



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:01 PM UTC

PDB ID : 7S3D / pdb_00007s3d
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:

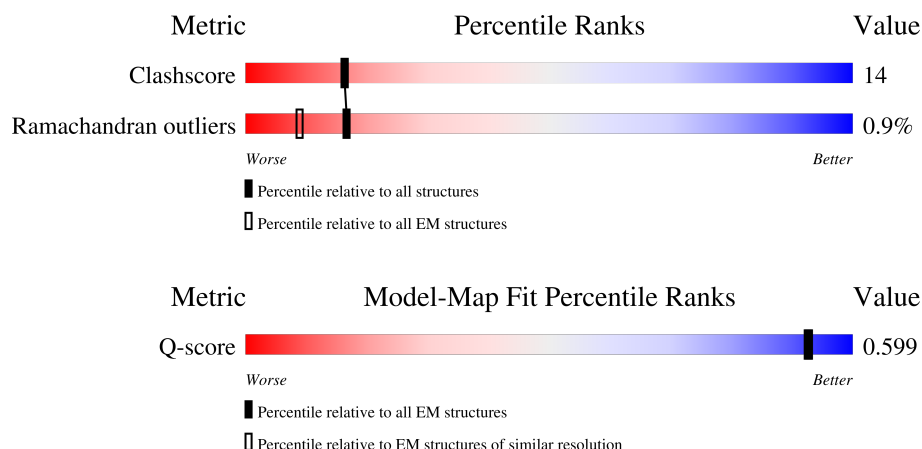
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.91 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.



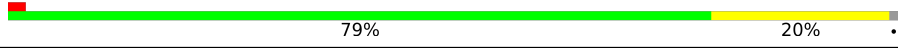
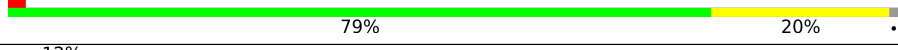
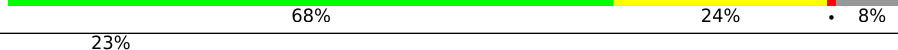
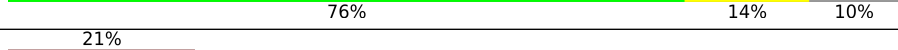
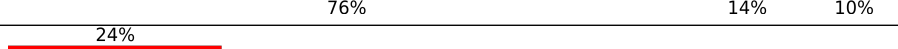
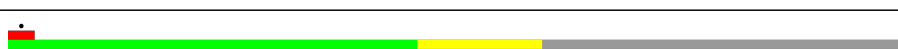
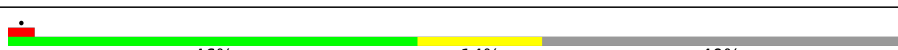
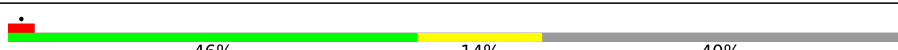
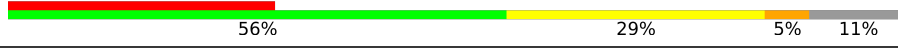
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	12972 (2.41 - 3.41)

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	 9% 71% 24% .
1	G	782	 9% 71% 24% .
1	a	782	 8% 70% 25% .
2	B	743	 78% 22%
2	H	743	 78% 22%

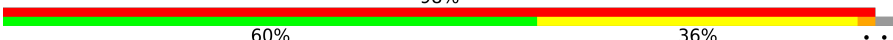
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Mol	Chain	Length	Quality of chain
2	b	743	
3	C	81	
3	N	81	
3	c	81	
4	D	155	
4	O	155	
4	d	155	
5	E	71	
5	P	71	
5	e	71	
6	F	168	
6	Q	168	
6	f	168	
7	I	70	
7	R	70	
7	i	70	
8	J	46	
8	S	46	
8	j	46	
9	K	84	
9	T	84	
9	k	84	
10	L	174	
10	U	174	
10	l	174	

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Mol	Chain	Length	Quality of chain
11	M	31	 77% 23%
11	V	31	 77% 23%
11	m	31	 77% 23%
12	W	99	 98% 60% 36% ..
12	X	99	 98% 60% 36% ..
12	x	99	 98% 60% 36% ..

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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	1124	X	-	-	-
14	CLA	A	1125	X	-	-	-
14	CLA	A	1126	X	-	-	-
14	CLA	A	1127	X	-	-	-
14	CLA	A	1128	X	-	-	-
14	CLA	A	1129	X	-	-	-
14	CLA	A	1130	X	-	-	-
14	CLA	A	1131	X	-	-	-
14	CLA	A	1132	X	-	-	-
14	CLA	A	1133	X	-	-	-
14	CLA	A	1134	X	-	-	-
14	CLA	A	1135	X	-	-	-
14	CLA	A	1136	X	-	-	-
14	CLA	A	1137	X	-	-	-
14	CLA	A	1138	X	-	-	-
14	CLA	A	1139	X	-	-	-
14	CLA	A	1140	X	-	-	-
14	CLA	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	1224	X	-	-	-
14	CLA	B	1225	X	-	-	-
14	CLA	B	1226	X	-	-	-
14	CLA	B	1227	X	-	-	-
14	CLA	B	1228	X	-	-	-
14	CLA	B	1229	X	-	-	-
14	CLA	B	1231	X	-	-	-
14	CLA	B	1232	X	-	-	-
14	CLA	B	1233	X	-	-	-
14	CLA	B	1234	X	-	-	-
14	CLA	B	1235	X	-	-	-
14	CLA	B	1236	X	-	-	-
14	CLA	B	1239	X	-	-	-
14	CLA	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	G	1128	X	-	-	-
14	CLA	G	1129	X	-	-	-
14	CLA	G	1130	X	-	-	-
14	CLA	G	1131	X	-	-	-
14	CLA	G	1132	X	-	-	-
14	CLA	G	1133	X	-	-	-
14	CLA	G	1134	X	-	-	-
14	CLA	G	1135	X	-	-	-
14	CLA	G	1136	X	-	-	-
14	CLA	G	1137	X	-	-	-
14	CLA	G	1138	X	-	-	-
14	CLA	G	1139	X	-	-	-
14	CLA	G	1140	X	-	-	-
14	CLA	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	H	1228	X	-	-	-
14	CLA	H	1229	X	-	-	-
14	CLA	H	1231	X	-	-	-
14	CLA	H	1232	X	-	-	-
14	CLA	H	1233	X	-	-	-
14	CLA	H	1234	X	-	-	-
14	CLA	H	1235	X	-	-	-
14	CLA	H	1236	X	-	-	-
14	CLA	H	1239	X	-	-	-
14	CLA	H	1240	X	-	-	-
14	CLA	K	1401	X	-	-	-
14	CLA	L	1501	X	-	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	-	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	1122	X	-	-	-
14	CLA	a	1123	X	-	-	-
14	CLA	a	1124	X	-	-	-
14	CLA	a	1125	X	-	-	-
14	CLA	a	1126	X	-	-	-
14	CLA	a	1127	X	-	-	-
14	CLA	a	1128	X	-	-	-
14	CLA	a	1129	X	-	-	-
14	CLA	a	1130	X	-	-	-
14	CLA	a	1131	X	-	-	-
14	CLA	a	1132	X	-	-	-
14	CLA	a	1133	X	-	-	-
14	CLA	a	1134	X	-	-	-
14	CLA	a	1135	X	-	-	-
14	CLA	a	1136	X	-	-	-
14	CLA	a	1137	X	-	-	-
14	CLA	a	1138	X	-	-	-
14	CLA	a	1139	X	-	-	-
14	CLA	a	1140	X	-	-	-
14	CLA	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	1222	X	-	-	-
14	CLA	b	1223	X	-	-	-
14	CLA	b	1224	X	-	-	-
14	CLA	b	1225	X	-	-	-
14	CLA	b	1226	X	-	-	-
14	CLA	b	1227	X	-	-	-
14	CLA	b	1228	X	-	-	-
14	CLA	b	1229	X	-	-	-
14	CLA	b	1231	X	-	-	-
14	CLA	b	1232	X	-	-	-
14	CLA	b	1233	X	-	-	-
14	CLA	b	1234	X	-	-	-
14	CLA	b	1235	X	-	-	-
14	CLA	b	1236	X	-	-	-
14	CLA	b	1239	X	-	-	-
14	CLA	b	1240	X	-	-	-
14	CLA	k	1401	X	-	-	-
14	CLA	l	1501	X	-	X	-
14	CLA	l	1502	X	-	-	-
14	CLA	l	1503	X	-	-	-
14	CLA	m	1501	X	-	-	-
15	F6C	A	1121	X	-	-	-
15	F6C	B	1207	X	-	-	-
15	F6C	B	1219	X	-	-	-
15	F6C	B	1230	X	-	-	-
15	F6C	B	1237	X	-	-	-
15	F6C	B	1238	X	-	-	-
15	F6C	G	1121	X	-	-	-
15	F6C	H	1207	X	-	-	-
15	F6C	H	1219	X	-	-	-
15	F6C	H	1230	X	-	-	-
15	F6C	H	1237	X	-	-	-
15	F6C	H	1238	X	-	-	-
15	F6C	a	1121	X	-	-	-
15	F6C	b	1207	X	-	-	-
15	F6C	b	1219	X	-	-	-
15	F6C	b	1230	X	-	-	-
15	F6C	b	1237	X	-	-	-
15	F6C	b	1238	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		

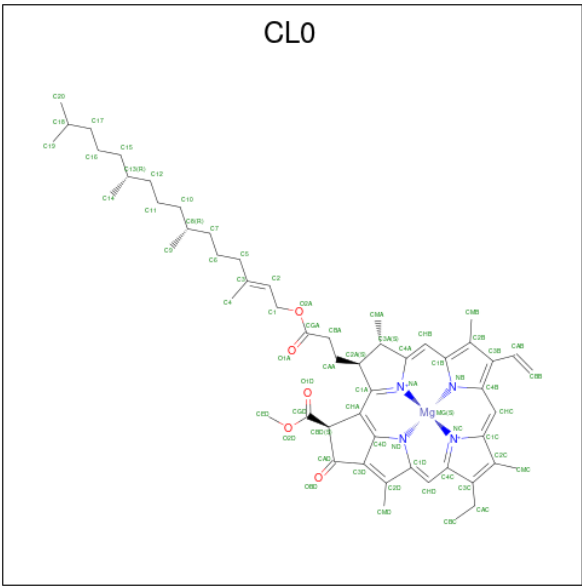
- Molecule 11 is a protein called Psam.

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.

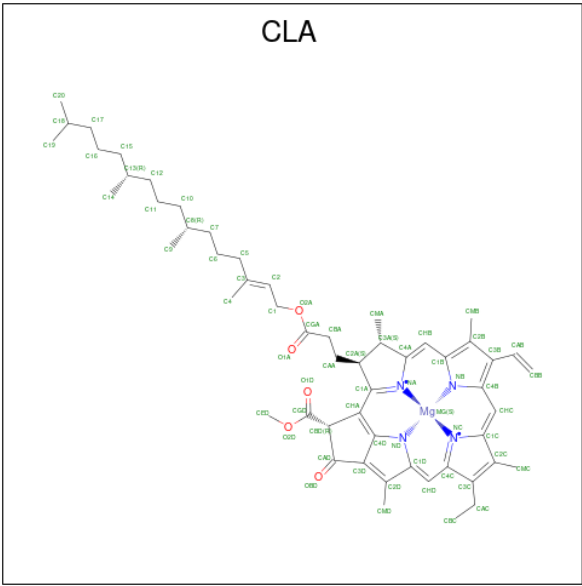
Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	97	Total	C	N	O	S	0	0
			649	405	107	132	5		
12	W	97	Total	C	N	O	S	0	0
			649	405	107	132	5		
12	x	97	Total	C	N	O	S	0	0
			649	405	107	132	5		

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



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

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



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

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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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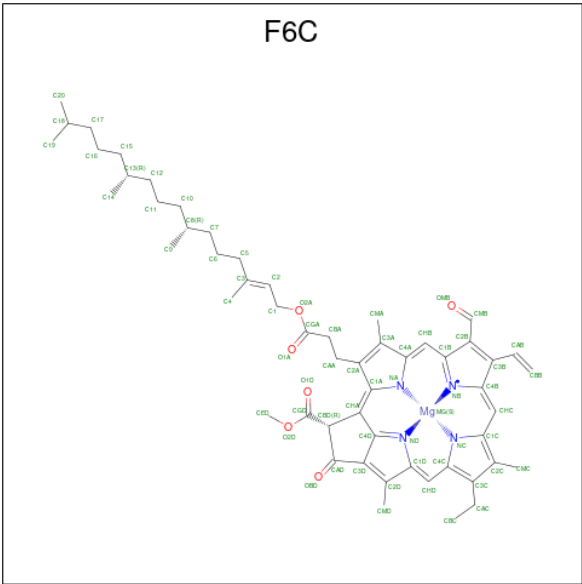
Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 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 (CCD ID: F6C) (formula: C₅₅H₆₈MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



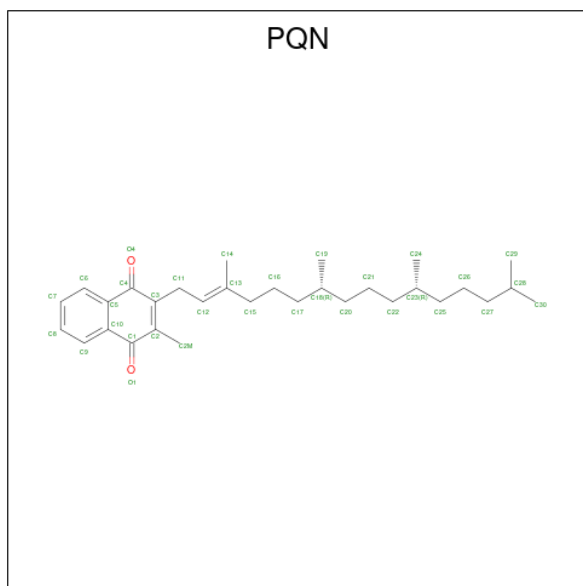
Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

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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 (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



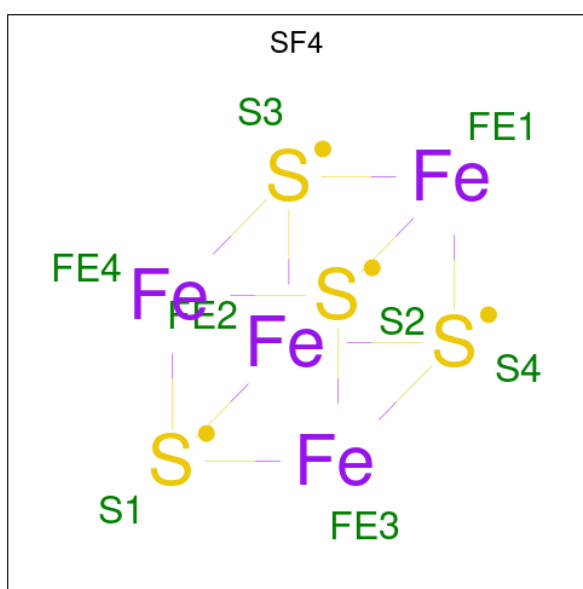
Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	C	O	0
			33	31	2	
16	B	1	Total	C	O	0
			33	31	2	

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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 (CCD ID: SF4) (formula: Fe_4S_4).



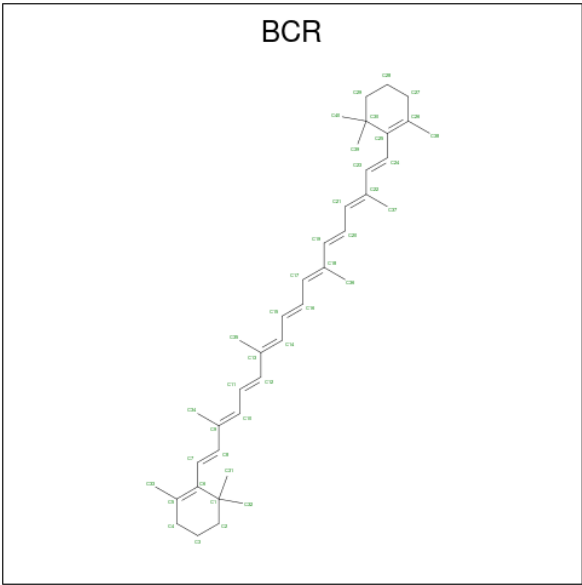
Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	Fe	S	0
			8	4	4	
17	C	1	Total	Fe	S	0
			8	4	4	
17	C	1	Total	Fe	S	0
			8	4	4	
17	G	1	Total	Fe	S	0
			8	4	4	
17	N	1	Total	Fe	S	0
			8	4	4	
17	N	1	Total	Fe	S	0
			8	4	4	
17	a	1	Total	Fe	S	0
			8	4	4	

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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 (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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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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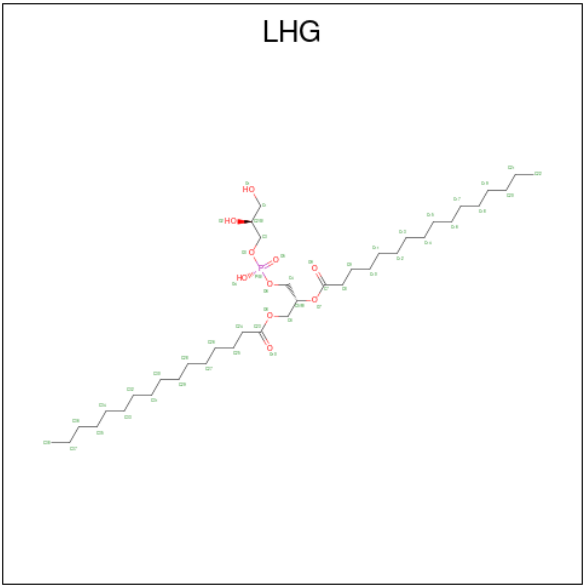
Mol	Chain	Residues	Atoms	AltConf
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	R	1	Total C 40 40	0
18	R	1	Total C 40 40	0
18	T	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	V	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 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 (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



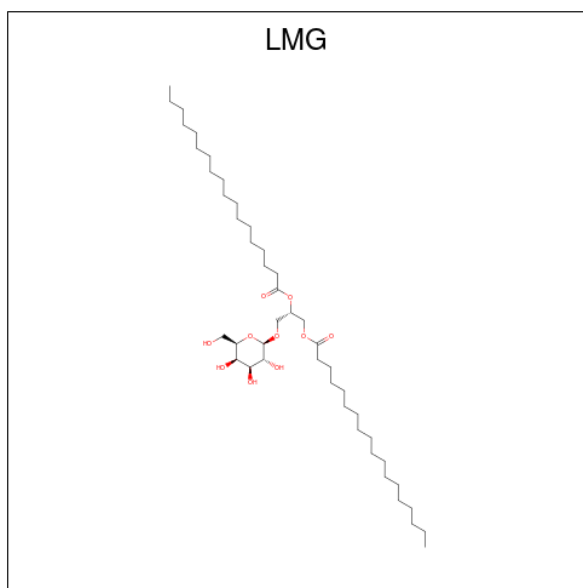
Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C O P 42 31 10 1	0
19	A	1	Total C O P 44 35 8 1	0
19	L	1	Total C O 25 20 5	0
19	L	1	Total C O P 49 38 10 1	0
19	G	1	Total C O P 42 31 10 1	0

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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 (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



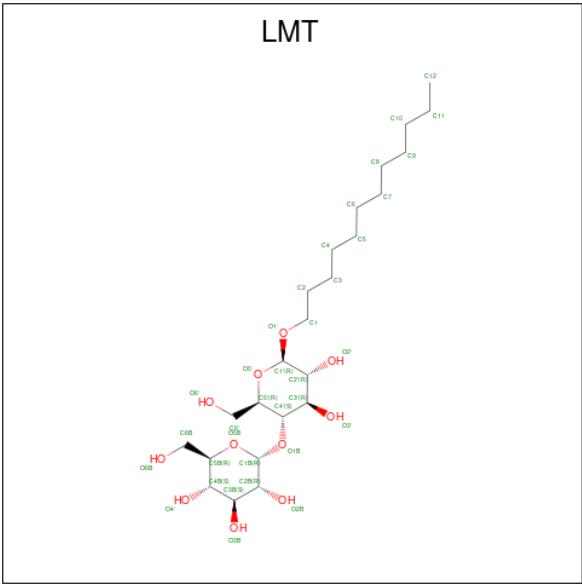
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O		0
			46	36	10		
20	B	1	Total	C	O		0
			46	36	10		
20	I	1	Total	C	O		0
			37	27	10		
20	G	1	Total	C	O		0
			46	36	10		

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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 (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

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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 (CCD ID: 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 (CCD ID: CA) (formula: Ca).

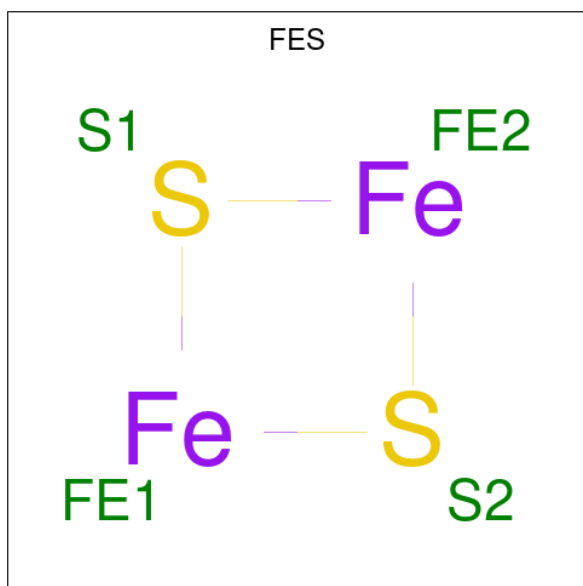
Mol	Chain	Residues	Atoms		AltConf
23	L	1	Total	Ca	0
			1	1	
23	U	1	Total	Ca	0
			1	1	

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

- Molecule 24 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: 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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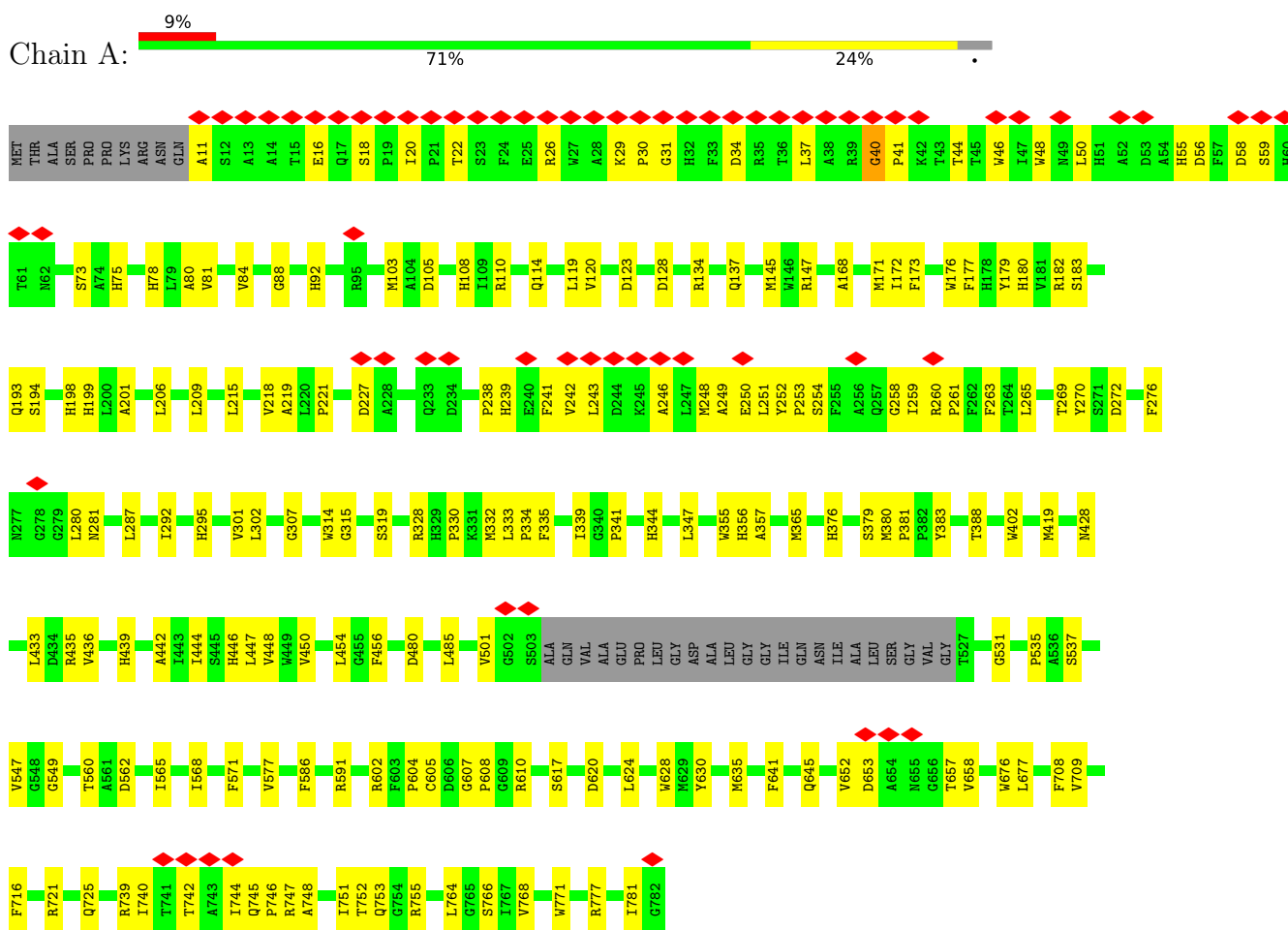
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Mol	Chain	Residues	Atoms		AltConf
25	L	15	Total 15	O 15	0
25	G	35	Total 35	O 35	0
25	H	35	Total 35	O 35	0
25	N	9	Total 9	O 9	0
25	O	13	Total 13	O 13	0
25	R	4	Total 4	O 4	0
25	U	15	Total 15	O 15	0
25	a	35	Total 35	O 35	0
25	b	35	Total 35	O 35	0
25	c	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

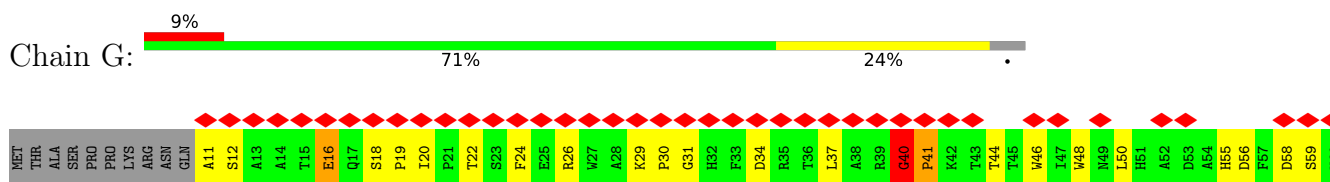
3 Residue-property plots

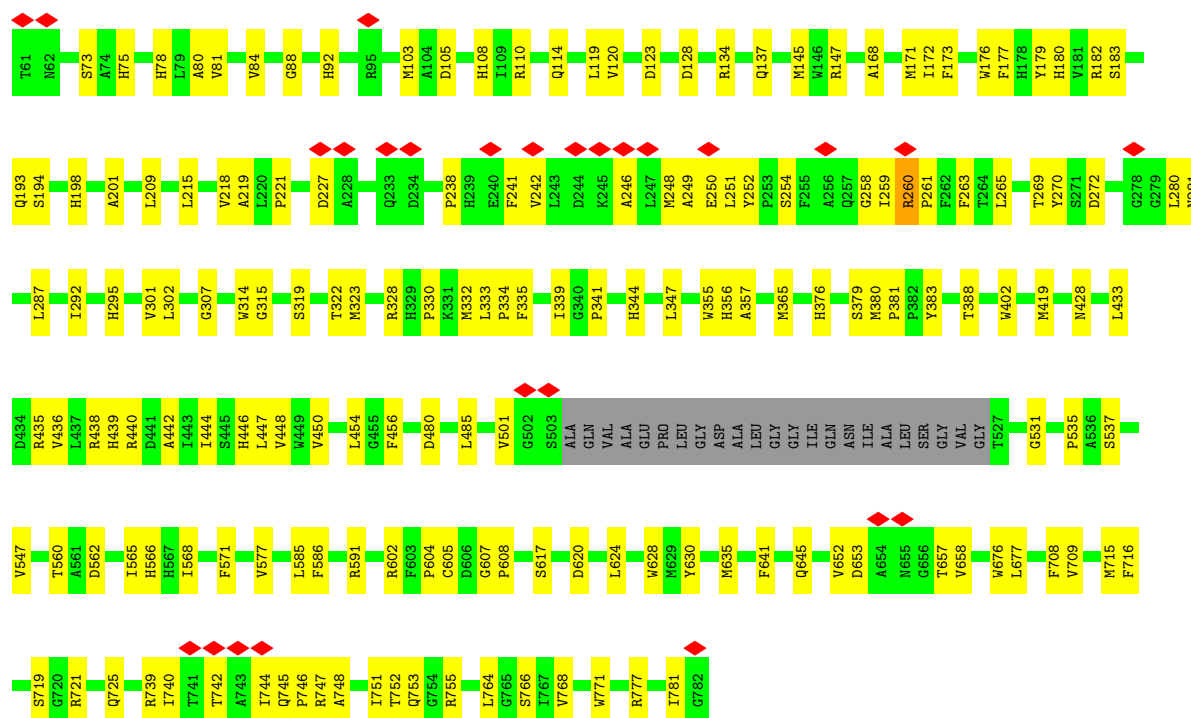
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

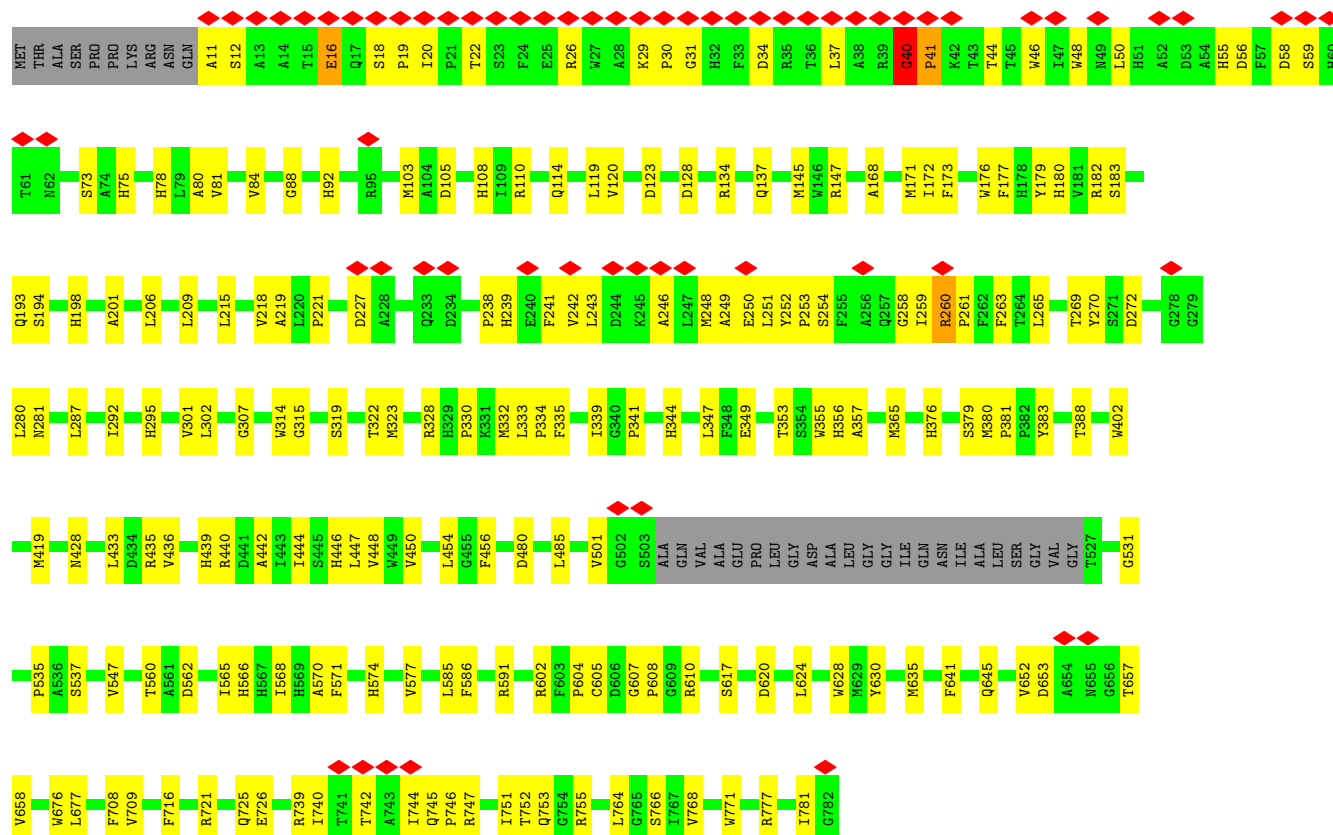


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

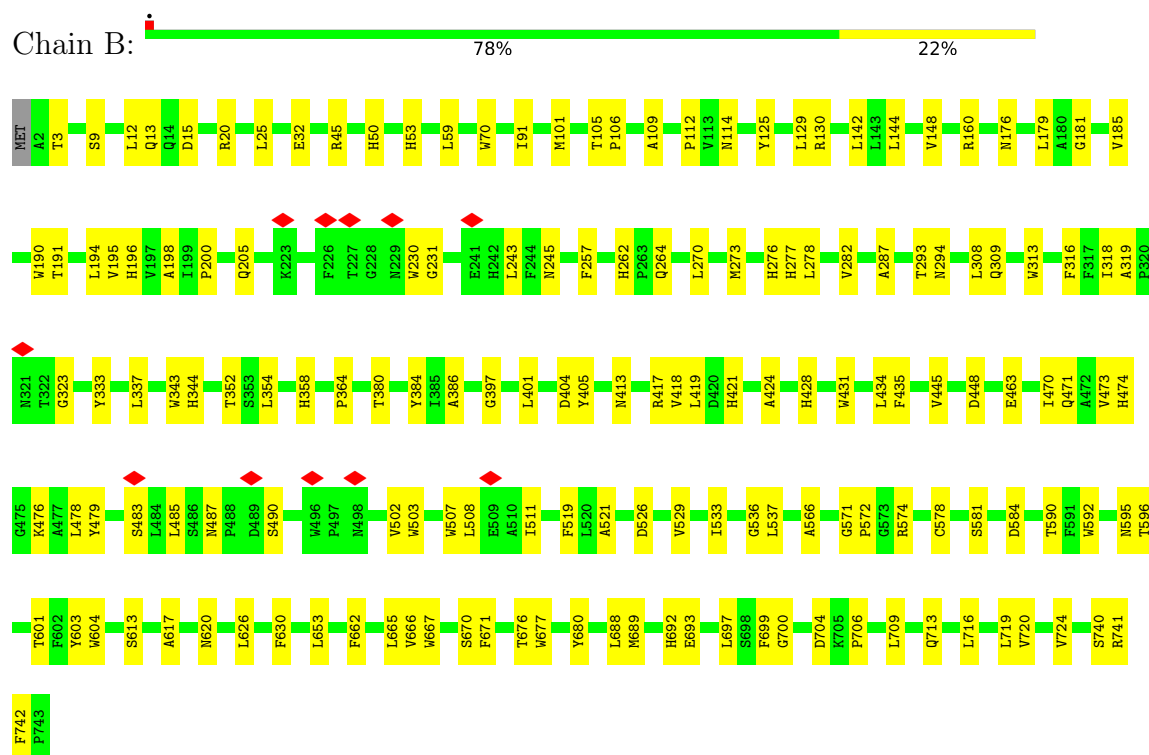




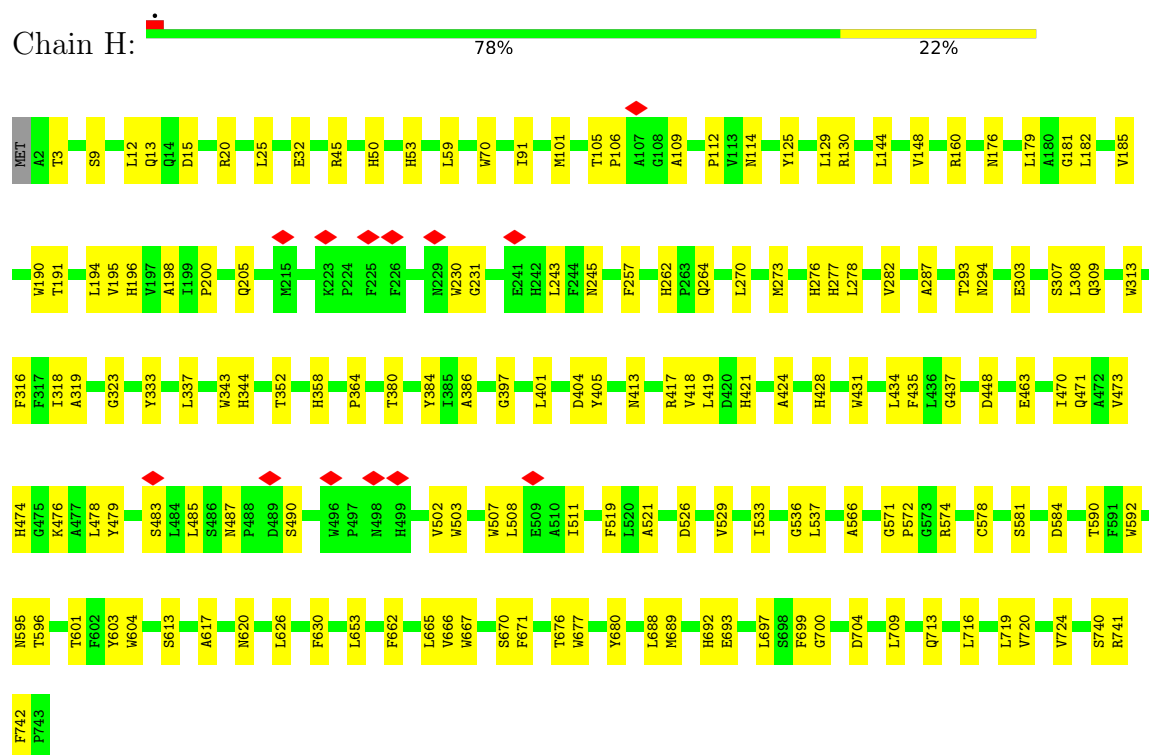
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

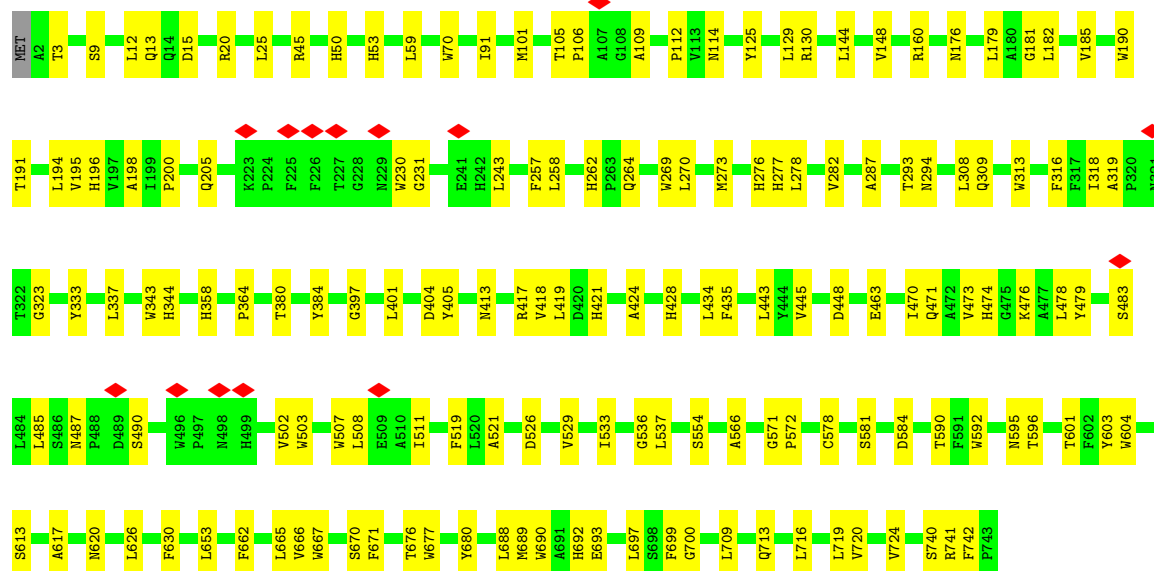


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



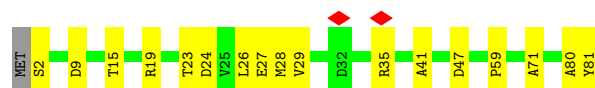
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:  79% 21%



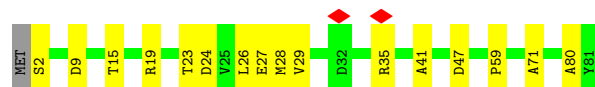
• Molecule 3: PsaC

Chain C:  78% 21%



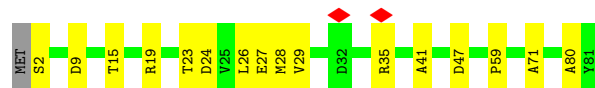
• Molecule 3: PsaC

Chain N:  79% 20%



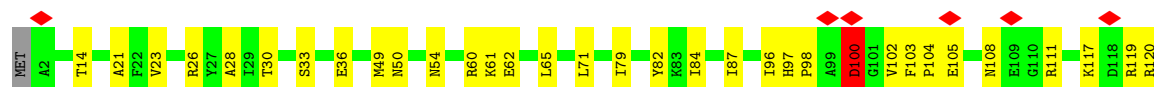
• Molecule 3: PsaC

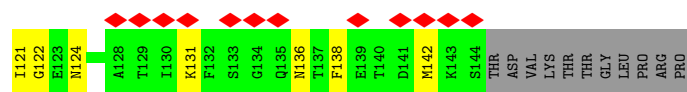
Chain c:  79% 20%



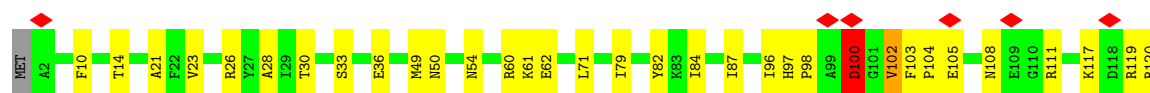
• Molecule 4: Photosystem I 16 kDa polypeptide

Chain D:  12% 66% 25% 8%

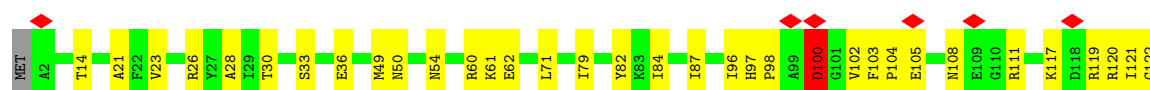




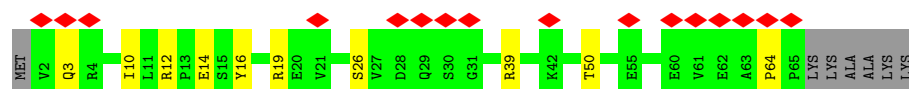
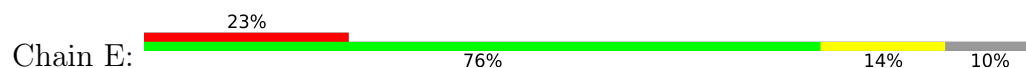
- Molecule 4: Photosystem I 16 kDa polypeptide



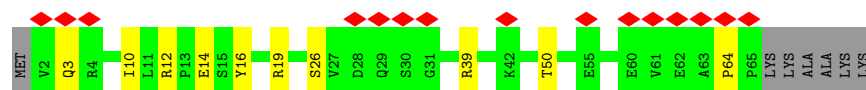
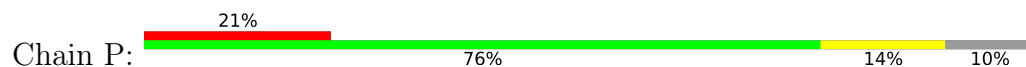
- Molecule 4: Photosystem I 16 kDa polypeptide



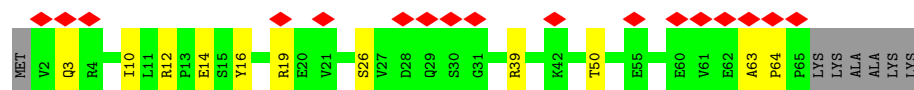
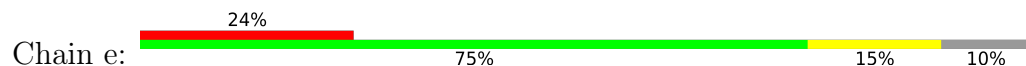
- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 5: Photosystem I reaction center subunit IV

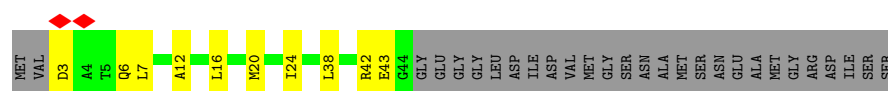


- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 6: PSI-F

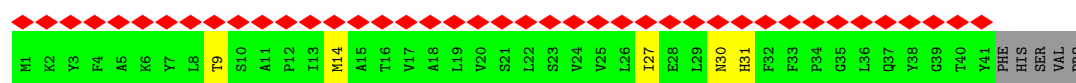
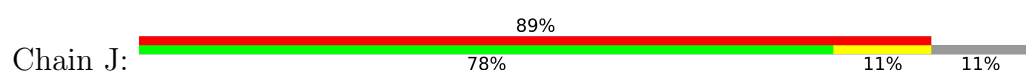




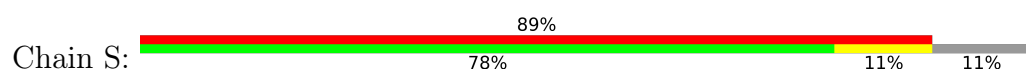
- Molecule 7: PsaI2



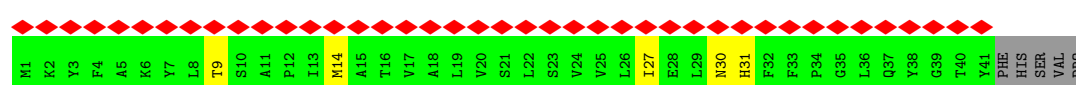
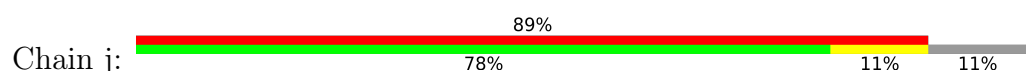
- Molecule 8: Photosystem I reaction center subunit IX



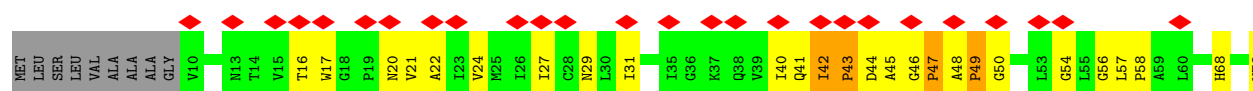
- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX

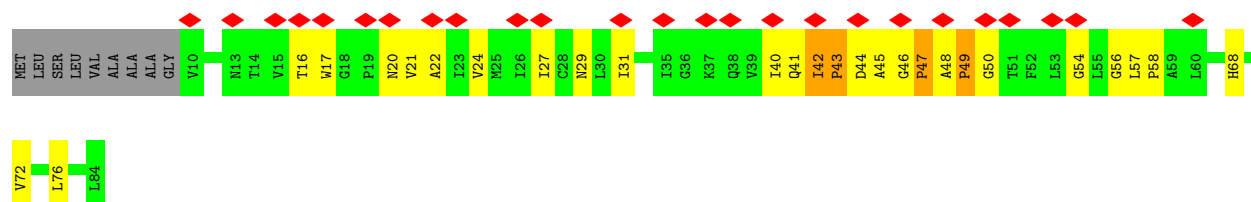


- Molecule 9: Photosystem I reaction center subunit PsaK

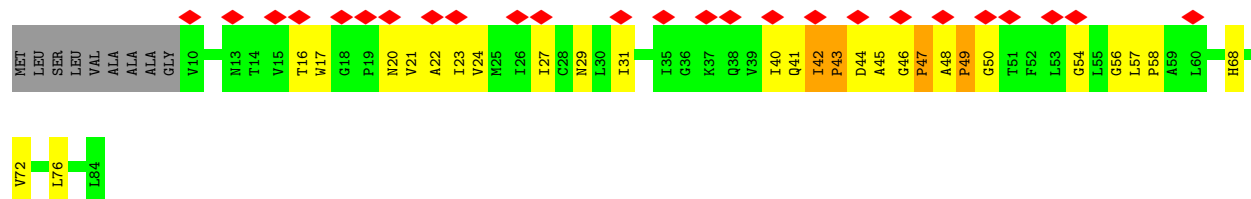


- Molecule 9: Photosystem I reaction center subunit PsaK

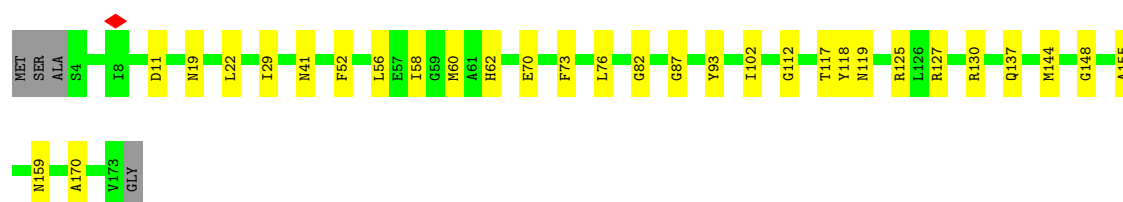
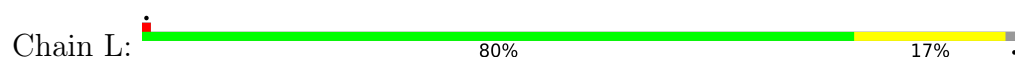




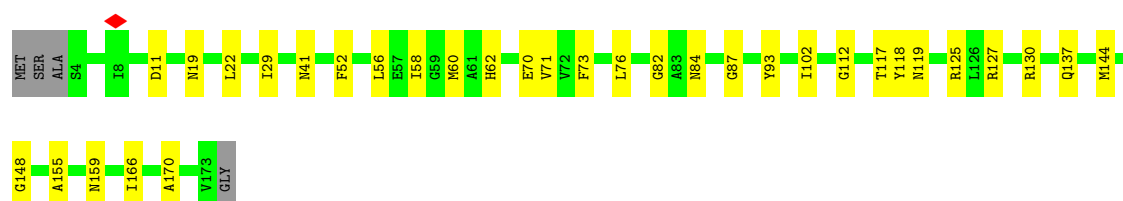
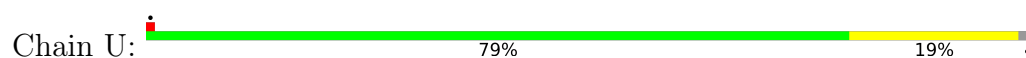
• Molecule 9: Photosystem I reaction center subunit PsaK



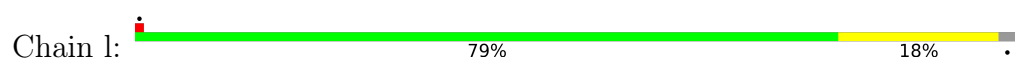
• Molecule 10: PSI subunit V



• Molecule 10: PSI subunit V



• Molecule 10: PSI subunit V



• Molecule 11: PsaM

Chain M:  77% 23%



- Molecule 11: Psam

Chain V:  77% 23%

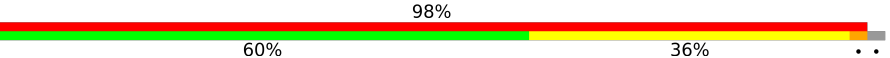


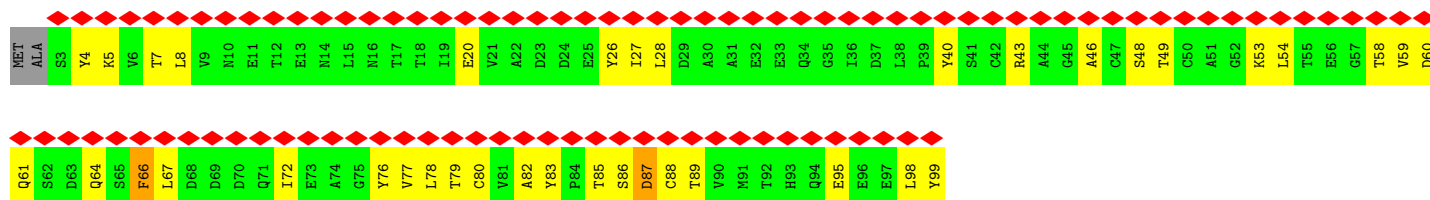
- Molecule 11: Psam

Chain m:  77% 23%

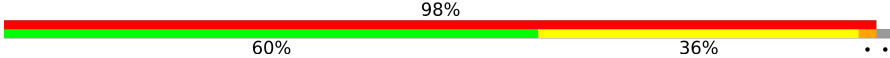


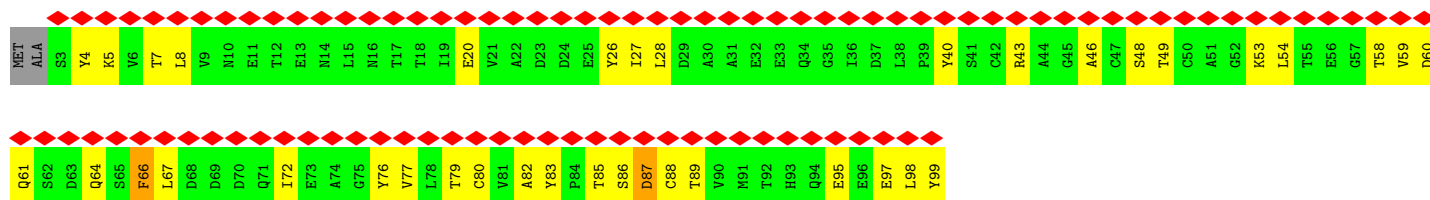
- Molecule 12: 2Fe-2S ferredoxin-type domain-containing protein

Chain X:  98% 60% 36% ..

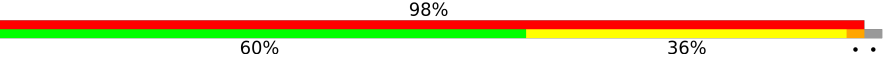


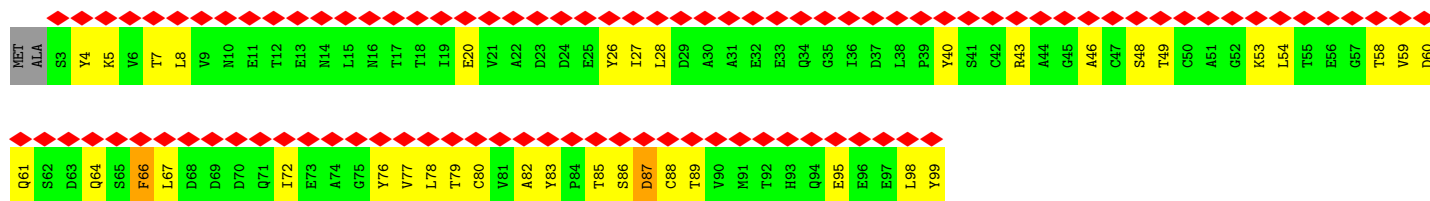
- Molecule 12: 2Fe-2S ferredoxin-type domain-containing protein

Chain W:  98% 60% 36% ..



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

Chain x:  98% 60% 36% ..



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 ($\text{\AA}$)	316.8, 316.8, 316.8	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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, F6C, CA, BCR, LMG, CL, LMT, CL0, CLA, PQN, LHG, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/6045	0.70	1/8233 (0.0%)
1	G	0.50	0/6045	0.70	1/8233 (0.0%)
1	a	0.50	0/6045	0.70	1/8233 (0.0%)
2	B	0.44	0/6124	0.65	1/8377 (0.0%)
2	H	0.44	0/6124	0.65	1/8377 (0.0%)
2	b	0.44	0/6124	0.65	1/8377 (0.0%)
3	C	0.42	0/608	0.64	0/823
3	N	0.42	0/608	0.64	0/823
3	c	0.41	0/608	0.65	0/823
4	D	0.45	0/1125	0.73	0/1515
4	O	0.45	0/1125	0.73	0/1515
4	d	0.46	0/1125	0.73	0/1515
5	E	0.29	0/517	0.51	0/702
5	P	0.29	0/517	0.51	0/702
5	e	0.29	0/517	0.51	0/702
6	F	0.33	0/847	0.74	1/1168 (0.1%)
6	Q	0.34	0/847	0.74	1/1168 (0.1%)
6	f	0.33	0/847	0.74	1/1168 (0.1%)
7	I	0.50	0/357	0.79	0/491
7	R	0.50	0/357	0.80	0/491
7	i	0.50	0/357	0.80	0/491
8	J	0.38	0/302	0.77	1/414 (0.2%)
8	S	0.38	0/302	0.77	1/414 (0.2%)
8	j	0.38	0/302	0.77	1/414 (0.2%)
9	K	0.66	0/526	1.21	2/724 (0.3%)
9	T	0.66	0/526	1.21	2/724 (0.3%)
9	k	0.66	0/526	1.21	2/724 (0.3%)
10	L	0.47	0/1322	0.64	0/1797
10	U	0.47	0/1322	0.64	0/1797
10	l	0.47	0/1322	0.64	0/1797
11	M	0.37	0/235	0.71	1/319 (0.3%)
11	V	0.37	0/235	0.70	1/319 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	m	0.37	0/235	0.71	1/319 (0.3%)
12	W	1.00	0/657	1.03	1/900 (0.1%)
12	X	1.00	0/657	1.04	1/900 (0.1%)
12	x	1.00	0/657	1.04	1/900 (0.1%)
All	All	0.49	0/55995	0.71	24/76389 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	42	ILE	C-N-CD	-14.41	65.92	125.00
9	k	42	ILE	C-N-CD	-14.41	65.92	125.00
9	T	42	ILE	C-N-CD	-14.40	65.96	125.00
6	Q	61	THR	C-N-CD	-14.37	66.07	125.00
6	f	61	THR	C-N-CD	-14.37	66.09	125.00

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5849	0	5643	198	0
1	G	5849	0	5643	198	0
1	a	5849	0	5643	203	0
2	B	5900	0	5643	131	0
2	H	5900	0	5643	132	0
2	b	5900	0	5643	129	0
3	C	598	0	573	16	0
3	N	598	0	573	15	0
3	c	598	0	573	16	0
4	D	1102	0	1082	40	0
4	O	1102	0	1082	41	0
4	d	1102	0	1082	37	0
5	E	506	0	501	10	0
5	P	506	0	501	10	0
5	e	506	0	501	11	0
6	F	826	0	703	25	0
6	Q	826	0	703	24	0
6	f	826	0	703	27	0
7	I	343	0	339	11	0
7	R	343	0	339	11	0
7	i	343	0	339	11	0
8	J	296	0	294	2	0
8	S	296	0	294	2	0
8	j	296	0	294	2	0
9	K	516	0	560	24	0
9	T	516	0	560	24	0
9	k	516	0	560	24	0
10	L	1291	0	1286	27	0
10	U	1291	0	1286	29	0
10	l	1291	0	1286	27	0
11	M	232	0	249	8	0
11	V	232	0	249	8	0
11	m	232	0	249	9	0
12	W	649	0	532	59	0
12	X	649	0	532	56	0
12	x	649	0	532	56	0
13	A	65	0	72	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	G	65	0	72	6	0
13	a	65	0	72	6	0
14	A	2330	0	2168	104	0
14	B	2255	0	2285	117	0
14	G	2330	0	2168	102	0
14	H	2255	0	2285	126	0
14	K	45	0	32	4	0
14	L	190	0	203	29	0
14	M	50	0	39	5	0
14	T	45	0	32	4	0
14	U	190	0	203	30	0
14	V	50	0	39	5	0
14	a	2330	0	2168	98	0
14	b	2255	0	2285	120	0
14	k	45	0	32	4	0
14	l	190	0	203	28	0
14	m	50	0	39	5	0
15	A	46	0	0	2	0
15	B	300	0	0	7	0
15	G	46	0	0	2	0
15	H	300	0	0	7	0
15	a	46	0	0	2	0
15	b	300	0	0	7	0
16	A	33	0	46	3	0
16	B	33	0	46	3	0
16	G	33	0	46	2	0
16	H	33	0	46	3	0
16	a	33	0	46	4	0
16	b	33	0	46	4	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
17	G	8	0	0	0	0
17	N	16	0	0	0	0
17	a	8	0	0	0	0
17	c	16	0	0	0	0
18	A	240	0	291	17	0
18	B	280	0	342	20	0
18	G	240	0	291	16	0
18	H	280	0	342	18	0
18	I	80	0	97	8	0
18	K	40	0	49	2	0
18	L	80	0	98	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	M	40	0	48	4	0
18	R	80	0	97	10	0
18	T	40	0	49	3	0
18	U	80	0	98	6	0
18	V	40	0	48	5	0
18	a	240	0	291	18	0
18	b	280	0	342	17	0
18	i	80	0	97	8	0
18	k	40	0	49	2	0
18	l	80	0	98	4	0
18	m	40	0	48	5	0
19	A	86	0	121	5	0
19	G	86	0	121	5	0
19	L	74	0	105	3	0
19	U	74	0	105	4	0
19	a	86	0	121	5	0
19	l	74	0	105	3	0
20	A	46	0	65	3	0
20	B	46	0	62	5	0
20	G	46	0	65	3	0
20	H	46	0	62	5	0
20	I	37	0	44	1	0
20	R	37	0	44	1	0
20	a	46	0	65	4	0
20	b	46	0	62	5	0
20	i	37	0	44	1	0
21	A	115	0	122	1	0
21	B	136	0	167	6	0
21	G	115	0	122	1	0
21	H	136	0	168	5	0
21	I	35	0	45	3	0
21	L	84	0	112	4	0
21	M	35	0	43	0	0
21	R	35	0	45	3	0
21	U	84	0	112	4	0
21	V	35	0	43	0	0
21	a	115	0	121	1	0
21	b	136	0	167	5	0
21	i	35	0	45	2	0
21	l	84	0	112	4	0
21	m	35	0	43	0	0
22	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	G	1	0	0	0	0
22	a	1	0	0	0	0
23	L	1	0	0	0	0
23	U	1	0	0	0	0
23	l	1	0	0	0	0
24	W	4	0	0	0	0
24	X	4	0	0	0	0
24	x	4	0	0	0	0
25	A	35	0	0	4	0
25	B	35	0	0	0	0
25	C	9	0	0	1	0
25	D	13	0	0	0	0
25	G	35	0	0	4	0
25	H	35	0	0	0	0
25	I	4	0	0	0	0
25	L	15	0	0	2	0
25	N	9	0	0	1	0
25	O	13	0	0	0	0
25	R	4	0	0	0	0
25	U	15	0	0	2	0
25	a	35	0	0	4	0
25	b	35	0	0	0	0
25	c	9	0	0	1	0
25	d	13	0	0	0	0
25	i	4	0	0	0	0
25	l	15	0	0	2	0
All	All	75150	0	72321	2094	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 2094 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:x:61:GLN:CD	12:x:77:VAL:HG12	1.51	1.34
14:L:1501:CLA:C20	14:L:1503:CLA:H141	1.58	1.33
14:U:1501:CLA:C20	14:U:1503:CLA:H141	1.58	1.33
12:X:61:GLN:CD	12:X:77:VAL:HG12	1.51	1.33
1:a:16:GLU:CB	1:a:182:ARG:CG	2.08	1.32

There are no symmetry-related clashes.

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	296/782 (38%)	290 (98%)	6 (2%)	0	100	100
1	G	745/782 (95%)	708 (95%)	31 (4%)	6 (1%)	16	43
1	a	745/782 (95%)	708 (95%)	31 (4%)	6 (1%)	16	43
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	11
4	O	141/155 (91%)	119 (84%)	17 (12%)	5 (4%)	3	11
4	d	141/155 (91%)	119 (84%)	17 (12%)	5 (4%)	3	11
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%)	3	11
6	Q	120/168 (71%)	106 (88%)	10 (8%)	4 (3%)	3	11
6	f	120/168 (71%)	106 (88%)	10 (8%)	4 (3%)	3	11
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
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%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	T	73/84 (87%)	57 (78%)	12 (16%)	4 (6%)	1	4
9	k	73/84 (87%)	57 (78%)	12 (16%)	4 (6%)	1	4
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%)	5	20
12	X	95/99 (96%)	80 (84%)	13 (14%)	2 (2%)	5	20
12	x	95/99 (96%)	80 (84%)	13 (14%)	2 (2%)	5	20
All	All	6541/7512 (87%)	6087 (93%)	397 (6%)	57 (1%)	16	40

5 of 57 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	G	1116	-	59,63,73	2.42	22 (37%)	70,101,113	2.62	26 (37%)
14	CLA	B	1222	25	69,73,73	2.20	21 (30%)	82,113,113	2.53	28 (34%)
18	BCR	A	4001	-	41,41,41	2.67	6 (14%)	56,56,56	6.73	16 (28%)
14	CLA	b	1202	-	69,73,73	2.21	21 (30%)	82,113,113	2.52	26 (31%)
14	CLA	b	1209	-	49,53,73	2.53	22 (44%)	58,89,113	2.67	22 (37%)
20	LMG	G	5003	-	46,46,55	1.37	5 (10%)	54,54,63	1.26	4 (7%)
14	CLA	a	1101	-	49,53,73	2.54	22 (44%)	58,89,113	2.82	24 (41%)
14	CLA	A	1129	-	54,58,73	2.49	19 (35%)	64,95,113	2.90	28 (43%)
21	LMT	U	6002	-	36,36,36	1.26	5 (13%)	47,47,47	1.23	7 (14%)
14	CLA	H	1211	-	69,73,73	2.23	23 (33%)	82,113,113	2.42	28 (34%)
21	LMT	H	6003	-	36,36,36	1.15	2 (5%)	47,47,47	1.62	8 (17%)
21	LMT	I	6001	-	36,36,36	1.15	5 (13%)	47,47,47	1.04	2 (4%)
14	CLA	a	1129	-	54,58,73	2.49	19 (35%)	64,95,113	2.90	28 (43%)
15	F6C	a	1121	-	52,54,74	3.10	25 (48%)	59,90,114	3.52	33 (55%)
18	BCR	a	4006	-	41,41,41	2.72	6 (14%)	56,56,56	6.73	23 (41%)
18	BCR	G	4006	-	41,41,41	2.72	6 (14%)	56,56,56	6.73	23 (41%)
19	LHG	A	5002	-	43,43,48	1.01	2 (4%)	46,48,54	1.15	3 (6%)
18	BCR	B	4006	-	41,41,41	2.63	6 (14%)	56,56,56	6.74	18 (32%)
14	CLA	H	1239	-	69,73,73	2.22	21 (30%)	82,113,113	2.49	30 (36%)
14	CLA	a	1125	-	69,73,73	2.16	20 (28%)	82,113,113	2.55	29 (35%)
14	CLA	a	1104	-	69,73,73	2.14	20 (28%)	82,113,113	2.63	27 (32%)
14	CLA	G	1126	-	64,68,73	2.33	21 (32%)	76,107,113	2.53	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	1013	-	64,68,73	2.30	21 (32%)	76,107,113	2.63	25 (32%)
14	CLA	U	1503	-	69,73,73	2.23	20 (28%)	82,113,113	2.43	26 (31%)
14	CLA	a	1103	-	69,73,73	2.20	21 (30%)	82,113,113	2.56	29 (35%)
20	LMG	B	5002	-	46,46,55	1.37	6 (13%)	54,54,63	1.25	6 (11%)
21	LMT	G	6002	-	29,29,36	1.42	6 (20%)	40,40,47	1.26	4 (10%)
14	CLA	a	1127	-	69,73,73	2.20	20 (28%)	82,113,113	2.40	23 (28%)
14	CLA	G	1101	-	49,53,73	2.54	22 (44%)	58,89,113	2.81	24 (41%)
14	CLA	B	1209	-	49,53,73	2.53	22 (44%)	58,89,113	2.67	22 (37%)
14	CLA	A	1139	-	49,53,73	2.54	23 (46%)	58,89,113	2.71	23 (39%)
18	BCR	H	4010	-	41,41,41	2.79	6 (14%)	56,56,56	7.03	20 (35%)
14	CLA	A	1109	-	69,73,73	2.24	23 (33%)	82,113,113	2.54	25 (30%)
17	SF4	c	3002	3	0,12,12	-	-	-	-	-
18	BCR	I	4018	-	41,41,41	2.73	7 (17%)	56,56,56	6.75	17 (30%)
19	LHG	A	5001	-	41,41,48	1.05	2 (4%)	44,47,54	0.99	2 (4%)
18	BCR	L	4019	-	41,41,41	2.84	6 (14%)	56,56,56	6.67	26 (46%)
14	CLA	b	1221	-	69,73,73	2.22	21 (30%)	82,113,113	2.47	26 (31%)
21	LMT	A	6003	-	33,33,36	1.19	5 (15%)	44,44,47	0.96	1 (2%)
14	CLA	a	1123	-	64,68,73	2.31	20 (31%)	76,107,113	2.62	27 (35%)
14	CLA	G	1129	-	54,58,73	2.49	19 (35%)	64,95,113	2.89	28 (43%)
14	CLA	G	1127	-	69,73,73	2.20	20 (28%)	82,113,113	2.39	24 (29%)
14	CLA	G	1104	-	69,73,73	2.14	20 (28%)	82,113,113	2.63	27 (32%)
15	F6C	b	1207	-	72,74,74	2.71	26 (36%)	83,114,114	3.16	35 (42%)
14	CLA	b	1022	-	59,63,73	2.37	19 (32%)	70,101,113	2.60	27 (38%)
14	CLA	B	1226	-	69,73,73	2.26	19 (27%)	82,113,113	2.44	26 (31%)
18	BCR	A	4005	-	41,41,41	2.78	6 (14%)	56,56,56	6.67	22 (39%)
14	CLA	G	1109	-	69,73,73	2.24	23 (33%)	82,113,113	2.53	25 (30%)
14	CLA	A	1108	-	49,53,73	2.57	21 (42%)	58,89,113	2.73	25 (43%)
15	F6C	B	1207	-	72,74,74	2.71	26 (36%)	83,114,114	3.15	36 (43%)
14	CLA	a	1106	1	64,68,73	2.29	21 (32%)	76,107,113	2.64	28 (36%)
17	SF4	N	3002	3	0,12,12	-	-	-	-	-
17	SF4	N	3003	3	0,12,12	-	-	-	-	-
14	CLA	b	1213	-	49,53,73	2.53	22 (44%)	58,89,113	2.81	23 (39%)
14	CLA	G	1120	-	49,53,73	2.48	20 (40%)	58,89,113	2.90	20 (34%)
14	CLA	a	1126	-	64,68,73	2.33	20 (31%)	76,107,113	2.53	23 (30%)
14	CLA	a	1012	25	69,73,73	2.21	19 (27%)	82,113,113	2.44	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	PQN	G	2001	-	34,34,34	1.53	2 (5%)	43,45,45	1.20	3 (6%)
14	CLA	G	1131	-	64,68,73	2.31	21 (32%)	76,107,113	2.58	24 (31%)
14	CLA	G	1112	-	59,63,73	2.42	22 (37%)	70,101,113	2.67	26 (37%)
14	CLA	G	1122	-	59,63,73	2.35	21 (35%)	70,101,113	2.61	27 (38%)
14	CLA	A	1106	1	64,68,73	2.29	20 (31%)	76,107,113	2.64	28 (36%)
14	CLA	H	1232	-	49,53,73	2.54	22 (44%)	58,89,113	2.74	23 (39%)
18	BCR	H	4004	-	41,41,41	2.64	6 (14%)	56,56,56	6.68	19 (33%)
14	CLA	M	1501	-	54,58,73	2.51	20 (37%)	64,95,113	2.74	27 (42%)
14	CLA	T	1401	-	49,53,73	2.56	22 (44%)	58,89,113	2.86	25 (43%)
14	CLA	l	1501	10	69,73,73	2.19	20 (28%)	82,113,113	2.49	26 (31%)
14	CLA	G	1119	-	69,73,73	2.22	19 (27%)	82,113,113	2.33	24 (29%)
21	LMT	l	6001	-	13,13,36	0.50	0	12,12,47	0.92	0
15	F6C	H	1207	-	72,74,74	2.70	26 (36%)	83,114,114	3.16	36 (43%)
14	CLA	A	1126	-	64,68,73	2.33	21 (32%)	76,107,113	2.53	23 (30%)
14	CLA	b	1205	-	69,73,73	2.18	20 (28%)	82,113,113	2.56	28 (34%)
14	CLA	B	1213	-	49,53,73	2.53	22 (44%)	58,89,113	2.81	23 (39%)
14	CLA	b	1208	-	64,68,73	2.32	21 (32%)	76,107,113	2.63	28 (36%)
17	SF4	C	3003	3	0,12,12	-	-	-	-	-
18	BCR	B	4017	-	41,41,41	2.81	6 (14%)	56,56,56	6.88	19 (33%)
14	CLA	b	1228	-	59,63,73	2.43	22 (37%)	70,101,113	2.53	29 (41%)
14	CLA	G	1128	-	64,68,73	2.33	19 (29%)	76,107,113	2.49	26 (34%)
14	CLA	a	1139	-	49,53,73	2.54	23 (46%)	58,89,113	2.71	23 (39%)
18	BCR	b	4006	-	41,41,41	2.63	6 (14%)	56,56,56	6.74	18 (32%)
14	CLA	b	1211	-	69,73,73	2.24	23 (33%)	82,113,113	2.43	28 (34%)
14	CLA	G	1105	-	49,53,73	2.55	20 (40%)	58,89,113	2.80	22 (37%)
14	CLA	H	1201	-	69,73,73	2.20	23 (33%)	82,113,113	2.61	28 (34%)
14	CLA	H	1022	-	59,63,73	2.37	19 (32%)	70,101,113	2.60	27 (38%)
15	F6C	B	1230	-	52,54,74	3.11	27 (51%)	59,90,114	3.62	30 (50%)
14	CLA	A	1103	-	69,73,73	2.20	21 (30%)	82,113,113	2.56	29 (35%)
21	LMT	a	6001	-	32,32,36	1.27	5 (15%)	43,43,47	1.11	5 (11%)
18	BCR	l	4019	-	41,41,41	2.84	6 (14%)	56,56,56	6.67	26 (46%)
18	BCR	l	4022	-	41,41,41	2.78	6 (14%)	56,56,56	6.56	21 (37%)
14	CLA	G	1106	1	64,68,73	2.29	20 (31%)	76,107,113	2.65	28 (36%)
14	CLA	b	1220	-	69,73,73	2.21	21 (30%)	82,113,113	2.46	23 (28%)
13	CL0	A	1011	-	58,73,73	3.07	20 (34%)	60,113,113	2.92	21 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	1013	-	64,68,73	2.30	21 (32%)	76,107,113	2.64	25 (32%)
18	BCR	B	4010	-	41,41,41	2.79	6 (14%)	56,56,56	7.03	20 (35%)
14	CLA	H	1222	25	69,73,73	2.20	21 (30%)	82,113,113	2.54	28 (34%)
14	CLA	A	1119	-	69,73,73	2.22	19 (27%)	82,113,113	2.33	24 (29%)
14	CLA	A	1133	1	64,68,73	2.30	21 (32%)	76,107,113	2.58	21 (27%)
14	CLA	H	1213	-	49,53,73	2.53	22 (44%)	58,89,113	2.81	23 (39%)
21	LMT	M	6000	-	36,36,36	1.16	6 (16%)	47,47,47	0.98	1 (2%)
14	CLA	B	1240	2	69,73,73	2.26	23 (33%)	82,113,113	2.48	24 (29%)
14	CLA	b	1212	-	49,53,73	2.50	21 (42%)	58,89,113	2.86	23 (39%)
18	BCR	H	4017	-	41,41,41	2.80	6 (14%)	56,56,56	6.88	19 (33%)
14	CLA	k	1401	-	49,53,73	2.57	21 (42%)	58,89,113	2.86	25 (43%)
14	CLA	A	1135	-	54,58,73	2.52	21 (38%)	64,95,113	2.78	27 (42%)
14	CLA	b	1240	2	69,73,73	2.27	23 (33%)	82,113,113	2.48	26 (31%)
19	LHG	L	5102	-	48,48,48	0.90	2 (4%)	51,54,54	1.05	3 (5%)
18	BCR	a	4003	-	41,41,41	2.74	6 (14%)	56,56,56	7.01	24 (42%)
21	LMT	A	6001	-	32,32,36	1.27	5 (15%)	43,43,47	1.11	5 (11%)
15	F6C	B	1219	-	62,64,74	2.92	30 (48%)	71,102,114	3.40	32 (45%)
14	CLA	G	1137	-	54,58,73	2.49	20 (37%)	64,95,113	2.82	24 (37%)
14	CLA	a	1135	-	54,58,73	2.52	21 (38%)	64,95,113	2.77	27 (42%)
14	CLA	A	1117	-	69,73,73	2.14	22 (31%)	82,113,113	2.49	32 (39%)
14	CLA	A	1141	-	49,53,73	2.52	23 (46%)	58,89,113	2.84	23 (39%)
14	CLA	H	1227	-	49,53,73	2.50	20 (40%)	58,89,113	2.82	21 (36%)
15	F6C	b	1238	25	72,74,74	2.71	25 (34%)	83,114,114	3.12	32 (38%)
14	CLA	G	1013	-	64,68,73	2.29	21 (32%)	76,107,113	2.64	25 (32%)
14	CLA	a	1131	-	64,68,73	2.30	21 (32%)	76,107,113	2.58	24 (31%)
15	F6C	G	1121	-	52,54,74	3.09	25 (48%)	59,90,114	3.52	33 (55%)
14	CLA	B	1221	-	69,73,73	2.22	21 (30%)	82,113,113	2.47	26 (31%)
14	CLA	a	1138	-	59,63,73	2.37	22 (37%)	70,101,113	2.75	28 (40%)
16	PQN	H	2002	-	34,34,34	1.59	2 (5%)	43,45,45	1.12	2 (4%)
19	LHG	G	5001	-	41,41,48	1.05	2 (4%)	44,47,54	0.99	2 (4%)
14	CLA	H	1240	2	69,73,73	2.26	23 (33%)	82,113,113	2.48	25 (30%)
21	LMT	V	6000	-	36,36,36	1.17	6 (16%)	47,47,47	0.98	1 (2%)
14	CLA	b	1235	-	64,68,73	2.28	21 (32%)	76,107,113	2.62	28 (36%)
21	LMT	U	6001	-	13,13,36	0.51	0	12,12,47	0.92	0
14	CLA	B	1224	-	69,73,73	2.22	20 (28%)	82,113,113	2.54	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	b	4014	-	41,41,41	2.62	7 (17%)	56,56,56	6.79	21 (37%)
14	CLA	b	1224	-	69,73,73	2.21	20 (28%)	82,113,113	2.53	26 (31%)
18	BCR	a	4002	-	41,41,41	2.65	6 (14%)	56,56,56	6.67	25 (44%)
14	CLA	b	1234	-	69,73,73	2.23	22 (31%)	82,113,113	2.42	26 (31%)
17	SF4	c	3003	3	0,12,12	-	-	-	-	-
14	CLA	G	1102	-	54,58,73	2.55	24 (44%)	64,95,113	2.78	28 (43%)
21	LMT	a	6003	-	33,33,36	1.18	4 (12%)	44,44,47	0.96	1 (2%)
14	CLA	B	1236	-	59,63,73	2.34	21 (35%)	70,101,113	2.80	27 (38%)
14	CLA	a	1107	-	49,53,73	2.52	19 (38%)	58,89,113	2.77	22 (37%)
14	CLA	B	1232	-	49,53,73	2.54	22 (44%)	58,89,113	2.75	23 (39%)
18	BCR	G	4005	-	41,41,41	2.78	6 (14%)	56,56,56	6.67	22 (39%)
19	LHG	L	5101	-	24,24,48	1.28	2 (8%)	26,26,54	1.50	4 (15%)
18	BCR	B	4004	-	41,41,41	2.64	6 (14%)	56,56,56	6.68	19 (33%)
14	CLA	A	1105	-	49,53,73	2.55	21 (42%)	58,89,113	2.80	22 (37%)
14	CLA	b	1021	-	69,73,73	2.20	21 (30%)	82,113,113	2.38	27 (32%)
18	BCR	H	4005	-	41,41,41	2.63	6 (14%)	56,56,56	6.68	20 (35%)
18	BCR	L	4022	-	41,41,41	2.78	6 (14%)	56,56,56	6.56	21 (37%)
14	CLA	H	1233	-	49,53,73	2.55	22 (44%)	58,89,113	2.76	24 (41%)
15	F6C	A	1121	-	52,54,74	3.09	25 (48%)	59,90,114	3.52	33 (55%)
14	CLA	L	1503	-	69,73,73	2.23	20 (28%)	82,113,113	2.43	26 (31%)
14	CLA	H	1210	-	69,73,73	2.20	22 (31%)	82,113,113	2.67	28 (34%)
18	BCR	i	4018	-	41,41,41	2.73	7 (17%)	56,56,56	6.75	16 (28%)
14	CLA	H	1212	-	49,53,73	2.50	21 (42%)	58,89,113	2.86	23 (39%)
14	CLA	a	1128	-	64,68,73	2.32	19 (29%)	76,107,113	2.48	26 (34%)
14	CLA	B	1235	-	64,68,73	2.29	21 (32%)	76,107,113	2.62	28 (36%)
18	BCR	b	4005	-	41,41,41	2.64	6 (14%)	56,56,56	6.68	20 (35%)
17	SF4	C	3002	3	0,12,12	-	-	-	-	-
14	CLA	H	1236	-	59,63,73	2.34	21 (35%)	70,101,113	2.80	27 (38%)
21	LMT	m	6000	-	36,36,36	1.16	6 (16%)	47,47,47	0.98	1 (2%)
24	FES	W	101	12	0,4,4	-	-	-	-	-
14	CLA	B	1215	-	64,68,73	2.26	21 (32%)	76,107,113	2.50	24 (31%)
14	CLA	b	1231	-	69,73,73	2.20	22 (31%)	82,113,113	2.47	24 (29%)
14	CLA	B	1202	-	69,73,73	2.21	21 (30%)	82,113,113	2.53	26 (31%)
14	CLA	b	1215	-	64,68,73	2.27	21 (32%)	76,107,113	2.50	24 (31%)
20	LMG	a	5003	-	46,46,55	1.37	5 (10%)	54,54,63	1.27	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	b	4010	-	41,41,41	2.79	6 (14%)	56,56,56	7.03	20 (35%)
16	PQN	B	2002	-	34,34,34	1.59	2 (5%)	43,45,45	1.12	2 (4%)
18	BCR	U	4022	-	41,41,41	2.77	6 (14%)	56,56,56	6.55	21 (37%)
24	FES	x	101	12	0,4,4	-	-	-	-	-
14	CLA	a	1140	-	59,63,73	2.41	21 (35%)	70,101,113	2.56	24 (34%)
18	BCR	b	4009	-	41,41,41	2.72	6 (14%)	56,56,56	6.67	25 (44%)
18	BCR	H	4014	-	41,41,41	2.62	6 (14%)	56,56,56	6.79	21 (37%)
14	CLA	G	1123	-	64,68,73	2.31	20 (31%)	76,107,113	2.61	27 (35%)
14	CLA	G	1134	1	49,53,73	2.52	21 (42%)	58,89,113	2.76	23 (39%)
14	CLA	H	1235	-	64,68,73	2.29	21 (32%)	76,107,113	2.61	28 (36%)
18	BCR	U	4019	-	41,41,41	2.84	6 (14%)	56,56,56	6.66	26 (46%)
21	LMT	a	6002	-	29,29,36	1.42	6 (20%)	40,40,47	1.26	4 (10%)
21	LMT	G	6003	-	33,33,36	1.19	4 (12%)	44,44,47	0.96	1 (2%)
18	BCR	V	4021	-	41,41,41	2.70	6 (14%)	56,56,56	6.78	19 (33%)
15	F6C	b	1219	-	62,64,74	2.91	29 (46%)	71,102,114	3.40	32 (45%)
14	CLA	H	1215	-	64,68,73	2.26	21 (32%)	76,107,113	2.50	24 (31%)
21	LMT	b	6002	-	36,36,36	1.18	6 (16%)	47,47,47	1.04	1 (2%)
14	CLA	G	1103	-	69,73,73	2.20	21 (30%)	82,113,113	2.56	29 (35%)
14	CLA	A	1115	-	69,73,73	2.24	20 (28%)	82,113,113	2.53	29 (35%)
21	LMT	l	6101	-	36,36,36	1.16	5 (13%)	47,47,47	1.34	4 (8%)
14	CLA	a	1112	-	59,63,73	2.42	22 (37%)	70,101,113	2.67	26 (37%)
21	LMT	b	6004	-	32,32,36	1.19	4 (12%)	43,43,47	1.19	4 (9%)
13	CL0	G	1011	-	58,73,73	3.08	20 (34%)	60,113,113	2.91	21 (35%)
15	F6C	H	1230	-	52,54,74	3.11	27 (51%)	59,90,114	3.62	30 (50%)
14	CLA	B	1210	-	69,73,73	2.20	22 (31%)	82,113,113	2.67	28 (34%)
21	LMT	B	6003	-	36,36,36	1.15	3 (8%)	47,47,47	1.62	8 (17%)
14	CLA	b	1227	-	49,53,73	2.50	20 (40%)	58,89,113	2.81	21 (36%)
14	CLA	b	1233	-	49,53,73	2.55	22 (44%)	58,89,113	2.76	25 (43%)
14	CLA	B	1212	-	49,53,73	2.51	21 (42%)	58,89,113	2.86	23 (39%)
14	CLA	A	1130	-	59,63,73	2.42	20 (33%)	70,101,113	2.50	25 (35%)
14	CLA	G	1139	-	49,53,73	2.54	24 (48%)	58,89,113	2.71	23 (39%)
14	CLA	a	1116	-	59,63,73	2.42	22 (37%)	70,101,113	2.63	25 (35%)
14	CLA	a	1109	-	69,73,73	2.24	23 (33%)	82,113,113	2.54	25 (30%)
14	CLA	G	1012	25	69,73,73	2.20	19 (27%)	82,113,113	2.44	28 (34%)
15	F6C	H	1219	-	62,64,74	2.92	30 (48%)	71,102,114	3.40	32 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	m	1501	-	54,58,73	2.51	20 (37%)	64,95,113	2.73	27 (42%)
21	LMT	U	6101	-	36,36,36	1.15	5 (13%)	47,47,47	1.34	4 (8%)
14	CLA	H	1220	-	69,73,73	2.21	21 (30%)	82,113,113	2.46	23 (28%)
21	LMT	B	6002	-	36,36,36	1.18	6 (16%)	47,47,47	1.03	1 (2%)
18	BCR	i	4020	-	41,41,41	2.90	7 (17%)	56,56,56	6.94	23 (41%)
14	CLA	A	1122	-	59,63,73	2.35	21 (35%)	70,101,113	2.61	27 (38%)
14	CLA	A	1120	-	49,53,73	2.48	20 (40%)	58,89,113	2.90	20 (34%)
21	LMT	L	6101	-	36,36,36	1.15	5 (13%)	47,47,47	1.34	4 (8%)
14	CLA	H	1202	-	69,73,73	2.21	21 (30%)	82,113,113	2.53	26 (31%)
21	LMT	H	6004	-	32,32,36	1.18	4 (12%)	43,43,47	1.18	4 (9%)
14	CLA	G	1110	-	49,53,73	2.55	20 (40%)	58,89,113	2.73	21 (36%)
14	CLA	a	1120	-	49,53,73	2.48	20 (40%)	58,89,113	2.90	20 (34%)
16	PQN	a	2001	-	34,34,34	1.53	2 (5%)	43,45,45	1.20	3 (6%)
14	CLA	A	1112	-	59,63,73	2.42	22 (37%)	70,101,113	2.67	26 (37%)
18	BCR	B	4005	-	41,41,41	2.63	6 (14%)	56,56,56	6.68	20 (35%)
18	BCR	B	4014	-	41,41,41	2.62	7 (17%)	56,56,56	6.79	21 (37%)
14	CLA	U	1502	-	64,68,73	2.28	20 (31%)	76,107,113	2.54	23 (30%)
14	CLA	G	1108	-	49,53,73	2.57	21 (42%)	58,89,113	2.73	24 (41%)
14	CLA	H	1221	-	69,73,73	2.22	21 (30%)	82,113,113	2.46	26 (31%)
18	BCR	R	4020	-	41,41,41	2.90	7 (17%)	56,56,56	6.93	22 (39%)
14	CLA	b	1210	-	69,73,73	2.21	22 (31%)	82,113,113	2.68	28 (34%)
18	BCR	I	4020	-	41,41,41	2.90	7 (17%)	56,56,56	6.94	22 (39%)
14	CLA	H	1224	-	69,73,73	2.22	20 (28%)	82,113,113	2.54	27 (32%)
14	CLA	b	1201	-	69,73,73	2.19	22 (31%)	82,113,113	2.61	28 (34%)
20	LMG	R	5006	-	37,37,55	1.15	3 (8%)	45,45,63	1.22	5 (11%)
20	LMG	i	5006	-	37,37,55	1.15	3 (8%)	45,45,63	1.22	5 (11%)
14	CLA	A	1111	-	64,68,73	2.29	21 (32%)	76,107,113	4.43	30 (39%)
14	CLA	A	1107	-	49,53,73	2.52	19 (38%)	58,89,113	2.77	22 (37%)
14	CLA	a	1136	-	69,73,73	2.20	22 (31%)	82,113,113	2.50	26 (31%)
15	F6C	b	1230	-	52,54,74	3.11	27 (51%)	59,90,114	3.62	30 (50%)
14	CLA	a	1105	-	49,53,73	2.55	21 (42%)	58,89,113	2.79	22 (37%)
18	BCR	K	4001	-	41,41,41	2.69	6 (14%)	56,56,56	6.61	22 (39%)
15	F6C	B	1237	25	72,74,74	2.64	25 (34%)	83,114,114	3.16	35 (42%)
14	CLA	a	1118	-	59,63,73	2.41	20 (33%)	70,101,113	2.65	24 (34%)
21	LMT	L	6001	-	13,13,36	0.51	0	12,12,47	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	H	1217	-	49,53,73	2.50	20 (40%)	58,89,113	2.81	22 (37%)
19	LHG	G	5002	-	43,43,48	1.00	2 (4%)	46,48,54	1.15	3 (6%)
14	CLA	H	1223	-	69,73,73	2.23	21 (30%)	82,113,113	2.51	28 (34%)
14	CLA	A	1140	-	59,63,73	2.41	21 (35%)	70,101,113	2.56	24 (34%)
14	CLA	H	1229	-	64,68,73	2.32	21 (32%)	76,107,113	2.59	26 (34%)
14	CLA	B	1021	-	69,73,73	2.20	21 (30%)	82,113,113	2.38	27 (32%)
18	BCR	b	4017	-	41,41,41	2.80	6 (14%)	56,56,56	6.88	19 (33%)
14	CLA	a	1133	1	64,68,73	2.30	21 (32%)	76,107,113	2.57	21 (27%)
14	CLA	B	1217	-	49,53,73	2.50	20 (40%)	58,89,113	2.81	23 (39%)
14	CLA	A	1125	-	69,73,73	2.16	20 (28%)	82,113,113	2.55	29 (35%)
14	CLA	H	1203	-	69,73,73	2.17	20 (28%)	82,113,113	2.55	25 (30%)
18	BCR	a	4004	-	41,41,41	2.80	6 (14%)	56,56,56	6.83	23 (41%)
14	CLA	l	1502	-	64,68,73	2.28	20 (31%)	76,107,113	2.54	22 (28%)
17	SF4	a	3001	2,1	0,12,12	-	-	-	-	-
20	LMG	b	5002	-	46,46,55	1.37	6 (13%)	54,54,63	1.25	6 (11%)
18	BCR	a	4005	-	41,41,41	2.78	6 (14%)	56,56,56	6.68	22 (39%)
14	CLA	A	1116	-	59,63,73	2.42	22 (37%)	70,101,113	2.62	25 (35%)
14	CLA	G	1113	-	49,53,73	2.53	21 (42%)	58,89,113	2.74	23 (39%)
15	F6C	H	1237	25	72,74,74	2.63	25 (34%)	83,114,114	3.17	35 (42%)
14	CLA	b	1206	-	69,73,73	2.22	20 (28%)	82,113,113	2.42	26 (31%)
14	CLA	B	1220	-	69,73,73	2.21	21 (30%)	82,113,113	2.46	23 (28%)
14	CLA	a	1108	-	49,53,73	2.56	21 (42%)	58,89,113	2.73	25 (43%)
14	CLA	H	1228	-	59,63,73	2.42	22 (37%)	70,101,113	2.52	29 (41%)
14	CLA	a	1141	-	49,53,73	2.52	23 (46%)	58,89,113	2.83	23 (39%)
18	BCR	G	4004	-	41,41,41	2.80	6 (14%)	56,56,56	6.83	23 (41%)
14	CLA	K	1401	-	49,53,73	2.56	22 (44%)	58,89,113	2.86	25 (43%)
14	CLA	G	1135	-	54,58,73	2.52	21 (38%)	64,95,113	2.78	27 (42%)
18	BCR	R	4018	-	41,41,41	2.73	7 (17%)	56,56,56	6.75	16 (28%)
14	CLA	B	1205	-	69,73,73	2.18	20 (28%)	82,113,113	2.55	28 (34%)
15	F6C	b	1237	25	72,74,74	2.64	25 (34%)	83,114,114	3.16	35 (42%)
14	CLA	G	1117	-	69,73,73	2.14	22 (31%)	82,113,113	2.49	33 (40%)
14	CLA	a	1124	25	59,63,73	2.38	21 (35%)	70,101,113	2.70	23 (32%)
14	CLA	H	1204	-	69,73,73	2.21	21 (30%)	82,113,113	2.50	25 (30%)
21	LMT	b	6003	-	36,36,36	1.15	3 (8%)	47,47,47	1.62	7 (14%)
18	BCR	T	4001	-	41,41,41	2.69	6 (14%)	56,56,56	6.61	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CL0	a	1011	-	58,73,73	3.07	20 (34%)	60,113,113	2.92	21 (35%)
14	CLA	G	1125	-	69,73,73	2.16	20 (28%)	82,113,113	2.55	29 (35%)
14	CLA	a	1102	-	54,58,73	2.55	25 (46%)	64,95,113	2.78	27 (42%)
14	CLA	H	1234	-	69,73,73	2.23	22 (31%)	82,113,113	2.42	26 (31%)
15	F6C	B	1238	25	72,74,74	2.71	25 (34%)	83,114,114	3.12	32 (38%)
19	LHG	a	5002	-	43,43,48	1.01	2 (4%)	46,48,54	1.15	3 (6%)
14	CLA	B	1223	-	69,73,73	2.23	21 (30%)	82,113,113	2.51	28 (34%)
19	LHG	l	5102	-	48,48,48	0.90	2 (4%)	51,54,54	1.05	3 (5%)
18	BCR	M	4021	-	41,41,41	2.70	6 (14%)	56,56,56	6.79	19 (33%)
14	CLA	a	1119	-	69,73,73	2.22	19 (27%)	82,113,113	2.33	24 (29%)
14	CLA	b	1203	-	69,73,73	2.17	20 (28%)	82,113,113	2.55	25 (30%)
14	CLA	V	1501	-	54,58,73	2.51	20 (37%)	64,95,113	2.74	27 (42%)
14	CLA	H	1218	-	49,53,73	2.51	20 (40%)	58,89,113	2.87	23 (39%)
14	CLA	H	1216	-	69,73,73	2.23	21 (30%)	82,113,113	2.30	22 (26%)
14	CLA	B	1203	-	69,73,73	2.17	20 (28%)	82,113,113	2.55	25 (30%)
14	CLA	a	1134	1	49,53,73	2.53	21 (42%)	58,89,113	2.76	23 (39%)
14	CLA	a	1111	-	64,68,73	2.29	22 (34%)	76,107,113	4.43	31 (40%)
18	BCR	A	4004	-	41,41,41	2.80	6 (14%)	56,56,56	6.83	23 (41%)
14	CLA	A	1012	25	69,73,73	2.21	19 (27%)	82,113,113	2.44	28 (34%)
14	CLA	A	1131	-	64,68,73	2.30	21 (32%)	76,107,113	2.57	24 (31%)
14	CLA	b	1023	-	69,73,73	2.24	21 (30%)	82,113,113	2.73	31 (37%)
21	LMT	A	6002	-	29,29,36	1.42	6 (20%)	40,40,47	1.26	4 (10%)
14	CLA	B	1228	-	59,63,73	2.43	22 (37%)	70,101,113	2.52	29 (41%)
14	CLA	G	1118	-	59,63,73	2.41	21 (35%)	70,101,113	2.66	24 (34%)
14	CLA	A	1101	-	49,53,73	2.54	22 (44%)	58,89,113	2.82	24 (41%)
15	F6C	H	1238	25	72,74,74	2.70	26 (36%)	83,114,114	3.11	32 (38%)
21	LMT	H	6002	-	36,36,36	1.18	6 (16%)	47,47,47	1.03	1 (2%)
14	CLA	A	1118	-	59,63,73	2.41	20 (33%)	70,101,113	2.66	24 (34%)
14	CLA	A	1123	-	64,68,73	2.31	20 (31%)	76,107,113	2.61	27 (35%)
14	CLA	B	1225	-	69,73,73	2.24	19 (27%)	82,113,113	2.33	21 (25%)
14	CLA	H	1231	-	69,73,73	2.20	22 (31%)	82,113,113	2.47	24 (29%)
14	CLA	B	1239	-	69,73,73	2.22	20 (28%)	82,113,113	2.49	29 (35%)
14	CLA	A	1110	-	49,53,73	2.54	20 (40%)	58,89,113	2.73	21 (36%)
14	CLA	B	1204	-	69,73,73	2.22	21 (30%)	82,113,113	2.50	26 (31%)
21	LMT	B	6001	-	36,36,36	1.16	5 (13%)	47,47,47	0.97	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	1217	-	49,53,73	2.50	20 (40%)	58,89,113	2.81	23 (39%)
14	CLA	b	1226	-	69,73,73	2.26	19 (27%)	82,113,113	2.44	26 (31%)
21	LMT	b	6001	-	36,36,36	1.16	5 (13%)	47,47,47	0.97	2 (4%)
14	CLA	b	1223	-	69,73,73	2.23	22 (31%)	82,113,113	2.51	29 (35%)
14	CLA	L	1501	10	69,73,73	2.19	20 (28%)	82,113,113	2.49	26 (31%)
14	CLA	G	1111	-	64,68,73	2.29	22 (34%)	76,107,113	4.43	30 (39%)
14	CLA	H	1208	-	64,68,73	2.32	21 (32%)	76,107,113	2.64	28 (36%)
14	CLA	B	1023	-	69,73,73	2.24	21 (30%)	82,113,113	2.73	31 (37%)
14	CLA	U	1501	10	69,73,73	2.19	20 (28%)	82,113,113	2.49	26 (31%)
21	LMT	l	6002	-	36,36,36	1.26	5 (13%)	47,47,47	1.24	7 (14%)
14	CLA	b	1214	-	64,68,73	2.35	21 (32%)	76,107,113	2.52	30 (39%)
14	CLA	B	1216	-	69,73,73	2.23	22 (31%)	82,113,113	2.30	22 (26%)
14	CLA	G	1136	-	69,73,73	2.20	22 (31%)	82,113,113	2.51	26 (31%)
14	CLA	a	1122	-	59,63,73	2.34	21 (35%)	70,101,113	2.61	26 (37%)
14	CLA	a	1137	-	54,58,73	2.49	20 (37%)	64,95,113	2.82	24 (37%)
21	LMT	H	6001	-	36,36,36	1.16	4 (11%)	47,47,47	0.97	2 (4%)
21	LMT	G	6001	-	32,32,36	1.27	5 (15%)	43,43,47	1.11	5 (11%)
14	CLA	H	1206	-	69,73,73	2.23	20 (28%)	82,113,113	2.42	26 (31%)
14	CLA	A	1137	-	54,58,73	2.49	20 (37%)	64,95,113	2.82	24 (37%)
14	CLA	a	1110	-	49,53,73	2.54	20 (40%)	58,89,113	2.73	21 (36%)
16	PQN	A	2001	-	34,34,34	1.53	2 (5%)	43,45,45	1.20	3 (6%)
14	CLA	G	1141	-	49,53,73	2.52	23 (46%)	58,89,113	2.83	23 (39%)
18	BCR	b	4004	-	41,41,41	2.64	6 (14%)	56,56,56	6.67	19 (33%)
14	CLA	b	1236	-	59,63,73	2.34	21 (35%)	70,101,113	2.80	27 (38%)
18	BCR	B	4009	-	41,41,41	2.72	6 (14%)	56,56,56	6.67	24 (42%)
14	CLA	G	1114	-	49,53,73	2.54	22 (44%)	58,89,113	2.72	20 (34%)
14	CLA	A	1114	-	49,53,73	2.54	22 (44%)	58,89,113	2.72	20 (34%)
14	CLA	b	1239	-	69,73,73	2.22	21 (30%)	82,113,113	2.50	30 (36%)
14	CLA	A	1132	-	69,73,73	2.19	21 (30%)	82,113,113	2.57	27 (32%)
14	CLA	l	1503	-	69,73,73	2.23	20 (28%)	82,113,113	2.43	26 (31%)
14	CLA	B	1234	-	69,73,73	2.23	22 (31%)	82,113,113	2.43	26 (31%)
14	CLA	H	1023	-	69,73,73	2.24	21 (30%)	82,113,113	2.73	31 (37%)
14	CLA	B	1231	-	69,73,73	2.20	22 (31%)	82,113,113	2.47	24 (29%)
14	CLA	A	1113	-	49,53,73	2.53	21 (42%)	58,89,113	2.74	23 (39%)
14	CLA	L	1502	-	64,68,73	2.28	20 (31%)	76,107,113	2.54	22 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	A	4006	-	41,41,41	2.72	6 (14%)	56,56,56	6.73	23 (41%)
14	CLA	b	1225	-	69,73,73	2.24	19 (27%)	82,113,113	2.32	21 (25%)
14	CLA	A	1136	-	69,73,73	2.20	22 (31%)	82,113,113	2.51	26 (31%)
17	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	a	1114	-	49,53,73	2.55	22 (44%)	58,89,113	2.72	21 (36%)
14	CLA	B	1218	-	49,53,73	2.51	20 (40%)	58,89,113	2.87	23 (39%)
14	CLA	H	1209	-	49,53,73	2.52	20 (40%)	58,89,113	2.67	22 (37%)
18	BCR	m	4021	-	41,41,41	2.70	6 (14%)	56,56,56	6.79	19 (33%)
19	LHG	U	5102	-	48,48,48	0.90	2 (4%)	51,54,54	1.05	3 (5%)
14	CLA	H	1205	-	69,73,73	2.18	20 (28%)	82,113,113	2.56	28 (34%)
14	CLA	B	1208	-	64,68,73	2.32	21 (32%)	76,107,113	2.64	28 (36%)
19	LHG	U	5101	-	24,24,48	1.27	2 (8%)	26,26,54	1.50	4 (15%)
14	CLA	H	1214	-	64,68,73	2.34	22 (34%)	76,107,113	2.51	30 (39%)
14	CLA	B	1211	-	69,73,73	2.24	23 (33%)	82,113,113	2.43	28 (34%)
14	CLA	A	1134	1	49,53,73	2.52	21 (42%)	58,89,113	2.75	23 (39%)
18	BCR	A	4002	-	41,41,41	2.64	6 (14%)	56,56,56	6.68	25 (44%)
18	BCR	H	4006	-	41,41,41	2.63	6 (14%)	56,56,56	6.74	18 (32%)
14	CLA	a	1130	-	59,63,73	2.43	20 (33%)	70,101,113	2.50	25 (35%)
14	CLA	G	1124	25	59,63,73	2.38	21 (35%)	70,101,113	2.70	23 (32%)
14	CLA	A	1127	-	69,73,73	2.20	20 (28%)	82,113,113	2.40	24 (29%)
14	CLA	A	1104	-	69,73,73	2.14	20 (28%)	82,113,113	2.63	27 (32%)
18	BCR	G	4001	-	41,41,41	2.67	6 (14%)	56,56,56	6.73	16 (28%)
14	CLA	A	1124	25	59,63,73	2.38	21 (35%)	70,101,113	2.70	24 (34%)
14	CLA	B	1227	-	49,53,73	2.50	20 (40%)	58,89,113	2.82	21 (36%)
14	CLA	a	1113	-	49,53,73	2.52	21 (42%)	58,89,113	2.74	23 (39%)
20	LMG	I	5006	-	37,37,55	1.15	3 (8%)	45,45,63	1.22	5 (11%)
20	LMG	H	5002	-	46,46,55	1.37	6 (13%)	54,54,63	1.25	6 (11%)
19	LHG	l	5101	-	24,24,48	1.28	2 (8%)	26,26,54	1.50	4 (15%)
14	CLA	A	1102	-	54,58,73	2.55	25 (46%)	64,95,113	2.77	28 (43%)
17	SF4	G	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	A	1138	-	59,63,73	2.37	22 (37%)	70,101,113	2.75	28 (40%)
14	CLA	H	1021	-	69,73,73	2.20	21 (30%)	82,113,113	2.38	27 (32%)
18	BCR	a	4001	-	41,41,41	2.67	6 (14%)	56,56,56	6.73	16 (28%)
18	BCR	k	4001	-	41,41,41	2.69	6 (14%)	56,56,56	6.61	22 (39%)
14	CLA	a	1117	-	69,73,73	2.14	22 (31%)	82,113,113	2.49	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	LHG	a	5001	-	41,41,48	1.06	2 (4%)	44,47,54	0.99	2 (4%)
14	CLA	b	1218	-	49,53,73	2.52	20 (40%)	58,89,113	2.88	23 (39%)
14	CLA	H	1225	-	69,73,73	2.24	19 (27%)	82,113,113	2.32	20 (24%)
14	CLA	A	1128	-	64,68,73	2.33	19 (29%)	76,107,113	2.48	26 (34%)
14	CLA	B	1206	-	69,73,73	2.22	20 (28%)	82,113,113	2.42	26 (31%)
14	CLA	G	1115	-	69,73,73	2.24	20 (28%)	82,113,113	2.53	29 (35%)
18	BCR	A	4003	-	41,41,41	2.74	6 (14%)	56,56,56	7.01	23 (41%)
18	BCR	G	4003	-	41,41,41	2.74	6 (14%)	56,56,56	7.01	22 (39%)
14	CLA	a	1132	-	69,73,73	2.20	21 (30%)	82,113,113	2.58	27 (32%)
21	LMT	A	6004	-	24,24,36	1.05	3 (12%)	29,29,47	1.08	1 (3%)
21	LMT	i	6001	-	36,36,36	1.16	6 (16%)	47,47,47	1.04	2 (4%)
21	LMT	a	6004	-	24,24,36	1.05	3 (12%)	29,29,47	1.07	1 (3%)
21	LMT	L	6002	-	36,36,36	1.26	5 (13%)	47,47,47	1.23	7 (14%)
21	LMT	B	6004	-	32,32,36	1.18	4 (12%)	43,43,47	1.18	4 (9%)
14	CLA	G	1140	-	59,63,73	2.41	21 (35%)	70,101,113	2.56	24 (34%)
14	CLA	B	1214	-	64,68,73	2.35	21 (32%)	76,107,113	2.52	30 (39%)
20	LMG	A	5003	-	46,46,55	1.37	5 (10%)	54,54,63	1.26	4 (7%)
14	CLA	G	1107	-	49,53,73	2.52	19 (38%)	58,89,113	2.77	22 (37%)
14	CLA	a	1115	-	69,73,73	2.24	20 (28%)	82,113,113	2.53	29 (35%)
14	CLA	B	1233	-	49,53,73	2.55	22 (44%)	58,89,113	2.75	25 (43%)
14	CLA	b	1204	-	69,73,73	2.21	21 (30%)	82,113,113	2.50	25 (30%)
18	BCR	G	4002	-	41,41,41	2.64	6 (14%)	56,56,56	6.67	25 (44%)
14	CLA	H	1226	-	69,73,73	2.26	19 (27%)	82,113,113	2.45	26 (31%)
18	BCR	H	4009	-	41,41,41	2.73	7 (17%)	56,56,56	6.67	24 (42%)
14	CLA	b	1232	-	49,53,73	2.54	22 (44%)	58,89,113	2.75	23 (39%)
14	CLA	G	1130	-	59,63,73	2.42	20 (33%)	70,101,113	2.49	25 (35%)
21	LMT	R	6001	-	36,36,36	1.15	5 (13%)	47,47,47	1.04	2 (4%)
14	CLA	G	1132	-	69,73,73	2.20	21 (30%)	82,113,113	2.57	27 (32%)
14	CLA	B	1201	-	69,73,73	2.19	23 (33%)	82,113,113	2.61	28 (34%)
16	PQN	b	2002	-	34,34,34	1.59	2 (5%)	43,45,45	1.12	2 (4%)
14	CLA	G	1133	1	64,68,73	2.30	20 (31%)	76,107,113	2.59	21 (27%)
14	CLA	B	1229	-	64,68,73	2.32	21 (32%)	76,107,113	2.58	26 (34%)
24	FES	X	101	12	0,4,4	-	-	-	-	-
14	CLA	b	1229	-	64,68,73	2.32	21 (32%)	76,107,113	2.58	26 (34%)
14	CLA	B	1022	-	59,63,73	2.37	19 (32%)	70,101,113	2.61	27 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	G	1138	-	59,63,73	2.37	22 (37%)	70,101,113	2.75	28 (40%)
14	CLA	b	1222	25	69,73,73	2.20	21 (30%)	82,113,113	2.54	28 (34%)
14	CLA	b	1216	-	69,73,73	2.23	21 (30%)	82,113,113	2.31	22 (26%)
21	LMT	G	6004	-	24,24,36	1.04	3 (12%)	29,29,47	1.08	1 (3%)

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	G	1116	-	1/1/13/20	14/27/103/115	-
14	CLA	B	1222	25	1/1/15/20	16/39/115/115	-
18	BCR	A	4001	-	-	12/29/63/63	0/2/2/2
14	CLA	b	1202	-	1/1/15/20	14/39/115/115	-
14	CLA	b	1209	-	1/1/11/20	4/15/91/115	-
20	LMG	G	5003	-	-	15/41/61/70	0/1/1/1
14	CLA	a	1101	-	1/1/11/20	8/15/91/115	-
14	CLA	A	1129	-	1/1/12/20	7/21/97/115	-
21	LMT	U	6002	-	-	6/21/61/61	0/2/2/2
14	CLA	H	1211	-	1/1/15/20	13/39/115/115	-
21	LMT	H	6003	-	-	10/21/61/61	0/2/2/2
21	LMT	I	6001	-	-	10/21/61/61	0/2/2/2
14	CLA	a	1129	-	1/1/12/20	7/21/97/115	-
15	F6C	a	1121	-	1/1/6/16	10/17/73/97	-
18	BCR	a	4006	-	-	15/29/63/63	0/2/2/2
18	BCR	G	4006	-	-	14/29/63/63	0/2/2/2
19	LHG	A	5002	-	-	24/45/45/53	-
18	BCR	B	4006	-	-	16/29/63/63	0/2/2/2
14	CLA	H	1239	-	1/1/15/20	22/39/115/115	-
14	CLA	a	1125	-	1/1/15/20	16/39/115/115	-
14	CLA	a	1104	-	1/1/15/20	18/39/115/115	-
14	CLA	G	1126	-	1/1/14/20	13/33/109/115	-
14	CLA	a	1013	-	1/1/14/20	8/33/109/115	-
14	CLA	U	1503	-	1/1/15/20	12/39/115/115	-
14	CLA	a	1103	-	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMG	B	5002	-	-	17/41/61/70	0/1/1/1
21	LMT	G	6002	-	-	8/14/54/61	0/2/2/2
14	CLA	a	1127	-	1/1/15/20	16/39/115/115	-
14	CLA	G	1101	-	1/1/11/20	8/15/91/115	-
14	CLA	B	1209	-	1/1/11/20	4/15/91/115	-
14	CLA	A	1139	-	1/1/11/20	6/15/91/115	-
18	BCR	H	4010	-	-	7/29/63/63	0/2/2/2
14	CLA	A	1109	-	1/1/15/20	15/39/115/115	-
17	SF4	c	3002	3	-	-	0/6/5/5
18	BCR	I	4018	-	-	11/29/63/63	0/2/2/2
19	LHG	A	5001	-	-	23/46/46/53	-
18	BCR	L	4019	-	-	9/29/63/63	0/2/2/2
14	CLA	b	1221	-	1/1/15/20	18/39/115/115	-
21	LMT	A	6003	-	-	7/18/58/61	0/2/2/2
14	CLA	a	1123	-	1/1/14/20	12/33/109/115	-
14	CLA	G	1129	-	1/1/12/20	7/21/97/115	-
14	CLA	G	1127	-	1/1/15/20	16/39/115/115	-
14	CLA	G	1104	-	1/1/15/20	18/39/115/115	-
15	F6C	b	1207	-	1/1/10/16	19/41/97/97	-
14	CLA	b	1022	-	1/1/13/20	10/27/103/115	-
14	CLA	B	1226	-	1/1/15/20	16/39/115/115	-
18	BCR	A	4005	-	-	10/29/63/63	0/2/2/2
14	CLA	G	1109	-	1/1/15/20	15/39/115/115	-
14	CLA	A	1108	-	1/1/11/20	3/15/91/115	-
15	F6C	B	1207	-	1/1/10/16	19/41/97/97	-
14	CLA	a	1106	1	1/1/14/20	10/33/109/115	-
17	SF4	N	3002	3	-	-	0/6/5/5
17	SF4	N	3003	3	-	-	0/6/5/5
14	CLA	b	1213	-	1/1/11/20	2/15/91/115	-
14	CLA	G	1120	-	1/1/11/20	5/15/91/115	-
14	CLA	a	1126	-	1/1/14/20	14/33/109/115	-
14	CLA	a	1012	25	1/1/15/20	9/39/115/115	-
16	PQN	G	2001	-	-	8/23/43/43	0/2/2/2
14	CLA	G	1131	-	1/1/14/20	14/33/109/115	-
14	CLA	G	1112	-	1/1/13/20	11/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1122	-	1/1/13/20	14/27/103/115	-
14	CLA	A	1106	1	1/1/14/20	10/33/109/115	-
14	CLA	H	1232	-	1/1/11/20	2/15/91/115	-
18	BCR	H	4004	-	-	11/29/63/63	0/2/2/2
14	CLA	M	1501	-	1/1/12/20	8/21/97/115	-
14	CLA	T	1401	-	1/1/11/20	11/15/91/115	-
14	CLA	l	1501	10	1/1/15/20	6/39/115/115	-
14	CLA	G	1119	-	1/1/15/20	14/39/115/115	-
21	LMT	l	6001	-	-	5/11/11/61	-
15	F6C	H	1207	-	1/1/10/16	19/41/97/97	-
14	CLA	A	1126	-	1/1/14/20	13/33/109/115	-
14	CLA	b	1205	-	1/1/15/20	15/39/115/115	-
14	CLA	B	1213	-	1/1/11/20	2/15/91/115	-
14	CLA	b	1208	-	1/1/14/20	9/33/109/115	-
17	SF4	C	3003	3	-	-	0/6/5/5
18	BCR	B	4017	-	-	15/29/63/63	0/2/2/2
14	CLA	b	1228	-	1/1/13/20	14/27/103/115	-
14	CLA	G	1128	-	1/1/14/20	15/33/109/115	-
14	CLA	a	1139	-	1/1/11/20	6/15/91/115	-
18	BCR	b	4006	-	-	16/29/63/63	0/2/2/2
14	CLA	b	1211	-	1/1/15/20	13/39/115/115	-
14	CLA	G	1105	-	1/1/11/20	3/15/91/115	-
14	CLA	H	1201	-	1/1/15/20	18/39/115/115	-
14	CLA	H	1022	-	1/1/13/20	10/27/103/115	-
15	F6C	B	1230	-	1/1/6/16	9/17/73/97	-
14	CLA	A	1103	-	1/1/15/20	18/39/115/115	-
21	LMT	a	6001	-	-	9/17/57/61	0/2/2/2
18	BCR	l	4019	-	-	9/29/63/63	0/2/2/2
18	BCR	l	4022	-	-	7/29/63/63	0/2/2/2
14	CLA	G	1106	1	1/1/14/20	10/33/109/115	-
14	CLA	b	1220	-	1/1/15/20	12/39/115/115	-
13	CL0	A	1011	-	3/3/20/25	16/37/135/135	-
14	CLA	A	1013	-	1/1/14/20	8/33/109/115	-
18	BCR	B	4010	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1222	25	1/1/15/20	16/39/115/115	-
14	CLA	A	1119	-	1/1/15/20	14/39/115/115	-
14	CLA	A	1133	1	1/1/14/20	19/33/109/115	-
14	CLA	H	1213	-	1/1/11/20	2/15/91/115	-
21	LMT	M	6000	-	-	5/21/61/61	0/2/2/2
14	CLA	B	1240	2	1/1/15/20	17/39/115/115	-
14	CLA	b	1212	-	1/1/11/20	5/15/91/115	-
18	BCR	H	4017	-	-	15/29/63/63	0/2/2/2
14	CLA	k	1401	-	1/1/11/20	11/15/91/115	-
14	CLA	A	1135	-	1/1/12/20	5/21/97/115	-
14	CLA	b	1240	2	1/1/15/20	17/39/115/115	-
19	LHG	L	5102	-	-	25/53/53/53	-
18	BCR	a	4003	-	-	9/29/63/63	0/2/2/2
21	LMT	A	6001	-	-	9/17/57/61	0/2/2/2
15	F6C	B	1219	-	1/1/8/16	16/29/85/97	-
14	CLA	G	1137	-	1/1/12/20	3/21/97/115	-
14	CLA	a	1135	-	1/1/12/20	5/21/97/115	-
14	CLA	A	1117	-	1/1/15/20	20/39/115/115	-
14	CLA	A	1141	-	1/1/11/20	11/15/91/115	-
14	CLA	H	1227	-	1/1/11/20	8/15/91/115	-
15	F6C	b	1238	25	1/1/10/16	15/41/97/97	-
14	CLA	G	1013	-	1/1/14/20	8/33/109/115	-
14	CLA	a	1131	-	1/1/14/20	14/33/109/115	-
15	F6C	G	1121	-	1/1/6/16	10/17/73/97	-
14	CLA	B	1221	-	1/1/15/20	18/39/115/115	-
14	CLA	a	1138	-	1/1/13/20	13/27/103/115	-
16	PQN	H	2002	-	-	7/23/43/43	0/2/2/2
19	LHG	G	5001	-	-	23/46/46/53	-
14	CLA	H	1240	2	1/1/15/20	17/39/115/115	-
21	LMT	V	6000	-	-	5/21/61/61	0/2/2/2
14	CLA	b	1235	-	1/1/14/20	12/33/109/115	-
21	LMT	U	6001	-	-	5/11/11/61	-
14	CLA	B	1224	-	1/1/15/20	19/39/115/115	-
18	BCR	b	4014	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	1224	-	1/1/15/20	19/39/115/115	-
18	BCR	a	4002	-	-	12/29/63/63	0/2/2/2
14	CLA	b	1234	-	1/1/15/20	16/39/115/115	-
21	LMT	a	6003	-	-	7/18/58/61	0/2/2/2
14	CLA	G	1102	-	1/1/12/20	8/21/97/115	-
17	SF4	c	3003	3	-	-	0/6/5/5
14	CLA	B	1236	-	1/1/13/20	15/27/103/115	-
14	CLA	a	1107	-	1/1/11/20	5/15/91/115	-
14	CLA	B	1232	-	1/1/11/20	2/15/91/115	-
18	BCR	G	4005	-	-	10/29/63/63	0/2/2/2
19	LHG	L	5101	-	-	15/26/26/53	-
18	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
14	CLA	A	1105	-	1/1/11/20	3/15/91/115	-
14	CLA	b	1021	-	1/1/15/20	12/39/115/115	-
18	BCR	H	4005	-	-	6/29/63/63	0/2/2/2
18	BCR	L	4022	-	-	7/29/63/63	0/2/2/2
14	CLA	H	1233	-	1/1/11/20	6/15/91/115	-
15	F6C	A	1121	-	1/1/6/16	10/17/73/97	-
14	CLA	L	1503	-	1/1/15/20	12/39/115/115	-
14	CLA	H	1210	-	1/1/15/20	14/39/115/115	-
18	BCR	i	4018	-	-	11/29/63/63	0/2/2/2
14	CLA	H	1212	-	1/1/11/20	5/15/91/115	-
14	CLA	a	1128	-	1/1/14/20	15/33/109/115	-
14	CLA	B	1235	-	1/1/14/20	12/33/109/115	-
18	BCR	b	4005	-	-	6/29/63/63	0/2/2/2
17	SF4	C	3002	3	-	-	0/6/5/5
14	CLA	H	1236	-	1/1/13/20	15/27/103/115	-
21	LMT	m	6000	-	-	5/21/61/61	0/2/2/2
24	FES	W	101	12	-	-	0/1/1/1
14	CLA	B	1215	-	1/1/14/20	13/33/109/115	-
14	CLA	b	1231	-	1/1/15/20	19/39/115/115	-
14	CLA	B	1202	-	1/1/15/20	14/39/115/115	-
14	CLA	b	1215	-	1/1/14/20	13/33/109/115	-
20	LMG	a	5003	-	-	15/41/61/70	0/1/1/1
18	BCR	b	4010	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	PQN	B	2002	-	-	7/23/43/43	0/2/2/2
18	BCR	U	4022	-	-	7/29/63/63	0/2/2/2
24	FES	x	101	12	-	-	0/1/1/1
14	CLA	a	1140	-	1/1/13/20	16/27/103/115	-
18	BCR	b	4009	-	-	4/29/63/63	0/2/2/2
18	BCR	H	4014	-	-	6/29/63/63	0/2/2/2
14	CLA	G	1123	-	1/1/14/20	11/33/109/115	-
14	CLA	G	1134	1	1/1/11/20	6/15/91/115	-
14	CLA	H	1235	-	1/1/14/20	12/33/109/115	-
18	BCR	U	4019	-	-	9/29/63/63	0/2/2/2
21	LMT	a	6002	-	-	8/14/54/61	0/2/2/2
21	LMT	G	6003	-	-	7/18/58/61	0/2/2/2
18	BCR	V	4021	-	-	14/29/63/63	0/2/2/2
15	F6C	b	1219	-	1/1/8/16	16/29/85/97	-
14	CLA	H	1215	-	1/1/14/20	13/33/109/115	-
21	LMT	b	6002	-	-	3/21/61/61	0/2/2/2
14	CLA	G	1103	-	1/1/15/20	18/39/115/115	-
14	CLA	A	1115	-	1/1/15/20	19/39/115/115	-
21	LMT	l	6101	-	-	8/21/61/61	0/2/2/2
14	CLA	a	1112	-	1/1/13/20	11/27/103/115	-
21	LMT	b	6004	-	-	10/17/57/61	0/2/2/2
13	CL0	G	1011	-	3/3/20/25	16/37/135/135	-
15	F6C	H	1230	-	1/1/6/16	9/17/73/97	-
14	CLA	B	1210	-	1/1/15/20	14/39/115/115	-
21	LMT	B	6003	-	-	10/21/61/61	0/2/2/2
14	CLA	b	1227	-	1/1/11/20	8/15/91/115	-
14	CLA	b	1233	-	1/1/11/20	6/15/91/115	-
14	CLA	B	1212	-	1/1/11/20	5/15/91/115	-
14	CLA	A	1130	-	1/1/13/20	9/27/103/115	-
14	CLA	G	1139	-	1/1/11/20	6/15/91/115	-
14	CLA	a	1116	-	1/1/13/20	14/27/103/115	-
14	CLA	a	1109	-	1/1/15/20	15/39/115/115	-
14	CLA	G	1012	25	1/1/15/20	9/39/115/115	-
15	F6C	H	1219	-	1/1/8/16	16/29/85/97	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	m	1501	-	1/1/12/20	8/21/97/115	-
21	LMT	U	6101	-	-	8/21/61/61	0/2/2/2
14	CLA	H	1220	-	1/1/15/20	13/39/115/115	-
21	LMT	B	6002	-	-	3/21/61/61	0/2/2/2
18	BCR	i	4020	-	-	7/29/63/63	0/2/2/2
14	CLA	A	1122	-	1/1/13/20	14/27/103/115	-
14	CLA	A	1120	-	1/1/11/20	5/15/91/115	-
21	LMT	L	6101	-	-	8/21/61/61	0/2/2/2
14	CLA	H	1202	-	1/1/15/20	14/39/115/115	-
21	LMT	H	6004	-	-	10/17/57/61	0/2/2/2
14	CLA	G	1110	-	1/1/11/20	3/15/91/115	-
14	CLA	a	1120	-	1/1/11/20	5/15/91/115	-
16	PQN	a	2001	-	-	8/23/43/43	0/2/2/2
14	CLA	A	1112	-	1/1/13/20	11/27/103/115	-
18	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
18	BCR	B	4014	-	-	6/29/63/63	0/2/2/2
14	CLA	U	1502	-	1/1/14/20	10/33/109/115	-
14	CLA	G	1108	-	1/1/11/20	3/15/91/115	-
14	CLA	H	1221	-	1/1/15/20	18/39/115/115	-
18	BCR	R	4020	-	-	7/29/63/63	0/2/2/2
14	CLA	b	1210	-	1/1/15/20	14/39/115/115	-
18	BCR	I	4020	-	-	7/29/63/63	0/2/2/2
14	CLA	H	1224	-	1/1/15/20	19/39/115/115	-
14	CLA	b	1201	-	1/1/15/20	18/39/115/115	-
20	LMG	R	5006	-	-	13/32/52/70	0/1/1/1
20	LMG	i	5006	-	-	13/32/52/70	0/1/1/1
14	CLA	A	1111	-	1/1/14/20	17/33/109/115	-
14	CLA	A	1107	-	1/1/11/20	5/15/91/115	-
14	CLA	a	1136	-	1/1/15/20	18/39/115/115	-
15	F6C	b	1230	-	1/1/6/16	9/17/73/97	-
14	CLA	a	1105	-	1/1/11/20	3/15/91/115	-
18	BCR	K	4001	-	-	16/29/63/63	0/2/2/2
15	F6C	B	1237	25	1/1/10/16	22/41/97/97	-
14	CLA	a	1118	-	1/1/13/20	12/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMT	L	6001	-	-	5/11/11/61	-
14	CLA	H	1217	-	1/1/11/20	8/15/91/115	-
19	LHG	G	5002	-	-	24/45/45/53	-
14	CLA	H	1223	-	1/1/15/20	11/39/115/115	-
14	CLA	A	1140	-	1/1/13/20	16/27/103/115	-
14	CLA	H	1229	-	1/1/14/20	13/33/109/115	-
14	CLA	B	1021	-	1/1/15/20	12/39/115/115	-
18	BCR	b	4017	-	-	15/29/63/63	0/2/2/2
14	CLA	a	1133	1	1/1/14/20	19/33/109/115	-
14	CLA	B	1217	-	1/1/11/20	8/15/91/115	-
14	CLA	A	1125	-	1/1/15/20	16/39/115/115	-
14	CLA	H	1203	-	1/1/15/20	23/39/115/115	-
18	BCR	a	4004	-	-	10/29/63/63	0/2/2/2
14	CLA	l	1502	-	1/1/14/20	10/33/109/115	-
20	LMG	b	5002	-	-	17/41/61/70	0/1/1/1
17	SF4	a	3001	2,1	-	-	0/6/5/5
18	BCR	a	4005	-	-	10/29/63/63	0/2/2/2
14	CLA	A	1116	-	1/1/13/20	14/27/103/115	-
14	CLA	G	1113	-	1/1/11/20	7/15/91/115	-
15	F6C	H	1237	25	1/1/10/16	22/41/97/97	-
14	CLA	b	1206	-	1/1/15/20	20/39/115/115	-
14	CLA	B	1220	-	1/1/15/20	13/39/115/115	-
14	CLA	a	1108	-	1/1/11/20	3/15/91/115	-
14	CLA	H	1228	-	1/1/13/20	14/27/103/115	-
14	CLA	a	1141	-	1/1/11/20	11/15/91/115	-
18	BCR	G	4004	-	-	10/29/63/63	0/2/2/2
14	CLA	K	1401	-	1/1/11/20	11/15/91/115	-
14	CLA	G	1135	-	1/1/12/20	5/21/97/115	-
18	BCR	R	4018	-	-	11/29/63/63	0/2/2/2
14	CLA	B	1205	-	1/1/15/20	15/39/115/115	-
15	F6C	b	1237	25	1/1/10/16	22/41/97/97	-
14	CLA	G	1117	-	1/1/15/20	20/39/115/115	-
14	CLA	a	1124	25	1/1/13/20	4/27/103/115	-
14	CLA	H	1204	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMT	b	6003	-	-	10/21/61/61	0/2/2/2
18	BCR	T	4001	-	-	16/29/63/63	0/2/2/2
13	CL0	a	1011	-	3/3/20/25	16/37/135/135	-
14	CLA	G	1125	-	1/1/15/20	17/39/115/115	-
14	CLA	a	1102	-	1/1/12/20	8/21/97/115	-
14	CLA	H	1234	-	1/1/15/20	16/39/115/115	-
15	F6C	B	1238	25	1/1/10/16	15/41/97/97	-
19	LHG	a	5002	-	-	24/45/45/53	-
14	CLA	B	1223	-	1/1/15/20	11/39/115/115	-
19	LHG	l	5102	-	-	25/53/53/53	-
18	BCR	M	4021	-	-	14/29/63/63	0/2/2/2
14	CLA	a	1119	-	1/1/15/20	14/39/115/115	-
14	CLA	b	1203	-	1/1/15/20	23/39/115/115	-
14	CLA	V	1501	-	1/1/12/20	8/21/97/115	-
14	CLA	H	1218	-	1/1/11/20	5/15/91/115	-
14	CLA	H	1216	-	1/1/15/20	20/39/115/115	-
14	CLA	B	1203	-	1/1/15/20	23/39/115/115	-
14	CLA	a	1134	1	1/1/11/20	6/15/91/115	-
14	CLA	a	1111	-	1/1/14/20	17/33/109/115	-
18	BCR	A	4004	-	-	10/29/63/63	0/2/2/2
14	CLA	A	1012	25	1/1/15/20	9/39/115/115	-
14	CLA	A	1131	-	1/1/14/20	14/33/109/115	-
14	CLA	b	1023	-	1/1/15/20	8/39/115/115	-
21	LMT	A	6002	-	-	8/14/54/61	0/2/2/2
14	CLA	B	1228	-	1/1/13/20	14/27/103/115	-
14	CLA	G	1118	-	1/1/13/20	12/27/103/115	-
14	CLA	A	1101	-	1/1/11/20	8/15/91/115	-
15	F6C	H	1238	25	1/1/10/16	15/41/97/97	-
21	LMT	H	6002	-	-	3/21/61/61	0/2/2/2
14	CLA	A	1118	-	1/1/13/20	12/27/103/115	-
14	CLA	A	1123	-	1/1/14/20	11/33/109/115	-
14	CLA	B	1225	-	1/1/15/20	16/39/115/115	-
14	CLA	H	1231	-	1/1/15/20	19/39/115/115	-
14	CLA	B	1239	-	1/1/15/20	22/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1110	-	1/1/11/20	3/15/91/115	-
14	CLA	B	1204	-	1/1/15/20	11/39/115/115	-
21	LMT	B	6001	-	-	7/21/61/61	0/2/2/2
14	CLA	b	1217	-	1/1/11/20	8/15/91/115	-
14	CLA	b	1226	-	1/1/15/20	16/39/115/115	-
21	LMT	b	6001	-	-	7/21/61/61	0/2/2/2
14	CLA	b	1223	-	1/1/15/20	11/39/115/115	-
14	CLA	L	1501	10	1/1/15/20	6/39/115/115	-
14	CLA	G	1111	-	1/1/14/20	17/33/109/115	-
14	CLA	H	1208	-	1/1/14/20	9/33/109/115	-
14	CLA	B	1023	-	1/1/15/20	8/39/115/115	-
14	CLA	U	1501	10	1/1/15/20	6/39/115/115	-
21	LMT	l	6002	-	-	6/21/61/61	0/2/2/2
14	CLA	b	1214	-	1/1/14/20	13/33/109/115	-
14	CLA	B	1216	-	1/1/15/20	20/39/115/115	-
14	CLA	G	1136	-	1/1/15/20	18/39/115/115	-
14	CLA	a	1122	-	1/1/13/20	14/27/103/115	-
14	CLA	a	1137	-	1/1/12/20	3/21/97/115	-
21	LMT	H	6001	-	-	7/21/61/61	0/2/2/2
21	LMT	G	6001	-	-	9/17/57/61	0/2/2/2
14	CLA	H	1206	-	1/1/15/20	20/39/115/115	-
14	CLA	A	1137	-	1/1/12/20	3/21/97/115	-
14	CLA	a	1110	-	1/1/11/20	3/15/91/115	-
16	PQN	A	2001	-	-	8/23/43/43	0/2/2/2
14	CLA	G	1141	-	1/1/11/20	11/15/91/115	-
18	BCR	b	4004	-	-	11/29/63/63	0/2/2/2
14	CLA	b	1236	-	1/1/13/20	15/27/103/115	-
18	BCR	B	4009	-	-	4/29/63/63	0/2/2/2
14	CLA	G	1114	-	1/1/11/20	6/15/91/115	-
14	CLA	A	1114	-	1/1/11/20	6/15/91/115	-
14	CLA	b	1239	-	1/1/15/20	22/39/115/115	-
14	CLA	A	1132	-	1/1/15/20	12/39/115/115	-
14	CLA	l	1503	-	1/1/15/20	12/39/115/115	-
14	CLA	B	1234	-	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1023	-	1/1/15/20	8/39/115/115	-
14	CLA	B	1231	-	1/1/15/20	19/39/115/115	-
14	CLA	A	1113	-	1/1/11/20	7/15/91/115	-
14	CLA	L	1502	-	1/1/14/20	10/33/109/115	-
18	BCR	A	4006	-	-	15/29/63/63	0/2/2/2
14	CLA	b	1225	-	1/1/15/20	16/39/115/115	-
14	CLA	A	1136	-	1/1/15/20	18/39/115/115	-
17	SF4	A	3001	2,1	-	-	0/6/5/5
14	CLA	a	1114	-	1/1/11/20	6/15/91/115	-
14	CLA	B	1218	-	1/1/11/20	5/15/91/115	-
14	CLA	H	1209	-	1/1/11/20	4/15/91/115	-
18	BCR	m	4021	-	-	14/29/63/63	0/2/2/2
19	LHG	U	5102	-	-	25/53/53/53	-
14	CLA	H	1205	-	1/1/15/20	15/39/115/115	-
14	CLA	B	1208	-	1/1/14/20	9/33/109/115	-
19	LHG	U	5101	-	-	15/26/26/53	-
14	CLA	H	1214	-	1/1/14/20	13/33/109/115	-
14	CLA	B	1211	-	1/1/15/20	13/39/115/115	-
14	CLA	A	1134	1	1/1/11/20	6/15/91/115	-
18	BCR	A	4002	-	-	12/29/63/63	0/2/2/2
18	BCR	H	4006	-	-	16/29/63/63	0/2/2/2
14	CLA	a	1130	-	1/1/13/20	9/27/103/115	-
14	CLA	G	1124	25	1/1/13/20	4/27/103/115	-
14	CLA	A	1127	-	1/1/15/20	16/39/115/115	-
14	CLA	A	1104	-	1/1/15/20	18/39/115/115	-
18	BCR	G	4001	-	-	12/29/63/63	0/2/2/2
14	CLA	A	1124	25	1/1/13/20	4/27/103/115	-
14	CLA	B	1227	-	1/1/11/20	8/15/91/115	-
14	CLA	a	1113	-	1/1/11/20	7/15/91/115	-
20	LMG	I	5006	-	-	13/32/52/70	0/1/1/1
20	LMG	H	5002	-	-	17/41/61/70	0/1/1/1
19	LHG	l	5101	-	-	14/26/26/53	-
14	CLA	A	1102	-	1/1/12/20	8/21/97/115	-
17	SF4	G	3001	2,1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1138	-	1/1/13/20	13/27/103/115	-
14	CLA	H	1021	-	1/1/15/20	12/39/115/115	-
18	BCR	a	4001	-	-	12/29/63/63	0/2/2/2
18	BCR	k	4001	-	-	16/29/63/63	0/2/2/2
14	CLA	a	1117	-	1/1/15/20	20/39/115/115	-
19	LHG	a	5001	-	-	23/46/46/53	-
14	CLA	b	1218	-	1/1/11/20	5/15/91/115	-
14	CLA	H	1225	-	1/1/15/20	16/39/115/115	-
14	CLA	A	1128	-	1/1/14/20	15/33/109/115	-
14	CLA	B	1206	-	1/1/15/20	20/39/115/115	-
14	CLA	G	1115	-	1/1/15/20	19/39/115/115	-
18	BCR	A	4003	-	-	9/29/63/63	0/2/2/2
18	BCR	G	4003	-	-	9/29/63/63	0/2/2/2
14	CLA	a	1132	-	1/1/15/20	12/39/115/115	-
21	LMT	A	6004	-	-	6/15/35/61	0/1/1/2
21	LMT	i	6001	-	-	10/21/61/61	0/2/2/2
21	LMT	a	6004	-	-	6/15/35/61	0/1/1/2
21	LMT	L	6002	-	-	6/21/61/61	0/2/2/2
21	LMT	B	6004	-	-	10/17/57/61	0/2/2/2
14	CLA	G	1140	-	1/1/13/20	16/27/103/115	-
14	CLA	B	1214	-	1/1/14/20	13/33/109/115	-
20	LMG	A	5003	-	-	15/41/61/70	0/1/1/1
14	CLA	G	1107	-	1/1/11/20	5/15/91/115	-
14	CLA	a	1115	-	1/1/15/20	19/39/115/115	-
14	CLA	B	1233	-	1/1/11/20	6/15/91/115	-
14	CLA	b	1204	-	1/1/15/20	11/39/115/115	-
18	BCR	G	4002	-	-	12/29/63/63	0/2/2/2
14	CLA	H	1226	-	1/1/15/20	16/39/115/115	-
18	BCR	H	4009	-	-	4/29/63/63	0/2/2/2
14	CLA	b	1232	-	1/1/11/20	2/15/91/115	-
14	CLA	G	1130	-	1/1/13/20	9/27/103/115	-
21	LMT	R	6001	-	-	10/21/61/61	0/2/2/2
14	CLA	G	1132	-	1/1/15/20	12/39/115/115	-
14	CLA	B	1201	-	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	PQN	b	2002	-	-	7/23/43/43	0/2/2/2
14	CLA	G	1133	1	1/1/14/20	19/33/109/115	-
14	CLA	B	1229	-	1/1/14/20	13/33/109/115	-
24	FES	X	101	12	-	-	0/1/1/1
14	CLA	b	1229	-	1/1/14/20	13/33/109/115	-
14	CLA	B	1022	-	1/1/13/20	10/27/103/115	-
14	CLA	G	1138	-	1/1/13/20	13/27/103/115	-
14	CLA	b	1222	25	1/1/15/20	15/39/115/115	-
14	CLA	b	1216	-	1/1/15/20	20/39/115/115	-
21	LMT	G	6004	-	-	6/15/35/61	0/1/1/2

The worst 5 of 6470 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	1121	F6C	C1A-CHA	10.09	1.51	1.35
15	A	1121	F6C	C1A-CHA	10.04	1.51	1.35
15	G	1121	F6C	C1A-CHA	10.01	1.51	1.35
15	b	1237	F6C	C1A-CHA	9.81	1.51	1.35
15	H	1237	F6C	C1A-CHA	9.80	1.51	1.35

The worst 5 of 8565 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	i	4020	BCR	C20-C21-C22	27.72	166.15	127.28
18	I	4020	BCR	C20-C21-C22	27.70	166.13	127.28
18	R	4020	BCR	C20-C21-C22	27.68	166.10	127.28
18	b	4010	BCR	C16-C17-C18	27.61	166.00	127.28
18	H	4010	BCR	C16-C17-C18	27.59	165.97	127.28

5 of 282 chirality outliers are listed below:

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

5 of 4628 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1011	CL0	CHA-CBD-CGD-O1D
13	G	1011	CL0	CHA-CBD-CGD-O1D
13	a	1011	CL0	CHA-CBD-CGD-O1D
14	A	1013	CLA	C1A-C2A-CAA-CBA
14	A	1013	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

354 monomers are involved in 980 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	1116	CLA	5	0
14	B	1222	CLA	5	0
18	A	4001	BCR	2	0
14	b	1202	CLA	7	0
14	b	1209	CLA	1	0
20	G	5003	LMG	3	0
14	a	1101	CLA	1	0
21	U	6002	LMT	2	0
14	H	1211	CLA	3	0
21	H	6003	LMT	1	0
21	I	6001	LMT	3	0
15	a	1121	F6C	2	0
18	a	4006	BCR	7	0
18	G	4006	BCR	7	0
19	A	5002	LHG	2	0
18	B	4006	BCR	2	0
14	H	1239	CLA	4	0
14	a	1125	CLA	2	0
14	a	1104	CLA	2	0
14	G	1126	CLA	5	0
14	a	1013	CLA	2	0
14	U	1503	CLA	16	0
14	a	1103	CLA	4	0
20	B	5002	LMG	5	0
14	a	1127	CLA	2	0
14	G	1101	CLA	1	0
14	B	1209	CLA	1	0
18	H	4010	BCR	2	0
14	A	1109	CLA	5	0
18	I	4018	BCR	4	0
19	A	5001	LHG	3	0
18	L	4019	BCR	3	0
14	b	1221	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	6003	LMT	1	0
14	a	1123	CLA	1	0
14	G	1127	CLA	1	0
14	G	1104	CLA	4	0
15	b	1207	F6C	1	0
14	b	1022	CLA	7	0
14	B	1226	CLA	1	0
14	G	1109	CLA	4	0
14	A	1108	CLA	7	0
15	B	1207	F6C	1	0
14	a	1106	CLA	4	0
14	b	1213	CLA	2	0
14	G	1120	CLA	1	0
14	a	1126	CLA	4	0
14	a	1012	CLA	4	0
16	G	2001	PQN	2	0
14	G	1131	CLA	3	0
14	G	1112	CLA	2	0
14	G	1122	CLA	3	0
14	A	1106	CLA	5	0
14	H	1232	CLA	1	0
18	H	4004	BCR	3	0
14	M	1501	CLA	5	0
14	T	1401	CLA	4	0
14	l	1501	CLA	21	0
14	G	1119	CLA	2	0
21	l	6001	LMT	1	0
15	H	1207	F6C	1	0
14	A	1126	CLA	6	0
14	b	1205	CLA	5	0
14	B	1213	CLA	2	0
14	b	1208	CLA	2	0
18	B	4017	BCR	3	0
14	b	1228	CLA	3	0
14	G	1128	CLA	2	0
18	b	4006	BCR	2	0
14	b	1211	CLA	4	0
14	G	1105	CLA	1	0
14	H	1201	CLA	8	0
14	H	1022	CLA	7	0
14	A	1103	CLA	4	0
18	l	4019	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	l	4022	BCR	2	0
14	G	1106	CLA	4	0
14	b	1220	CLA	3	0
13	A	1011	CL0	6	0
14	A	1013	CLA	2	0
18	B	4010	BCR	2	0
14	H	1222	CLA	6	0
14	A	1119	CLA	2	0
14	A	1133	CLA	1	0
14	H	1213	CLA	2	0
14	B	1240	CLA	1	0
14	b	1212	CLA	1	0
18	H	4017	BCR	3	0
14	k	1401	CLA	4	0
14	A	1135	CLA	2	0
14	b	1240	CLA	1	0
19	L	5102	LHG	1	0
18	a	4003	BCR	3	0
15	B	1219	F6C	6	0
14	a	1135	CLA	2	0
14	A	1117	CLA	2	0
14	A	1141	CLA	2	0
14	H	1227	CLA	5	0
14	G	1013	CLA	3	0
14	a	1131	CLA	3	0
15	G	1121	F6C	2	0
14	B	1221	CLA	10	0
16	H	2002	PQN	3	0
19	G	5001	LHG	3	0
14	H	1240	CLA	2	0
14	b	1235	CLA	4	0
21	U	6001	LMT	1	0
14	B	1224	CLA	6	0
18	b	4014	BCR	3	0
14	b	1224	CLA	8	0
18	a	4002	BCR	3	0
14	b	1234	CLA	5	0
14	G	1102	CLA	1	0
21	a	6003	LMT	1	0
14	B	1236	CLA	3	0
14	a	1107	CLA	1	0
18	G	4005	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	L	5101	LHG	2	0
18	B	4004	BCR	4	0
14	A	1105	CLA	1	0
18	H	4005	BCR	3	0
18	L	4022	BCR	3	0
15	A	1121	F6C	2	0
14	L	1503	CLA	16	0
14	H	1210	CLA	4	0
18	i	4018	BCR	4	0
14	H	1212	CLA	1	0
14	a	1128	CLA	2	0
14	B	1235	CLA	4	0
18	b	4005	BCR	3	0
14	H	1236	CLA	4	0
14	B	1215	CLA	4	0
14	b	1231	CLA	4	0
14	B	1202	CLA	6	0
14	b	1215	CLA	4	0
20	a	5003	LMG	4	0
18	b	4010	BCR	1	0
16	B	2002	PQN	3	0
18	U	4022	BCR	3	0
18	b	4009	BCR	4	0
18	H	4014	BCR	3	0
14	G	1123	CLA	2	0
14	G	1134	CLA	3	0
14	H	1235	CLA	5	0
18	U	4019	BCR	3	0
21	G	6003	LMT	1	0
18	V	4021	BCR	5	0
15	b	1219	F6C	6	0
14	H	1215	CLA	4	0
21	b	6002	LMT	1	0
14	G	1103	CLA	5	0
14	A	1115	CLA	8	0
21	l	6101	LMT	1	0
14	a	1112	CLA	1	0
21	b	6004	LMT	2	0
13	G	1011	CL0	6	0
14	B	1210	CLA	3	0
21	B	6003	LMT	2	0
14	b	1227	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	1233	CLA	1	0
14	B	1212	CLA	1	0
14	A	1130	CLA	3	0
14	a	1116	CLA	5	0
14	a	1109	CLA	5	0
14	G	1012	CLA	4	0
15	H	1219	F6C	6	0
14	m	1501	CLA	5	0
21	U	6101	LMT	1	0
14	H	1220	CLA	4	0
21	B	6002	LMT	1	0
18	i	4020	BCR	4	0
14	A	1122	CLA	3	0
14	A	1120	CLA	1	0
21	L	6101	LMT	1	0
14	H	1202	CLA	6	0
21	H	6004	LMT	2	0
14	a	1120	CLA	1	0
16	a	2001	PQN	4	0
14	A	1112	CLA	3	0
18	B	4005	BCR	3	0
18	B	4014	BCR	3	0
14	U	1502	CLA	3	0
14	G	1108	CLA	8	0
14	H	1221	CLA	10	0
18	R	4020	BCR	5	0
14	b	1210	CLA	3	0
18	I	4020	BCR	4	0
14	H	1224	CLA	7	0
14	b	1201	CLA	6	0
20	R	5006	LMG	1	0
20	i	5006	LMG	1	0
14	A	1111	CLA	5	0
14	A	1107	CLA	1	0
14	a	1136	CLA	4	0
14	a	1105	CLA	1	0
18	K	4001	BCR	2	0
14	a	1118	CLA	2	0
21	L	6001	LMT	1	0
14	H	1217	CLA	3	0
19	G	5002	LHG	2	0
14	H	1223	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	1140	CLA	1	0
14	H	1229	CLA	4	0
18	b	4017	BCR	2	0
14	a	1133	CLA	1	0
14	B	1217	CLA	3	0
14	A	1125	CLA	2	0
14	H	1203	CLA	5	0
18	a	4004	BCR	3	0
14	l	1502	CLA	2	0
20	b	5002	LMG	5	0
18	a	4005	BCR	1	0
14	A	1116	CLA	6	0
14	G	1113	CLA	11	0
14	b	1206	CLA	6	0
14	B	1220	CLA	3	0
14	a	1108	CLA	8	0
14	H	1228	CLA	2	0
14	a	1141	CLA	2	0
18	G	4004	BCR	3	0
14	K	1401	CLA	4	0
14	G	1135	CLA	2	0
18	R	4018	BCR	5	0
14	B	1205	CLA	6	0
14	G	1117	CLA	2	0
14	a	1124	CLA	3	0
14	H	1204	CLA	4	0
21	b	6003	LMT	1	0
18	T	4001	BCR	3	0
13	a	1011	CL0	6	0
14	G	1125	CLA	1	0
14	a	1102	CLA	1	0
14	H	1234	CLA	4	0
19	a	5002	LHG	2	0
14	B	1223	CLA	3	0
19	l	5102	LHG	1	0
18	M	4021	BCR	4	0
14	a	1119	CLA	2	0
14	b	1203	CLA	4	0
14	V	1501	CLA	5	0
14	H	1218	CLA	2	0
14	H	1216	CLA	6	0
14	B	1203	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a	1134	CLA	3	0
14	a	1111	CLA	5	0
18	A	4004	BCR	3	0
14	A	1012	CLA	4	0
14	A	1131	CLA	3	0
14	b	1023	CLA	4	0
14	B	1228	CLA	2	0
14	G	1118	CLA	2	0
14	A	1101	CLA	1	0
21	H	6002	LMT	1	0
14	A	1118	CLA	2	0
14	A	1123	CLA	2	0
14	B	1225	CLA	4	0
14	H	1231	CLA	2	0
14	B	1239	CLA	3	0
14	B	1204	CLA	4	0
21	B	6001	LMT	1	0
14	b	1217	CLA	3	0
14	b	1226	CLA	3	0
21	b	6001	LMT	1	0
14	b	1223	CLA	3	0
14	L	1501	CLA	21	0
14	G	1111	CLA	5	0
14	H	1208	CLA	1	0
14	B	1023	CLA	5	0
14	U	1501	CLA	21	0
21	l	6002	LMT	2	0
14	b	1214	CLA	3	0
14	B	1216	CLA	7	0
14	G	1136	CLA	3	0
14	a	1122	CLA	3	0
21	H	6001	LMT	1	0
14	H	1206	CLA	6	0
16	A	2001	PQN	3	0
14	G	1141	CLA	2	0
18	b	4004	BCR	2	0
14	b	1236	CLA	3	0
18	B	4009	BCR	3	0
14	b	1239	CLA	2	0
14	A	1132	CLA	3	0
14	l	1503	CLA	16	0
14	B	1234	CLA	5	0

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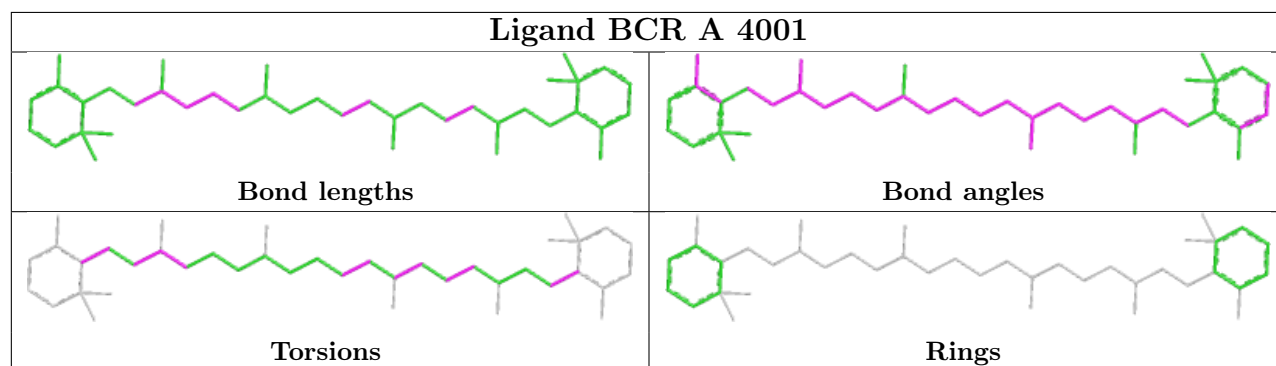
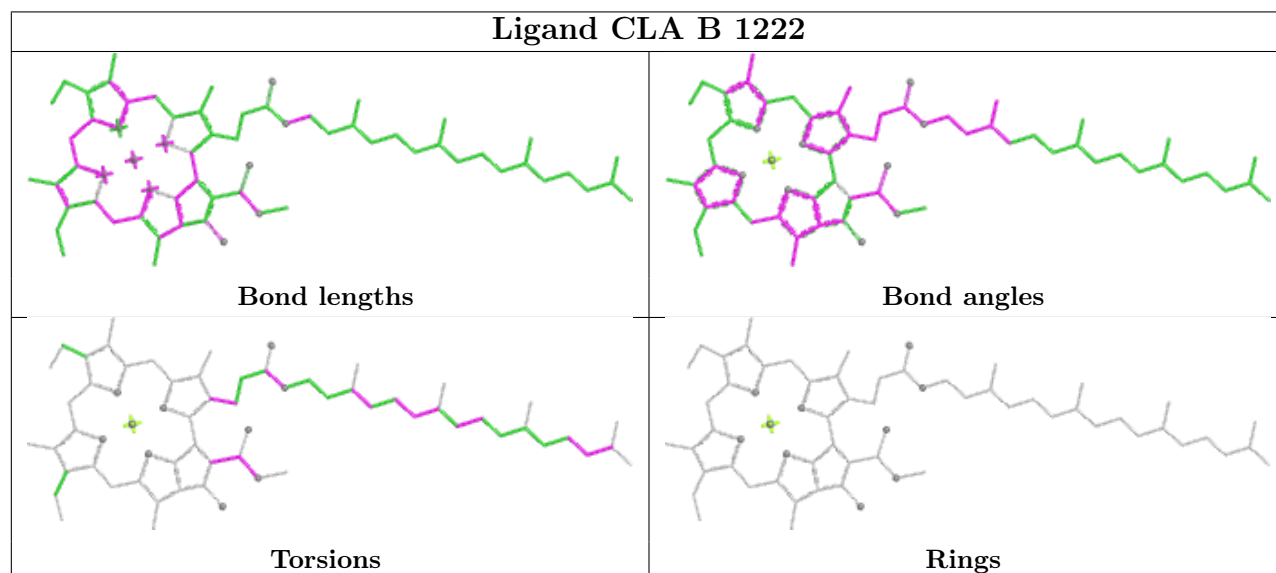
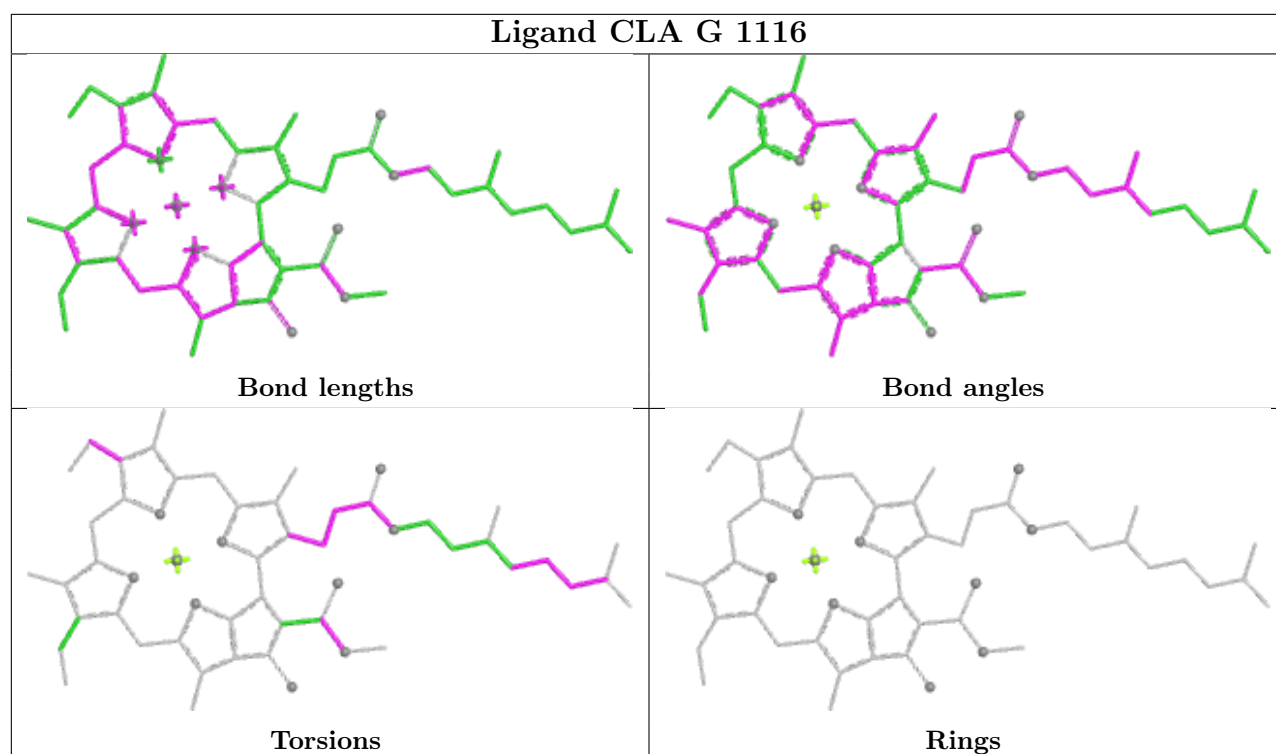
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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14	B	1231	CLA	2	0
14	A	1113	CLA	12	0
14	L	1502	CLA	3	0
18	A	4006	BCR	7	0
14	b	1225	CLA	5	0
14	A	1136	CLA	3	0
14	B	1218	CLA	2	0
14	H	1209	CLA	1	0
18	m	4021	BCR	5	0
19	U	5102	LHG	1	0
14	H	1205	CLA	5	0
14	B	1208	CLA	2	0
19	U	5101	LHG	3	0
14	H	1214	CLA	4	0
14	B	1211	CLA	4	0
14	A	1134	CLA	3	0
18	A	4002	BCR	3	0
18	H	4006	BCR	2	0
14	a	1130	CLA	3	0
14	G	1124	CLA	3	0
14	A	1127	CLA	1	0
14	A	1104	CLA	2	0
18	G	4001	BCR	1	0
14	A	1124	CLA	3	0
14	B	1227	CLA	4	0
14	a	1113	CLA	11	0
20	I	5006	LMG	1	0
20	H	5002	LMG	5	0
19	l	5101	LHG	2	0
14	A	1102	CLA	1	0
14	A	1138	CLA	1	0
18	a	4001	BCR	1	0
18	k	4001	BCR	2	0
14	a	1117	CLA	1	0
19	a	5001	LHG	3	0
14	b	1218	CLA	1	0
14	H	1225	CLA	5	0
14	A	1128	CLA	1	0
14	B	1206	CLA	7	0
14	G	1115	CLA	5	0
18	A	4003	BCR	2	0

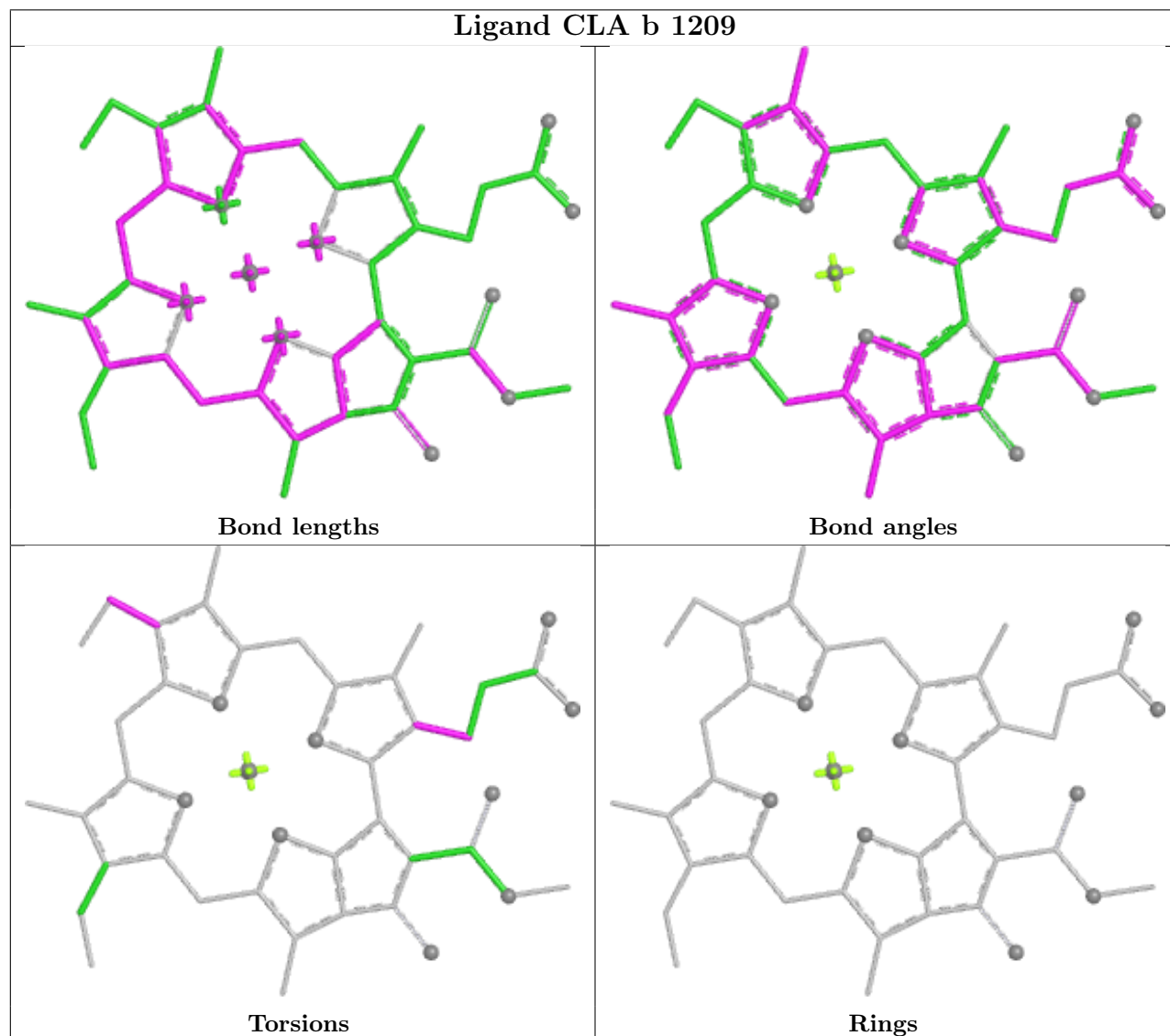
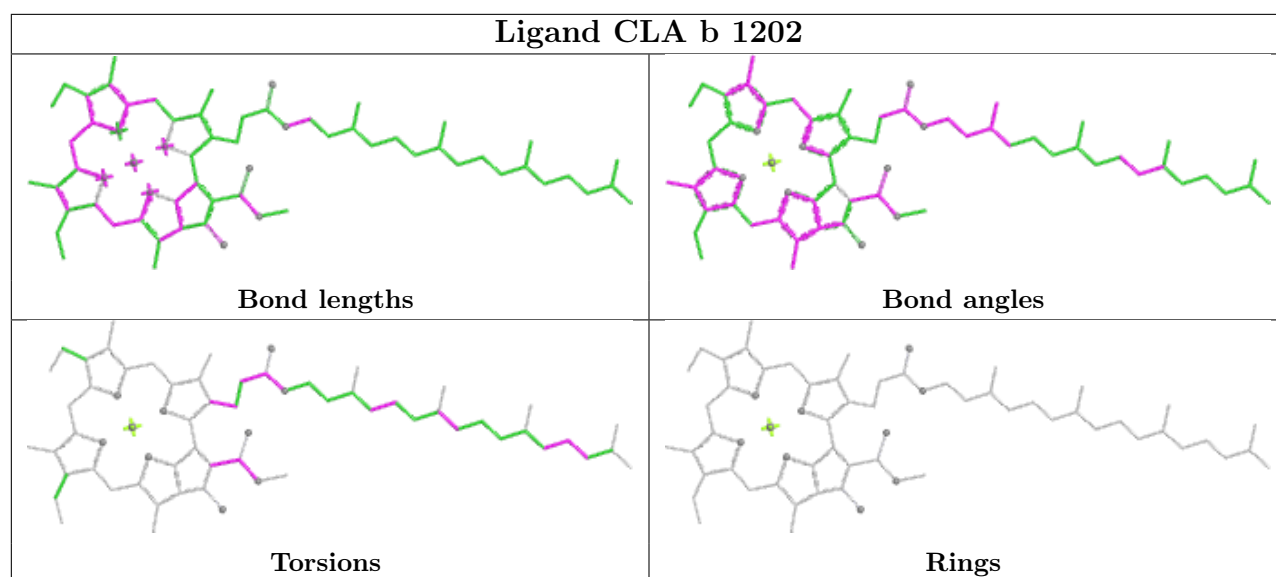
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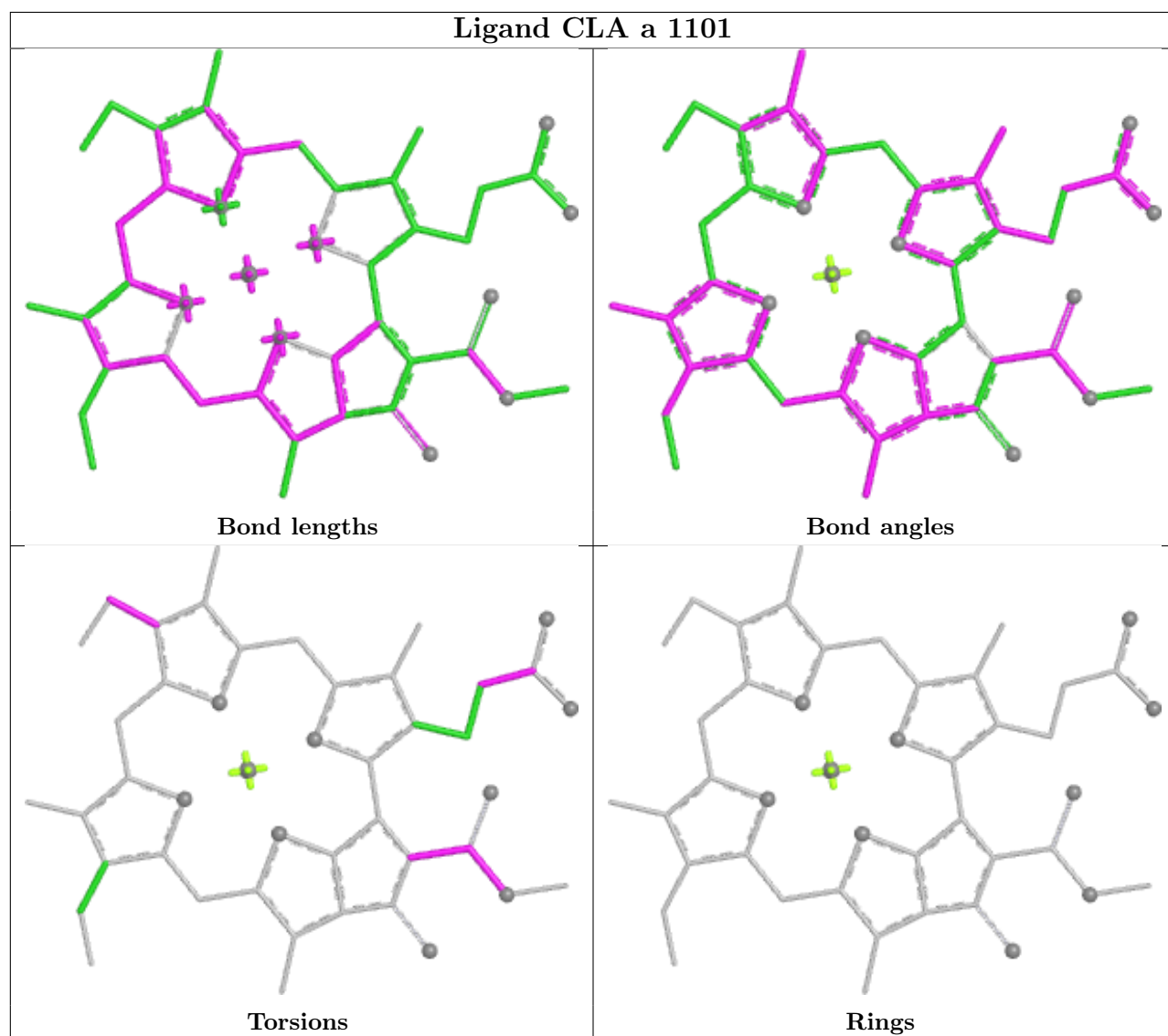
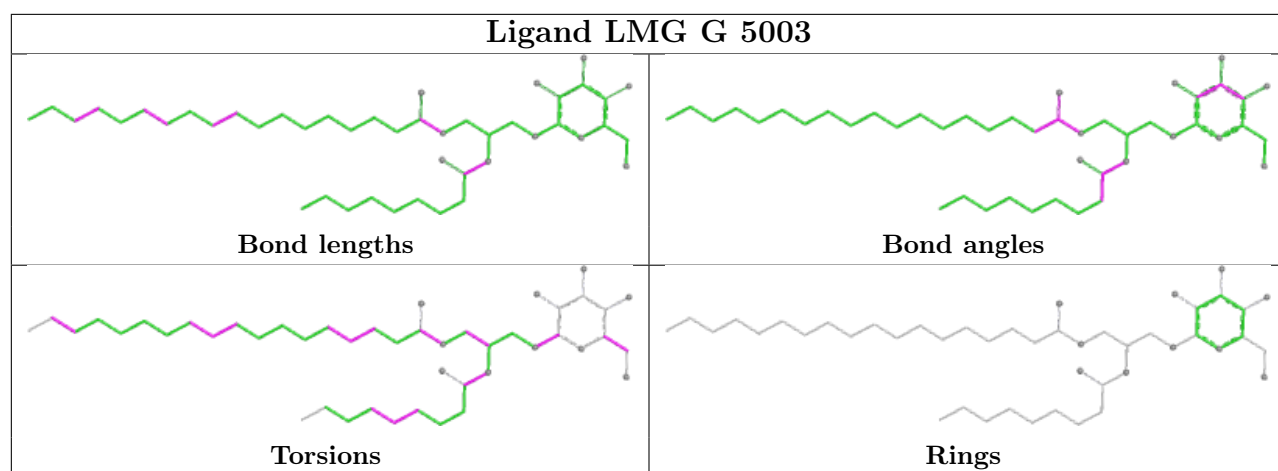
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	G	4003	BCR	2	0
14	a	1132	CLA	4	0
21	i	6001	LMT	2	0
21	L	6002	LMT	2	0
21	B	6004	LMT	2	0
14	G	1140	CLA	2	0
14	B	1214	CLA	4	0
20	A	5003	LMG	3	0
14	G	1107	CLA	1	0
14	a	1115	CLA	8	0
14	b	1204	CLA	4	0
18	G	4002	BCR	2	0
14	H	1226	CLA	3	0
18	H	4009	BCR	2	0
14	b	1232	CLA	1	0
14	G	1130	CLA	3	0
21	R	6001	LMT	3	0
14	G	1132	CLA	4	0
14	B	1201	CLA	6	0
16	b	2002	PQN	4	0
14	G	1133	CLA	2	0
14	B	1229	CLA	5	0
14	b	1229	CLA	3	0
14	B	1022	CLA	6	0
14	G	1138	CLA	1	0
14	b	1222	CLA	5	0
14	b	1216	CLA	7	0

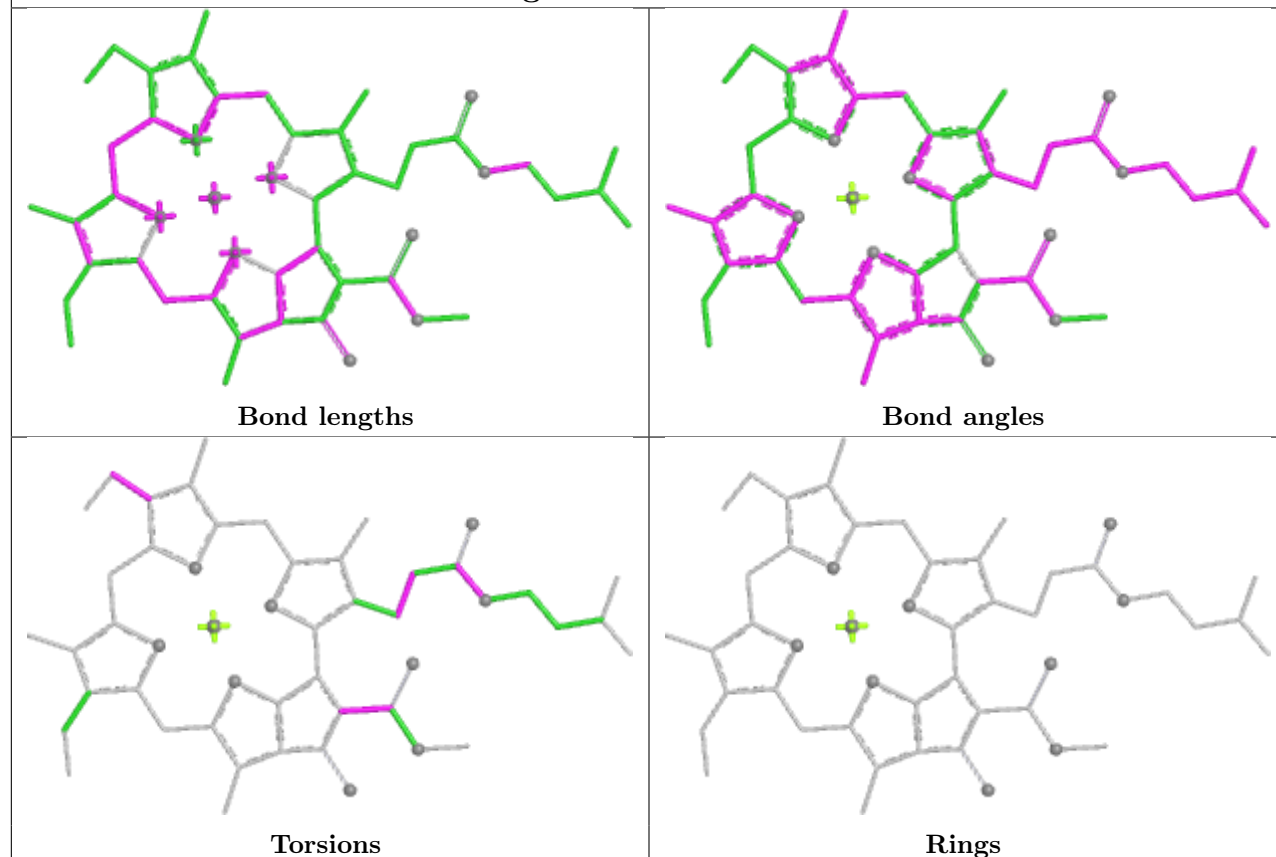
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



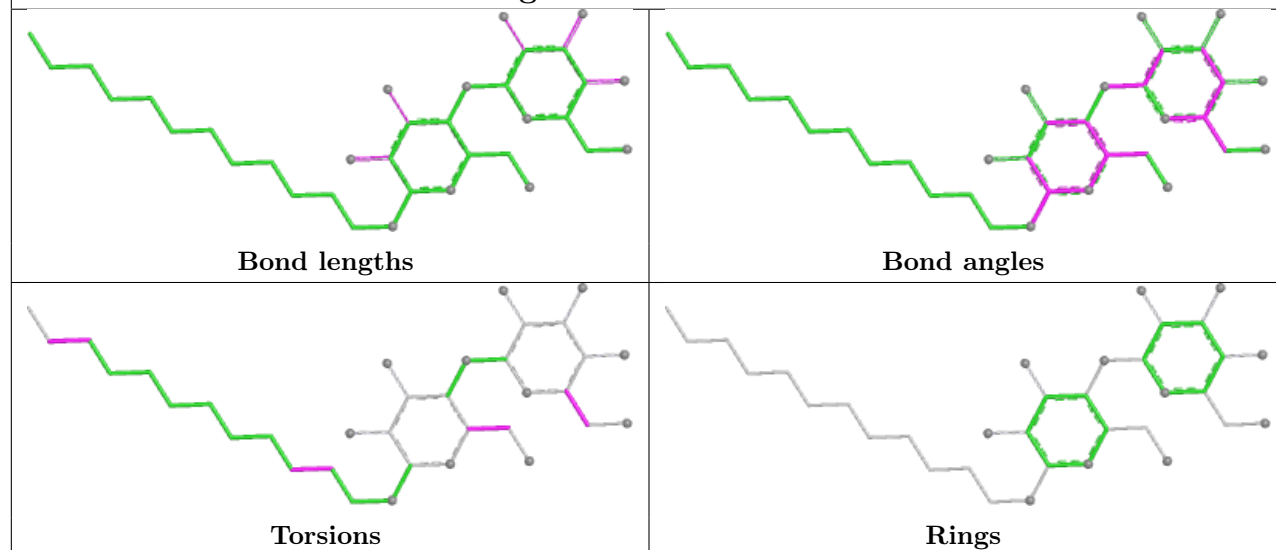


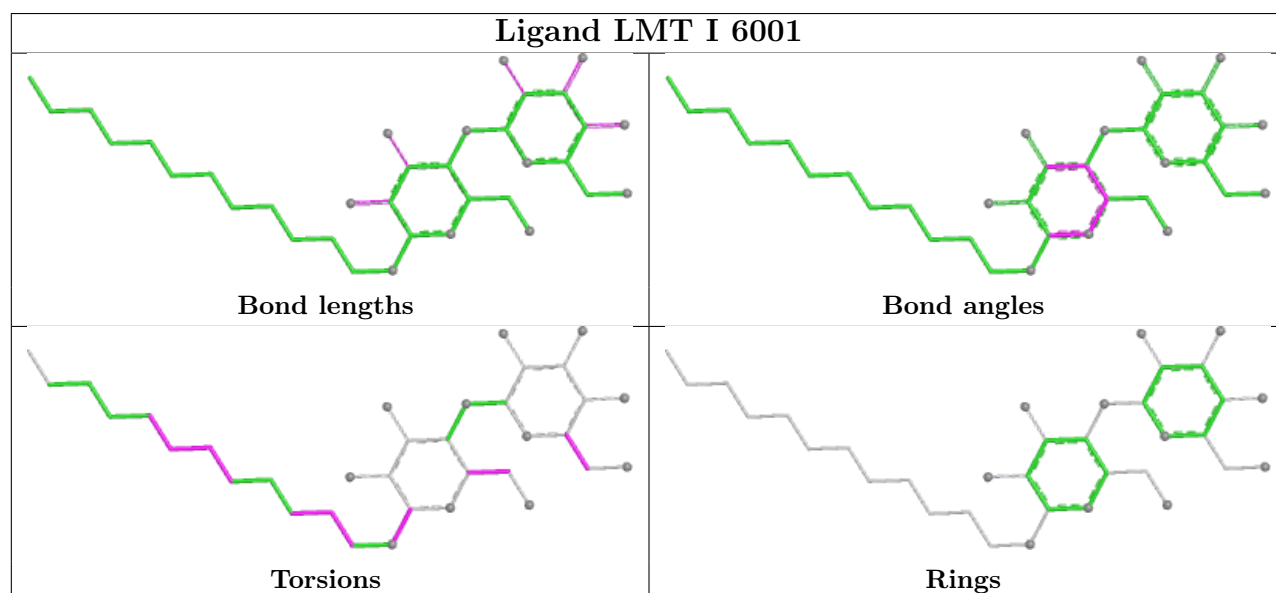
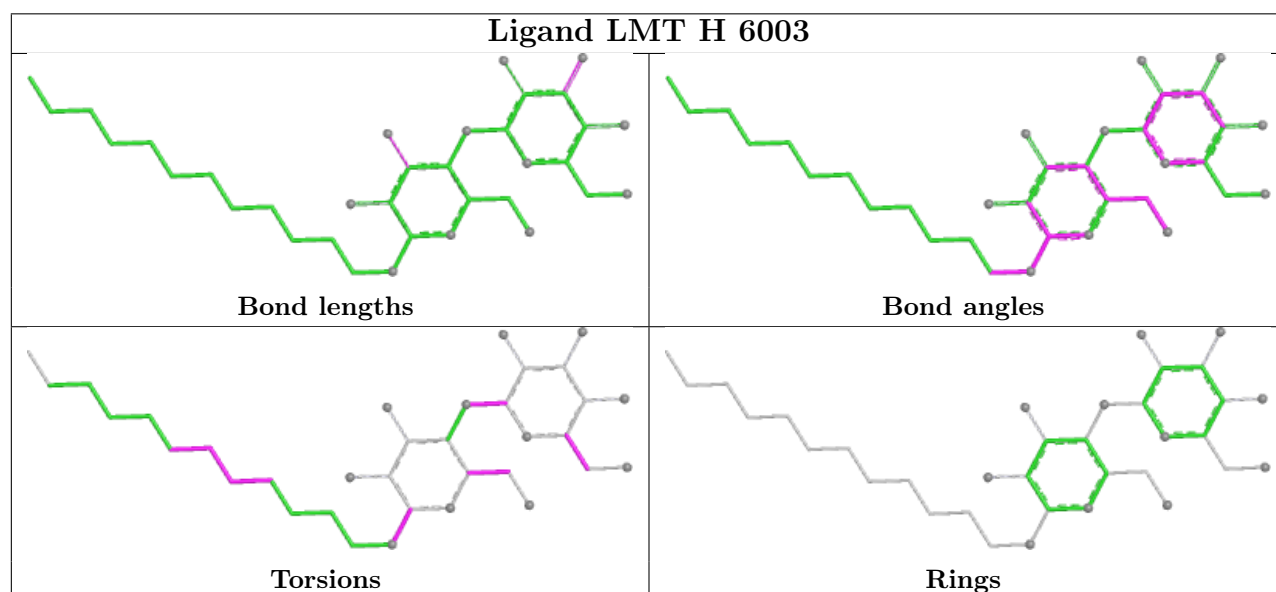
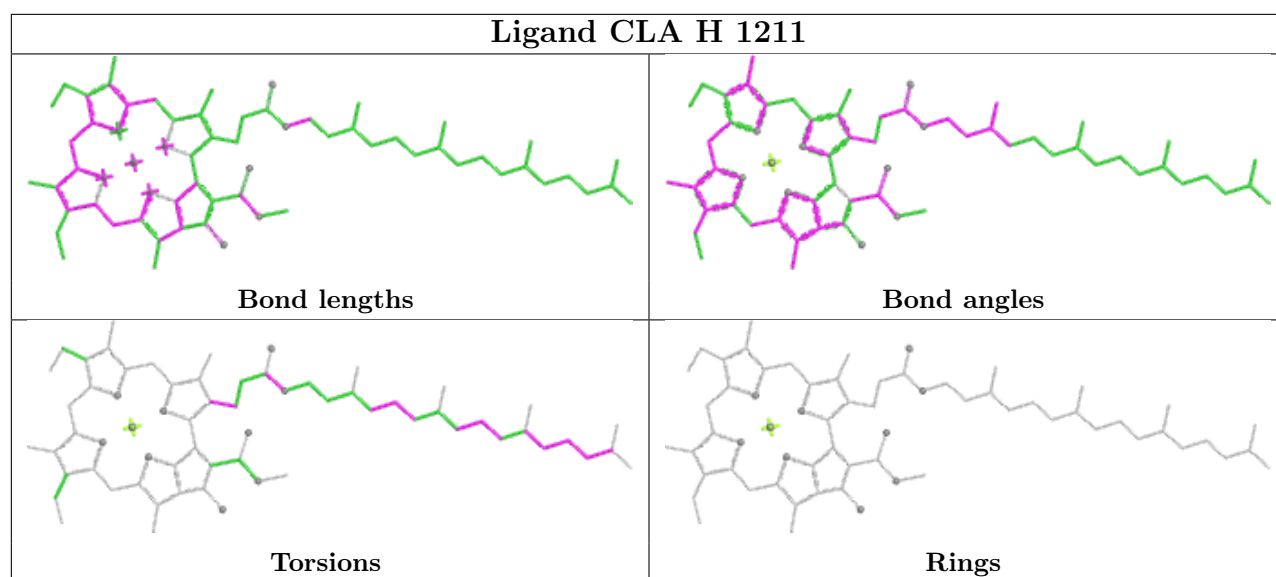


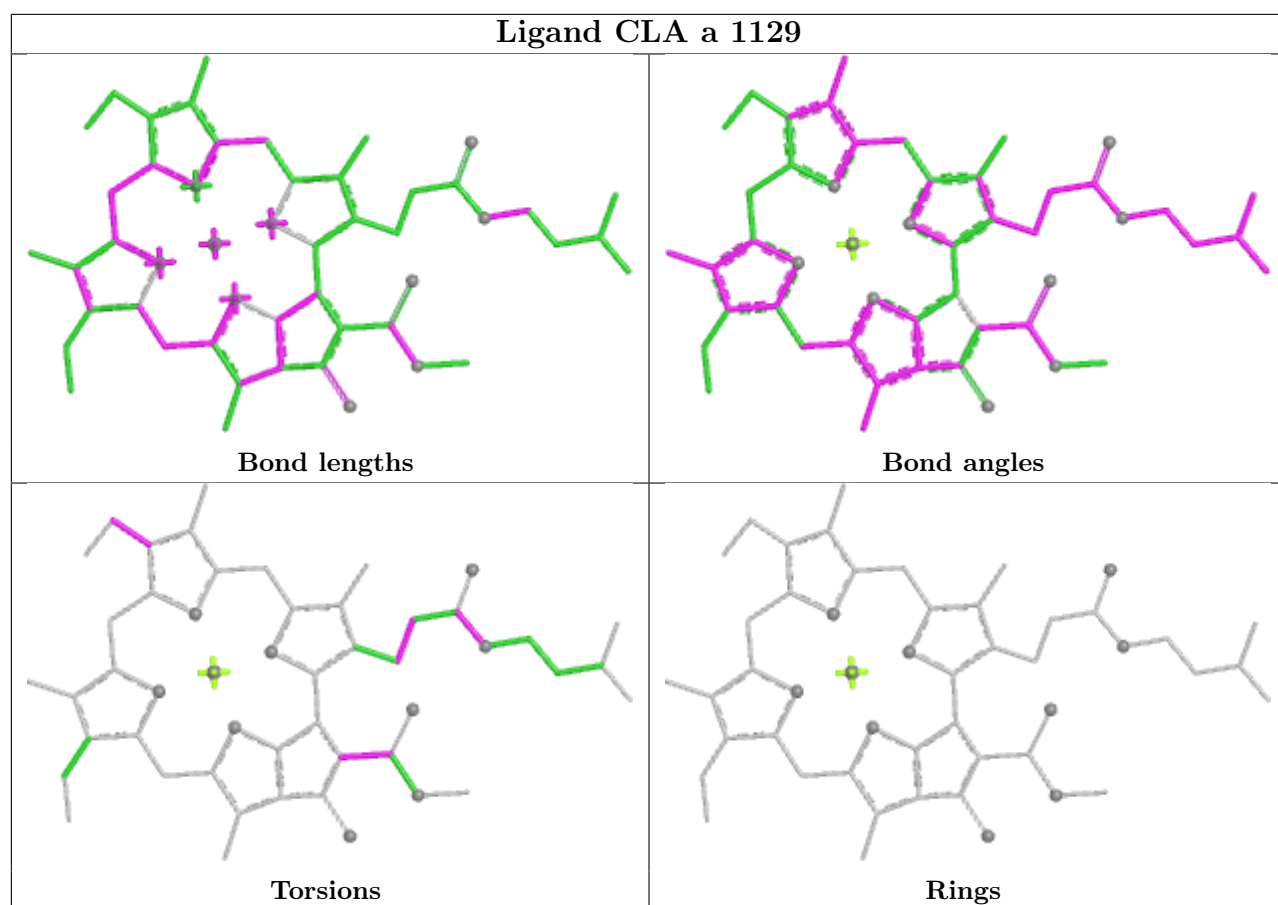
Ligand CLA A 1129



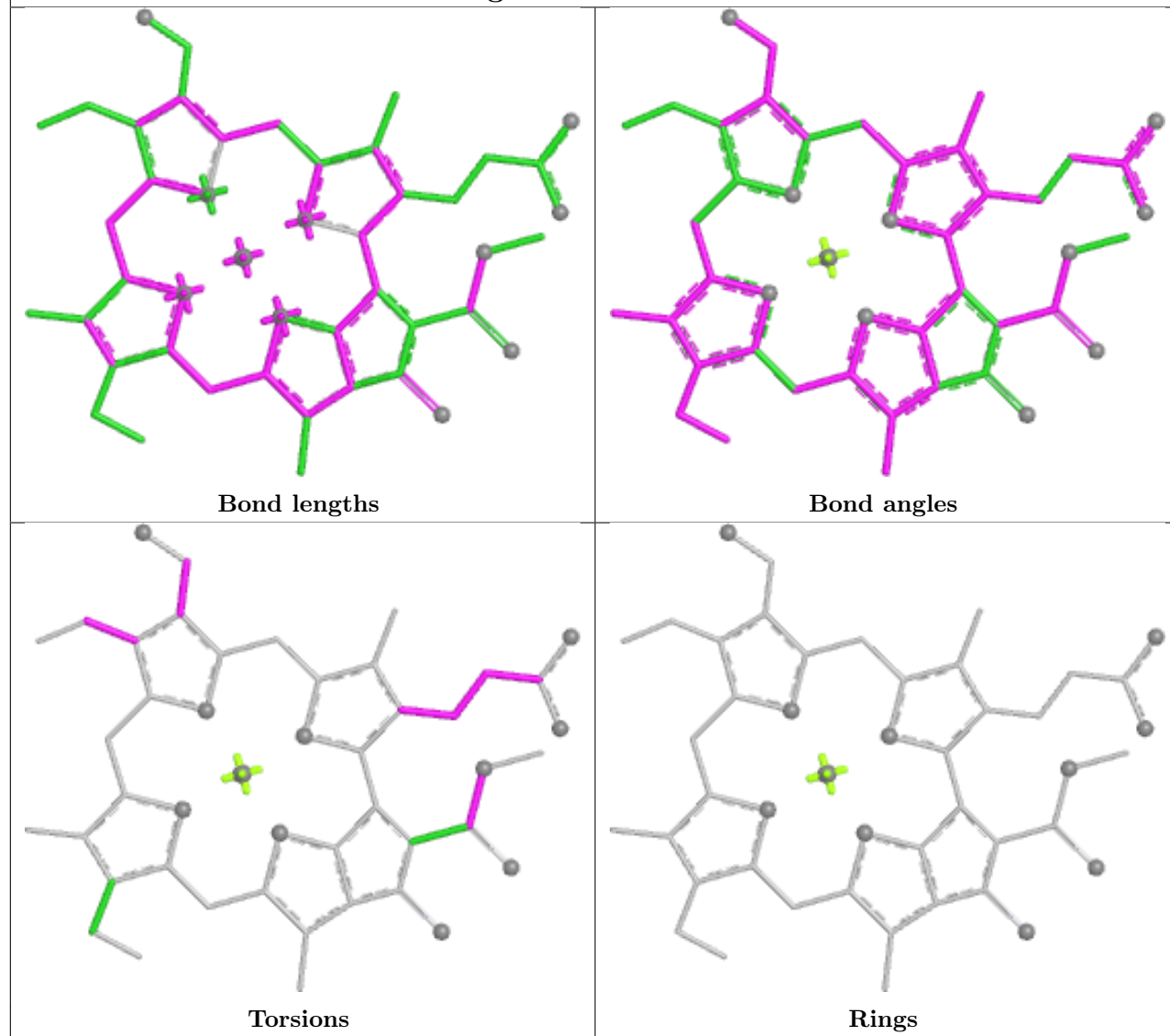
Ligand LMT U 6002



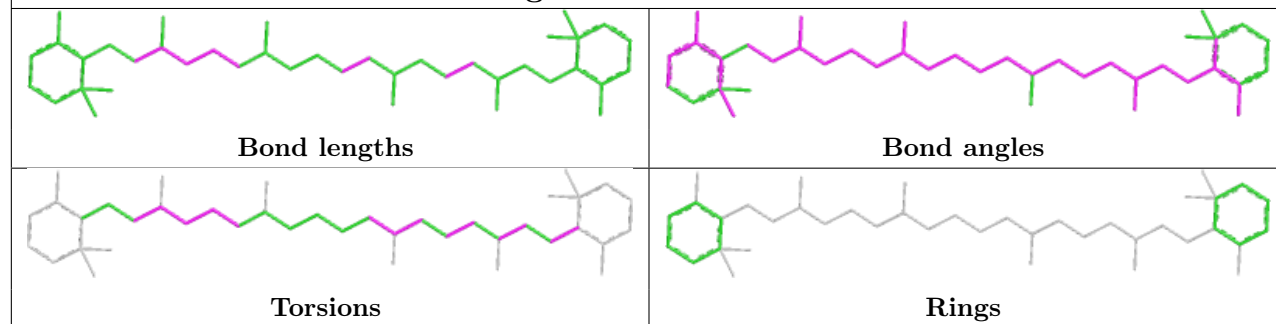


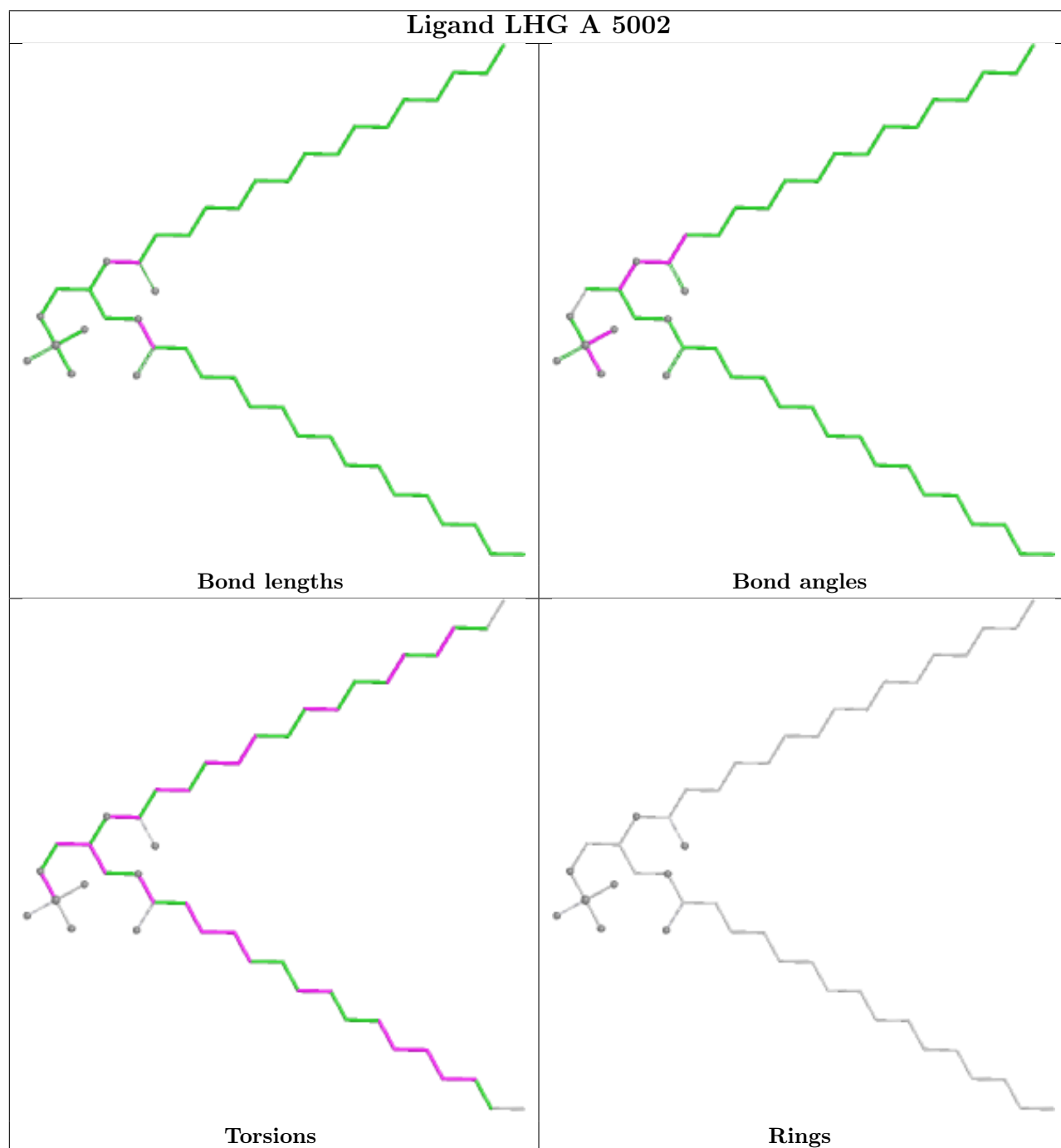
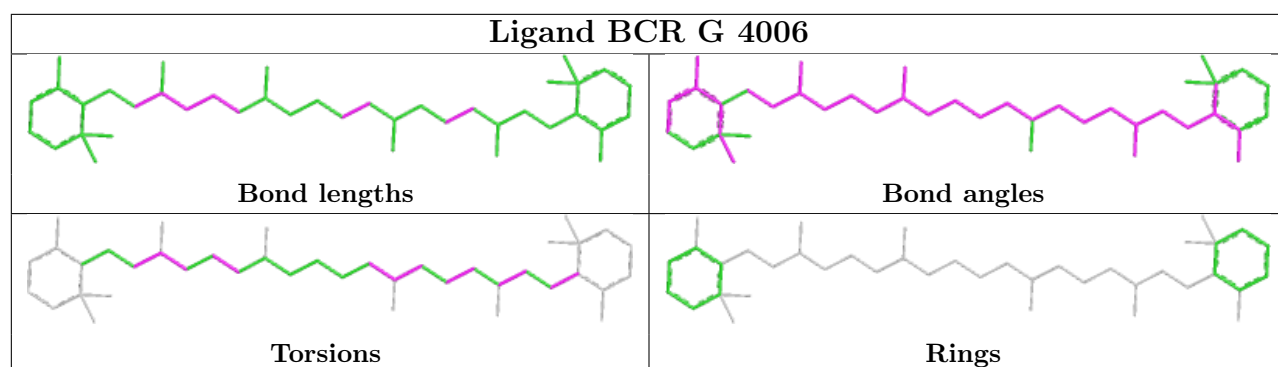


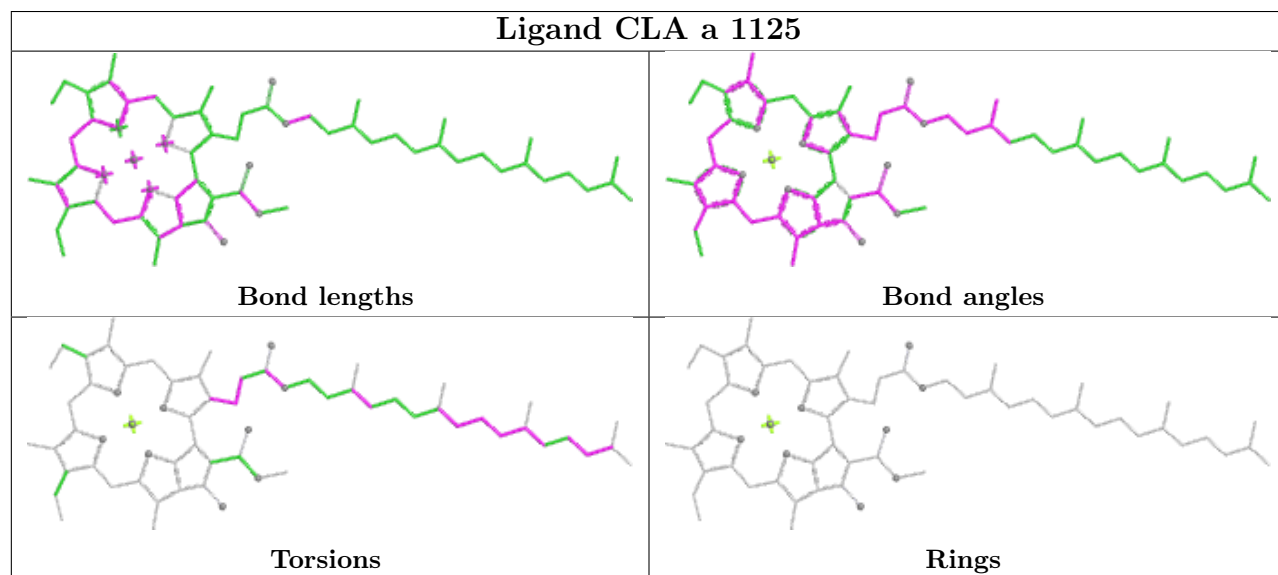
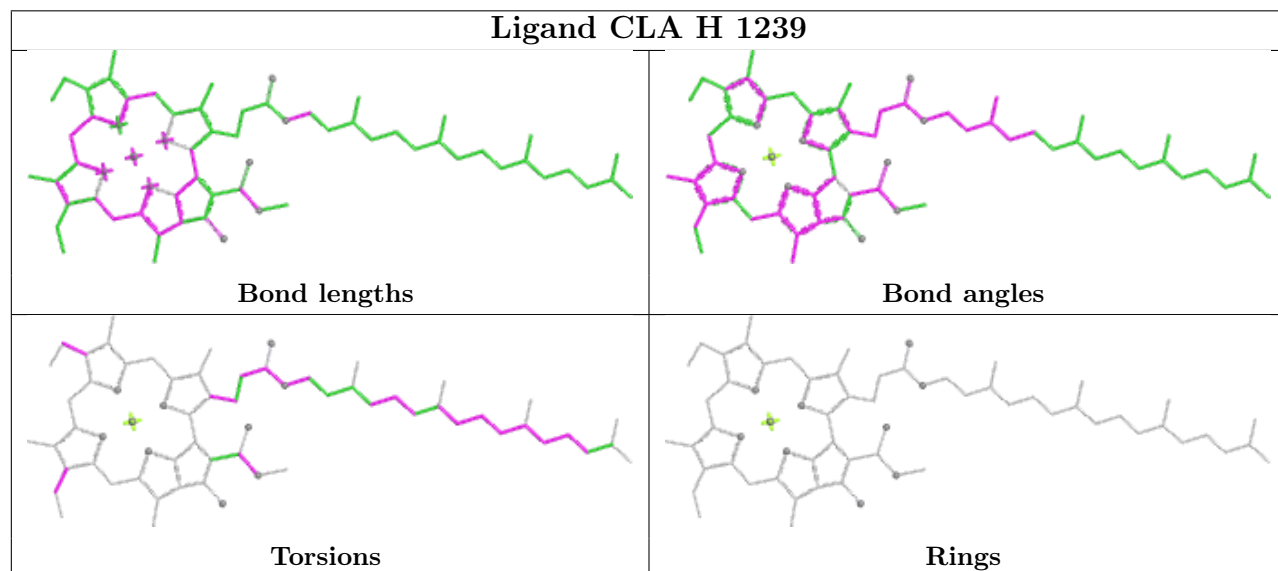
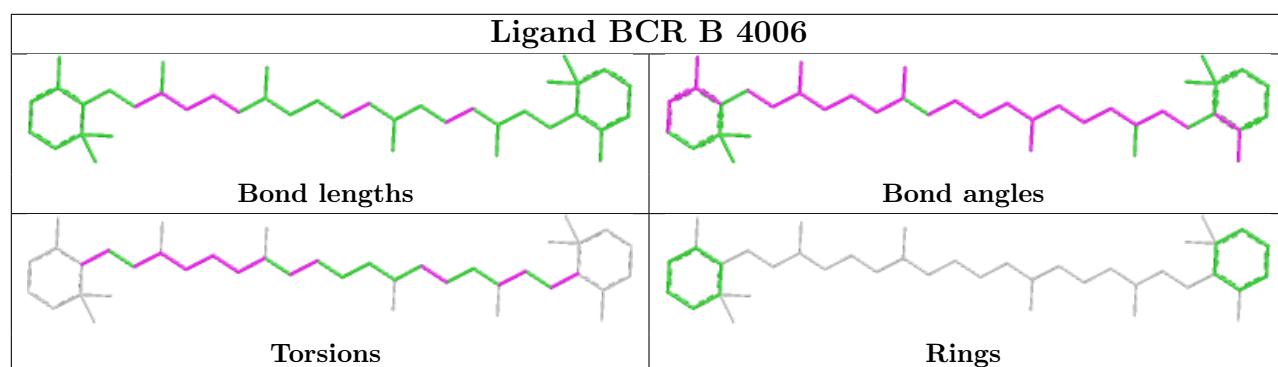
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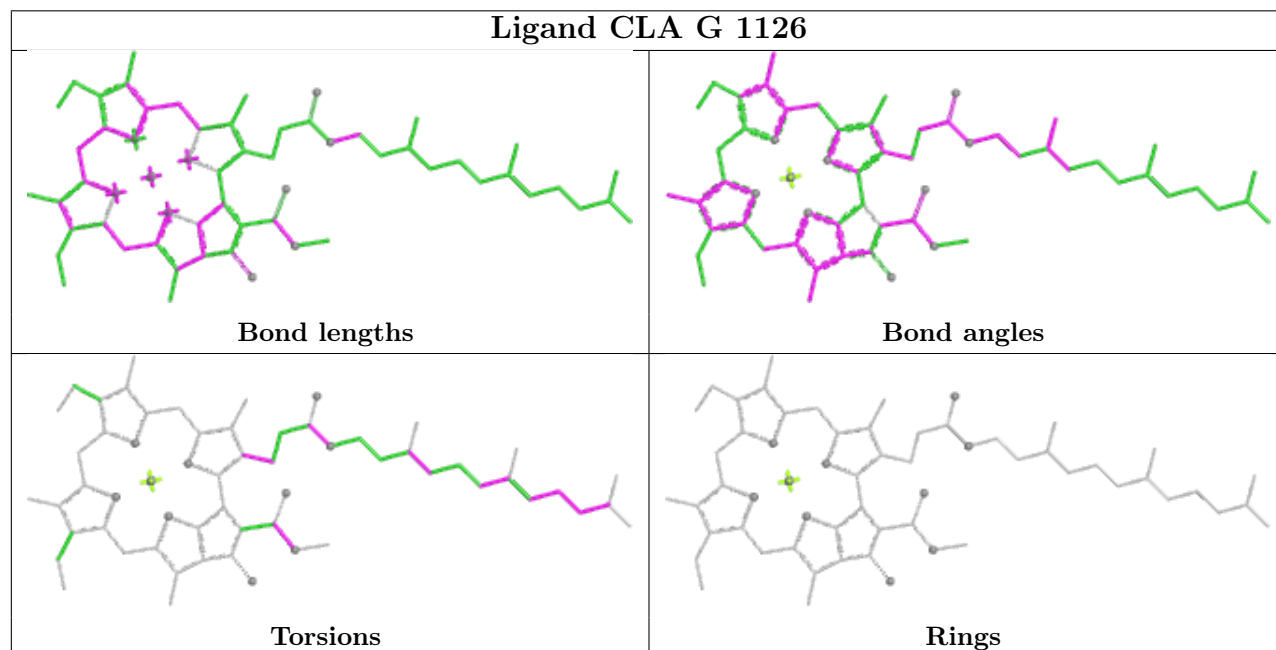
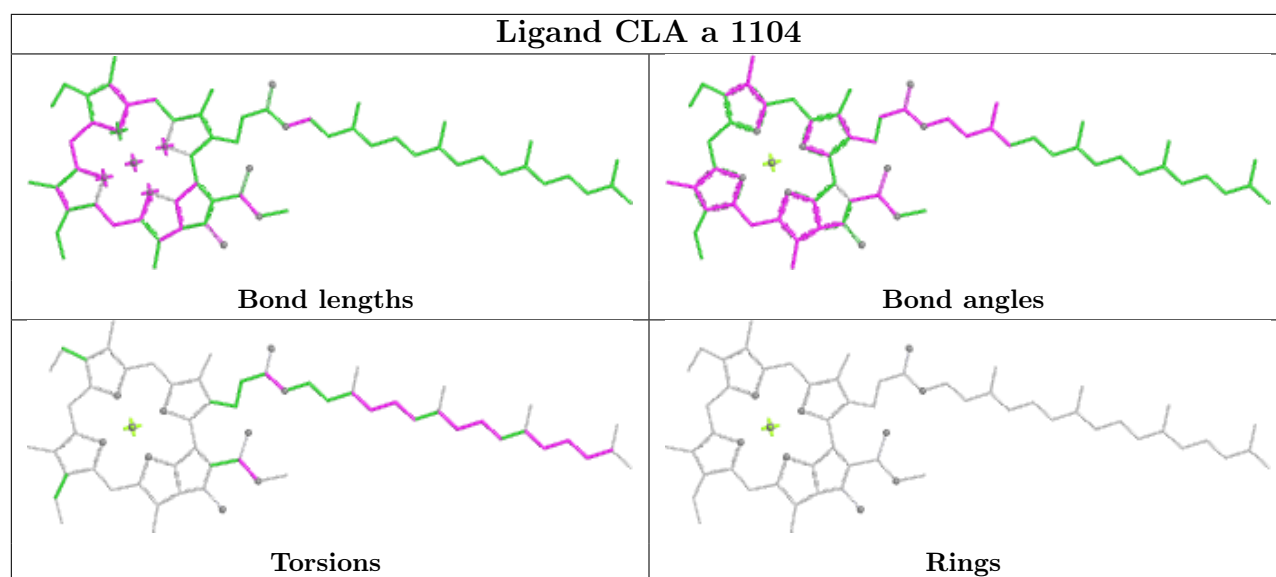


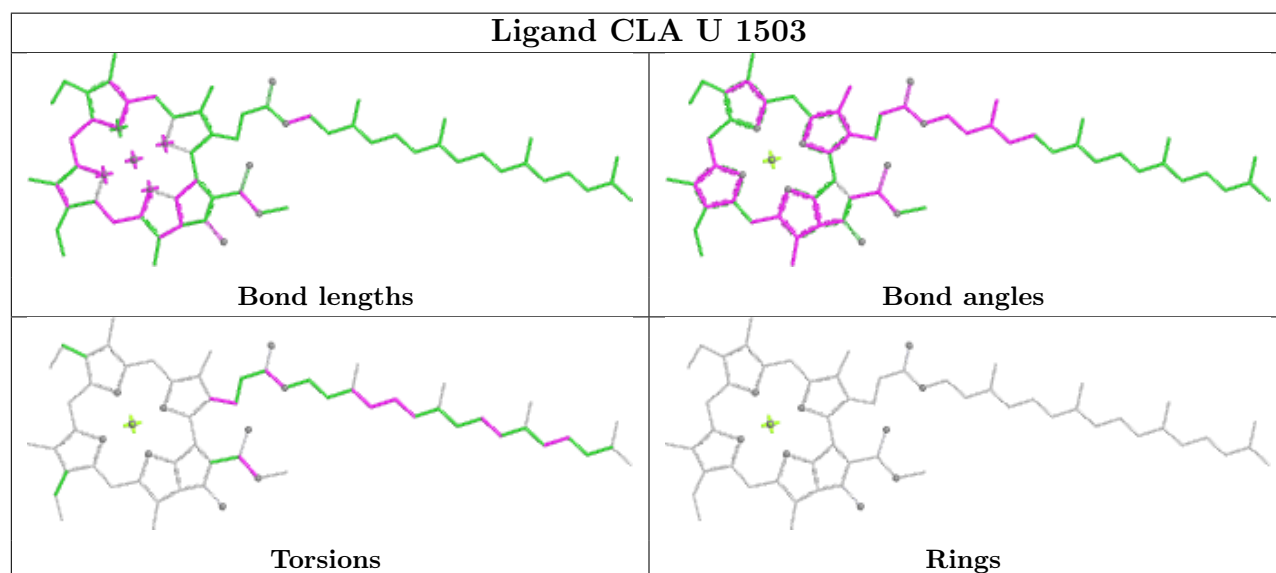
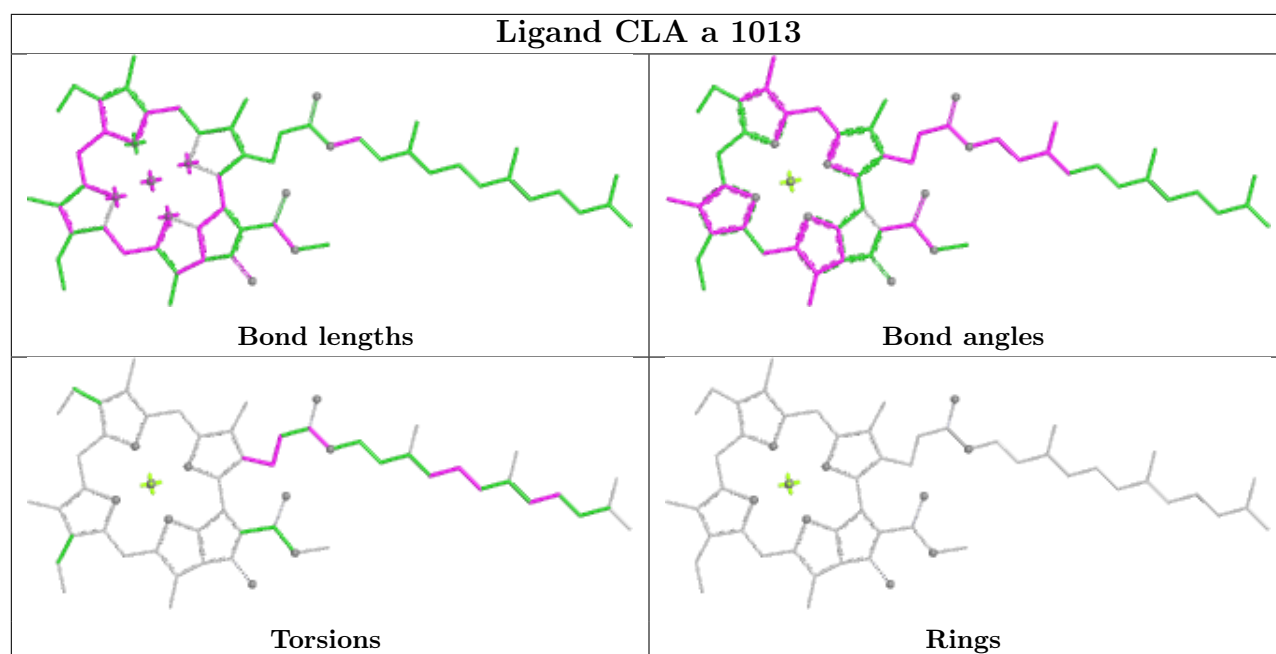
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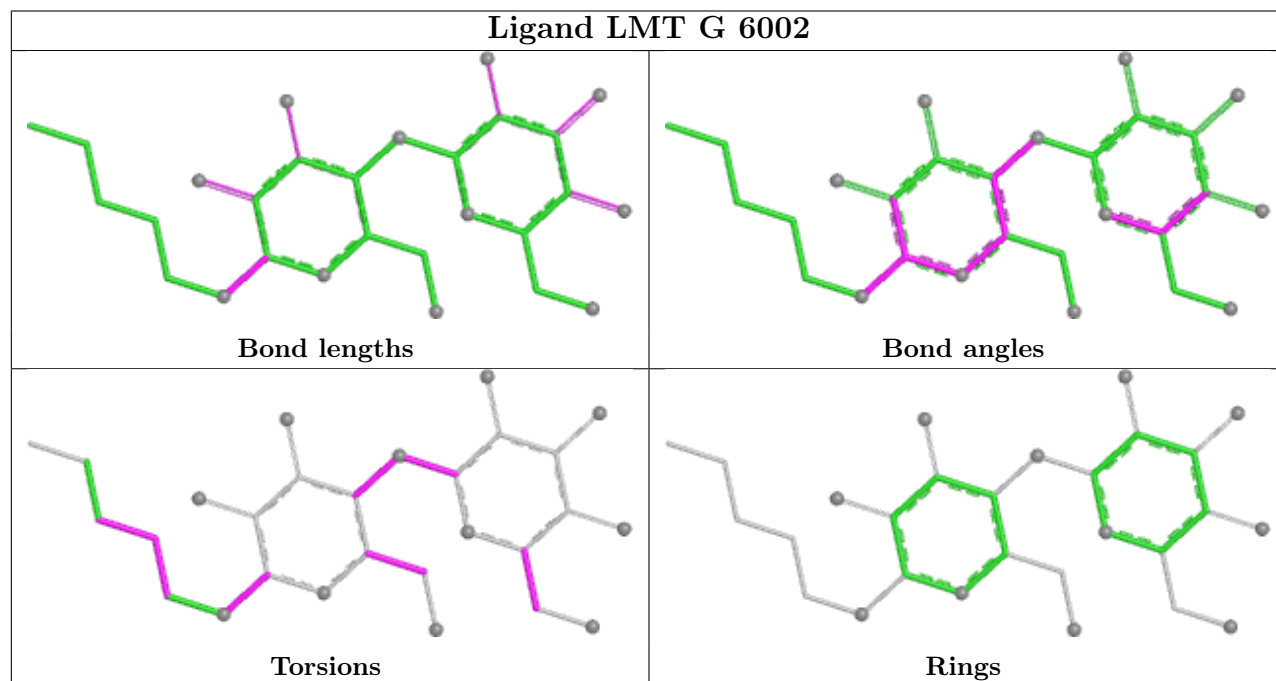
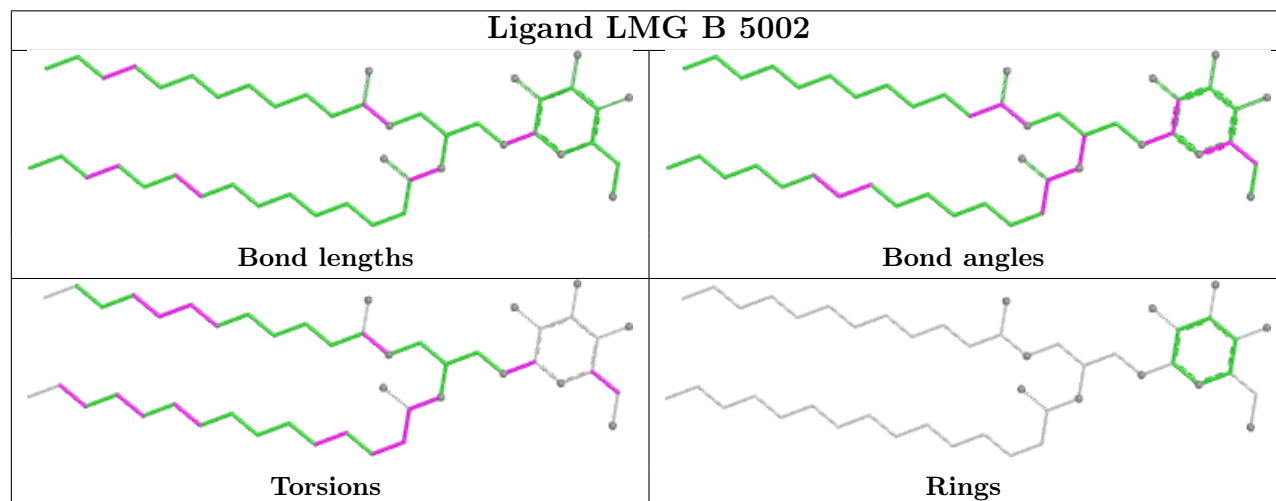
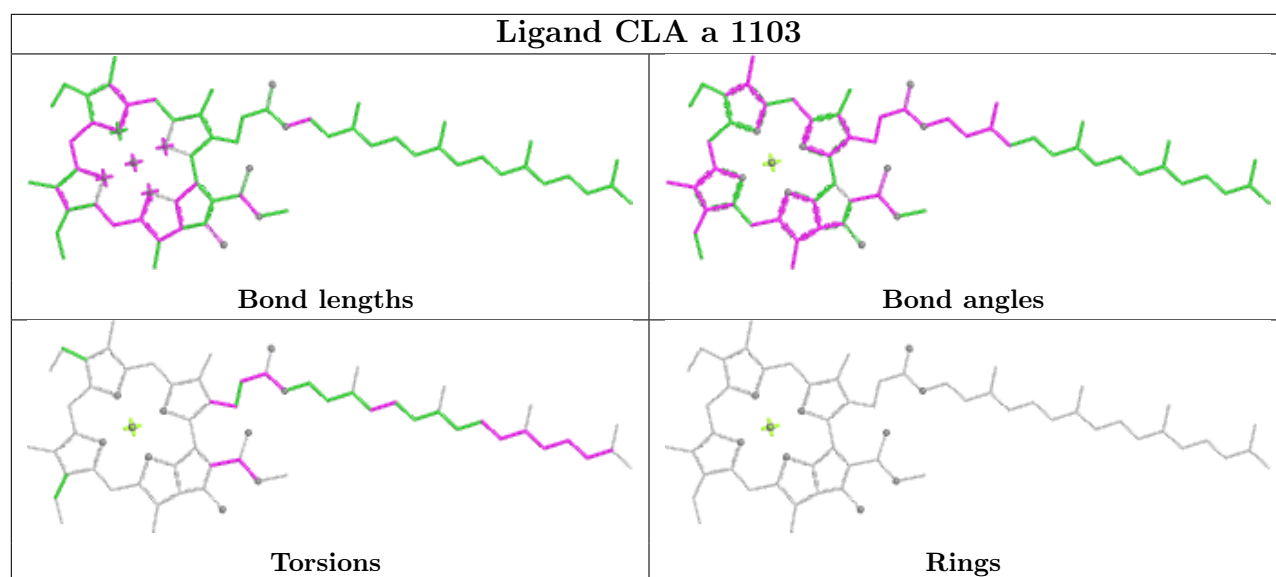


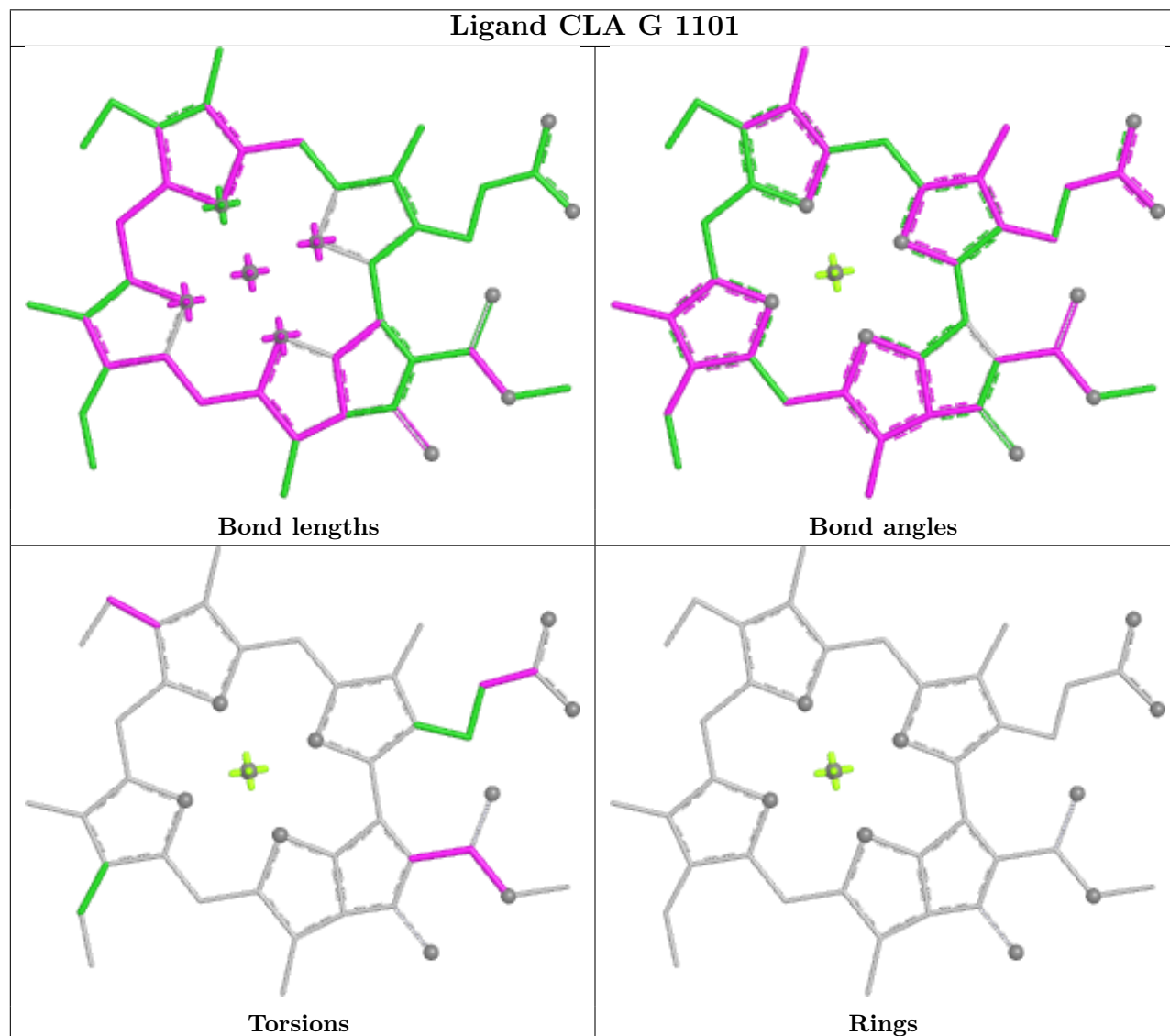
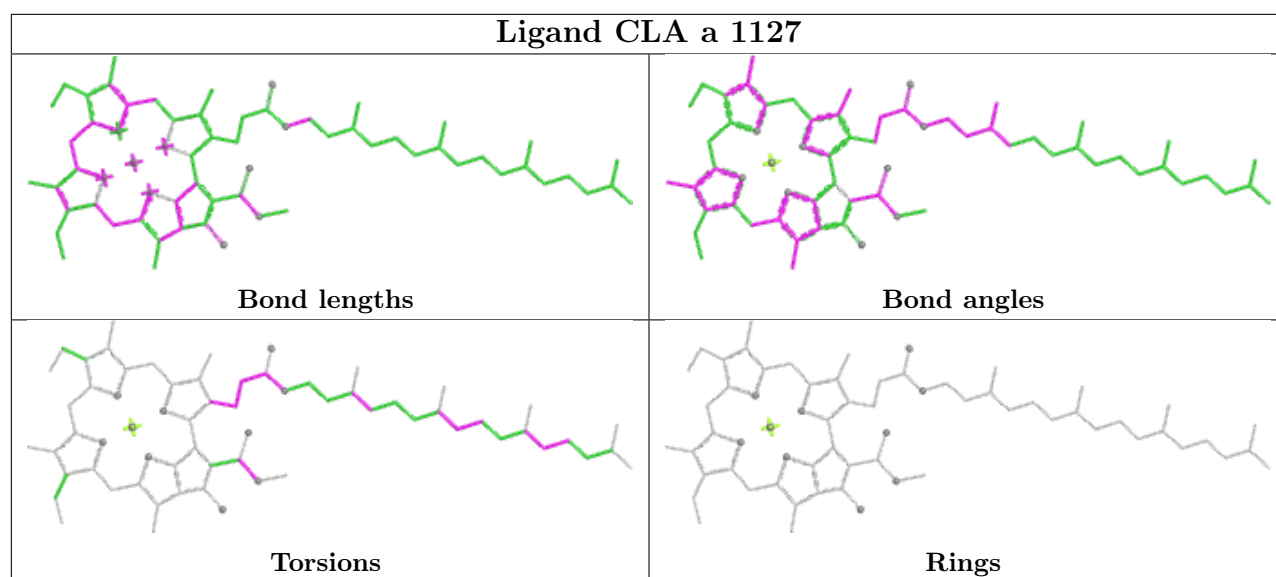


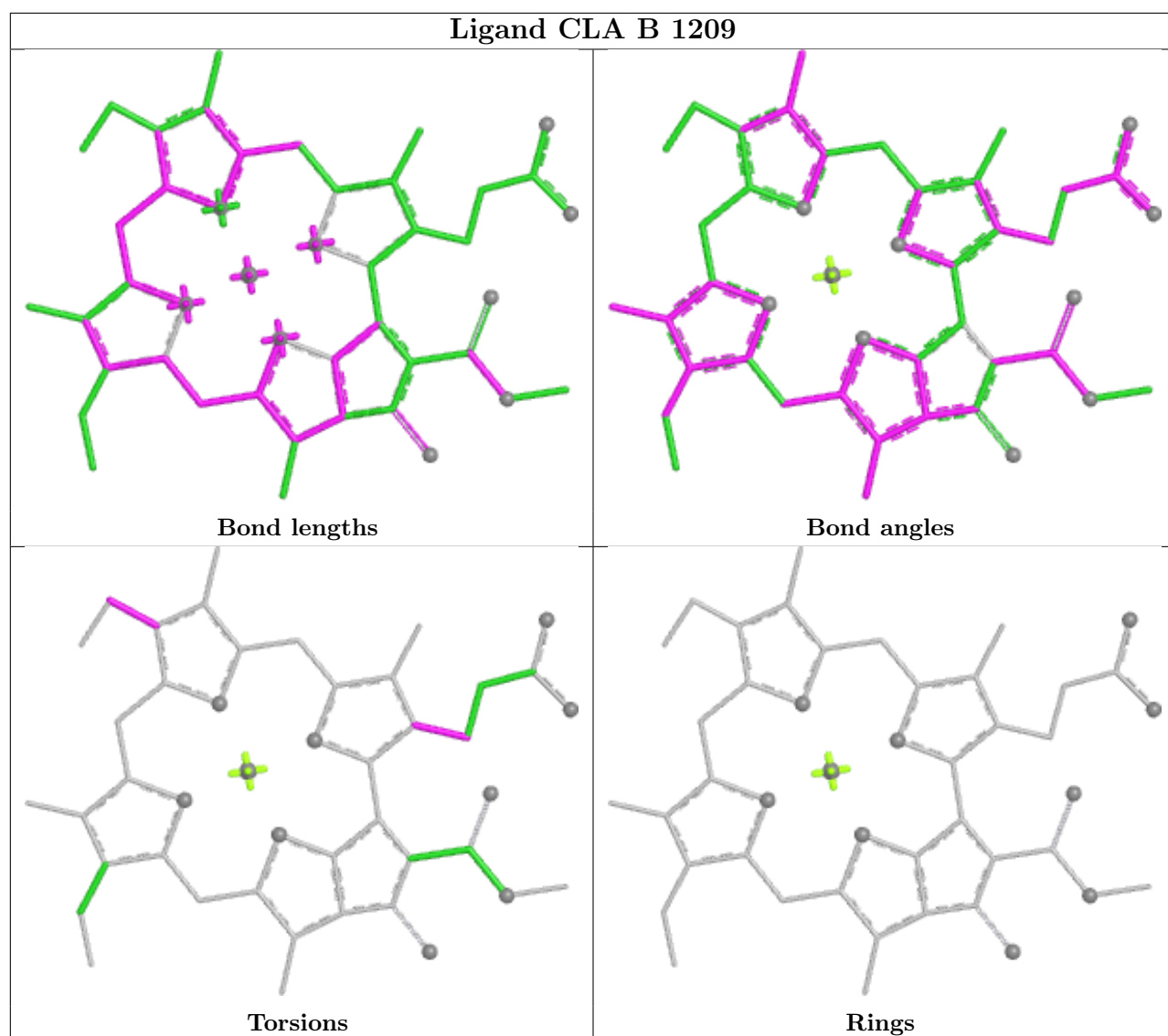




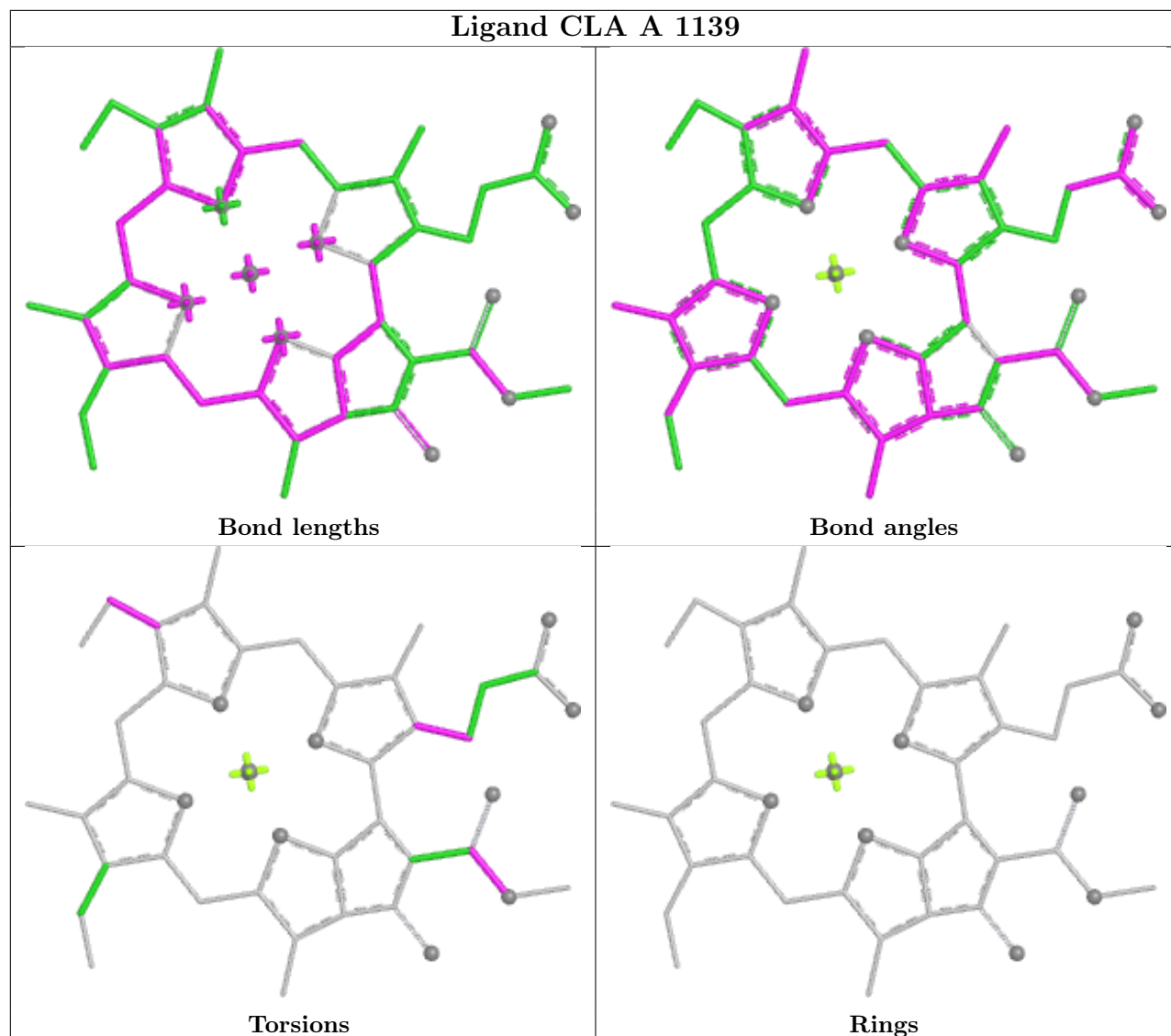




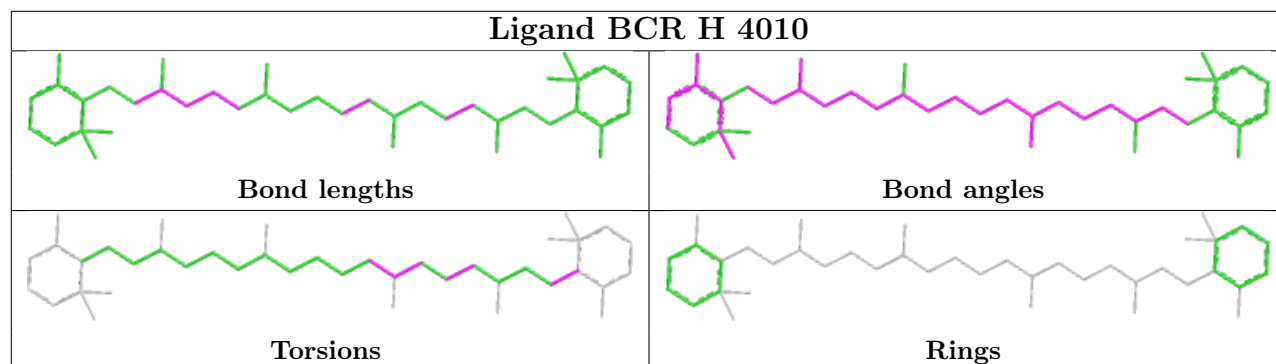


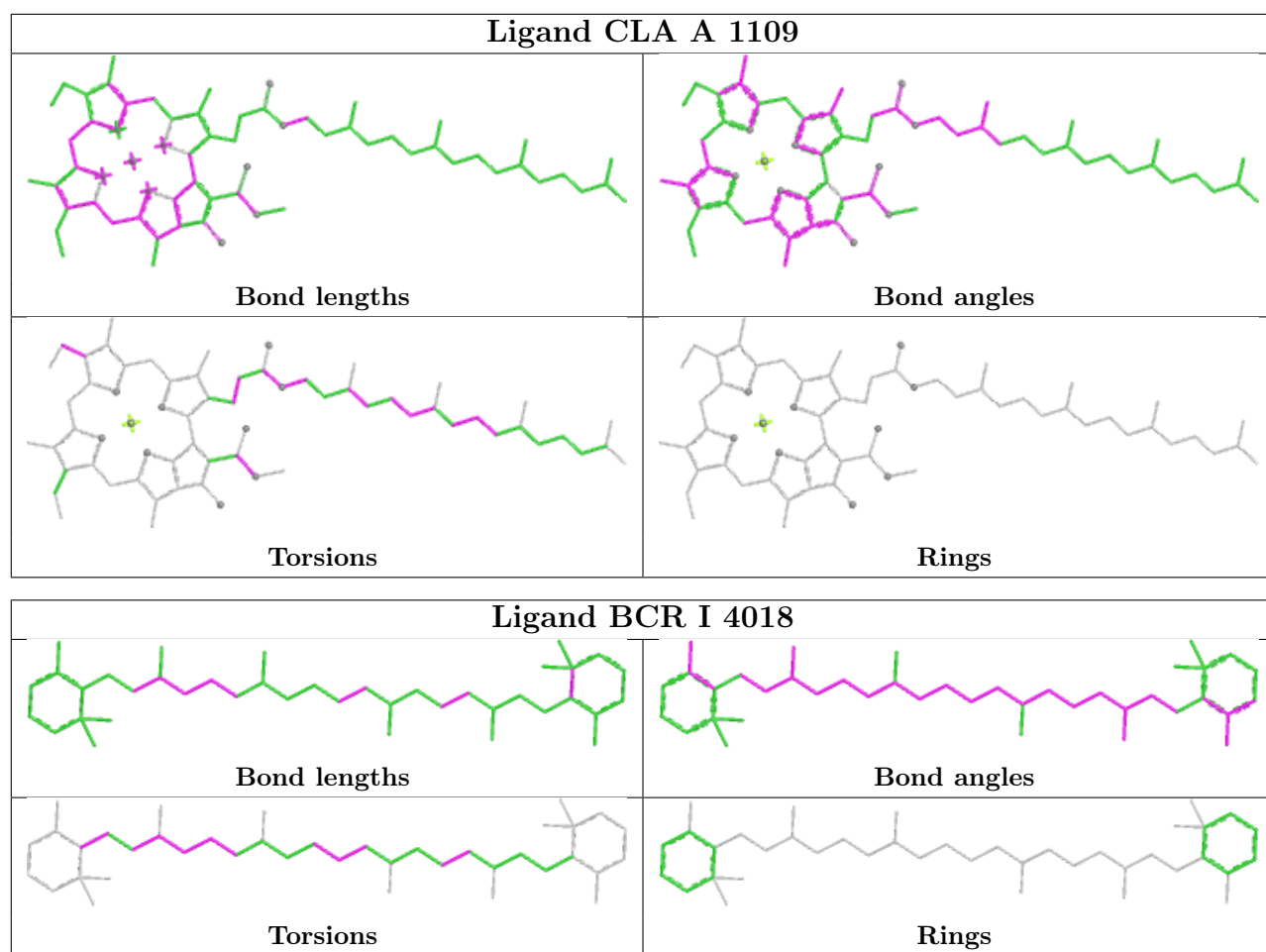


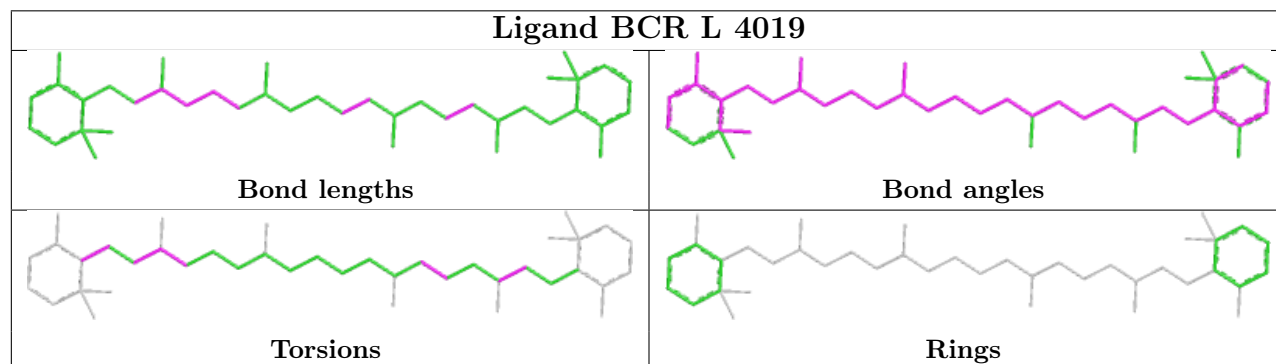
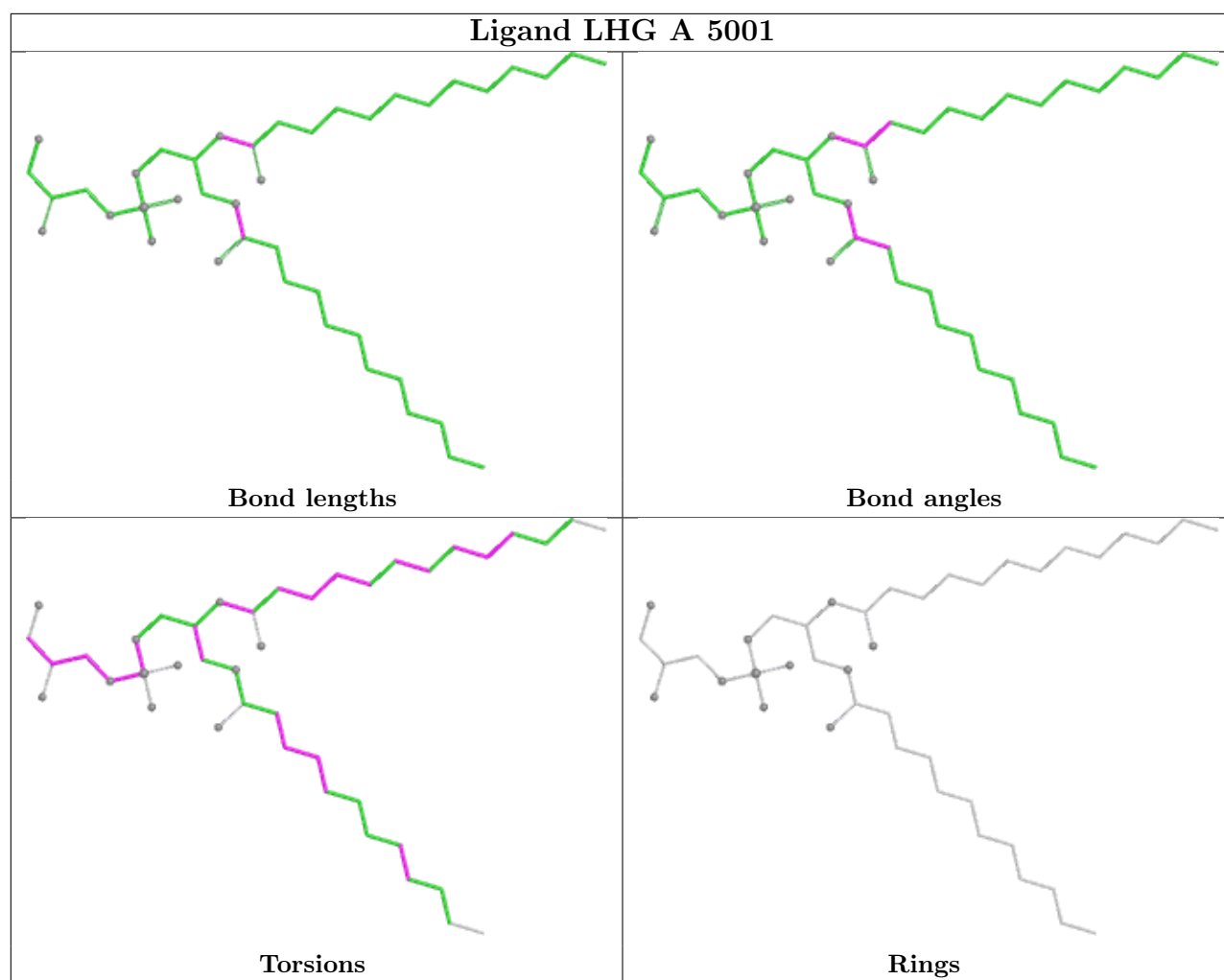
Ligand CLA A 1139

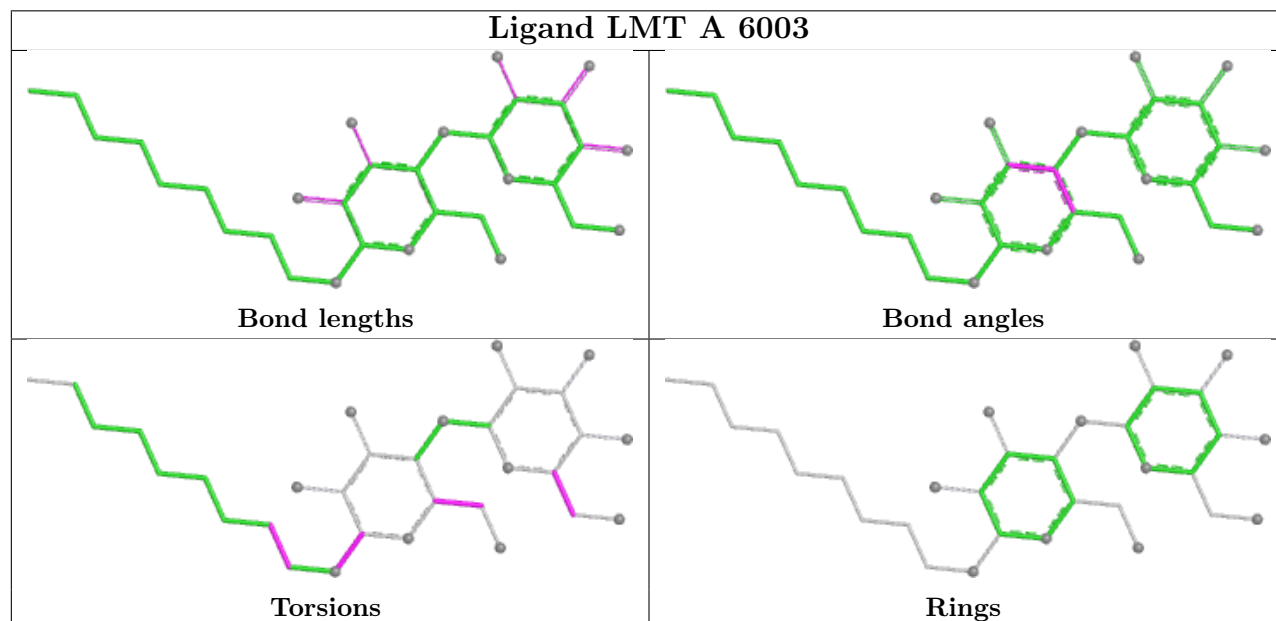
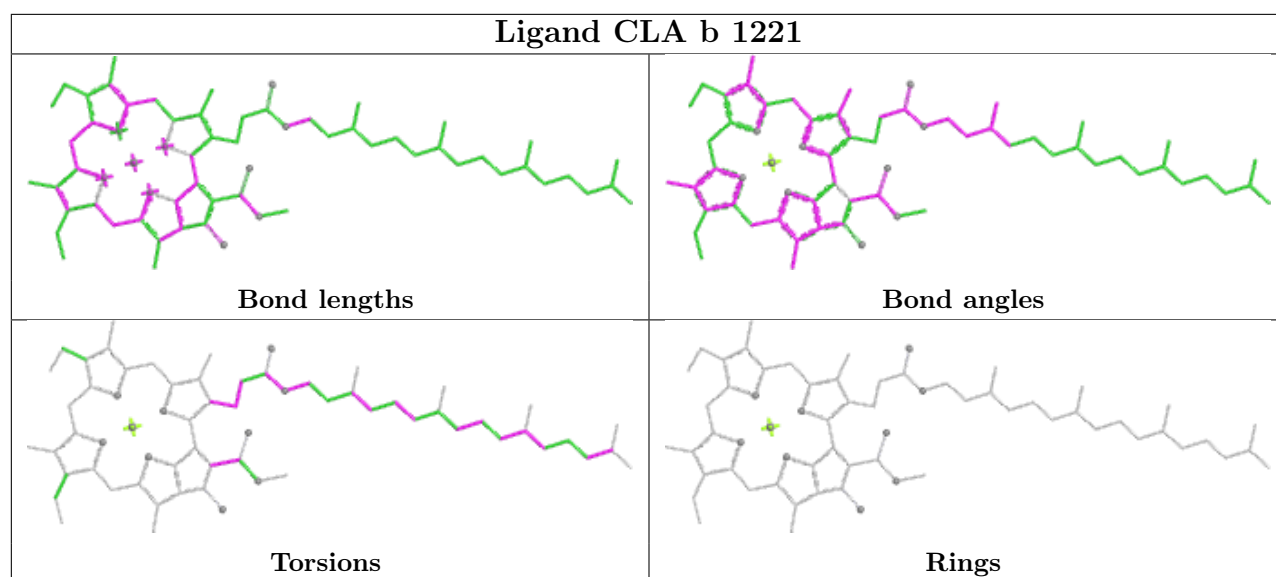


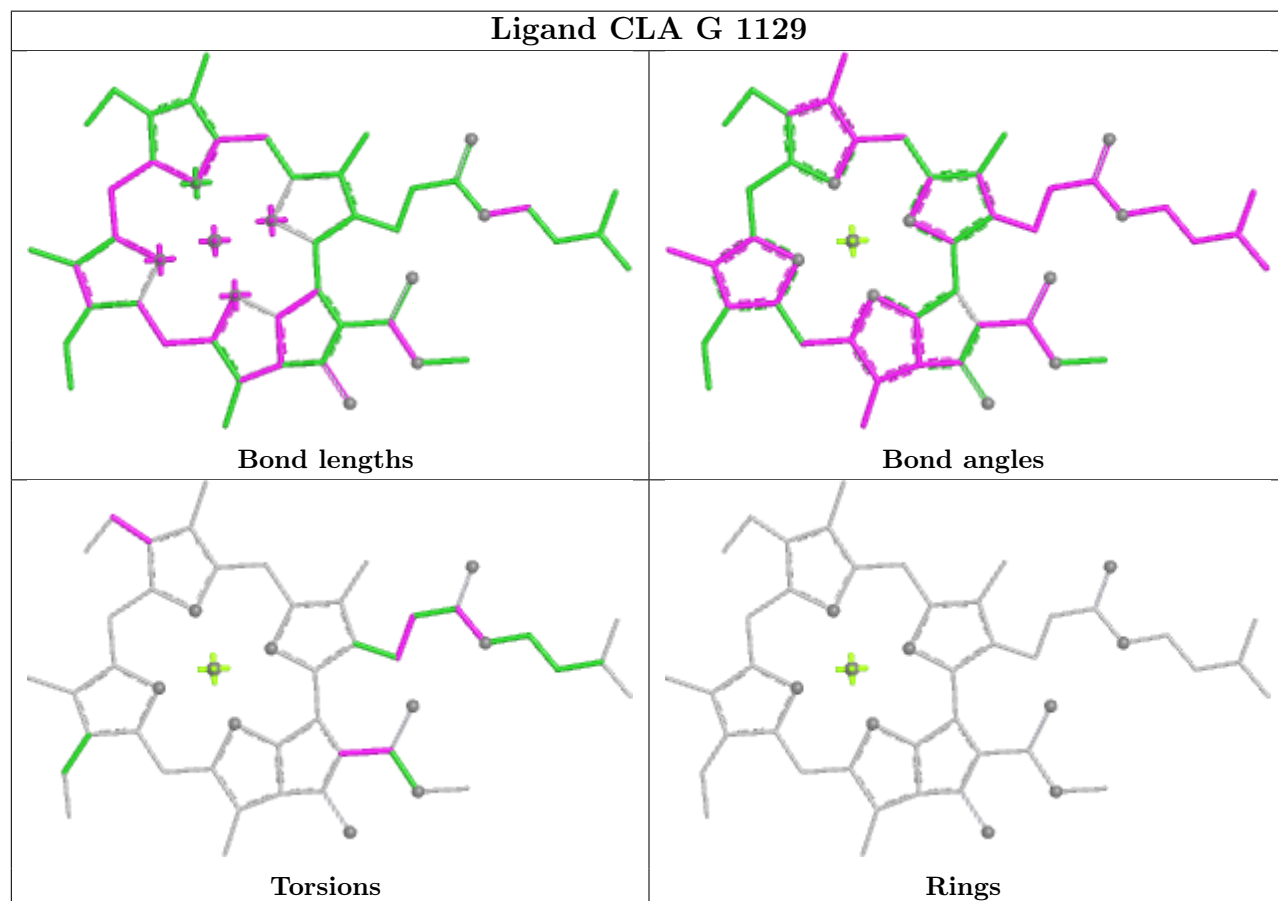
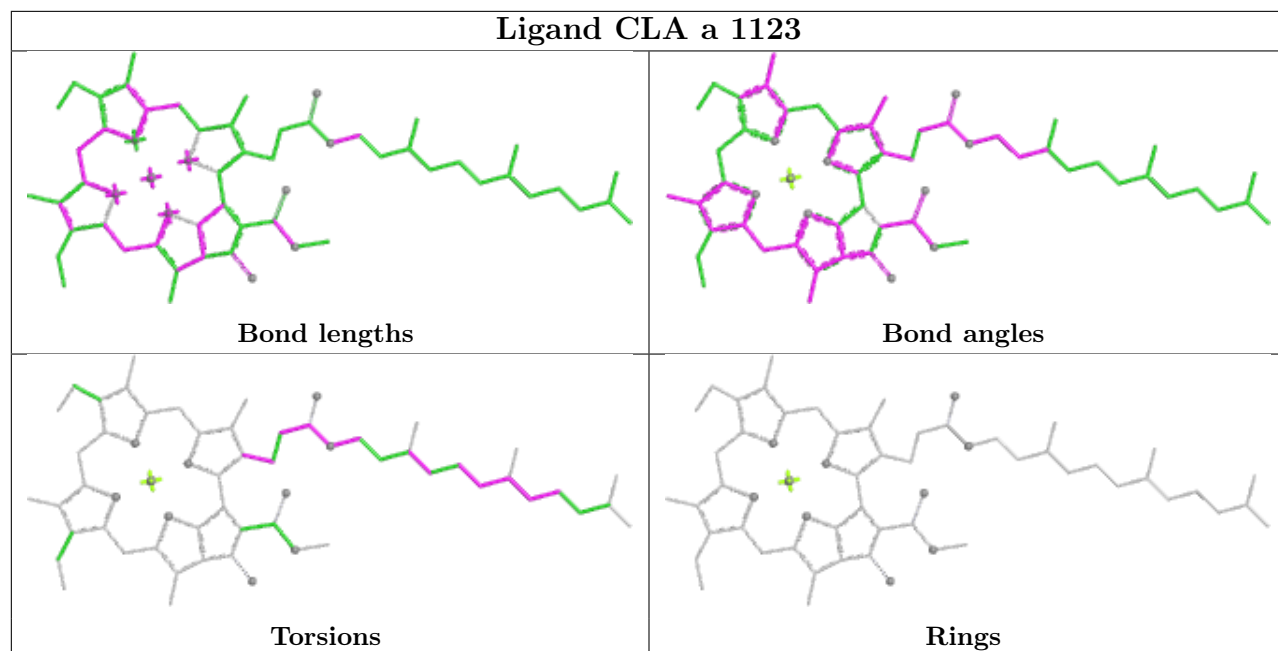
Ligand BCR H 4010

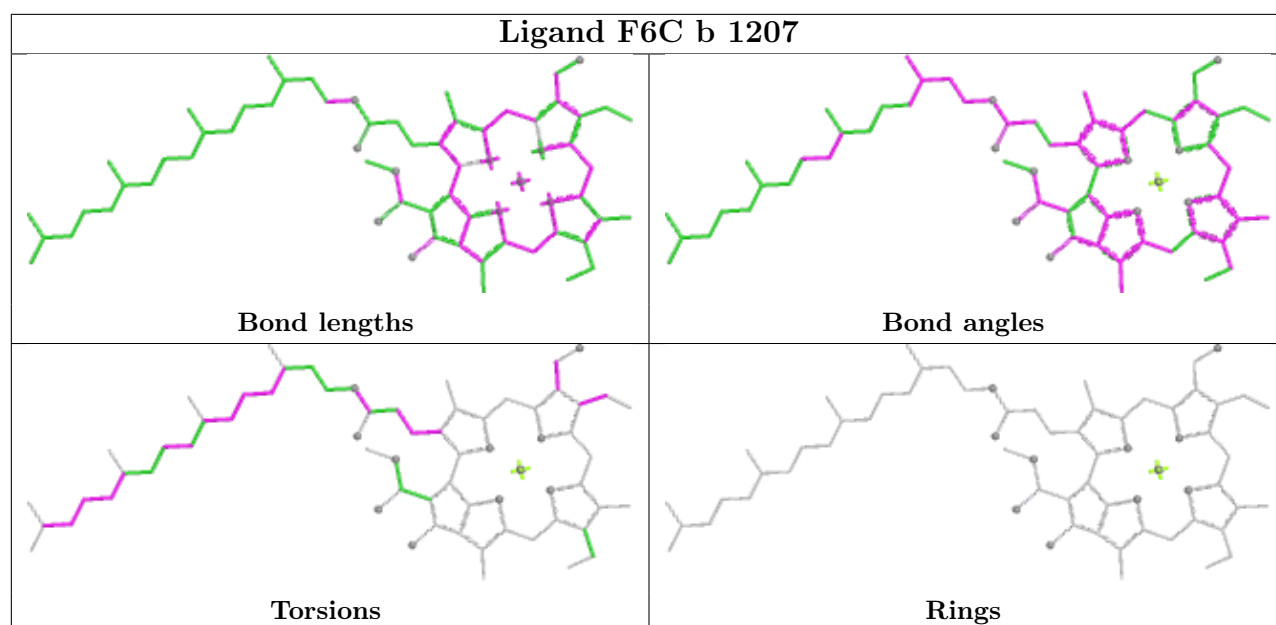
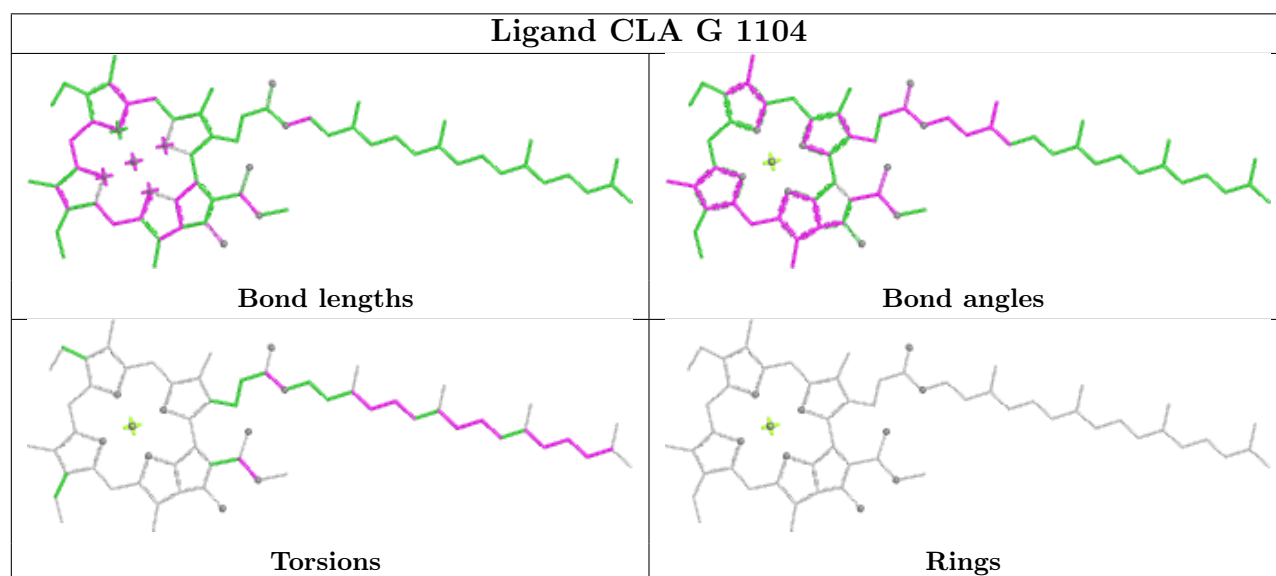
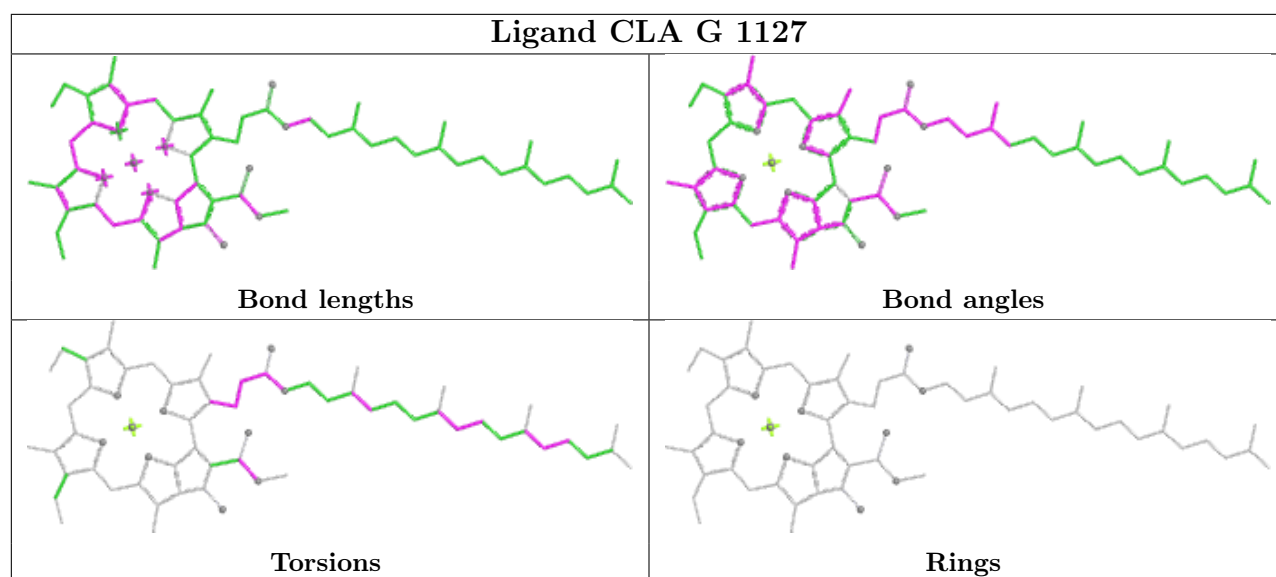


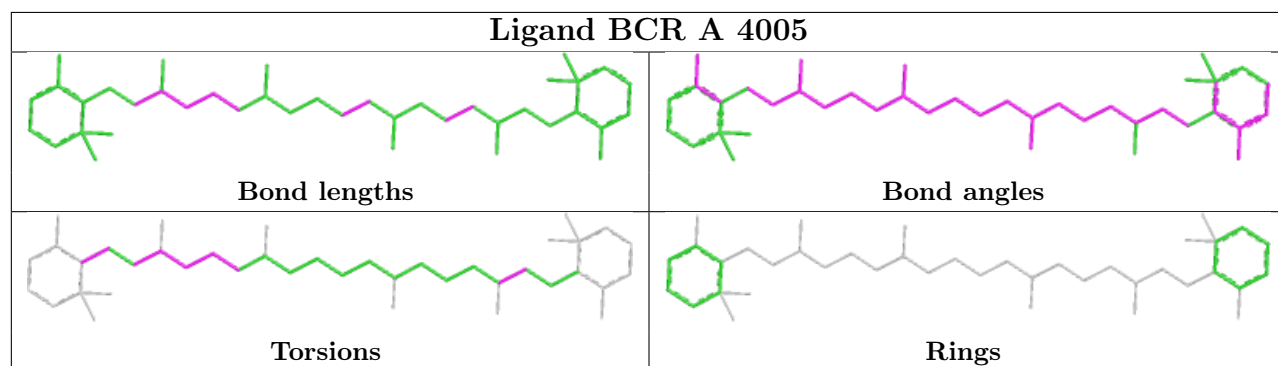
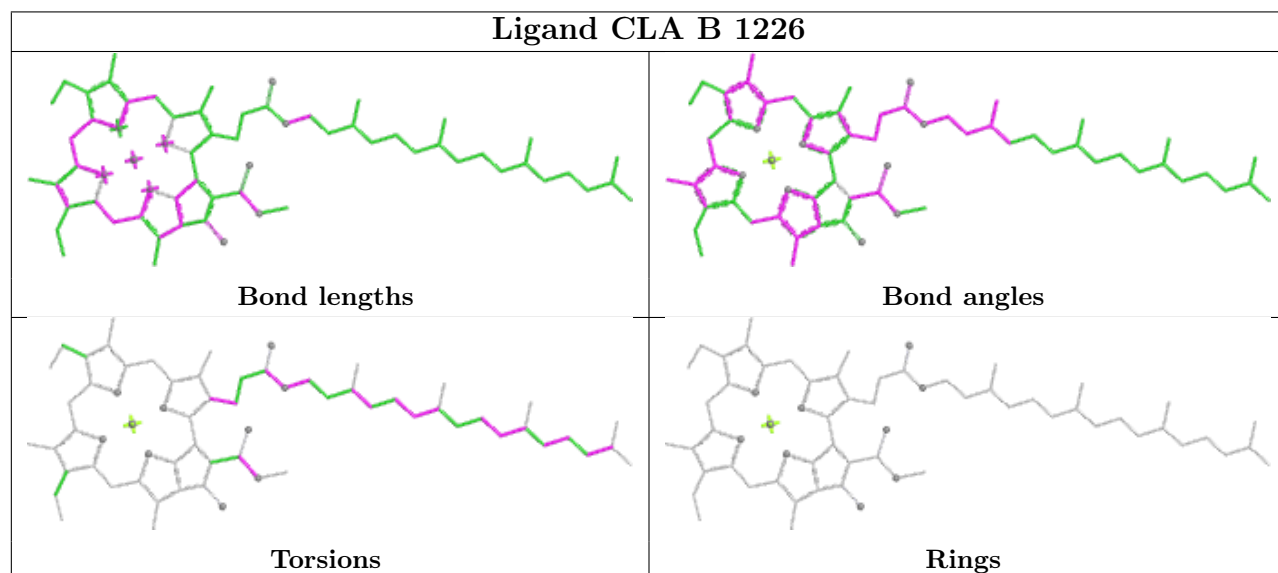
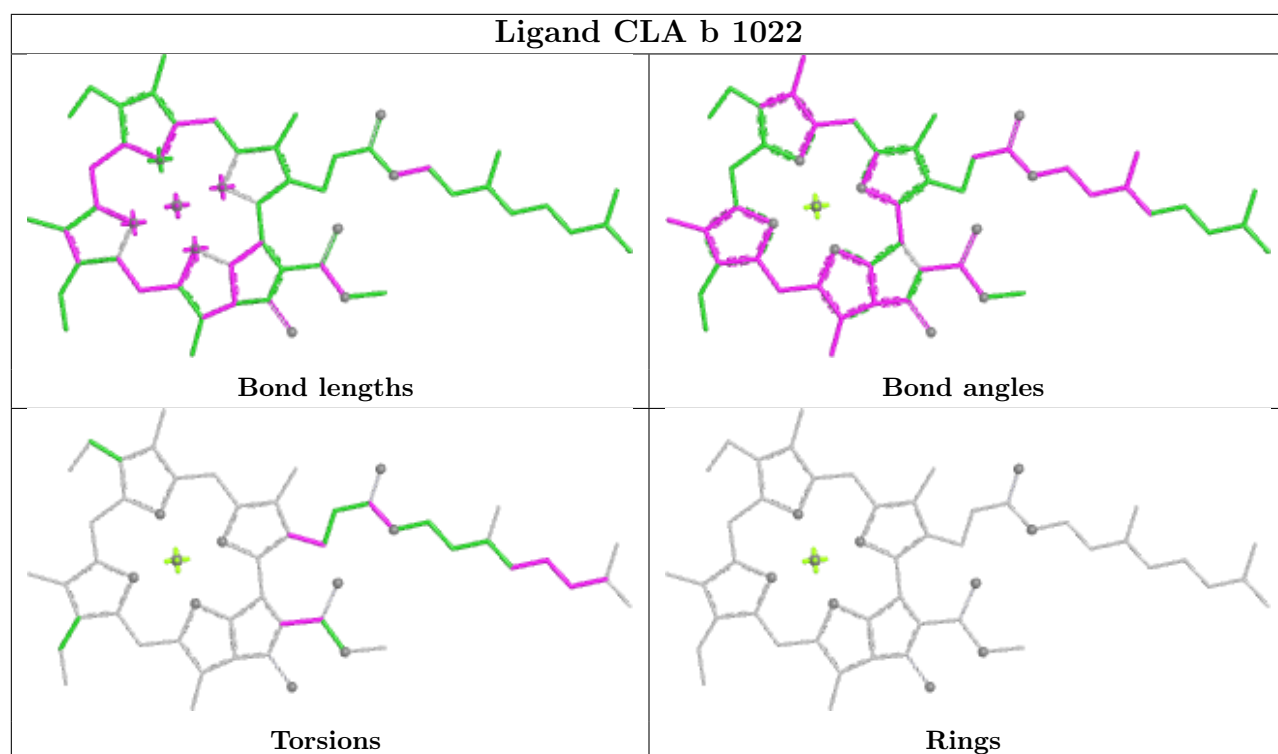




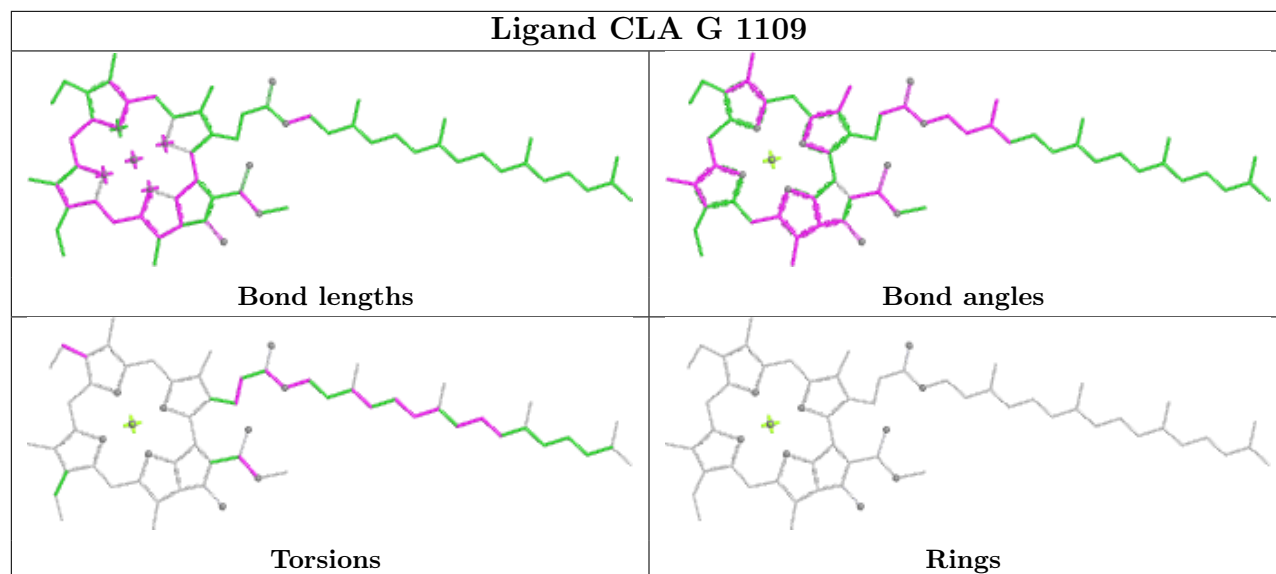




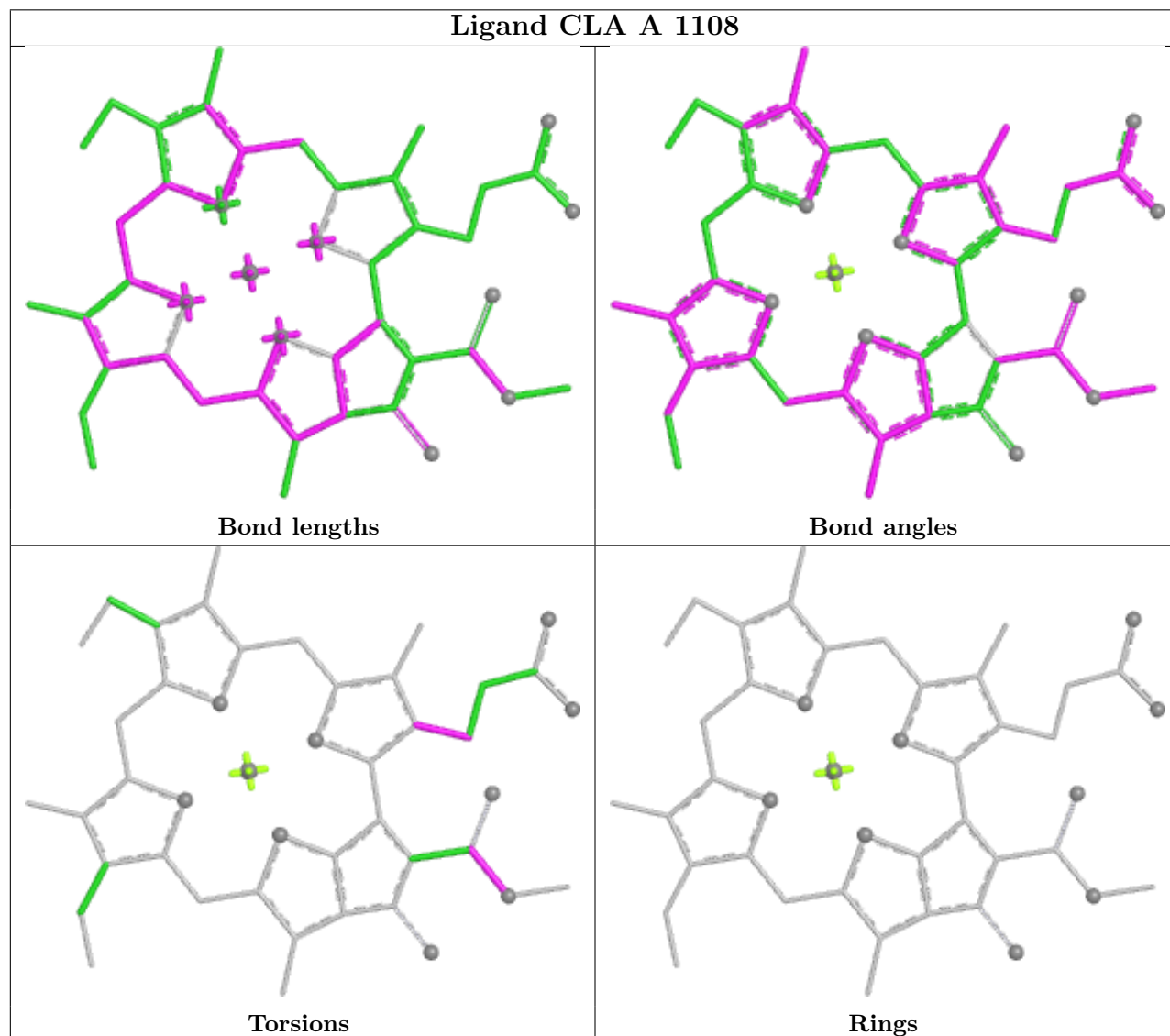


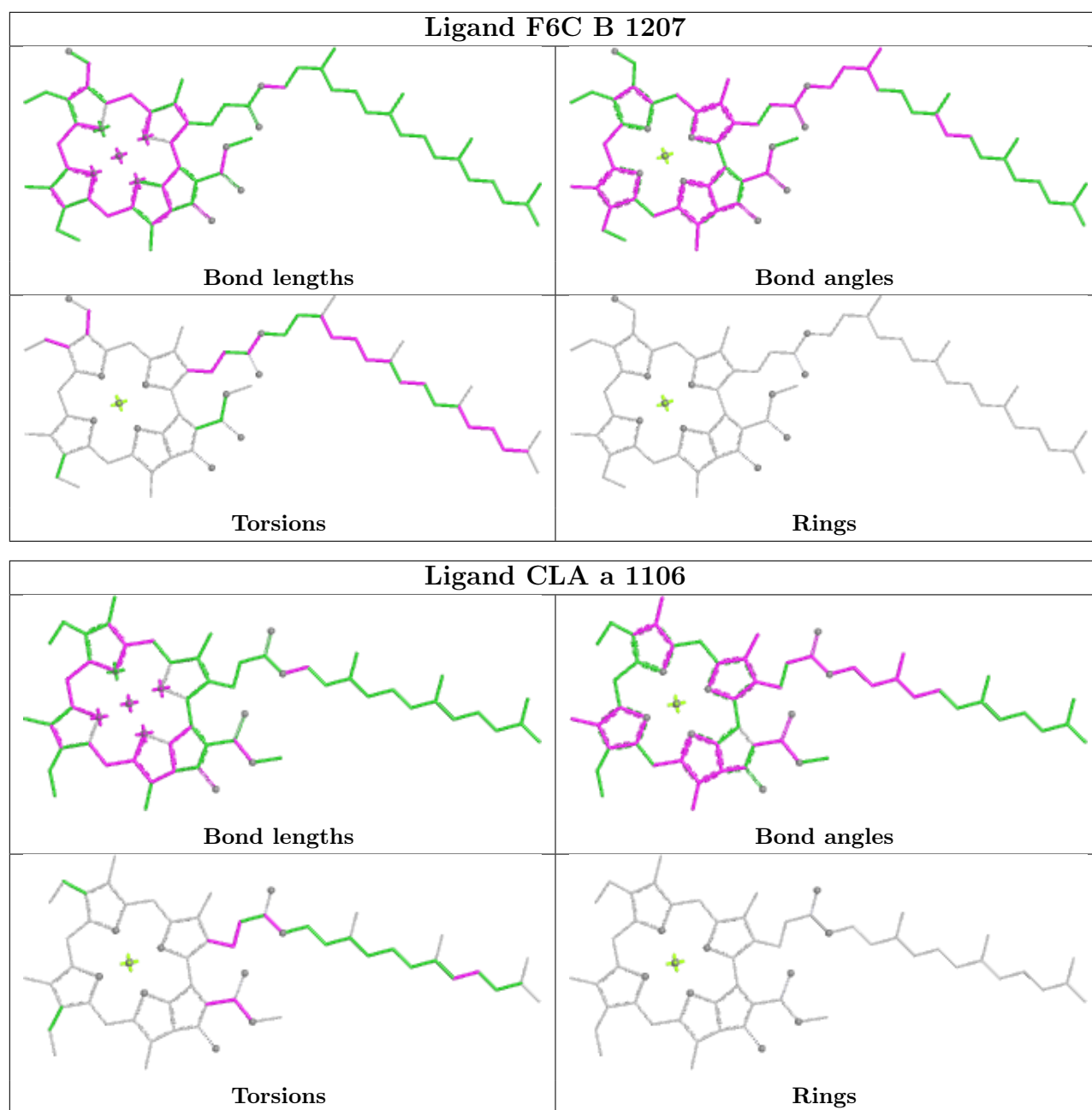


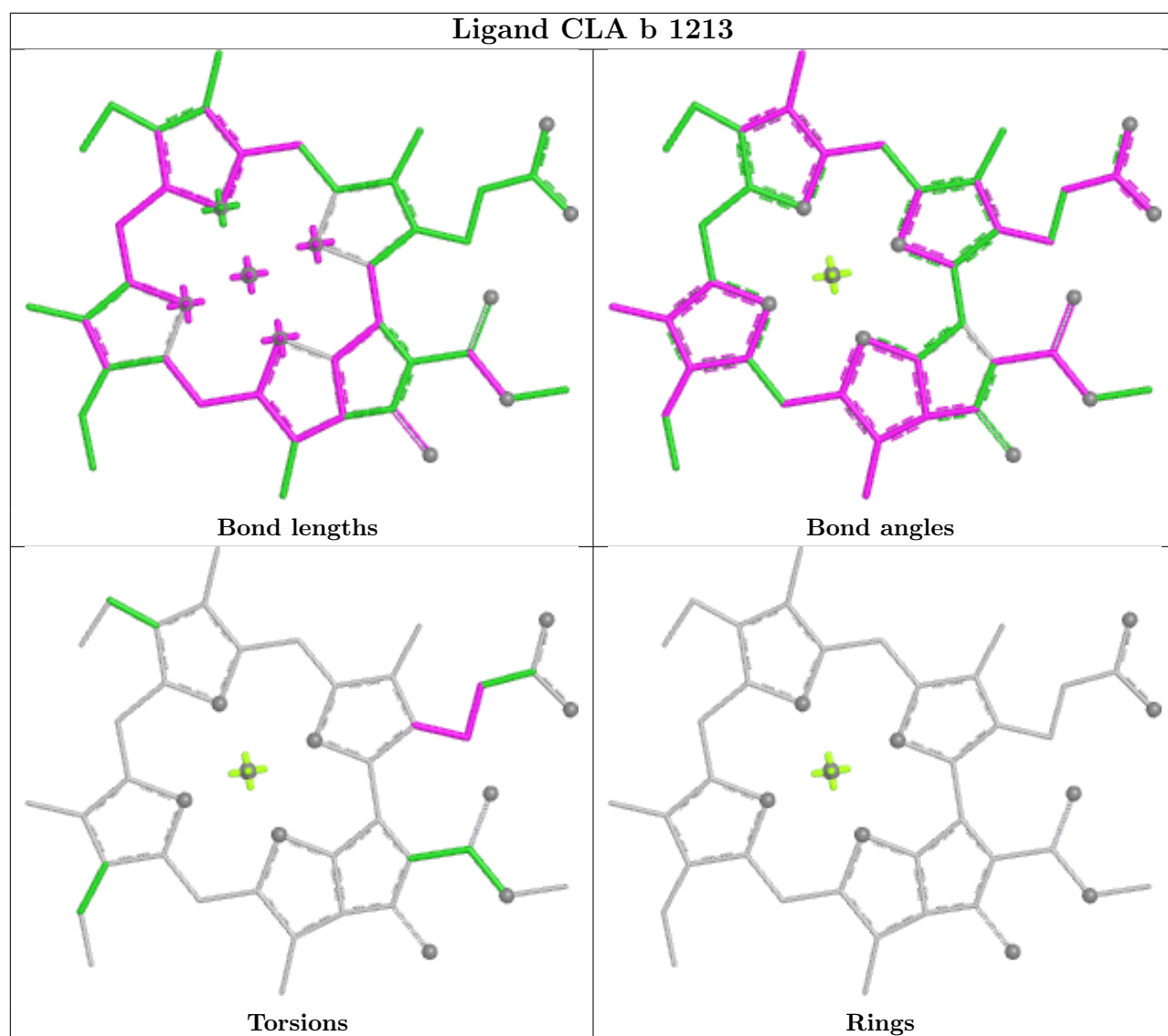
Ligand CLA G 1109



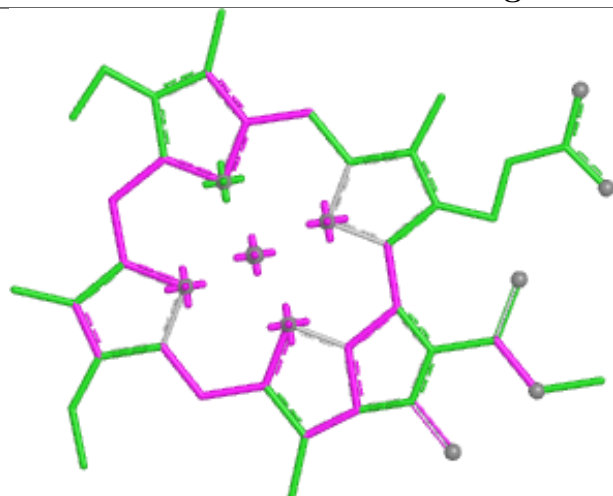
Ligand CLA A 1108



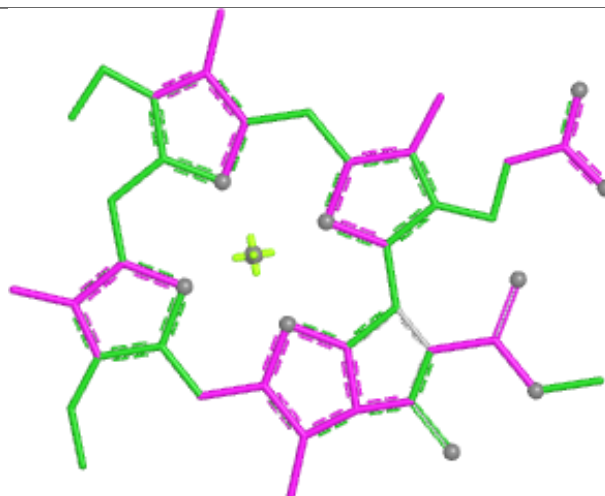




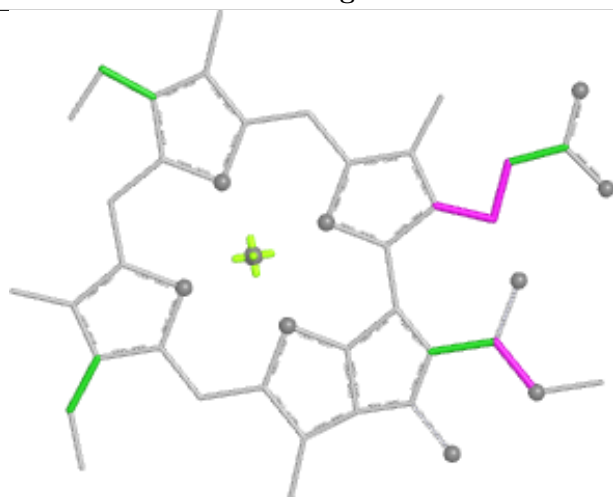
Ligand CLA G 1120



Bond lengths



Bond angles

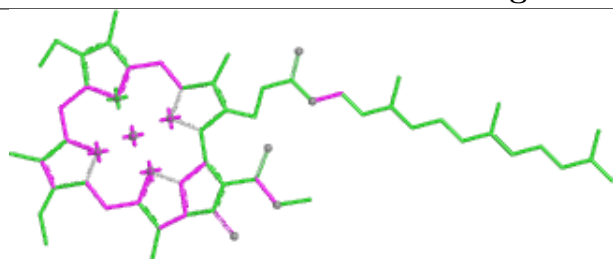


Torsions

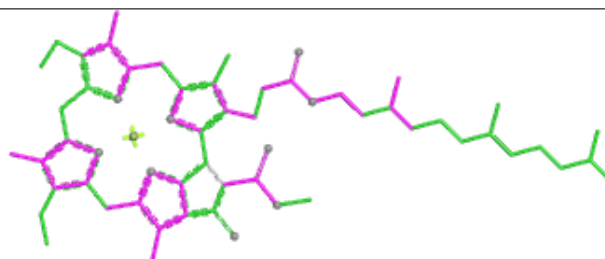


Rings

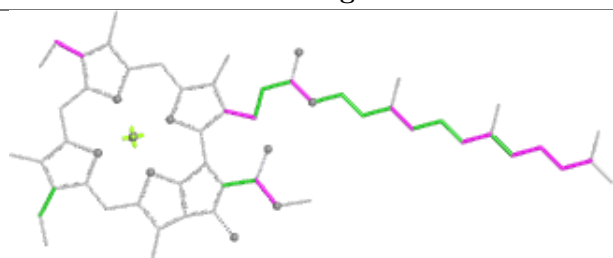
Ligand CLA a 1126



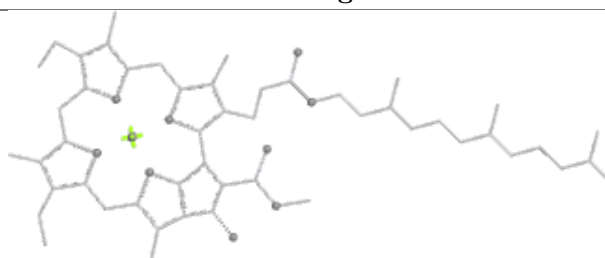
Bond lengths



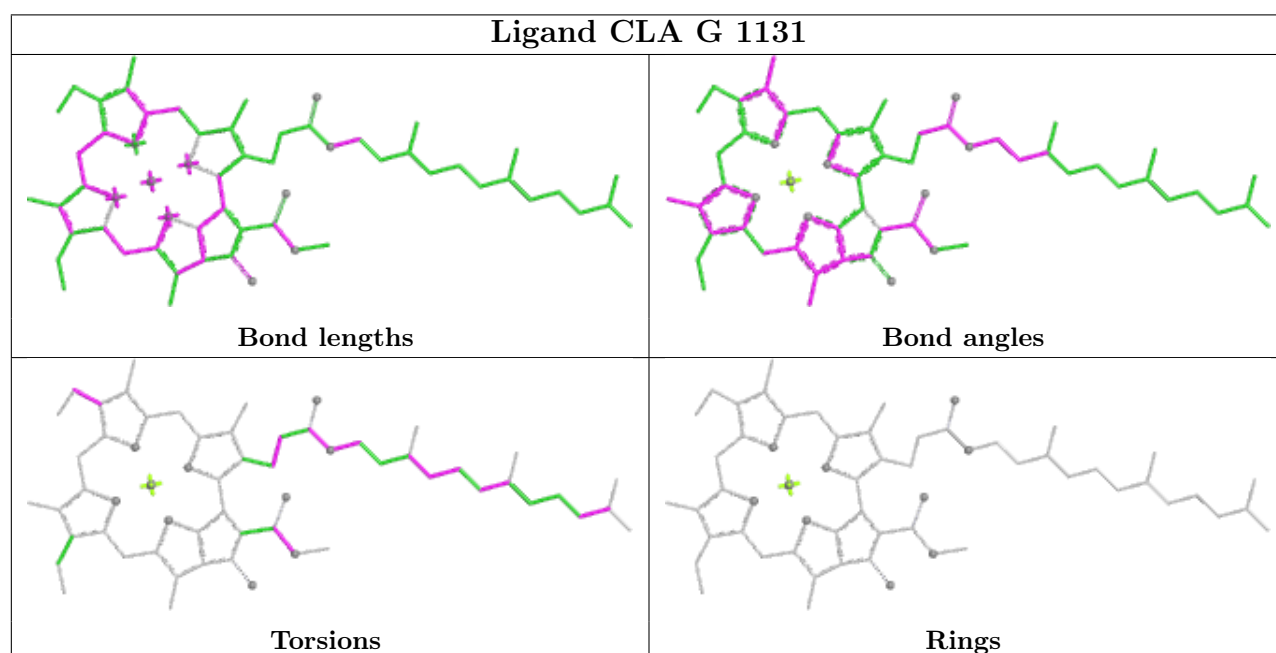
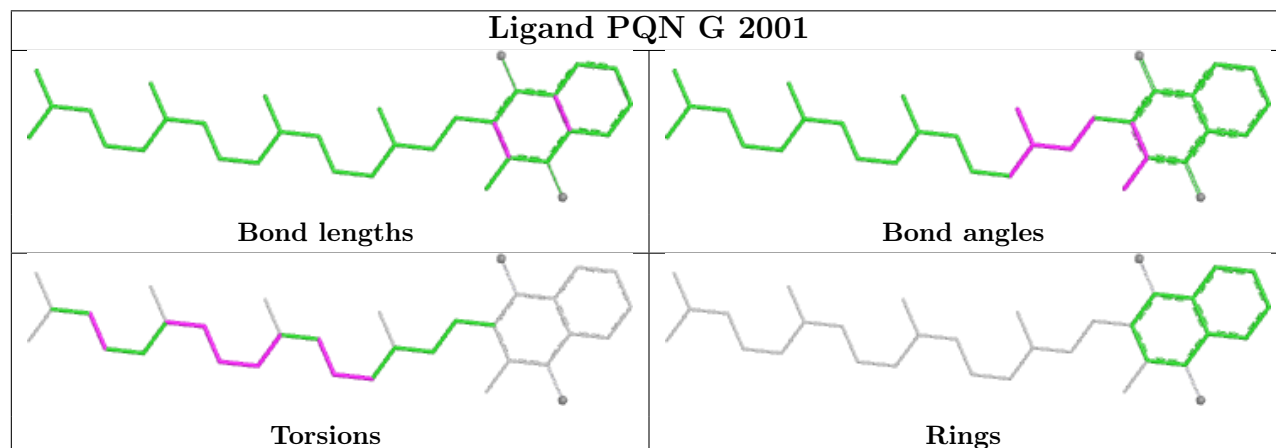
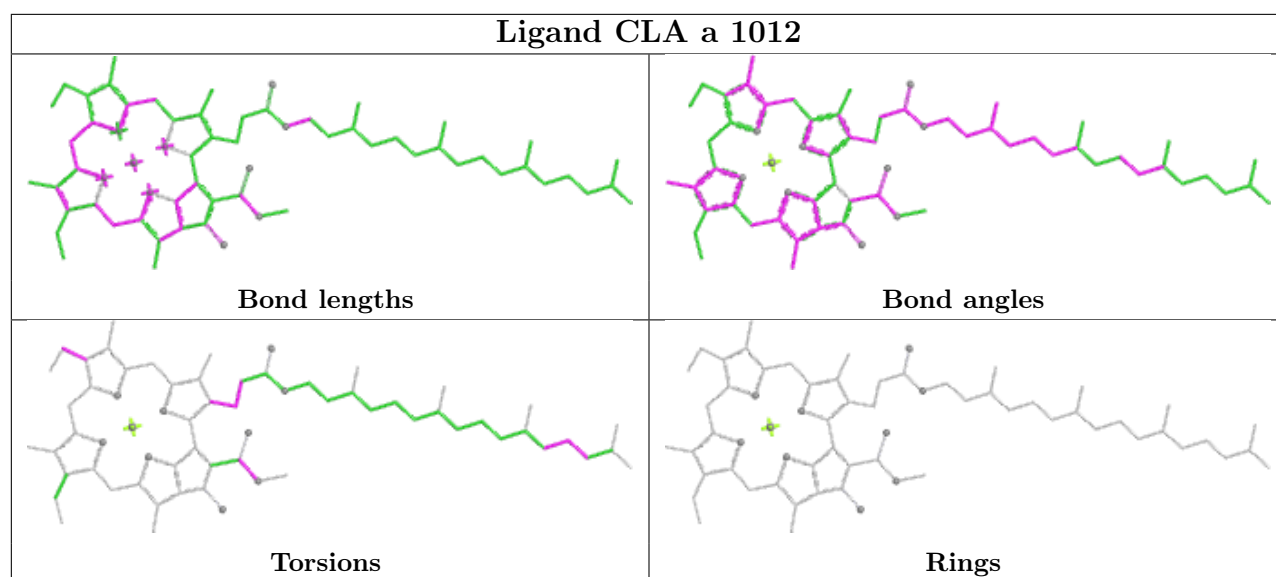
Bond angles

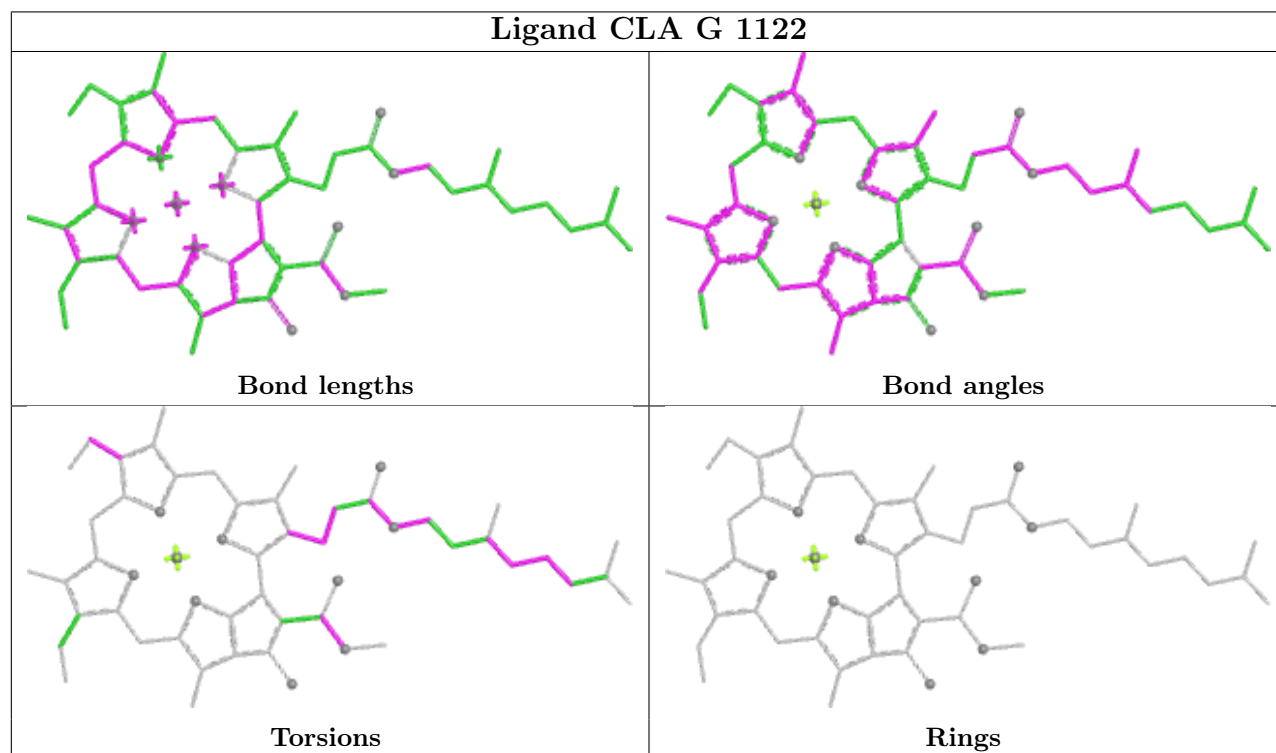
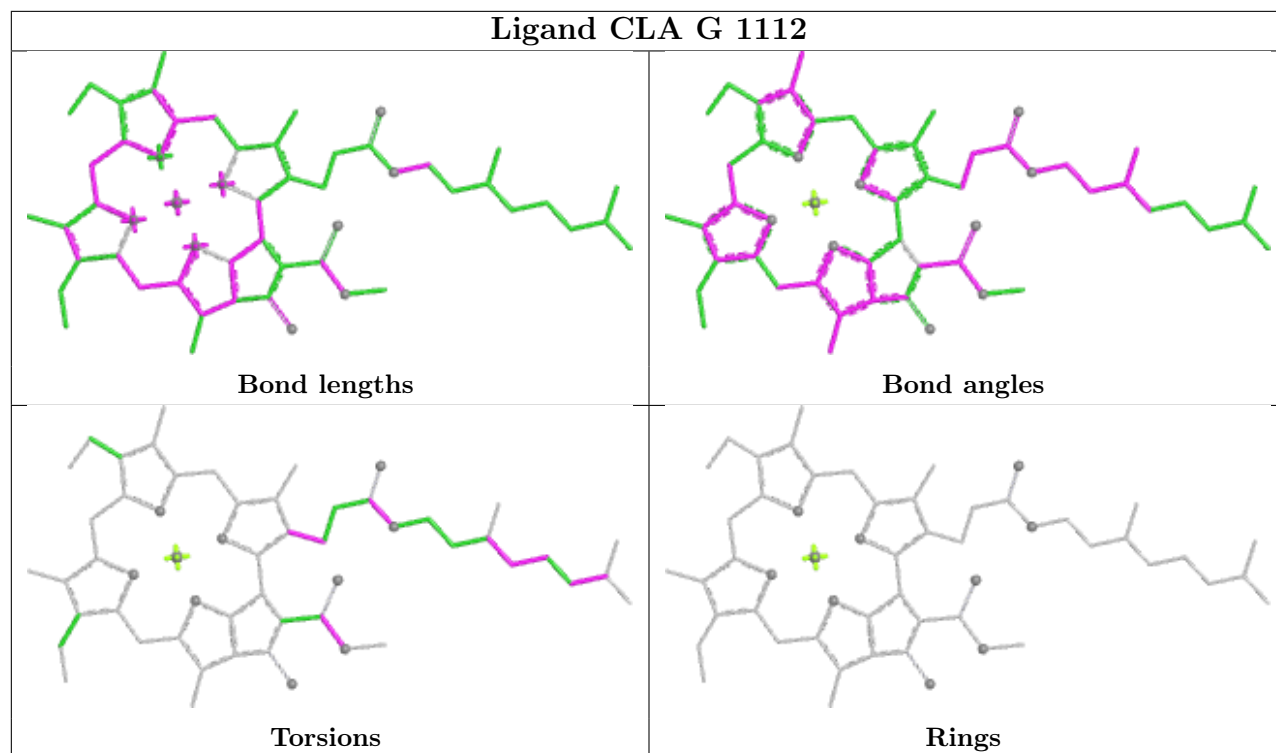


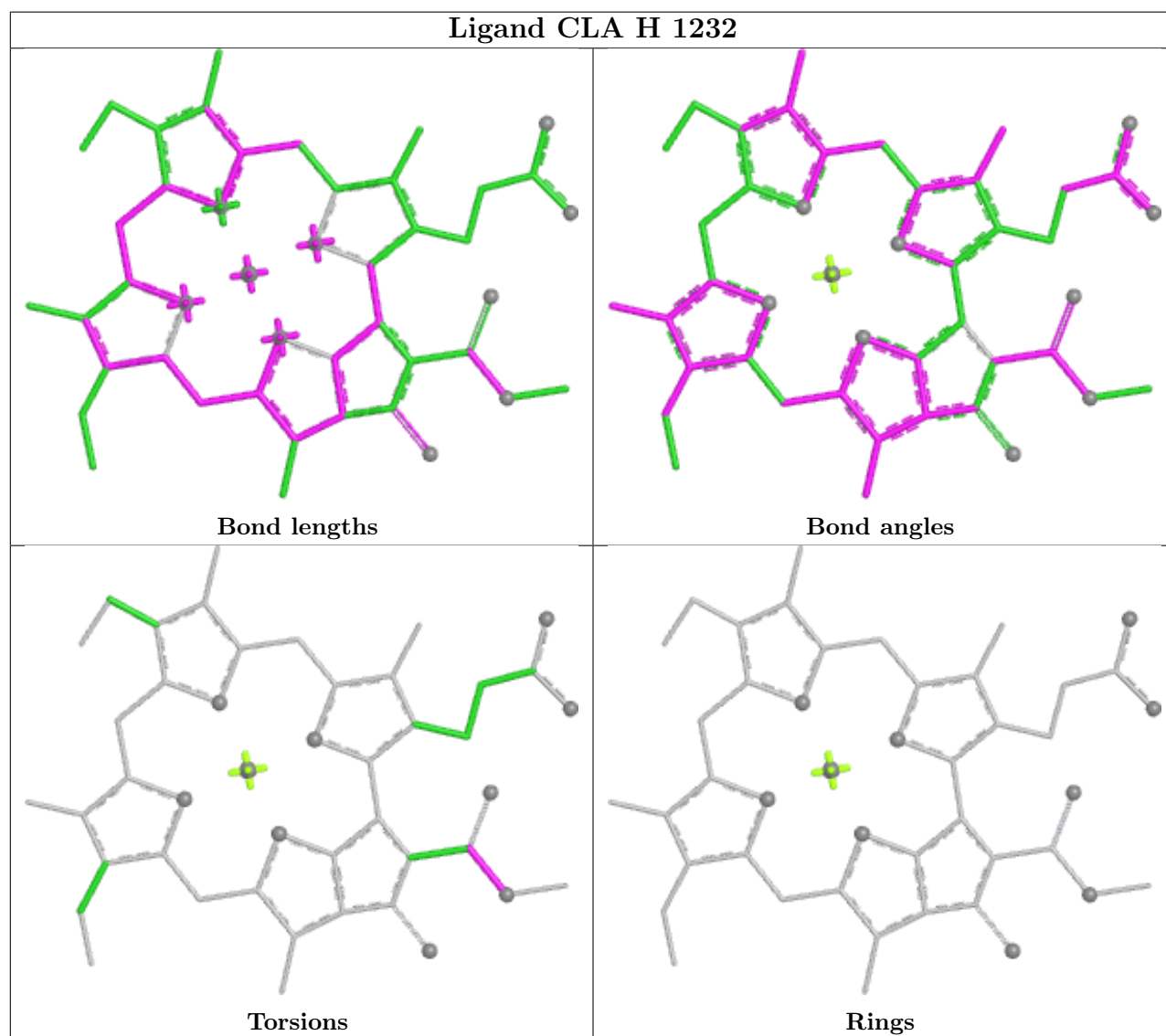
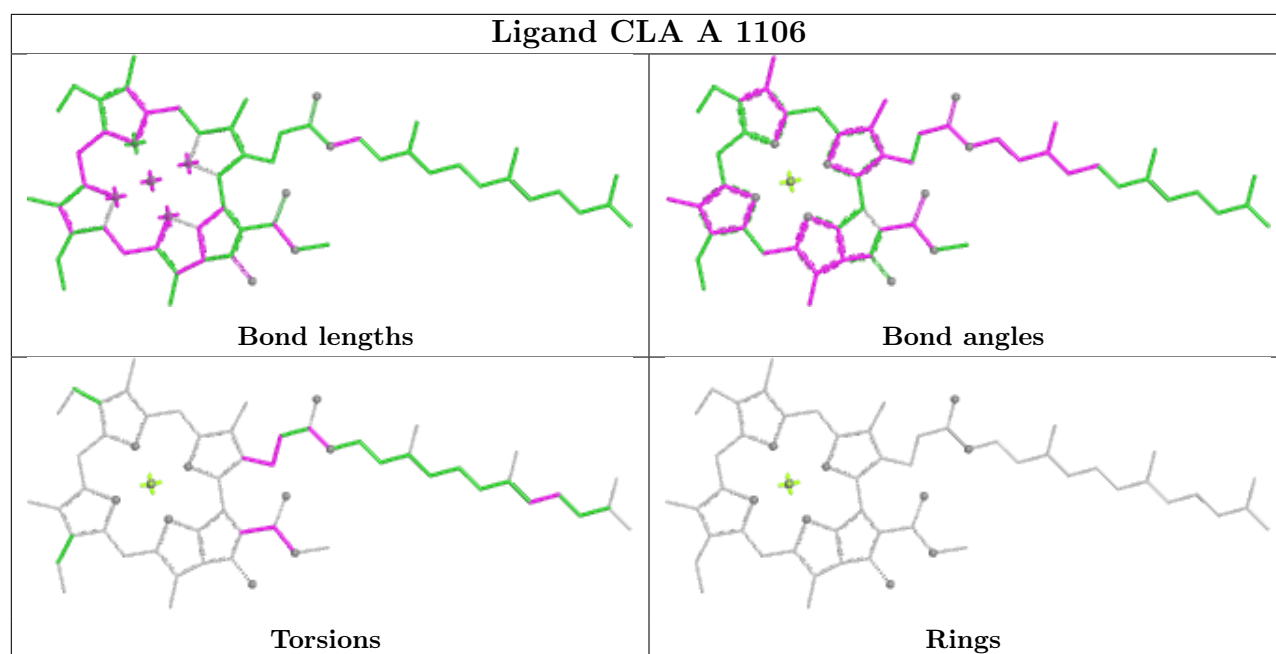
Torsions

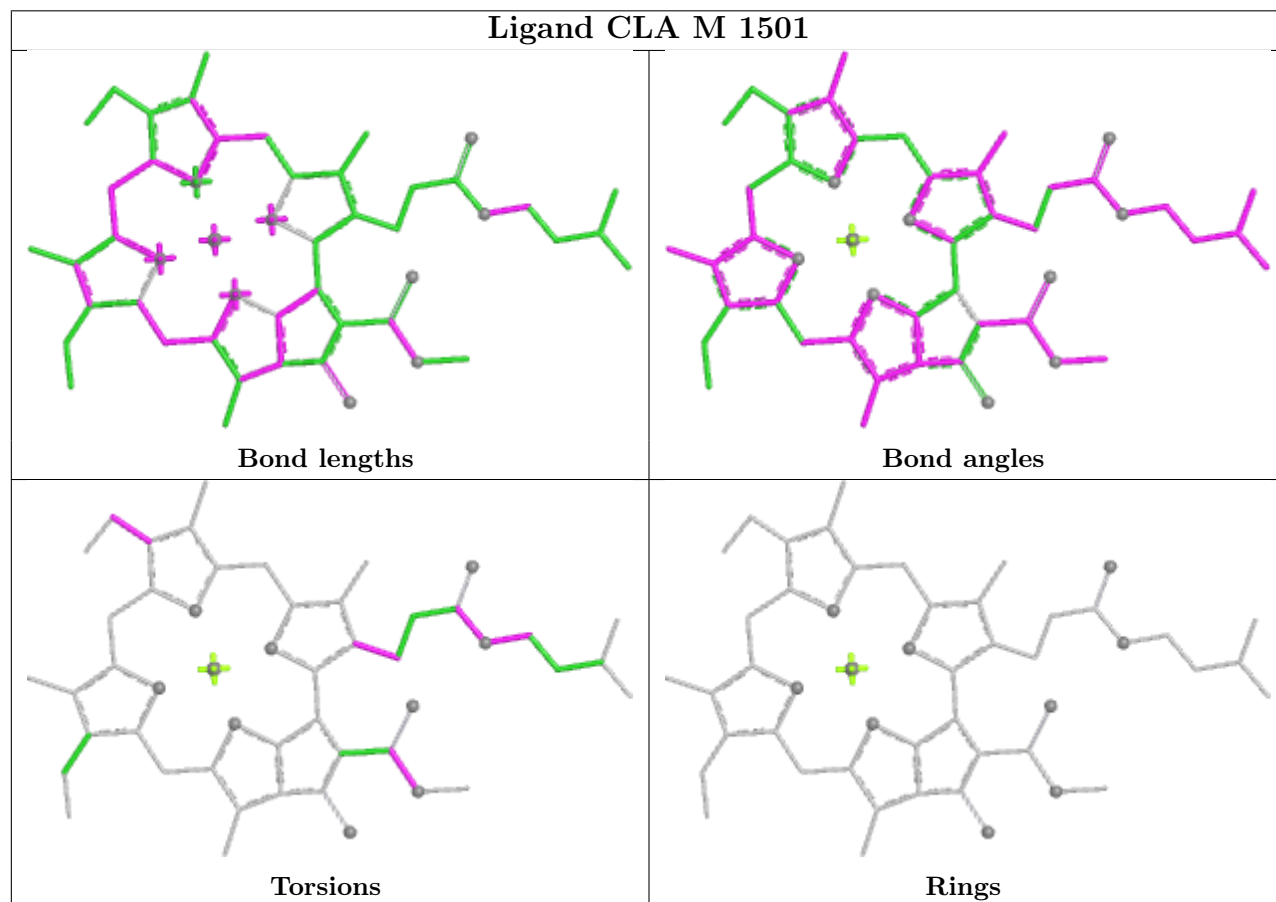
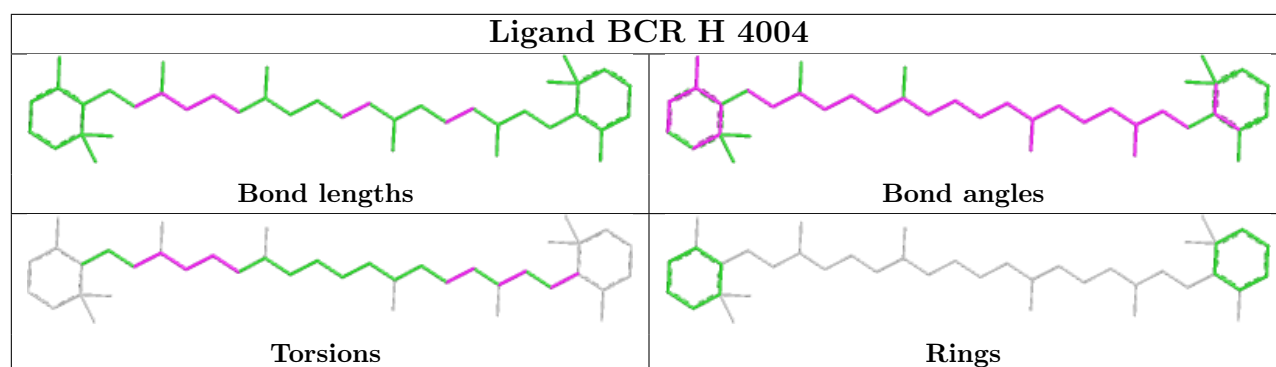


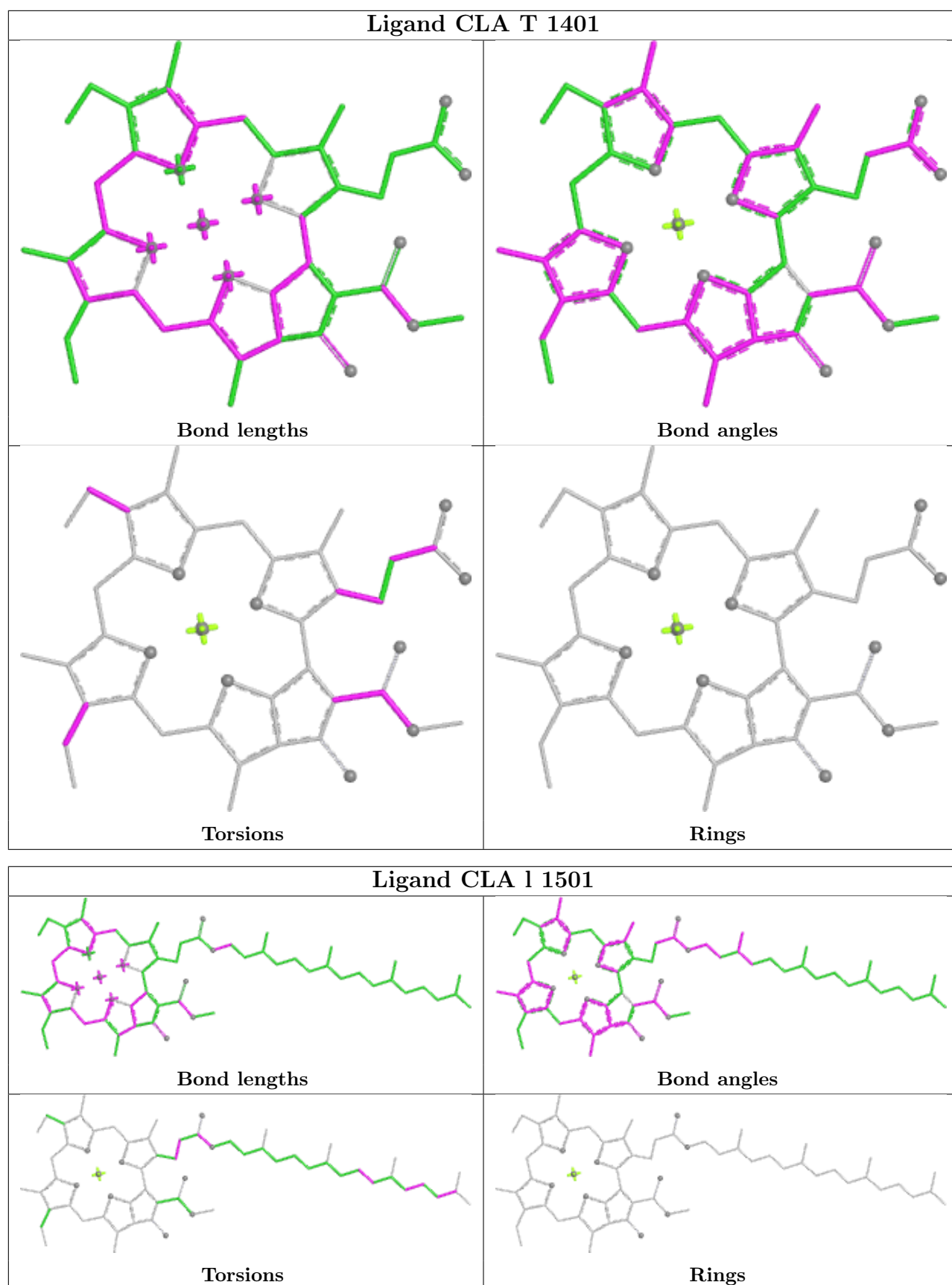
Rings

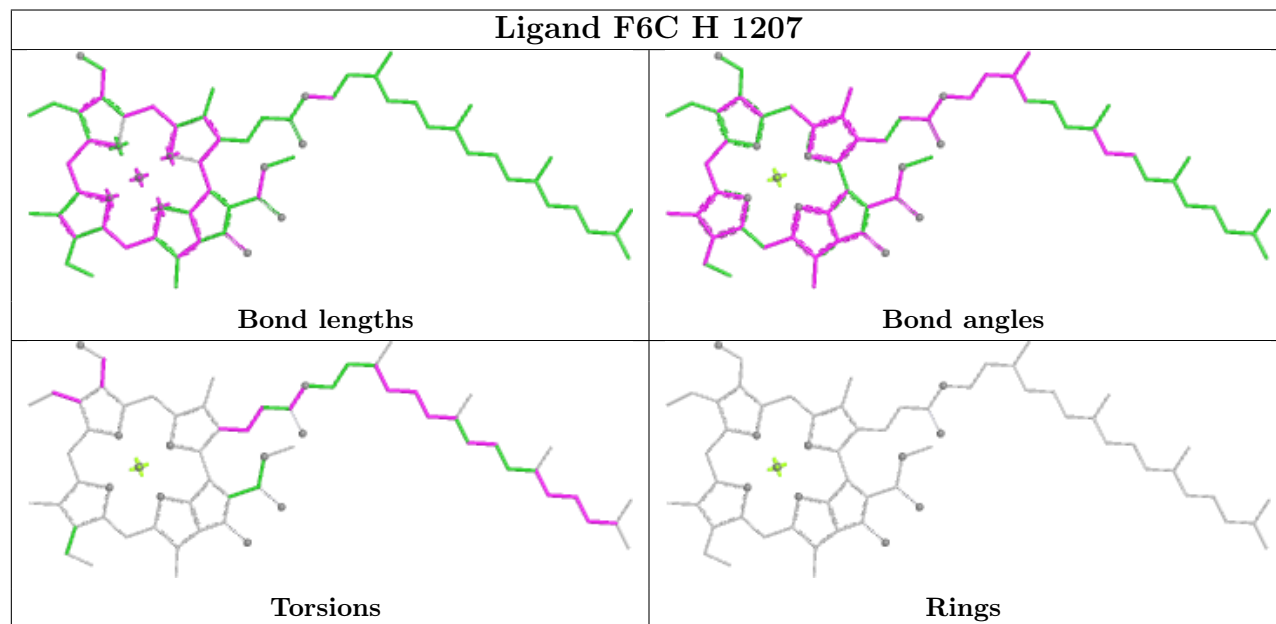
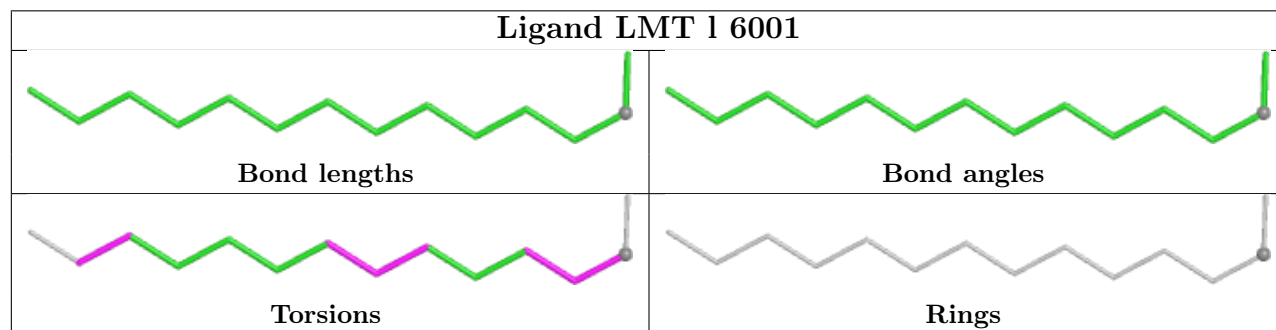
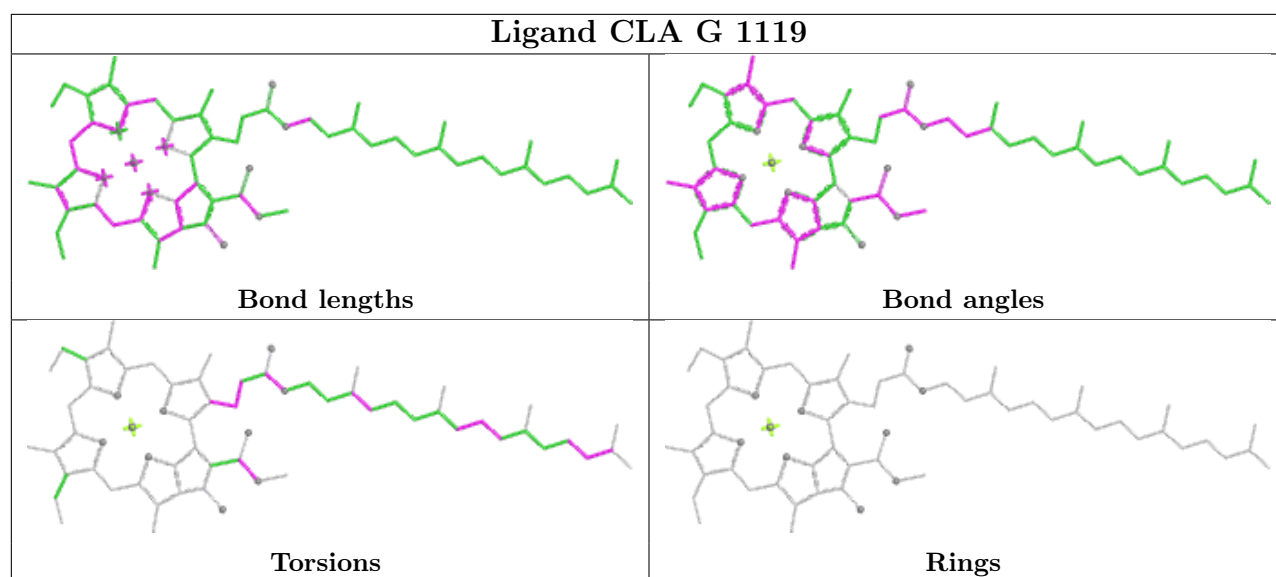


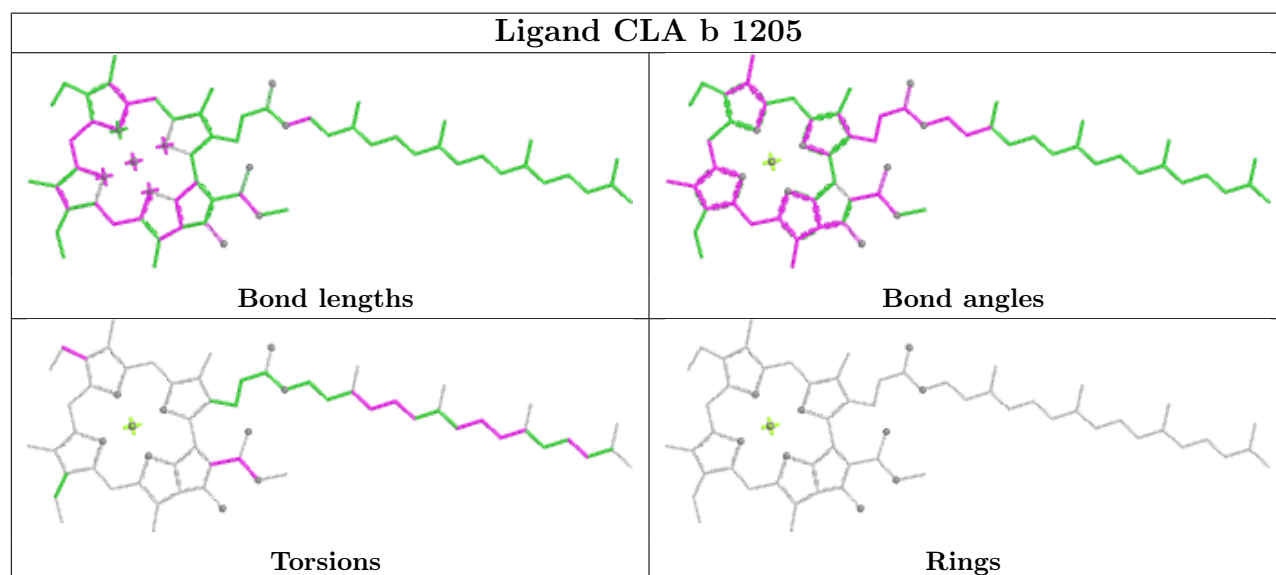
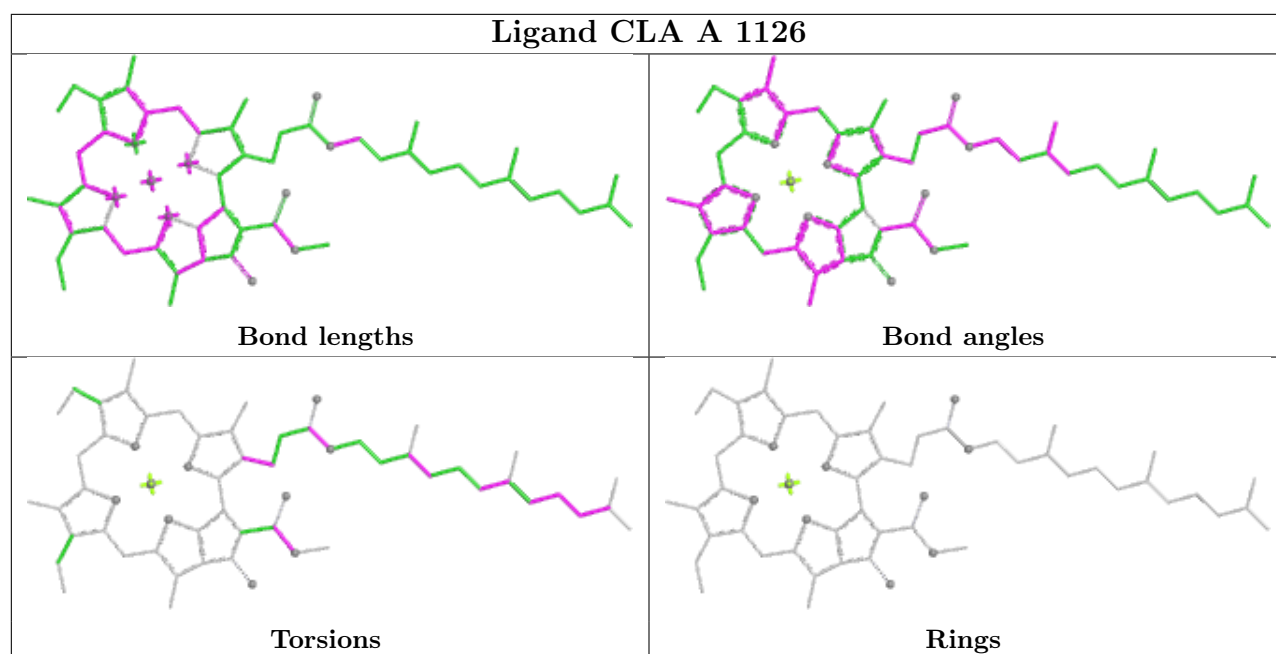




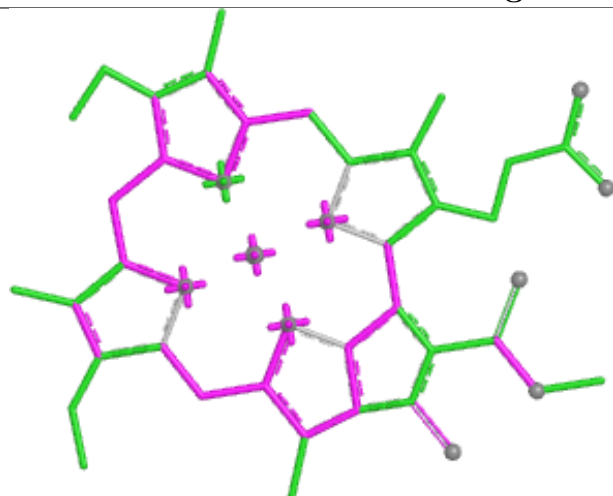




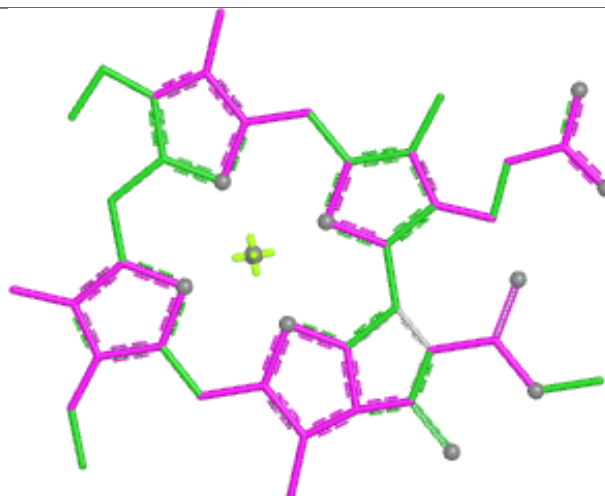




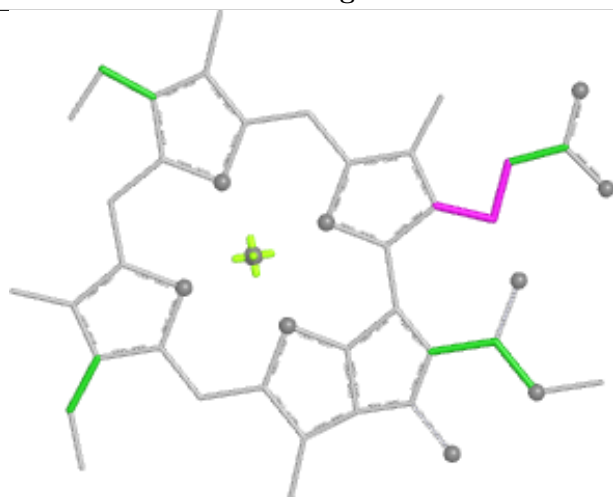
Ligand CLA B 1213



Bond lengths



Bond angles

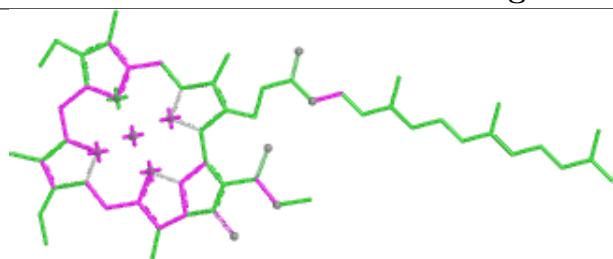


Torsions

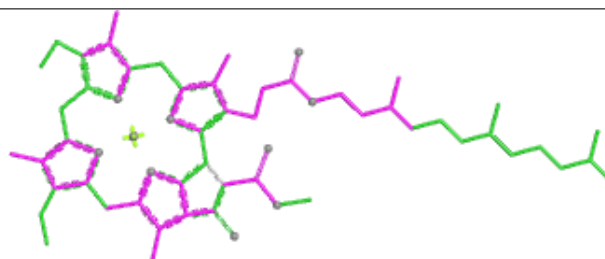


Rings

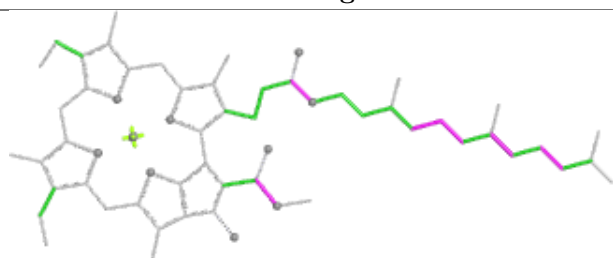
Ligand CLA b 1208



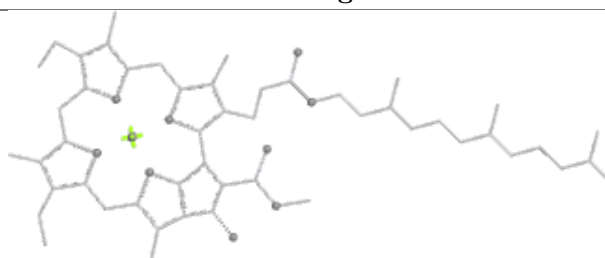
Bond lengths



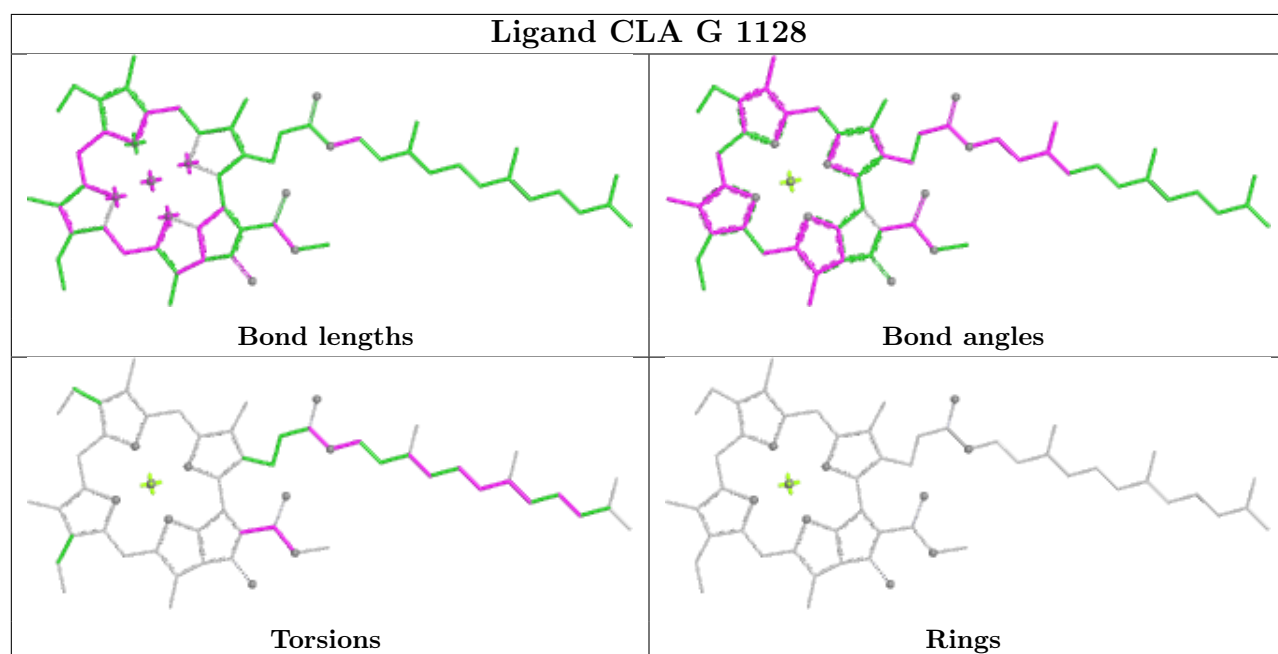
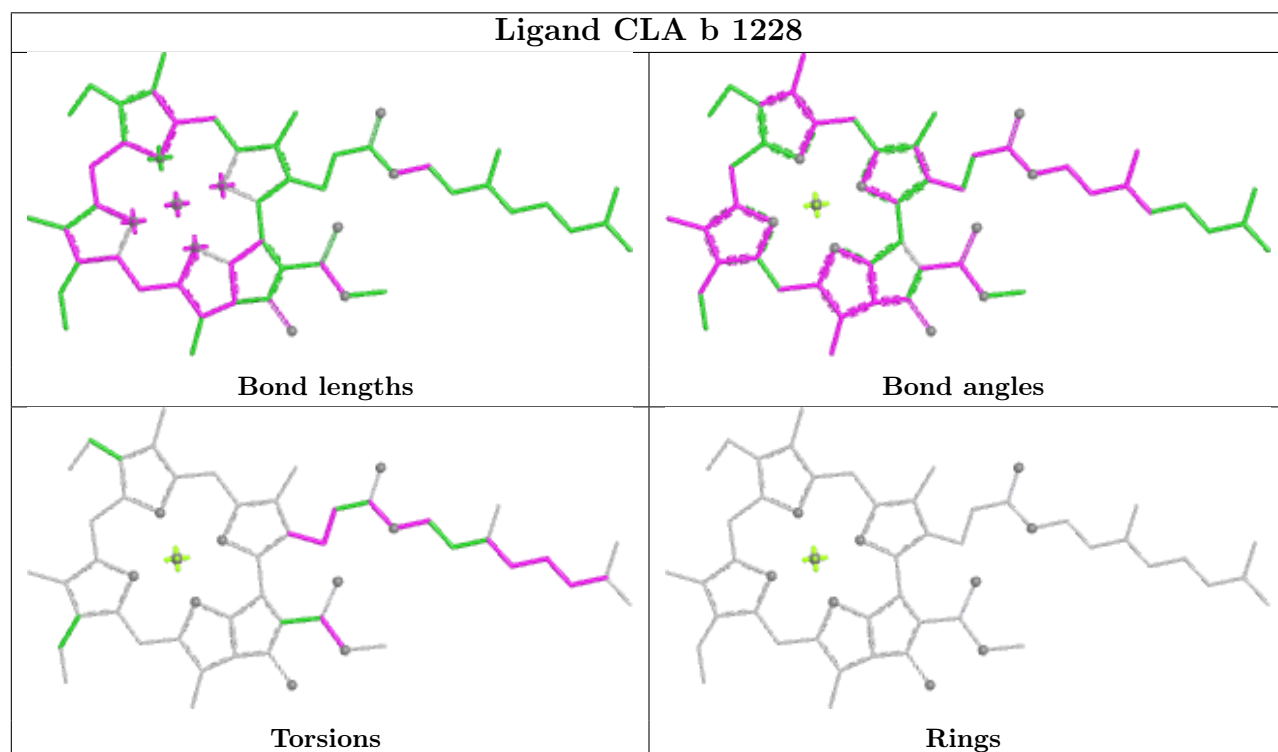
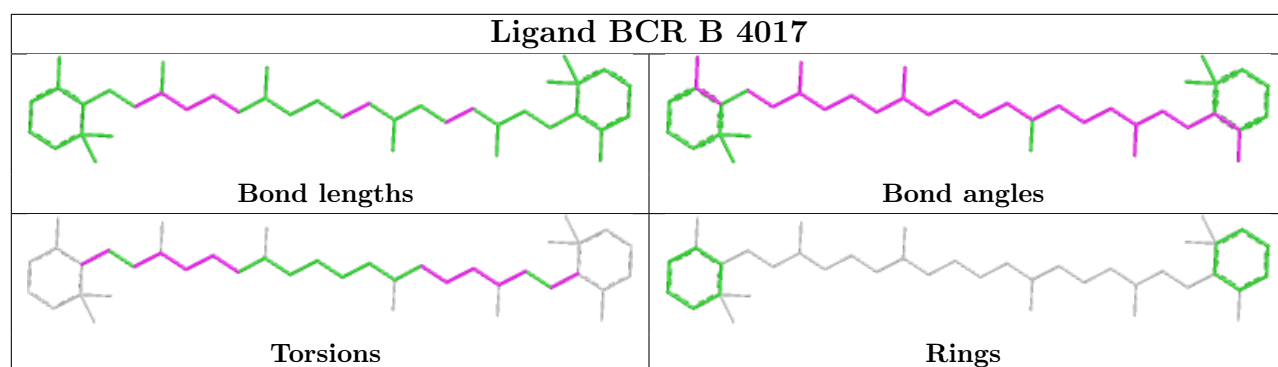
Bond angles

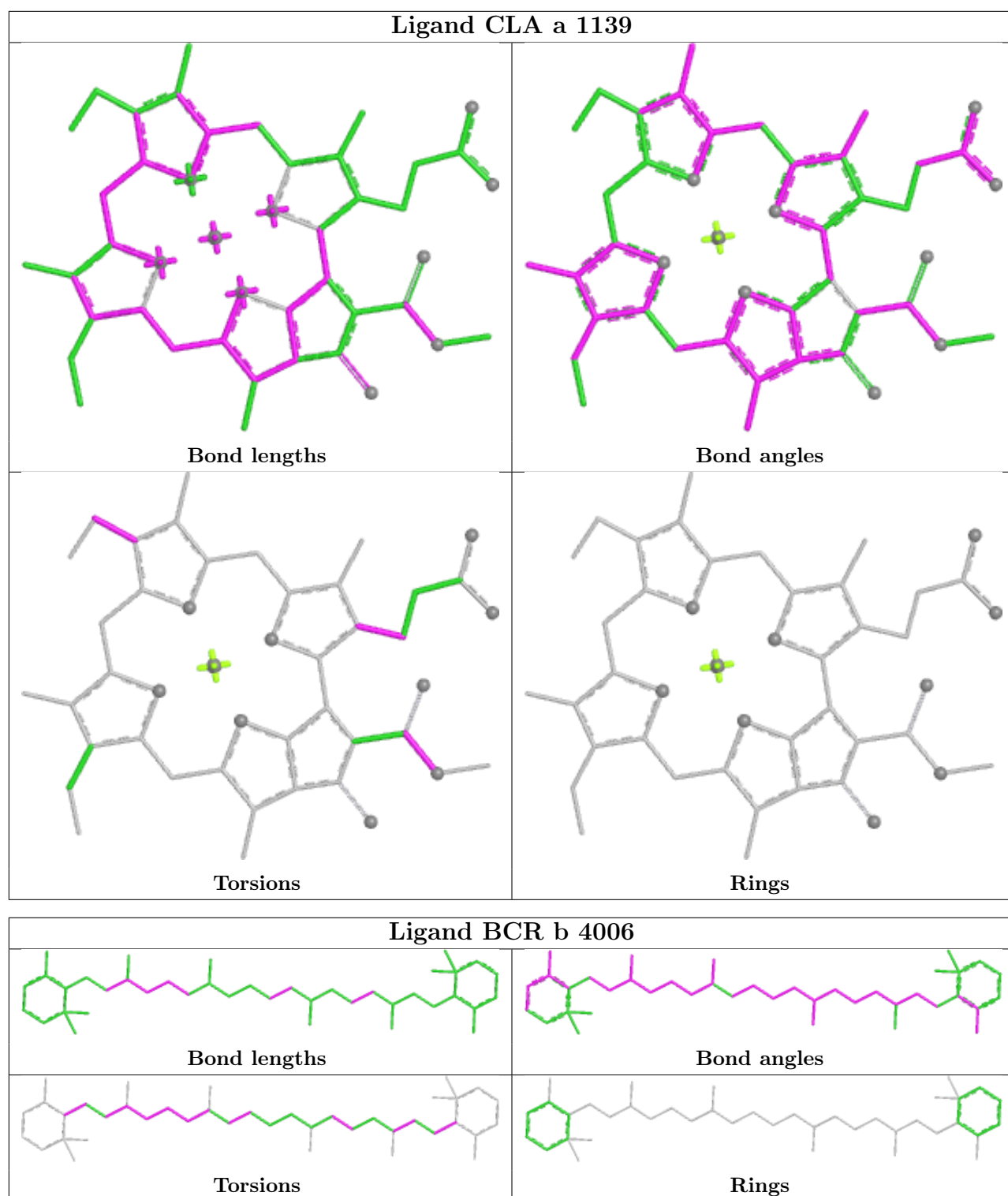


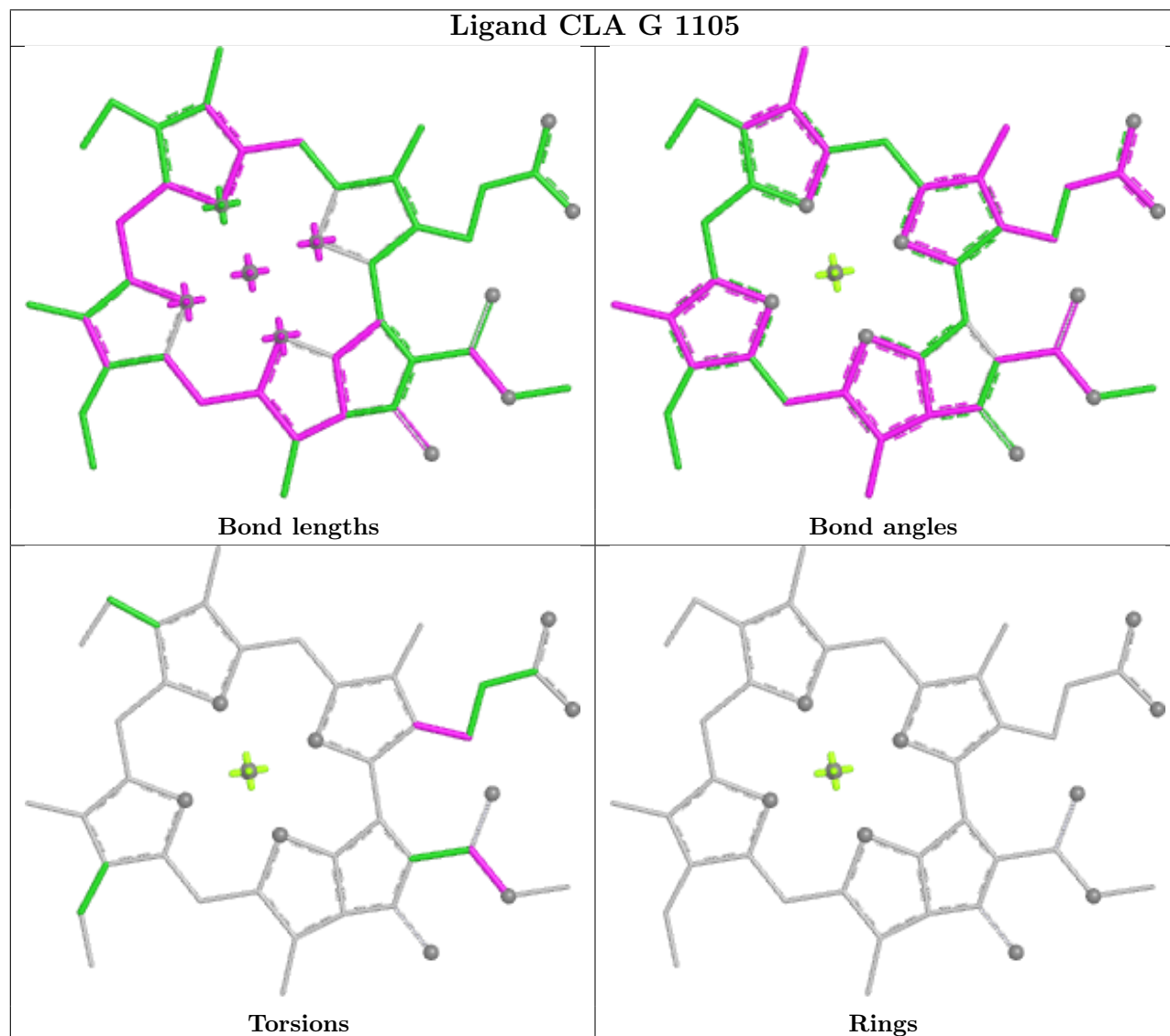
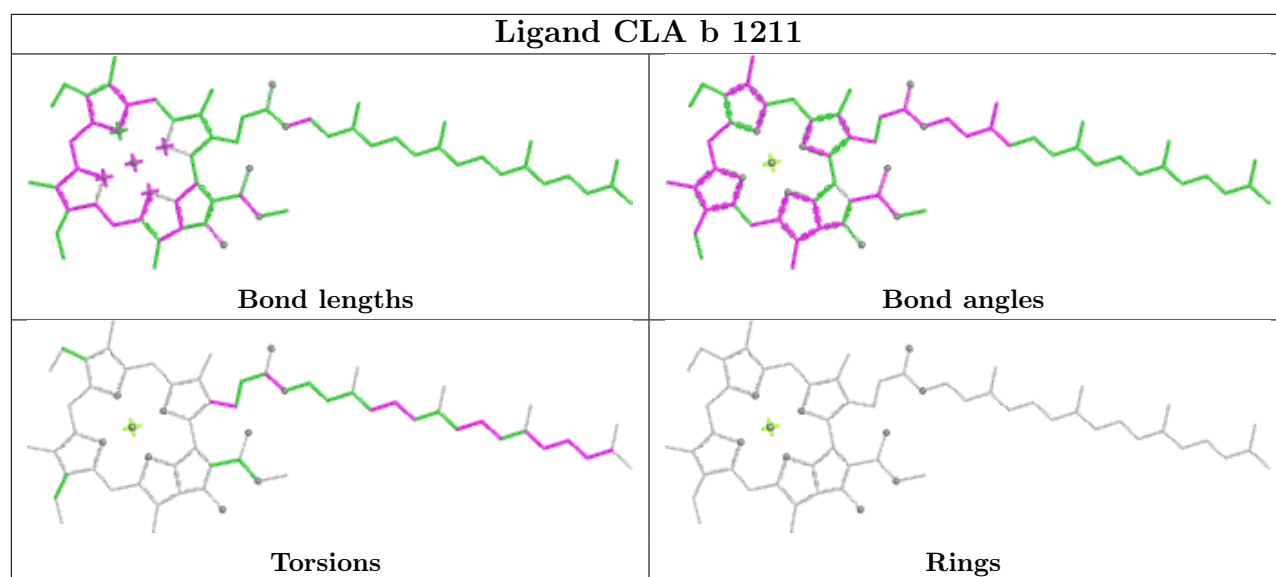
Torsions

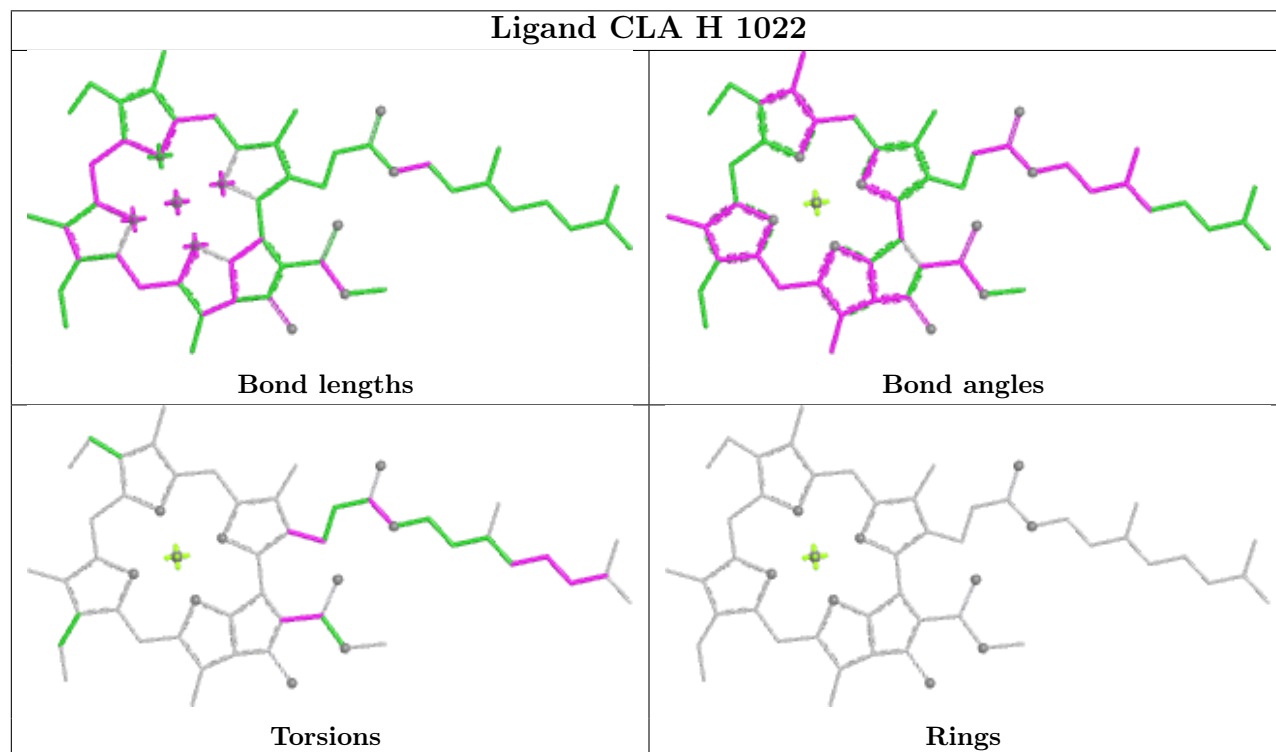
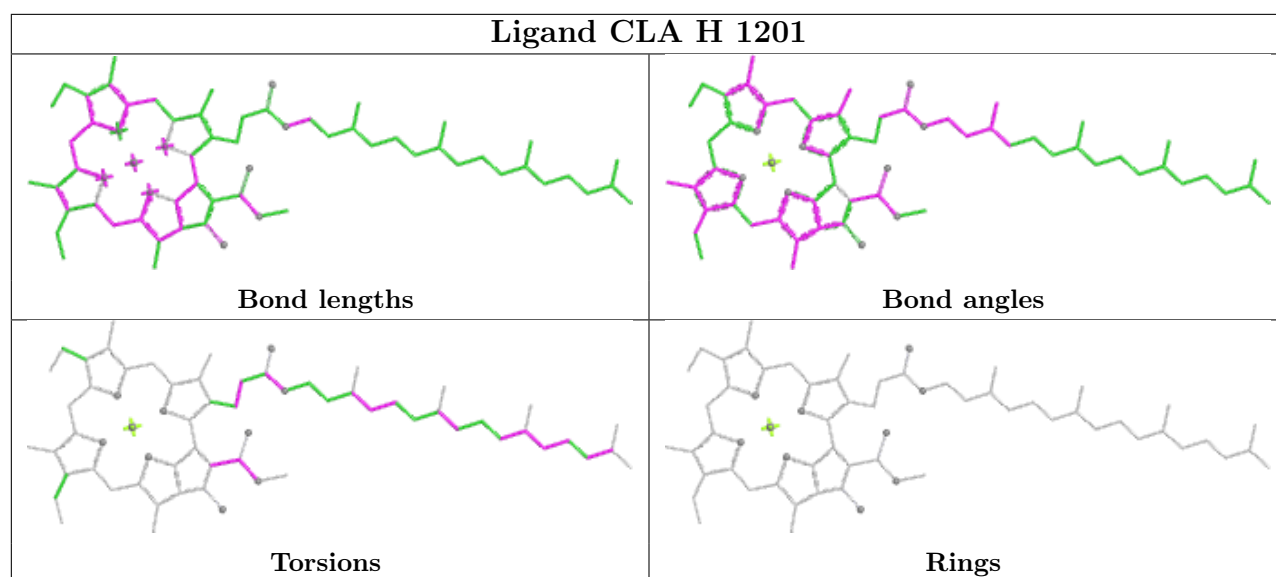


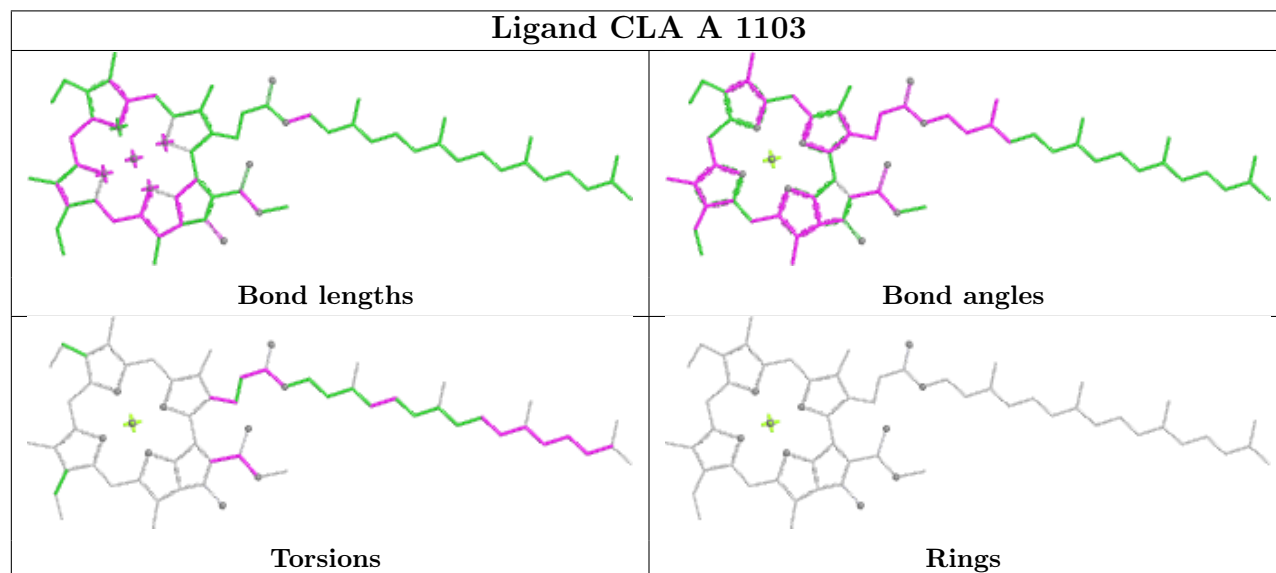
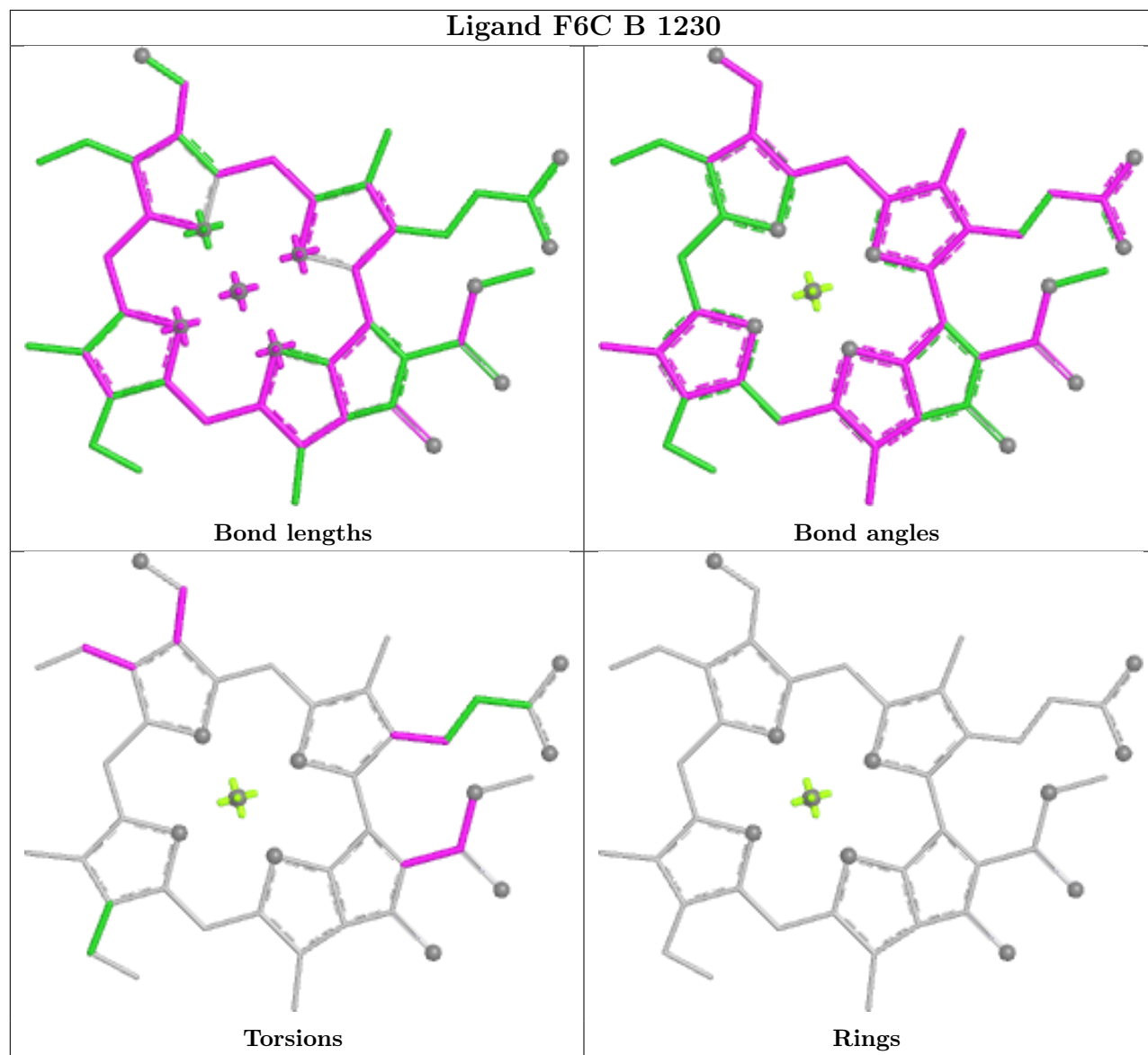
Rings

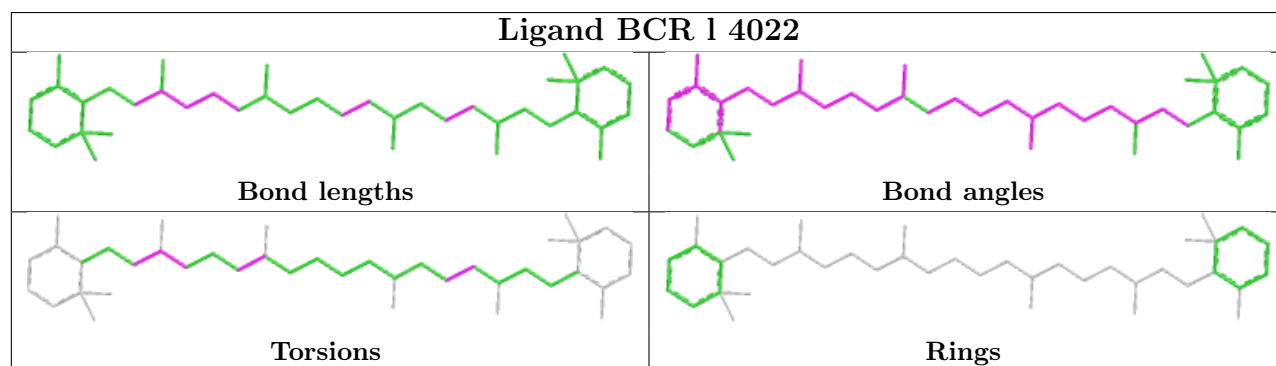
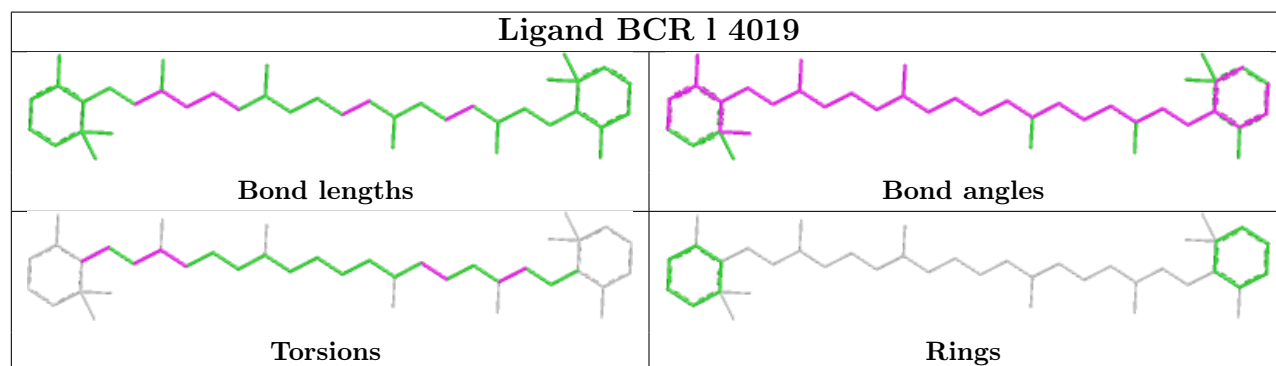
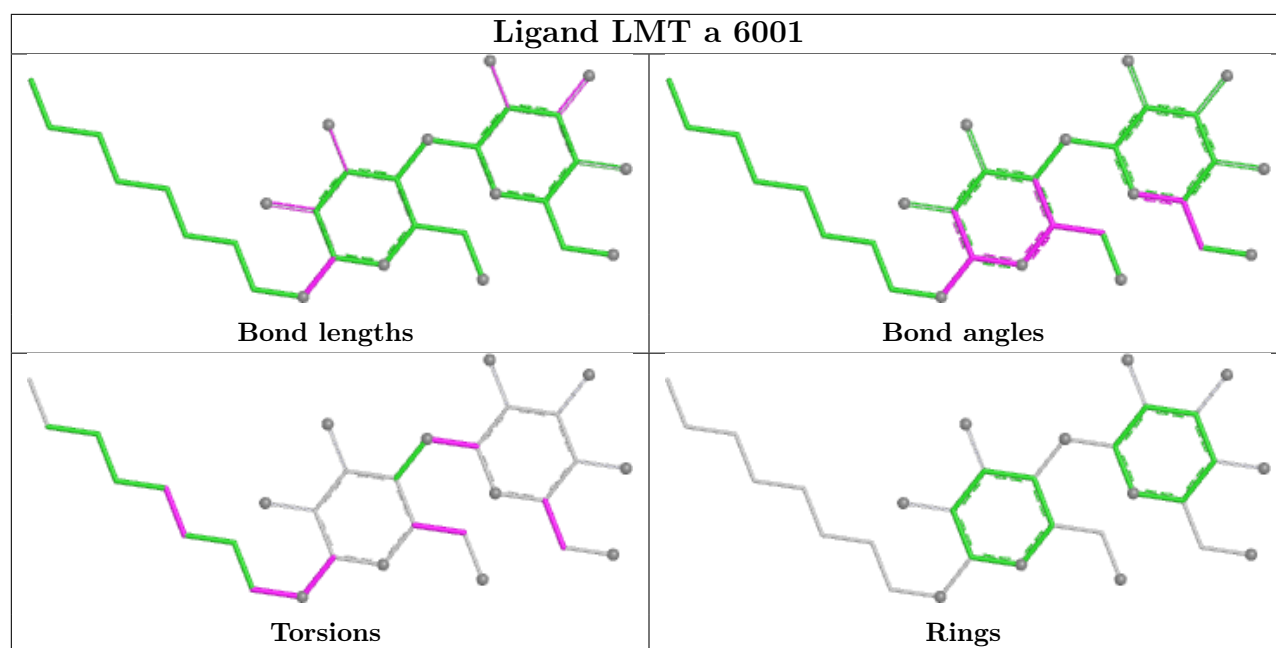


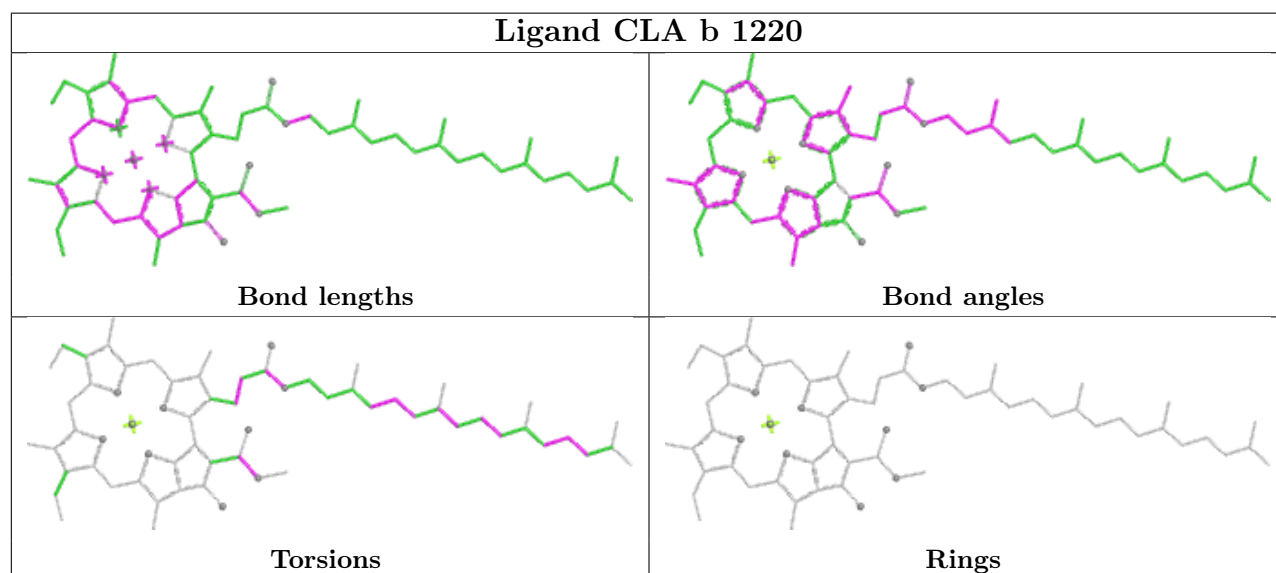
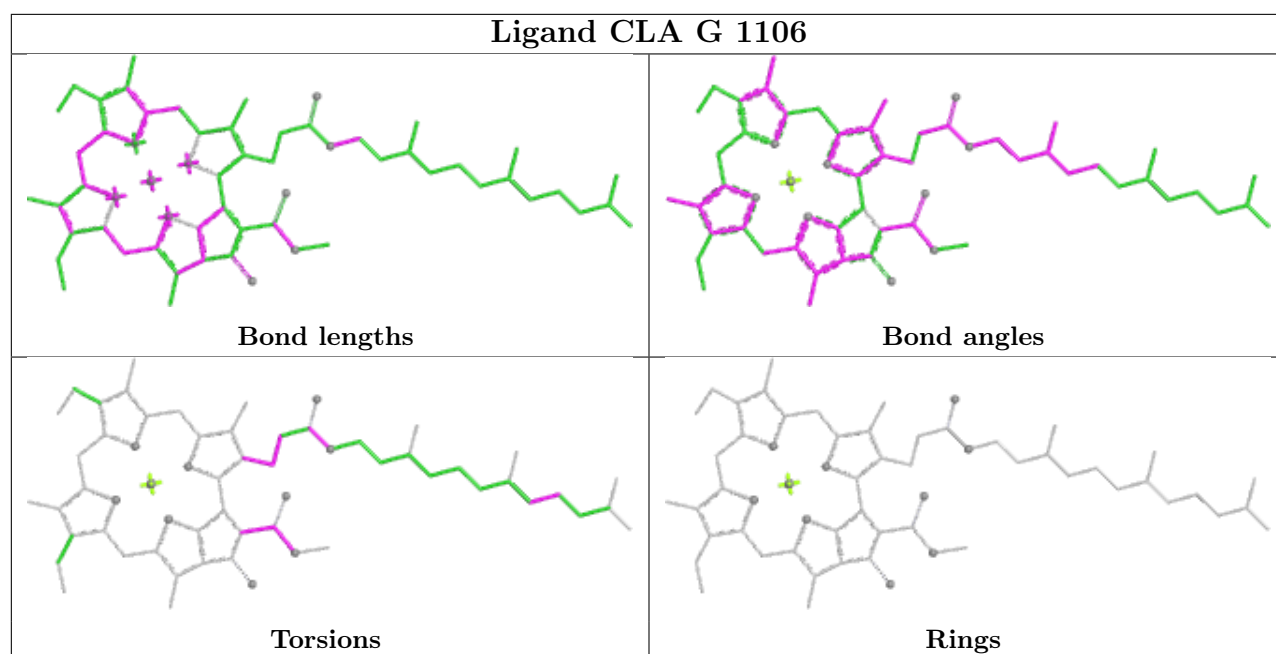


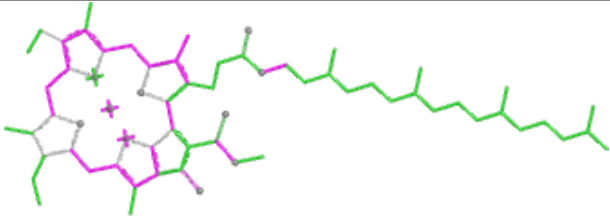
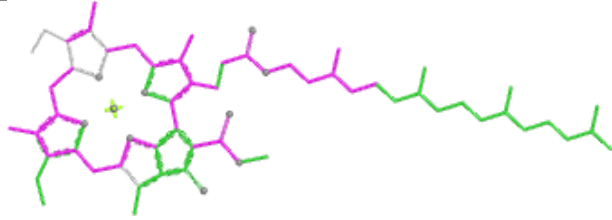
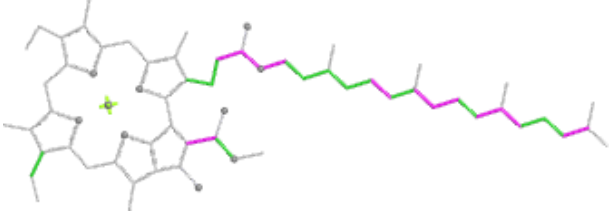
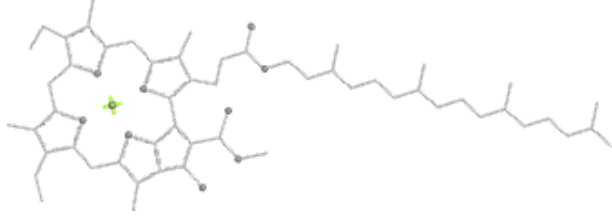
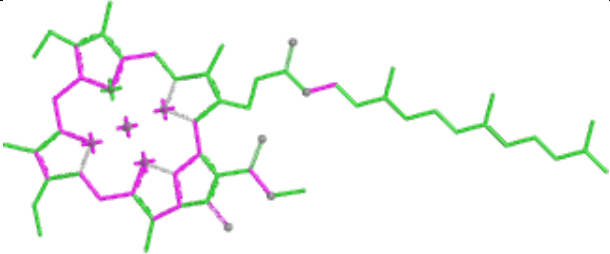
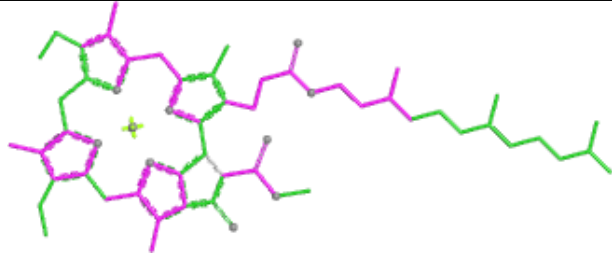
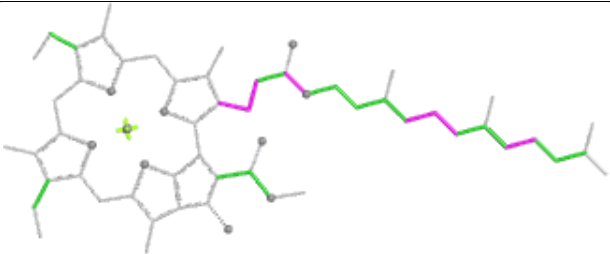
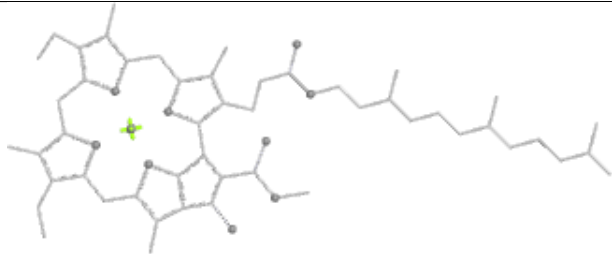
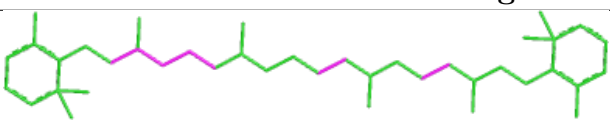
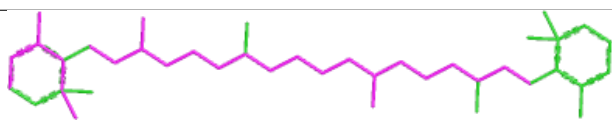
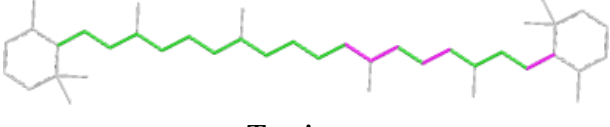
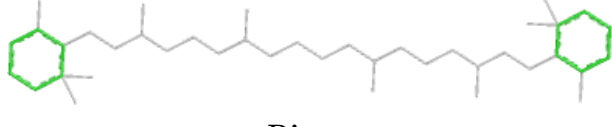


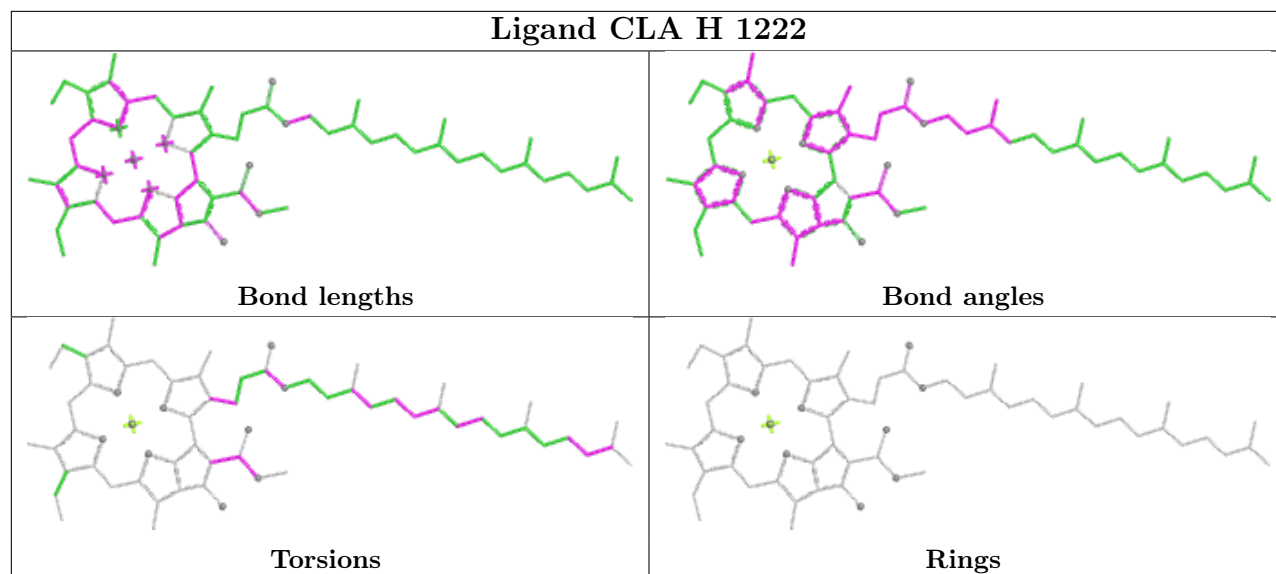
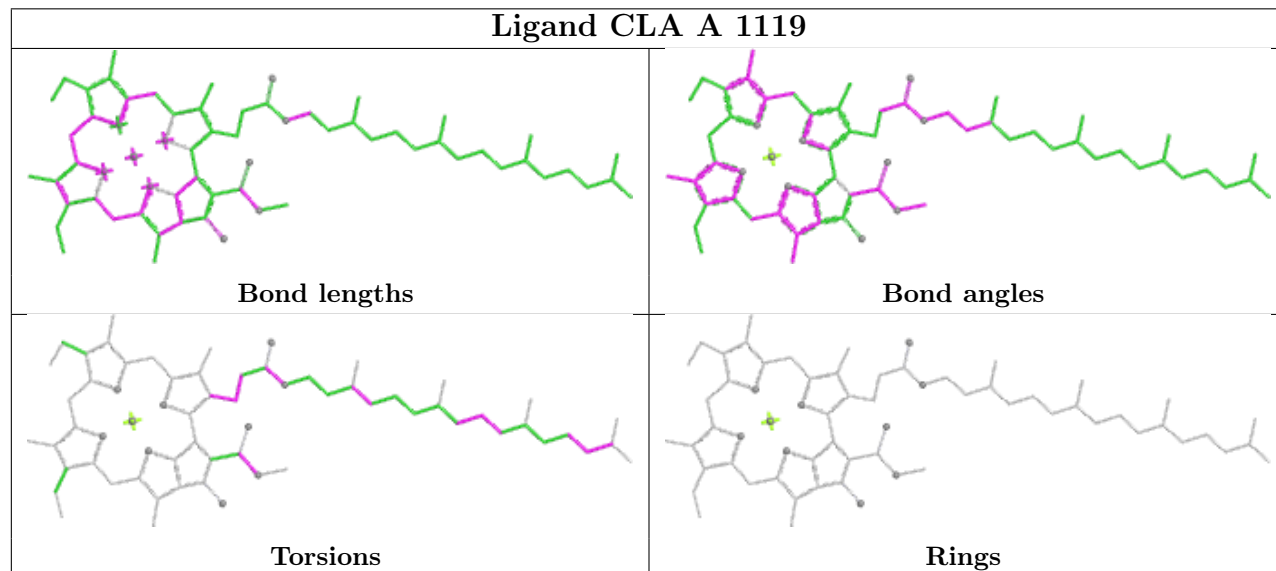


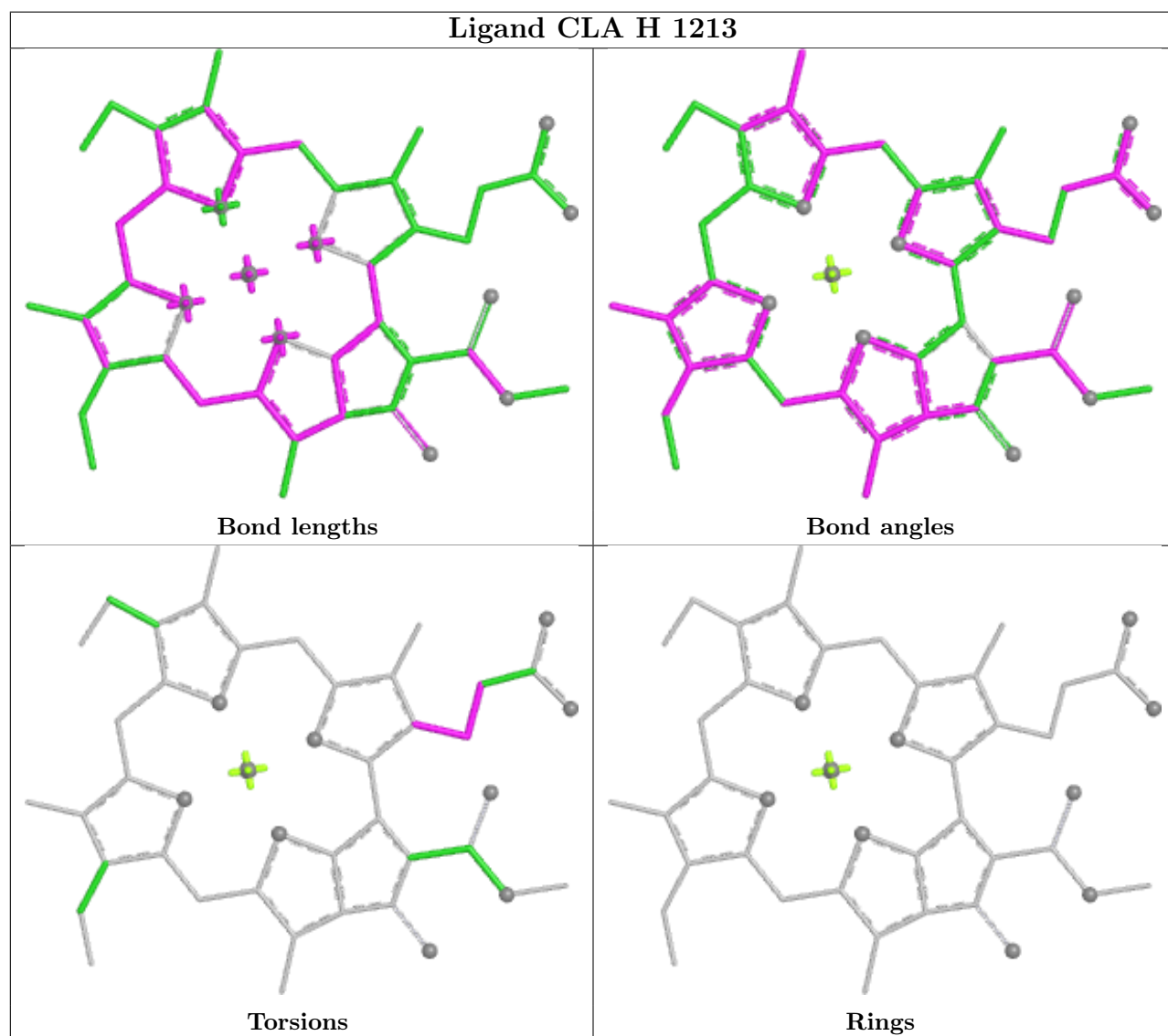
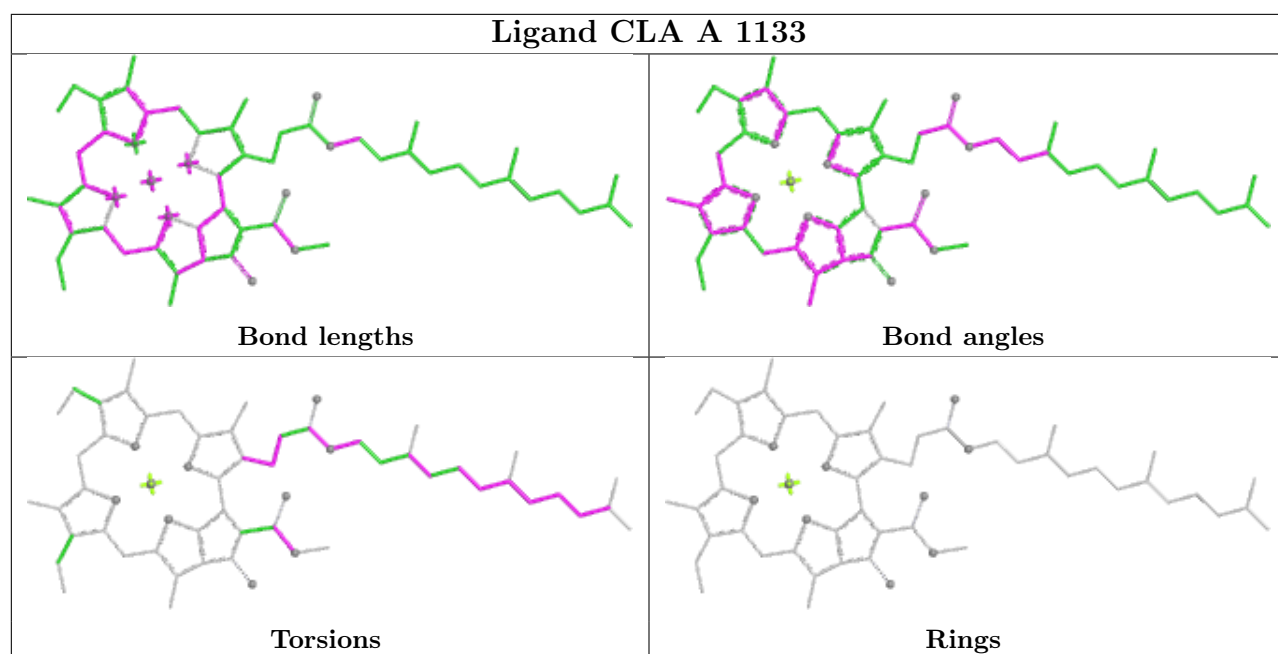


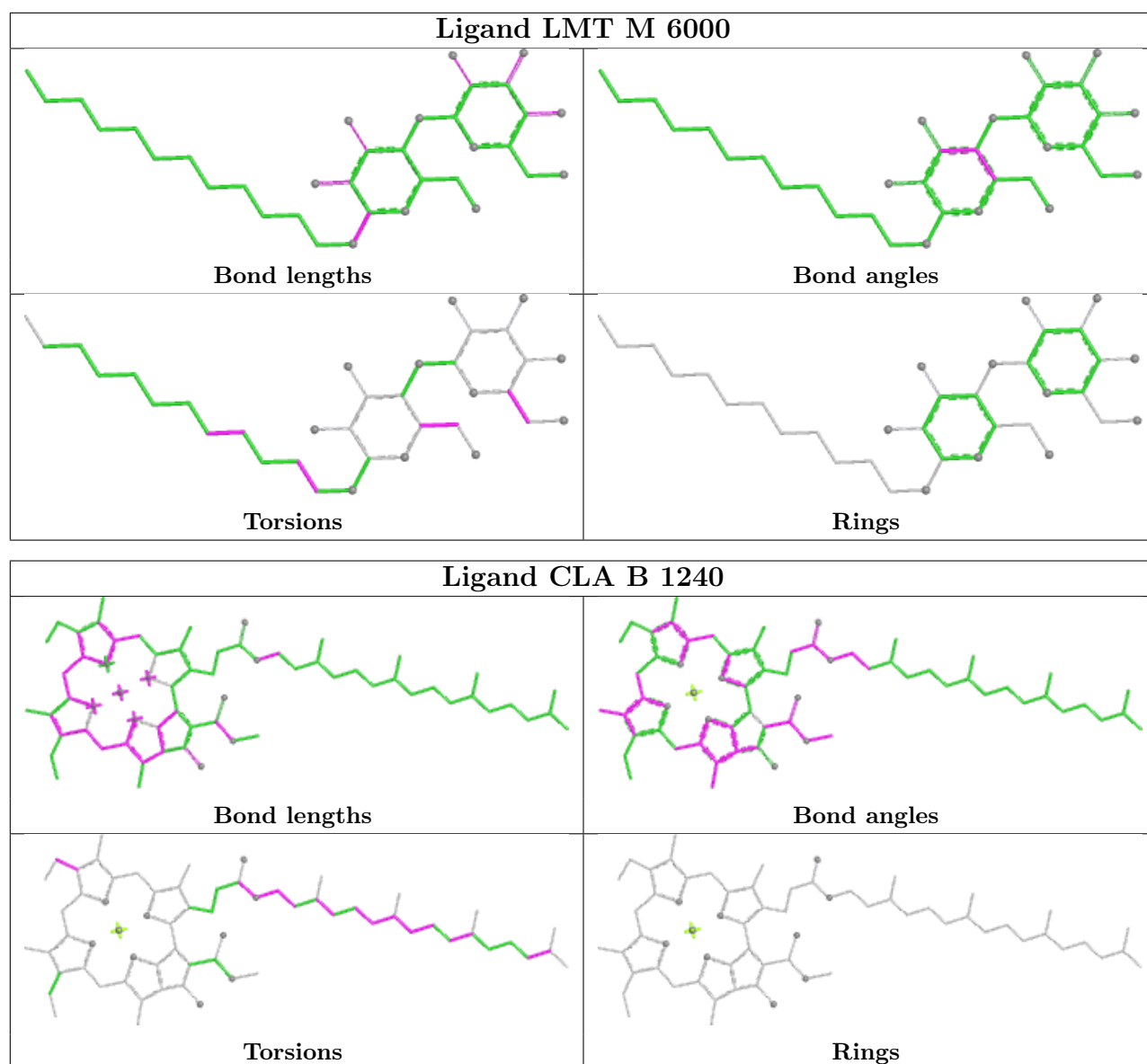


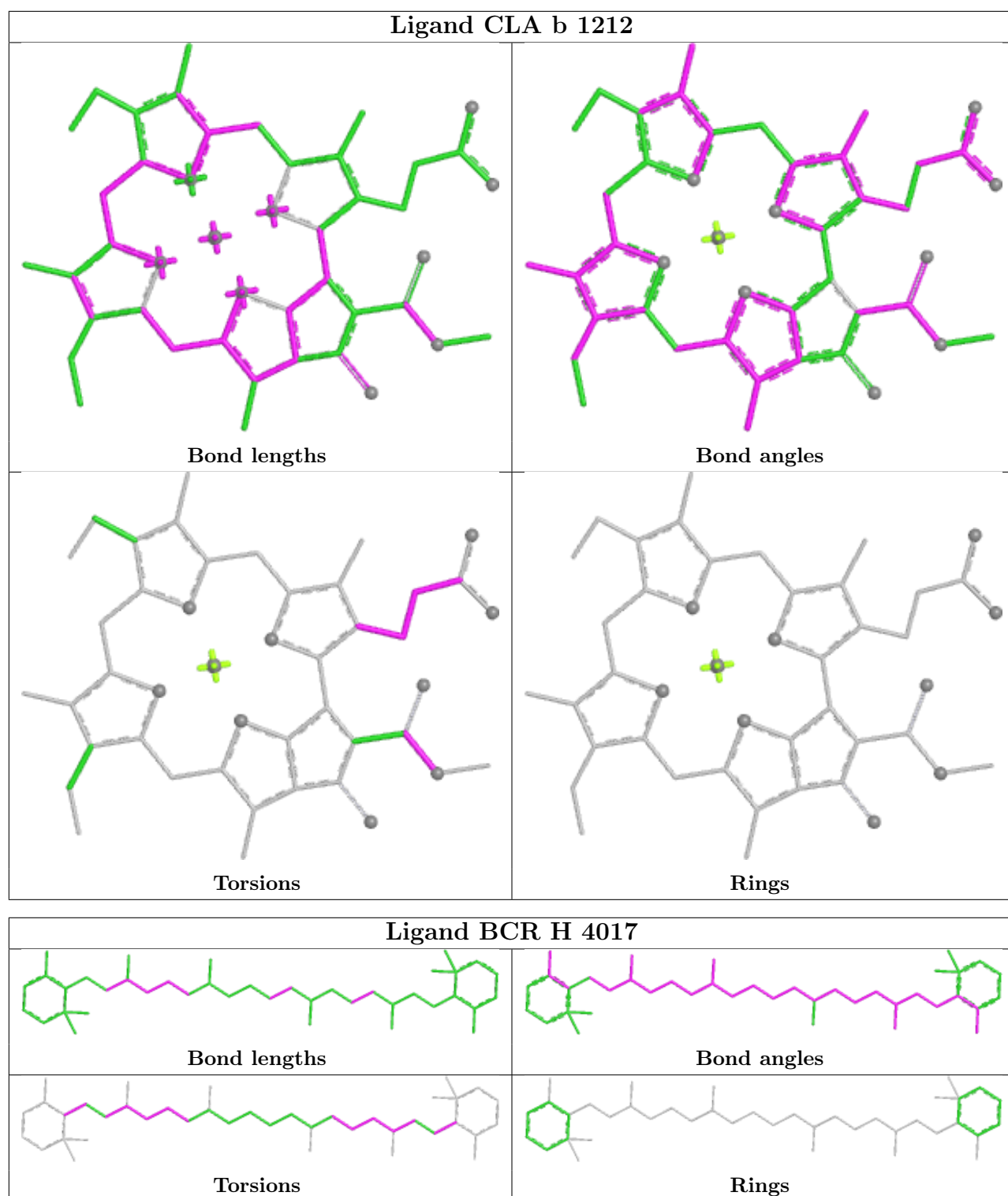


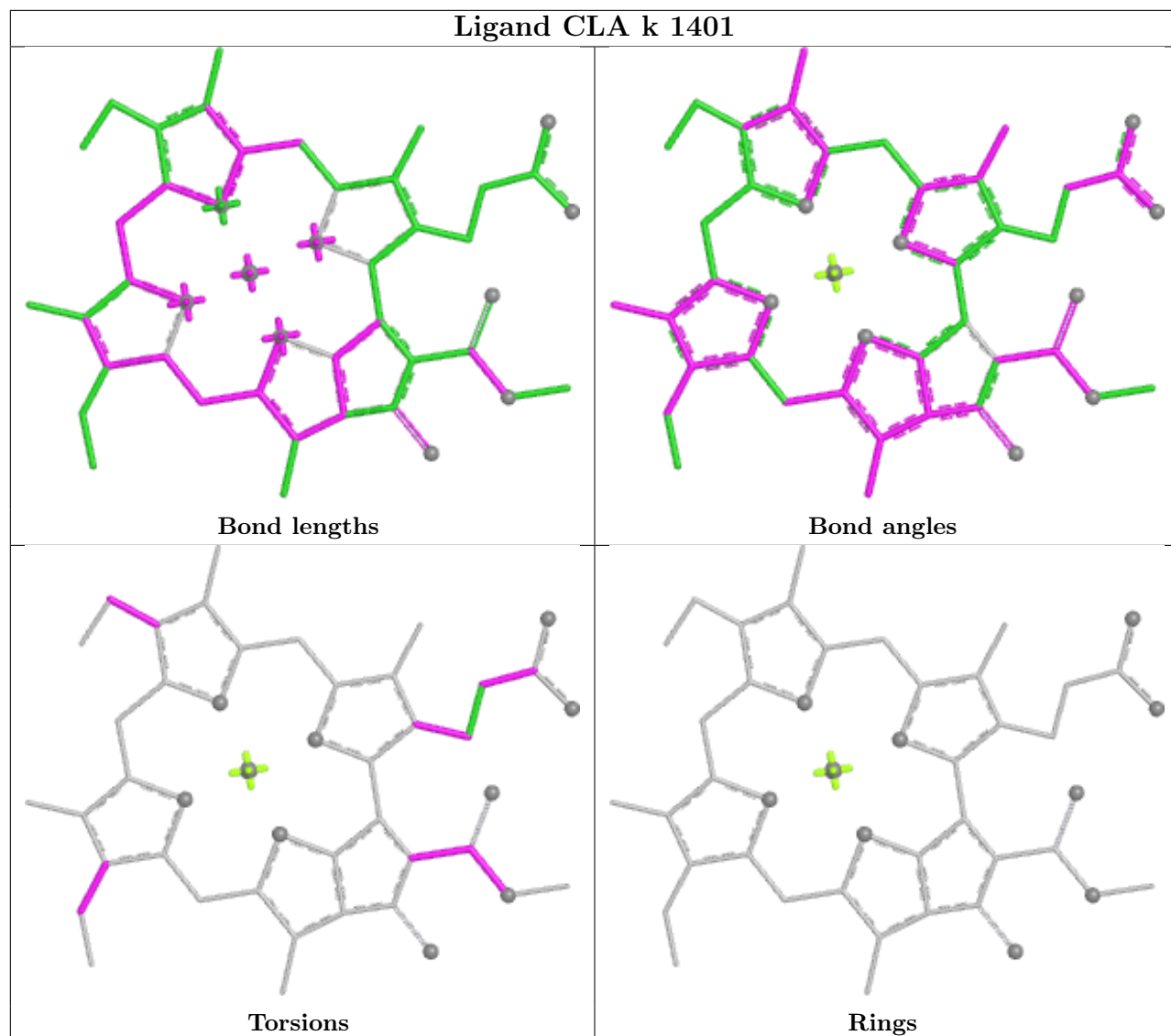
Ligand CL0 A 1011	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 1013	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 4010	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 1222**Ligand CLA A 1119**

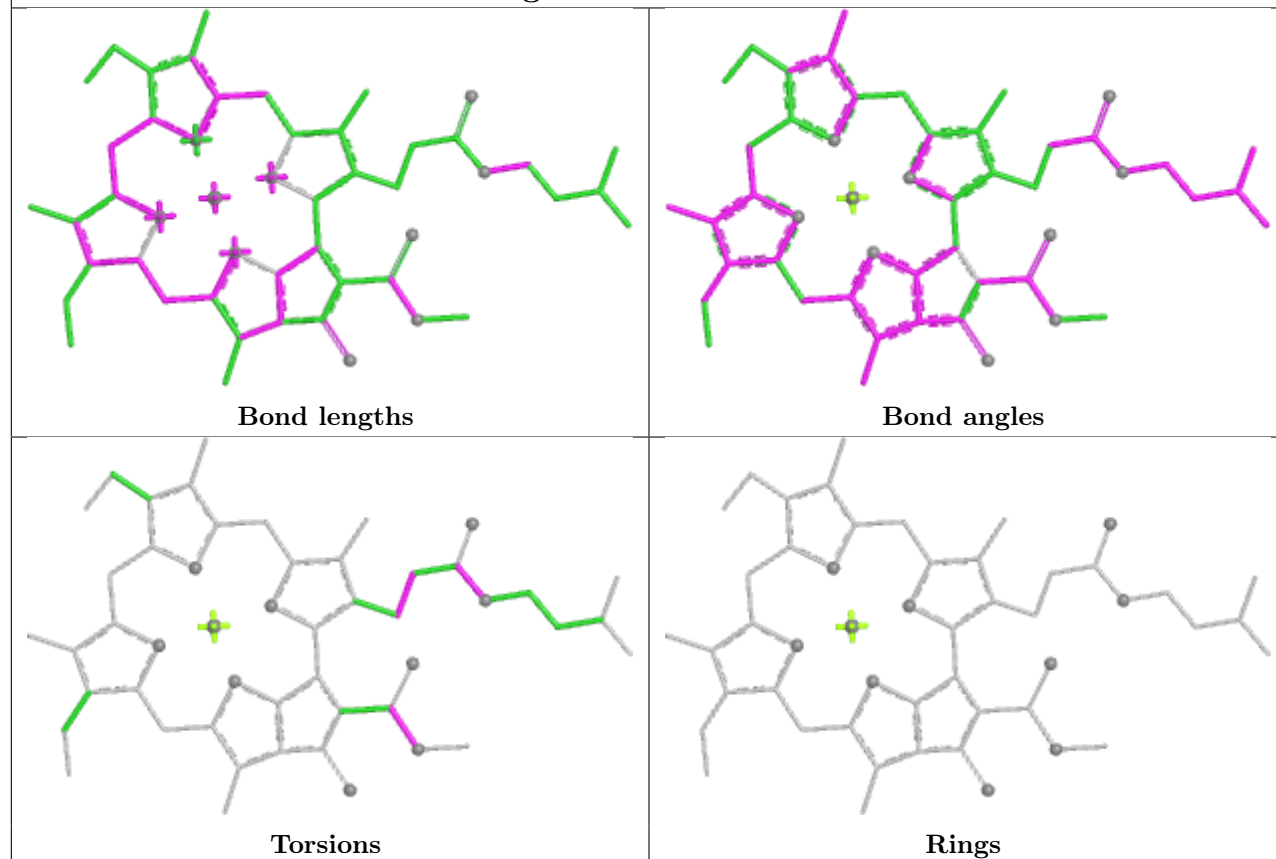




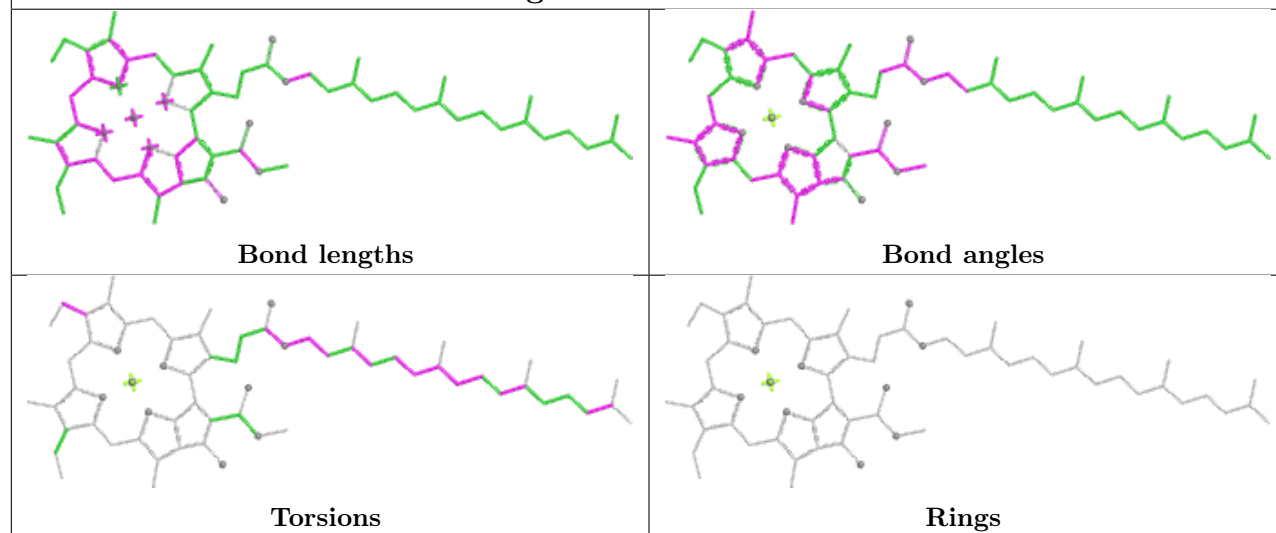


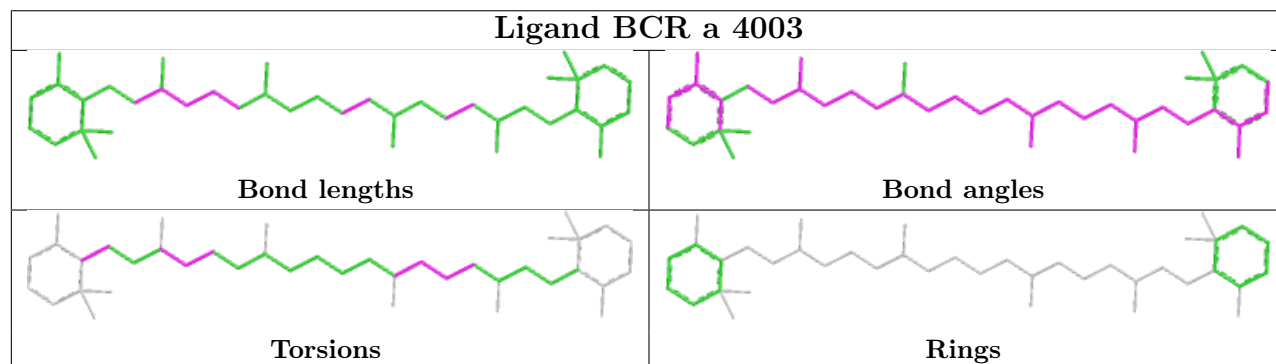
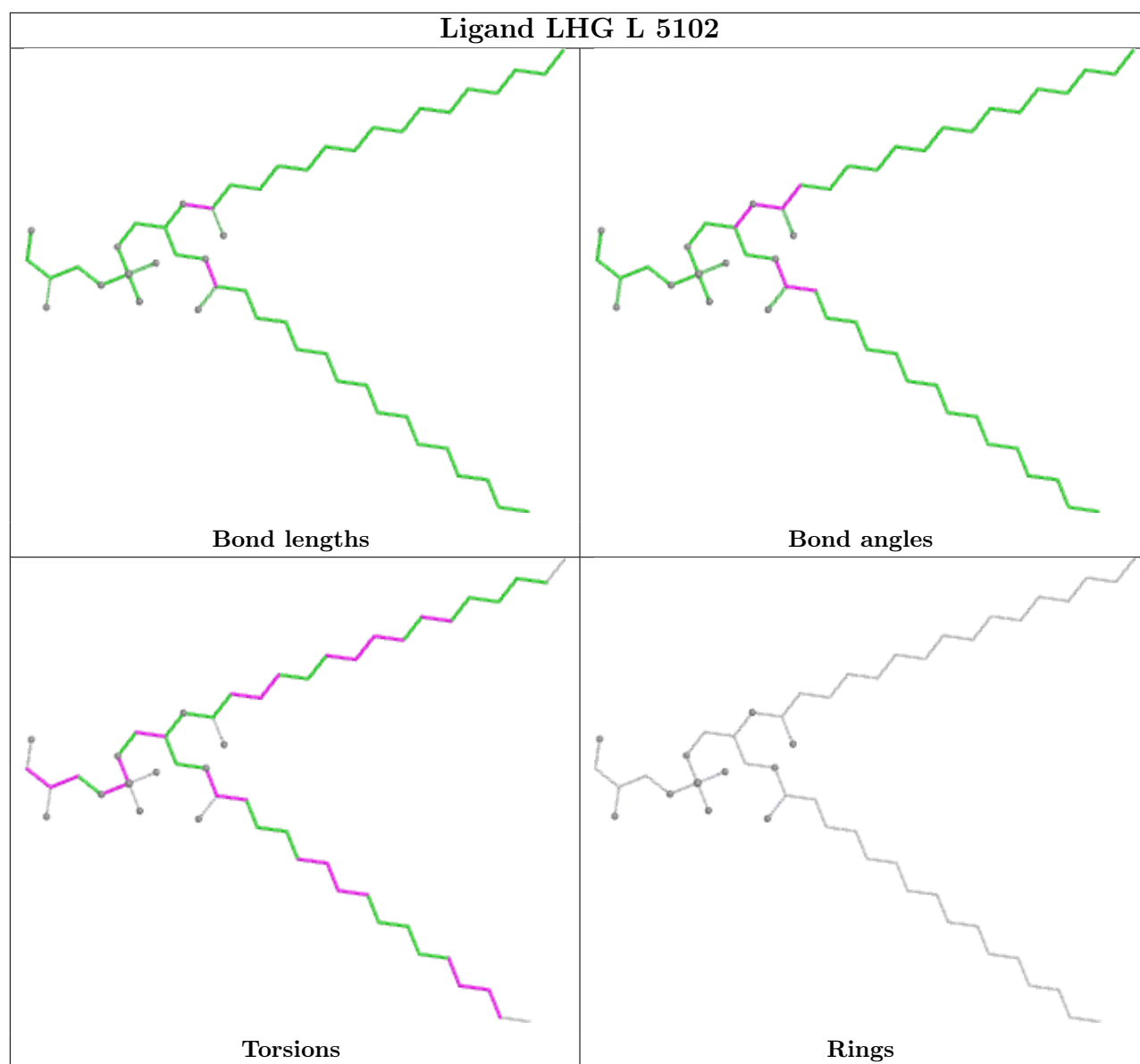


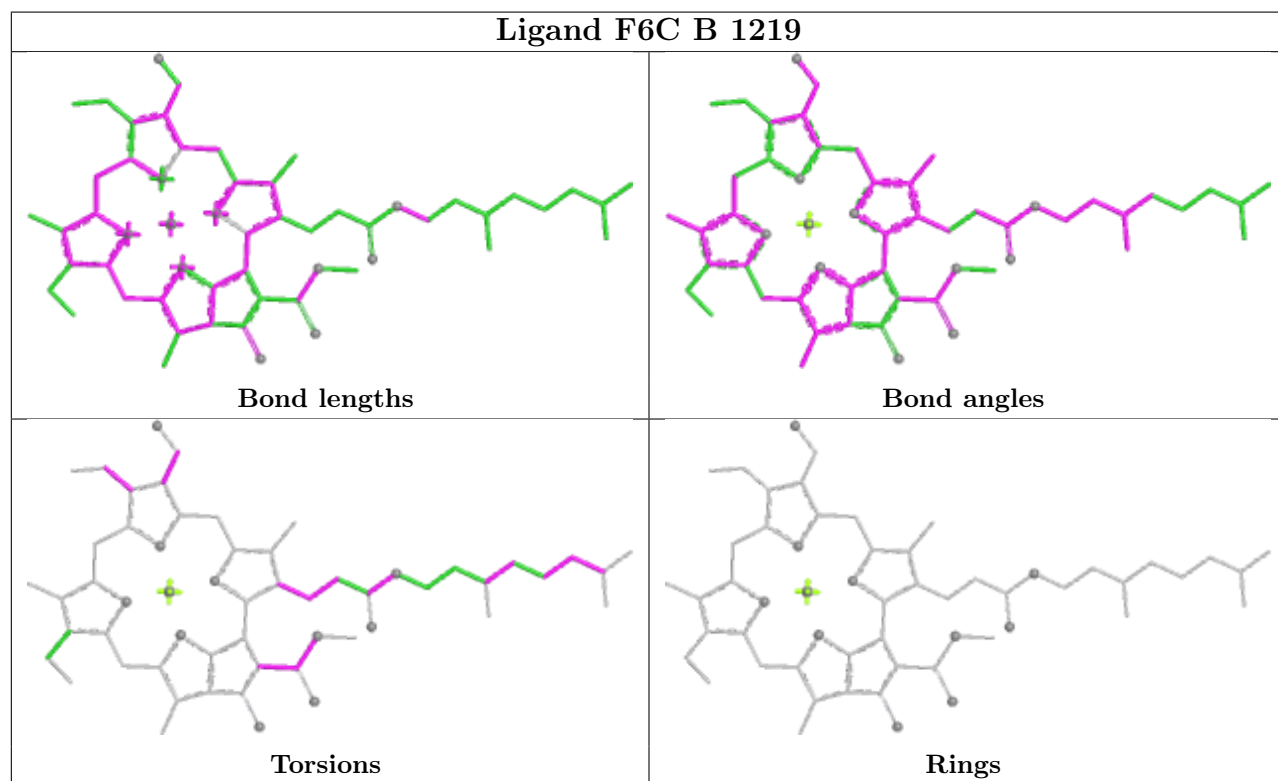
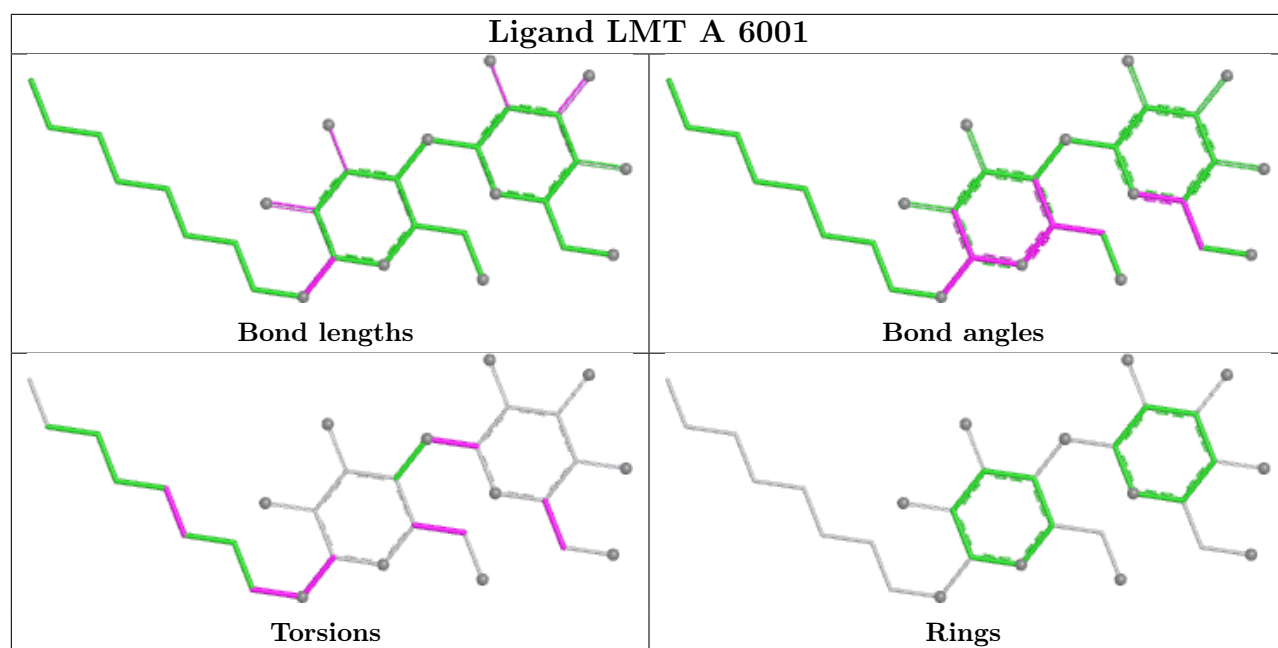
Ligand CLA A 1135

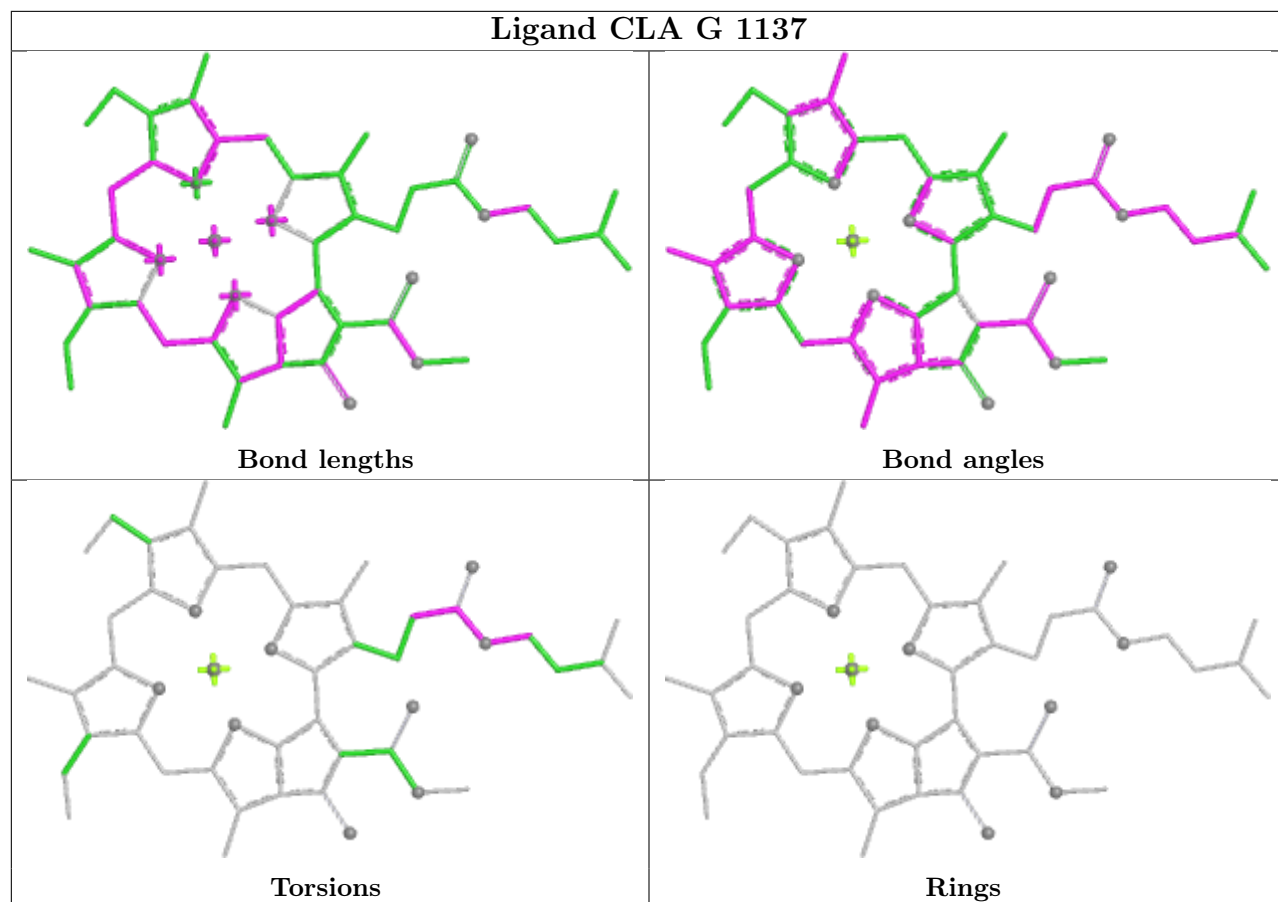


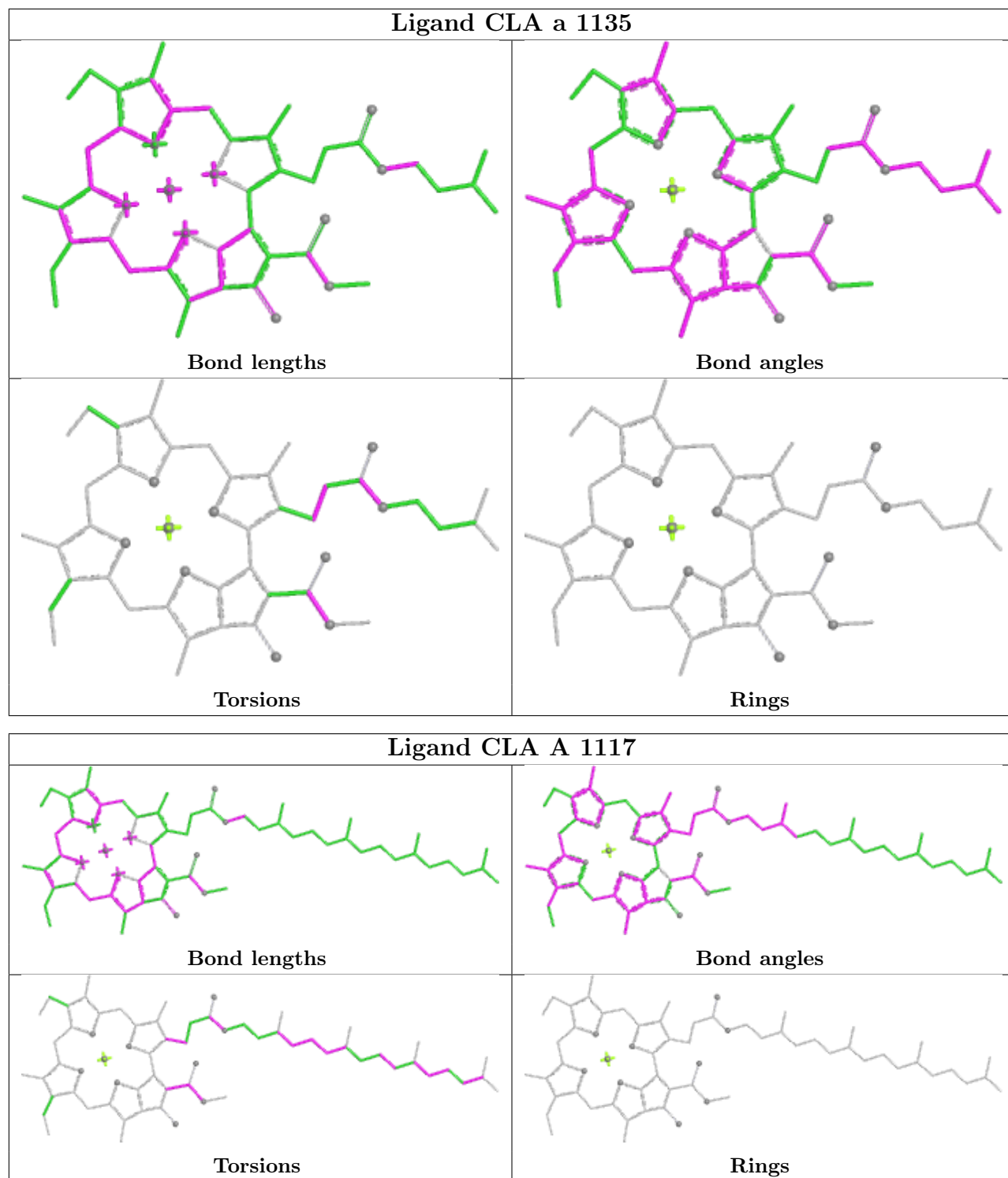
Ligand CLA b 1240



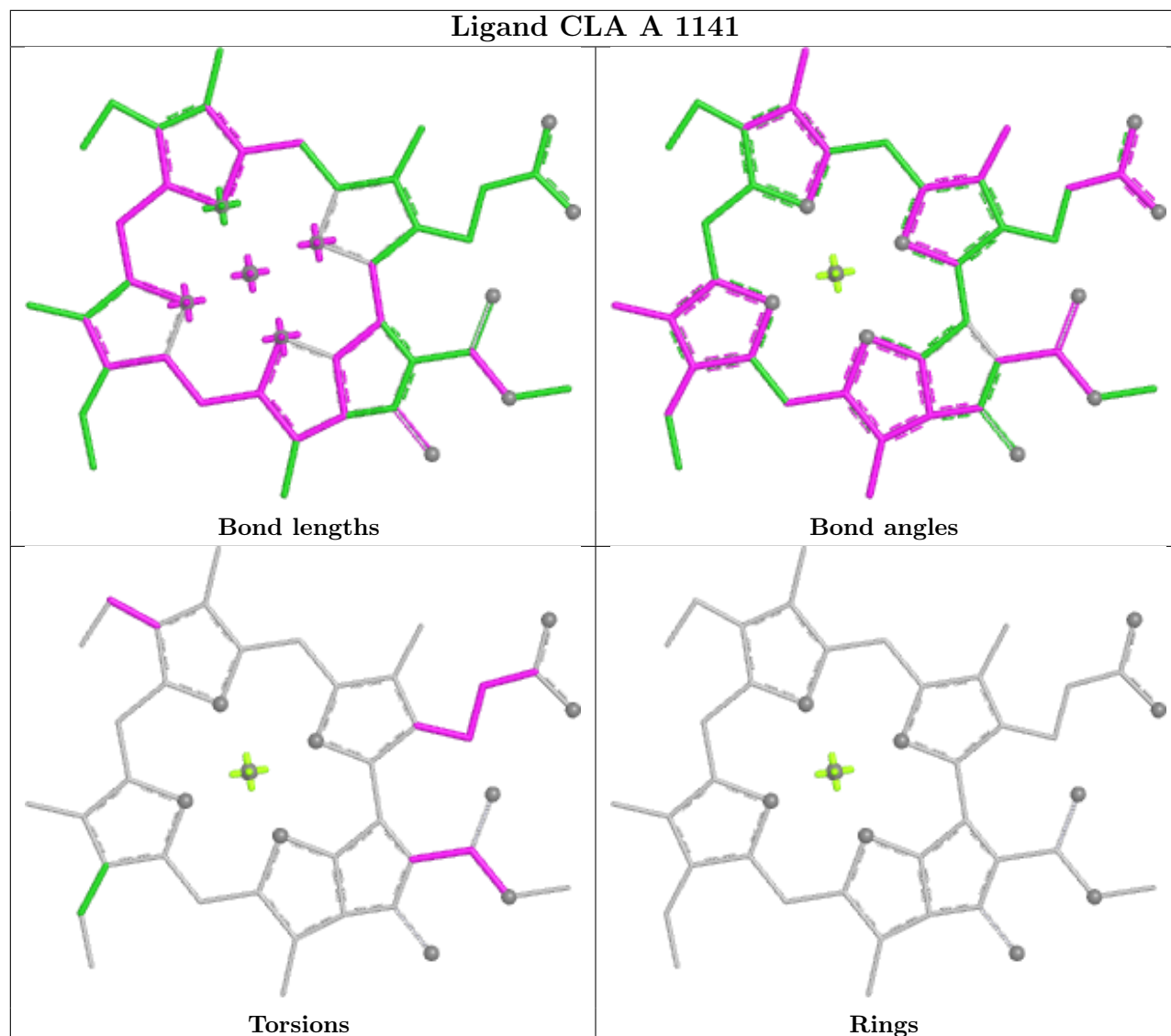


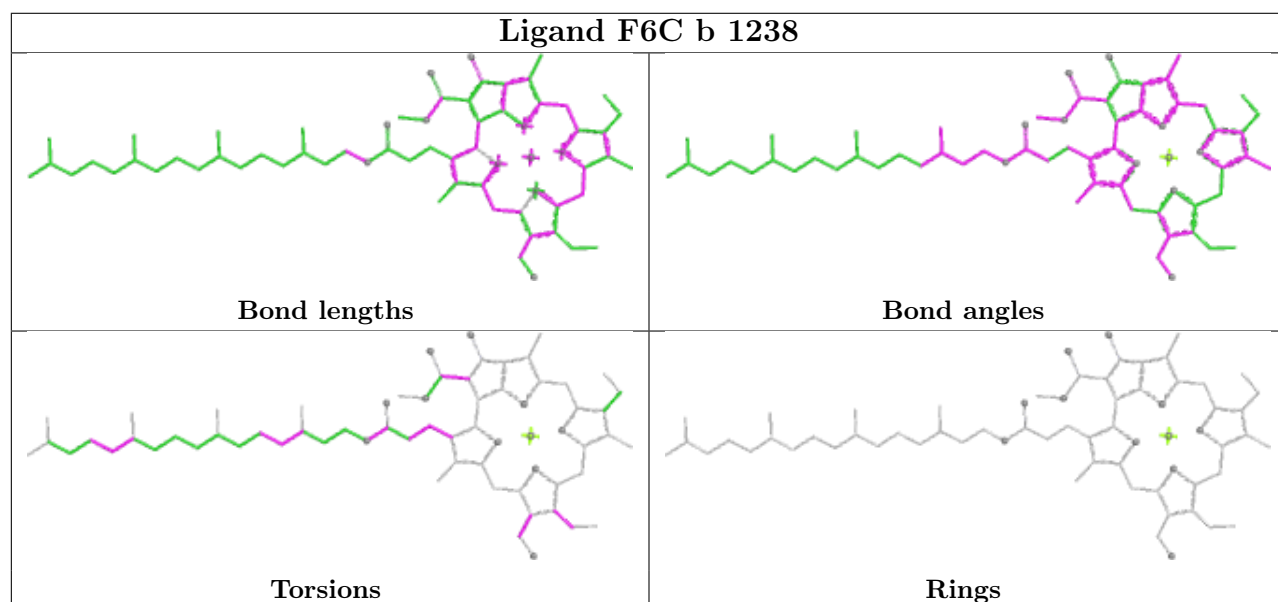
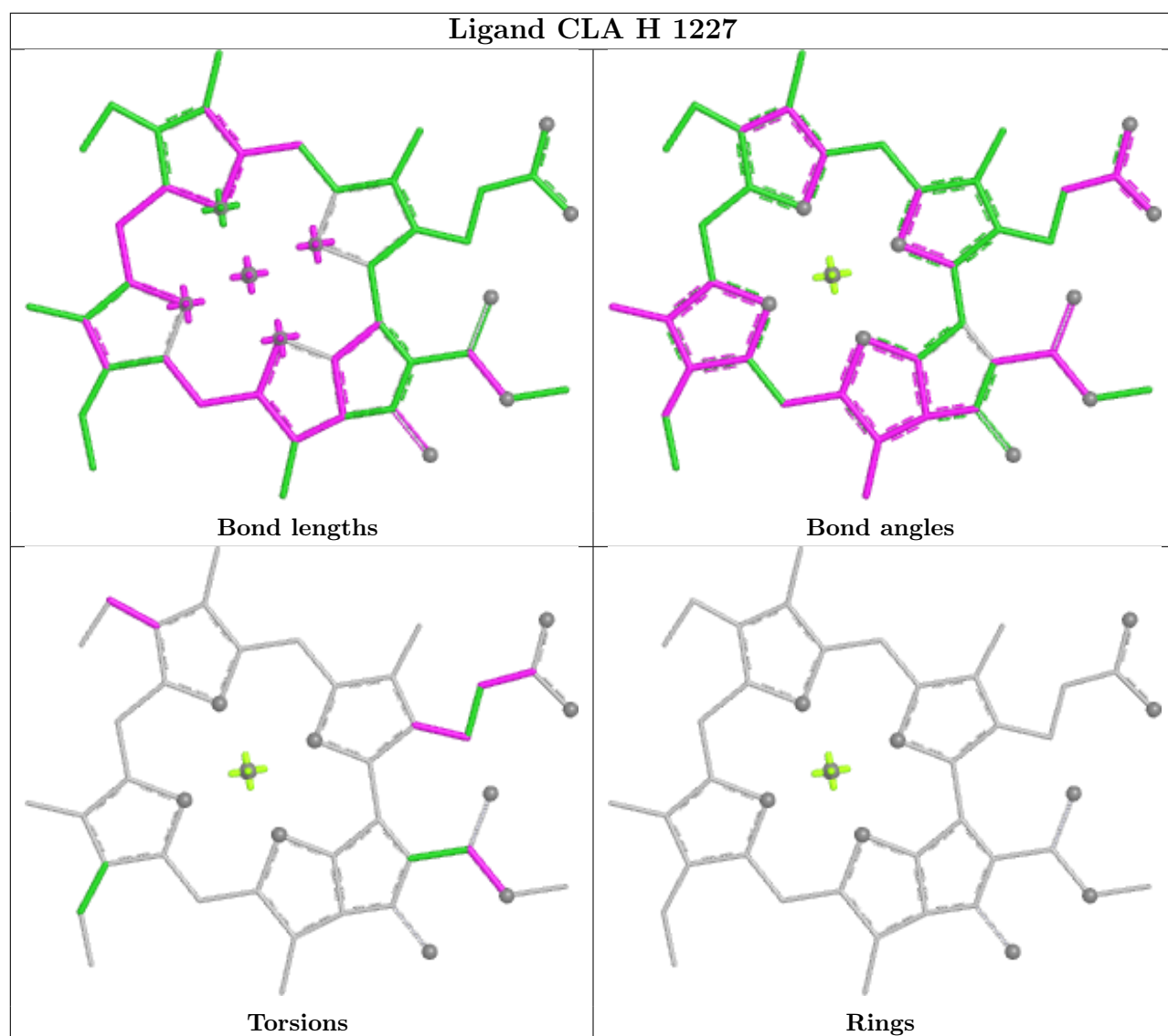


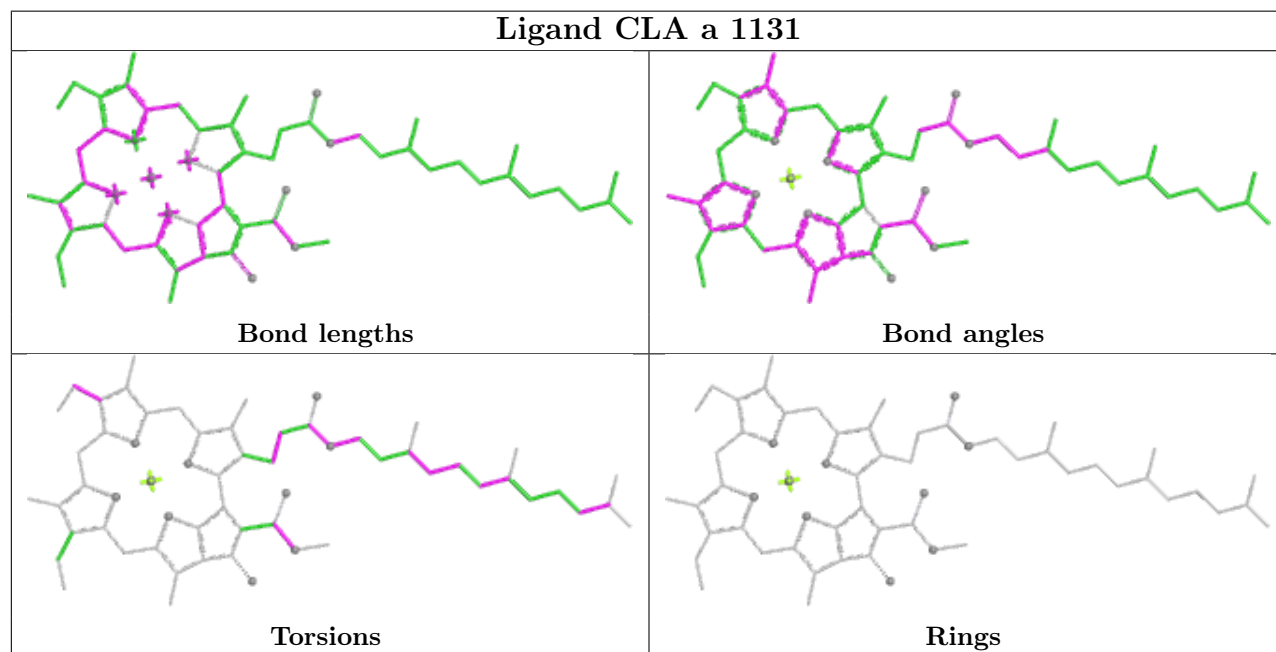
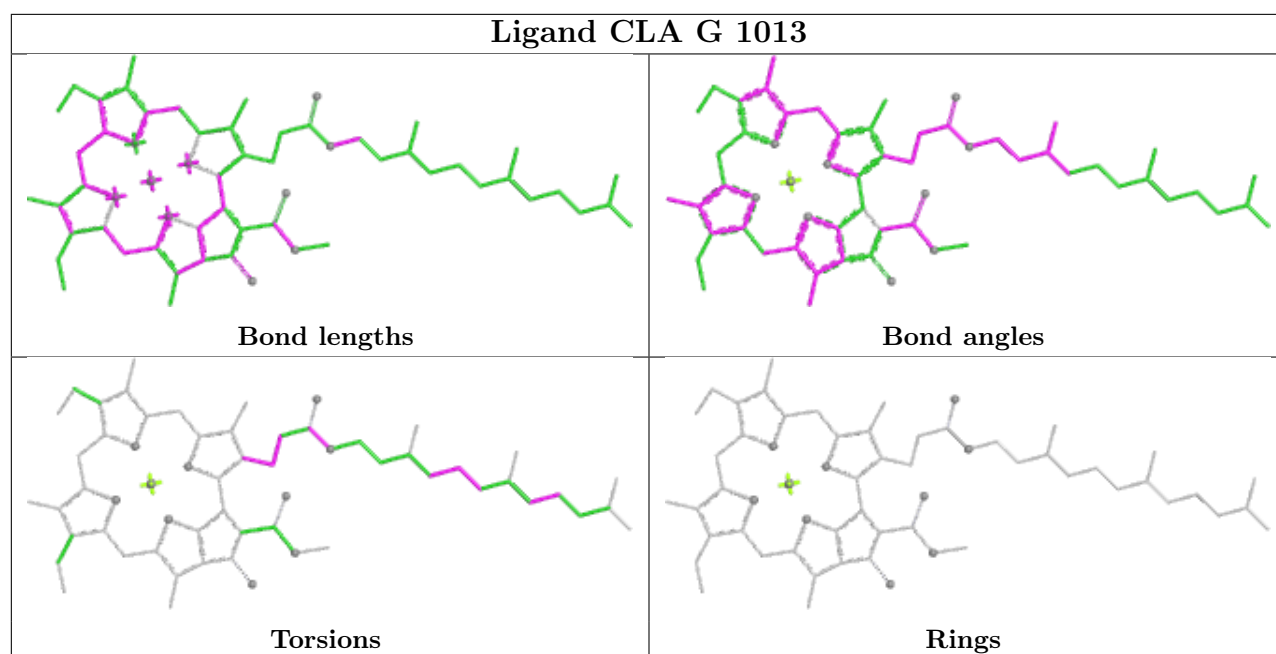


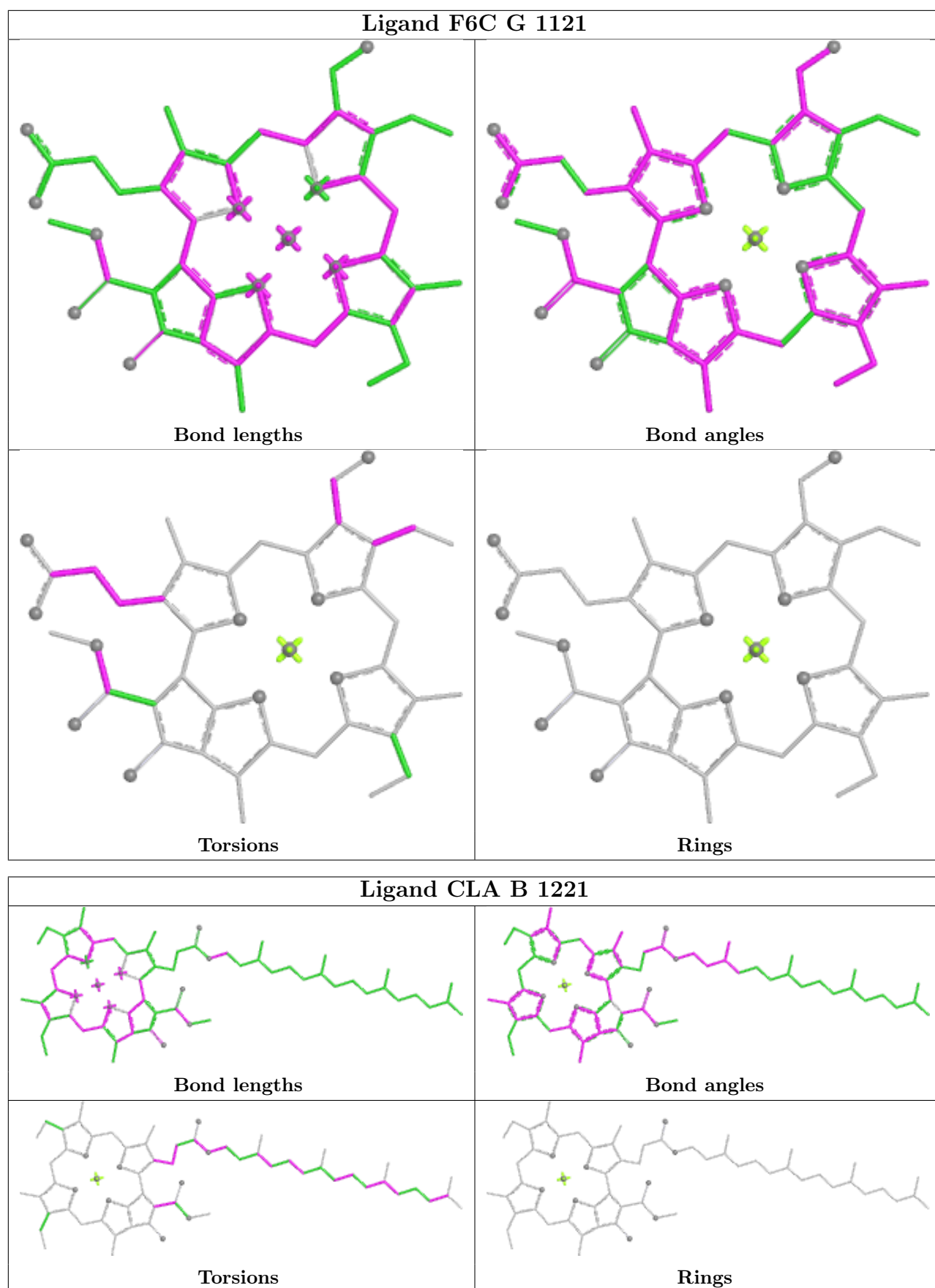


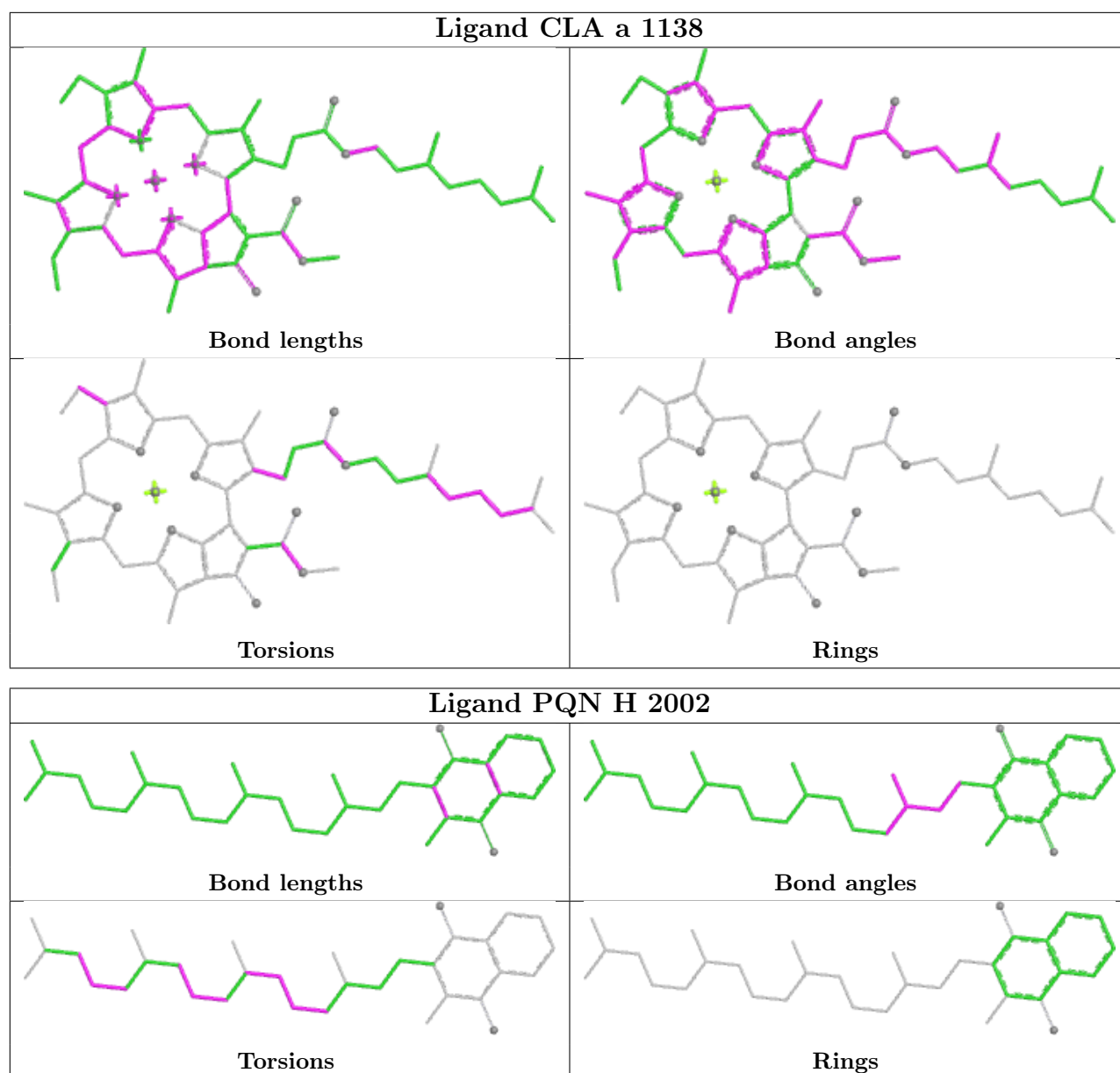
Ligand CLA A 1141

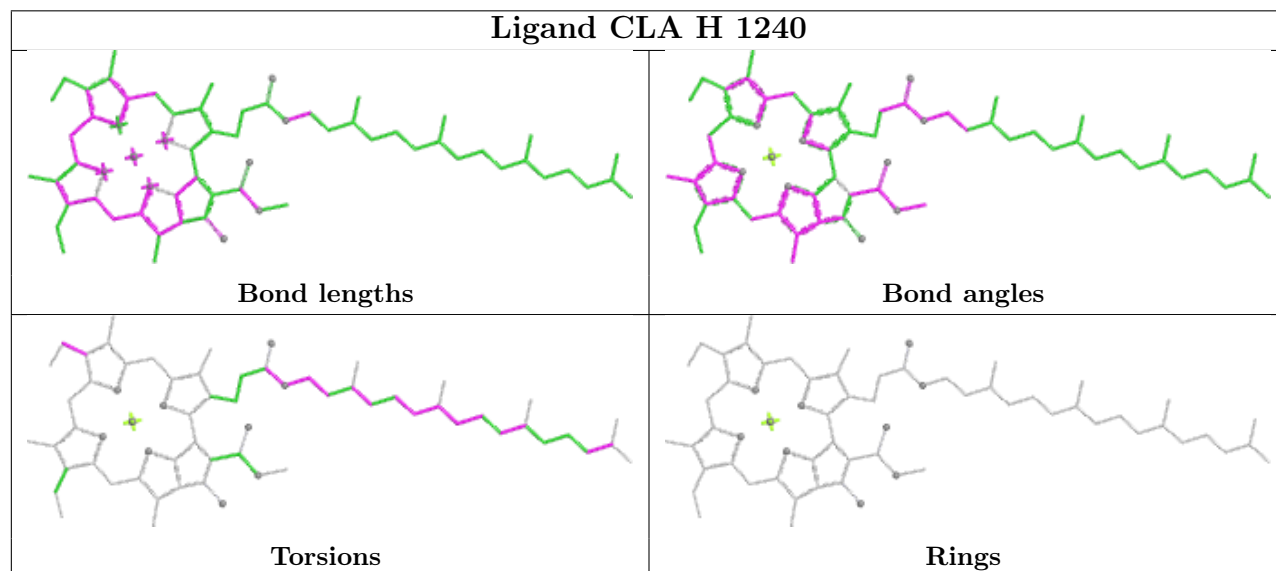
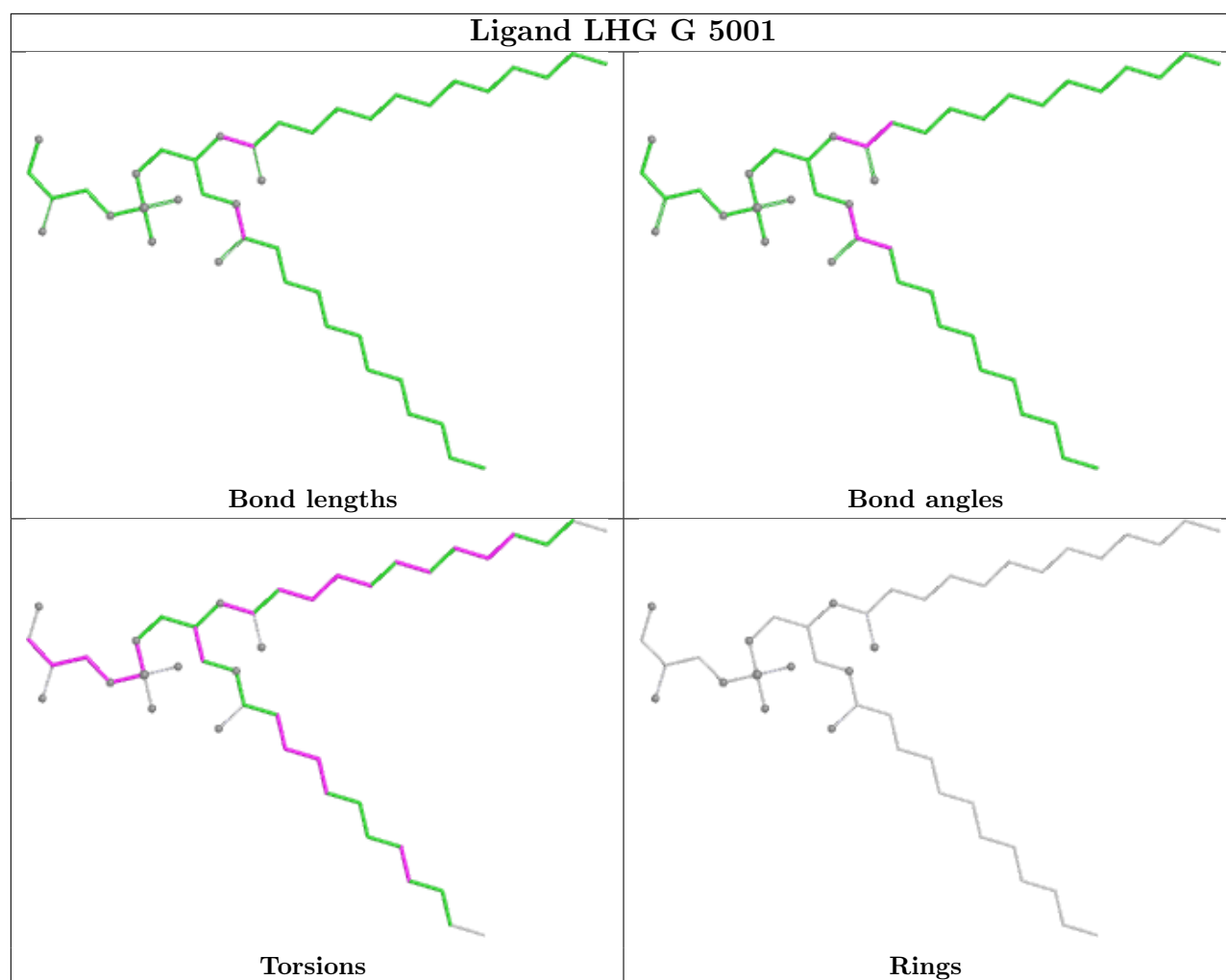


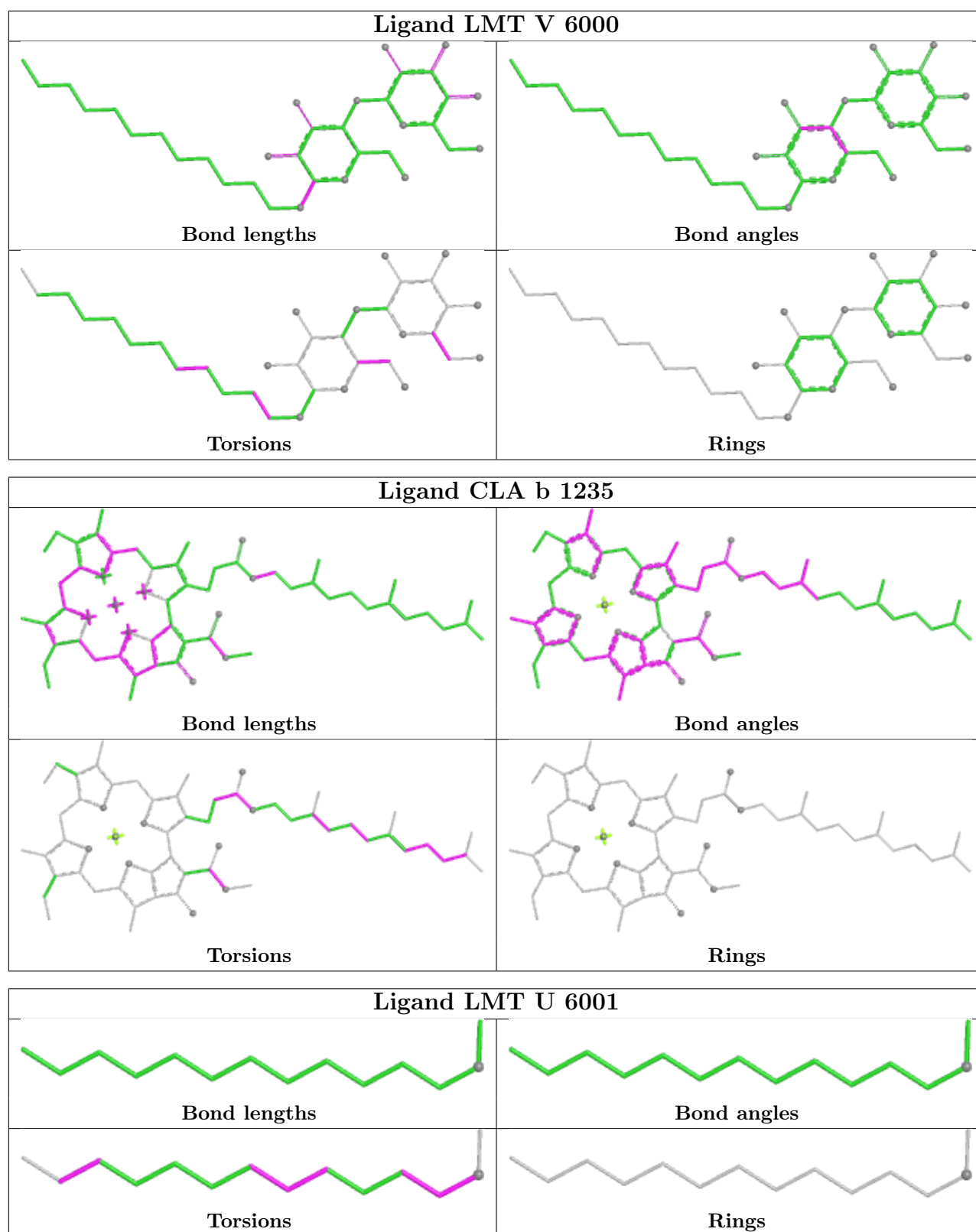


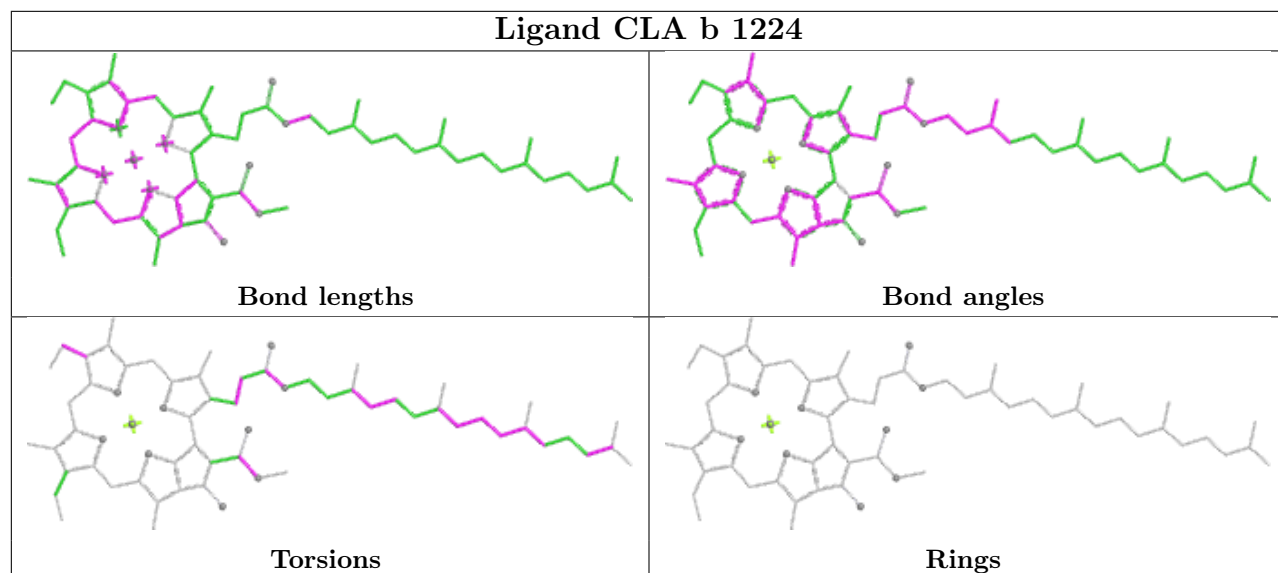
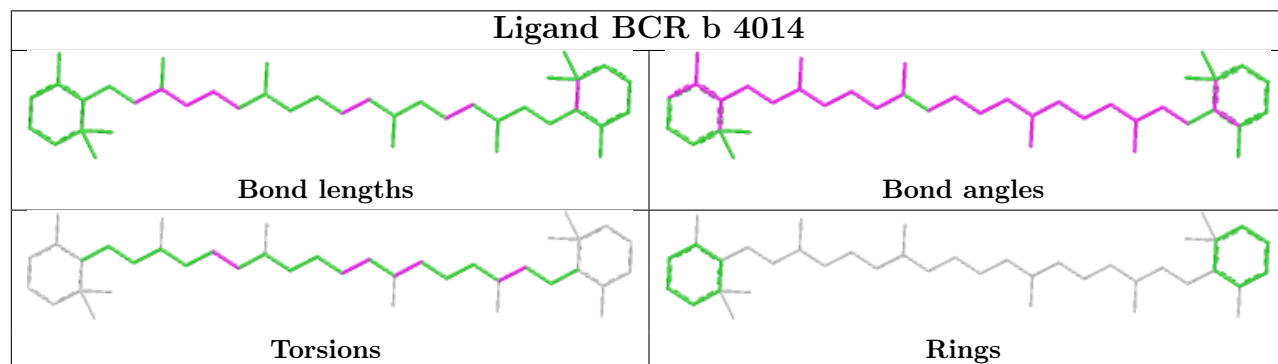
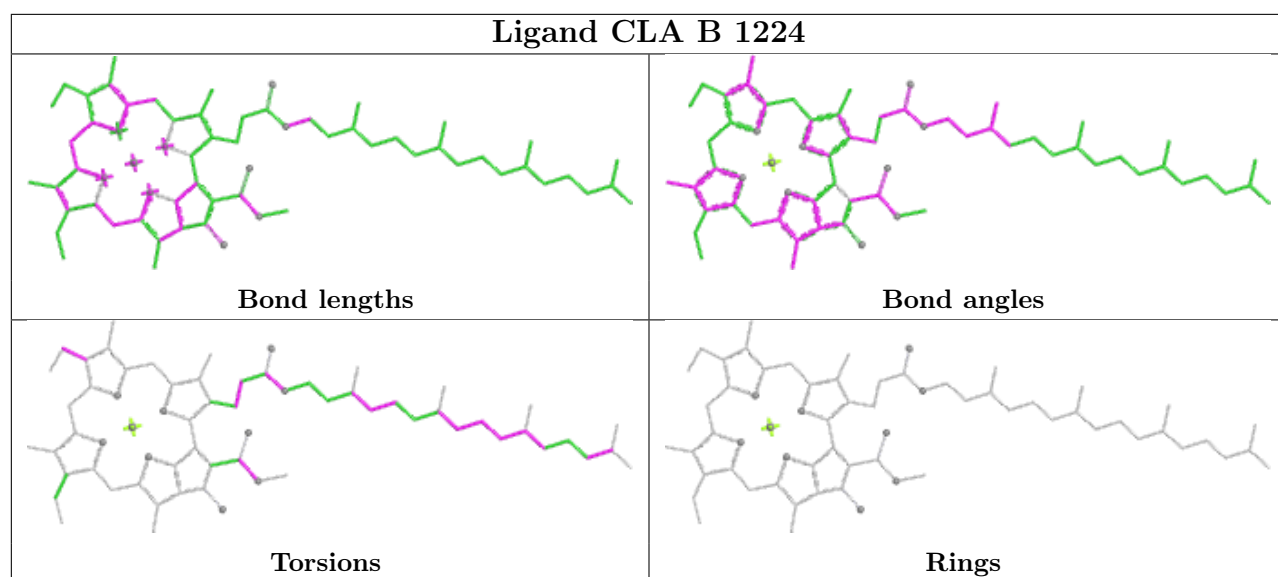


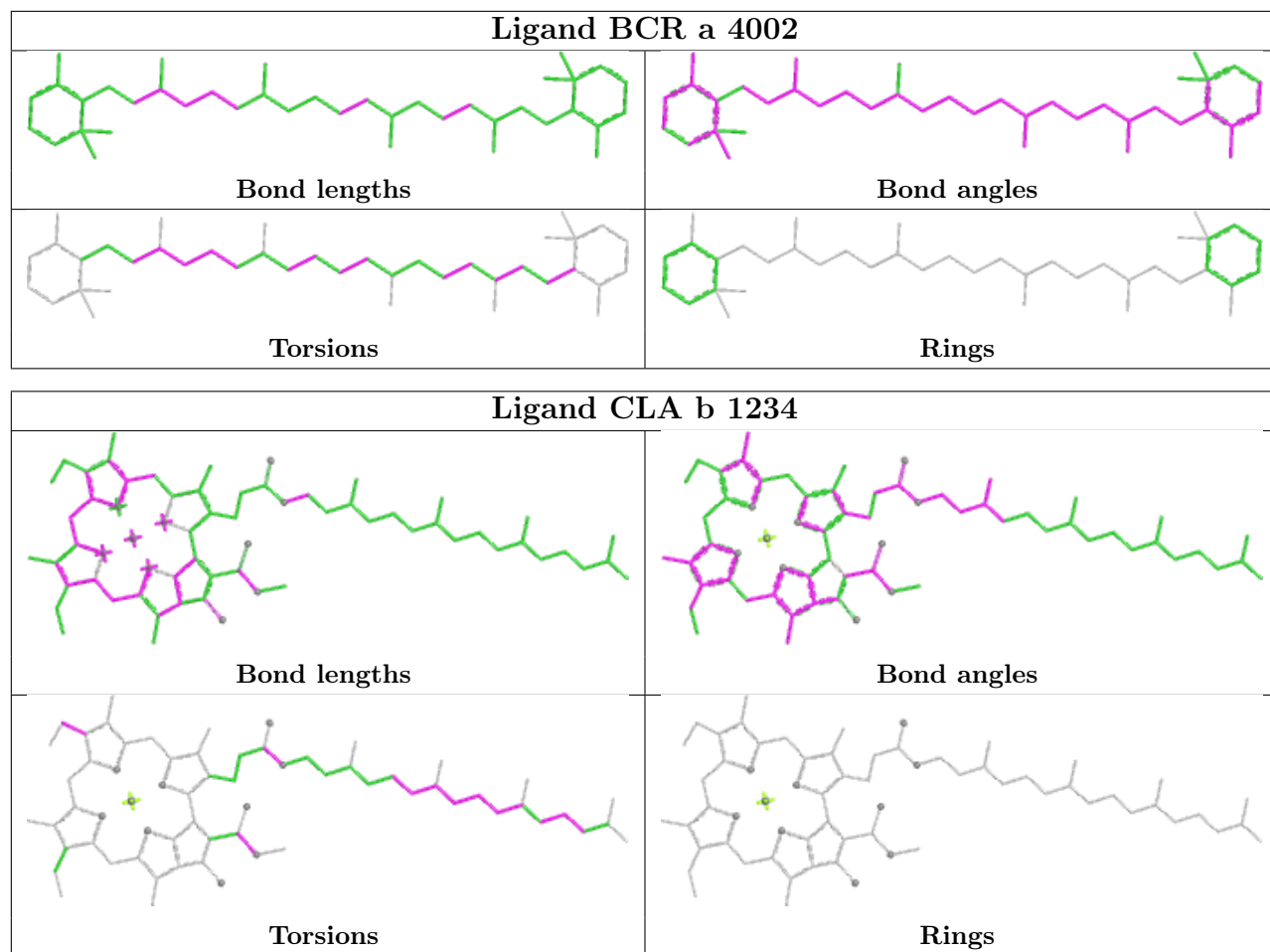




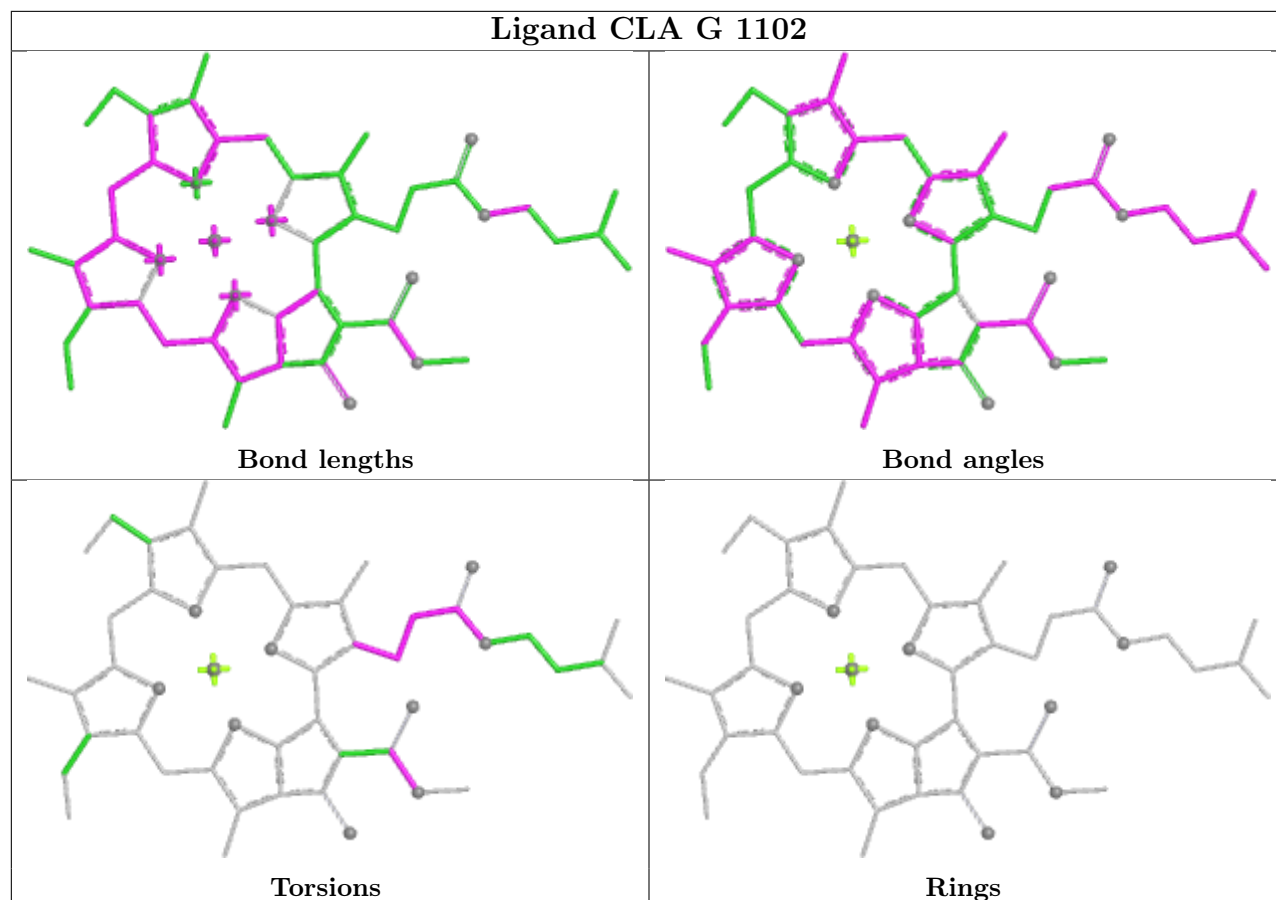




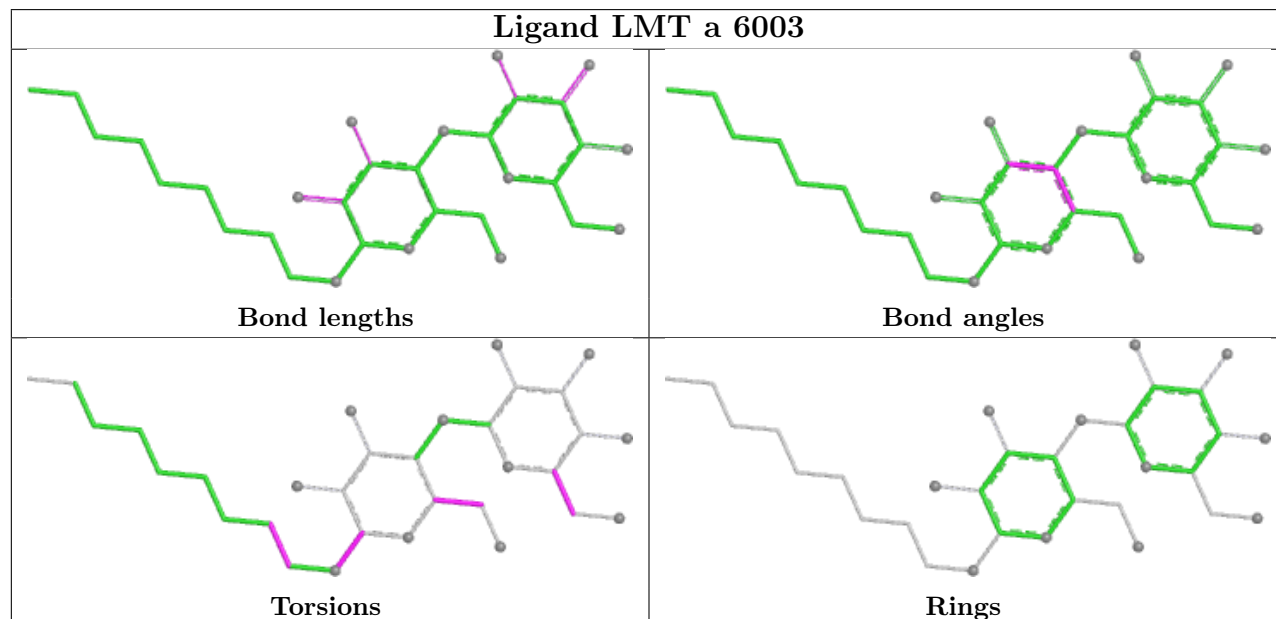


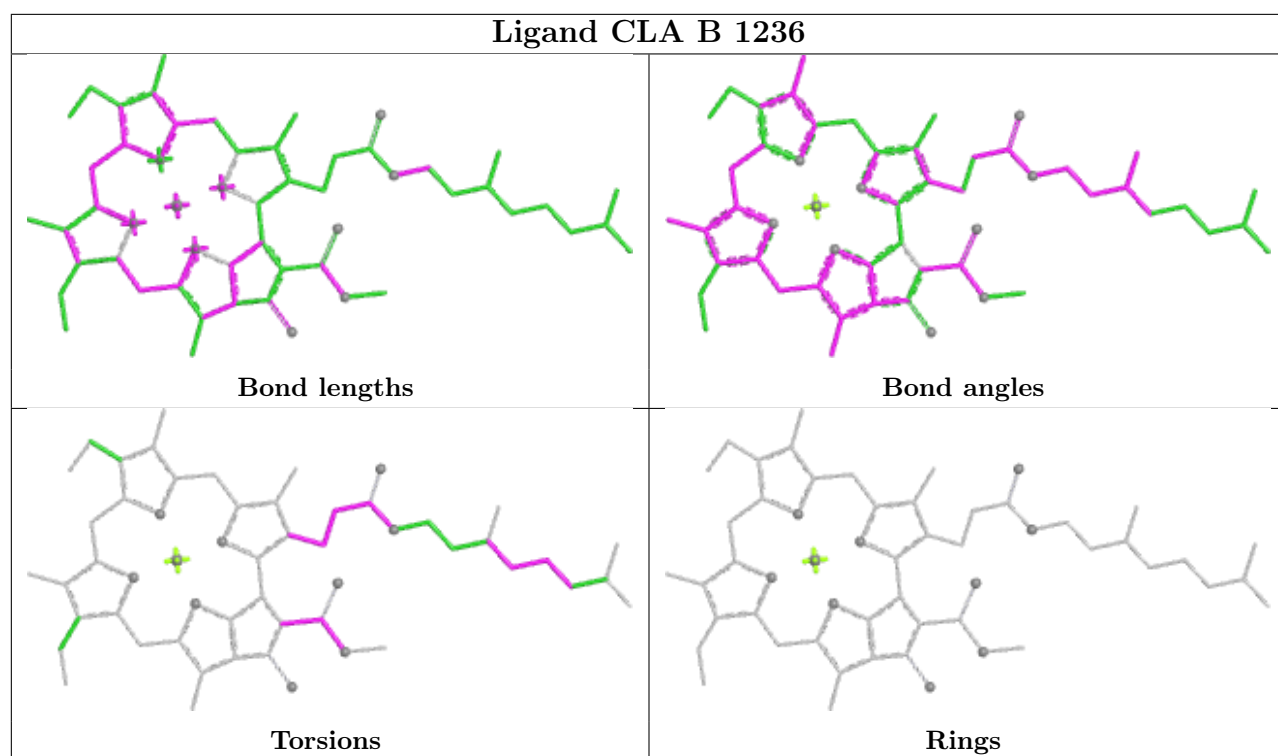


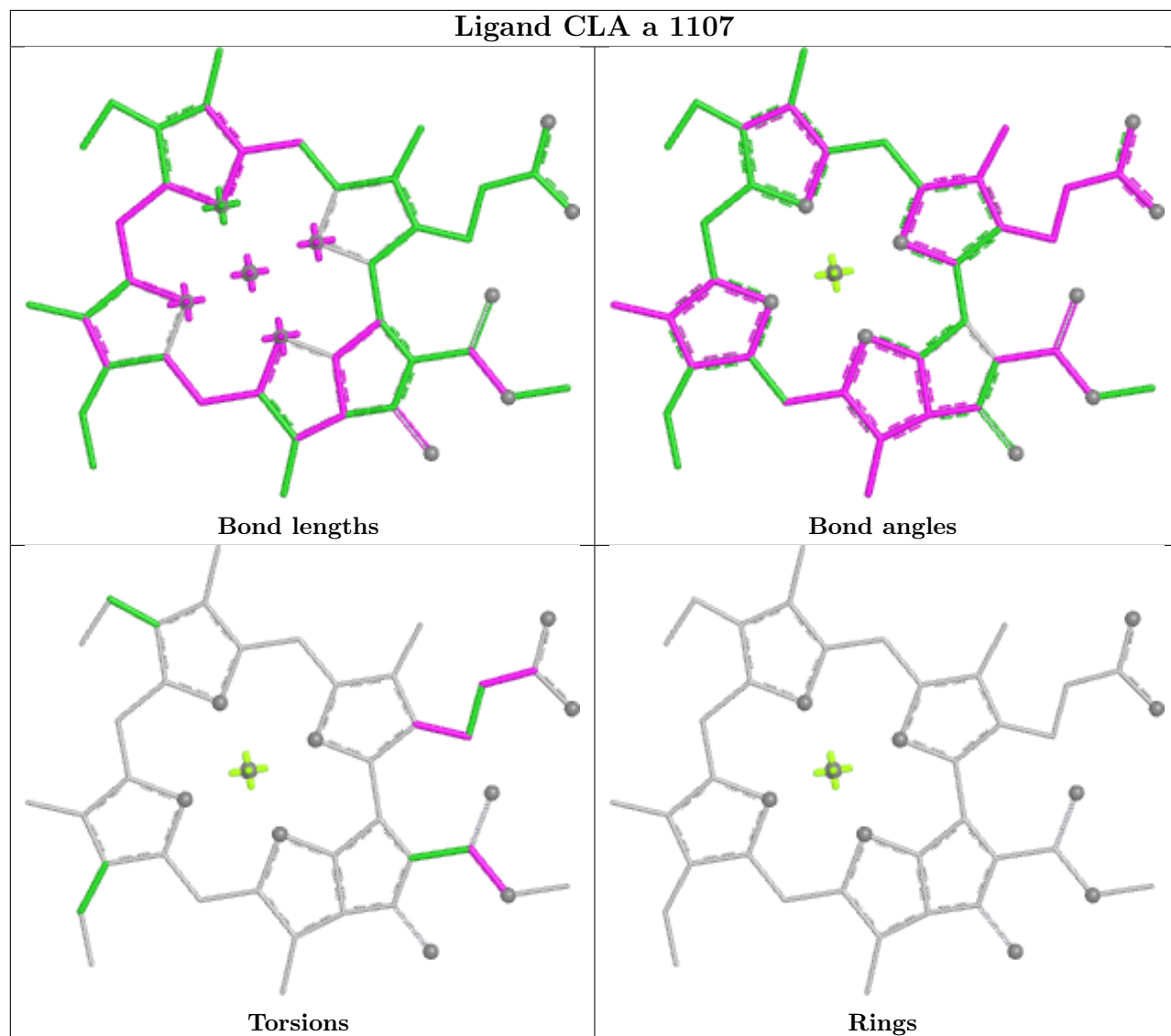
Ligand CLA G 1102

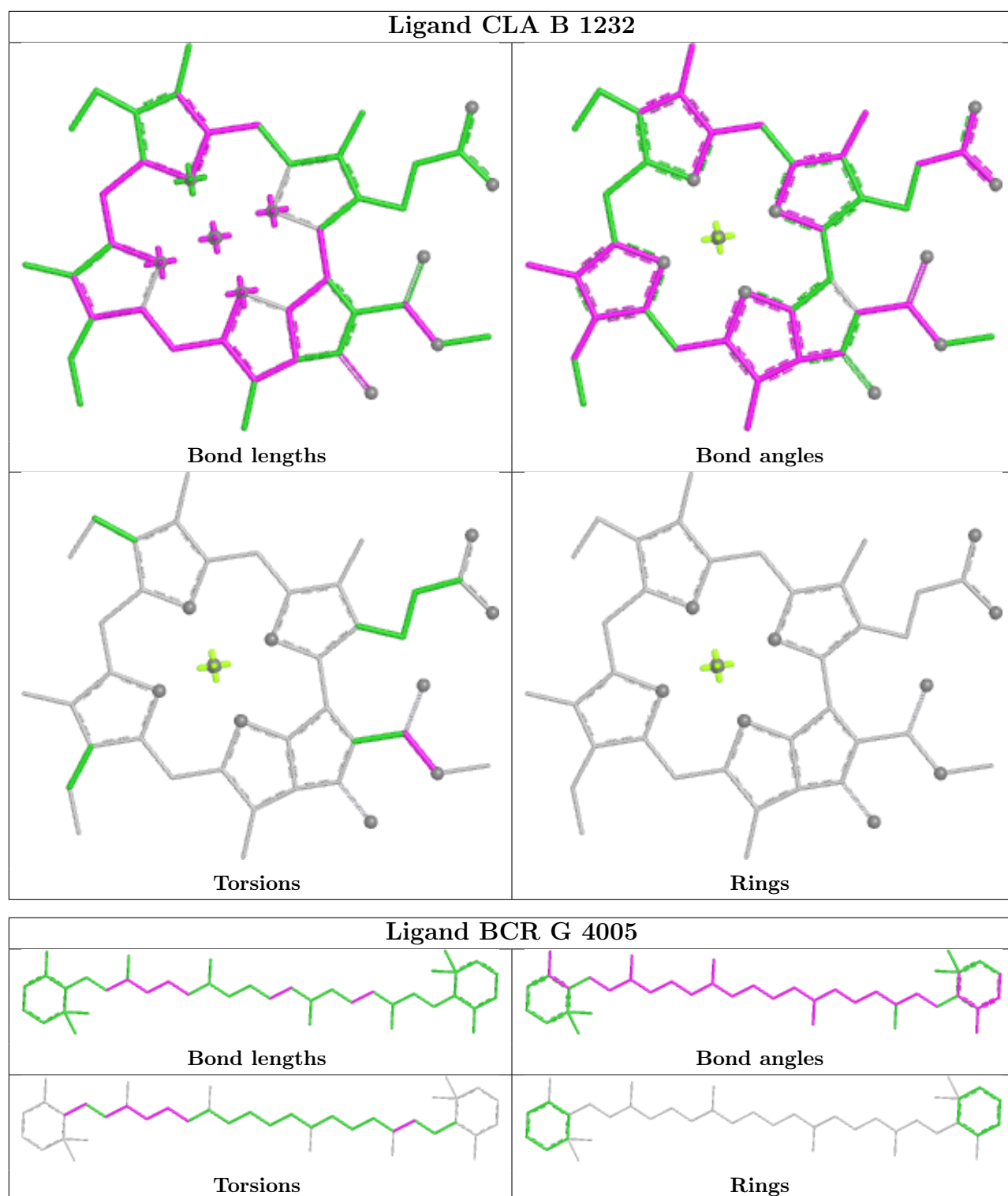


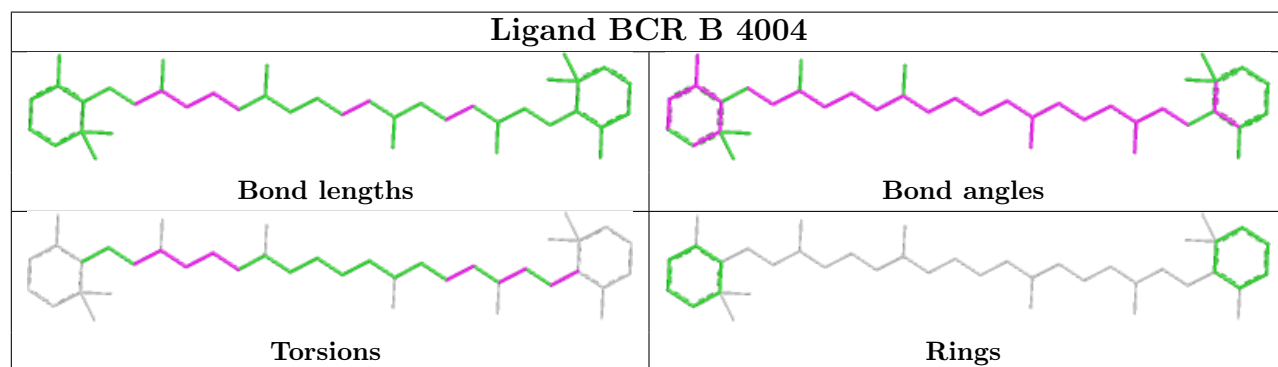
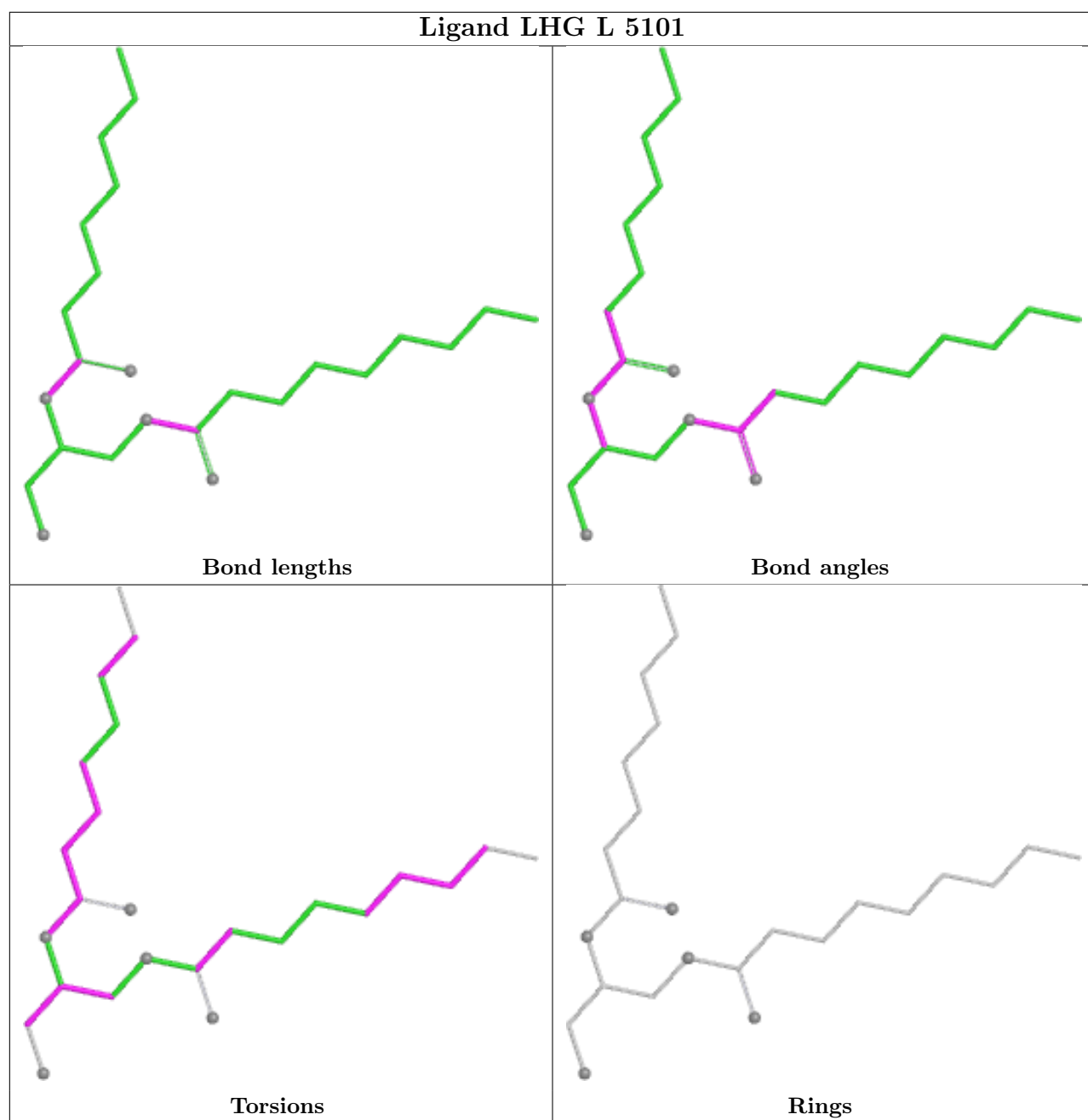
Ligand LMT a 6003

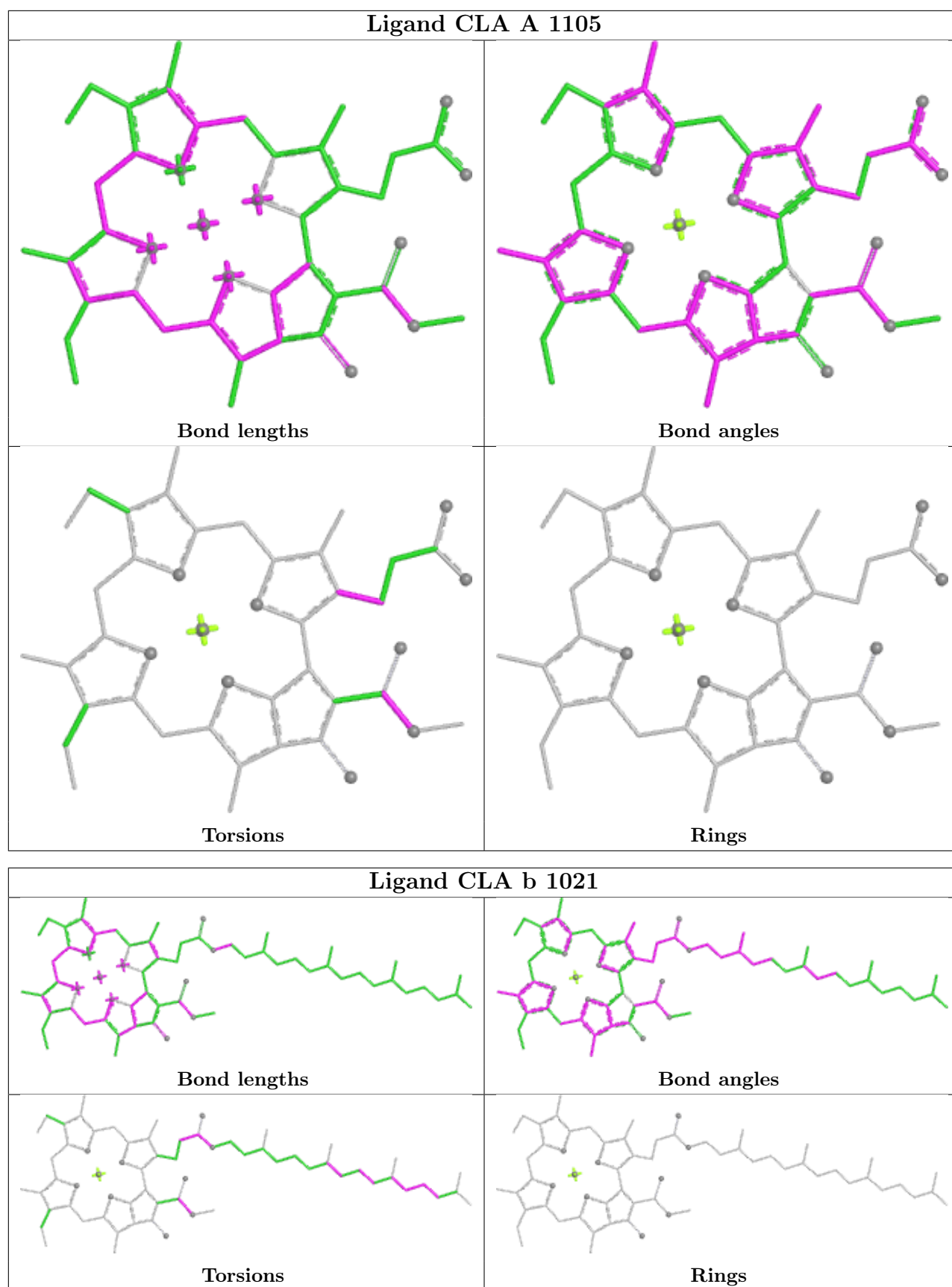


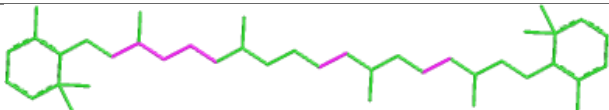
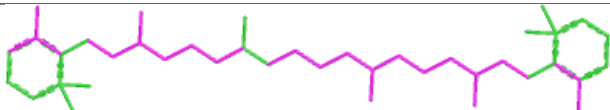
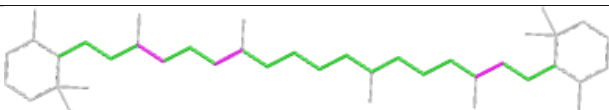
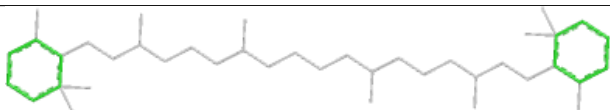


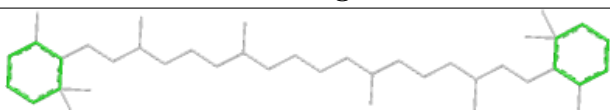




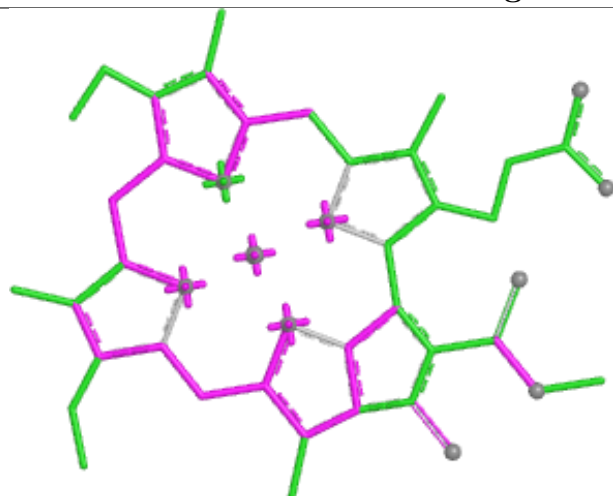




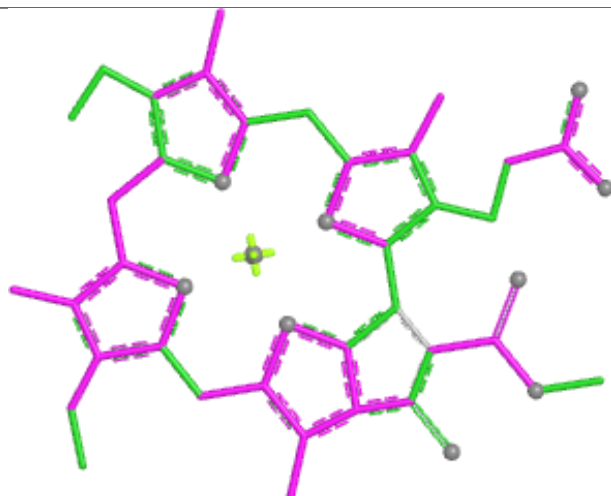
Ligand BCR H 4005	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR L 4022	
	
Bond lengths	Bond angles
	
Torsions	Rings

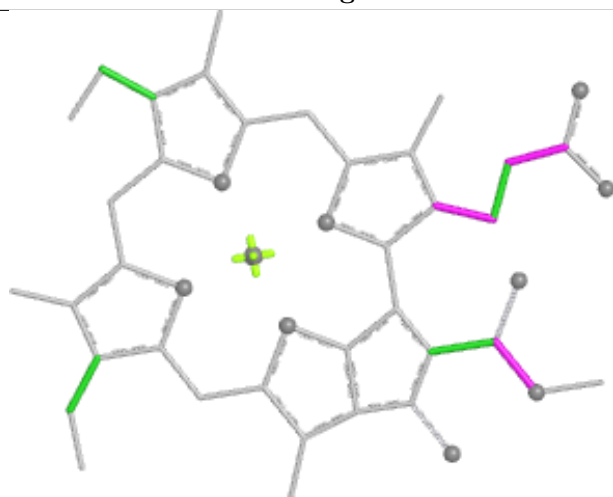
Ligand CLA H 1233



Bond lengths



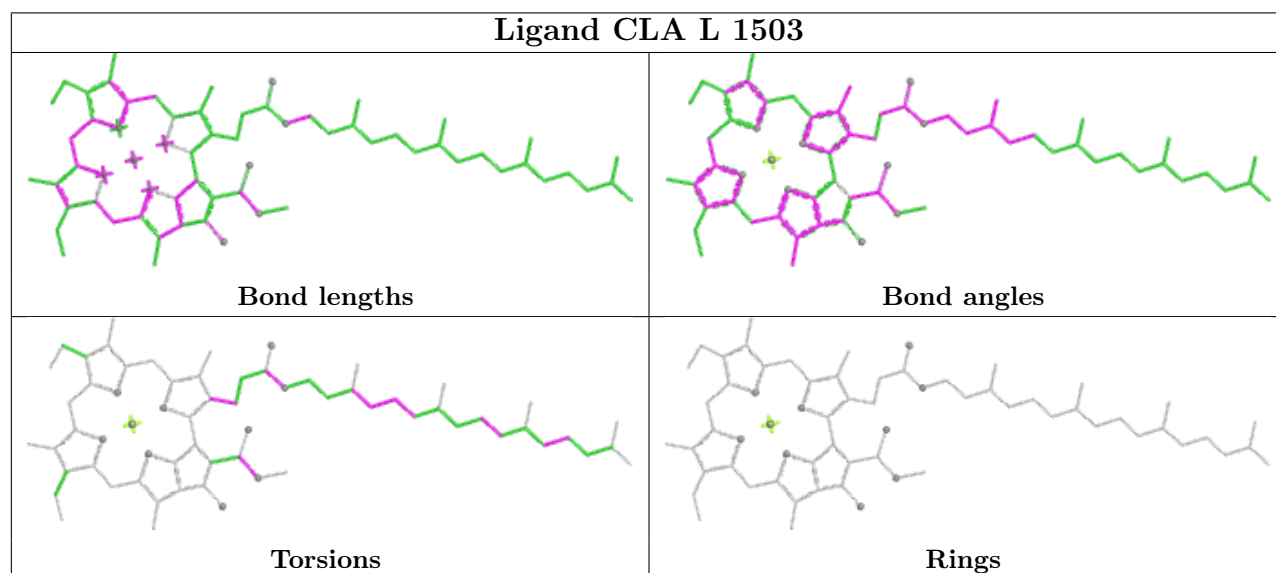
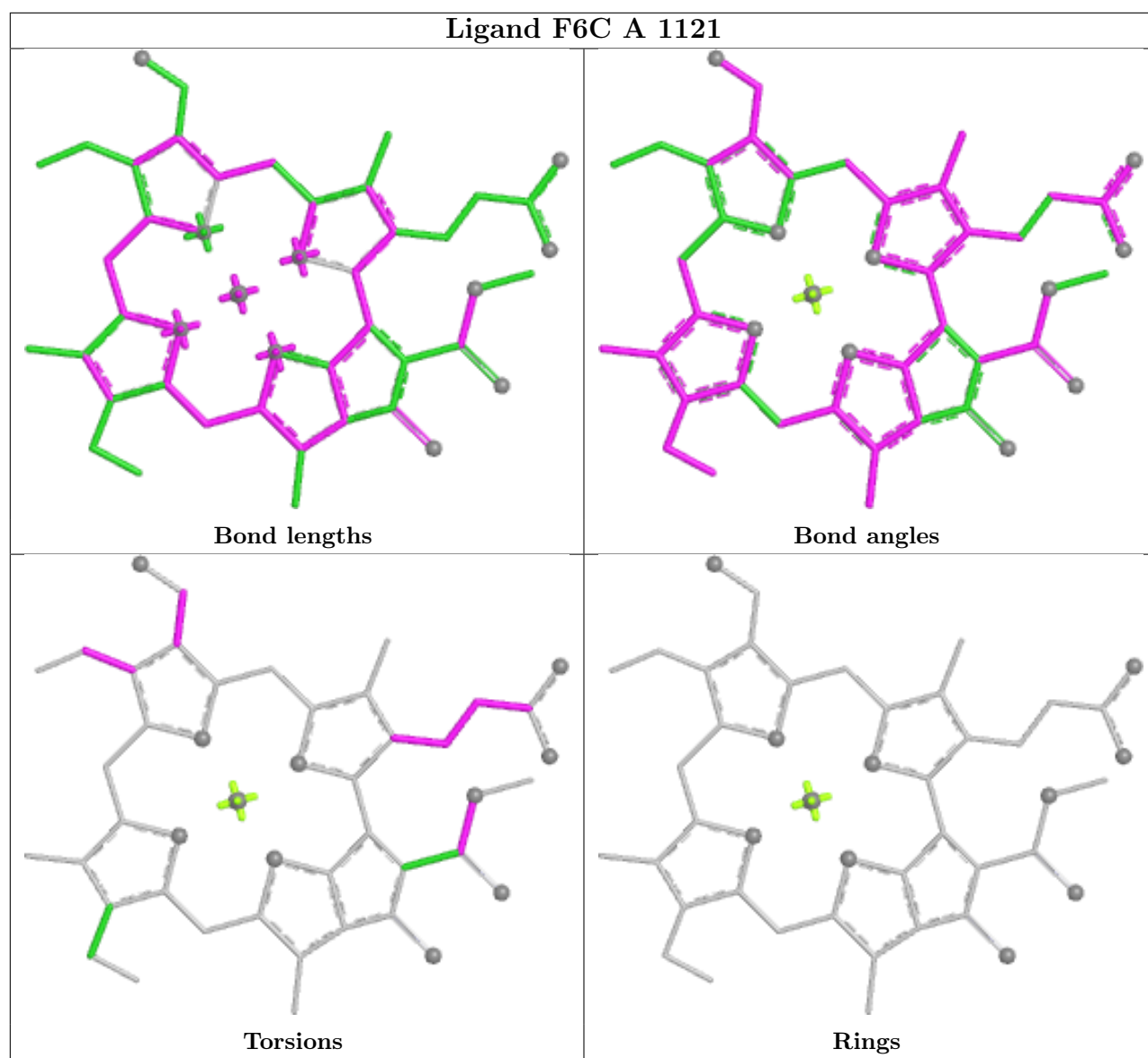
Bond angles

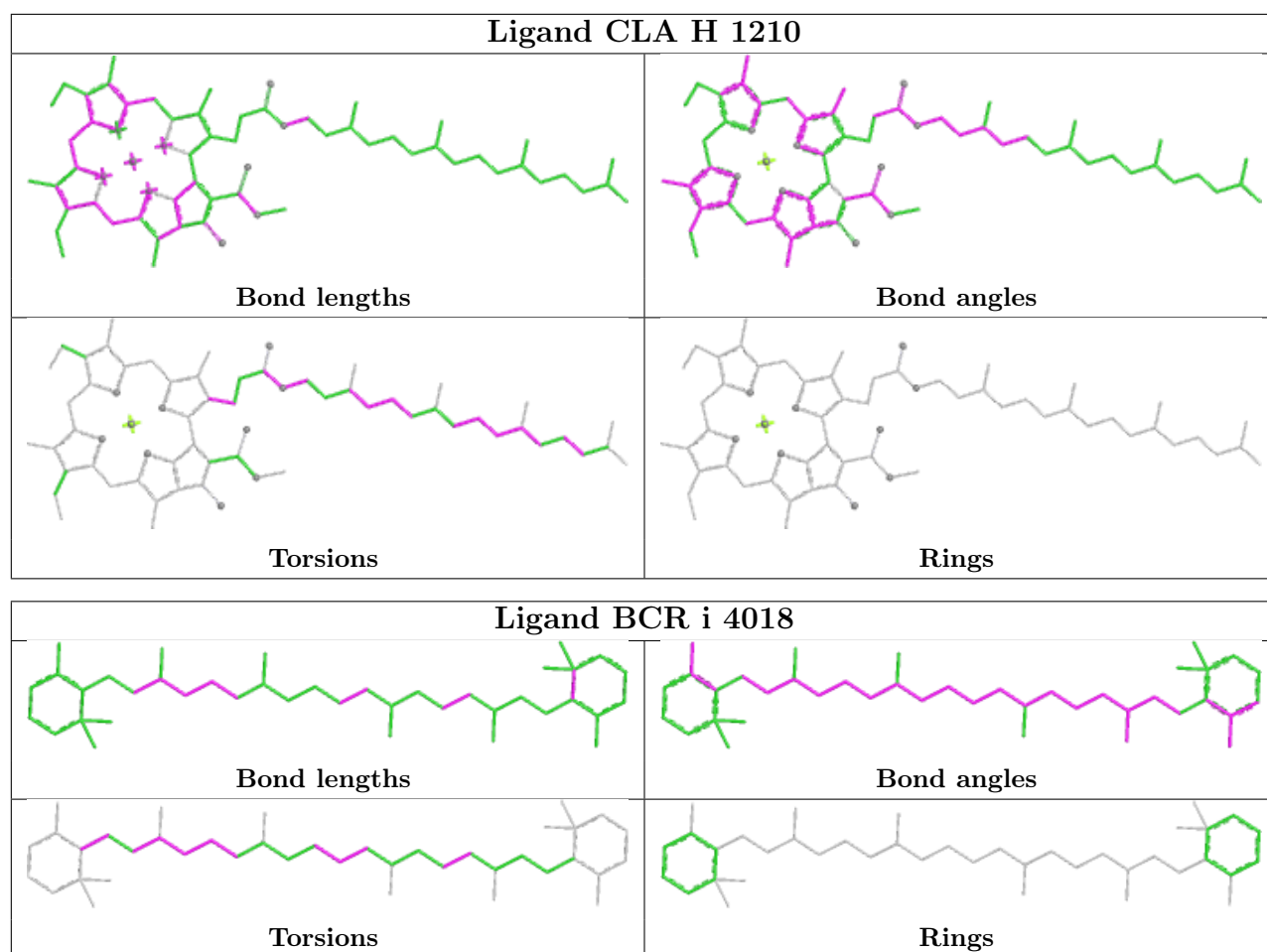


Torsions

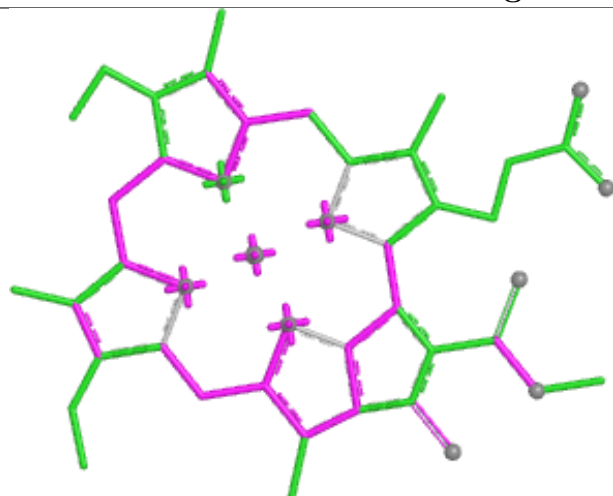


Rings

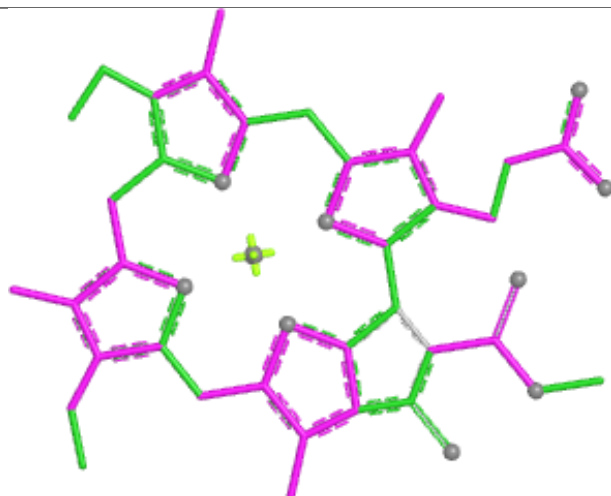




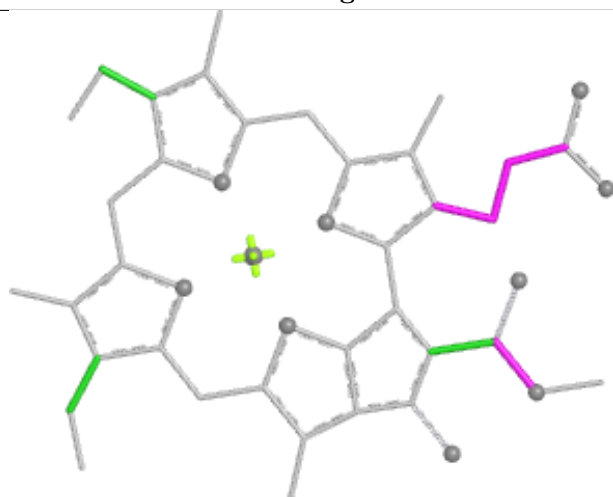
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Bond lengths



Bond angles

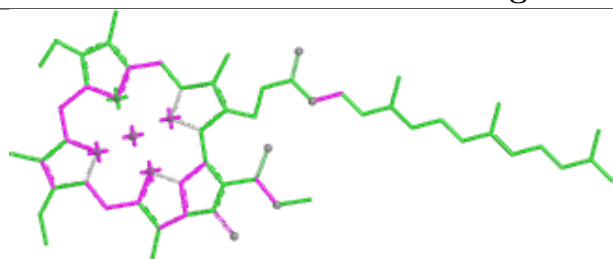


Torsions

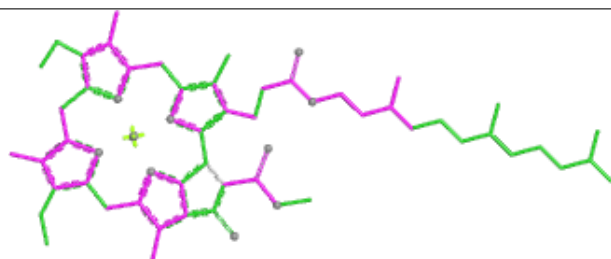


Rings

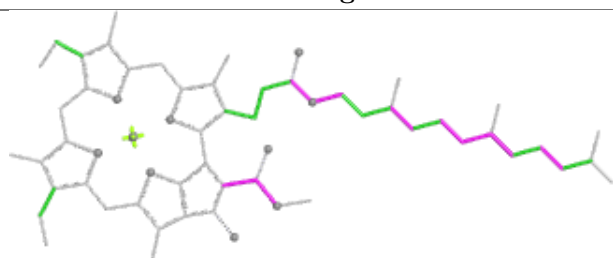
Ligand CLA a 1128



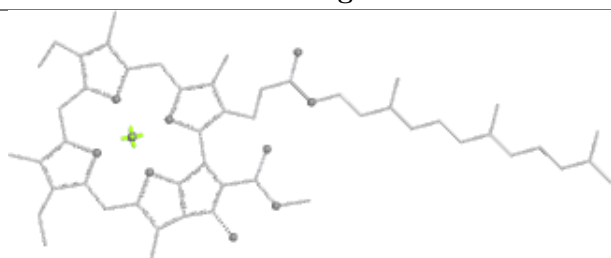
Bond lengths



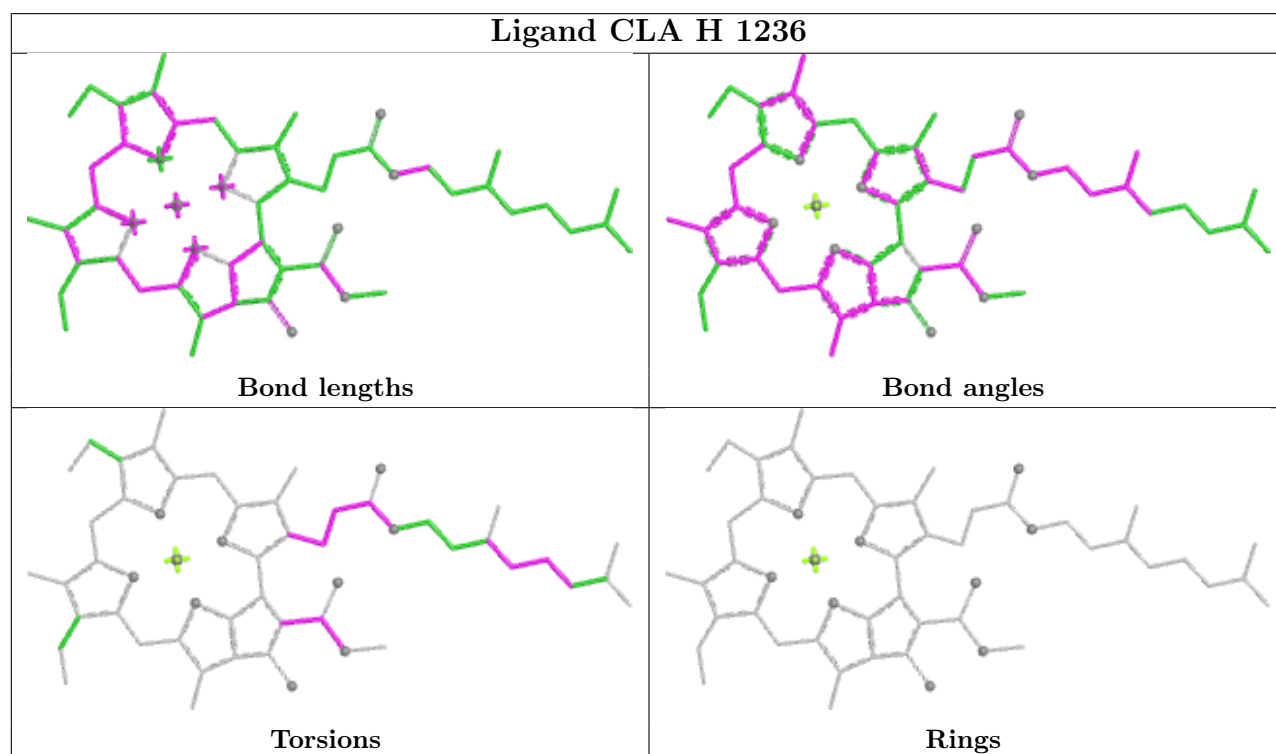
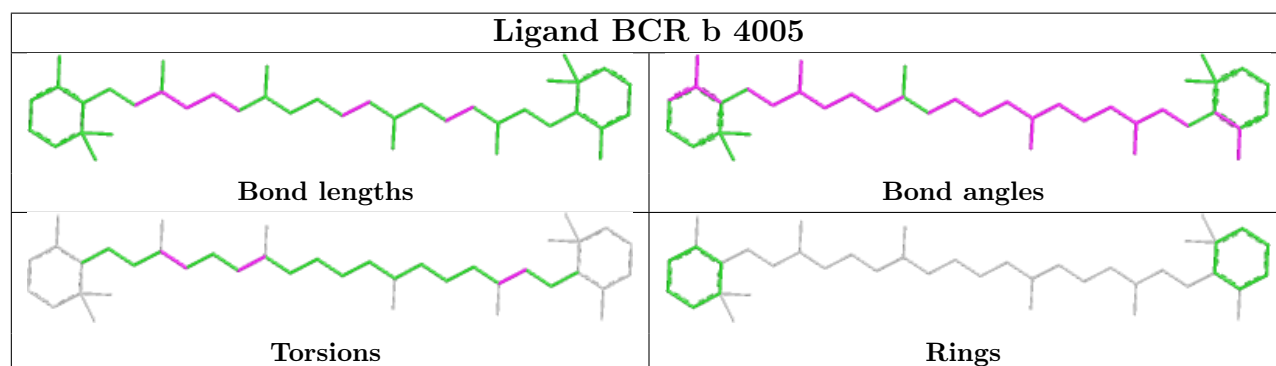
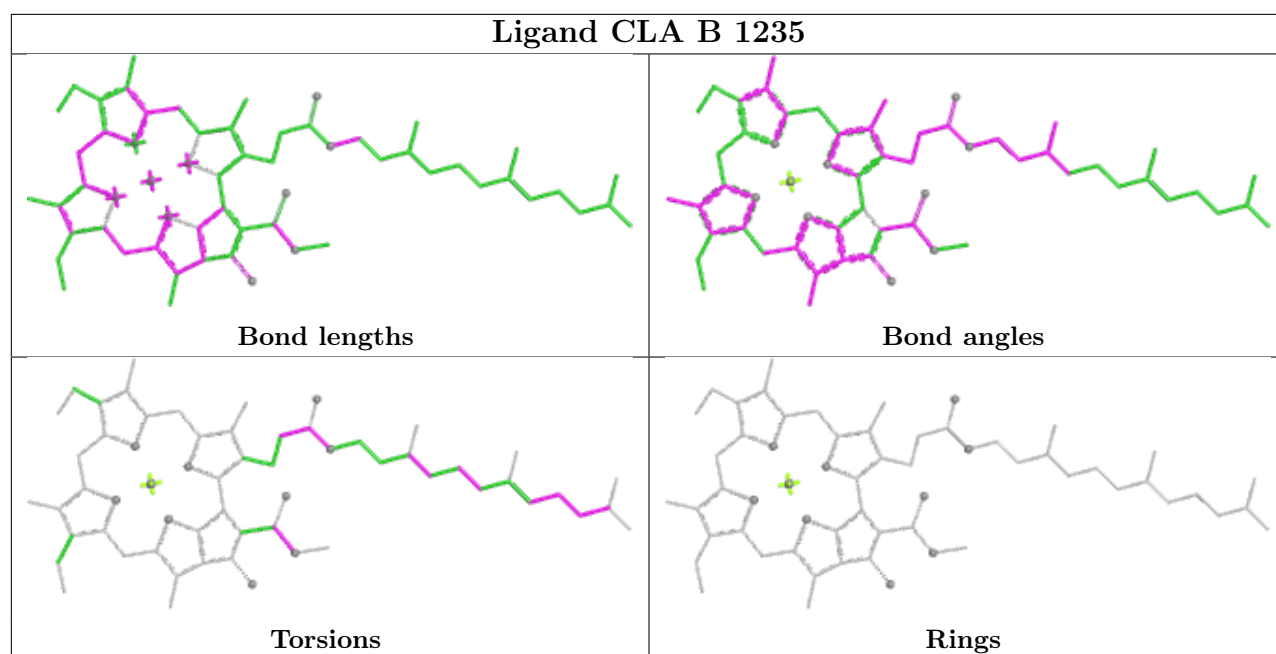
Bond angles

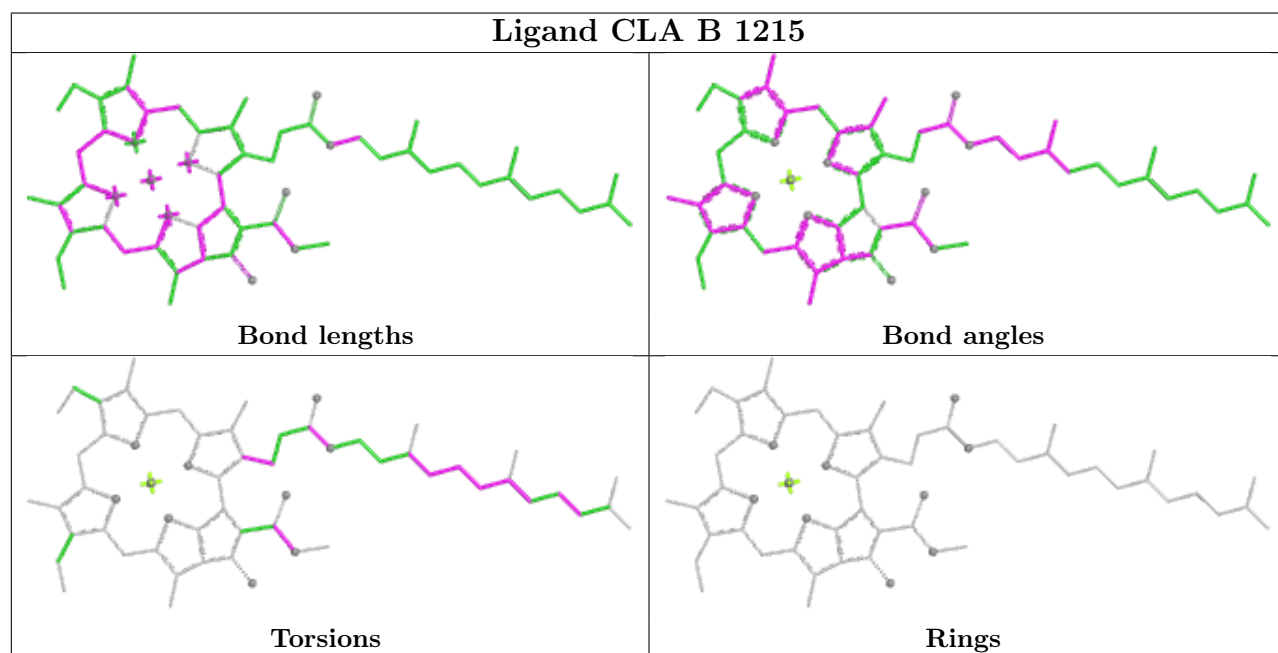
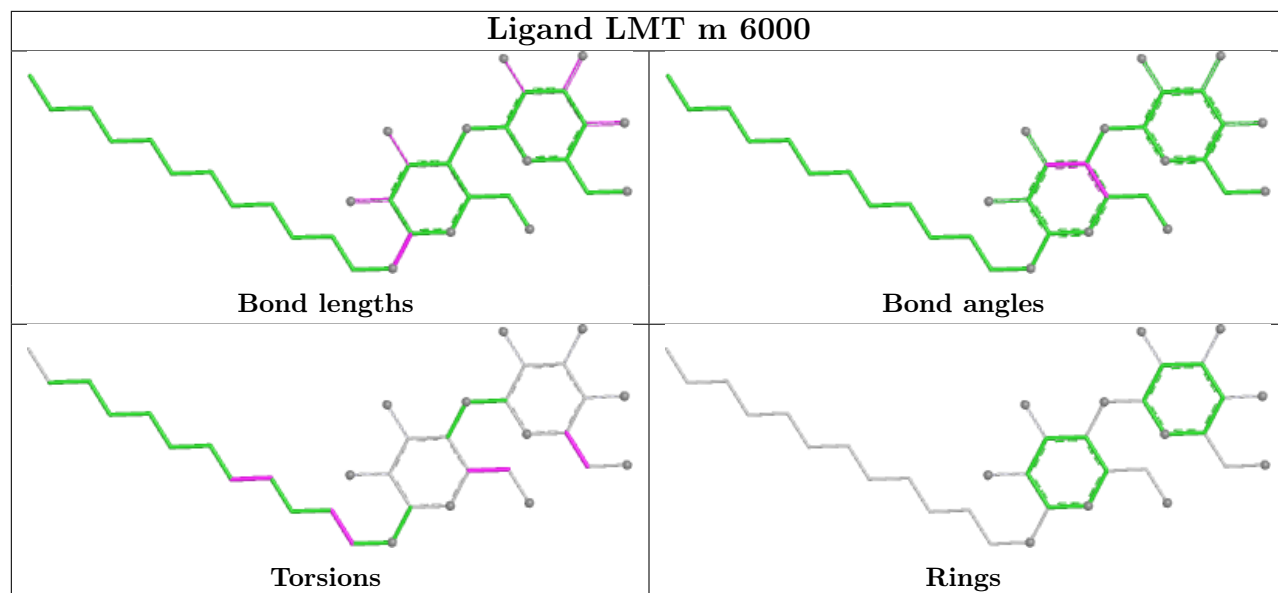


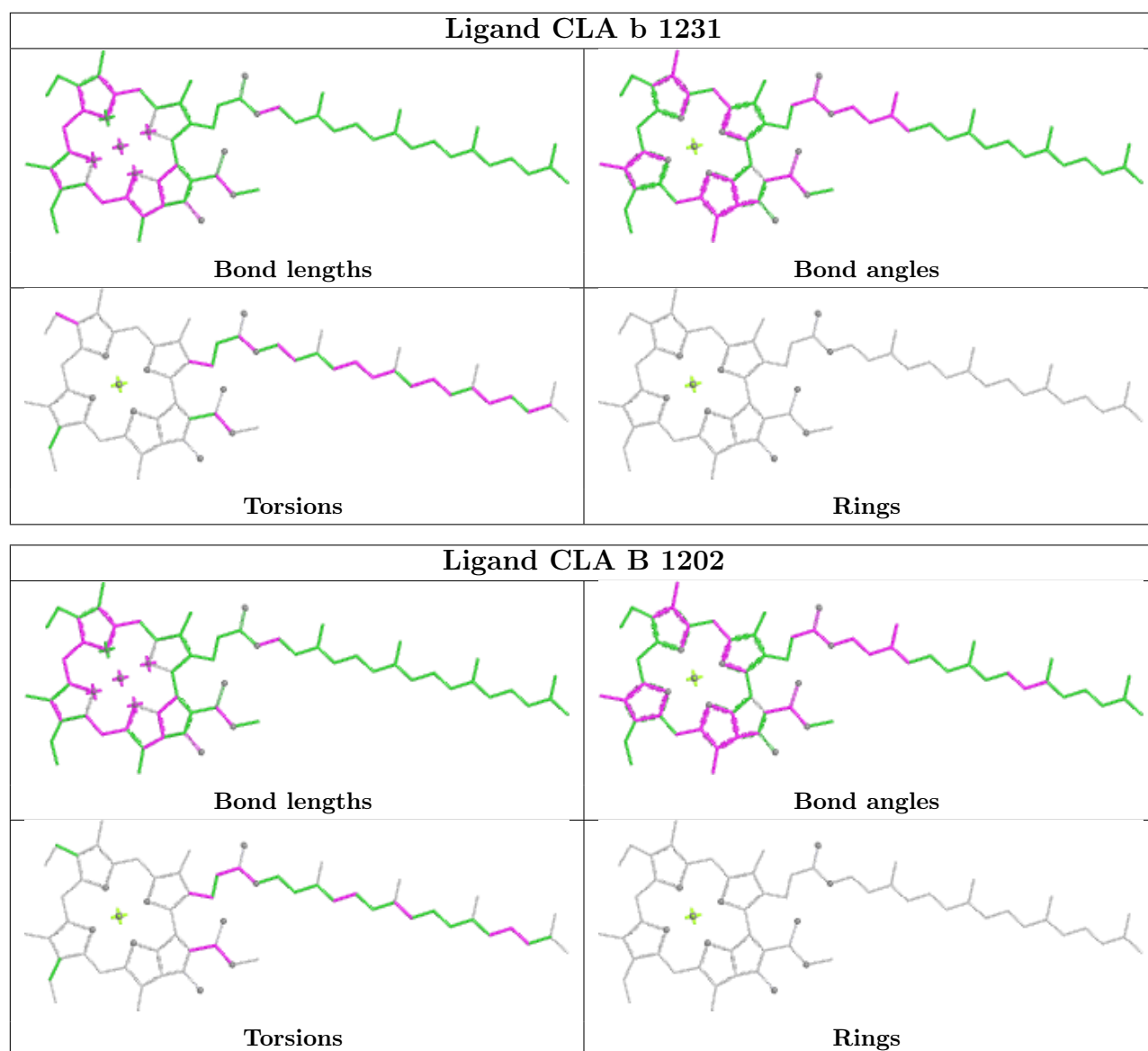
Torsions

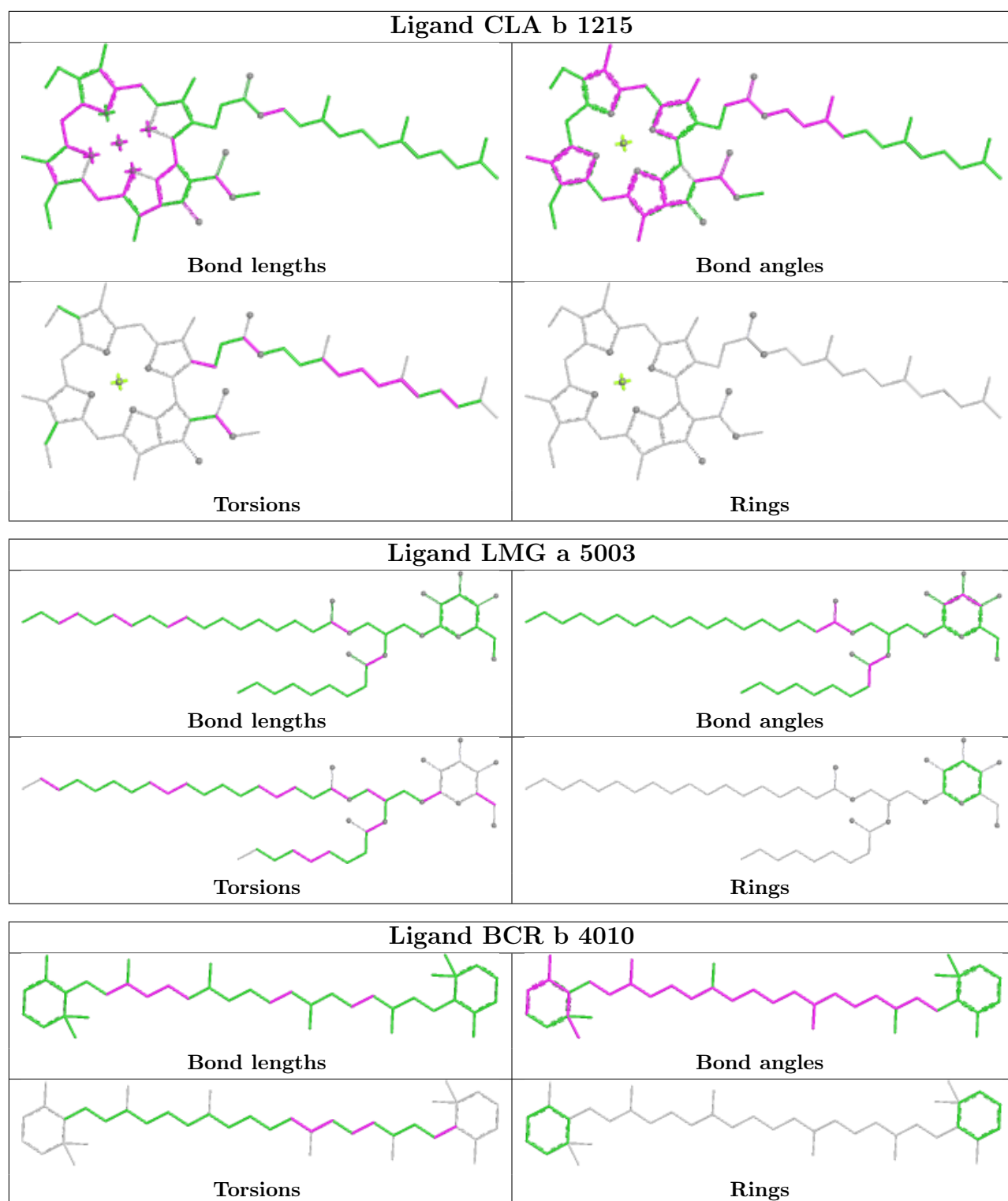


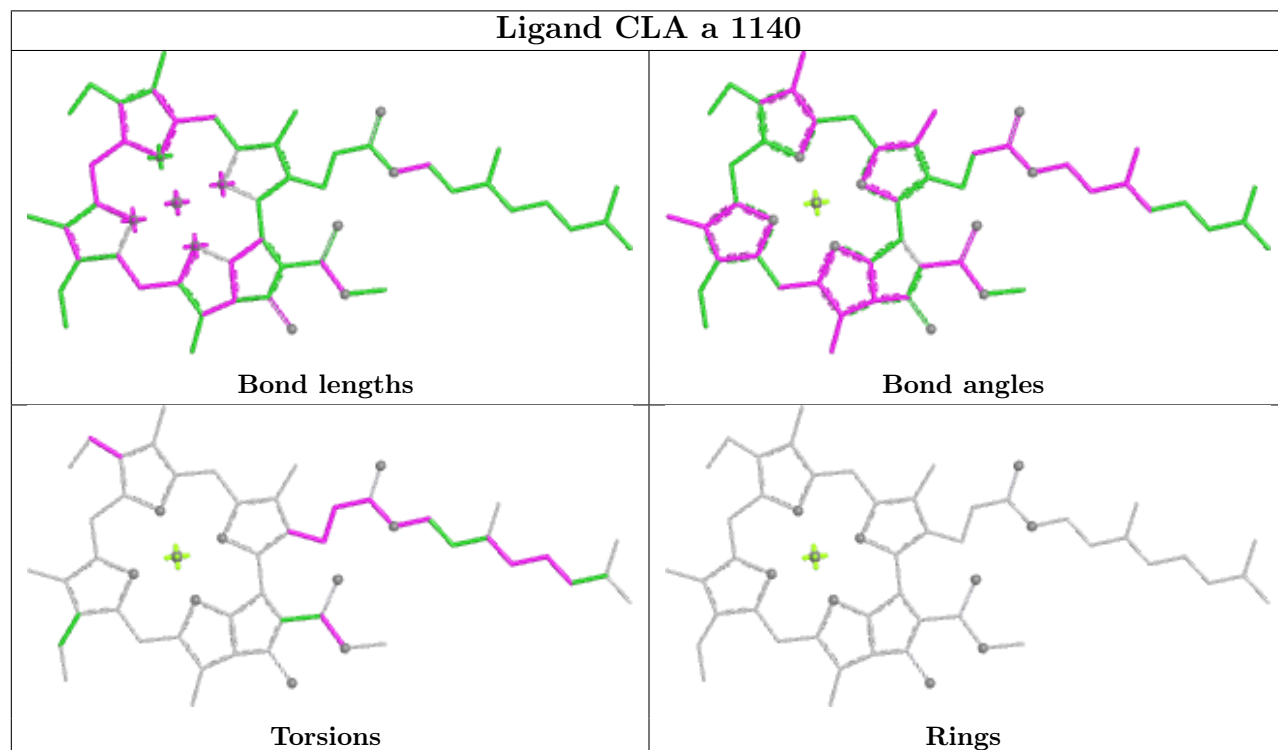
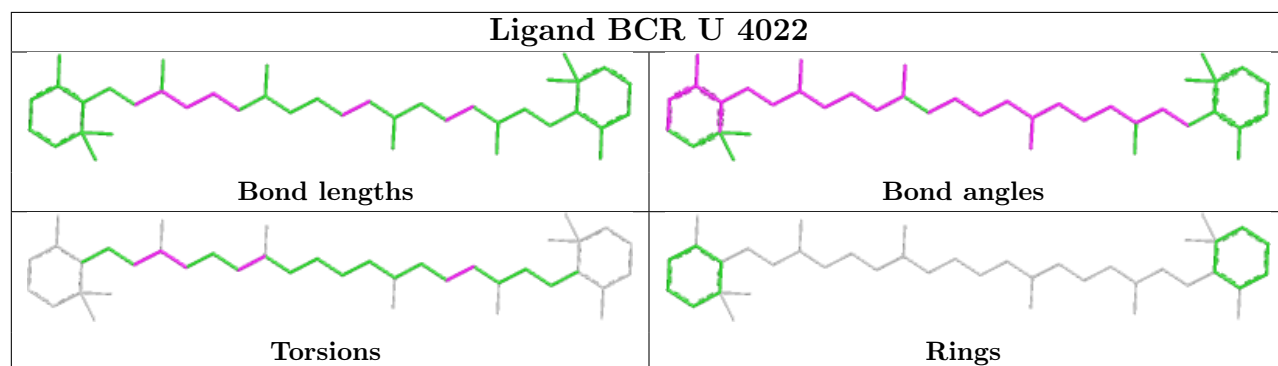
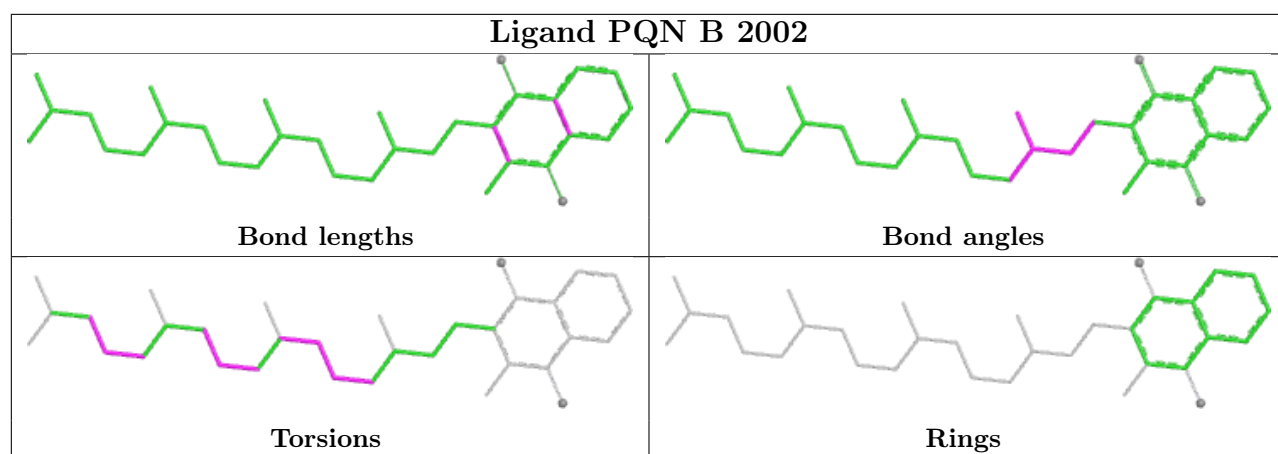
Rings

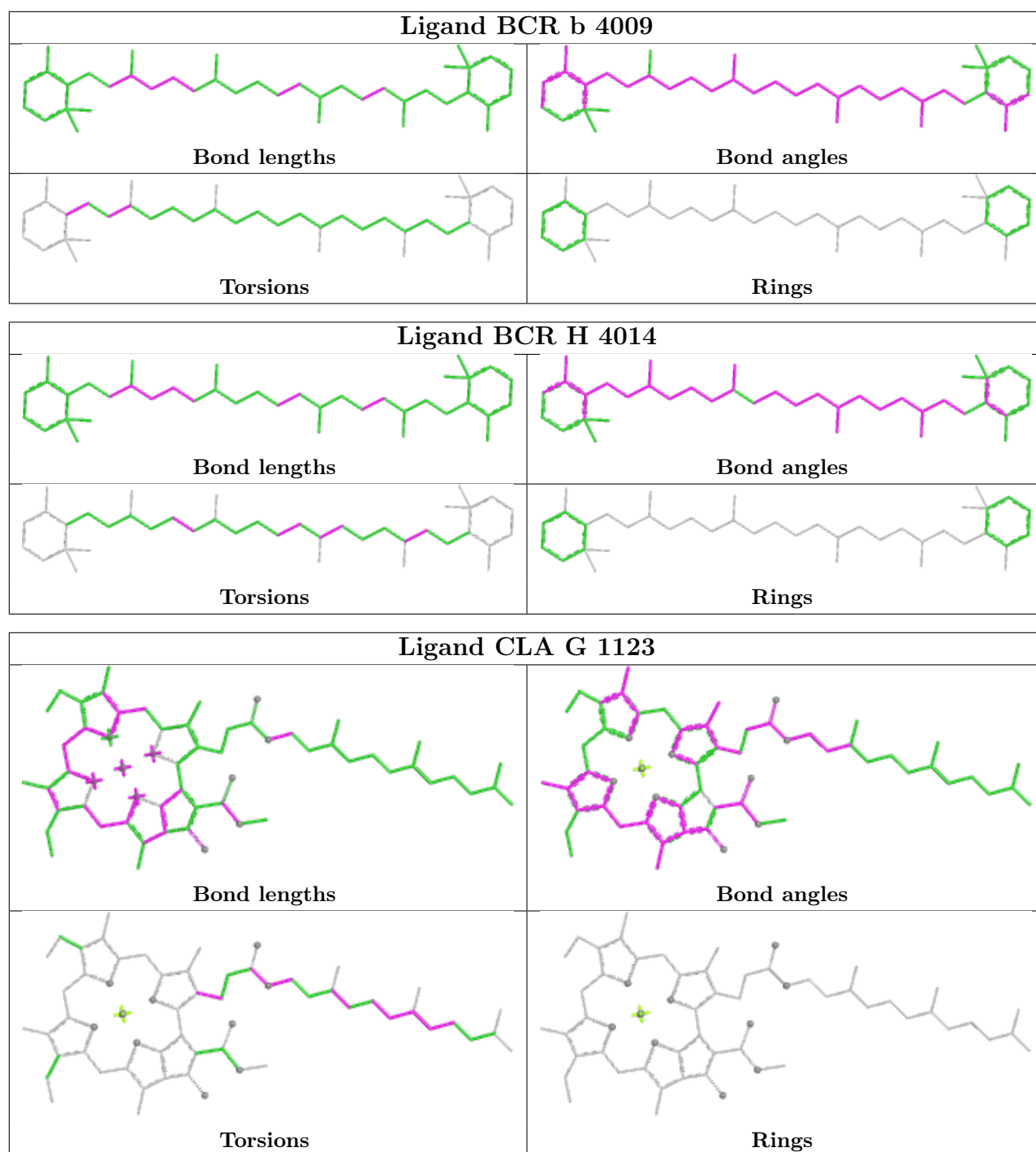




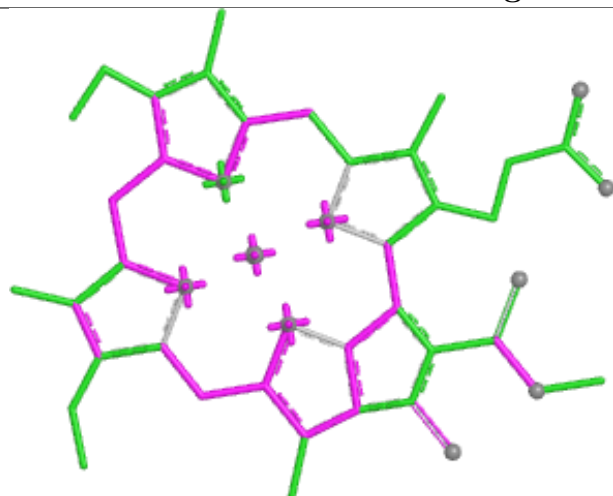




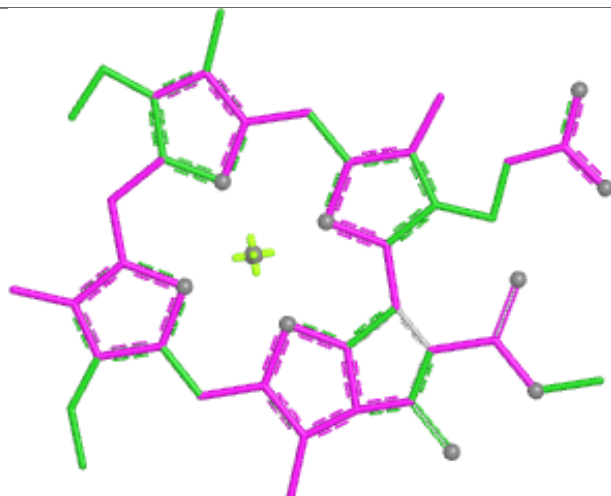




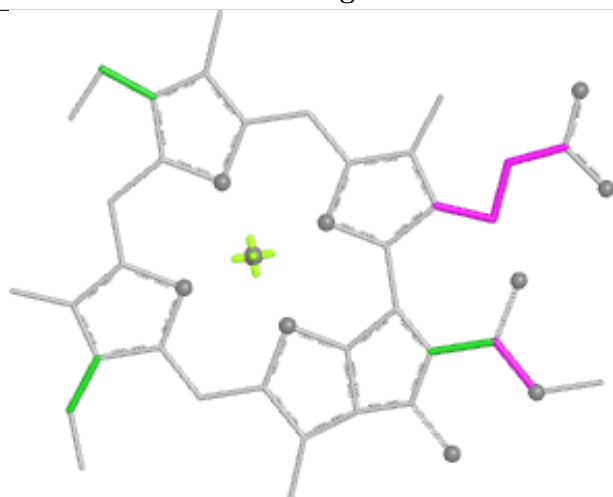
Ligand CLA G 1134



Bond lengths



Bond angles

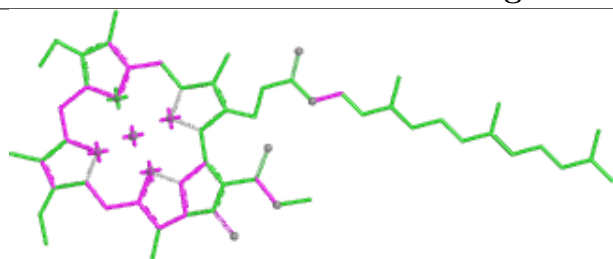


Torsions

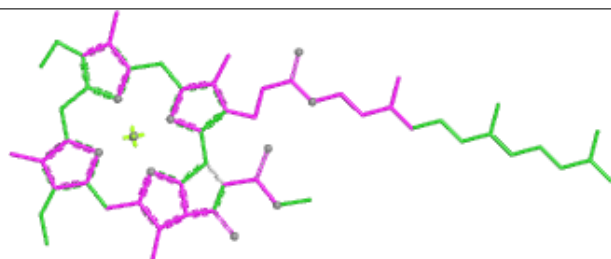


Rings

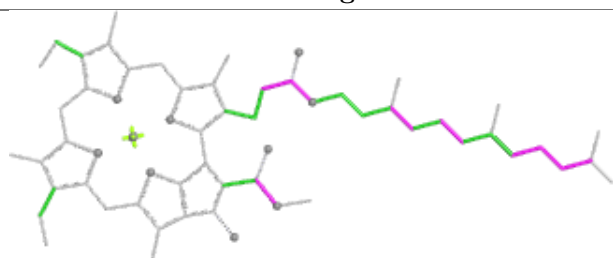
Ligand CLA H 1235



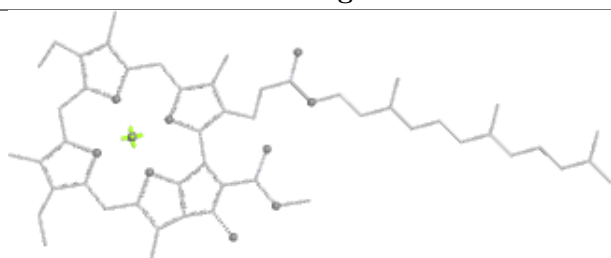
Bond lengths



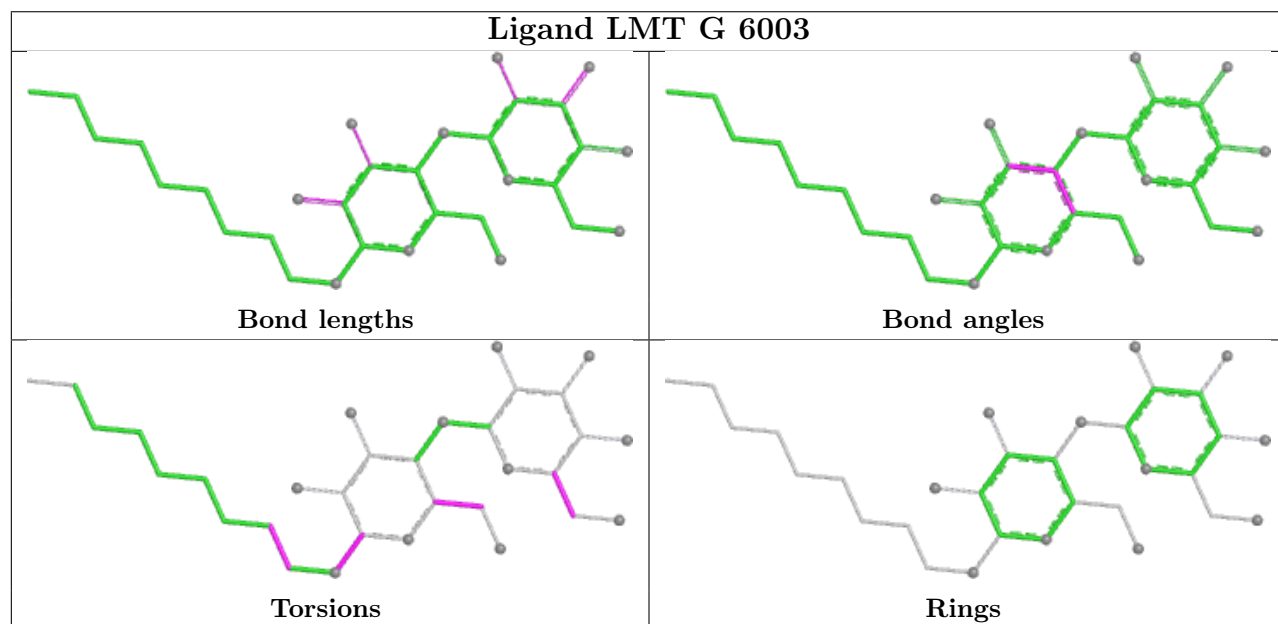
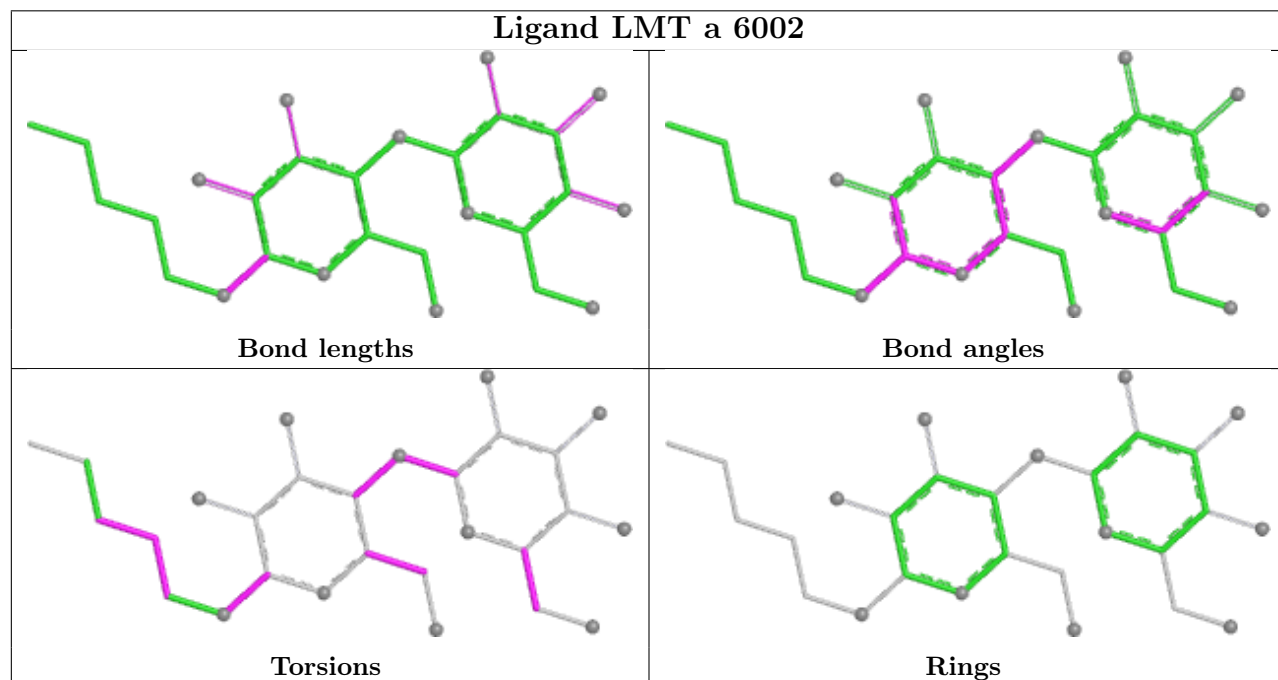
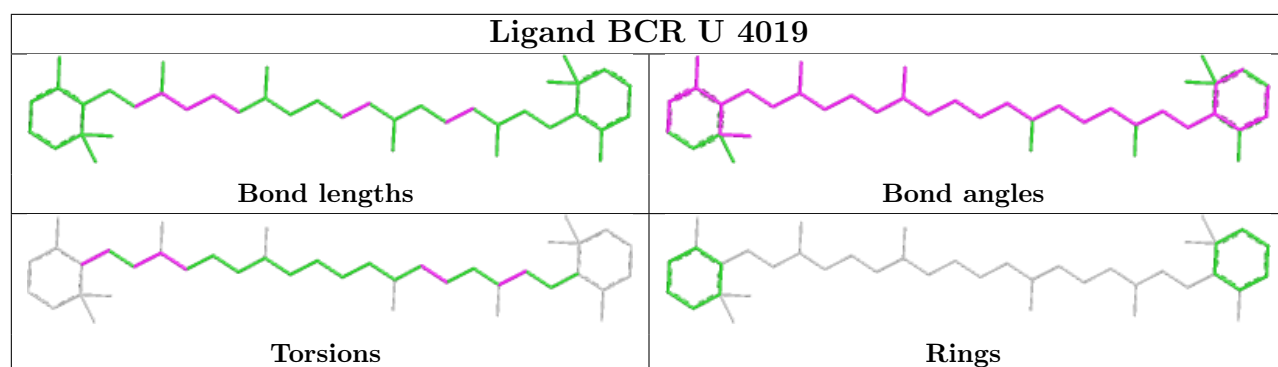
Bond angles

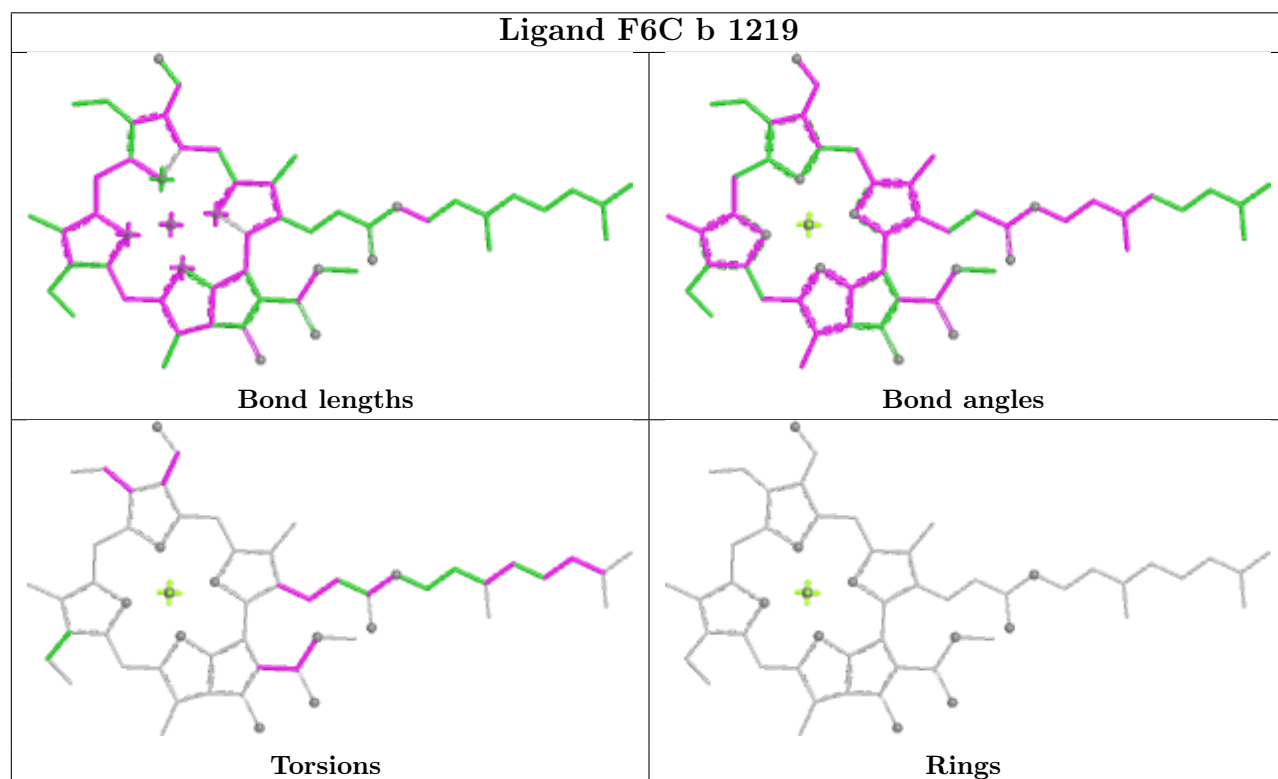
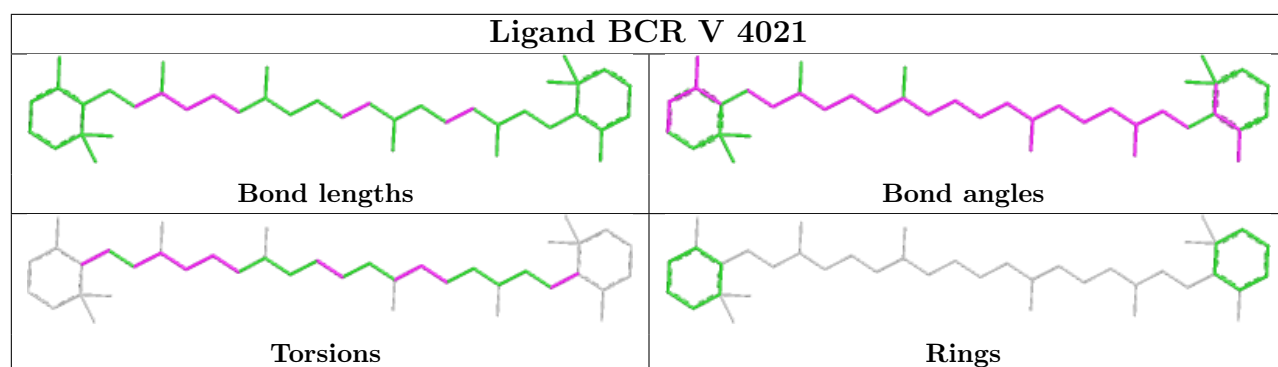


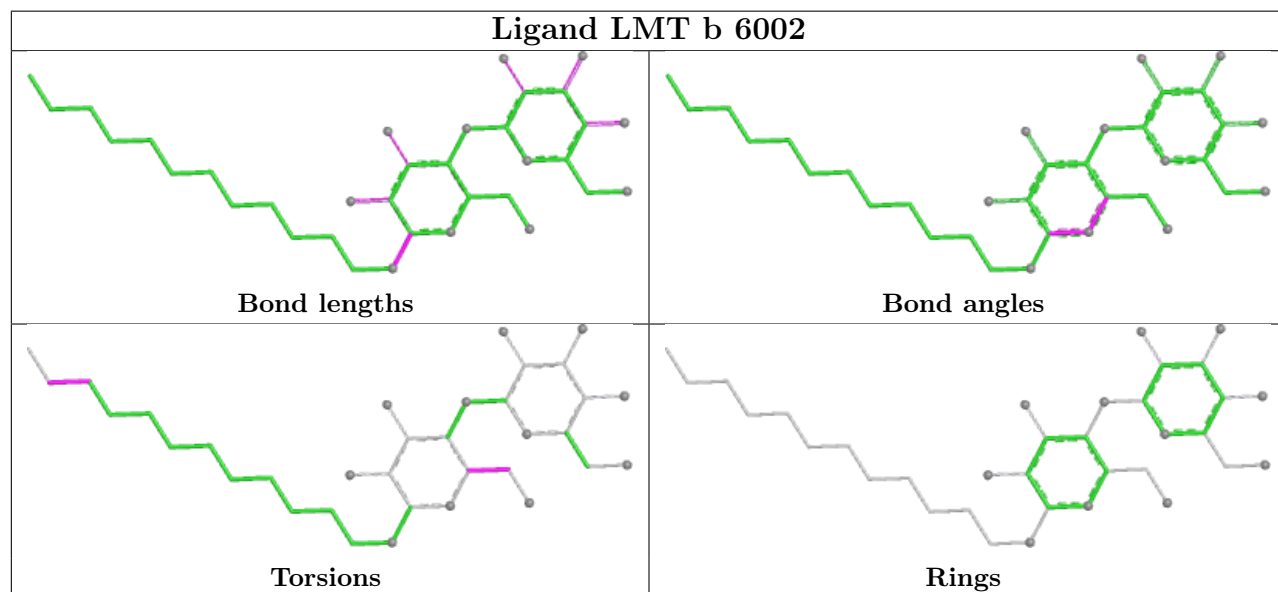
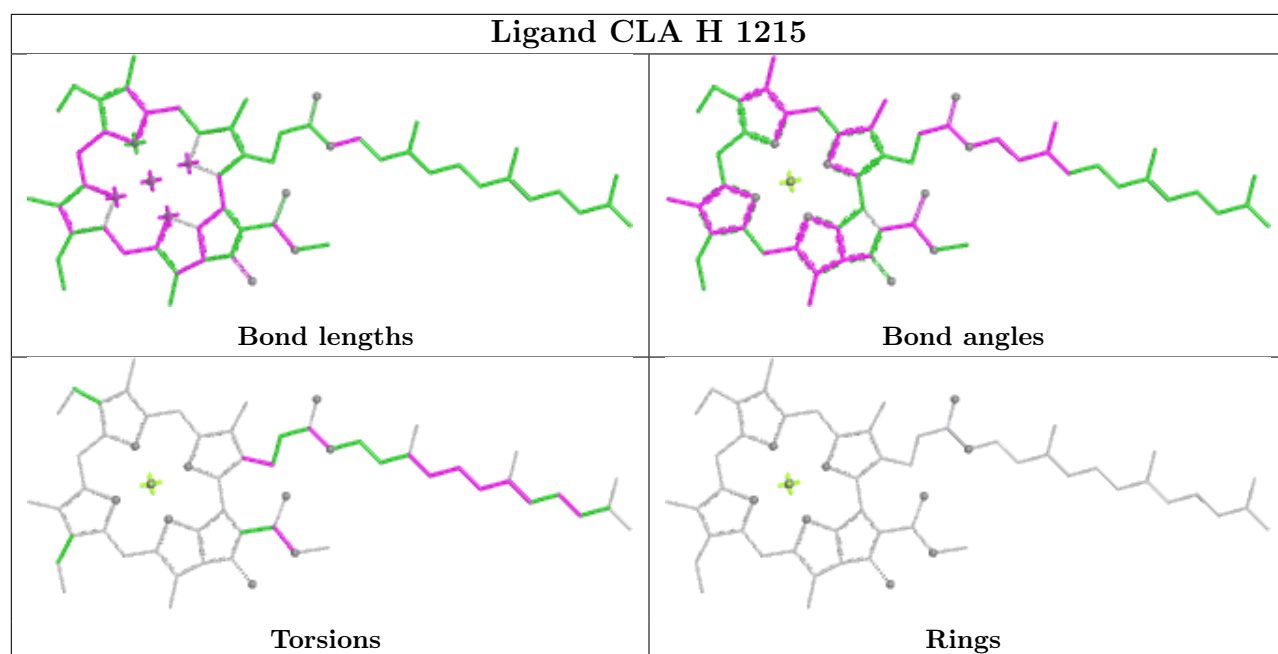
Torsions

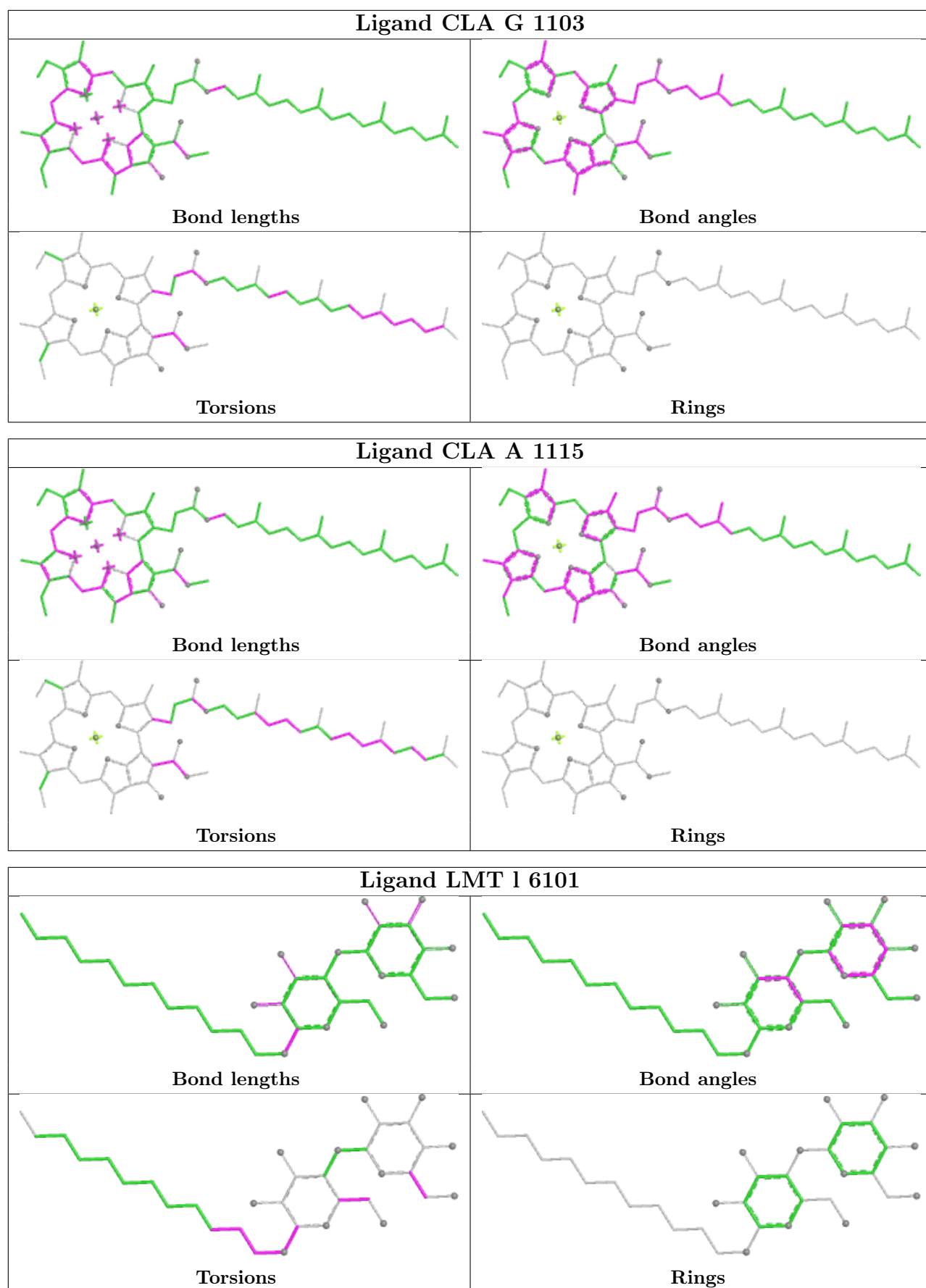


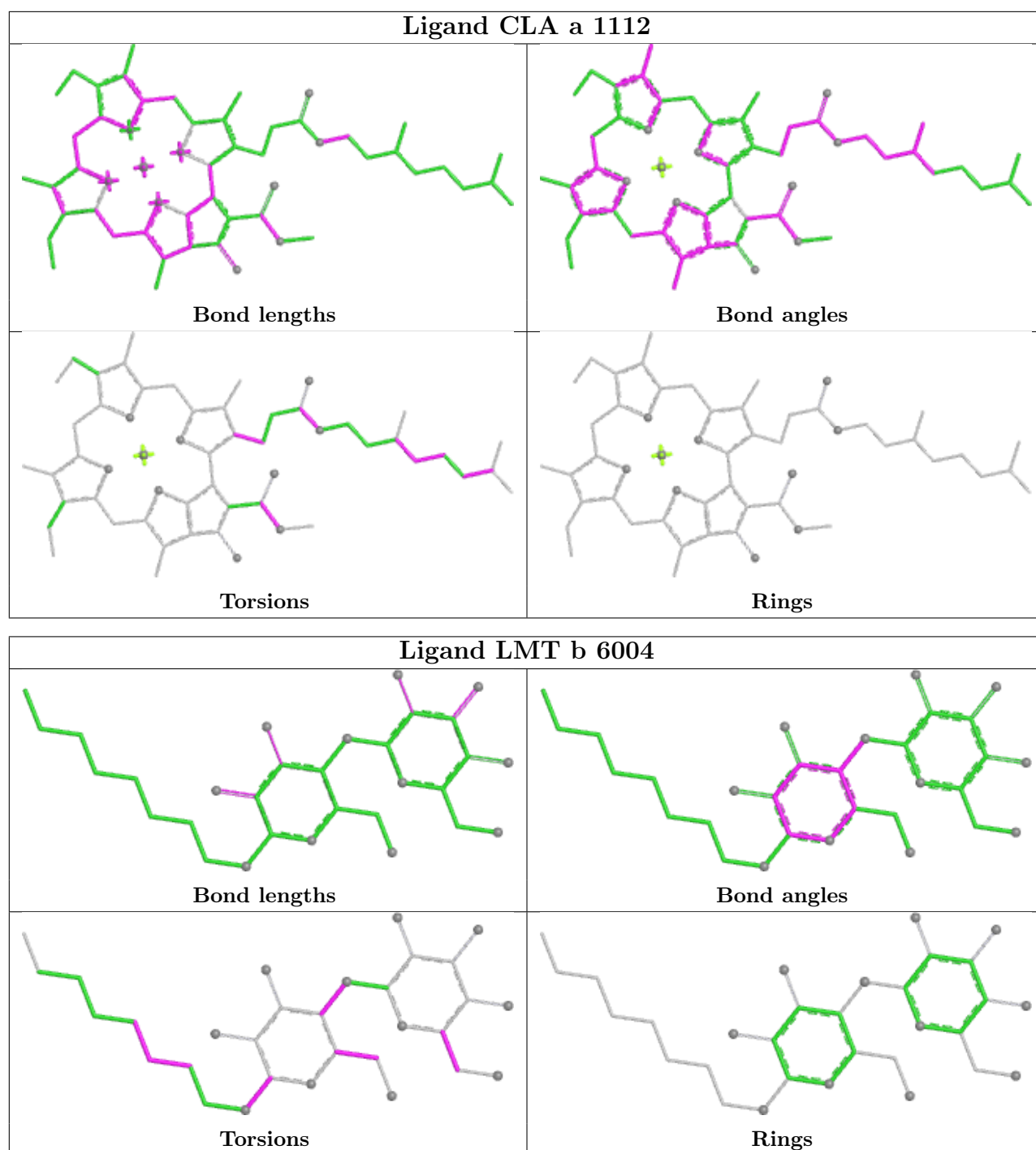
Rings

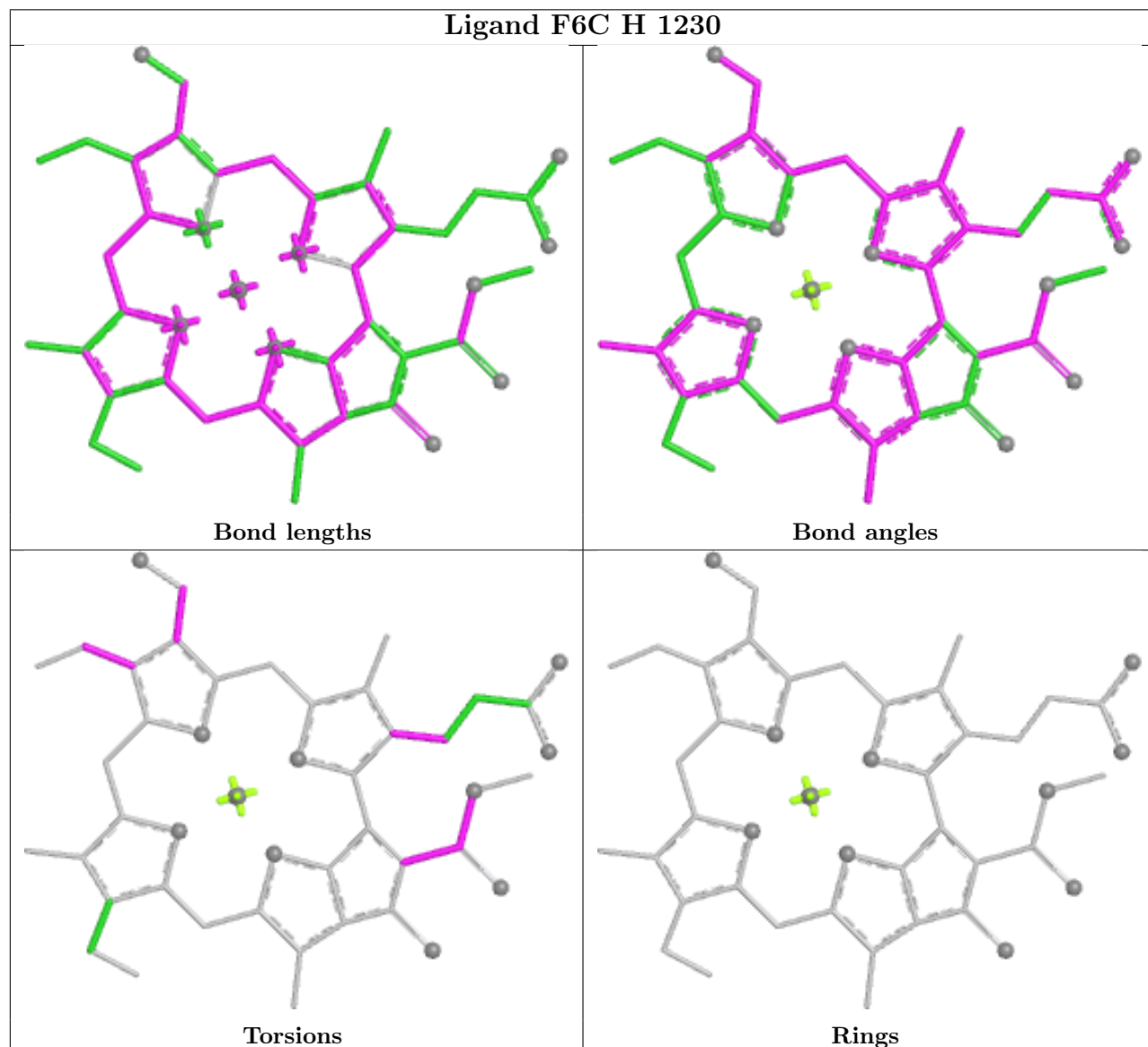
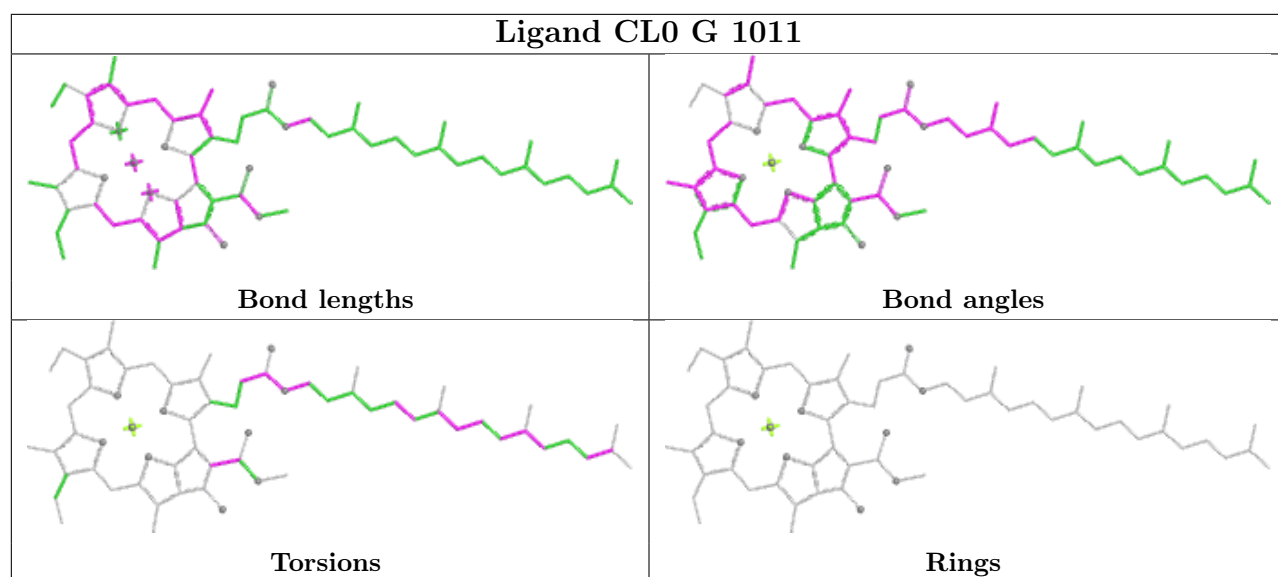


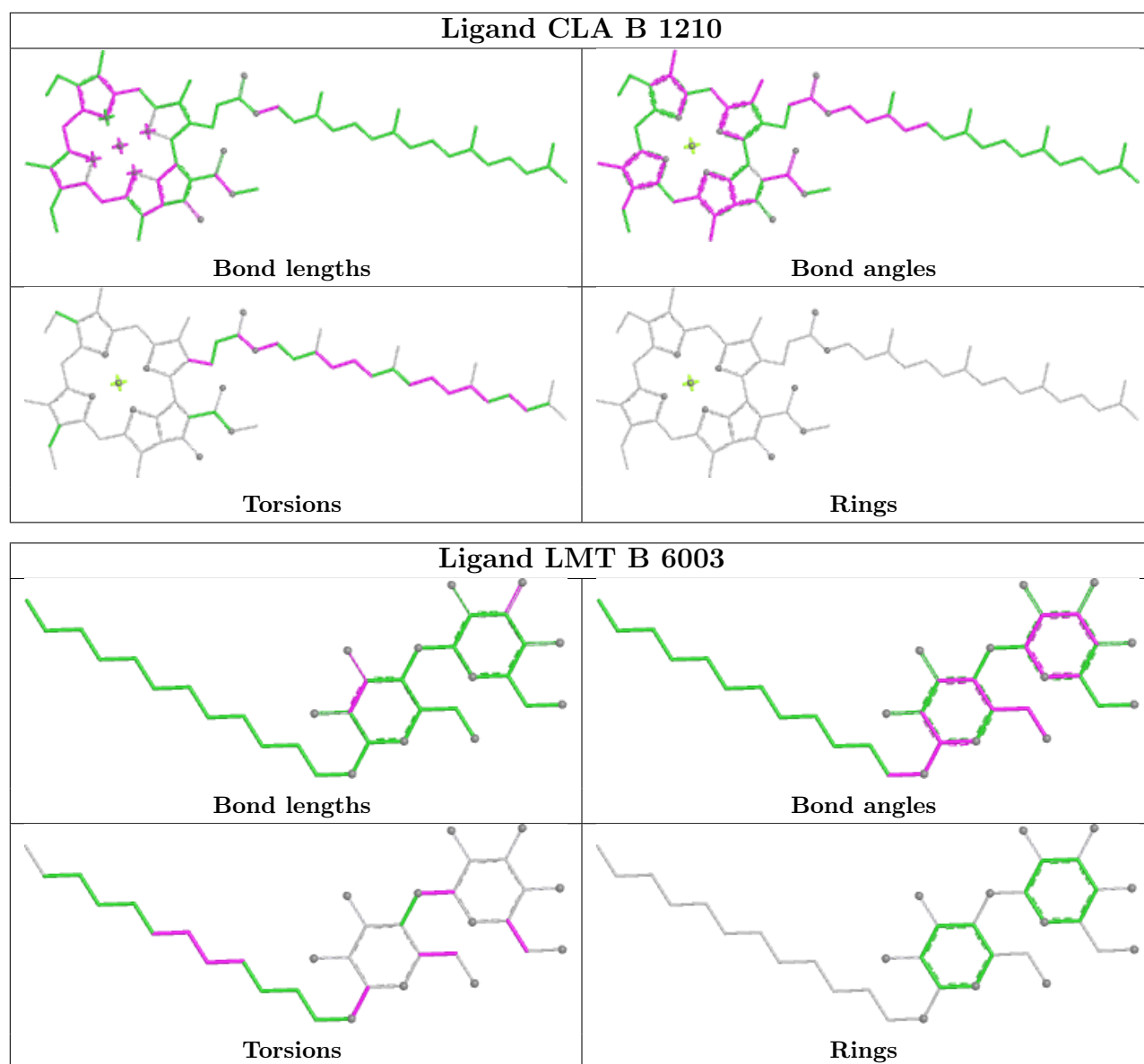


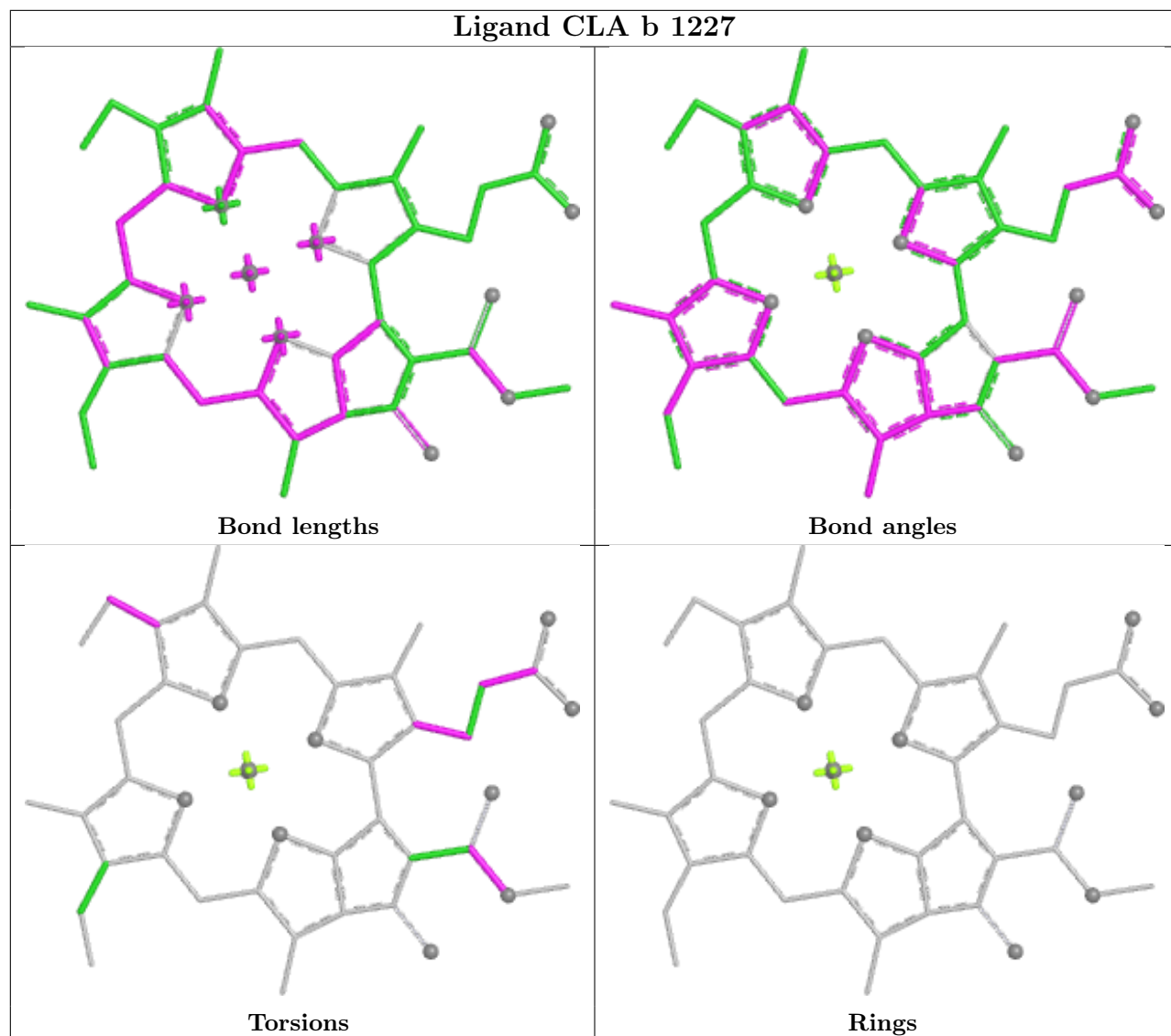


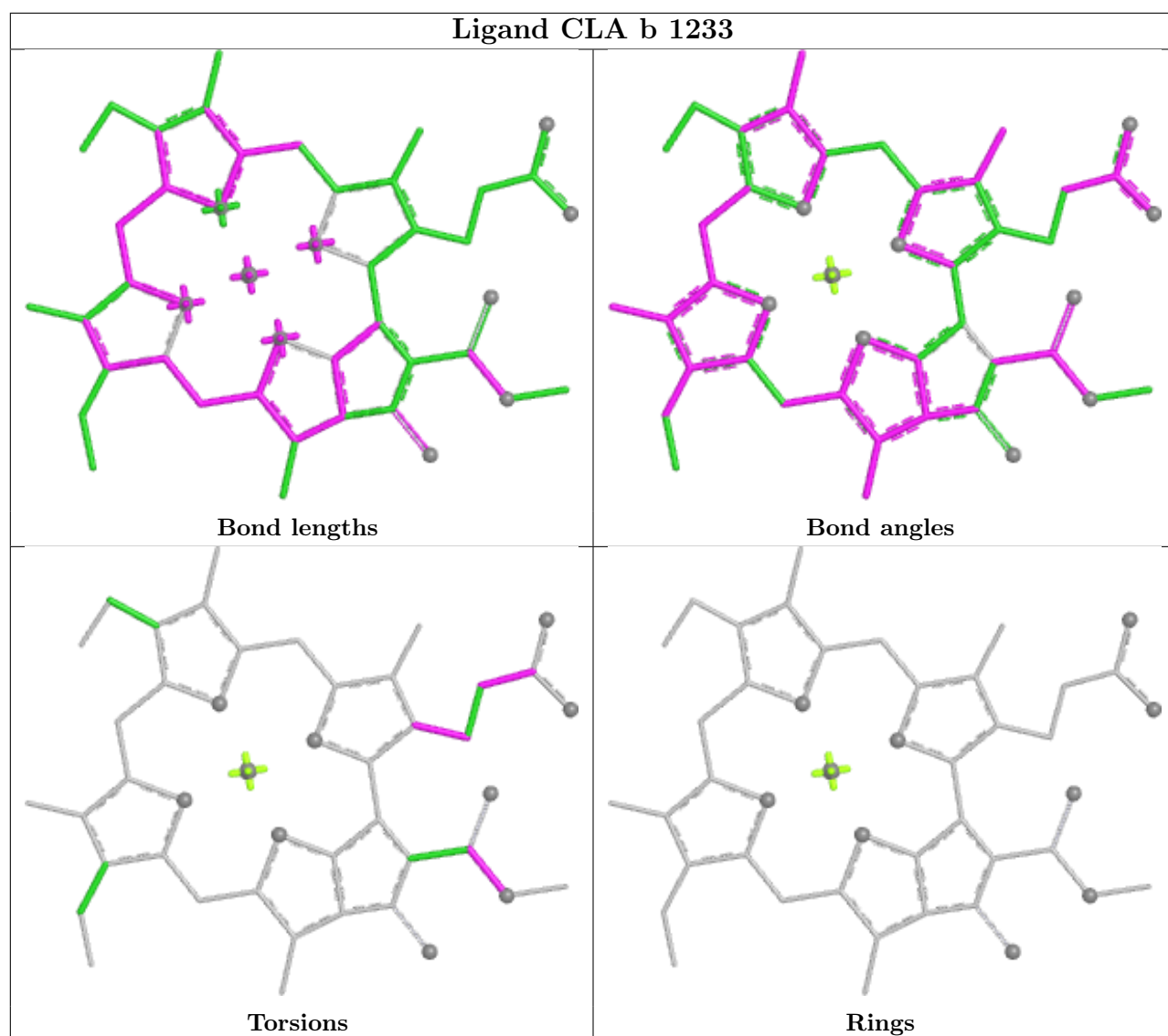


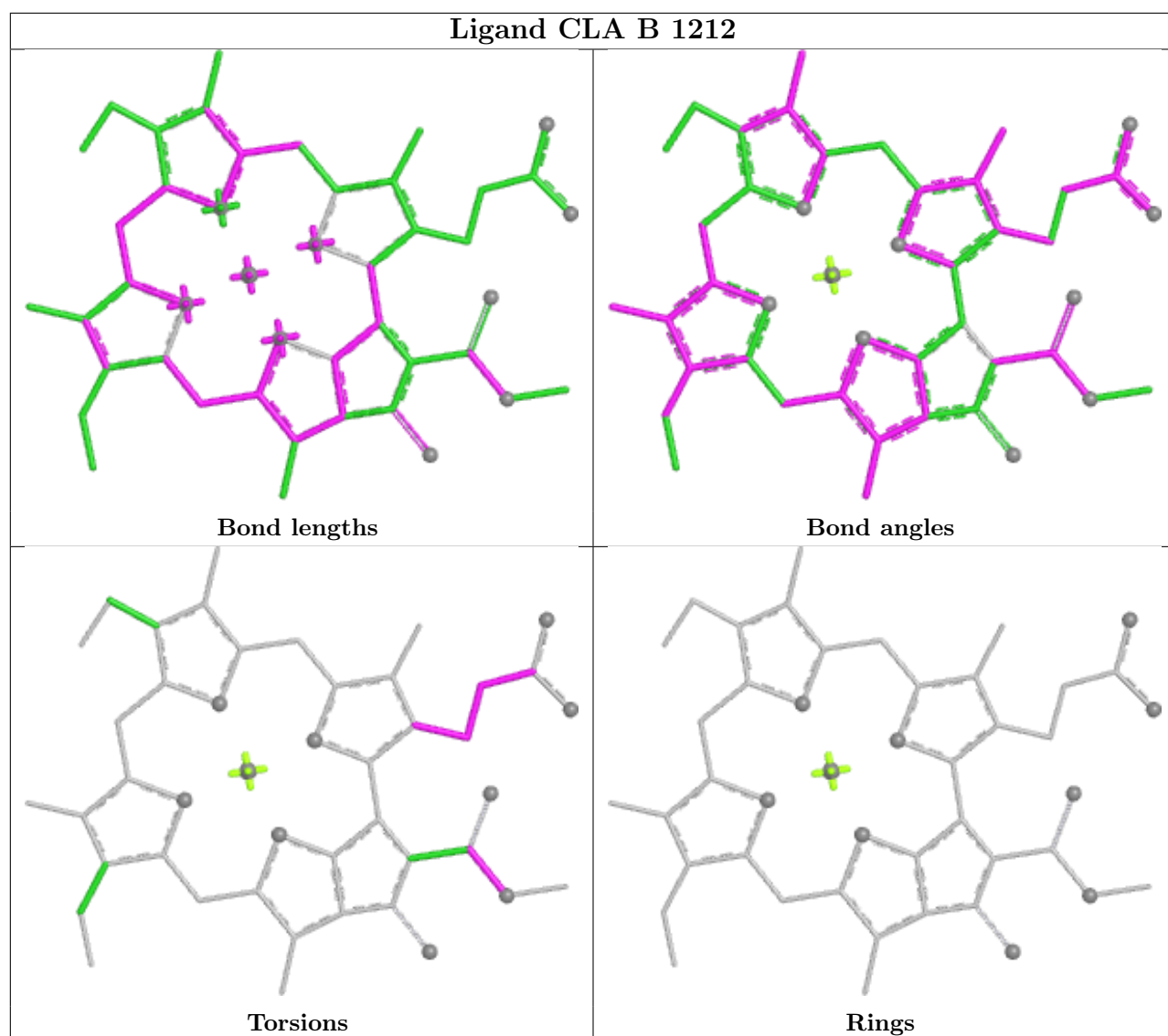


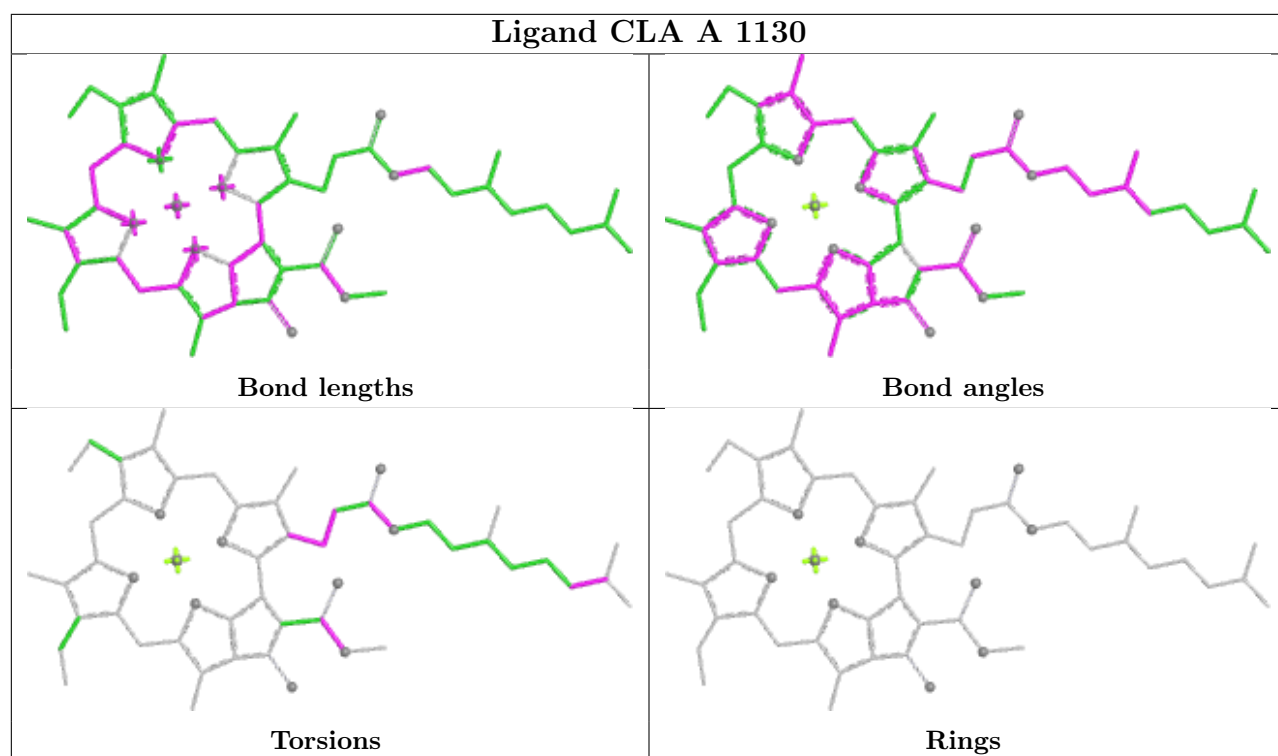




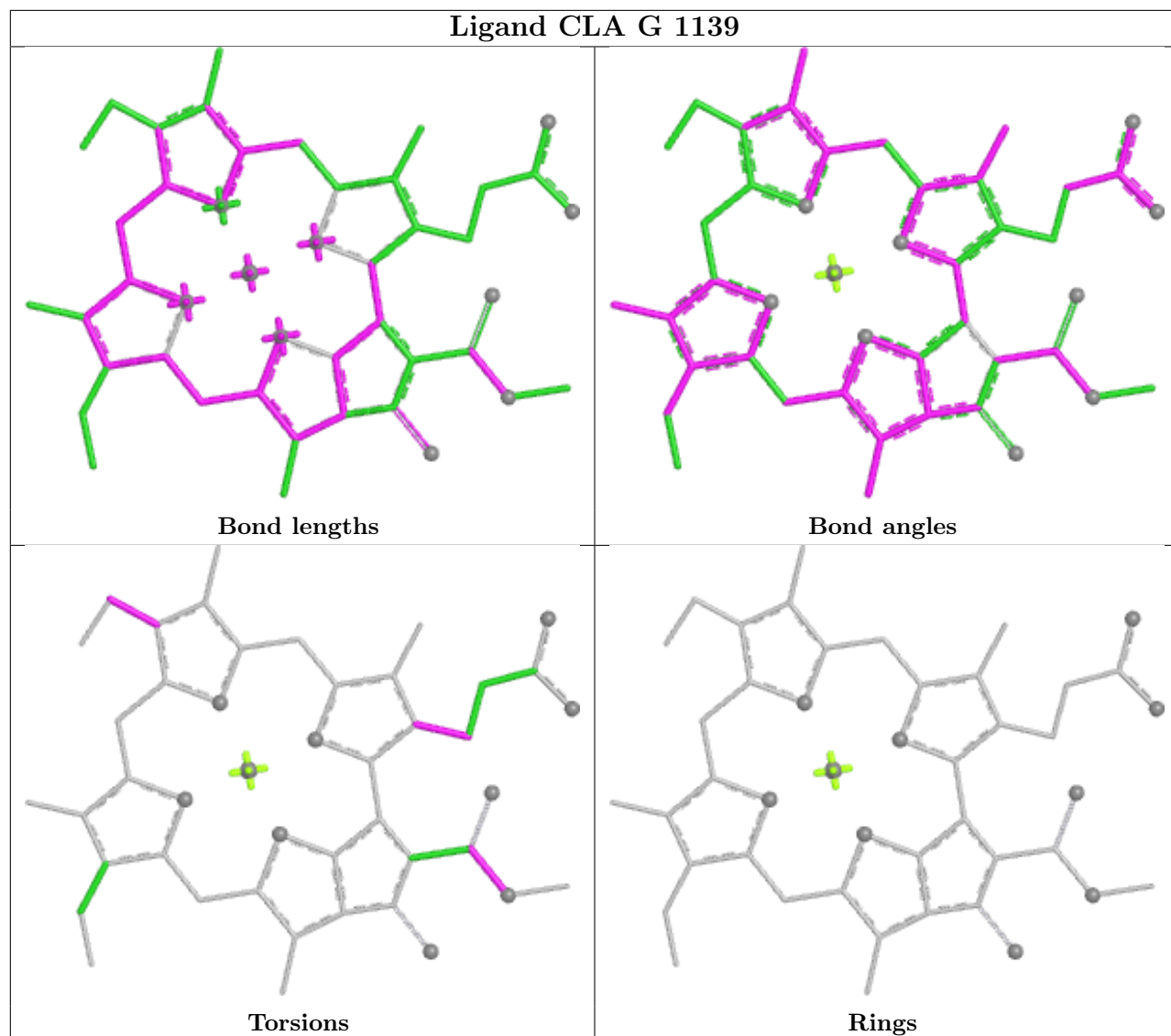


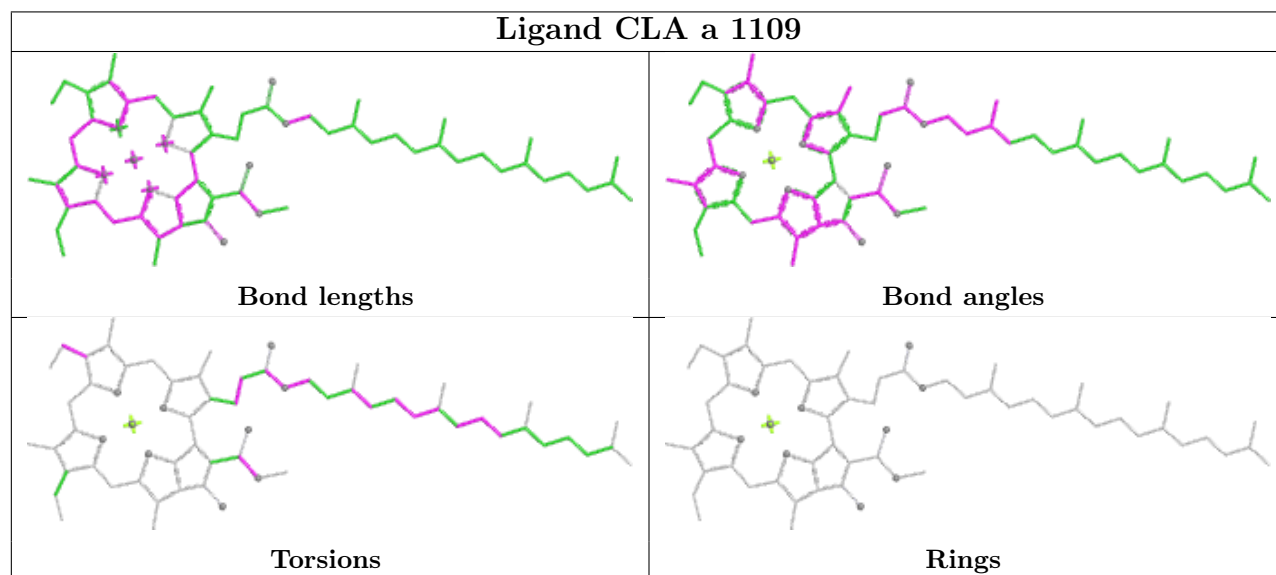
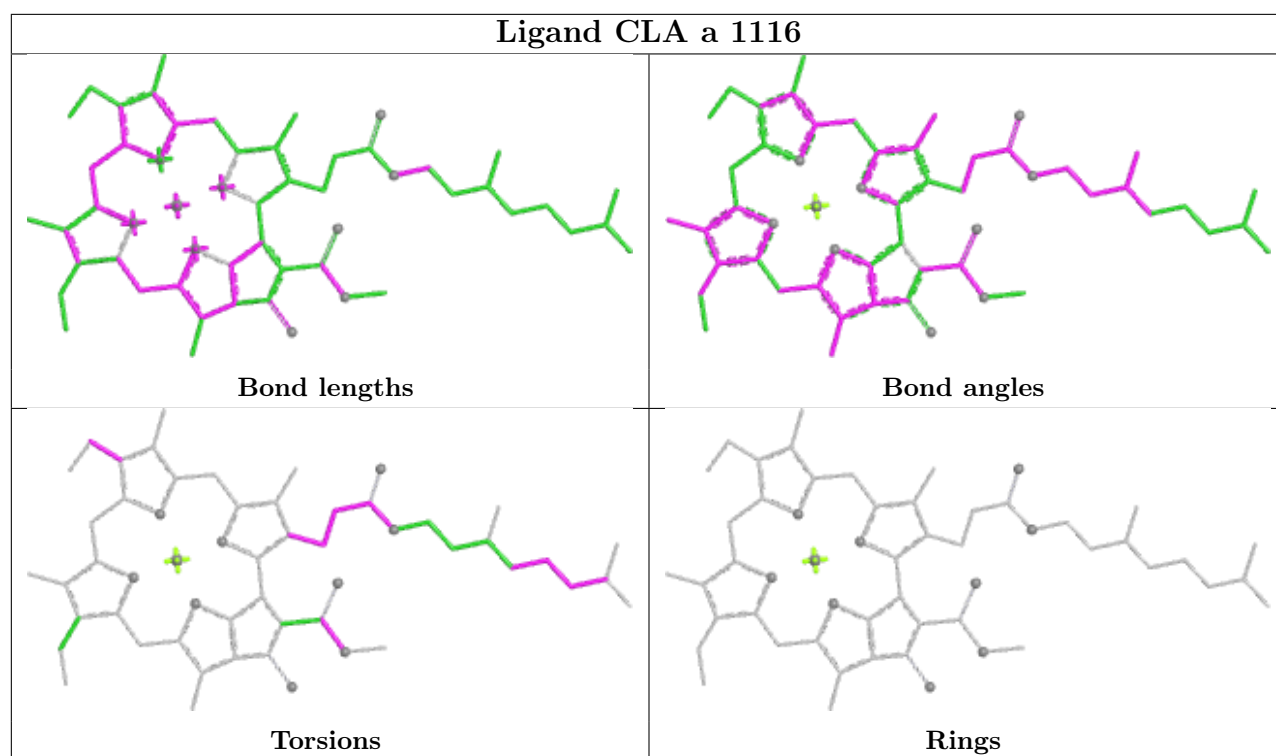


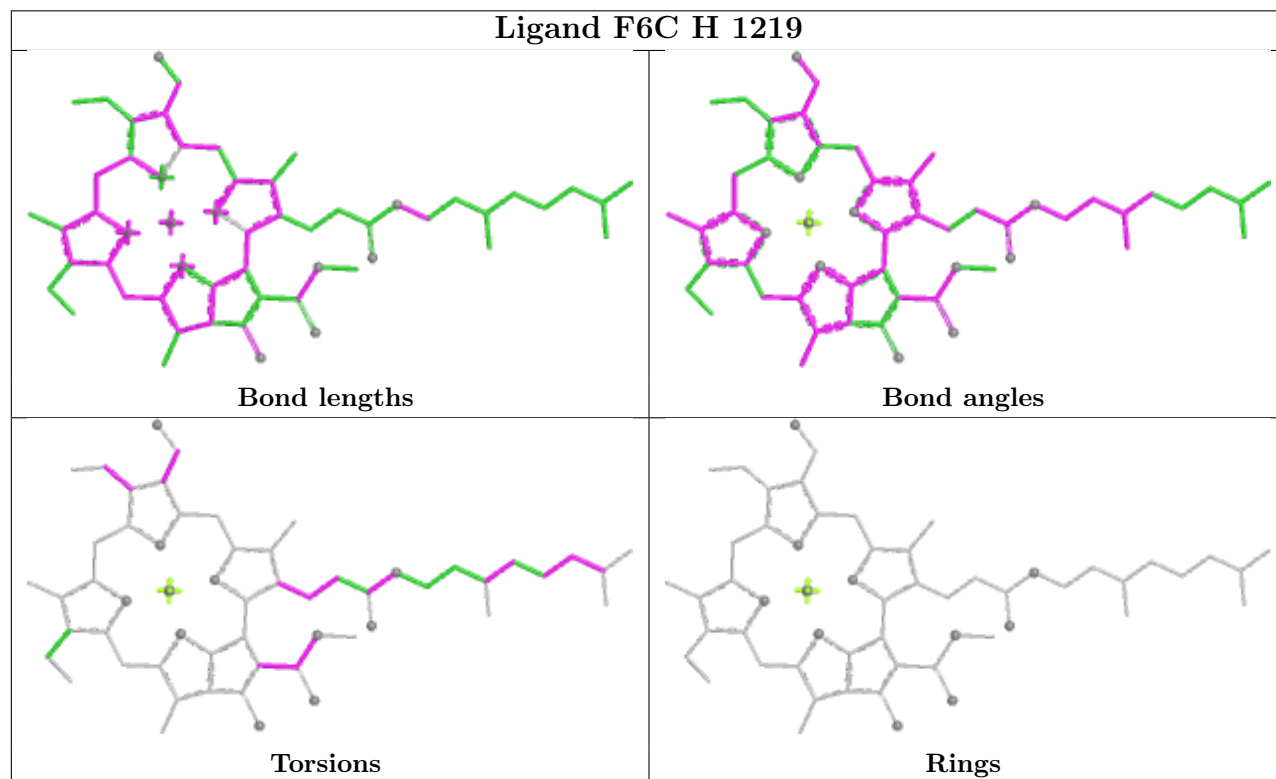
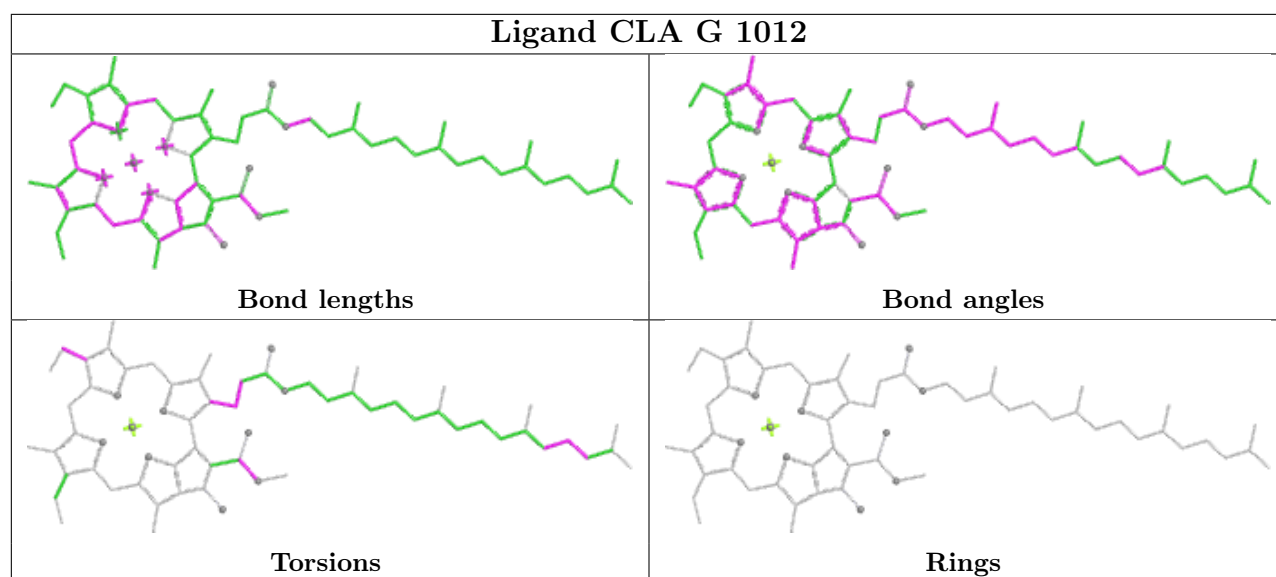


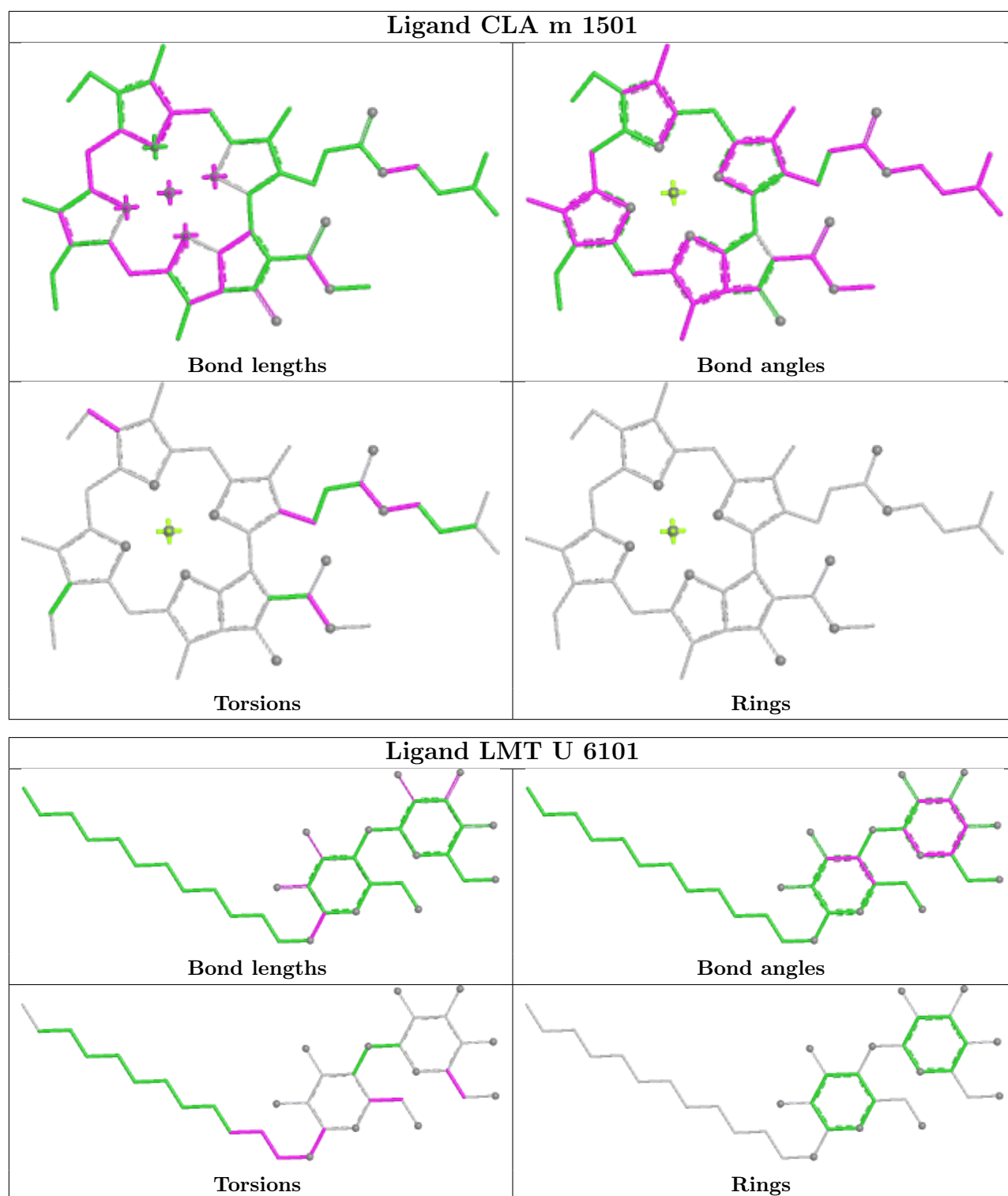


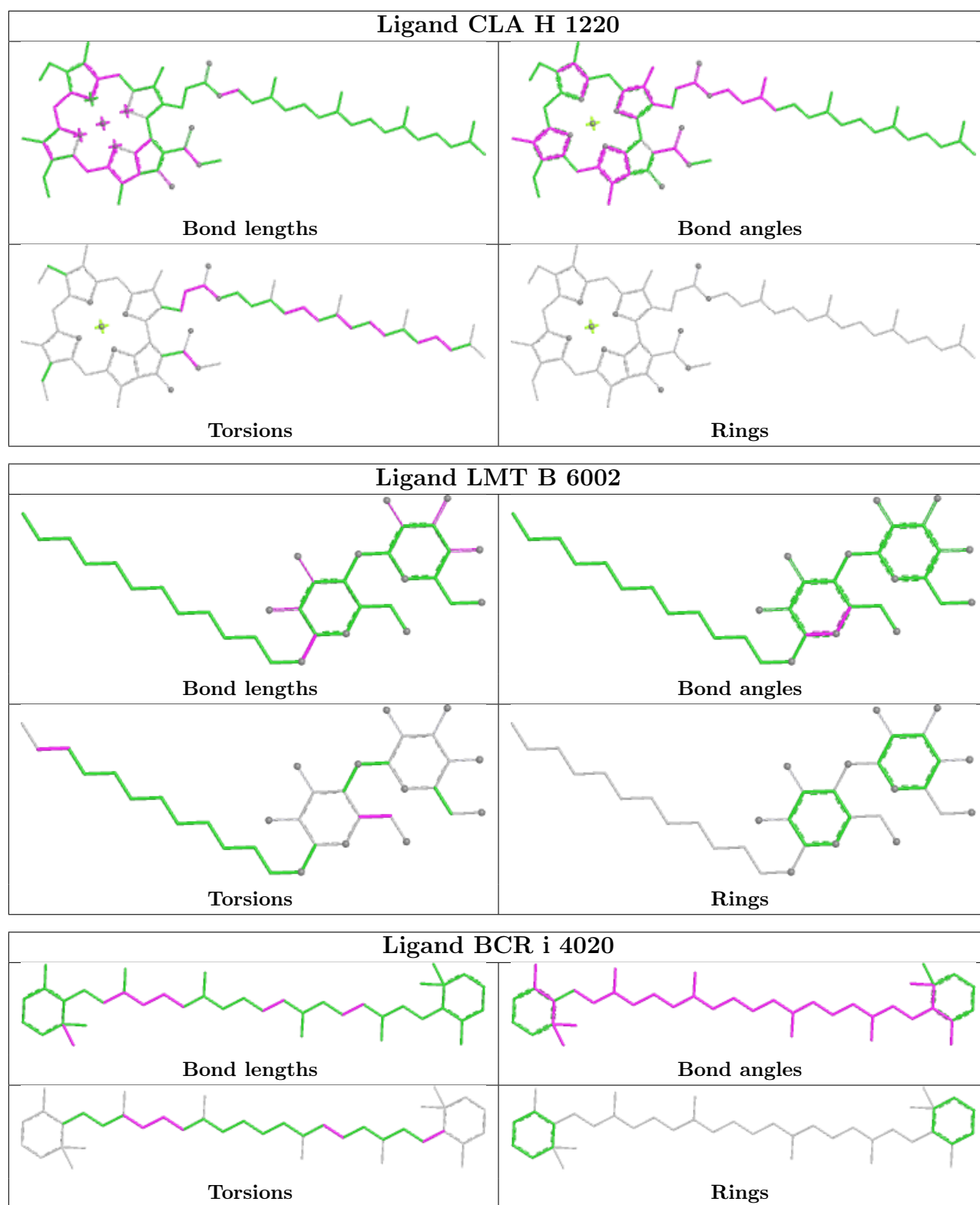
Ligand CLA G 1139

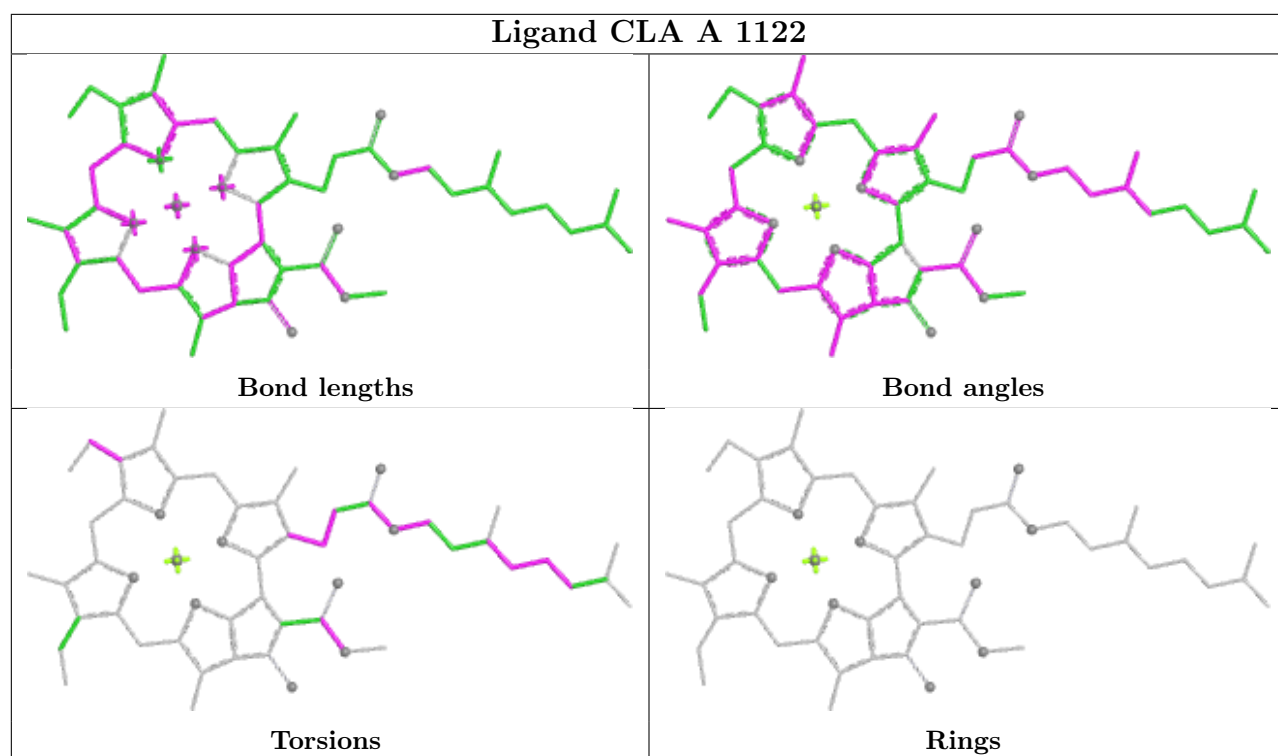


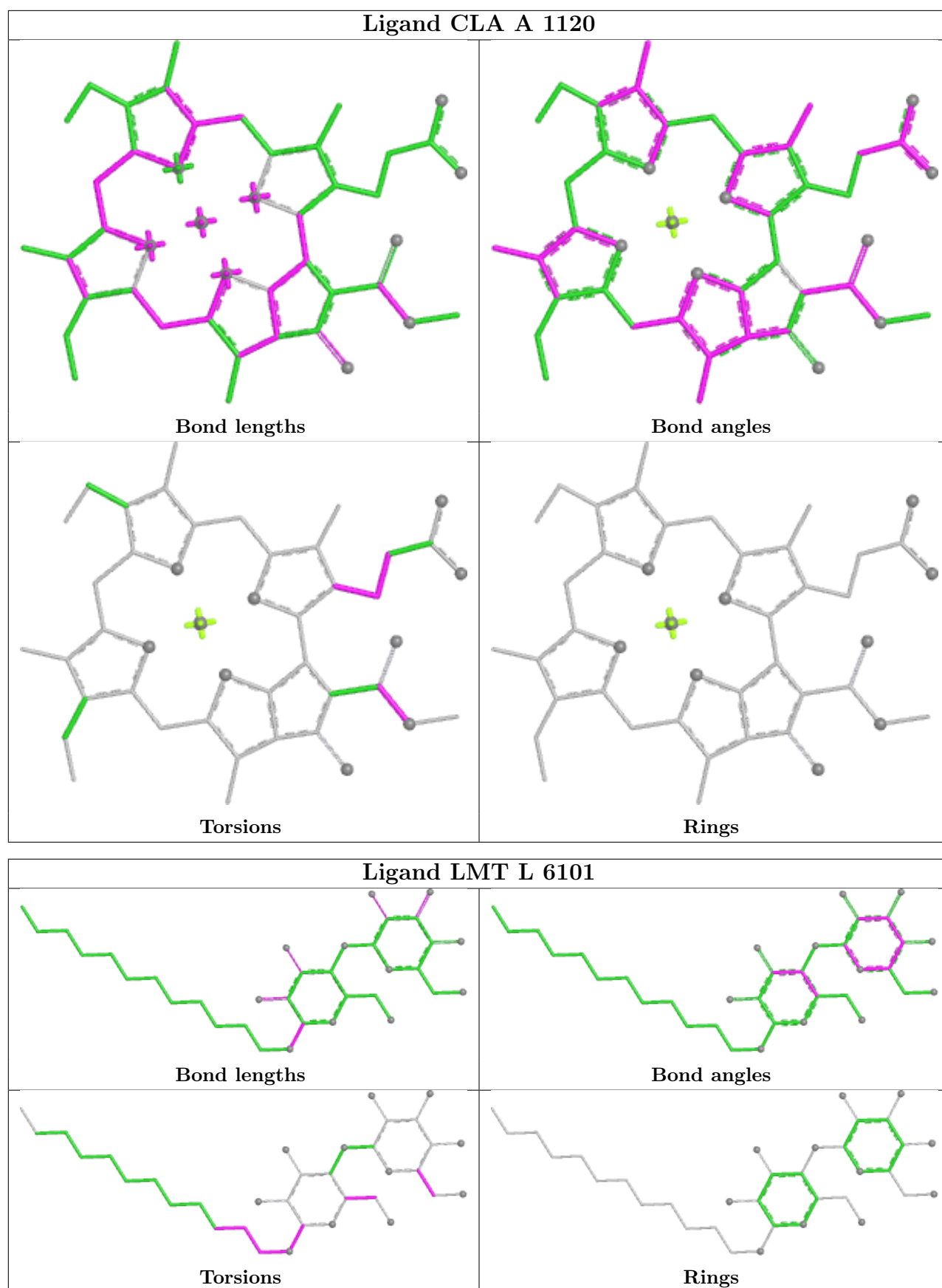


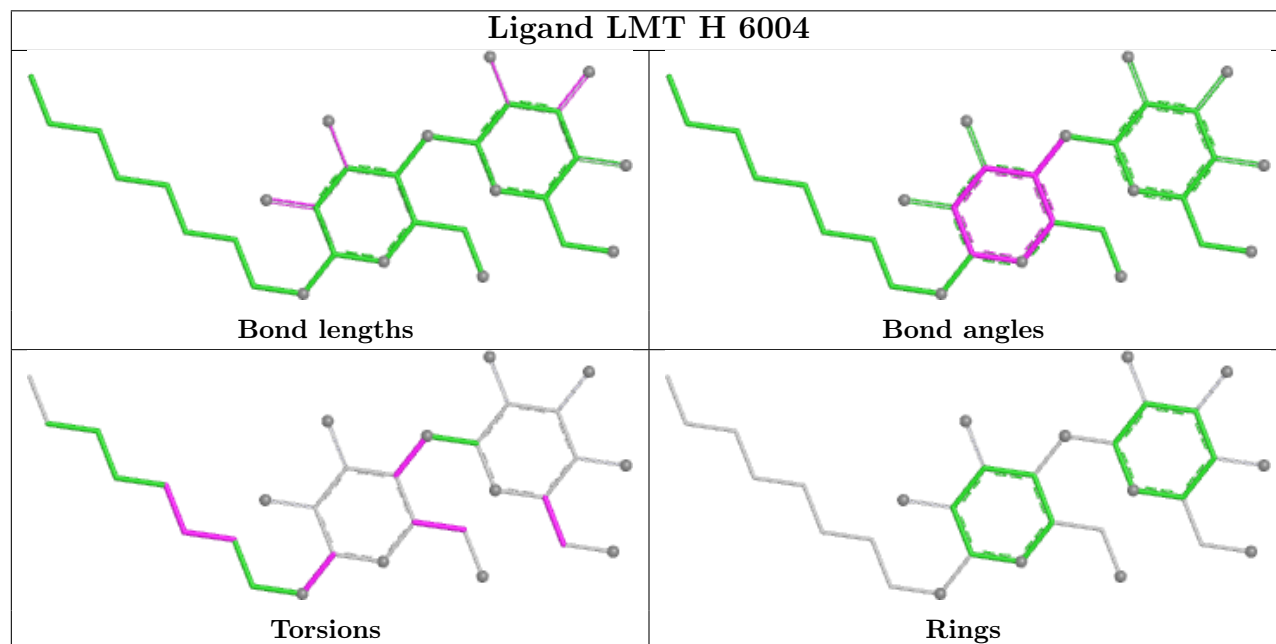
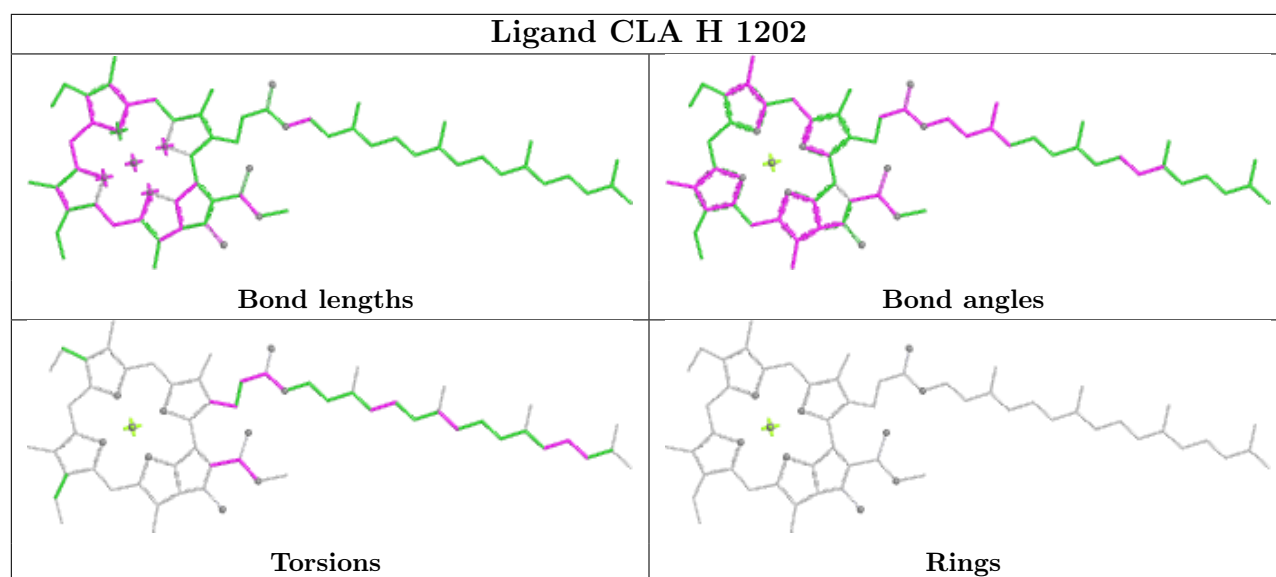




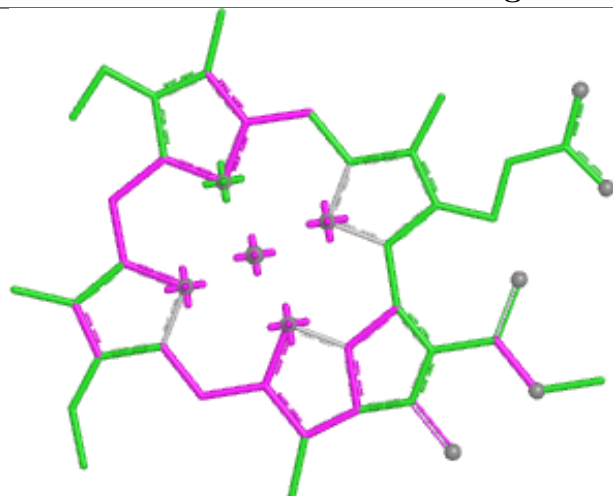




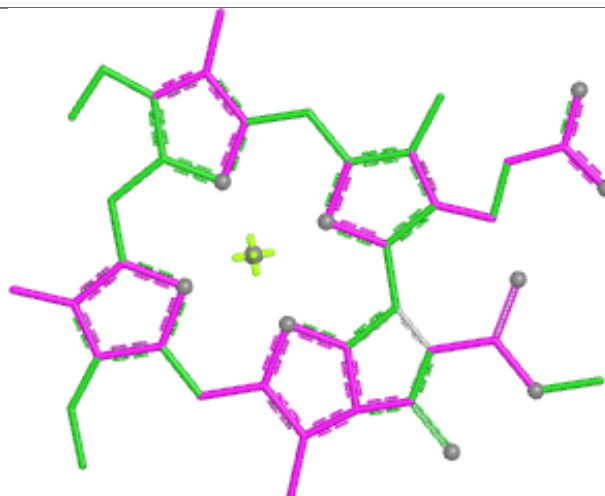




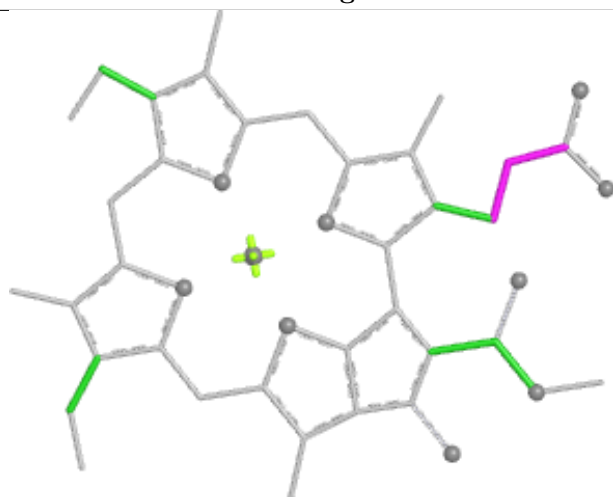
Ligand CLA G 1110



Bond lengths



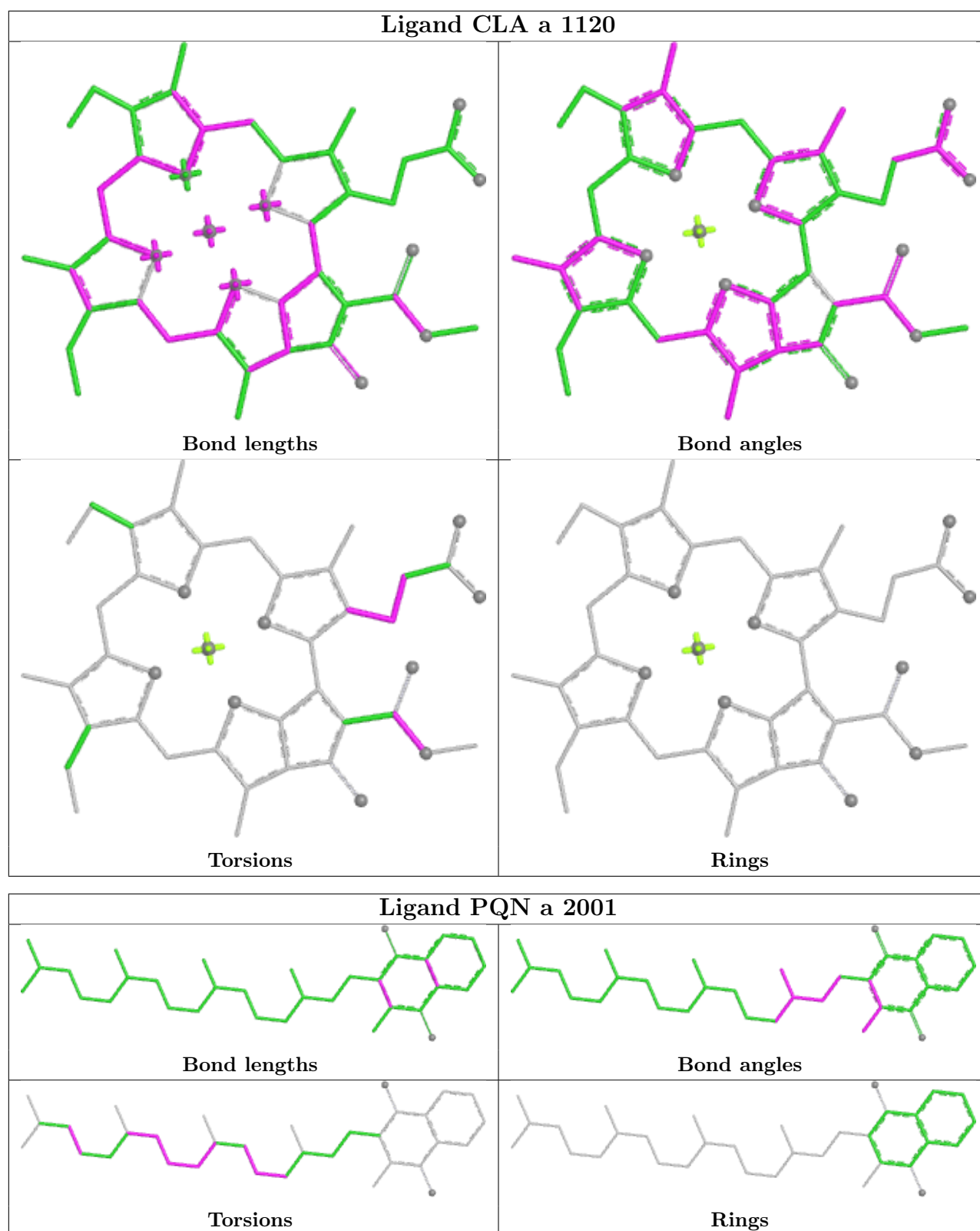
Bond angles

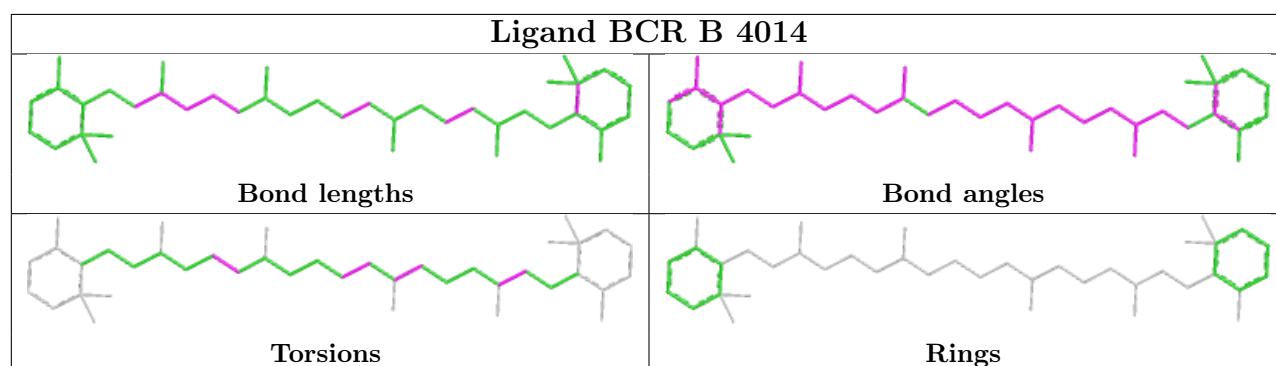
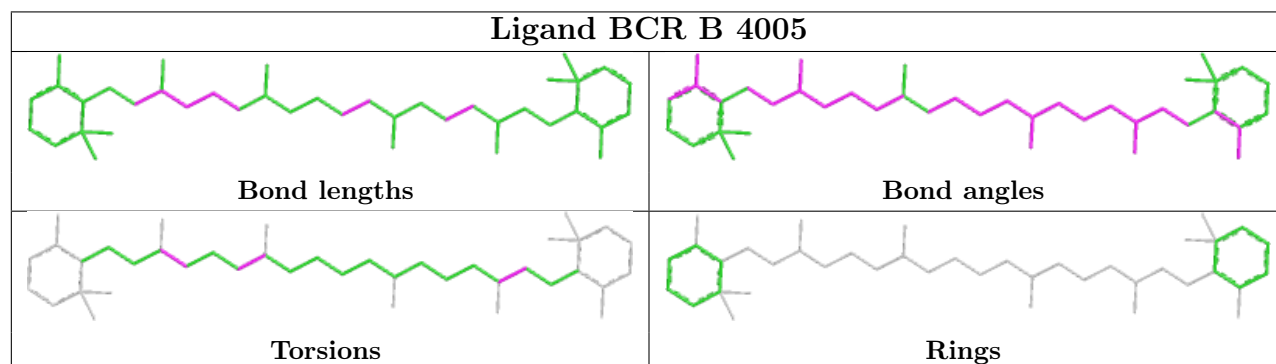
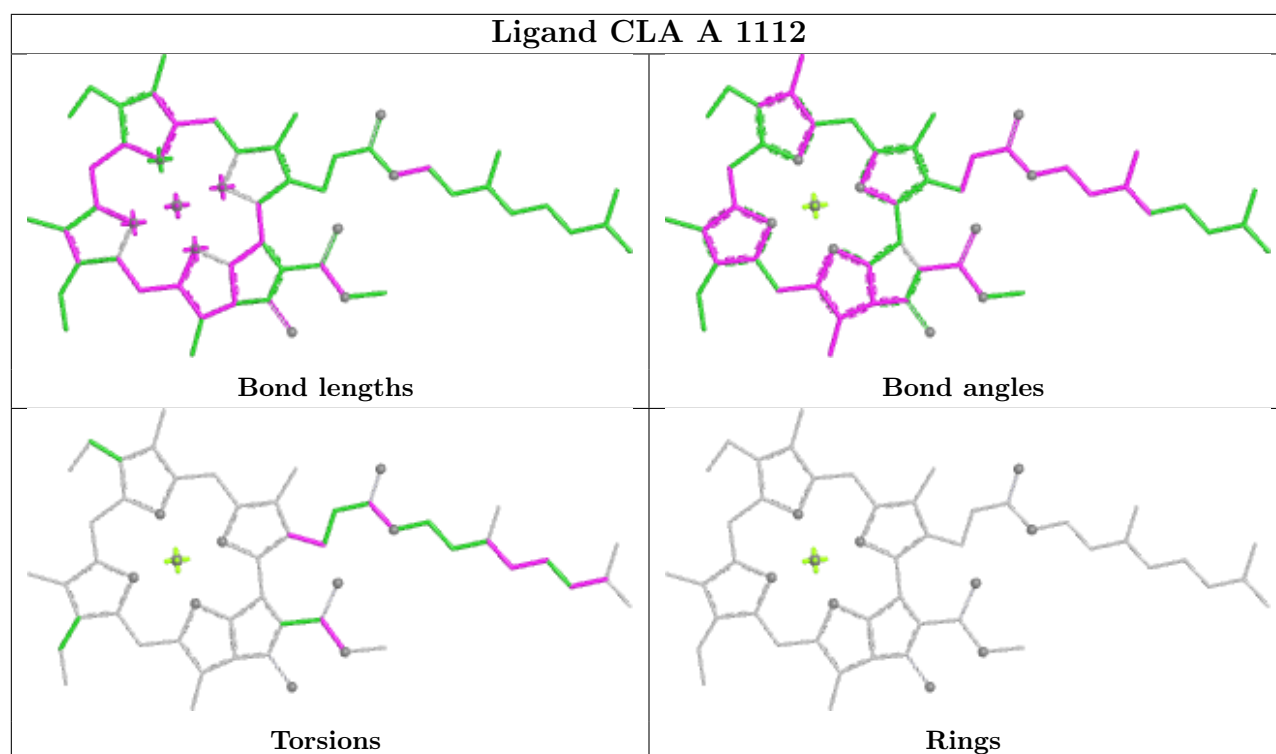


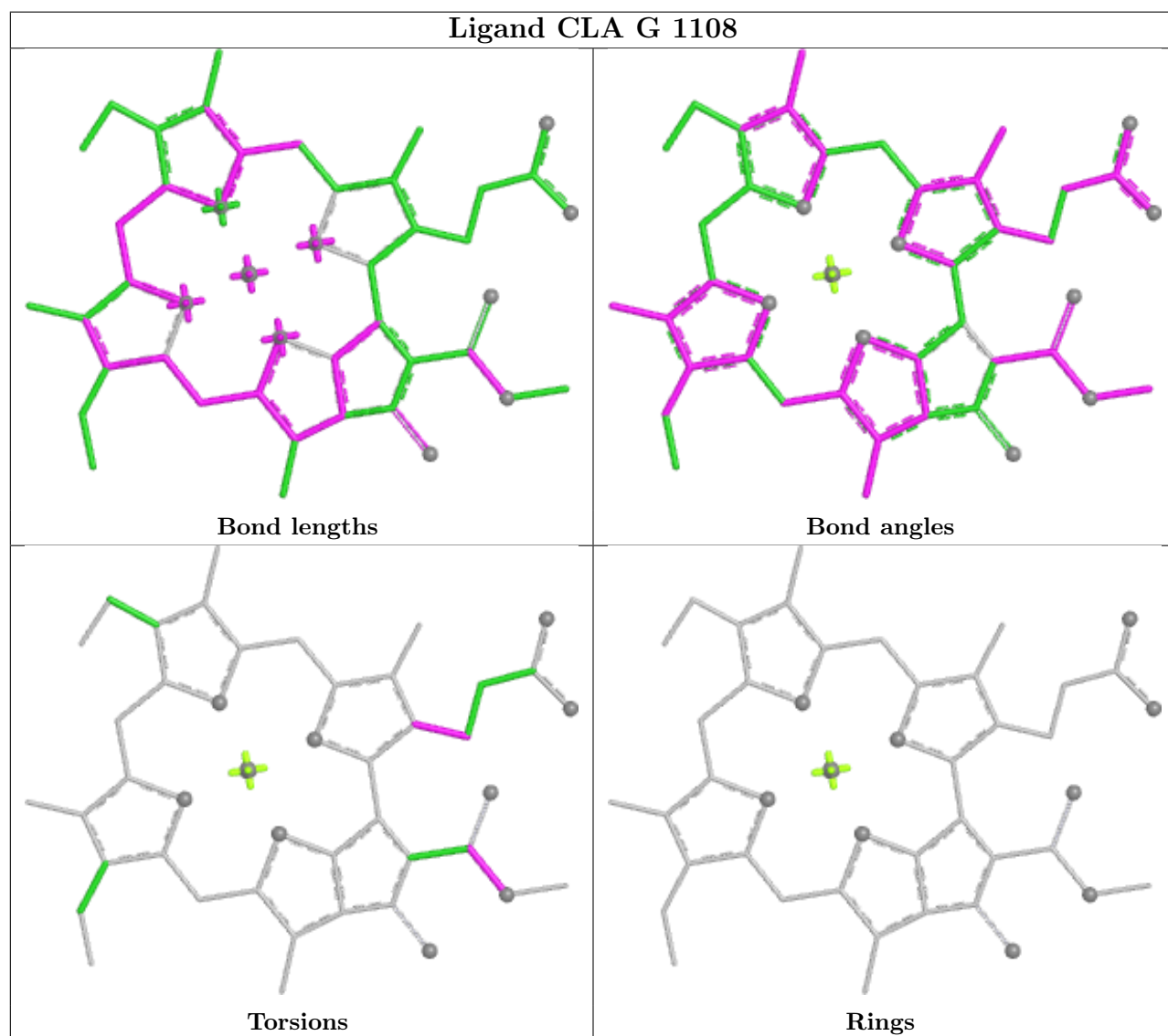
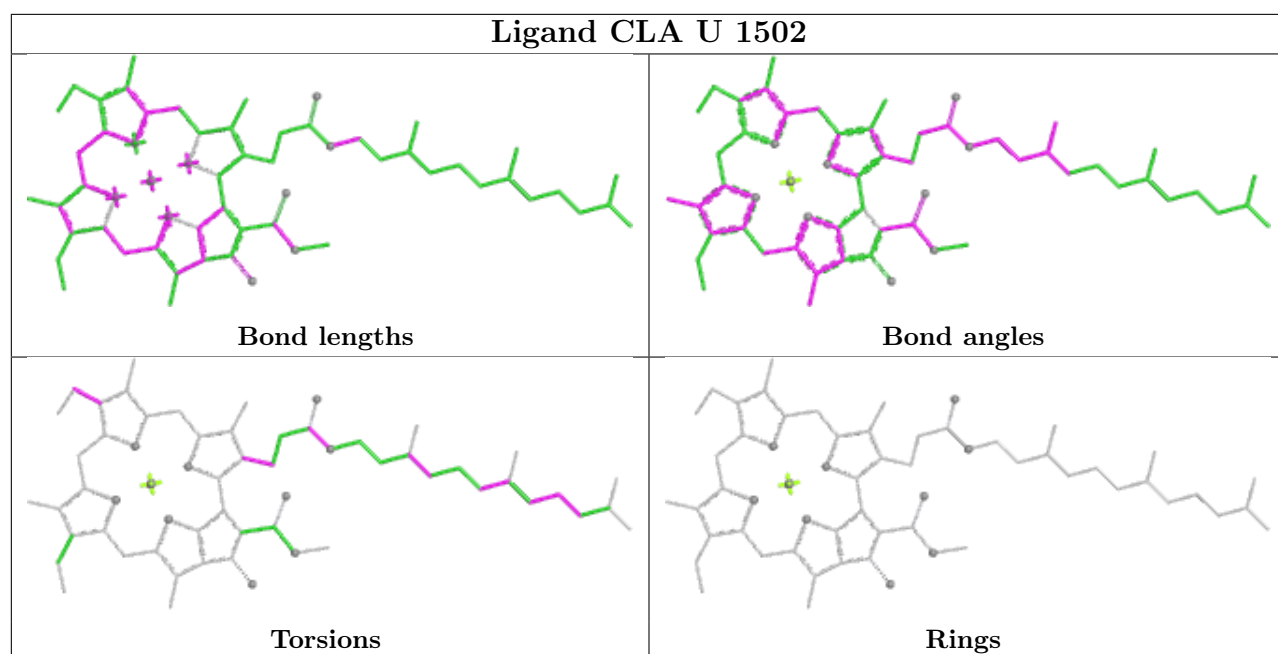
Torsions

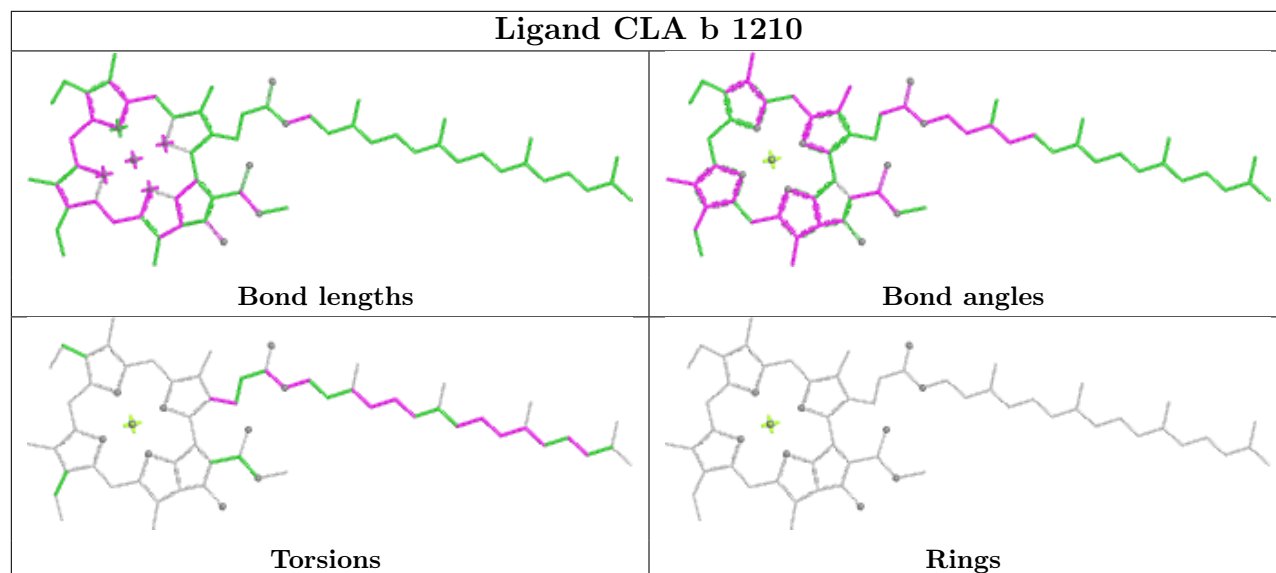
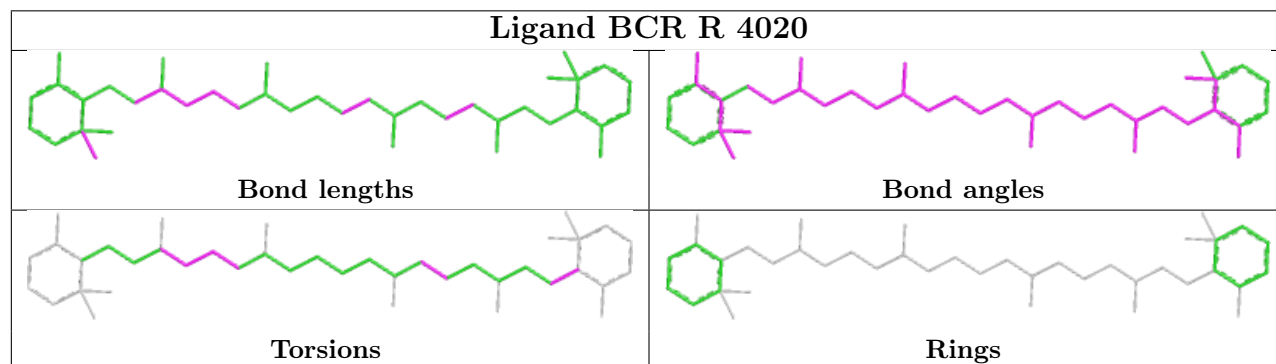
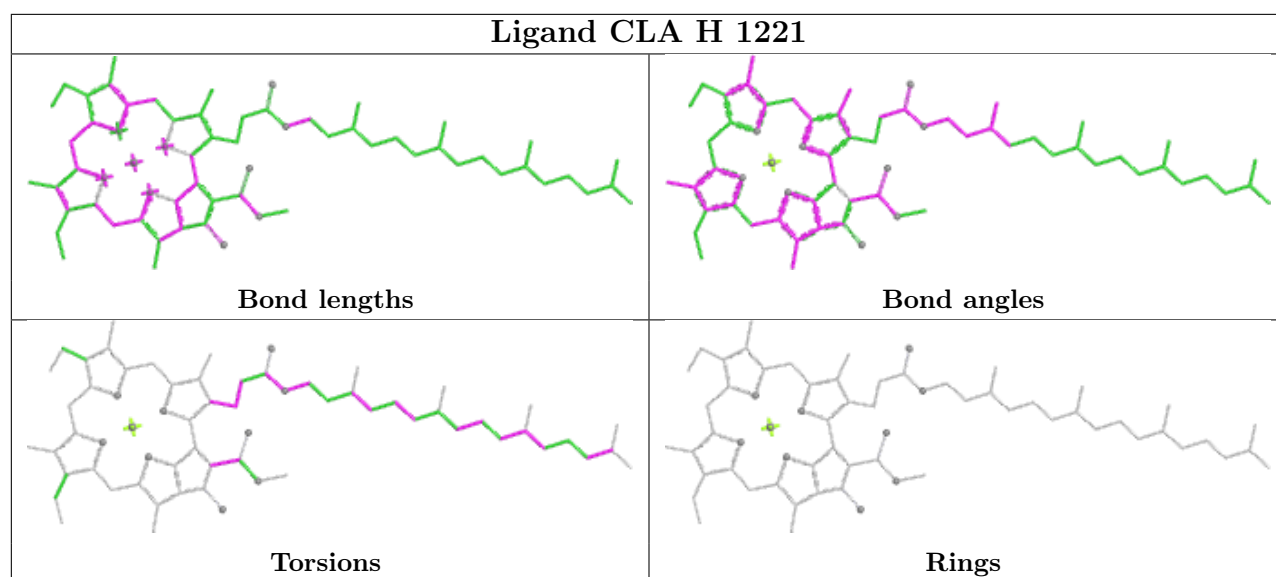


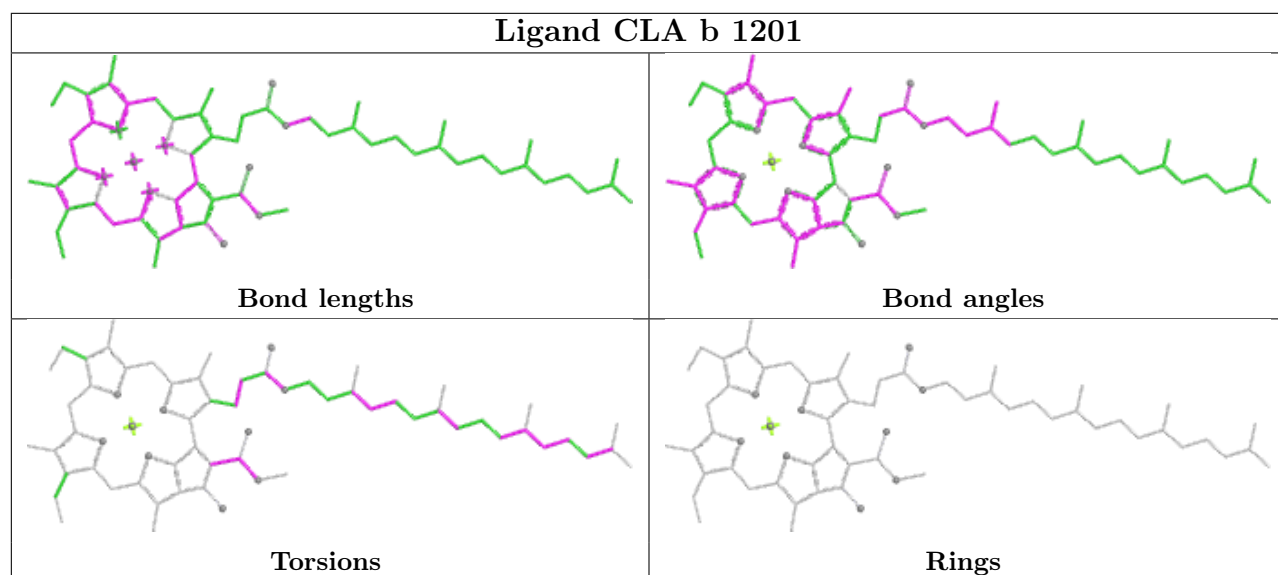
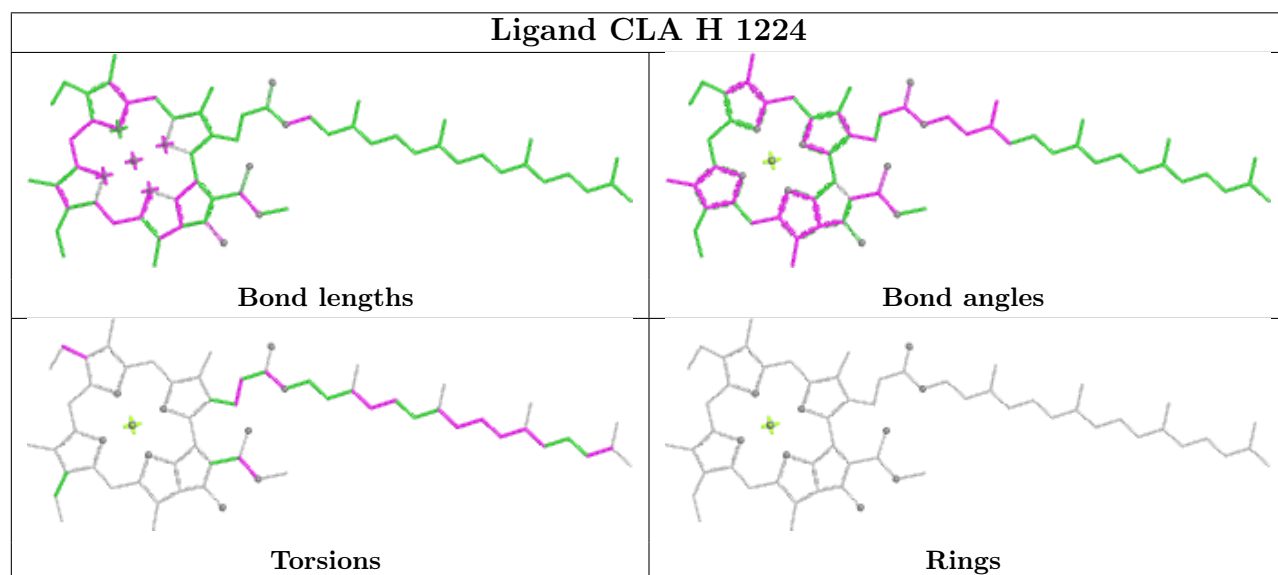
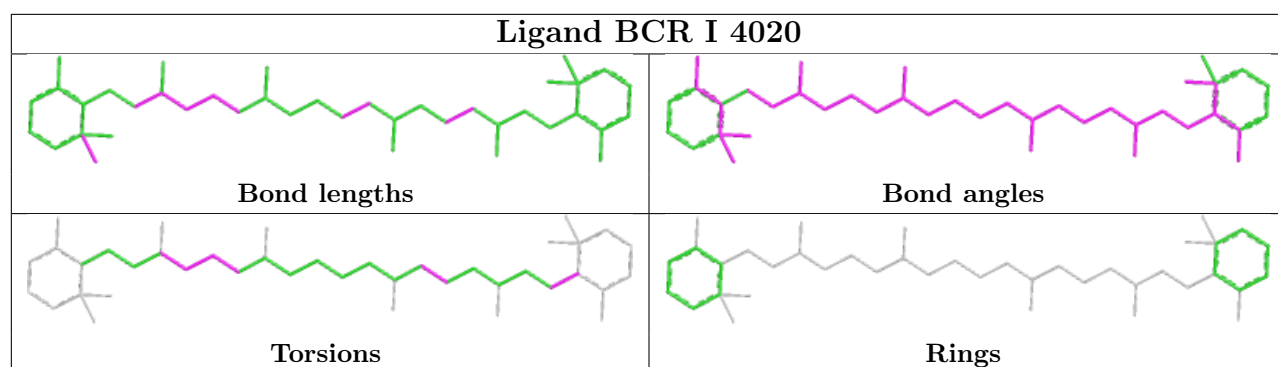
Rings

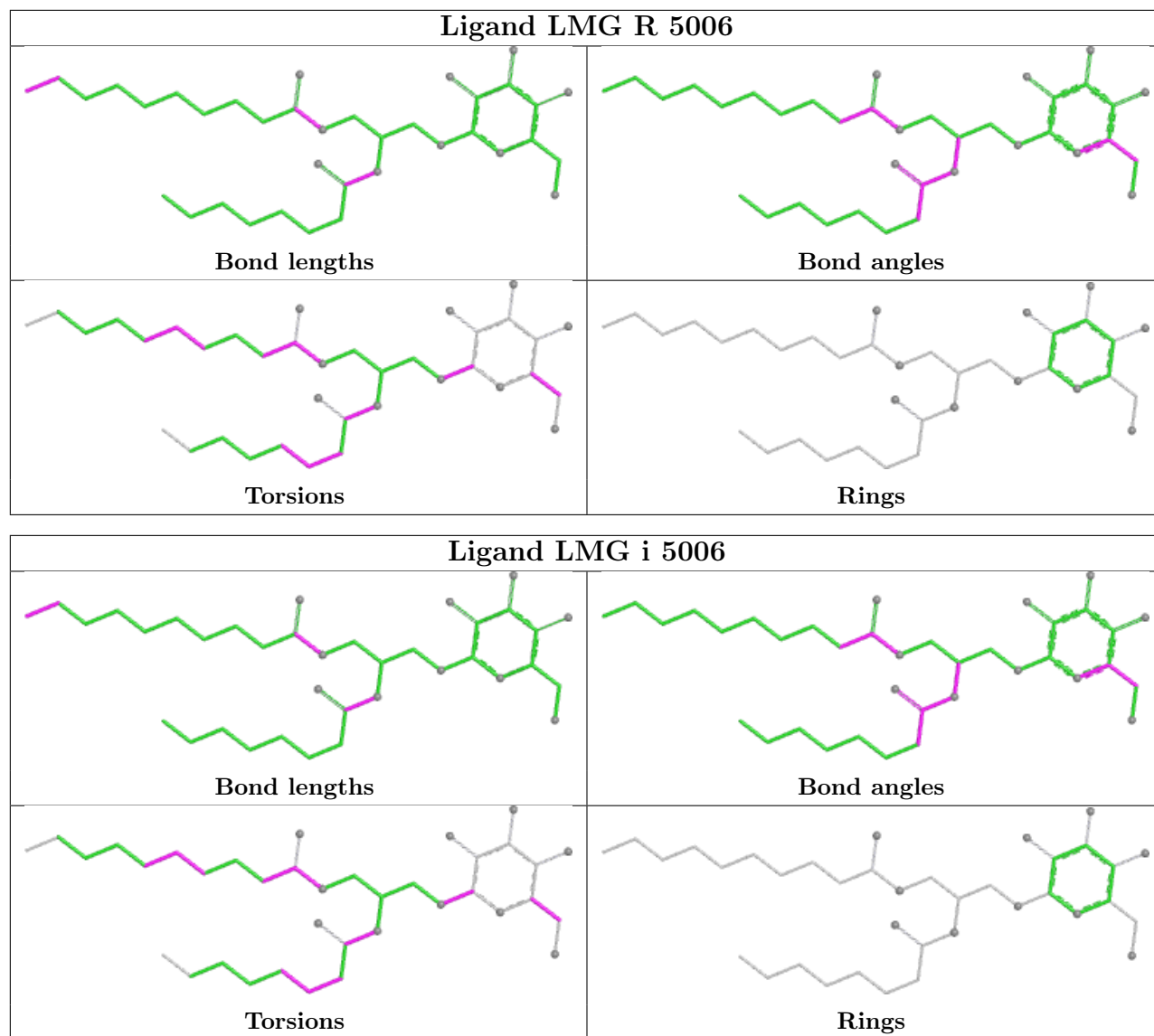


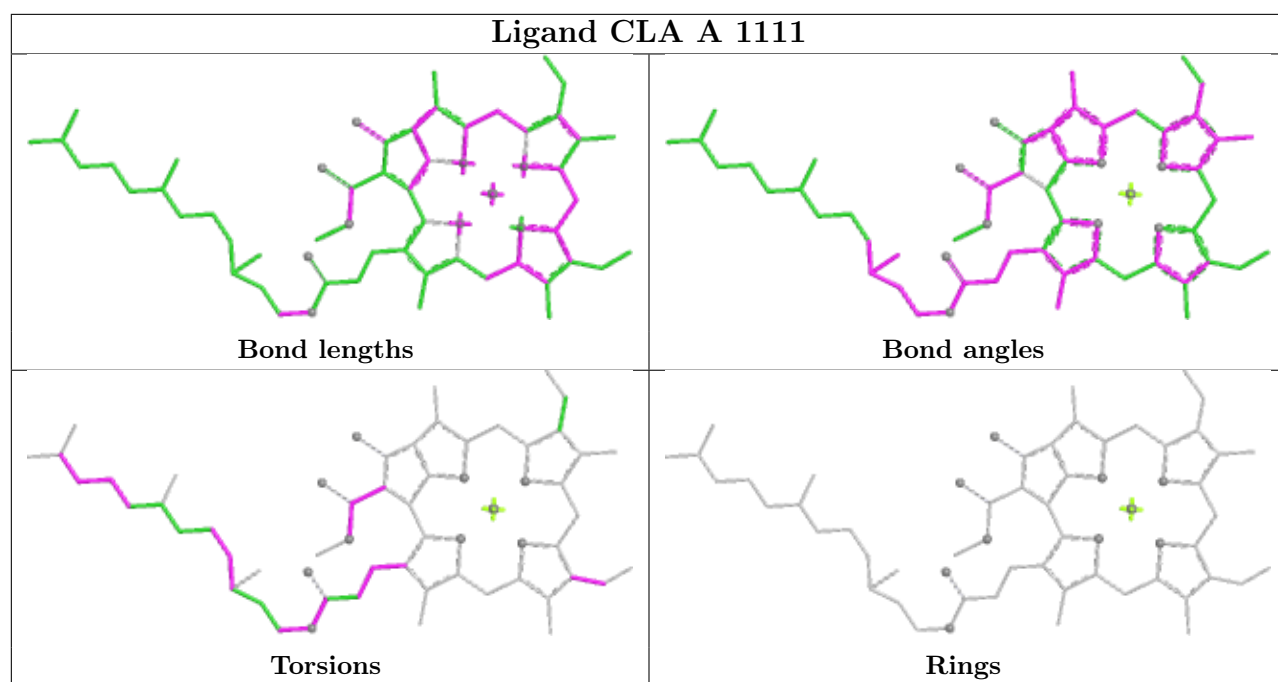




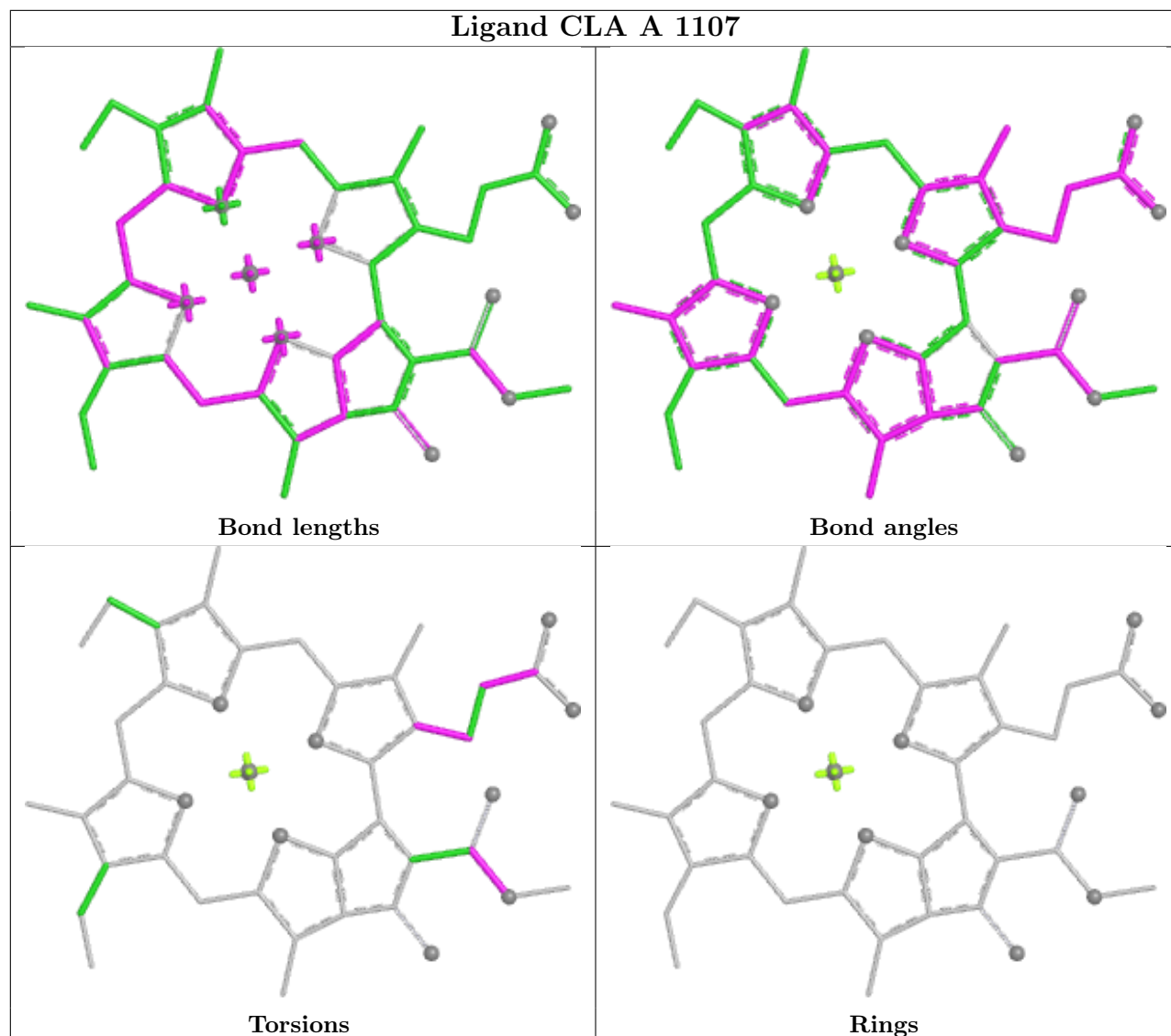




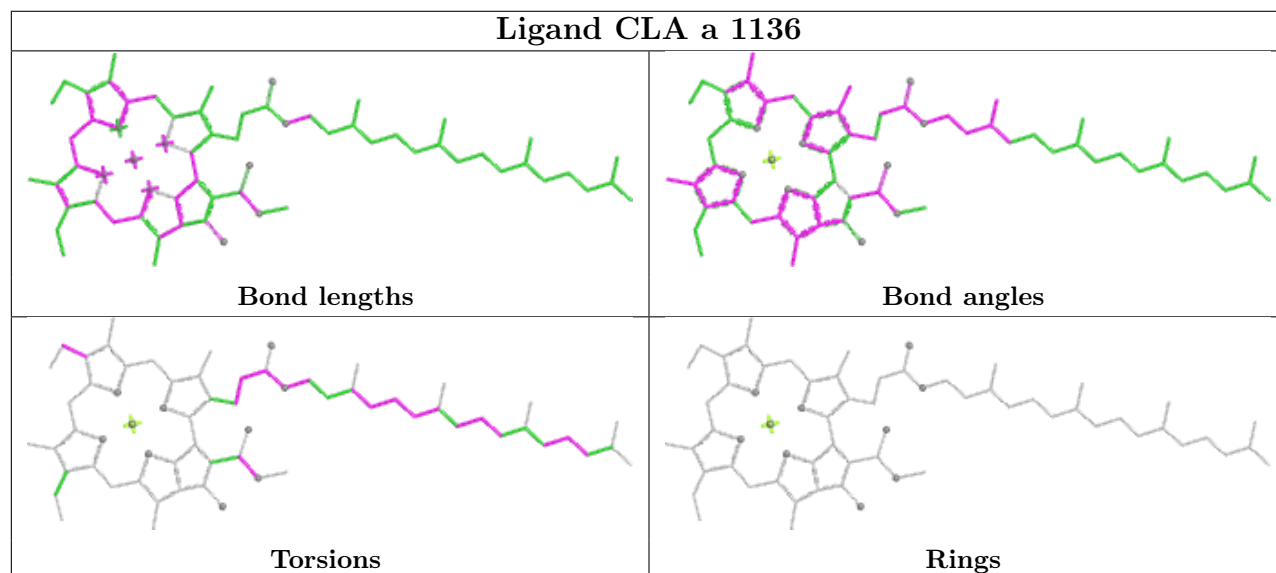


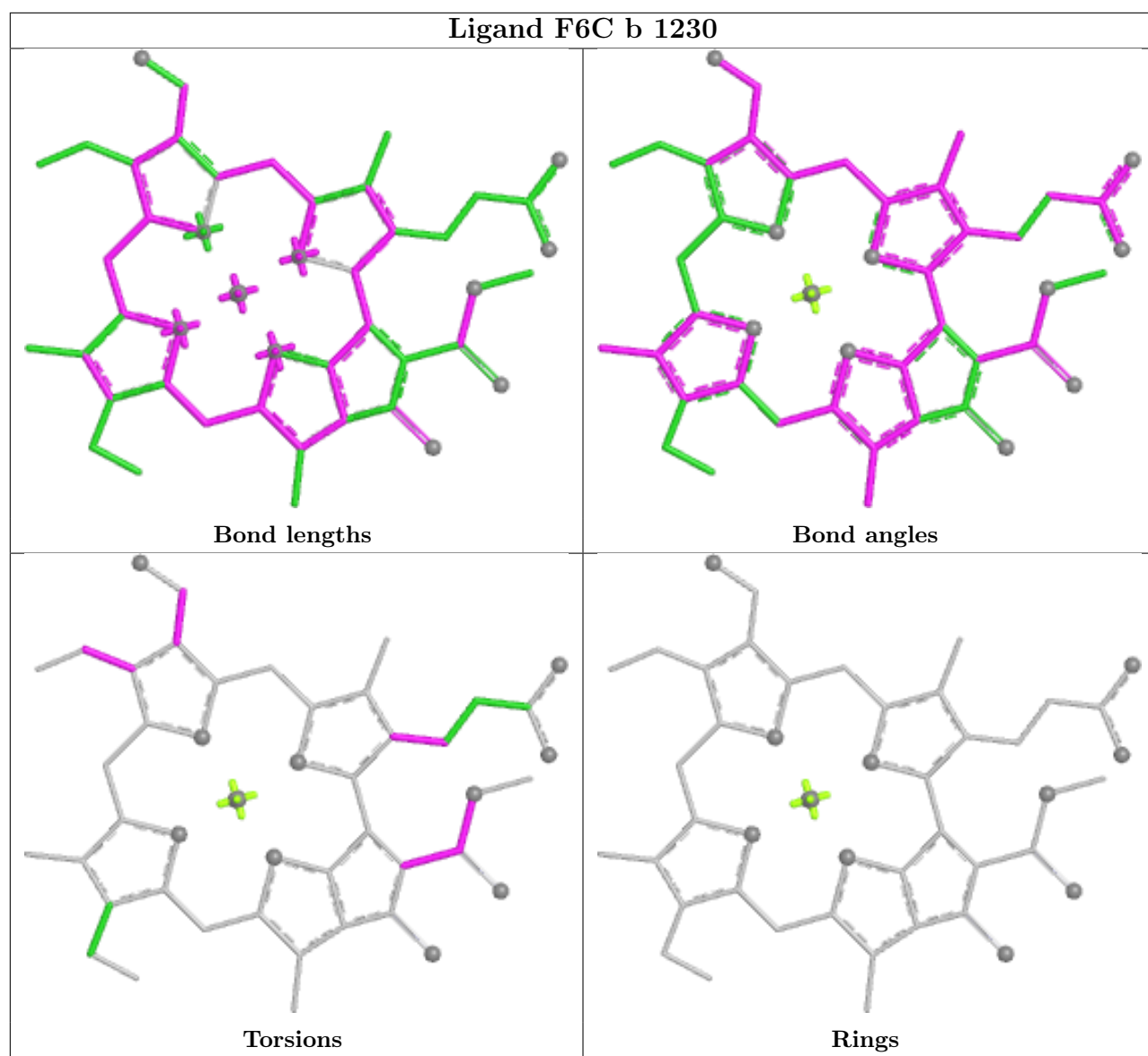


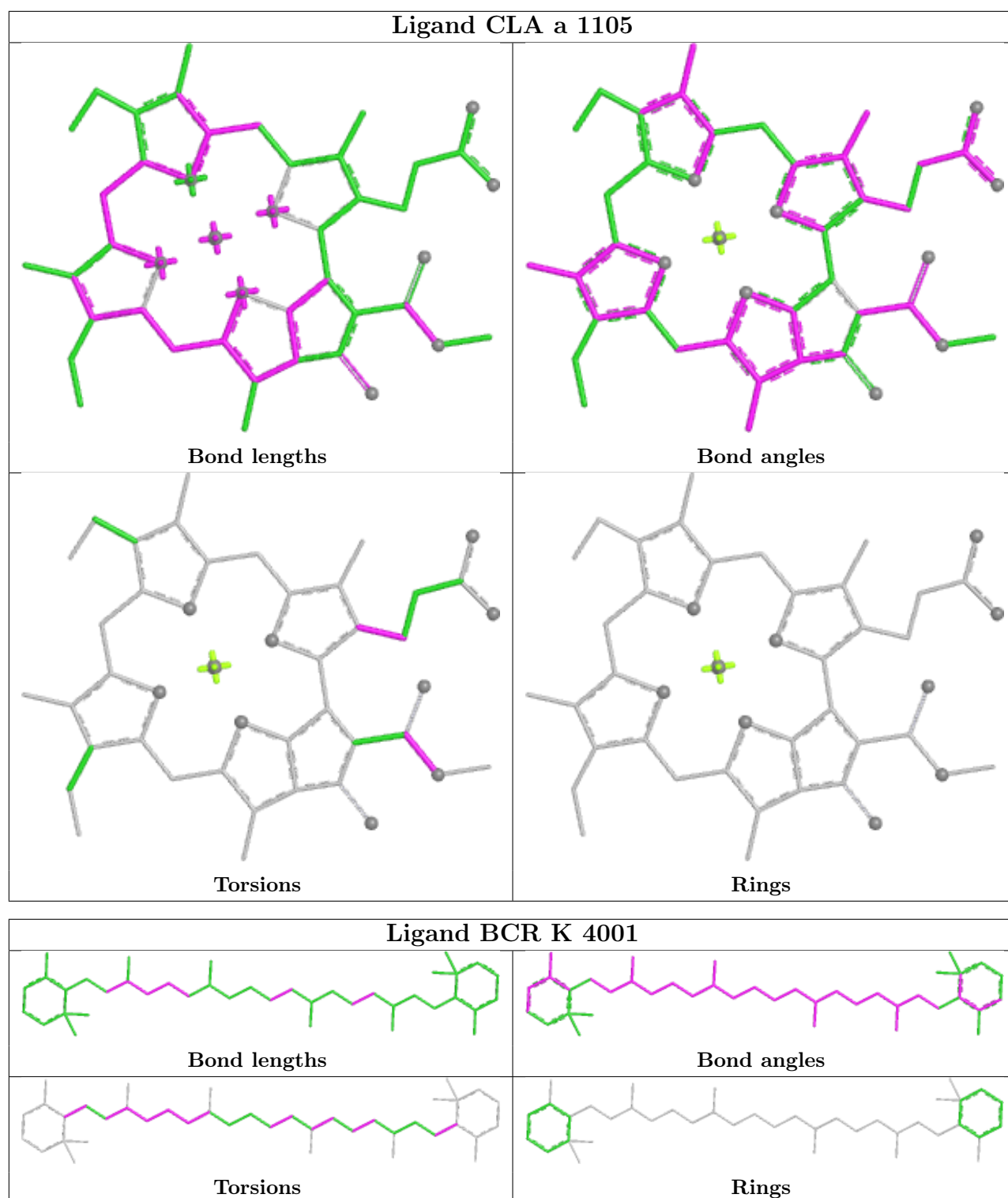
Ligand CLA A 1107

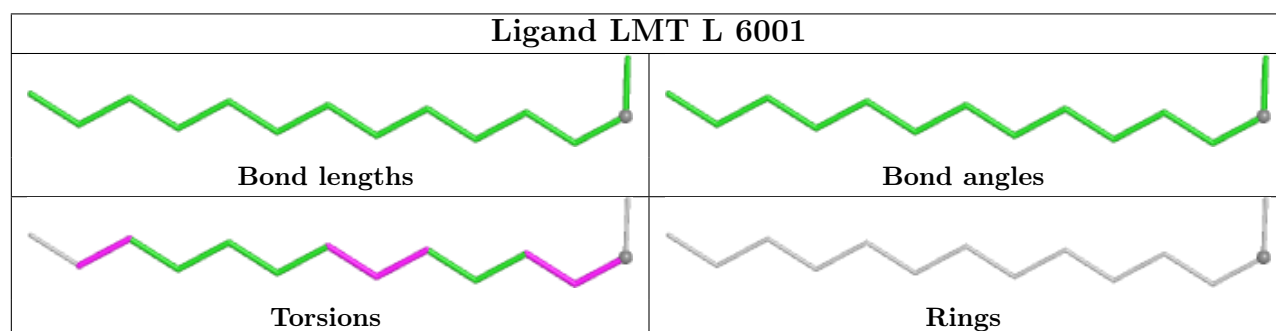
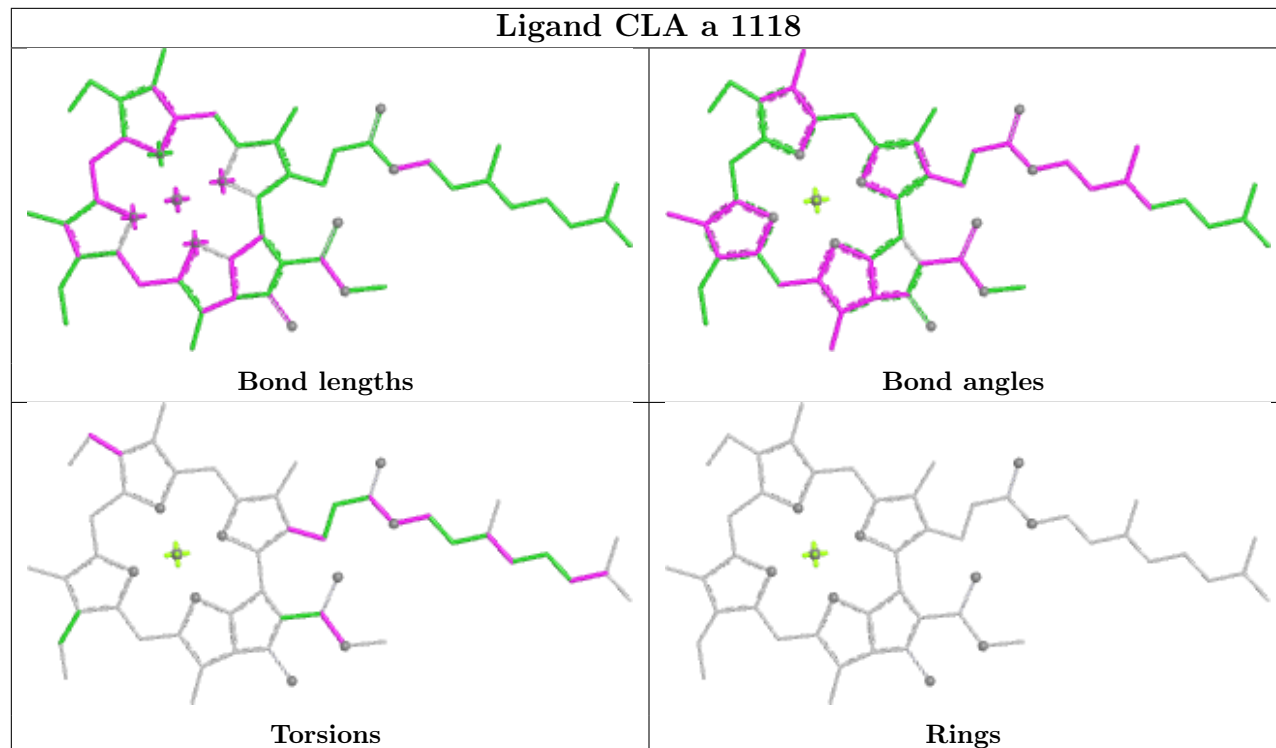
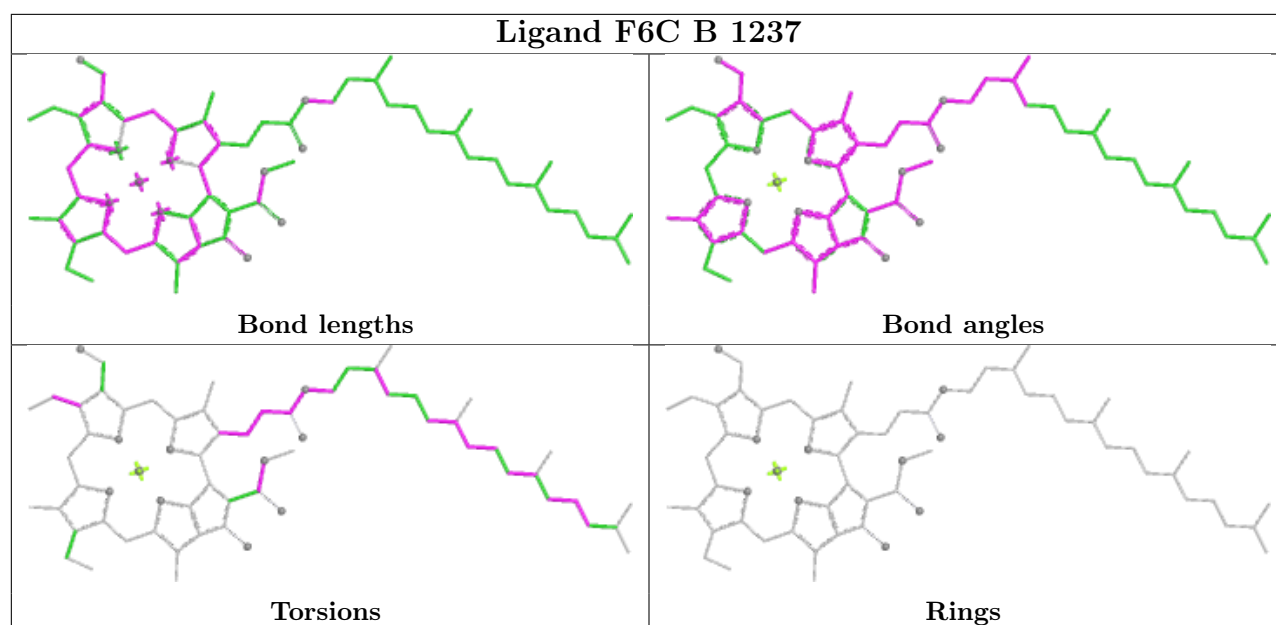


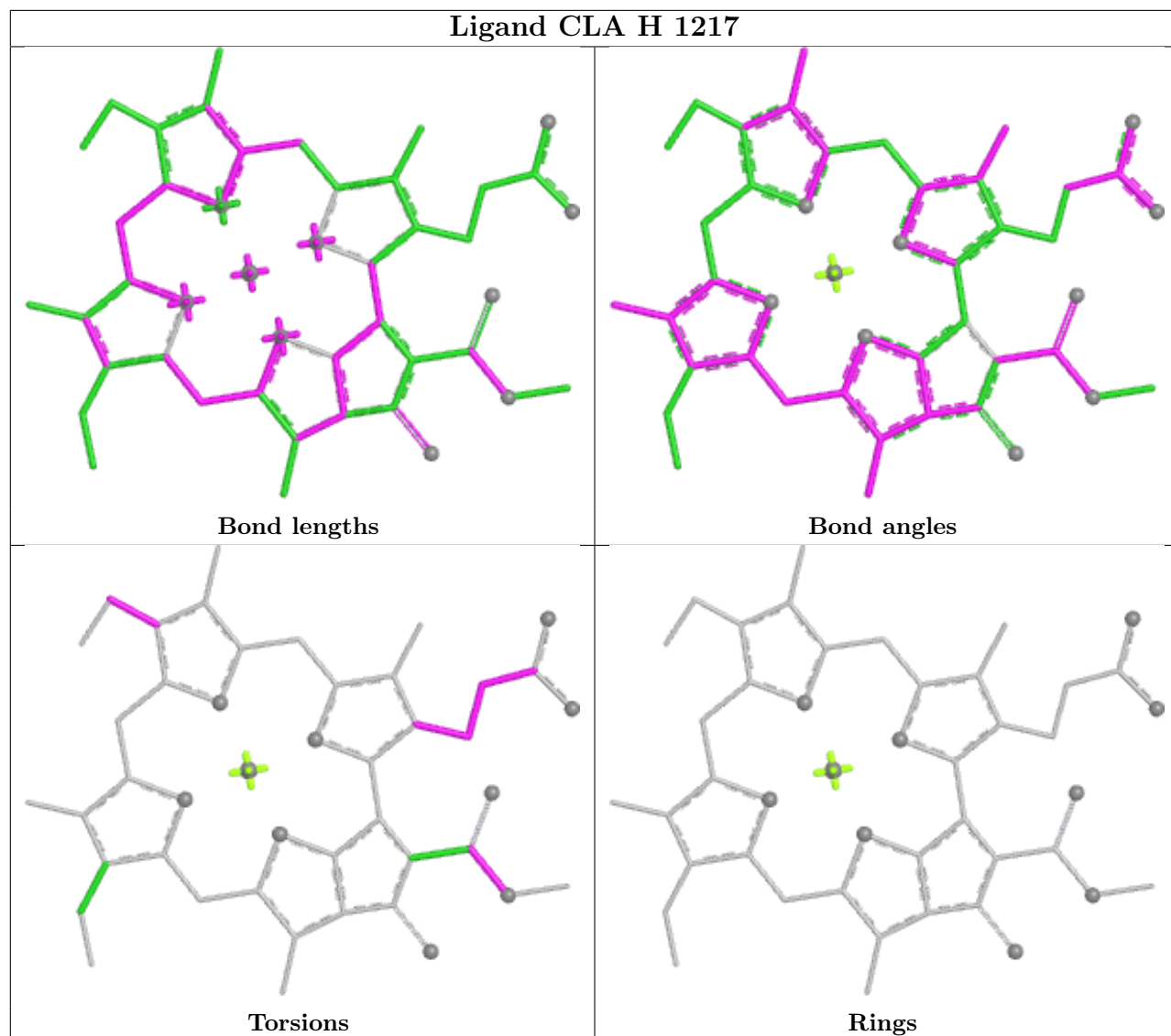
Ligand CLA a 1136

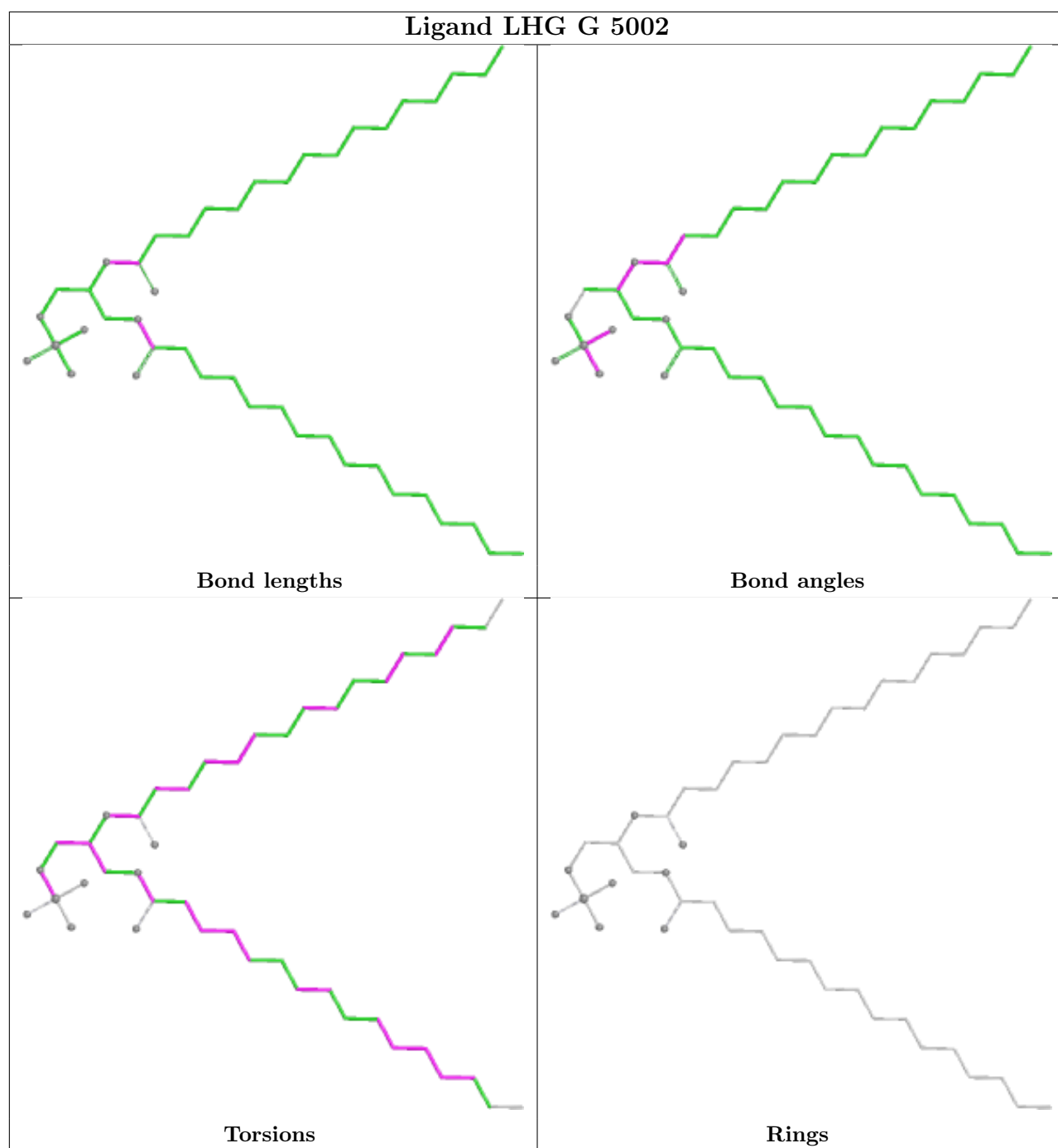


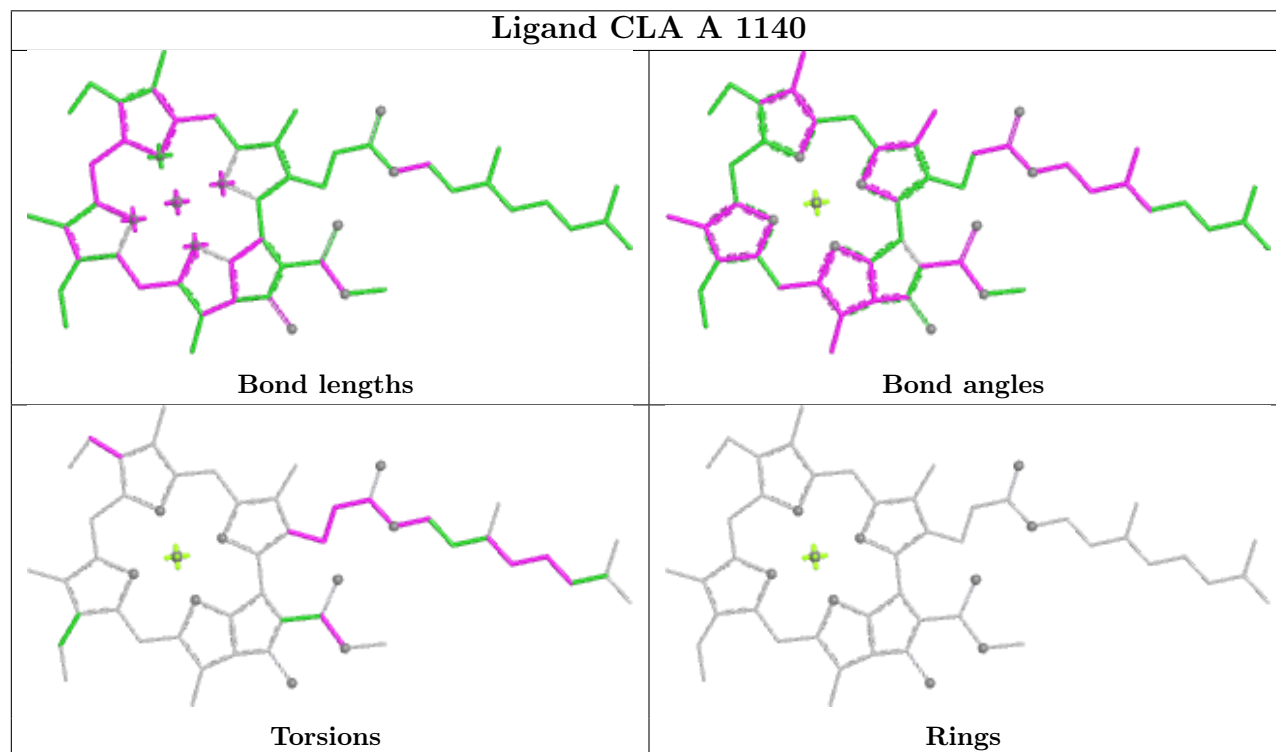
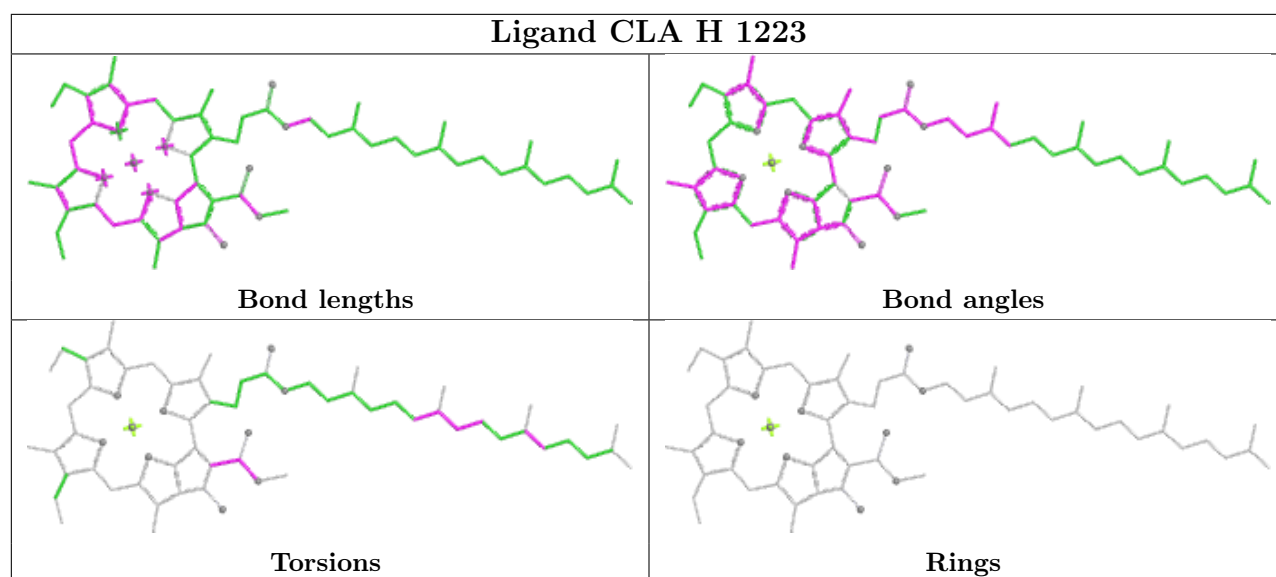


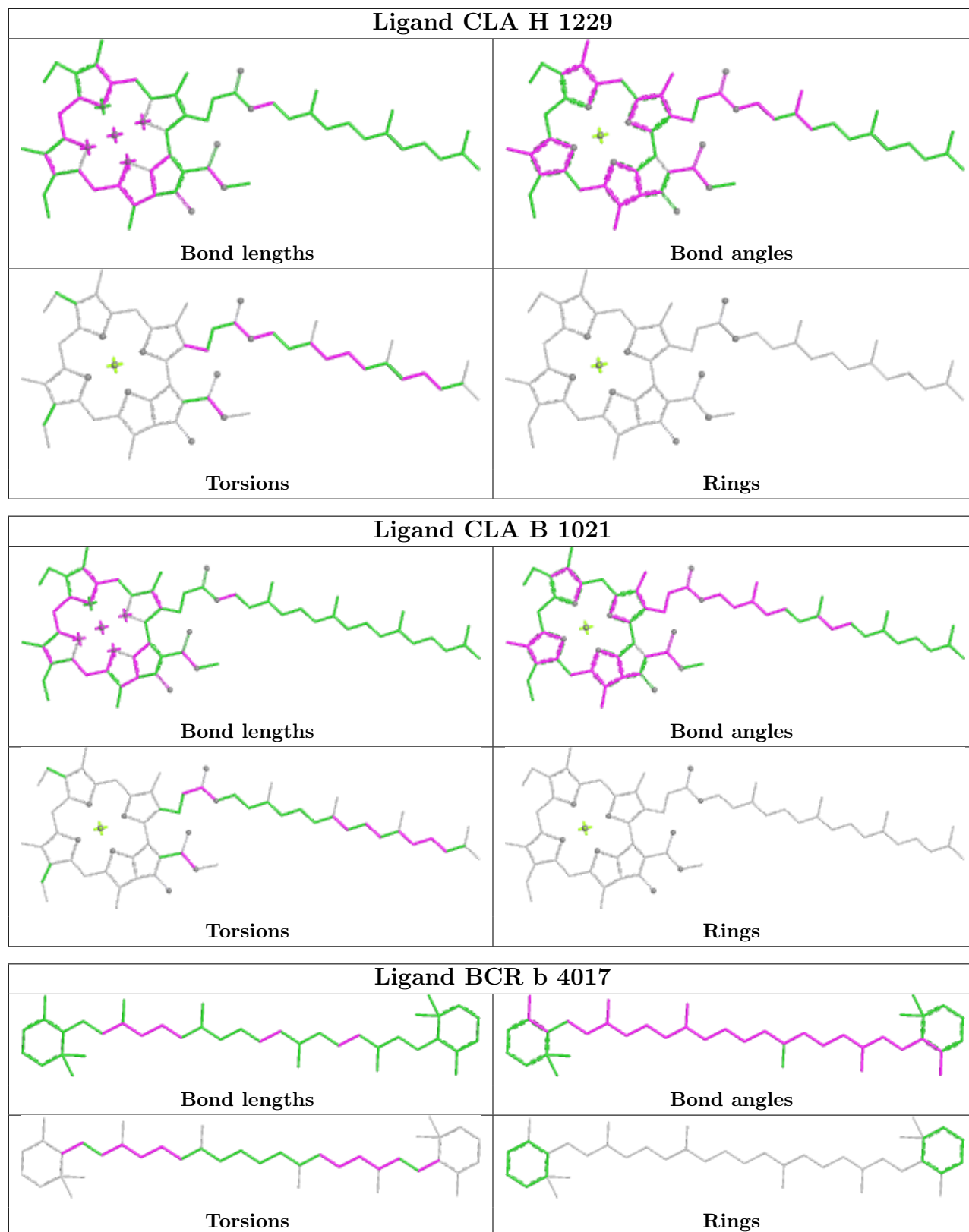


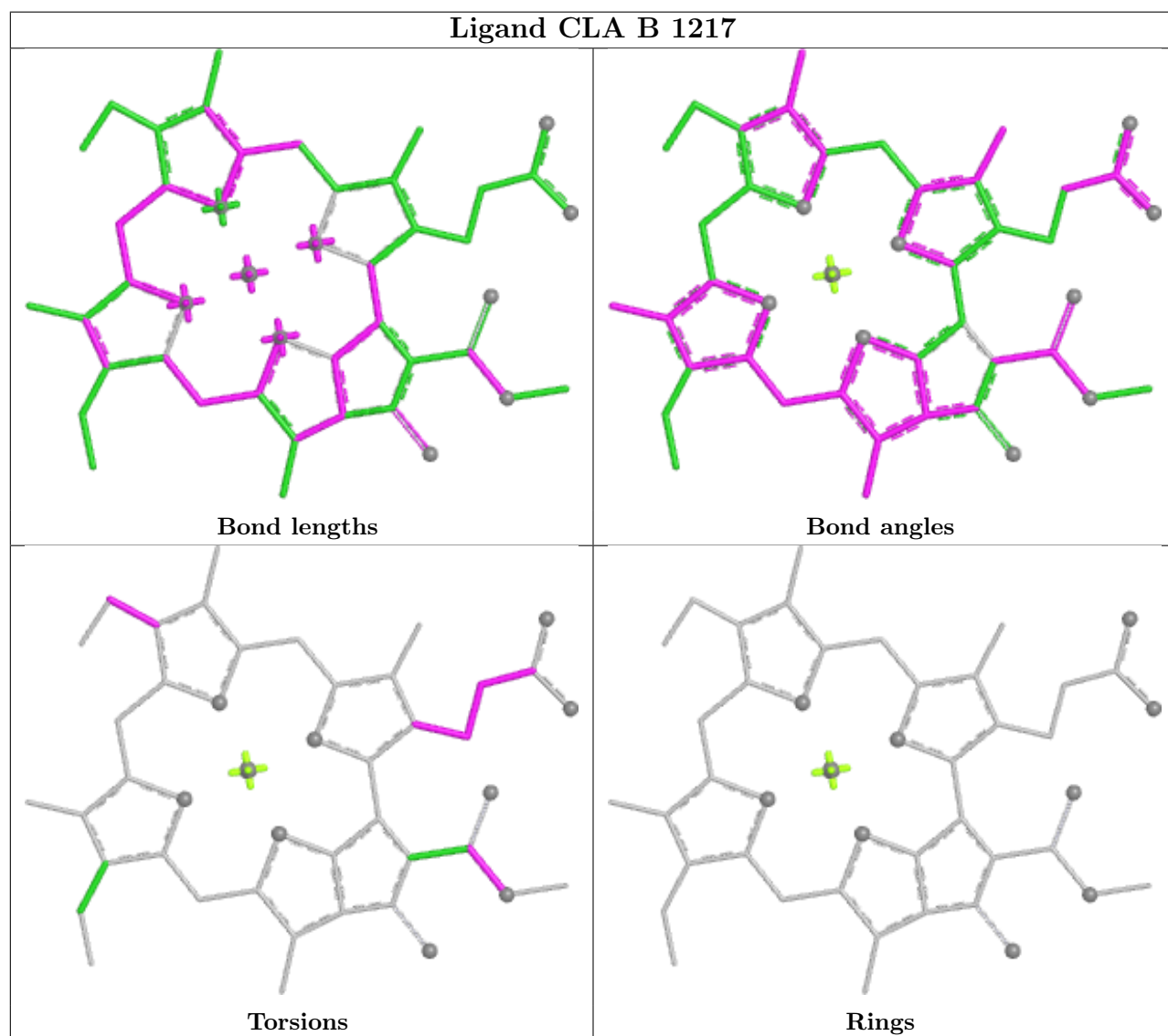
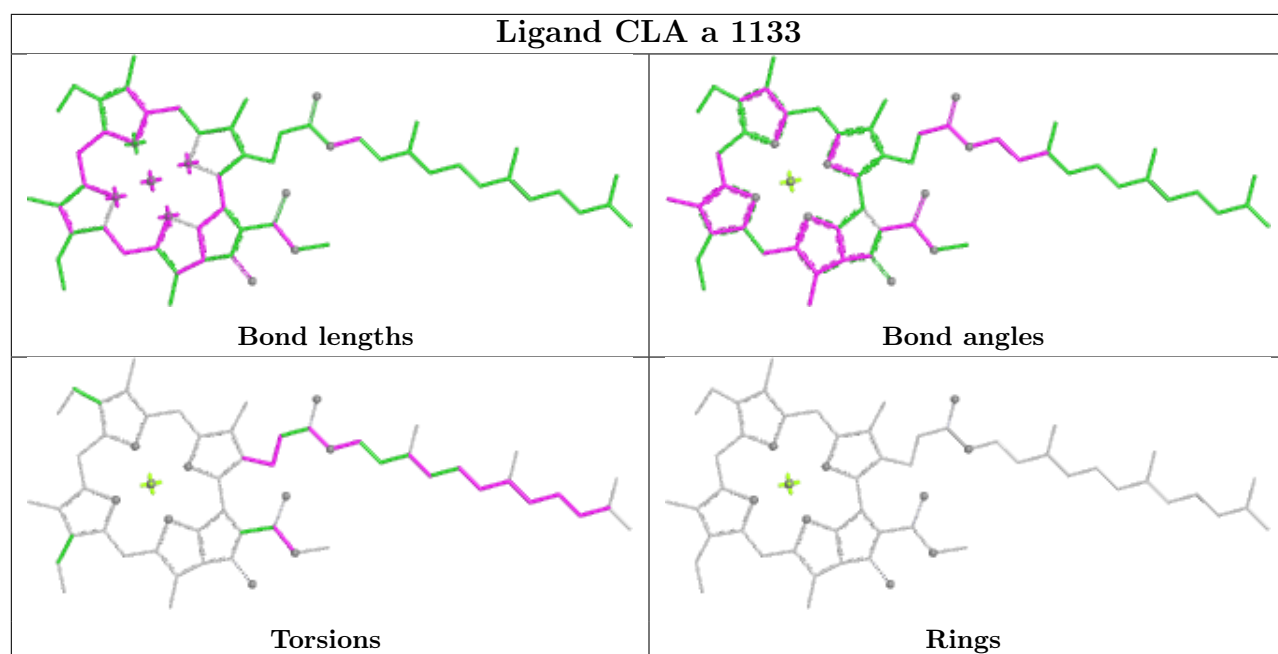


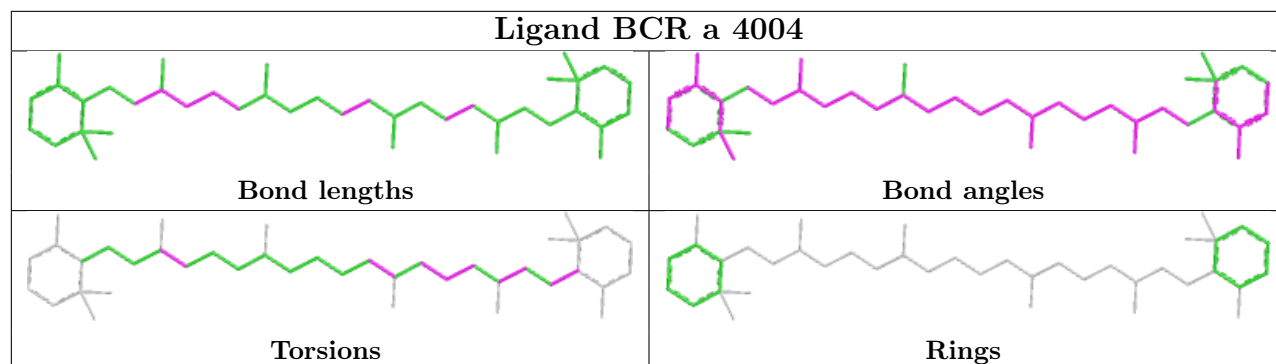
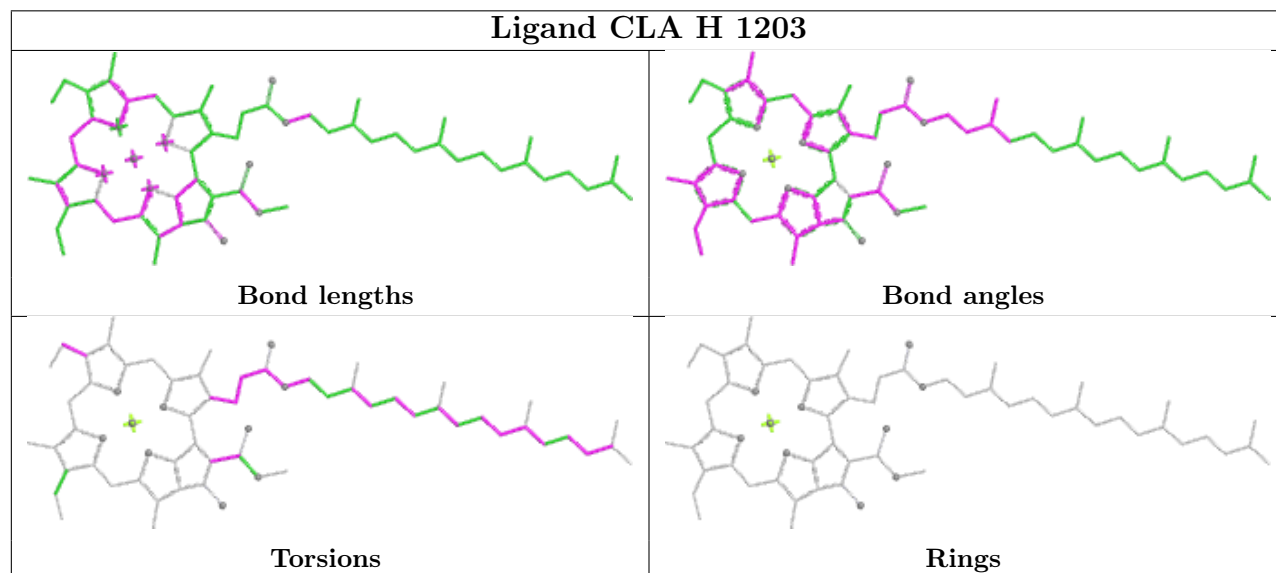
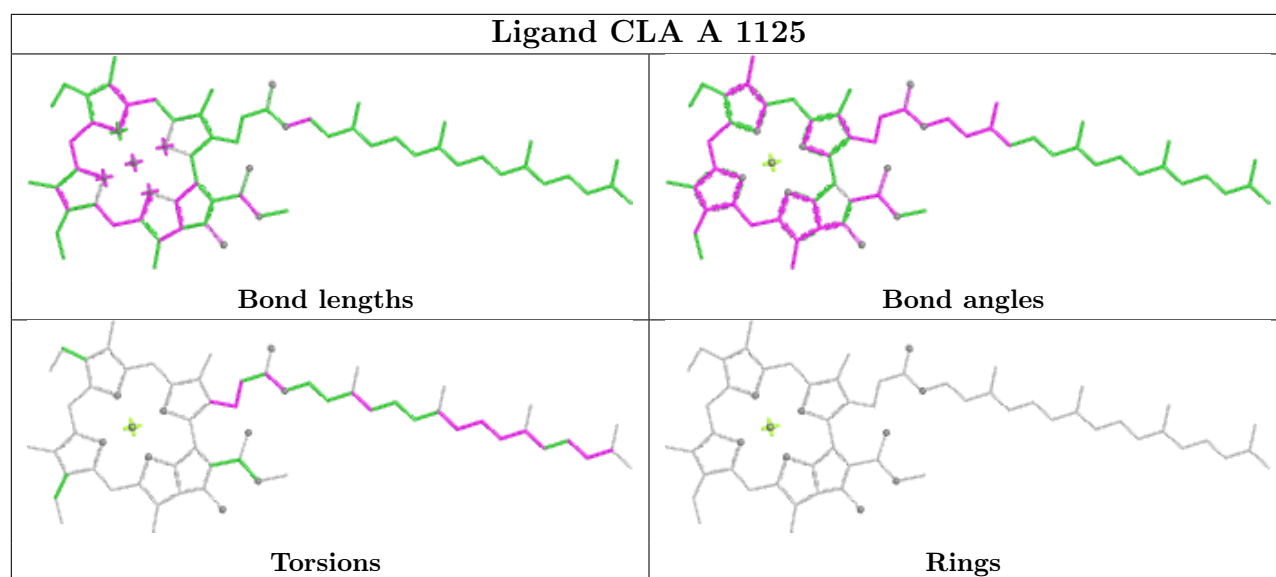


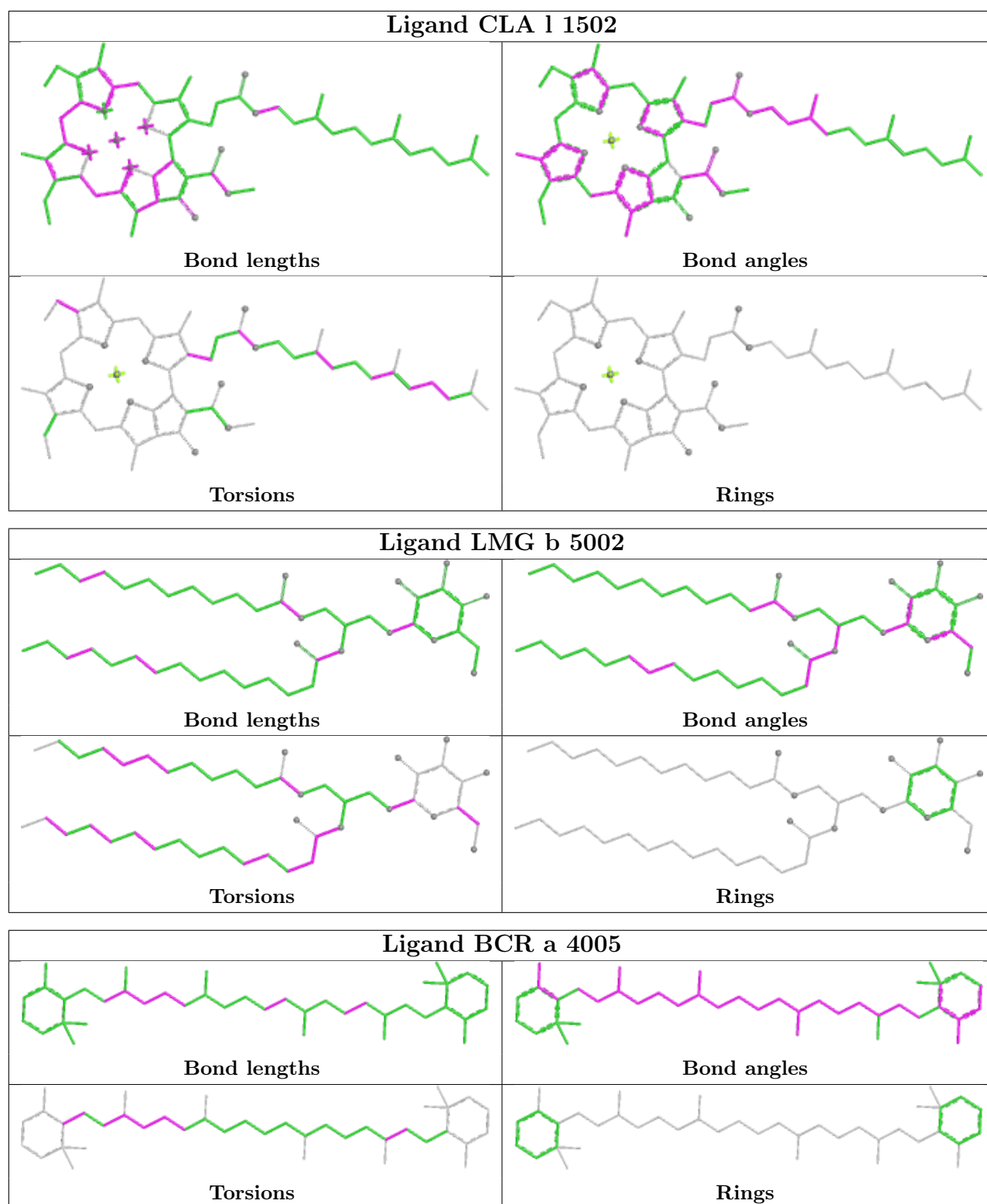


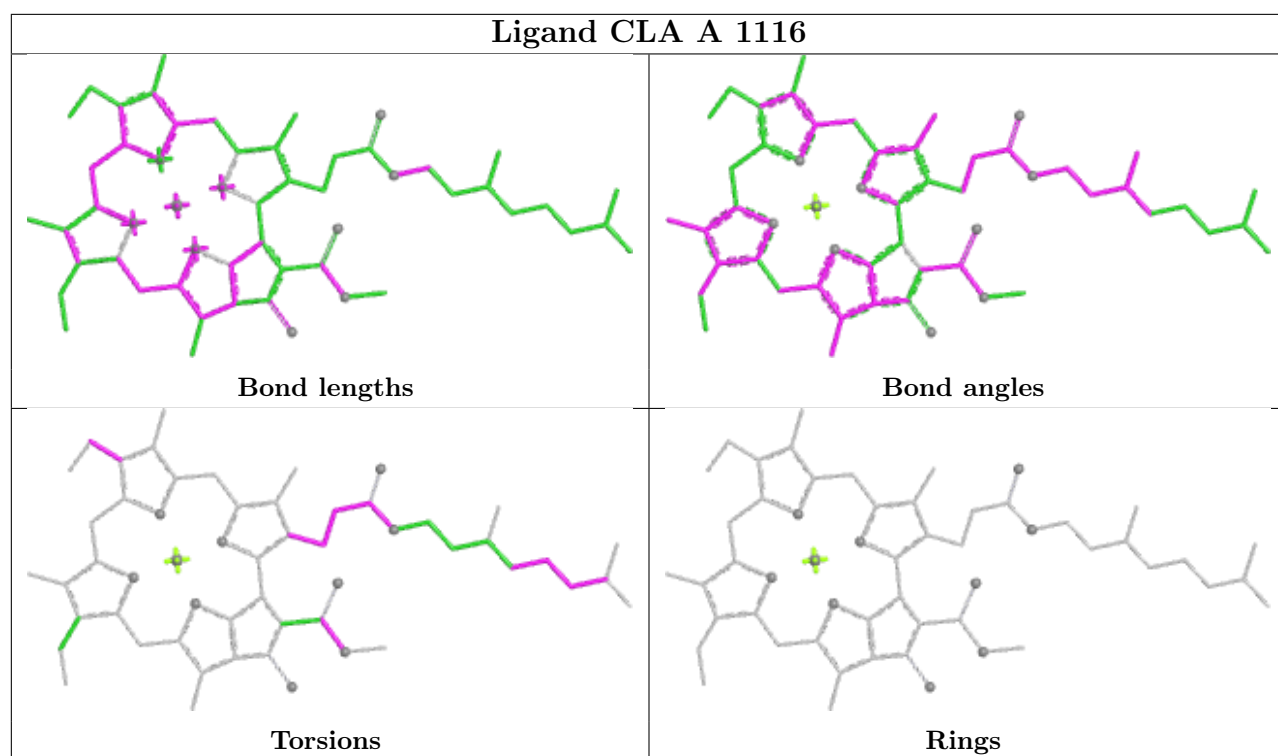




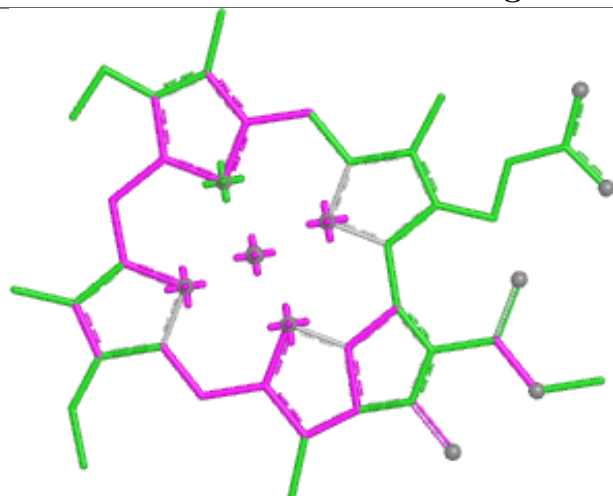




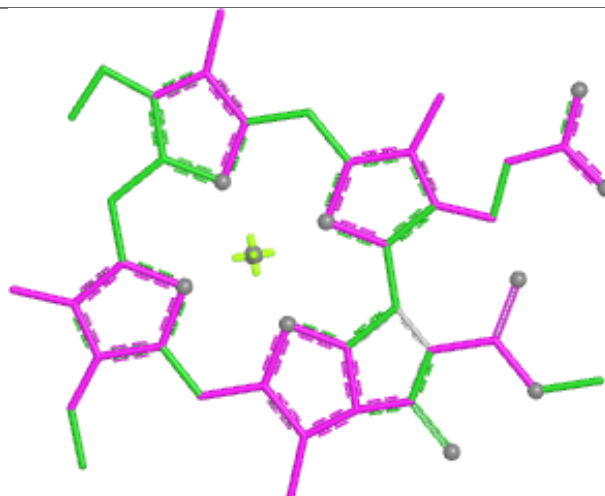




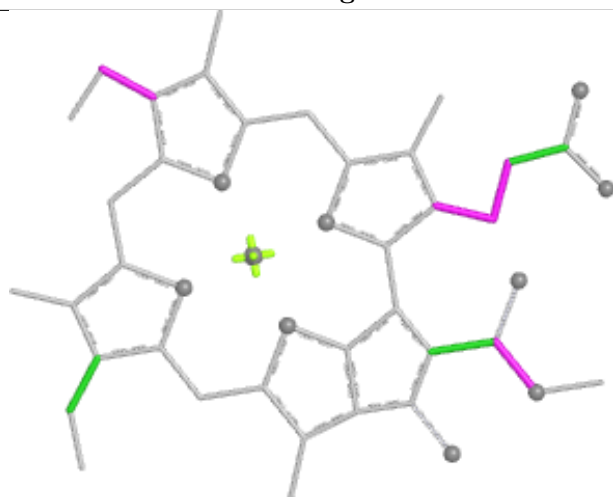
Ligand CLA G 1113



Bond lengths



Bond angles

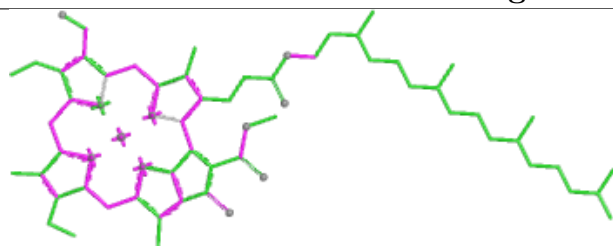


Torsions

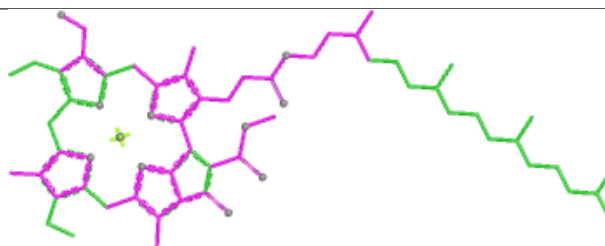


Rings

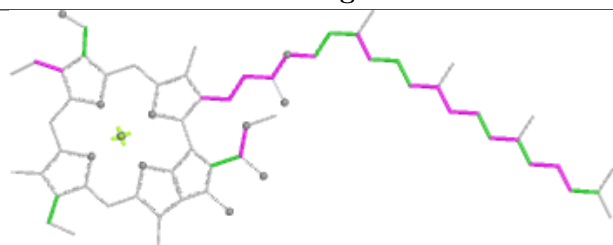
Ligand F6C H 1237



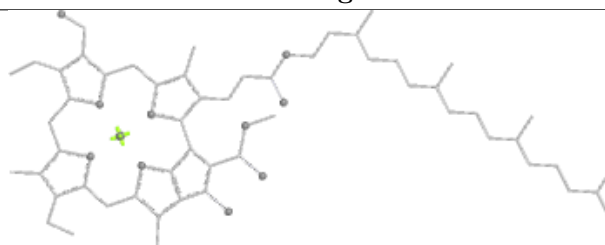
Bond lengths



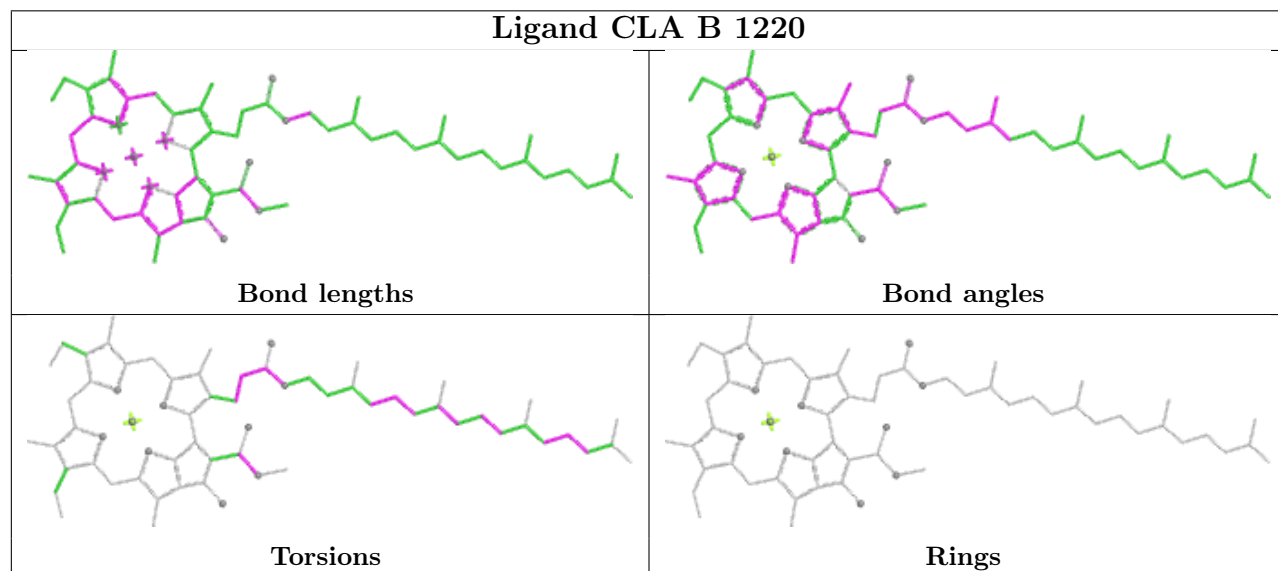
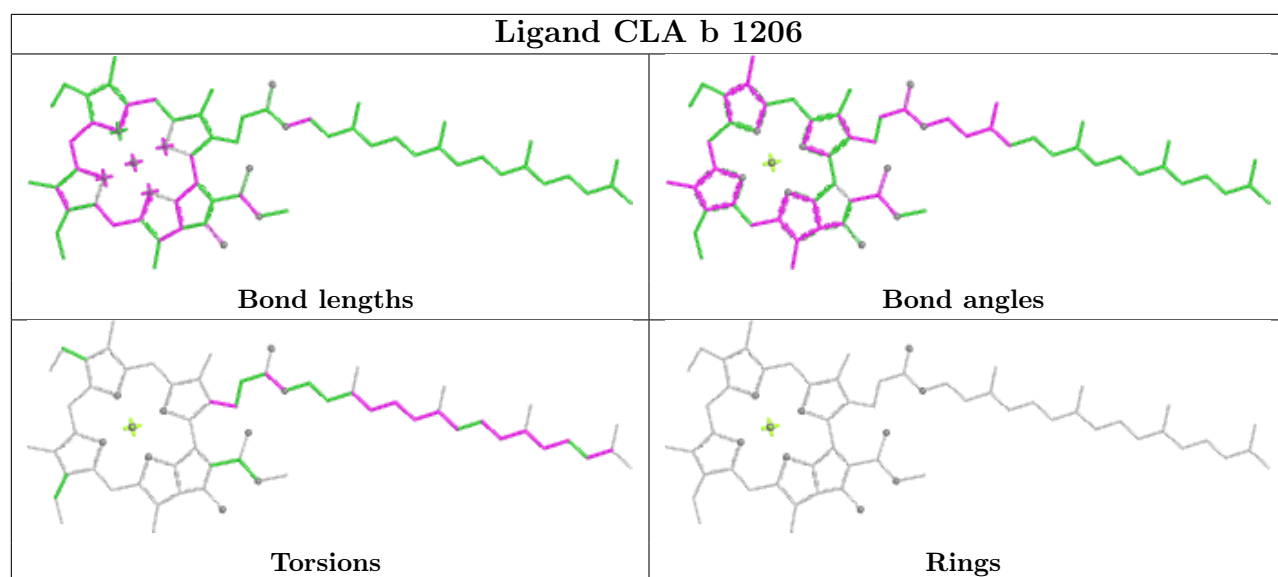
Bond angles

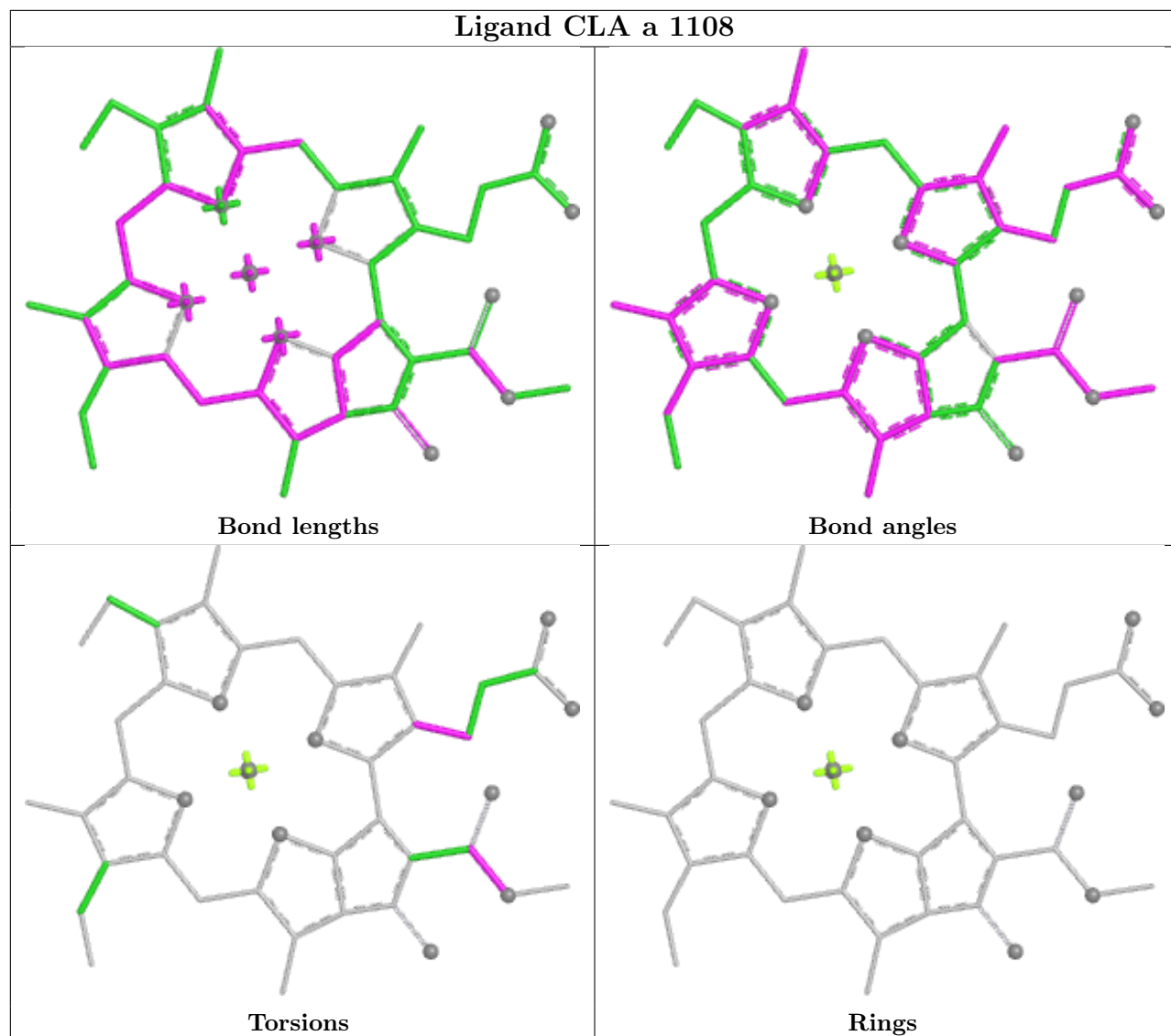


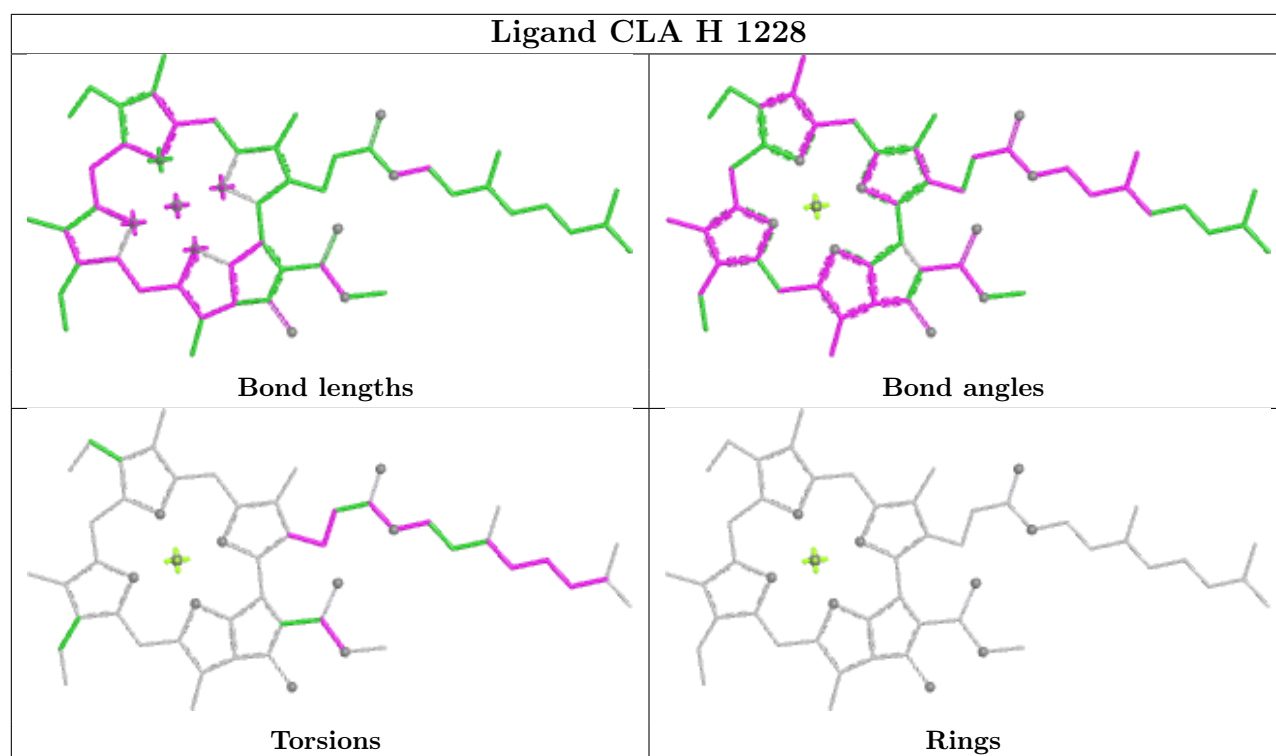
Torsions

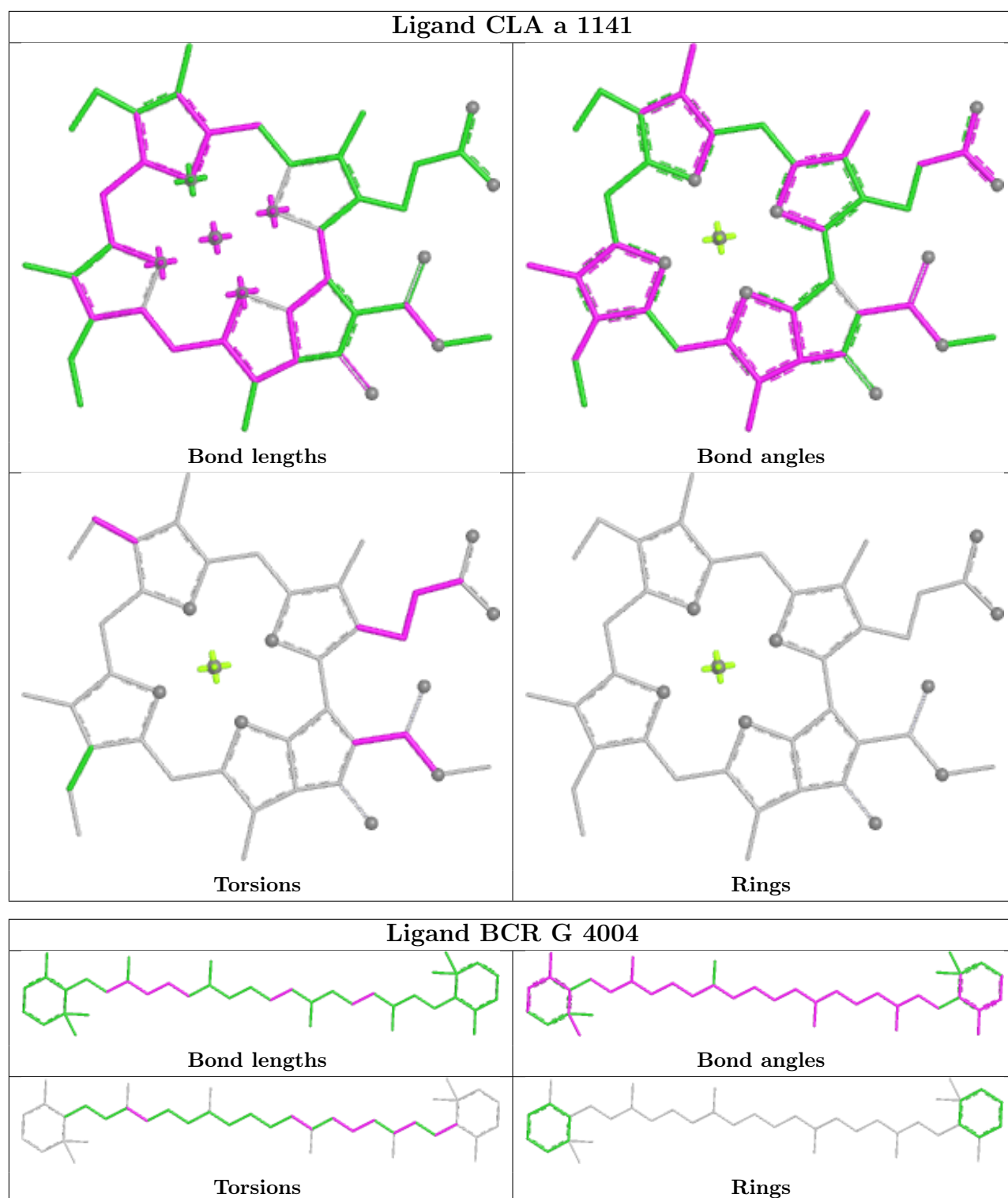


Rings

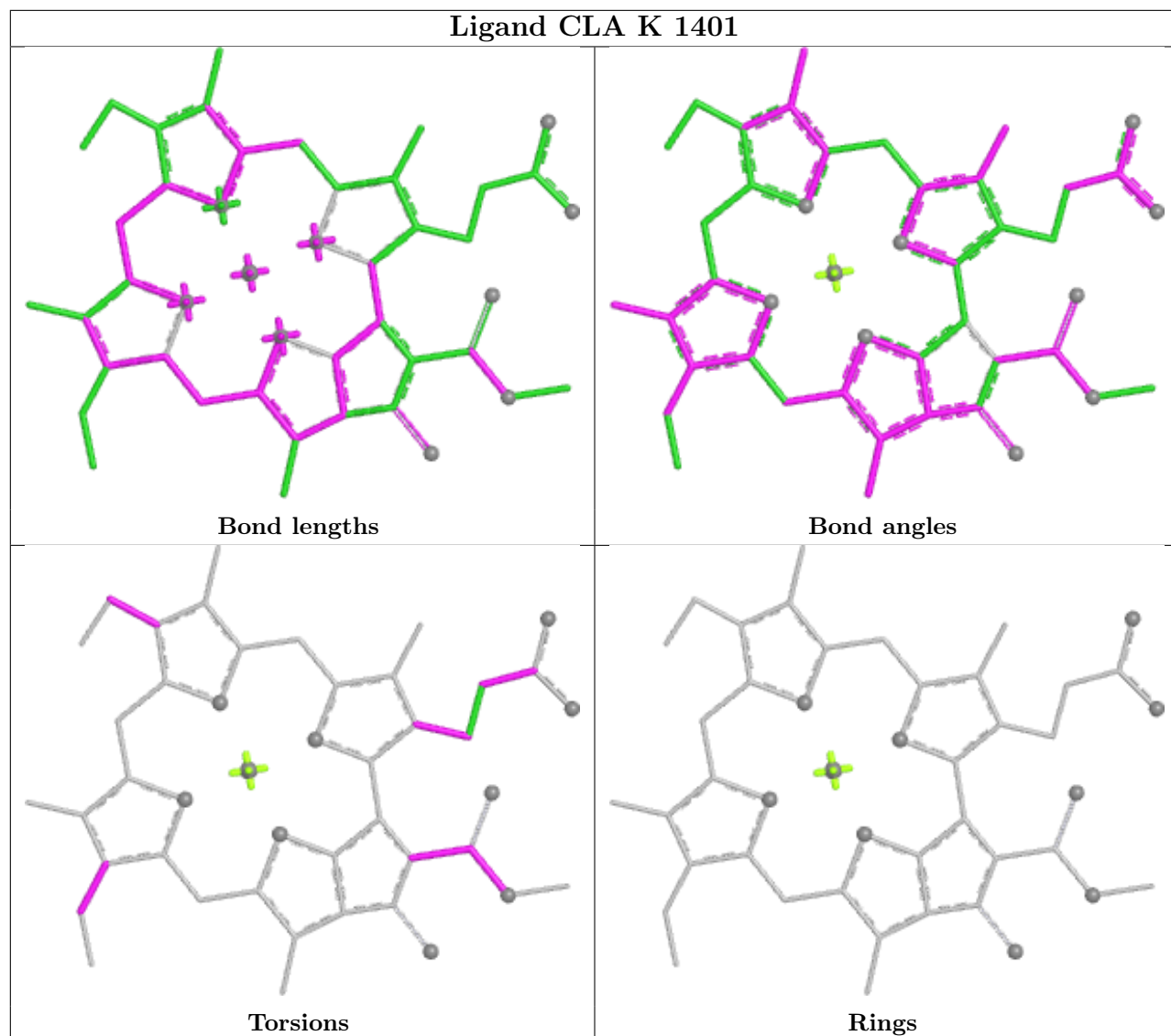




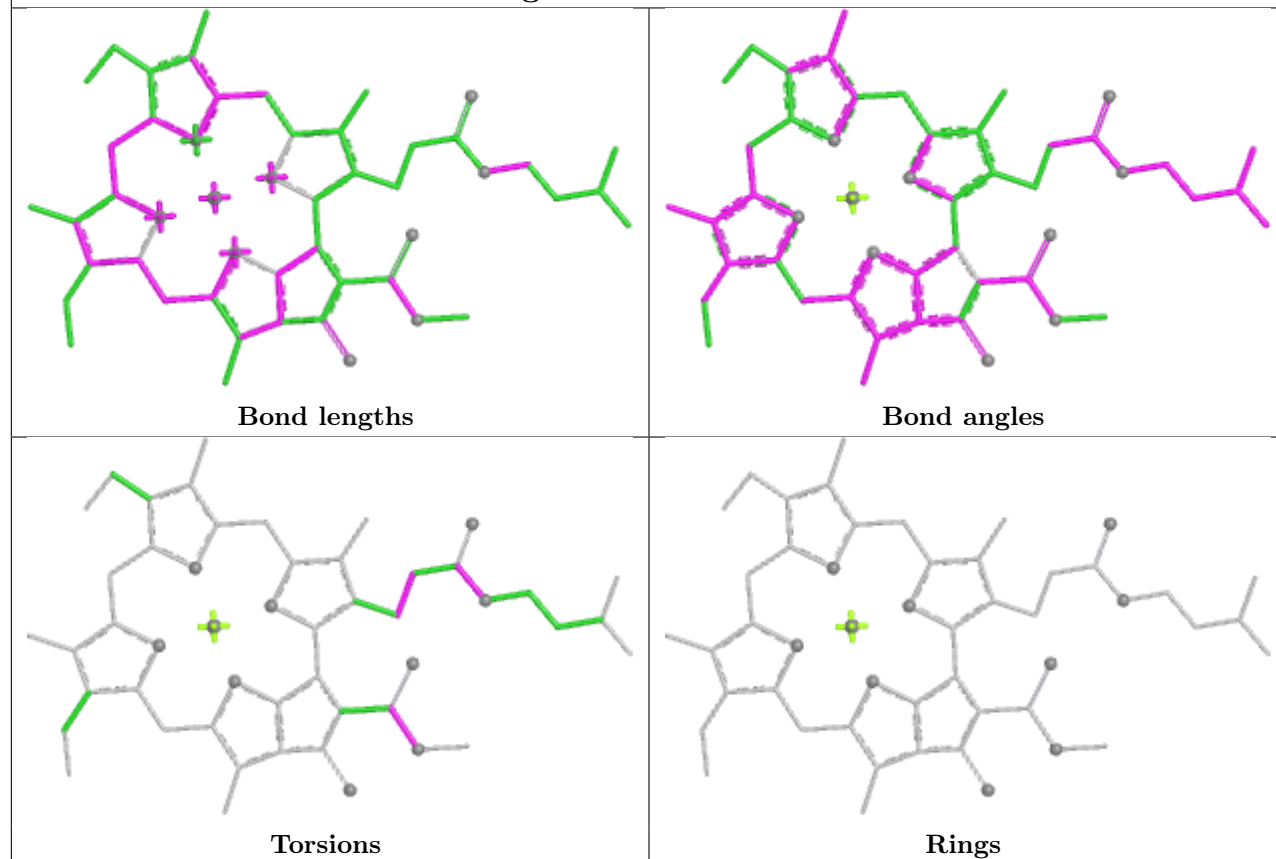




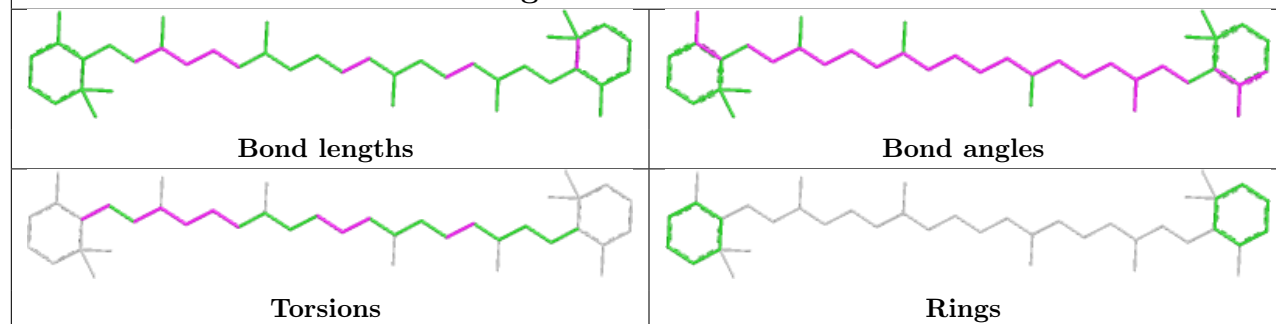
Ligand CLA K 1401

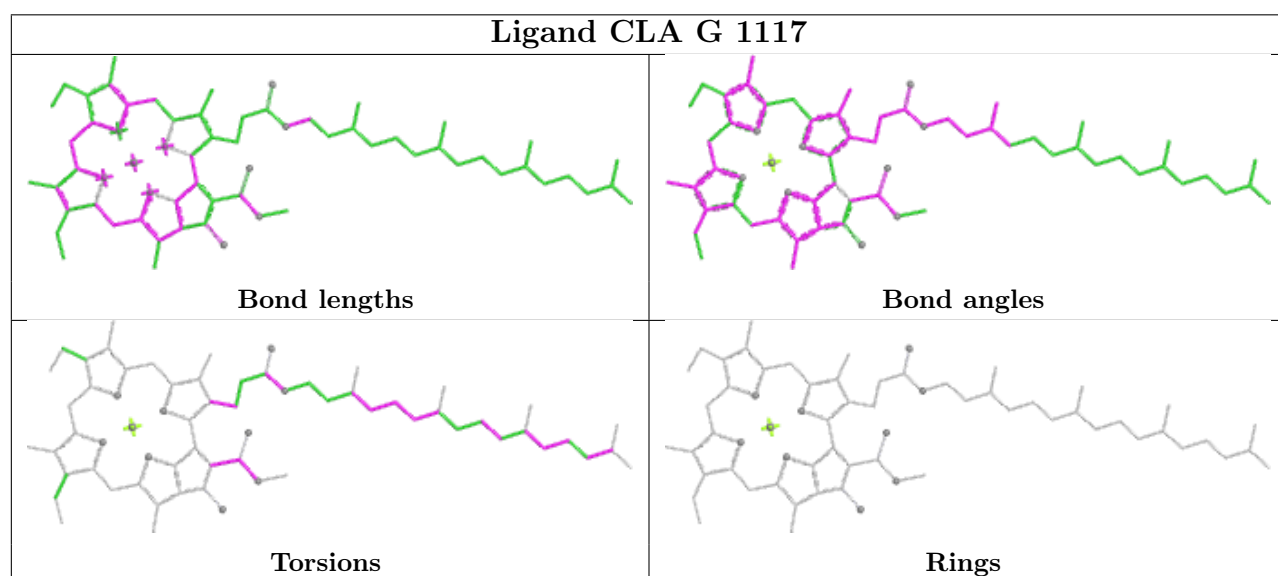
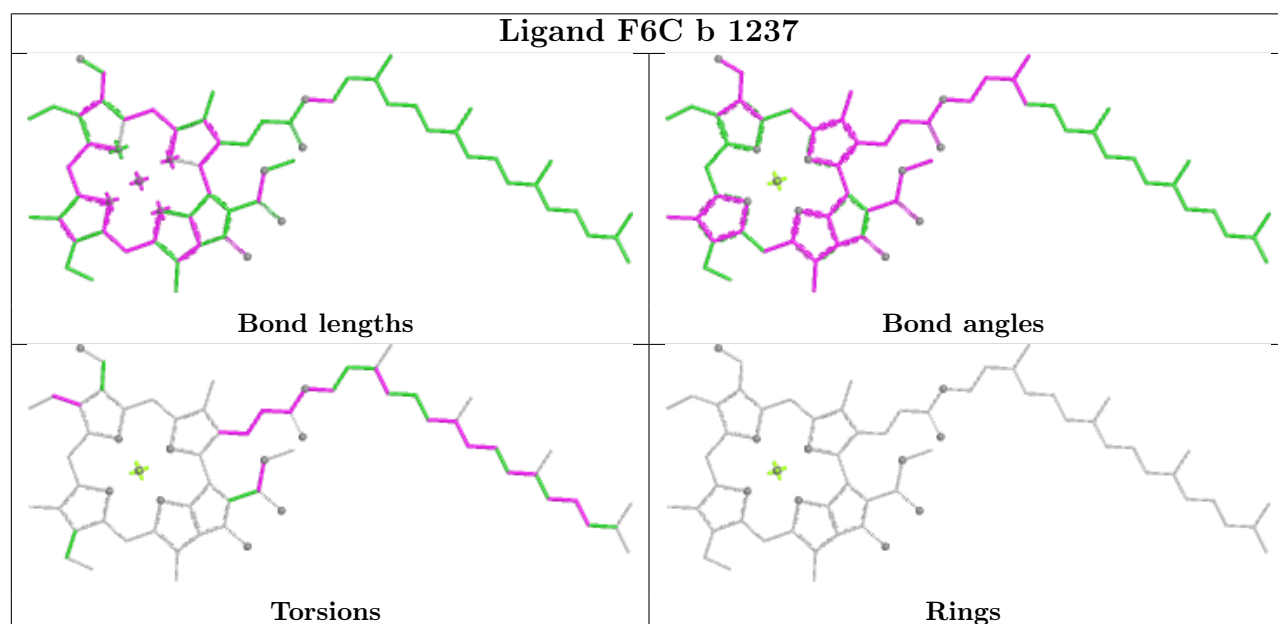
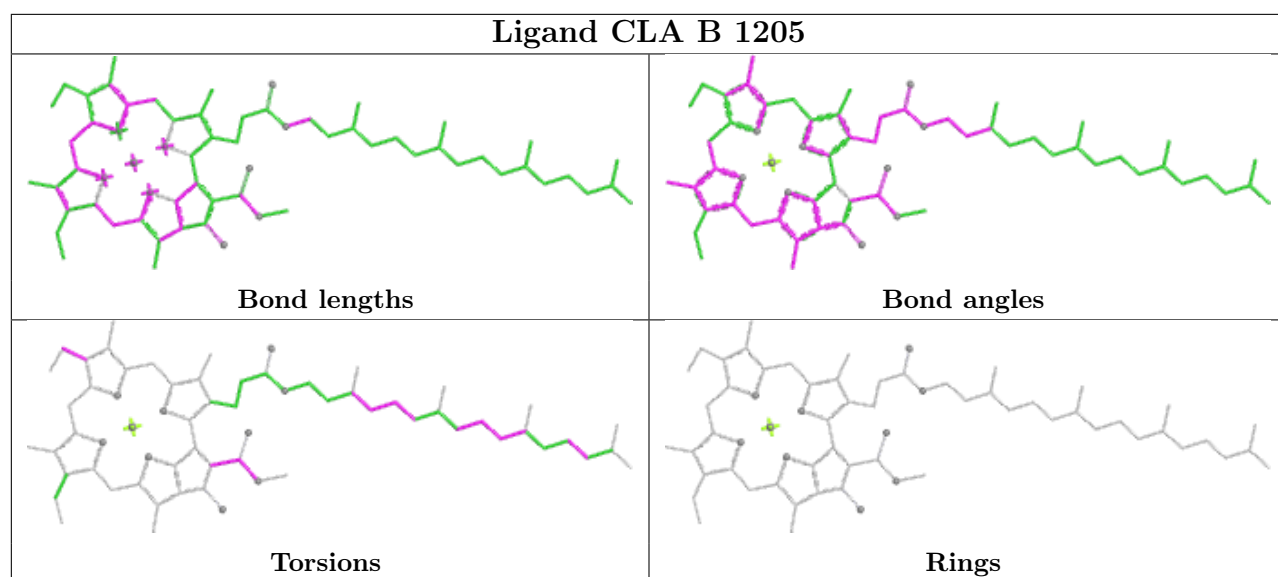


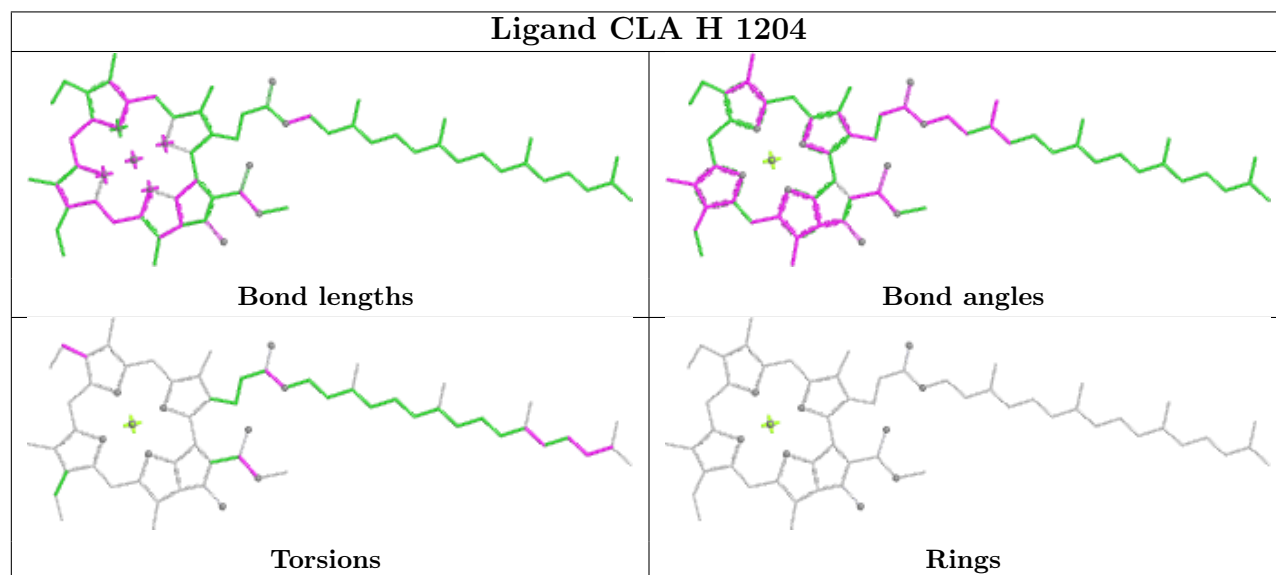
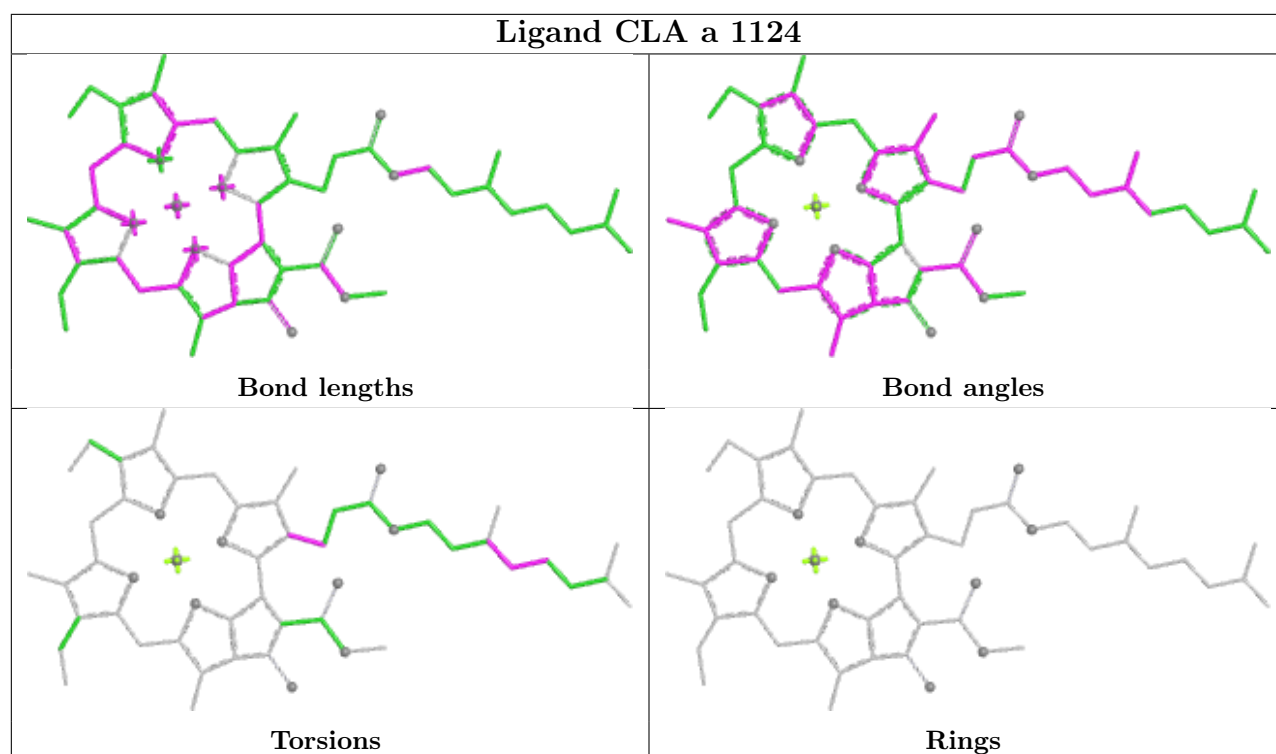
Ligand CLA G 1135

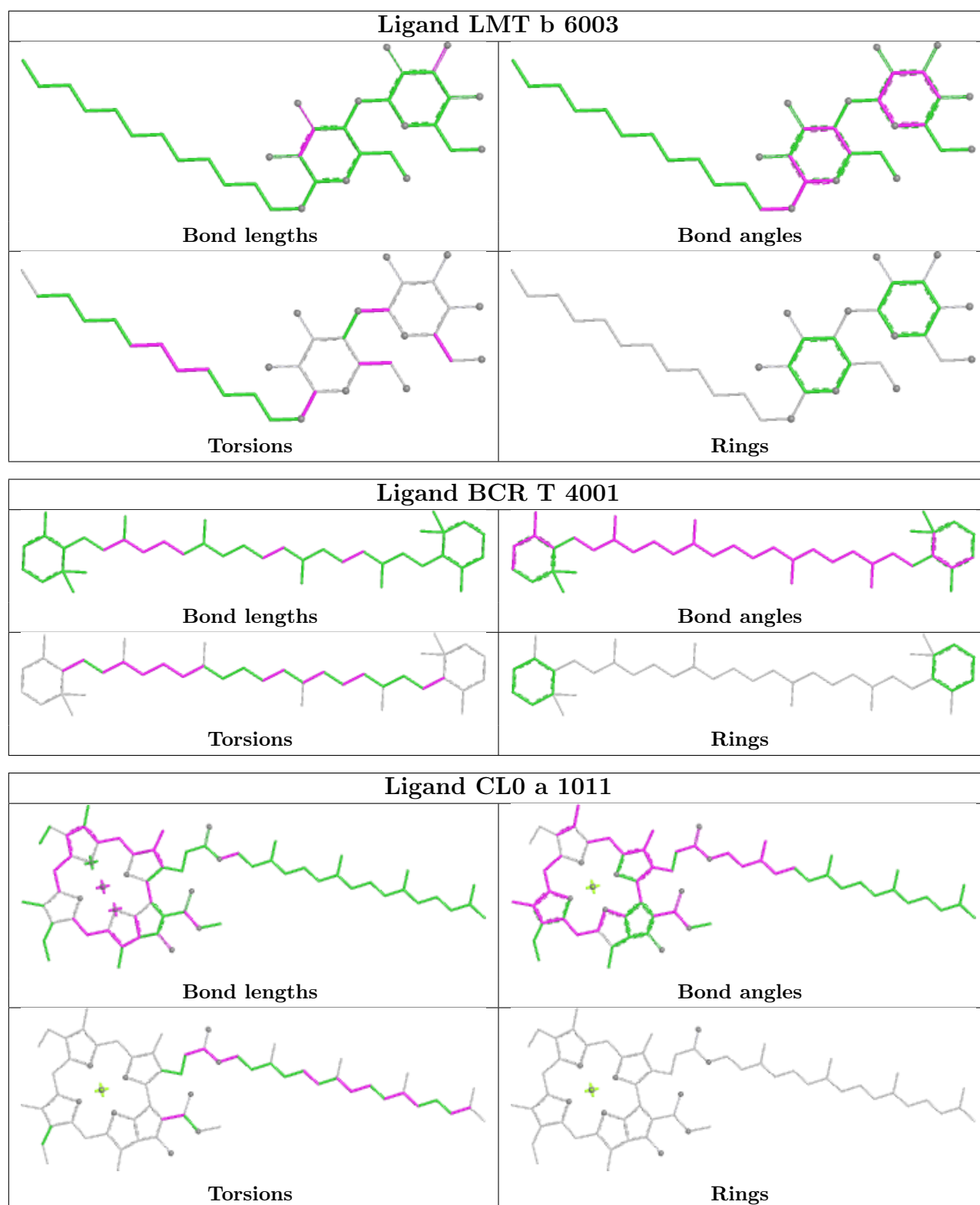


Ligand BCR R 4018

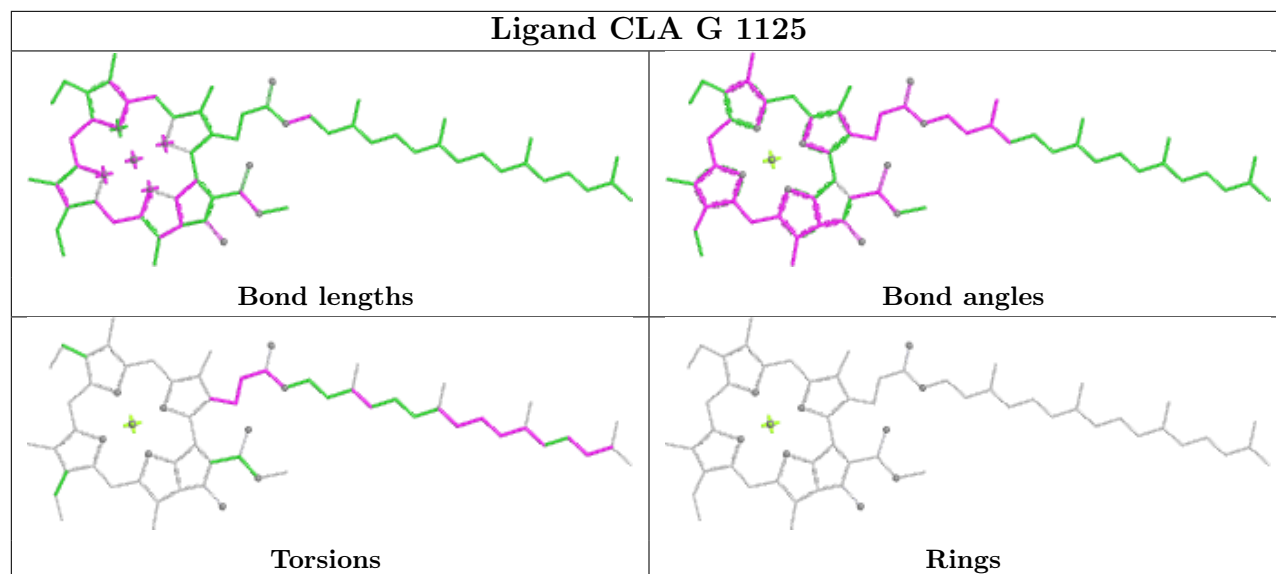




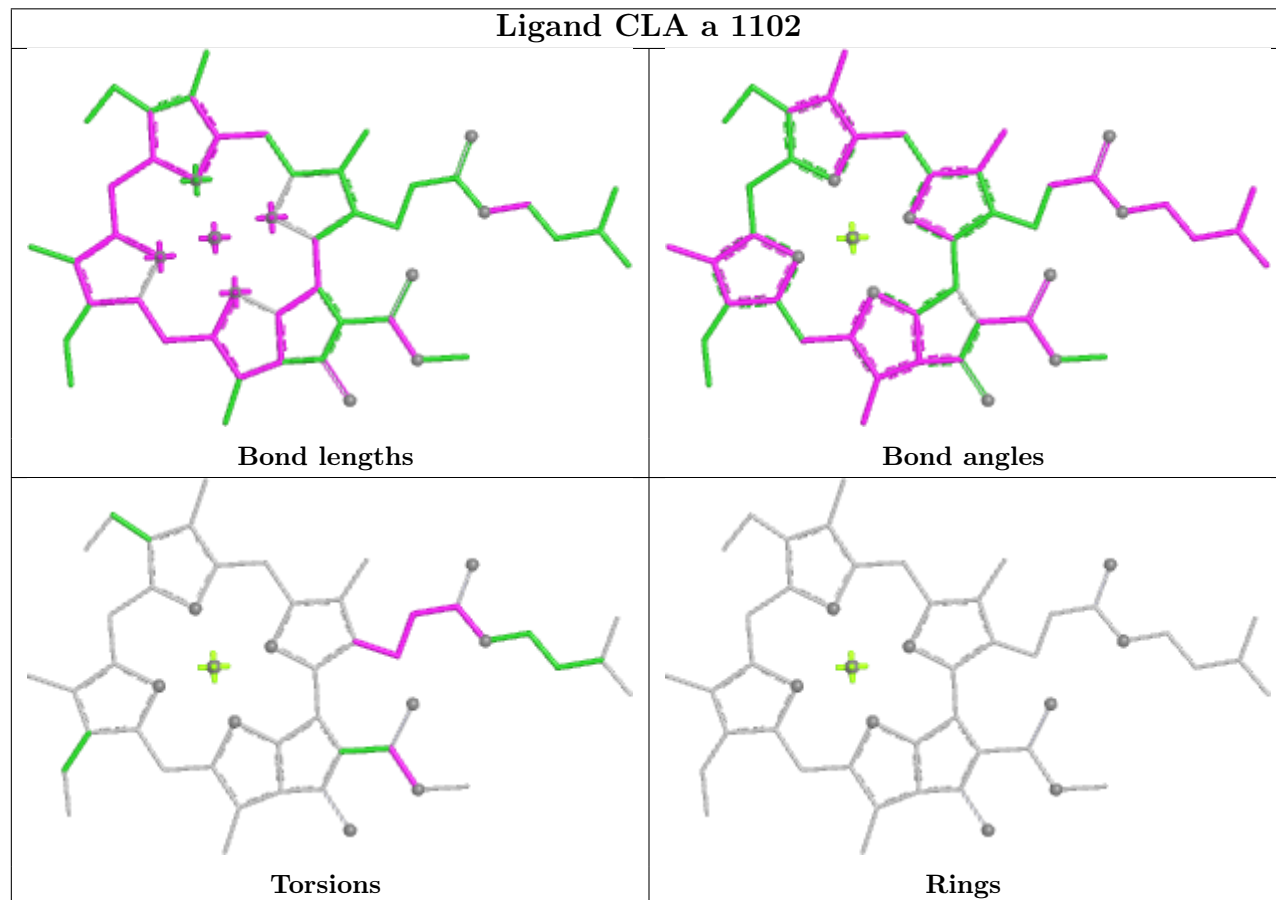


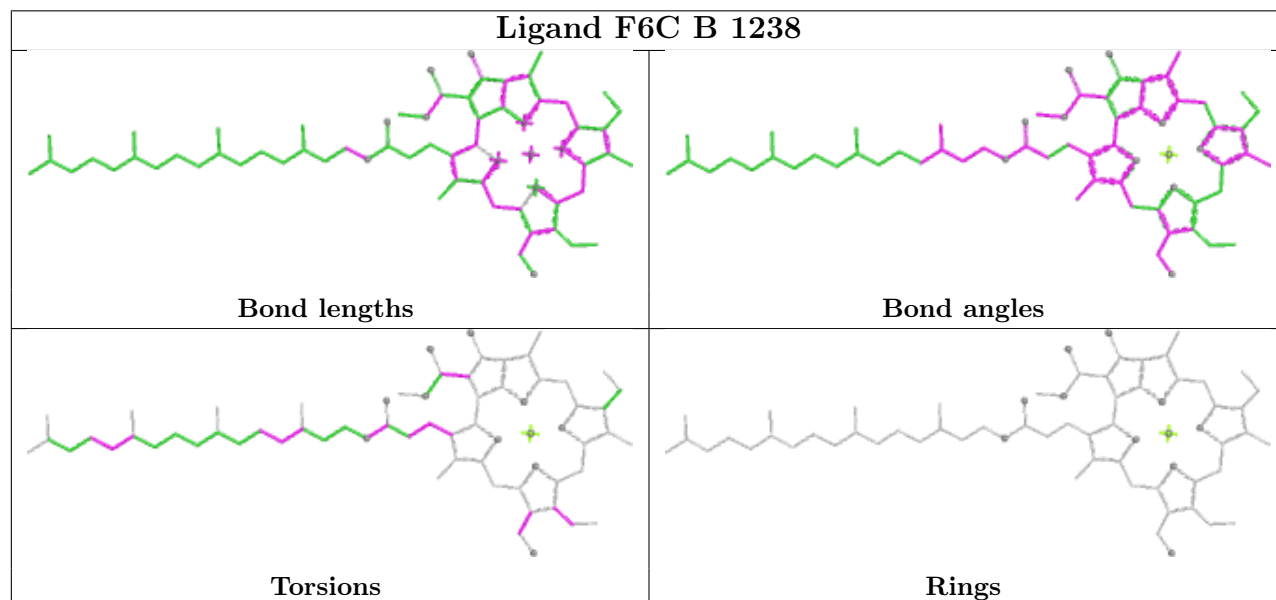
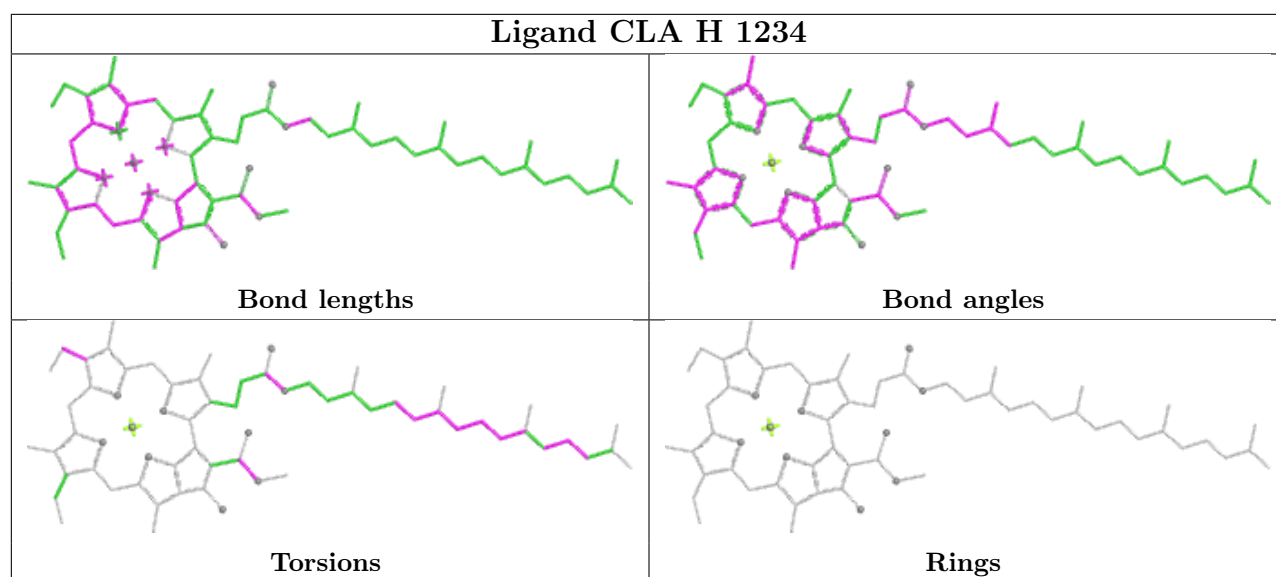


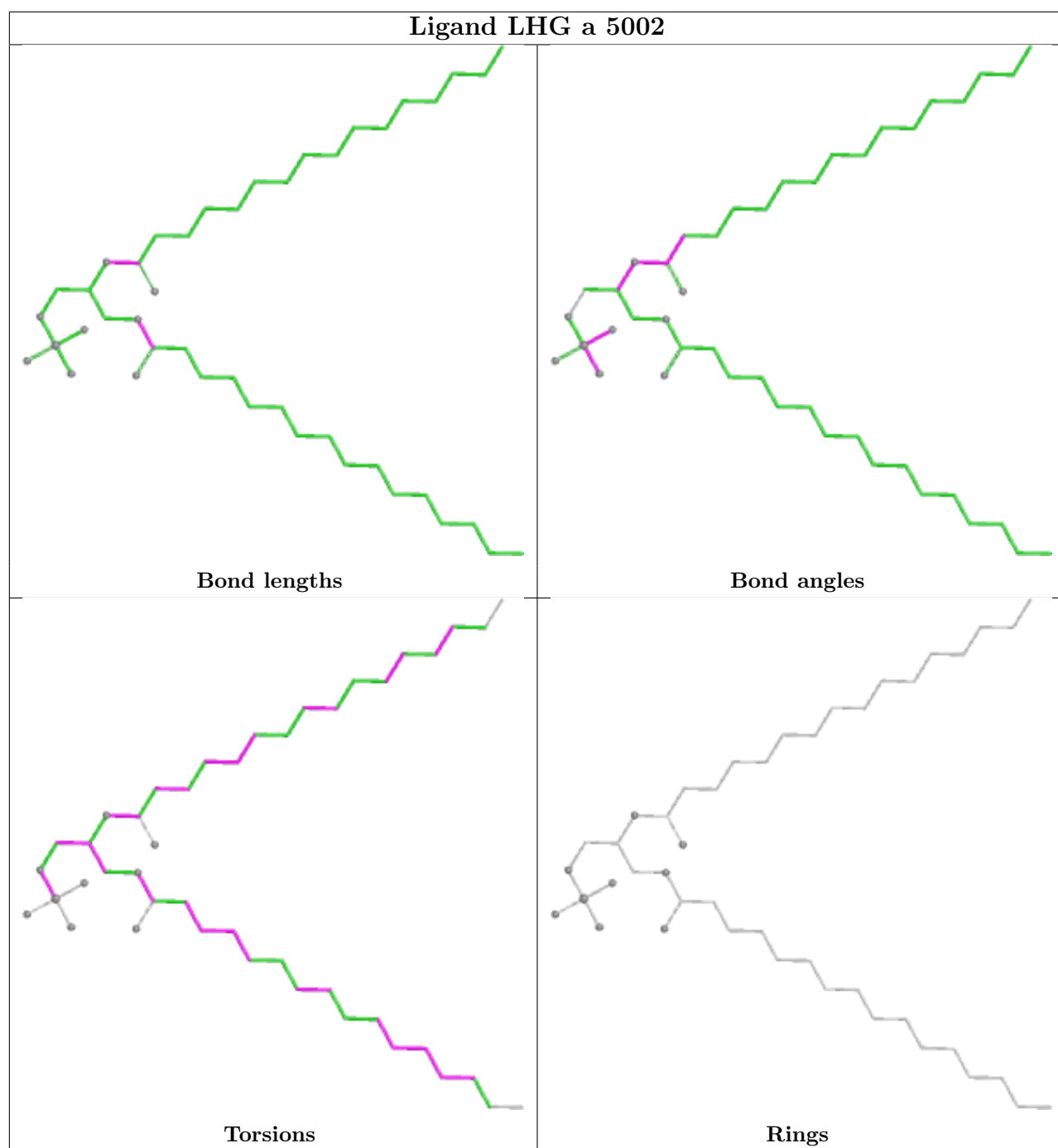
Ligand CLA G 1125

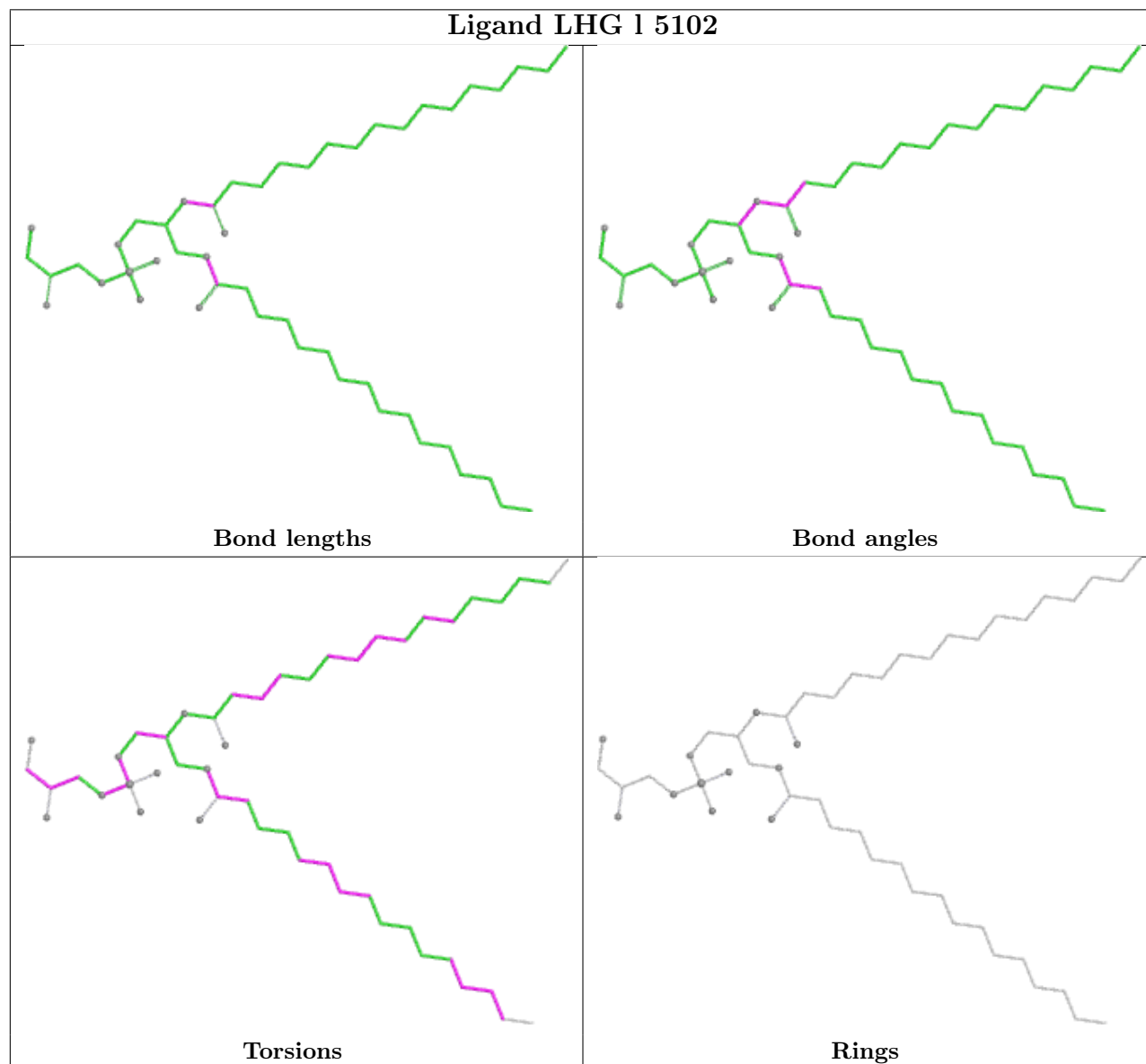
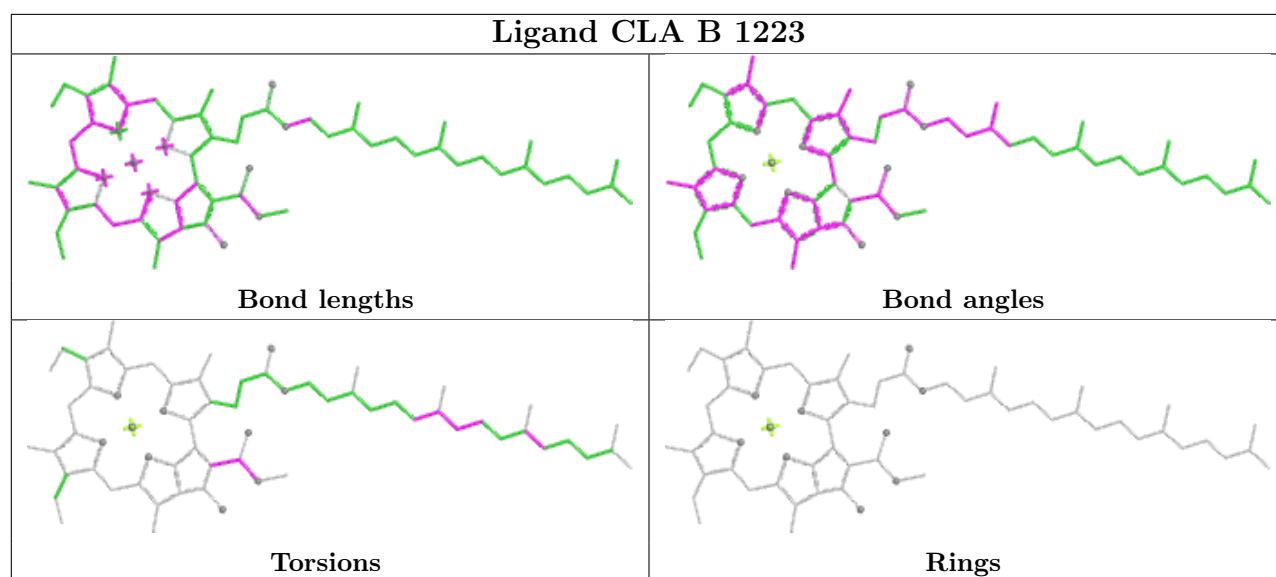


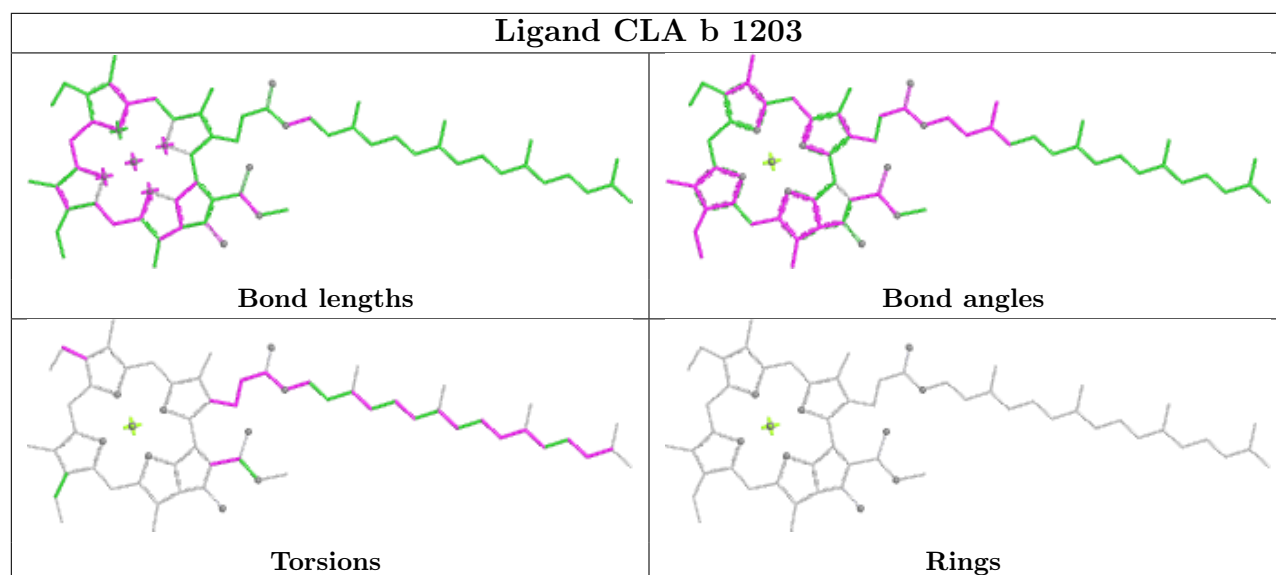
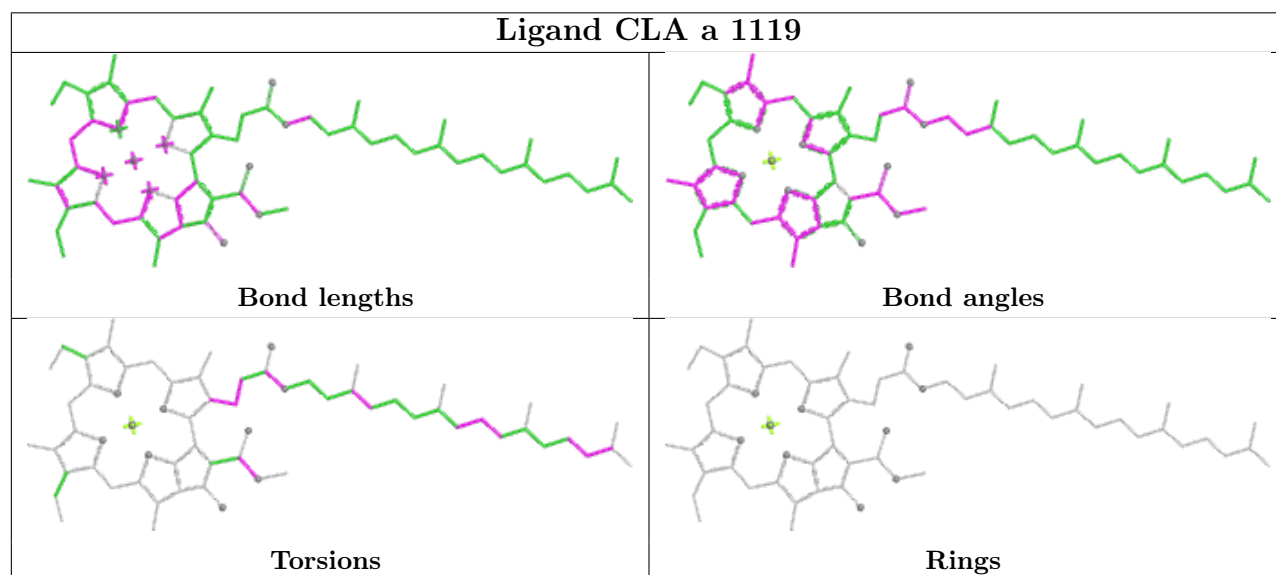
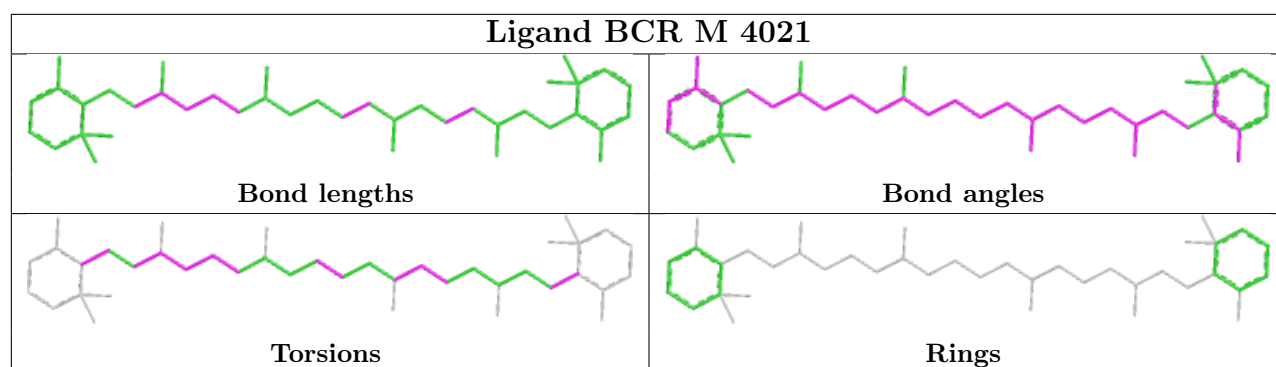
Ligand CLA a 1102

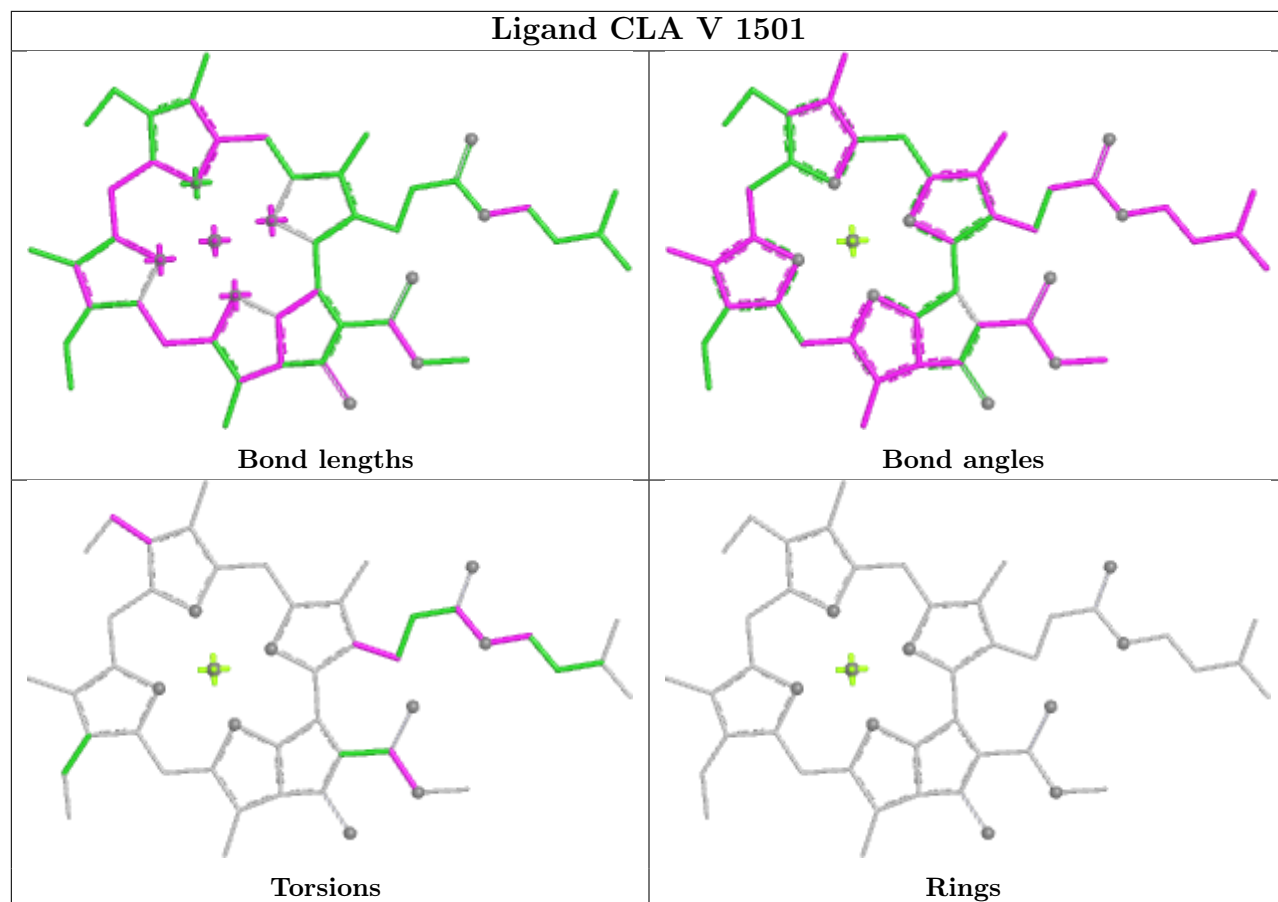




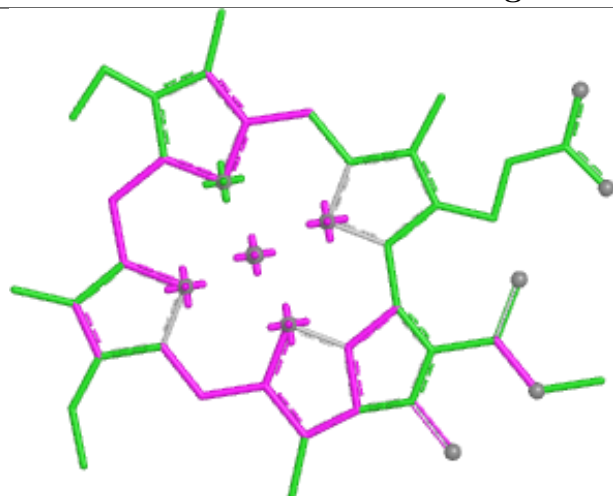




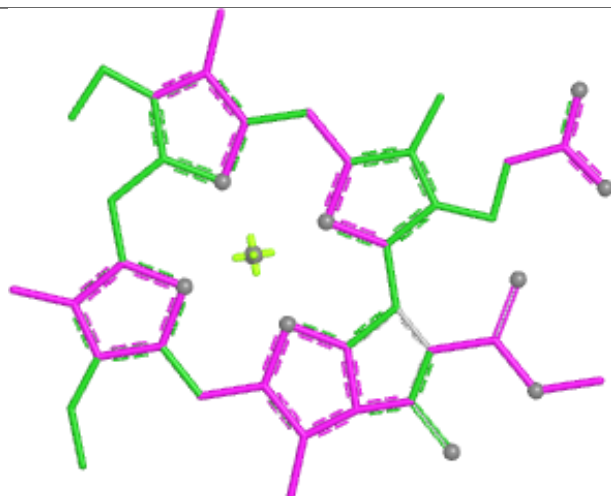




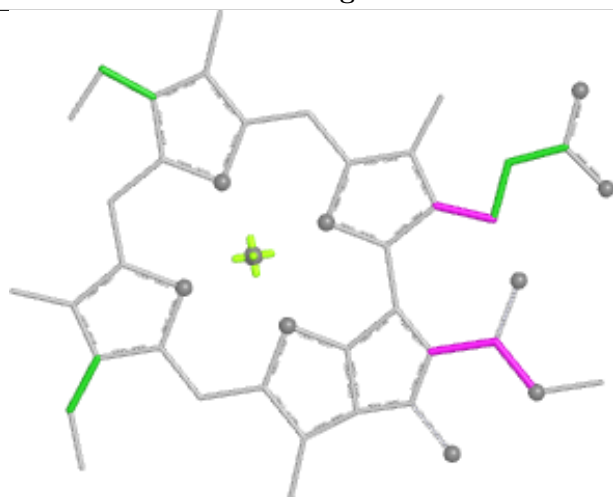
Ligand CLA H 1218



Bond lengths



Bond angles

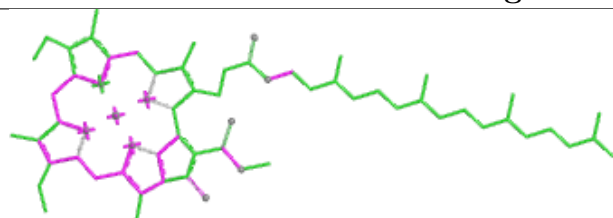


Torsions

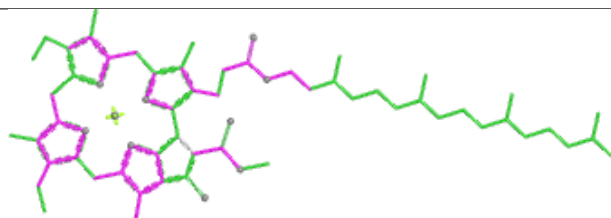


Rings

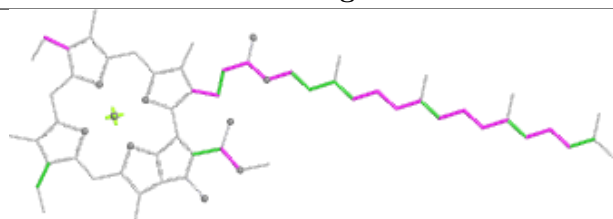
Ligand CLA H 1216



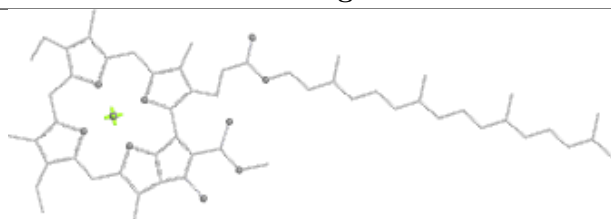
Bond lengths



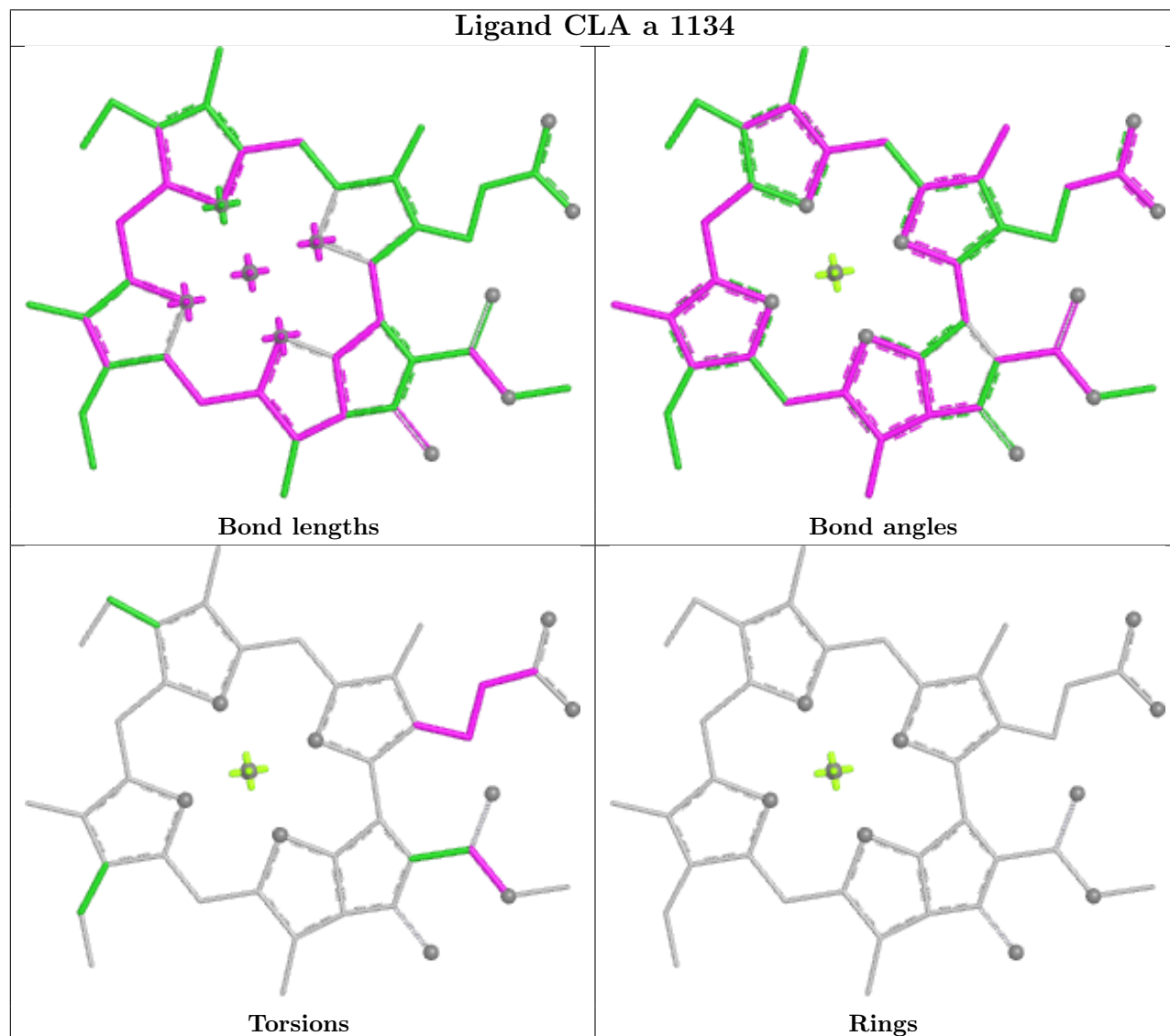
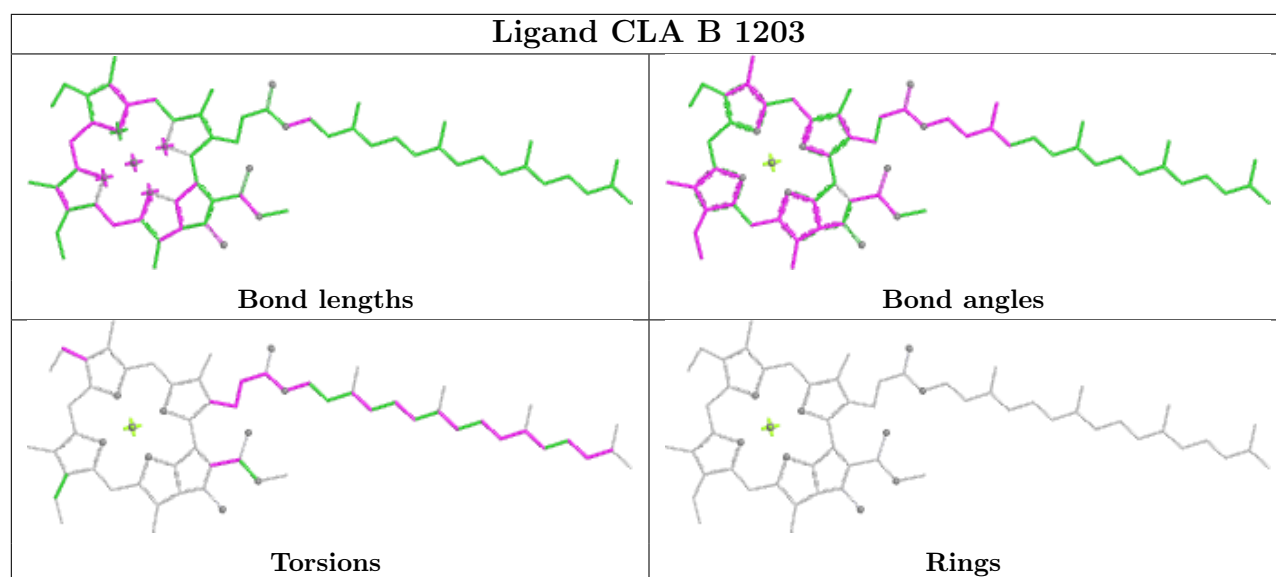
Bond angles

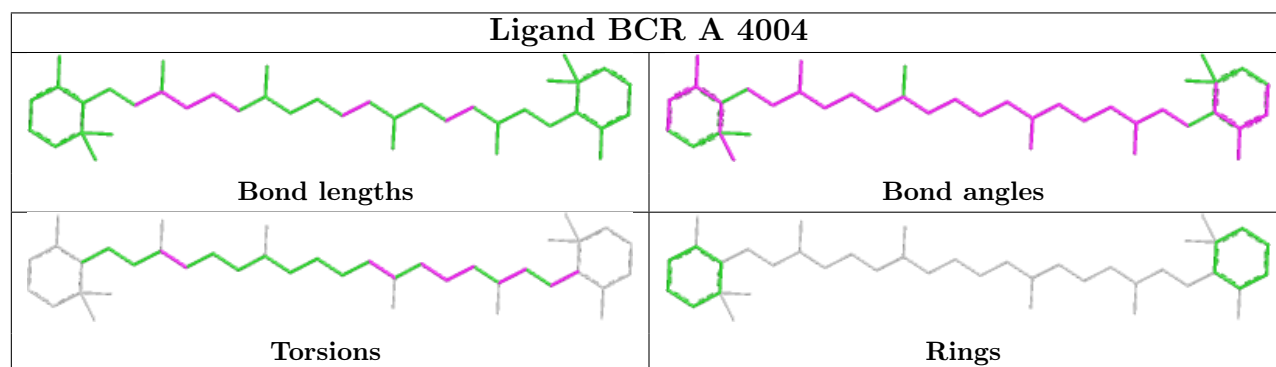
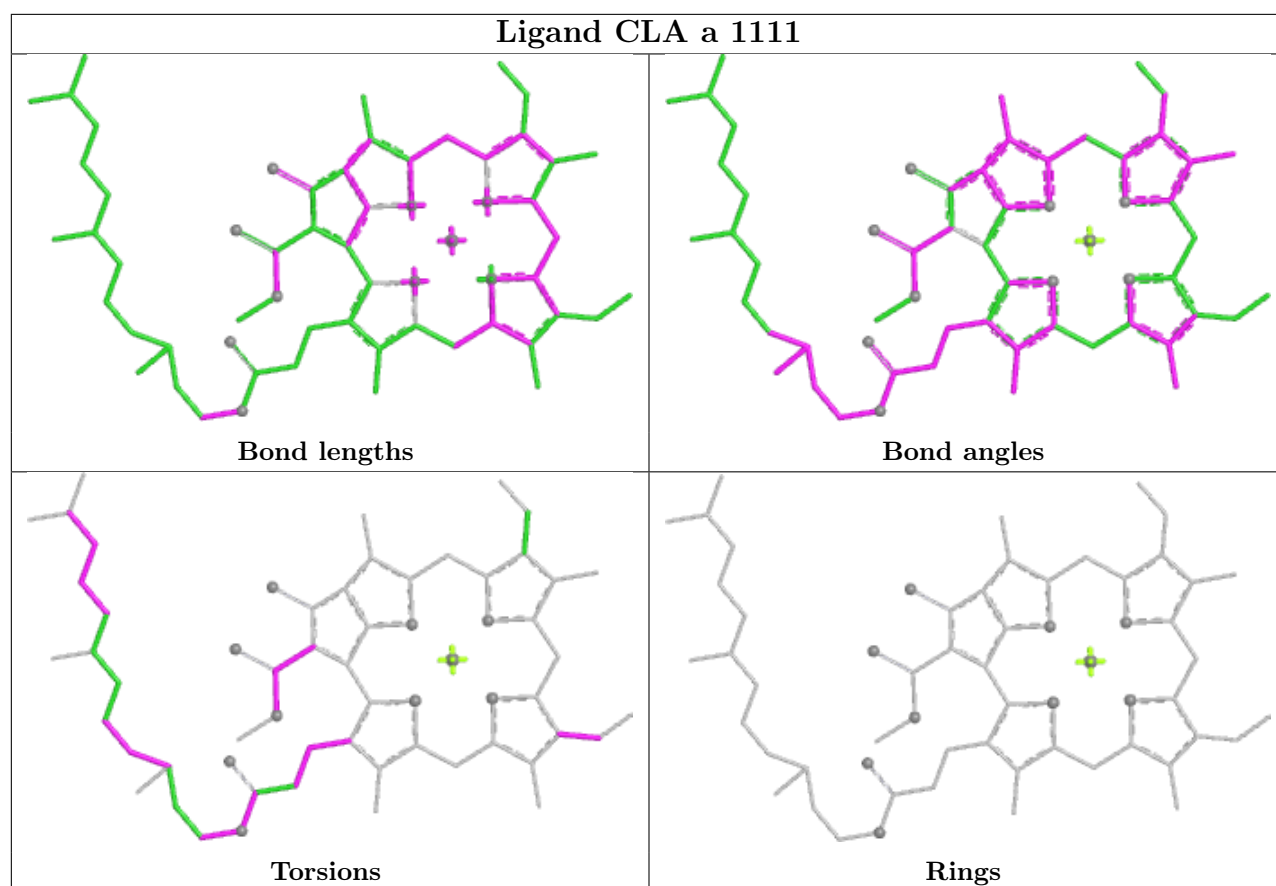


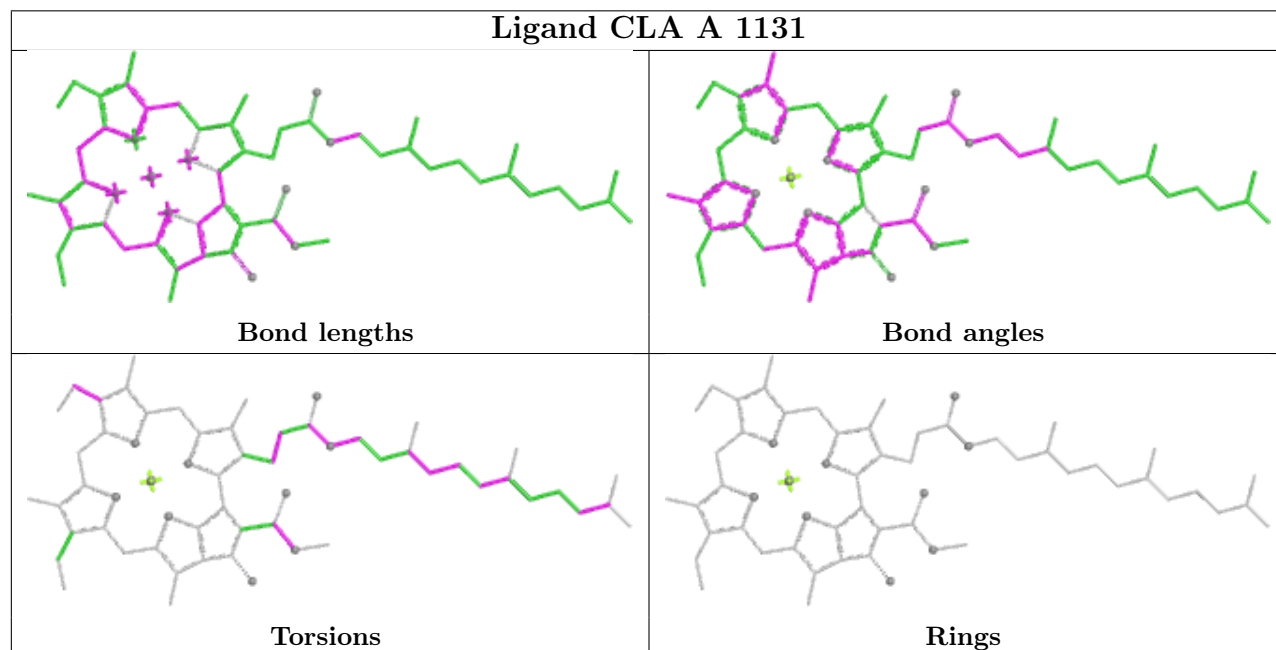
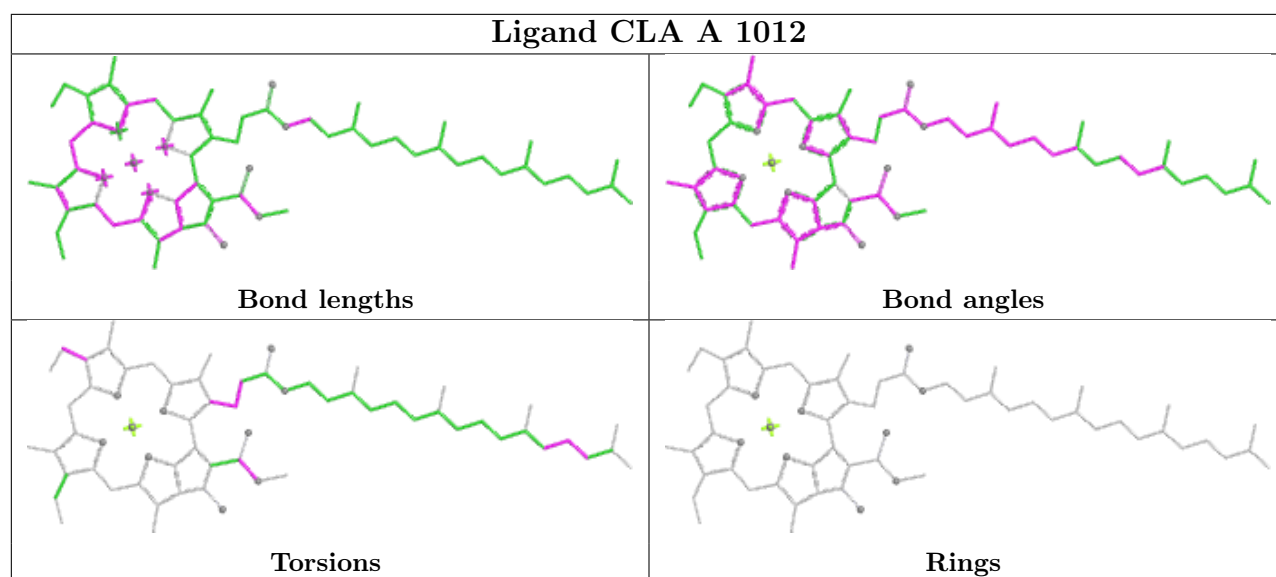
Torsions

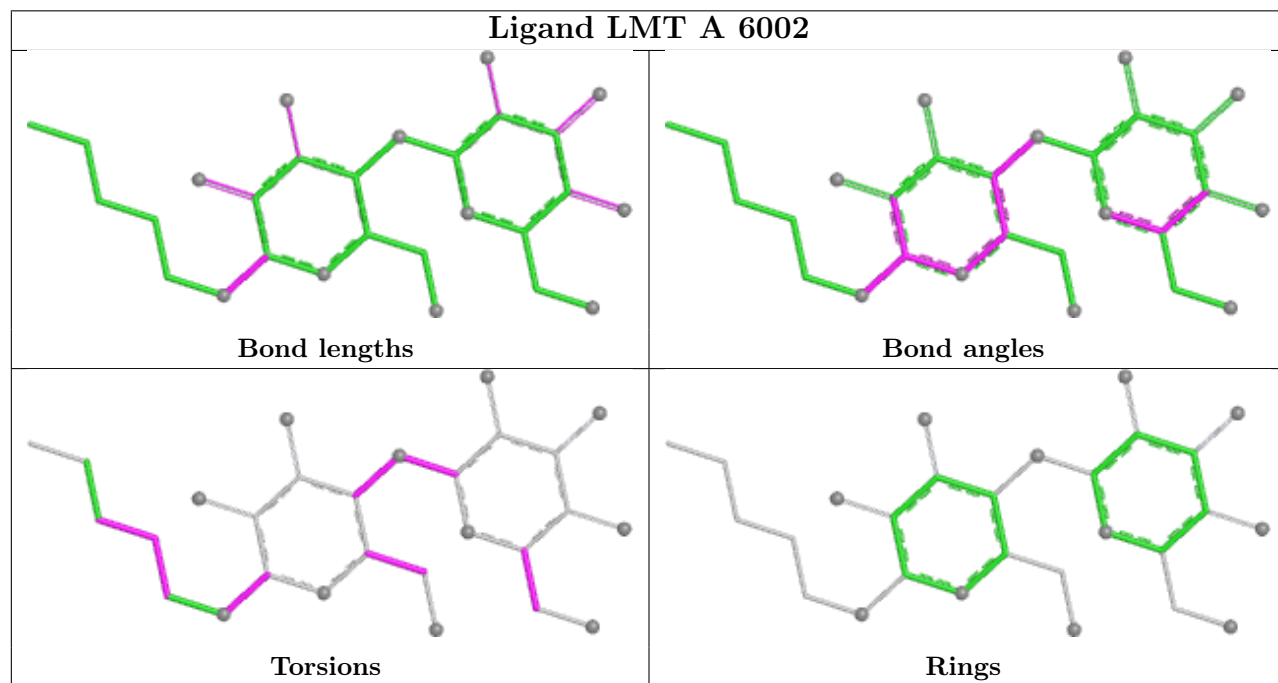
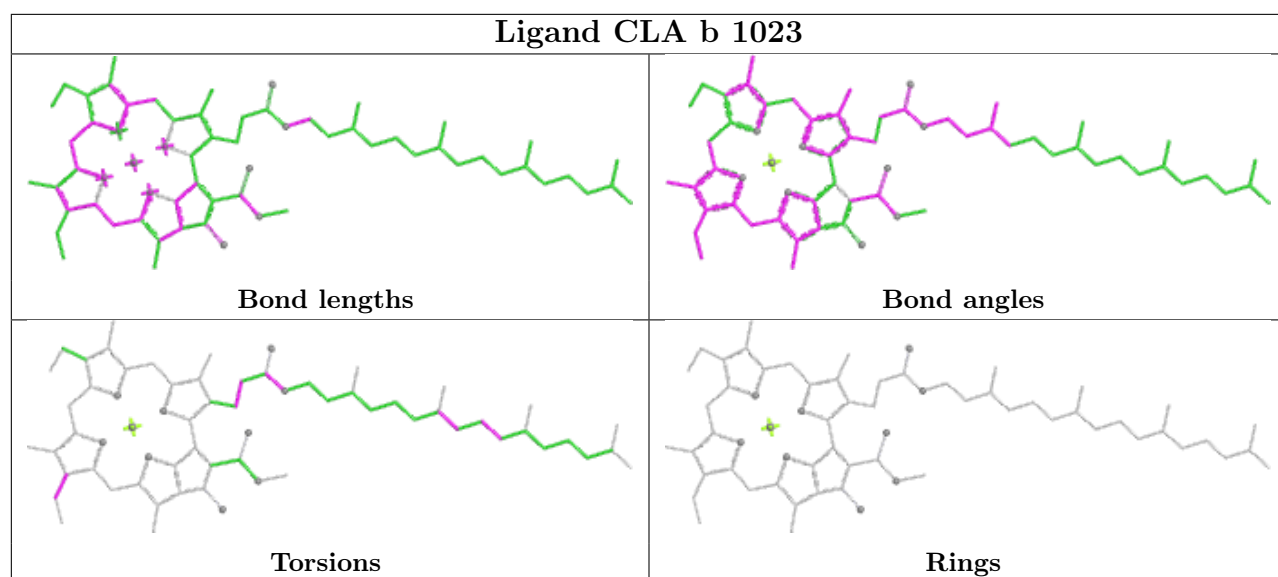


Rings

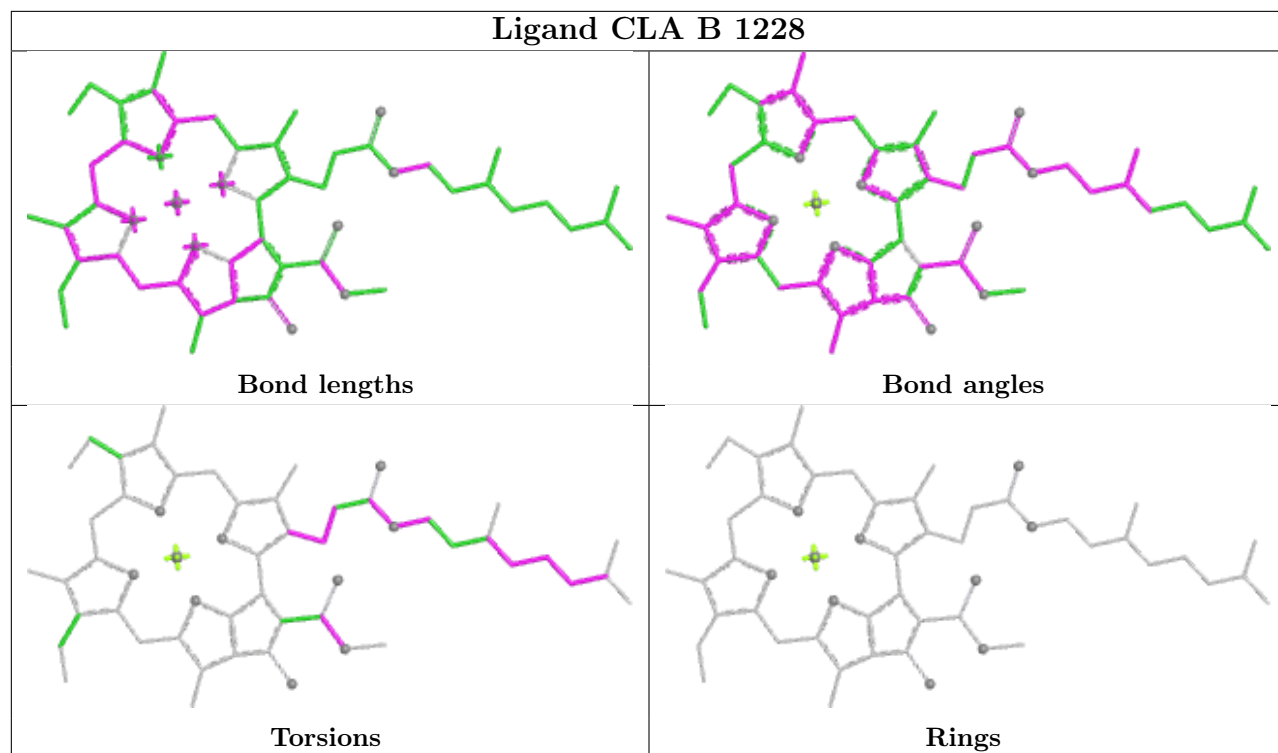




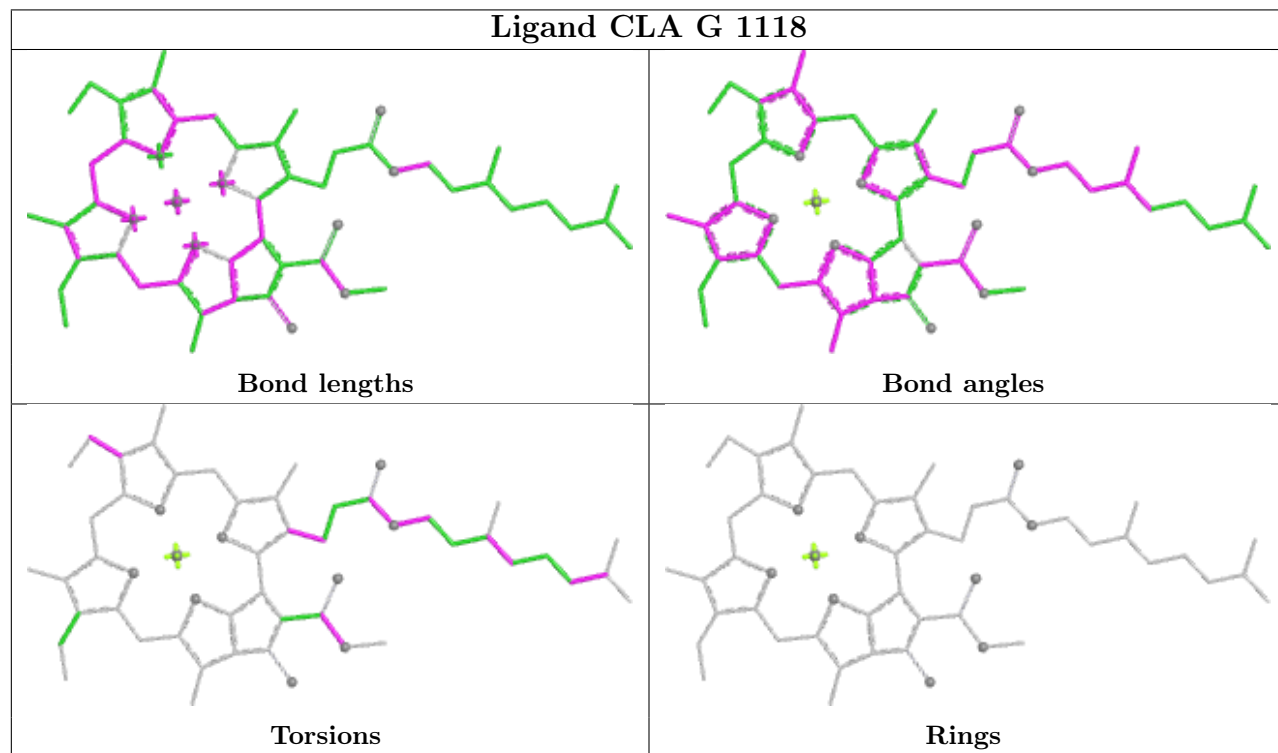




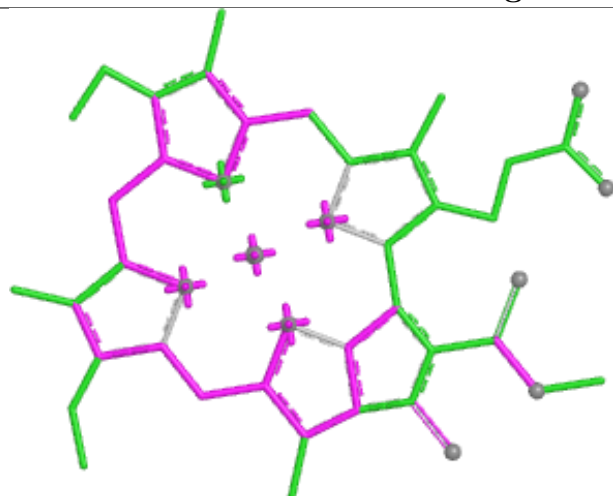
Ligand CLA B 1228



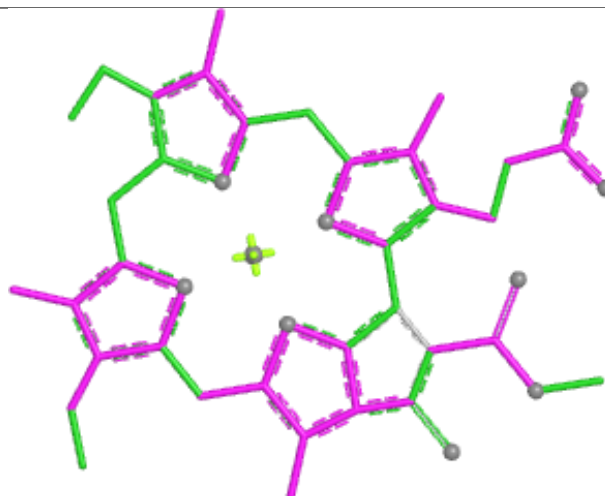
Ligand CLA G 1118



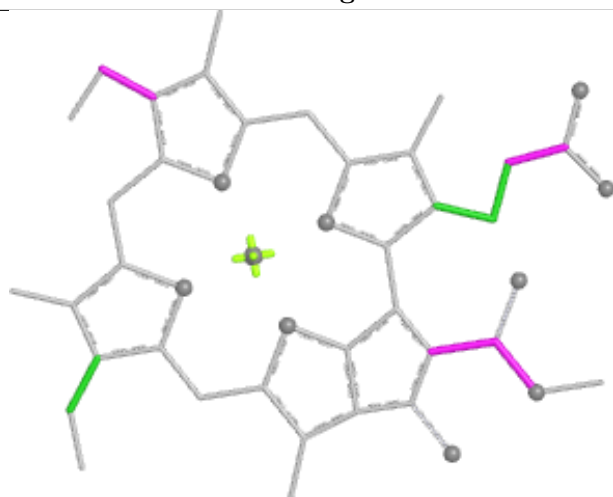
Ligand CLA A 1101



Bond lengths



Bond angles

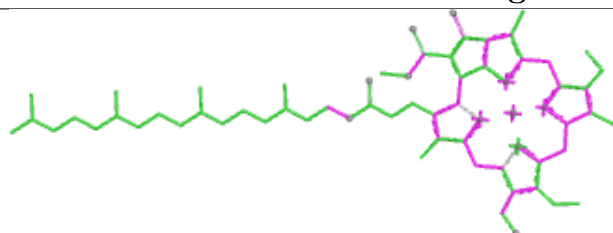


Torsions

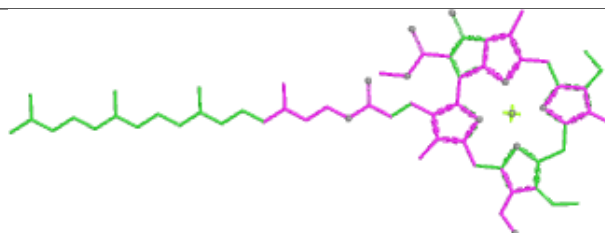


Rings

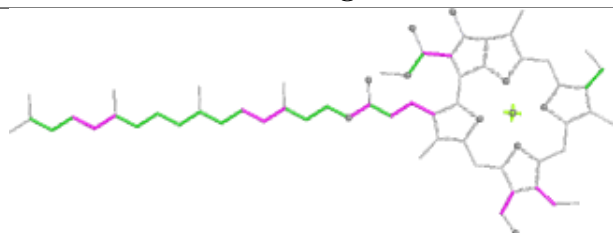
Ligand F6C H 1238



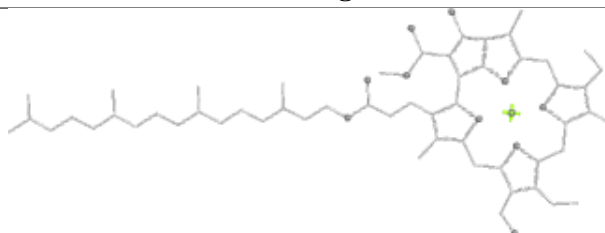
Bond lengths



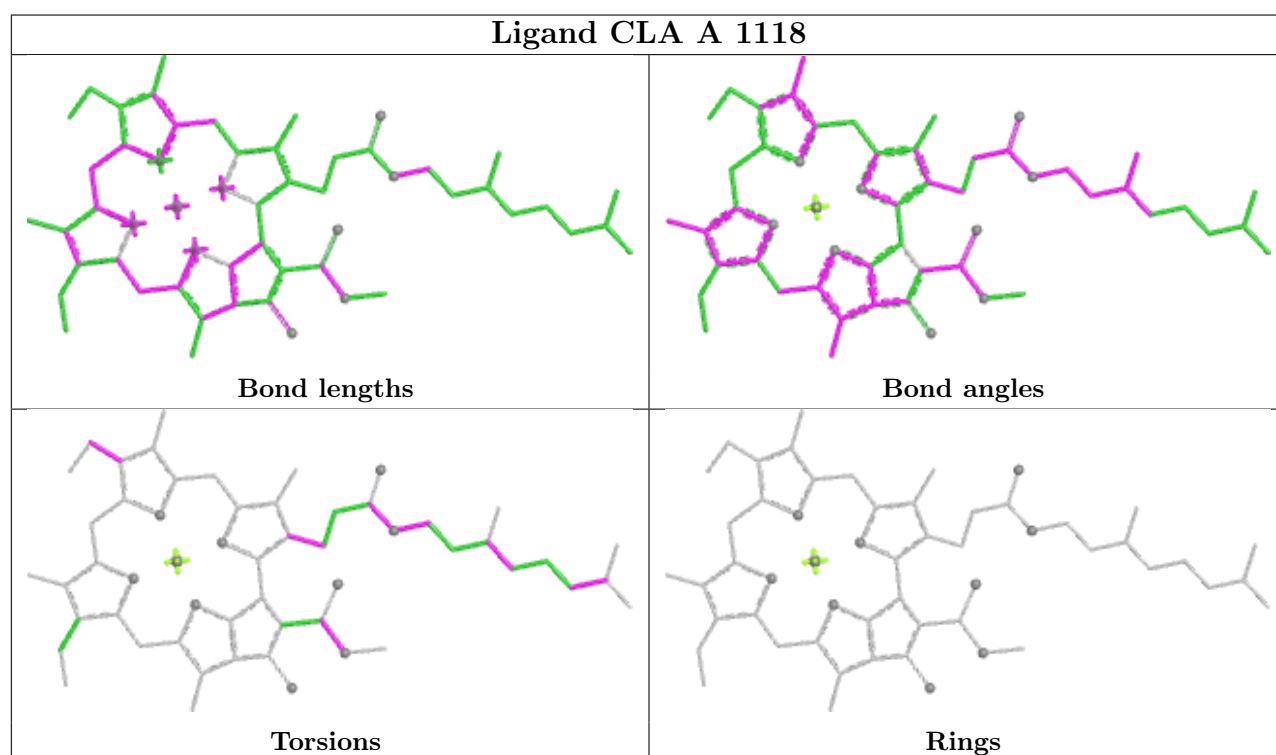
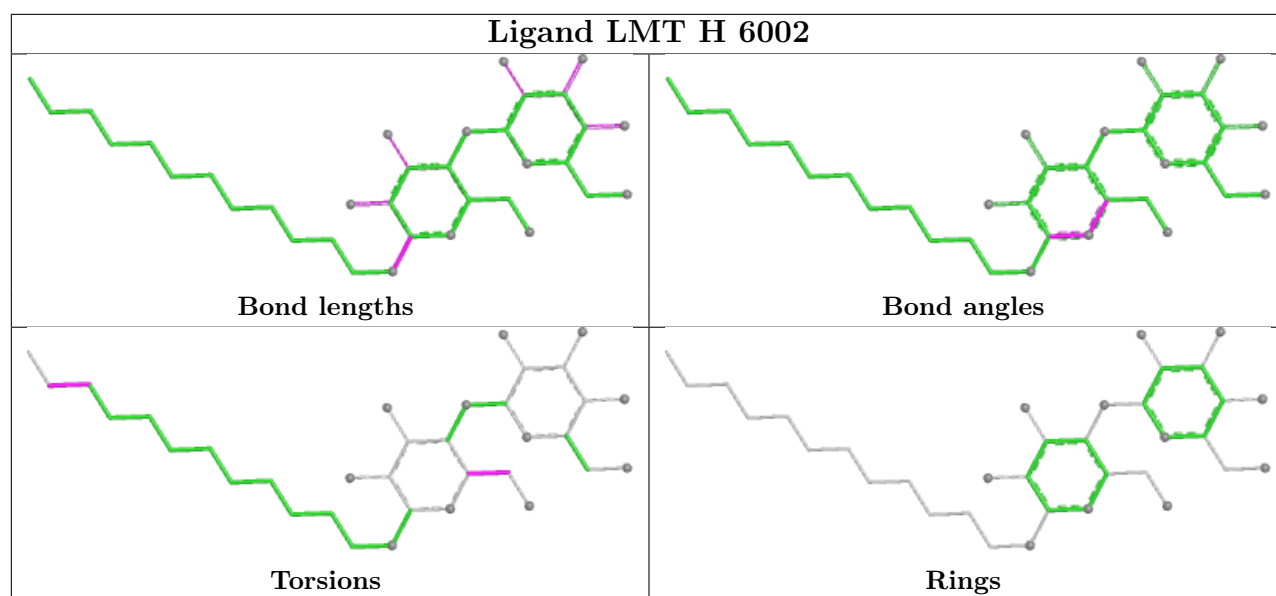
Bond angles

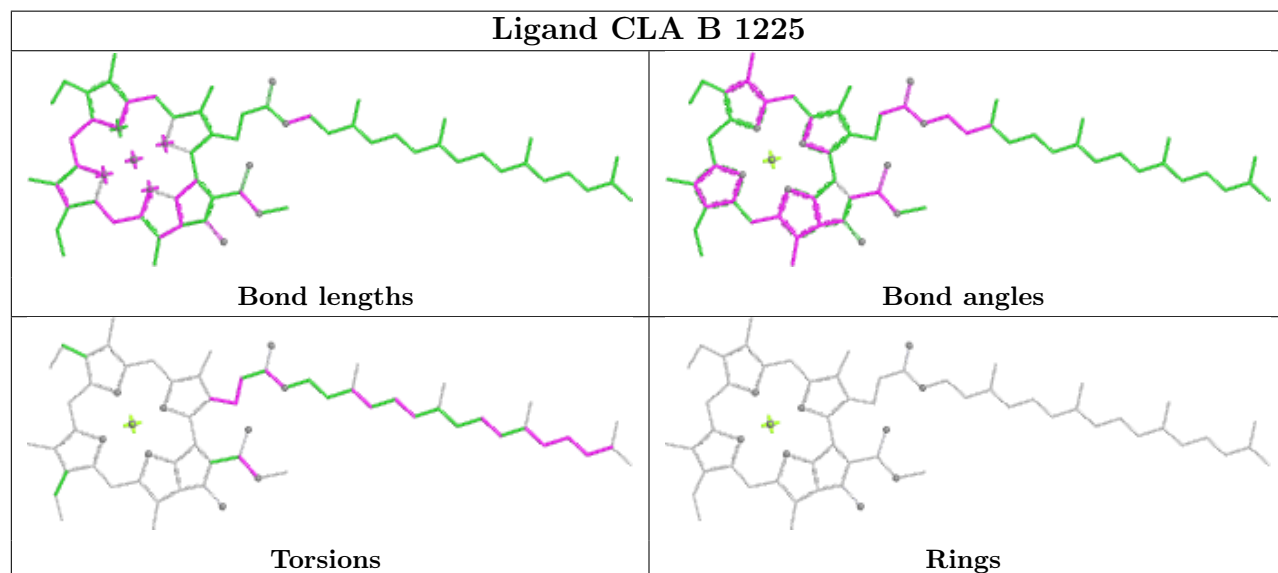
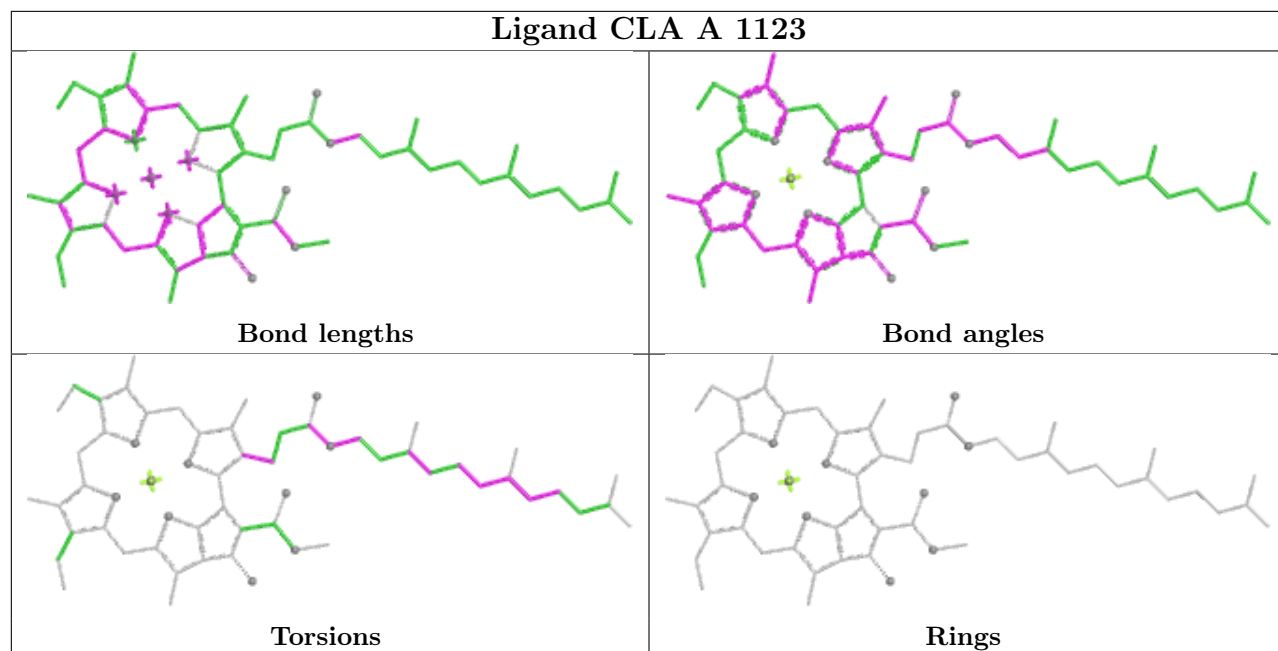


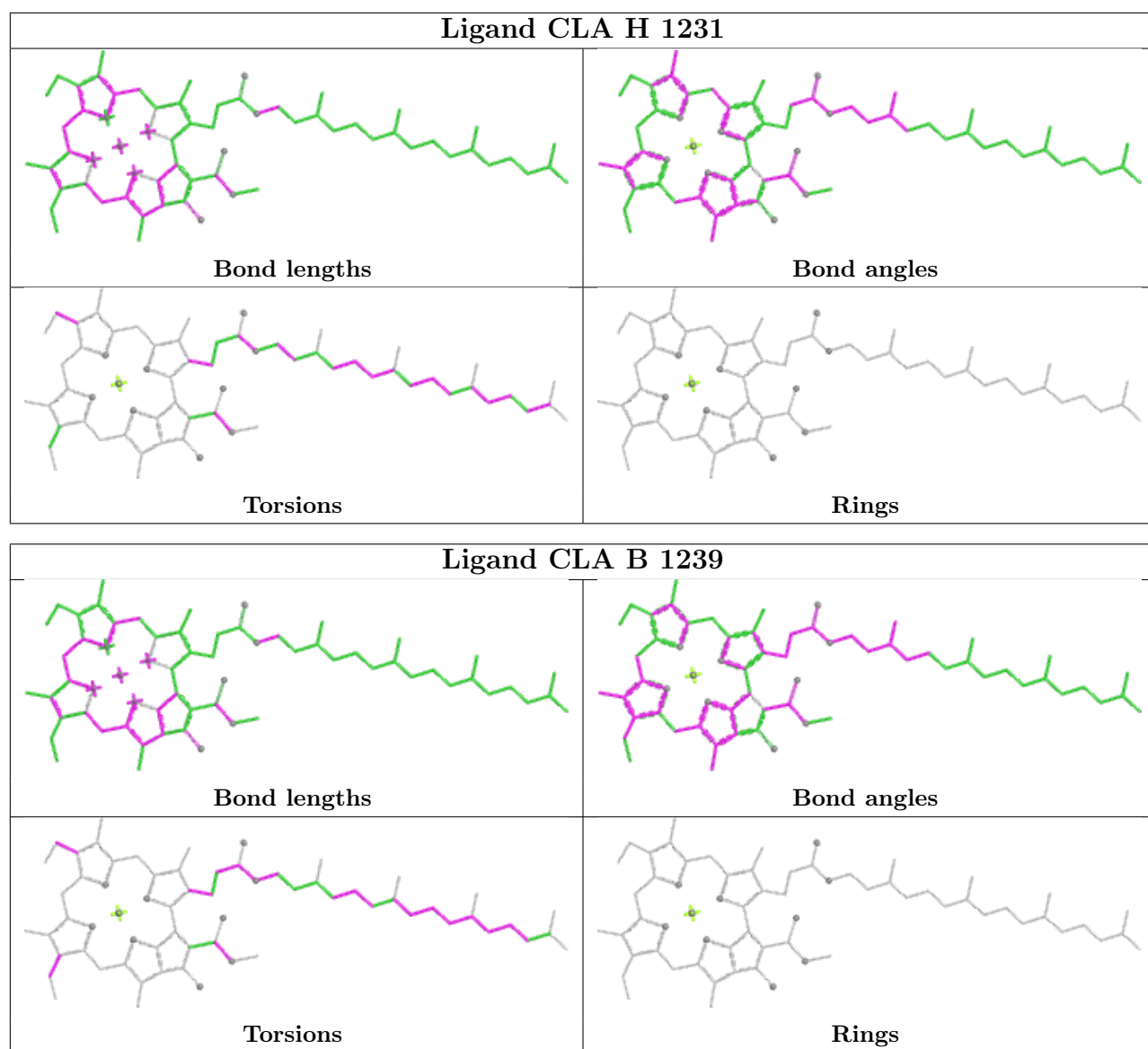
Torsions



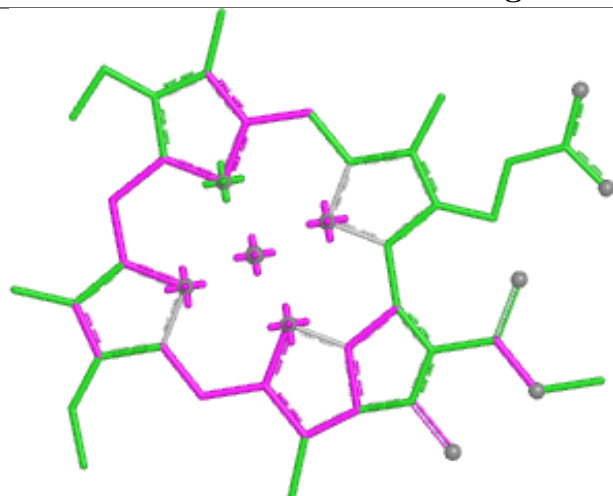
Rings



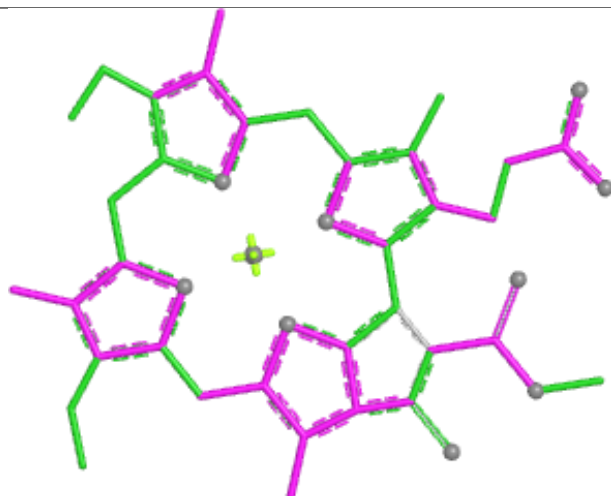




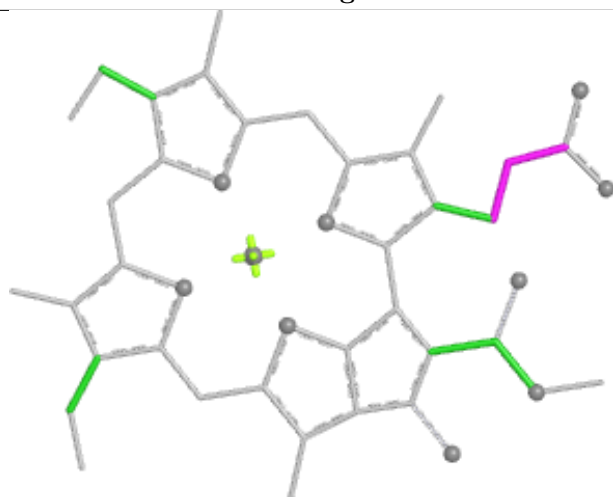
Ligand CLA A 1110



Bond lengths



Bond angles

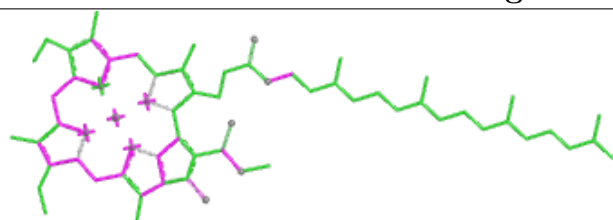


Torsions

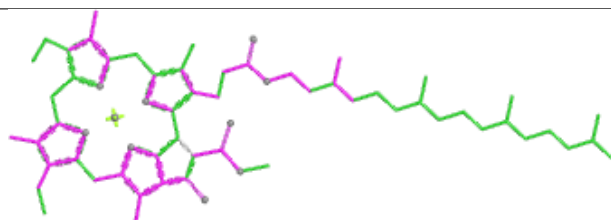


Rings

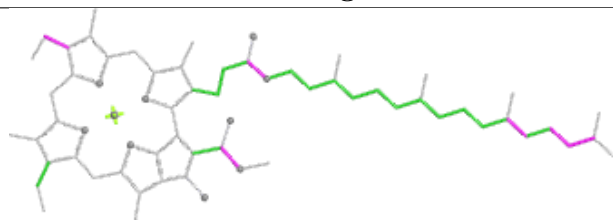
Ligand CLA B 1204



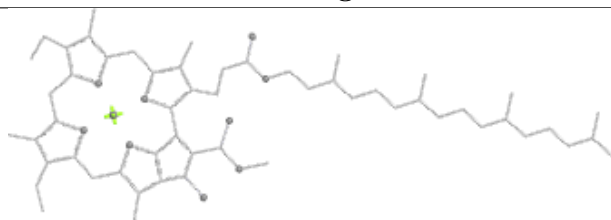
Bond lengths



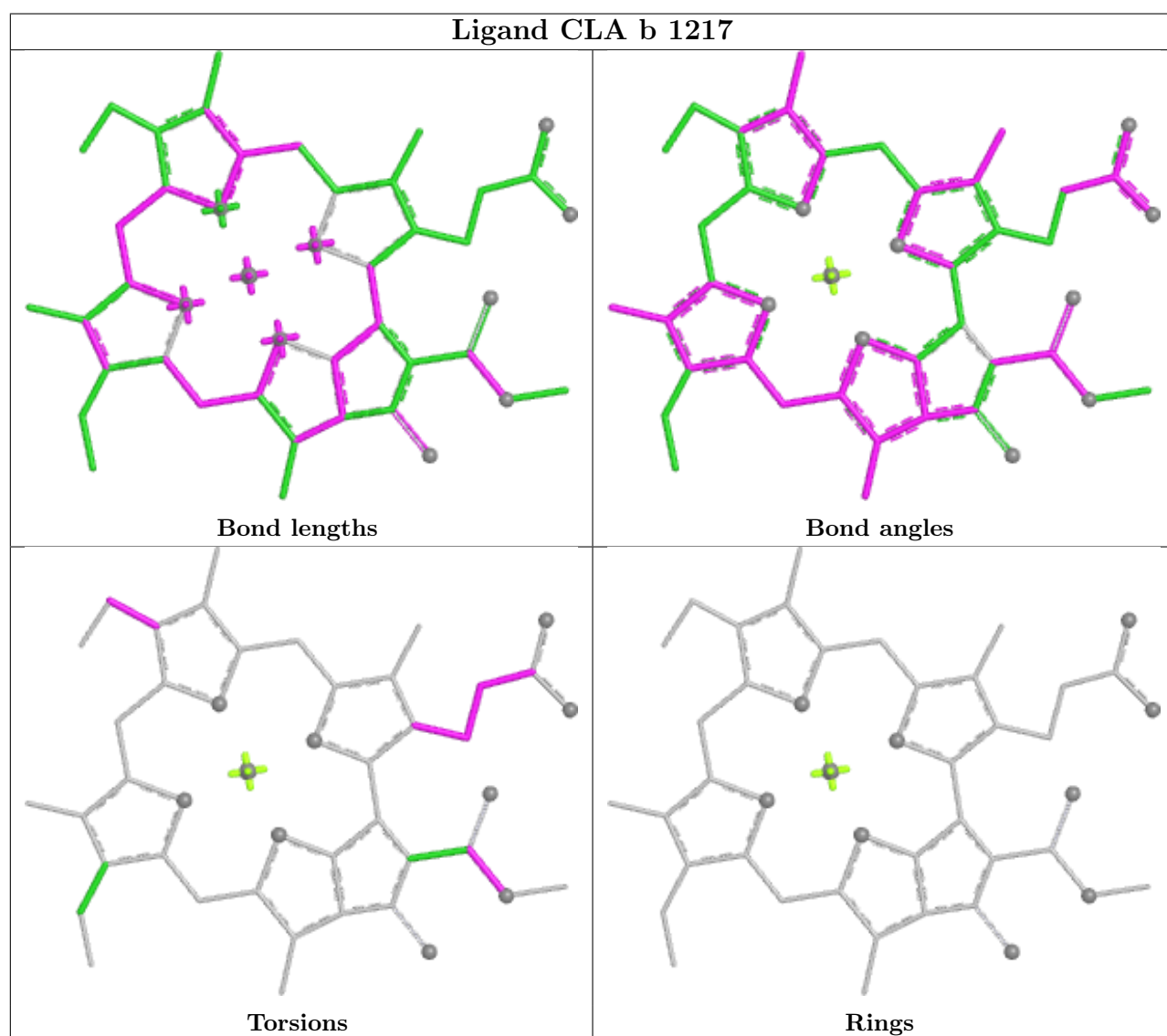
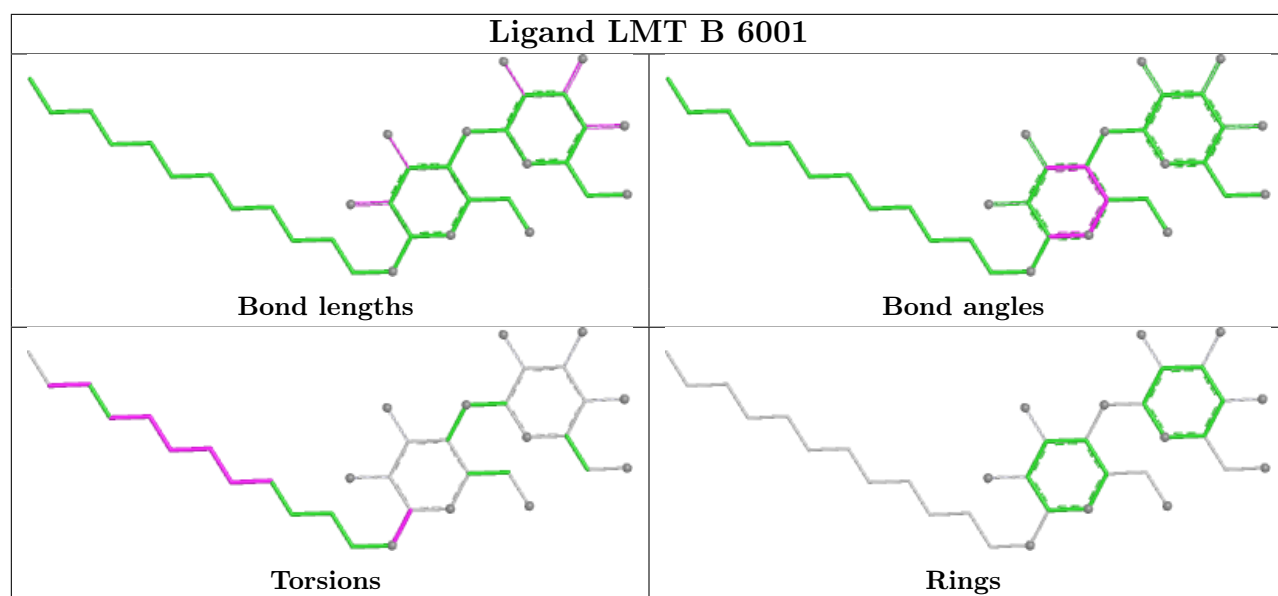
Bond angles

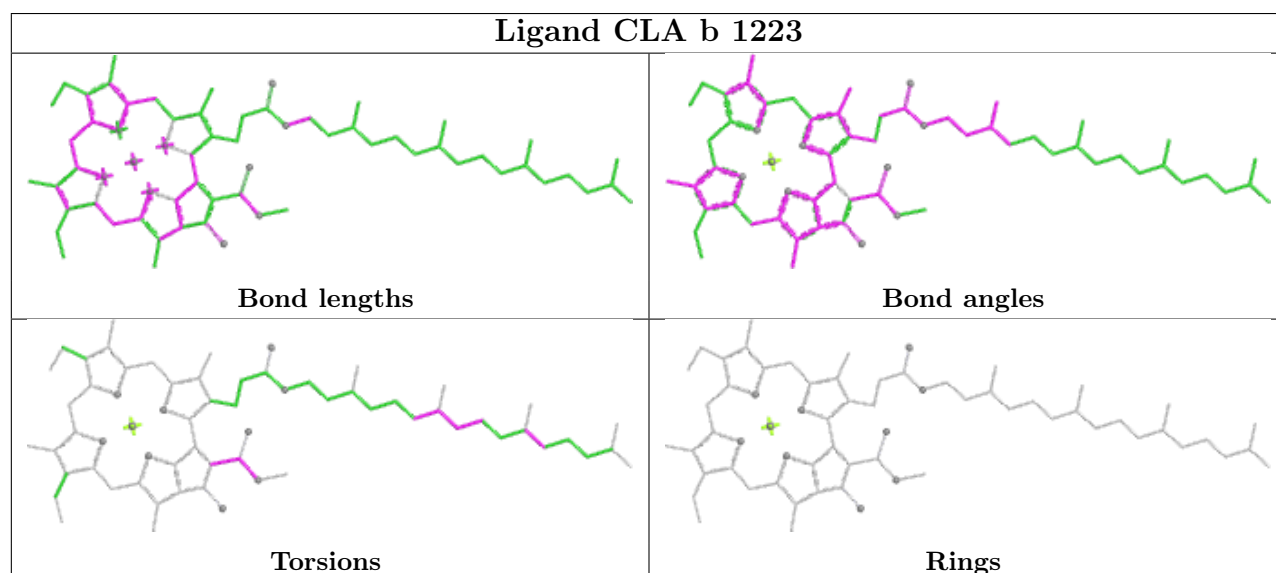
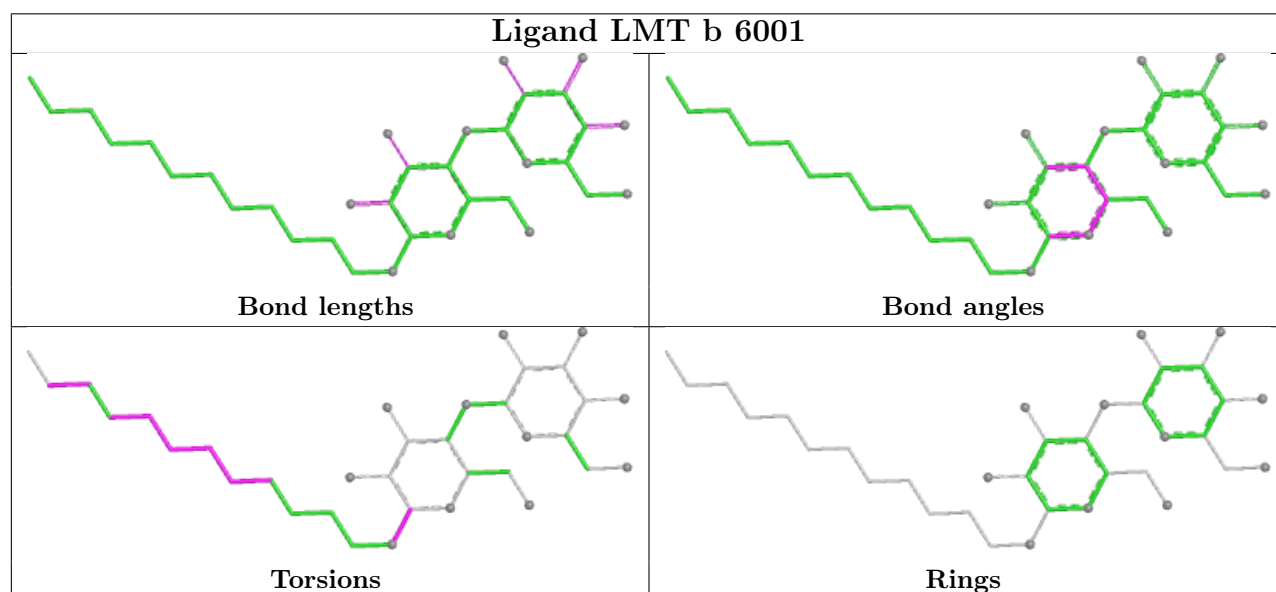
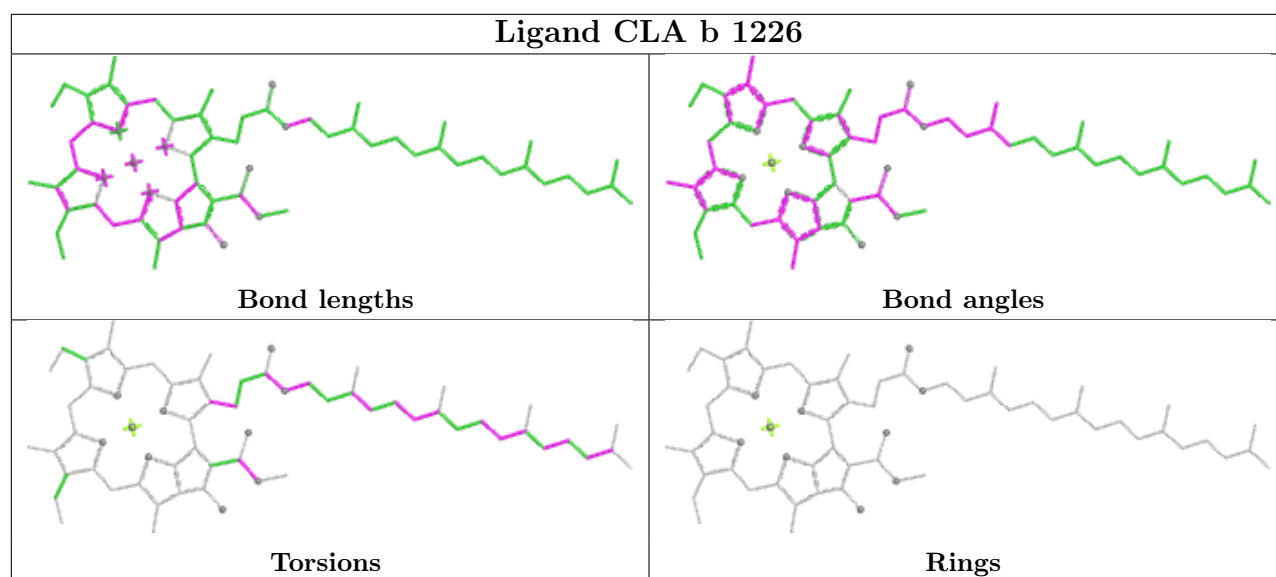


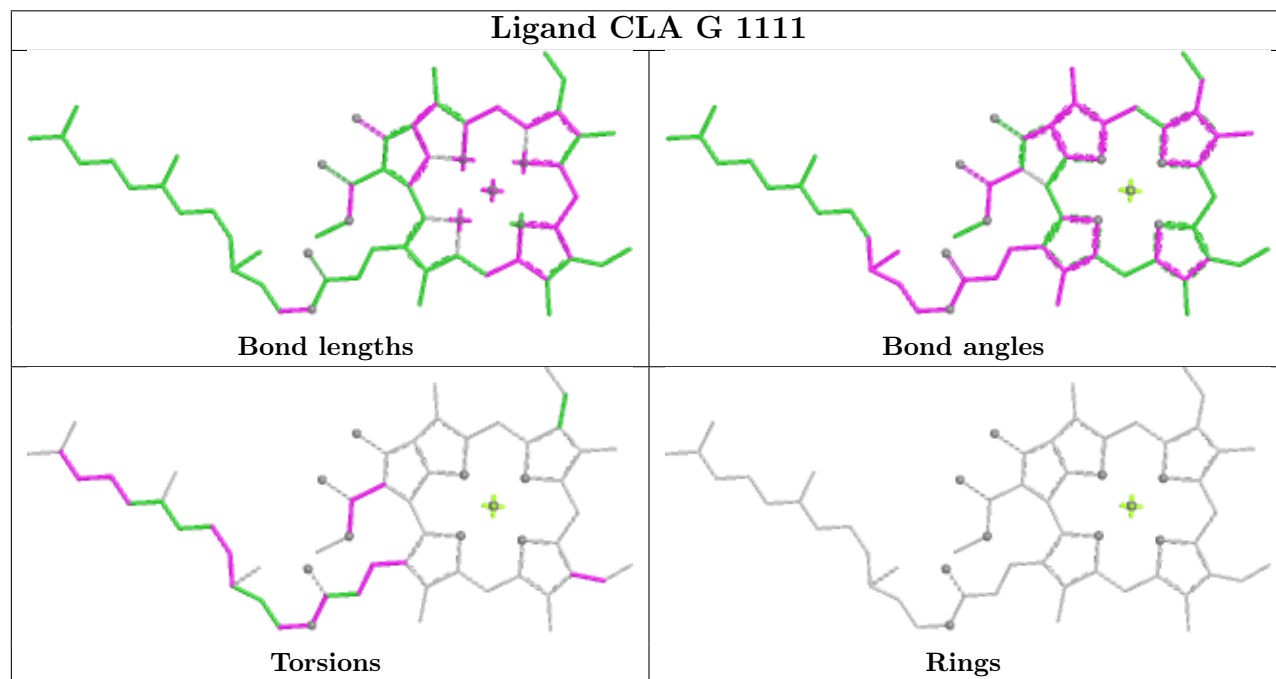
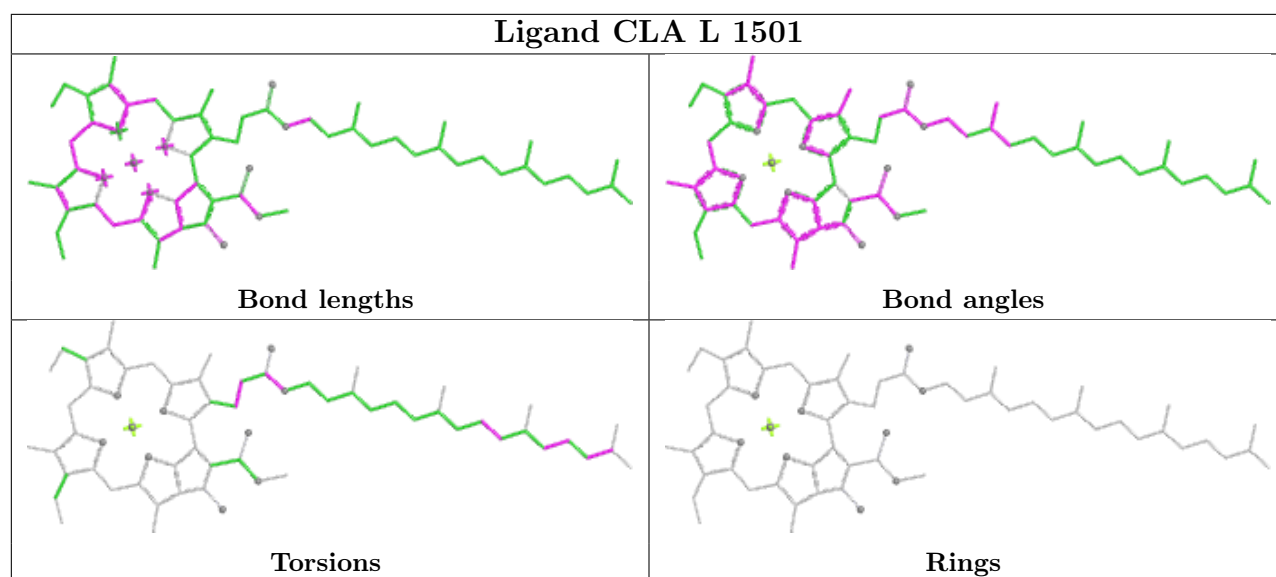
Torsions

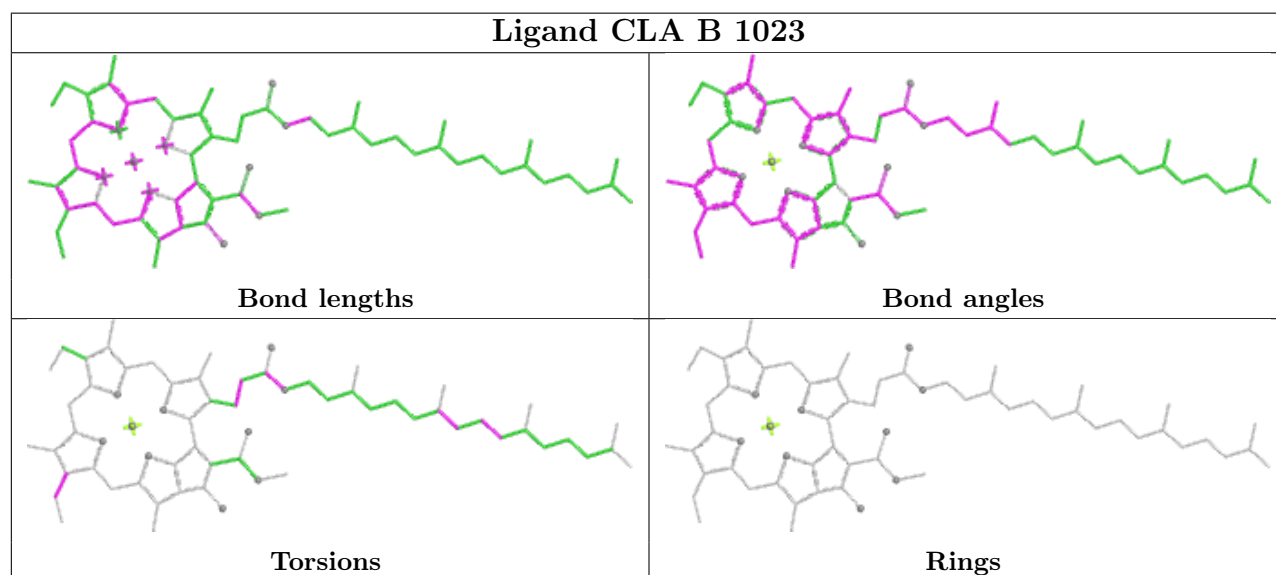
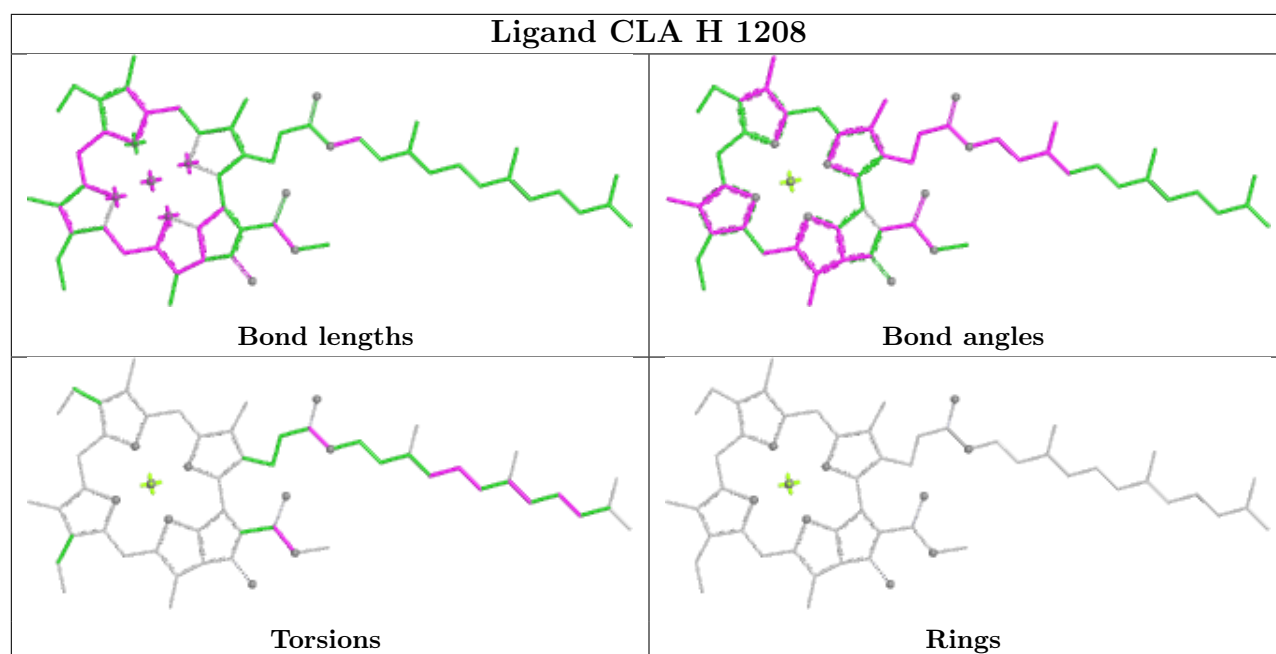


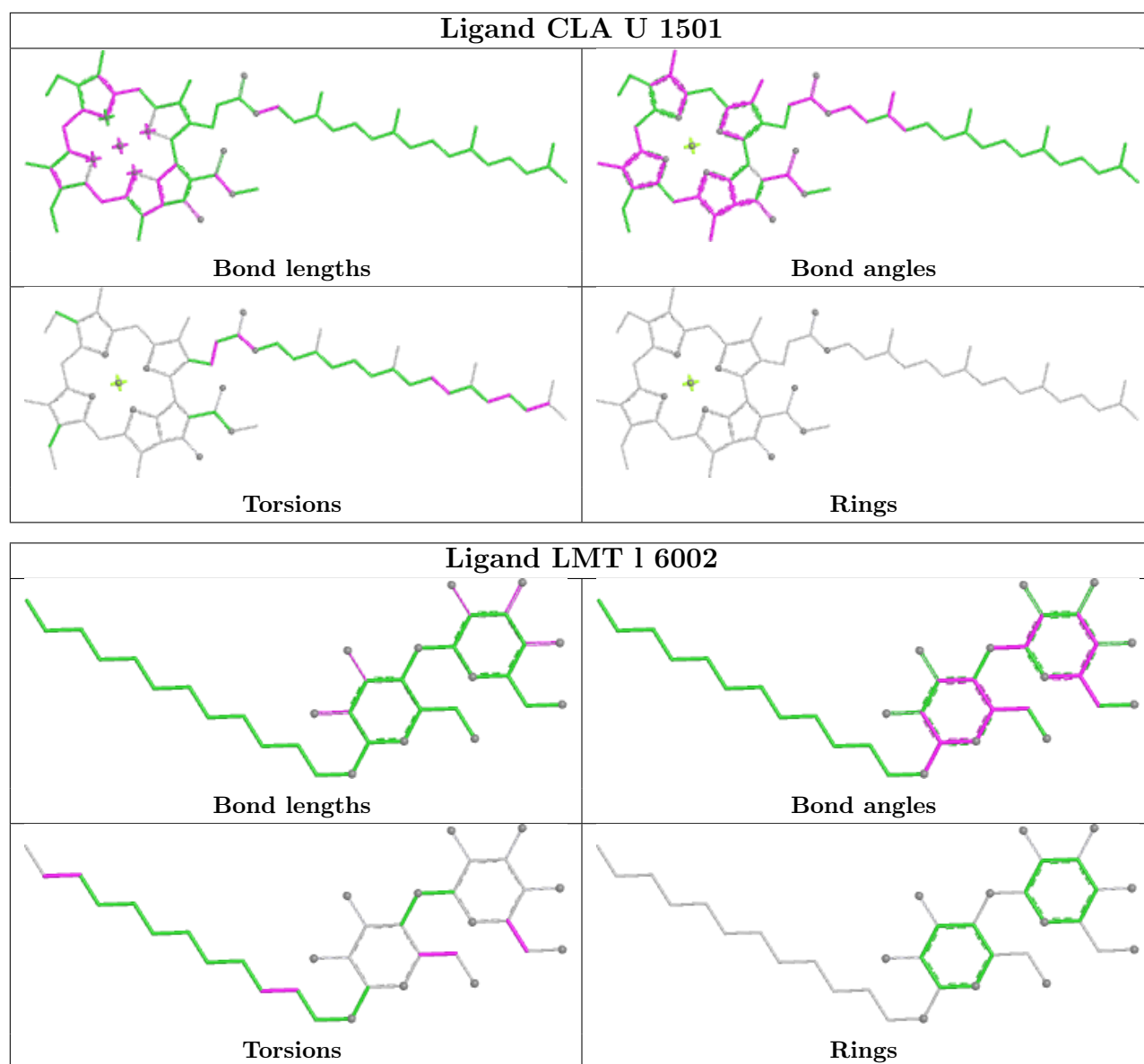
Rings

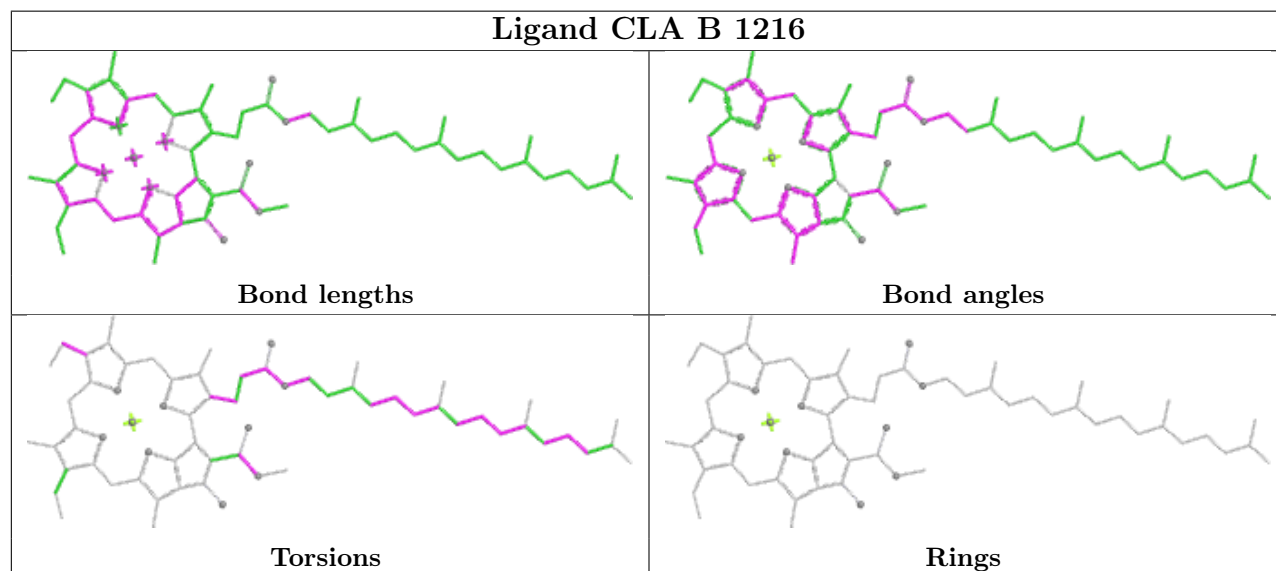
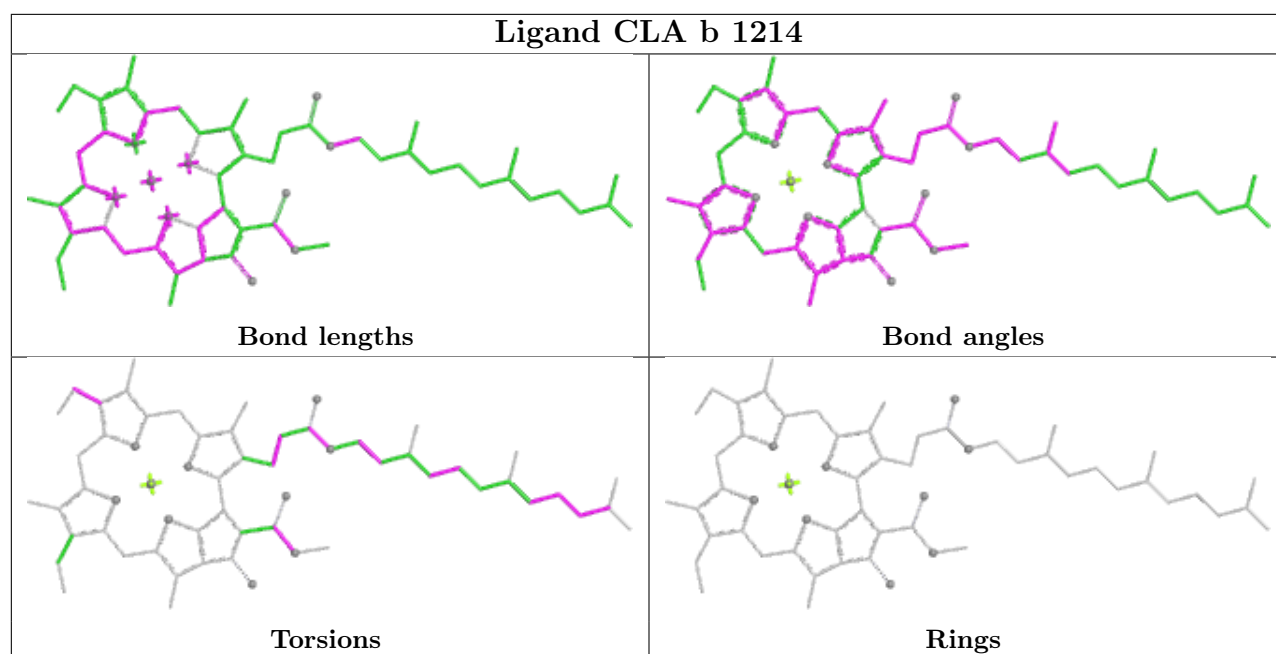


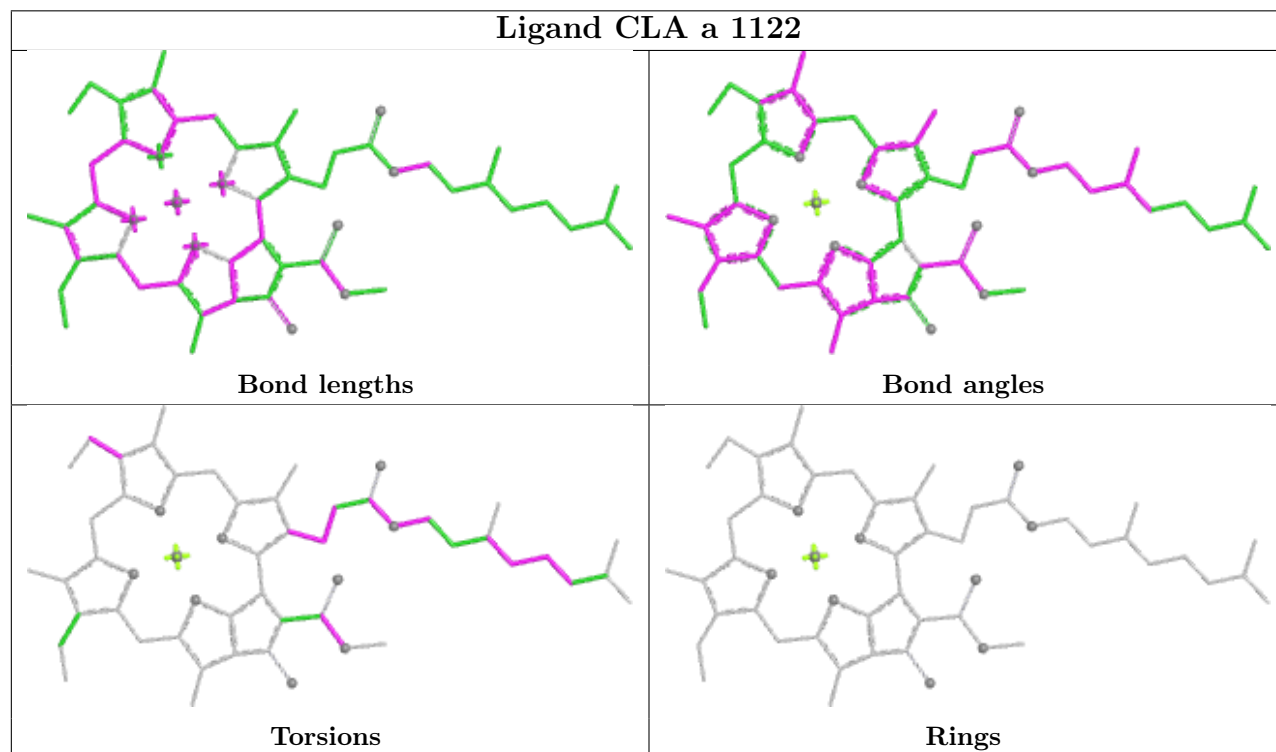
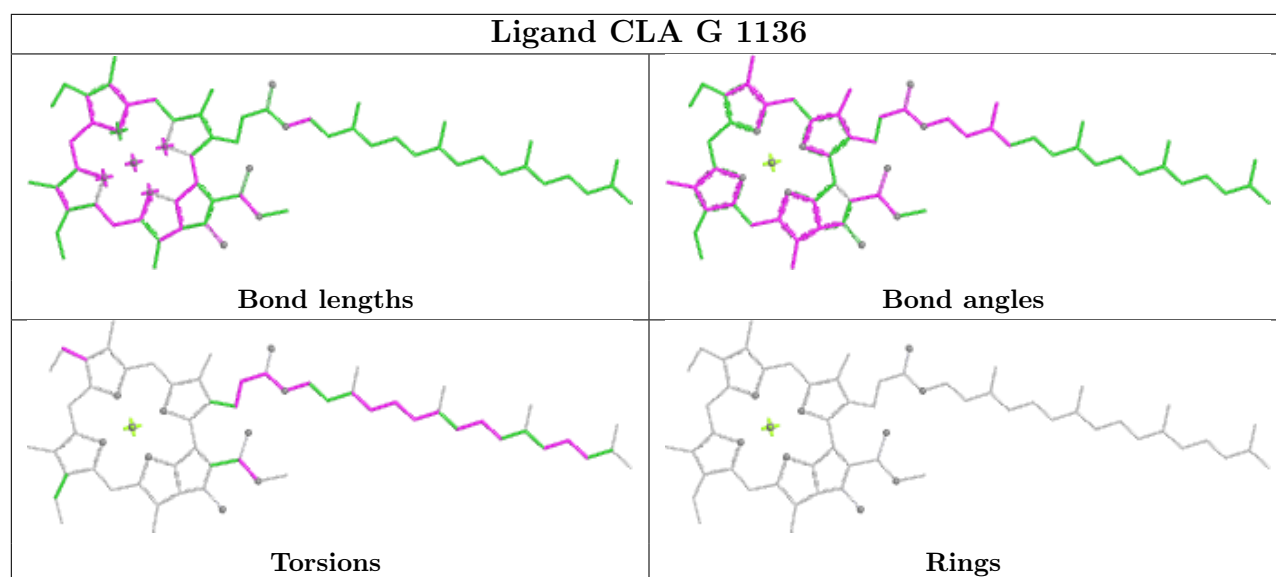


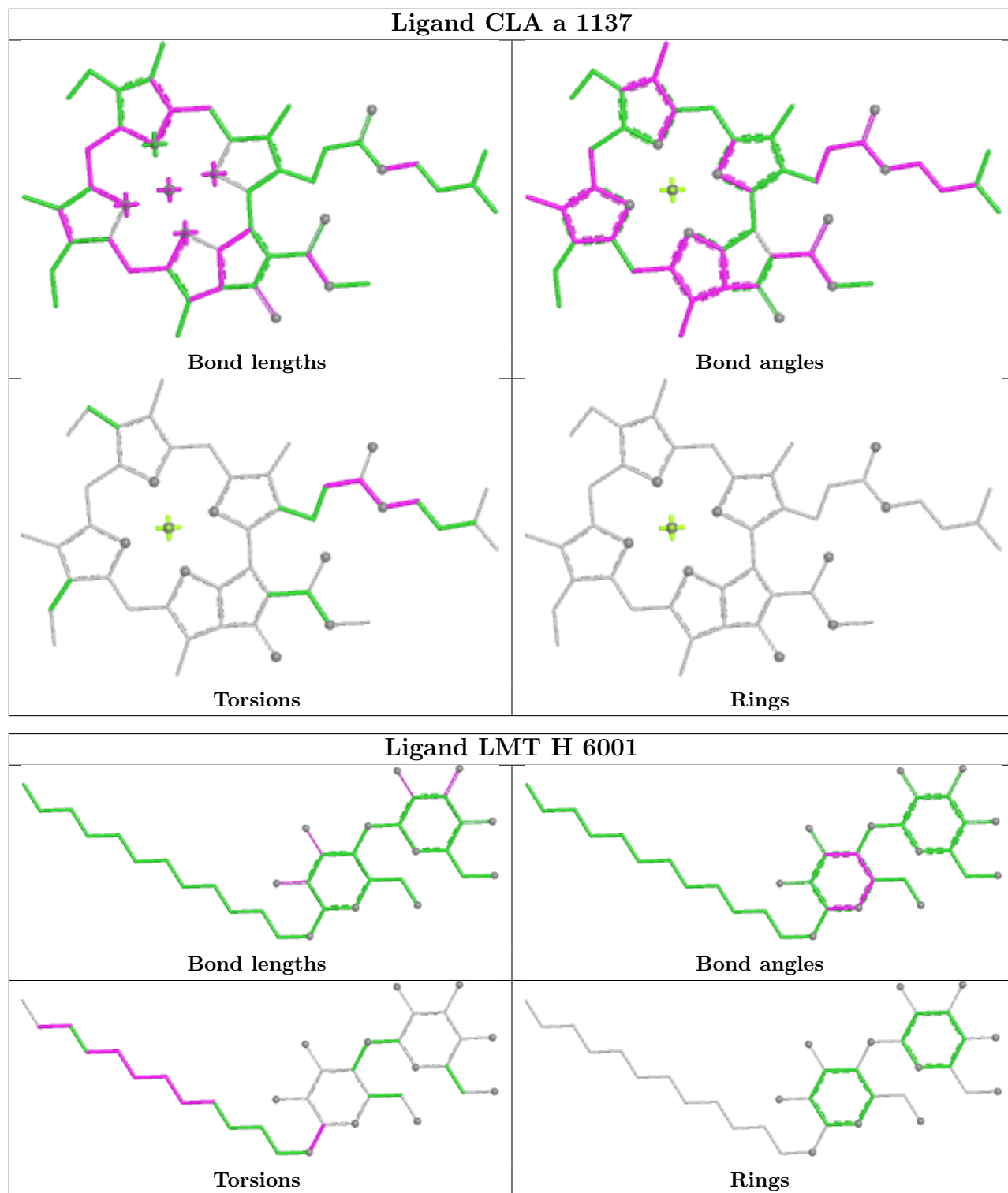


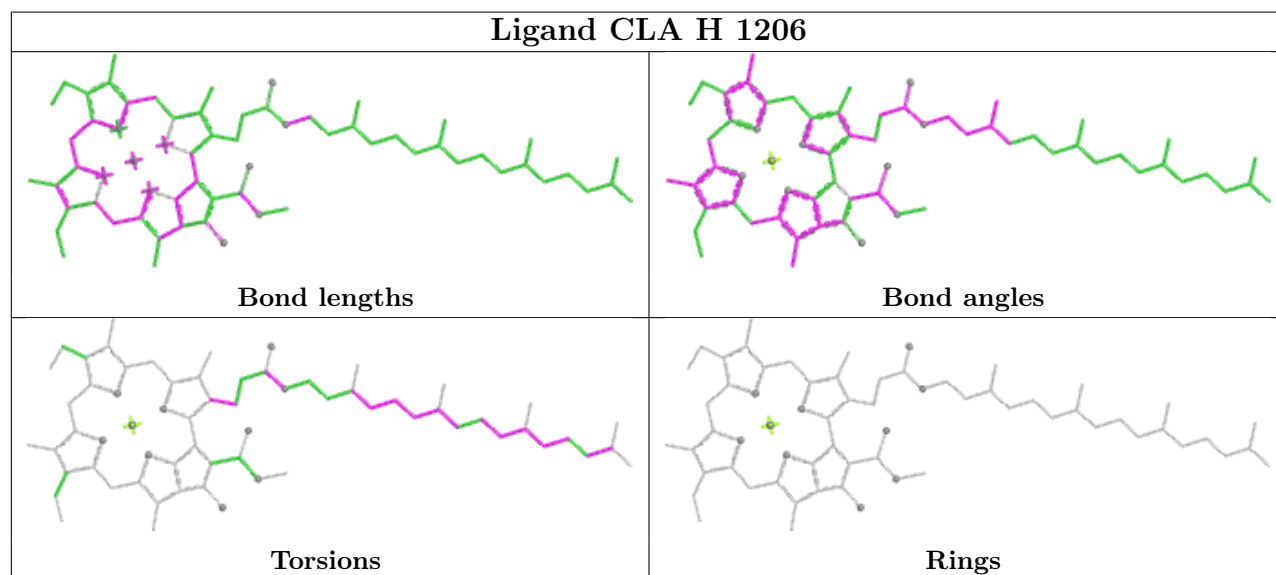
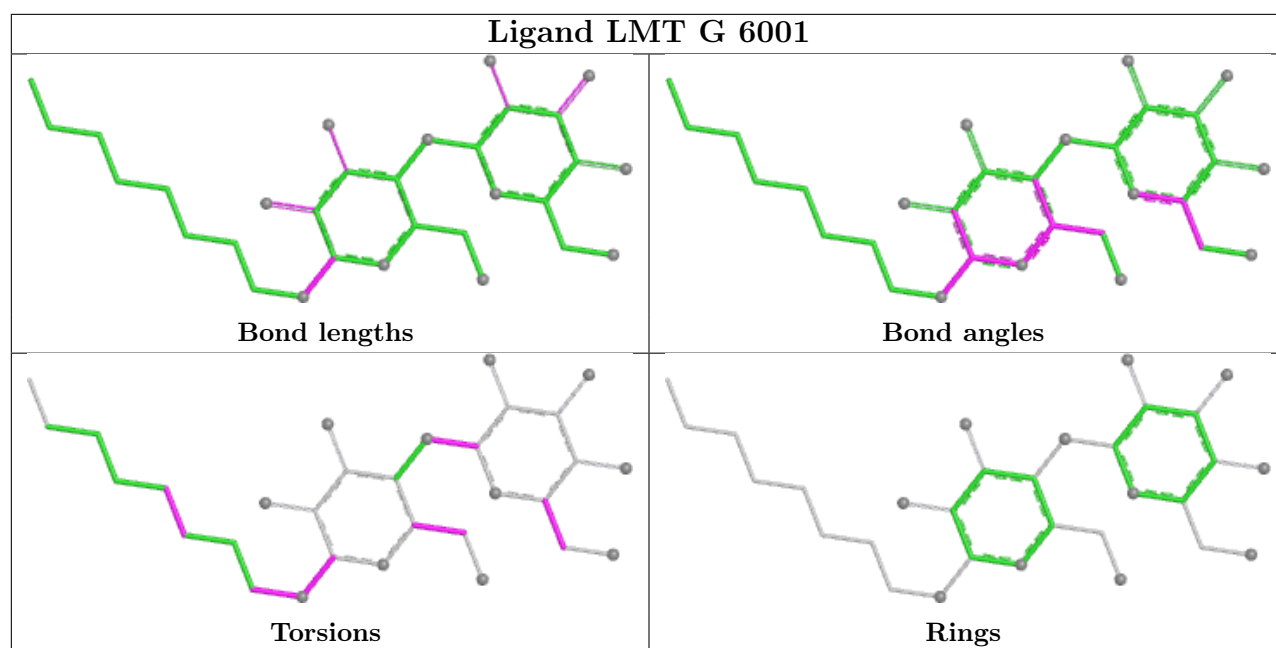




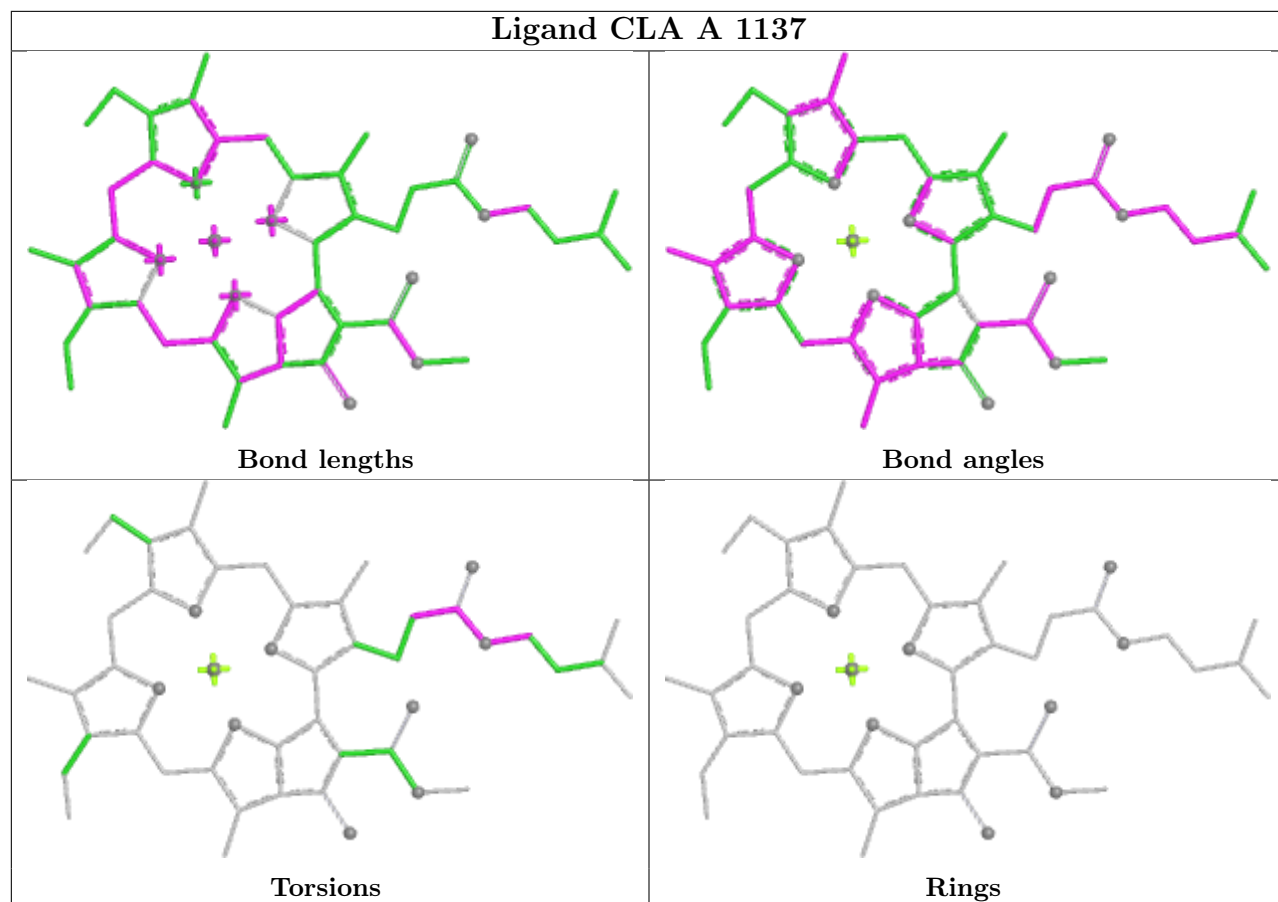


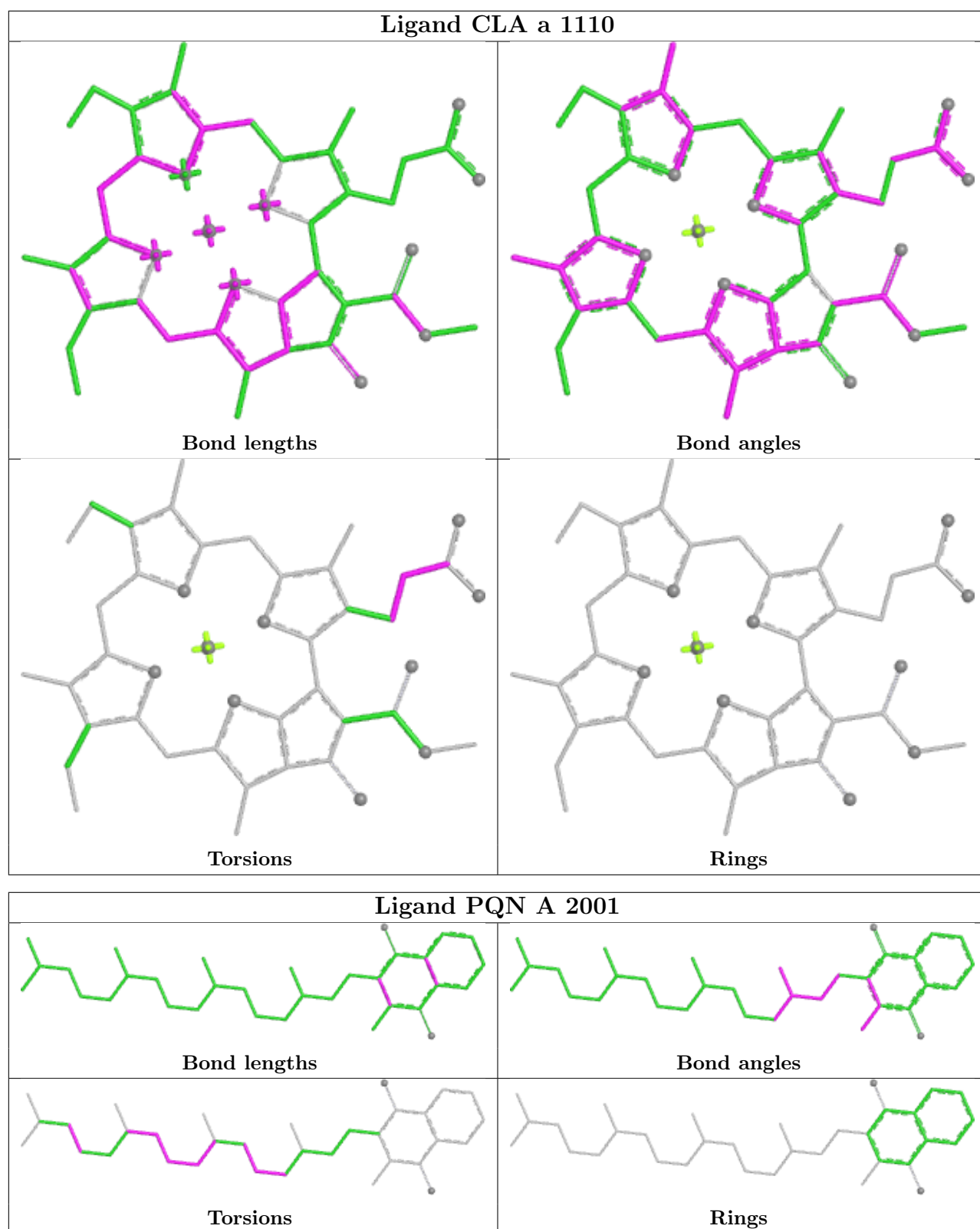


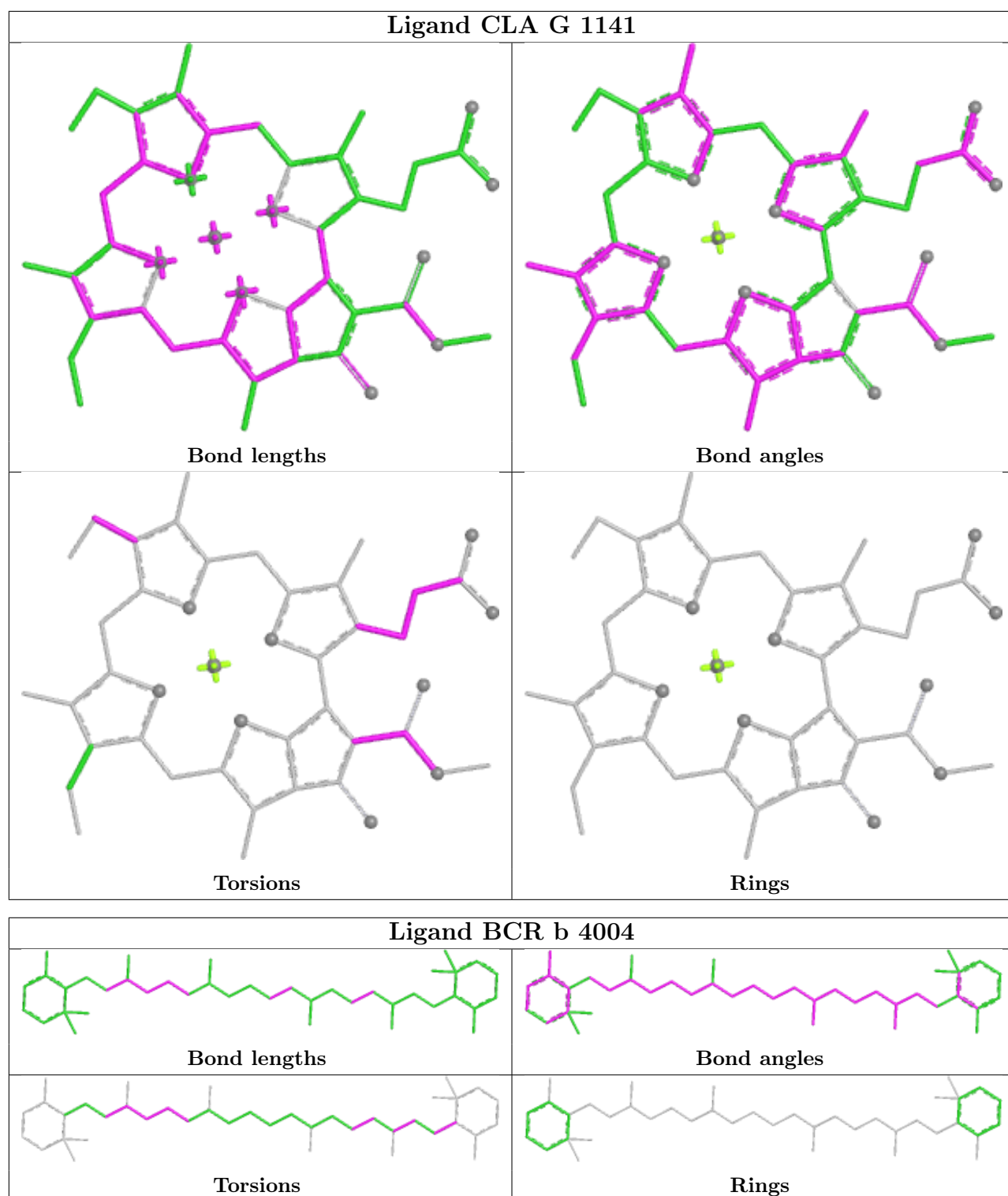


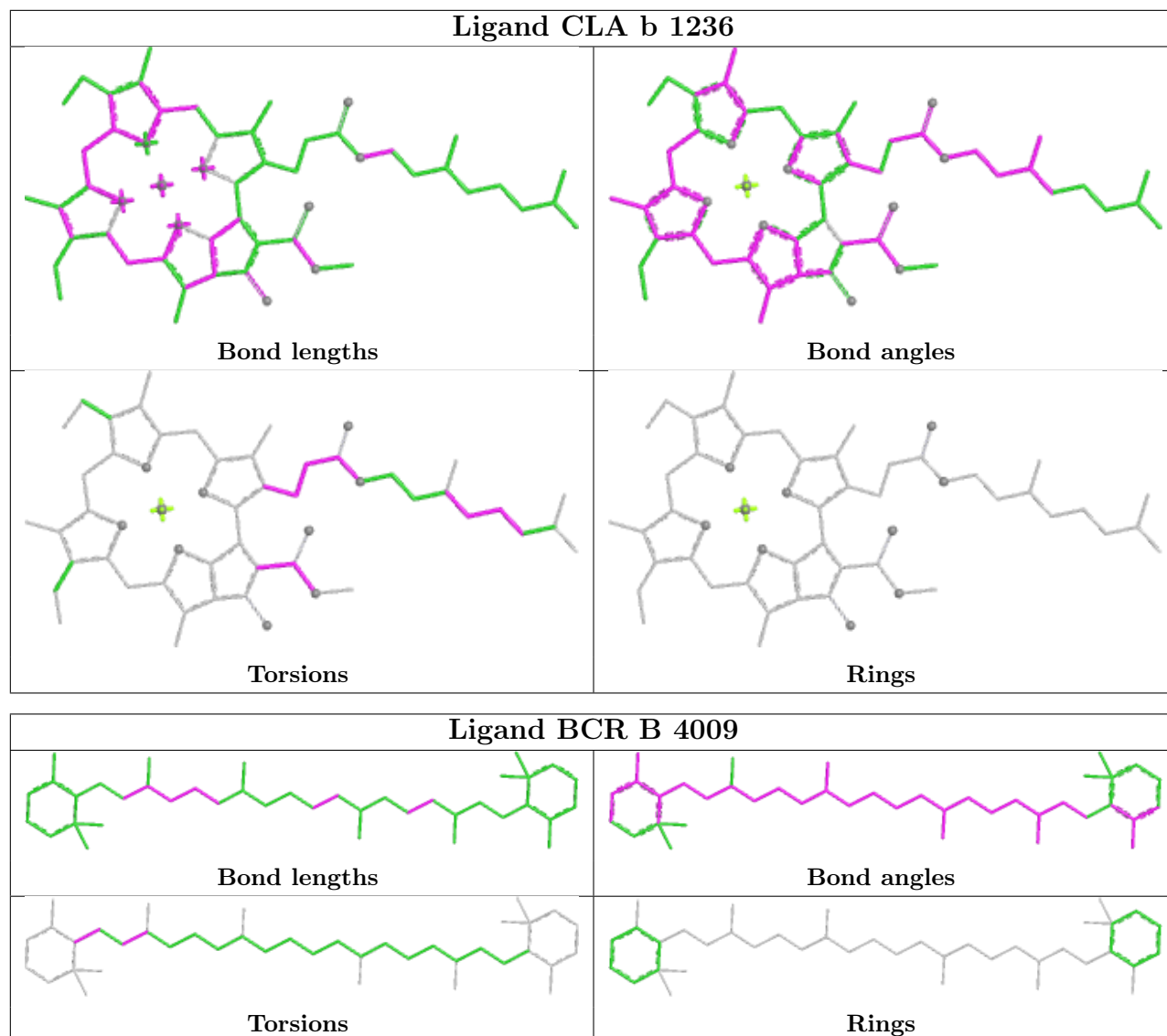


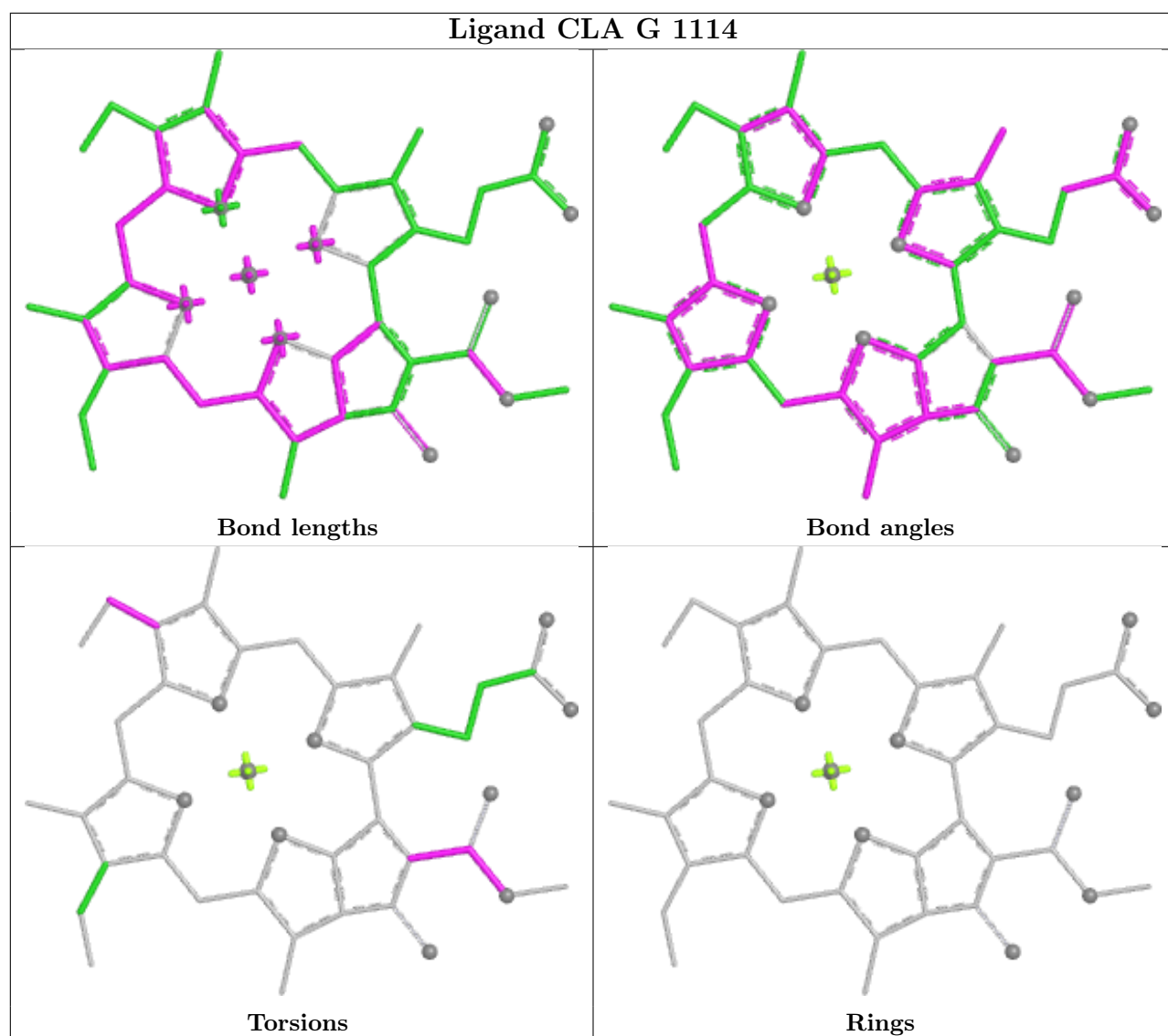
Ligand CLA A 1137



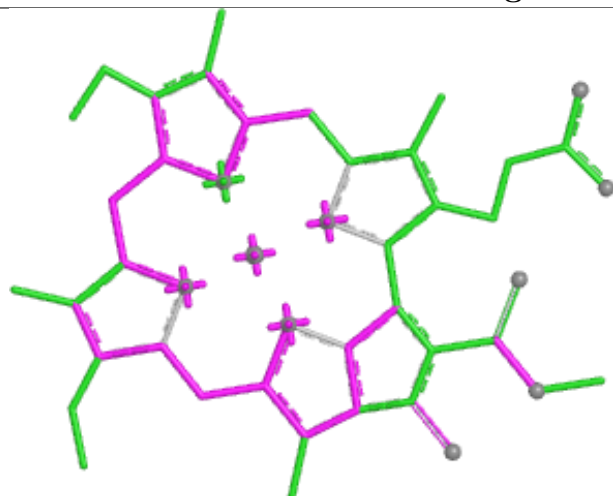




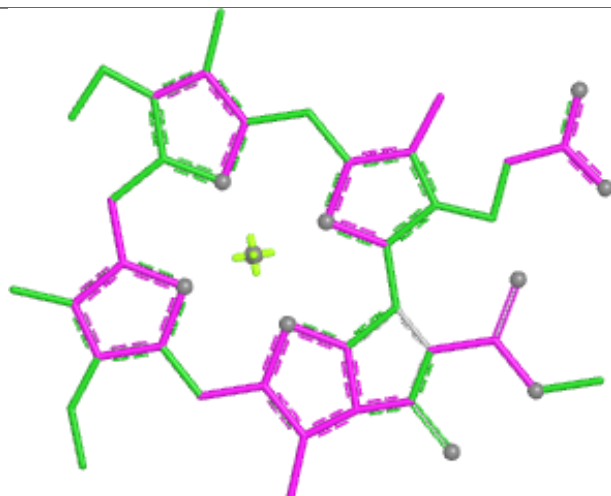




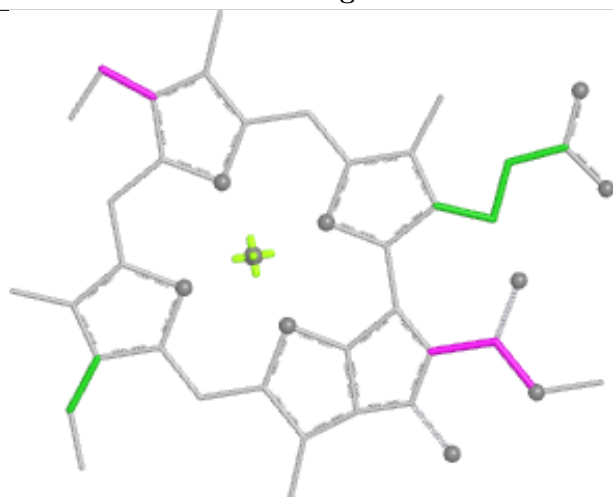
Ligand CLA A 1114



Bond lengths



Bond angles

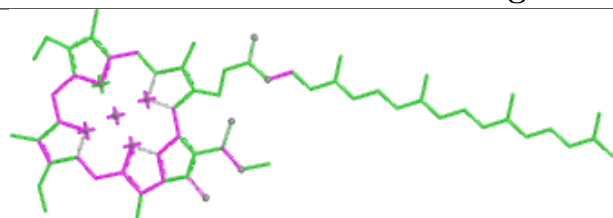


Torsions

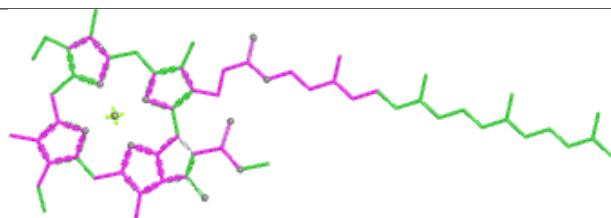


Rings

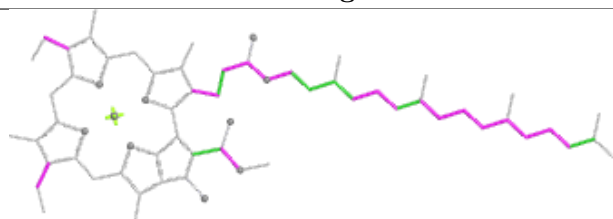
Ligand CLA b 1239



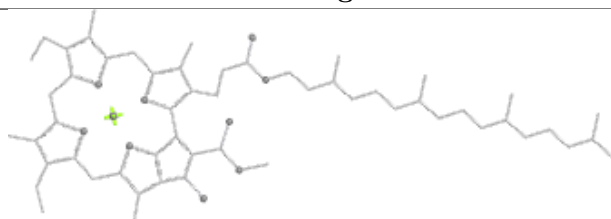
Bond lengths



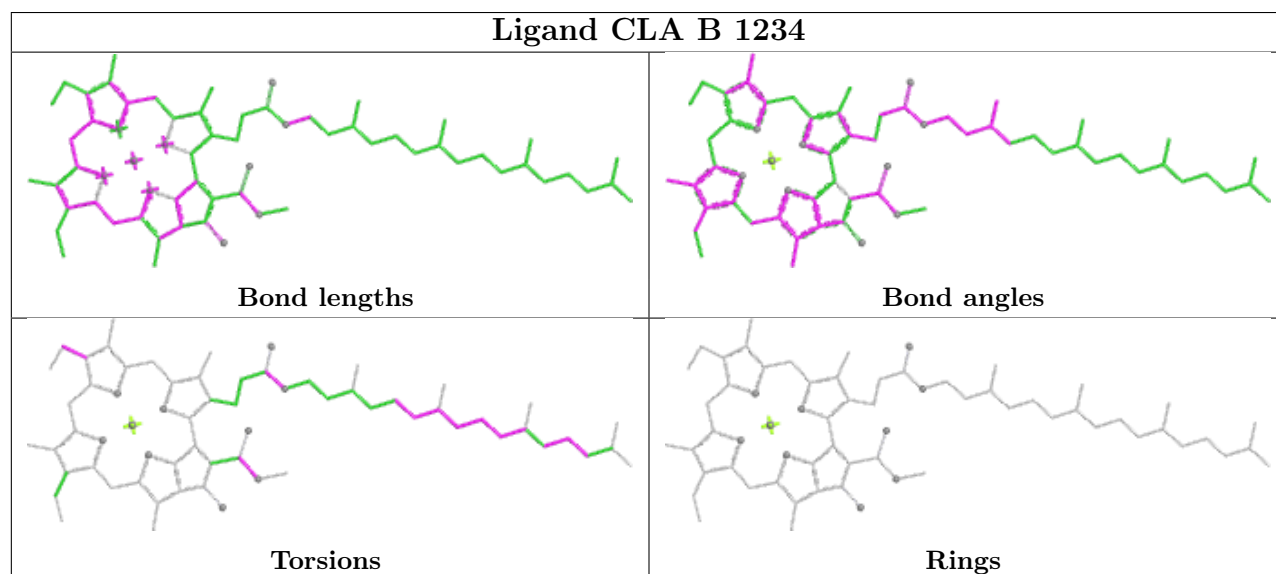
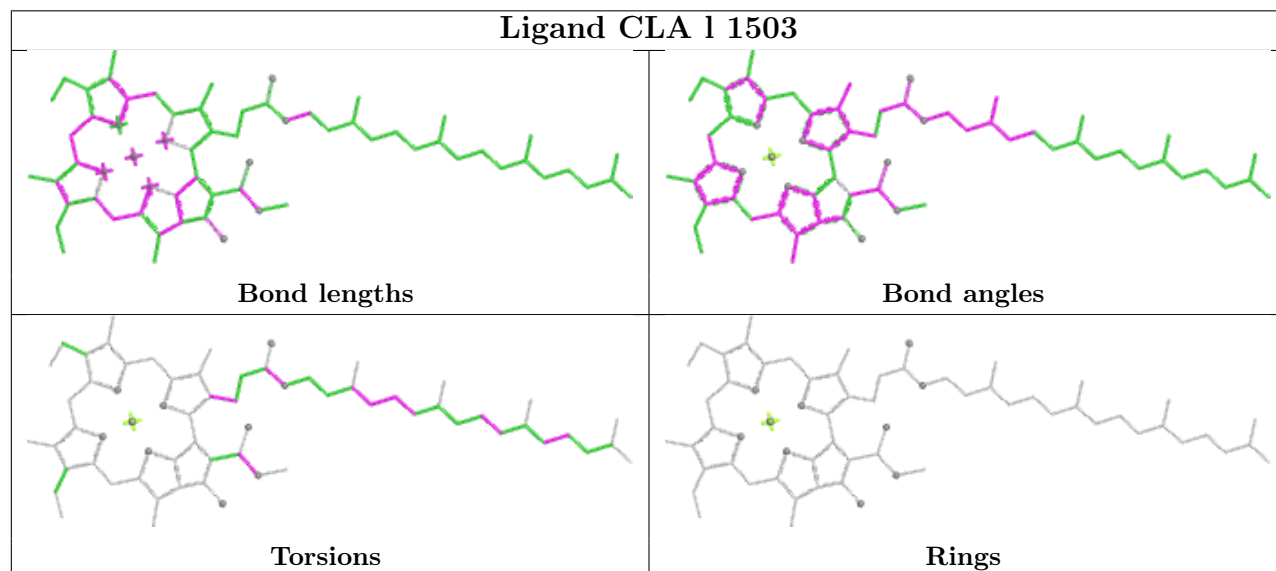
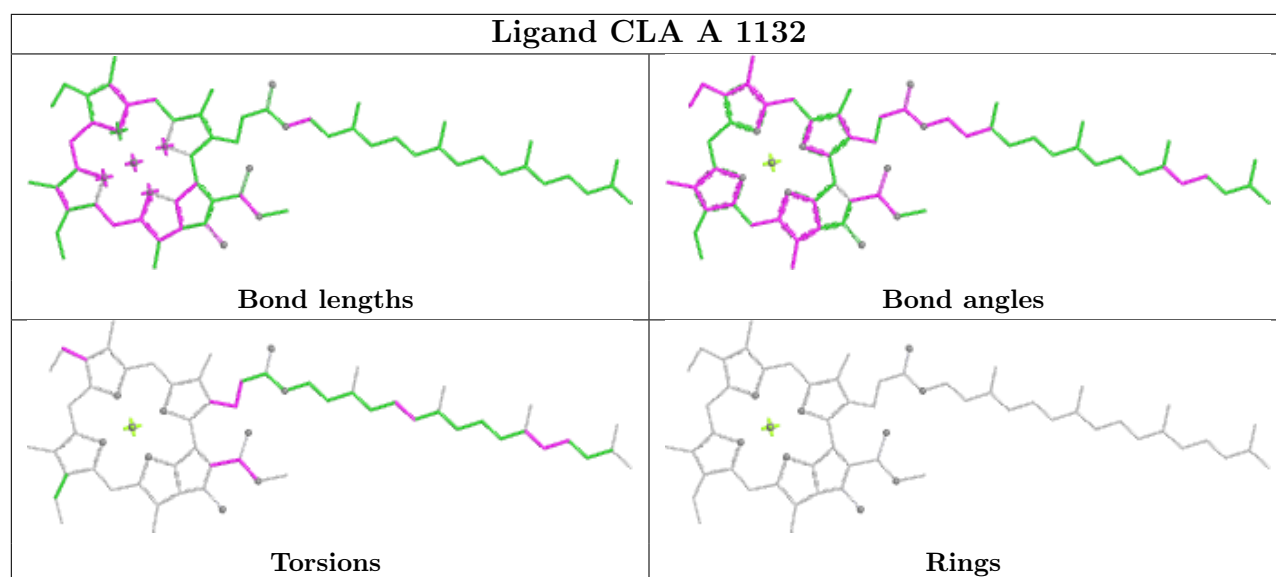
Bond angles

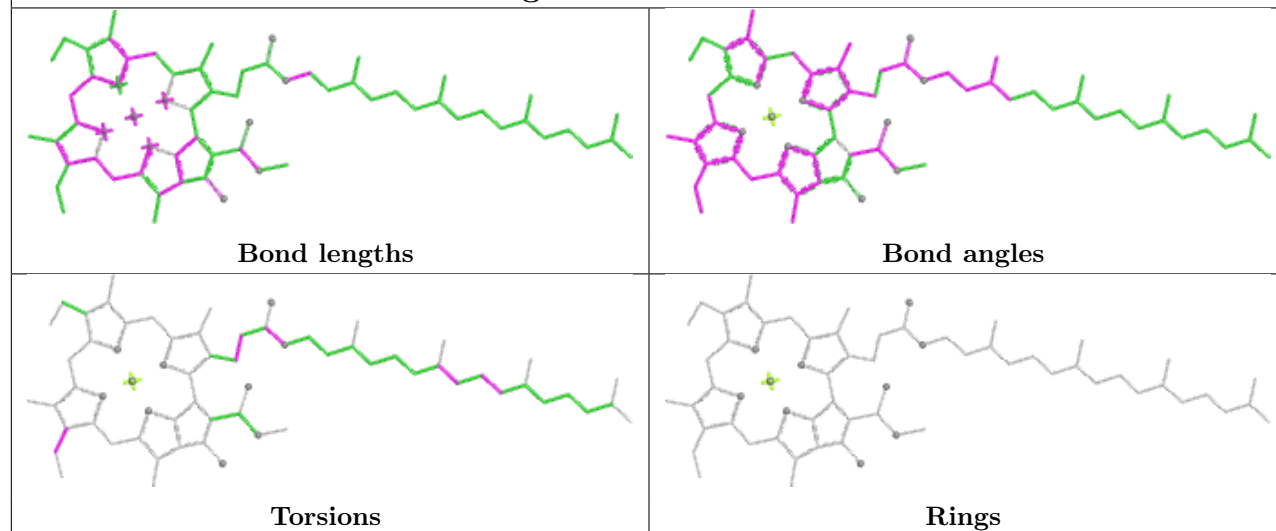
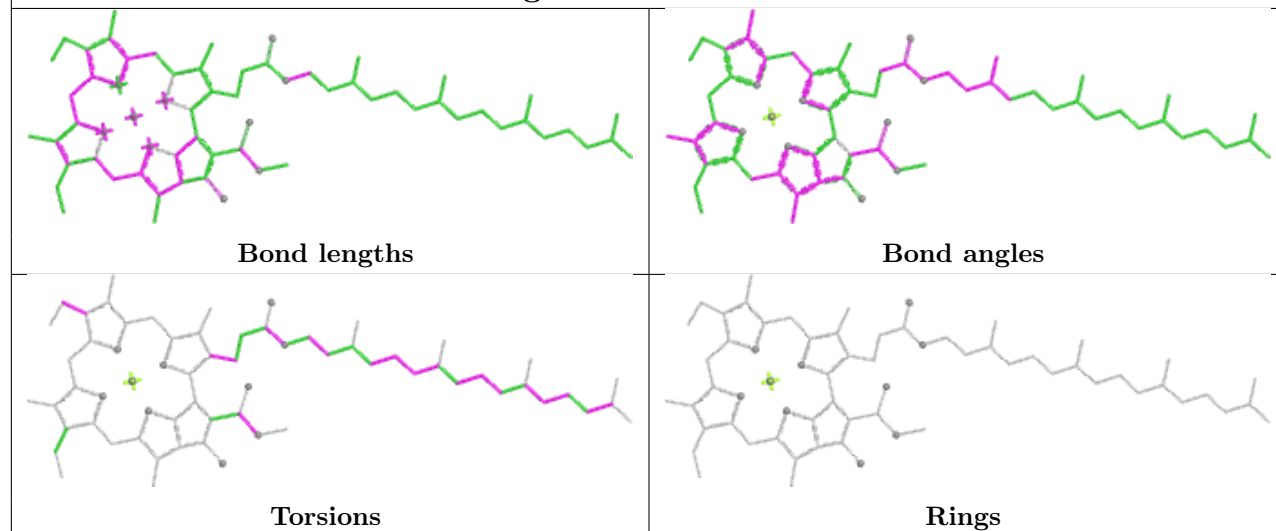


Torsions

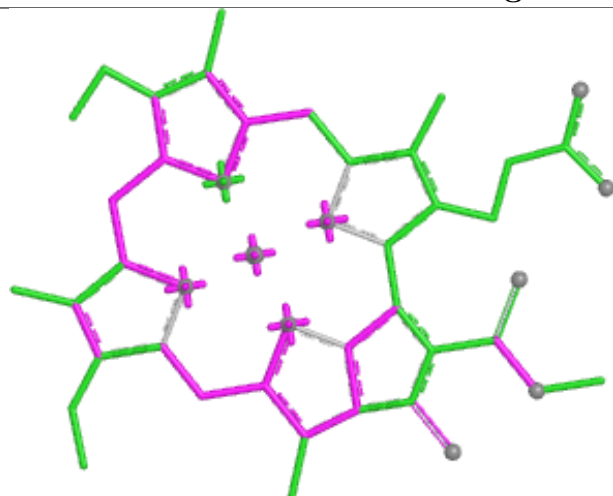


Rings

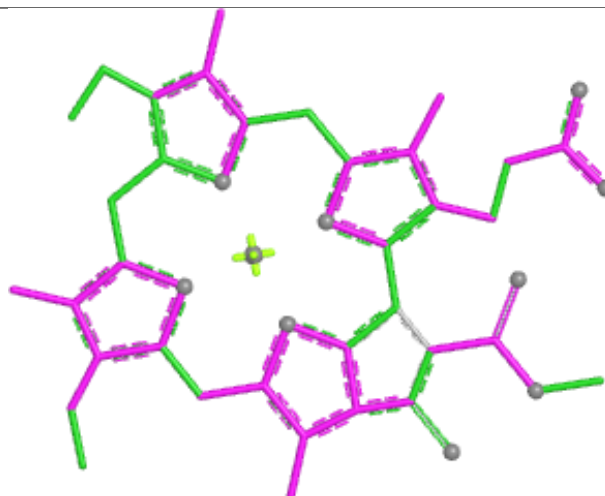


Ligand CLA H 1023**Ligand CLA B 1231**

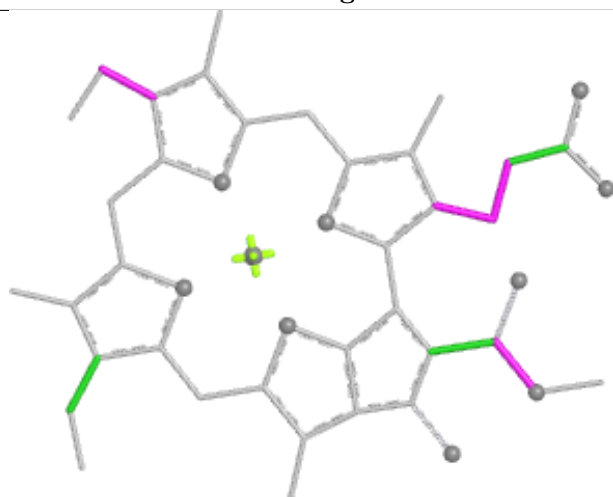
Ligand CLA A 1113



Bond lengths



Bond angles

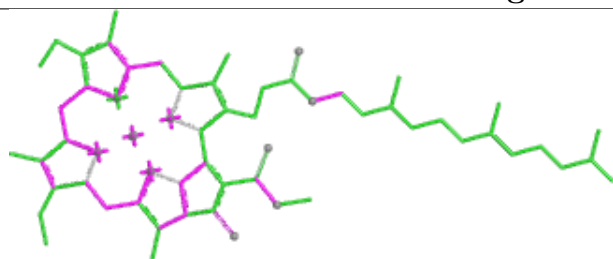


Torsions

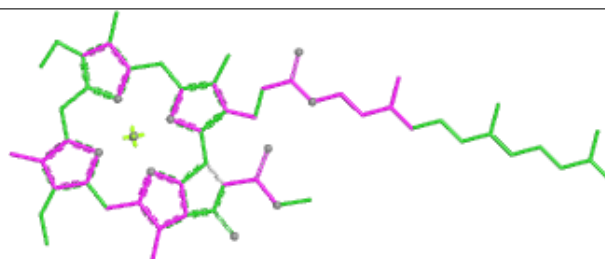


Rings

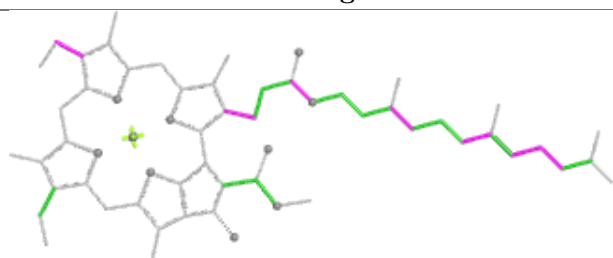
Ligand CLA L 1502



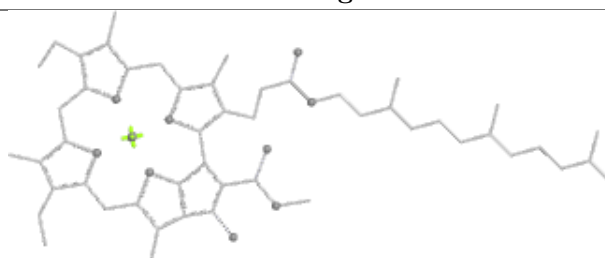
Bond lengths



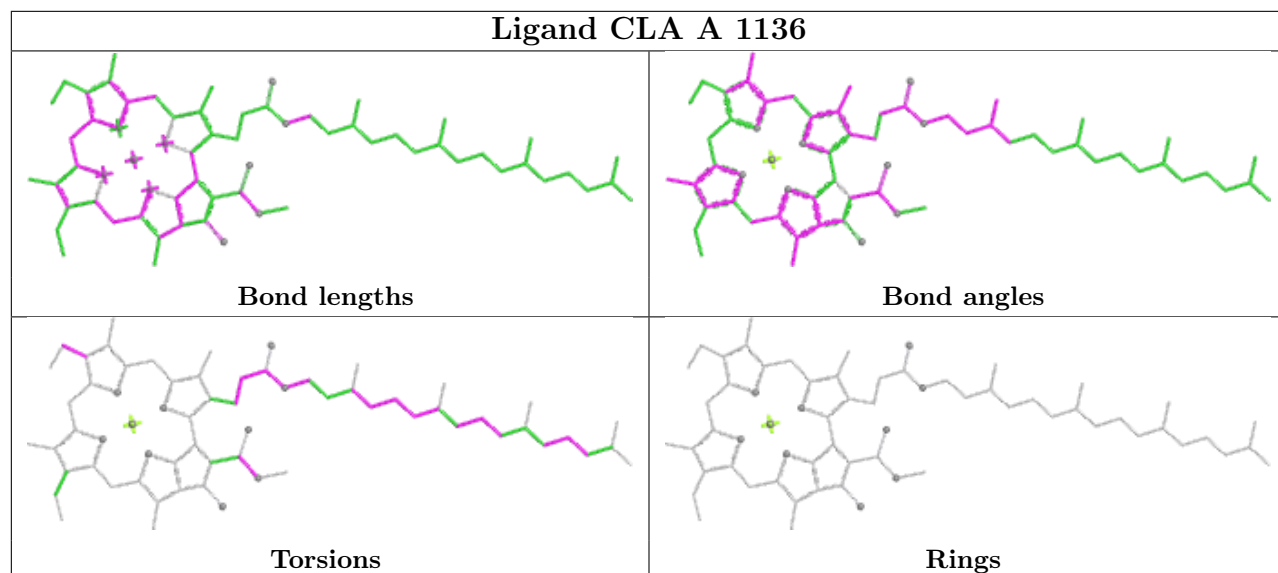
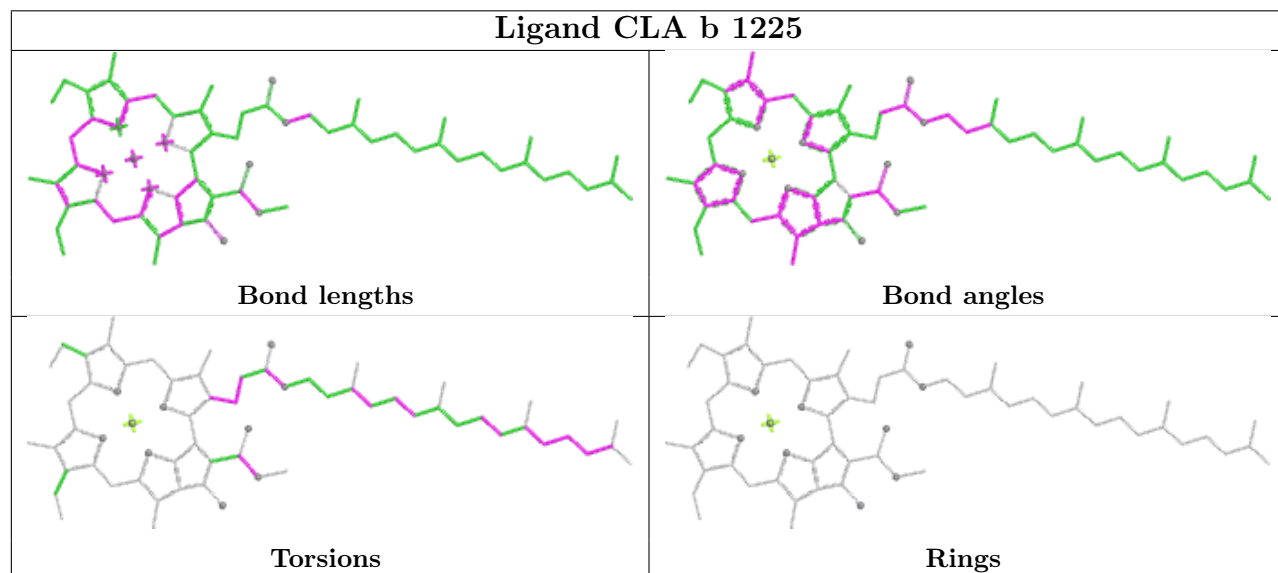
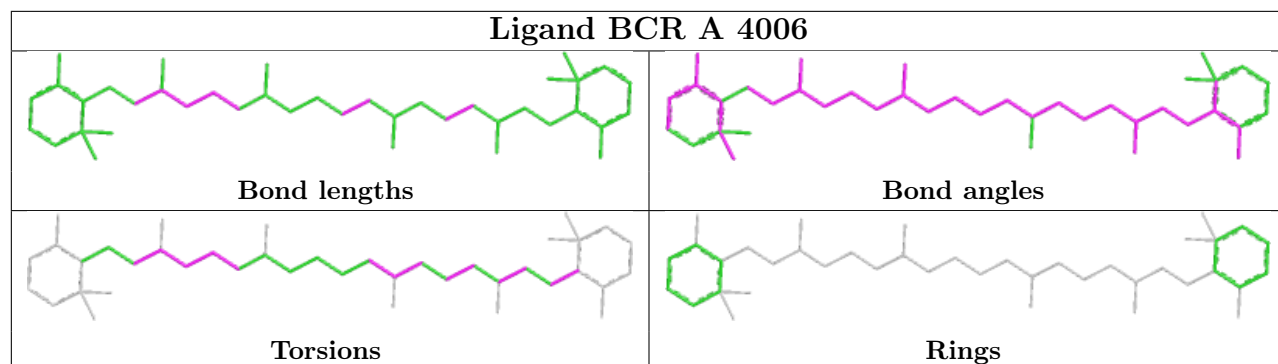
Bond angles

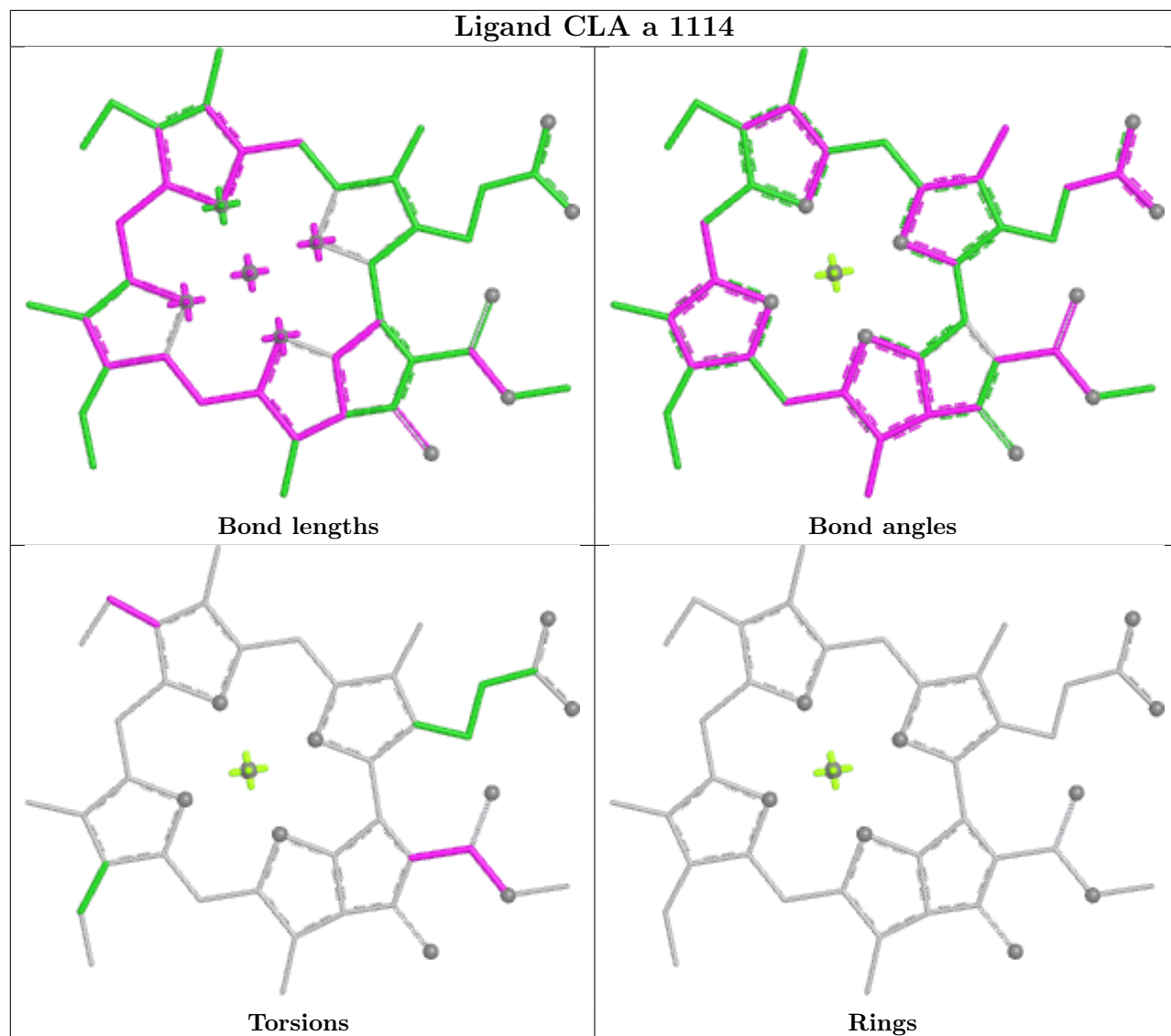


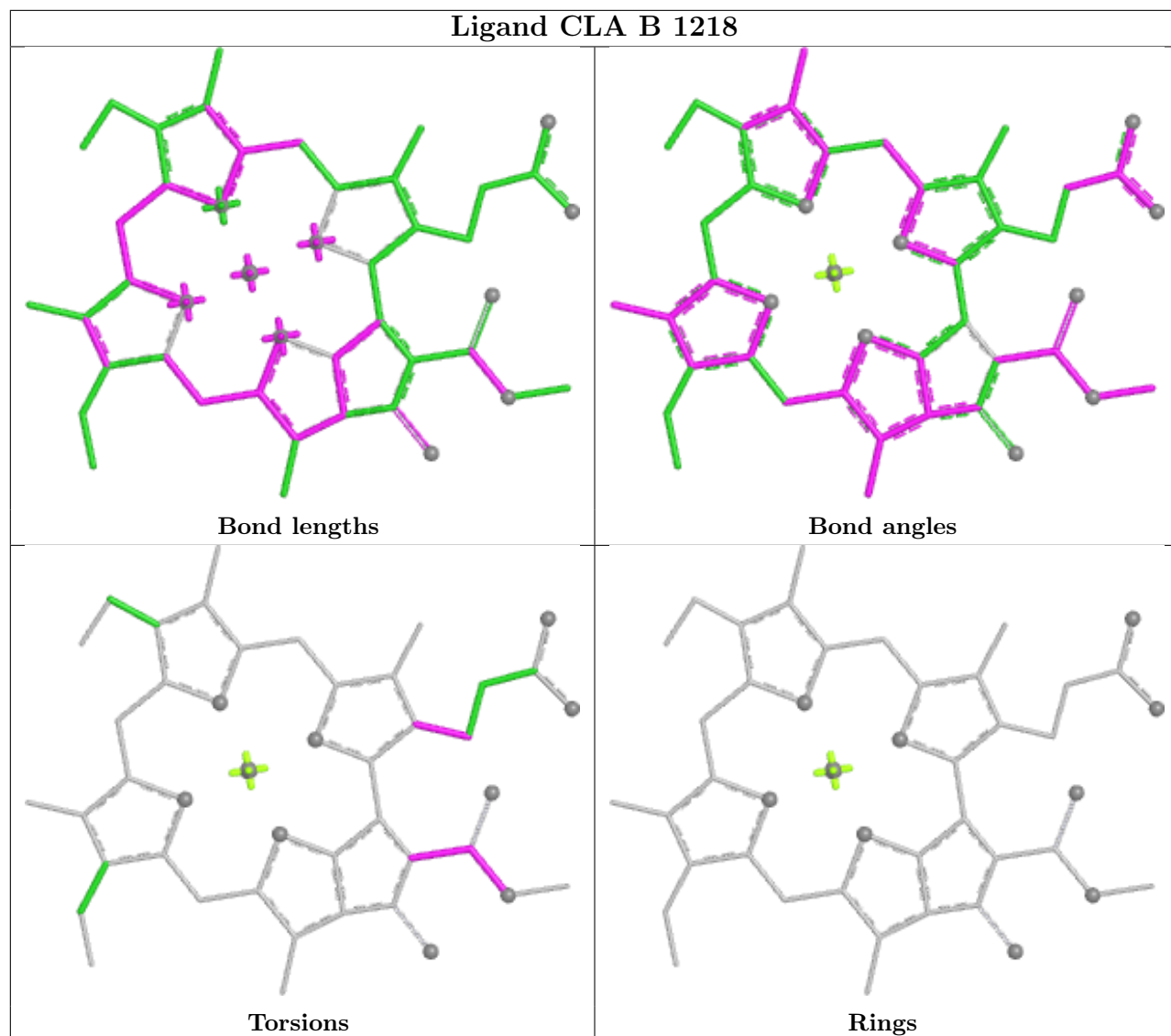
Torsions

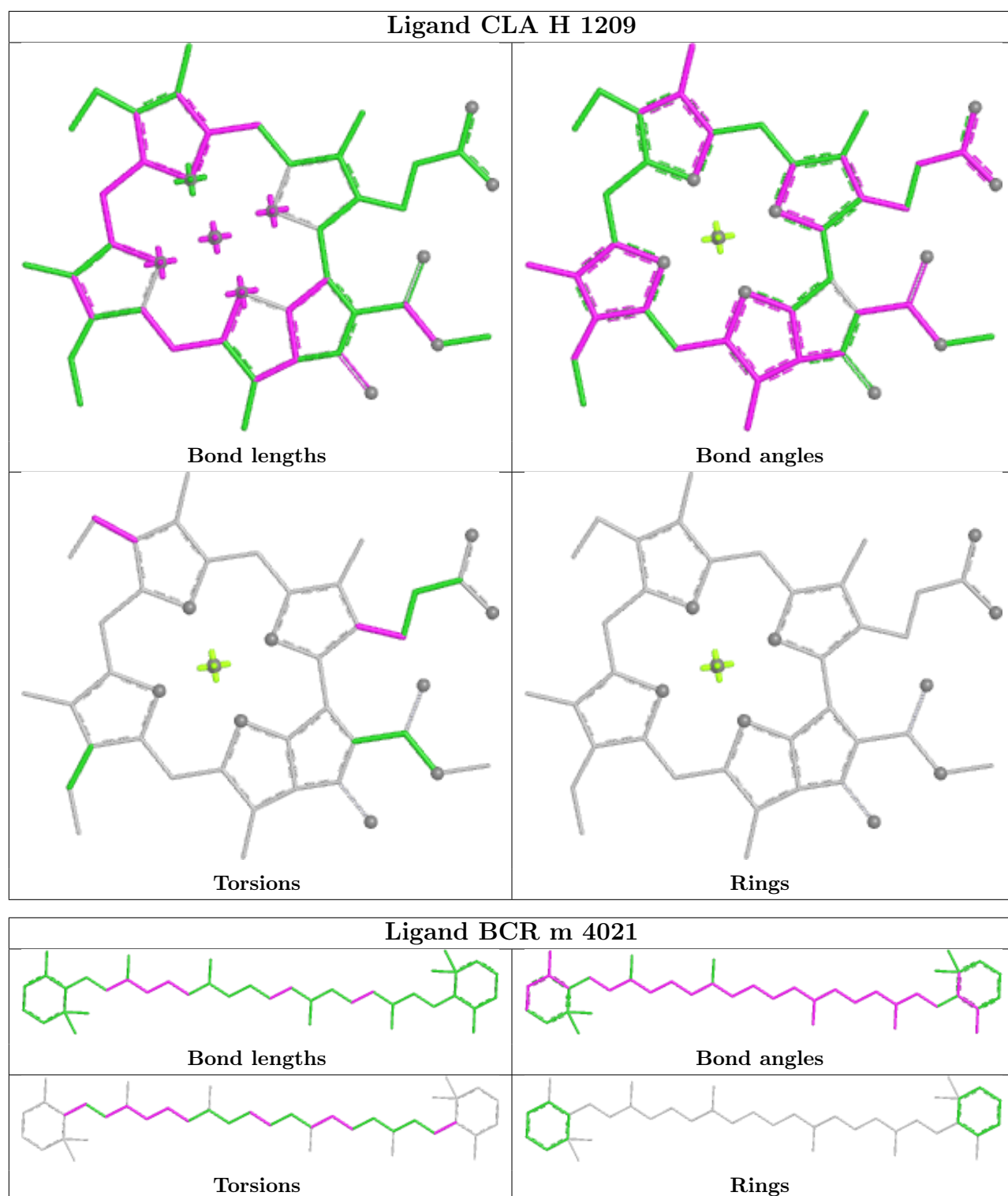


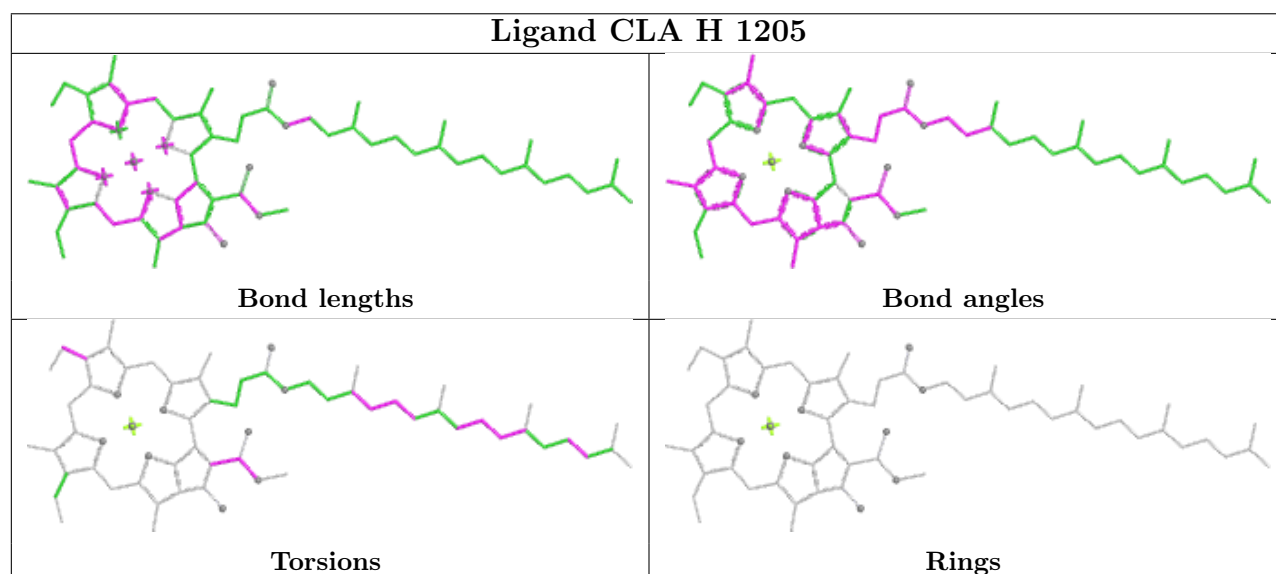
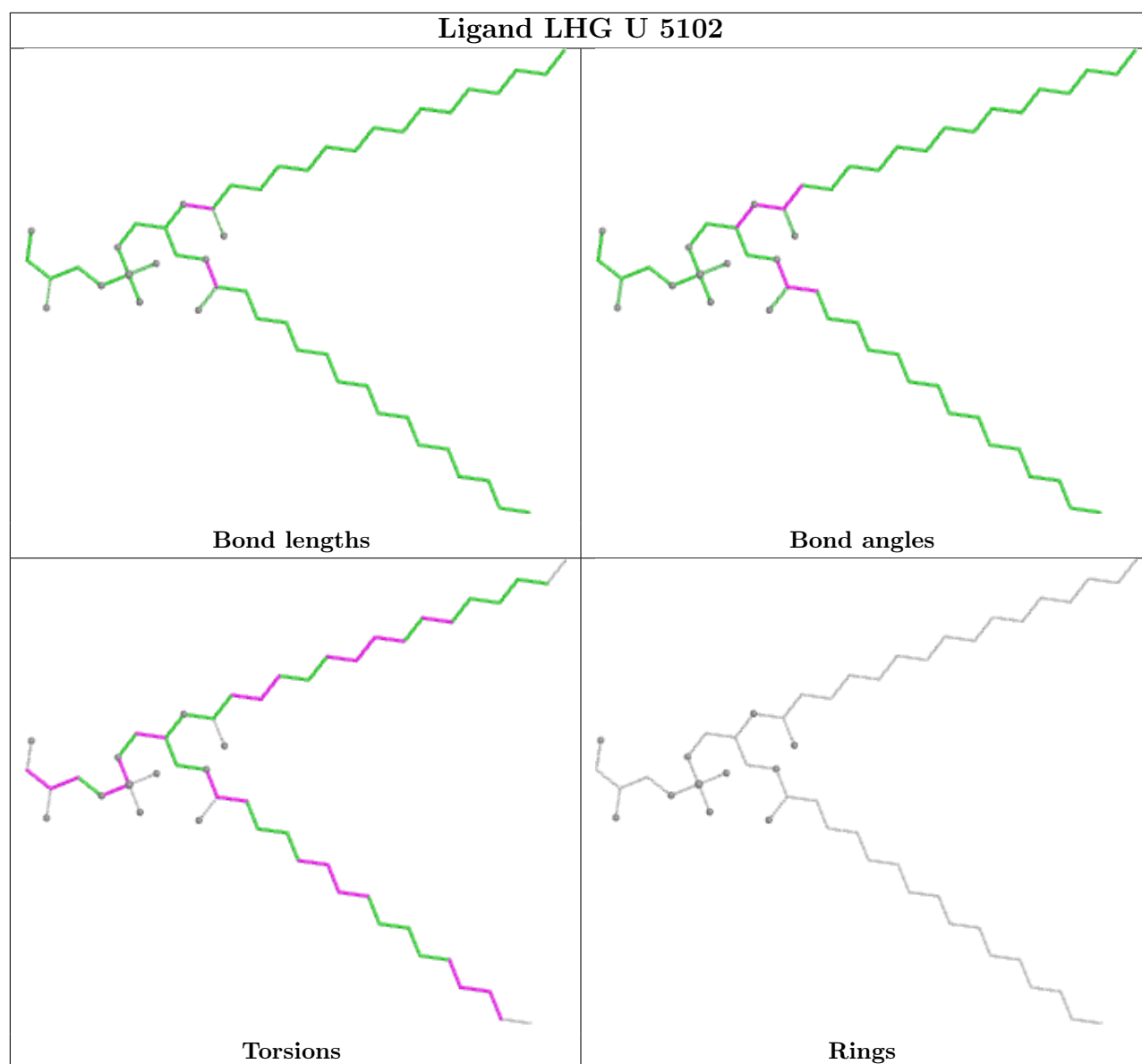
Rings

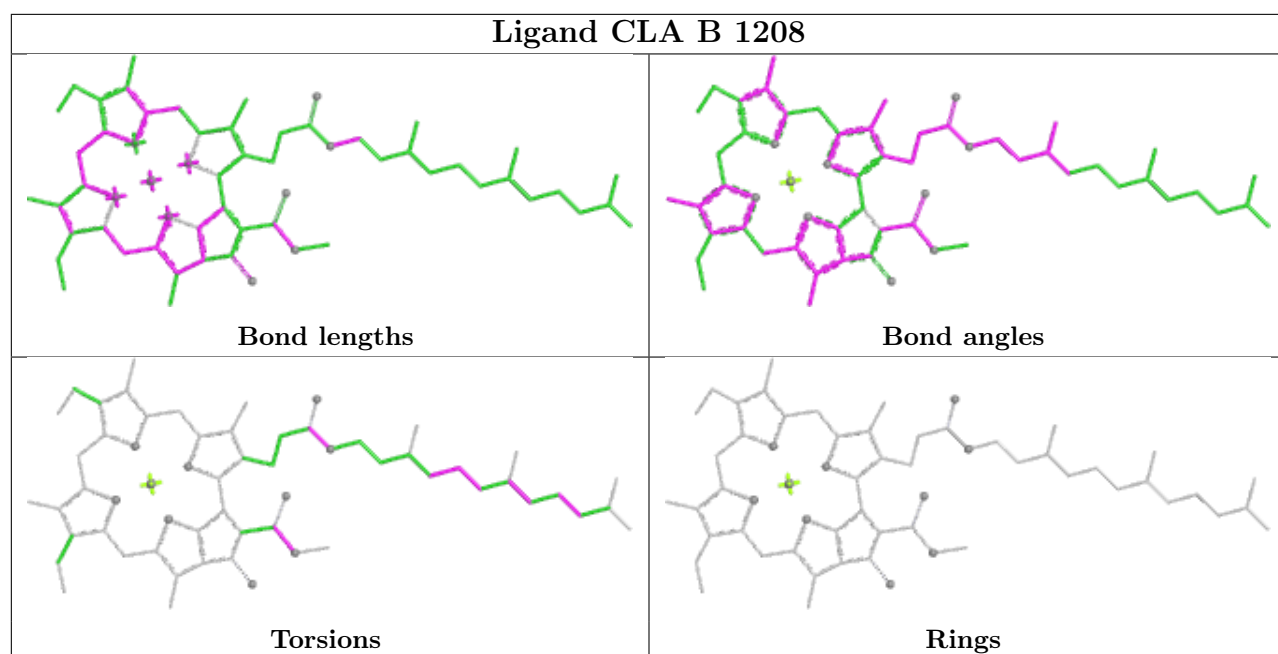


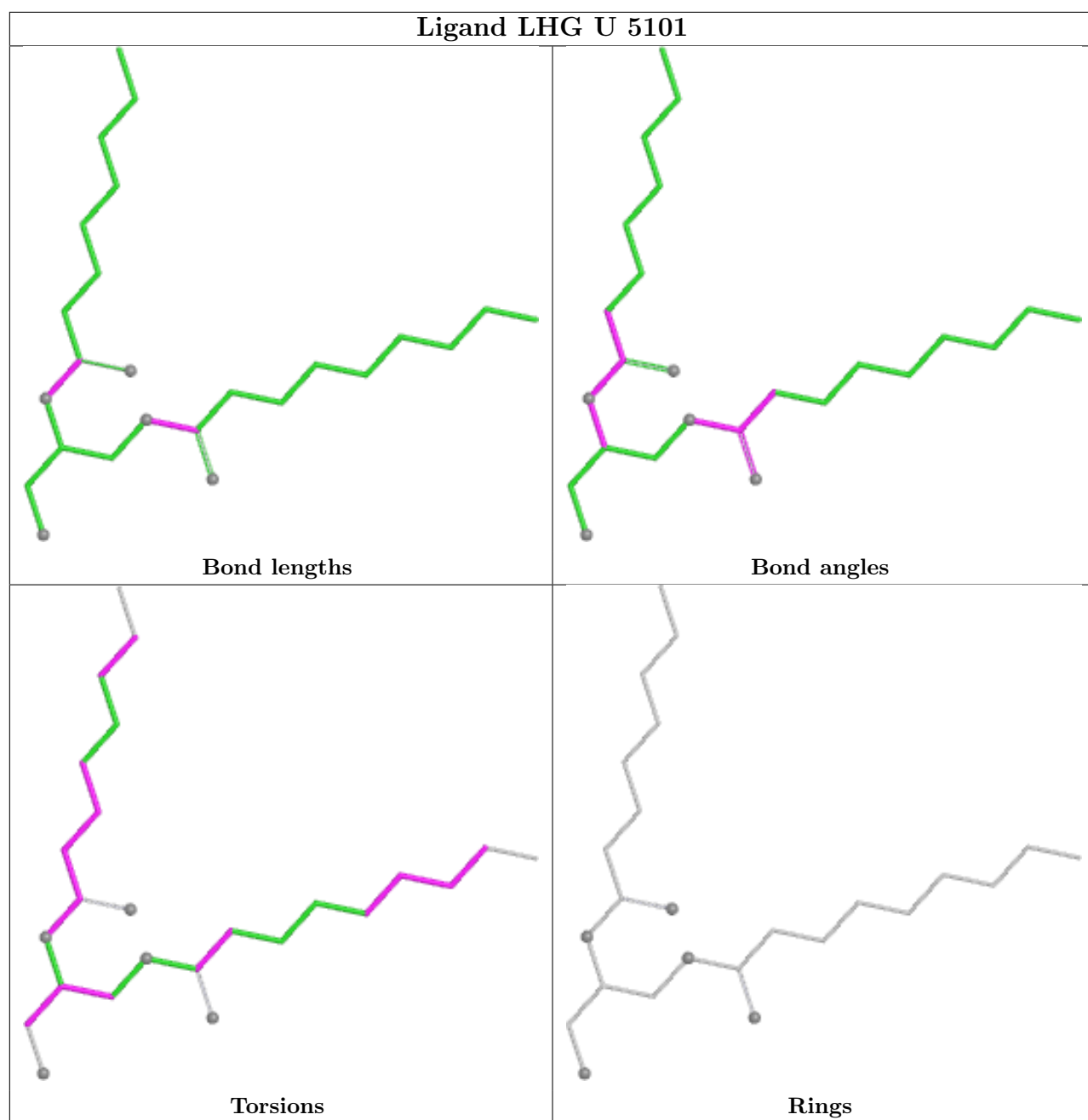


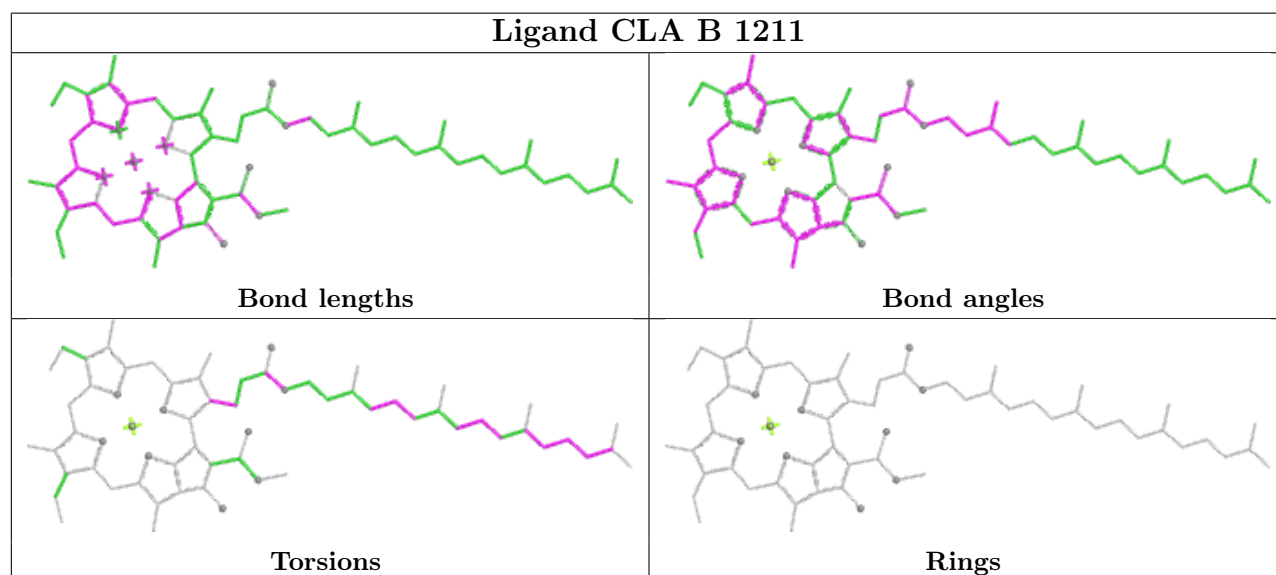
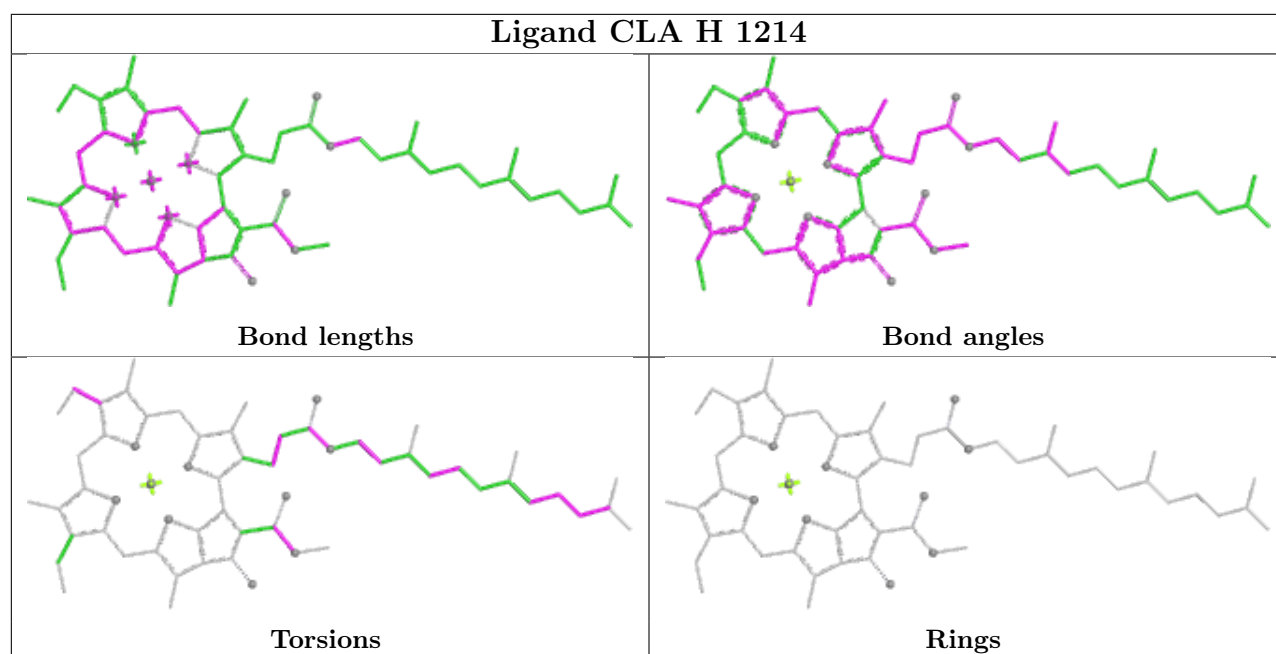




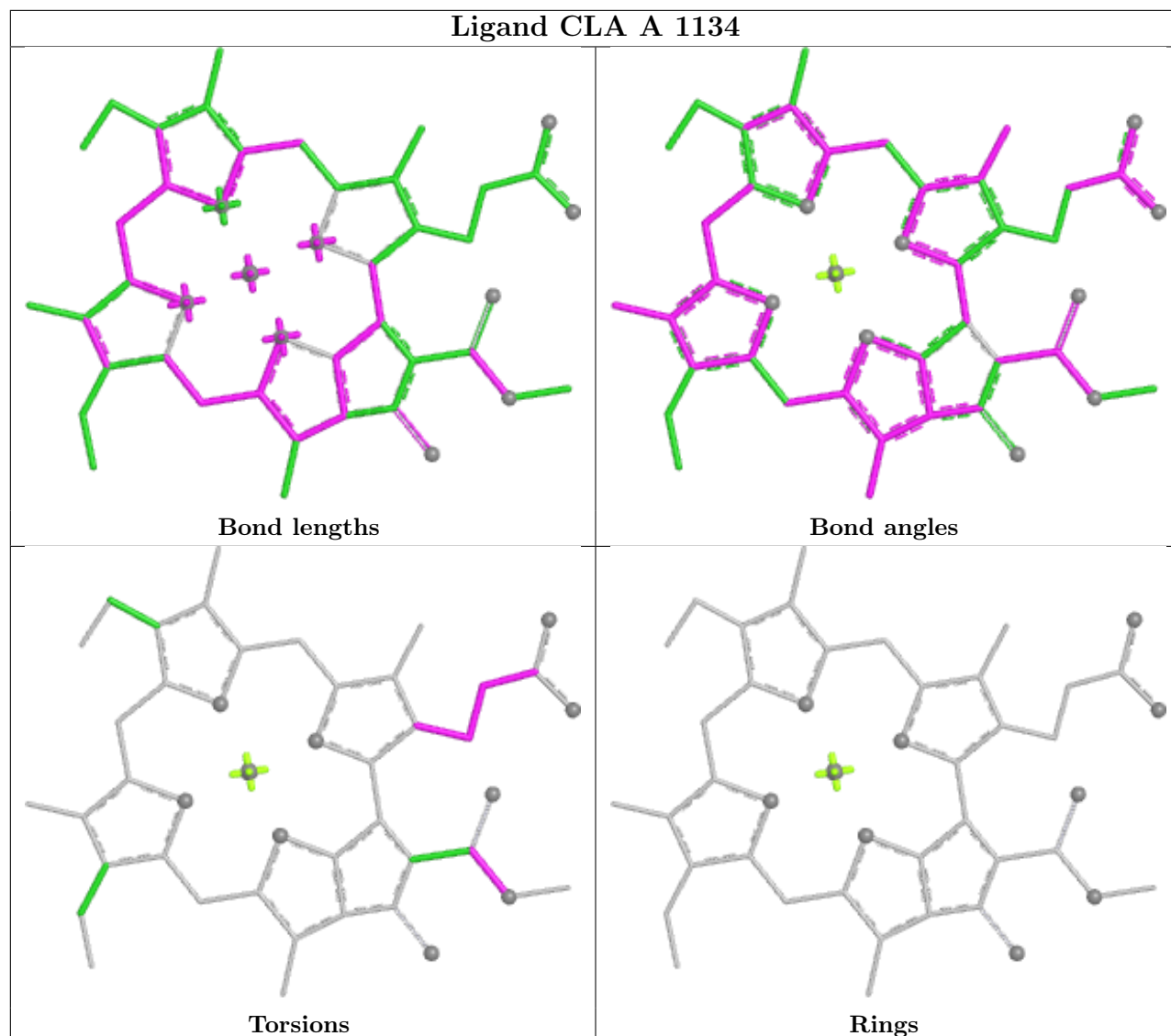




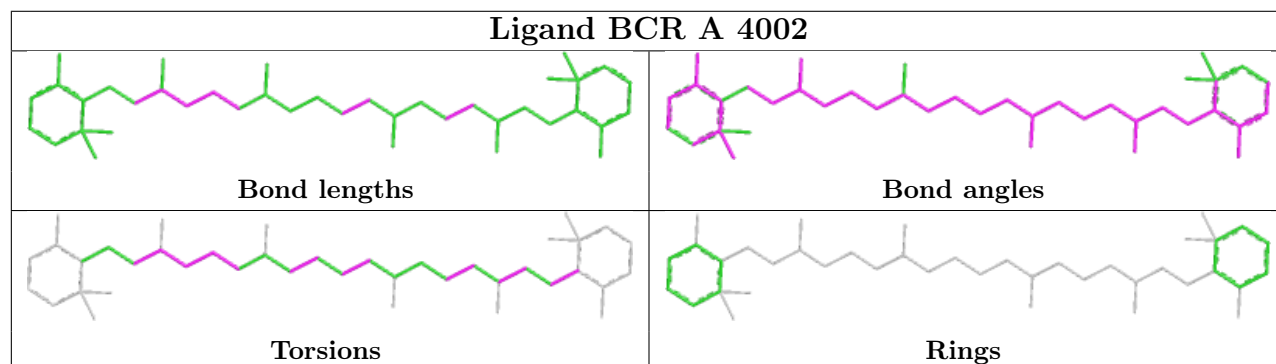


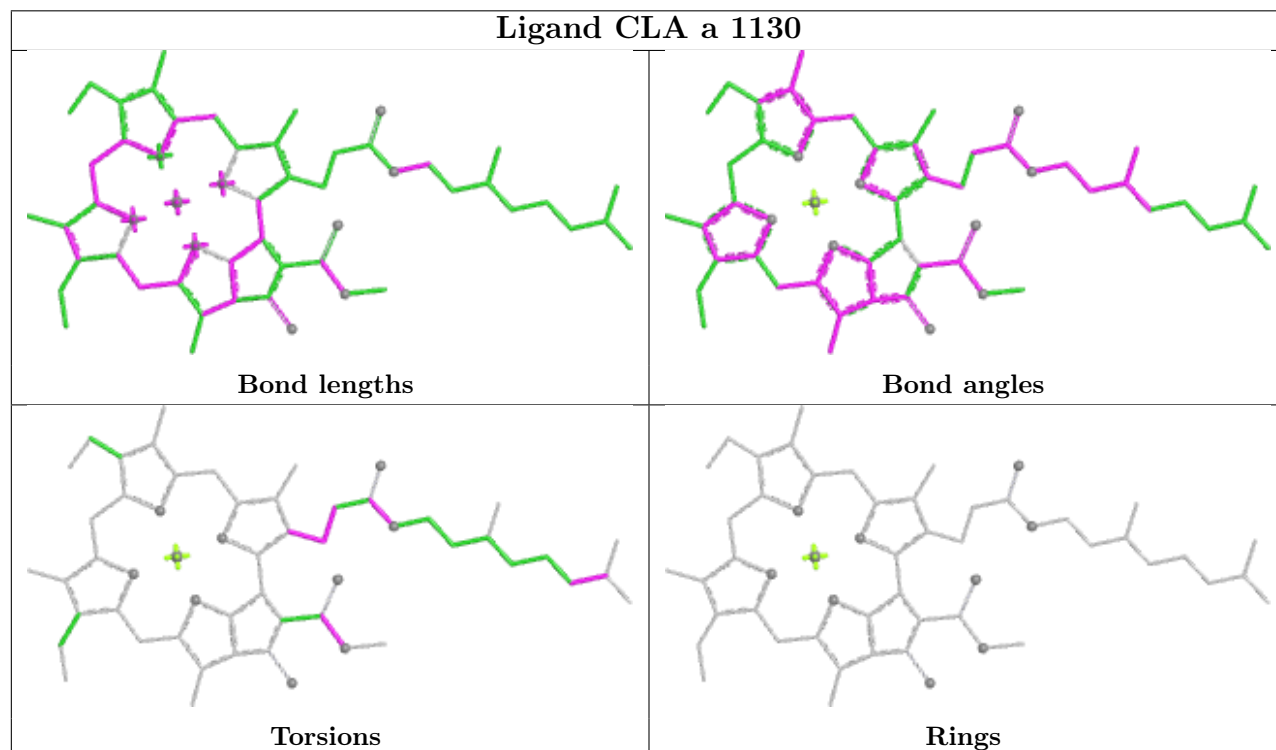
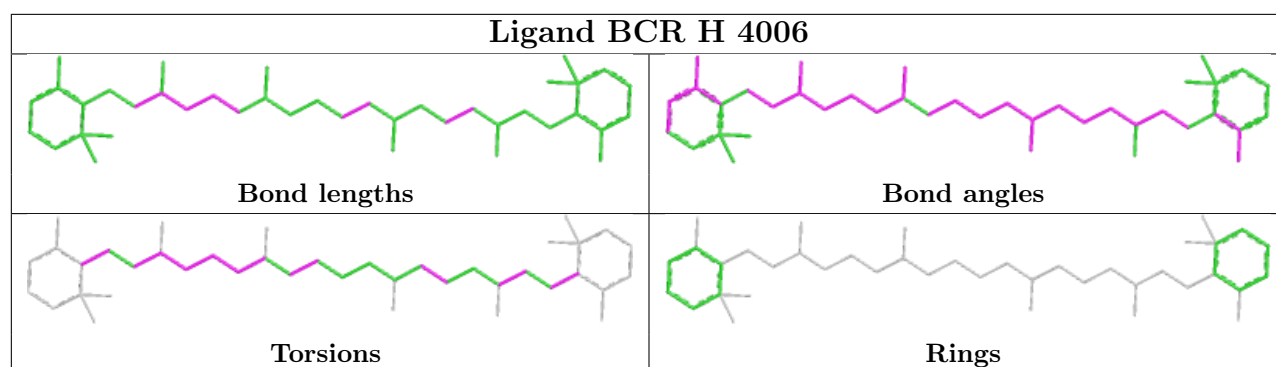


Ligand CLA A 1134

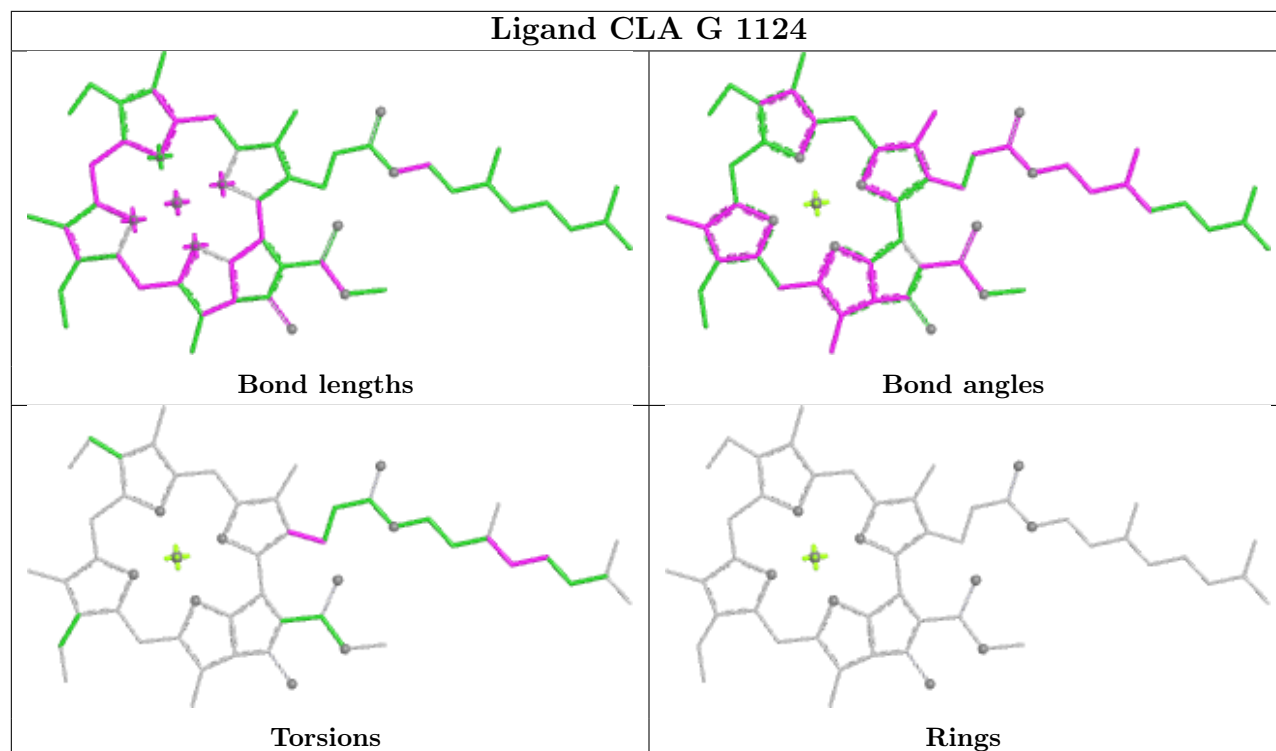


Ligand BCR A 4002

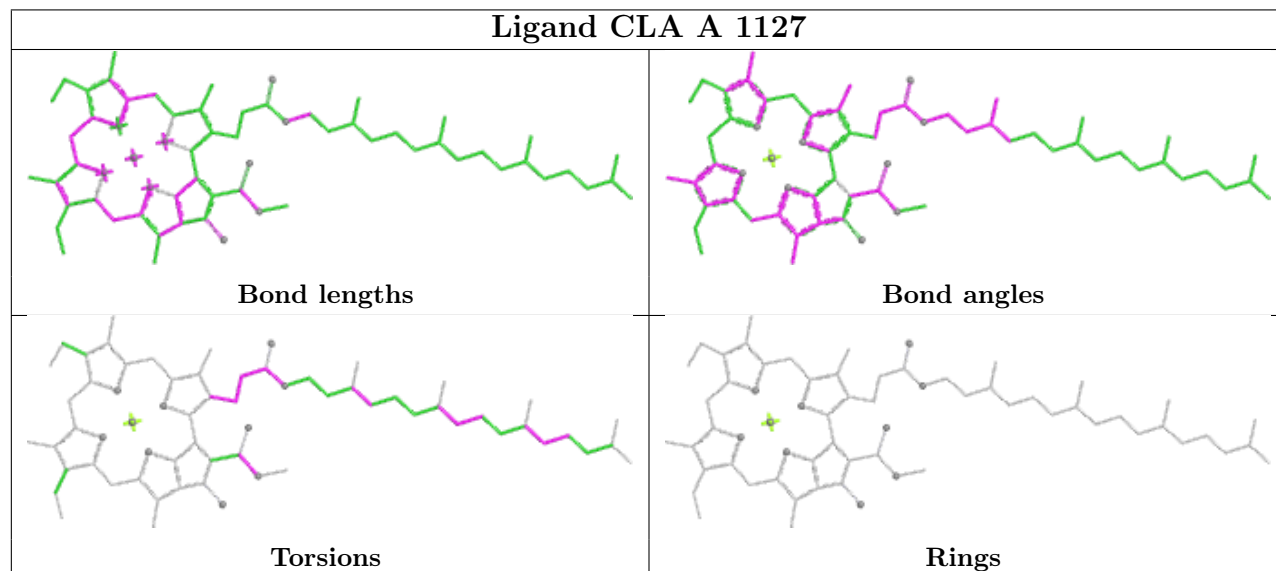


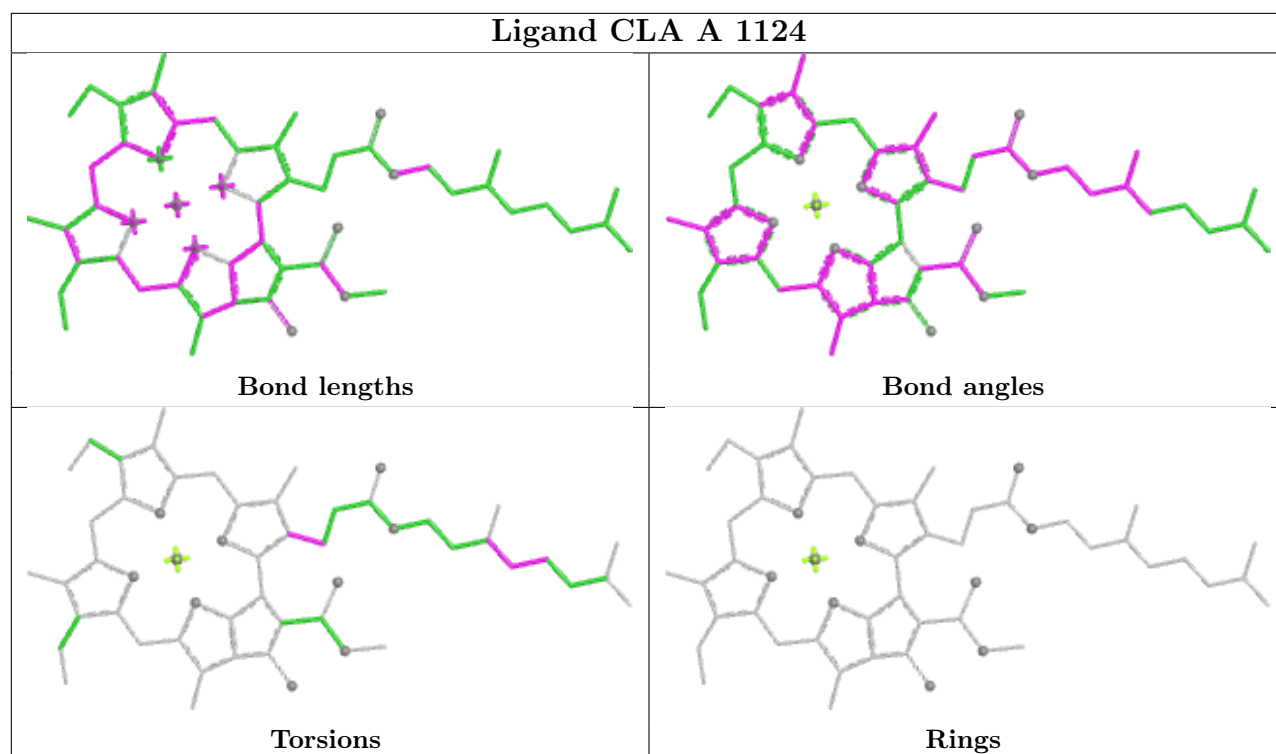
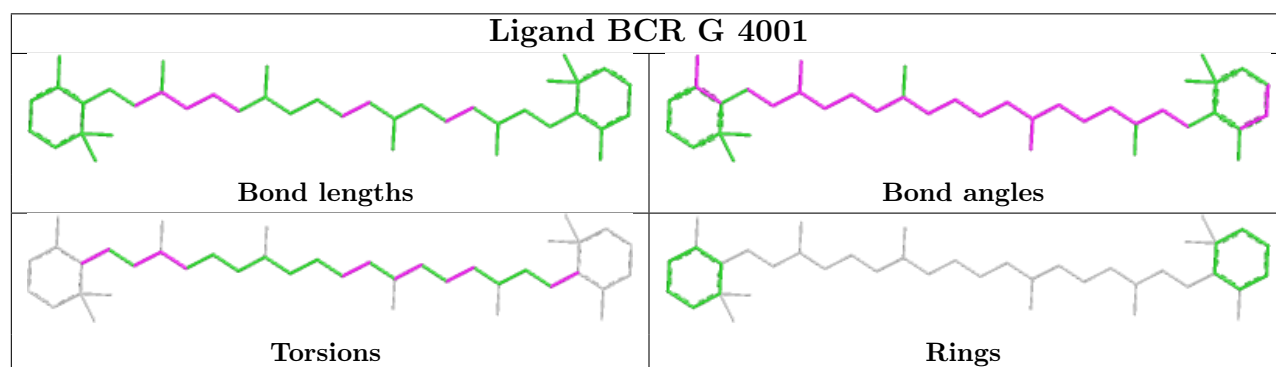
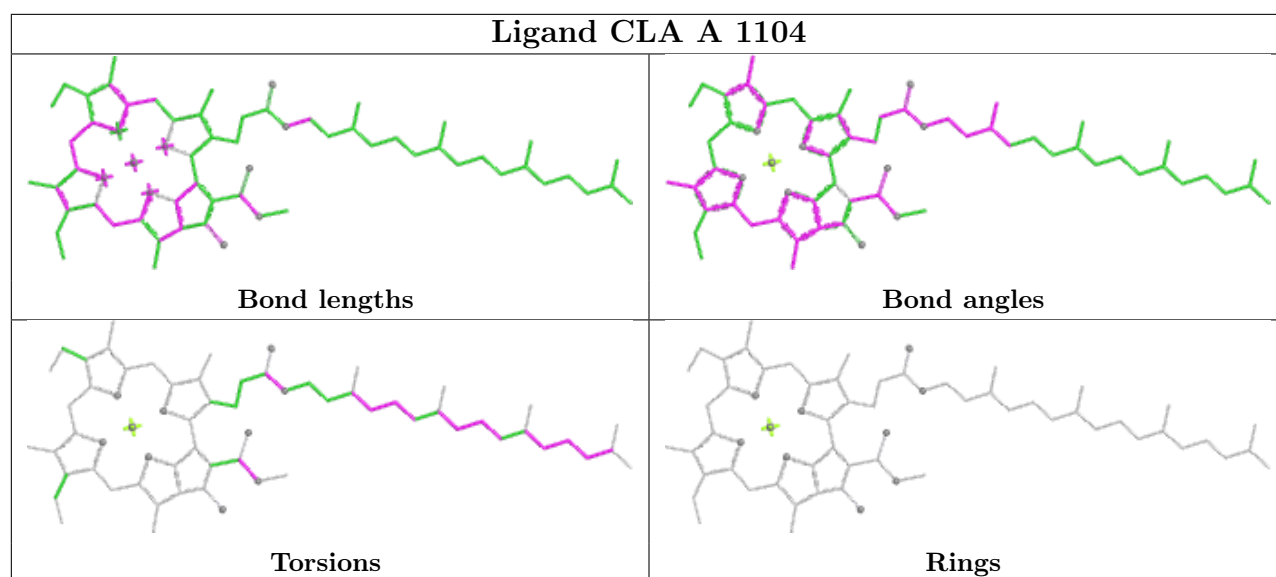


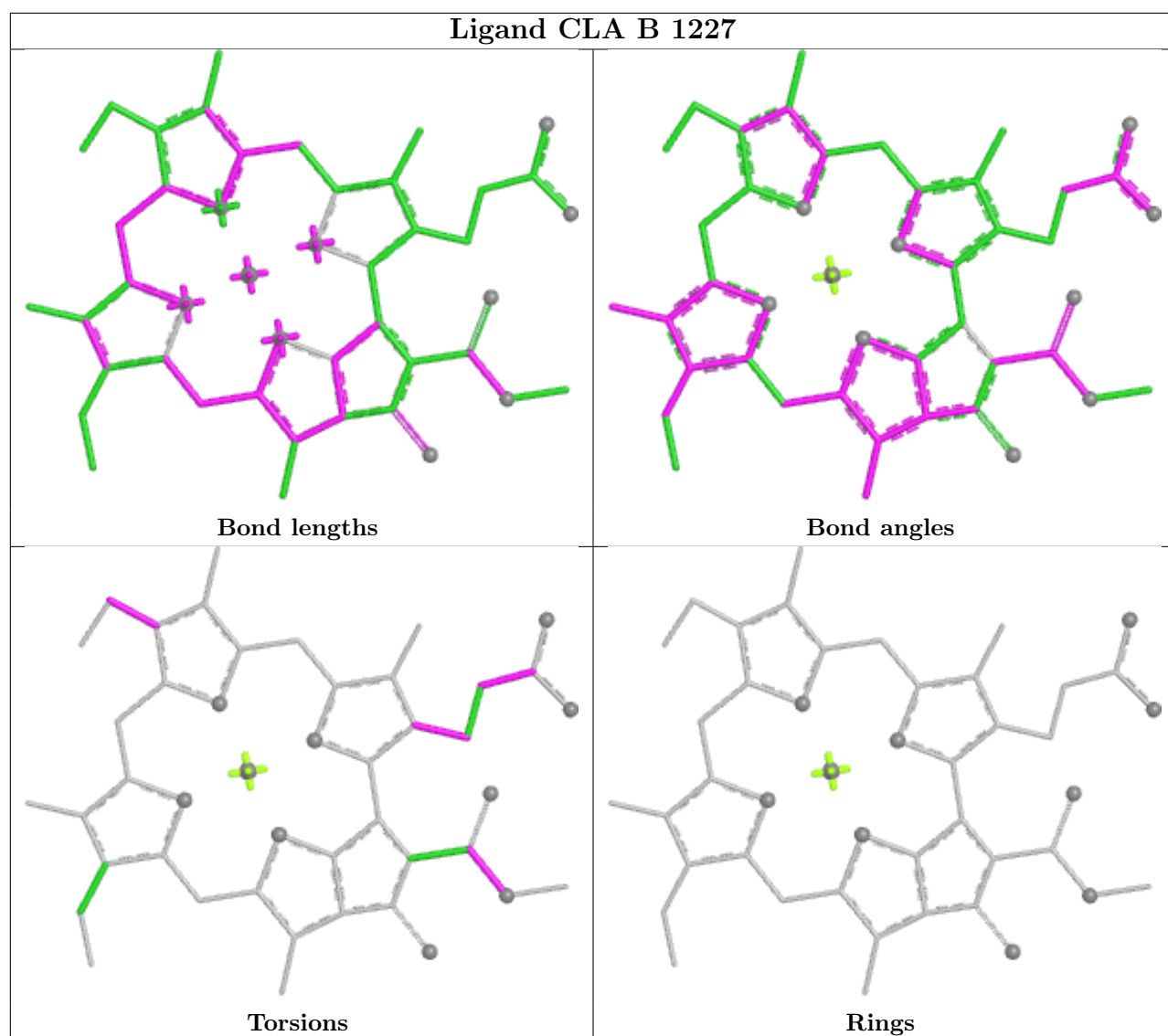
Ligand CLA G 1124

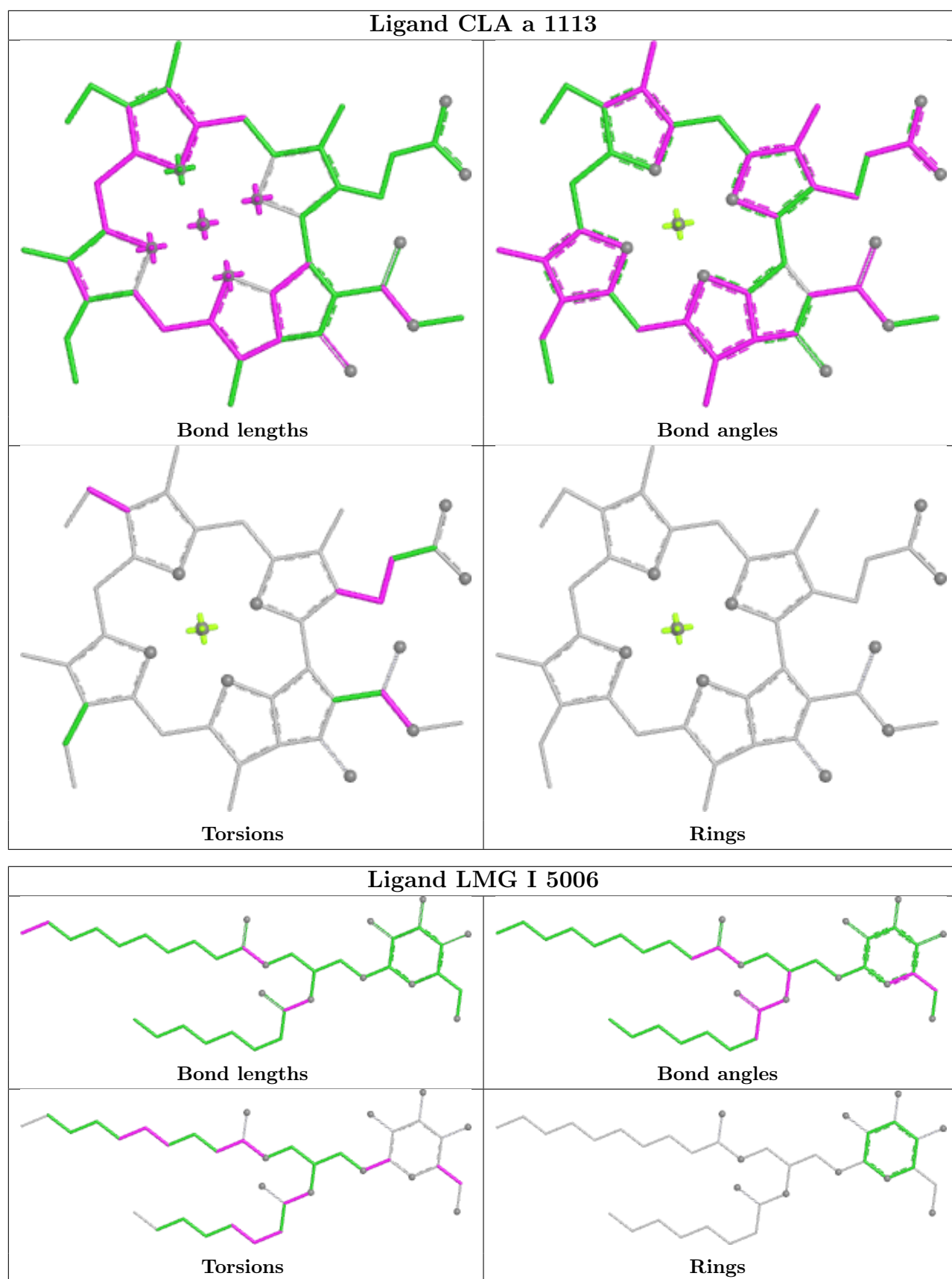


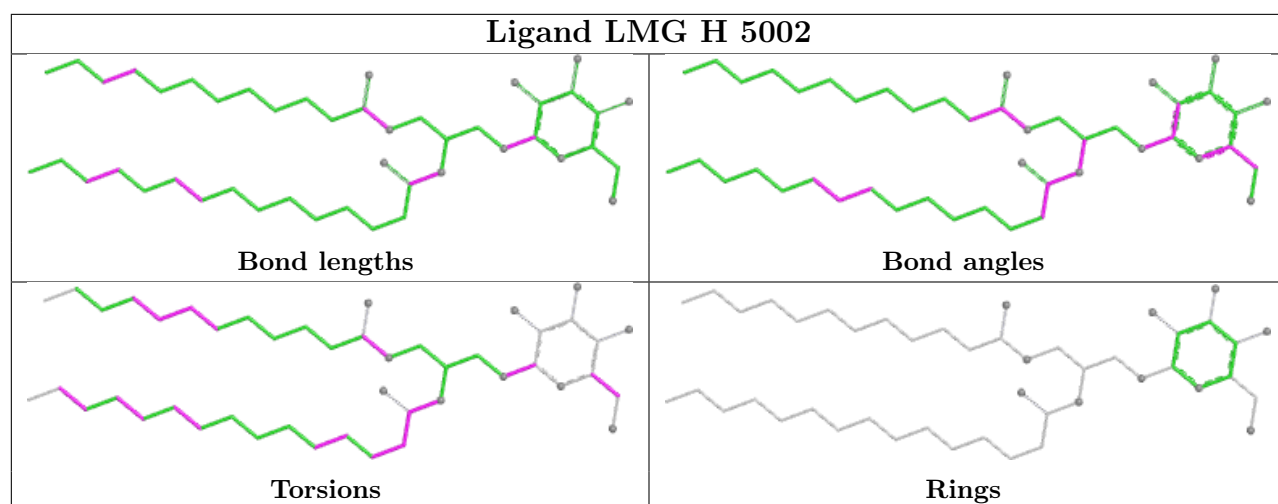
Ligand CLA A 1127

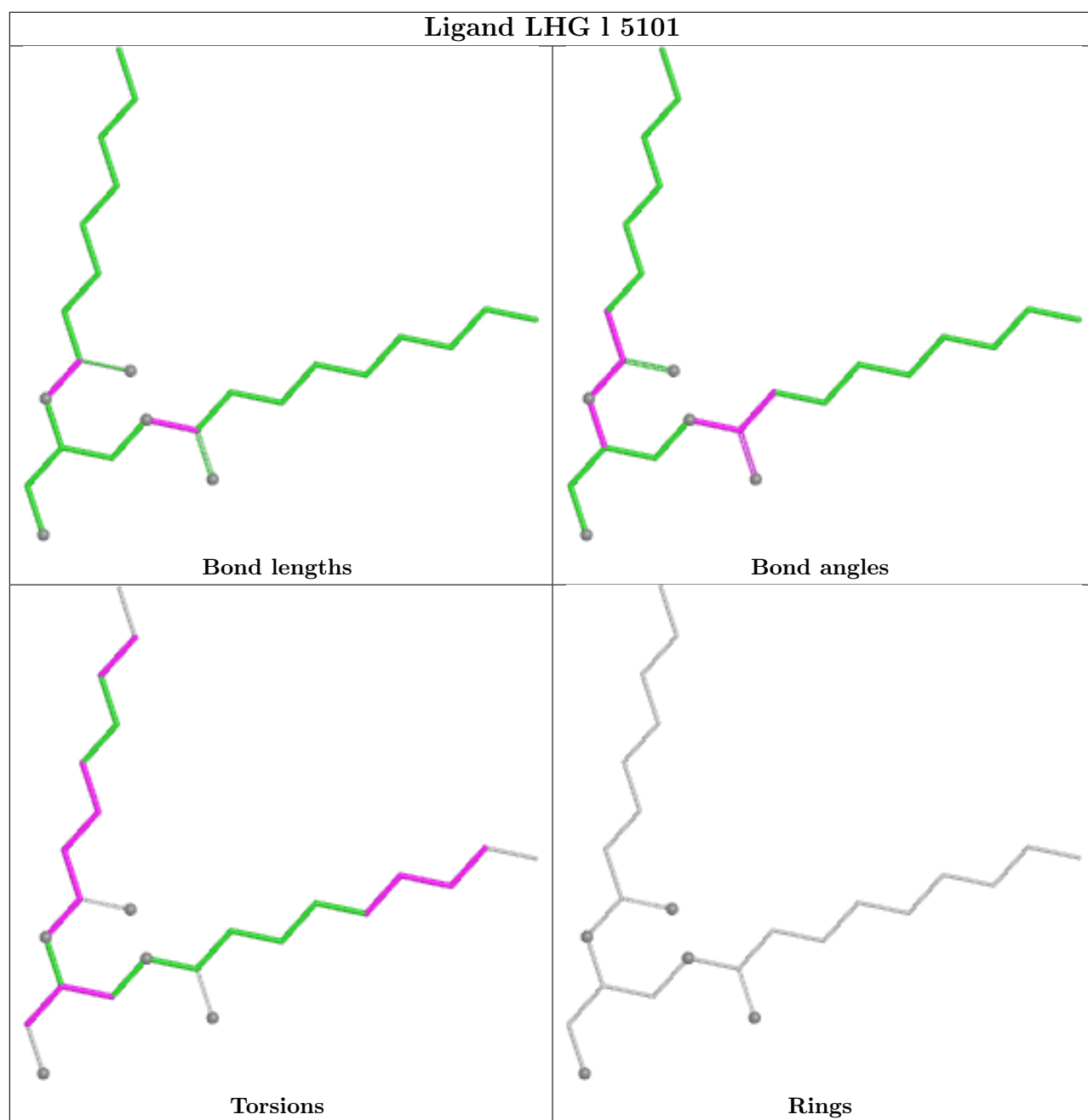




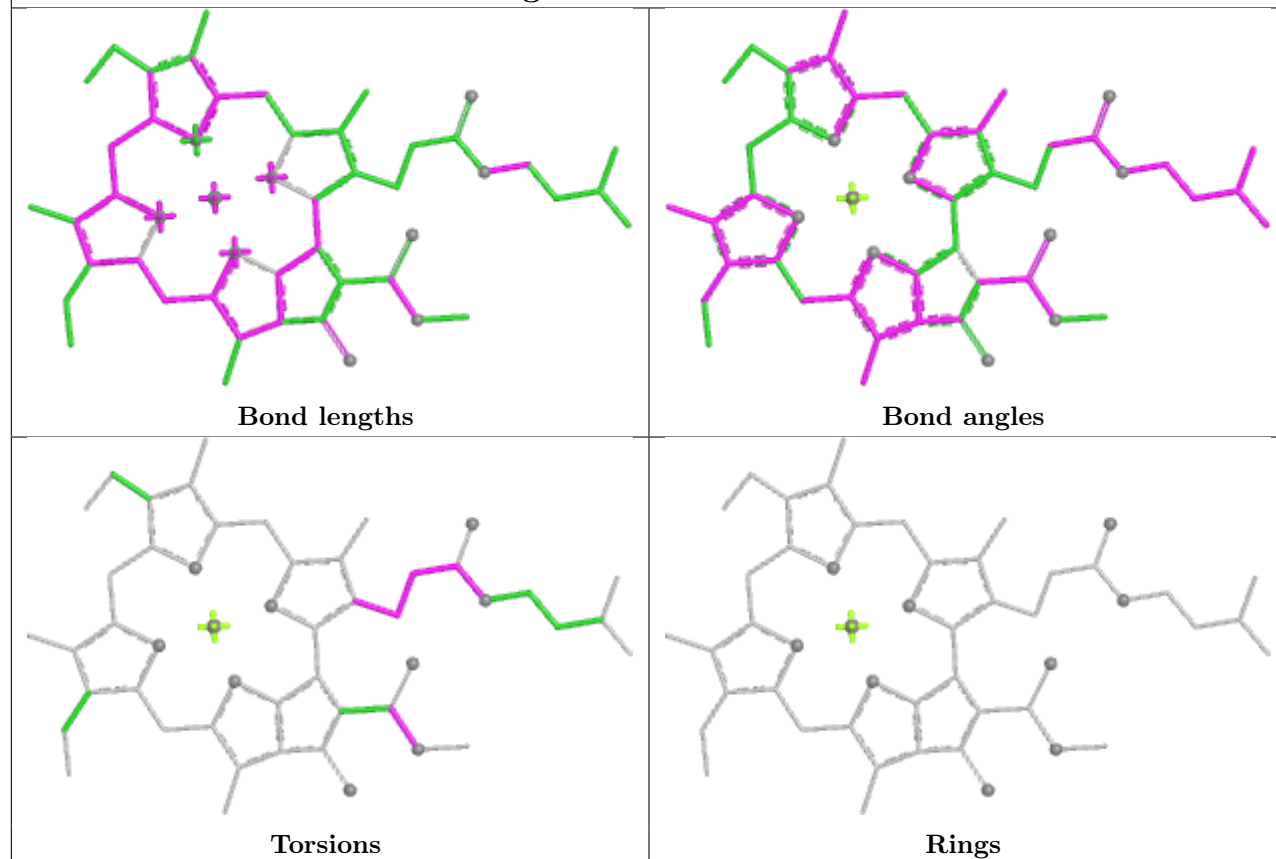




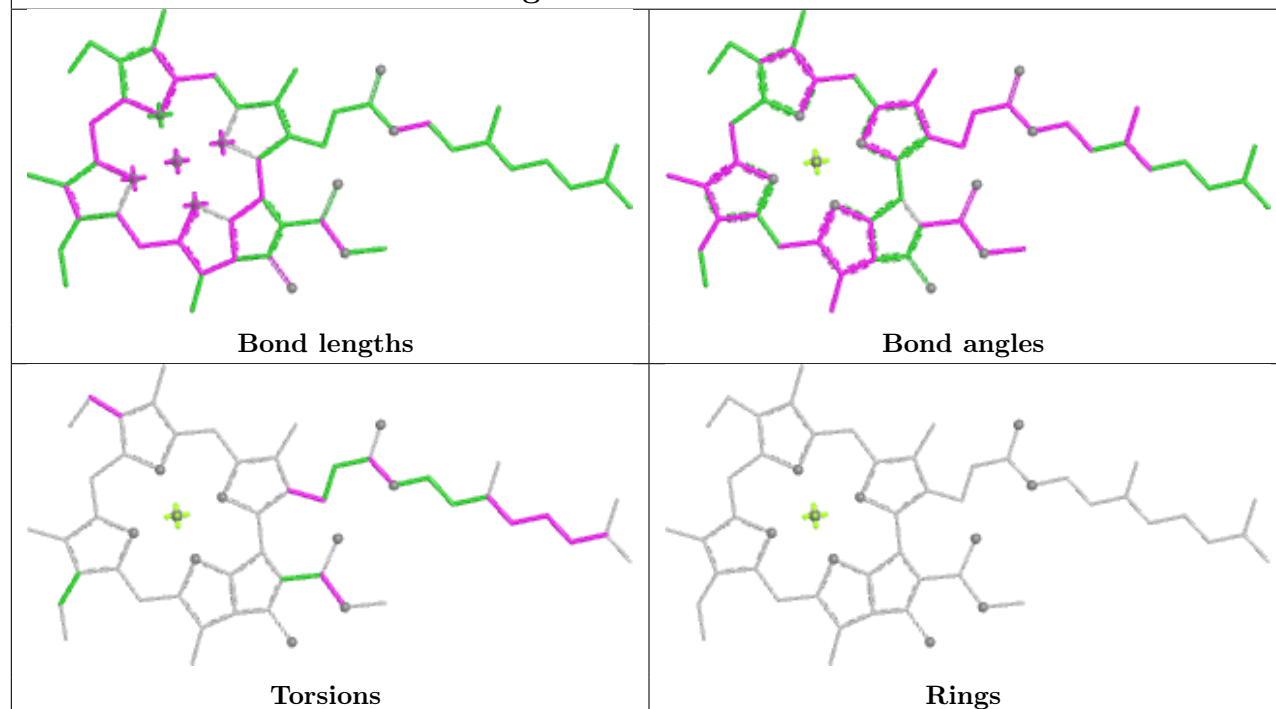


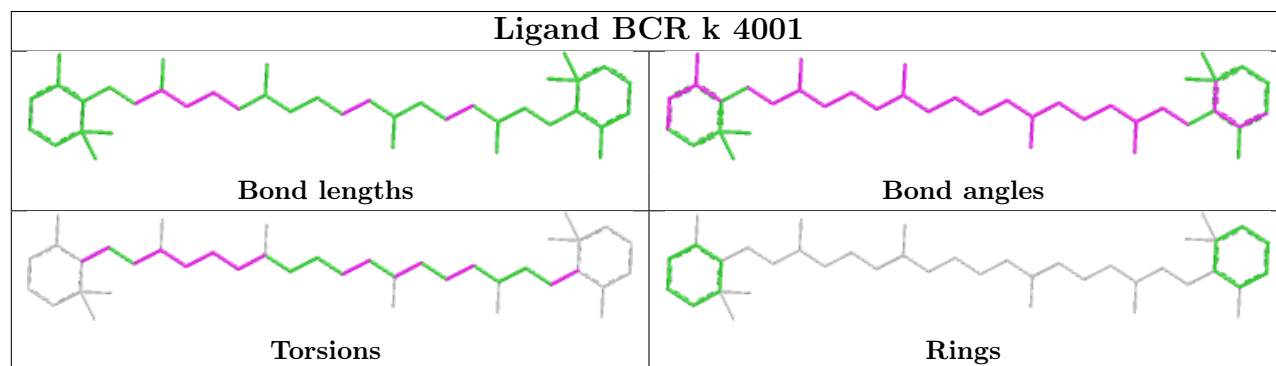
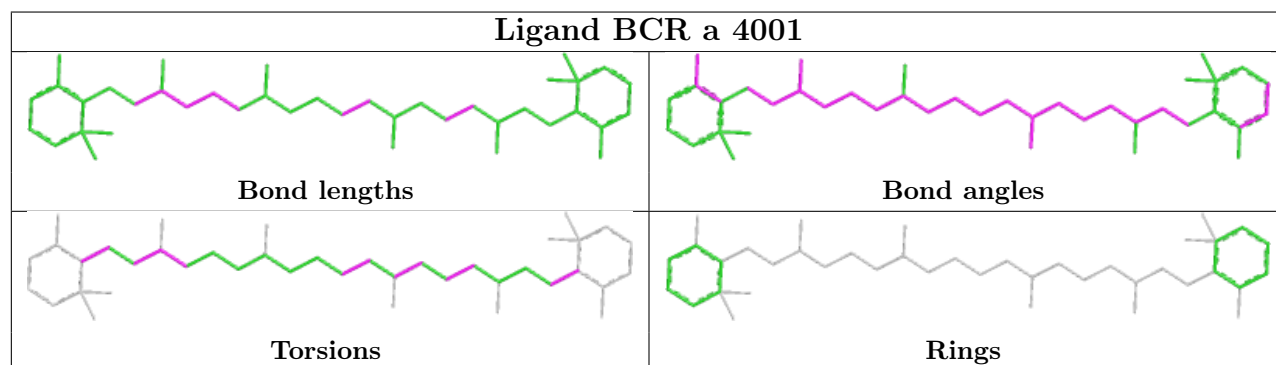
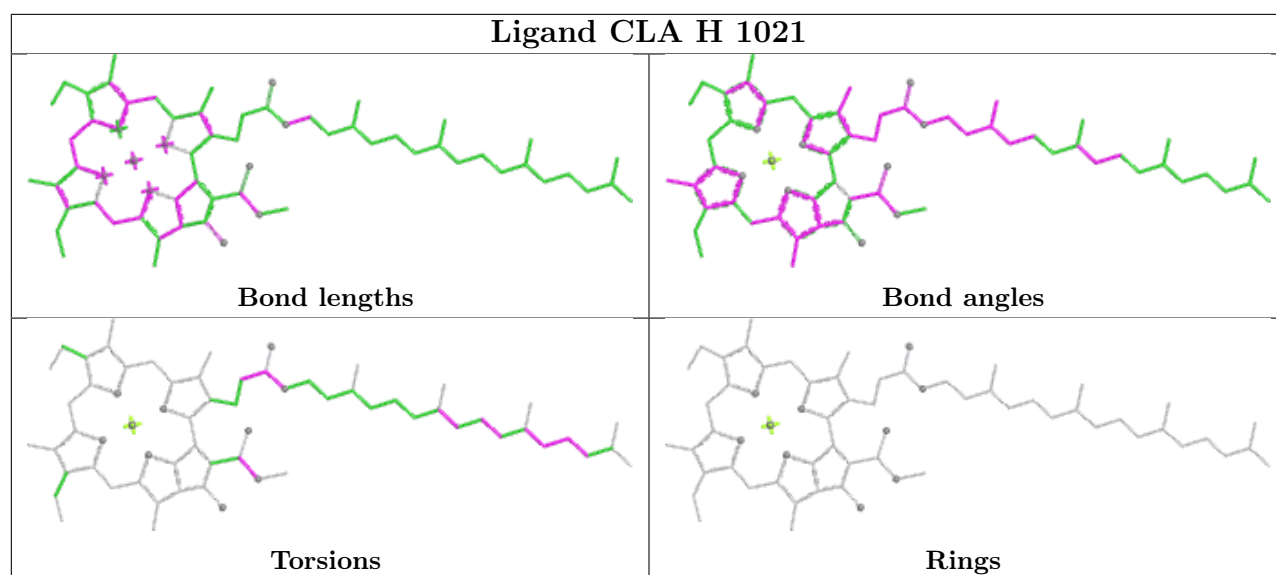


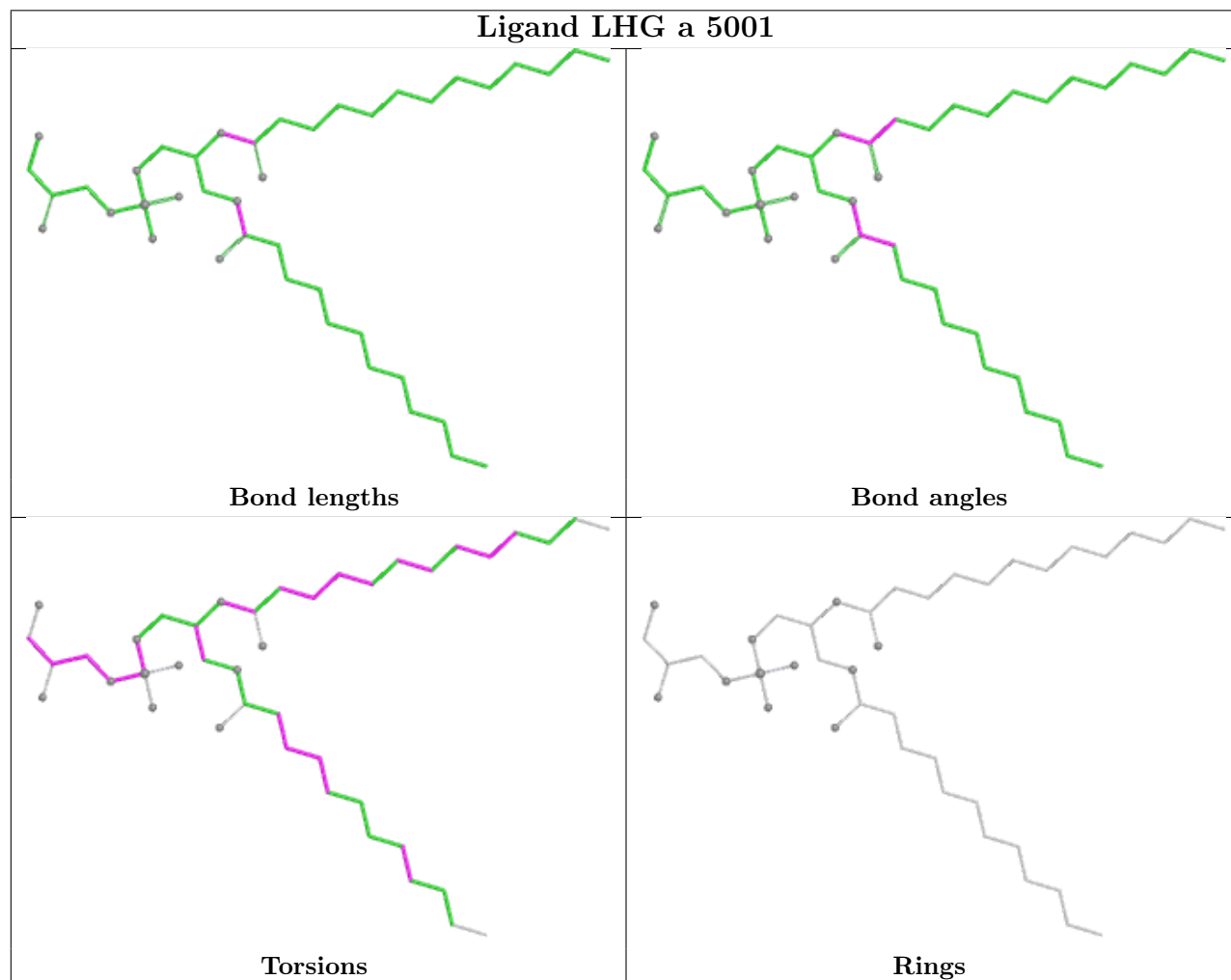
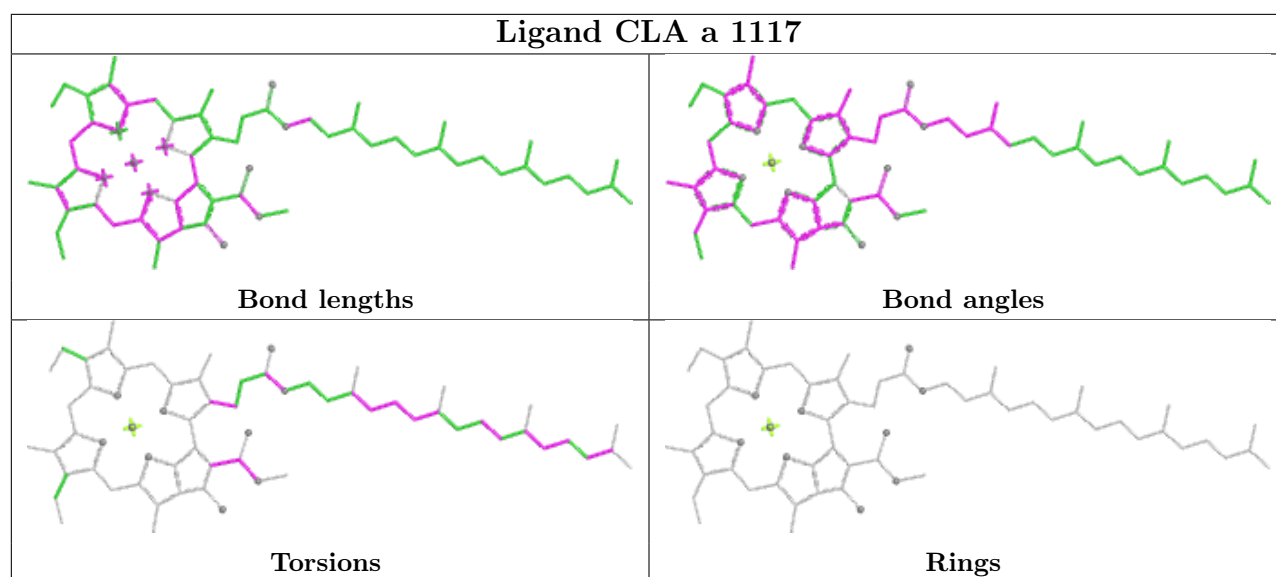
Ligand CLA A 1102

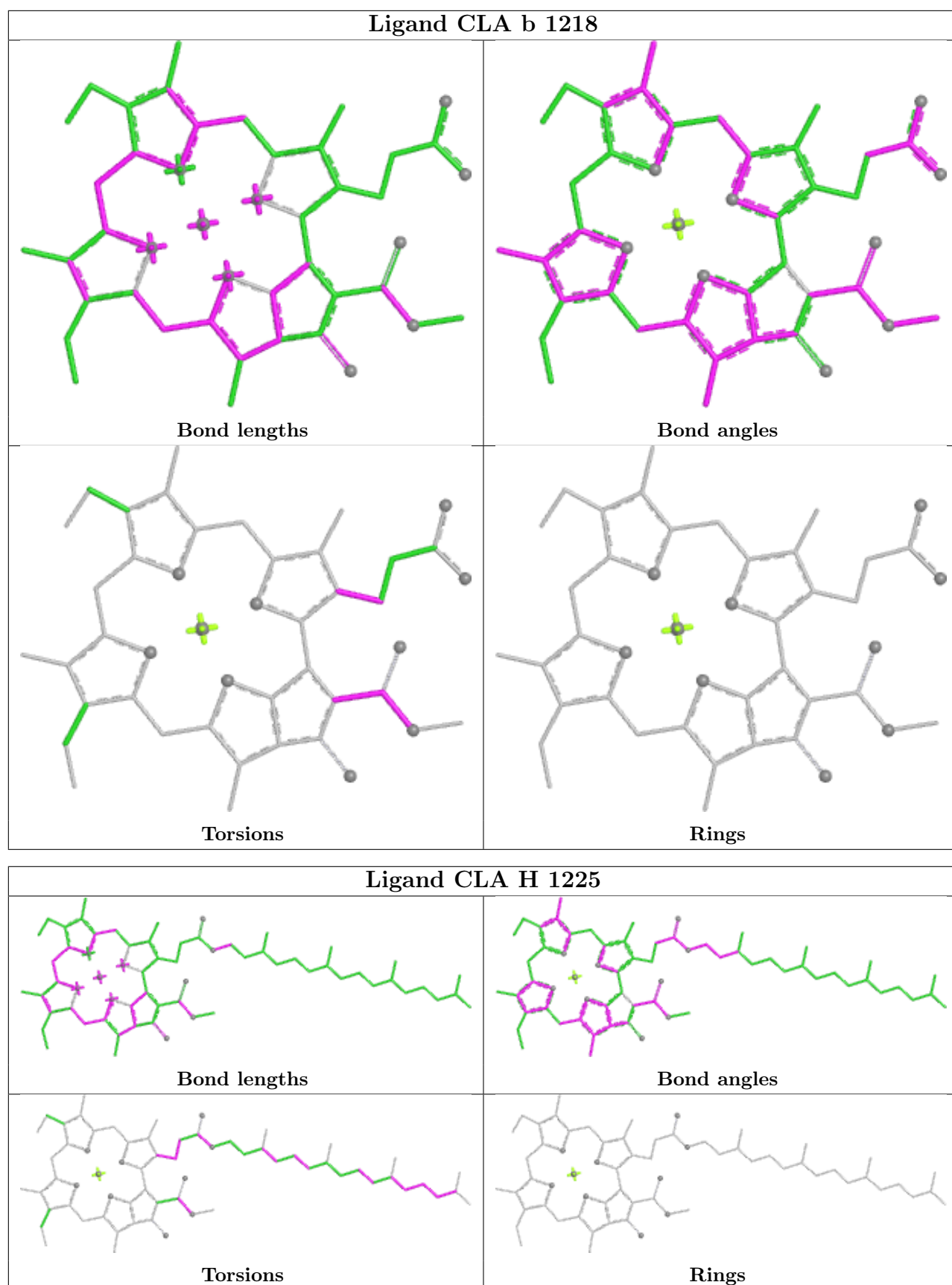


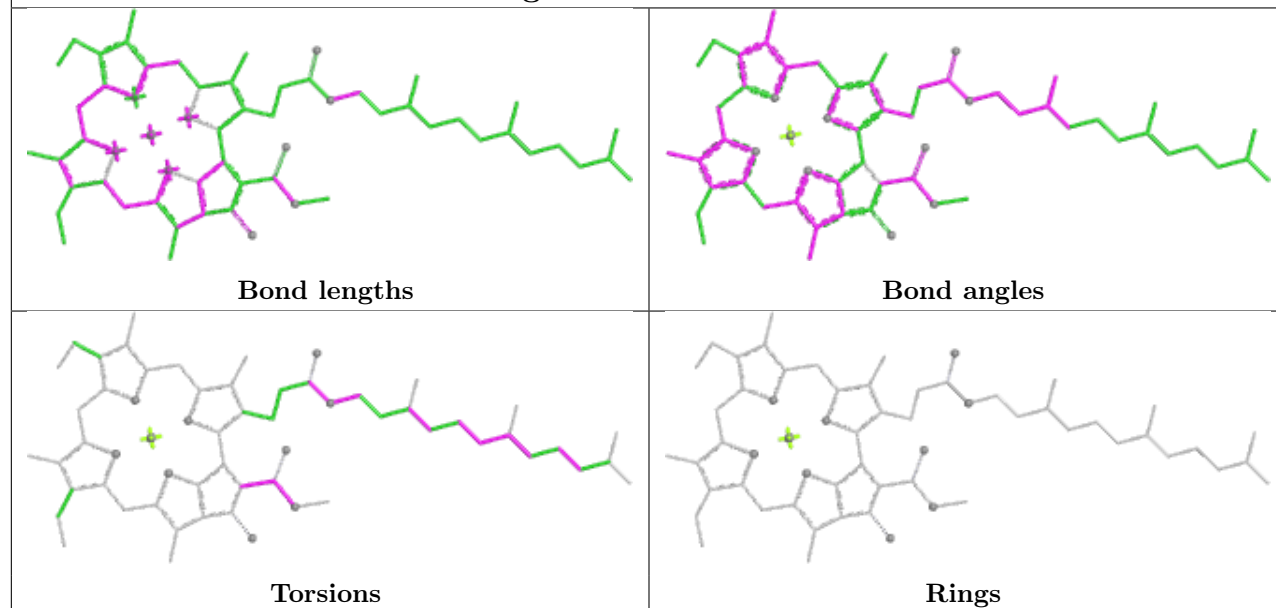
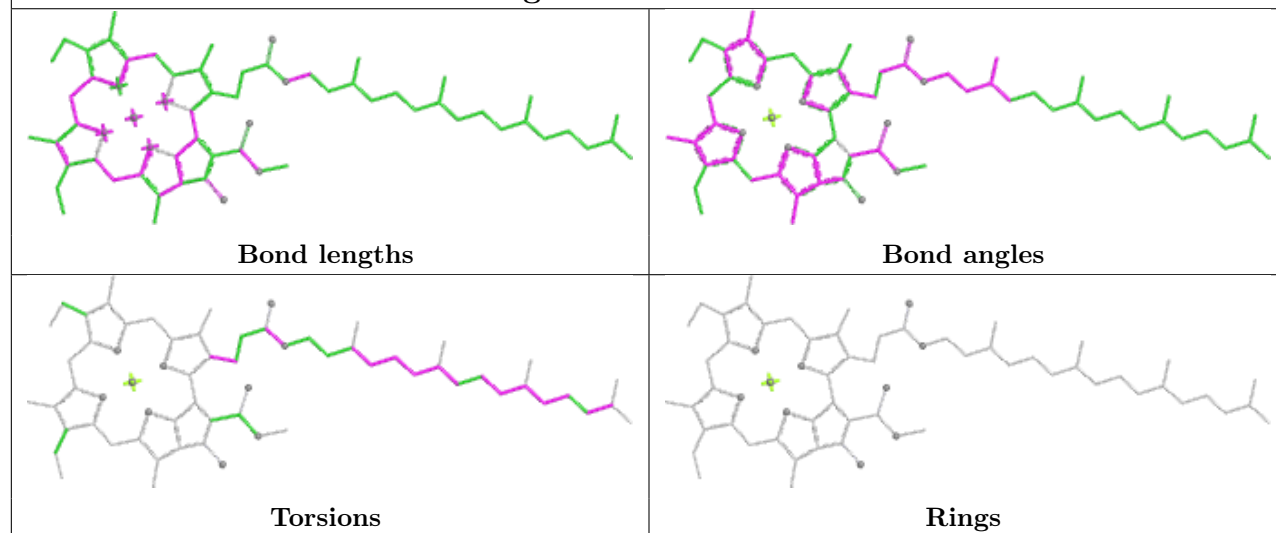
Ligand CLA A 1138

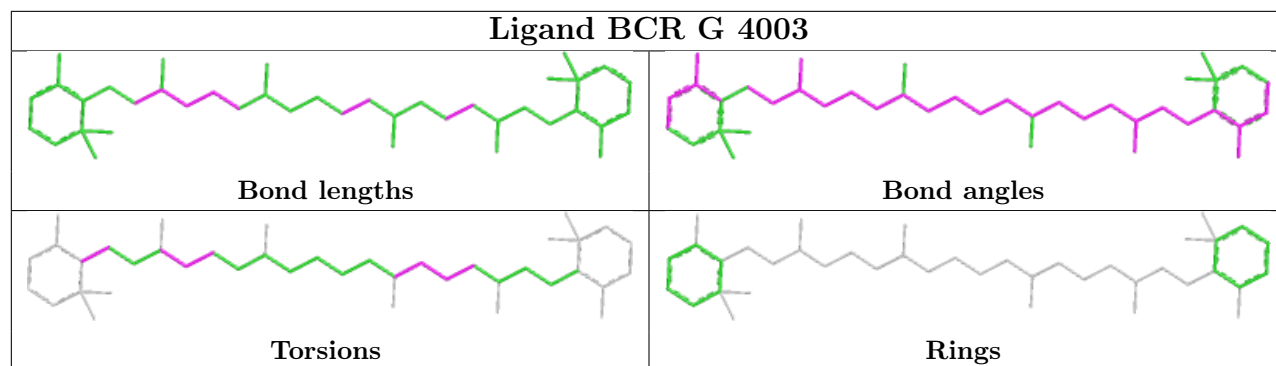
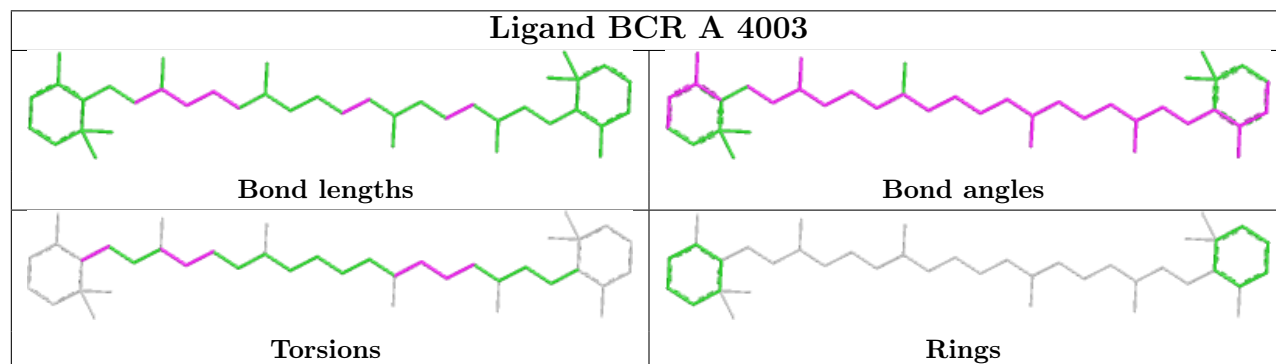
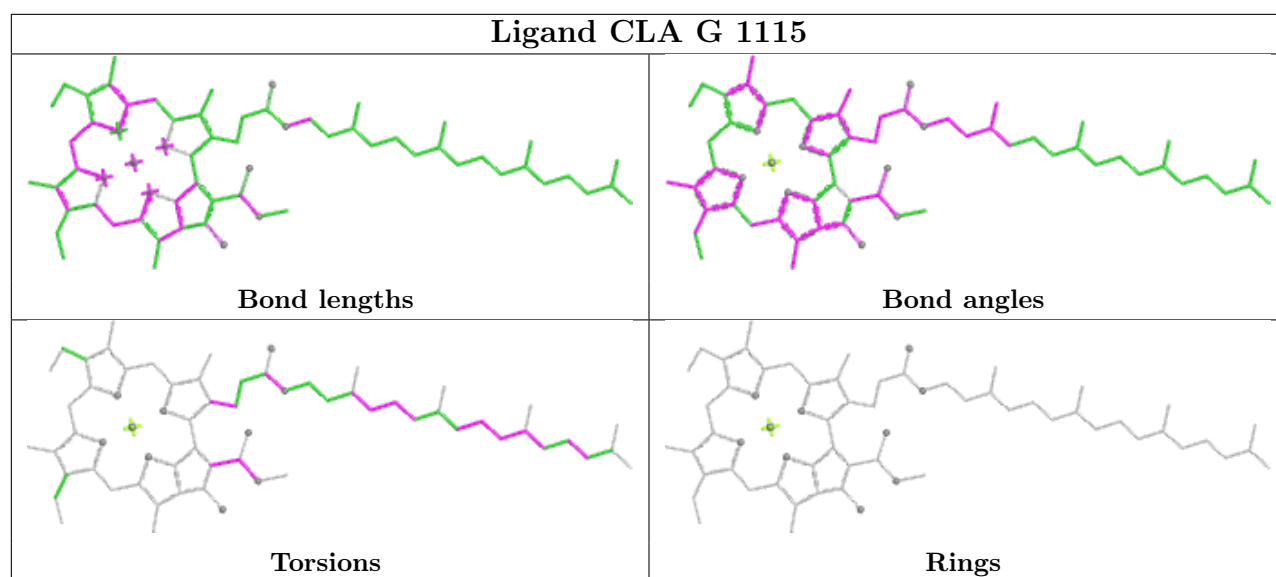


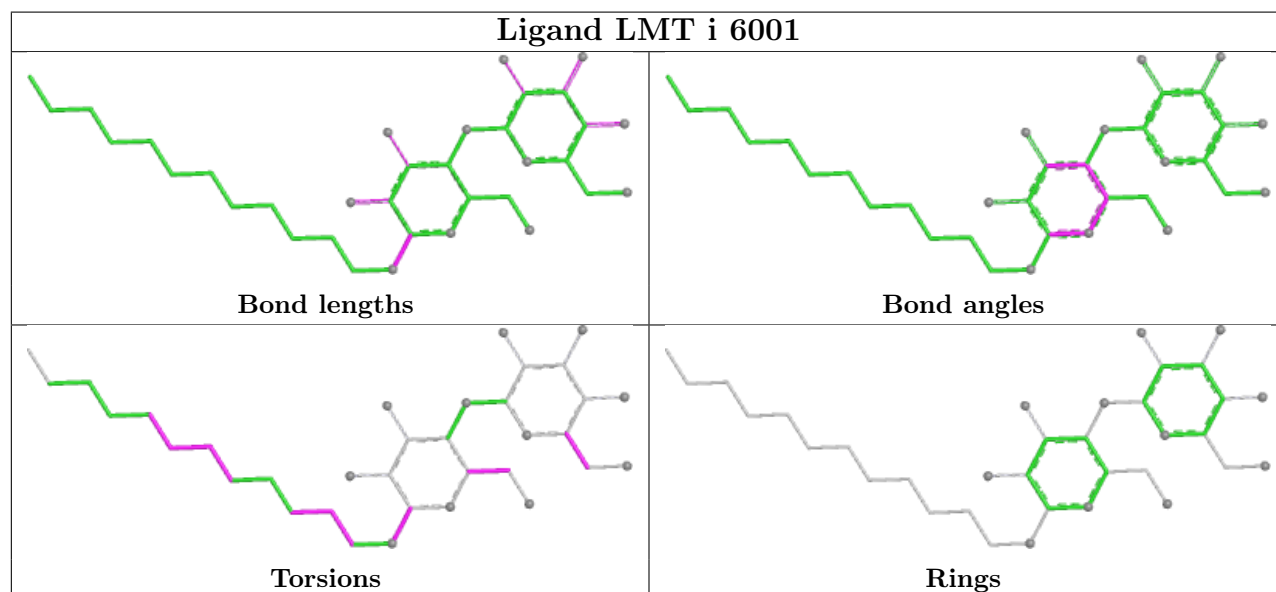
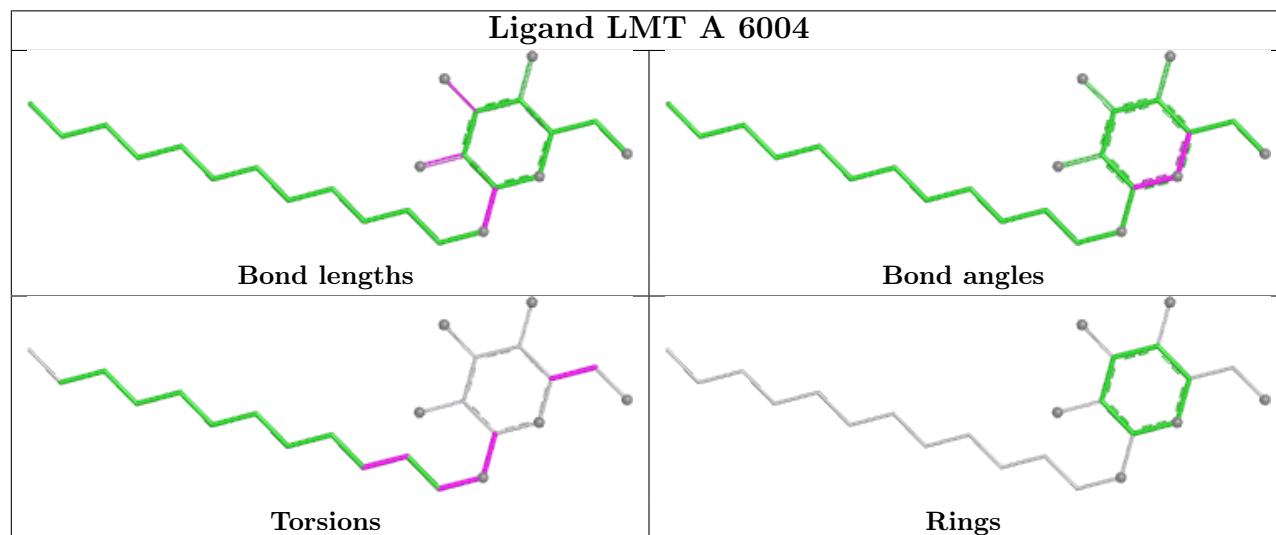
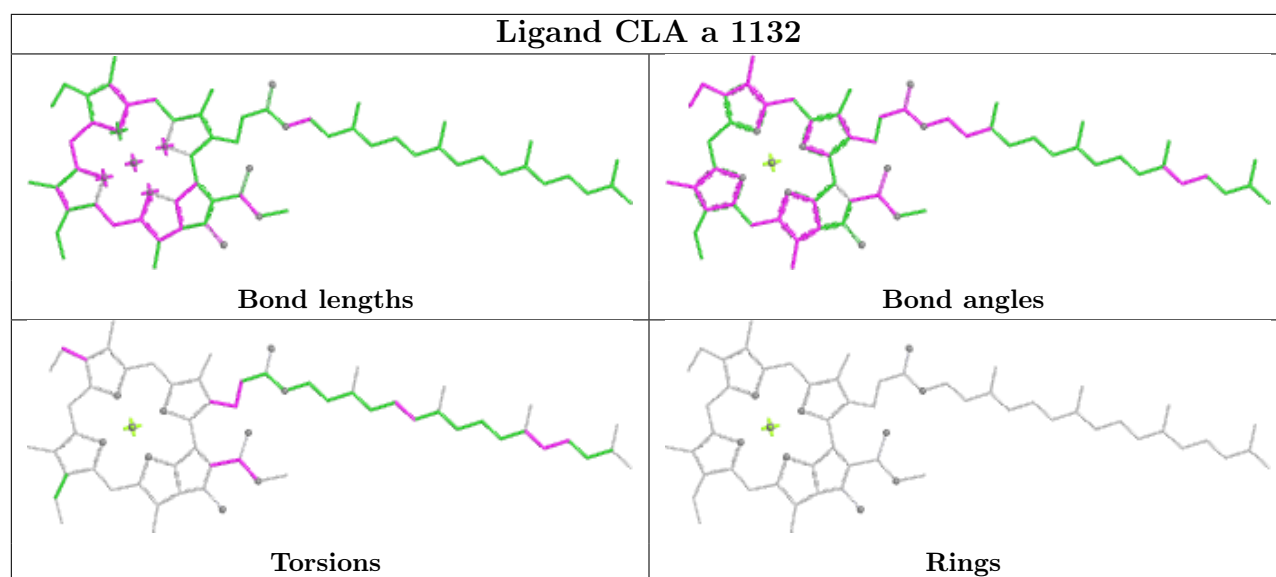


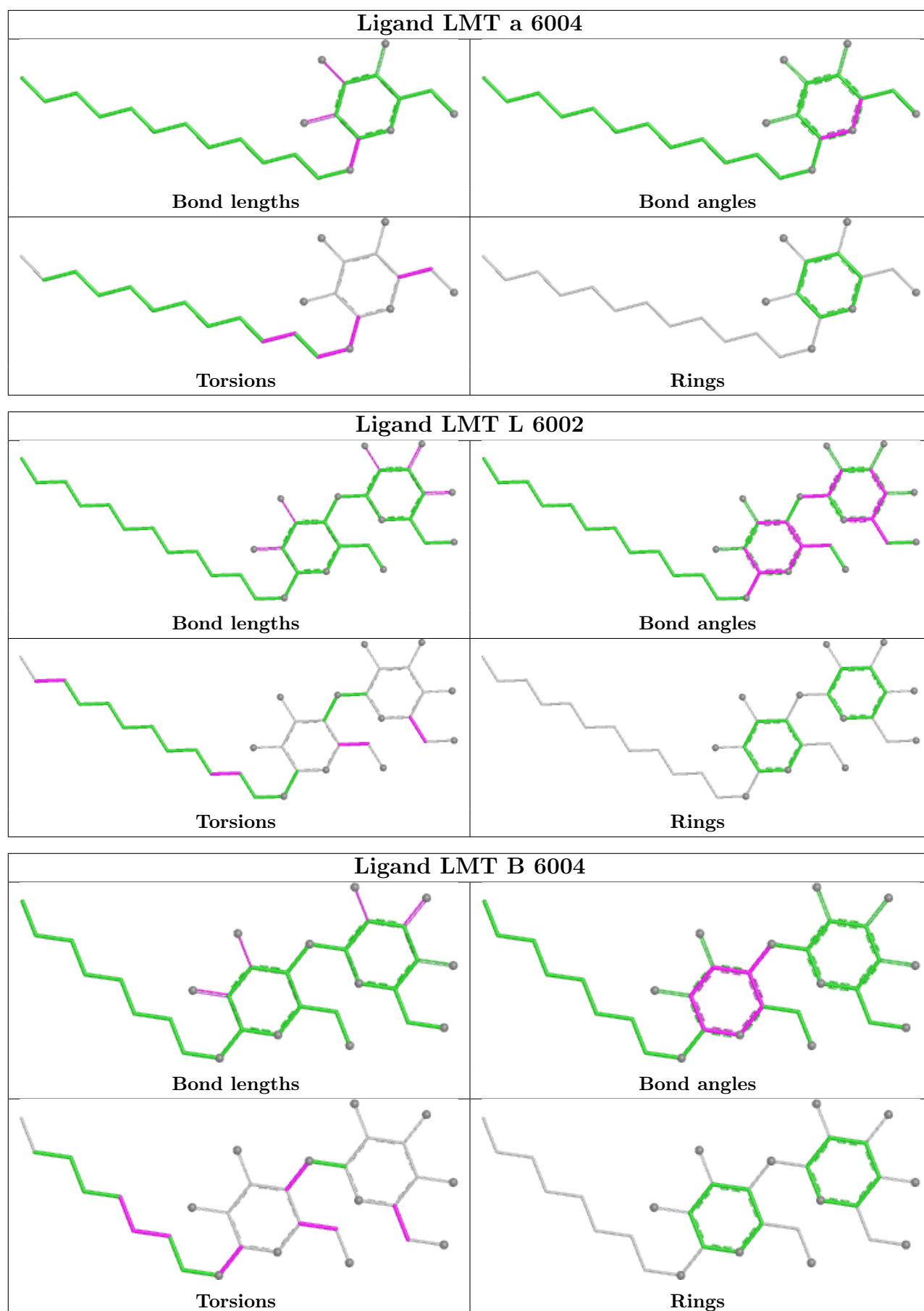




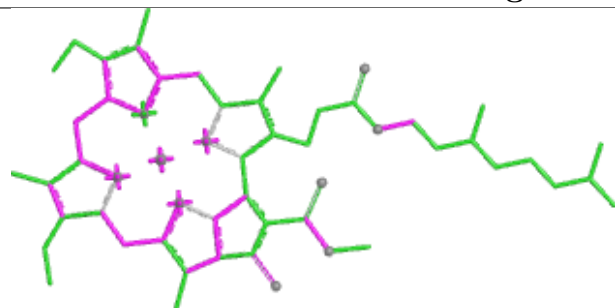
Ligand CLA A 1128**Ligand CLA B 1206**



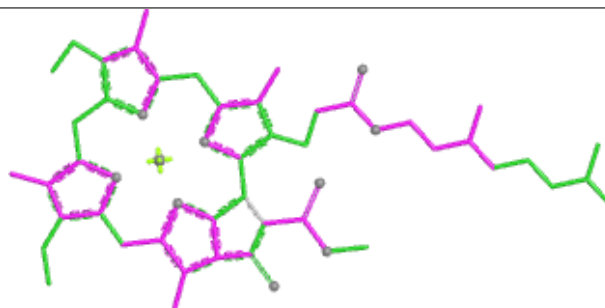




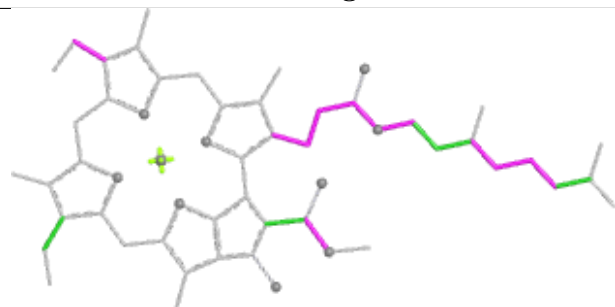
Ligand CLA G 1140



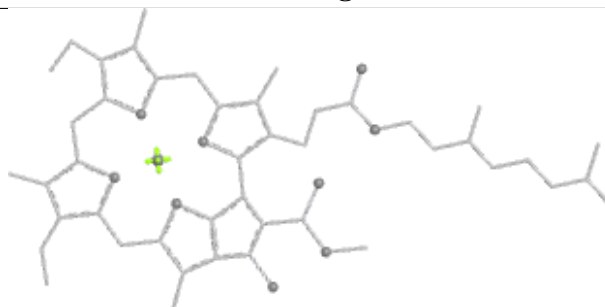
Bond lengths



Bond angles

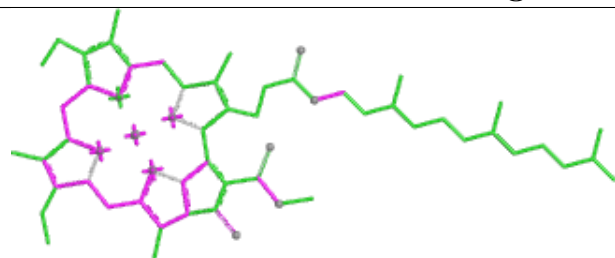


Torsions

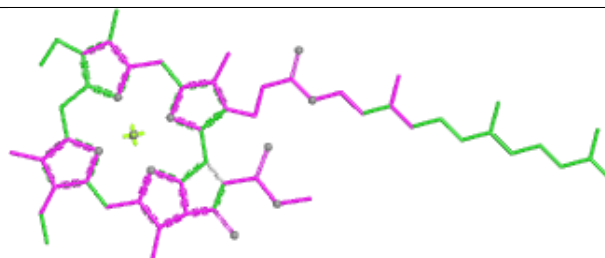


Rings

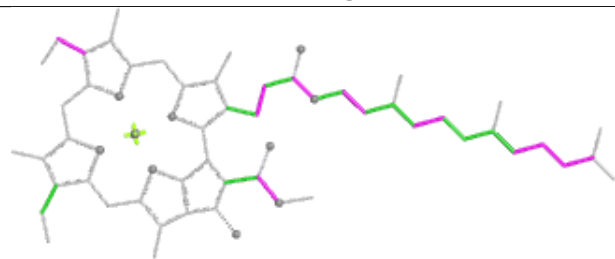
Ligand CLA B 1214



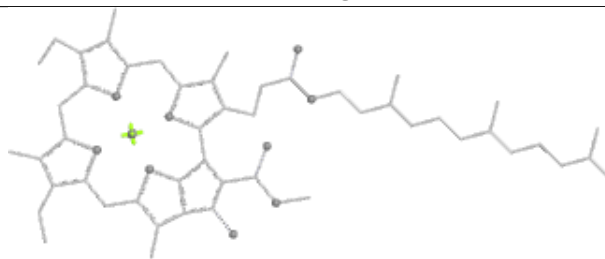
Bond lengths



Bond angles

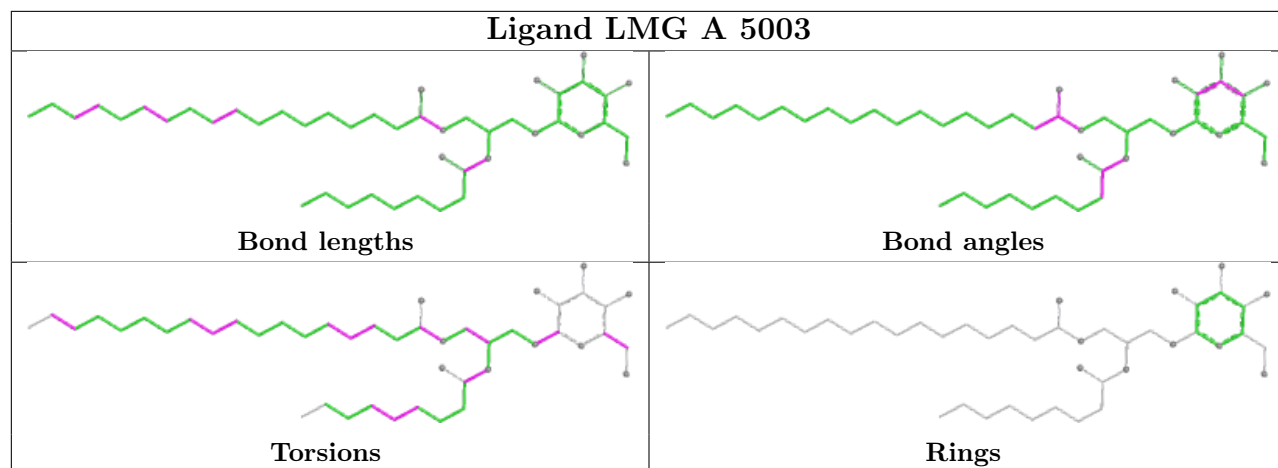


Torsions

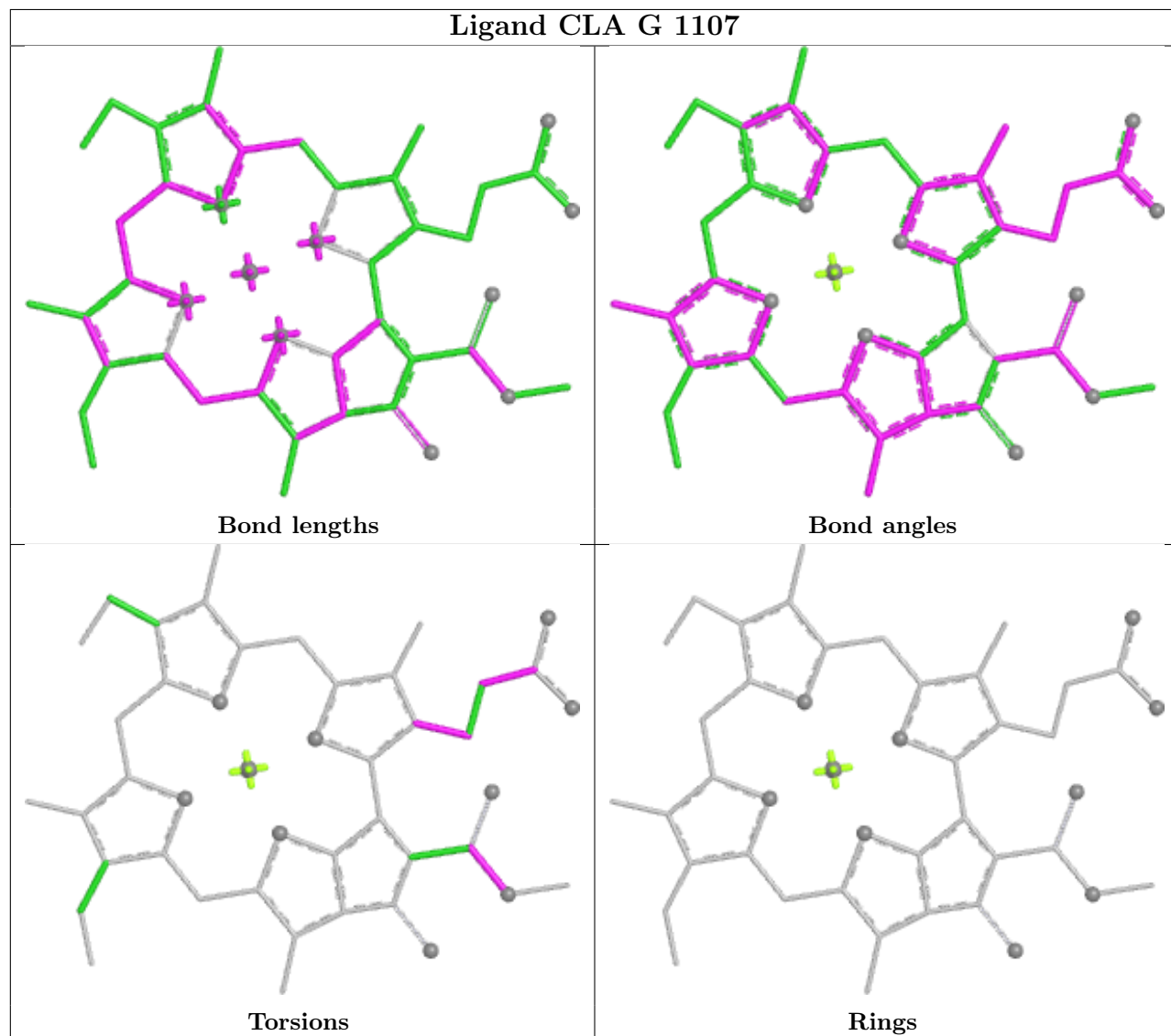


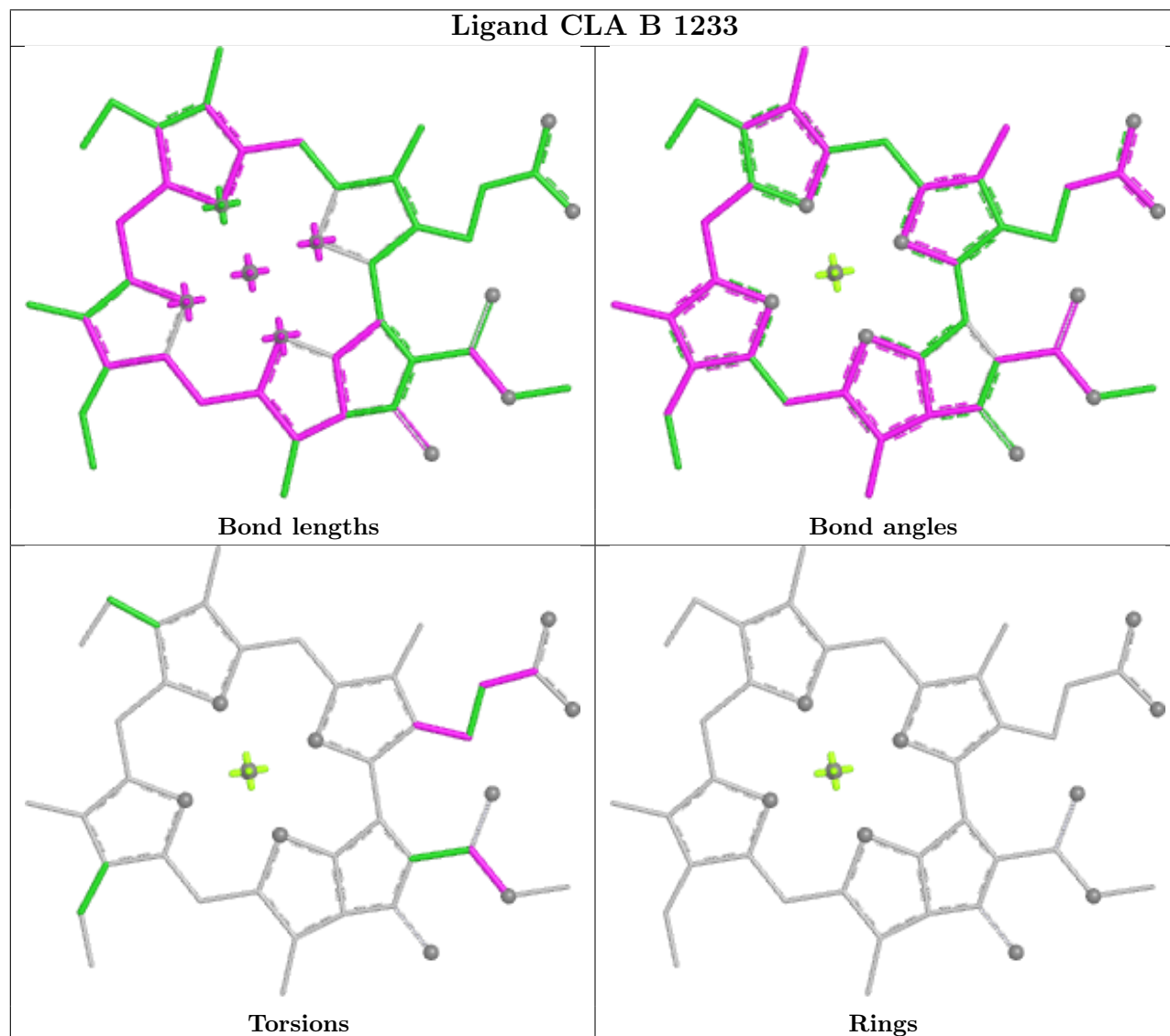
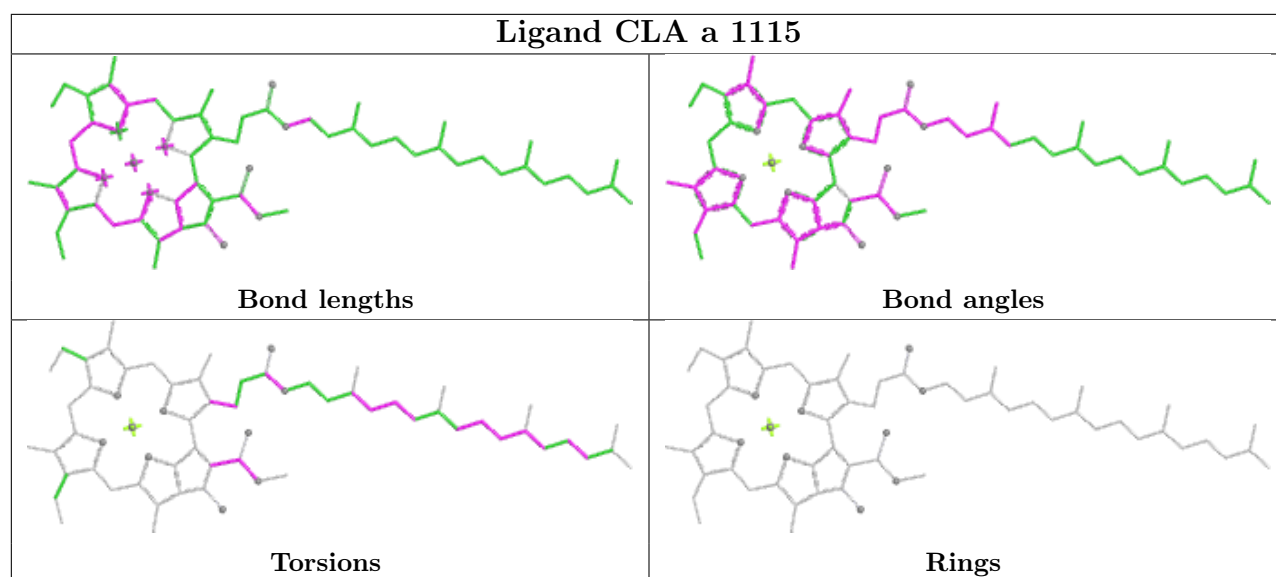
Rings

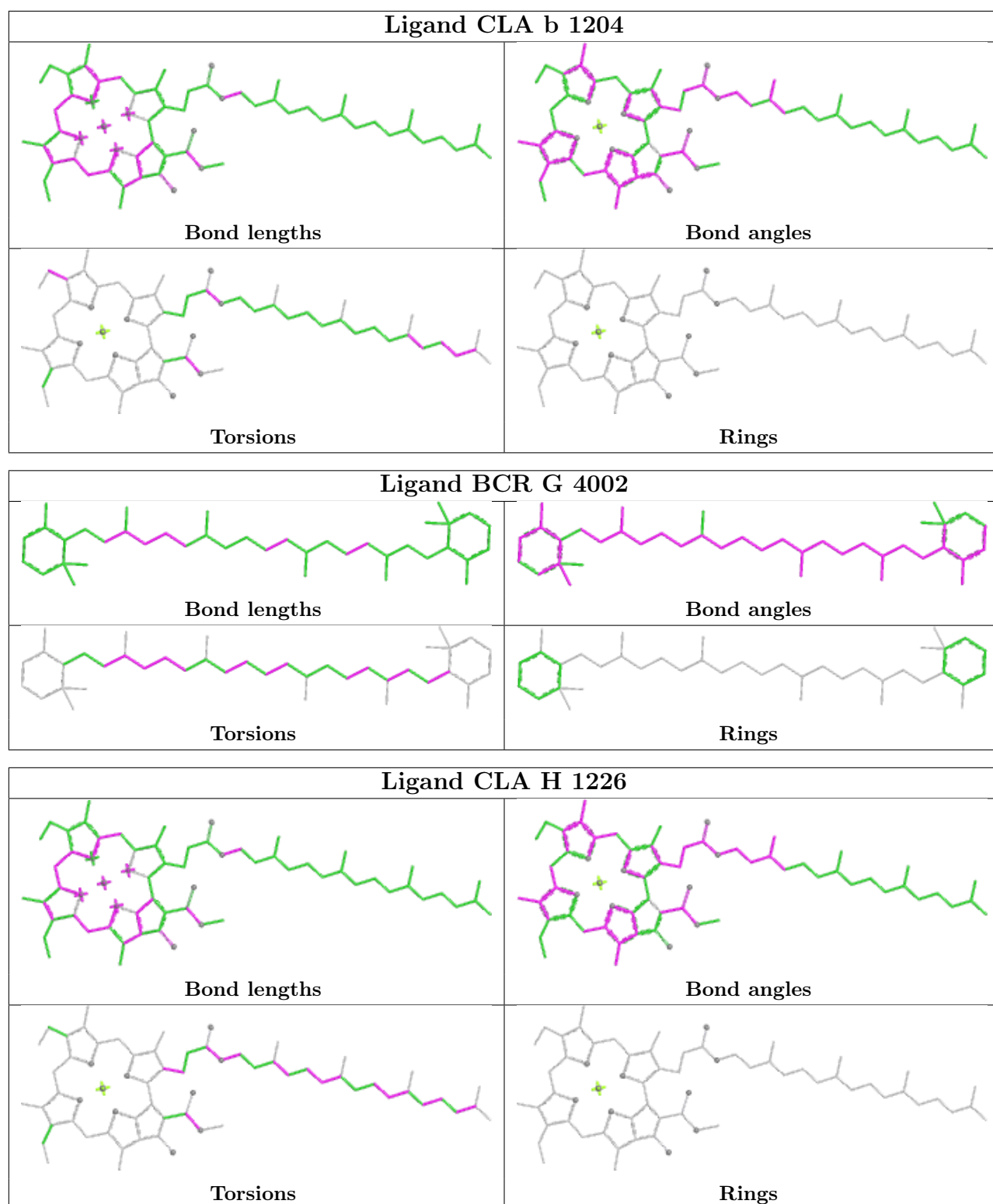
Ligand LMG A 5003

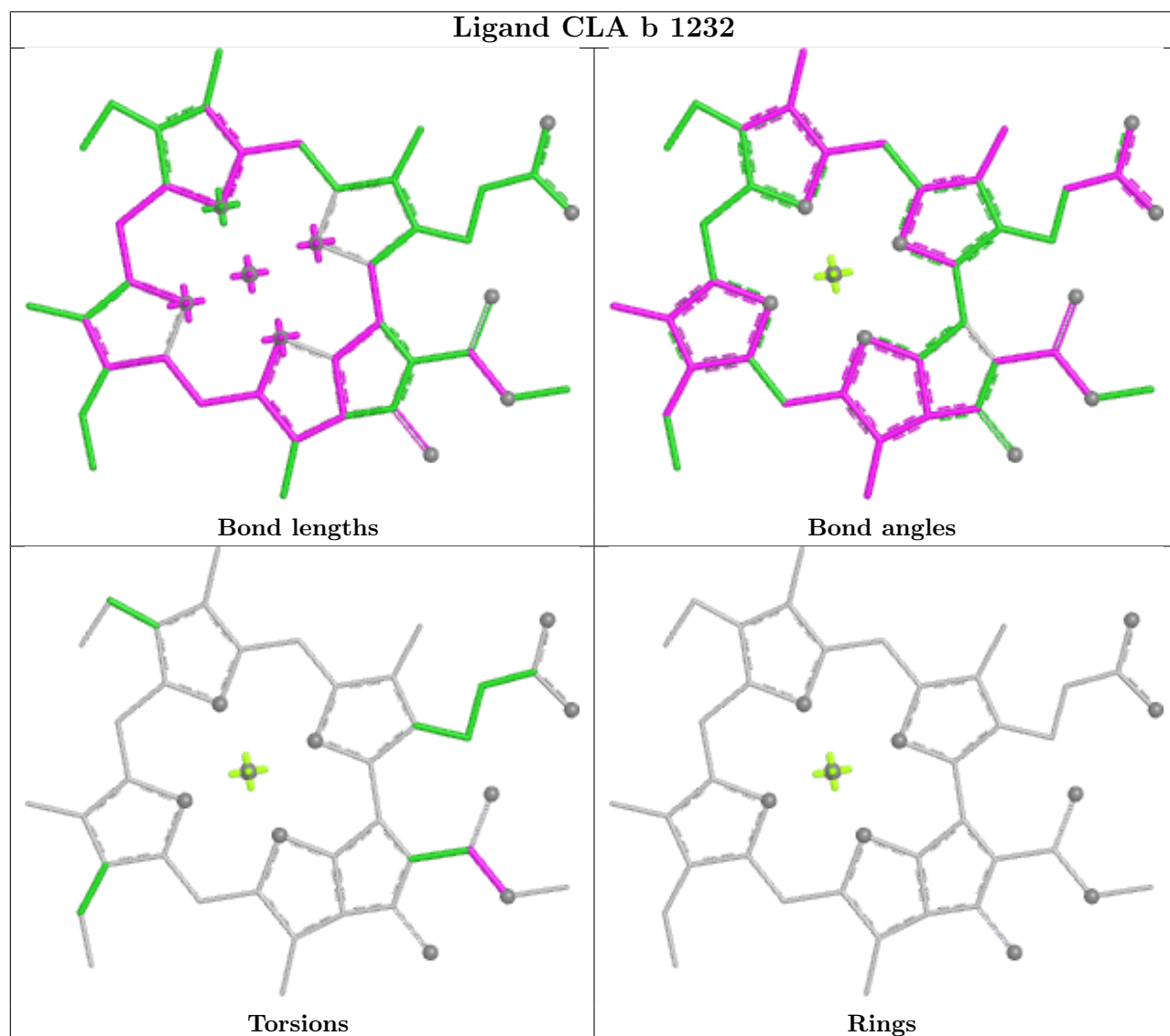
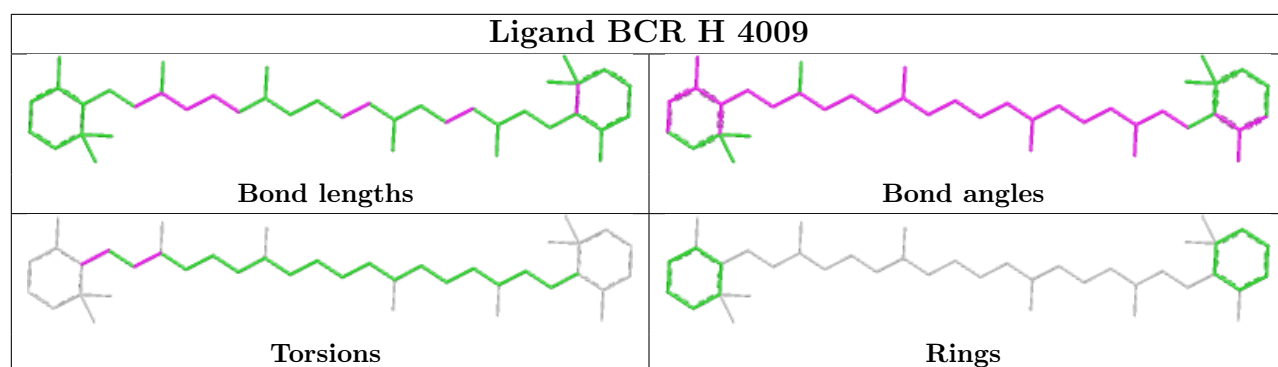


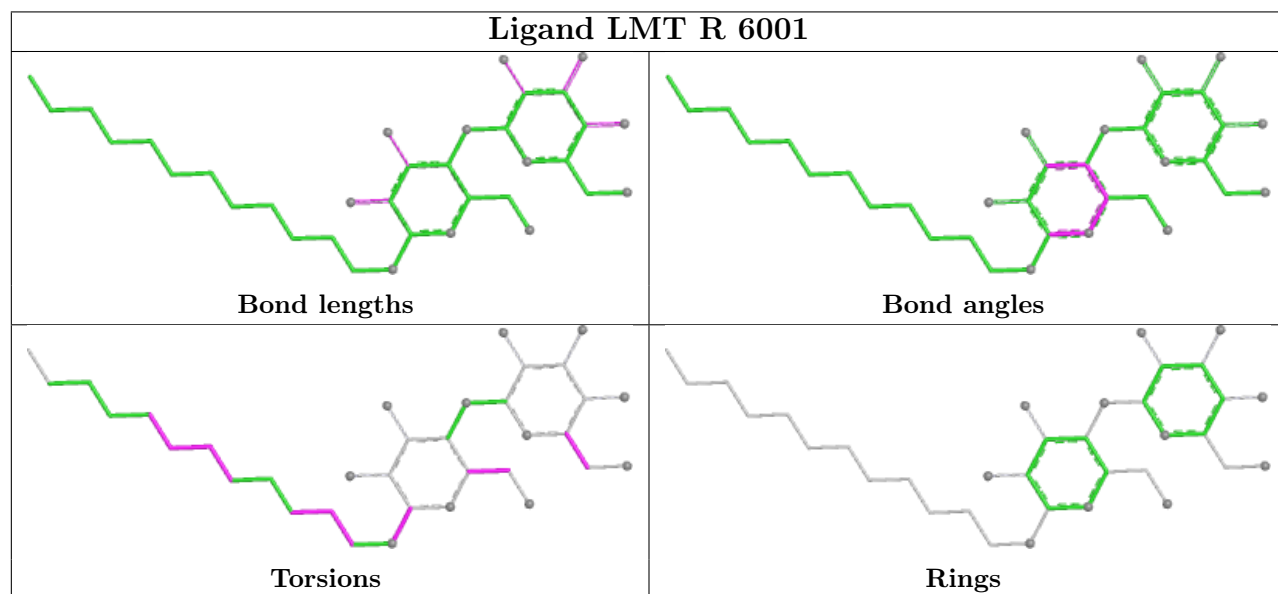
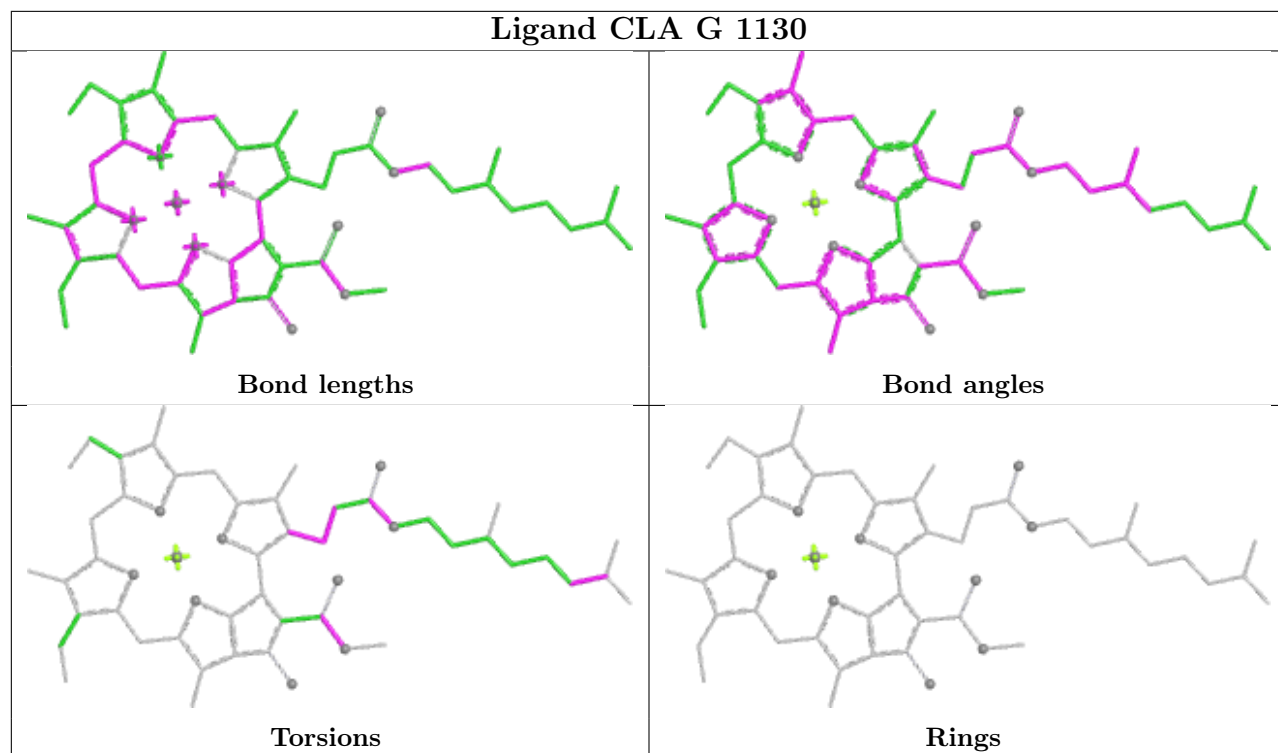
Ligand CLA G 1107

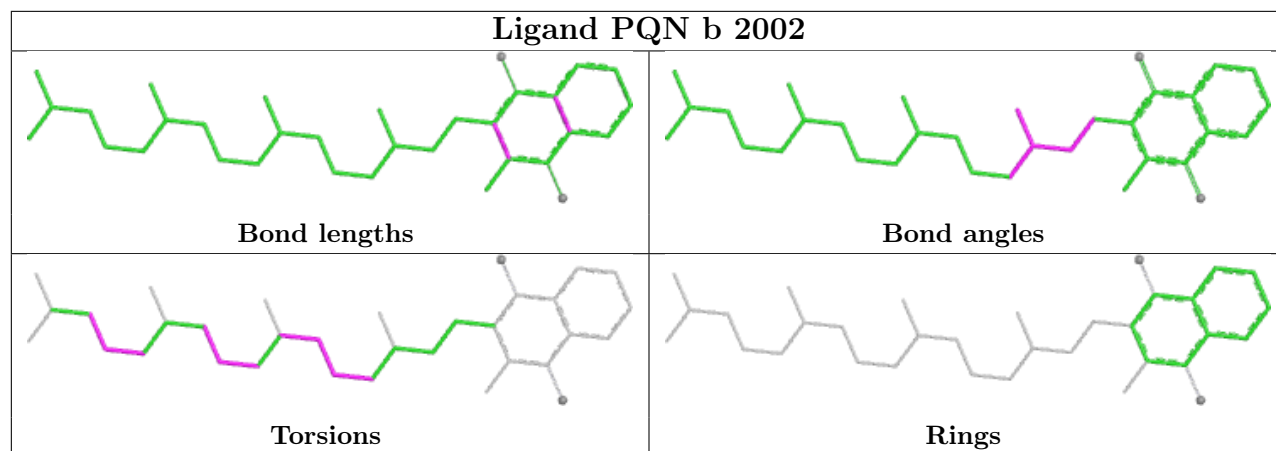
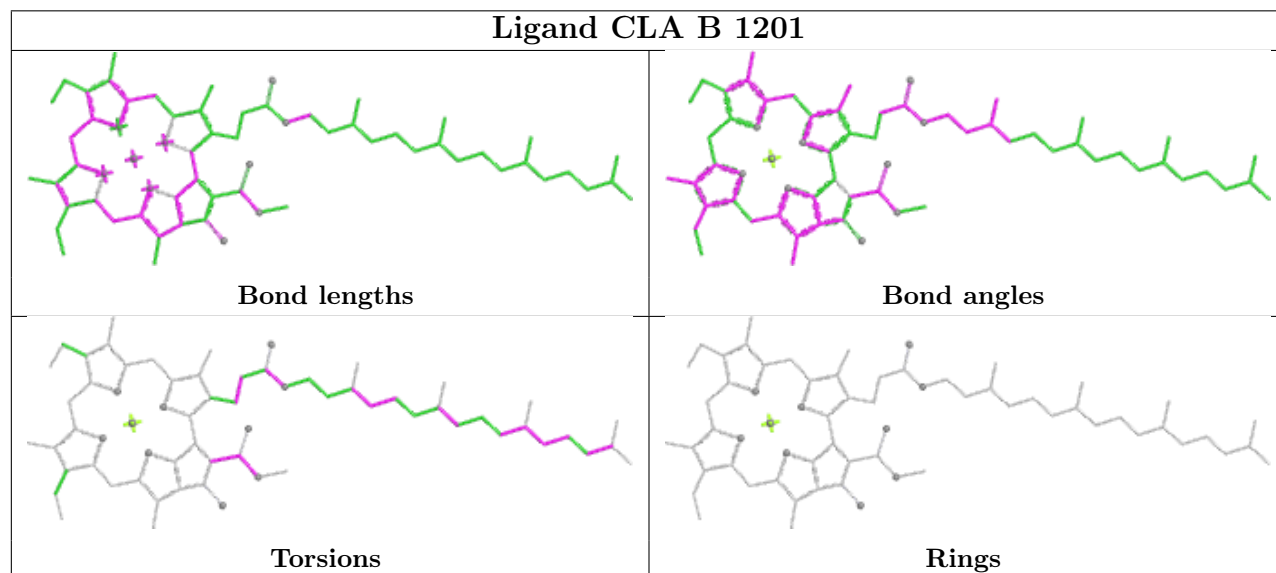
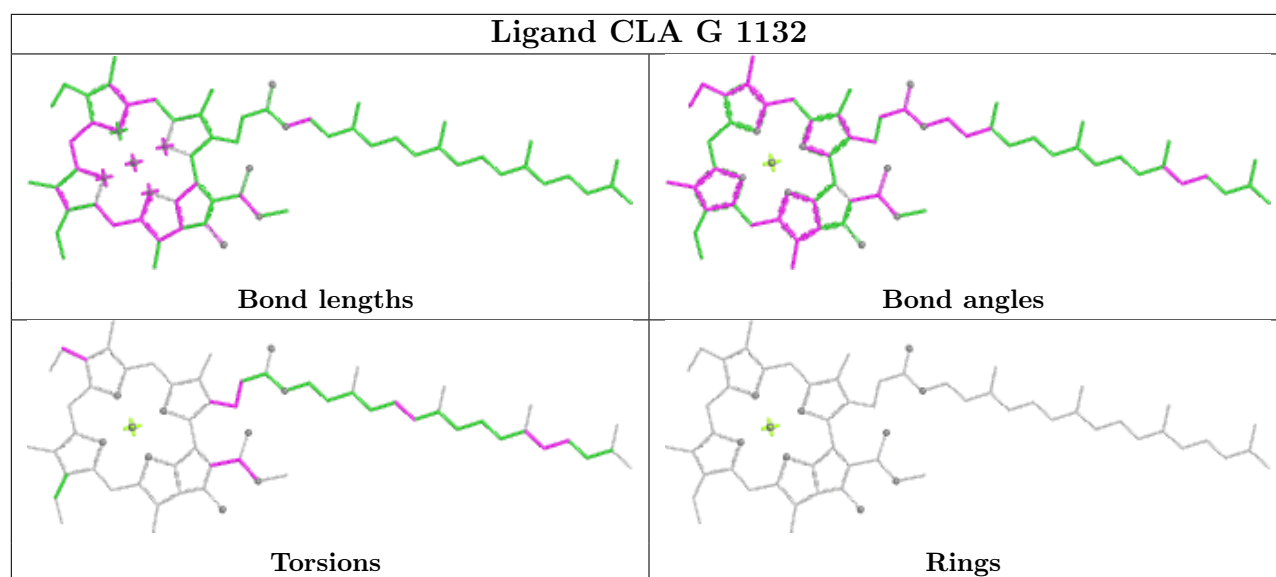


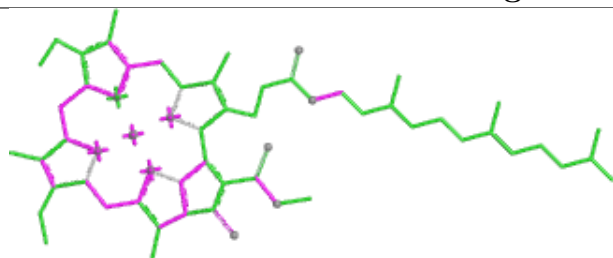
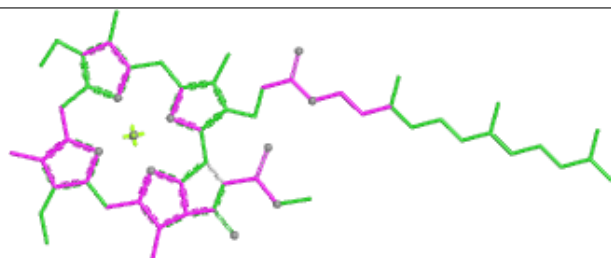
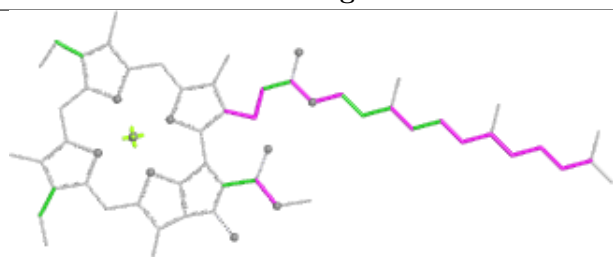
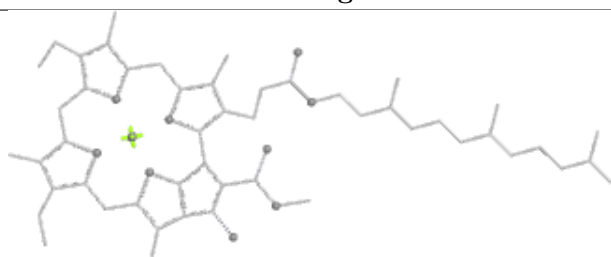
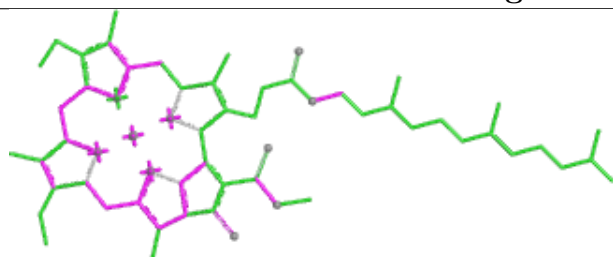
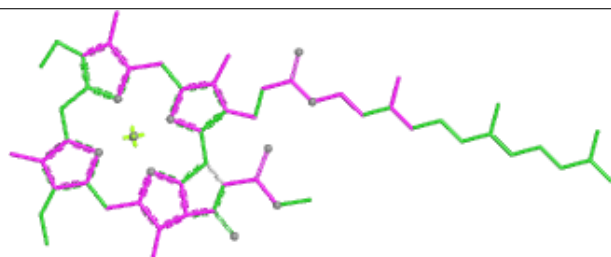
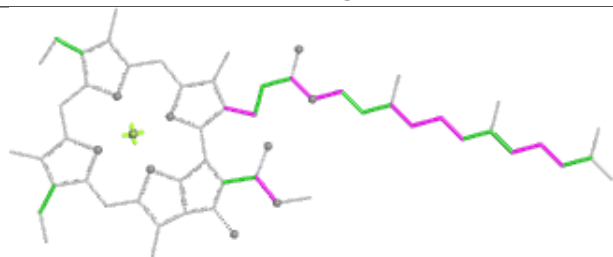
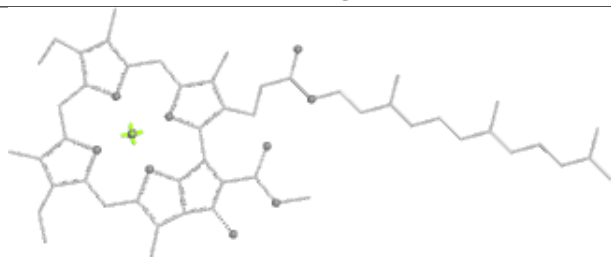


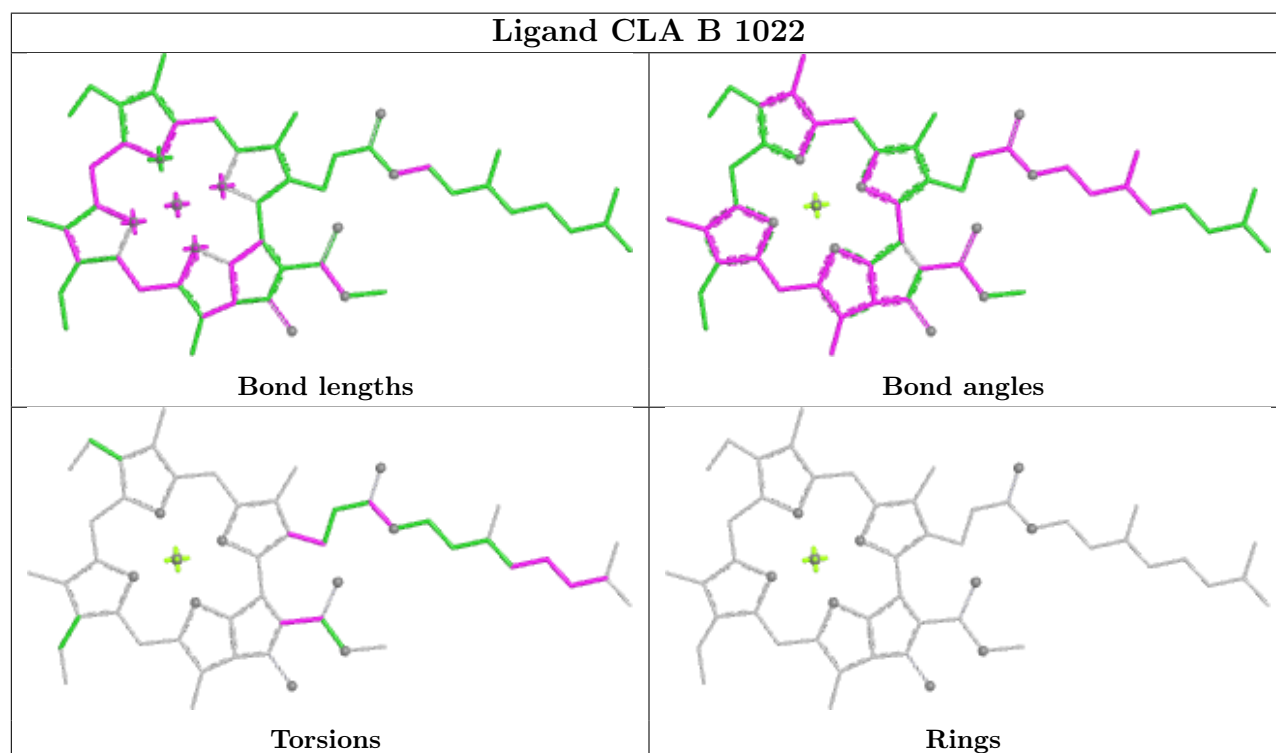
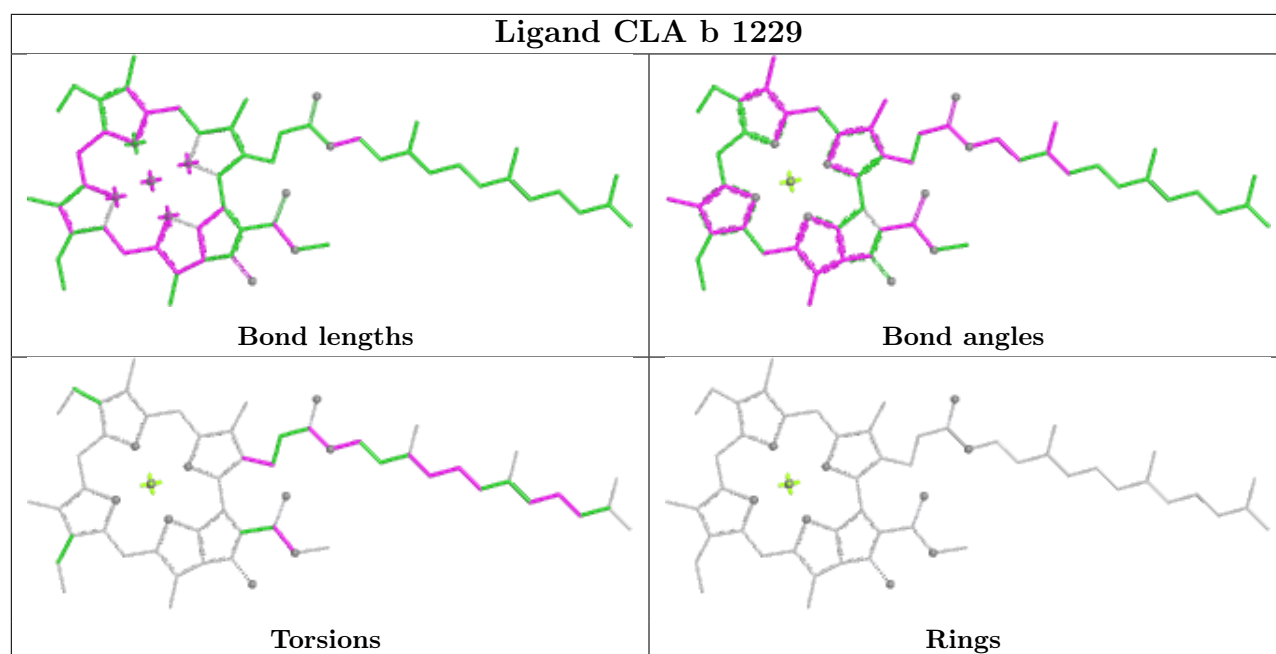


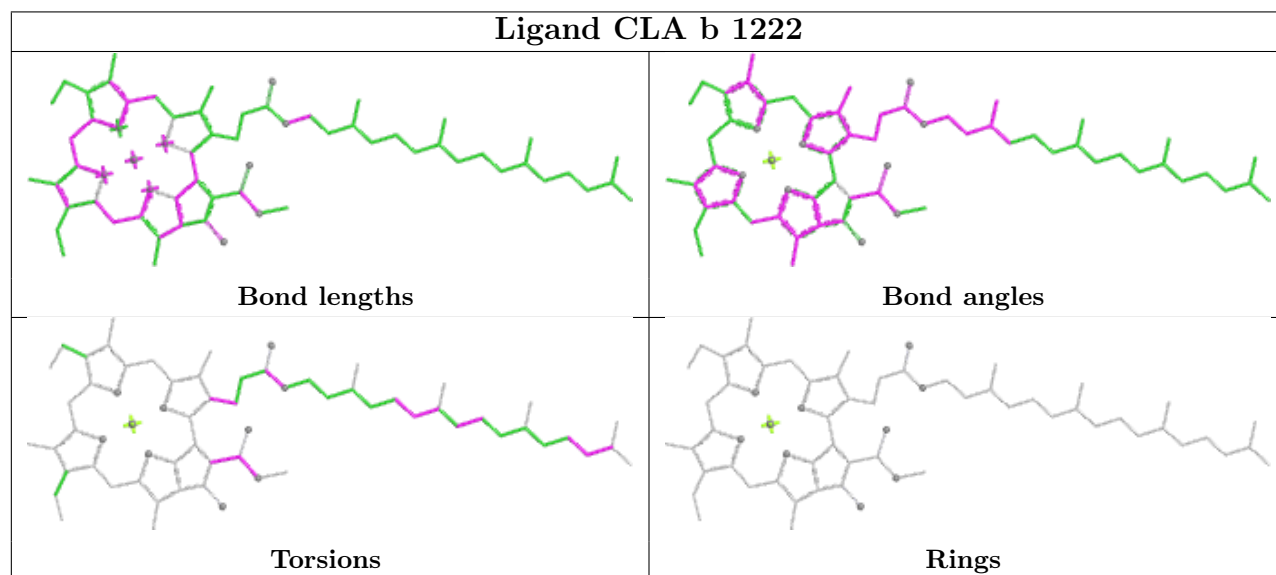
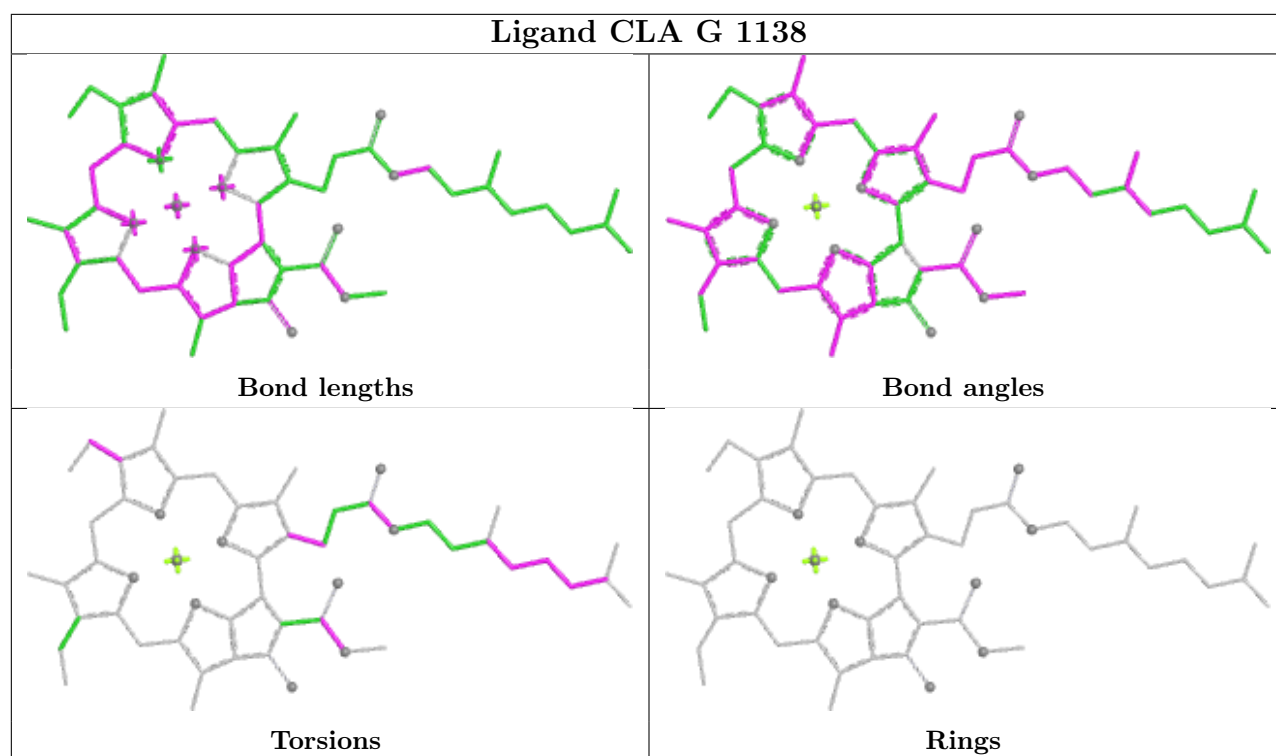


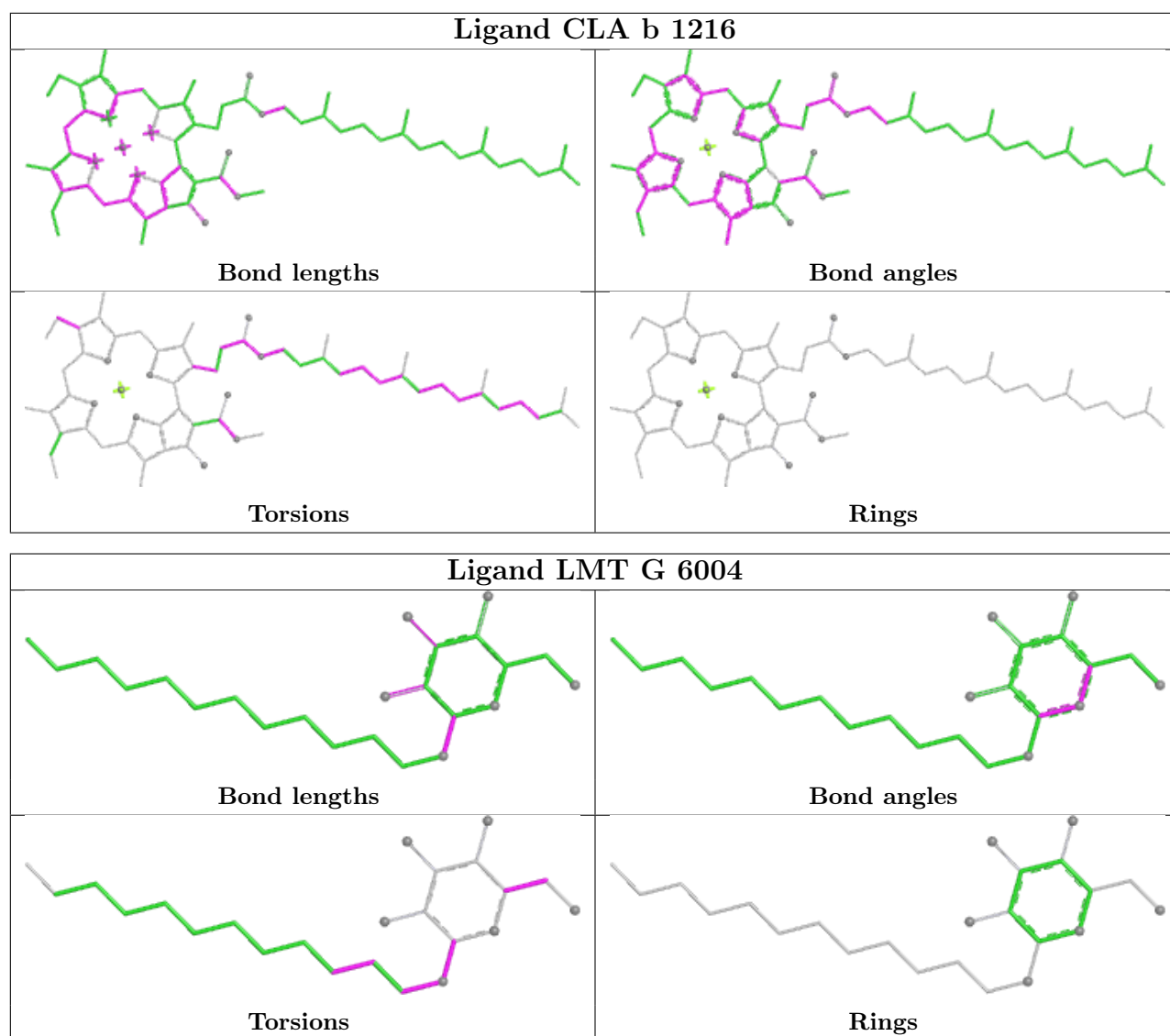




Ligand CLA G 1133**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 1229****Bond lengths****Bond angles****Torsions****Rings**







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

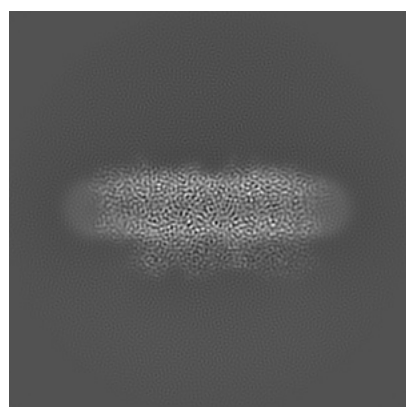
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24821. These allow visual inspection of the internal detail of the map and identification of artifacts.

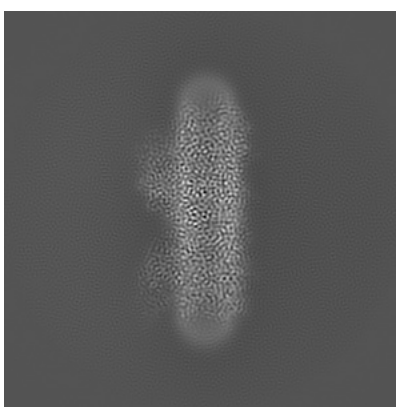
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

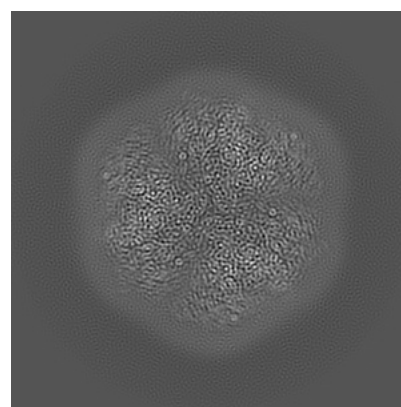
6.1.1 Primary map



X



Y

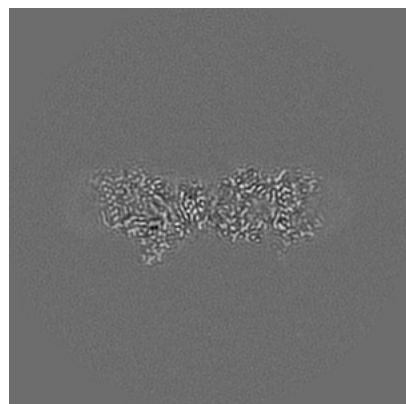


Z

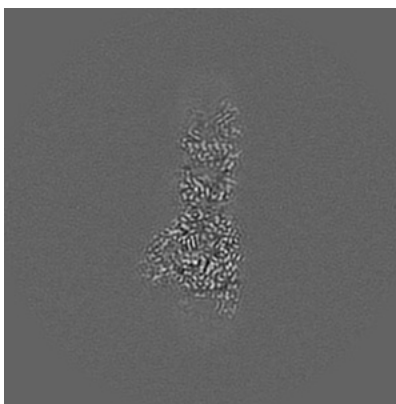
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

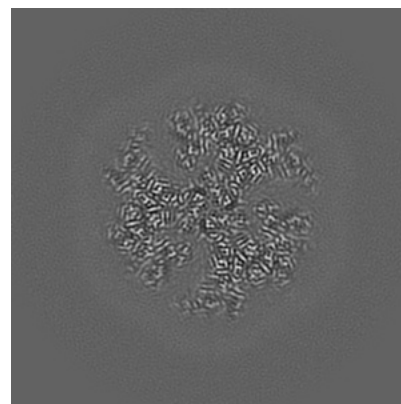
6.2.1 Primary map



X Index: 192



Y Index: 192

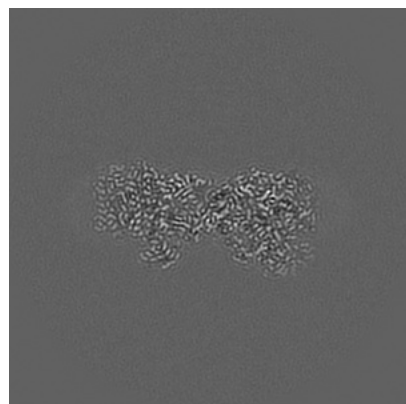


Z Index: 192

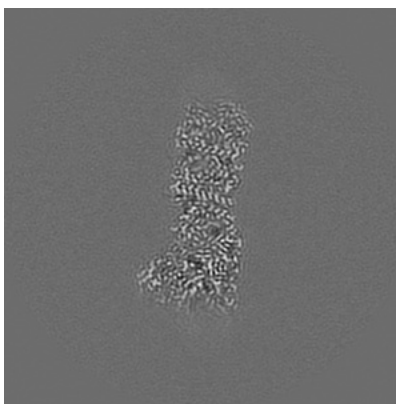
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

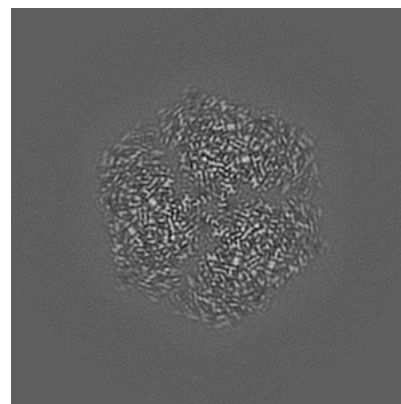
6.3.1 Primary map



X Index: 212



Y Index: 180

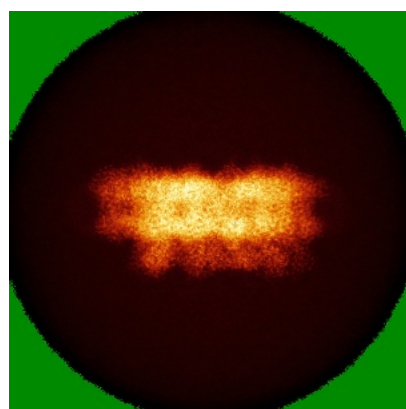


Z Index: 212

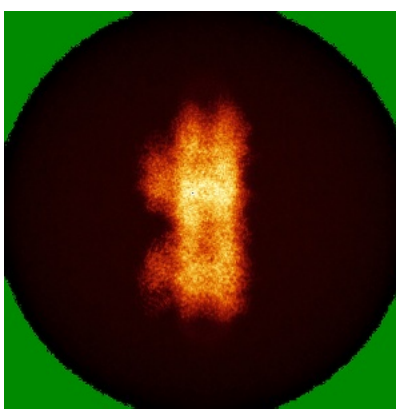
The images above show the largest variance slices of the map in three orthogonal directions.

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

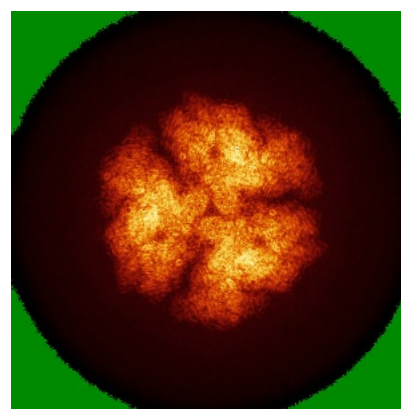
6.4.1 Primary map



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

This section was not generated.

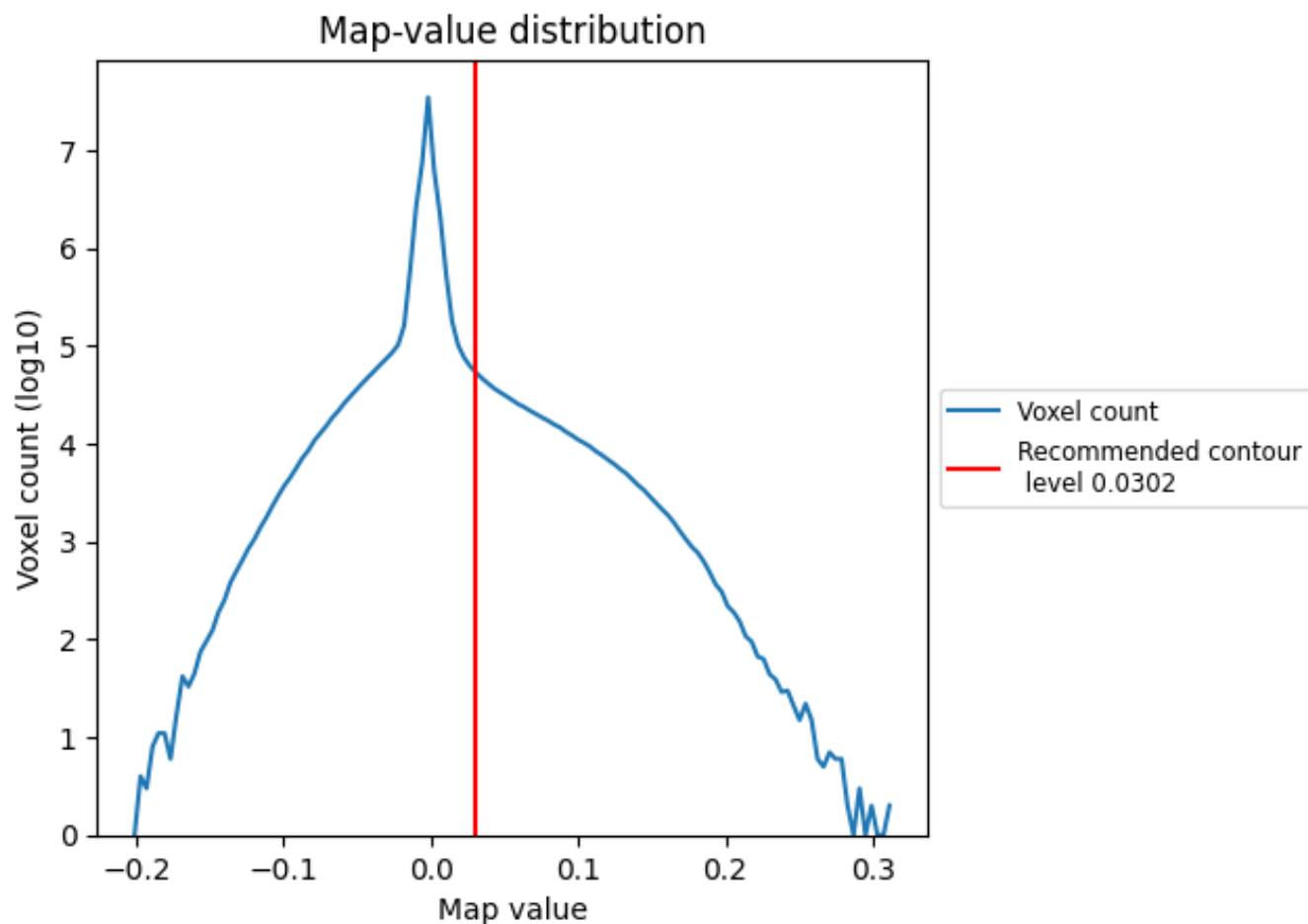
6.6 Mask visualisation

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

7 Map analysis [i](#)

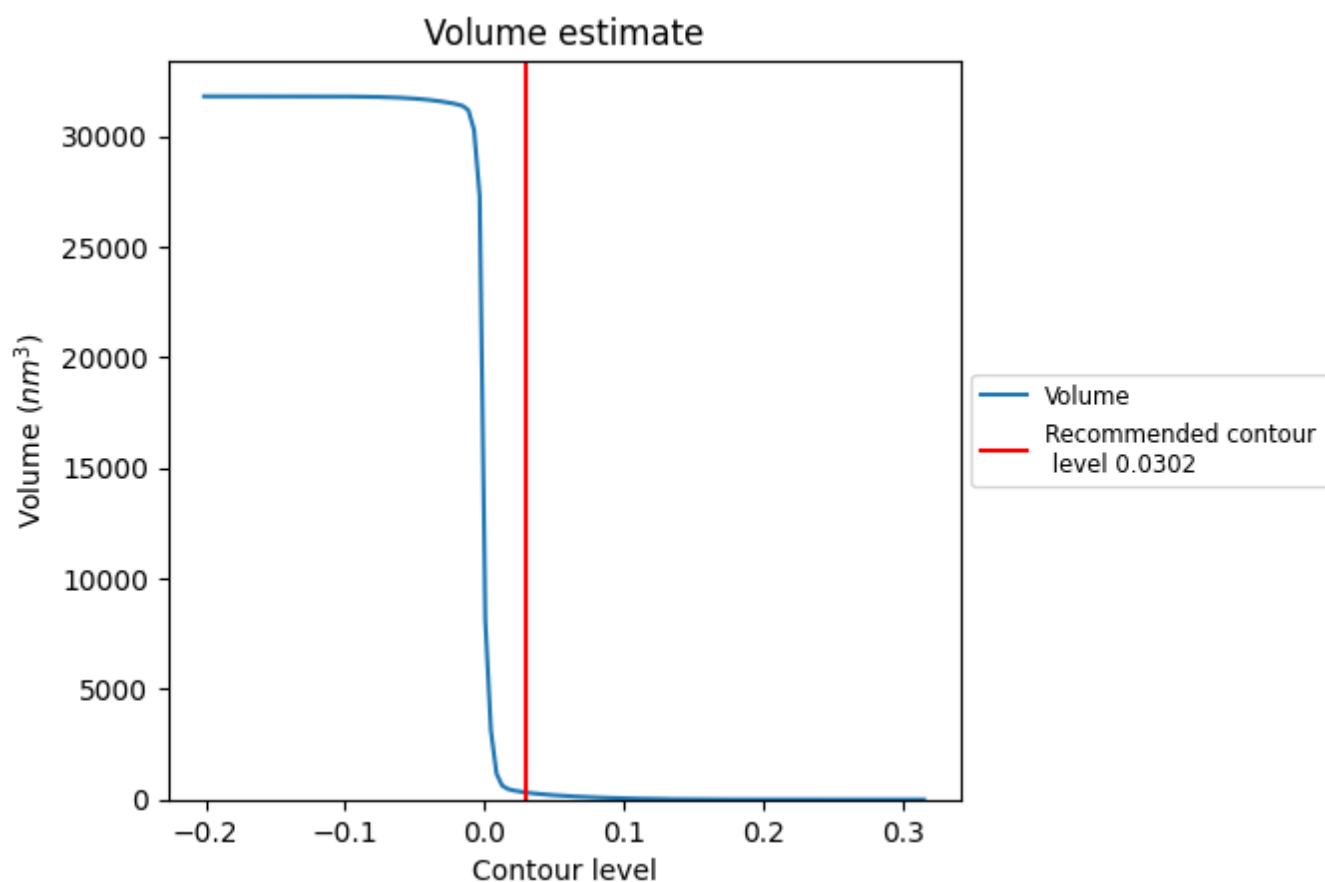
This section contains the results of statistical analysis of the map.

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.

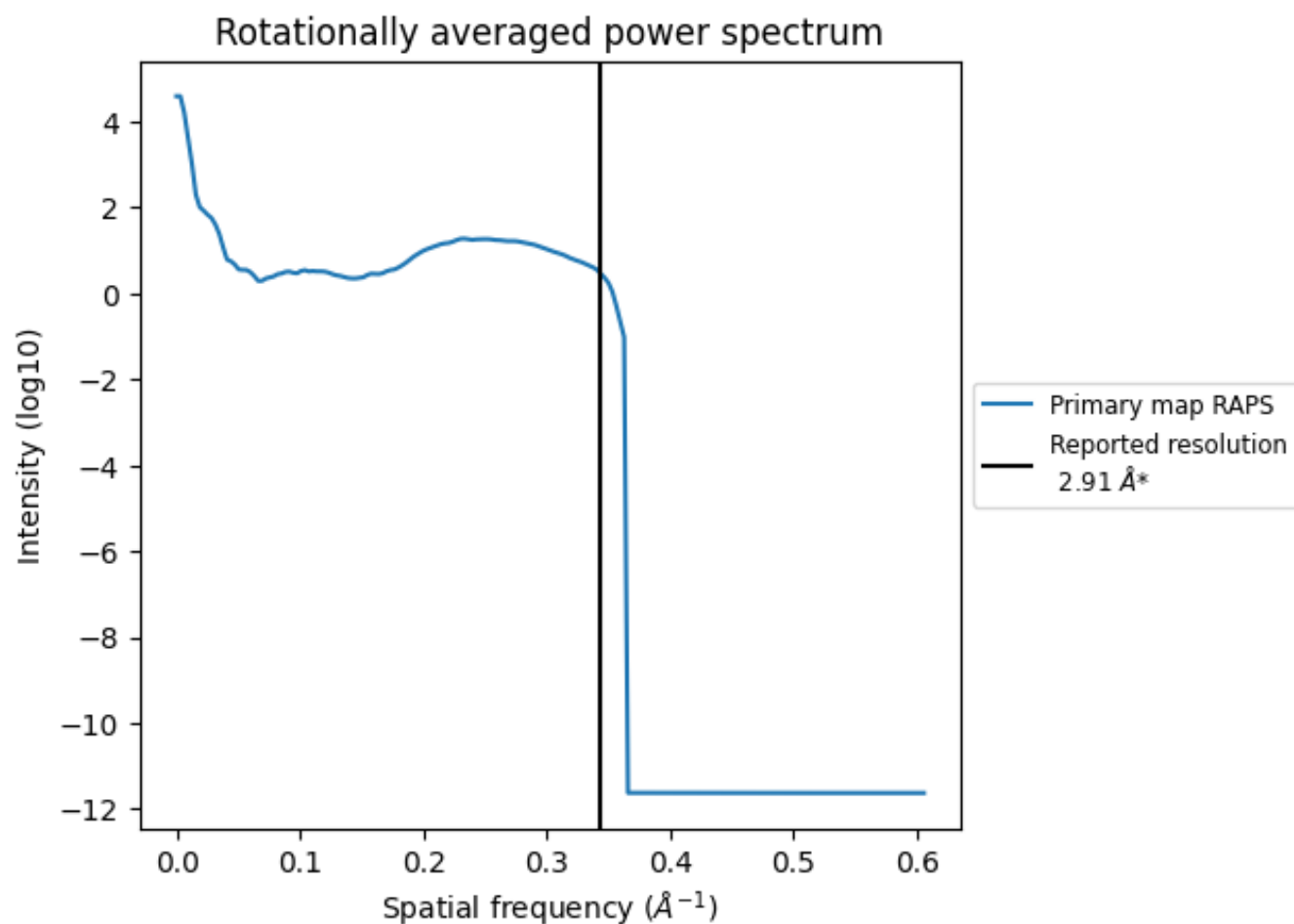
7.2 Volume estimate [i](#)



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 ⓘ

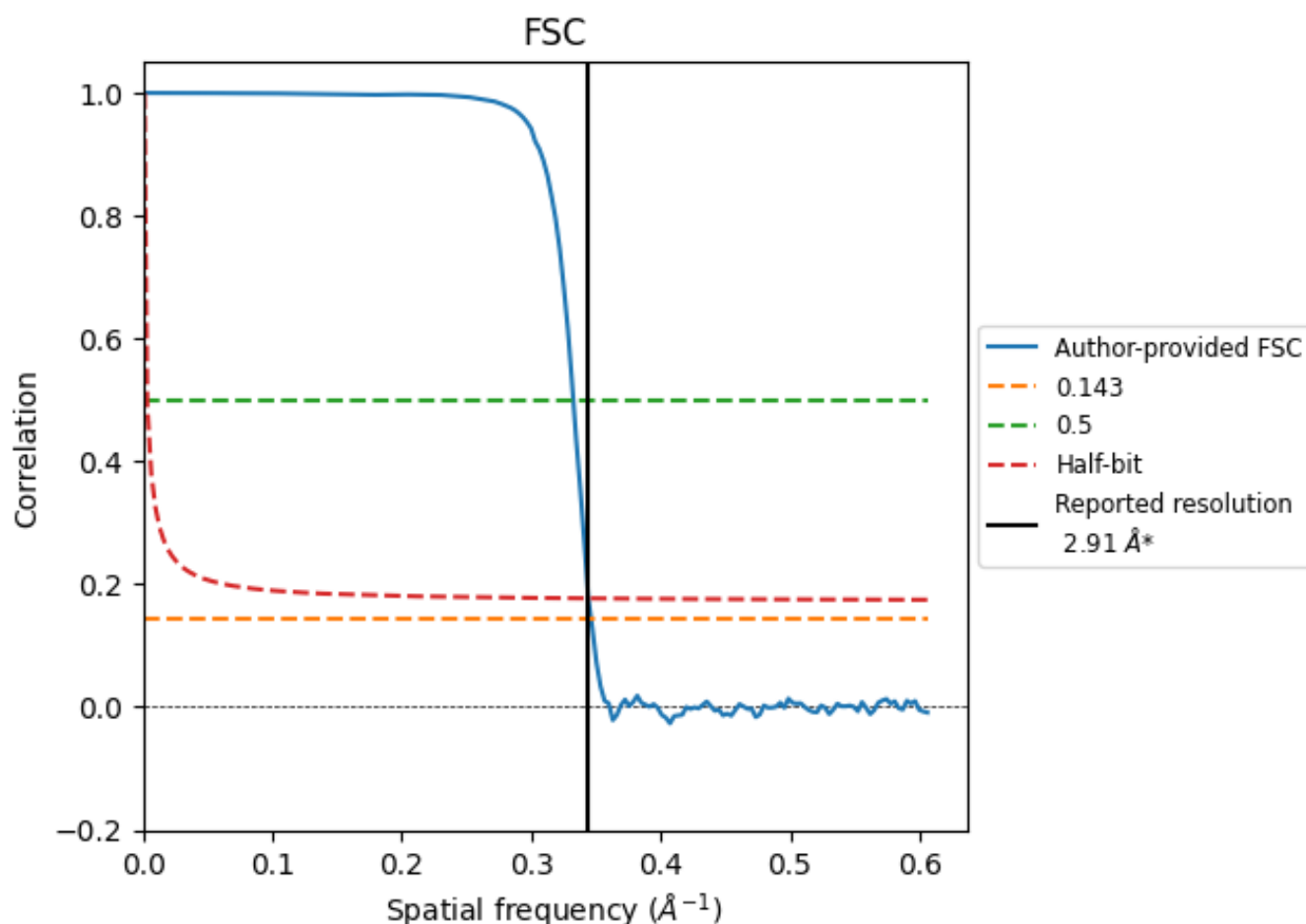


*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

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.

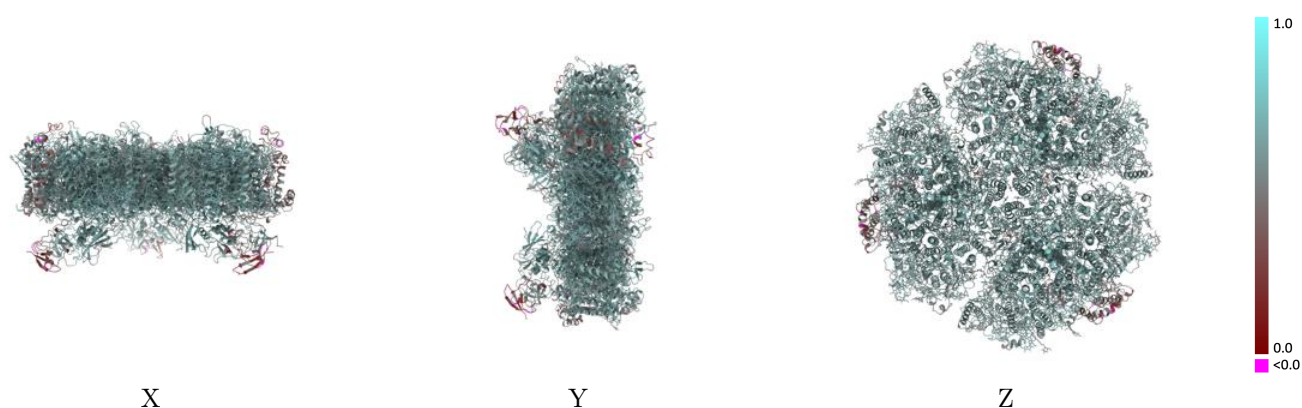
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD 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](#)

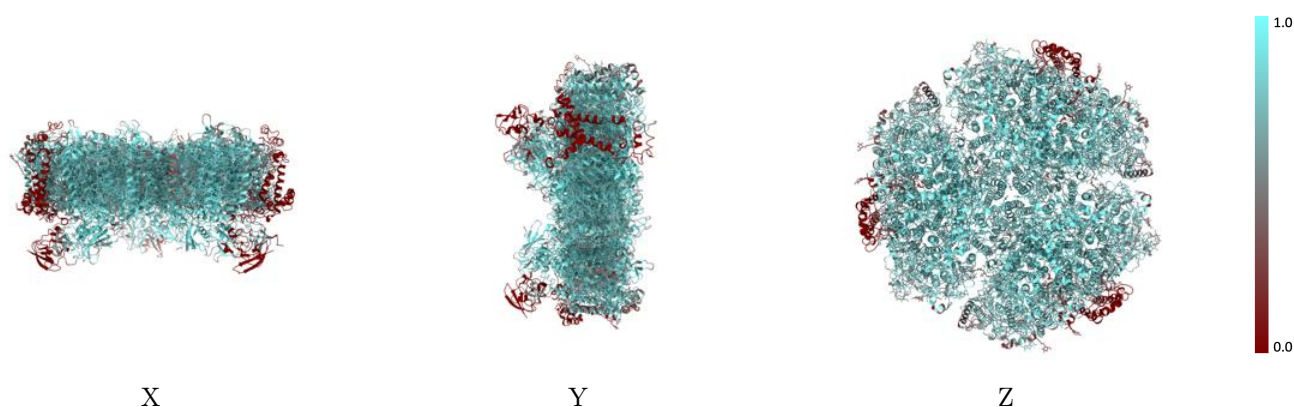
This section was not generated.

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



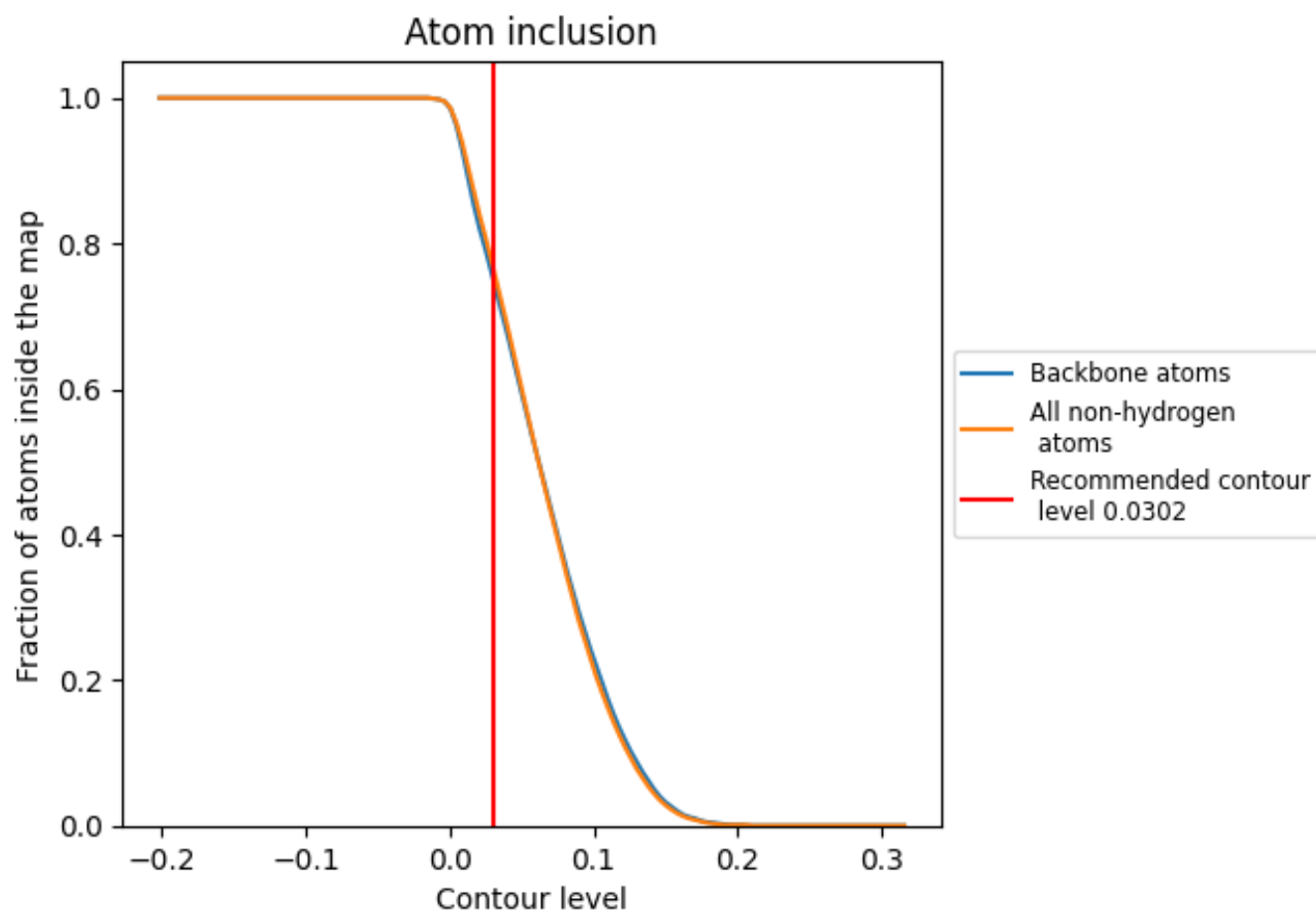
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0302).

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