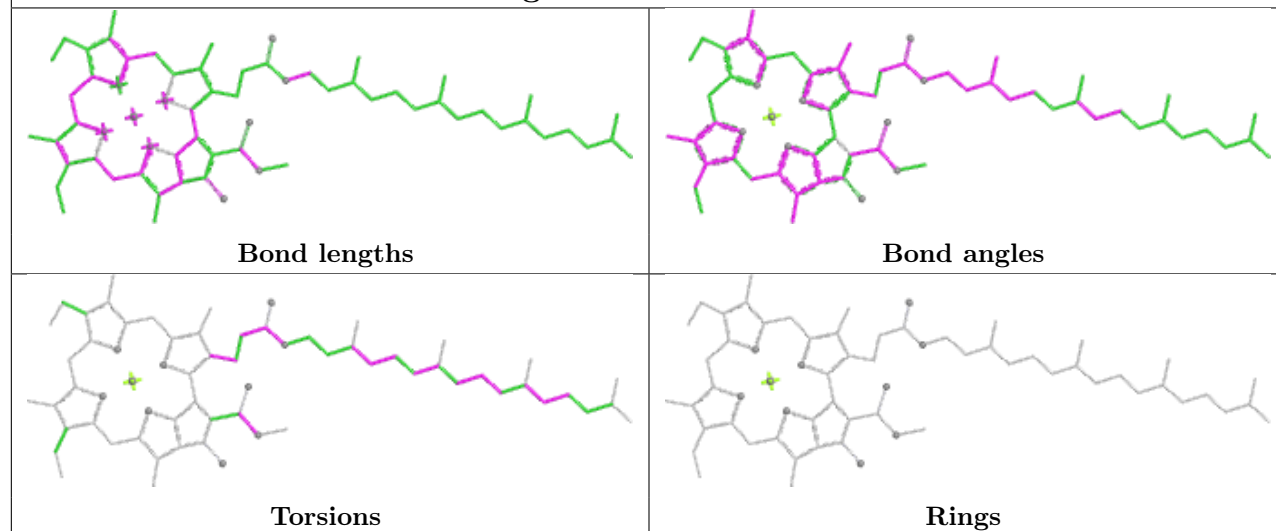


Ligand CLA H 1232

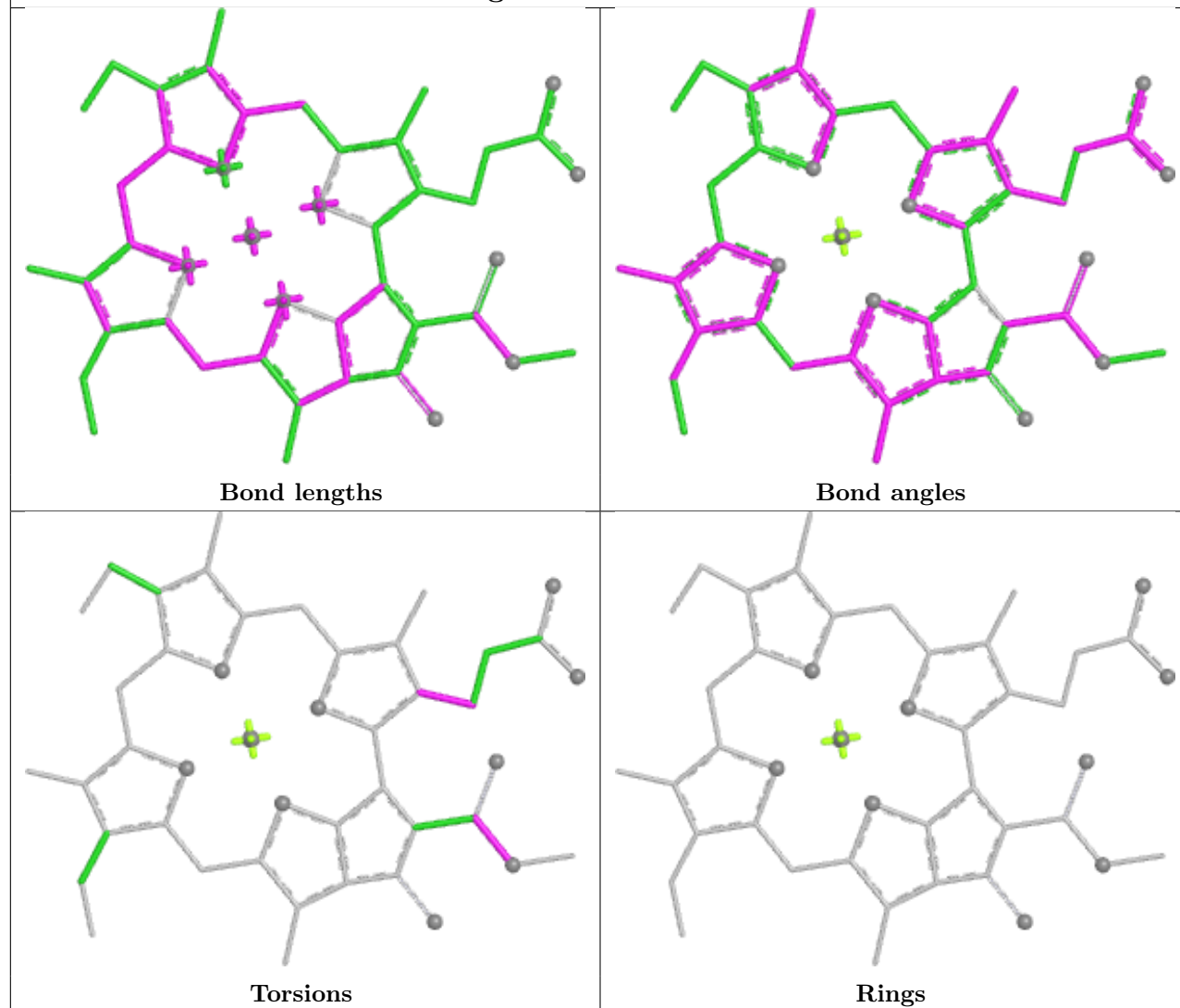


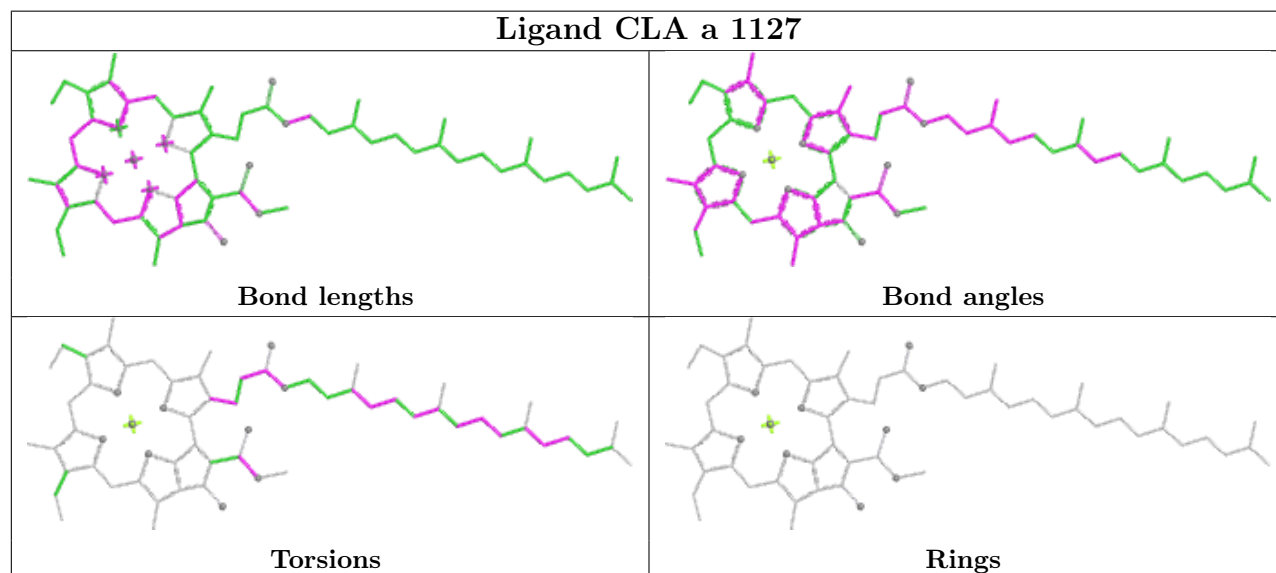
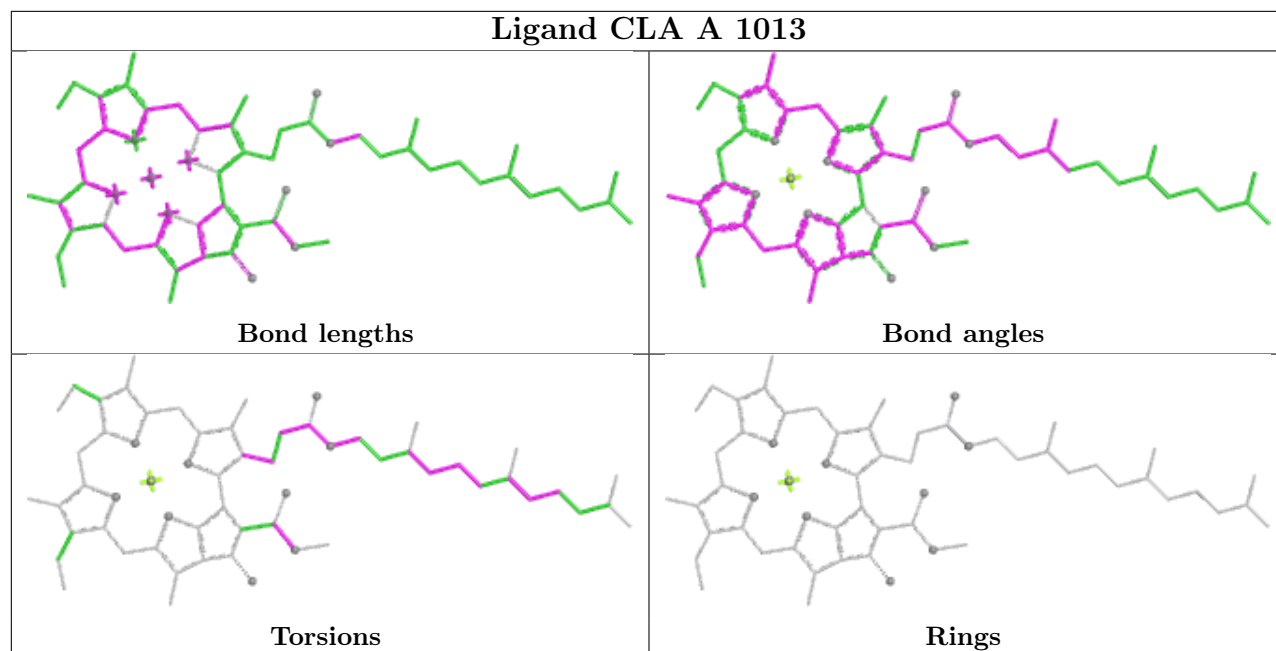


Ligand CLA A 1127

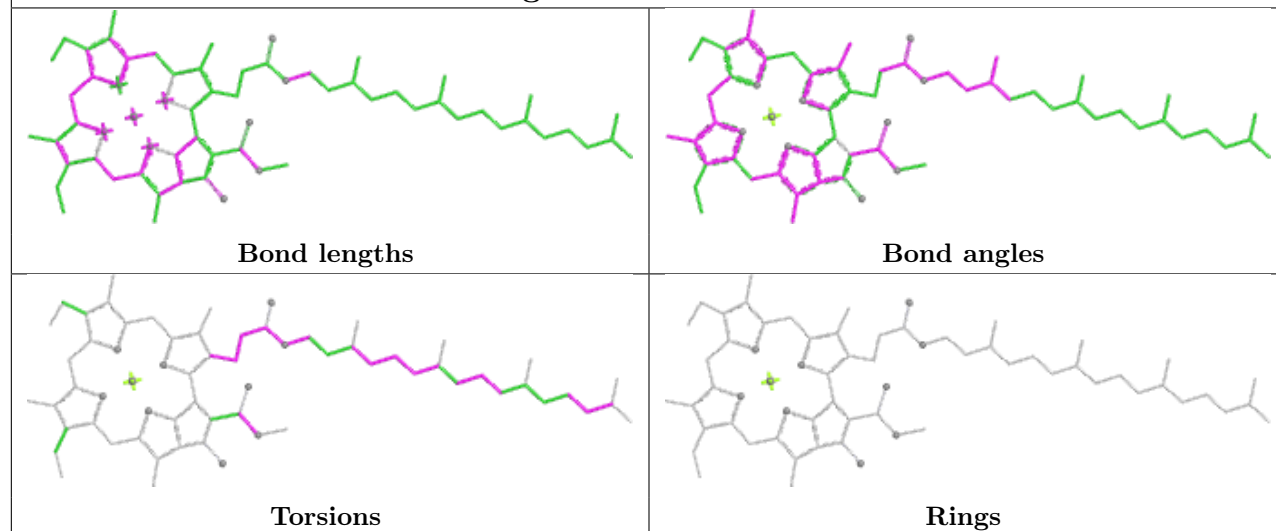


Ligand CLA a 1139

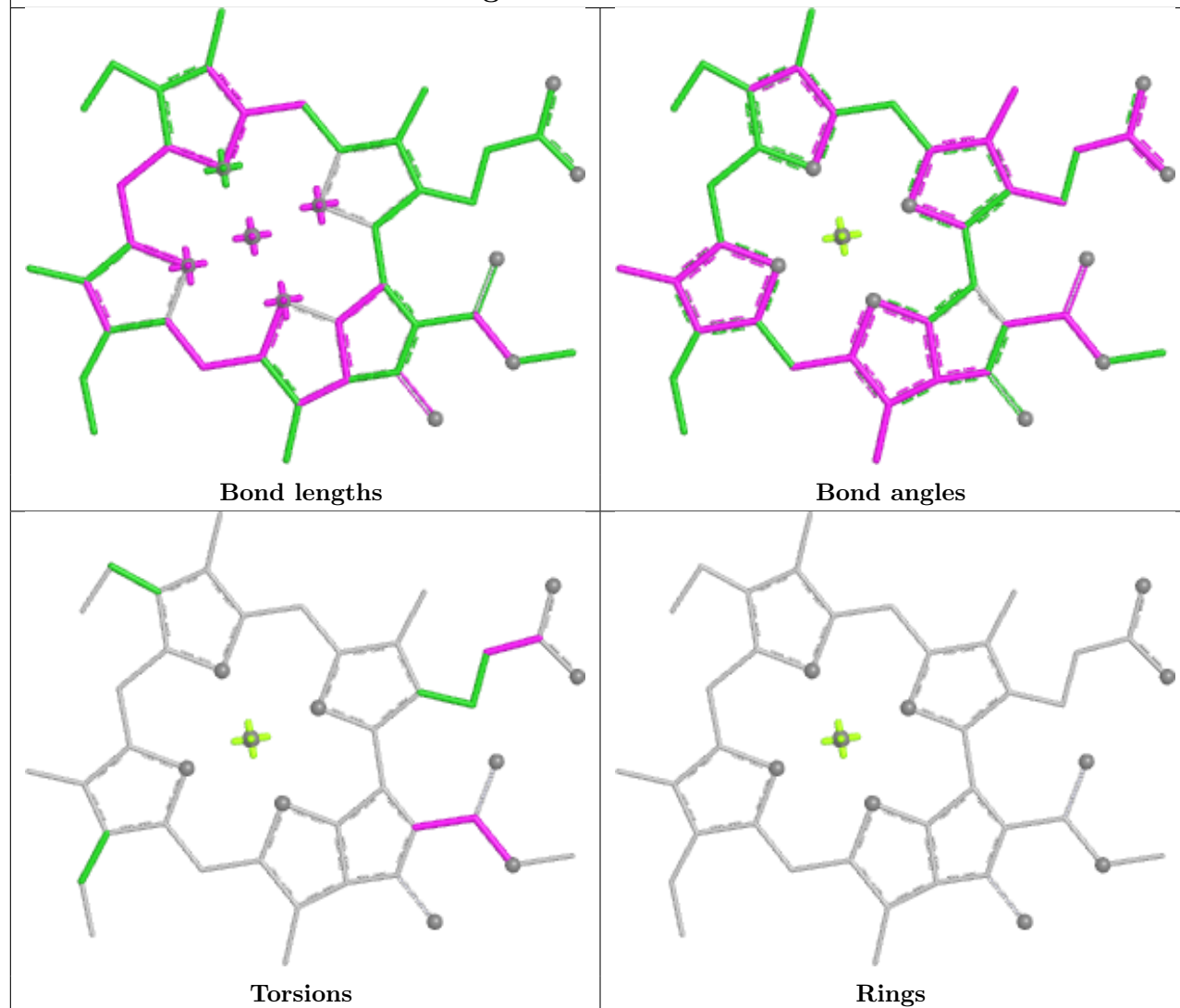


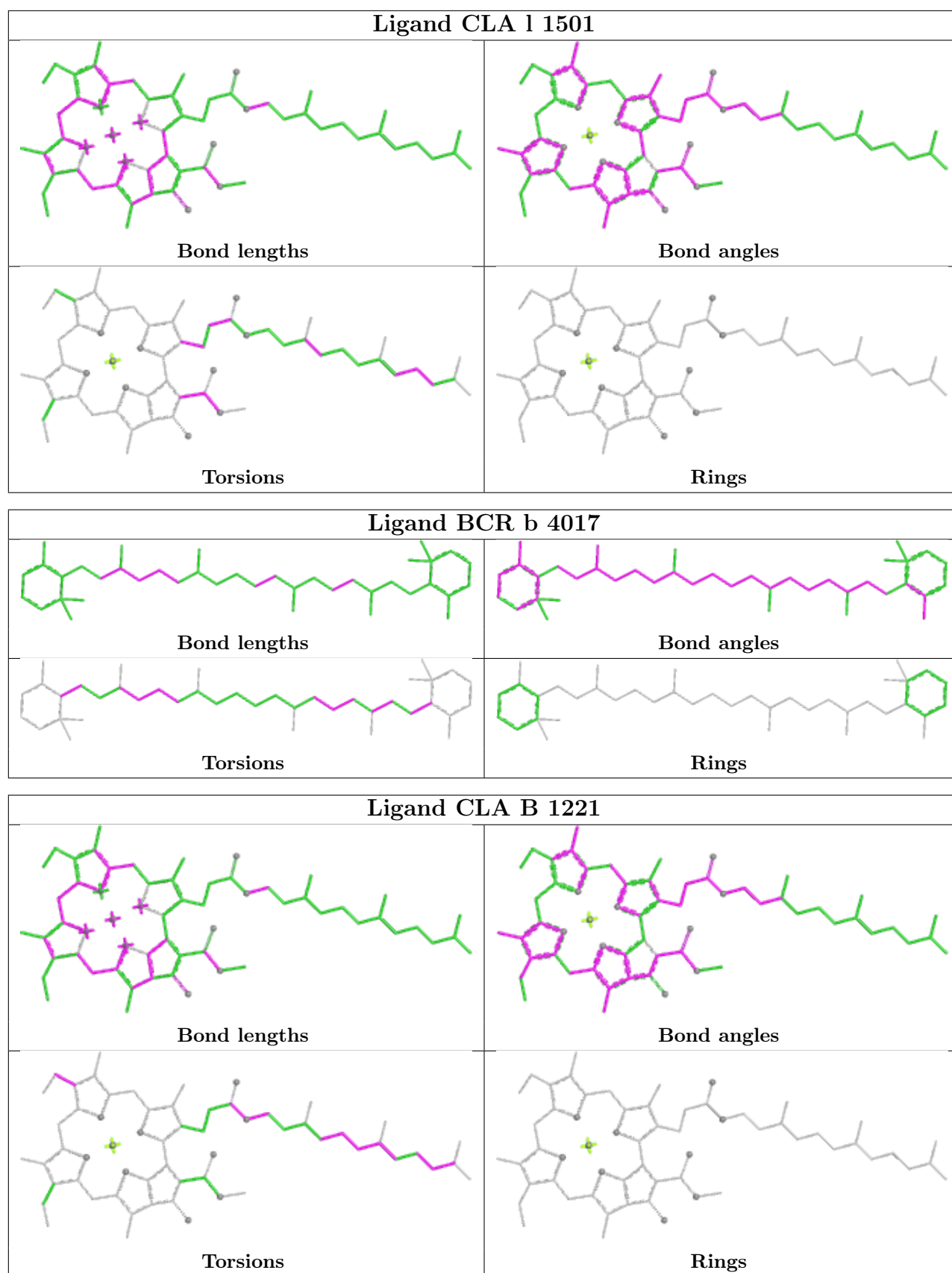


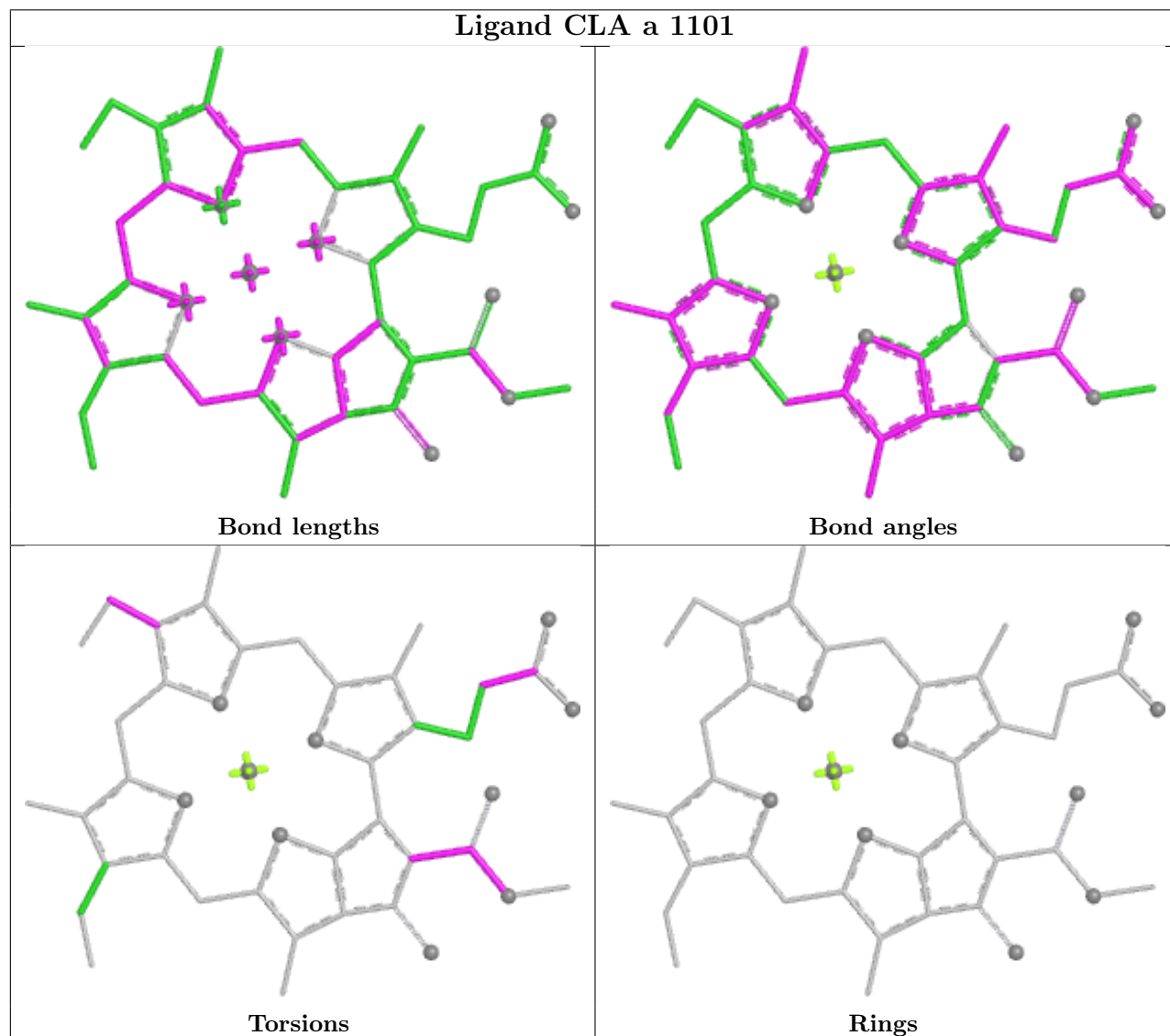
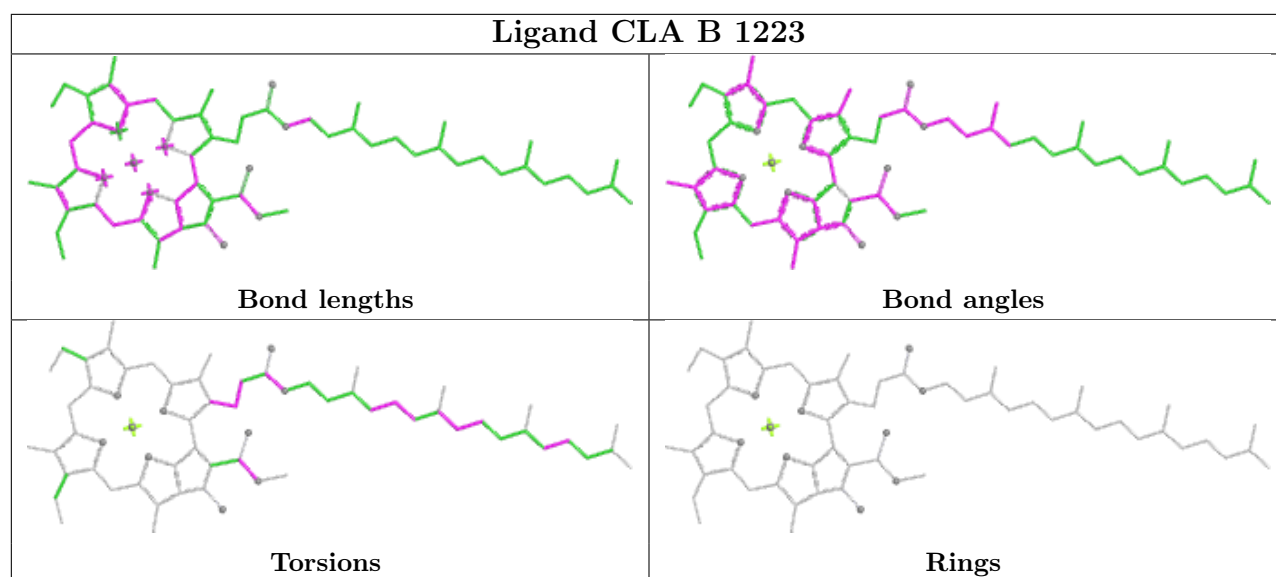
Ligand CLA A 1140

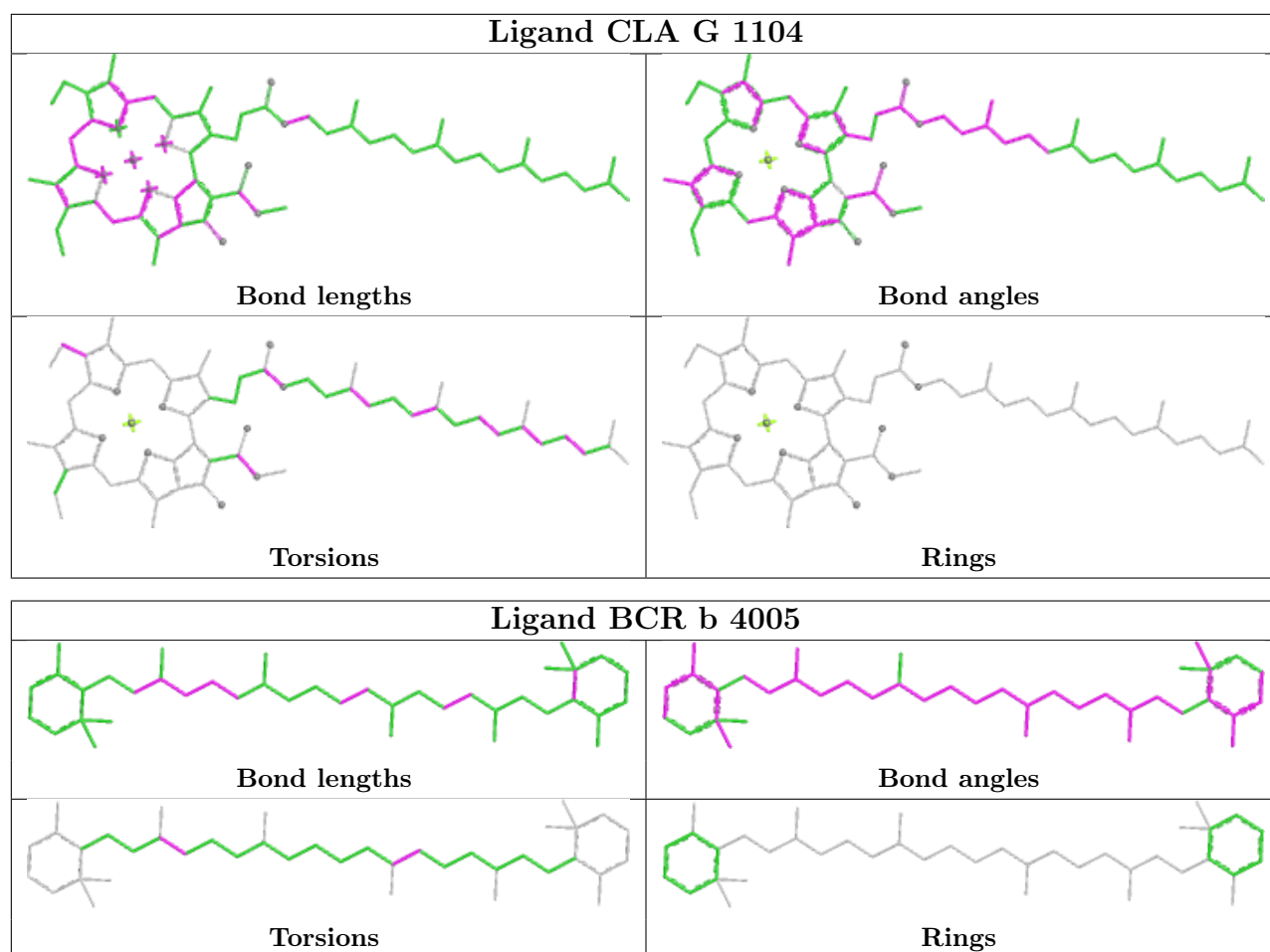


Ligand CLA H 1218









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	K	1
9	T	1
9	k	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	44:UNK	C	69:VAL	N	11.74
1	T	44:UNK	C	69:VAL	N	11.74
1	k	44:UNK	C	69:VAL	N	11.74

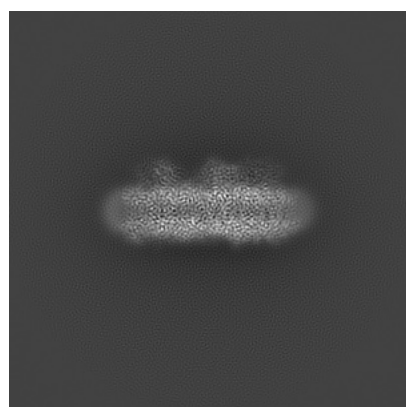
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20397. These allow visual inspection of the internal detail of the map and identification of artifacts.

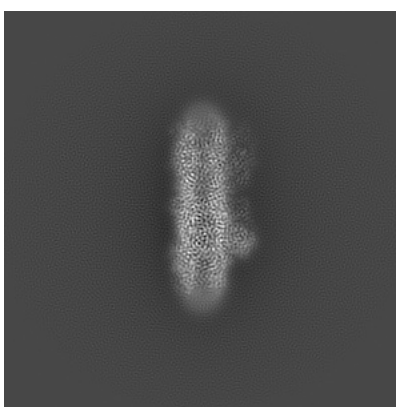
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

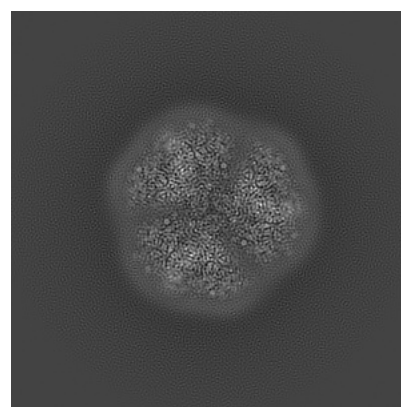
6.1.1 Primary map



X



Y

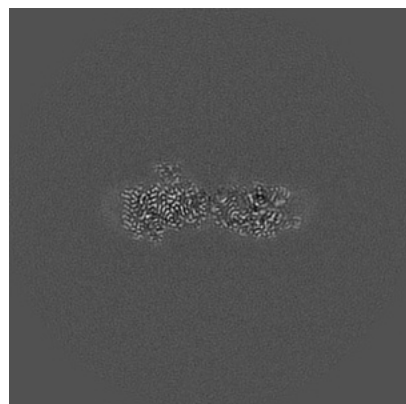


Z

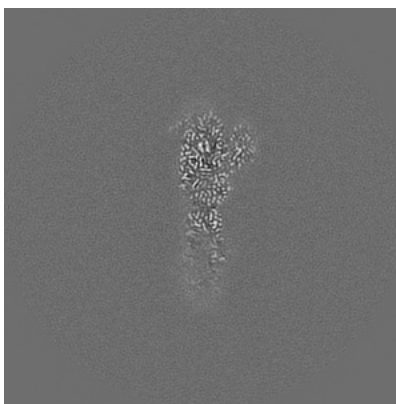
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

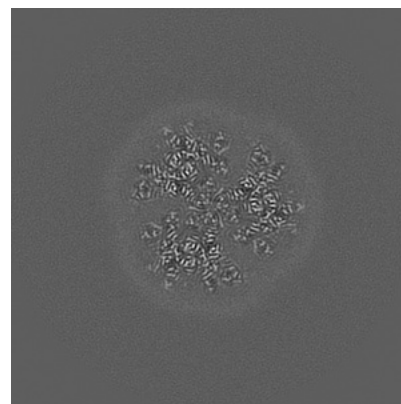
6.2.1 Primary map



X Index: 200



Y Index: 200

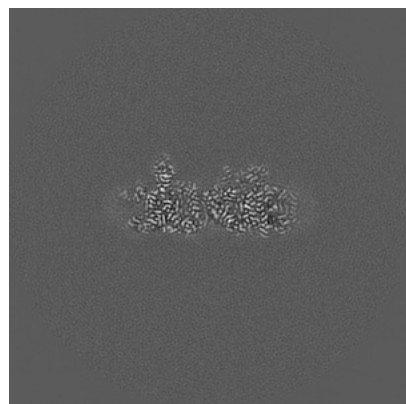


Z Index: 200

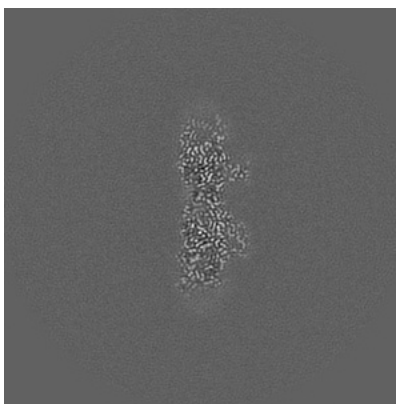
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

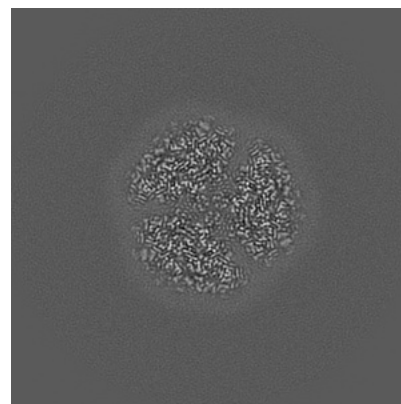
6.3.1 Primary map



X Index: 180



Y Index: 216

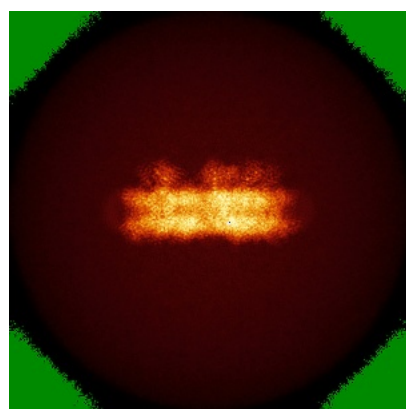


Z Index: 188

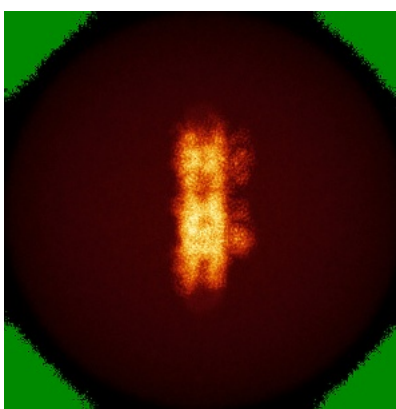
The images above show the largest variance slices of the map in three orthogonal directions.

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

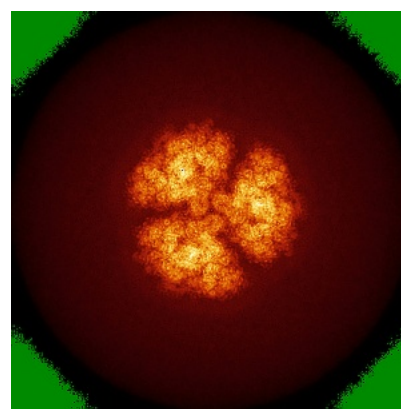
6.4.1 Primary map



X



Y

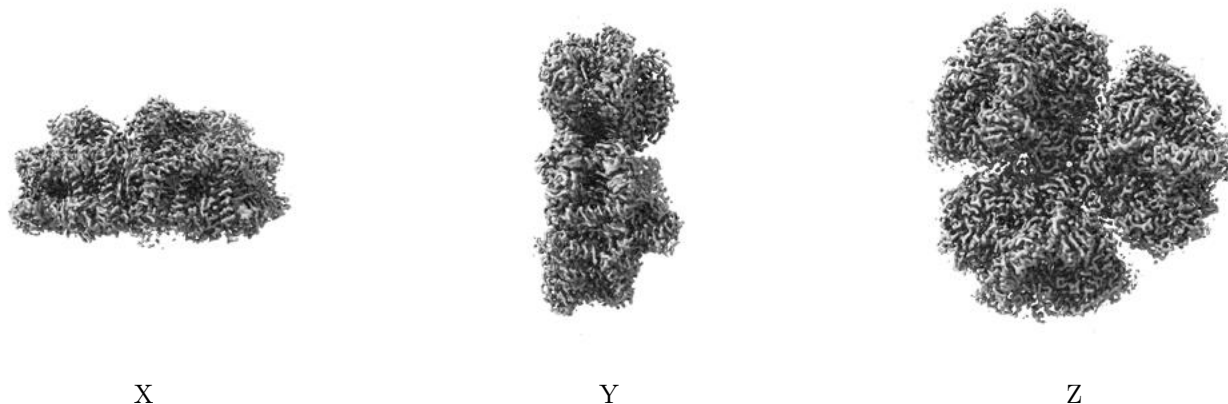


Z

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 0.0293. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

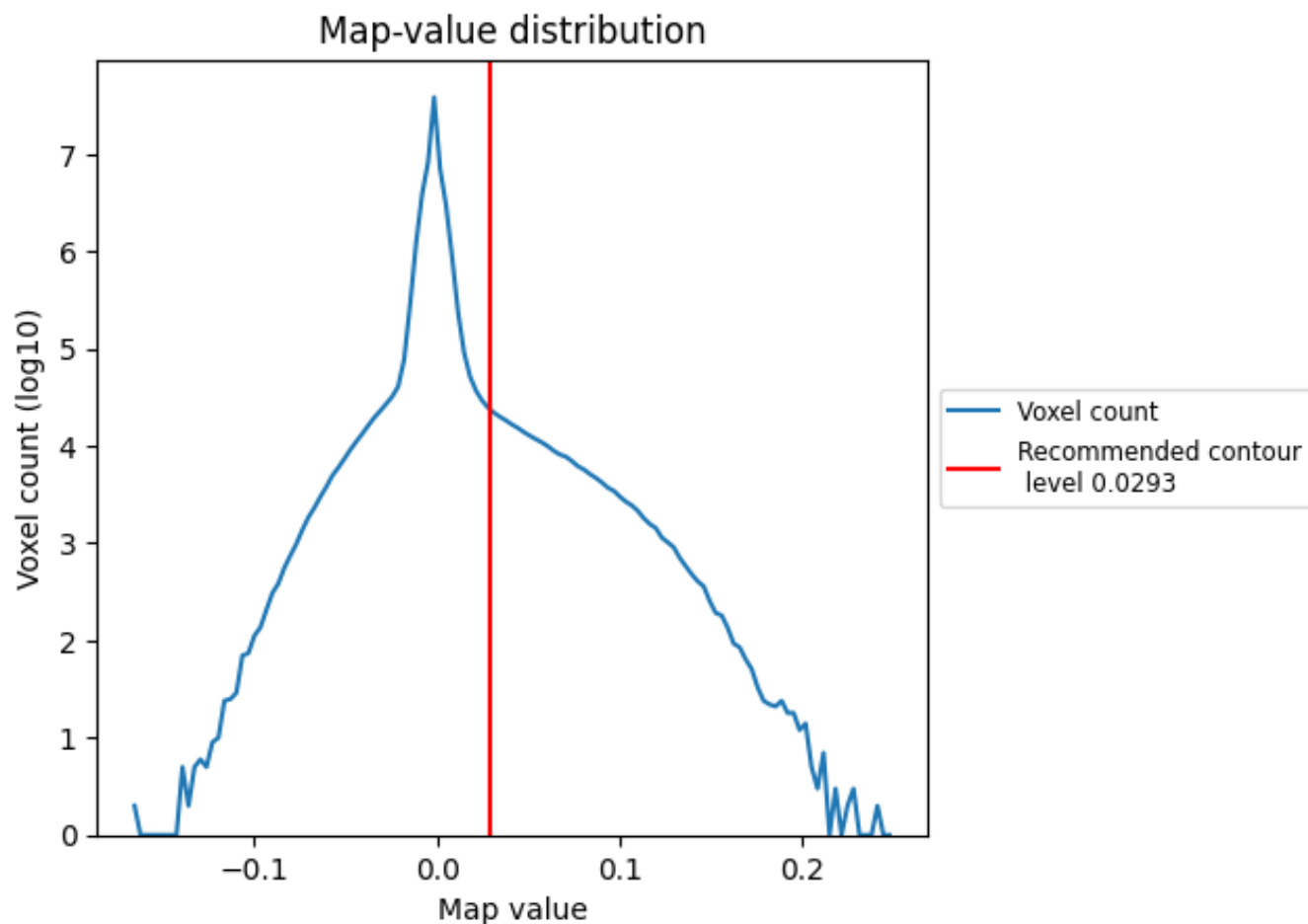
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

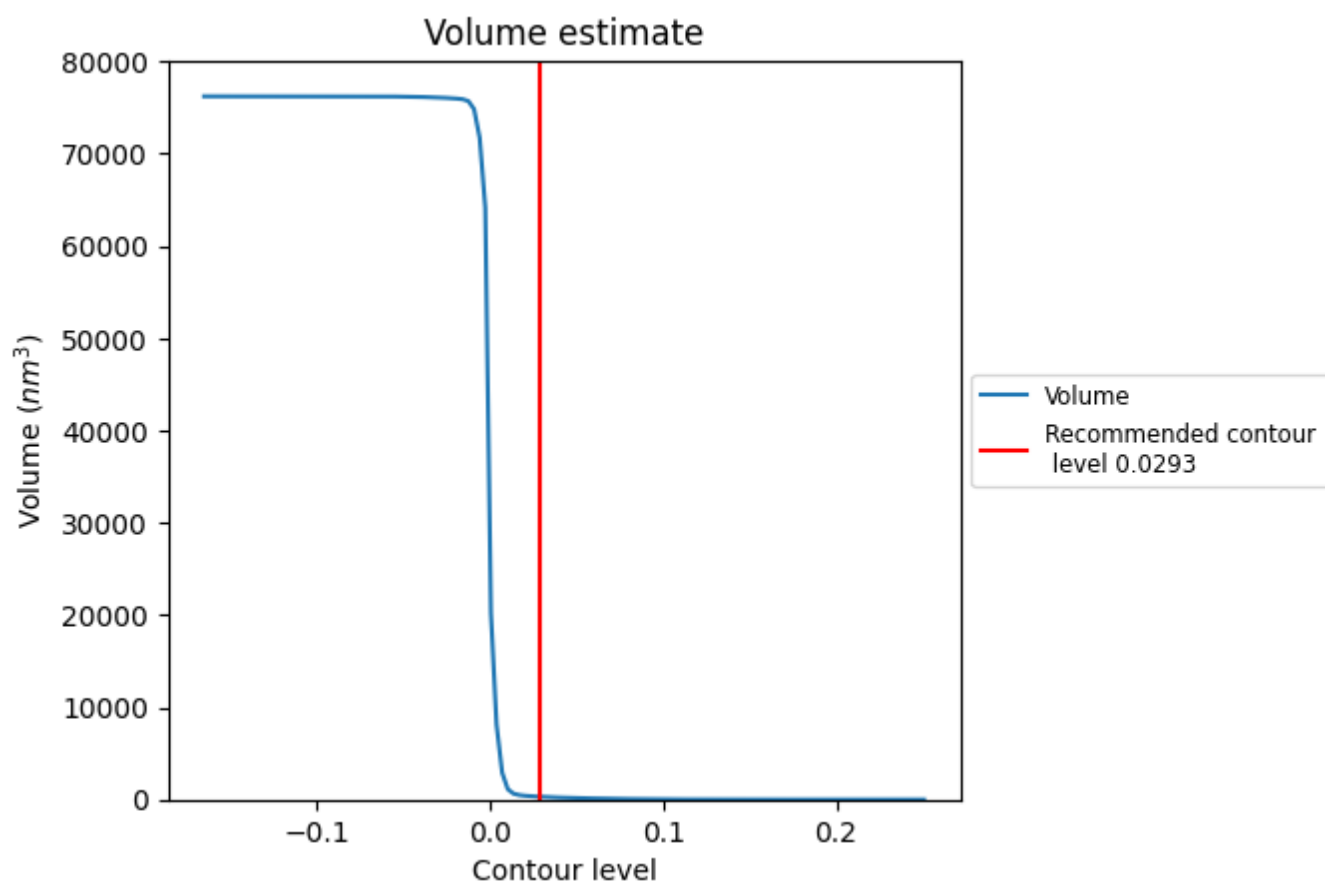
This section contains the results of statistical analysis of the map.

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.

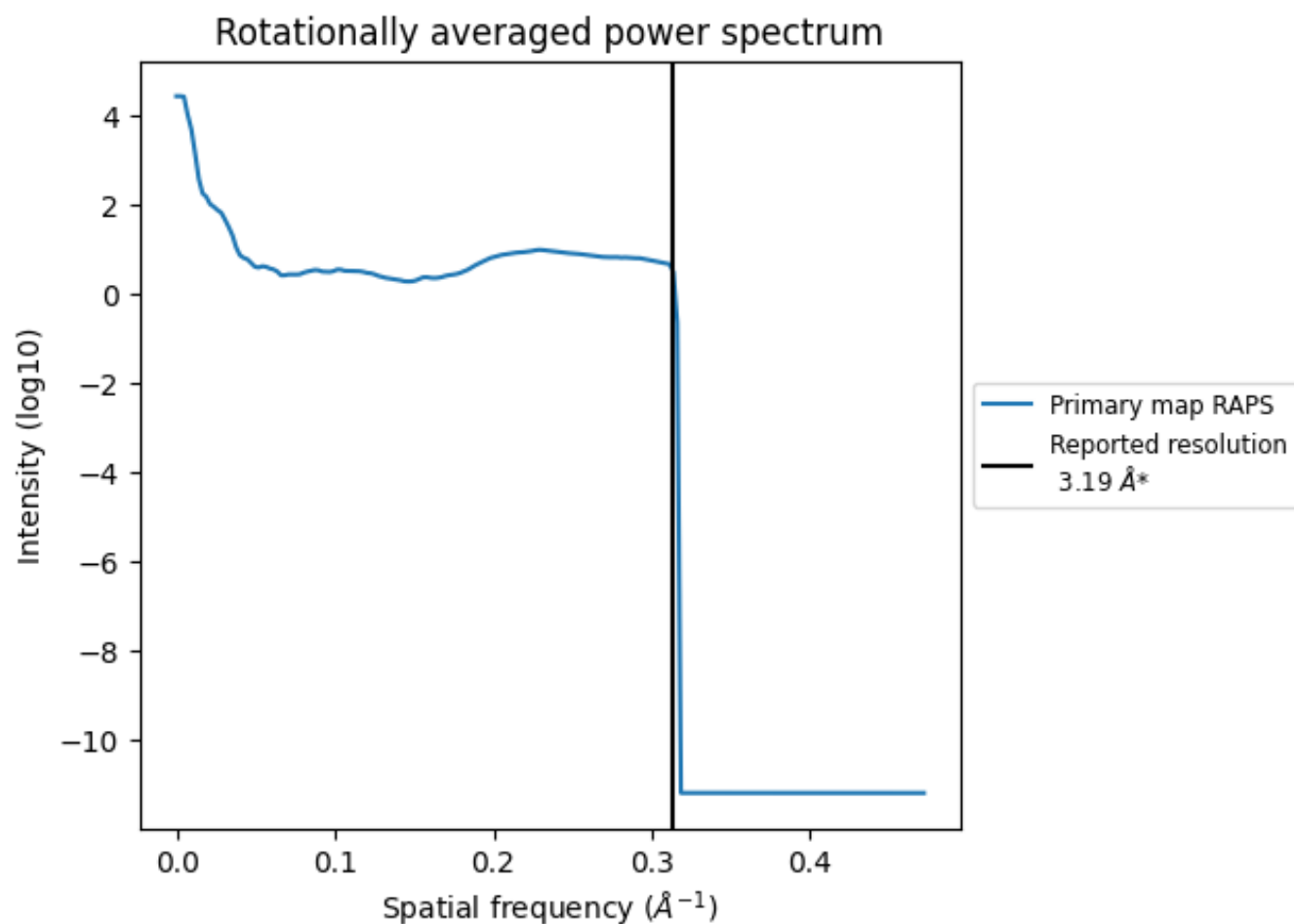
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 301 nm³; this corresponds to an approximate mass of 272 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 ⓘ

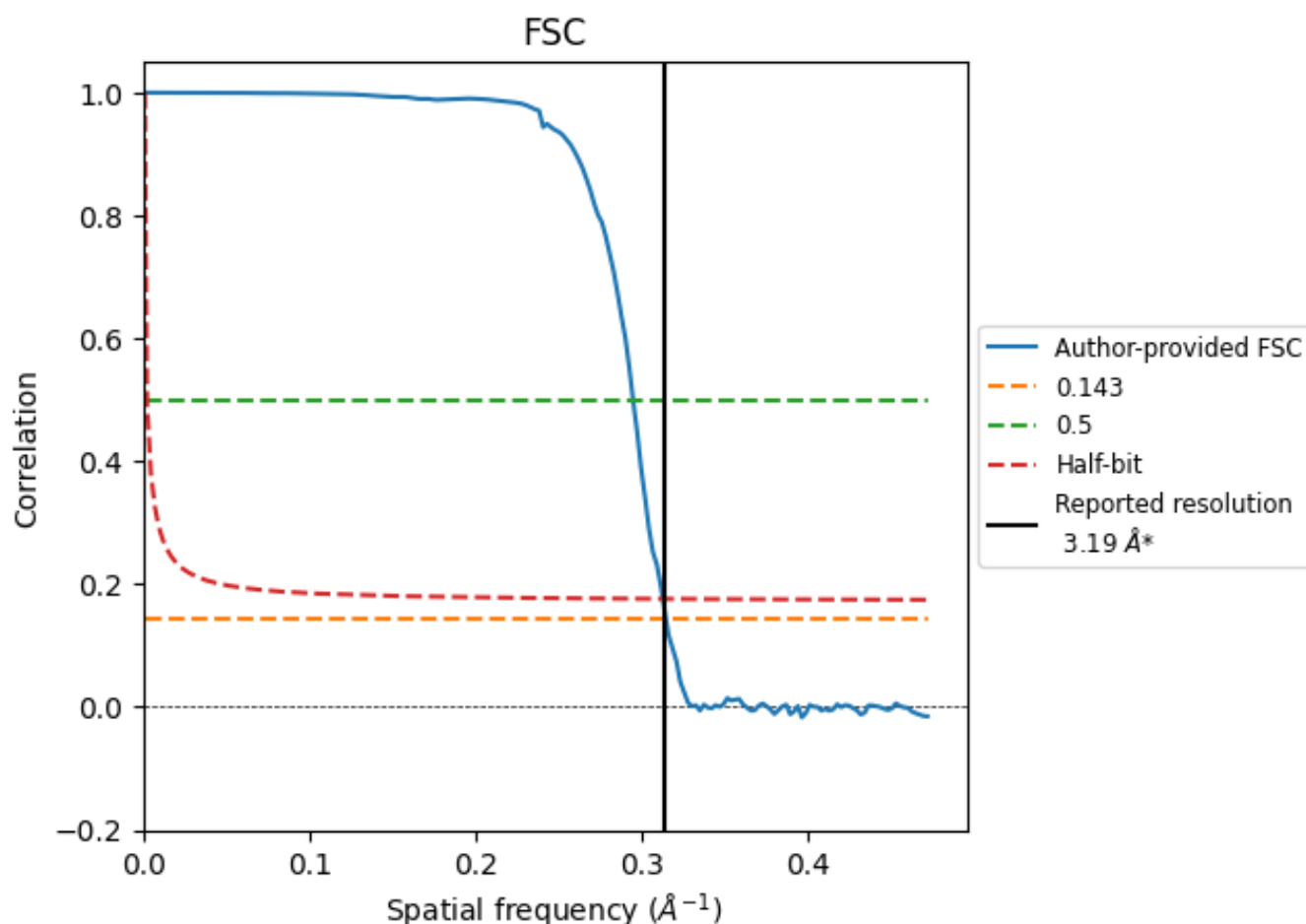


*Reported resolution corresponds to spatial frequency of 0.313 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.313 Å⁻¹

8.2 Resolution estimates [i](#)

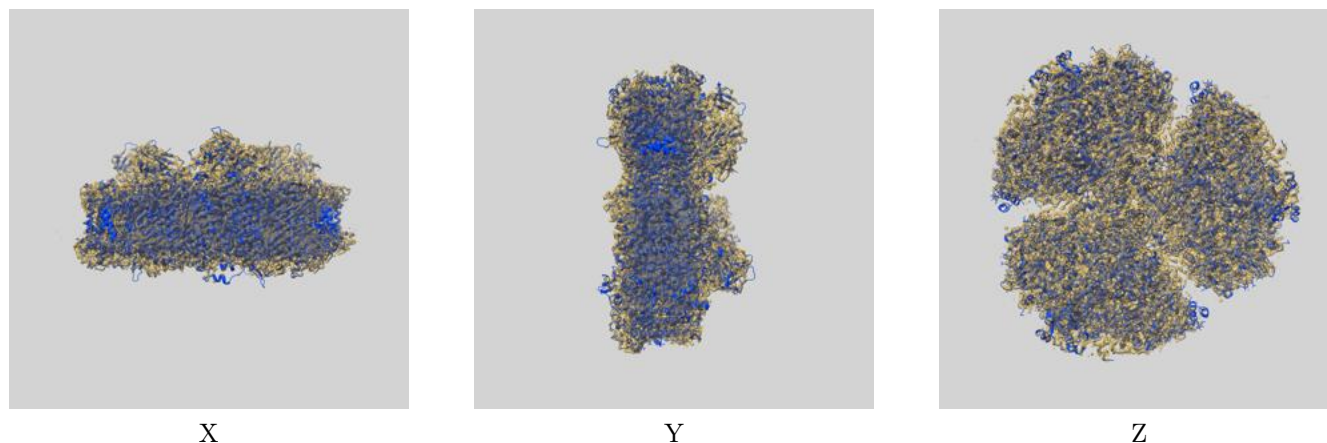
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.19	-	-
Author-provided FSC curve	3.18	3.39	3.20
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

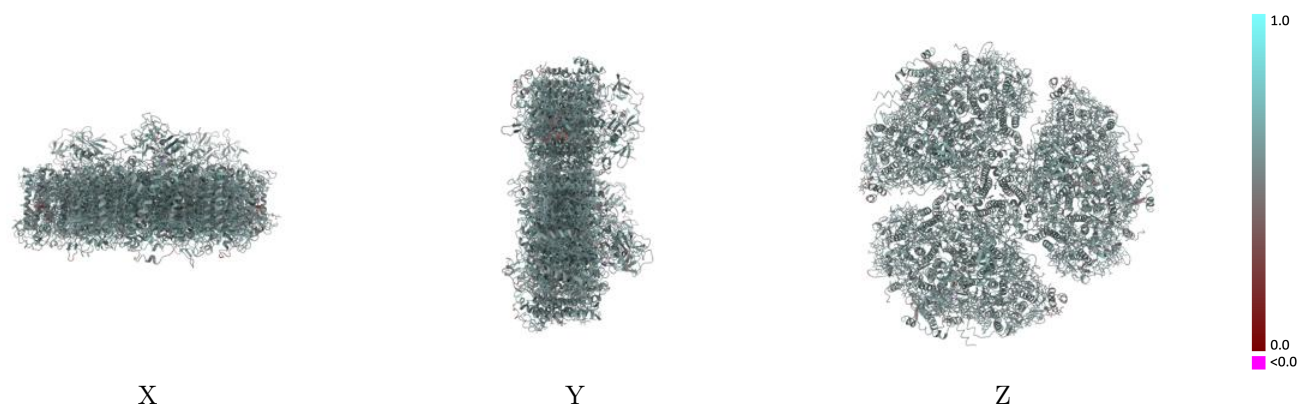
This section contains information regarding the fit between EMDB map EMD-20397 and PDB model 6PNJ. Per-residue inclusion information can be found in section 3 on page 31.

9.1 Map-model overlay [i](#)



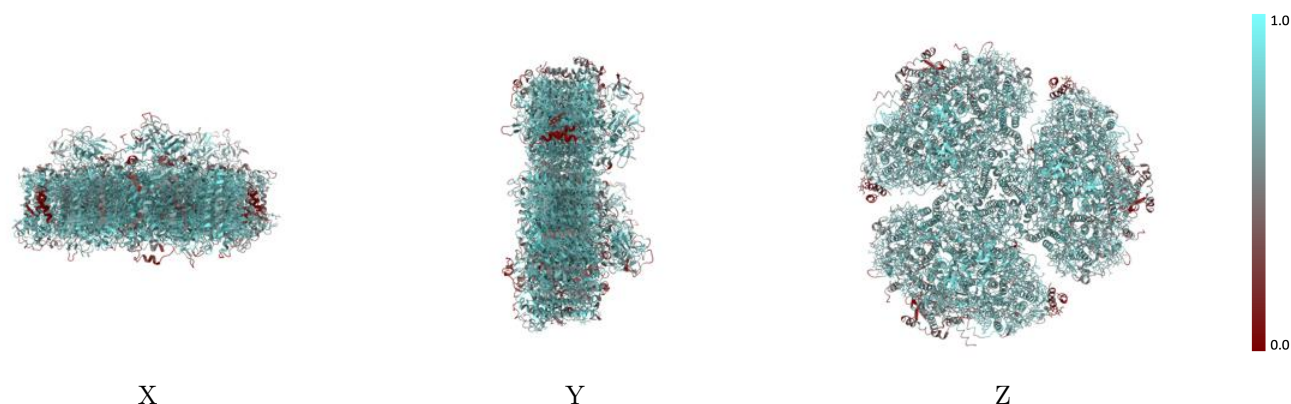
The images above show the 3D surface view of the map at the recommended contour level 0.0293 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



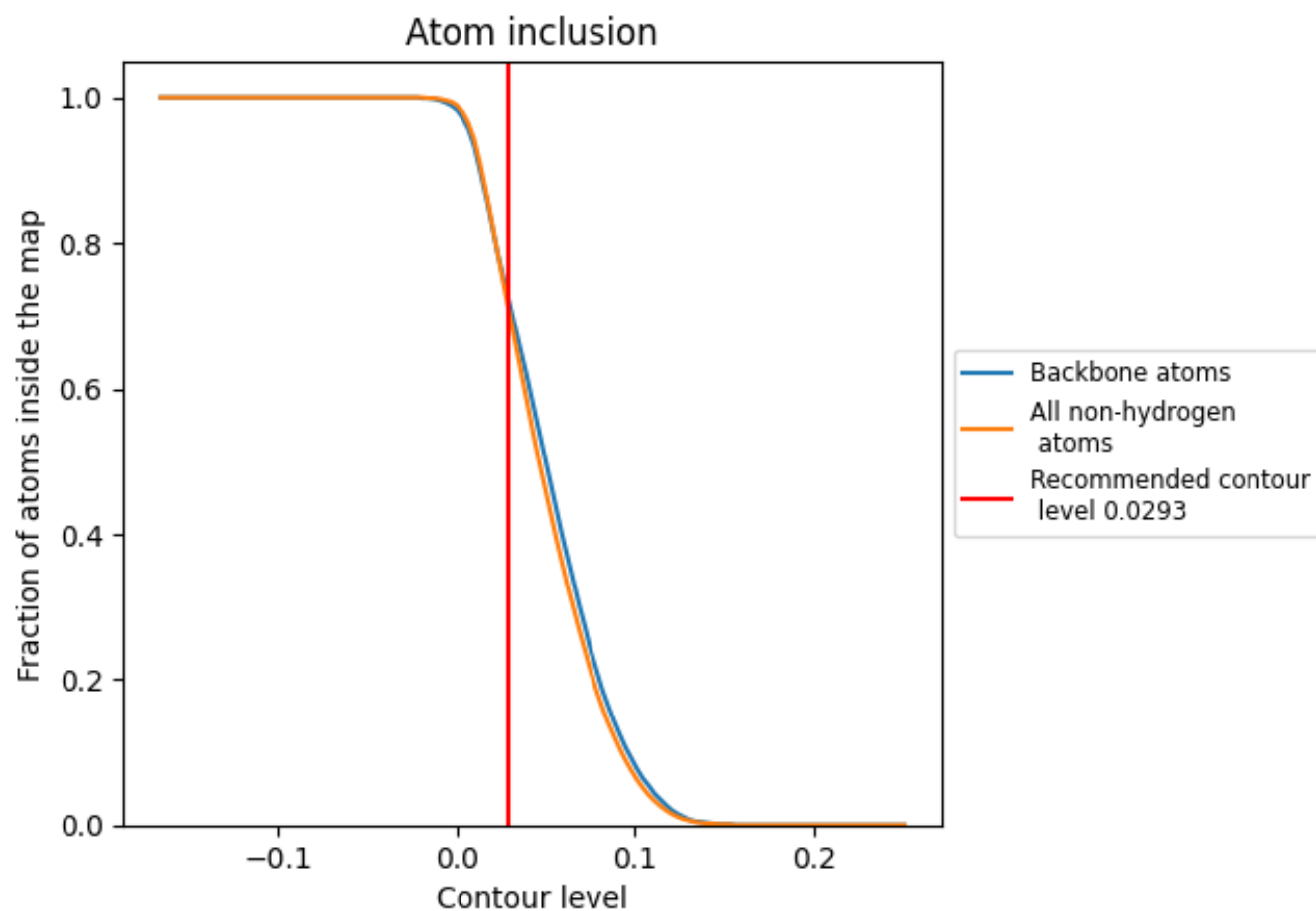
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0293).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 71% 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 (0.0293) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7110	 0.5660
A	 0.7590	 0.5750
B	 0.7530	 0.5760
C	 0.7520	 0.5500
D	 0.6200	 0.5530
E	 0.5200	 0.5330
F	 0.3820	 0.5160
G	 0.7580	 0.5750
H	 0.7530	 0.5760
I	 0.7530	 0.5820
J	 0.4310	 0.4890
K	 0.0660	 0.4440
L	 0.7380	 0.5700
M	 0.6640	 0.5450
N	 0.7440	 0.5490
O	 0.6220	 0.5540
P	 0.5200	 0.5320
Q	 0.3800	 0.5180
R	 0.7580	 0.5850
S	 0.4230	 0.4950
T	 0.0660	 0.4420
U	 0.7340	 0.5690
V	 0.6790	 0.5460
W	 0.4870	 0.5130
X	 0.5090	 0.5110
a	 0.7600	 0.5740
b	 0.7550	 0.5760
c	 0.7390	 0.5500
d	 0.6170	 0.5540
e	 0.5110	 0.5280
f	 0.3870	 0.5190
i	 0.7550	 0.5860
j	 0.4310	 0.4910
k	 0.0660	 0.4450
l	 0.7320	 0.5700



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
m	 0.6820	 0.5490
x	 0.5050	 0.5150