



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 01:45 AM UTC

PDB ID : 7LX0 / pdb_00007lx0
EMDB ID : EMD-23563
Title : Quantitative assessment of chlorophyll types in cryo-EM maps of photosystem I acclimated to far-red light
Authors : Gisriel, C.J.; Wang, J.
Deposited on : 2021-03-02
Resolution : 2.96 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.dev132
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) : 2.49

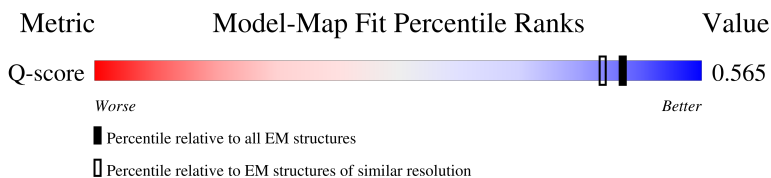
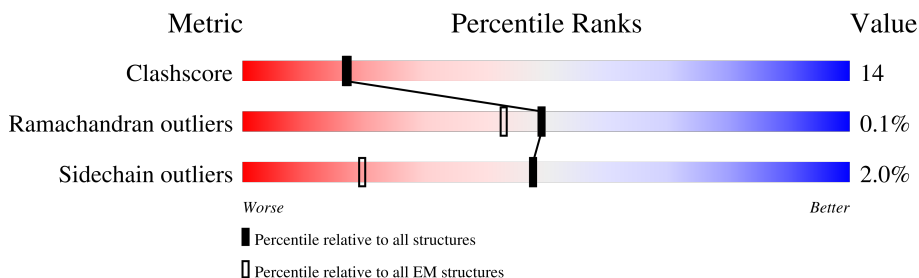
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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.



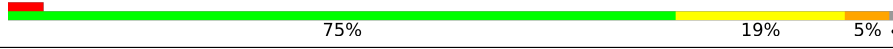
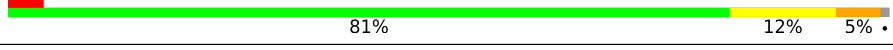
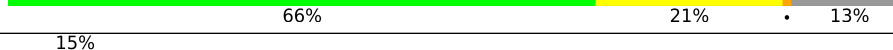
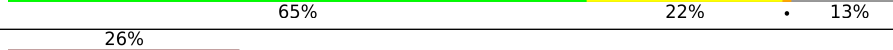
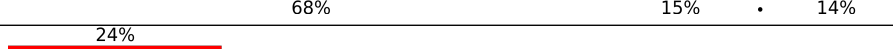
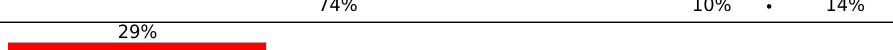
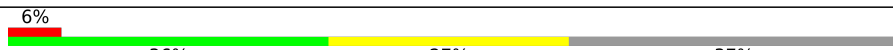
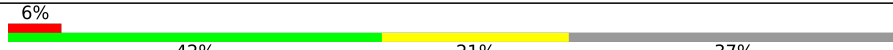
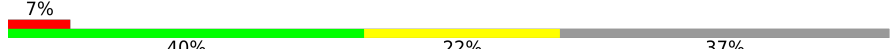
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13155 (2.46 - 3.46)

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	 6% 69% 27% 5%
1	G	788	 6% 69% 26% 5%
1	a	788	 6% 69% 27% 5%
2	B	741	 1% 72% 28%

Continued on next page...

Continued from previous page...

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	49	
9	T	49	
9	k	49	
10	L	174	
10	U	174	

Continued on next page...

Continued from previous page...

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
13	CL0	A	1011	X	-	-	-
13	CL0	G	1011	X	-	-	-
13	CL0	a	1011	X	-	-	-
14	CLA	A	1012	X	-	-	-
14	CLA	A	1013	X	-	-	-
14	CLA	A	1101	X	-	-	-
14	CLA	A	1102	X	-	-	-
14	CLA	A	1103	X	-	-	-
14	CLA	A	1104	X	-	-	-
14	CLA	A	1105	X	-	-	-
14	CLA	A	1106	X	-	-	-
14	CLA	A	1107	X	-	-	-
14	CLA	A	1108	X	-	-	-
14	CLA	A	1109	X	-	-	-
14	CLA	A	1110	X	-	-	-
14	CLA	A	1111	X	-	-	-
14	CLA	A	1112	X	-	-	-
14	CLA	A	1113	X	-	-	-
14	CLA	A	1114	X	-	-	-
14	CLA	A	1115	X	-	-	-
14	CLA	A	1116	X	-	-	-
14	CLA	A	1117	X	-	-	-
14	CLA	A	1118	X	-	-	-
14	CLA	A	1119	X	-	-	-
14	CLA	A	1120	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	1122	X	-	-	-
14	CLA	A	1123	X	-	-	-
14	CLA	A	1124	X	-	-	-
14	CLA	A	1125	X	-	-	-
14	CLA	A	1126	X	-	-	-
14	CLA	A	1127	X	-	-	-
14	CLA	A	1128	X	-	-	-
14	CLA	A	1129	X	-	-	-
14	CLA	A	1130	X	-	-	-
14	CLA	A	1131	X	-	-	-
14	CLA	A	1132	X	-	-	-
14	CLA	A	1133	X	-	-	-
14	CLA	A	1134	X	-	-	-
14	CLA	A	1135	X	-	-	-
14	CLA	A	1136	X	-	-	-
14	CLA	A	1137	X	-	-	-
14	CLA	A	1138	X	-	-	-
14	CLA	A	1139	X	-	-	-
14	CLA	A	1140	X	-	-	-
14	CLA	B	1021	X	-	-	-
14	CLA	B	1022	X	-	-	-
14	CLA	B	1023	X	-	-	-
14	CLA	B	1201	X	-	-	-
14	CLA	B	1202	X	-	-	-
14	CLA	B	1203	X	-	-	-
14	CLA	B	1204	X	-	-	-
14	CLA	B	1205	X	-	-	-
14	CLA	B	1206	X	-	-	-
14	CLA	B	1208	X	-	-	-
14	CLA	B	1209	X	-	-	-
14	CLA	B	1210	X	-	-	-
14	CLA	B	1211	X	-	-	-
14	CLA	B	1212	X	-	-	-
14	CLA	B	1213	X	-	-	-
14	CLA	B	1214	X	-	-	-
14	CLA	B	1215	X	-	-	-
14	CLA	B	1216	X	-	-	-
14	CLA	B	1217	X	-	-	-
14	CLA	B	1218	X	-	-	-
14	CLA	B	1219	X	-	-	-
14	CLA	B	1220	X	-	-	-
14	CLA	B	1221	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	1222	X	-	-	-
14	CLA	B	1223	X	-	-	-
14	CLA	B	1224	X	-	-	-
14	CLA	B	1225	X	-	-	-
14	CLA	B	1226	X	-	-	-
14	CLA	B	1227	X	-	-	-
14	CLA	B	1228	X	-	-	-
14	CLA	B	1229	X	-	-	-
14	CLA	B	1231	X	-	-	-
14	CLA	B	1232	X	-	-	-
14	CLA	B	1233	X	-	-	-
14	CLA	B	1234	X	-	-	-
14	CLA	B	1235	X	-	-	-
14	CLA	B	1236	X	-	-	-
14	CLA	B	1239	X	-	-	-
14	CLA	G	1012	X	-	-	-
14	CLA	G	1013	X	-	-	-
14	CLA	G	1101	X	-	-	-
14	CLA	G	1102	X	-	-	-
14	CLA	G	1103	X	-	-	-
14	CLA	G	1104	X	-	-	-
14	CLA	G	1105	X	-	-	-
14	CLA	G	1106	X	-	-	-
14	CLA	G	1107	X	-	-	-
14	CLA	G	1108	X	-	-	-
14	CLA	G	1109	X	-	-	-
14	CLA	G	1110	X	-	-	-
14	CLA	G	1111	X	-	-	-
14	CLA	G	1112	X	-	-	-
14	CLA	G	1113	X	-	-	-
14	CLA	G	1114	X	-	-	-
14	CLA	G	1115	X	-	-	-
14	CLA	G	1116	X	-	-	-
14	CLA	G	1117	X	-	-	-
14	CLA	G	1118	X	-	-	-
14	CLA	G	1119	X	-	-	-
14	CLA	G	1120	X	-	-	-
14	CLA	G	1122	X	-	-	-
14	CLA	G	1123	X	-	-	-
14	CLA	G	1124	X	-	-	-
14	CLA	G	1125	X	-	-	-
14	CLA	G	1126	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	G	1127	X	-	-	-
14	CLA	G	1128	X	-	-	-
14	CLA	G	1129	X	-	-	-
14	CLA	G	1130	X	-	-	-
14	CLA	G	1131	X	-	-	-
14	CLA	G	1132	X	-	-	-
14	CLA	G	1133	X	-	-	-
14	CLA	G	1134	X	-	-	-
14	CLA	G	1135	X	-	-	-
14	CLA	G	1136	X	-	-	-
14	CLA	G	1137	X	-	-	-
14	CLA	G	1138	X	-	-	-
14	CLA	G	1139	X	-	-	-
14	CLA	G	1140	X	-	-	-
14	CLA	H	1021	X	-	-	-
14	CLA	H	1022	X	-	-	-
14	CLA	H	1023	X	-	-	-
14	CLA	H	1201	X	-	-	-
14	CLA	H	1202	X	-	-	-
14	CLA	H	1203	X	-	-	-
14	CLA	H	1204	X	-	-	-
14	CLA	H	1205	X	-	-	-
14	CLA	H	1206	X	-	-	-
14	CLA	H	1208	X	-	-	-
14	CLA	H	1209	X	-	-	-
14	CLA	H	1210	X	-	-	-
14	CLA	H	1211	X	-	-	-
14	CLA	H	1212	X	-	-	-
14	CLA	H	1213	X	-	-	-
14	CLA	H	1214	X	-	-	-
14	CLA	H	1215	X	-	-	-
14	CLA	H	1216	X	-	-	-
14	CLA	H	1217	X	-	-	-
14	CLA	H	1218	X	-	-	-
14	CLA	H	1219	X	-	-	-
14	CLA	H	1220	X	-	-	-
14	CLA	H	1221	X	-	-	-
14	CLA	H	1222	X	-	-	-
14	CLA	H	1223	X	-	-	-
14	CLA	H	1224	X	-	-	-
14	CLA	H	1225	X	-	-	-
14	CLA	H	1226	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	H	1227	X	-	-	-
14	CLA	H	1228	X	-	-	-
14	CLA	H	1229	X	-	-	-
14	CLA	H	1231	X	-	-	-
14	CLA	H	1232	X	-	-	-
14	CLA	H	1233	X	-	-	-
14	CLA	H	1234	X	-	-	-
14	CLA	H	1235	X	-	-	-
14	CLA	H	1236	X	-	-	-
14	CLA	H	1239	X	-	-	-
14	CLA	K	1401	X	-	-	-
14	CLA	L	1501	X	-	-	-
14	CLA	L	1502	X	-	-	-
14	CLA	L	1503	X	-	-	-
14	CLA	T	1401	X	-	-	-
14	CLA	U	1501	X	-	-	-
14	CLA	U	1502	X	-	-	-
14	CLA	U	1503	X	-	-	-
14	CLA	W	1701	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	a	1012	X	-	-	-
14	CLA	a	1013	X	-	-	-
14	CLA	a	1101	X	-	-	-
14	CLA	a	1102	X	-	-	-
14	CLA	a	1103	X	-	-	-
14	CLA	a	1104	X	-	-	-
14	CLA	a	1105	X	-	-	-
14	CLA	a	1106	X	-	-	-
14	CLA	a	1107	X	-	-	-
14	CLA	a	1108	X	-	-	-
14	CLA	a	1109	X	-	-	-
14	CLA	a	1110	X	-	-	-
14	CLA	a	1111	X	-	-	-
14	CLA	a	1112	X	-	-	-
14	CLA	a	1113	X	-	-	-
14	CLA	a	1114	X	-	-	-
14	CLA	a	1115	X	-	-	-
14	CLA	a	1116	X	-	-	-
14	CLA	a	1117	X	-	-	-
14	CLA	a	1118	X	-	-	-
14	CLA	a	1119	X	-	-	-
14	CLA	a	1120	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	1122	X	-	-	-
14	CLA	a	1123	X	-	-	-
14	CLA	a	1124	X	-	-	-
14	CLA	a	1125	X	-	-	-
14	CLA	a	1126	X	-	-	-
14	CLA	a	1127	X	-	-	-
14	CLA	a	1128	X	-	-	-
14	CLA	a	1129	X	-	-	-
14	CLA	a	1130	X	-	-	-
14	CLA	a	1131	X	-	-	-
14	CLA	a	1132	X	-	-	-
14	CLA	a	1133	X	-	-	-
14	CLA	a	1134	X	-	-	-
14	CLA	a	1135	X	-	-	-
14	CLA	a	1136	X	-	-	-
14	CLA	a	1137	X	-	-	-
14	CLA	a	1138	X	-	-	-
14	CLA	a	1139	X	-	-	-
14	CLA	a	1140	X	-	-	-
14	CLA	b	1021	X	-	-	-
14	CLA	b	1022	X	-	-	-
14	CLA	b	1023	X	-	-	-
14	CLA	b	1201	X	-	-	-
14	CLA	b	1202	X	-	-	-
14	CLA	b	1203	X	-	-	-
14	CLA	b	1204	X	-	-	-
14	CLA	b	1205	X	-	-	-
14	CLA	b	1206	X	-	-	-
14	CLA	b	1208	X	-	-	-
14	CLA	b	1209	X	-	-	-
14	CLA	b	1210	X	-	-	-
14	CLA	b	1211	X	-	-	-
14	CLA	b	1212	X	-	-	-
14	CLA	b	1213	X	-	-	-
14	CLA	b	1214	X	-	-	-
14	CLA	b	1215	X	-	-	-
14	CLA	b	1216	X	-	-	-
14	CLA	b	1217	X	-	-	-
14	CLA	b	1218	X	-	-	-
14	CLA	b	1219	X	-	-	-
14	CLA	b	1220	X	-	-	-
14	CLA	b	1221	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	1222	X	-	-	-
14	CLA	b	1223	X	-	-	-
14	CLA	b	1224	X	-	-	-
14	CLA	b	1225	X	-	-	-
14	CLA	b	1226	X	-	-	-
14	CLA	b	1227	X	-	-	-
14	CLA	b	1228	X	-	-	-
14	CLA	b	1229	X	-	-	-
14	CLA	b	1231	X	-	-	-
14	CLA	b	1232	X	-	-	-
14	CLA	b	1233	X	-	-	-
14	CLA	b	1234	X	-	-	-
14	CLA	b	1235	X	-	-	-
14	CLA	b	1236	X	-	-	-
14	CLA	b	1239	X	-	-	-
14	CLA	k	1401	X	-	-	-
14	CLA	l	1501	X	-	-	-
14	CLA	l	1502	X	-	-	-
14	CLA	l	1503	X	-	-	-
14	CLA	x	1701	X	-	-	-
15	F6C	A	1121	X	-	-	-
15	F6C	B	1207	X	-	-	-
15	F6C	B	1230	X	-	-	-
15	F6C	B	1237	X	-	-	-
15	F6C	B	1238	X	-	-	-
15	F6C	G	1121	X	-	-	-
15	F6C	H	1207	X	-	-	-
15	F6C	H	1230	X	-	-	-
15	F6C	H	1237	X	-	-	-
15	F6C	H	1238	X	-	-	-
15	F6C	a	1121	X	-	-	-
15	F6C	b	1207	X	-	-	-
15	F6C	b	1230	X	-	-	-
15	F6C	b	1237	X	-	-	-
15	F6C	b	1238	X	-	-	-

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 72462 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	G	751	Total	C	N	O	S	0	0
			5931	3892	1013	993	33		
1	a	751	Total	C	N	O	S	0	0
			5931	3892	1013	993	33		
1	A	751	Total	C	N	O	S	0	0
			5931	3892	1013	993	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	739	Total	C	N	O	S	0	0
			5913	3896	997	1002	18		
2	b	739	Total	C	N	O	S	0	0
			5913	3896	997	1002	18		
2	B	739	Total	C	N	O	S	0	0
			5913	3896	997	1002	18		

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	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	P	62	Total	C	N	O		0	0
			497	313	88	96			
5	e	62	Total	C	N	O		0	0
			497	313	88	96			
5	E	62	Total	C	N	O		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	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		
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	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		
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
R	1	MET	-	initiating methionine	UNP A0A2N6MR25
i	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	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		
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	T	44	Total	C	N	O	S	0	0
			253	161	46	45	1		
9	k	44	Total	C	N	O	S	0	0
			253	161	46	45	1		
9	K	44	Total	C	N	O	S	0	0
			253	161	46	45	1		

- Molecule 10 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	163	Total	C	N	O	S	0	0
			1227	792	207	223	5		
10	l	163	Total	C	N	O	S	0	0
			1227	792	207	223	5		
10	L	163	Total	C	N	O	S	0	0
			1227	792	207	223	5		

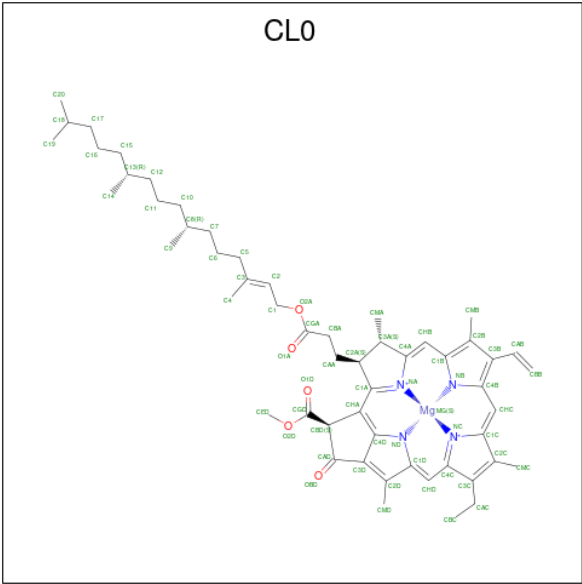
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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

- Molecule 12 is a protein called Photosystem one PsaX.

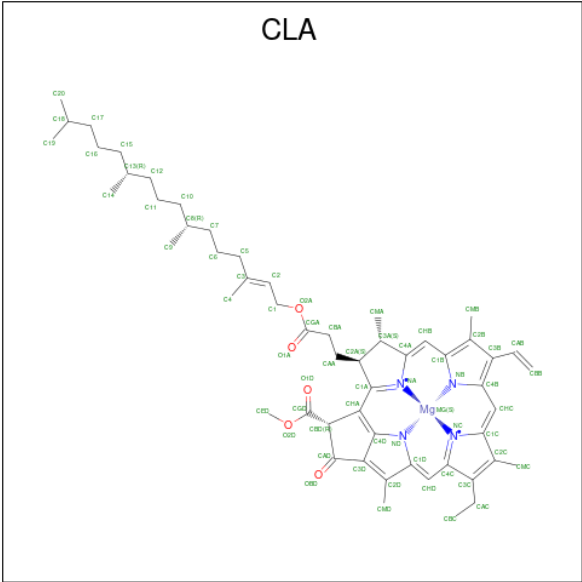
Mol	Chain	Residues	Atoms				AltConf	Trace
12	W	29	Total	C	N	O	0	0
			246	172	36	38		
12	x	29	Total	C	N	O	0	0
			246	172	36	38		
12	X	29	Total	C	N	O	0	0
			246	172	36	38		

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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 50	C 40	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
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 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 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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 50	C 40	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 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 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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 50	C 40	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 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 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

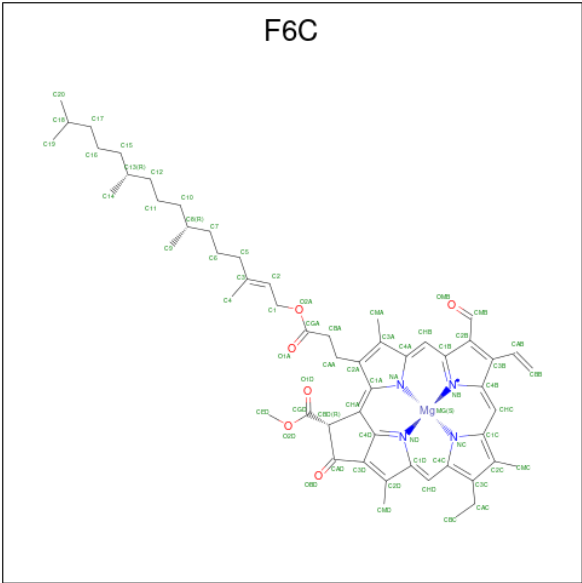
Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 15 is Chlorophyll F (CCD ID: F6C) (formula: C₅₅H₆₈MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



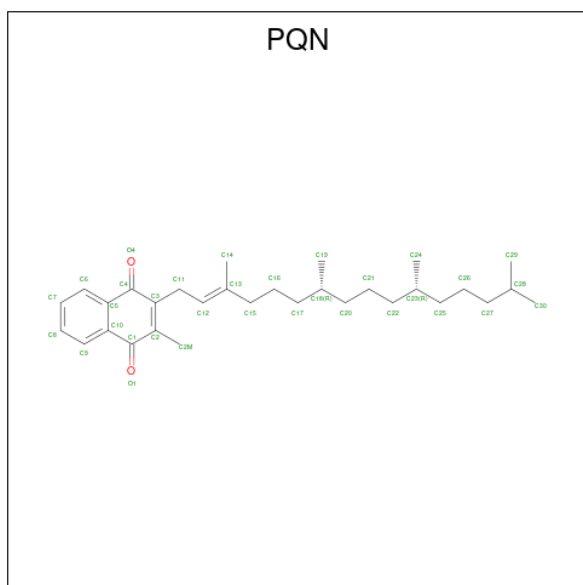
Mol	Chain	Residues	Atoms					AltConf
15	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

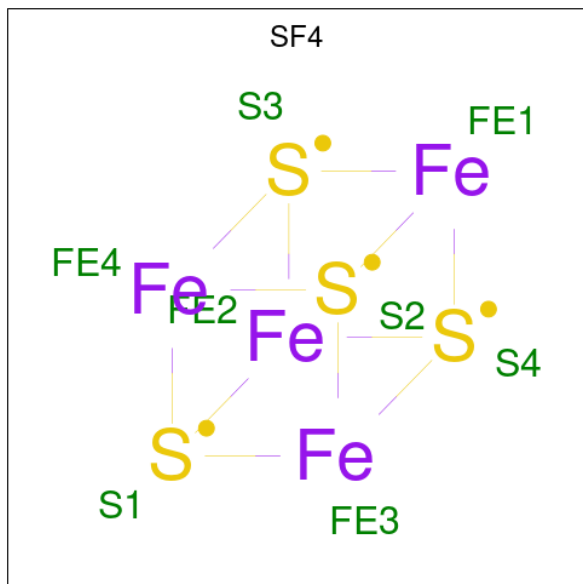
Mol	Chain	Residues	Atoms					AltConf
15	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			66	55	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
			66	55	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 16 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
16	G	1	Total	C	O	0
			33	31	2	
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	
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: Fe_4S_4).



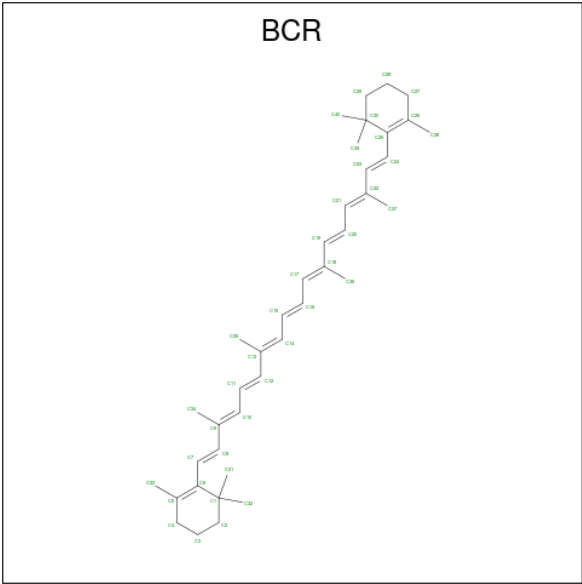
Mol	Chain	Residues	Atoms			AltConf
17	G	1	Total	Fe	S	0
			8	4	4	
17	N	1	Total	Fe	S	0
			8	4	4	
17	N	1	Total	Fe	S	0
			8	4	4	
17	a	1	Total	Fe	S	0
			8	4	4	
17	c	1	Total	Fe	S	0
			8	4	4	
17	c	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

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	

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



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
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	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

Continued on next page...

Continued from previous page...

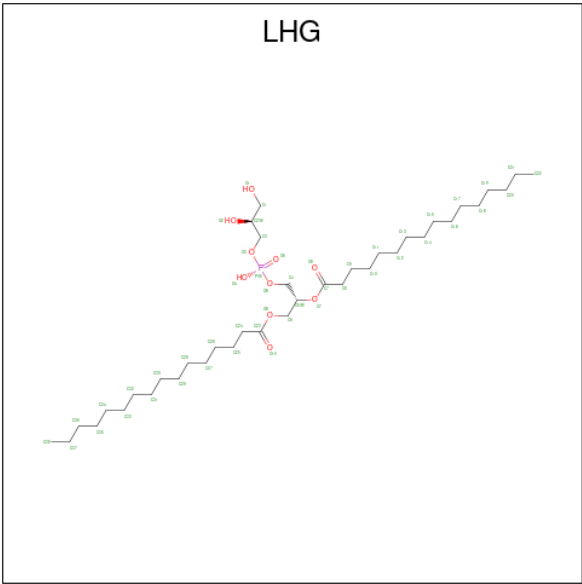
Mol	Chain	Residues	Atoms	AltConf
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	i	1	Total C 40 40	0
18	i	1	Total C 40 40	0
18	l	1	Total C 40 40	0
18	l	1	Total C 40 40	0
18	m	1	Total C 40 40	0
18	A	1	Total C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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
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	
18	B	1	Total	C	0
			40	40	
18	I	1	Total	C	0
			40	40	
18	I	1	Total	C	0
			40	40	
18	L	1	Total	C	0
			40	40	
18	L	1	Total	C	0
			40	40	
18	M	1	Total	C	0
			40	40	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



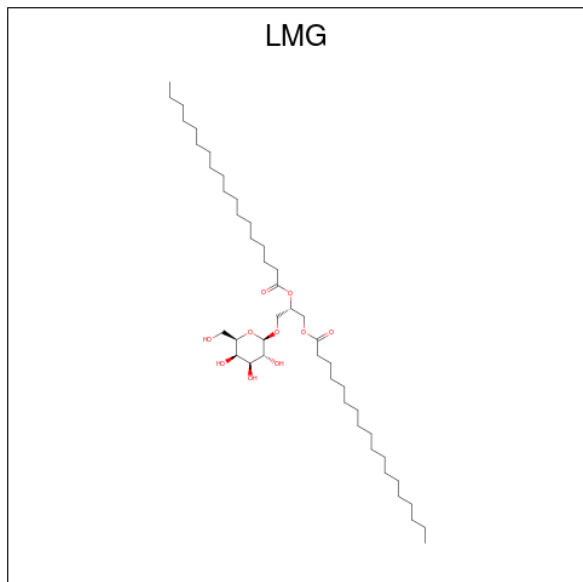
Mol	Chain	Residues	Atoms				AltConf
19	G	1	Total	C	O	P	0
			42	31	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
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	
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: $C_{45}H_{86}O_{10}$).



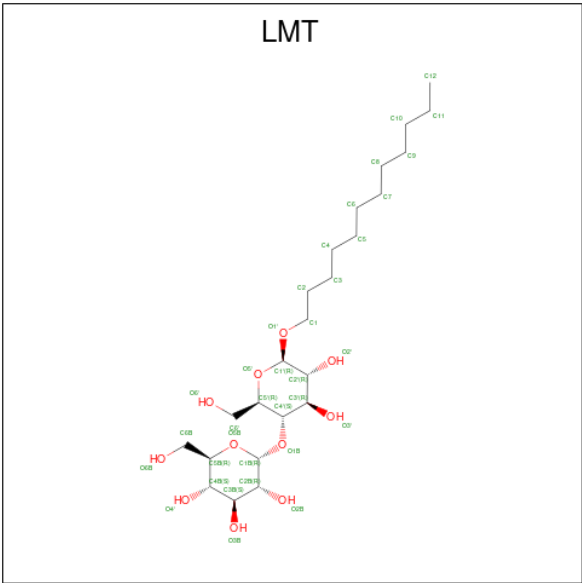
Mol	Chain	Residues	Atoms				AltConf
20	G	1	Total	C	O		0
			46	36	10		
20	H	1	Total	C	O		0
			46	36	10		
20	R	1	Total	C	O		0
			37	27	10		
20	U	1	Total	C	O		0
			50	40	10		
20	a	1	Total	C	O		0
			46	36	10		
20	b	1	Total	C	O		0
			46	36	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
20	i	1	Total	C	O	0
			37	27	10	
20	l	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	G	1	Total	C	O	0
			31	20	11	
21	G	1	Total	C	O	0
			28	17	11	
21	a	1	Total	C	O	0
			31	20	11	
21	a	1	Total	C	O	0
			28	17	11	
21	A	1	Total	C	O	0
			31	20	11	

Continued on next page...

Continued from previous page...

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

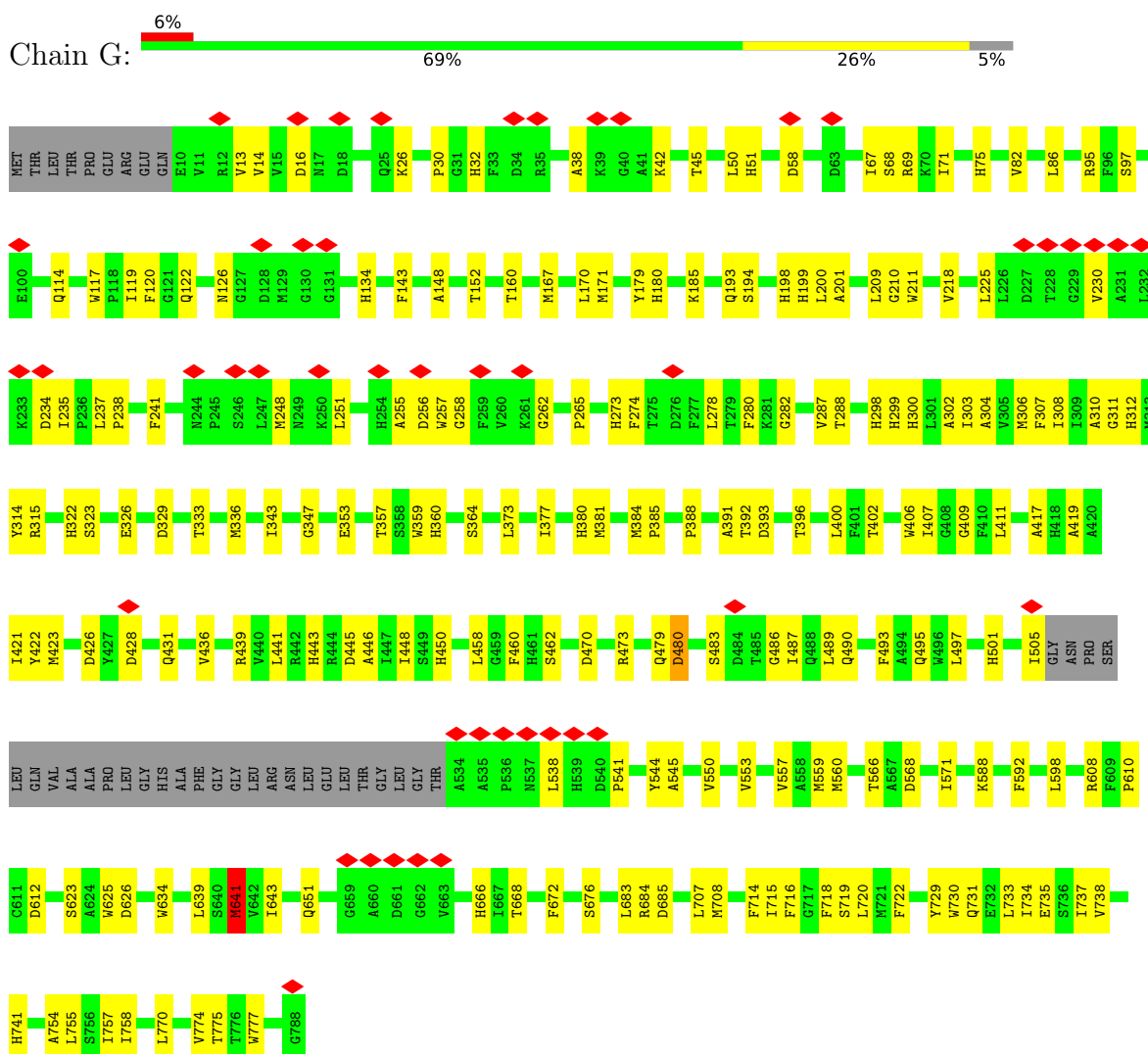
- Molecule 22 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

3 Residue-property plots

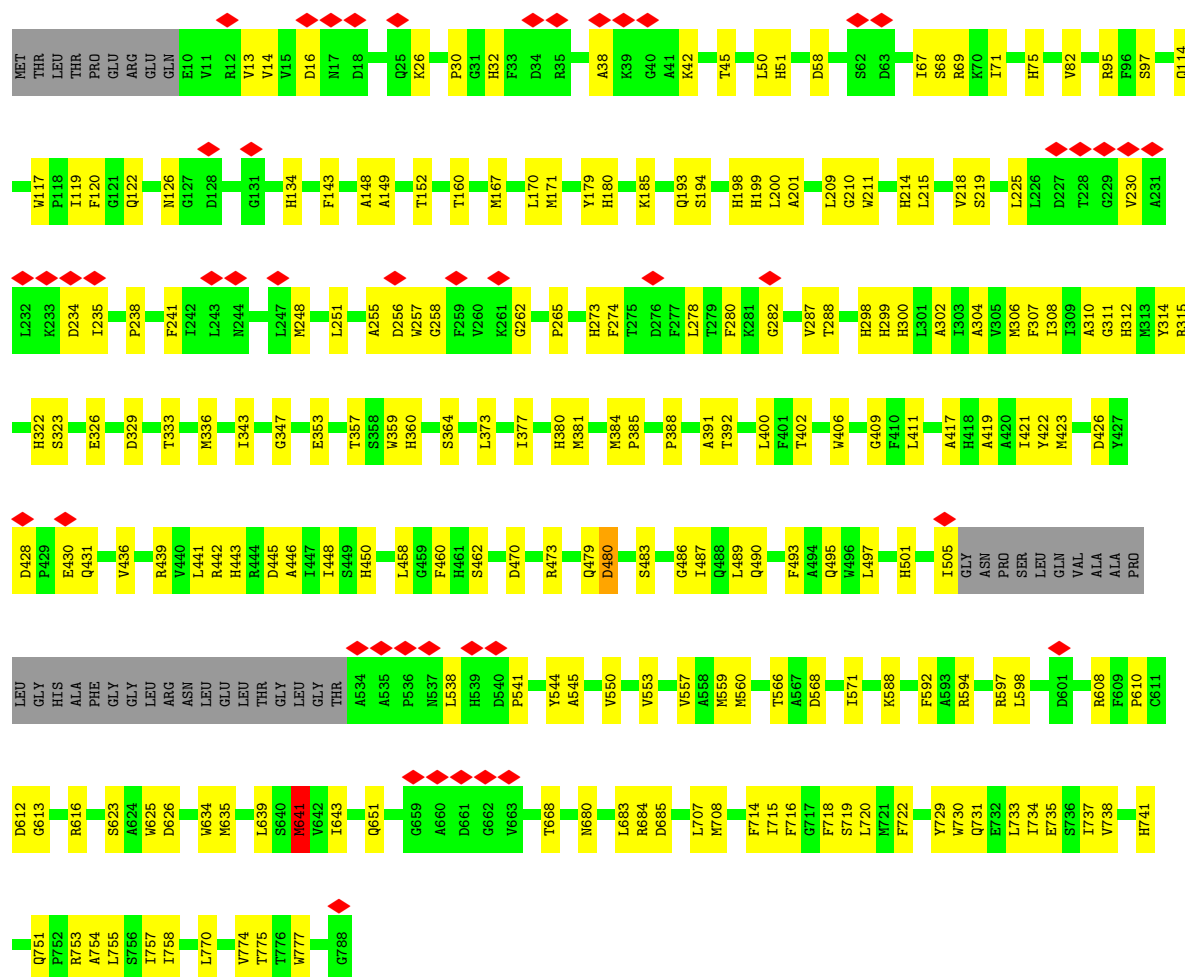
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

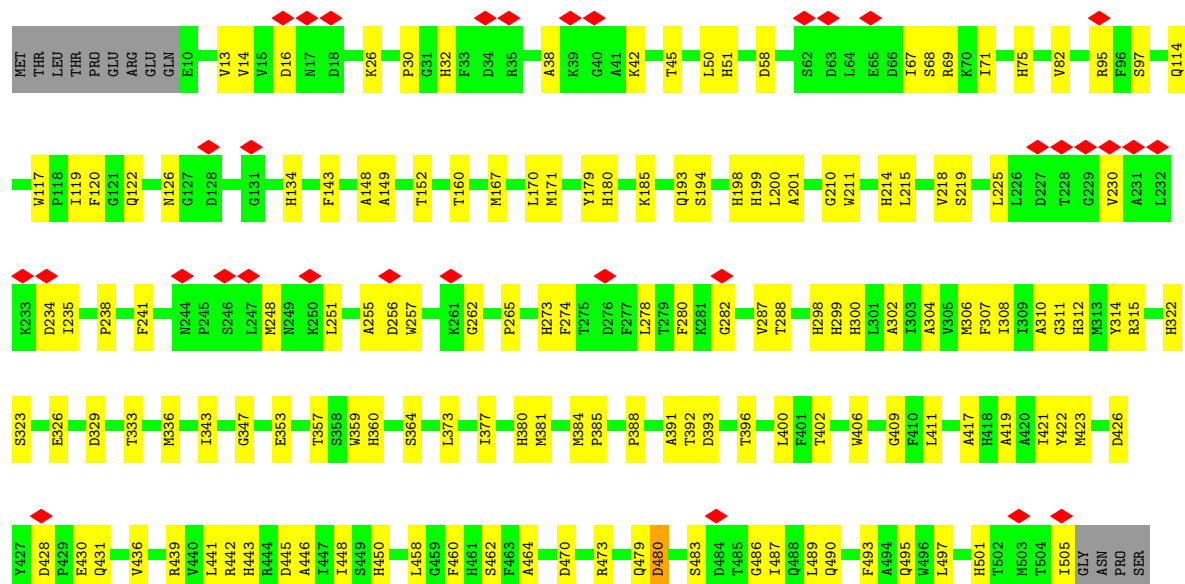


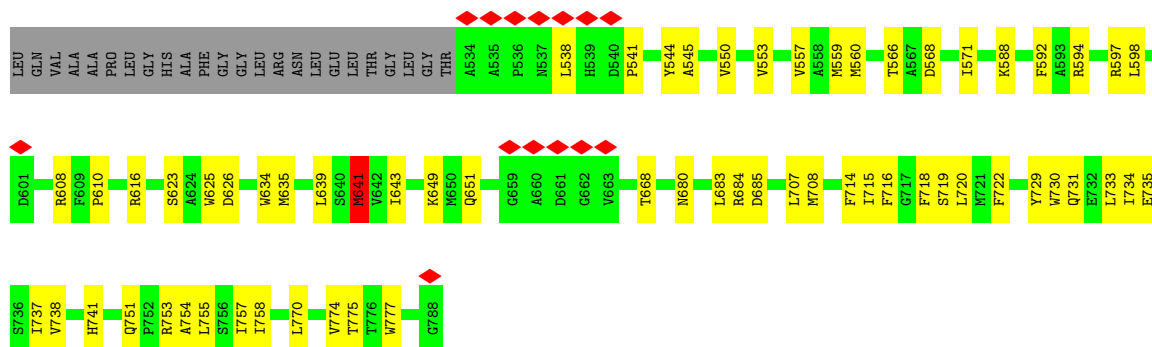
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





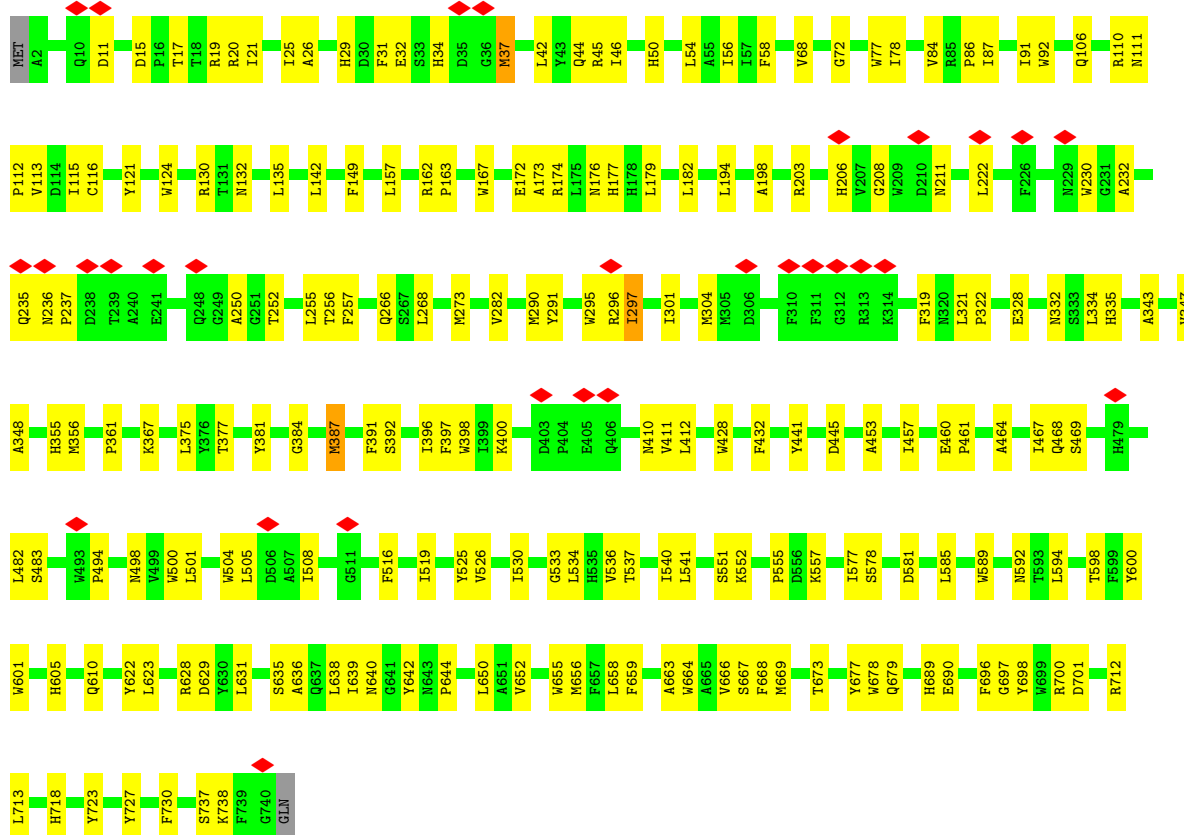
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





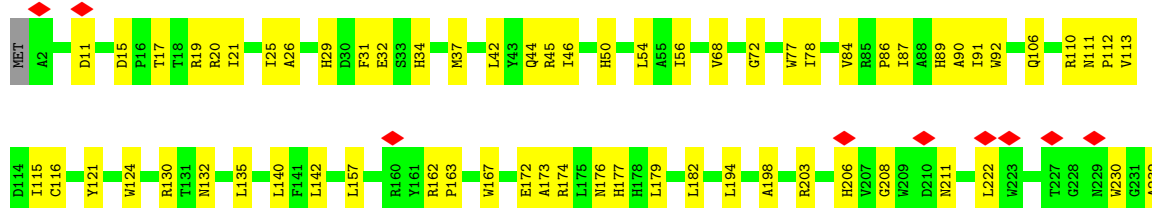
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

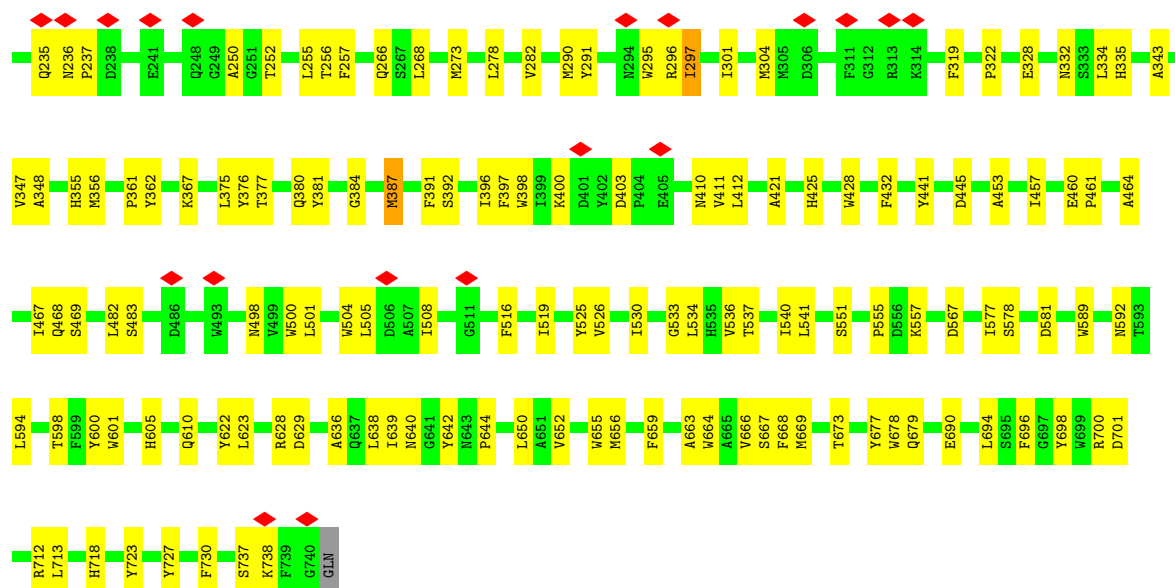
Chain H: 72% 27%



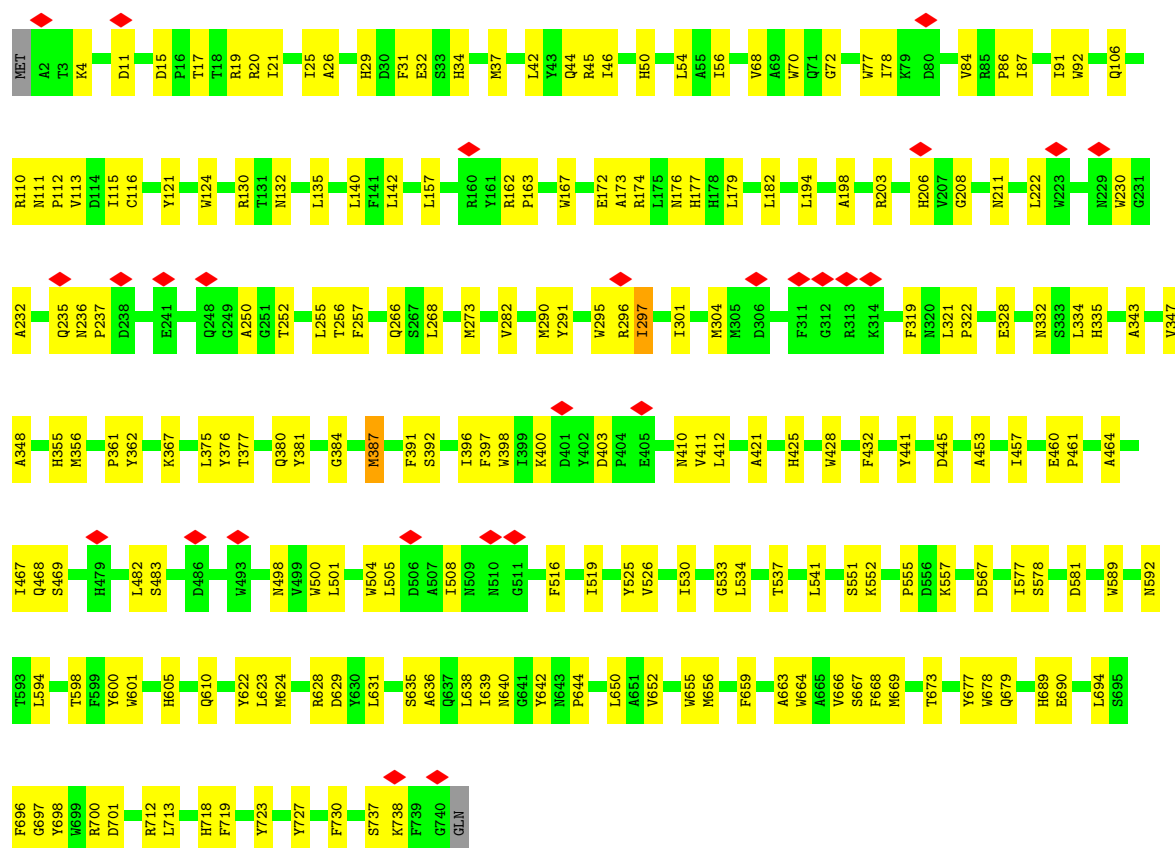
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 72% 27%

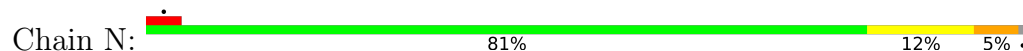




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

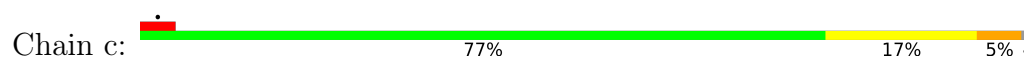


• Molecule 3: Photosystem I iron-sulfur center

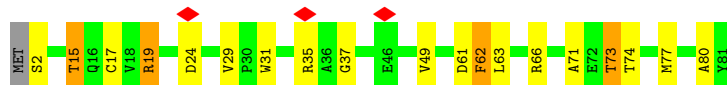
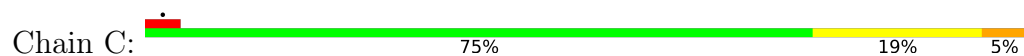




- Molecule 3: Photosystem I iron-sulfur center



- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I protein Psad

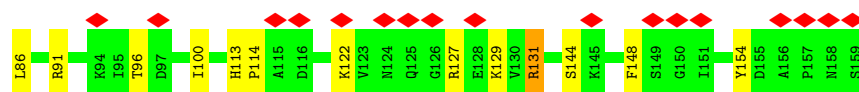


- Molecule 4: Photosystem I protein Psad

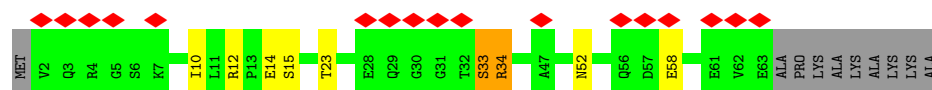
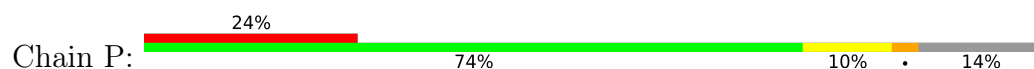


- Molecule 4: Photosystem I protein Psad

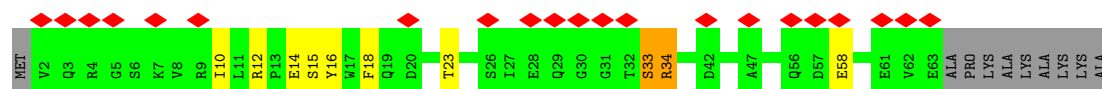




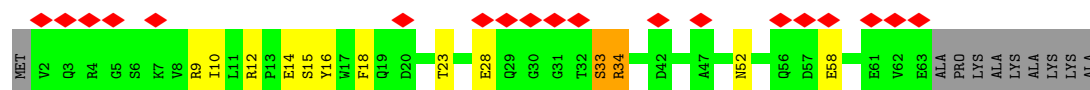
• Molecule 5: Photosystem I reaction center subunit IV



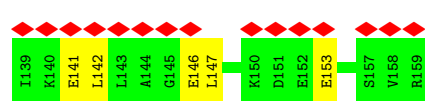
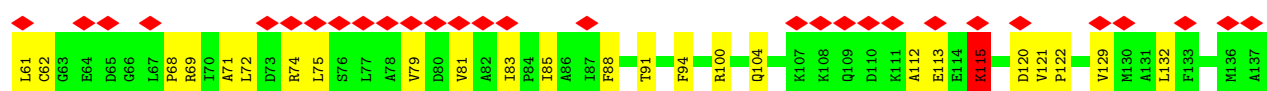
• Molecule 5: Photosystem I reaction center subunit IV



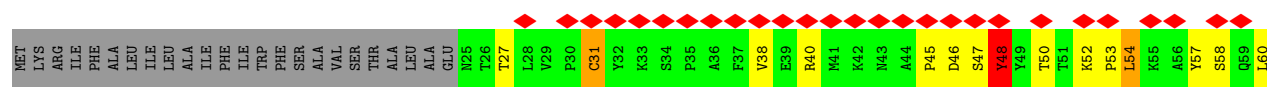
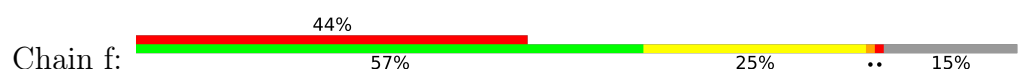
• Molecule 5: Photosystem I reaction center subunit IV

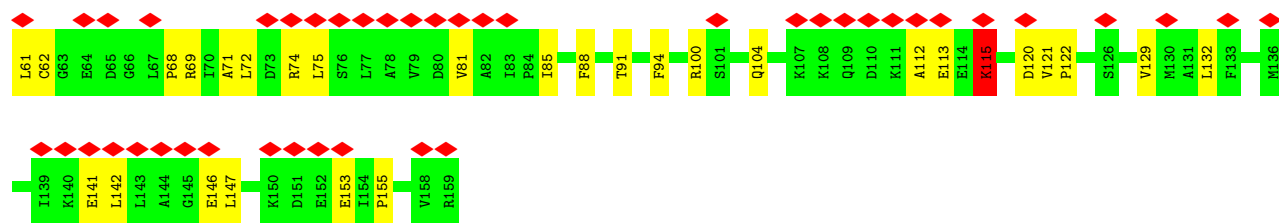


• Molecule 6: Photosystem I reaction center protein PsaF subunit III

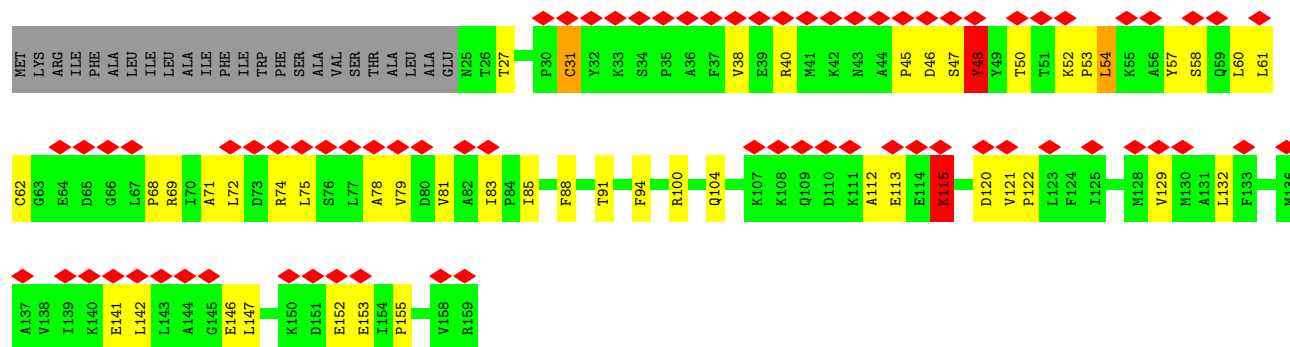


• Molecule 6: Photosystem I reaction center protein PsaF subunit III

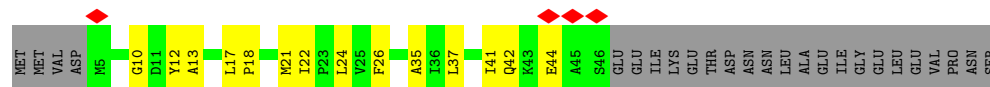
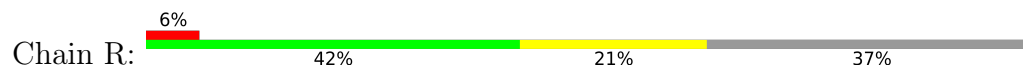




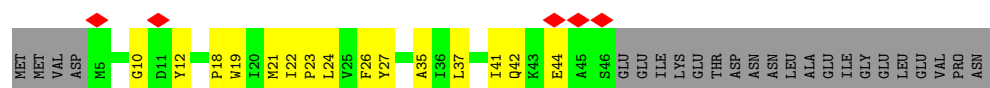
• Molecule 6: Photosystem I reaction center protein PsaF subunit III



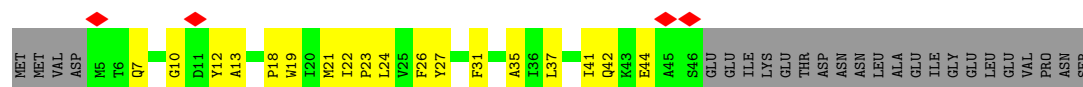
• Molecule 7: photosystem I subunit VIII



• Molecule 7: photosystem I subunit VIII

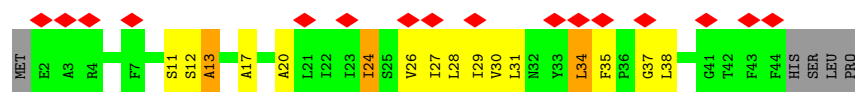


• Molecule 7: photosystem I subunit VIII

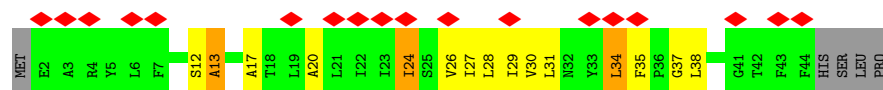
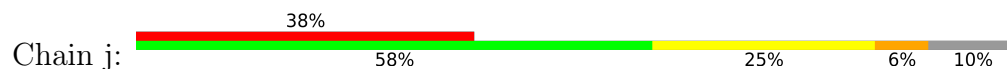


• Molecule 8: Photosystem I reaction centre subunit IX / PsaJ

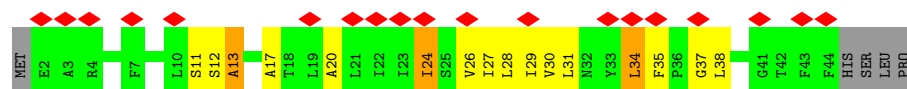




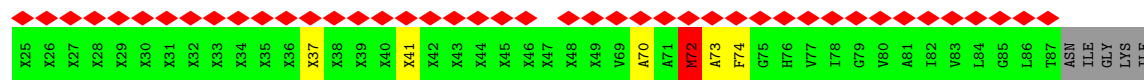
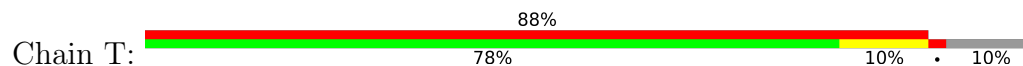
- Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



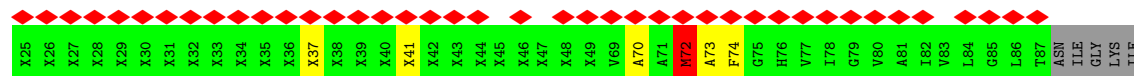
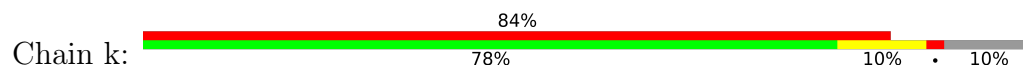
- Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



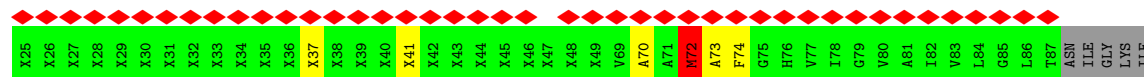
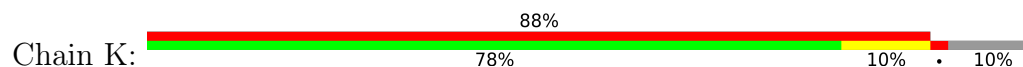
- Molecule 9: Photosystem I reaction center subunit PsaK



- Molecule 9: Photosystem I reaction center subunit PsaK



- Molecule 9: Photosystem I reaction center subunit PsaK

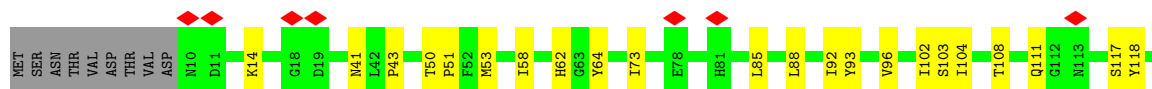


- Molecule 10: PSI subunit V





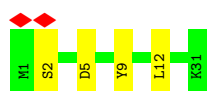
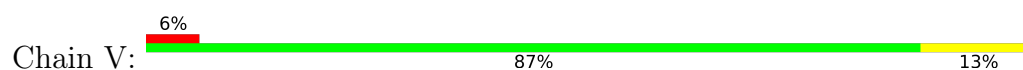
- Molecule 10: PSI subunit V



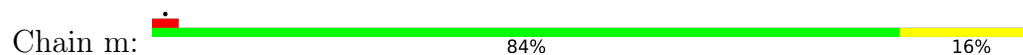
- Molecule 10: PSI subunit V



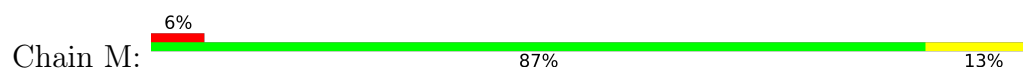
- Molecule 11: Photosystem I reaction center subunit XII



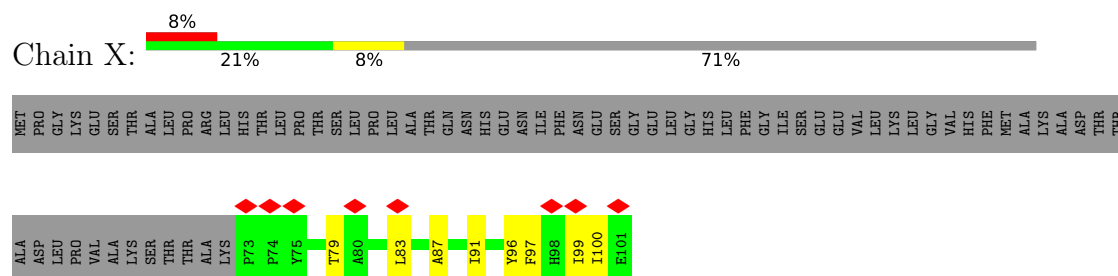
- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 12: Photosystem one Psax



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	201104	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.328	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	0.324	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	381.6013, 381.6013, 381.6013	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.49063, 1.49063, 1.49063	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/6138	0.50	1/8362 (0.0%)
1	G	0.49	0/6138	0.49	1/8362 (0.0%)
1	a	0.49	0/6138	0.49	1/8362 (0.0%)
2	B	0.50	0/6135	0.48	0/8385
2	H	0.50	0/6135	0.48	0/8385
2	b	0.50	0/6135	0.48	0/8385
3	C	0.52	0/611	0.76	2/828 (0.2%)
3	N	0.52	0/611	0.76	2/828 (0.2%)
3	c	0.52	0/611	0.76	2/828 (0.2%)
4	D	0.41	0/1116	0.58	0/1505
4	O	0.41	0/1116	0.58	0/1505
4	d	0.41	0/1116	0.58	0/1505
5	E	0.35	0/506	0.62	2/686 (0.3%)
5	P	0.35	0/506	0.62	2/686 (0.3%)
5	e	0.34	0/506	0.62	2/686 (0.3%)
6	F	0.35	0/1084	0.73	5/1470 (0.3%)
6	Q	0.35	0/1084	0.74	5/1470 (0.3%)
6	f	0.35	0/1084	0.74	5/1470 (0.3%)
7	I	0.51	0/365	0.66	0/502
7	R	0.50	0/365	0.67	0/502
7	i	0.50	0/365	0.66	0/502
8	J	0.31	0/353	0.85	2/482 (0.4%)
8	S	0.31	0/353	0.85	2/482 (0.4%)
8	j	0.31	0/353	0.85	0/482
9	K	0.22	0/129	1.03	2/175 (1.1%)
9	T	0.22	0/129	1.03	2/175 (1.1%)
9	k	0.22	0/129	1.03	2/175 (1.1%)
10	L	0.50	0/1255	0.76	4/1702 (0.2%)
10	U	0.50	0/1255	0.76	4/1702 (0.2%)
10	l	0.50	0/1255	0.76	4/1702 (0.2%)
11	M	0.37	0/250	0.57	0/340
11	V	0.38	0/250	0.57	0/340

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	m	0.37	0/250	0.57	0/340
12	W	0.26	0/256	0.41	0/350
12	X	0.26	0/256	0.41	0/350
12	x	0.26	0/256	0.41	0/350
All	All	0.47	0/54594	0.57	52/74361 (0.1%)

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	2
6	Q	0	2
6	f	0	2
8	J	0	1
8	S	0	1
8	j	0	1
10	L	0	1
10	U	0	1
10	l	0	1
All	All	0	15

There are no bond length outliers.

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	132	ARG	CG-CD-NE	12.10	138.61	112.00
10	L	132	ARG	CG-CD-NE	12.08	138.57	112.00
10	l	132	ARG	CG-CD-NE	12.07	138.55	112.00
10	l	132	ARG	CD-NE-CZ	9.51	137.72	124.40
10	L	132	ARG	CD-NE-CZ	9.50	137.70	124.40

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	333	THR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
6	Q	47	SER	Peptide
6	Q	48	TYR	Peptide
8	S	35	PHE	Peptide
10	U	132	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5931	0	5774	169	0
1	G	5931	0	5774	162	0
1	a	5931	0	5774	169	0
2	B	5913	0	5669	174	0
2	H	5913	0	5669	170	0
2	b	5913	0	5669	170	0
3	C	601	0	577	15	0
3	N	601	0	577	11	0
3	c	601	0	577	15	0
4	D	1092	0	1098	29	0
4	O	1092	0	1098	27	0
4	d	1092	0	1098	30	0
5	E	497	0	482	10	0
5	P	497	0	482	7	0
5	e	497	0	482	7	0
6	F	1060	0	1091	32	0
6	Q	1060	0	1091	27	0
6	f	1060	0	1091	30	0
7	I	350	0	354	19	0
7	R	350	0	354	12	0
7	i	350	0	354	14	0
8	J	344	0	360	10	0
8	S	344	0	360	10	0
8	j	344	0	360	11	0
9	K	253	0	168	5	0
9	T	253	0	168	5	0
9	k	253	0	168	5	0
10	L	1227	0	1239	33	0
10	U	1227	0	1239	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	l	1227	0	1239	32	0
11	M	245	0	259	4	0
11	V	245	0	259	5	0
11	m	245	0	259	6	0
12	W	246	0	246	6	0
12	X	246	0	246	5	0
12	x	246	0	246	5	0
13	A	65	0	72	4	0
13	G	65	0	72	4	0
13	a	65	0	72	4	0
14	A	2315	0	2200	116	0
14	B	2220	0	2213	155	0
14	G	2315	0	2200	112	0
14	H	2220	0	2213	154	0
14	K	45	0	32	0	0
14	L	190	0	203	13	0
14	T	45	0	32	0	0
14	U	190	0	203	12	0
14	W	55	0	49	5	0
14	X	55	0	49	5	0
14	a	2315	0	2200	116	0
14	b	2220	0	2213	159	0
14	k	45	0	32	0	0
14	l	190	0	203	12	0
14	x	55	0	49	3	0
15	A	46	0	0	0	0
15	B	244	0	0	3	0
15	G	46	0	0	0	0
15	H	244	0	0	2	0
15	a	46	0	0	0	0
15	b	244	0	0	2	0
16	A	33	0	46	11	0
16	B	33	0	46	6	0
16	G	33	0	46	8	0
16	H	33	0	46	6	0
16	a	33	0	46	10	0
16	b	33	0	46	5	0
17	A	8	0	0	0	0
17	C	16	0	0	1	0
17	G	8	0	0	0	0
17	N	16	0	0	1	0
17	a	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	c	16	0	0	1	0
18	A	240	0	293	18	0
18	B	360	0	438	32	0
18	G	240	0	293	21	0
18	H	360	0	438	33	0
18	I	80	0	96	11	0
18	L	80	0	97	9	0
18	M	40	0	48	4	0
18	R	80	0	96	10	0
18	U	80	0	97	7	0
18	V	40	0	48	4	0
18	a	240	0	293	21	0
18	b	360	0	438	33	0
18	i	80	0	96	8	0
18	l	80	0	97	8	0
18	m	40	0	48	5	0
19	A	42	0	54	3	0
19	B	44	0	61	1	0
19	G	42	0	54	2	0
19	H	44	0	61	3	0
19	a	42	0	54	3	0
19	b	44	0	61	0	0
20	A	46	0	65	5	0
20	B	46	0	62	4	0
20	G	46	0	65	5	0
20	H	46	0	62	4	0
20	I	37	0	44	1	0
20	L	50	0	70	5	0
20	R	37	0	44	4	0
20	U	50	0	70	3	0
20	a	46	0	65	2	0
20	b	46	0	62	4	0
20	i	37	0	44	1	0
20	l	50	0	70	4	0
21	A	59	0	58	1	0
21	G	59	0	57	1	0
21	a	59	0	58	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	72462	0	70691	1973	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 14.

The worst 5 of 1973 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)
1:G:406:TRP:CD1	14:G:1126:CLA:HAB	2.09	0.87
1:A:406:TRP:CD1	14:A:1126:CLA:HAB	2.09	0.87
1:a:406:TRP:CD1	14:a:1126:CLA:HAB	2.09	0.87
14:B:1204:CLA:H43	7:I:21:MET:HE1	1.56	0.86
14:H:1205:CLA:H102	14:H:1205:CLA:H2	1.58	0.86

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	747/788 (95%)	707 (95%)	40 (5%)	0	100	100
1	G	747/788 (95%)	707 (95%)	40 (5%)	0	100	100
1	a	747/788 (95%)	707 (95%)	40 (5%)	0	100	100
2	B	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	H	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	b	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
3	C	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	26
3	N	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	26
3	c	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
4	D	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
4	O	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
4	d	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
5	E	60/72 (83%)	57 (95%)	3 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	P	60/72 (83%)	57 (95%)	3 (5%)	0	100	100
5	e	60/72 (83%)	57 (95%)	3 (5%)	0	100	100
6	F	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	16	37
6	Q	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	16	37
6	f	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	16	37
7	I	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
7	R	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
7	i	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
8	J	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	4	13
8	S	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	4	13
8	j	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	4	13
9	K	17/49 (35%)	17 (100%)	0	0	100	100
9	T	17/49 (35%)	17 (100%)	0	0	100	100
9	k	17/49 (35%)	17 (100%)	0	0	100	100
10	L	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
10	U	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
10	l	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	V	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
12	W	27/101 (27%)	27 (100%)	0	0	100	100
12	X	27/101 (27%)	27 (100%)	0	0	100	100
12	x	27/101 (27%)	27 (100%)	0	0	100	100
All	All	6621/7410 (89%)	6240 (94%)	373 (6%)	8 (0%)	49	72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	Q	48	TYR
6	f	48	TYR
6	F	48	TYR
3	N	63	LEU
8	S	13	ALA

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	613/641 (96%)	607 (99%)	6 (1%)	68	82
1	G	613/641 (96%)	607 (99%)	6 (1%)	68	82
1	a	613/641 (96%)	607 (99%)	6 (1%)	68	82
2	B	595/597 (100%)	590 (99%)	5 (1%)	73	85
2	H	595/597 (100%)	590 (99%)	5 (1%)	73	85
2	b	595/597 (100%)	590 (99%)	5 (1%)	73	85
3	C	68/69 (99%)	64 (94%)	4 (6%)	18	41
3	N	68/69 (99%)	64 (94%)	4 (6%)	18	41
3	c	68/69 (99%)	64 (94%)	4 (6%)	18	41
4	D	115/132 (87%)	111 (96%)	4 (4%)	32	57
4	O	115/132 (87%)	111 (96%)	4 (4%)	32	57
4	d	115/132 (87%)	111 (96%)	4 (4%)	32	57
5	E	54/60 (90%)	51 (94%)	3 (6%)	19	43
5	P	54/60 (90%)	51 (94%)	3 (6%)	19	43
5	e	54/60 (90%)	51 (94%)	3 (6%)	19	43
6	F	115/134 (86%)	107 (93%)	8 (7%)	14	34
6	Q	115/134 (86%)	107 (93%)	8 (7%)	14	34
6	f	115/134 (86%)	107 (93%)	8 (7%)	14	34
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%)	33 (92%)	3 (8%)	10	27
8	S	36/42 (86%)	33 (92%)	3 (8%)	10	27
8	j	36/42 (86%)	33 (92%)	3 (8%)	10	27
9	K	12/16 (75%)	11 (92%)	1 (8%)	10	27
9	T	12/16 (75%)	11 (92%)	1 (8%)	10	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	k	12/16 (75%)	11 (92%)	1 (8%)	10	27
10	L	128/138 (93%)	125 (98%)	3 (2%)	44	67
10	U	128/138 (93%)	125 (98%)	3 (2%)	44	67
10	l	128/138 (93%)	125 (98%)	3 (2%)	44	67
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	5469/5997 (91%)	5358 (98%)	111 (2%)	48	71

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	34	ARG
10	L	132	ARG
10	l	14	LYS
10	L	123	LYS
6	F	54	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	206	HIS
1	A	25	GLN
2	B	691	GLN
2	b	242	HIS
4	d	70	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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
15	F6C	B	1230	-	52,54,74	3.04	27 (51%)	59,90,114	3.65	30 (50%)
14	CLA	b	1220	-	59,63,73	2.38	20 (33%)	70,101,113	2.74	26 (37%)
14	CLA	A	1113	-	49,53,73	2.48	20 (40%)	58,89,113	2.76	25 (43%)
14	CLA	G	1013	-	64,68,73	2.28	21 (32%)	76,107,113	2.60	26 (34%)
14	CLA	b	1226	-	69,73,73	2.23	19 (27%)	82,113,113	2.35	27 (32%)
14	CLA	G	1118	-	59,63,73	2.38	21 (35%)	70,101,113	2.65	30 (42%)
16	PQN	A	2001	-	34,34,34	1.47	2 (5%)	43,45,45	1.28	6 (13%)
14	CLA	A	1136	-	69,73,73	2.19	20 (28%)	82,113,113	2.49	25 (30%)
21	LMT	A	6001	-	32,32,36	1.25	5 (15%)	43,43,47	1.06	2 (4%)
16	PQN	B	2002	-	34,34,34	1.50	2 (5%)	43,45,45	1.28	3 (6%)
18	BCR	A	4008	-	41,41,41	2.90	7 (17%)	56,56,56	6.61	20 (35%)
14	CLA	b	1224	-	69,73,73	2.20	20 (28%)	82,113,113	2.47	24 (29%)
14	CLA	H	1217	-	59,63,73	2.36	20 (33%)	70,101,113	2.67	24 (34%)
14	CLA	a	1132	-	69,73,73	2.18	20 (28%)	82,113,113	2.61	27 (32%)
14	CLA	G	1132	-	69,73,73	2.19	20 (28%)	82,113,113	2.62	27 (32%)
19	LHG	B	5004	-	43,43,48	0.96	2 (4%)	46,49,54	1.14	3 (6%)
15	F6C	B	1207	-	72,74,74	2.66	26 (36%)	83,114,114	3.33	33 (39%)
19	LHG	A	5001	-	41,41,48	0.99	2 (4%)	44,47,54	1.12	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	1133	-	64,68,73	2.29	21 (32%)	76,107,113	2.61	26 (34%)
14	CLA	a	1134	-	49,53,73	2.57	21 (42%)	58,89,113	2.75	25 (43%)
14	CLA	b	1235	-	64,68,73	2.29	20 (31%)	76,107,113	2.56	28 (36%)
14	CLA	a	1124	-	59,63,73	2.37	19 (32%)	70,101,113	2.74	28 (40%)
14	CLA	H	1225	-	69,73,73	2.23	19 (27%)	82,113,113	2.34	22 (26%)
14	CLA	L	1503	-	69,73,73	2.21	20 (28%)	82,113,113	2.47	27 (32%)
15	F6C	B	1238	-	72,74,74	2.63	23 (31%)	83,114,114	3.21	34 (40%)
14	CLA	H	1219	-	49,53,73	2.52	22 (44%)	58,89,113	2.76	23 (39%)
14	CLA	G	1138	-	64,68,73	2.31	20 (31%)	76,107,113	2.52	27 (35%)
18	BCR	H	4014	-	41,41,41	2.81	8 (19%)	56,56,56	6.59	24 (42%)
14	CLA	a	1111	-	64,68,73	2.27	20 (31%)	76,107,113	4.44	29 (38%)
14	CLA	A	1115	-	69,73,73	2.20	20 (28%)	82,113,113	2.59	28 (34%)
14	CLA	b	1222	-	69,73,73	2.21	20 (28%)	82,113,113	2.54	29 (35%)
18	BCR	R	4020	-	41,41,41	2.94	8 (19%)	56,56,56	6.92	22 (39%)
15	F6C	G	1121	-	52,54,74	3.04	24 (46%)	59,90,114	3.58	32 (54%)
14	CLA	G	1113	-	49,53,73	2.48	20 (40%)	58,89,113	2.76	25 (43%)
18	BCR	L	4019	-	41,41,41	2.75	6 (14%)	56,56,56	7.19	28 (50%)
14	CLA	a	1128	-	64,68,73	2.31	19 (29%)	76,107,113	2.51	26 (34%)
14	CLA	B	1217	-	59,63,73	2.36	20 (33%)	70,101,113	2.68	24 (34%)
14	CLA	b	1215	-	64,68,73	2.26	19 (29%)	76,107,113	2.48	24 (31%)
14	CLA	H	1221	-	69,73,73	2.19	20 (28%)	82,113,113	2.42	27 (32%)
14	CLA	H	1213	-	69,73,73	2.21	20 (28%)	82,113,113	2.50	24 (29%)
14	CLA	H	1021	-	69,73,73	2.17	21 (30%)	82,113,113	2.43	26 (31%)
18	BCR	H	4009	-	41,41,41	2.75	7 (17%)	56,56,56	6.58	20 (35%)
18	BCR	I	4018	-	41,41,41	2.84	7 (17%)	56,56,56	6.73	25 (44%)
14	CLA	a	1126	-	64,68,73	2.30	19 (29%)	76,107,113	2.55	29 (38%)
14	CLA	W	1701	-	59,63,73	2.37	20 (33%)	70,101,113	2.62	26 (37%)
18	BCR	b	4013	-	41,41,41	2.62	6 (14%)	56,56,56	6.87	21 (37%)
14	CLA	G	1124	-	59,63,73	2.38	21 (35%)	70,101,113	2.74	28 (40%)
14	CLA	B	1221	-	69,73,73	2.19	20 (28%)	82,113,113	2.43	27 (32%)
14	CLA	a	1102	-	64,68,73	2.29	20 (31%)	76,107,113	2.58	26 (34%)
14	CLA	a	1107	1	49,53,73	2.49	19 (38%)	58,89,113	2.71	23 (39%)
14	CLA	G	1120	-	49,53,73	2.45	19 (38%)	58,89,113	2.81	22 (37%)
14	CLA	H	1216	-	69,73,73	2.21	22 (31%)	82,113,113	2.42	28 (34%)
14	CLA	a	1122	-	59,63,73	2.36	20 (33%)	70,101,113	2.65	28 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	1203	-	69,73,73	2.17	20 (28%)	82,113,113	2.53	24 (29%)
14	CLA	b	1232	-	49,53,73	2.50	19 (38%)	58,89,113	2.70	23 (39%)
14	CLA	H	1239	-	69,73,73	2.23	20 (28%)	82,113,113	2.57	34 (41%)
19	LHG	G	5001	-	41,41,48	1.00	2 (4%)	44,47,54	1.11	3 (6%)
20	LMG	H	5002	-	46,46,55	1.34	5 (10%)	54,54,63	1.27	4 (7%)
18	BCR	H	4017	-	41,41,41	2.80	7 (17%)	56,56,56	6.90	20 (35%)
14	CLA	B	1205	-	69,73,73	2.16	20 (28%)	82,113,113	2.51	25 (30%)
14	CLA	a	1106	-	64,68,73	2.26	20 (31%)	76,107,113	2.66	27 (35%)
14	CLA	H	1214	-	69,73,73	2.23	21 (30%)	82,113,113	2.46	31 (37%)
14	CLA	H	1226	-	69,73,73	2.23	19 (27%)	82,113,113	2.35	27 (32%)
14	CLA	b	1023	-	69,73,73	2.19	21 (30%)	82,113,113	2.65	29 (35%)
18	BCR	a	4007	-	41,41,41	2.87	8 (19%)	56,56,56	6.72	24 (42%)
13	CL0	a	1011	-	58,73,73	3.06	21 (36%)	60,113,113	2.96	21 (35%)
14	CLA	A	1117	-	69,73,73	2.17	20 (28%)	82,113,113	2.52	28 (34%)
14	CLA	a	1112	-	59,63,73	2.38	20 (33%)	70,101,113	2.66	27 (38%)
15	F6C	b	1230	-	52,54,74	3.04	27 (51%)	59,90,114	3.65	30 (50%)
14	CLA	a	1129	-	54,58,73	2.49	20 (37%)	64,95,113	2.74	24 (37%)
14	CLA	G	1102	-	64,68,73	2.29	20 (31%)	76,107,113	2.57	26 (34%)
14	CLA	G	1115	-	69,73,73	2.20	20 (28%)	82,113,113	2.59	28 (34%)
14	CLA	A	1013	-	64,68,73	2.28	21 (32%)	76,107,113	2.61	27 (35%)
14	CLA	a	1117	-	69,73,73	2.18	20 (28%)	82,113,113	2.51	28 (34%)
14	CLA	a	1139	-	49,53,73	2.49	20 (40%)	58,89,113	2.71	24 (41%)
14	CLA	G	1111	-	64,68,73	2.27	20 (31%)	76,107,113	4.44	29 (38%)
14	CLA	H	1223	-	69,73,73	2.18	20 (28%)	82,113,113	2.55	29 (35%)
14	CLA	G	1135	-	64,68,73	2.28	20 (31%)	76,107,113	2.55	27 (35%)
14	CLA	B	1208	-	69,73,73	2.20	20 (28%)	82,113,113	2.44	27 (32%)
14	CLA	G	1123	-	64,68,73	2.30	20 (31%)	76,107,113	2.51	27 (35%)
18	BCR	H	4016	-	41,41,41	2.74	6 (14%)	56,56,56	6.81	19 (33%)
14	CLA	A	1105	-	49,53,73	2.50	20 (40%)	58,89,113	2.80	23 (39%)
14	CLA	H	1022	-	69,73,73	2.19	20 (28%)	82,113,113	2.53	29 (35%)
14	CLA	H	1231	2	59,63,73	2.37	20 (33%)	70,101,113	2.62	25 (35%)
14	CLA	x	1701	-	59,63,73	2.38	20 (33%)	70,101,113	2.63	26 (37%)
19	LHG	b	5004	-	43,43,48	0.97	2 (4%)	46,49,54	1.14	3 (6%)
14	CLA	H	1220	-	59,63,73	2.37	20 (33%)	70,101,113	2.74	26 (37%)
18	BCR	i	4020	-	41,41,41	2.94	8 (19%)	56,56,56	6.92	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMG	U	5007	-	50,50,55	1.45	7 (14%)	58,58,63	1.10	2 (3%)
17	SF4	A	3001	1,2	0,12,12	-	-	-		
14	CLA	B	1212	-	49,53,73	2.46	19 (38%)	58,89,113	2.73	20 (34%)
14	CLA	A	1128	-	64,68,73	2.31	19 (29%)	76,107,113	2.50	27 (35%)
14	CLA	a	1109	-	69,73,73	2.19	20 (28%)	82,113,113	2.51	27 (32%)
18	BCR	H	4013	-	41,41,41	2.62	6 (14%)	56,56,56	6.87	21 (37%)
14	CLA	b	1204	-	69,73,73	2.22	20 (28%)	82,113,113	2.48	29 (35%)
14	CLA	G	1129	-	54,58,73	2.49	20 (37%)	64,95,113	2.74	24 (37%)
19	LHG	H	5004	-	43,43,48	0.96	2 (4%)	46,49,54	1.14	3 (6%)
14	CLA	H	1224	-	69,73,73	2.20	20 (28%)	82,113,113	2.46	24 (29%)
14	CLA	G	1107	1	49,53,73	2.49	19 (38%)	58,89,113	2.71	23 (39%)
14	CLA	H	1202	-	64,68,73	2.22	20 (31%)	76,107,113	2.59	28 (36%)
14	CLA	A	1130	-	59,63,73	2.39	19 (32%)	70,101,113	2.61	28 (40%)
15	F6C	b	1238	-	72,74,74	2.63	23 (31%)	83,114,114	3.21	34 (40%)
14	CLA	b	1201	-	59,63,73	2.37	20 (33%)	70,101,113	2.74	25 (35%)
14	CLA	G	1106	-	64,68,73	2.26	20 (31%)	76,107,113	2.66	27 (35%)
14	CLA	a	1127	-	69,73,73	2.20	20 (28%)	82,113,113	2.46	24 (29%)
14	CLA	H	1210	-	69,73,73	2.22	22 (31%)	82,113,113	2.64	30 (36%)
18	BCR	a	4003	-	41,41,41	2.69	6 (14%)	56,56,56	6.70	22 (39%)
14	CLA	H	1205	-	69,73,73	2.17	20 (28%)	82,113,113	2.51	26 (31%)
18	BCR	m	4021	-	41,41,41	2.76	7 (17%)	56,56,56	6.81	16 (28%)
14	CLA	b	1217	-	59,63,73	2.35	20 (33%)	70,101,113	2.67	24 (34%)
21	LMT	a	6001	-	32,32,36	1.24	5 (15%)	43,43,47	1.06	2 (4%)
14	CLA	b	1022	-	69,73,73	2.18	20 (28%)	82,113,113	2.53	29 (35%)
15	F6C	H	1207	-	72,74,74	2.66	26 (36%)	83,114,114	3.33	33 (39%)
14	CLA	G	1122	-	59,63,73	2.36	20 (33%)	70,101,113	2.66	28 (40%)
14	CLA	B	1233	-	49,53,73	2.51	20 (40%)	58,89,113	2.76	22 (37%)
18	BCR	a	4011	-	41,41,41	2.80	7 (17%)	56,56,56	6.69	28 (50%)
14	CLA	a	1110	-	49,53,73	2.48	19 (38%)	58,89,113	2.72	22 (37%)
18	BCR	V	4021	-	41,41,41	2.77	7 (17%)	56,56,56	6.82	16 (28%)
14	CLA	H	1222	-	69,73,73	2.21	20 (28%)	82,113,113	2.54	29 (35%)
14	CLA	a	1119	-	69,73,73	2.21	22 (31%)	82,113,113	2.47	25 (30%)
14	CLA	B	1225	-	69,73,73	2.23	19 (27%)	82,113,113	2.34	23 (28%)
14	CLA	H	1232	-	49,53,73	2.50	19 (38%)	58,89,113	2.70	23 (39%)
14	CLA	H	1215	-	64,68,73	2.26	19 (29%)	76,107,113	2.48	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	F6C	b	1207	-	72,74,74	2.67	26 (36%)	83,114,114	3.33	33 (39%)
14	CLA	A	1122	-	59,63,73	2.36	20 (33%)	70,101,113	2.66	28 (40%)
18	BCR	B	4010	-	41,41,41	2.86	6 (14%)	56,56,56	6.84	20 (35%)
18	BCR	G	4008	-	41,41,41	2.90	7 (17%)	56,56,56	6.61	20 (35%)
14	CLA	a	1130	-	59,63,73	2.39	19 (32%)	70,101,113	2.61	28 (40%)
18	BCR	H	4006	-	41,41,41	2.67	6 (14%)	56,56,56	6.76	21 (37%)
20	LMG	A	5005	-	46,46,55	1.38	5 (10%)	54,54,63	1.10	2 (3%)
14	CLA	H	1203	-	69,73,73	2.17	20 (28%)	82,113,113	2.53	24 (29%)
14	CLA	b	1209	-	49,53,73	2.49	21 (42%)	58,89,113	2.84	23 (39%)
14	CLA	H	1234	-	69,73,73	2.17	20 (28%)	82,113,113	2.45	24 (29%)
14	CLA	G	1110	-	49,53,73	2.49	19 (38%)	58,89,113	2.73	22 (37%)
14	CLA	B	1236	-	49,53,73	2.47	20 (40%)	58,89,113	2.78	22 (37%)
14	CLA	B	1229	-	64,68,73	2.29	21 (32%)	76,107,113	2.62	27 (35%)
14	CLA	A	1133	-	64,68,73	2.29	20 (31%)	76,107,113	2.61	26 (34%)
14	CLA	G	1119	-	69,73,73	2.20	22 (31%)	82,113,113	2.47	24 (29%)
14	CLA	A	1114	-	49,53,73	2.52	21 (42%)	58,89,113	2.72	21 (36%)
14	CLA	A	1102	-	64,68,73	2.29	20 (31%)	76,107,113	2.58	26 (34%)
14	CLA	G	1134	-	49,53,73	2.56	21 (42%)	58,89,113	2.75	24 (41%)
18	BCR	B	4017	-	41,41,41	2.80	7 (17%)	56,56,56	6.90	20 (35%)
13	CL0	A	1011	-	58,73,73	3.06	21 (36%)	60,113,113	2.96	21 (35%)
14	CLA	A	1111	-	64,68,73	2.27	20 (31%)	76,107,113	4.44	29 (38%)
14	CLA	B	1216	-	69,73,73	2.20	22 (31%)	82,113,113	2.41	28 (34%)
14	CLA	b	1208	-	69,73,73	2.21	20 (28%)	82,113,113	2.44	27 (32%)
14	CLA	G	1012	-	69,73,73	2.20	19 (27%)	82,113,113	2.54	29 (35%)
14	CLA	b	1234	-	69,73,73	2.18	20 (28%)	82,113,113	2.45	24 (29%)
15	F6C	a	1121	-	52,54,74	3.05	24 (46%)	59,90,114	3.57	32 (54%)
14	CLA	b	1233	-	49,53,73	2.51	21 (42%)	58,89,113	2.76	21 (36%)
14	CLA	H	1236	-	49,53,73	2.48	20 (40%)	58,89,113	2.77	22 (37%)
14	CLA	G	1103	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	24 (31%)
14	CLA	B	1213	-	69,73,73	2.20	20 (28%)	82,113,113	2.50	24 (29%)
14	CLA	b	1212	-	49,53,73	2.46	19 (38%)	58,89,113	2.74	20 (34%)
14	CLA	H	1201	-	59,63,73	2.37	20 (33%)	70,101,113	2.75	25 (35%)
14	CLA	b	1214	-	69,73,73	2.23	21 (30%)	82,113,113	2.46	31 (37%)
14	CLA	U	1502	-	64,68,73	2.24	20 (31%)	76,107,113	2.60	24 (31%)
14	CLA	G	1101	-	49,53,73	2.45	20 (40%)	58,89,113	2.81	22 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	k	1401	-	49,53,73	2.52	22 (44%)	58,89,113	2.80	23 (39%)
14	CLA	H	1218	-	49,53,73	2.53	19 (38%)	58,89,113	2.65	21 (36%)
14	CLA	G	1133	-	64,68,73	2.29	20 (31%)	76,107,113	2.61	26 (34%)
14	CLA	G	1104	-	69,73,73	2.15	20 (28%)	82,113,113	2.62	25 (30%)
18	BCR	a	4001	-	41,41,41	2.73	6 (14%)	56,56,56	6.76	23 (41%)
14	CLA	B	1022	-	69,73,73	2.18	20 (28%)	82,113,113	2.53	29 (35%)
14	CLA	A	1116	-	59,63,73	2.40	20 (33%)	70,101,113	2.69	30 (42%)
18	BCR	M	4021	-	41,41,41	2.77	7 (17%)	56,56,56	6.82	16 (28%)
21	LMT	A	6002	-	29,29,36	1.36	6 (20%)	40,40,47	1.18	4 (10%)
14	CLA	A	1135	-	64,68,73	2.28	20 (31%)	76,107,113	2.54	27 (35%)
17	SF4	C	3003	3	0,12,12	-	-	-	-	-
14	CLA	B	1231	2	59,63,73	2.38	20 (33%)	70,101,113	2.63	25 (35%)
14	CLA	G	1128	-	64,68,73	2.30	19 (29%)	76,107,113	2.50	26 (34%)
14	CLA	b	1223	-	69,73,73	2.18	20 (28%)	82,113,113	2.54	29 (35%)
14	CLA	A	1127	-	69,73,73	2.19	20 (28%)	82,113,113	2.46	24 (29%)
14	CLA	B	1202	-	64,68,73	2.22	20 (31%)	76,107,113	2.58	28 (36%)
14	CLA	a	1137	-	54,58,73	2.47	20 (37%)	64,95,113	2.89	27 (42%)
18	BCR	A	4003	-	41,41,41	2.69	7 (17%)	56,56,56	6.71	22 (39%)
14	CLA	b	1218	-	49,53,73	2.53	19 (38%)	58,89,113	2.65	21 (36%)
18	BCR	G	4001	-	41,41,41	2.73	6 (14%)	56,56,56	6.76	23 (41%)
14	CLA	b	1231	2	59,63,73	2.38	20 (33%)	70,101,113	2.63	25 (35%)
14	CLA	G	1131	-	64,68,73	2.29	20 (31%)	76,107,113	2.55	24 (31%)
14	CLA	G	1112	-	59,63,73	2.39	20 (33%)	70,101,113	2.66	27 (38%)
14	CLA	a	1115	-	69,73,73	2.20	20 (28%)	82,113,113	2.59	28 (34%)
14	CLA	B	1206	2	49,53,73	2.48	18 (36%)	58,89,113	2.60	23 (39%)
14	CLA	b	1227	-	49,53,73	2.54	20 (40%)	58,89,113	2.70	23 (39%)
14	CLA	b	1211	-	69,73,73	2.20	21 (30%)	82,113,113	2.50	25 (30%)
14	CLA	G	1117	-	69,73,73	2.18	20 (28%)	82,113,113	2.52	28 (34%)
18	BCR	B	4006	-	41,41,41	2.66	6 (14%)	56,56,56	6.77	21 (37%)
14	CLA	b	1205	-	69,73,73	2.17	20 (28%)	82,113,113	2.50	25 (30%)
14	CLA	a	1118	-	59,63,73	2.38	21 (35%)	70,101,113	2.65	30 (42%)
20	LMG	L	5007	-	50,50,55	1.45	7 (14%)	58,58,63	1.10	2 (3%)
14	CLA	a	1101	-	49,53,73	2.45	19 (38%)	58,89,113	2.81	22 (37%)
14	CLA	a	1138	-	64,68,73	2.31	20 (31%)	76,107,113	2.51	25 (32%)
14	CLA	A	1118	-	59,63,73	2.38	21 (35%)	70,101,113	2.65	30 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	1220	-	59,63,73	2.37	20 (33%)	70,101,113	2.74	26 (37%)
14	CLA	b	1206	2	49,53,73	2.49	18 (36%)	58,89,113	2.61	23 (39%)
15	F6C	H	1237	-	72,74,74	2.60	23 (31%)	83,114,114	3.18	33 (39%)
14	CLA	A	1125	-	69,73,73	2.17	20 (28%)	82,113,113	2.56	26 (31%)
17	SF4	c	3002	3	0,12,12	-	-	-	-	-
14	CLA	a	1104	-	69,73,73	2.15	20 (28%)	82,113,113	2.62	25 (30%)
18	BCR	B	4009	-	41,41,41	2.75	7 (17%)	56,56,56	6.58	20 (35%)
14	CLA	b	1229	-	64,68,73	2.29	20 (31%)	76,107,113	2.62	27 (35%)
14	CLA	A	1120	-	49,53,73	2.45	19 (38%)	58,89,113	2.81	22 (37%)
14	CLA	B	1224	-	69,73,73	2.20	20 (28%)	82,113,113	2.47	24 (29%)
14	CLA	B	1228	-	59,63,73	2.38	22 (37%)	70,101,113	2.65	28 (40%)
16	PQN	b	2002	-	34,34,34	1.51	2 (5%)	43,45,45	1.28	3 (6%)
18	BCR	a	4002	-	41,41,41	2.74	6 (14%)	56,56,56	6.43	28 (50%)
20	LMG	R	5006	-	37,37,55	1.14	3 (8%)	45,45,63	1.21	4 (8%)
18	BCR	b	4010	-	41,41,41	2.86	6 (14%)	56,56,56	6.84	20 (35%)
14	CLA	a	1116	-	59,63,73	2.40	20 (33%)	70,101,113	2.68	30 (42%)
14	CLA	G	1140	-	69,73,73	2.20	21 (30%)	82,113,113	2.42	26 (31%)
14	CLA	l	1501	10	69,73,73	2.19	20 (28%)	82,113,113	2.41	25 (30%)
14	CLA	B	1210	-	69,73,73	2.21	21 (30%)	82,113,113	2.64	29 (35%)
18	BCR	B	4014	-	41,41,41	2.81	8 (19%)	56,56,56	6.59	24 (42%)
18	BCR	B	4013	-	41,41,41	2.62	6 (14%)	56,56,56	6.87	21 (37%)
14	CLA	H	1209	-	49,53,73	2.50	21 (42%)	58,89,113	2.85	23 (39%)
14	CLA	a	1131	-	64,68,73	2.29	20 (31%)	76,107,113	2.54	23 (30%)
14	CLA	A	1138	-	64,68,73	2.31	20 (31%)	76,107,113	2.52	27 (35%)
17	SF4	C	3002	3	0,12,12	-	-	-	-	-
15	F6C	A	1121	-	52,54,74	3.05	24 (46%)	59,90,114	3.57	32 (54%)
14	CLA	A	1101	-	49,53,73	2.45	19 (38%)	58,89,113	2.80	22 (37%)
17	SF4	N	3002	3	0,12,12	-	-	-	-	-
18	BCR	G	4002	-	41,41,41	2.74	6 (14%)	56,56,56	6.43	28 (50%)
14	CLA	B	1222	-	69,73,73	2.22	20 (28%)	82,113,113	2.54	29 (35%)
18	BCR	U	4019	-	41,41,41	2.75	6 (14%)	56,56,56	7.19	28 (50%)
14	CLA	G	1136	-	69,73,73	2.19	20 (28%)	82,113,113	2.48	25 (30%)
18	BCR	B	4016	-	41,41,41	2.74	6 (14%)	56,56,56	6.81	18 (32%)
14	CLA	A	1104	-	69,73,73	2.15	20 (28%)	82,113,113	2.62	25 (30%)
18	BCR	b	4014	-	41,41,41	2.81	8 (19%)	56,56,56	6.59	25 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	L	1502	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	24 (31%)
17	SF4	c	3003	3	0,12,12	-	-	-		
14	CLA	B	1215	-	64,68,73	2.26	19 (29%)	76,107,113	2.48	24 (31%)
14	CLA	H	1212	-	49,53,73	2.46	19 (38%)	58,89,113	2.74	20 (34%)
14	CLA	A	1124	-	59,63,73	2.38	19 (32%)	70,101,113	2.74	28 (40%)
14	CLA	b	1221	-	69,73,73	2.18	20 (28%)	82,113,113	2.42	27 (32%)
18	BCR	H	4005	-	41,41,41	2.77	8 (19%)	56,56,56	6.74	24 (42%)
18	BCR	b	4009	-	41,41,41	2.75	7 (17%)	56,56,56	6.58	20 (35%)
14	CLA	B	1219	-	49,53,73	2.53	22 (44%)	58,89,113	2.76	23 (39%)
18	BCR	G	4003	-	41,41,41	2.69	6 (14%)	56,56,56	6.71	22 (39%)
14	CLA	B	1232	-	49,53,73	2.50	19 (38%)	58,89,113	2.71	22 (37%)
14	CLA	H	1204	-	69,73,73	2.22	20 (28%)	82,113,113	2.48	29 (35%)
14	CLA	B	1214	-	69,73,73	2.23	21 (30%)	82,113,113	2.46	31 (37%)
14	CLA	b	1225	-	69,73,73	2.23	19 (27%)	82,113,113	2.34	23 (28%)
14	CLA	a	1140	-	69,73,73	2.19	21 (30%)	82,113,113	2.42	25 (30%)
14	CLA	B	1021	-	69,73,73	2.17	21 (30%)	82,113,113	2.44	25 (30%)
18	BCR	l	4022	-	41,41,41	2.85	7 (17%)	56,56,56	6.65	22 (39%)
14	CLA	a	1105	-	49,53,73	2.50	21 (42%)	58,89,113	2.79	23 (39%)
14	CLA	H	1208	-	69,73,73	2.21	20 (28%)	82,113,113	2.44	26 (31%)
18	BCR	A	4001	-	41,41,41	2.73	6 (14%)	56,56,56	6.76	23 (41%)
14	CLA	H	1206	2	49,53,73	2.49	18 (36%)	58,89,113	2.61	23 (39%)
14	CLA	A	1131	-	64,68,73	2.29	20 (31%)	76,107,113	2.54	24 (31%)
18	BCR	b	4017	-	41,41,41	2.79	7 (17%)	56,56,56	6.89	20 (35%)
14	CLA	B	1209	-	49,53,73	2.50	20 (40%)	58,89,113	2.85	23 (39%)
14	CLA	B	1023	-	69,73,73	2.19	21 (30%)	82,113,113	2.65	29 (35%)
14	CLA	A	1126	-	64,68,73	2.31	20 (31%)	76,107,113	2.56	29 (38%)
17	SF4	a	3001	1,2	0,12,12	-	-	-		
14	CLA	G	1125	-	69,73,73	2.17	20 (28%)	82,113,113	2.56	26 (31%)
14	CLA	G	1130	-	59,63,73	2.38	19 (32%)	70,101,113	2.61	29 (41%)
14	CLA	B	1223	-	69,73,73	2.18	20 (28%)	82,113,113	2.55	30 (36%)
18	BCR	H	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.65	25 (44%)
14	CLA	a	1108	-	49,53,73	2.51	20 (40%)	58,89,113	2.73	24 (41%)
14	CLA	B	1226	-	69,73,73	2.22	19 (27%)	82,113,113	2.35	27 (32%)
15	F6C	B	1237	-	72,74,74	2.60	23 (31%)	83,114,114	3.18	33 (39%)
14	CLA	G	1105	-	49,53,73	2.50	21 (42%)	58,89,113	2.80	23 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	G	1139	-	49,53,73	2.49	20 (40%)	58,89,113	2.71	24 (41%)
14	CLA	b	1228	-	59,63,73	2.38	22 (37%)	70,101,113	2.65	28 (40%)
18	BCR	B	4005	-	41,41,41	2.77	7 (17%)	56,56,56	6.74	23 (41%)
14	CLA	a	1103	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	25 (32%)
18	BCR	l	4019	-	41,41,41	2.76	6 (14%)	56,56,56	7.19	28 (50%)
14	CLA	A	1140	-	69,73,73	2.19	21 (30%)	82,113,113	2.41	25 (30%)
14	CLA	A	1112	-	59,63,73	2.38	20 (33%)	70,101,113	2.65	27 (38%)
14	CLA	A	1129	-	54,58,73	2.48	20 (37%)	64,95,113	2.73	24 (37%)
15	F6C	H	1238	-	72,74,74	2.63	23 (31%)	83,114,114	3.21	34 (40%)
18	BCR	b	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.65	25 (44%)
14	CLA	X	1701	-	59,63,73	2.38	20 (33%)	70,101,113	2.63	26 (37%)
18	BCR	b	4005	-	41,41,41	2.77	7 (17%)	56,56,56	6.74	24 (42%)
14	CLA	A	1139	-	49,53,73	2.49	20 (40%)	58,89,113	2.71	24 (41%)
14	CLA	G	1108	-	49,53,73	2.51	20 (40%)	58,89,113	2.73	24 (41%)
14	CLA	B	1239	-	69,73,73	2.23	20 (28%)	82,113,113	2.57	34 (41%)
18	BCR	I	4020	-	41,41,41	2.94	8 (19%)	56,56,56	6.92	22 (39%)
14	CLA	G	1126	-	64,68,73	2.30	19 (29%)	76,107,113	2.57	29 (38%)
18	BCR	B	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.65	25 (44%)
14	CLA	H	1227	-	49,53,73	2.54	20 (40%)	58,89,113	2.70	23 (39%)
16	PQN	G	2001	-	34,34,34	1.47	2 (5%)	43,45,45	1.28	6 (13%)
14	CLA	A	1123	-	64,68,73	2.30	20 (31%)	76,107,113	2.50	27 (35%)
14	CLA	a	1113	-	49,53,73	2.47	20 (40%)	58,89,113	2.76	24 (41%)
18	BCR	A	4007	-	41,41,41	2.87	8 (19%)	56,56,56	6.72	24 (42%)
20	LMG	a	5005	-	46,46,55	1.38	5 (10%)	54,54,63	1.10	2 (3%)
15	F6C	H	1230	-	52,54,74	3.04	27 (51%)	59,90,114	3.65	30 (50%)
18	BCR	b	4016	-	41,41,41	2.74	6 (14%)	56,56,56	6.81	19 (33%)
14	CLA	U	1503	-	69,73,73	2.21	20 (28%)	82,113,113	2.47	28 (34%)
14	CLA	H	1023	-	69,73,73	2.19	21 (30%)	82,113,113	2.65	29 (35%)
21	LMT	G	6001	-	32,32,36	1.25	5 (15%)	43,43,47	1.06	2 (4%)
14	CLA	a	1012	-	69,73,73	2.20	19 (27%)	82,113,113	2.54	29 (35%)
14	CLA	H	1235	-	64,68,73	2.29	20 (31%)	76,107,113	2.56	28 (36%)
14	CLA	a	1114	-	49,53,73	2.52	21 (42%)	58,89,113	2.73	22 (37%)
14	CLA	A	1107	1	49,53,73	2.48	19 (38%)	58,89,113	2.71	23 (39%)
14	CLA	U	1501	10	69,73,73	2.19	20 (28%)	82,113,113	2.41	25 (30%)
18	BCR	R	4018	-	41,41,41	2.83	7 (17%)	56,56,56	6.73	25 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	U	4022	-	41,41,41	2.85	7 (17%)	56,56,56	6.64	22 (39%)
20	LMG	i	5006	-	37,37,55	1.13	3 (8%)	45,45,63	1.21	4 (8%)
18	BCR	A	4002	-	41,41,41	2.74	6 (14%)	56,56,56	6.43	28 (50%)
14	CLA	b	1021	-	69,73,73	2.17	21 (30%)	82,113,113	2.44	25 (30%)
14	CLA	A	1106	-	64,68,73	2.26	20 (31%)	76,107,113	2.66	27 (35%)
20	LMG	G	5005	-	46,46,55	1.37	5 (10%)	54,54,63	1.10	2 (3%)
18	BCR	A	4011	-	41,41,41	2.80	7 (17%)	56,56,56	6.69	28 (50%)
14	CLA	a	1123	-	64,68,73	2.30	20 (31%)	76,107,113	2.50	27 (35%)
14	CLA	A	1109	-	69,73,73	2.19	20 (28%)	82,113,113	2.51	26 (31%)
14	CLA	b	1236	-	49,53,73	2.47	20 (40%)	58,89,113	2.77	22 (37%)
14	CLA	a	1135	-	64,68,73	2.29	20 (31%)	76,107,113	2.55	27 (35%)
14	CLA	G	1114	-	49,53,73	2.52	21 (42%)	58,89,113	2.72	21 (36%)
14	CLA	A	1110	-	49,53,73	2.49	19 (38%)	58,89,113	2.72	22 (37%)
18	BCR	i	4018	-	41,41,41	2.84	7 (17%)	56,56,56	6.73	25 (44%)
14	CLA	L	1501	10	69,73,73	2.19	20 (28%)	82,113,113	2.41	25 (30%)
14	CLA	A	1119	-	69,73,73	2.21	22 (31%)	82,113,113	2.47	26 (31%)
18	BCR	L	4022	-	41,41,41	2.85	6 (14%)	56,56,56	6.64	22 (39%)
14	CLA	b	1210	-	69,73,73	2.22	22 (31%)	82,113,113	2.64	30 (36%)
14	CLA	b	1239	-	69,73,73	2.23	20 (28%)	82,113,113	2.57	34 (41%)
14	CLA	H	1229	-	64,68,73	2.29	21 (32%)	76,107,113	2.61	27 (35%)
14	CLA	A	1134	-	49,53,73	2.56	21 (42%)	58,89,113	2.76	24 (41%)
14	CLA	l	1502	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	24 (31%)
14	CLA	b	1216	-	69,73,73	2.21	22 (31%)	82,113,113	2.42	28 (34%)
14	CLA	B	1204	-	69,73,73	2.22	20 (28%)	82,113,113	2.47	29 (35%)
14	CLA	H	1233	-	49,53,73	2.51	21 (42%)	58,89,113	2.76	22 (37%)
14	CLA	B	1235	-	64,68,73	2.29	20 (31%)	76,107,113	2.57	28 (36%)
14	CLA	A	1012	-	69,73,73	2.20	19 (27%)	82,113,113	2.53	29 (35%)
18	BCR	G	4007	-	41,41,41	2.87	8 (19%)	56,56,56	6.72	24 (42%)
13	CL0	G	1011	-	58,73,73	3.06	21 (36%)	60,113,113	2.96	21 (35%)
15	F6C	b	1237	-	72,74,74	2.59	24 (33%)	83,114,114	3.17	33 (39%)
16	PQN	a	2001	-	34,34,34	1.46	2 (5%)	43,45,45	1.28	6 (13%)
14	CLA	a	1136	-	69,73,73	2.19	19 (27%)	82,113,113	2.48	26 (31%)
14	CLA	B	1234	-	69,73,73	2.17	20 (28%)	82,113,113	2.45	24 (29%)
14	CLA	A	1103	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	25 (32%)
14	CLA	b	1213	-	69,73,73	2.21	20 (28%)	82,113,113	2.50	24 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMT	a	6002	-	29,29,36	1.36	6 (20%)	40,40,47	1.18	4 (10%)
17	SF4	G	3001	1,2	0,12,12	-	-	-		
14	CLA	G	1116	-	59,63,73	2.39	20 (33%)	70,101,113	2.67	30 (42%)
14	CLA	T	1401	-	49,53,73	2.52	22 (44%)	58,89,113	2.81	23 (39%)
14	CLA	l	1503	-	69,73,73	2.21	20 (28%)	82,113,113	2.47	27 (32%)
14	CLA	b	1219	-	49,53,73	2.52	22 (44%)	58,89,113	2.76	23 (39%)
14	CLA	H	1211	-	69,73,73	2.20	21 (30%)	82,113,113	2.50	25 (30%)
14	CLA	G	1109	-	69,73,73	2.19	20 (28%)	82,113,113	2.51	26 (31%)
18	BCR	a	4008	-	41,41,41	2.90	6 (14%)	56,56,56	6.61	20 (35%)
16	PQN	H	2002	-	34,34,34	1.51	2 (5%)	43,45,45	1.28	4 (9%)
14	CLA	B	1201	-	59,63,73	2.37	20 (33%)	70,101,113	2.75	25 (35%)
20	LMG	I	5006	-	37,37,55	1.13	3 (8%)	45,45,63	1.21	4 (8%)
14	CLA	A	1137	-	54,58,73	2.47	20 (37%)	64,95,113	2.88	27 (42%)
14	CLA	K	1401	-	49,53,73	2.53	22 (44%)	58,89,113	2.81	23 (39%)
21	LMT	G	6002	-	29,29,36	1.36	6 (20%)	40,40,47	1.18	4 (10%)
14	CLA	a	1013	-	64,68,73	2.28	21 (32%)	76,107,113	2.61	26 (34%)
14	CLA	B	1203	-	69,73,73	2.17	20 (28%)	82,113,113	2.53	23 (28%)
14	CLA	b	1202	-	64,68,73	2.22	21 (32%)	76,107,113	2.59	28 (36%)
17	SF4	N	3003	3	0,12,12	-	-	-		
20	LMG	B	5002	-	46,46,55	1.34	5 (10%)	54,54,63	1.27	4 (7%)
14	CLA	A	1132	-	69,73,73	2.19	20 (28%)	82,113,113	2.61	27 (32%)
19	LHG	a	5001	-	41,41,48	0.99	2 (4%)	44,47,54	1.11	3 (6%)
14	CLA	a	1125	-	69,73,73	2.18	20 (28%)	82,113,113	2.56	26 (31%)
14	CLA	G	1127	-	69,73,73	2.20	20 (28%)	82,113,113	2.46	24 (29%)
20	LMG	l	5007	-	50,50,55	1.45	7 (14%)	58,58,63	1.10	2 (3%)
18	BCR	H	4010	-	41,41,41	2.86	6 (14%)	56,56,56	6.84	20 (35%)
14	CLA	a	1120	-	49,53,73	2.46	19 (38%)	58,89,113	2.82	22 (37%)
14	CLA	B	1218	-	49,53,73	2.54	19 (38%)	58,89,113	2.66	21 (36%)
14	CLA	A	1108	-	49,53,73	2.51	20 (40%)	58,89,113	2.74	24 (41%)
14	CLA	G	1137	-	54,58,73	2.47	20 (37%)	64,95,113	2.89	27 (42%)
20	LMG	b	5002	-	46,46,55	1.34	5 (10%)	54,54,63	1.27	4 (7%)
18	BCR	b	4006	-	41,41,41	2.67	6 (14%)	56,56,56	6.76	21 (37%)
14	CLA	B	1227	-	49,53,73	2.54	20 (40%)	58,89,113	2.70	24 (41%)
14	CLA	B	1211	-	69,73,73	2.20	21 (30%)	82,113,113	2.49	25 (30%)
14	CLA	H	1228	-	59,63,73	2.38	22 (37%)	70,101,113	2.66	28 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	G	4011	-	41,41,41	2.80	7 (17%)	56,56,56	6.69	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
15	F6C	B	1230	-	1/1/6/16	8/17/73/97	-
14	CLA	b	1220	-	1/1/13/20	10/27/103/115	-
14	CLA	A	1113	-	1/1/11/20	9/15/91/115	-
14	CLA	G	1013	-	1/1/14/20	12/33/109/115	-
14	CLA	b	1226	-	1/1/15/20	11/39/115/115	-
14	CLA	G	1118	-	1/1/13/20	10/27/103/115	-
16	PQN	A	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	A	1136	-	1/1/15/20	19/39/115/115	-
21	LMT	A	6001	-	-	6/17/57/61	0/2/2/2
16	PQN	B	2002	-	-	12/23/43/43	0/2/2/2
18	BCR	A	4008	-	-	12/29/63/63	0/2/2/2
14	CLA	b	1224	-	1/1/15/20	16/39/115/115	-
14	CLA	H	1217	-	1/1/13/20	13/27/103/115	-
14	CLA	a	1132	-	1/1/15/20	14/39/115/115	-
14	CLA	G	1132	-	1/1/15/20	14/39/115/115	-
19	LHG	B	5004	-	-	25/48/48/53	-
15	F6C	B	1207	-	1/1/10/16	20/41/97/97	-
19	LHG	A	5001	-	-	23/46/46/53	-
14	CLA	a	1133	-	1/1/14/20	9/33/109/115	-
14	CLA	a	1134	-	1/1/11/20	5/15/91/115	-
14	CLA	b	1235	-	1/1/14/20	12/33/109/115	-
14	CLA	a	1124	-	1/1/13/20	11/27/103/115	-
14	CLA	H	1225	-	1/1/15/20	15/39/115/115	-
14	CLA	L	1503	-	1/1/15/20	15/39/115/115	-
15	F6C	B	1238	-	1/1/10/16	16/41/97/97	-
14	CLA	H	1219	-	1/1/11/20	5/15/91/115	-
14	CLA	G	1138	-	1/1/14/20	15/33/109/115	-
18	BCR	H	4014	-	-	7/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	1111	-	1/1/14/20	13/33/109/115	-
14	CLA	A	1115	-	1/1/15/20	20/39/115/115	-
14	CLA	b	1222	-	1/1/15/20	17/39/115/115	-
18	BCR	R	4020	-	-	12/29/63/63	0/2/2/2
15	F6C	G	1121	-	1/1/6/16	9/17/73/97	-
14	CLA	G	1113	-	1/1/11/20	9/15/91/115	-
18	BCR	L	4019	-	-	12/29/63/63	0/2/2/2
14	CLA	a	1128	-	1/1/14/20	15/33/109/115	-
14	CLA	B	1217	-	1/1/13/20	13/27/103/115	-
14	CLA	b	1215	-	1/1/14/20	18/33/109/115	-
14	CLA	H	1221	-	1/1/15/20	11/39/115/115	-
14	CLA	H	1213	-	1/1/15/20	16/39/115/115	-
14	CLA	H	1021	-	1/1/15/20	20/39/115/115	-
18	BCR	H	4009	-	-	8/29/63/63	0/2/2/2
18	BCR	I	4018	-	-	8/29/63/63	0/2/2/2
14	CLA	a	1126	-	1/1/14/20	21/33/109/115	-
14	CLA	W	1701	-	1/1/13/20	11/27/103/115	-
18	BCR	b	4013	-	-	11/29/63/63	0/2/2/2
14	CLA	G	1124	-	1/1/13/20	11/27/103/115	-
14	CLA	B	1221	-	1/1/15/20	10/39/115/115	-
14	CLA	a	1102	-	1/1/14/20	14/33/109/115	-
14	CLA	a	1107	1	1/1/11/20	5/15/91/115	-
14	CLA	G	1120	-	1/1/11/20	9/15/91/115	-
14	CLA	H	1216	-	1/1/15/20	21/39/115/115	-
14	CLA	a	1122	-	1/1/13/20	13/27/103/115	-
14	CLA	b	1203	-	1/1/15/20	17/39/115/115	-
14	CLA	b	1232	-	1/1/11/20	2/15/91/115	-
14	CLA	H	1239	-	1/1/15/20	22/39/115/115	-
19	LHG	G	5001	-	-	23/46/46/53	-
20	LMG	H	5002	-	-	12/41/61/70	0/1/1/1
18	BCR	H	4017	-	-	13/29/63/63	0/2/2/2
14	CLA	B	1205	-	1/1/15/20	10/39/115/115	-
14	CLA	a	1106	-	1/1/14/20	13/33/109/115	-
14	CLA	H	1214	-	1/1/15/20	17/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1226	-	1/1/15/20	11/39/115/115	-
14	CLA	b	1023	-	1/1/15/20	15/39/115/115	-
18	BCR	a	4007	-	-	12/29/63/63	0/2/2/2
13	CL0	a	1011	-	3/3/20/25	10/37/135/135	-
14	CLA	A	1117	-	1/1/15/20	19/39/115/115	-
14	CLA	a	1112	-	1/1/13/20	14/27/103/115	-
15	F6C	b	1230	-	1/1/6/16	8/17/73/97	-
14	CLA	a	1129	-	1/1/12/20	7/21/97/115	-
14	CLA	G	1102	-	1/1/14/20	14/33/109/115	-
14	CLA	G	1115	-	1/1/15/20	20/39/115/115	-
14	CLA	A	1013	-	1/1/14/20	12/33/109/115	-
14	CLA	a	1117	-	1/1/15/20	19/39/115/115	-
14	CLA	a	1139	-	1/1/11/20	4/15/91/115	-
14	CLA	G	1111	-	1/1/14/20	13/33/109/115	-
14	CLA	H	1223	-	1/1/15/20	17/39/115/115	-
14	CLA	G	1135	-	1/1/14/20	14/33/109/115	-
14	CLA	B	1208	-	1/1/15/20	16/39/115/115	-
14	CLA	G	1123	-	1/1/14/20	13/33/109/115	-
18	BCR	H	4016	-	-	10/29/63/63	0/2/2/2
14	CLA	A	1105	-	1/1/11/20	4/15/91/115	-
14	CLA	H	1022	-	1/1/15/20	19/39/115/115	-
14	CLA	H	1231	2	1/1/13/20	7/27/103/115	-
14	CLA	x	1701	-	1/1/13/20	11/27/103/115	-
19	LHG	b	5004	-	-	25/48/48/53	-
14	CLA	H	1220	-	1/1/13/20	10/27/103/115	-
18	BCR	i	4020	-	-	12/29/63/63	0/2/2/2
20	LMG	U	5007	-	-	14/45/65/70	0/1/1/1
17	SF4	A	3001	1,2	-	-	0/6/5/5
14	CLA	B	1212	-	1/1/11/20	4/15/91/115	-
14	CLA	A	1128	-	1/1/14/20	15/33/109/115	-
14	CLA	a	1109	-	1/1/15/20	19/39/115/115	-
18	BCR	H	4013	-	-	11/29/63/63	0/2/2/2
14	CLA	b	1204	-	1/1/15/20	16/39/115/115	-
14	CLA	G	1129	-	1/1/12/20	7/21/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LHG	H	5004	-	-	25/48/48/53	-
14	CLA	H	1224	-	1/1/15/20	16/39/115/115	-
14	CLA	G	1107	1	1/1/11/20	5/15/91/115	-
14	CLA	H	1202	-	1/1/14/20	14/33/109/115	-
14	CLA	A	1130	-	1/1/13/20	9/27/103/115	-
15	F6C	b	1238	-	1/1/10/16	16/41/97/97	-
14	CLA	b	1201	-	1/1/13/20	7/27/103/115	-
14	CLA	G	1106	-	1/1/14/20	13/33/109/115	-
14	CLA	a	1127	-	1/1/15/20	13/39/115/115	-
14	CLA	H	1210	-	1/1/15/20	14/39/115/115	-
18	BCR	a	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	H	1205	-	1/1/15/20	10/39/115/115	-
18	BCR	m	4021	-	-	18/29/63/63	0/2/2/2
14	CLA	b	1217	-	1/1/13/20	13/27/103/115	-
21	LMT	a	6001	-	-	7/17/57/61	0/2/2/2
14	CLA	b	1022	-	1/1/15/20	19/39/115/115	-
15	F6C	H	1207	-	1/1/10/16	20/41/97/97	-
14	CLA	G	1122	-	1/1/13/20	12/27/103/115	-
14	CLA	B	1233	-	1/1/11/20	7/15/91/115	-
18	BCR	a	4011	-	-	17/29/63/63	0/2/2/2
14	CLA	a	1110	-	1/1/11/20	7/15/91/115	-
18	BCR	V	4021	-	-	18/29/63/63	0/2/2/2
14	CLA	H	1222	-	1/1/15/20	17/39/115/115	-
14	CLA	a	1119	-	1/1/15/20	9/39/115/115	-
14	CLA	B	1225	-	1/1/15/20	15/39/115/115	-
14	CLA	H	1232	-	1/1/11/20	2/15/91/115	-
14	CLA	H	1215	-	1/1/14/20	18/33/109/115	-
15	F6C	b	1207	-	1/1/10/16	20/41/97/97	-
14	CLA	A	1122	-	1/1/13/20	13/27/103/115	-
18	BCR	B	4010	-	-	10/29/63/63	0/2/2/2
18	BCR	G	4008	-	-	12/29/63/63	0/2/2/2
14	CLA	a	1130	-	1/1/13/20	9/27/103/115	-
18	BCR	H	4006	-	-	10/29/63/63	0/2/2/2
20	LMG	A	5005	-	-	19/41/61/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1203	-	1/1/15/20	17/39/115/115	-
14	CLA	b	1209	-	1/1/11/20	5/15/91/115	-
14	CLA	H	1234	-	1/1/15/20	18/39/115/115	-
14	CLA	G	1110	-	1/1/11/20	7/15/91/115	-
14	CLA	B	1236	-	1/1/11/20	3/15/91/115	-
14	CLA	B	1229	-	1/1/14/20	14/33/109/115	-
14	CLA	A	1133	-	1/1/14/20	9/33/109/115	-
14	CLA	G	1119	-	1/1/15/20	9/39/115/115	-
14	CLA	A	1114	-	1/1/11/20	11/15/91/115	-
14	CLA	A	1102	-	1/1/14/20	14/33/109/115	-
14	CLA	G	1134	-	1/1/11/20	5/15/91/115	-
18	BCR	B	4017	-	-	13/29/63/63	0/2/2/2
13	CL0	A	1011	-	3/3/20/25	10/37/135/135	-
14	CLA	A	1111	-	1/1/14/20	13/33/109/115	-
14	CLA	B	1216	-	1/1/15/20	21/39/115/115	-
14	CLA	b	1208	-	1/1/15/20	16/39/115/115	-
14	CLA	G	1012	-	1/1/15/20	11/39/115/115	-
14	CLA	b	1234	-	1/1/15/20	18/39/115/115	-
15	F6C	a	1121	-	1/1/6/16	9/17/73/97	-
14	CLA	b	1233	-	1/1/11/20	7/15/91/115	-
14	CLA	H	1236	-	1/1/11/20	3/15/91/115	-
14	CLA	G	1103	-	1/1/14/20	13/33/109/115	-
14	CLA	B	1213	-	1/1/15/20	16/39/115/115	-
14	CLA	b	1212	-	1/1/11/20	4/15/91/115	-
14	CLA	H	1201	-	1/1/13/20	7/27/103/115	-
14	CLA	b	1214	-	1/1/15/20	17/39/115/115	-
14	CLA	U	1502	-	1/1/14/20	11/33/109/115	-
14	CLA	G	1101	-	1/1/11/20	8/15/91/115	-
14	CLA	k	1401	-	1/1/11/20	9/15/91/115	-
14	CLA	H	1218	-	1/1/11/20	6/15/91/115	-
14	CLA	G	1133	-	1/1/14/20	9/33/109/115	-
14	CLA	G	1104	-	1/1/15/20	9/39/115/115	-
18	BCR	a	4001	-	-	14/29/63/63	0/2/2/2
14	CLA	B	1022	-	1/1/15/20	19/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1116	-	1/1/13/20	12/27/103/115	-
18	BCR	M	4021	-	-	18/29/63/63	0/2/2/2
21	LMT	A	6002	-	-	8/14/54/61	0/2/2/2
14	CLA	A	1135	-	1/1/14/20	14/33/109/115	-
17	SF4	C	3003	3	-	-	0/6/5/5
14	CLA	B	1231	2	1/1/13/20	7/27/103/115	-
14	CLA	G	1128	-	1/1/14/20	15/33/109/115	-
14	CLA	b	1223	-	1/1/15/20	17/39/115/115	-
14	CLA	A	1127	-	1/1/15/20	13/39/115/115	-
14	CLA	B	1202	-	1/1/14/20	14/33/109/115	-
14	CLA	a	1137	-	1/1/12/20	5/21/97/115	-
18	BCR	A	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	b	1218	-	1/1/11/20	6/15/91/115	-
18	BCR	G	4001	-	-	14/29/63/63	0/2/2/2
14	CLA	b	1231	2	1/1/13/20	7/27/103/115	-
14	CLA	G	1131	-	1/1/14/20	14/33/109/115	-
14	CLA	G	1112	-	1/1/13/20	14/27/103/115	-
14	CLA	a	1115	-	1/1/15/20	20/39/115/115	-
14	CLA	B	1206	2	1/1/11/20	5/15/91/115	-
14	CLA	b	1227	-	1/1/11/20	7/15/91/115	-
14	CLA	b	1211	-	1/1/15/20	18/39/115/115	-
14	CLA	G	1117	-	1/1/15/20	19/39/115/115	-
18	BCR	B	4006	-	-	10/29/63/63	0/2/2/2
14	CLA	b	1205	-	1/1/15/20	10/39/115/115	-
14	CLA	a	1118	-	1/1/13/20	10/27/103/115	-
20	LMG	L	5007	-	-	15/45/65/70	0/1/1/1
14	CLA	a	1101	-	1/1/11/20	8/15/91/115	-
14	CLA	a	1138	-	1/1/14/20	15/33/109/115	-
14	CLA	A	1118	-	1/1/13/20	10/27/103/115	-
14	CLA	B	1220	-	1/1/13/20	10/27/103/115	-
14	CLA	b	1206	2	1/1/11/20	5/15/91/115	-
15	F6C	H	1237	-	1/1/10/16	18/41/97/97	-
14	CLA	A	1125	-	1/1/15/20	18/39/115/115	-
17	SF4	c	3002	3	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	1104	-	1/1/15/20	9/39/115/115	-
18	BCR	B	4009	-	-	8/29/63/63	0/2/2/2
14	CLA	b	1229	-	1/1/14/20	14/33/109/115	-
14	CLA	A	1120	-	1/1/11/20	9/15/91/115	-
14	CLA	B	1224	-	1/1/15/20	16/39/115/115	-
14	CLA	B	1228	-	1/1/13/20	14/27/103/115	-
16	PQN	b	2002	-	-	12/23/43/43	0/2/2/2
18	BCR	a	4002	-	-	6/29/63/63	0/2/2/2
20	LMG	R	5006	-	-	10/32/52/70	0/1/1/1
18	BCR	b	4010	-	-	10/29/63/63	0/2/2/2
14	CLA	a	1116	-	1/1/13/20	12/27/103/115	-
14	CLA	G	1140	-	1/1/15/20	21/39/115/115	-
14	CLA	l	1501	10	1/1/15/20	12/39/115/115	-
14	CLA	B	1210	-	1/1/15/20	14/39/115/115	-
18	BCR	B	4014	-	-	7/29/63/63	0/2/2/2
18	BCR	B	4013	-	-	11/29/63/63	0/2/2/2
14	CLA	H	1209	-	1/1/11/20	5/15/91/115	-
14	CLA	a	1131	-	1/1/14/20	14/33/109/115	-
14	CLA	A	1138	-	1/1/14/20	15/33/109/115	-
17	SF4	C	3002	3	-	-	0/6/5/5
15	F6C	A	1121	-	1/1/6/16	9/17/73/97	-
14	CLA	A	1101	-	1/1/11/20	8/15/91/115	-
17	SF4	N	3002	3	-	-	0/6/5/5
18	BCR	G	4002	-	-	6/29/63/63	0/2/2/2
14	CLA	B	1222	-	1/1/15/20	17/39/115/115	-
18	BCR	U	4019	-	-	12/29/63/63	0/2/2/2
14	CLA	G	1136	-	1/1/15/20	19/39/115/115	-
18	BCR	B	4016	-	-	10/29/63/63	0/2/2/2
14	CLA	A	1104	-	1/1/15/20	9/39/115/115	-
18	BCR	b	4014	-	-	7/29/63/63	0/2/2/2
14	CLA	L	1502	-	1/1/14/20	11/33/109/115	-
17	SF4	c	3003	3	-	-	0/6/5/5
14	CLA	B	1215	-	1/1/14/20	18/33/109/115	-
14	CLA	H	1212	-	1/1/11/20	4/15/91/115	-
14	CLA	A	1124	-	1/1/13/20	11/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	1221	-	1/1/15/20	10/39/115/115	-
18	BCR	H	4005	-	-	4/29/63/63	0/2/2/2
18	BCR	b	4009	-	-	8/29/63/63	0/2/2/2
14	CLA	B	1219	-	1/1/11/20	5/15/91/115	-
18	BCR	G	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	B	1232	-	1/1/11/20	2/15/91/115	-
14	CLA	H	1204	-	1/1/15/20	16/39/115/115	-
14	CLA	B	1214	-	1/1/15/20	17/39/115/115	-
14	CLA	b	1225	-	1/1/15/20	15/39/115/115	-
14	CLA	a	1140	-	1/1/15/20	21/39/115/115	-
14	CLA	B	1021	-	1/1/15/20	20/39/115/115	-
18	BCR	l	4022	-	-	6/29/63/63	0/2/2/2
14	CLA	a	1105	-	1/1/11/20	4/15/91/115	-
14	CLA	H	1208	-	1/1/15/20	16/39/115/115	-
18	BCR	A	4001	-	-	14/29/63/63	0/2/2/2
14	CLA	H	1206	2	1/1/11/20	5/15/91/115	-
14	CLA	A	1131	-	1/1/14/20	14/33/109/115	-
18	BCR	b	4017	-	-	13/29/63/63	0/2/2/2
14	CLA	B	1209	-	1/1/11/20	5/15/91/115	-
14	CLA	B	1023	-	1/1/15/20	15/39/115/115	-
14	CLA	A	1126	-	1/1/14/20	21/33/109/115	-
17	SF4	a	3001	1,2	-	-	0/6/5/5
14	CLA	G	1125	-	1/1/15/20	18/39/115/115	-
14	CLA	G	1130	-	1/1/13/20	9/27/103/115	-
14	CLA	B	1223	-	1/1/15/20	17/39/115/115	-
18	BCR	H	4004	-	-	7/29/63/63	0/2/2/2
14	CLA	a	1108	-	1/1/11/20	4/15/91/115	-
14	CLA	B	1226	-	1/1/15/20	11/39/115/115	-
15	F6C	B	1237	-	1/1/10/16	18/41/97/97	-
14	CLA	G	1105	-	1/1/11/20	4/15/91/115	-
14	CLA	G	1139	-	1/1/11/20	4/15/91/115	-
14	CLA	b	1228	-	1/1/13/20	14/27/103/115	-
18	BCR	B	4005	-	-	4/29/63/63	0/2/2/2
14	CLA	a	1103	-	1/1/14/20	13/33/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	l	4019	-	-	12/29/63/63	0/2/2/2
14	CLA	A	1140	-	1/1/15/20	21/39/115/115	-
14	CLA	A	1112	-	1/1/13/20	14/27/103/115	-
14	CLA	A	1129	-	1/1/12/20	7/21/97/115	-
15	F6C	H	1238	-	1/1/10/16	16/41/97/97	-
18	BCR	b	4004	-	-	7/29/63/63	0/2/2/2
14	CLA	X	1701	-	1/1/13/20	11/27/103/115	-
18	BCR	b	4005	-	-	4/29/63/63	0/2/2/2
14	CLA	A	1139	-	1/1/11/20	4/15/91/115	-
14	CLA	G	1108	-	1/1/11/20	4/15/91/115	-
14	CLA	B	1239	-	1/1/15/20	22/39/115/115	-
18	BCR	I	4020	-	-	12/29/63/63	0/2/2/2
14	CLA	G	1126	-	1/1/14/20	21/33/109/115	-
18	BCR	B	4004	-	-	7/29/63/63	0/2/2/2
14	CLA	H	1227	-	1/1/11/20	7/15/91/115	-
16	PQN	G	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	A	1123	-	1/1/14/20	13/33/109/115	-
14	CLA	a	1113	-	1/1/11/20	9/15/91/115	-
18	BCR	A	4007	-	-	12/29/63/63	0/2/2/2
20	LMG	a	5005	-	-	19/41/61/70	0/1/1/1
15	F6C	H	1230	-	1/1/6/16	8/17/73/97	-
18	BCR	b	4016	-	-	10/29/63/63	0/2/2/2
14	CLA	U	1503	-	1/1/15/20	15/39/115/115	-
14	CLA	H	1023	-	1/1/15/20	15/39/115/115	-
21	LMT	G	6001	-	-	7/17/57/61	0/2/2/2
14	CLA	a	1012	-	1/1/15/20	11/39/115/115	-
14	CLA	H	1235	-	1/1/14/20	12/33/109/115	-
14	CLA	a	1114	-	1/1/11/20	11/15/91/115	-
14	CLA	A	1107	1	1/1/11/20	5/15/91/115	-
14	CLA	U	1501	10	1/1/15/20	12/39/115/115	-
18	BCR	R	4018	-	-	8/29/63/63	0/2/2/2
18	BCR	U	4022	-	-	6/29/63/63	0/2/2/2
20	LMG	i	5006	-	-	10/32/52/70	0/1/1/1
18	BCR	A	4002	-	-	6/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	1021	-	1/1/15/20	20/39/115/115	-
14	CLA	A	1106	-	1/1/14/20	13/33/109/115	-
20	LMG	G	5005	-	-	19/41/61/70	0/1/1/1
18	BCR	A	4011	-	-	17/29/63/63	0/2/2/2
14	CLA	a	1123	-	1/1/14/20	13/33/109/115	-
14	CLA	A	1109	-	1/1/15/20	19/39/115/115	-
14	CLA	b	1236	-	1/1/11/20	3/15/91/115	-
14	CLA	a	1135	-	1/1/14/20	14/33/109/115	-
14	CLA	G	1114	-	1/1/11/20	11/15/91/115	-
14	CLA	A	1110	-	1/1/11/20	7/15/91/115	-
18	BCR	i	4018	-	-	8/29/63/63	0/2/2/2
14	CLA	L	1501	10	1/1/15/20	12/39/115/115	-
14	CLA	A	1119	-	1/1/15/20	9/39/115/115	-
18	BCR	L	4022	-	-	6/29/63/63	0/2/2/2
14	CLA	b	1210	-	1/1/15/20	14/39/115/115	-
14	CLA	b	1239	-	1/1/15/20	22/39/115/115	-
14	CLA	H	1229	-	1/1/14/20	14/33/109/115	-
14	CLA	A	1134	-	1/1/11/20	5/15/91/115	-
14	CLA	l	1502	-	1/1/14/20	11/33/109/115	-
14	CLA	b	1216	-	1/1/15/20	21/39/115/115	-
14	CLA	B	1204	-	1/1/15/20	15/39/115/115	-
14	CLA	H	1233	-	1/1/11/20	7/15/91/115	-
14	CLA	B	1235	-	1/1/14/20	12/33/109/115	-
14	CLA	A	1012	-	1/1/15/20	11/39/115/115	-
18	BCR	G	4007	-	-	12/29/63/63	0/2/2/2
13	CL0	G	1011	-	3/3/20/25	10/37/135/135	-
15	F6C	b	1237	-	1/1/10/16	18/41/97/97	-
16	PQN	a	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	a	1136	-	1/1/15/20	19/39/115/115	-
14	CLA	B	1234	-	1/1/15/20	18/39/115/115	-
14	CLA	A	1103	-	1/1/14/20	13/33/109/115	-
14	CLA	b	1213	-	1/1/15/20	16/39/115/115	-
21	LMT	a	6002	-	-	8/14/54/61	0/2/2/2
17	SF4	G	3001	1,2	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1116	-	1/1/13/20	12/27/103/115	-
14	CLA	T	1401	-	1/1/11/20	9/15/91/115	-
14	CLA	l	1503	-	1/1/15/20	15/39/115/115	-
14	CLA	b	1219	-	1/1/11/20	5/15/91/115	-
14	CLA	H	1211	-	1/1/15/20	18/39/115/115	-
14	CLA	G	1109	-	1/1/15/20	19/39/115/115	-
18	BCR	a	4008	-	-	12/29/63/63	0/2/2/2
16	PQN	H	2002	-	-	12/23/43/43	0/2/2/2
14	CLA	B	1201	-	1/1/13/20	7/27/103/115	-
20	LMG	I	5006	-	-	10/32/52/70	0/1/1/1
14	CLA	A	1137	-	1/1/12/20	5/21/97/115	-
14	CLA	K	1401	-	1/1/11/20	9/15/91/115	-
21	LMT	G	6002	-	-	7/14/54/61	0/2/2/2
14	CLA	a	1013	-	1/1/14/20	12/33/109/115	-
14	CLA	B	1203	-	1/1/15/20	17/39/115/115	-
14	CLA	b	1202	-	1/1/14/20	14/33/109/115	-
20	LMG	B	5002	-	-	13/41/61/70	0/1/1/1
17	SF4	N	3003	3	-	-	0/6/5/5
14	CLA	A	1132	-	1/1/15/20	14/39/115/115	-
19	LHG	a	5001	-	-	23/46/46/53	-
14	CLA	a	1125	-	1/1/15/20	18/39/115/115	-
14	CLA	G	1127	-	1/1/15/20	13/39/115/115	-
20	LMG	l	5007	-	-	14/45/65/70	0/1/1/1
18	BCR	H	4010	-	-	10/29/63/63	0/2/2/2
14	CLA	a	1120	-	1/1/11/20	9/15/91/115	-
14	CLA	B	1218	-	1/1/11/20	6/15/91/115	-
14	CLA	A	1108	-	1/1/11/20	4/15/91/115	-
14	CLA	G	1137	-	1/1/12/20	5/21/97/115	-
20	LMG	b	5002	-	-	13/41/61/70	0/1/1/1
18	BCR	b	4006	-	-	10/29/63/63	0/2/2/2
14	CLA	B	1227	-	1/1/11/20	7/15/91/115	-
14	CLA	B	1211	-	1/1/15/20	18/39/115/115	-
14	CLA	H	1228	-	1/1/13/20	14/27/103/115	-
18	BCR	G	4011	-	-	17/29/63/63	0/2/2/2

The worst 5 of 6019 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	1230	F6C	C1A-CHA	9.56	1.50	1.35
15	B	1230	F6C	C1A-CHA	9.54	1.50	1.35
15	H	1230	F6C	C1A-CHA	9.53	1.50	1.35
15	b	1207	F6C	C1A-CHA	9.52	1.50	1.35
15	H	1207	F6C	C1A-CHA	9.51	1.50	1.35

The worst 5 of 8492 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	H	4010	BCR	C16-C17-C18	26.23	164.06	127.28
18	b	4010	BCR	C16-C17-C18	26.18	164.00	127.28
18	B	4010	BCR	C16-C17-C18	26.16	163.97	127.28
18	H	4017	BCR	C20-C21-C22	24.75	161.99	127.28
18	B	4017	BCR	C20-C21-C22	24.75	161.99	127.28

5 of 276 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	G	1011	CL0	NC
13	G	1011	CL0	NA
13	G	1011	CL0	ND
13	a	1011	CL0	NC
13	a	1011	CL0	NA

5 of 4356 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	1013	CLA	C1A-C2A-CAA-CBA
14	G	1013	CLA	C3A-C2A-CAA-CBA
14	G	1013	CLA	C11-C10-C8-C9
14	G	1101	CLA	CHA-CBD-CGD-O1D
14	G	1101	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

325 monomers are involved in 1089 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1230	F6C	1	0
14	b	1220	CLA	3	0
14	A	1113	CLA	1	0
14	G	1013	CLA	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	1226	CLA	1	0
14	G	1118	CLA	1	0
16	A	2001	PQN	11	0
14	A	1136	CLA	5	0
21	A	6001	LMT	1	0
16	B	2002	PQN	6	0
18	A	4008	BCR	5	0
14	b	1224	CLA	8	0
14	H	1217	CLA	2	0
14	a	1132	CLA	6	0
14	G	1132	CLA	5	0
19	B	5004	LHG	1	0
15	B	1207	F6C	1	0
19	A	5001	LHG	3	0
14	a	1133	CLA	1	0
14	a	1134	CLA	2	0
14	b	1235	CLA	2	0
14	a	1124	CLA	6	0
14	H	1225	CLA	5	0
14	L	1503	CLA	6	0
15	B	1238	F6C	1	0
14	H	1219	CLA	4	0
14	G	1138	CLA	5	0
18	H	4014	BCR	2	0
14	a	1111	CLA	6	0
14	A	1115	CLA	5	0
14	b	1222	CLA	9	0
18	R	4020	BCR	5	0
14	G	1113	CLA	2	0
18	L	4019	BCR	3	0
14	a	1128	CLA	2	0
14	B	1217	CLA	2	0
14	b	1215	CLA	3	0
14	H	1221	CLA	9	0
14	H	1213	CLA	5	0
14	H	1021	CLA	7	0
18	H	4009	BCR	7	0
18	I	4018	BCR	2	0
14	a	1126	CLA	5	0
14	W	1701	CLA	5	0
18	b	4013	BCR	2	0
14	G	1124	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	1221	CLA	9	0
14	a	1102	CLA	2	0
14	a	1107	CLA	2	0
14	G	1120	CLA	2	0
14	H	1216	CLA	7	0
14	a	1122	CLA	2	0
14	b	1203	CLA	5	0
14	b	1232	CLA	1	0
14	H	1239	CLA	2	0
19	G	5001	LHG	2	0
20	H	5002	LMG	4	0
18	H	4017	BCR	4	0
14	B	1205	CLA	11	0
14	a	1106	CLA	4	0
14	H	1214	CLA	3	0
14	H	1226	CLA	2	0
14	b	1023	CLA	9	0
18	a	4007	BCR	1	0
13	a	1011	CL0	4	0
14	A	1117	CLA	4	0
14	a	1112	CLA	3	0
15	b	1230	F6C	1	0
14	a	1129	CLA	1	0
14	G	1102	CLA	1	0
14	G	1115	CLA	5	0
14	A	1013	CLA	4	0
14	a	1117	CLA	3	0
14	a	1139	CLA	1	0
14	G	1111	CLA	6	0
14	H	1223	CLA	4	0
14	G	1135	CLA	3	0
14	B	1208	CLA	3	0
14	G	1123	CLA	2	0
18	H	4016	BCR	3	0
14	H	1022	CLA	6	0
14	H	1231	CLA	4	0
14	x	1701	CLA	3	0
14	H	1220	CLA	3	0
18	i	4020	BCR	5	0
20	U	5007	LMG	3	0
14	B	1212	CLA	3	0
14	A	1128	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a	1109	CLA	3	0
18	H	4013	BCR	3	0
14	b	1204	CLA	4	0
14	G	1129	CLA	1	0
19	H	5004	LHG	3	0
14	H	1224	CLA	8	0
14	G	1107	CLA	2	0
14	H	1202	CLA	4	0
15	b	1238	F6C	1	0
14	b	1201	CLA	6	0
14	G	1106	CLA	2	0
14	a	1127	CLA	3	0
14	H	1210	CLA	12	0
18	a	4003	BCR	2	0
14	H	1205	CLA	12	0
18	m	4021	BCR	5	0
14	b	1217	CLA	2	0
14	b	1022	CLA	6	0
14	G	1122	CLA	2	0
18	a	4011	BCR	6	0
14	a	1110	CLA	1	0
18	V	4021	BCR	4	0
14	H	1222	CLA	10	0
14	a	1119	CLA	5	0
14	B	1225	CLA	6	0
14	H	1232	CLA	1	0
14	H	1215	CLA	4	0
14	A	1122	CLA	1	0
18	B	4010	BCR	9	0
18	G	4008	BCR	5	0
18	H	4006	BCR	4	0
20	A	5005	LMG	5	0
14	H	1203	CLA	5	0
14	H	1234	CLA	10	0
14	B	1236	CLA	6	0
14	B	1229	CLA	4	0
14	A	1133	CLA	1	0
14	G	1119	CLA	6	0
14	A	1114	CLA	1	0
14	A	1102	CLA	2	0
14	G	1134	CLA	2	0
18	B	4017	BCR	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	1011	CL0	4	0
14	A	1111	CLA	5	0
14	B	1216	CLA	9	0
14	b	1208	CLA	4	0
14	G	1012	CLA	3	0
14	b	1234	CLA	9	0
14	H	1236	CLA	6	0
14	G	1103	CLA	5	0
14	B	1213	CLA	5	0
14	b	1212	CLA	4	0
14	H	1201	CLA	2	0
14	b	1214	CLA	3	0
14	U	1502	CLA	2	0
14	G	1133	CLA	1	0
14	G	1104	CLA	3	0
18	a	4001	BCR	5	0
14	B	1022	CLA	6	0
14	A	1116	CLA	9	0
18	M	4021	BCR	4	0
14	A	1135	CLA	3	0
17	C	3003	SF4	1	0
14	B	1231	CLA	3	0
14	G	1128	CLA	1	0
14	b	1223	CLA	5	0
14	A	1127	CLA	3	0
14	B	1202	CLA	4	0
14	a	1137	CLA	1	0
18	A	4003	BCR	1	0
18	G	4001	BCR	5	0
14	b	1231	CLA	3	0
14	G	1131	CLA	5	0
14	G	1112	CLA	2	0
14	a	1115	CLA	4	0
14	B	1206	CLA	4	0
14	b	1227	CLA	4	0
14	b	1211	CLA	4	0
14	G	1117	CLA	4	0
18	B	4006	BCR	4	0
14	b	1205	CLA	11	0
14	a	1118	CLA	1	0
20	L	5007	LMG	5	0
14	a	1138	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	1118	CLA	1	0
14	B	1220	CLA	3	0
14	b	1206	CLA	5	0
14	A	1125	CLA	4	0
14	a	1104	CLA	2	0
18	B	4009	BCR	7	0
14	b	1229	CLA	5	0
14	A	1120	CLA	2	0
14	B	1224	CLA	9	0
14	B	1228	CLA	5	0
16	b	2002	PQN	5	0
18	a	4002	BCR	1	0
20	R	5006	LMG	4	0
18	b	4010	BCR	9	0
14	a	1116	CLA	8	0
14	G	1140	CLA	7	0
14	l	1501	CLA	6	0
14	B	1210	CLA	11	0
18	B	4014	BCR	4	0
18	B	4013	BCR	3	0
14	a	1131	CLA	5	0
14	A	1138	CLA	5	0
18	G	4002	BCR	3	0
14	B	1222	CLA	11	0
18	U	4019	BCR	2	0
14	G	1136	CLA	5	0
18	B	4016	BCR	2	0
14	A	1104	CLA	3	0
18	b	4014	BCR	5	0
14	L	1502	CLA	4	0
17	c	3003	SF4	1	0
14	B	1215	CLA	4	0
14	H	1212	CLA	3	0
14	A	1124	CLA	5	0
14	b	1221	CLA	10	0
18	H	4005	BCR	3	0
18	b	4009	BCR	6	0
14	B	1219	CLA	4	0
18	G	4003	BCR	2	0
14	B	1232	CLA	1	0
14	H	1204	CLA	7	0
14	B	1214	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	1225	CLA	6	0
14	a	1140	CLA	8	0
14	B	1021	CLA	7	0
18	l	4022	BCR	6	0
14	H	1208	CLA	2	0
18	A	4001	BCR	5	0
14	H	1206	CLA	5	0
14	A	1131	CLA	5	0
18	b	4017	BCR	3	0
14	B	1023	CLA	6	0
14	A	1126	CLA	4	0
14	G	1125	CLA	3	0
14	B	1223	CLA	5	0
18	H	4004	BCR	1	0
14	a	1108	CLA	1	0
14	B	1226	CLA	1	0
14	G	1139	CLA	1	0
14	b	1228	CLA	5	0
18	B	4005	BCR	3	0
14	a	1103	CLA	5	0
18	l	4019	BCR	2	0
14	A	1140	CLA	8	0
14	A	1112	CLA	3	0
14	A	1129	CLA	1	0
15	H	1238	F6C	1	0
18	b	4004	BCR	1	0
14	X	1701	CLA	5	0
18	b	4005	BCR	4	0
14	A	1139	CLA	1	0
14	G	1108	CLA	1	0
14	B	1239	CLA	4	0
18	I	4020	BCR	9	0
14	G	1126	CLA	4	0
14	H	1227	CLA	3	0
16	G	2001	PQN	8	0
14	A	1123	CLA	2	0
14	a	1113	CLA	2	0
18	A	4007	BCR	1	0
20	a	5005	LMG	2	0
15	H	1230	F6C	1	0
18	b	4016	BCR	2	0
14	U	1503	CLA	7	0

Continued on next page...

Continued from previous page...

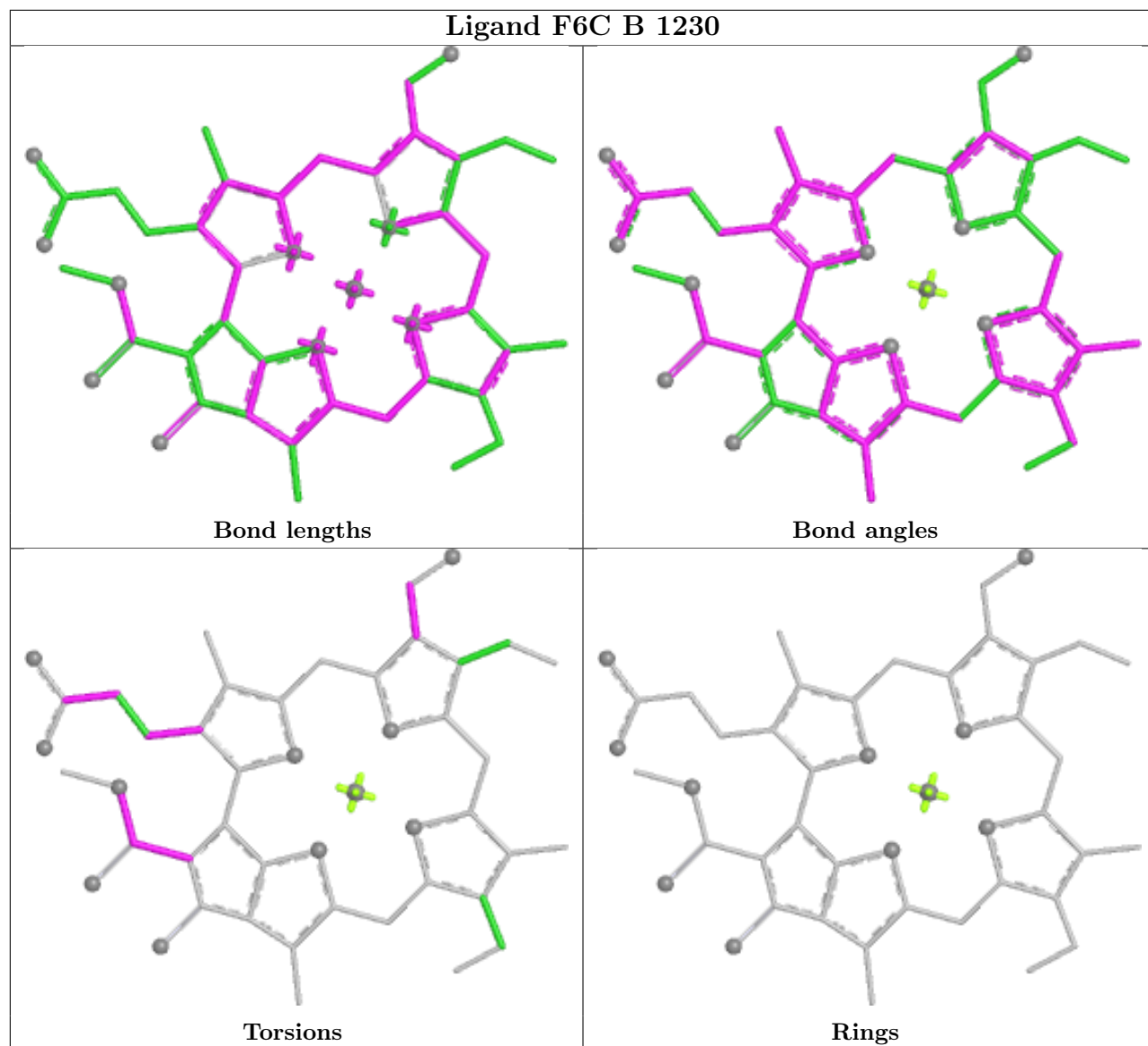
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	1023	CLA	7	0
21	G	6001	LMT	1	0
14	a	1012	CLA	5	0
14	H	1235	CLA	2	0
14	A	1107	CLA	2	0
14	U	1501	CLA	6	0
18	R	4018	BCR	5	0
18	U	4022	BCR	5	0
20	i	5006	LMG	1	0
18	A	4002	BCR	2	0
14	b	1021	CLA	8	0
14	A	1106	CLA	2	0
20	G	5005	LMG	5	0
18	A	4011	BCR	4	0
14	a	1123	CLA	2	0
14	A	1109	CLA	3	0
14	b	1236	CLA	7	0
14	a	1135	CLA	3	0
18	i	4018	BCR	3	0
14	L	1501	CLA	6	0
14	A	1119	CLA	7	0
18	L	4022	BCR	6	0
14	b	1210	CLA	10	0
14	b	1239	CLA	3	0
14	H	1229	CLA	4	0
14	A	1134	CLA	2	0
14	l	1502	CLA	3	0
14	b	1216	CLA	9	0
14	B	1204	CLA	5	0
14	H	1233	CLA	1	0
14	B	1235	CLA	2	0
14	A	1012	CLA	5	0
18	G	4007	BCR	1	0
13	G	1011	CL0	4	0
16	a	2001	PQN	10	0
14	a	1136	CLA	6	0
14	B	1234	CLA	9	0
14	A	1103	CLA	5	0
14	b	1213	CLA	4	0
14	G	1116	CLA	7	0
14	l	1503	CLA	6	0
14	b	1219	CLA	3	0

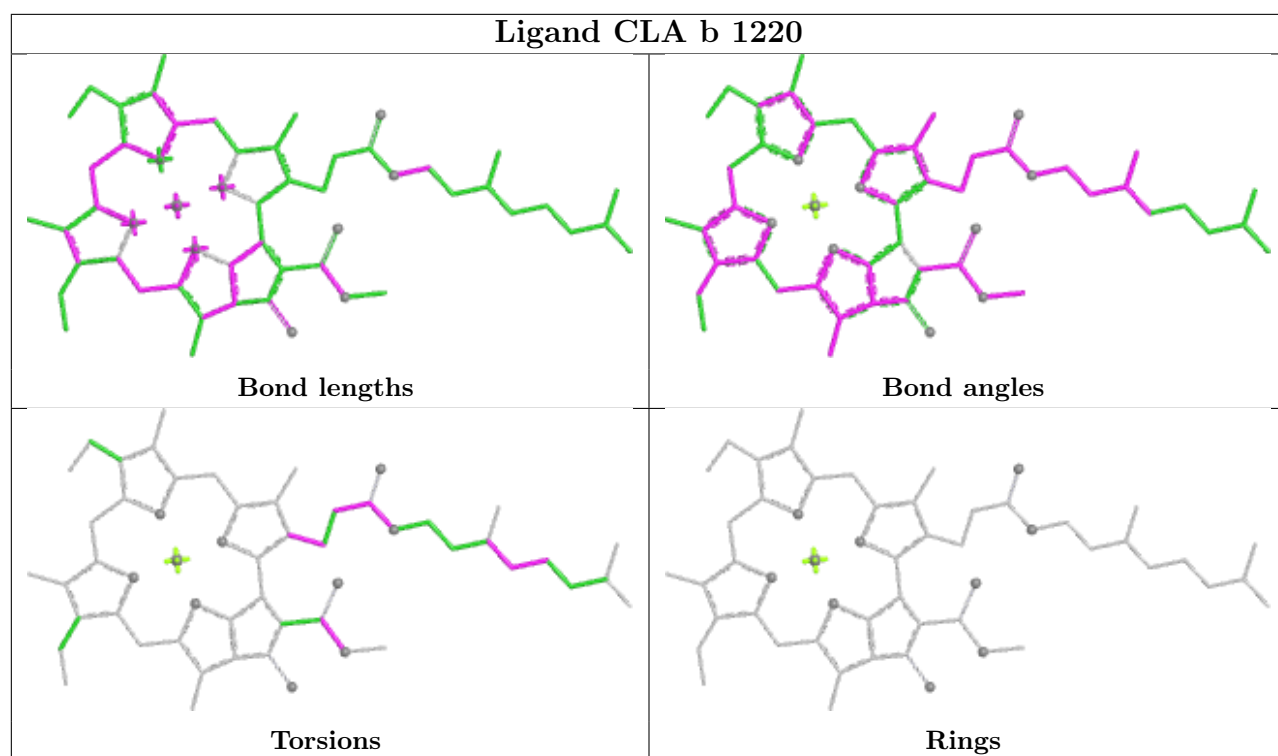
Continued on next page...

Continued from previous page...

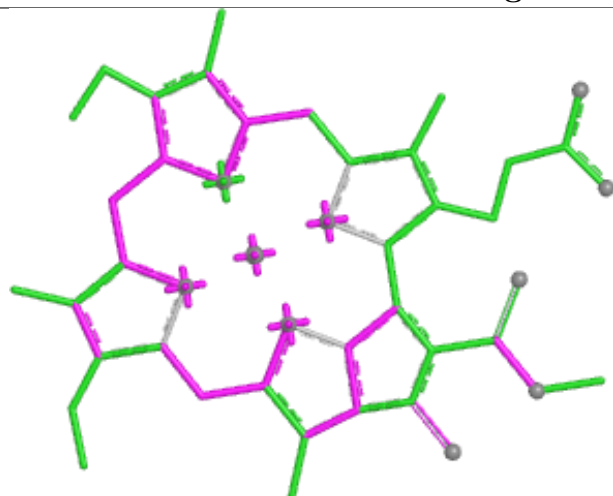
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	1211	CLA	4	0
14	G	1109	CLA	4	0
18	a	4008	BCR	6	0
16	H	2002	PQN	6	0
14	B	1201	CLA	4	0
20	I	5006	LMG	1	0
14	A	1137	CLA	1	0
14	a	1013	CLA	4	0
14	B	1203	CLA	4	0
14	b	1202	CLA	4	0
17	N	3003	SF4	1	0
20	B	5002	LMG	4	0
14	A	1132	CLA	6	0
19	a	5001	LHG	3	0
14	a	1125	CLA	4	0
14	G	1127	CLA	3	0
20	I	5007	LMG	4	0
18	H	4010	BCR	9	0
14	a	1120	CLA	2	0
14	A	1108	CLA	1	0
14	G	1137	CLA	1	0
20	b	5002	LMG	4	0
18	b	4006	BCR	4	0
14	B	1227	CLA	3	0
14	B	1211	CLA	5	0
14	H	1228	CLA	5	0
18	G	4011	BCR	5	0

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

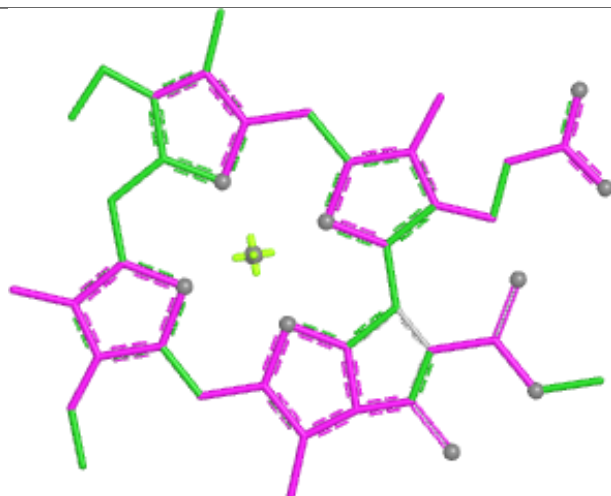




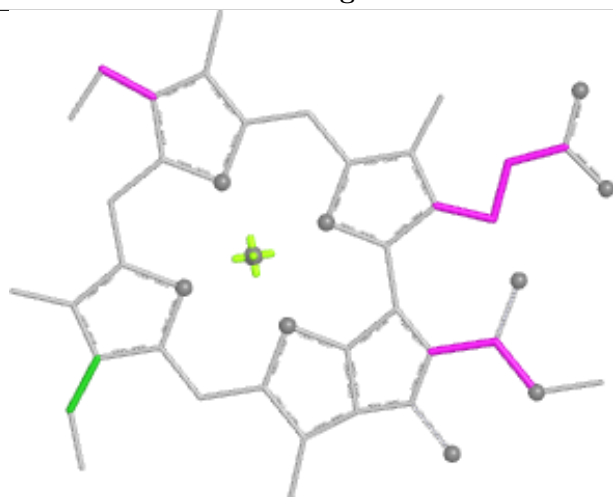
Ligand CLA A 1113



Bond lengths



Bond angles

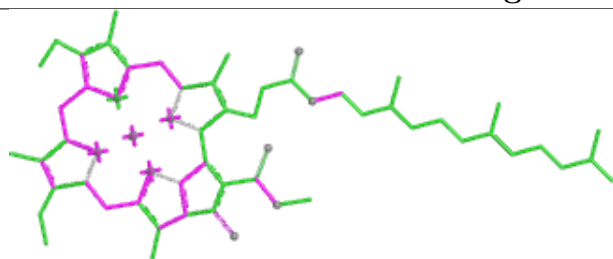


Torsions

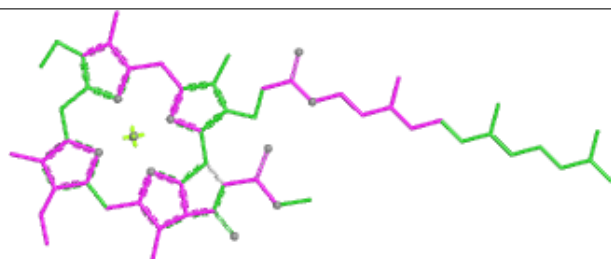


Rings

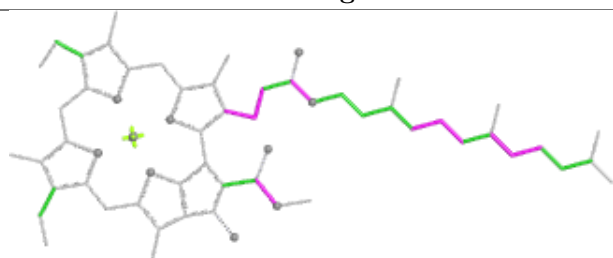
Ligand CLA G 1013



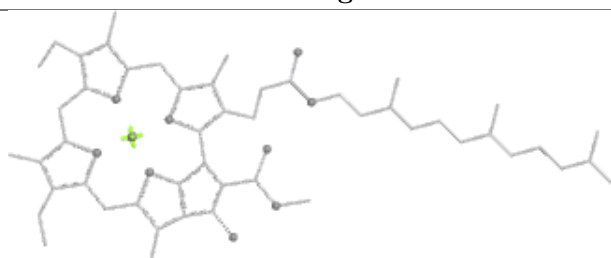
Bond lengths



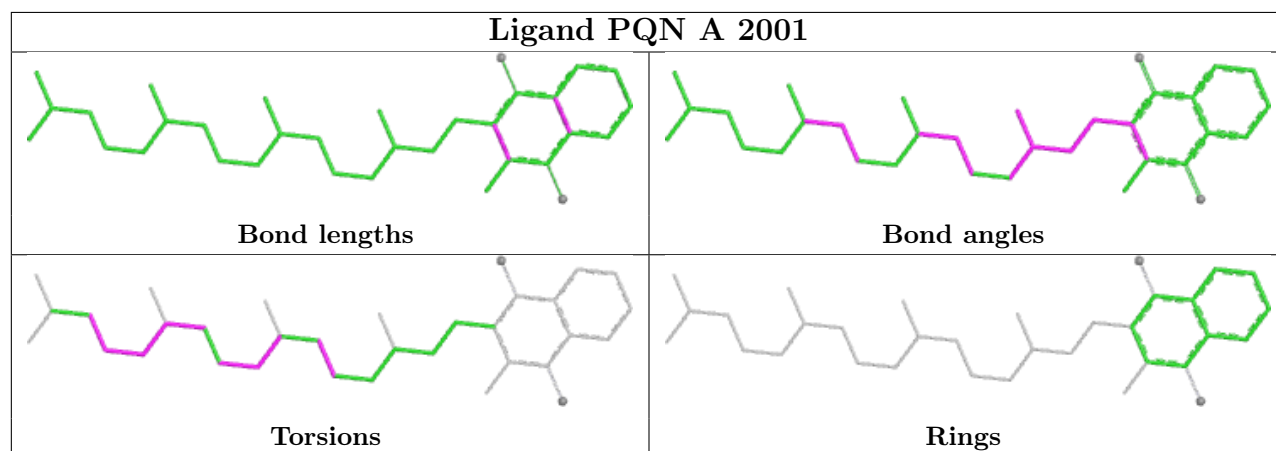
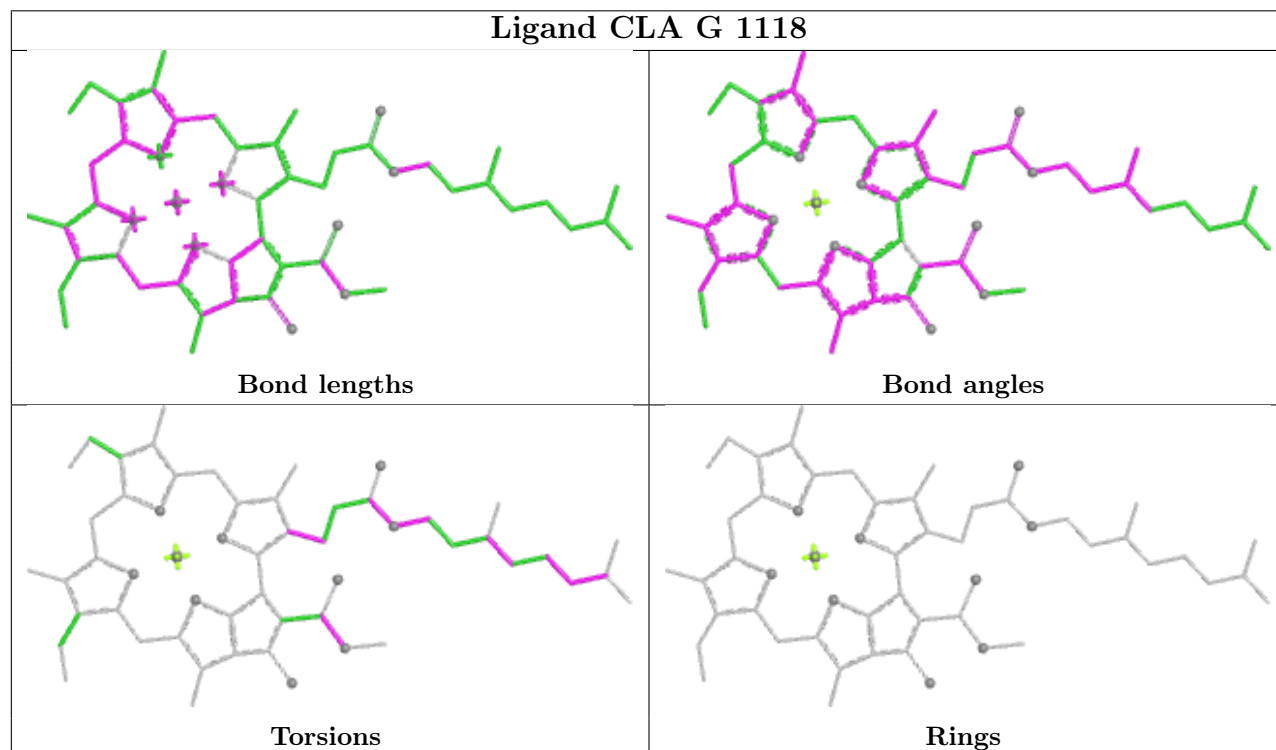
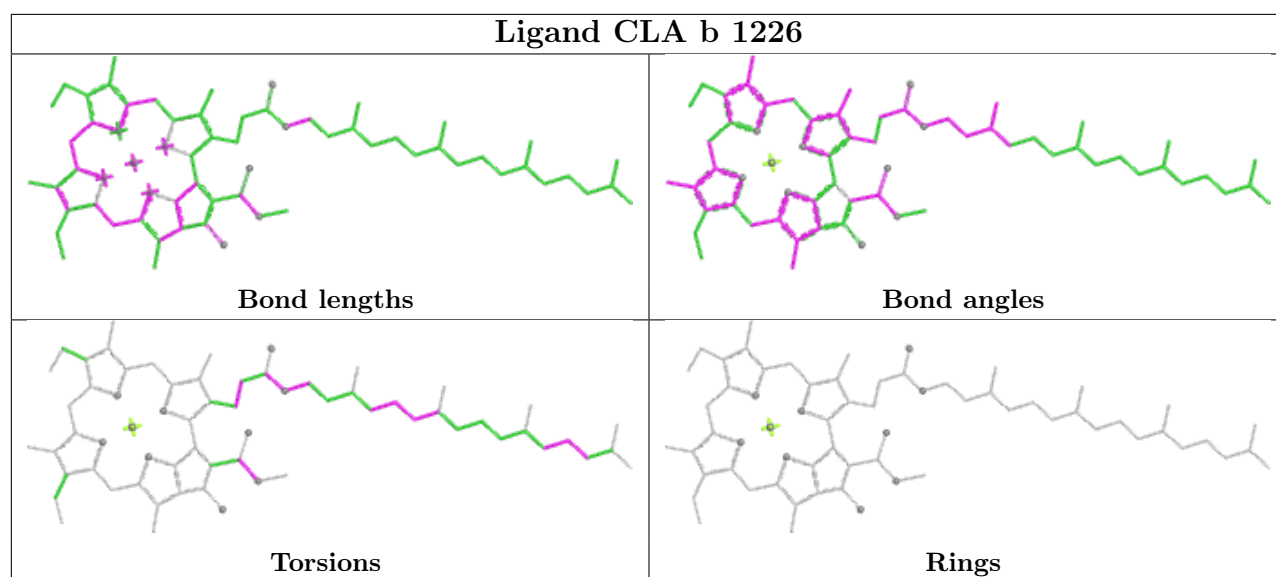
Bond angles

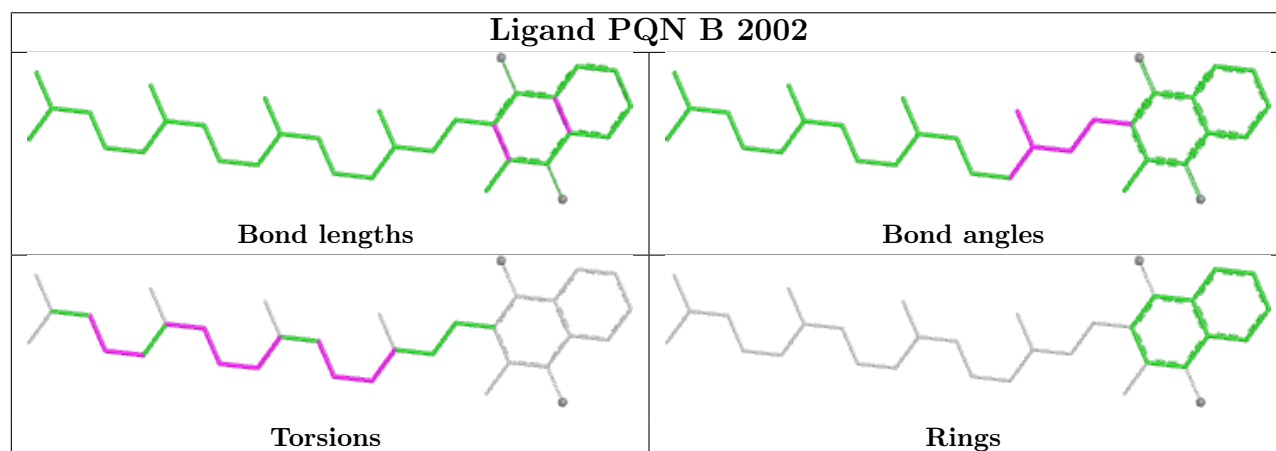
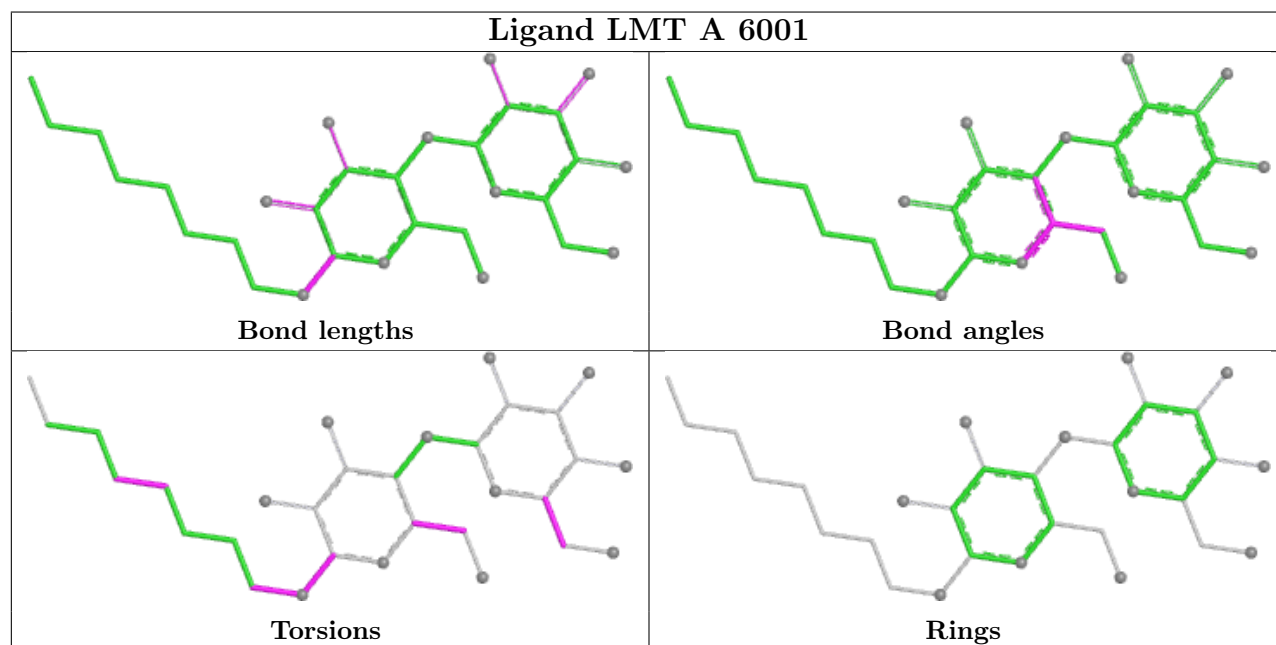
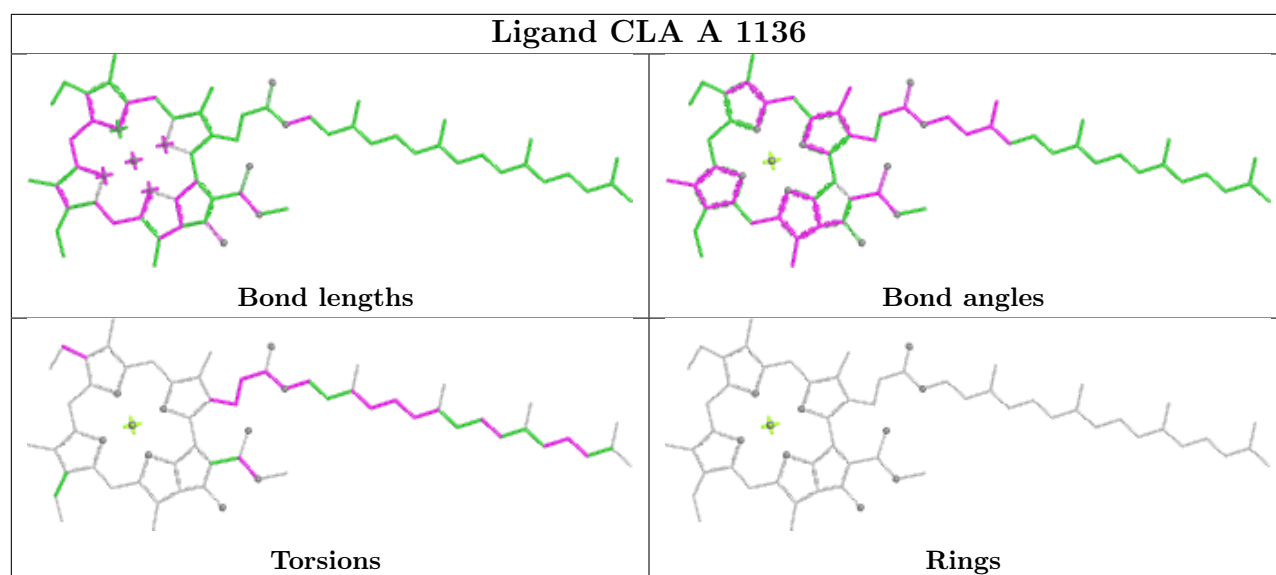


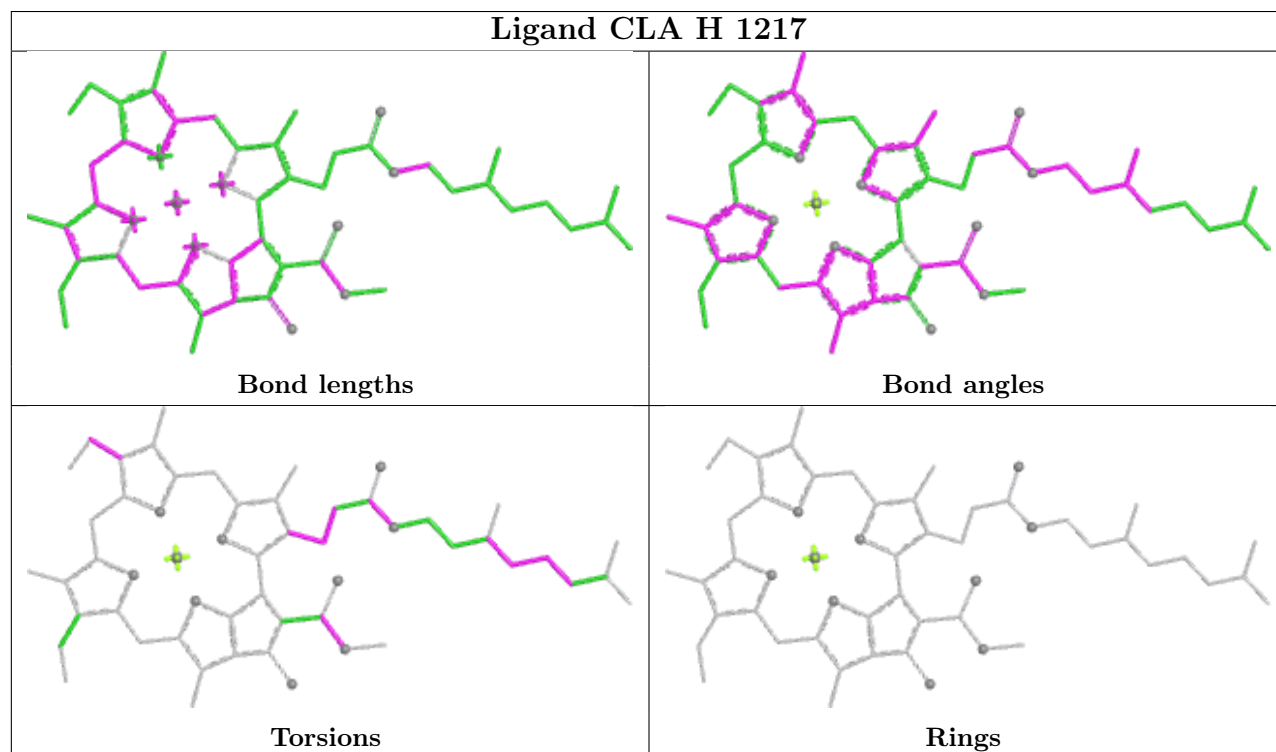
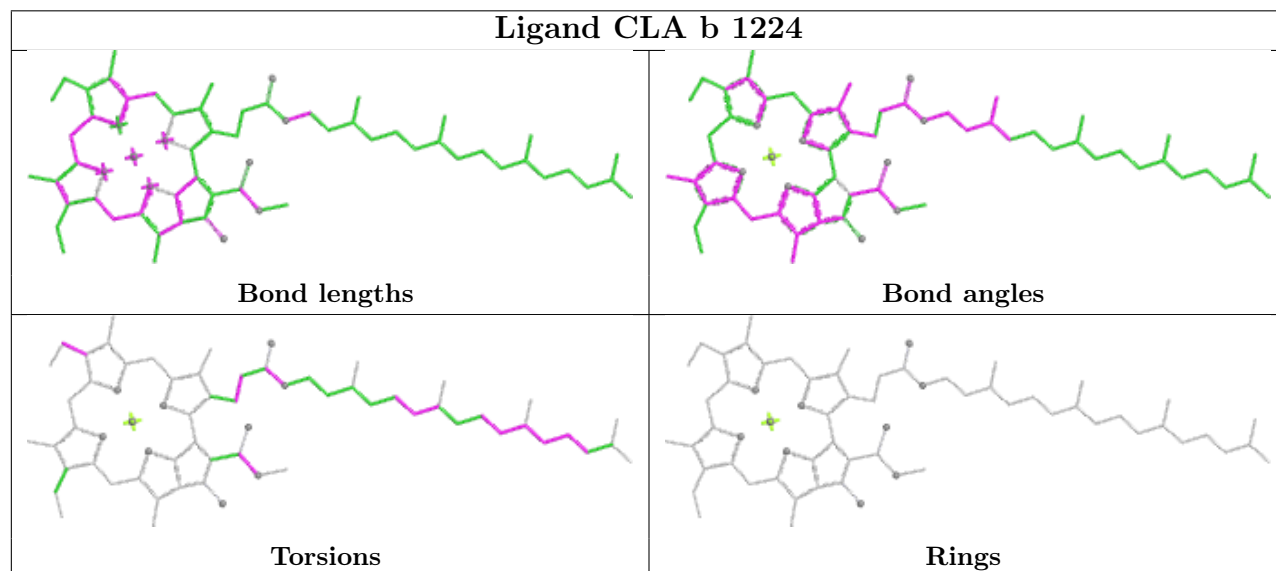
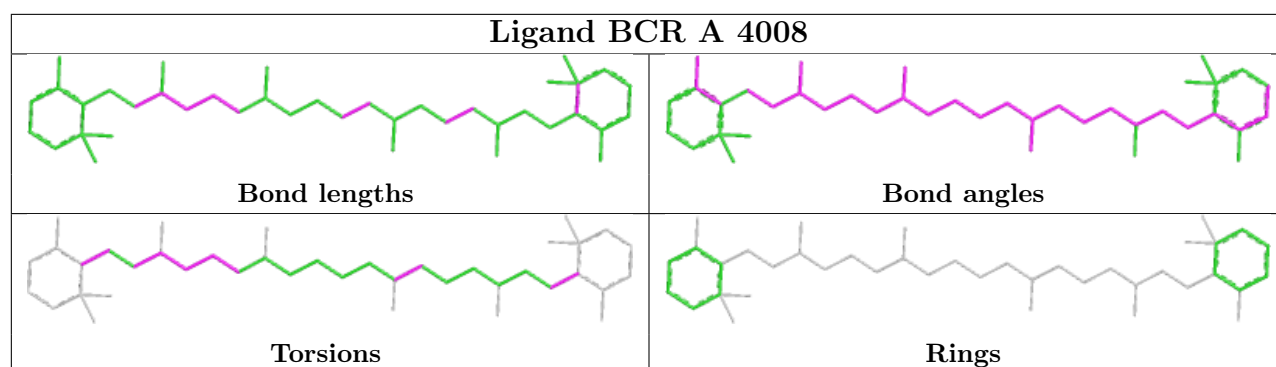
Torsions

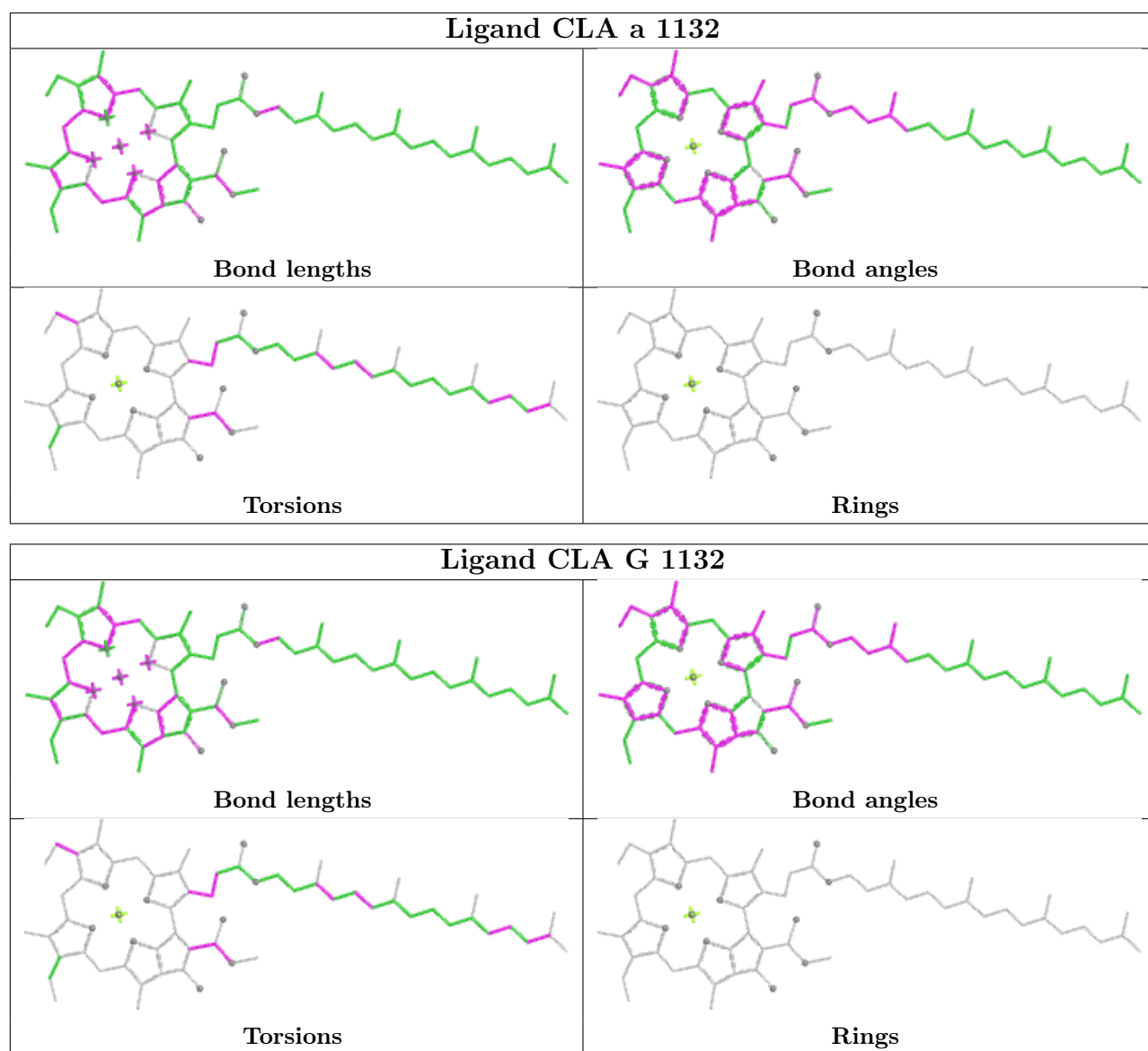


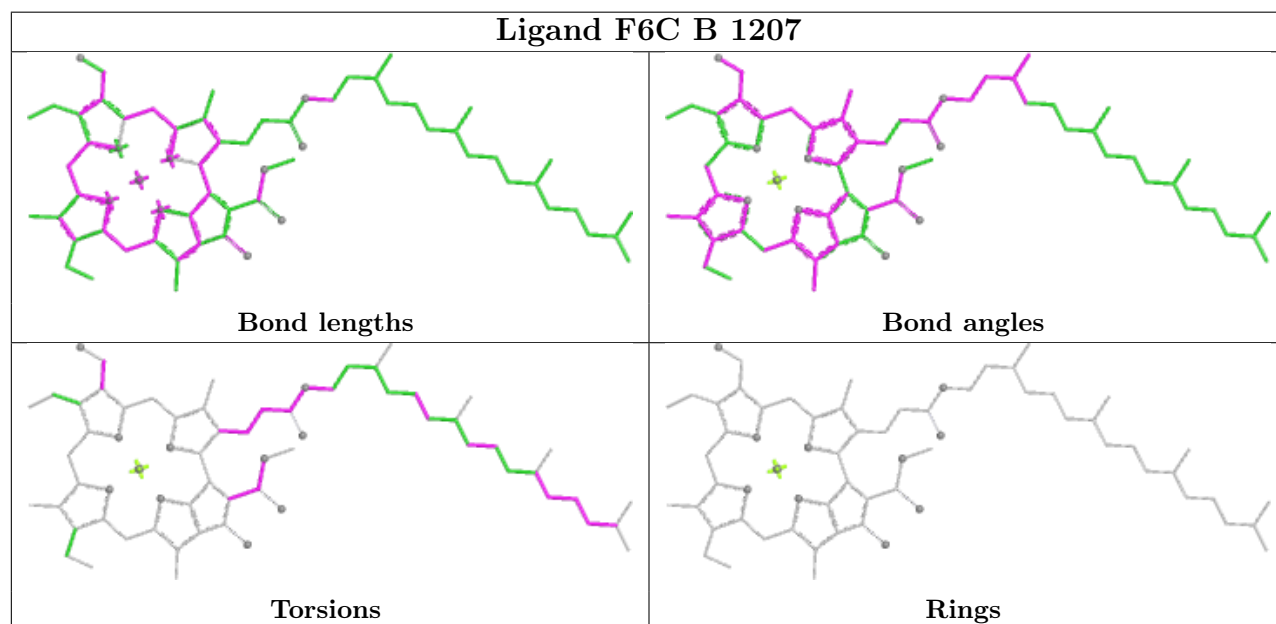
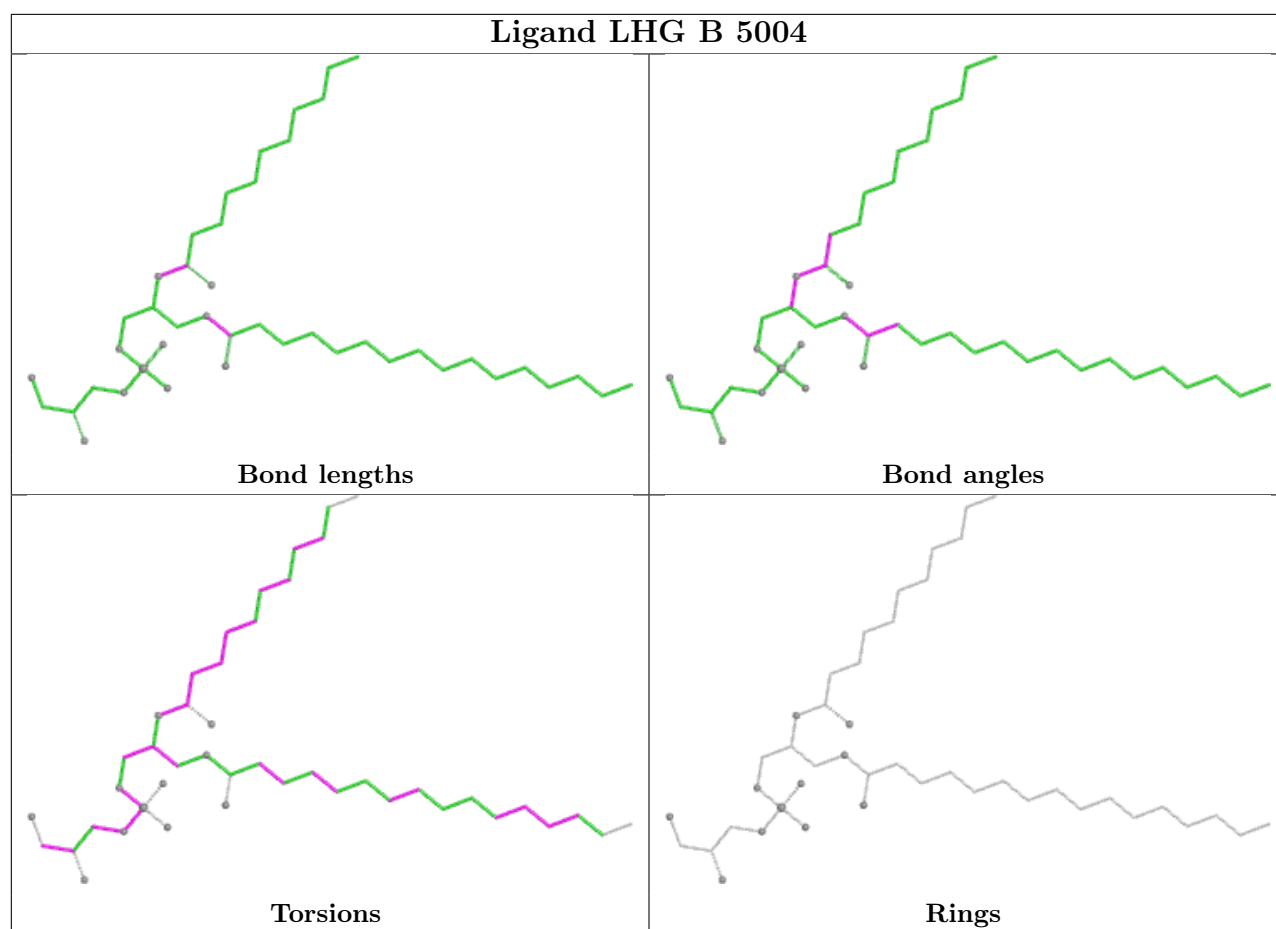
Rings

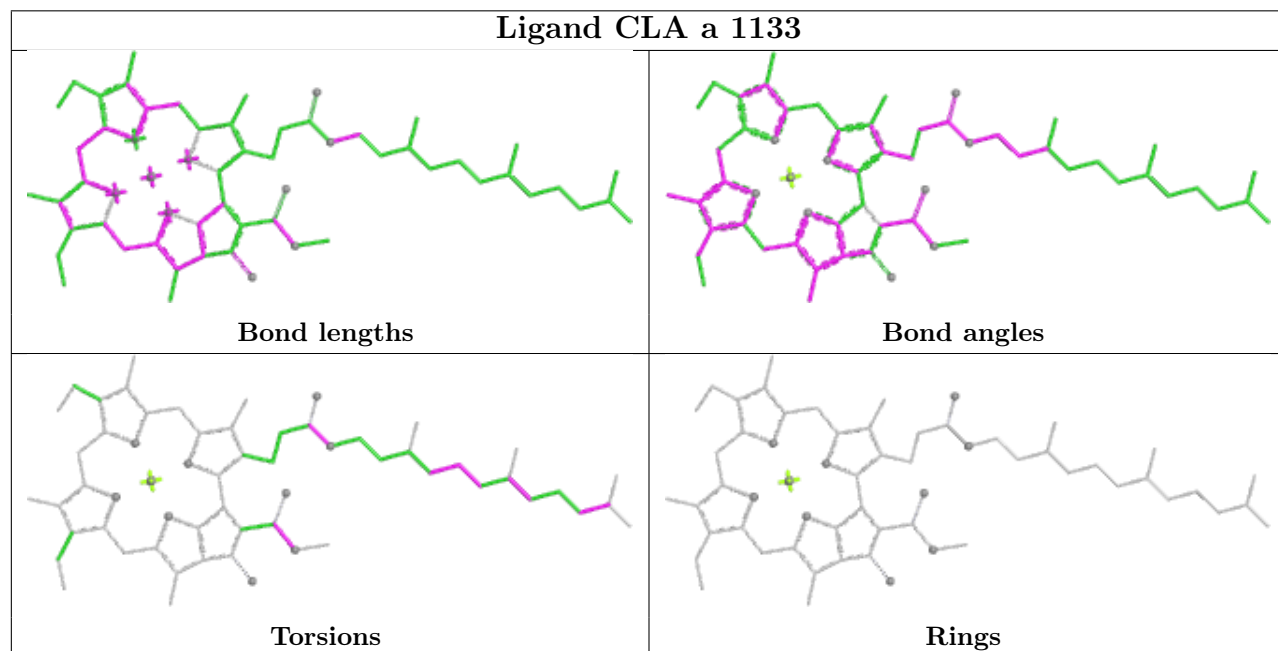
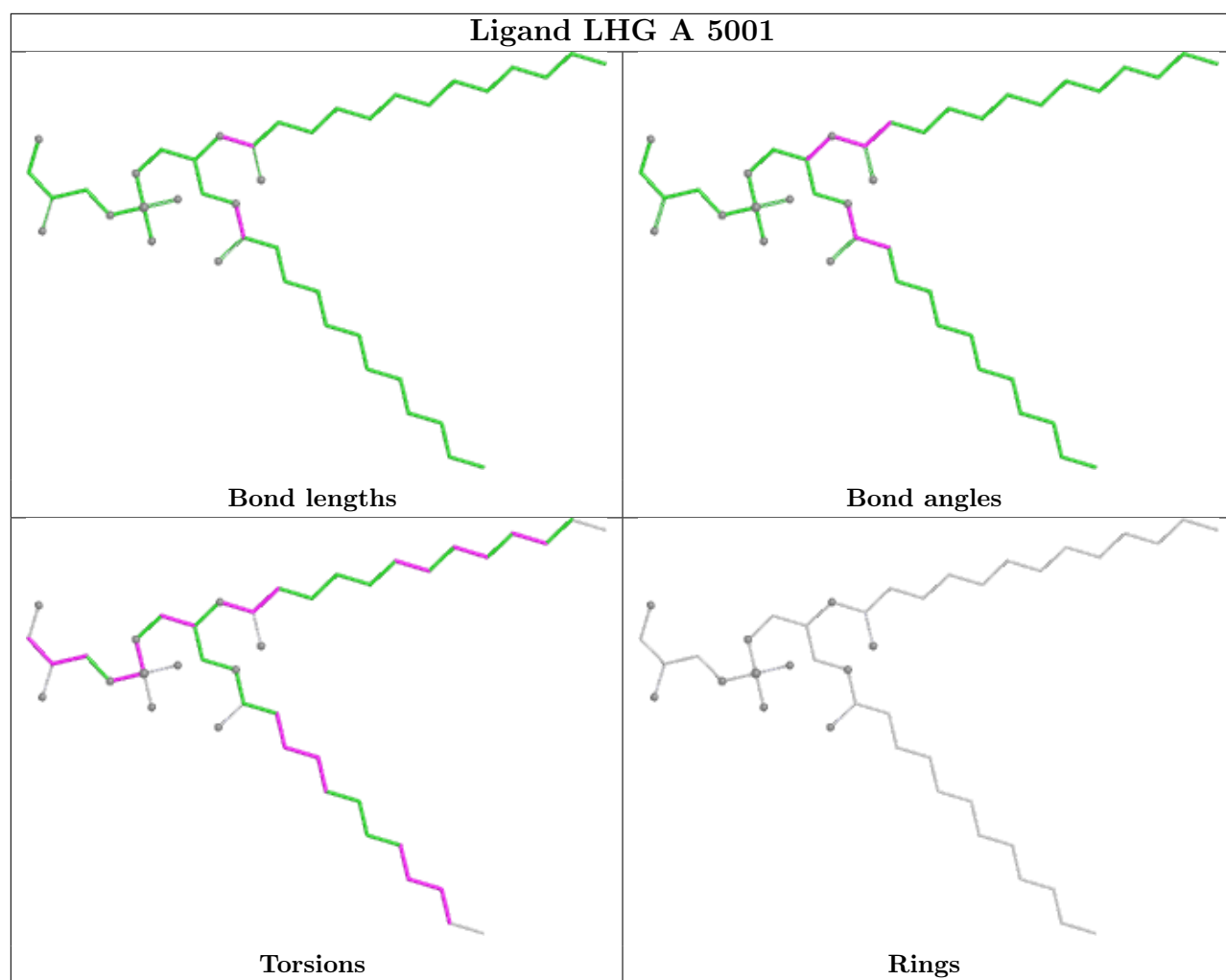


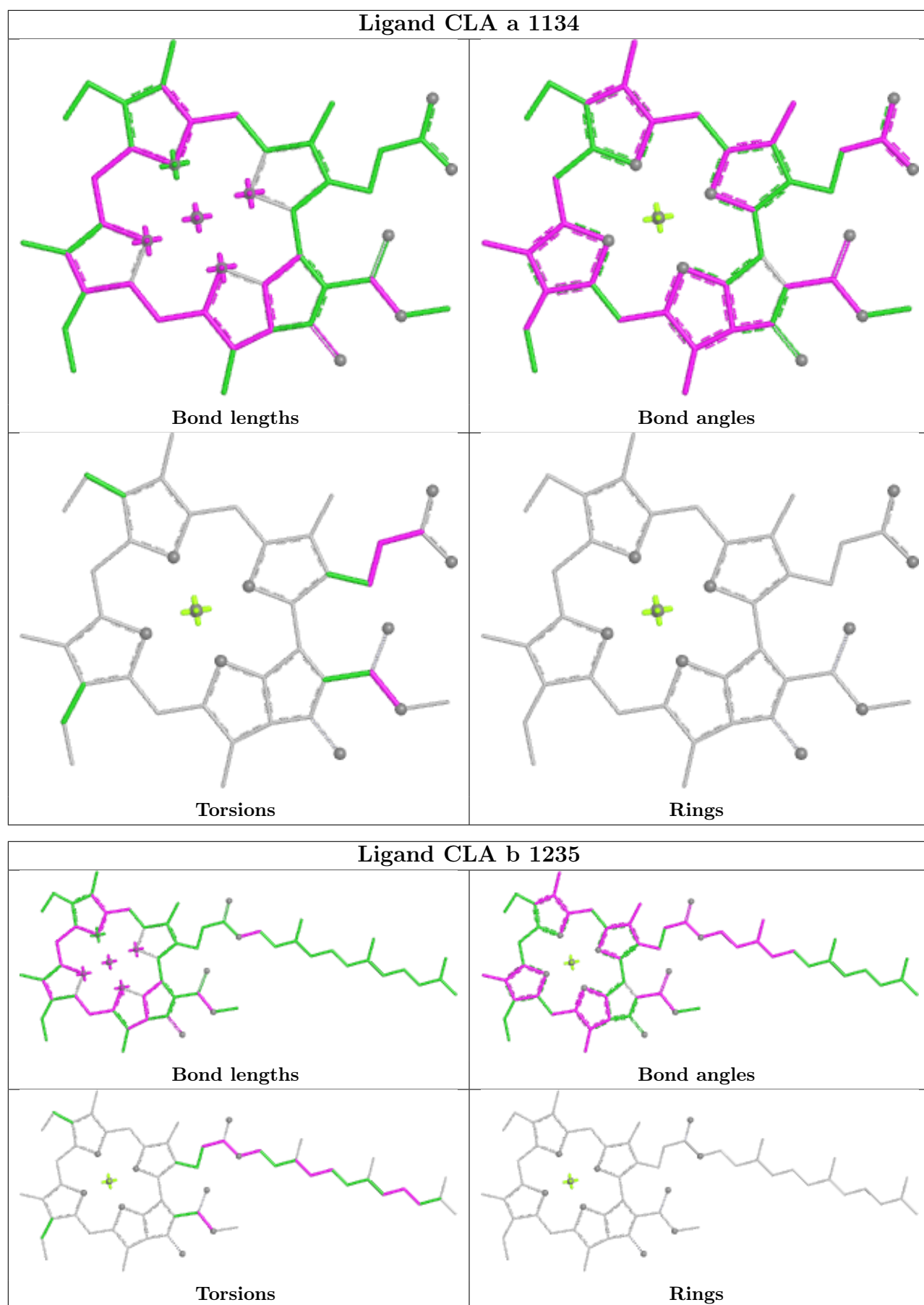


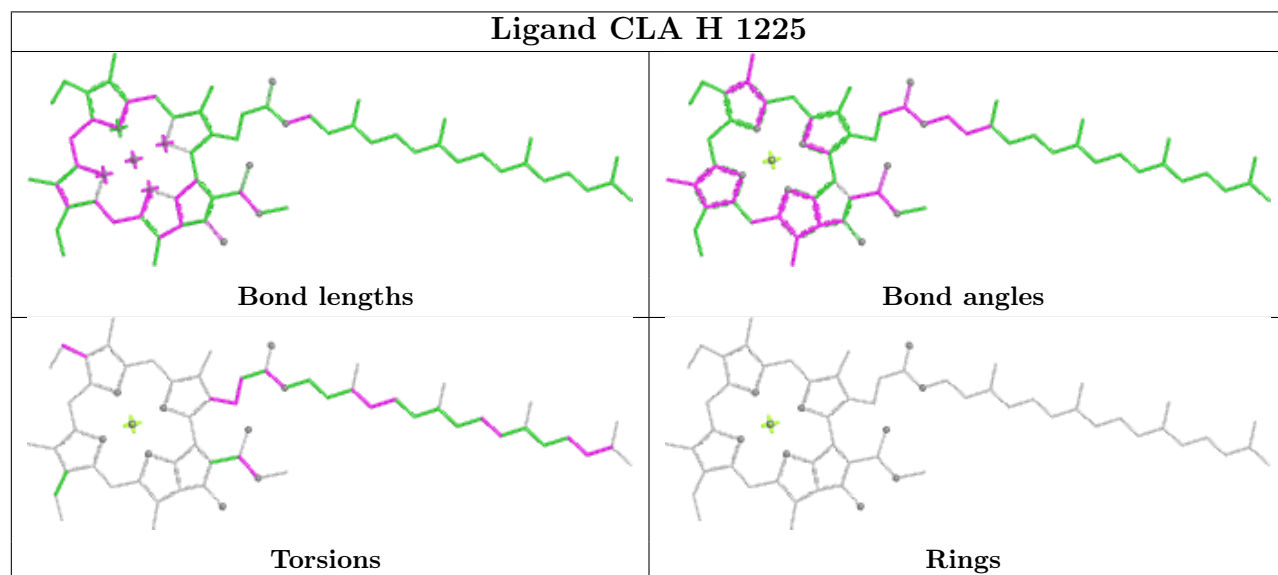
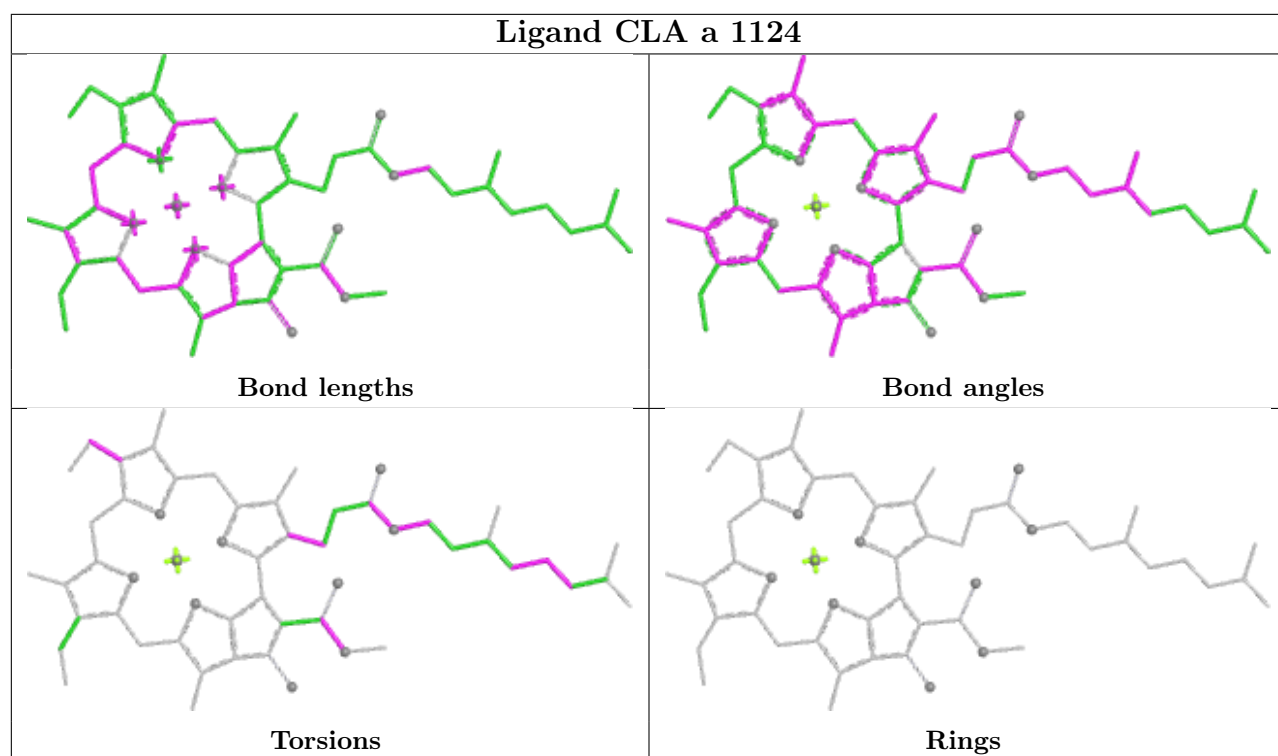


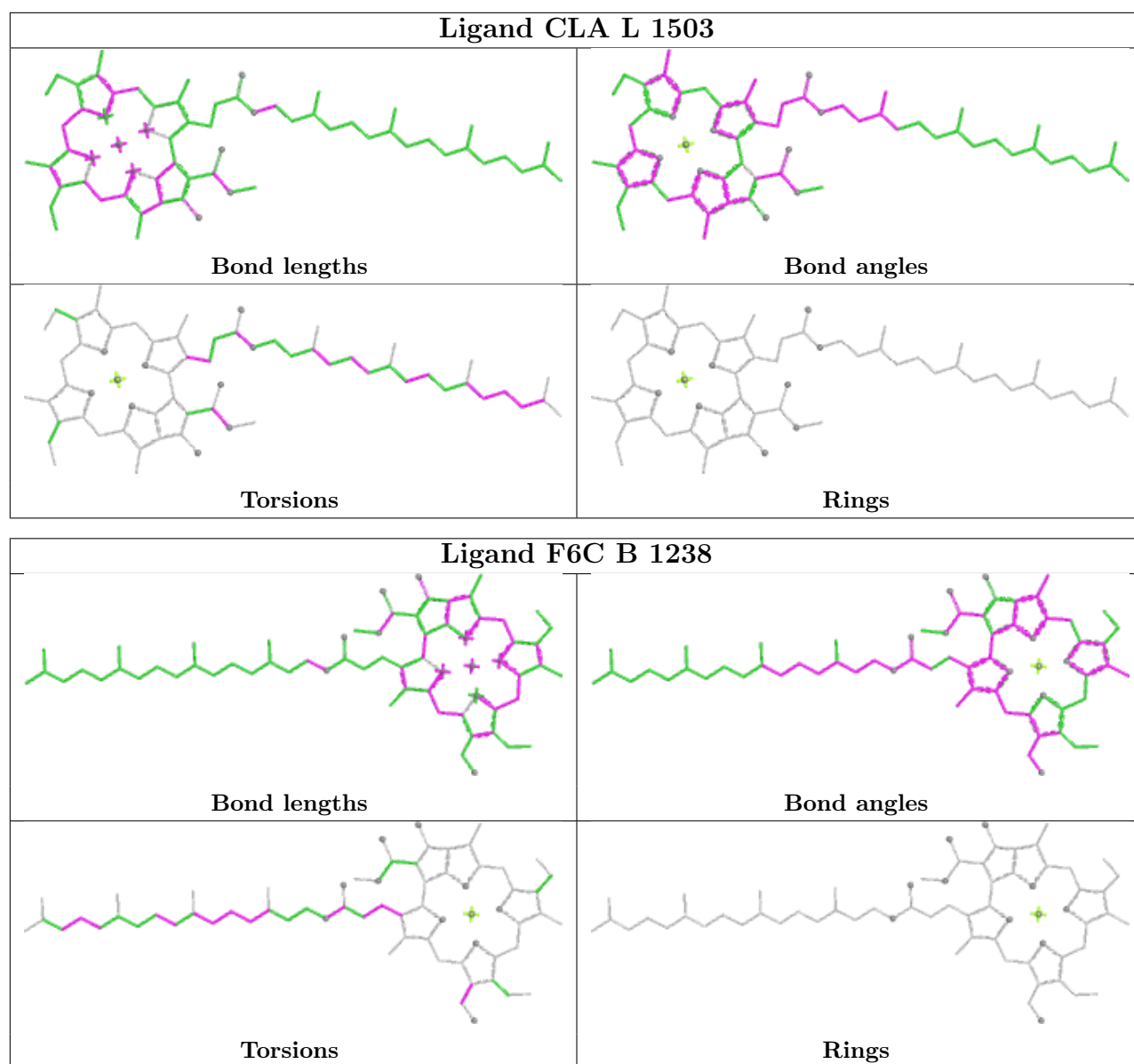




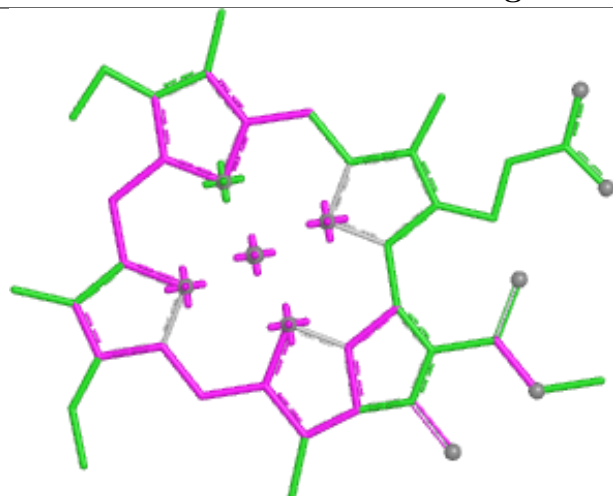




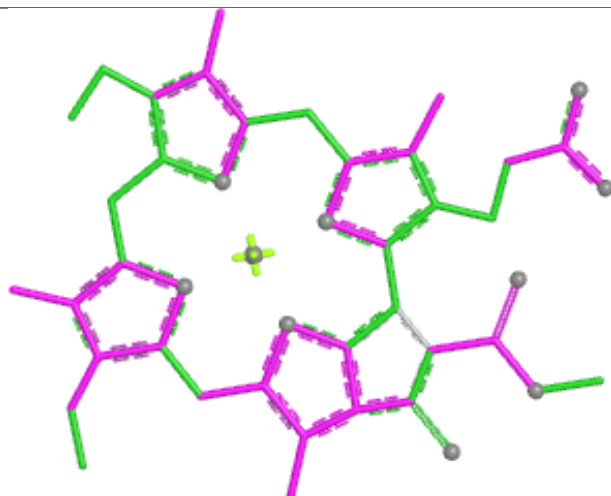




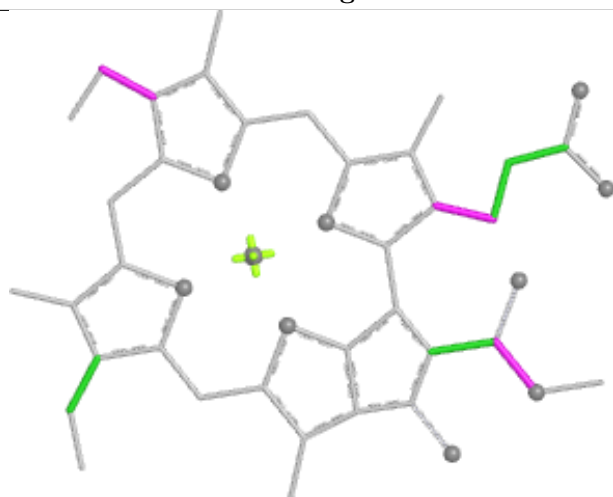
Ligand CLA H 1219



Bond lengths



Bond angles

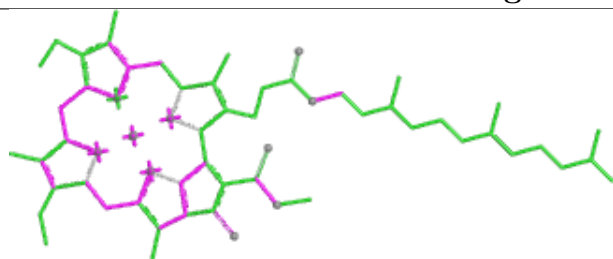


Torsions

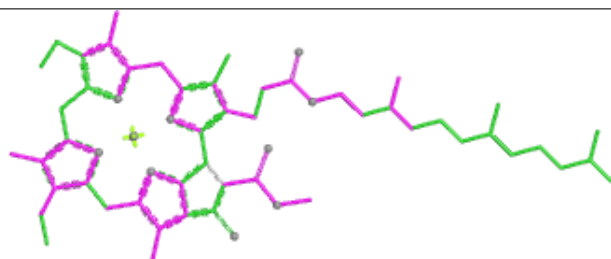


Rings

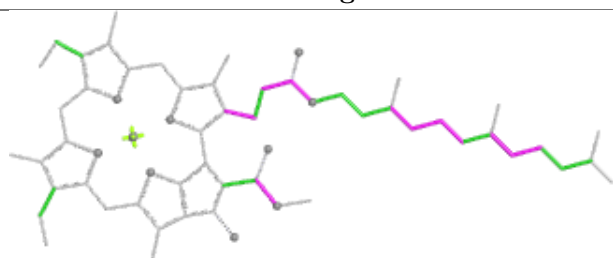
Ligand CLA G 1138



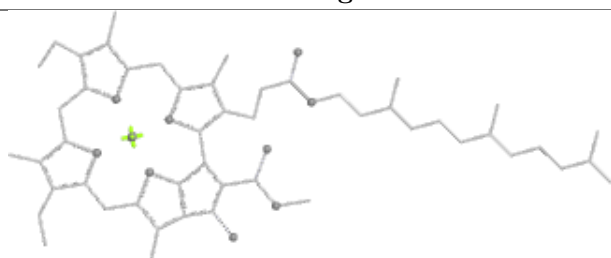
Bond lengths



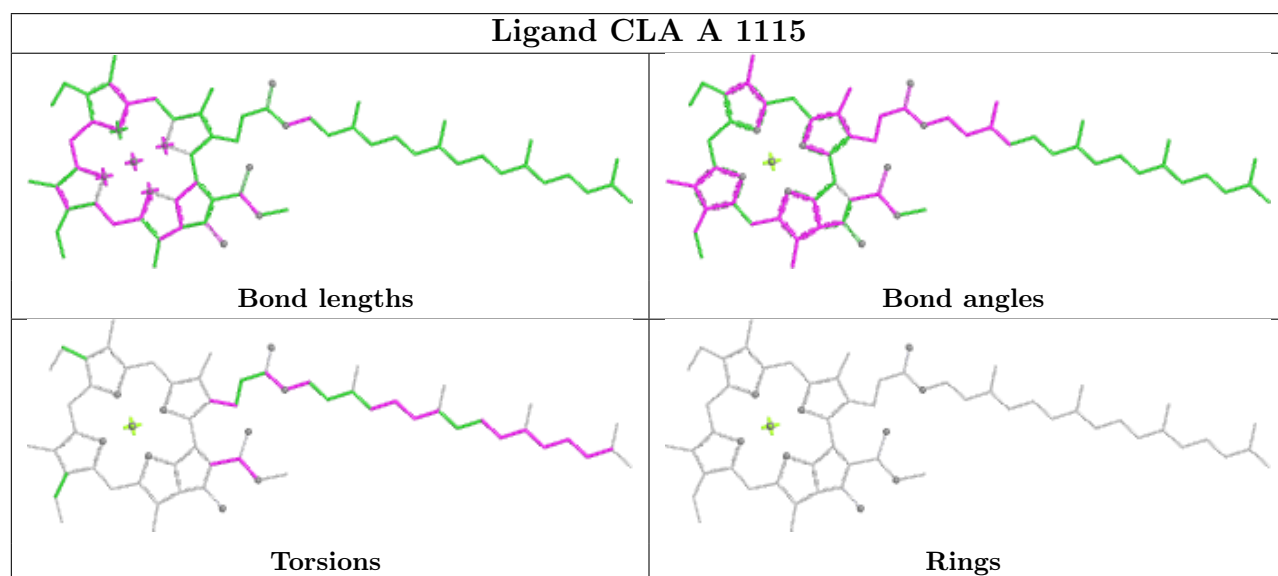
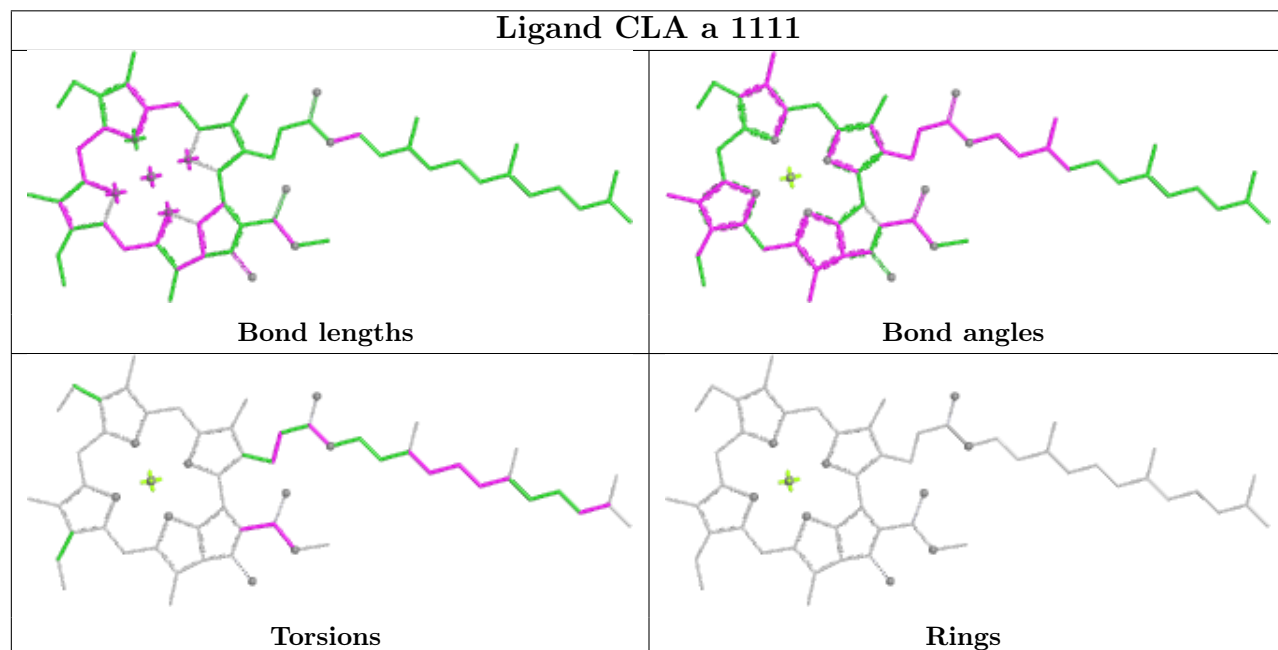
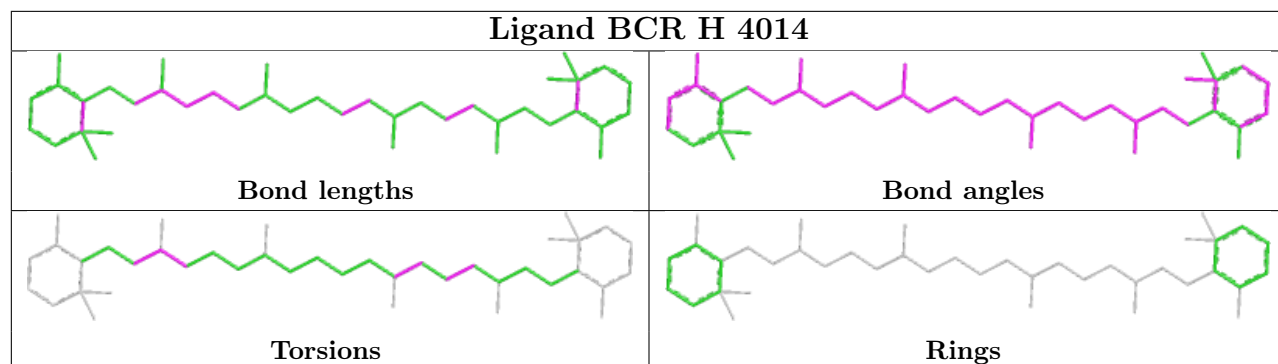
Bond angles

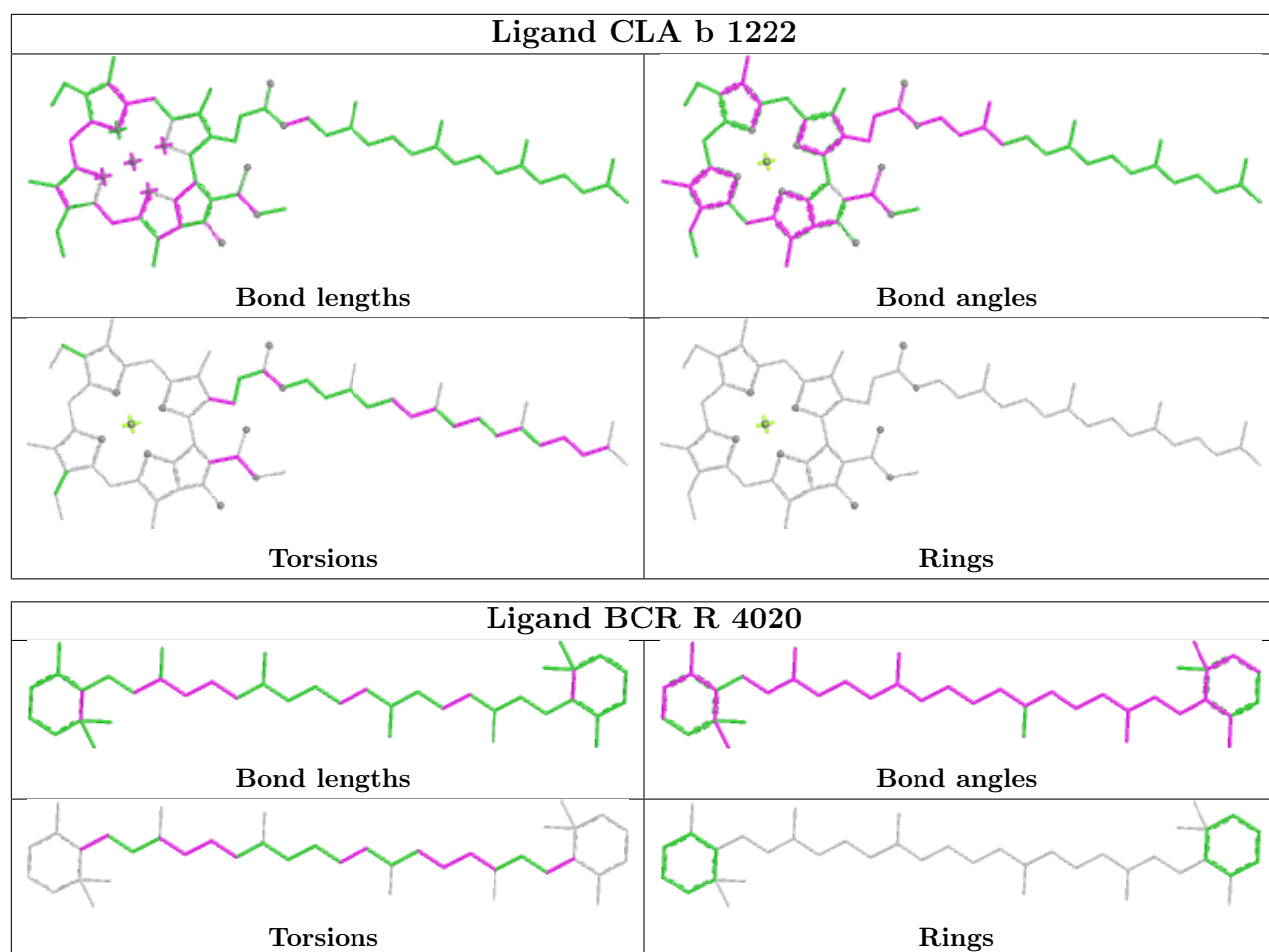


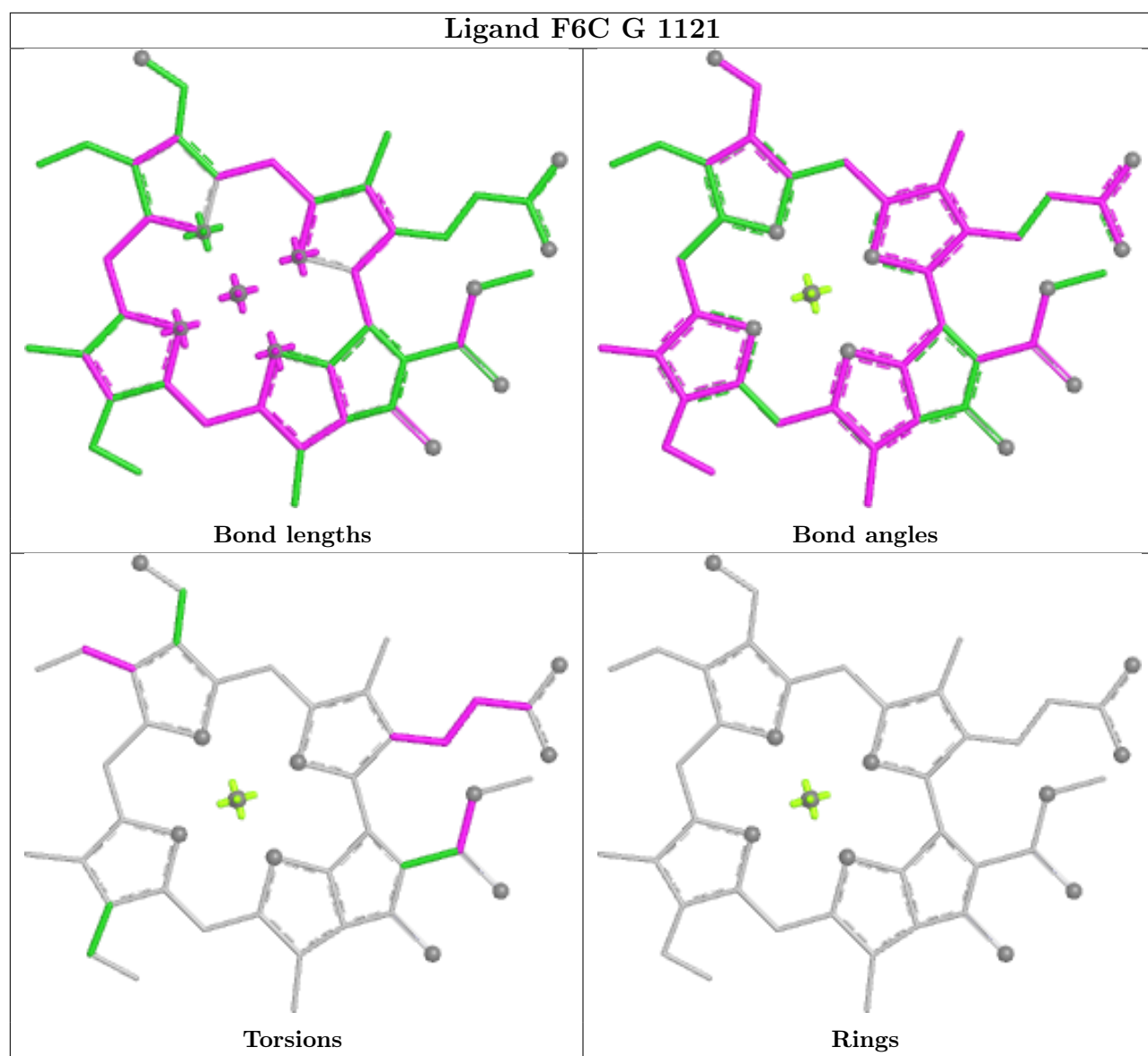
Torsions

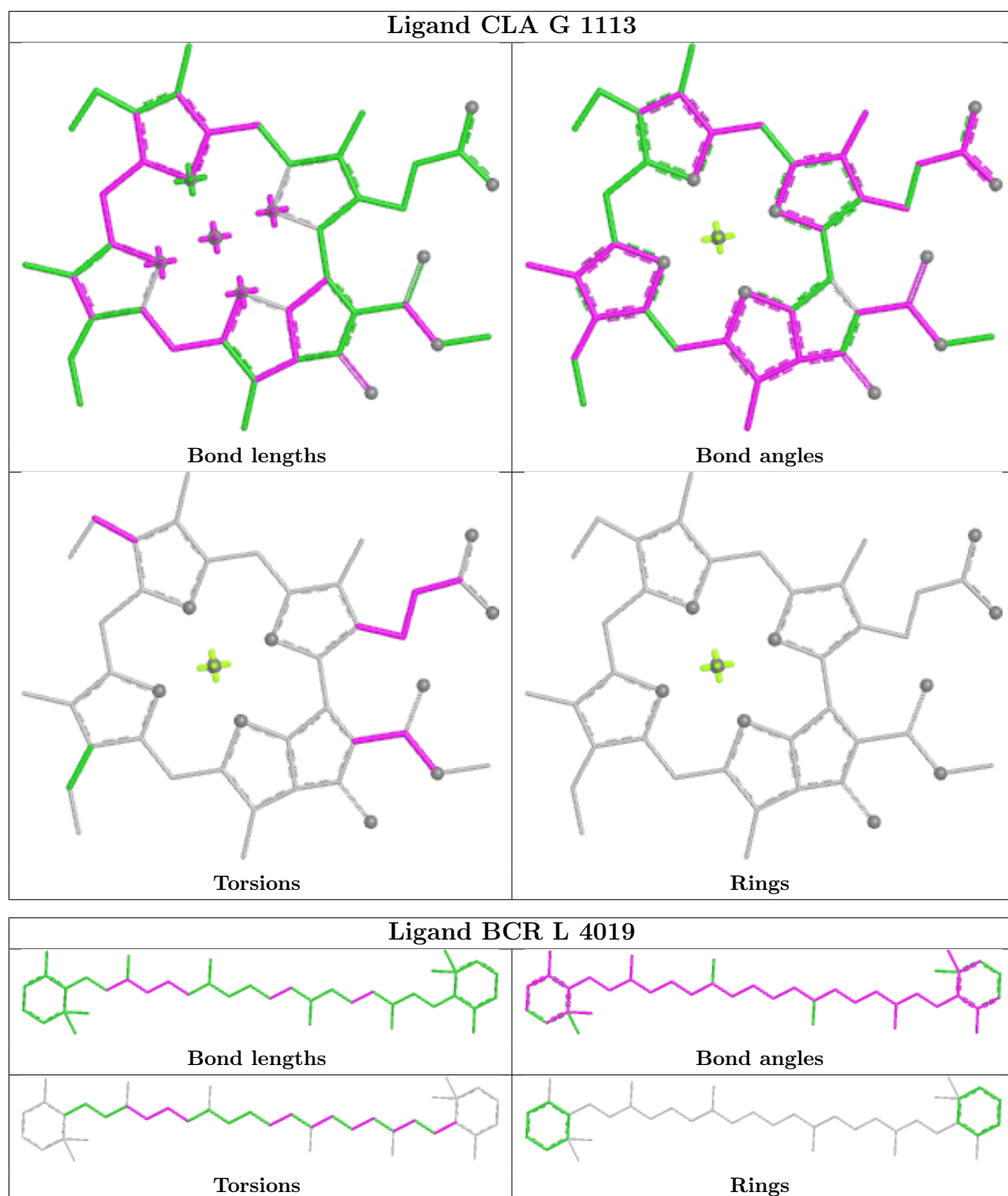


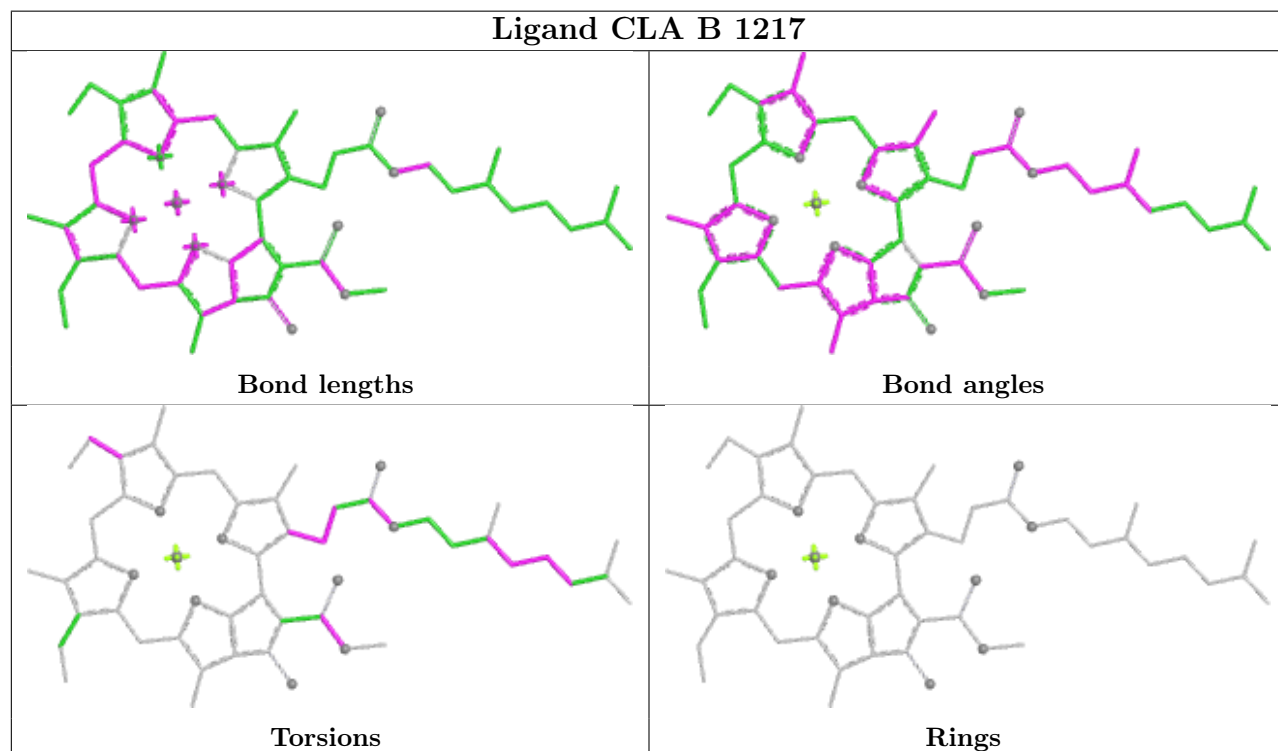
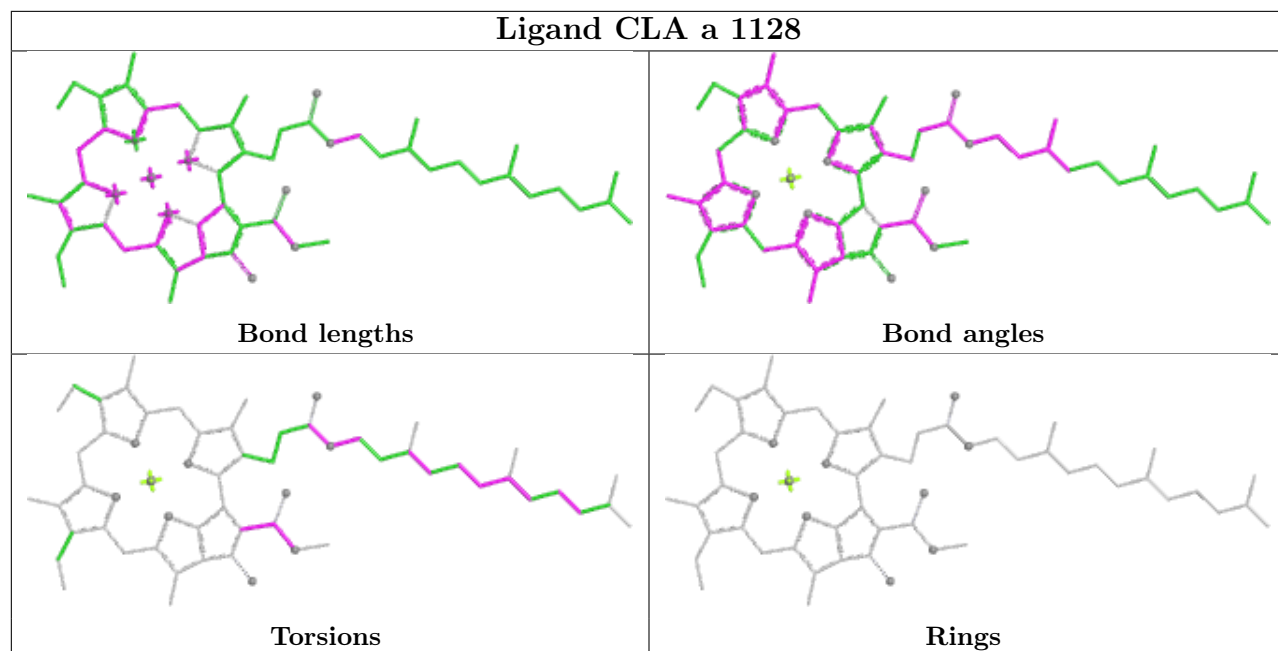
Rings

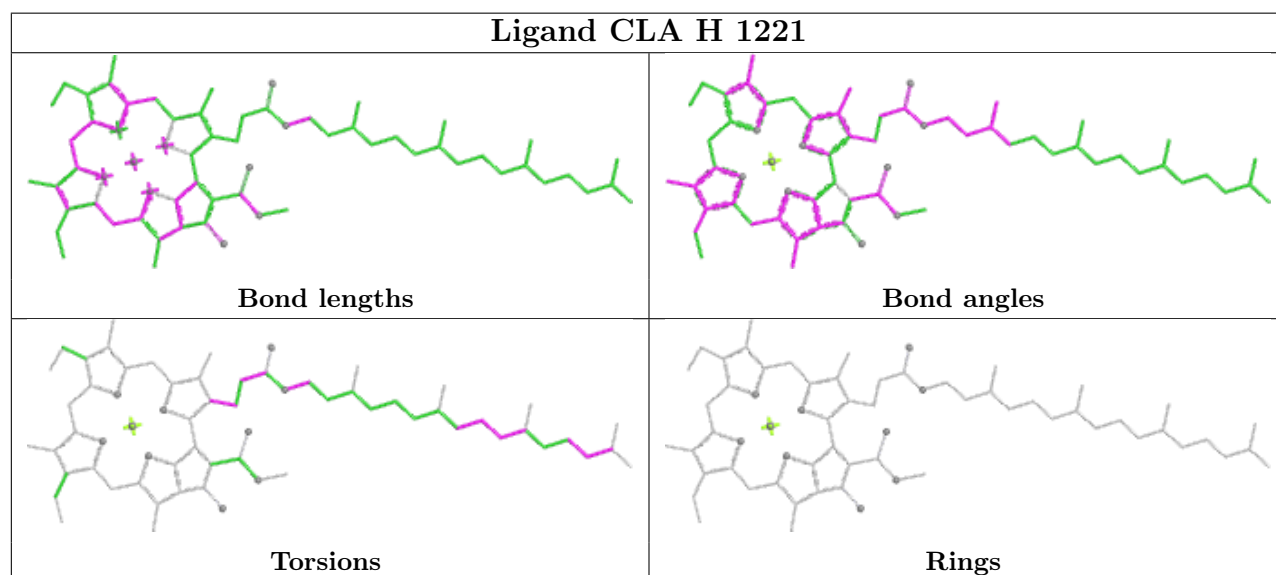
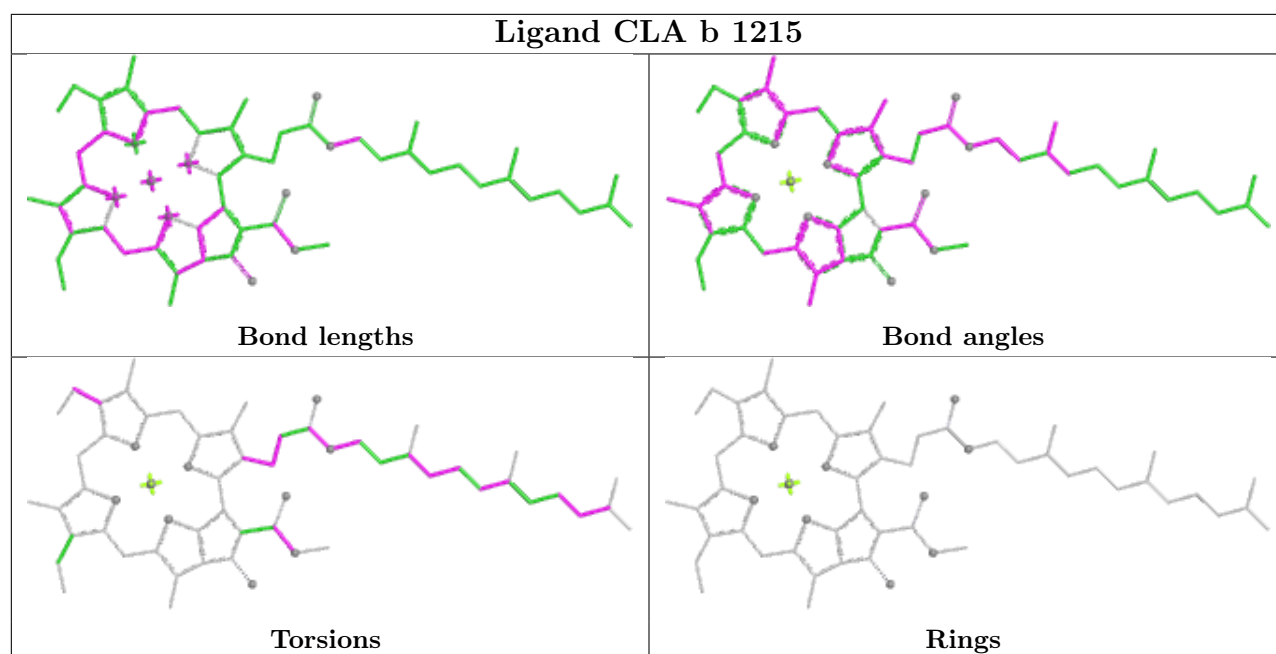


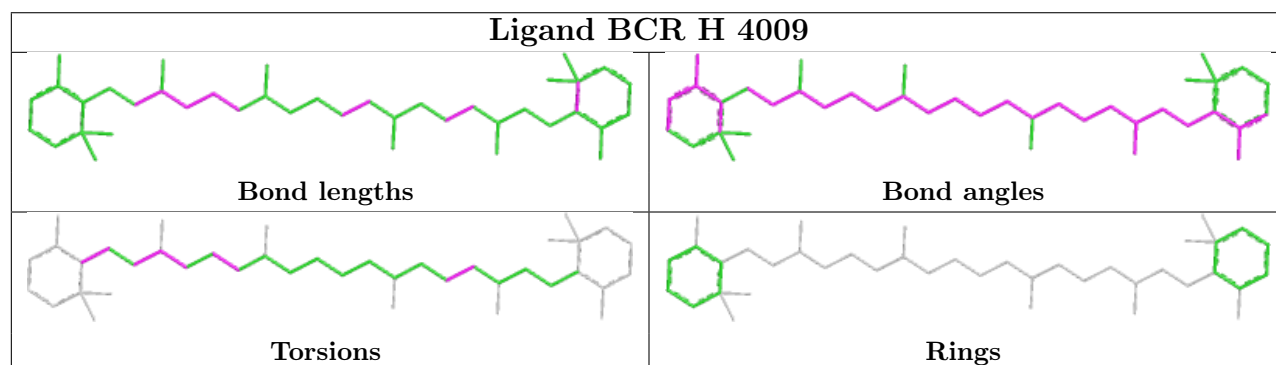
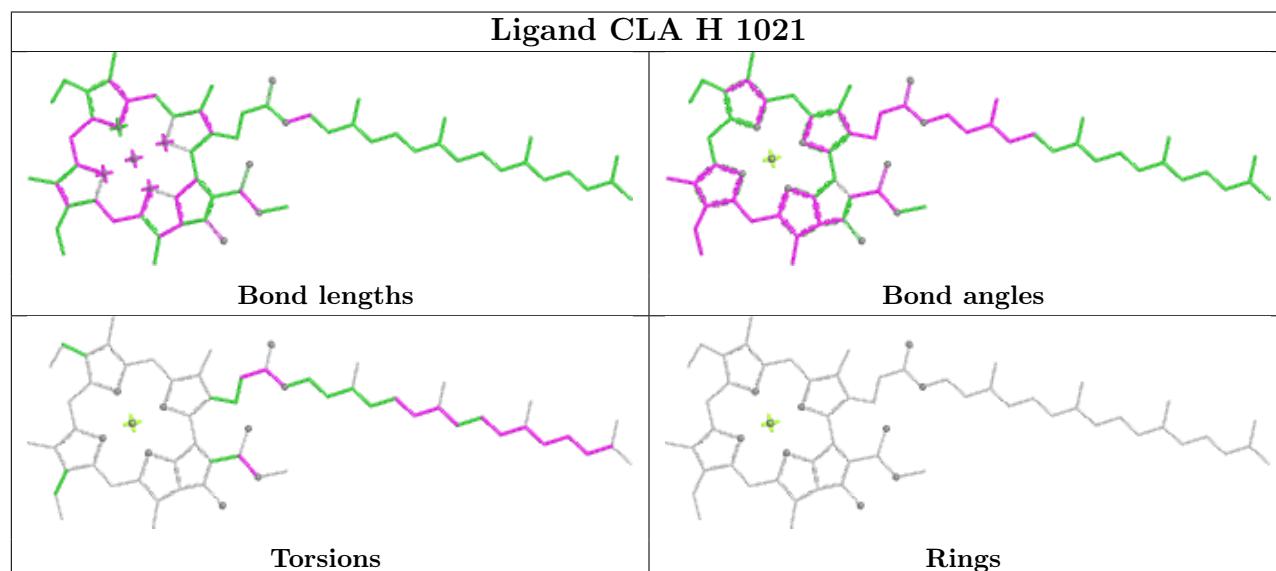
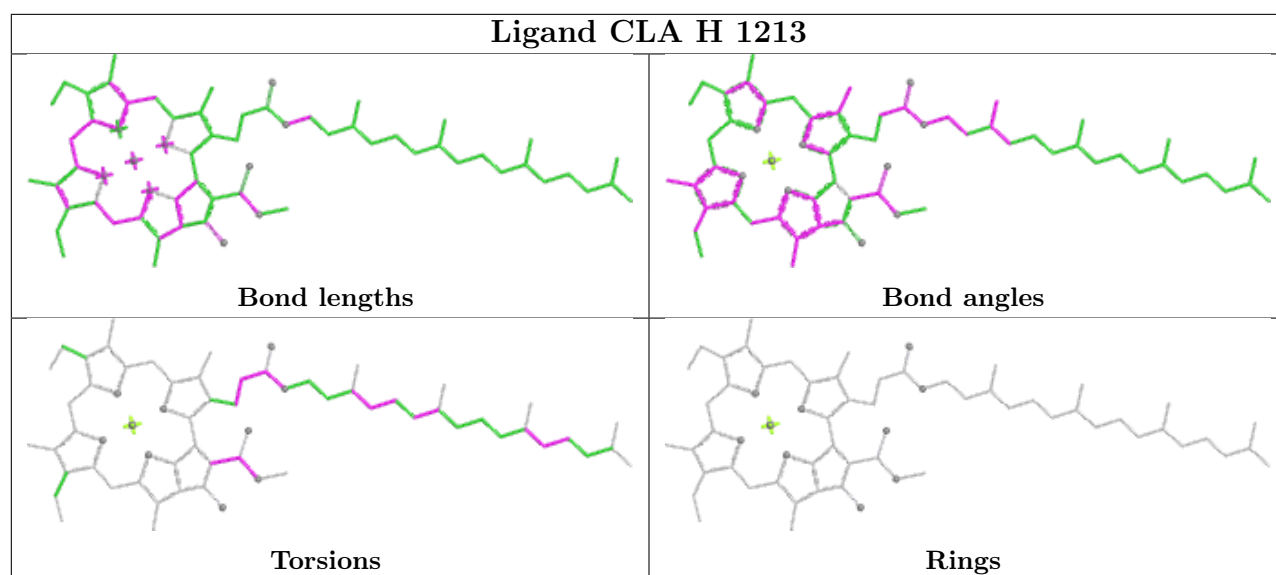


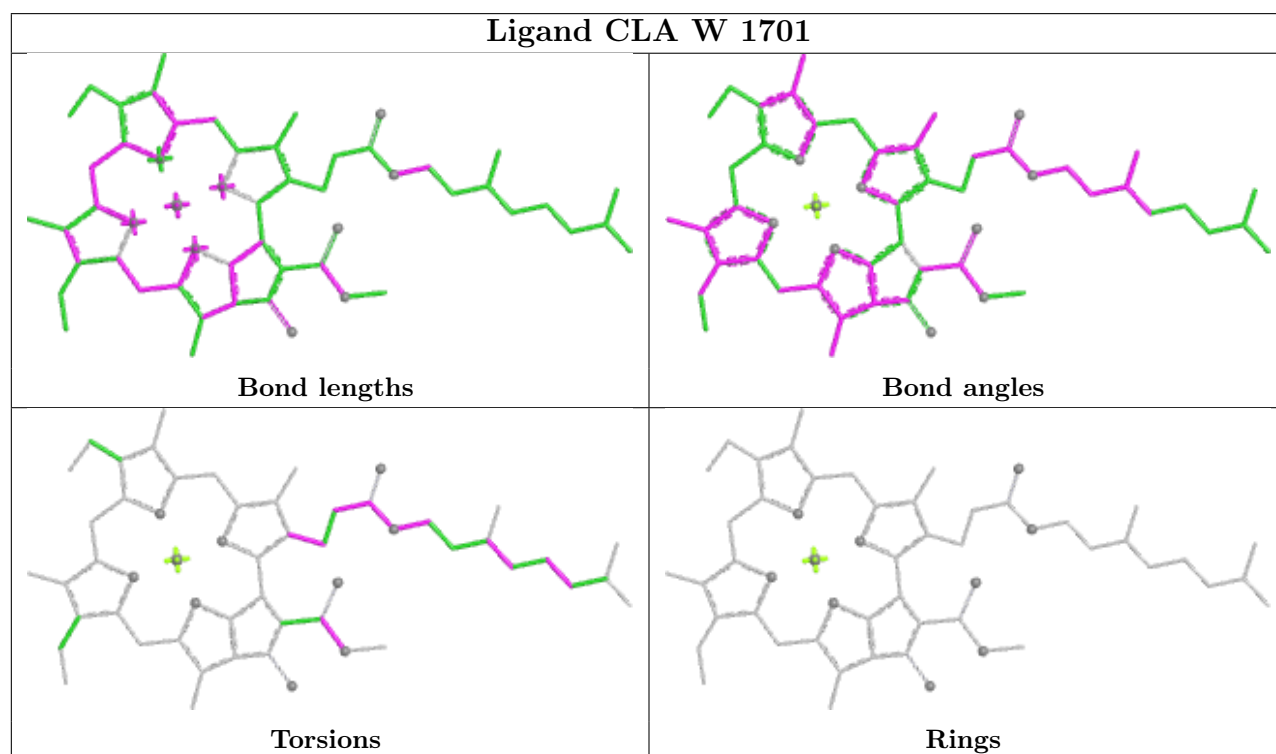
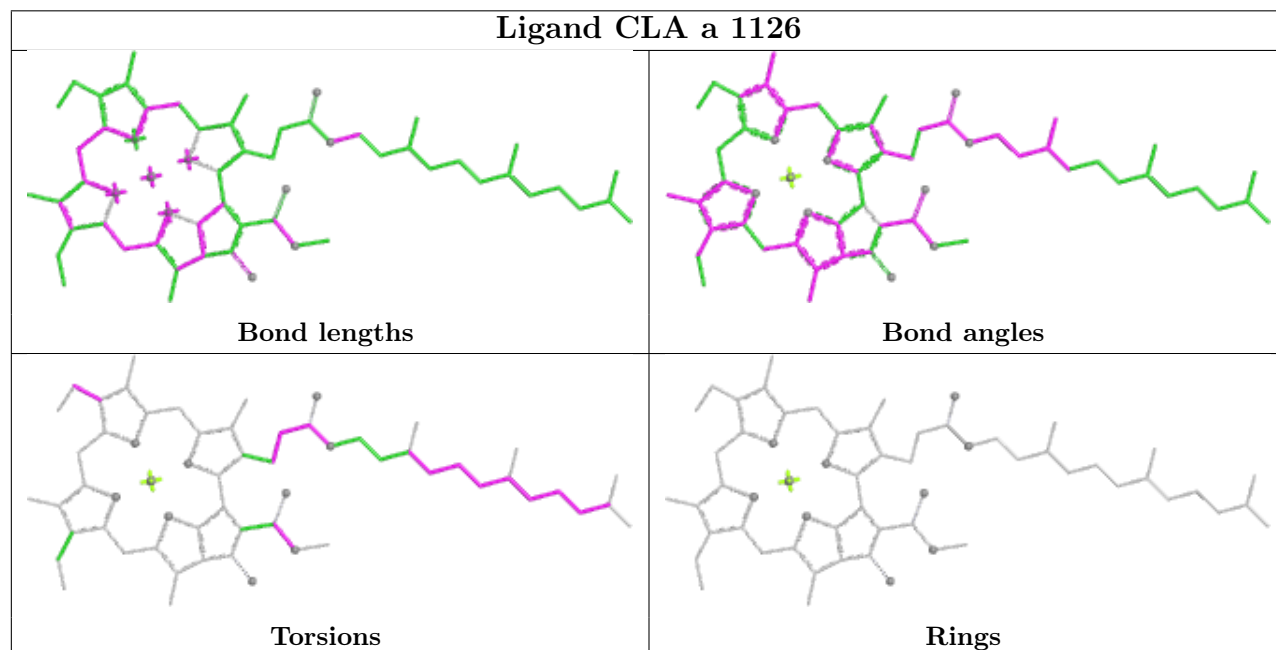
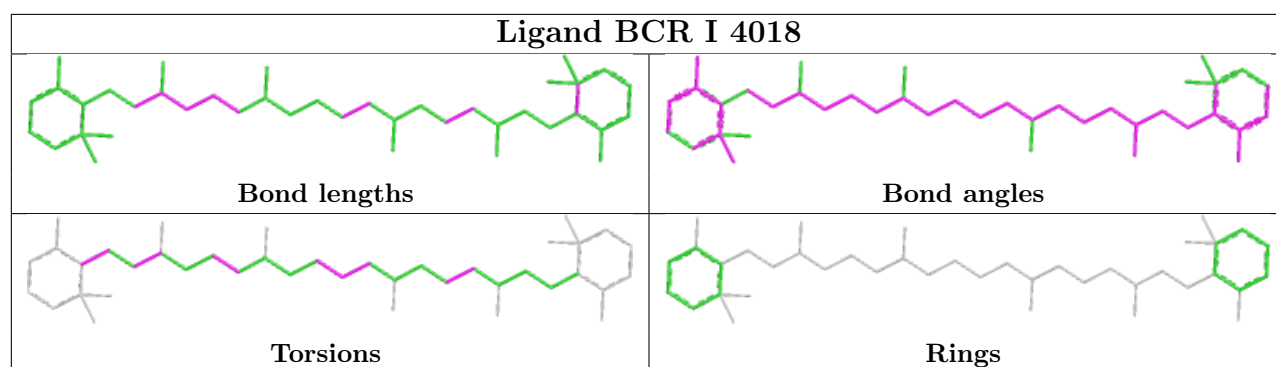


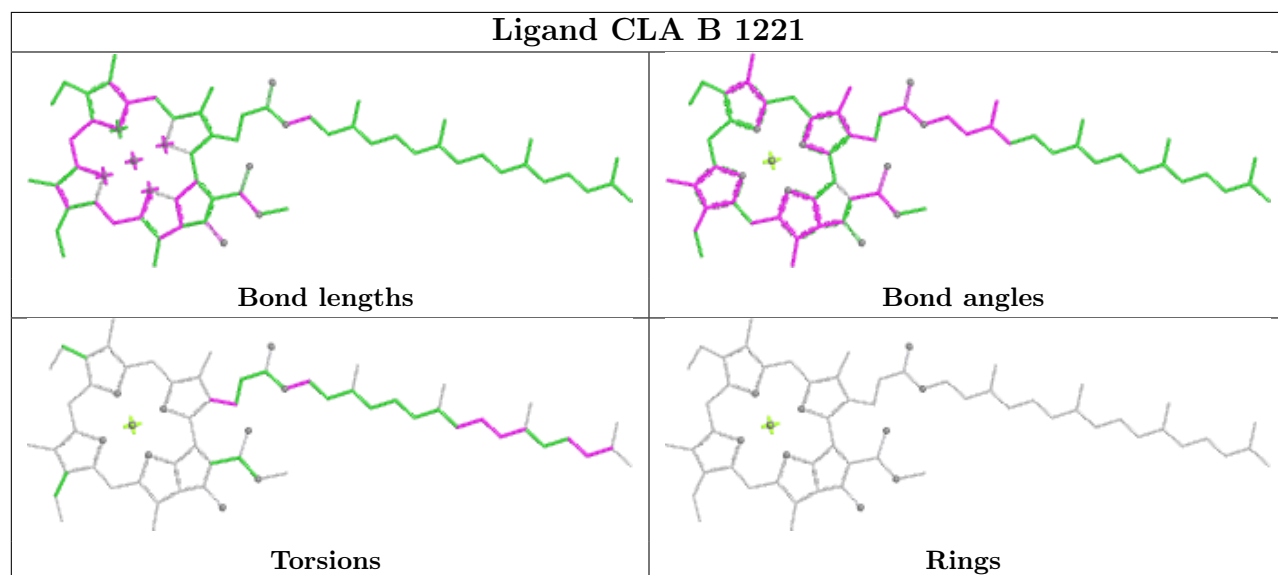
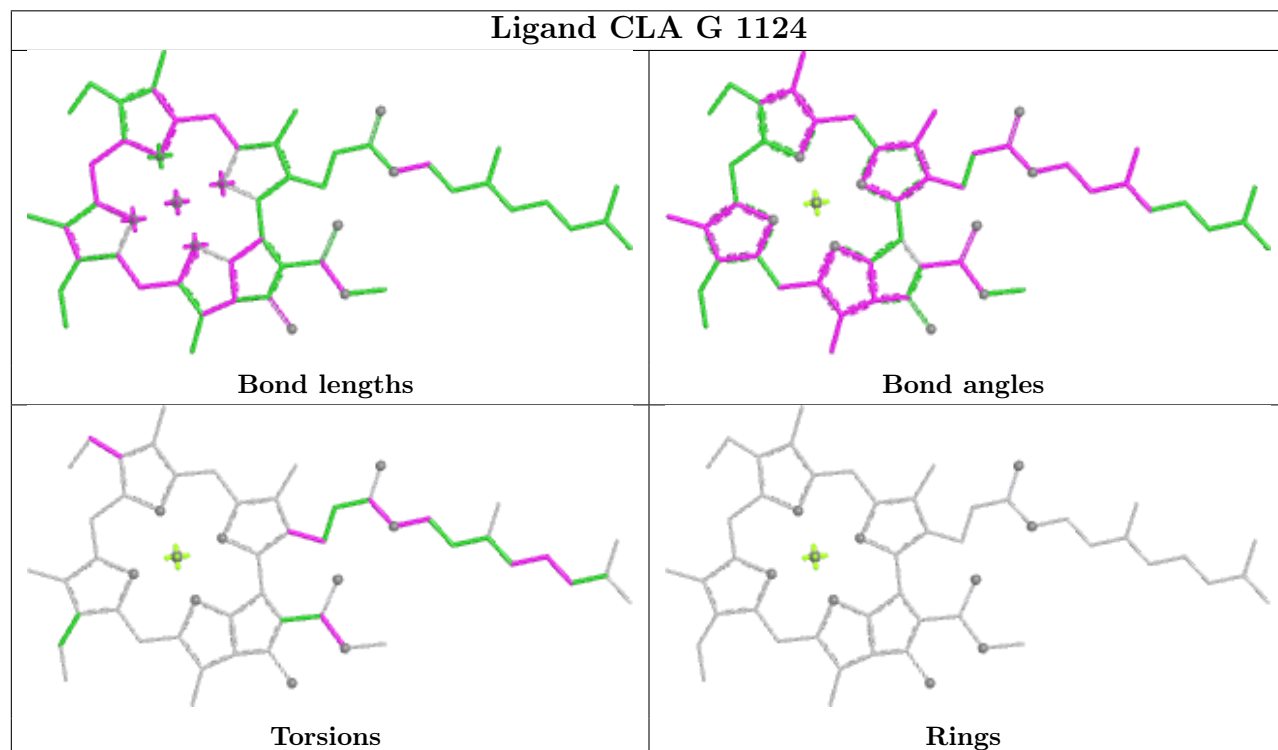
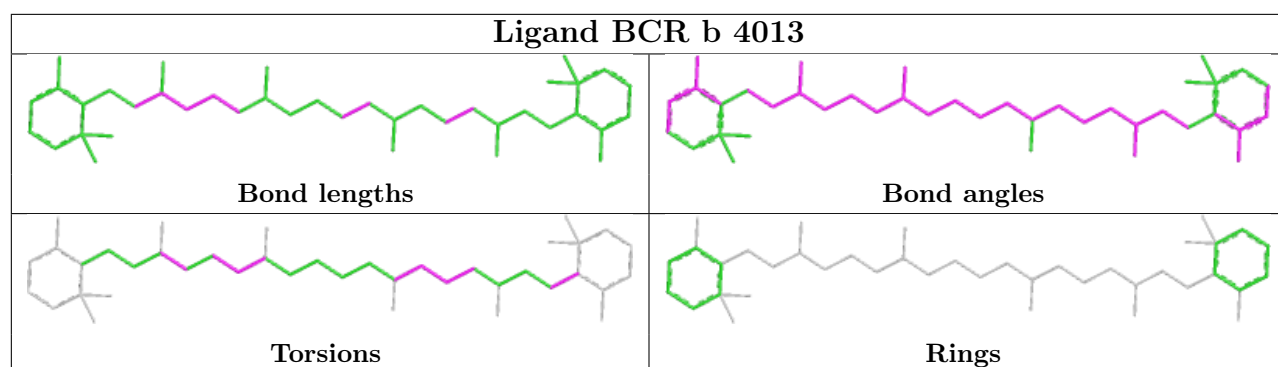


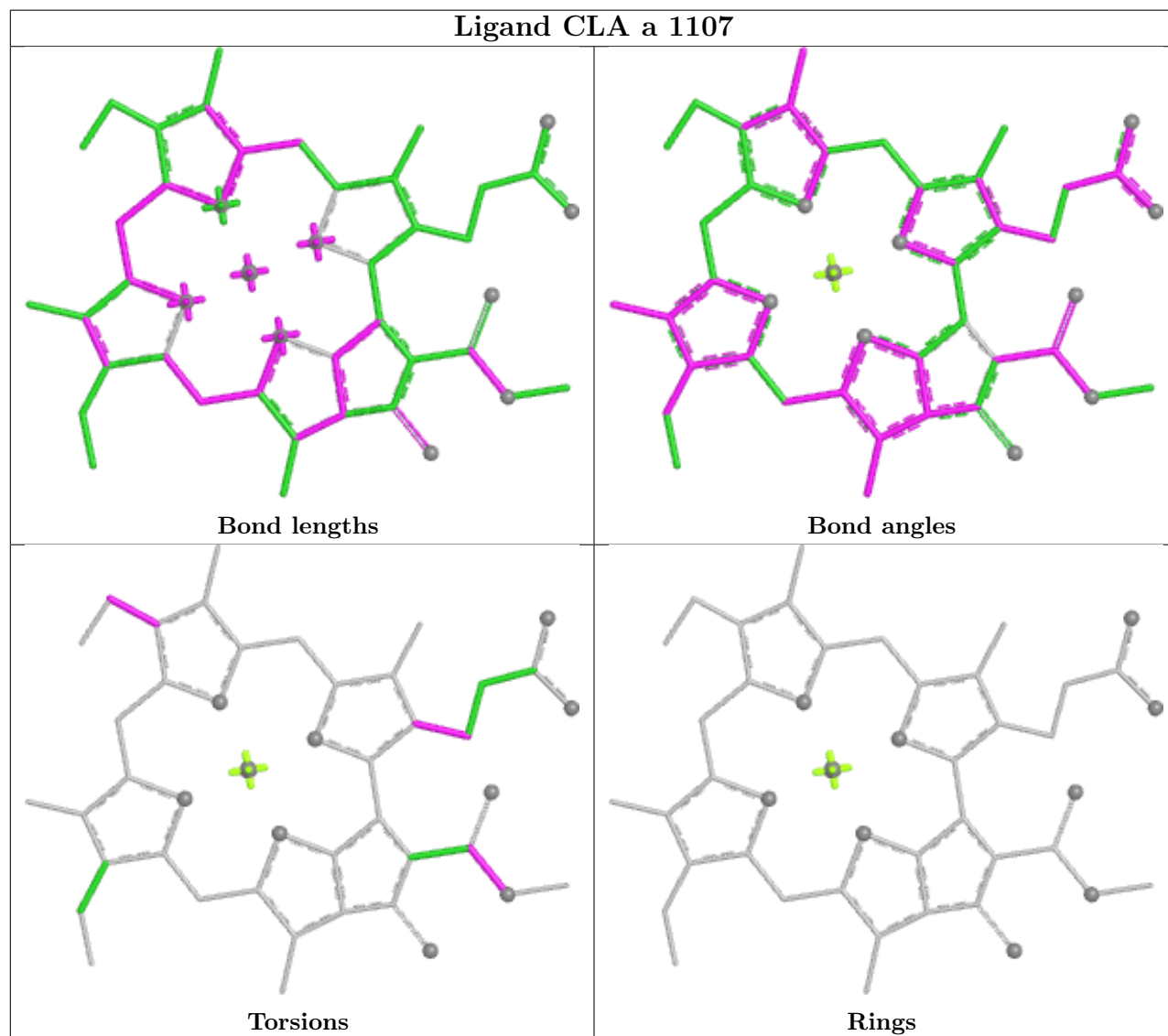
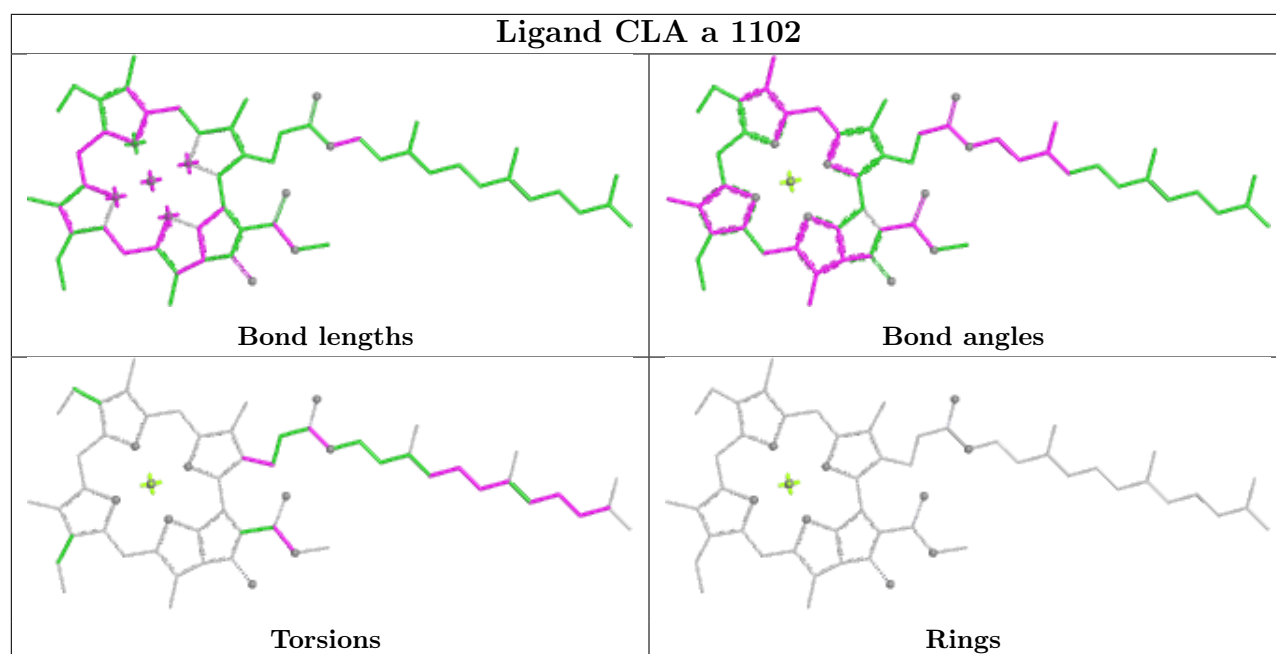




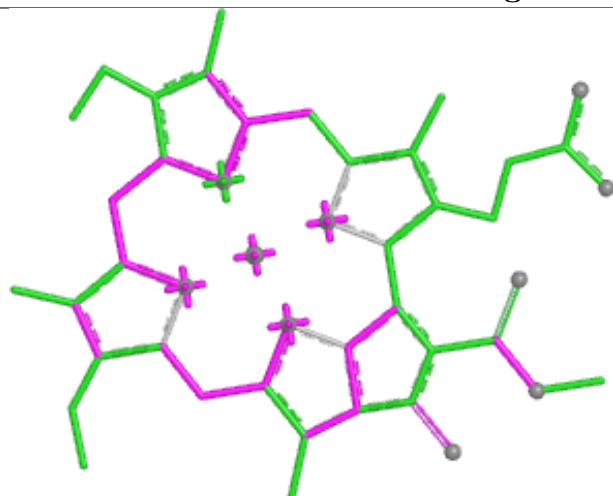




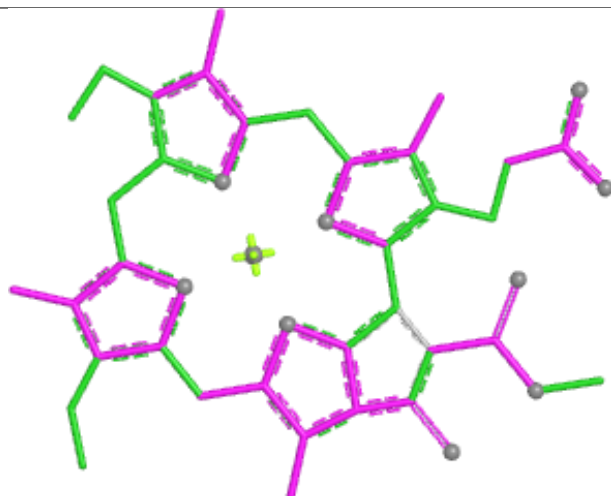




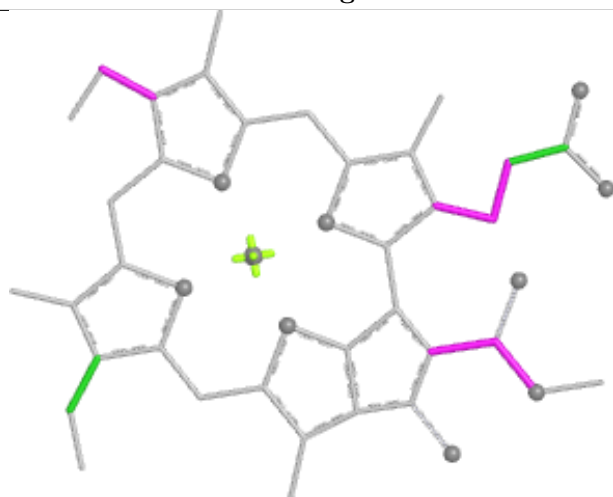
Ligand CLA G 1120



Bond lengths



Bond angles

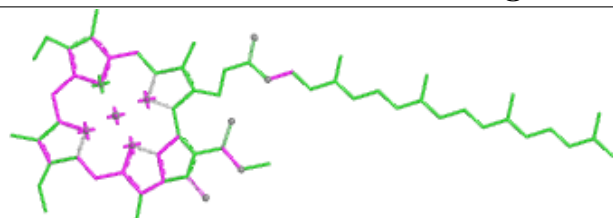


Torsions

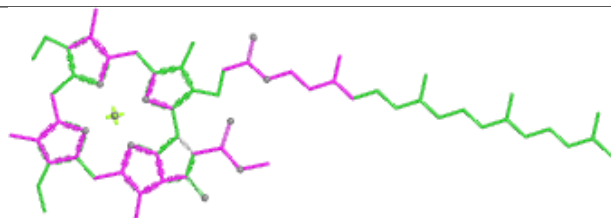


Rings

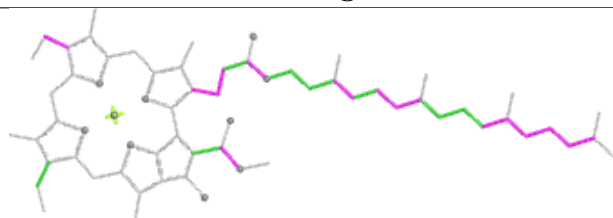
Ligand CLA H 1216



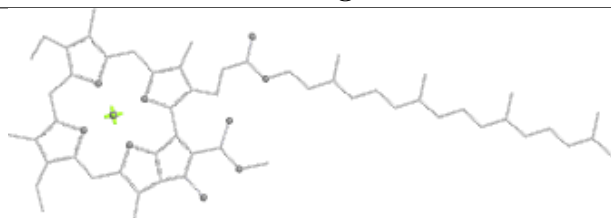
Bond lengths



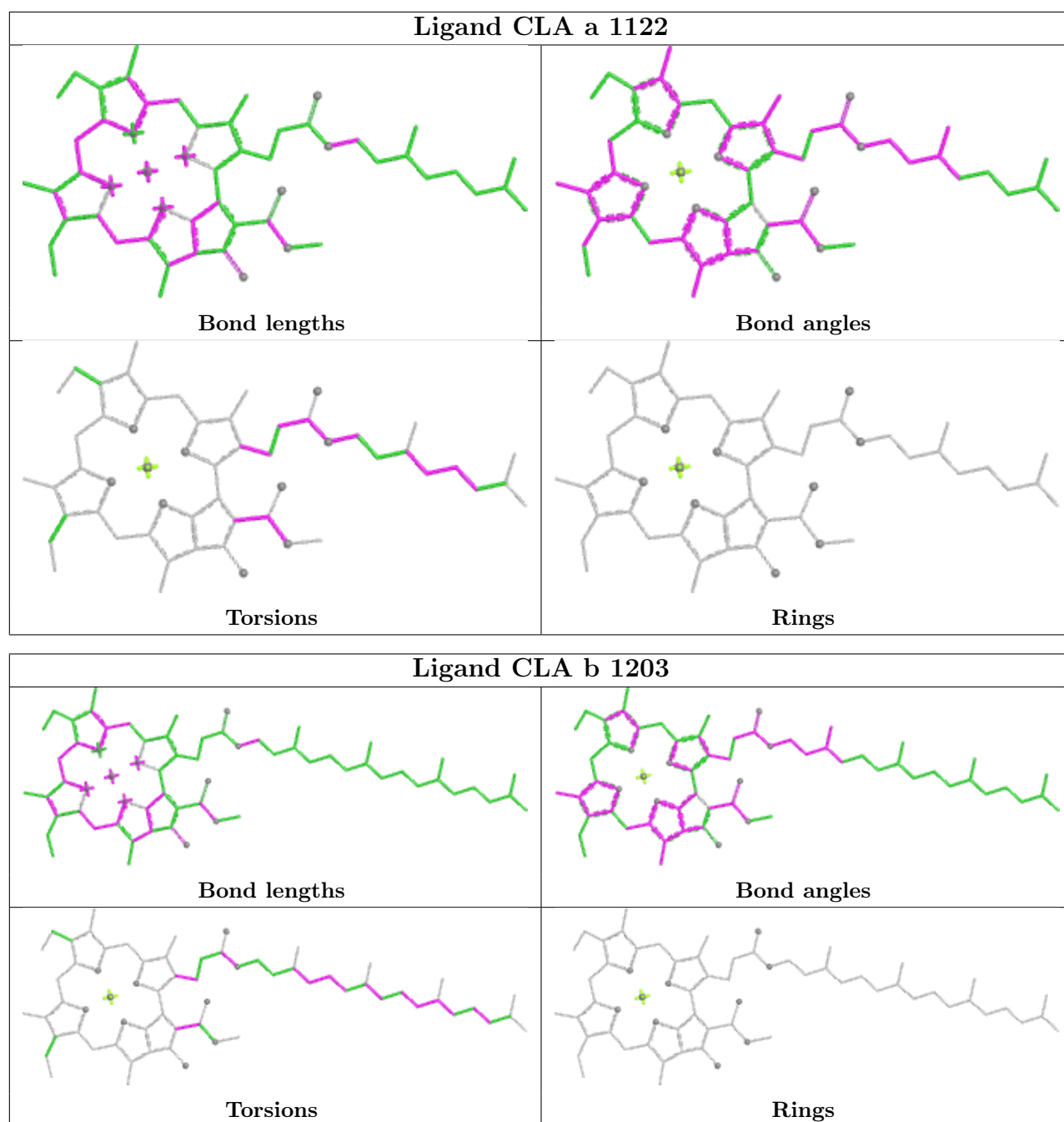
Bond angles

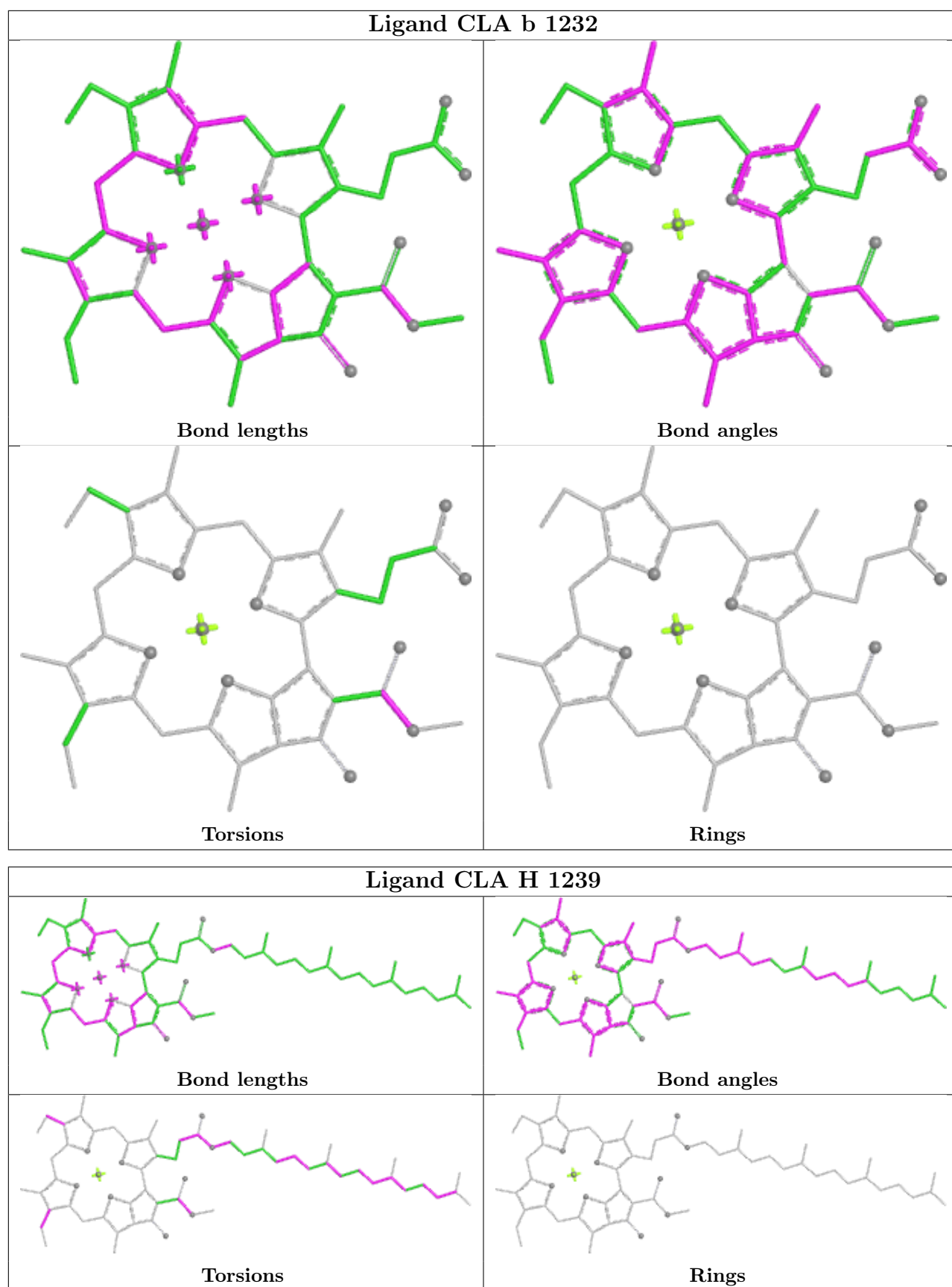


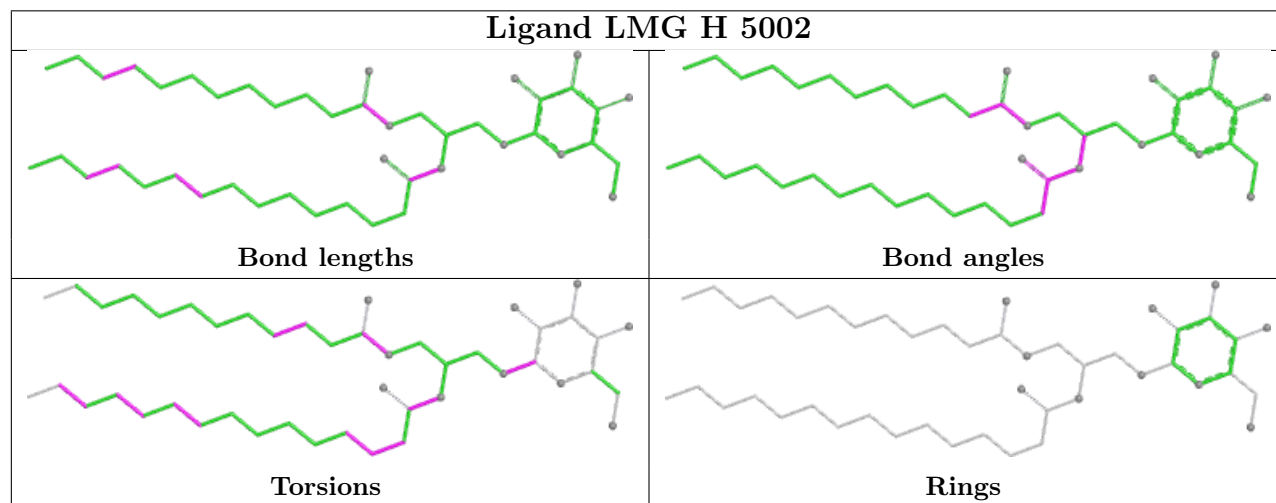
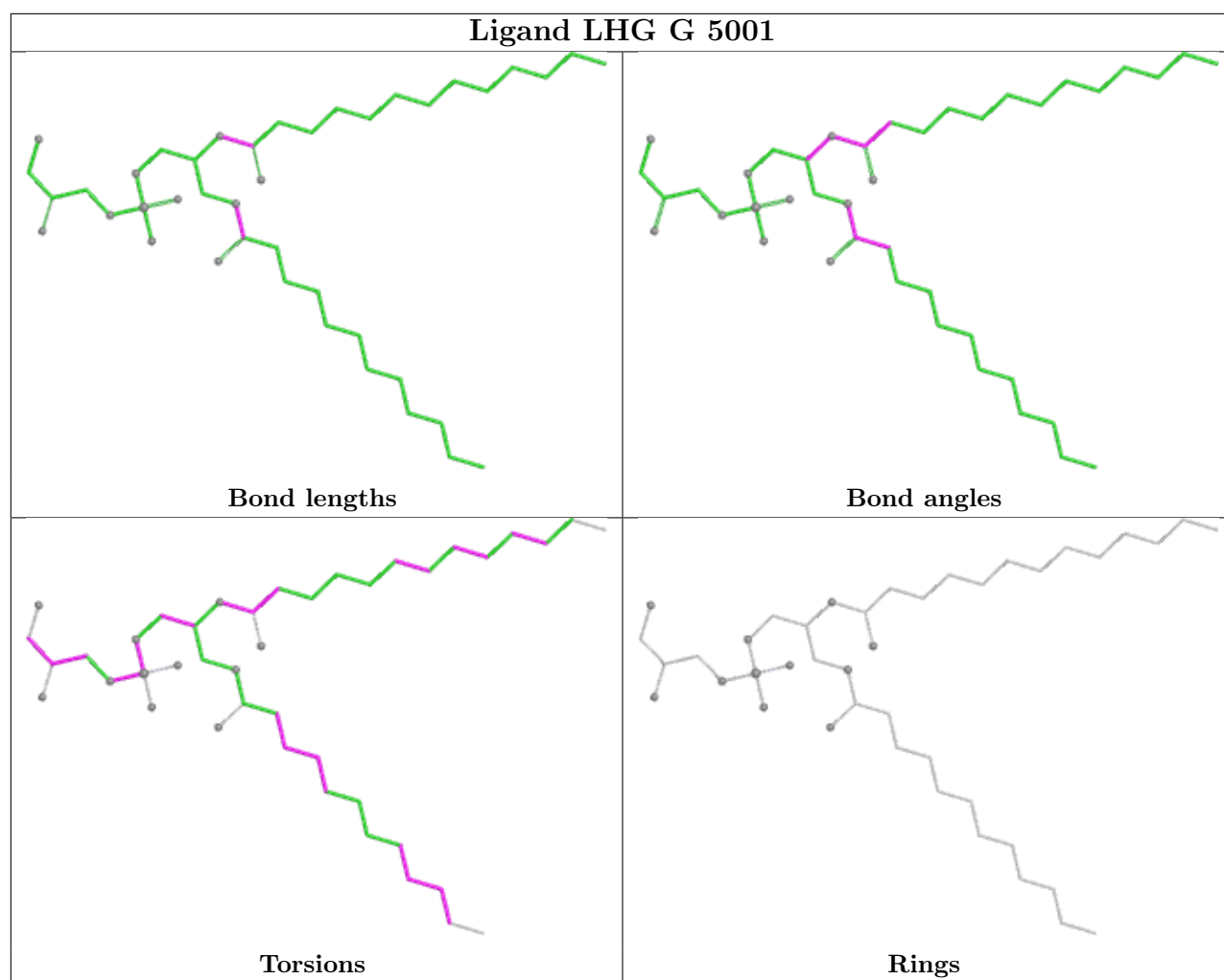
Torsions

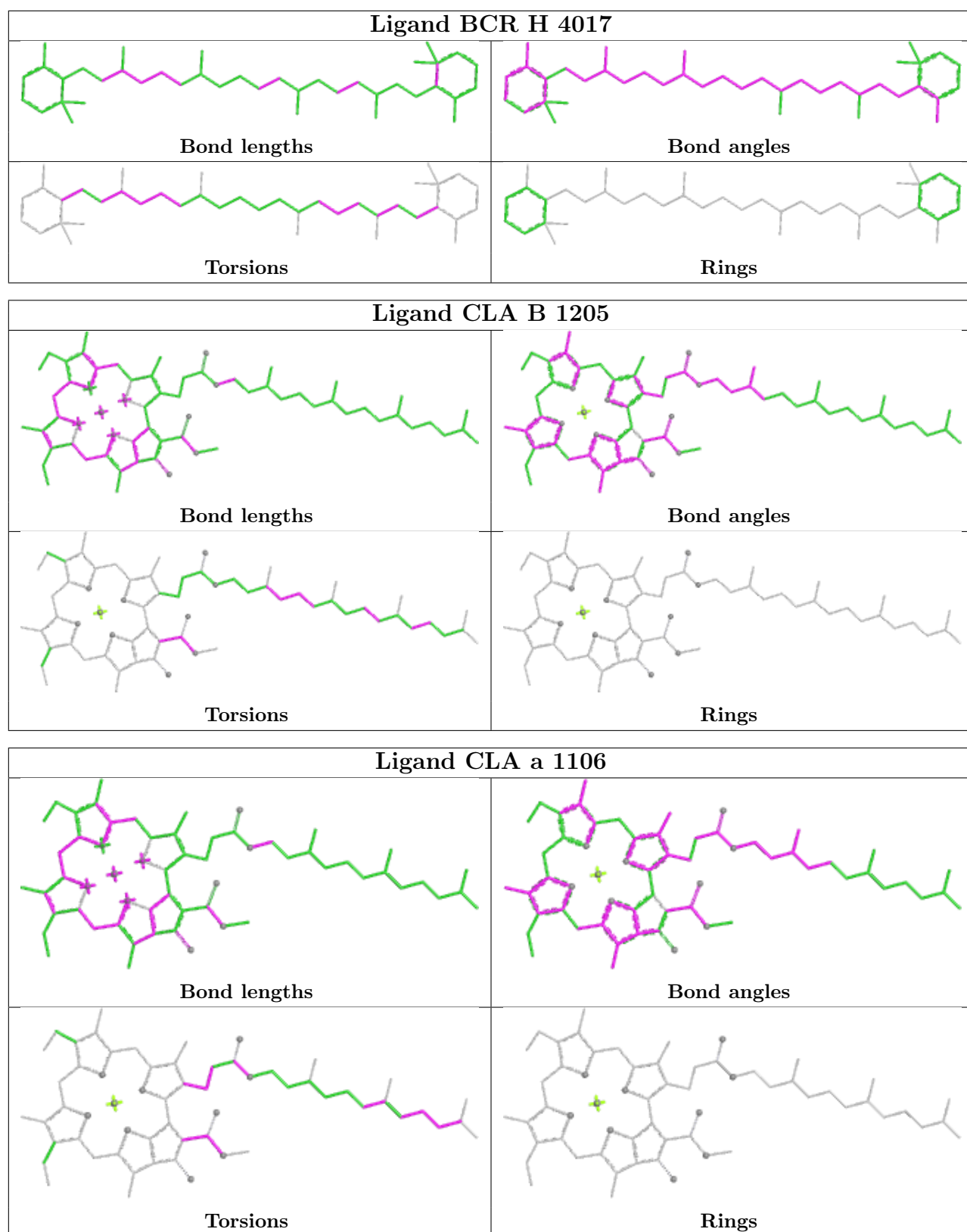


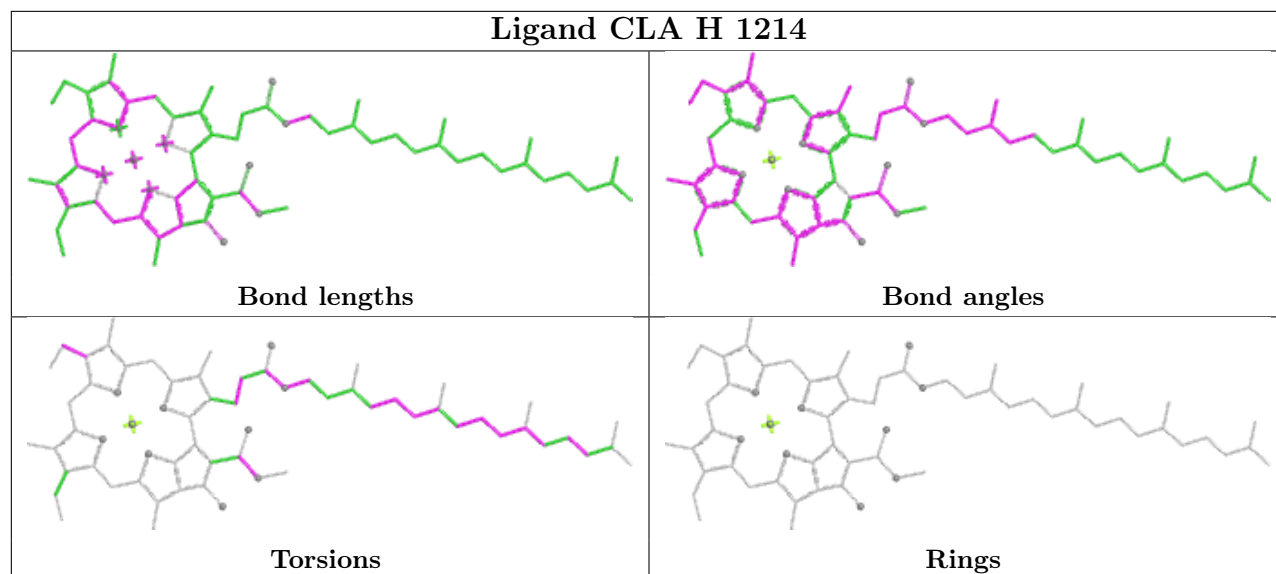
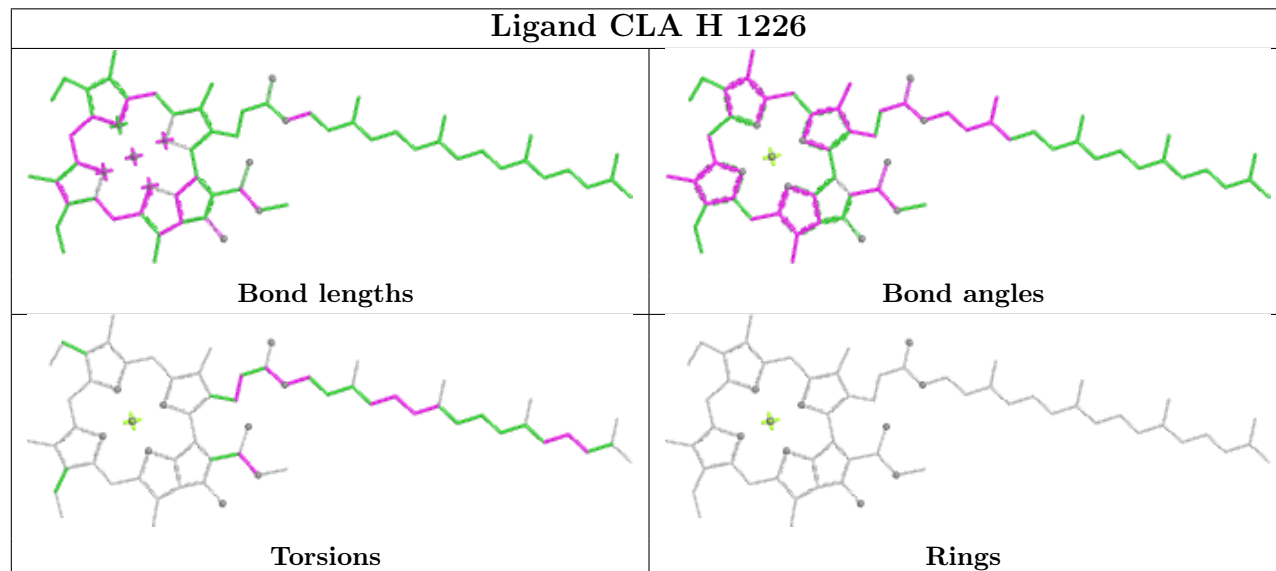
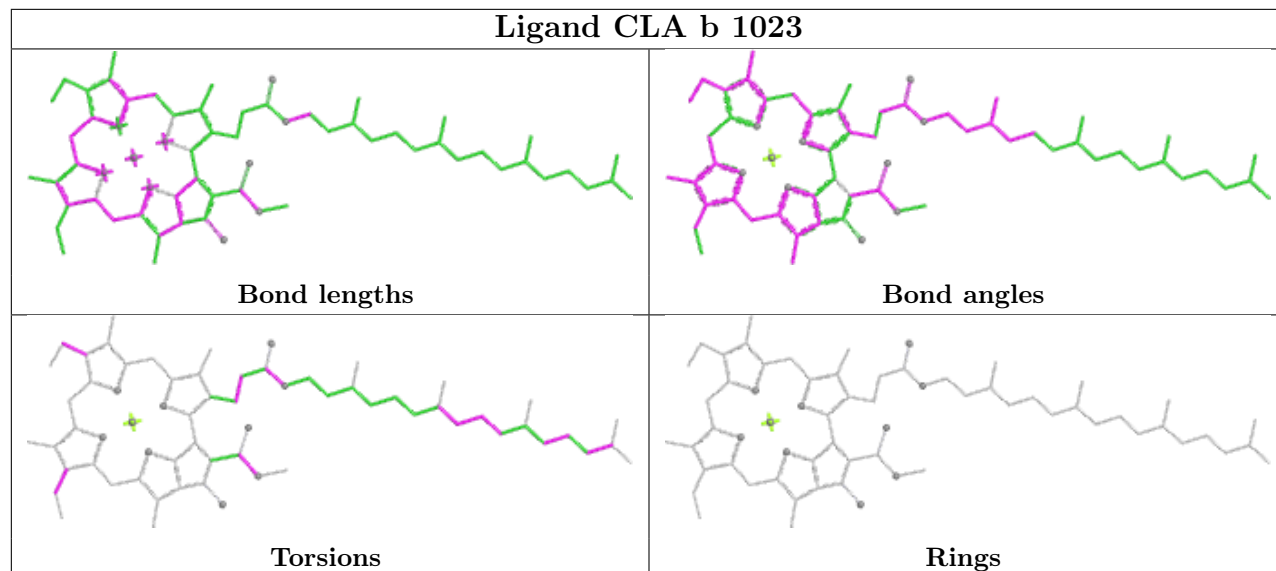
Rings

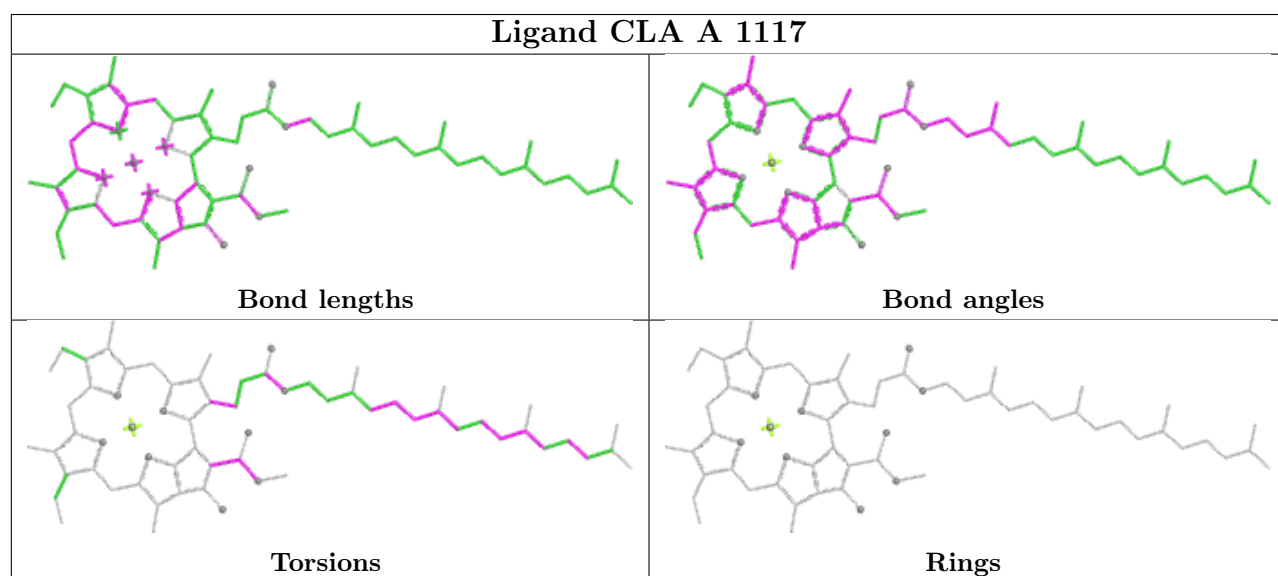
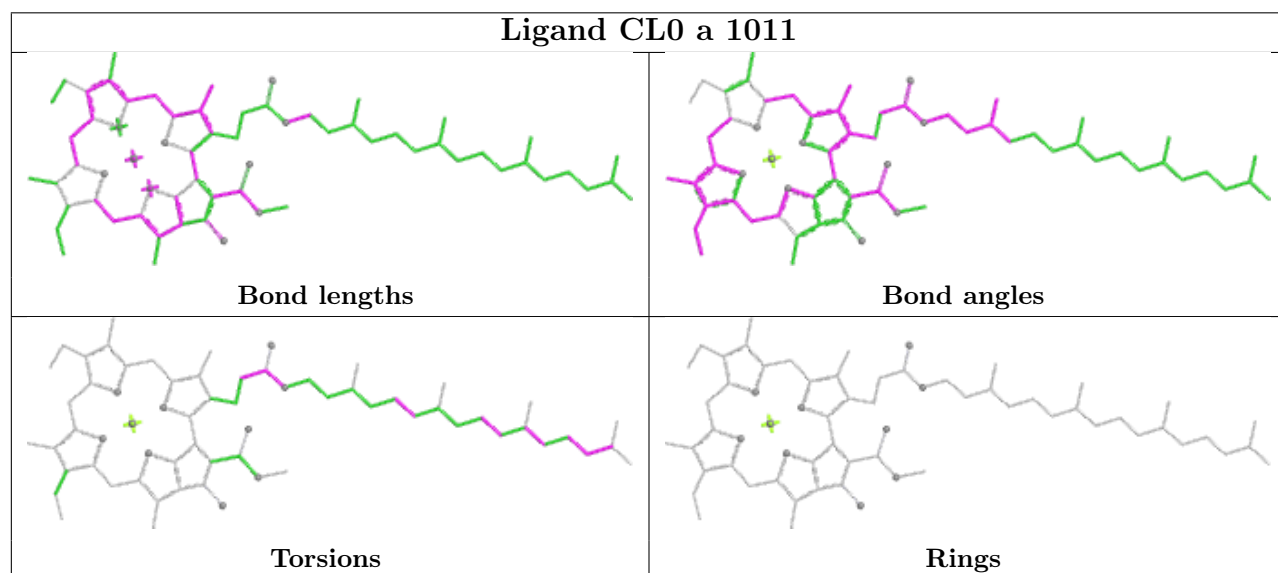
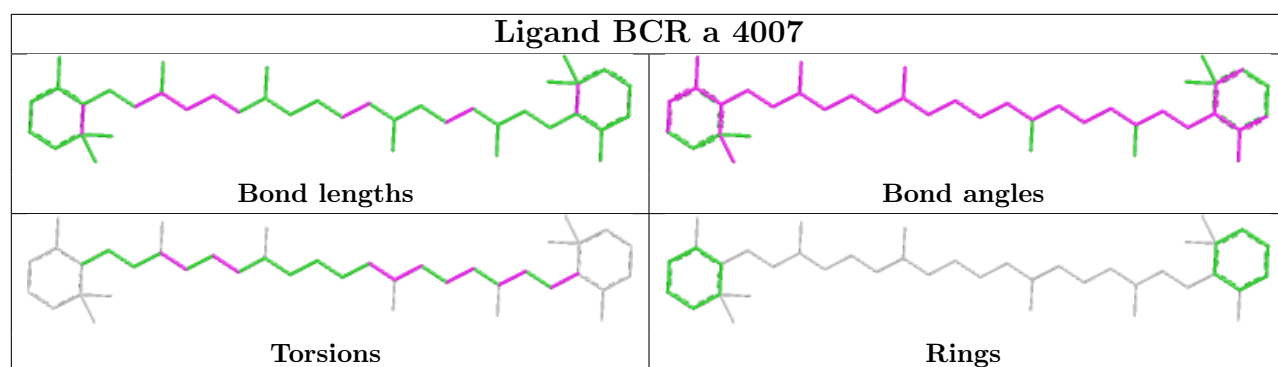


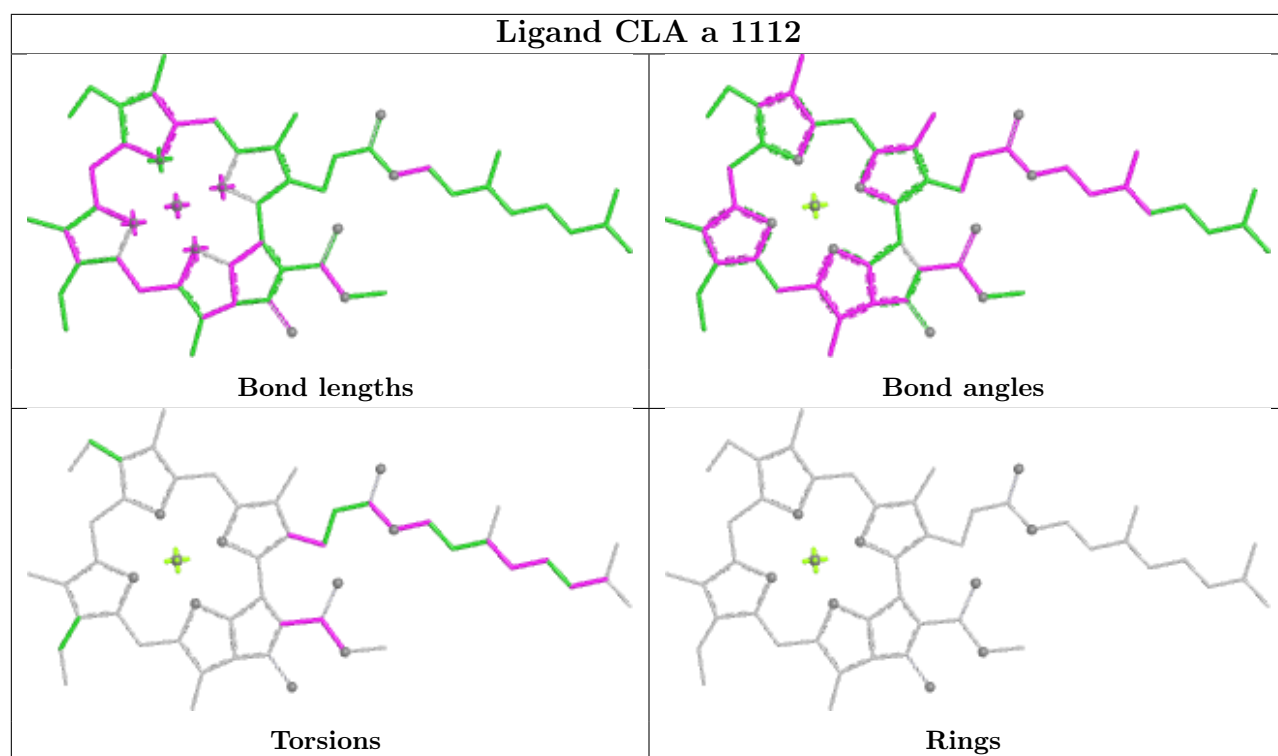


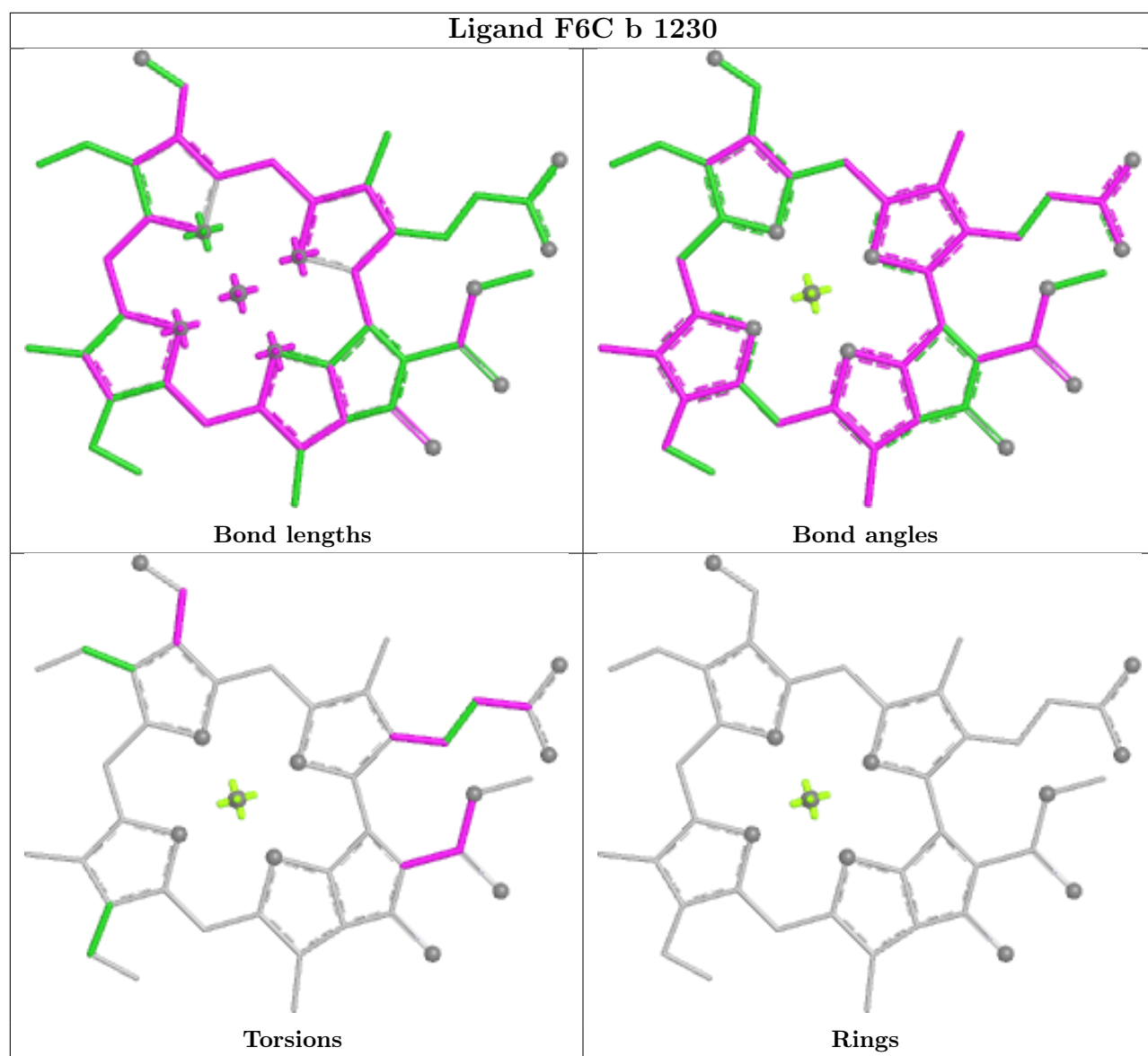


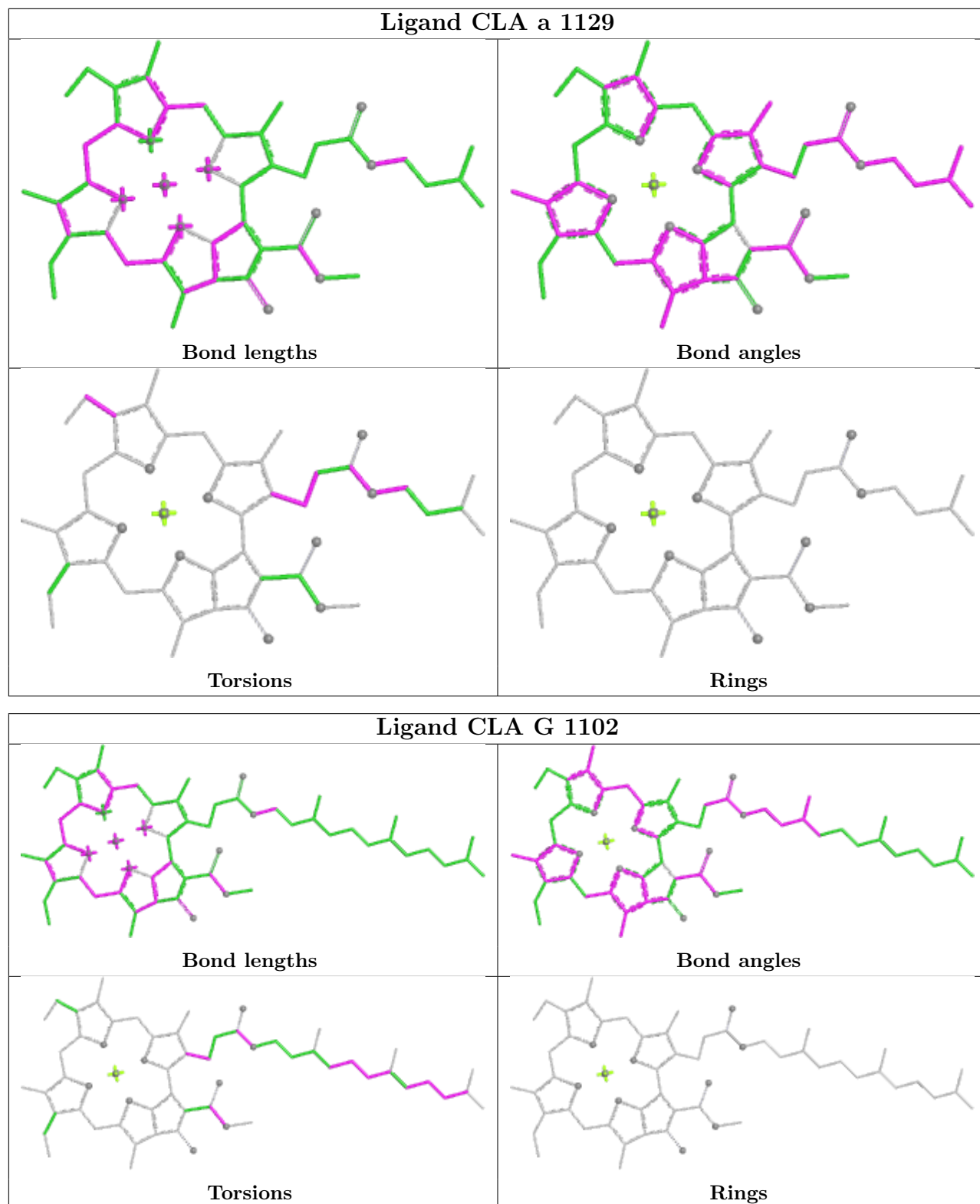


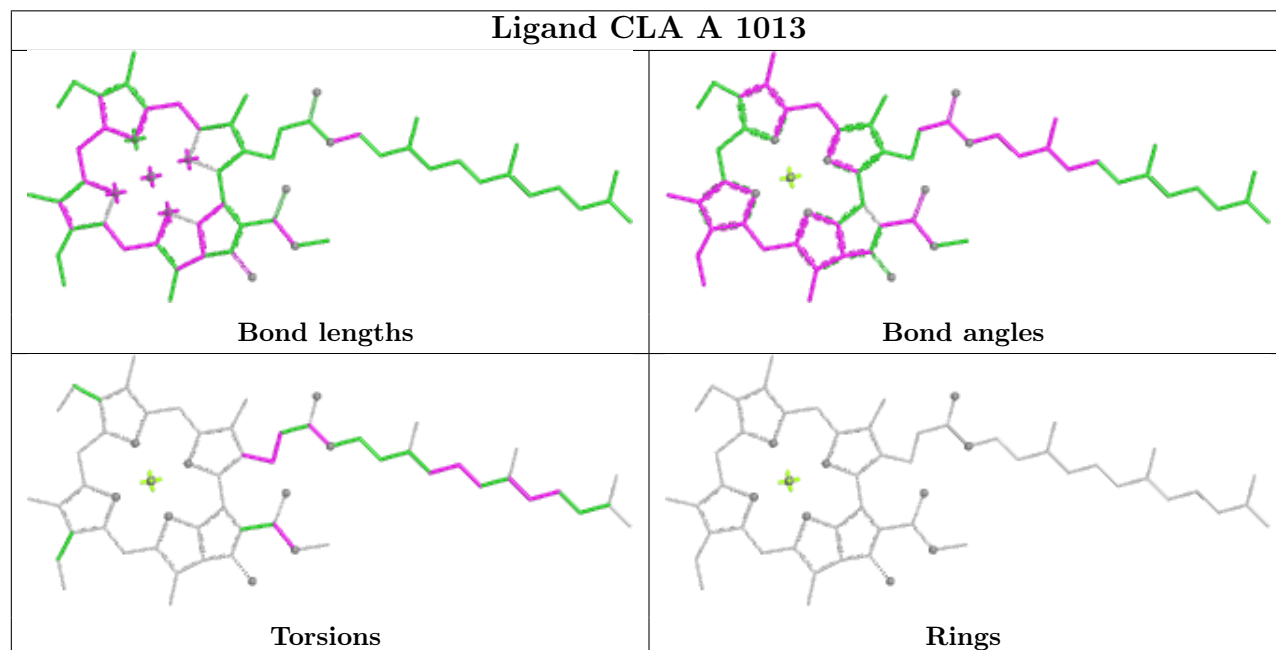
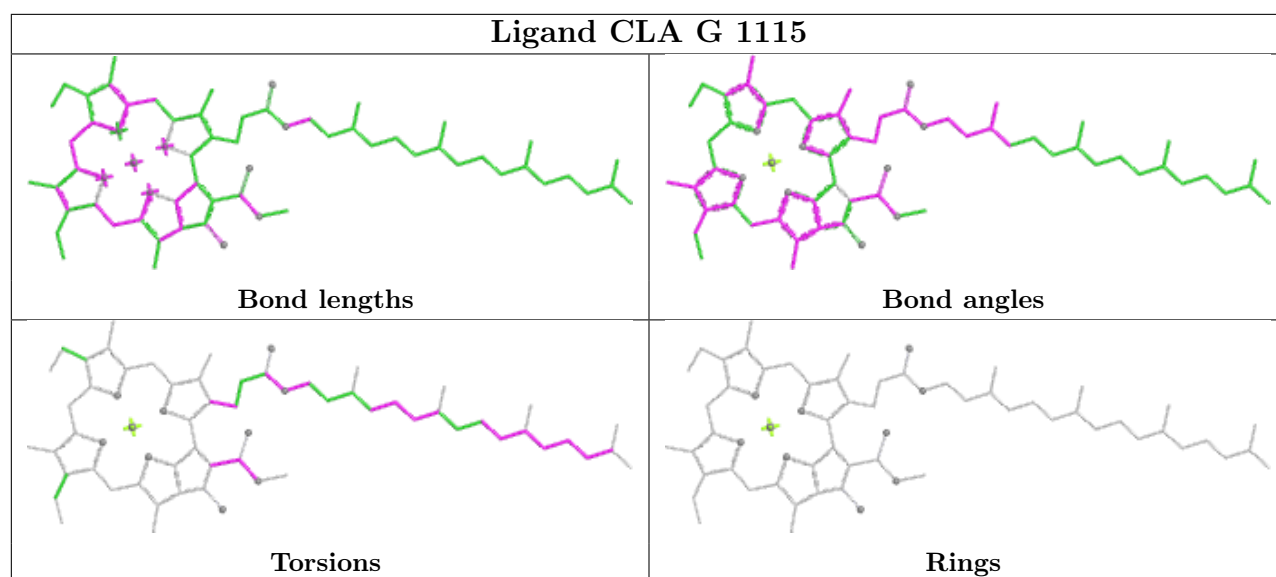
Ligand CLA H 1214**Ligand CLA H 1226****Ligand CLA b 1023**

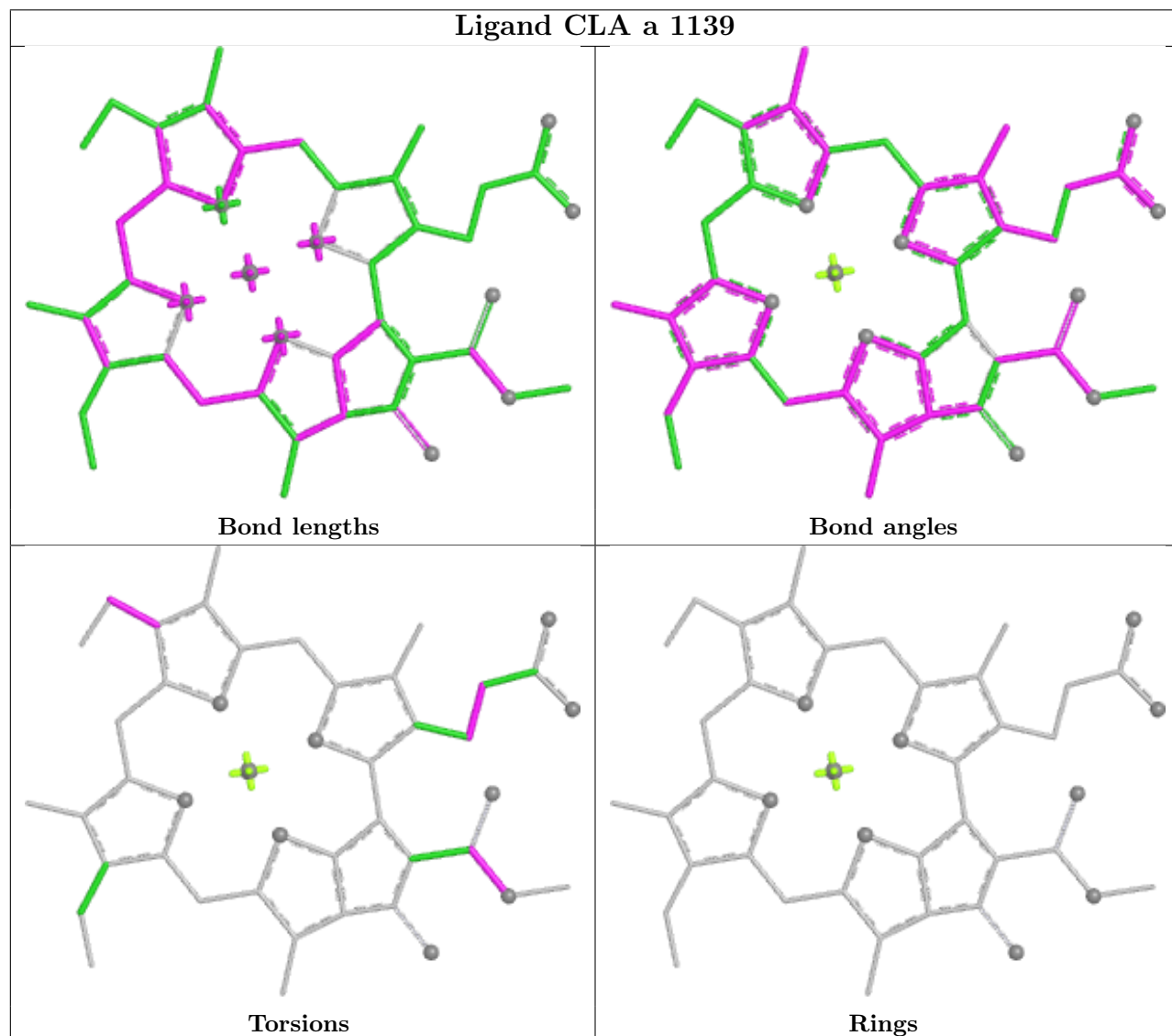
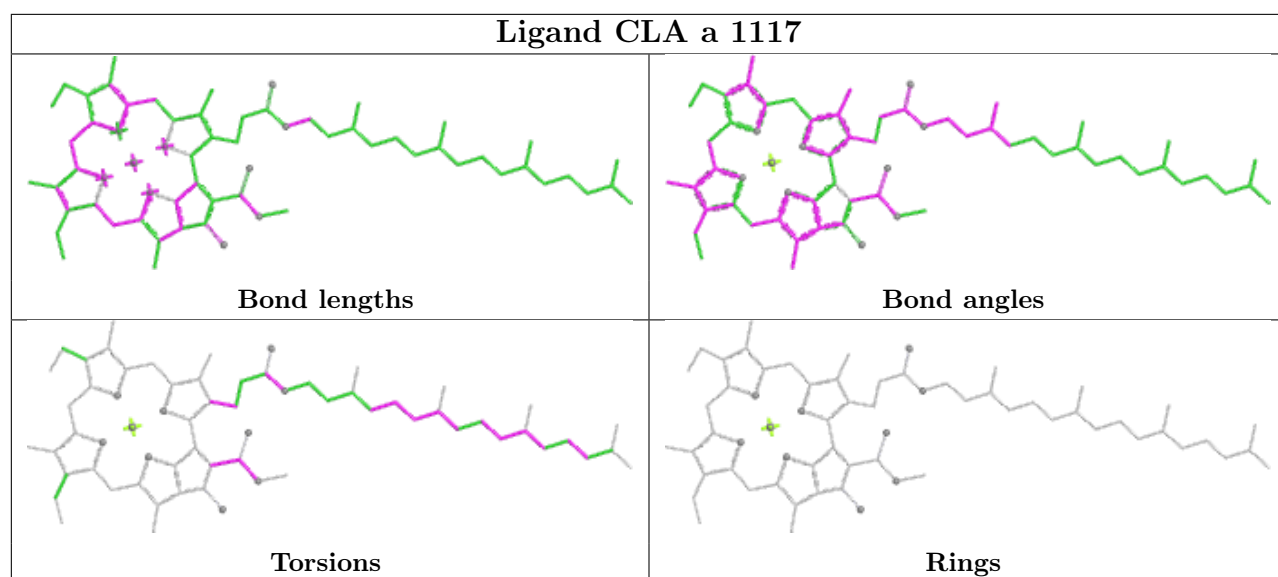


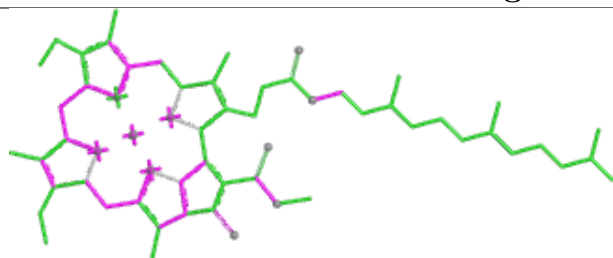
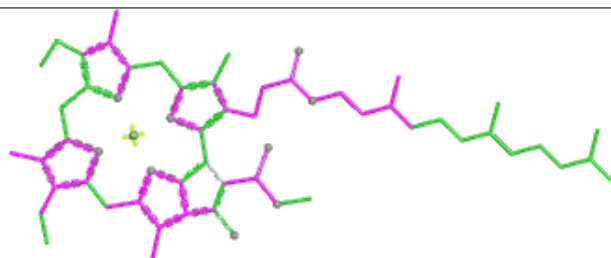
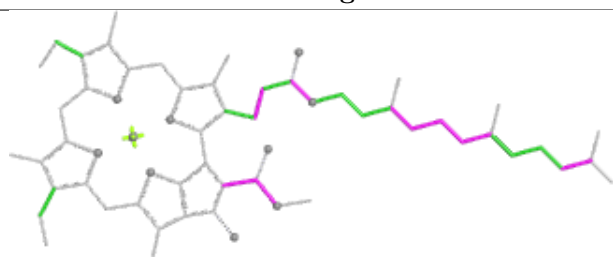
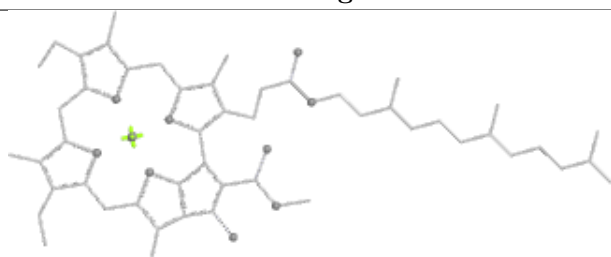
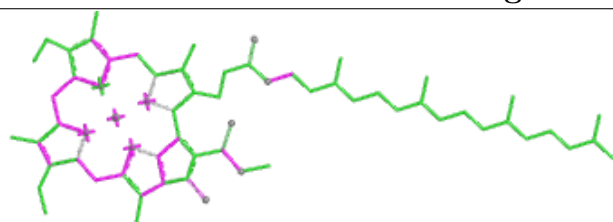
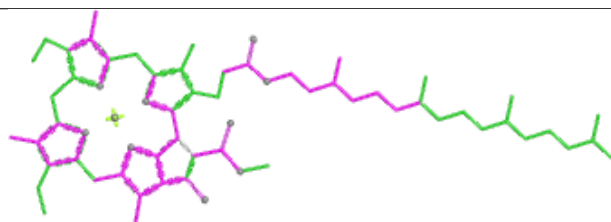
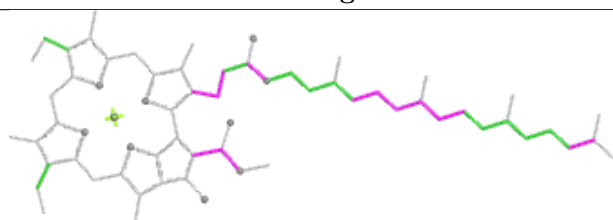
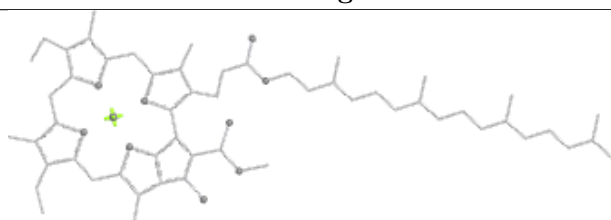


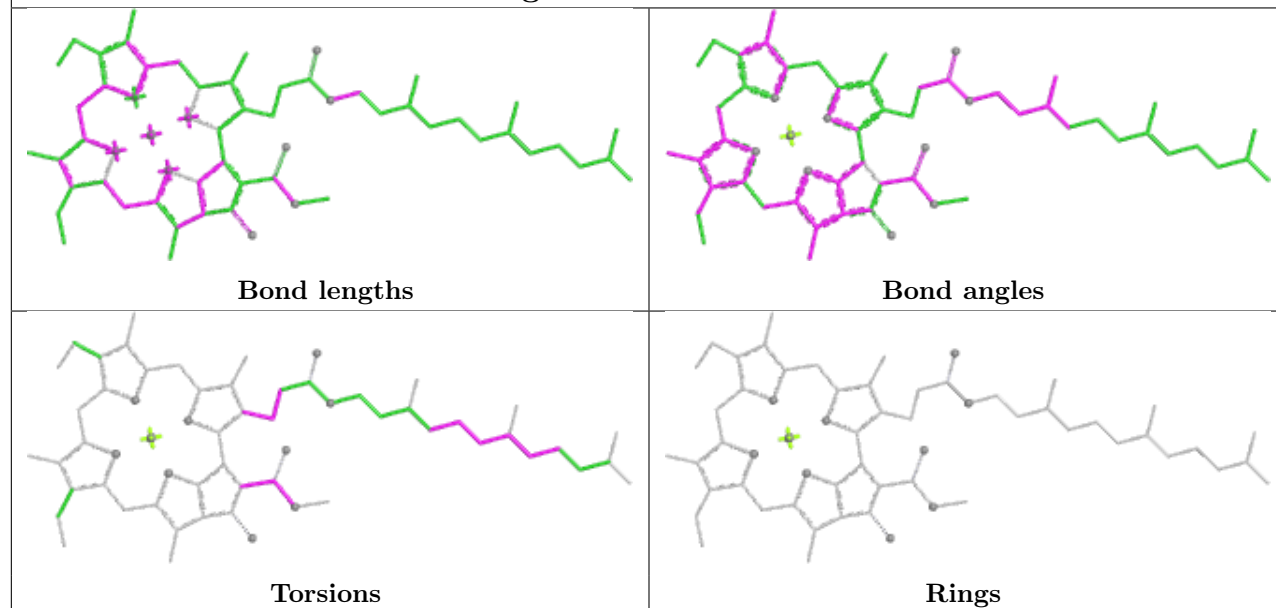
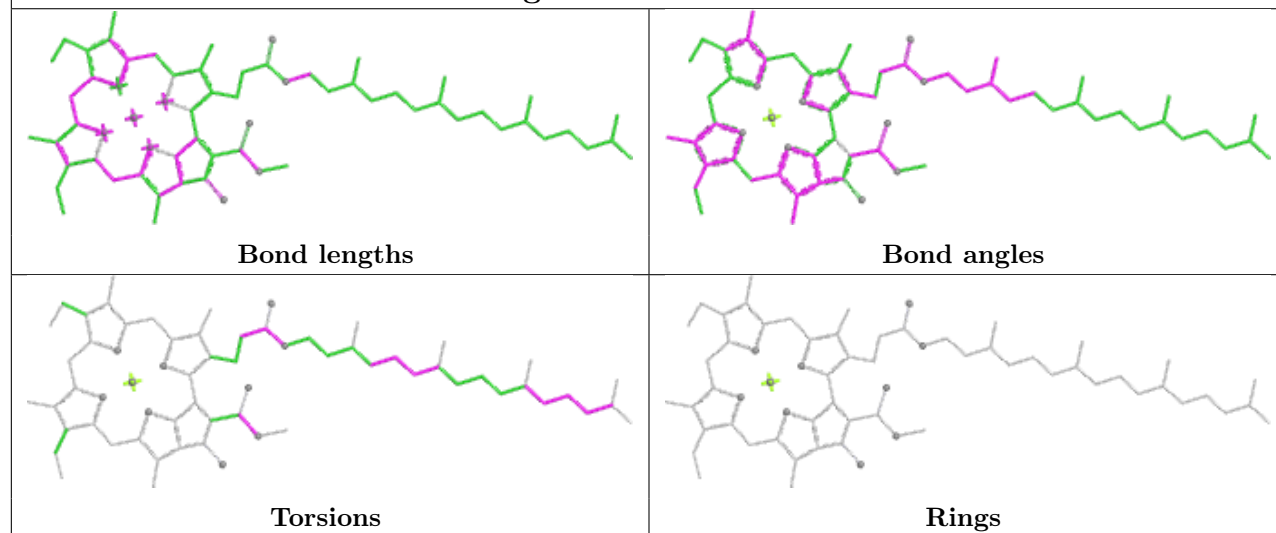


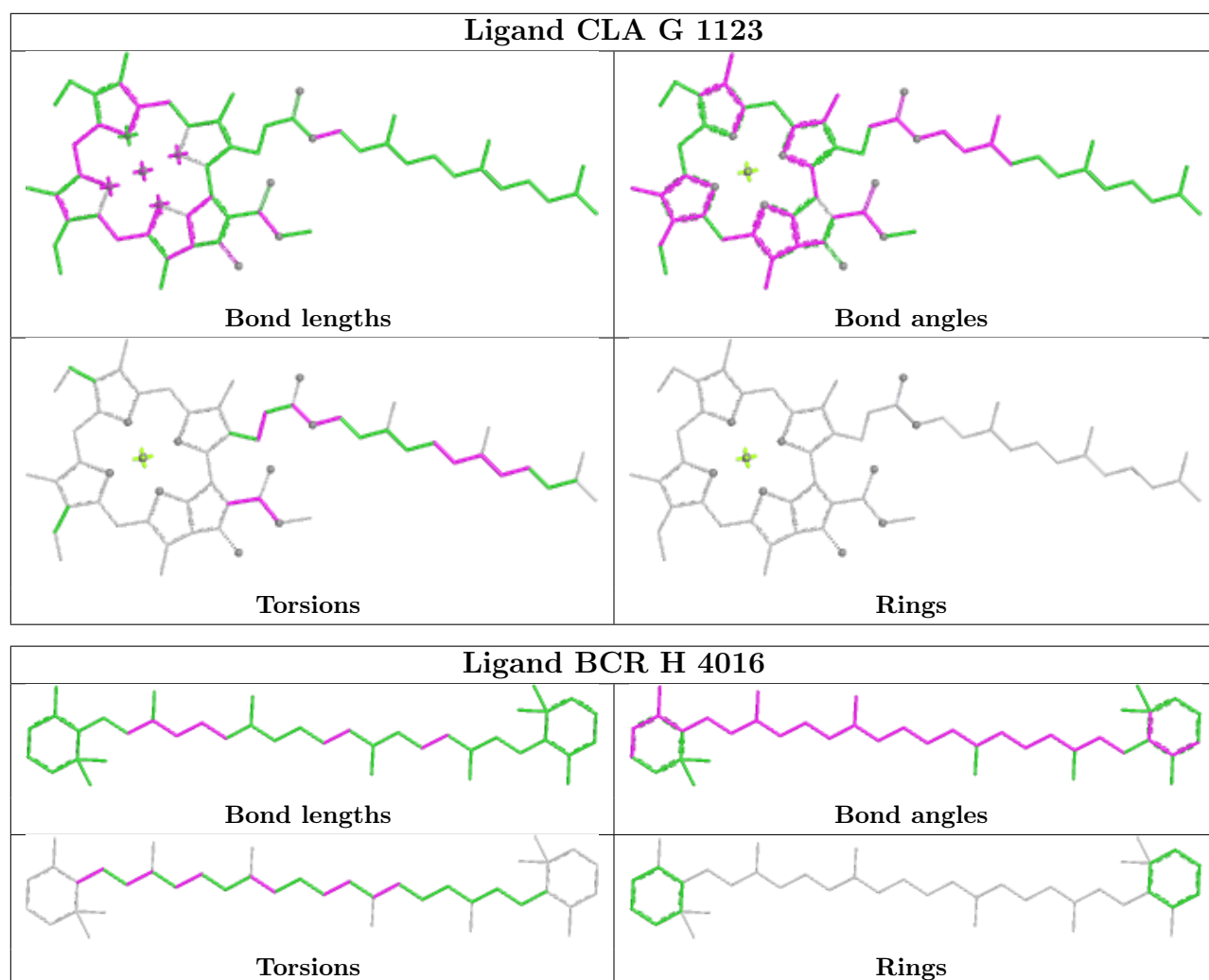




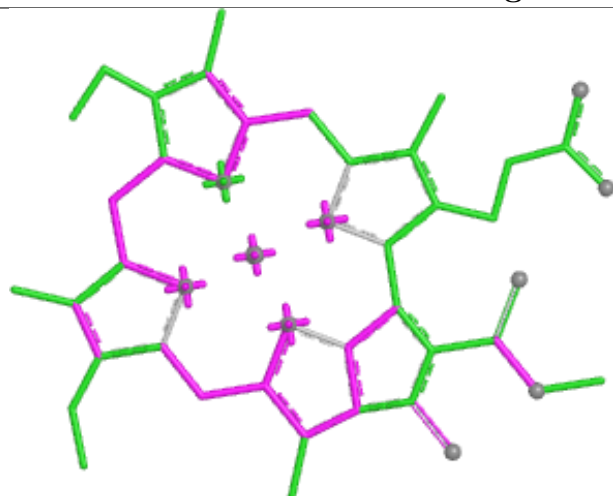


Ligand CLA G 1111**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA H 1223****Bond lengths****Bond angles****Torsions****Rings**

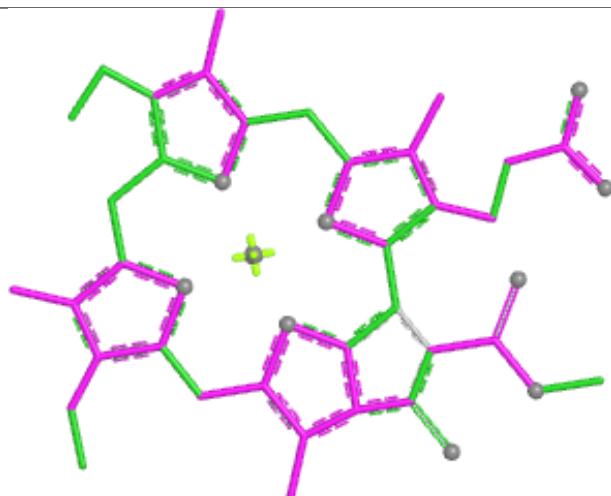
Ligand CLA G 1135**Ligand CLA B 1208**



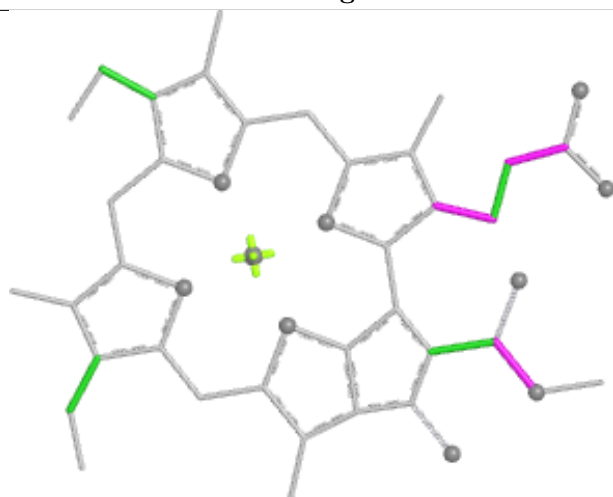
Ligand CLA A 1105



Bond lengths



Bond angles

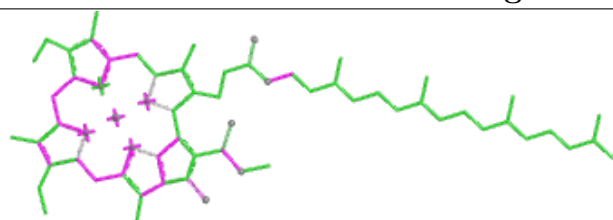


Torsions

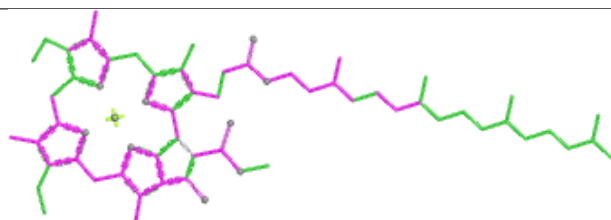


Rings

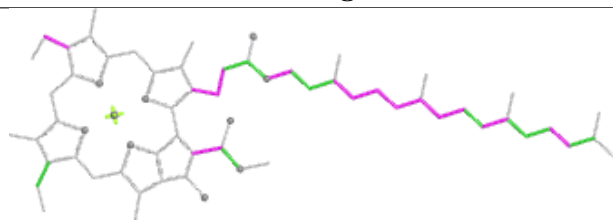
Ligand CLA H 1022



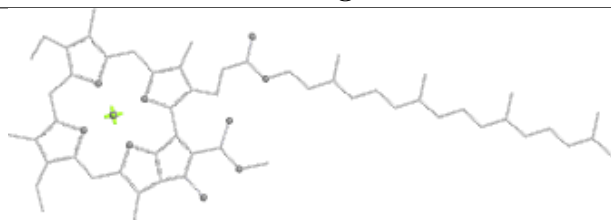
Bond lengths



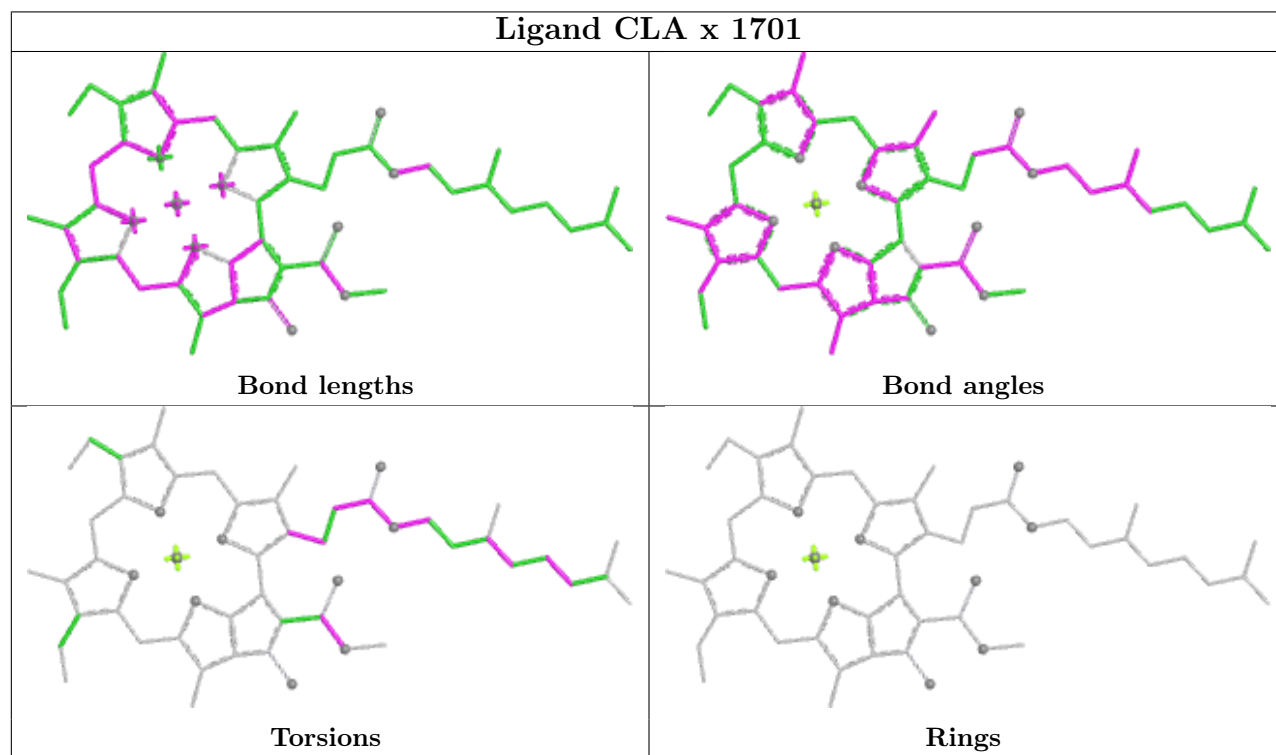
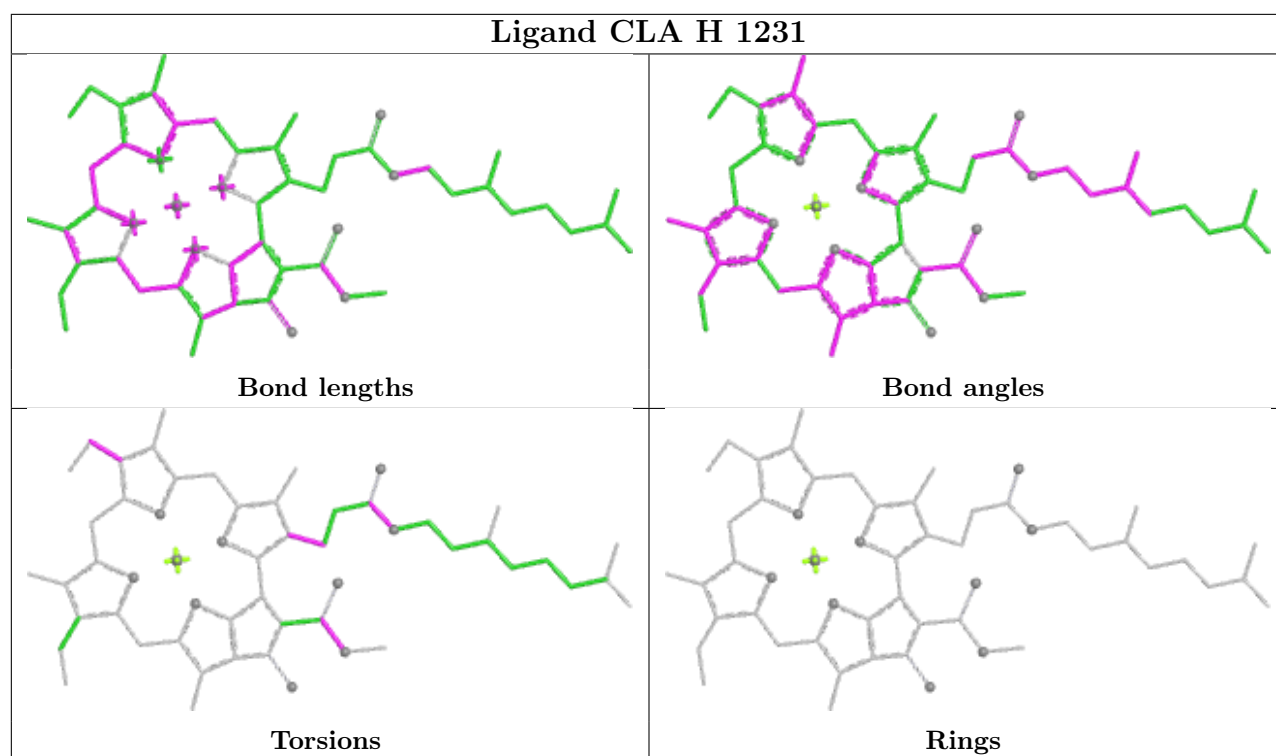
Bond angles

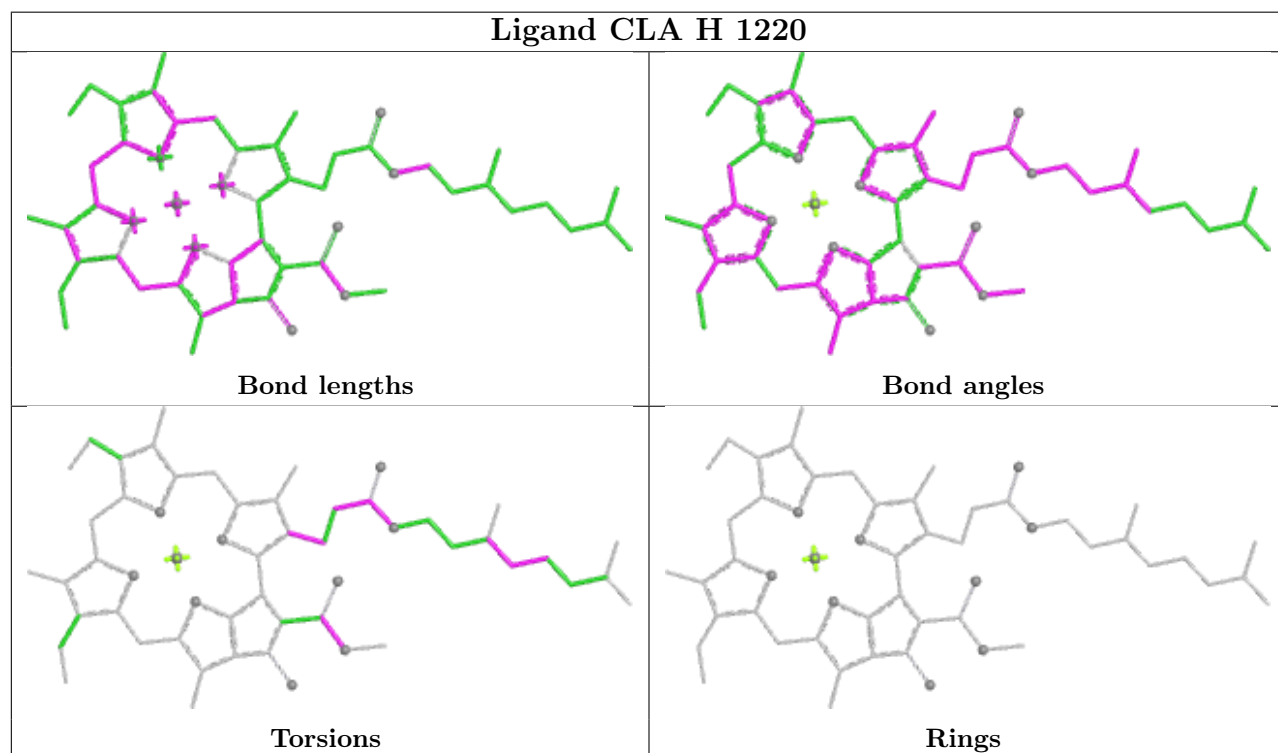
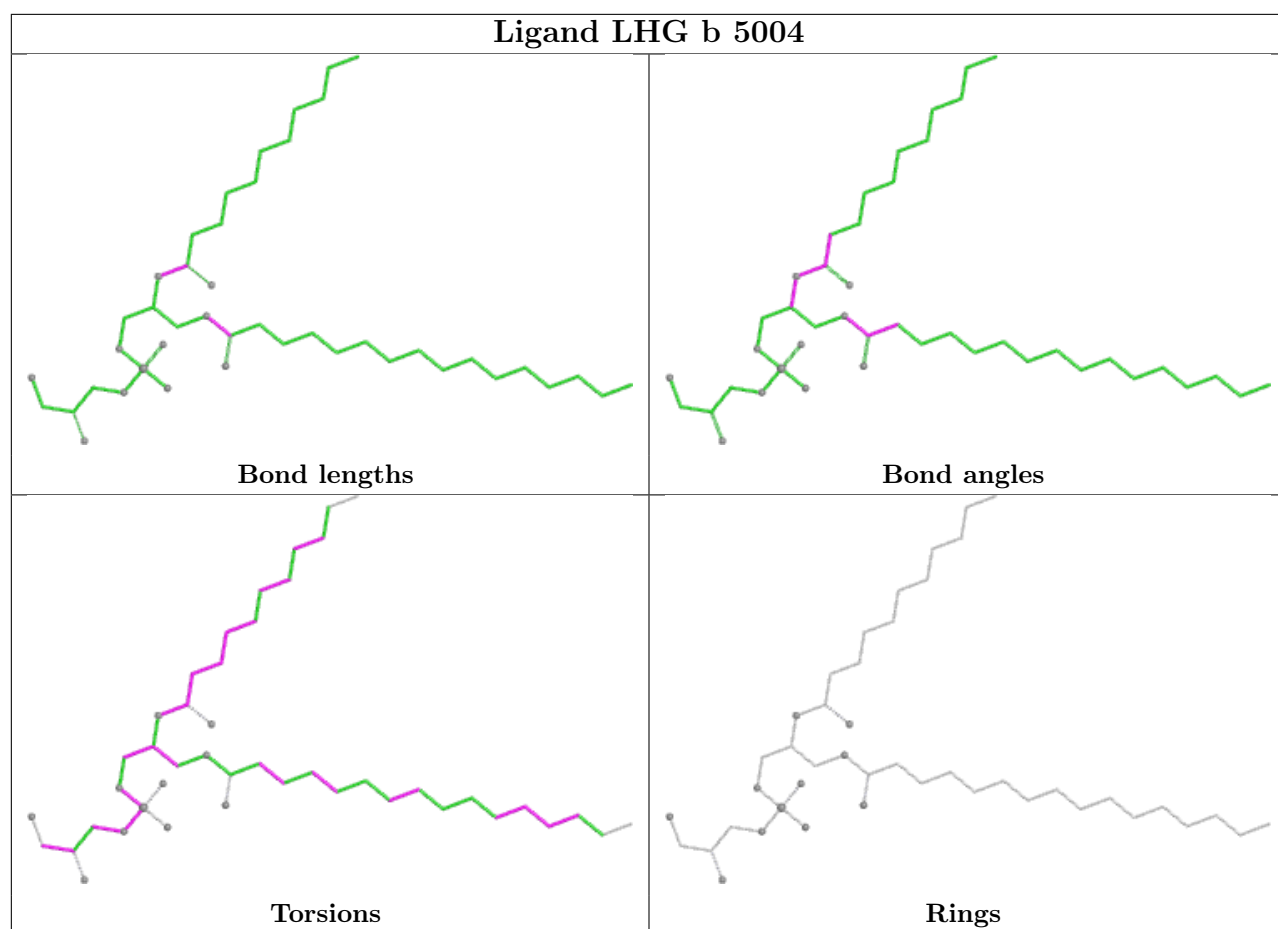


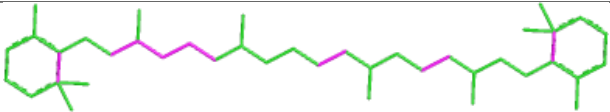
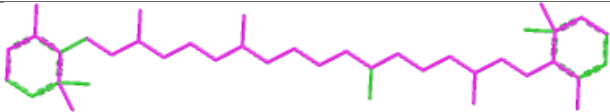
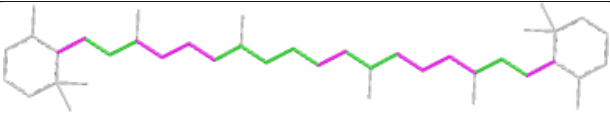
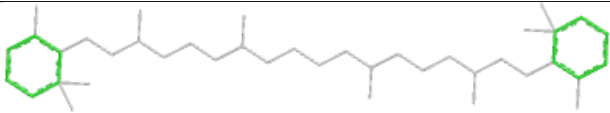
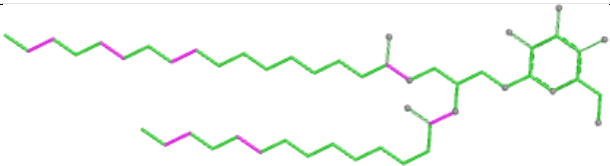
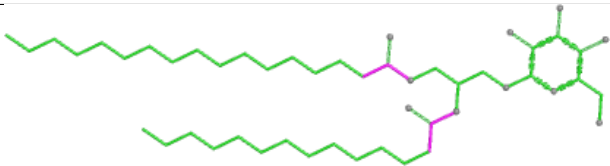
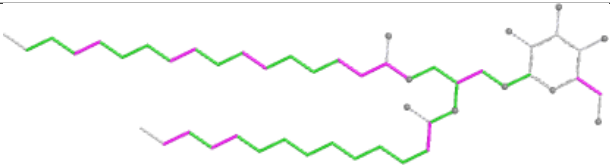
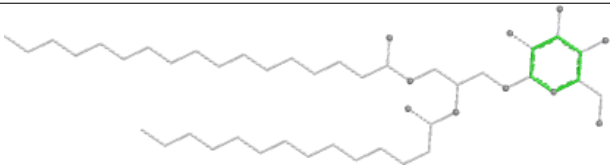
Torsions



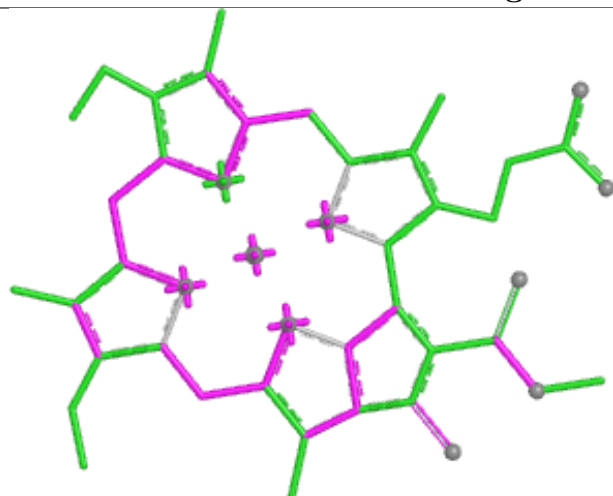
Rings



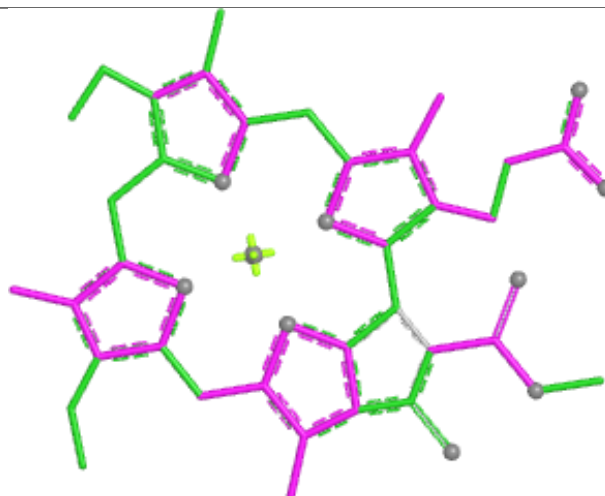


Ligand BCR i 4020	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG U 5007	
 Bond lengths	 Bond angles
 Torsions	 Rings

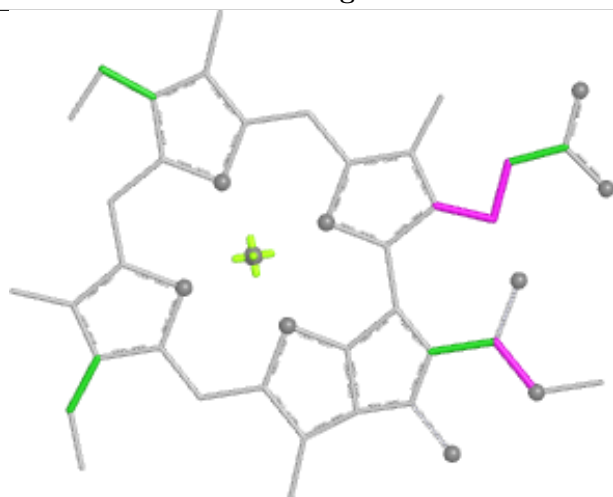
Ligand CLA B 1212



Bond lengths



Bond angles

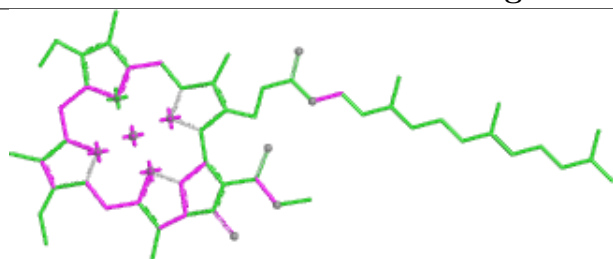


Torsions

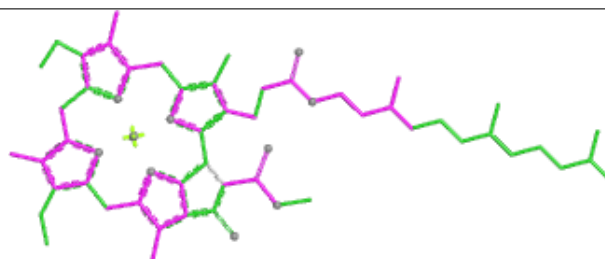


Rings

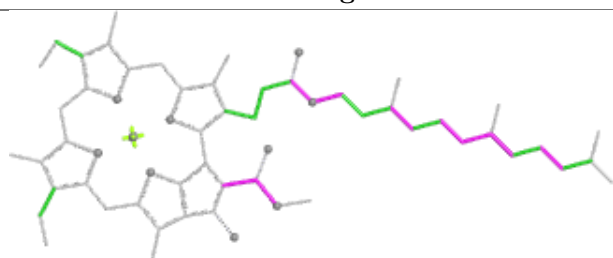
Ligand CLA A 1128



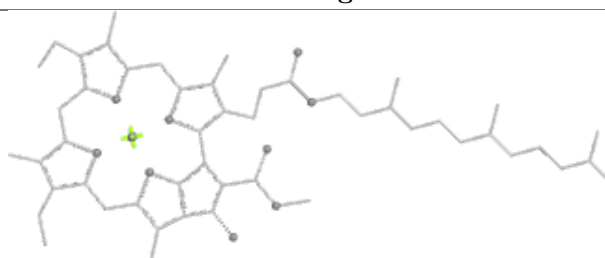
Bond lengths



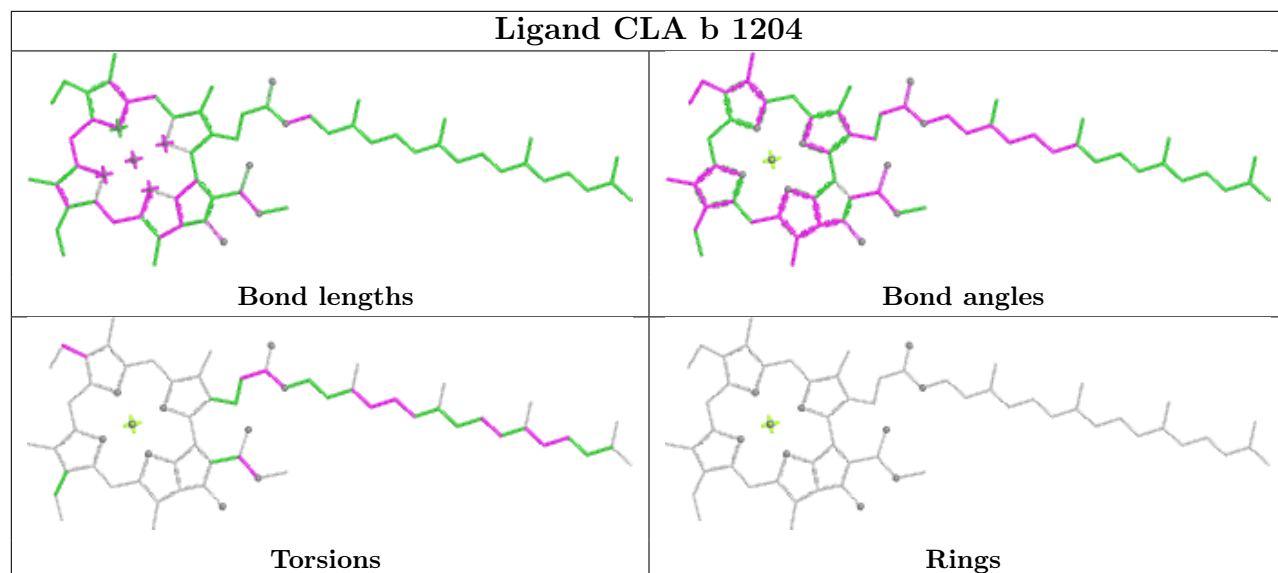
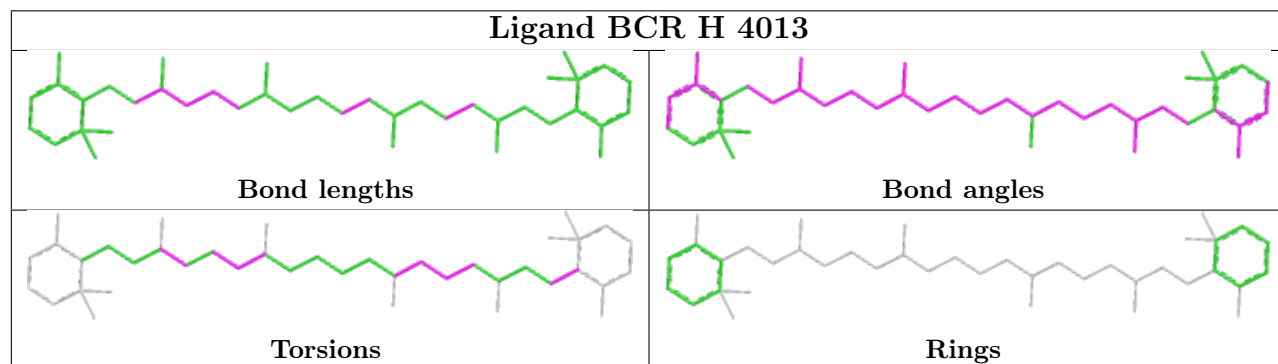
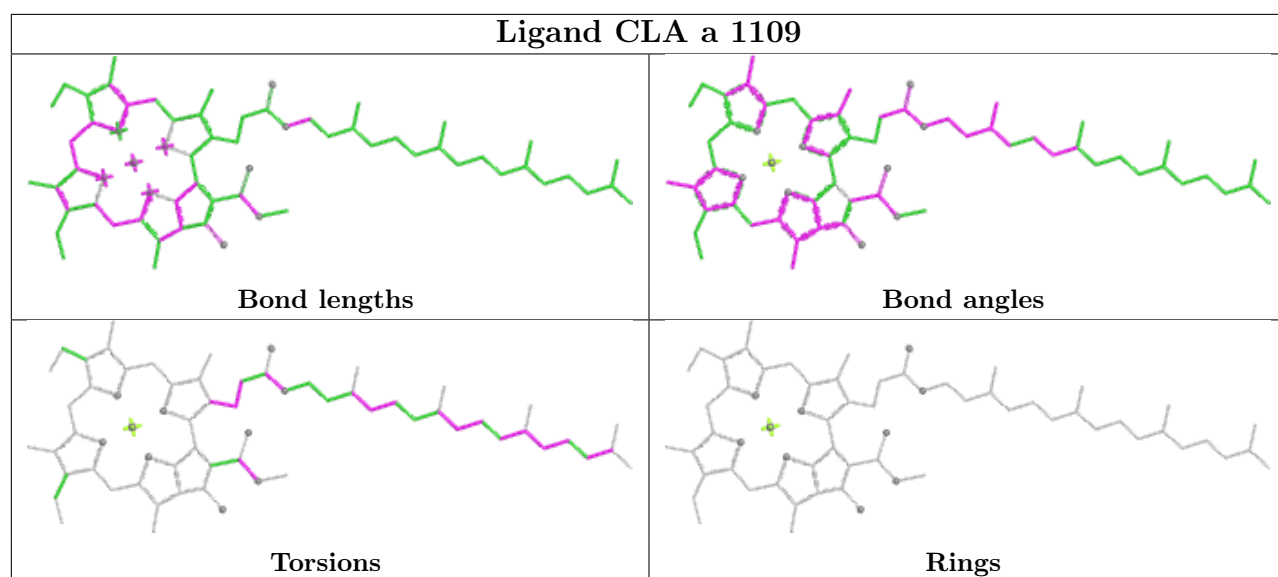
Bond angles

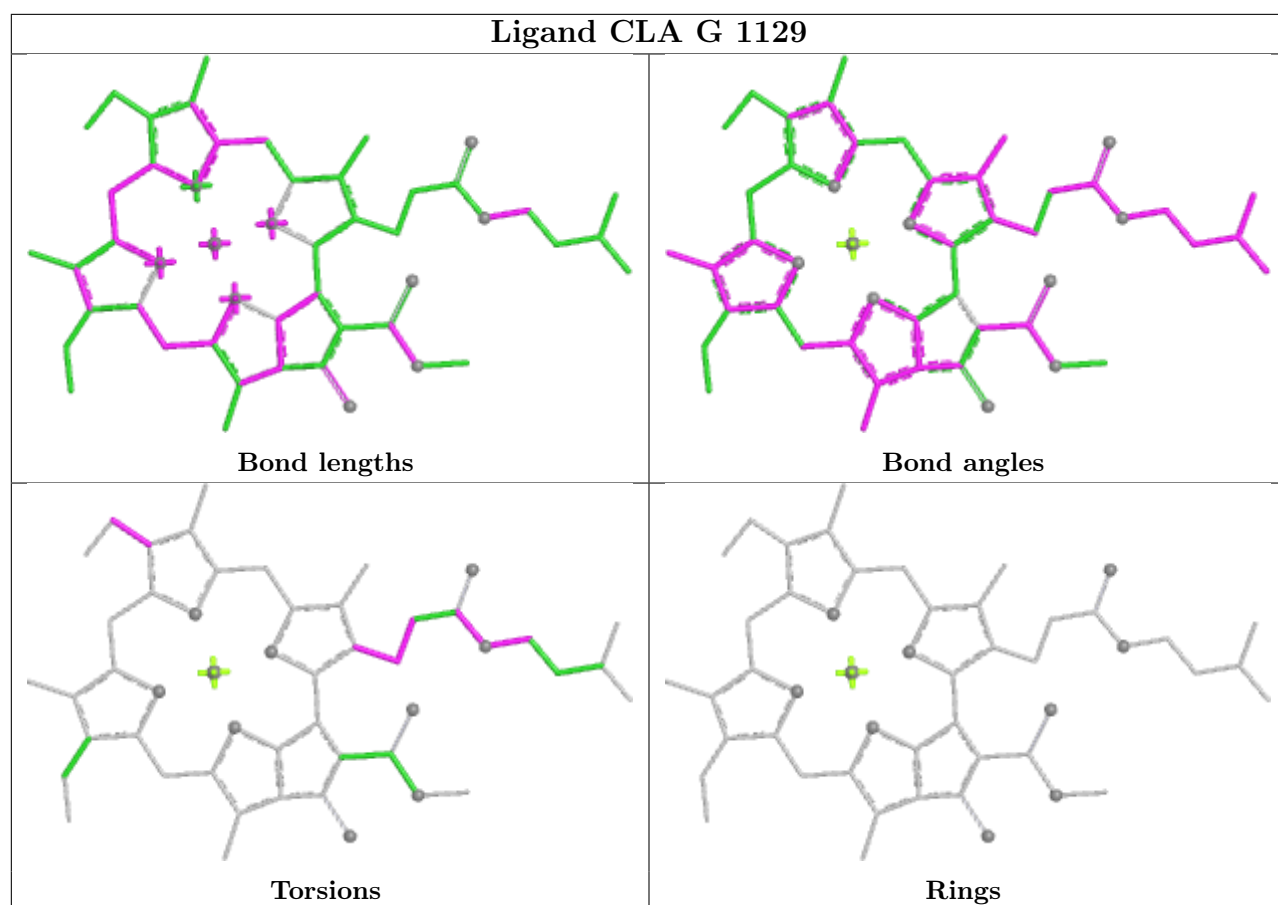


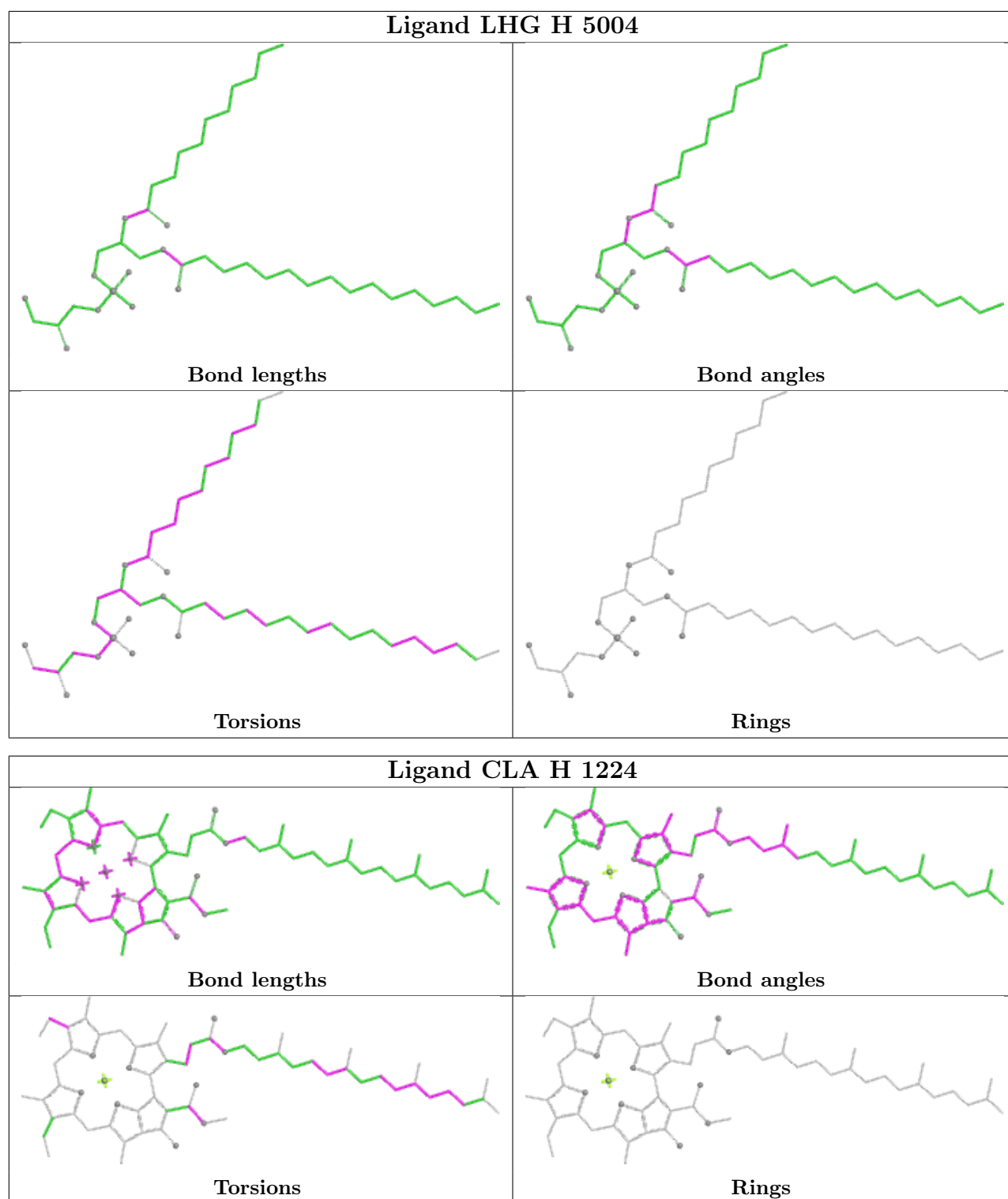
Torsions



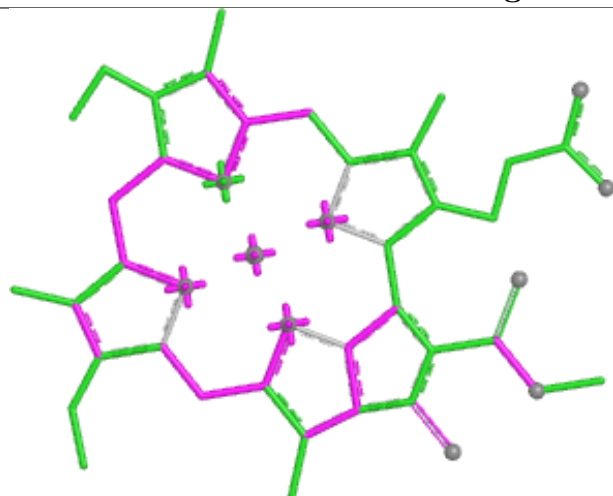
Rings



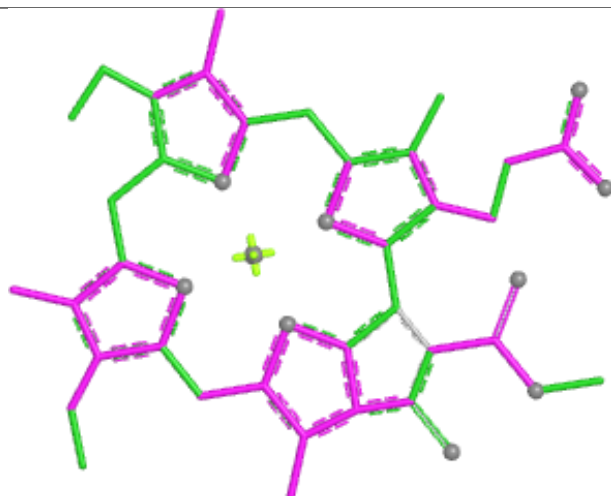




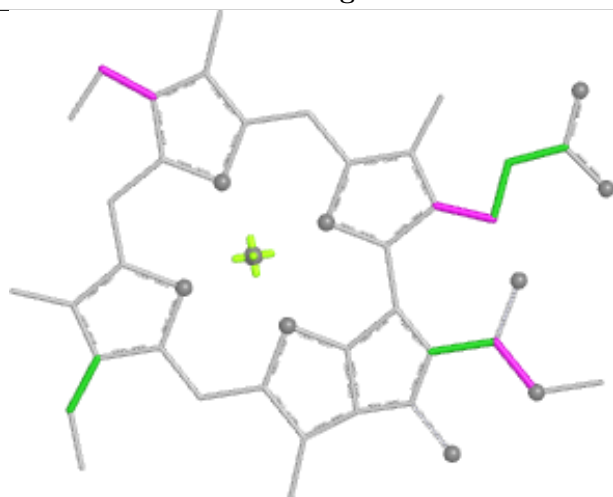
Ligand CLA G 1107



Bond lengths



Bond angles

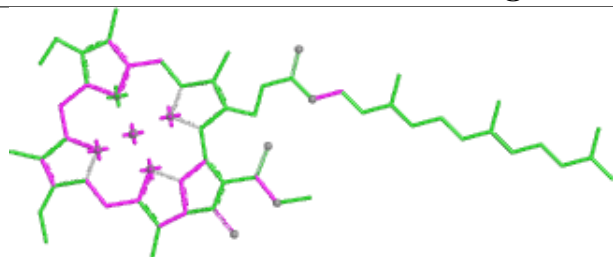


Torsions

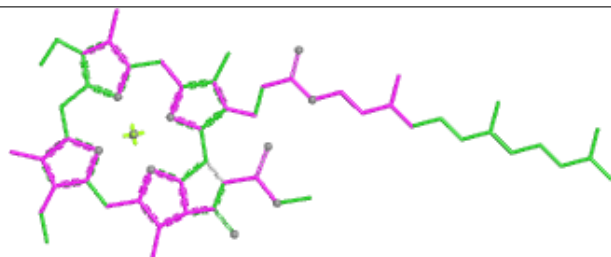


Rings

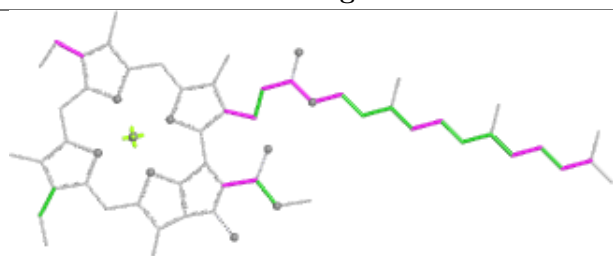
Ligand CLA H 1202



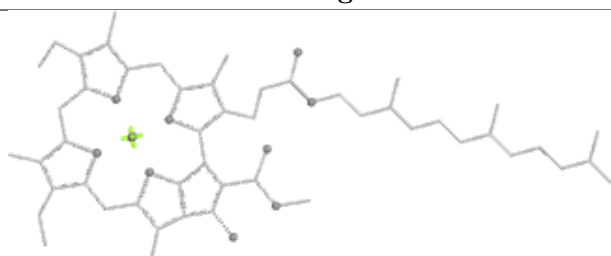
Bond lengths



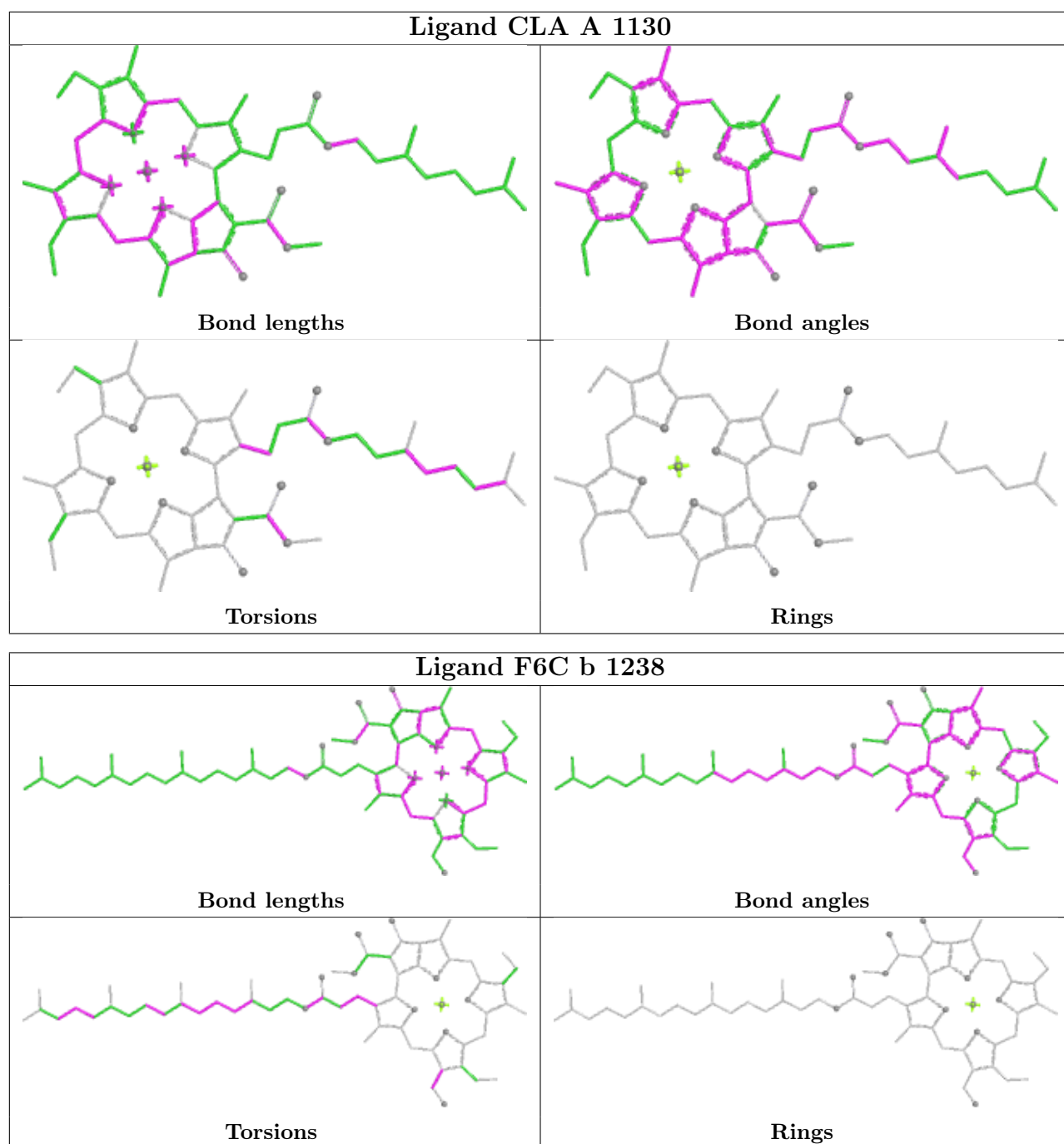
Bond angles

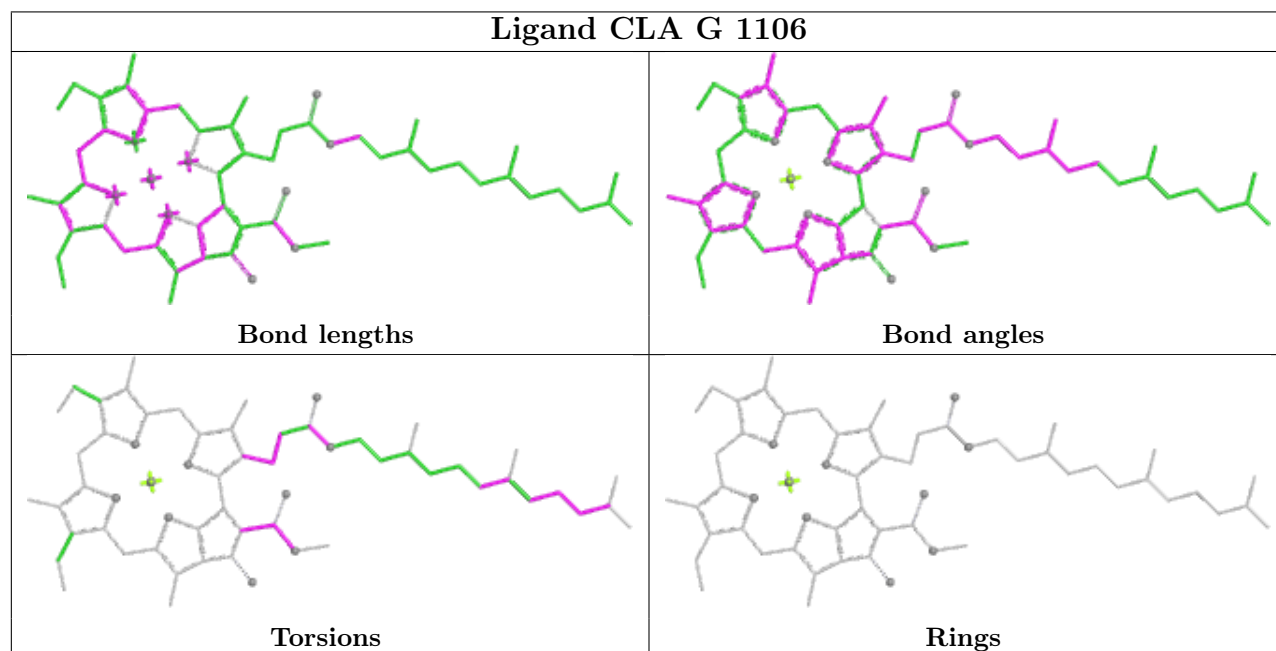
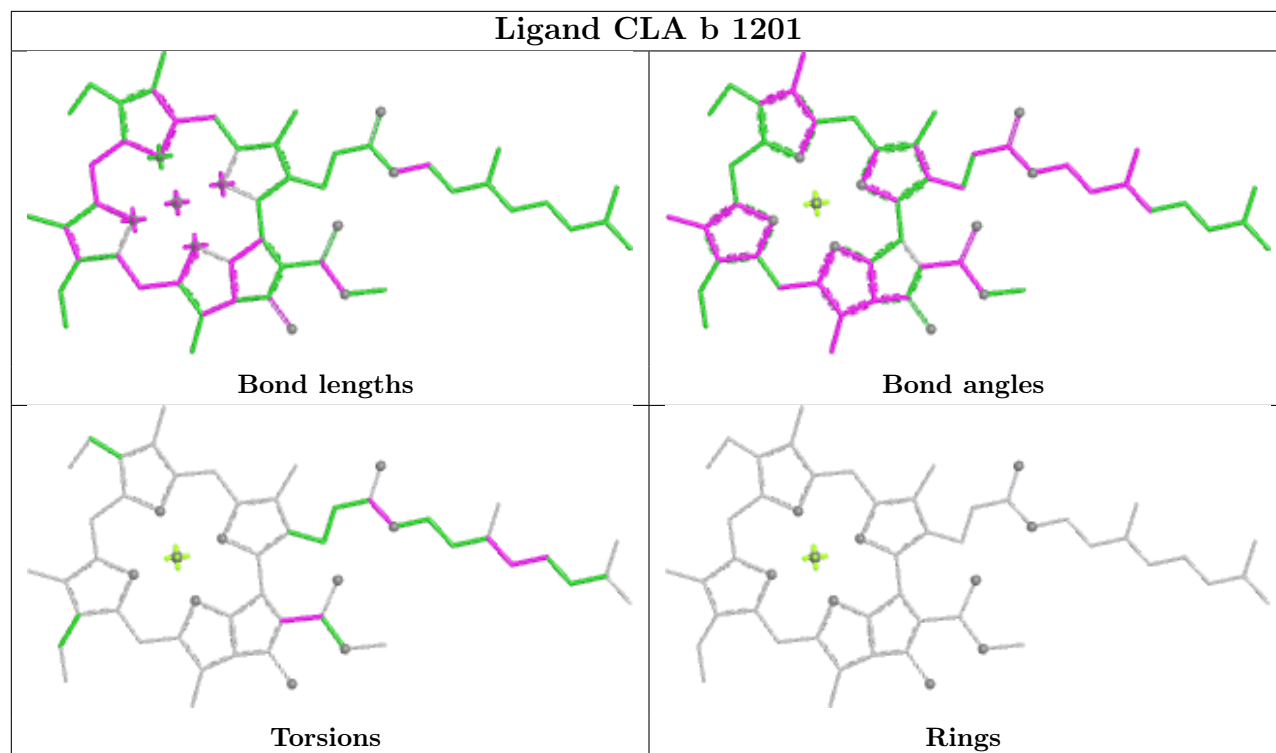


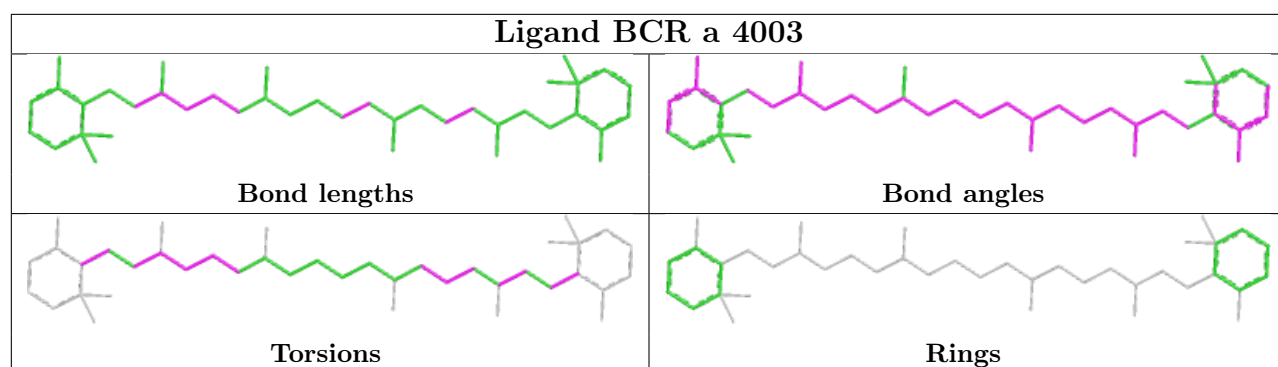
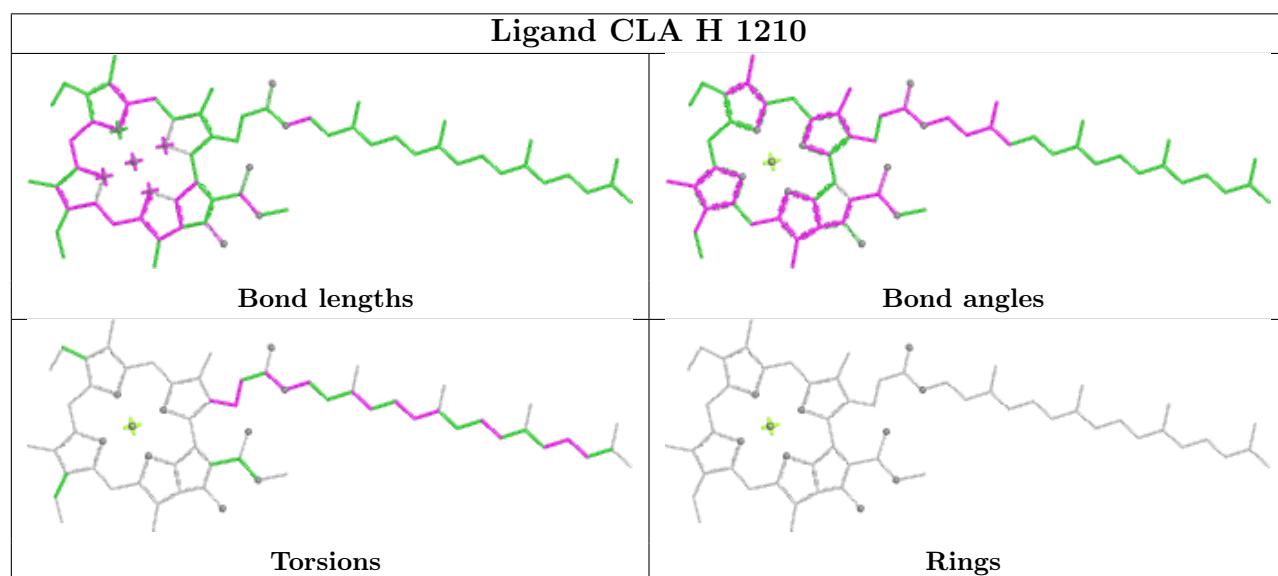
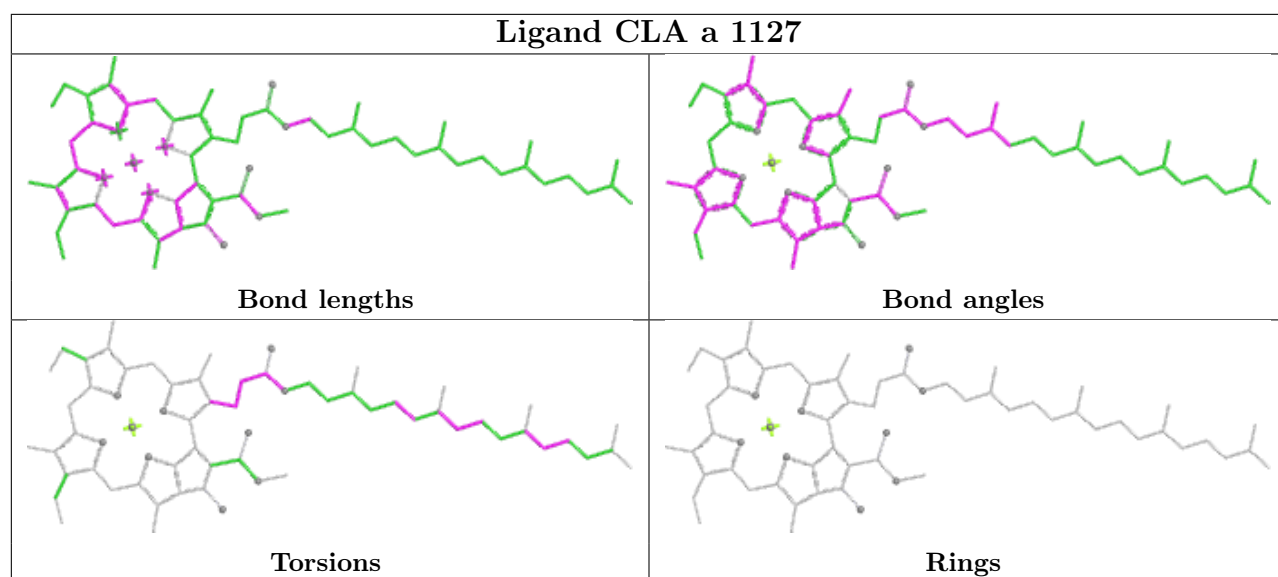
Torsions

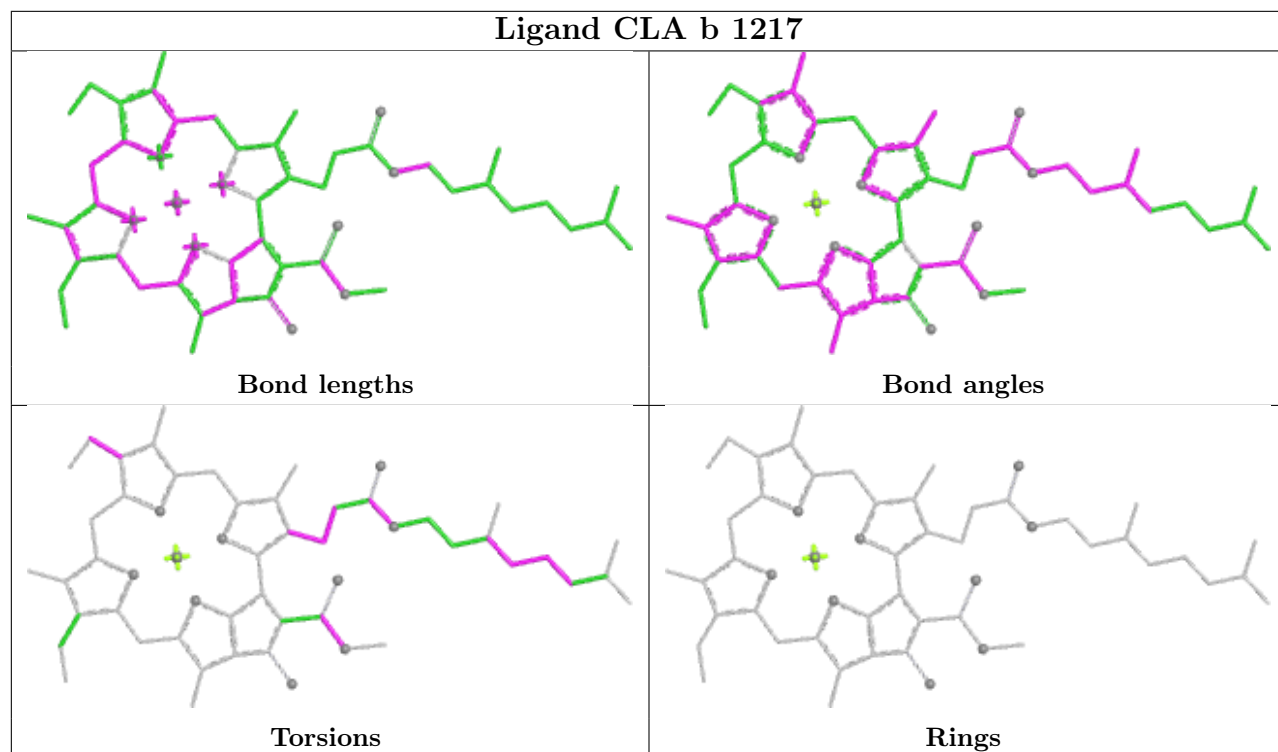
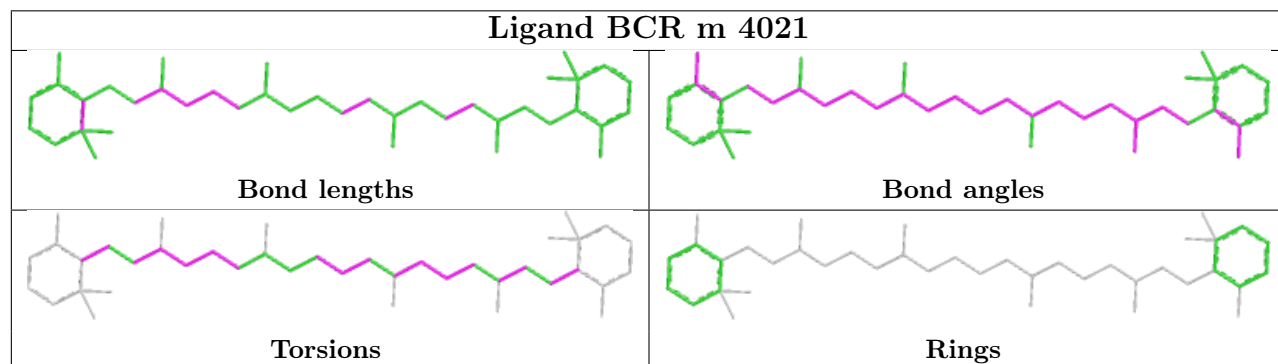
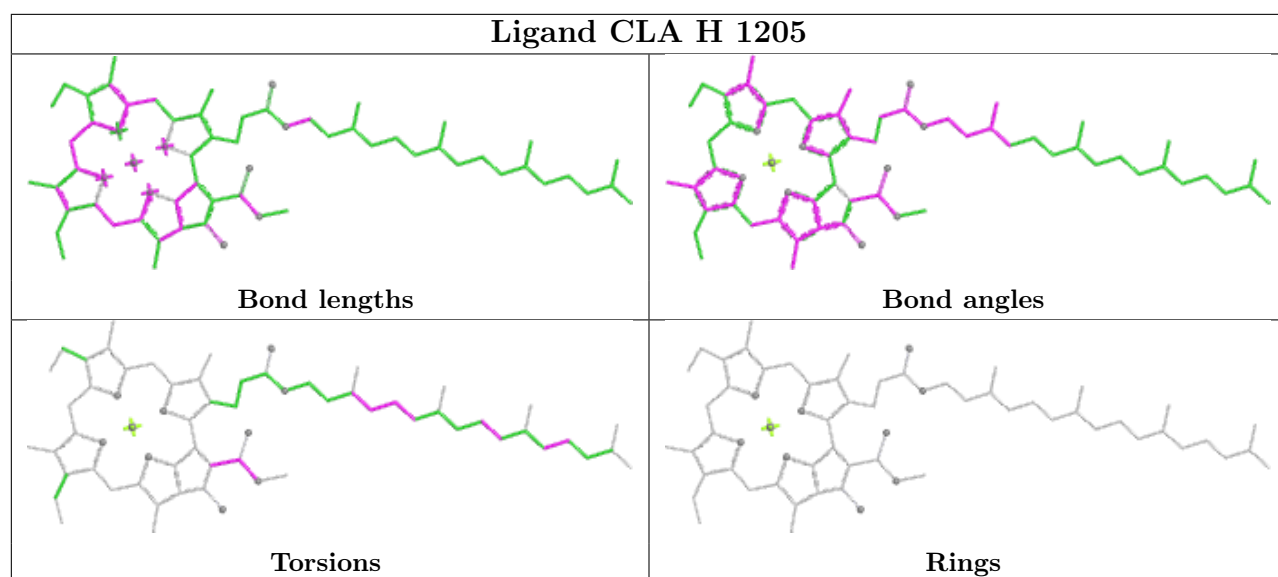


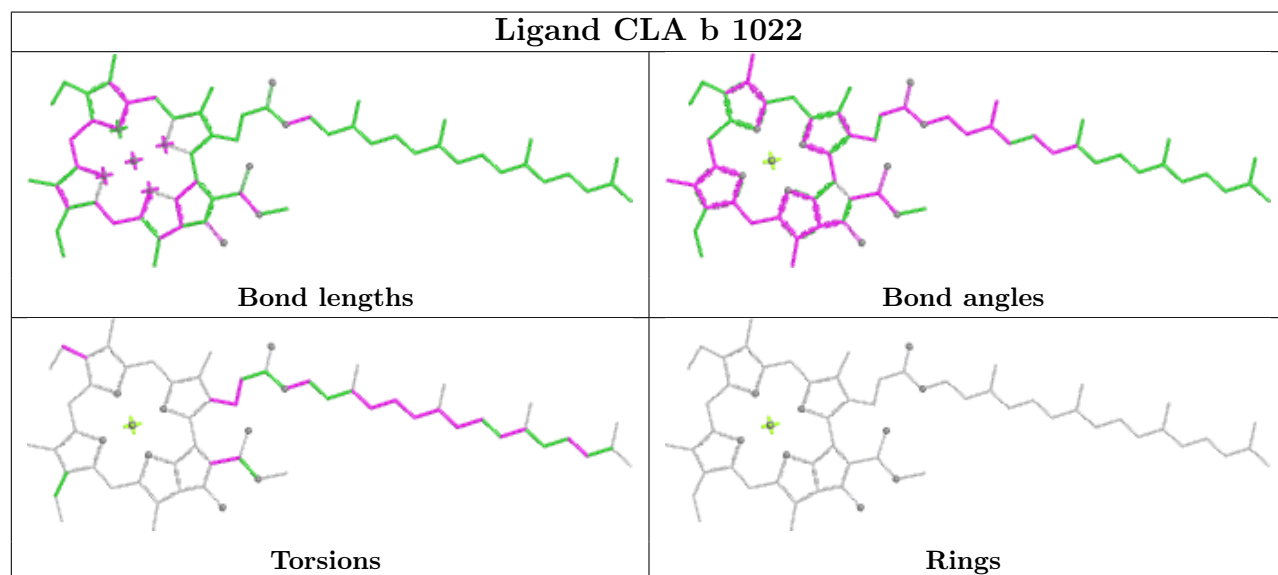
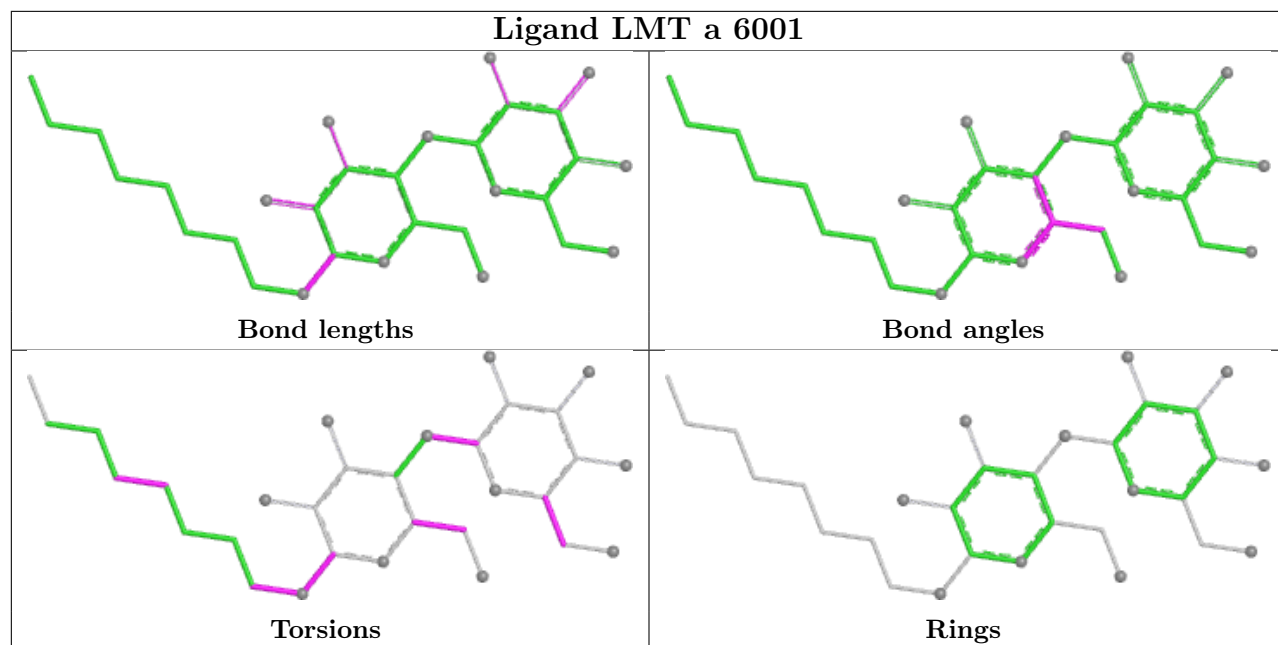
Rings

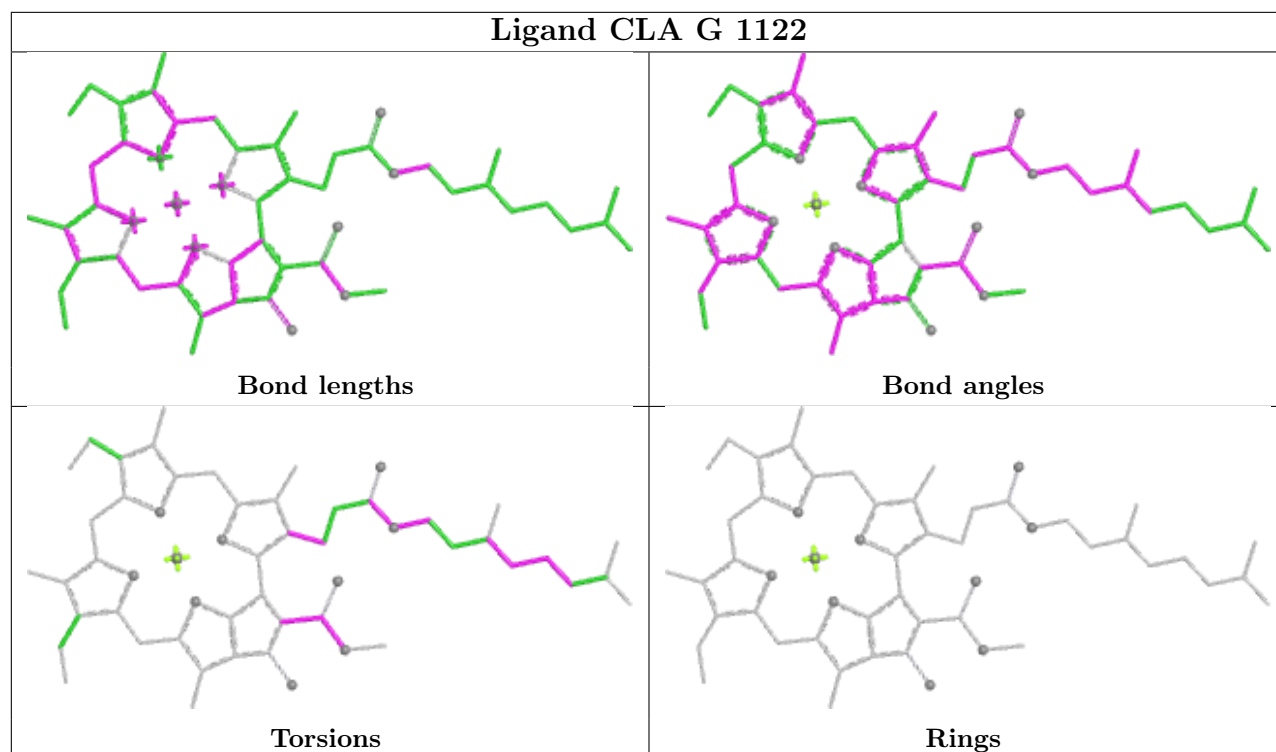
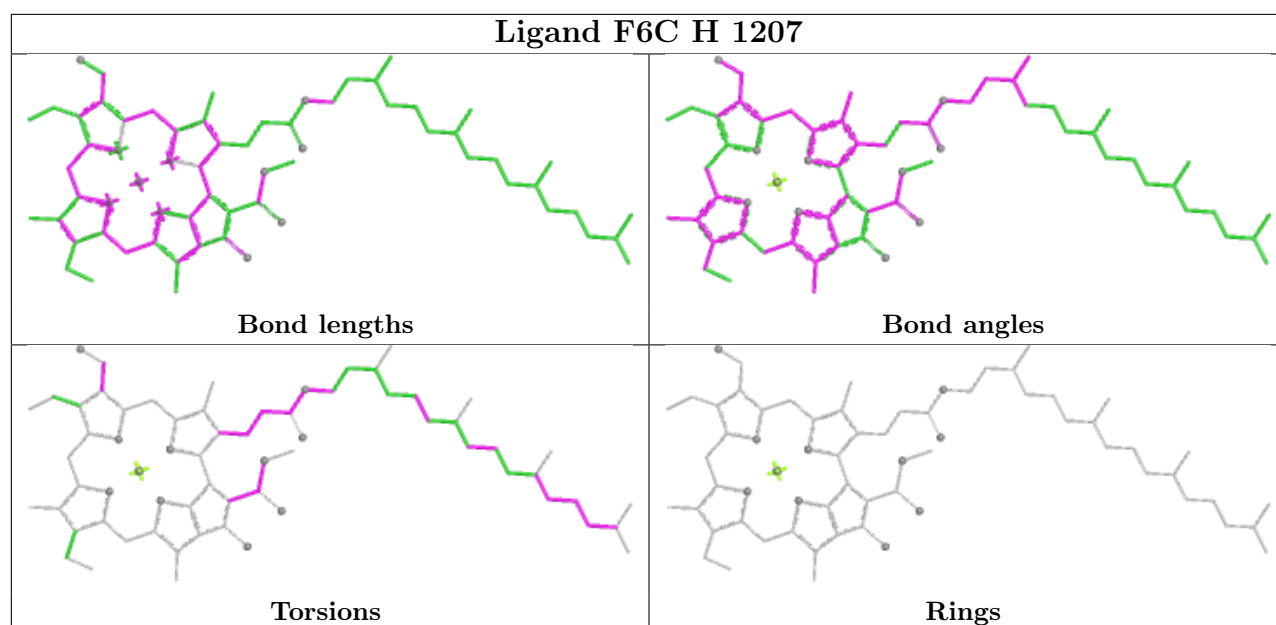


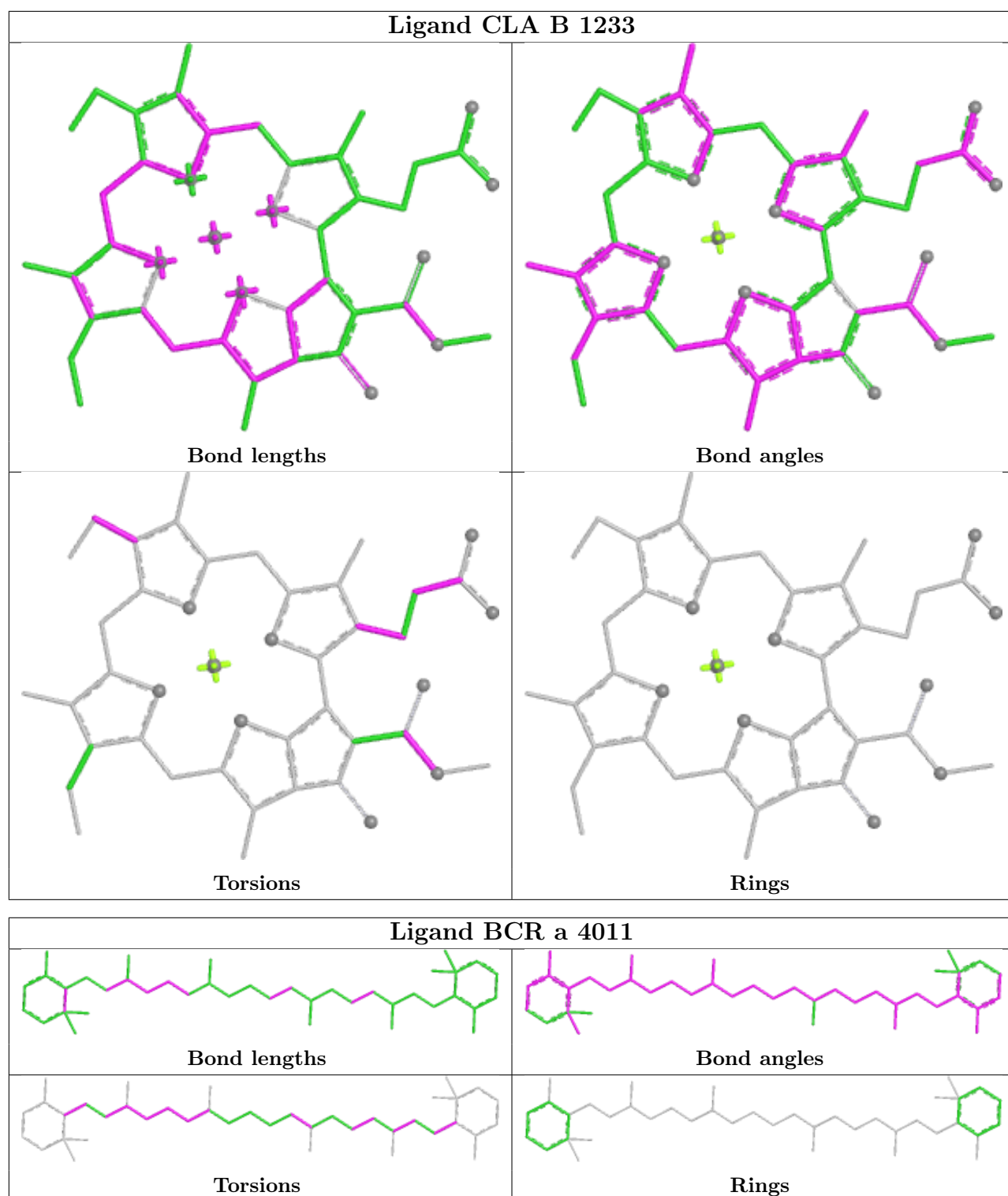


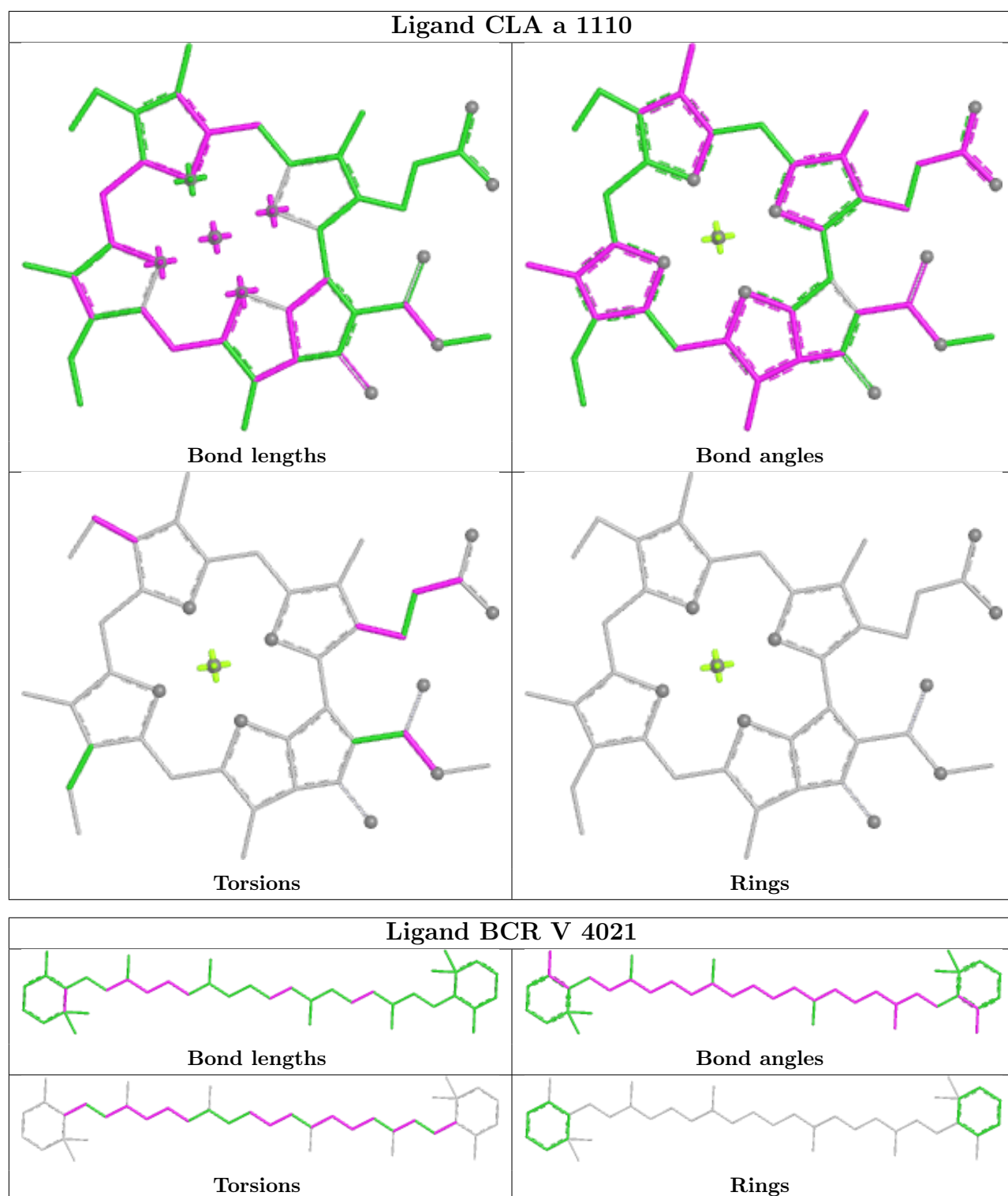


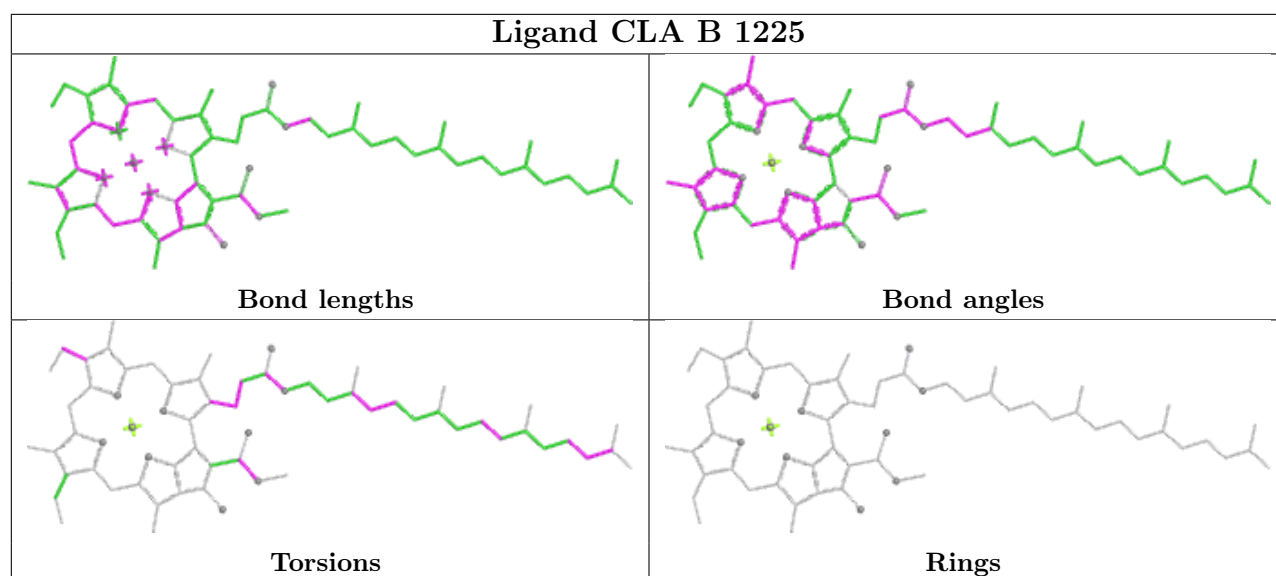
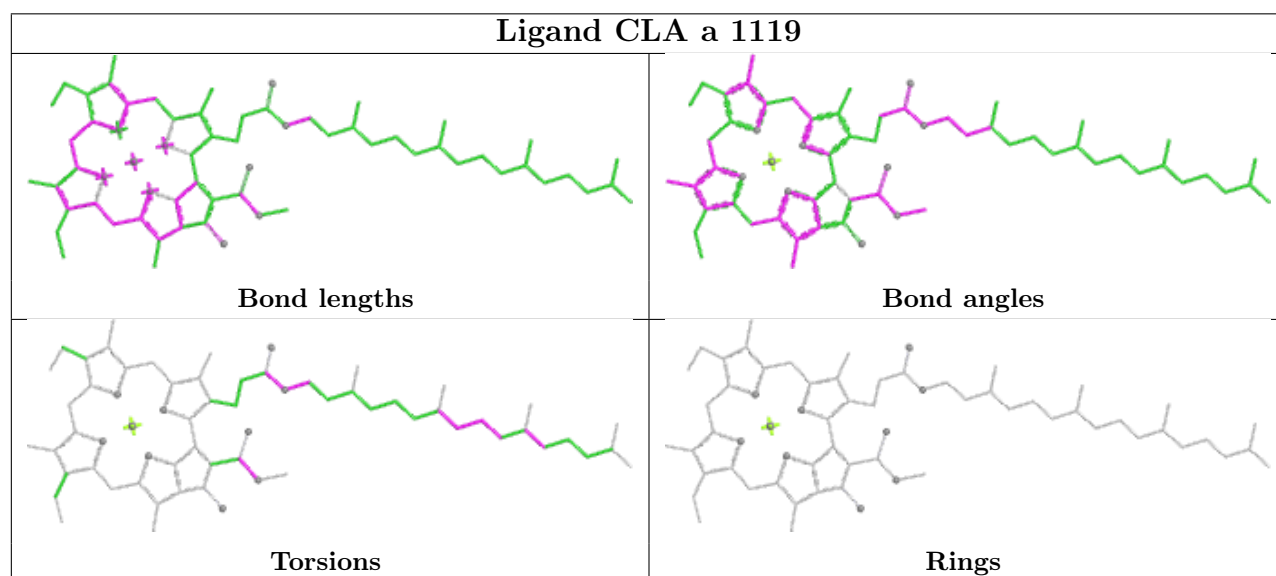
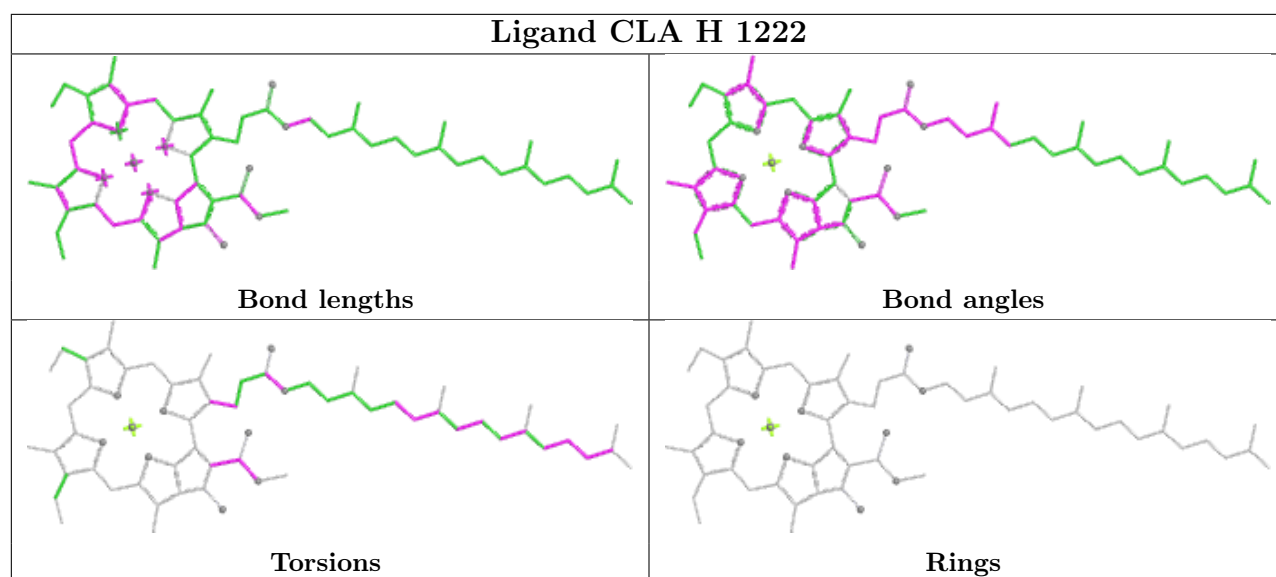




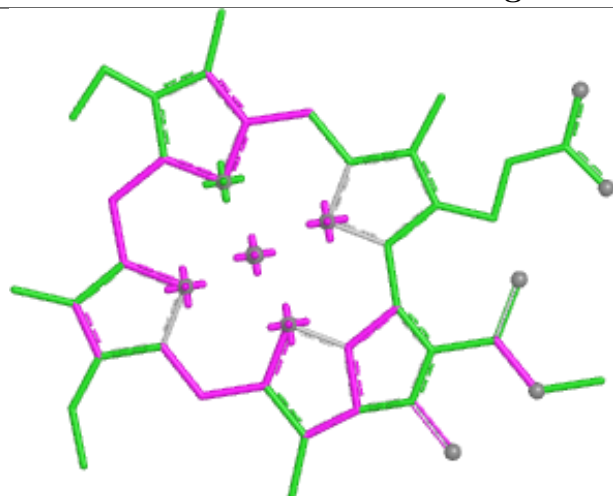




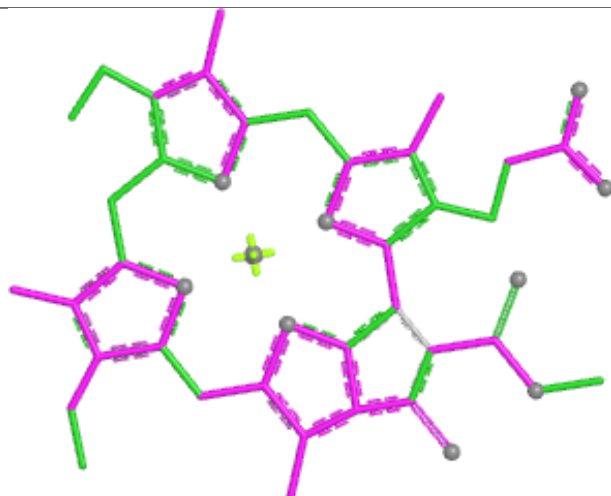




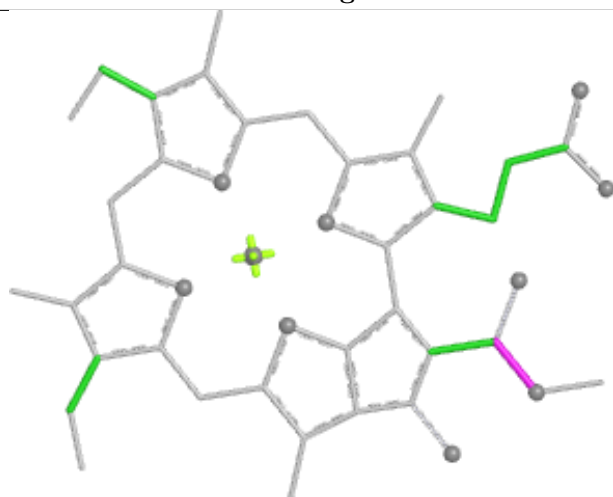
Ligand CLA H 1232



Bond lengths



Bond angles

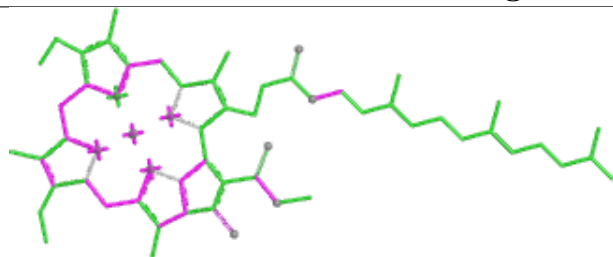


Torsions

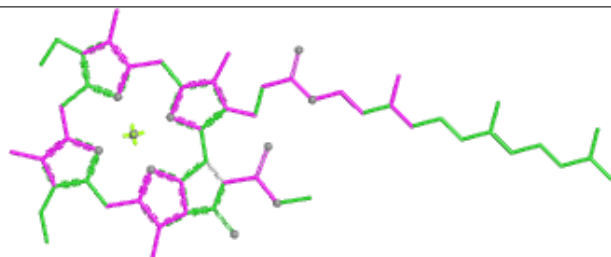


Rings

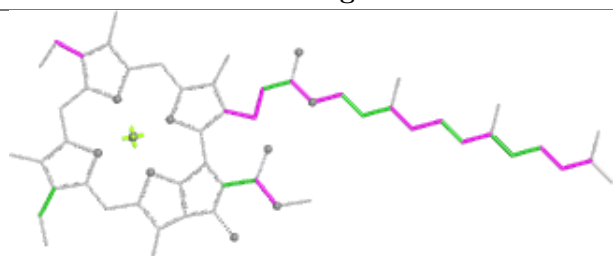
Ligand CLA H 1215



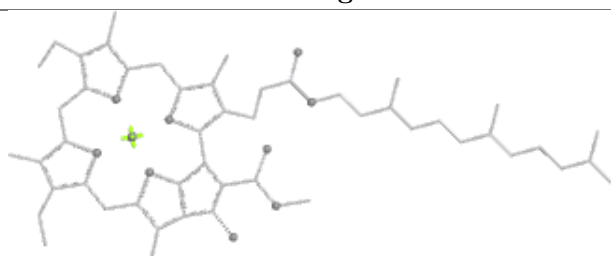
Bond lengths



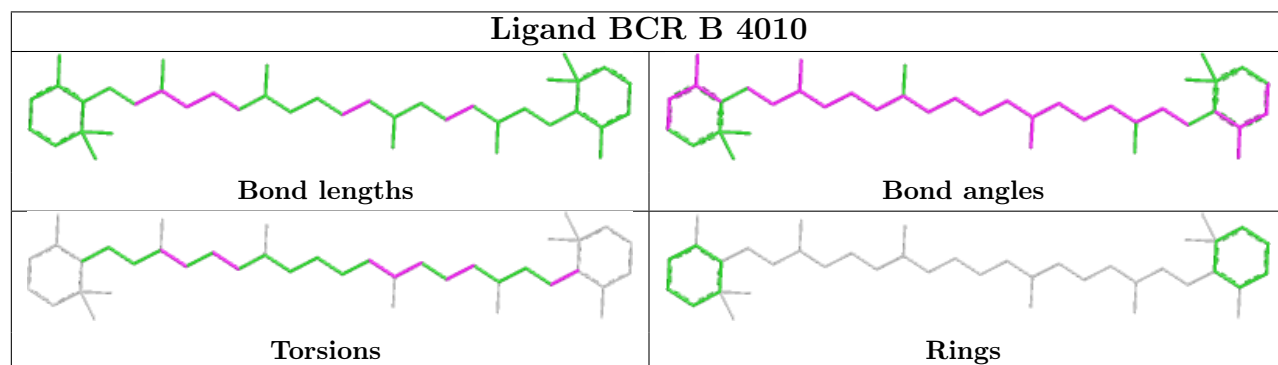
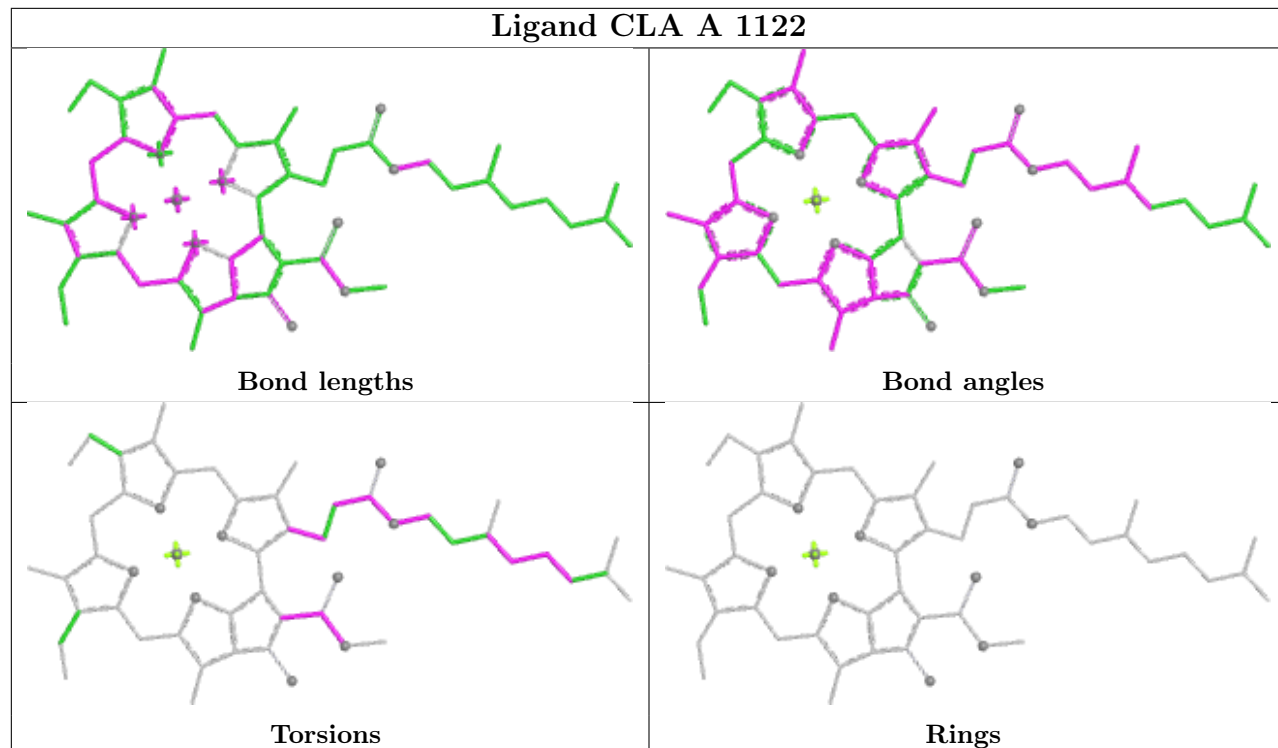
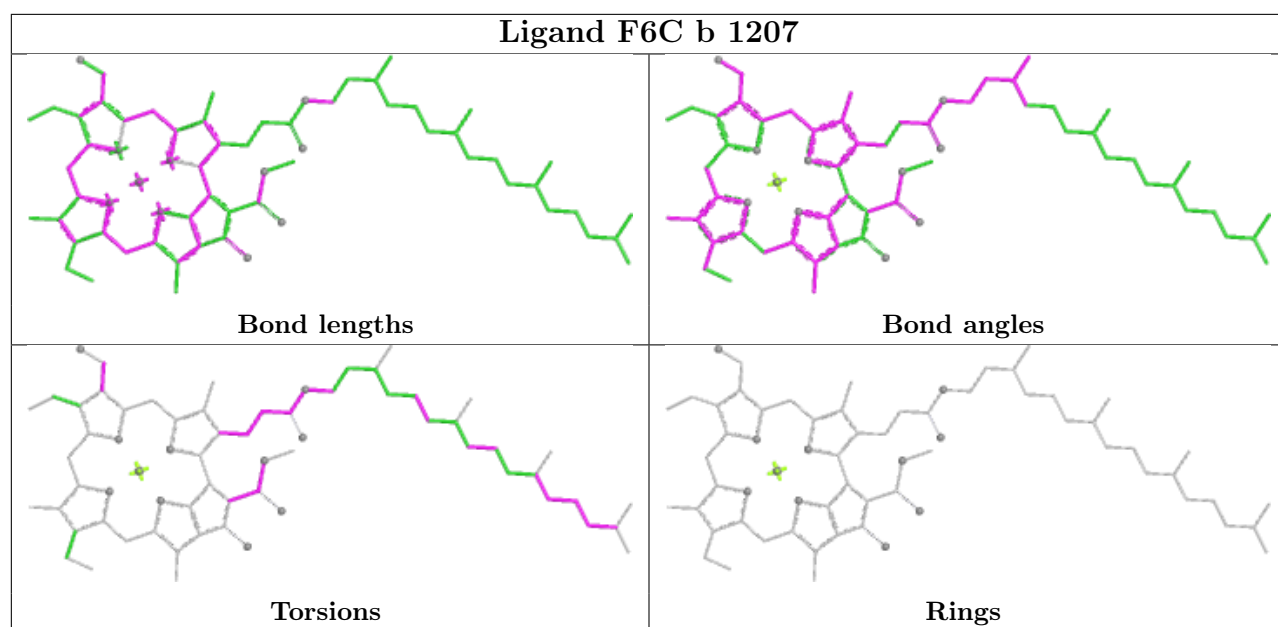
Bond angles

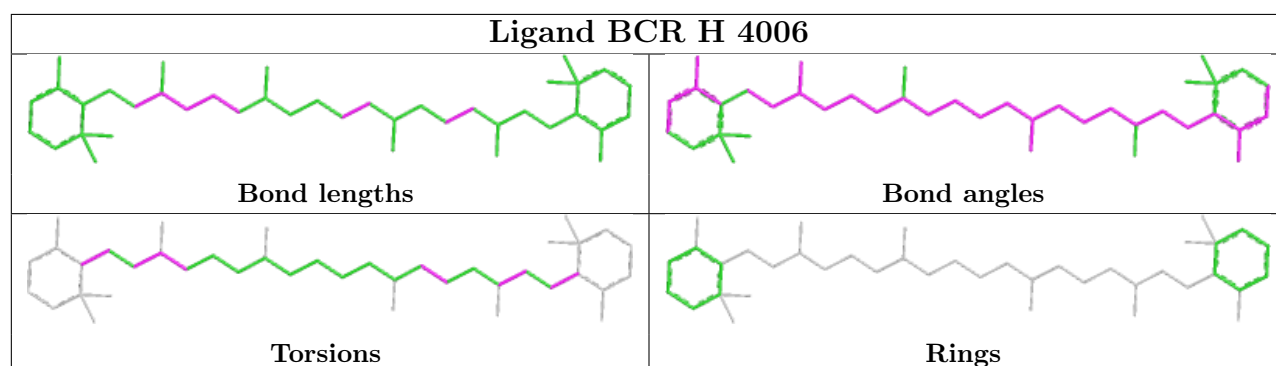
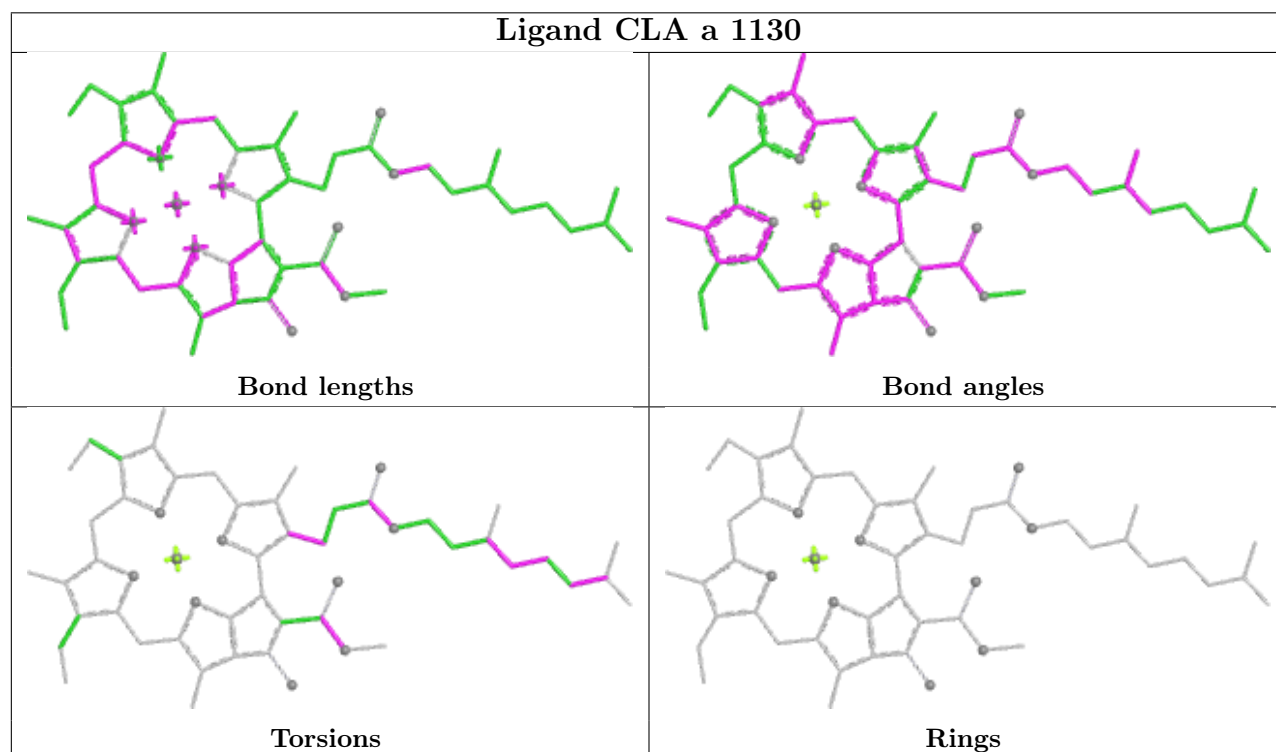
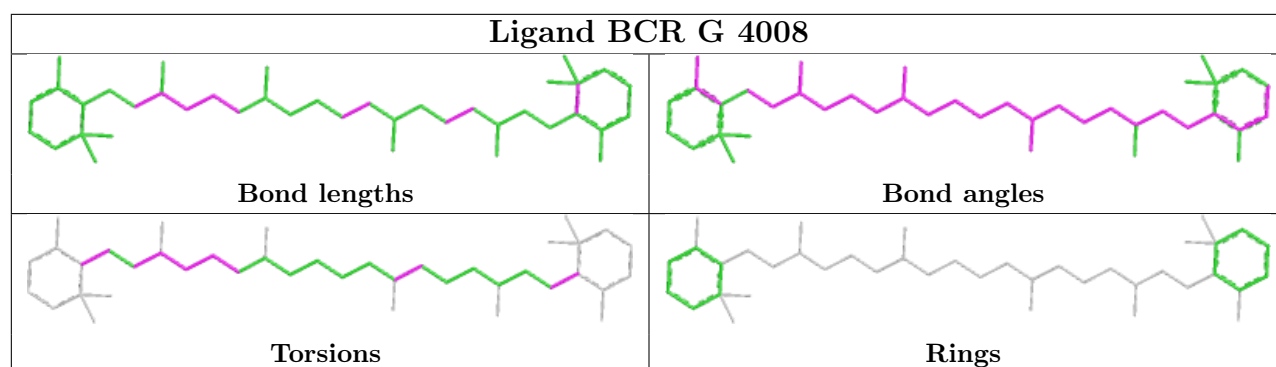


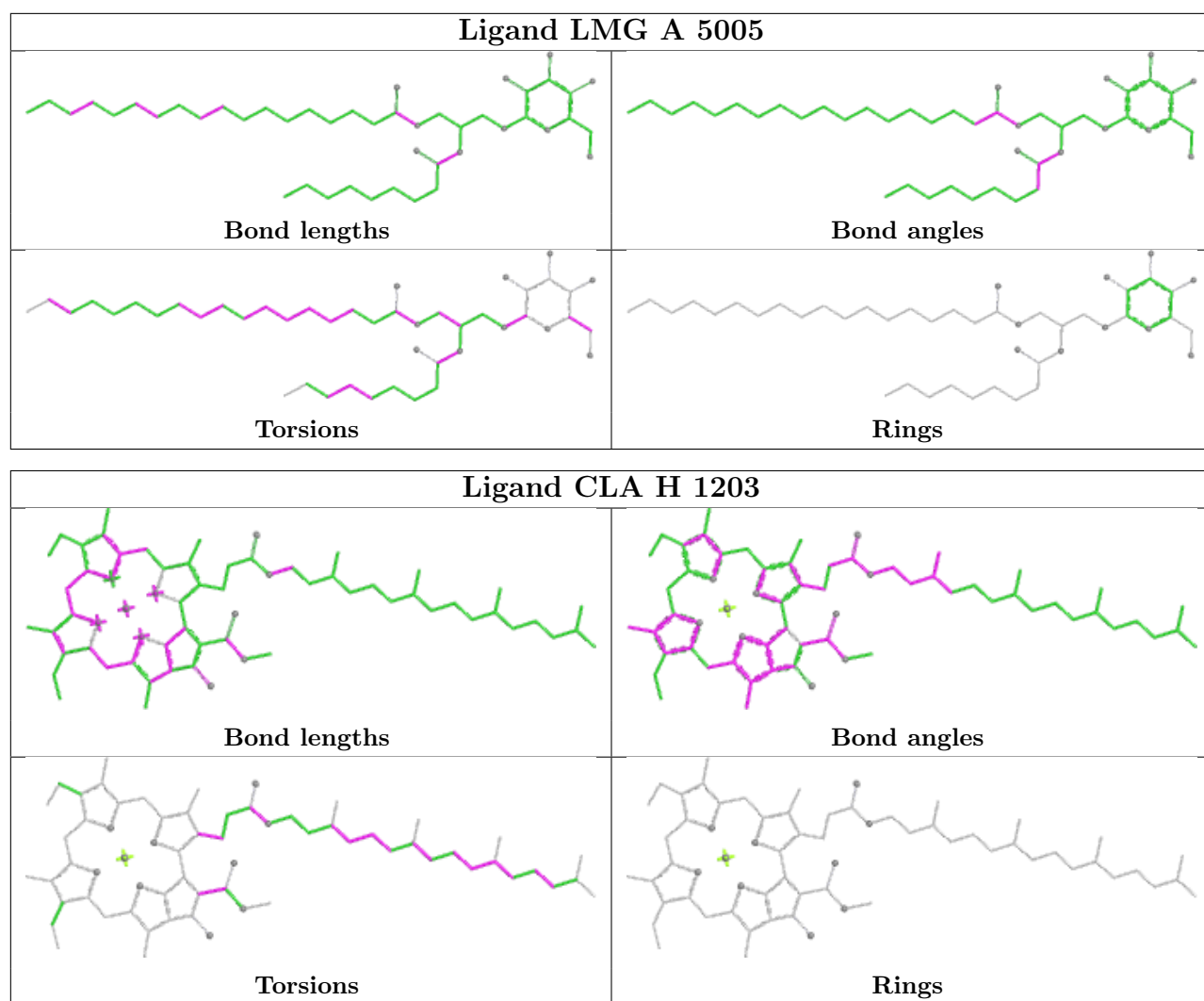
Torsions

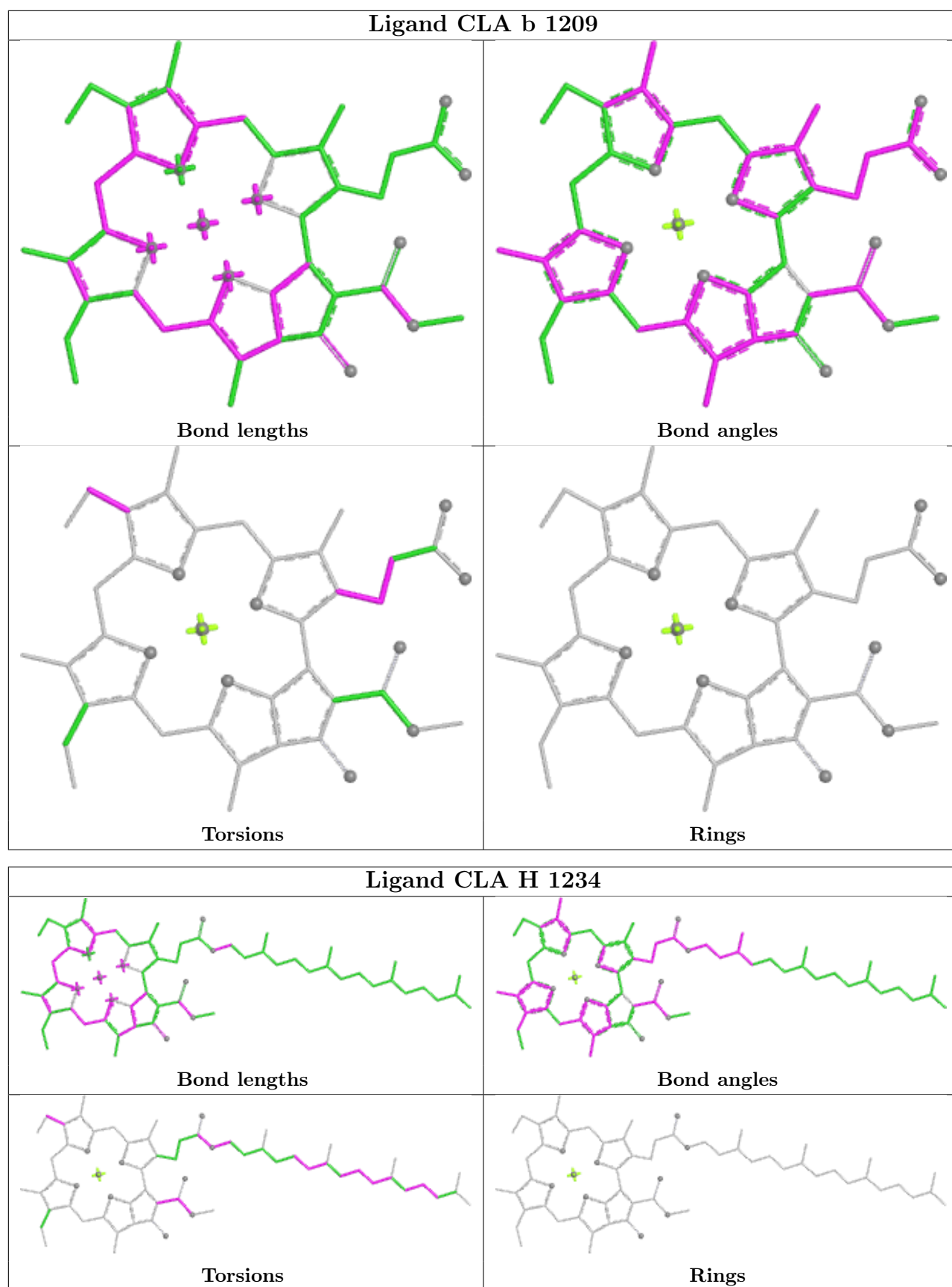


Rings

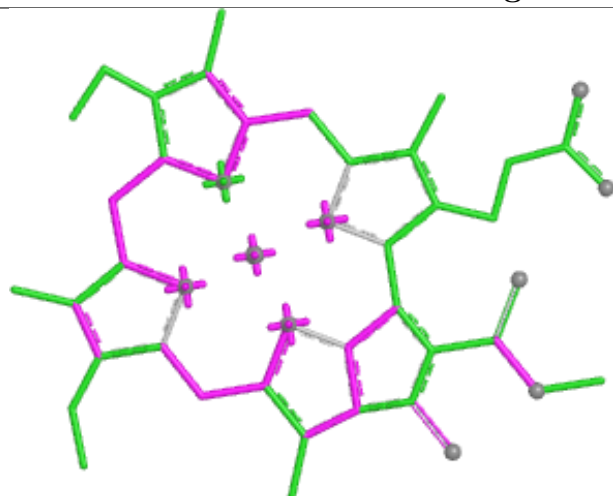




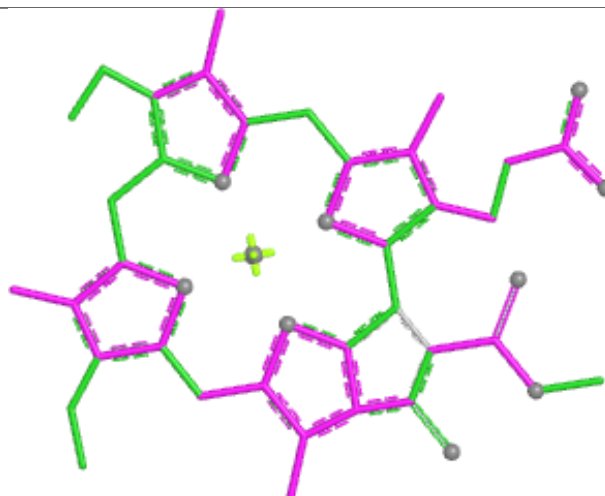




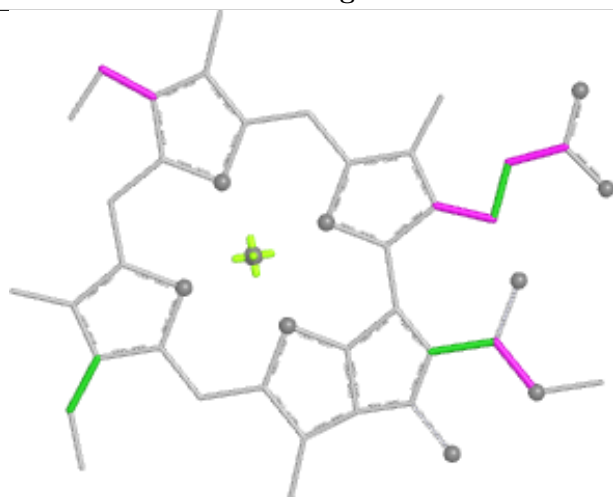
Ligand CLA G 1110



Bond lengths



Bond angles

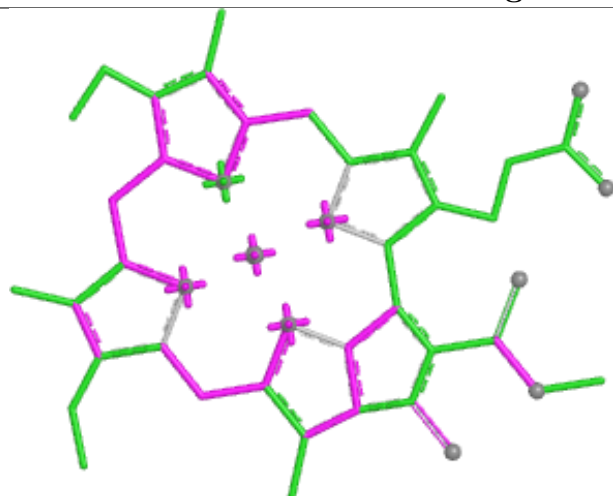


Torsions

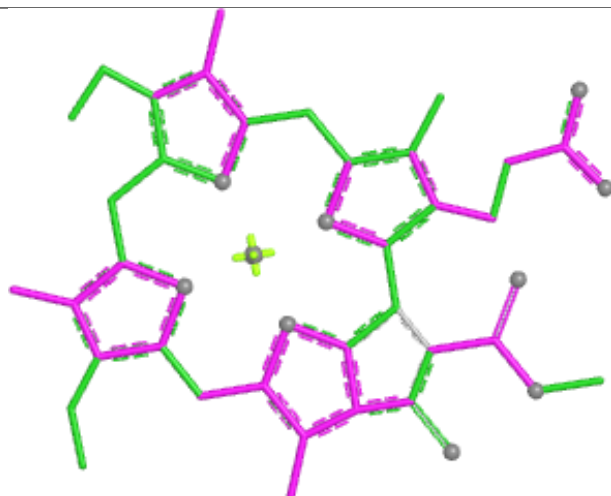


Rings

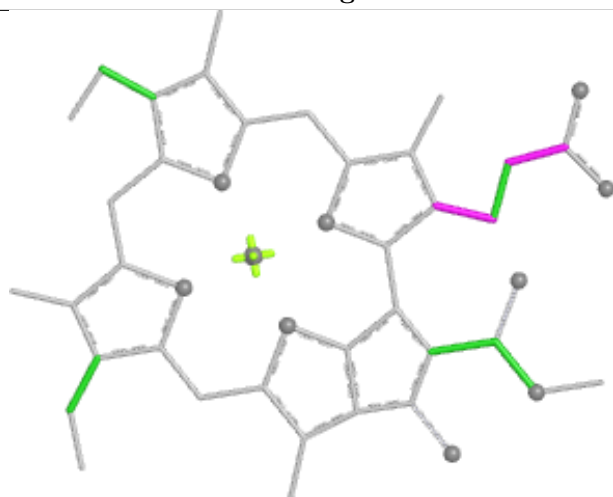
Ligand CLA B 1236



Bond lengths



Bond angles

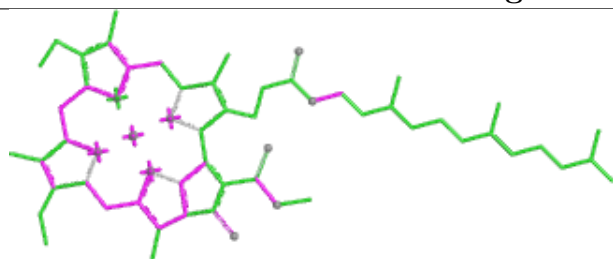


Torsions

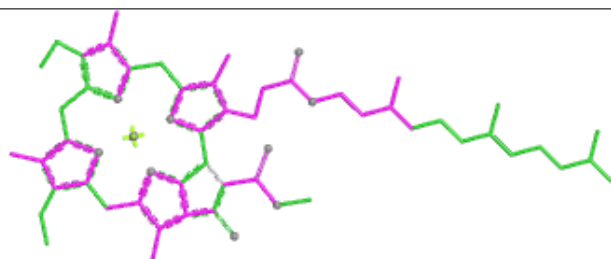


Rings

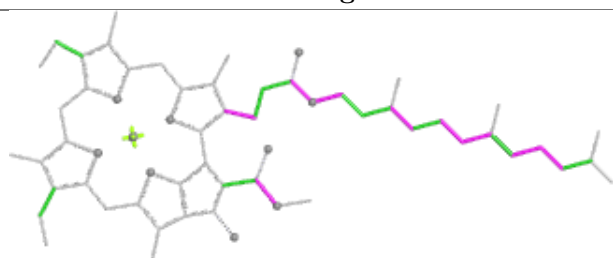
Ligand CLA B 1229



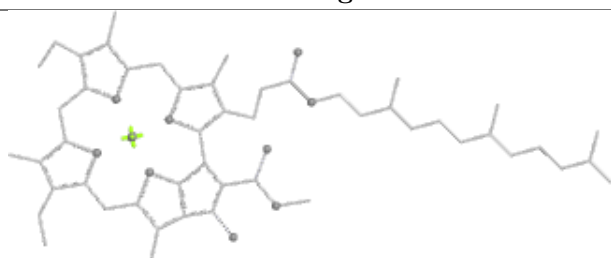
Bond lengths



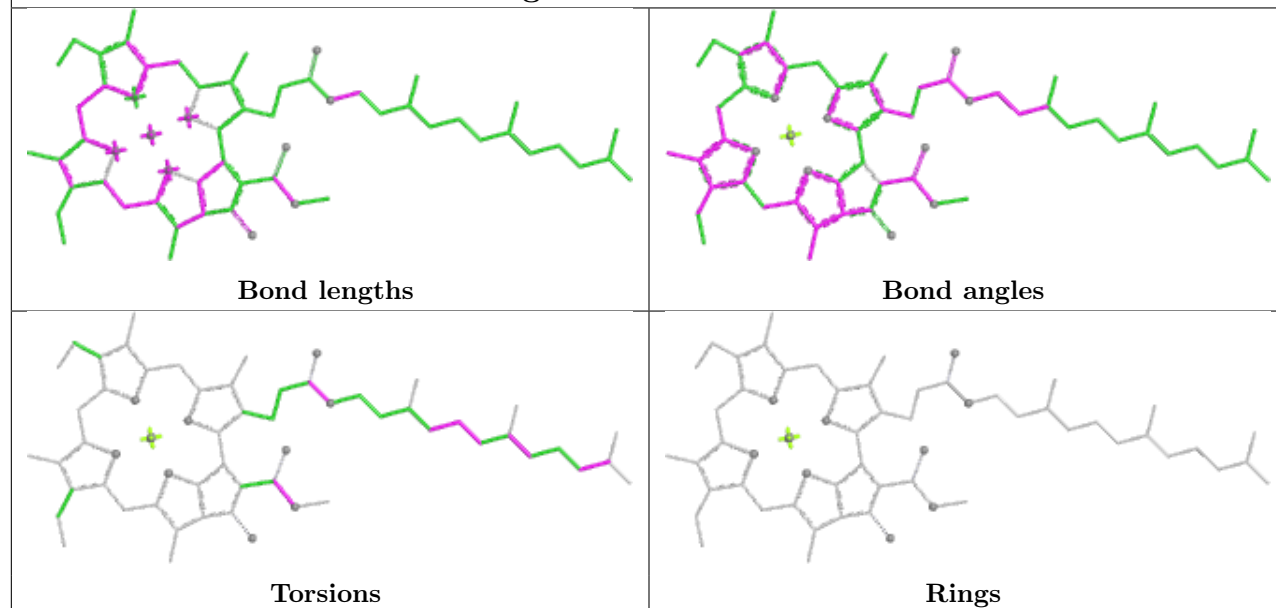
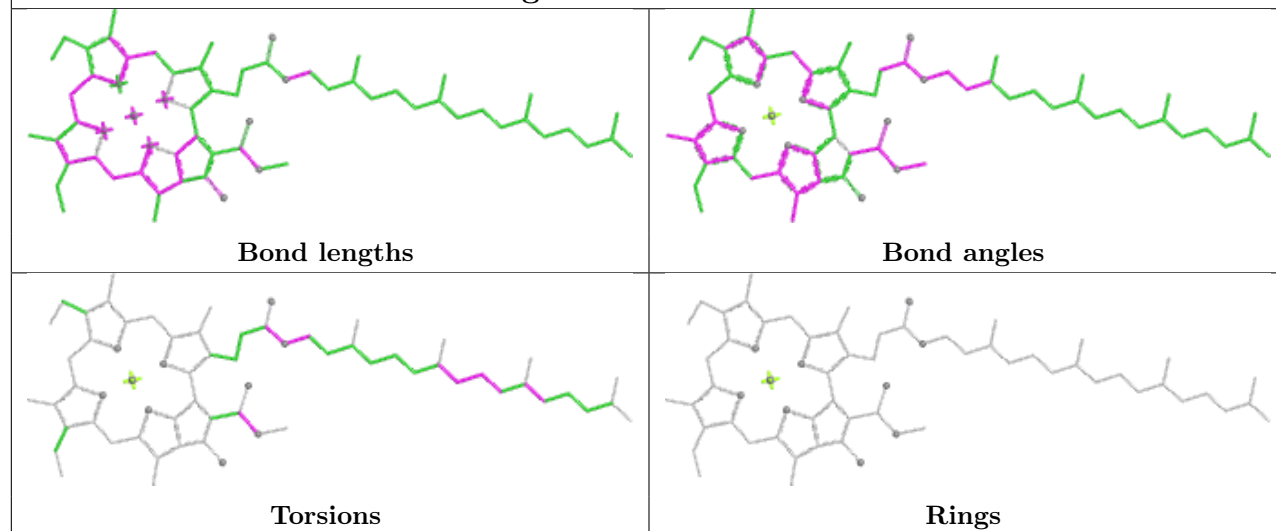
Bond angles



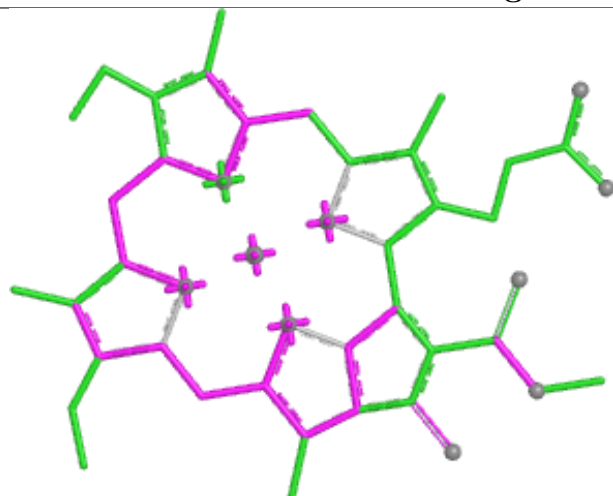
Torsions



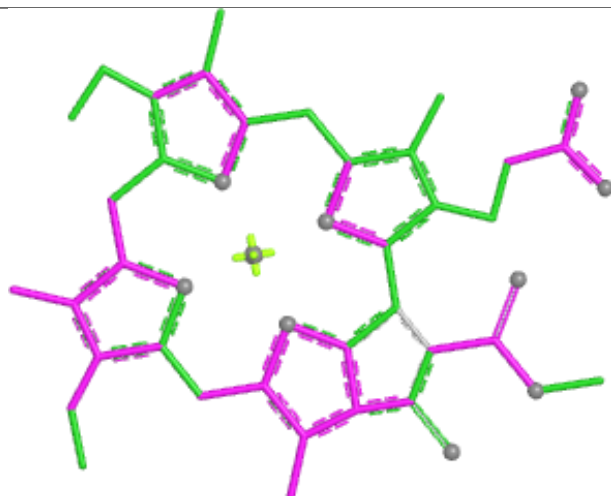
Rings

Ligand CLA A 1133**Ligand CLA G 1119**

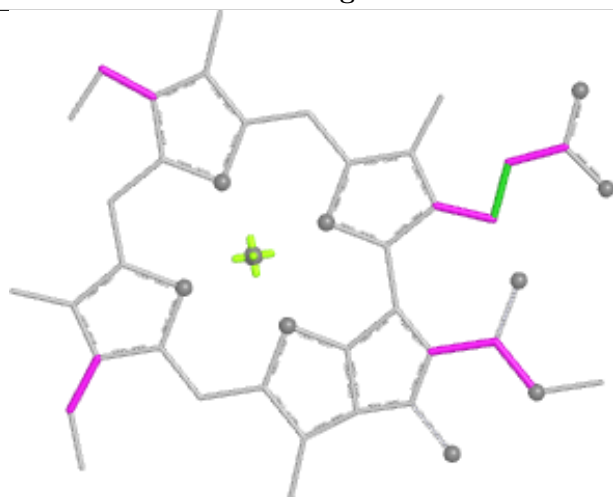
Ligand CLA A 1114



Bond lengths



Bond angles

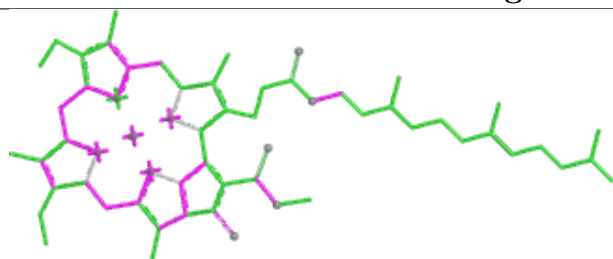


Torsions

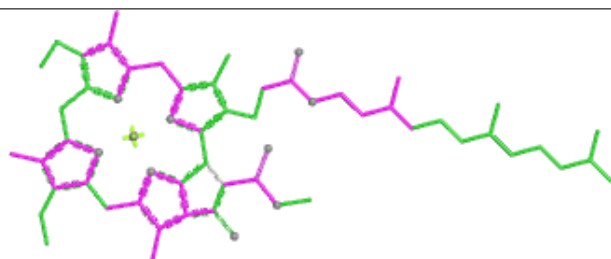


Rings

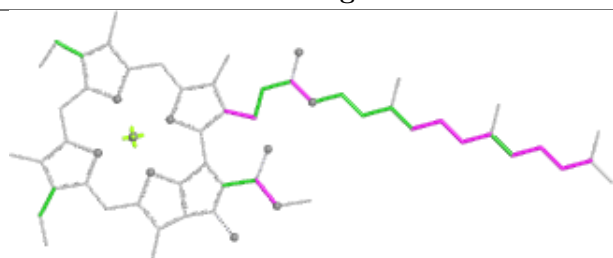
Ligand CLA A 1102



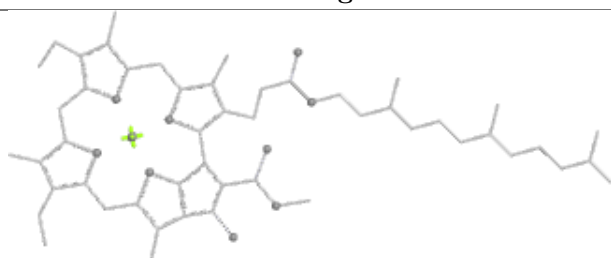
Bond lengths



Bond angles

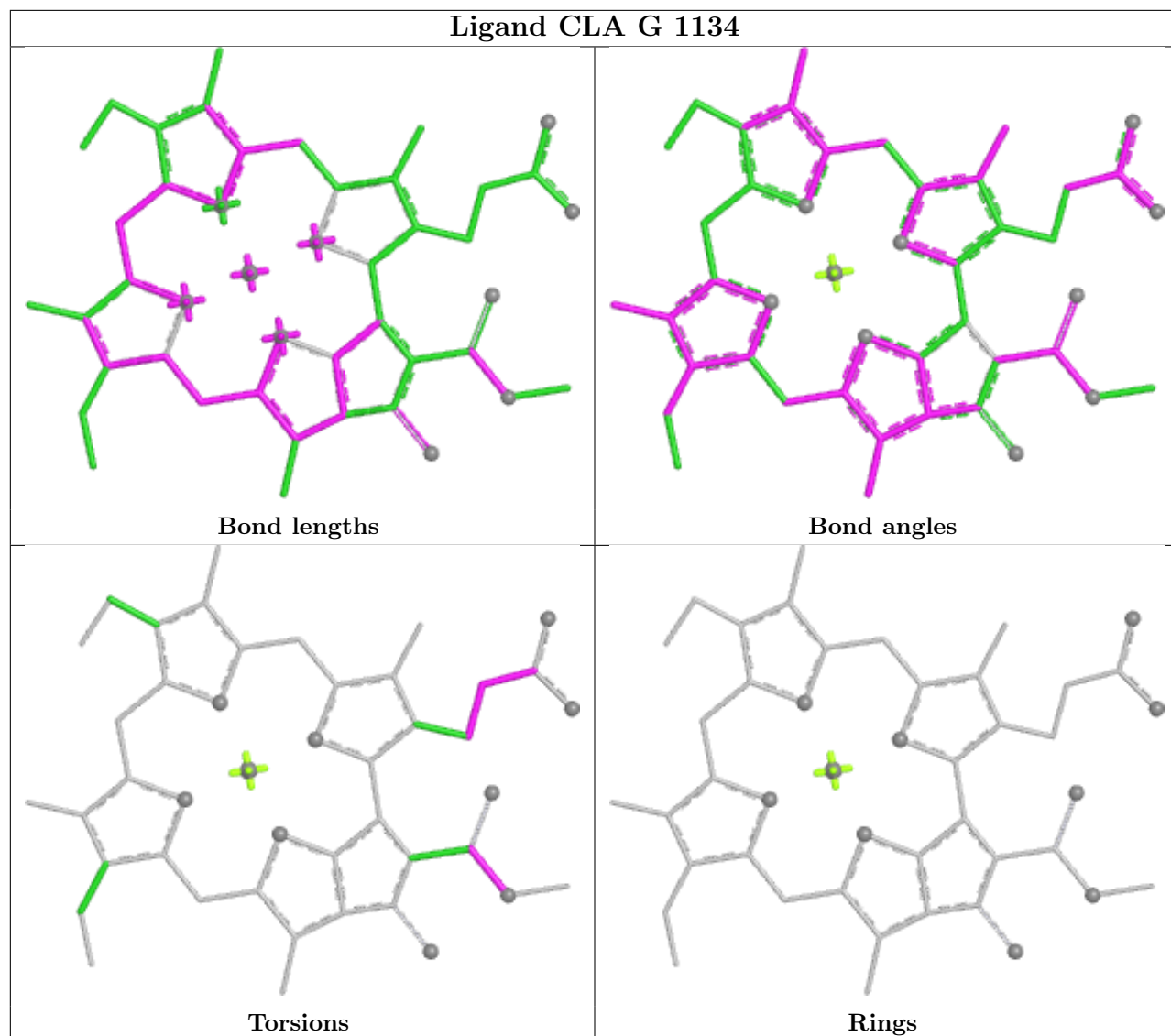


Torsions

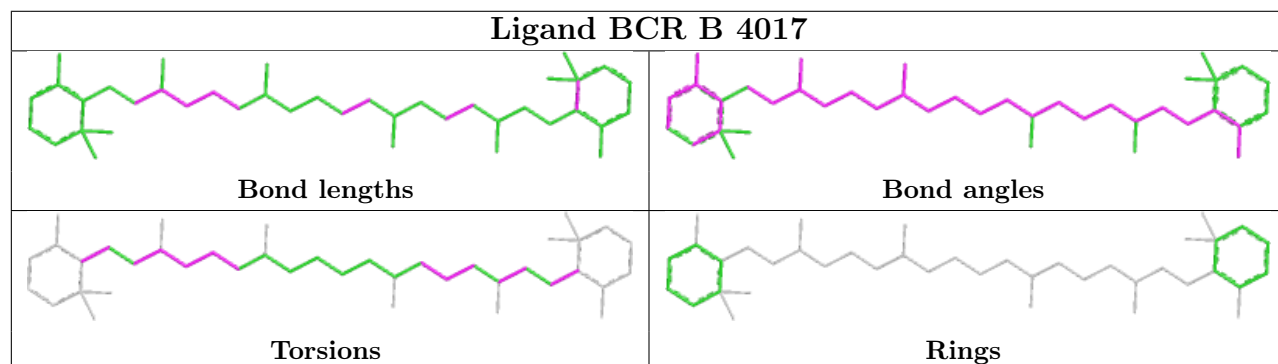


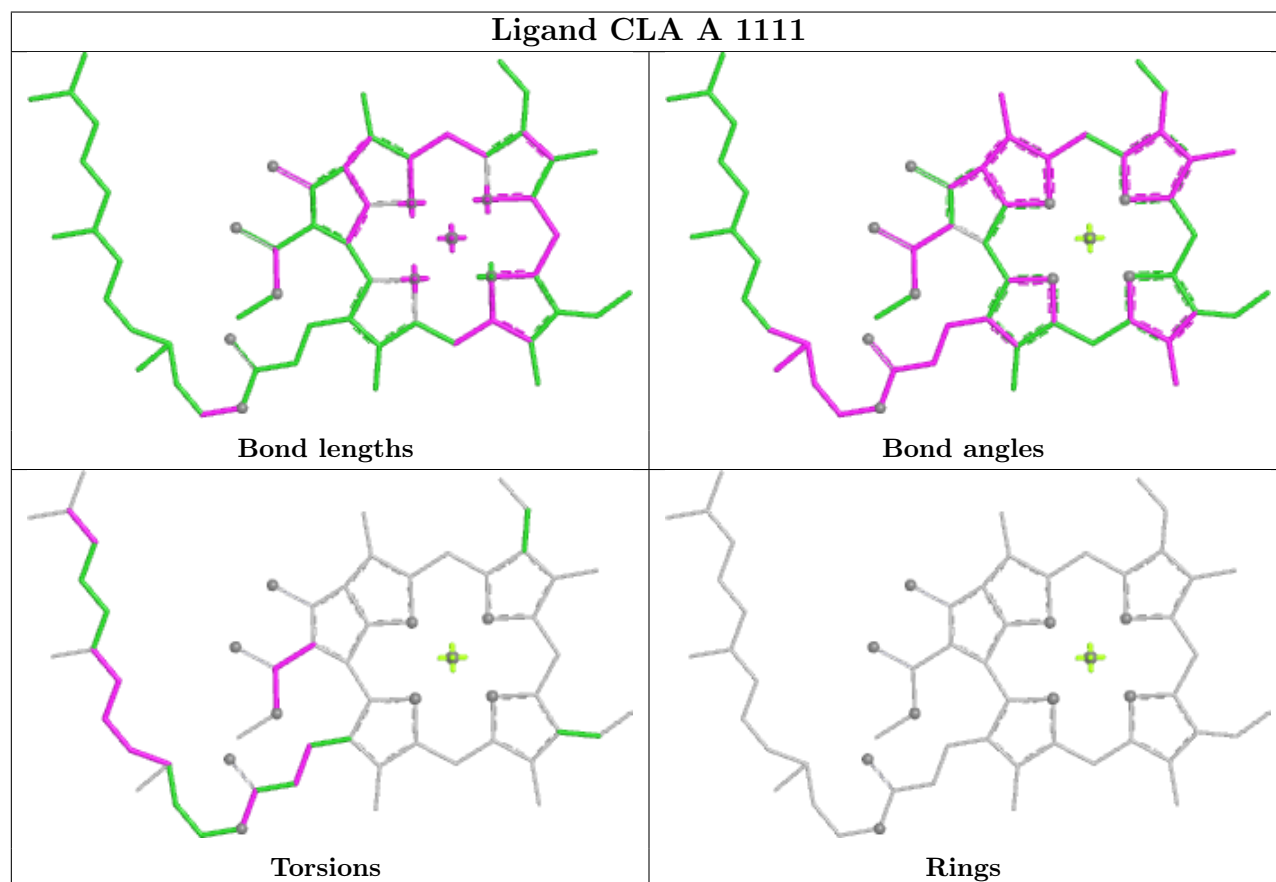
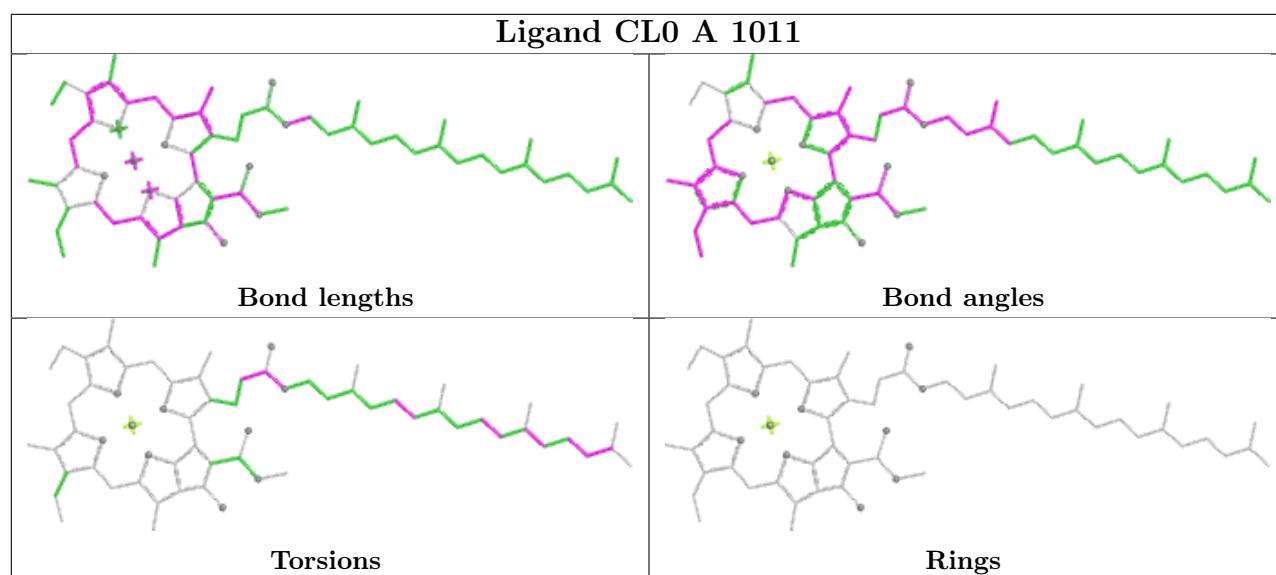
Rings

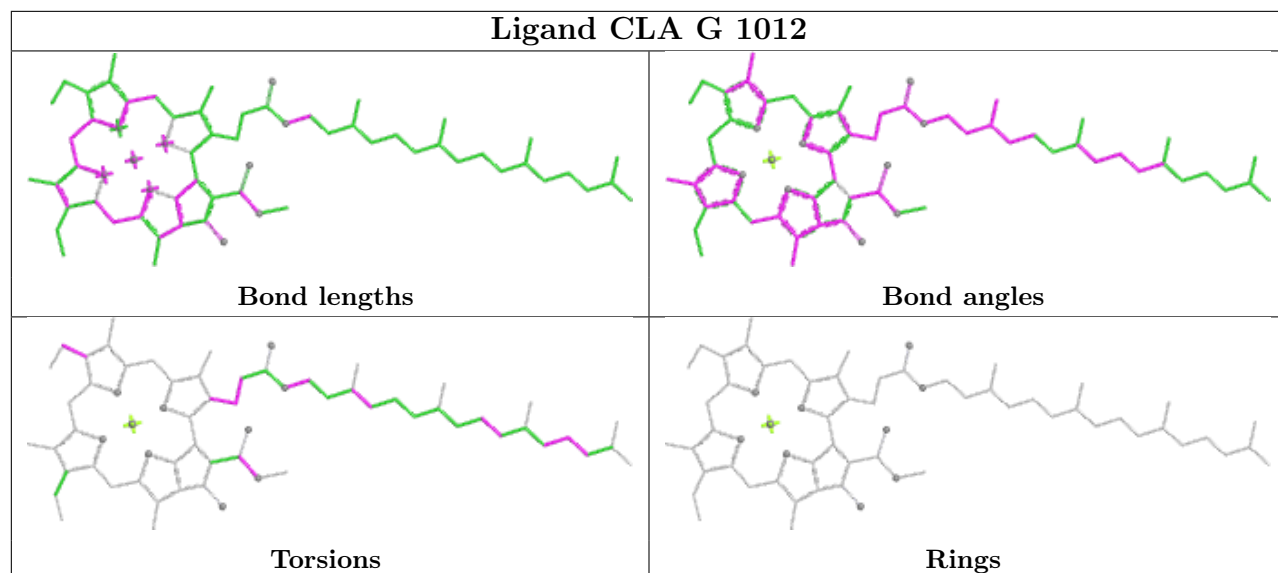
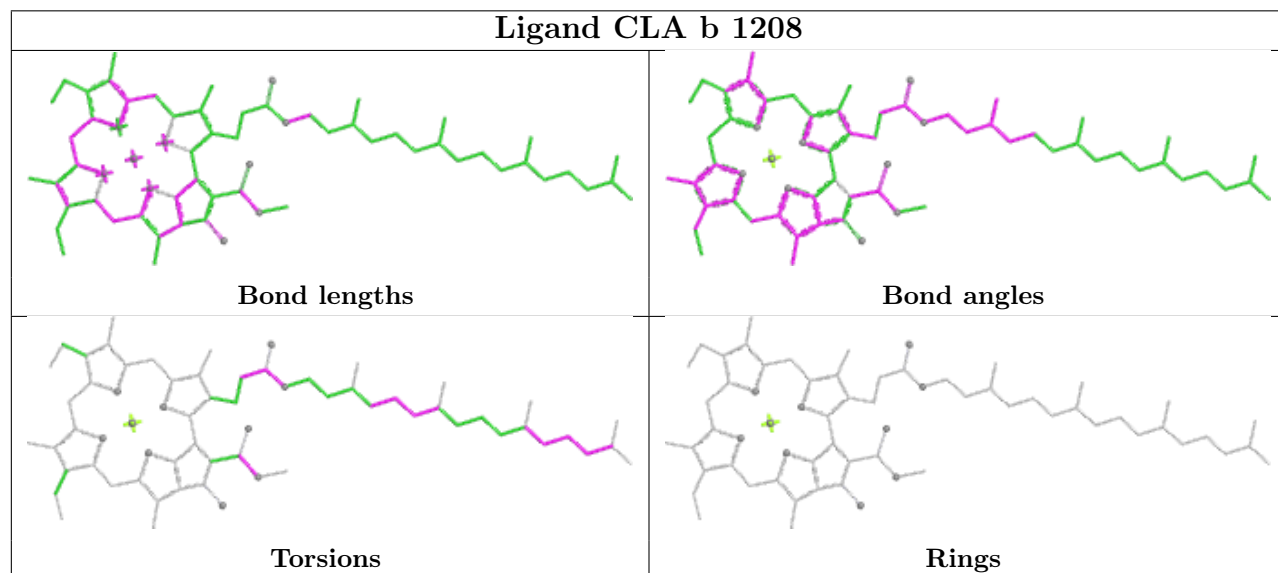
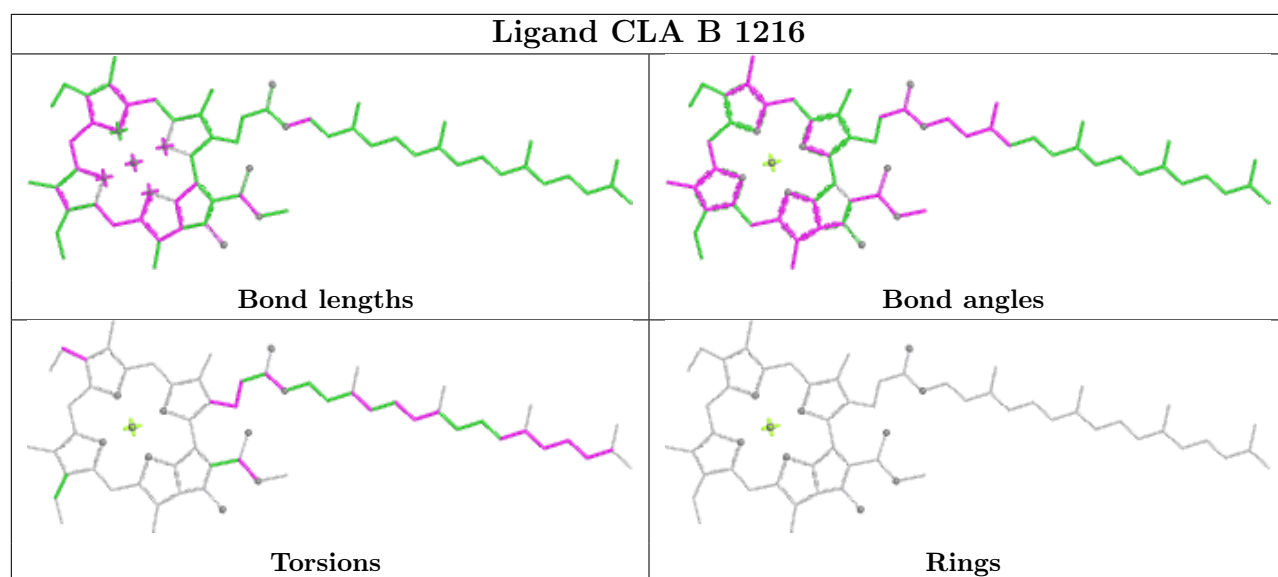
Ligand CLA G 1134

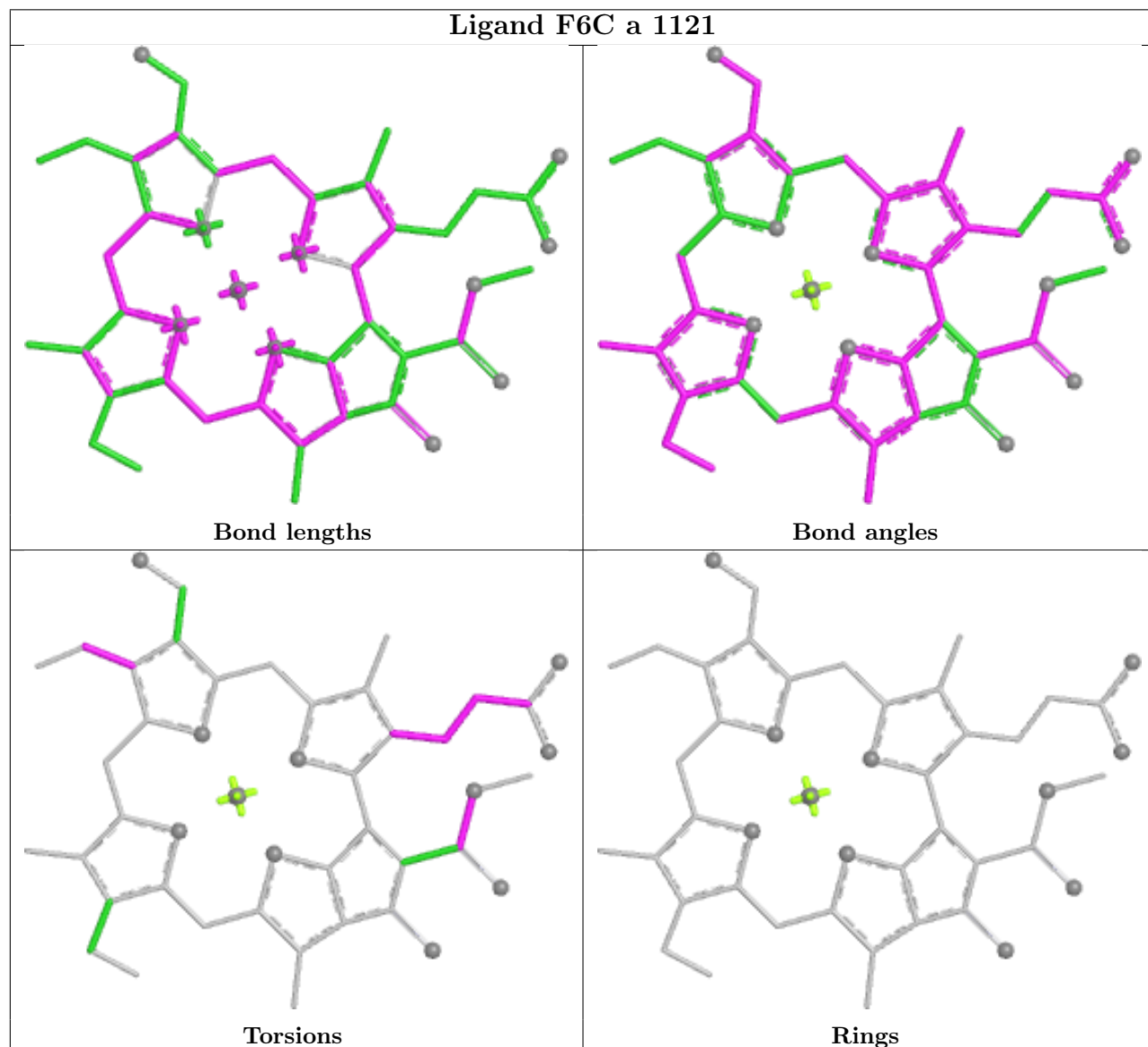
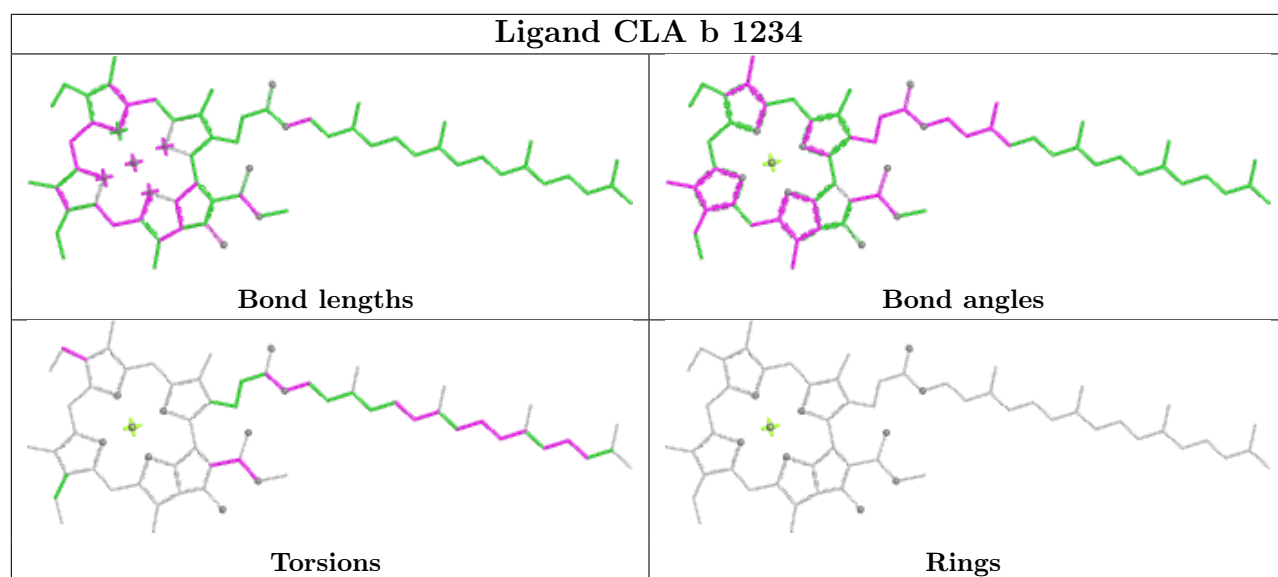


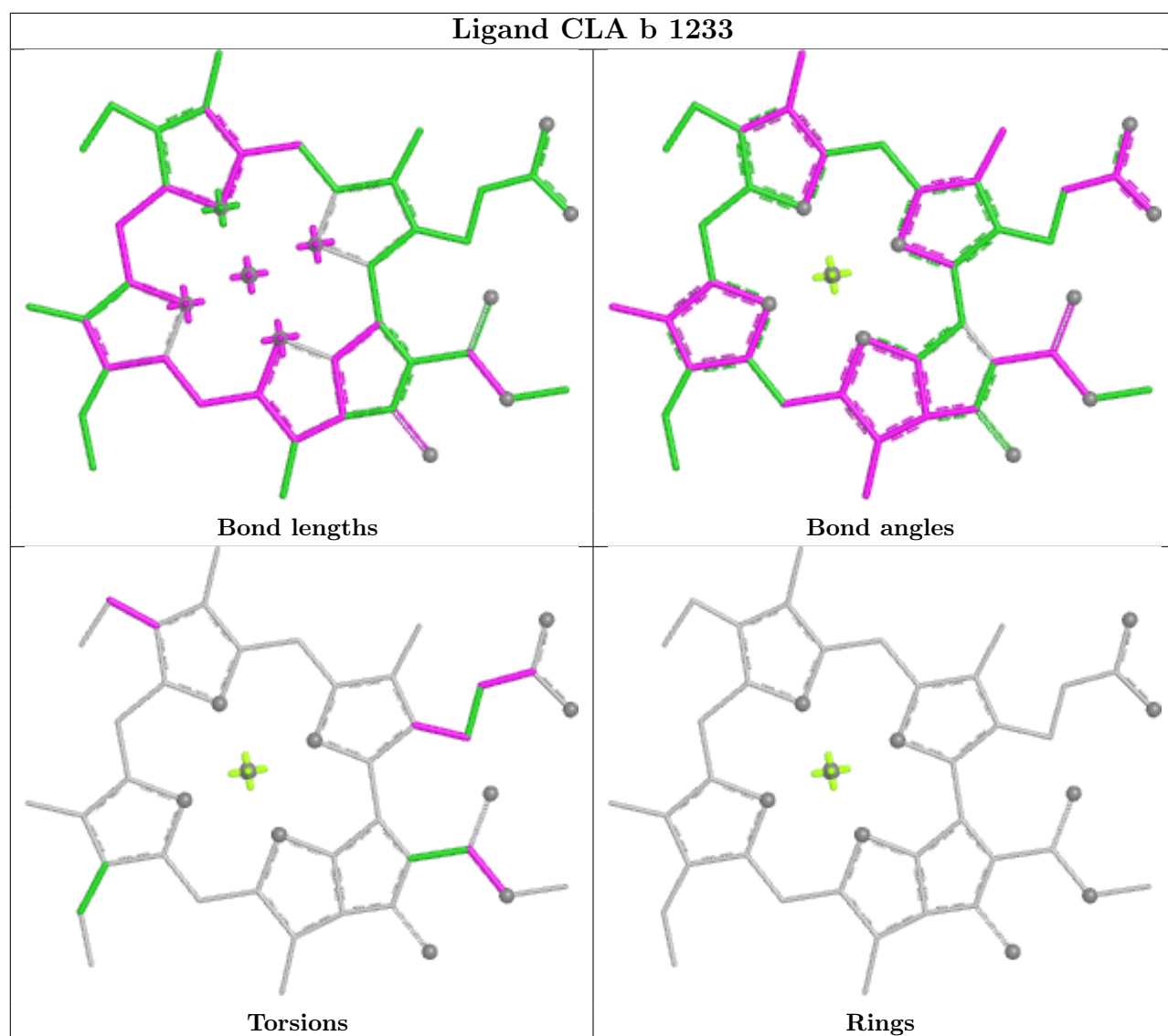
Ligand BCR B 4017



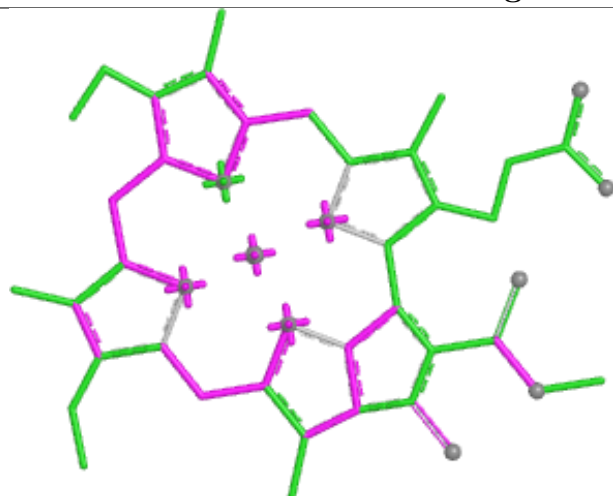




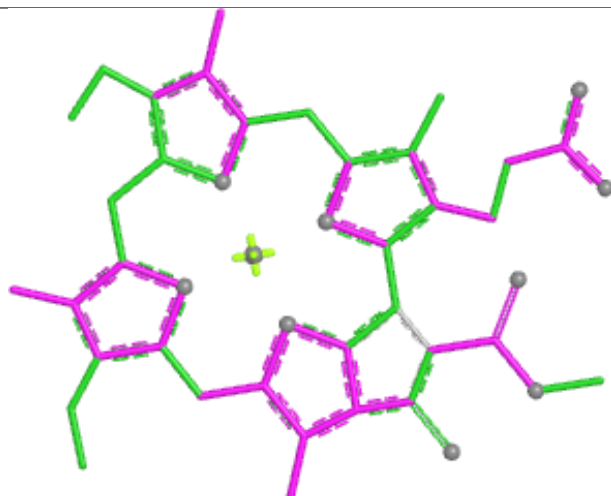




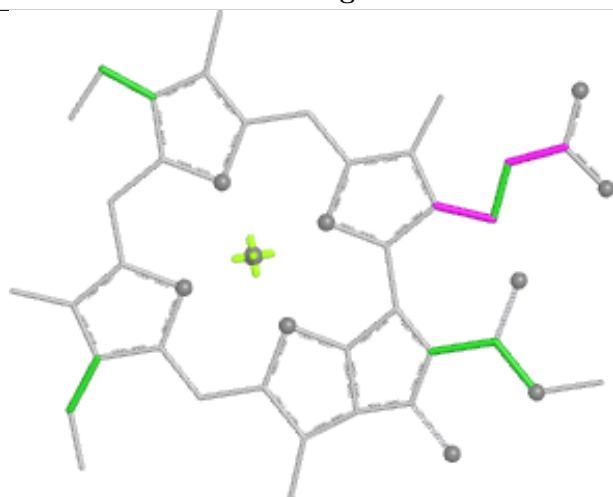
Ligand CLA H 1236



Bond lengths



Bond angles

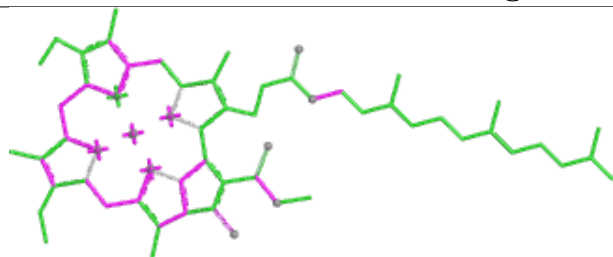


Torsions

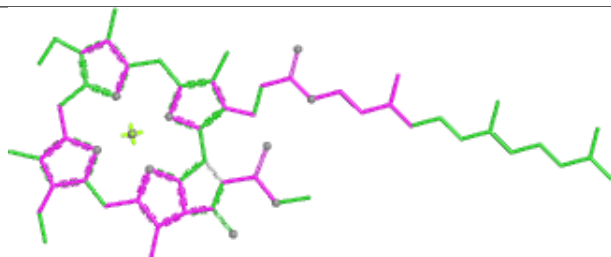


Rings

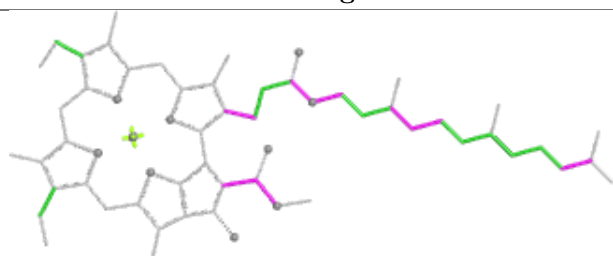
Ligand CLA G 1103



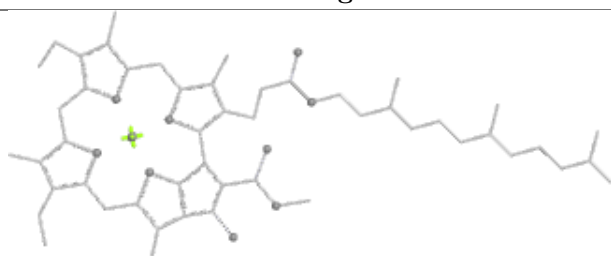
Bond lengths



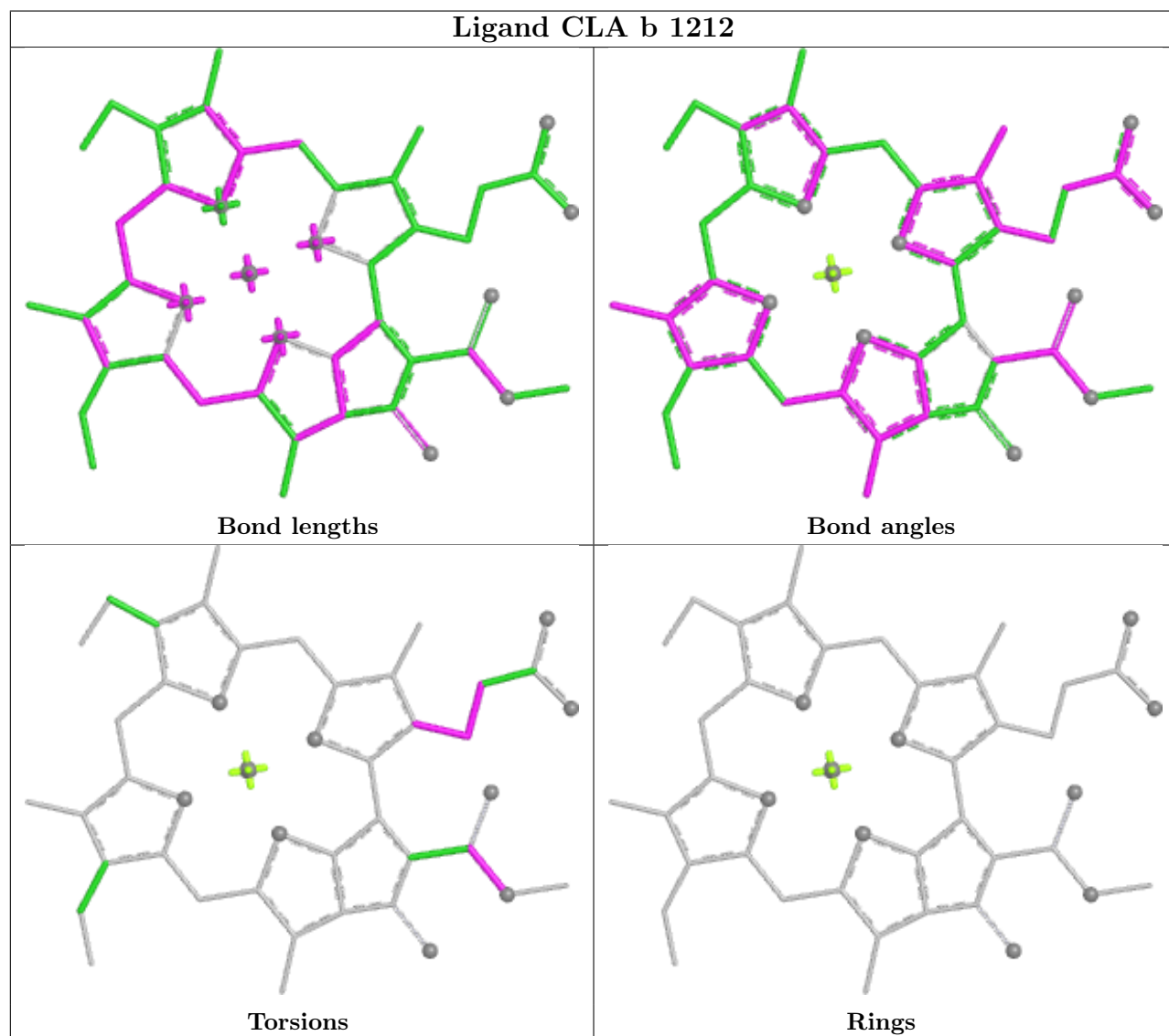
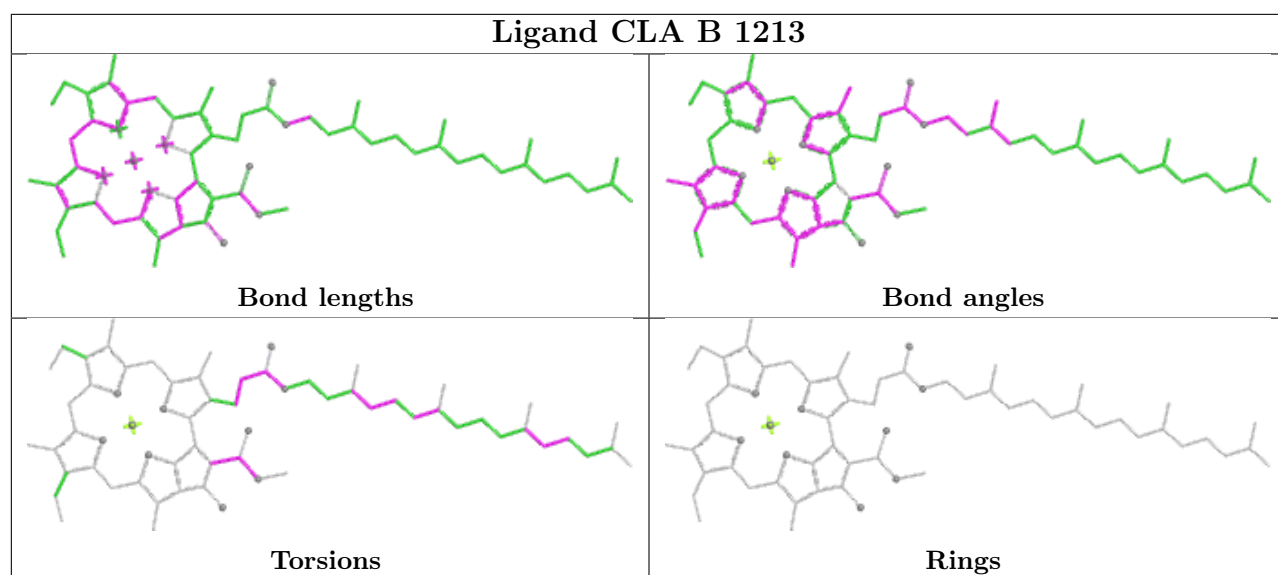
Bond angles



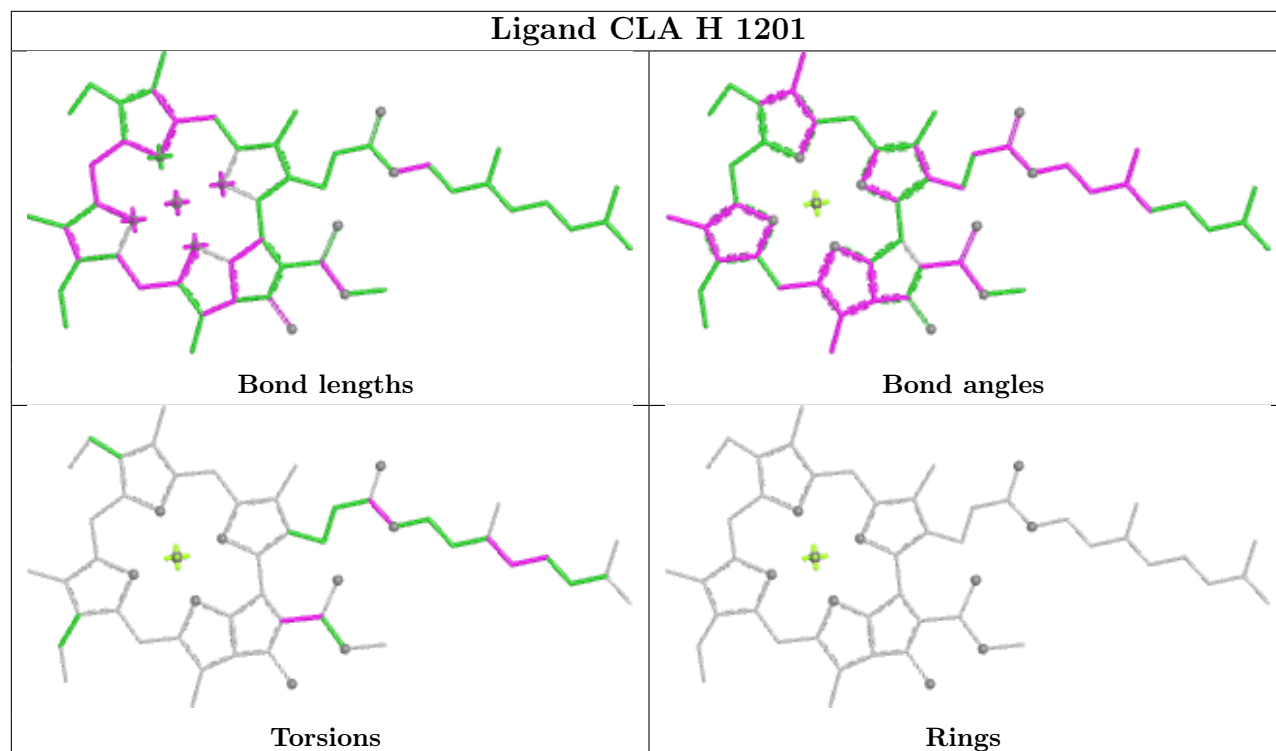
Torsions



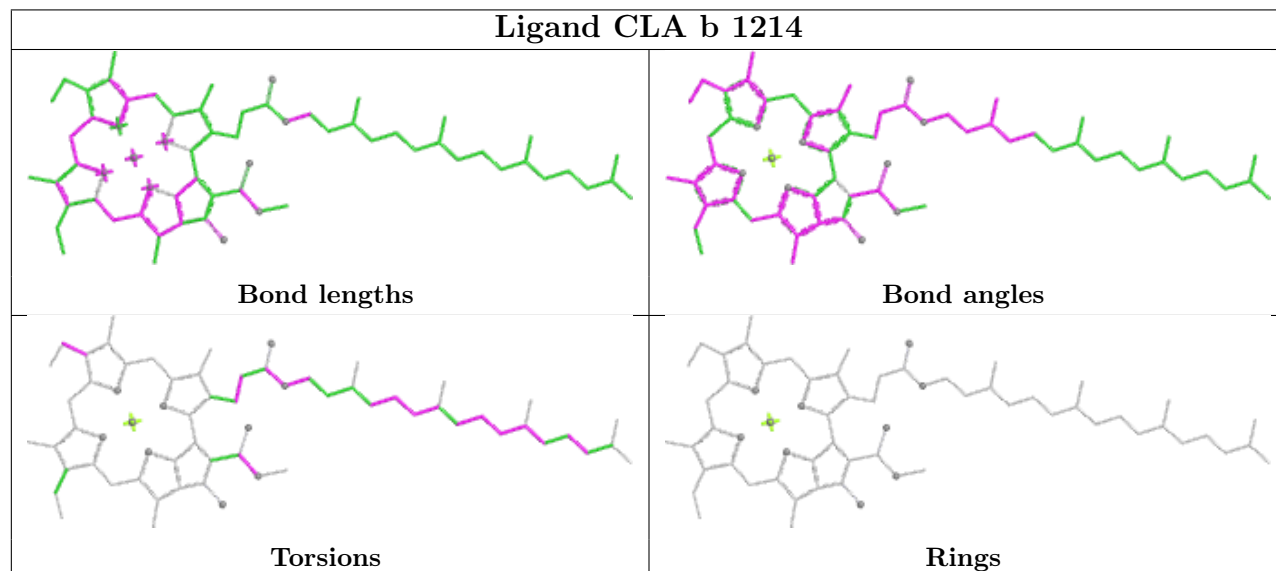
Rings



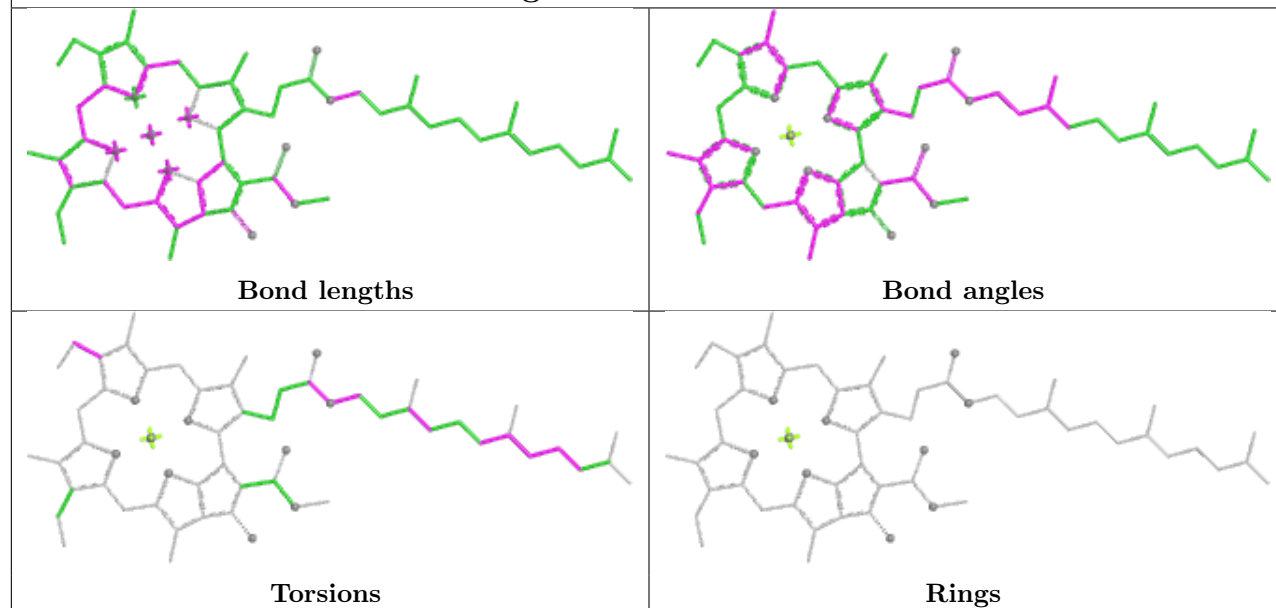
Ligand CLA H 1201



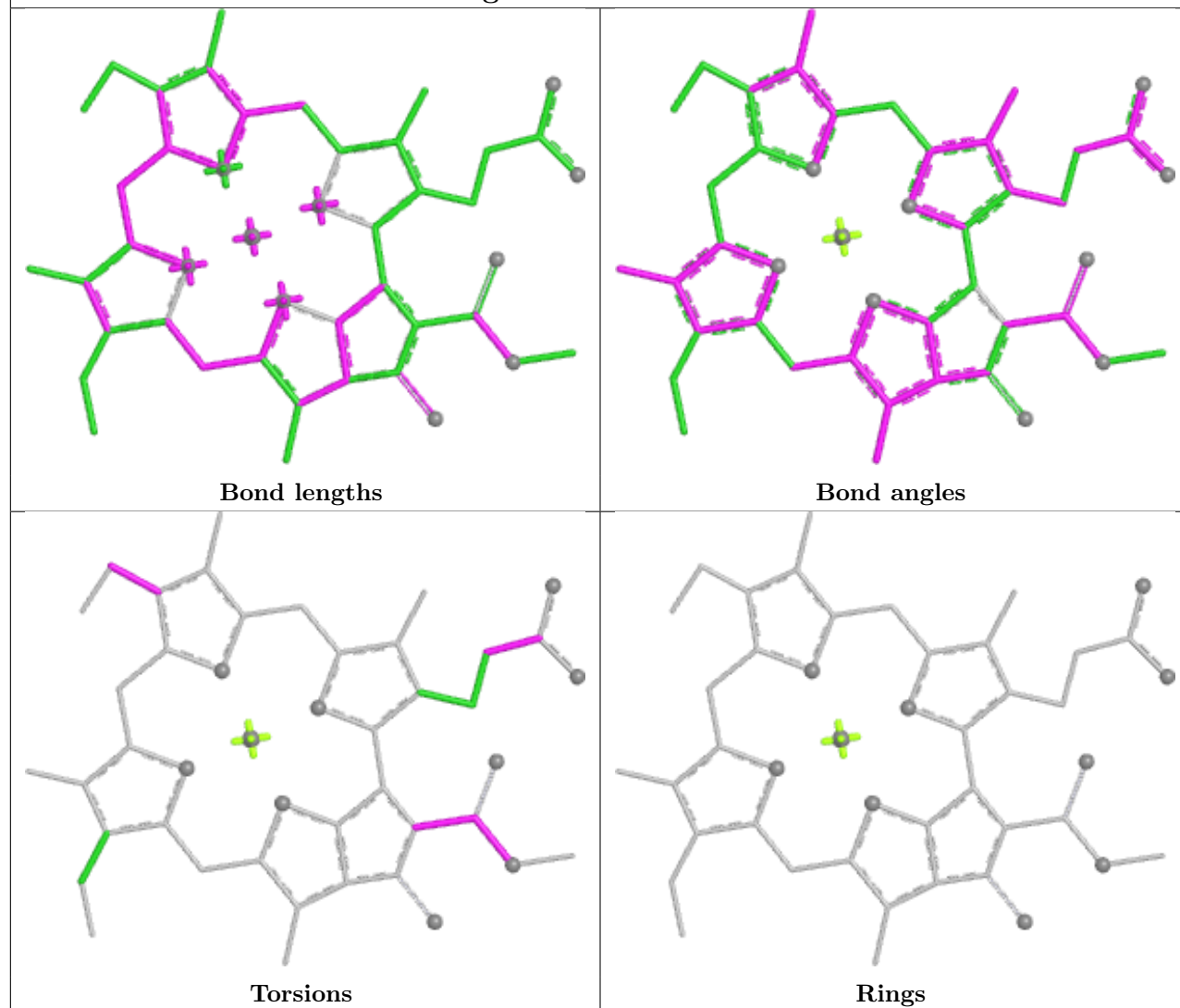
Ligand CLA b 1214

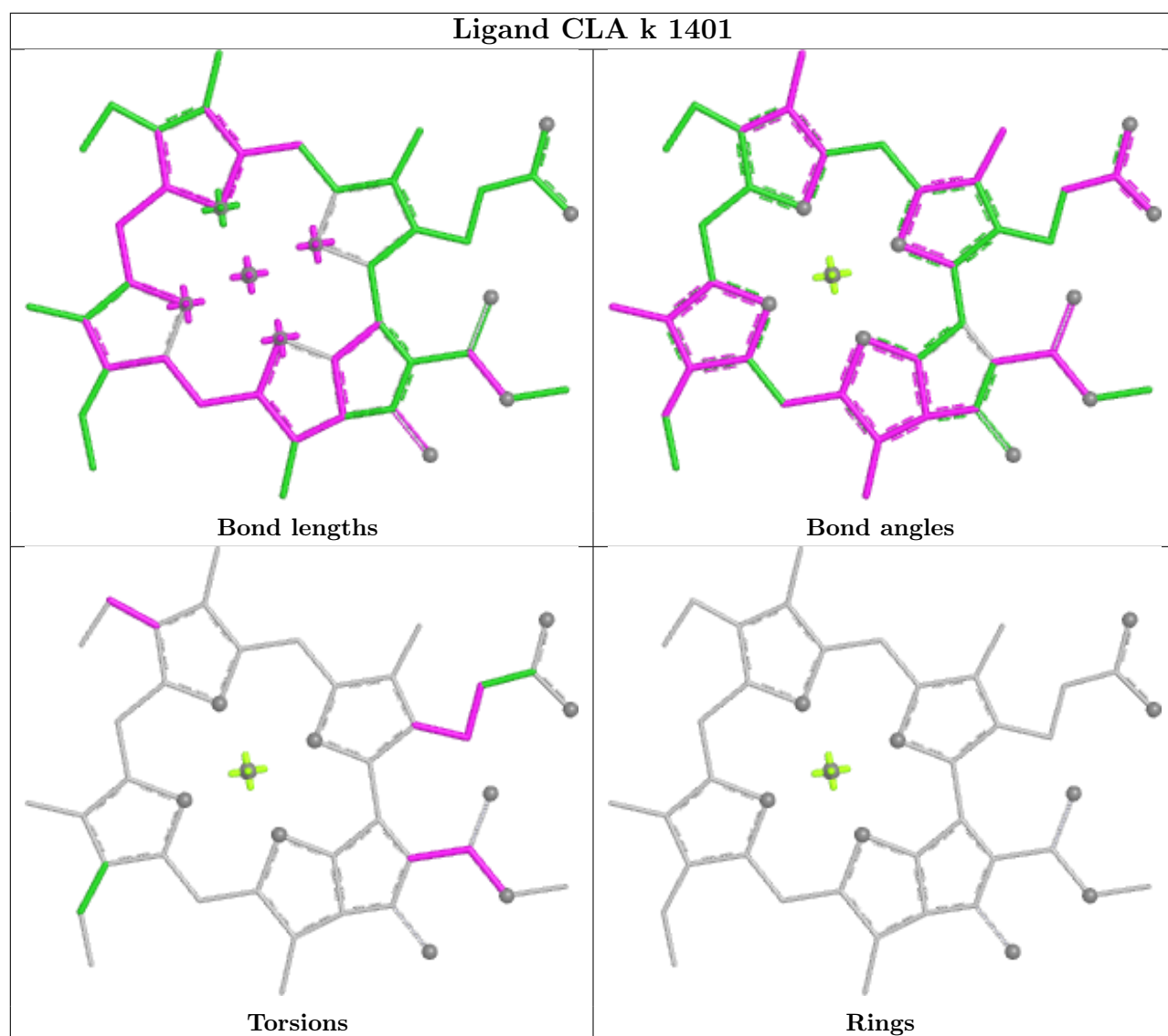


Ligand CLA U 1502

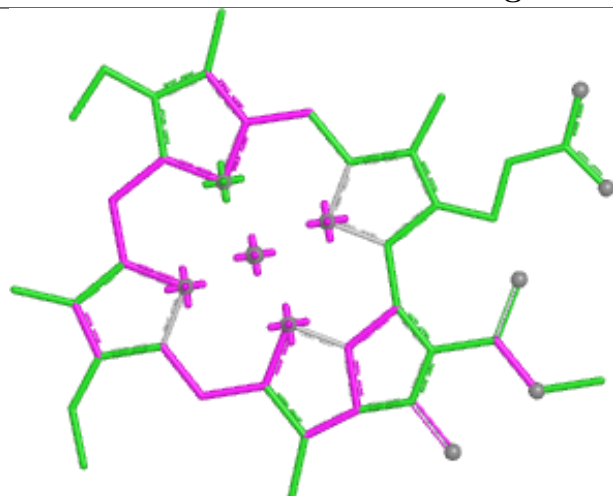


Ligand CLA G 1101

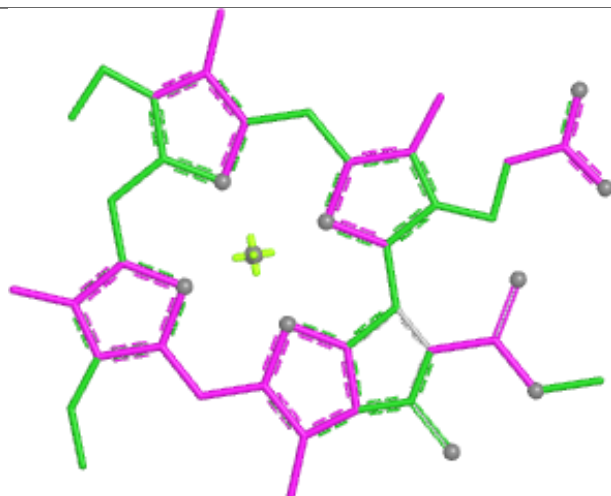




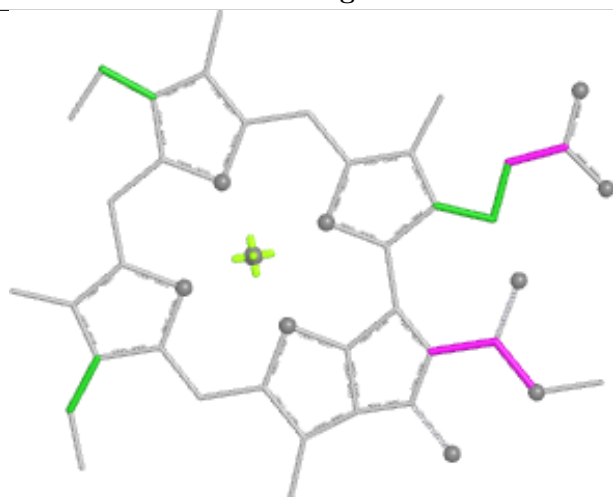
Ligand CLA H 1218



Bond lengths



Bond angles

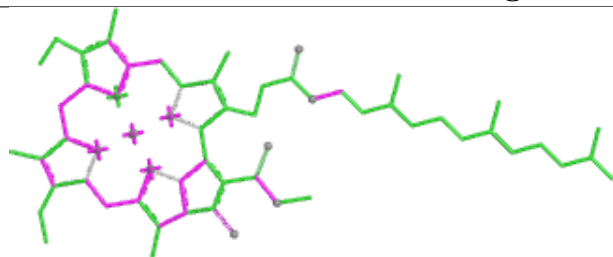


Torsions

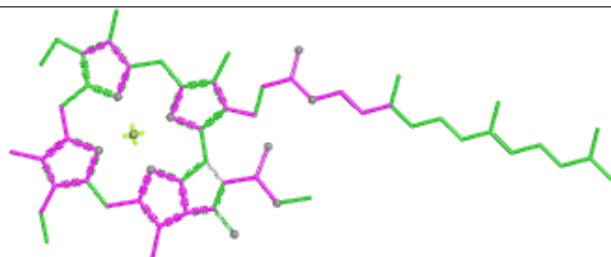


Rings

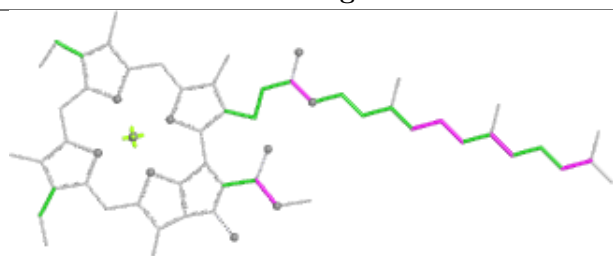
Ligand CLA G 1133



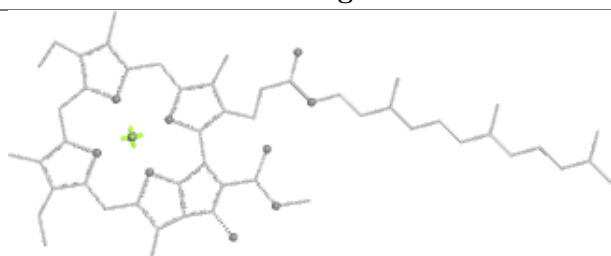
Bond lengths



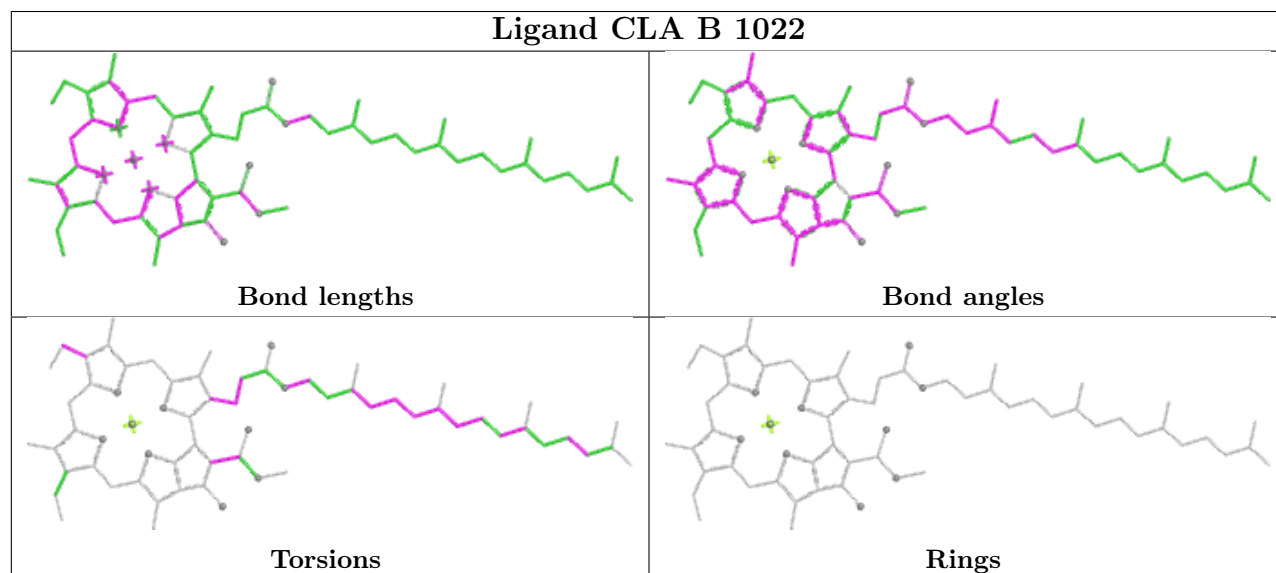
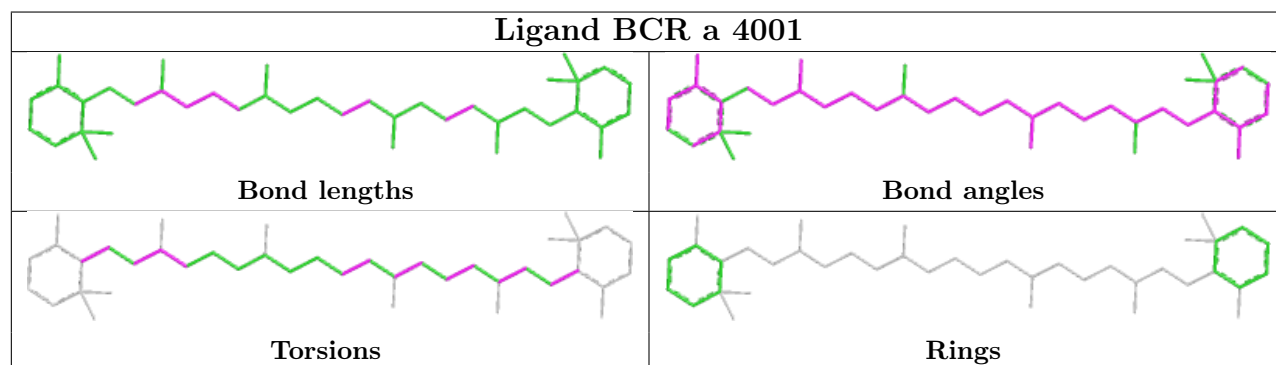
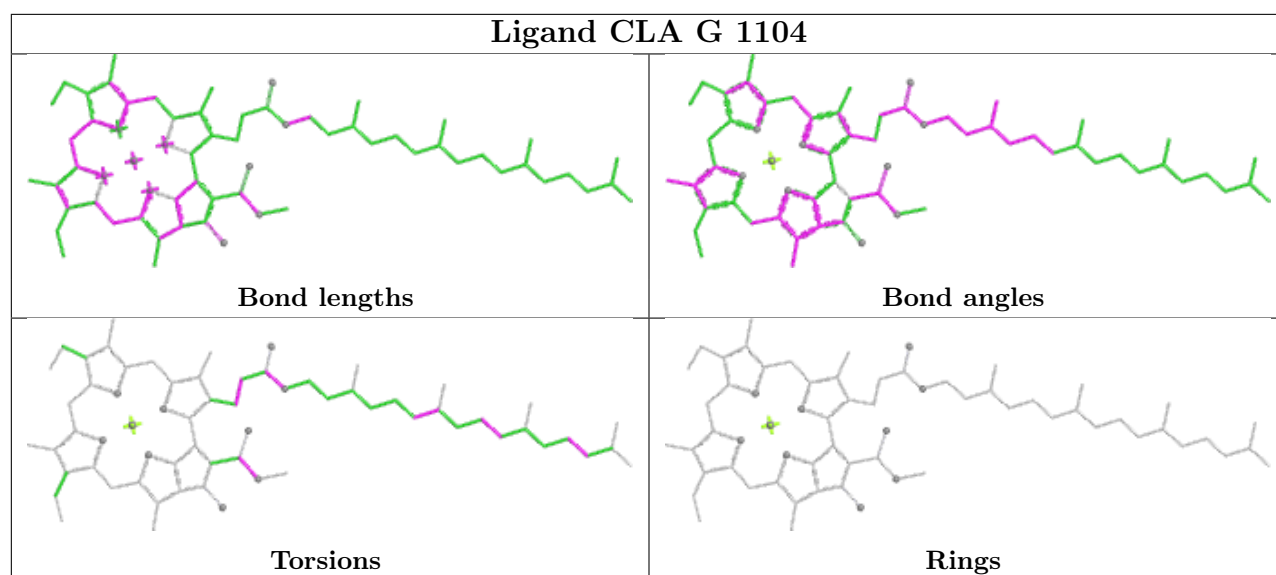
Bond angles

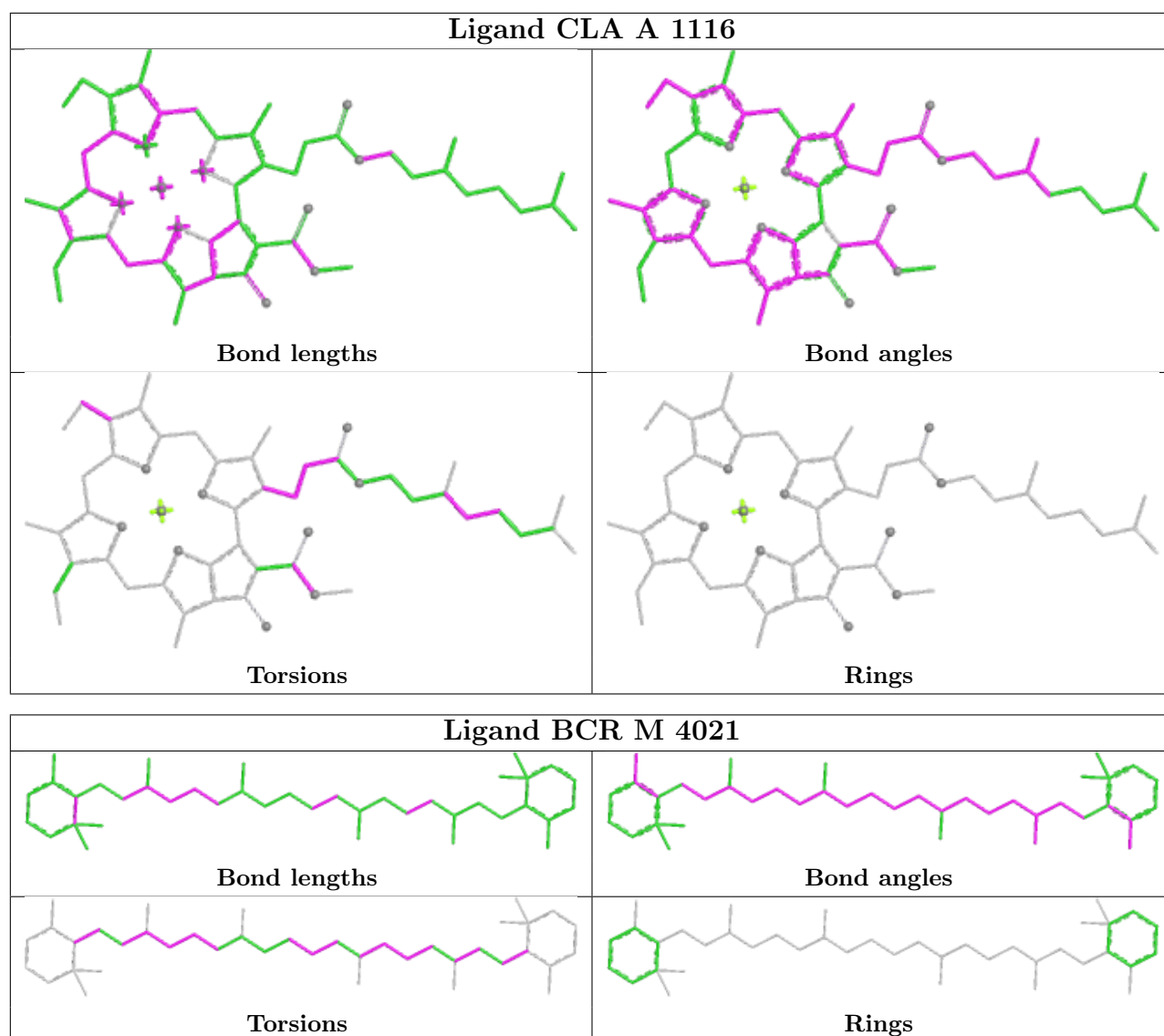


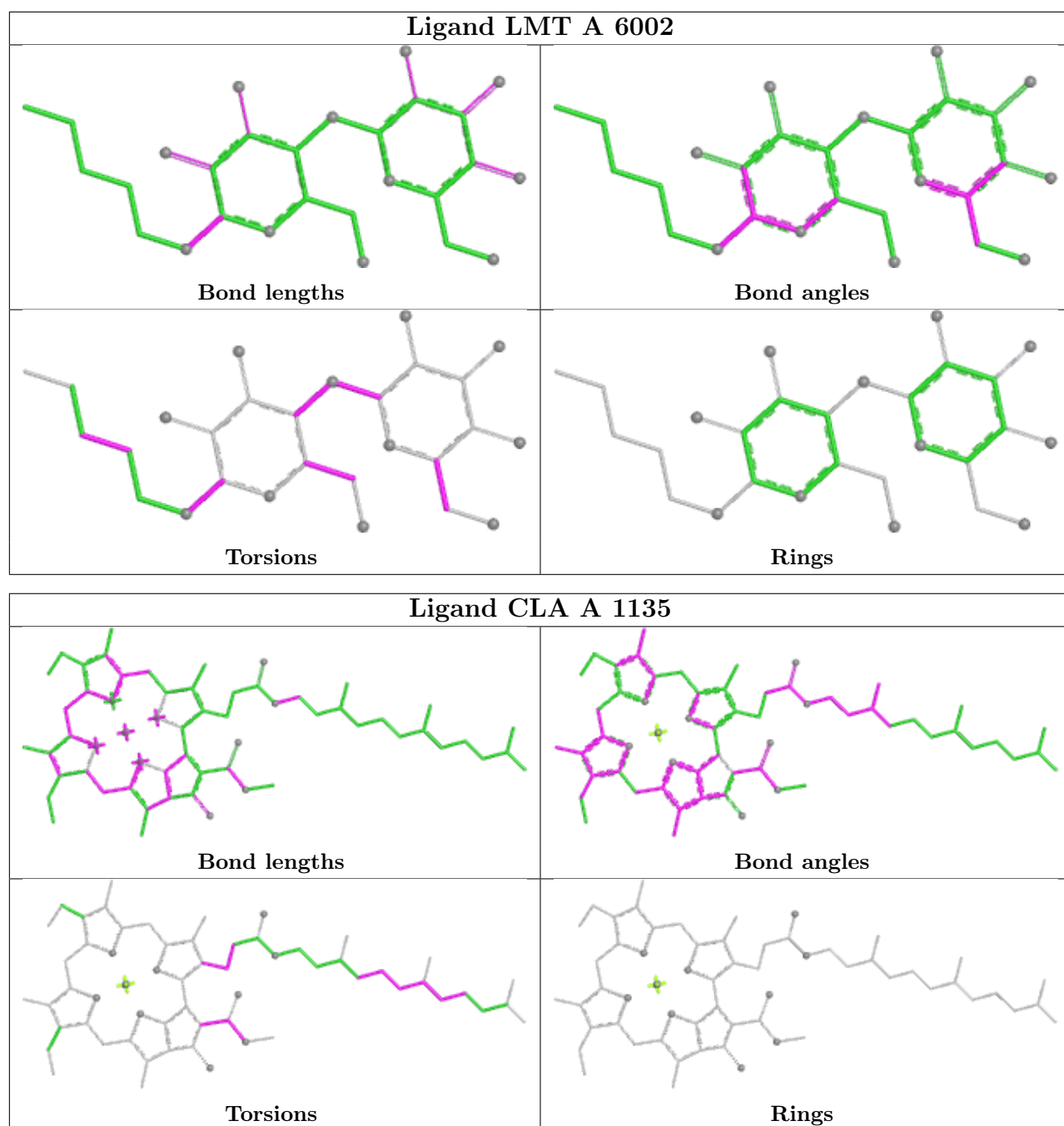
Torsions



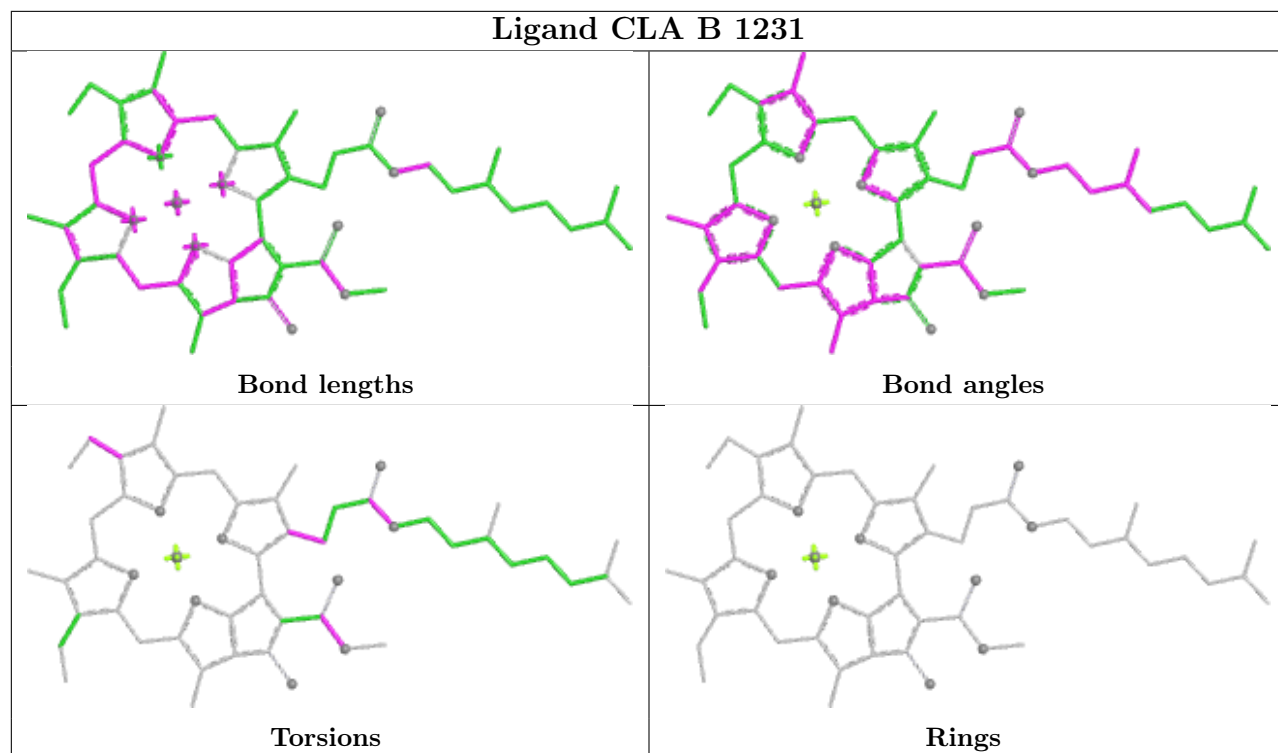
Rings



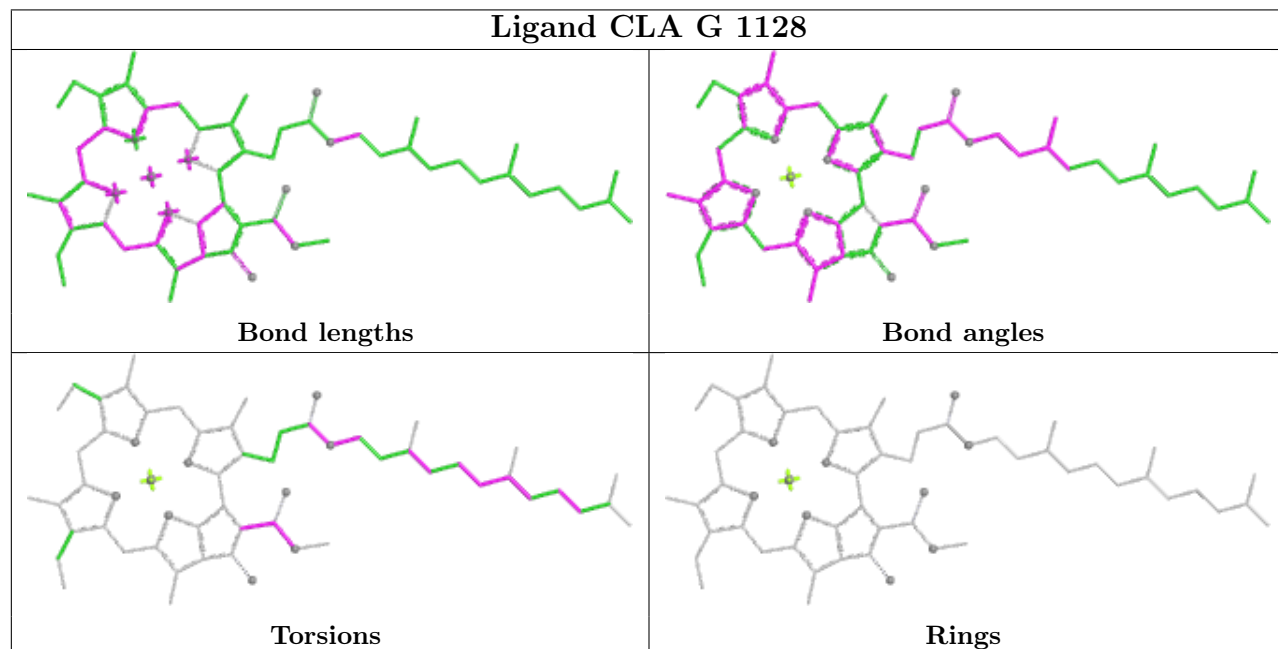


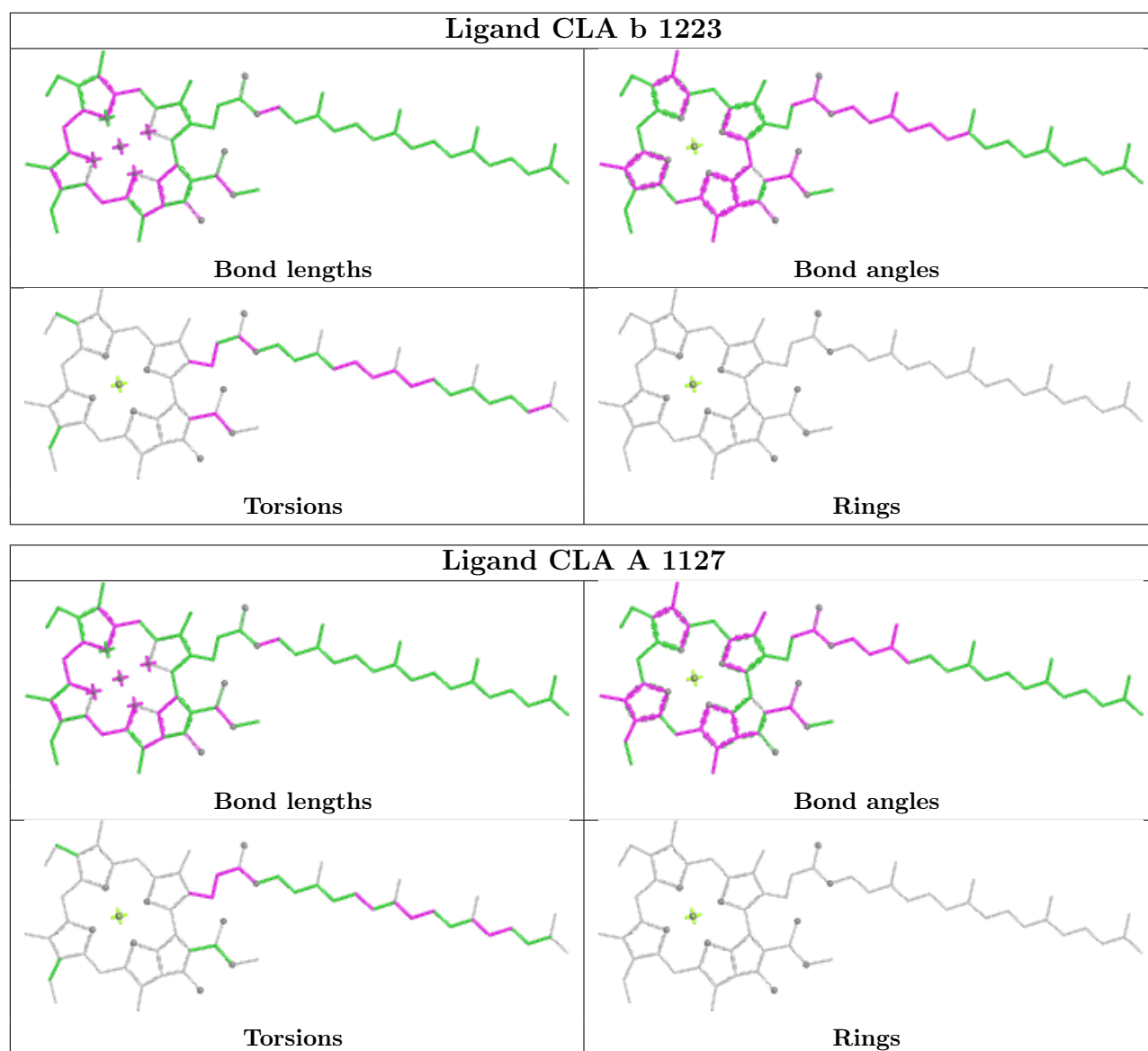


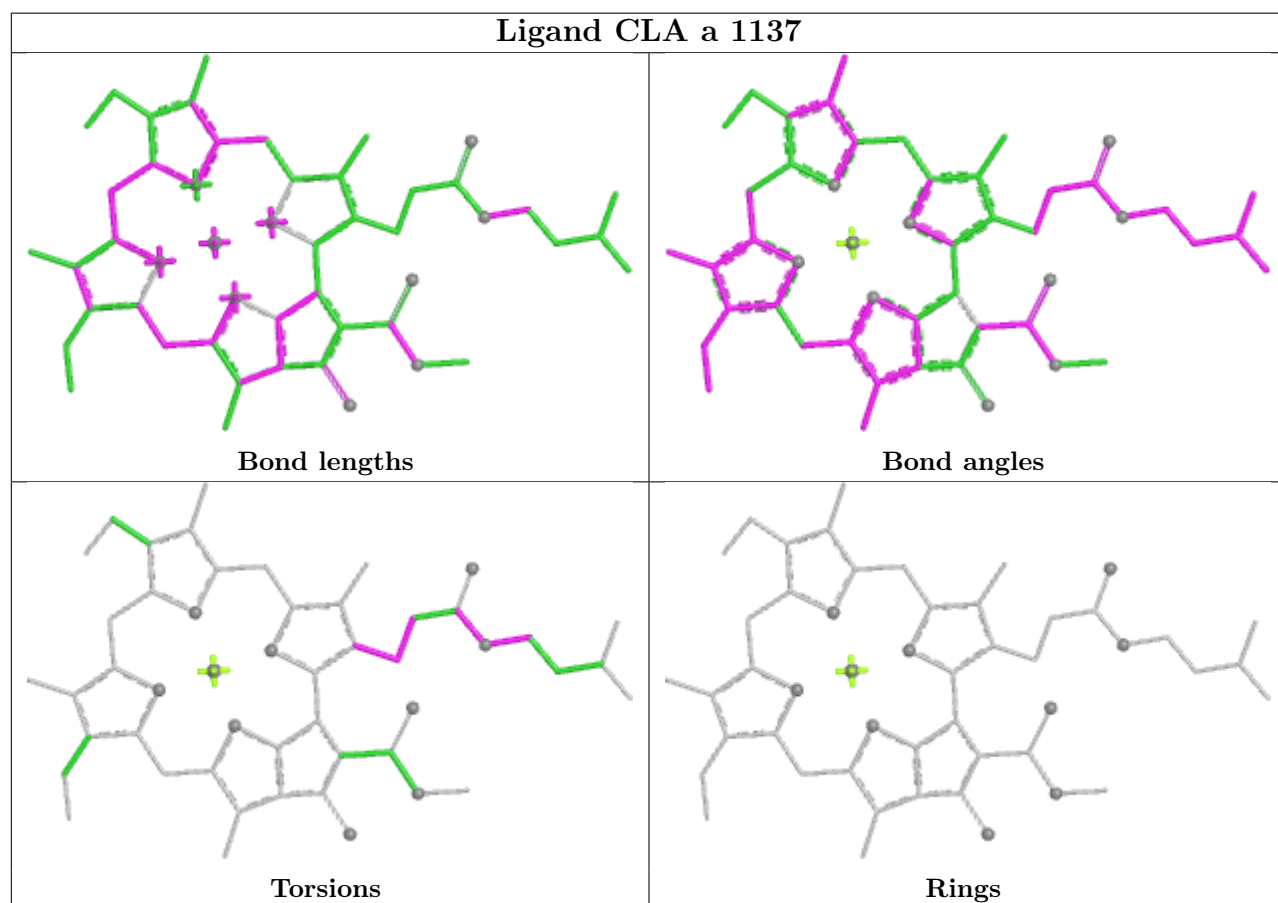
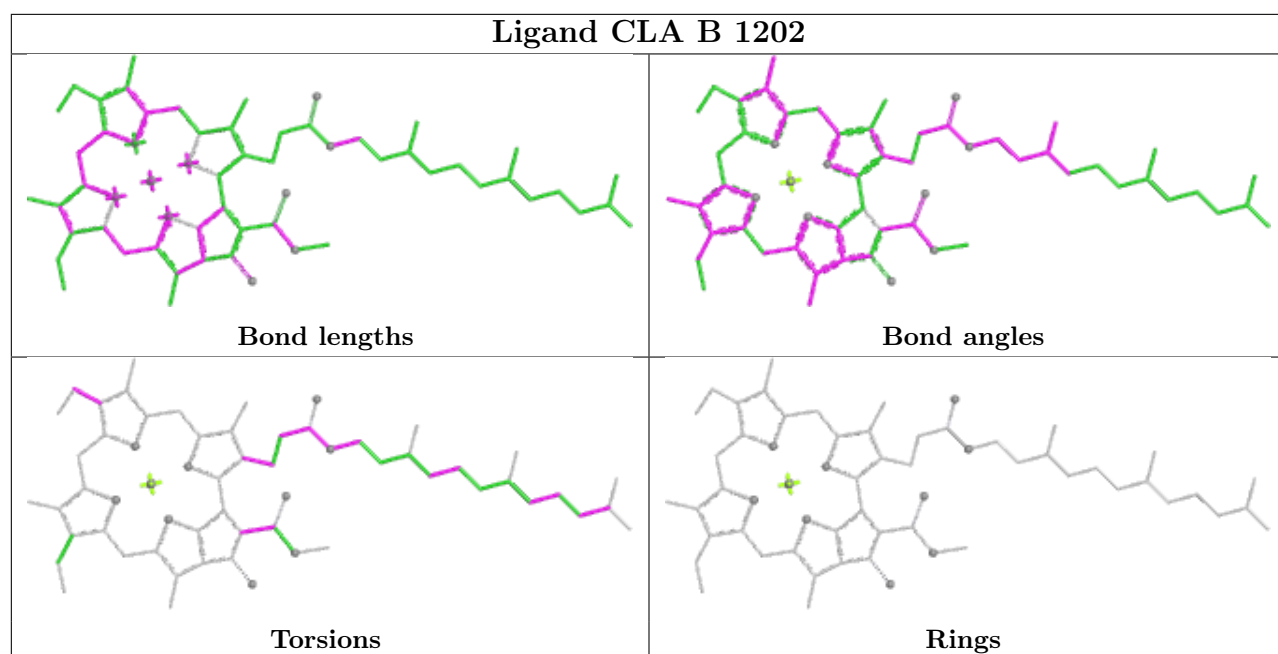
Ligand CLA B 1231

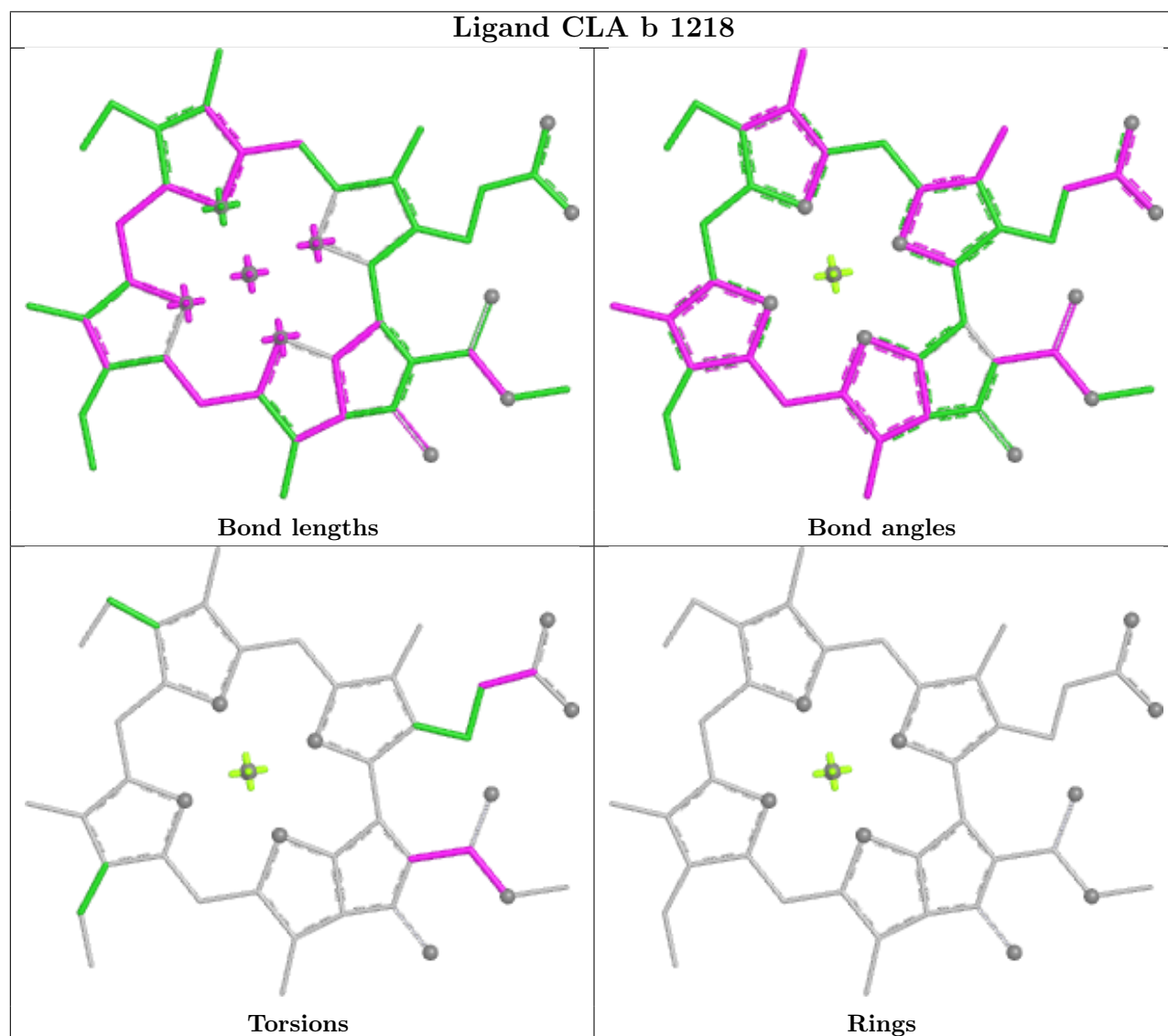
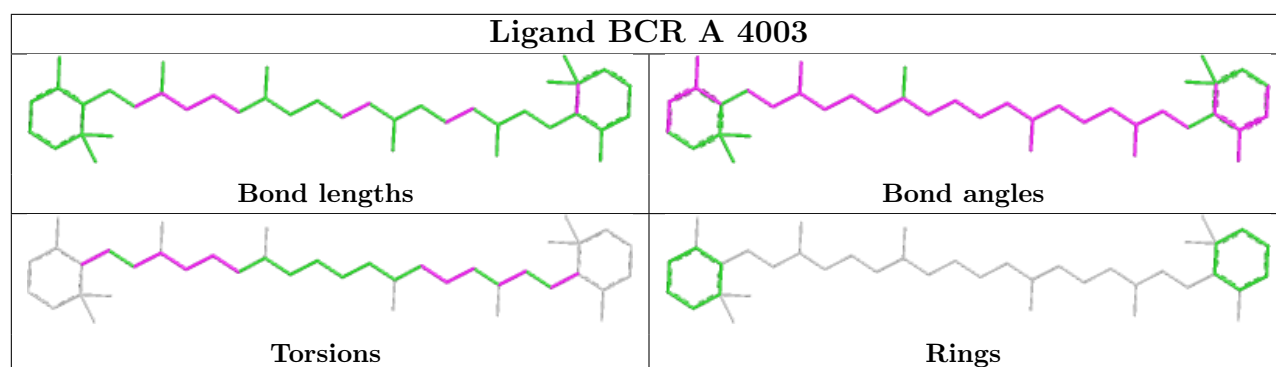


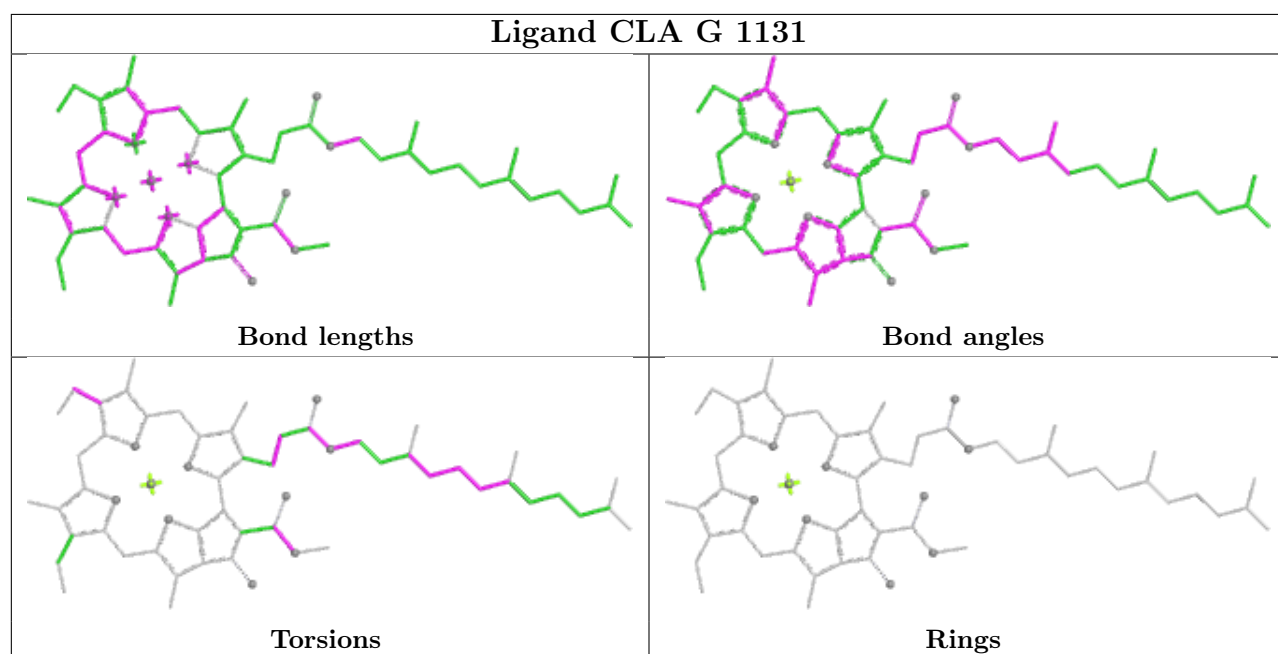
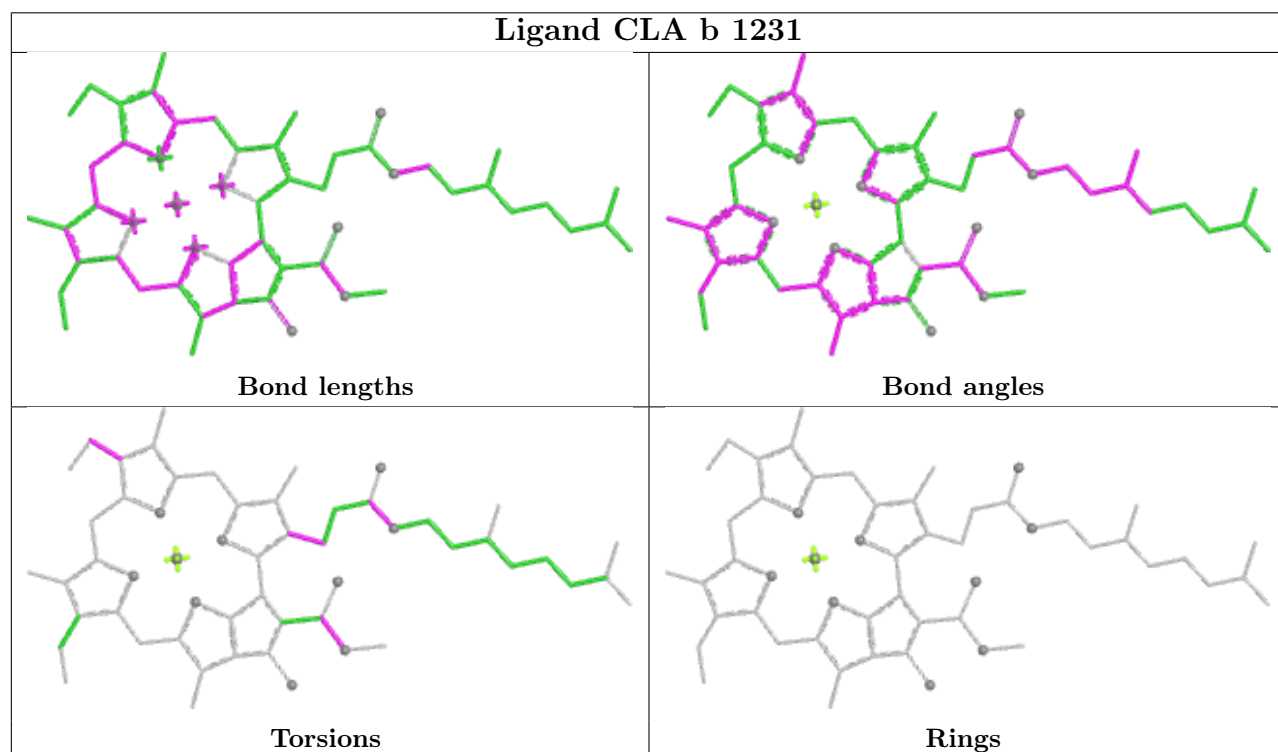
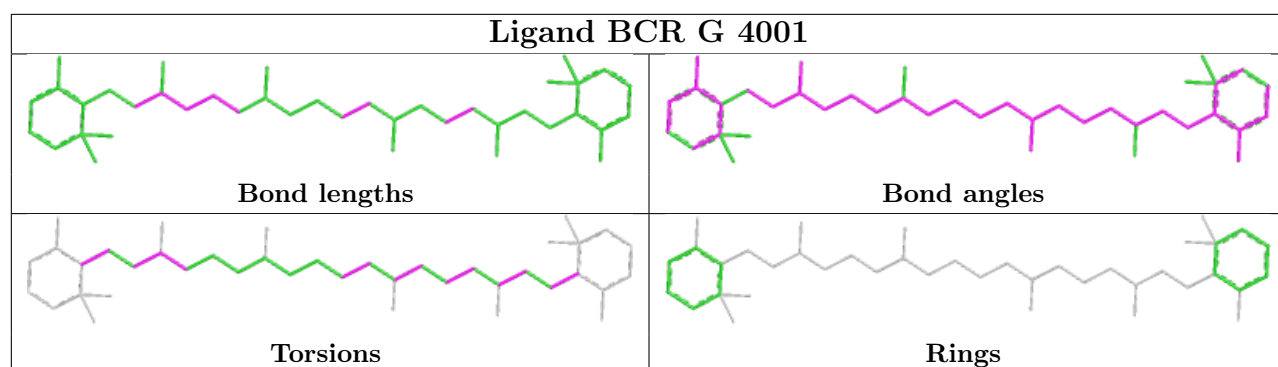
Ligand CLA G 1128



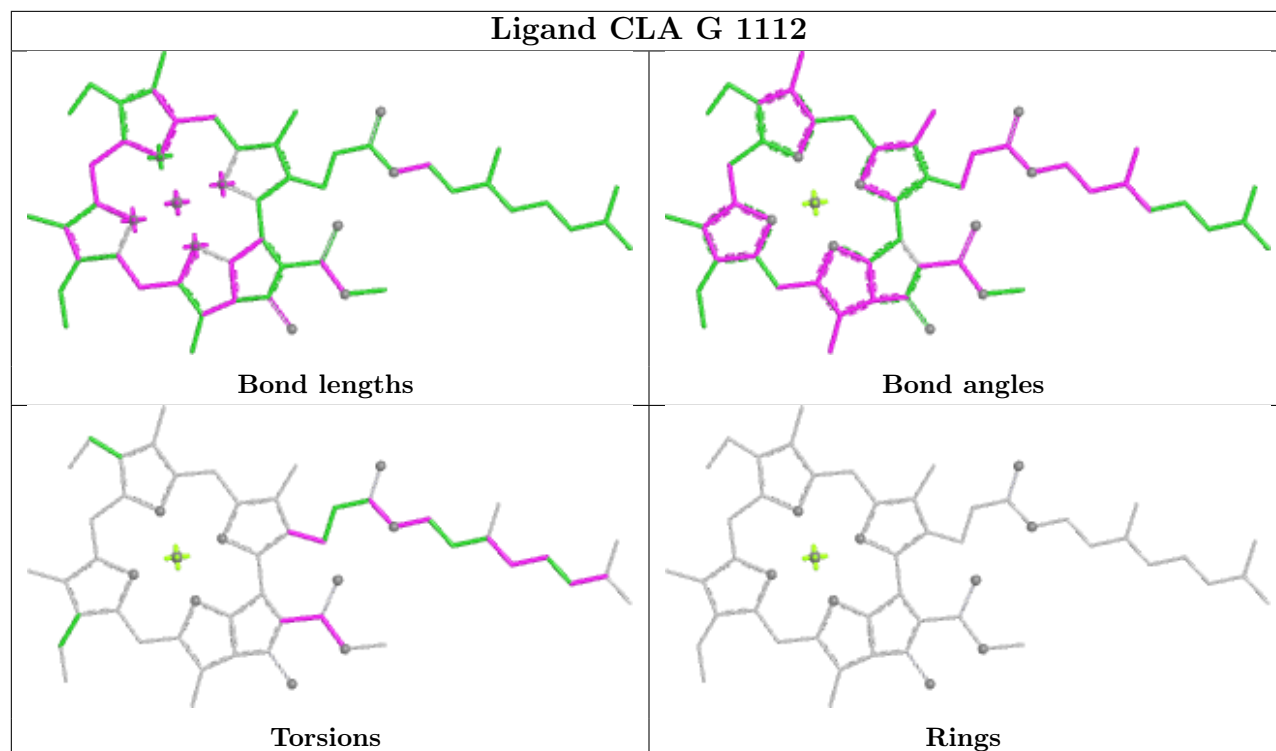




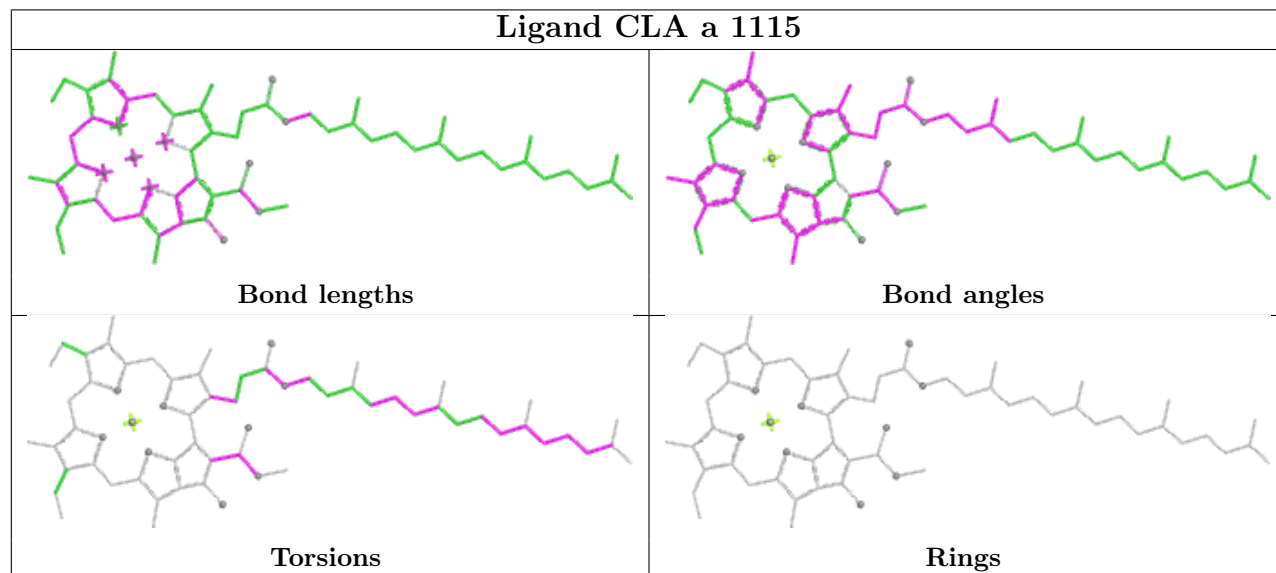


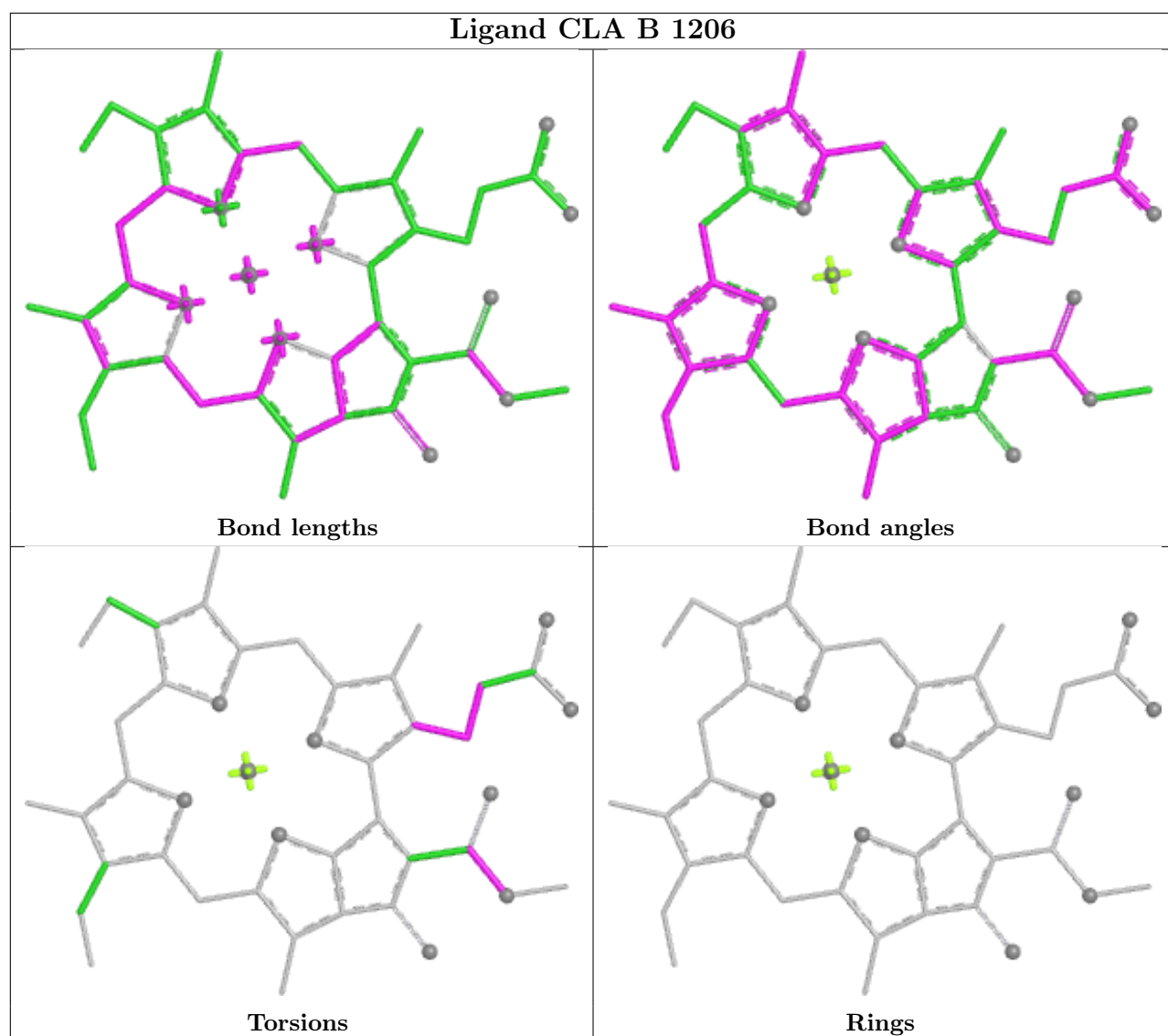


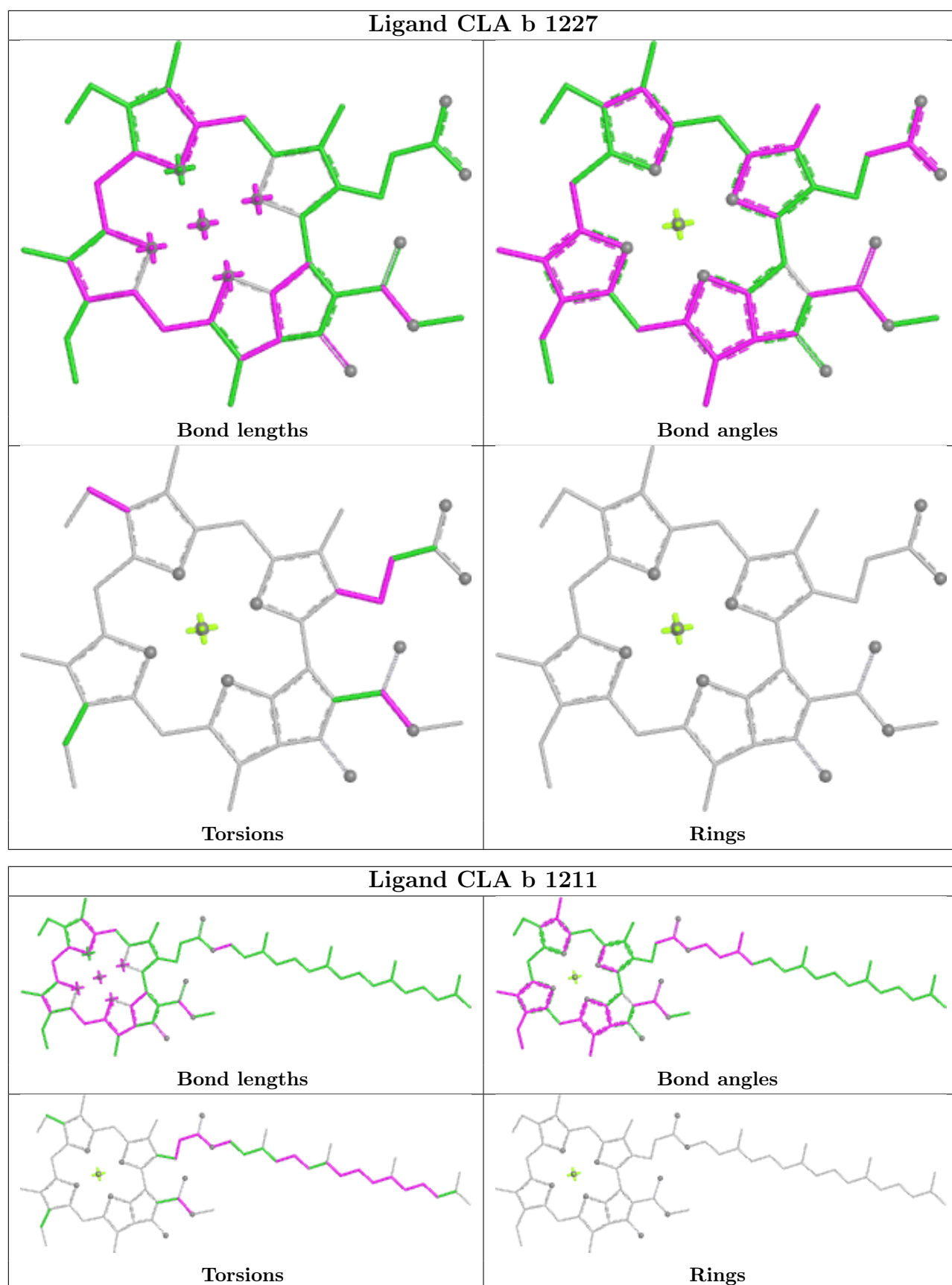
Ligand CLA G 1112

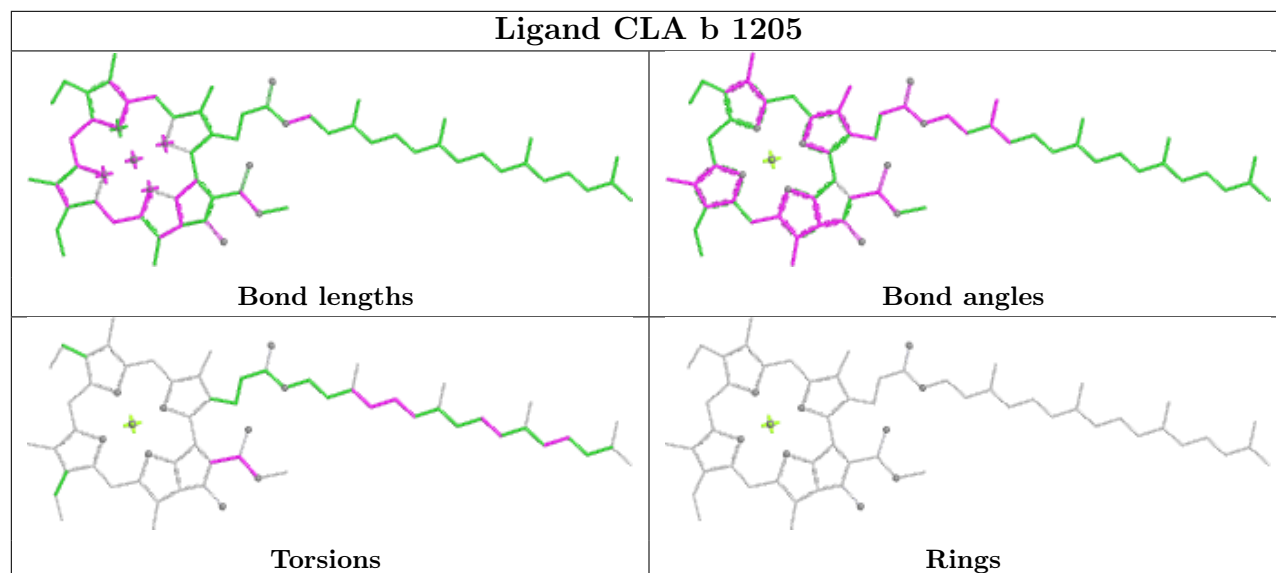
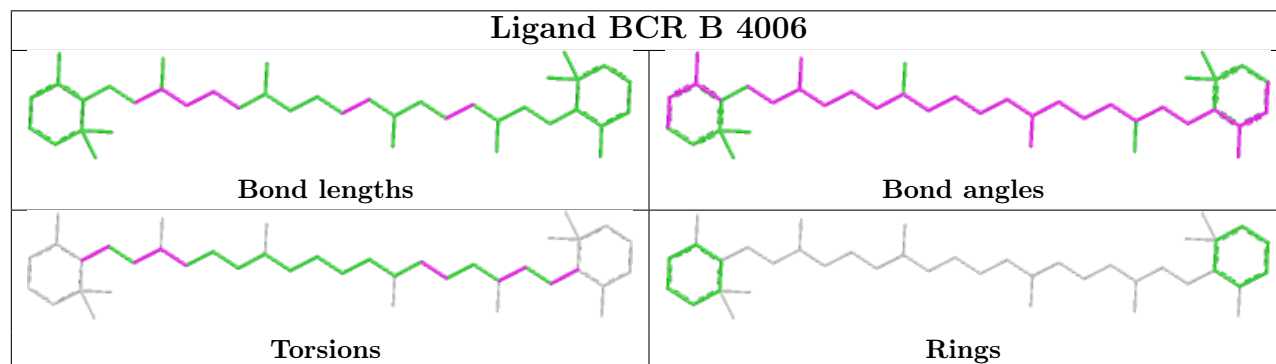
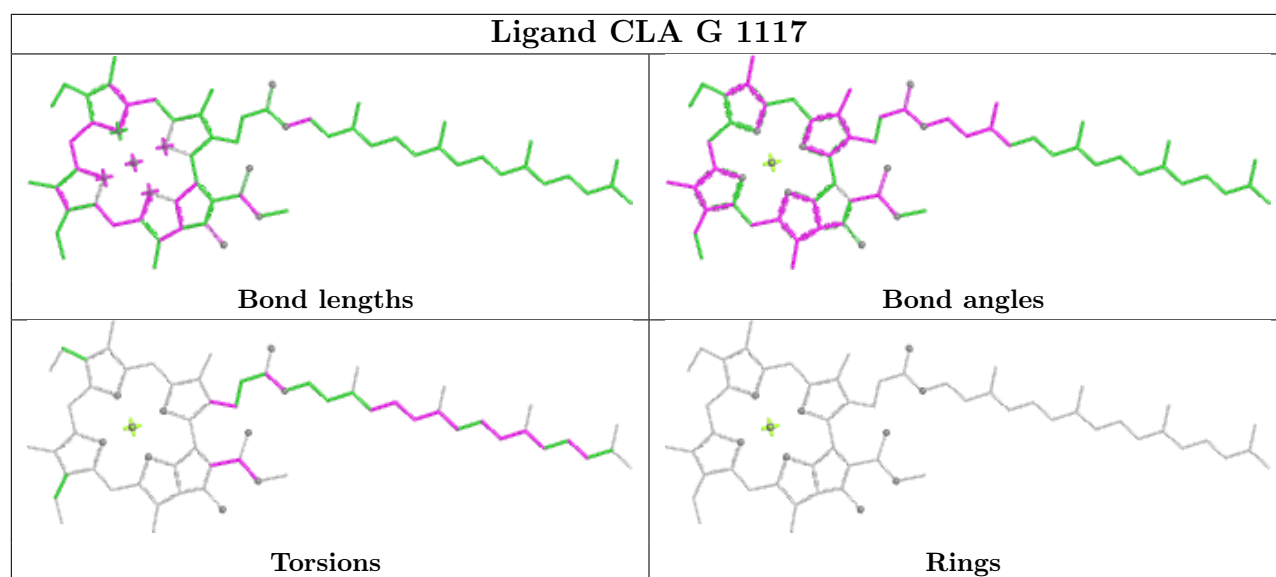


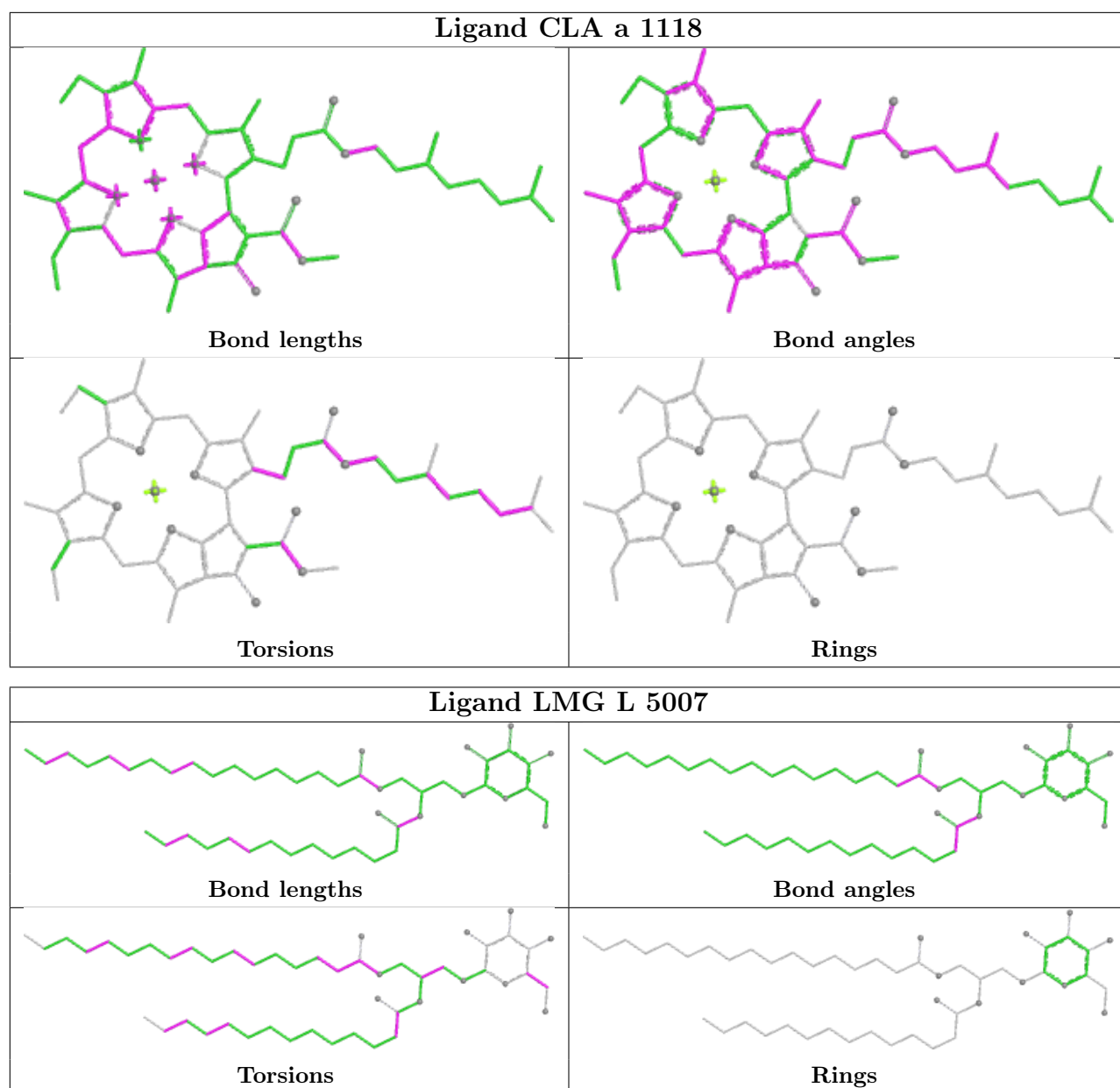
Ligand CLA a 1115

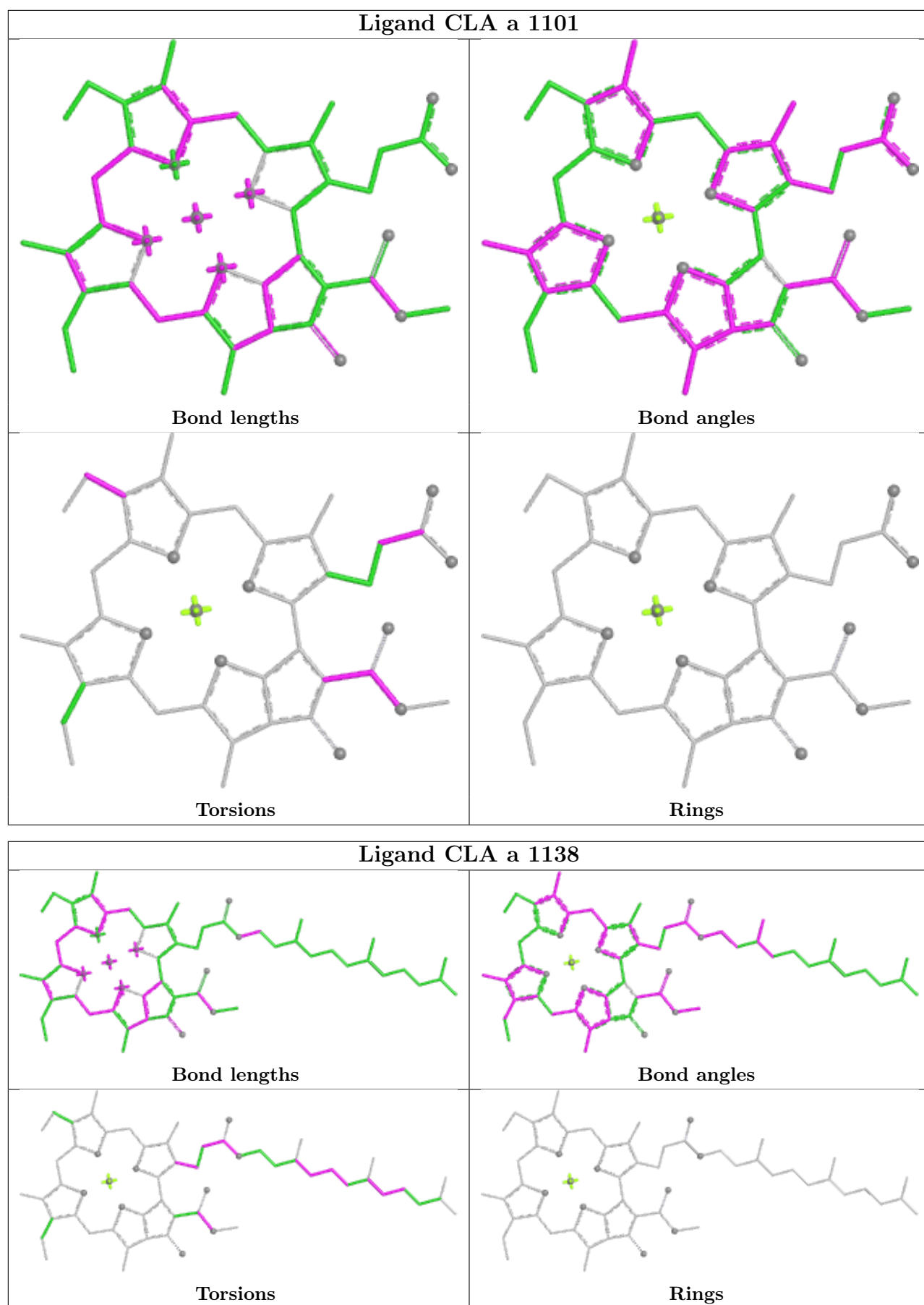




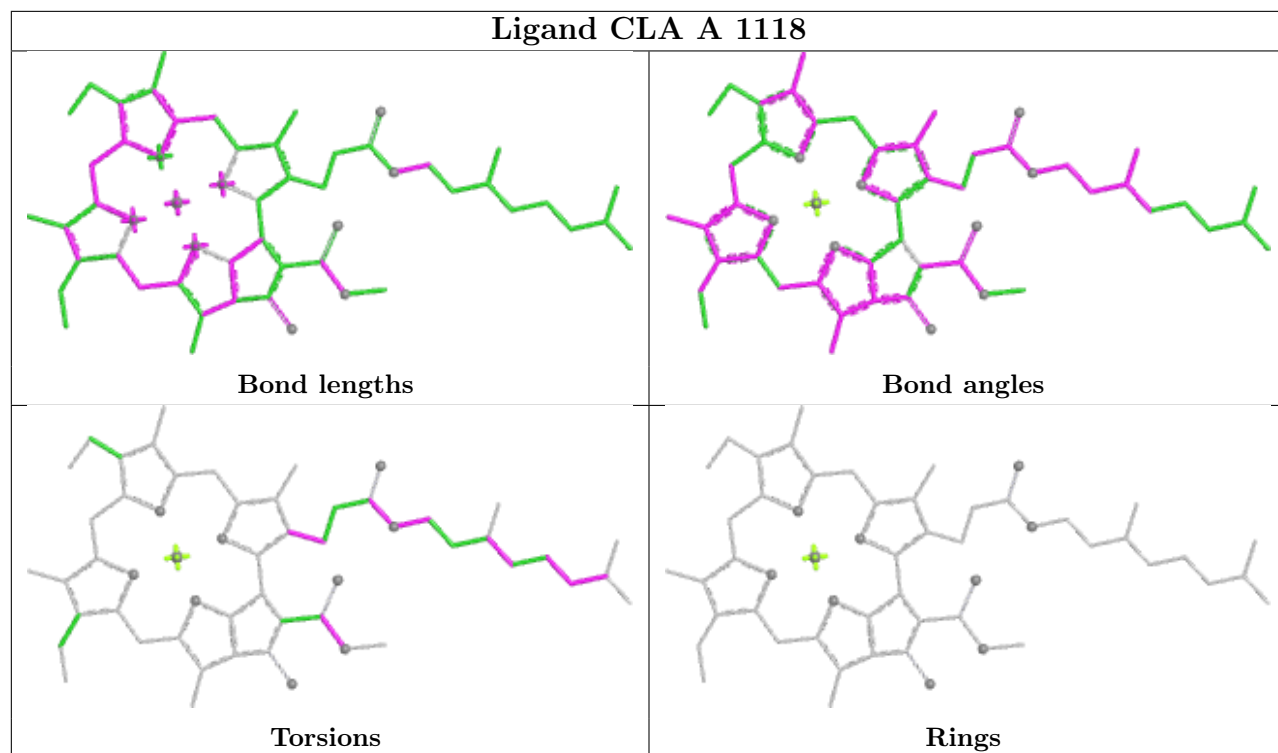




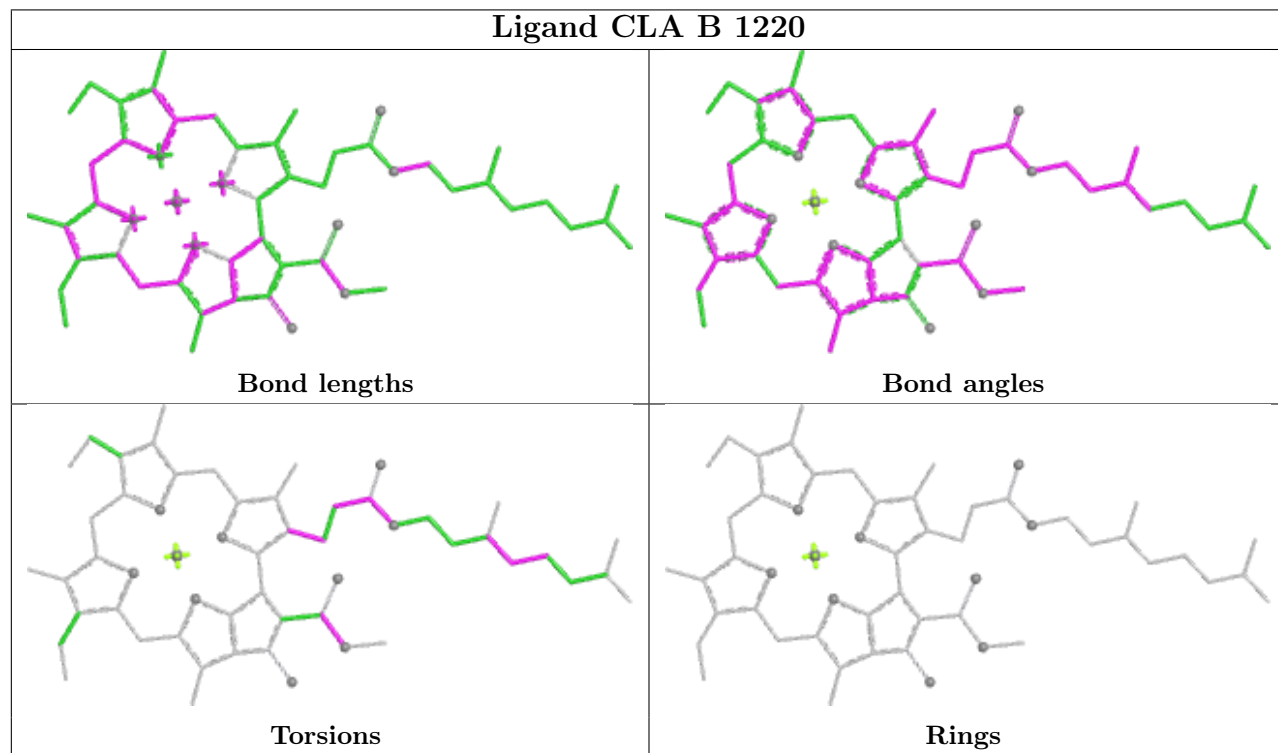


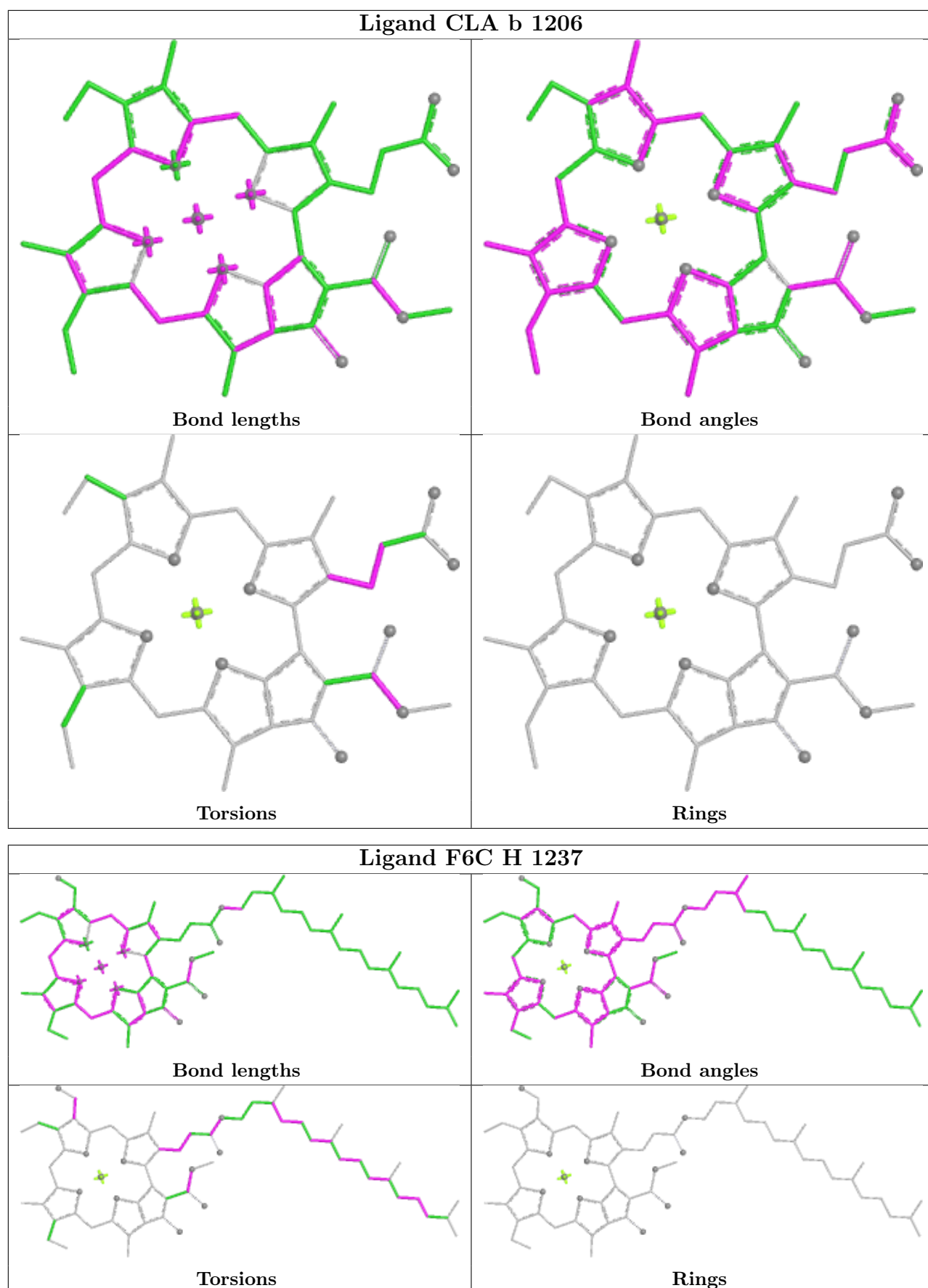


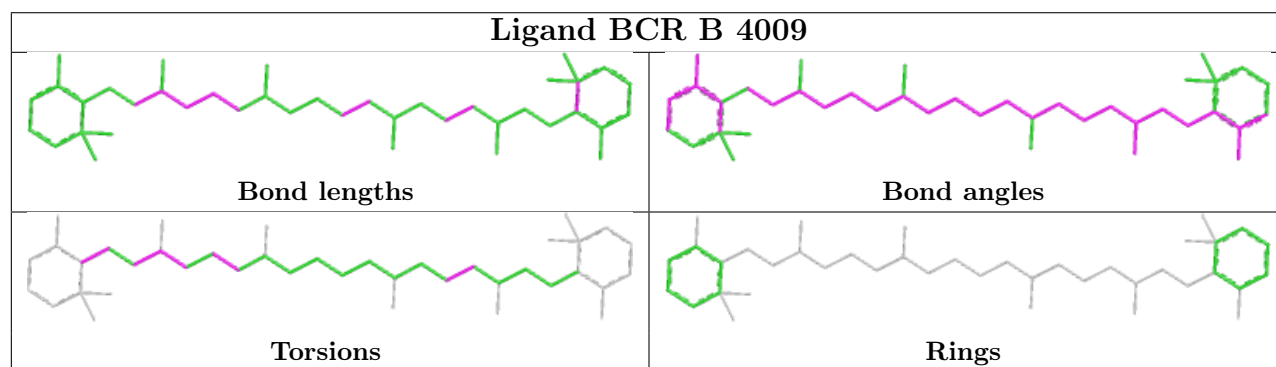
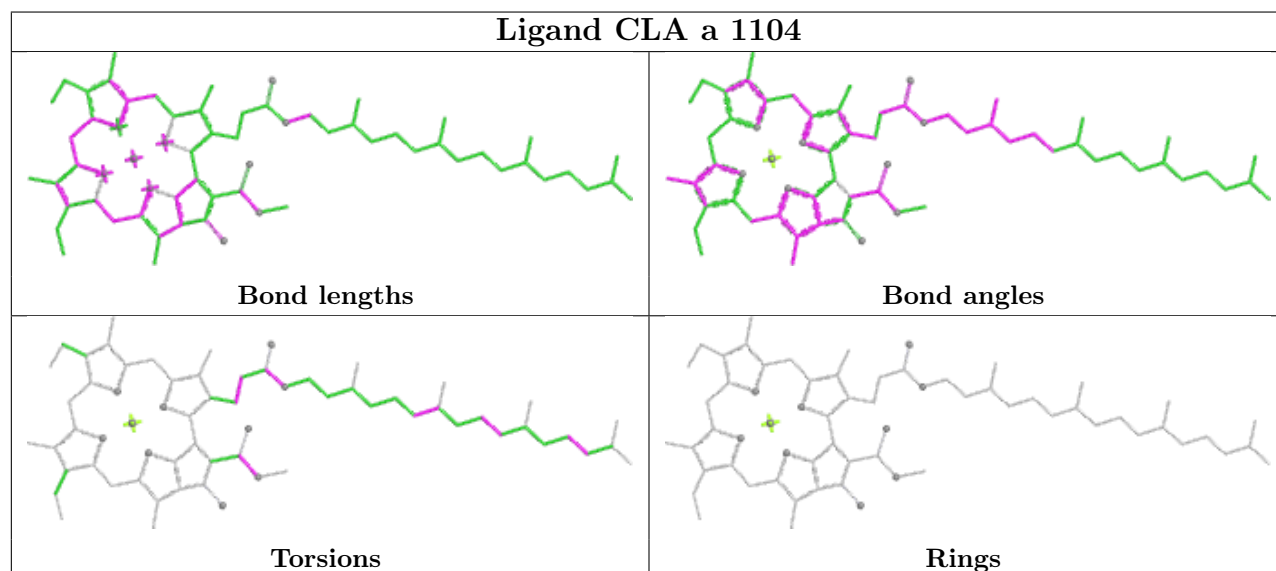
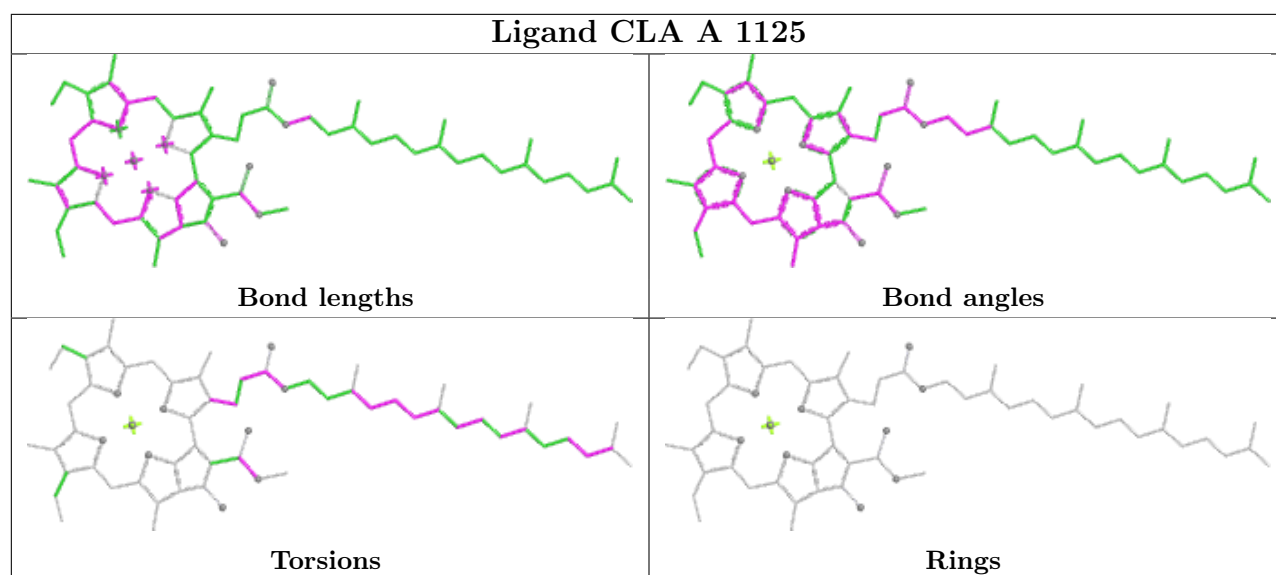
Ligand CLA A 1118

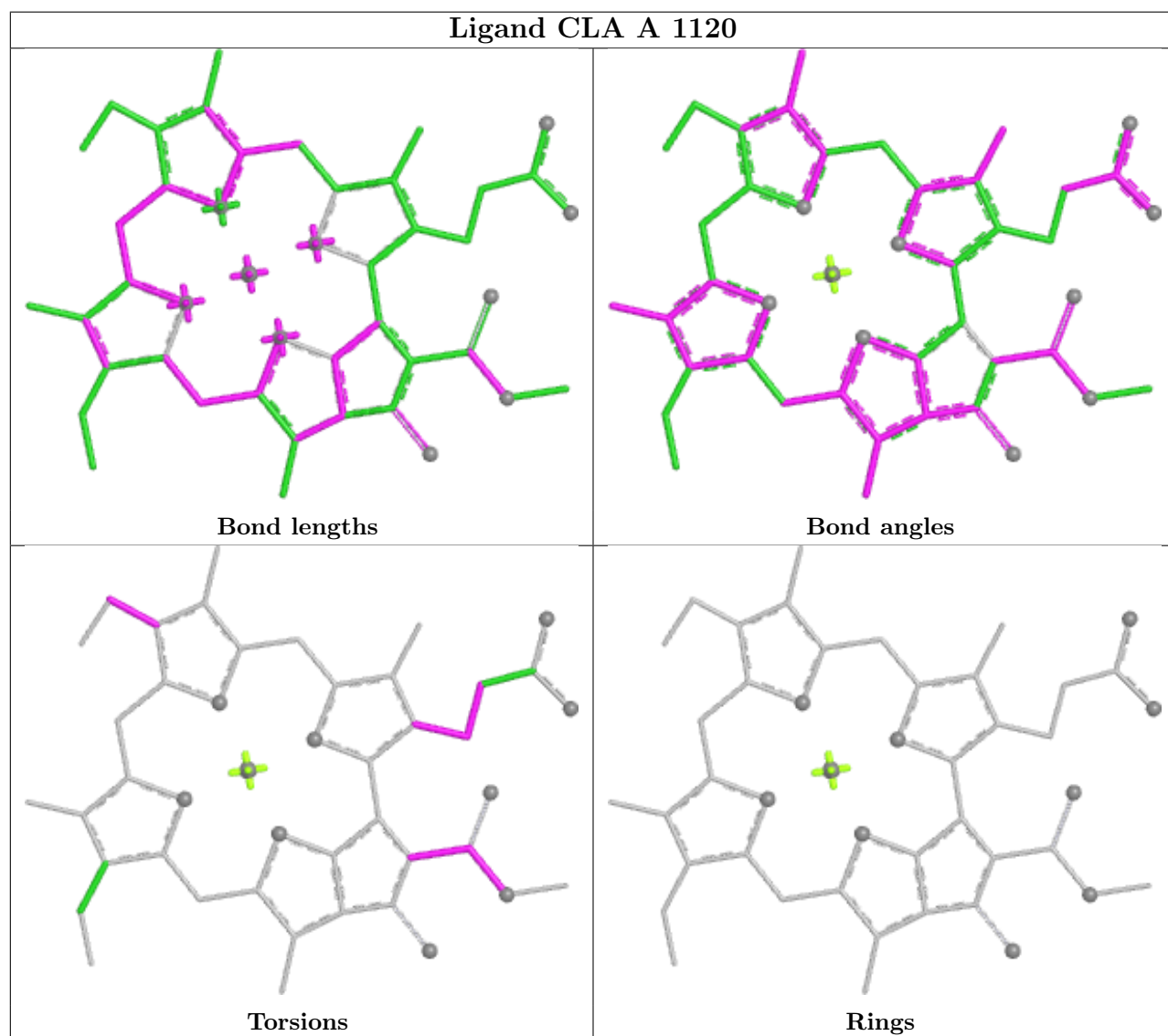
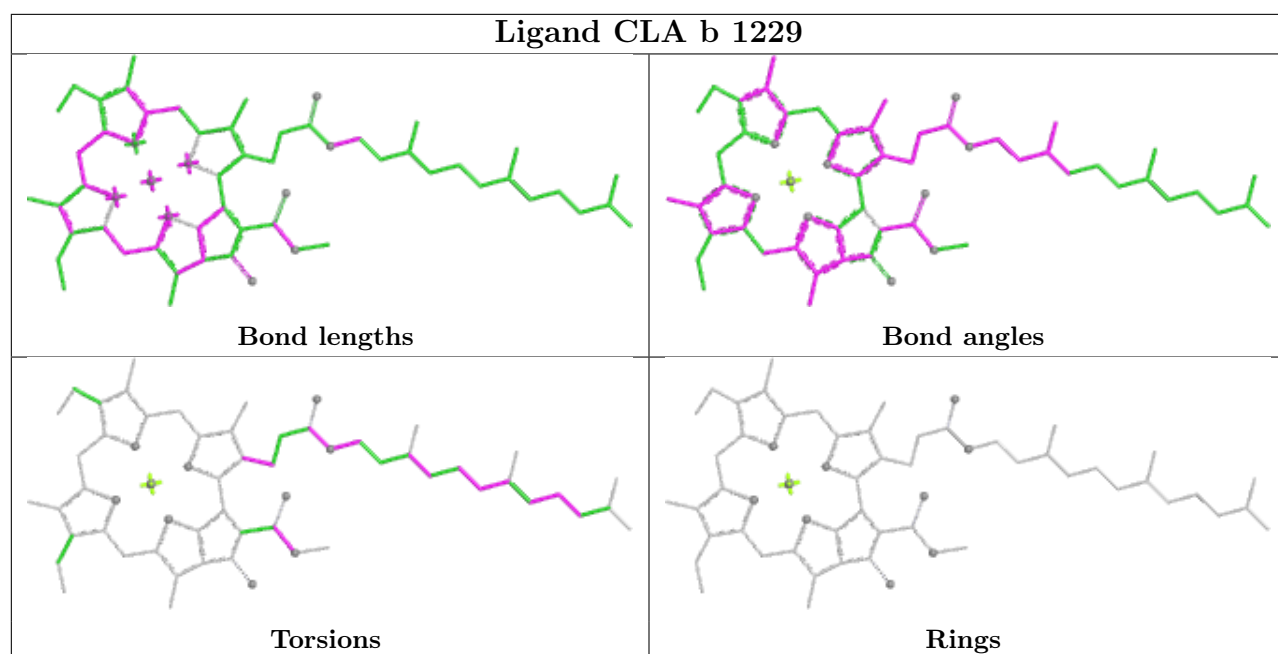


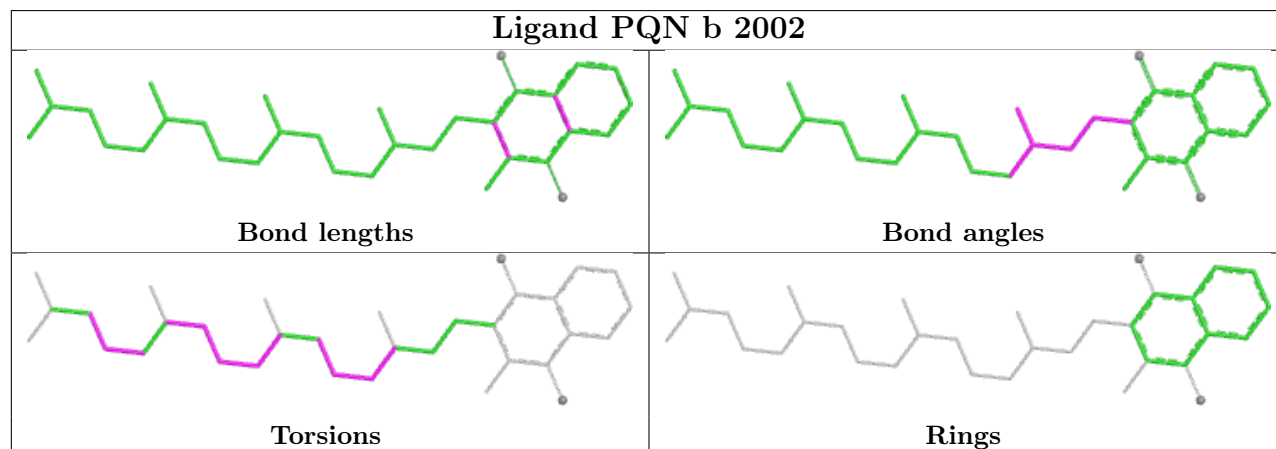
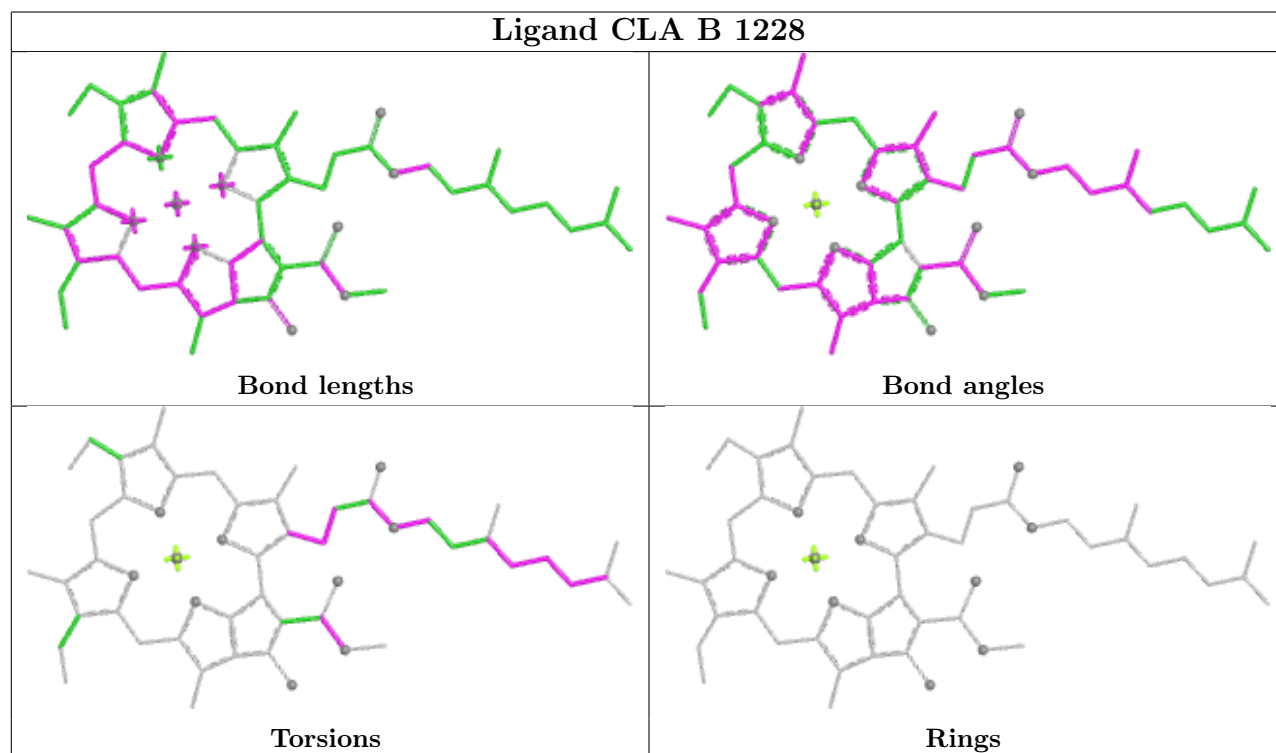
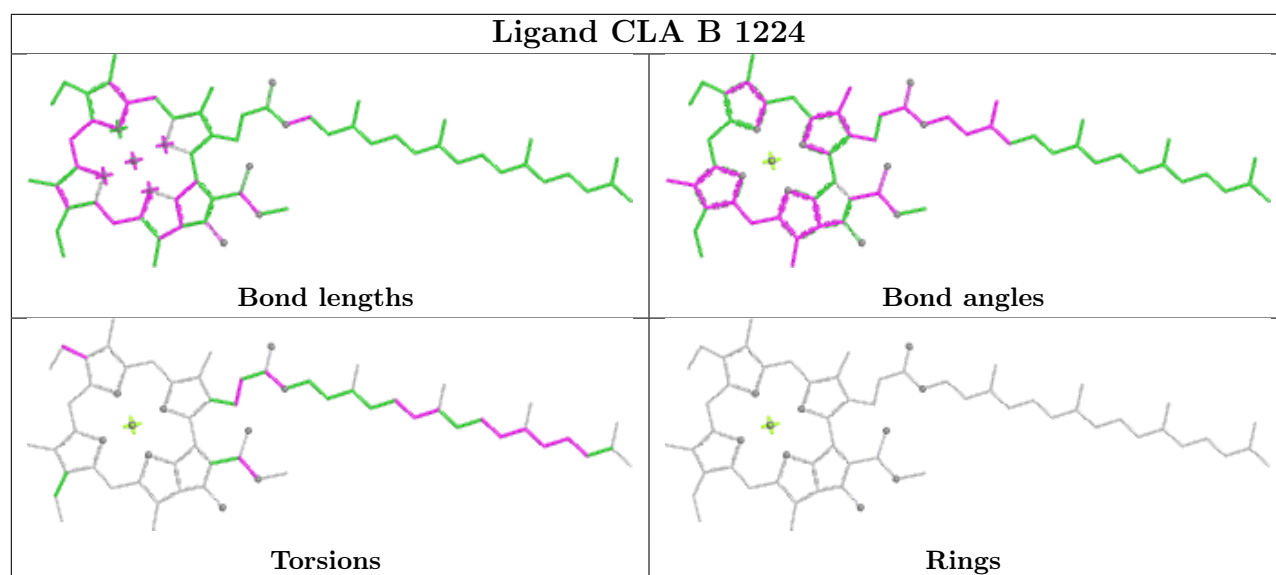
Ligand CLA B 1220

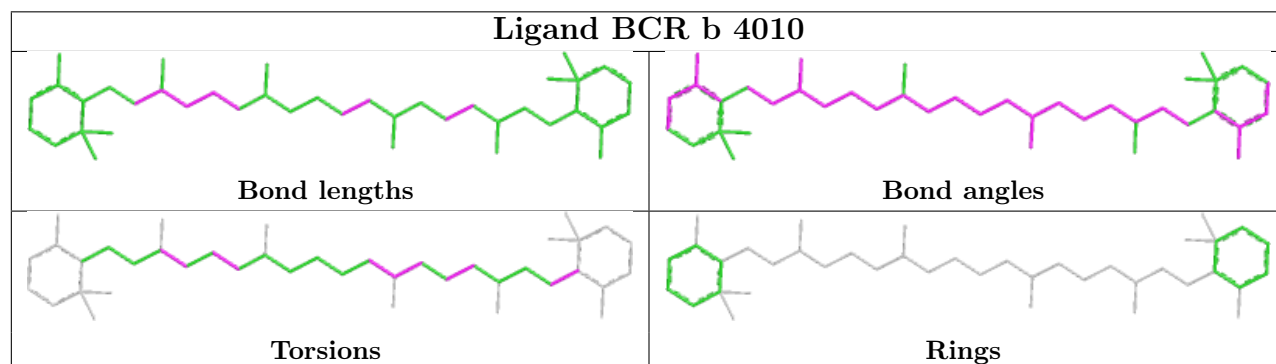
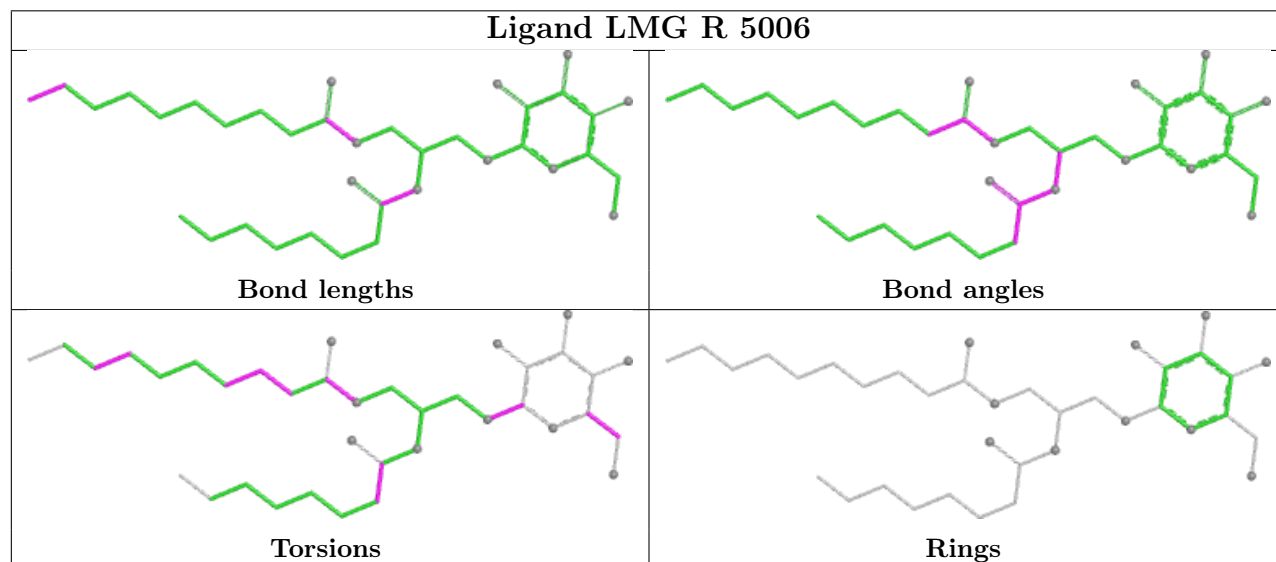
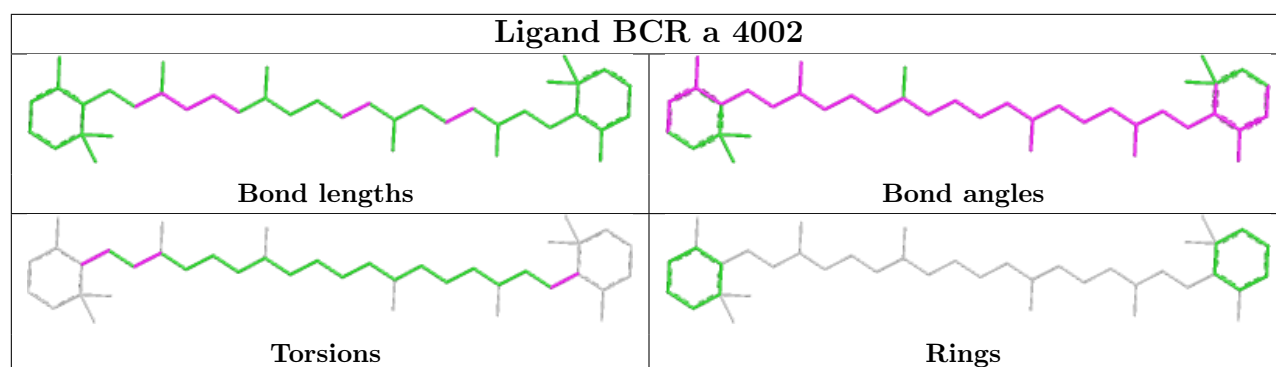


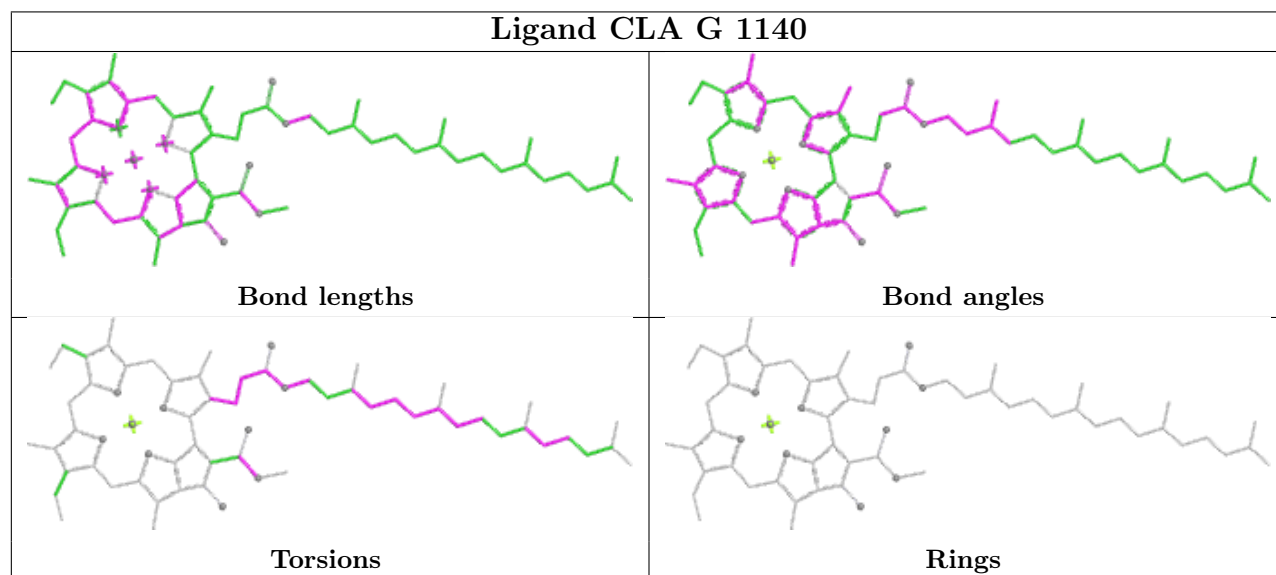
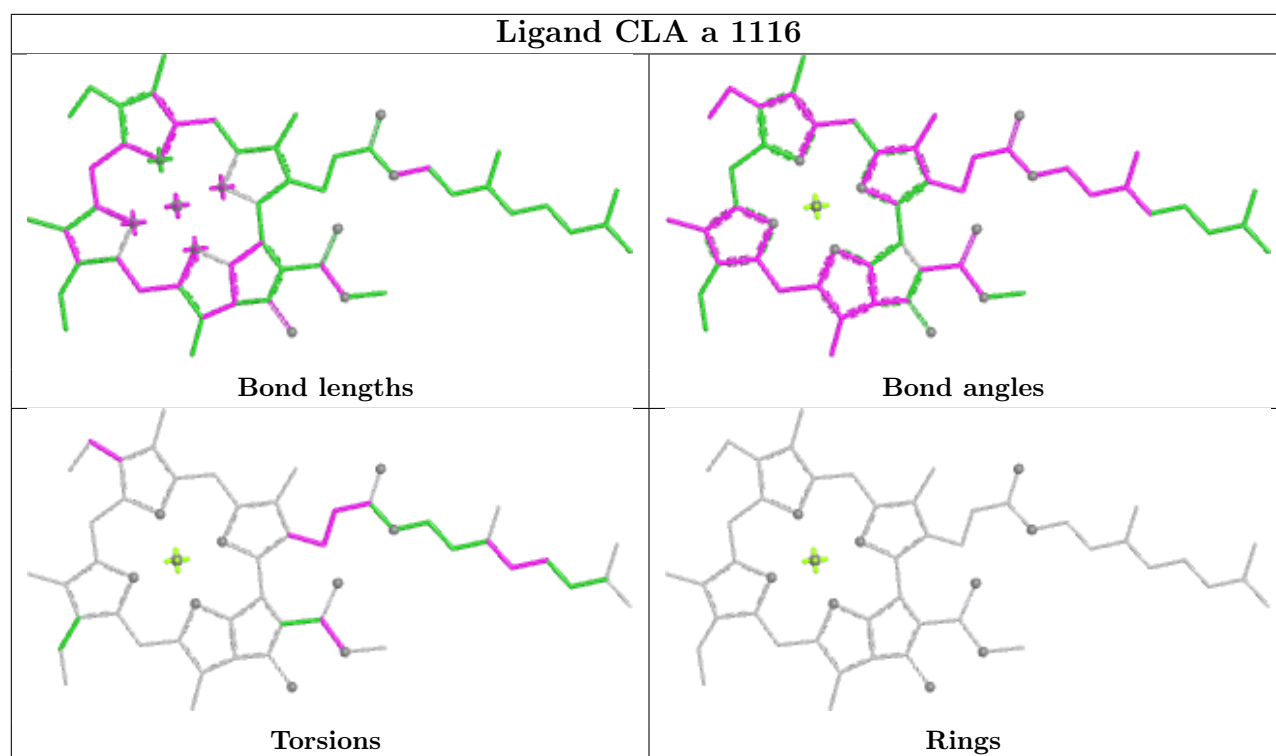


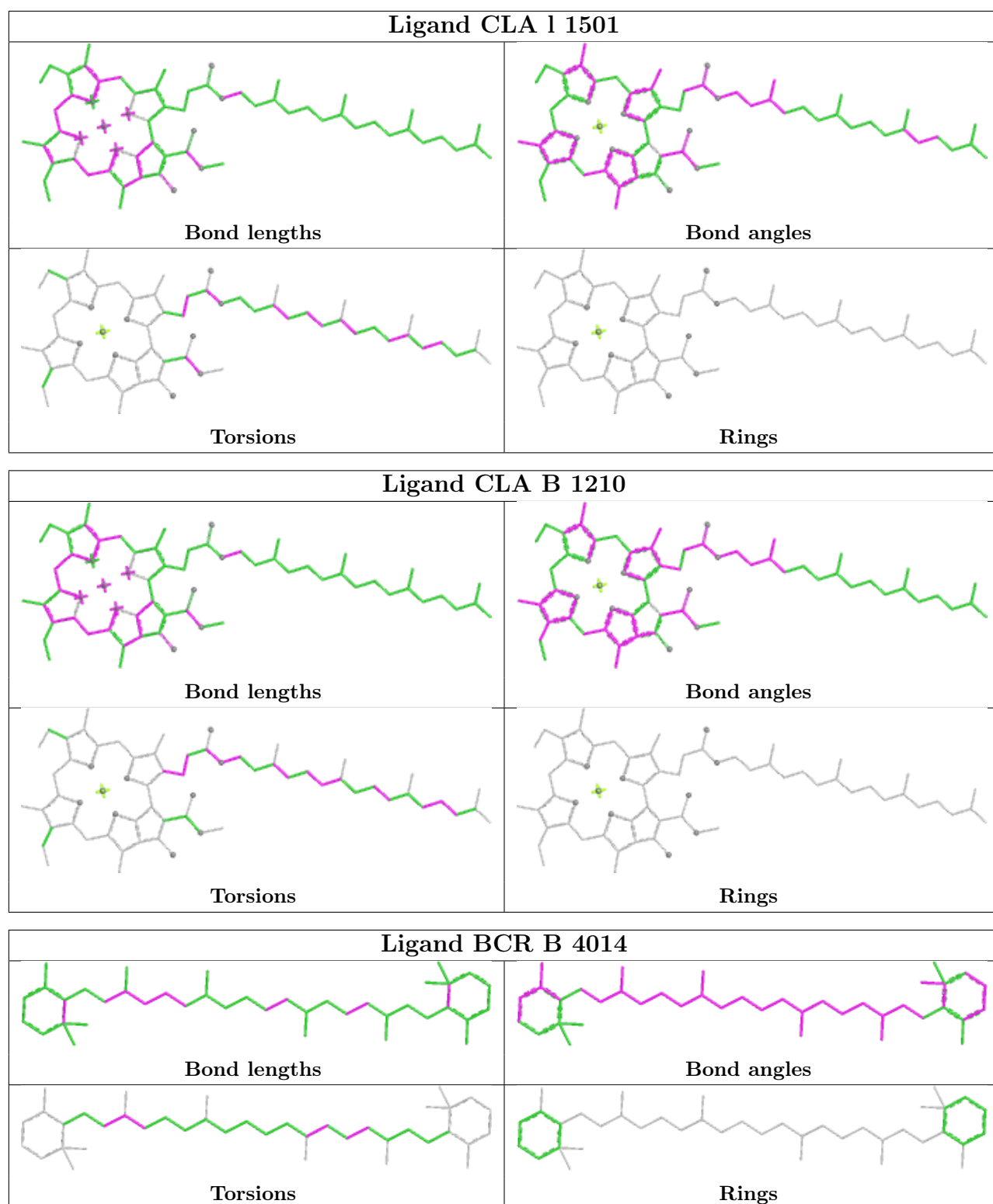


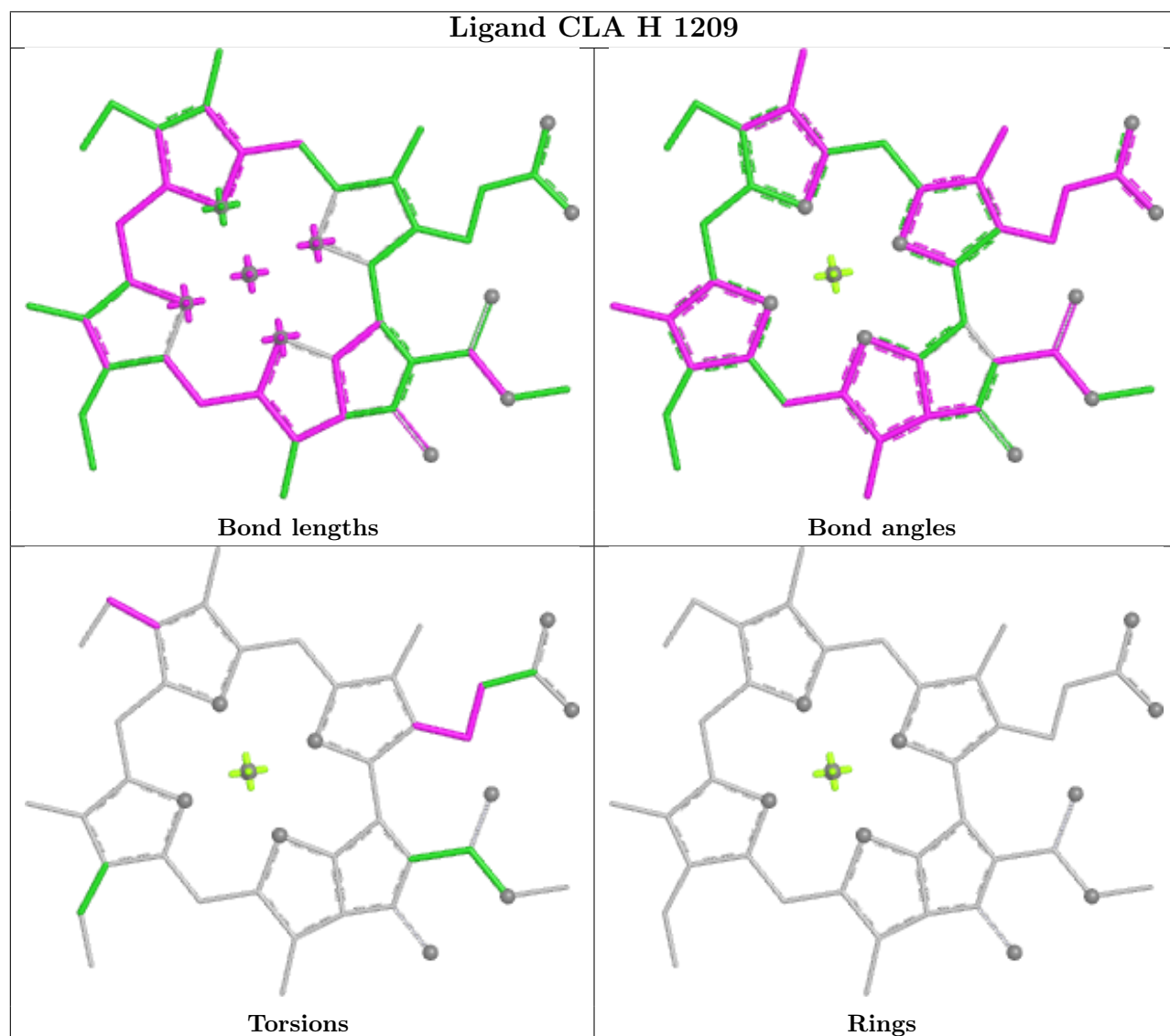
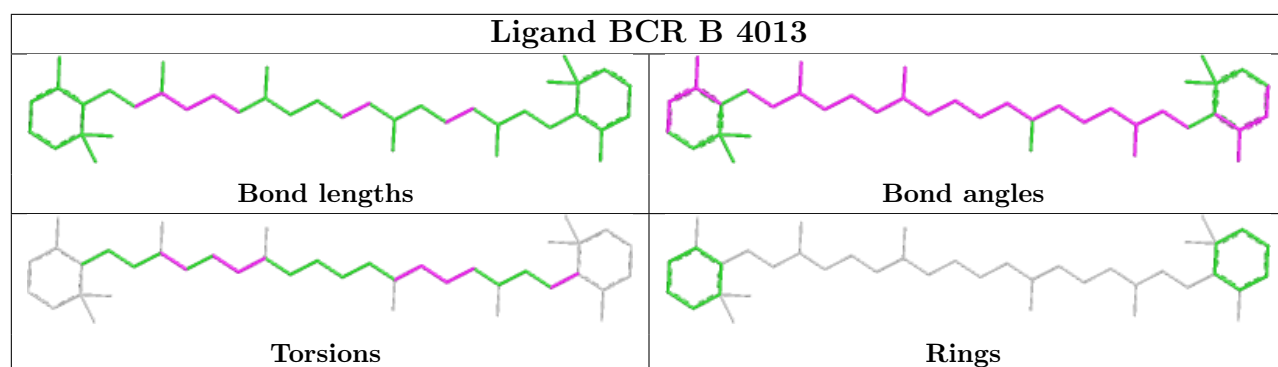


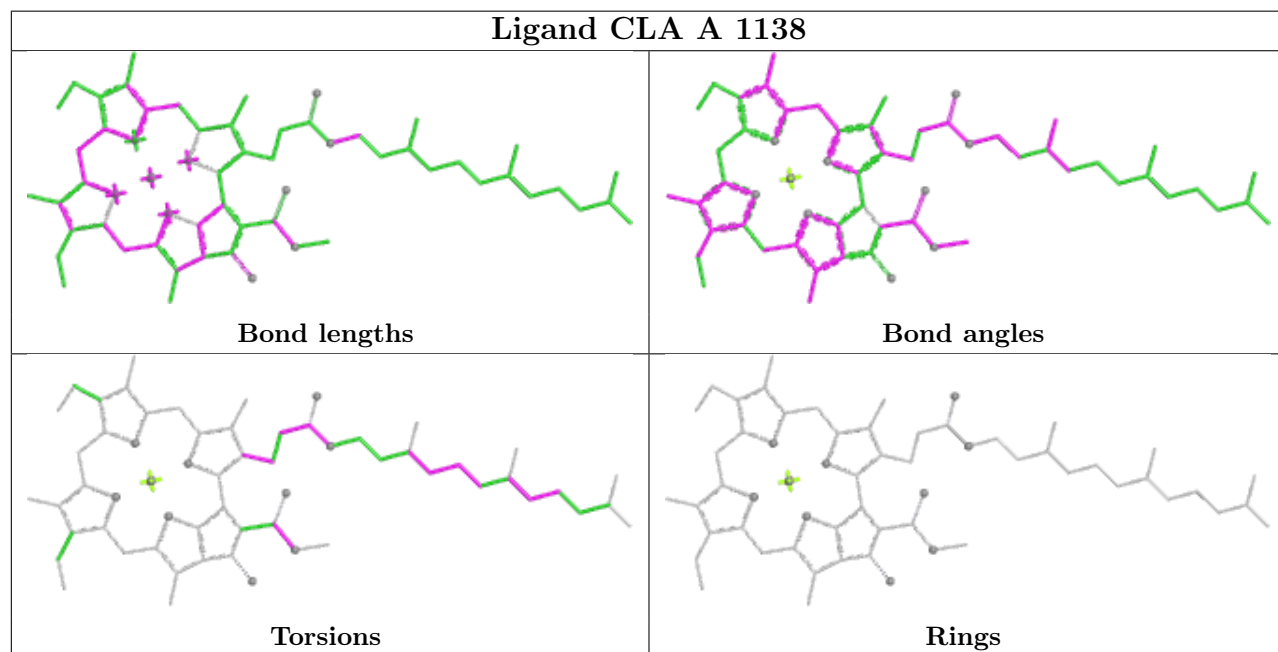
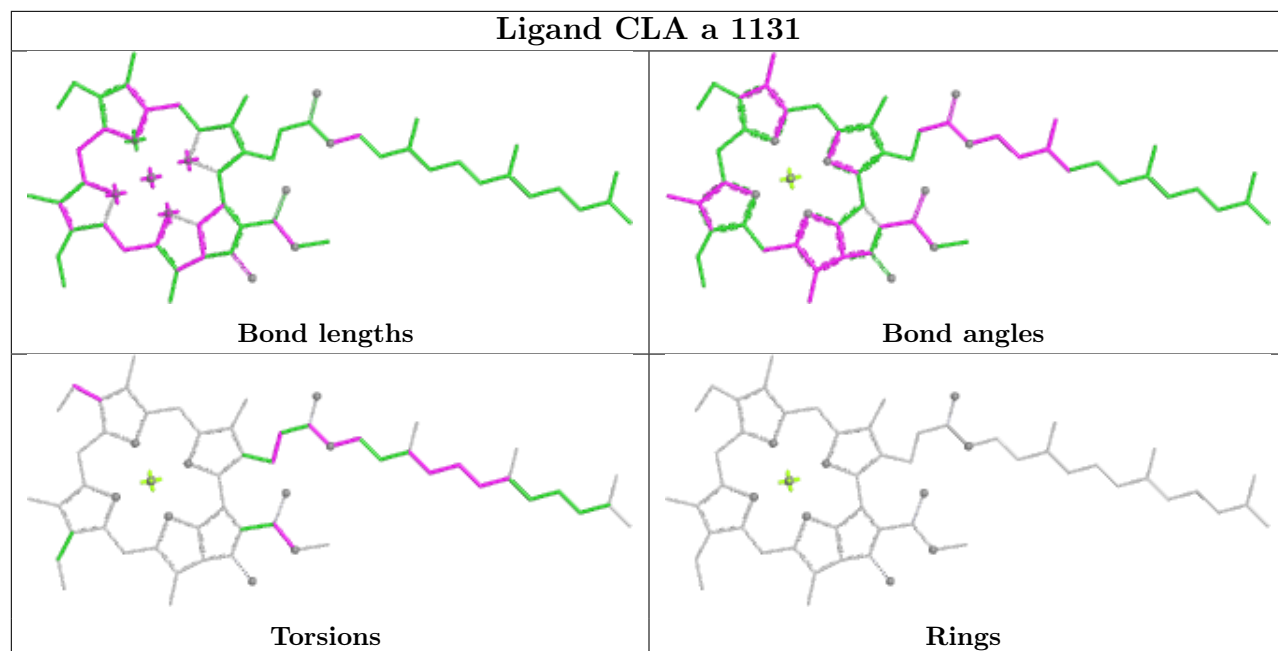


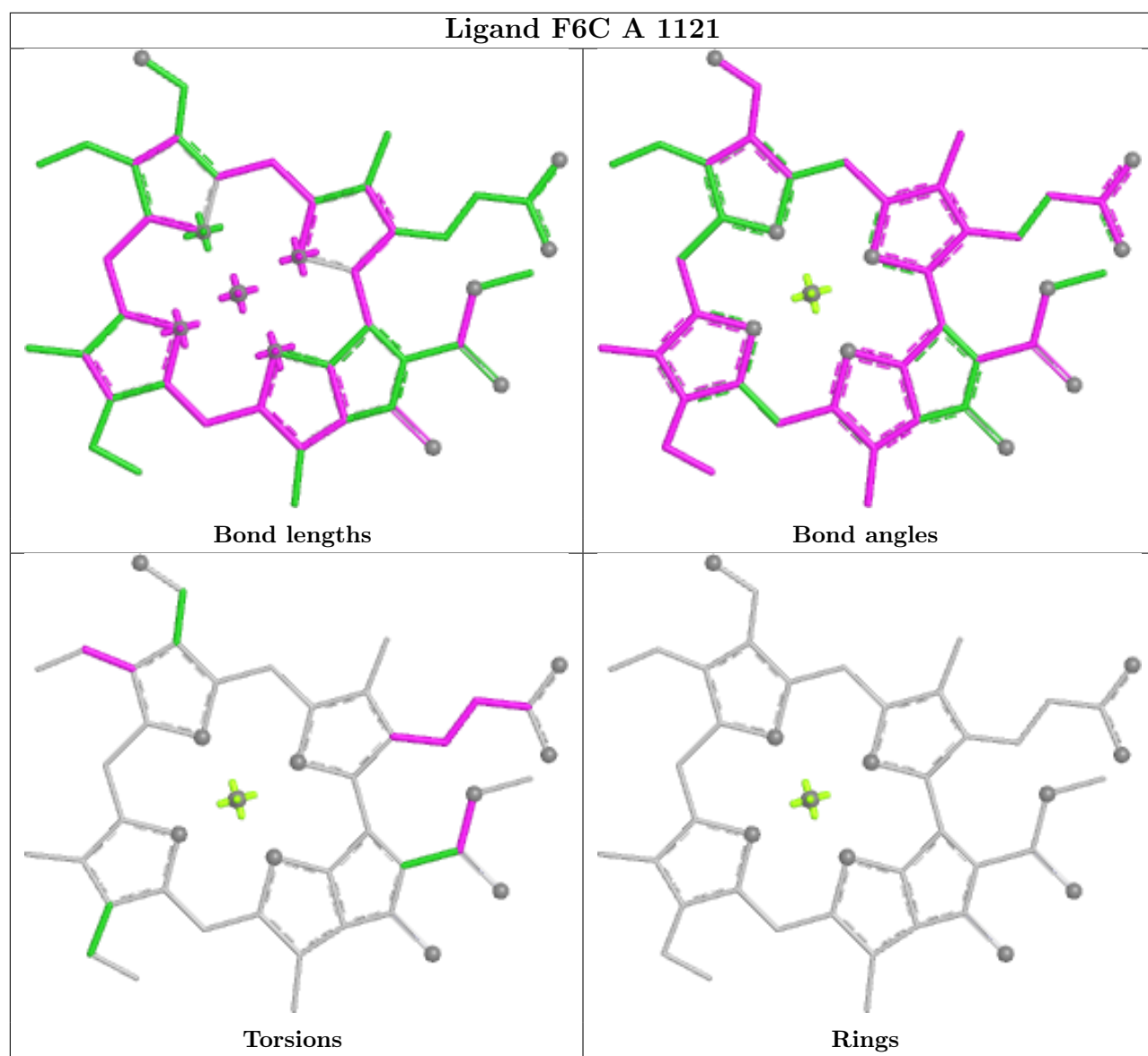


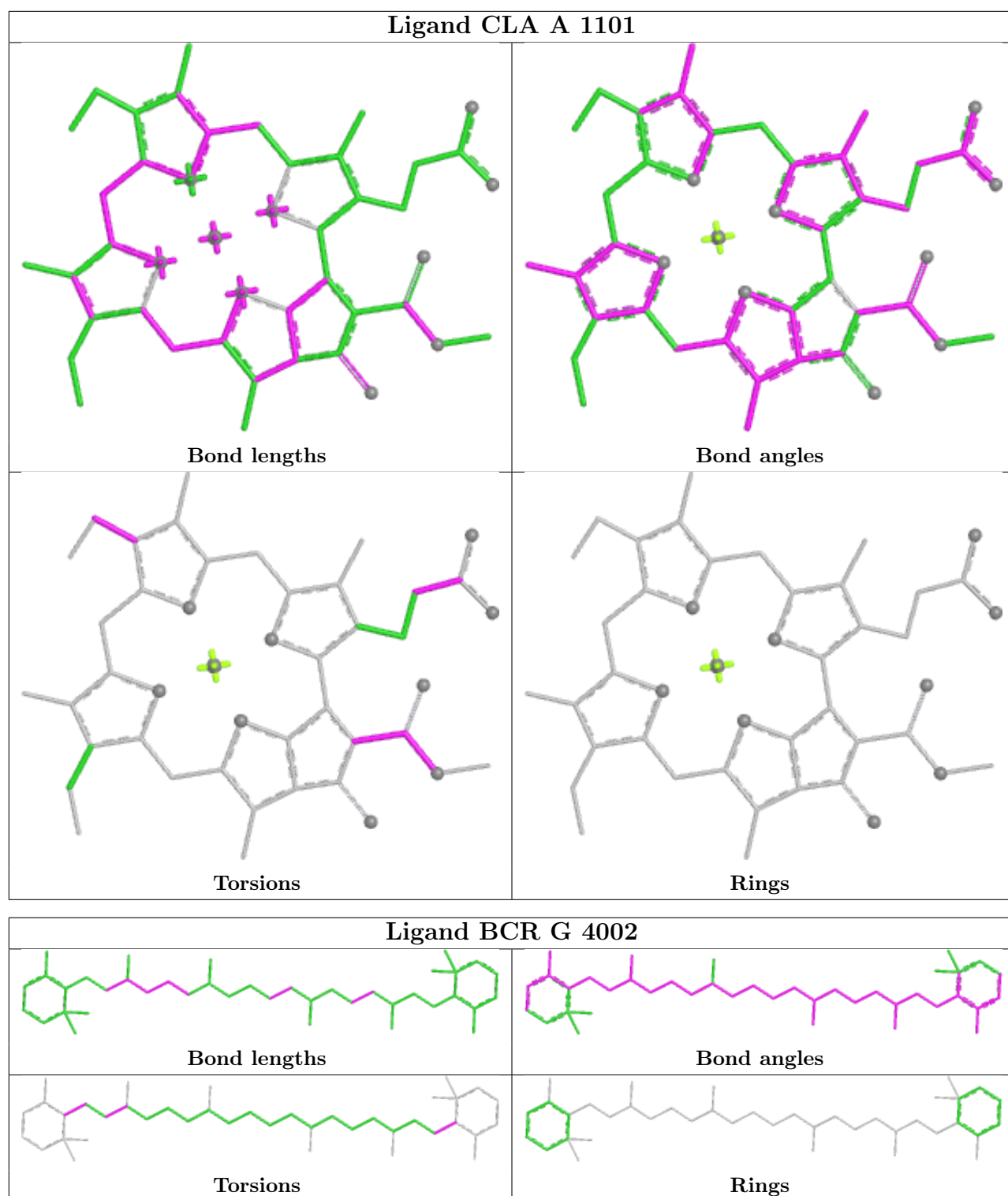


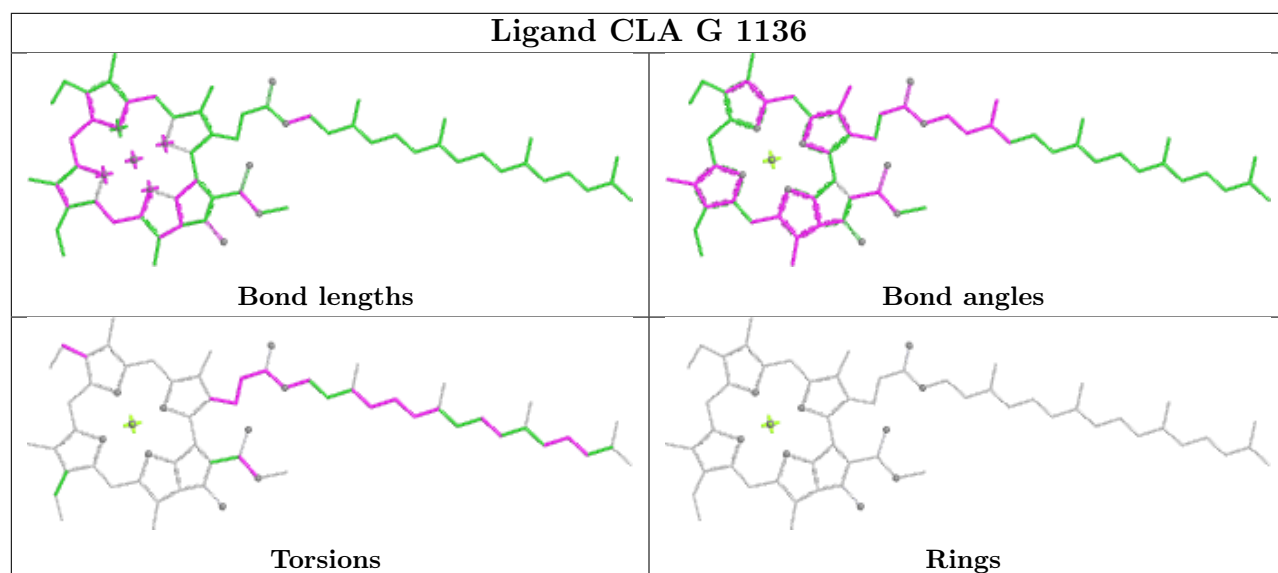
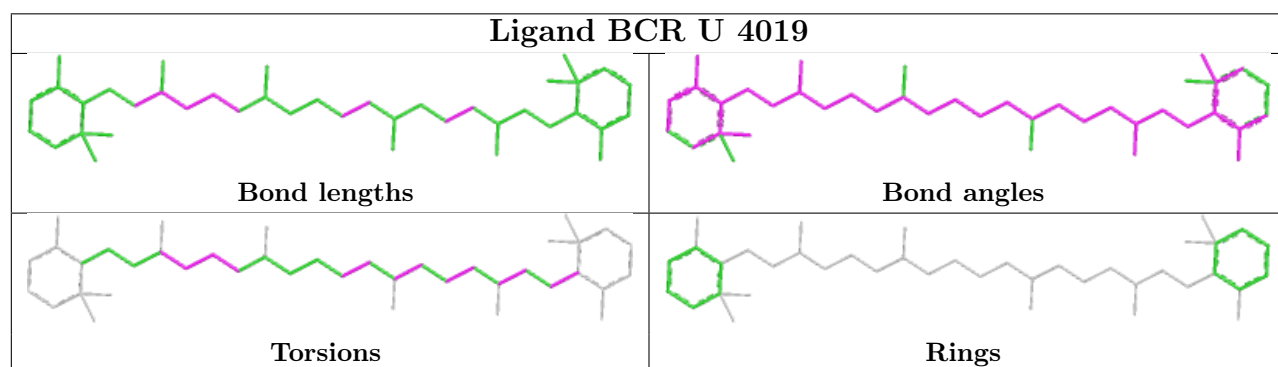
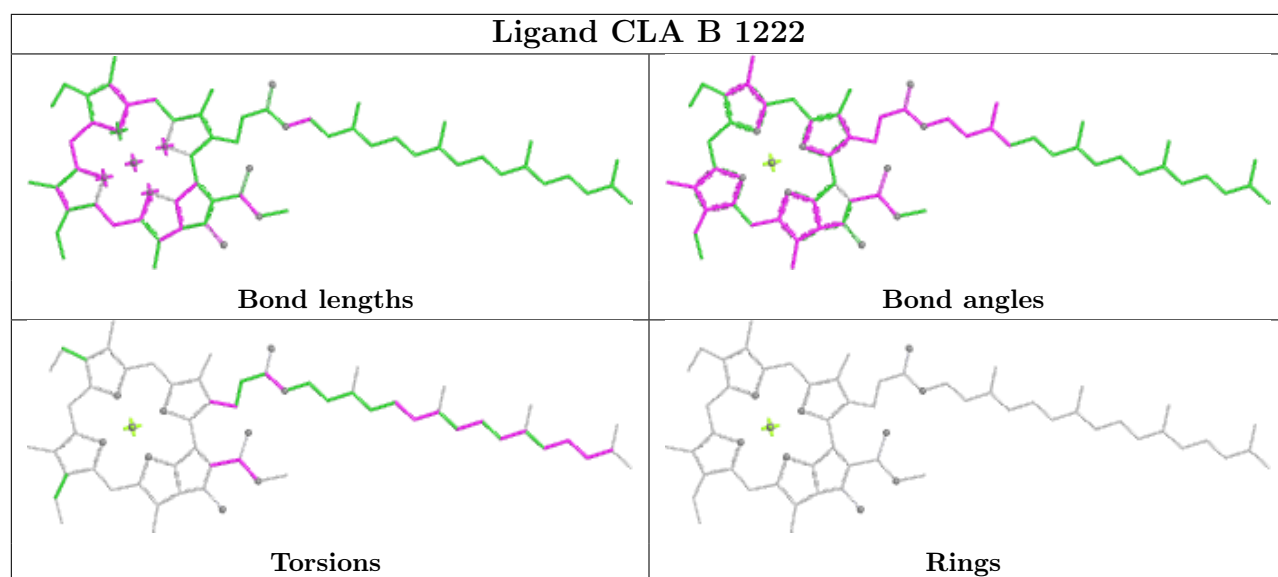


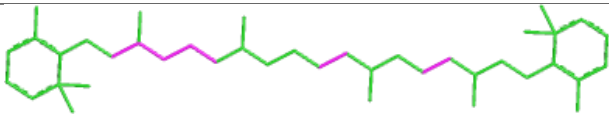
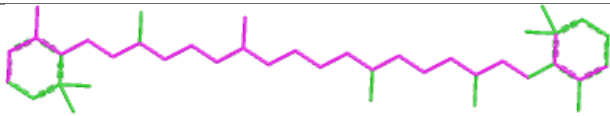
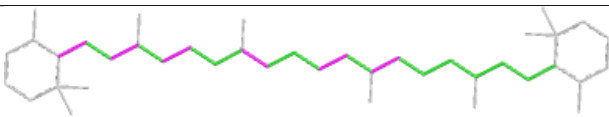
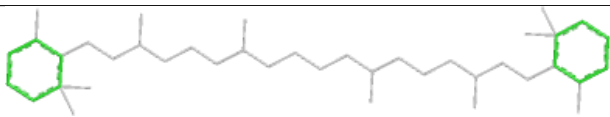


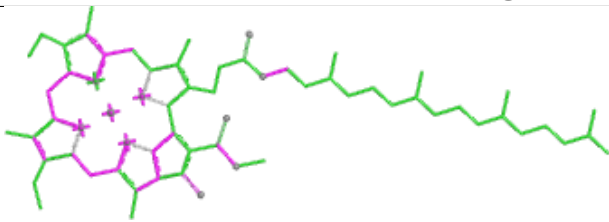
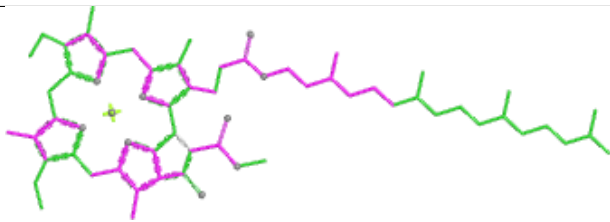
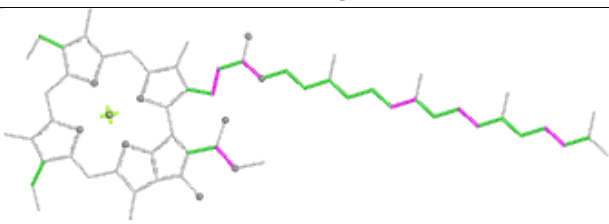
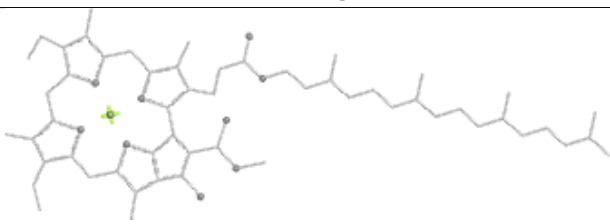


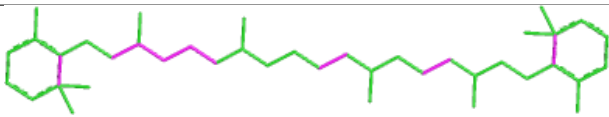
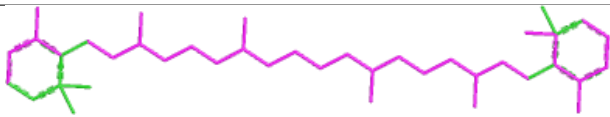
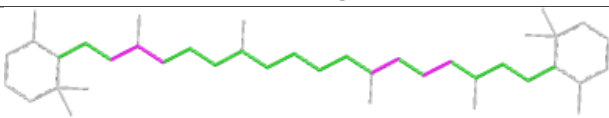
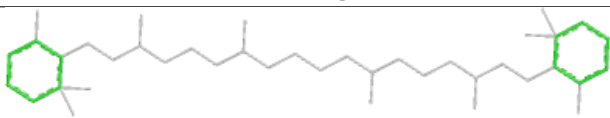


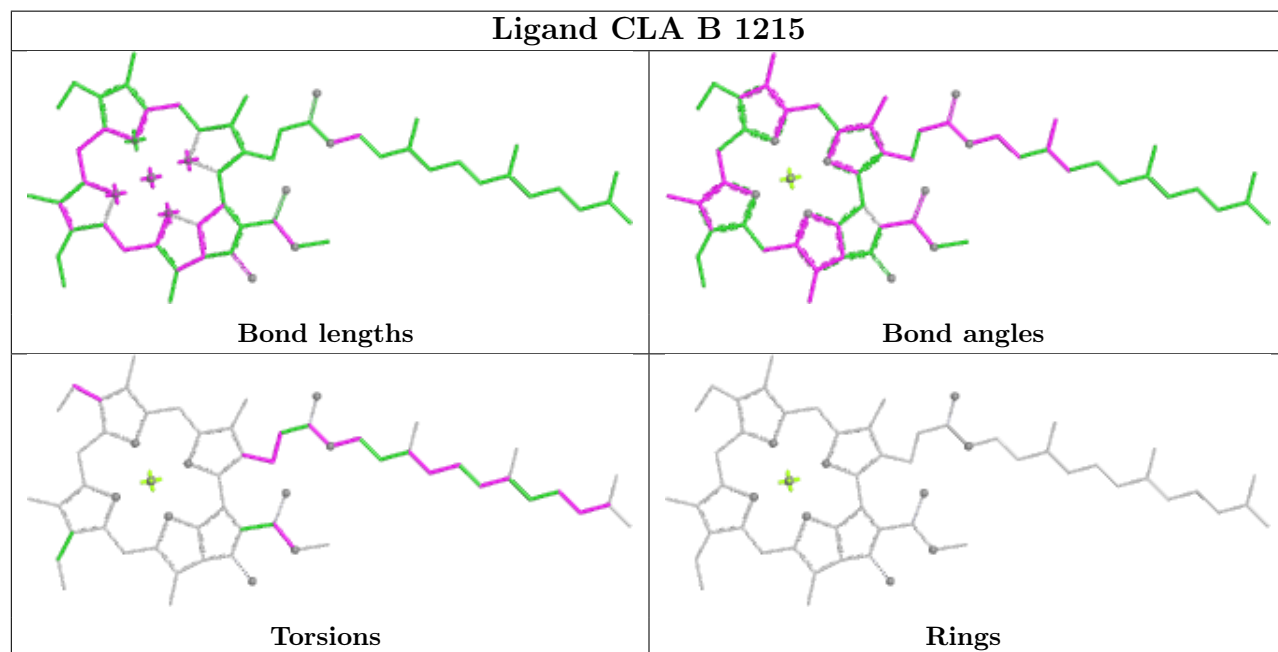
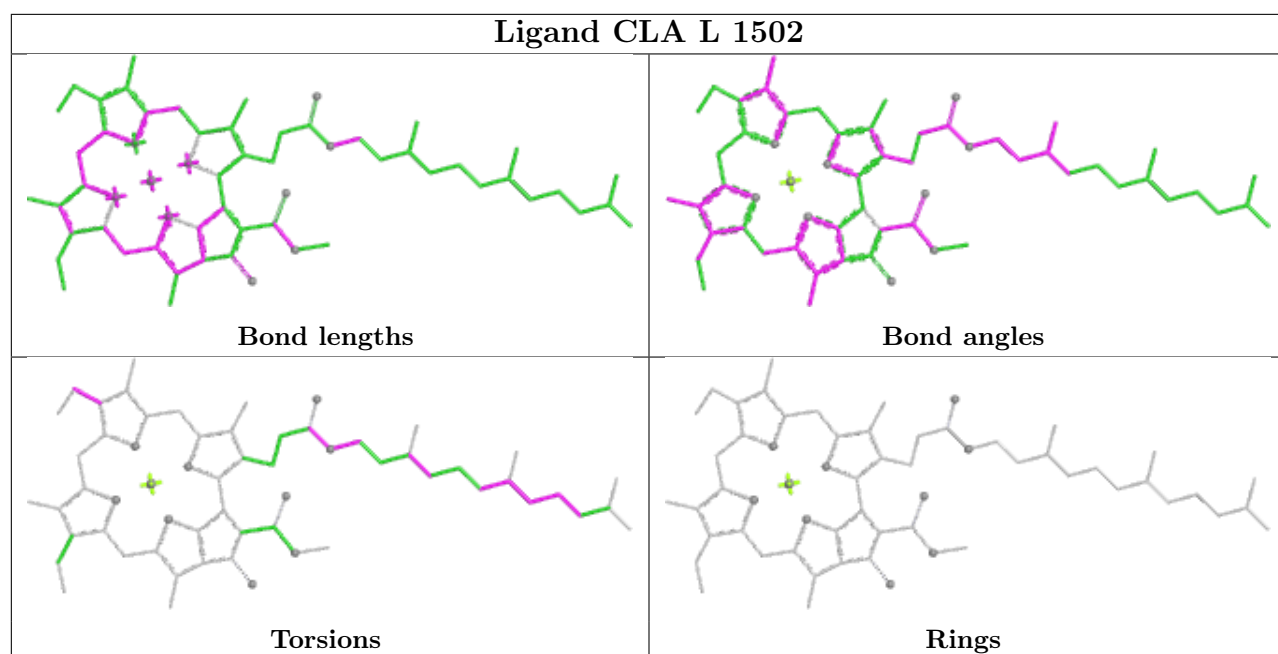




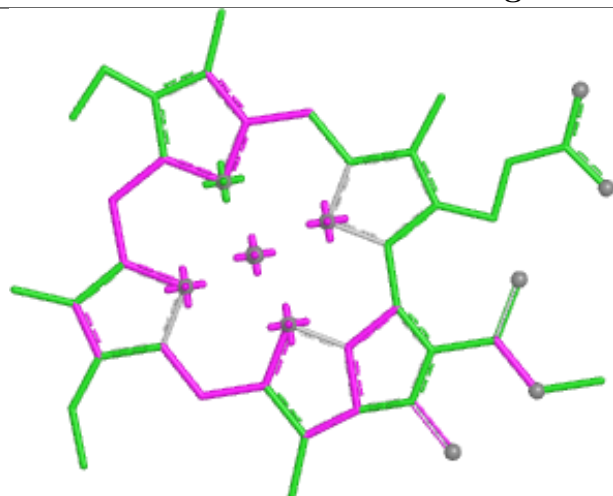
Ligand BCR B 4016	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1104	
	
Bond lengths	Bond angles
	
Torsions	Rings

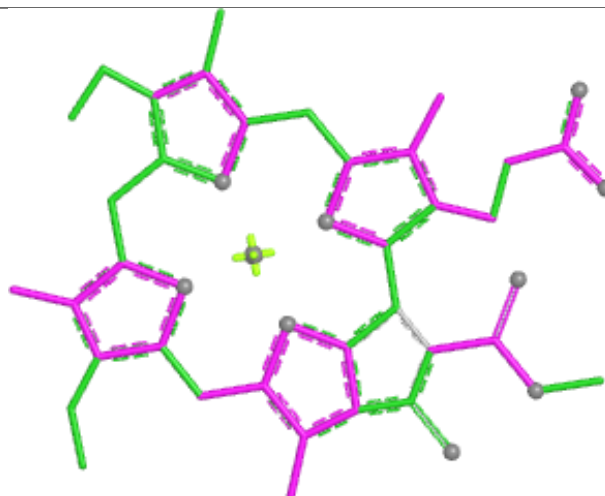
Ligand BCR b 4014	
	
Bond lengths	Bond angles
	
Torsions	Rings



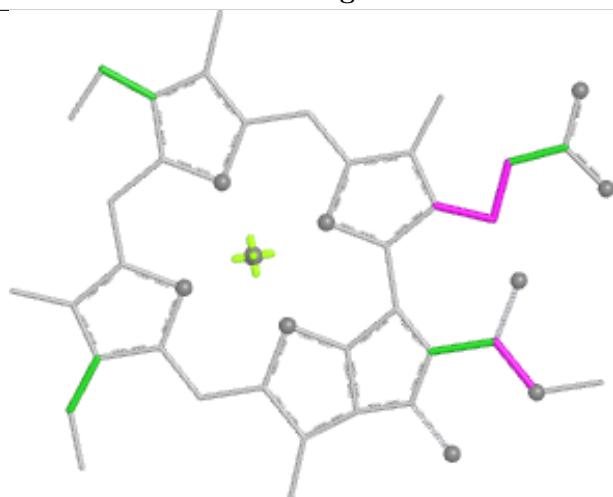
Ligand CLA H 1212



Bond lengths



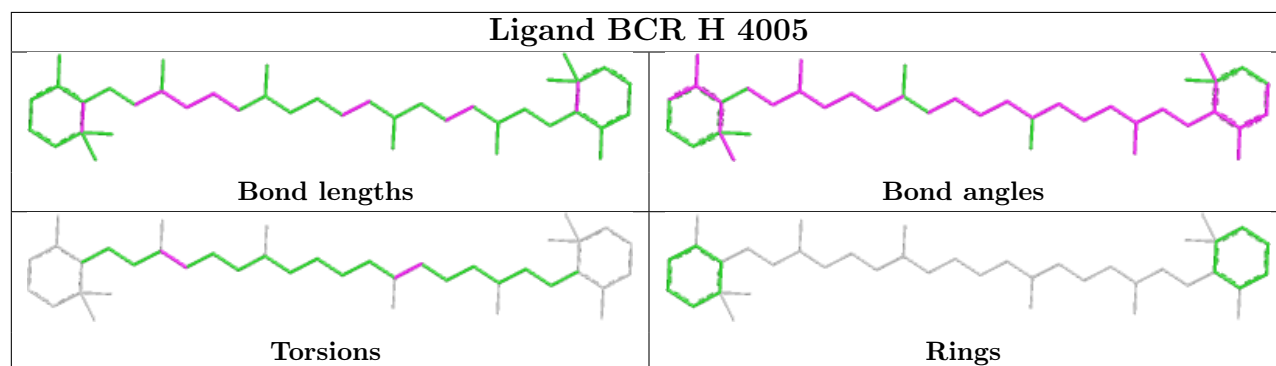
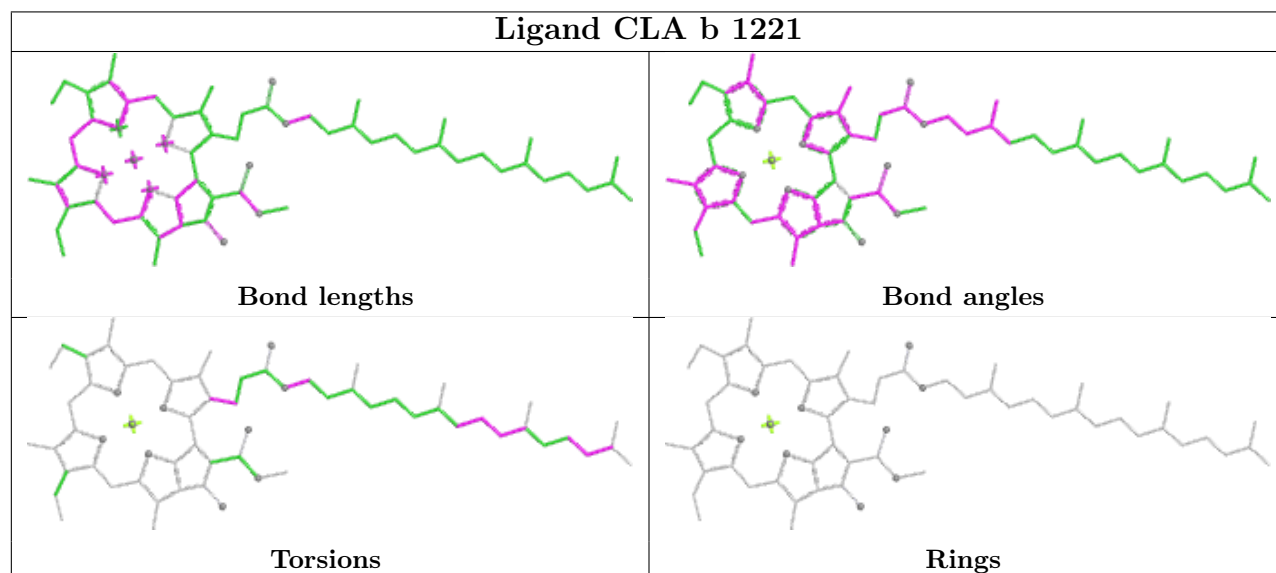
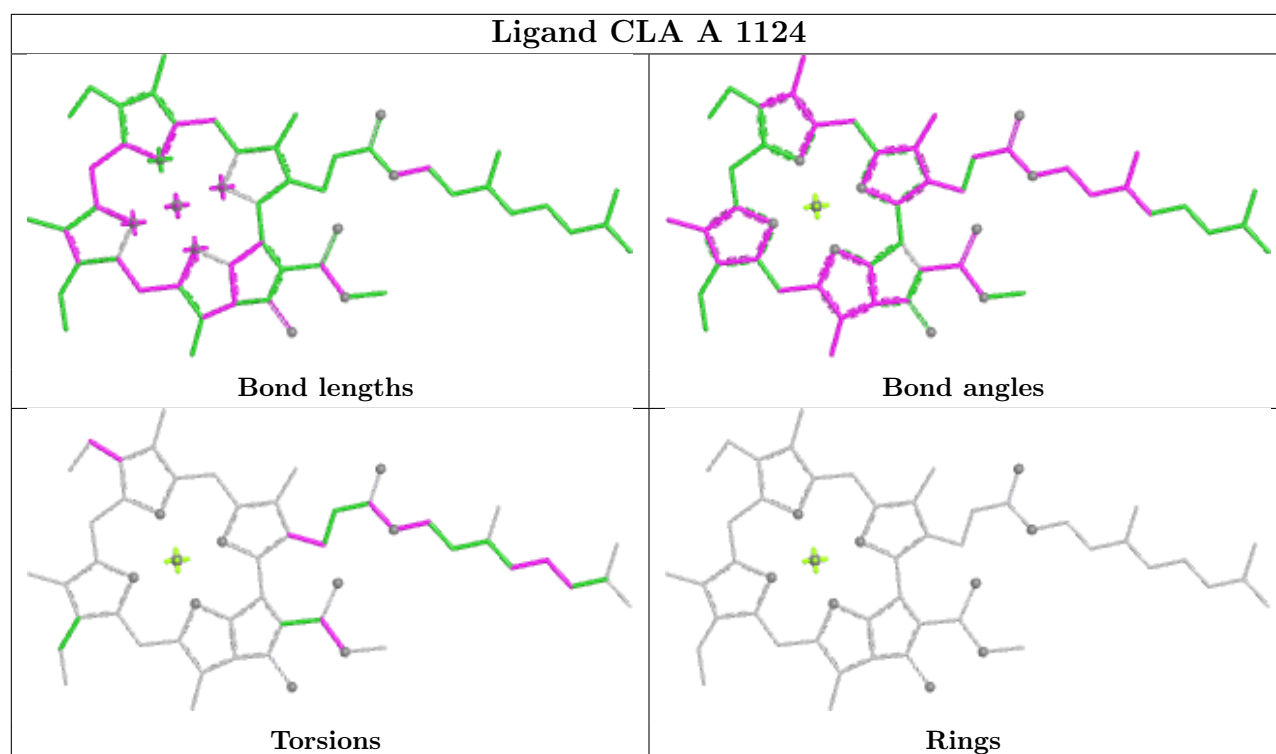
Bond angles

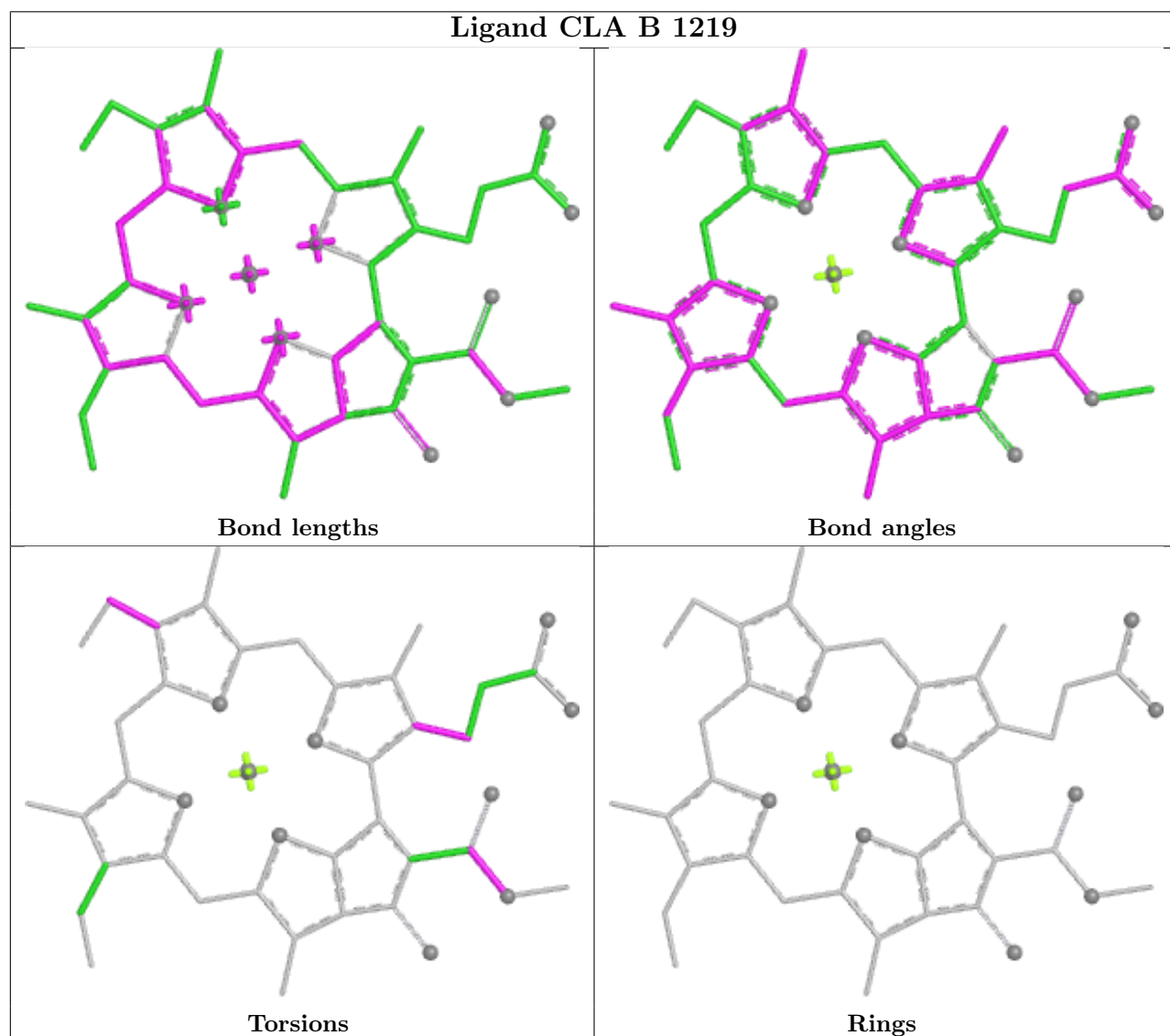
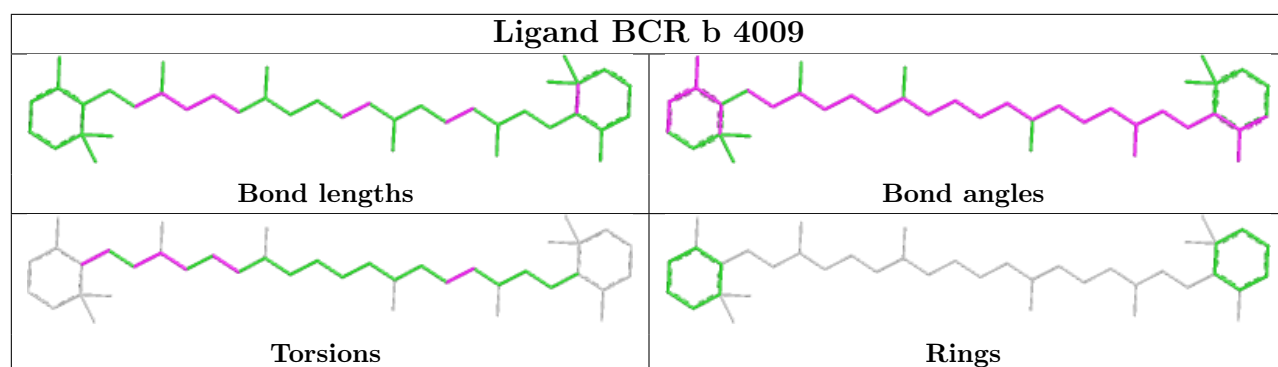


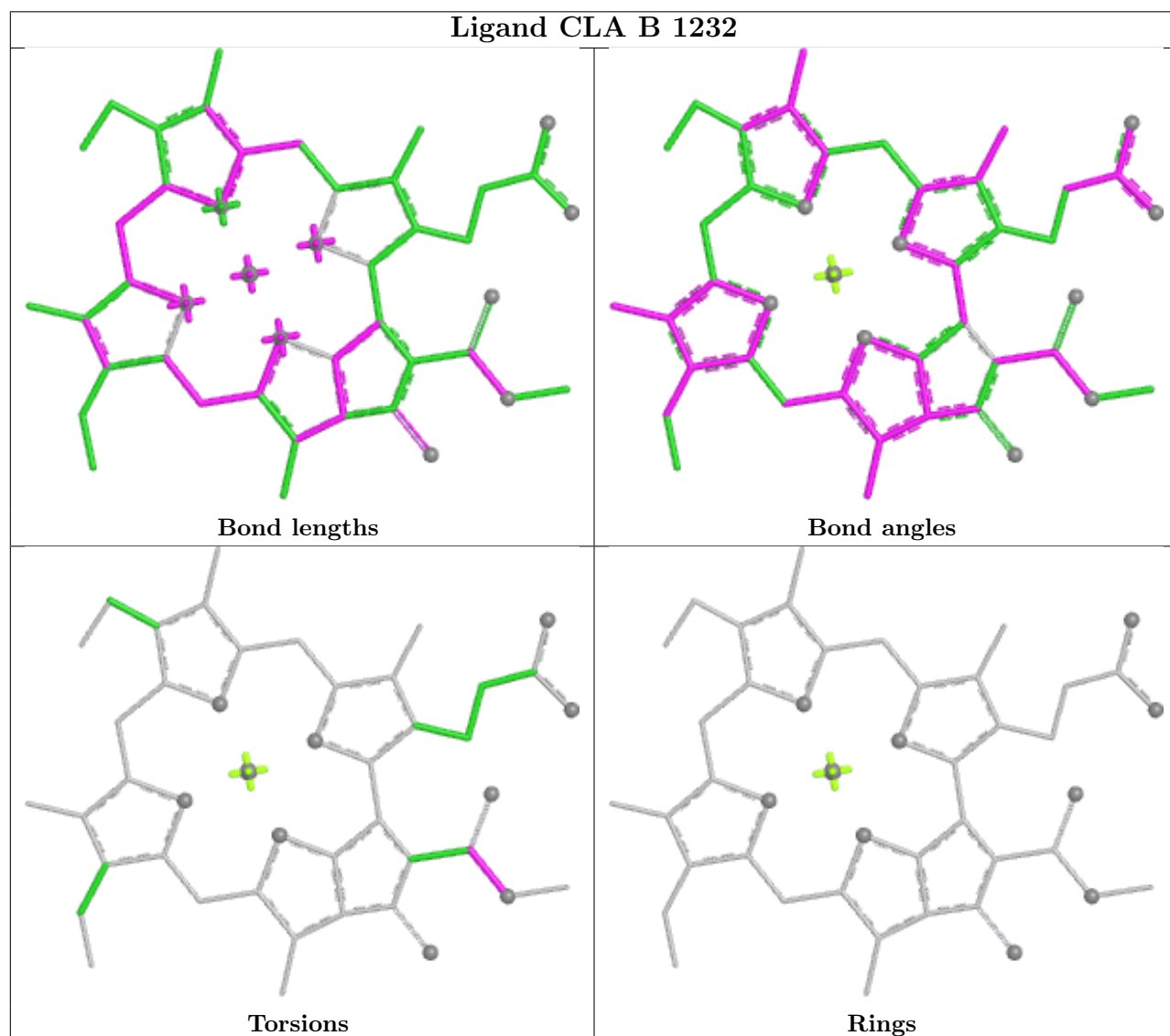
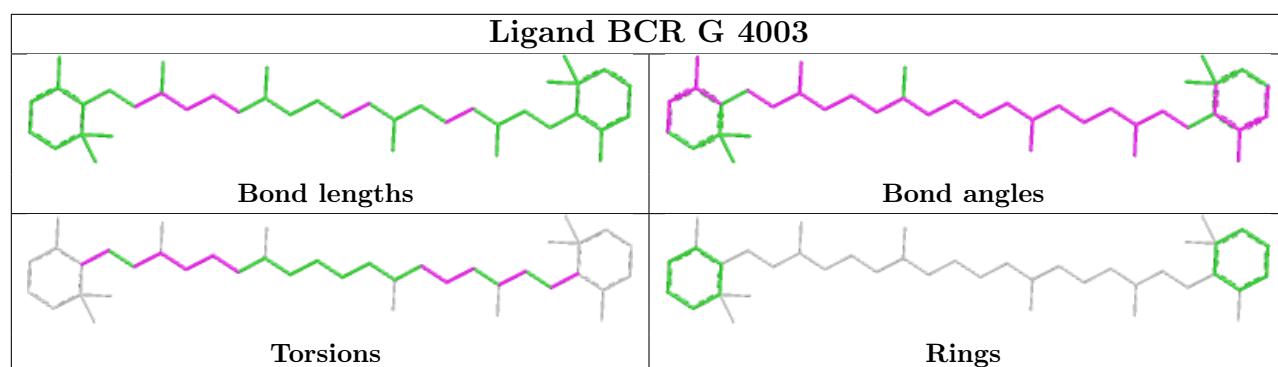
Torsions

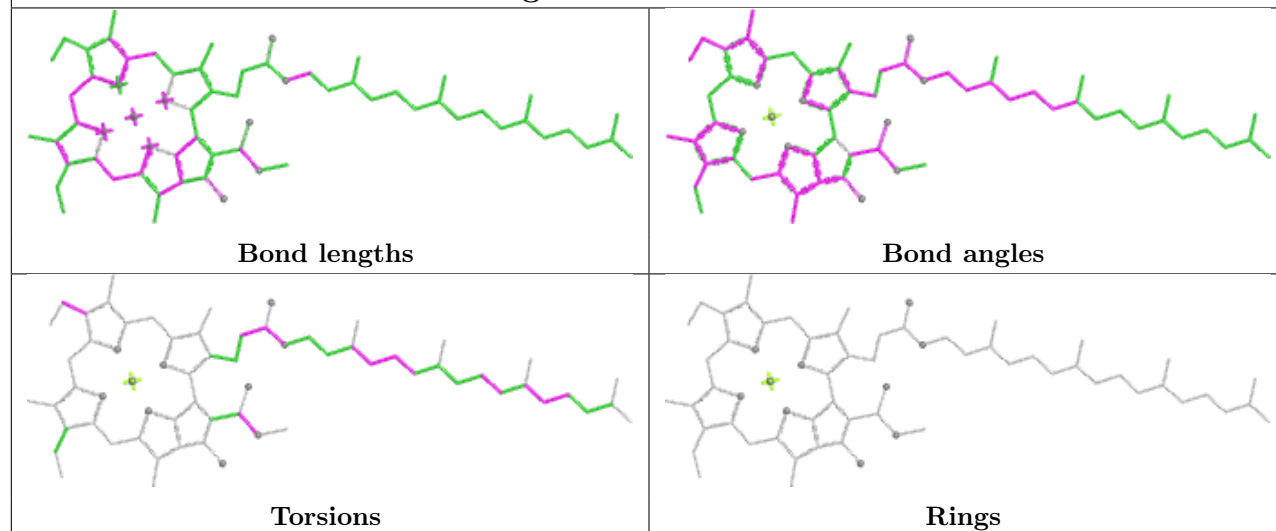
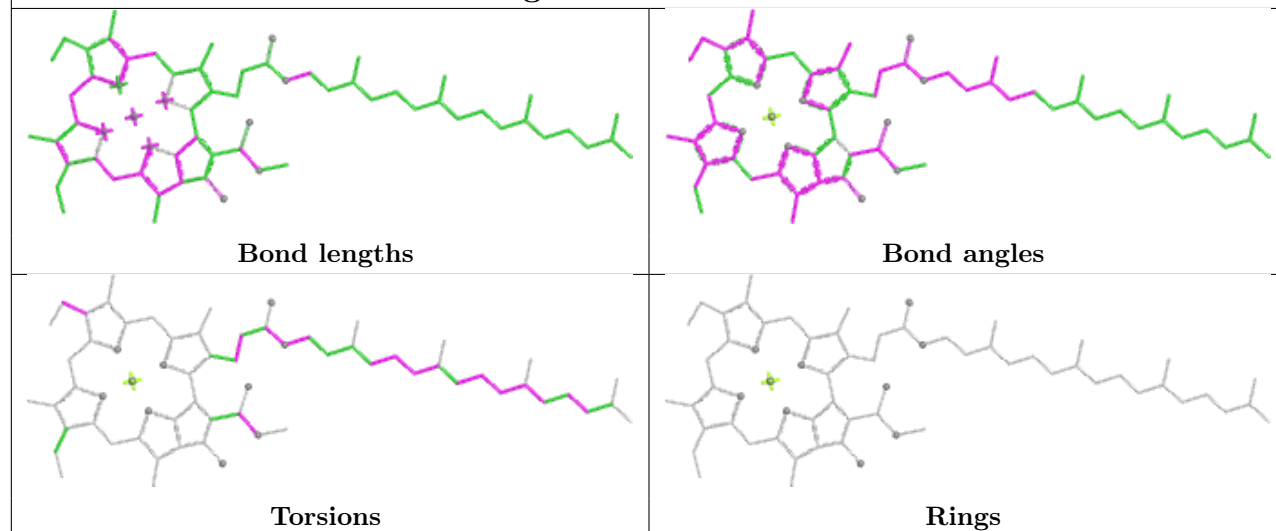
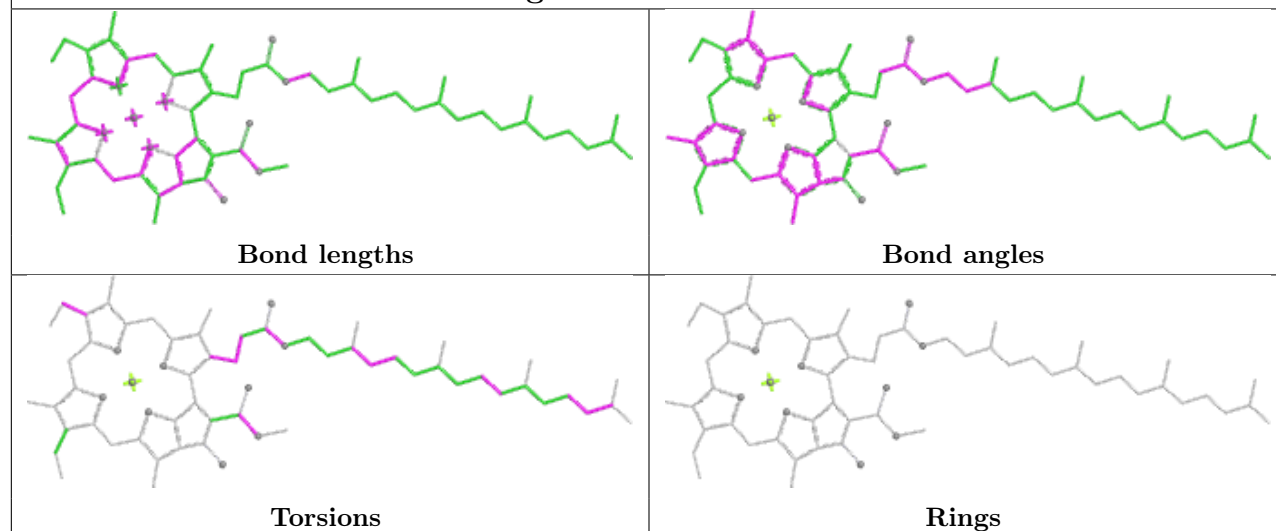


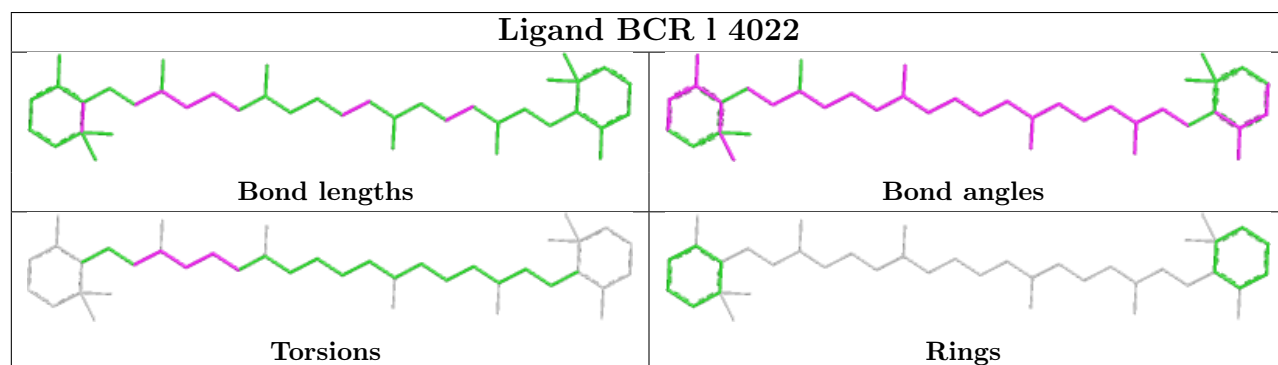
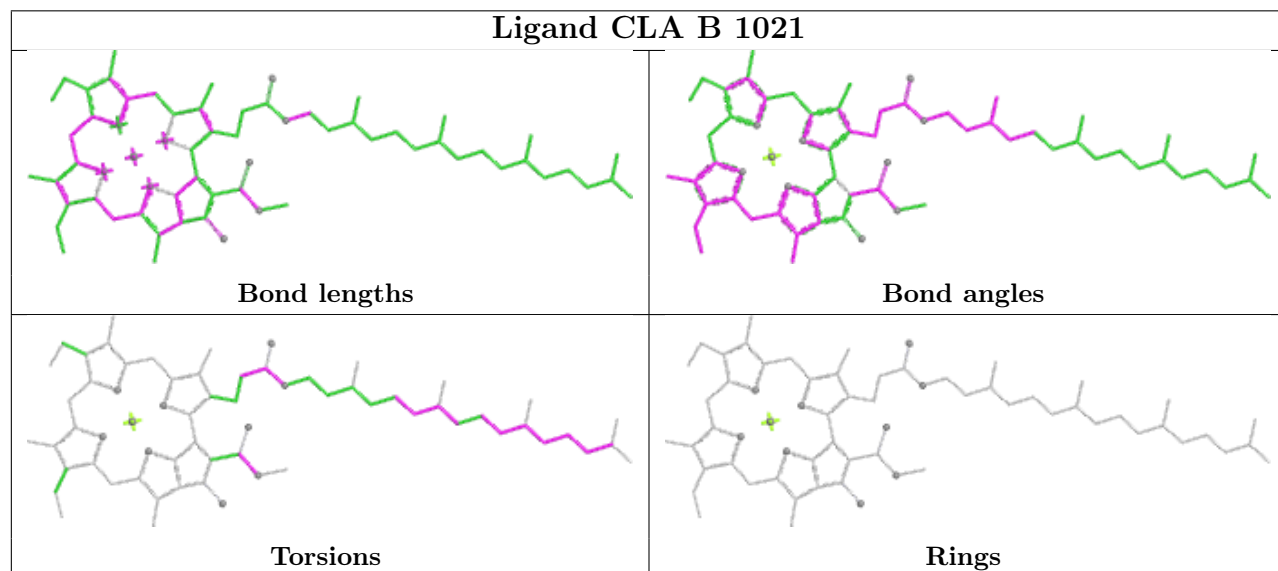
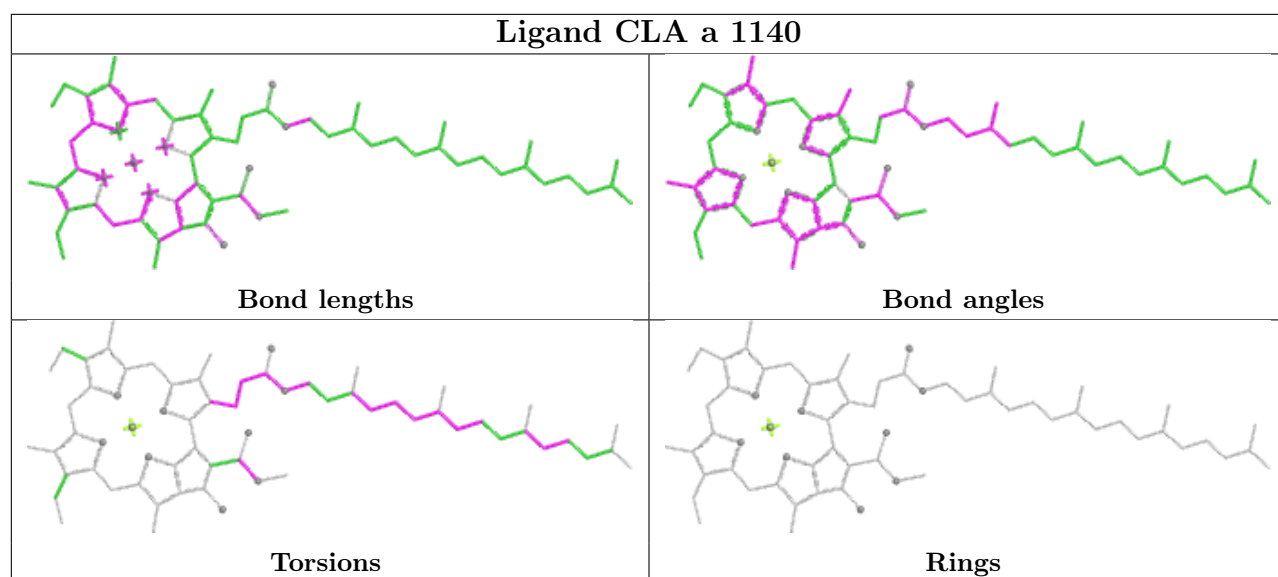
Rings

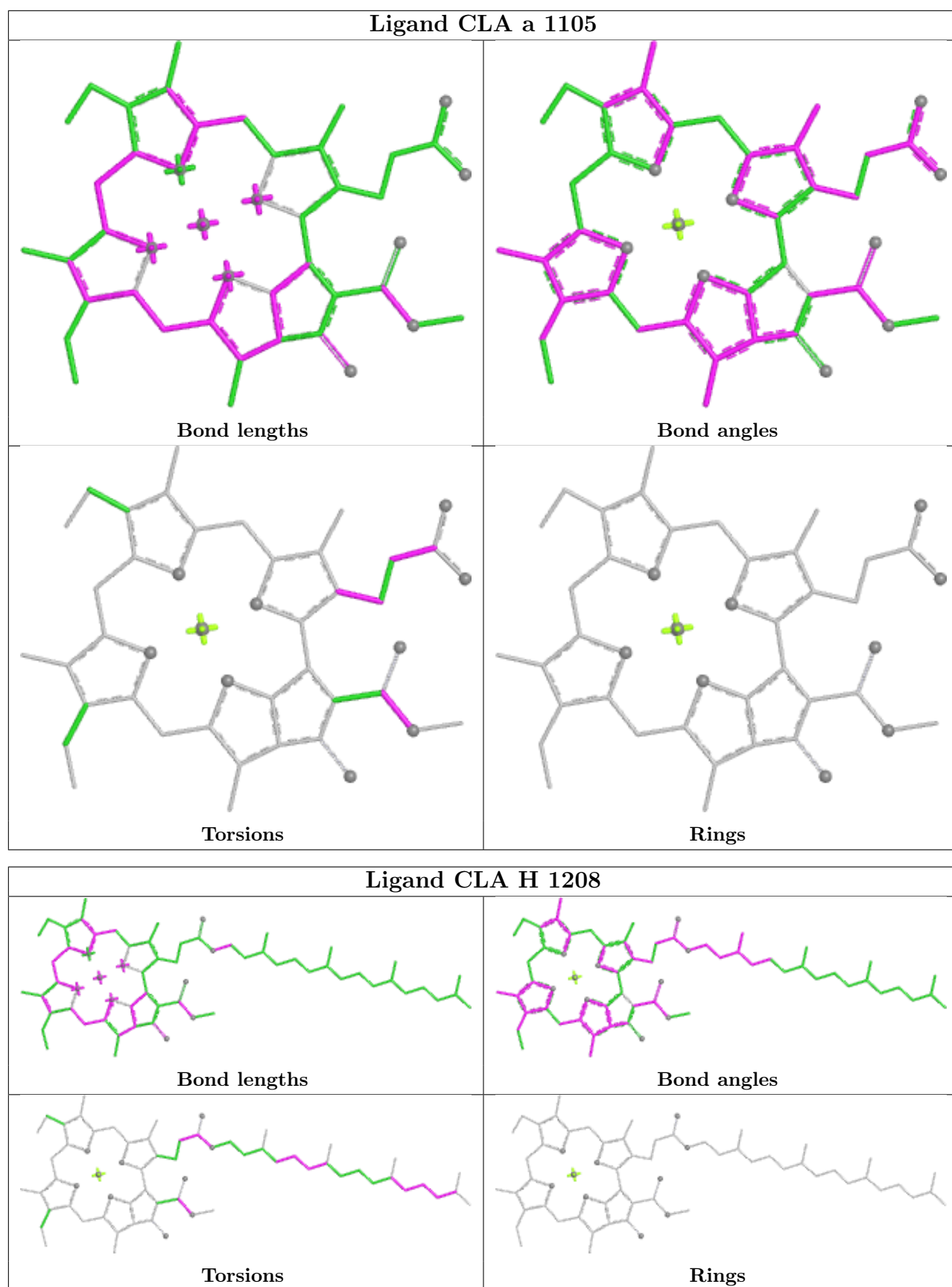


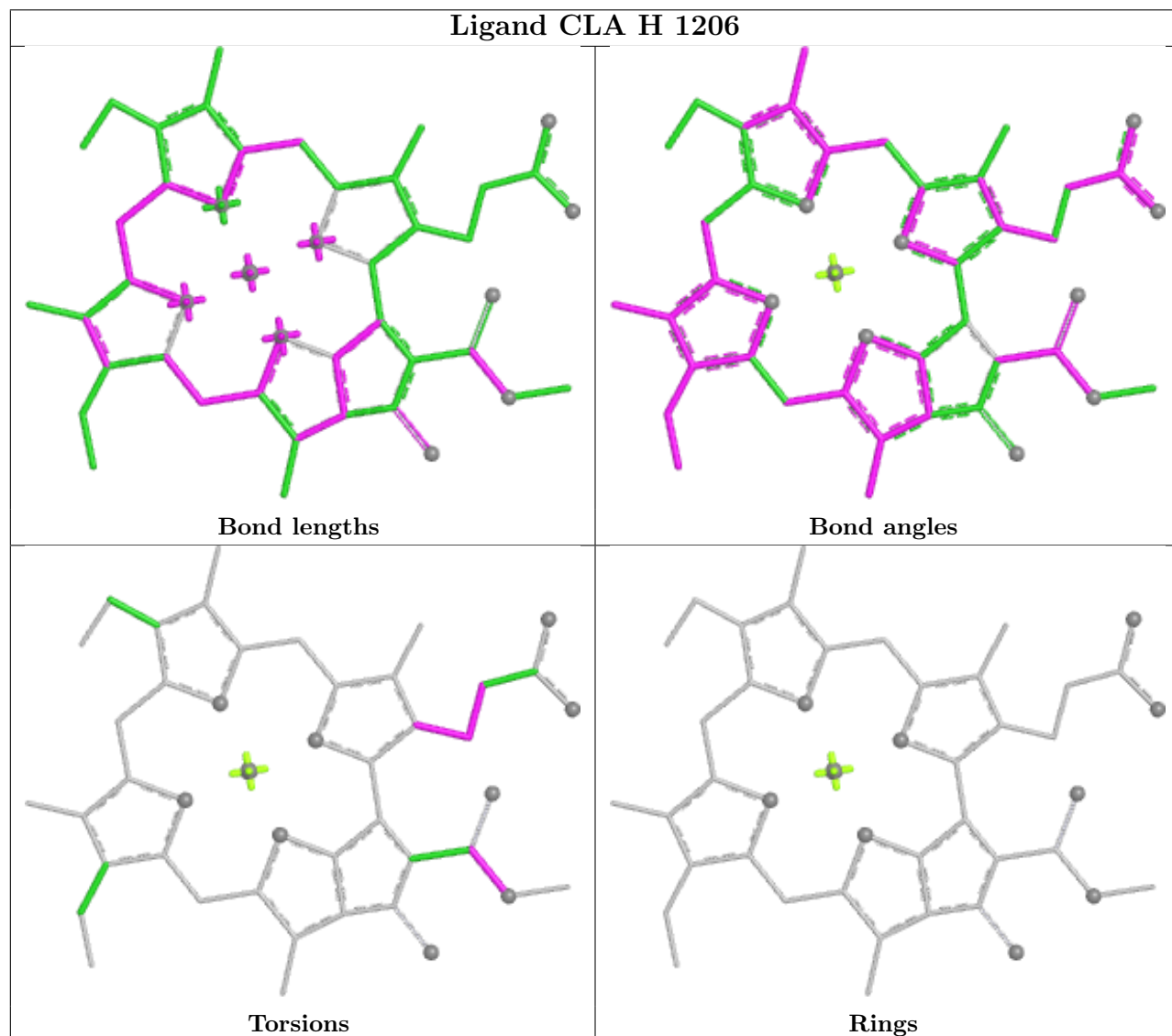
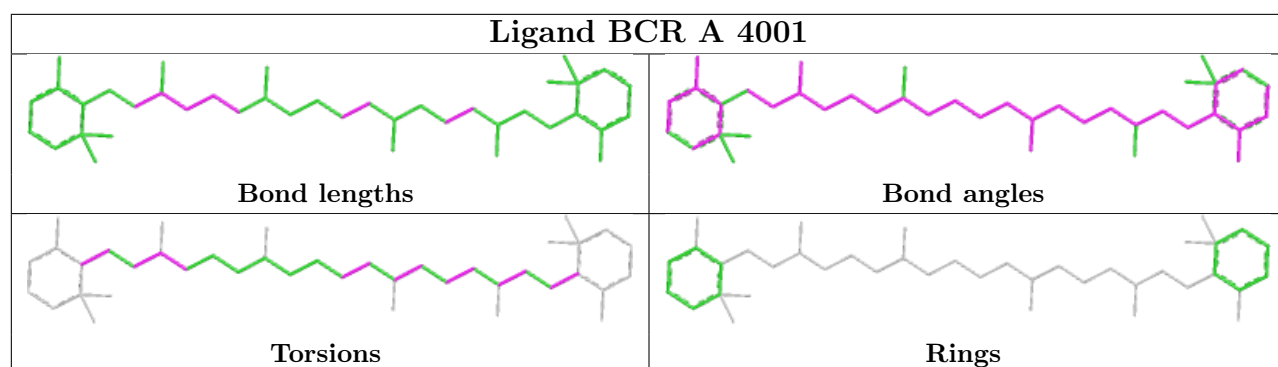


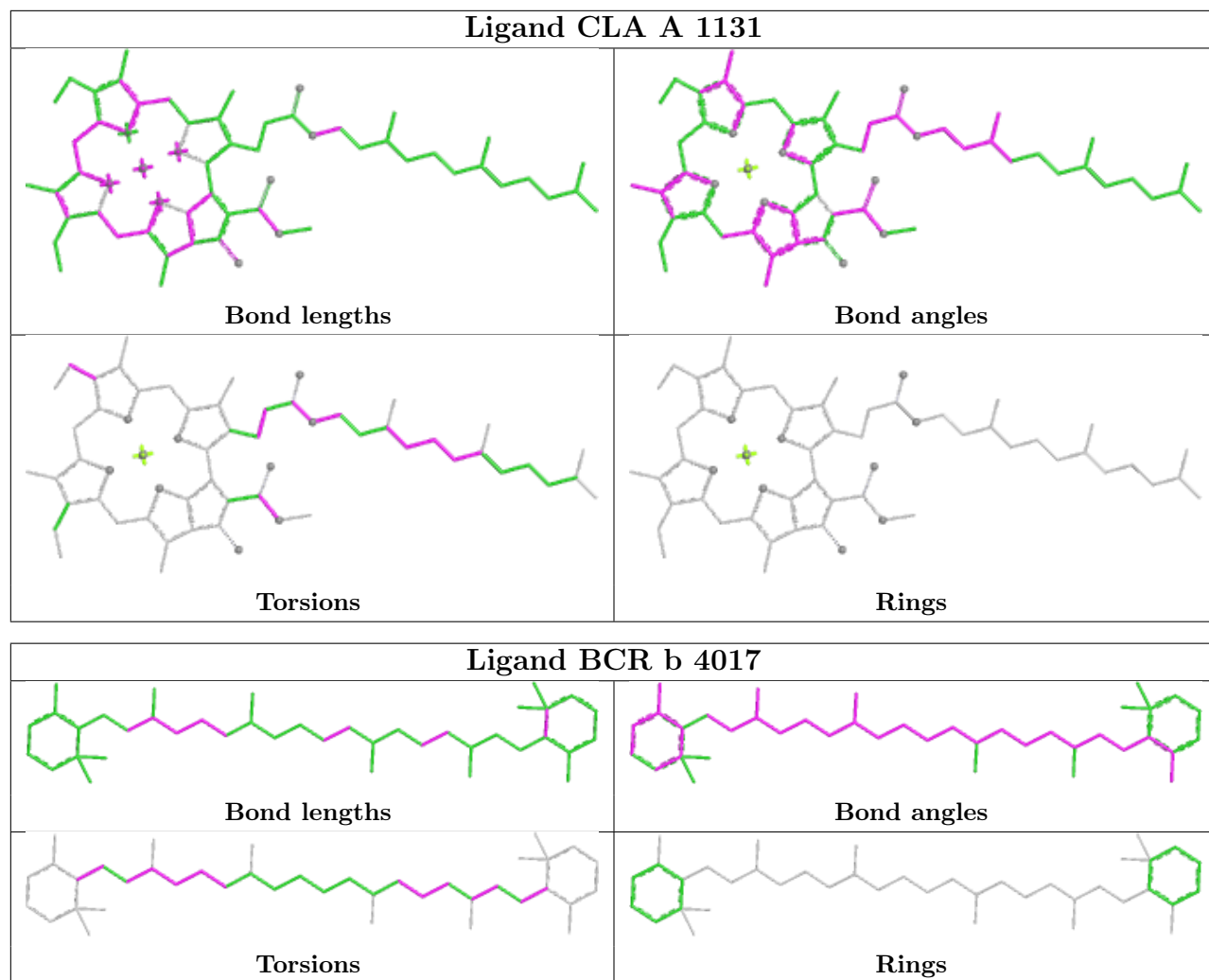


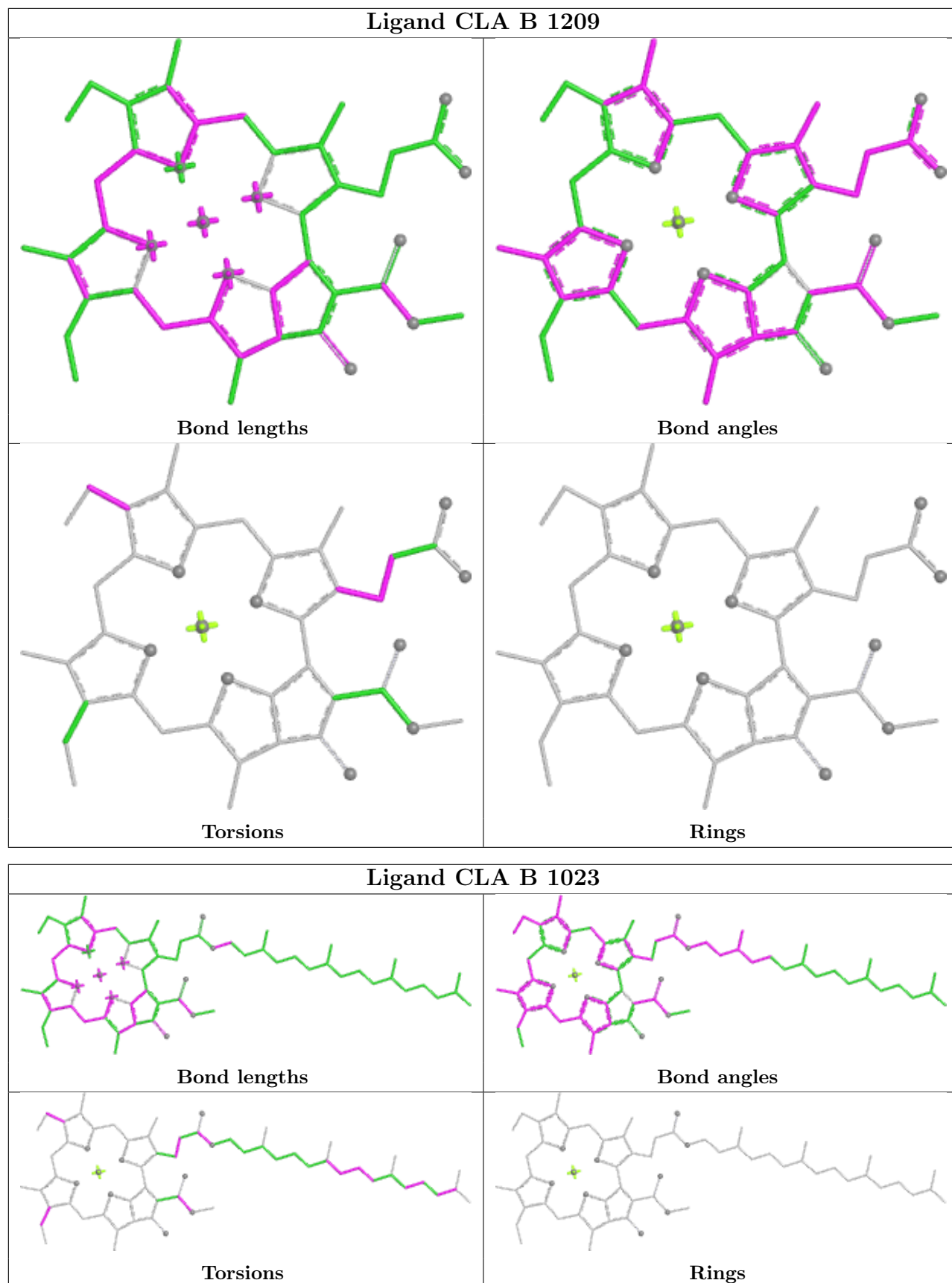
Ligand CLA H 1204**Ligand CLA B 1214****Ligand CLA b 1225**

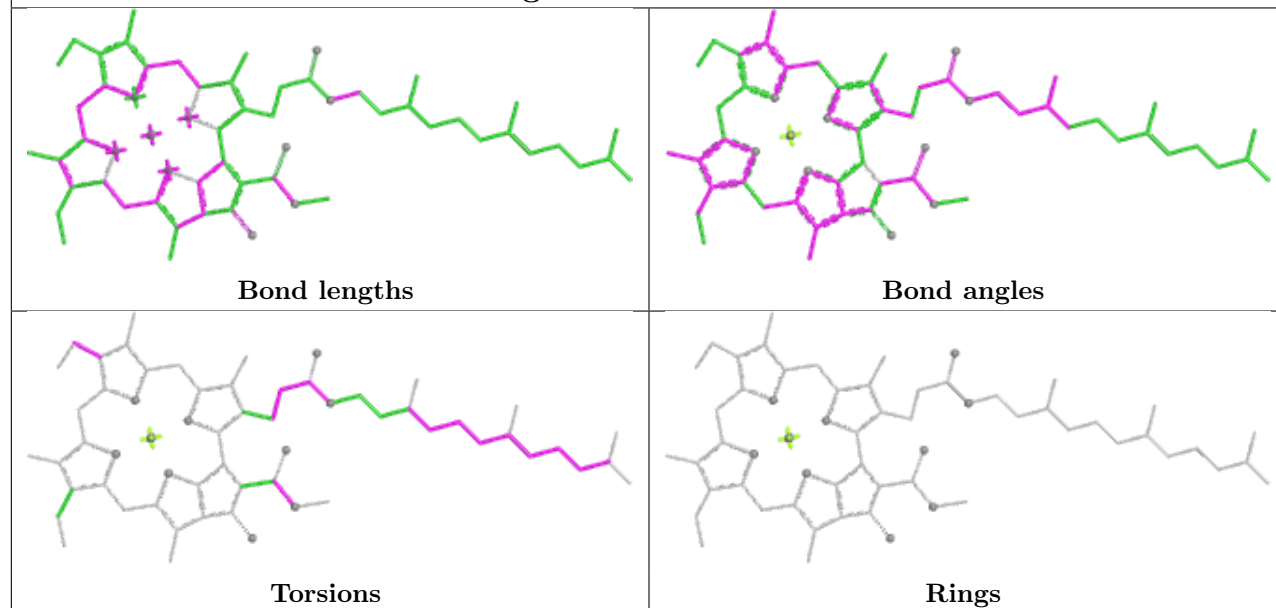
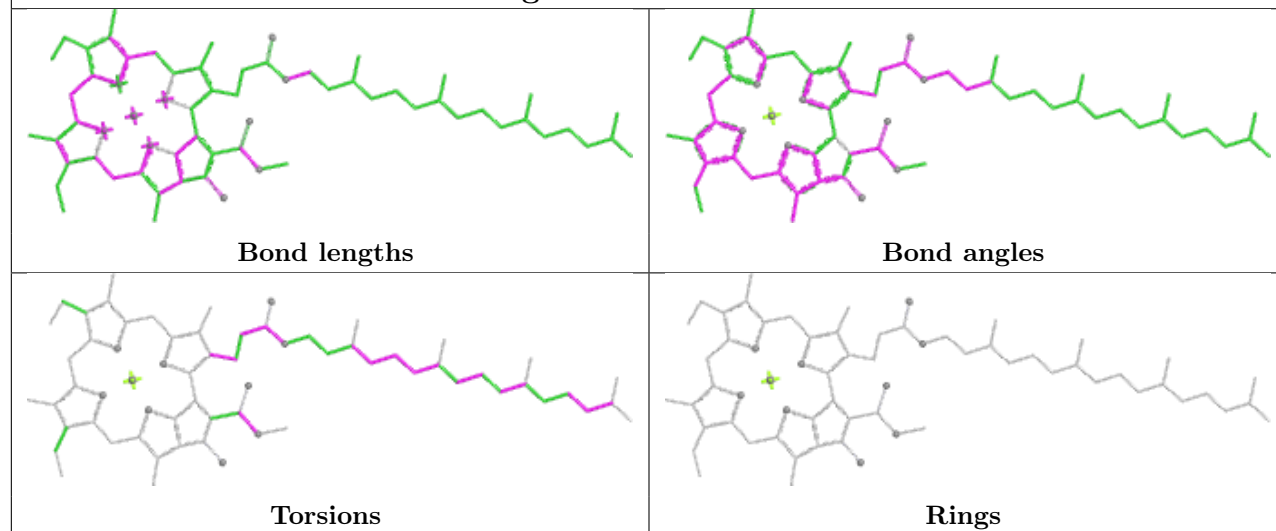


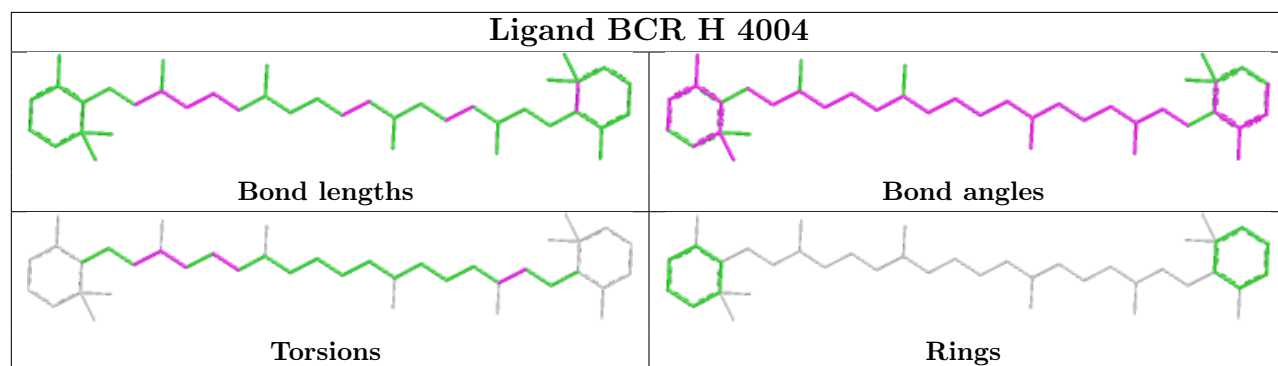
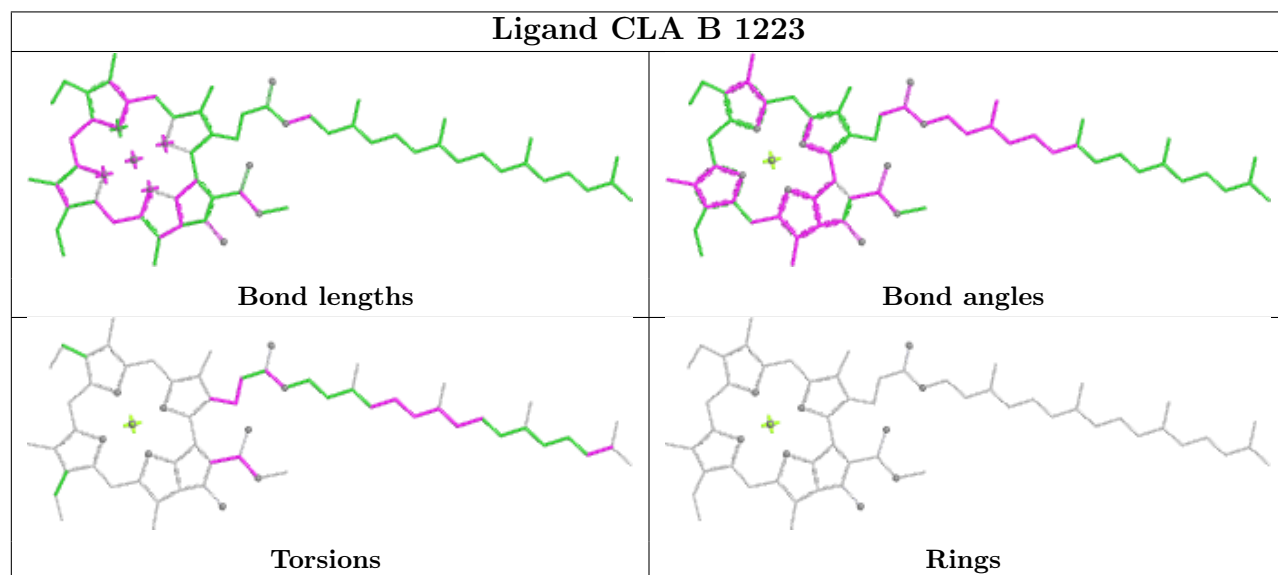
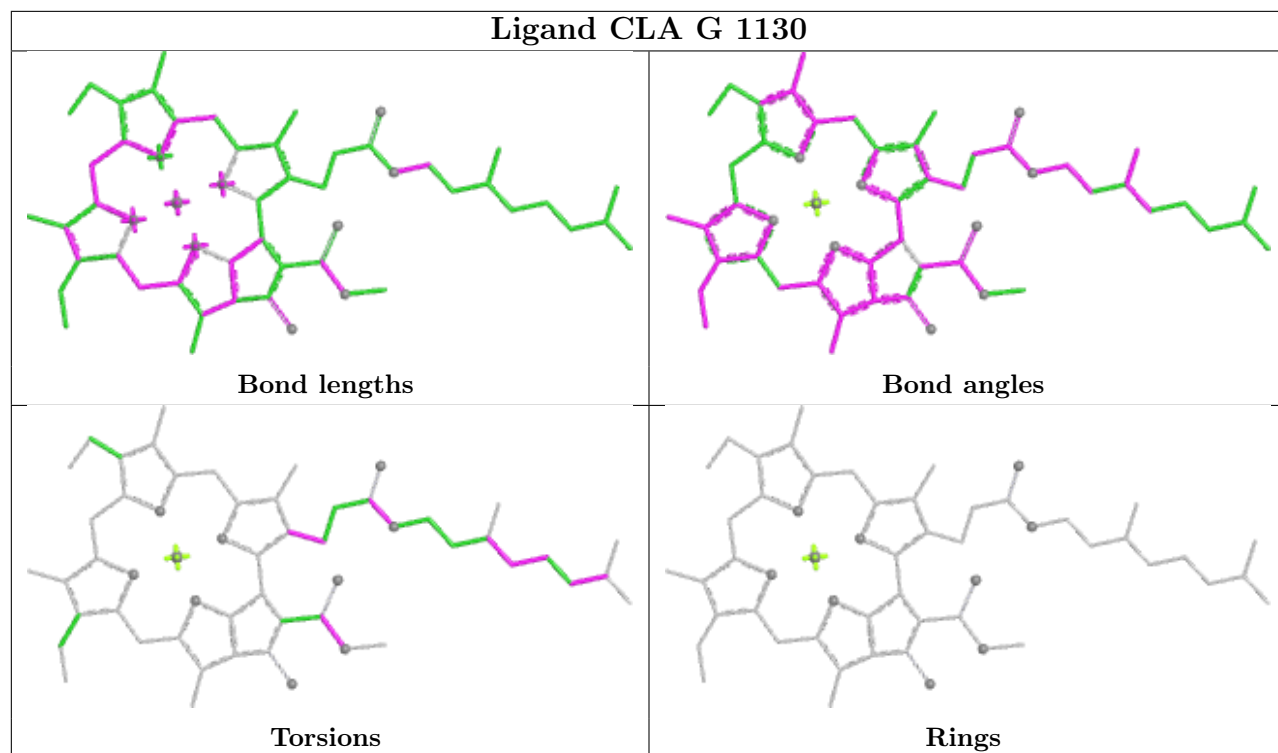


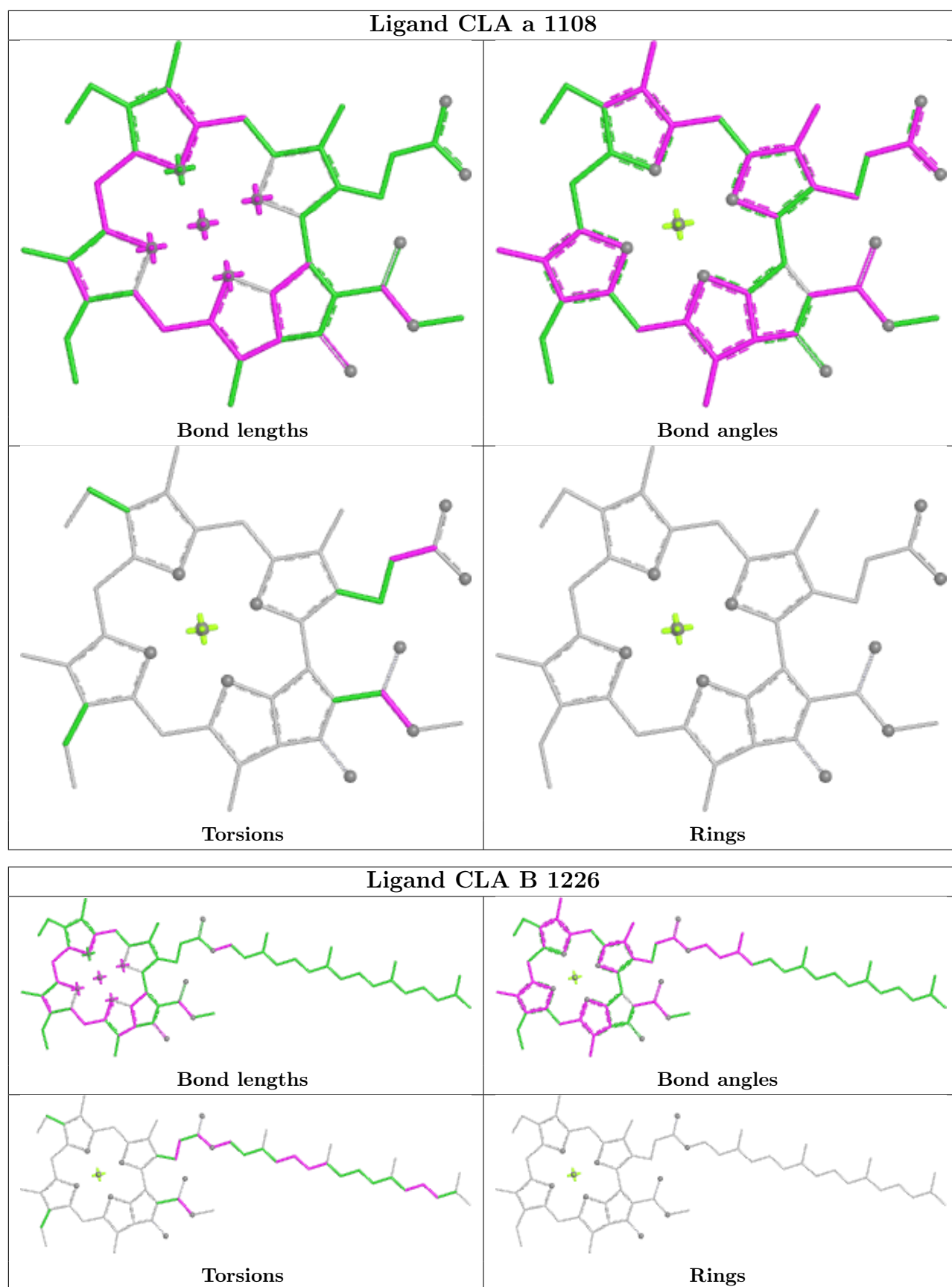


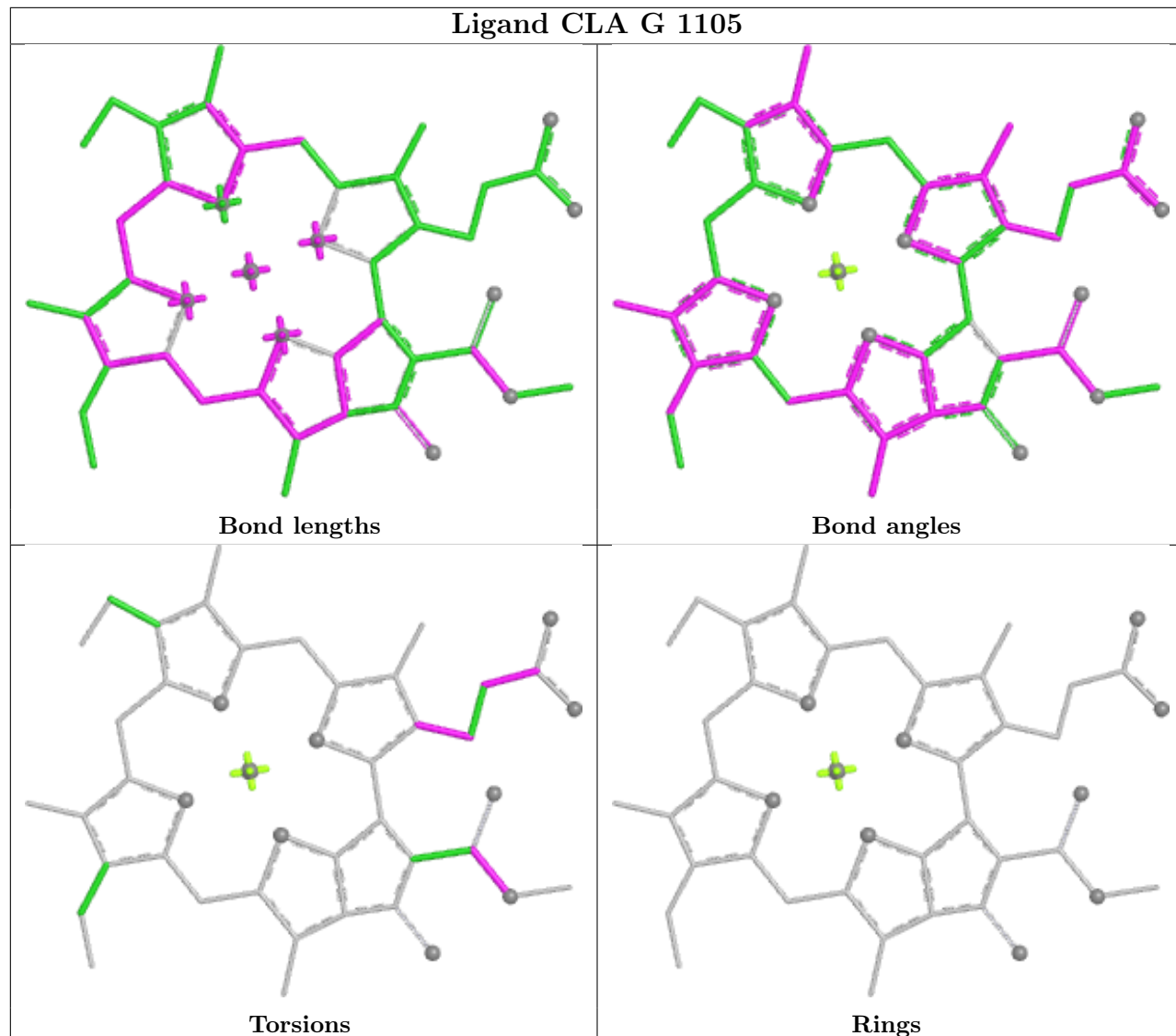
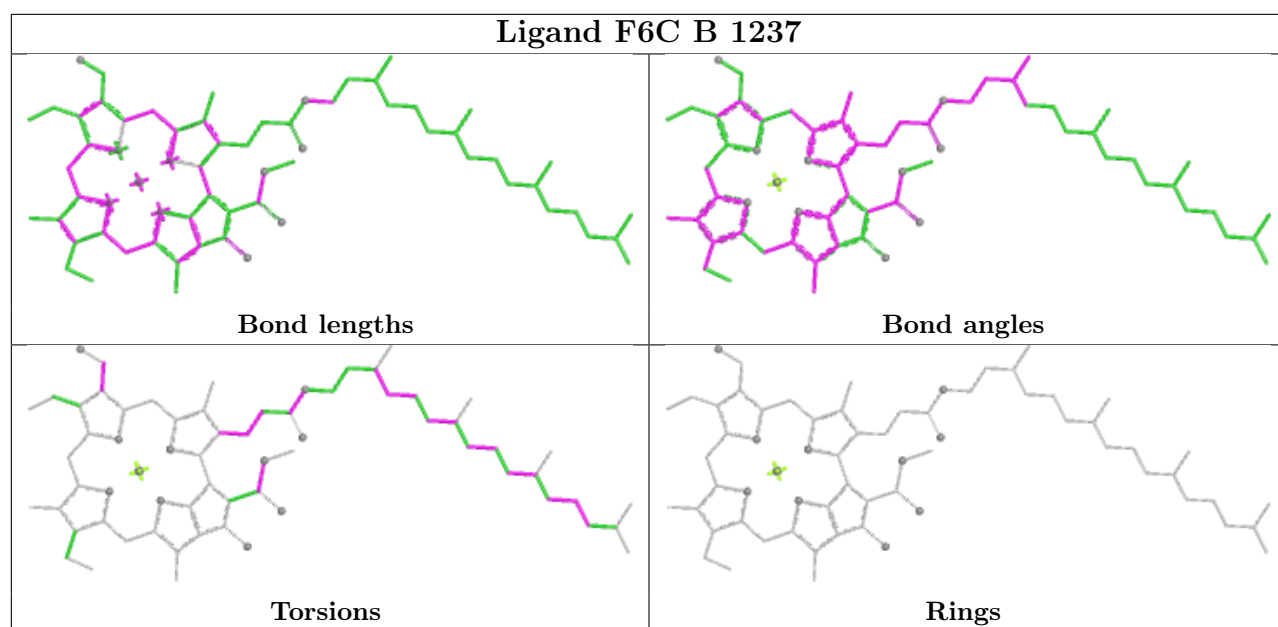




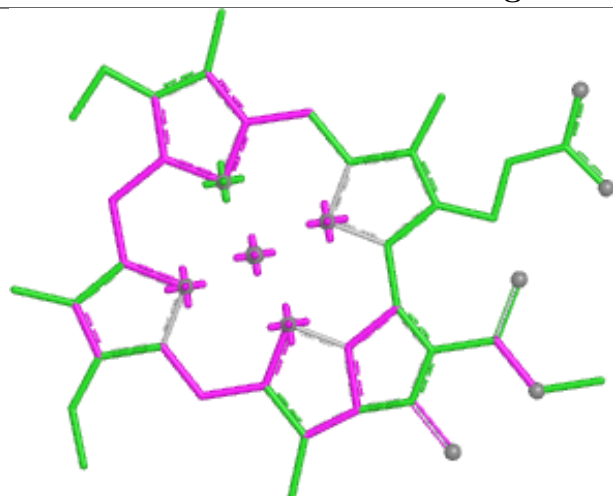
Ligand CLA A 1126**Ligand CLA G 1125**



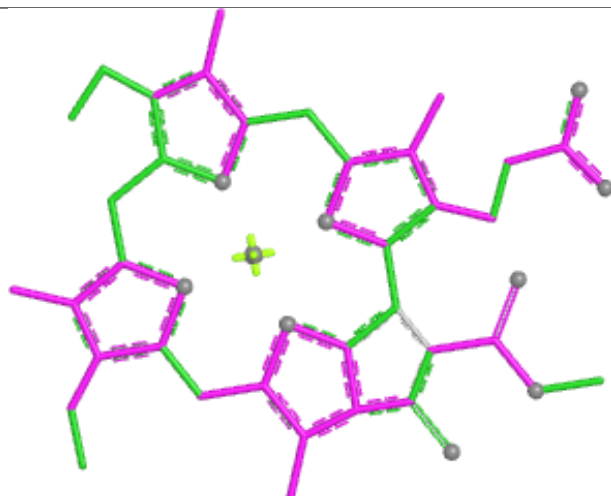




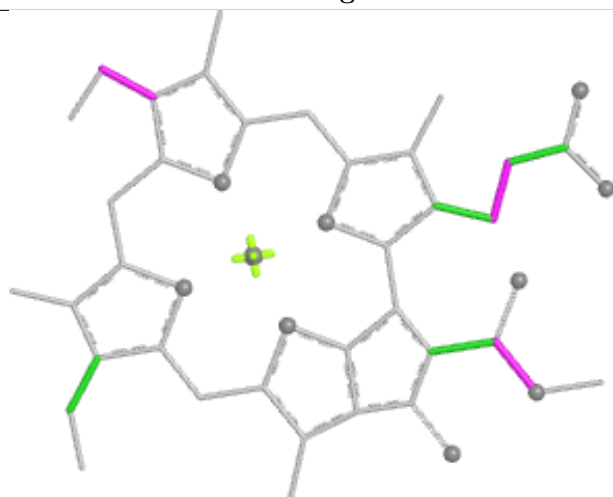
Ligand CLA G 1139



Bond lengths



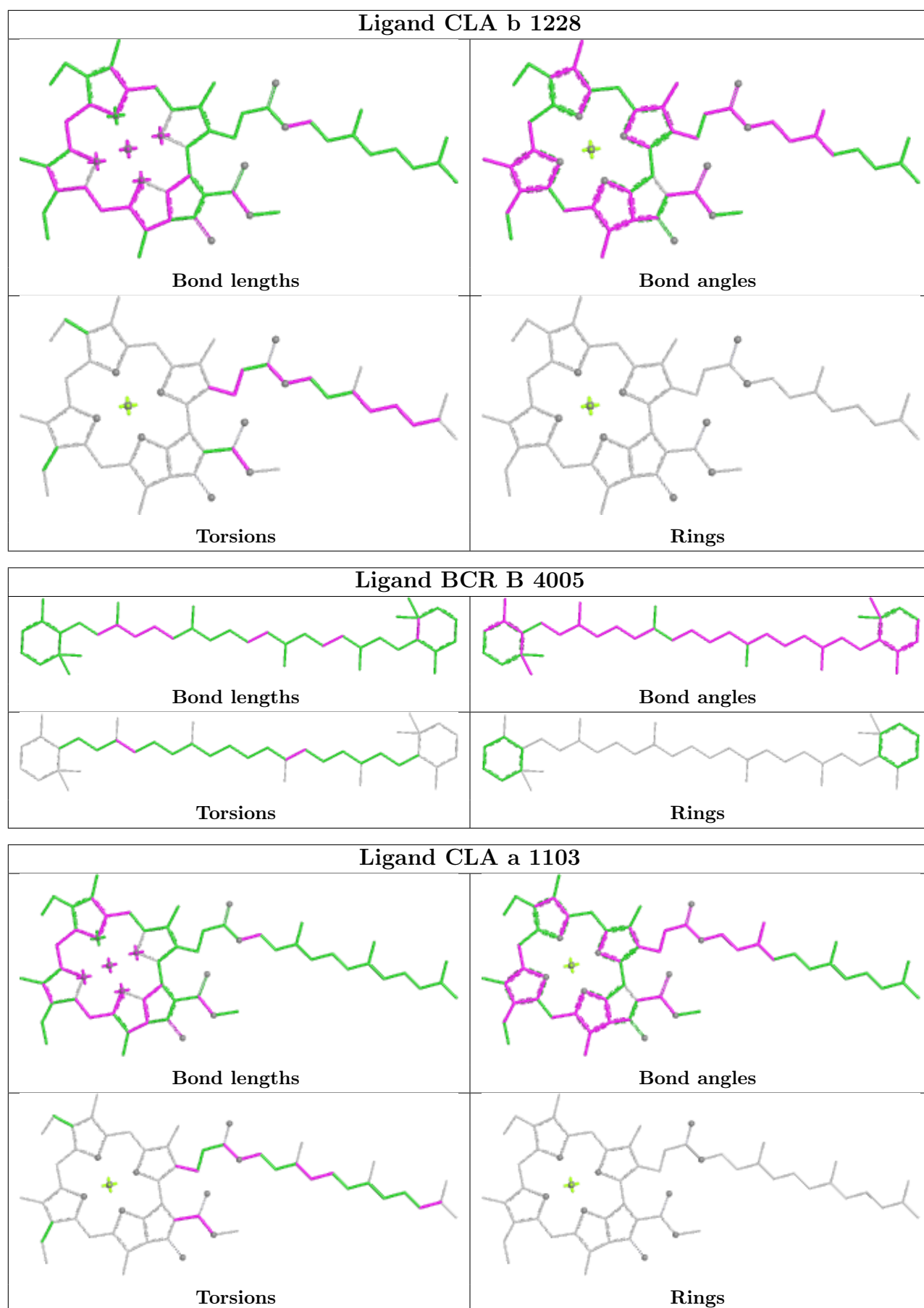
Bond angles

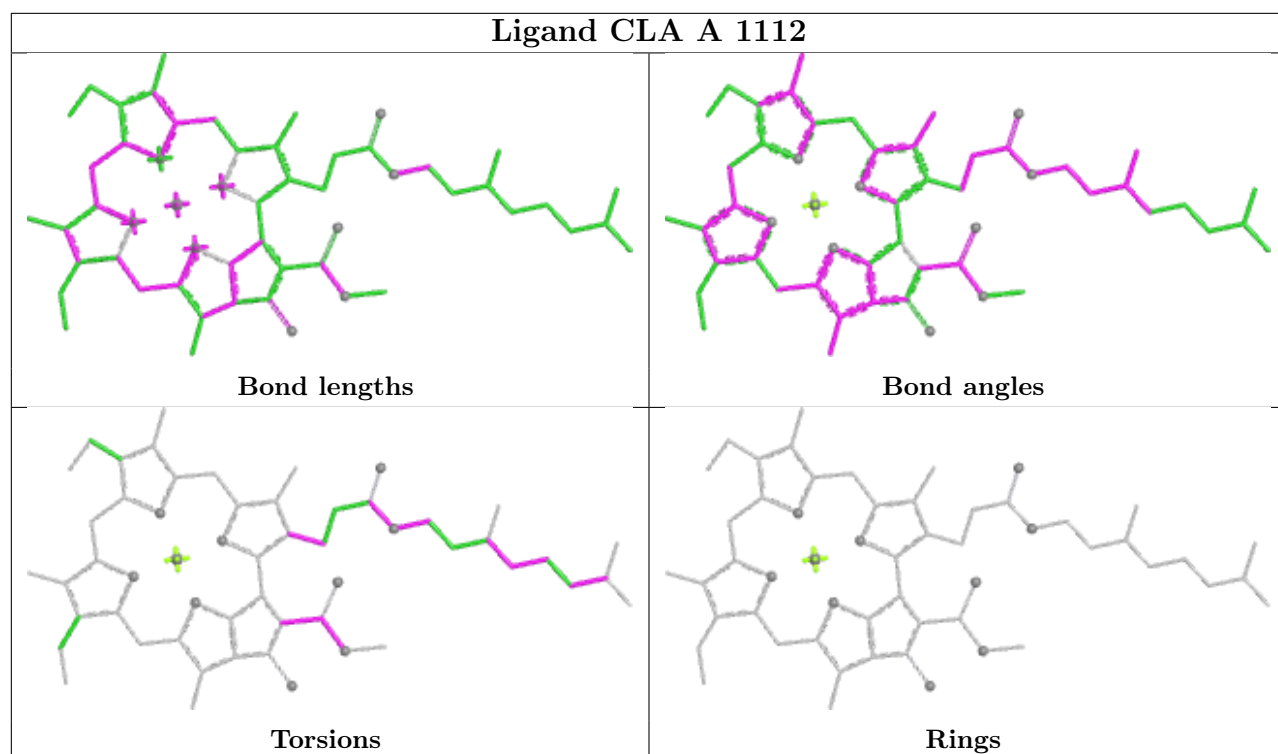
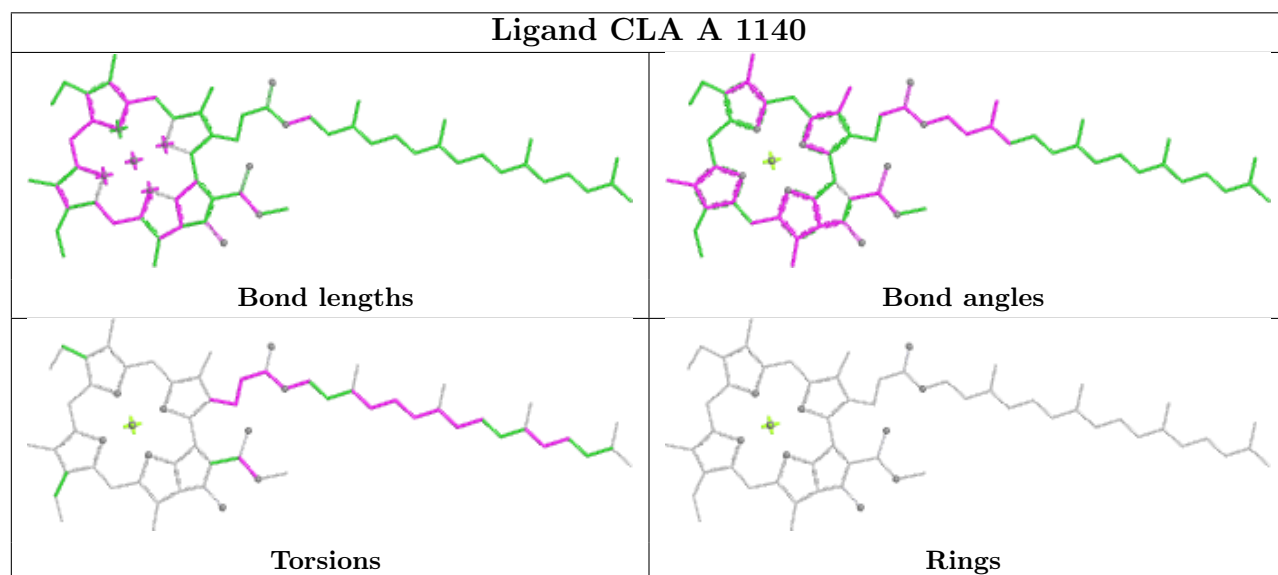
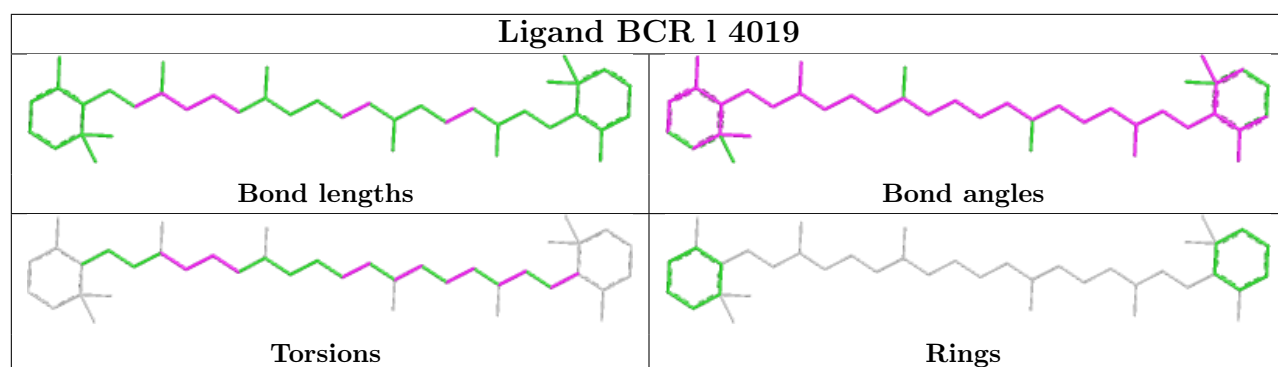


Torsions

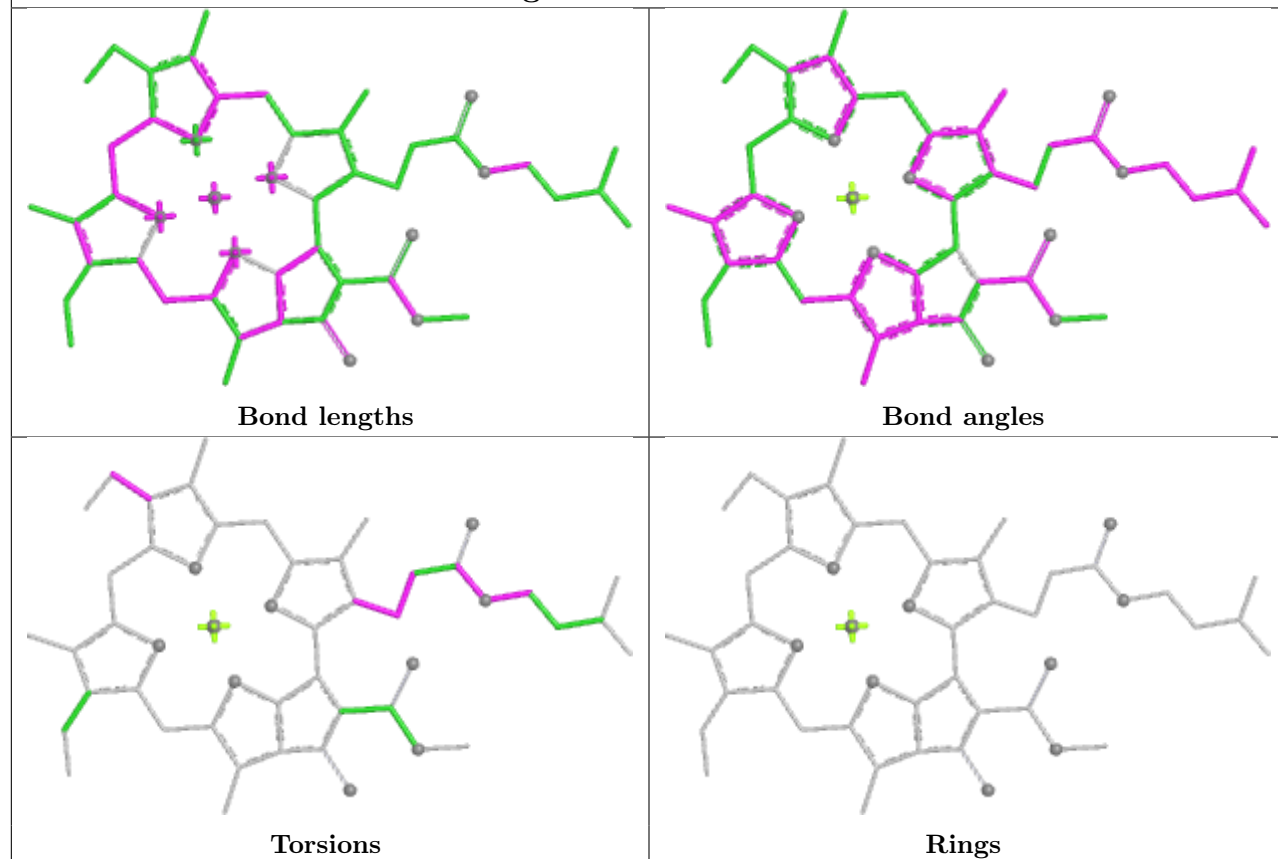


Rings

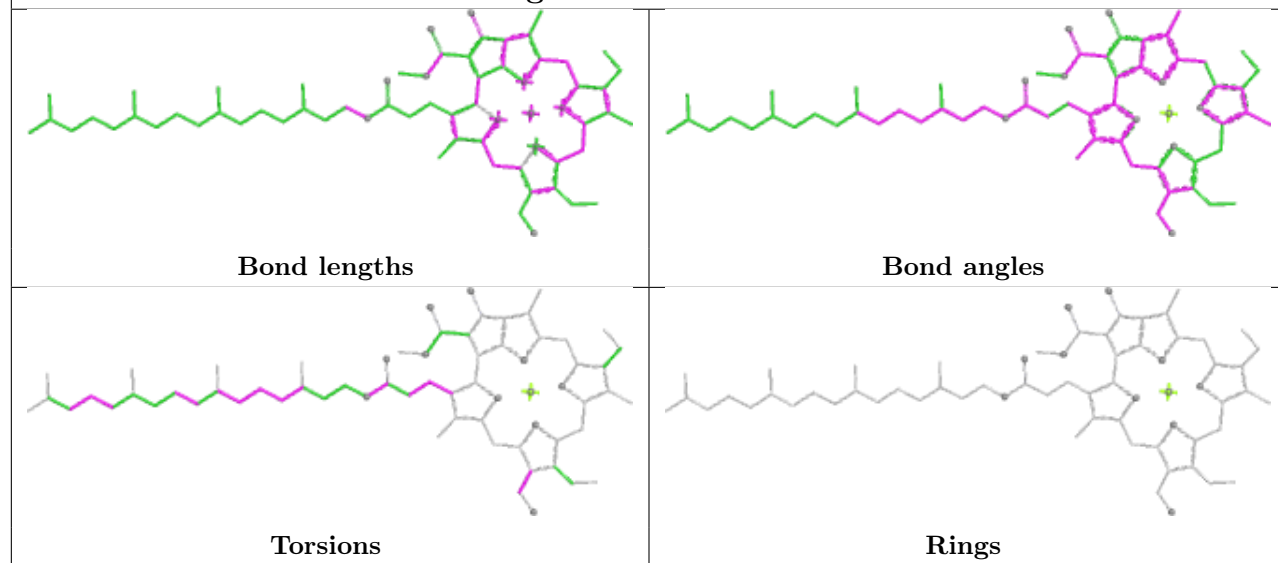


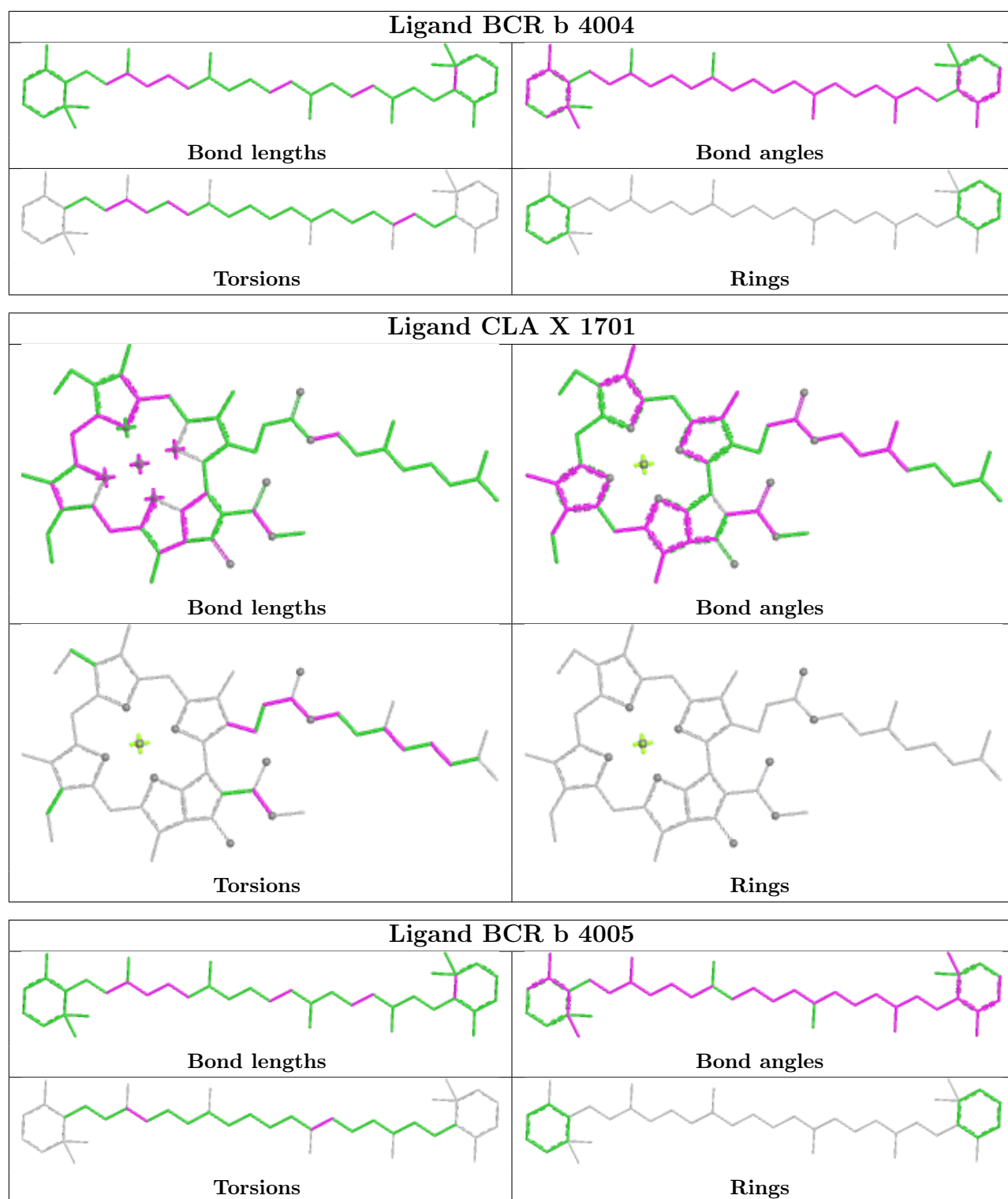


Ligand CLA A 1129

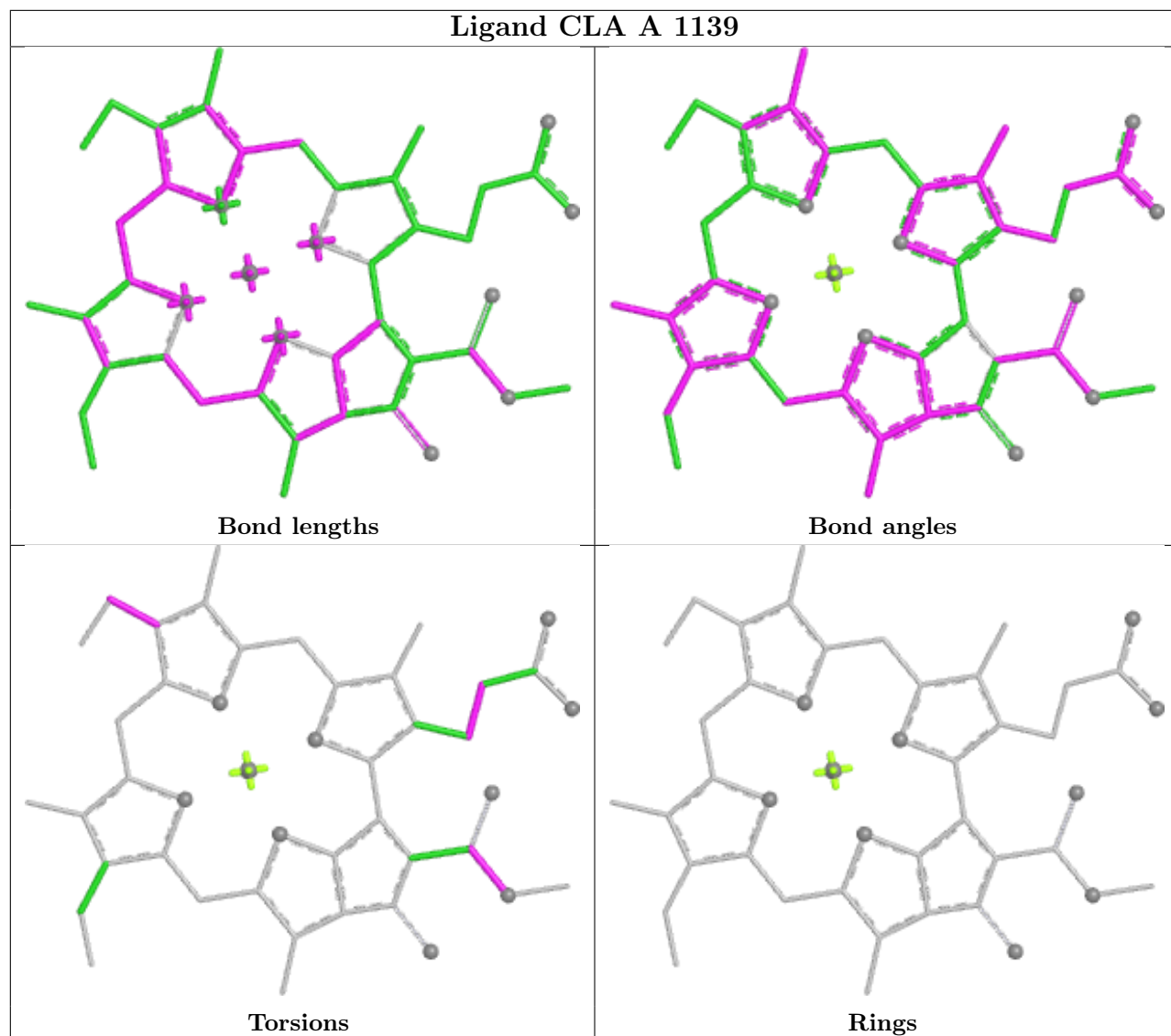


Ligand F6C H 1238

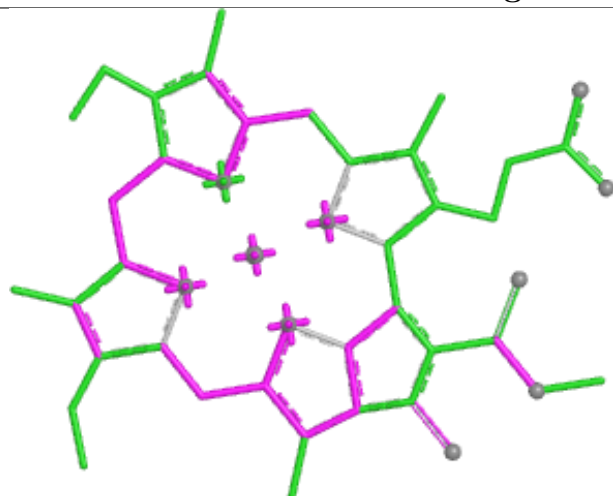




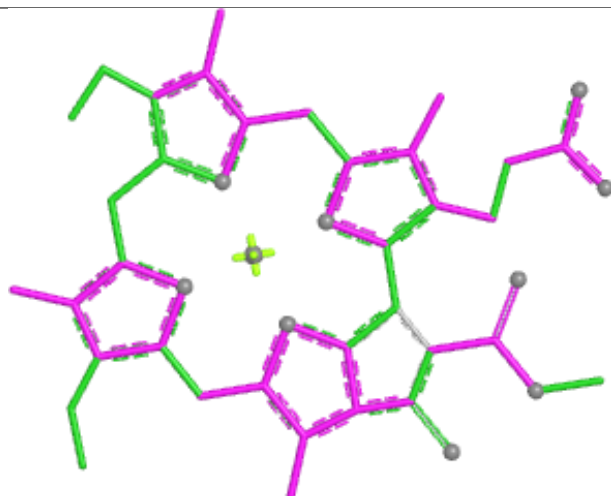
Ligand CLA A 1139



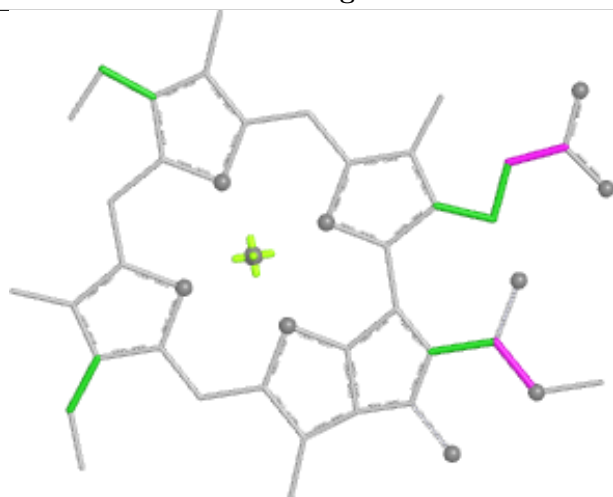
Ligand CLA G 1108



Bond lengths



Bond angles

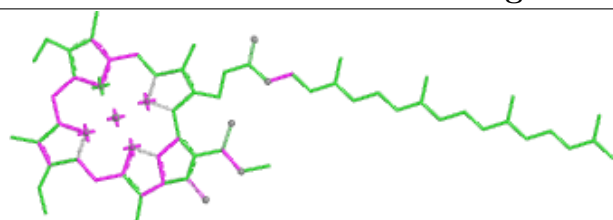


Torsions

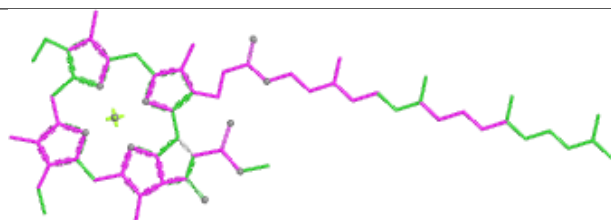


Rings

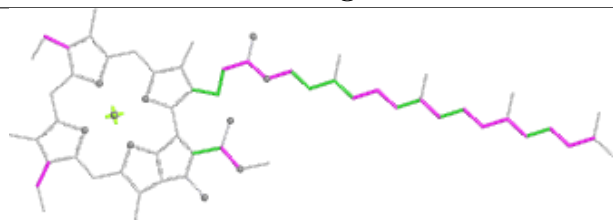
Ligand CLA B 1239



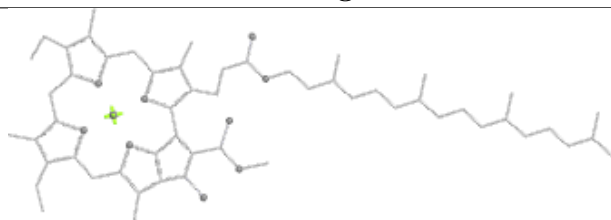
Bond lengths



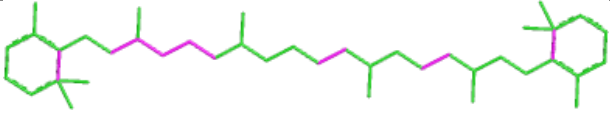
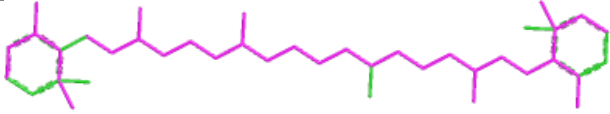
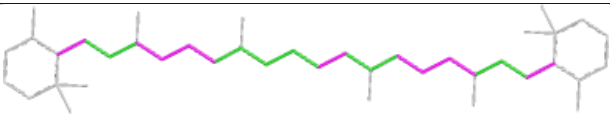
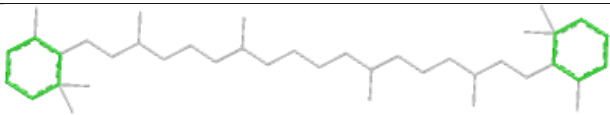
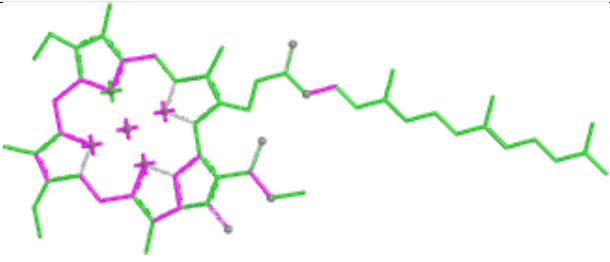
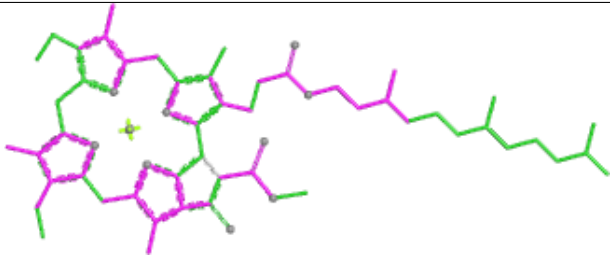
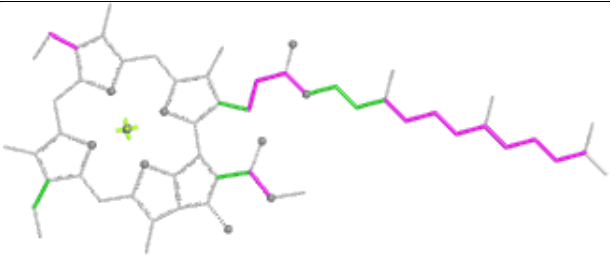
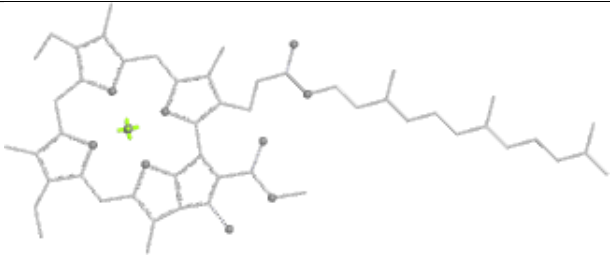
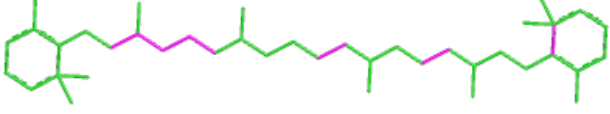
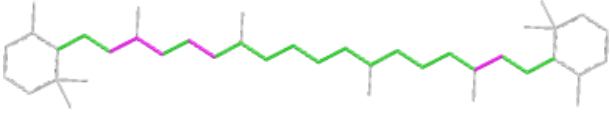
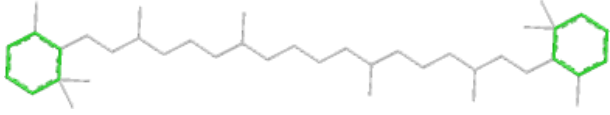
Bond angles

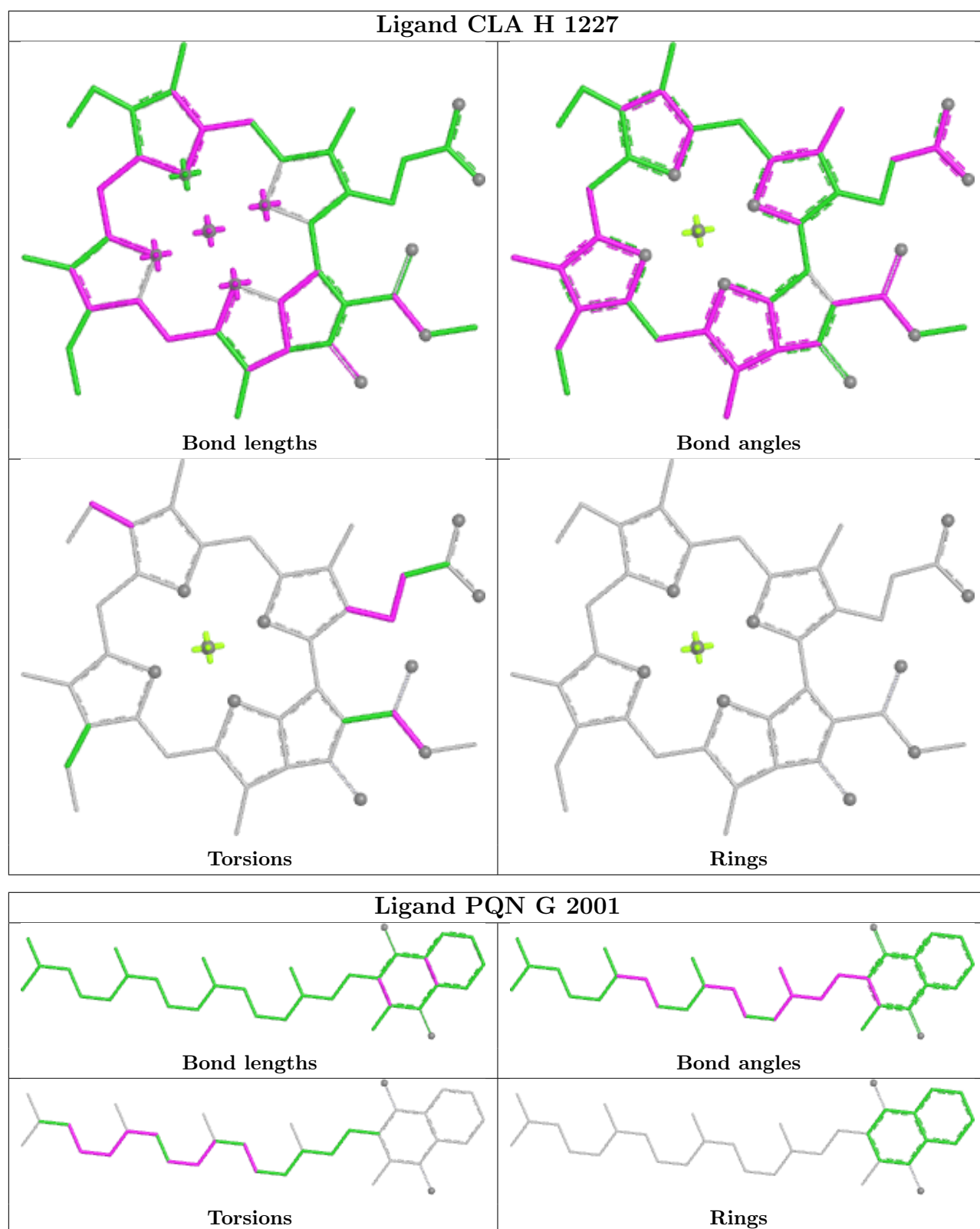


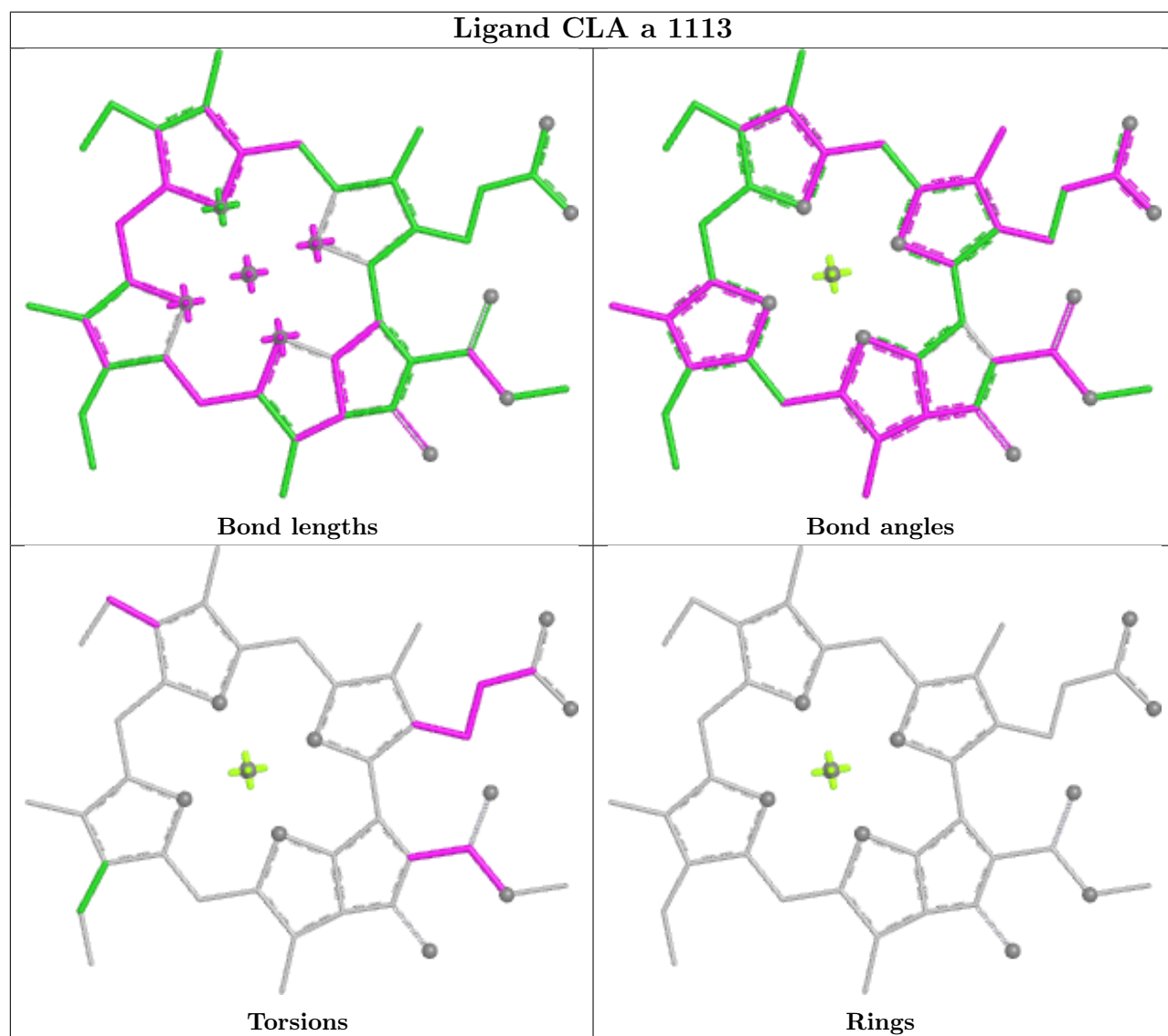
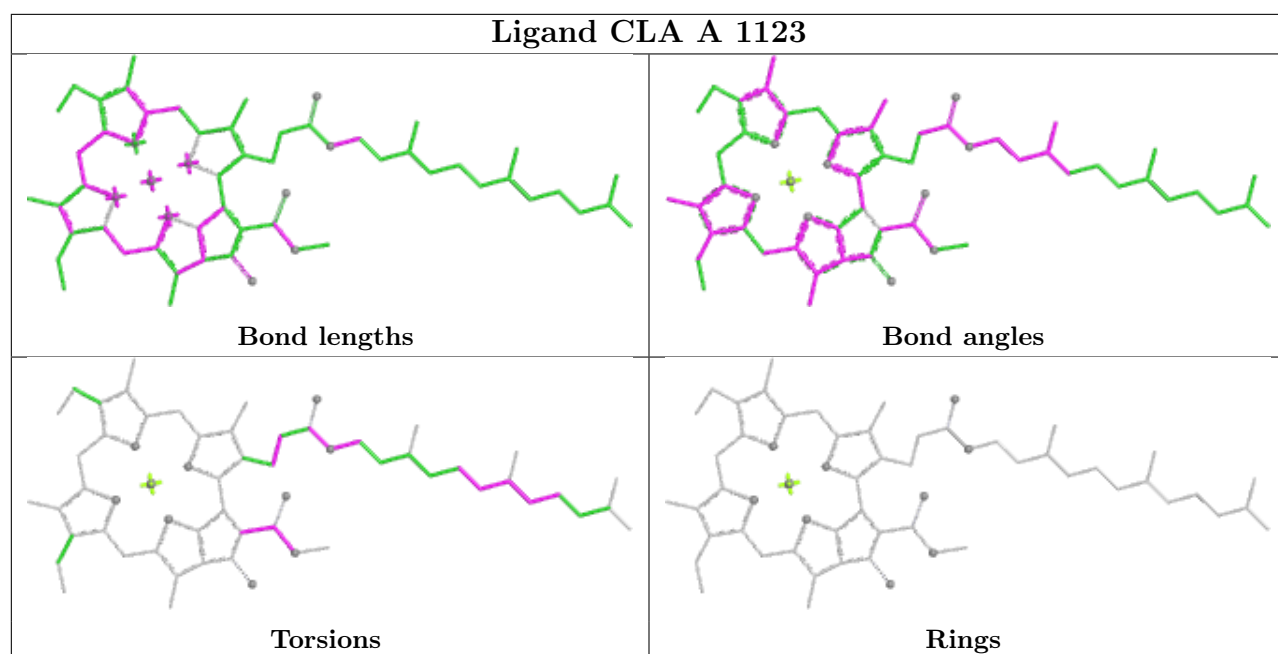
Torsions

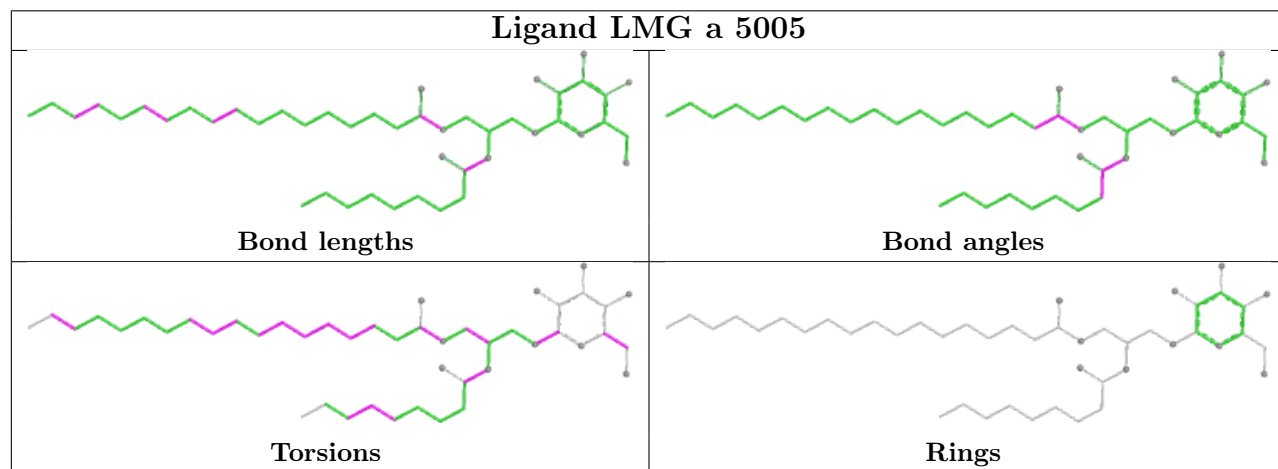
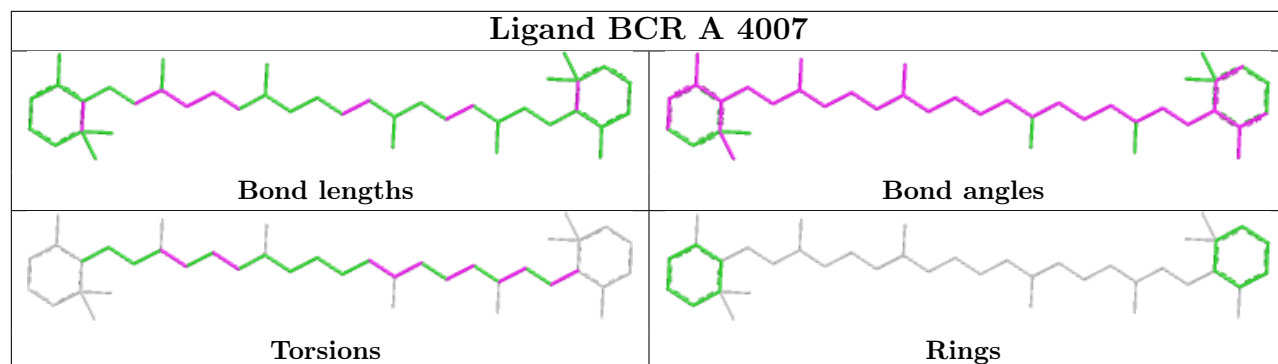


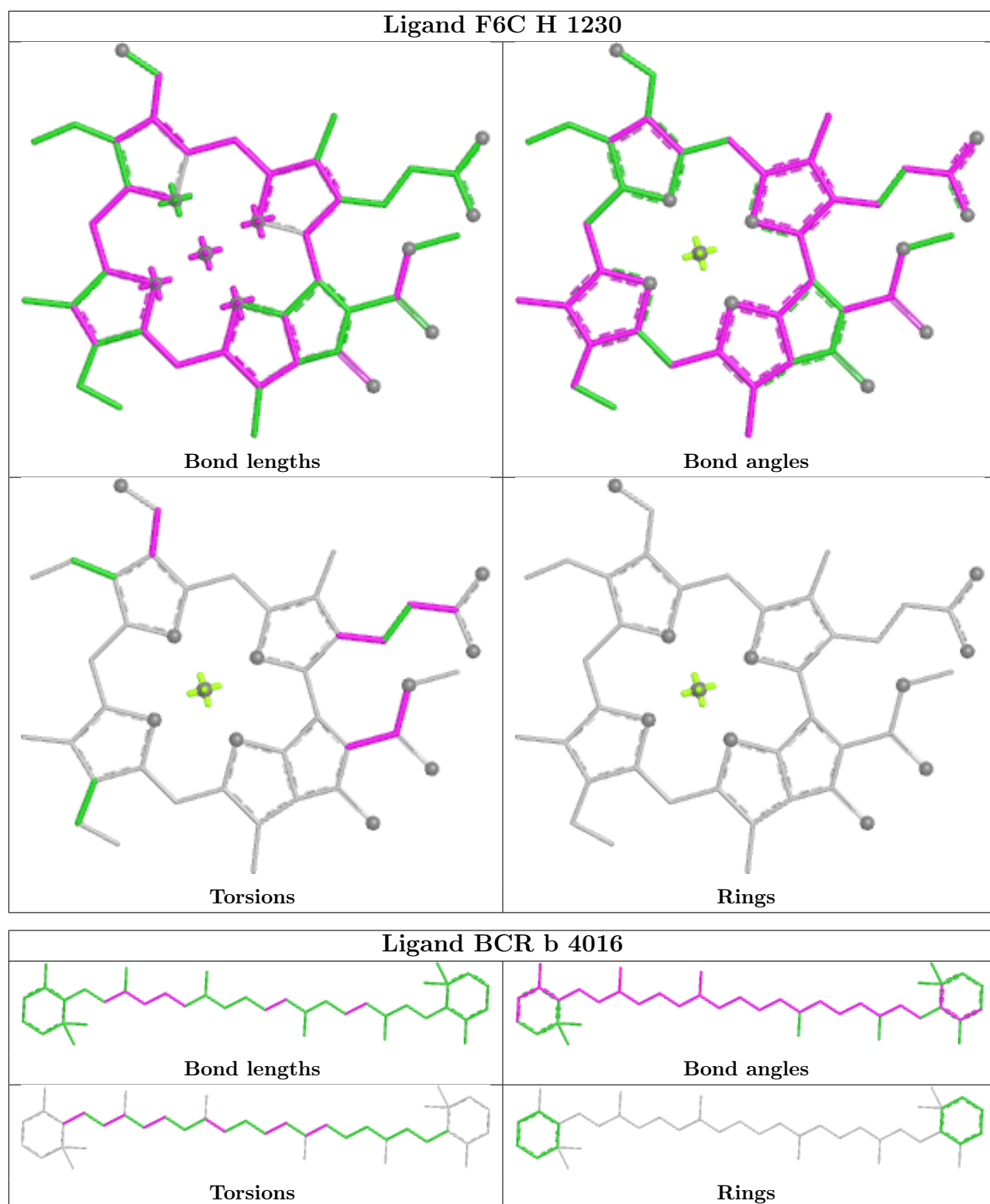
Rings

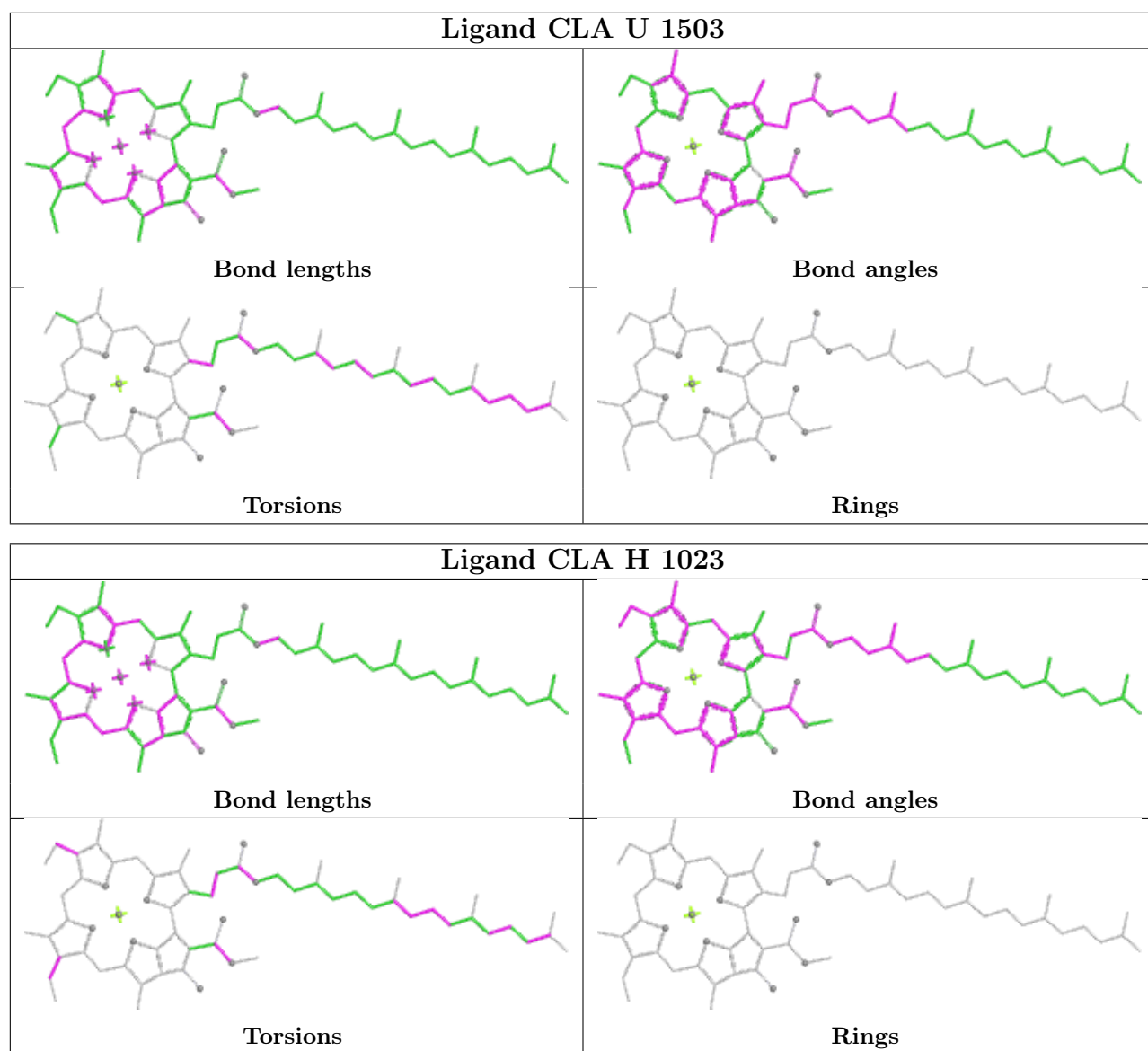
Ligand BCR I 4020	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA G 1126	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 4004	
 Bond lengths	 Bond angles
 Torsions	 Rings

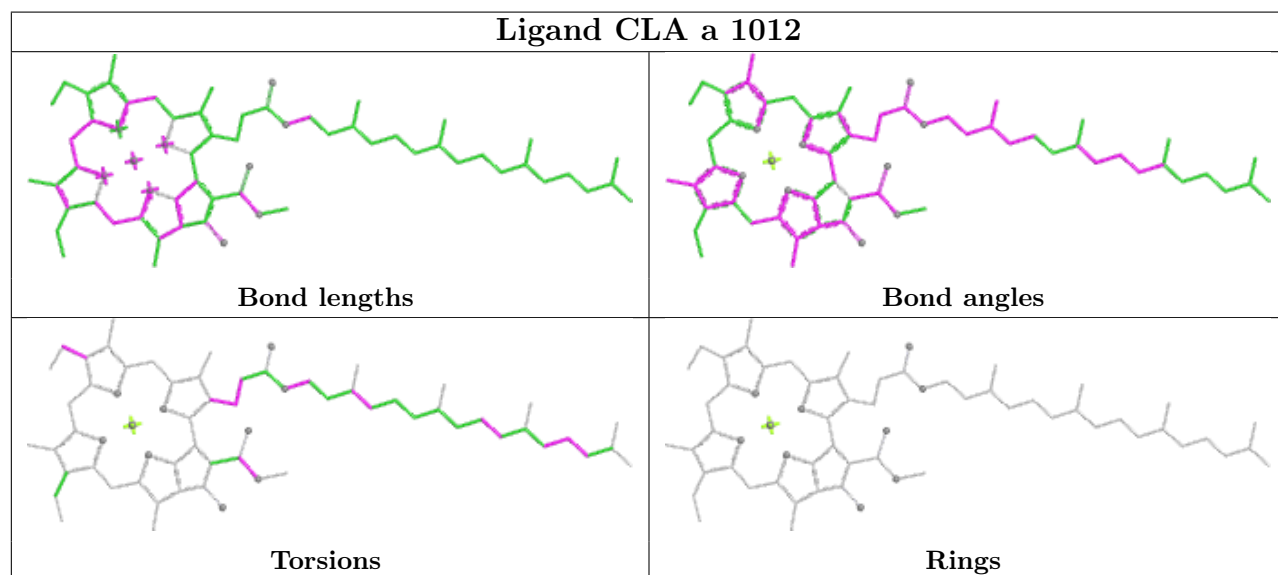
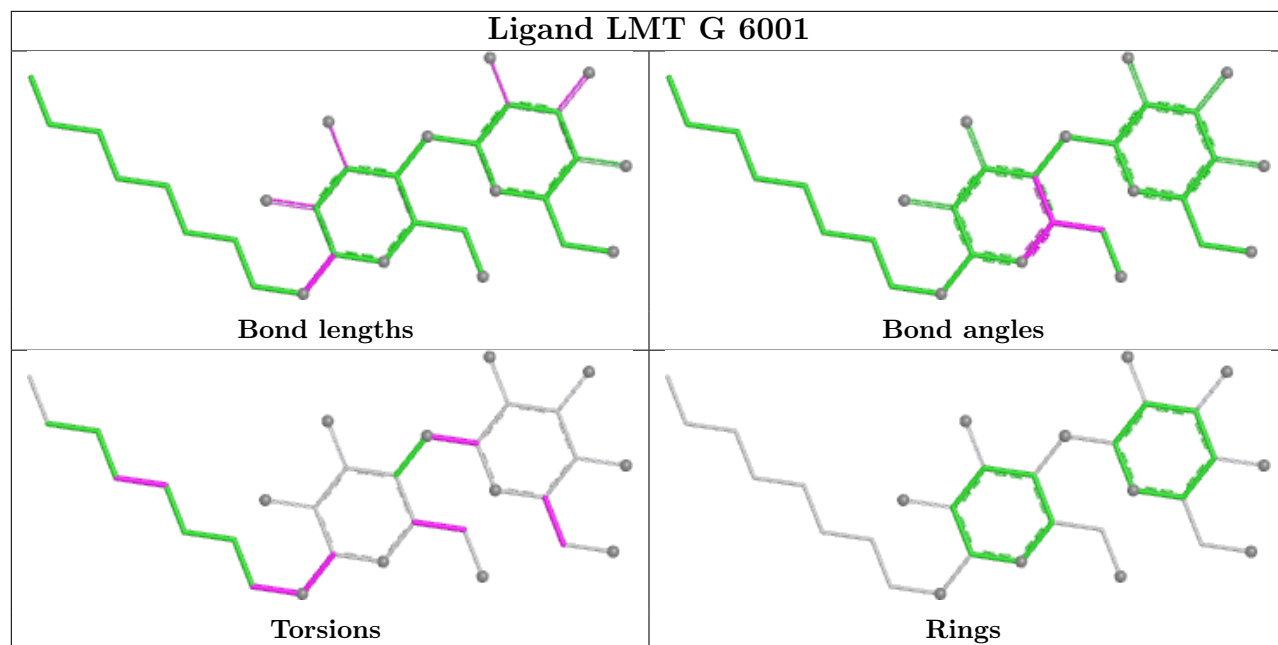




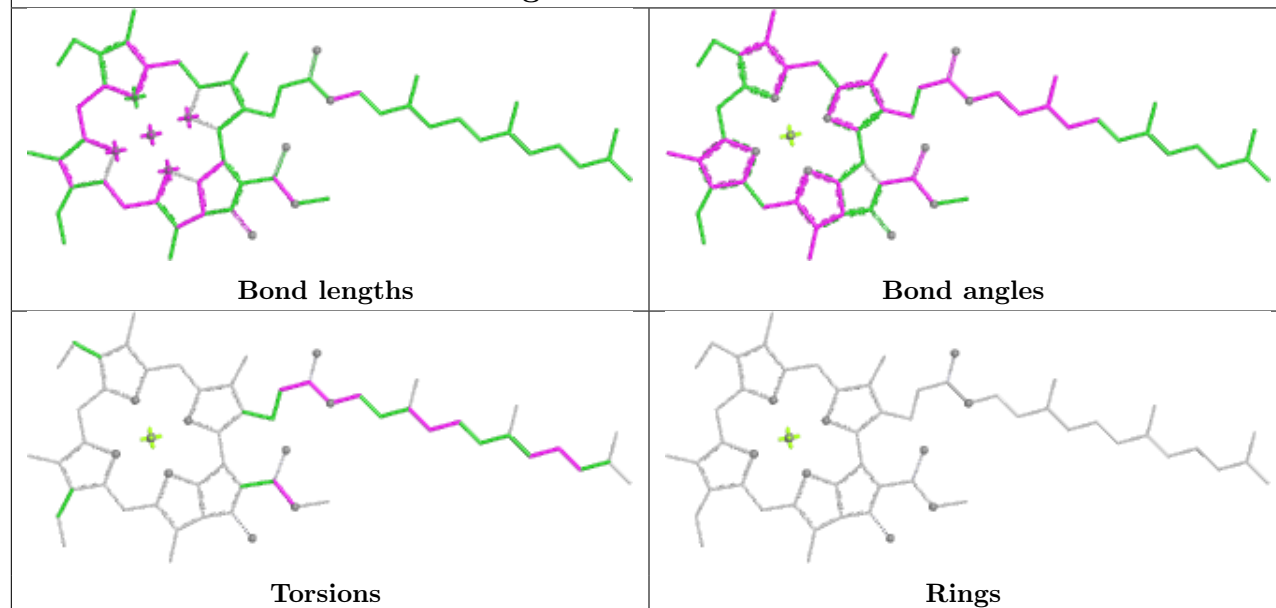




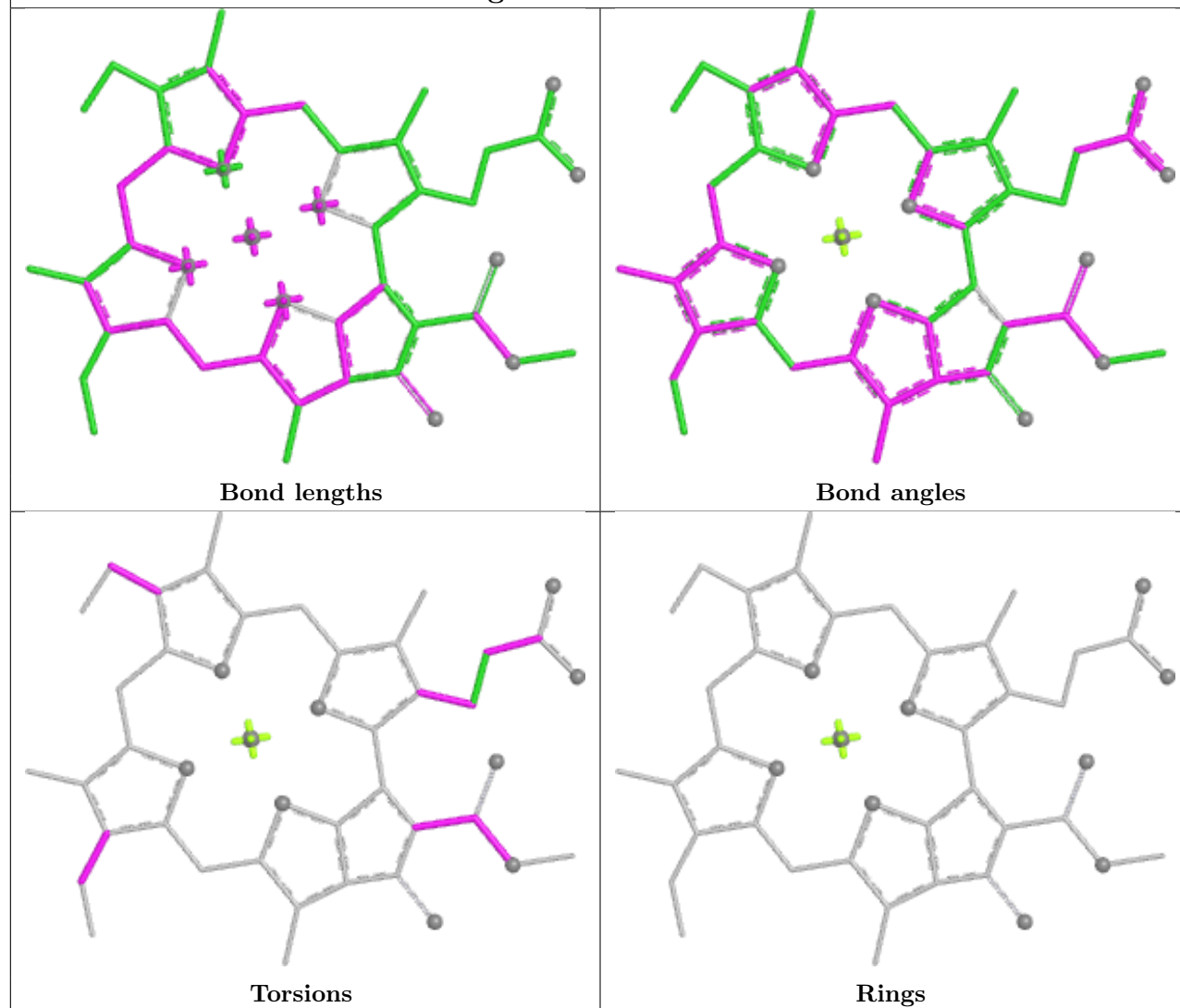




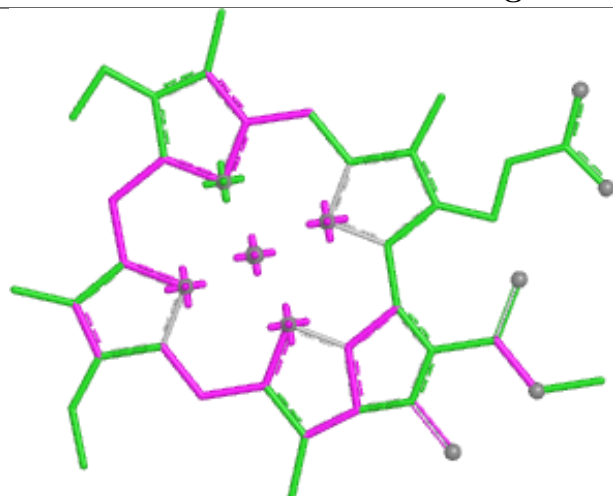
Ligand CLA H 1235



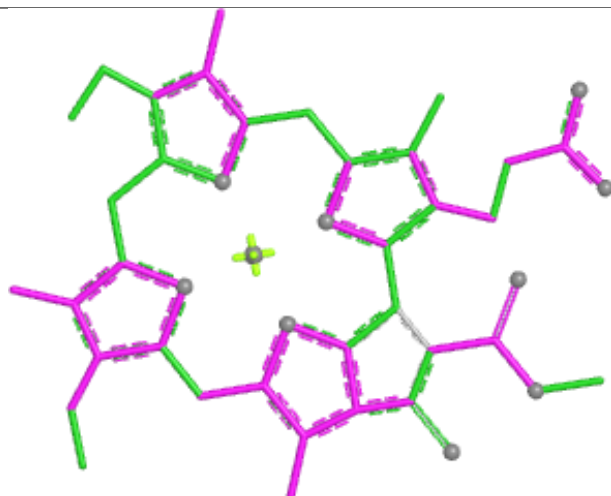
Ligand CLA a 1114



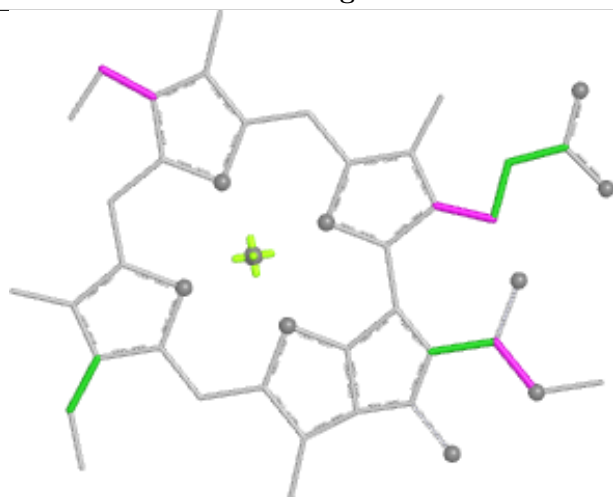
Ligand CLA A 1107



Bond lengths



Bond angles

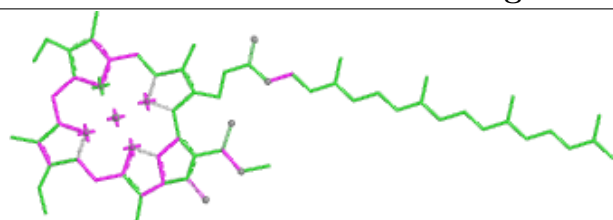


Torsions

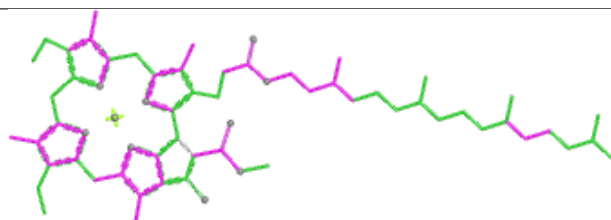


Rings

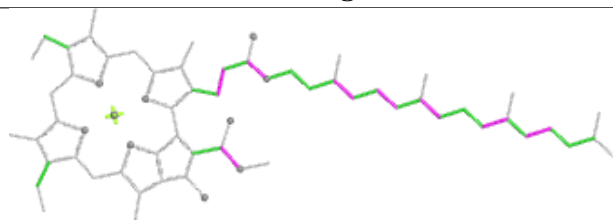
Ligand CLA U 1501



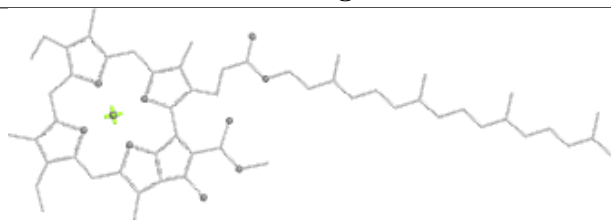
Bond lengths



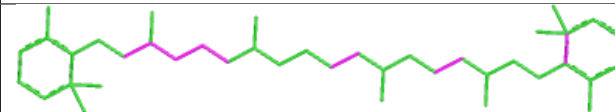
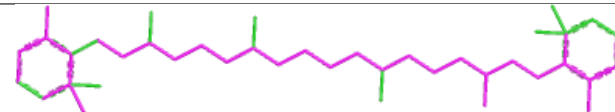
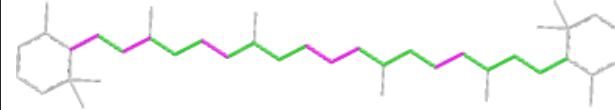
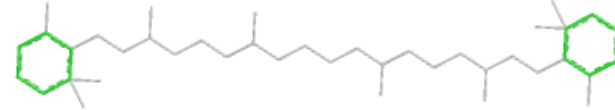
Bond angles

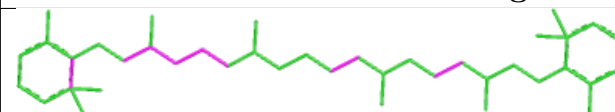
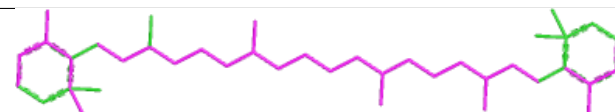
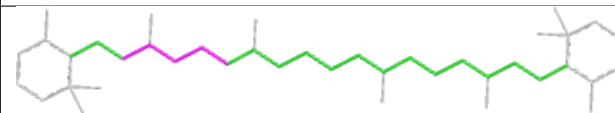
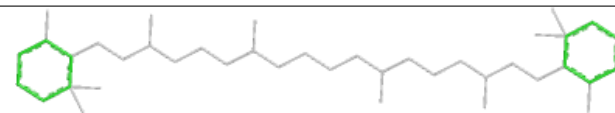


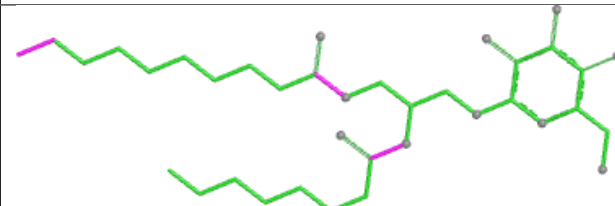
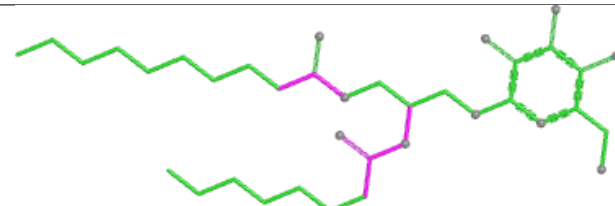
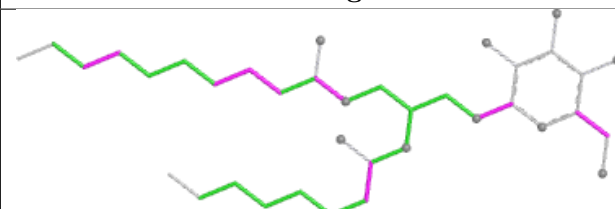
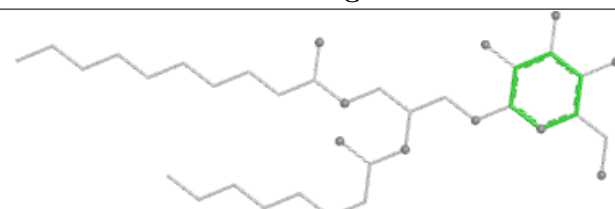
Torsions

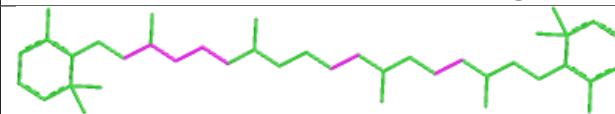
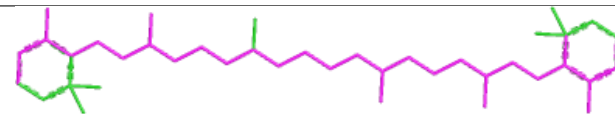
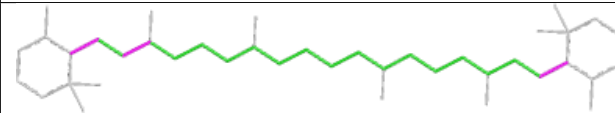
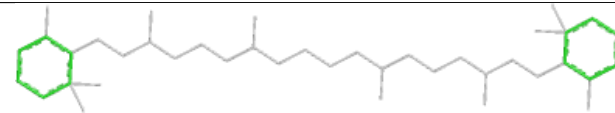


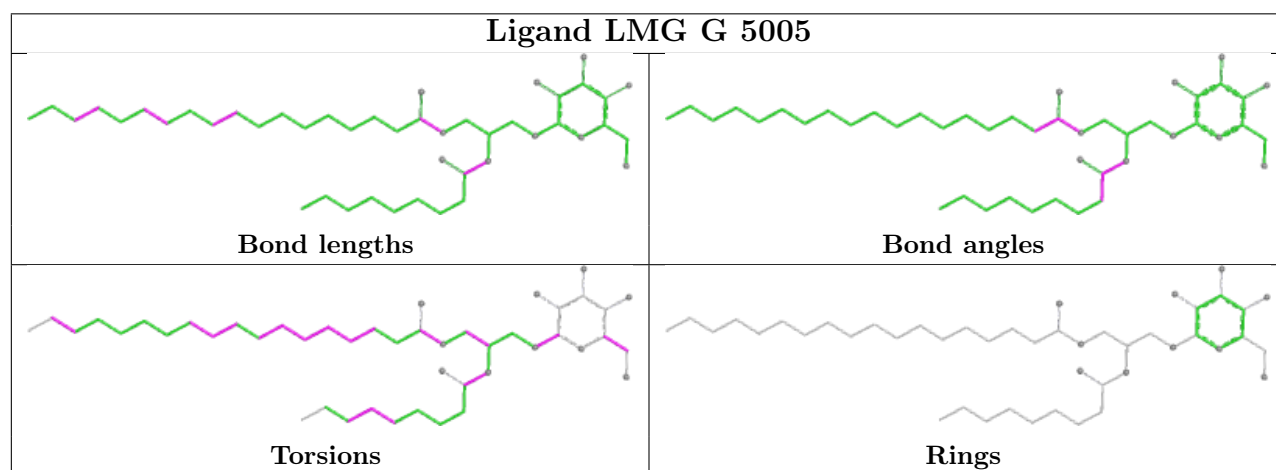
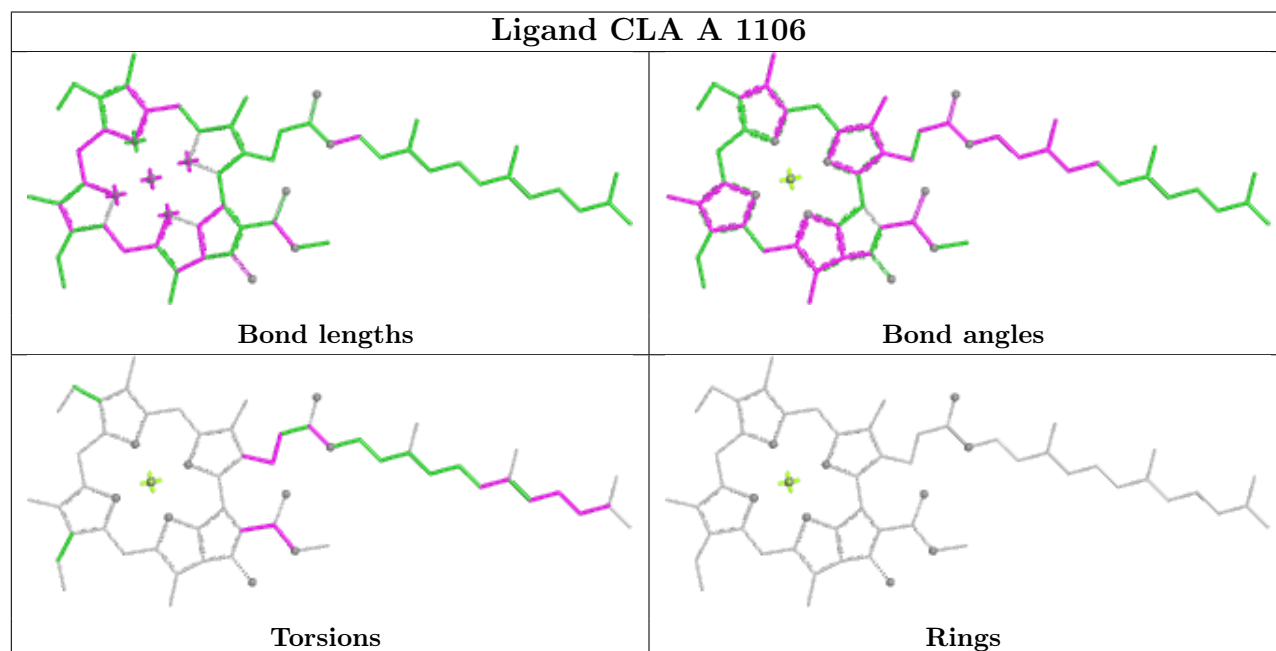
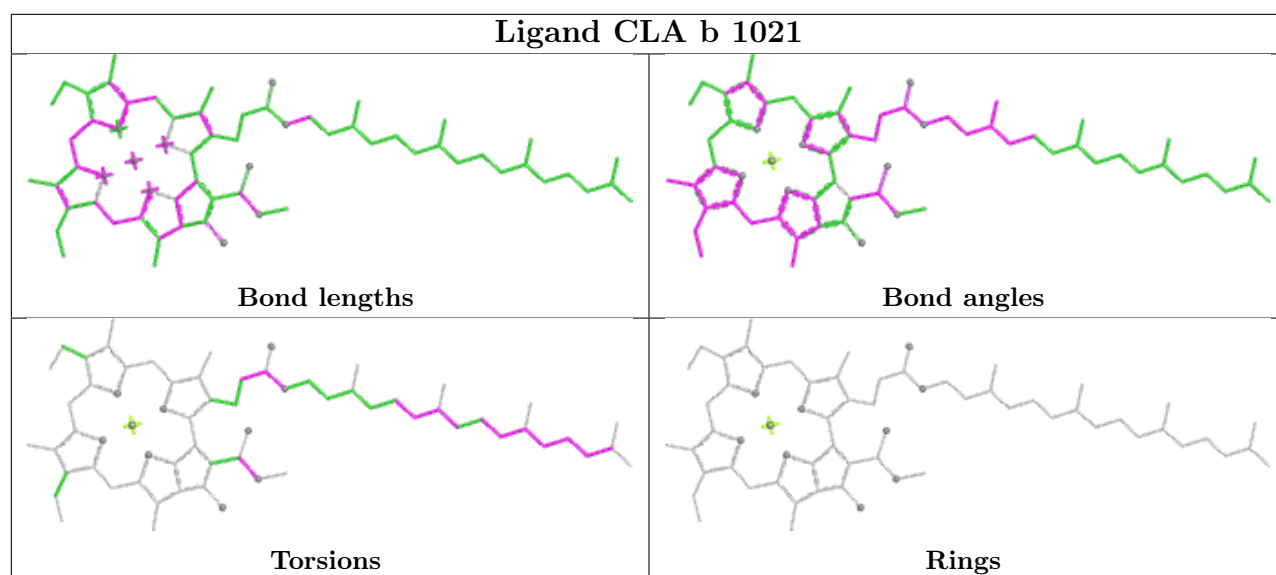
Rings

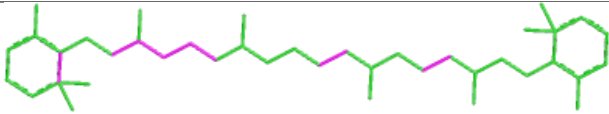
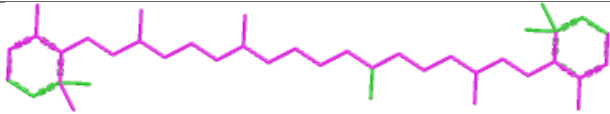
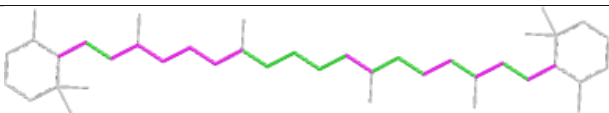
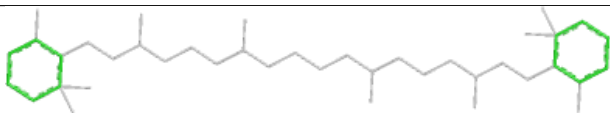
Ligand BCR R 4018	
	
Bond lengths	Bond angles
	
Torsions	Rings

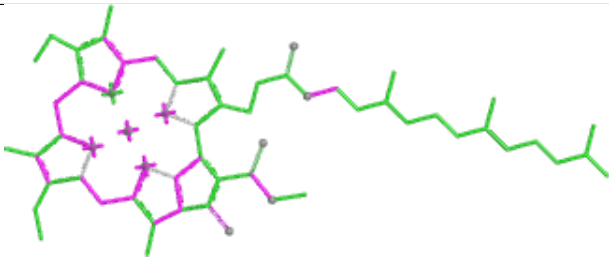
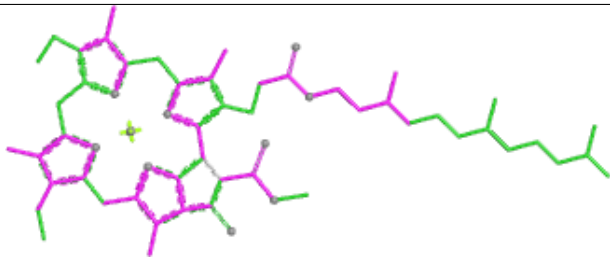
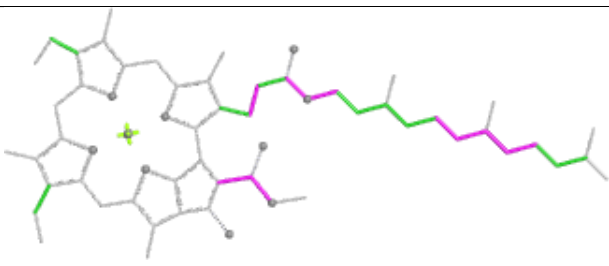
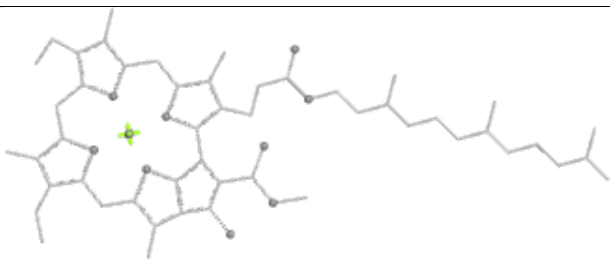
Ligand BCR U 4022	
	
Bond lengths	Bond angles
	
Torsions	Rings

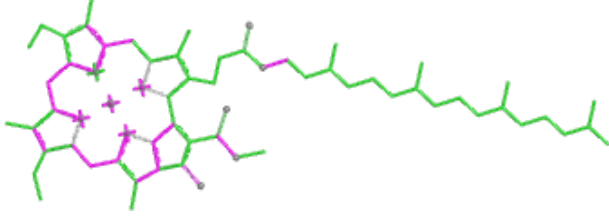
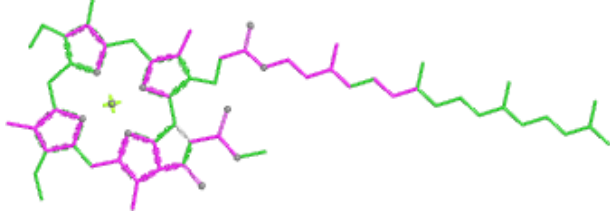
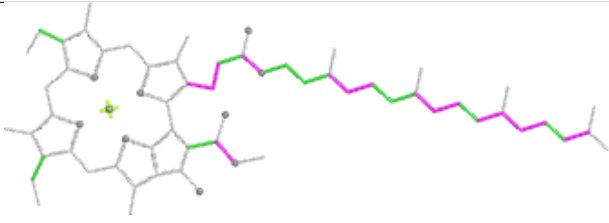
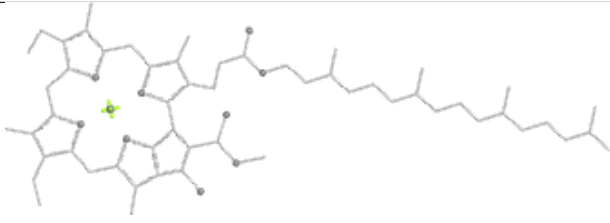
Ligand LMG i 5006	
	
Bond lengths	Bond angles
	
Torsions	Rings

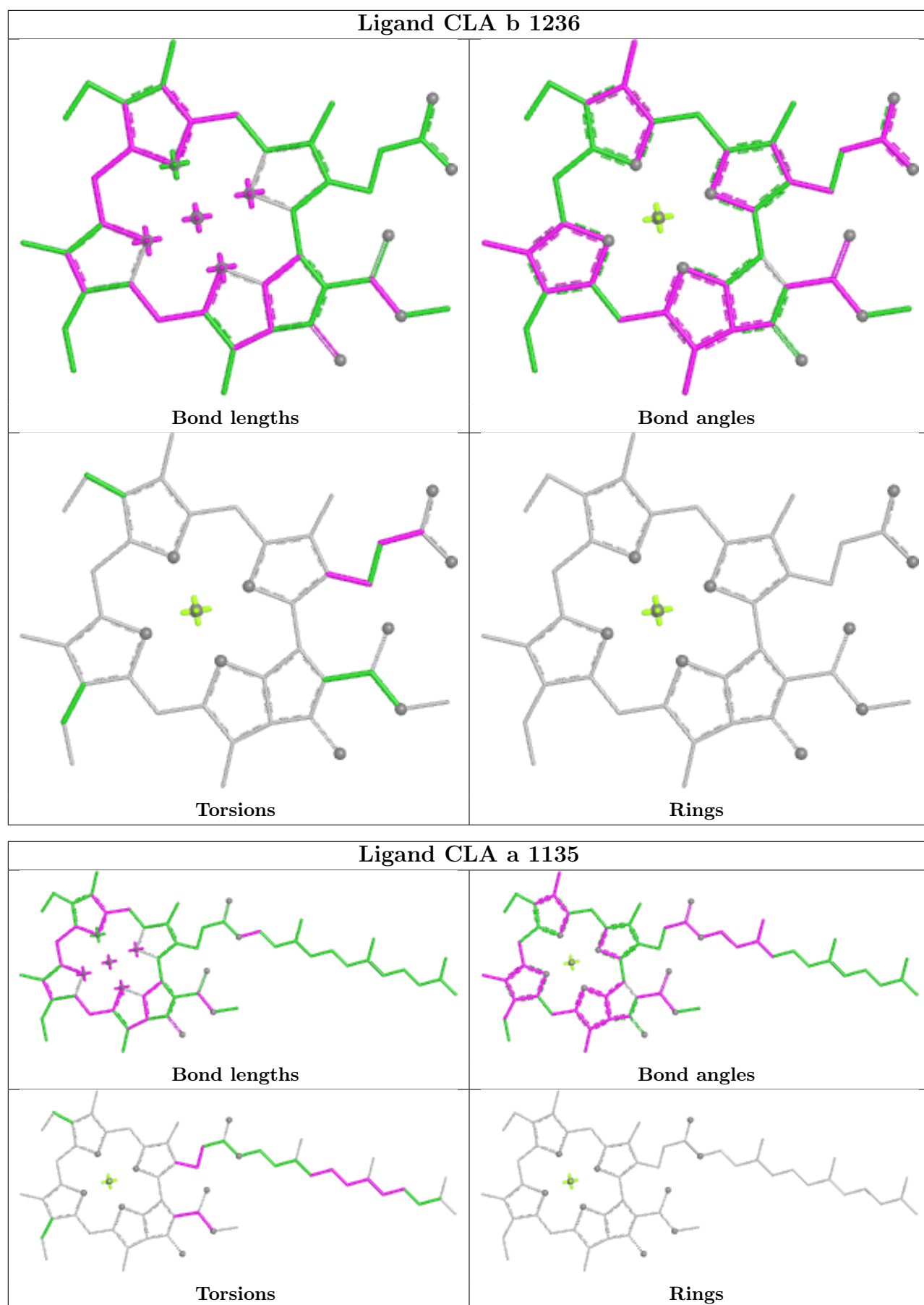
Ligand BCR A 4002	
	
Bond lengths	Bond angles
	
Torsions	Rings



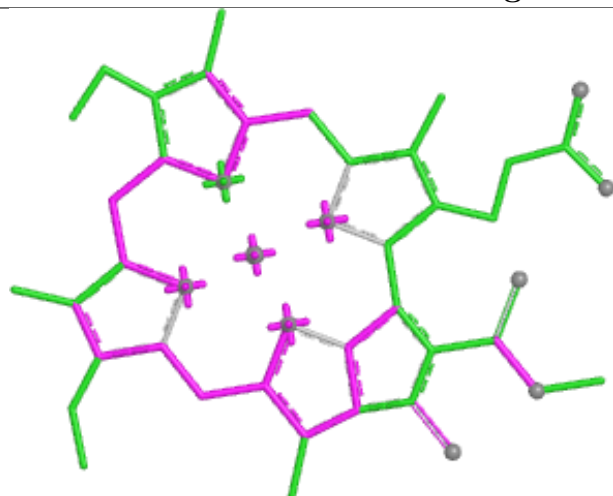
Ligand BCR A 4011	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 1123	
	
Bond lengths	Bond angles
	
Torsions	Rings

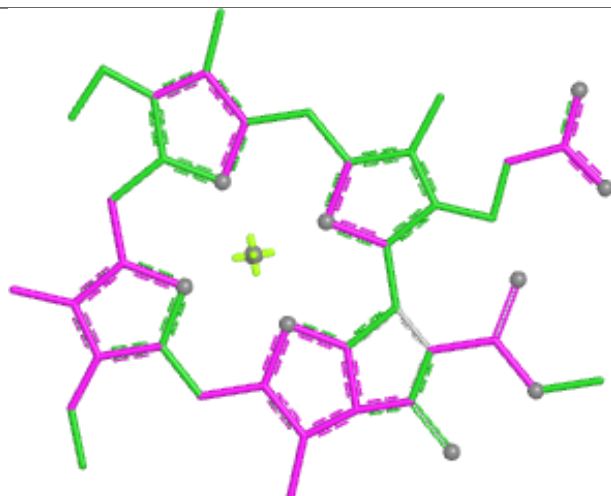
Ligand CLA A 1109	
	
Bond lengths	Bond angles
	
Torsions	Rings



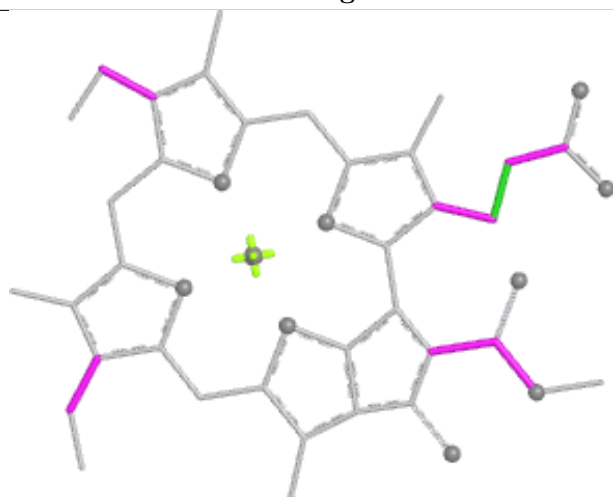
Ligand CLA G 1114



Bond lengths



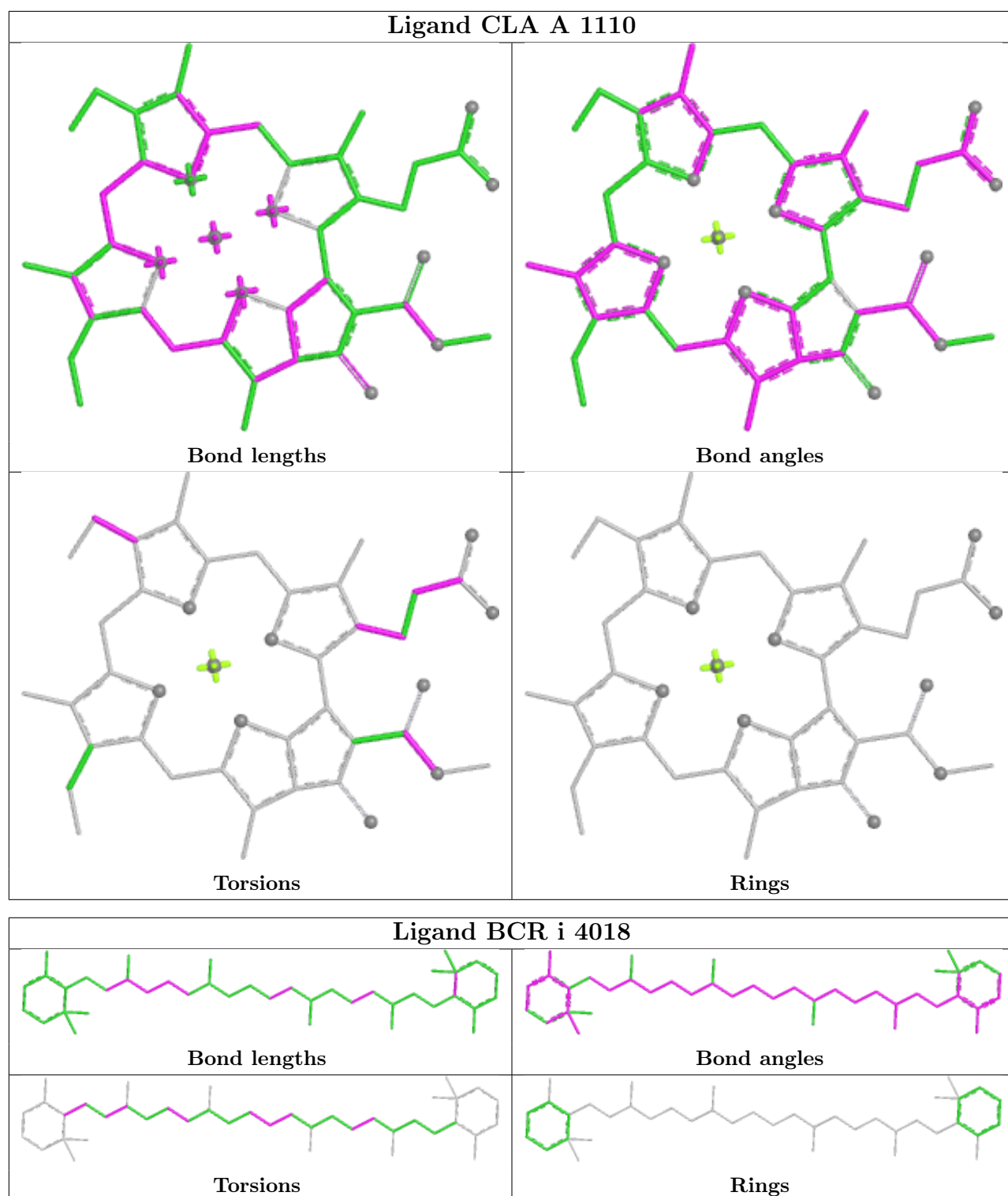
Bond angles

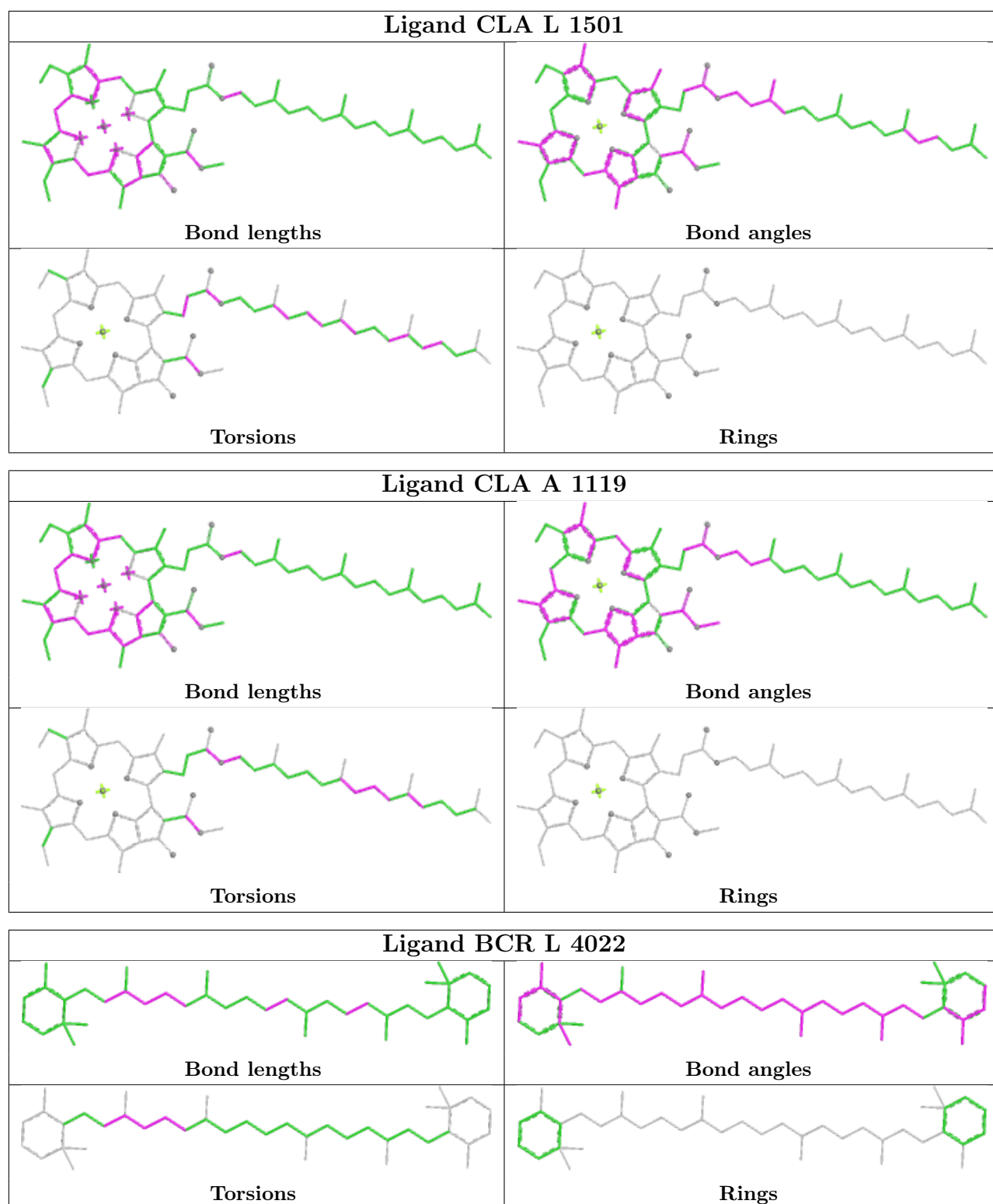


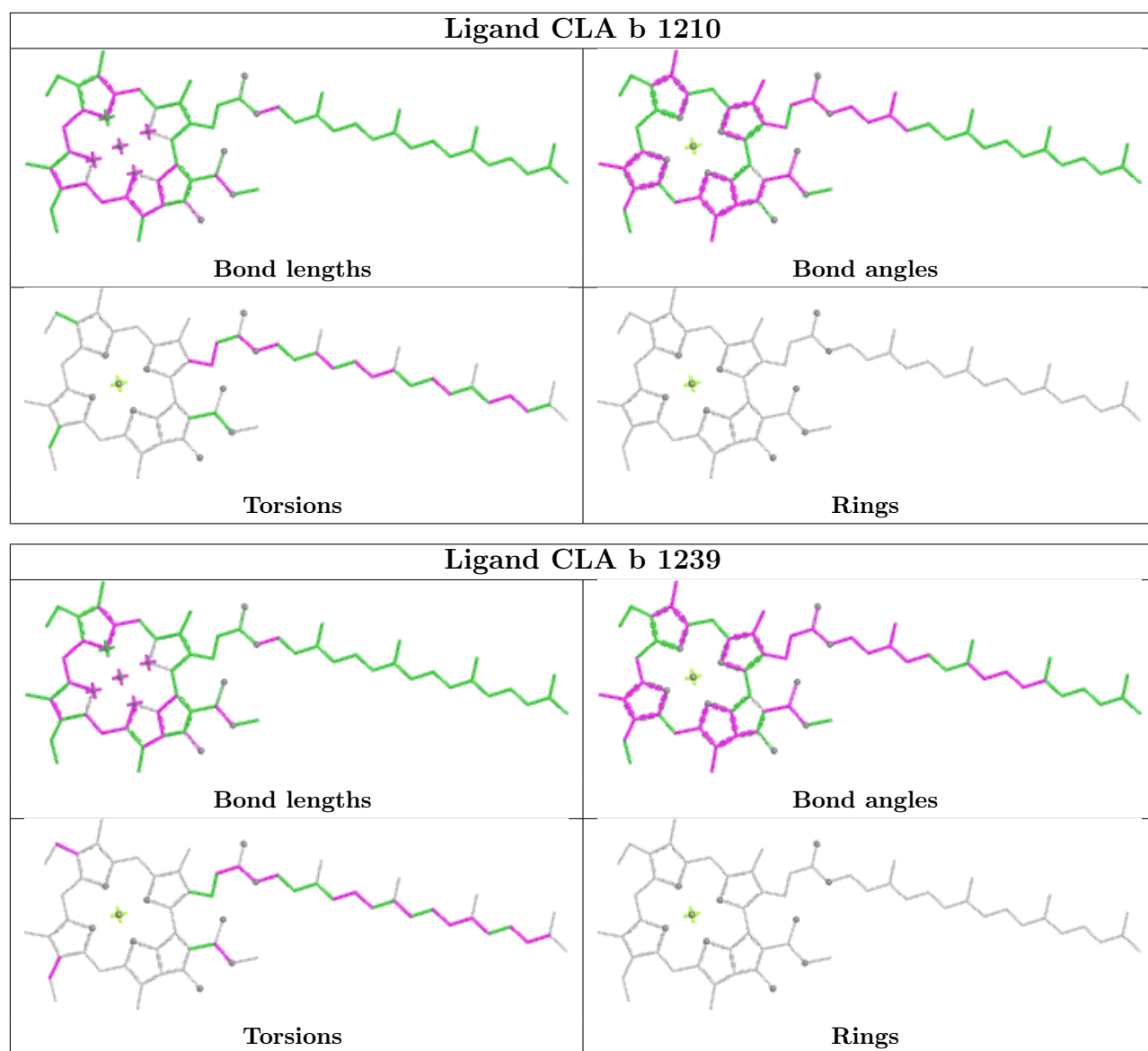
Torsions



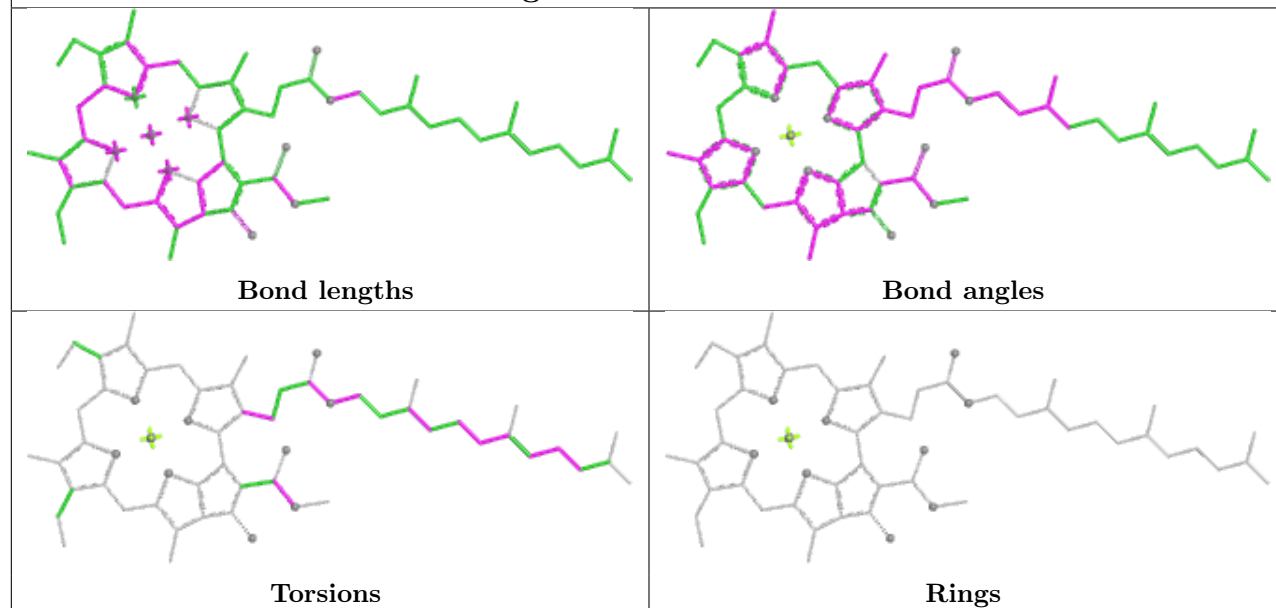
Rings



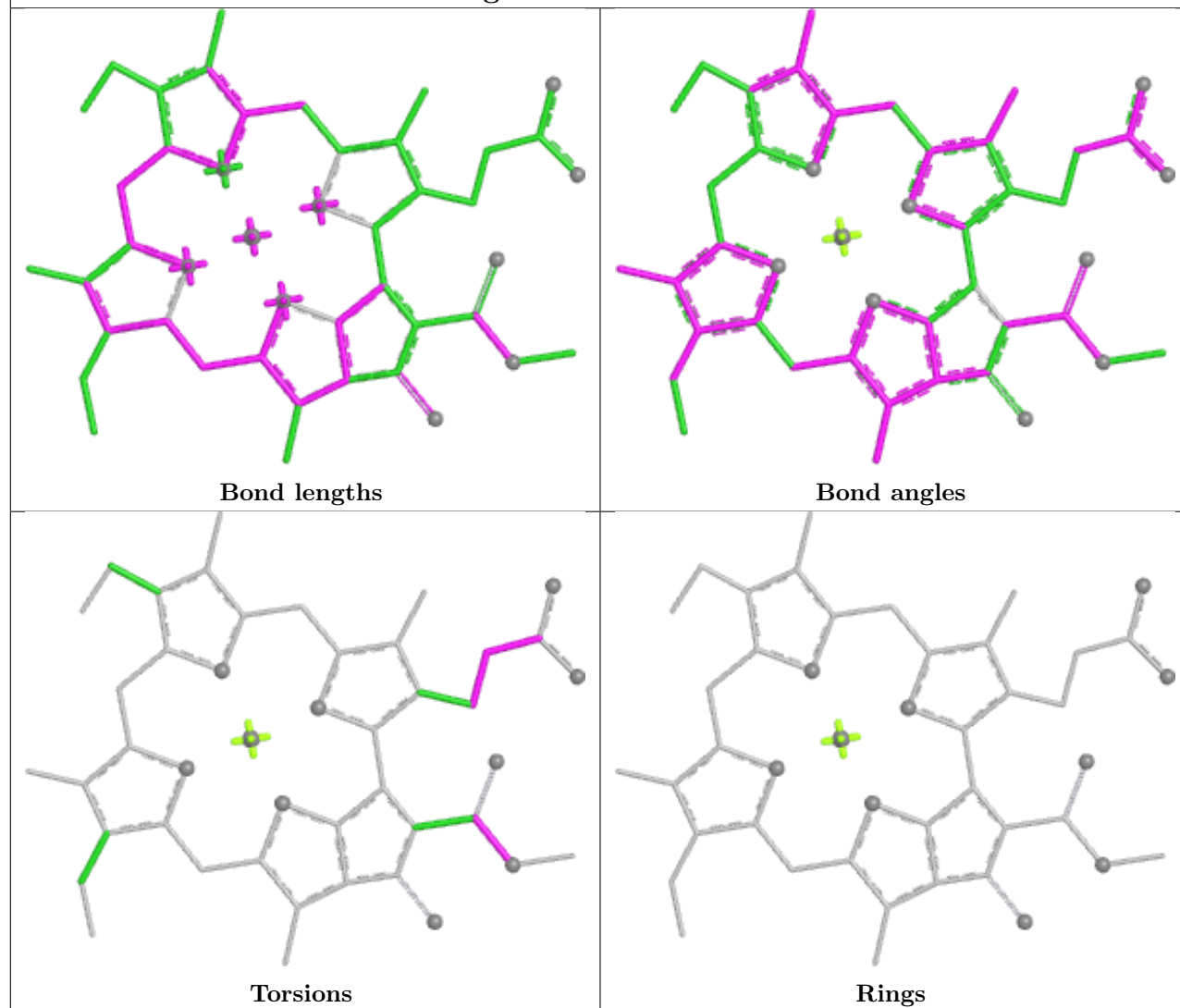


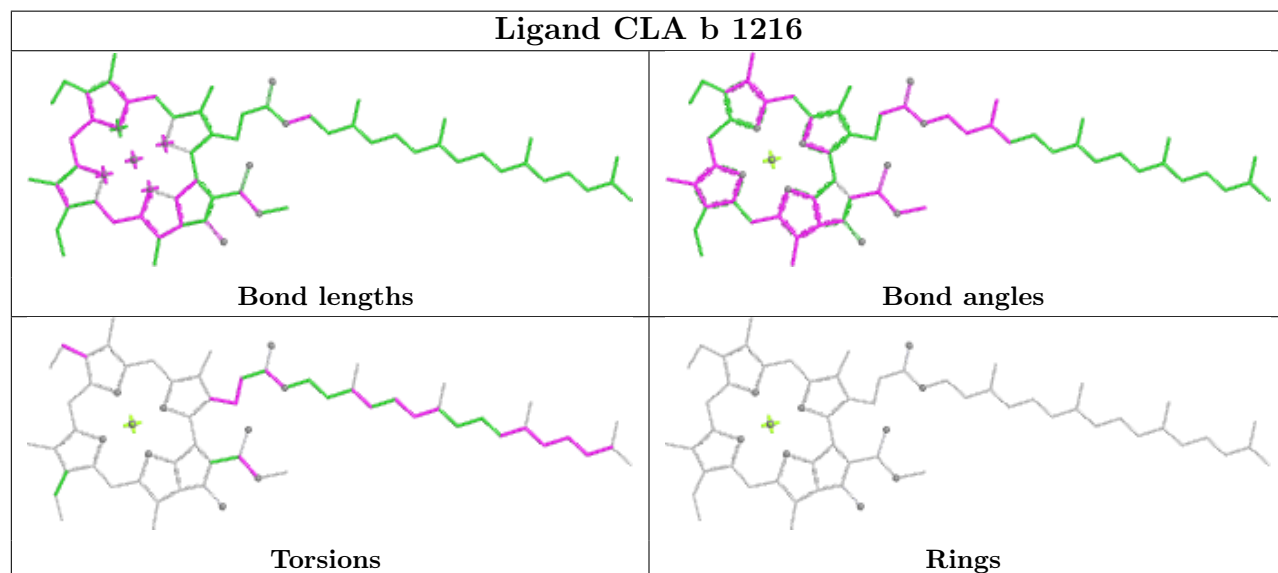
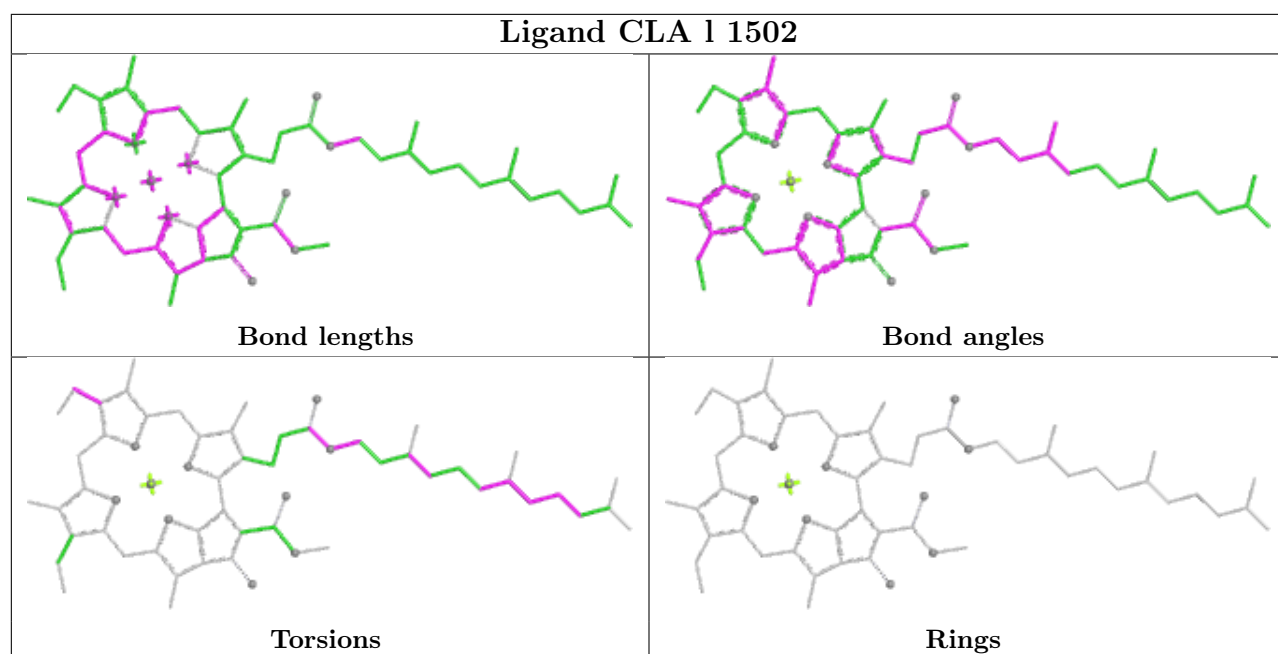


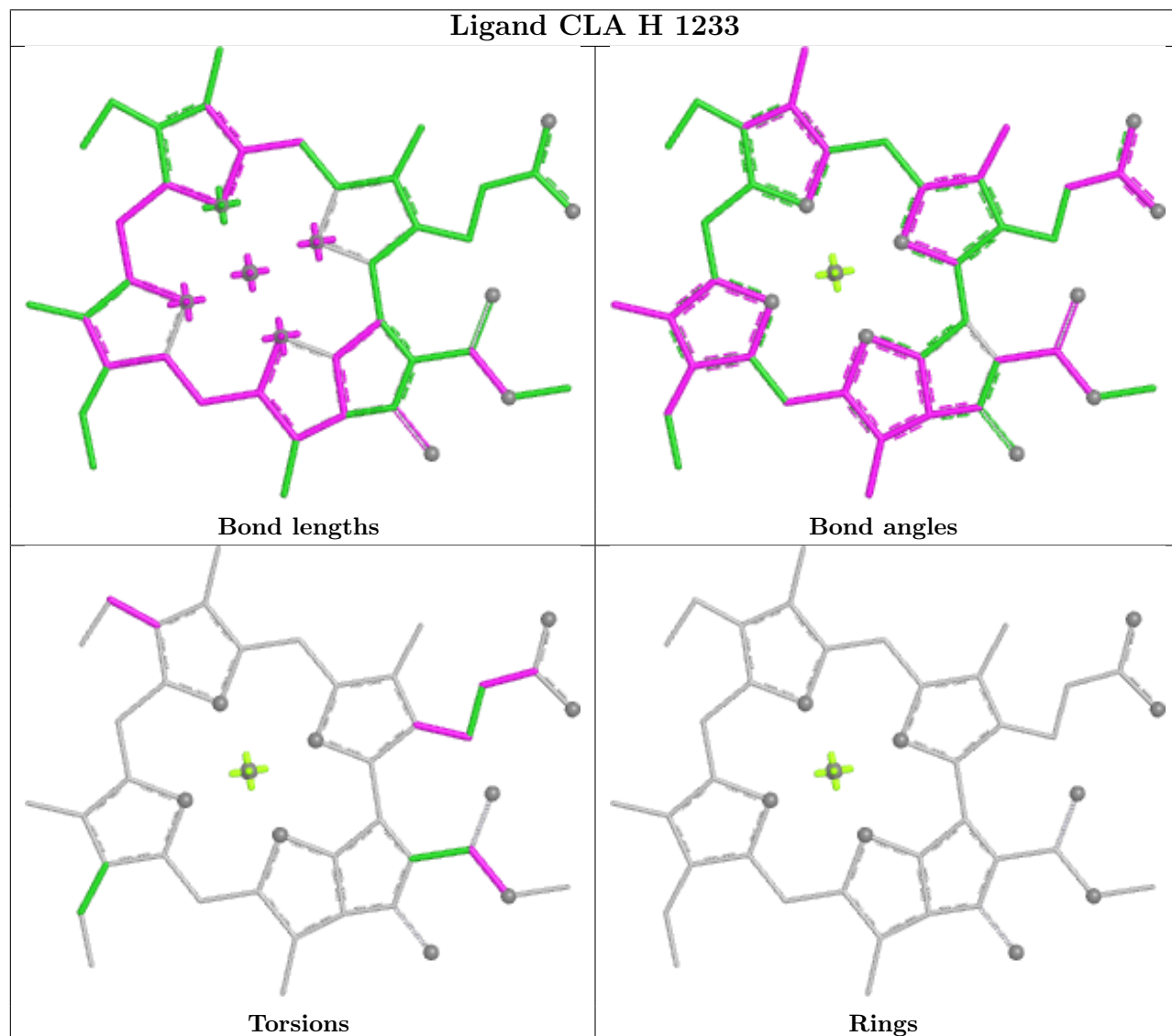
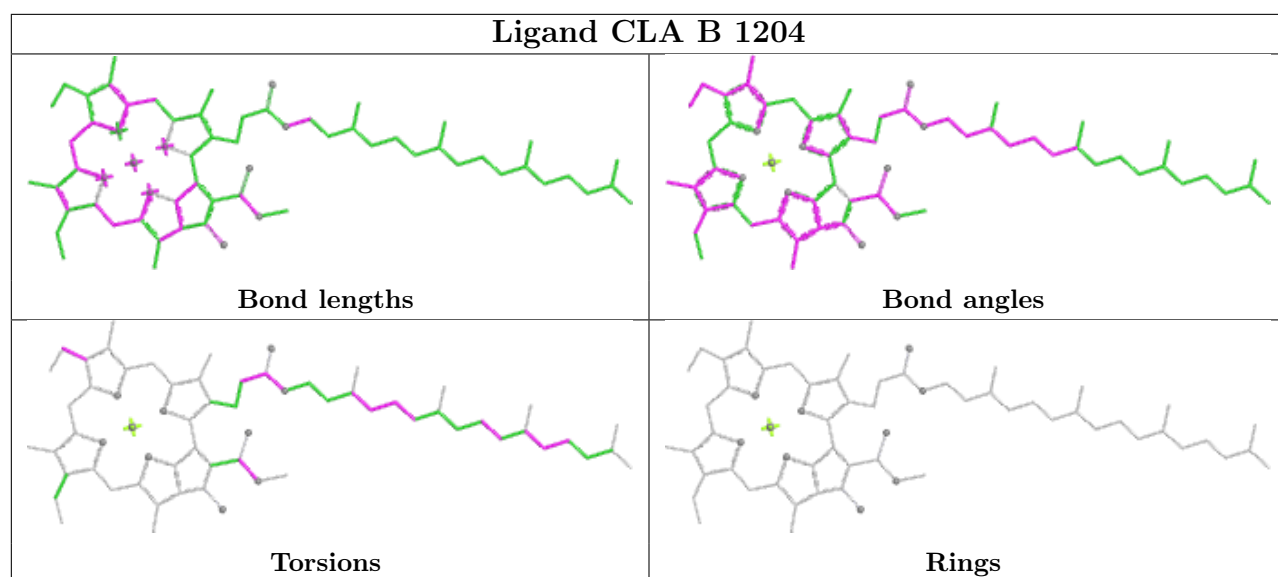
Ligand CLA H 1229

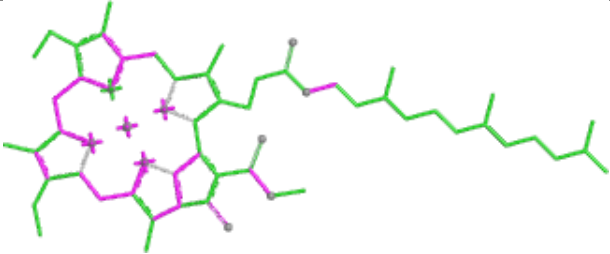
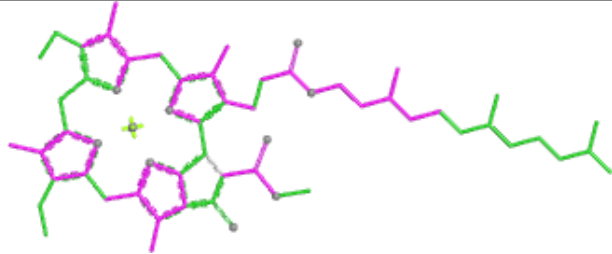
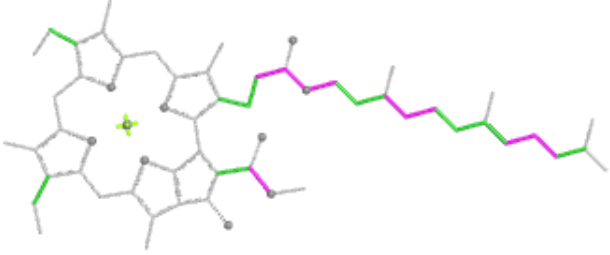
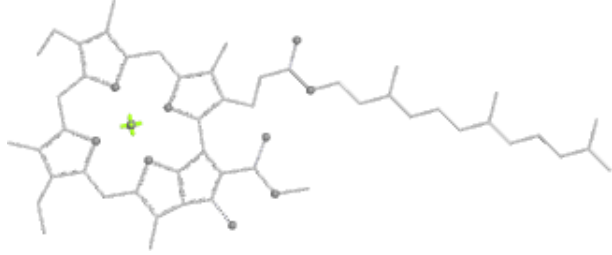
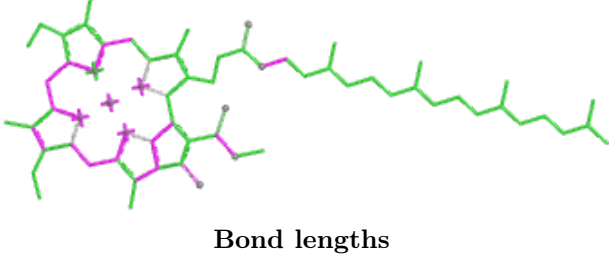
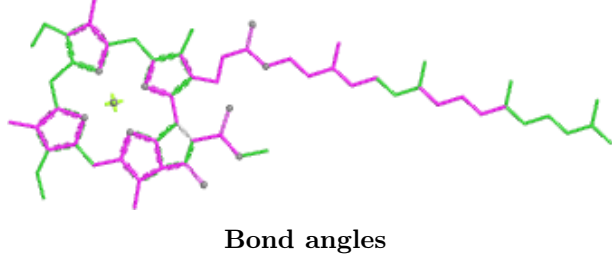
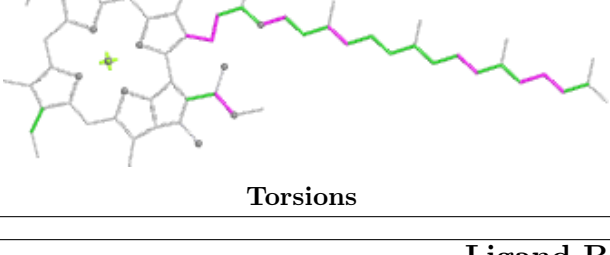
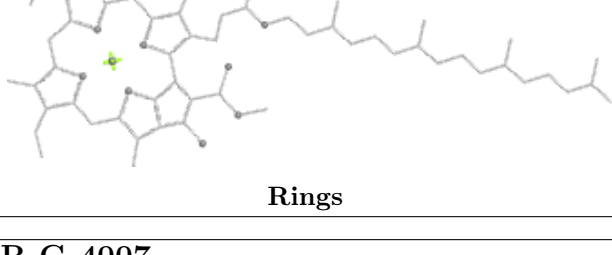
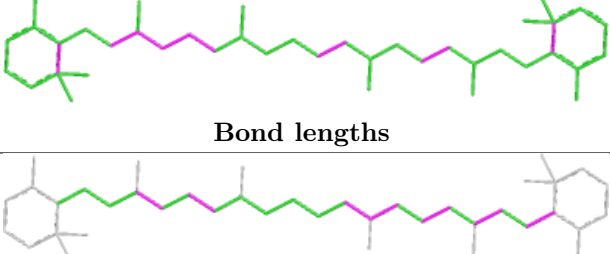
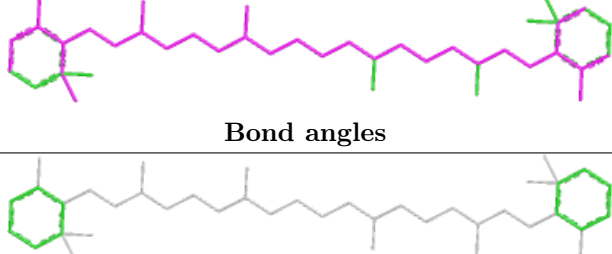


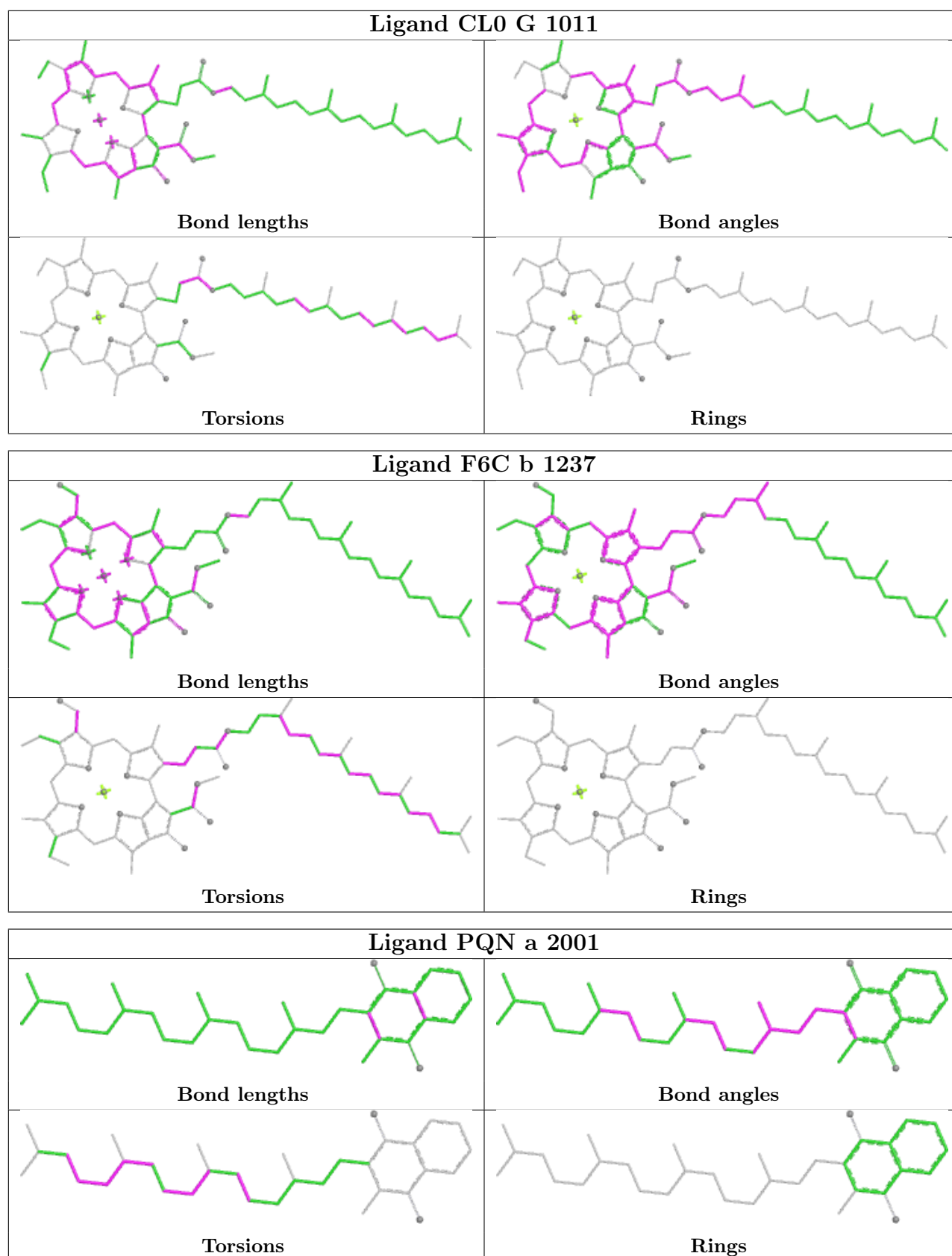
Ligand CLA A 1134

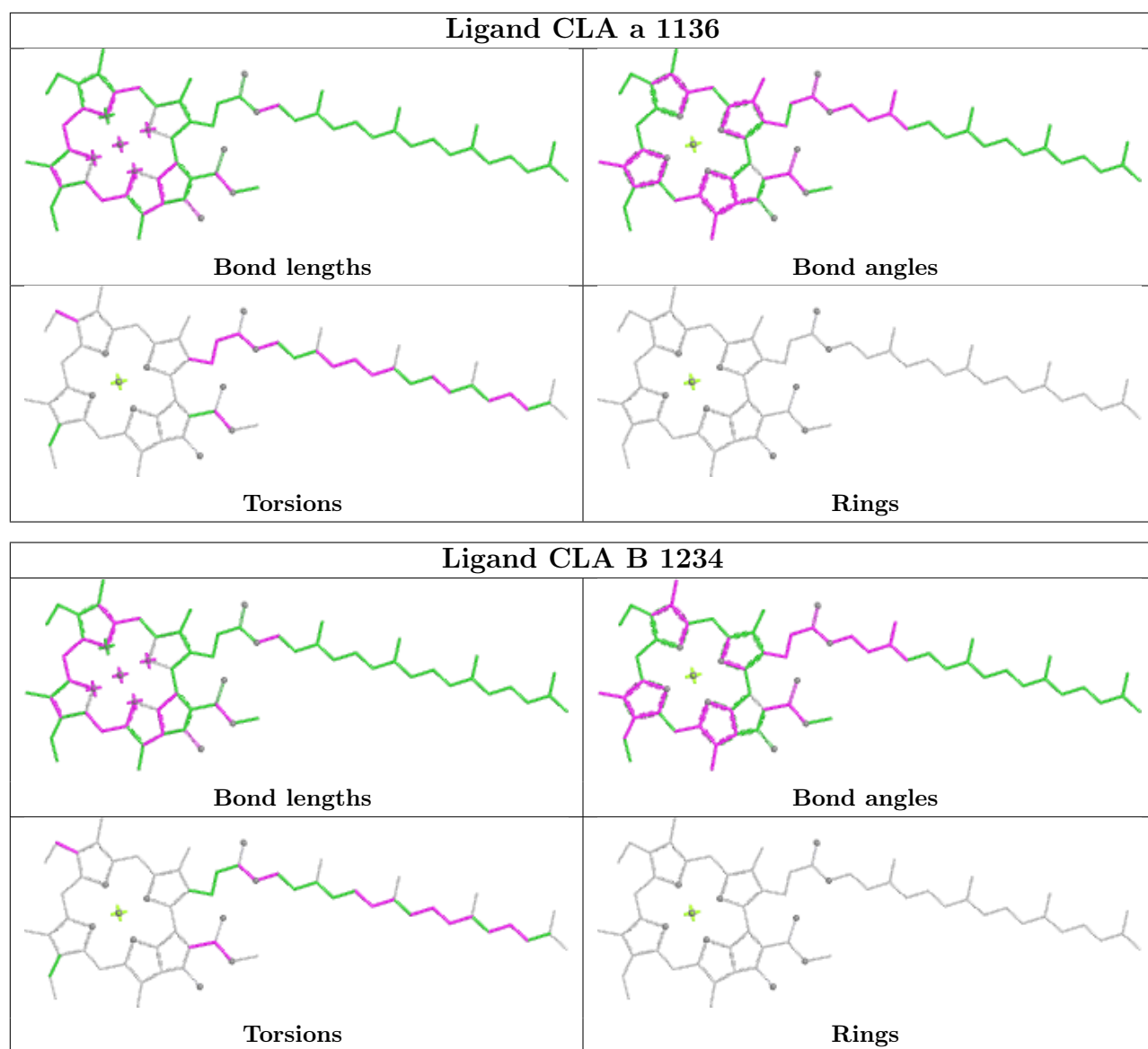


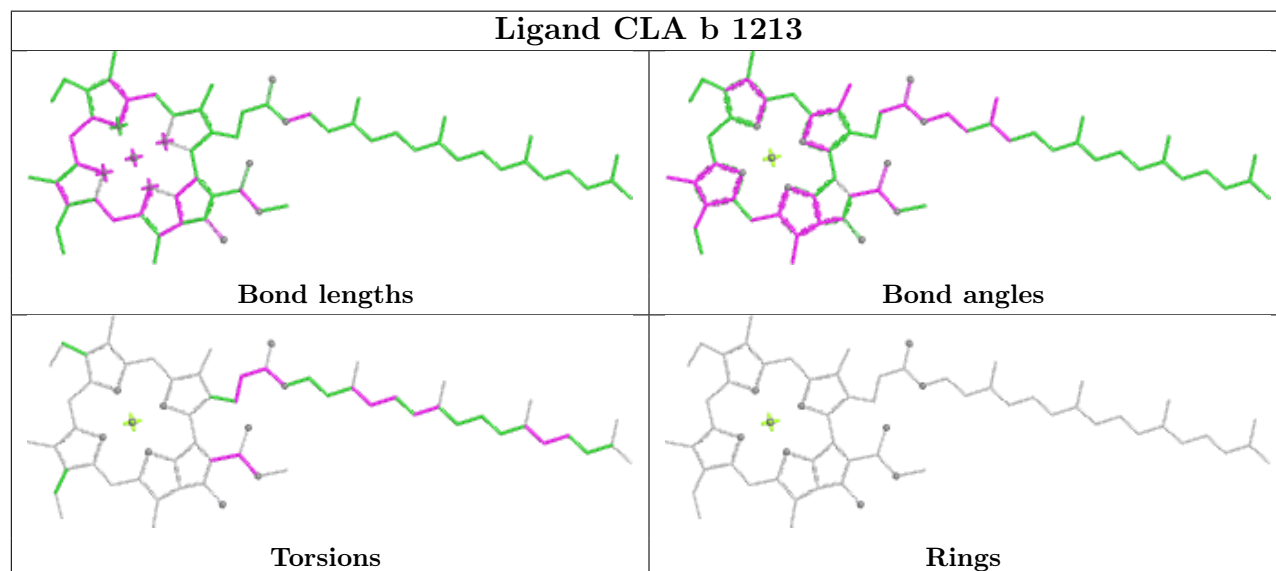
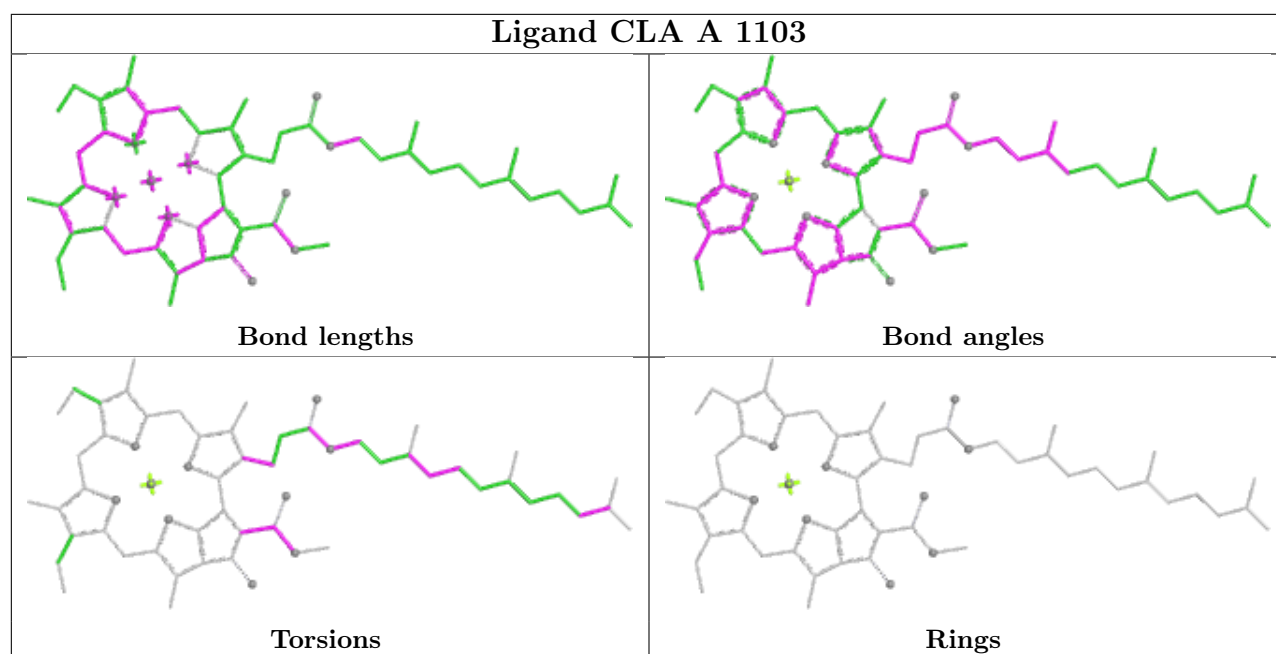


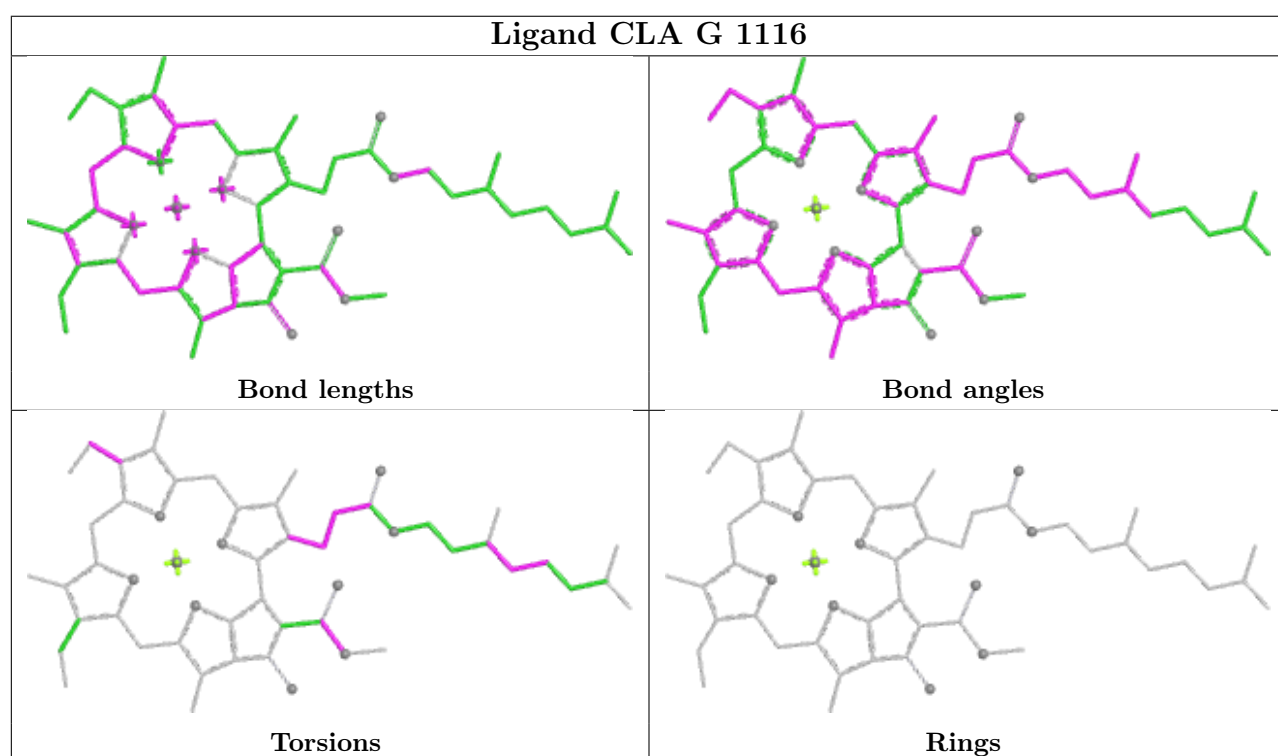
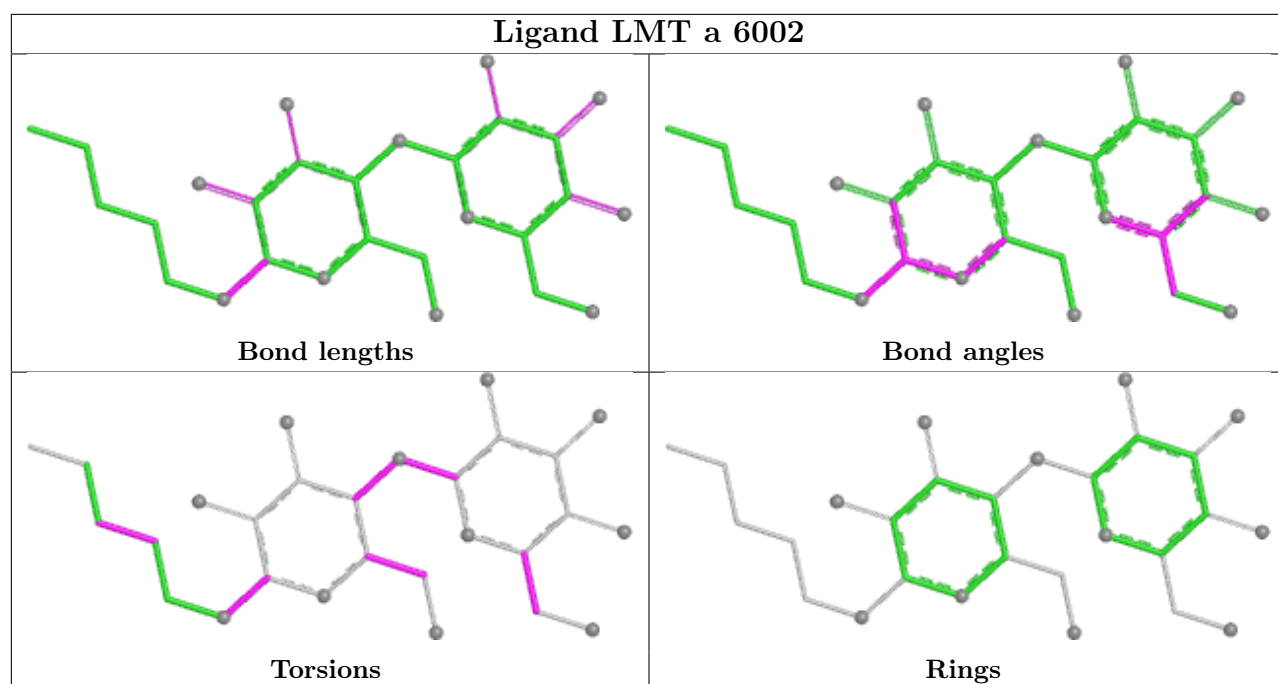


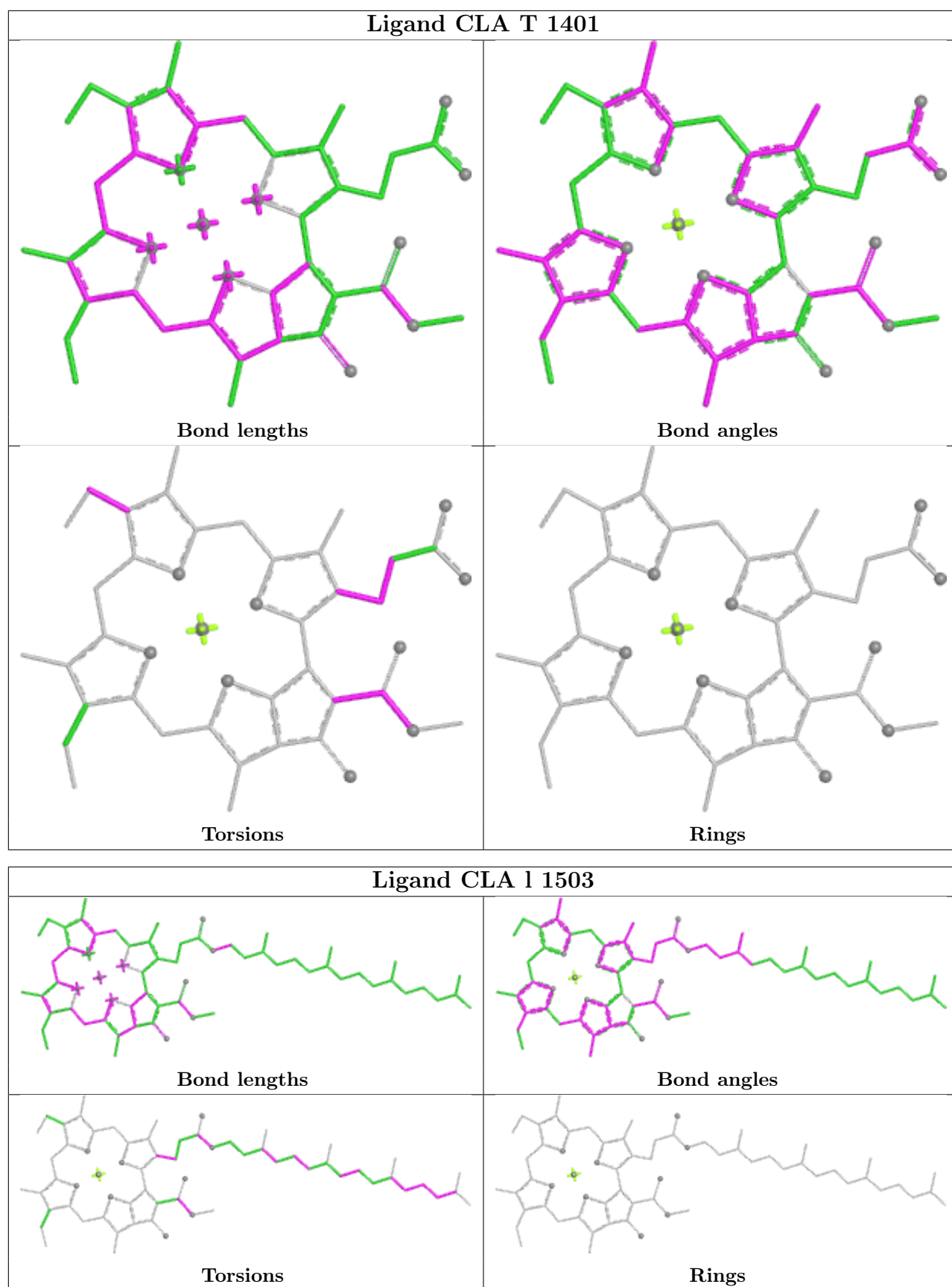
Ligand CLA B 1235	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA A 1012	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR G 4007	
	
Bond lengths	Bond angles
	
Torsions	Rings

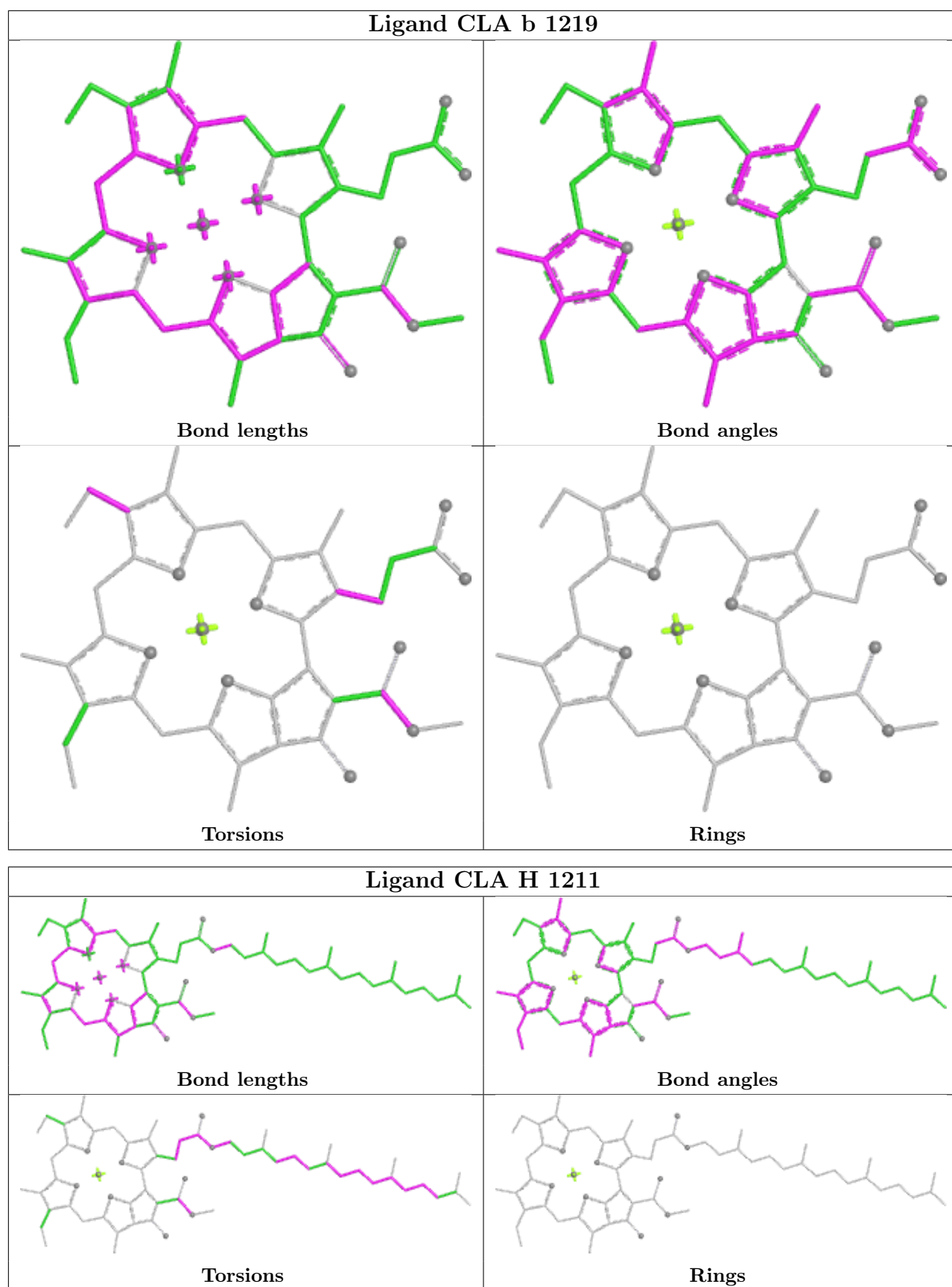


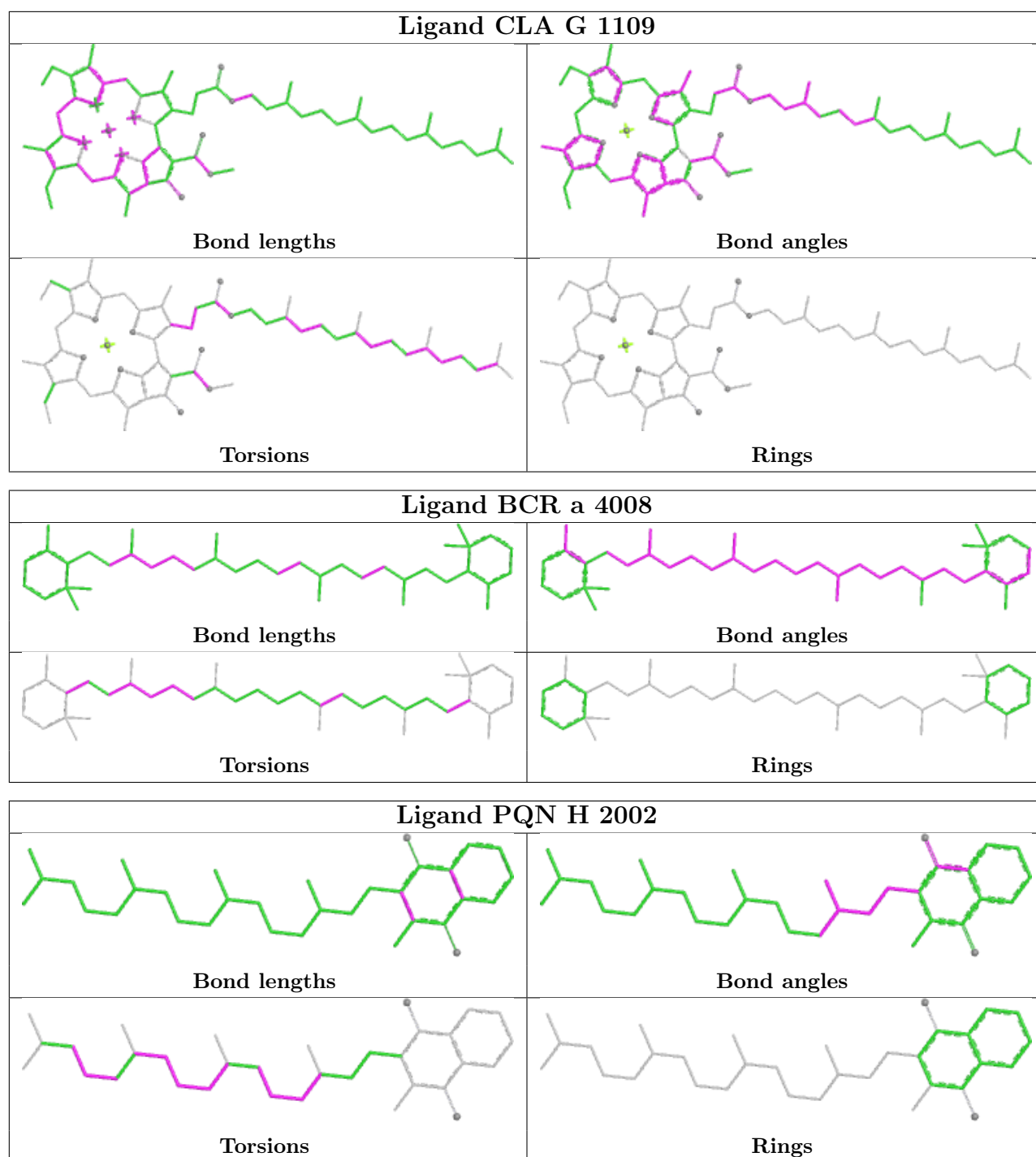


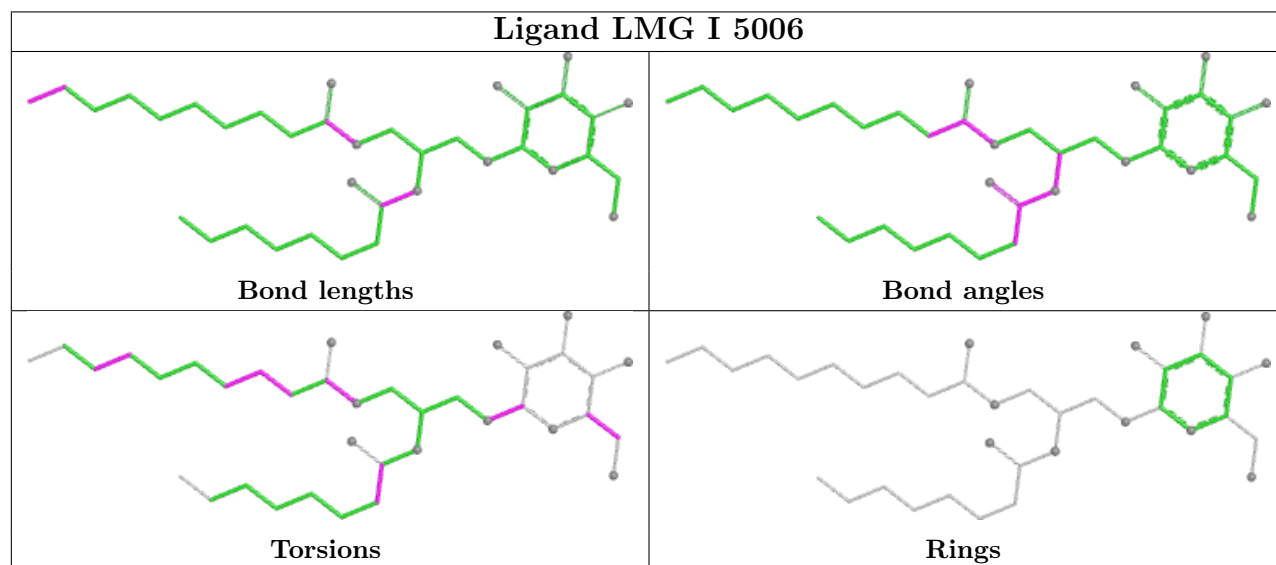
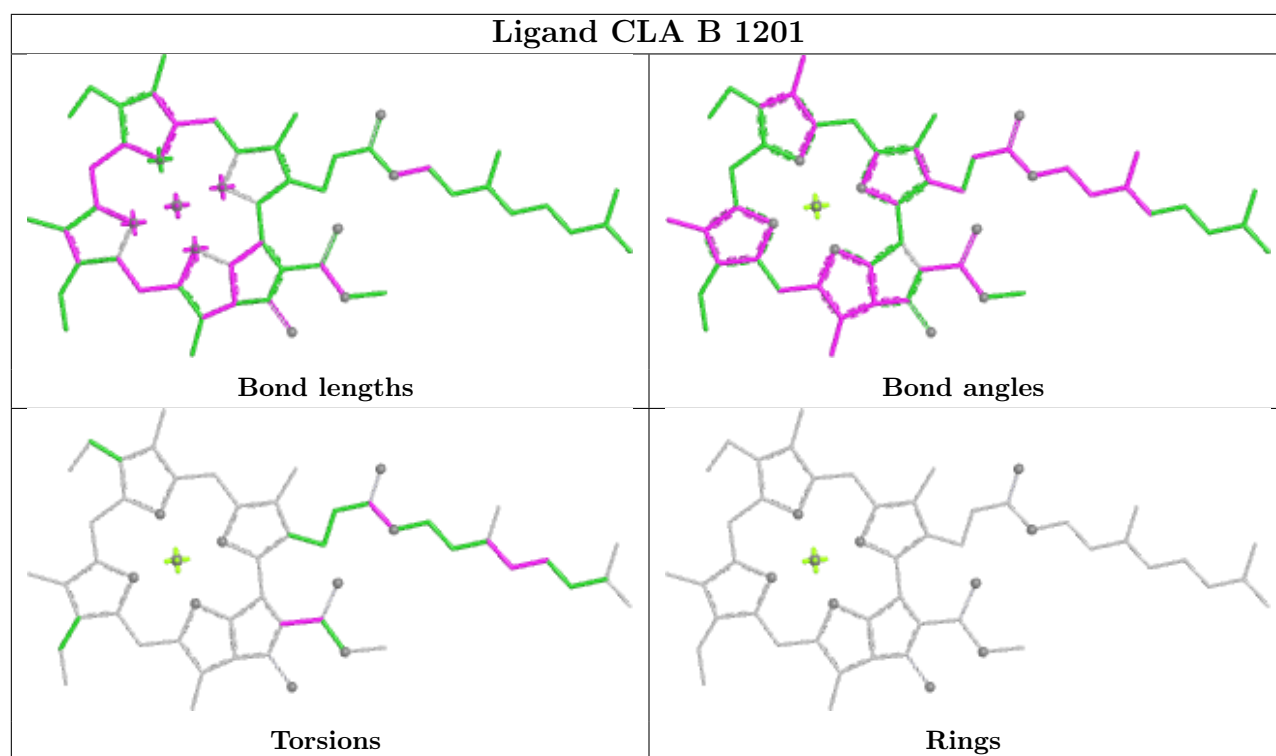




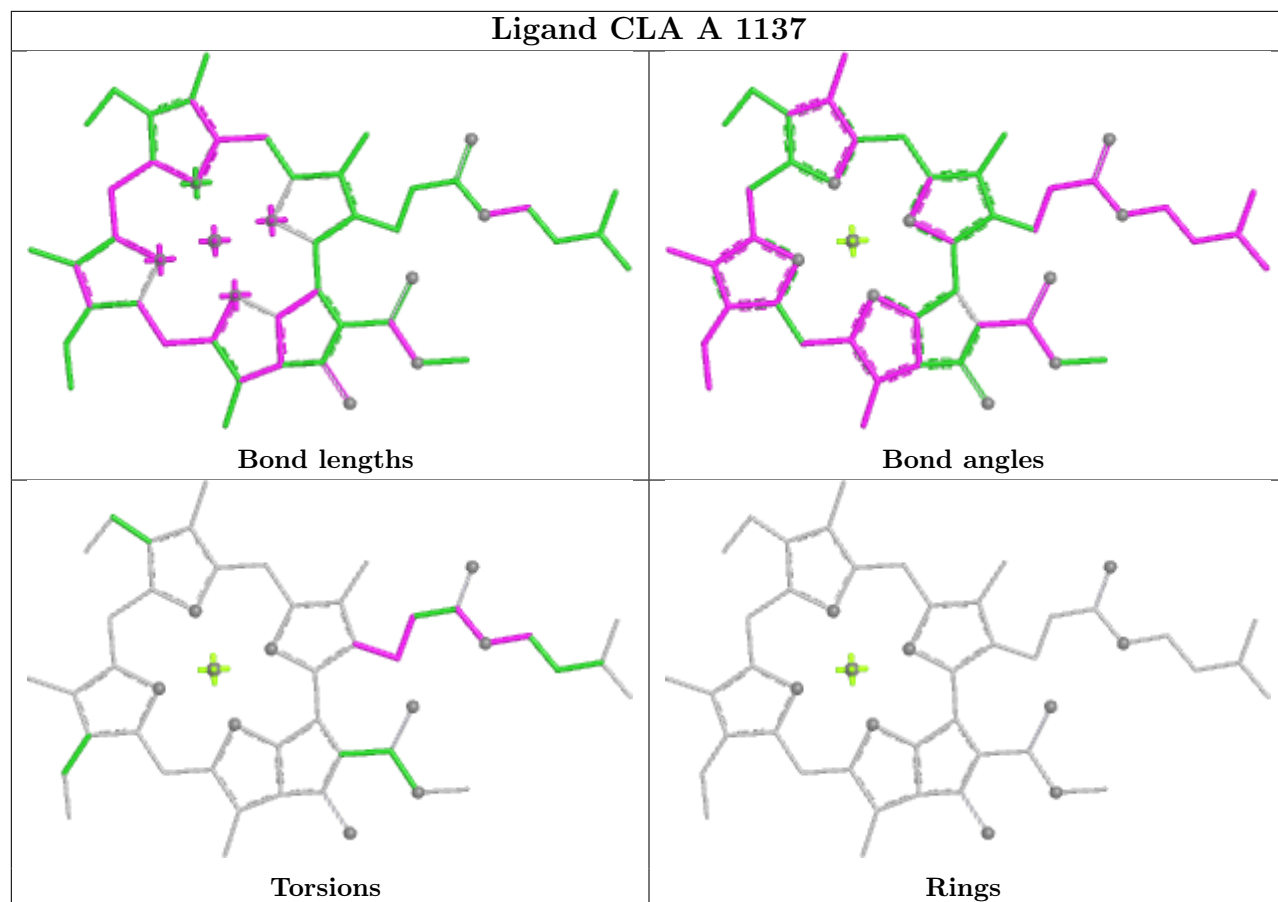




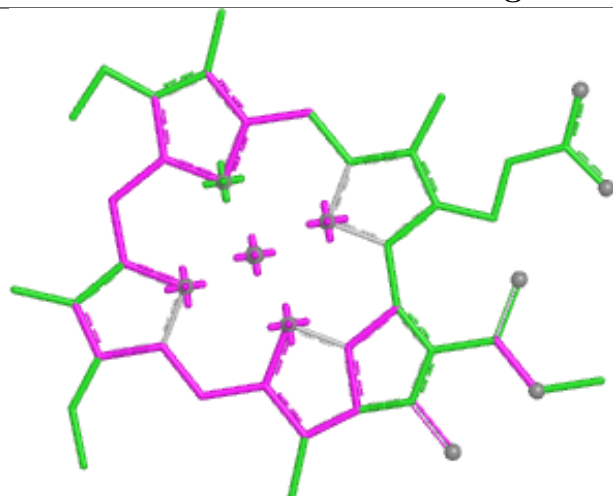




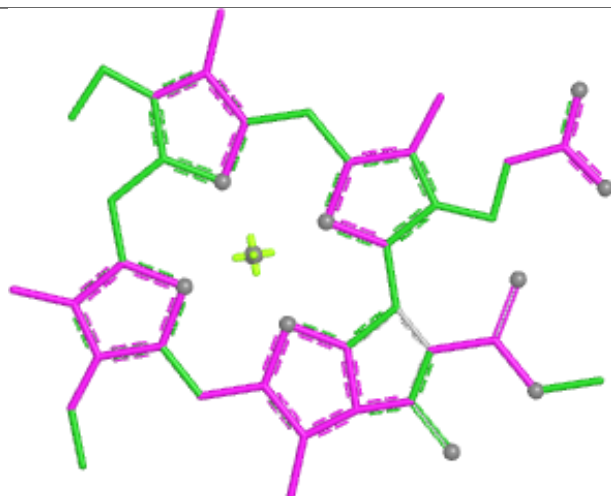
Ligand CLA A 1137



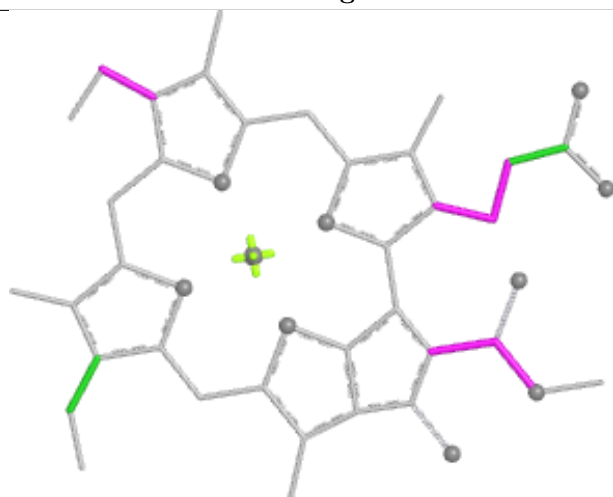
Ligand CLA K 1401



Bond lengths



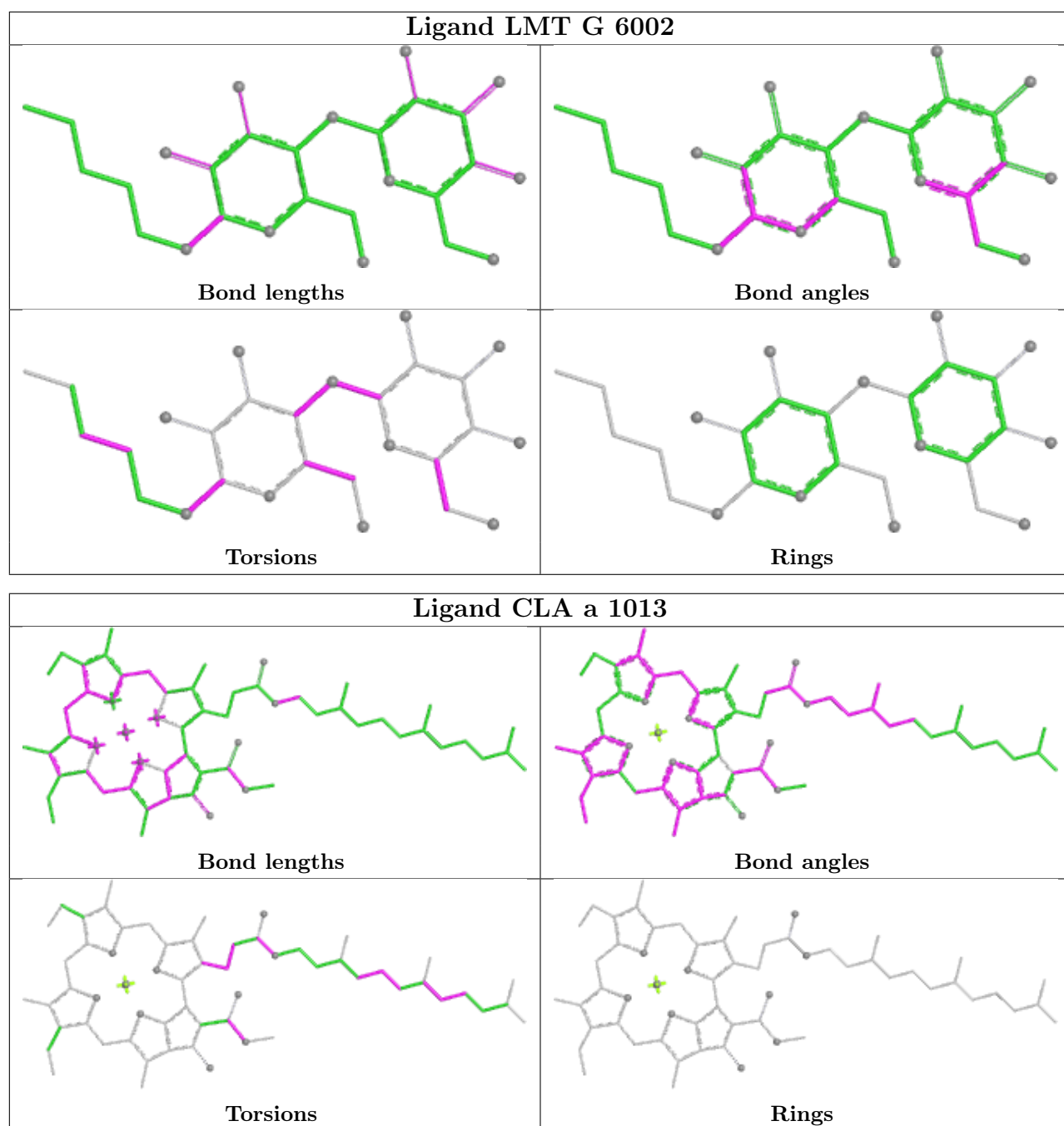
Bond angles

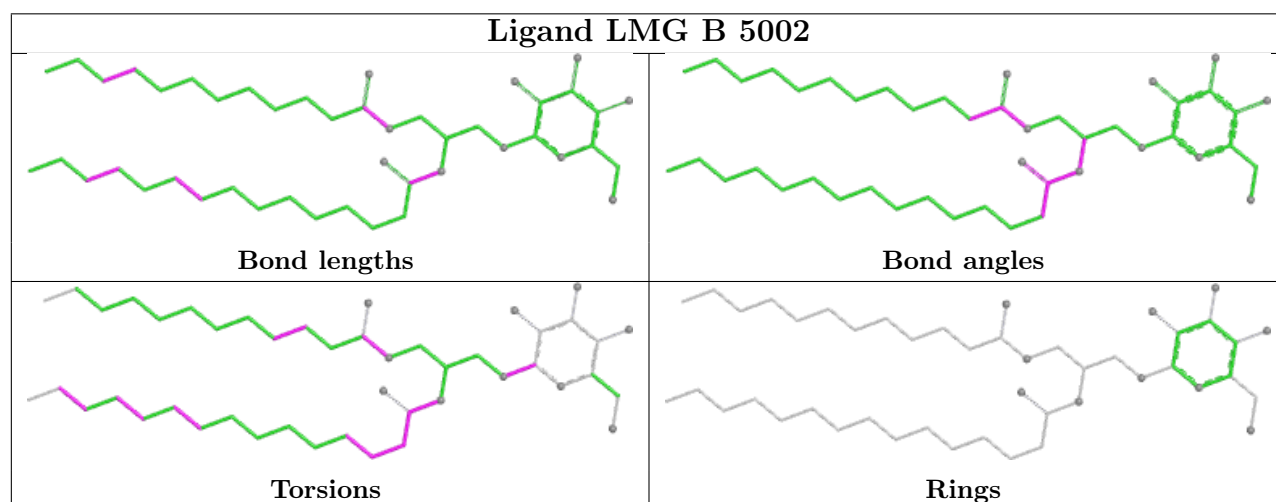
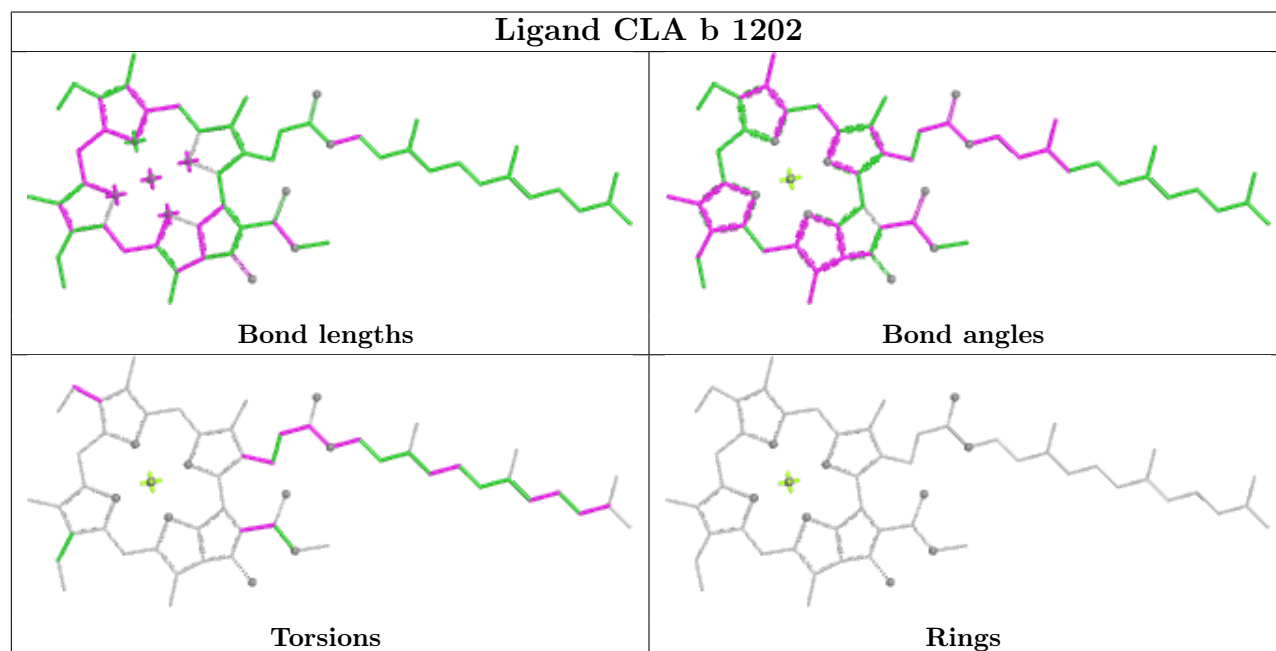
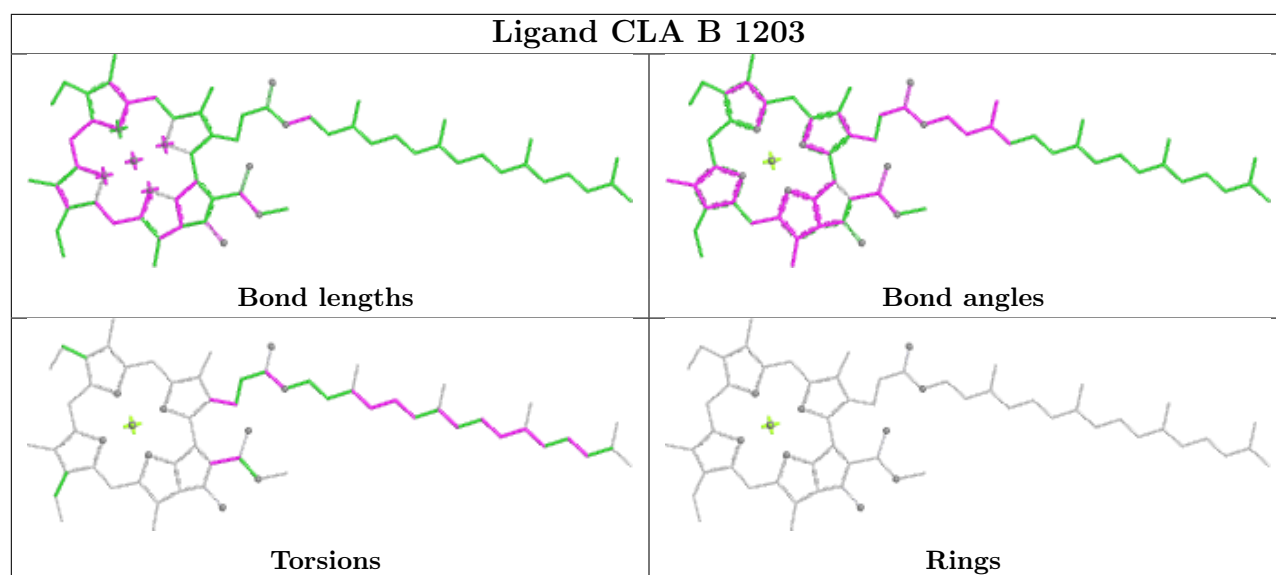


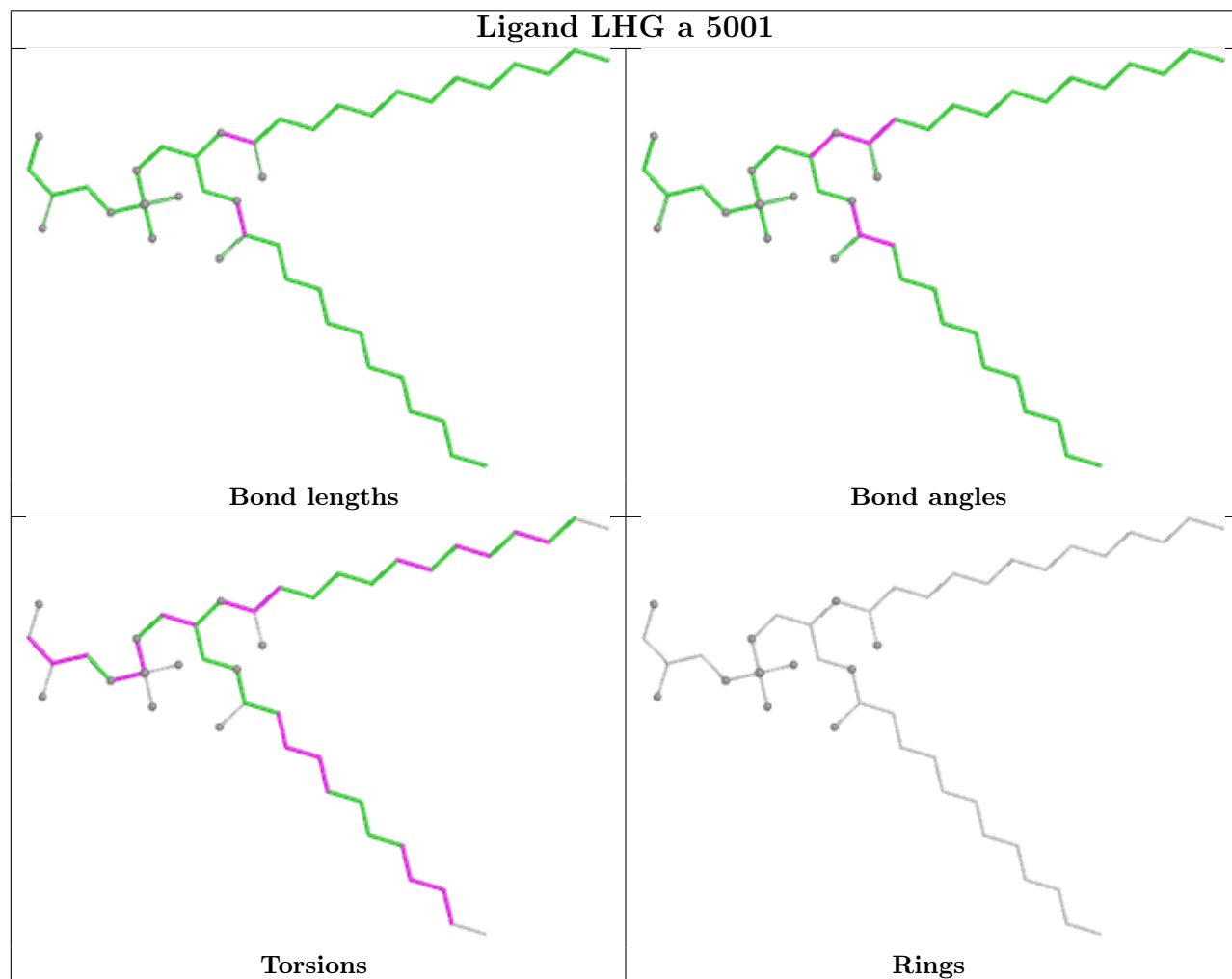
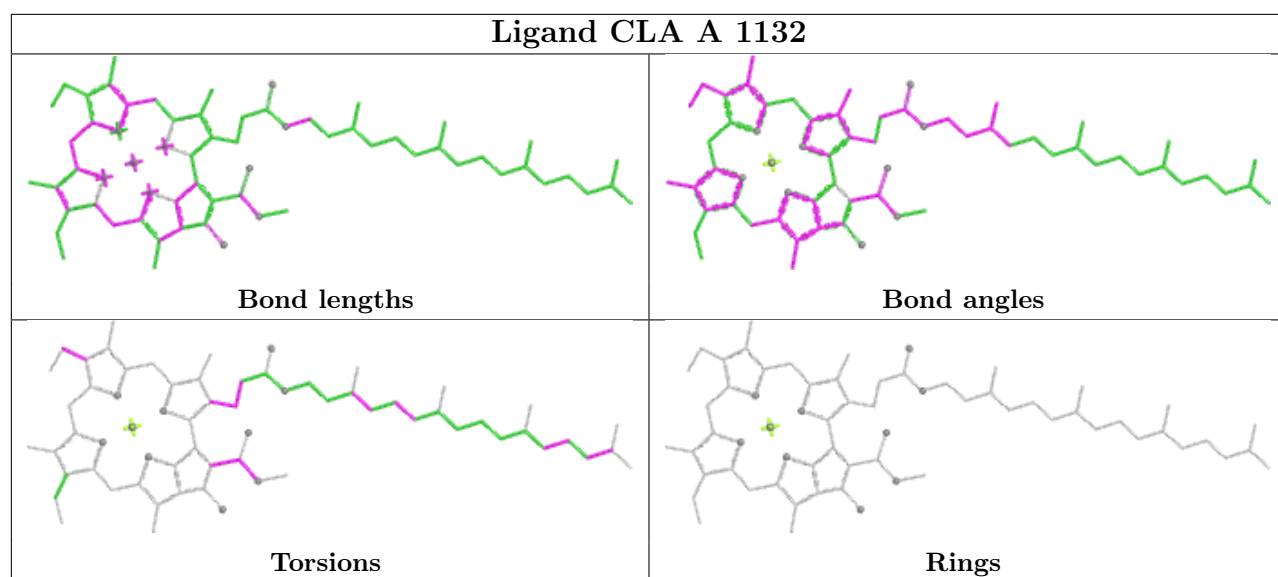
Torsions

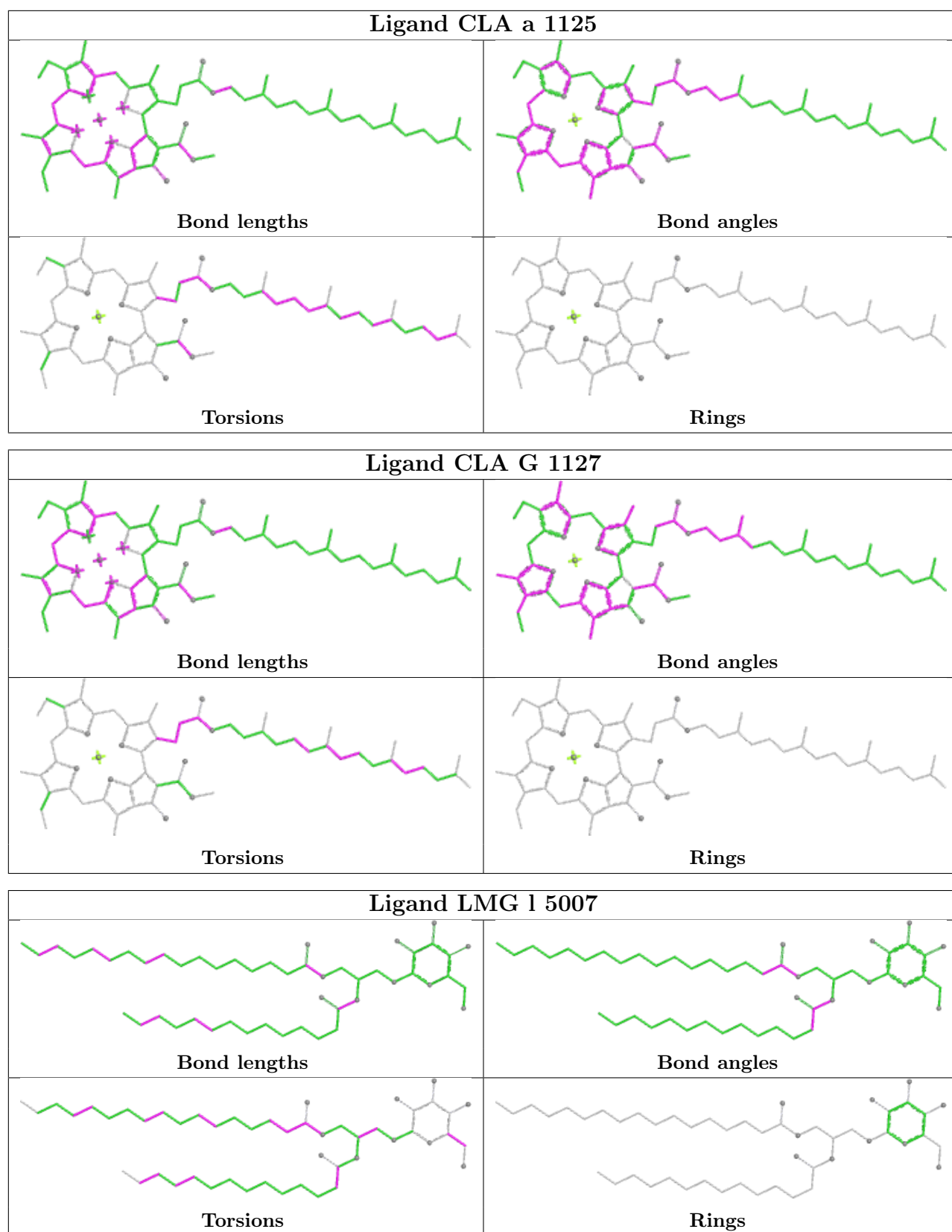


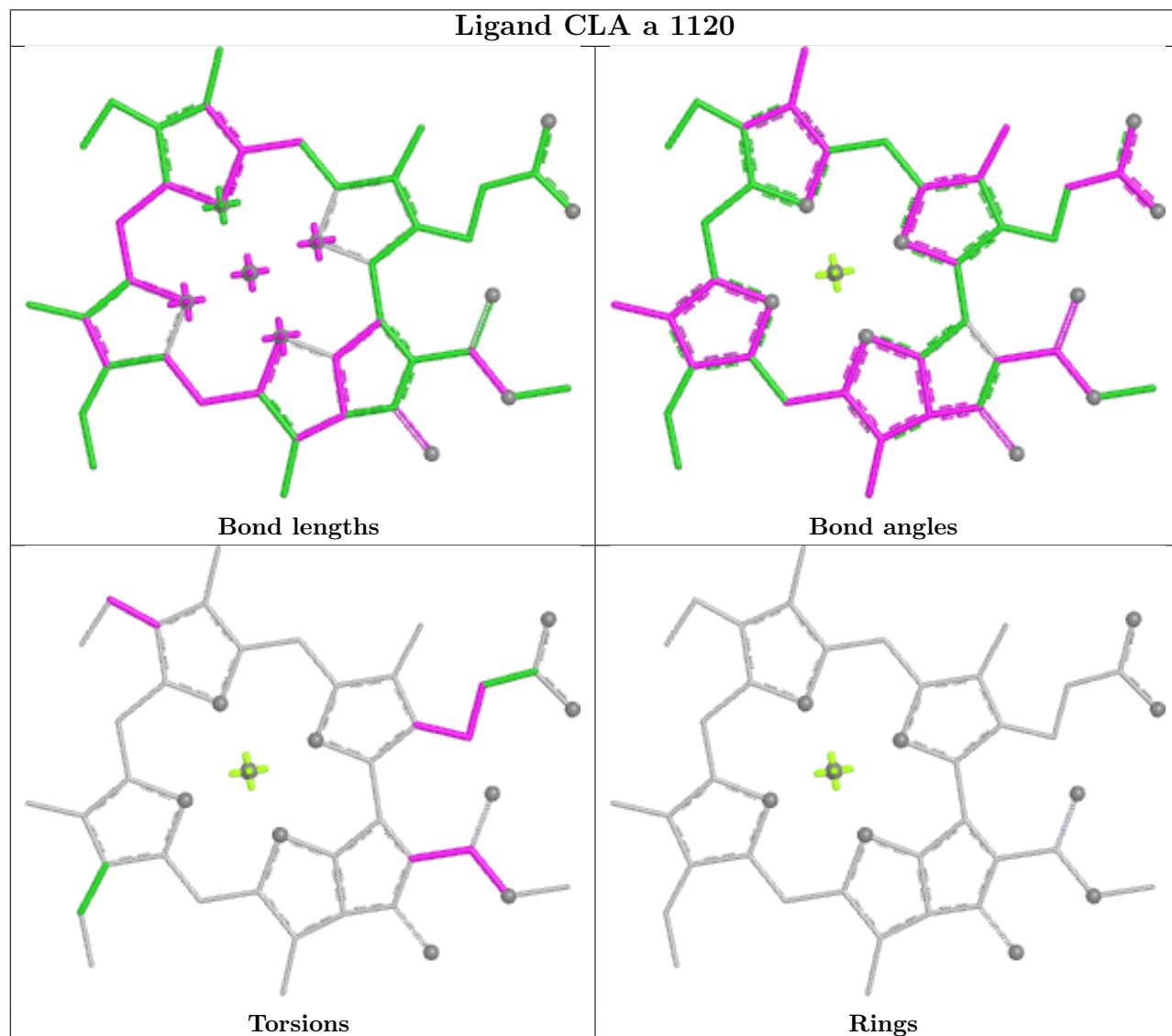
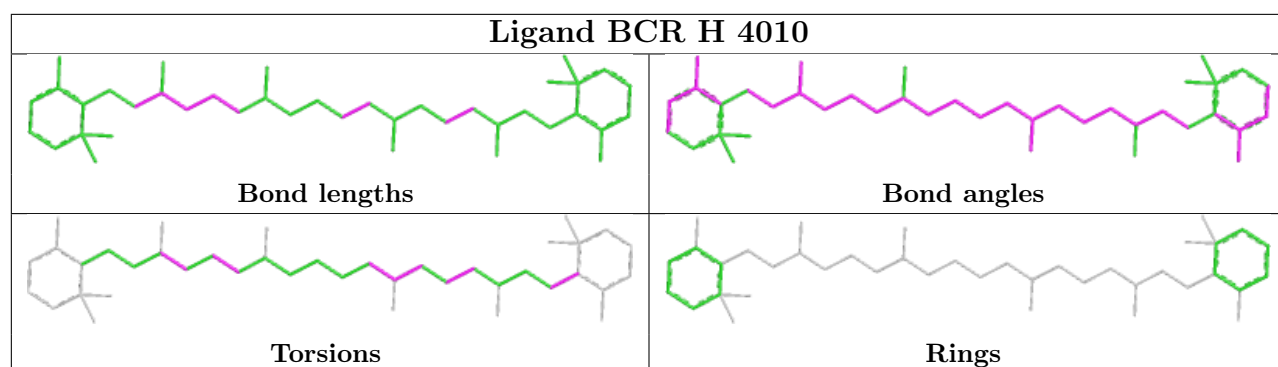
Rings

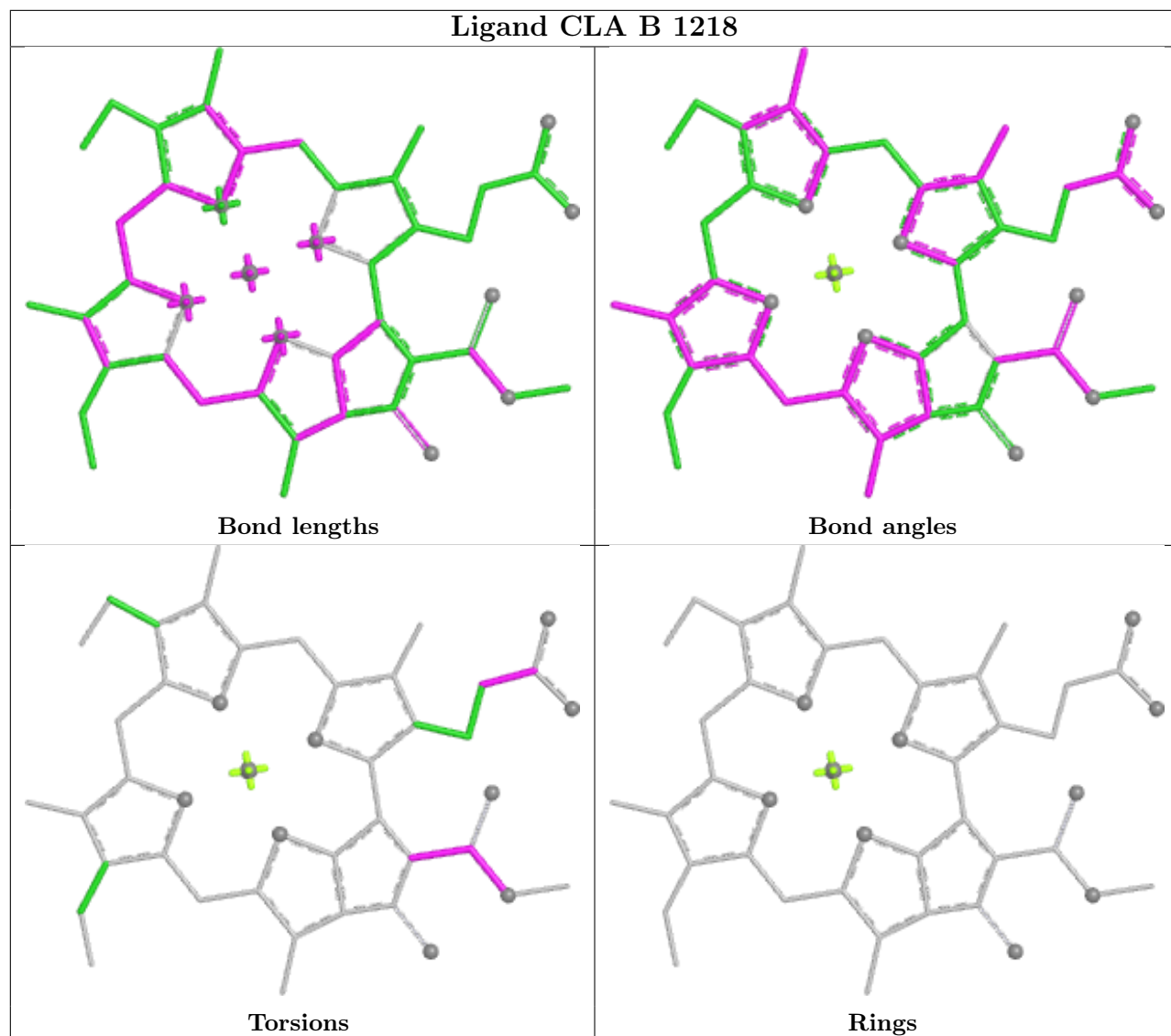




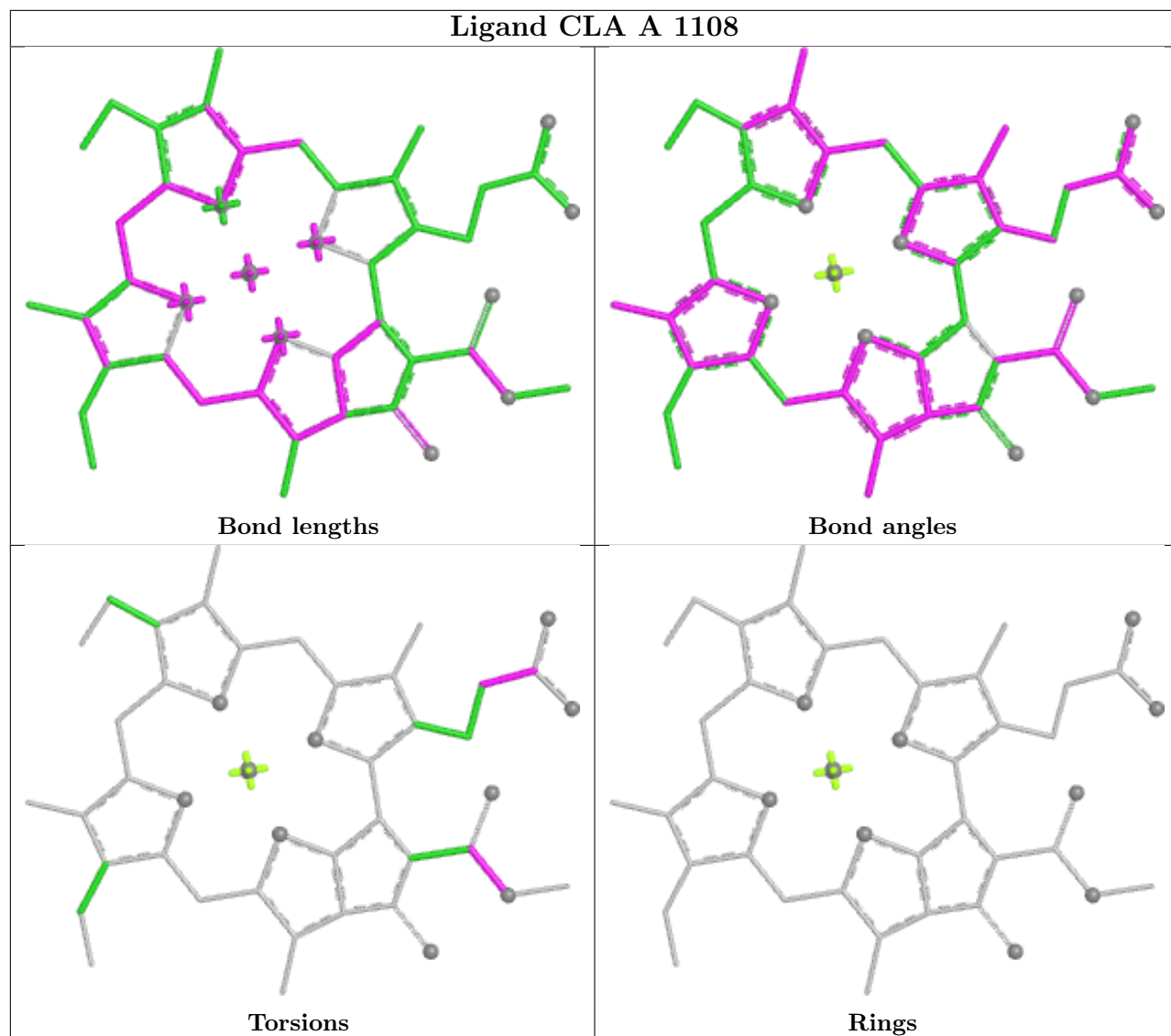




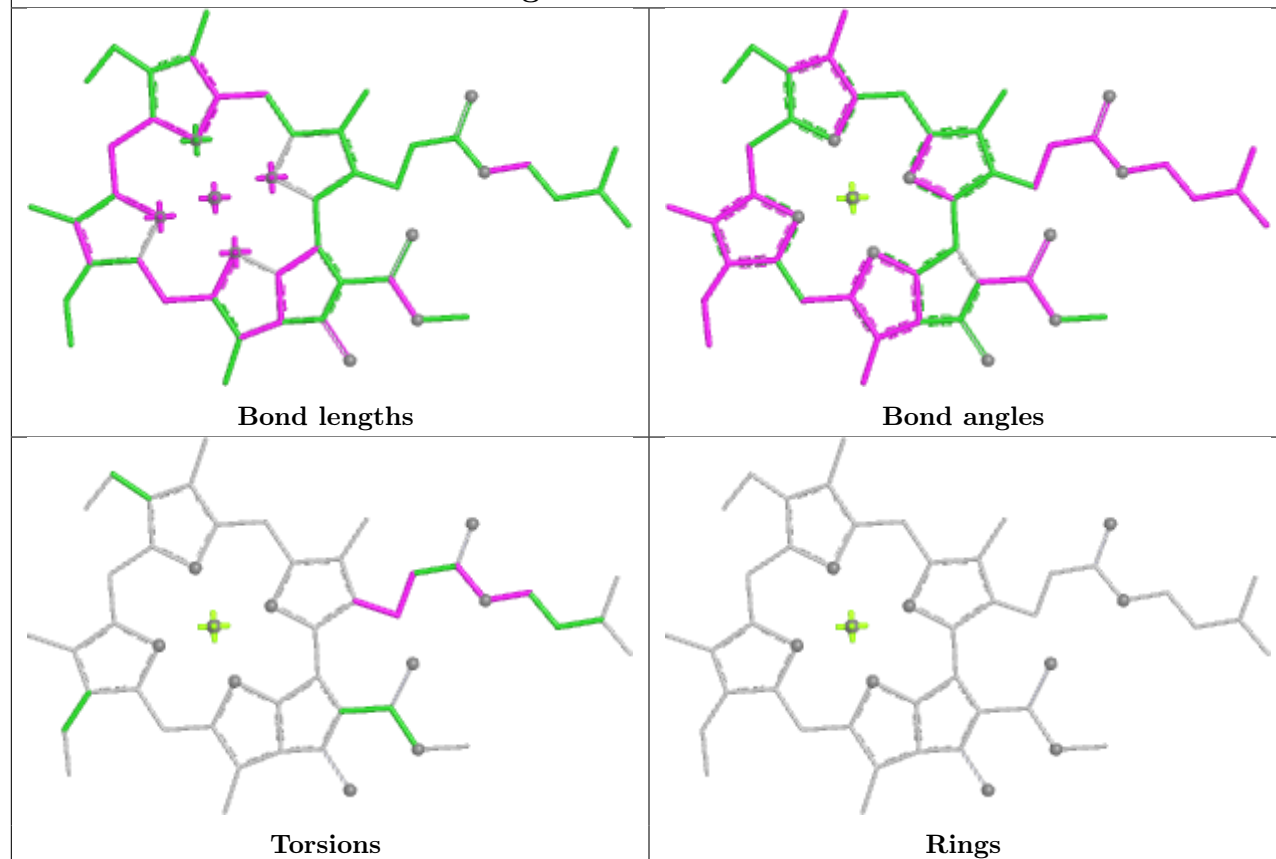




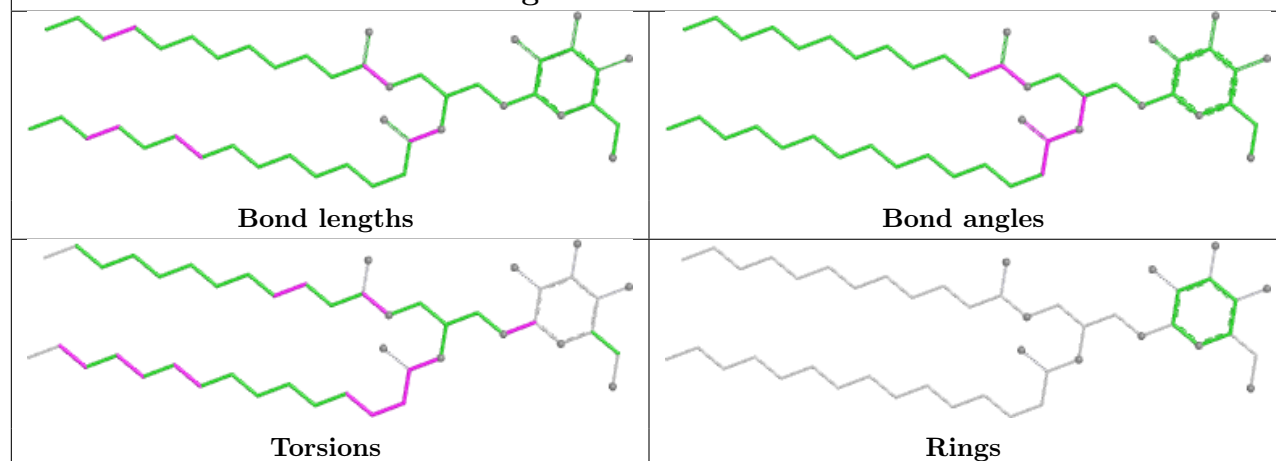
Ligand CLA A 1108



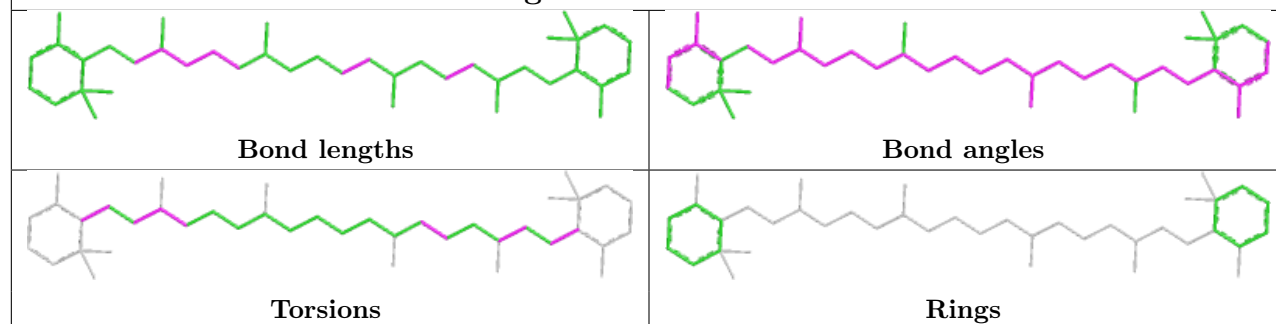
Ligand CLA G 1137

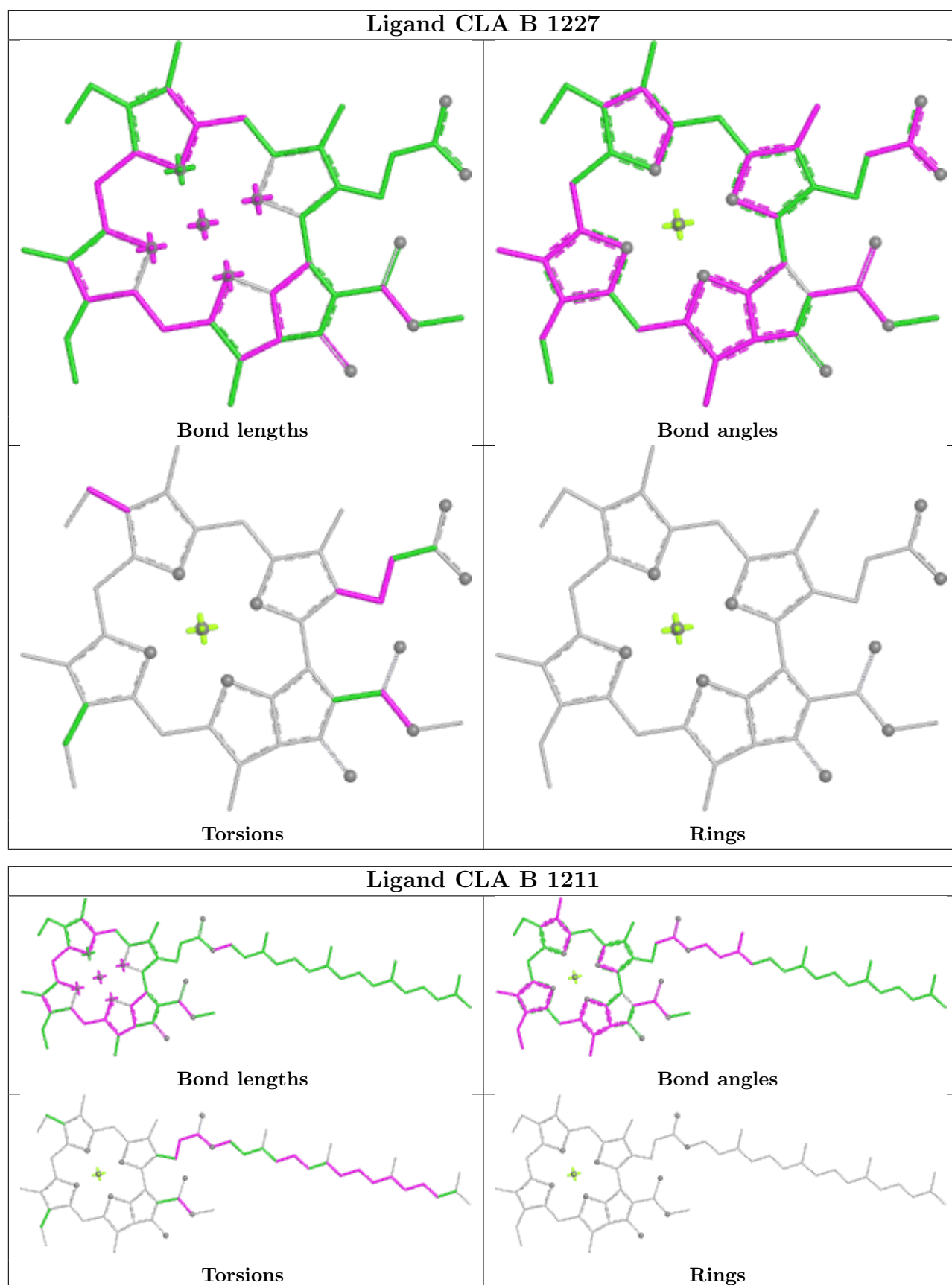


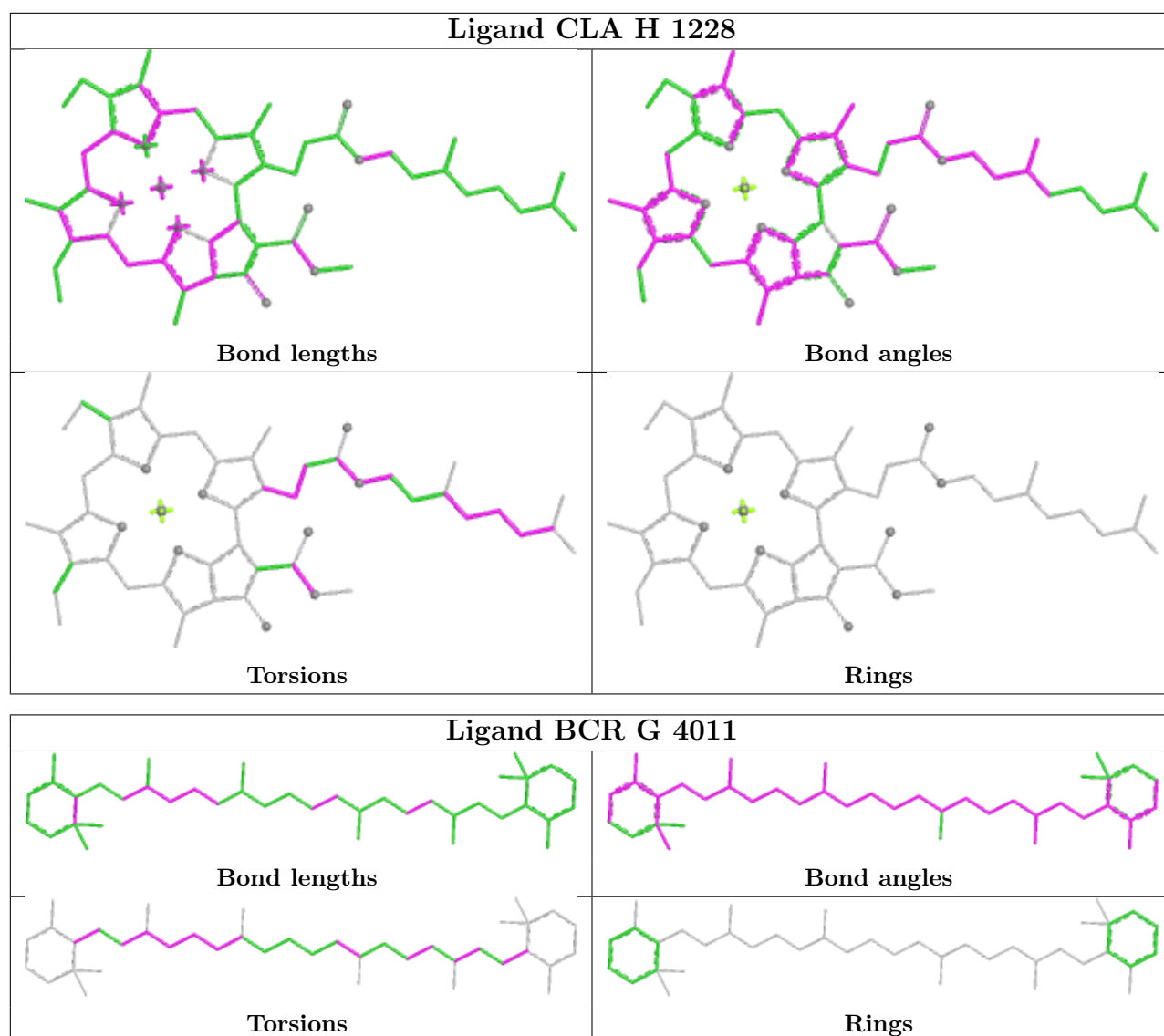
Ligand LMG b 5002



Ligand BCR b 4006







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	T	1
9	k	1
9	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	49:UNK	C	69:VAL	N	9.76
1	k	49:UNK	C	69:VAL	N	9.75
1	K	49:UNK	C	69:VAL	N	9.75

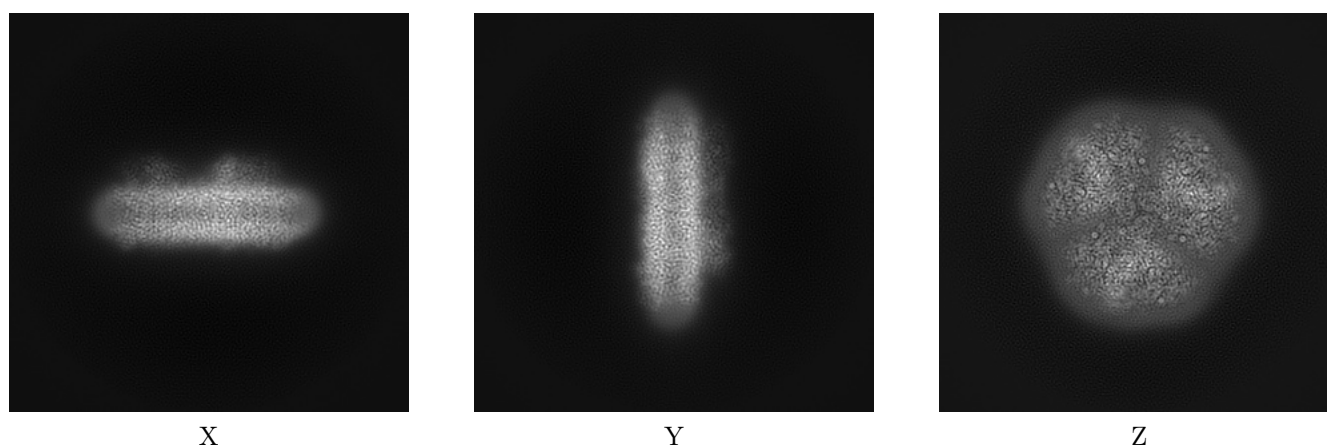
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23563. 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](#)

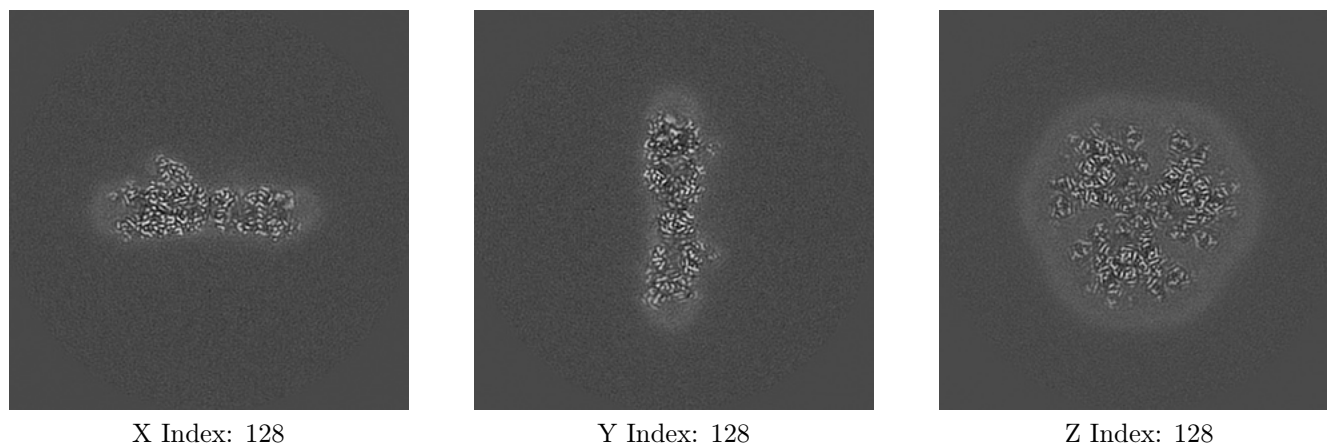
6.1.1 Primary map



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

6.2 Central slices [i](#)

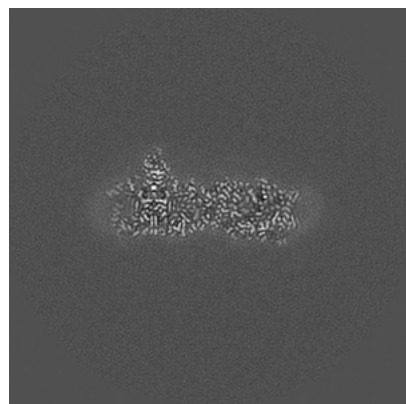
6.2.1 Primary map



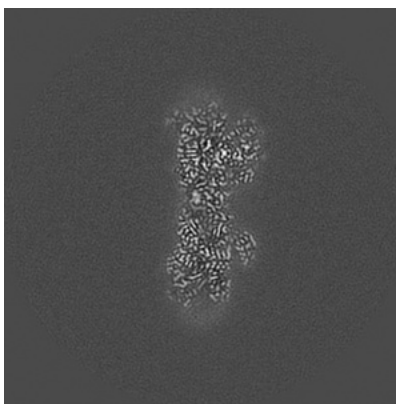
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

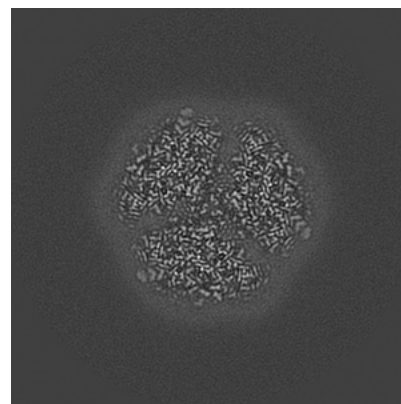
6.3.1 Primary map



X Index: 121



Y Index: 140

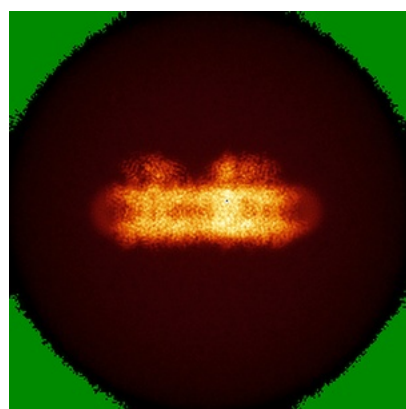


Z Index: 120

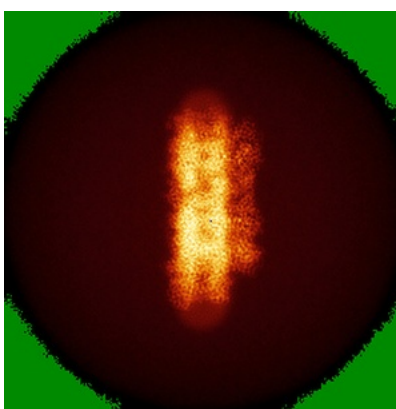
The images above show the largest variance slices of the map in three orthogonal directions.

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

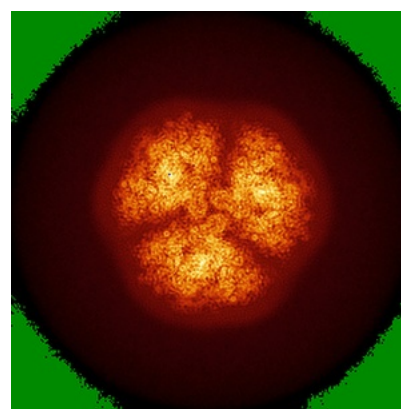
6.4.1 Primary map



X



Y

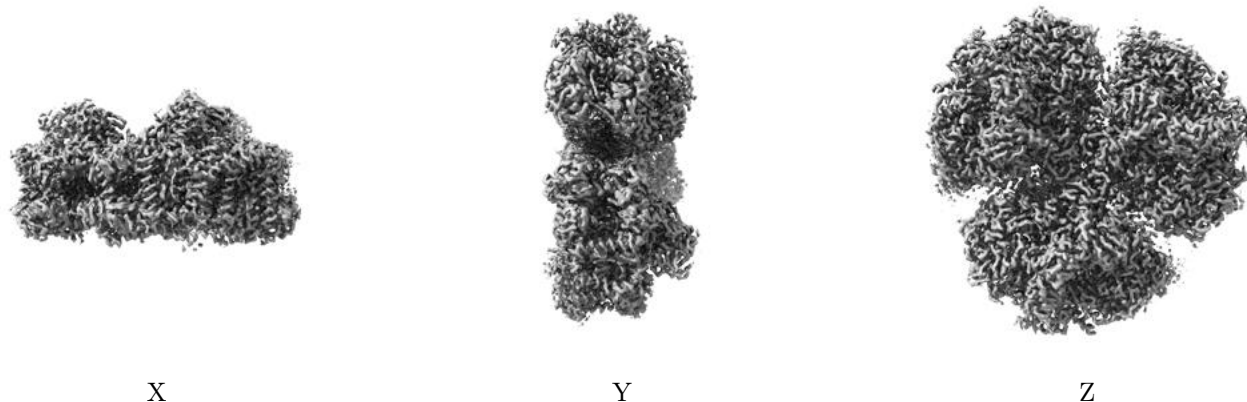


Z

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

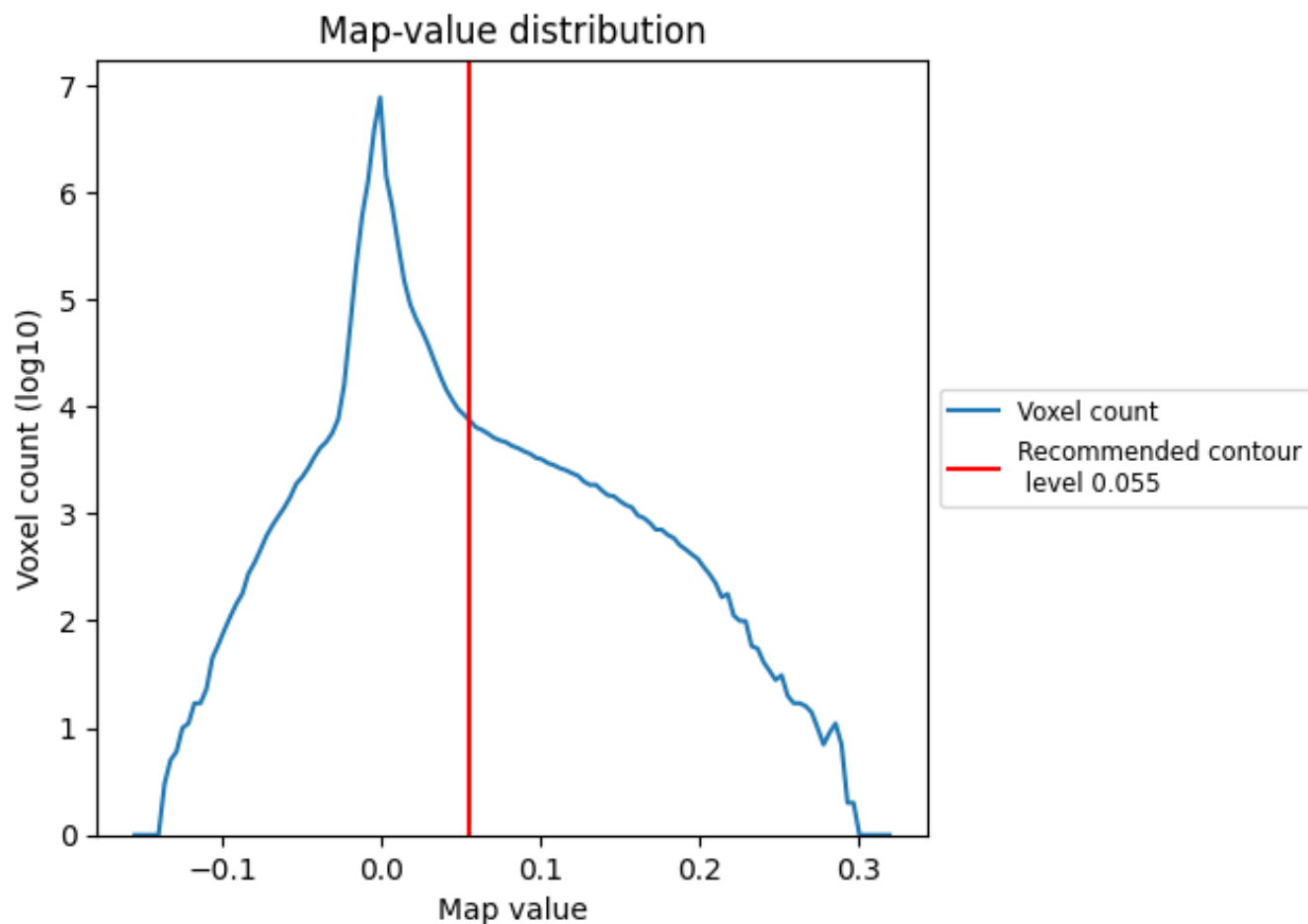
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

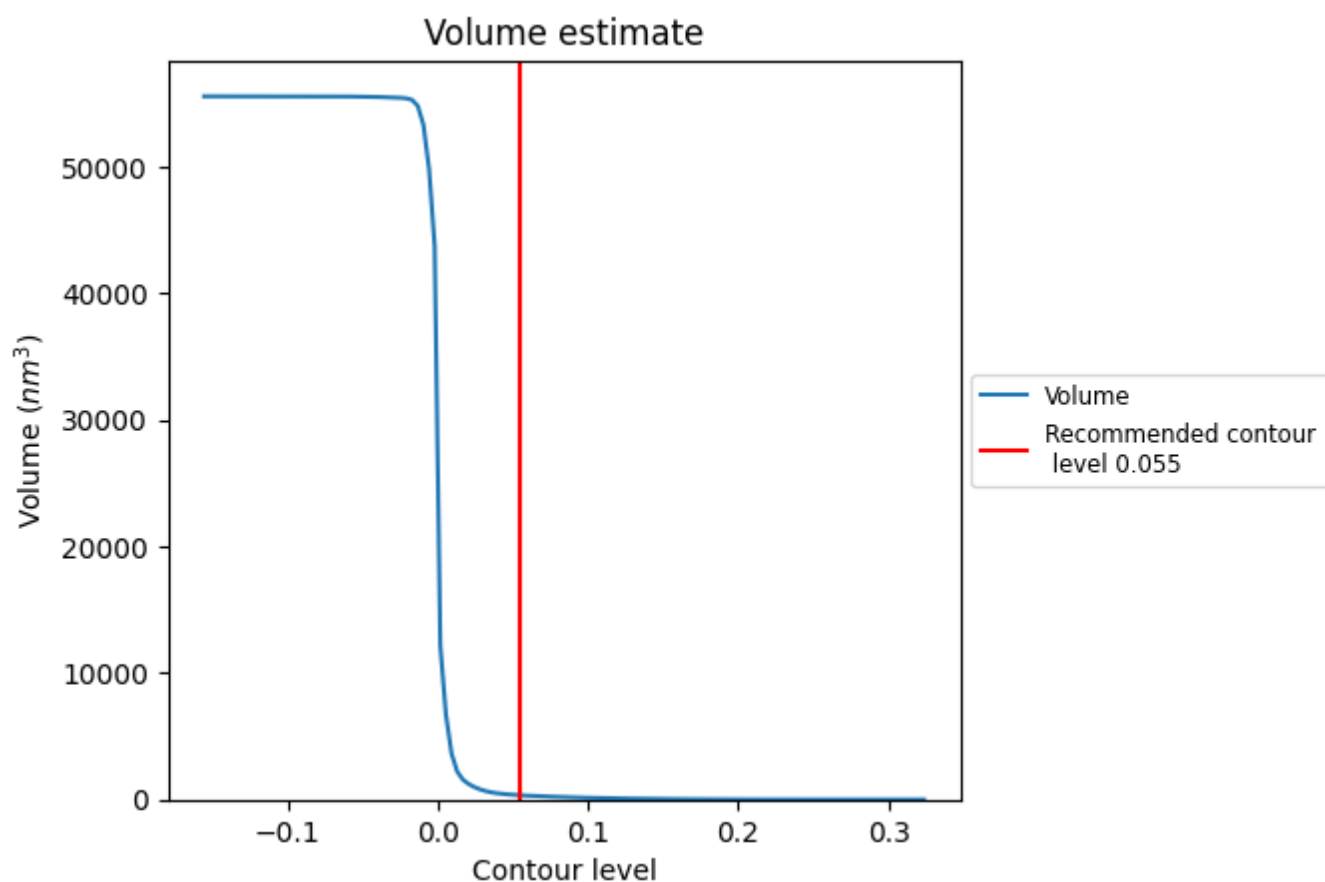
This section contains the results of statistical analysis of the map.

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.

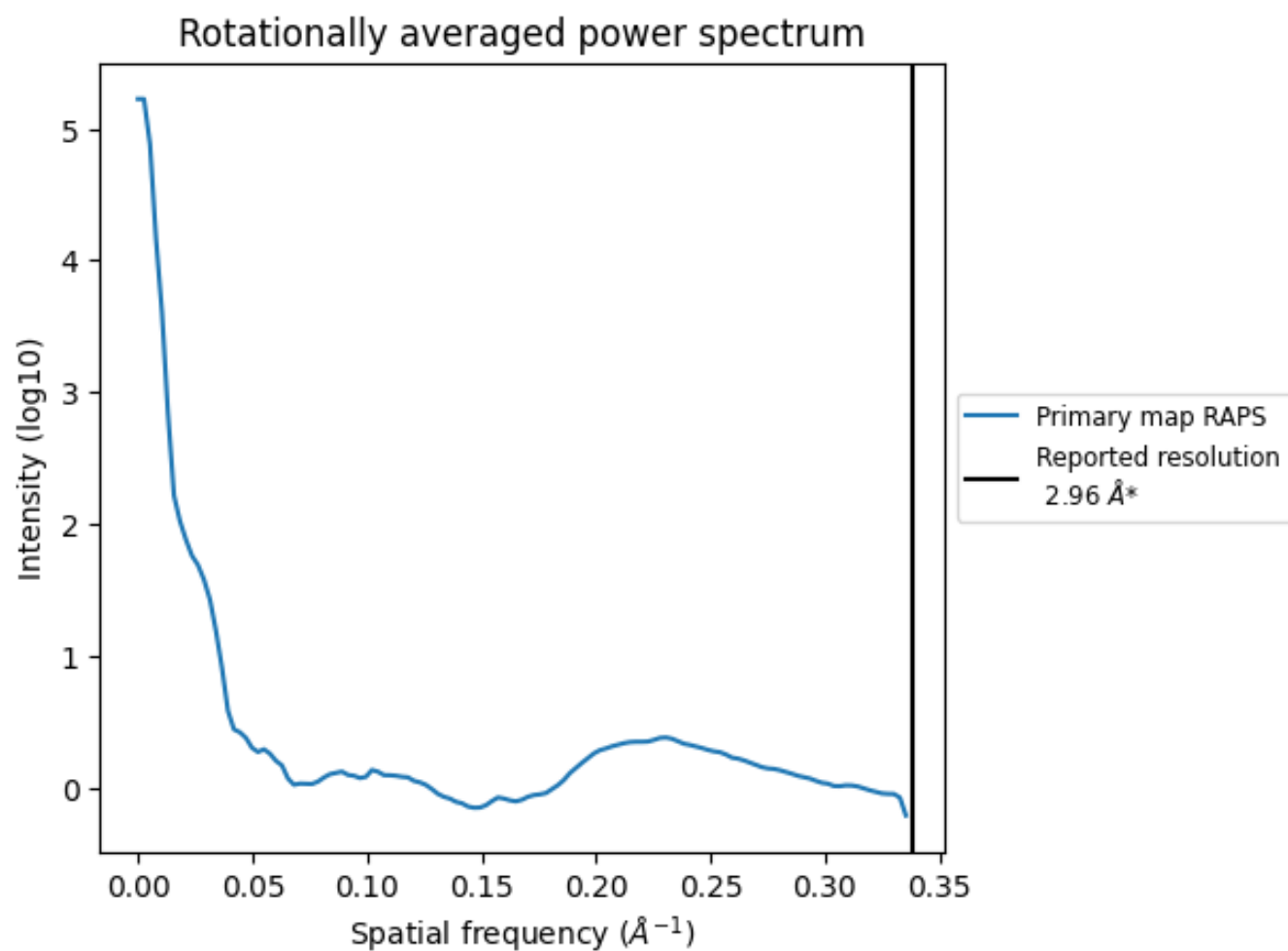
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339 nm³; this corresponds to an approximate mass of 306 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 ⓘ

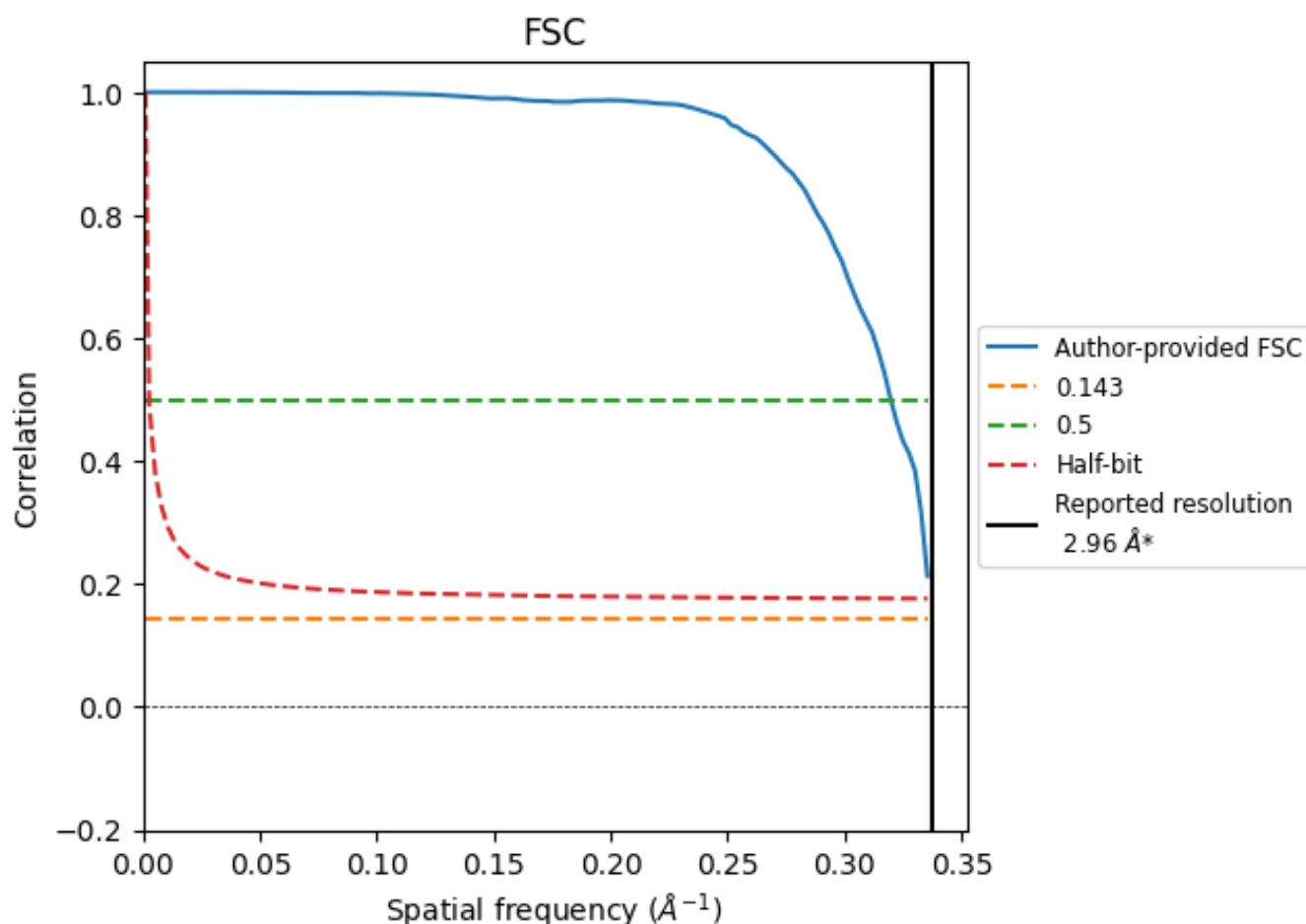


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 Å⁻¹

8.2 Resolution estimates [i](#)

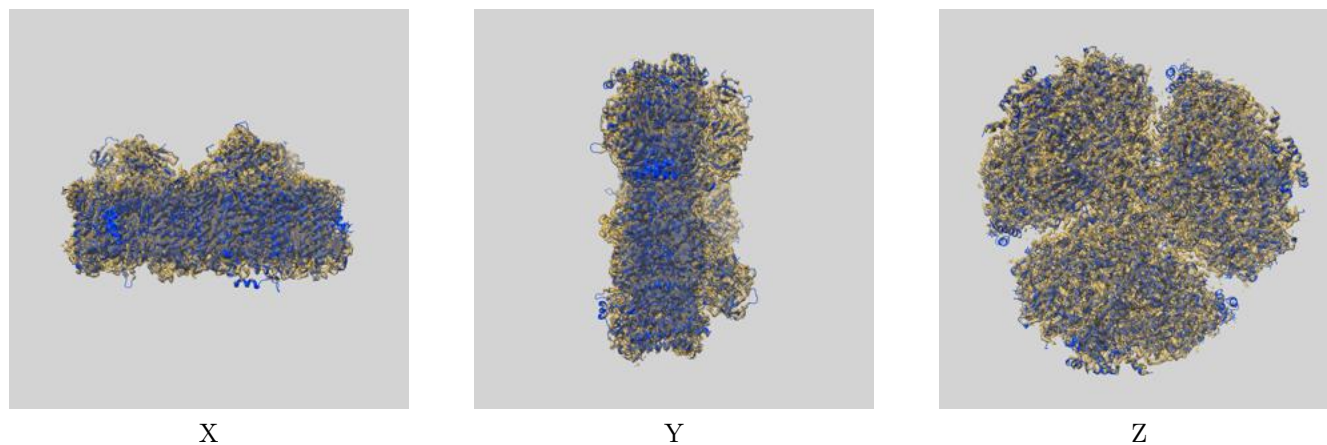
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	-	3.13	-
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

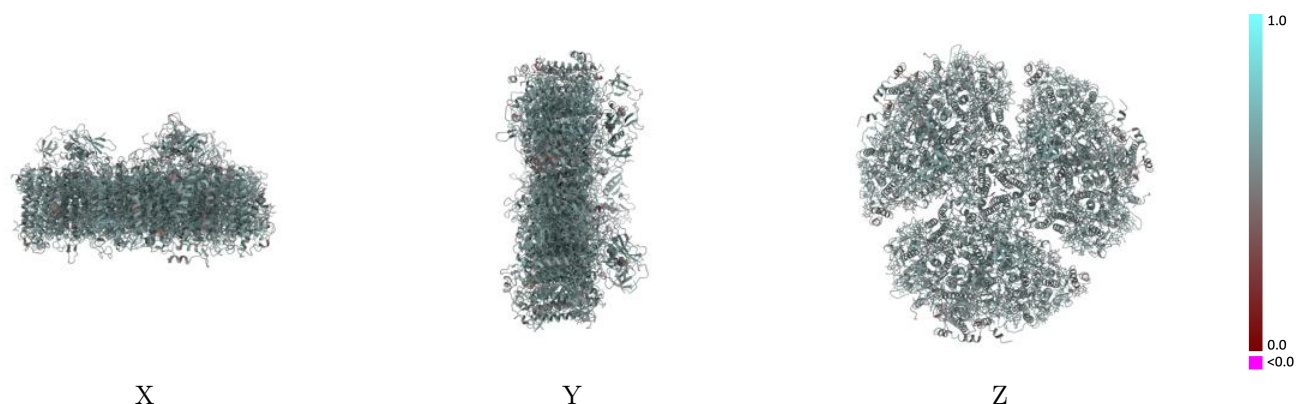
This section contains information regarding the fit between EMDB map EMD-23563 and PDB model 7LX0. Per-residue inclusion information can be found in section [3](#) on page [37](#).

9.1 Map-model overlay [i](#)



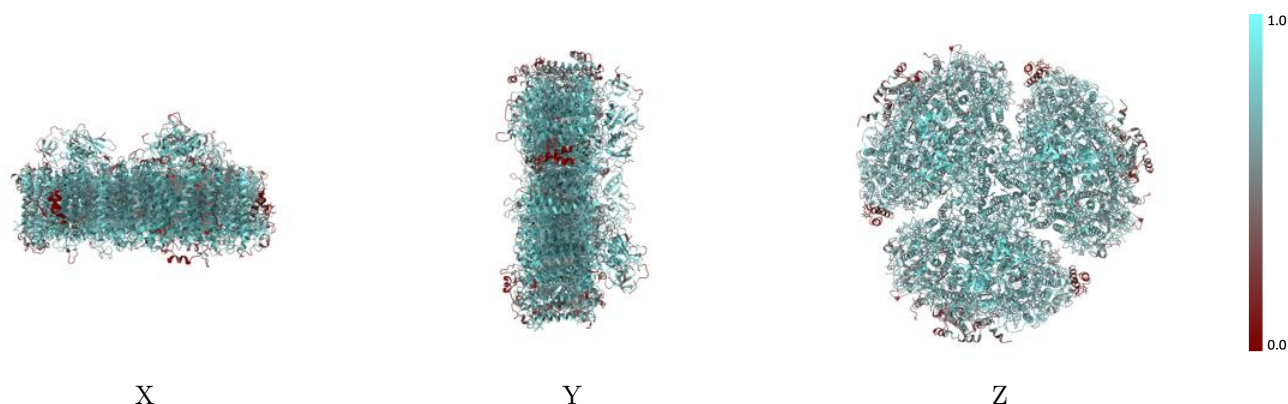
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



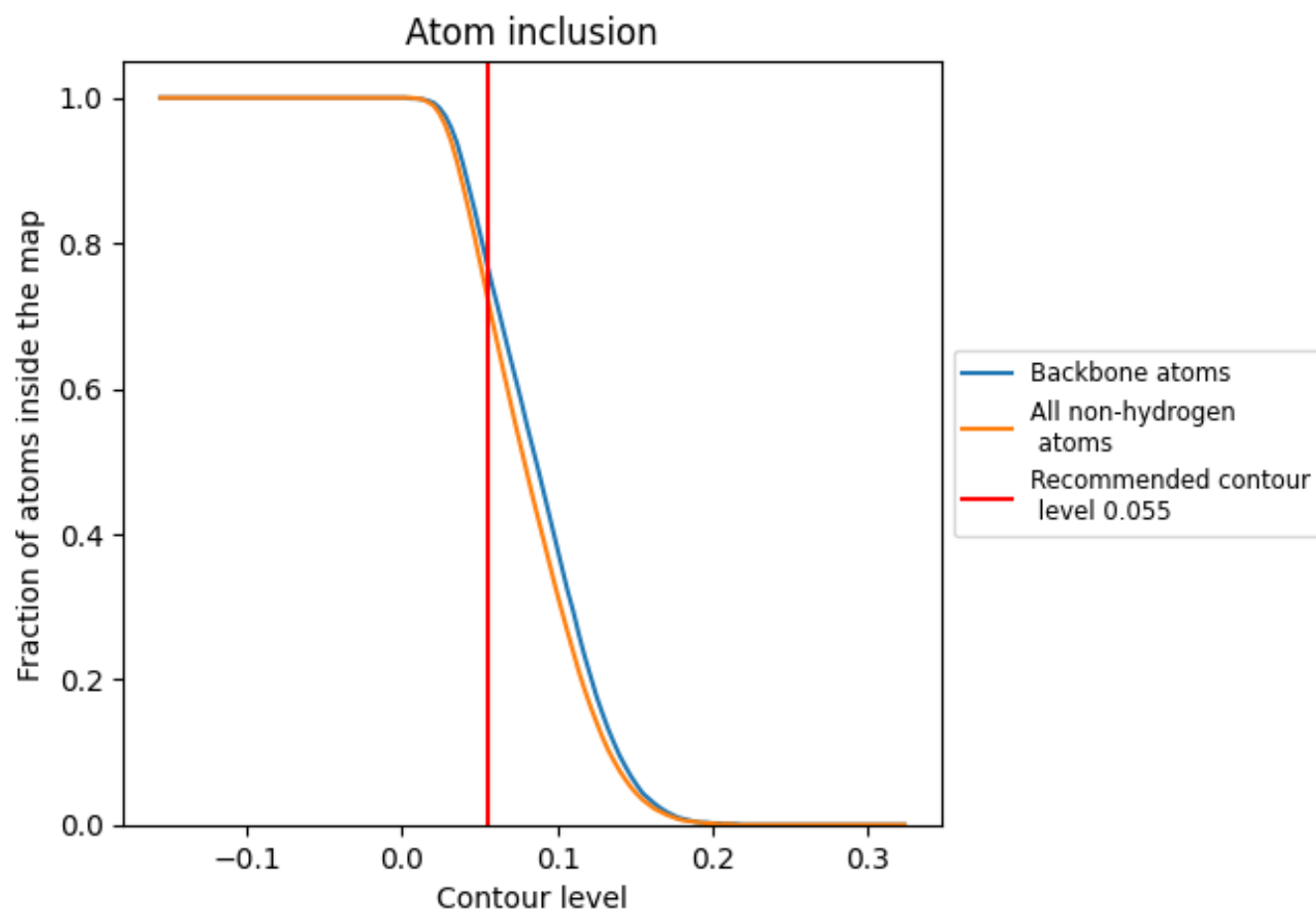
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 73% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7260	 0.5650
A	 0.7680	 0.5740
B	 0.7700	 0.5740
C	 0.7790	 0.5640
D	 0.6530	 0.5490
E	 0.5630	 0.5200
F	 0.3940	 0.4990
G	 0.7700	 0.5750
H	 0.7680	 0.5770
I	 0.7960	 0.5720
J	 0.4490	 0.4770
K	 0.0920	 0.4640
L	 0.7760	 0.5720
M	 0.7000	 0.5480
N	 0.7850	 0.5550
O	 0.6520	 0.5470
P	 0.5610	 0.5160
Q	 0.3970	 0.5010
R	 0.7830	 0.5670
S	 0.4580	 0.4730
T	 0.0710	 0.4560
U	 0.7790	 0.5690
V	 0.7110	 0.5530
W	 0.4910	 0.4970
X	 0.4810	 0.4960
a	 0.7690	 0.5770
b	 0.7650	 0.5770
c	 0.7870	 0.5610
d	 0.6450	 0.5480
e	 0.5400	 0.5100
f	 0.3960	 0.4930
i	 0.7920	 0.5750
j	 0.4410	 0.4730
k	 0.1050	 0.4620
l	 0.7700	 0.5720



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
m	 0.7000	 0.5580
x	 0.4780	 0.4930