



wwPDB EM Validation Summary Report ⓘ

May 26, 2024 – 02:03 PM EDT

PDB ID : 7S3D
EMDB ID : EMD-24821
Title : Structure of photosystem I with bound ferredoxin from *Synechococcus* sp. PCC 7335 acclimated to far-red light
Authors : Gisriel, C.J.; Flesher, D.A.; Shen, G.; Wang, J.; Ho, M.; Brudvig, G.W.; Bryant, D.A.
Deposited on : 2021-09-05
Resolution : 2.91 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:

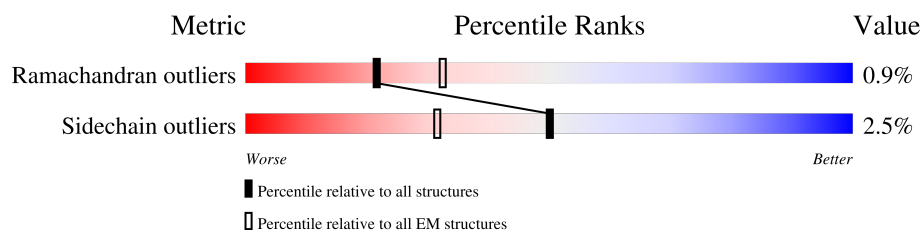
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 2.91 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	782	<div> <div>9%</div> <div>93%</div> <div>..</div> </div>
1	G	782	<div> <div>9%</div> <div>93%</div> <div>..</div> </div>
1	a	782	<div> <div>8%</div> <div>93%</div> <div>..</div> </div>
2	B	743	<div> <div>99%</div> <div>.</div> </div>
2	H	743	<div> <div>99%</div> <div>.</div> </div>
2	b	743	<div> <div>99%</div> <div>.</div> </div>
3	C	81	<div> <div>98%</div> <div>..</div> </div>
3	N	81	<div> <div>98%</div> <div>..</div> </div>
3	c	81	<div> <div>98%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	155	
4	O	155	
4	d	155	
5	E	71	
5	P	71	
5	e	71	
6	F	168	
6	Q	168	
6	f	168	
7	I	70	
7	R	70	
7	i	70	
8	J	46	
8	S	46	
8	j	46	
9	K	84	
9	T	84	
9	k	84	
10	L	174	
10	U	174	
10	l	174	
11	M	31	
11	V	31	
11	m	31	
12	W	99	

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Mol	Chain	Length	Quality of chain
12	X	99	<div> <div>98%</div> <div>83%15%</div> </div>
12	x	99	<div> <div>98%</div> <div>83%15%</div> </div>

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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	A	1141	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	1220	X	-	-	-
14	CLA	B	1221	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	B	1240	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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	G	1141	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	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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	H	1235	X	-	-	-
14	CLA	H	1236	X	-	-	-
14	CLA	H	1239	X	-	-	-
14	CLA	H	1240	X	-	-	-
14	CLA	K	1401	X	-	-	-
14	CLA	L	1501	X	-	-	-
14	CLA	L	1502	X	-	-	-
14	CLA	L	1503	X	-	-	-
14	CLA	M	1501	X	-	-	-
14	CLA	T	1401	X	-	-	-
14	CLA	U	1501	X	-	-	-
14	CLA	U	1502	X	-	-	-
14	CLA	U	1503	X	-	-	-
14	CLA	V	1501	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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	a	1141	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	1220	X	-	-	-
14	CLA	b	1221	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	b	1240	X	-	-	-
14	CLA	k	1401	X	-	-	-
14	CLA	l	1501	X	-	-	-
14	CLA	l	1502	X	-	-	-
14	CLA	l	1503	X	-	-	-
14	CLA	m	1501	X	-	-	-

2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 75150 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	749	Total	C	N	O	S	0	0
			5849	3818	1005	991	35		
1	G	749	Total	C	N	O	S	0	0
			5849	3818	1005	991	35		
1	a	749	Total	C	N	O	S	0	0
			5849	3818	1005	991	35		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	742	Total	C	N	O	S	0	0
			5900	3883	988	1008	21		
2	H	742	Total	C	N	O	S	0	0
			5900	3883	988	1008	21		
2	b	742	Total	C	N	O	S	0	0
			5900	3883	988	1008	21		

- Molecule 3 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			598	365	105	117	11		
3	N	80	Total	C	N	O	S	0	0
			598	365	105	117	11		
3	c	80	Total	C	N	O	S	0	0
			598	365	105	117	11		

- Molecule 4 is a protein called Photosystem I 16 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1102	695	189	213	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	143	Total	C	N	O	S	0	0
			1102	695	189	213	5		
4	d	143	Total	C	N	O	S	0	0
			1102	695	189	213	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	64	Total	C	N	O		0	0
			506	322	89	95			
5	P	64	Total	C	N	O		0	0
			506	322	89	95			
5	e	64	Total	C	N	O		0	0
			506	322	89	95			

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	124	Total	C	N	O	S	0	0
			826	542	134	148	2		
6	Q	124	Total	C	N	O	S	0	0
			826	542	134	148	2		
6	f	124	Total	C	N	O	S	0	0
			826	542	134	148	2		

- Molecule 7 is a protein called PsaI2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	42	Total	C	N	O	S	0	0
			343	237	49	55	2		
7	R	42	Total	C	N	O	S	0	0
			343	237	49	55	2		
7	i	42	Total	C	N	O	S	0	0
			343	237	49	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			296	197	46	52	1		
8	S	41	Total	C	N	O	S	0	0
			296	197	46	52	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	41	Total	C	N	O	S	0	0
			296	197	46	52	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	75	Total	C	N	O	S	0	0
			516	343	85	86	2		
9	T	75	Total	C	N	O	S	0	0
			516	343	85	86	2		
9	k	75	Total	C	N	O	S	0	0
			516	343	85	86	2		

- Molecule 10 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	170	Total	C	N	O	S	0	0
			1291	830	220	238	3		
10	U	170	Total	C	N	O	S	0	0
			1291	830	220	238	3		
10	l	170	Total	C	N	O	S	0	0
			1291	830	220	238	3		

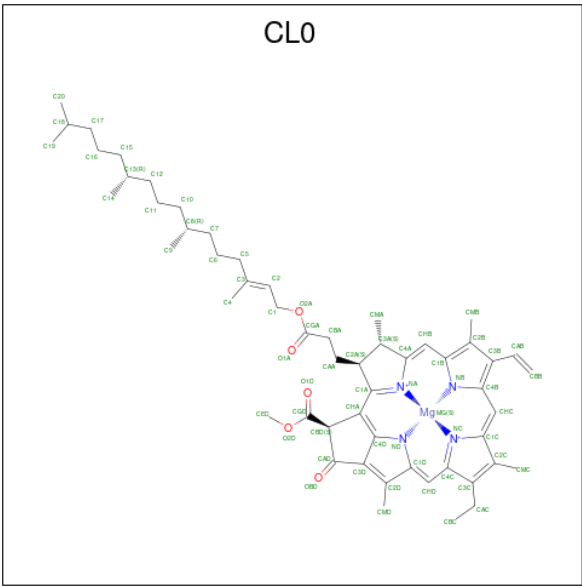
- Molecule 11 is a protein called Psam.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			232	156	35	40	1		
11	V	31	Total	C	N	O	S	0	0
			232	156	35	40	1		
11	m	31	Total	C	N	O	S	0	0
			232	156	35	40	1		

- Molecule 12 is a protein called 2Fe-2S ferredoxin-type domain-containing protein.

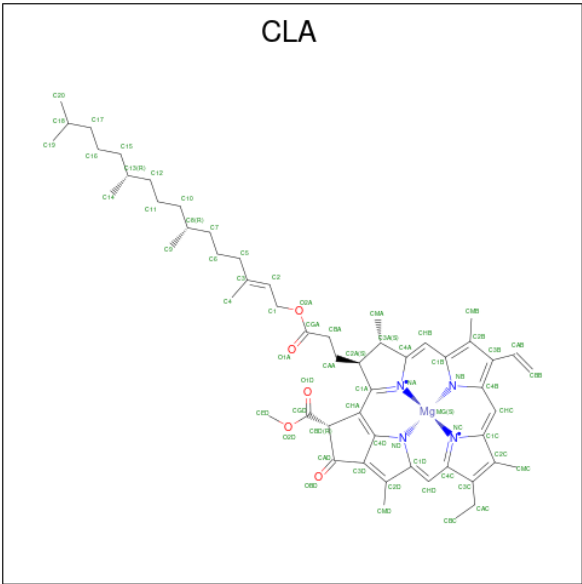
Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	97	Total	C	N	O	S	0	0
			649	405	107	132	5		
12	W	97	Total	C	N	O	S	0	0
			649	405	107	132	5		
12	x	97	Total	C	N	O	S	0	0
			649	405	107	132	5		

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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

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

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

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

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

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

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

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

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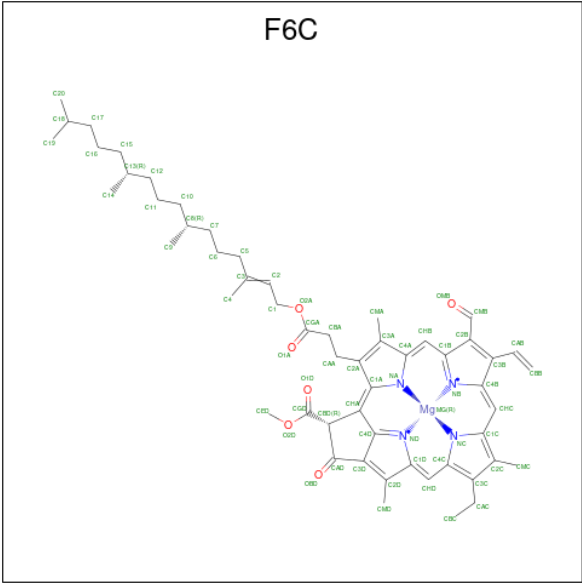
Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total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

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

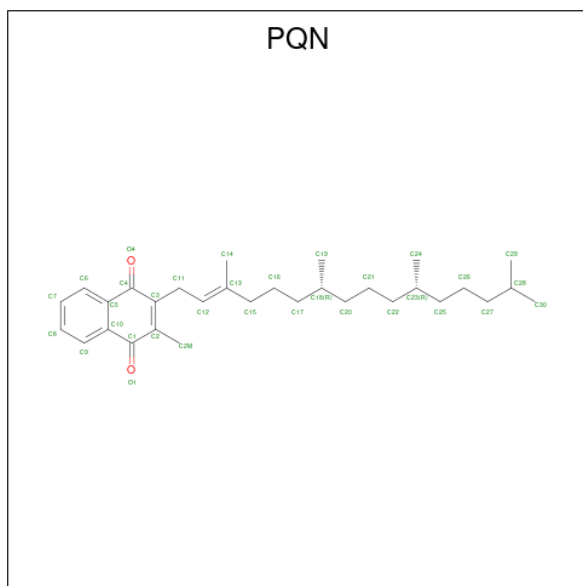
- Molecule 15 is Chlorophyll F (three-letter code: F6C) (formula: C₅₅H₆₈MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
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	
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
			56	45	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 (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



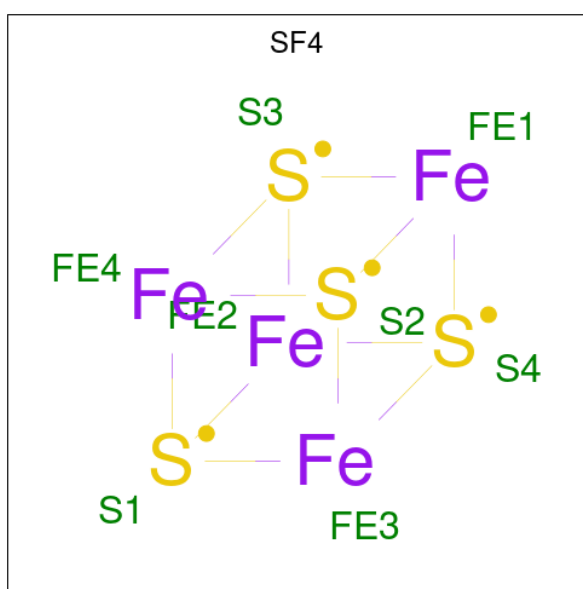
Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	C	O	0
			33	31	2	
16	B	1	Total	C	O	0
			33	31	2	

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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	

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



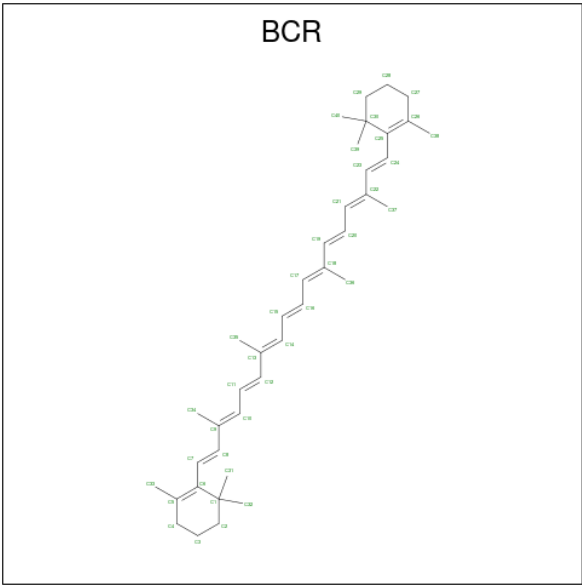
Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	Fe	S	0
			8	4	4	
17	C	1	Total	Fe	S	0
			8	4	4	
17	C	1	Total	Fe	S	0
			8	4	4	
17	G	1	Total	Fe	S	0
			8	4	4	
17	N	1	Total	Fe	S	0
			8	4	4	
17	N	1	Total	Fe	S	0
			8	4	4	
17	a	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
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 (three-letter code: BCR) (formula: C₄₀H₅₆).



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

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

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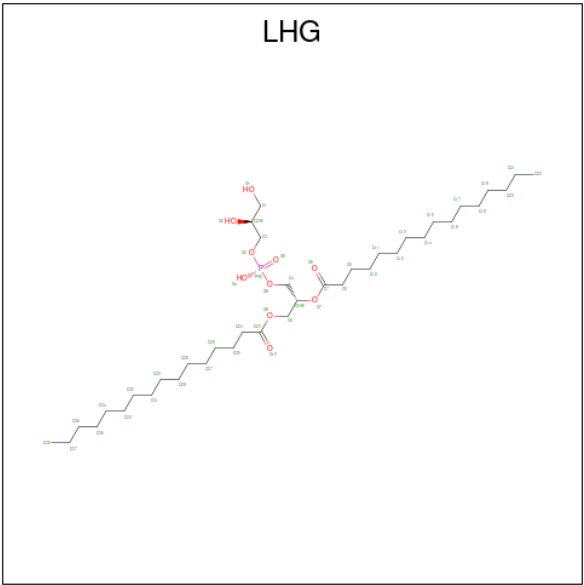
Mol	Chain	Residues	Atoms	AltConf
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	R	1	Total C 40 40	0
18	R	1	Total C 40 40	0
18	T	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	V	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C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

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

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



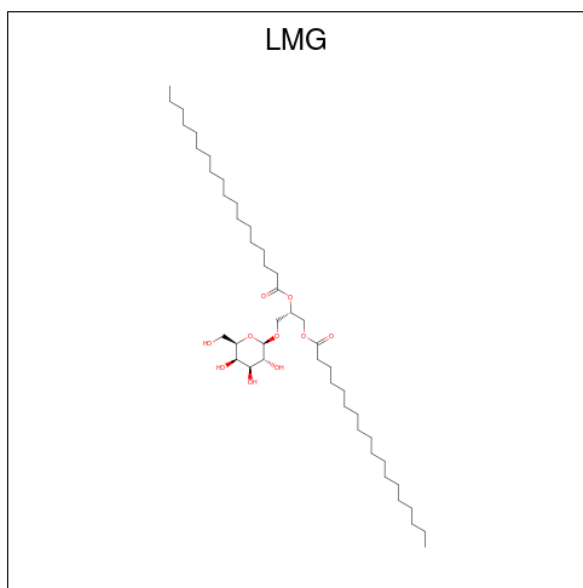
Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C O P 42 31 10 1	0
19	A	1	Total C O P 44 35 8 1	0
19	L	1	Total C O 25 20 5	0
19	L	1	Total C O P 49 38 10 1	0
19	G	1	Total C O P 42 31 10 1	0

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Mol	Chain	Residues	Atoms				AltConf
19	G	1	Total	C	O	P	0
			44	35	8	1	
19	U	1	Total	C	O		0
			25	20	5		
19	U	1	Total	C	O	P	0
			49	38	10	1	
19	a	1	Total	C	O	P	0
			42	31	10	1	
19	a	1	Total	C	O	P	0
			44	35	8	1	
19	l	1	Total	C	O		0
			25	20	5		
19	l	1	Total	C	O	P	0
			49	38	10	1	

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



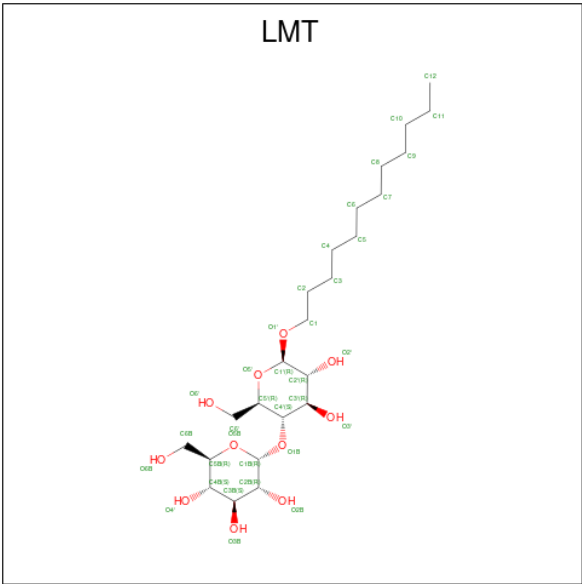
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			46	36	10	
20	B	1	Total	C	O	0
			46	36	10	
20	I	1	Total	C	O	0
			37	27	10	
20	G	1	Total	C	O	0
			46	36	10	

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Mol	Chain	Residues	Atoms			AltConf
20	H	1	Total	C	O	0
			46	36	10	
20	R	1	Total	C	O	0
			37	27	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	

- Molecule 21 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			31	20	11	
21	A	1	Total	C	O	0
			28	17	11	
21	A	1	Total	C	O	0
			32	21	11	
21	A	1	Total	C	O	0
			24	18	6	
21	B	1	Total	C	O	0
			35	24	11	
21	B	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
21	B	1	Total 35	C 24	O 11	0
21	B	1	Total 31	C 20	O 11	0
21	I	1	Total 35	C 24	O 11	0
21	L	1	Total 14	C 13	O 1	0
21	L	1	Total 35	C 24	O 11	0
21	L	1	Total 35	C 24	O 11	0
21	M	1	Total 35	C 24	O 11	0
21	G	1	Total 31	C 20	O 11	0
21	G	1	Total 28	C 17	O 11	0
21	G	1	Total 32	C 21	O 11	0
21	G	1	Total 24	C 18	O 6	0
21	H	1	Total 35	C 24	O 11	0
21	H	1	Total 35	C 24	O 11	0
21	H	1	Total 35	C 24	O 11	0
21	H	1	Total 31	C 20	O 11	0
21	R	1	Total 35	C 24	O 11	0
21	U	1	Total 14	C 13	O 1	0
21	U	1	Total 35	C 24	O 11	0
21	U	1	Total 35	C 24	O 11	0
21	V	1	Total 35	C 24	O 11	0
21	a	1	Total 31	C 20	O 11	0

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Mol	Chain	Residues	Atoms			AltConf
21	a	1	Total	C	O	0
			28	17	11	
21	a	1	Total	C	O	0
			32	21	11	
21	a	1	Total	C	O	0
			24	18	6	
21	b	1	Total	C	O	0
			35	24	11	
21	b	1	Total	C	O	0
			35	24	11	
21	b	1	Total	C	O	0
			35	24	11	
21	b	1	Total	C	O	0
			31	20	11	
21	i	1	Total	C	O	0
			35	24	11	
21	l	1	Total	C	O	0
			14	13	1	
21	l	1	Total	C	O	0
			35	24	11	
21	l	1	Total	C	O	0
			35	24	11	
21	m	1	Total	C	O	0
			35	24	11	

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	Cl	0
			1	1	
22	G	1	Total	Cl	0
			1	1	
22	a	1	Total	Cl	0
			1	1	

- Molecule 23 is CALCIUM ION (three-letter code: CA) (formula: Ca).

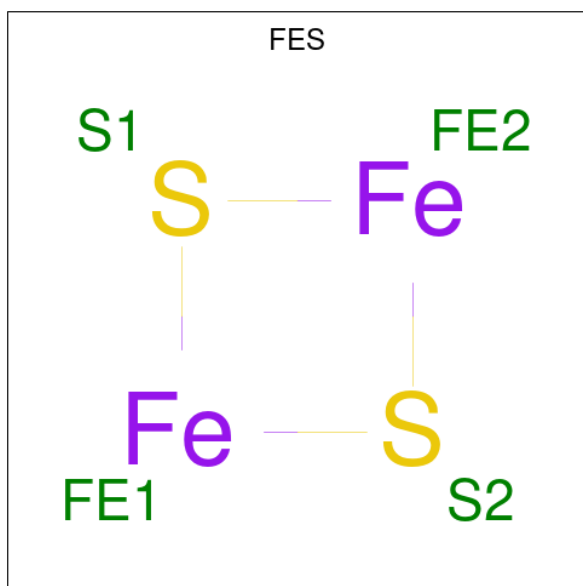
Mol	Chain	Residues	Atoms		AltConf
23	L	1	Total	Ca	0
			1	1	
23	U	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
23	1	1	Total	Ca	0
			1	1	

- Molecule 24 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
24	X	1	Total	Fe	S	0
			4	2	2	
24	W	1	Total	Fe	S	0
			4	2	2	
24	x	1	Total	Fe	S	0
			4	2	2	

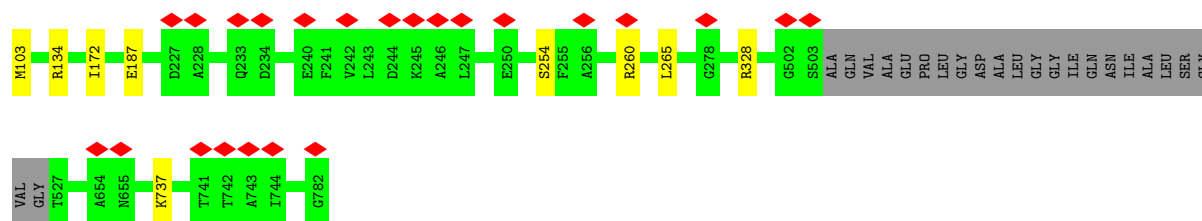
- Molecule 25 is water.

Mol	Chain	Residues	Atoms		AltConf
25	A	35	Total	O	0
			35	35	
25	B	35	Total	O	0
			35	35	
25	C	9	Total	O	0
			9	9	
25	D	13	Total	O	0
			13	13	
25	I	4	Total	O	0
			4	4	

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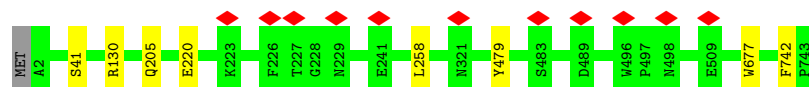
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Mol	Chain	Residues	Atoms		AltConf
25	L	15	Total 15	O 15	0
25	G	35	Total 35	O 35	0
25	H	35	Total 35	O 35	0
25	N	9	Total 9	O 9	0
25	O	13	Total 13	O 13	0
25	R	4	Total 4	O 4	0
25	U	15	Total 15	O 15	0
25	a	35	Total 35	O 35	0
25	b	35	Total 35	O 35	0
25	c	9	Total 9	O 9	0
25	d	13	Total 13	O 13	0
25	i	4	Total 4	O 4	0
25	l	15	Total 15	O 15	0



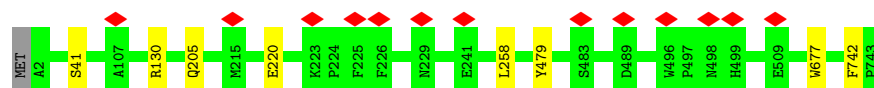
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 99%



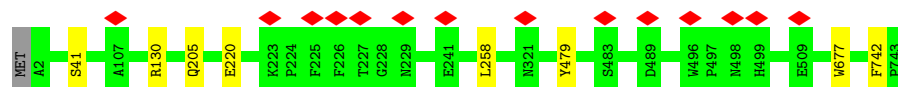
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain H: 99%



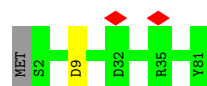
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 99%



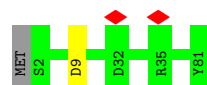
- Molecule 3: PsaC

Chain C: 98%



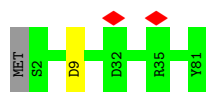
- Molecule 3: PsaC

Chain N: 98%

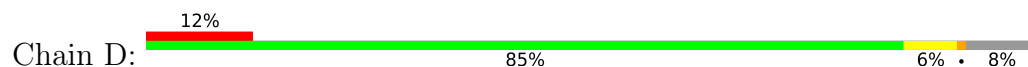


- Molecule 3: PsaC

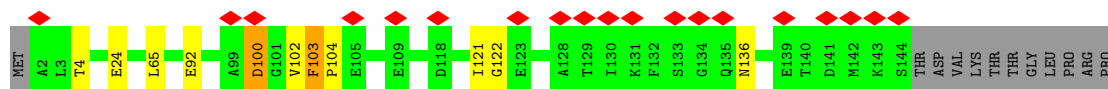
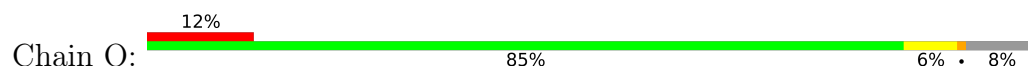
Chain c: 98%



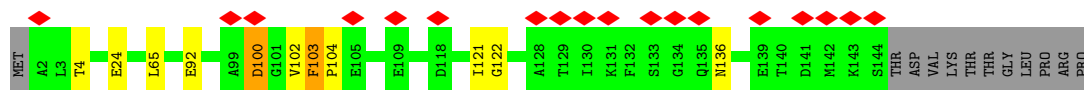
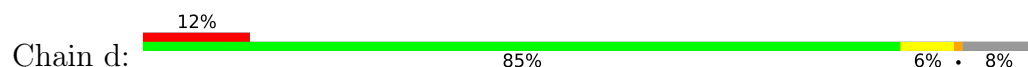
- Molecule 4: Photosystem I 16 kDa polypeptide



- Molecule 4: Photosystem I 16 kDa polypeptide



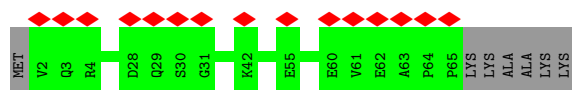
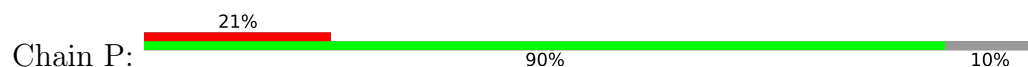
- Molecule 4: Photosystem I 16 kDa polypeptide



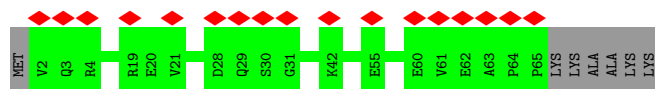
- Molecule 5: Photosystem I reaction center subunit IV



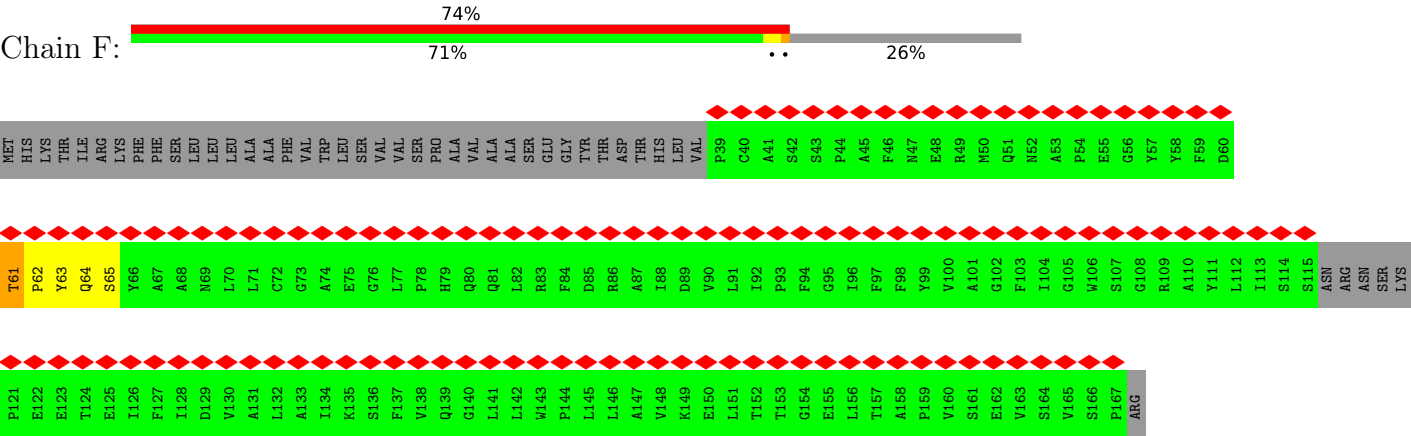
- Molecule 5: Photosystem I reaction center subunit IV



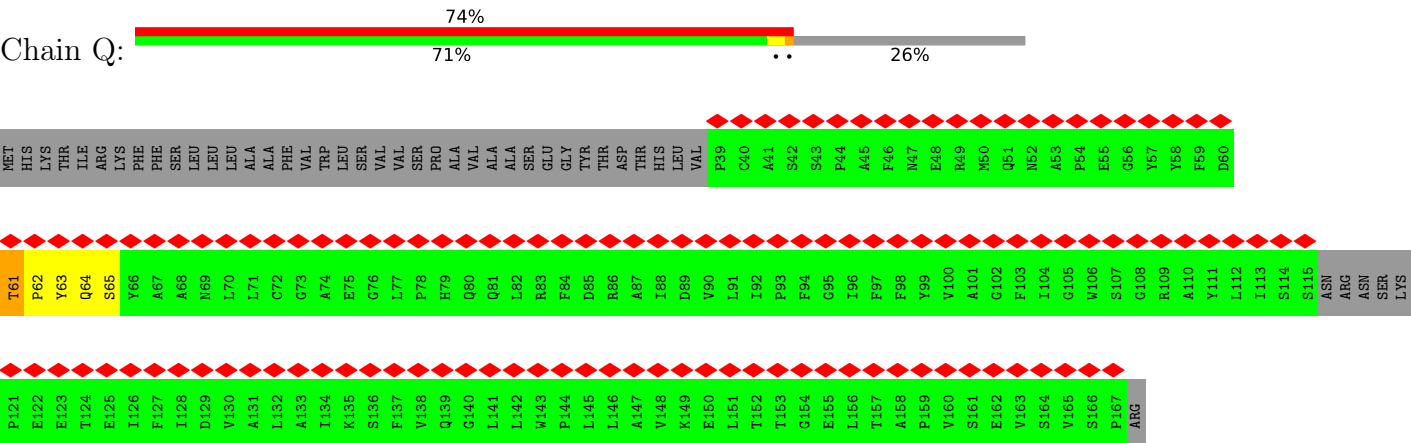
- Molecule 5: Photosystem I reaction center subunit IV



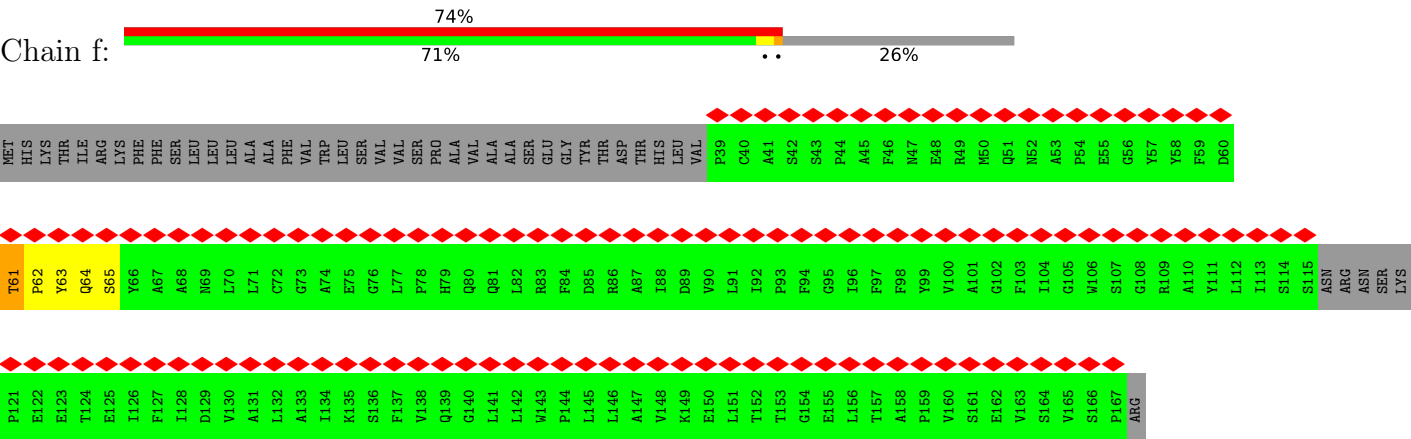
- Molecule 6: PSI-F



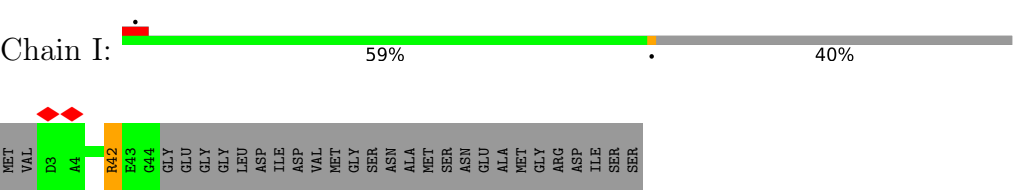
• Molecule 6: PSI-F



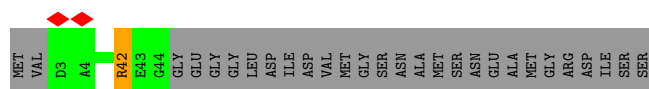
• Molecule 6: PSI-F



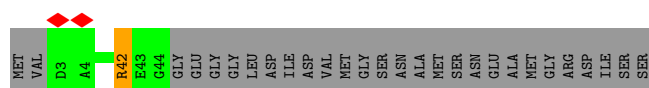
• Molecule 7: PsaI2



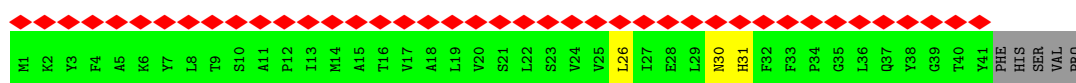
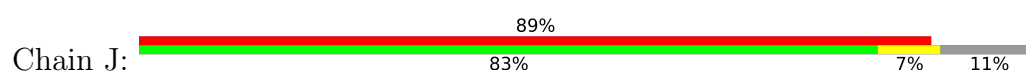
• Molecule 7: PsaI2



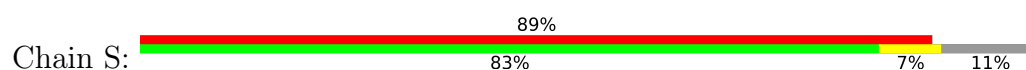
- Molecule 7: PsaI2



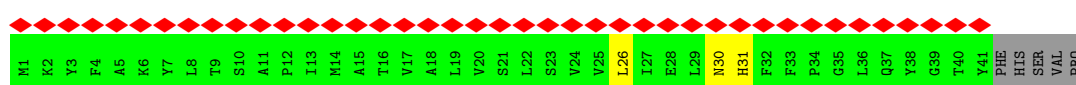
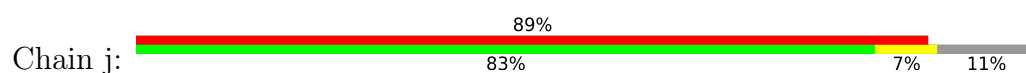
- Molecule 8: Photosystem I reaction center subunit IX



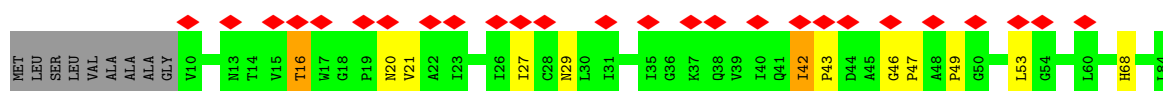
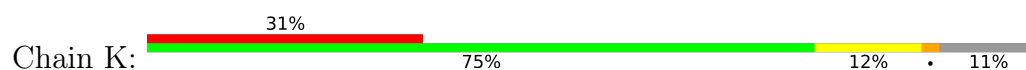
- Molecule 8: Photosystem I reaction center subunit IX



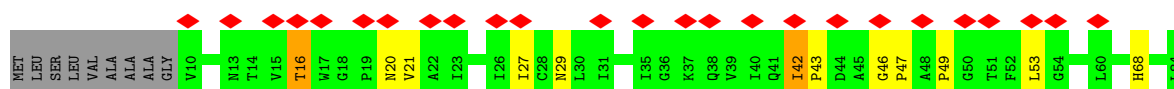
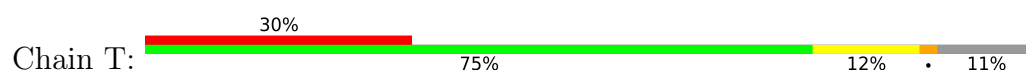
- Molecule 8: Photosystem I reaction center subunit IX



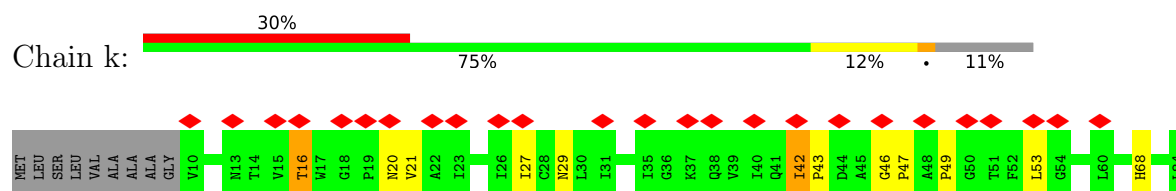
- Molecule 9: Photosystem I reaction center subunit PsaK



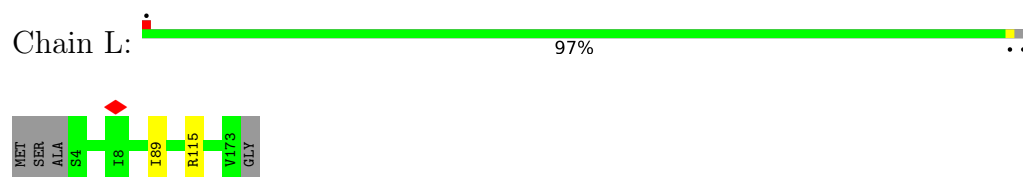
- Molecule 9: Photosystem I reaction center subunit PsaK



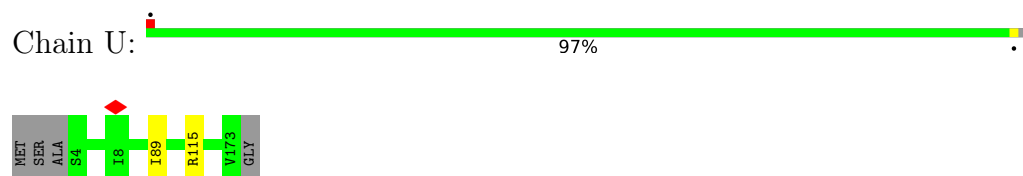
- Molecule 9: Photosystem I reaction center subunit PsaK



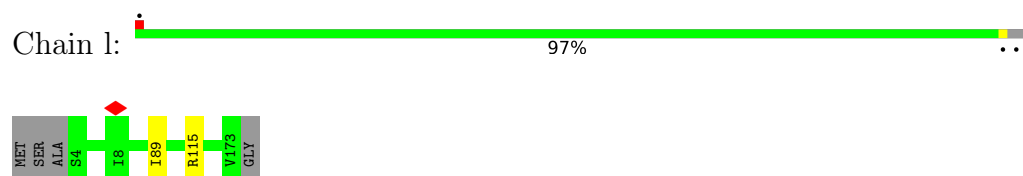
- Molecule 10: PSI subunit V



- Molecule 10: PSI subunit V



- Molecule 10: PSI subunit V



- Molecule 11: PsaM



There are no outlier residues recorded for this chain.

- Molecule 11: PsaM



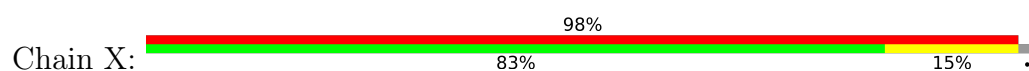
There are no outlier residues recorded for this chain.

- Molecule 11: PsaM



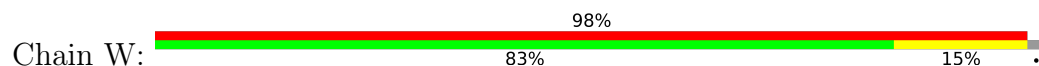
There are no outlier residues recorded for this chain.

- Molecule 12: 2Fe-2S ferredoxin-type domain-containing protein

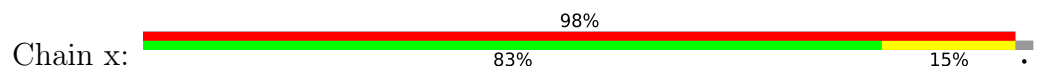




- Molecule 12: 2Fe-2S ferredoxin-type domain-containing protein



- Molecule 12: 2Fe-2S ferredoxin-type domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	286672	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 ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.315	Depositor
Minimum map value	-0.201	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0302	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.48	0/6045	0.62	4/8233 (0.0%)
1	G	0.49	0/6045	0.62	5/8233 (0.1%)
1	a	0.48	0/6045	0.62	4/8233 (0.0%)
2	B	0.47	0/6124	0.59	1/8377 (0.0%)
2	H	0.47	0/6124	0.59	1/8377 (0.0%)
2	b	0.47	0/6124	0.59	1/8377 (0.0%)
3	C	0.50	0/608	0.65	1/823 (0.1%)
3	N	0.50	0/608	0.65	1/823 (0.1%)
3	c	0.50	0/608	0.65	1/823 (0.1%)
4	D	0.44	0/1125	0.63	1/1515 (0.1%)
4	O	0.44	0/1125	0.63	1/1515 (0.1%)
4	d	0.44	0/1125	0.63	1/1515 (0.1%)
5	E	0.38	0/517	0.48	0/702
5	P	0.38	0/517	0.48	0/702
5	e	0.38	0/517	0.48	0/702
6	F	0.31	0/847	0.90	1/1168 (0.1%)
6	Q	0.31	0/847	0.90	1/1168 (0.1%)
6	f	0.31	0/847	0.90	1/1168 (0.1%)
7	I	0.52	0/357	0.83	1/491 (0.2%)
7	R	0.52	0/357	0.83	1/491 (0.2%)
7	i	0.52	0/357	0.83	1/491 (0.2%)
8	J	0.31	0/302	0.71	1/414 (0.2%)
8	S	0.31	0/302	0.72	1/414 (0.2%)
8	j	0.31	0/302	0.71	1/414 (0.2%)
9	K	0.47	0/526	1.37	3/724 (0.4%)
9	T	0.47	0/526	1.37	3/724 (0.4%)
9	k	0.47	0/526	1.37	3/724 (0.4%)
10	L	0.50	0/1322	0.59	1/1797 (0.1%)
10	U	0.50	0/1322	0.59	1/1797 (0.1%)
10	l	0.50	0/1322	0.59	1/1797 (0.1%)
11	M	0.34	0/235	0.62	0/319
11	V	0.34	0/235	0.62	0/319

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	m	0.34	0/235	0.62	0/319
12	W	0.66	0/657	0.58	0/900
12	X	0.66	0/657	0.58	0/900
12	x	0.67	0/657	0.58	0/900
All	All	0.48	0/55995	0.66	43/76389 (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
2	B	0	2
2	H	0	2
2	b	0	2
4	D	0	2
4	O	0	2
4	d	0	2
All	All	0	12

There are no bond length outliers.

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	42	ILE	C-N-CD	-24.85	65.92	120.60
9	k	42	ILE	C-N-CD	-24.85	65.92	120.60
9	T	42	ILE	C-N-CD	-24.84	65.96	120.60
6	Q	61	THR	C-N-CD	-24.79	66.07	120.60
6	f	61	THR	C-N-CD	-24.78	66.09	120.60

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	677	TRP	Peptide
2	B	742	PHE	Mainchain
4	D	100	ASP	Peptide
4	D	136	ASN	Peptide
2	H	677	TRP	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	745/782 (95%)	708 (95%)	31 (4%)	6 (1%)	19	49
1	G	745/782 (95%)	708 (95%)	31 (4%)	6 (1%)	19	49
1	a	745/782 (95%)	708 (95%)	31 (4%)	6 (1%)	19	49
2	B	740/743 (100%)	703 (95%)	37 (5%)	0	100	100
2	H	740/743 (100%)	702 (95%)	38 (5%)	0	100	100
2	b	740/743 (100%)	702 (95%)	38 (5%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	N	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	141/155 (91%)	119 (84%)	17 (12%)	5 (4%)	3	13
4	O	141/155 (91%)	119 (84%)	17 (12%)	5 (4%)	3	13
4	d	141/155 (91%)	119 (84%)	17 (12%)	5 (4%)	3	13
5	E	62/71 (87%)	60 (97%)	2 (3%)	0	100	100
5	P	62/71 (87%)	60 (97%)	2 (3%)	0	100	100
5	e	62/71 (87%)	60 (97%)	2 (3%)	0	100	100
6	F	120/168 (71%)	106 (88%)	10 (8%)	4 (3%)	4	14
6	Q	120/168 (71%)	106 (88%)	10 (8%)	4 (3%)	4	14
6	f	120/168 (71%)	106 (88%)	10 (8%)	4 (3%)	4	14
7	I	40/70 (57%)	36 (90%)	4 (10%)	0	100	100
7	R	40/70 (57%)	36 (90%)	4 (10%)	0	100	100
7	i	40/70 (57%)	36 (90%)	4 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	39/46 (85%)	34 (87%)	5 (13%)	0	100	100
8	S	39/46 (85%)	34 (87%)	5 (13%)	0	100	100
8	j	39/46 (85%)	34 (87%)	5 (13%)	0	100	100
9	K	73/84 (87%)	57 (78%)	12 (16%)	4 (6%)	2	5
9	T	73/84 (87%)	57 (78%)	12 (16%)	4 (6%)	2	5
9	k	73/84 (87%)	57 (78%)	12 (16%)	4 (6%)	2	5
10	L	168/174 (97%)	165 (98%)	3 (2%)	0	100	100
10	U	168/174 (97%)	165 (98%)	3 (2%)	0	100	100
10	l	168/174 (97%)	165 (98%)	3 (2%)	0	100	100
11	M	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	V	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	m	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
12	W	95/99 (96%)	80 (84%)	13 (14%)	2 (2%)	7	24
12	X	95/99 (96%)	80 (84%)	13 (14%)	2 (2%)	7	24
12	x	95/99 (96%)	80 (84%)	13 (14%)	2 (2%)	7	24
All	All	6990/7512 (93%)	6505 (93%)	422 (6%)	63 (1%)	21	46

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	PRO
6	F	62	PRO
9	K	43	PRO
9	K	47	PRO
1	G	41	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	593/626 (95%)	582 (98%)	11 (2%)	57	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	593/626 (95%)	582 (98%)	11 (2%)	57	83
1	a	593/626 (95%)	582 (98%)	11 (2%)	57	83
2	B	598/599 (100%)	593 (99%)	5 (1%)	81	93
2	H	598/599 (100%)	593 (99%)	5 (1%)	81	93
2	b	598/599 (100%)	593 (99%)	5 (1%)	81	93
3	C	67/68 (98%)	67 (100%)	0	100	100
3	N	67/68 (98%)	67 (100%)	0	100	100
3	c	67/68 (98%)	67 (100%)	0	100	100
4	D	115/127 (91%)	110 (96%)	5 (4%)	29	61
4	O	115/127 (91%)	110 (96%)	5 (4%)	29	61
4	d	115/127 (91%)	110 (96%)	5 (4%)	29	61
5	E	56/61 (92%)	56 (100%)	0	100	100
5	P	56/61 (92%)	56 (100%)	0	100	100
5	e	56/61 (92%)	56 (100%)	0	100	100
6	F	63/140 (45%)	62 (98%)	1 (2%)	62	85
6	Q	63/140 (45%)	62 (98%)	1 (2%)	62	85
6	f	63/140 (45%)	62 (98%)	1 (2%)	62	85
7	I	33/54 (61%)	32 (97%)	1 (3%)	41	73
7	R	33/54 (61%)	32 (97%)	1 (3%)	41	73
7	i	33/54 (61%)	32 (97%)	1 (3%)	41	73
8	J	29/40 (72%)	27 (93%)	2 (7%)	15	40
8	S	29/40 (72%)	27 (93%)	2 (7%)	15	40
8	j	29/40 (72%)	27 (93%)	2 (7%)	15	40
9	K	53/59 (90%)	46 (87%)	7 (13%)	4	11
9	T	53/59 (90%)	46 (87%)	7 (13%)	4	11
9	k	53/59 (90%)	46 (87%)	7 (13%)	4	11
10	L	135/137 (98%)	134 (99%)	1 (1%)	84	95
10	U	135/137 (98%)	134 (99%)	1 (1%)	84	95
10	l	135/137 (98%)	134 (99%)	1 (1%)	84	95
11	M	23/24 (96%)	23 (100%)	0	100	100
11	V	23/24 (96%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	m	23/24 (96%)	23 (100%)	0	100	100
12	W	52/85 (61%)	39 (75%)	13 (25%)	0	1
12	X	52/85 (61%)	39 (75%)	13 (25%)	0	1
12	x	52/85 (61%)	39 (75%)	13 (25%)	0	1
All	All	5451/6060 (90%)	5313 (98%)	138 (2%)	50	77

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	j	30	ASN
9	k	21	VAL
12	x	59	VAL
1	G	37	LEU
1	G	36	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
10	U	14	GLN
1	a	428	ASN
10	U	172	ASN
1	a	108	HIS
1	a	745	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 417 ligands modelled in this entry, 6 are monoatomic - leaving 411 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
14	CLA	H	1233	-	45,53,73	2.56	19 (42%)	52,89,113	2.90	20 (38%)
14	CLA	G	1113	-	45,53,73	2.55	18 (40%)	52,89,113	2.88	21 (40%)
14	CLA	a	1113	-	45,53,73	2.54	18 (40%)	52,89,113	2.87	20 (38%)
14	CLA	A	1117	-	65,73,73	2.15	19 (29%)	76,113,113	2.62	28 (36%)
14	CLA	A	1129	-	50,58,73	2.51	19 (38%)	58,95,113	3.08	25 (43%)
18	BCR	M	4021	-	41,41,41	2.91	6 (14%)	56,56,56	6.65	19 (33%)
15	F6C	b	1230	-	49,54,74	3.18	25 (51%)	46,90,114	3.79	25 (54%)
14	CLA	U	1501	10	65,73,73	2.18	18 (27%)	76,113,113	2.61	23 (30%)
14	CLA	A	1140	-	55,63,73	2.42	18 (32%)	64,101,113	2.69	21 (32%)
21	LMT	l	6001	-	13,13,36	0.44	0	12,12,47	0.91	0
18	BCR	L	4019	-	41,41,41	3.09	7 (17%)	56,56,56	6.50	28 (50%)
14	CLA	B	1214	-	60,68,73	2.34	21 (35%)	70,107,113	2.67	28 (40%)
21	LMT	l	6002	-	36,36,36	1.29	5 (13%)	47,47,47	1.22	7 (14%)
14	CLA	b	1224	-	65,73,73	2.22	17 (26%)	76,113,113	2.64	23 (30%)
21	LMT	a	6002	-	29,29,36	1.46	6 (20%)	40,40,47	1.23	4 (10%)
14	CLA	A	1114	-	45,53,73	2.58	19 (42%)	52,89,113	2.88	19 (36%)
14	CLA	H	1226	-	65,73,73	2.27	18 (27%)	76,113,113	2.63	24 (31%)
18	BCR	b	4009	-	41,41,41	2.93	6 (14%)	56,56,56	6.51	23 (41%)
14	CLA	H	1022	-	55,63,73	2.38	18 (32%)	64,101,113	2.73	24 (37%)
18	BCR	H	4017	-	41,41,41	3.05	8 (19%)	56,56,56	6.71	20 (35%)
14	CLA	b	1236	-	55,63,73	2.32	18 (32%)	64,101,113	2.98	23 (35%)
14	CLA	G	1119	-	65,73,73	2.23	18 (27%)	76,113,113	2.48	21 (27%)
14	CLA	a	1128	-	60,68,73	2.34	19 (31%)	70,107,113	2.69	23 (32%)
18	BCR	B	4017	-	41,41,41	3.05	8 (19%)	56,56,56	6.71	20 (35%)
14	CLA	b	1023	-	65,73,73	2.24	20 (30%)	76,113,113	2.86	30 (39%)
18	BCR	L	4022	-	41,41,41	3.00	6 (14%)	56,56,56	6.39	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	1226	-	65,73,73	2.27	18 (27%)	76,113,113	2.62	24 (31%)
14	CLA	H	1214	-	60,68,73	2.34	21 (35%)	70,107,113	2.66	28 (40%)
18	BCR	A	4006	-	41,41,41	2.94	6 (14%)	56,56,56	6.57	24 (42%)
14	CLA	A	1130	-	55,63,73	2.46	19 (34%)	64,101,113	2.66	21 (32%)
14	CLA	G	1129	-	50,58,73	2.51	19 (38%)	58,95,113	3.08	25 (43%)
14	CLA	A	1122	-	55,63,73	2.35	19 (34%)	64,101,113	2.71	24 (37%)
18	BCR	B	4006	-	41,41,41	2.82	6 (14%)	56,56,56	6.58	18 (32%)
19	LHG	a	5002	-	43,43,48	1.00	2 (4%)	47,48,54	1.13	2 (4%)
14	CLA	K	1401	-	45,53,73	2.59	19 (42%)	52,89,113	3.03	23 (44%)
14	CLA	b	1203	-	65,73,73	2.17	19 (29%)	76,113,113	2.69	22 (28%)
14	CLA	B	1211	-	65,73,73	2.24	20 (30%)	76,113,113	2.53	25 (32%)
14	CLA	A	1104	-	65,73,73	2.15	19 (29%)	76,113,113	2.79	24 (31%)
14	CLA	A	1131	-	60,68,73	2.30	19 (31%)	70,107,113	2.72	21 (30%)
14	CLA	a	1117	-	65,73,73	2.15	19 (29%)	76,113,113	2.62	28 (36%)
14	CLA	b	1233	-	45,53,73	2.57	19 (42%)	52,89,113	2.91	20 (38%)
14	CLA	G	1105	-	45,53,73	2.61	18 (40%)	52,89,113	2.94	20 (38%)
15	F6C	B	1219	-	59,64,74	2.96	26 (44%)	58,102,114	3.52	27 (46%)
18	BCR	B	4004	-	41,41,41	2.82	6 (14%)	56,56,56	6.52	22 (39%)
16	PQN	A	2001	-	34,34,34	1.50	2 (5%)	42,45,45	1.19	4 (9%)
14	CLA	A	1132	-	65,73,73	2.18	18 (27%)	76,113,113	2.64	23 (30%)
14	CLA	b	1234	-	65,73,73	2.22	19 (29%)	76,113,113	2.54	24 (31%)
15	F6C	H	1238	25	69,74,74	2.73	24 (34%)	70,114,114	3.11	29 (41%)
18	BCR	G	4006	-	41,41,41	2.94	6 (14%)	56,56,56	6.57	23 (41%)
14	CLA	H	1021	-	65,73,73	2.22	19 (29%)	76,113,113	2.47	27 (35%)
14	CLA	B	1208	-	60,68,73	2.34	19 (31%)	70,107,113	2.76	26 (37%)
14	CLA	H	1211	-	65,73,73	2.23	20 (30%)	76,113,113	2.52	25 (32%)
15	F6C	B	1207	-	69,74,74	2.75	24 (34%)	70,114,114	3.16	28 (40%)
14	CLA	G	1123	-	60,68,73	2.33	18 (30%)	70,107,113	2.77	24 (34%)
14	CLA	G	1133	1	60,68,73	2.32	18 (30%)	70,107,113	2.77	20 (28%)
14	CLA	A	1126	-	60,68,73	2.33	17 (28%)	70,107,113	2.58	20 (28%)
14	CLA	a	1138	-	55,63,73	2.38	20 (36%)	64,101,113	2.89	26 (40%)
14	CLA	G	1127	-	65,73,73	2.22	19 (29%)	76,113,113	2.53	21 (27%)
21	LMT	b	6002	-	36,36,36	1.21	6 (16%)	47,47,47	1.03	1 (2%)
14	CLA	b	1206	-	65,73,73	2.23	19 (29%)	76,113,113	2.61	24 (31%)
14	CLA	a	1132	-	65,73,73	2.19	18 (27%)	76,113,113	2.65	23 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	T	1401	-	45,53,73	2.59	20 (44%)	52,89,113	3.03	22 (42%)
15	F6C	H	1219	-	59,64,74	2.96	26 (44%)	58,102,114	3.52	28 (48%)
14	CLA	B	1232	-	45,53,73	2.58	20 (44%)	52,89,113	2.89	20 (38%)
18	BCR	H	4004	-	41,41,41	2.83	6 (14%)	56,56,56	6.52	22 (39%)
14	CLA	A	1139	-	45,53,73	2.56	20 (44%)	52,89,113	2.84	20 (38%)
14	CLA	a	1124	25	55,63,73	2.40	19 (34%)	64,101,113	2.82	21 (32%)
14	CLA	H	1204	-	65,73,73	2.21	19 (29%)	76,113,113	2.59	23 (30%)
14	CLA	G	1108	-	45,53,73	2.62	19 (42%)	52,89,113	2.91	21 (40%)
14	CLA	L	1501	10	65,73,73	2.18	18 (27%)	76,113,113	2.61	23 (30%)
24	FES	x	101	12	0,4,4	-	-	-	-	-
14	CLA	G	1125	-	65,73,73	2.16	18 (27%)	76,113,113	2.69	23 (30%)
14	CLA	V	1501	-	50,58,73	2.53	18 (36%)	58,95,113	2.91	24 (41%)
14	CLA	b	1201	-	65,73,73	2.20	20 (30%)	76,113,113	2.71	25 (32%)
18	BCR	K	4001	-	41,41,41	2.90	6 (14%)	56,56,56	6.45	22 (39%)
14	CLA	A	1118	-	55,63,73	2.42	18 (32%)	64,101,113	2.79	22 (34%)
13	CL0	G	1011	-	65,73,73	2.26	20 (30%)	76,113,113	2.54	25 (32%)
20	LMG	H	5002	-	46,46,55	1.29	6 (13%)	54,54,63	1.24	6 (11%)
14	CLA	a	1102	-	50,58,73	2.59	21 (42%)	58,95,113	2.96	24 (41%)
15	F6C	H	1207	-	69,74,74	2.75	24 (34%)	70,114,114	3.17	27 (38%)
18	BCR	R	4018	-	41,41,41	2.94	6 (14%)	56,56,56	6.59	16 (28%)
18	BCR	b	4014	-	41,41,41	2.81	6 (14%)	56,56,56	6.63	20 (35%)
19	LHG	U	5101	-	24,24,48	1.27	2 (8%)	26,26,54	1.48	4 (15%)
17	SF4	C	3002	3	0,12,12	-	-	-	-	-
18	BCR	l	4019	-	41,41,41	3.08	7 (17%)	56,56,56	6.50	28 (50%)
20	LMG	B	5002	-	46,46,55	1.29	6 (13%)	54,54,63	1.24	6 (11%)
14	CLA	B	1215	-	60,68,73	2.27	19 (31%)	70,107,113	2.62	20 (28%)
14	CLA	G	1122	-	55,63,73	2.35	19 (34%)	64,101,113	2.71	25 (39%)
14	CLA	a	1129	-	50,58,73	2.52	19 (38%)	58,95,113	3.08	25 (43%)
14	CLA	H	1232	-	45,53,73	2.58	20 (44%)	52,89,113	2.89	20 (38%)
14	CLA	B	1223	-	65,73,73	2.23	18 (27%)	76,113,113	2.62	26 (34%)
20	LMG	i	5006	-	37,37,55	1.13	3 (8%)	45,45,63	1.21	5 (11%)
14	CLA	G	1101	-	45,53,73	2.57	19 (42%)	52,89,113	2.94	22 (42%)
14	CLA	A	1111	-	60,68,73	2.29	18 (30%)	70,107,113	4.77	28 (40%)
14	CLA	B	1239	-	65,73,73	2.23	19 (29%)	76,113,113	2.63	27 (35%)
18	BCR	m	4021	-	41,41,41	2.91	6 (14%)	56,56,56	6.64	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMT	A	6002	-	29,29,36	1.46	6 (20%)	40,40,47	1.24	4 (10%)
14	CLA	a	1105	-	45,53,73	2.61	19 (42%)	52,89,113	2.94	20 (38%)
14	CLA	b	1235	-	60,68,73	2.29	19 (31%)	70,107,113	2.76	26 (37%)
13	CL0	A	1011	-	65,73,73	2.26	20 (30%)	76,113,113	2.54	25 (32%)
14	CLA	A	1124	25	55,63,73	2.40	18 (32%)	64,101,113	2.83	21 (32%)
14	CLA	L	1502	-	60,68,73	2.27	18 (30%)	70,107,113	2.69	21 (30%)
18	BCR	b	4004	-	41,41,41	2.82	6 (14%)	56,56,56	6.51	22 (39%)
14	CLA	A	1115	-	65,73,73	2.26	18 (27%)	76,113,113	2.64	26 (34%)
14	CLA	a	1101	-	45,53,73	2.58	19 (42%)	52,89,113	2.95	22 (42%)
14	CLA	H	1210	-	65,73,73	2.21	18 (27%)	76,113,113	2.82	25 (32%)
14	CLA	H	1215	-	60,68,73	2.27	19 (31%)	70,107,113	2.62	20 (28%)
18	BCR	k	4001	-	41,41,41	2.89	6 (14%)	56,56,56	6.45	22 (39%)
14	CLA	m	1501	-	50,58,73	2.52	18 (36%)	58,95,113	2.91	24 (41%)
14	CLA	b	1220	-	65,73,73	2.22	19 (29%)	76,113,113	2.57	22 (28%)
14	CLA	G	1131	-	60,68,73	2.31	19 (31%)	70,107,113	2.72	21 (30%)
14	CLA	B	1213	-	45,53,73	2.58	19 (42%)	52,89,113	2.93	20 (38%)
14	CLA	a	1116	-	55,63,73	2.42	19 (34%)	64,101,113	2.75	23 (35%)
14	CLA	b	1022	-	55,63,73	2.38	17 (30%)	64,101,113	2.73	24 (37%)
14	CLA	H	1223	-	65,73,73	2.23	18 (27%)	76,113,113	2.62	26 (34%)
21	LMT	m	6000	-	36,36,36	1.19	6 (16%)	47,47,47	0.97	1 (2%)
21	LMT	U	6002	-	36,36,36	1.29	5 (13%)	47,47,47	1.21	7 (14%)
14	CLA	G	1126	-	60,68,73	2.34	17 (28%)	70,107,113	2.59	20 (28%)
14	CLA	a	1127	-	65,73,73	2.22	19 (29%)	76,113,113	2.54	21 (27%)
14	CLA	b	1205	-	65,73,73	2.17	17 (26%)	76,113,113	2.67	24 (31%)
14	CLA	a	1139	-	45,53,73	2.57	20 (44%)	52,89,113	2.84	20 (38%)
15	F6C	b	1207	-	69,74,74	2.75	24 (34%)	70,114,114	3.17	28 (40%)
21	LMT	U	6101	-	36,36,36	1.18	5 (13%)	47,47,47	1.32	4 (8%)
14	CLA	G	1141	-	45,53,73	2.54	20 (44%)	52,89,113	2.97	21 (40%)
14	CLA	G	1117	-	65,73,73	2.14	19 (29%)	76,113,113	2.62	29 (38%)
18	BCR	G	4003	-	41,41,41	2.95	6 (14%)	56,56,56	6.84	25 (44%)
14	CLA	G	1111	-	60,68,73	2.29	18 (30%)	70,107,113	4.77	28 (40%)
14	CLA	a	1104	-	65,73,73	2.15	19 (29%)	76,113,113	2.79	24 (31%)
20	LMG	a	5003	-	46,46,55	1.29	5 (10%)	54,54,63	1.25	4 (7%)
14	CLA	H	1231	-	65,73,73	2.19	19 (29%)	76,113,113	2.57	21 (27%)
14	CLA	a	1131	-	60,68,73	2.30	19 (31%)	70,107,113	2.72	22 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	H	1229	-	60,68,73	2.33	19 (31%)	70,107,113	2.70	23 (32%)
14	CLA	G	1137	-	50,58,73	2.52	18 (36%)	58,95,113	3.01	22 (37%)
20	LMG	G	5003	-	46,46,55	1.29	5 (10%)	54,54,63	1.25	4 (7%)
14	CLA	a	1125	-	65,73,73	2.16	18 (27%)	76,113,113	2.69	23 (30%)
14	CLA	a	1126	-	60,68,73	2.33	17 (28%)	70,107,113	2.59	20 (28%)
14	CLA	L	1503	-	65,73,73	2.23	19 (29%)	76,113,113	2.56	23 (30%)
14	CLA	a	1119	-	65,73,73	2.22	18 (27%)	76,113,113	2.48	21 (27%)
14	CLA	H	1213	-	45,53,73	2.58	19 (42%)	52,89,113	2.94	20 (38%)
18	BCR	H	4014	-	41,41,41	2.81	6 (14%)	56,56,56	6.63	20 (35%)
18	BCR	I	4018	-	41,41,41	2.94	6 (14%)	56,56,56	6.59	16 (28%)
21	LMT	A	6003	-	33,33,36	1.22	5 (15%)	44,44,47	0.95	1 (2%)
15	F6C	H	1230	-	49,54,74	3.18	25 (51%)	46,90,114	3.80	25 (54%)
14	CLA	G	1134	1	45,53,73	2.55	20 (44%)	52,89,113	2.92	20 (38%)
15	F6C	B	1230	-	49,54,74	3.18	25 (51%)	46,90,114	3.79	25 (54%)
14	CLA	B	1226	-	65,73,73	2.27	18 (27%)	76,113,113	2.62	24 (31%)
18	BCR	b	4017	-	41,41,41	3.05	8 (19%)	56,56,56	6.72	20 (35%)
15	F6C	G	1121	-	49,54,74	3.13	24 (48%)	46,90,114	3.77	27 (58%)
17	SF4	G	3001	1,2	0,12,12	-	-	-	-	-
19	LHG	A	5002	-	43,43,48	1.00	2 (4%)	47,48,54	1.14	2 (4%)
18	BCR	a	4005	-	41,41,41	3.03	7 (17%)	56,56,56	6.52	23 (41%)
14	CLA	B	1229	-	60,68,73	2.33	19 (31%)	70,107,113	2.69	23 (32%)
19	LHG	G	5001	-	41,41,48	1.05	2 (4%)	44,47,54	0.98	2 (4%)
14	CLA	H	1221	-	65,73,73	2.24	20 (30%)	76,113,113	2.55	23 (30%)
14	CLA	G	1120	-	45,53,73	2.53	18 (40%)	52,89,113	3.11	19 (36%)
14	CLA	b	1211	-	65,73,73	2.24	20 (30%)	76,113,113	2.52	25 (32%)
14	CLA	B	1216	-	65,73,73	2.21	19 (29%)	76,113,113	2.42	21 (27%)
14	CLA	G	1130	-	55,63,73	2.46	19 (34%)	64,101,113	2.65	21 (32%)
21	LMT	b	6003	-	36,36,36	1.18	4 (11%)	47,47,47	1.60	7 (14%)
14	CLA	A	1137	-	50,58,73	2.52	18 (36%)	58,95,113	3.01	22 (37%)
14	CLA	G	1107	-	45,53,73	2.56	17 (37%)	52,89,113	2.93	21 (40%)
14	CLA	a	1141	-	45,53,73	2.54	20 (44%)	52,89,113	2.98	21 (40%)
15	F6C	b	1237	25	69,74,74	2.68	23 (33%)	70,114,114	3.17	30 (42%)
14	CLA	B	1228	-	55,63,73	2.45	20 (36%)	64,101,113	2.66	26 (40%)
17	SF4	c	3003	3	0,12,12	-	-	-	-	-
14	CLA	B	1021	-	65,73,73	2.22	19 (29%)	76,113,113	2.47	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	H	1228	-	55,63,73	2.44	20 (36%)	64,101,113	2.66	26 (40%)
14	CLA	A	1105	-	45,53,73	2.61	18 (40%)	52,89,113	2.94	20 (38%)
14	CLA	G	1114	-	45,53,73	2.57	19 (42%)	52,89,113	2.89	19 (36%)
18	BCR	a	4006	-	41,41,41	2.94	6 (14%)	56,56,56	6.58	24 (42%)
14	CLA	H	1220	-	65,73,73	2.22	19 (29%)	76,113,113	2.58	22 (28%)
19	LHG	L	5102	-	48,48,48	0.90	2 (4%)	51,54,54	1.04	3 (5%)
14	CLA	B	1222	25	65,73,73	2.22	19 (29%)	76,113,113	2.66	24 (31%)
14	CLA	G	1110	-	45,53,73	2.61	18 (40%)	52,89,113	2.89	19 (36%)
14	CLA	B	1212	-	45,53,73	2.55	19 (42%)	52,89,113	2.97	22 (42%)
14	CLA	a	1120	-	45,53,73	2.53	18 (40%)	52,89,113	3.10	19 (36%)
19	LHG	U	5102	-	48,48,48	0.90	2 (4%)	51,54,54	1.04	3 (5%)
14	CLA	U	1502	-	60,68,73	2.28	18 (30%)	70,107,113	2.69	21 (30%)
14	CLA	A	1134	1	45,53,73	2.54	20 (44%)	52,89,113	2.92	20 (38%)
18	BCR	H	4010	-	41,41,41	3.03	7 (17%)	56,56,56	6.86	21 (37%)
19	LHG	A	5001	-	41,41,48	1.05	2 (4%)	44,47,54	0.98	2 (4%)
14	CLA	B	1209	-	45,53,73	2.56	18 (40%)	52,89,113	2.80	20 (38%)
18	BCR	H	4006	-	41,41,41	2.82	6 (14%)	56,56,56	6.58	18 (32%)
14	CLA	a	1133	1	60,68,73	2.31	19 (31%)	70,107,113	2.75	20 (28%)
18	BCR	B	4010	-	41,41,41	3.03	7 (17%)	56,56,56	6.85	21 (37%)
21	LMT	B	6003	-	36,36,36	1.18	4 (11%)	47,47,47	1.60	7 (14%)
14	CLA	b	1213	-	45,53,73	2.58	19 (42%)	52,89,113	2.93	20 (38%)
14	CLA	B	1204	-	65,73,73	2.21	19 (29%)	76,113,113	2.60	23 (30%)
14	CLA	H	1216	-	65,73,73	2.21	19 (29%)	76,113,113	2.41	21 (27%)
15	F6C	B	1238	25	69,74,74	2.73	24 (34%)	70,114,114	3.12	29 (41%)
14	CLA	G	1115	-	65,73,73	2.26	18 (27%)	76,113,113	2.64	26 (34%)
14	CLA	A	1107	-	45,53,73	2.57	17 (37%)	52,89,113	2.92	21 (40%)
15	F6C	b	1219	-	59,64,74	2.96	26 (44%)	58,102,114	3.52	27 (46%)
17	SF4	N	3003	3	0,12,12	-	-	-	-	-
18	BCR	U	4019	-	41,41,41	3.09	7 (17%)	56,56,56	6.49	28 (50%)
19	LHG	L	5101	-	24,24,48	1.27	2 (8%)	26,26,54	1.48	4 (15%)
18	BCR	a	4001	-	41,41,41	2.88	6 (14%)	56,56,56	6.56	17 (30%)
14	CLA	H	1205	-	65,73,73	2.18	17 (26%)	76,113,113	2.67	24 (31%)
17	SF4	c	3002	3	0,12,12	-	-	-	-	-
14	CLA	b	1222	25	65,73,73	2.21	19 (29%)	76,113,113	2.67	25 (32%)
14	CLA	a	1108	-	45,53,73	2.61	19 (42%)	52,89,113	2.90	22 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	1111	-	60,68,73	2.30	18 (30%)	70,107,113	4.77	27 (38%)
21	LMT	B	6004	-	32,32,36	1.22	5 (15%)	43,43,47	1.16	4 (9%)
14	CLA	H	1222	25	65,73,73	2.22	19 (29%)	76,113,113	2.67	24 (31%)
18	BCR	B	4014	-	41,41,41	2.81	6 (14%)	56,56,56	6.63	20 (35%)
21	LMT	H	6001	-	36,36,36	1.19	5 (13%)	47,47,47	0.96	1 (2%)
18	BCR	V	4021	-	41,41,41	2.91	6 (14%)	56,56,56	6.64	19 (33%)
14	CLA	A	1112	-	55,63,73	2.44	20 (36%)	64,101,113	2.79	22 (34%)
13	CL0	a	1011	-	65,73,73	2.26	20 (30%)	76,113,113	2.54	25 (32%)
14	CLA	B	1217	-	45,53,73	2.53	18 (40%)	52,89,113	2.95	20 (38%)
21	LMT	U	6001	-	13,13,36	0.44	0	12,12,47	0.90	0
21	LMT	b	6004	-	32,32,36	1.22	5 (15%)	43,43,47	1.17	4 (9%)
14	CLA	G	1138	-	55,63,73	2.38	20 (36%)	64,101,113	2.89	26 (40%)
21	LMT	G	6003	-	33,33,36	1.22	5 (15%)	44,44,47	0.95	1 (2%)
20	LMG	R	5006	-	37,37,55	1.13	3 (8%)	45,45,63	1.21	5 (11%)
14	CLA	b	1227	-	45,53,73	2.52	18 (40%)	52,89,113	2.99	19 (36%)
14	CLA	H	1209	-	45,53,73	2.55	18 (40%)	52,89,113	2.80	20 (38%)
14	CLA	l	1501	10	65,73,73	2.18	18 (27%)	76,113,113	2.60	23 (30%)
21	LMT	I	6001	-	36,36,36	1.18	5 (13%)	47,47,47	1.03	2 (4%)
14	CLA	H	1208	-	60,68,73	2.33	19 (31%)	70,107,113	2.76	26 (37%)
14	CLA	H	1227	-	45,53,73	2.53	18 (40%)	52,89,113	3.00	19 (36%)
16	PQN	B	2002	-	34,34,34	1.55	2 (5%)	42,45,45	1.12	2 (4%)
14	CLA	B	1227	-	45,53,73	2.53	18 (40%)	52,89,113	2.99	19 (36%)
14	CLA	H	1023	-	65,73,73	2.24	20 (30%)	76,113,113	2.85	30 (39%)
20	LMG	A	5003	-	46,46,55	1.29	5 (10%)	54,54,63	1.25	4 (7%)
14	CLA	G	1109	-	65,73,73	2.24	20 (30%)	76,113,113	2.66	23 (30%)
14	CLA	l	1503	-	65,73,73	2.23	19 (29%)	76,113,113	2.56	23 (30%)
14	CLA	H	1240	2	65,73,73	2.27	20 (30%)	76,113,113	2.59	22 (28%)
21	LMT	G	6004	-	24,24,36	1.05	3 (12%)	29,29,47	1.07	2 (6%)
14	CLA	H	1217	-	45,53,73	2.53	18 (40%)	52,89,113	2.95	20 (38%)
21	LMT	L	6001	-	13,13,36	0.44	0	12,12,47	0.90	0
18	BCR	A	4004	-	41,41,41	3.04	6 (14%)	56,56,56	6.67	25 (44%)
21	LMT	H	6004	-	32,32,36	1.21	4 (12%)	43,43,47	1.16	4 (9%)
14	CLA	A	1133	1	60,68,73	2.31	18 (30%)	70,107,113	2.76	20 (28%)
21	LMT	M	6000	-	36,36,36	1.19	6 (16%)	47,47,47	0.97	1 (2%)
16	PQN	G	2001	-	34,34,34	1.50	2 (5%)	42,45,45	1.19	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	1141	-	45,53,73	2.55	20 (44%)	52,89,113	2.98	21 (40%)
20	LMG	b	5002	-	46,46,55	1.29	6 (13%)	54,54,63	1.24	6 (11%)
15	F6C	b	1238	25	69,74,74	2.74	24 (34%)	70,114,114	3.12	29 (41%)
20	LMG	I	5006	-	37,37,55	1.13	3 (8%)	45,45,63	1.21	5 (11%)
14	CLA	a	1114	-	45,53,73	2.58	19 (42%)	52,89,113	2.88	19 (36%)
21	LMT	B	6001	-	36,36,36	1.19	5 (13%)	47,47,47	0.96	2 (4%)
18	BCR	I	4020	-	41,41,41	3.17	9 (21%)	56,56,56	6.78	21 (37%)
14	CLA	B	1221	-	65,73,73	2.24	19 (29%)	76,113,113	2.55	23 (30%)
14	CLA	b	1223	-	65,73,73	2.23	18 (27%)	76,113,113	2.62	26 (34%)
14	CLA	A	1119	-	65,73,73	2.23	18 (27%)	76,113,113	2.49	21 (27%)
14	CLA	A	1128	-	60,68,73	2.35	19 (31%)	70,107,113	2.69	23 (32%)
18	BCR	A	4002	-	41,41,41	2.85	6 (14%)	56,56,56	6.53	25 (44%)
21	LMT	b	6001	-	36,36,36	1.18	5 (13%)	47,47,47	0.96	2 (4%)
14	CLA	A	1136	-	65,73,73	2.19	19 (29%)	76,113,113	2.62	22 (28%)
18	BCR	B	4005	-	41,41,41	2.83	6 (14%)	56,56,56	6.53	20 (35%)
18	BCR	B	4009	-	41,41,41	2.94	6 (14%)	56,56,56	6.51	23 (41%)
14	CLA	B	1231	-	65,73,73	2.19	19 (29%)	76,113,113	2.57	21 (27%)
21	LMT	A	6004	-	24,24,36	1.06	3 (12%)	29,29,47	1.07	2 (6%)
14	CLA	B	1202	-	65,73,73	2.22	18 (27%)	76,113,113	2.62	24 (31%)
21	LMT	L	6101	-	36,36,36	1.18	5 (13%)	47,47,47	1.32	4 (8%)
19	LHG	l	5102	-	48,48,48	0.90	2 (4%)	51,54,54	1.04	3 (5%)
18	BCR	a	4003	-	41,41,41	2.95	6 (14%)	56,56,56	6.84	25 (44%)
14	CLA	G	1013	-	60,68,73	2.30	19 (31%)	70,107,113	2.80	22 (31%)
17	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
14	CLA	G	1135	-	50,58,73	2.56	20 (40%)	58,95,113	2.95	25 (43%)
14	CLA	B	1023	-	65,73,73	2.24	20 (30%)	76,113,113	2.85	30 (39%)
21	LMT	i	6001	-	36,36,36	1.18	5 (13%)	47,47,47	1.03	2 (4%)
14	CLA	A	1110	-	45,53,73	2.60	18 (40%)	52,89,113	2.89	19 (36%)
14	CLA	B	1224	-	65,73,73	2.22	17 (26%)	76,113,113	2.64	24 (31%)
14	CLA	b	1239	-	65,73,73	2.23	19 (29%)	76,113,113	2.63	27 (35%)
18	BCR	G	4001	-	41,41,41	2.88	6 (14%)	56,56,56	6.56	17 (30%)
21	LMT	G	6001	-	32,32,36	1.30	6 (18%)	43,43,47	1.10	5 (11%)
14	CLA	G	1102	-	50,58,73	2.59	21 (42%)	58,95,113	2.96	24 (41%)
21	LMT	G	6002	-	29,29,36	1.46	6 (20%)	40,40,47	1.23	4 (10%)
14	CLA	b	1232	-	45,53,73	2.58	20 (44%)	52,89,113	2.89	20 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	H	1225	-	65,73,73	2.26	19 (29%)	76,113,113	2.48	19 (25%)
14	CLA	b	1202	-	65,73,73	2.22	18 (27%)	76,113,113	2.61	24 (31%)
18	BCR	i	4018	-	41,41,41	2.94	6 (14%)	56,56,56	6.59	16 (28%)
18	BCR	G	4005	-	41,41,41	3.02	7 (17%)	56,56,56	6.51	23 (41%)
14	CLA	B	1220	-	65,73,73	2.22	19 (29%)	76,113,113	2.57	22 (28%)
21	LMT	H	6002	-	36,36,36	1.20	6 (16%)	47,47,47	1.02	1 (2%)
14	CLA	a	1134	1	45,53,73	2.55	20 (44%)	52,89,113	2.93	20 (38%)
14	CLA	G	1106	1	60,68,73	2.31	18 (30%)	70,107,113	2.77	25 (35%)
14	CLA	B	1225	-	65,73,73	2.27	19 (29%)	76,113,113	2.48	19 (25%)
18	BCR	H	4005	-	41,41,41	2.83	6 (14%)	56,56,56	6.53	20 (35%)
21	LMT	B	6002	-	36,36,36	1.20	6 (16%)	47,47,47	1.02	1 (2%)
14	CLA	A	1125	-	65,73,73	2.16	18 (27%)	76,113,113	2.69	23 (30%)
15	F6C	a	1121	-	49,54,74	3.13	24 (48%)	46,90,114	3.77	27 (58%)
18	BCR	H	4009	-	41,41,41	2.94	6 (14%)	56,56,56	6.51	23 (41%)
14	CLA	b	1217	-	45,53,73	2.53	18 (40%)	52,89,113	2.96	20 (38%)
14	CLA	H	1202	-	65,73,73	2.22	18 (27%)	76,113,113	2.61	24 (31%)
14	CLA	G	1124	25	55,63,73	2.40	18 (32%)	64,101,113	2.83	21 (32%)
14	CLA	A	1103	-	65,73,73	2.21	18 (27%)	76,113,113	2.64	26 (34%)
18	BCR	G	4002	-	41,41,41	2.85	6 (14%)	56,56,56	6.52	25 (44%)
19	LHG	a	5001	-	41,41,48	1.05	2 (4%)	44,47,54	0.98	2 (4%)
21	LMT	R	6001	-	36,36,36	1.17	5 (13%)	47,47,47	1.03	2 (4%)
14	CLA	G	1136	-	65,73,73	2.19	19 (29%)	76,113,113	2.62	22 (28%)
21	LMT	L	6002	-	36,36,36	1.29	5 (13%)	47,47,47	1.21	7 (14%)
14	CLA	B	1210	-	65,73,73	2.21	19 (29%)	76,113,113	2.82	25 (32%)
14	CLA	A	1012	25	65,73,73	2.19	17 (26%)	76,113,113	2.52	25 (32%)
14	CLA	a	1109	-	65,73,73	2.24	20 (30%)	76,113,113	2.67	23 (30%)
14	CLA	k	1401	-	45,53,73	2.59	19 (42%)	52,89,113	3.03	22 (42%)
24	FES	X	101	12	0,4,4	-	-	-	-	-
14	CLA	H	1224	-	65,73,73	2.23	17 (26%)	76,113,113	2.65	24 (31%)
14	CLA	a	1130	-	55,63,73	2.46	19 (34%)	64,101,113	2.66	21 (32%)
14	CLA	H	1234	-	65,73,73	2.22	19 (29%)	76,113,113	2.54	24 (31%)
14	CLA	B	1240	2	65,73,73	2.27	20 (30%)	76,113,113	2.59	22 (28%)
18	BCR	G	4004	-	41,41,41	3.04	6 (14%)	56,56,56	6.67	25 (44%)
18	BCR	A	4001	-	41,41,41	2.88	6 (14%)	56,56,56	6.56	17 (30%)
14	CLA	a	1013	-	60,68,73	2.31	19 (31%)	70,107,113	2.79	22 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	1234	-	65,73,73	2.22	19 (29%)	76,113,113	2.54	24 (31%)
14	CLA	b	1240	2	65,73,73	2.27	20 (30%)	76,113,113	2.59	22 (28%)
14	CLA	A	1102	-	50,58,73	2.59	21 (42%)	58,95,113	2.95	24 (41%)
14	CLA	H	1203	-	65,73,73	2.17	19 (29%)	76,113,113	2.69	22 (28%)
14	CLA	A	1106	1	60,68,73	2.31	18 (30%)	70,107,113	2.76	25 (35%)
14	CLA	B	1206	-	65,73,73	2.23	18 (27%)	76,113,113	2.60	24 (31%)
14	CLA	a	1110	-	45,53,73	2.60	18 (40%)	52,89,113	2.89	19 (36%)
18	BCR	U	4022	-	41,41,41	3.00	6 (14%)	56,56,56	6.39	22 (39%)
24	FES	W	101	12	0,4,4	-	-	-	-	-
14	CLA	H	1235	-	60,68,73	2.29	19 (31%)	70,107,113	2.76	26 (37%)
18	BCR	a	4004	-	41,41,41	3.04	6 (14%)	56,56,56	6.66	25 (44%)
14	CLA	b	1212	-	45,53,73	2.54	19 (42%)	52,89,113	2.97	22 (42%)
14	CLA	G	1012	25	65,73,73	2.19	17 (26%)	76,113,113	2.52	25 (32%)
14	CLA	G	1128	-	60,68,73	2.35	19 (31%)	70,107,113	2.70	23 (32%)
14	CLA	b	1216	-	65,73,73	2.22	19 (29%)	76,113,113	2.42	21 (27%)
18	BCR	i	4020	-	41,41,41	3.17	9 (21%)	56,56,56	6.78	21 (37%)
14	CLA	a	1115	-	65,73,73	2.26	18 (27%)	76,113,113	2.64	26 (34%)
14	CLA	b	1229	-	60,68,73	2.33	19 (31%)	70,107,113	2.69	23 (32%)
19	LHG	G	5002	-	43,43,48	1.00	2 (4%)	47,48,54	1.14	2 (4%)
14	CLA	M	1501	-	50,58,73	2.53	18 (36%)	58,95,113	2.91	24 (41%)
14	CLA	a	1107	-	45,53,73	2.56	17 (37%)	52,89,113	2.92	21 (40%)
14	CLA	b	1204	-	65,73,73	2.21	19 (29%)	76,113,113	2.59	23 (30%)
18	BCR	b	4006	-	41,41,41	2.82	6 (14%)	56,56,56	6.58	18 (32%)
14	CLA	A	1108	-	45,53,73	2.62	19 (42%)	52,89,113	2.91	22 (42%)
14	CLA	B	1201	-	65,73,73	2.20	20 (30%)	76,113,113	2.71	25 (32%)
14	CLA	b	1231	-	65,73,73	2.18	19 (29%)	76,113,113	2.57	21 (27%)
17	SF4	N	3002	3	0,12,12	-	-	-	-	-
14	CLA	B	1203	-	65,73,73	2.17	19 (29%)	76,113,113	2.69	22 (28%)
14	CLA	A	1109	-	65,73,73	2.24	20 (30%)	76,113,113	2.67	23 (30%)
14	CLA	a	1123	-	60,68,73	2.33	18 (30%)	70,107,113	2.77	24 (34%)
14	CLA	H	1206	-	65,73,73	2.24	19 (29%)	76,113,113	2.60	24 (31%)
14	CLA	G	1132	-	65,73,73	2.19	18 (27%)	76,113,113	2.64	23 (30%)
14	CLA	b	1215	-	60,68,73	2.28	19 (31%)	70,107,113	2.62	20 (28%)
14	CLA	a	1137	-	50,58,73	2.52	18 (36%)	58,95,113	3.01	22 (37%)
14	CLA	G	1140	-	55,63,73	2.42	18 (32%)	64,101,113	2.69	20 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	1116	-	55,63,73	2.42	19 (34%)	64,101,113	2.75	22 (34%)
14	CLA	b	1209	-	45,53,73	2.56	18 (40%)	52,89,113	2.80	20 (38%)
21	LMT	a	6003	-	33,33,36	1.22	5 (15%)	44,44,47	0.95	1 (2%)
14	CLA	H	1212	-	45,53,73	2.54	18 (40%)	52,89,113	2.96	22 (42%)
14	CLA	A	1127	-	65,73,73	2.22	19 (29%)	76,113,113	2.54	21 (27%)
14	CLA	B	1205	-	65,73,73	2.17	17 (26%)	76,113,113	2.67	24 (31%)
21	LMT	l	6101	-	36,36,36	1.18	5 (13%)	47,47,47	1.32	4 (8%)
14	CLA	G	1103	-	65,73,73	2.21	18 (27%)	76,113,113	2.64	26 (34%)
18	BCR	R	4020	-	41,41,41	3.17	9 (21%)	56,56,56	6.77	21 (37%)
14	CLA	b	1225	-	65,73,73	2.26	19 (29%)	76,113,113	2.48	19 (25%)
18	BCR	a	4002	-	41,41,41	2.85	6 (14%)	56,56,56	6.52	25 (44%)
14	CLA	a	1122	-	55,63,73	2.35	19 (34%)	64,101,113	2.71	24 (37%)
14	CLA	A	1101	-	45,53,73	2.57	19 (42%)	52,89,113	2.94	22 (42%)
14	CLA	H	1201	-	65,73,73	2.20	20 (30%)	76,113,113	2.71	25 (32%)
14	CLA	a	1136	-	65,73,73	2.19	19 (29%)	76,113,113	2.61	22 (28%)
16	PQN	b	2002	-	34,34,34	1.55	2 (5%)	42,45,45	1.12	2 (4%)
14	CLA	b	1208	-	60,68,73	2.34	19 (31%)	70,107,113	2.75	26 (37%)
21	LMT	a	6004	-	24,24,36	1.06	3 (12%)	29,29,47	1.07	2 (6%)
17	SF4	a	3001	1,2	0,12,12	-	-	-	-	-
14	CLA	a	1112	-	55,63,73	2.44	20 (36%)	64,101,113	2.80	22 (34%)
16	PQN	a	2001	-	34,34,34	1.50	2 (5%)	42,45,45	1.19	4 (9%)
14	CLA	G	1112	-	55,63,73	2.44	20 (36%)	64,101,113	2.79	22 (34%)
14	CLA	b	1210	-	65,73,73	2.21	19 (29%)	76,113,113	2.82	25 (32%)
14	CLA	A	1135	-	50,58,73	2.56	20 (40%)	58,95,113	2.95	25 (43%)
15	F6C	B	1237	25	69,74,74	2.68	23 (33%)	70,114,114	3.17	30 (42%)
17	SF4	C	3003	3	0,12,12	-	-	-	-	-
14	CLA	b	1218	-	45,53,73	2.57	18 (40%)	52,89,113	3.09	21 (40%)
21	LMT	A	6001	-	32,32,36	1.30	6 (18%)	43,43,47	1.10	5 (11%)
14	CLA	A	1120	-	45,53,73	2.53	18 (40%)	52,89,113	3.11	19 (36%)
14	CLA	B	1218	-	45,53,73	2.57	18 (40%)	52,89,113	3.08	21 (40%)
14	CLA	b	1021	-	65,73,73	2.22	19 (29%)	76,113,113	2.47	27 (35%)
14	CLA	A	1113	-	45,53,73	2.55	18 (40%)	52,89,113	2.87	21 (40%)
14	CLA	b	1221	-	65,73,73	2.24	19 (29%)	76,113,113	2.55	23 (30%)
14	CLA	B	1235	-	60,68,73	2.29	19 (31%)	70,107,113	2.77	26 (37%)
14	CLA	a	1012	25	65,73,73	2.20	17 (26%)	76,113,113	2.52	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	1214	-	60,68,73	2.34	21 (35%)	70,107,113	2.66	28 (40%)
16	PQN	H	2002	-	34,34,34	1.56	2 (5%)	42,45,45	1.12	2 (4%)
14	CLA	a	1103	-	65,73,73	2.21	18 (27%)	76,113,113	2.64	26 (34%)
14	CLA	A	1138	-	55,63,73	2.38	20 (36%)	64,101,113	2.89	26 (40%)
18	BCR	l	4022	-	41,41,41	3.01	6 (14%)	56,56,56	6.40	22 (39%)
18	BCR	A	4003	-	41,41,41	2.96	6 (14%)	56,56,56	6.84	25 (44%)
18	BCR	A	4005	-	41,41,41	3.02	6 (14%)	56,56,56	6.52	23 (41%)
14	CLA	B	1233	-	45,53,73	2.57	19 (42%)	52,89,113	2.90	20 (38%)
19	LHG	l	5101	-	24,24,48	1.27	2 (8%)	26,26,54	1.48	4 (15%)
14	CLA	b	1228	-	55,63,73	2.45	20 (36%)	64,101,113	2.66	26 (40%)
14	CLA	a	1135	-	50,58,73	2.56	20 (40%)	58,95,113	2.94	24 (41%)
14	CLA	B	1236	-	55,63,73	2.33	18 (32%)	64,101,113	2.98	23 (35%)
14	CLA	G	1116	-	55,63,73	2.41	19 (34%)	64,101,113	2.74	22 (34%)
14	CLA	G	1118	-	55,63,73	2.42	18 (32%)	64,101,113	2.80	22 (34%)
21	LMT	V	6000	-	36,36,36	1.19	6 (16%)	47,47,47	0.97	1 (2%)
14	CLA	H	1236	-	55,63,73	2.33	19 (34%)	64,101,113	2.98	23 (35%)
18	BCR	b	4010	-	41,41,41	3.03	7 (17%)	56,56,56	6.86	21 (37%)
14	CLA	G	1139	-	45,53,73	2.56	20 (44%)	52,89,113	2.84	20 (38%)
14	CLA	H	1218	-	45,53,73	2.57	18 (40%)	52,89,113	3.08	21 (40%)
21	LMT	a	6001	-	32,32,36	1.31	6 (18%)	43,43,47	1.10	5 (11%)
14	CLA	a	1118	-	55,63,73	2.42	18 (32%)	64,101,113	2.79	22 (34%)
15	F6C	H	1237	25	69,74,74	2.68	23 (33%)	70,114,114	3.18	30 (42%)
18	BCR	T	4001	-	41,41,41	2.90	6 (14%)	56,56,56	6.45	22 (39%)
14	CLA	U	1503	-	65,73,73	2.23	19 (29%)	76,113,113	2.56	23 (30%)
14	CLA	l	1502	-	60,68,73	2.27	18 (30%)	70,107,113	2.69	21 (30%)
14	CLA	a	1140	-	55,63,73	2.42	18 (32%)	64,101,113	2.69	21 (32%)
14	CLA	A	1123	-	60,68,73	2.32	18 (30%)	70,107,113	2.77	24 (34%)
18	BCR	b	4005	-	41,41,41	2.84	6 (14%)	56,56,56	6.53	20 (35%)
14	CLA	a	1106	1	60,68,73	2.31	19 (31%)	70,107,113	2.76	25 (35%)
14	CLA	G	1104	-	65,73,73	2.15	19 (29%)	76,113,113	2.80	24 (31%)
15	F6C	A	1121	-	49,54,74	3.13	24 (48%)	46,90,114	3.77	27 (58%)
14	CLA	H	1239	-	65,73,73	2.23	20 (30%)	76,113,113	2.62	28 (36%)
21	LMT	H	6003	-	36,36,36	1.18	3 (8%)	47,47,47	1.60	7 (14%)
14	CLA	B	1022	-	55,63,73	2.38	18 (32%)	64,101,113	2.74	24 (37%)
14	CLA	A	1013	-	60,68,73	2.30	19 (31%)	70,107,113	2.80	22 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1233	-	1/1/11/20	8/13/91/115	-
14	CLA	G	1113	-	1/1/11/20	7/13/91/115	-
14	CLA	a	1113	-	1/1/11/20	7/13/91/115	-
14	CLA	A	1117	-	1/1/15/20	21/37/115/115	-
14	CLA	A	1129	-	1/1/12/20	6/19/97/115	-
18	BCR	M	4021	-	-	14/29/63/63	0/2/2/2
15	F6C	b	1230	-	-	9/17/73/97	-
14	CLA	U	1501	10	1/1/15/20	8/37/115/115	-
14	CLA	A	1140	-	1/1/13/20	14/25/103/115	-
21	LMT	l	6001	-	-	5/11/11/61	-
18	BCR	L	4019	-	-	10/29/63/63	0/2/2/2
14	CLA	B	1214	-	1/1/14/20	11/31/109/115	-
21	LMT	l	6002	-	-	6/21/61/61	0/2/2/2
14	CLA	b	1224	-	1/1/15/20	19/37/115/115	-
21	LMT	a	6002	-	-	9/14/54/61	0/2/2/2
14	CLA	A	1114	-	1/1/11/20	4/13/91/115	-
14	CLA	H	1226	-	1/1/15/20	18/37/115/115	-
18	BCR	b	4009	-	-	4/29/63/63	0/2/2/2
14	CLA	H	1022	-	1/1/13/20	11/25/103/115	-
18	BCR	H	4017	-	-	15/29/63/63	0/2/2/2
14	CLA	b	1236	-	1/1/13/20	15/25/103/115	-
14	CLA	G	1119	-	1/1/15/20	16/37/115/115	-
14	CLA	a	1128	-	1/1/14/20	15/31/109/115	-
18	BCR	B	4017	-	-	15/29/63/63	0/2/2/2
14	CLA	b	1023	-	1/1/15/20	10/37/115/115	-
18	BCR	L	4022	-	-	8/29/63/63	0/2/2/2
14	CLA	b	1226	-	1/1/15/20	18/37/115/115	-
14	CLA	H	1214	-	1/1/14/20	11/31/109/115	-
18	BCR	A	4006	-	-	16/29/63/63	0/2/2/2
14	CLA	A	1130	-	1/1/13/20	9/25/103/115	-
14	CLA	G	1129	-	1/1/12/20	6/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1122	-	1/1/13/20	12/25/103/115	-
18	BCR	B	4006	-	-	16/29/63/63	0/2/2/2
19	LHG	a	5002	-	-	24/45/45/53	-
14	CLA	K	1401	-	1/1/11/20	9/13/91/115	-
14	CLA	b	1203	-	1/1/15/20	22/37/115/115	-
14	CLA	B	1211	-	1/1/15/20	15/37/115/115	-
14	CLA	A	1104	-	1/1/15/20	19/37/115/115	-
14	CLA	A	1131	-	1/1/14/20	12/31/109/115	-
14	CLA	a	1117	-	1/1/15/20	21/37/115/115	-
14	CLA	b	1233	-	1/1/11/20	8/13/91/115	-
14	CLA	G	1105	-	1/1/11/20	3/13/91/115	-
15	F6C	B	1219	-	-	15/29/85/97	-
18	BCR	B	4004	-	-	12/29/63/63	0/2/2/2
16	PQN	A	2001	-	-	8/23/43/43	0/2/2/2
14	CLA	A	1132	-	1/1/15/20	10/37/115/115	-
14	CLA	b	1234	-	1/1/15/20	15/37/115/115	-
15	F6C	H	1238	25	-	15/41/97/97	-
18	BCR	G	4006	-	-	16/29/63/63	0/2/2/2
14	CLA	H	1021	-	1/1/15/20	14/37/115/115	-
14	CLA	B	1208	-	1/1/14/20	9/31/109/115	-
14	CLA	H	1211	-	1/1/15/20	15/37/115/115	-
15	F6C	B	1207	-	-	19/41/97/97	-
14	CLA	G	1123	-	1/1/14/20	14/31/109/115	-
14	CLA	G	1133	1	1/1/14/20	21/31/109/115	-
14	CLA	A	1126	-	1/1/14/20	15/31/109/115	-
14	CLA	a	1138	-	1/1/13/20	13/25/103/115	-
14	CLA	G	1127	-	1/1/15/20	18/37/115/115	-
21	LMT	b	6002	-	-	3/21/61/61	0/2/2/2
14	CLA	b	1206	-	1/1/15/20	20/37/115/115	-
14	CLA	a	1132	-	1/1/15/20	10/37/115/115	-
14	CLA	T	1401	-	1/1/11/20	9/13/91/115	-
15	F6C	H	1219	-	-	15/29/85/97	-
14	CLA	B	1232	-	1/1/11/20	2/13/91/115	-
18	BCR	H	4004	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1139	-	1/1/11/20	8/13/91/115	-
14	CLA	a	1124	25	1/1/13/20	5/25/103/115	-
14	CLA	H	1204	-	1/1/15/20	11/37/115/115	-
14	CLA	G	1108	-	1/1/11/20	5/13/91/115	-
14	CLA	L	1501	10	1/1/15/20	8/37/115/115	-
24	FES	x	101	12	-	-	0/1/1/1
14	CLA	G	1125	-	1/1/15/20	20/37/115/115	-
14	CLA	V	1501	-	1/1/12/20	6/19/97/115	-
14	CLA	b	1201	-	1/1/15/20	18/37/115/115	-
18	BCR	K	4001	-	-	16/29/63/63	0/2/2/2
14	CLA	A	1118	-	1/1/13/20	11/25/103/115	-
13	CL0	G	1011	-	3/3/20/25	15/37/135/135	-
20	LMG	H	5002	-	-	17/41/61/70	0/1/1/1
14	CLA	a	1102	-	1/1/12/20	10/19/97/115	-
15	F6C	H	1207	-	-	19/41/97/97	-
18	BCR	R	4018	-	-	11/29/63/63	0/2/2/2
18	BCR	b	4014	-	-	6/29/63/63	0/2/2/2
19	LHG	U	5101	-	-	15/26/26/53	-
17	SF4	C	3002	3	-	-	0/6/5/5
18	BCR	l	4019	-	-	10/29/63/63	0/2/2/2
20	LMG	B	5002	-	-	17/41/61/70	0/1/1/1
14	CLA	B	1215	-	1/1/14/20	16/31/109/115	-
14	CLA	G	1122	-	1/1/13/20	12/25/103/115	-
14	CLA	a	1129	-	1/1/12/20	6/19/97/115	-
14	CLA	H	1232	-	1/1/11/20	2/13/91/115	-
14	CLA	B	1223	-	1/1/15/20	11/37/115/115	-
20	LMG	i	5006	-	-	13/32/52/70	0/1/1/1
14	CLA	G	1101	-	1/1/11/20	6/13/91/115	-
14	CLA	A	1111	-	1/1/14/20	16/31/109/115	-
14	CLA	B	1239	-	1/1/15/20	20/37/115/115	-
18	BCR	m	4021	-	-	14/29/63/63	0/2/2/2
21	LMT	A	6002	-	-	9/14/54/61	0/2/2/2
14	CLA	a	1105	-	1/1/11/20	3/13/91/115	-
14	CLA	b	1235	-	1/1/14/20	14/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CL0	A	1011	-	3/3/20/25	15/37/135/135	-
14	CLA	A	1124	25	1/1/13/20	5/25/103/115	-
14	CLA	L	1502	-	1/1/14/20	10/31/109/115	-
18	BCR	b	4004	-	-	12/29/63/63	0/2/2/2
14	CLA	A	1115	-	1/1/15/20	19/37/115/115	-
14	CLA	a	1101	-	1/1/11/20	6/13/91/115	-
14	CLA	H	1210	-	1/1/15/20	17/37/115/115	-
14	CLA	H	1215	-	1/1/14/20	16/31/109/115	-
18	BCR	k	4001	-	-	16/29/63/63	0/2/2/2
14	CLA	m	1501	-	1/1/12/20	6/19/97/115	-
14	CLA	b	1220	-	1/1/15/20	14/37/115/115	-
14	CLA	G	1131	-	1/1/14/20	12/31/109/115	-
14	CLA	B	1213	-	1/1/11/20	2/13/91/115	-
14	CLA	a	1116	-	1/1/13/20	12/25/103/115	-
14	CLA	b	1022	-	1/1/13/20	11/25/103/115	-
14	CLA	H	1223	-	1/1/15/20	11/37/115/115	-
21	LMT	m	6000	-	-	5/21/61/61	0/2/2/2
21	LMT	U	6002	-	-	6/21/61/61	0/2/2/2
14	CLA	G	1126	-	1/1/14/20	15/31/109/115	-
14	CLA	a	1127	-	1/1/15/20	18/37/115/115	-
14	CLA	b	1205	-	1/1/15/20	13/37/115/115	-
14	CLA	a	1139	-	1/1/11/20	8/13/91/115	-
15	F6C	b	1207	-	-	19/41/97/97	-
21	LMT	U	6101	-	-	8/21/61/61	0/2/2/2
14	CLA	G	1141	-	1/1/11/20	10/13/91/115	-
14	CLA	G	1117	-	1/1/15/20	21/37/115/115	-
18	BCR	G	4003	-	-	9/29/63/63	0/2/2/2
14	CLA	G	1111	-	1/1/14/20	16/31/109/115	-
14	CLA	a	1104	-	1/1/15/20	19/37/115/115	-
20	LMG	a	5003	-	-	15/41/61/70	0/1/1/1
14	CLA	H	1231	-	1/1/15/20	17/37/115/115	-
14	CLA	a	1131	-	1/1/14/20	12/31/109/115	-
14	CLA	H	1229	-	1/1/14/20	15/31/109/115	-
14	CLA	G	1137	-	1/1/12/20	6/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMG	G	5003	-	-	15/41/61/70	0/1/1/1
14	CLA	a	1125	-	1/1/15/20	20/37/115/115	-
14	CLA	a	1126	-	1/1/14/20	15/31/109/115	-
14	CLA	L	1503	-	1/1/15/20	13/37/115/115	-
14	CLA	a	1119	-	1/1/15/20	16/37/115/115	-
14	CLA	H	1213	-	1/1/11/20	2/13/91/115	-
18	BCR	H	4014	-	-	6/29/63/63	0/2/2/2
18	BCR	I	4018	-	-	11/29/63/63	0/2/2/2
21	LMT	A	6003	-	-	7/18/58/61	0/2/2/2
15	F6C	H	1230	-	-	9/17/73/97	-
14	CLA	G	1134	1	1/1/11/20	9/13/91/115	-
15	F6C	B	1230	-	-	9/17/73/97	-
14	CLA	B	1226	-	1/1/15/20	18/37/115/115	-
18	BCR	b	4017	-	-	15/29/63/63	0/2/2/2
15	F6C	G	1121	-	-	10/17/73/97	-
19	LHG	A	5002	-	-	24/45/45/53	-
17	SF4	G	3001	1,2	-	-	0/6/5/5
18	BCR	a	4005	-	-	10/29/63/63	0/2/2/2
14	CLA	B	1229	-	1/1/14/20	15/31/109/115	-
19	LHG	G	5001	-	-	23/46/46/53	-
14	CLA	H	1221	-	1/1/15/20	20/37/115/115	-
14	CLA	G	1120	-	1/1/11/20	6/13/91/115	-
14	CLA	b	1211	-	1/1/15/20	15/37/115/115	-
14	CLA	B	1216	-	1/1/15/20	18/37/115/115	-
14	CLA	G	1130	-	1/1/13/20	9/25/103/115	-
21	LMT	b	6003	-	-	11/21/61/61	0/2/2/2
14	CLA	A	1137	-	1/1/12/20	6/19/97/115	-
14	CLA	G	1107	-	1/1/11/20	5/13/91/115	-
14	CLA	a	1141	-	1/1/11/20	10/13/91/115	-
15	F6C	b	1237	25	-	24/41/97/97	-
14	CLA	B	1228	-	1/1/13/20	15/25/103/115	-
17	SF4	c	3003	3	-	-	0/6/5/5
14	CLA	B	1021	-	1/1/15/20	14/37/115/115	-
14	CLA	H	1228	-	1/1/13/20	15/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1105	-	1/1/11/20	3/13/91/115	-
14	CLA	G	1114	-	1/1/11/20	4/13/91/115	-
18	BCR	a	4006	-	-	16/29/63/63	0/2/2/2
14	CLA	H	1220	-	1/1/15/20	14/37/115/115	-
19	LHG	L	5102	-	-	26/53/53/53	-
14	CLA	B	1222	25	1/1/15/20	15/37/115/115	-
14	CLA	G	1110	-	1/1/11/20	4/13/91/115	-
14	CLA	B	1212	-	1/1/11/20	8/13/91/115	-
14	CLA	a	1120	-	1/1/11/20	6/13/91/115	-
19	LHG	U	5102	-	-	26/53/53/53	-
14	CLA	U	1502	-	1/1/14/20	10/31/109/115	-
14	CLA	A	1134	1	1/1/11/20	9/13/91/115	-
18	BCR	H	4010	-	-	7/29/63/63	0/2/2/2
19	LHG	A	5001	-	-	23/46/46/53	-
14	CLA	B	1209	-	1/1/11/20	2/13/91/115	-
18	BCR	H	4006	-	-	16/29/63/63	0/2/2/2
14	CLA	a	1133	1	1/1/14/20	21/31/109/115	-
18	BCR	B	4010	-	-	7/29/63/63	0/2/2/2
21	LMT	B	6003	-	-	11/21/61/61	0/2/2/2
14	CLA	b	1213	-	1/1/11/20	2/13/91/115	-
14	CLA	B	1204	-	1/1/15/20	11/37/115/115	-
14	CLA	H	1216	-	1/1/15/20	18/37/115/115	-
15	F6C	B	1238	25	-	15/41/97/97	-
14	CLA	G	1115	-	1/1/15/20	19/37/115/115	-
14	CLA	A	1107	-	1/1/11/20	5/13/91/115	-
15	F6C	b	1219	-	-	15/29/85/97	-
17	SF4	N	3003	3	-	-	0/6/5/5
18	BCR	U	4019	-	-	9/29/63/63	0/2/2/2
19	LHG	L	5101	-	-	15/26/26/53	-
18	BCR	a	4001	-	-	12/29/63/63	0/2/2/2
14	CLA	H	1205	-	1/1/15/20	13/37/115/115	-
17	SF4	c	3002	3	-	-	0/6/5/5
14	CLA	b	1222	25	1/1/15/20	15/37/115/115	-
14	CLA	a	1108	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	1111	-	1/1/14/20	16/31/109/115	-
21	LMT	B	6004	-	-	10/17/57/61	0/2/2/2
14	CLA	H	1222	25	1/1/15/20	15/37/115/115	-
18	BCR	B	4014	-	-	6/29/63/63	0/2/2/2
21	LMT	H	6001	-	-	7/21/61/61	0/2/2/2
18	BCR	V	4021	-	-	14/29/63/63	0/2/2/2
14	CLA	A	1112	-	1/1/13/20	12/25/103/115	-
13	CL0	a	1011	-	3/3/20/25	15/37/135/135	-
14	CLA	B	1217	-	1/1/11/20	7/13/91/115	-
21	LMT	U	6001	-	-	5/11/11/61	-
21	LMT	b	6004	-	-	10/17/57/61	0/2/2/2
14	CLA	G	1138	-	1/1/13/20	13/25/103/115	-
21	LMT	G	6003	-	-	7/18/58/61	0/2/2/2
20	LMG	R	5006	-	-	13/32/52/70	0/1/1/1
14	CLA	b	1227	-	1/1/11/20	7/13/91/115	-
14	CLA	H	1209	-	1/1/11/20	2/13/91/115	-
14	CLA	l	1501	10	1/1/15/20	8/37/115/115	-
21	LMT	I	6001	-	-	11/21/61/61	0/2/2/2
14	CLA	H	1208	-	1/1/14/20	9/31/109/115	-
14	CLA	H	1227	-	1/1/11/20	7/13/91/115	-
16	PQN	B	2002	-	-	9/23/43/43	0/2/2/2
14	CLA	B	1227	-	1/1/11/20	7/13/91/115	-
14	CLA	H	1023	-	1/1/15/20	10/37/115/115	-
20	LMG	A	5003	-	-	15/41/61/70	0/1/1/1
14	CLA	G	1109	-	1/1/15/20	13/37/115/115	-
14	CLA	l	1503	-	1/1/15/20	13/37/115/115	-
14	CLA	H	1240	2	1/1/15/20	18/37/115/115	-
21	LMT	G	6004	-	-	6/15/35/61	0/1/1/2
14	CLA	H	1217	-	1/1/11/20	7/13/91/115	-
21	LMT	L	6001	-	-	5/11/11/61	-
18	BCR	A	4004	-	-	11/29/63/63	0/2/2/2
21	LMT	H	6004	-	-	10/17/57/61	0/2/2/2
14	CLA	A	1133	1	1/1/14/20	21/31/109/115	-
21	LMT	M	6000	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	PQN	G	2001	-	-	8/23/43/43	0/2/2/2
14	CLA	A	1141	-	1/1/11/20	10/13/91/115	-
20	LMG	b	5002	-	-	17/41/61/70	0/1/1/1
15	F6C	b	1238	25	-	15/41/97/97	-
20	LMG	I	5006	-	-	13/32/52/70	0/1/1/1
14	CLA	a	1114	-	1/1/11/20	4/13/91/115	-
21	LMT	B	6001	-	-	7/21/61/61	0/2/2/2
18	BCR	I	4020	-	-	9/29/63/63	0/2/2/2
14	CLA	B	1221	-	1/1/15/20	20/37/115/115	-
14	CLA	b	1223	-	1/1/15/20	11/37/115/115	-
14	CLA	A	1119	-	1/1/15/20	16/37/115/115	-
14	CLA	A	1128	-	1/1/14/20	15/31/109/115	-
18	BCR	A	4002	-	-	12/29/63/63	0/2/2/2
21	LMT	b	6001	-	-	7/21/61/61	0/2/2/2
14	CLA	A	1136	-	1/1/15/20	18/37/115/115	-
18	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
18	BCR	B	4009	-	-	4/29/63/63	0/2/2/2
14	CLA	B	1231	-	1/1/15/20	17/37/115/115	-
21	LMT	A	6004	-	-	6/15/35/61	0/1/1/2
14	CLA	B	1202	-	1/1/15/20	16/37/115/115	-
21	LMT	L	6101	-	-	8/21/61/61	0/2/2/2
19	LHG	l	5102	-	-	26/53/53/53	-
18	BCR	a	4003	-	-	9/29/63/63	0/2/2/2
14	CLA	G	1013	-	1/1/14/20	10/31/109/115	-
17	SF4	A	3001	1,2	-	-	0/6/5/5
14	CLA	G	1135	-	1/1/12/20	8/19/97/115	-
14	CLA	B	1023	-	1/1/15/20	10/37/115/115	-
21	LMT	i	6001	-	-	11/21/61/61	0/2/2/2
14	CLA	A	1110	-	1/1/11/20	4/13/91/115	-
14	CLA	B	1224	-	1/1/15/20	19/37/115/115	-
14	CLA	b	1239	-	1/1/15/20	20/37/115/115	-
18	BCR	G	4001	-	-	12/29/63/63	0/2/2/2
21	LMT	G	6001	-	-	9/17/57/61	0/2/2/2
14	CLA	G	1102	-	1/1/12/20	10/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMT	G	6002	-	-	9/14/54/61	0/2/2/2
14	CLA	b	1232	-	1/1/11/20	2/13/91/115	-
14	CLA	H	1225	-	1/1/15/20	18/37/115/115	-
14	CLA	b	1202	-	1/1/15/20	16/37/115/115	-
18	BCR	i	4018	-	-	11/29/63/63	0/2/2/2
18	BCR	G	4005	-	-	10/29/63/63	0/2/2/2
14	CLA	B	1220	-	1/1/15/20	14/37/115/115	-
21	LMT	H	6002	-	-	3/21/61/61	0/2/2/2
14	CLA	a	1134	1	1/1/11/20	9/13/91/115	-
14	CLA	G	1106	1	1/1/14/20	10/31/109/115	-
14	CLA	B	1225	-	1/1/15/20	18/37/115/115	-
18	BCR	H	4005	-	-	6/29/63/63	0/2/2/2
21	LMT	B	6002	-	-	3/21/61/61	0/2/2/2
14	CLA	A	1125	-	1/1/15/20	20/37/115/115	-
15	F6C	a	1121	-	-	10/17/73/97	-
18	BCR	H	4009	-	-	4/29/63/63	0/2/2/2
14	CLA	b	1217	-	1/1/11/20	7/13/91/115	-
14	CLA	H	1202	-	1/1/15/20	16/37/115/115	-
14	CLA	G	1124	25	1/1/13/20	5/25/103/115	-
14	CLA	A	1103	-	1/1/15/20	23/37/115/115	-
18	BCR	G	4002	-	-	12/29/63/63	0/2/2/2
19	LHG	a	5001	-	-	23/46/46/53	-
21	LMT	R	6001	-	-	11/21/61/61	0/2/2/2
14	CLA	G	1136	-	1/1/15/20	18/37/115/115	-
21	LMT	L	6002	-	-	6/21/61/61	0/2/2/2
14	CLA	B	1210	-	1/1/15/20	17/37/115/115	-
14	CLA	A	1012	25	1/1/15/20	7/37/115/115	-
14	CLA	a	1109	-	1/1/15/20	13/37/115/115	-
14	CLA	k	1401	-	1/1/11/20	9/13/91/115	-
24	FES	X	101	12	-	-	0/1/1/1
14	CLA	H	1224	-	1/1/15/20	19/37/115/115	-
14	CLA	a	1130	-	1/1/13/20	9/25/103/115	-
14	CLA	H	1234	-	1/1/15/20	15/37/115/115	-
14	CLA	B	1240	2	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	G	4004	-	-	11/29/63/63	0/2/2/2
18	BCR	A	4001	-	-	12/29/63/63	0/2/2/2
14	CLA	a	1013	-	1/1/14/20	10/31/109/115	-
14	CLA	B	1234	-	1/1/15/20	15/37/115/115	-
14	CLA	b	1240	2	1/1/15/20	18/37/115/115	-
14	CLA	A	1102	-	1/1/12/20	10/19/97/115	-
14	CLA	H	1203	-	1/1/15/20	22/37/115/115	-
14	CLA	A	1106	1	1/1/14/20	10/31/109/115	-
14	CLA	B	1206	-	1/1/15/20	20/37/115/115	-
14	CLA	a	1110	-	1/1/11/20	4/13/91/115	-
18	BCR	U	4022	-	-	8/29/63/63	0/2/2/2
24	FES	W	101	12	-	-	0/1/1/1
14	CLA	H	1235	-	1/1/14/20	14/31/109/115	-
18	BCR	a	4004	-	-	11/29/63/63	0/2/2/2
14	CLA	b	1212	-	1/1/11/20	8/13/91/115	-
14	CLA	G	1012	25	1/1/15/20	7/37/115/115	-
14	CLA	G	1128	-	1/1/14/20	15/31/109/115	-
14	CLA	b	1216	-	1/1/15/20	18/37/115/115	-
18	BCR	i	4020	-	-	9/29/63/63	0/2/2/2
14	CLA	a	1115	-	1/1/15/20	19/37/115/115	-
14	CLA	b	1229	-	1/1/14/20	15/31/109/115	-
19	LHG	G	5002	-	-	24/45/45/53	-
14	CLA	M	1501	-	1/1/12/20	6/19/97/115	-
14	CLA	a	1107	-	1/1/11/20	5/13/91/115	-
14	CLA	b	1204	-	1/1/15/20	11/37/115/115	-
18	BCR	b	4006	-	-	16/29/63/63	0/2/2/2
14	CLA	A	1108	-	1/1/11/20	5/13/91/115	-
14	CLA	B	1201	-	1/1/15/20	18/37/115/115	-
14	CLA	b	1231	-	1/1/15/20	17/37/115/115	-
17	SF4	N	3002	3	-	-	0/6/5/5
14	CLA	B	1203	-	1/1/15/20	22/37/115/115	-
14	CLA	A	1109	-	1/1/15/20	13/37/115/115	-
14	CLA	a	1123	-	1/1/14/20	14/31/109/115	-
14	CLA	H	1206	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1132	-	1/1/15/20	10/37/115/115	-
14	CLA	b	1215	-	1/1/14/20	16/31/109/115	-
14	CLA	a	1137	-	1/1/12/20	6/19/97/115	-
14	CLA	G	1140	-	1/1/13/20	14/25/103/115	-
14	CLA	A	1116	-	1/1/13/20	12/25/103/115	-
14	CLA	b	1209	-	1/1/11/20	2/13/91/115	-
21	LMT	a	6003	-	-	7/18/58/61	0/2/2/2
14	CLA	H	1212	-	1/1/11/20	8/13/91/115	-
14	CLA	A	1127	-	1/1/15/20	18/37/115/115	-
14	CLA	B	1205	-	1/1/15/20	13/37/115/115	-
21	LMT	l	6101	-	-	8/21/61/61	0/2/2/2
14	CLA	G	1103	-	1/1/15/20	23/37/115/115	-
18	BCR	R	4020	-	-	9/29/63/63	0/2/2/2
14	CLA	b	1225	-	1/1/15/20	17/37/115/115	-
18	BCR	a	4002	-	-	12/29/63/63	0/2/2/2
14	CLA	a	1122	-	1/1/13/20	12/25/103/115	-
14	CLA	A	1101	-	1/1/11/20	6/13/91/115	-
14	CLA	H	1201	-	1/1/15/20	18/37/115/115	-
14	CLA	a	1136	-	1/1/15/20	18/37/115/115	-
16	PQN	b	2002	-	-	9/23/43/43	0/2/2/2
14	CLA	b	1208	-	1/1/14/20	9/31/109/115	-
21	LMT	a	6004	-	-	6/15/35/61	0/1/1/2
17	SF4	a	3001	1,2	-	-	0/6/5/5
14	CLA	a	1112	-	1/1/13/20	12/25/103/115	-
16	PQN	a	2001	-	-	8/23/43/43	0/2/2/2
14	CLA	G	1112	-	1/1/13/20	12/25/103/115	-
14	CLA	b	1210	-	1/1/15/20	17/37/115/115	-
14	CLA	A	1135	-	1/1/12/20	8/19/97/115	-
15	F6C	B	1237	25	-	24/41/97/97	-
17	SF4	C	3003	3	-	-	0/6/5/5
14	CLA	b	1218	-	1/1/11/20	6/13/91/115	-
21	LMT	A	6001	-	-	9/17/57/61	0/2/2/2
14	CLA	A	1120	-	1/1/11/20	6/13/91/115	-
14	CLA	B	1218	-	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	1021	-	1/1/15/20	14/37/115/115	-
14	CLA	A	1113	-	1/1/11/20	7/13/91/115	-
14	CLA	b	1221	-	1/1/15/20	20/37/115/115	-
14	CLA	B	1235	-	1/1/14/20	14/31/109/115	-
14	CLA	a	1012	25	1/1/15/20	7/37/115/115	-
14	CLA	b	1214	-	1/1/14/20	11/31/109/115	-
16	PQN	H	2002	-	-	9/23/43/43	0/2/2/2
14	CLA	a	1103	-	1/1/15/20	23/37/115/115	-
14	CLA	A	1138	-	1/1/13/20	13/25/103/115	-
18	BCR	l	4022	-	-	8/29/63/63	0/2/2/2
18	BCR	A	4003	-	-	9/29/63/63	0/2/2/2
18	BCR	A	4005	-	-	10/29/63/63	0/2/2/2
14	CLA	B	1233	-	1/1/11/20	8/13/91/115	-
19	LHG	l	5101	-	-	15/26/26/53	-
14	CLA	b	1228	-	1/1/13/20	15/25/103/115	-
14	CLA	a	1135	-	1/1/12/20	8/19/97/115	-
14	CLA	B	1236	-	1/1/13/20	15/25/103/115	-
14	CLA	G	1116	-	1/1/13/20	12/25/103/115	-
14	CLA	G	1118	-	1/1/13/20	11/25/103/115	-
21	LMT	V	6000	-	-	5/21/61/61	0/2/2/2
14	CLA	H	1236	-	1/1/13/20	15/25/103/115	-
18	BCR	b	4010	-	-	7/29/63/63	0/2/2/2
14	CLA	G	1139	-	1/1/11/20	8/13/91/115	-
14	CLA	H	1218	-	1/1/11/20	6/13/91/115	-
21	LMT	a	6001	-	-	9/17/57/61	0/2/2/2
14	CLA	a	1118	-	1/1/13/20	11/25/103/115	-
15	F6C	H	1237	25	-	24/41/97/97	-
18	BCR	T	4001	-	-	16/29/63/63	0/2/2/2
14	CLA	U	1503	-	1/1/15/20	13/37/115/115	-
14	CLA	l	1502	-	1/1/14/20	10/31/109/115	-
14	CLA	a	1140	-	1/1/13/20	14/25/103/115	-
14	CLA	A	1123	-	1/1/14/20	14/31/109/115	-
18	BCR	b	4005	-	-	6/29/63/63	0/2/2/2
14	CLA	a	1106	1	1/1/14/20	10/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1104	-	1/1/15/20	19/37/115/115	-
15	F6C	A	1121	-	-	10/17/73/97	-
14	CLA	H	1239	-	1/1/15/20	20/37/115/115	-
21	LMT	H	6003	-	-	11/21/61/61	0/2/2/2
14	CLA	B	1022	-	1/1/13/20	11/25/103/115	-
14	CLA	A	1013	-	1/1/14/20	10/31/109/115	-

The worst 5 of 5905 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	1207	F6C	MG-NA	9.22	2.24	2.05
15	H	1207	F6C	MG-NA	9.19	2.24	2.05
15	B	1207	F6C	MG-NA	9.18	2.24	2.05
15	H	1219	F6C	MG-NA	9.11	2.23	2.05
15	B	1219	F6C	MG-NA	9.08	2.23	2.05

The worst 5 of 7844 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	i	4020	BCR	C20-C21-C22	27.22	166.15	127.31
18	I	4020	BCR	C20-C21-C22	27.20	166.13	127.31
18	R	4020	BCR	C20-C21-C22	27.18	166.10	127.31
18	b	4010	BCR	C16-C17-C18	27.11	166.00	127.31
18	H	4010	BCR	C16-C17-C18	27.09	165.97	127.31

5 of 264 chirality outliers are listed below:

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

5 of 4777 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	1013	CLA	C1A-C2A-CAA-CBA
14	A	1013	CLA	C3A-C2A-CAA-CBA
14	A	1101	CLA	CHA-CBD-CGD-O2D

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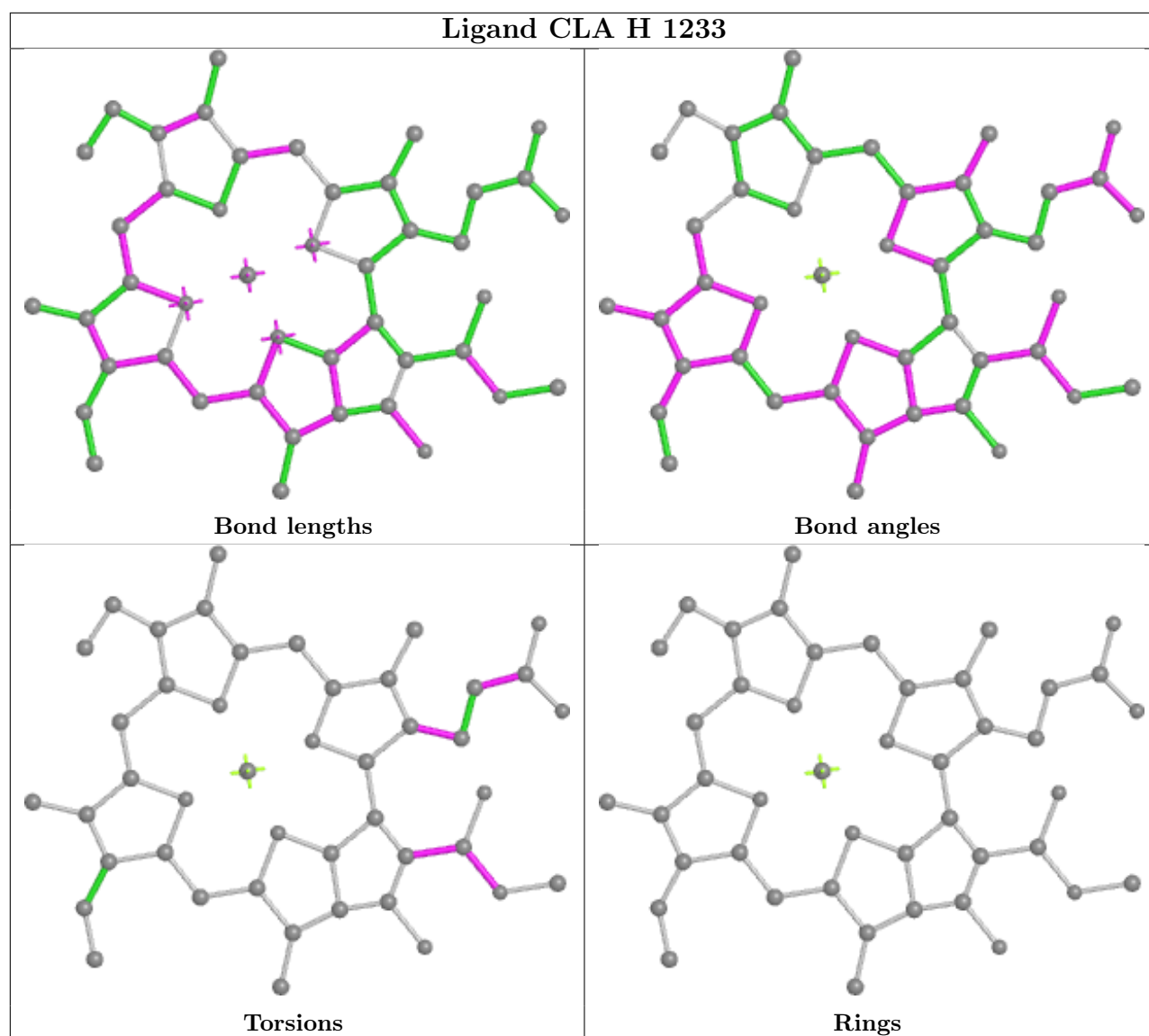
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Mol	Chain	Res	Type	Atoms
14	A	1102	CLA	CHA-CBD-CGD-O1D
14	A	1102	CLA	CHA-CBD-CGD-O2D

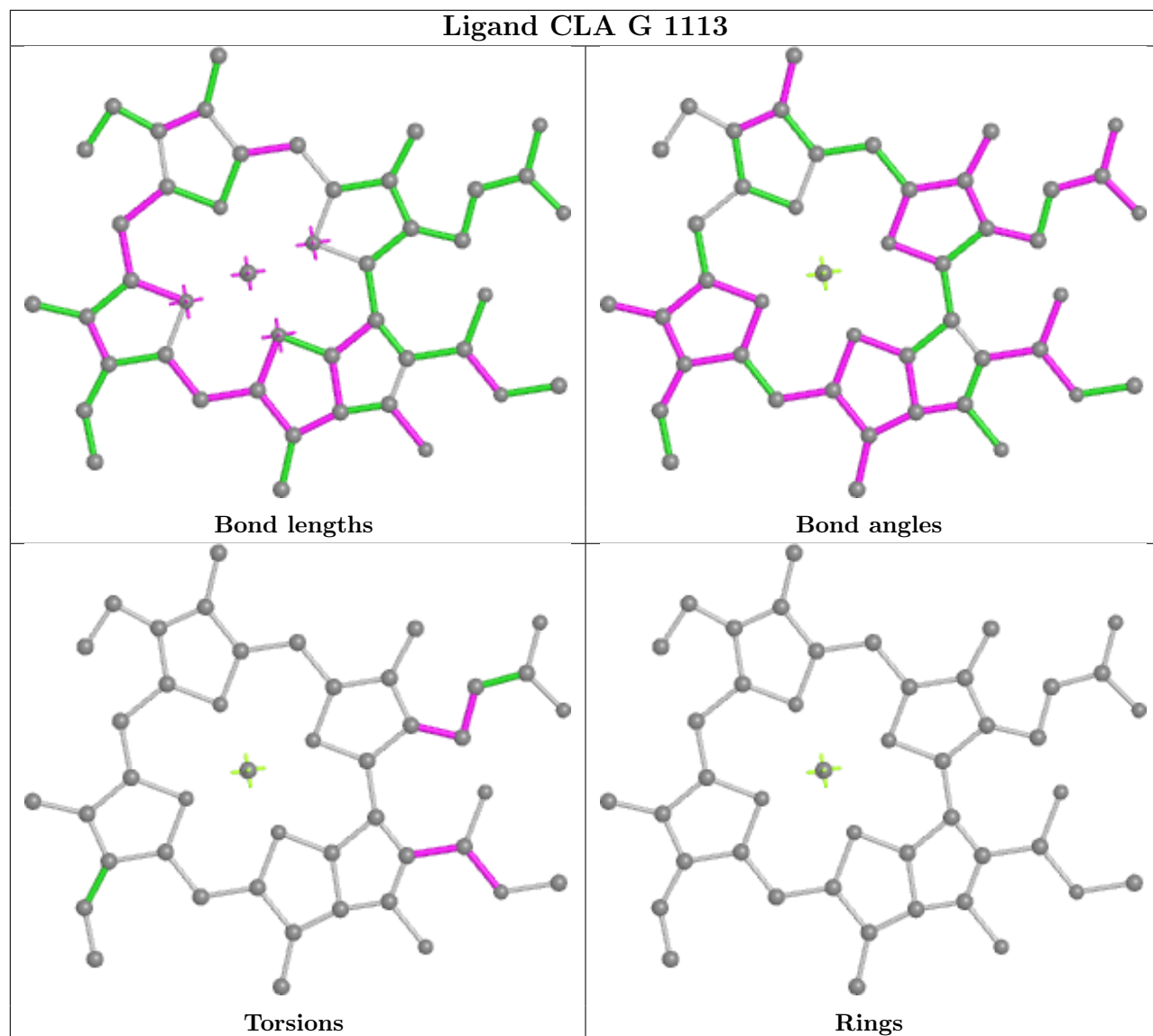
There are no ring outliers.

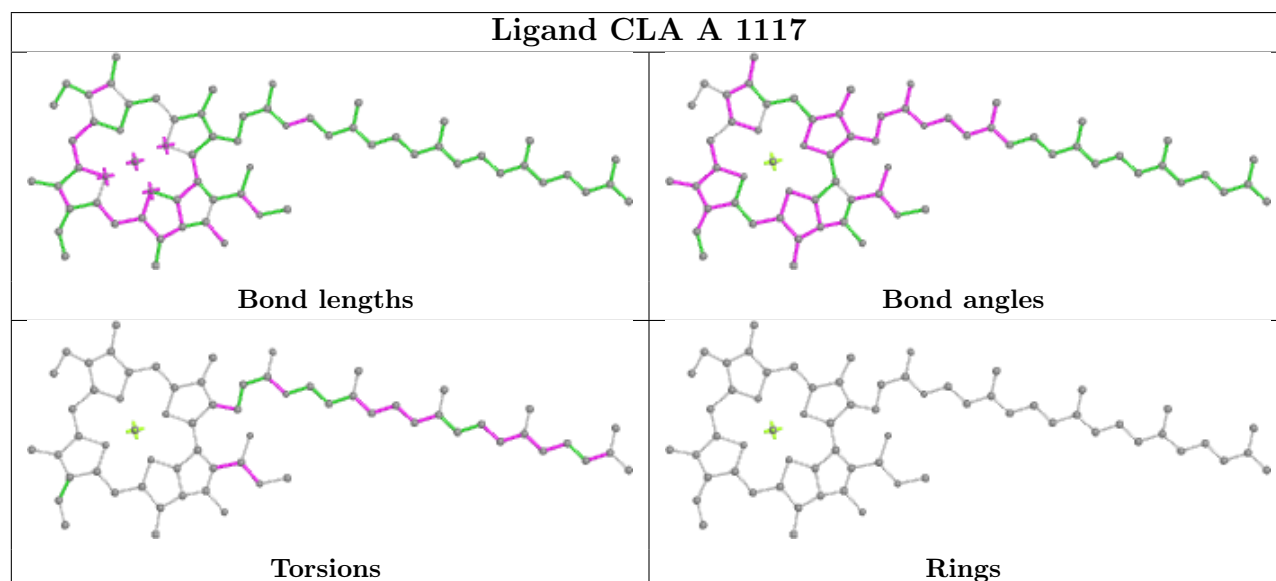
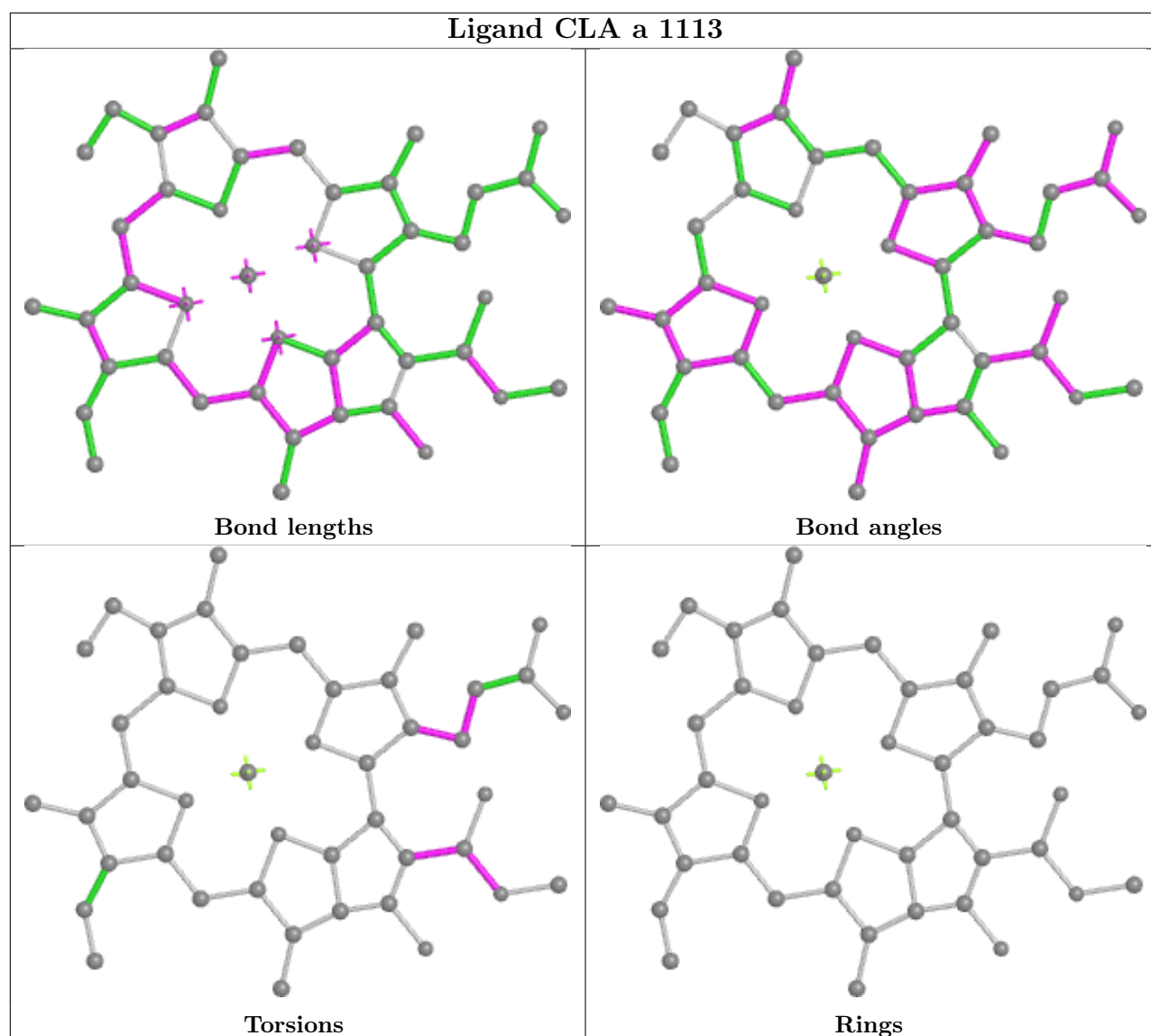
No monomer is involved in short contacts.

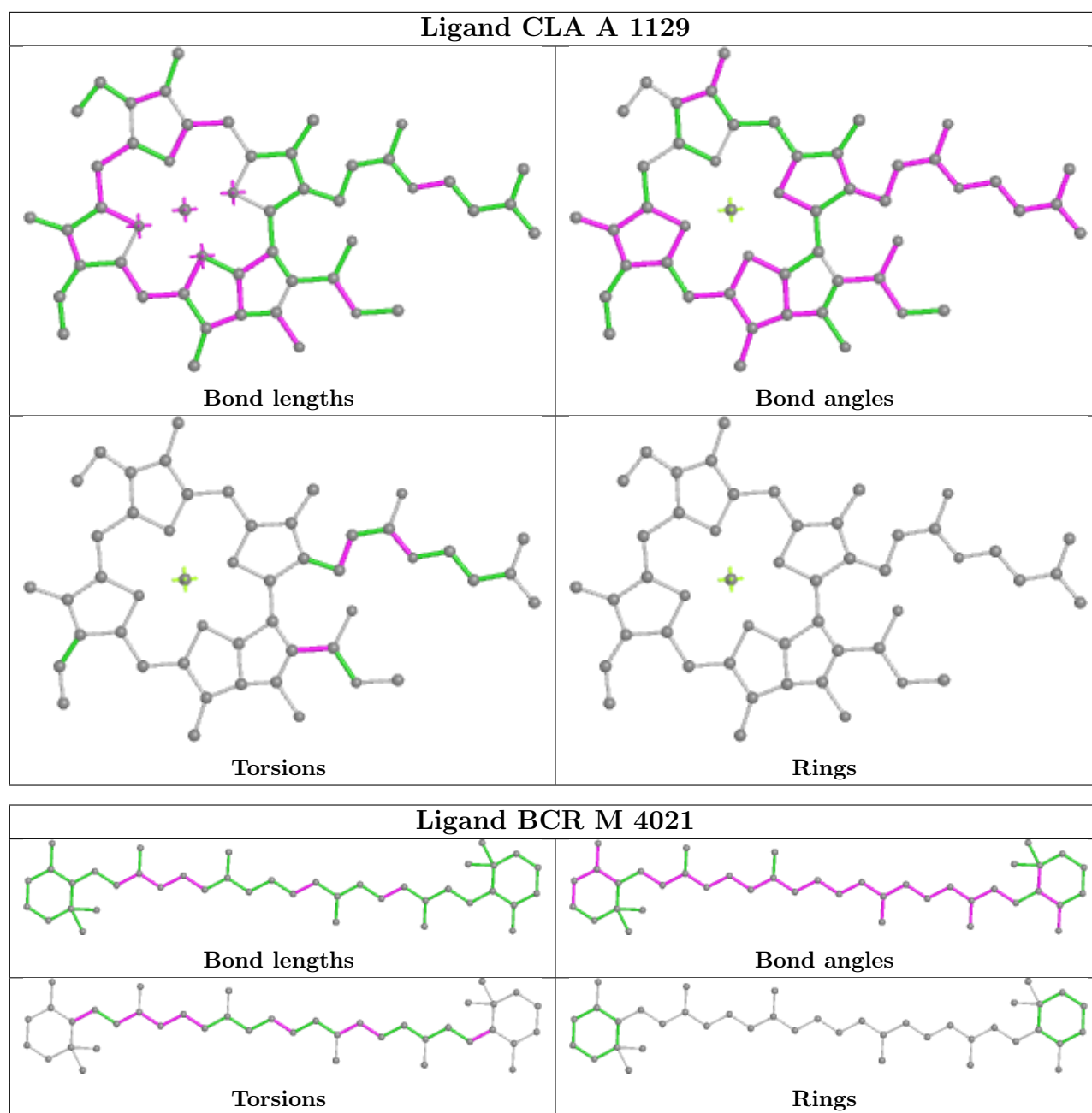
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

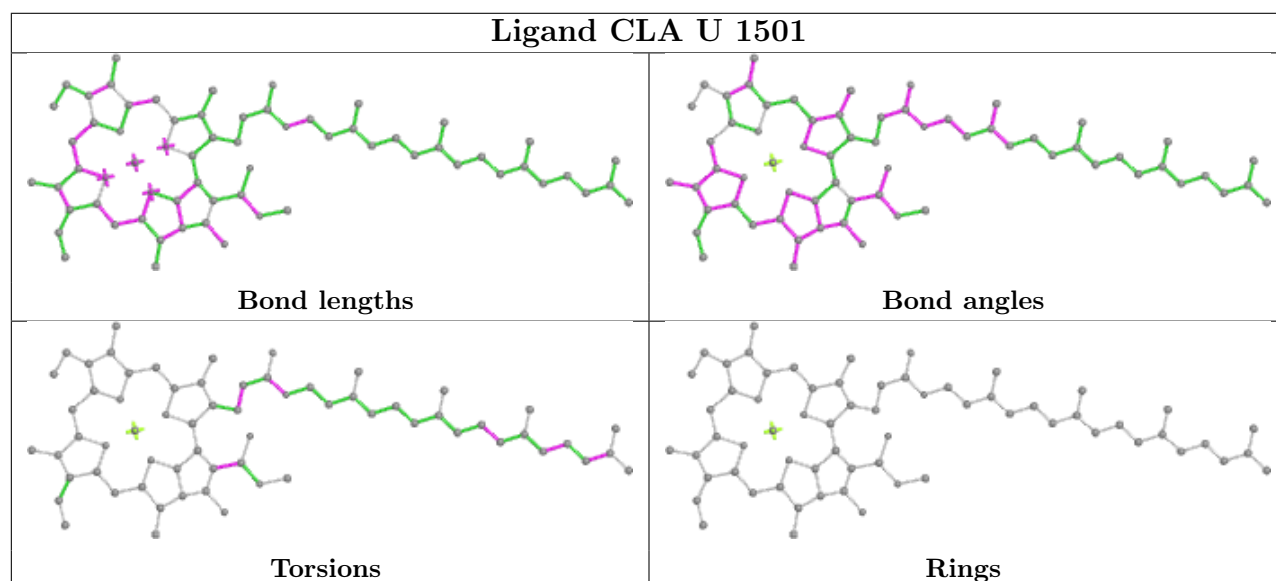
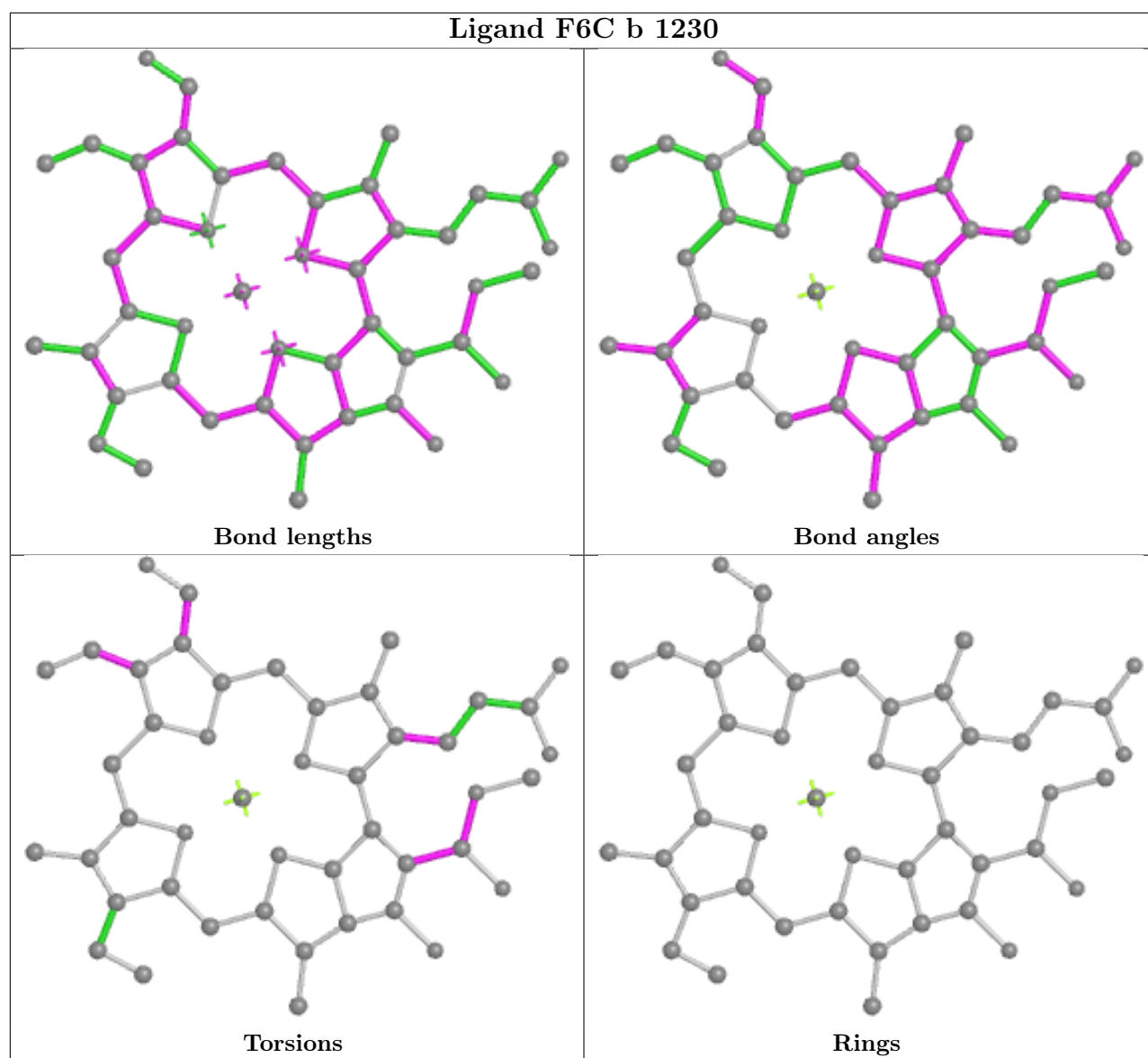


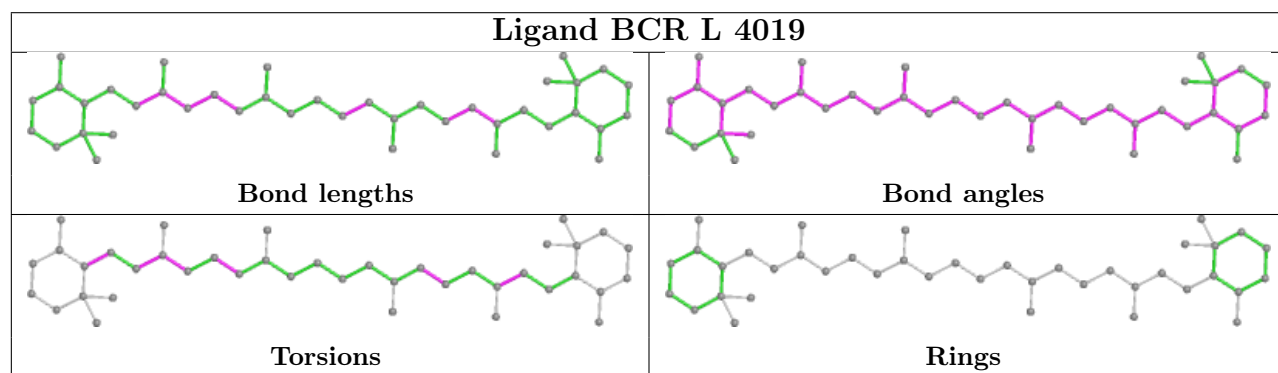
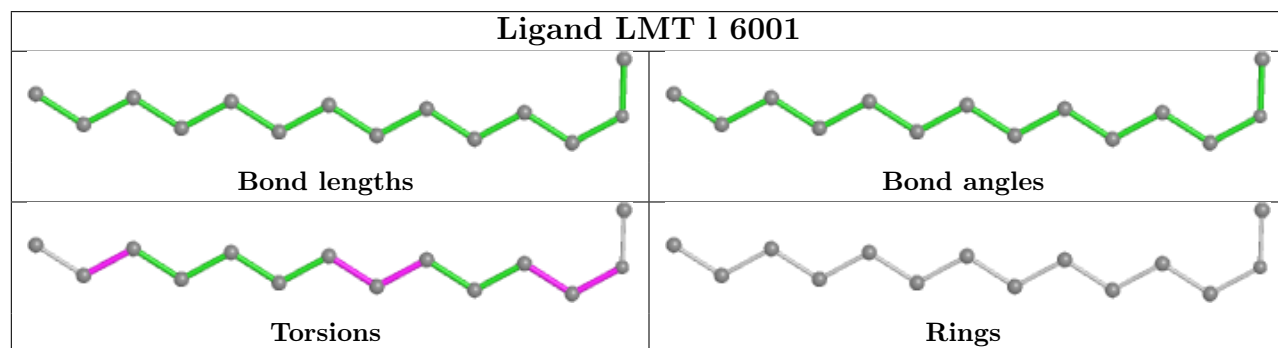
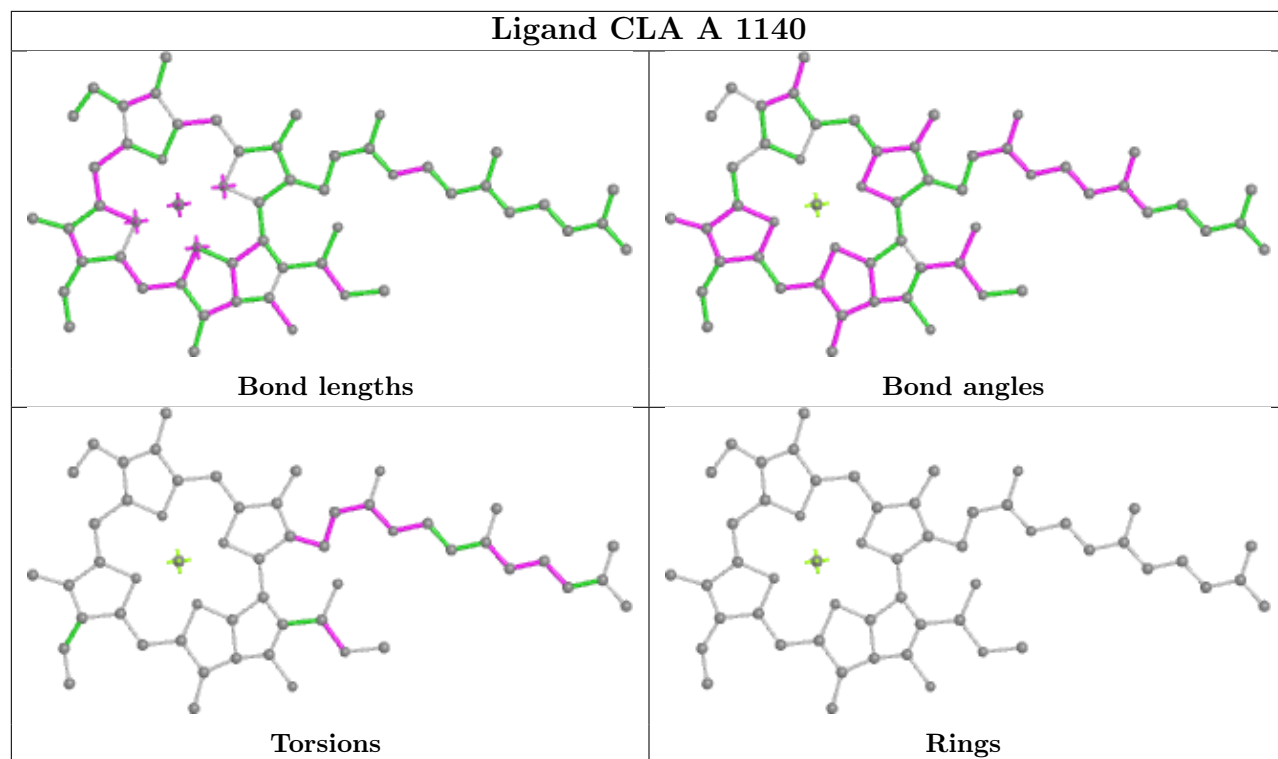
Ligand CLA G 1113

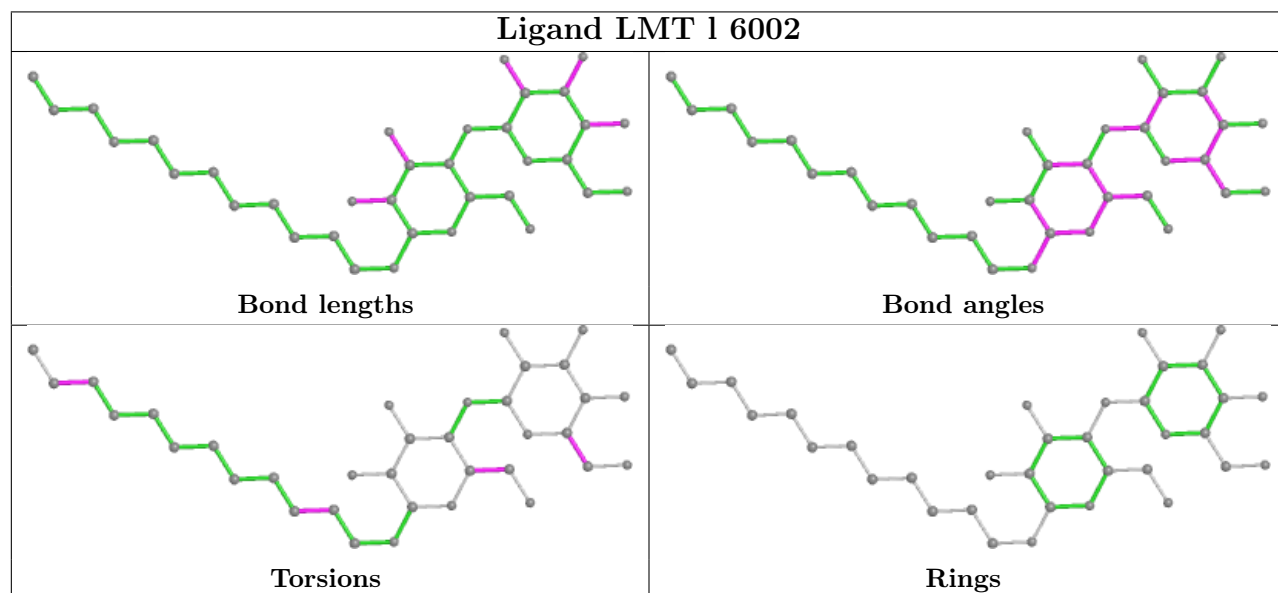
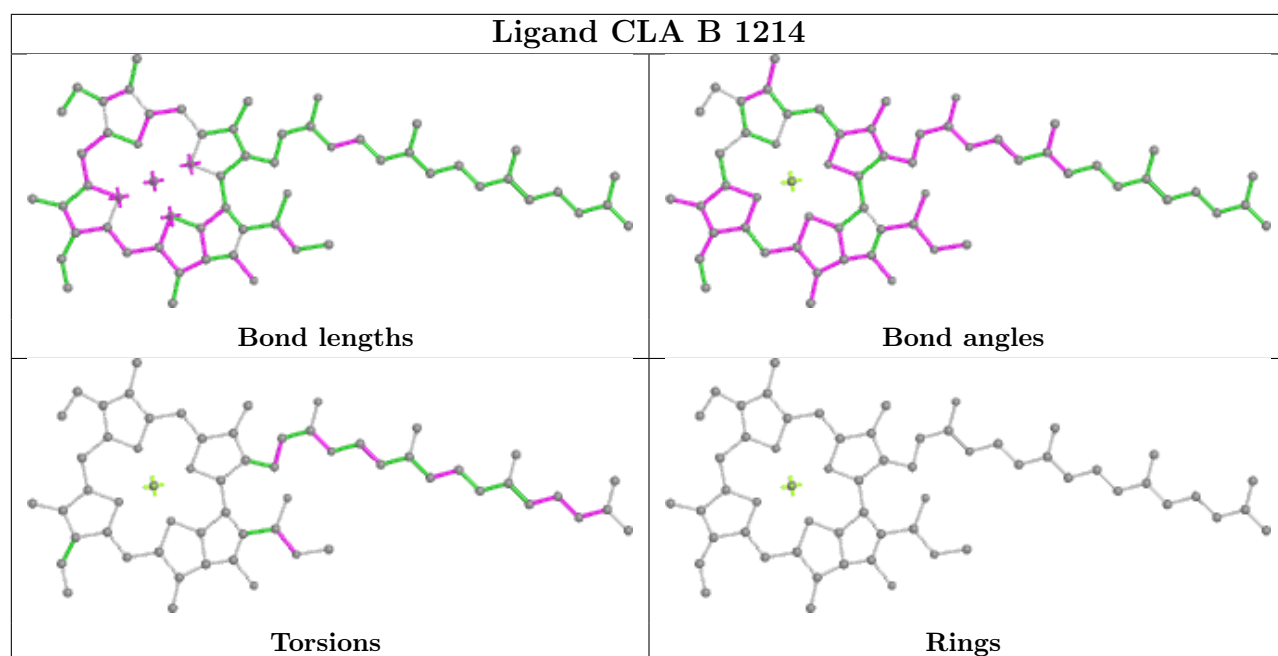


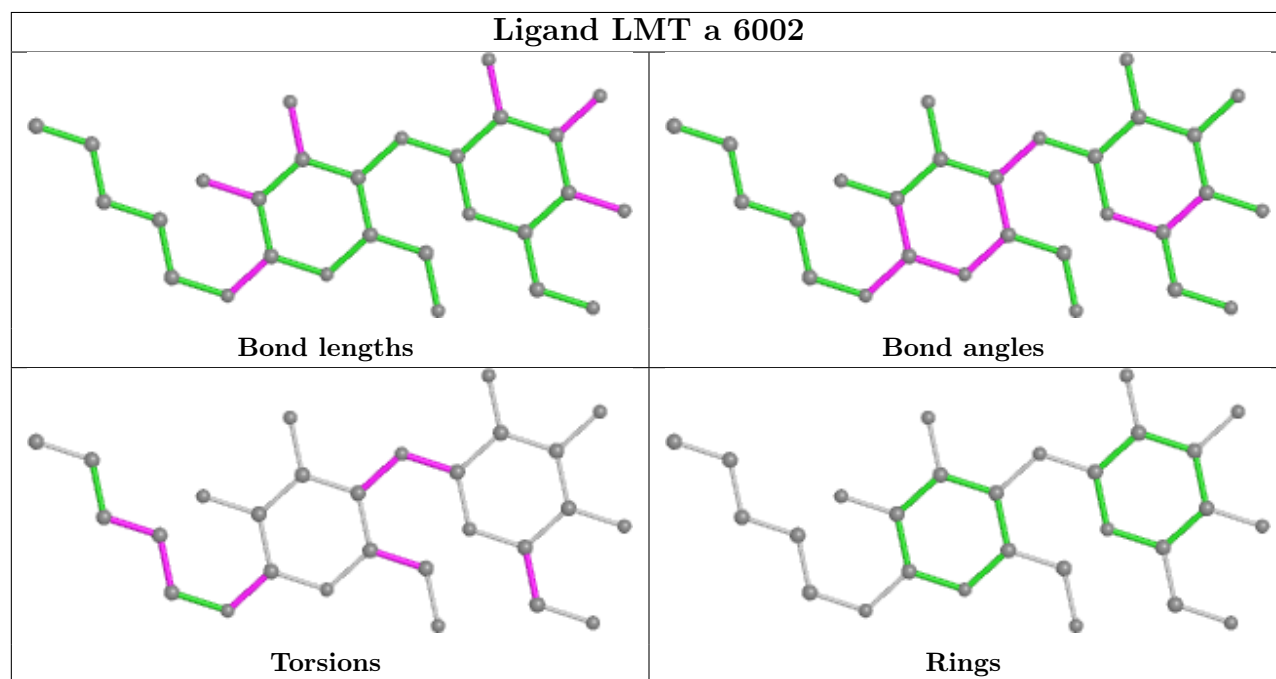
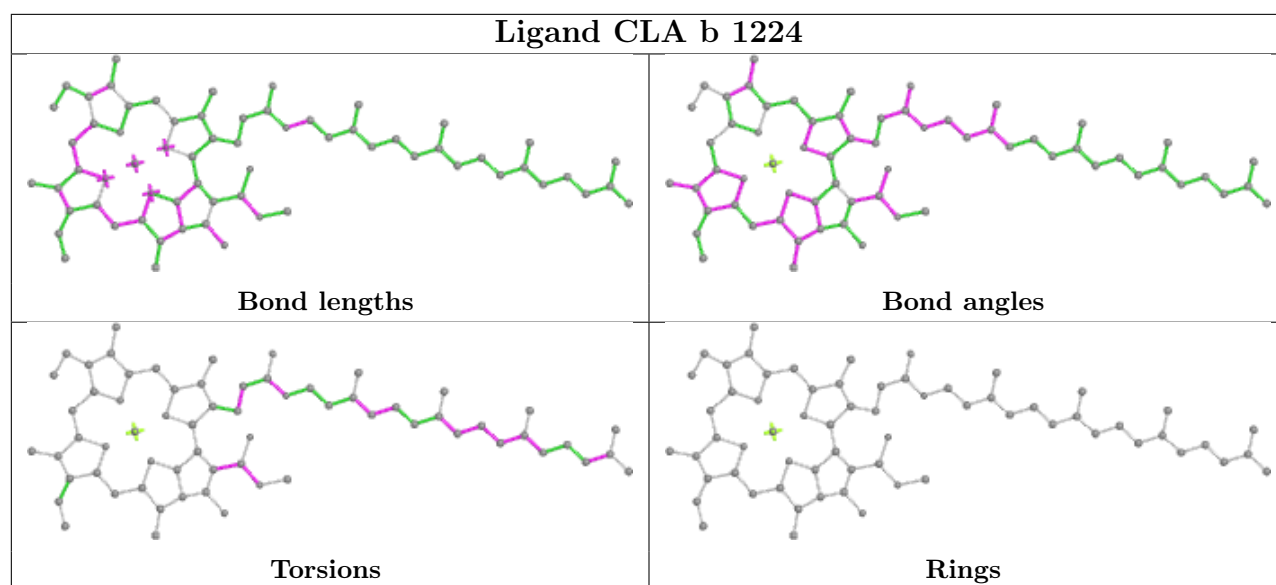




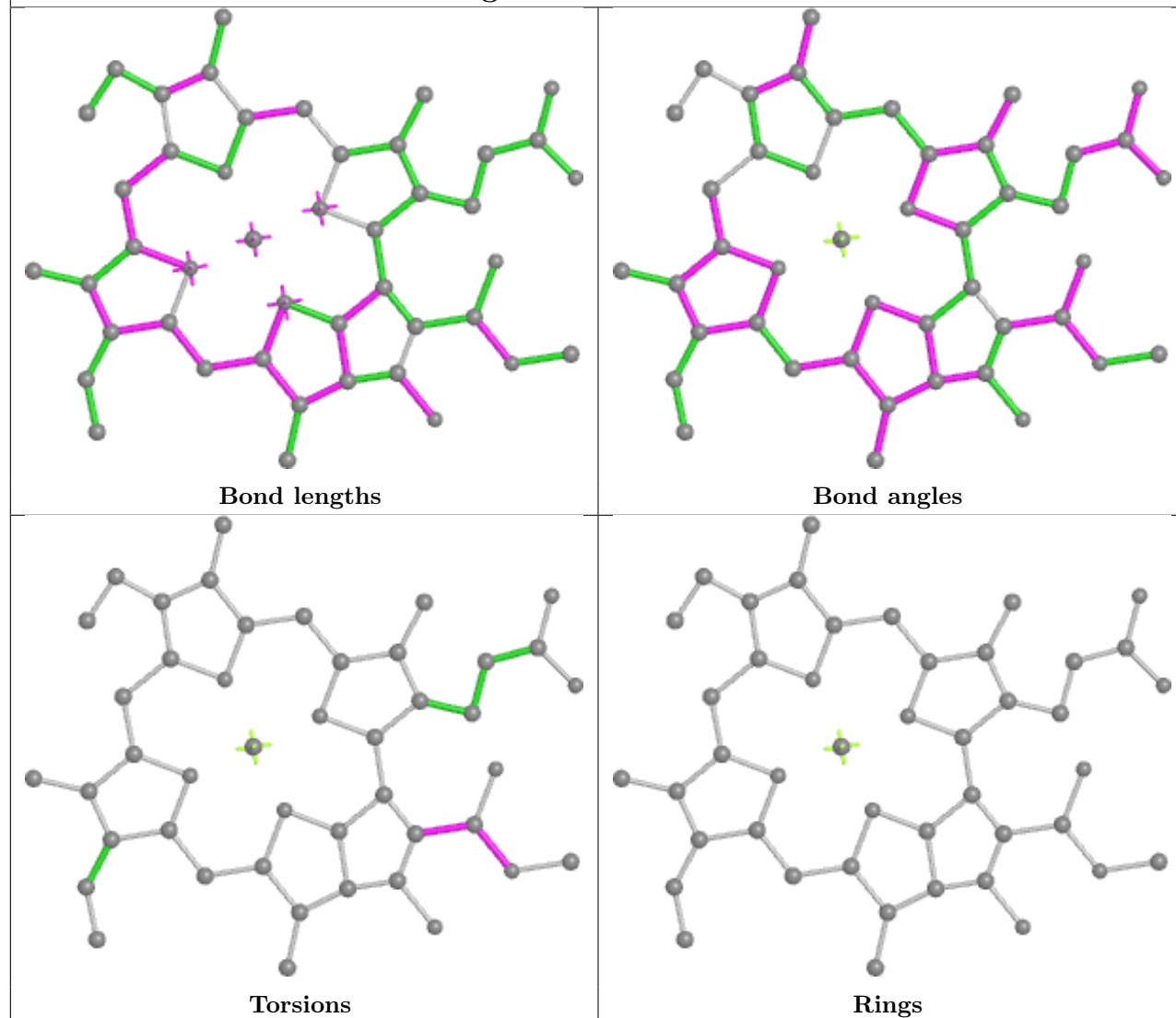




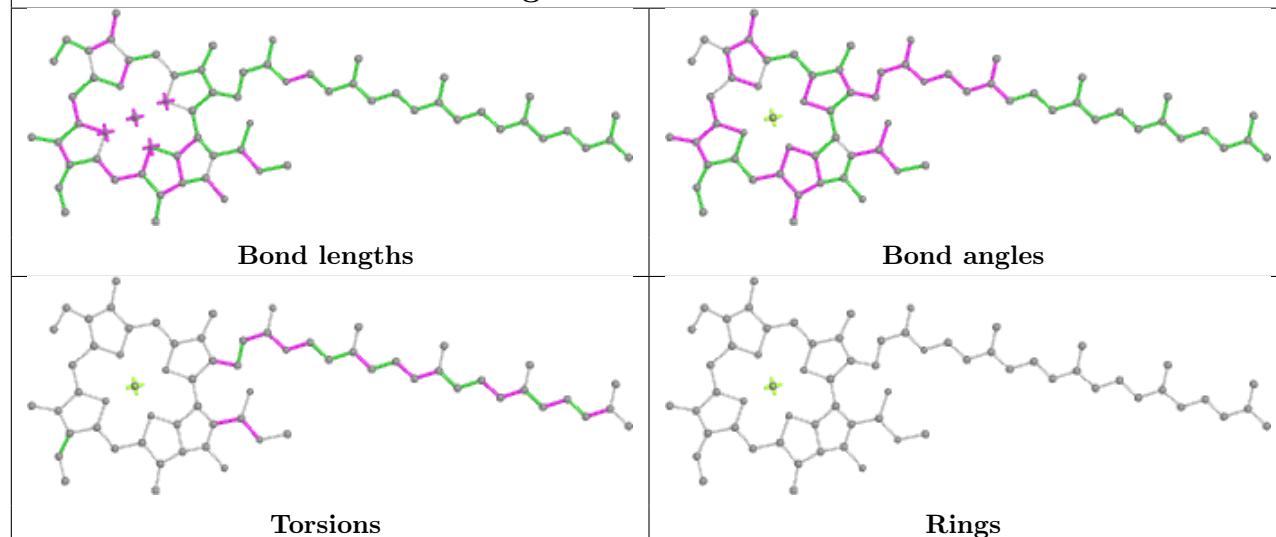


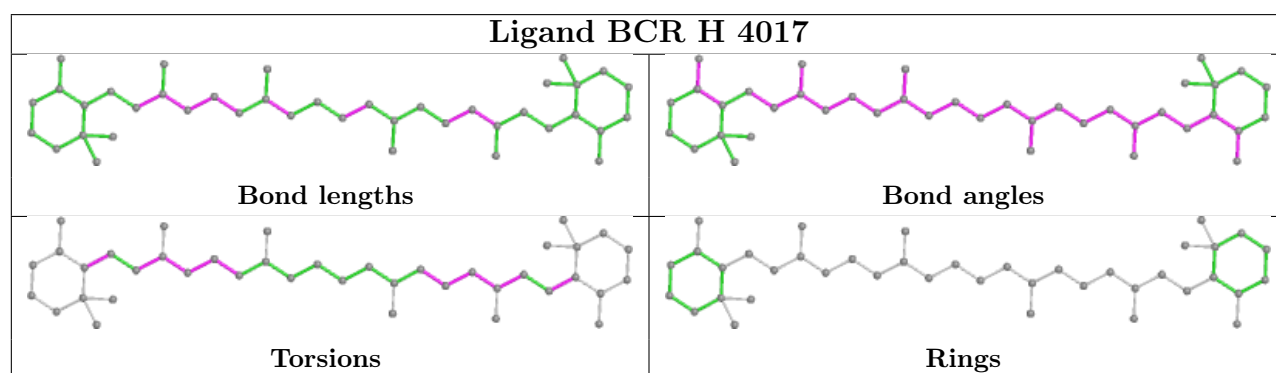
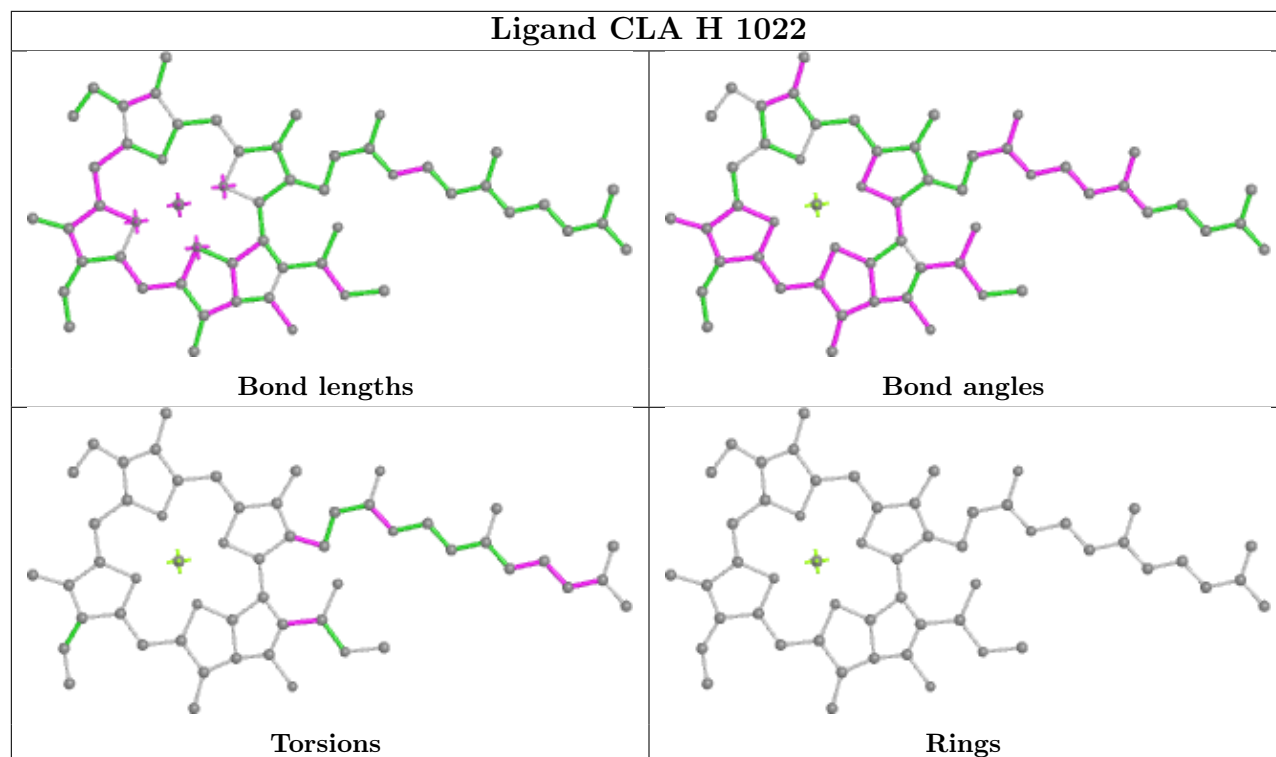
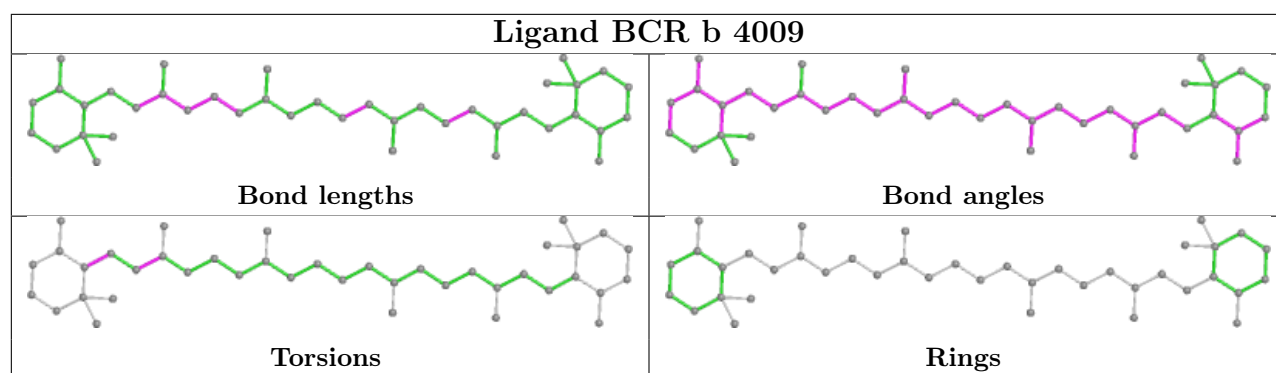


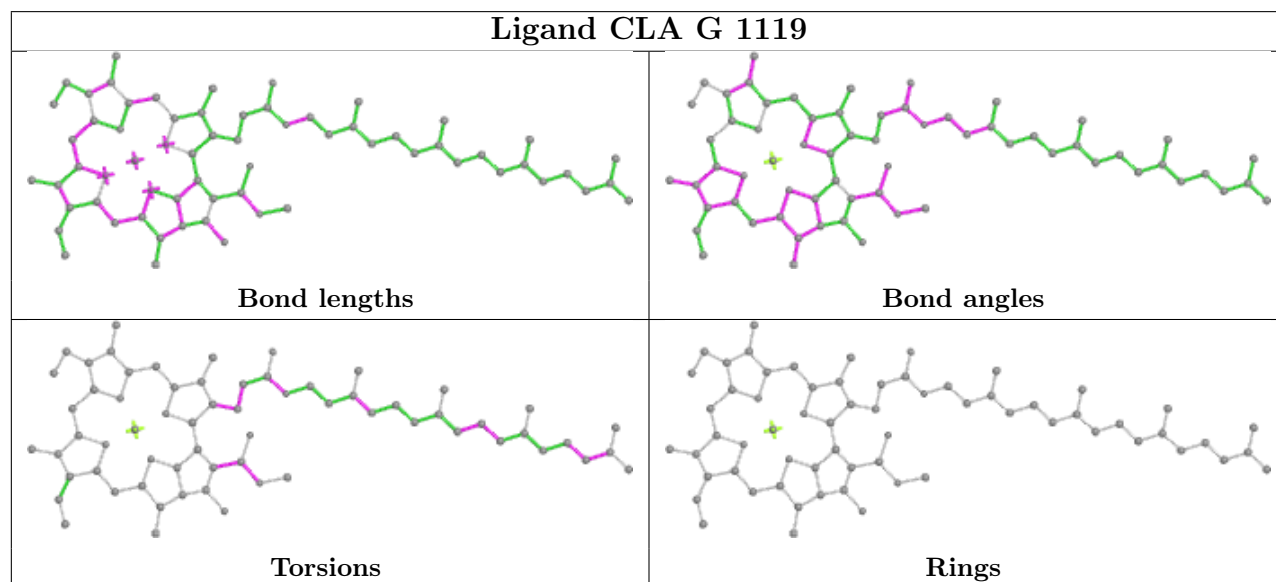
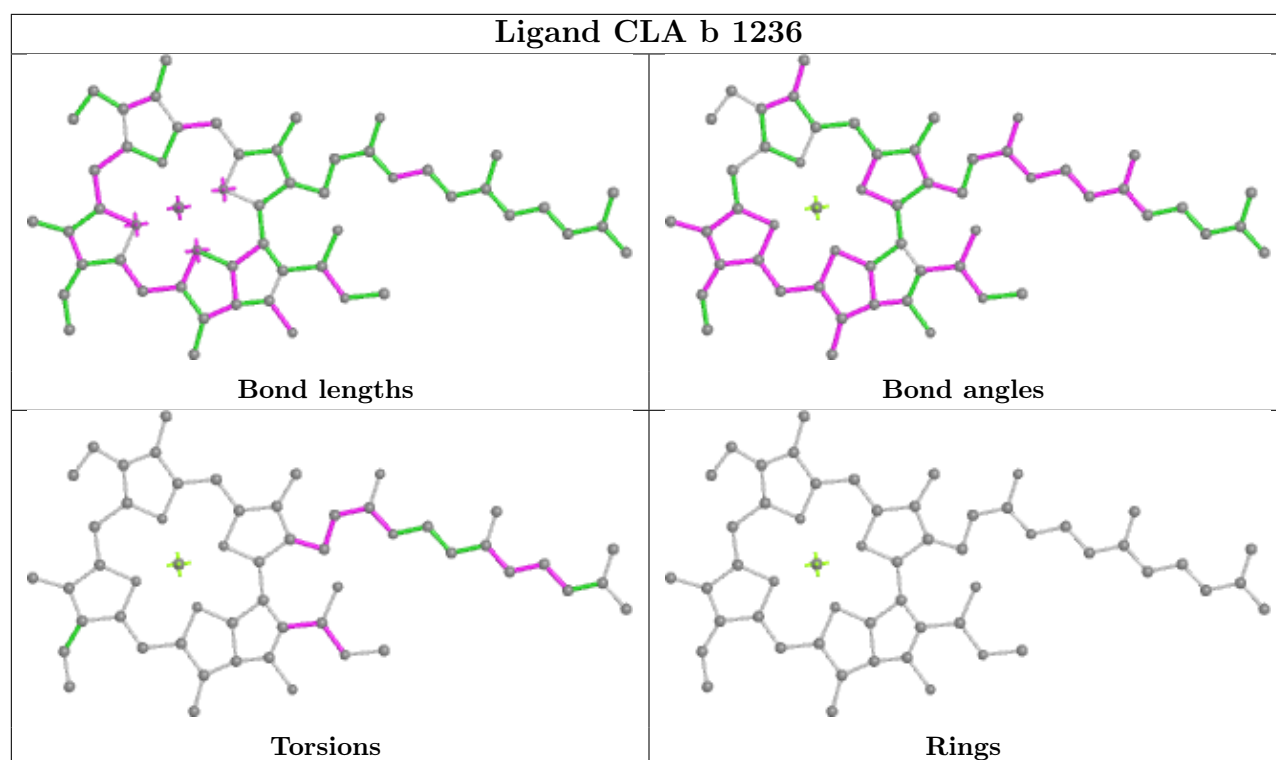
Ligand CLA A 1114

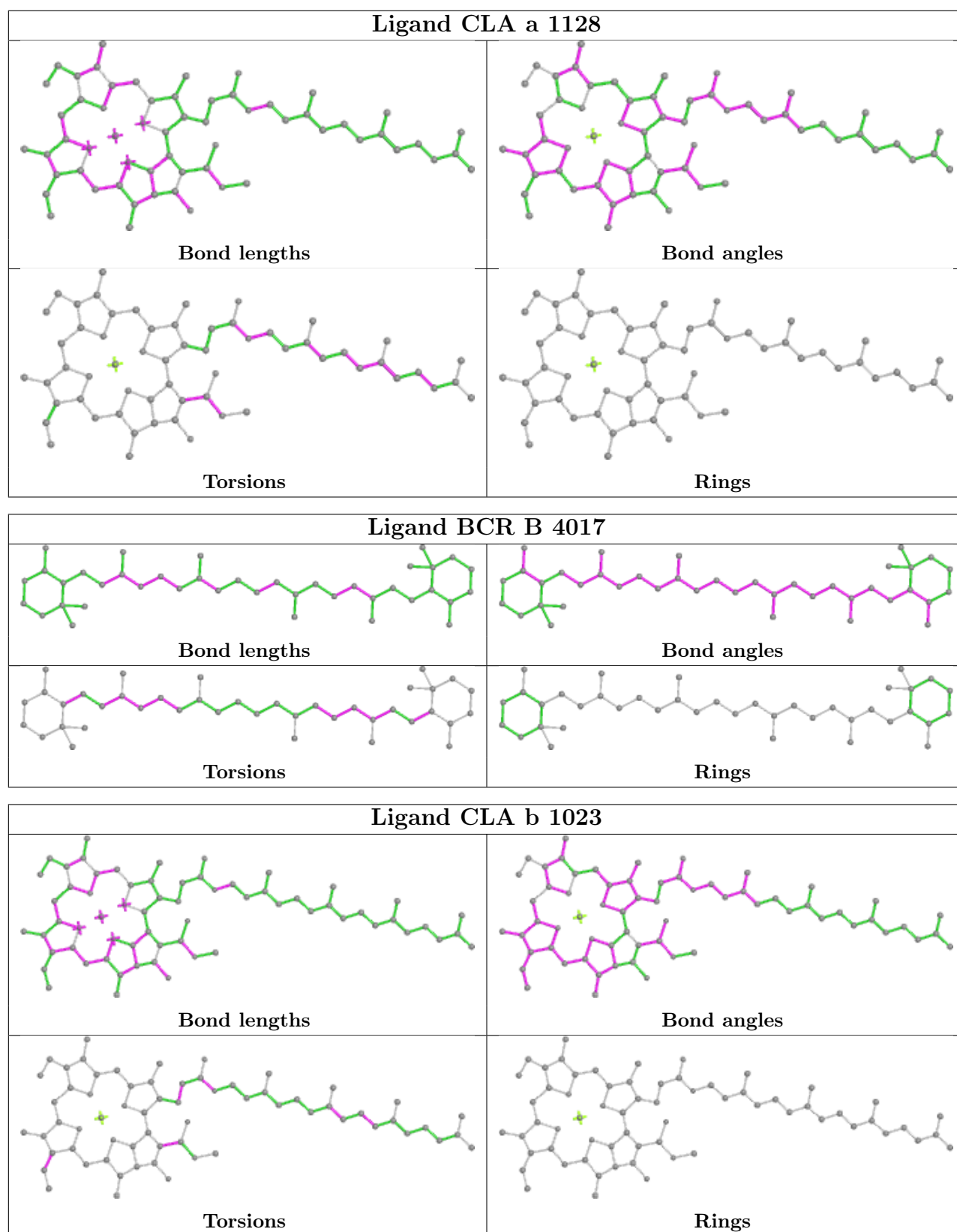


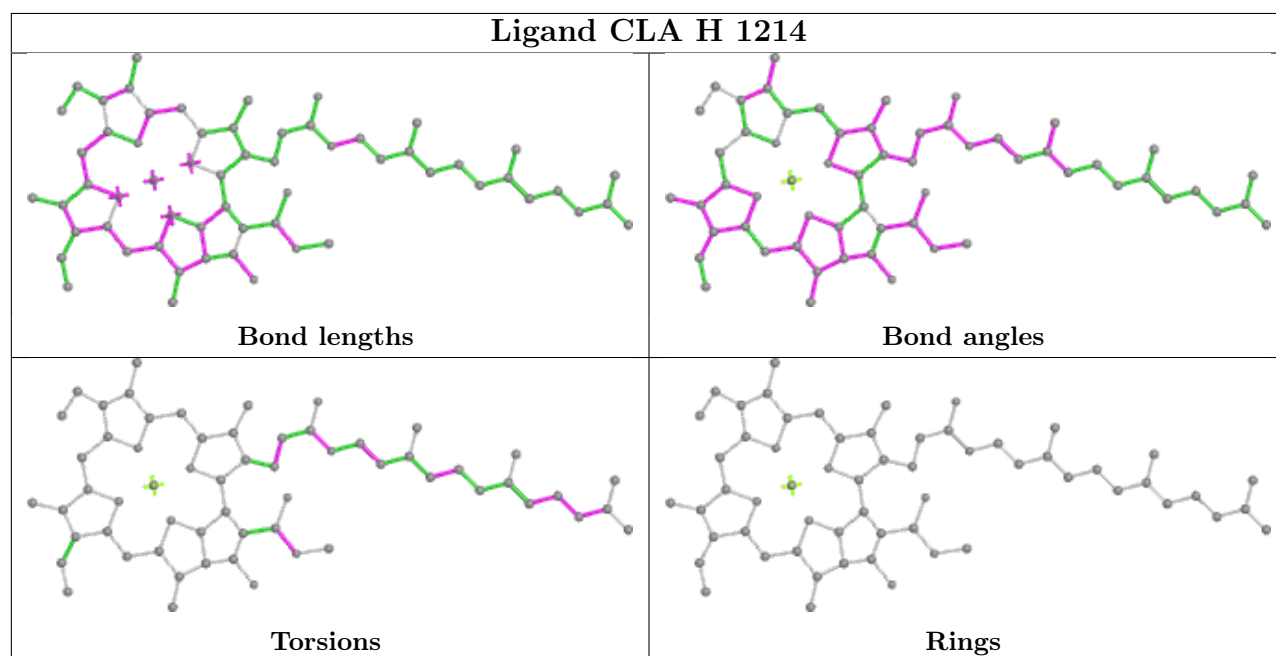
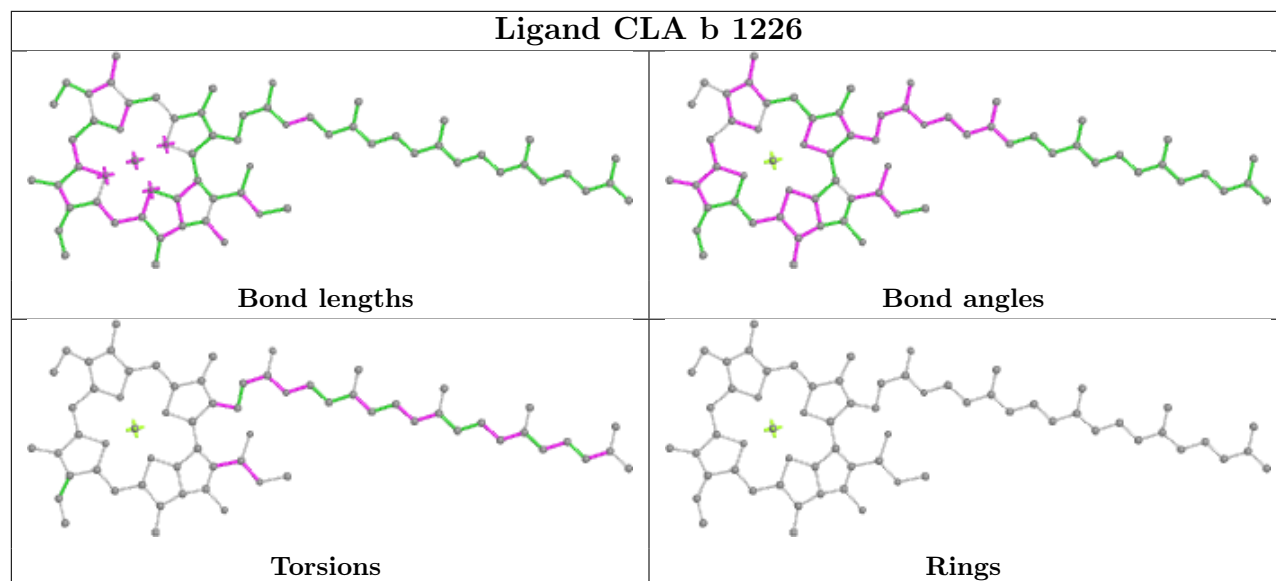
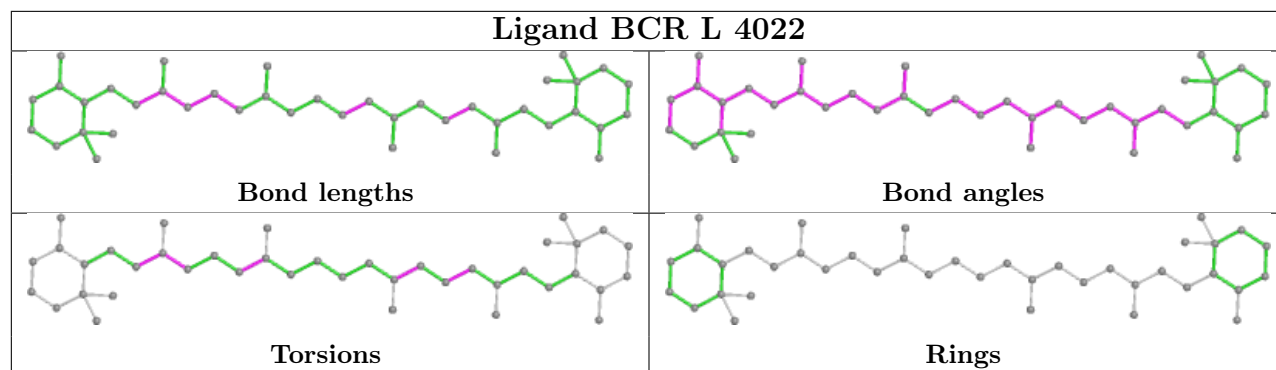
Ligand CLA H 1226

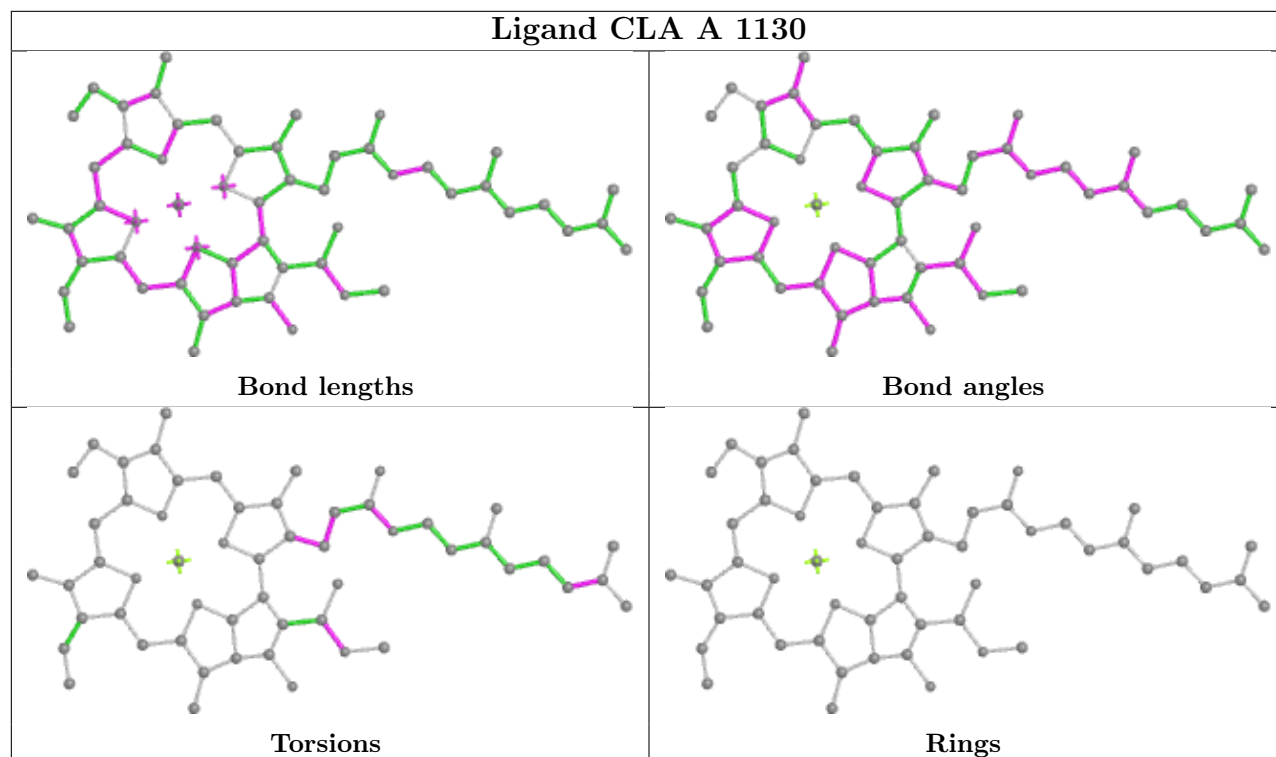
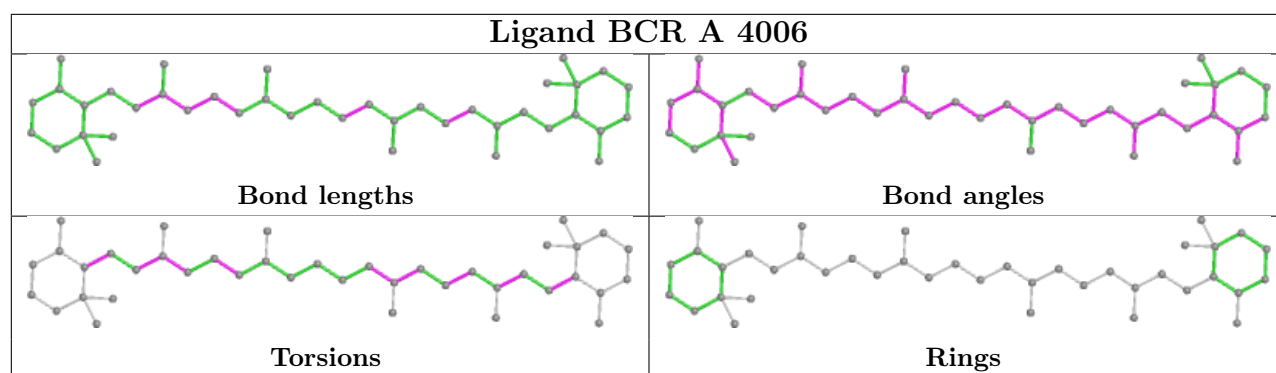




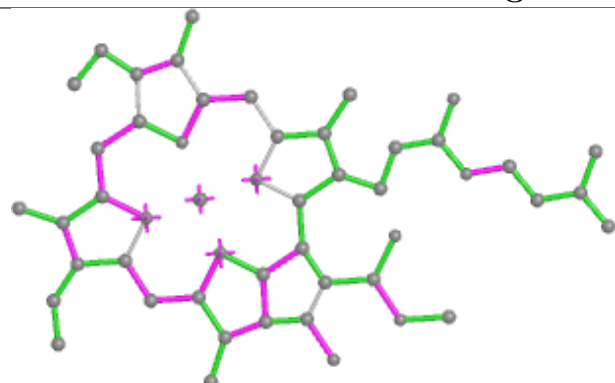




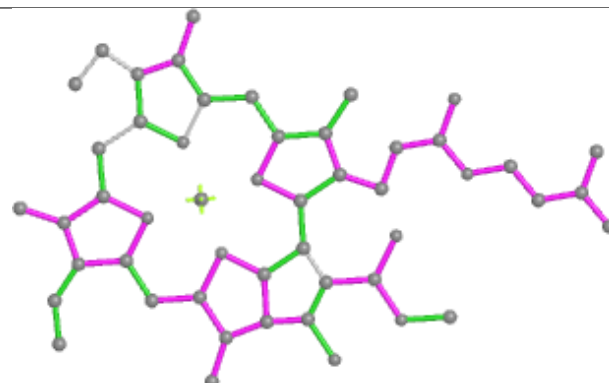




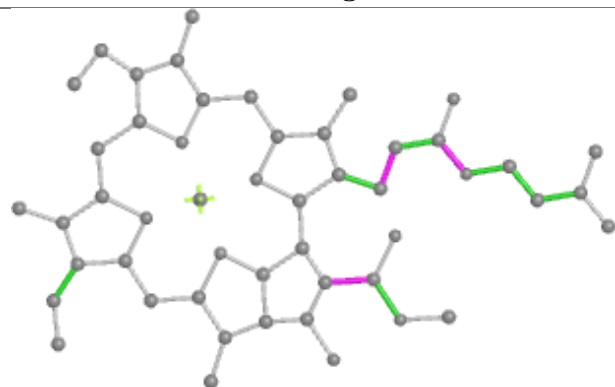
Ligand CLA G 1129



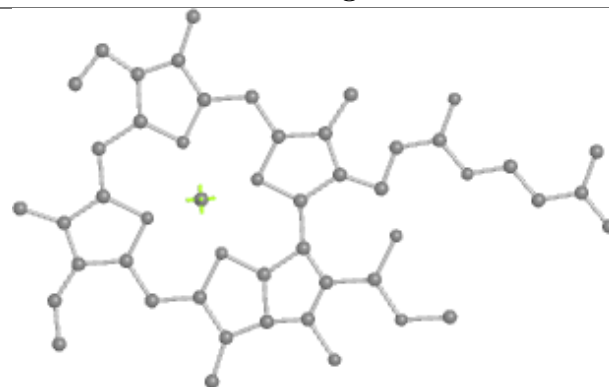
Bond lengths



Bond angles

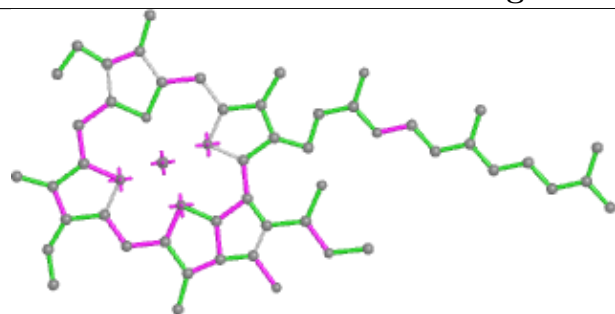


Torsions

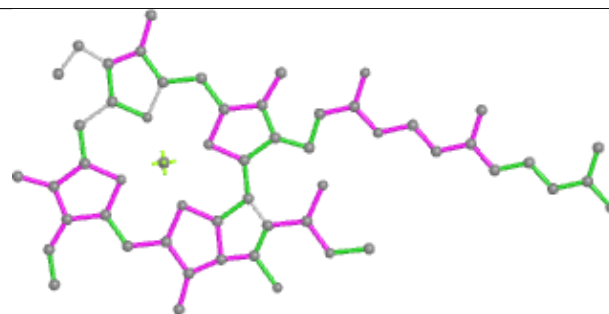


Rings

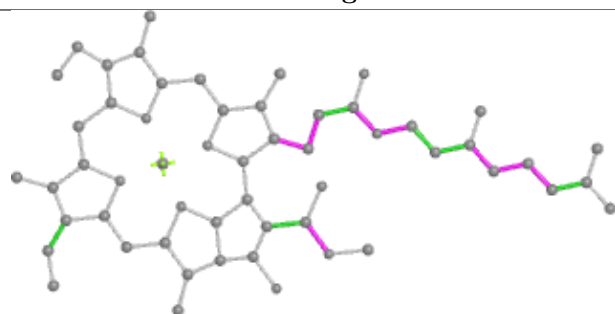
Ligand CLA A 1122



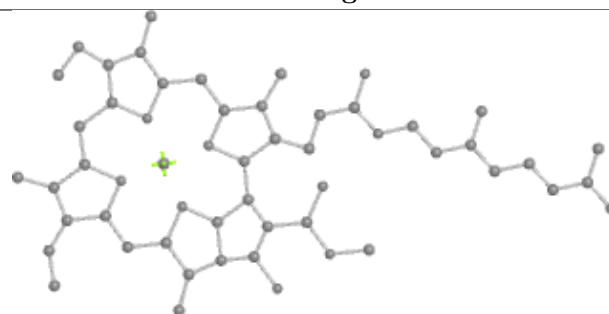
Bond lengths



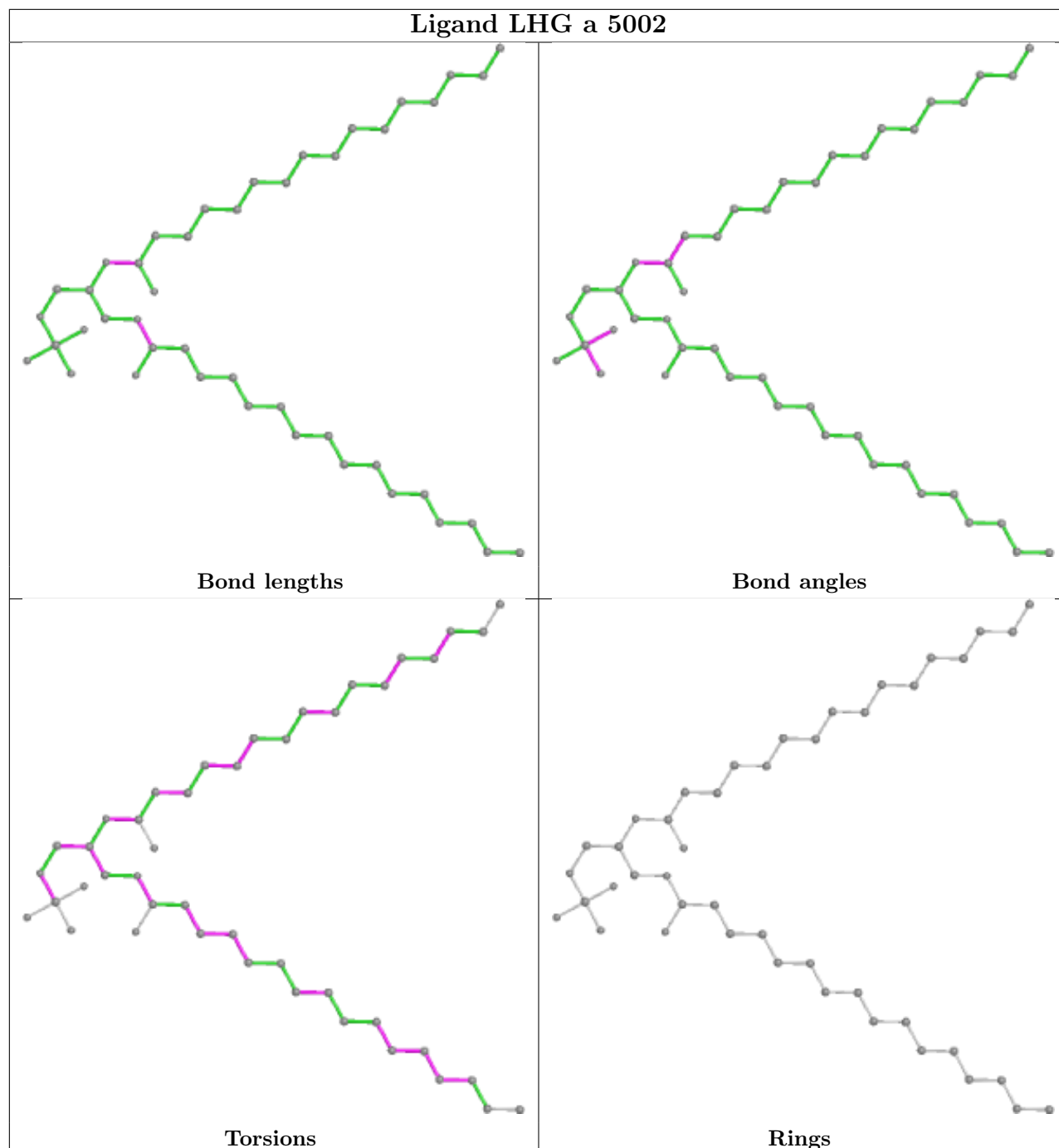
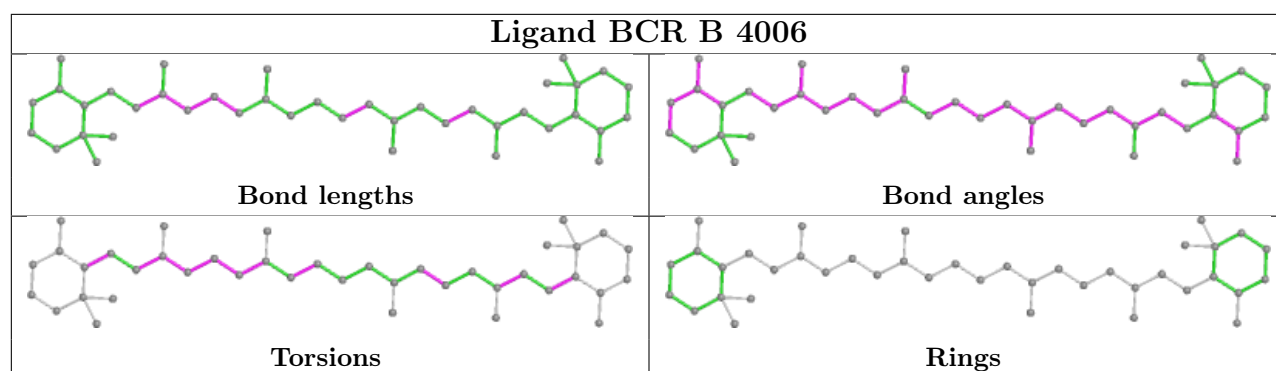
Bond angles



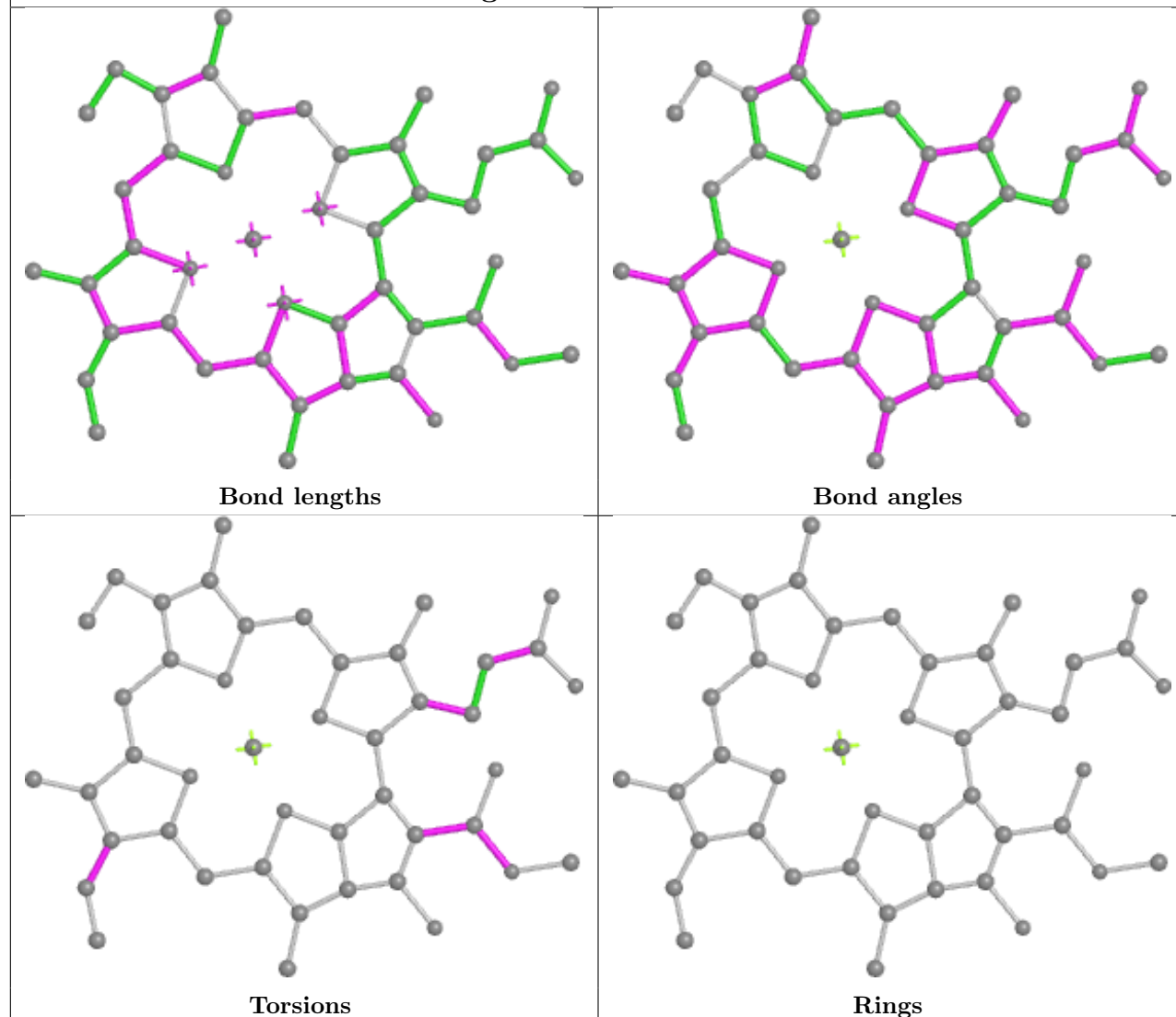
Torsions



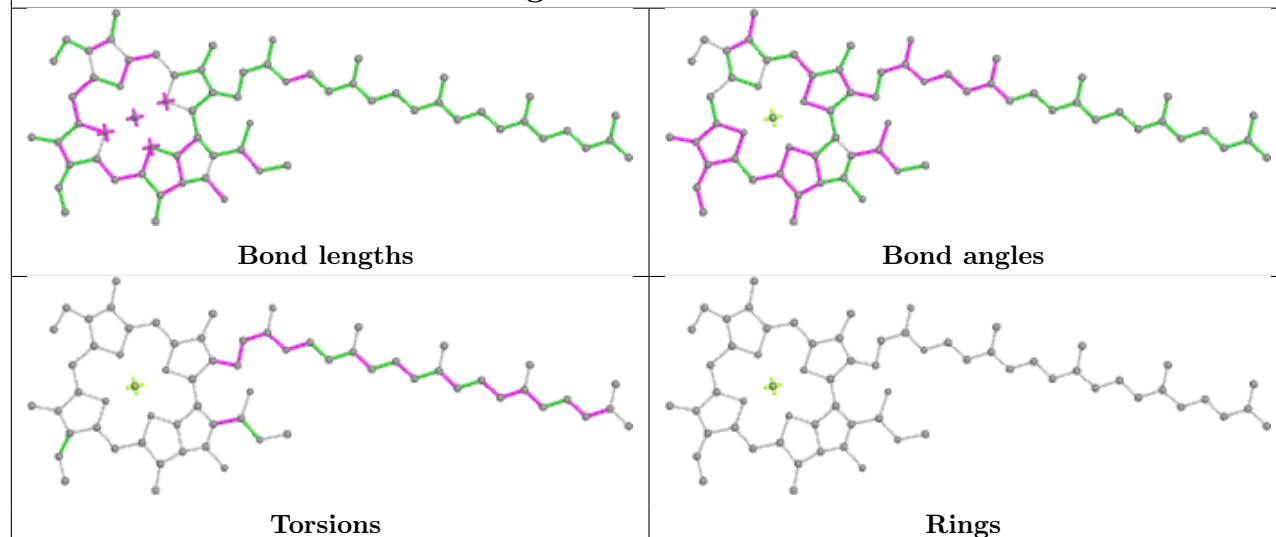
Rings

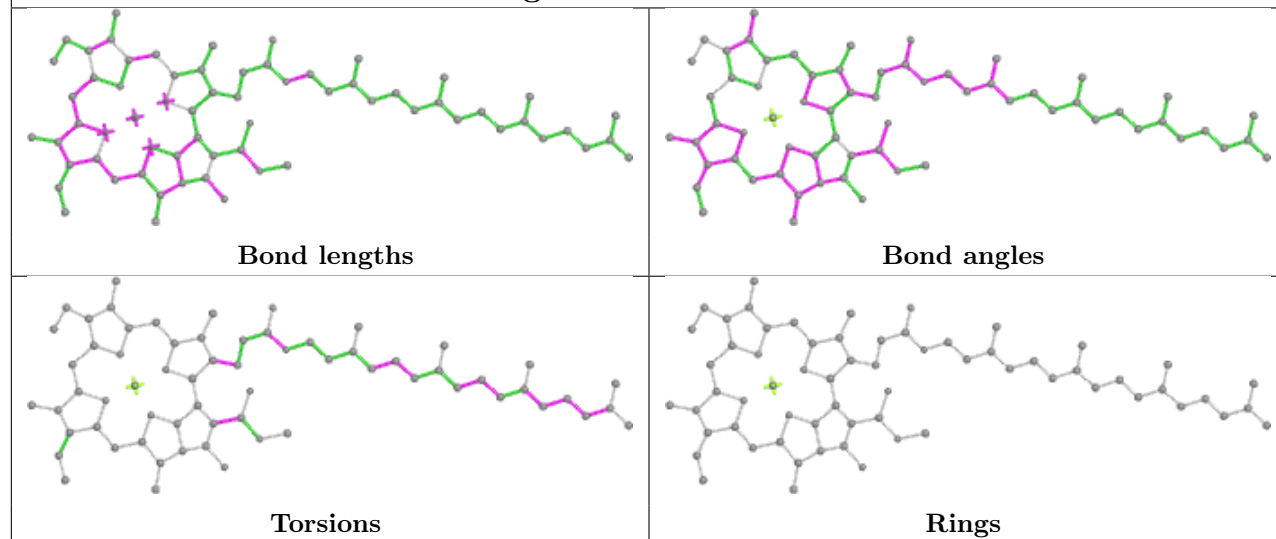
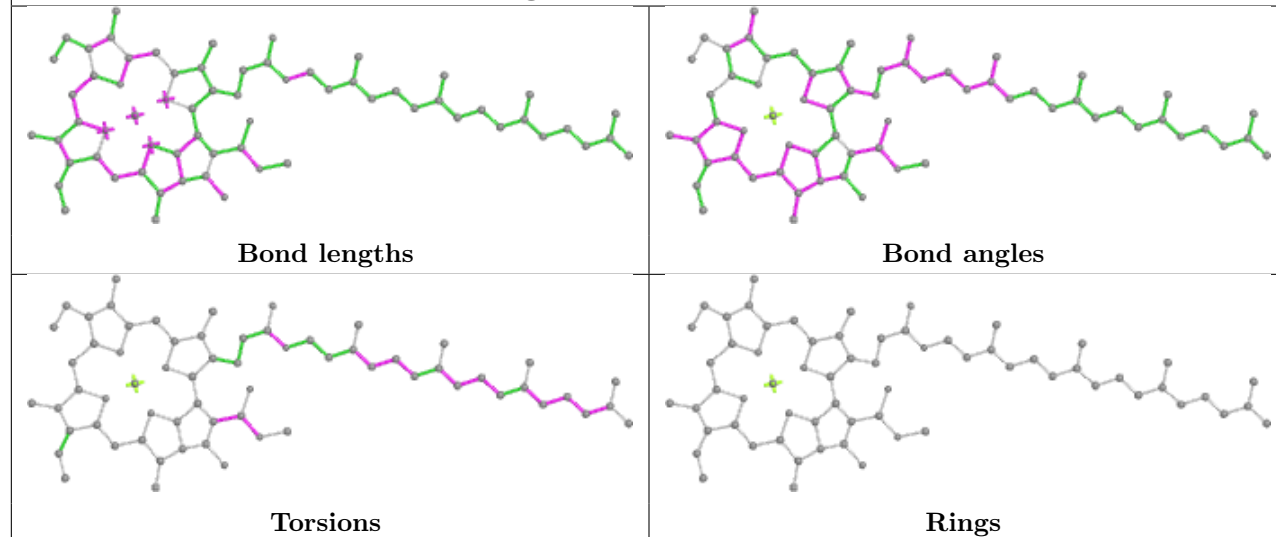


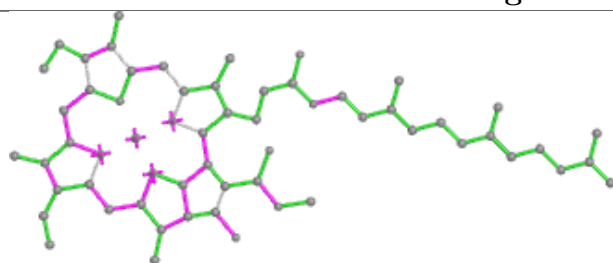
Ligand CLA K 1401



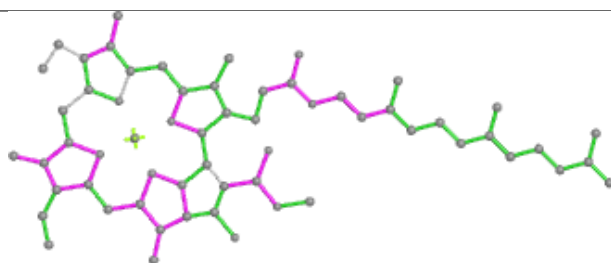
Ligand CLA b 1203



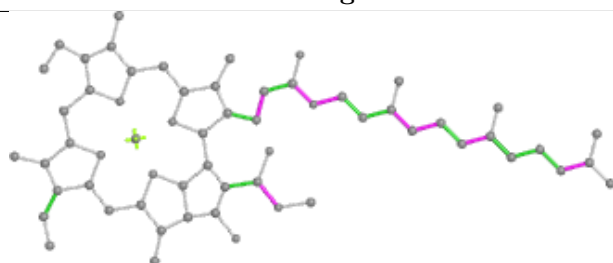
Ligand CLA B 1211**Ligand CLA A 1104**

Ligand CLA A 1131

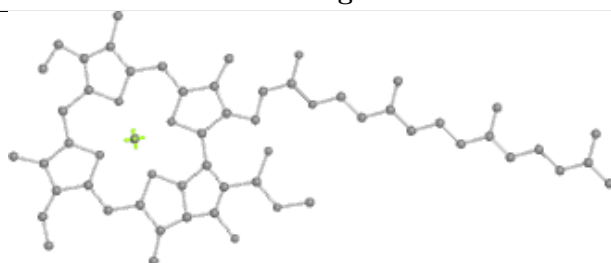
Bond lengths



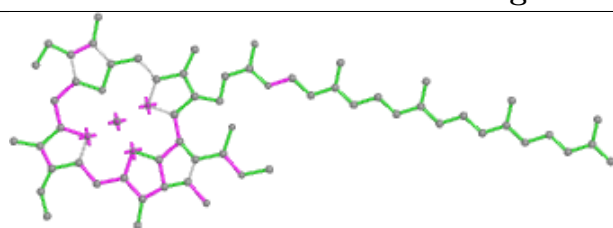
Bond angles



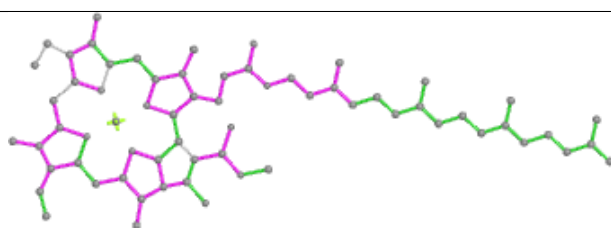
Torsions



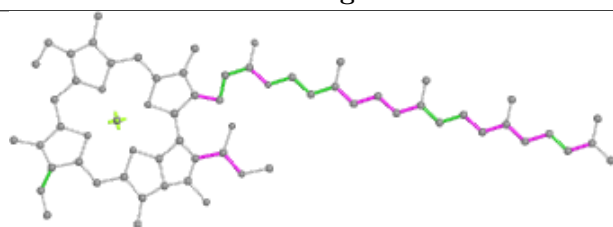
Rings

Ligand CLA a 1117

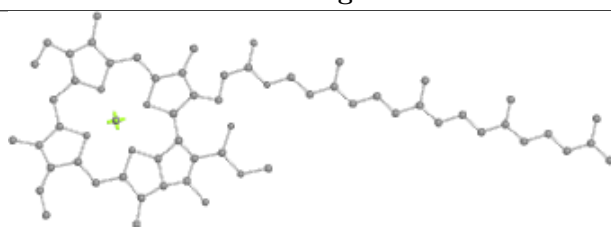
Bond lengths



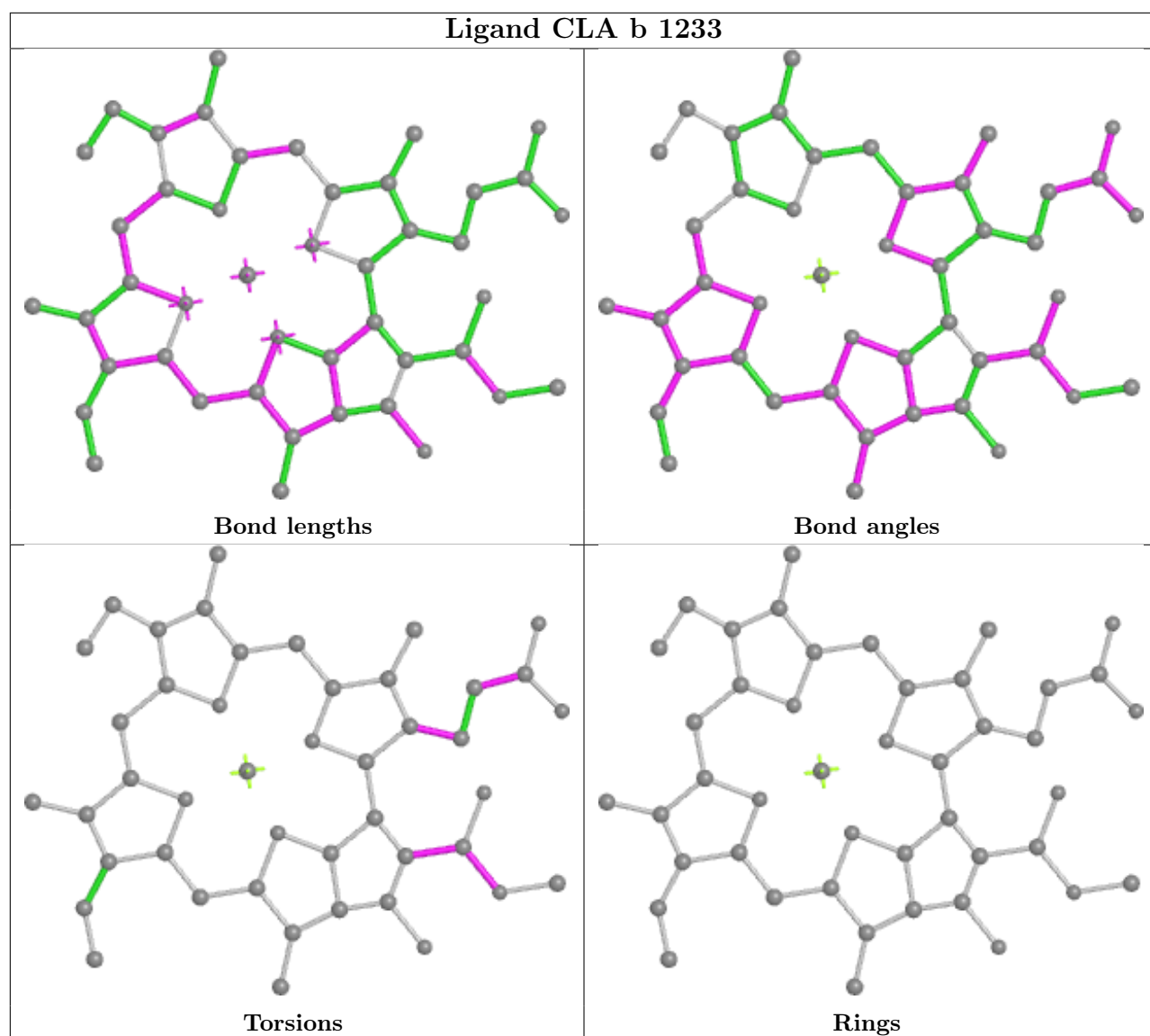
Bond angles



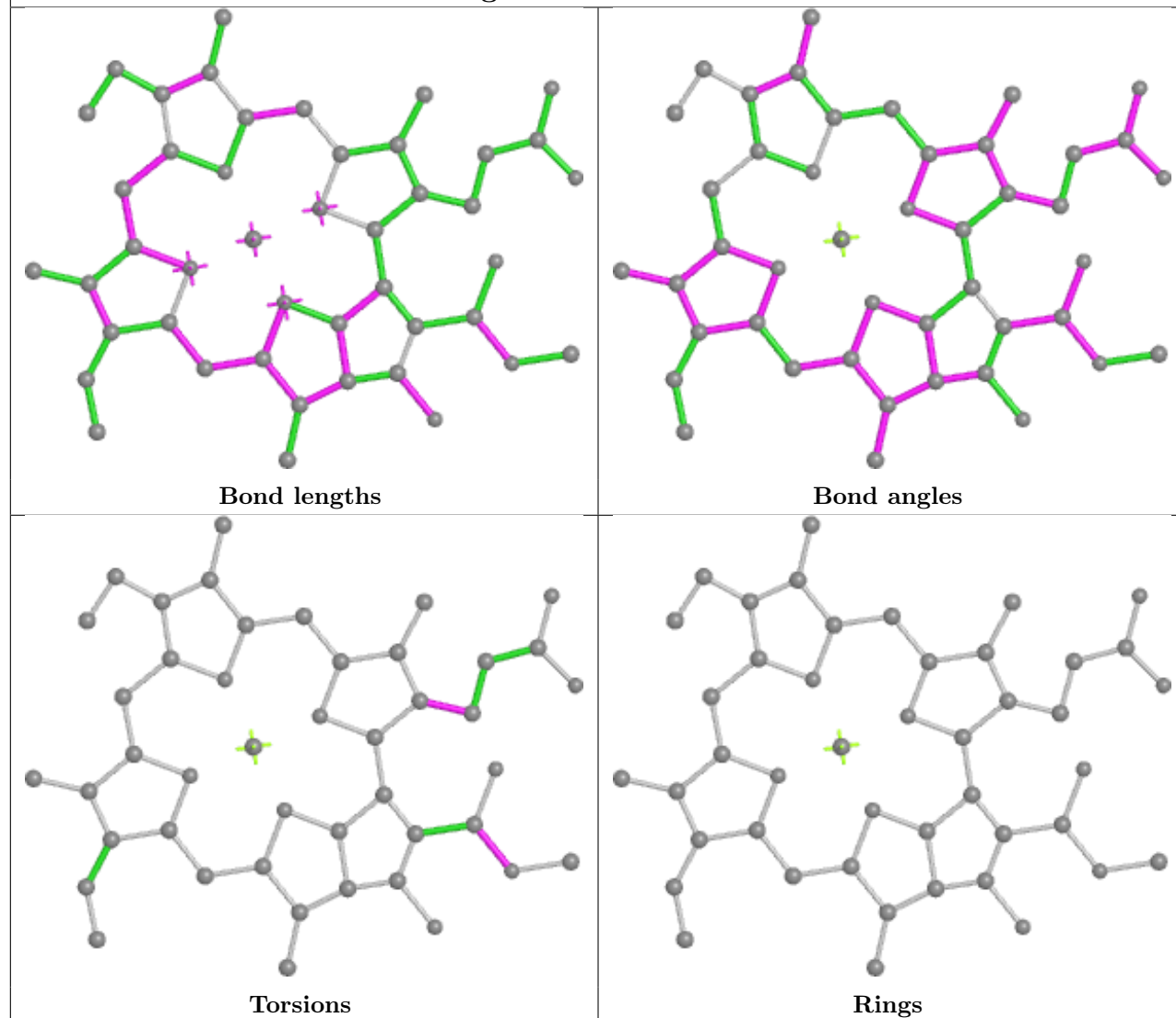
Torsions

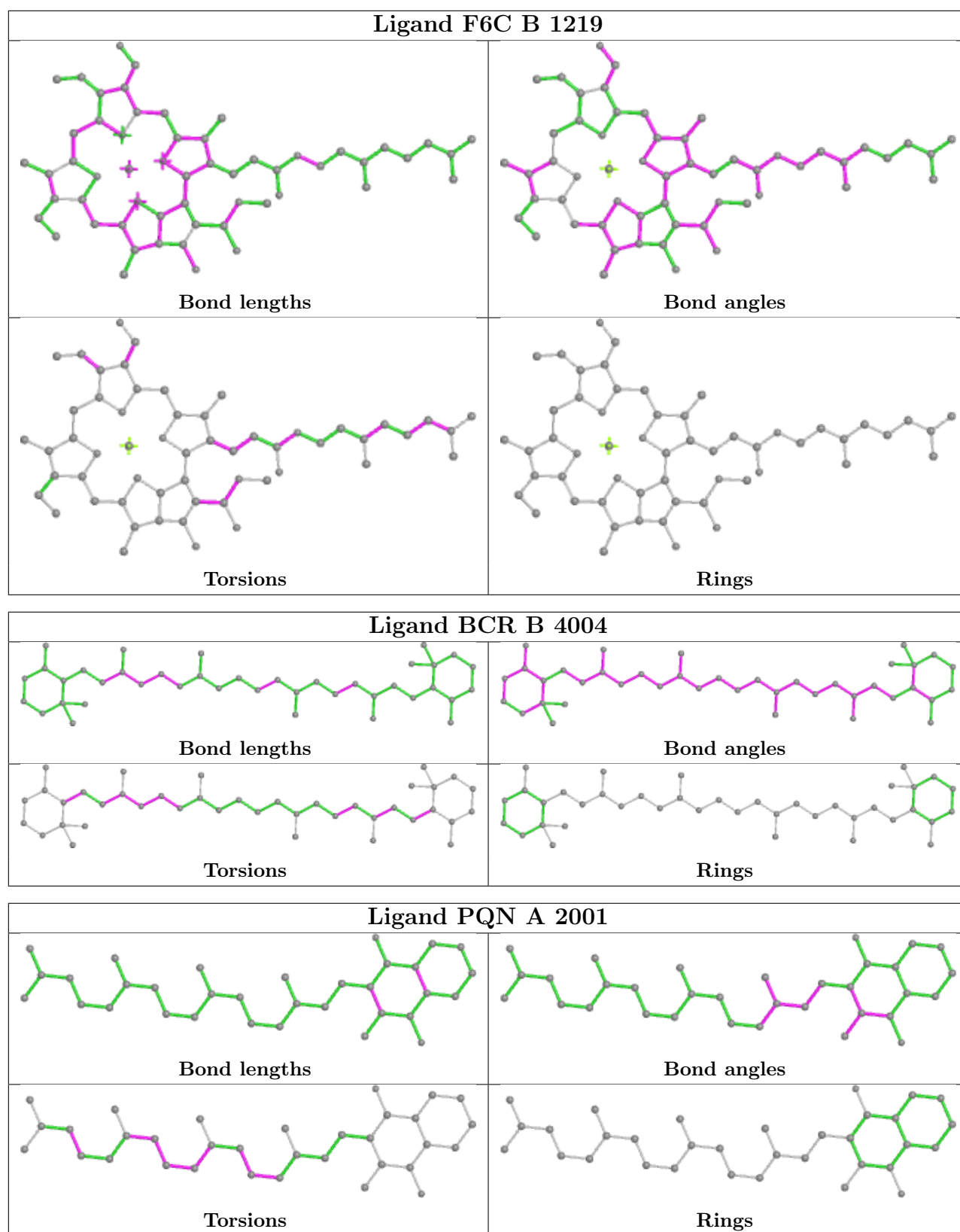


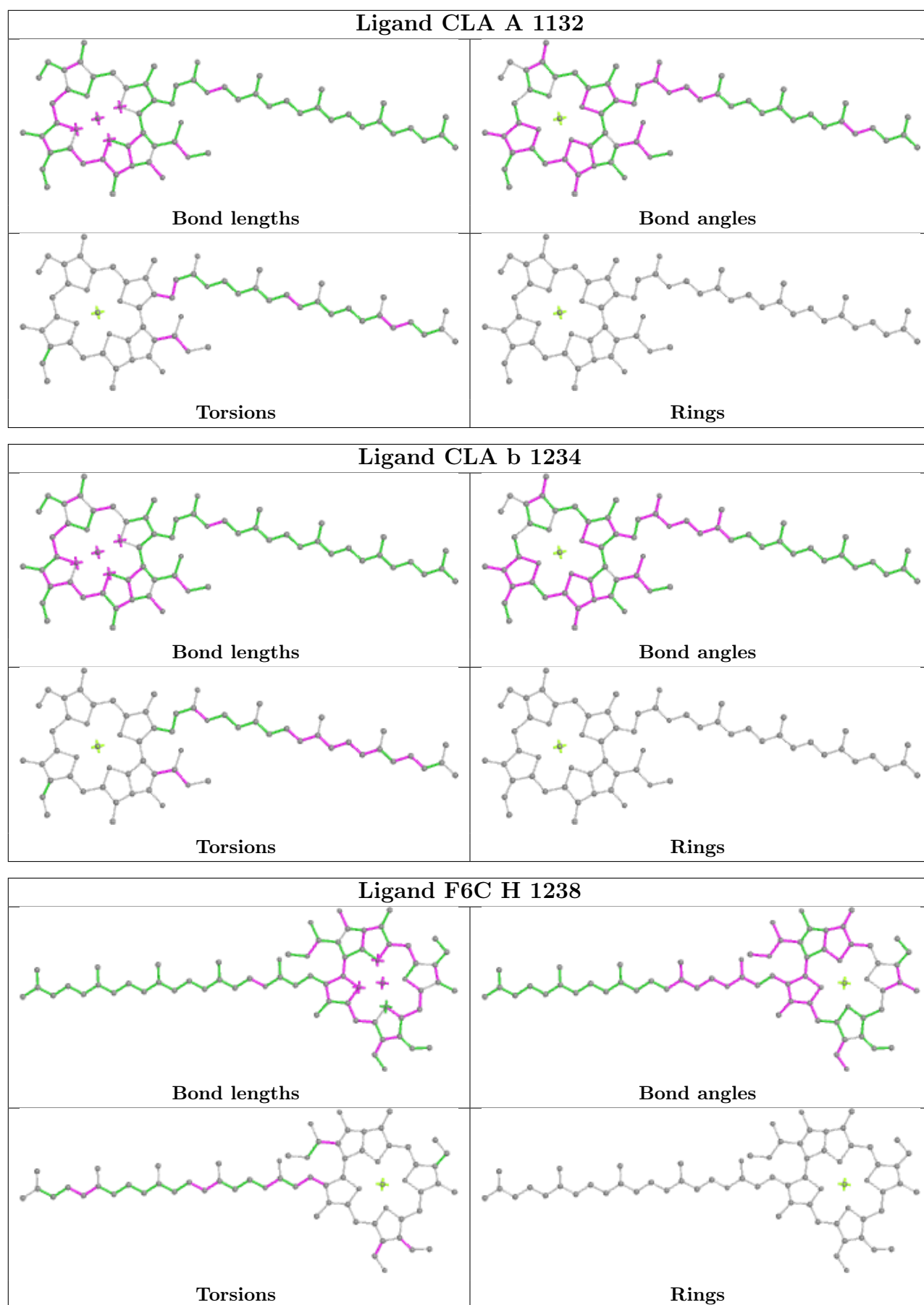
Rings

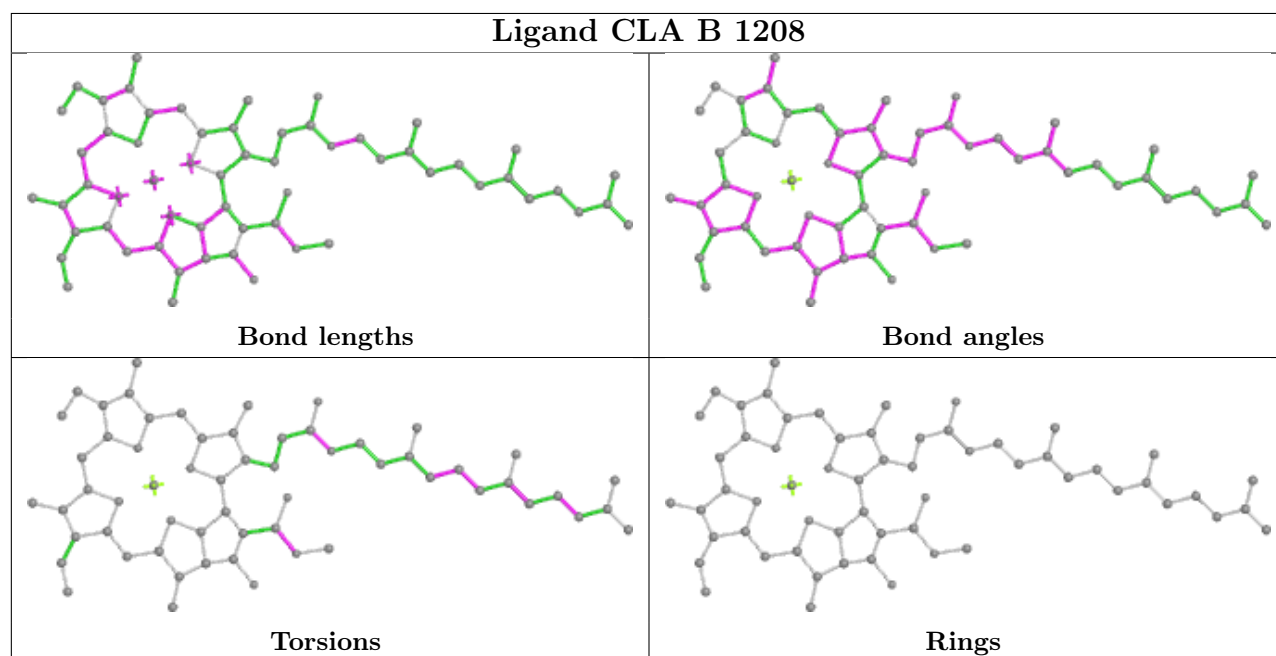
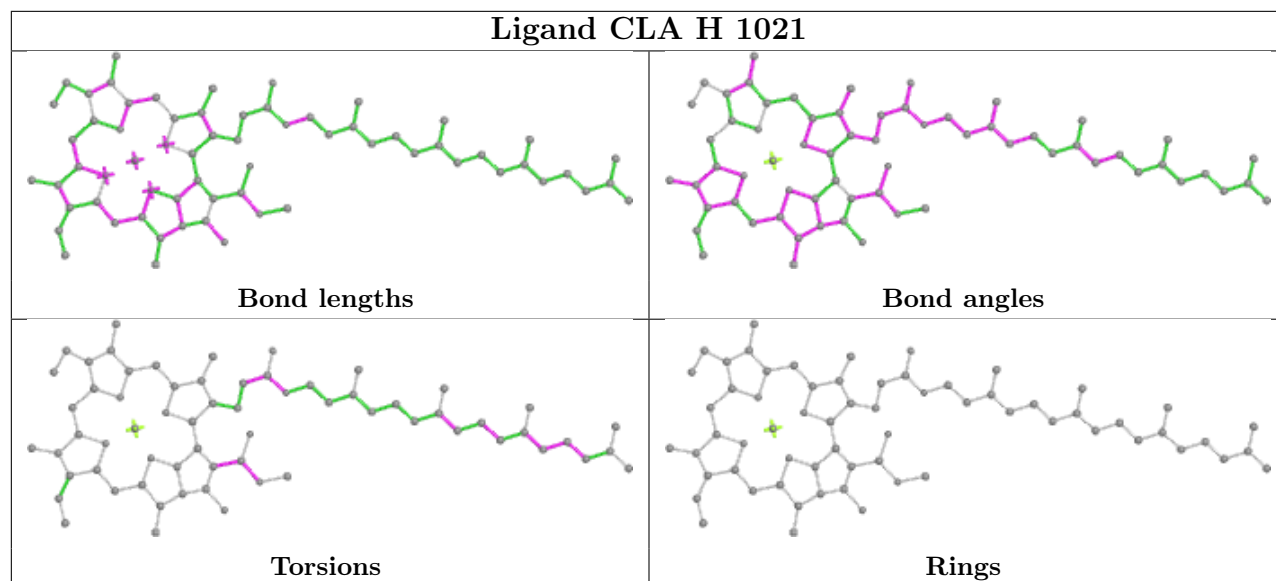
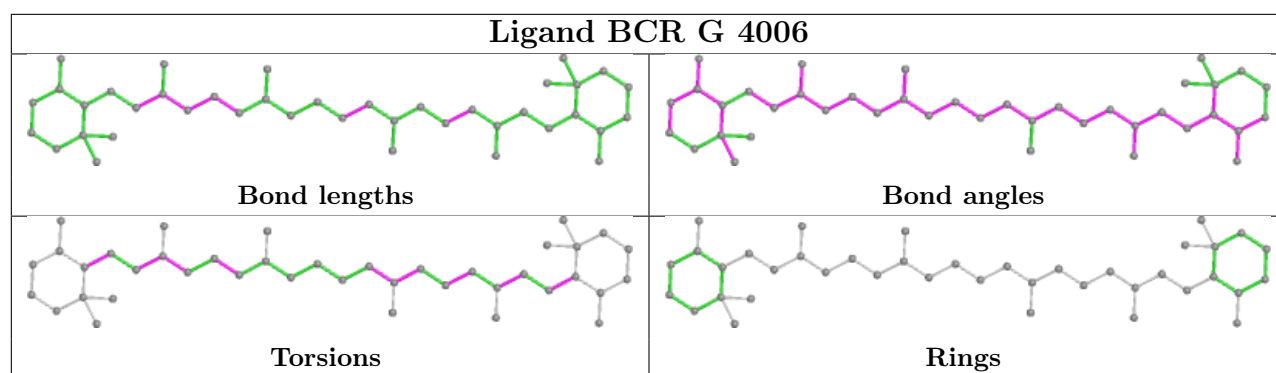


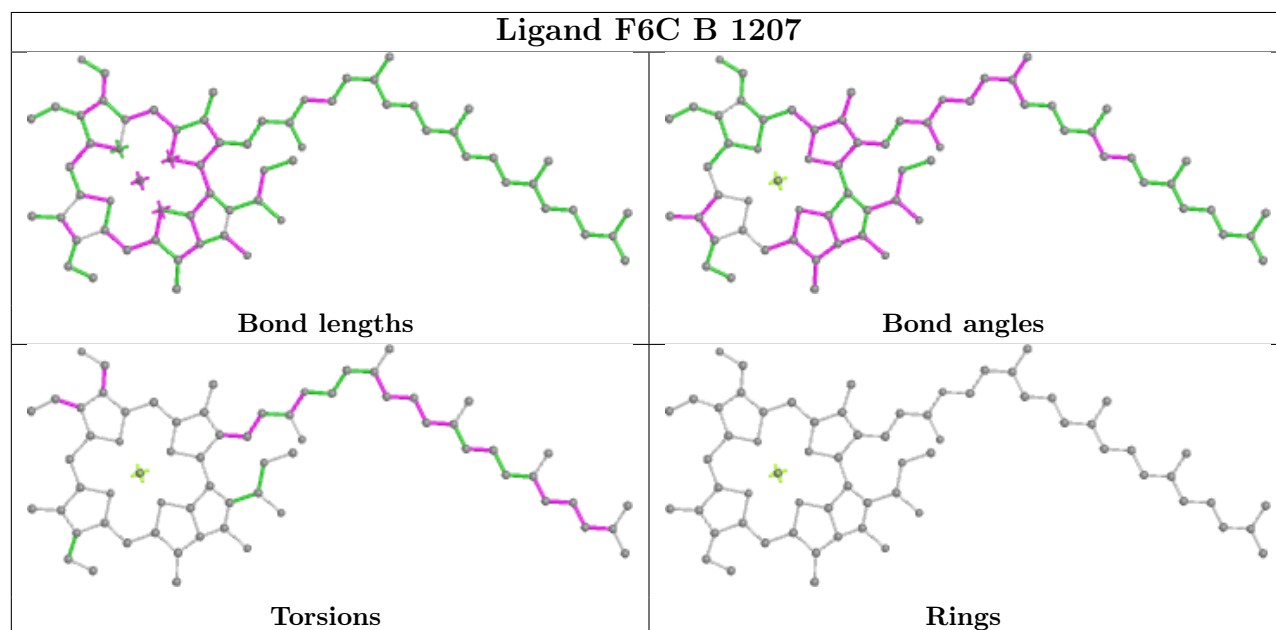
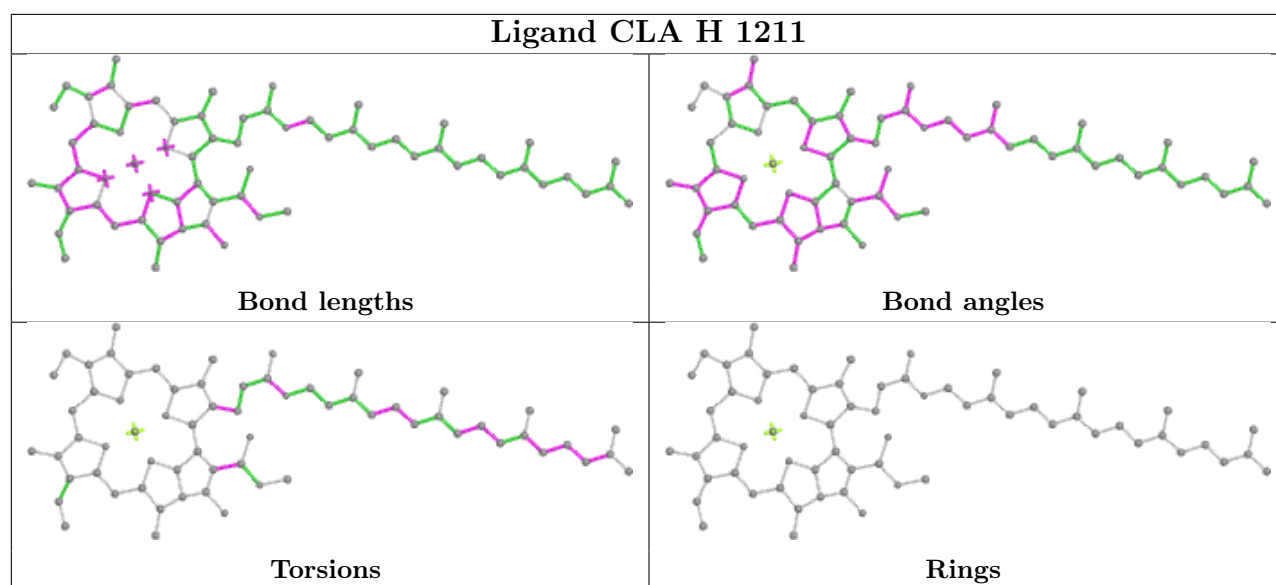
Ligand CLA G 1105

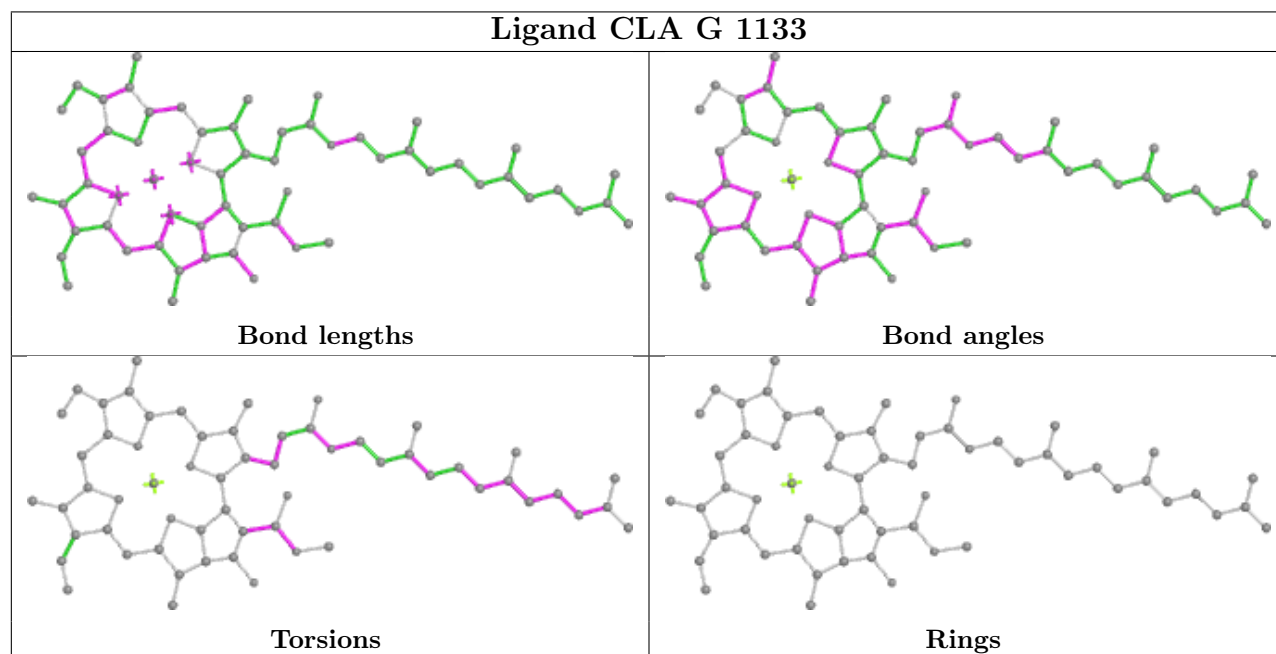
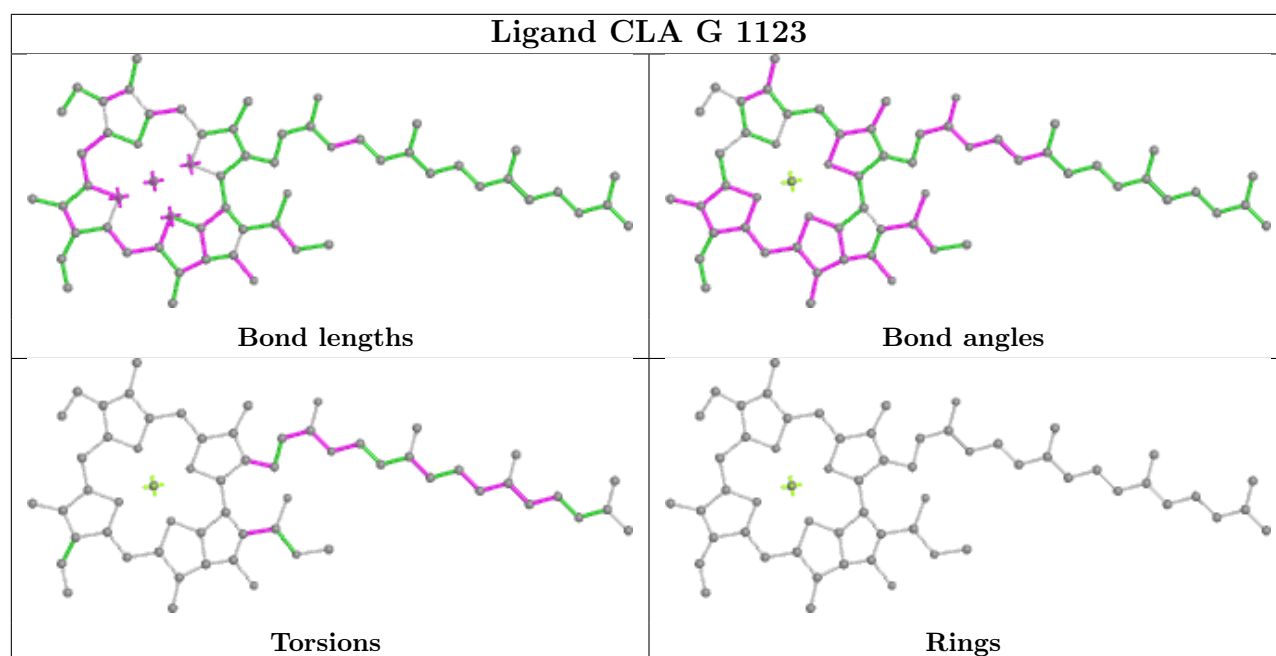




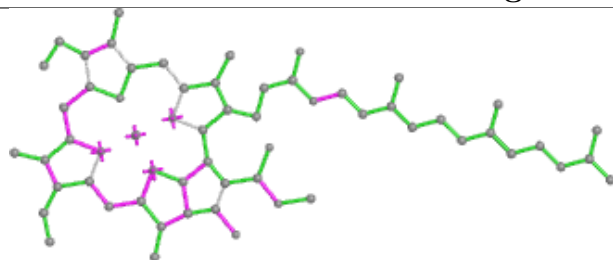




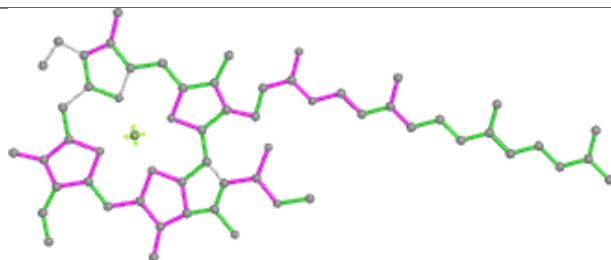




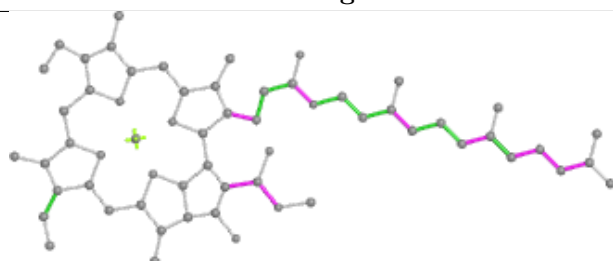
Ligand CLA A 1126



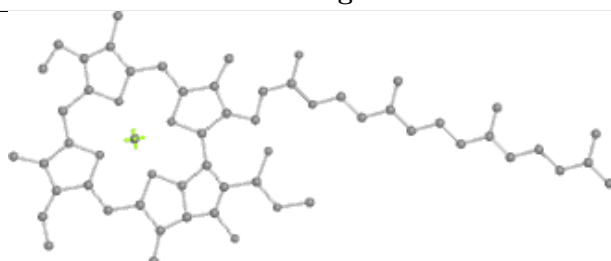
Bond lengths



Bond angles

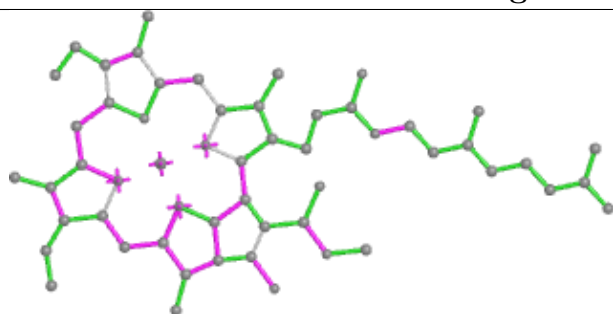


Torsions

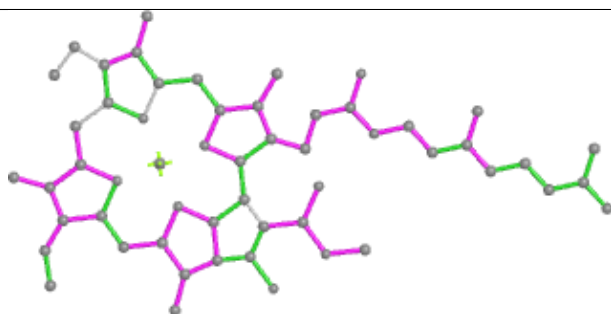


Rings

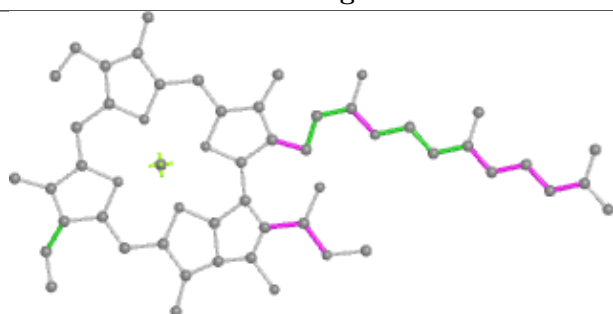
Ligand CLA a 1138



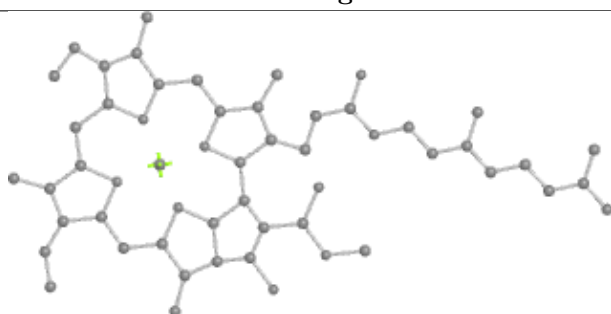
Bond lengths



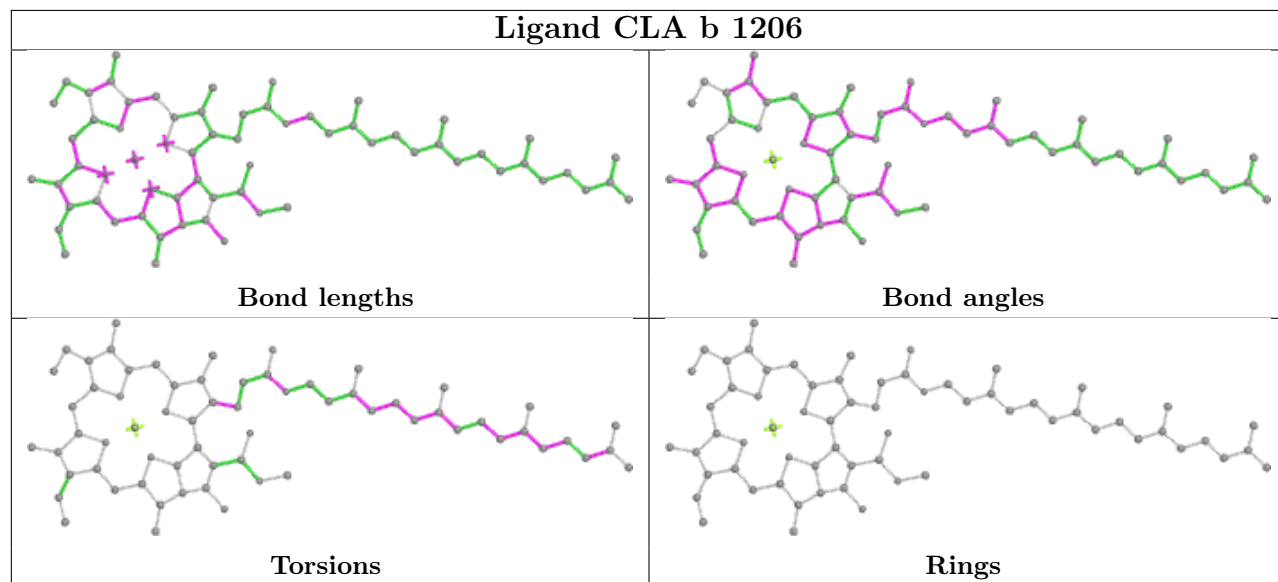
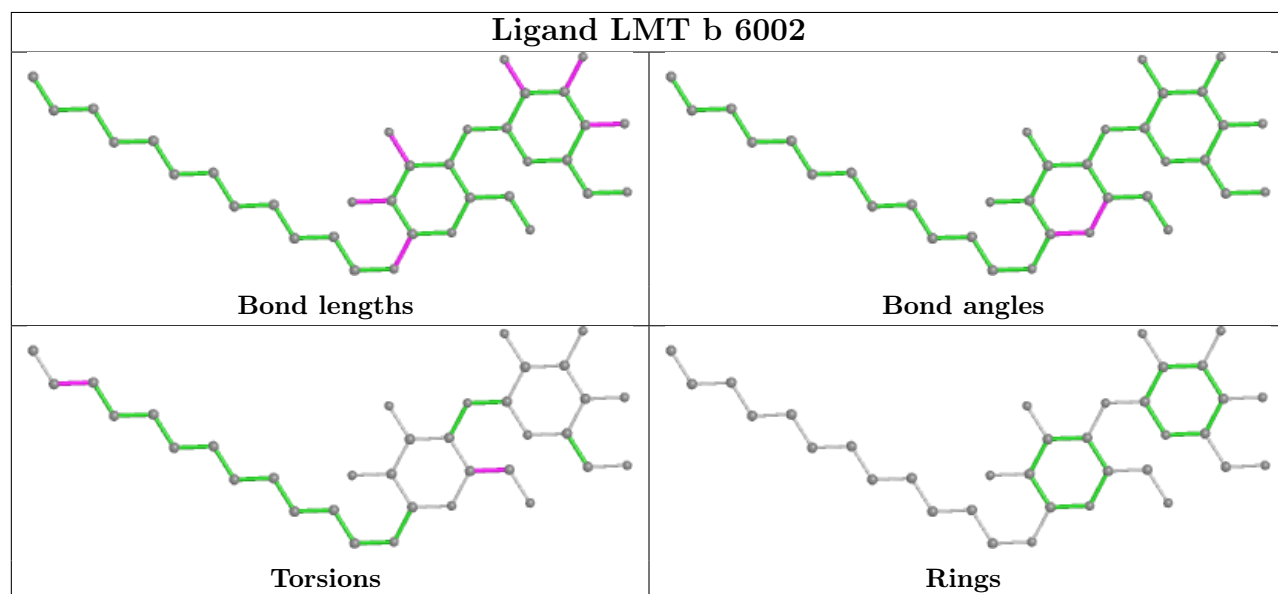
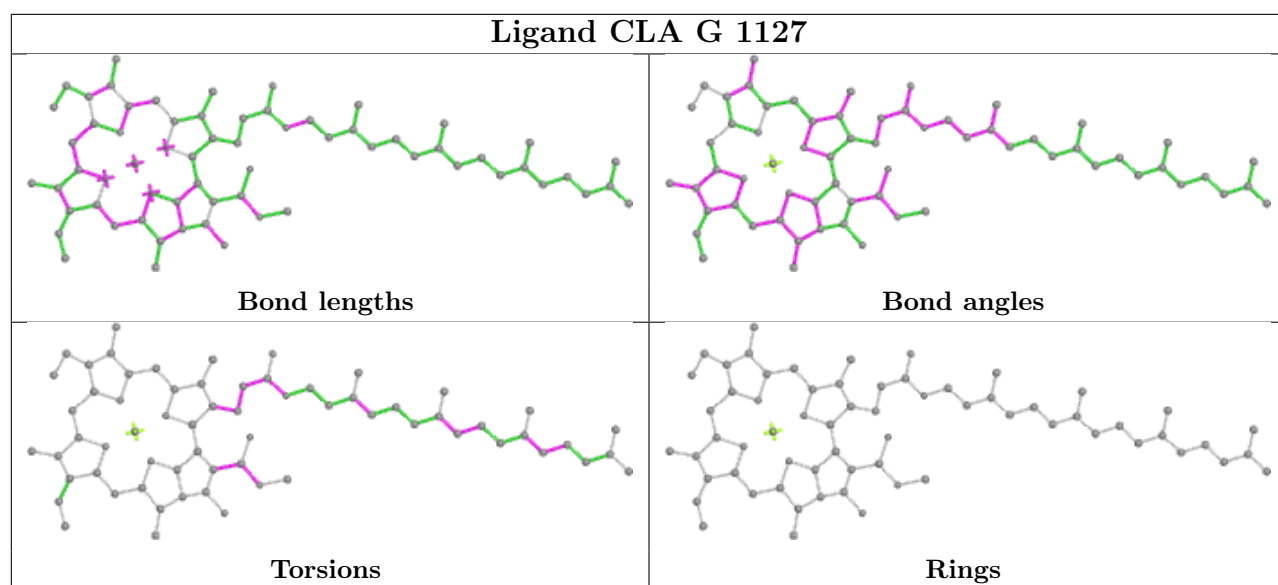
Bond angles

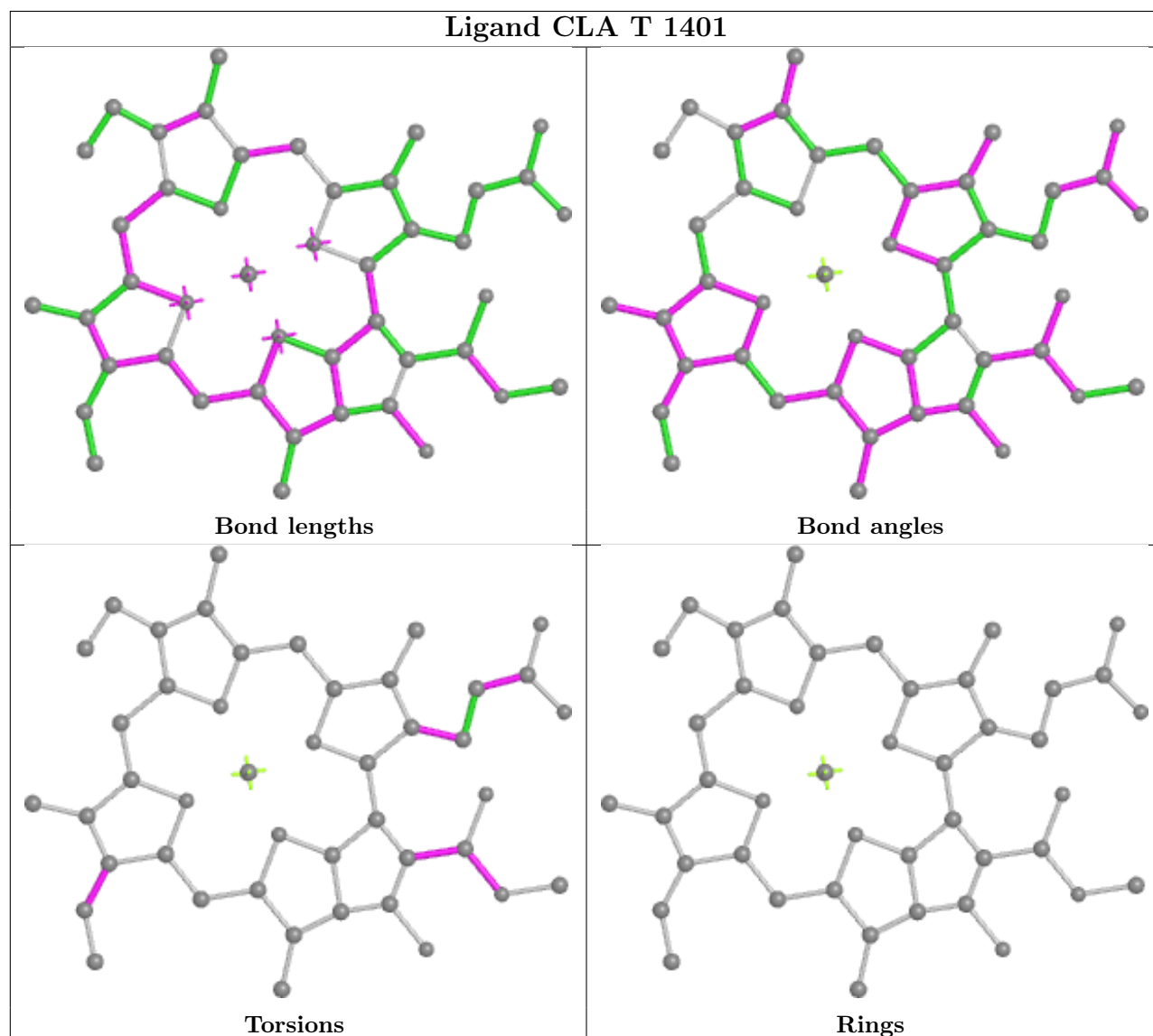
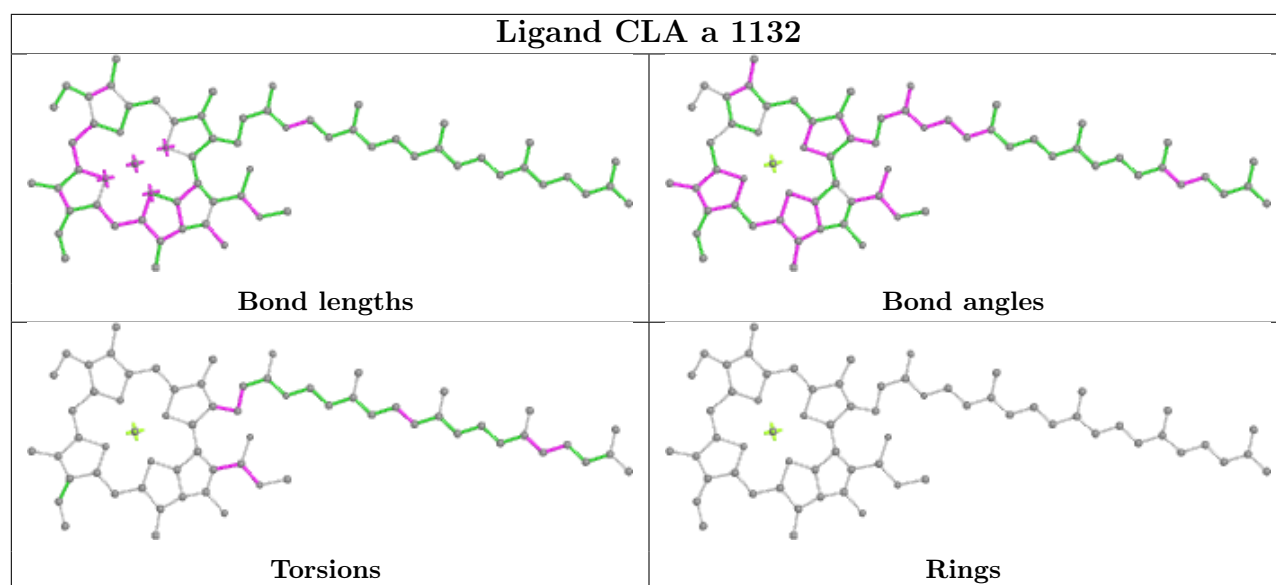


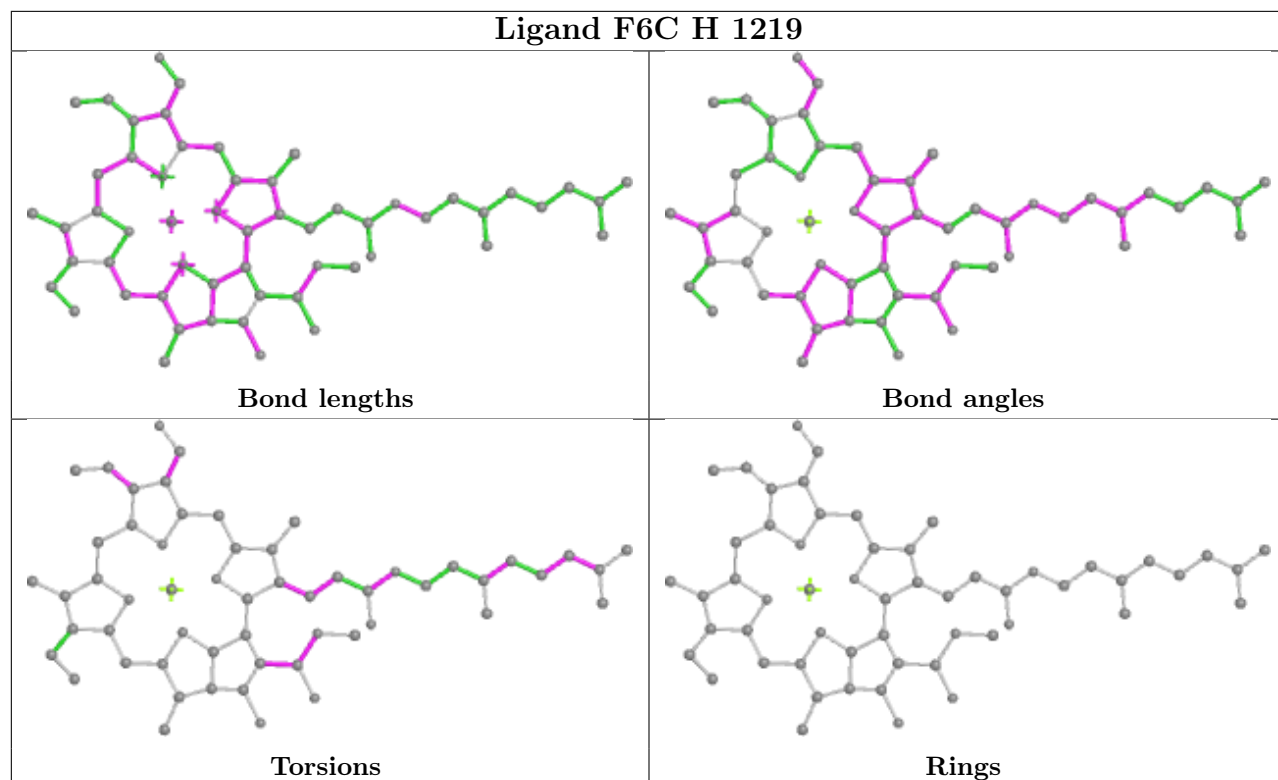
Torsions

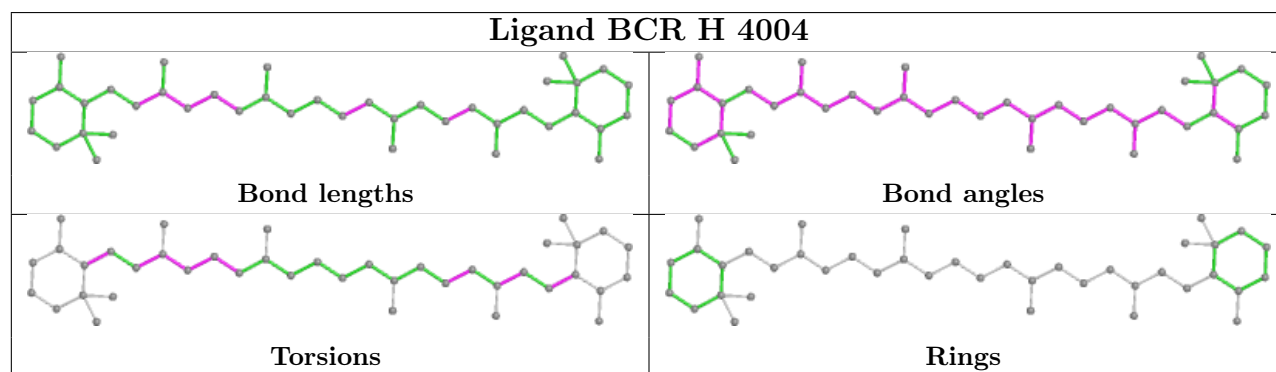
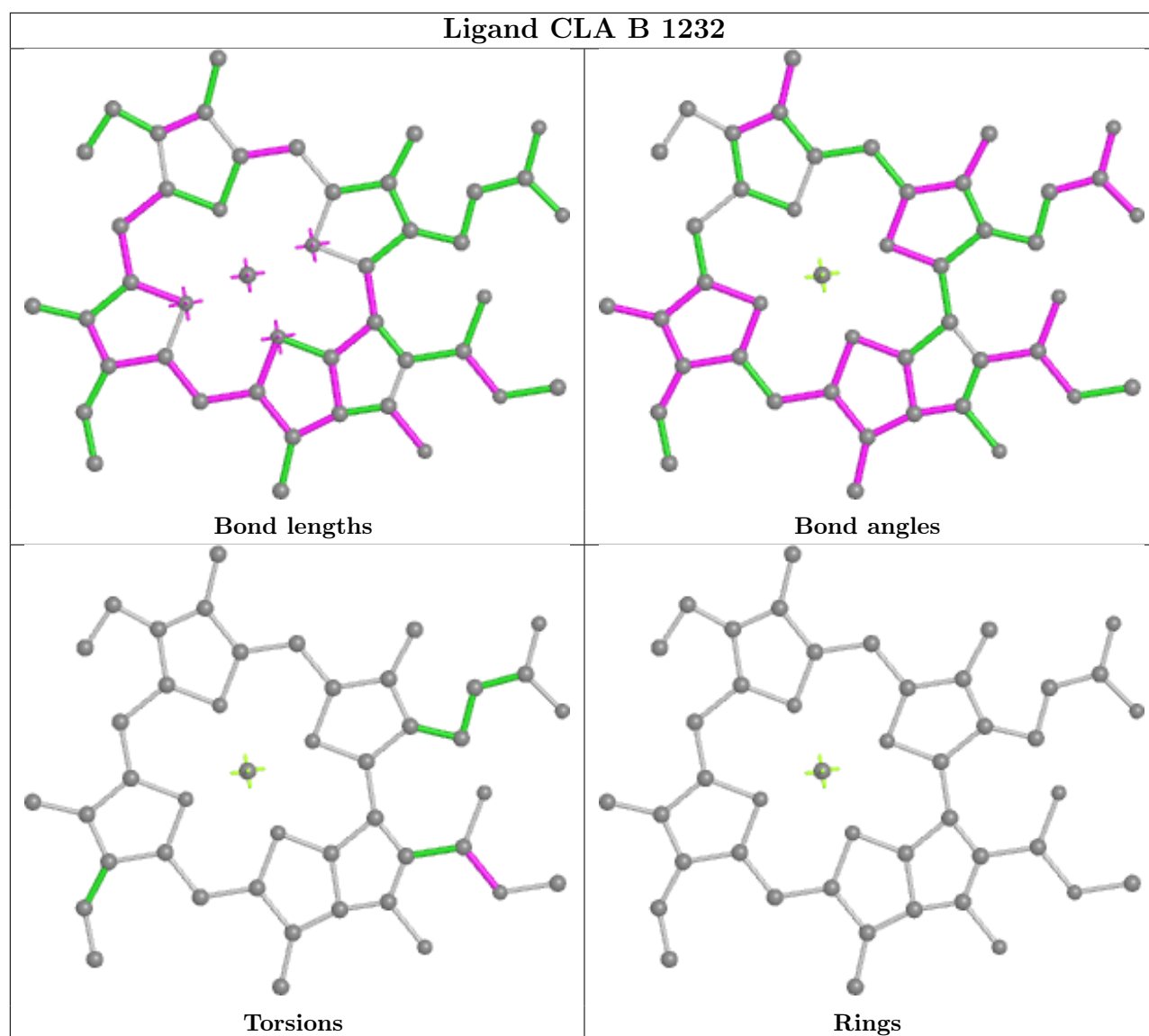


Rings

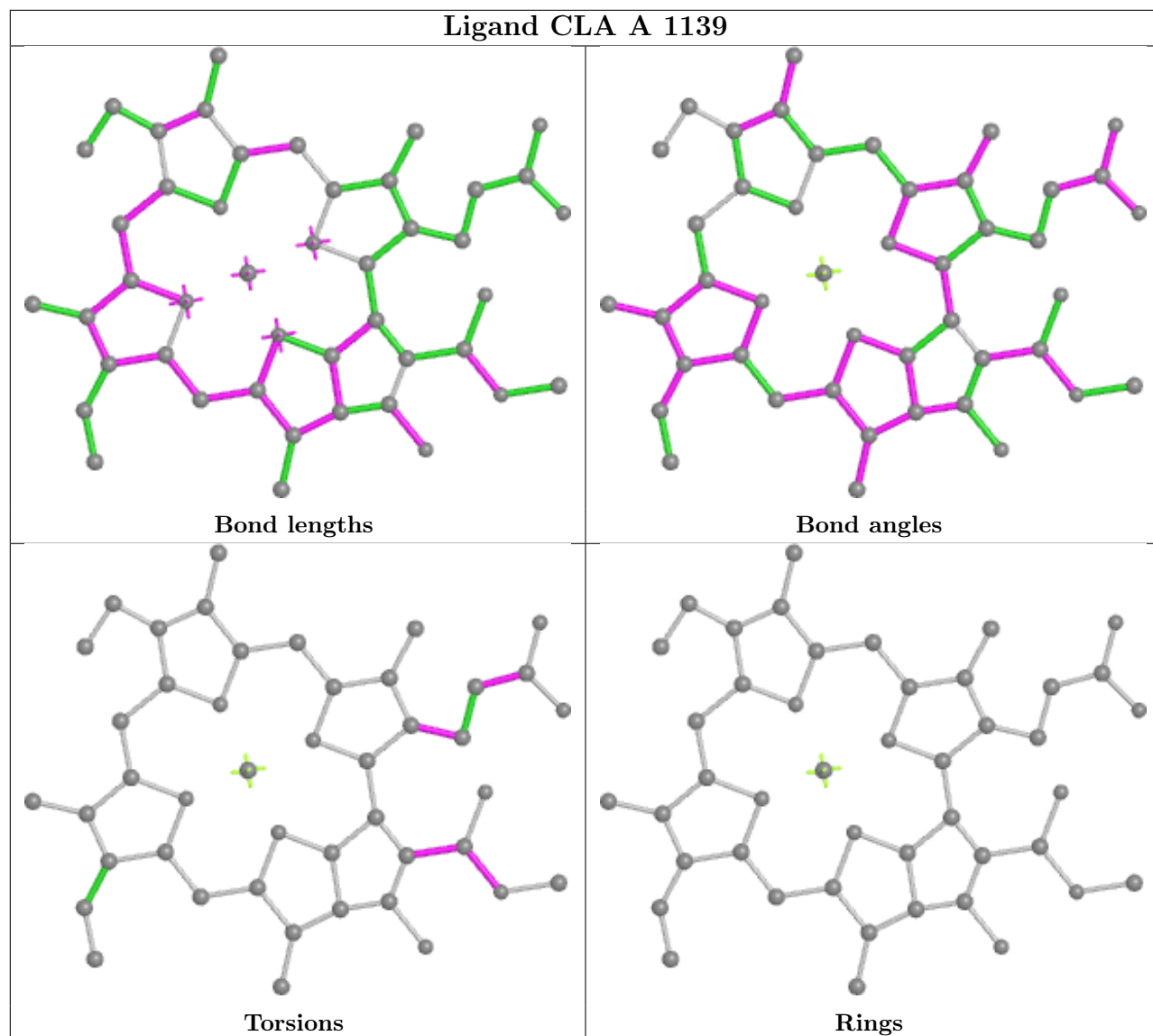


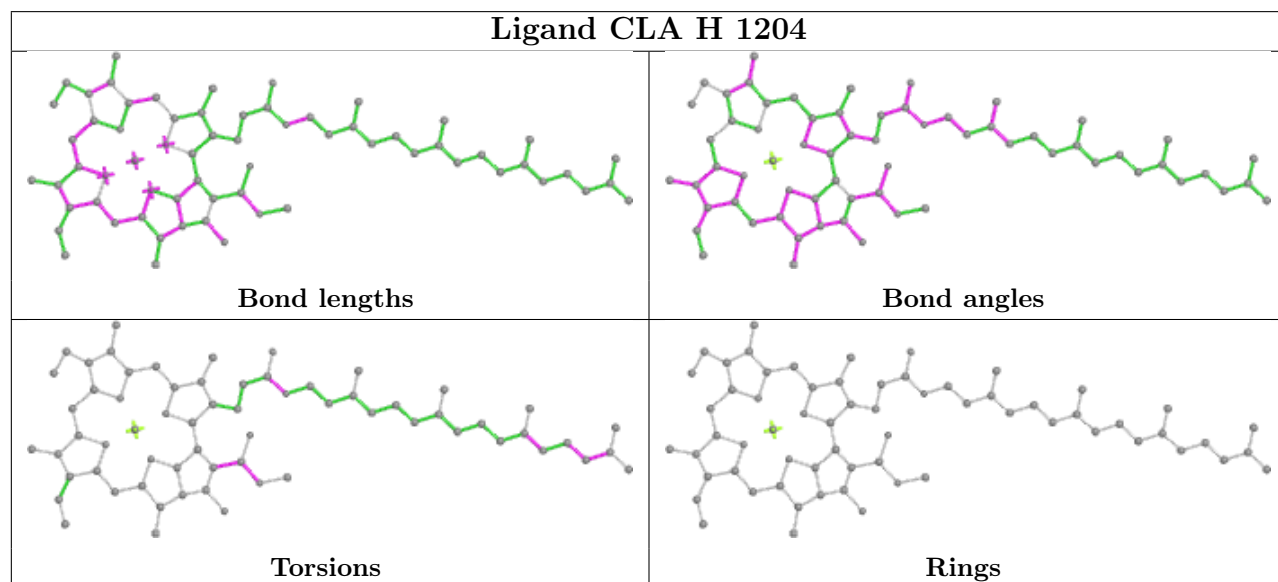
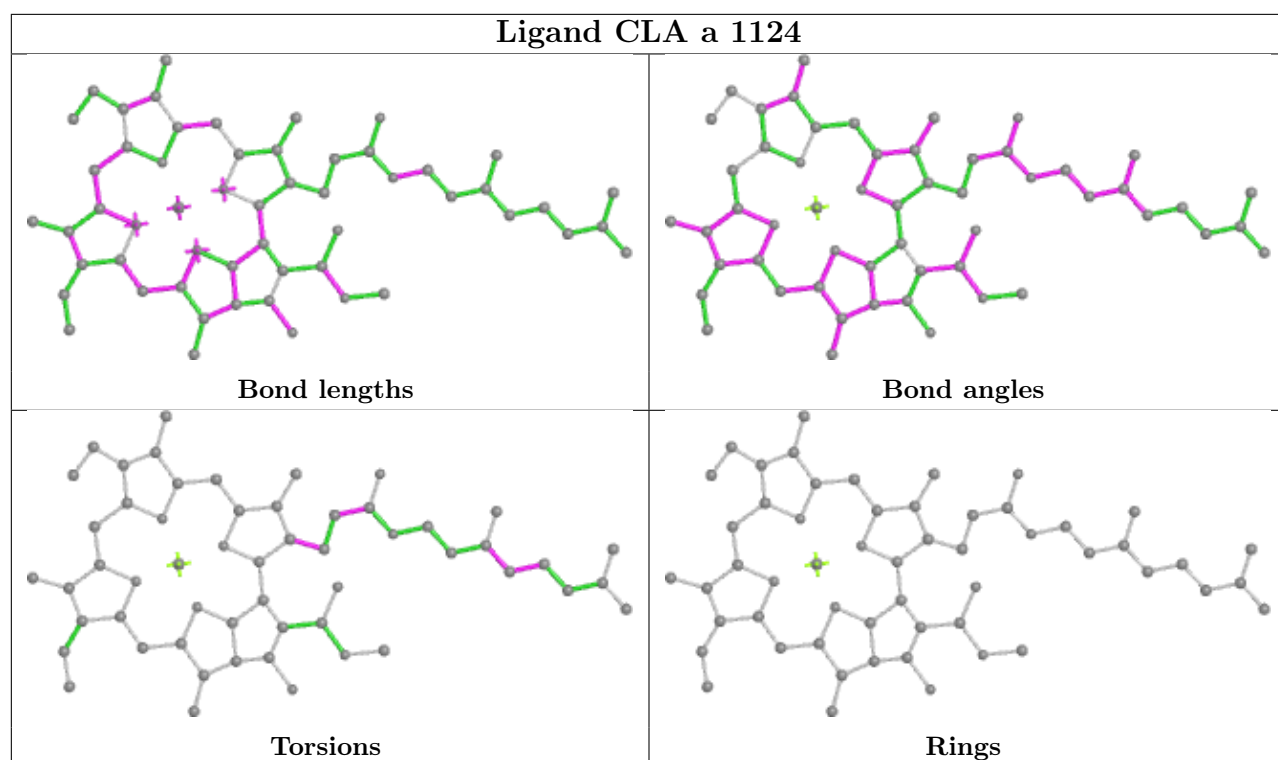




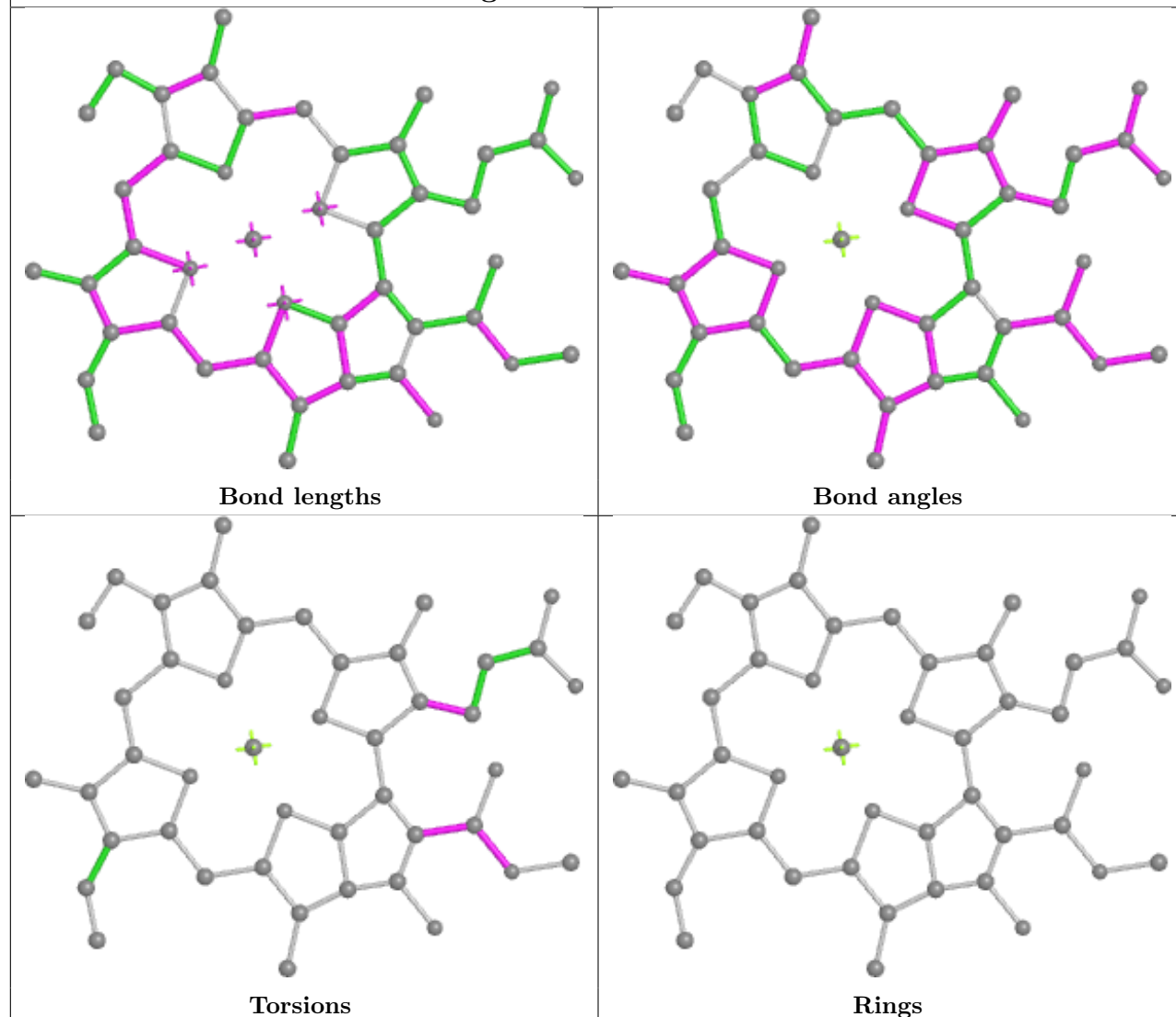


Ligand CLA A 1139

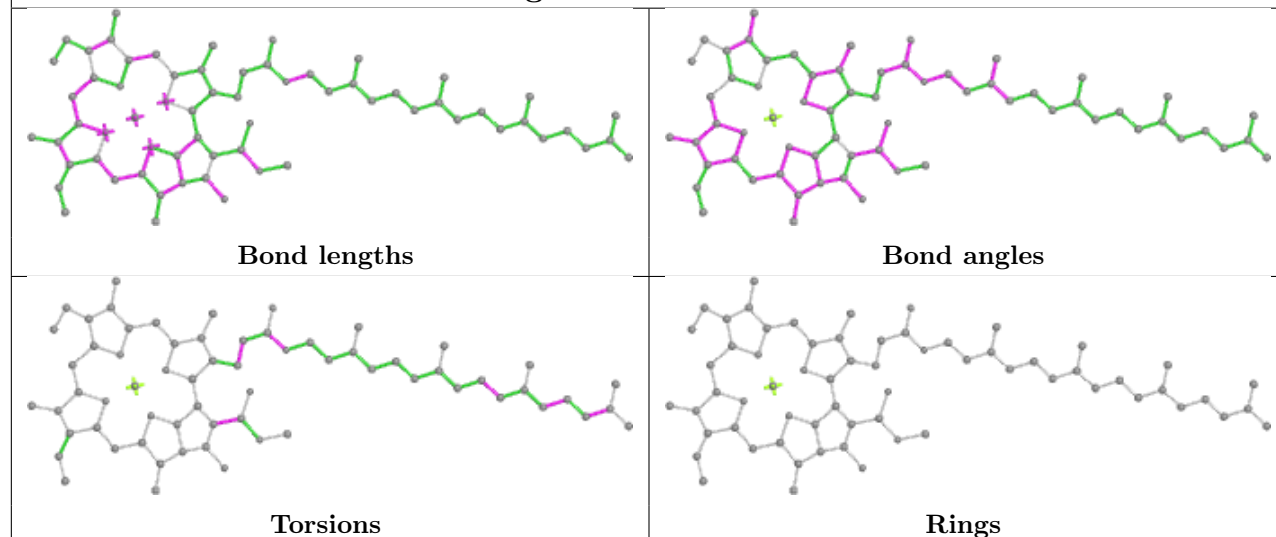




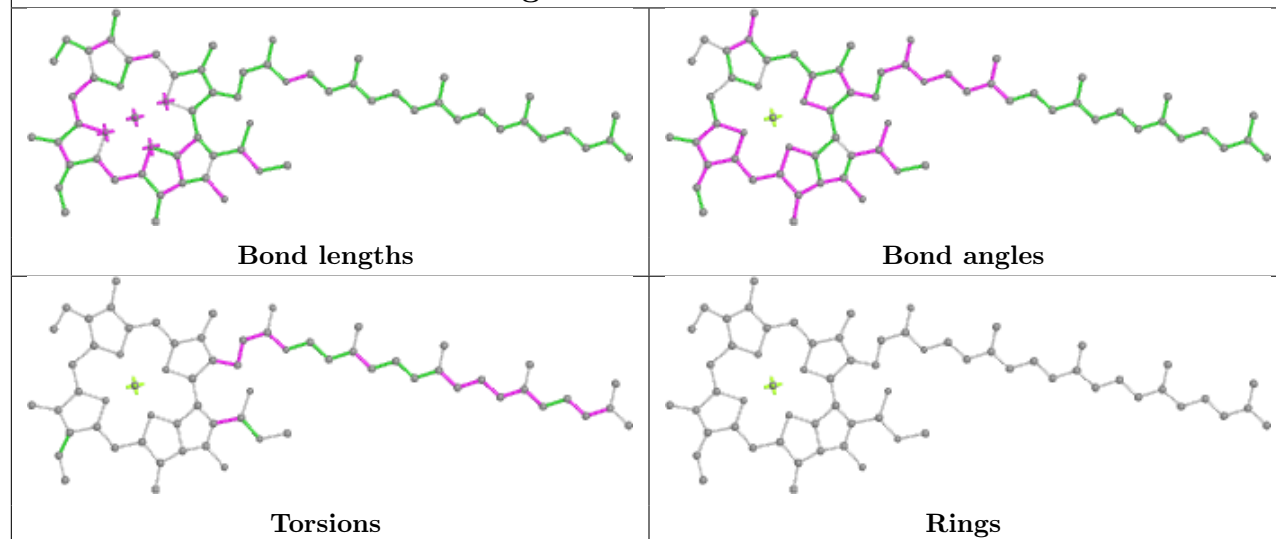
Ligand CLA G 1108



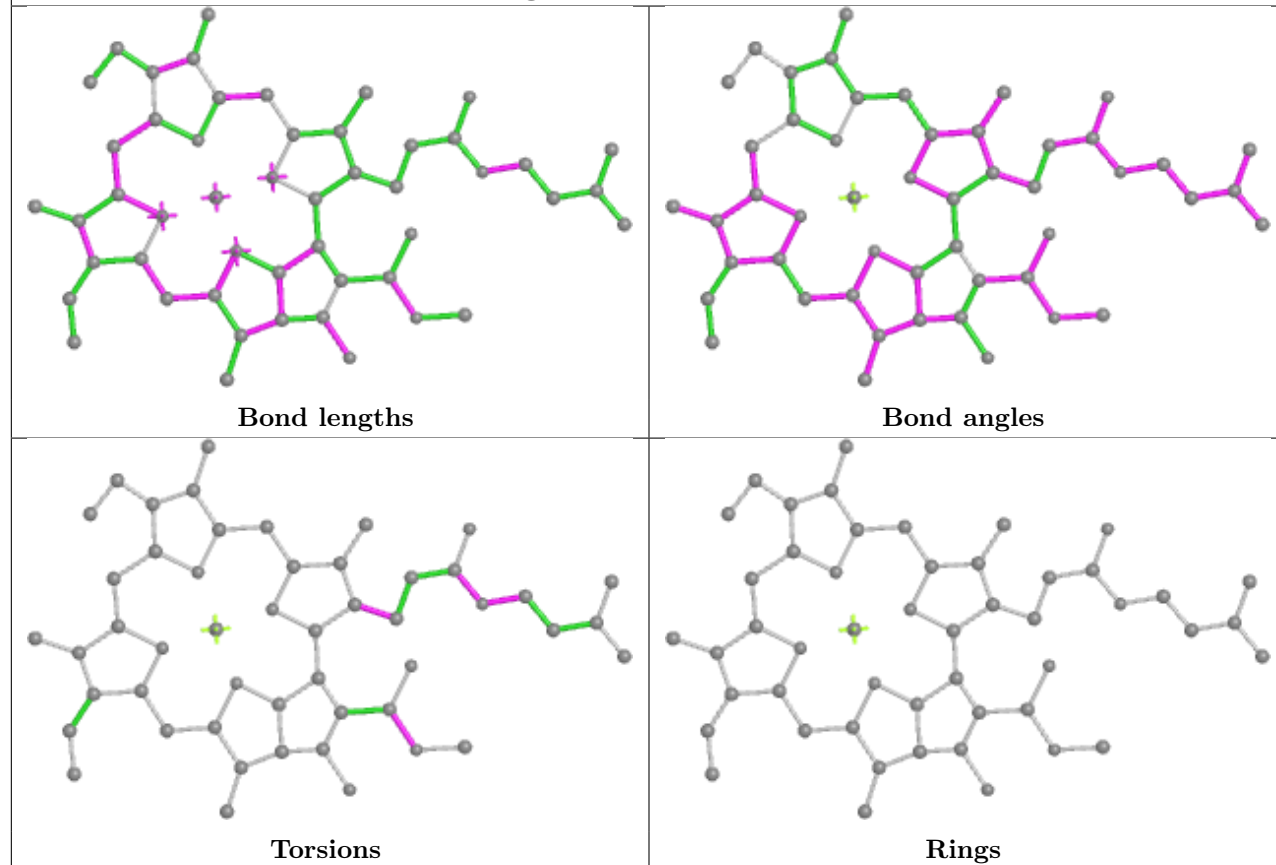
Ligand CLA L 1501

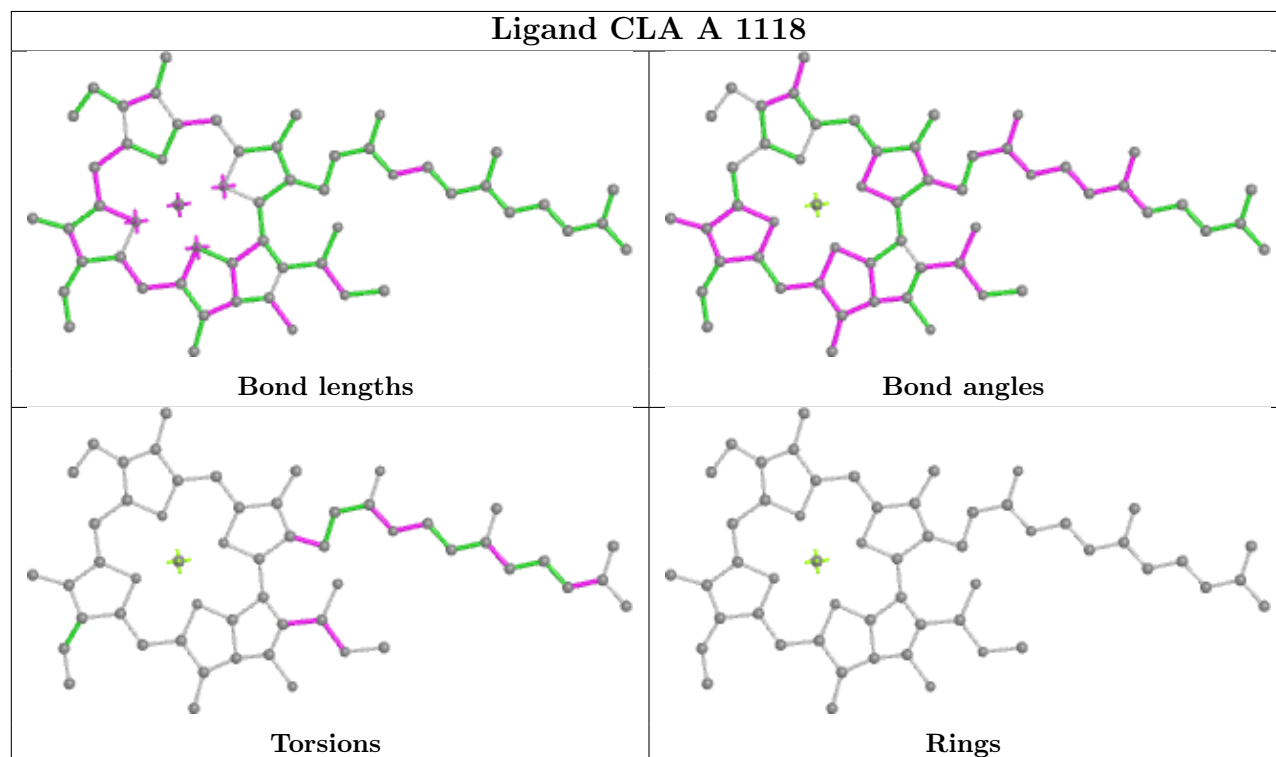
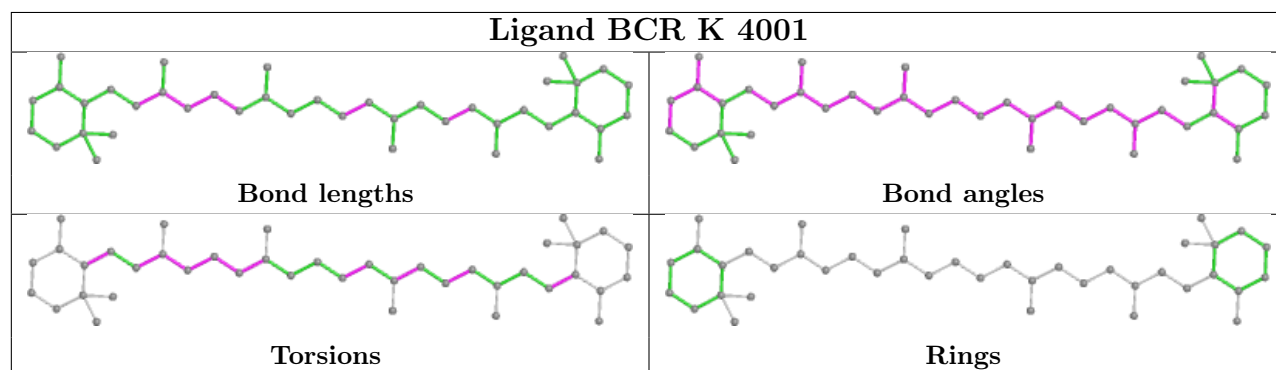
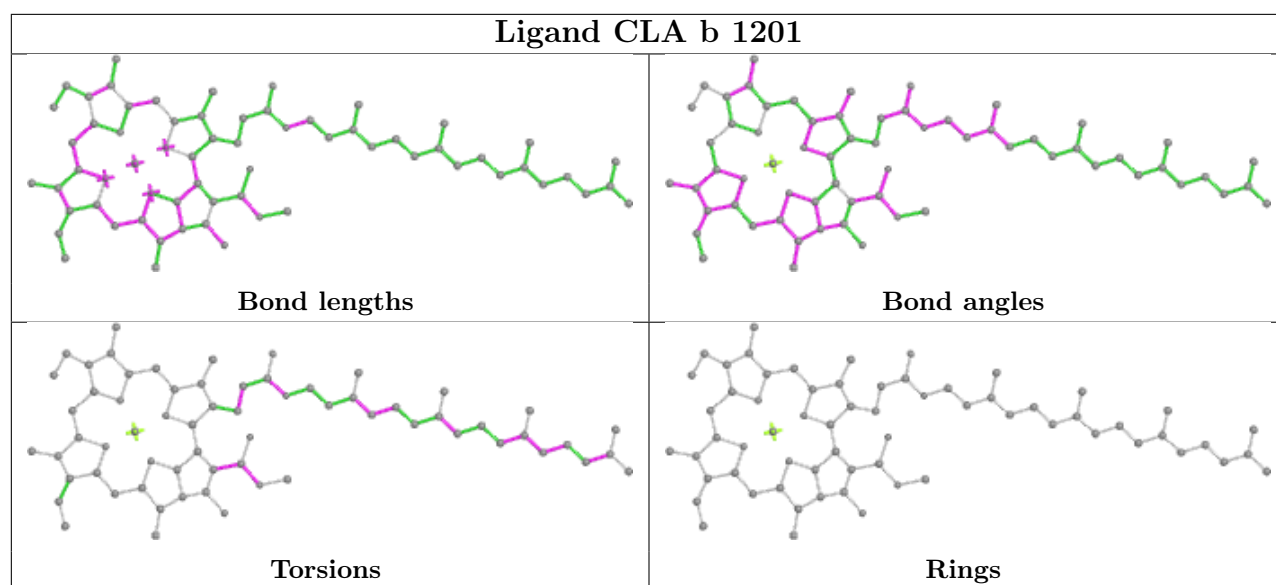


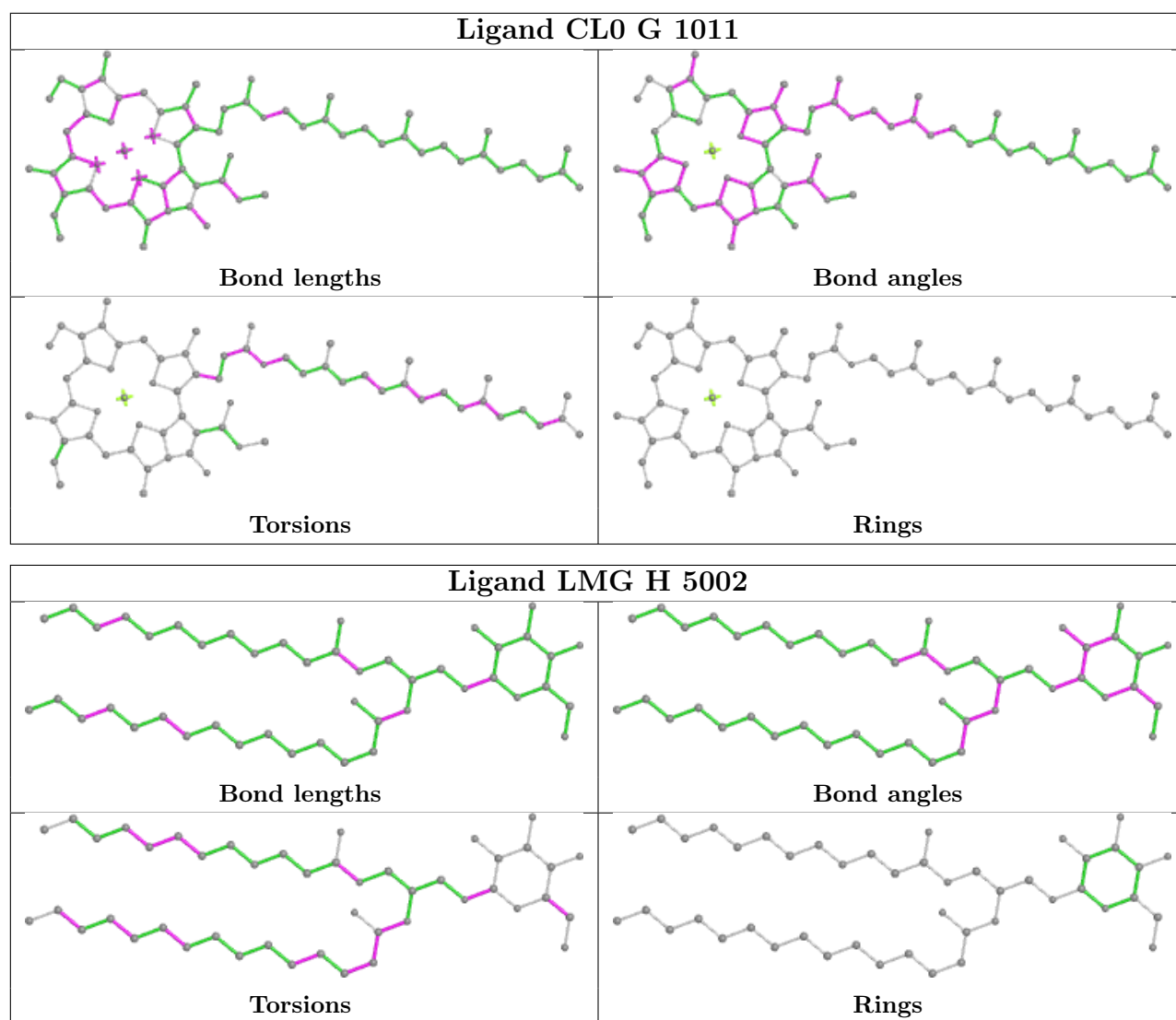
Ligand CLA G 1125

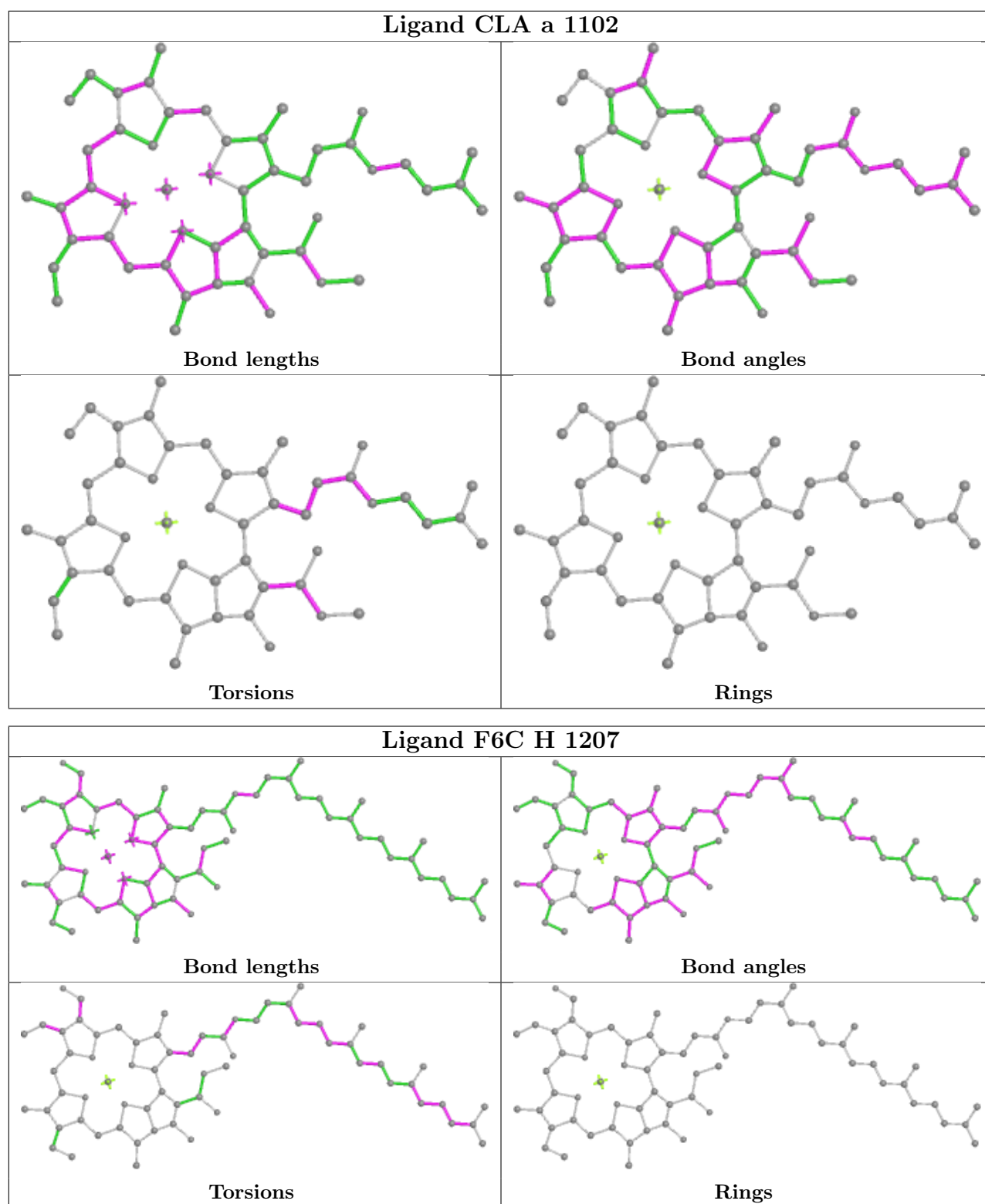


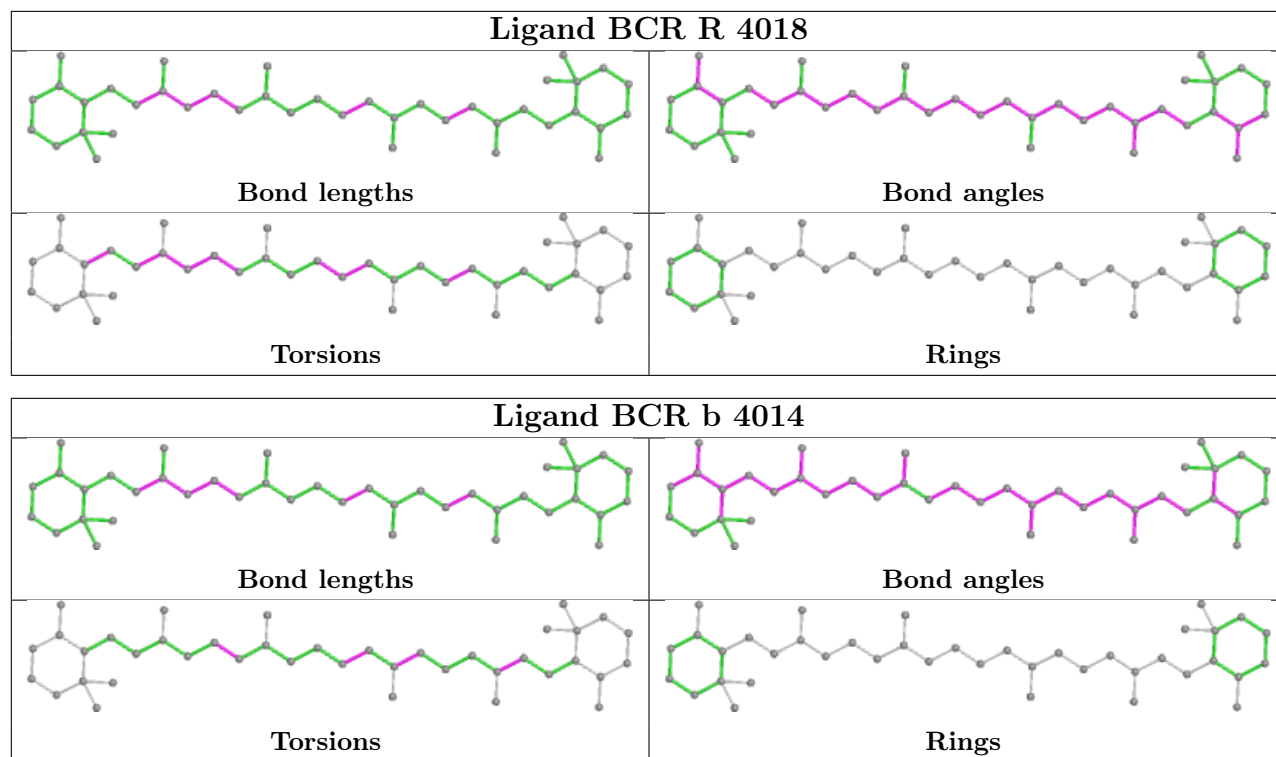
Ligand CLA V 1501

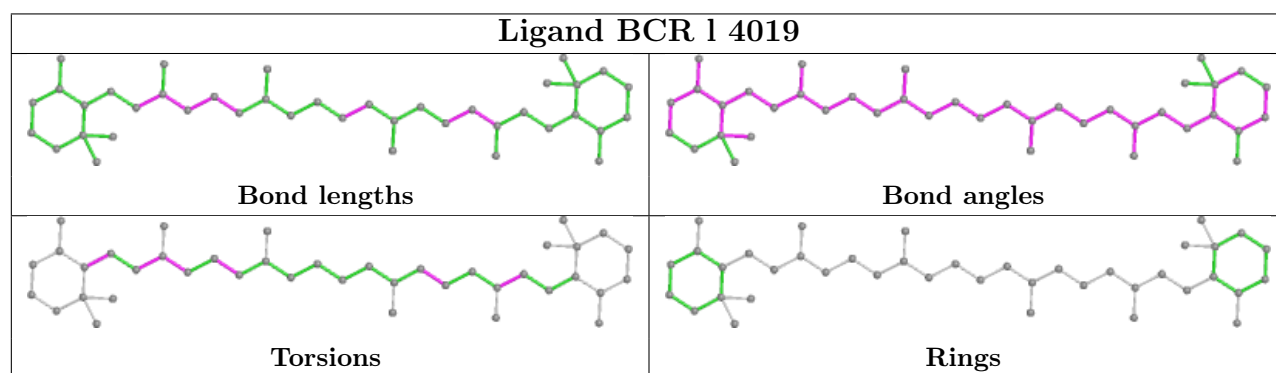
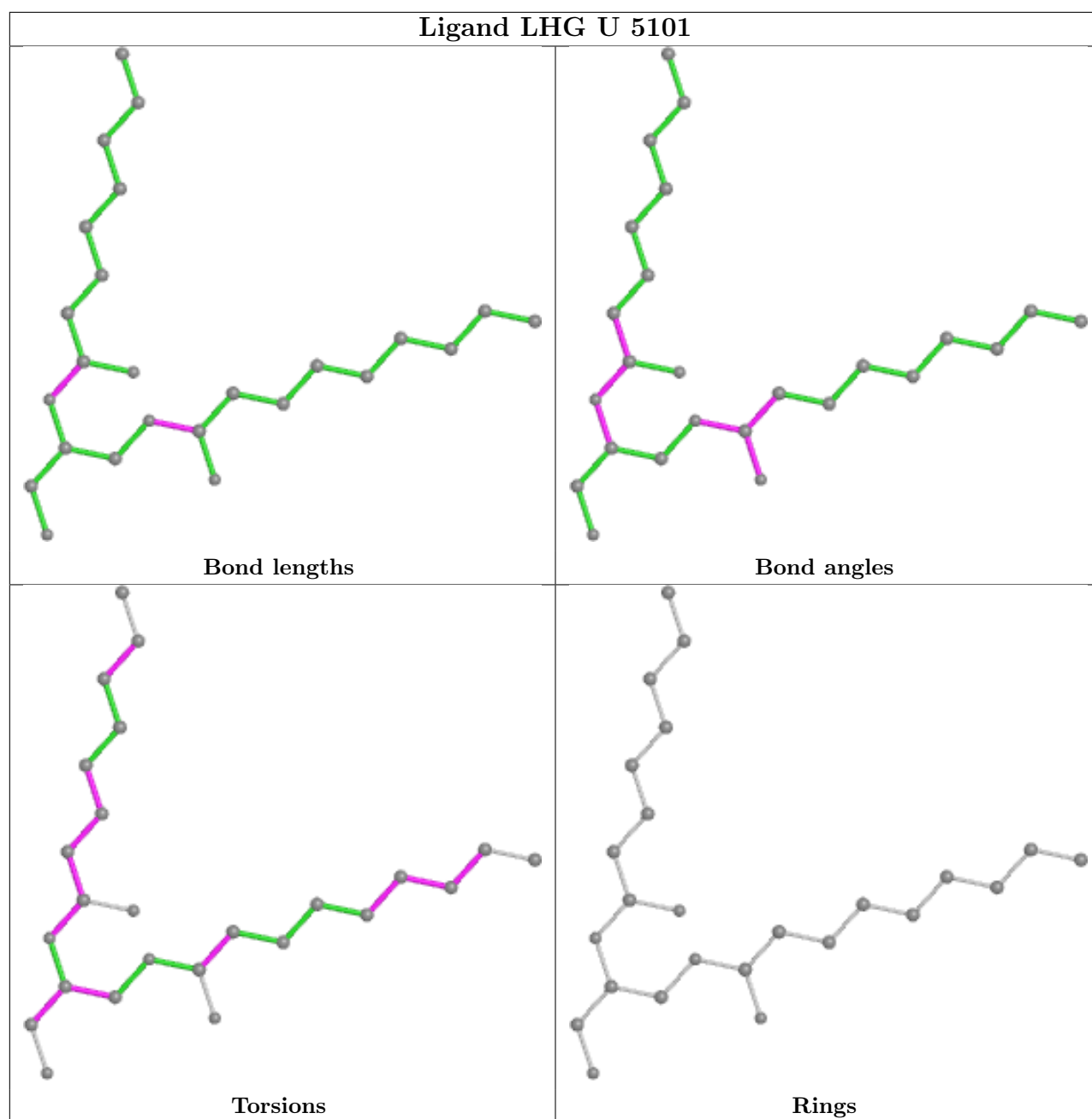


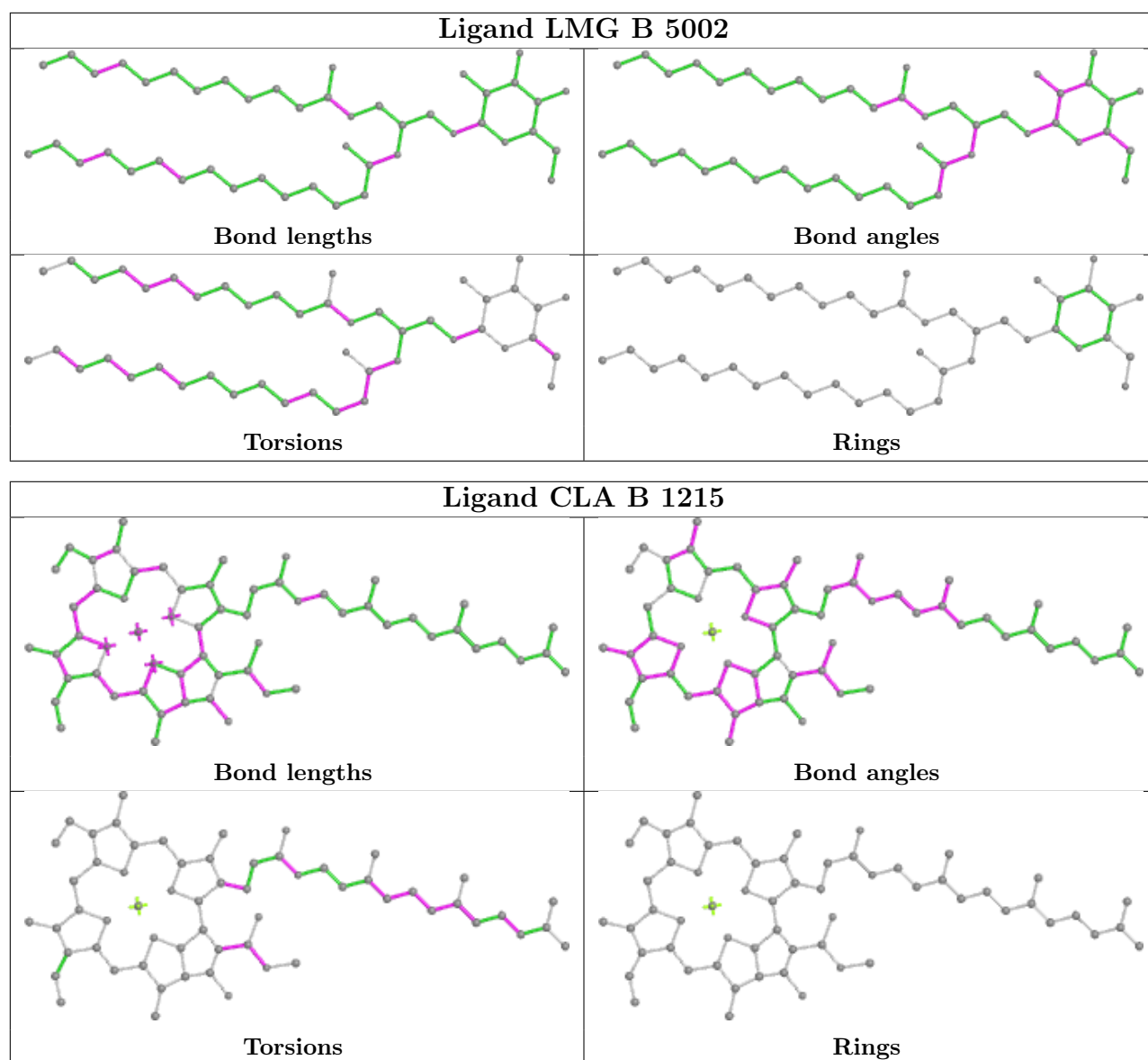




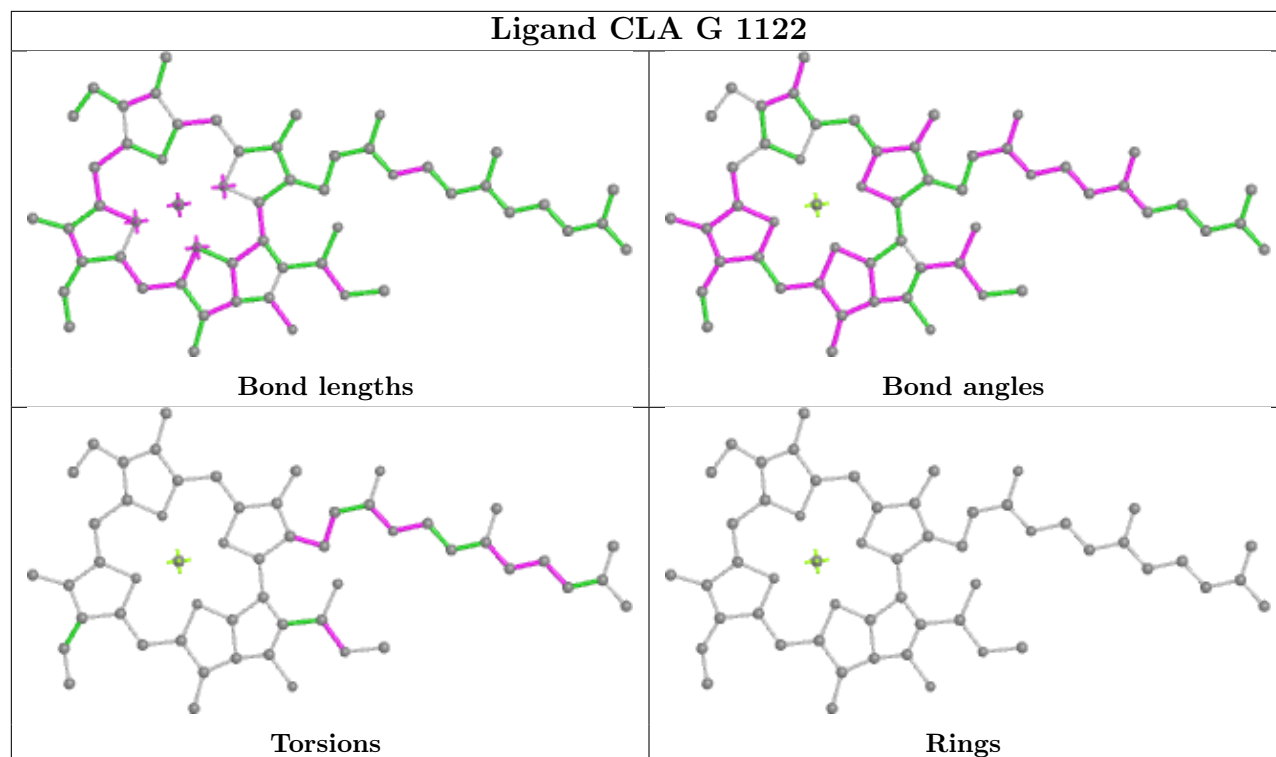




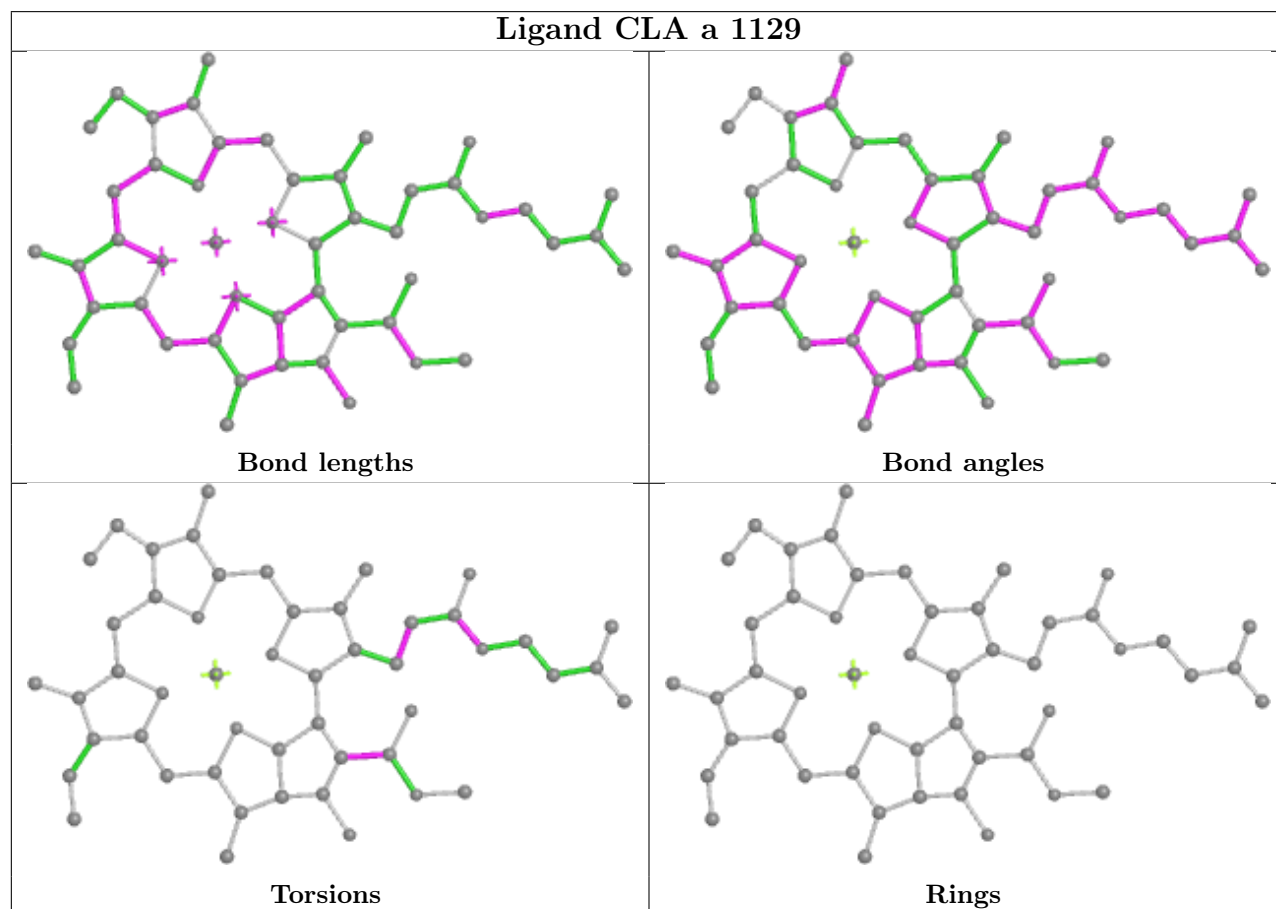




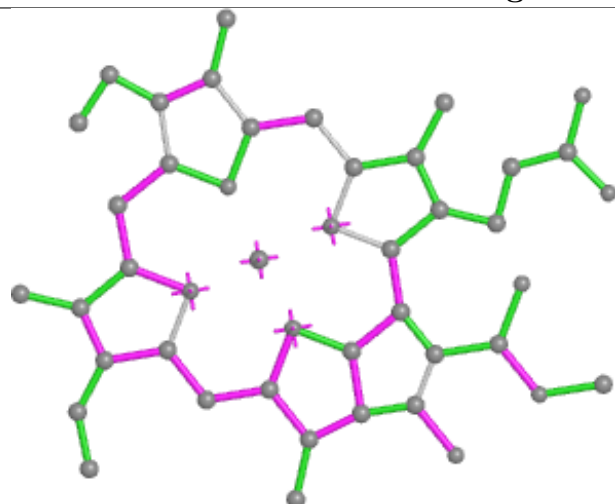
Ligand CLA G 1122



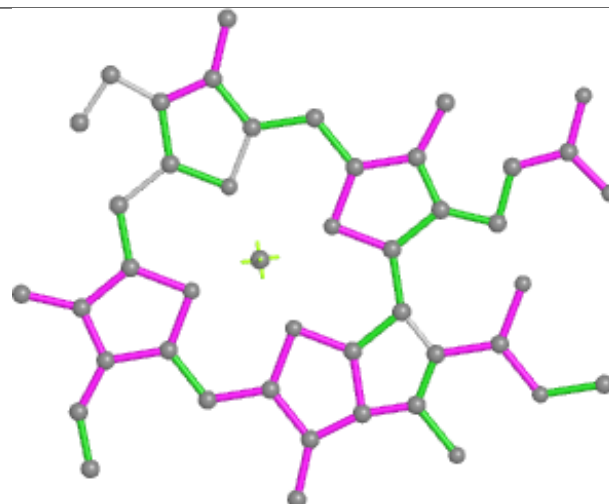
Ligand CLA a 1129



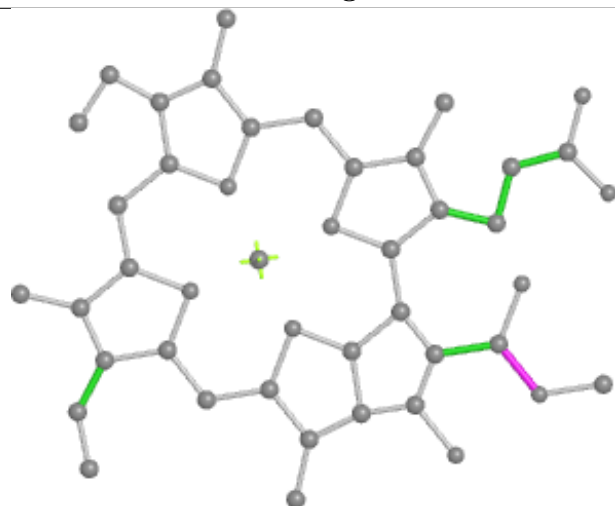
Ligand CLA H 1232



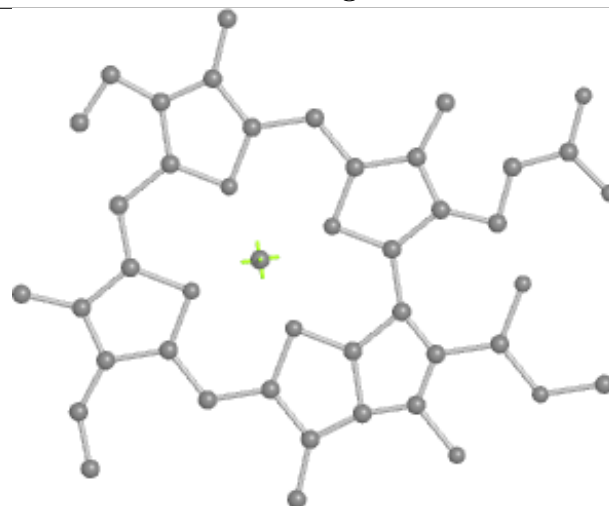
Bond lengths



Bond angles

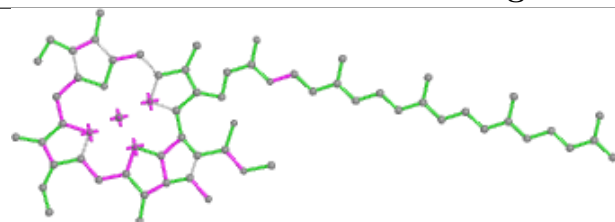


Torsions

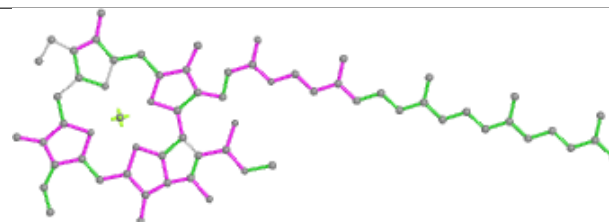


Rings

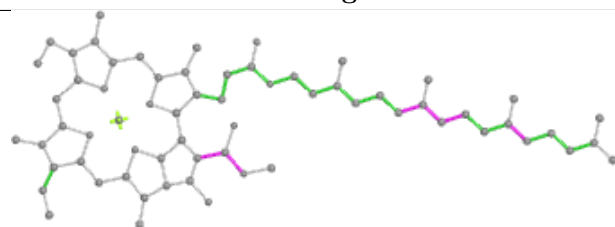
Ligand CLA B 1223



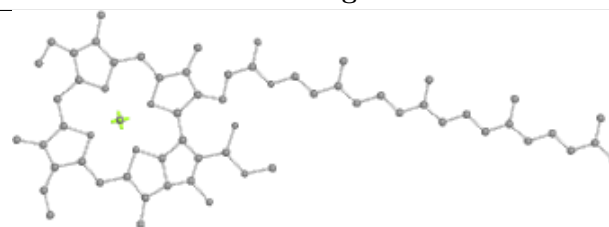
Bond lengths



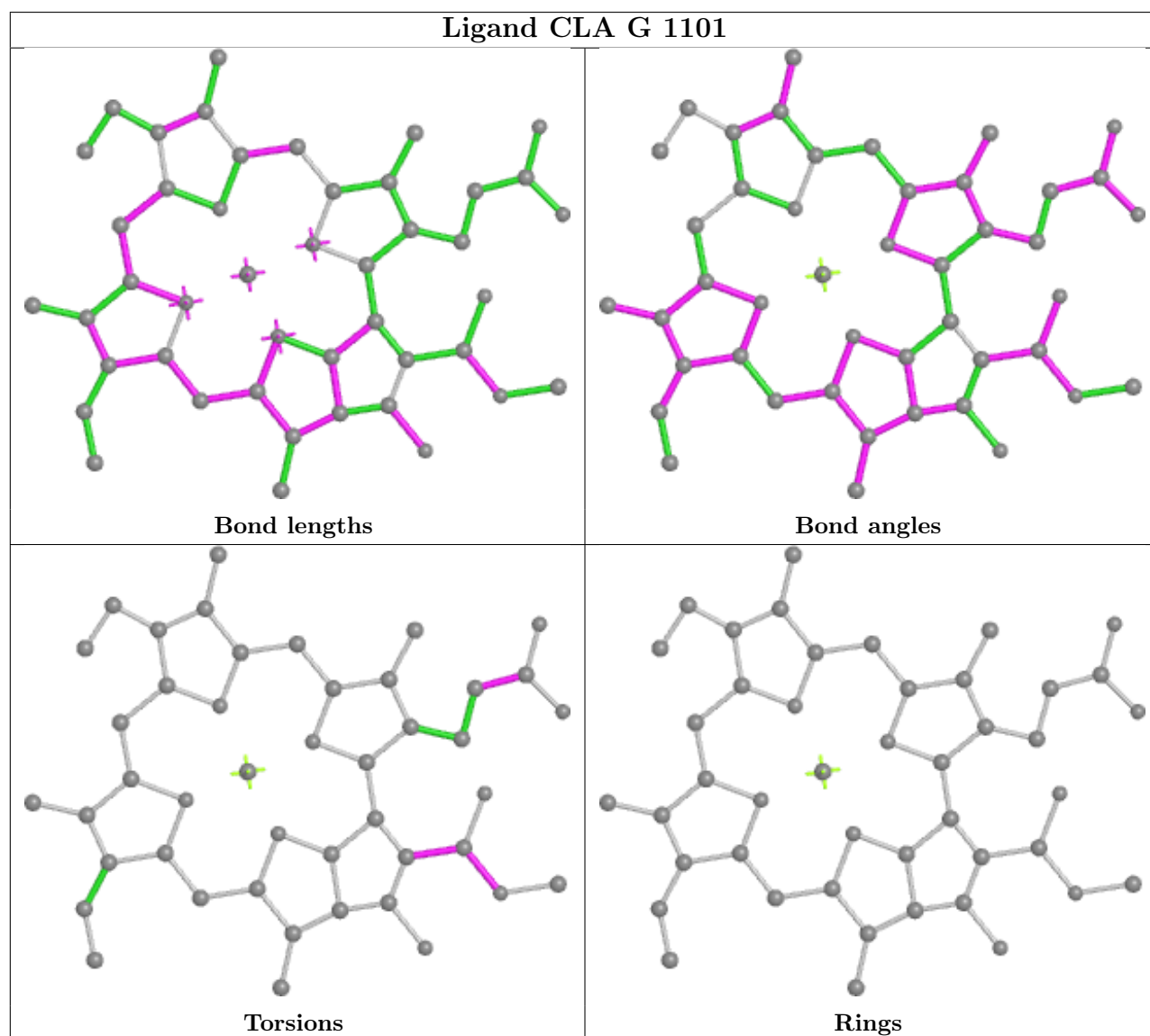
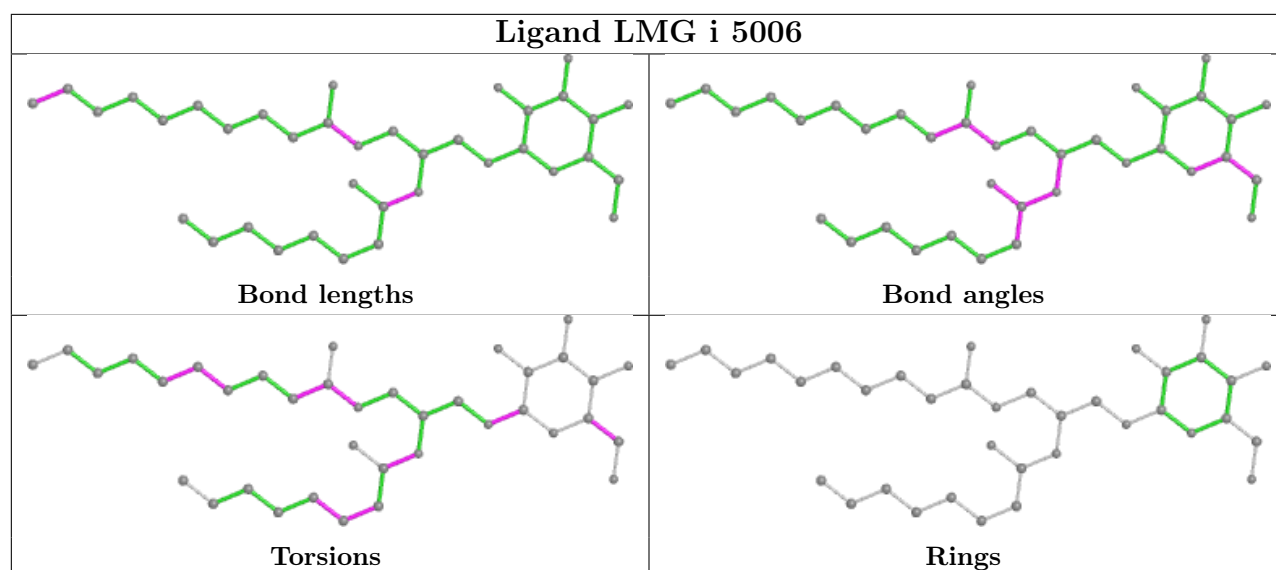
Bond angles

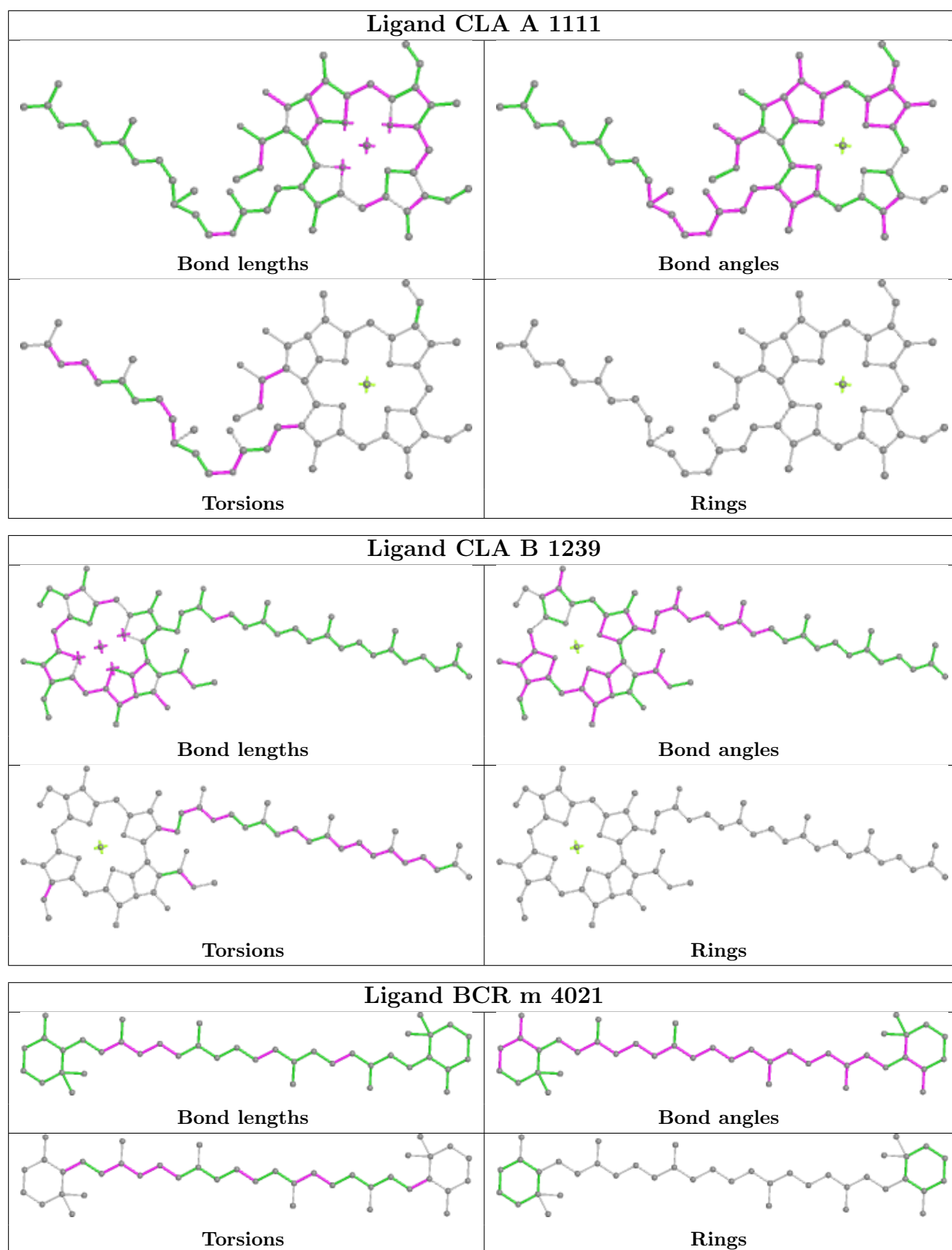


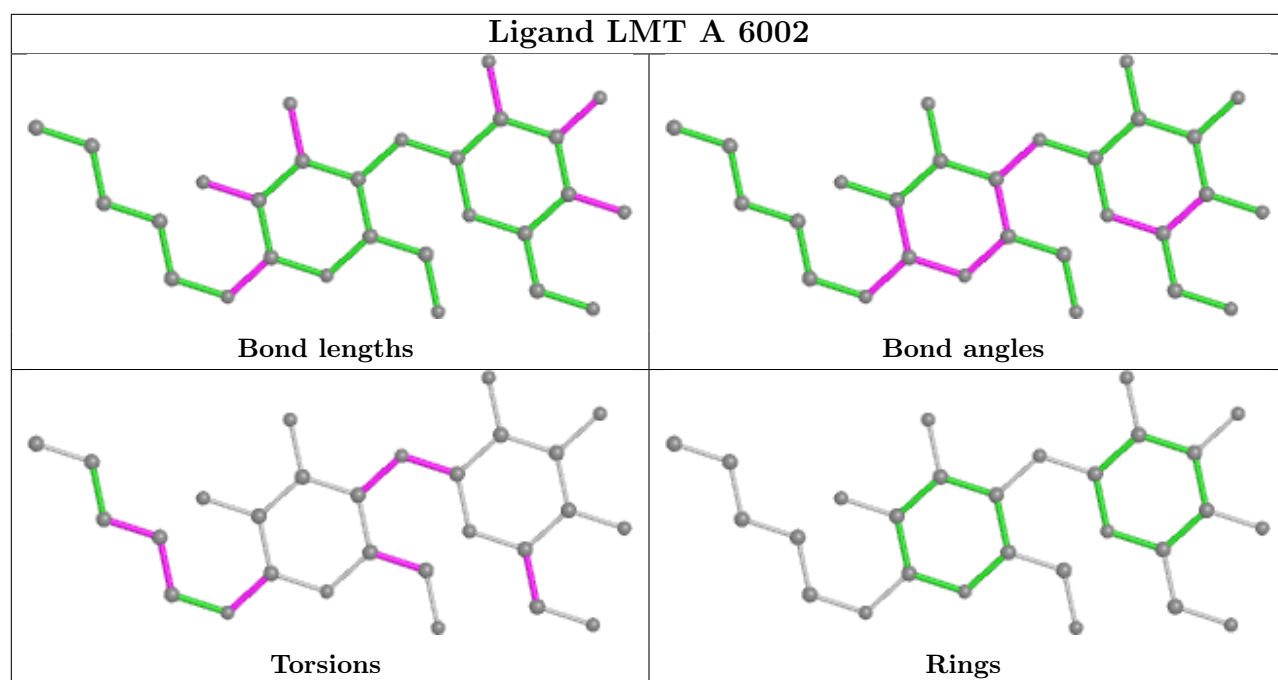
Torsions

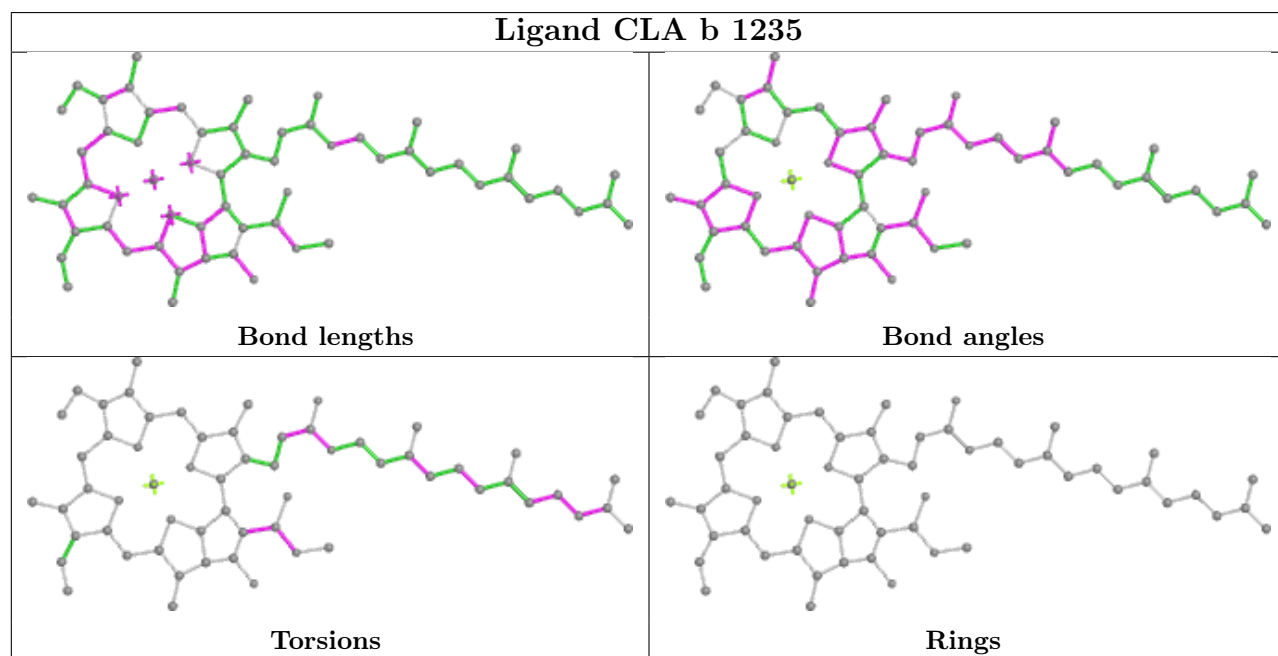
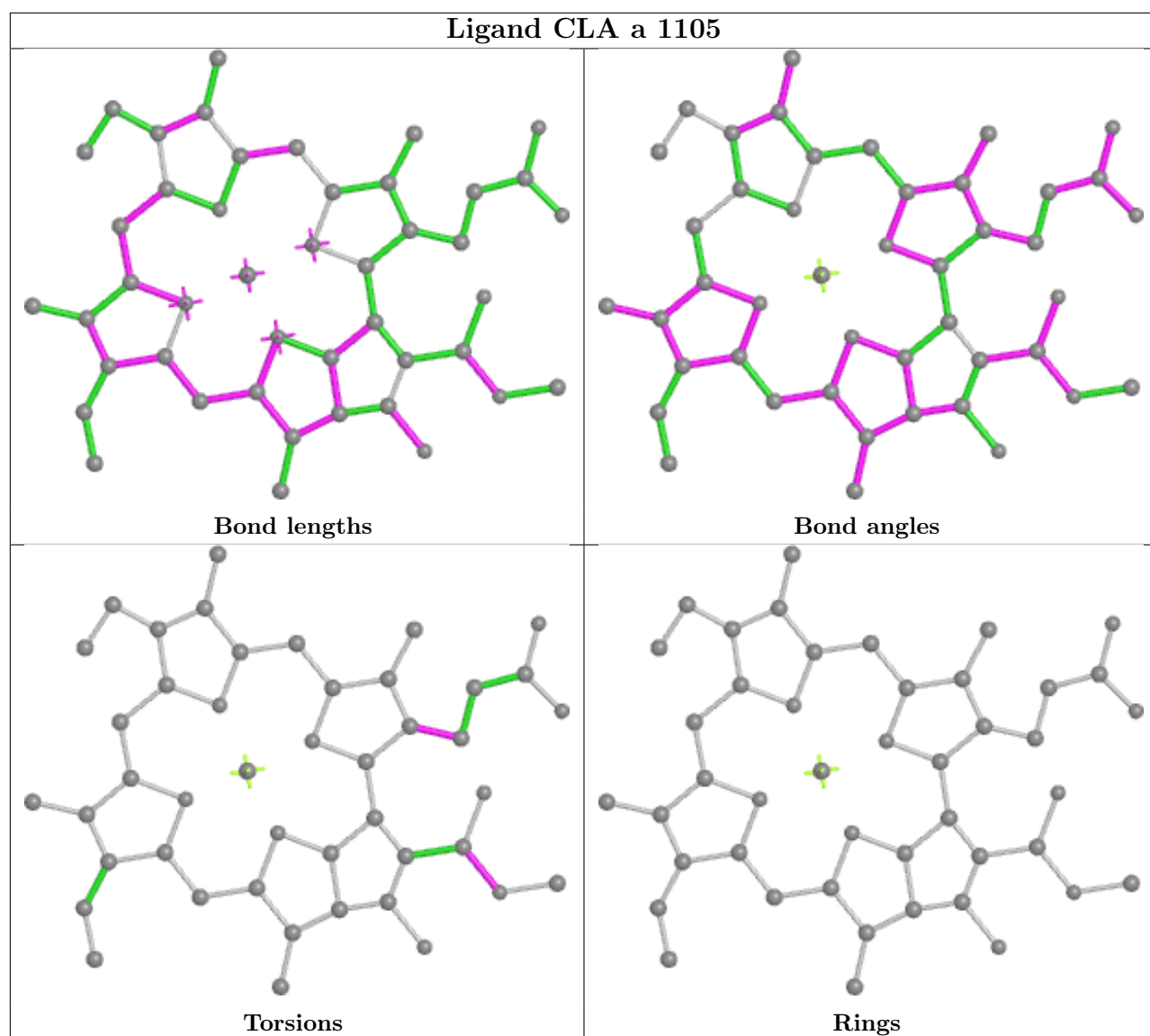


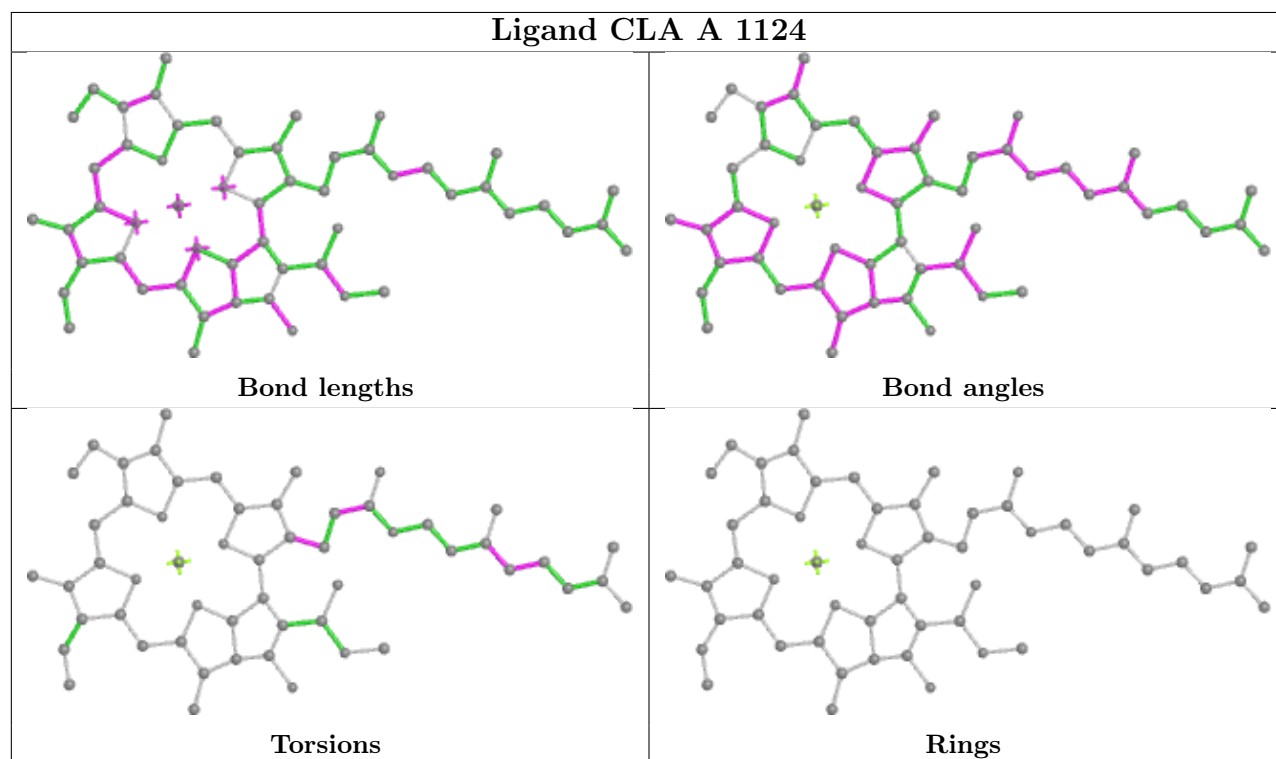
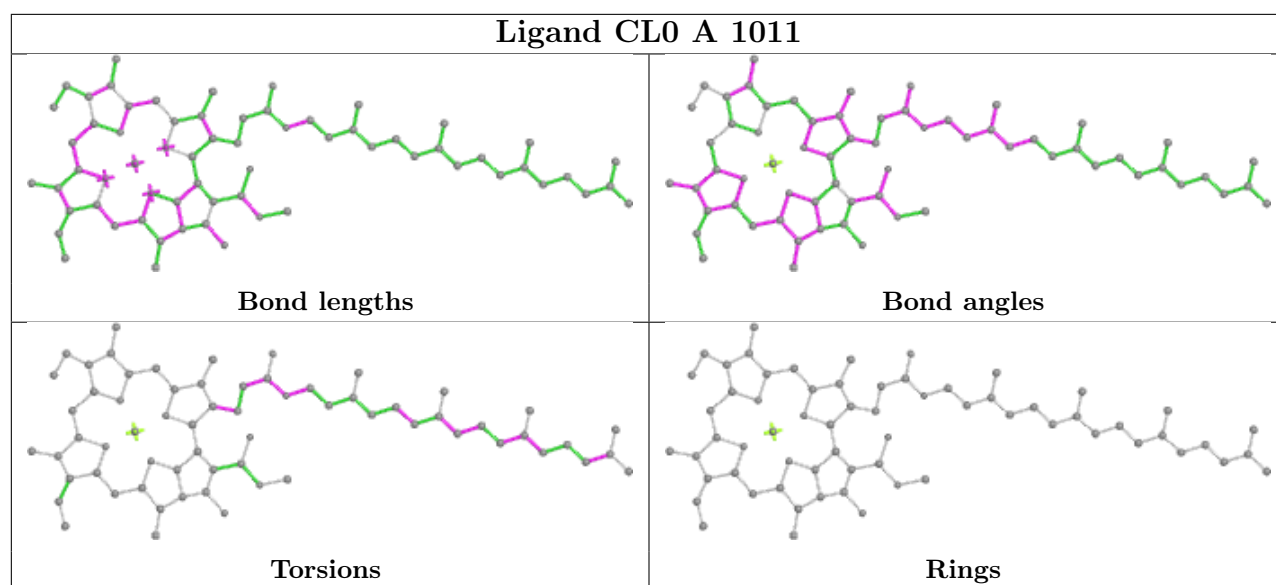
Rings

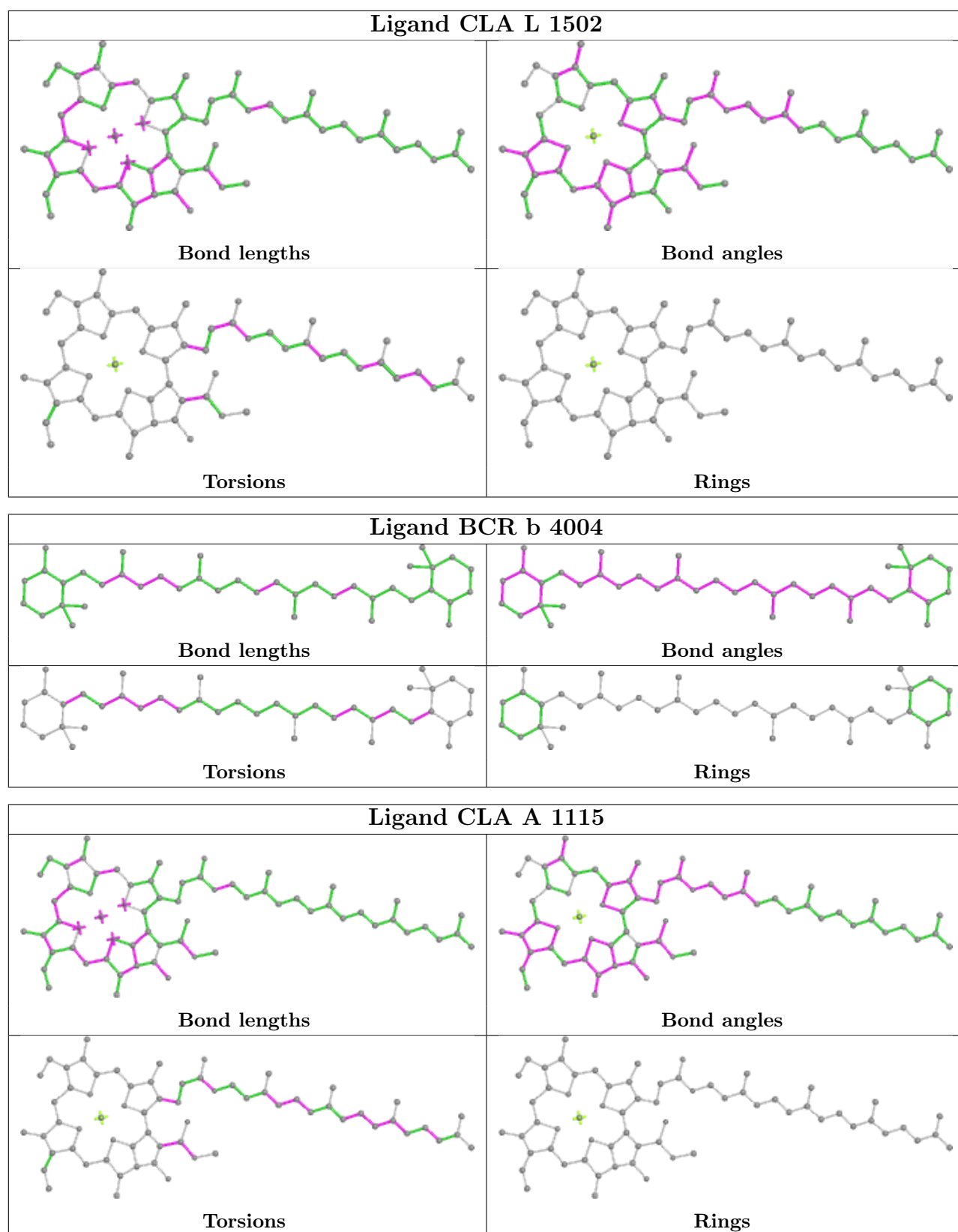


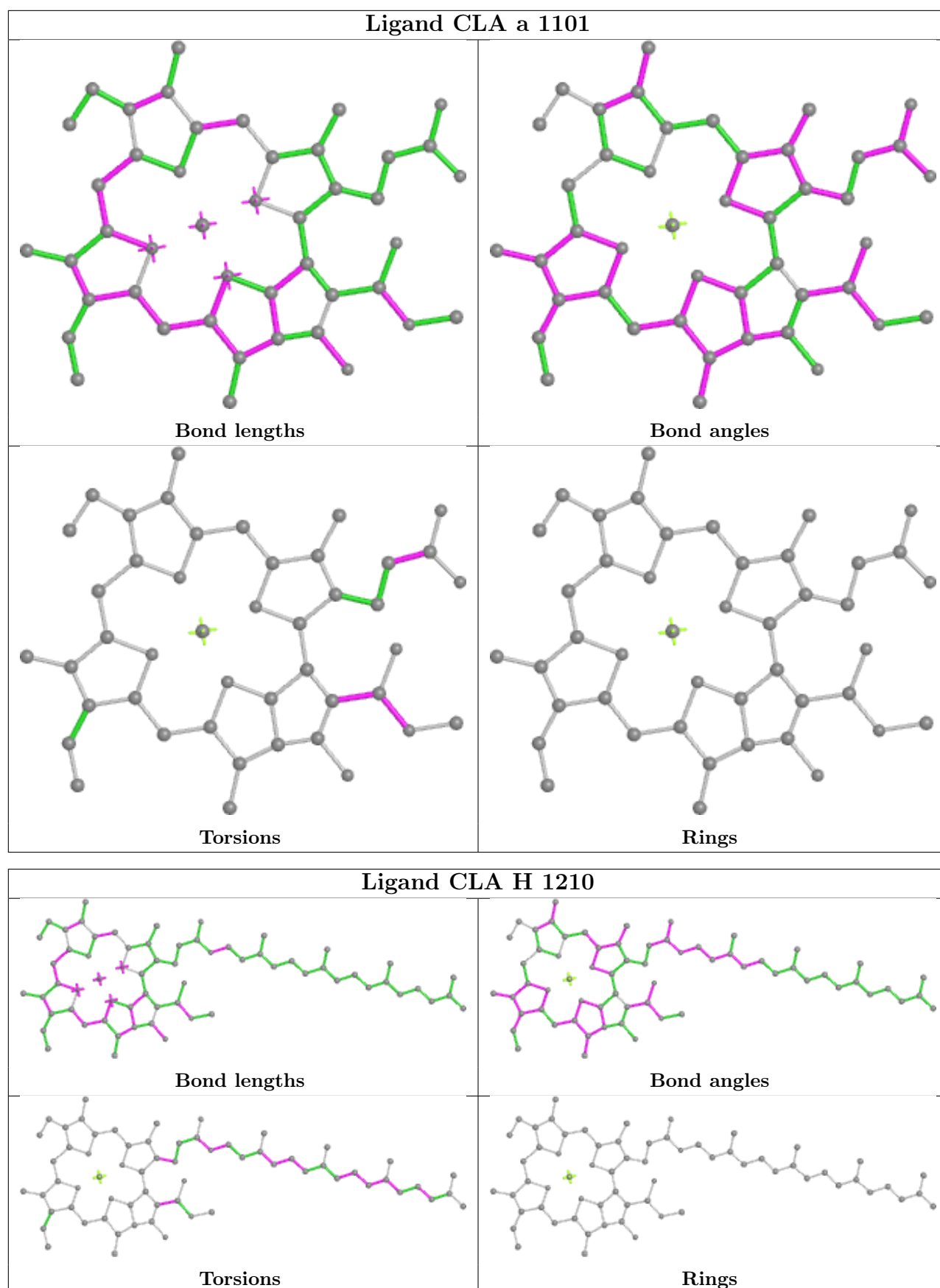


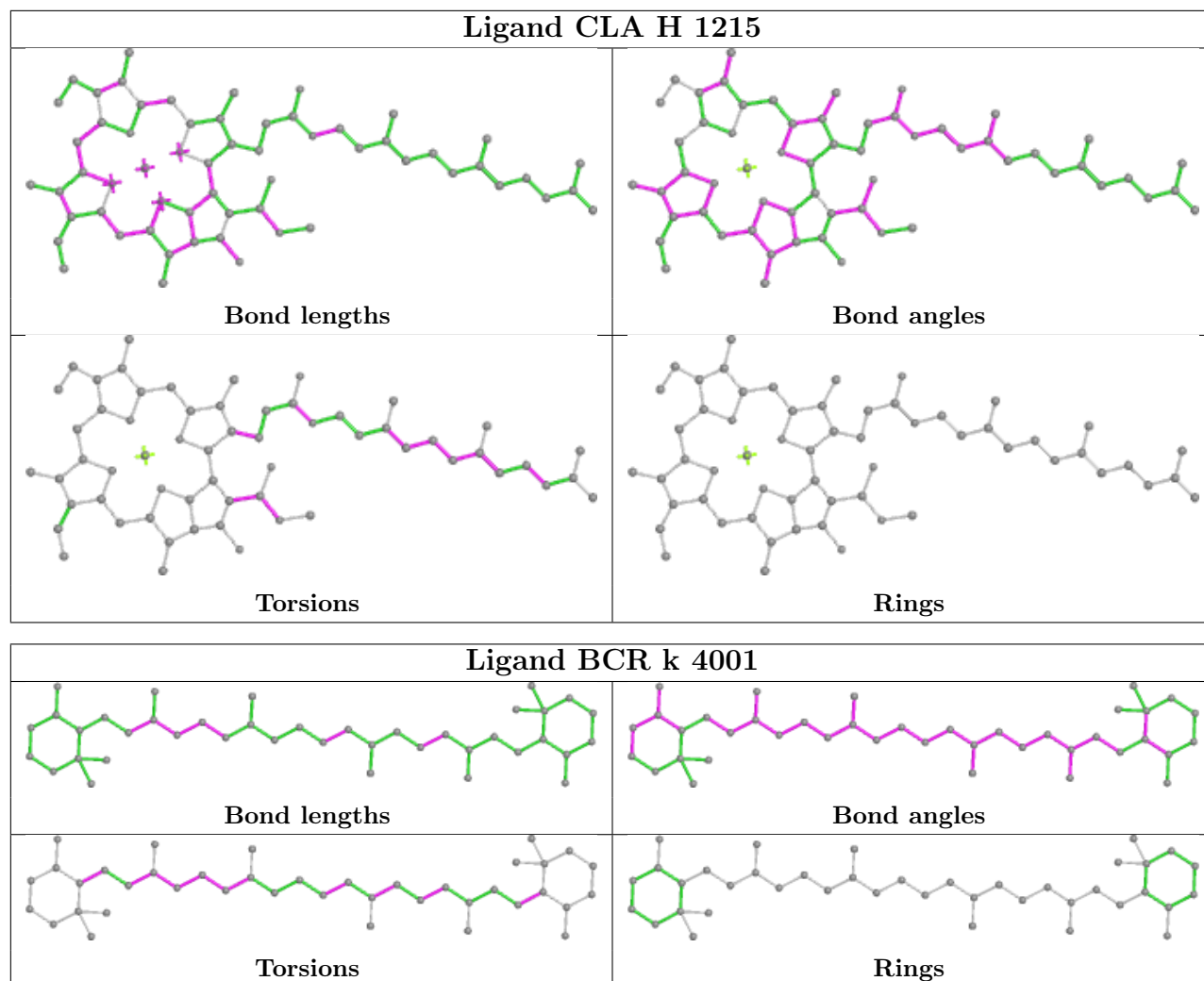


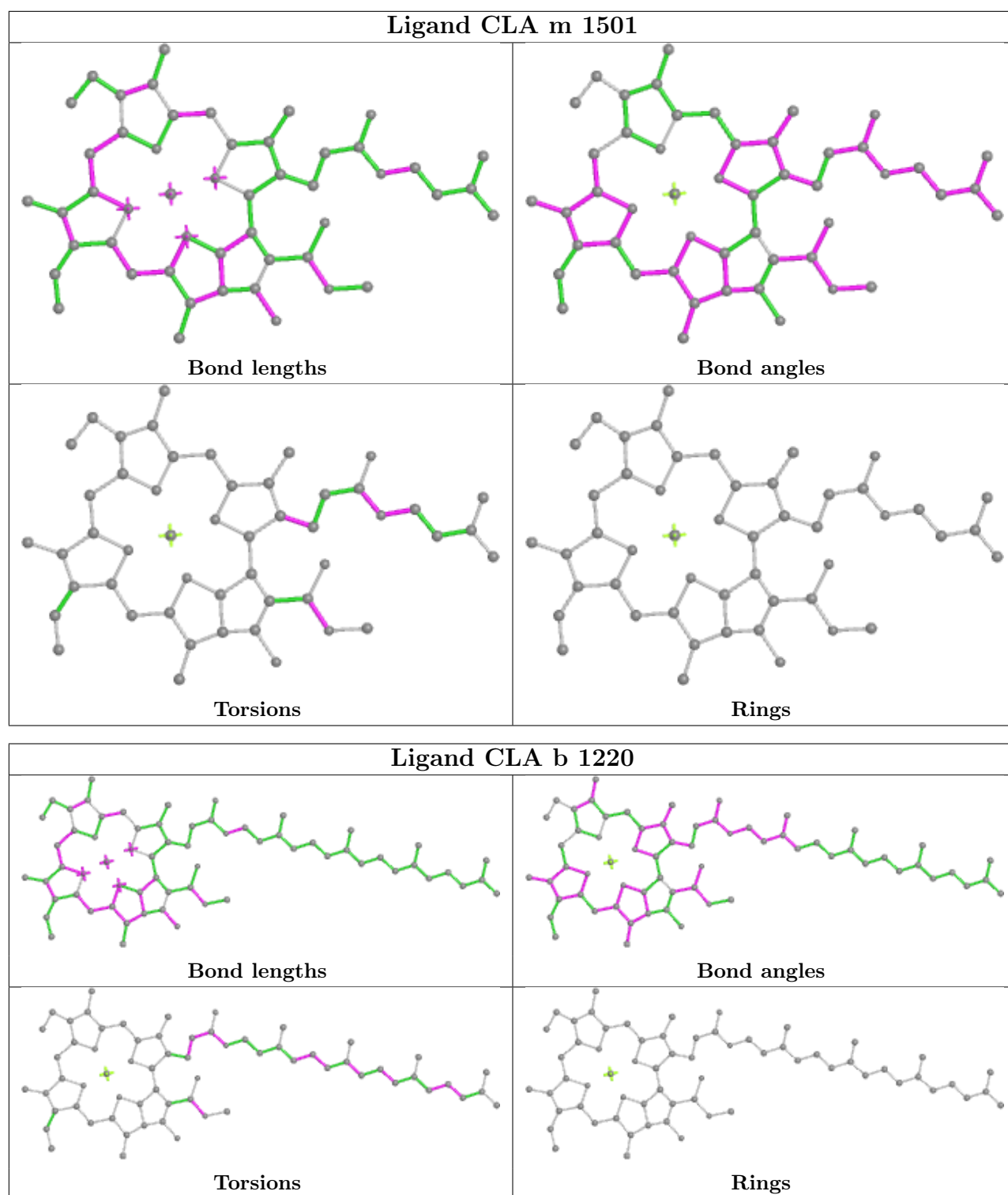




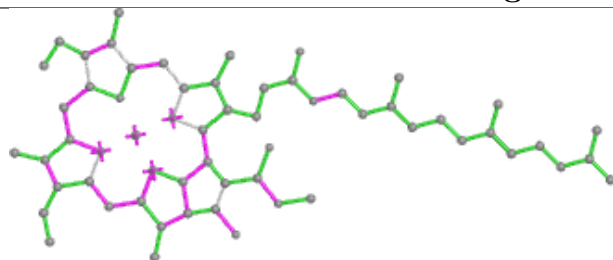




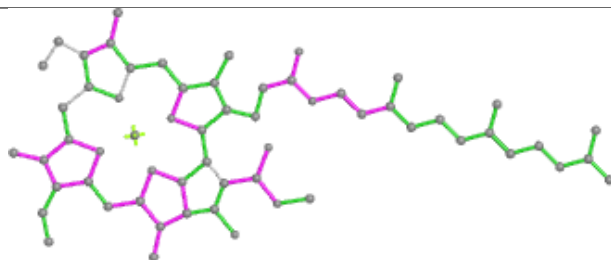




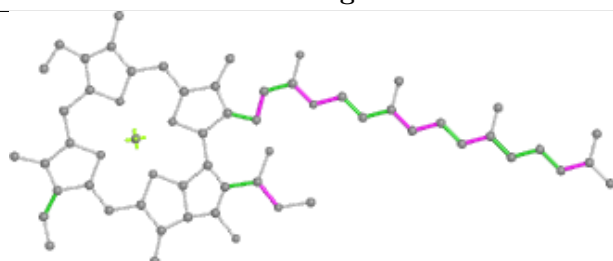
Ligand CLA G 1131



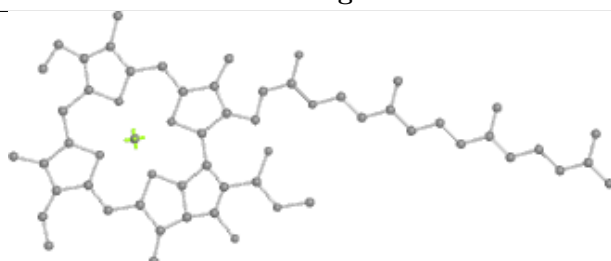
Bond lengths



Bond angles

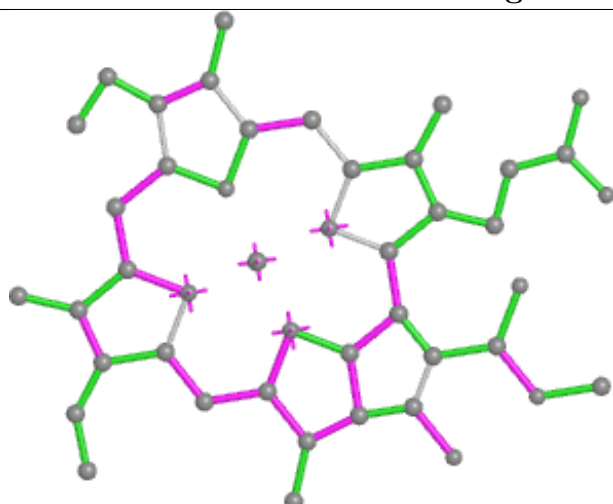


Torsions

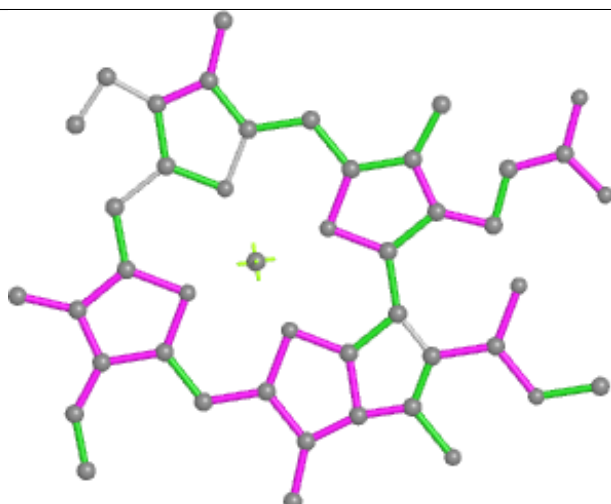


Rings

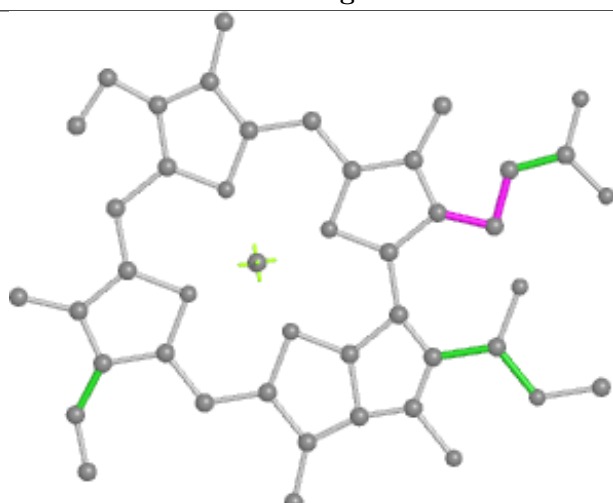
Ligand CLA B 1213



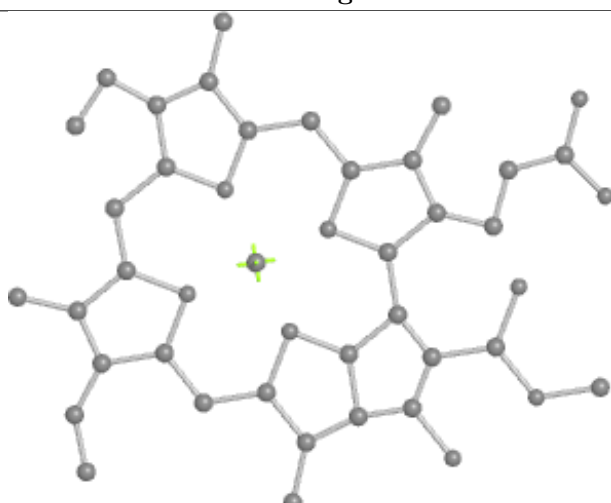
Bond lengths



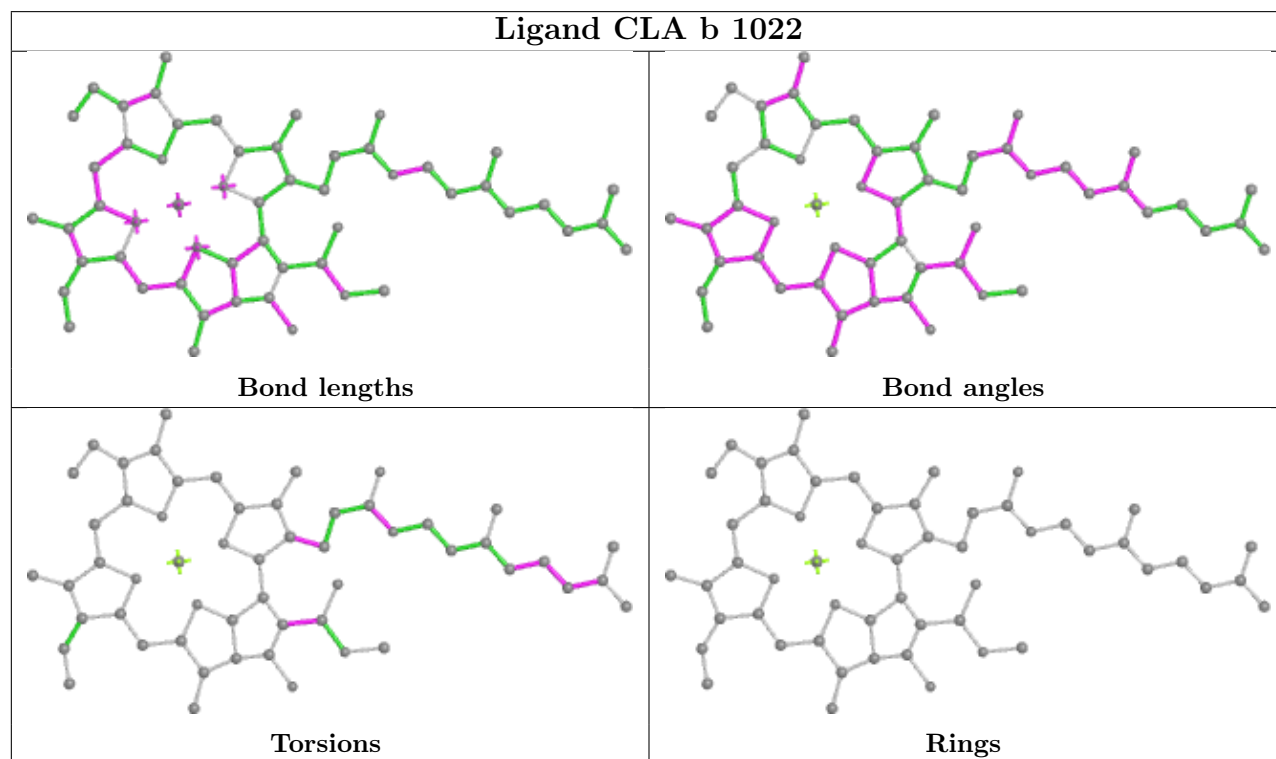
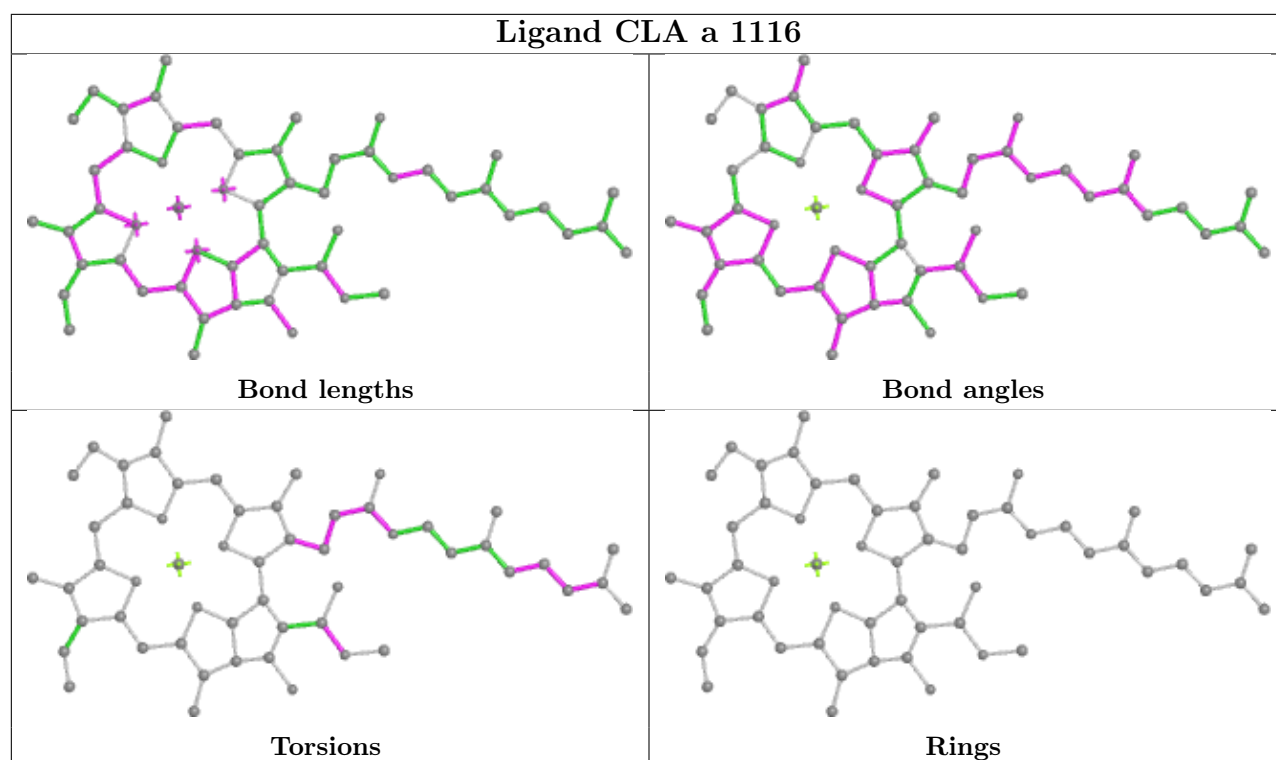
Bond angles

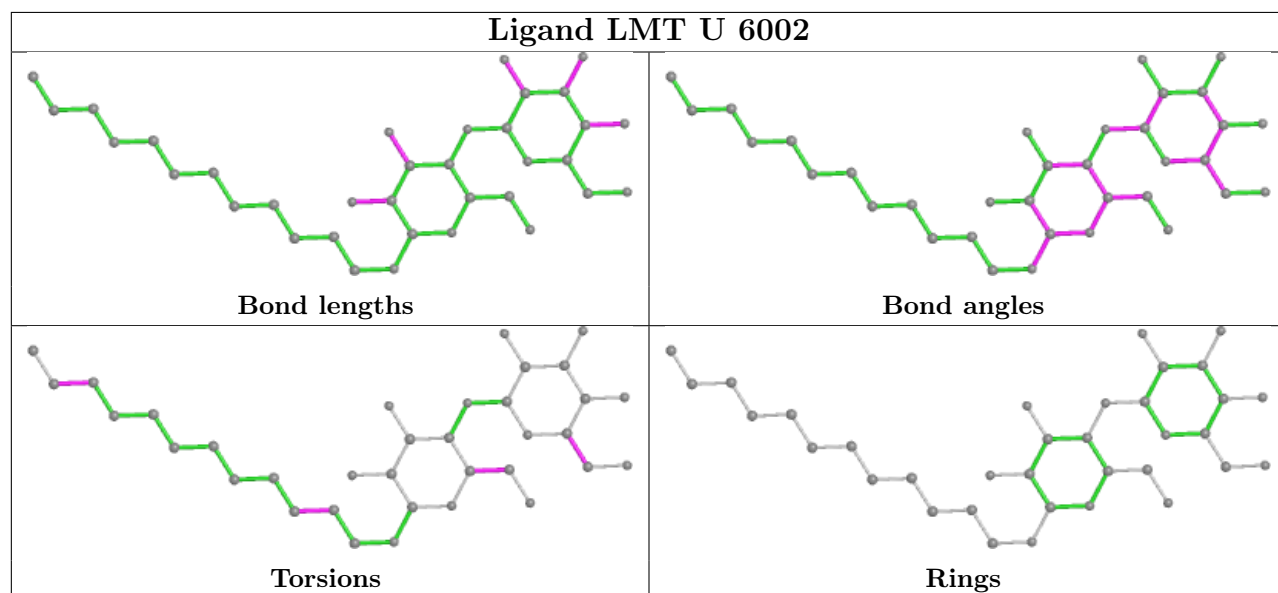
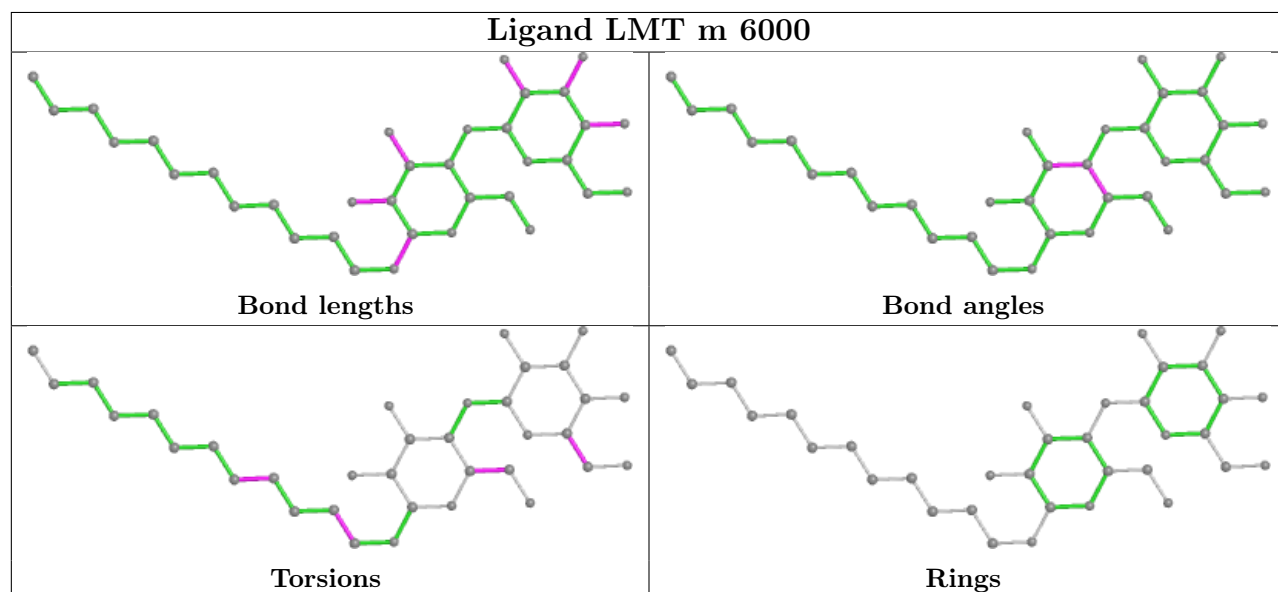
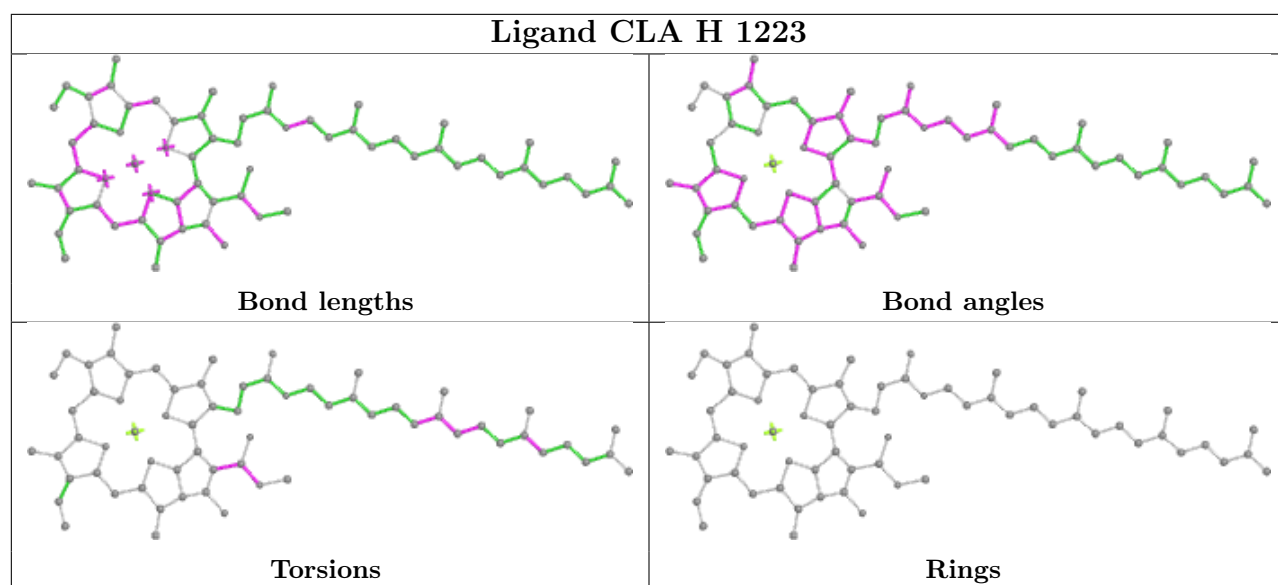


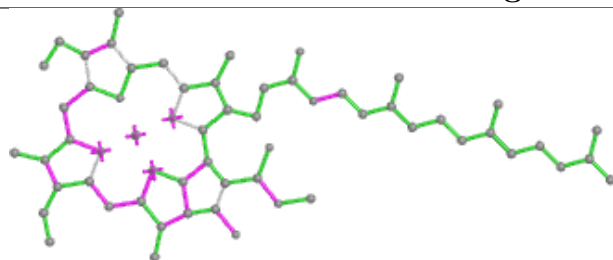
Torsions



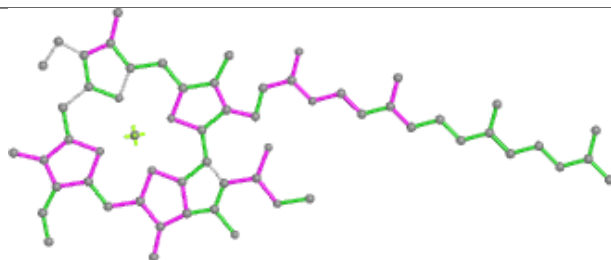
Rings



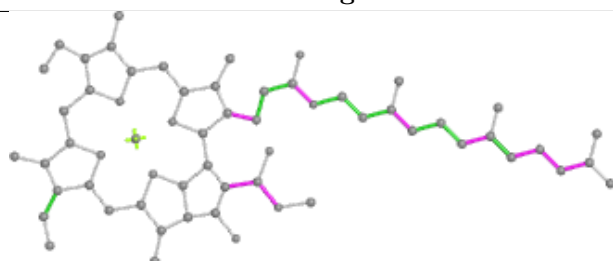


Ligand CLA G 1126

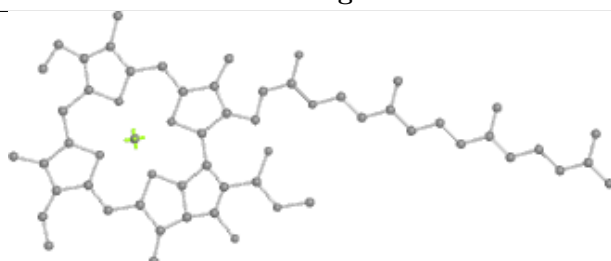
Bond lengths



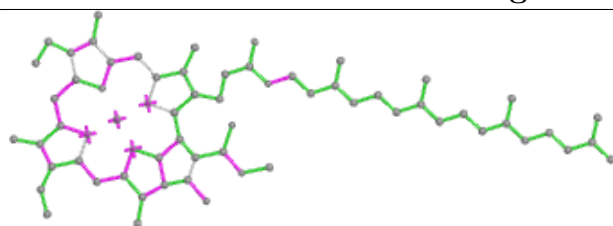
Bond angles



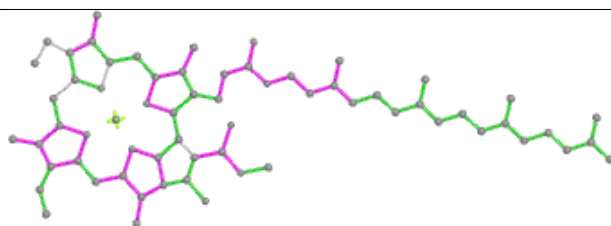
Torsions



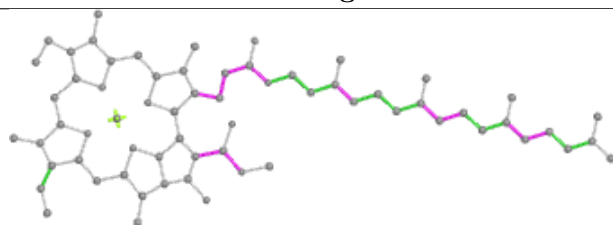
Rings

Ligand CLA a 1127

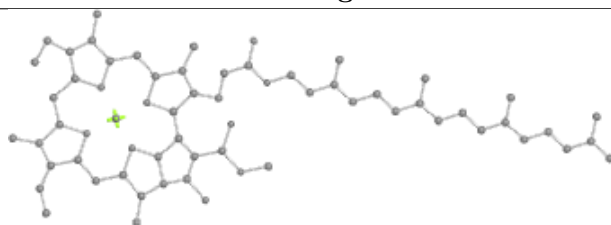
Bond lengths



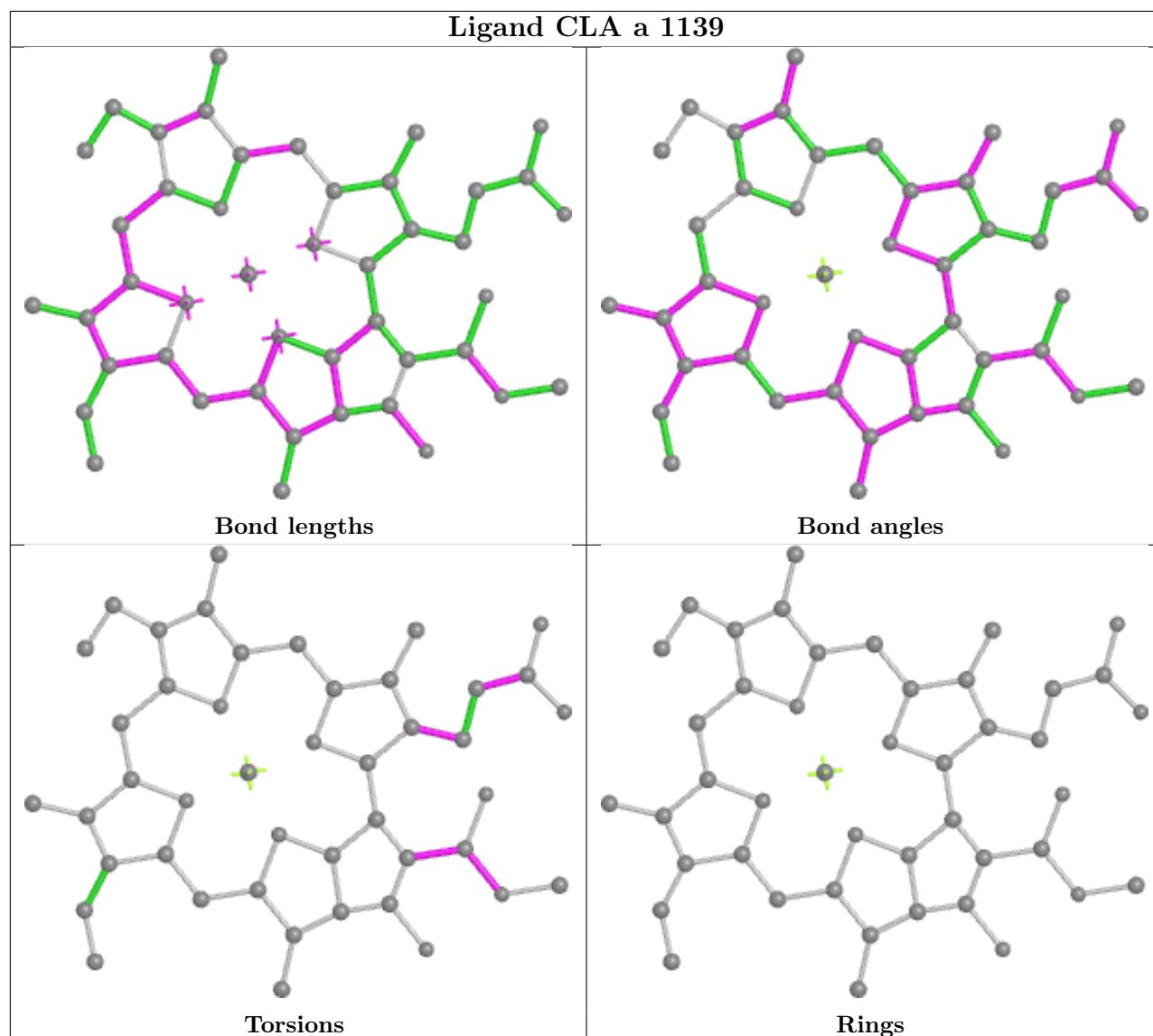
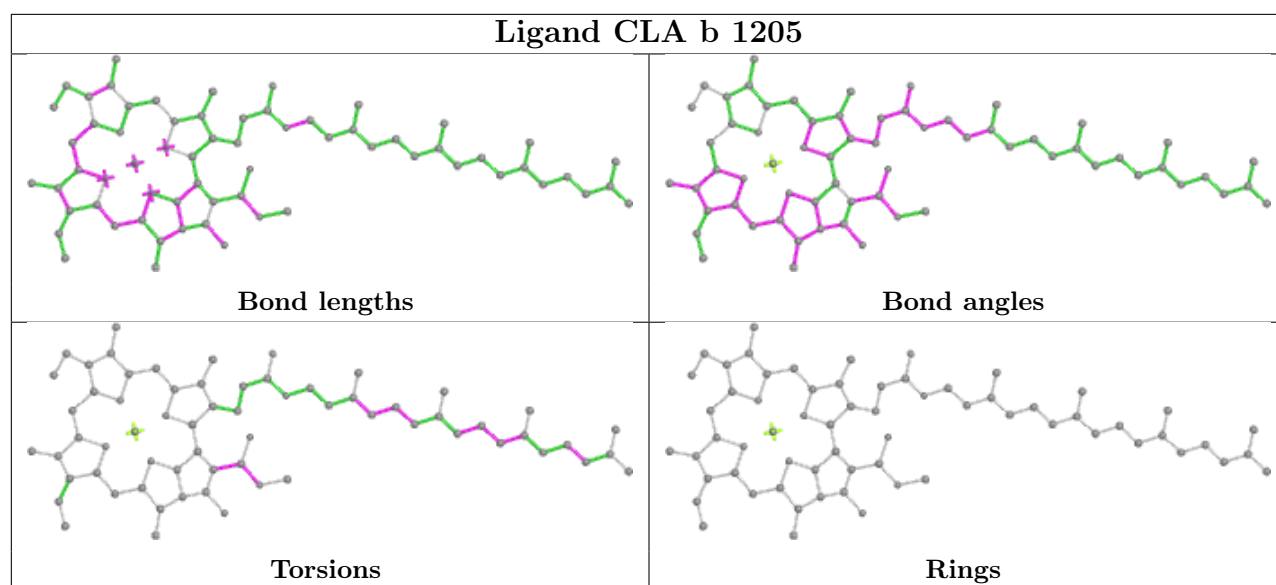
Bond angles

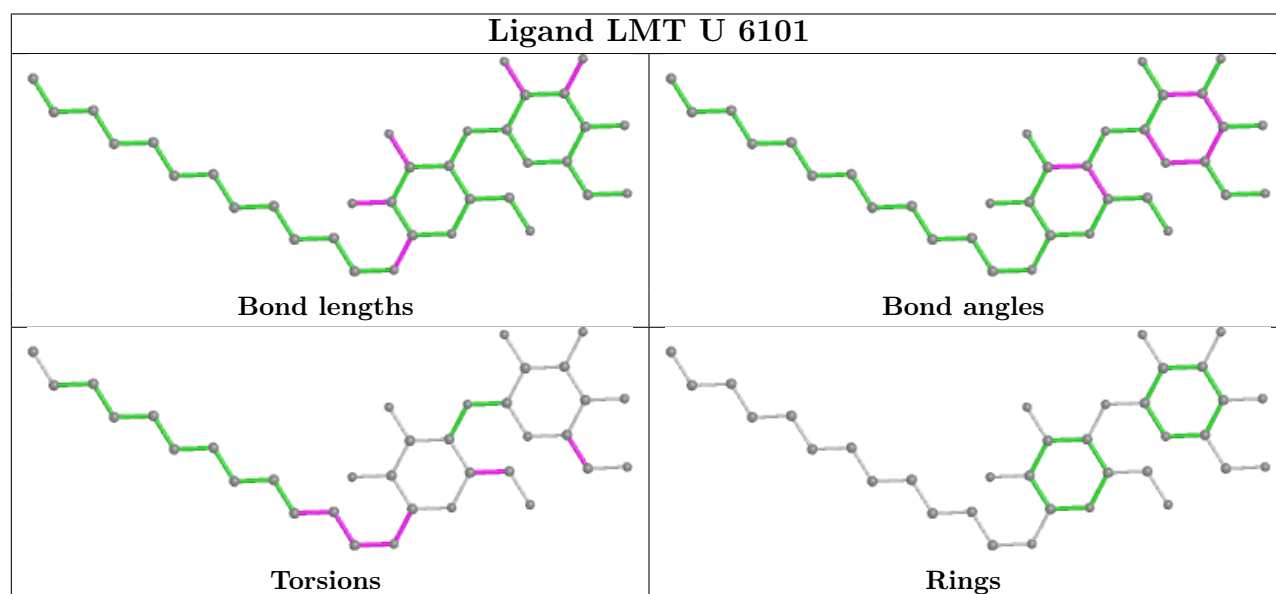
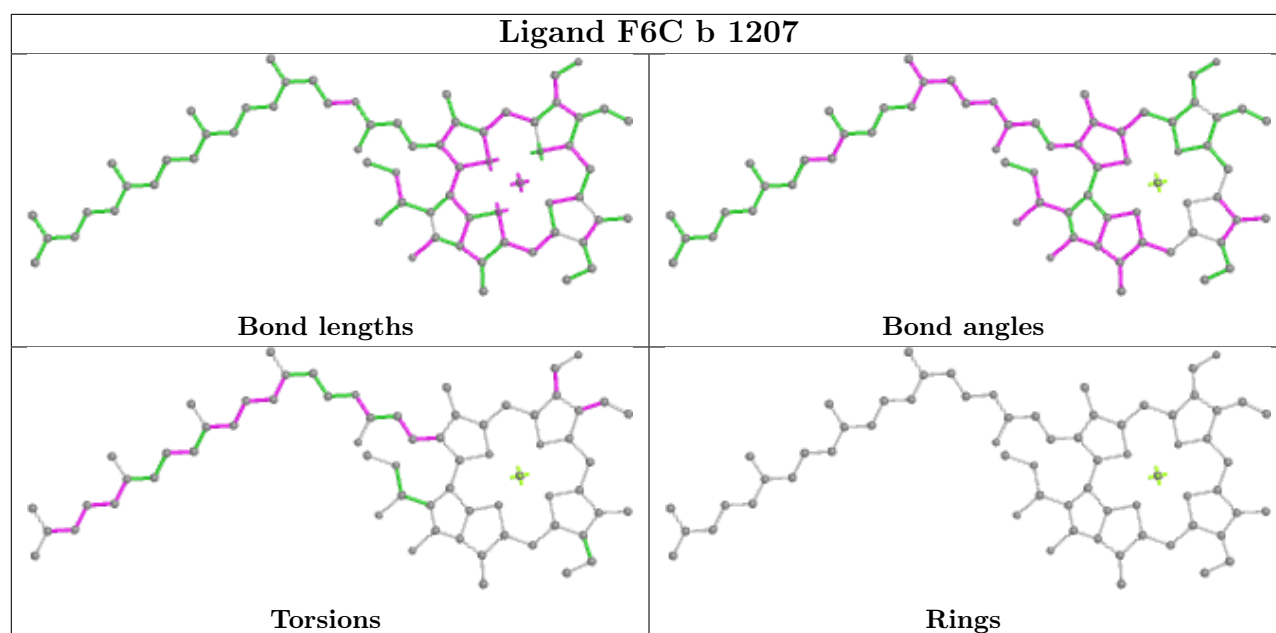


Torsions

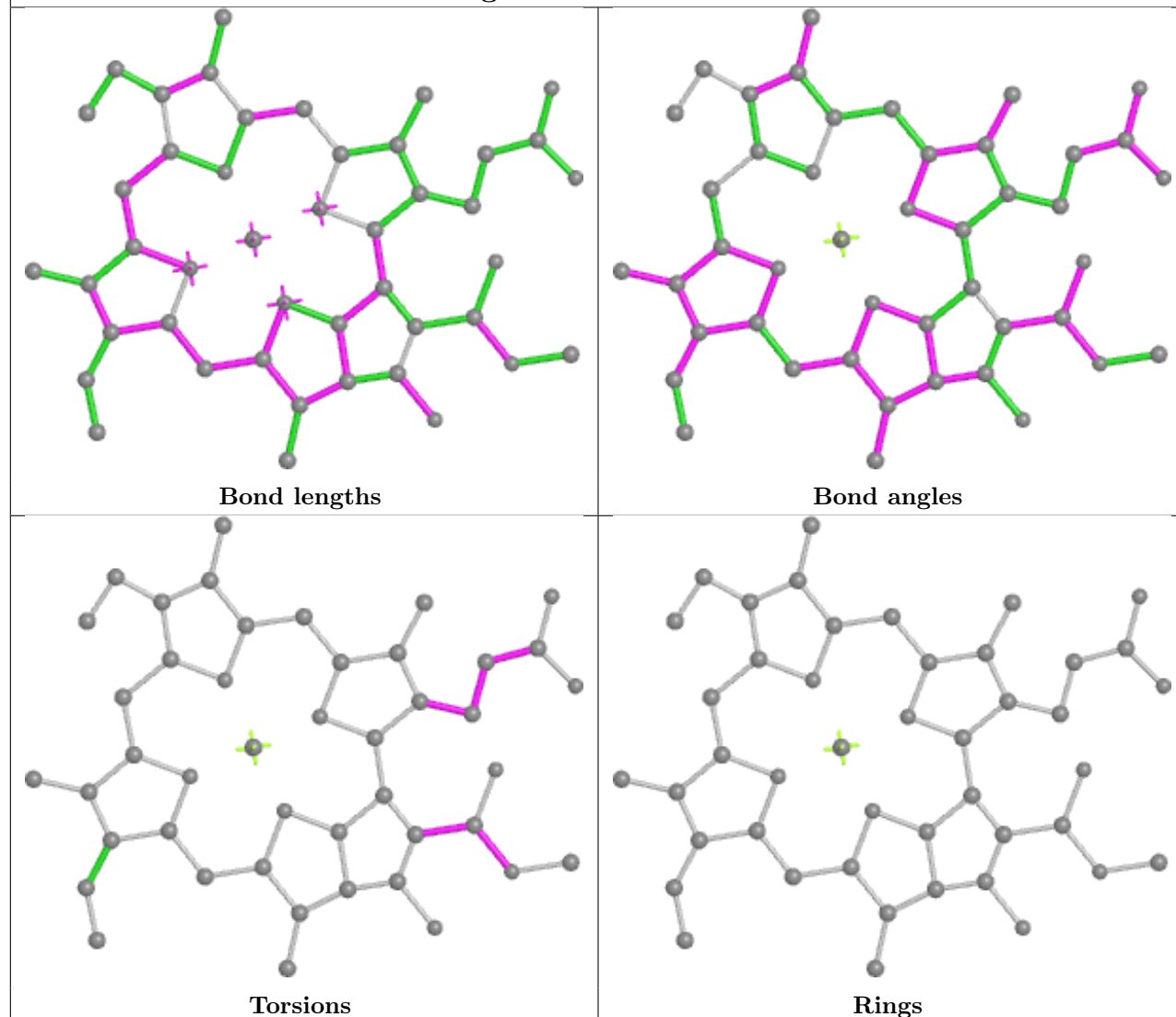


Rings

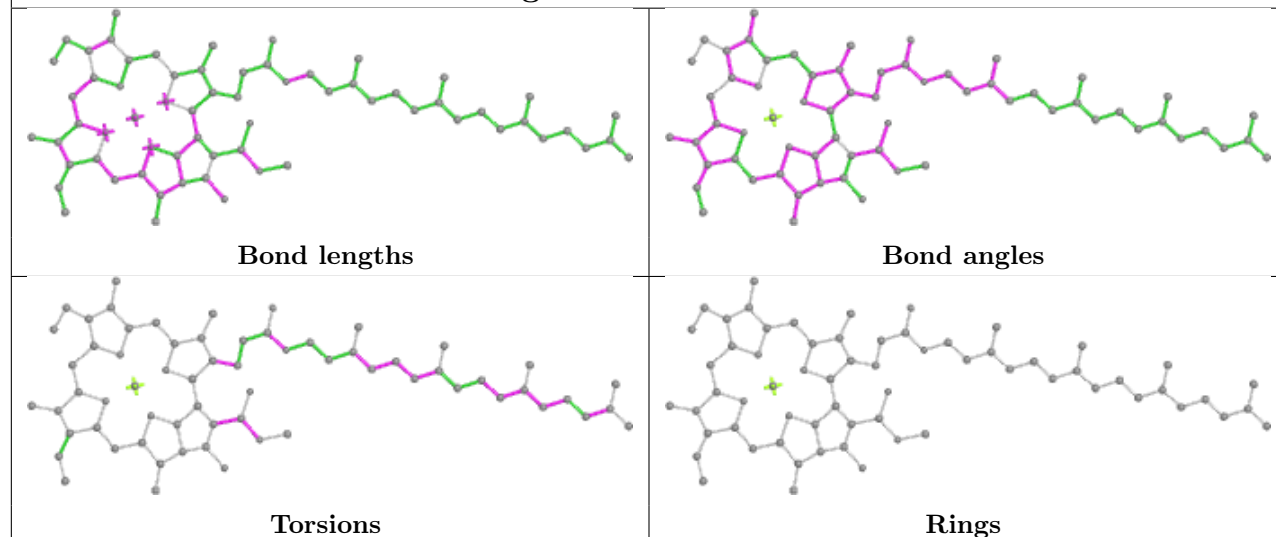


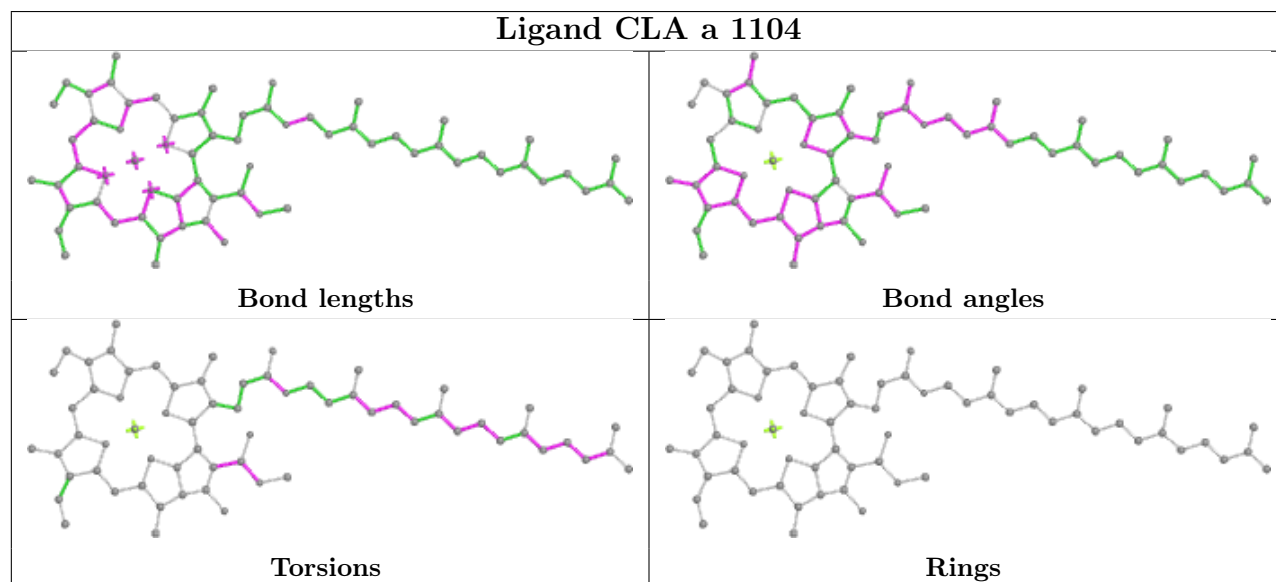
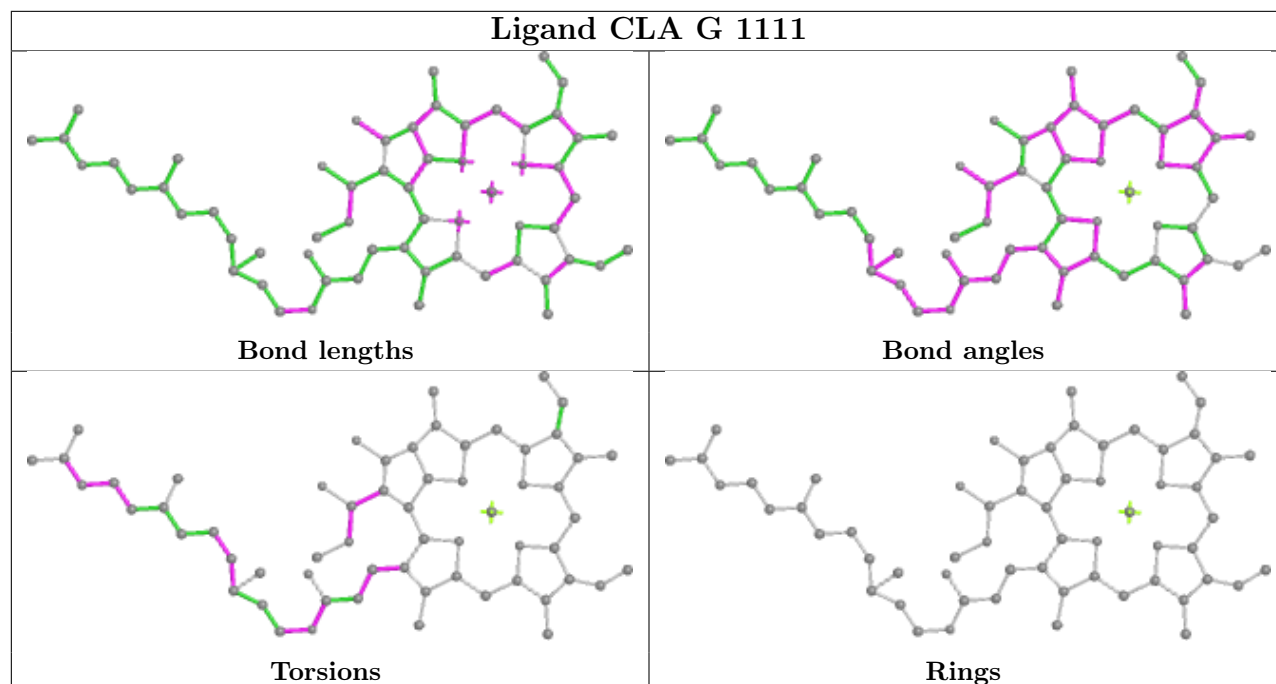
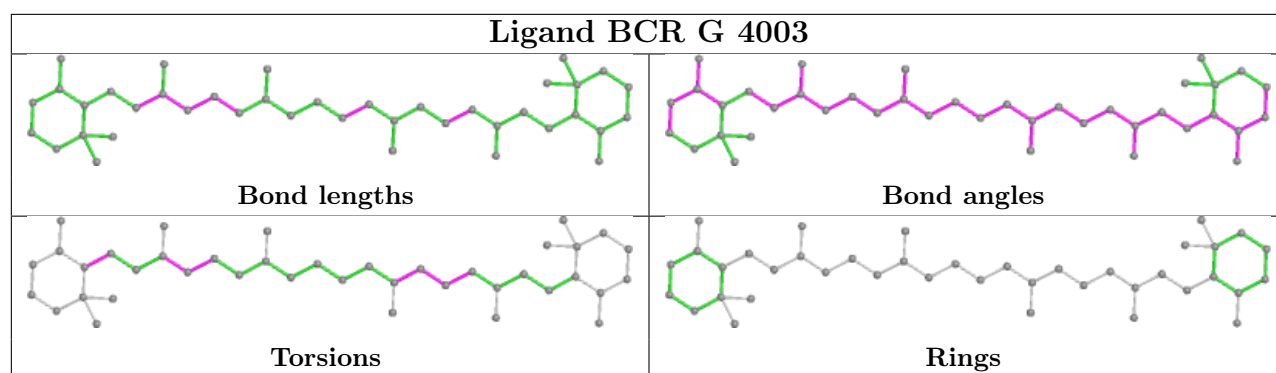


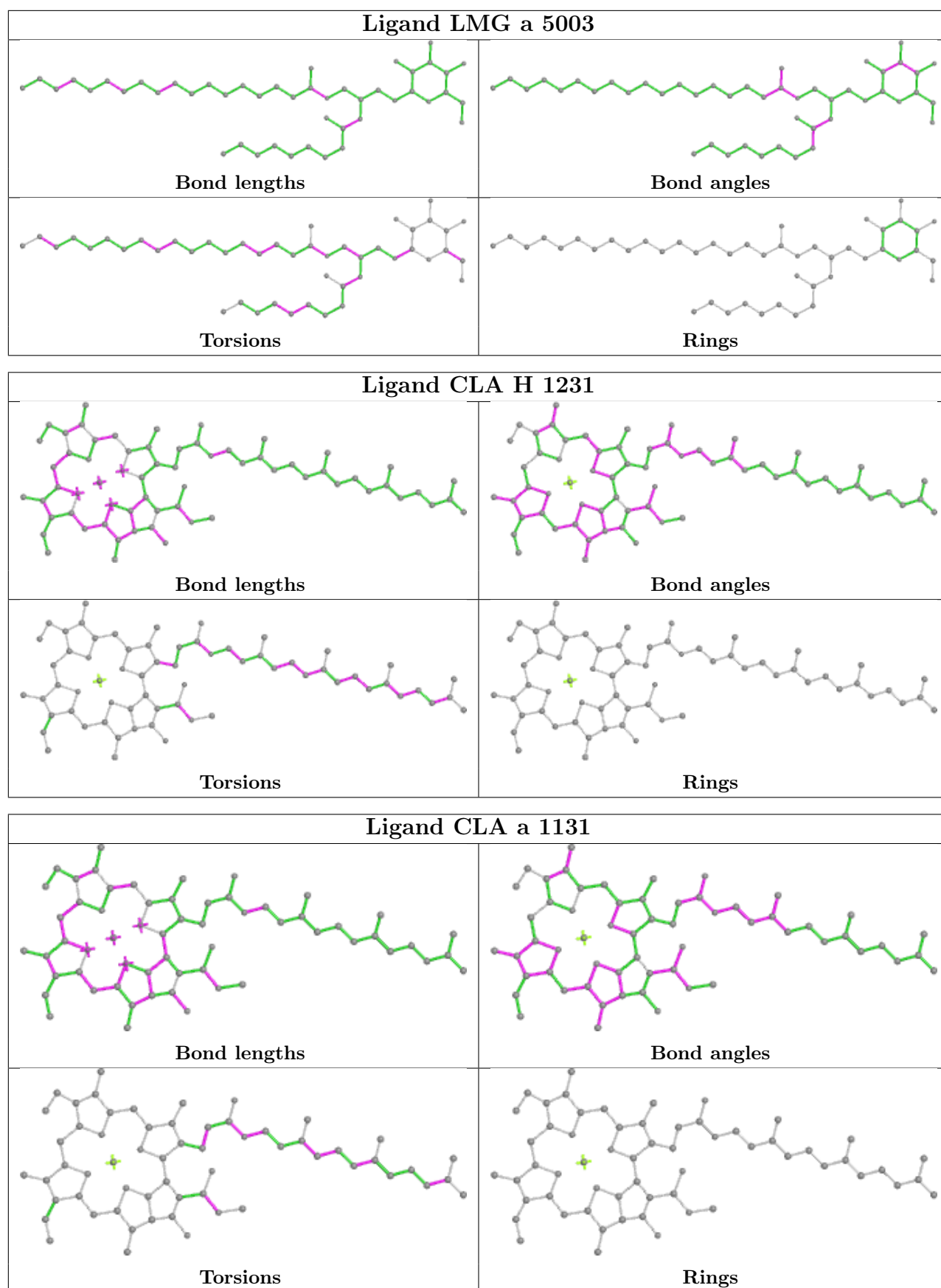
Ligand CLA G 1141



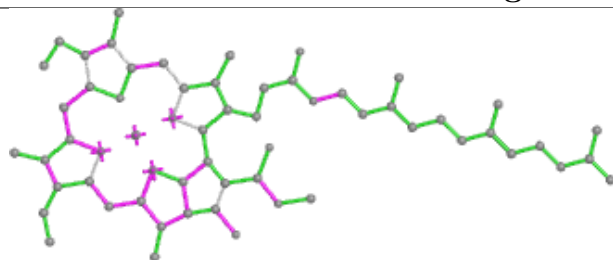
Ligand CLA G 1117



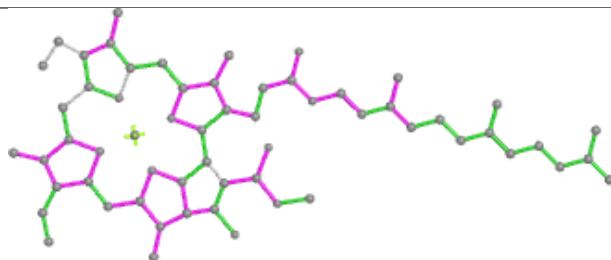




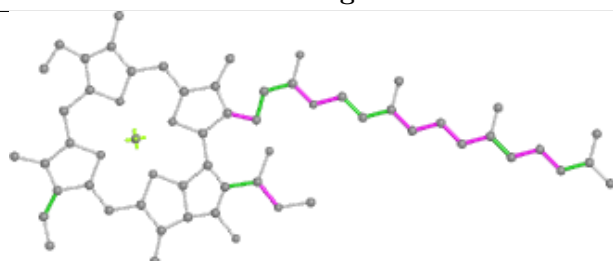
Ligand CLA H 1229



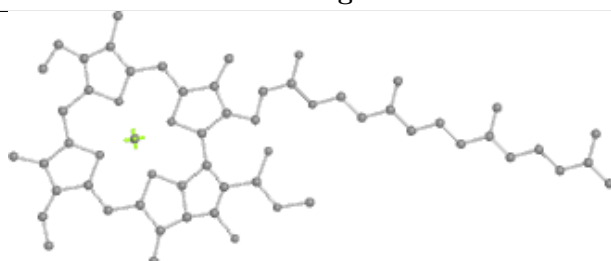
Bond lengths



Bond angles

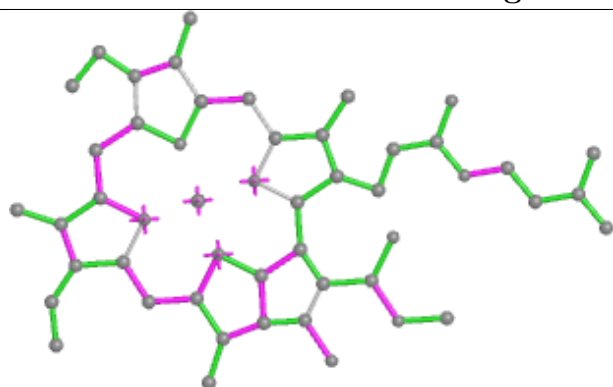


Torsions

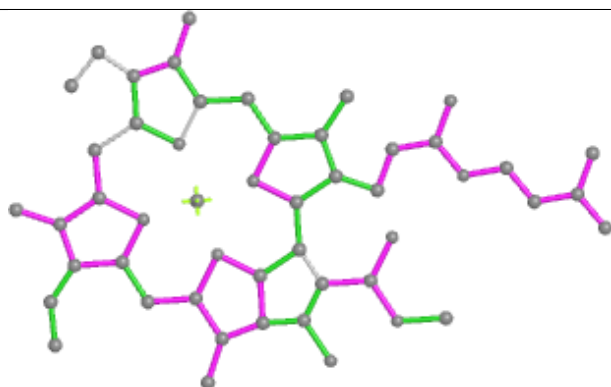


Rings

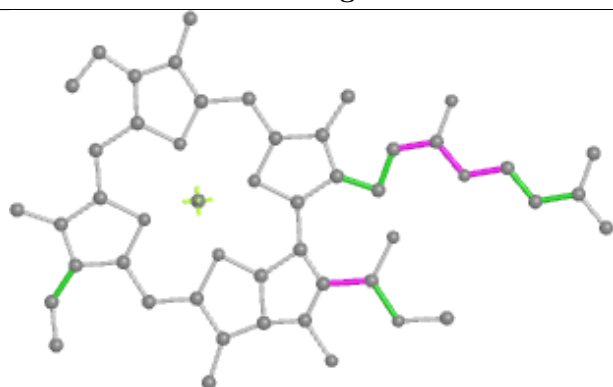
Ligand CLA G 1137



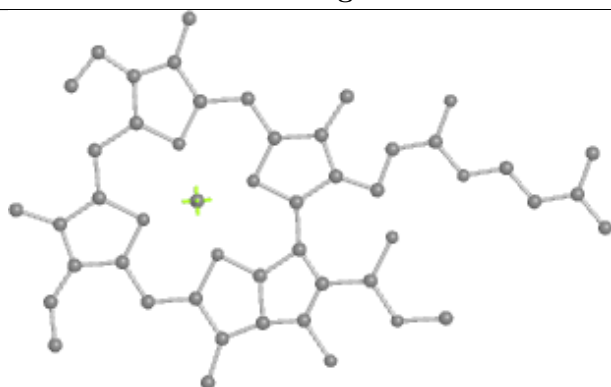
Bond lengths



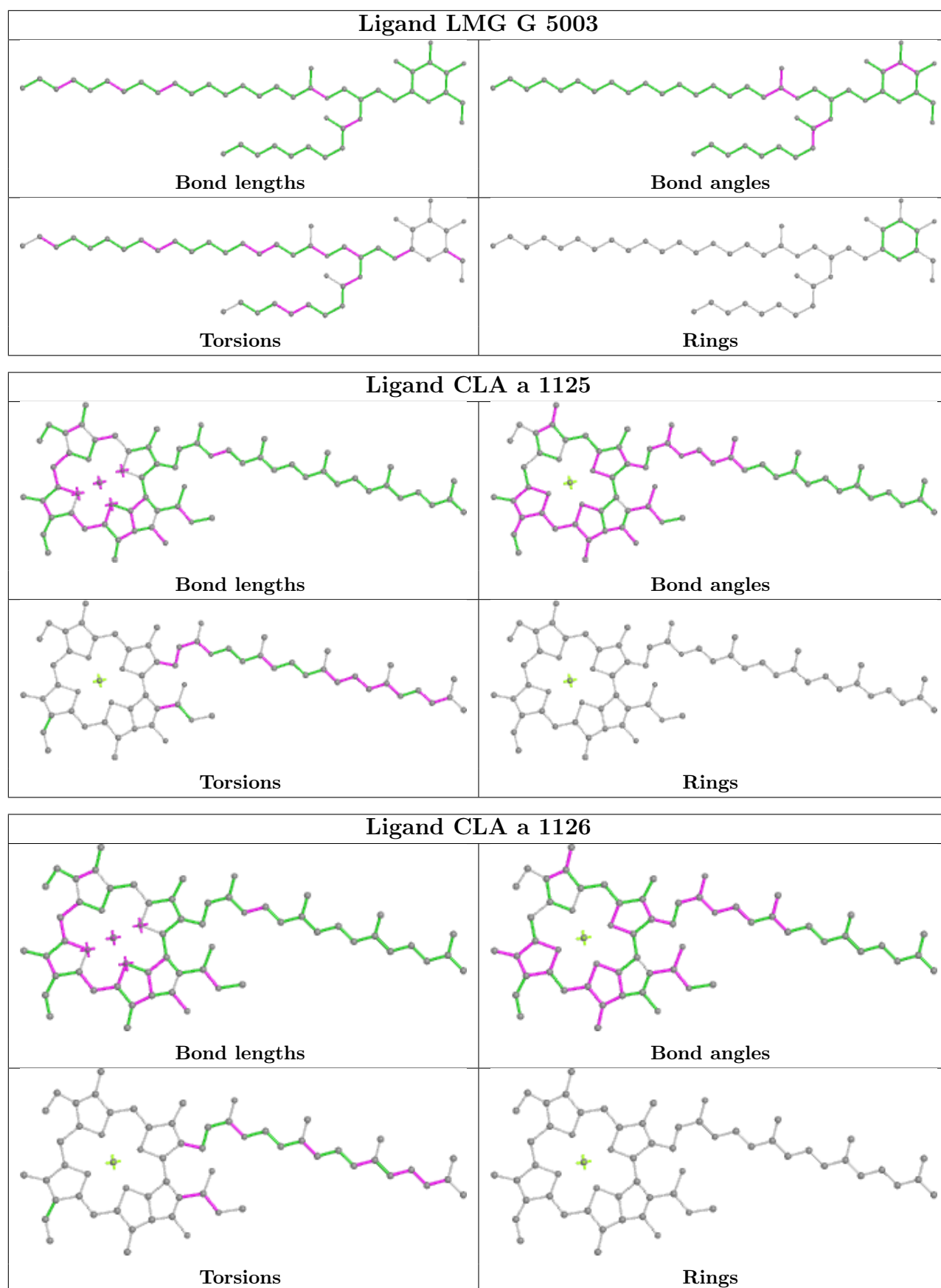
Bond angles

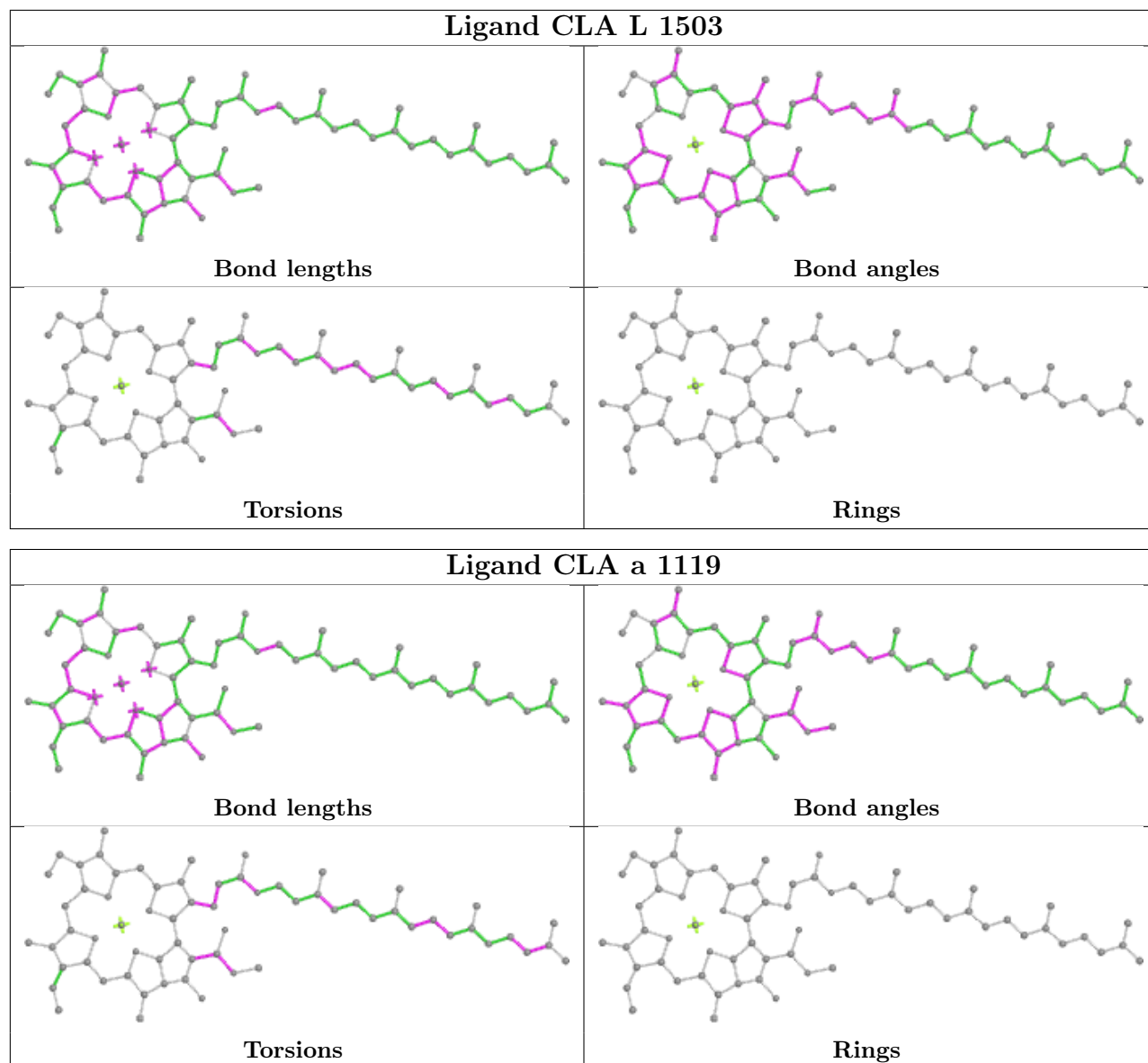


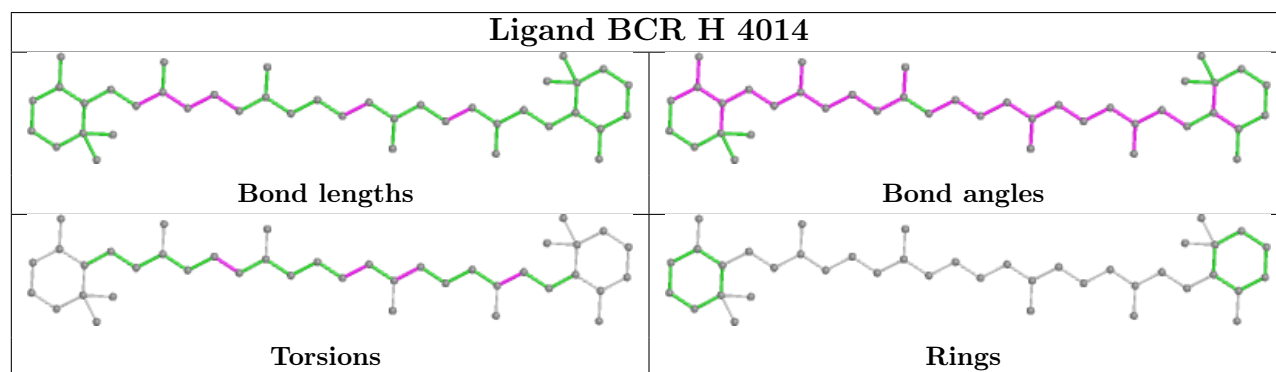
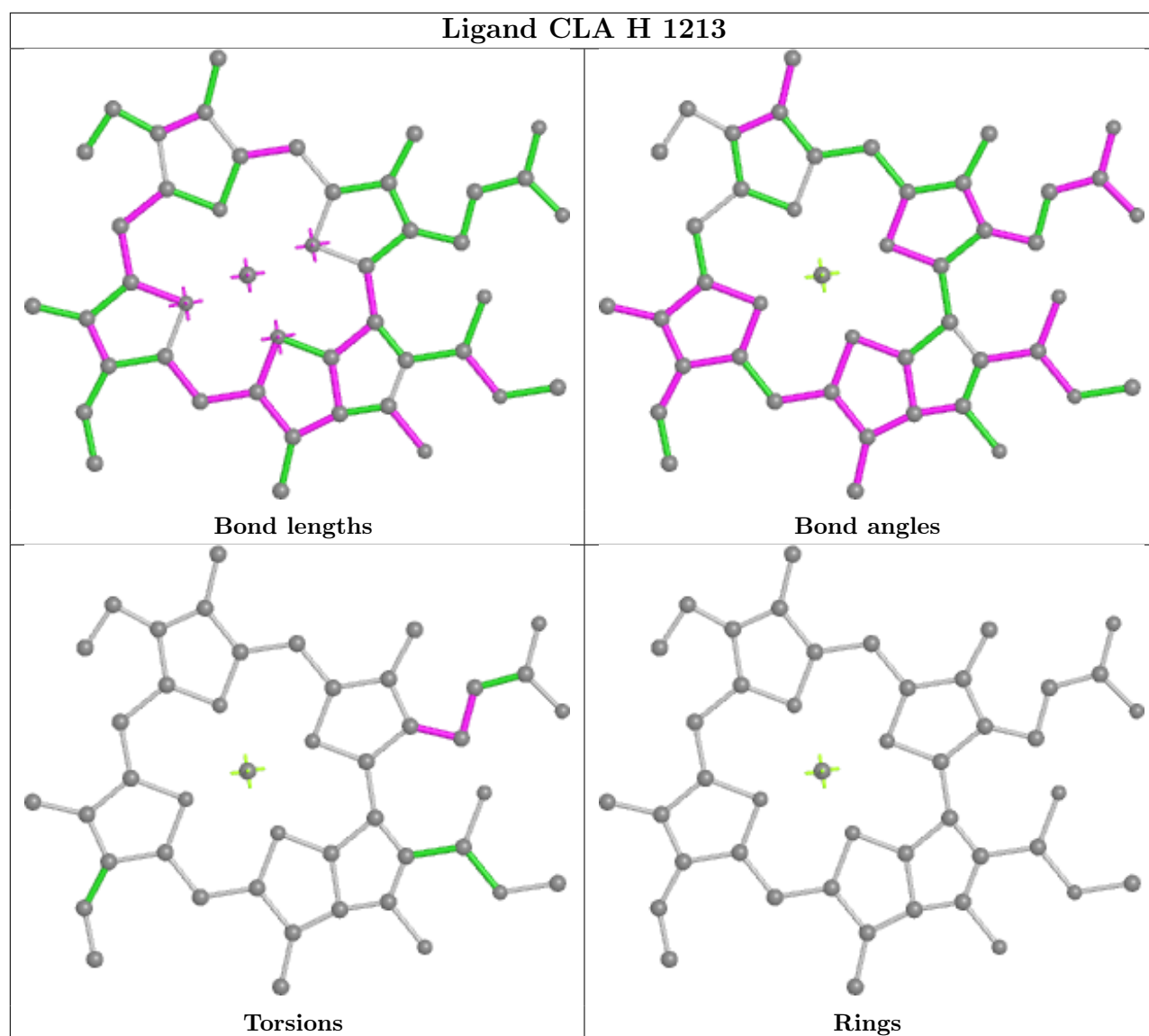
Torsions

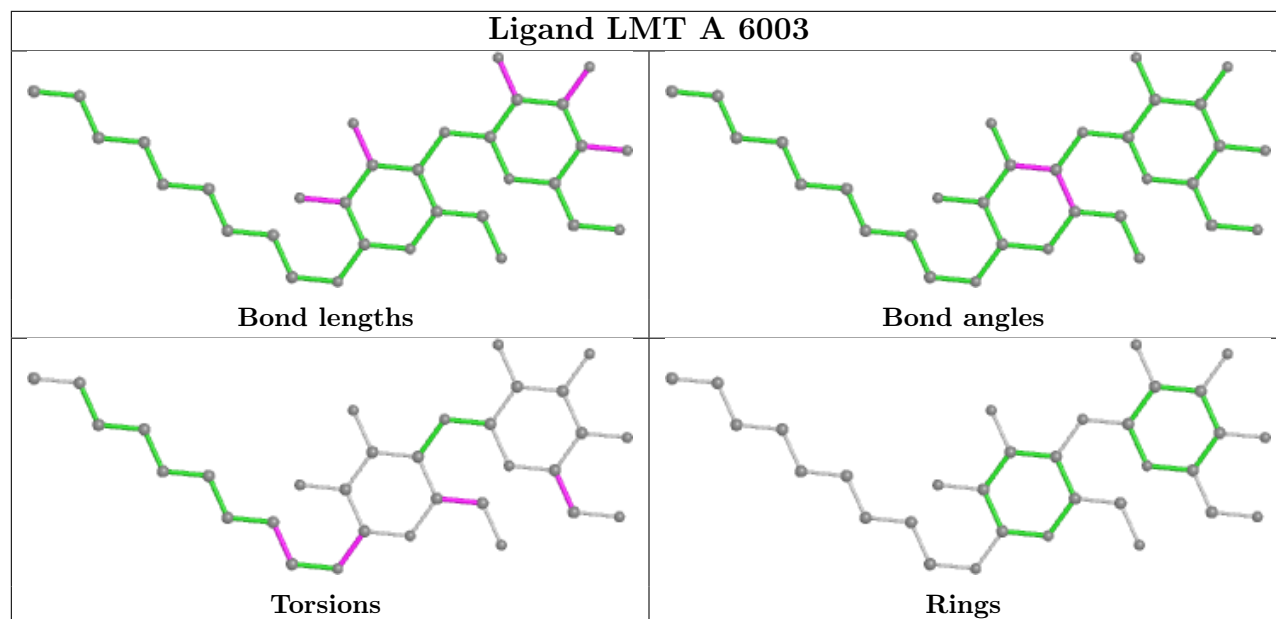
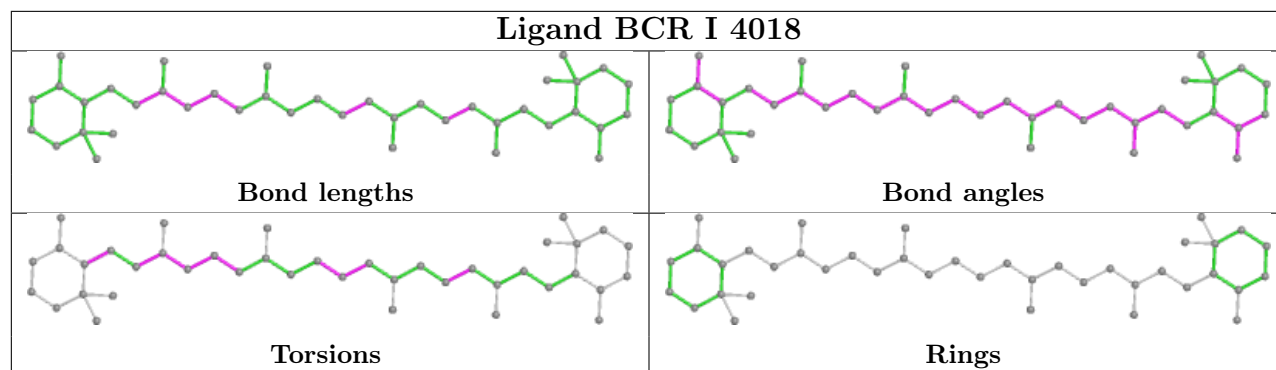


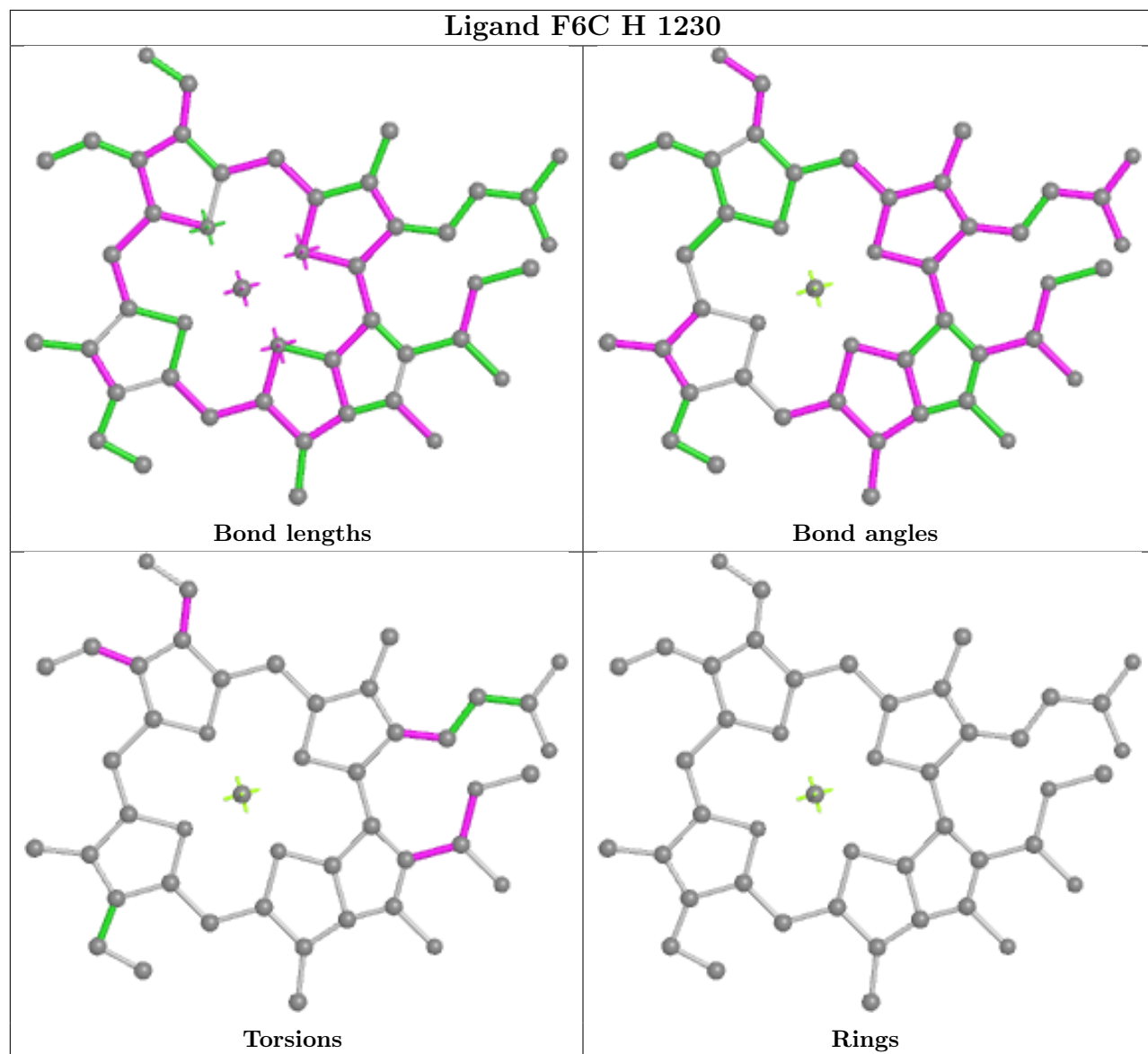
Rings



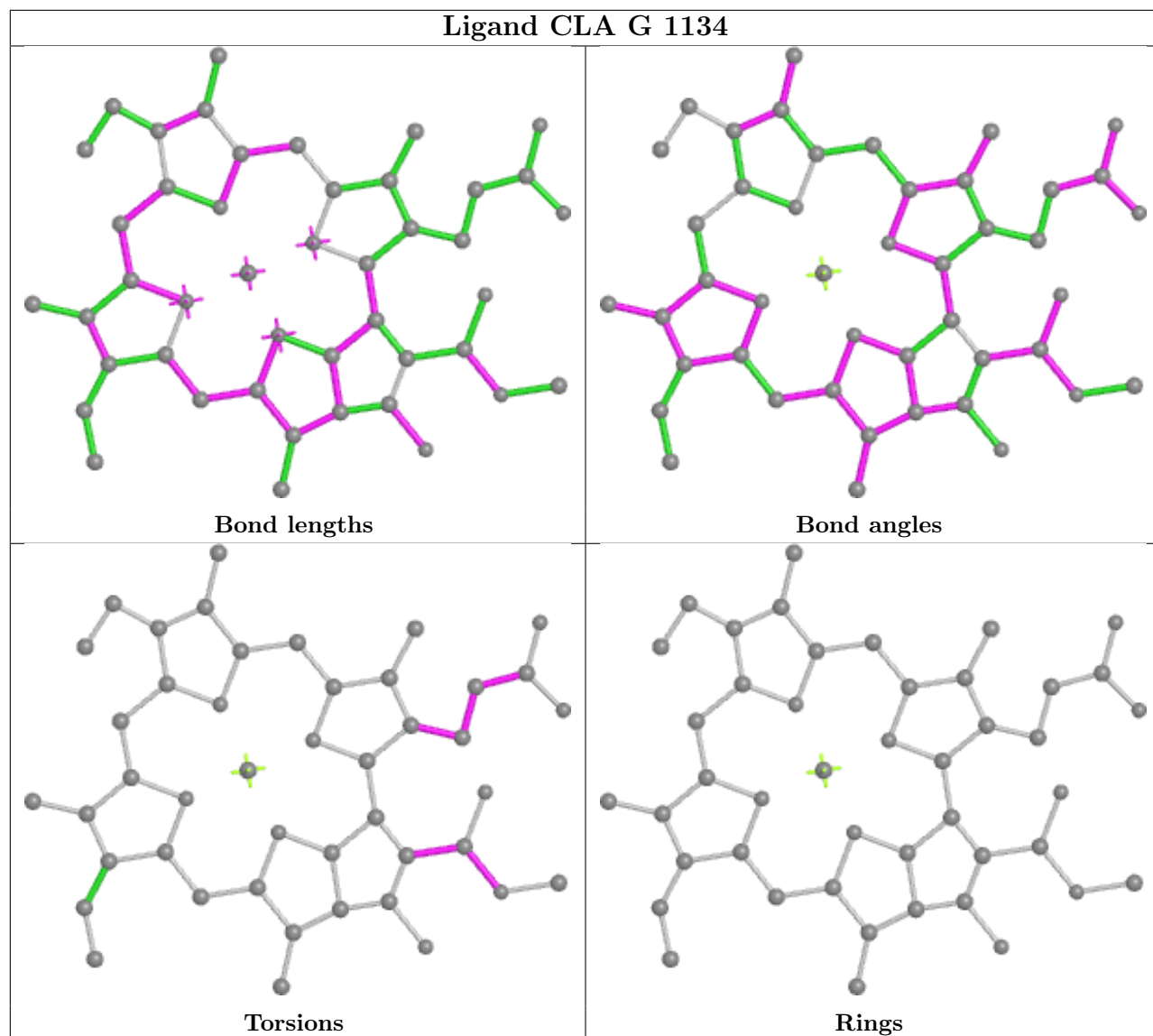


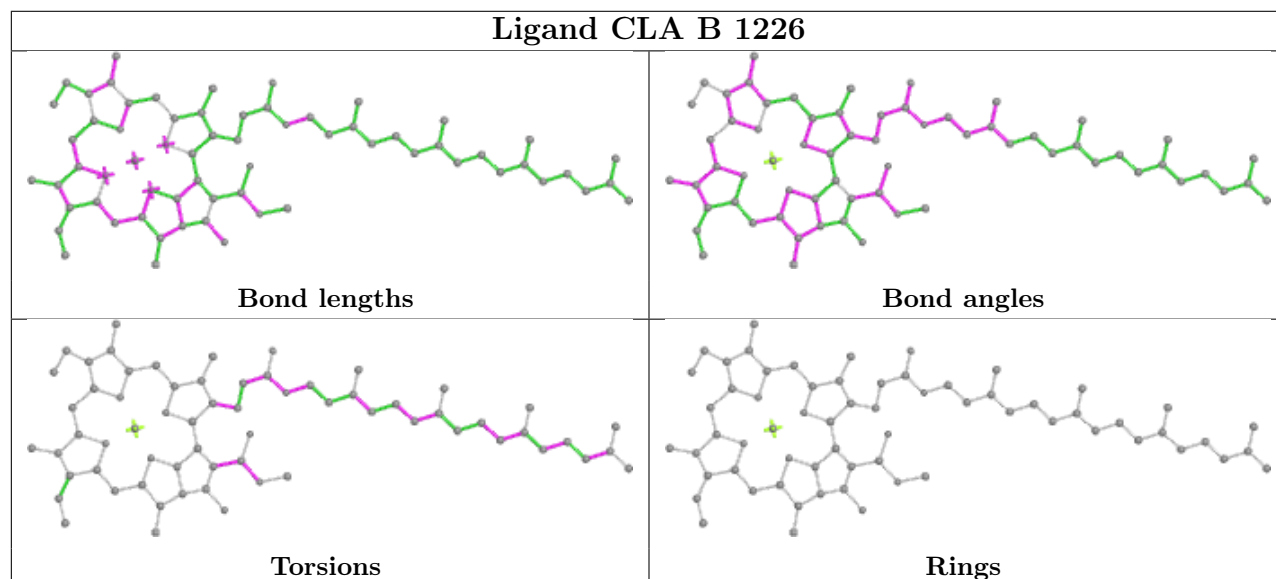
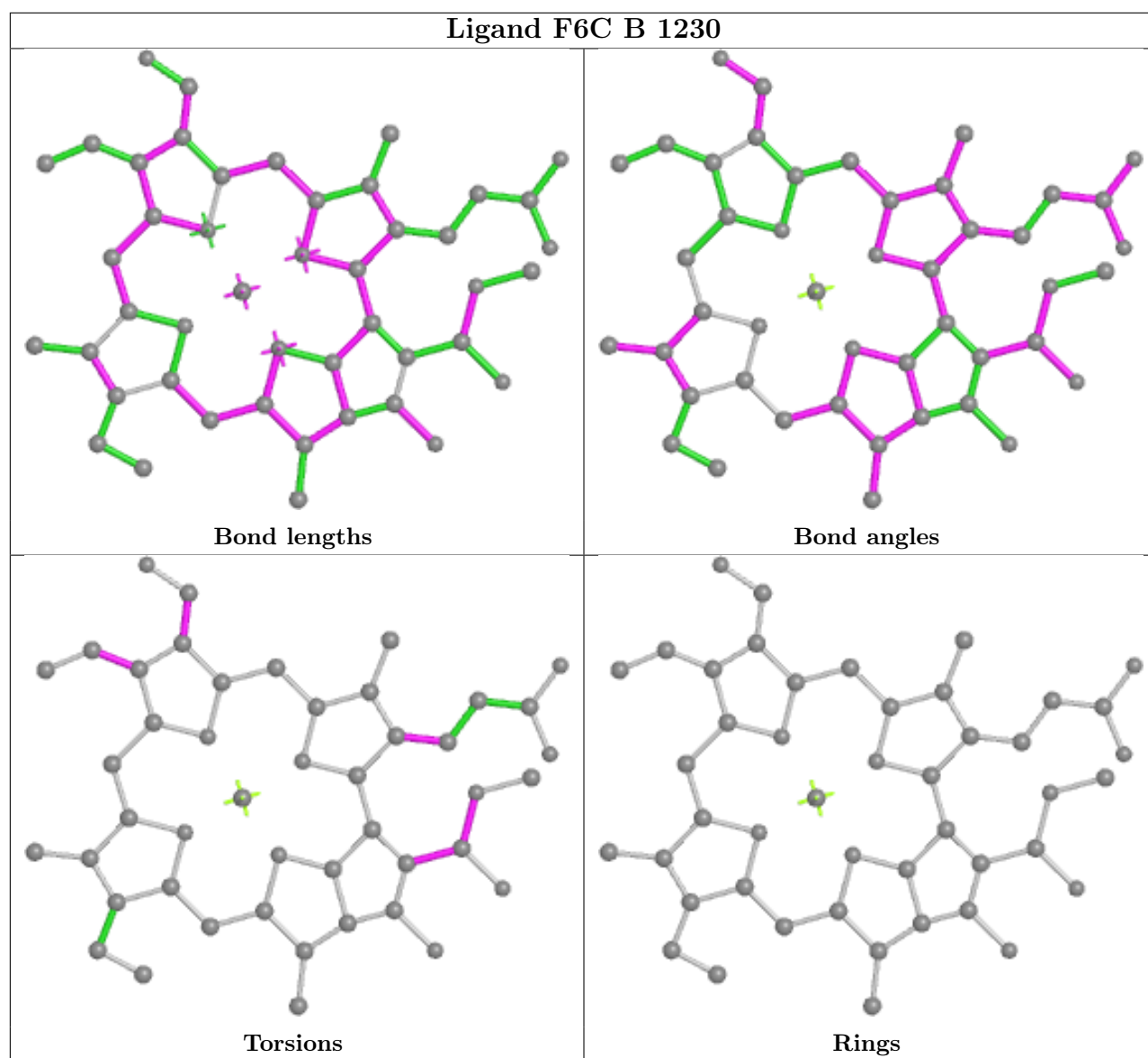


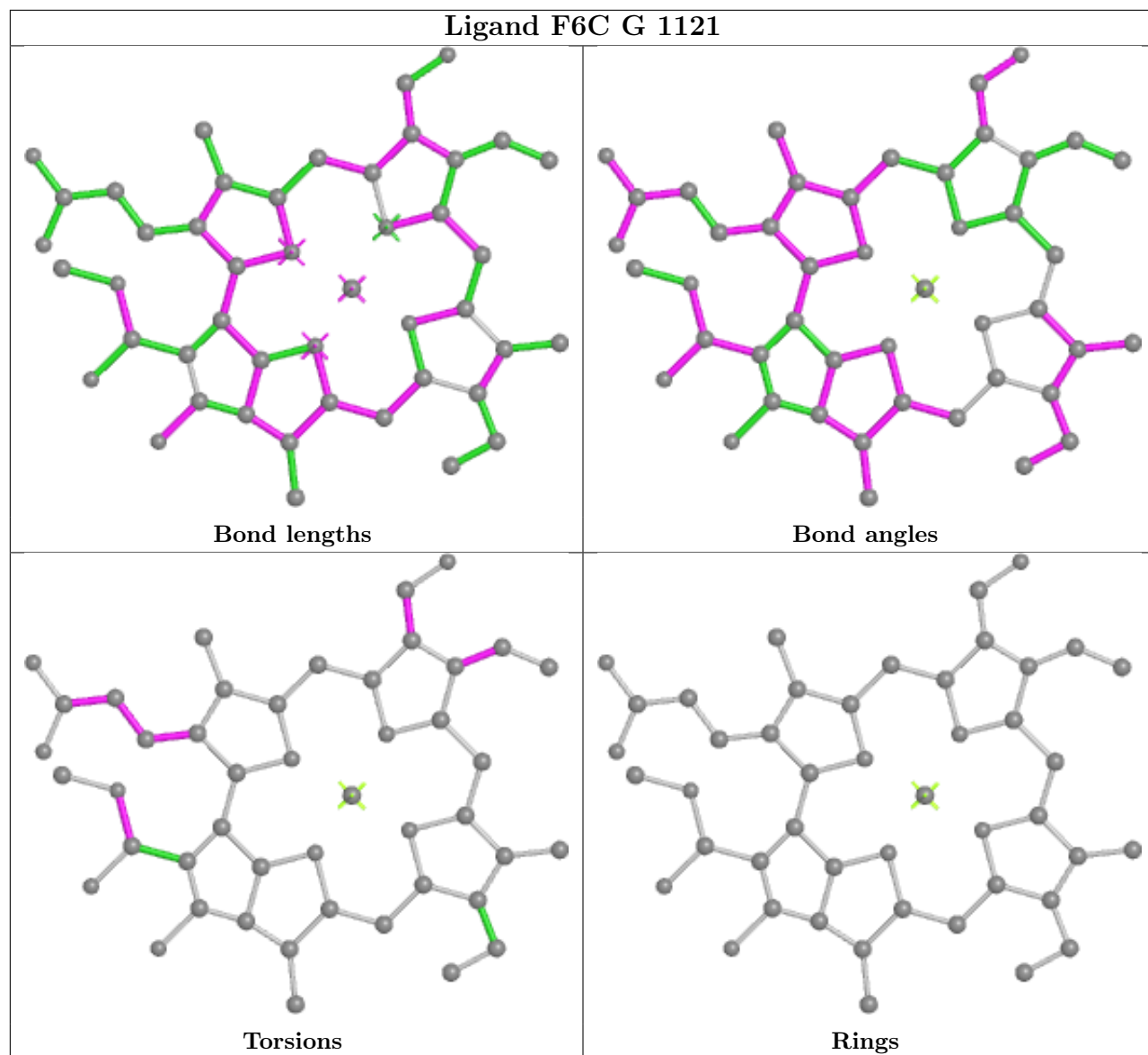
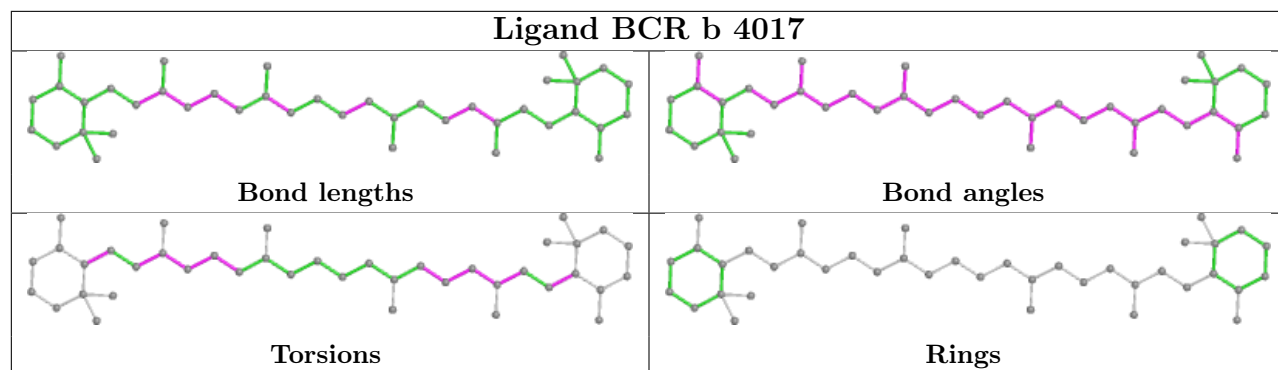


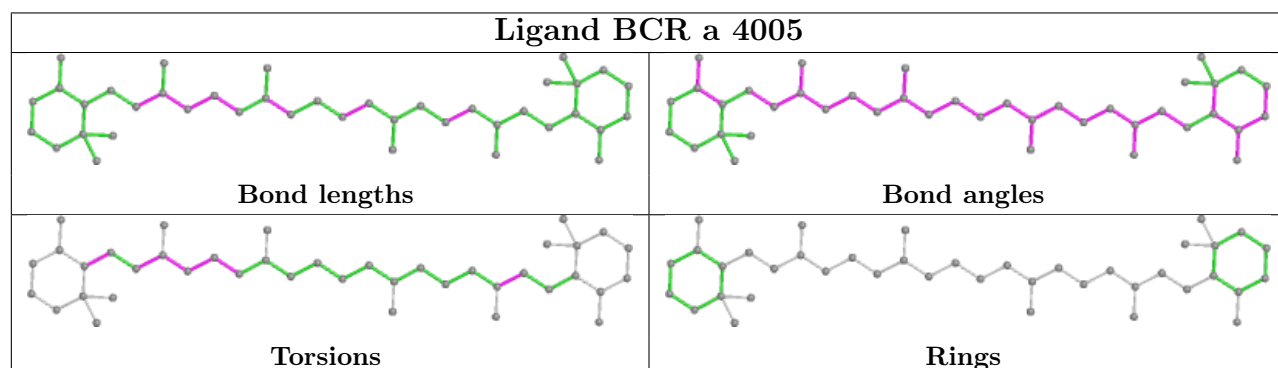
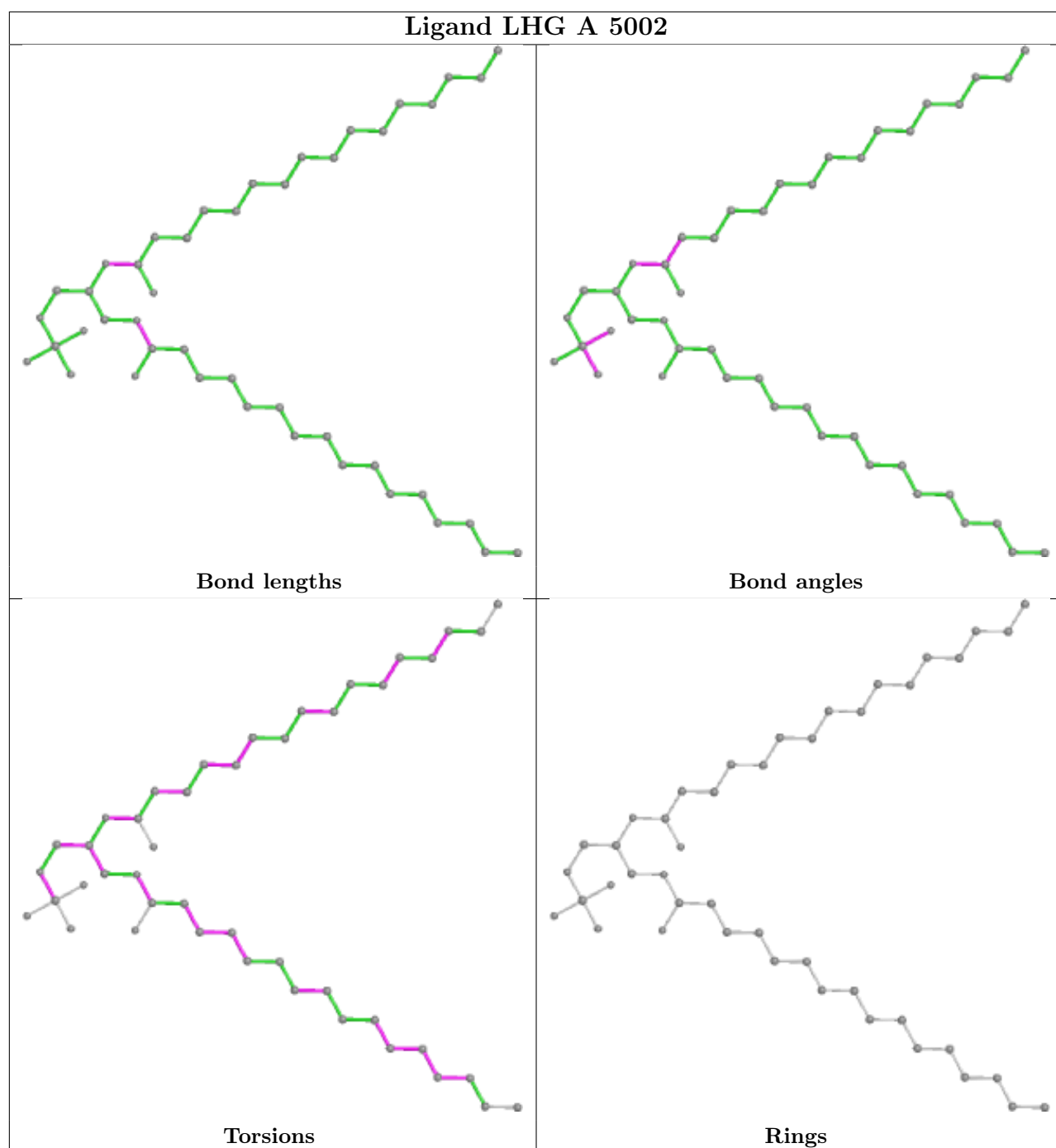


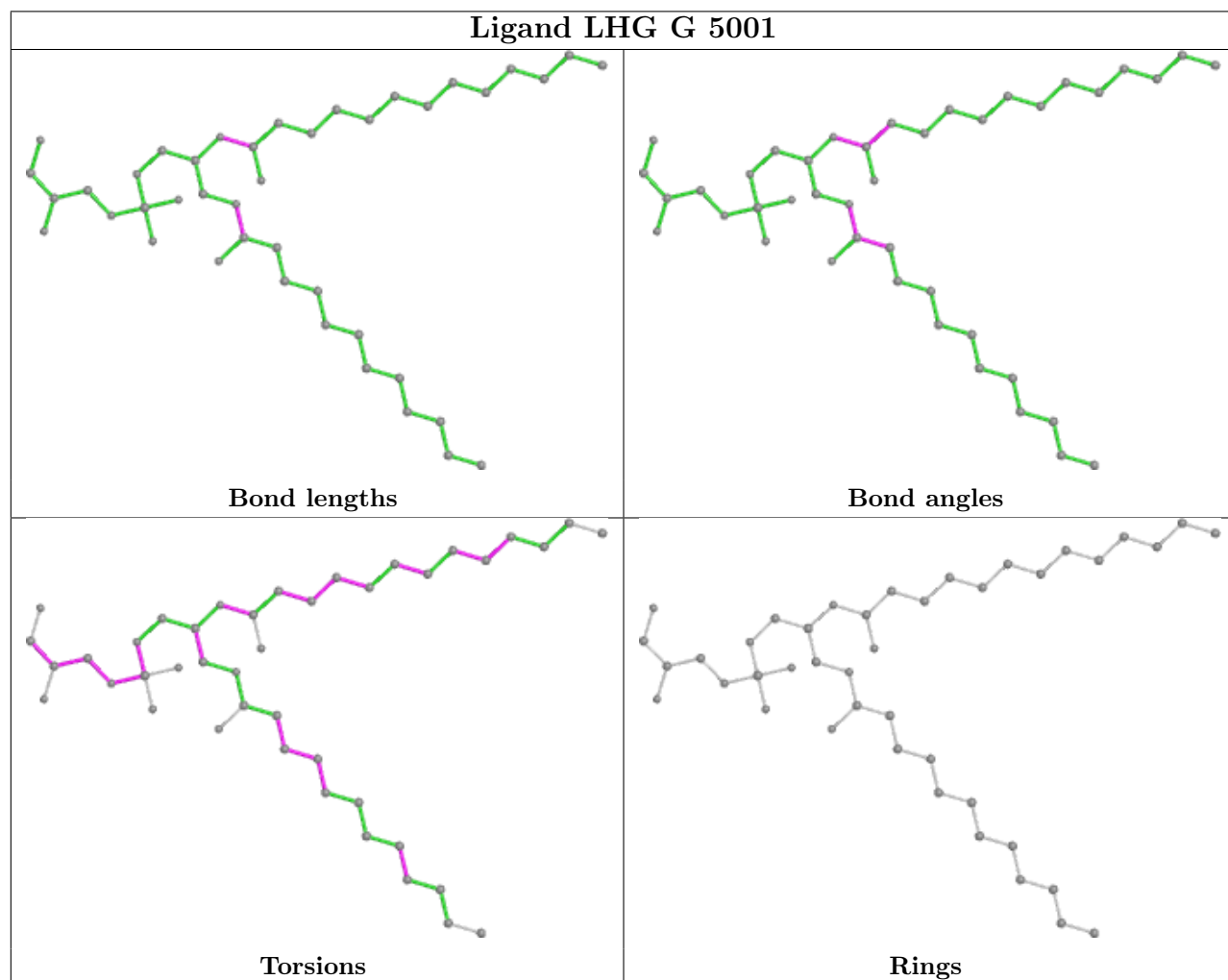
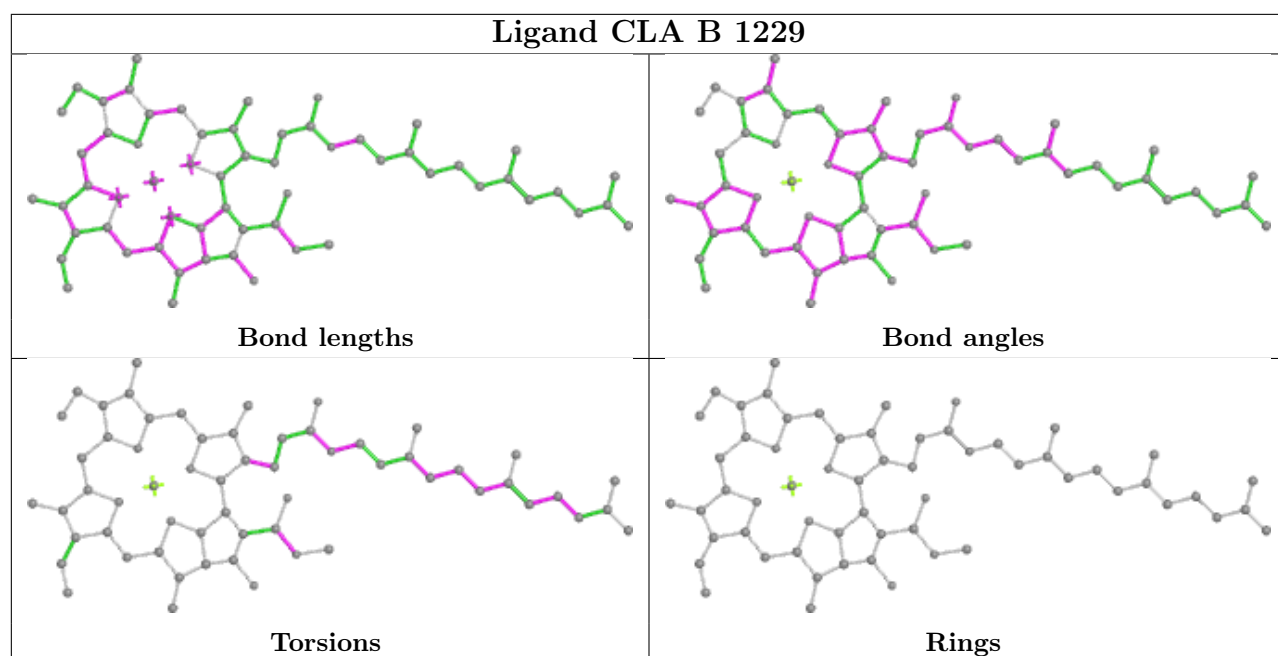
Ligand CLA G 1134



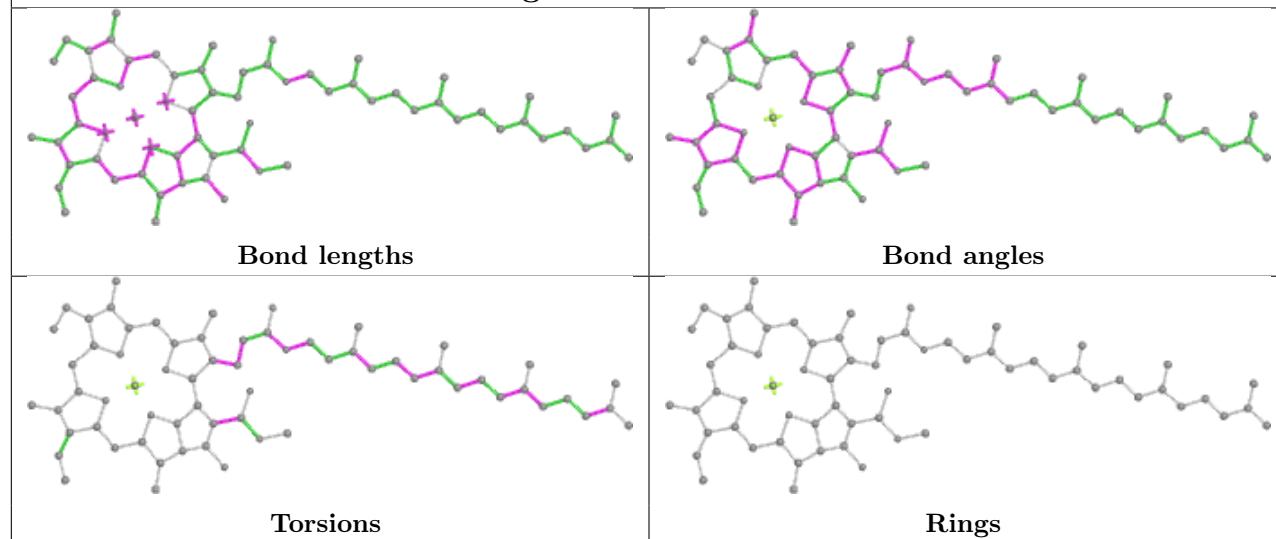




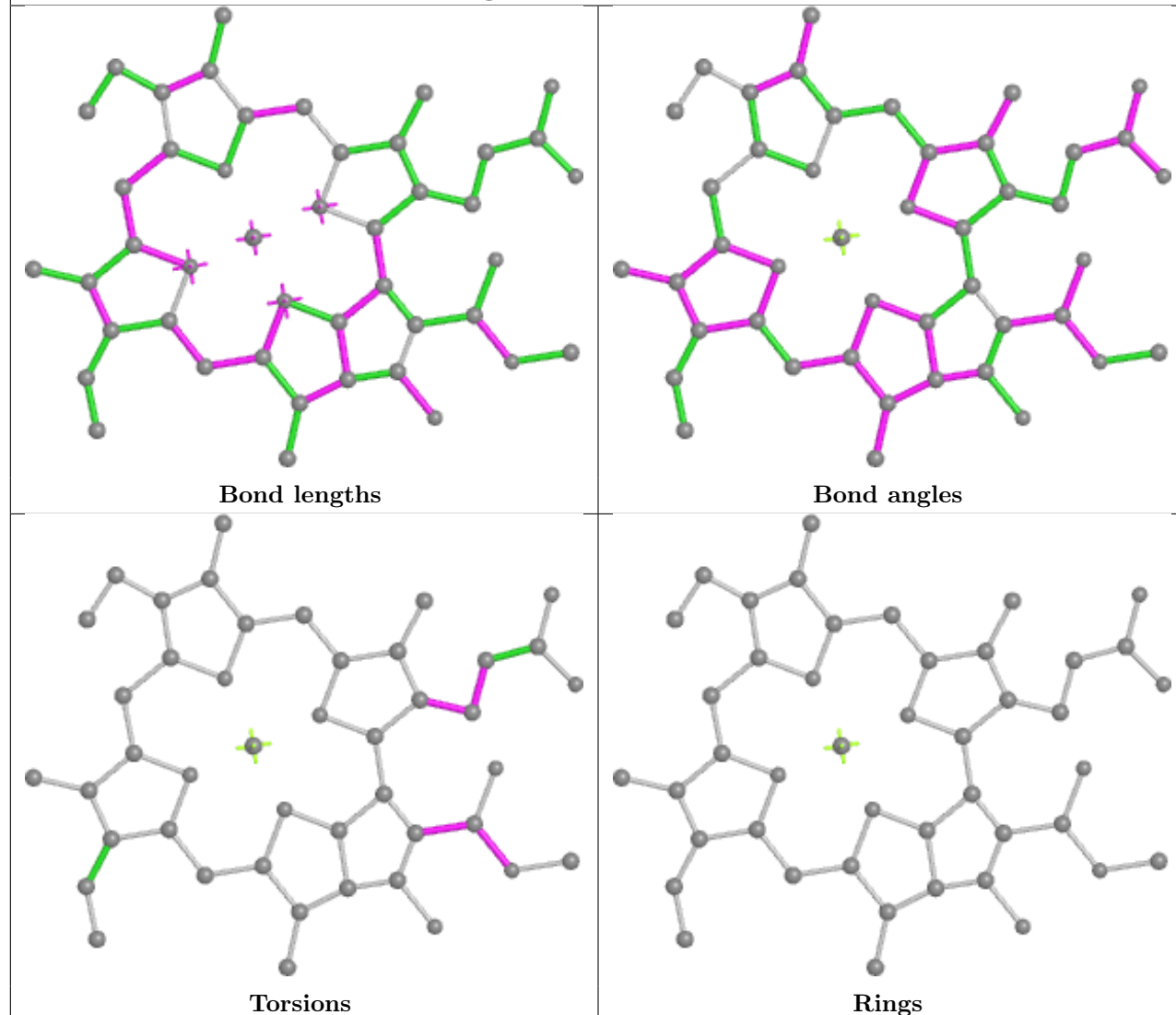


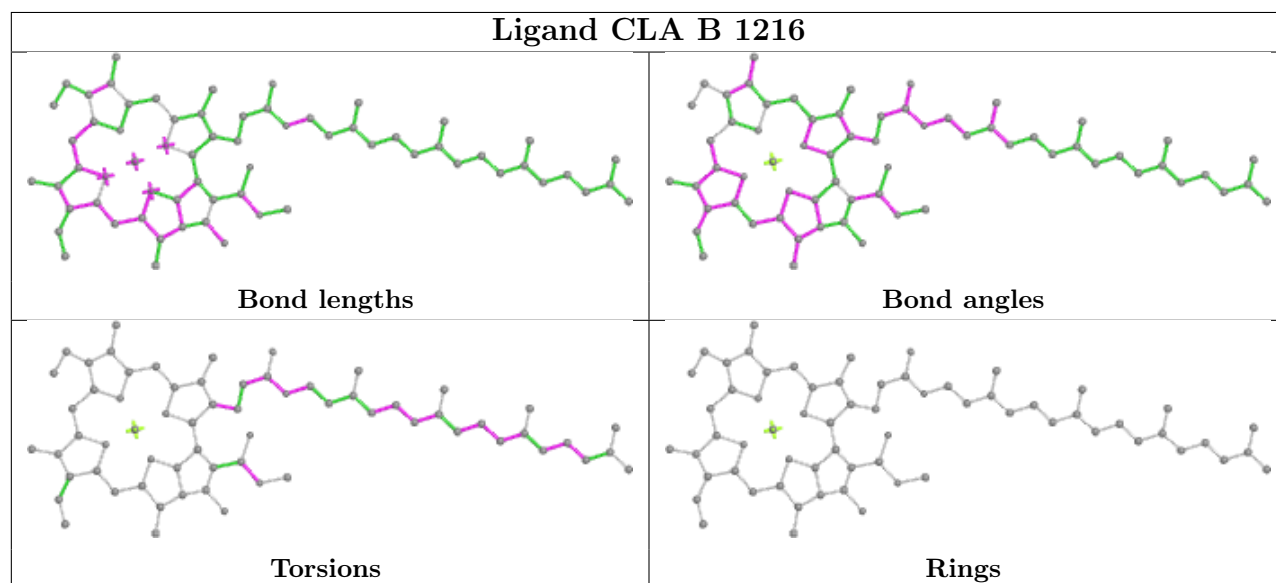
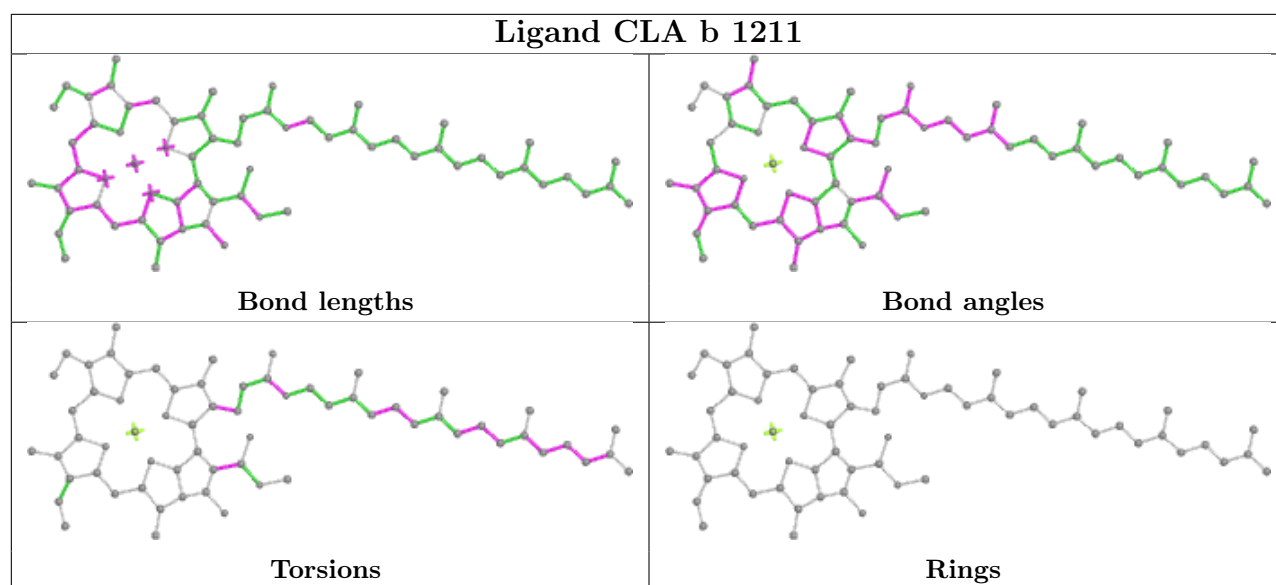


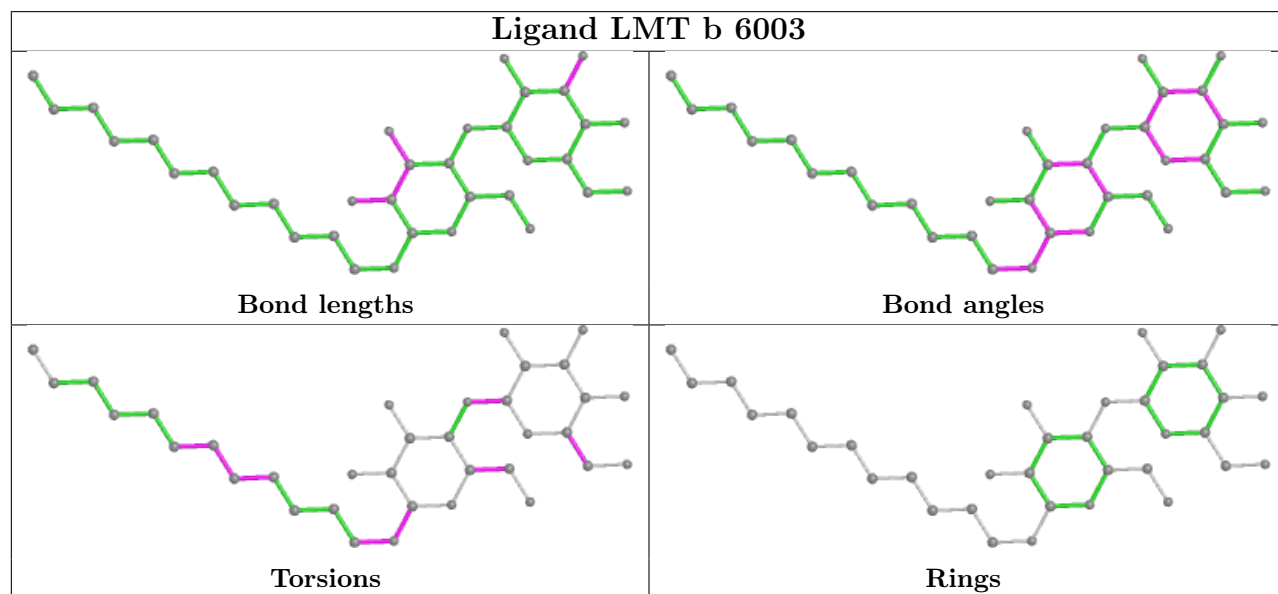
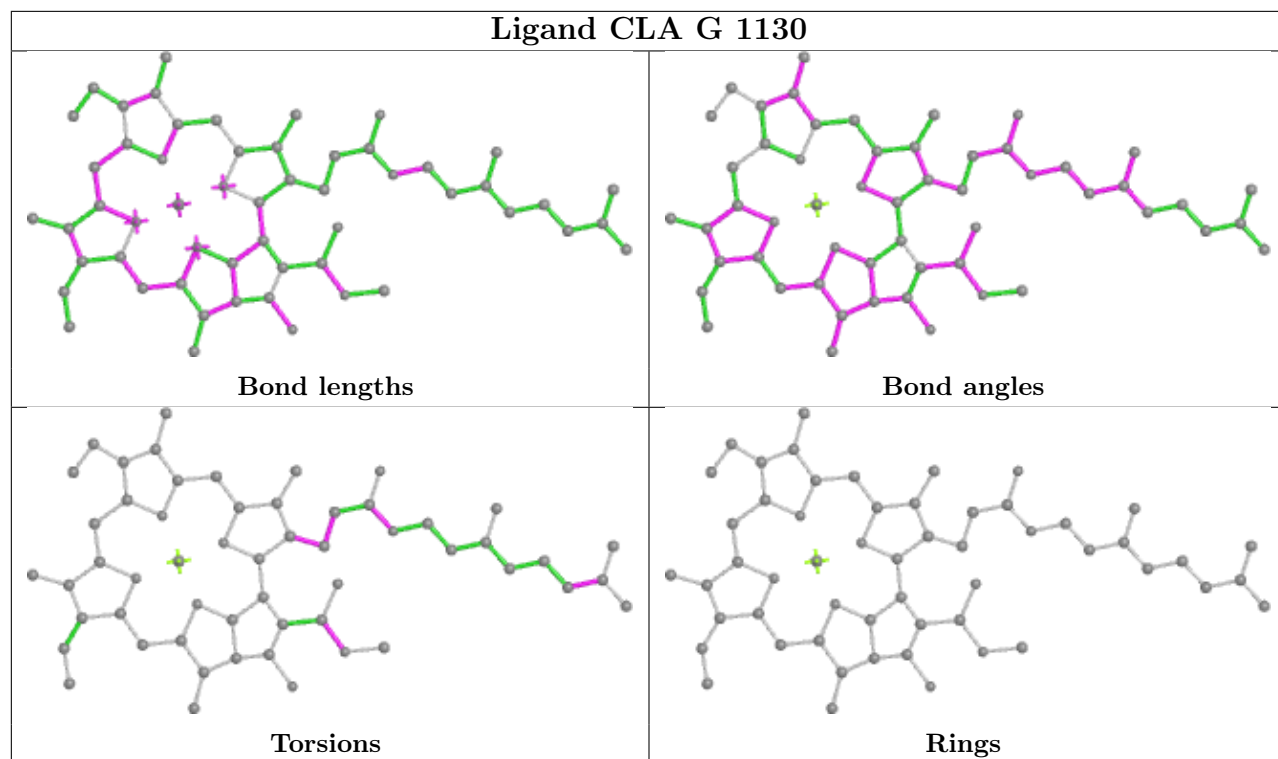
Ligand CLA H 1221



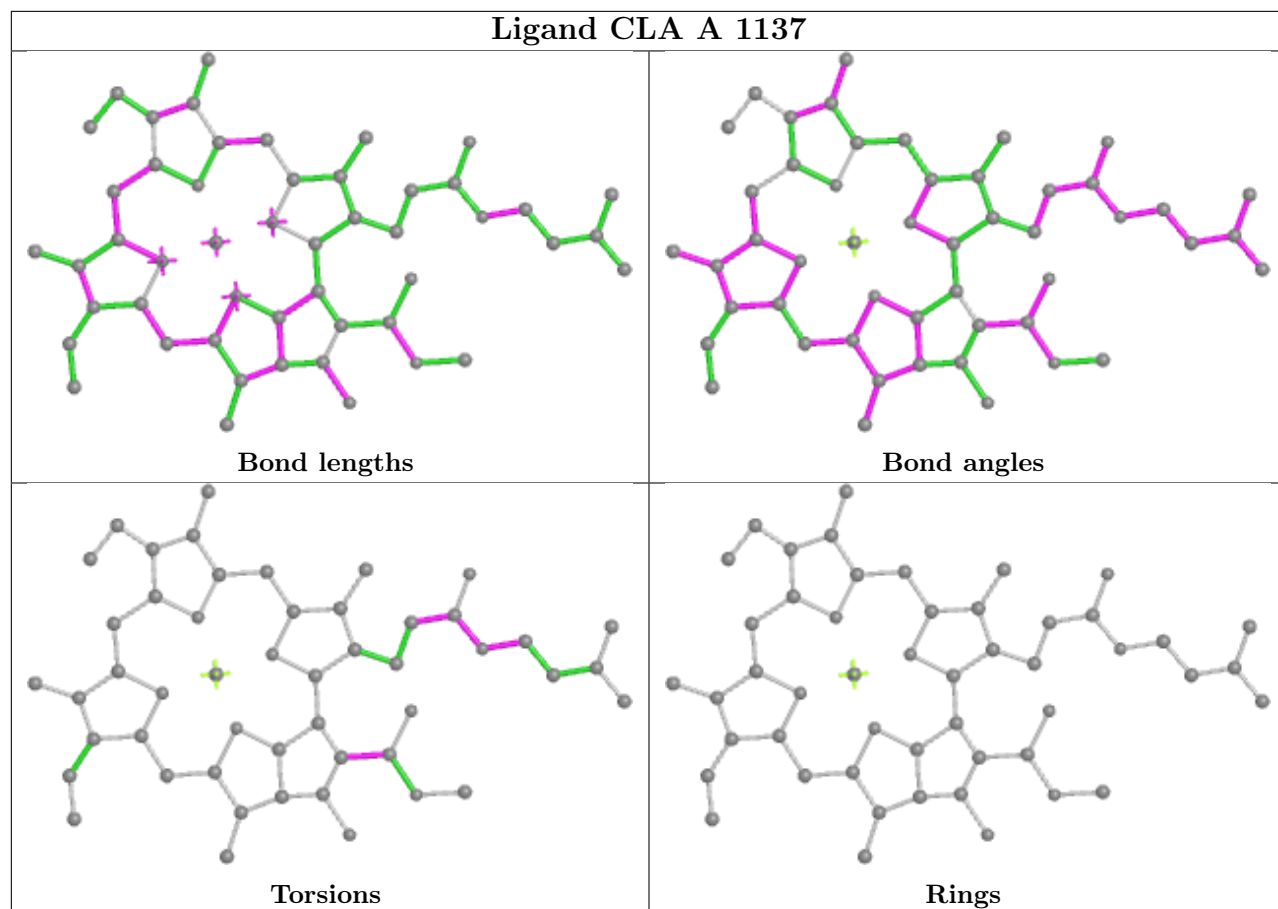
Ligand CLA G 1120



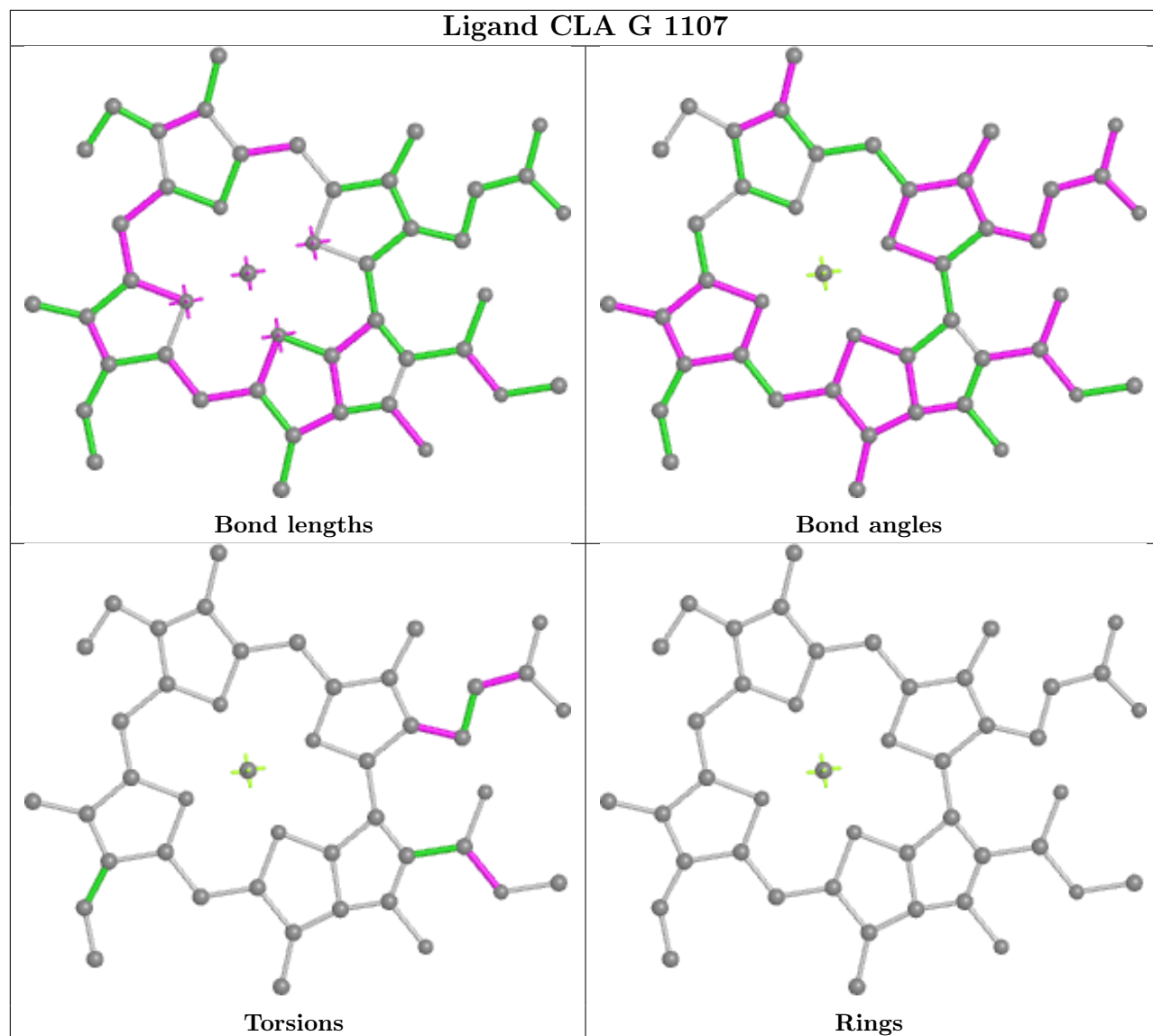


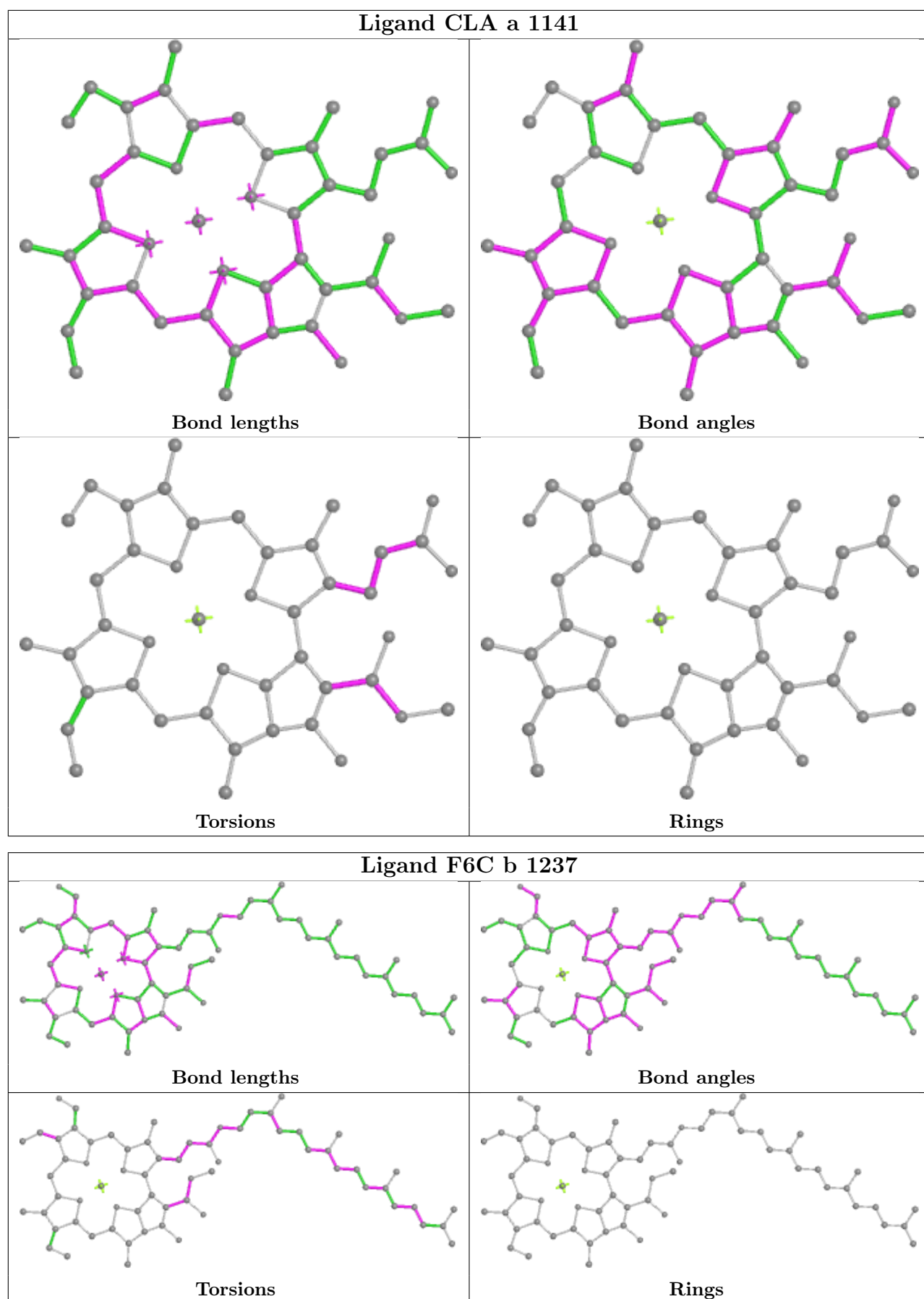


Ligand CLA A 1137

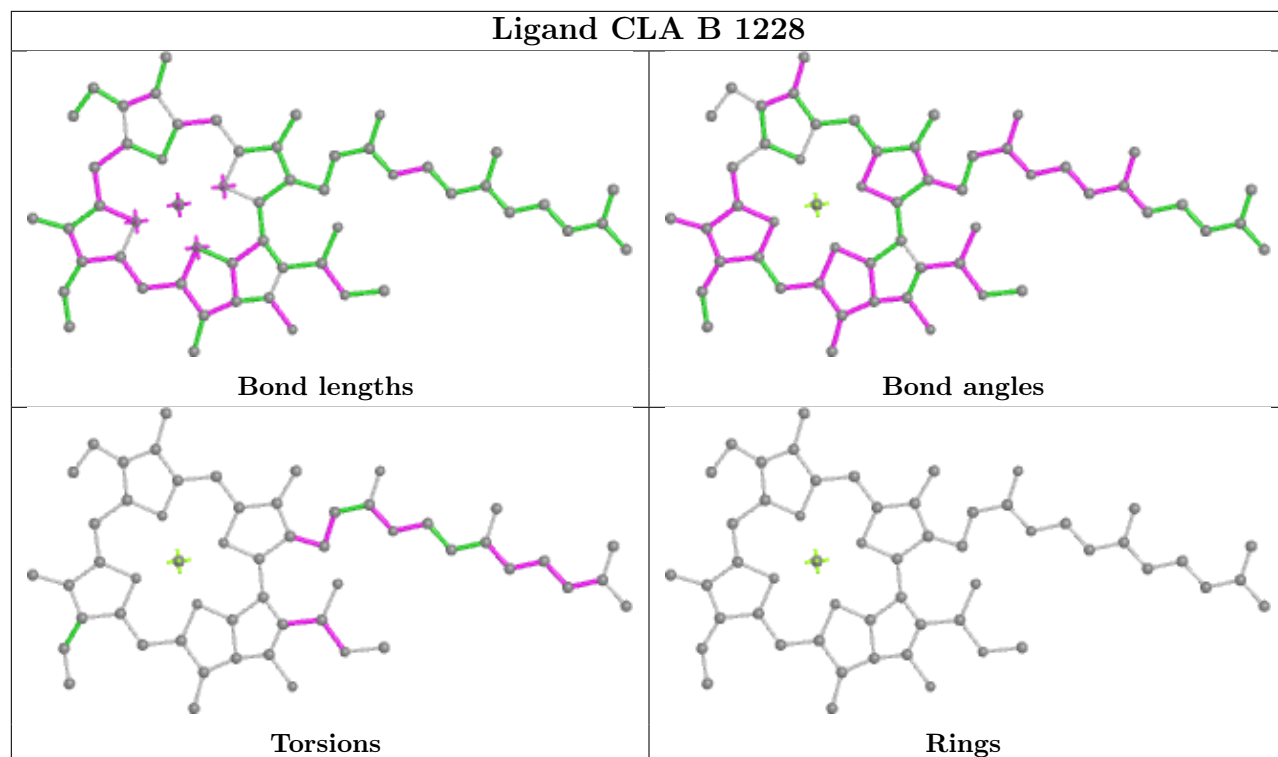


Ligand CLA G 1107

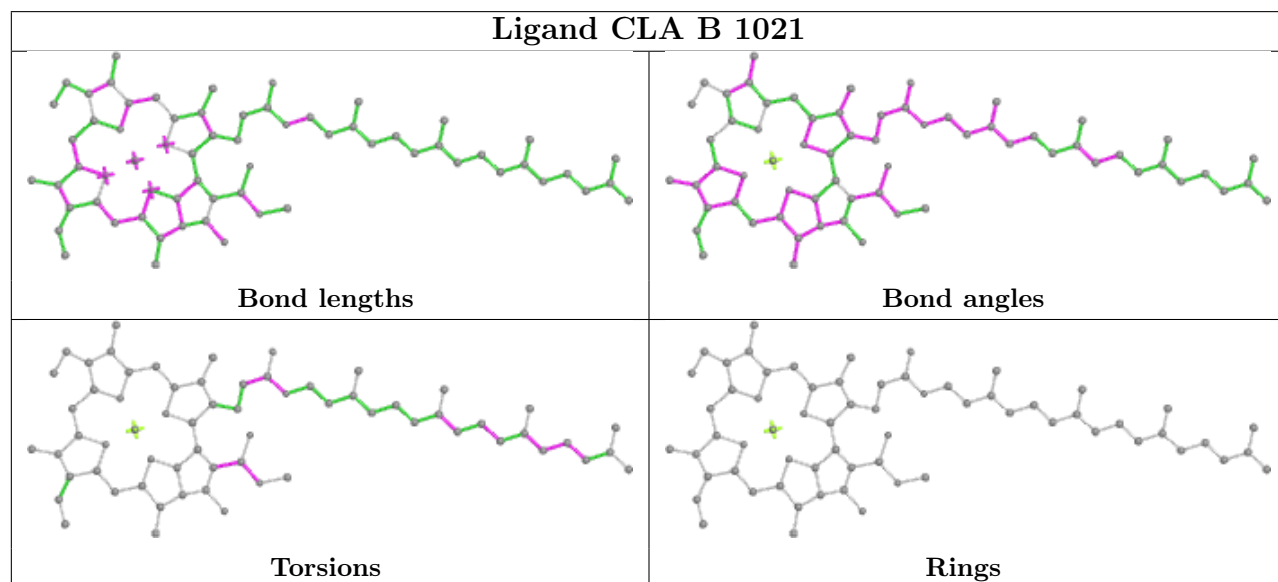


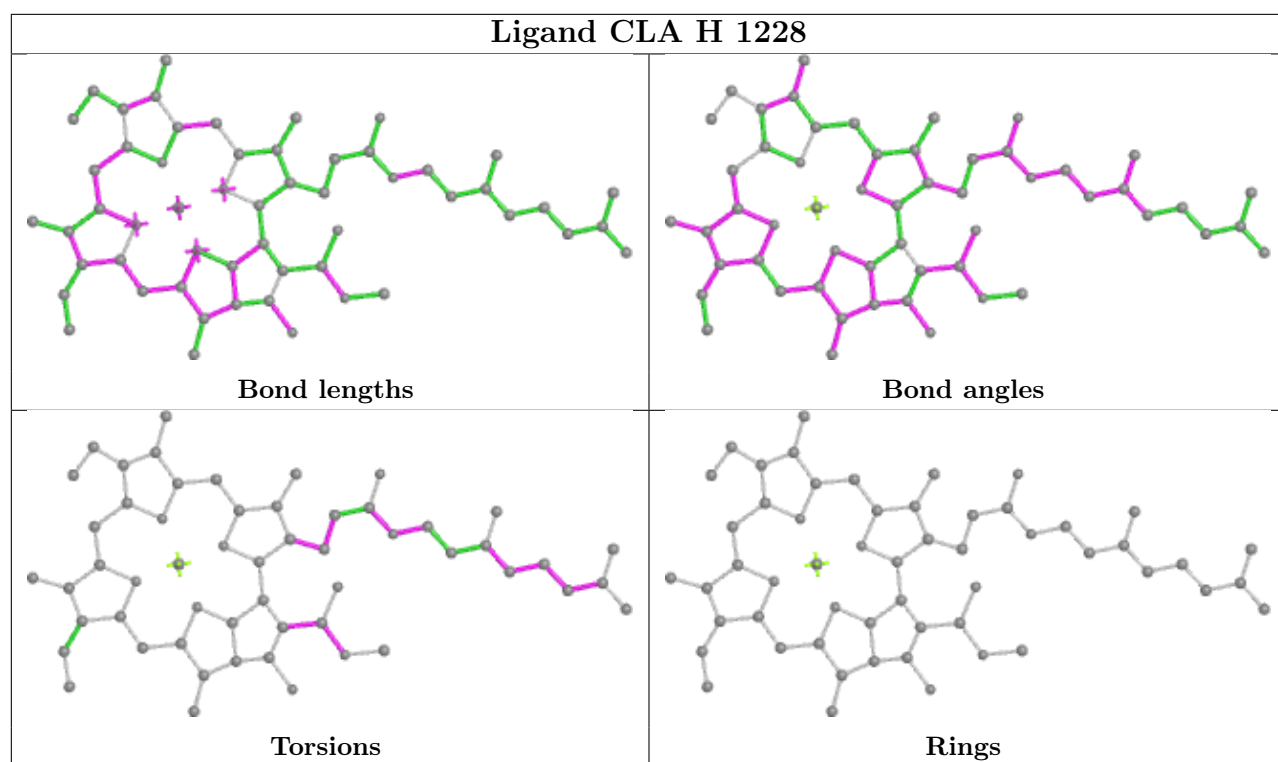


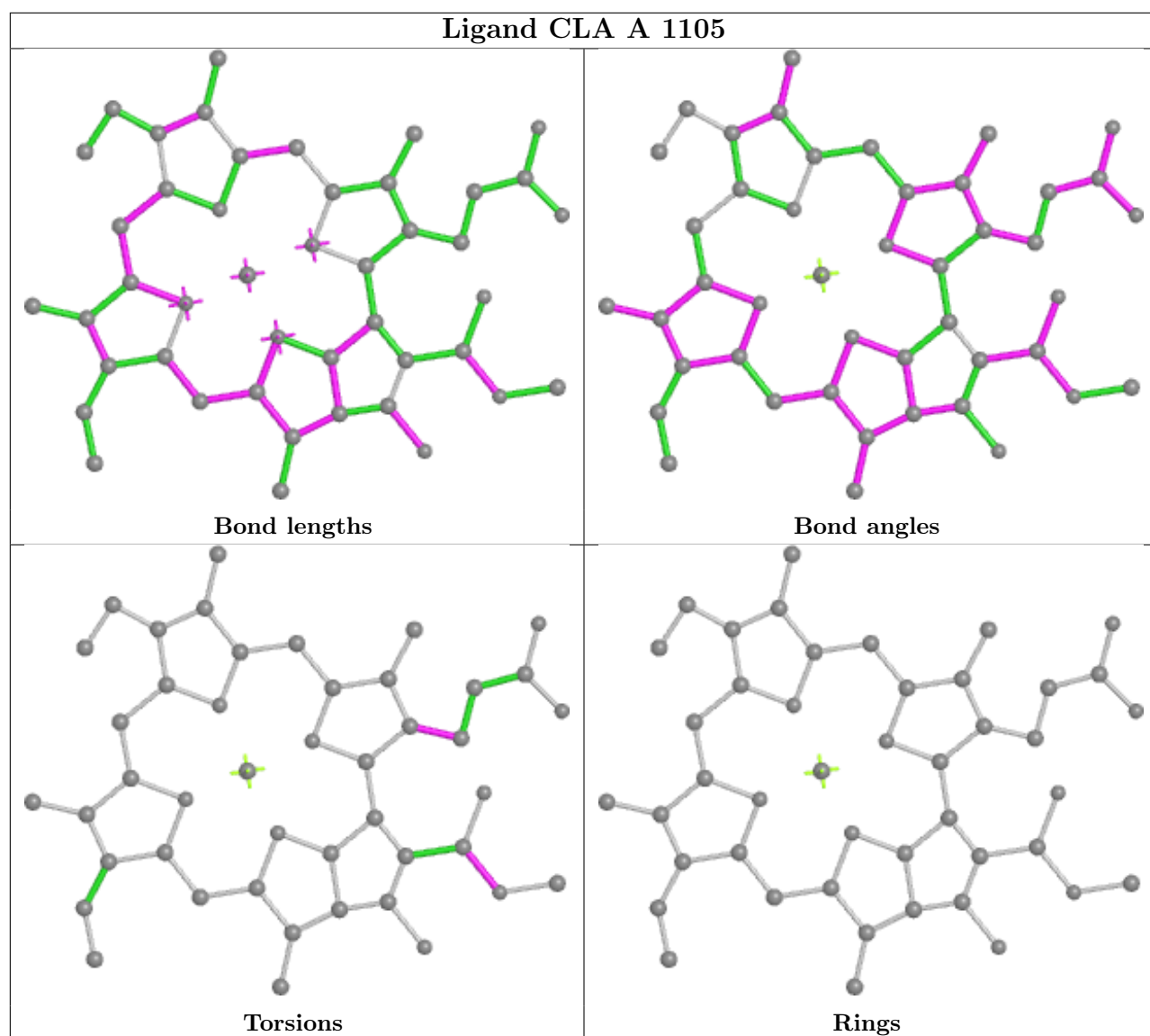
Ligand CLA B 1228

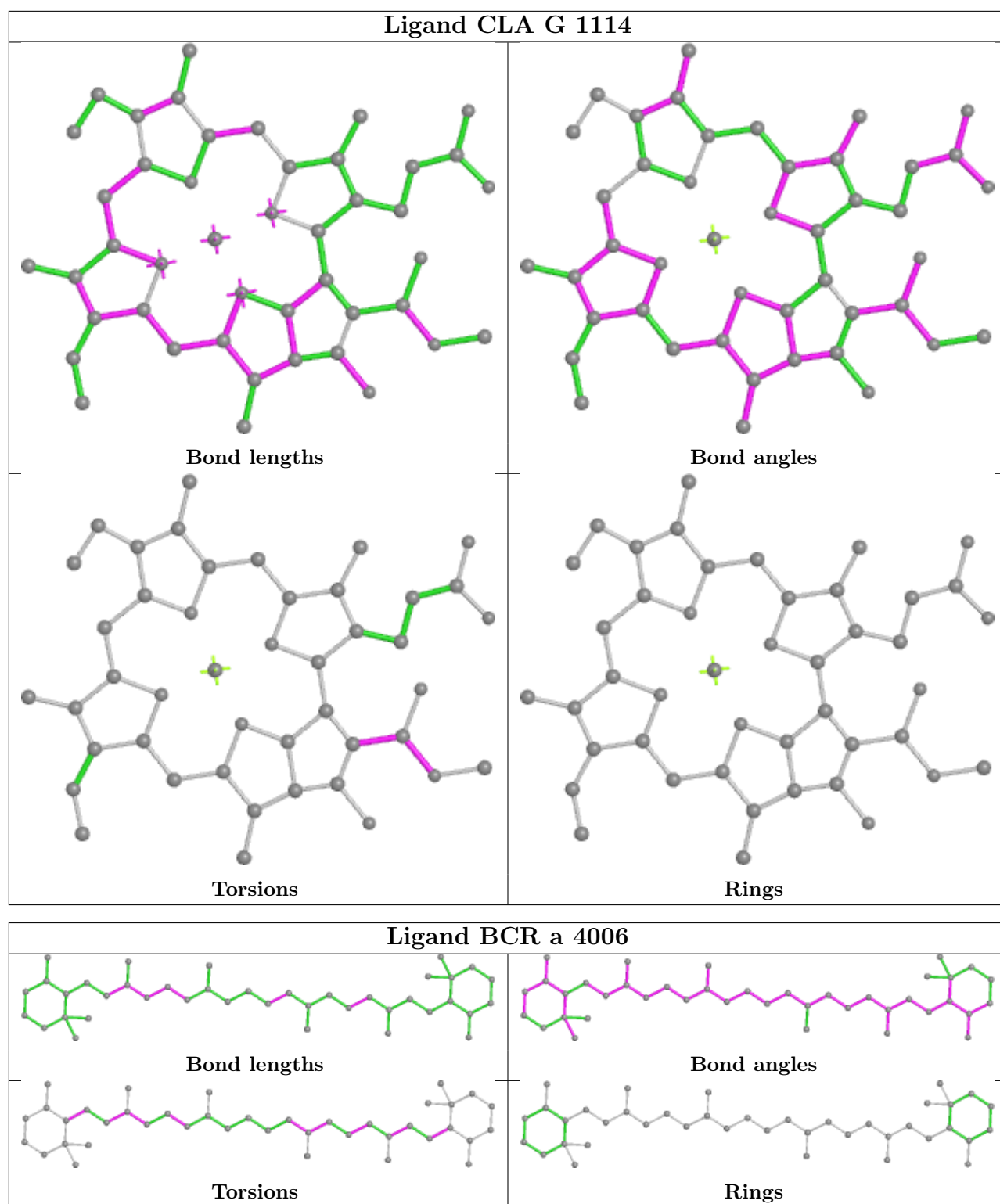


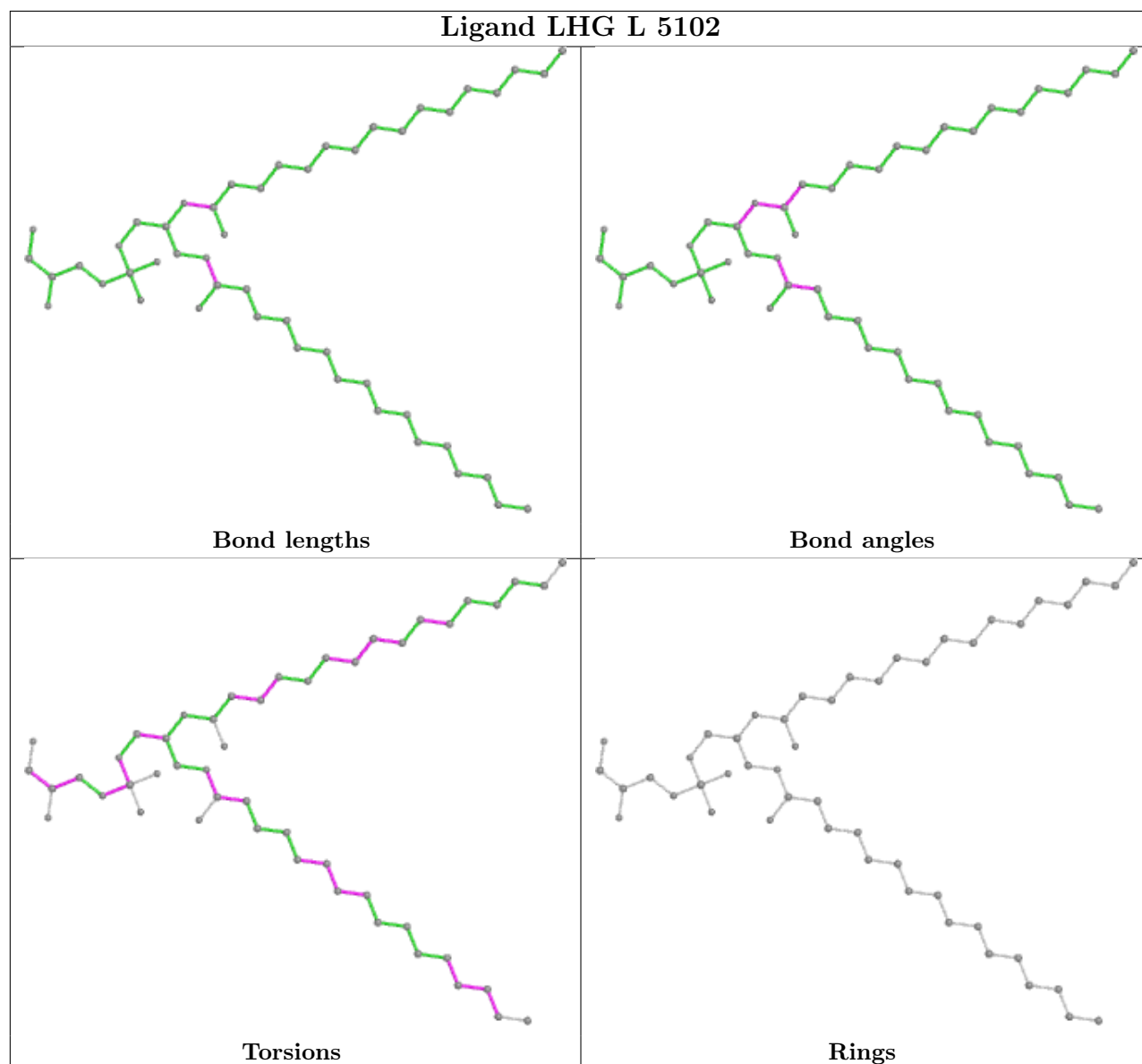
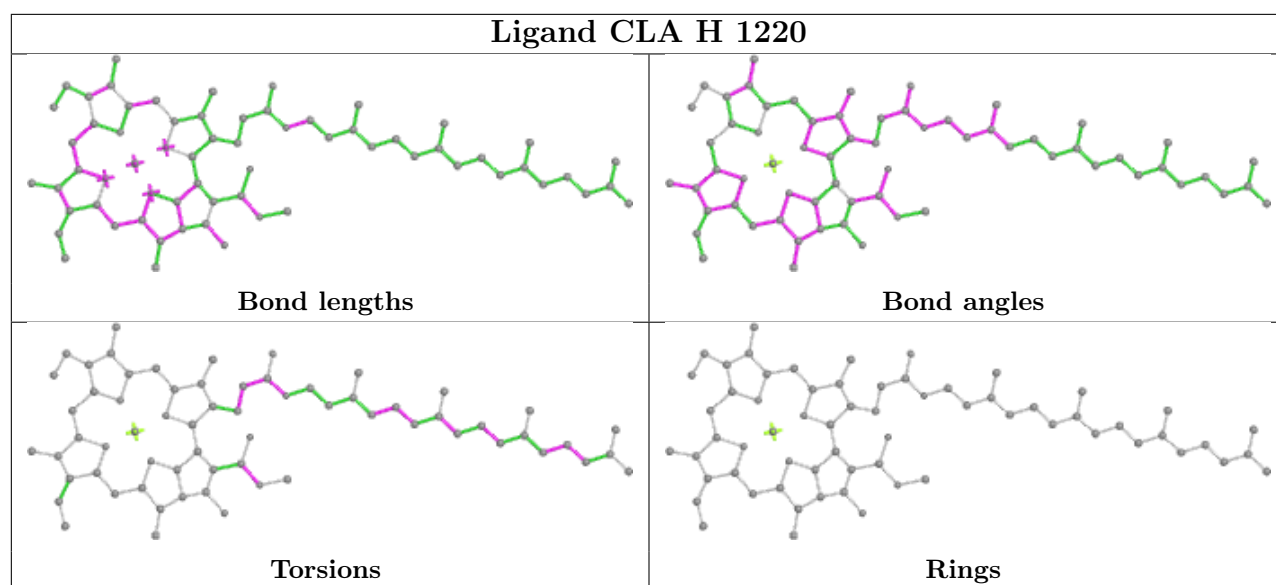
Ligand CLA B 1021



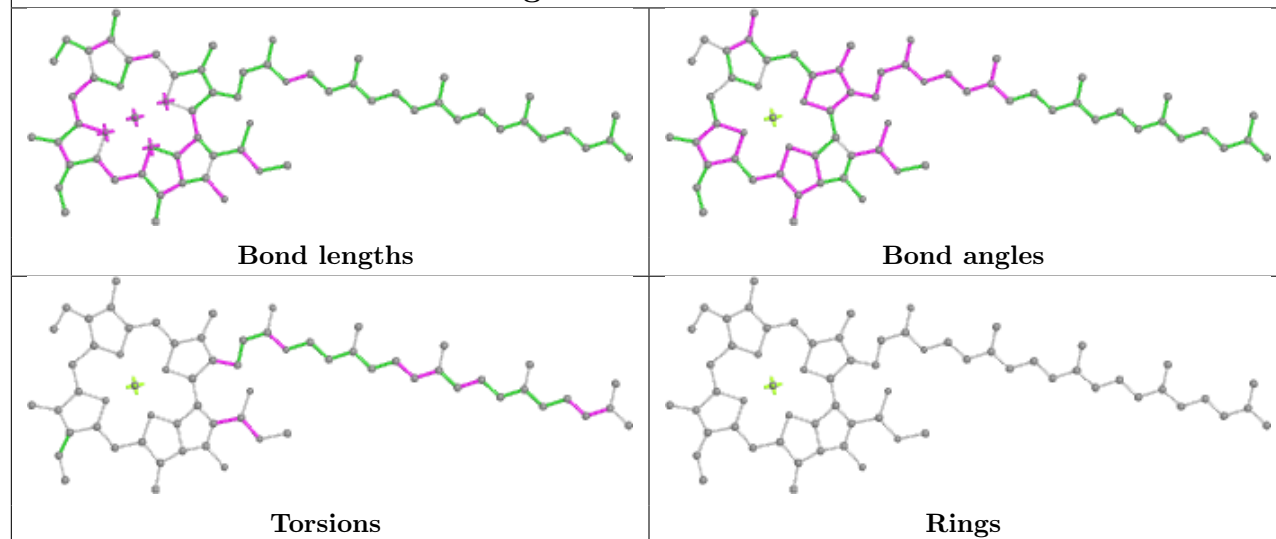




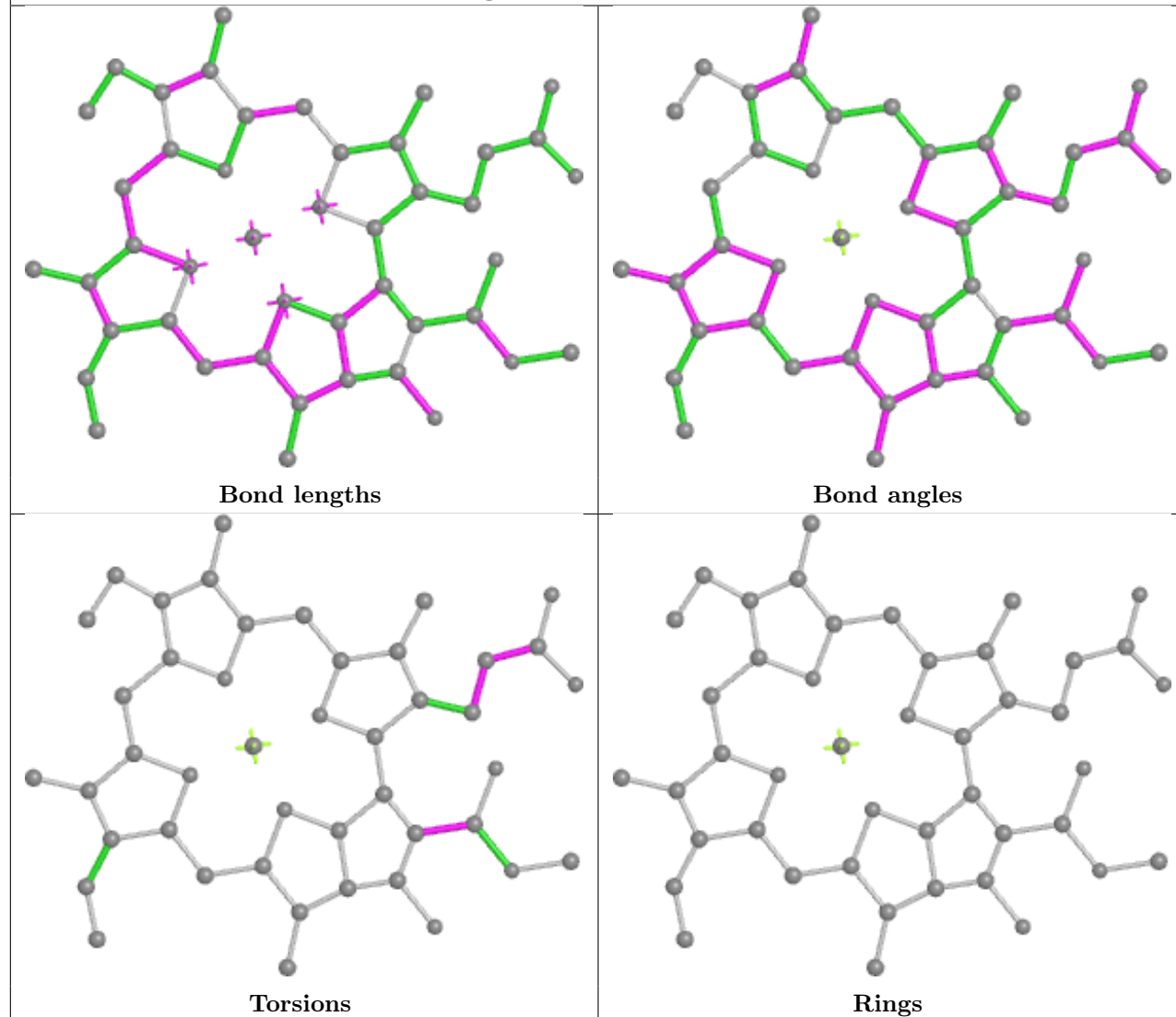


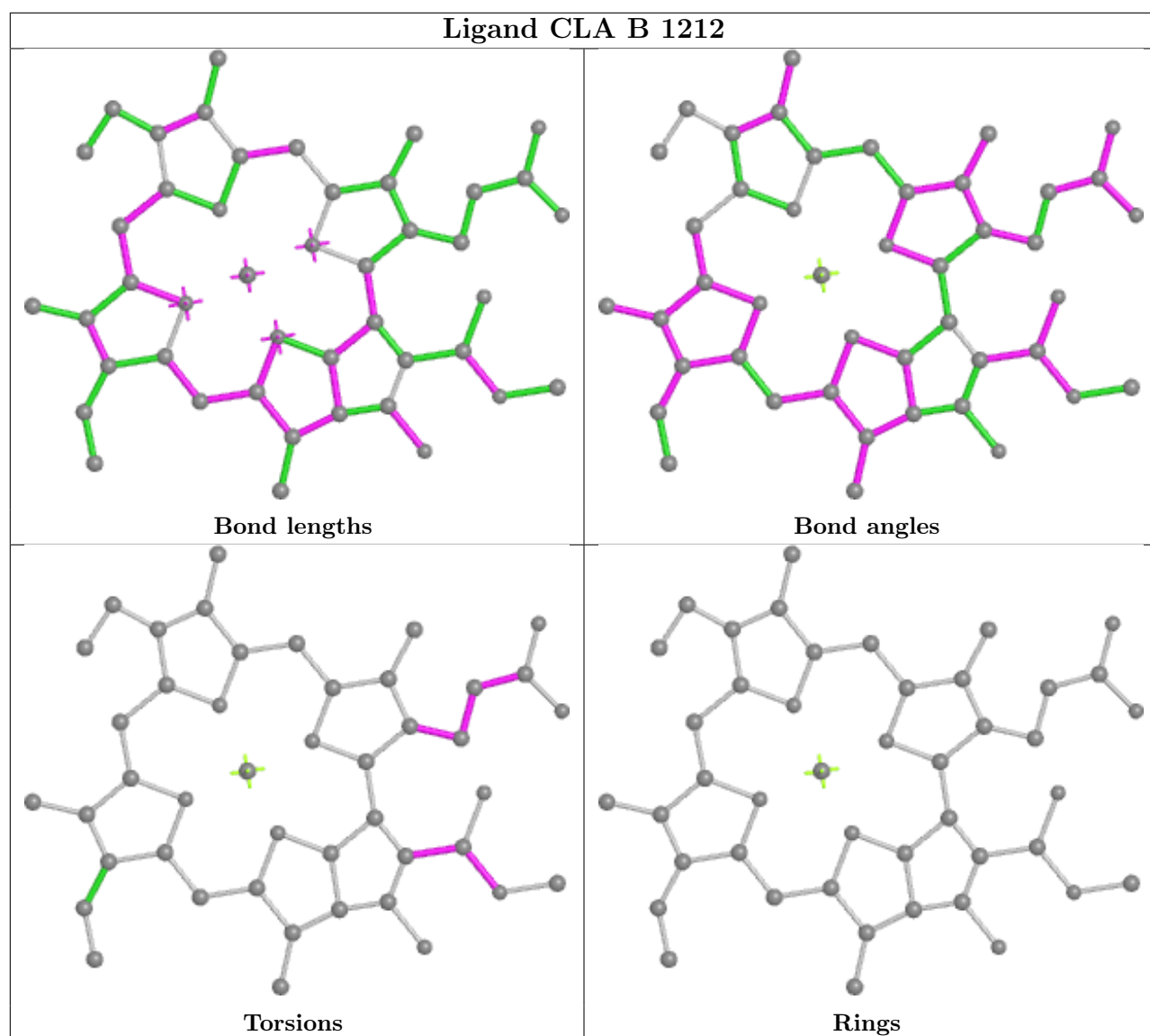


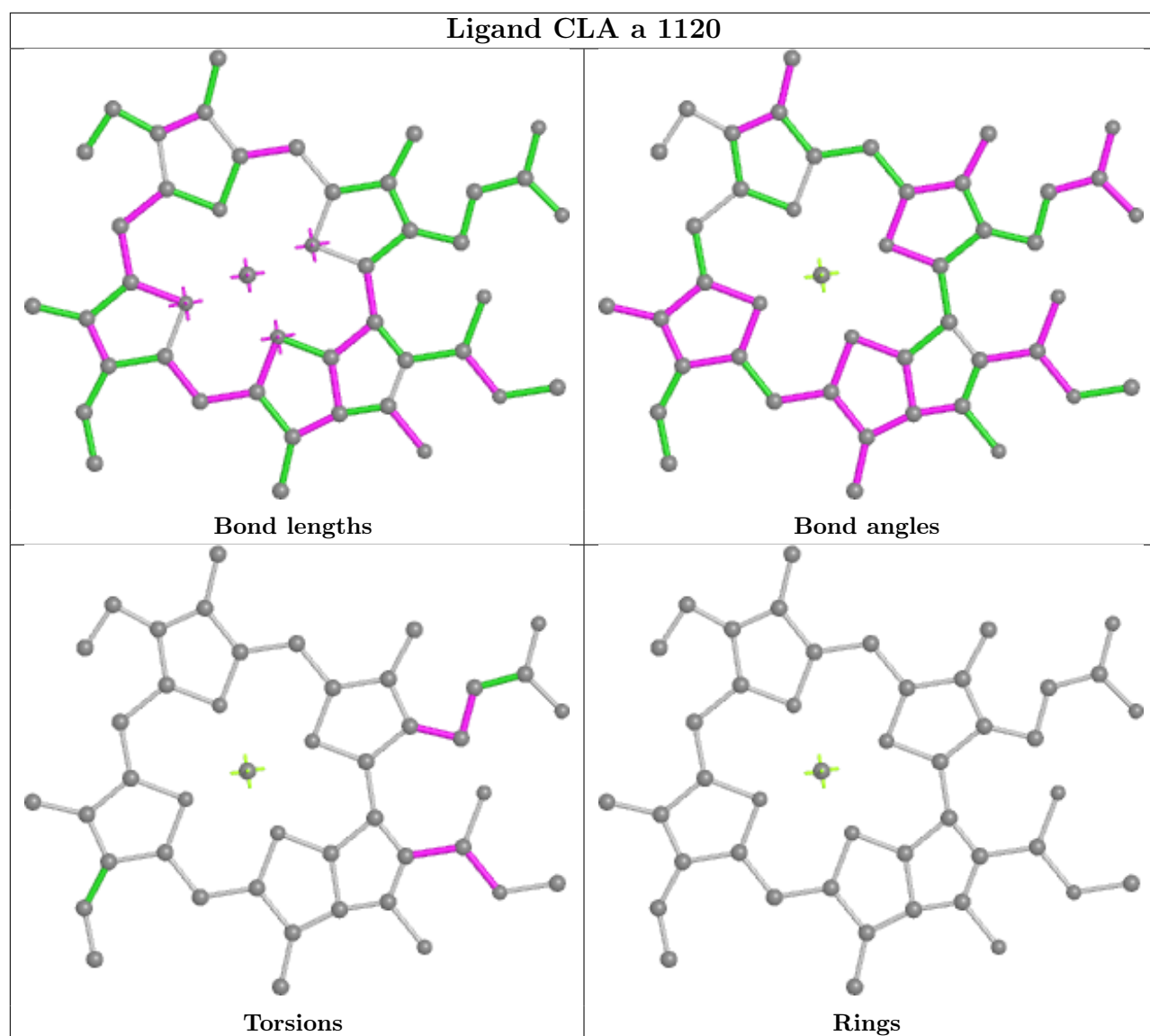
Ligand CLA B 1222

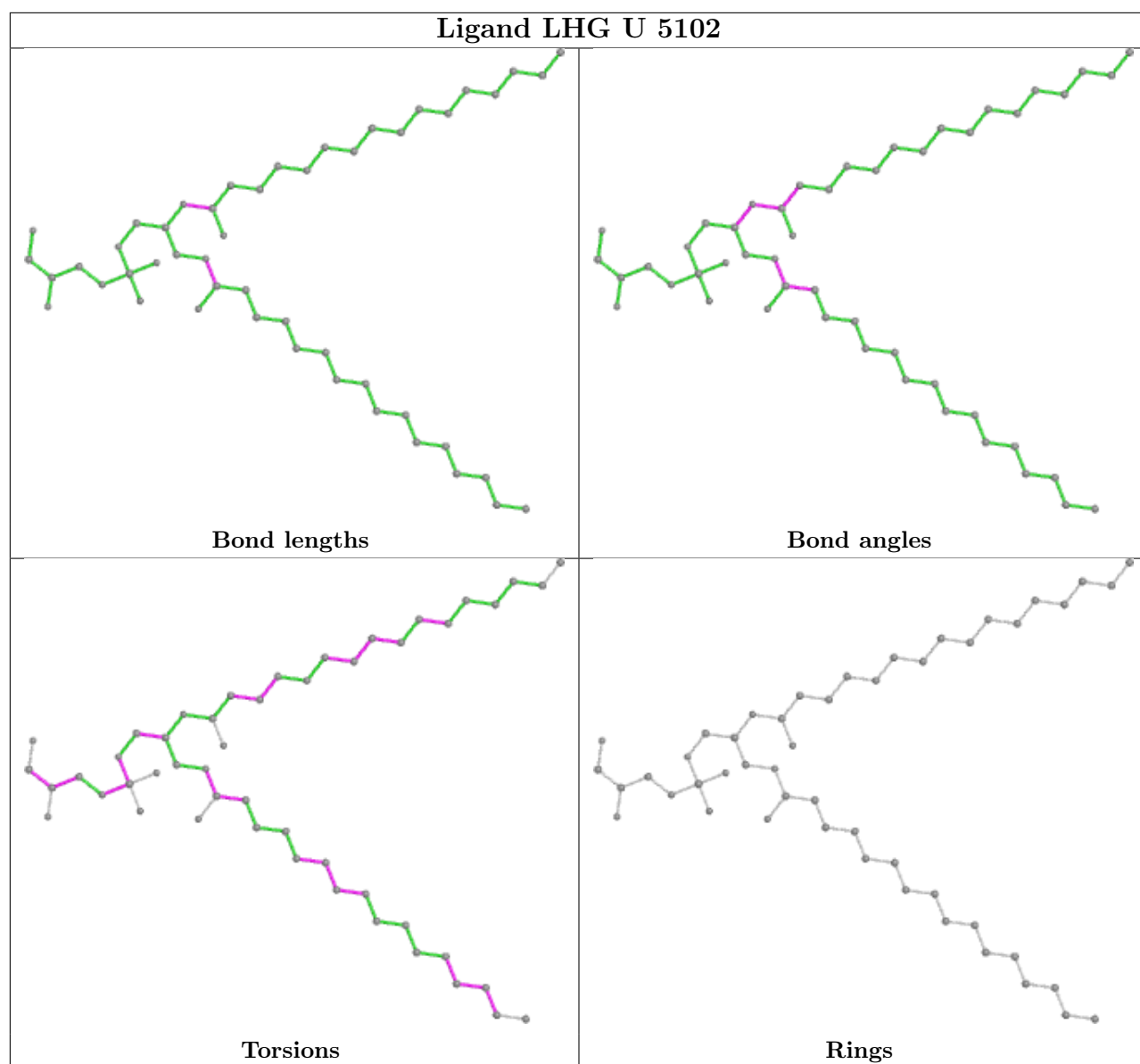


Ligand CLA G 1110

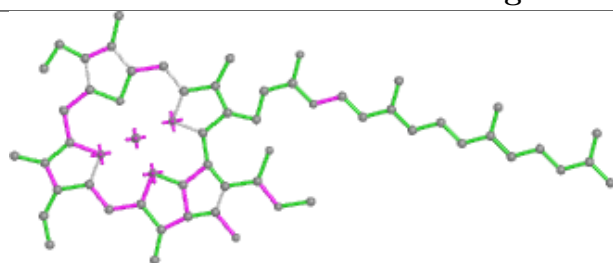




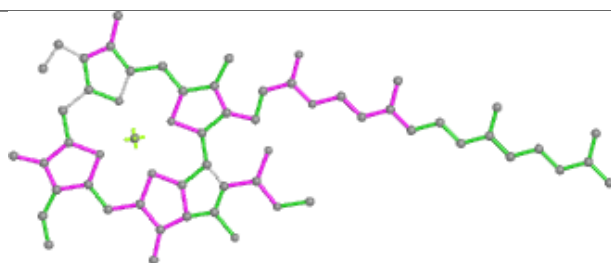




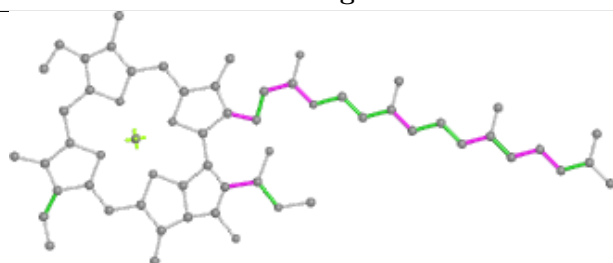
Ligand CLA U 1502



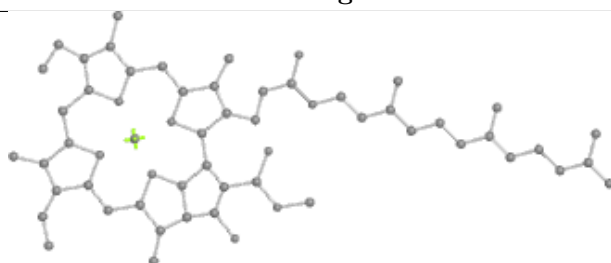
Bond lengths



Bond angles

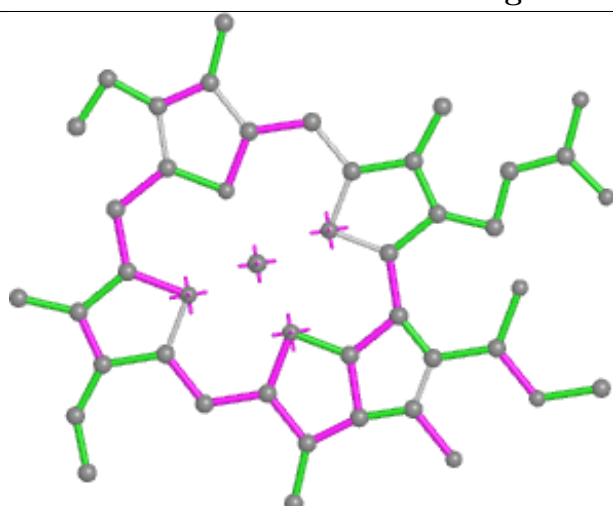


Torsions

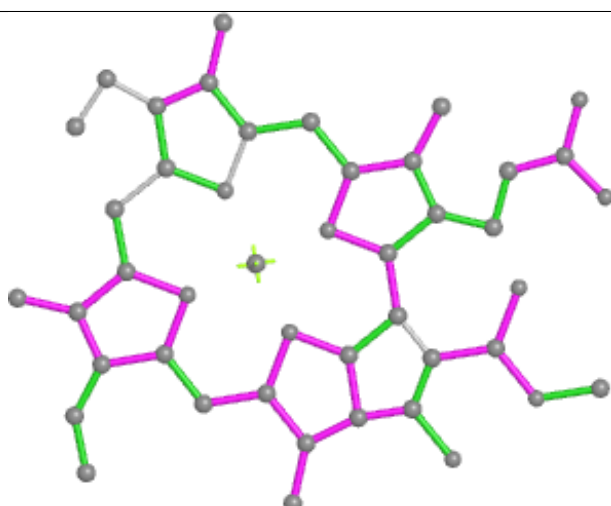


Rings

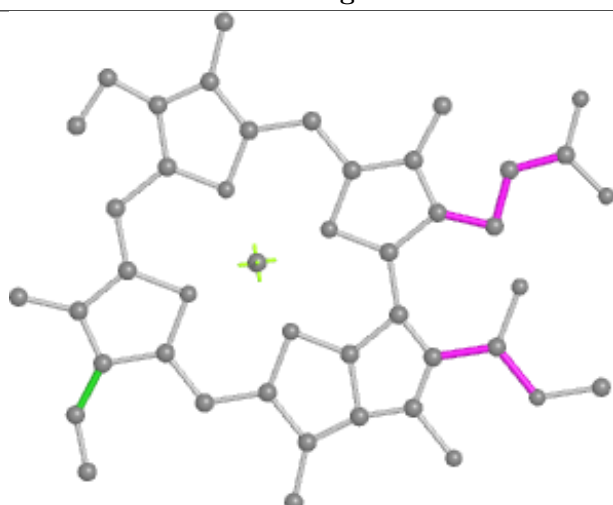
Ligand CLA A 1134



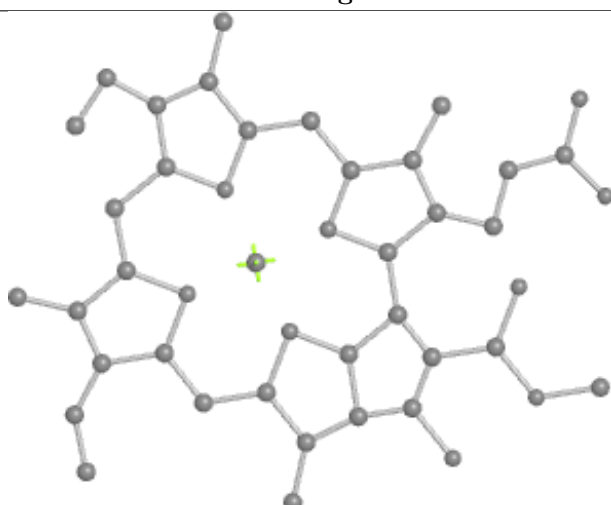
Bond lengths



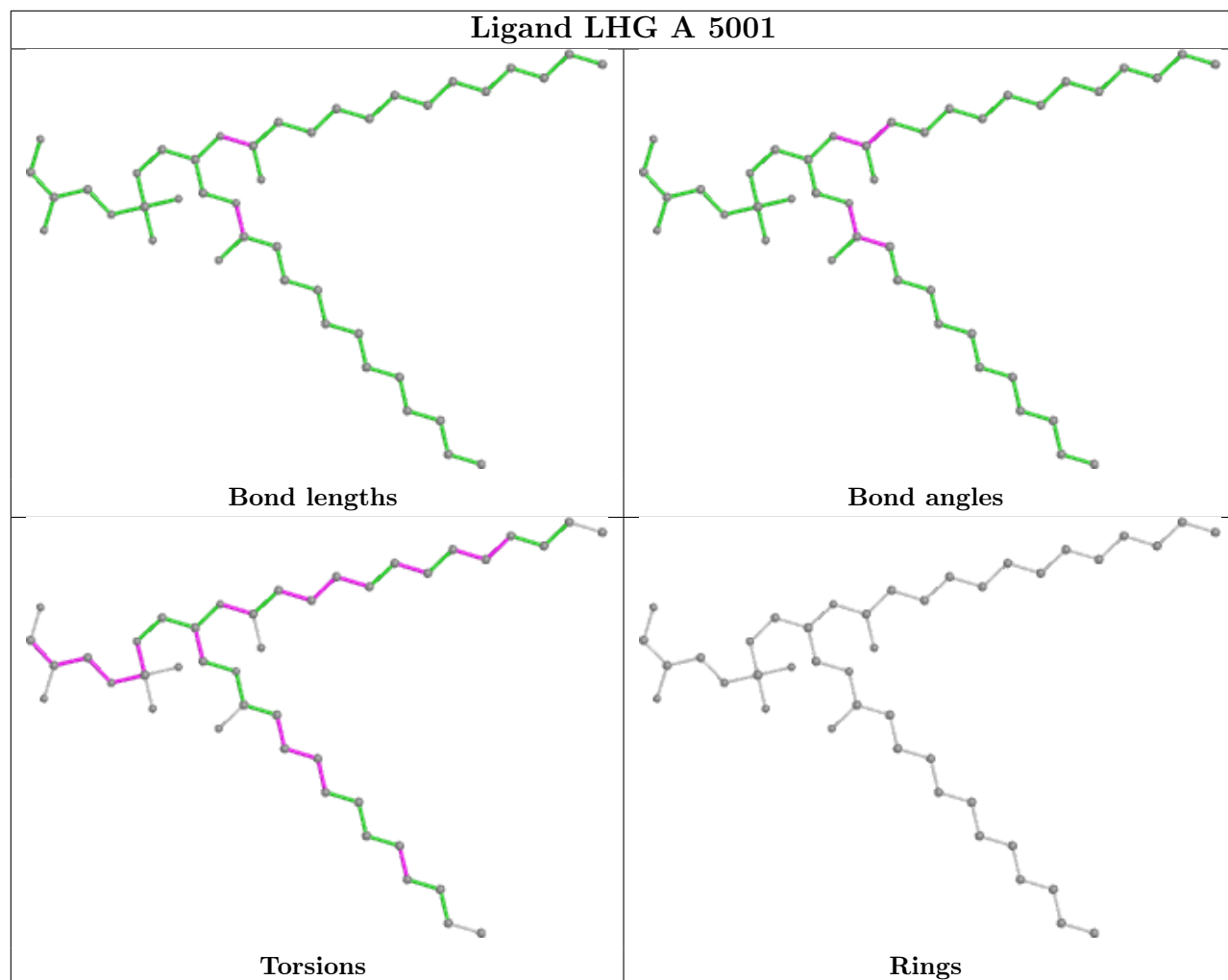
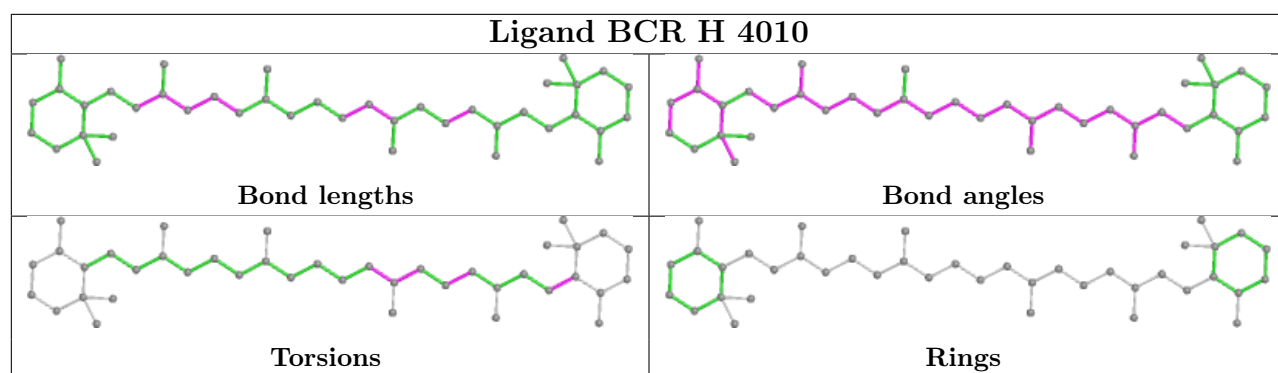
Bond angles

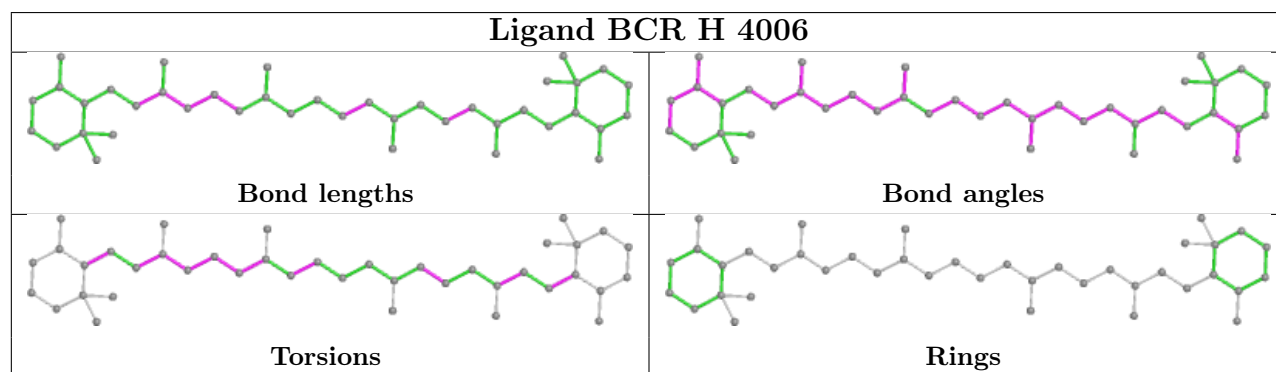
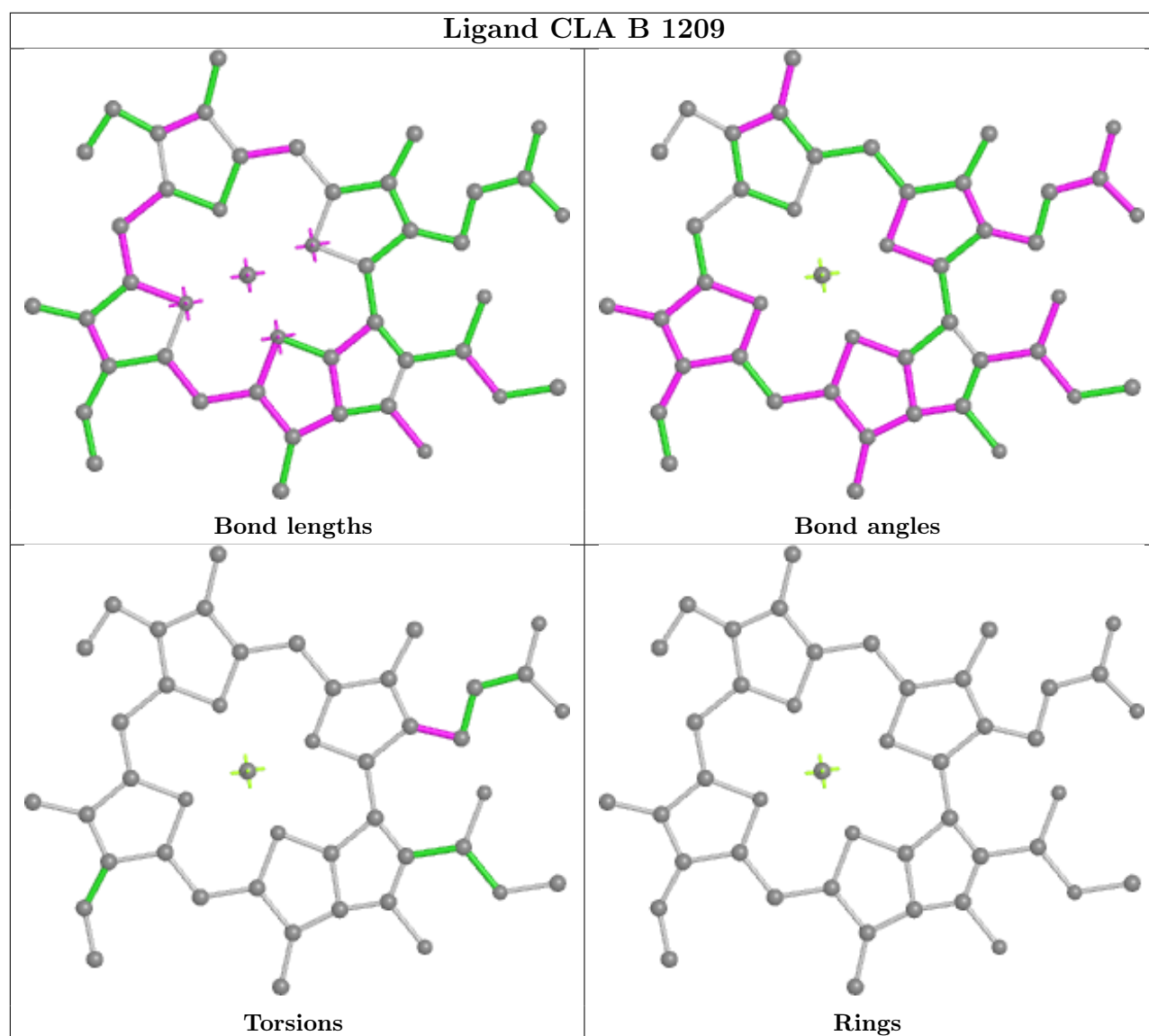


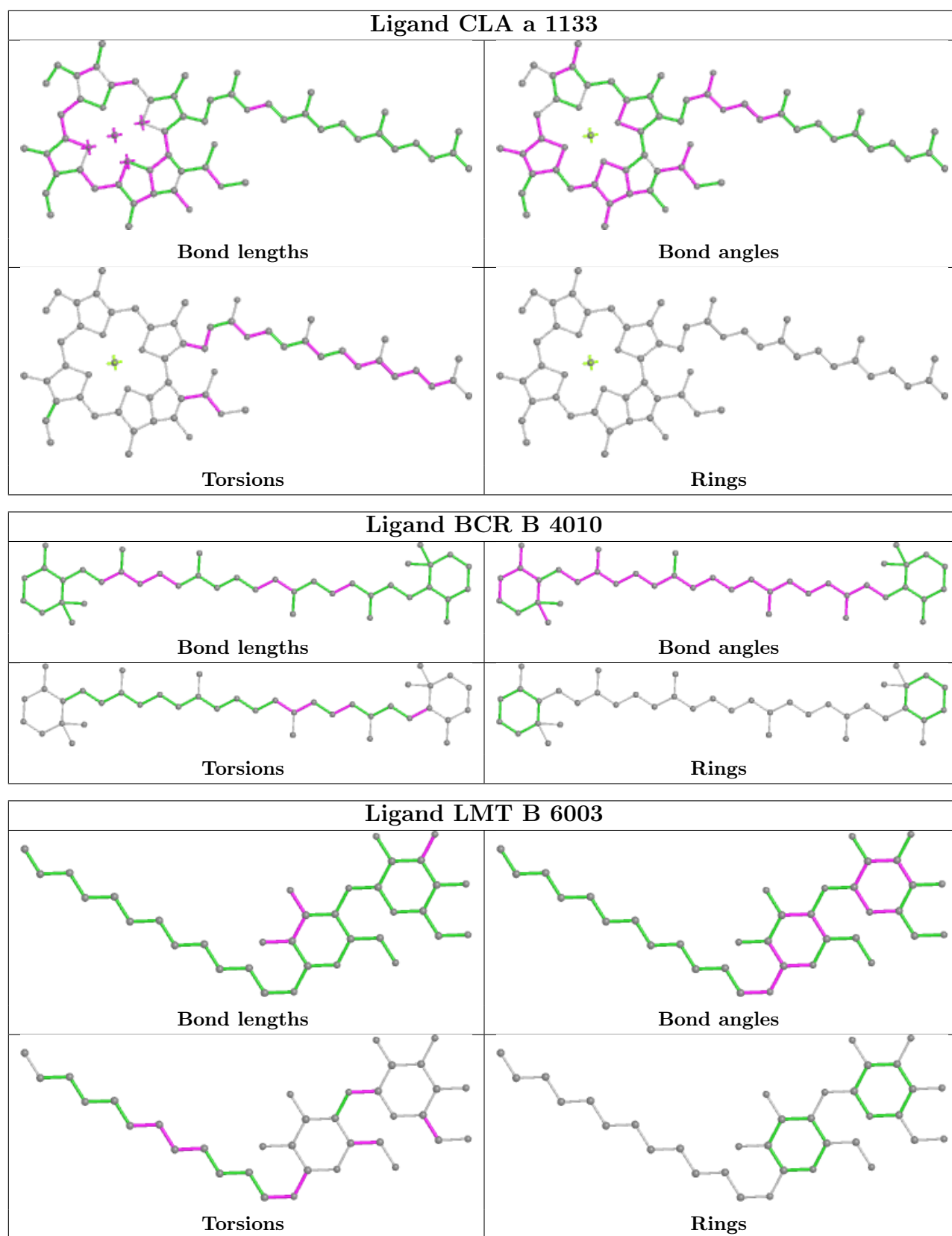
Torsions

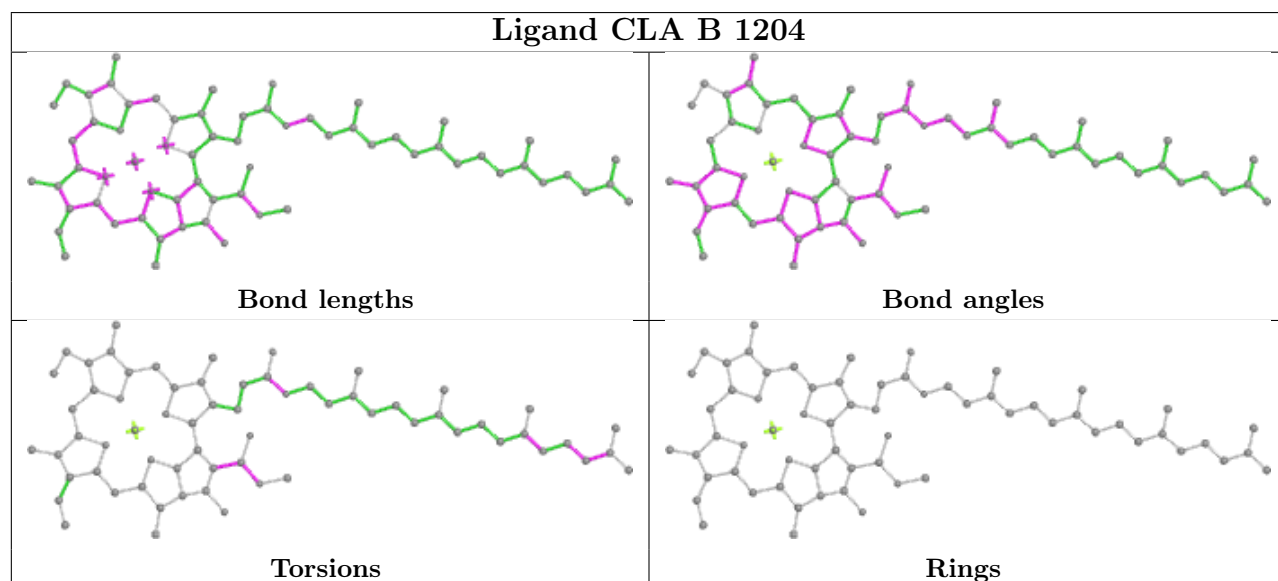
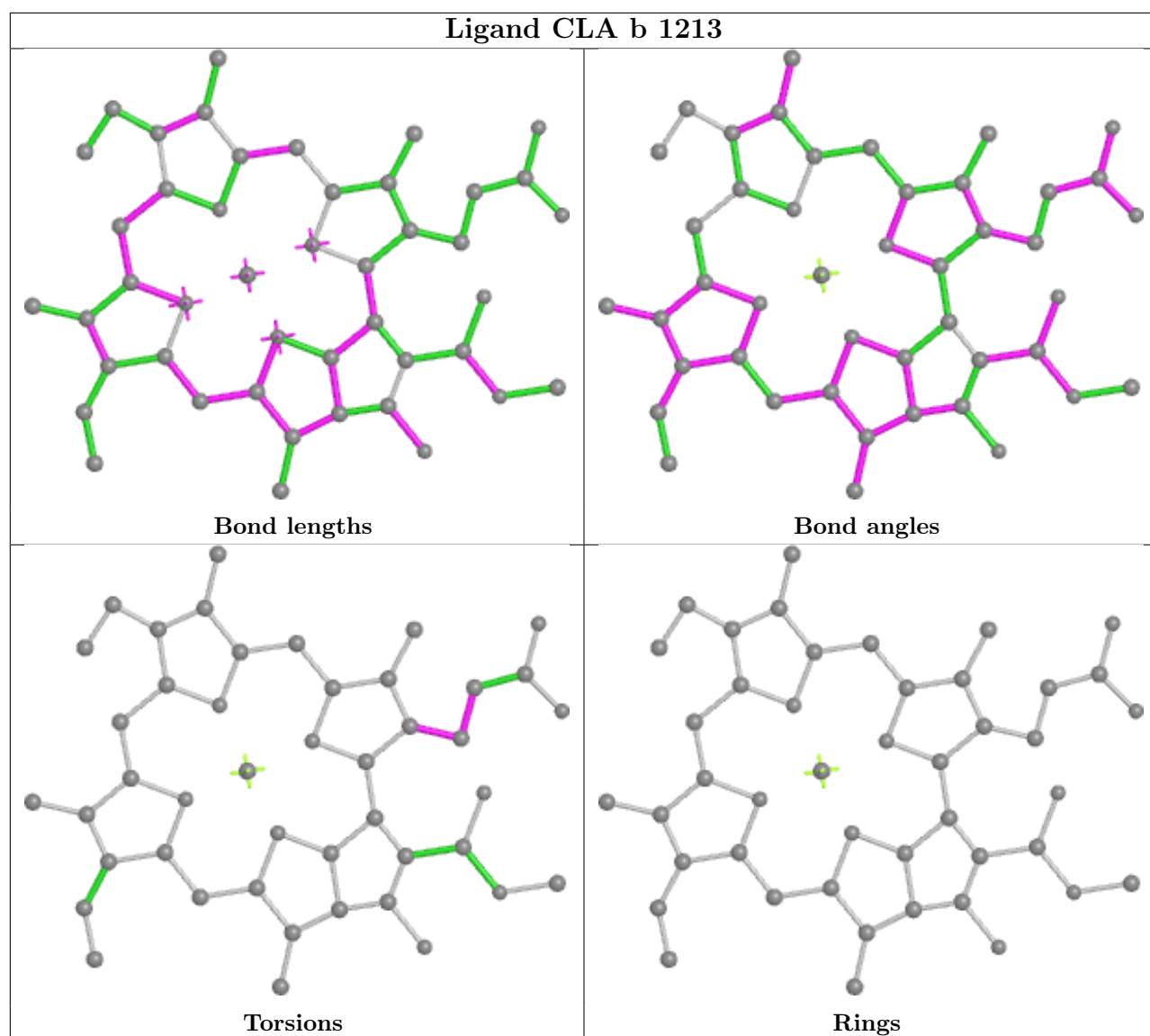


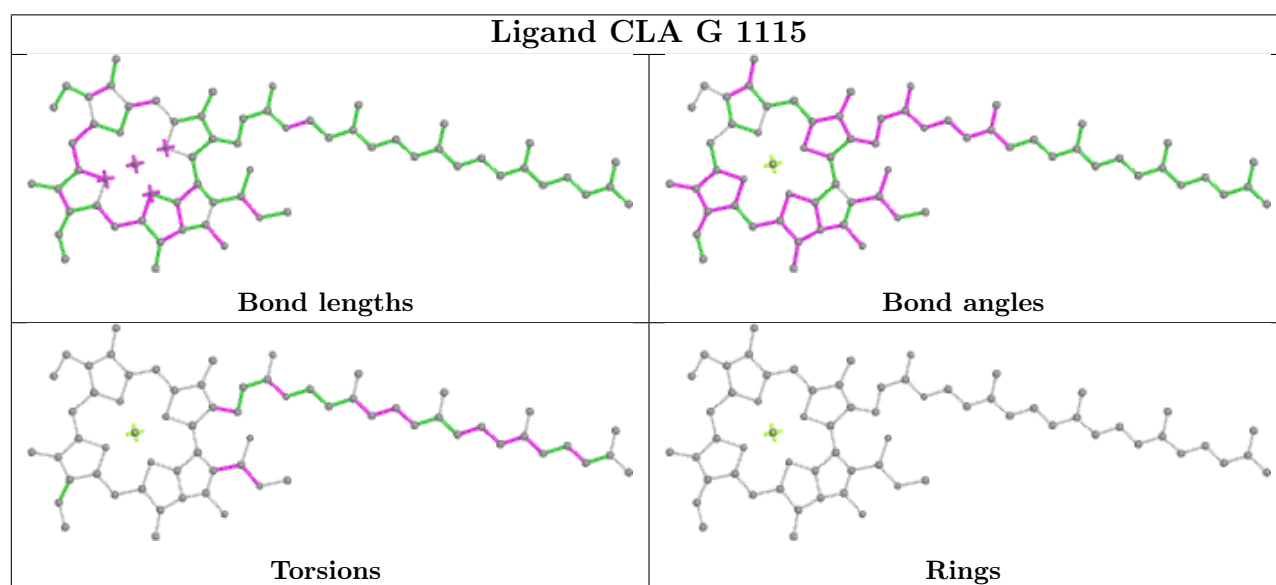
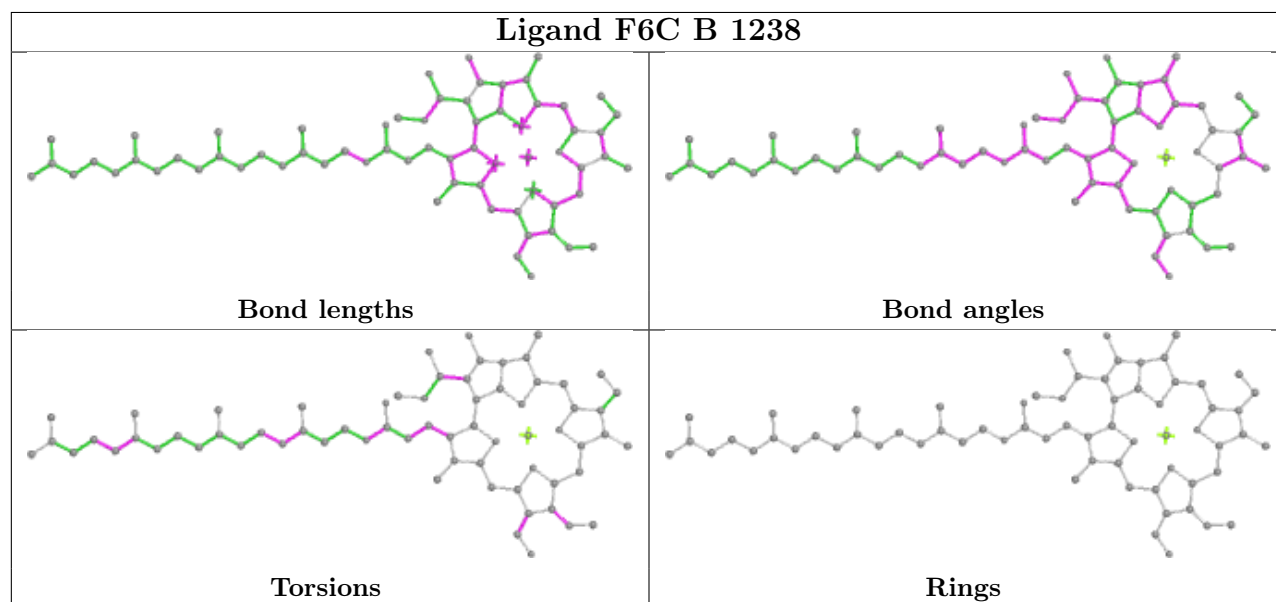
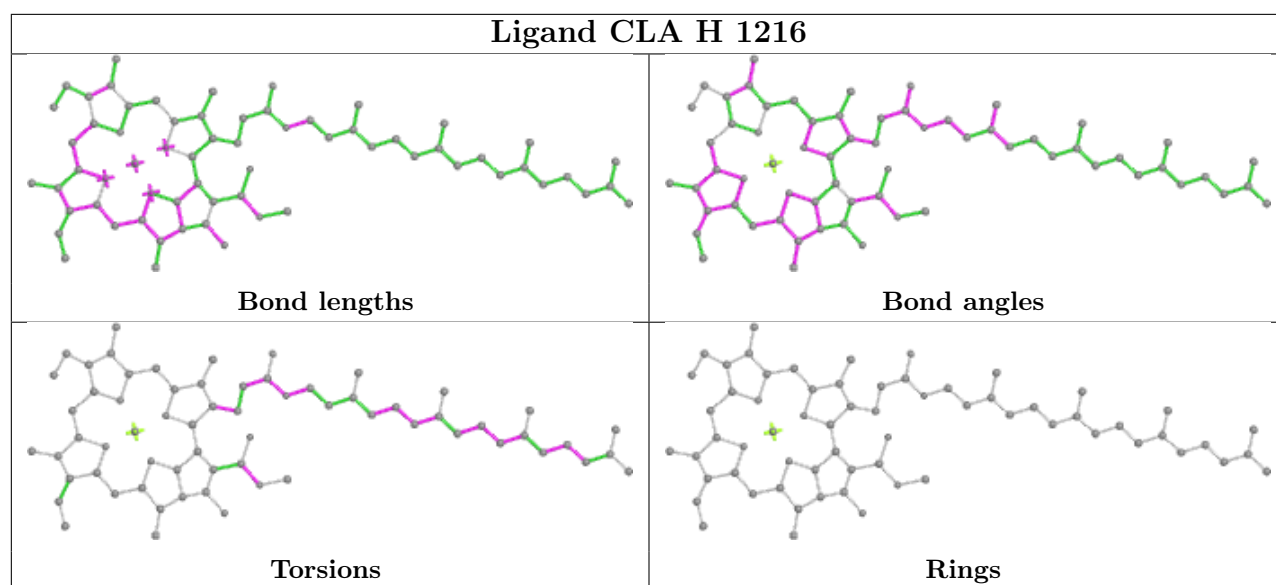
Rings

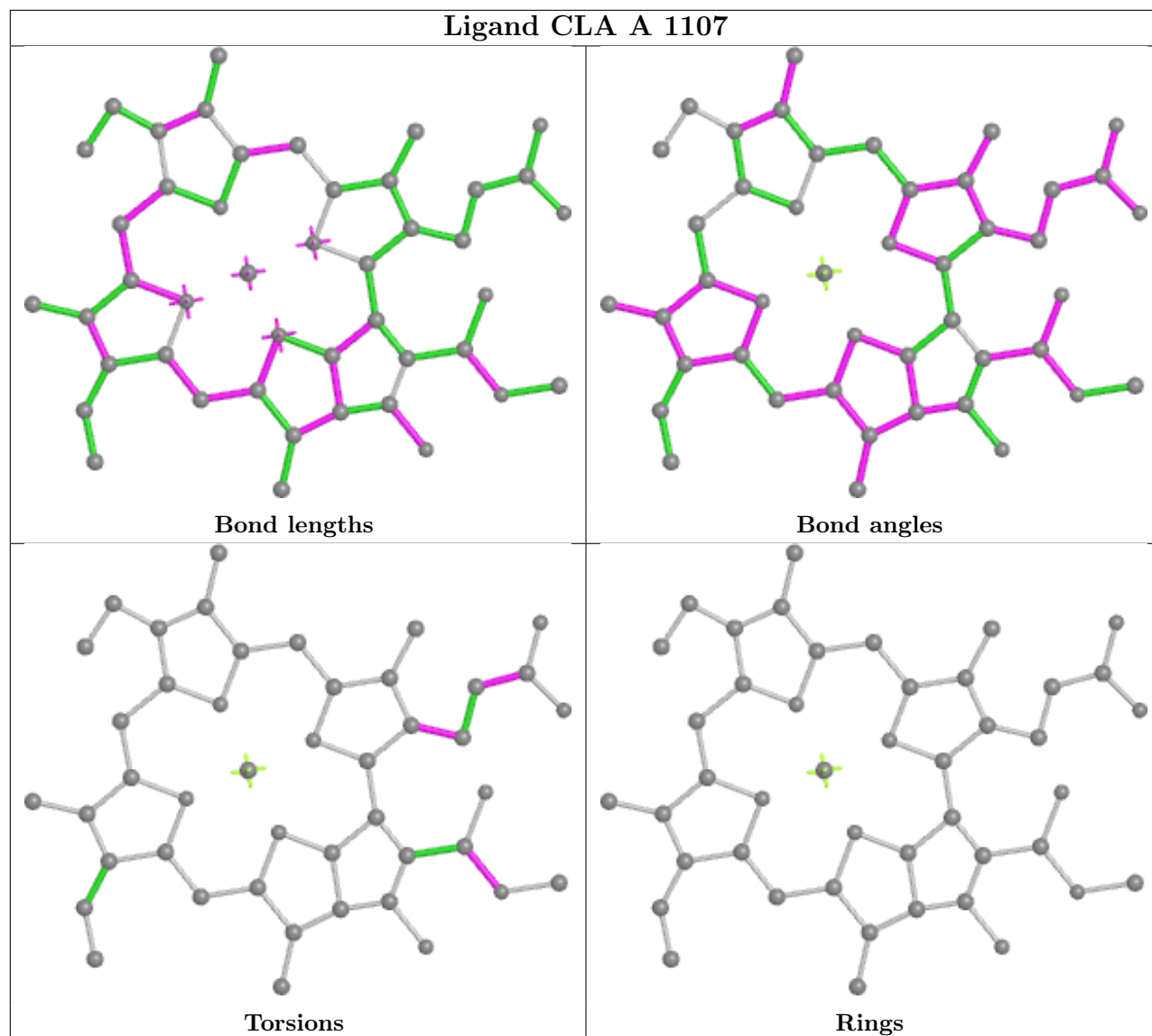


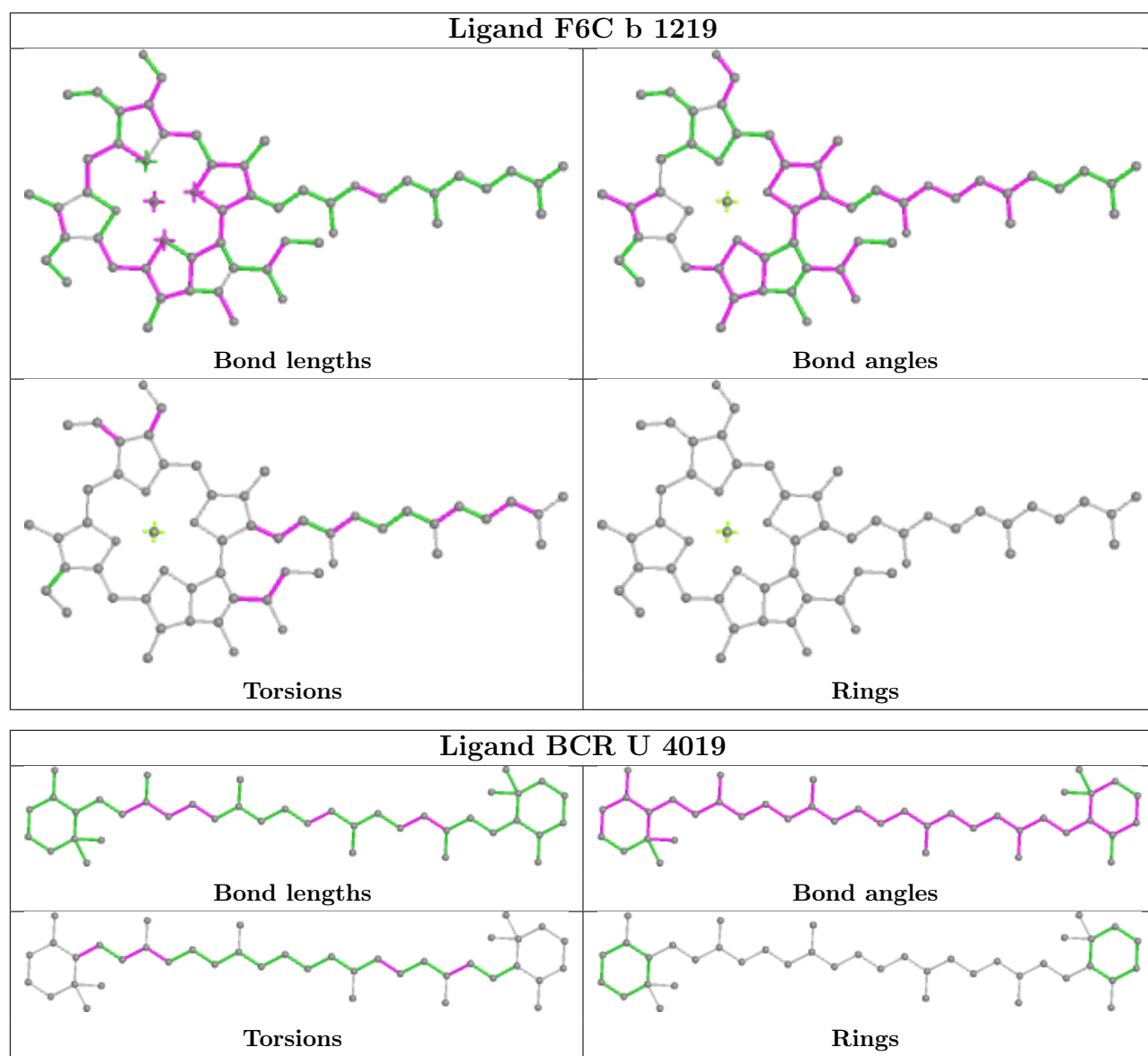


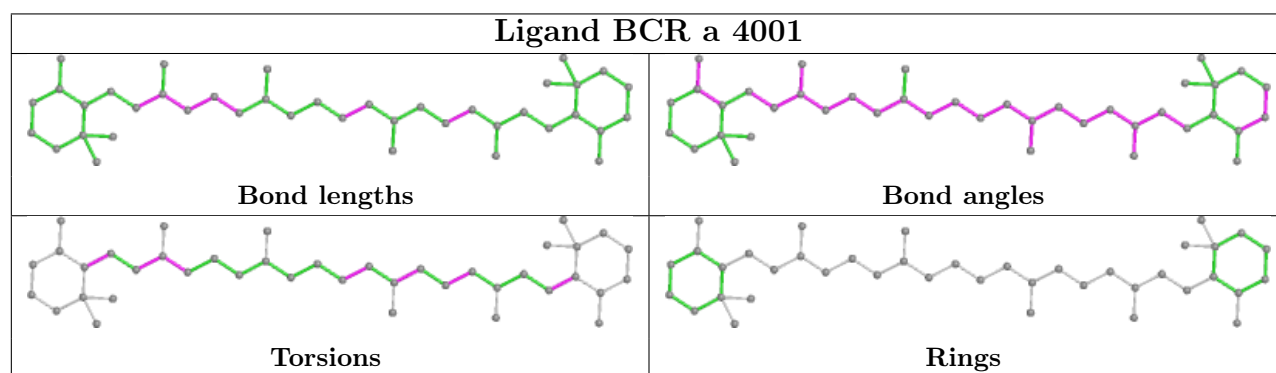
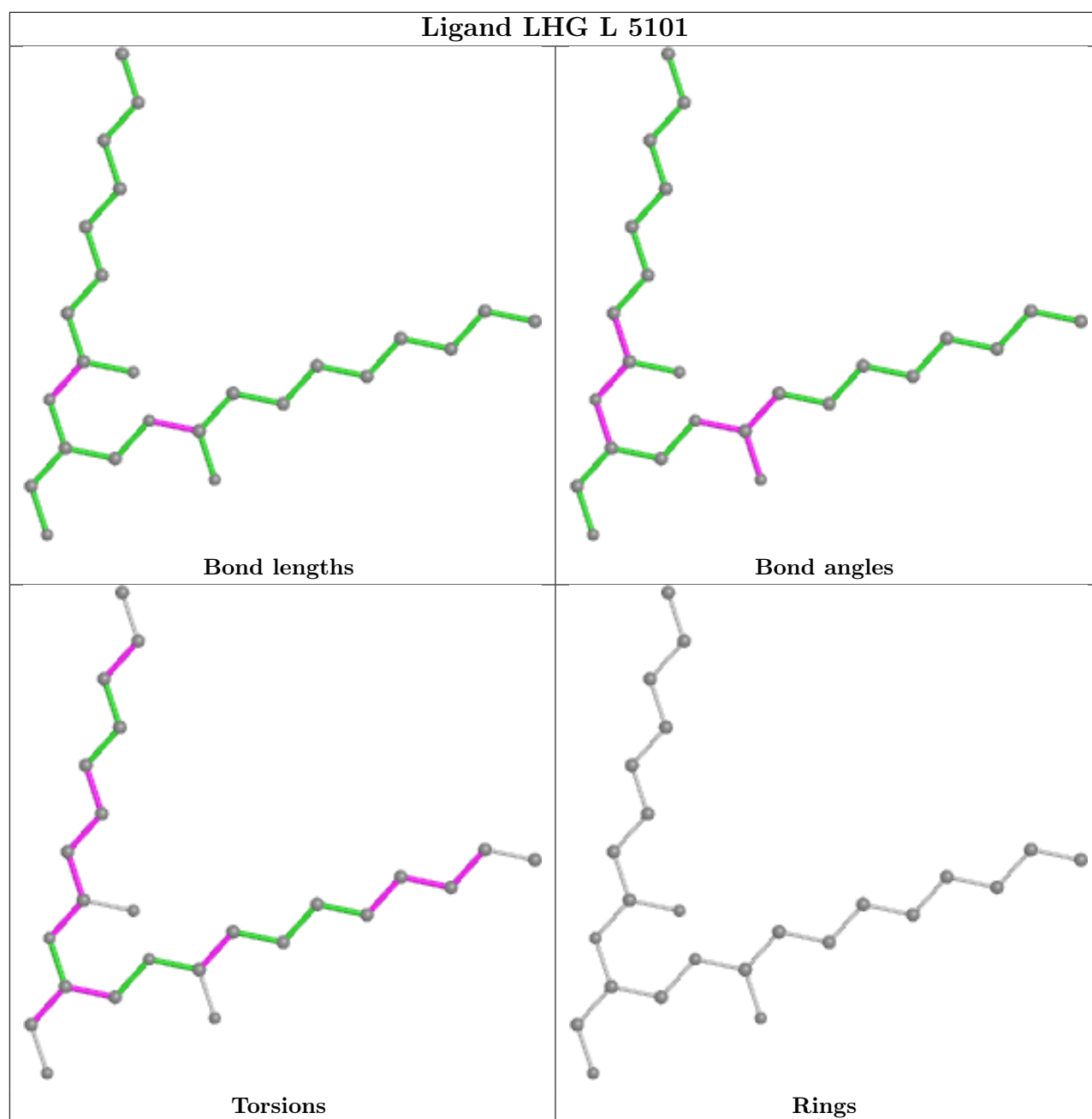


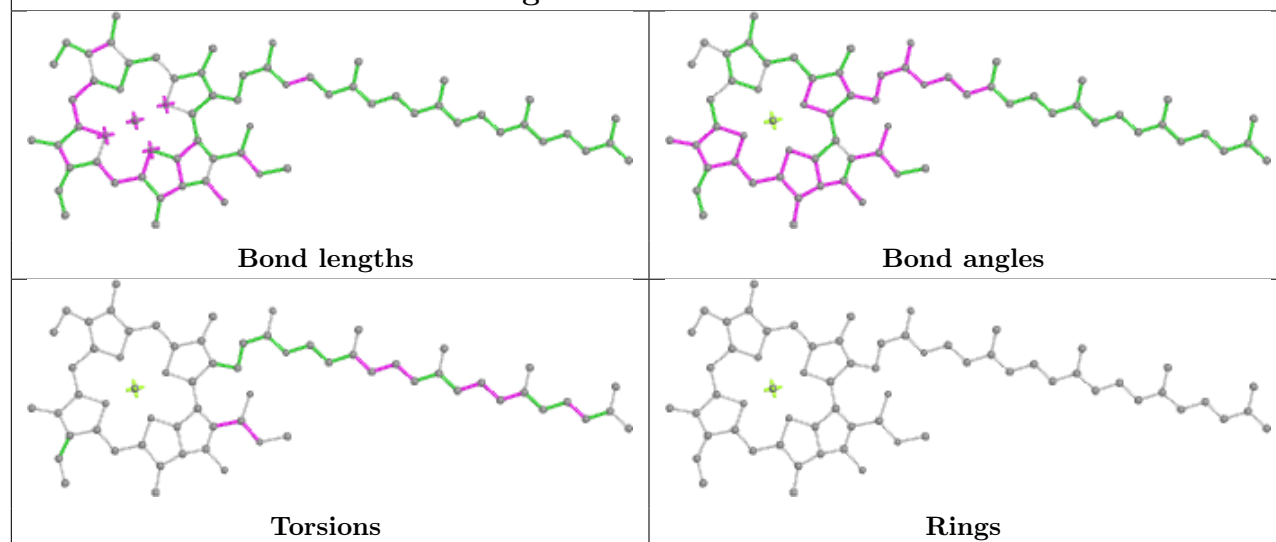
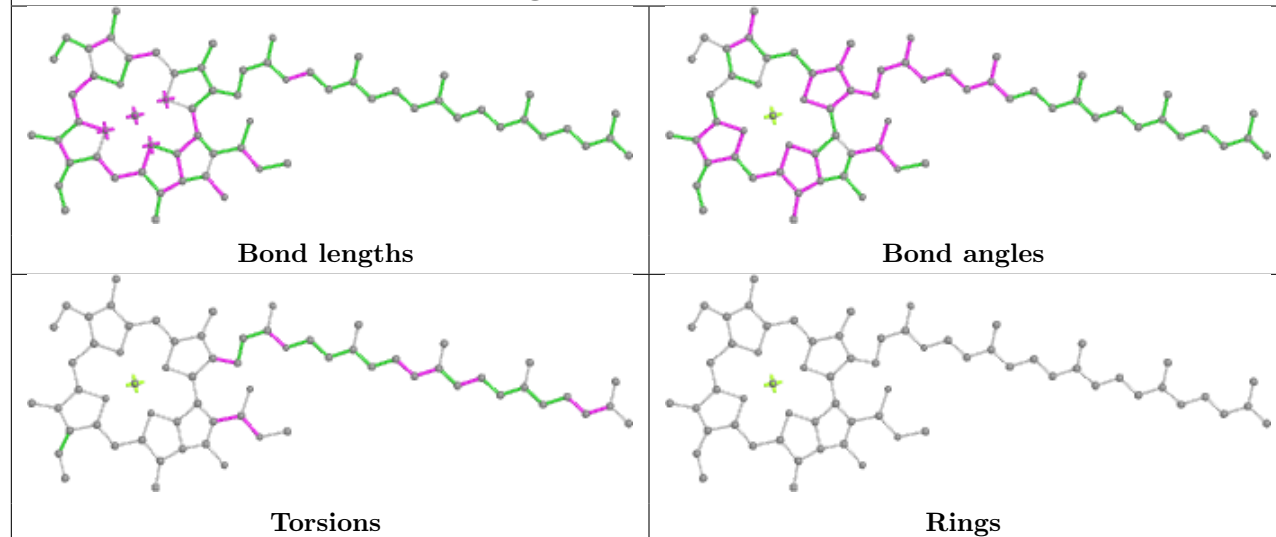


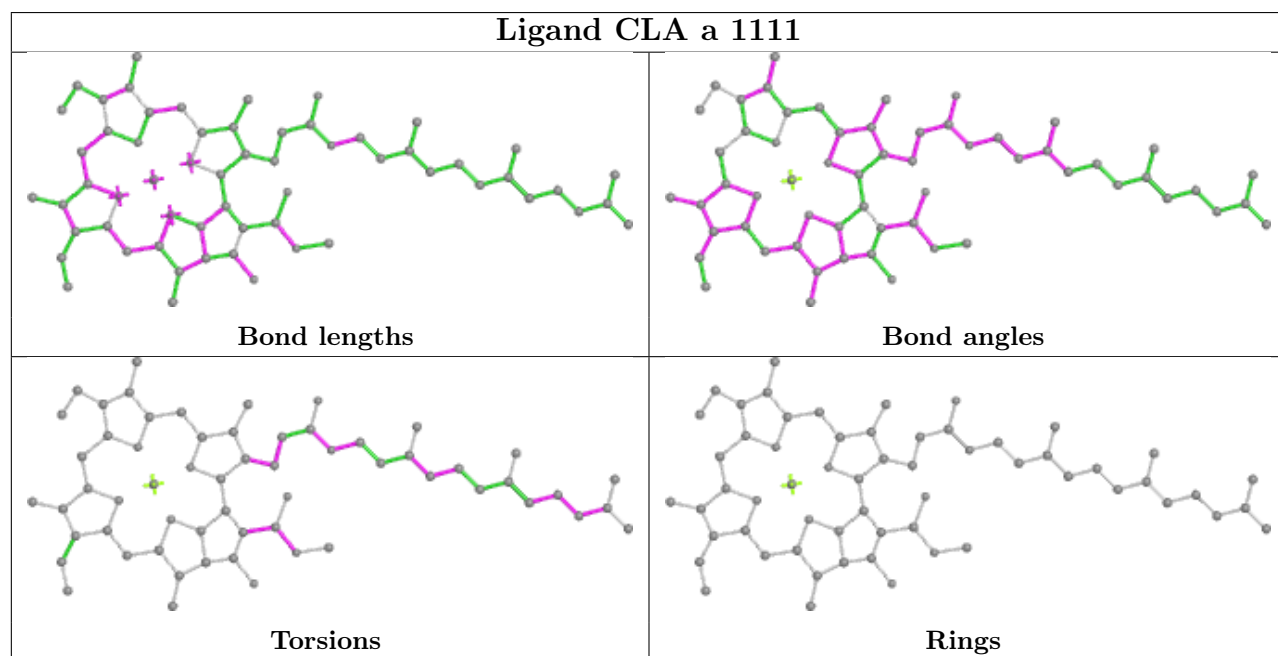
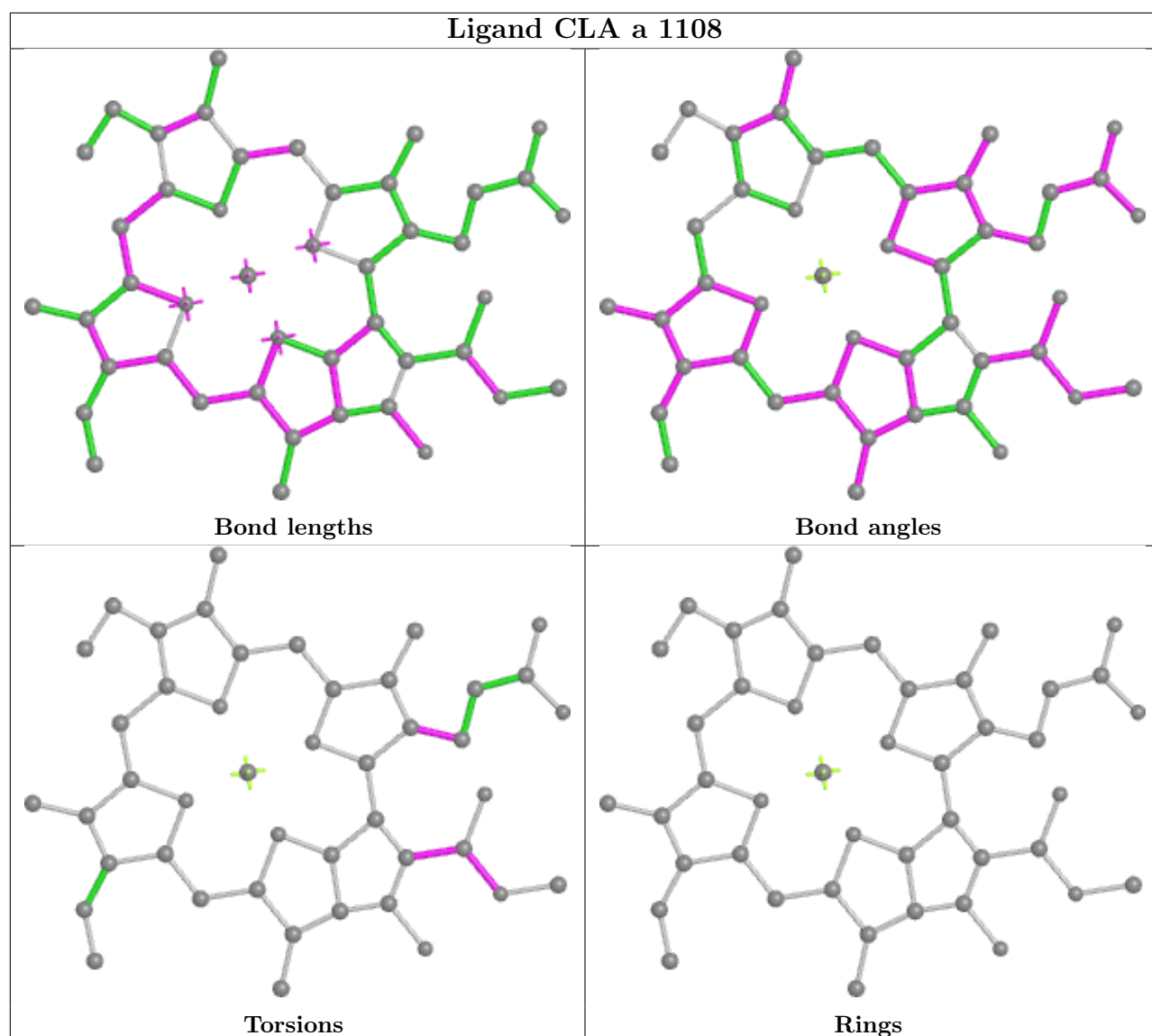


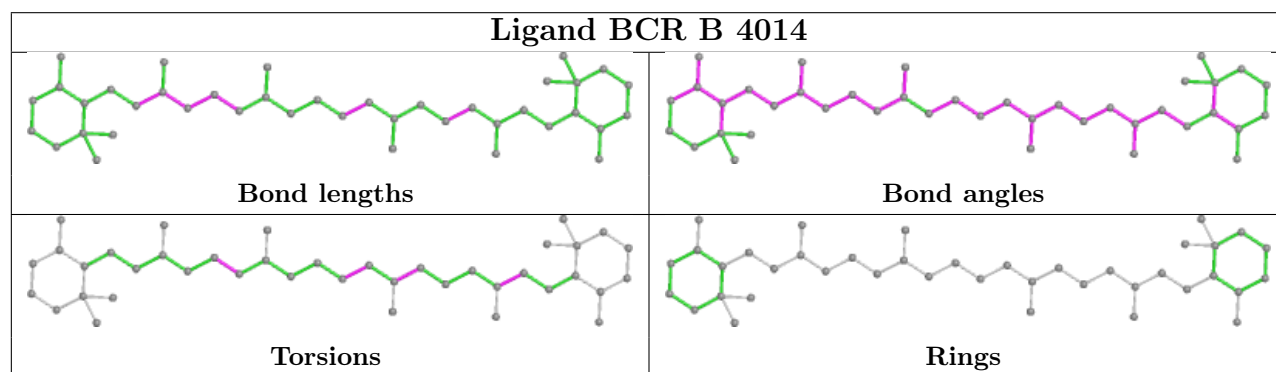
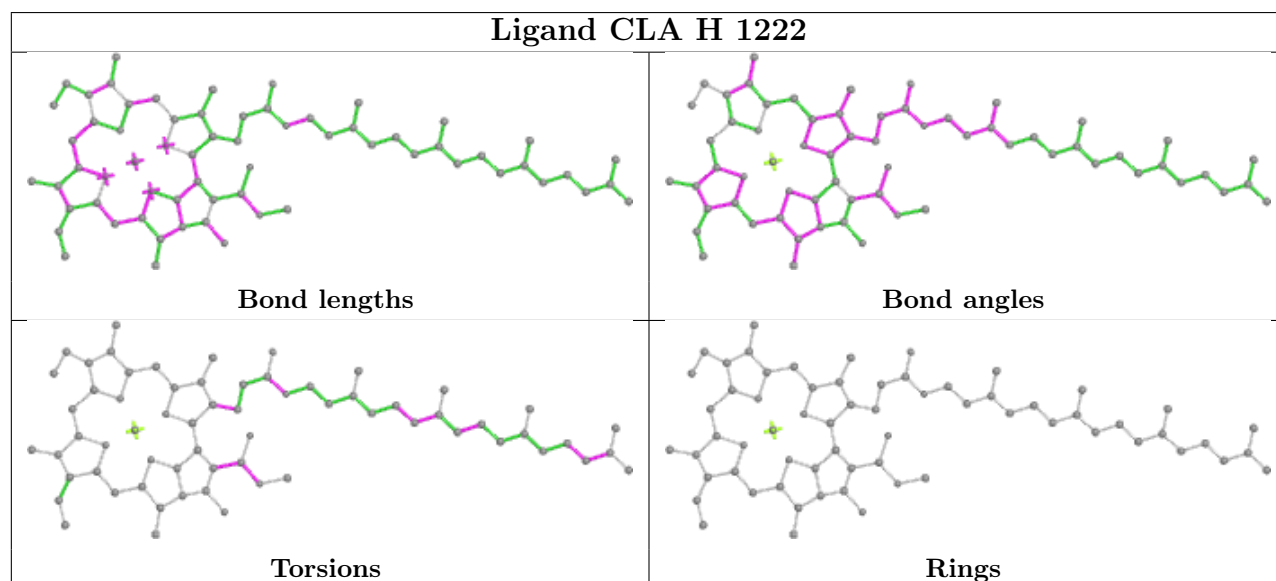
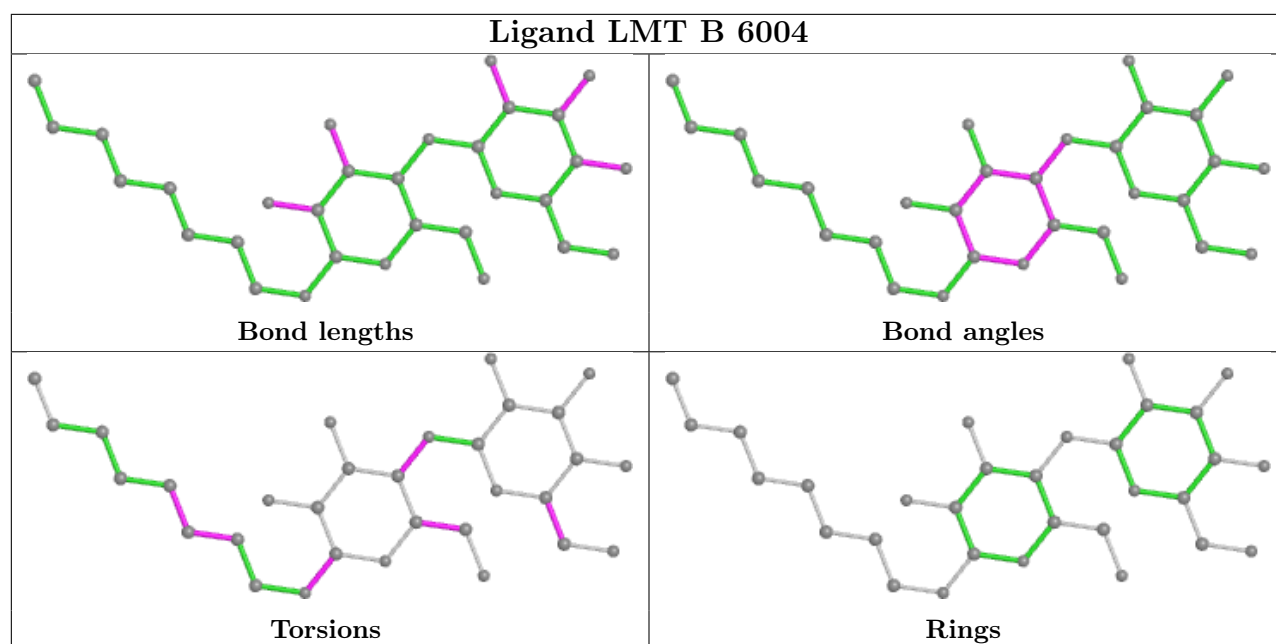


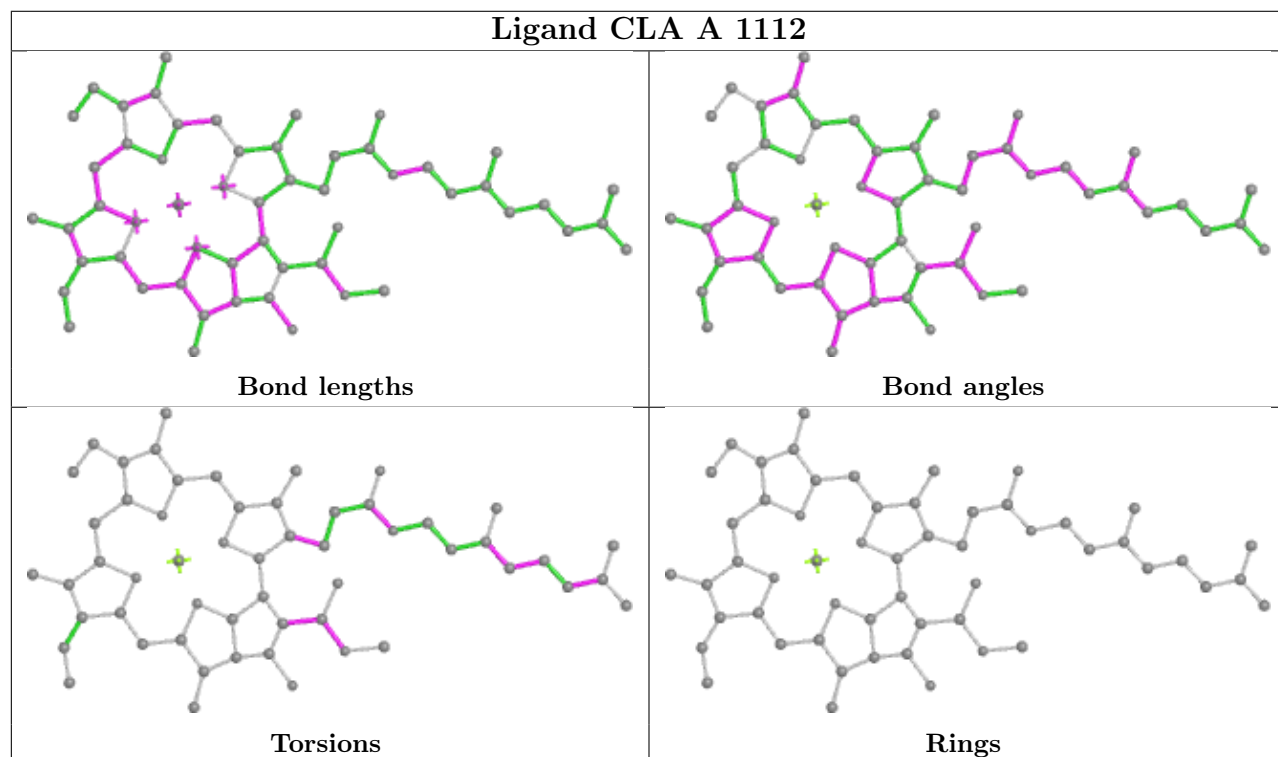
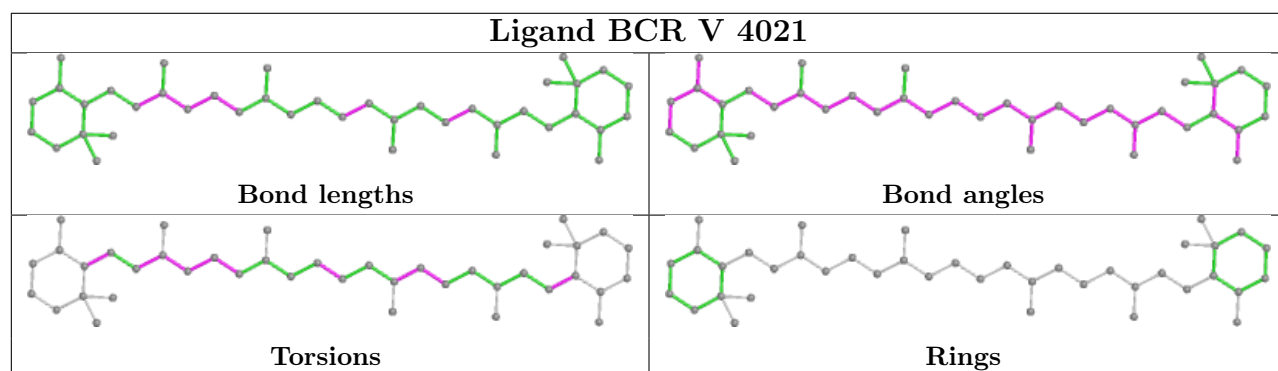
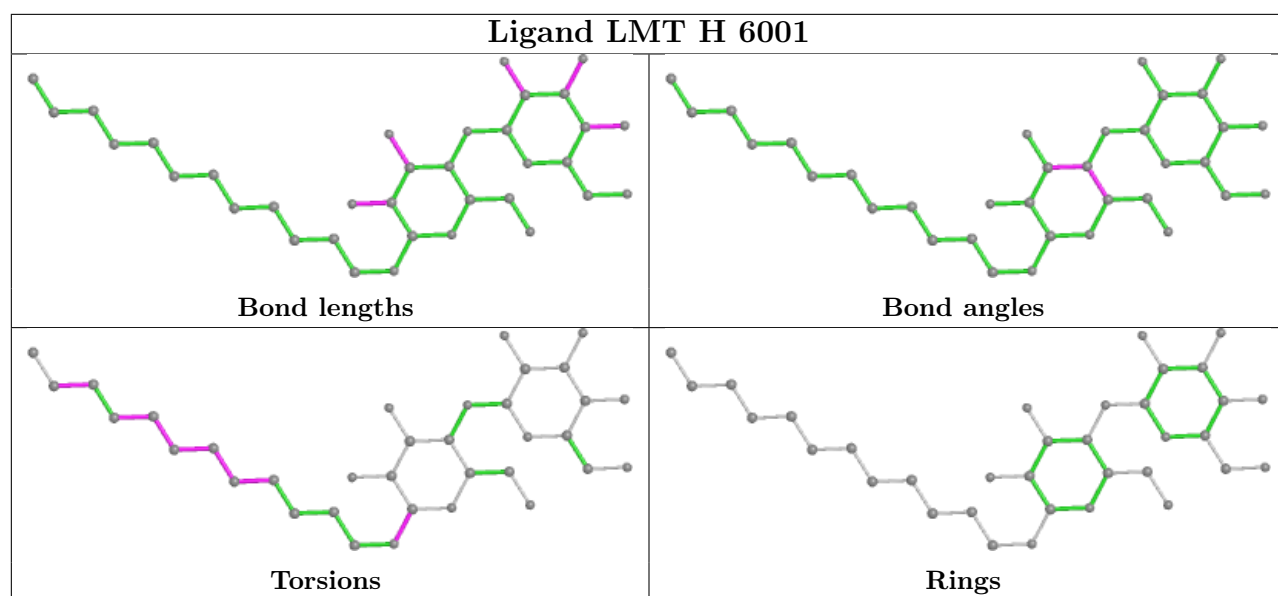




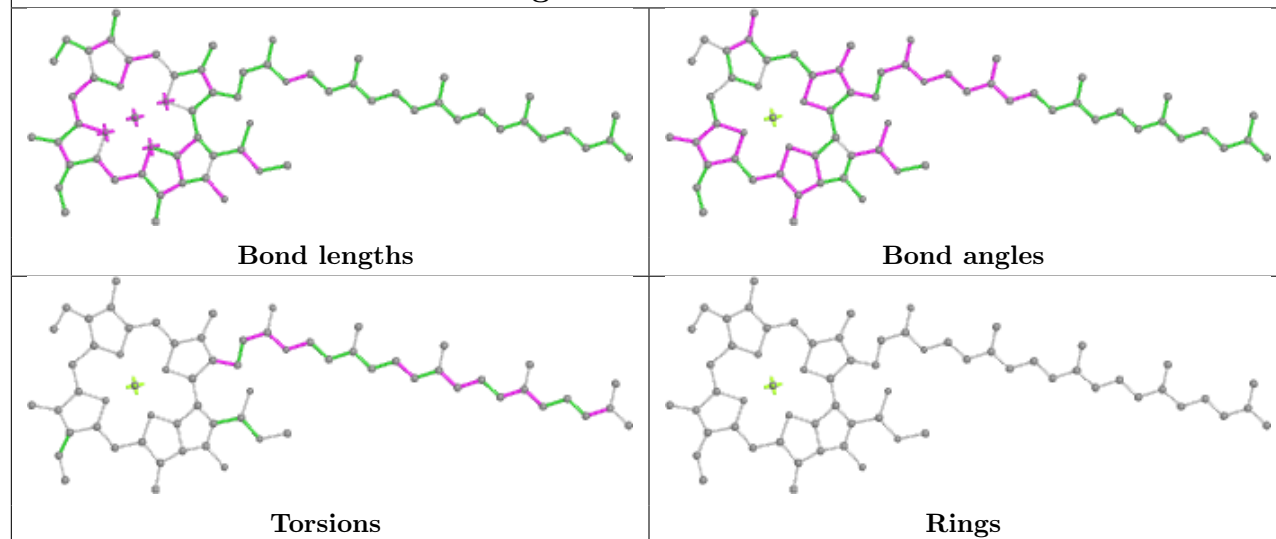
Ligand CLA H 1205**Ligand CLA b 1222**



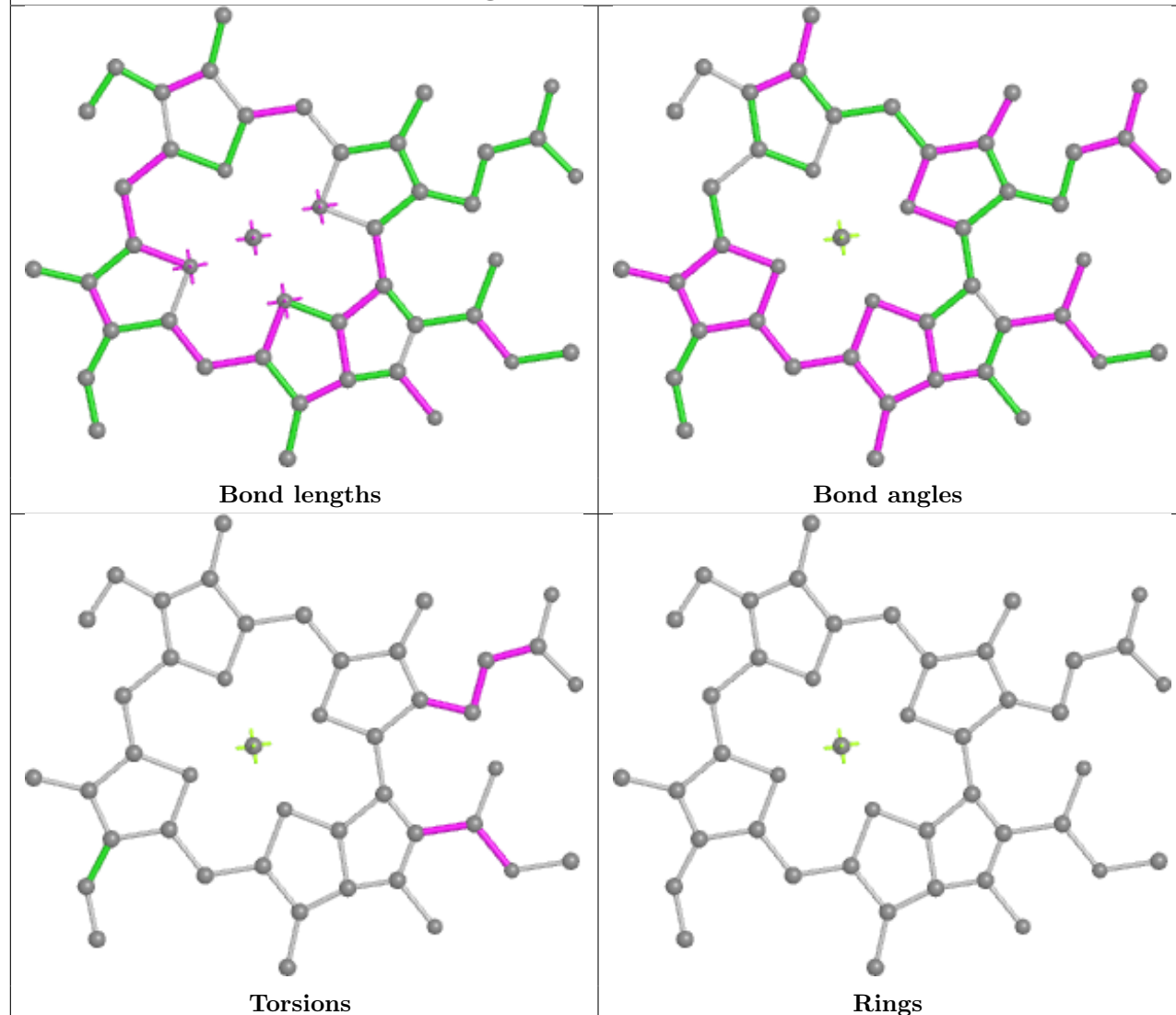


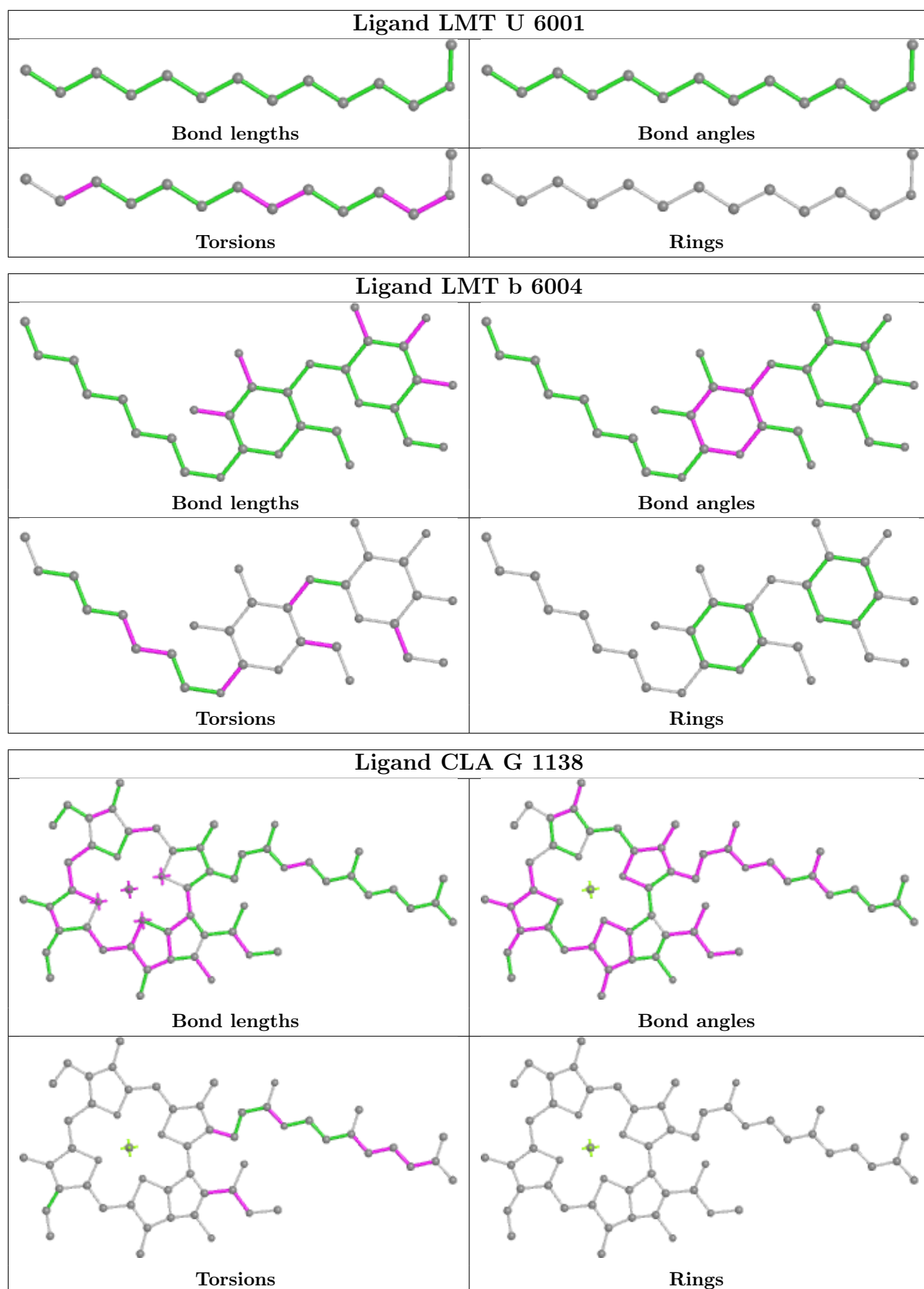


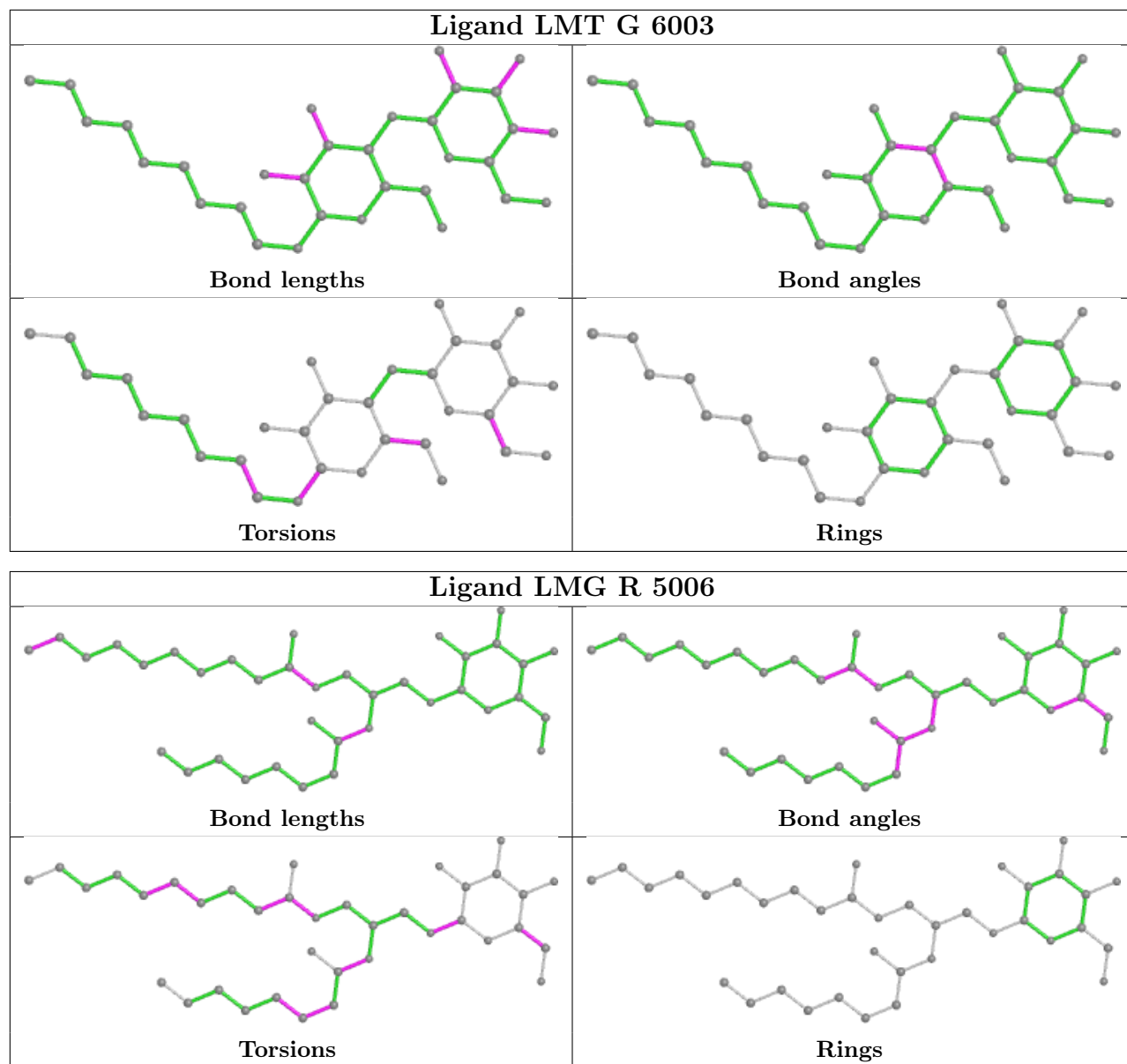
Ligand CL0 a 1011

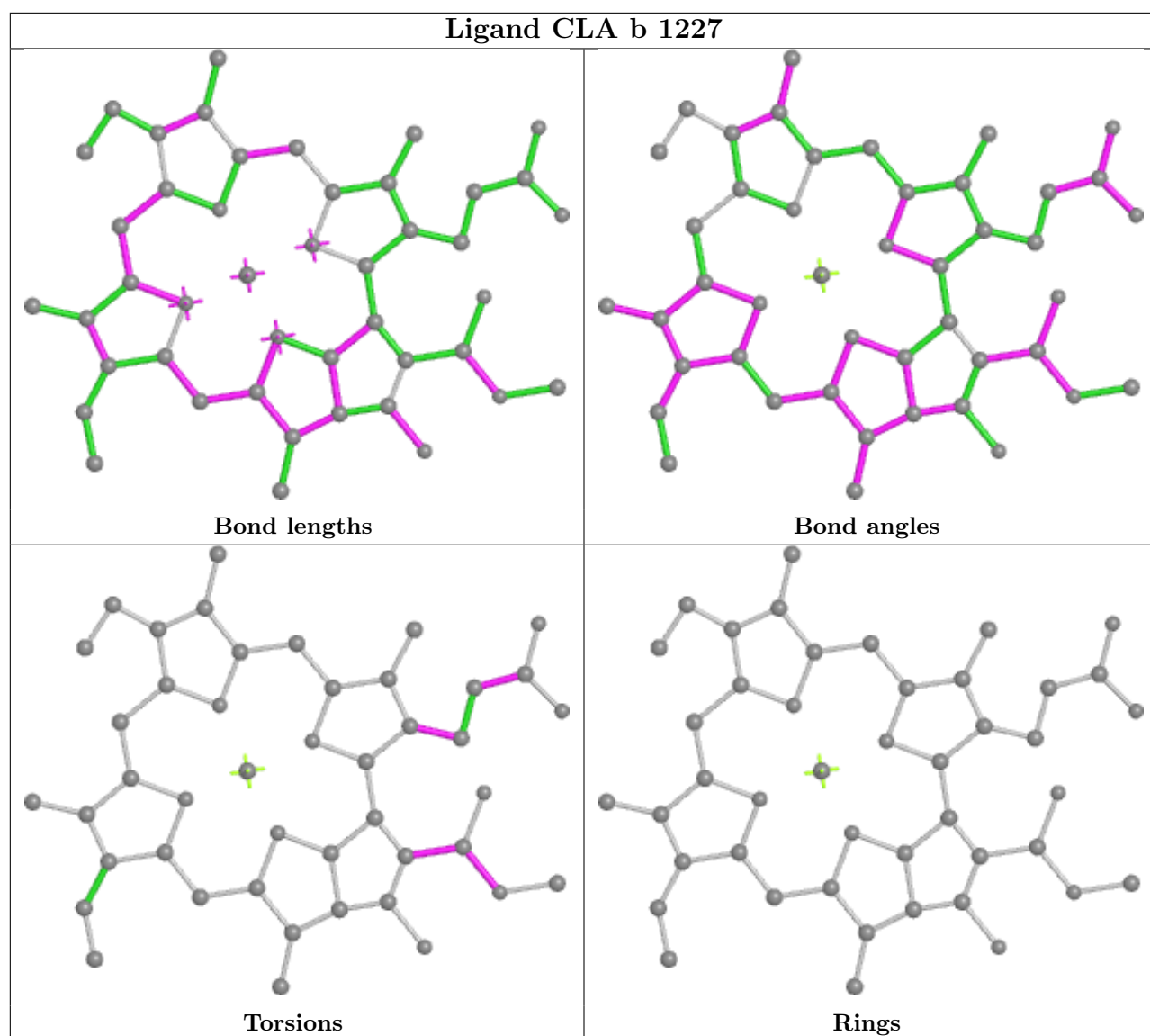


Ligand CLA B 1217

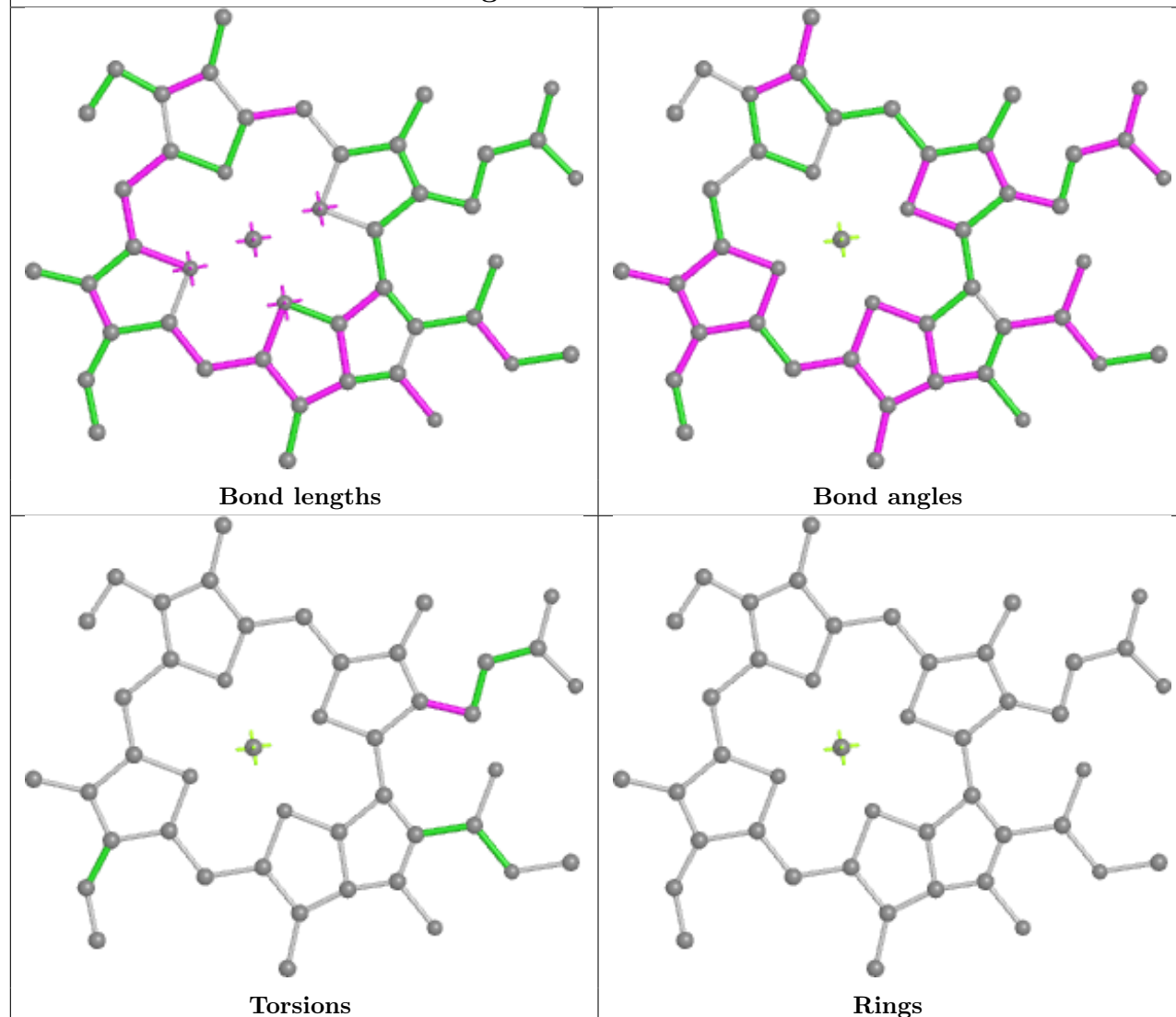




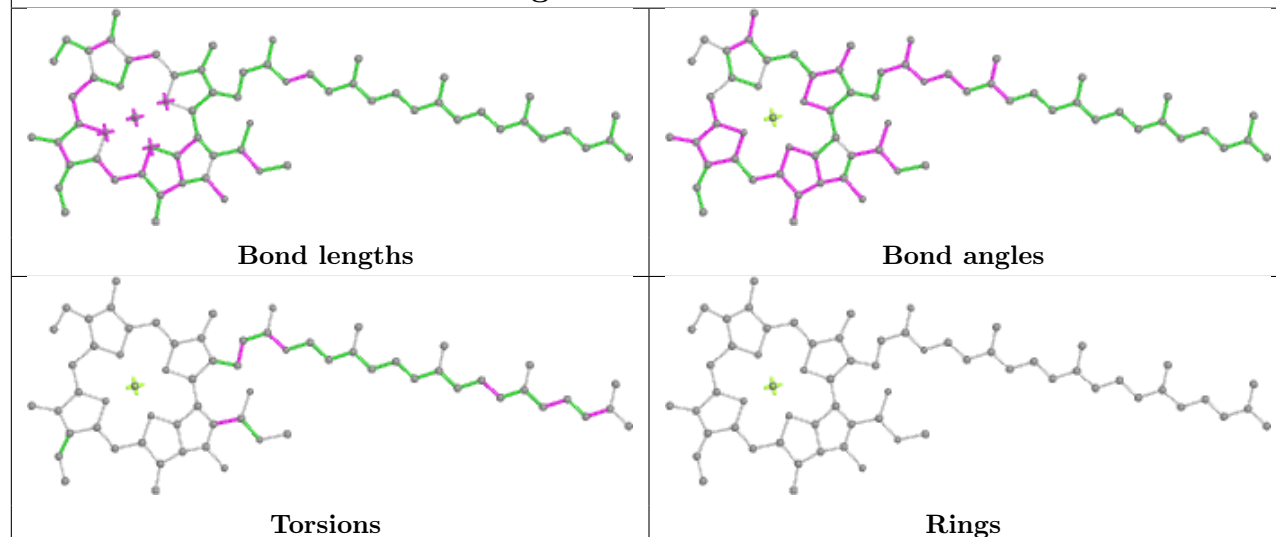


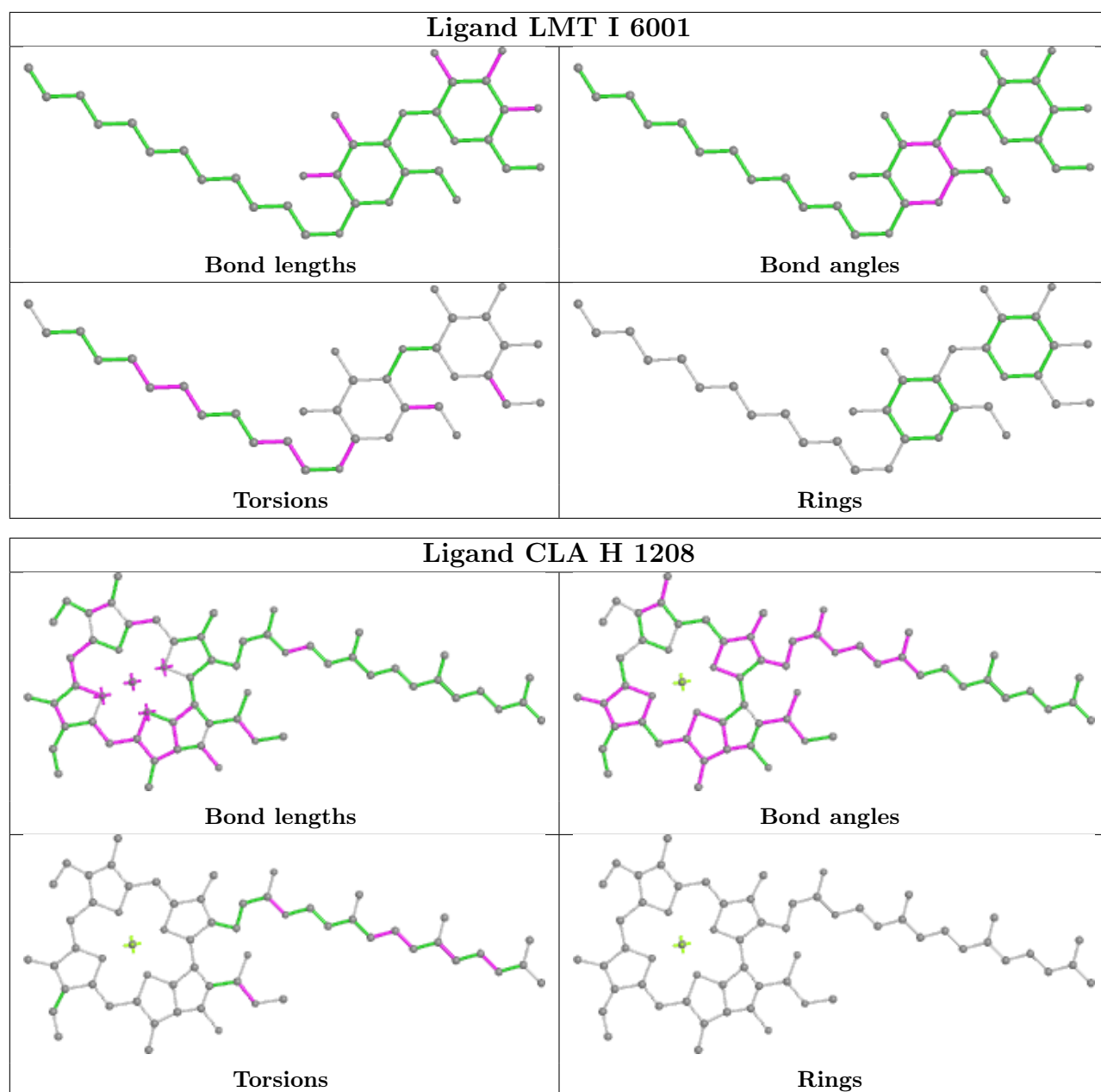


Ligand CLA H 1209

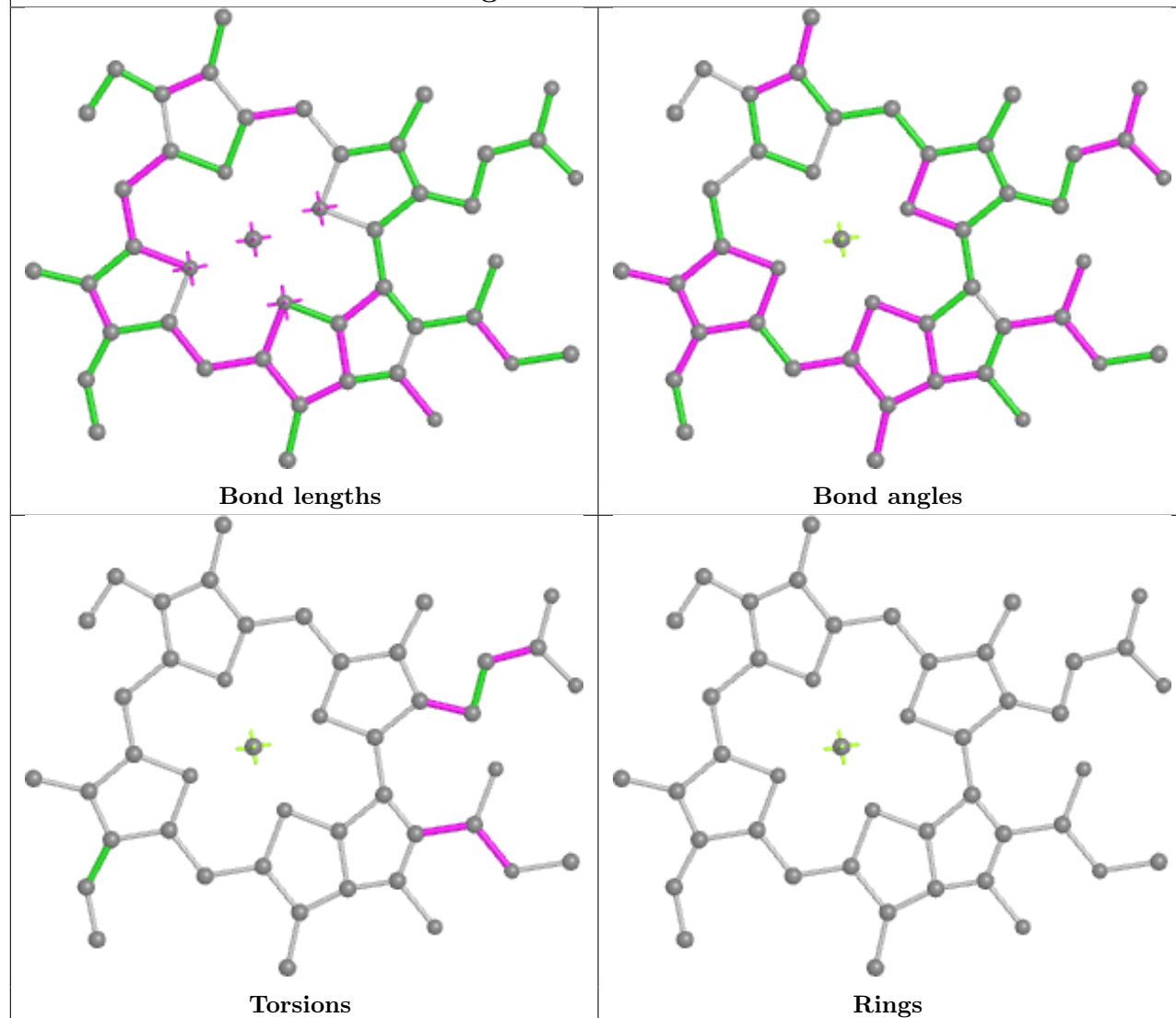


Ligand CLA I 1501

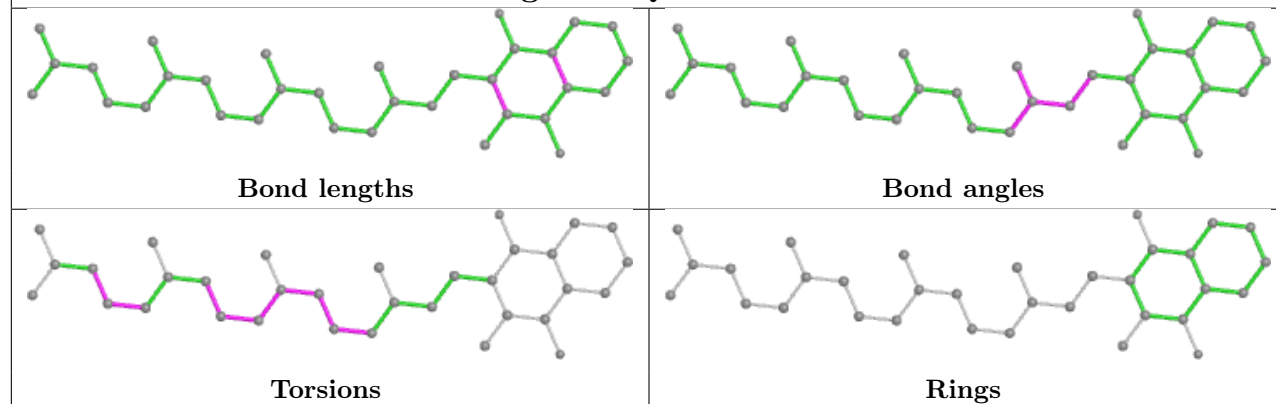




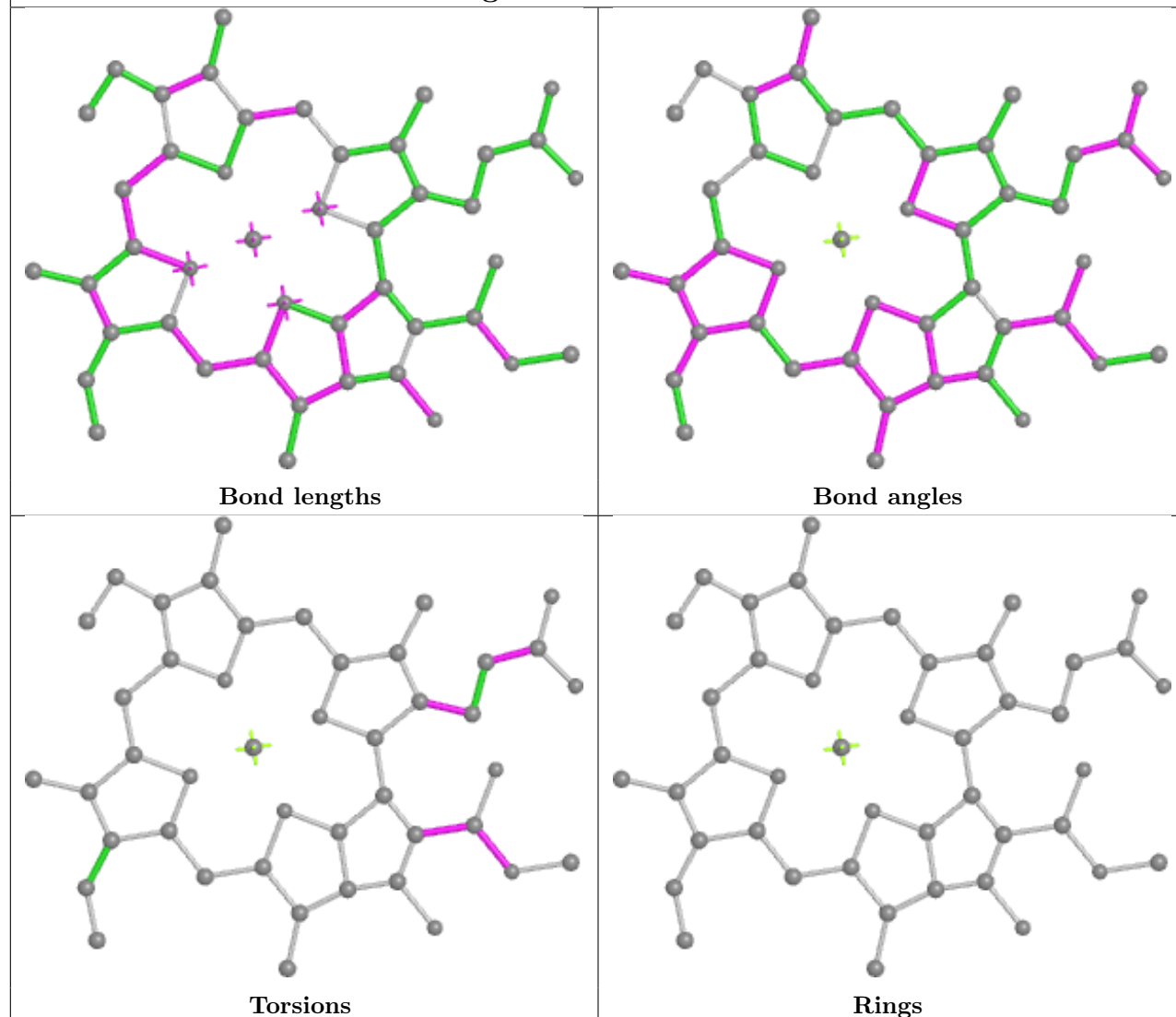
Ligand CLA H 1227



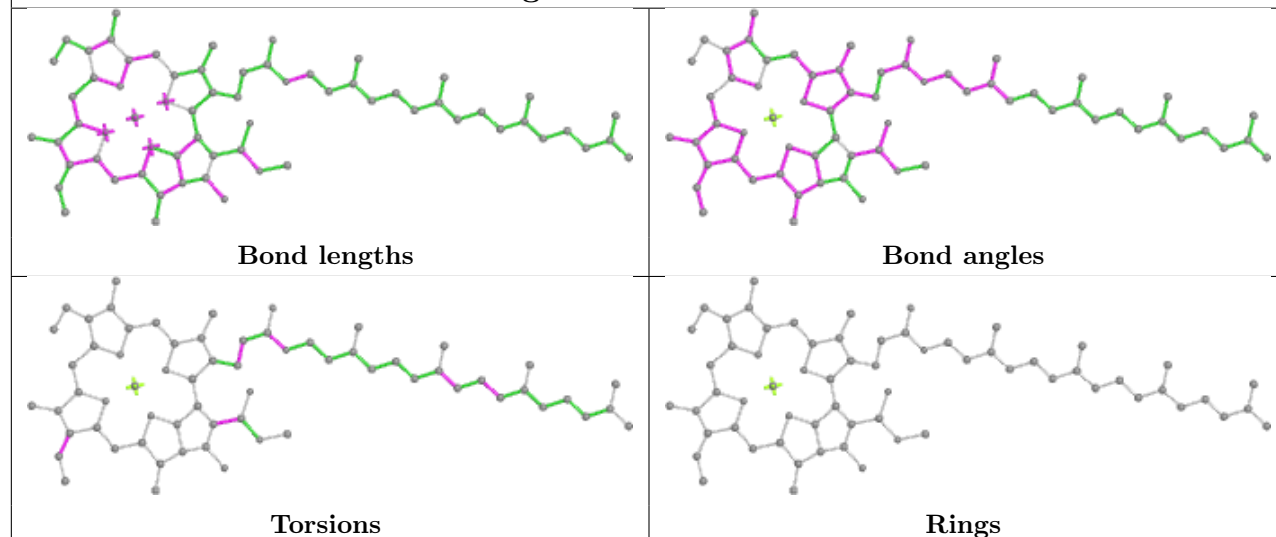
Ligand PQN B 2002

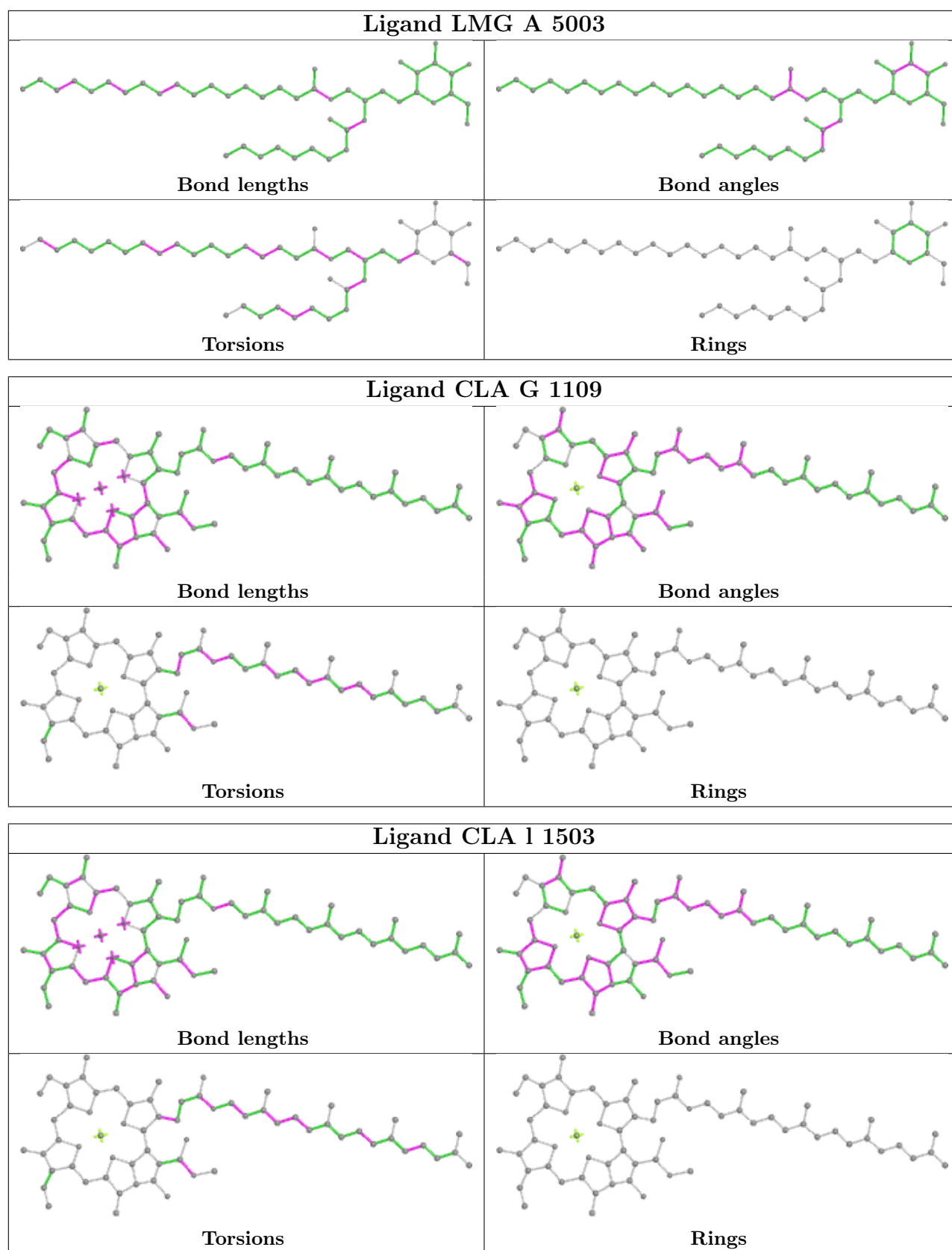


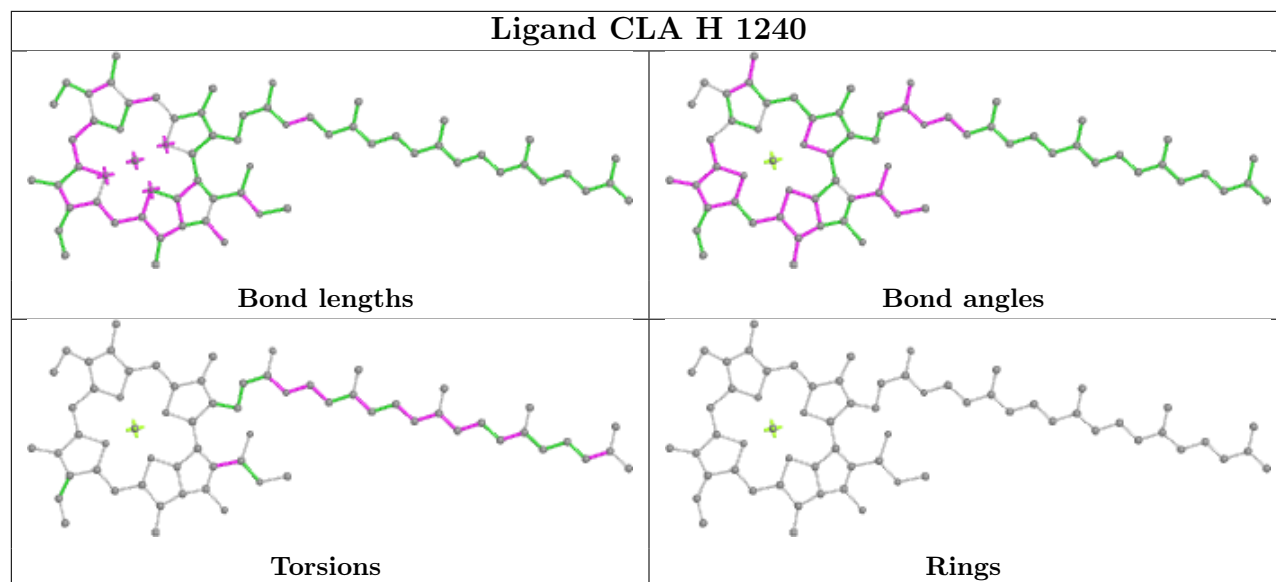
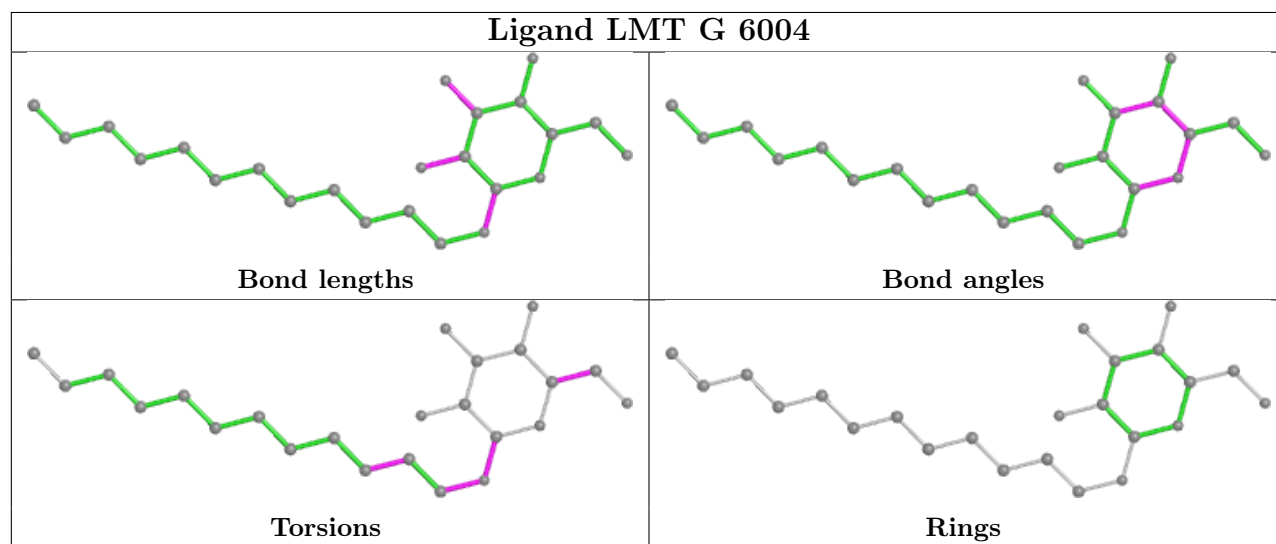
Ligand CLA B 1227



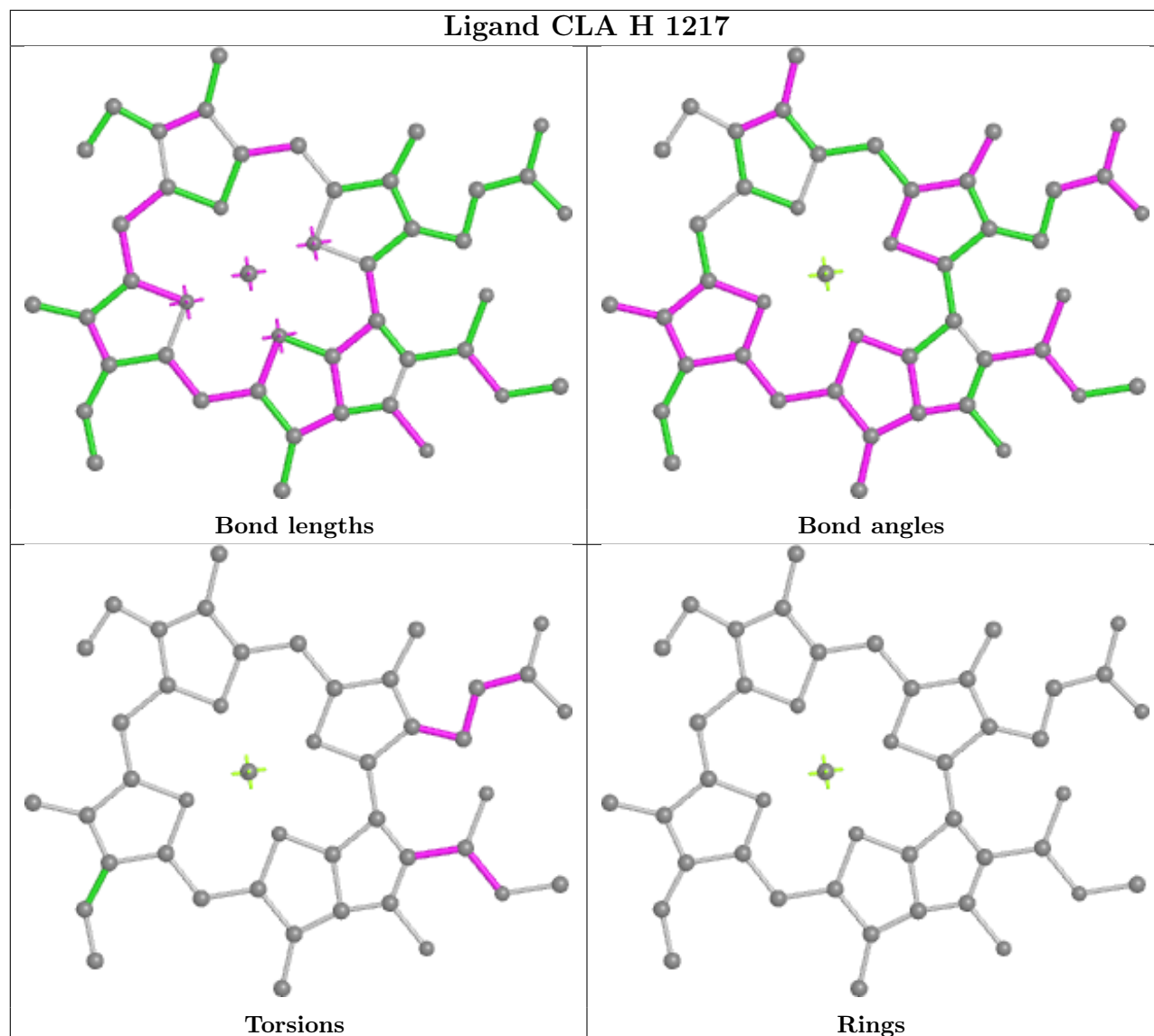
Ligand CLA H 1023



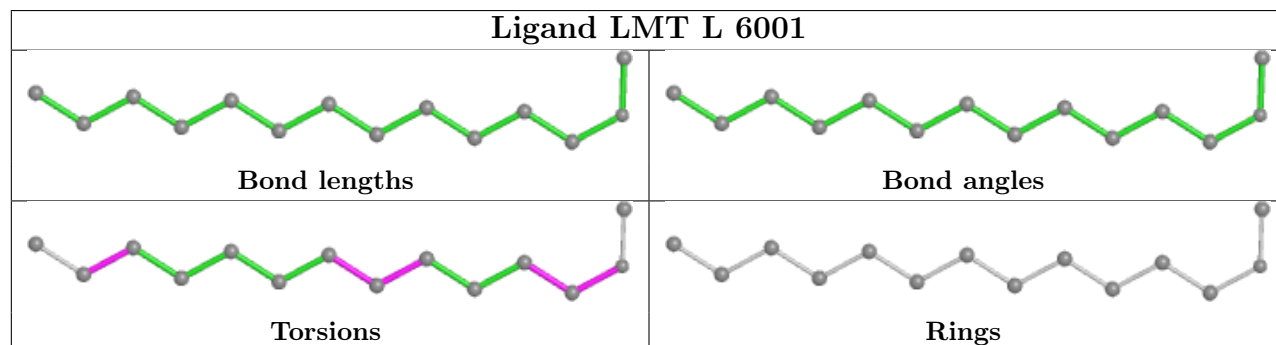


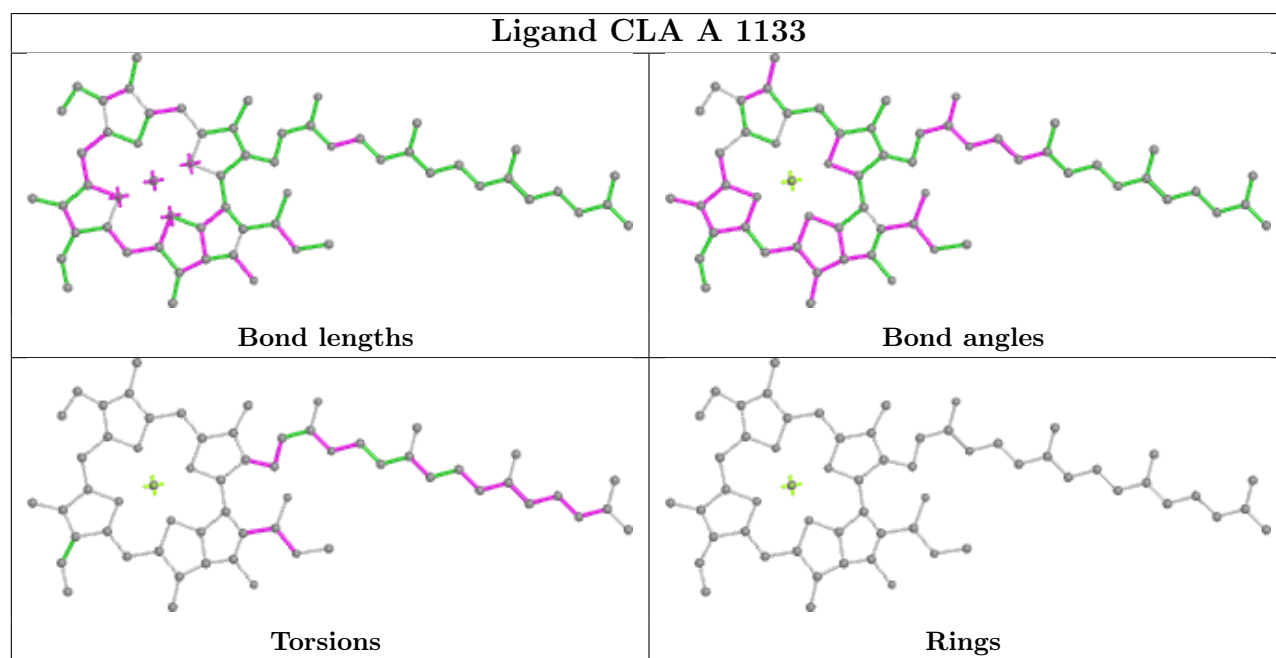
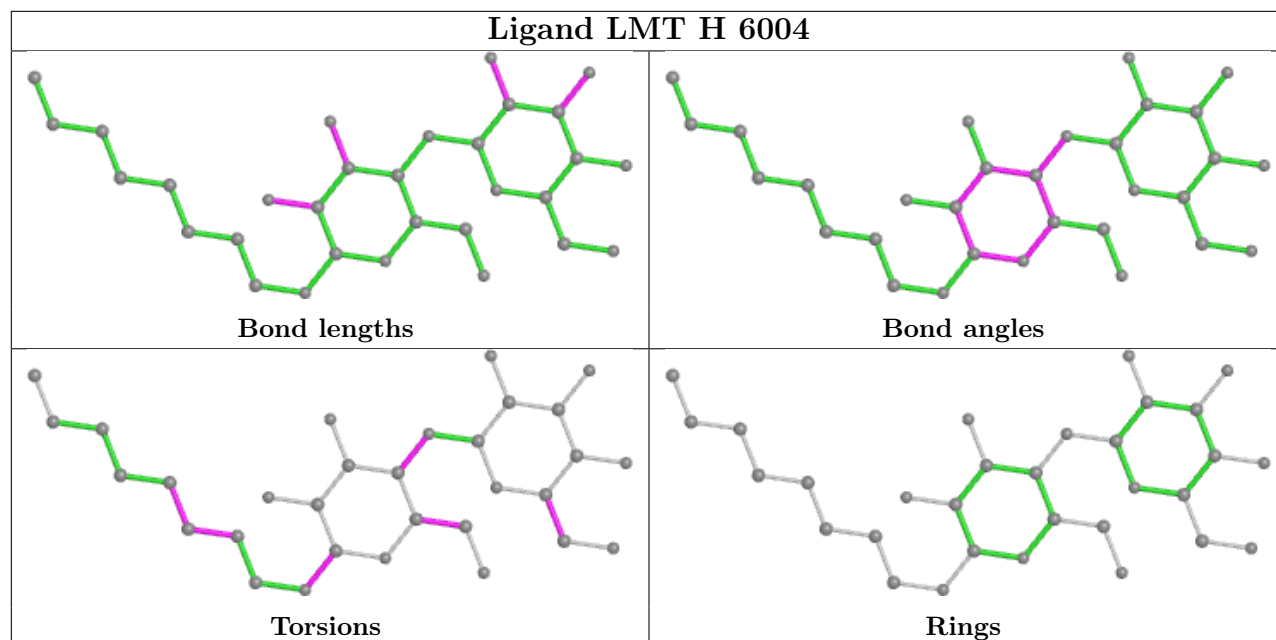
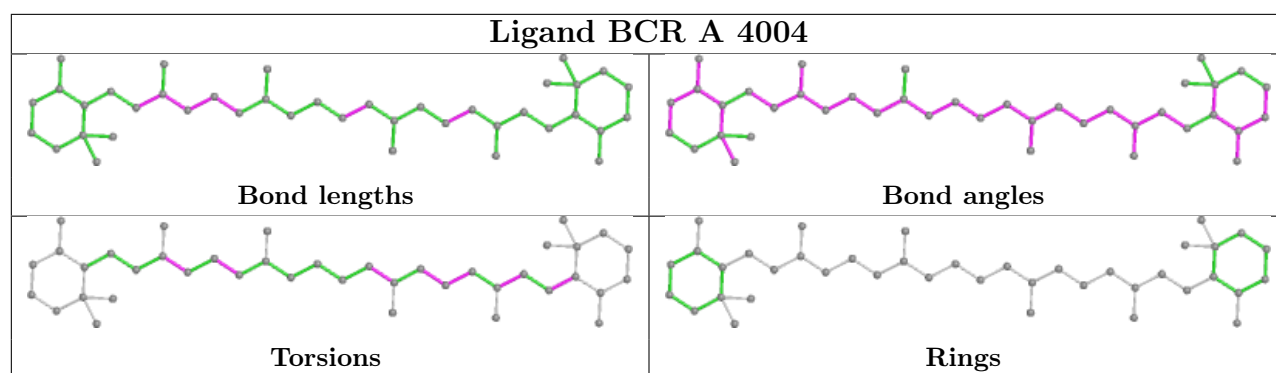
Ligand CLA H 1240**Ligand LMT G 6004**

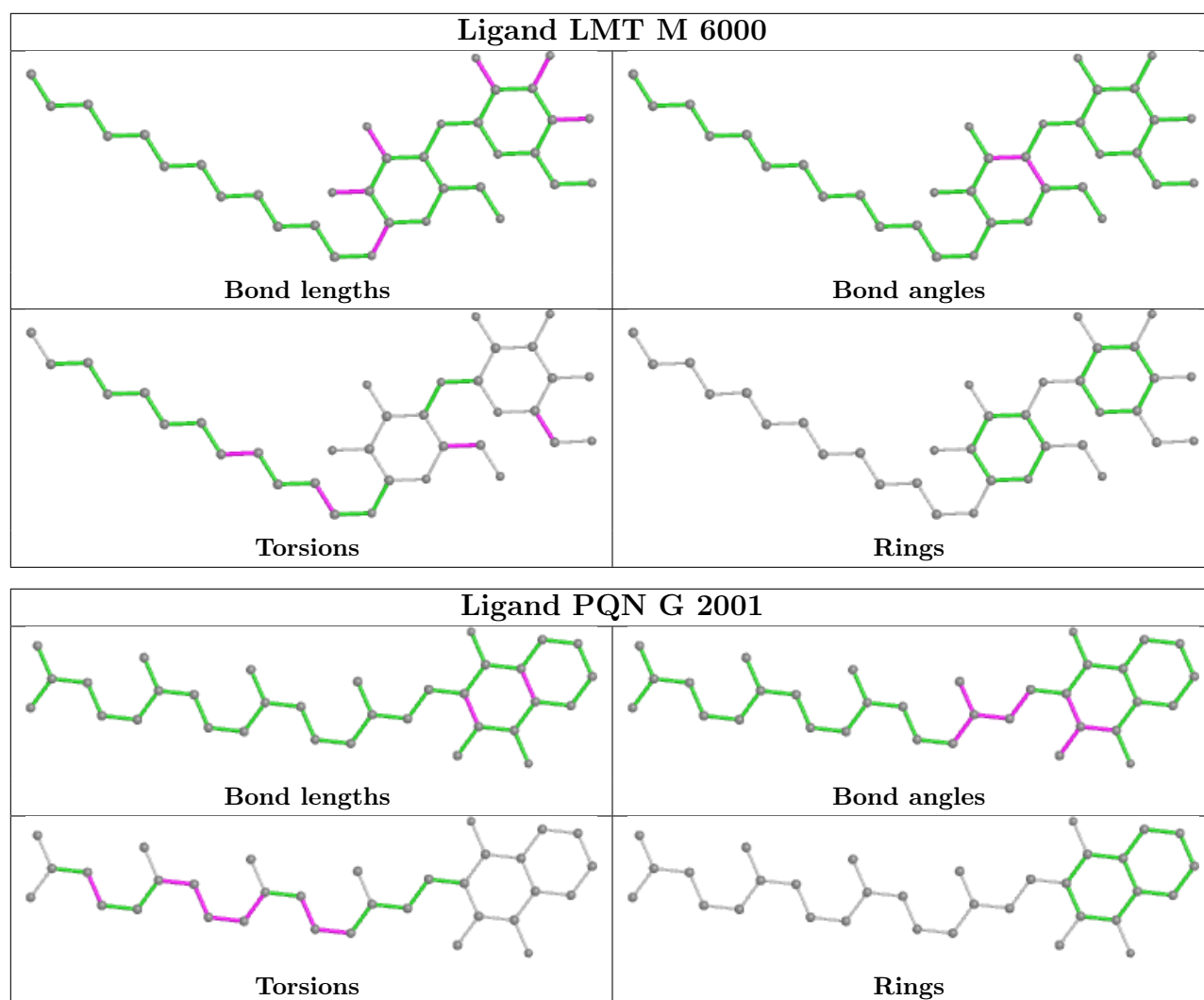
Ligand CLA H 1217

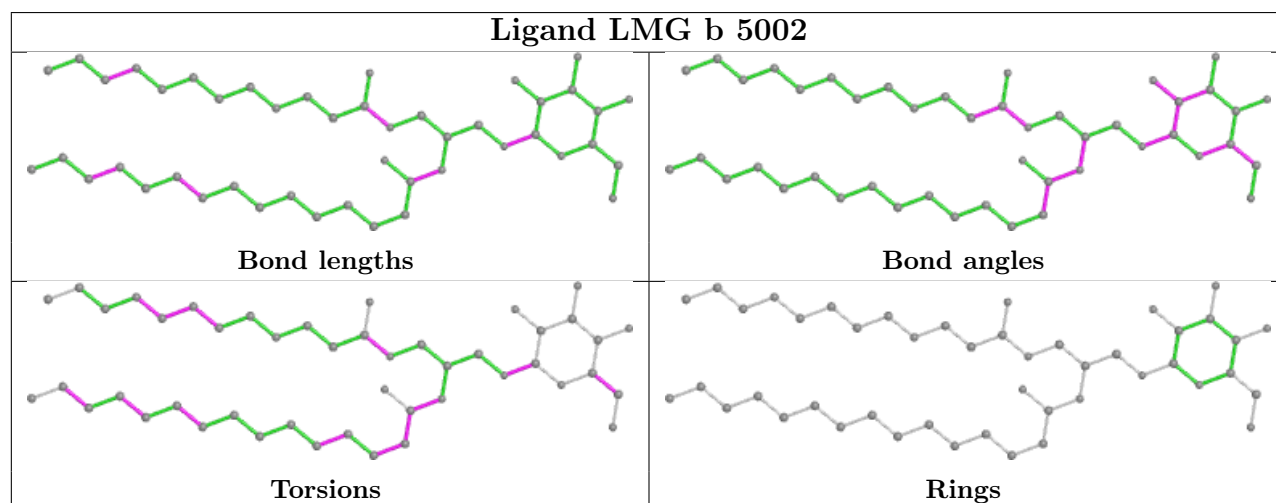
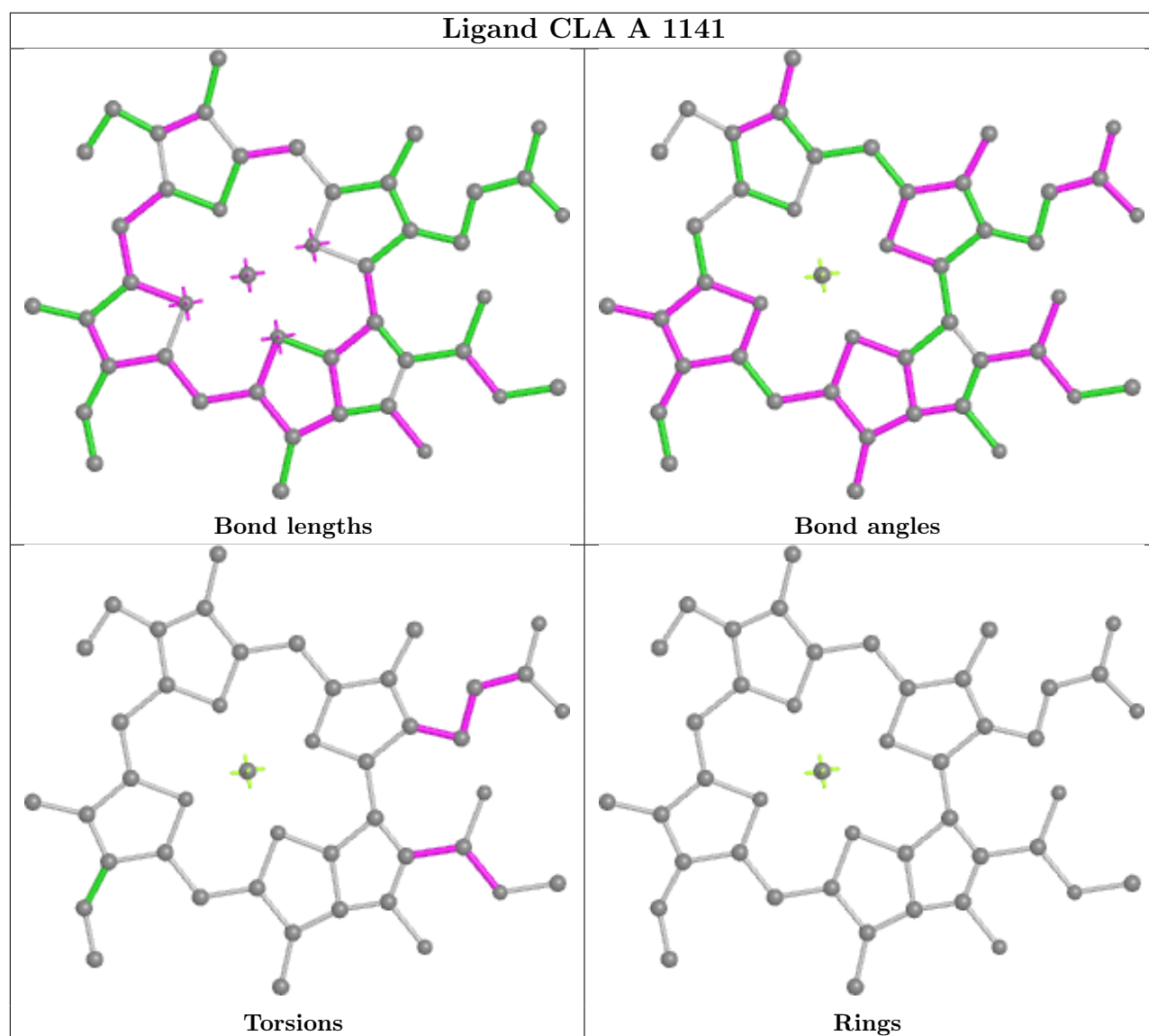


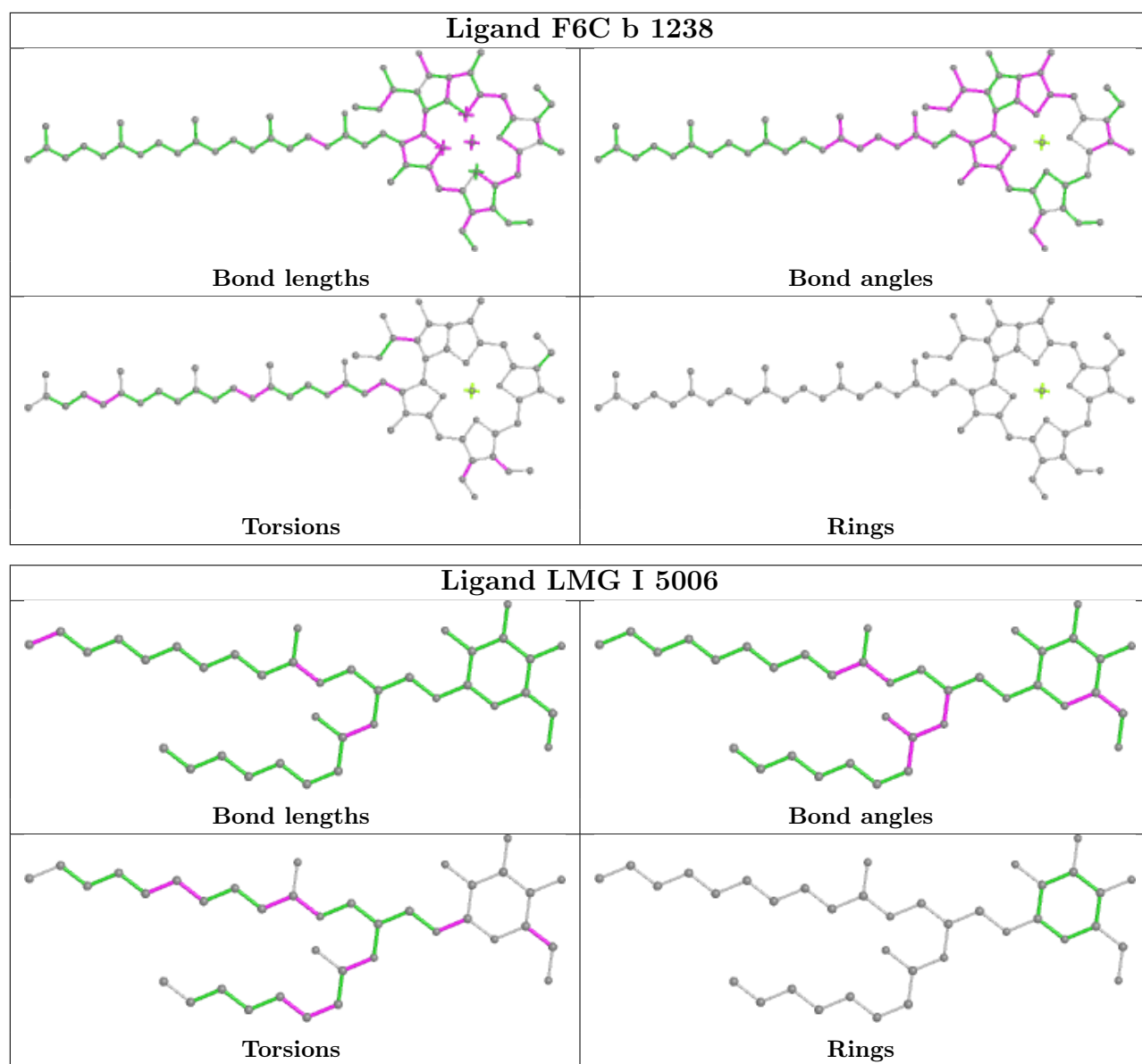
Ligand LMT L 6001

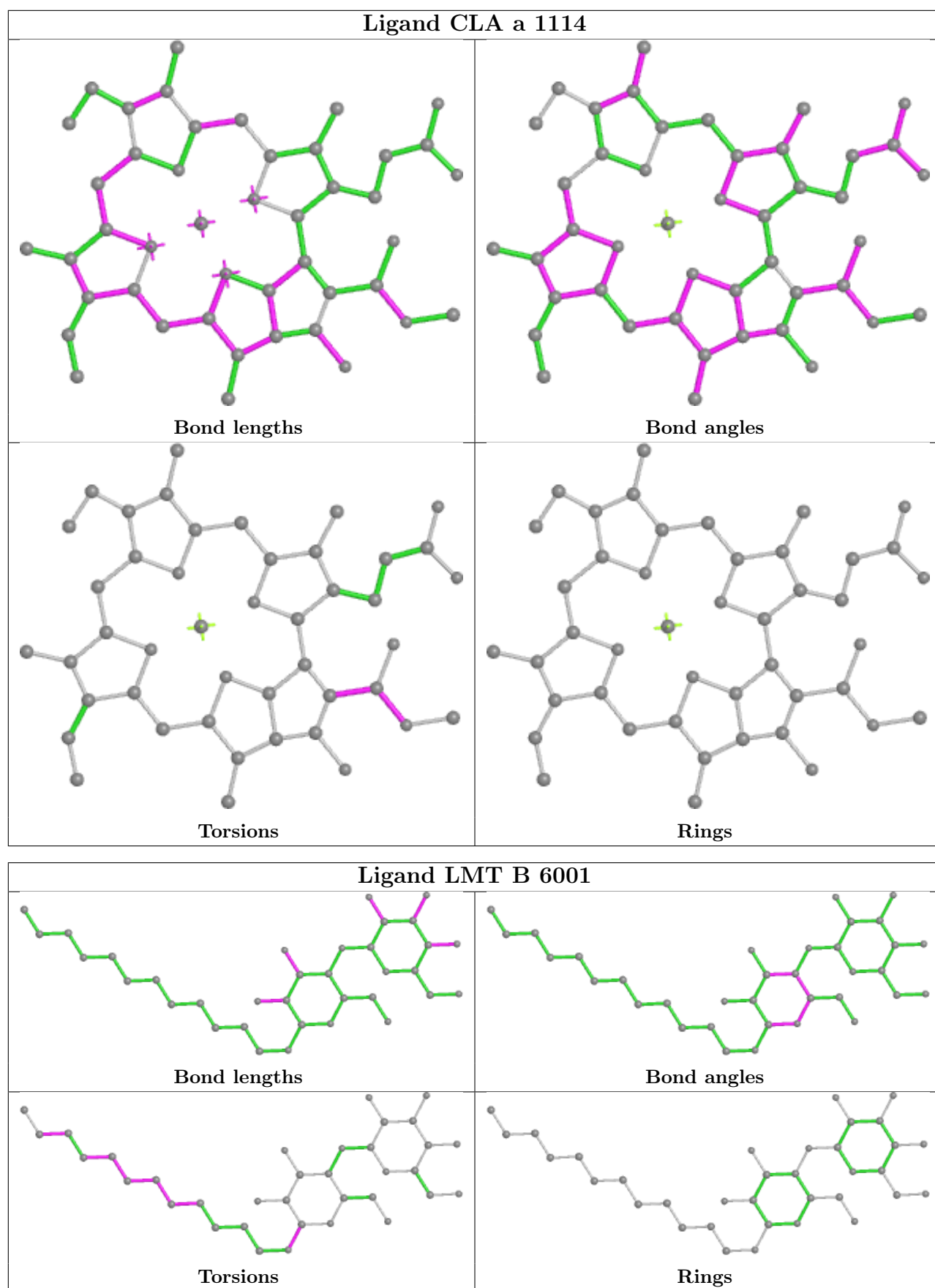


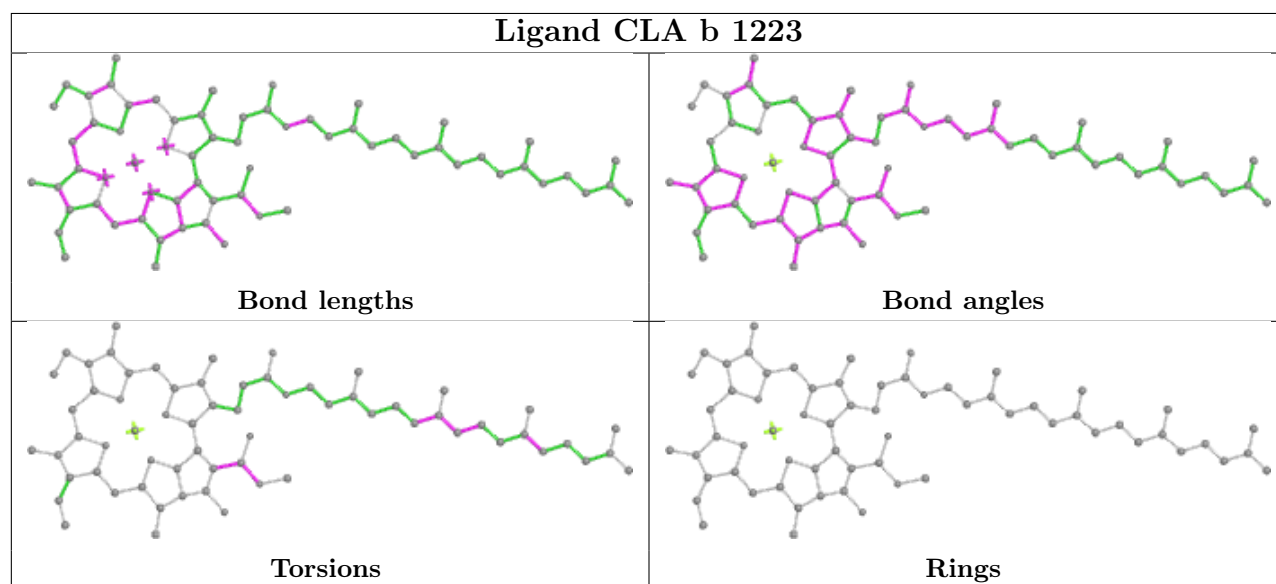
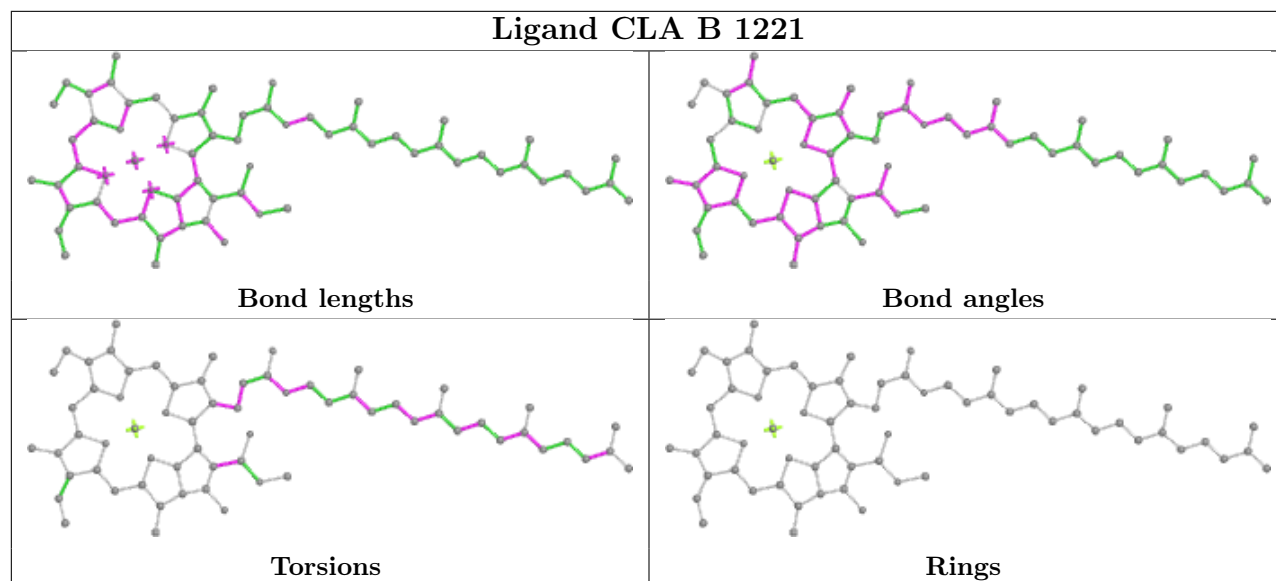
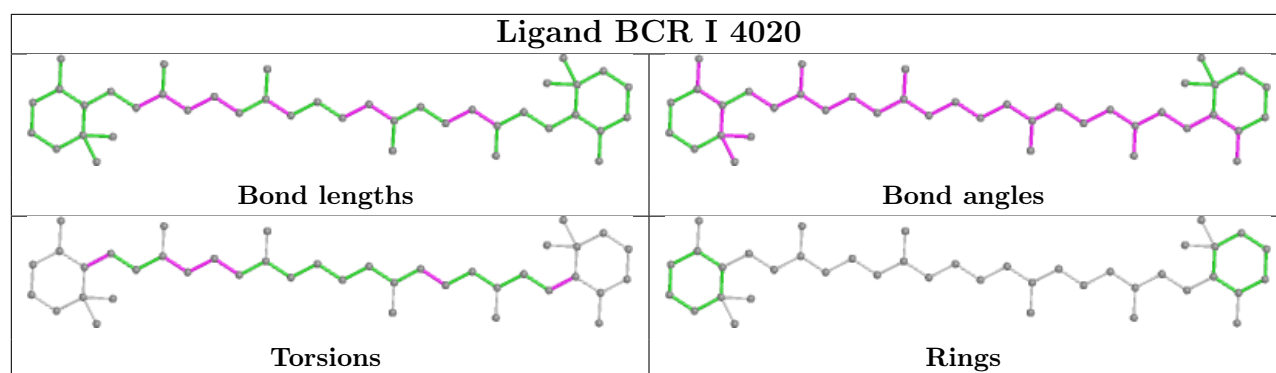


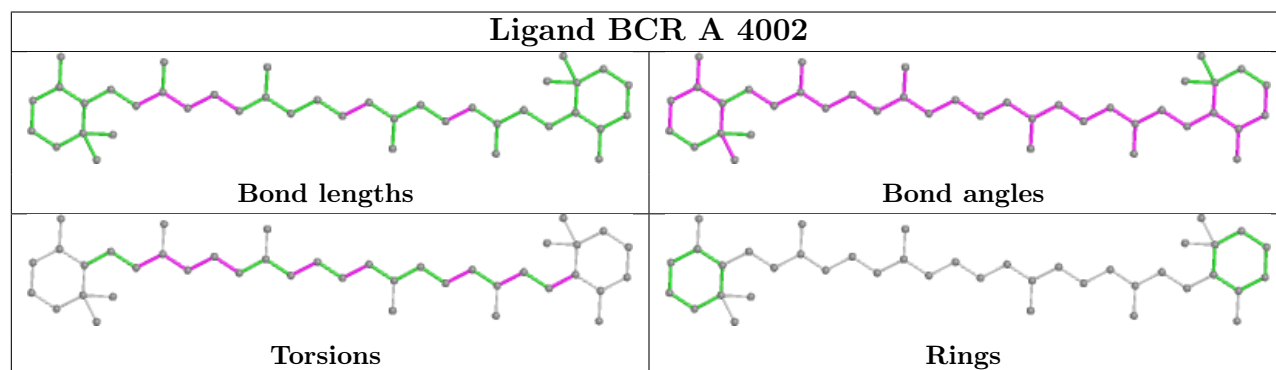
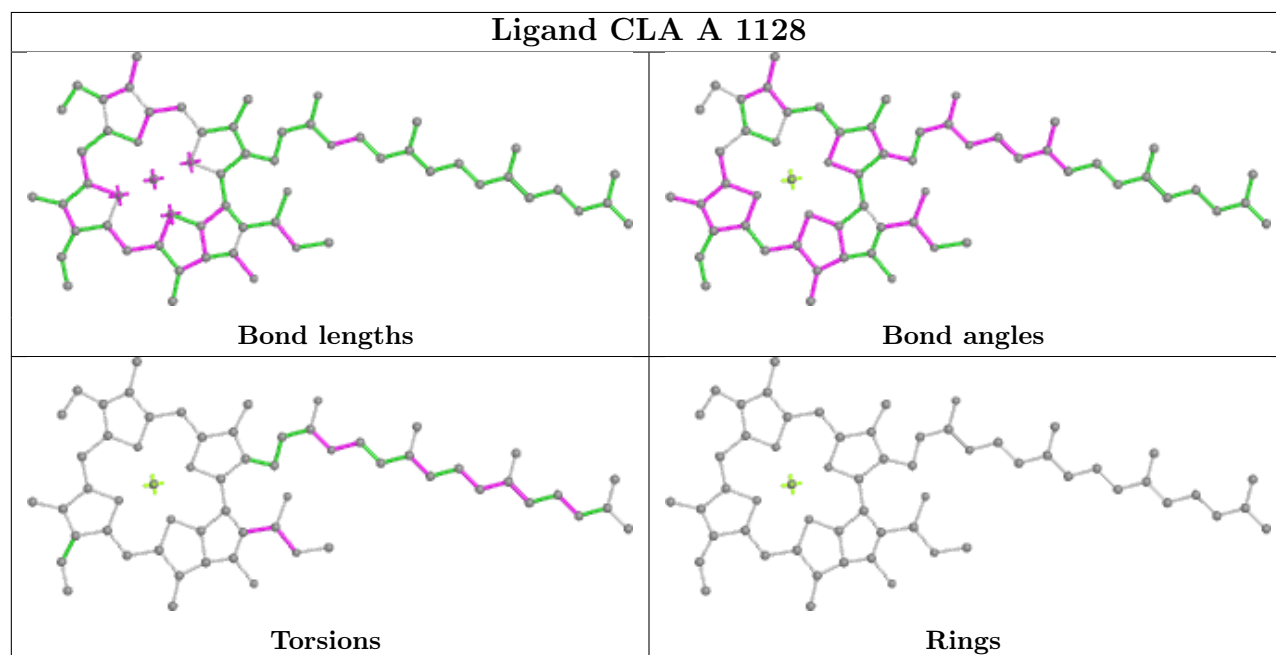
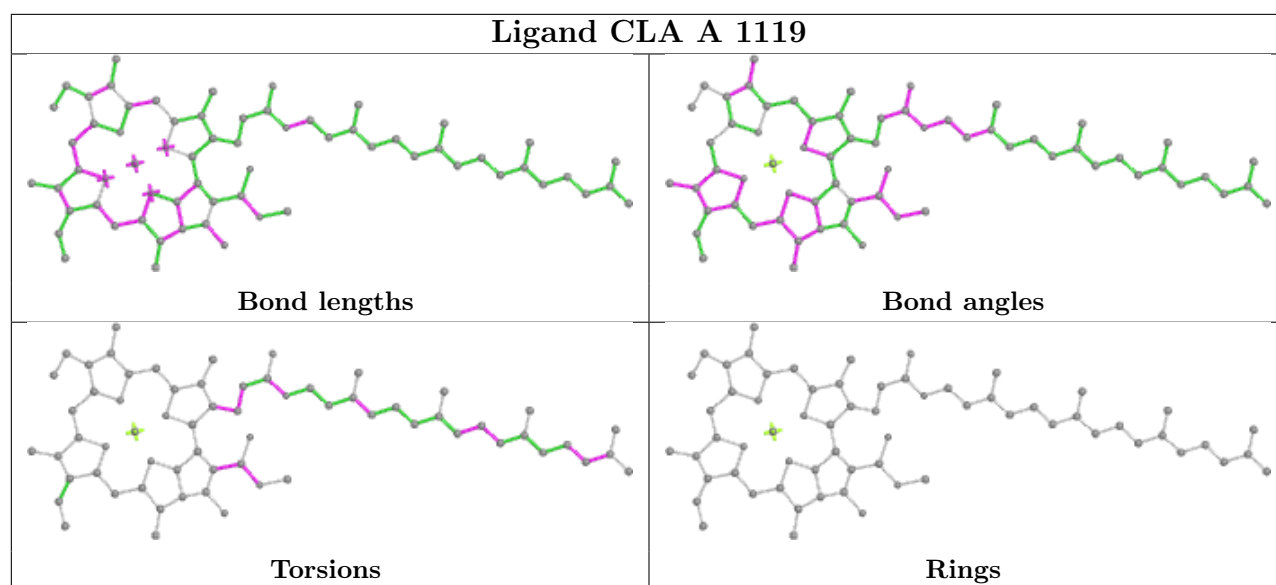


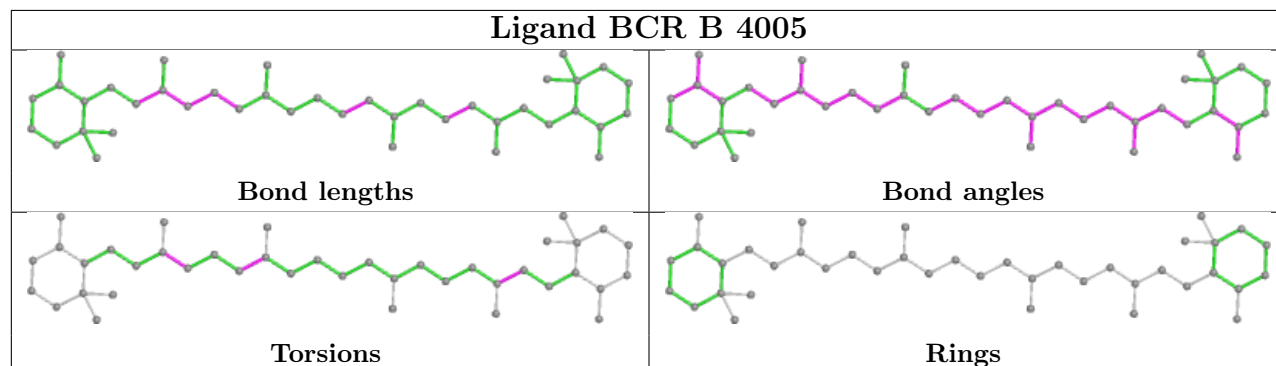
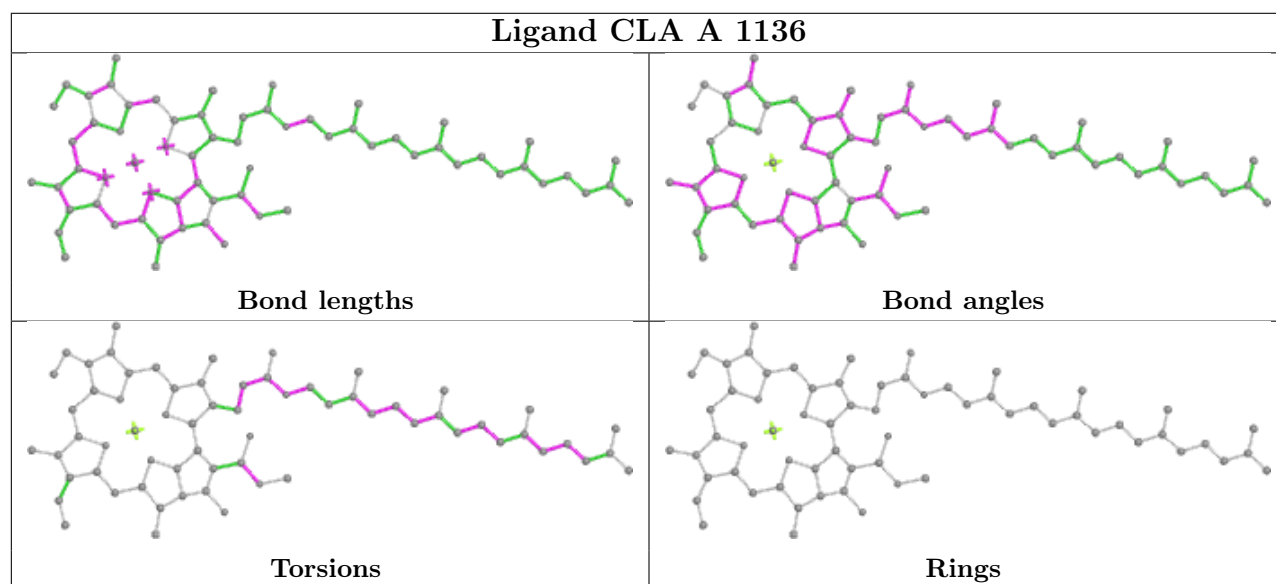
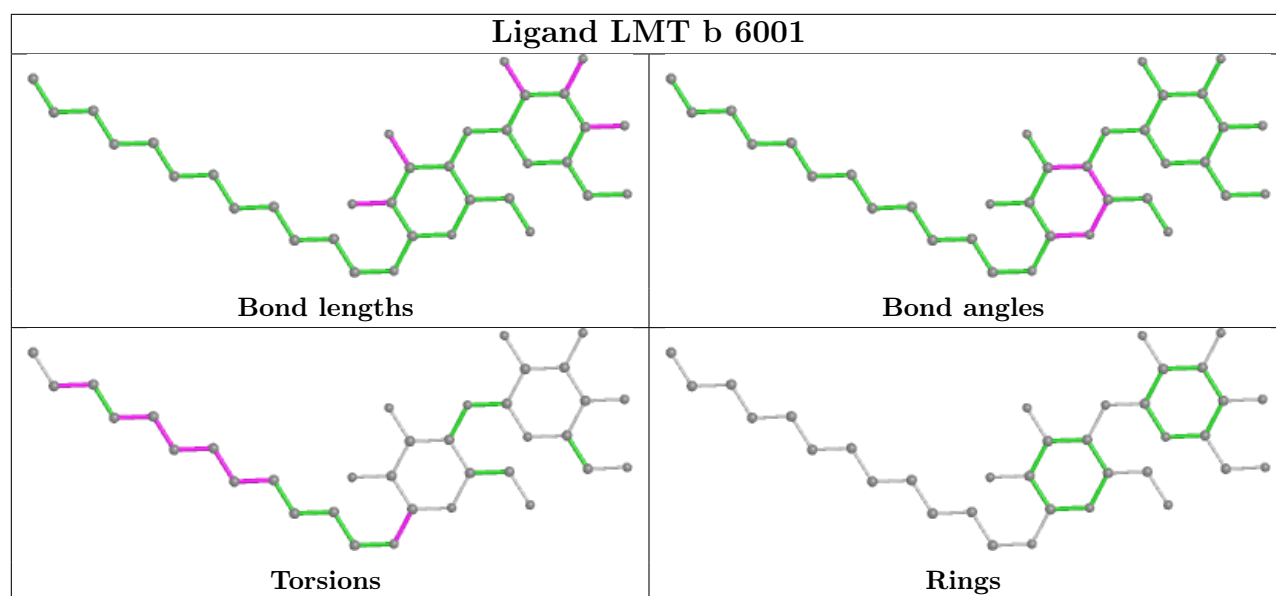


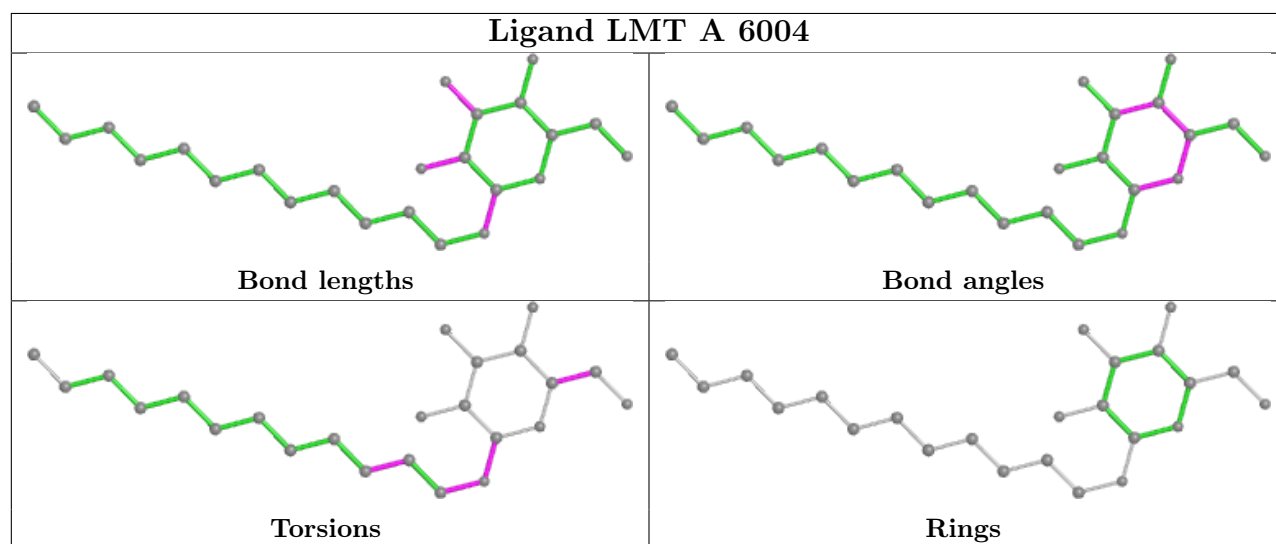
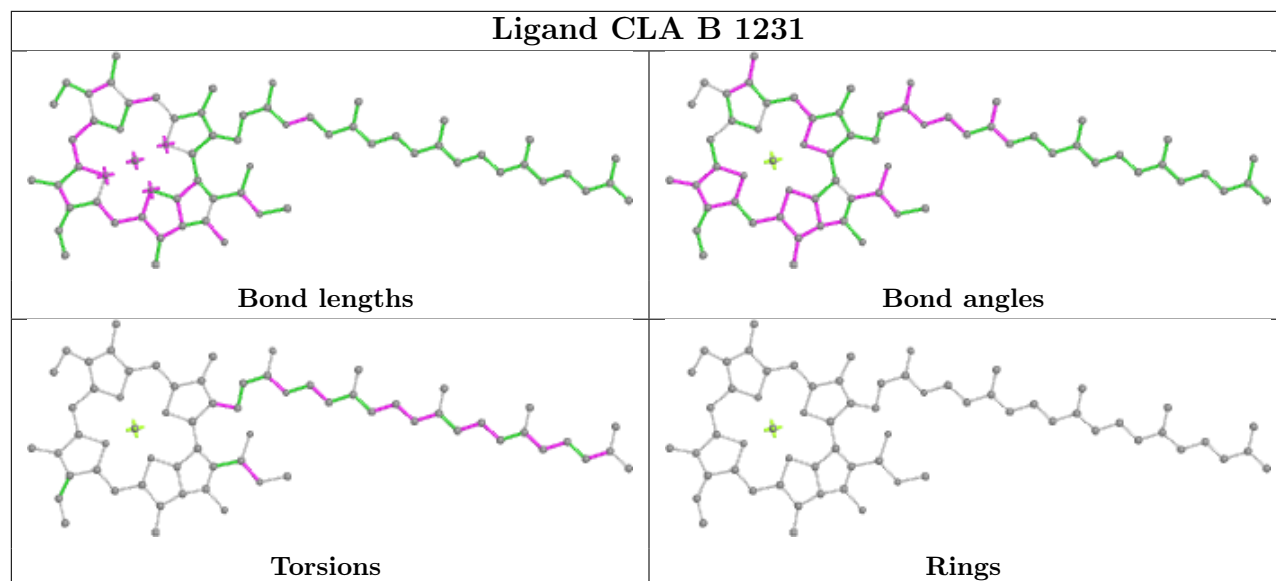
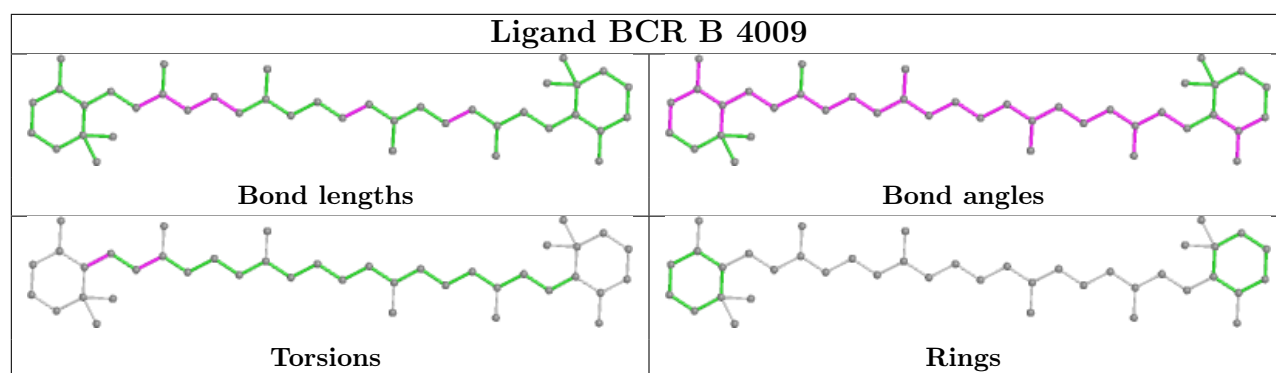


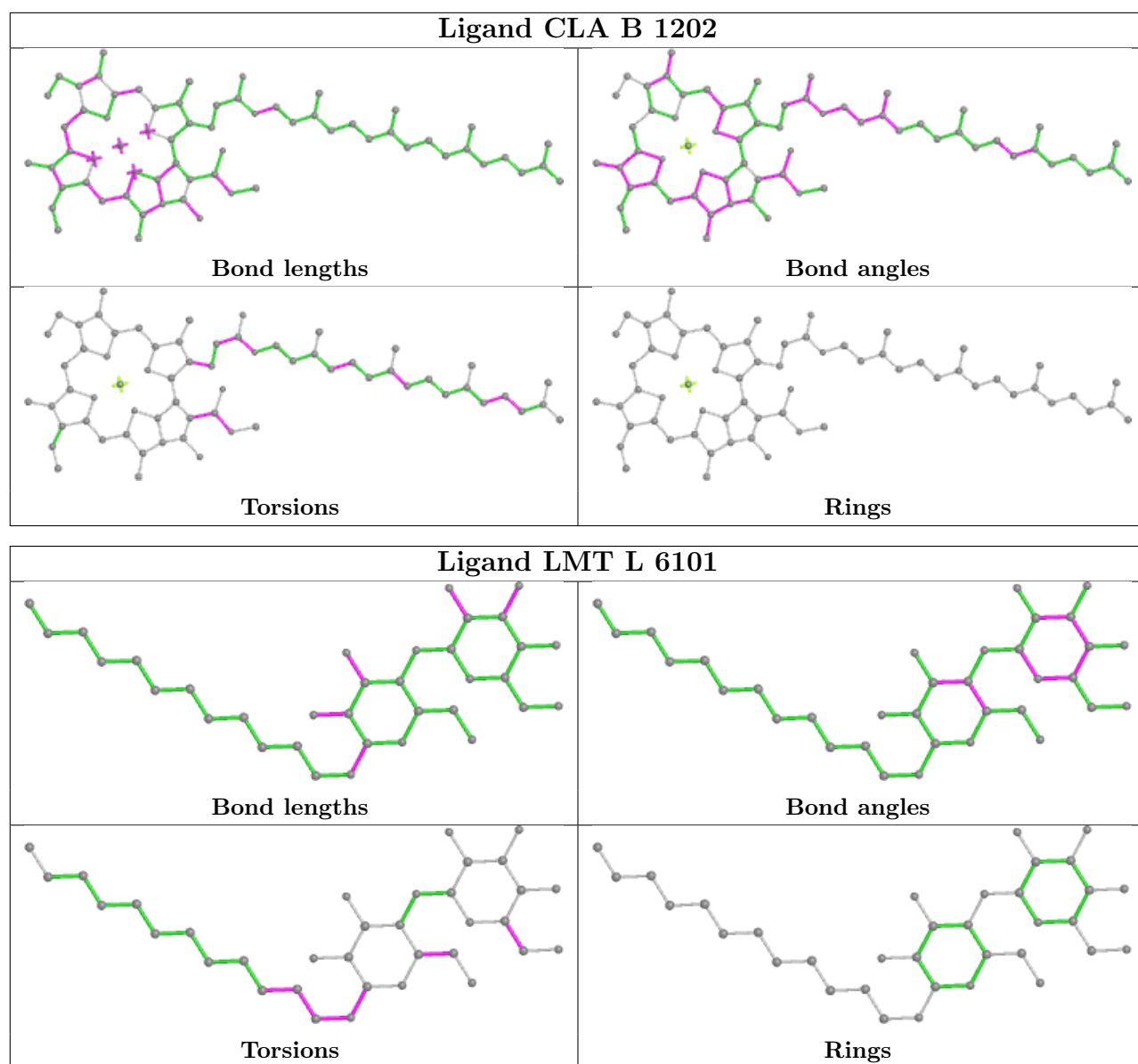


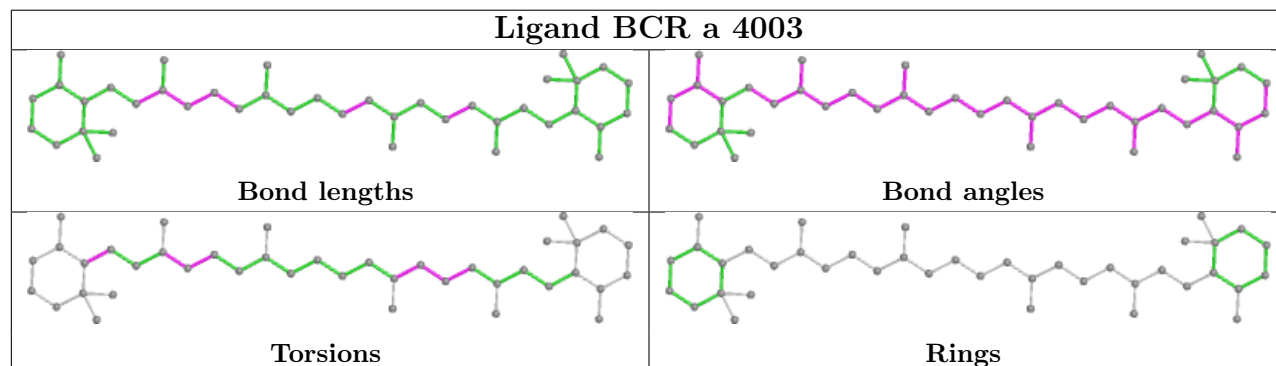
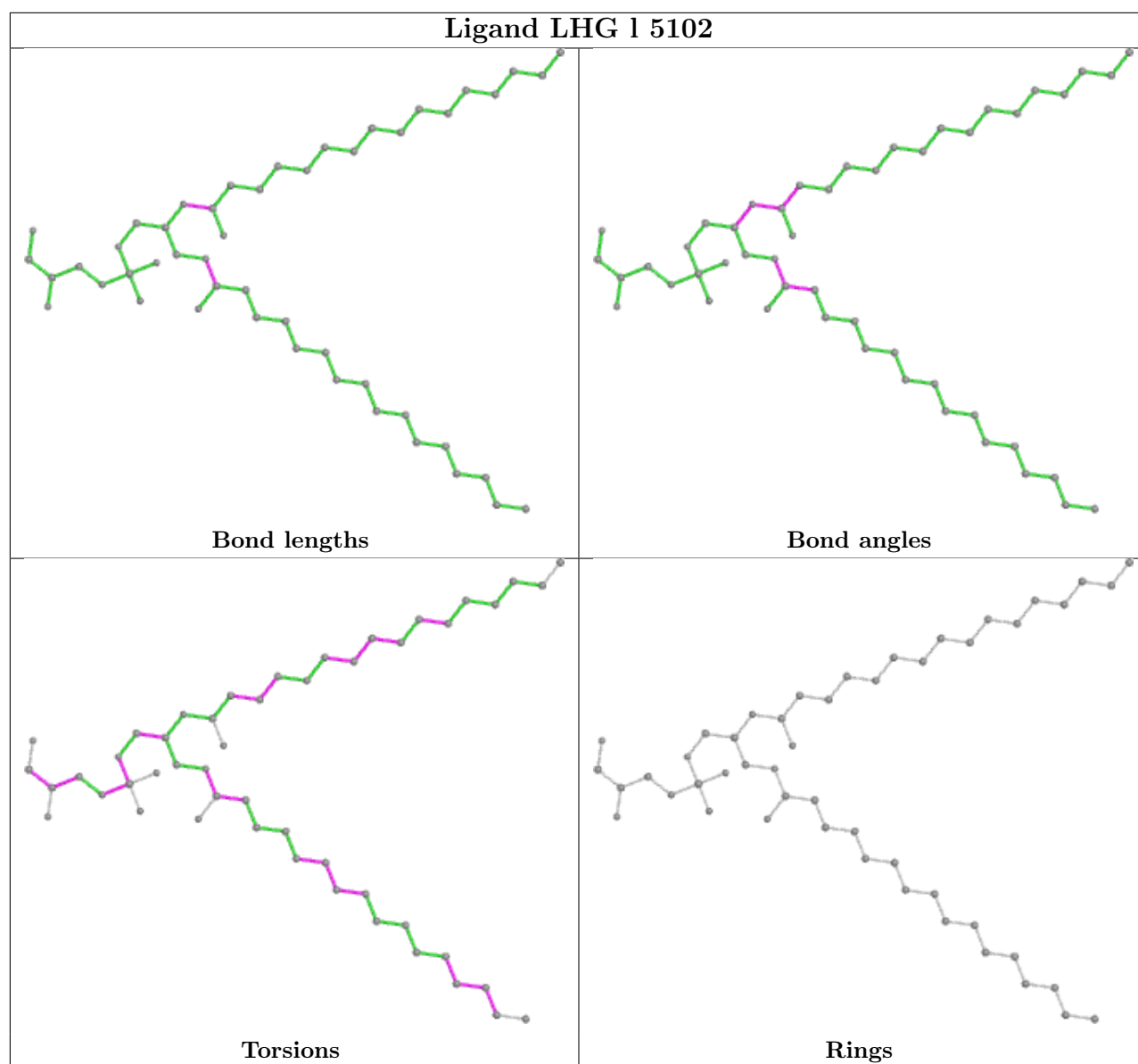




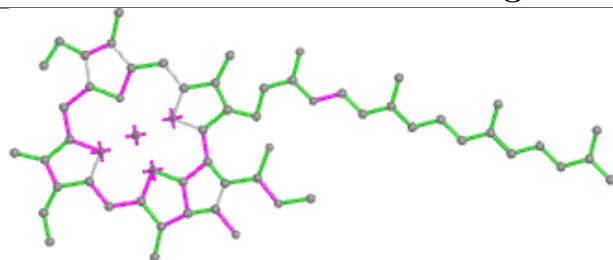




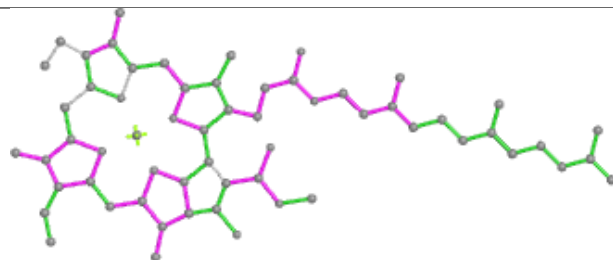




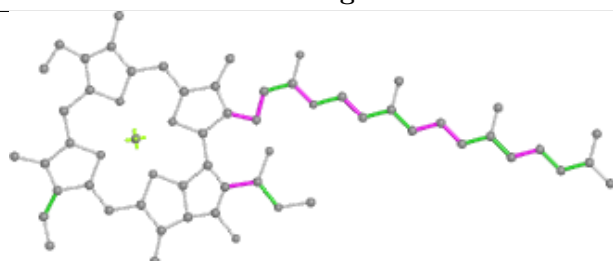
Ligand CLA G 1013



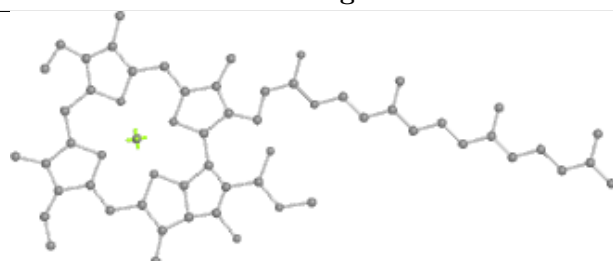
Bond lengths



Bond angles

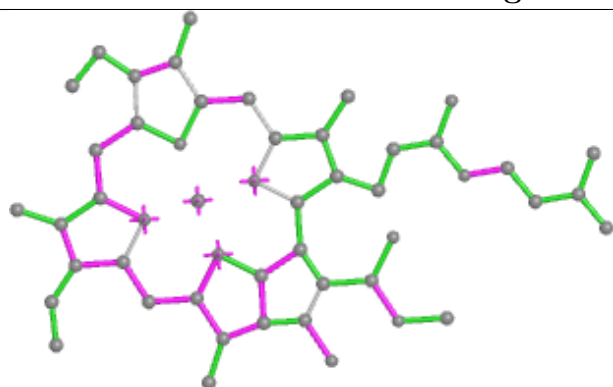


Torsions

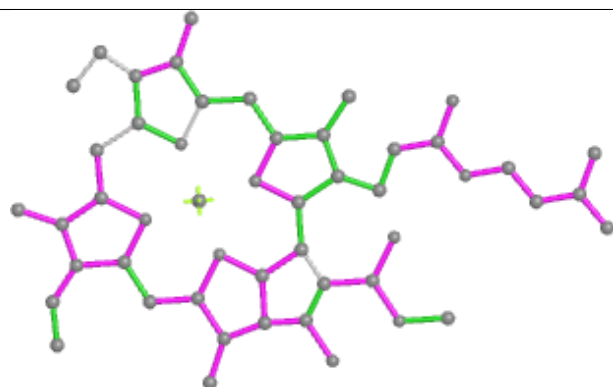


Rings

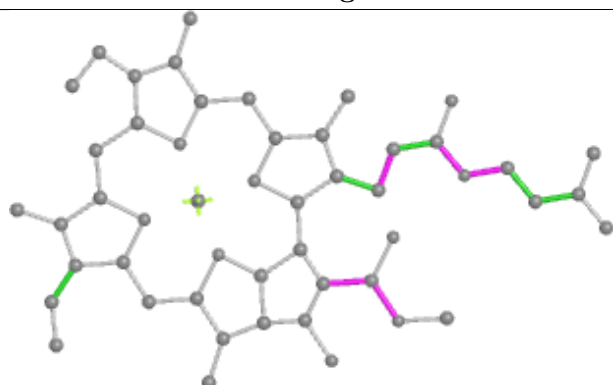
Ligand CLA G 1135



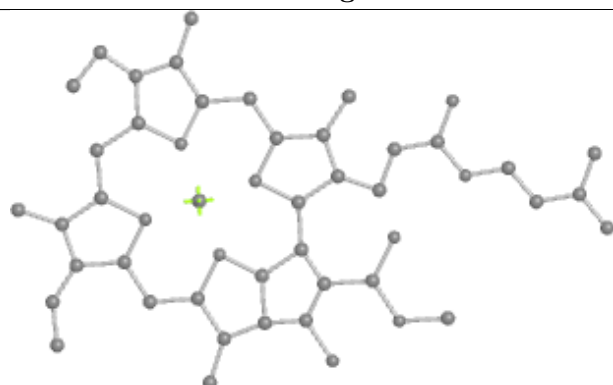
Bond lengths



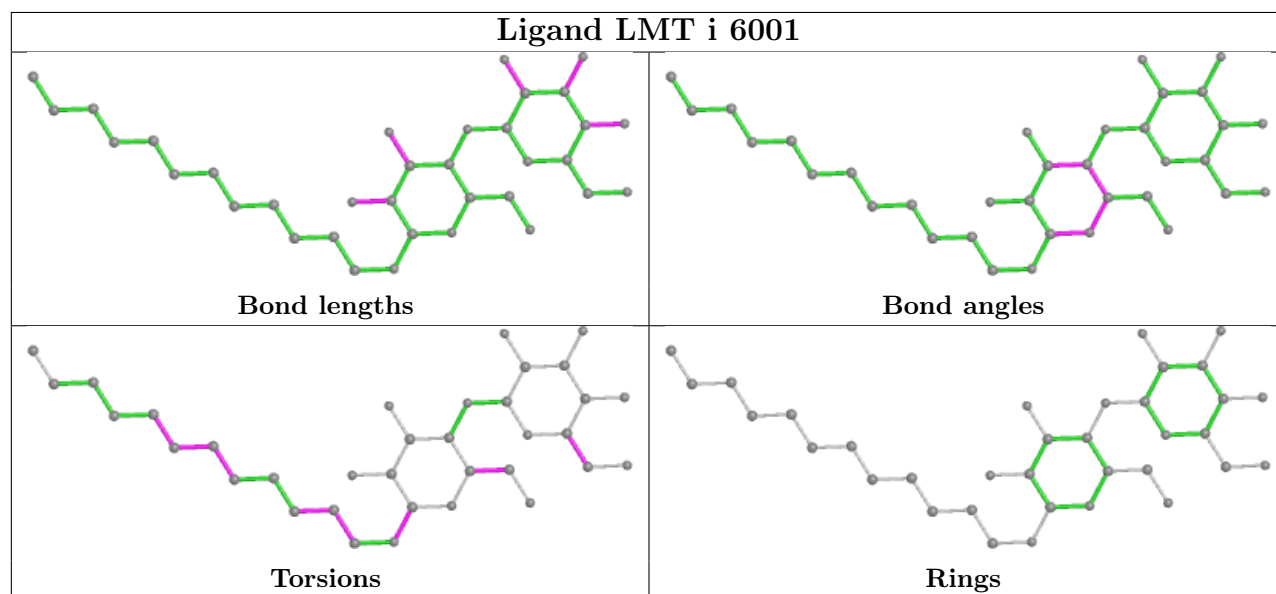
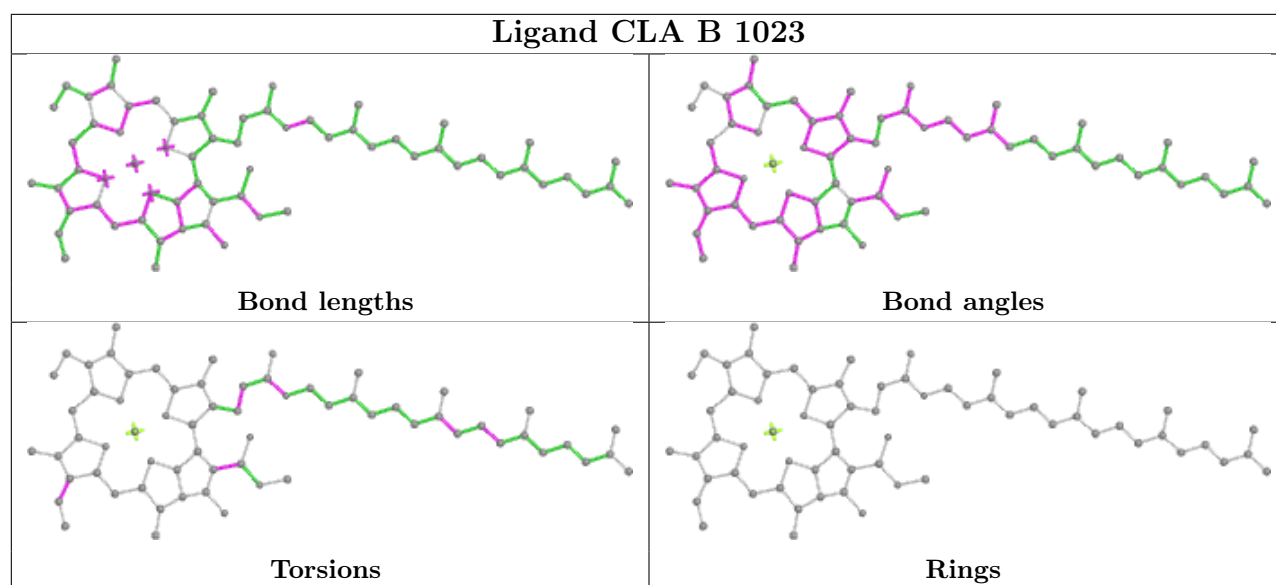
Bond angles



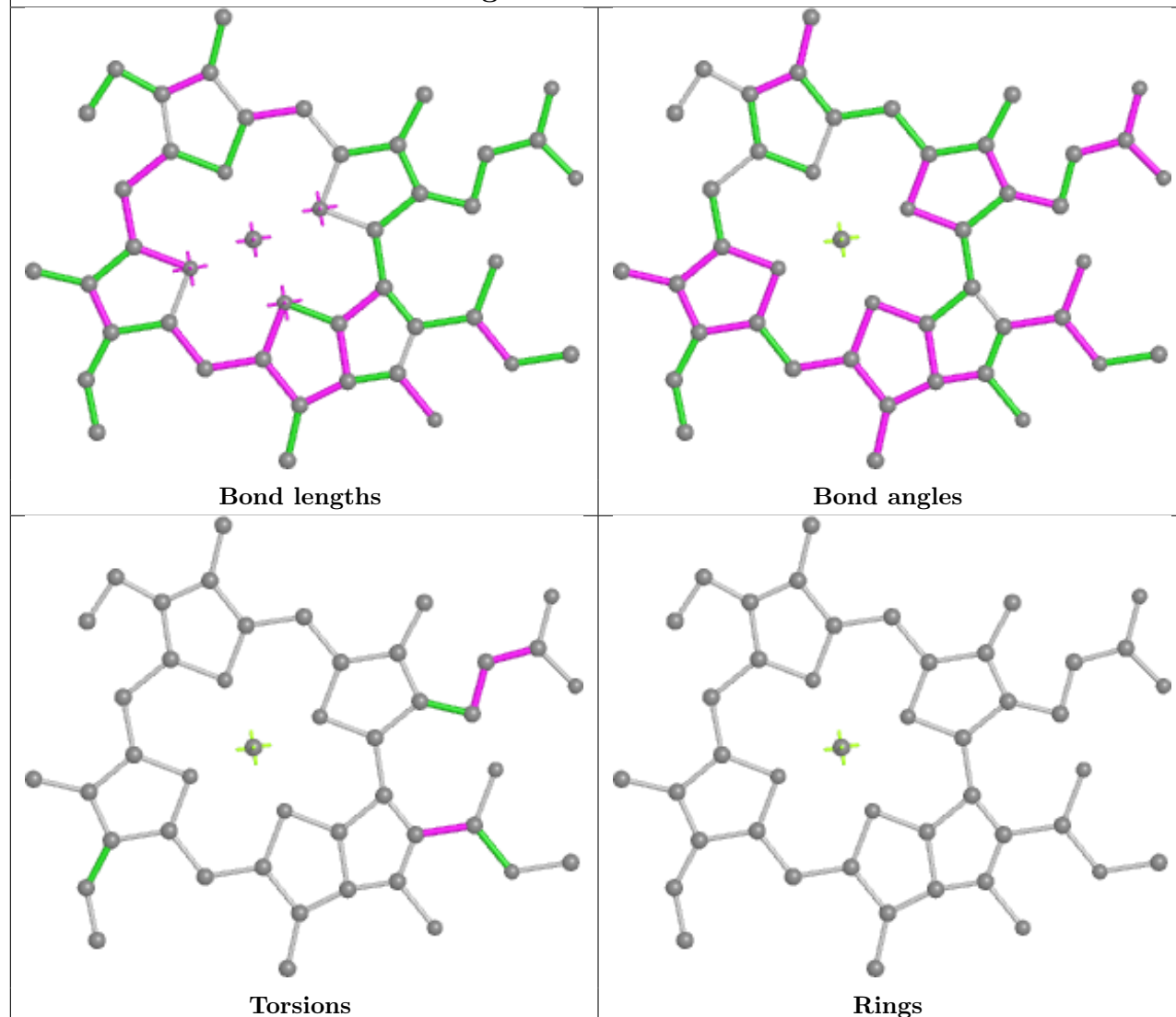
Torsions



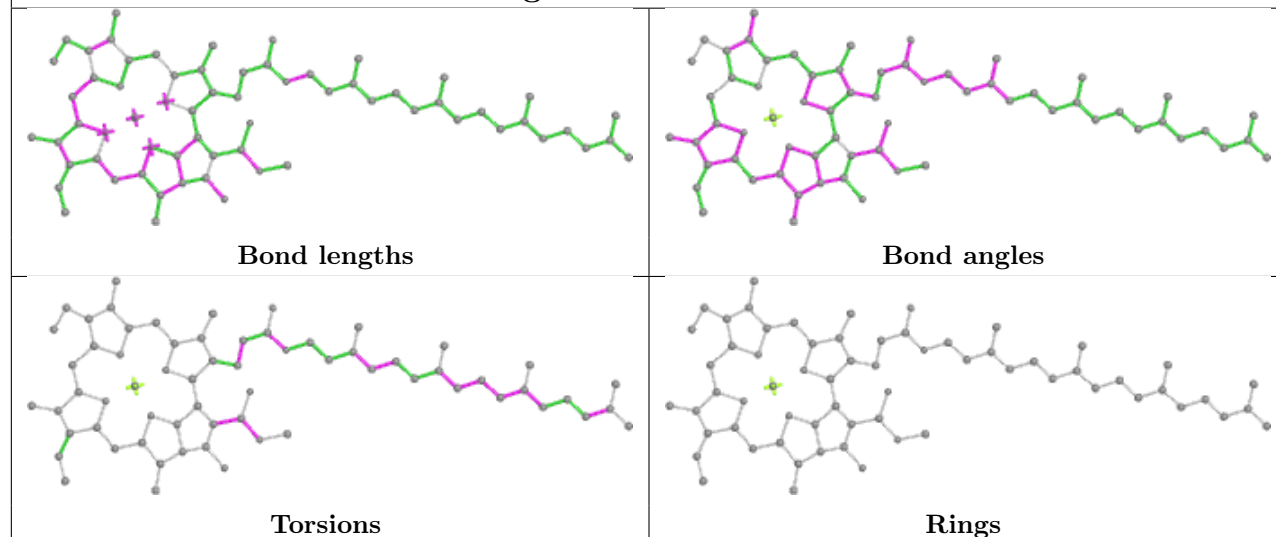
Rings

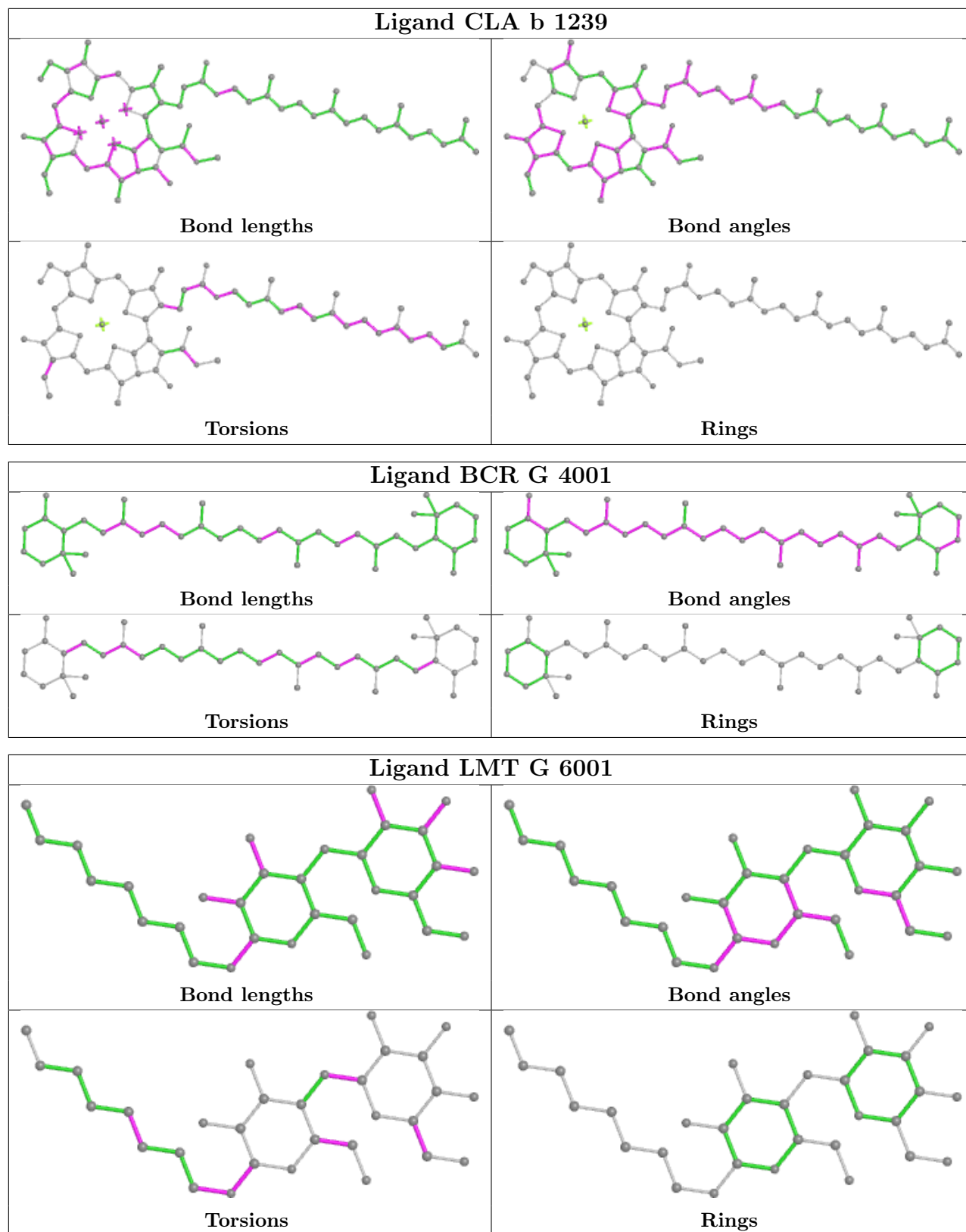


Ligand CLA A 1110

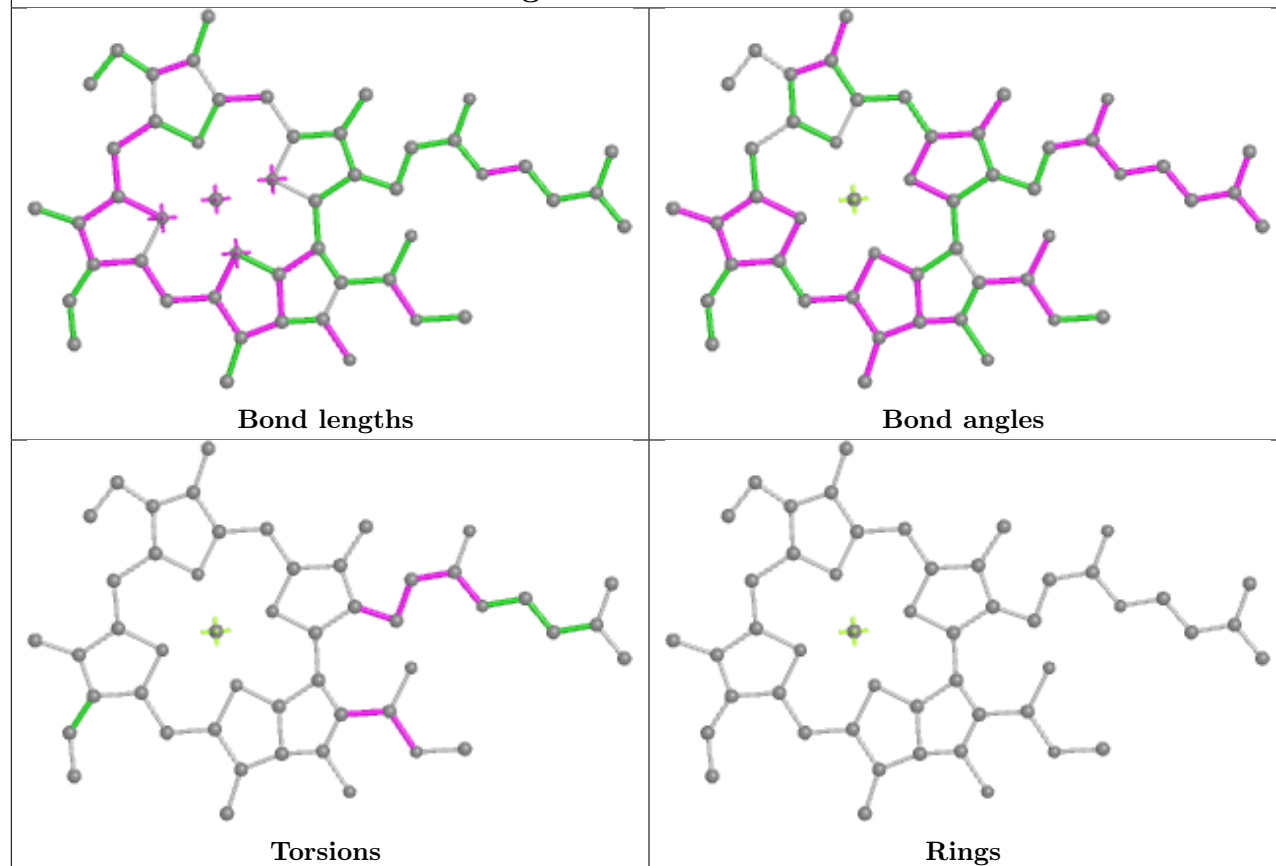


Ligand CLA B 1224

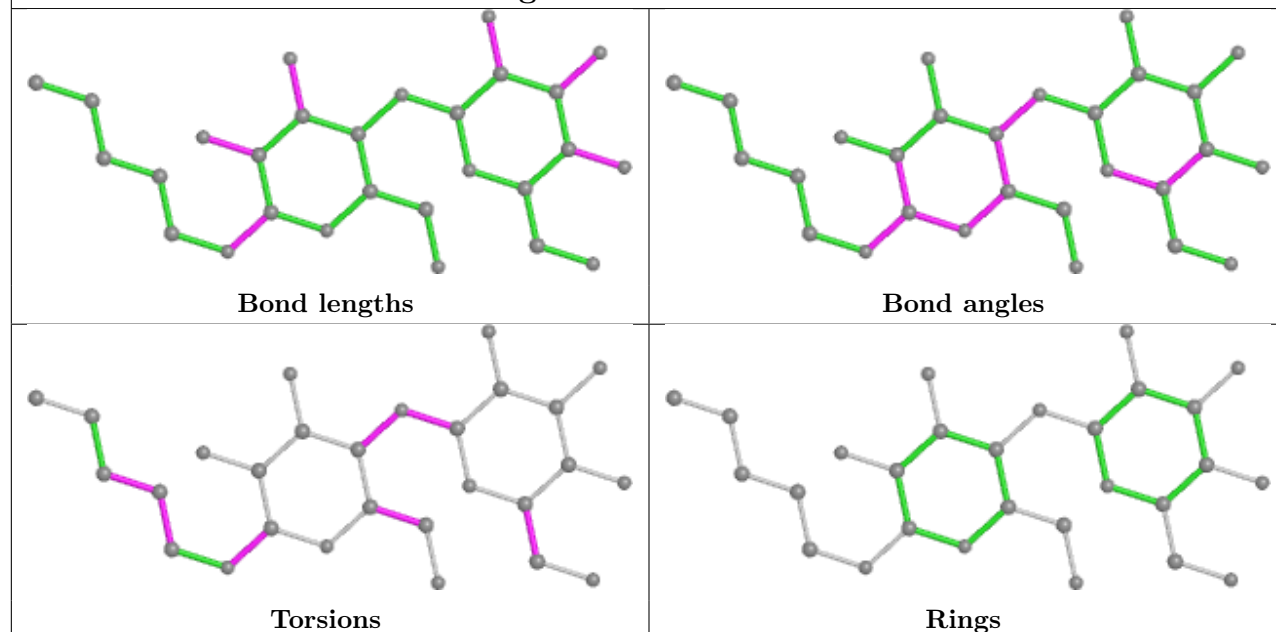


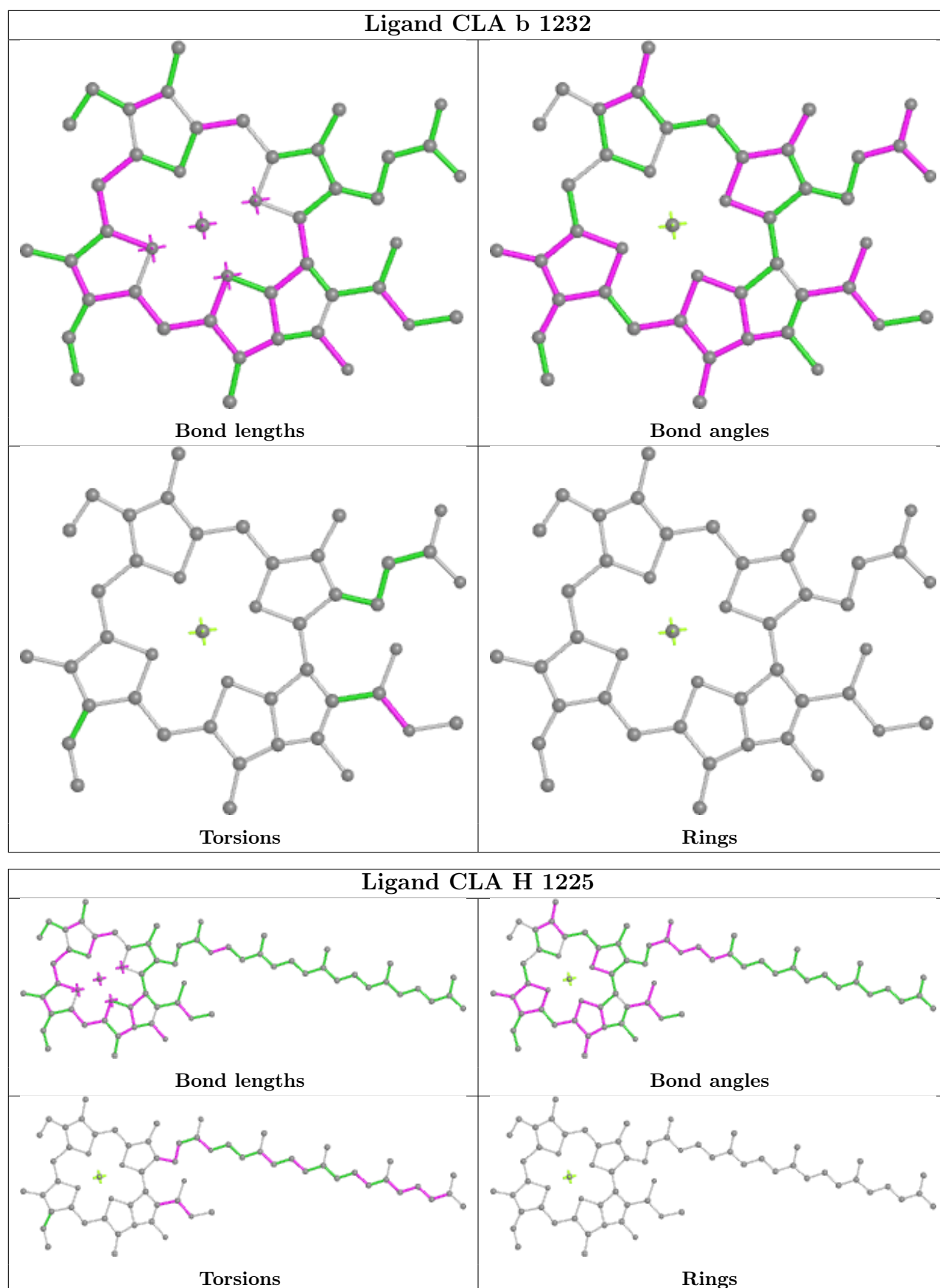


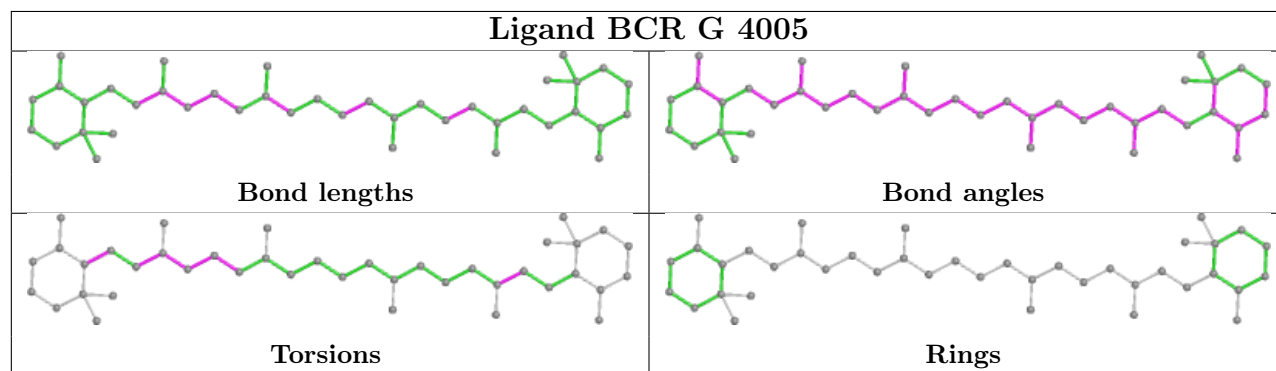
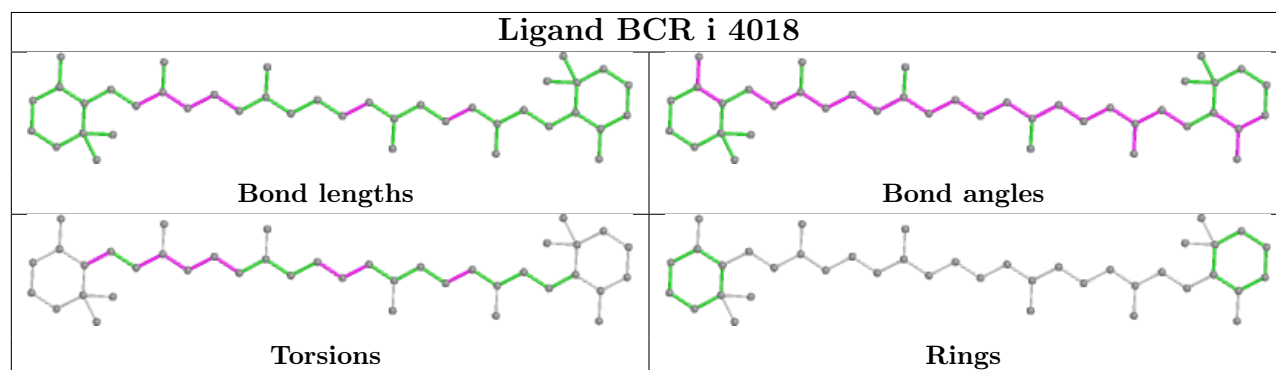
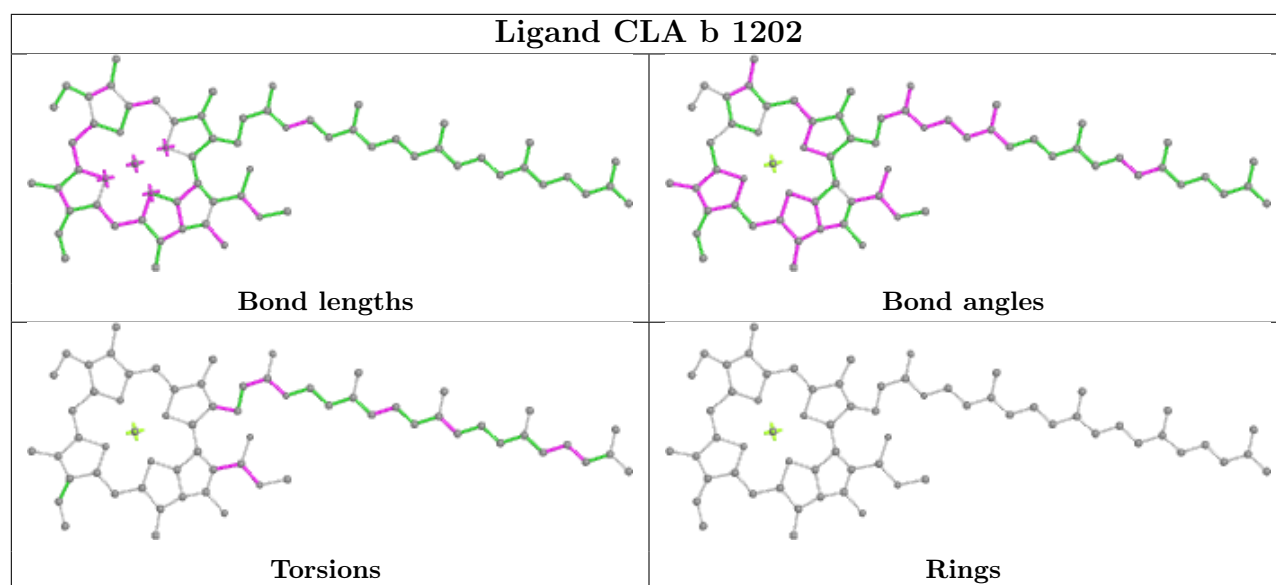
Ligand CLA G 1102

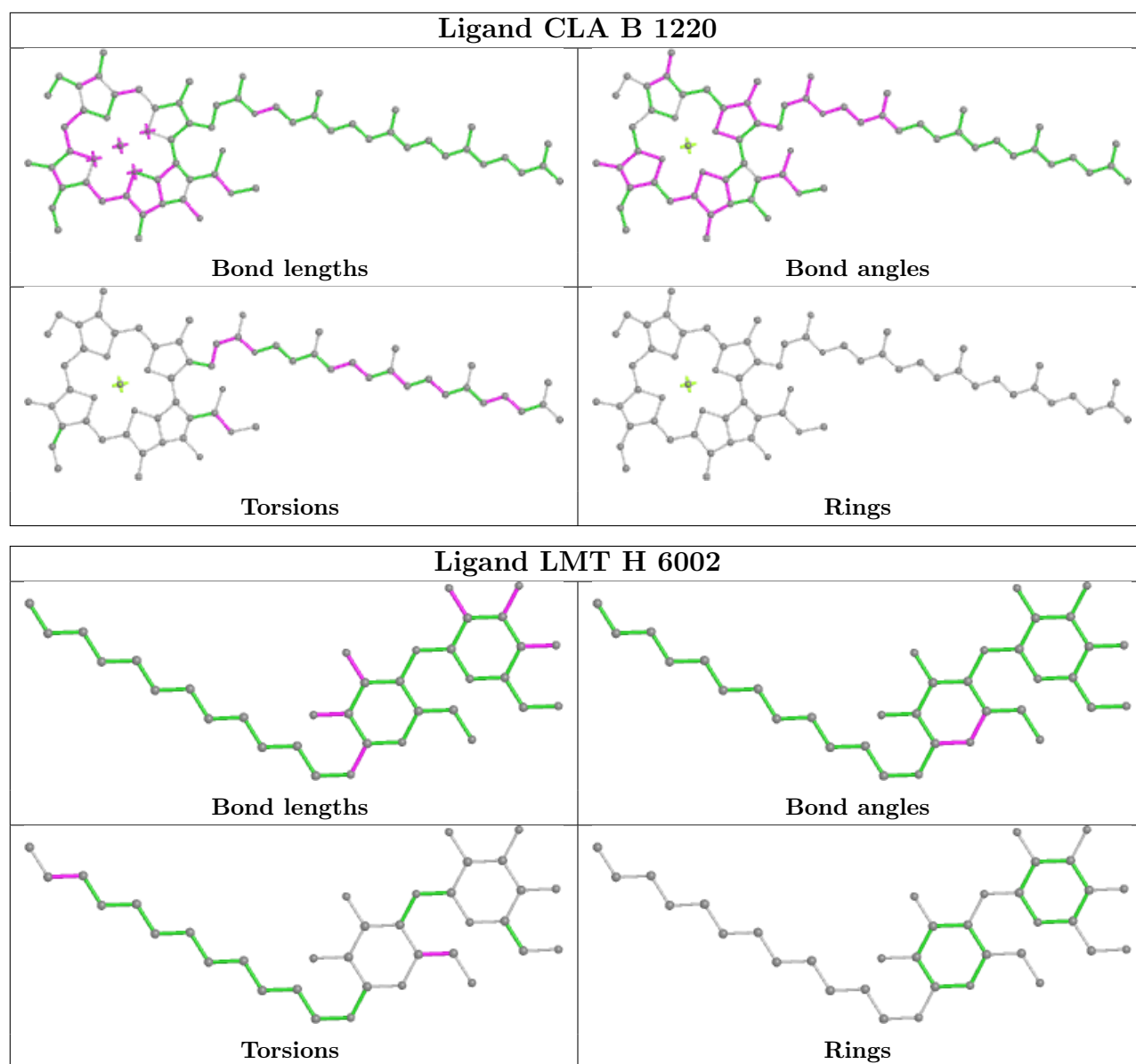


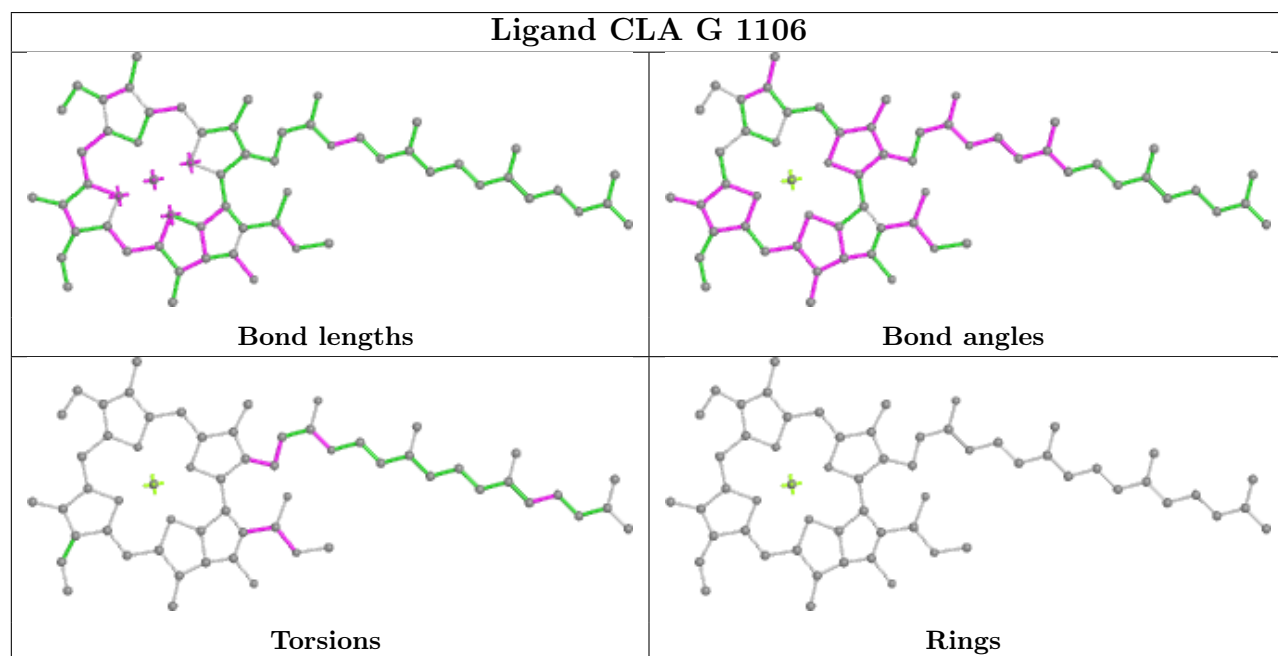
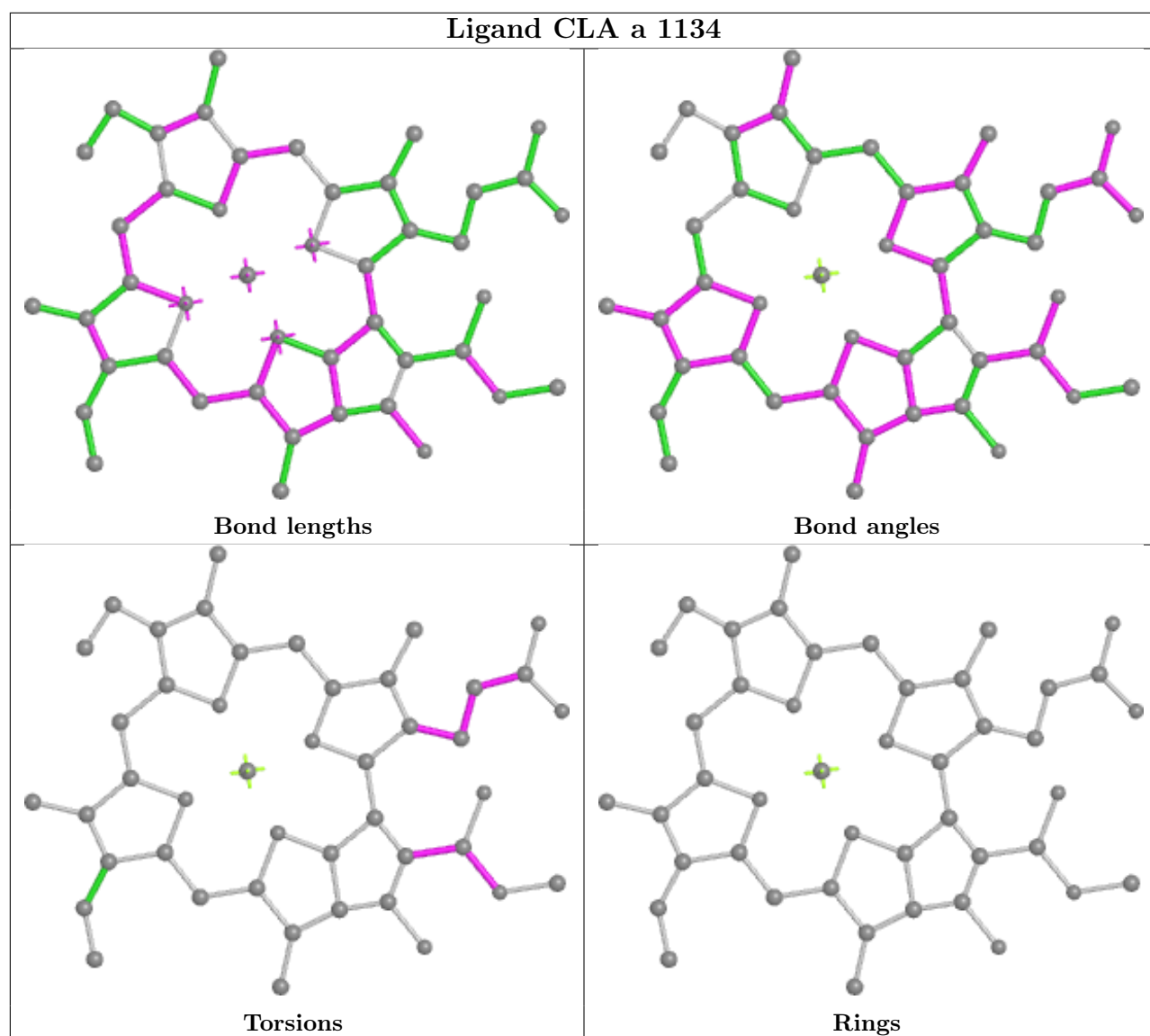
Ligand LMT G 6002

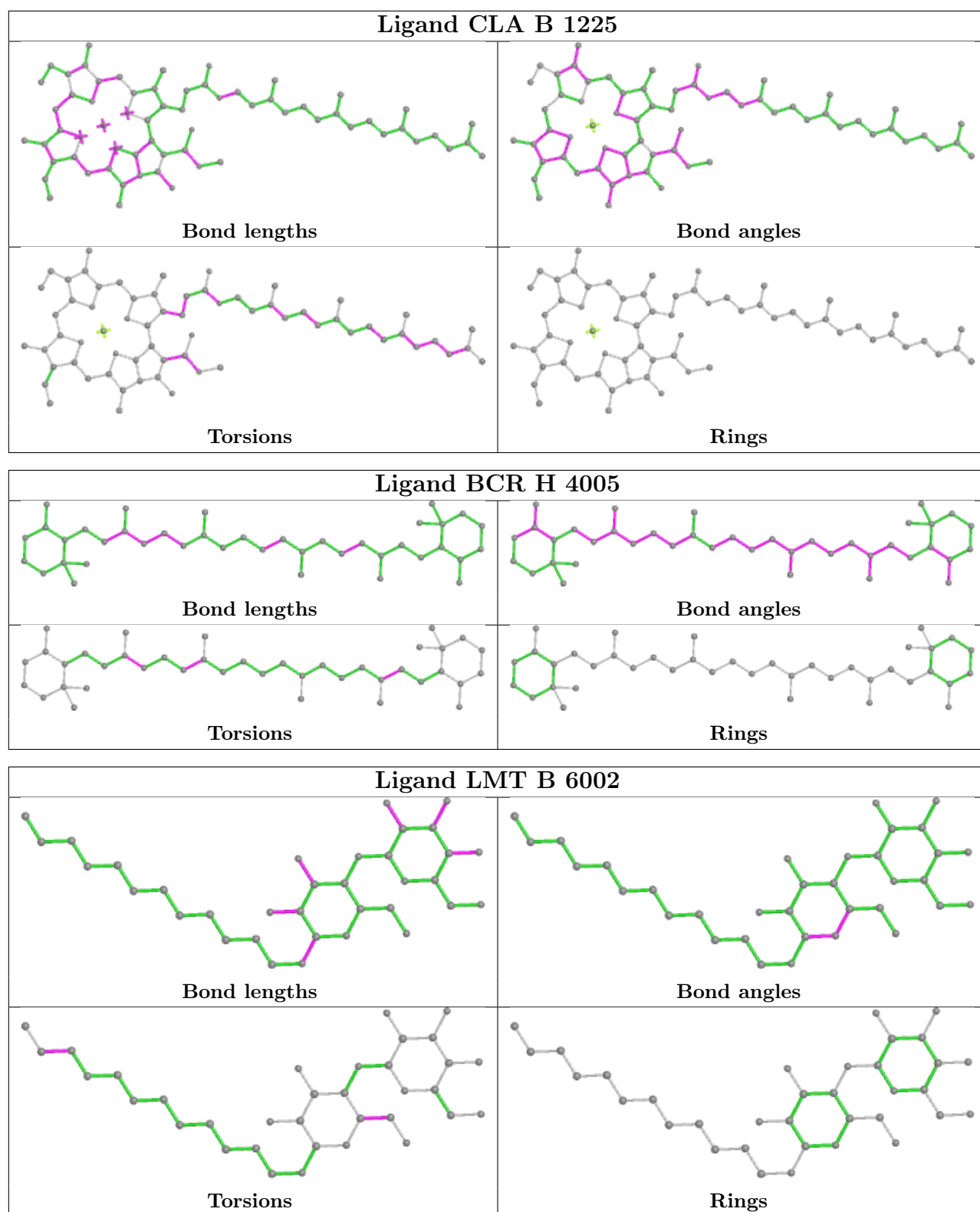




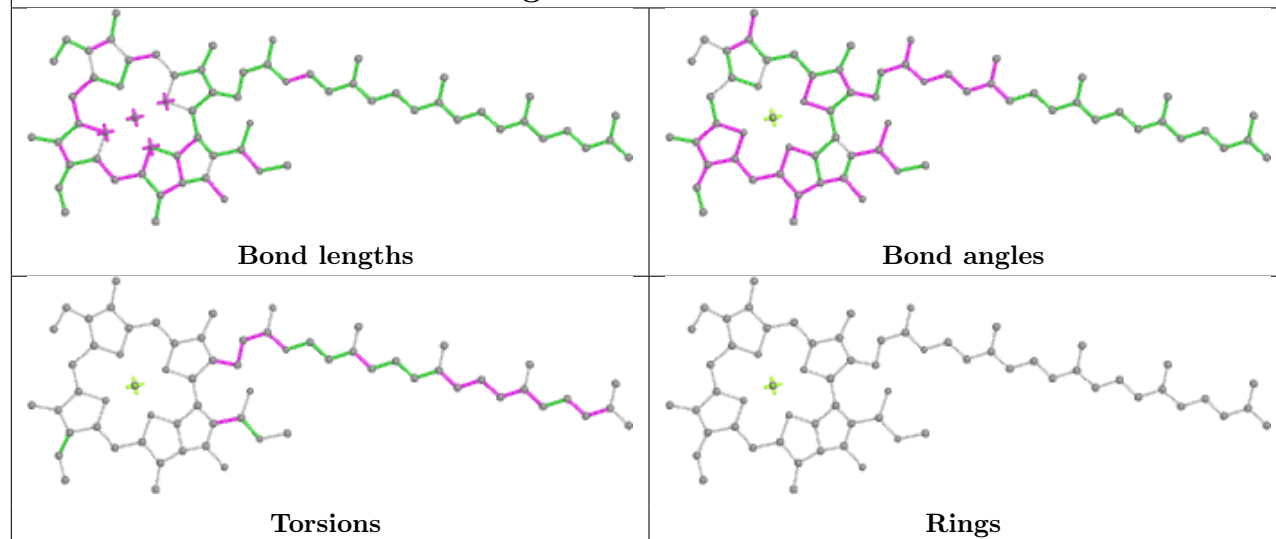




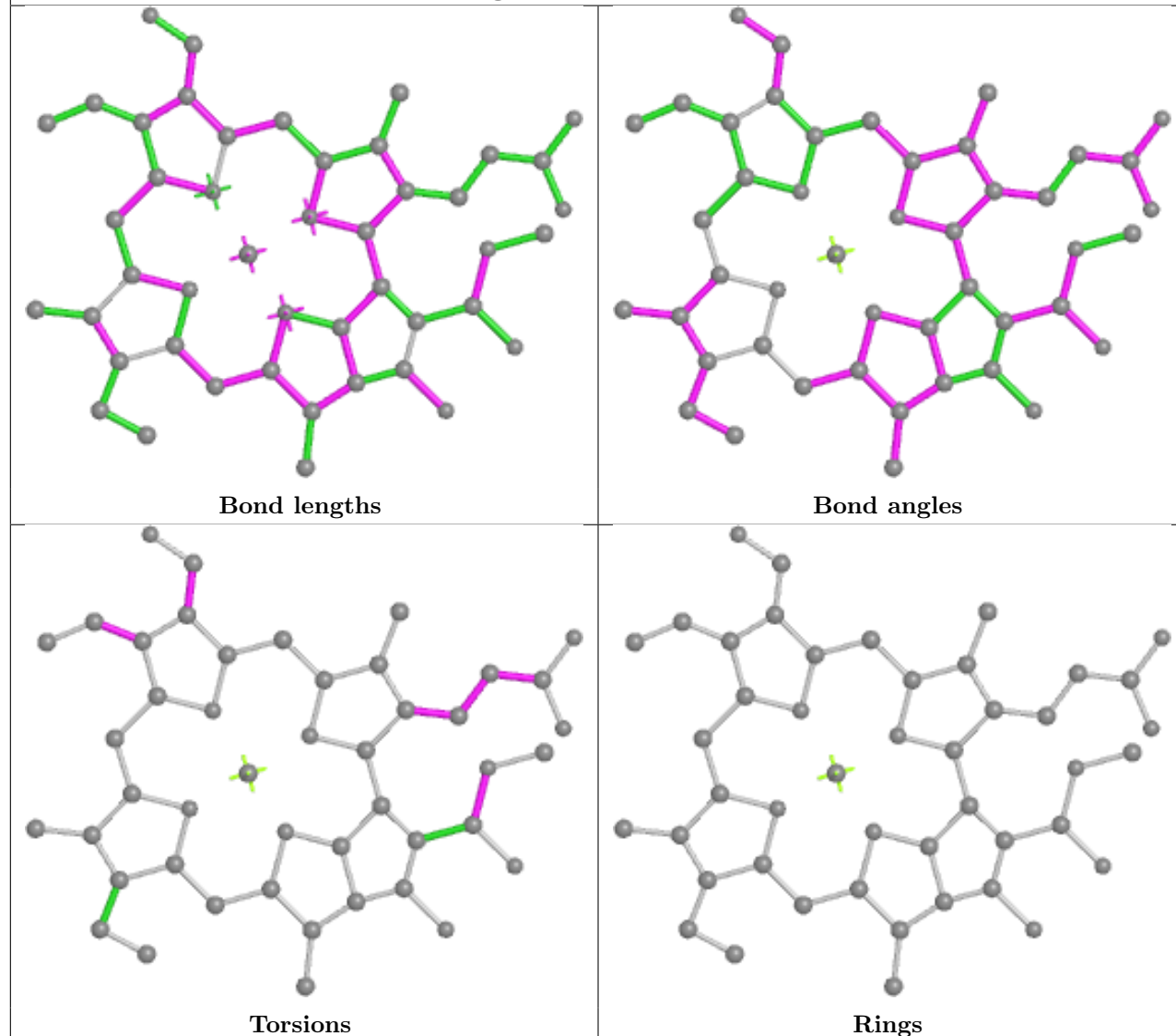


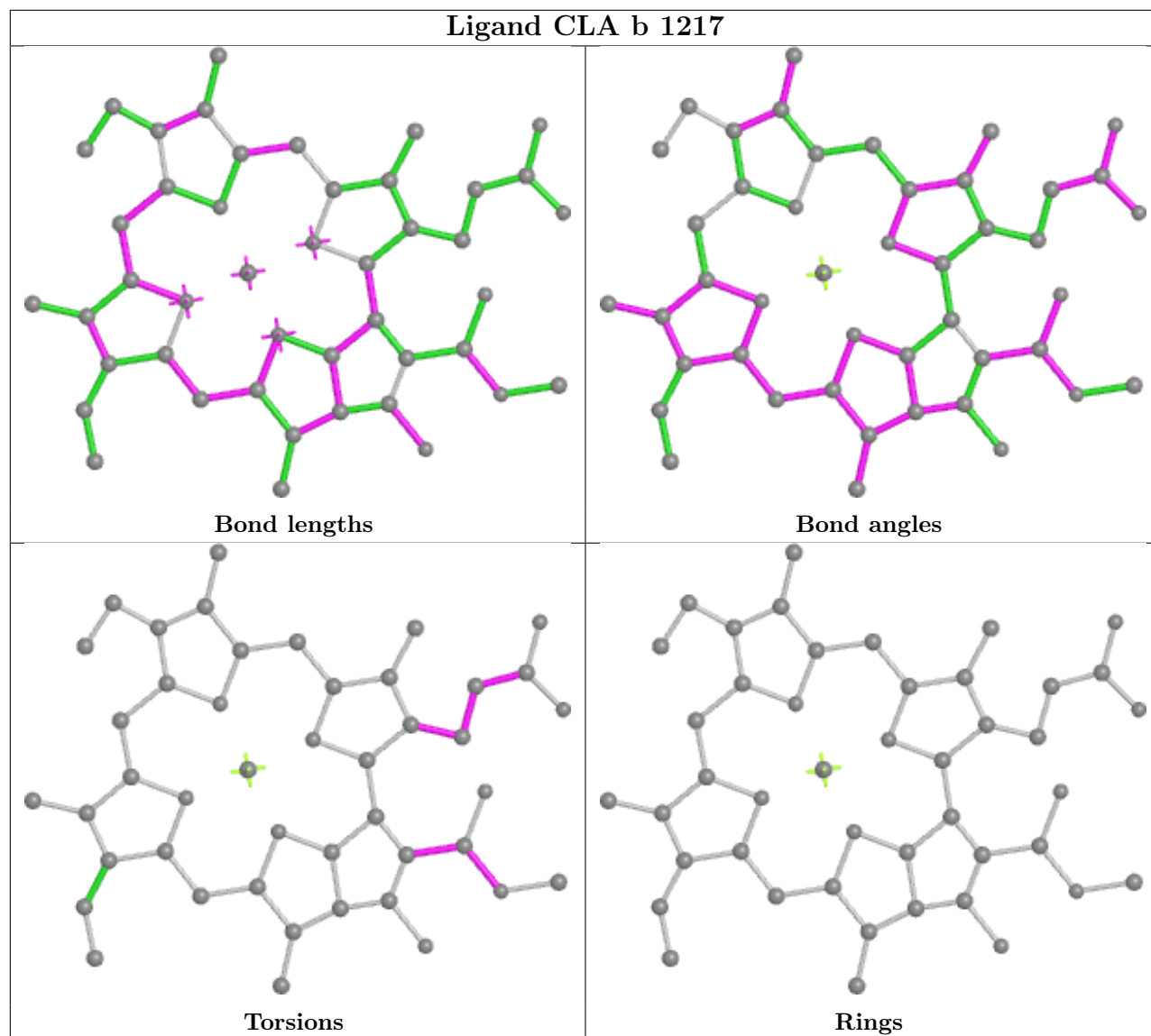
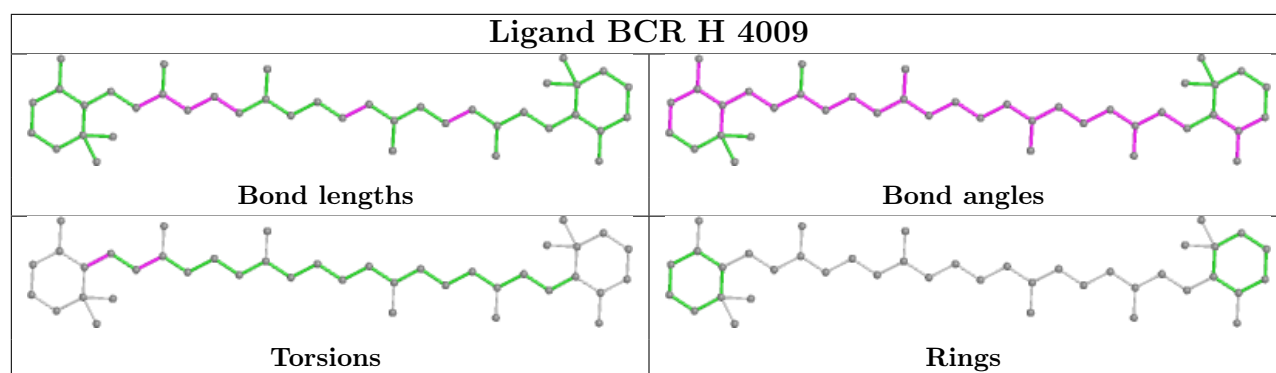


Ligand CLA A 1125

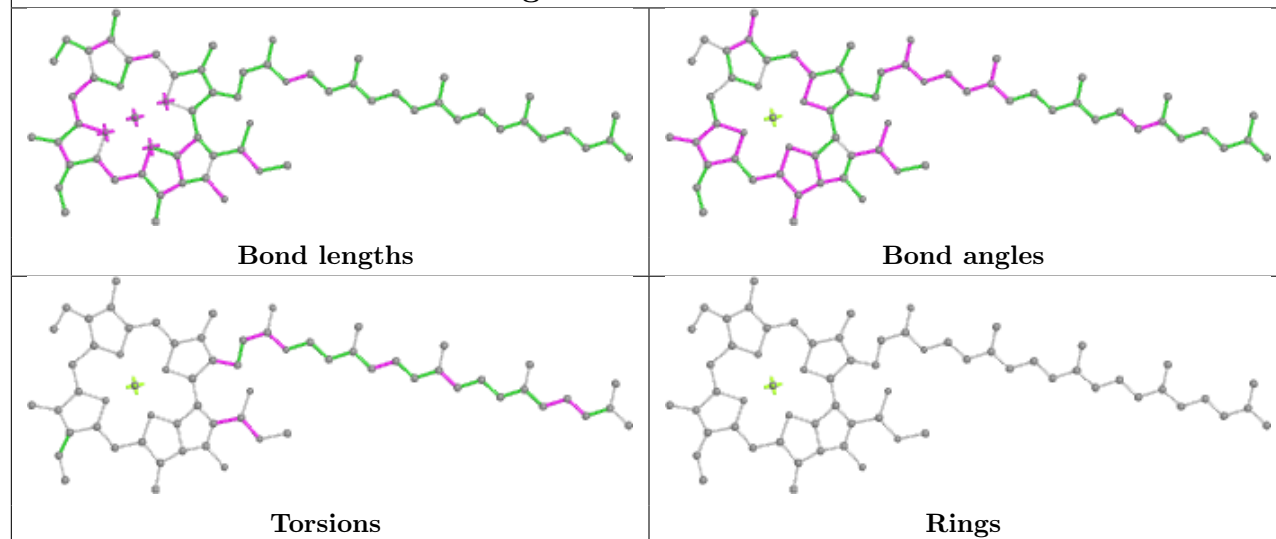


Ligand F6C a 1121

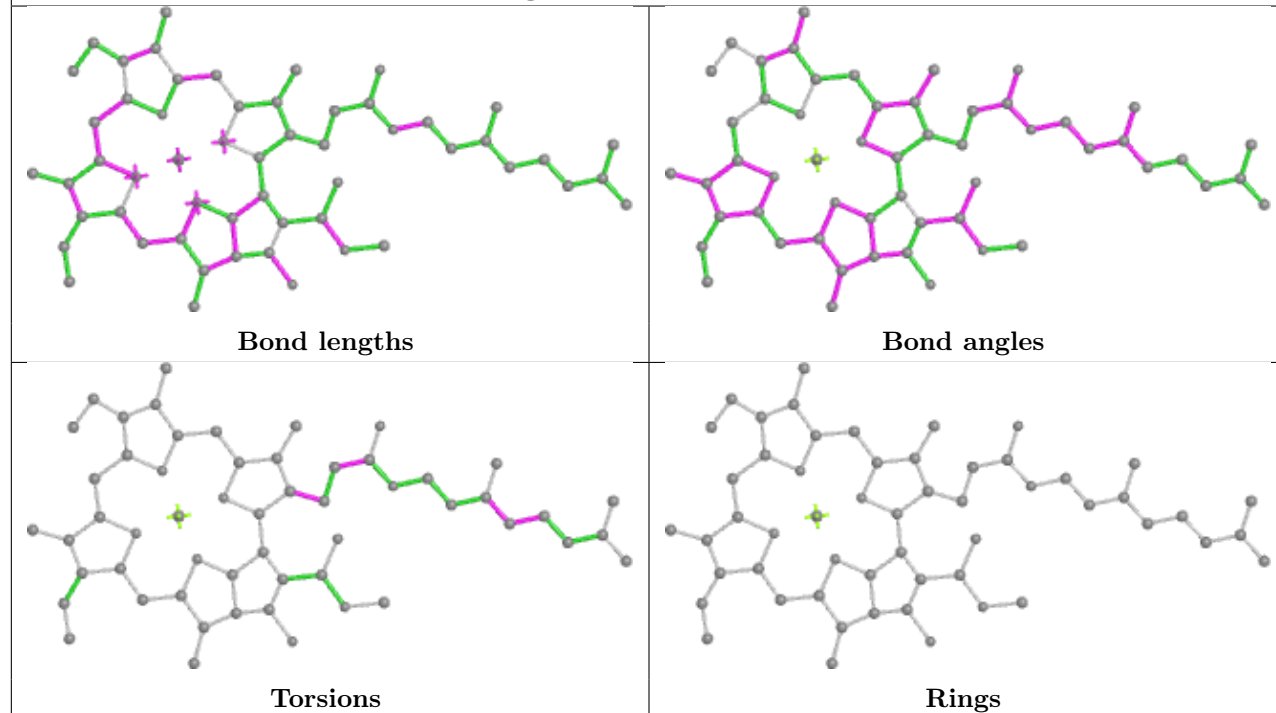


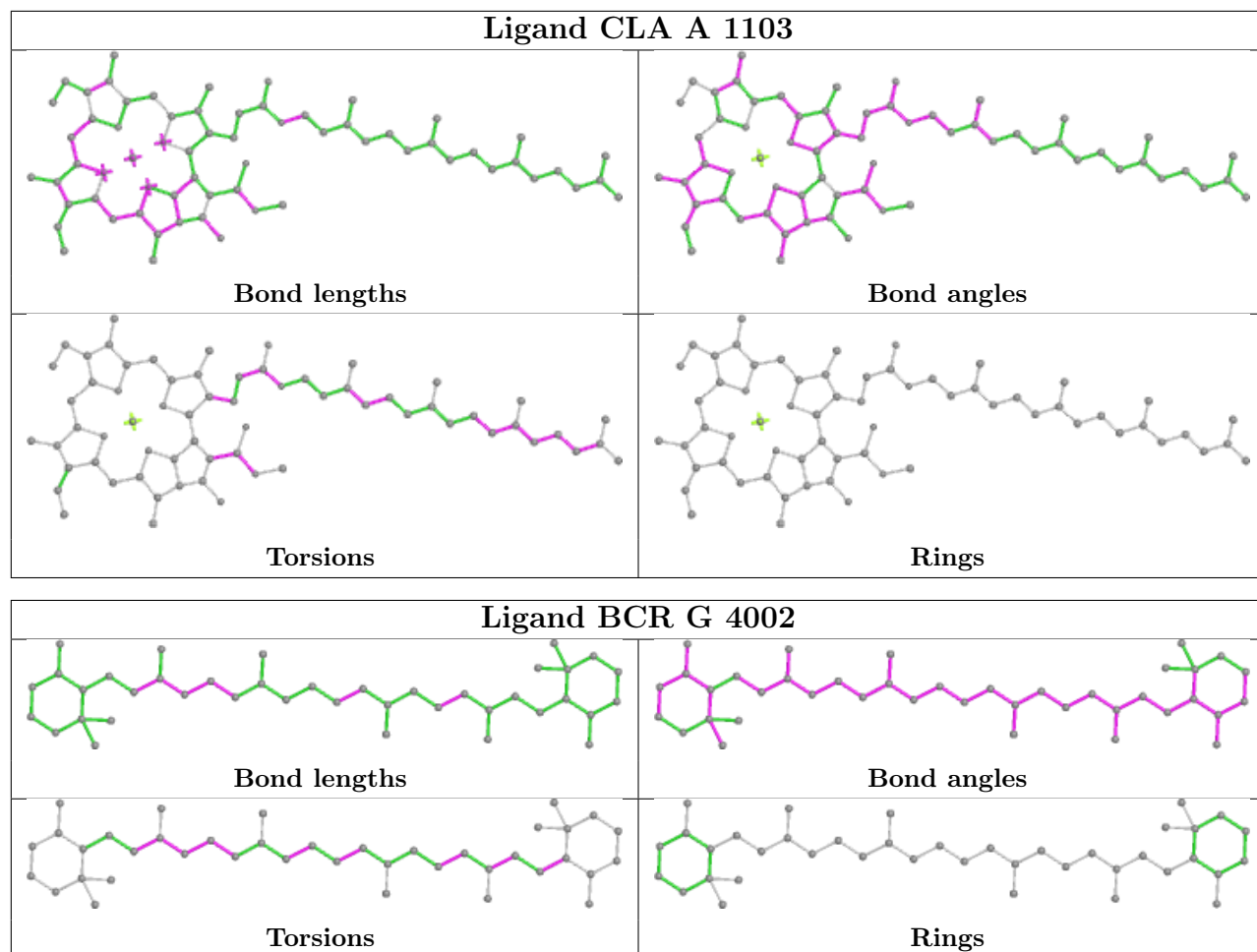


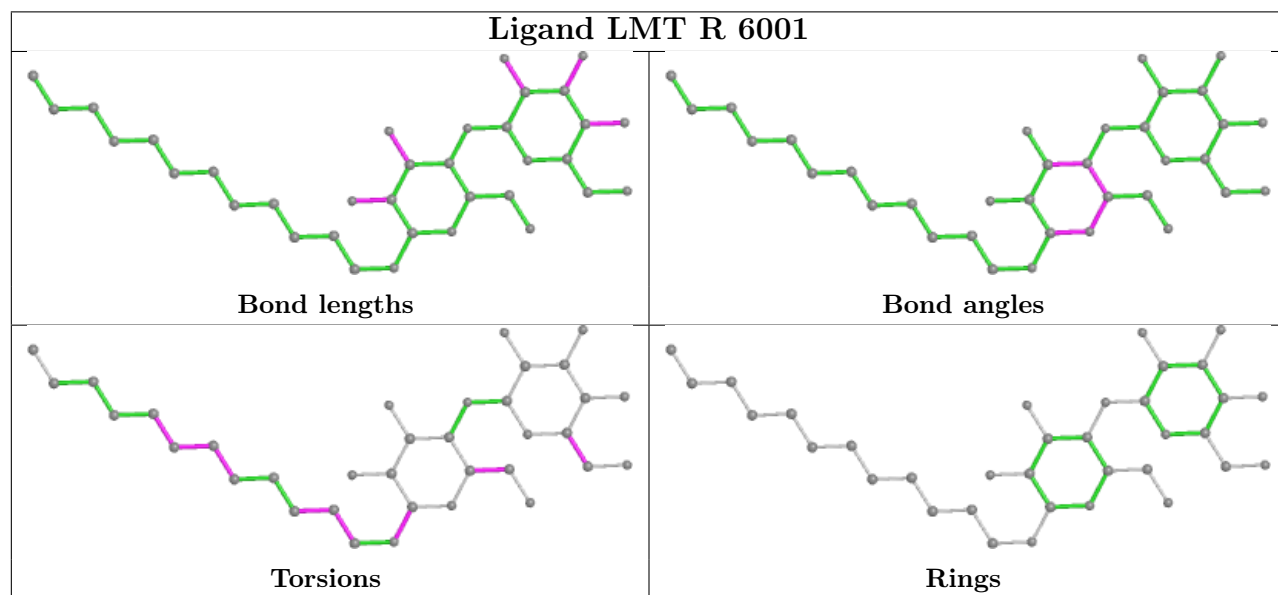
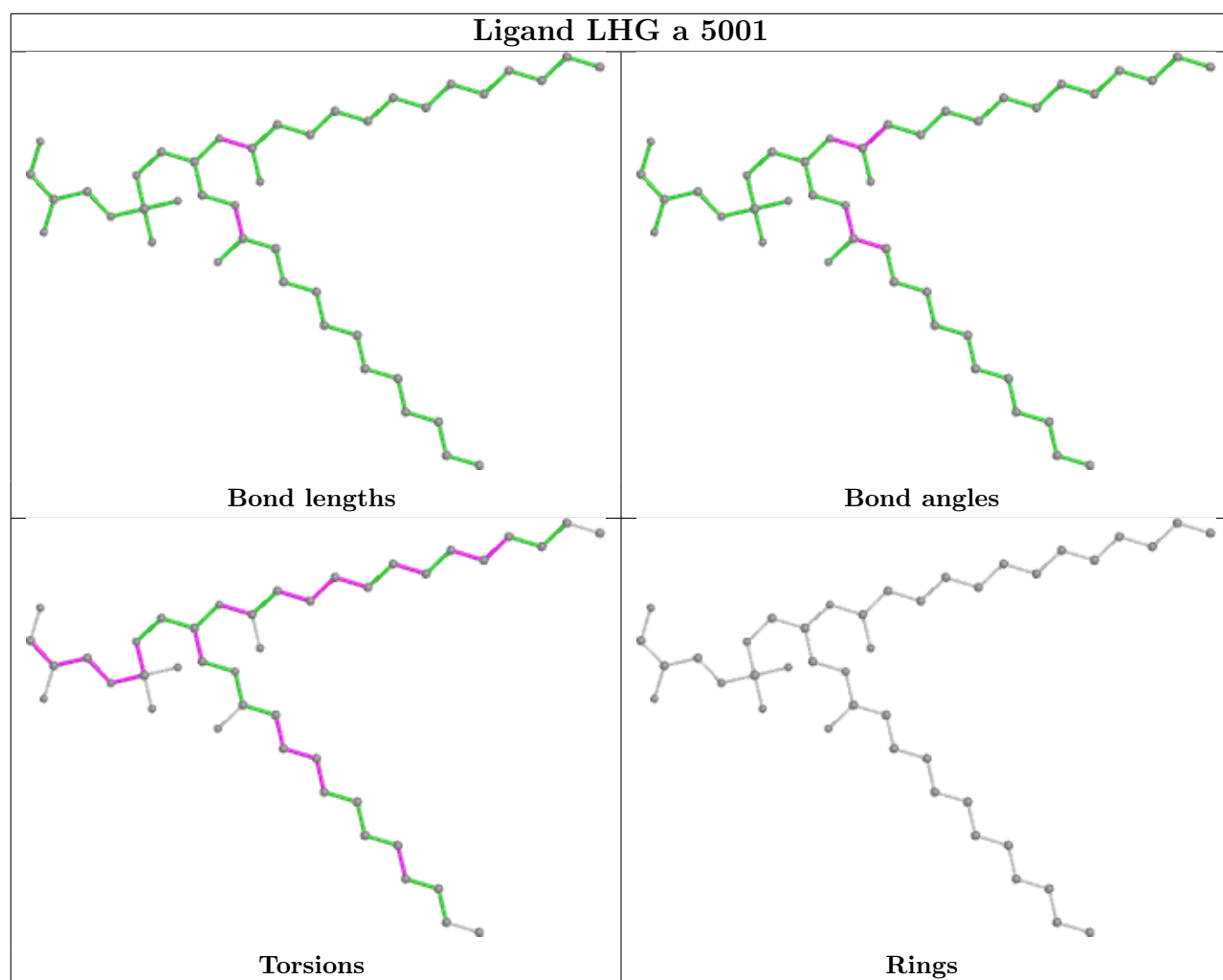
Ligand CLA H 1202

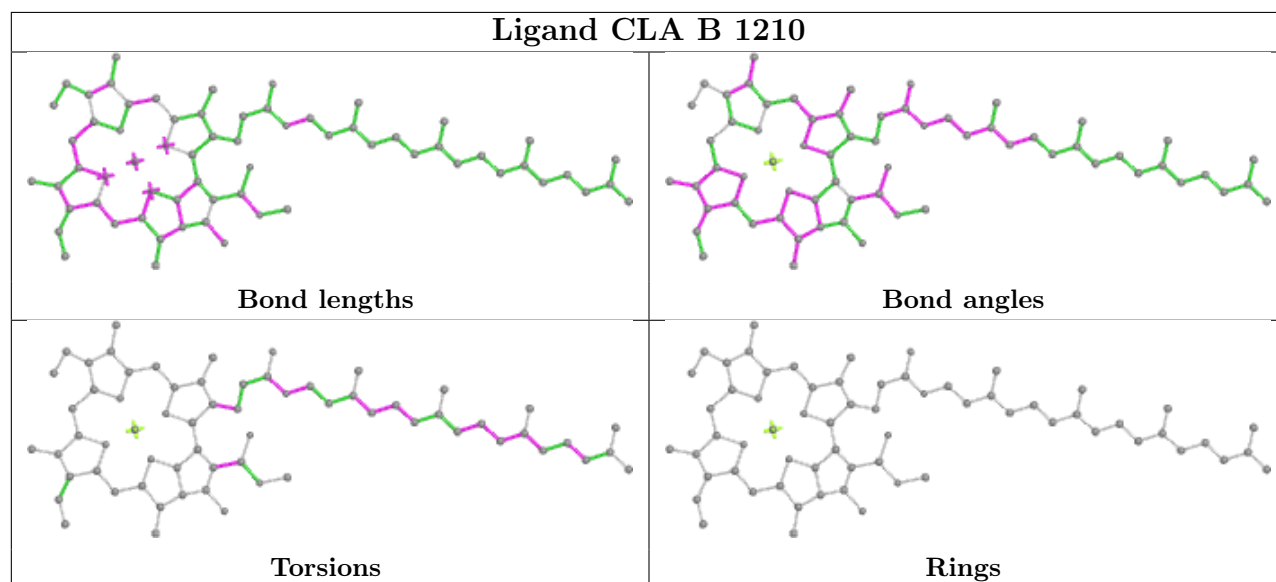
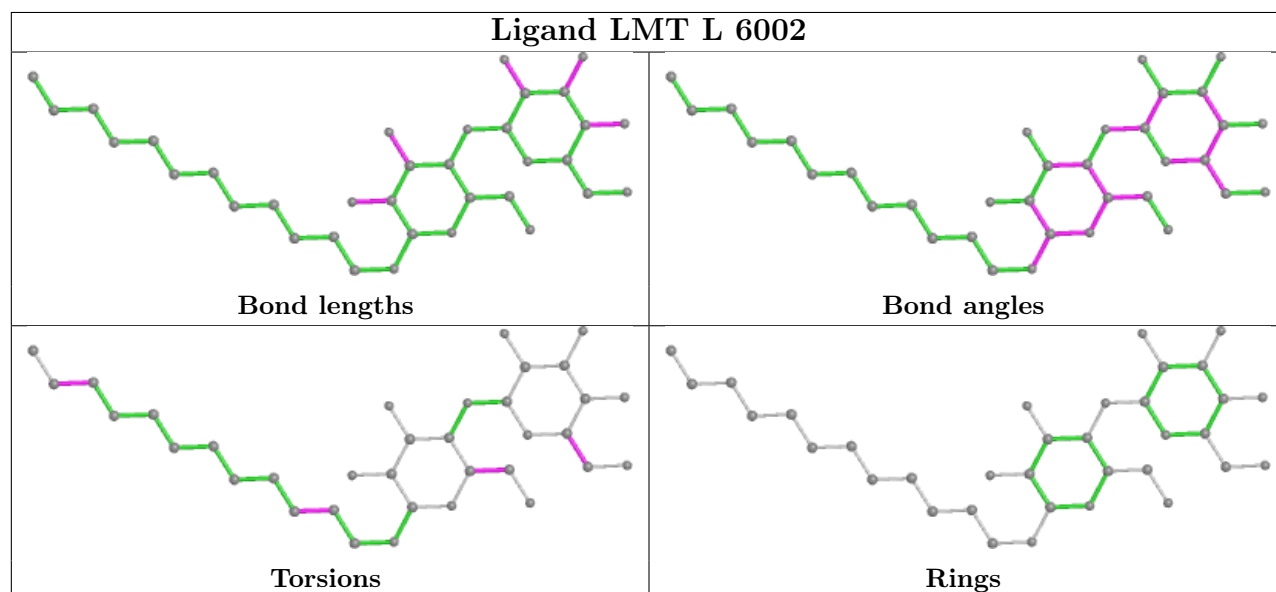
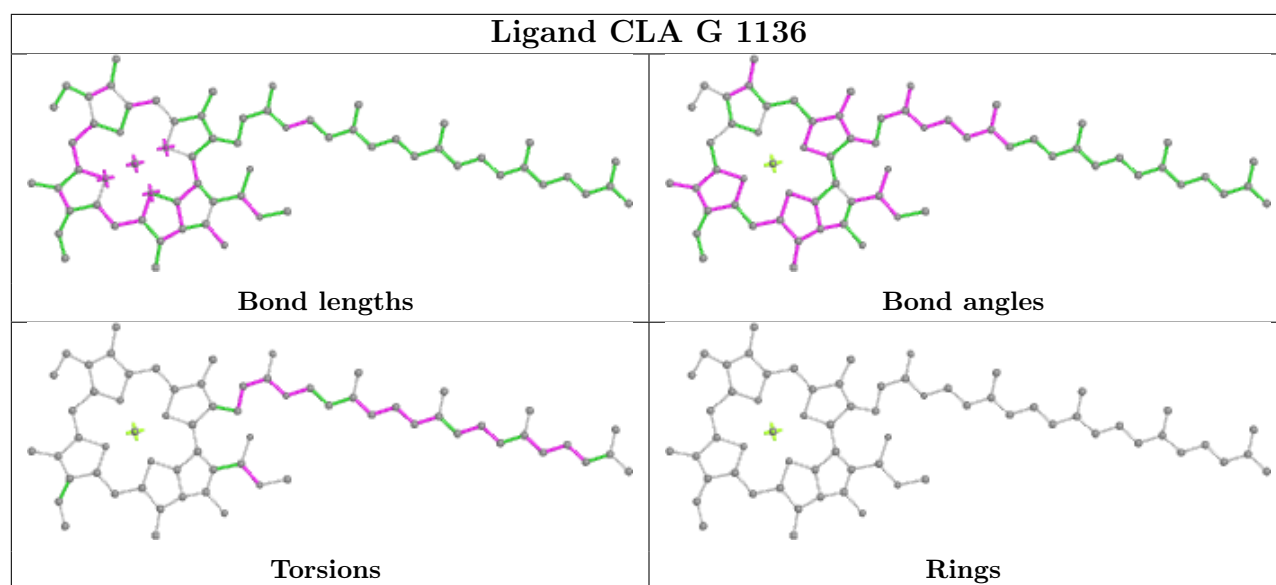


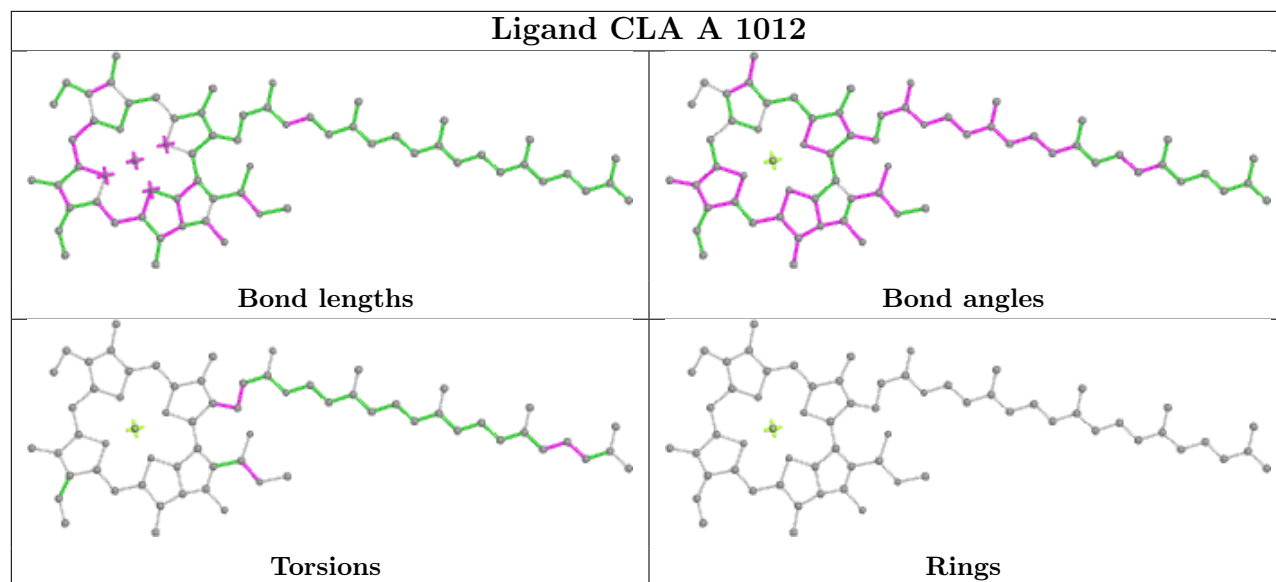
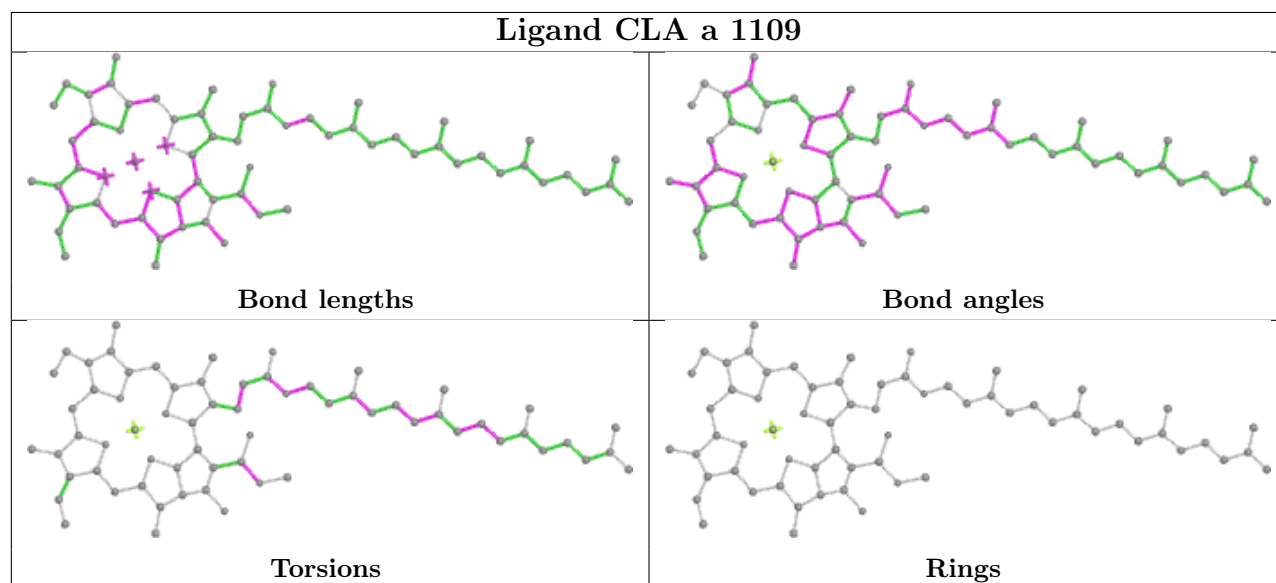
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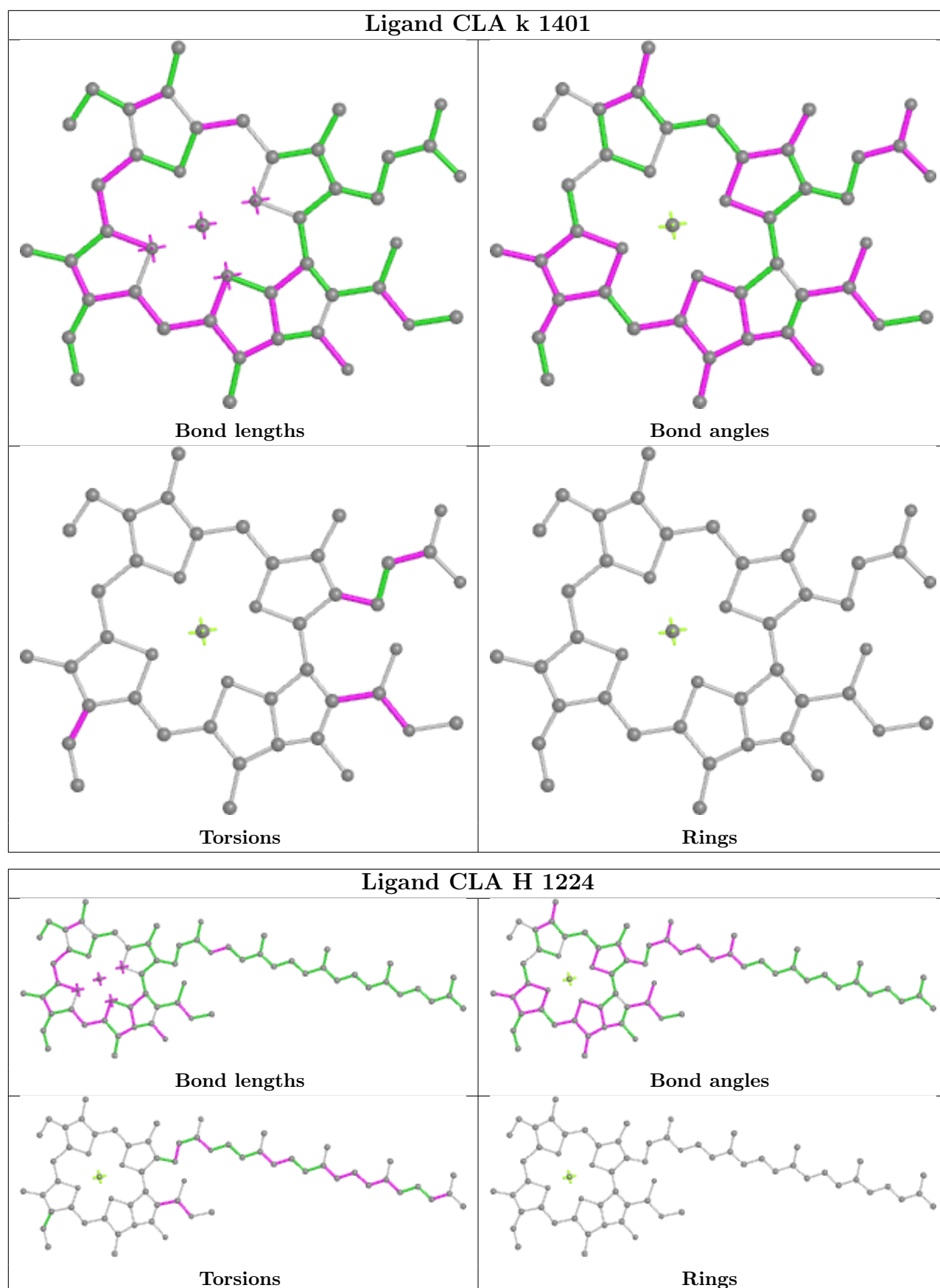


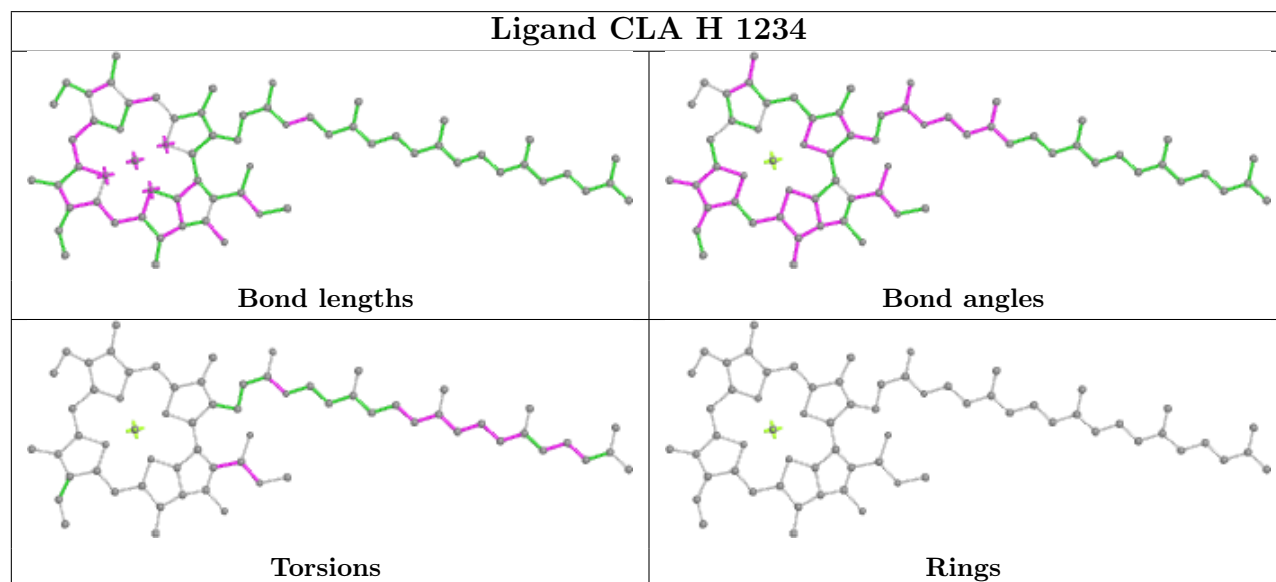
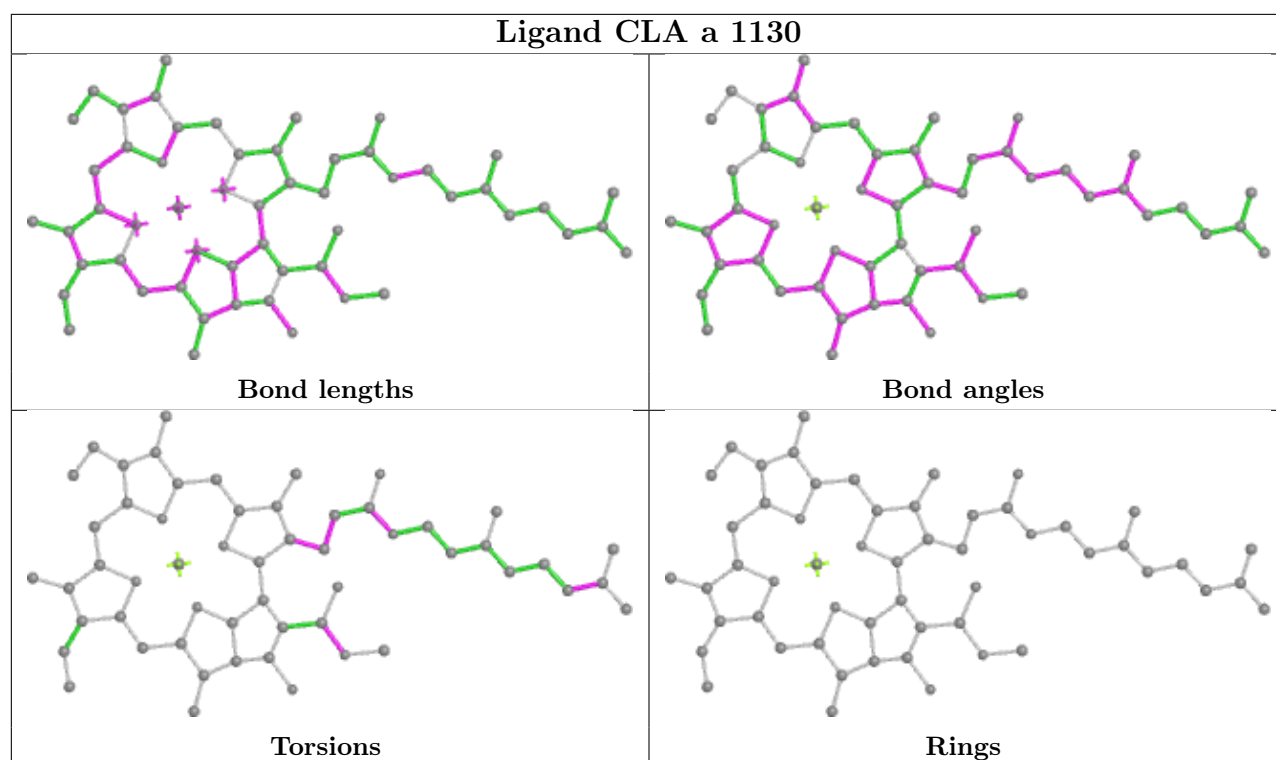


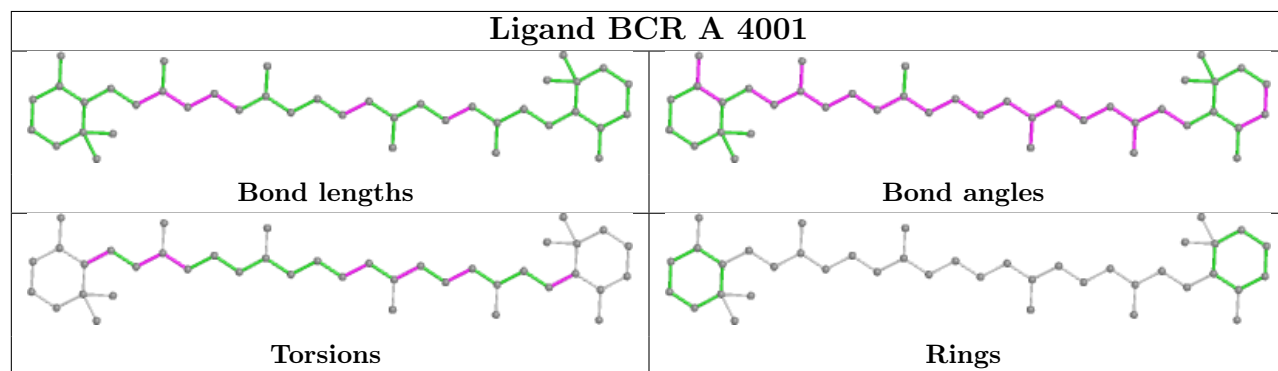
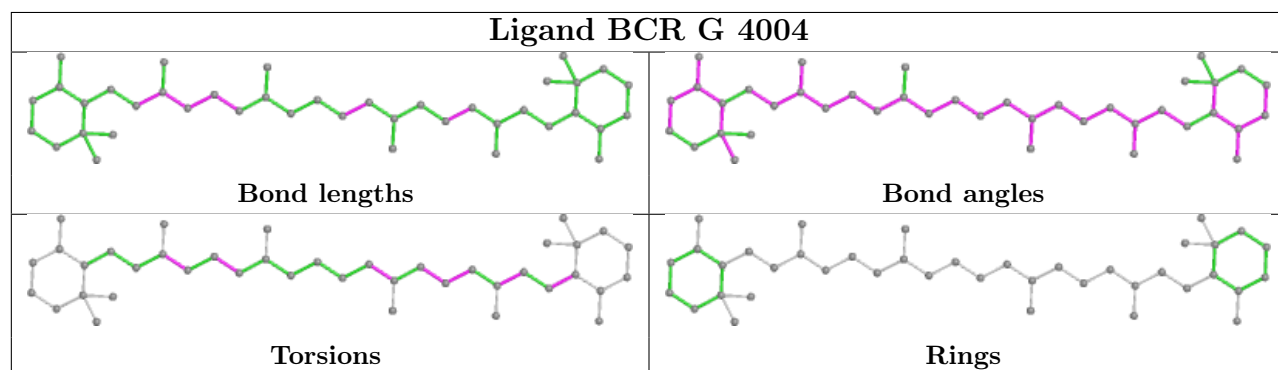
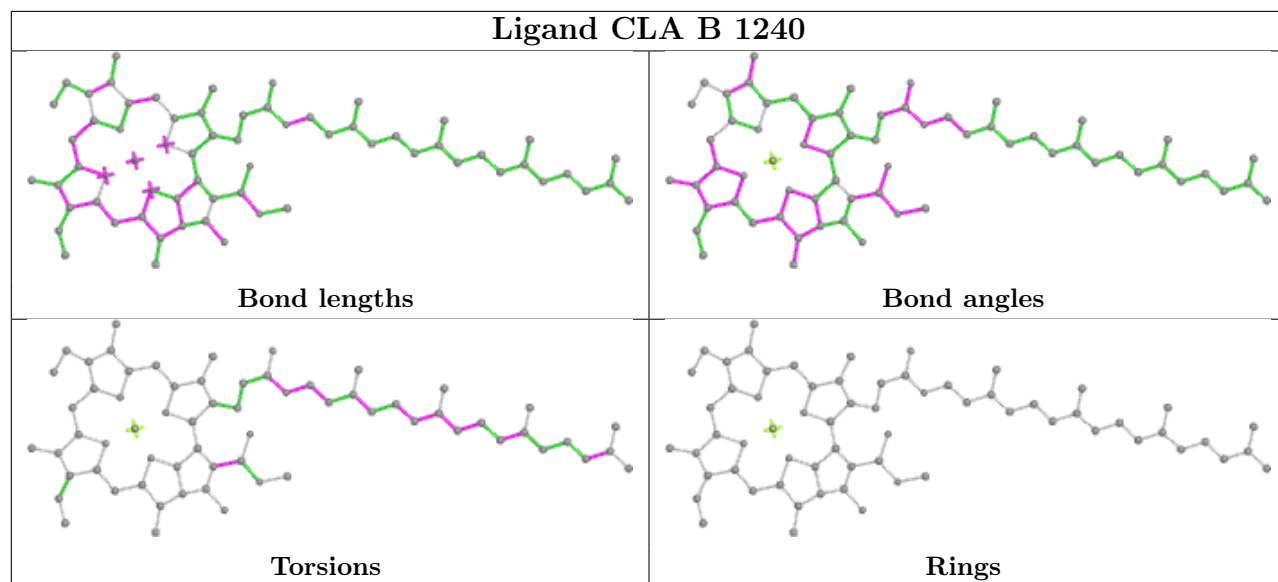


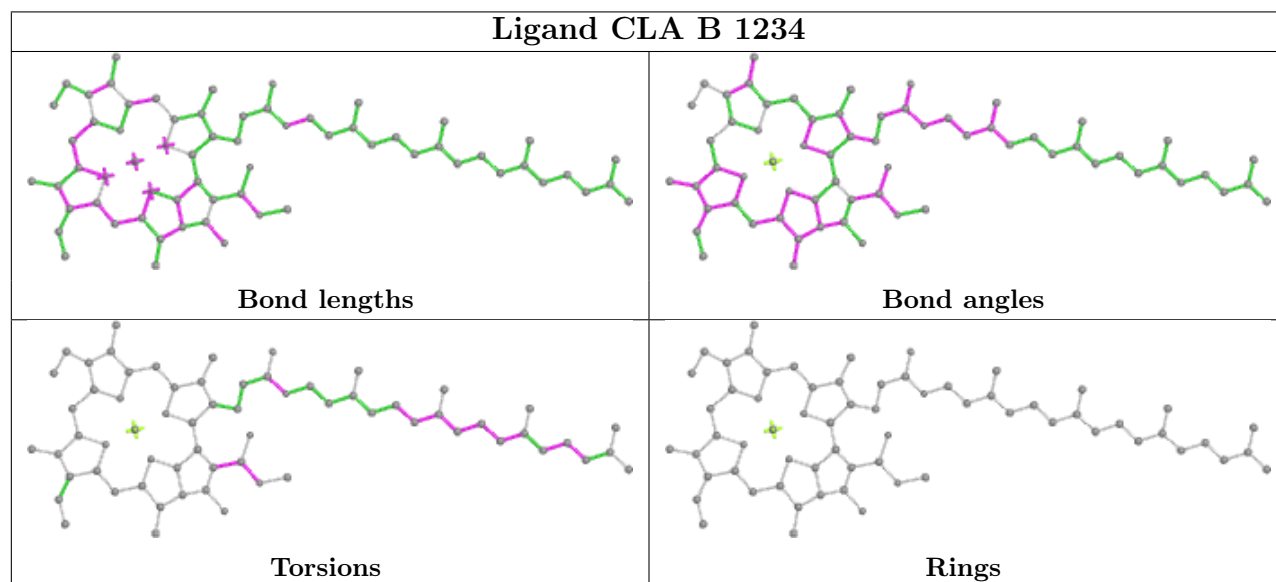
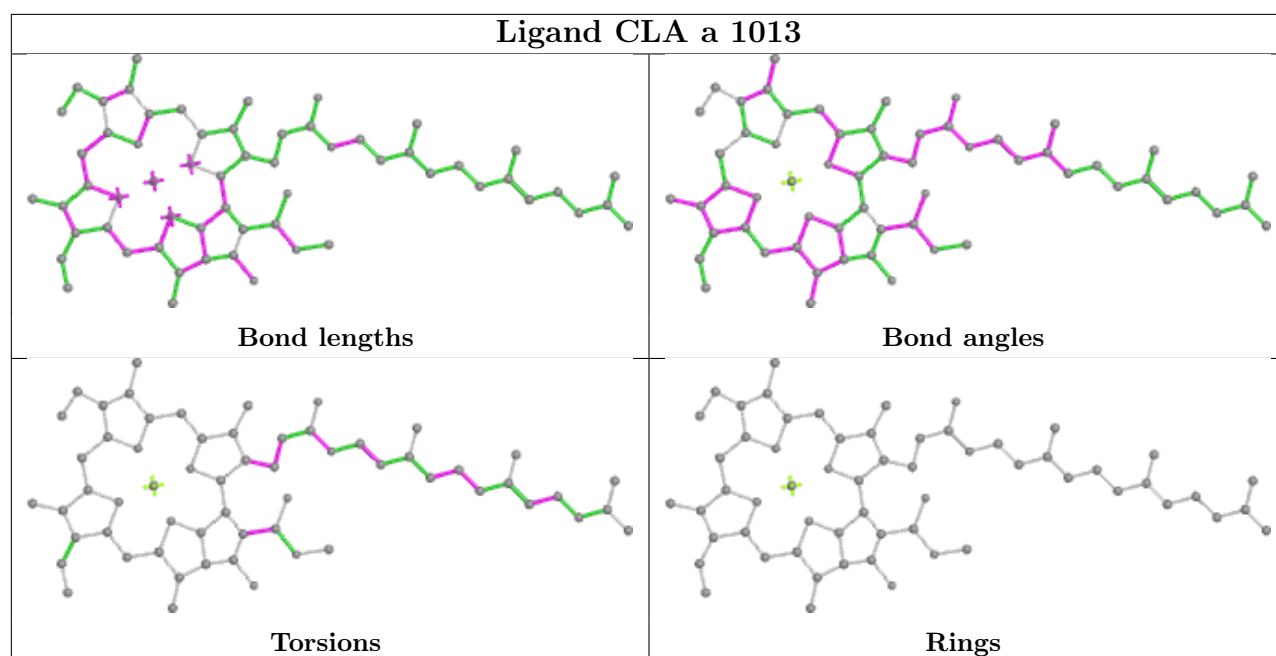


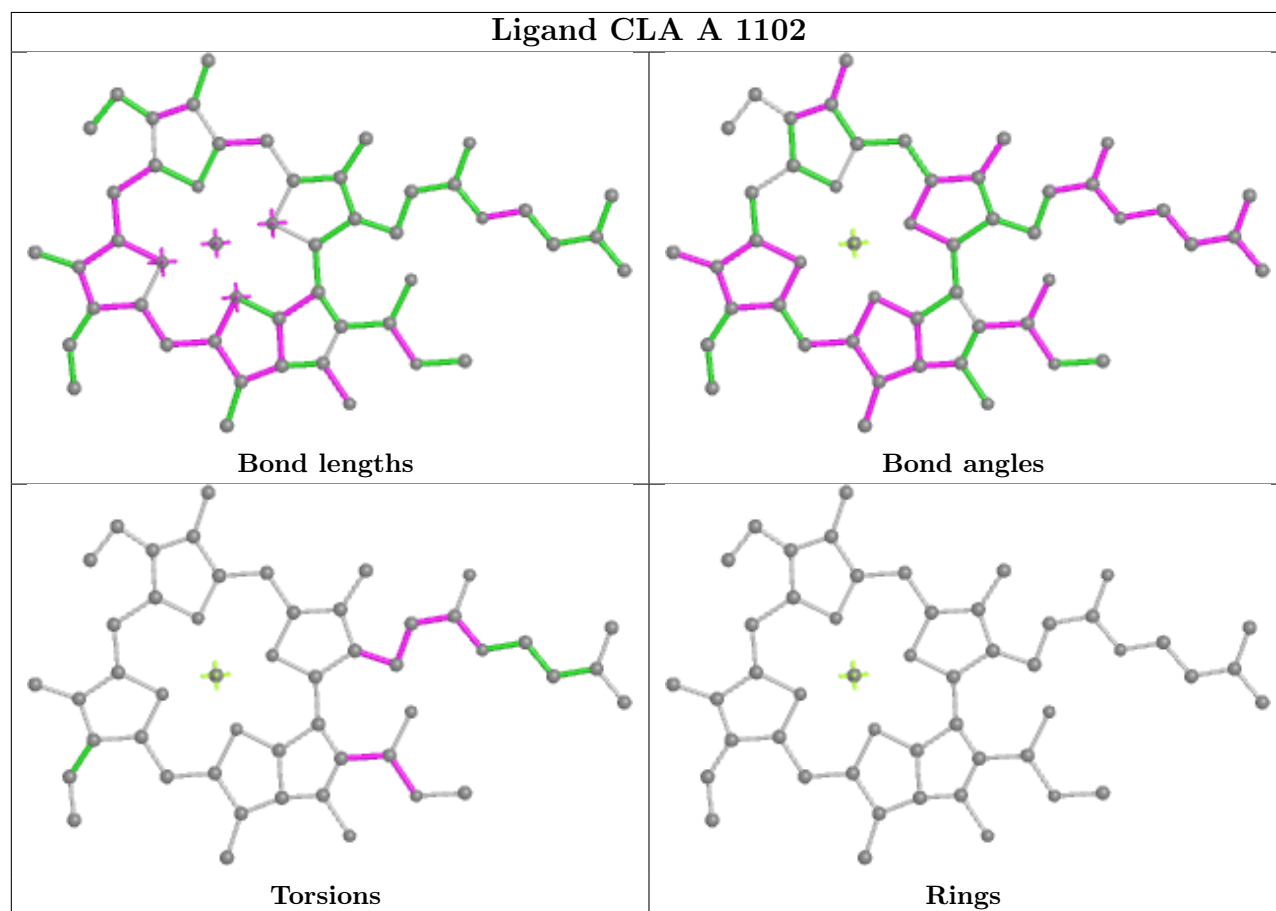
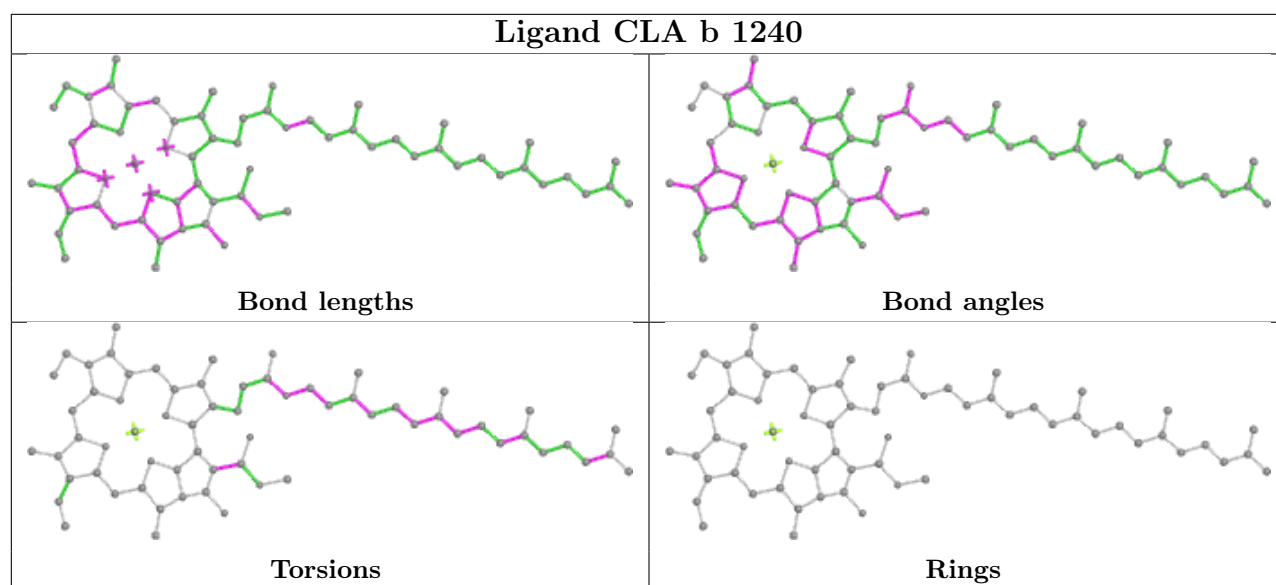
Ligand CLA A 1012**Ligand CLA a 1109**

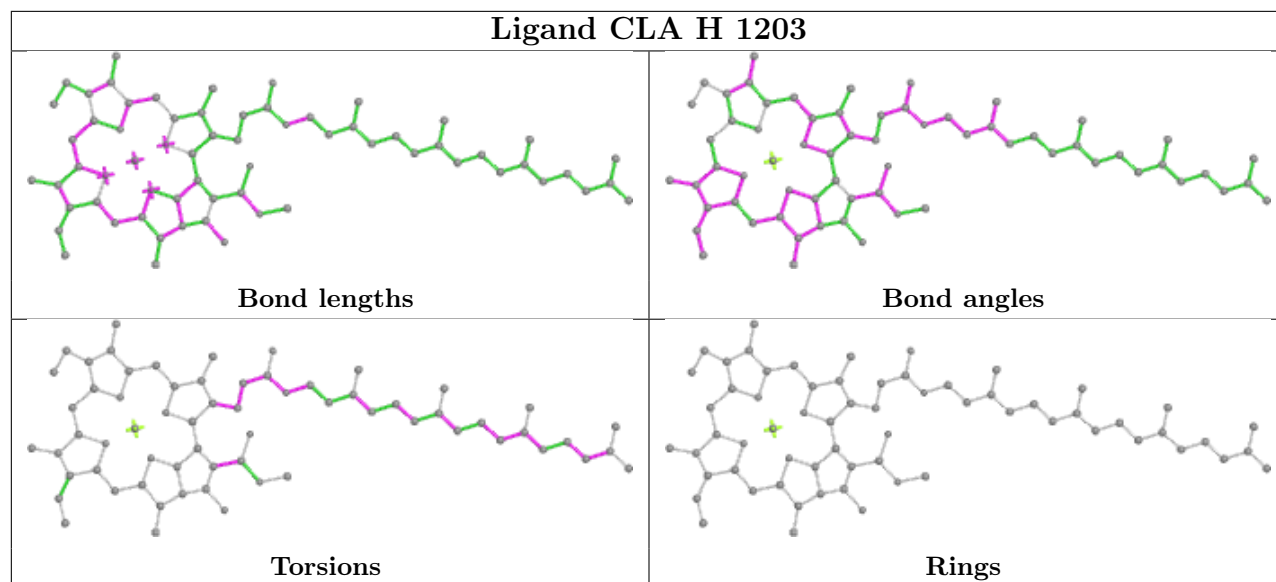
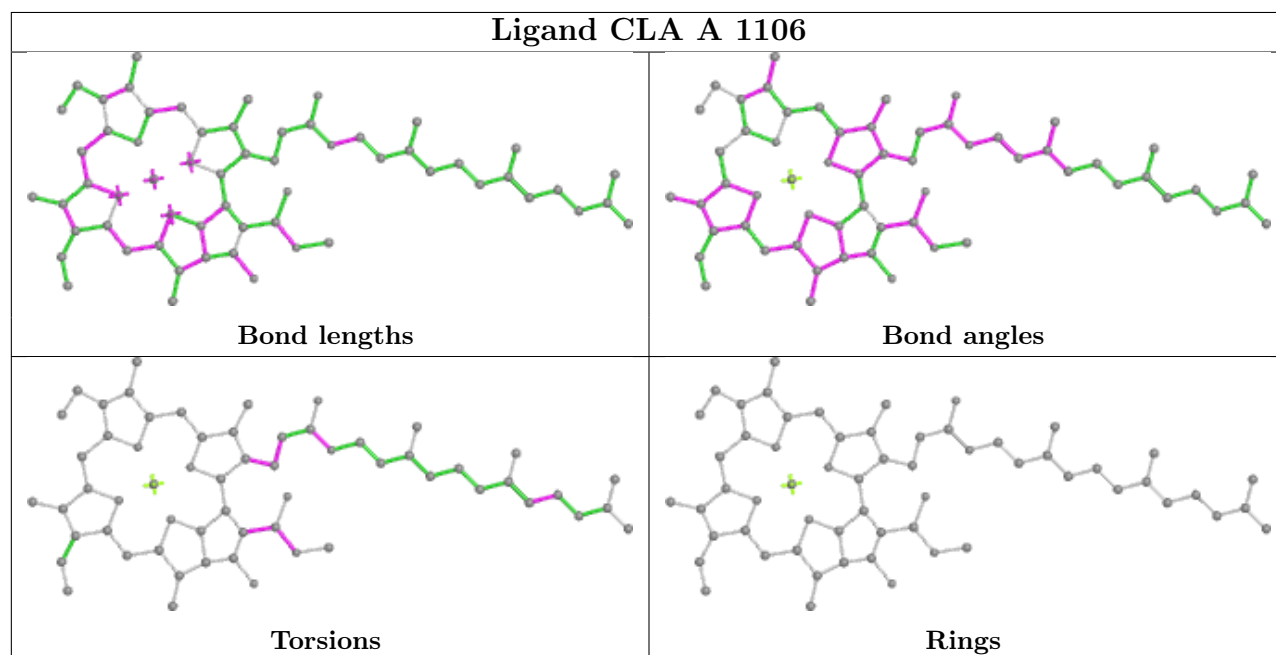


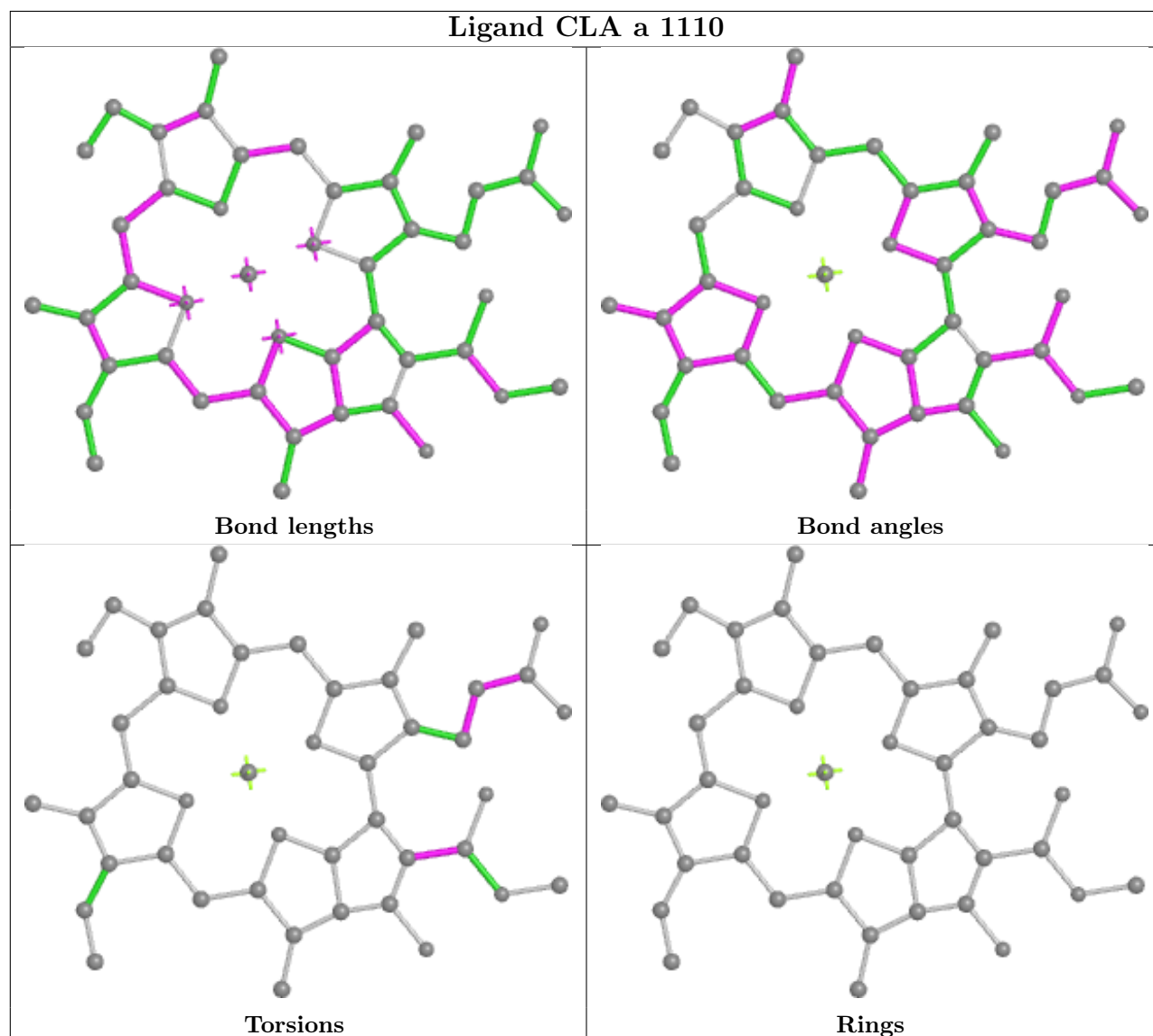
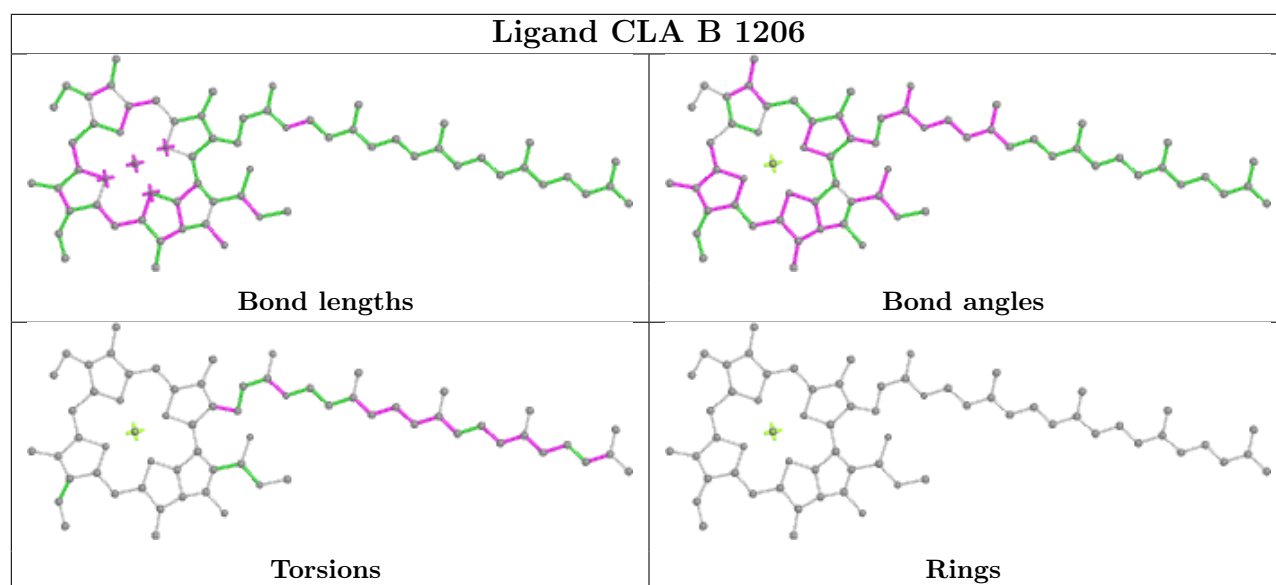


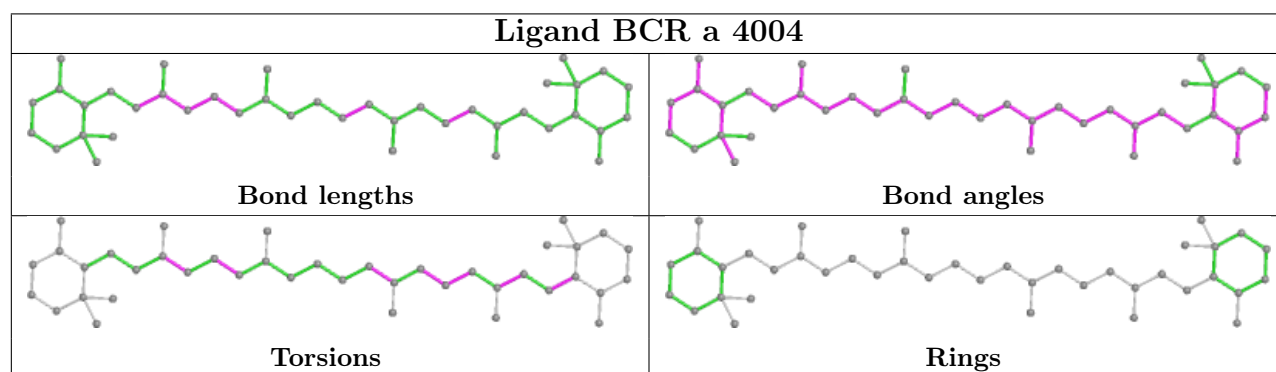
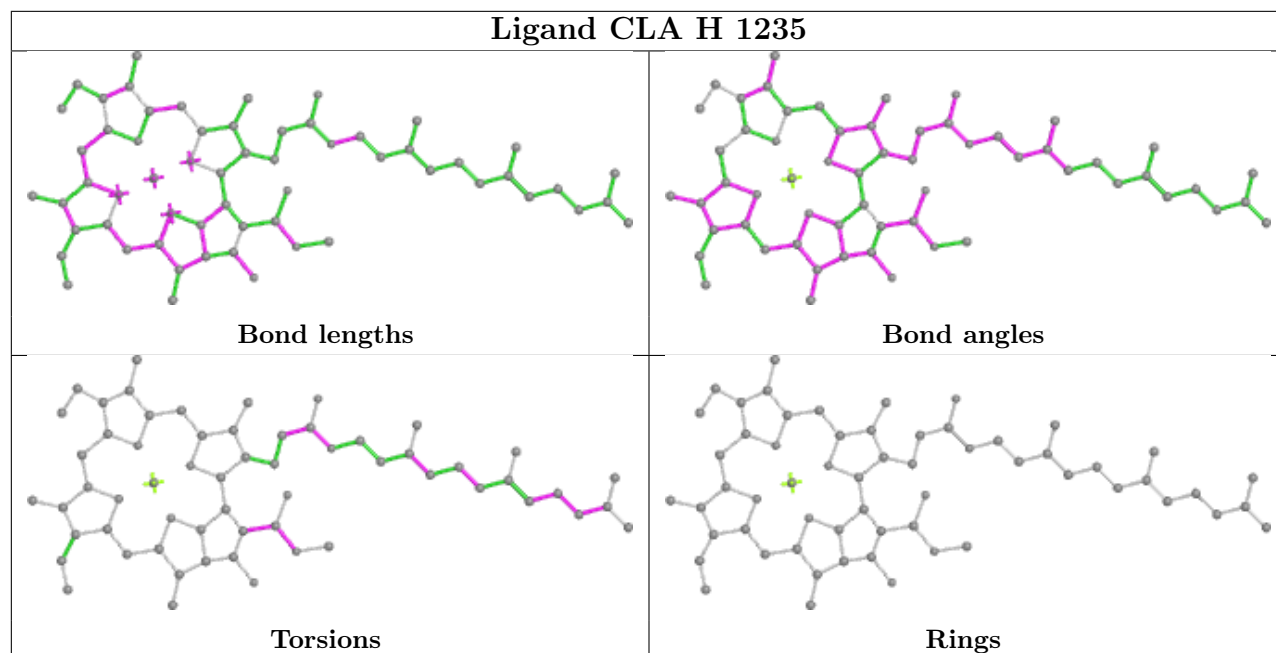
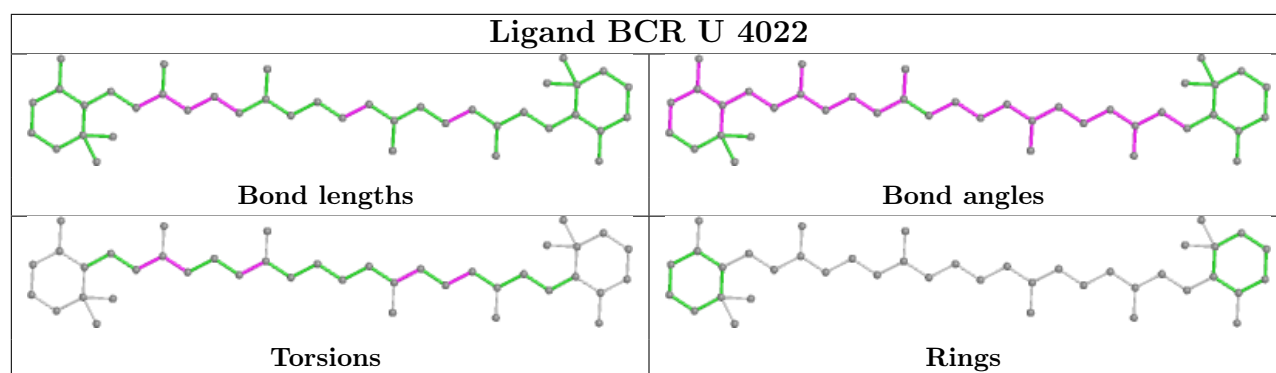


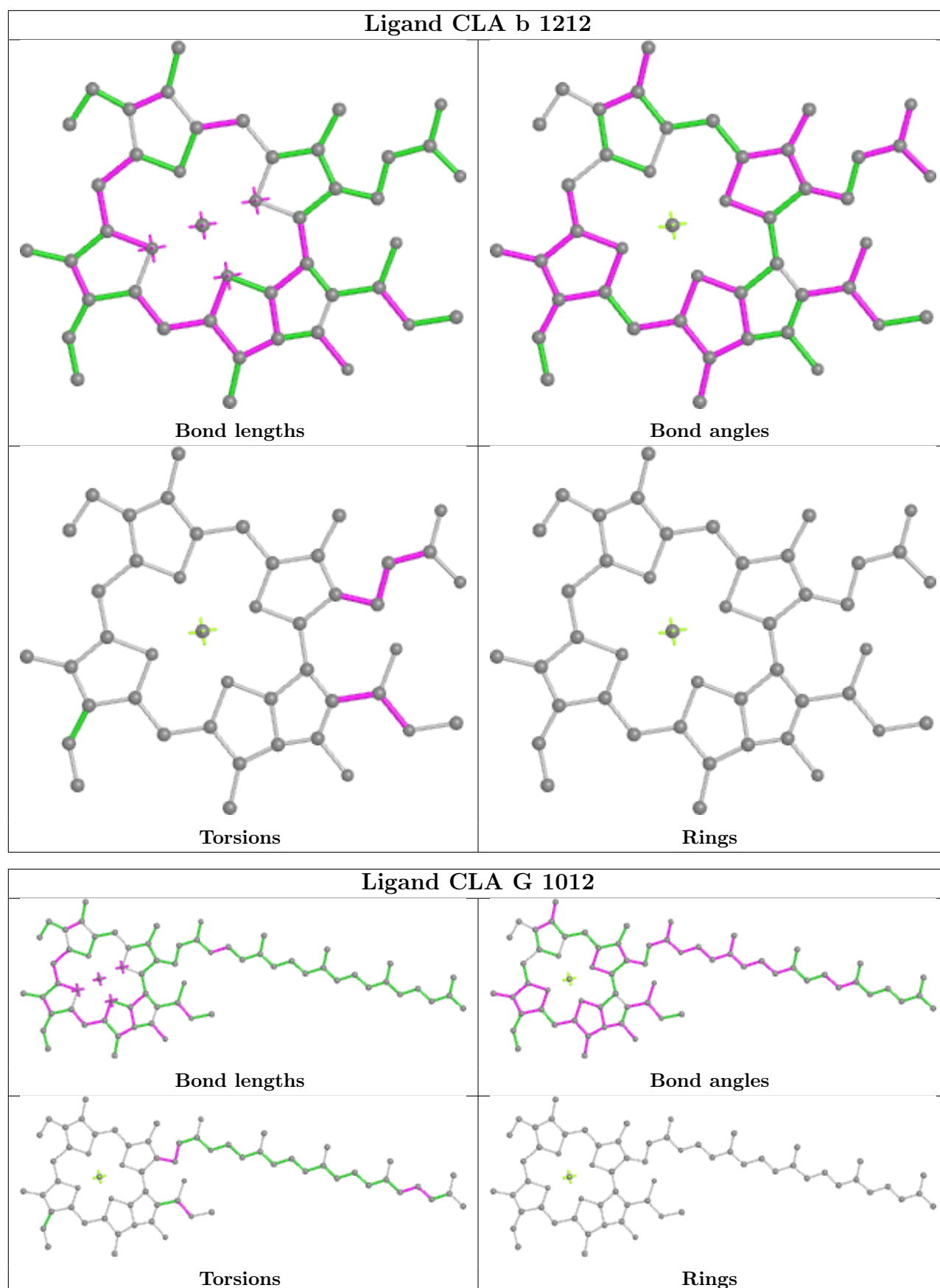


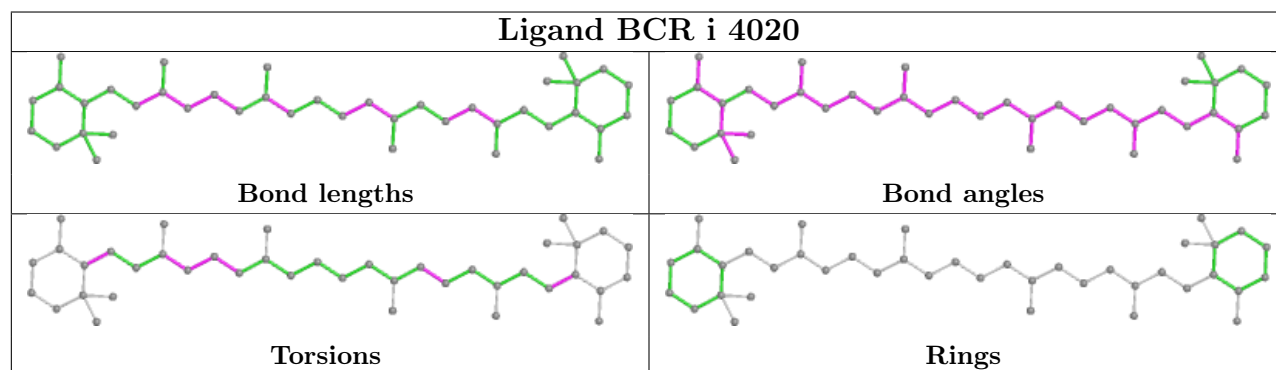
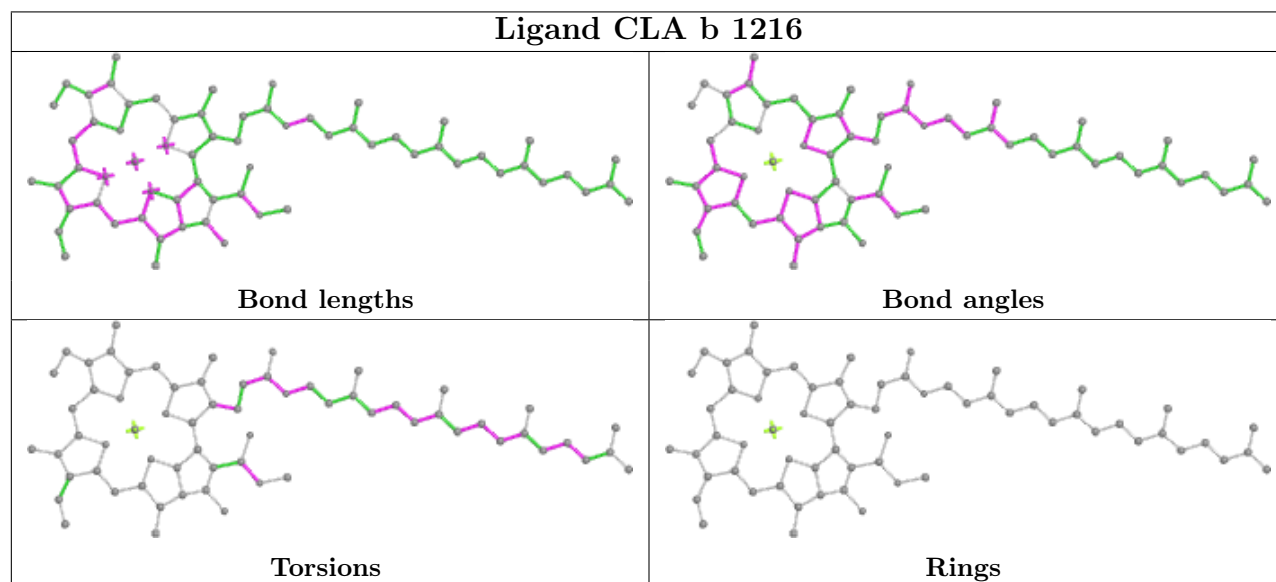
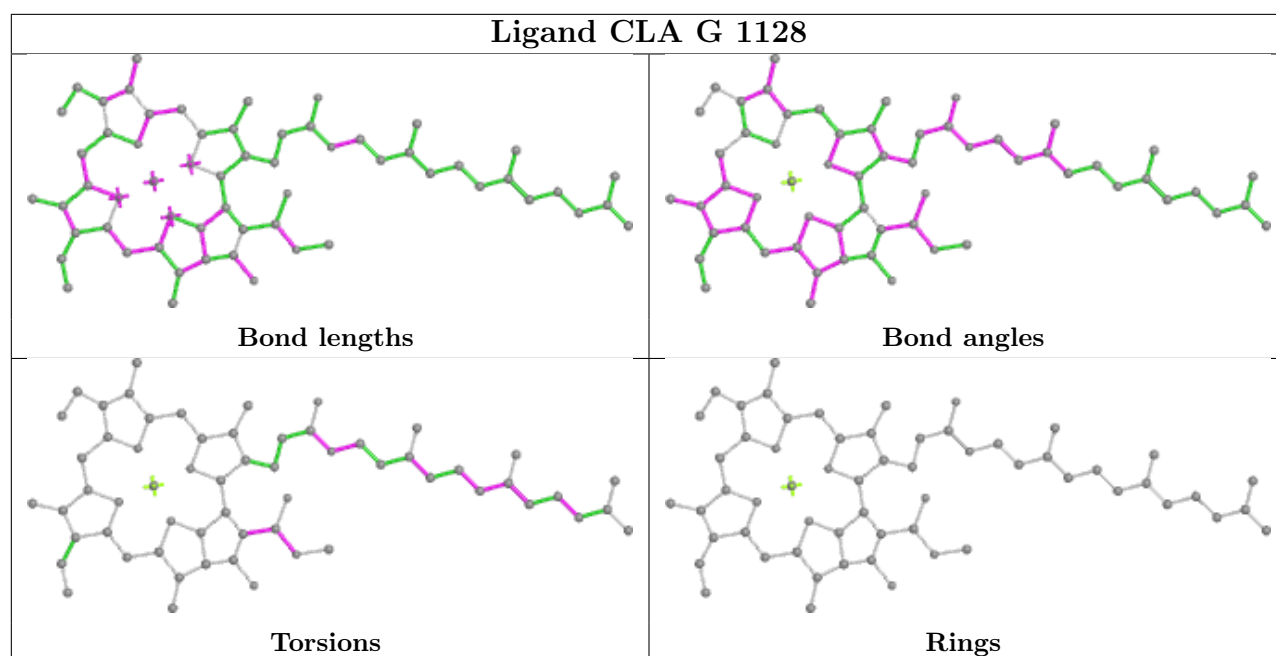


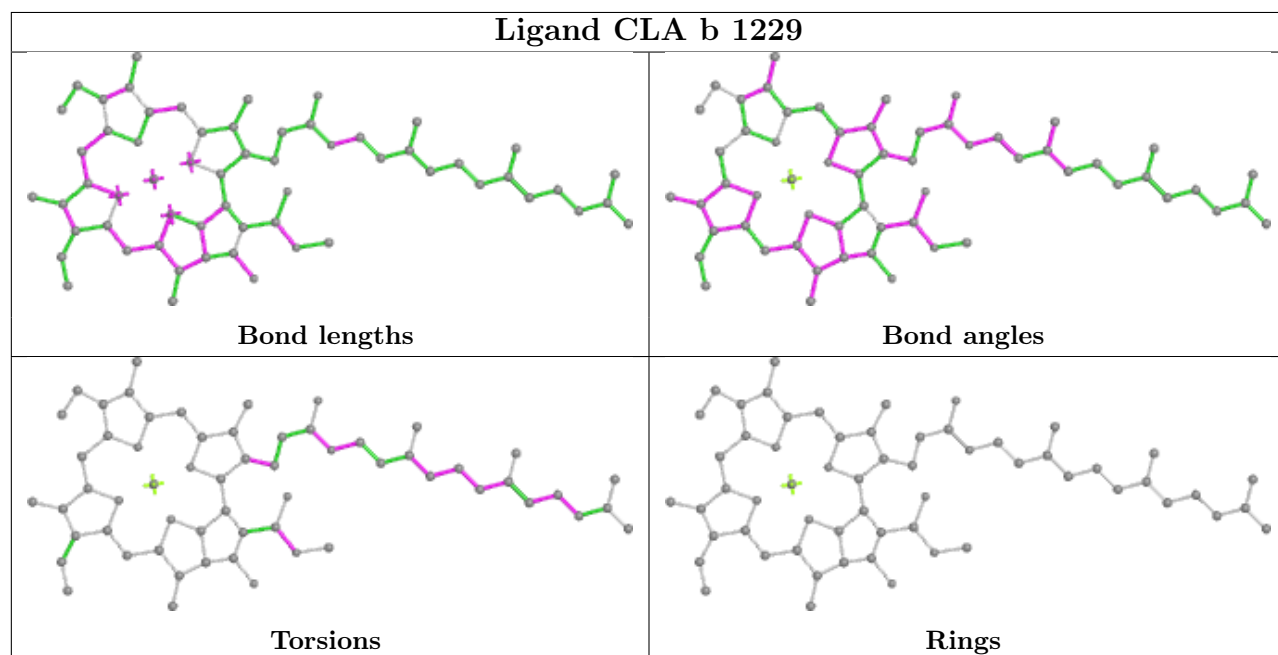
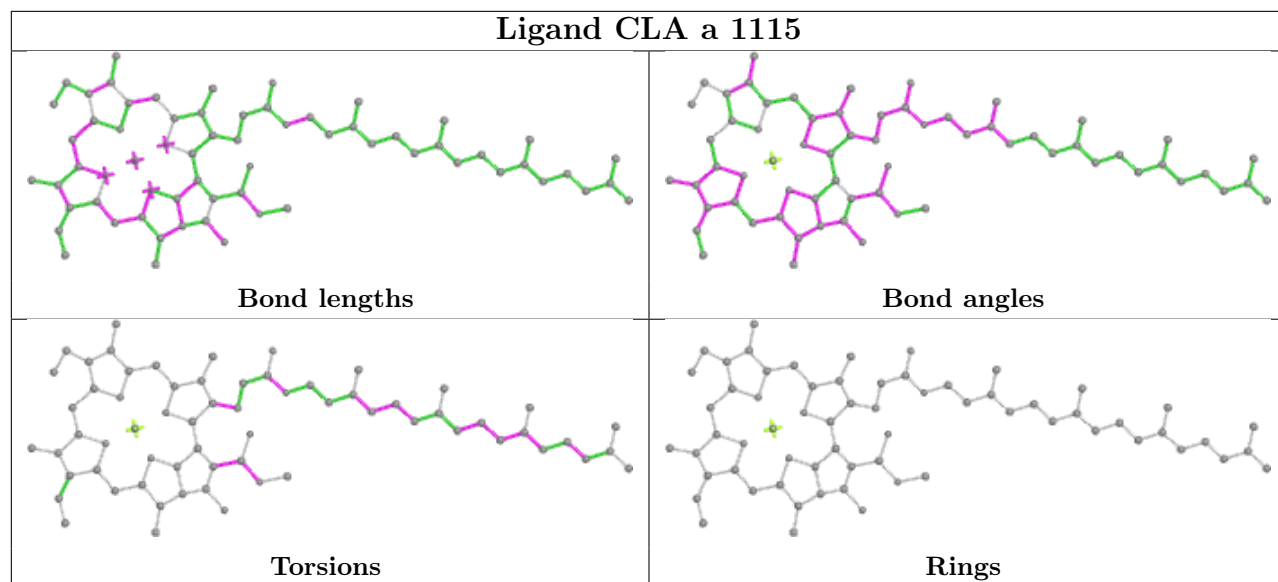
Ligand CLA H 1203**Ligand CLA A 1106**

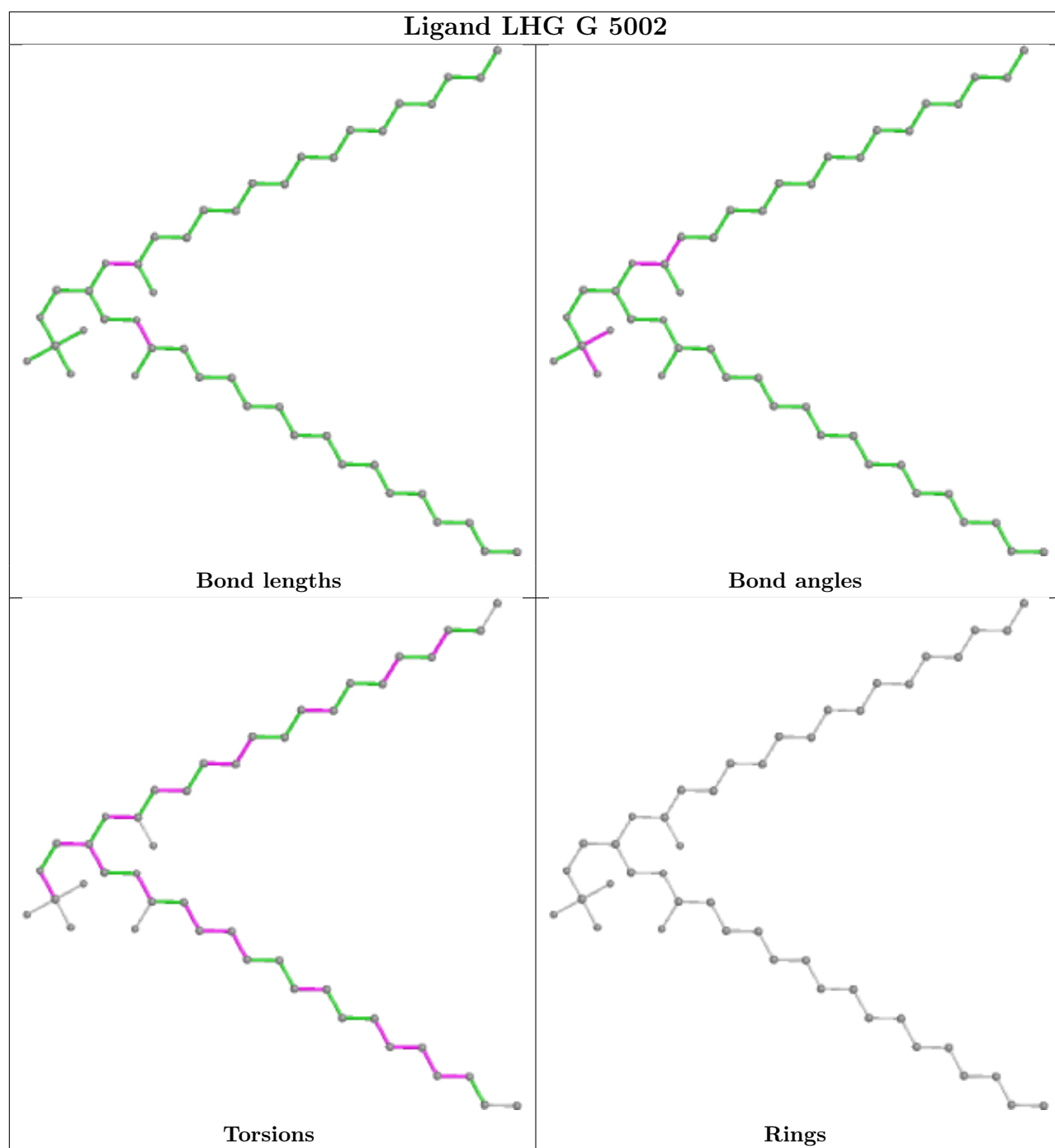




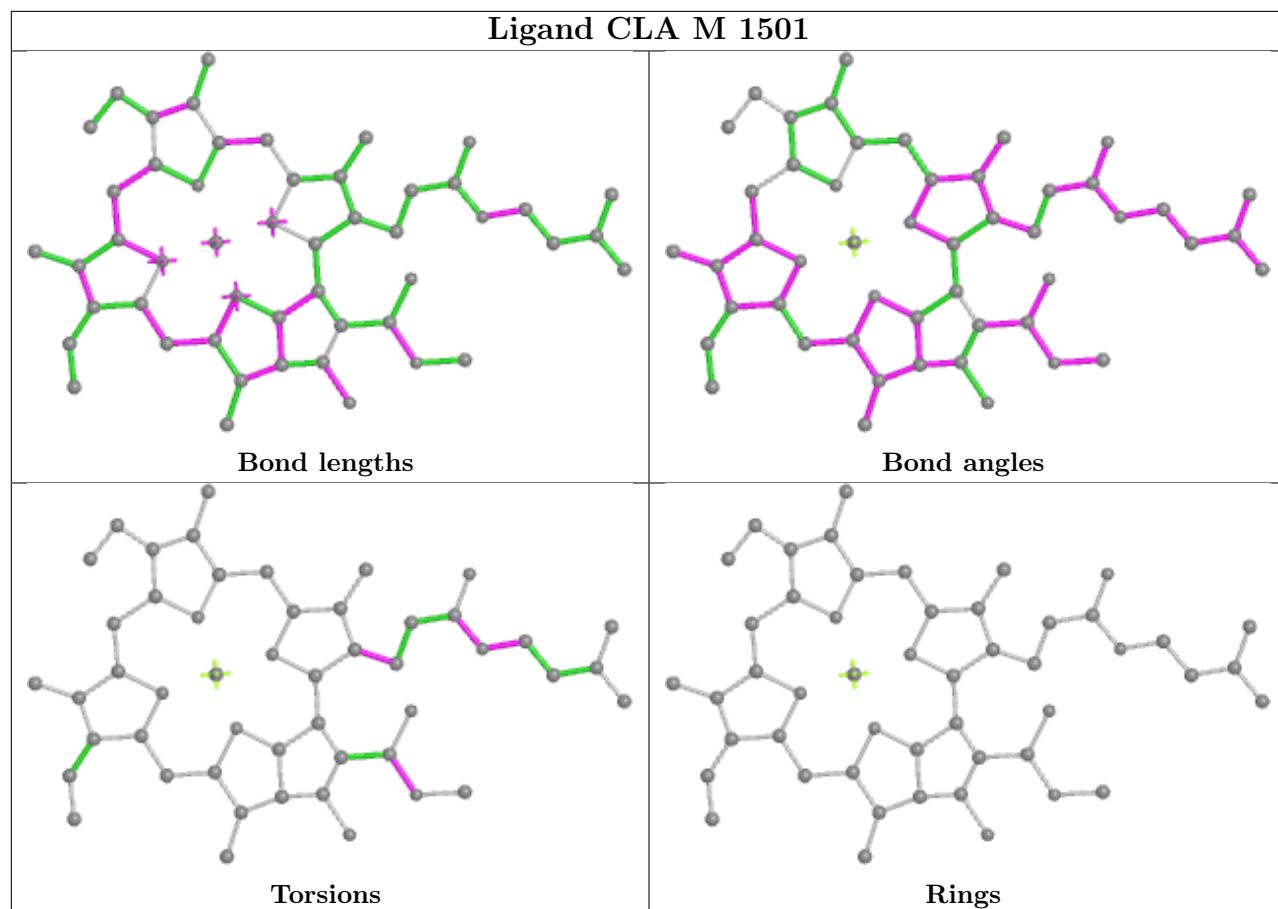


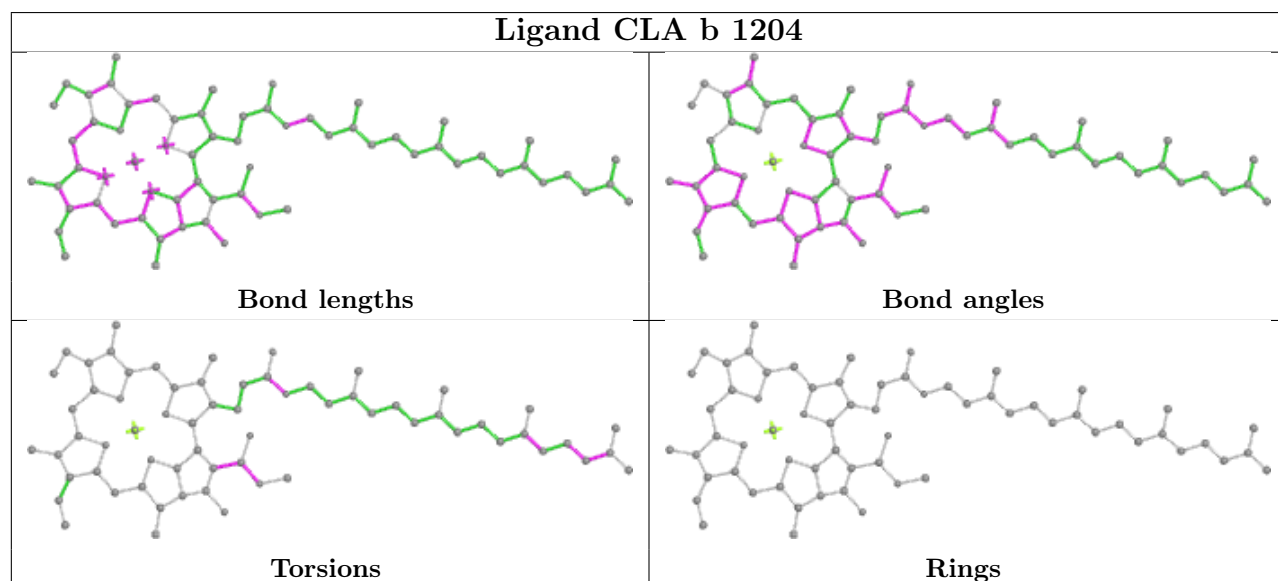
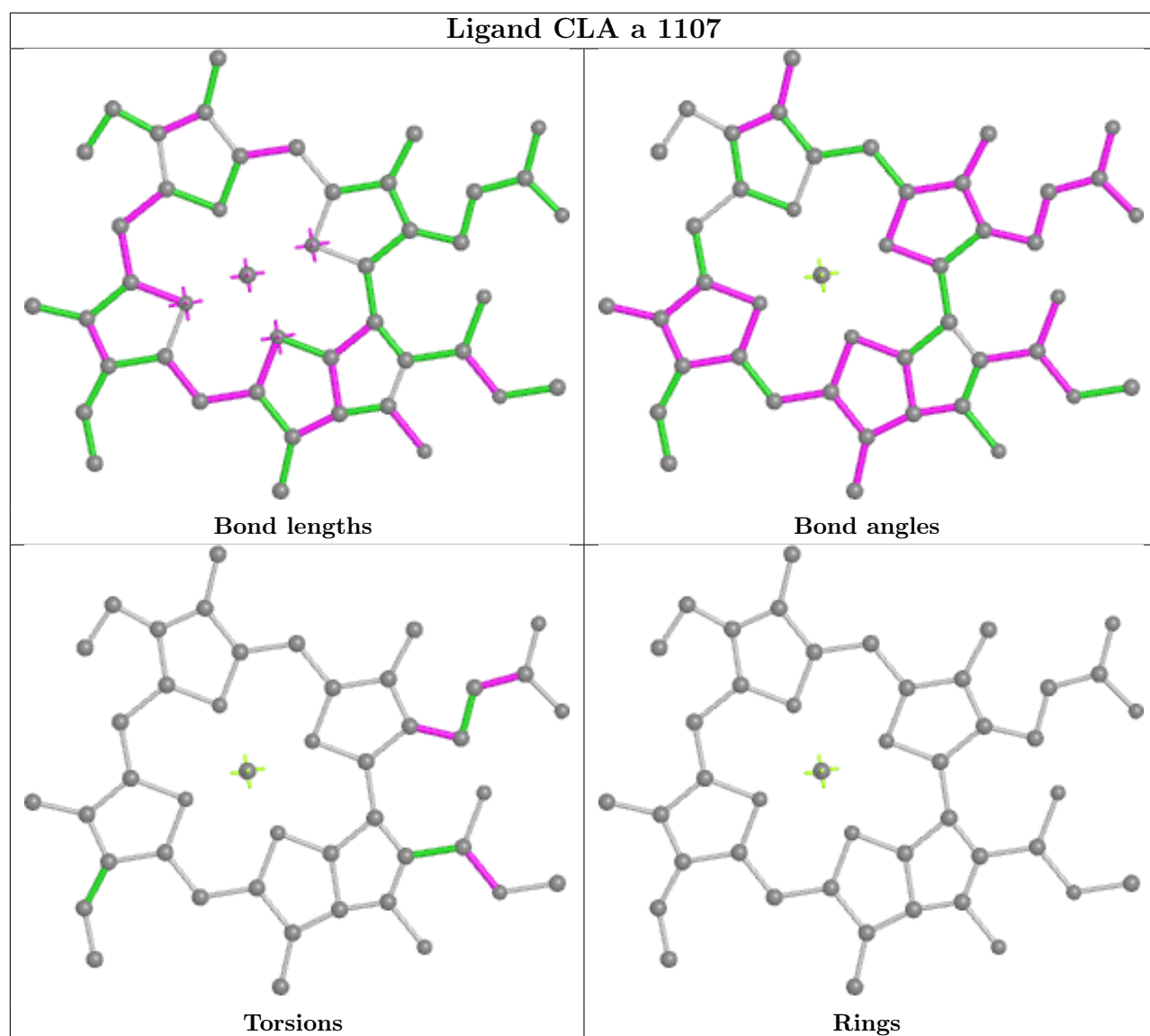


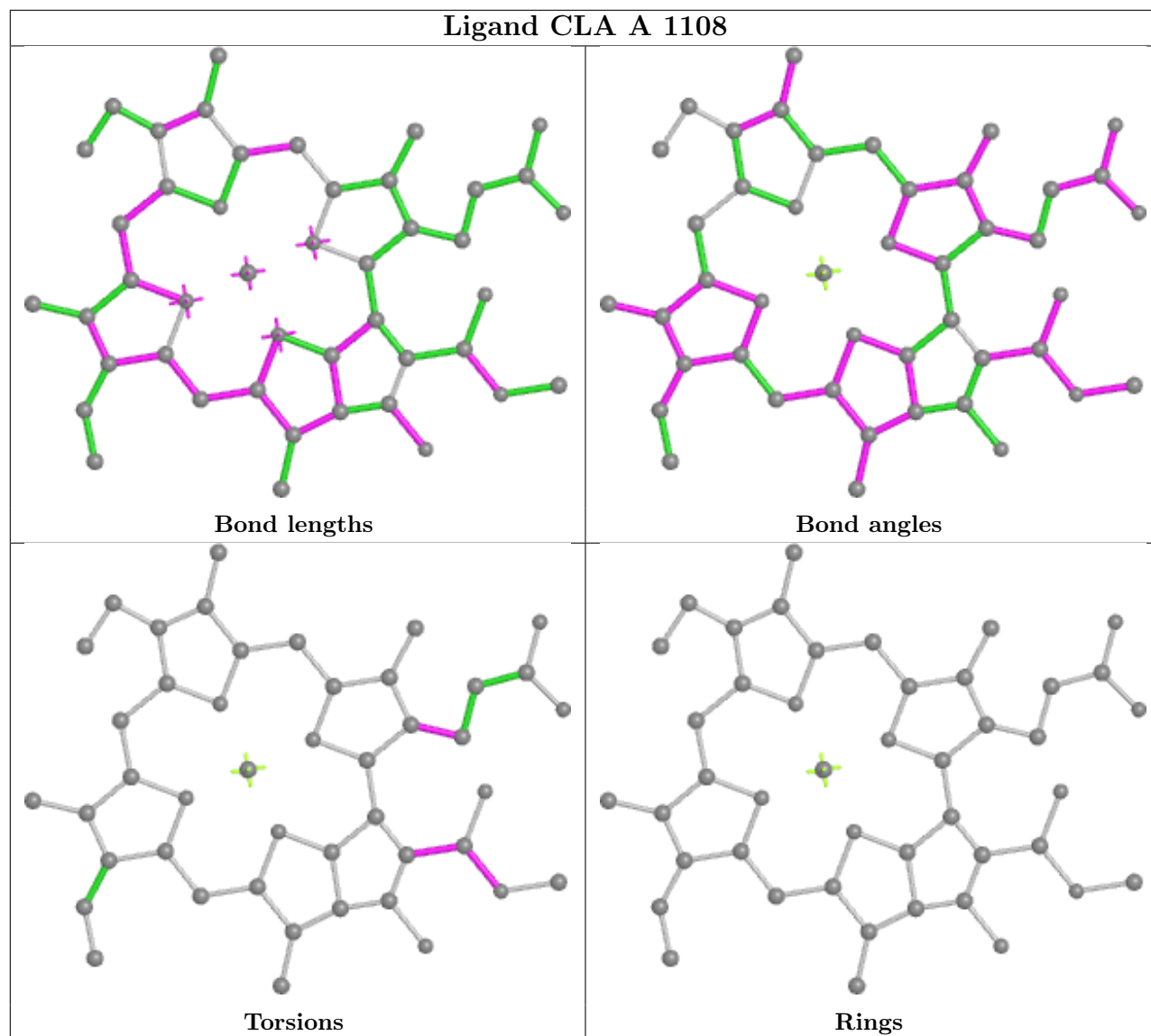
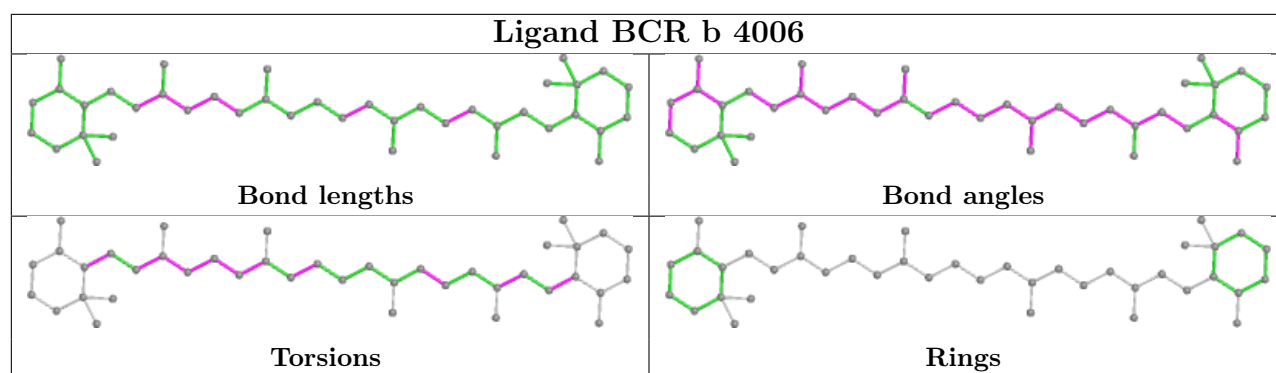


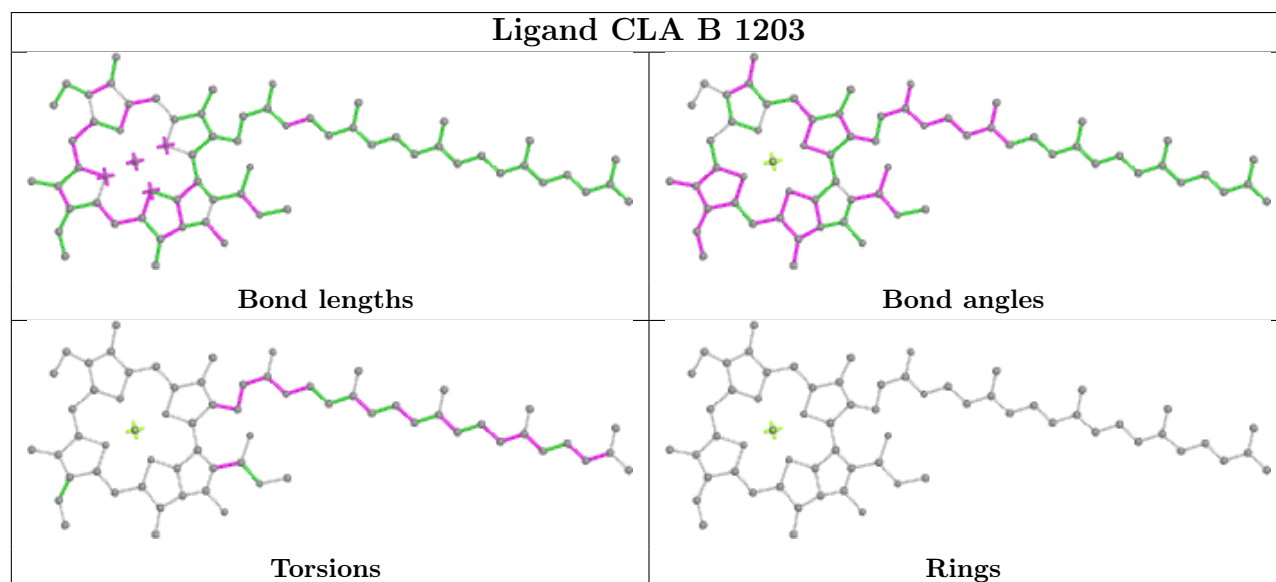
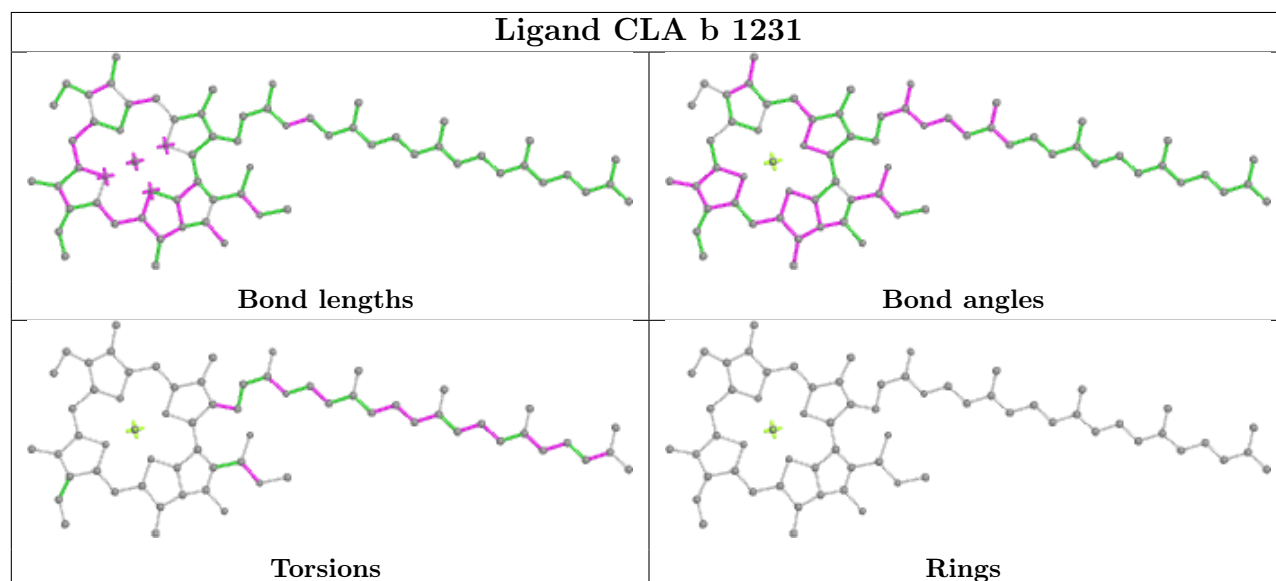
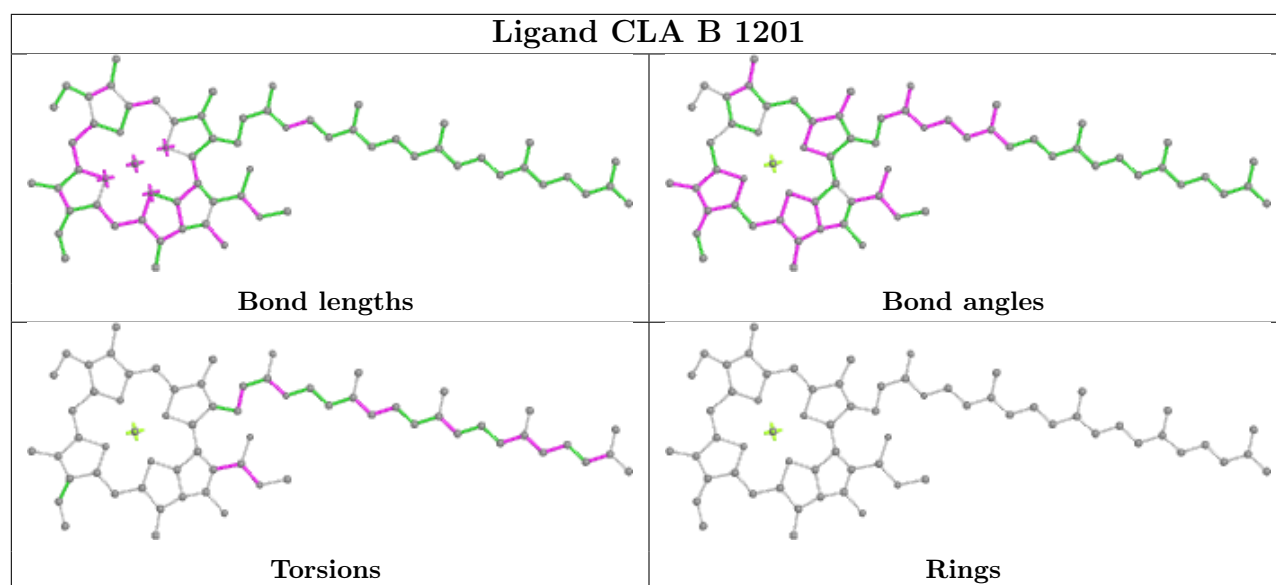


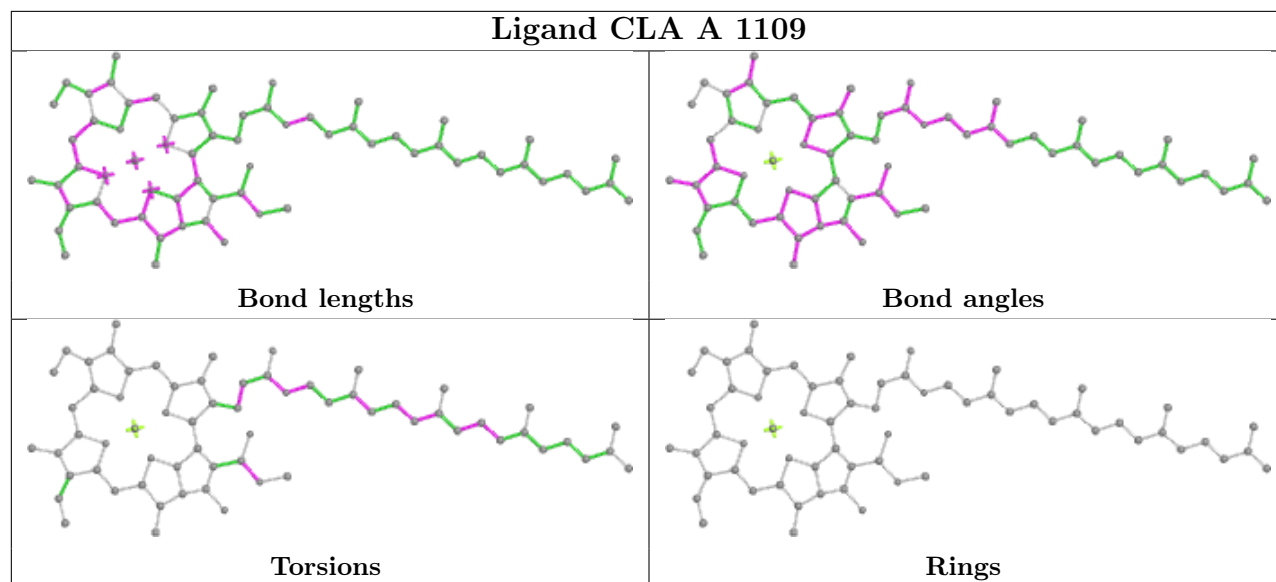
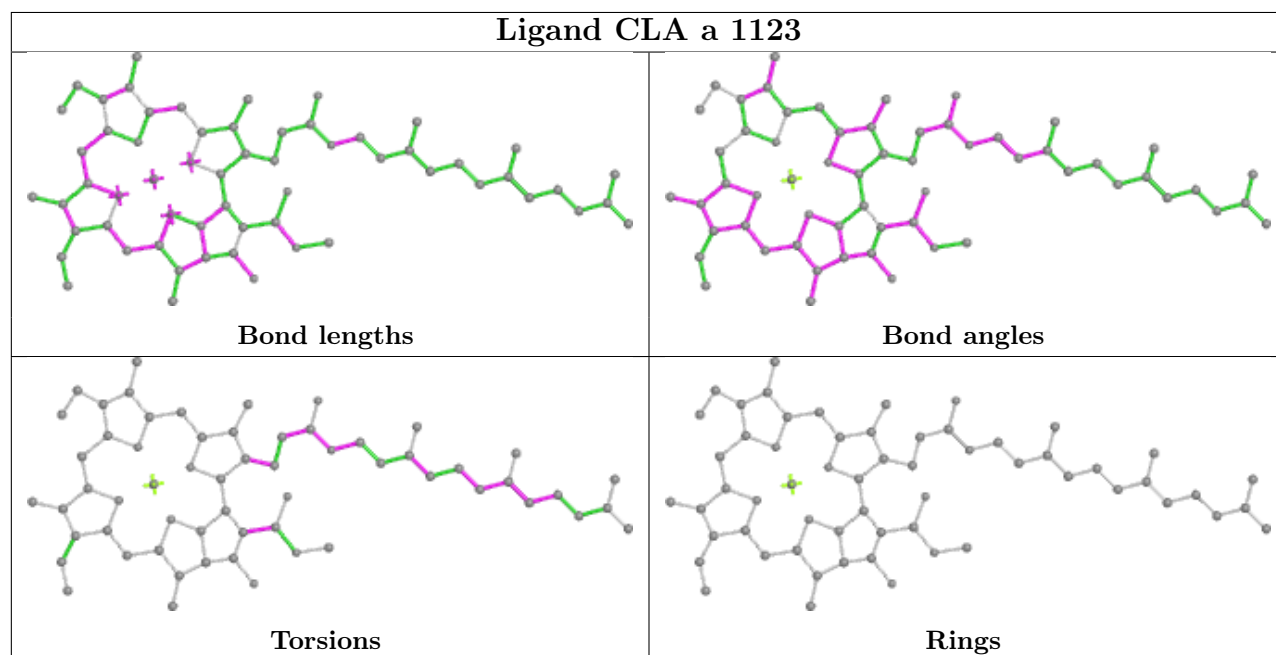
Ligand CLA M 1501

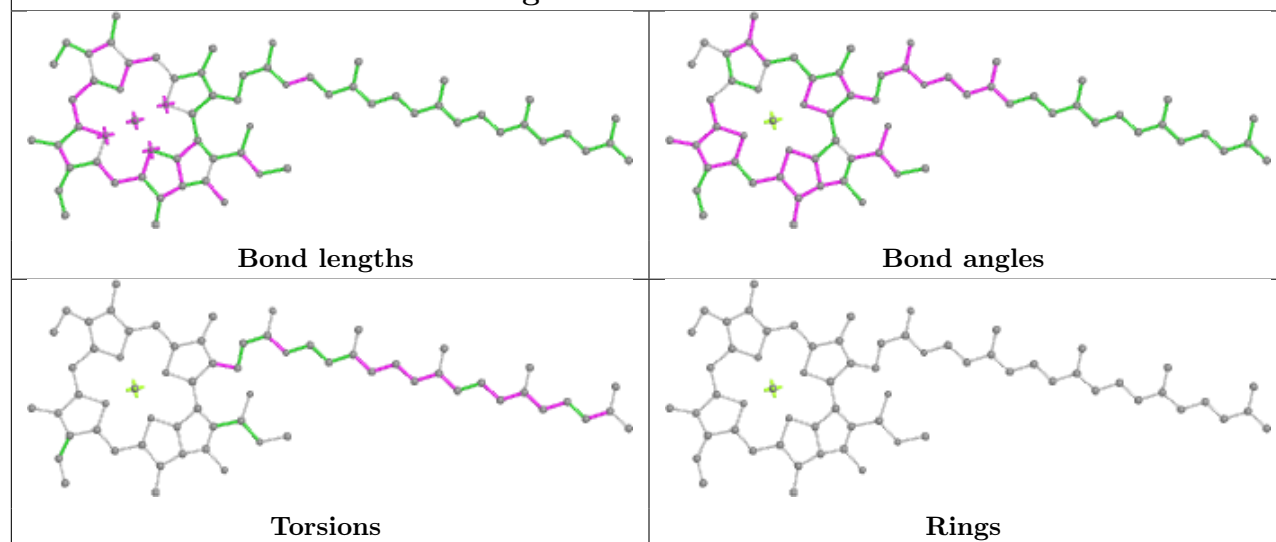
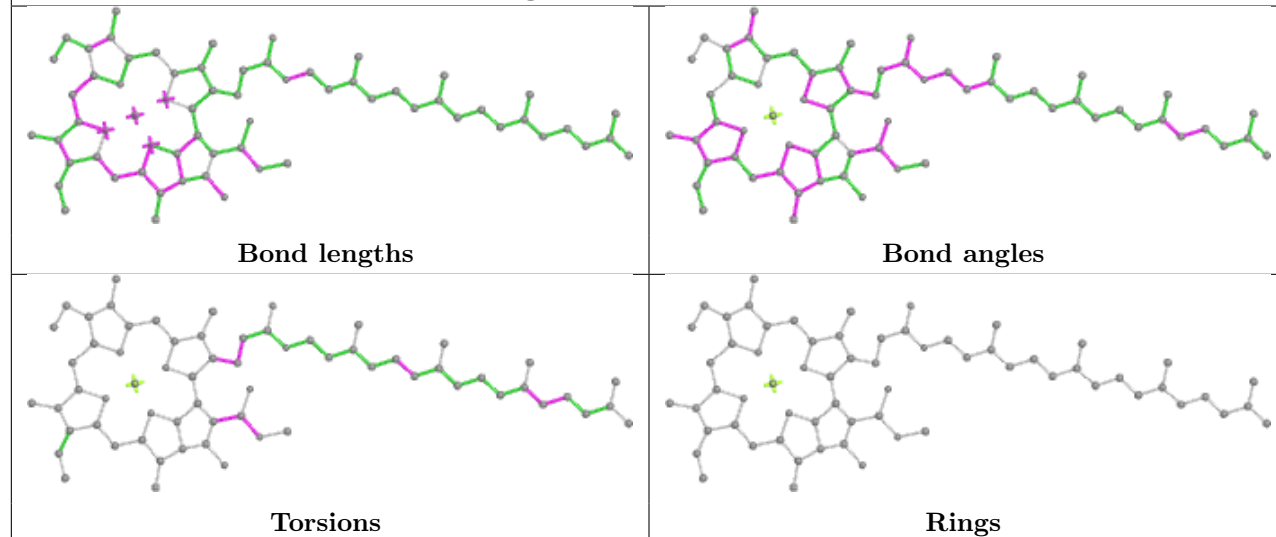


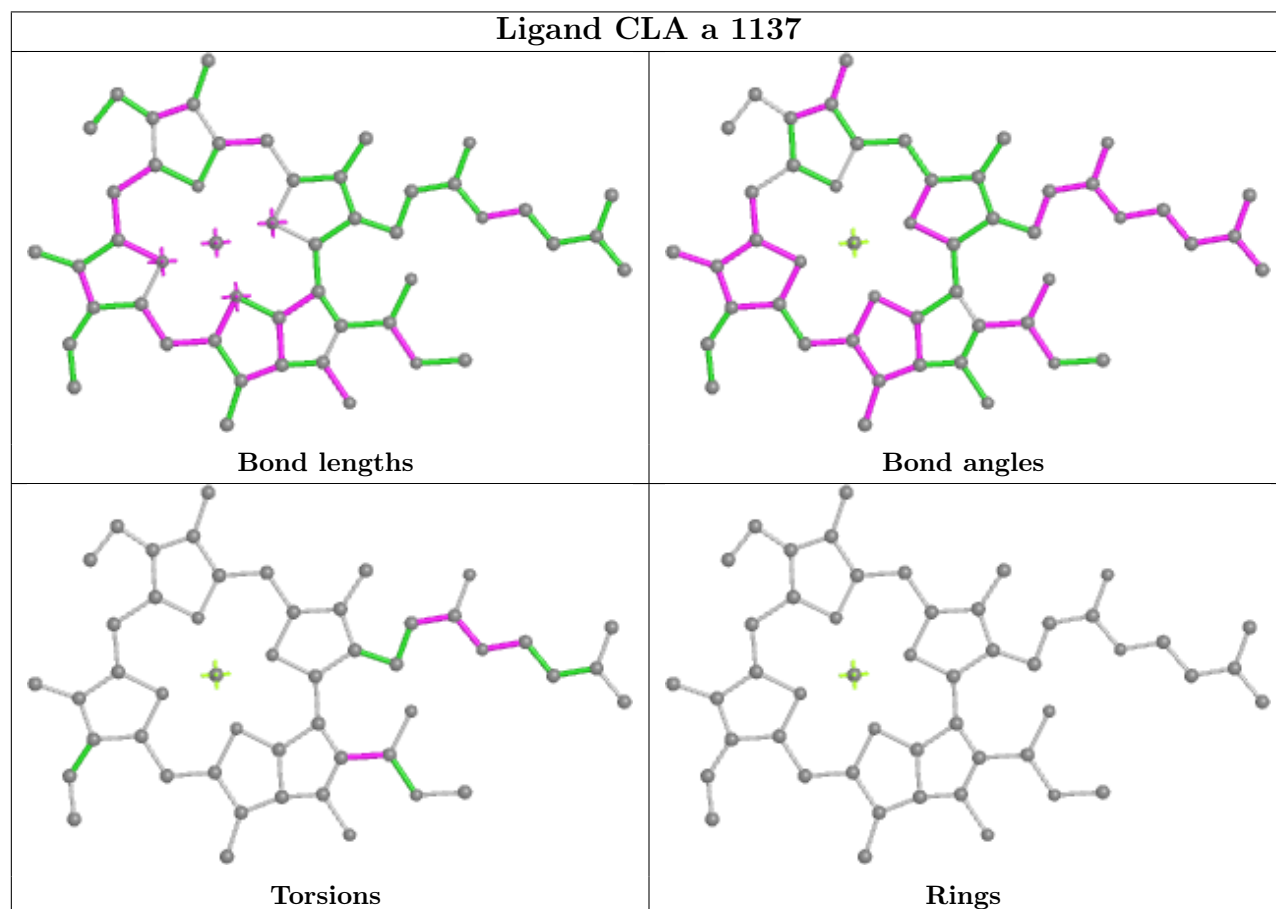
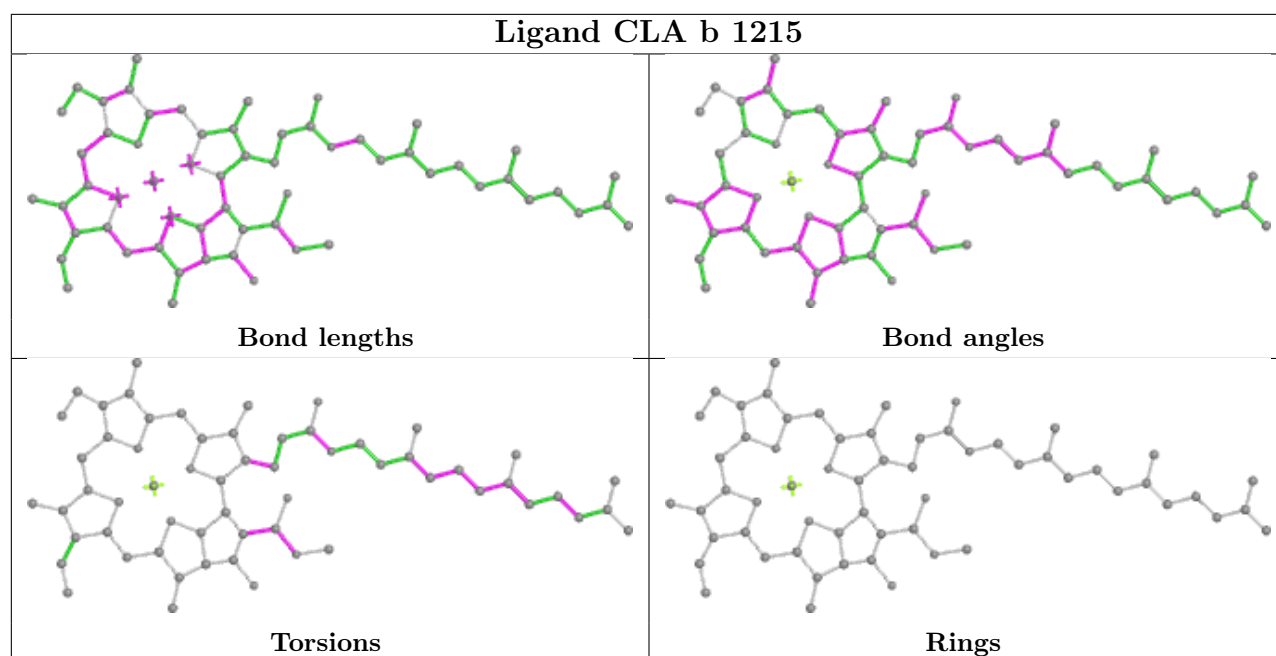




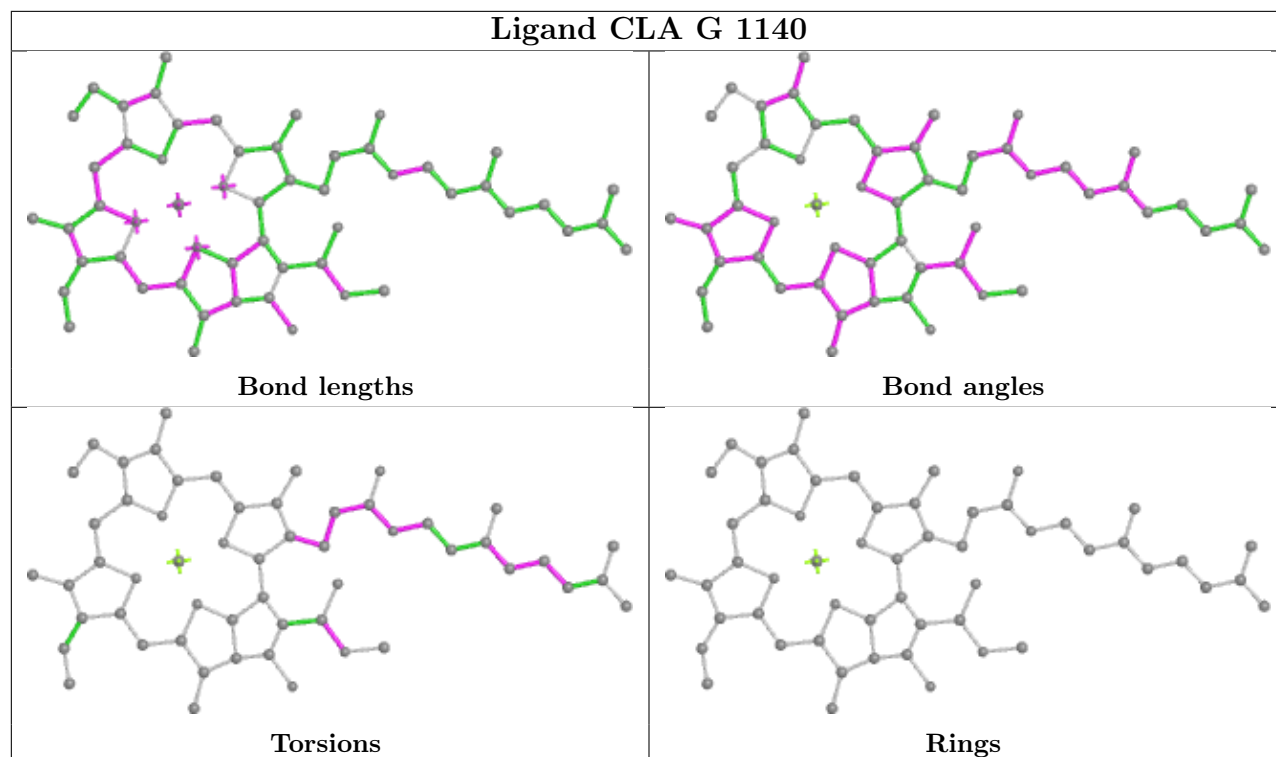


Ligand CLA A 1109**Ligand CLA a 1123**

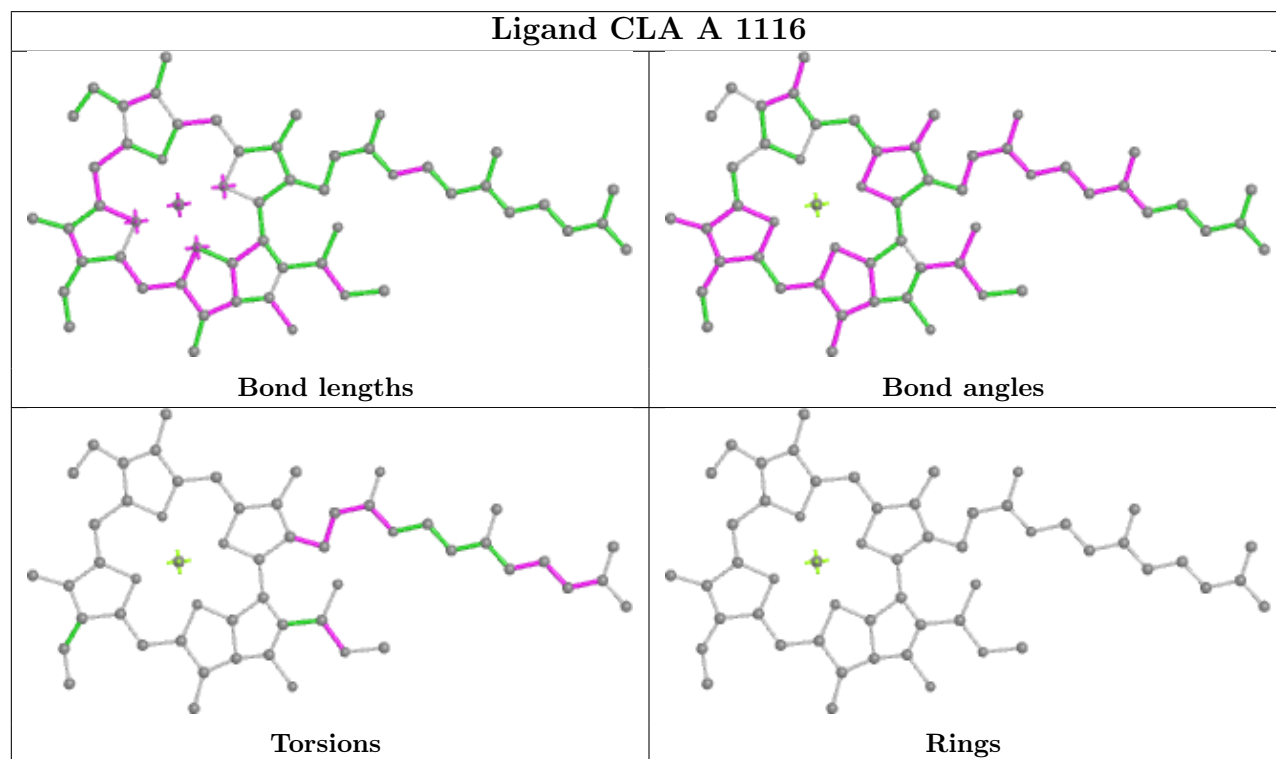
Ligand CLA H 1206**Ligand CLA G 1132**

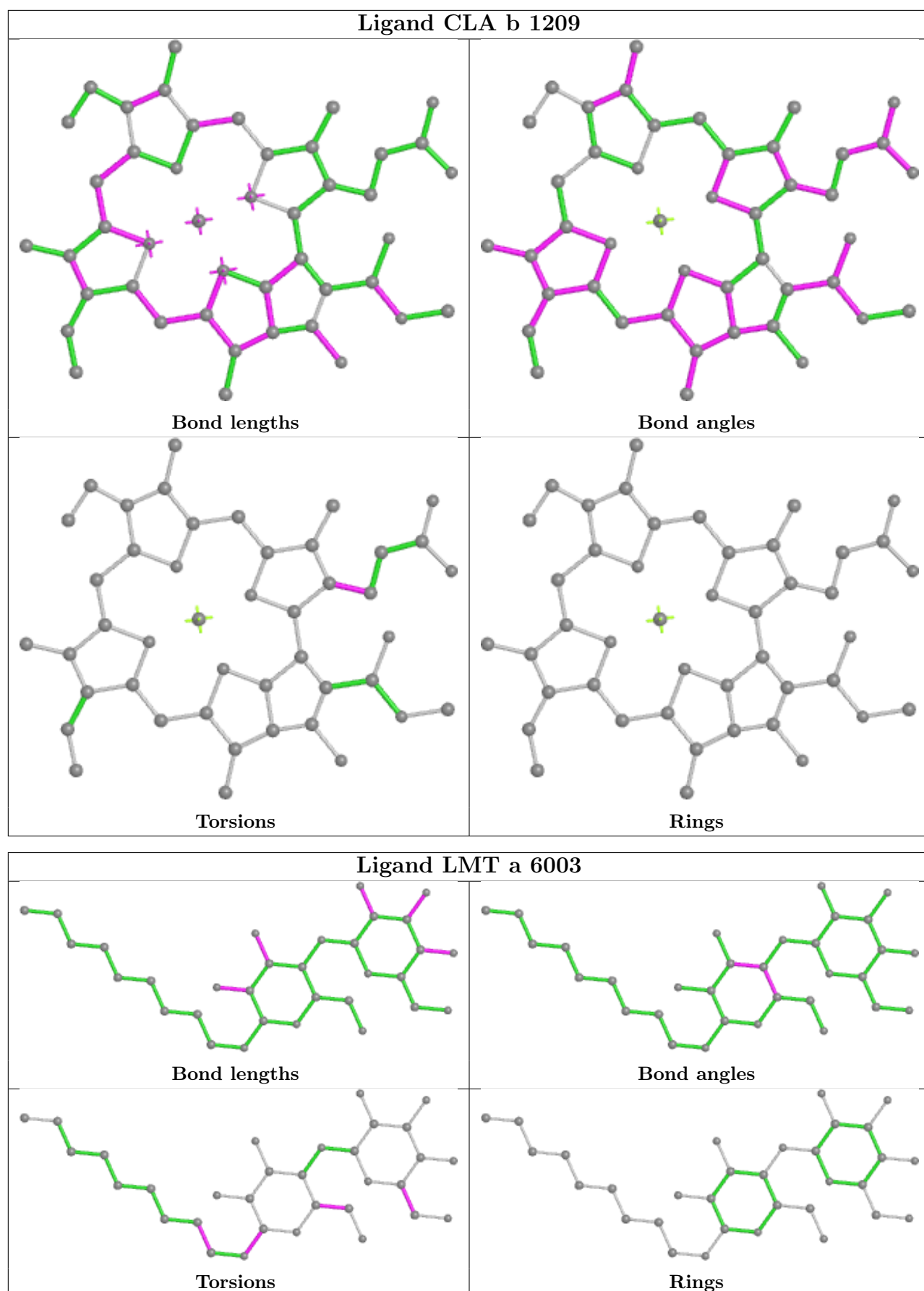


Ligand CLA G 1140

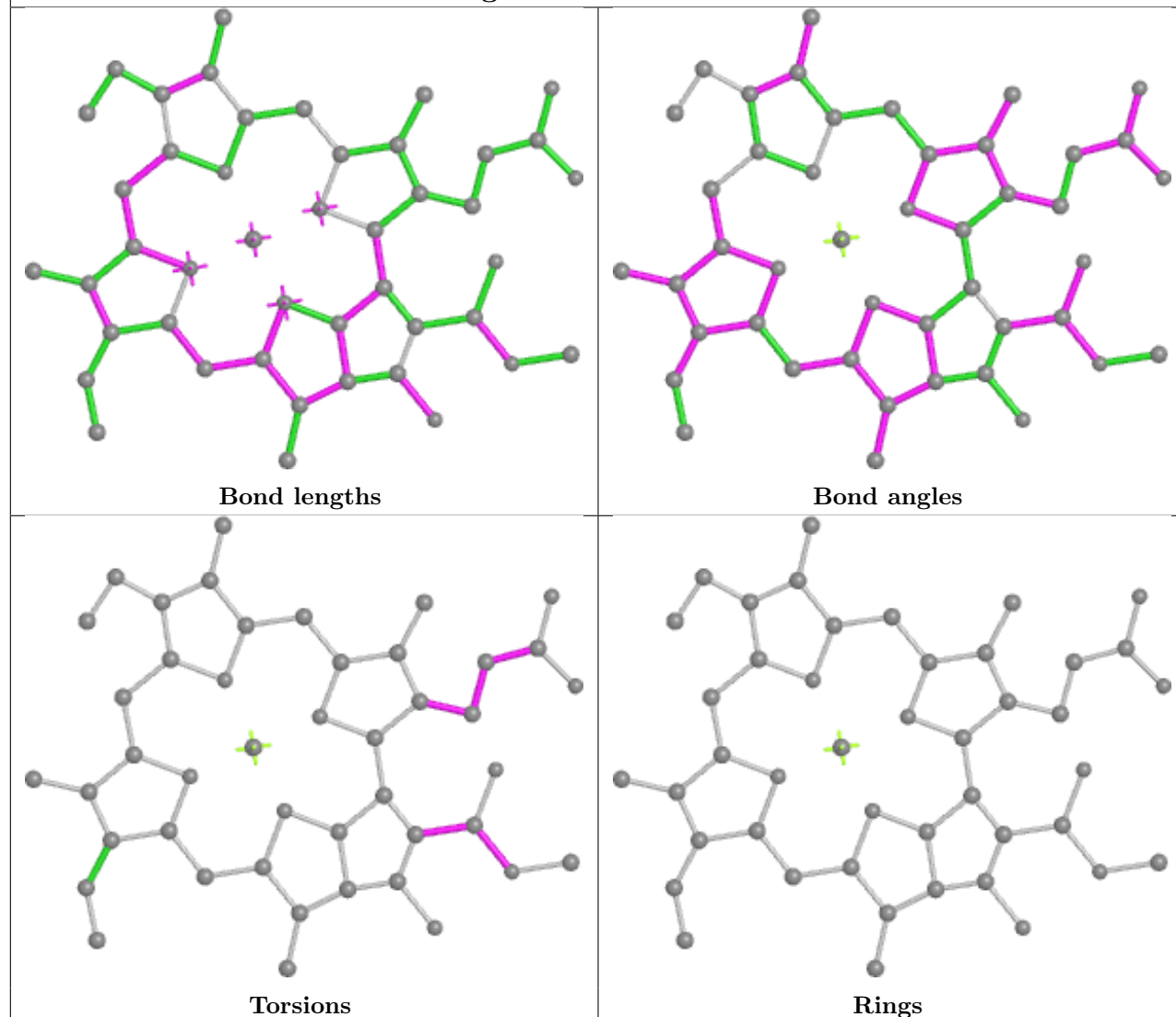


Ligand CLA A 1116

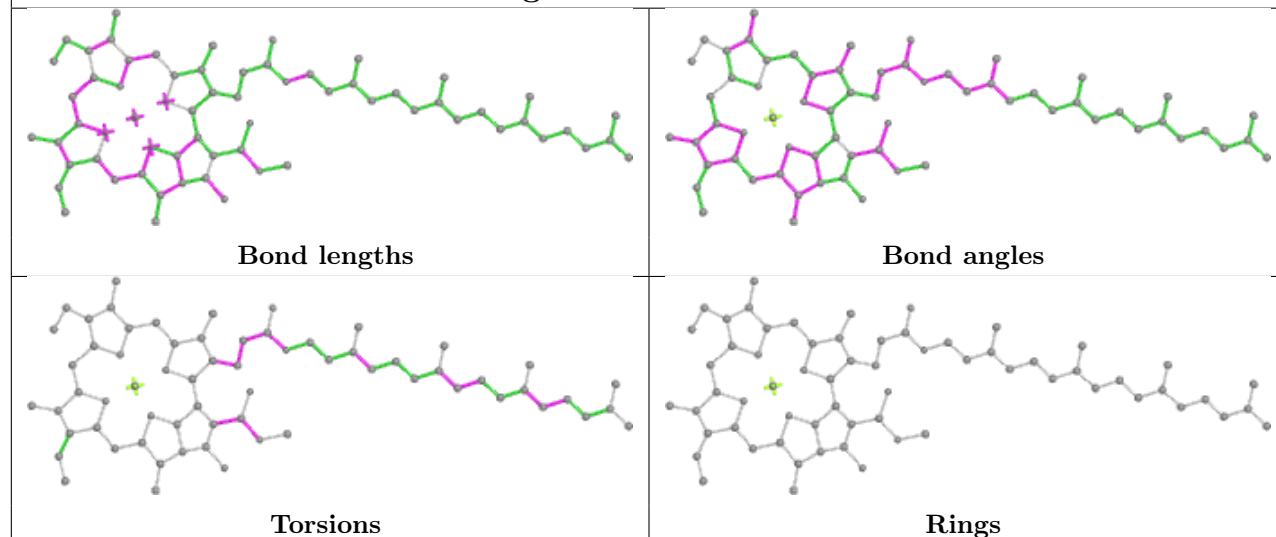


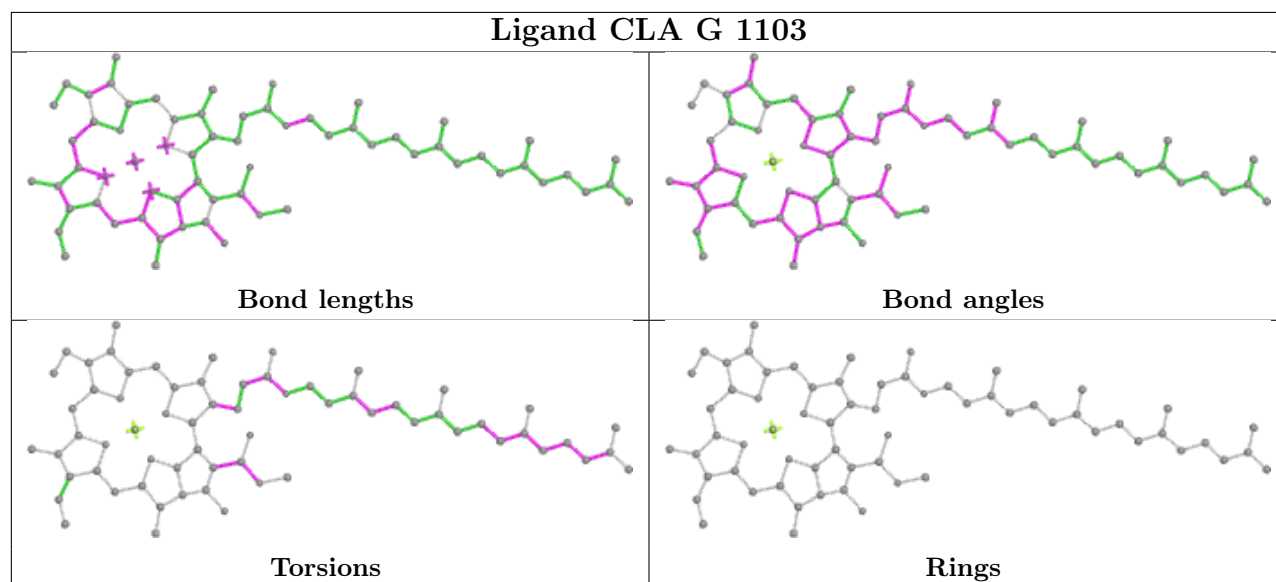
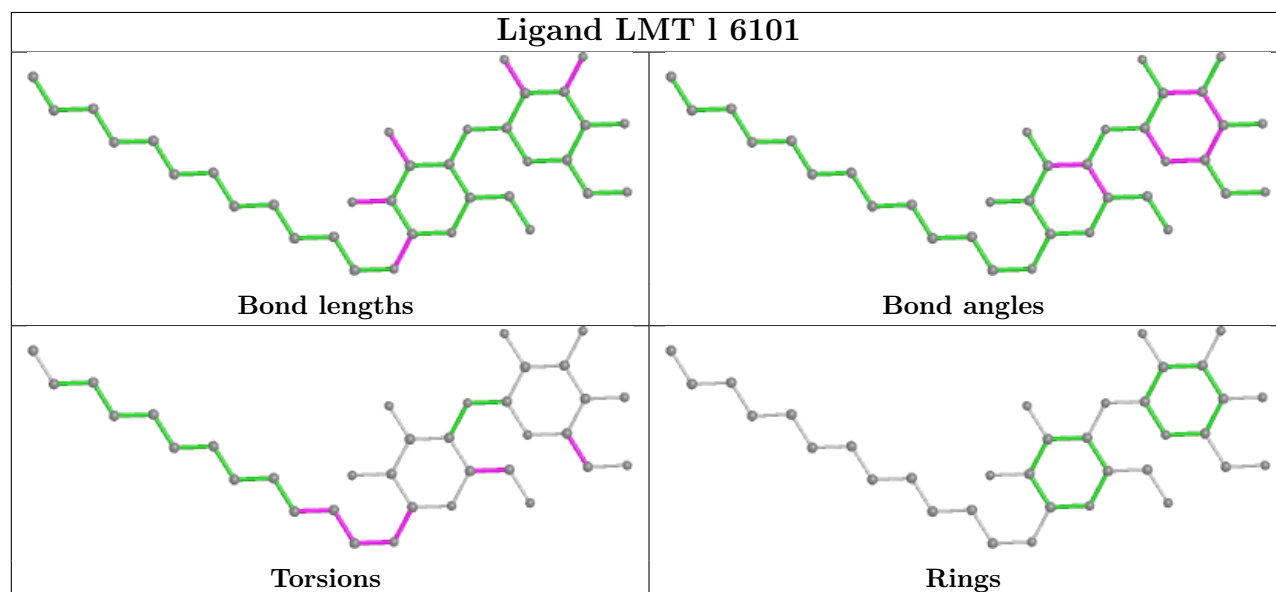
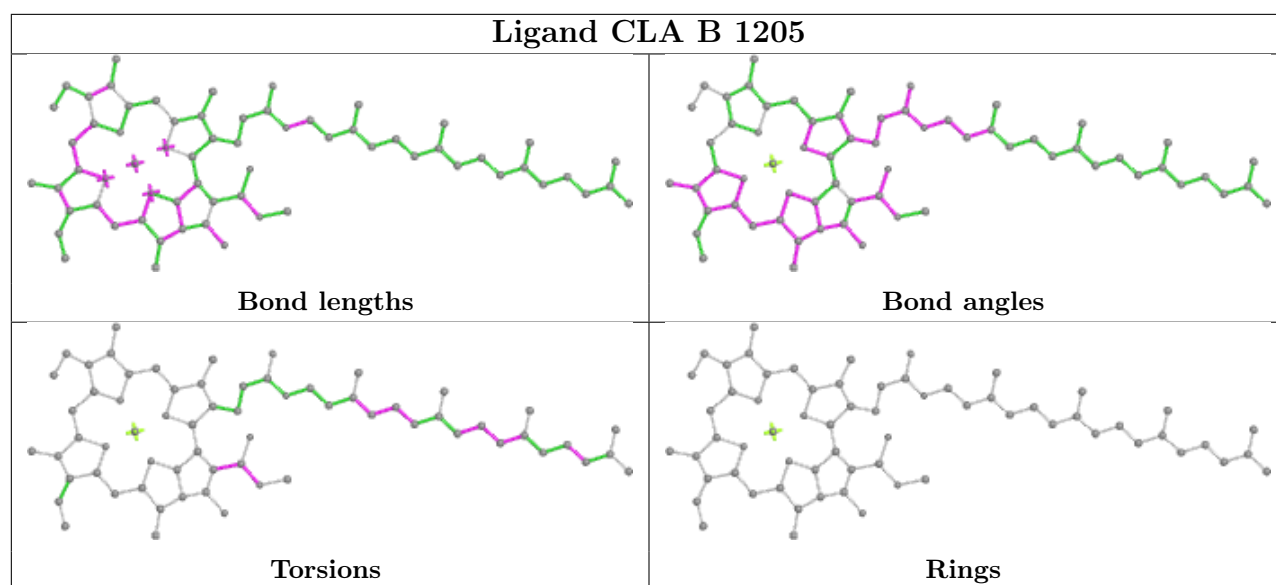


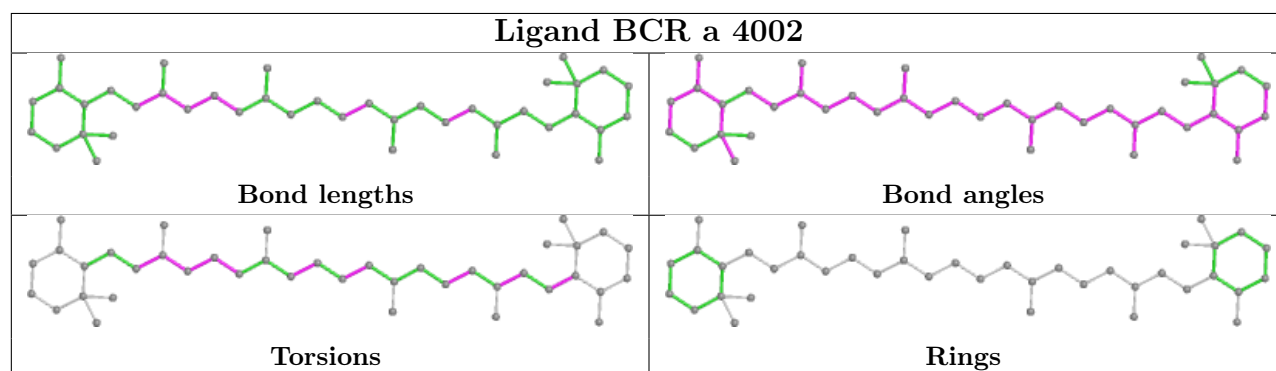
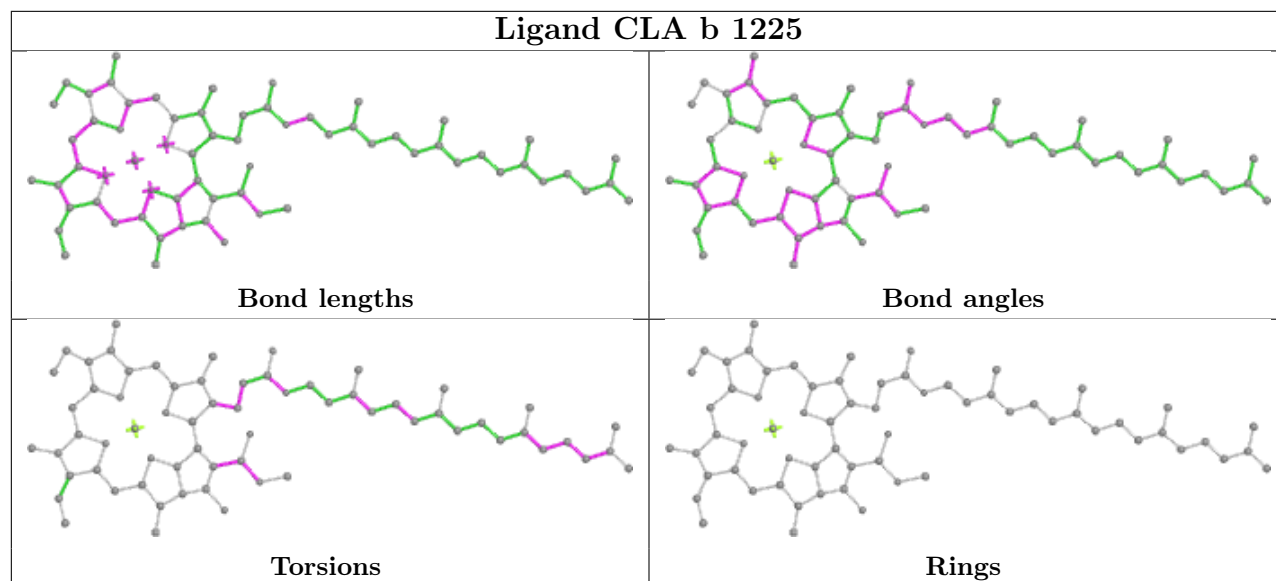
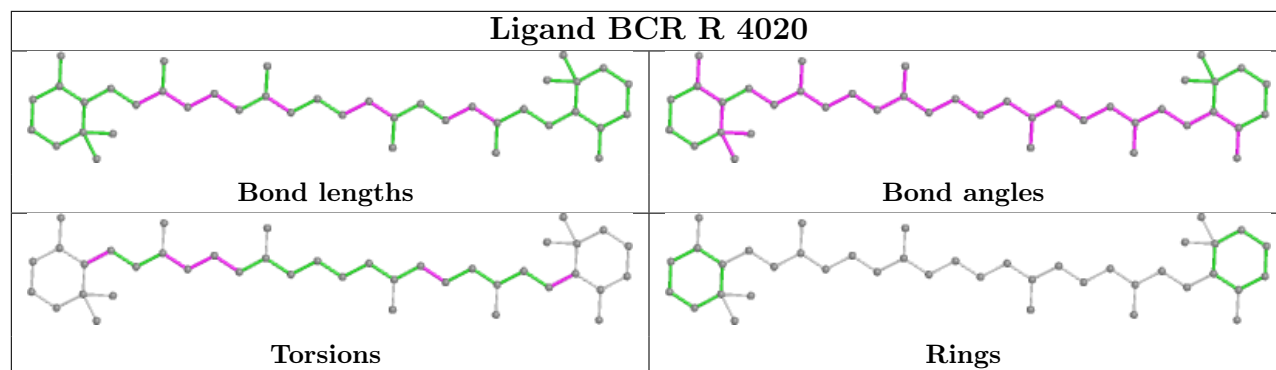
Ligand CLA H 1212

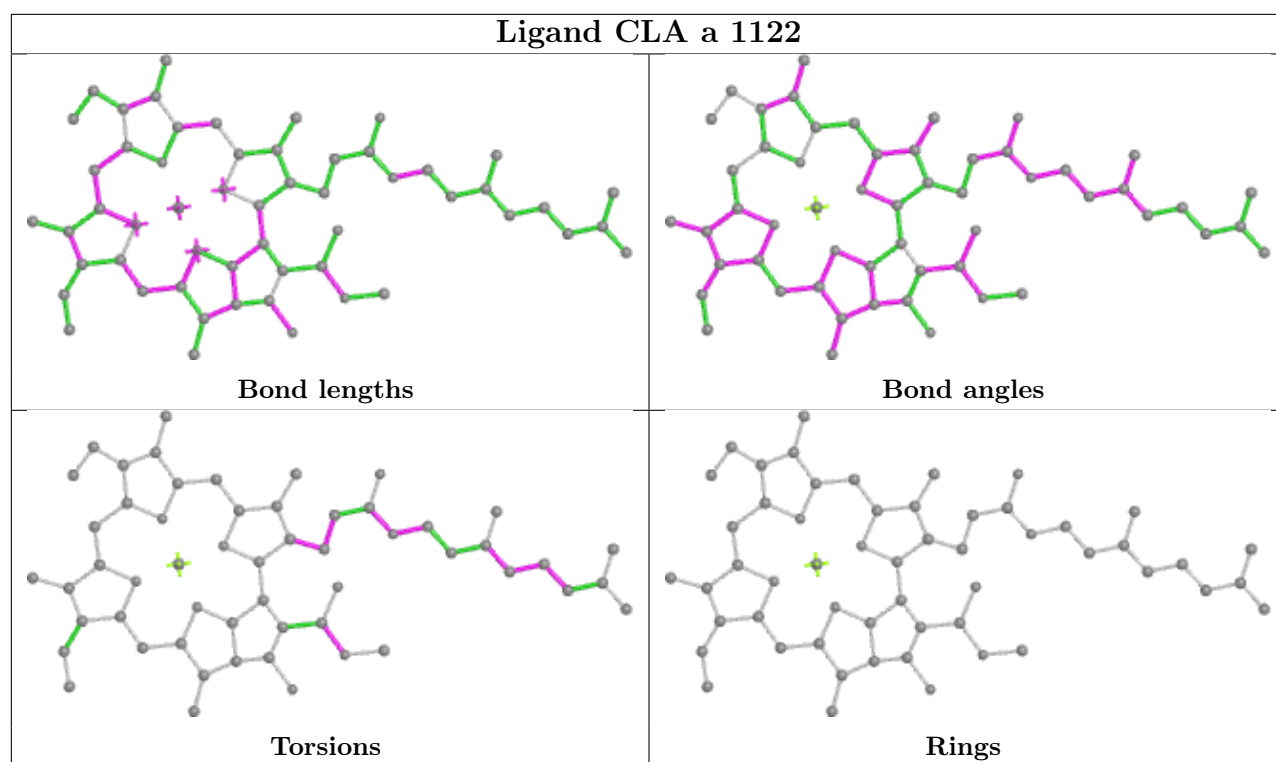


Ligand CLA A 1127

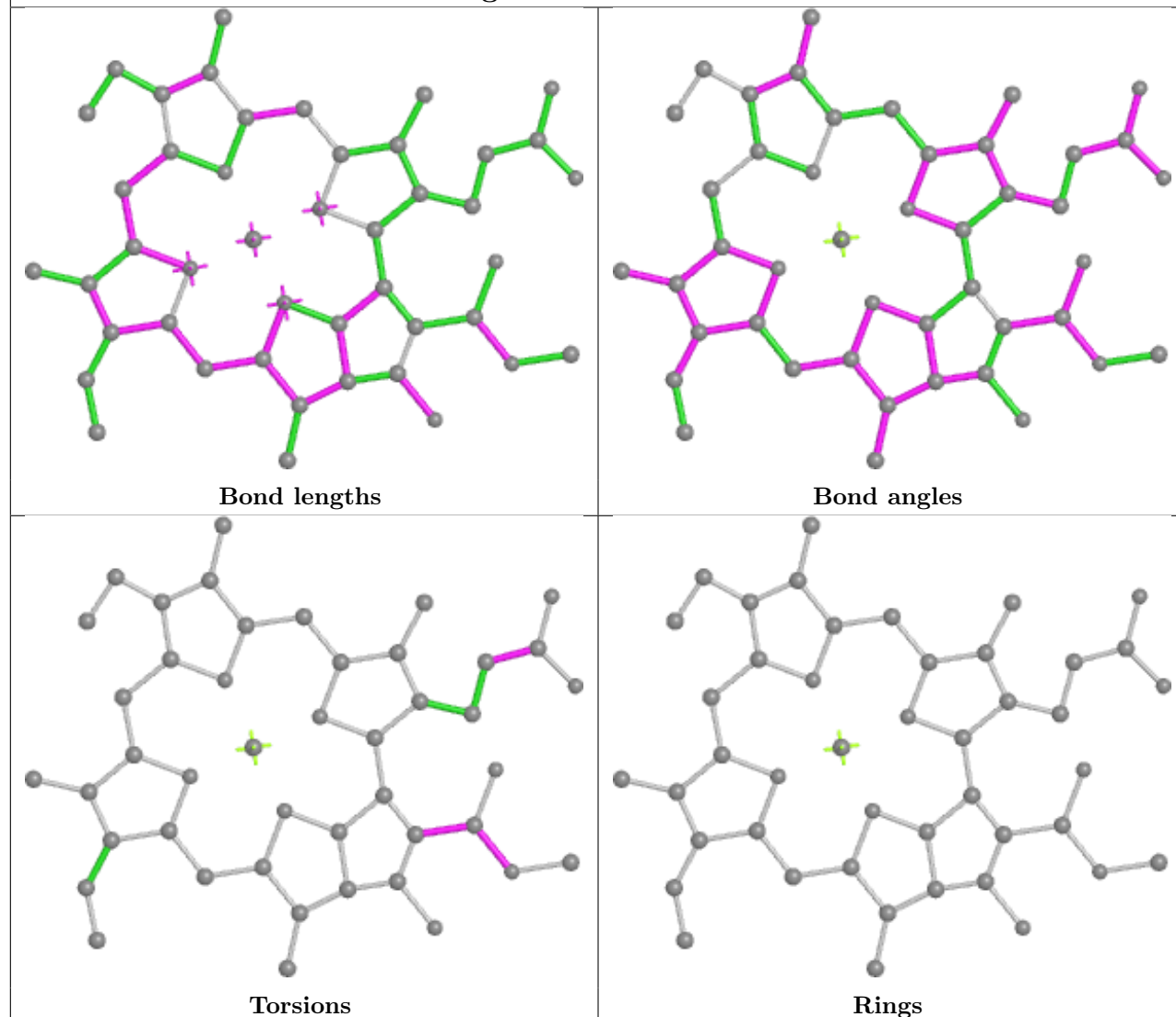




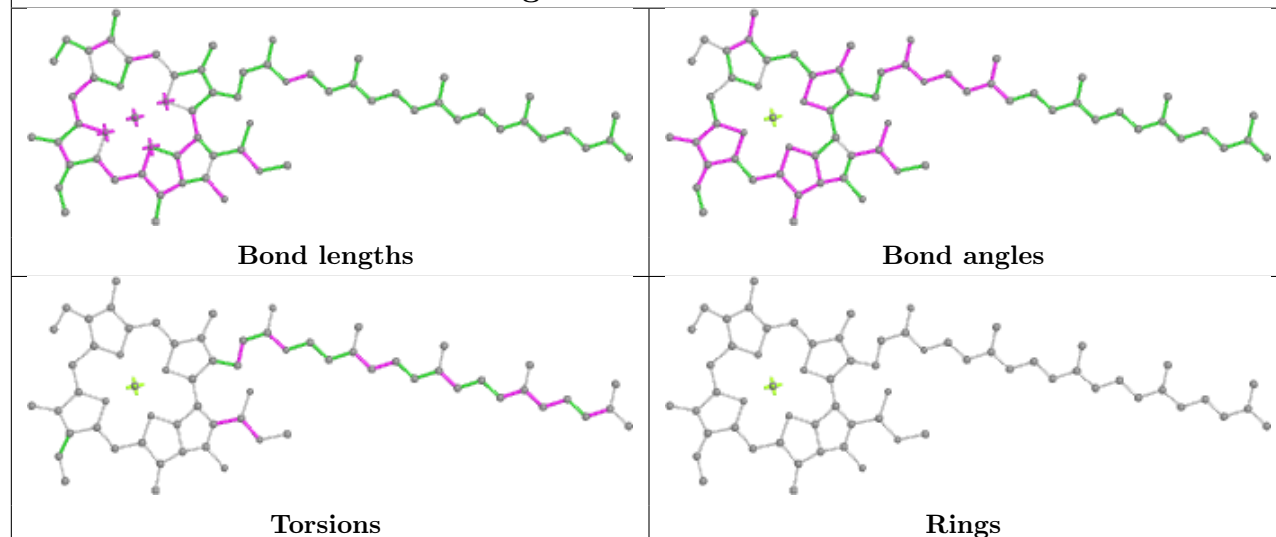


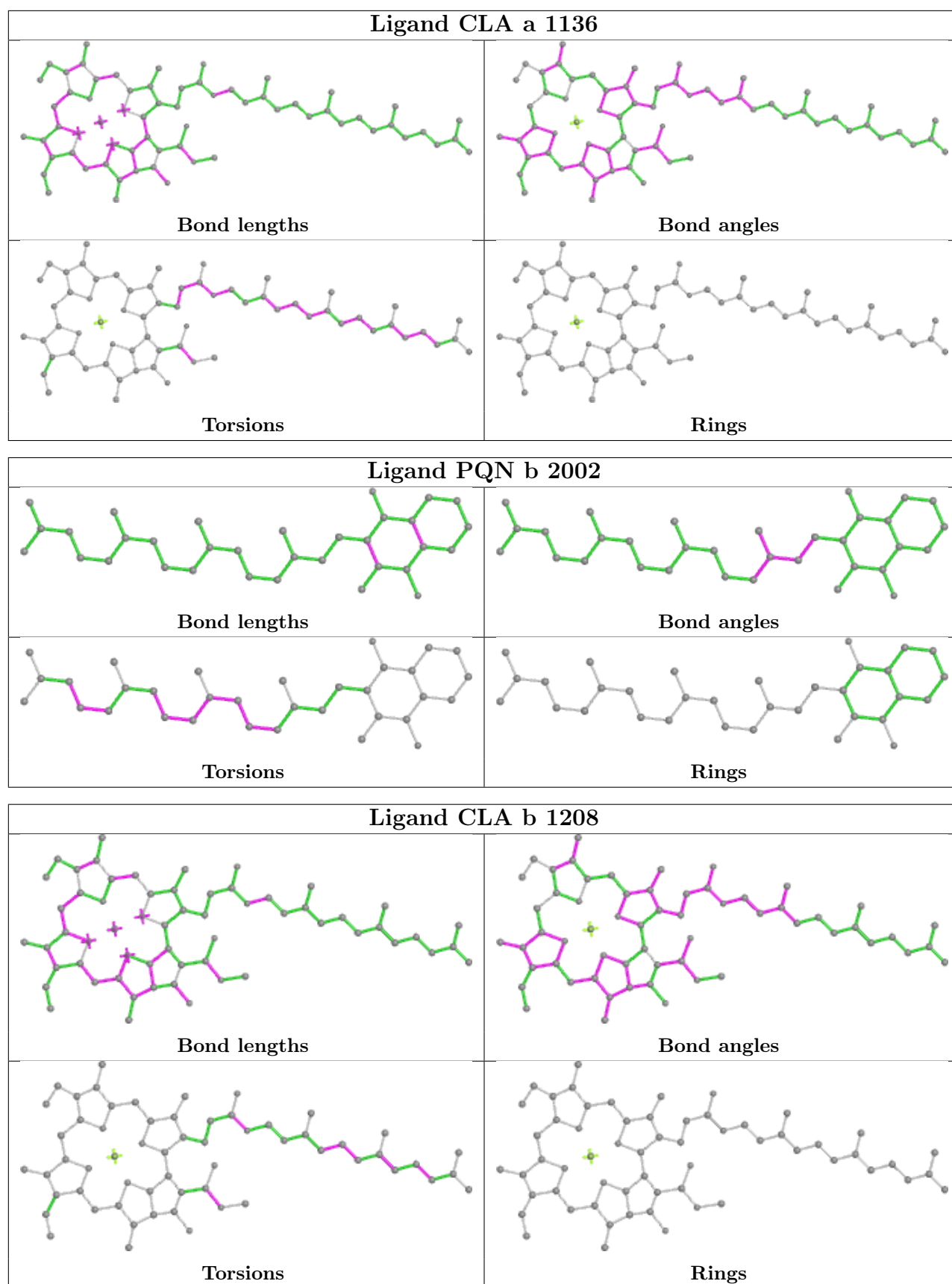


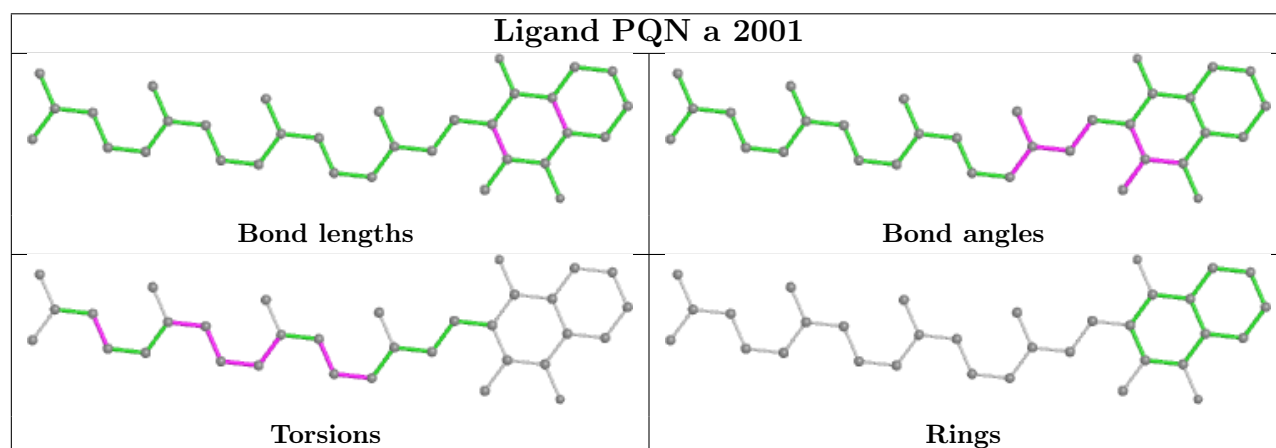
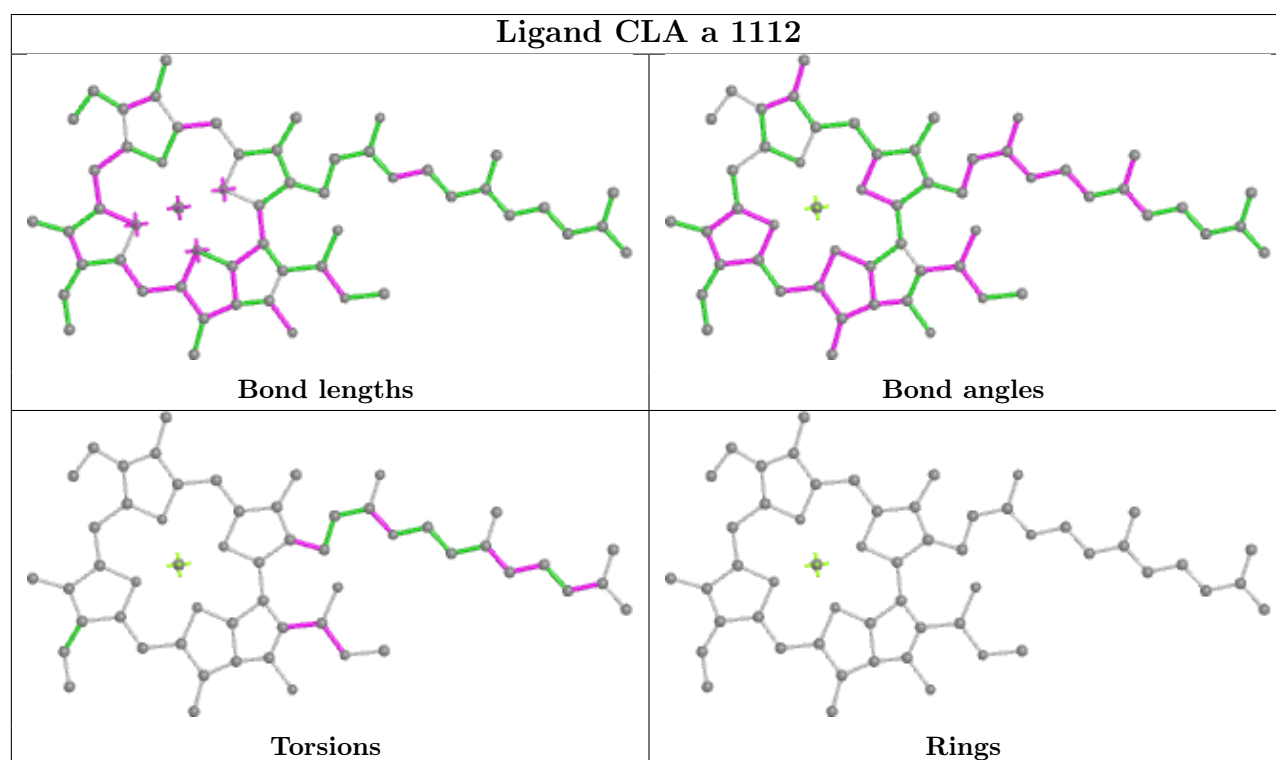
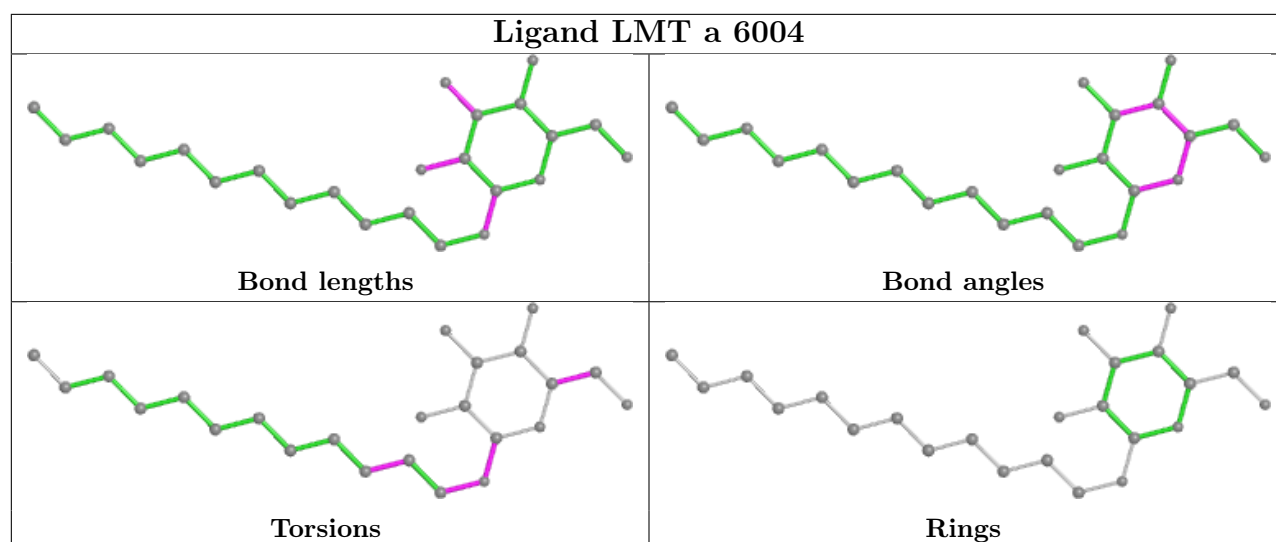
Ligand CLA A 1101

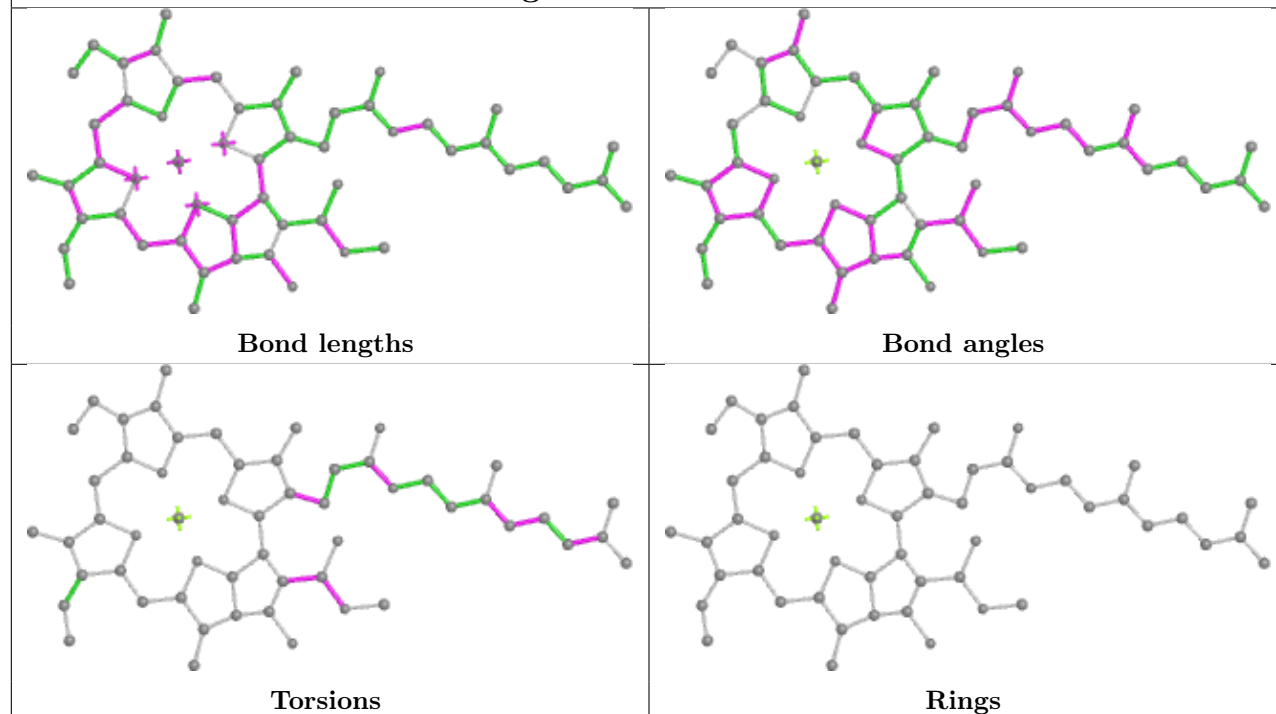
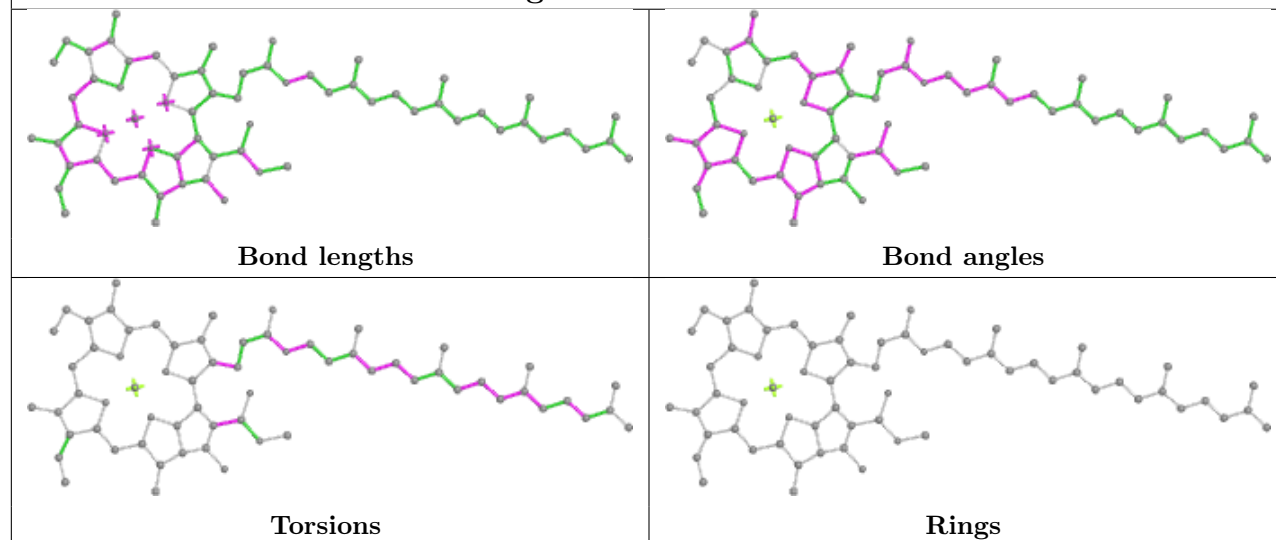


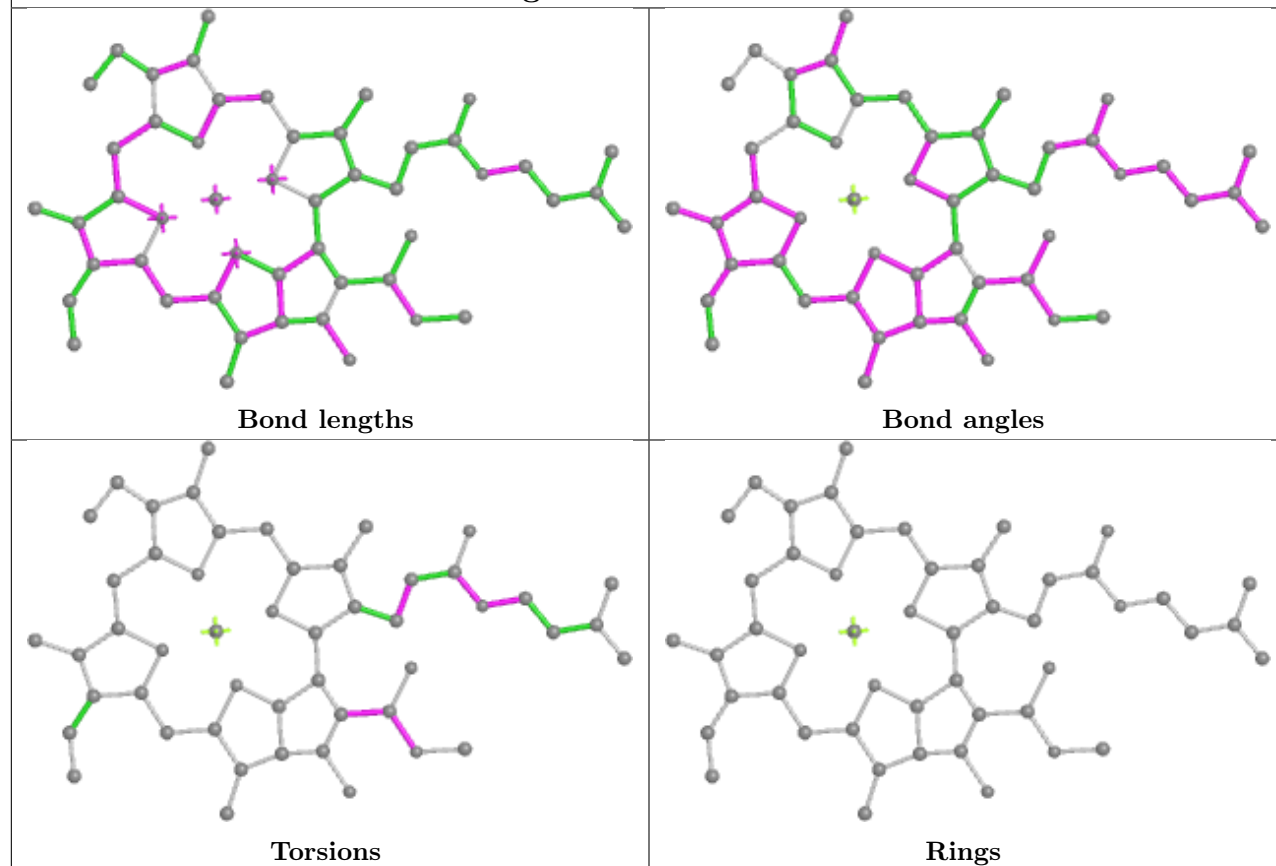
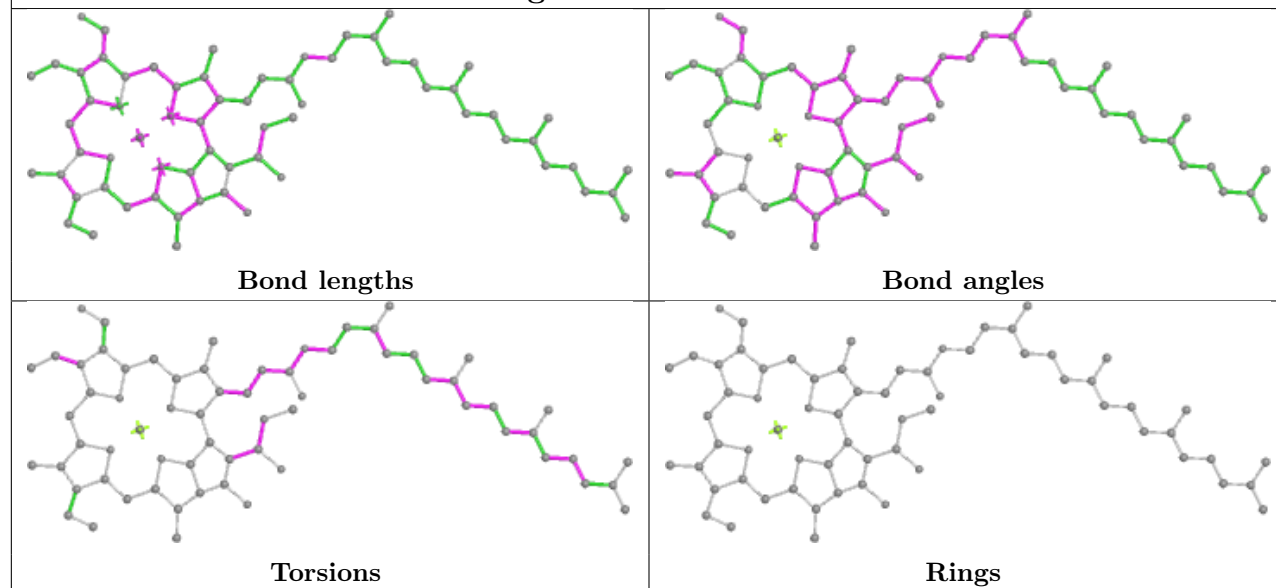
Ligand CLA H 1201

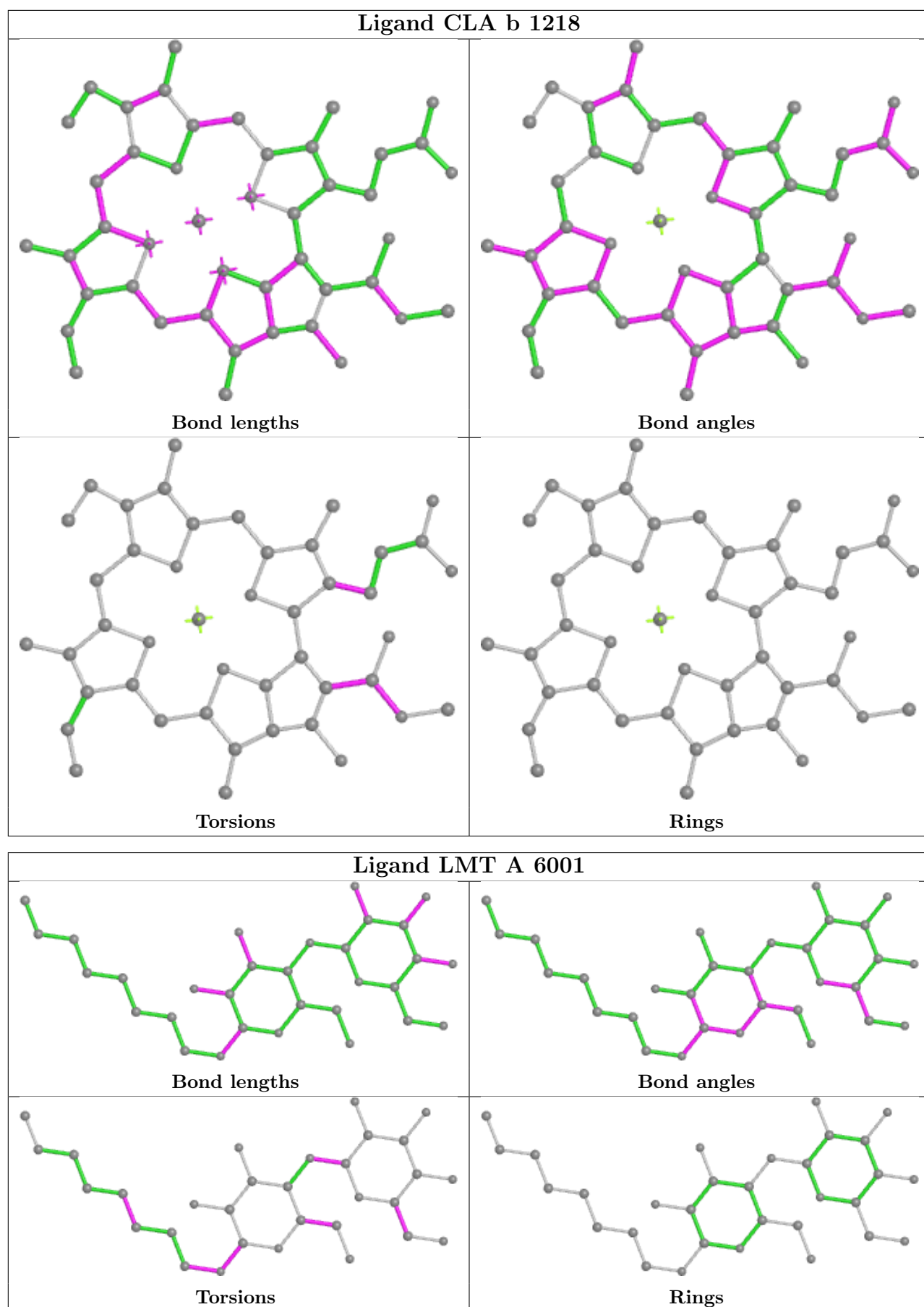




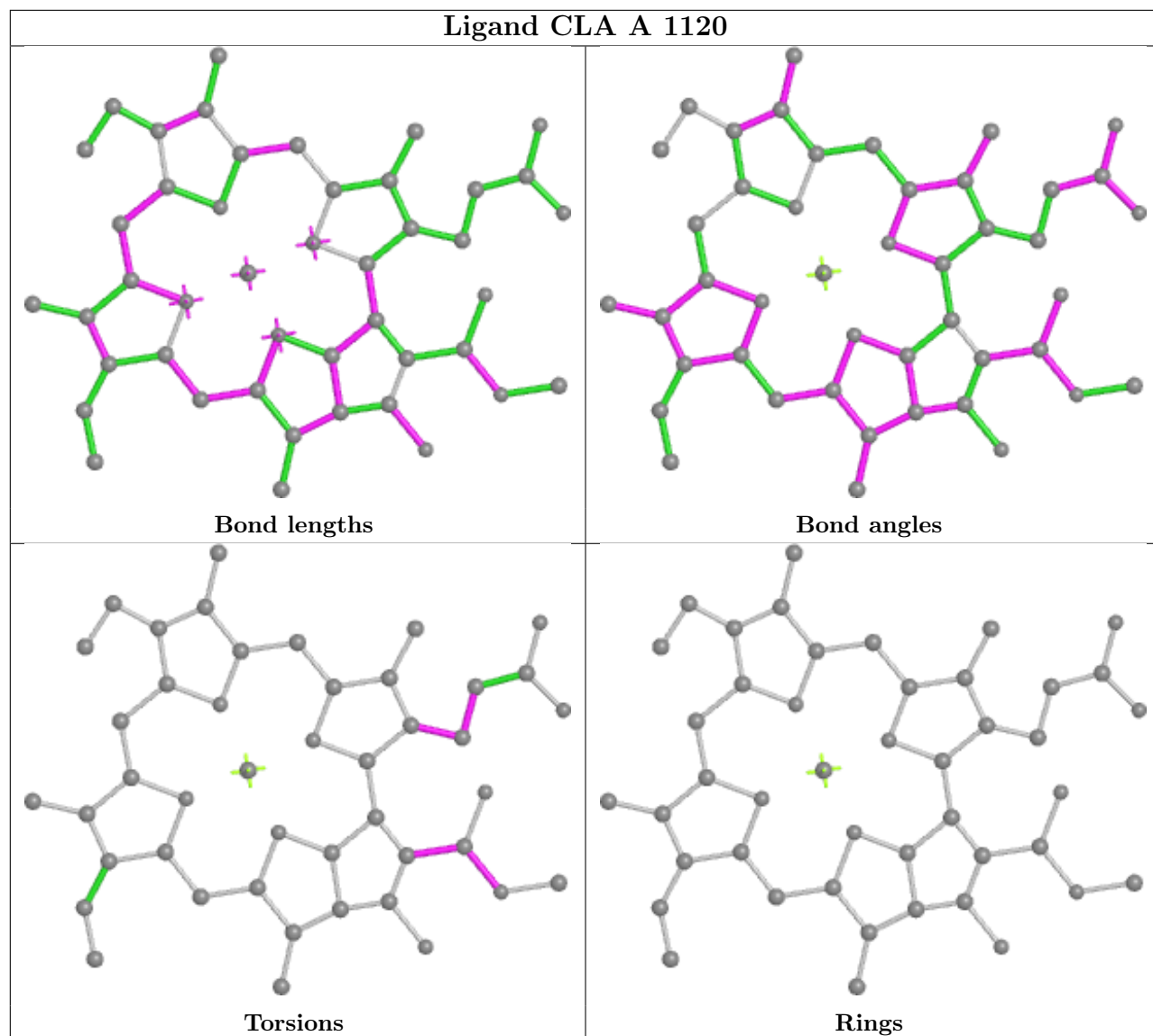


Ligand CLA G 1112**Ligand CLA b 1210**

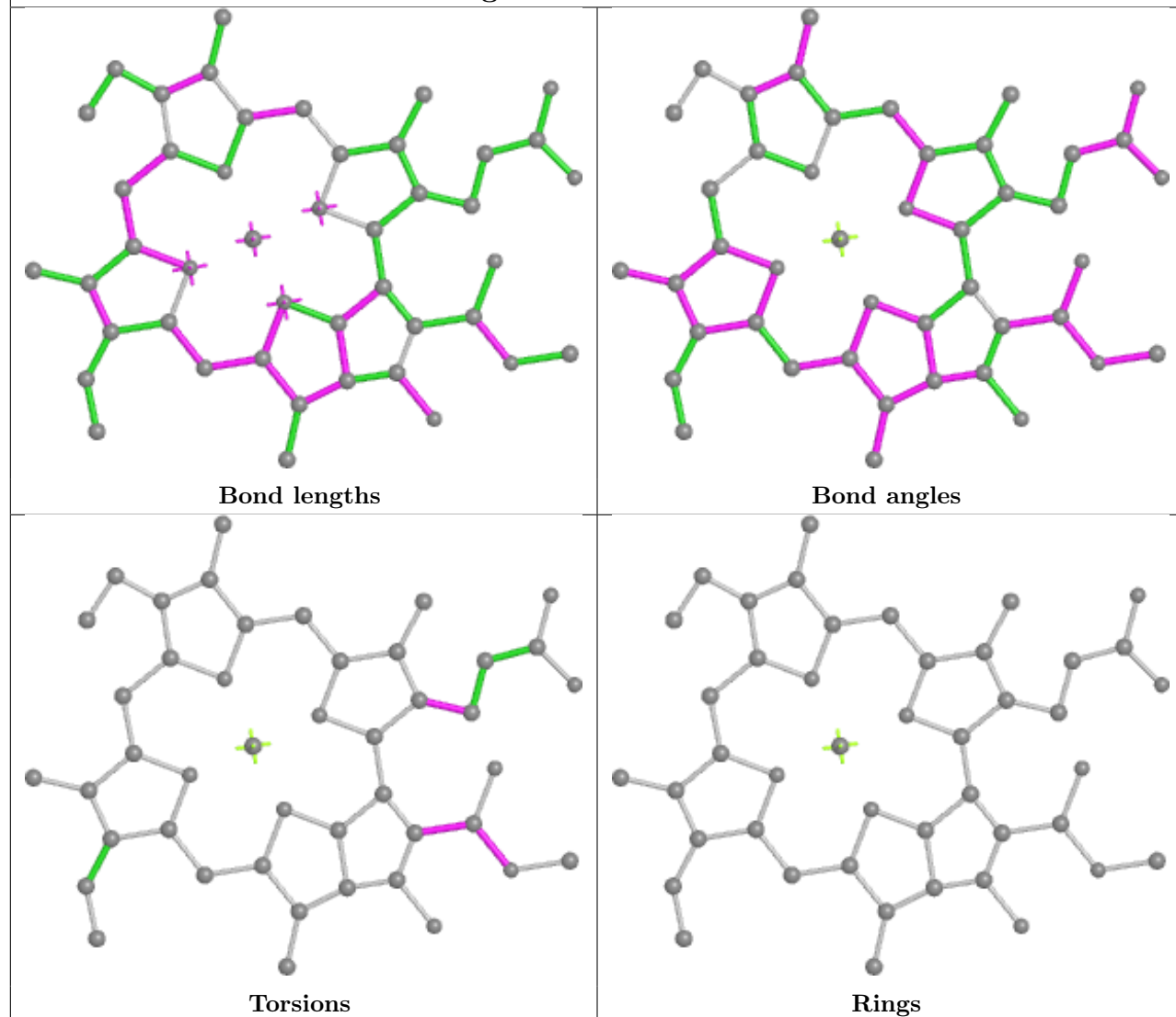
Ligand CLA A 1135**Ligand F6C B 1237**



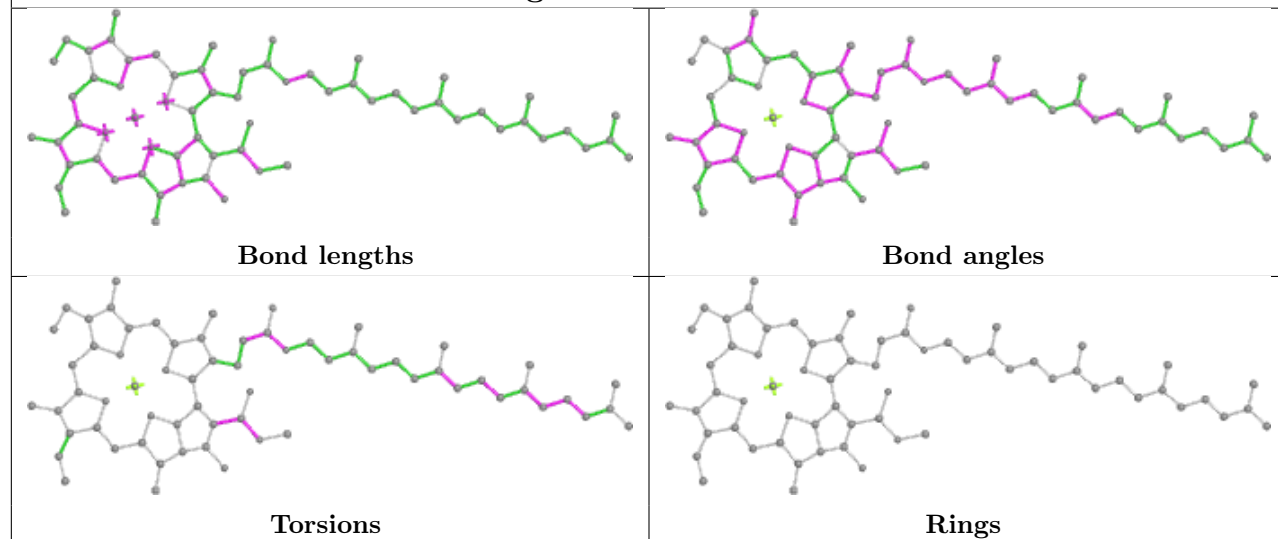
Ligand CLA A 1120



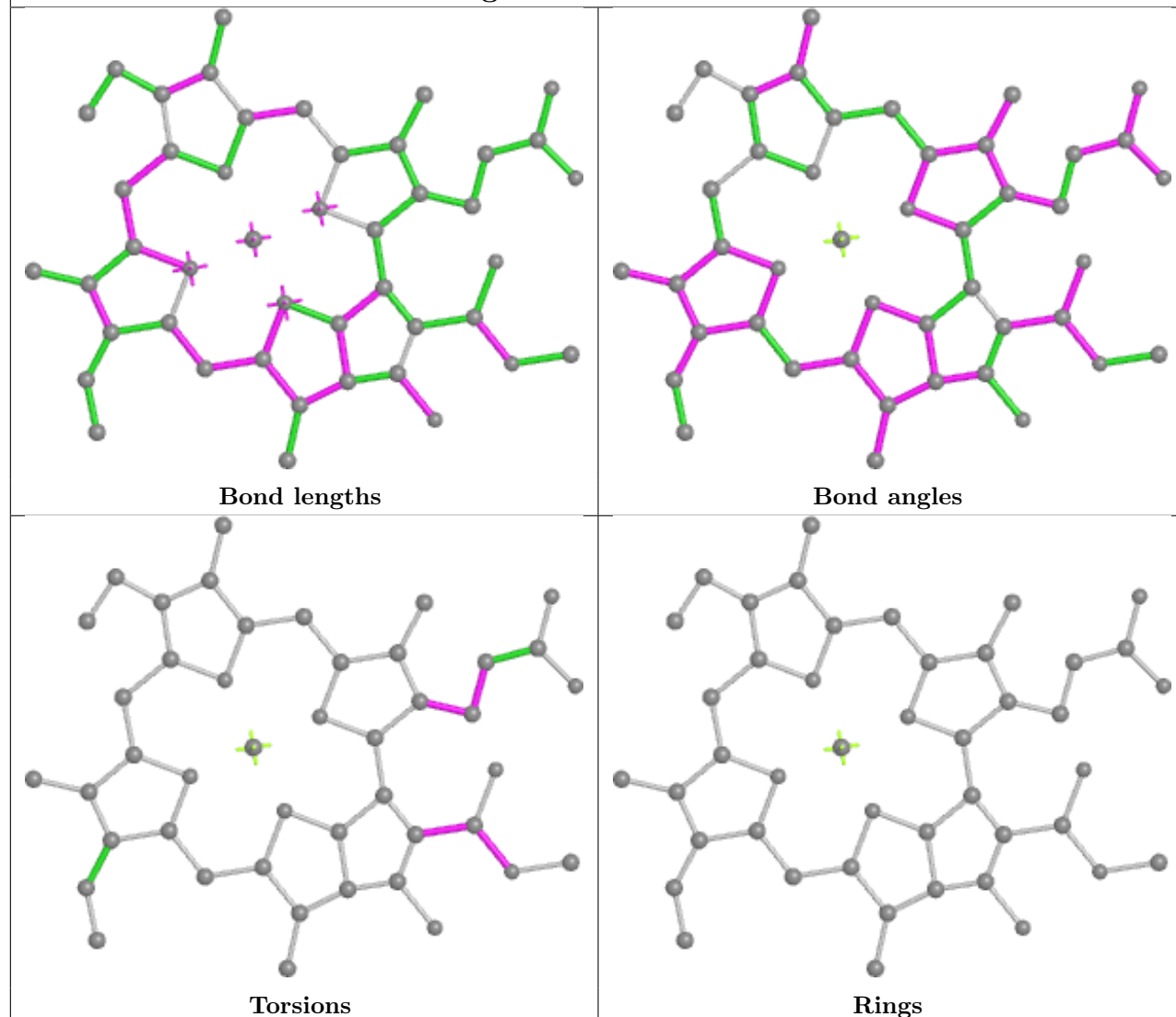
Ligand CLA B 1218



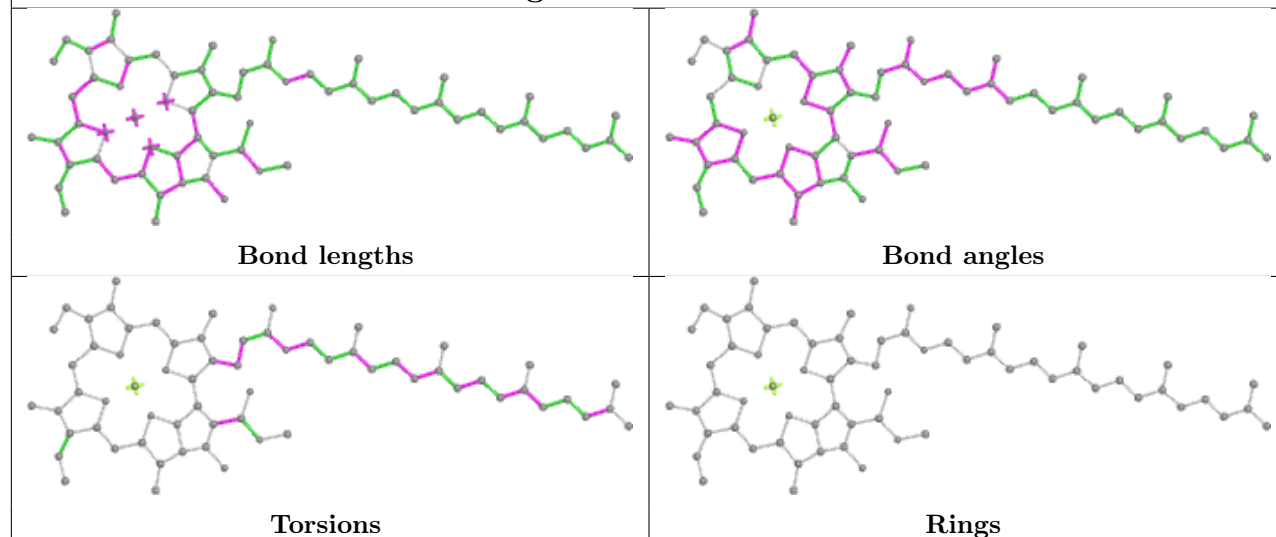
Ligand CLA b 1021

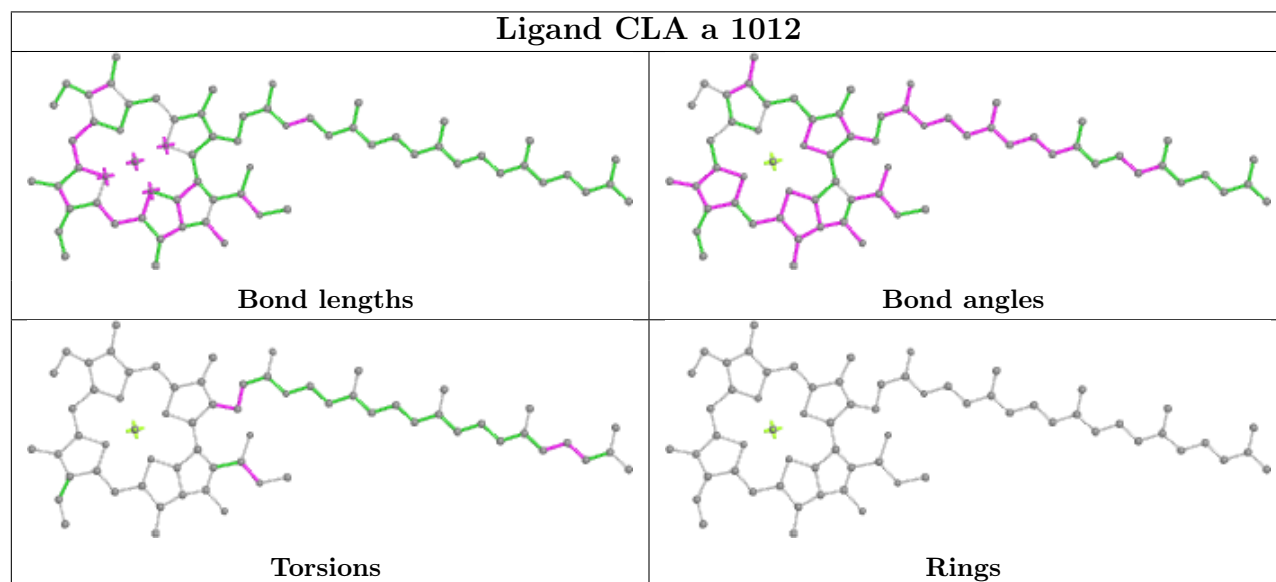
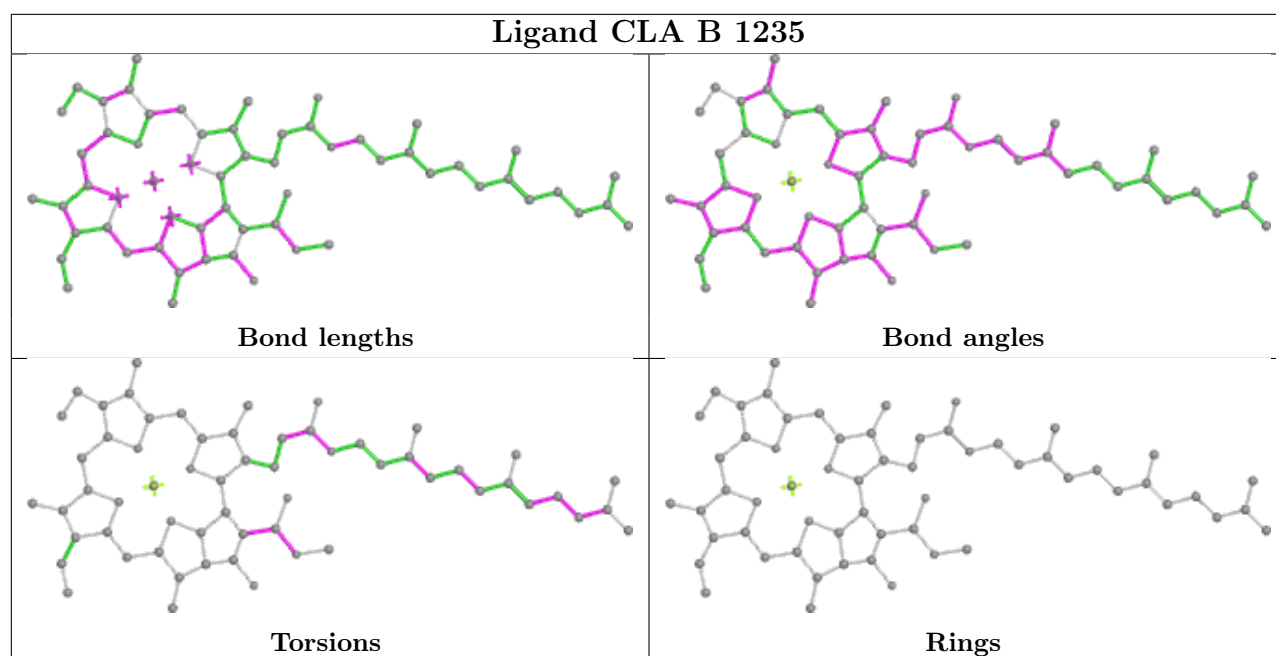


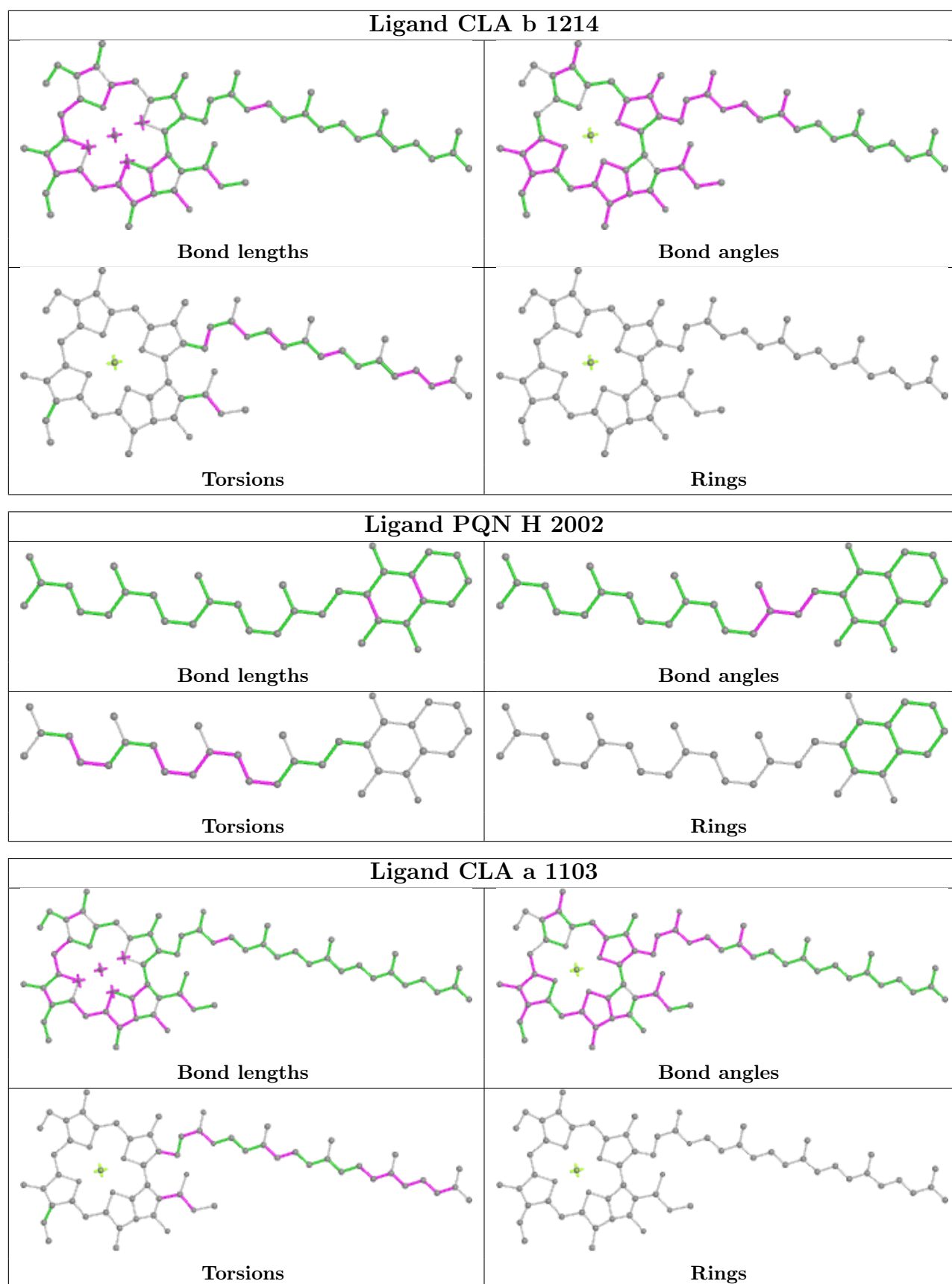
Ligand CLA A 1113

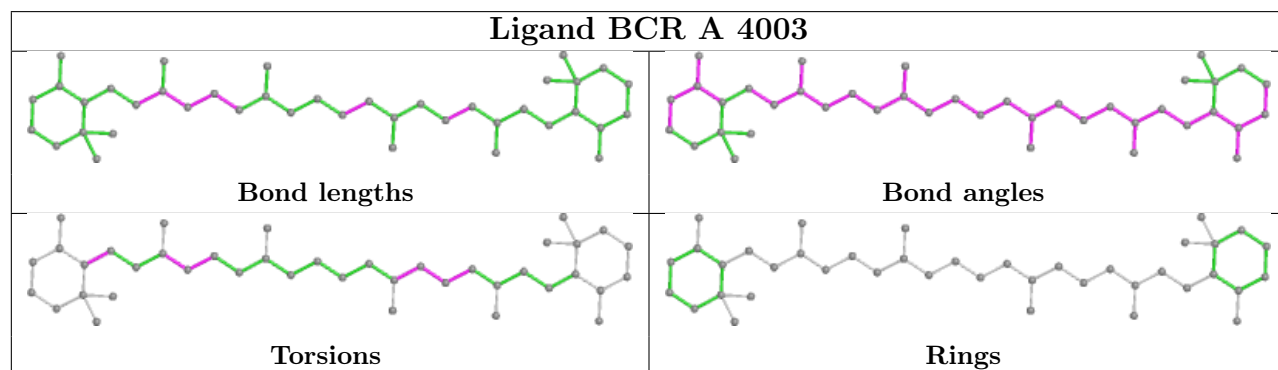
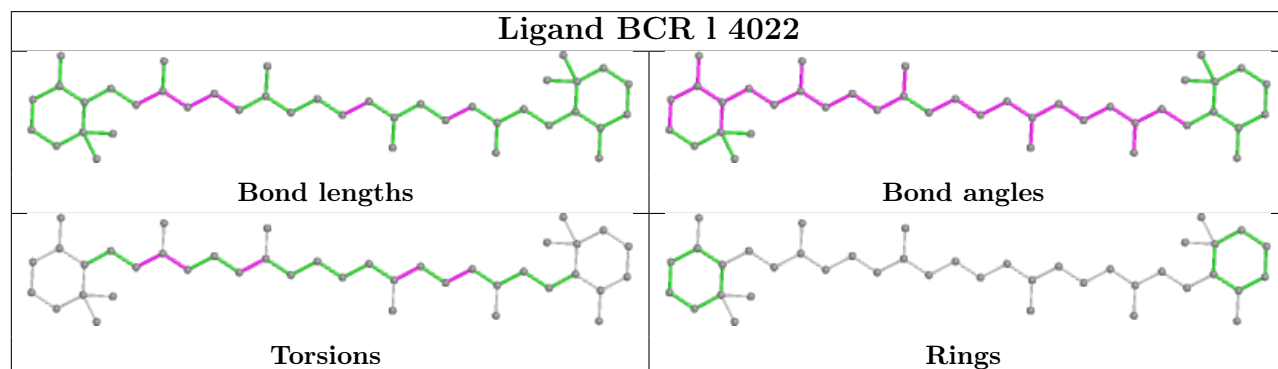
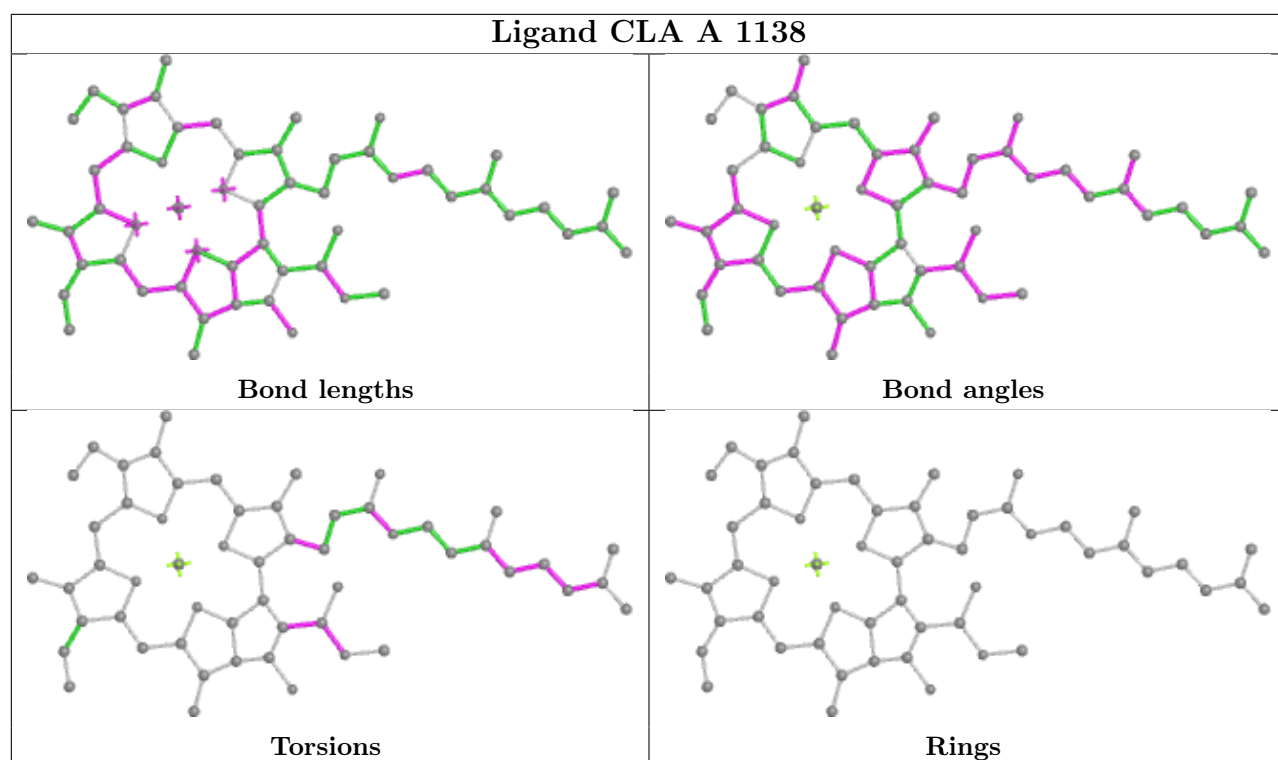


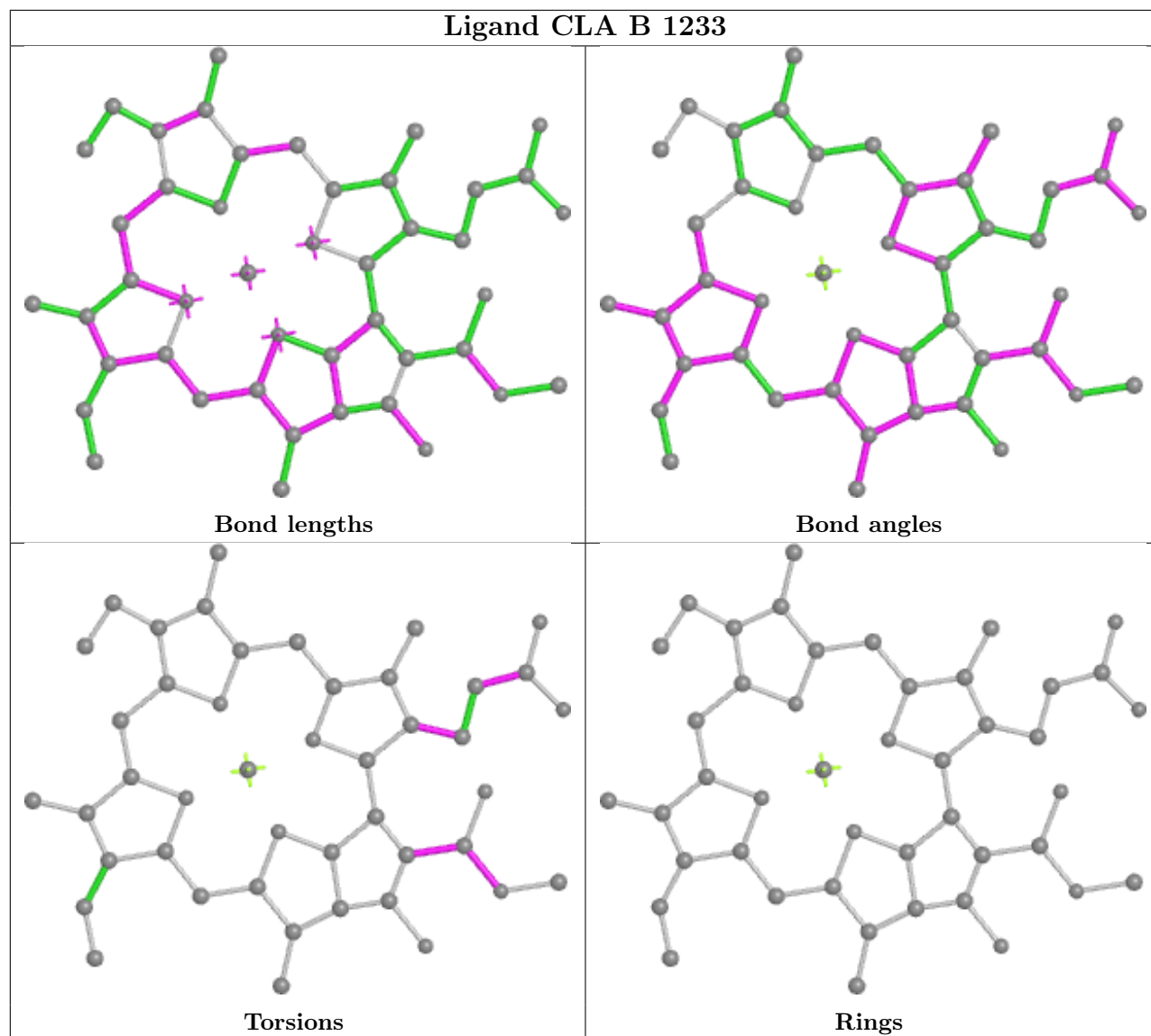
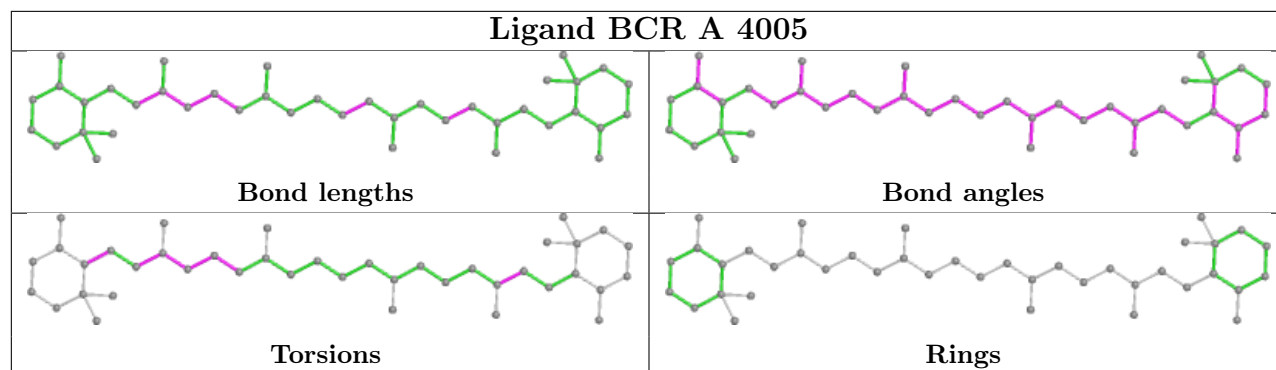
Ligand CLA b 1221

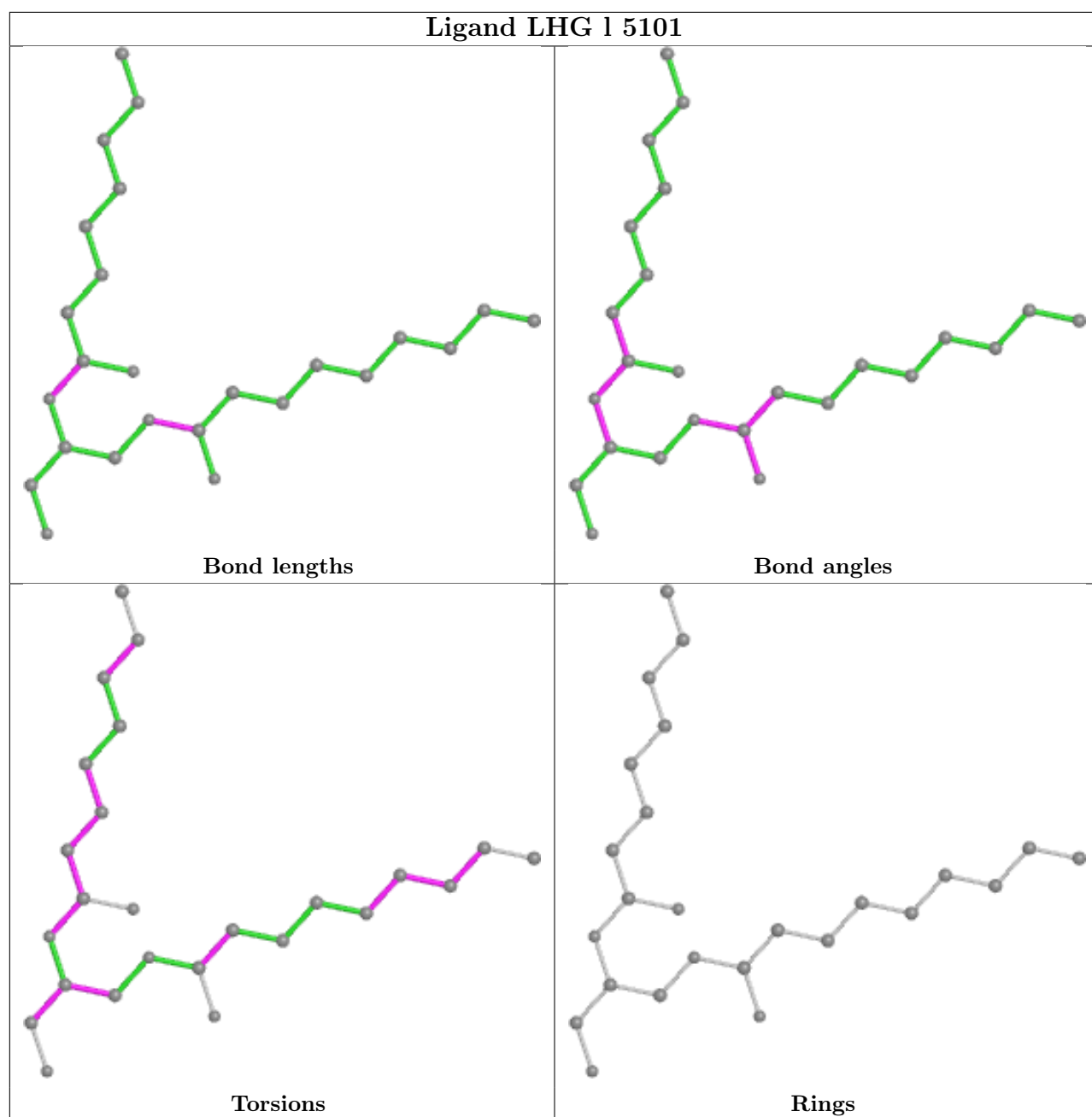


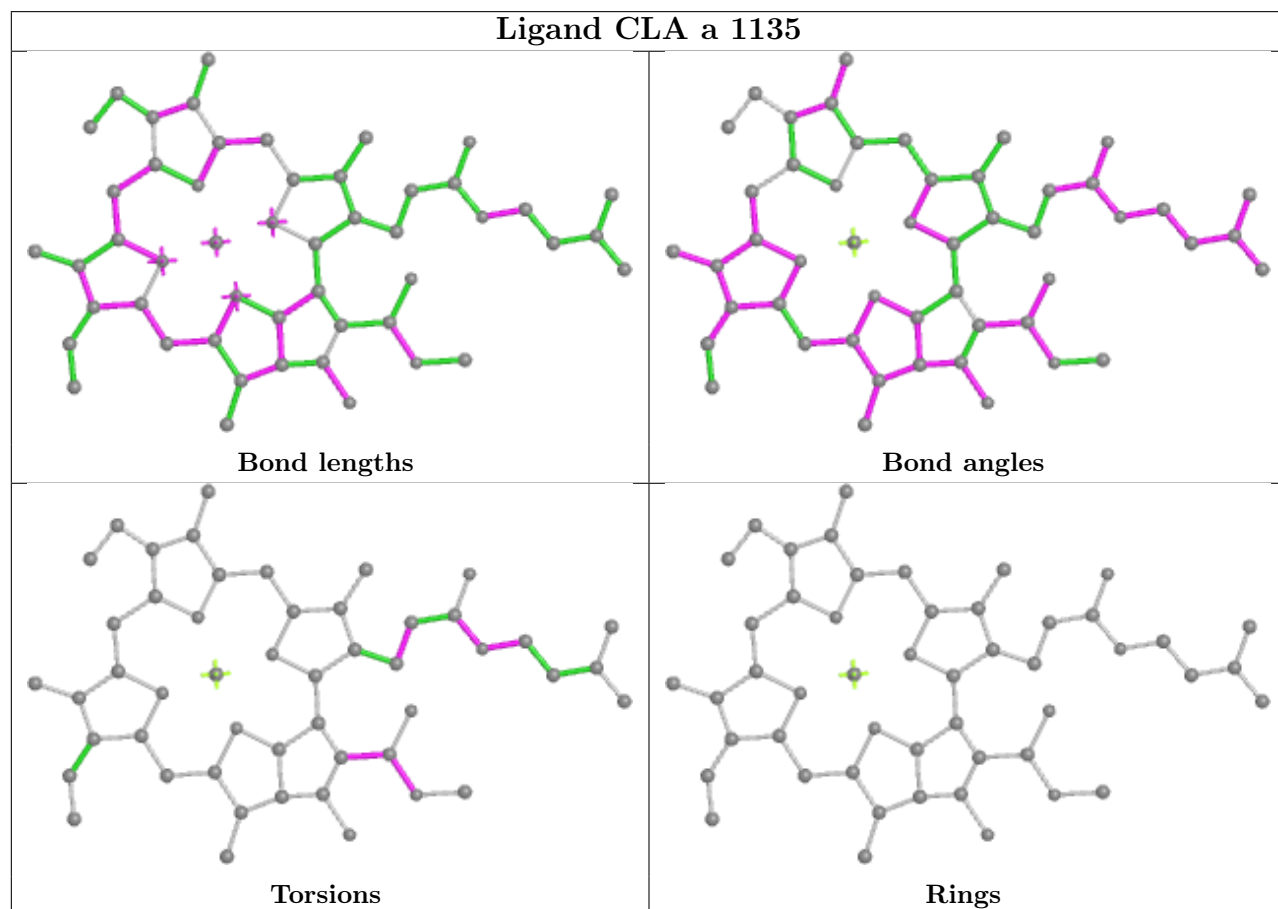
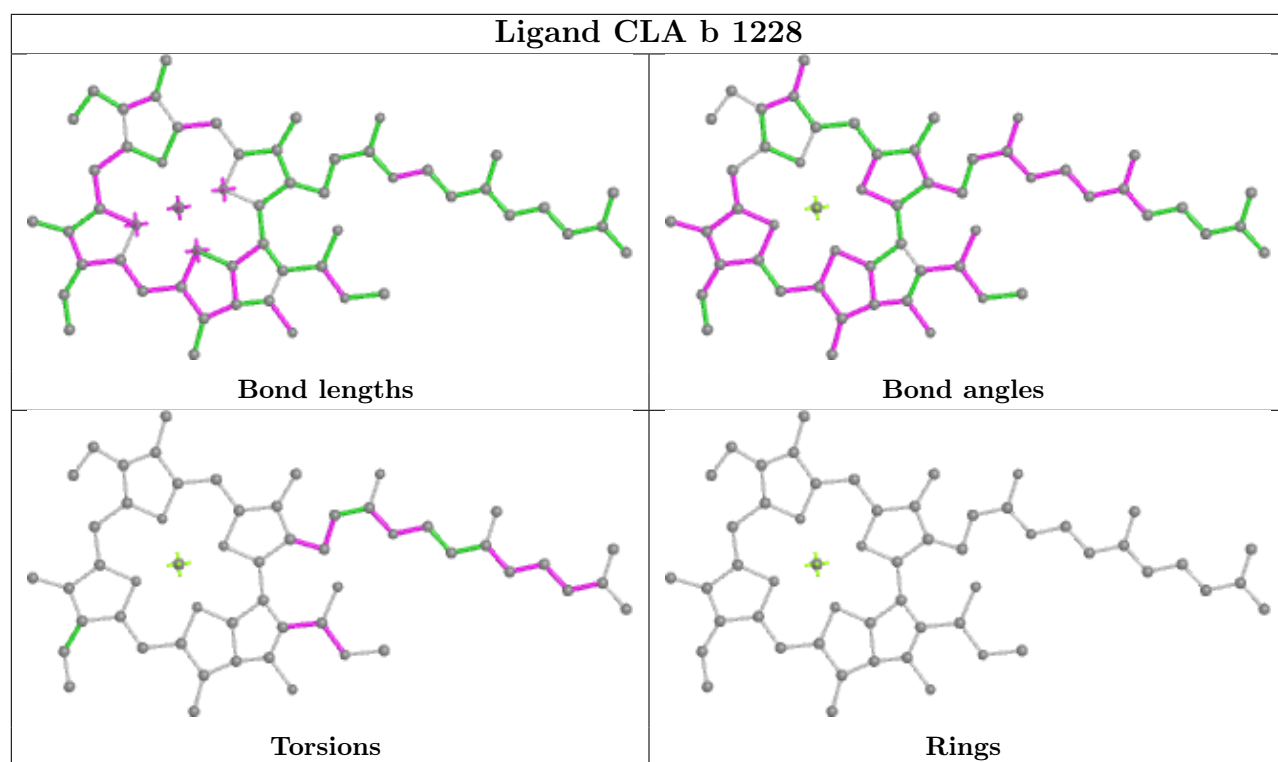




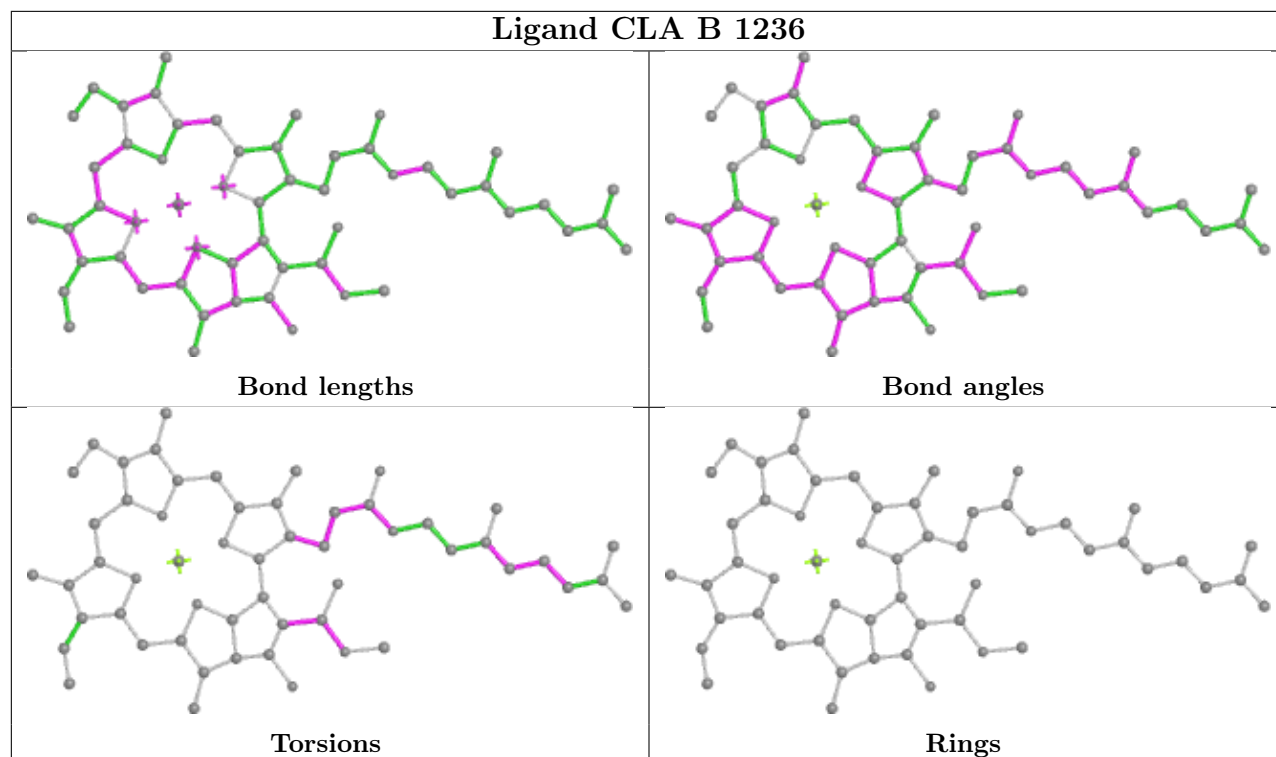




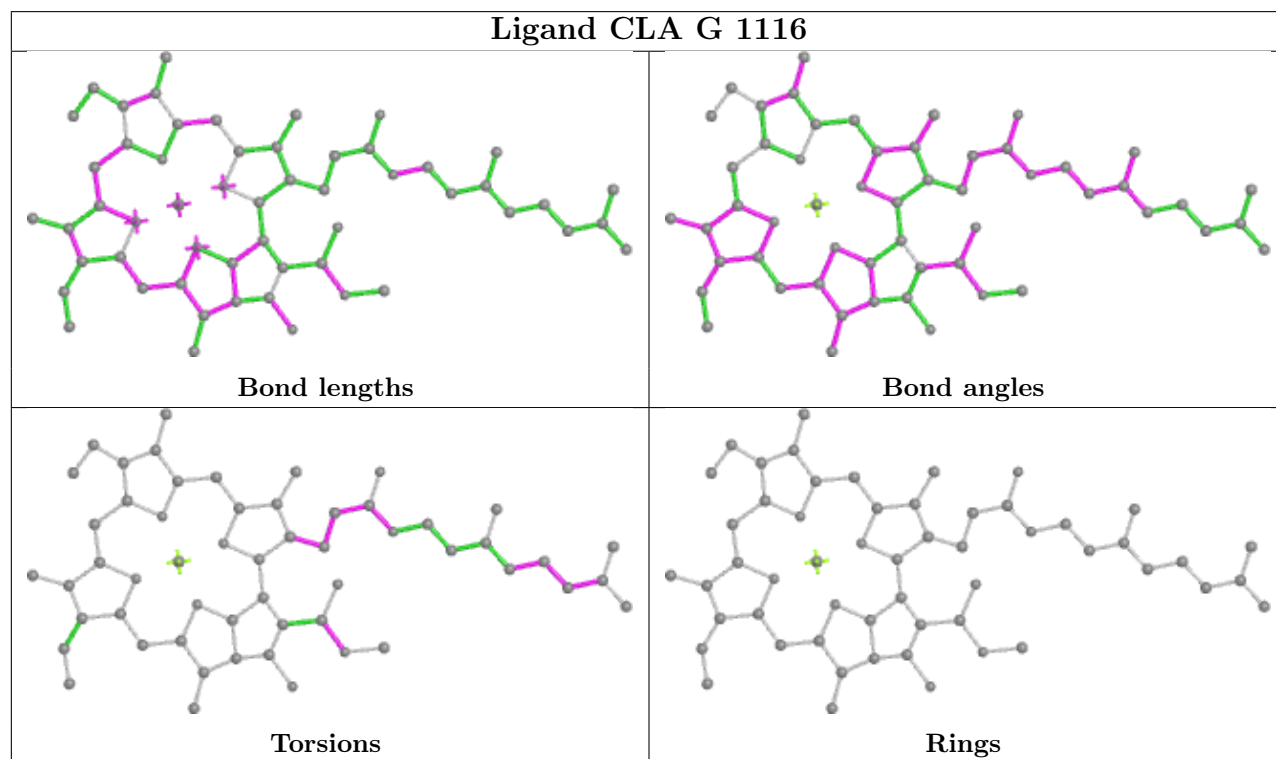


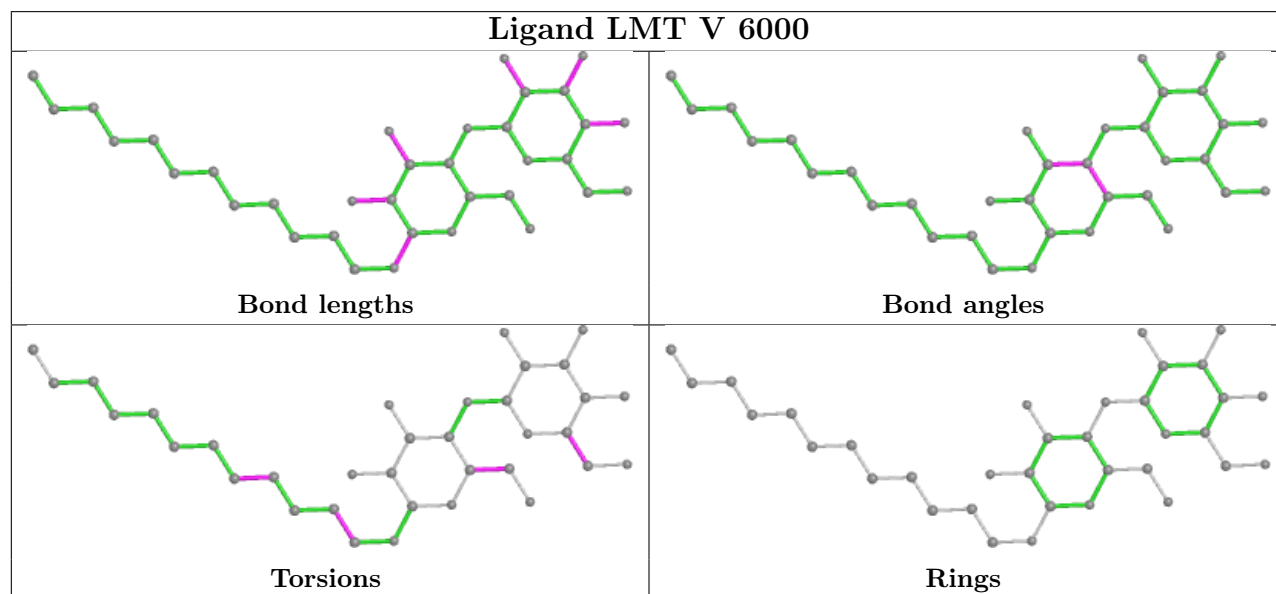
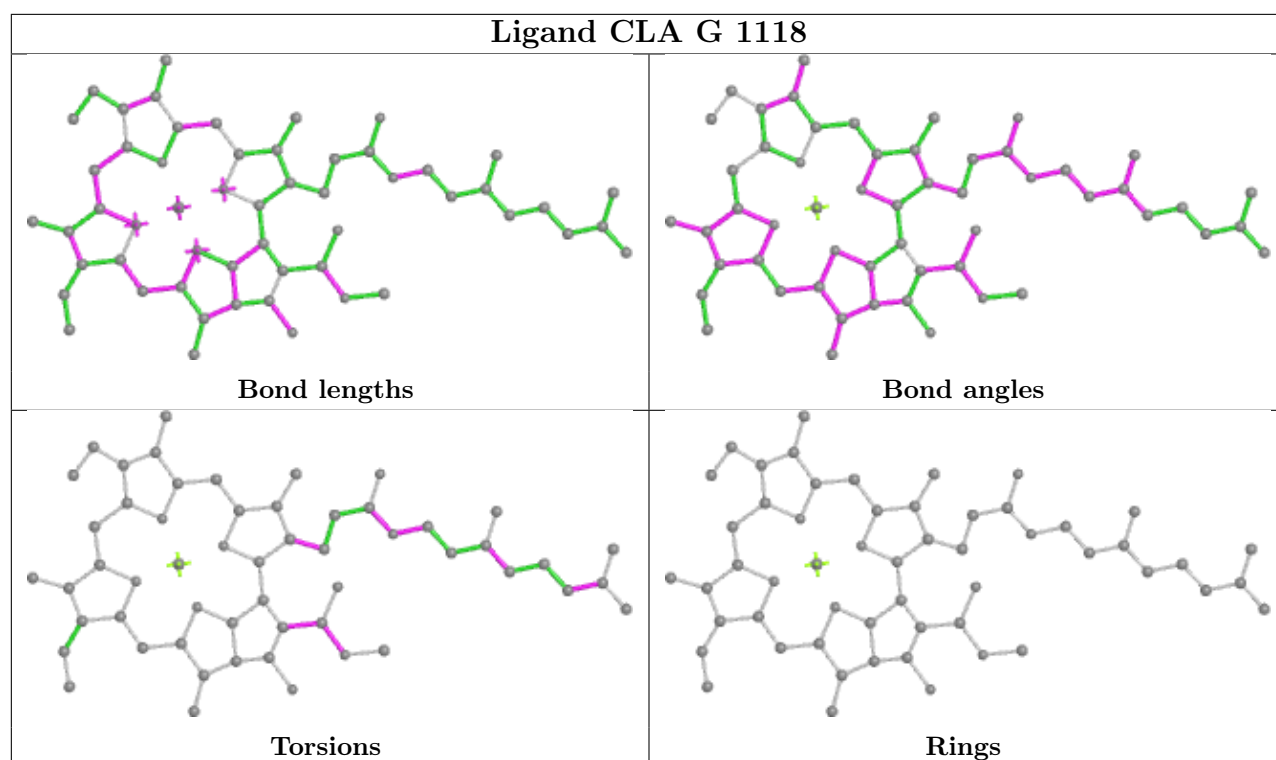


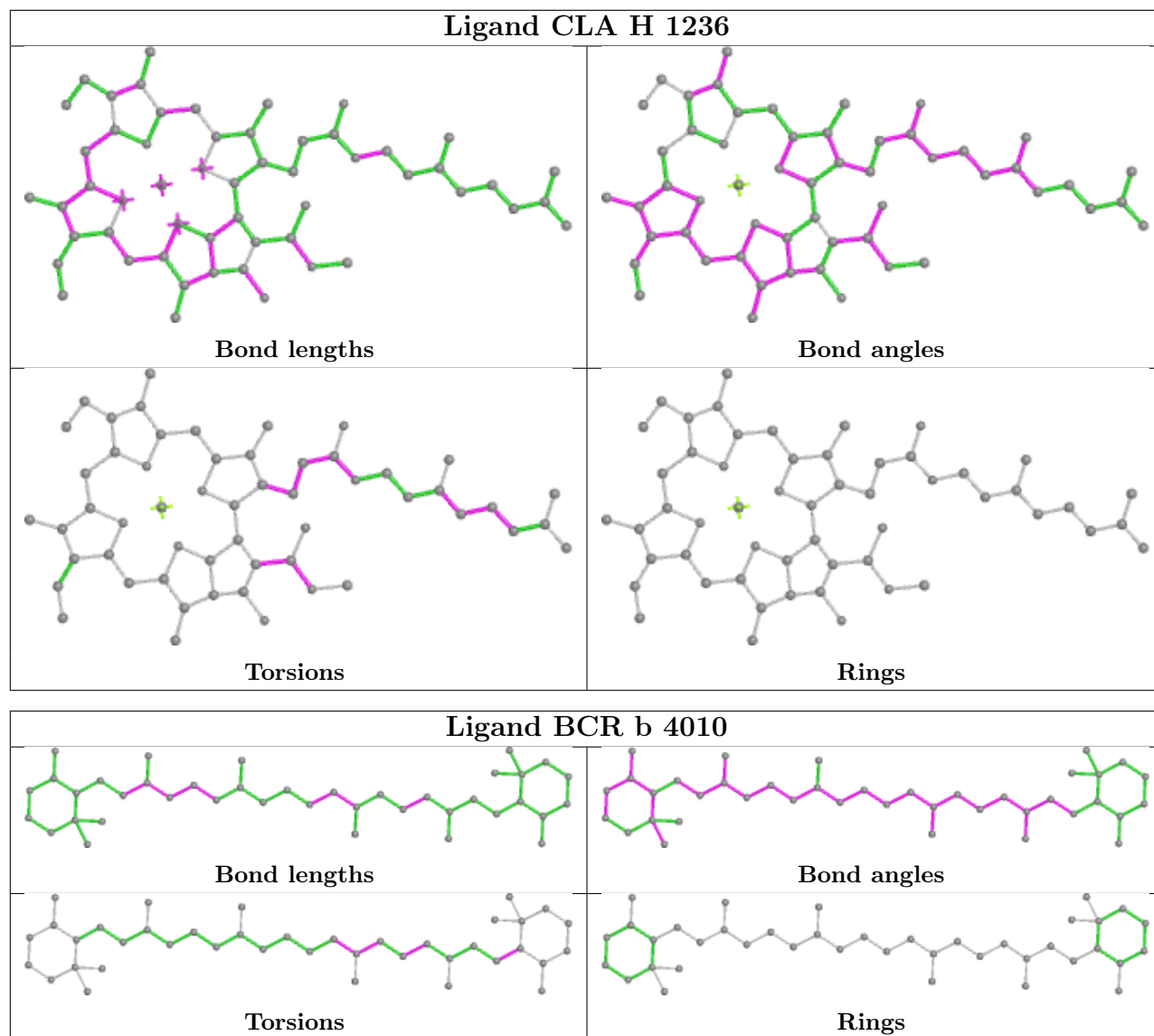
Ligand CLA B 1236



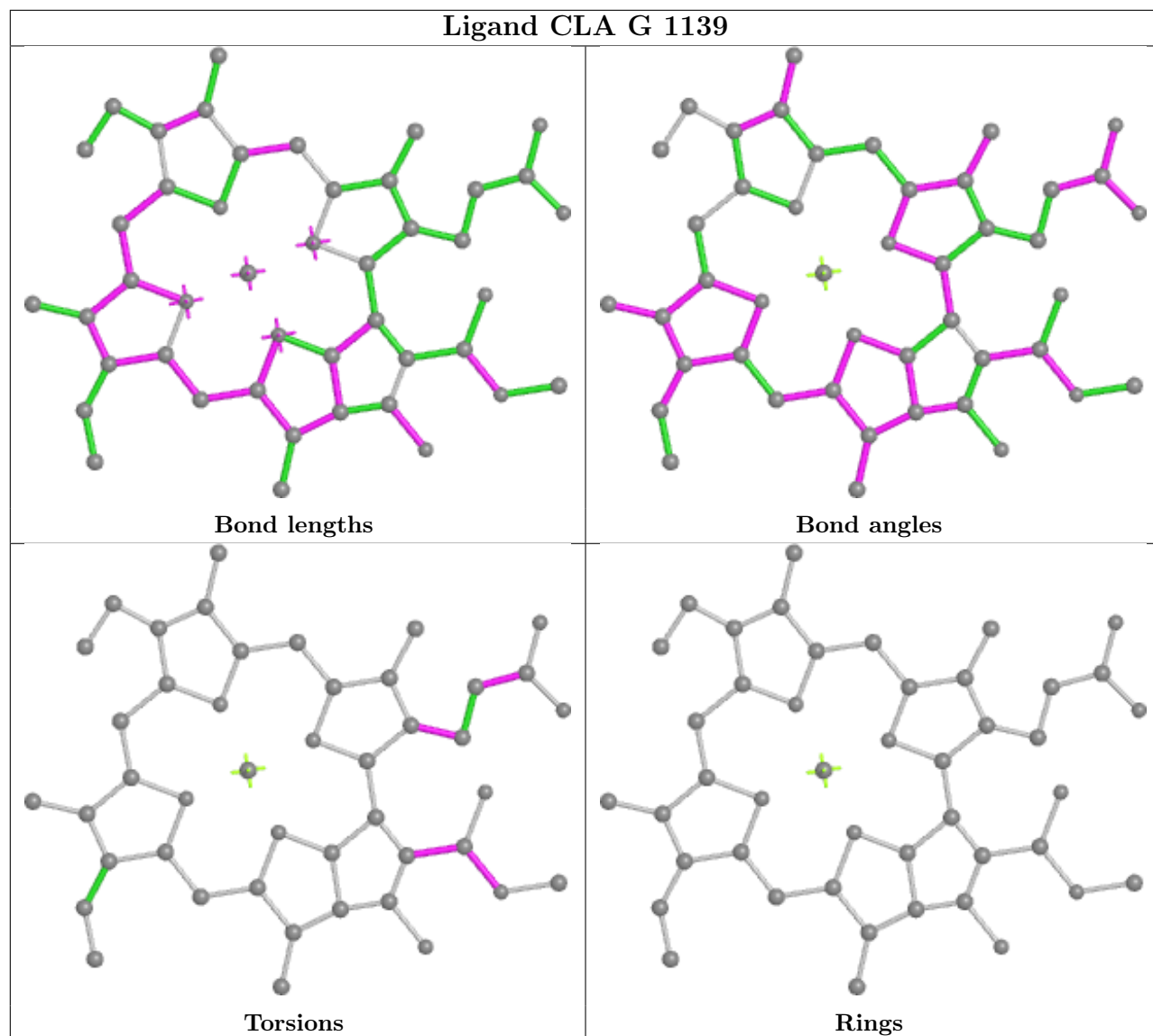
Ligand CLA G 1116



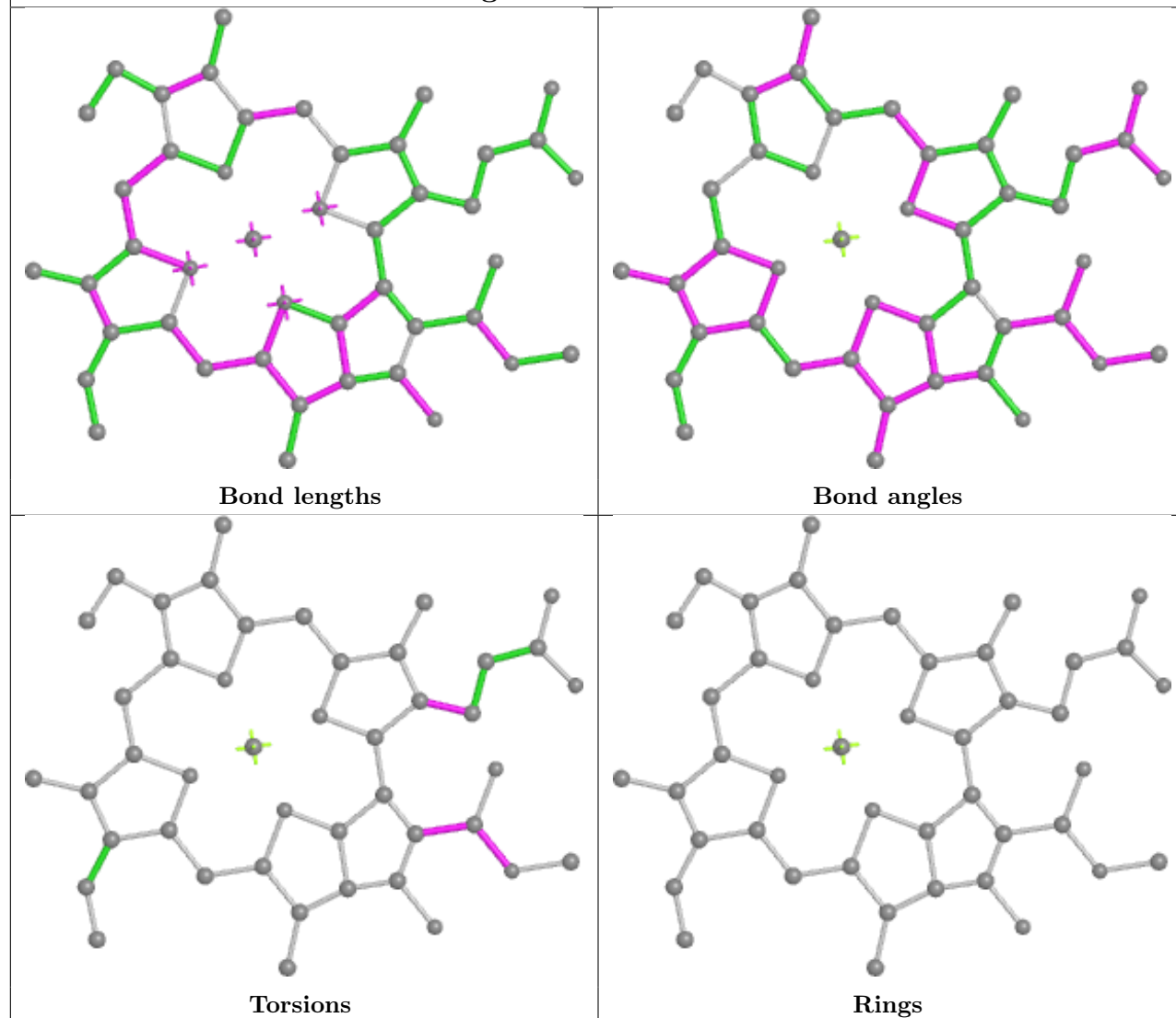




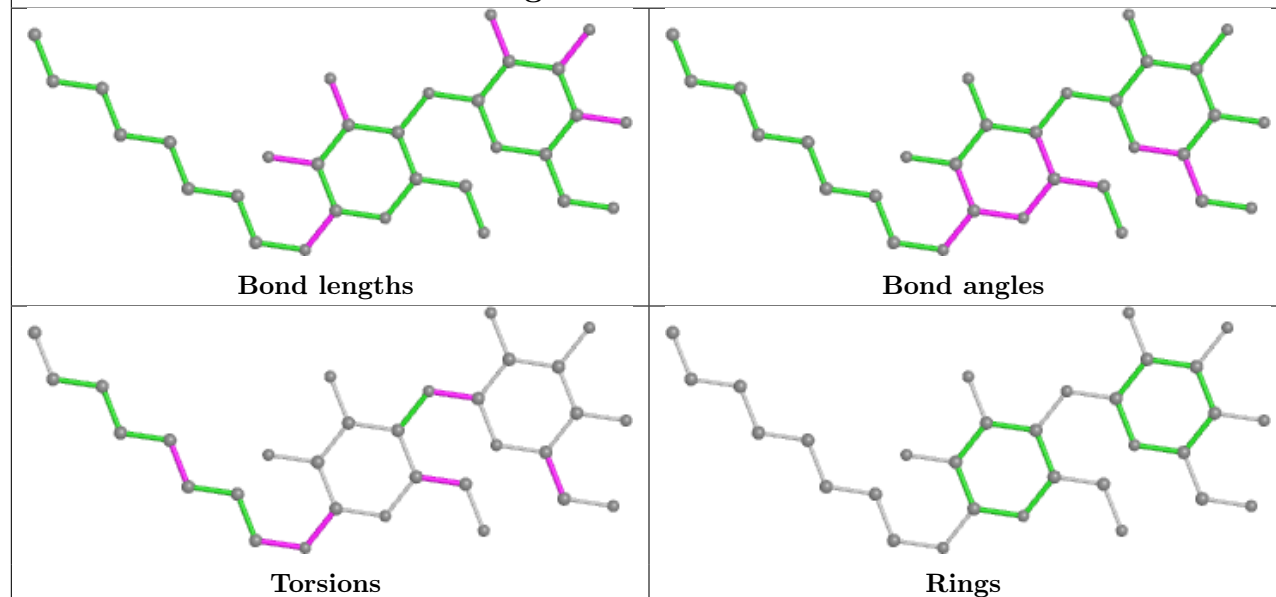
Ligand CLA G 1139

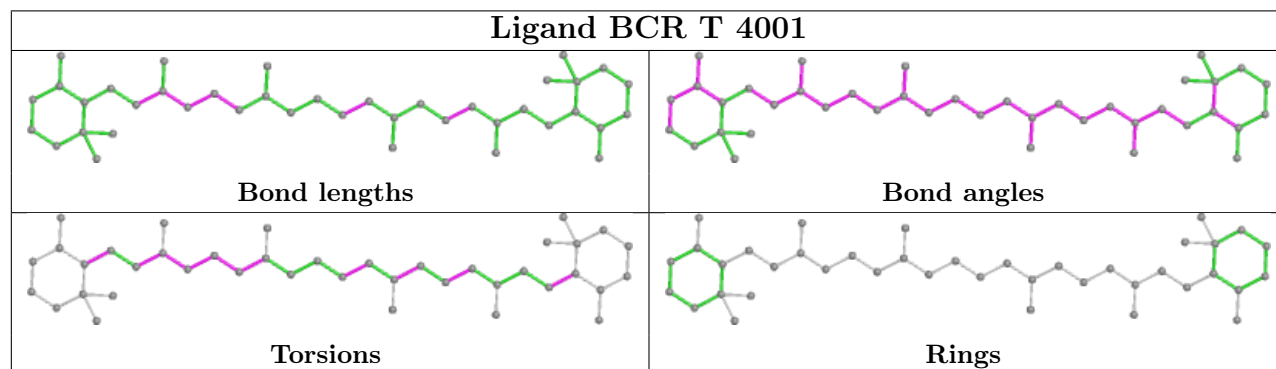
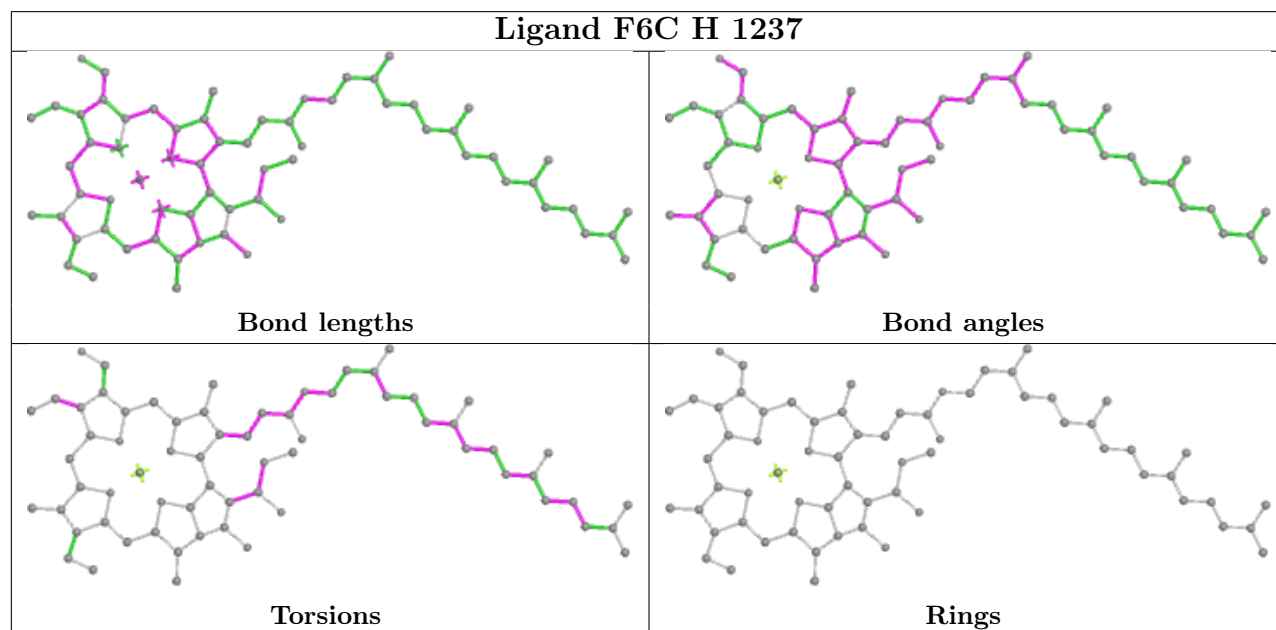
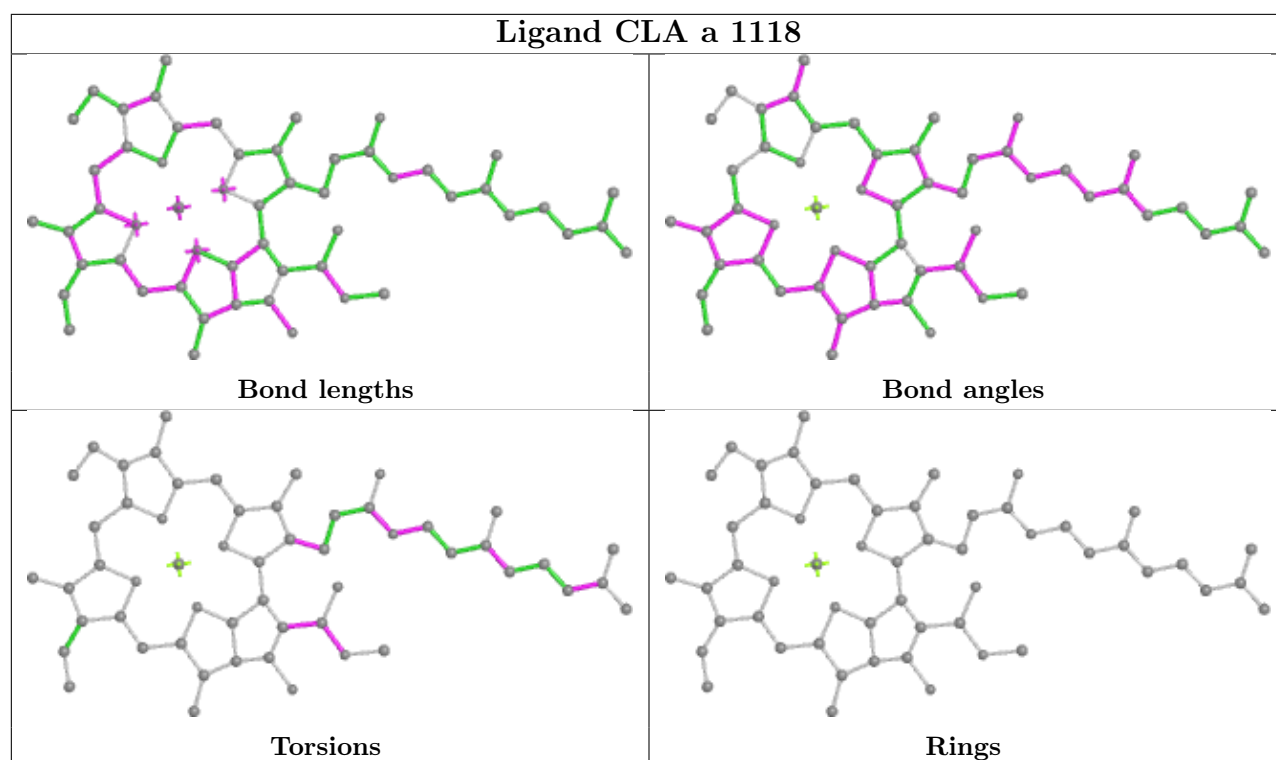


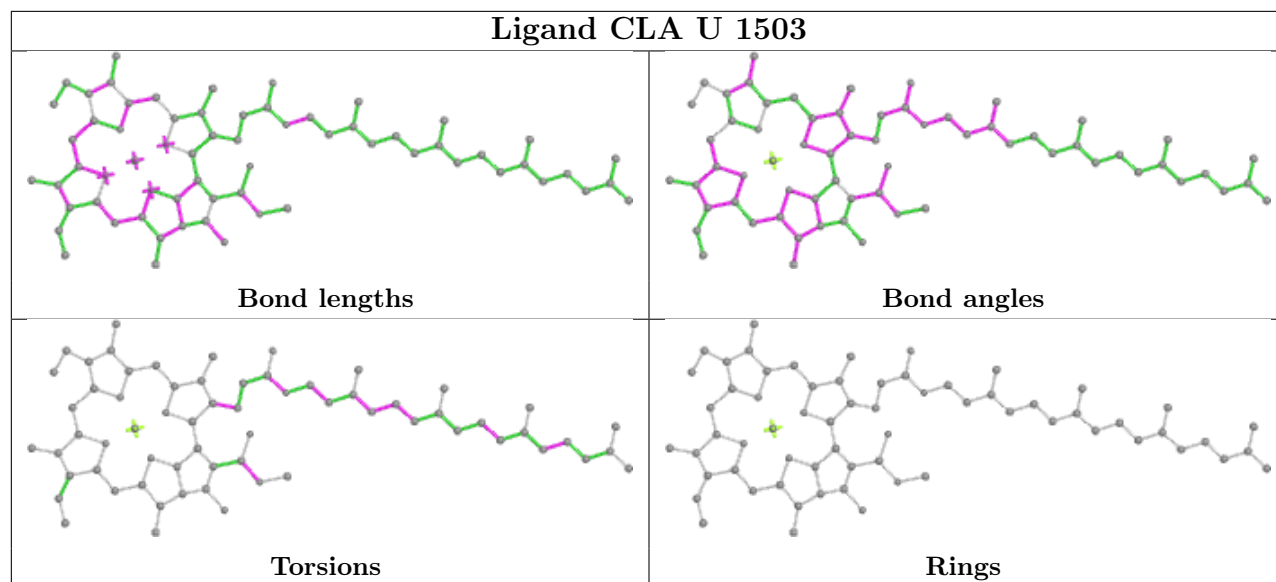
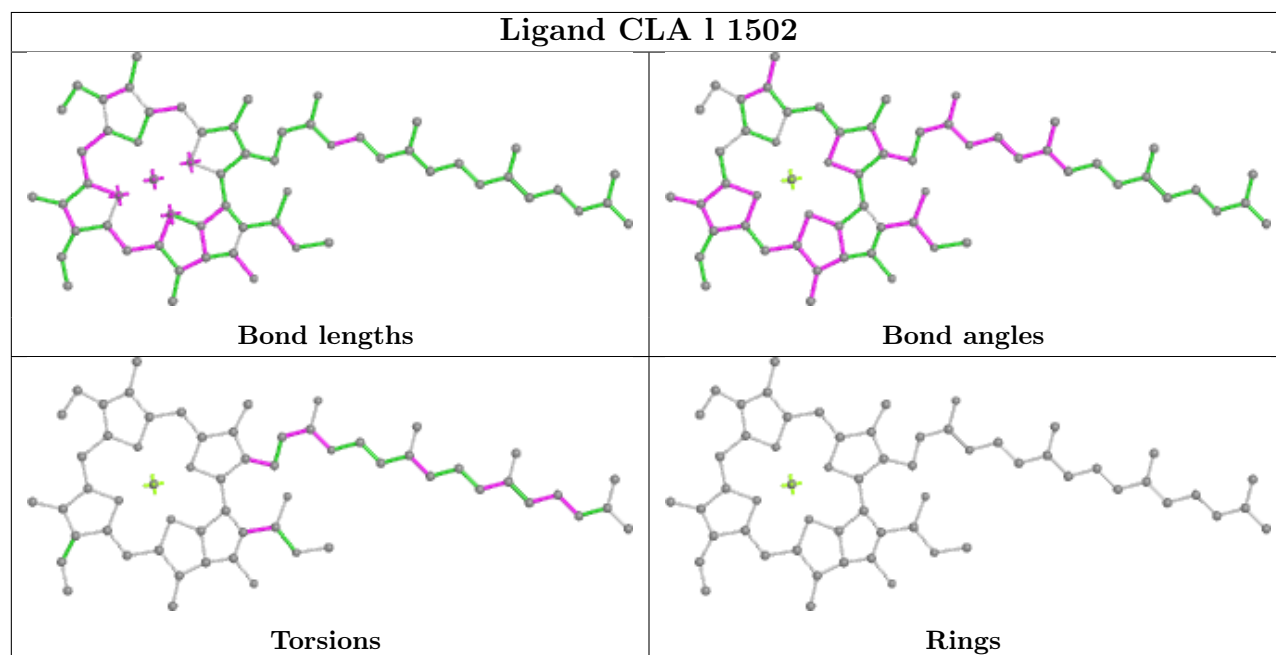
Ligand CLA H 1218

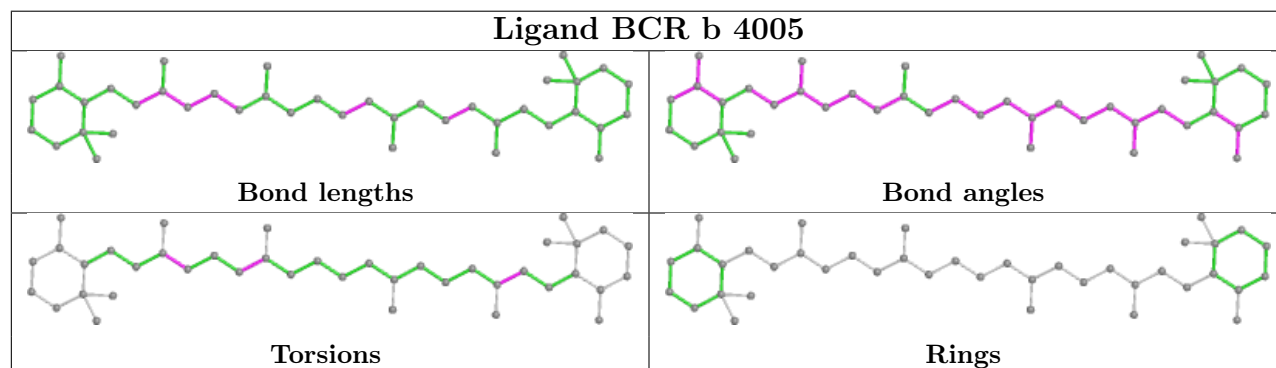
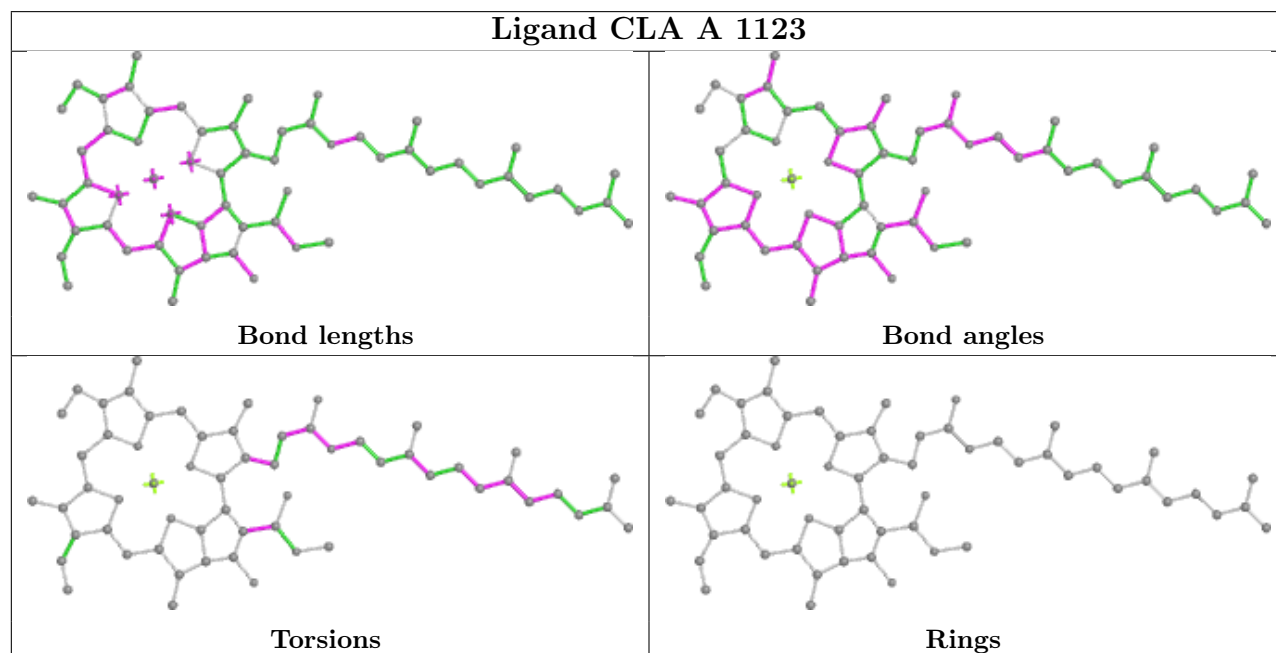
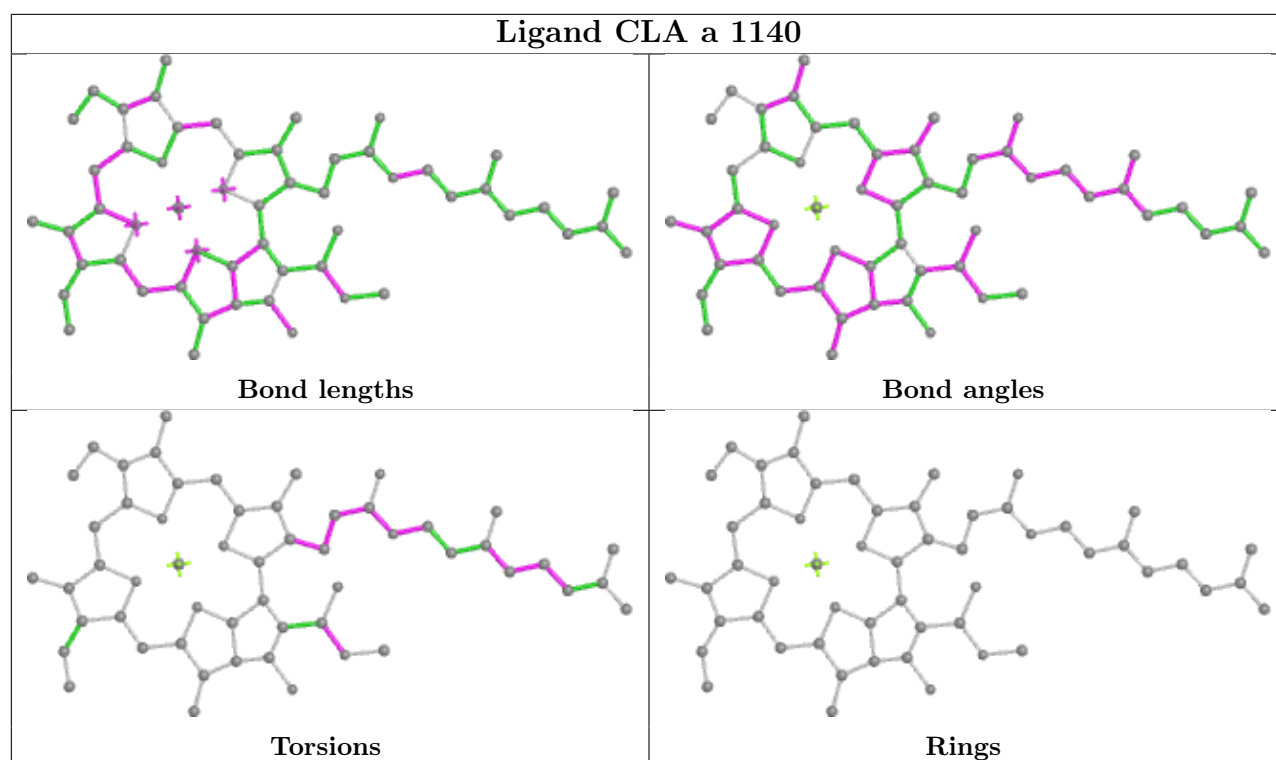


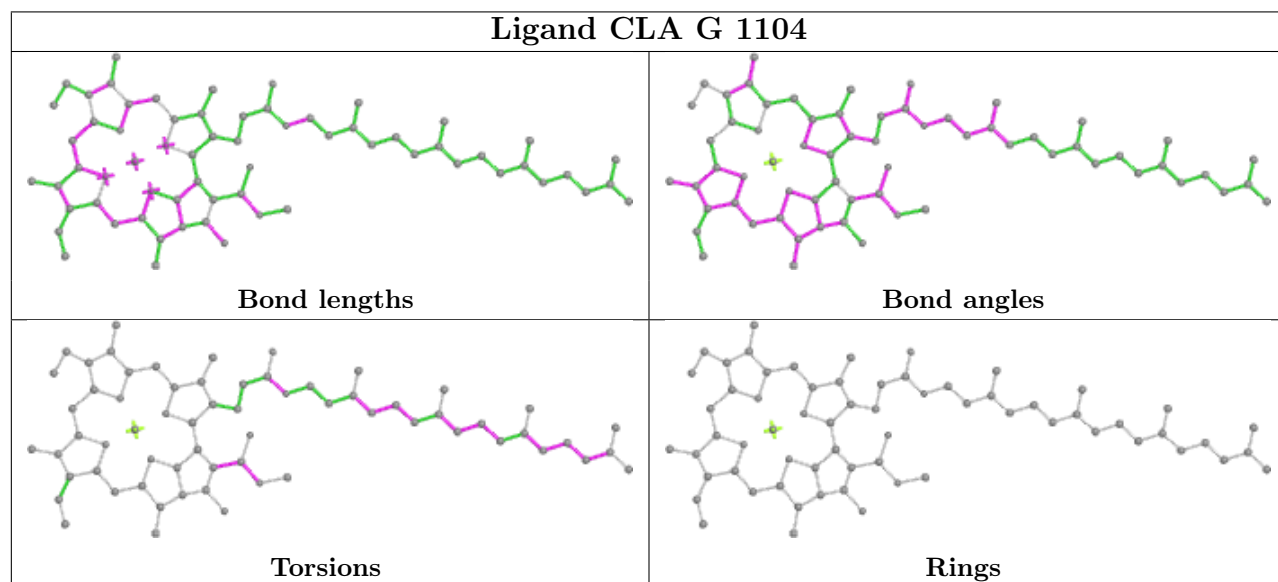
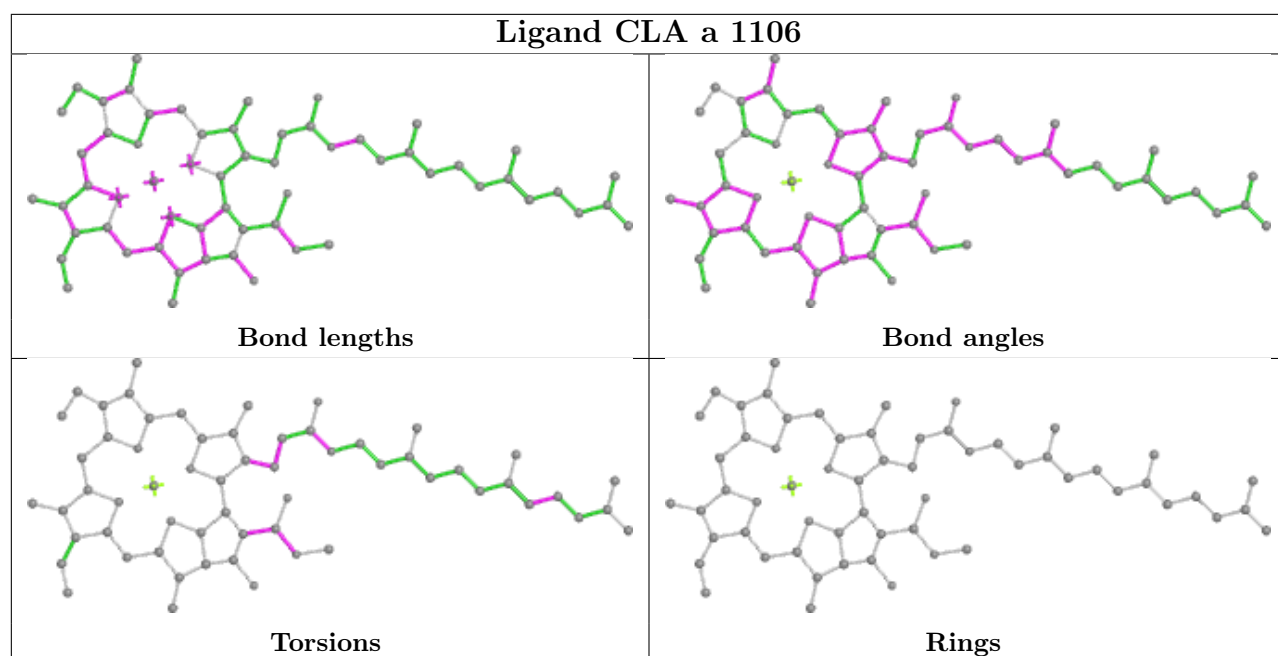
Ligand LMT a 6001

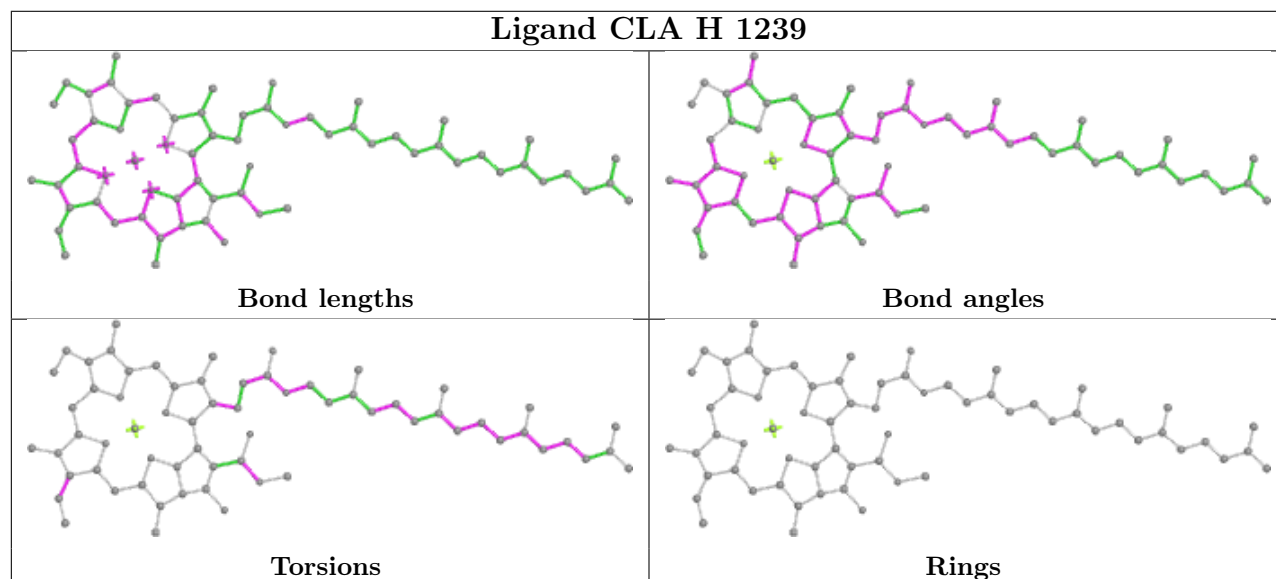
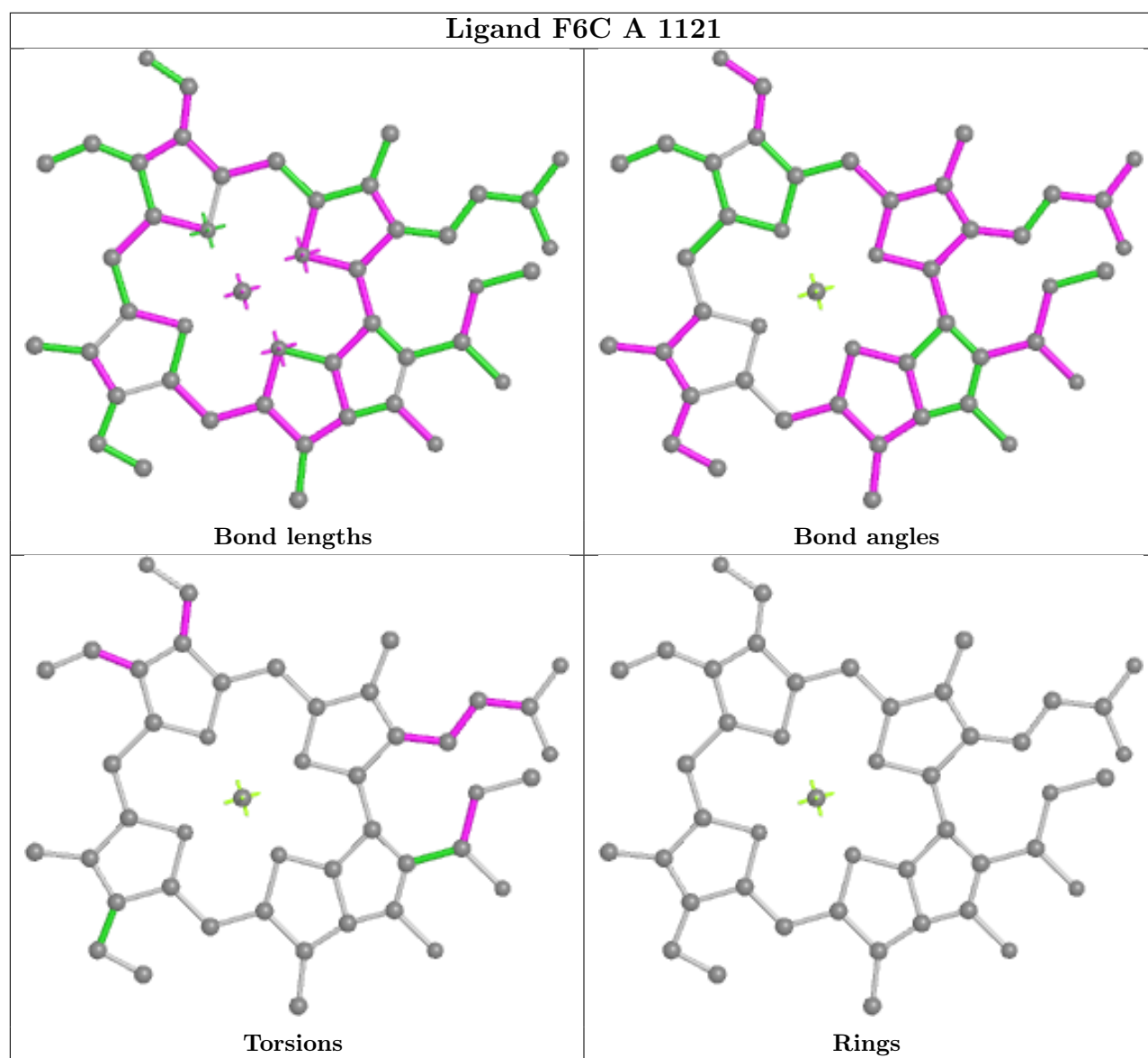


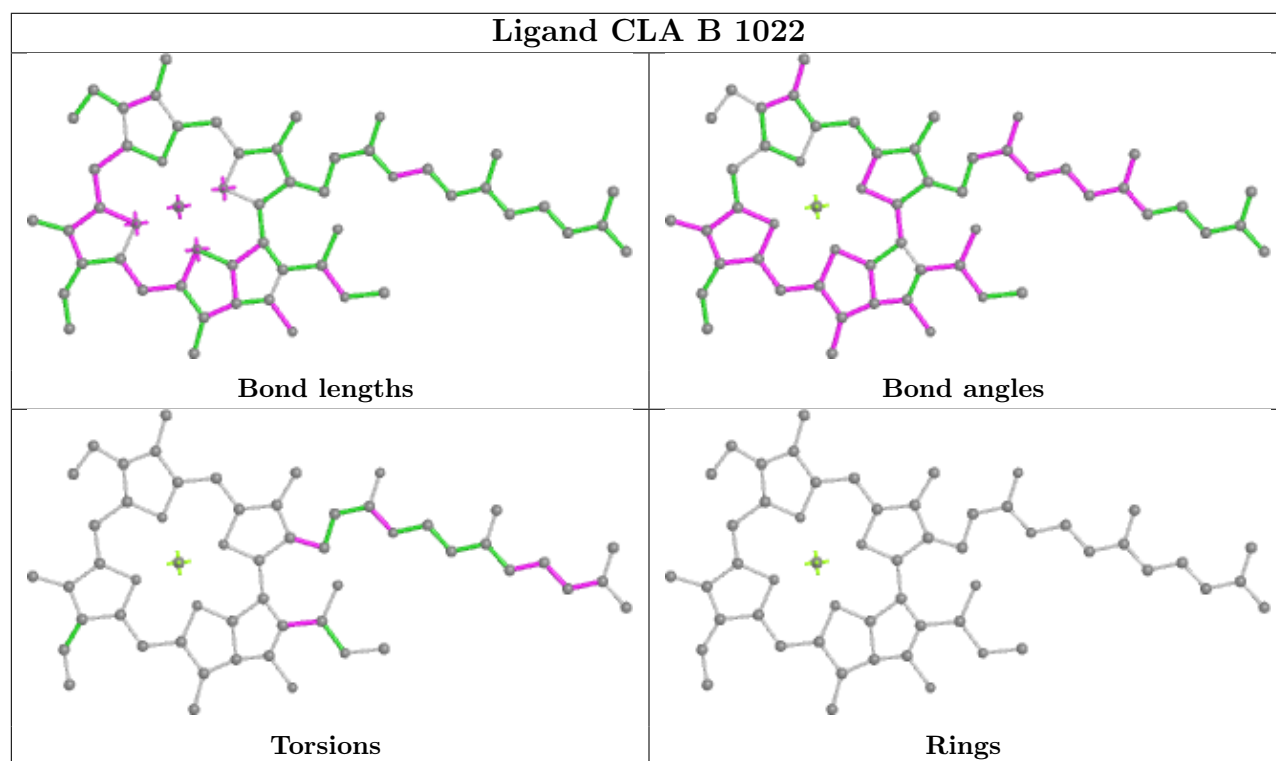
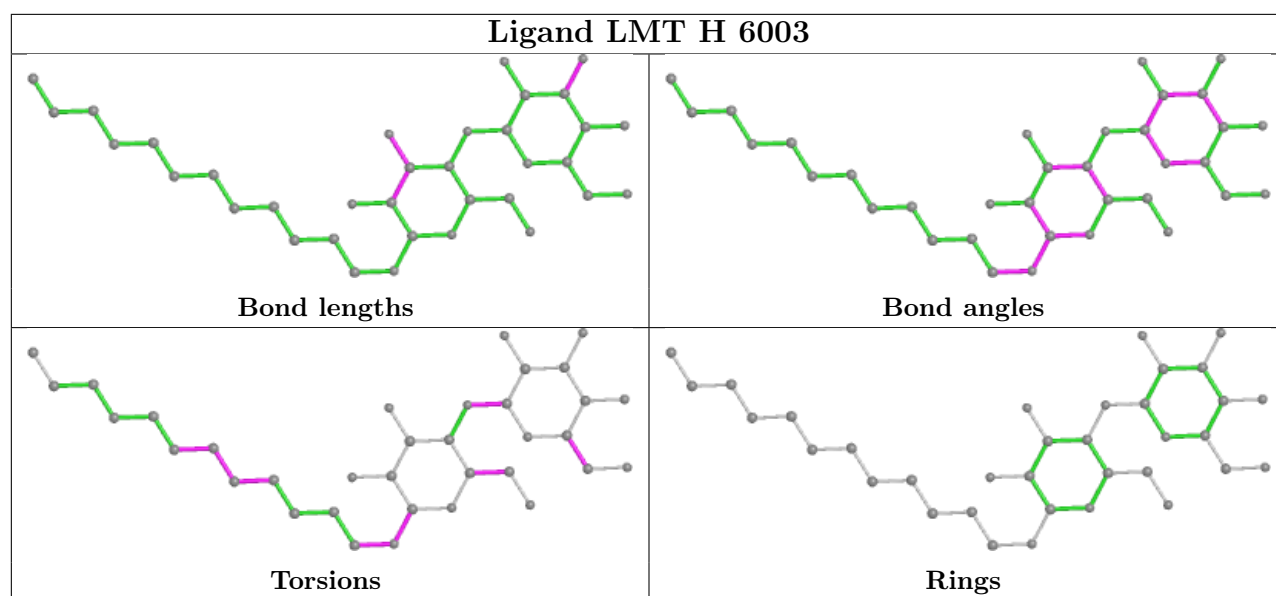


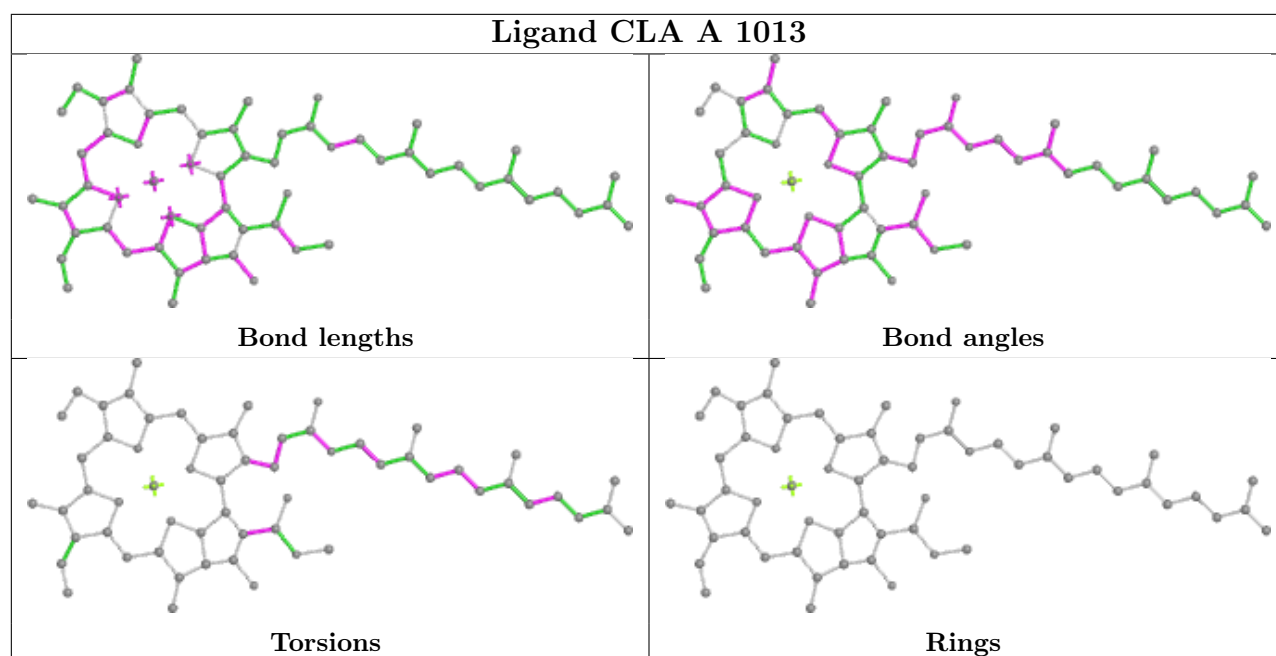
Ligand CLA U 1503**Ligand CLA I 1502**











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

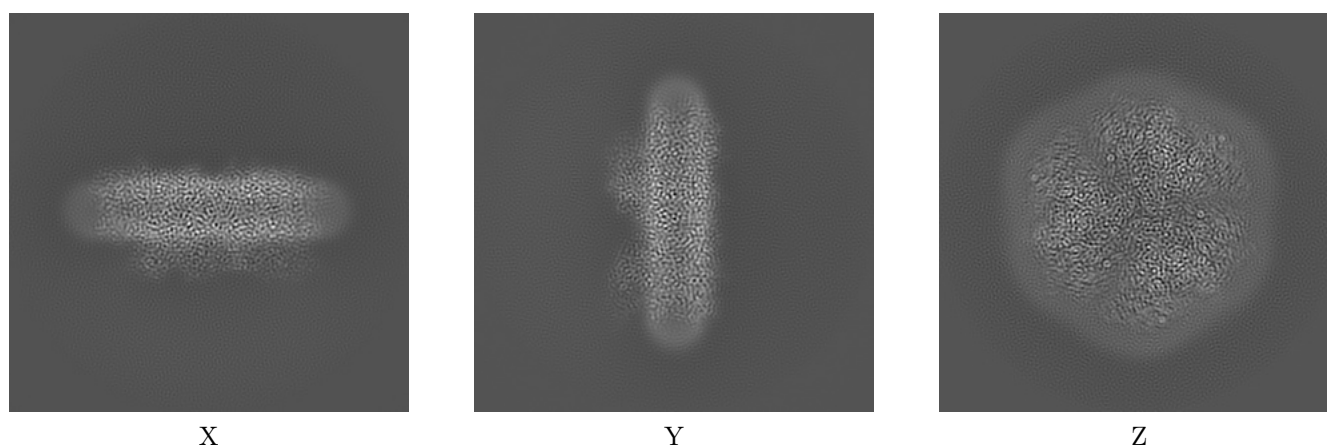
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24821. 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](#)

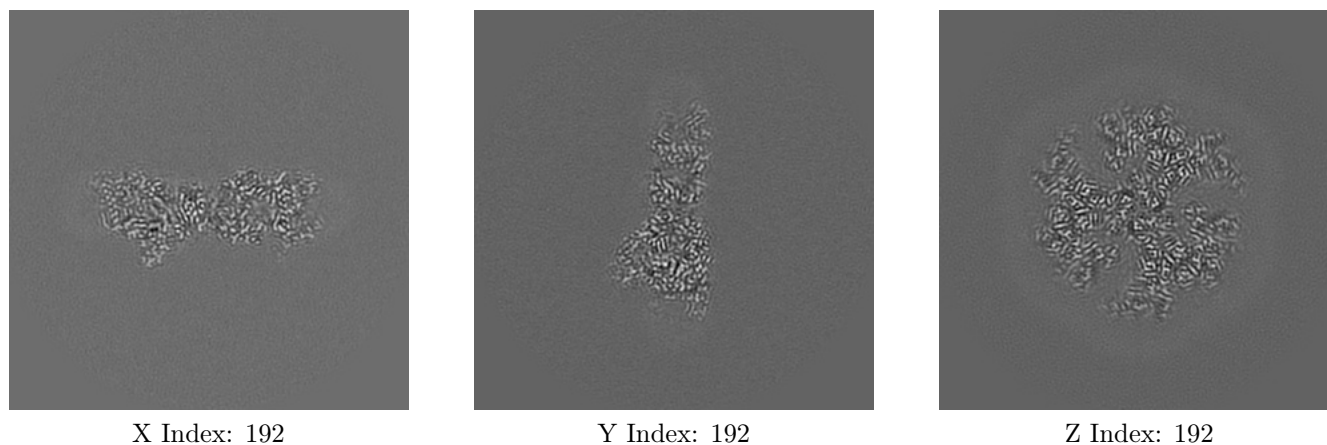
6.1.1 Primary map



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

6.2 Central slices [i](#)

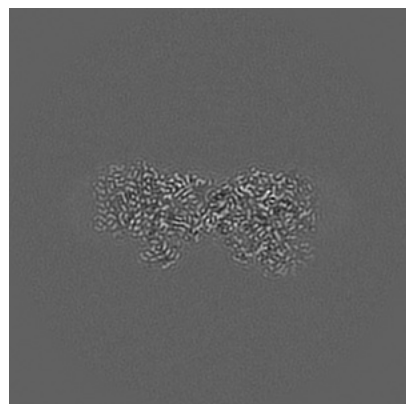
6.2.1 Primary map



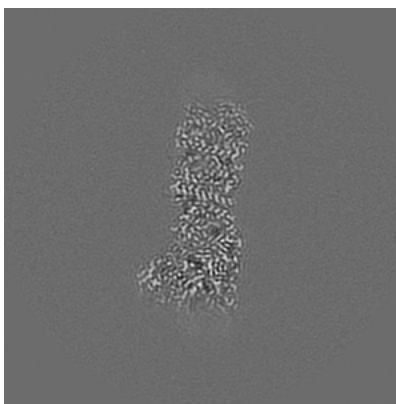
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

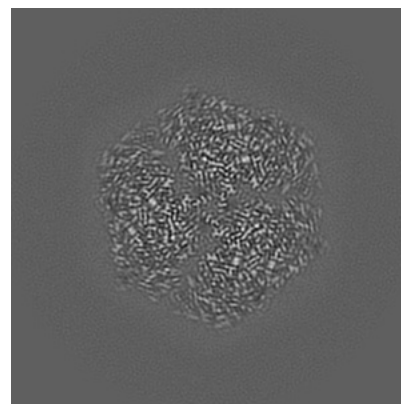
6.3.1 Primary map



X Index: 212



Y Index: 180

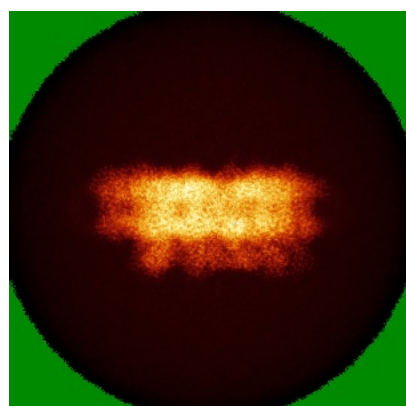


Z Index: 212

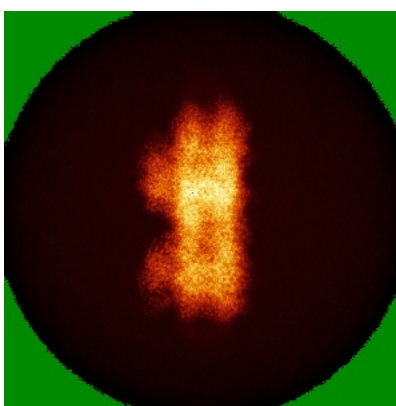
The images above show the largest variance slices of the map in three orthogonal directions.

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

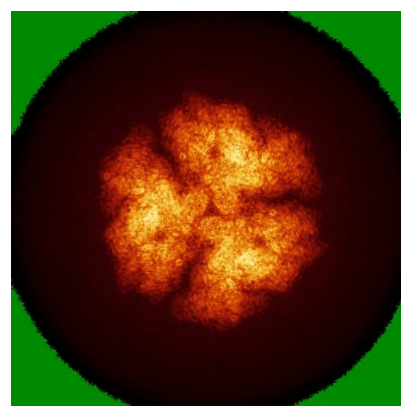
6.4.1 Primary map



X



Y

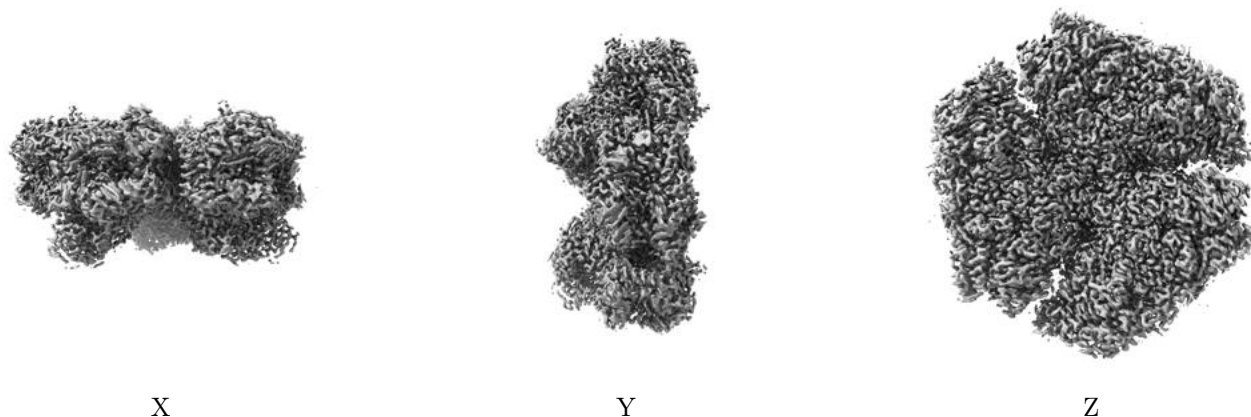


Z

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 0.0302. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

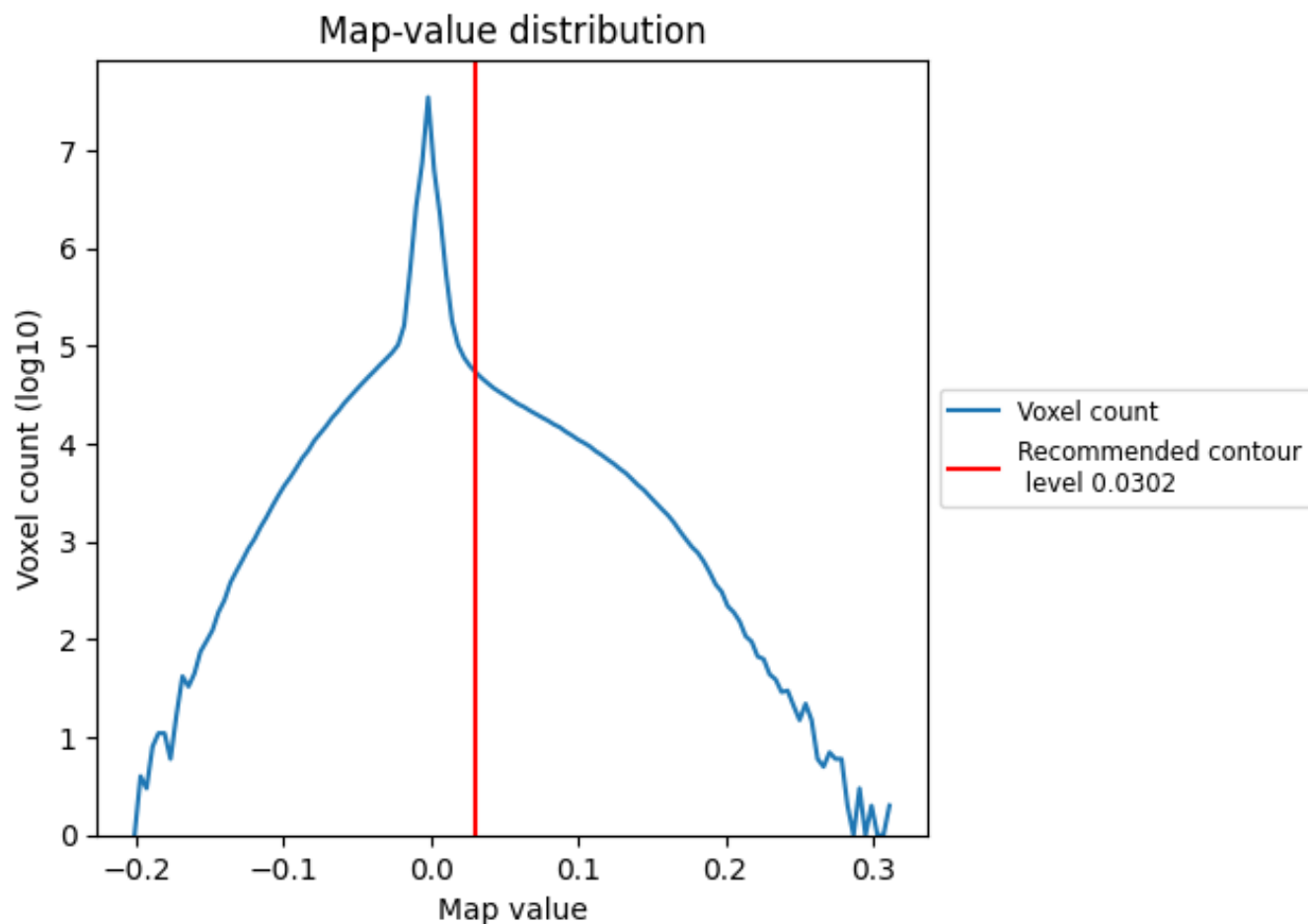
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

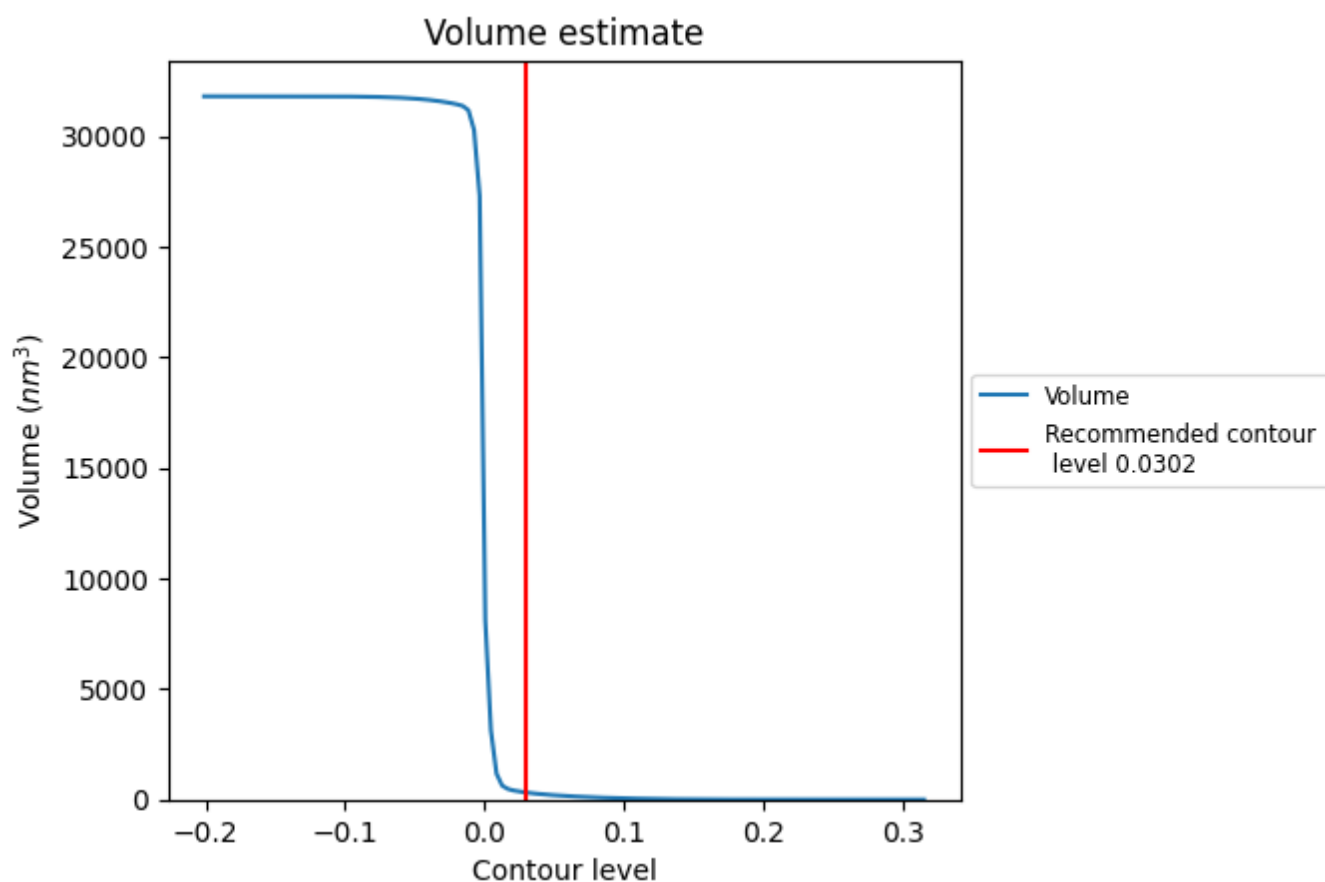
This section contains the results of statistical analysis of the map.

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.

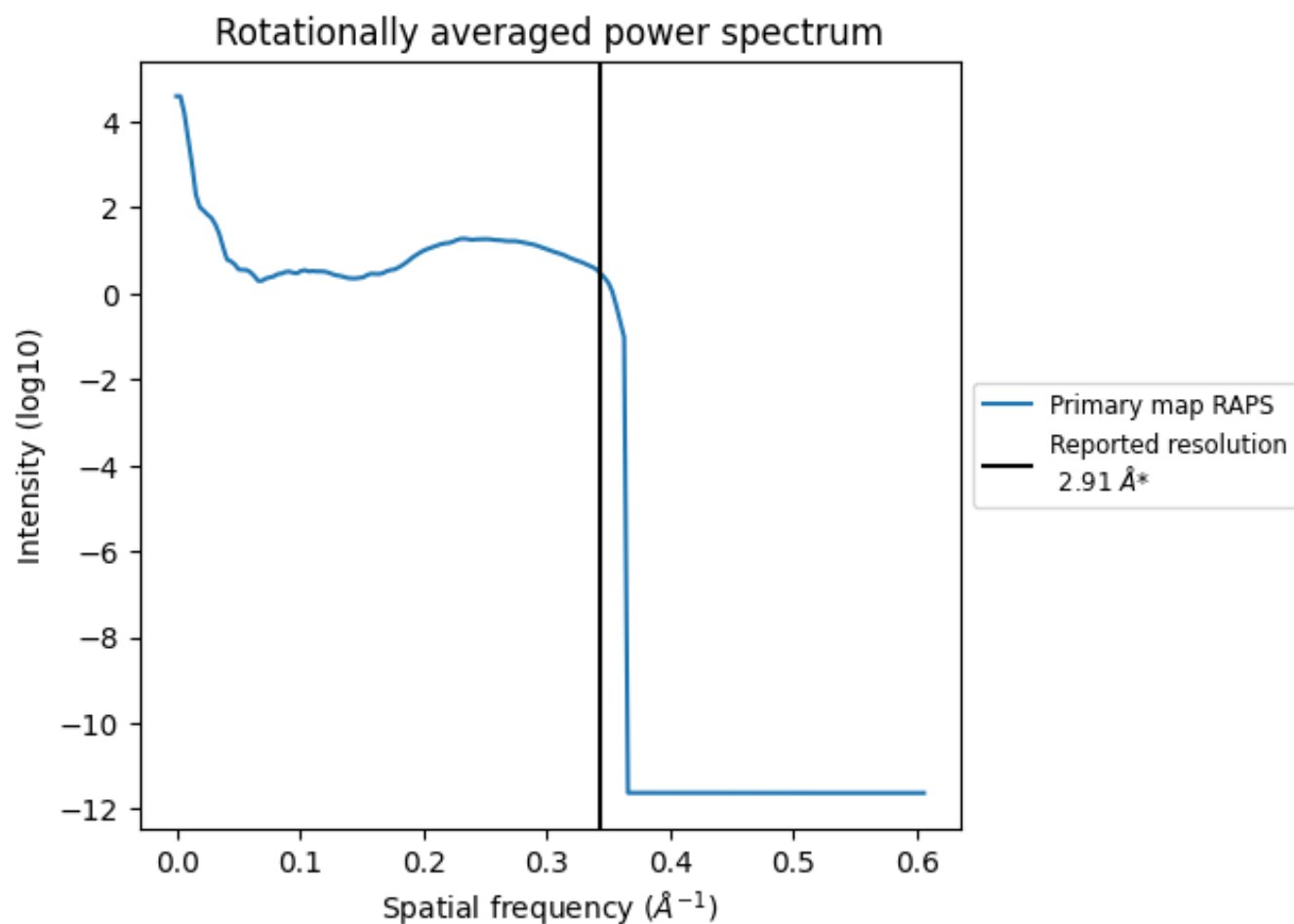
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 317 nm^3 ; this corresponds to an approximate mass of 286 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 ⓘ

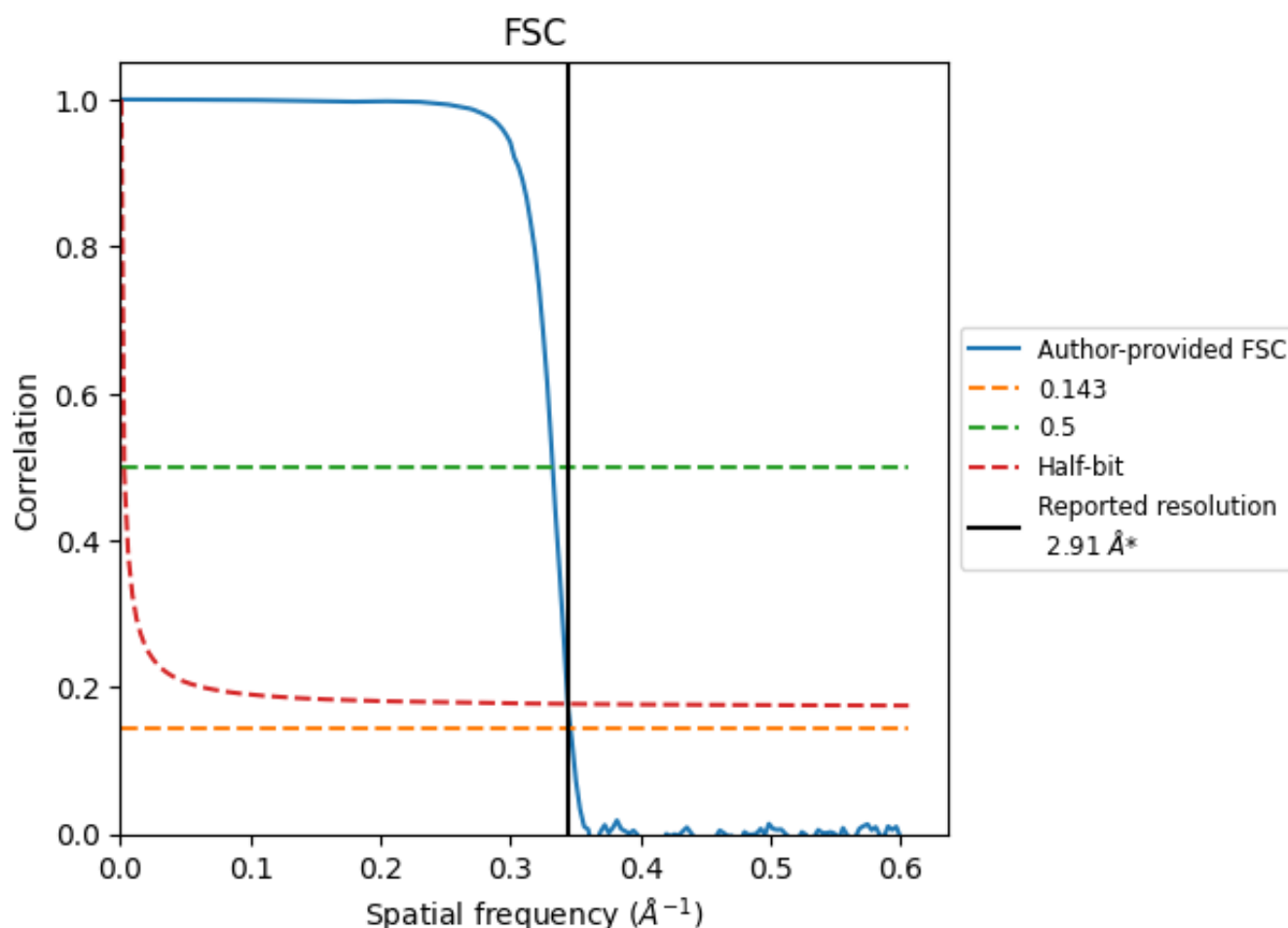


*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

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 0.344 Å⁻¹

8.2 Resolution estimates [i](#)

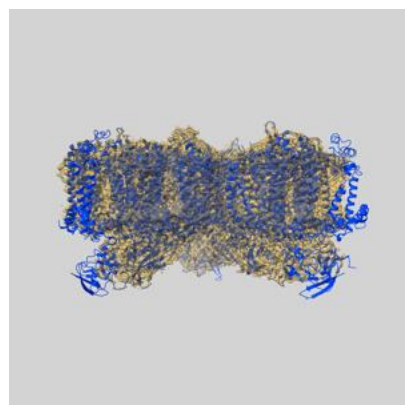
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.89	3.01	2.91
Unmasked-calculated*	-	-	-

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

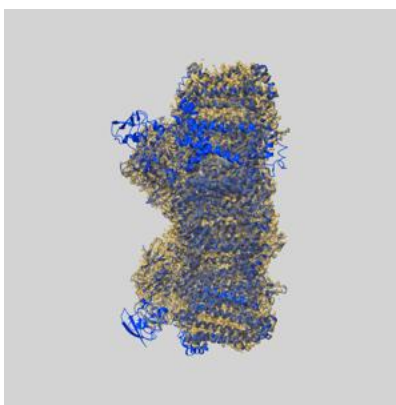
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24821 and PDB model 7S3D. Per-residue inclusion information can be found in [section 3](#) on [page 40](#).

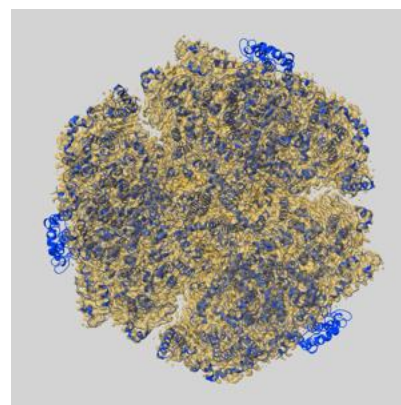
9.1 Map-model overlay [i](#)



X



Y



Z

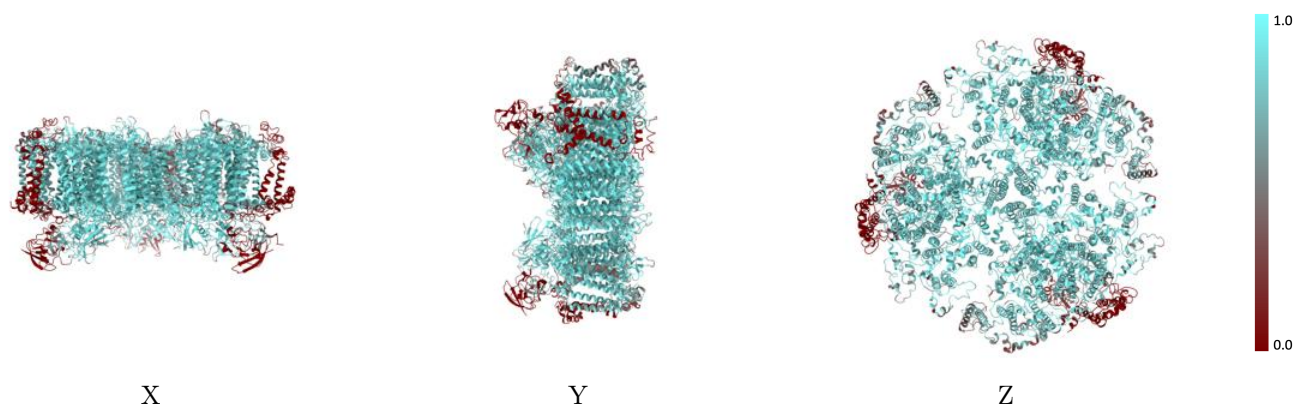
The images above show the 3D surface view of the map at the recommended contour level 0.0302 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



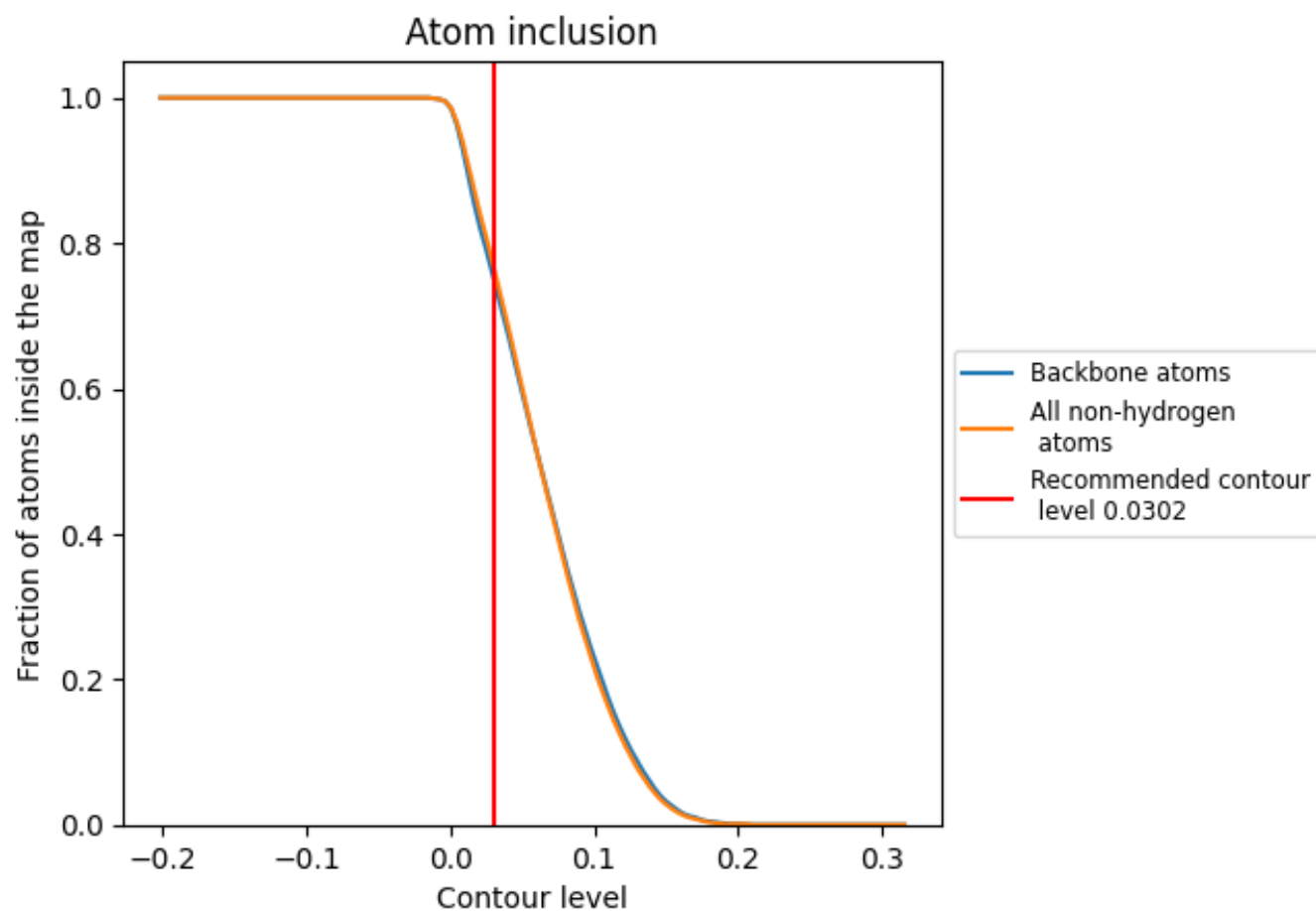
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0302).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 77% 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 (0.0302) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7670	 0.5990
A	 0.8190	 0.6180
B	 0.8490	 0.6180
C	 0.9230	 0.6330
D	 0.7650	 0.5910
E	 0.5790	 0.5940
F	 0.0060	 0.4060
G	 0.8200	 0.6180
H	 0.8490	 0.6180
I	 0.8910	 0.6310
J	 0.0070	 0.4470
K	 0.4810	 0.5480
L	 0.9190	 0.6310
M	 0.8230	 0.6080
N	 0.9150	 0.6340
O	 0.7600	 0.5920
P	 0.5810	 0.5900
Q	 0.0050	 0.4060
R	 0.8970	 0.6320
S	 0.0070	 0.4420
T	 0.4760	 0.5470
U	 0.9190	 0.6310
V	 0.8200	 0.6090
W	 0.0000	 0.3220
X	 0.0020	 0.3220
a	 0.8210	 0.6180
b	 0.8490	 0.6160
c	 0.9210	 0.6320
d	 0.7640	 0.5910
e	 0.5710	 0.5880
f	 0.0050	 0.4080
i	 0.8950	 0.6300
j	 0.0070	 0.4380
k	 0.4830	 0.5460
l	 0.9170	 0.6310



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Chain	Atom inclusion	Q-score
m	 0.8290	 0.6040
x	 0.0020	 0.3230