



## wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 03:28 AM EST

PDB ID : 6NWA  
EMDB ID : EMD-0524  
Title : The structure of the photosystem I IsiA super-complex  
Authors : Toporik, H.; Li, J.; Williams, D.; Chiu, P.L.; Mazor, Y.  
Deposited on : 2019-02-06  
Resolution : 3.48 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

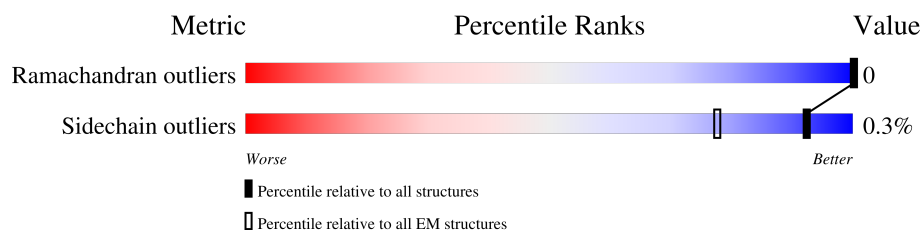
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

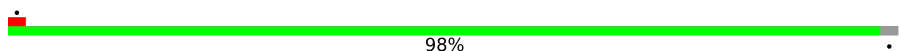
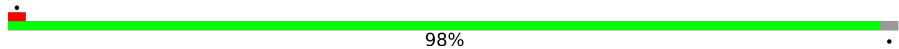
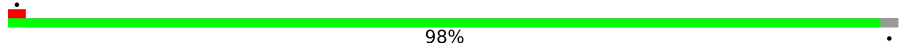
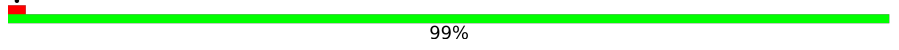
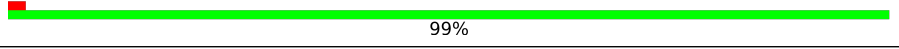
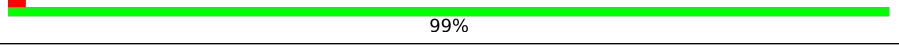
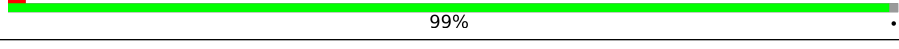
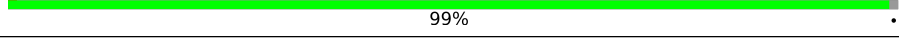
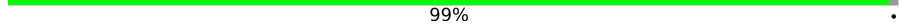
The reported resolution of this entry is 3.48 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	751	 98% .
1	H	751	 98% .
1	a	751	 98% .
2	B	731	 99% .
2	G	731	 99% .
2	b	731	 99% .
3	C	81	 99% .
3	N	81	 99% .
3	c	81	 99% .

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Mol	Chain	Length	Quality of chain
4	D	141	
4	O	141	
4	d	141	
5	E	74	
5	P	74	
5	e	74	
6	F	165	
6	Q	165	
6	f	165	
7	I	40	
7	R	40	
7	i	40	
8	J	40	
8	S	40	
8	j	40	
9	L	157	
9	U	157	
9	l	157	
10	M	31	
10	V	31	
10	m	31	
11	W	342	
11	X	342	
11	Y	342	
11	Z	342	

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Mol	Chain	Length	Quality of chain
11	g	342	
11	h	342	
11	n	342	
11	o	342	
11	p	342	
11	q	342	
11	r	342	
11	s	342	
11	t	342	
11	u	342	
11	v	342	
11	w	342	
11	x	342	
11	y	342	
12	K	86	
12	T	86	
12	k	86	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL0	A	1011	X	-	-	-
15	CL0	H	1011	X	-	-	-
15	CL0	a	1011	X	-	-	-
16	CLA	A	1013	X	-	-	-
16	CLA	A	1022	X	-	-	-
16	CLA	A	1101	X	-	-	-
16	CLA	A	1102	X	-	-	-
16	CLA	A	1103	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	A	1104	X	-	-	-
16	CLA	A	1105	X	-	-	-
16	CLA	A	1106	X	-	-	-
16	CLA	A	1107	X	-	-	-
16	CLA	A	1108	X	-	-	-
16	CLA	A	1109	X	-	-	-
16	CLA	A	1110	X	-	-	-
16	CLA	A	1111	X	-	-	-
16	CLA	A	1112	X	-	-	-
16	CLA	A	1113	X	-	-	-
16	CLA	A	1114	X	-	-	-
16	CLA	A	1115	X	-	-	-
16	CLA	A	1116	X	-	-	-
16	CLA	A	1117	X	-	-	-
16	CLA	A	1118	X	-	-	-
16	CLA	A	1119	X	-	-	-
16	CLA	A	1120	X	-	-	-
16	CLA	A	1121	X	-	-	-
16	CLA	A	1122	X	-	-	-
16	CLA	A	1123	X	-	-	-
16	CLA	A	1124	X	-	-	-
16	CLA	A	1125	X	-	-	-
16	CLA	A	1126	X	-	-	-
16	CLA	A	1127	X	-	-	-
16	CLA	A	1128	X	-	-	-
16	CLA	A	1129	X	-	-	-
16	CLA	A	1130	X	-	-	-
16	CLA	A	1131	X	-	-	-
16	CLA	A	1132	X	-	-	-
16	CLA	A	1133	X	-	-	-
16	CLA	A	1134	X	-	-	-
16	CLA	A	1135	X	-	-	-
16	CLA	A	1136	X	-	-	-
16	CLA	A	1137	X	-	-	-
16	CLA	A	1138	X	-	-	-
16	CLA	A	1139	X	-	-	-
16	CLA	A	1140	X	-	-	-
16	CLA	A	1237	X	-	-	-
16	CLA	A	1402	X	-	-	-
16	CLA	A	1801	X	-	-	-
16	CLA	B	1012	X	-	-	-
16	CLA	B	1021	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	B	1023	X	-	-	-
16	CLA	B	1201	X	-	-	-
16	CLA	B	1202	X	-	-	-
16	CLA	B	1203	X	-	-	-
16	CLA	B	1204	X	-	-	-
16	CLA	B	1205	X	-	-	-
16	CLA	B	1206	X	-	-	-
16	CLA	B	1207	X	-	-	-
16	CLA	B	1208	X	-	-	-
16	CLA	B	1209	X	-	-	-
16	CLA	B	1210	X	-	-	-
16	CLA	B	1211	X	-	-	-
16	CLA	B	1212	X	-	-	-
16	CLA	B	1213	X	-	-	-
16	CLA	B	1214	X	-	-	-
16	CLA	B	1215	X	-	-	-
16	CLA	B	1216	X	-	-	-
16	CLA	B	1217	X	-	-	-
16	CLA	B	1218	X	-	-	-
16	CLA	B	1219	X	-	-	-
16	CLA	B	1220	X	-	-	-
16	CLA	B	1221	X	-	-	-
16	CLA	B	1222	X	-	-	-
16	CLA	B	1223	X	-	-	-
16	CLA	B	1224	X	-	-	-
16	CLA	B	1225	X	-	-	-
16	CLA	B	1226	X	-	-	-
16	CLA	B	1227	X	-	-	-
16	CLA	B	1228	X	-	-	-
16	CLA	B	1229	X	-	-	-
16	CLA	B	1230	X	-	-	-
16	CLA	B	1231	X	-	-	-
16	CLA	B	1232	X	-	-	-
16	CLA	B	1234	X	-	-	-
16	CLA	B	1235	X	-	-	-
16	CLA	B	1236	X	-	-	-
16	CLA	B	1238	X	-	-	-
16	CLA	B	1239	X	-	-	-
16	CLA	B	1240	X	-	-	-
16	CLA	F	1301	X	-	-	-
16	CLA	F	1302	X	-	-	-
16	CLA	G	1012	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	G	1021	X	-	-	-
16	CLA	G	1023	X	-	-	-
16	CLA	G	1201	X	-	-	-
16	CLA	G	1202	X	-	-	-
16	CLA	G	1203	X	-	-	-
16	CLA	G	1204	X	-	-	-
16	CLA	G	1205	X	-	-	-
16	CLA	G	1206	X	-	-	-
16	CLA	G	1207	X	-	-	-
16	CLA	G	1208	X	-	-	-
16	CLA	G	1209	X	-	-	-
16	CLA	G	1210	X	-	-	-
16	CLA	G	1211	X	-	-	-
16	CLA	G	1212	X	-	-	-
16	CLA	G	1213	X	-	-	-
16	CLA	G	1214	X	-	-	-
16	CLA	G	1215	X	-	-	-
16	CLA	G	1216	X	-	-	-
16	CLA	G	1217	X	-	-	-
16	CLA	G	1218	X	-	-	-
16	CLA	G	1219	X	-	-	-
16	CLA	G	1220	X	-	-	-
16	CLA	G	1221	X	-	-	-
16	CLA	G	1222	X	-	-	-
16	CLA	G	1223	X	-	-	-
16	CLA	G	1224	X	-	-	-
16	CLA	G	1225	X	-	-	-
16	CLA	G	1226	X	-	-	-
16	CLA	G	1227	X	-	-	-
16	CLA	G	1228	X	-	-	-
16	CLA	G	1229	X	-	-	-
16	CLA	G	1230	X	-	-	-
16	CLA	G	1231	X	-	-	-
16	CLA	G	1232	X	-	-	-
16	CLA	G	1234	X	-	-	-
16	CLA	G	1235	X	-	-	-
16	CLA	G	1236	X	-	-	-
16	CLA	G	1238	X	-	-	-
16	CLA	G	1239	X	-	-	-
16	CLA	G	1240	X	-	-	-
16	CLA	H	1013	X	-	-	-
16	CLA	H	1022	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	H	1101	X	-	-	-
16	CLA	H	1102	X	-	-	-
16	CLA	H	1103	X	-	-	-
16	CLA	H	1104	X	-	-	-
16	CLA	H	1105	X	-	-	-
16	CLA	H	1106	X	-	-	-
16	CLA	H	1107	X	-	-	-
16	CLA	H	1108	X	-	-	-
16	CLA	H	1109	X	-	-	-
16	CLA	H	1110	X	-	-	-
16	CLA	H	1111	X	-	-	-
16	CLA	H	1112	X	-	-	-
16	CLA	H	1113	X	-	-	-
16	CLA	H	1114	X	-	-	-
16	CLA	H	1115	X	-	-	-
16	CLA	H	1116	X	-	-	-
16	CLA	H	1117	X	-	-	-
16	CLA	H	1118	X	-	-	-
16	CLA	H	1119	X	-	-	-
16	CLA	H	1120	X	-	-	-
16	CLA	H	1121	X	-	-	-
16	CLA	H	1122	X	-	-	-
16	CLA	H	1123	X	-	-	-
16	CLA	H	1124	X	-	-	-
16	CLA	H	1125	X	-	-	-
16	CLA	H	1126	X	-	-	-
16	CLA	H	1127	X	-	-	-
16	CLA	H	1128	X	-	-	-
16	CLA	H	1129	X	-	-	-
16	CLA	H	1130	X	-	-	-
16	CLA	H	1131	X	-	-	-
16	CLA	H	1132	X	-	-	-
16	CLA	H	1133	X	-	-	-
16	CLA	H	1134	X	-	-	-
16	CLA	H	1135	X	-	-	-
16	CLA	H	1136	X	-	-	-
16	CLA	H	1137	X	-	-	-
16	CLA	H	1138	X	-	-	-
16	CLA	H	1139	X	-	-	-
16	CLA	H	1140	X	-	-	-
16	CLA	H	1237	X	-	-	-
16	CLA	H	1402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	H	1801	X	-	-	-
16	CLA	J	1302	X	-	-	-
16	CLA	J	1303	X	-	-	-
16	CLA	K	1401	X	-	-	-
16	CLA	L	1501	X	-	-	-
16	CLA	L	1502	X	-	-	-
16	CLA	L	1503	X	-	-	-
16	CLA	Q	1301	X	-	-	-
16	CLA	Q	1302	X	-	-	-
16	CLA	S	1302	X	-	-	-
16	CLA	S	1303	X	-	-	-
16	CLA	T	1401	X	-	-	-
16	CLA	U	1501	X	-	-	-
16	CLA	U	1502	X	-	-	-
16	CLA	U	1503	X	-	-	-
16	CLA	W	501	X	-	-	-
16	CLA	W	502	X	-	-	-
16	CLA	W	503	X	-	-	-
16	CLA	W	504	X	-	-	-
16	CLA	W	505	X	-	-	-
16	CLA	W	506	X	-	-	-
16	CLA	W	507	X	-	-	-
16	CLA	W	508	X	-	-	-
16	CLA	W	509	X	-	-	-
16	CLA	W	510	X	-	-	-
16	CLA	W	511	X	-	-	-
16	CLA	W	512	X	-	-	-
16	CLA	W	513	X	-	-	-
16	CLA	W	514	X	-	-	-
16	CLA	W	515	X	-	-	-
16	CLA	W	516	X	-	-	-
16	CLA	W	517	X	-	-	-
16	CLA	X	501	X	-	-	-
16	CLA	X	502	X	-	-	-
16	CLA	X	503	X	-	-	-
16	CLA	X	504	X	-	-	-
16	CLA	X	505	X	-	-	-
16	CLA	X	506	X	-	-	-
16	CLA	X	507	X	-	-	-
16	CLA	X	508	X	-	-	-
16	CLA	X	509	X	-	-	-
16	CLA	X	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	X	511	X	-	-	-
16	CLA	X	512	X	-	-	-
16	CLA	X	513	X	-	-	-
16	CLA	X	514	X	-	-	-
16	CLA	X	515	X	-	-	-
16	CLA	X	516	X	-	-	-
16	CLA	X	517	X	-	-	-
16	CLA	Y	501	X	-	-	-
16	CLA	Y	502	X	-	-	-
16	CLA	Y	503	X	-	-	-
16	CLA	Y	504	X	-	-	-
16	CLA	Y	505	X	-	-	-
16	CLA	Y	506	X	-	-	-
16	CLA	Y	507	X	-	-	-
16	CLA	Y	508	X	-	-	-
16	CLA	Y	509	X	-	-	-
16	CLA	Y	510	X	-	-	-
16	CLA	Y	511	X	-	-	-
16	CLA	Y	512	X	-	-	-
16	CLA	Y	513	X	-	-	-
16	CLA	Y	514	X	-	-	-
16	CLA	Y	515	X	-	-	-
16	CLA	Y	516	X	-	-	-
16	CLA	Y	517	X	-	-	-
16	CLA	Z	501	X	-	-	-
16	CLA	Z	502	X	-	-	-
16	CLA	Z	503	X	-	-	-
16	CLA	Z	504	X	-	-	-
16	CLA	Z	505	X	-	-	-
16	CLA	Z	506	X	-	-	-
16	CLA	Z	507	X	-	-	-
16	CLA	Z	508	X	-	-	-
16	CLA	Z	509	X	-	-	-
16	CLA	Z	510	X	-	-	-
16	CLA	Z	511	X	-	-	-
16	CLA	Z	512	X	-	-	-
16	CLA	Z	513	X	-	-	-
16	CLA	Z	514	X	-	-	-
16	CLA	Z	515	X	-	-	-
16	CLA	Z	516	X	-	-	-
16	CLA	Z	517	X	-	-	-
16	CLA	a	1013	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	a	1022	X	-	-	-
16	CLA	a	1101	X	-	-	-
16	CLA	a	1102	X	-	-	-
16	CLA	a	1103	X	-	-	-
16	CLA	a	1104	X	-	-	-
16	CLA	a	1105	X	-	-	-
16	CLA	a	1106	X	-	-	-
16	CLA	a	1107	X	-	-	-
16	CLA	a	1108	X	-	-	-
16	CLA	a	1109	X	-	-	-
16	CLA	a	1110	X	-	-	-
16	CLA	a	1111	X	-	-	-
16	CLA	a	1112	X	-	-	-
16	CLA	a	1113	X	-	-	-
16	CLA	a	1114	X	-	-	-
16	CLA	a	1115	X	-	-	-
16	CLA	a	1116	X	-	-	-
16	CLA	a	1117	X	-	-	-
16	CLA	a	1118	X	-	-	-
16	CLA	a	1119	X	-	-	-
16	CLA	a	1120	X	-	-	-
16	CLA	a	1121	X	-	-	-
16	CLA	a	1122	X	-	-	-
16	CLA	a	1123	X	-	-	-
16	CLA	a	1124	X	-	-	-
16	CLA	a	1125	X	-	-	-
16	CLA	a	1126	X	-	-	-
16	CLA	a	1127	X	-	-	-
16	CLA	a	1128	X	-	-	-
16	CLA	a	1129	X	-	-	-
16	CLA	a	1130	X	-	-	-
16	CLA	a	1131	X	-	-	-
16	CLA	a	1132	X	-	-	-
16	CLA	a	1133	X	-	-	-
16	CLA	a	1134	X	-	-	-
16	CLA	a	1135	X	-	-	-
16	CLA	a	1136	X	-	-	-
16	CLA	a	1137	X	-	-	-
16	CLA	a	1138	X	-	-	-
16	CLA	a	1139	X	-	-	-
16	CLA	a	1140	X	-	-	-
16	CLA	a	1237	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	a	1402	X	-	-	-
16	CLA	a	1801	X	-	-	-
16	CLA	b	1012	X	-	-	-
16	CLA	b	1021	X	-	-	-
16	CLA	b	1023	X	-	-	-
16	CLA	b	1201	X	-	-	-
16	CLA	b	1202	X	-	-	-
16	CLA	b	1203	X	-	-	-
16	CLA	b	1204	X	-	-	-
16	CLA	b	1205	X	-	-	-
16	CLA	b	1206	X	-	-	-
16	CLA	b	1207	X	-	-	-
16	CLA	b	1208	X	-	-	-
16	CLA	b	1209	X	-	-	-
16	CLA	b	1210	X	-	-	-
16	CLA	b	1211	X	-	-	-
16	CLA	b	1212	X	-	-	-
16	CLA	b	1213	X	-	-	-
16	CLA	b	1214	X	-	-	-
16	CLA	b	1215	X	-	-	-
16	CLA	b	1216	X	-	-	-
16	CLA	b	1217	X	-	-	-
16	CLA	b	1218	X	-	-	-
16	CLA	b	1219	X	-	-	-
16	CLA	b	1220	X	-	-	-
16	CLA	b	1221	X	-	-	-
16	CLA	b	1222	X	-	-	-
16	CLA	b	1223	X	-	-	-
16	CLA	b	1224	X	-	-	-
16	CLA	b	1225	X	-	-	-
16	CLA	b	1226	X	-	-	-
16	CLA	b	1227	X	-	-	-
16	CLA	b	1228	X	-	-	-
16	CLA	b	1229	X	-	-	-
16	CLA	b	1230	X	-	-	-
16	CLA	b	1231	X	-	-	-
16	CLA	b	1232	X	-	-	-
16	CLA	b	1234	X	-	-	-
16	CLA	b	1235	X	-	-	-
16	CLA	b	1236	X	-	-	-
16	CLA	b	1238	X	-	-	-
16	CLA	b	1239	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	b	1240	X	-	-	-
16	CLA	f	1301	X	-	-	-
16	CLA	f	1302	X	-	-	-
16	CLA	g	501	X	-	-	-
16	CLA	g	502	X	-	-	-
16	CLA	g	503	X	-	-	-
16	CLA	g	504	X	-	-	-
16	CLA	g	505	X	-	-	-
16	CLA	g	506	X	-	-	-
16	CLA	g	507	X	-	-	-
16	CLA	g	508	X	-	-	-
16	CLA	g	509	X	-	-	-
16	CLA	g	510	X	-	-	-
16	CLA	g	511	X	-	-	-
16	CLA	g	512	X	-	-	-
16	CLA	g	513	X	-	-	-
16	CLA	g	514	X	-	-	-
16	CLA	g	515	X	-	-	-
16	CLA	g	516	X	-	-	-
16	CLA	g	517	X	-	-	-
16	CLA	h	501	X	-	-	-
16	CLA	h	502	X	-	-	-
16	CLA	h	503	X	-	-	-
16	CLA	h	504	X	-	-	-
16	CLA	h	505	X	-	-	-
16	CLA	h	506	X	-	-	-
16	CLA	h	507	X	-	-	-
16	CLA	h	508	X	-	-	-
16	CLA	h	509	X	-	-	-
16	CLA	h	510	X	-	-	-
16	CLA	h	511	X	-	-	-
16	CLA	h	512	X	-	-	-
16	CLA	h	513	X	-	-	-
16	CLA	h	514	X	-	-	-
16	CLA	h	515	X	-	-	-
16	CLA	h	516	X	-	-	-
16	CLA	h	517	X	-	-	-
16	CLA	j	1302	X	-	-	-
16	CLA	j	1303	X	-	-	-
16	CLA	k	1401	X	-	-	-
16	CLA	l	1501	X	-	-	-
16	CLA	l	1502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	l	1503	X	-	-	-
16	CLA	n	501	X	-	-	-
16	CLA	n	502	X	-	-	-
16	CLA	n	503	X	-	-	-
16	CLA	n	504	X	-	-	-
16	CLA	n	505	X	-	-	-
16	CLA	n	506	X	-	-	-
16	CLA	n	507	X	-	-	-
16	CLA	n	508	X	-	-	-
16	CLA	n	509	X	-	-	-
16	CLA	n	510	X	-	-	-
16	CLA	n	511	X	-	-	-
16	CLA	n	512	X	-	-	-
16	CLA	n	513	X	-	-	-
16	CLA	n	514	X	-	-	-
16	CLA	n	515	X	-	-	-
16	CLA	n	516	X	-	-	-
16	CLA	n	517	X	-	-	-
16	CLA	o	501	X	-	-	-
16	CLA	o	502	X	-	-	-
16	CLA	o	503	X	-	-	-
16	CLA	o	504	X	-	-	-
16	CLA	o	505	X	-	-	-
16	CLA	o	506	X	-	-	-
16	CLA	o	507	X	-	-	-
16	CLA	o	508	X	-	-	-
16	CLA	o	509	X	-	-	-
16	CLA	o	510	X	-	-	-
16	CLA	o	511	X	-	-	-
16	CLA	o	512	X	-	-	-
16	CLA	o	513	X	-	-	-
16	CLA	o	514	X	-	-	-
16	CLA	o	515	X	-	-	-
16	CLA	o	516	X	-	-	-
16	CLA	o	517	X	-	-	-
16	CLA	p	501	X	-	-	-
16	CLA	p	502	X	-	-	-
16	CLA	p	503	X	-	-	-
16	CLA	p	504	X	-	-	-
16	CLA	p	505	X	-	-	-
16	CLA	p	506	X	-	-	-
16	CLA	p	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	p	508	X	-	-	-
16	CLA	p	509	X	-	-	-
16	CLA	p	510	X	-	-	-
16	CLA	p	511	X	-	-	-
16	CLA	p	512	X	-	-	-
16	CLA	p	513	X	-	-	-
16	CLA	p	514	X	-	-	-
16	CLA	p	515	X	-	-	-
16	CLA	p	516	X	-	-	-
16	CLA	p	517	X	-	-	-
16	CLA	q	501	X	-	-	-
16	CLA	q	502	X	-	-	-
16	CLA	q	503	X	-	-	-
16	CLA	q	504	X	-	-	-
16	CLA	q	505	X	-	-	-
16	CLA	q	506	X	-	-	-
16	CLA	q	507	X	-	-	-
16	CLA	q	508	X	-	-	-
16	CLA	q	509	X	-	-	-
16	CLA	q	510	X	-	-	-
16	CLA	q	511	X	-	-	-
16	CLA	q	512	X	-	-	-
16	CLA	q	513	X	-	-	-
16	CLA	q	514	X	-	-	-
16	CLA	q	515	X	-	-	-
16	CLA	q	516	X	-	-	-
16	CLA	q	517	X	-	-	-
16	CLA	r	501	X	-	-	-
16	CLA	r	502	X	-	-	-
16	CLA	r	503	X	-	-	-
16	CLA	r	504	X	-	-	-
16	CLA	r	505	X	-	-	-
16	CLA	r	506	X	-	-	-
16	CLA	r	507	X	-	-	-
16	CLA	r	508	X	-	-	-
16	CLA	r	509	X	-	-	-
16	CLA	r	510	X	-	-	-
16	CLA	r	511	X	-	-	-
16	CLA	r	512	X	-	-	-
16	CLA	r	513	X	-	-	-
16	CLA	r	514	X	-	-	-
16	CLA	r	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	r	516	X	-	-	-
16	CLA	r	517	X	-	-	-
16	CLA	s	501	X	-	-	-
16	CLA	s	502	X	-	-	-
16	CLA	s	503	X	-	-	-
16	CLA	s	504	X	-	-	-
16	CLA	s	505	X	-	-	-
16	CLA	s	506	X	-	-	-
16	CLA	s	507	X	-	-	-
16	CLA	s	508	X	-	-	-
16	CLA	s	509	X	-	-	-
16	CLA	s	510	X	-	-	-
16	CLA	s	511	X	-	-	-
16	CLA	s	512	X	-	-	-
16	CLA	s	513	X	-	-	-
16	CLA	s	514	X	-	-	-
16	CLA	s	515	X	-	-	-
16	CLA	s	516	X	-	-	-
16	CLA	s	517	X	-	-	-
16	CLA	t	501	X	-	-	-
16	CLA	t	502	X	-	-	-
16	CLA	t	503	X	-	-	-
16	CLA	t	504	X	-	-	-
16	CLA	t	505	X	-	-	-
16	CLA	t	506	X	-	-	-
16	CLA	t	507	X	-	-	-
16	CLA	t	508	X	-	-	-
16	CLA	t	509	X	-	-	-
16	CLA	t	510	X	-	-	-
16	CLA	t	511	X	-	-	-
16	CLA	t	512	X	-	-	-
16	CLA	t	513	X	-	-	-
16	CLA	t	514	X	-	-	-
16	CLA	t	515	X	-	-	-
16	CLA	t	516	X	-	-	-
16	CLA	t	517	X	-	-	-
16	CLA	u	501	X	-	-	-
16	CLA	u	502	X	-	-	-
16	CLA	u	503	X	-	-	-
16	CLA	u	504	X	-	-	-
16	CLA	u	505	X	-	-	-
16	CLA	u	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	u	507	X	-	-	-
16	CLA	u	508	X	-	-	-
16	CLA	u	509	X	-	-	-
16	CLA	u	510	X	-	-	-
16	CLA	u	511	X	-	-	-
16	CLA	u	512	X	-	-	-
16	CLA	u	513	X	-	-	-
16	CLA	u	514	X	-	-	-
16	CLA	u	515	X	-	-	-
16	CLA	u	516	X	-	-	-
16	CLA	u	517	X	-	-	-
16	CLA	v	501	X	-	-	-
16	CLA	v	502	X	-	-	-
16	CLA	v	503	X	-	-	-
16	CLA	v	504	X	-	-	-
16	CLA	v	505	X	-	-	-
16	CLA	v	506	X	-	-	-
16	CLA	v	507	X	-	-	-
16	CLA	v	508	X	-	-	-
16	CLA	v	509	X	-	-	-
16	CLA	v	510	X	-	-	-
16	CLA	v	511	X	-	-	-
16	CLA	v	512	X	-	-	-
16	CLA	v	513	X	-	-	-
16	CLA	v	514	X	-	-	-
16	CLA	v	515	X	-	-	-
16	CLA	v	516	X	-	-	-
16	CLA	v	517	X	-	-	-
16	CLA	w	501	X	-	-	-
16	CLA	w	502	X	-	-	-
16	CLA	w	503	X	-	-	-
16	CLA	w	504	X	-	-	-
16	CLA	w	505	X	-	-	-
16	CLA	w	506	X	-	-	-
16	CLA	w	507	X	-	-	-
16	CLA	w	508	X	-	-	-
16	CLA	w	509	X	-	-	-
16	CLA	w	510	X	-	-	-
16	CLA	w	511	X	-	-	-
16	CLA	w	512	X	-	-	-
16	CLA	w	513	X	-	-	-
16	CLA	w	514	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	w	515	X	-	-	-
16	CLA	w	516	X	-	-	-
16	CLA	w	517	X	-	-	-
16	CLA	x	501	X	-	-	-
16	CLA	x	502	X	-	-	-
16	CLA	x	503	X	-	-	-
16	CLA	x	504	X	-	-	-
16	CLA	x	505	X	-	-	-
16	CLA	x	506	X	-	-	-
16	CLA	x	507	X	-	-	-
16	CLA	x	508	X	-	-	-
16	CLA	x	509	X	-	-	-
16	CLA	x	510	X	-	-	-
16	CLA	x	511	X	-	-	-
16	CLA	x	512	X	-	-	-
16	CLA	x	513	X	-	-	-
16	CLA	x	514	X	-	-	-
16	CLA	x	515	X	-	-	-
16	CLA	x	516	X	-	-	-
16	CLA	x	517	X	-	-	-
16	CLA	y	501	X	-	-	-
16	CLA	y	502	X	-	-	-
16	CLA	y	503	X	-	-	-
16	CLA	y	504	X	-	-	-
16	CLA	y	505	X	-	-	-
16	CLA	y	506	X	-	-	-
16	CLA	y	507	X	-	-	-
16	CLA	y	508	X	-	-	-
16	CLA	y	509	X	-	-	-
16	CLA	y	510	X	-	-	-
16	CLA	y	511	X	-	-	-
16	CLA	y	512	X	-	-	-
16	CLA	y	513	X	-	-	-
16	CLA	y	514	X	-	-	-
16	CLA	y	515	X	-	-	-
16	CLA	y	516	X	-	-	-
16	CLA	y	517	X	-	-	-



## 2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 137509 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	739	Total	C	N	O	S	0	0
			5786	3790	984	985	27		
1	a	739	Total	C	N	O	S	0	0
			5786	3790	984	985	27		
1	H	739	Total	C	N	O	S	0	0
			5786	3790	984	985	27		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	604	VAL	ILE	conflict	UNP P29254
a	604	VAL	ILE	conflict	UNP P29254
H	604	VAL	ILE	conflict	UNP P29254

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	729	Total	C	N	O	S	0	0
			5766	3796	967	988	15		
2	b	729	Total	C	N	O	S	0	0
			5766	3796	967	988	15		
2	G	729	Total	C	N	O	S	0	0
			5766	3796	967	988	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	c	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	N	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	141	Total	C	N	O	S	0	0
			1098	694	189	211	4		
4	d	141	Total	C	N	O	S	0	0
			1098	694	189	211	4		
4	O	141	Total	C	N	O	S	0	0
			1098	694	189	211	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	69	Total	C	N	O	0	0
			542	340	96	106		
5	e	69	Total	C	N	O	0	0
			542	340	96	106		
5	P	69	Total	C	N	O	0	0
			542	340	96	106		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	139	Total	C	N	O	S	0	0
			1069	689	179	197	4		
6	f	139	Total	C	N	O	S	0	0
			1069	689	179	197	4		
6	Q	139	Total	C	N	O	S	0	0
			1069	689	179	197	4		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	37	Total	C	N	O	S	0	0
			293	200	41	49	3		
7	i	37	Total	C	N	O	S	0	0
			293	200	41	49	3		
7	R	37	Total	C	N	O	S	0	0
			293	200	41	49	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O	S	0	0
			308	208	46	52	2		
8	j	39	Total	C	N	O	S	0	0
			308	208	46	52	2		
8	S	39	Total	C	N	O	S	0	0
			308	208	46	52	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	154	Total	C	N	O	S	0	0
			1156	753	188	213	2		
9	l	154	Total	C	N	O	S	0	0
			1156	753	188	213	2		
9	U	154	Total	C	N	O	S	0	0
			1156	753	188	213	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
10	m	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
10	V	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 11 is a protein called Iron stress-induced chlorophyll-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	329	Total	C	N	O	S	0	0
			2478	1656	401	417	4		
11	X	339	Total	C	N	O	S	0	0
			2605	1732	424	444	5		
11	Y	340	Total	C	N	O	S	0	0
			2608	1735	424	444	5		
11	Z	337	Total	C	N	O	S	0	0
			2582	1717	421	439	5		
11	g	332	Total	C	N	O	S	0	0
			2531	1686	411	430	4		
11	y	317	Total	C	N	O	S	0	0
			2416	1613	395	404	4		

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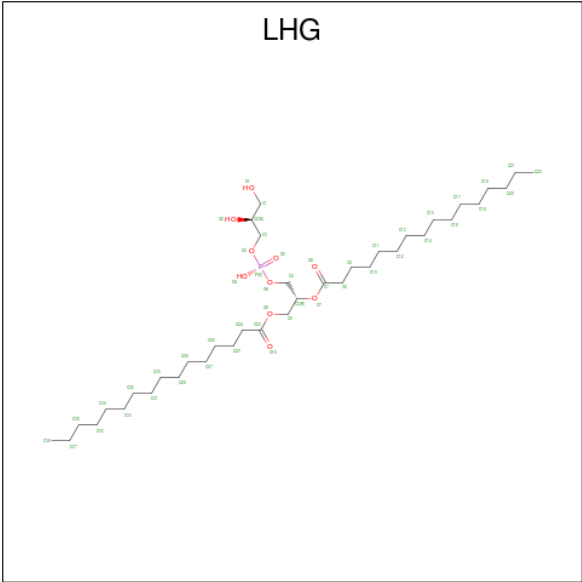
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Mol	Chain	Residues	Atoms					AltConf	Trace
11	n	329	Total	C	N	O	S	0	0
			2475	1655	401	415	4		
11	o	339	Total	C	N	O	S	0	0
			2605	1732	424	444	5		
11	p	340	Total	C	N	O	S	0	0
			2609	1735	424	445	5		
11	q	337	Total	C	N	O	S	0	0
			2582	1717	421	439	5		
11	r	332	Total	C	N	O	S	0	0
			2531	1686	411	430	4		
11	h	317	Total	C	N	O	S	0	0
			2416	1613	395	404	4		
11	t	329	Total	C	N	O	S	0	0
			2478	1656	401	417	4		
11	u	339	Total	C	N	O	S	0	0
			2605	1732	424	444	5		
11	s	340	Total	C	N	O	S	0	0
			2609	1735	424	445	5		
11	w	337	Total	C	N	O	S	0	0
			2582	1717	421	439	5		
11	x	332	Total	C	N	O	S	0	0
			2531	1686	411	430	4		
11	v	317	Total	C	N	O	S	0	0
			2416	1613	395	404	4		

- Molecule 12 is a protein called Photosystem I reaction center subunit PsaK 1.

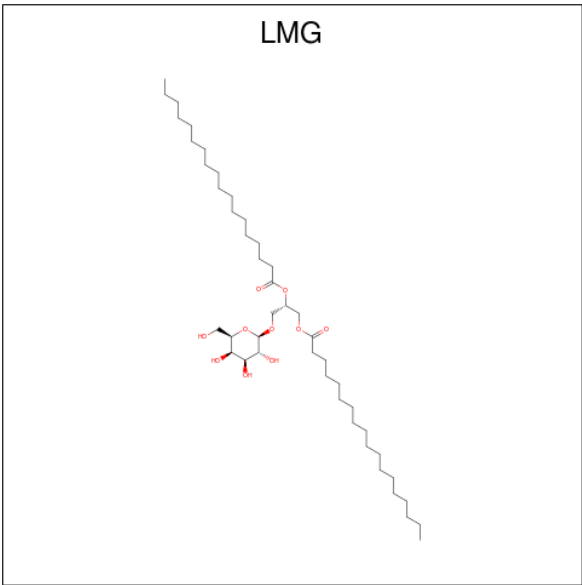
Mol	Chain	Residues	Atoms					AltConf	Trace
12	k	70	Total	C	N	O	S	0	0
			485	317	80	84	4		
12	K	70	Total	C	N	O	S	0	0
			485	317	80	84	4		
12	T	70	Total	C	N	O	S	0	0
			485	317	80	84	4		

- Molecule 13 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			70	48	20	2	
13	A	1	Total	C	O	P	0
			70	48	20	2	
13	I	1	Total	C	O	P	0
			44	33	10	1	
13	a	1	Total	C	O	P	0
			70	48	20	2	
13	a	1	Total	C	O	P	0
			70	48	20	2	
13	i	1	Total	C	O	P	0
			44	33	10	1	
13	H	1	Total	C	O	P	0
			70	48	20	2	
13	H	1	Total	C	O	P	0
			70	48	20	2	
13	R	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 14 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



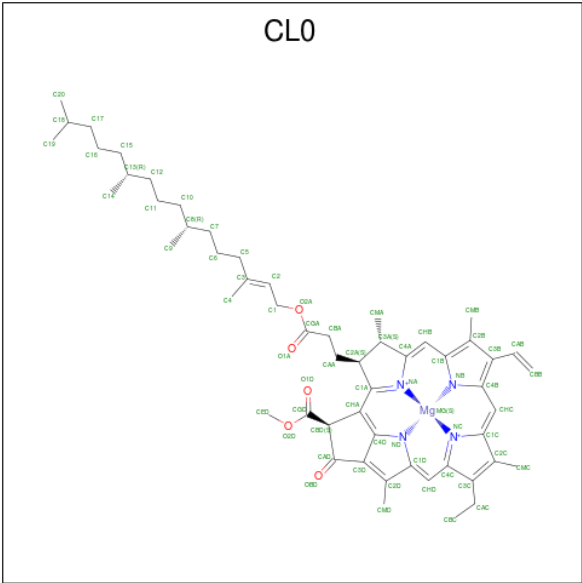
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			116	86	30	
14	A	1	Total	C	O	0
			116	86	30	
14	A	1	Total	C	O	0
			116	86	30	
14	B	1	Total	C	O	0
			43	33	10	
14	Y	1	Total	C	O	0
			39	29	10	
14	a	1	Total	C	O	0
			115	85	30	
14	a	1	Total	C	O	0
			115	85	30	
14	a	1	Total	C	O	0
			115	85	30	
14	b	1	Total	C	O	0
			43	33	10	
14	p	1	Total	C	O	0
			39	29	10	
14	H	1	Total	C	O	0
			116	86	30	
14	H	1	Total	C	O	0
			116	86	30	
14	H	1	Total	C	O	0
			116	86	30	
14	G	1	Total	C	O	0
			43	33	10	

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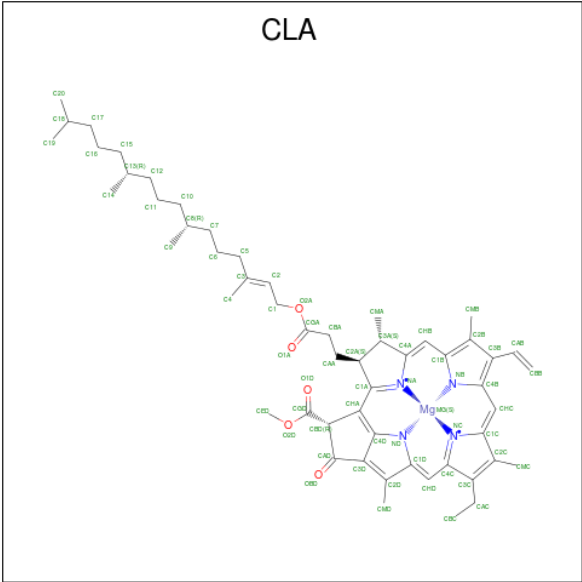
Mol	Chain	Residues	Atoms			AltConf
14	s	1	Total	C	O	0
			39	29	10	

- Molecule 15 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

- Molecule 16 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	A	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	B	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	
16	B	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	
16	B	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	
16	B	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	
16	B	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	
16	B	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	
16	B	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	
16	B	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	
16	B	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	
16	B	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	B	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	F	1	Total 72	C 57	Mg 2	N 8	O 5	0
16	F	1	Total 72	C 57	Mg 2	N 8	O 5	0
16	J	1	Total 82	C 66	Mg 2	N 8	O 6	0
16	J	1	Total 82	C 66	Mg 2	N 8	O 6	0
16	L	1	Total 195	C 165	Mg 3	N 12	O 15	0
16	L	1	Total 195	C 165	Mg 3	N 12	O 15	0
16	L	1	Total 195	C 165	Mg 3	N 12	O 15	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0

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Mol	Chain	Residues	Atoms					AltConf
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	W	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0

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Mol	Chain	Residues	Atoms					AltConf
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	X	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	Y	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	Y	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	Y	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	Y	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	Y	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	Y	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	Y	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	Y	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	Y	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	Y	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	Y	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	Y	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	Y	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	Y	1	Total 952	C 782	Mg 17	N 68	O 85	0

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Mol	Chain	Residues	Atoms					AltConf
16	Y	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	Y	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	Y	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	Y	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	Z	1	Total	C	Mg	N	O	0
			943	773	17	68	85	

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Mol	Chain	Residues	Atoms					AltConf
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	g	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0

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Mol	Chain	Residues	Atoms					AltConf
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	y	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	a	1	Total 2600	C 2152	Mg 45	N 180	O 223	0
16	a	1	Total 2600	C 2152	Mg 45	N 180	O 223	0
16	a	1	Total 2600	C 2152	Mg 45	N 180	O 223	0
16	a	1	Total 2600	C 2152	Mg 45	N 180	O 223	0
16	a	1	Total 2600	C 2152	Mg 45	N 180	O 223	0
16	a	1	Total 2600	C 2152	Mg 45	N 180	O 223	0
16	a	1	Total 2600	C 2152	Mg 45	N 180	O 223	0
16	a	1	Total 2600	C 2152	Mg 45	N 180	O 223	0

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Mol	Chain	Residues	Atoms					AltConf
16	a	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	a	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	a	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	a	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	a	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	a	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	a	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	a	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	a	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	a	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	a	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	a	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	a	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	b	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	
16	b	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	
16	b	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	
16	b	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	
16	b	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	

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Mol	Chain	Residues	Atoms					AltConf
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms					AltConf
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	b	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	l	1	Total 195	C 165	Mg 3	N 12	O 15	0
16	l	1	Total 195	C 165	Mg 3	N 12	O 15	0
16	l	1	Total 195	C 165	Mg 3	N 12	O 15	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0

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Mol	Chain	Residues	Atoms					AltConf
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	n	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0

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Mol	Chain	Residues	Atoms					AltConf
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	o	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	p	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	p	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	p	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	p	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	p	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	p	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	p	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	p	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	p	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	p	1	Total 952	C 782	Mg 17	N 68	O 85	0

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Mol	Chain	Residues	Atoms					AltConf
16	p	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	p	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	p	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	p	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	p	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	p	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	

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Mol	Chain	Residues	Atoms					AltConf
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	q	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	r	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	r	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	r	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	r	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	r	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	r	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	r	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	r	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	r	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	r	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	r	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	r	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	r	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	h	1	Total	C	Mg	N	O	0
			933	763	17	68	85	

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Mol	Chain	Residues	Atoms					AltConf
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	h	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	H	1	Total 2600	C 2152	Mg 45	N 180	O 223	0
16	H	1	Total 2600	C 2152	Mg 45	N 180	O 223	0
16	H	1	Total 2600	C 2152	Mg 45	N 180	O 223	0
16	H	1	Total 2600	C 2152	Mg 45	N 180	O 223	0
16	H	1	Total 2600	C 2152	Mg 45	N 180	O 223	0

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Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	H	1	Total	C	Mg	N	O	0
			2600	2152	45	180	223	
16	G	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	
16	G	1	Total	C	Mg	N	O	0
			2344	1934	41	164	205	

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Mol	Chain	Residues	Atoms					AltConf
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms					AltConf
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	G	1	Total 2344	C 1934	Mg 41	N 164	O 205	0
16	U	1	Total 195	C 165	Mg 3	N 12	O 15	0
16	U	1	Total 195	C 165	Mg 3	N 12	O 15	0
16	U	1	Total 195	C 165	Mg 3	N 12	O 15	0



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Mol	Chain	Residues	Atoms					AltConf
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	t	1	Total 947	C 777	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0

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Mol	Chain	Residues	Atoms					AltConf
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	u	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	s	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	s	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	s	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	s	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	s	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	s	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	s	1	Total 952	C 782	Mg 17	N 68	O 85	0
16	s	1	Total 952	C 782	Mg 17	N 68	O 85	0

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Mol	Chain	Residues	Atoms					AltConf
16	s	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	s	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	s	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	s	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	s	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	s	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	s	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	s	1	Total	C	Mg	N	O	0
			952	782	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	

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Mol	Chain	Residues	Atoms					AltConf
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	w	1	Total	C	Mg	N	O	0
			943	773	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	
16	x	1	Total	C	Mg	N	O	0
			923	753	17	68	85	

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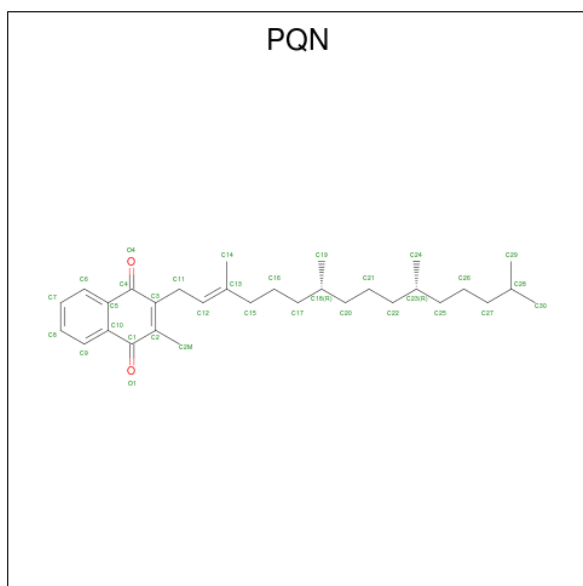
Mol	Chain	Residues	Atoms					AltConf
16	x	1	Total 923	C 753	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	v	1	Total 933	C 763	Mg 17	N 68	O 85	0
16	f	1	Total 72	C 57	Mg 2	N 8	O 5	0
16	f	1	Total 72	C 57	Mg 2	N 8	O 5	0
16	Q	1	Total 72	C 57	Mg 2	N 8	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	Q	1	Total	C	Mg	N	O	0
			72	57	2	8	5	
16	j	1	Total	C	Mg	N	O	0
			82	66	2	8	6	
16	j	1	Total	C	Mg	N	O	0
			82	66	2	8	6	
16	S	1	Total	C	Mg	N	O	0
			82	66	2	8	6	
16	S	1	Total	C	Mg	N	O	0
			82	66	2	8	6	
16	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 17 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ).



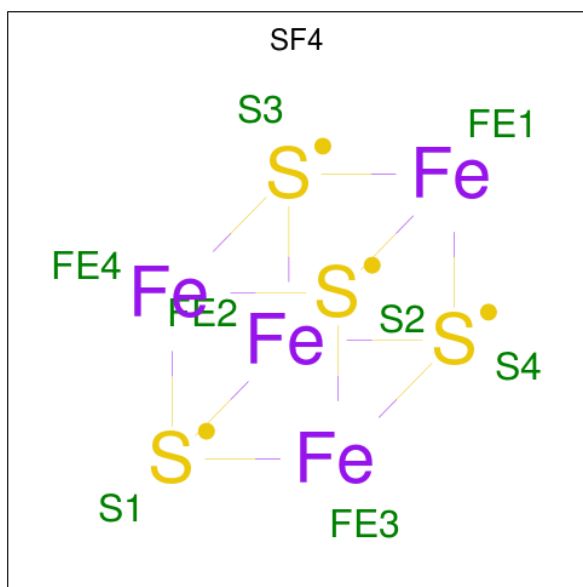
Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	C	O	0
			33	31	2	
17	B	1	Total	C	O	0
			33	31	2	
17	a	1	Total	C	O	0
			33	31	2	
17	b	1	Total	C	O	0
			33	31	2	

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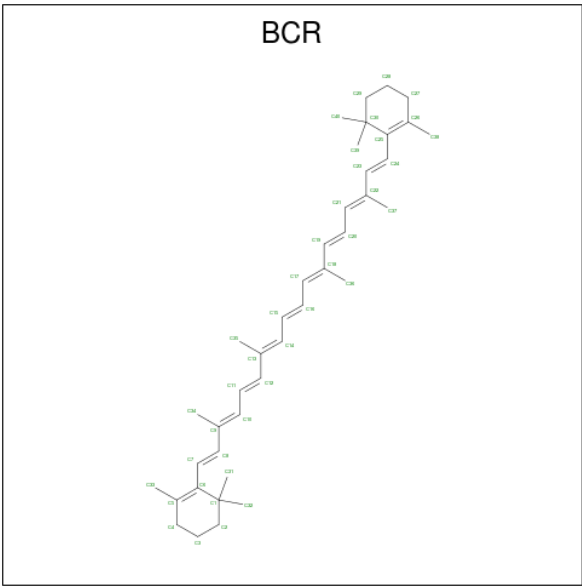
Mol	Chain	Residues	Atoms			AltConf
17	H	1	Total	C	O	0
			33	31	2	
17	G	1	Total	C	O	0
			33	31	2	

- Molecule 18 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			16	8	8	
18	C	1	Total	Fe	S	0
			16	8	8	
18	a	1	Total	Fe	S	0
			8	4	4	
18	H	1	Total	Fe	S	0
			8	4	4	
18	c	1	Total	Fe	S	0
			16	8	8	
18	c	1	Total	Fe	S	0
			16	8	8	
18	N	1	Total	Fe	S	0
			16	8	8	
18	N	1	Total	Fe	S	0
			16	8	8	

- Molecule 19 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	C	0
			240	240	
19	A	1	Total	C	0
			240	240	
19	A	1	Total	C	0
			240	240	
19	A	1	Total	C	0
			240	240	
19	A	1	Total	C	0
			240	240	
19	A	1	Total	C	0
			240	240	
19	B	1	Total	C	0
			265	265	
19	B	1	Total	C	0
			265	265	
19	B	1	Total	C	0
			265	265	
19	B	1	Total	C	0
			265	265	
19	B	1	Total	C	0
			265	265	
19	B	1	Total	C	0
			265	265	

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Mol	Chain	Residues	Atoms		AltConf
19	F	1	Total 40	C 40	0
19	I	1	Total 80	C 80	0
19	I	1	Total 80	C 80	0
19	J	1	Total 120	C 120	0
19	J	1	Total 120	C 120	0
19	J	1	Total 120	C 120	0
19	L	1	Total 80	C 80	0
19	L	1	Total 80	C 80	0
19	M	1	Total 40	C 40	0
19	W	1	Total 80	C 80	0
19	W	1	Total 80	C 80	0
19	X	1	Total 160	C 160	0
19	X	1	Total 160	C 160	0
19	X	1	Total 160	C 160	0
19	X	1	Total 160	C 160	0
19	Y	1	Total 160	C 160	0
19	Y	1	Total 160	C 160	0
19	Y	1	Total 160	C 160	0
19	Y	1	Total 160	C 160	0
19	Z	1	Total 160	C 160	0
19	Z	1	Total 160	C 160	0

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Mol	Chain	Residues	Atoms		AltConf
19	Z	1	Total 160	C 160	0
19	Z	1	Total 160	C 160	0
19	g	1	Total 160	C 160	0
19	g	1	Total 160	C 160	0
19	g	1	Total 160	C 160	0
19	g	1	Total 160	C 160	0
19	y	1	Total 160	C 160	0
19	y	1	Total 160	C 160	0
19	y	1	Total 160	C 160	0
19	y	1	Total 160	C 160	0
19	a	1	Total 240	C 240	0
19	a	1	Total 240	C 240	0
19	a	1	Total 240	C 240	0
19	a	1	Total 240	C 240	0
19	a	1	Total 240	C 240	0
19	a	1	Total 240	C 240	0
19	b	1	Total 265	C 265	0
19	b	1	Total 265	C 265	0
19	b	1	Total 265	C 265	0
19	b	1	Total 265	C 265	0
19	b	1	Total 265	C 265	0

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Mol	Chain	Residues	Atoms	AltConf
19	b	1	Total C 265 265	0
19	b	1	Total C 265 265	0
19	i	1	Total C 80 80	0
19	i	1	Total C 80 80	0
19	k	1	Total C 40 40	0
19	l	1	Total C 80 80	0
19	l	1	Total C 80 80	0
19	m	1	Total C 40 40	0
19	n	1	Total C 80 80	0
19	n	1	Total C 80 80	0
19	o	1	Total C 160 160	0
19	o	1	Total C 160 160	0
19	o	1	Total C 160 160	0
19	o	1	Total C 160 160	0
19	p	1	Total C 160 160	0
19	p	1	Total C 160 160	0
19	p	1	Total C 160 160	0
19	p	1	Total C 160 160	0
19	q	1	Total C 160 160	0
19	q	1	Total C 160 160	0
19	q	1	Total C 160 160	0

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Mol	Chain	Residues	Atoms	AltConf
19	q	1	Total C 160 160	0
19	r	1	Total C 160 160	0
19	r	1	Total C 160 160	0
19	r	1	Total C 160 160	0
19	r	1	Total C 160 160	0
19	h	1	Total C 160 160	0
19	h	1	Total C 160 160	0
19	h	1	Total C 160 160	0
19	h	1	Total C 160 160	0
19	H	1	Total C 240 240	0
19	H	1	Total C 240 240	0
19	H	1	Total C 240 240	0
19	H	1	Total C 240 240	0
19	H	1	Total C 240 240	0
19	H	1	Total C 240 240	0
19	H	1	Total C 240 240	0
19	G	1	Total C 265 265	0
19	G	1	Total C 265 265	0
19	G	1	Total C 265 265	0
19	G	1	Total C 265 265	0
19	G	1	Total C 265 265	0
19	G	1	Total C 265 265	0

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Mol	Chain	Residues	Atoms	AltConf
19	G	1	Total C 265 265	0
19	R	1	Total C 80 80	0
19	R	1	Total C 80 80	0
19	U	1	Total C 80 80	0
19	U	1	Total C 80 80	0
19	V	1	Total C 40 40	0
19	t	1	Total C 80 80	0
19	t	1	Total C 80 80	0
19	u	1	Total C 160 160	0
19	u	1	Total C 160 160	0
19	u	1	Total C 160 160	0
19	u	1	Total C 160 160	0
19	s	1	Total C 160 160	0
19	s	1	Total C 160 160	0
19	s	1	Total C 160 160	0
19	s	1	Total C 160 160	0
19	w	1	Total C 160 160	0
19	w	1	Total C 160 160	0
19	w	1	Total C 160 160	0
19	w	1	Total C 160 160	0
19	x	1	Total C 160 160	0

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Mol	Chain	Residues	Atoms		AltConf
19	x	1	Total 160	C 160	0
19	x	1	Total 160	C 160	0
19	x	1	Total 160	C 160	0
19	v	1	Total 160	C 160	0
19	v	1	Total 160	C 160	0
19	v	1	Total 160	C 160	0
19	v	1	Total 160	C 160	0
19	f	1	Total 40	C 40	0
19	Q	1	Total 40	C 40	0
19	j	1	Total 120	C 120	0
19	j	1	Total 120	C 120	0
19	j	1	Total 120	C 120	0
19	S	1	Total 120	C 120	0
19	S	1	Total 120	C 120	0
19	S	1	Total 120	C 120	0
19	K	1	Total 40	C 40	0
19	T	1	Total 40	C 40	0

- Molecule 20 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			AltConf
20	L	1	Total 35	C 24	O 11	0
20	l	1	Total 35	C 24	O 11	0
20	U	1	Total 35	C 24	O 11	0

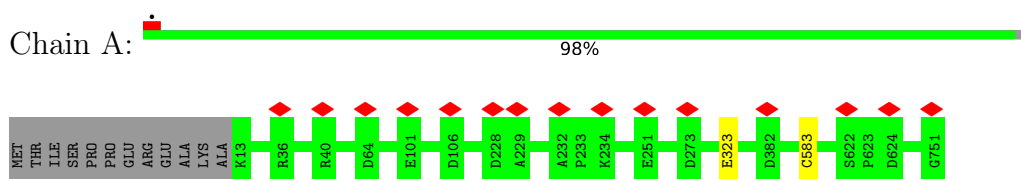
- Molecule 21 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
21	L	1	Total Ca 1 1	0
21	l	1	Total Ca 1 1	0
21	U	1	Total Ca 1 1	0

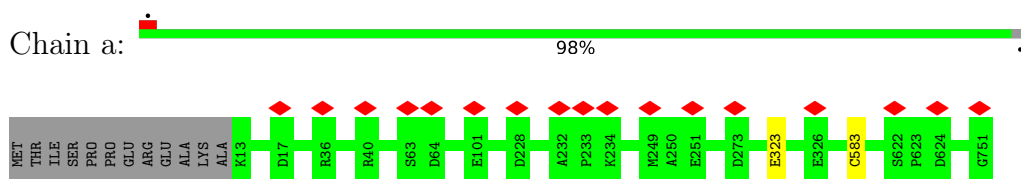
### 3 Residue-property plots [i](#)

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.

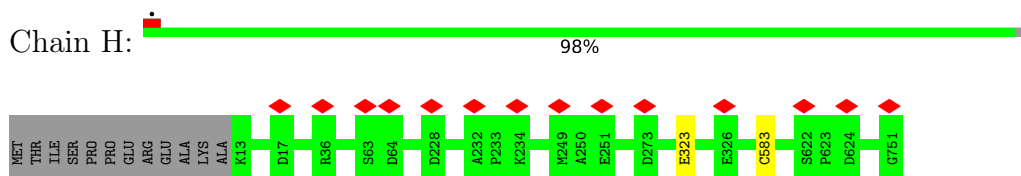
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



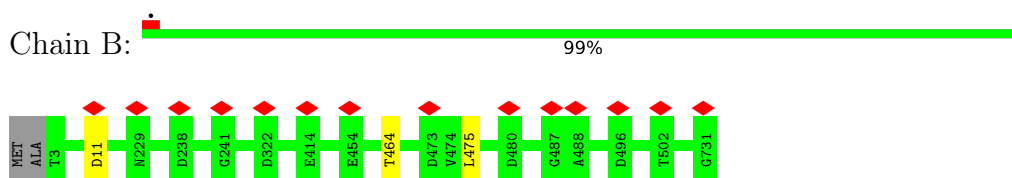
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



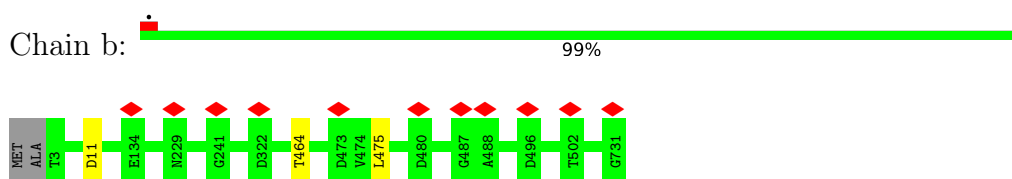
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

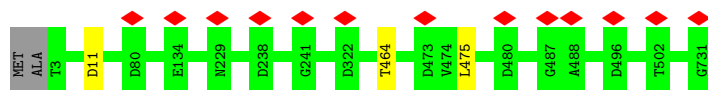


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



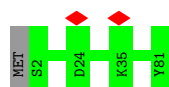
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain G:  99%



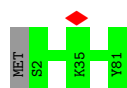
- Molecule 3: Photosystem I iron-sulfur center

Chain C:  99%



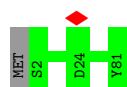
- Molecule 3: Photosystem I iron-sulfur center

Chain c:  99%



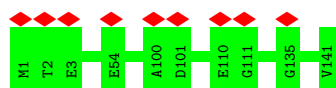
- Molecule 3: Photosystem I iron-sulfur center

Chain N:  99%



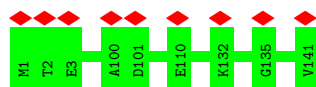
- Molecule 4: Photosystem I reaction center subunit II

Chain D:  6% 100%



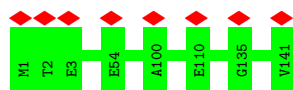
- Molecule 4: Photosystem I reaction center subunit II

Chain d:  6% 100%

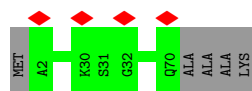
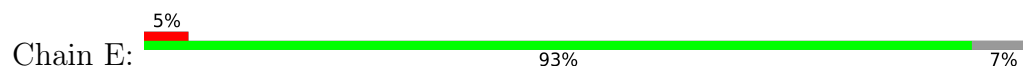


- Molecule 4: Photosystem I reaction center subunit II

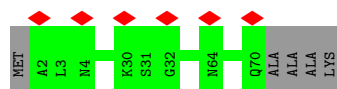
Chain O:  6% 100%



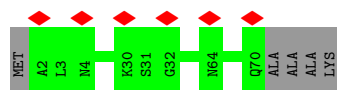
- Molecule 5: Photosystem I reaction center subunit IV



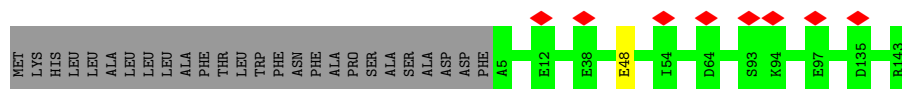
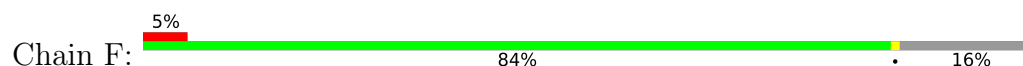
- Molecule 5: Photosystem I reaction center subunit IV



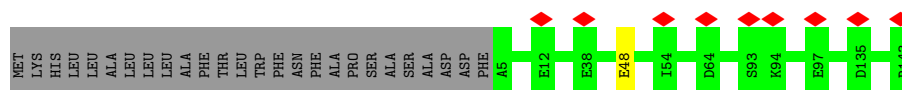
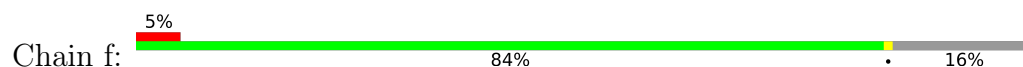
- Molecule 5: Photosystem I reaction center subunit IV



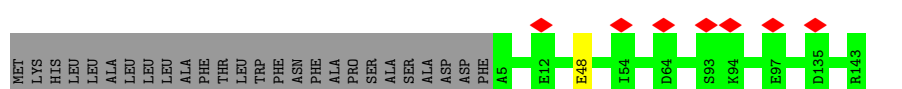
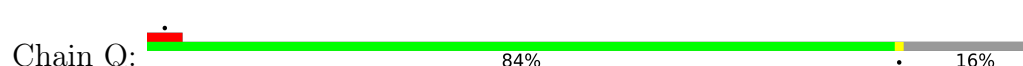
- Molecule 6: Photosystem I reaction center subunit III



- Molecule 6: Photosystem I reaction center subunit III



- Molecule 6: Photosystem I reaction center subunit III



- Molecule 7: Photosystem I reaction center subunit VIII



Chain I:  92% 8%



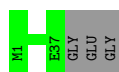
- Molecule 7: Photosystem I reaction center subunit VIII

Chain i:  92% 8%



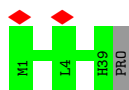
- Molecule 7: Photosystem I reaction center subunit VIII

Chain R:  92% 8%



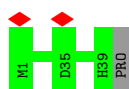
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  5% 98% .



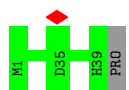
- Molecule 8: Photosystem I reaction center subunit IX

Chain j:  5% 98% .



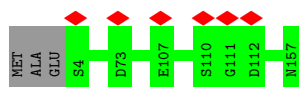
- Molecule 8: Photosystem I reaction center subunit IX

Chain S:  5% 98% .



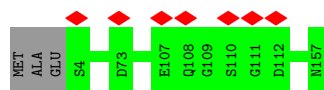
- Molecule 9: Photosystem I reaction center subunit XI

Chain L:  5% 98% .



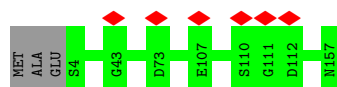
- Molecule 9: Photosystem I reaction center subunit XI

Chain I:  98%



- Molecule 9: Photosystem I reaction center subunit XI

Chain U:  98%



- Molecule 10: Photosystem I reaction center subunit XII

Chain M:  6% 94% 6%



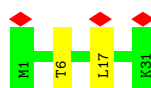
- Molecule 10: Photosystem I reaction center subunit XII

Chain m:  6% 94% 6%



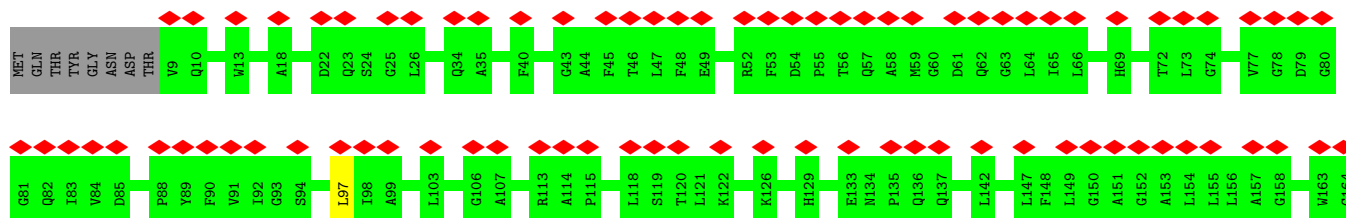
- Molecule 10: Photosystem I reaction center subunit XII

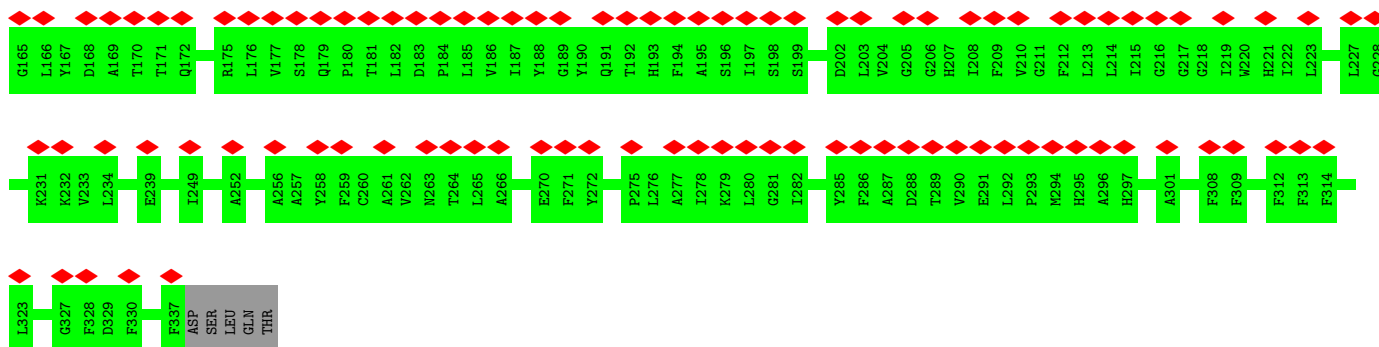
Chain V:  10% 94% 6%



- Molecule 11: Iron stress-induced chlorophyll-binding protein

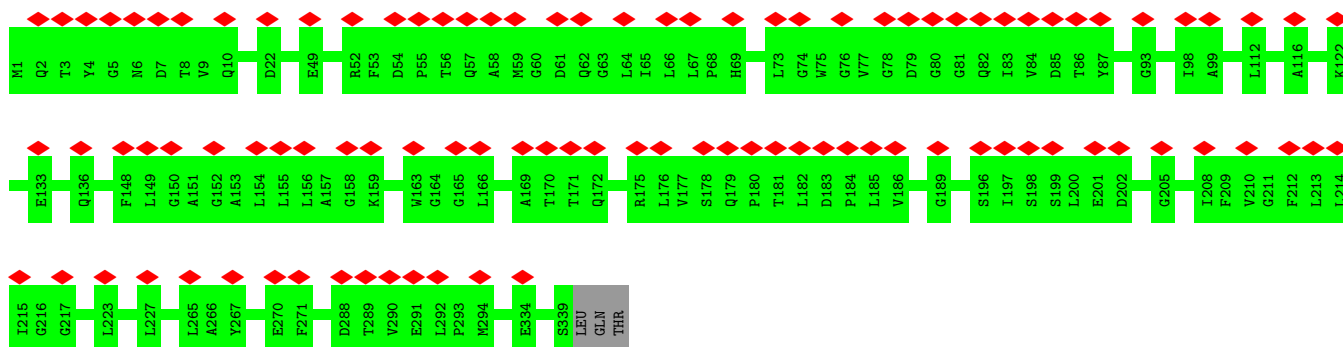
Chain W:  52% 96%





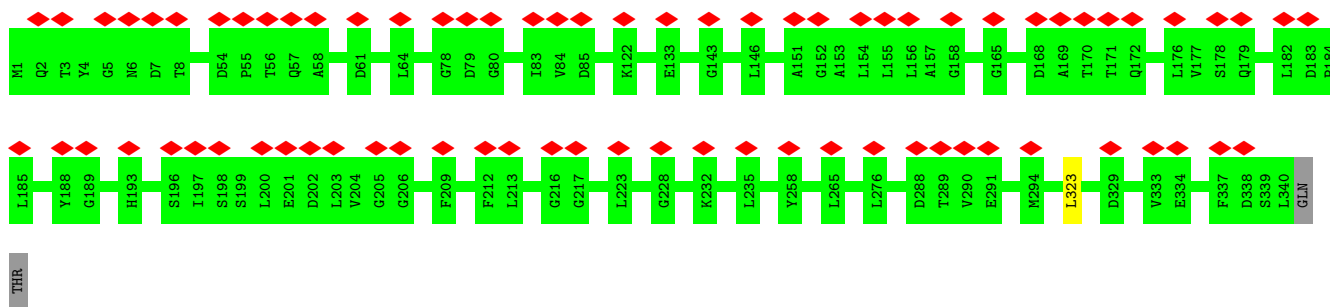
- Molecule 11: Iron stress-induced chlorophyll-binding protein

Chain X: 29% 99%



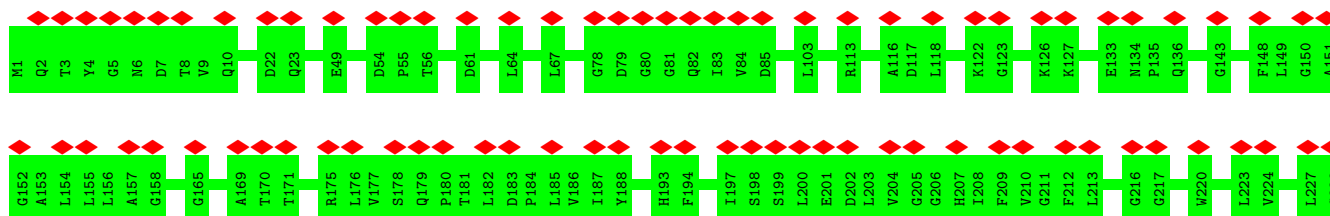
- Molecule 11: Iron stress-induced chlorophyll-binding protein

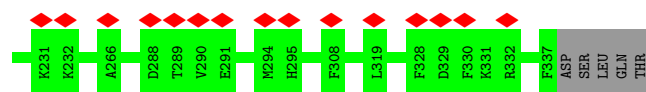
Chain Y: 22% 99%



- Molecule 11: Iron stress-induced chlorophyll-binding protein

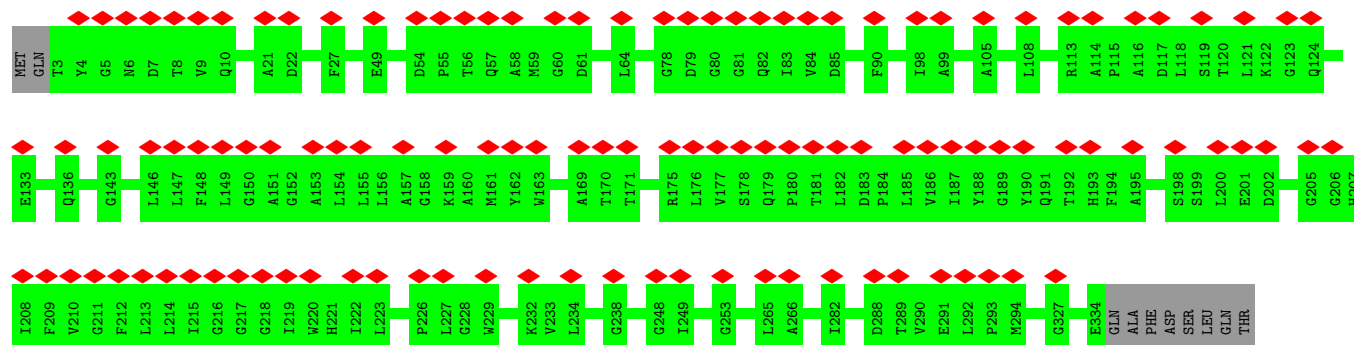
Chain Z: 28% 99%





- Molecule 11: Iron stress-induced chlorophyll-binding protein

Chain g: 35% 97%



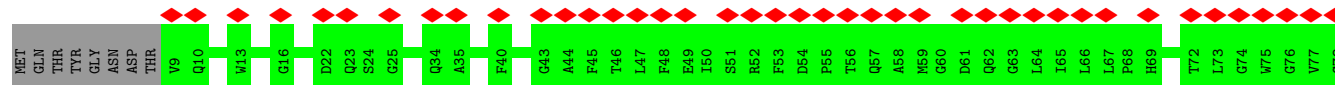
- Molecule 11: Iron stress-induced chlorophyll-binding protein

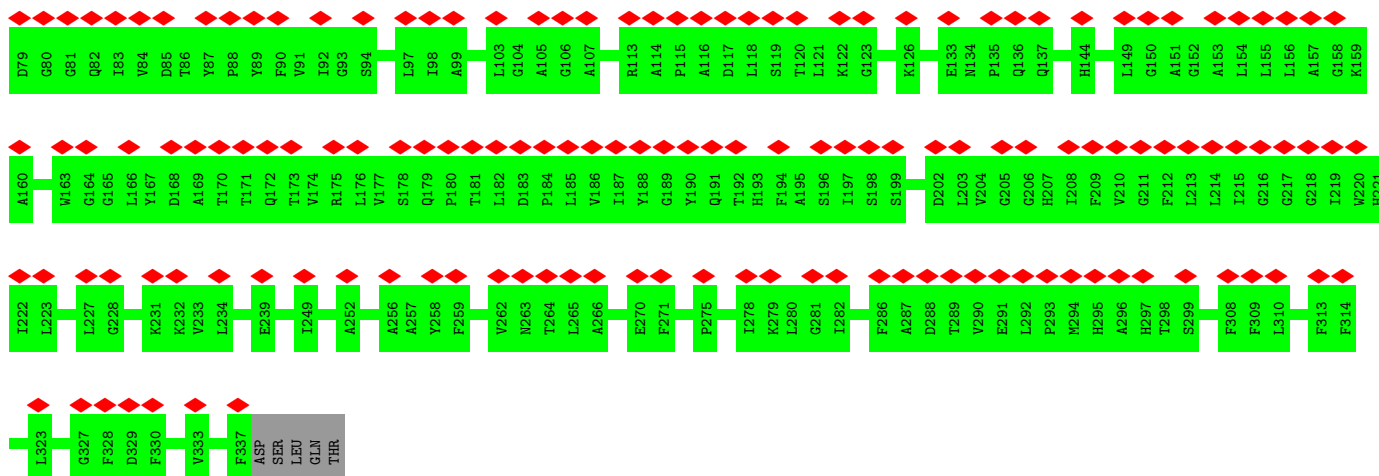
Chain y: 50% 93% 7%



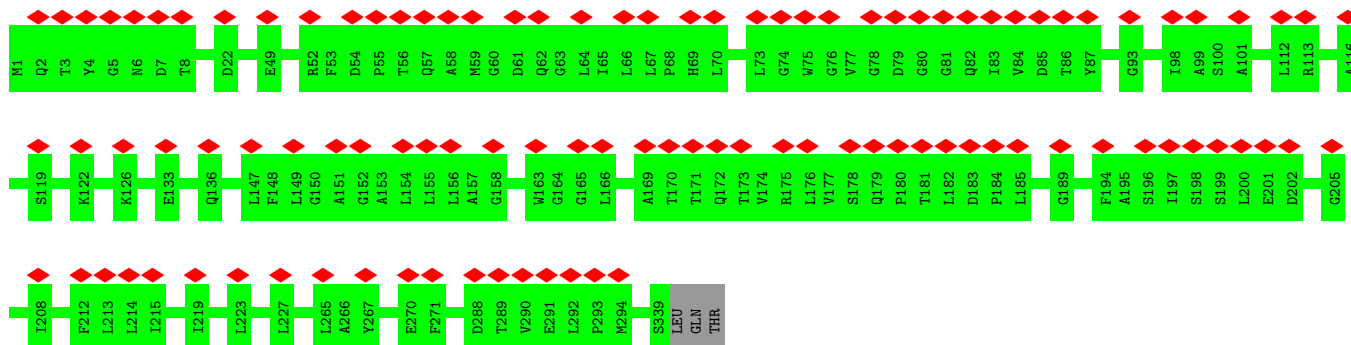
- Molecule 11: Iron stress-induced chlorophyll-binding protein

Chain n: 54% 96%

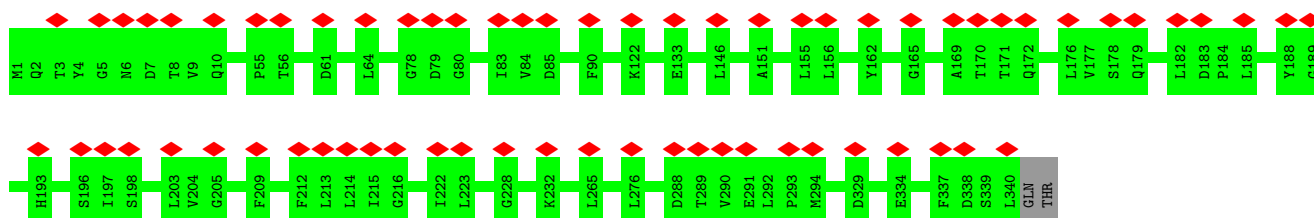




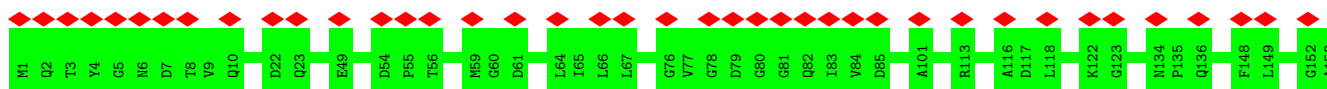
- Molecule 11: Iron stress-induced chlorophyll-binding protein

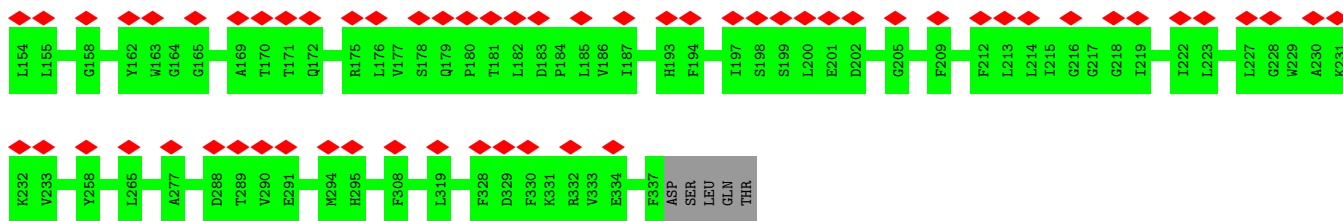


- Molecule 11: Iron stress-induced chlorophyll-binding protein

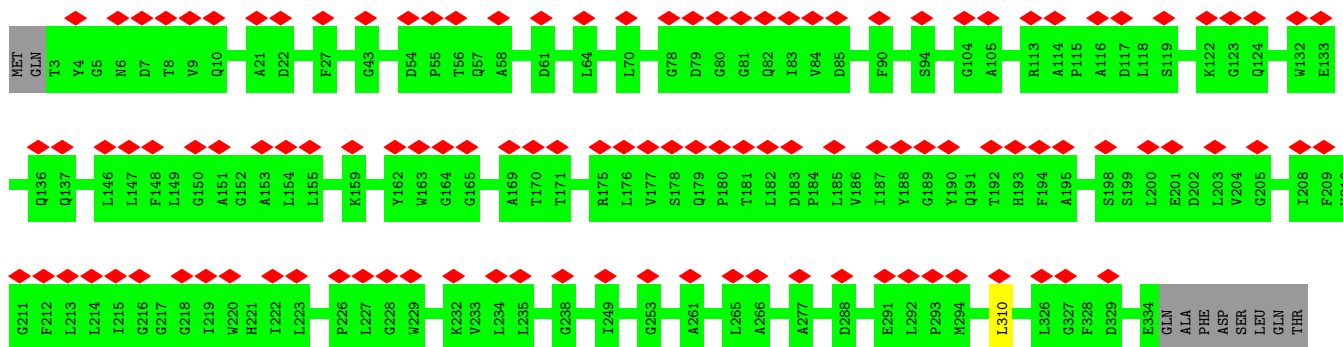


- Molecule 11: Iron stress-induced chlorophyll-binding protein

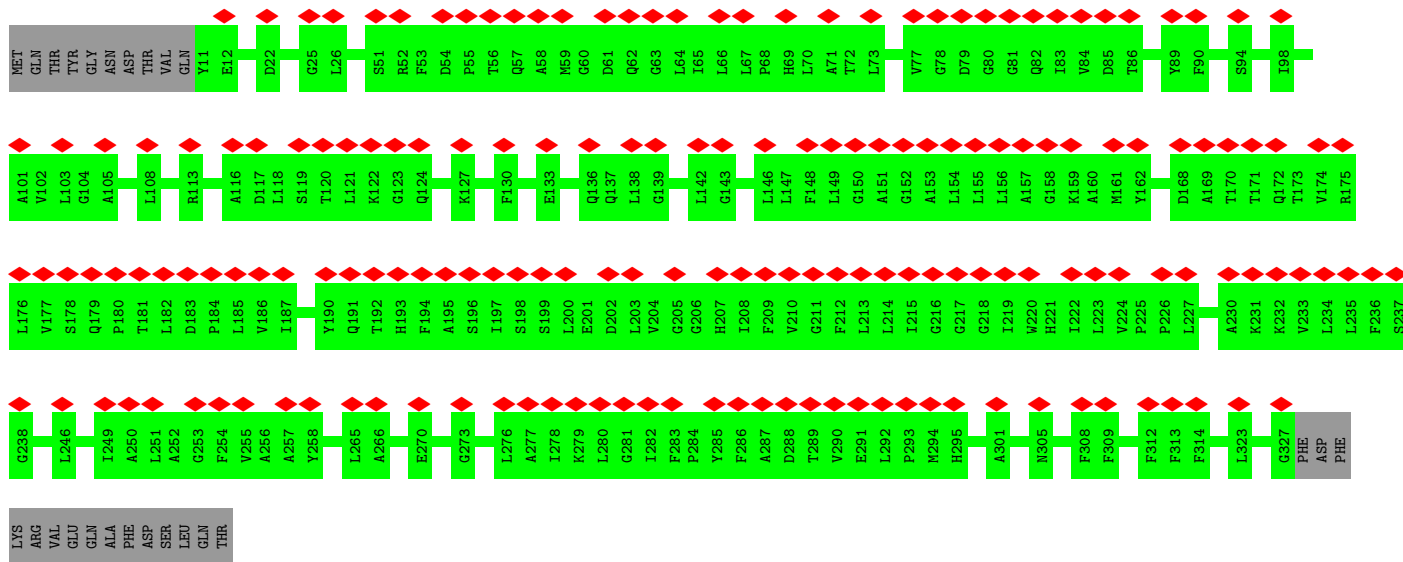
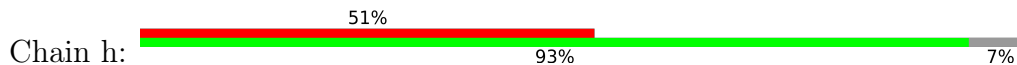




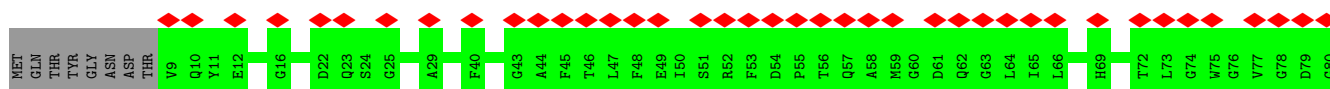
• Molecule 11: Iron stress-induced chlorophyll-binding protein

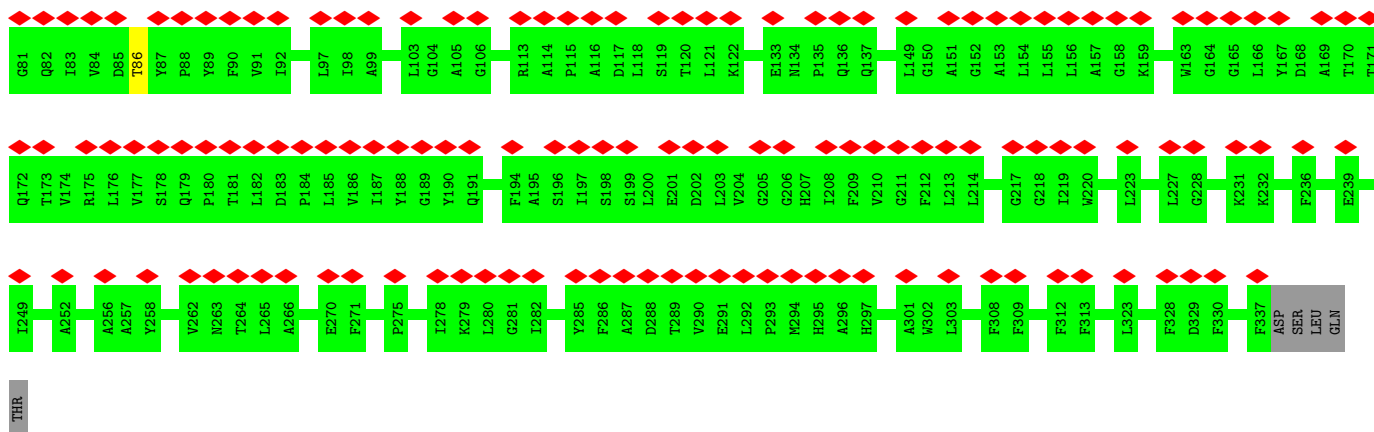


• Molecule 11: Iron stress-induced chlorophyll-binding protein

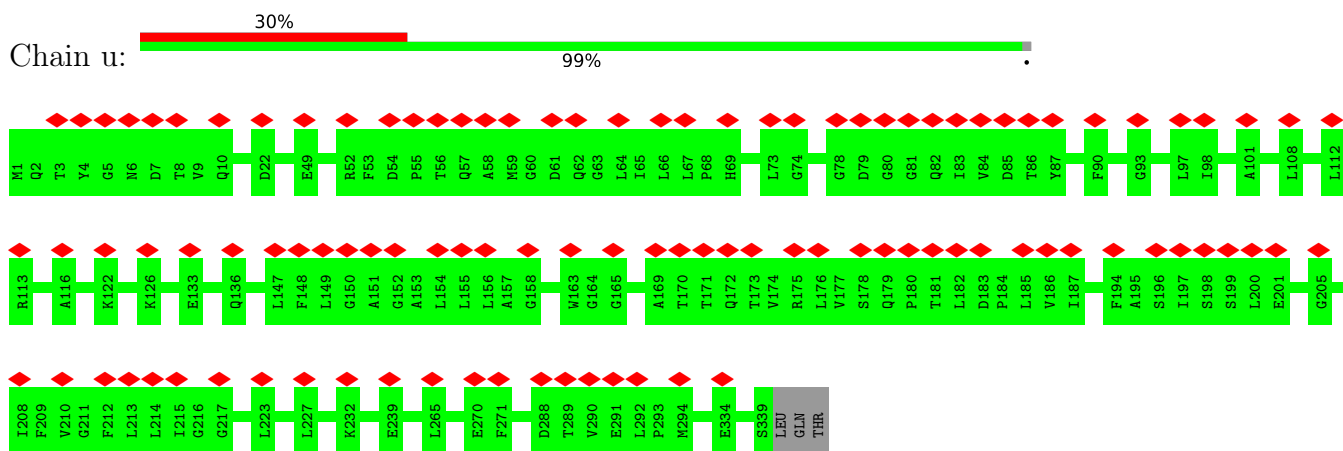


• Molecule 11: Iron stress-induced chlorophyll-binding protein

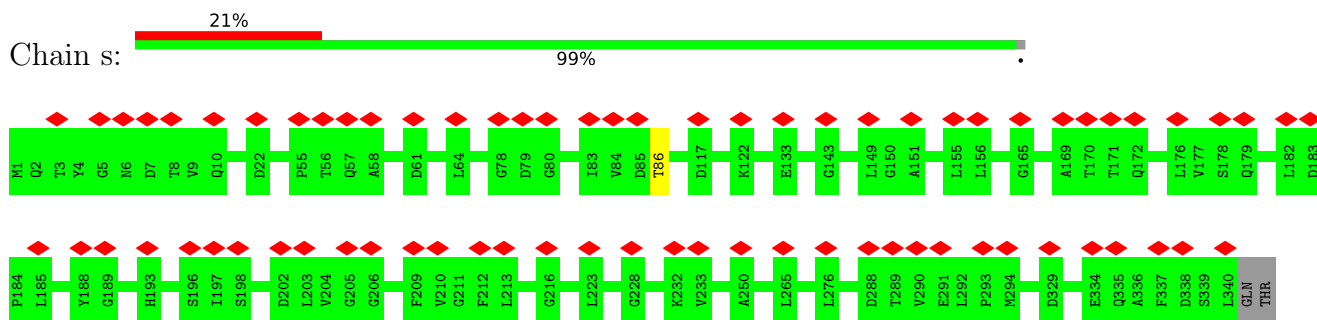




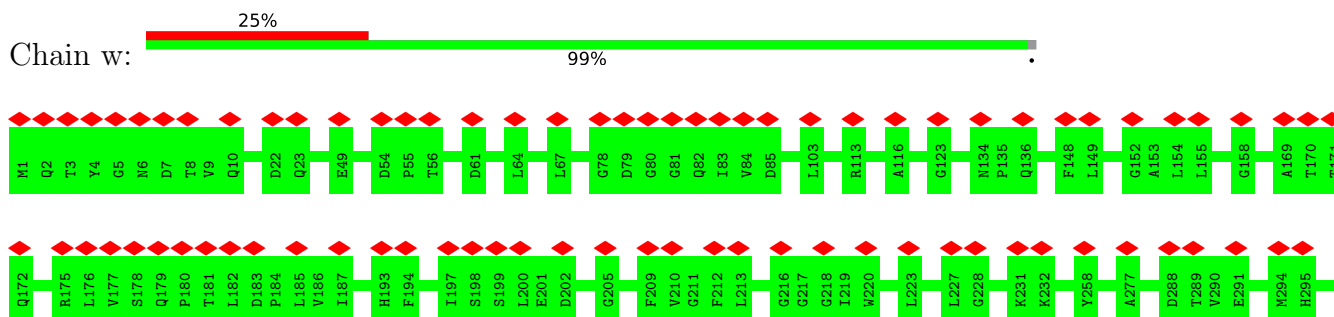
• Molecule 11: Iron stress-induced chlorophyll-binding protein

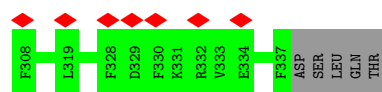


• Molecule 11: Iron stress-induced chlorophyll-binding protein



• Molecule 11: Iron stress-induced chlorophyll-binding protein

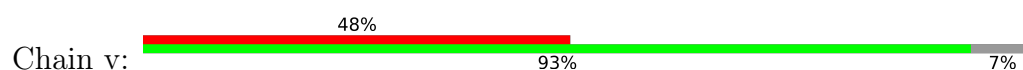




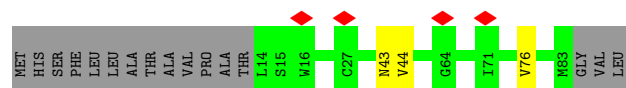
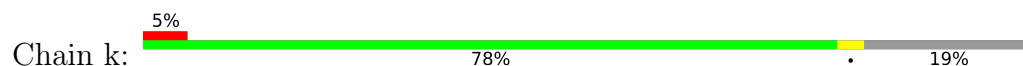
- Molecule 11: Iron stress-induced chlorophyll-binding protein



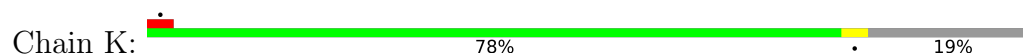
- Molecule 11: Iron stress-induced chlorophyll-binding protein



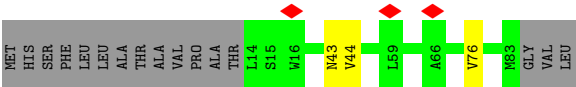
- Molecule 12: Photosystem I reaction center subunit Psak 1



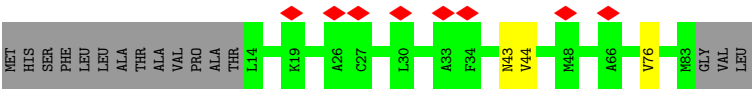
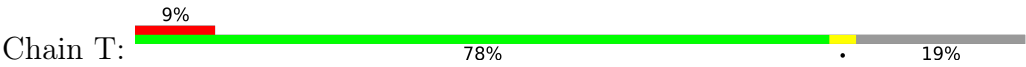
- Molecule 12: Photosystem I reaction center subunit Psak 1







● Molecule 12: Photosystem I reaction center subunit PsaK 1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	74000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.151	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	512.0, 512.0, 512.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.024, 1.024, 1.024	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, LMT, LHG, CA, BCR, PQN, CLA, CL0, 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	0.32	0/5984	0.47	0/8157
1	H	0.32	0/5984	0.47	0/8157
1	a	0.32	0/5984	0.47	0/8157
2	B	0.34	0/5977	0.49	1/8173 (0.0%)
2	G	0.34	0/5977	0.49	1/8173 (0.0%)
2	b	0.34	0/5977	0.49	1/8173 (0.0%)
3	C	0.36	0/610	0.61	0/826
3	N	0.36	0/610	0.61	0/826
3	c	0.36	0/610	0.61	0/826
4	D	0.29	0/1122	0.48	0/1513
4	O	0.29	0/1122	0.49	0/1513
4	d	0.29	0/1122	0.48	0/1513
5	E	0.30	0/551	0.48	0/745
5	P	0.30	0/551	0.49	0/745
5	e	0.30	0/551	0.48	0/745
6	F	0.30	0/1098	0.51	0/1495
6	Q	0.30	0/1098	0.51	0/1495
6	f	0.30	0/1098	0.51	0/1495
7	I	0.33	0/304	0.59	0/416
7	R	0.33	0/304	0.59	0/416
7	i	0.33	0/304	0.59	0/416
8	J	0.29	0/316	0.50	0/428
8	S	0.28	0/316	0.50	0/428
8	j	0.29	0/316	0.50	0/428
9	L	0.33	0/1186	0.53	0/1611
9	U	0.33	0/1186	0.53	0/1611
9	l	0.33	0/1186	0.53	0/1611
10	M	0.28	0/241	0.59	1/326 (0.3%)
10	V	0.29	0/241	0.59	1/326 (0.3%)
10	m	0.28	0/241	0.59	1/326 (0.3%)
11	W	0.28	0/2565	0.51	1/3512 (0.0%)
11	X	0.29	0/2695	0.49	0/3685

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	Y	0.30	0/2698	0.50	1/3691 (0.0%)
11	Z	0.29	0/2670	0.51	0/3650
11	g	0.28	0/2618	0.52	0/3582
11	h	0.27	0/2501	0.51	0/3423
11	n	0.27	0/2562	0.48	0/3508
11	o	0.27	0/2695	0.47	0/3685
11	p	0.28	0/2699	0.47	0/3692
11	q	0.28	0/2670	0.48	0/3650
11	r	0.27	0/2618	0.49	0/3582
11	s	0.28	0/2699	0.47	0/3692
11	t	0.27	0/2565	0.49	0/3512
11	u	0.27	0/2695	0.46	0/3685
11	v	0.27	0/2501	0.50	0/3423
11	w	0.28	0/2670	0.48	0/3650
11	x	0.28	0/2618	0.49	0/3582
11	y	0.28	0/2501	0.52	0/3423
12	K	0.30	0/495	0.55	0/672
12	T	0.30	0/495	0.55	0/672
12	k	0.30	0/495	0.55	0/672
All	All	0.30	0/100892	0.49	8/137713 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	m	17	LEU	CA-CB-CG	6.79	130.93	115.30
10	M	17	LEU	CA-CB-CG	6.78	130.89	115.30
10	V	17	LEU	CA-CB-CG	6.78	130.89	115.30
11	Y	323	LEU	CA-CB-CG	5.71	128.43	115.30
11	W	97	LEU	CA-CB-CG	5.38	127.67	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	737/751 (98%)	711 (96%)	26 (4%)	0	100	100
1	H	737/751 (98%)	711 (96%)	26 (4%)	0	100	100
1	a	737/751 (98%)	711 (96%)	26 (4%)	0	100	100
2	B	727/731 (100%)	699 (96%)	28 (4%)	0	100	100
2	G	727/731 (100%)	699 (96%)	28 (4%)	0	100	100
2	b	727/731 (100%)	699 (96%)	28 (4%)	0	100	100
3	C	78/81 (96%)	68 (87%)	10 (13%)	0	100	100
3	N	78/81 (96%)	68 (87%)	10 (13%)	0	100	100
3	c	78/81 (96%)	68 (87%)	10 (13%)	0	100	100
4	D	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
4	O	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
4	d	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
5	E	67/74 (90%)	63 (94%)	4 (6%)	0	100	100
5	P	67/74 (90%)	63 (94%)	4 (6%)	0	100	100
5	e	67/74 (90%)	63 (94%)	4 (6%)	0	100	100
6	F	137/165 (83%)	133 (97%)	4 (3%)	0	100	100
6	Q	137/165 (83%)	133 (97%)	4 (3%)	0	100	100
6	f	137/165 (83%)	133 (97%)	4 (3%)	0	100	100
7	I	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
7	R	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
7	i	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
8	J	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
8	S	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
8	j	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
9	L	152/157 (97%)	145 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	U	152/157 (97%)	145 (95%)	7 (5%)	0	100	100
9	l	152/157 (97%)	145 (95%)	7 (5%)	0	100	100
10	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
10	V	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
10	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	W	327/342 (96%)	313 (96%)	14 (4%)	0	100	100
11	X	337/342 (98%)	324 (96%)	13 (4%)	0	100	100
11	Y	338/342 (99%)	323 (96%)	15 (4%)	0	100	100
11	Z	335/342 (98%)	328 (98%)	7 (2%)	0	100	100
11	g	330/342 (96%)	320 (97%)	10 (3%)	0	100	100
11	h	315/342 (92%)	303 (96%)	12 (4%)	0	100	100
11	n	327/342 (96%)	309 (94%)	18 (6%)	0	100	100
11	o	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
11	p	338/342 (99%)	327 (97%)	11 (3%)	0	100	100
11	q	335/342 (98%)	325 (97%)	10 (3%)	0	100	100
11	r	330/342 (96%)	319 (97%)	11 (3%)	0	100	100
11	s	338/342 (99%)	326 (96%)	12 (4%)	0	100	100
11	t	327/342 (96%)	314 (96%)	13 (4%)	0	100	100
11	u	337/342 (98%)	324 (96%)	13 (4%)	0	100	100
11	v	315/342 (92%)	306 (97%)	9 (3%)	0	100	100
11	w	335/342 (98%)	321 (96%)	14 (4%)	0	100	100
11	x	330/342 (96%)	319 (97%)	11 (3%)	0	100	100
11	y	315/342 (92%)	305 (97%)	10 (3%)	0	100	100
12	K	68/86 (79%)	61 (90%)	7 (10%)	0	100	100
12	T	68/86 (79%)	61 (90%)	7 (10%)	0	100	100
12	k	68/86 (79%)	61 (90%)	7 (10%)	0	100	100
All	All	12564/13047 (96%)	12054 (96%)	510 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	593/603 (98%)	591 (100%)	2 (0%)	92	97
1	H	593/603 (98%)	591 (100%)	2 (0%)	92	97
1	a	593/603 (98%)	591 (100%)	2 (0%)	92	97
2	B	581/583 (100%)	579 (100%)	2 (0%)	92	97
2	G	581/583 (100%)	579 (100%)	2 (0%)	92	97
2	b	581/583 (100%)	579 (100%)	2 (0%)	92	97
3	C	68/69 (99%)	68 (100%)	0	100	100
3	N	68/69 (99%)	68 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	D	115/116 (99%)	115 (100%)	0	100	100
4	O	115/116 (99%)	115 (100%)	0	100	100
4	d	115/116 (99%)	115 (100%)	0	100	100
5	E	58/60 (97%)	58 (100%)	0	100	100
5	P	58/60 (97%)	58 (100%)	0	100	100
5	e	58/60 (97%)	58 (100%)	0	100	100
6	F	112/137 (82%)	111 (99%)	1 (1%)	78	91
6	Q	112/137 (82%)	111 (99%)	1 (1%)	78	91
6	f	112/137 (82%)	111 (99%)	1 (1%)	78	91
7	I	31/32 (97%)	31 (100%)	0	100	100
7	R	31/32 (97%)	31 (100%)	0	100	100
7	i	31/32 (97%)	31 (100%)	0	100	100
8	J	33/35 (94%)	33 (100%)	0	100	100
8	S	33/35 (94%)	33 (100%)	0	100	100
8	j	33/35 (94%)	33 (100%)	0	100	100
9	L	116/118 (98%)	116 (100%)	0	100	100
9	U	116/118 (98%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	l	116/118 (98%)	116 (100%)	0	100	100
10	M	25/25 (100%)	24 (96%)	1 (4%)	31	62
10	V	25/25 (100%)	24 (96%)	1 (4%)	31	62
10	m	25/25 (100%)	24 (96%)	1 (4%)	31	62
11	W	232/260 (89%)	232 (100%)	0	100	100
11	X	252/260 (97%)	252 (100%)	0	100	100
11	Y	251/260 (96%)	251 (100%)	0	100	100
11	Z	249/260 (96%)	249 (100%)	0	100	100
11	g	243/260 (94%)	243 (100%)	0	100	100
11	h	231/260 (89%)	231 (100%)	0	100	100
11	n	231/260 (89%)	231 (100%)	0	100	100
11	o	252/260 (97%)	252 (100%)	0	100	100
11	p	252/260 (97%)	252 (100%)	0	100	100
11	q	249/260 (96%)	249 (100%)	0	100	100
11	r	243/260 (94%)	242 (100%)	1 (0%)	91	96
11	s	252/260 (97%)	251 (100%)	1 (0%)	91	96
11	t	232/260 (89%)	231 (100%)	1 (0%)	91	96
11	u	252/260 (97%)	252 (100%)	0	100	100
11	v	231/260 (89%)	231 (100%)	0	100	100
11	w	249/260 (96%)	249 (100%)	0	100	100
11	x	243/260 (94%)	243 (100%)	0	100	100
11	y	231/260 (89%)	231 (100%)	0	100	100
12	K	48/62 (77%)	45 (94%)	3 (6%)	18	50
12	T	48/62 (77%)	45 (94%)	3 (6%)	18	50
12	k	48/62 (77%)	45 (94%)	3 (6%)	18	50
All	All	9715/10200 (95%)	9685 (100%)	30 (0%)	92	97

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	r	310	LEU
12	T	43	ASN
2	G	11	ASP

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Mol	Chain	Res	Type
12	T	76	VAL
12	K	43	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
11	q	6	ASN
5	P	59	ASN
2	G	450	GLN
5	P	4	ASN
11	w	305	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 771 ligands modelled in this entry, 3 are monoatomic - leaving 768 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	$\# Z  > 2$
16	CLA	H	1107	-	50,58,73	1.64	8 (16%)	58,95,113	1.81	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	u	505	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	8 (10%)
19	BCR	H	4011	-	41,41,41	1.11	2 (4%)	56,56,56	1.36	8 (14%)
13	LHG	A	849	-	42,42,48	0.67	1 (2%)	45,48,54	1.23	4 (8%)
19	BCR	W	601	-	41,41,41	1.04	2 (4%)	56,56,56	1.33	8 (14%)
16	CLA	H	1123	-	65,73,73	1.47	6 (9%)	76,113,113	1.52	9 (11%)
19	BCR	p	602	-	41,41,41	1.04	2 (4%)	56,56,56	1.36	8 (14%)
16	CLA	a	1117	-	65,73,73	1.42	7 (10%)	76,113,113	1.51	7 (9%)
16	CLA	W	507	-	60,68,73	1.56	6 (10%)	70,107,113	1.44	8 (11%)
16	CLA	b	1212	-	45,53,73	1.72	6 (13%)	52,89,113	1.71	9 (17%)
16	CLA	x	505	-	46,54,73	1.74	6 (13%)	53,90,113	1.64	8 (15%)
19	BCR	L	4022	-	41,41,41	1.09	1 (2%)	56,56,56	1.53	12 (21%)
16	CLA	x	509	-	60,68,73	1.54	6 (10%)	70,107,113	1.47	8 (11%)
16	CLA	o	517	-	55,63,73	1.57	7 (12%)	64,101,113	1.64	8 (12%)
16	CLA	A	1134	-	45,53,73	1.78	8 (17%)	52,89,113	1.73	10 (19%)
16	CLA	A	1402	-	42,49,73	1.80	6 (14%)	48,83,113	1.67	6 (12%)
19	BCR	o	602	-	41,41,41	1.02	2 (4%)	56,56,56	1.35	7 (12%)
19	BCR	x	602	-	41,41,41	1.00	2 (4%)	56,56,56	1.33	7 (12%)
19	BCR	G	4005	-	41,41,41	1.12	2 (4%)	56,56,56	1.40	7 (12%)
16	CLA	X	505	-	65,73,73	1.49	7 (10%)	76,113,113	1.41	8 (10%)
16	CLA	p	506	-	60,68,73	1.52	8 (13%)	70,107,113	1.50	8 (11%)
15	CL0	a	1011	-	65,73,73	1.45	9 (13%)	76,113,113	1.66	14 (18%)
16	CLA	H	1112	-	45,53,73	1.70	7 (15%)	52,89,113	1.81	8 (15%)
19	BCR	F	4016	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	7 (12%)
16	CLA	b	1232	-	45,53,73	1.80	6 (13%)	52,89,113	1.67	7 (13%)
16	CLA	a	1125	-	65,73,73	1.43	8 (12%)	76,113,113	1.54	9 (11%)
19	BCR	U	4022	-	41,41,41	1.10	1 (2%)	56,56,56	1.53	12 (21%)
16	CLA	G	1213	-	55,63,73	1.57	7 (12%)	64,101,113	1.54	8 (12%)
19	BCR	b	4006	-	25,25,41	1.08	2 (8%)	33,33,56	1.42	7 (21%)
16	CLA	Z	506	-	60,68,73	1.53	7 (11%)	70,107,113	1.50	7 (10%)
16	CLA	H	1138	-	65,73,73	1.44	9 (13%)	76,113,113	1.53	10 (13%)
16	CLA	b	1211	-	65,73,73	1.43	7 (10%)	76,113,113	1.48	8 (10%)
16	CLA	b	1222	-	55,63,73	1.59	9 (16%)	64,101,113	1.56	9 (14%)
16	CLA	G	1201	-	54,62,73	1.59	7 (12%)	62,99,113	1.69	9 (14%)
16	CLA	J	1303	-	38,45,73	1.86	7 (18%)	43,78,113	1.77	7 (16%)
16	CLA	L	1503	-	65,73,73	1.42	7 (10%)	76,113,113	1.50	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	b	1208	-	45,53,73	1.75	7 (15%)	52,89,113	1.67	8 (15%)
16	CLA	b	1217	-	45,53,73	1.76	6 (13%)	52,89,113	1.64	6 (11%)
16	CLA	Z	513	-	50,58,73	1.67	6 (12%)	58,95,113	1.57	8 (13%)
16	CLA	a	1104	-	65,73,73	1.47	7 (10%)	76,113,113	1.50	7 (9%)
19	BCR	J	4012	-	41,41,41	1.15	2 (4%)	56,56,56	1.40	7 (12%)
16	CLA	H	1108	-	45,53,73	1.73	7 (15%)	52,89,113	1.72	7 (13%)
16	CLA	W	513	-	50,58,73	1.68	6 (12%)	58,95,113	1.57	9 (15%)
17	PQN	H	2001	-	34,34,34	0.35	0	42,45,45	1.18	4 (9%)
19	BCR	B	4004	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	5 (8%)
16	CLA	Z	511	-	65,73,73	1.44	7 (10%)	76,113,113	1.57	9 (11%)
16	CLA	w	508	-	55,63,73	1.59	6 (10%)	64,101,113	1.54	7 (10%)
16	CLA	a	1111	-	55,63,73	1.58	9 (16%)	64,101,113	1.55	9 (14%)
16	CLA	v	517	-	55,63,73	1.63	6 (10%)	64,101,113	1.51	9 (14%)
16	CLA	s	517	-	55,63,73	1.59	6 (10%)	64,101,113	1.53	7 (10%)
19	BCR	a	4001	-	41,41,41	1.13	2 (4%)	56,56,56	1.35	9 (16%)
16	CLA	A	1131	-	65,73,73	1.44	9 (13%)	76,113,113	1.52	11 (14%)
16	CLA	v	507	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
19	BCR	t	603	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	8 (14%)
16	CLA	H	1135	-	51,59,73	1.61	9 (17%)	59,96,113	1.60	8 (13%)
16	CLA	Y	505	-	65,73,73	1.49	8 (12%)	76,113,113	1.48	9 (11%)
16	CLA	G	1203	-	65,73,73	1.47	7 (10%)	76,113,113	1.48	8 (10%)
16	CLA	t	501	-	50,58,73	1.67	5 (10%)	58,95,113	1.54	10 (17%)
16	CLA	t	513	-	50,58,73	1.66	6 (12%)	58,95,113	1.57	9 (15%)
16	CLA	v	503	-	46,54,73	1.75	6 (13%)	53,90,113	1.62	7 (13%)
20	LMT	U	4101	-	36,36,36	1.15	5 (13%)	47,47,47	1.06	4 (8%)
16	CLA	X	504	-	60,68,73	1.55	7 (11%)	70,107,113	1.47	8 (11%)
16	CLA	H	1130	-	65,73,73	1.45	9 (13%)	76,113,113	1.48	9 (11%)
16	CLA	B	1206	-	65,73,73	1.44	7 (10%)	76,113,113	1.60	8 (10%)
16	CLA	r	505	-	46,54,73	1.75	5 (10%)	53,90,113	1.63	8 (15%)
19	BCR	r	603	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	7 (12%)
17	PQN	B	2002	-	34,34,34	0.37	0	42,45,45	1.17	2 (4%)
19	BCR	r	602	-	41,41,41	1.00	2 (4%)	56,56,56	1.32	7 (12%)
16	CLA	G	1012	-	60,68,73	1.58	10 (16%)	70,107,113	1.51	12 (17%)
16	CLA	b	1219	-	45,53,73	1.74	6 (13%)	52,89,113	1.72	9 (17%)
16	CLA	H	1102	-	56,64,73	1.56	7 (12%)	65,102,113	1.67	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	BCR	b	4017	-	41,41,41	1.17	2 (4%)	56,56,56	1.31	7 (12%)
16	CLA	v	515	-	60,68,73	1.53	6 (10%)	70,107,113	1.50	7 (10%)
16	CLA	l	1501	-	65,73,73	1.45	7 (10%)	76,113,113	1.50	9 (11%)
14	LMG	A	4201	-	32,32,55	1.01	1 (3%)	40,40,63	1.12	3 (7%)
16	CLA	u	503	-	46,54,73	1.74	7 (15%)	53,90,113	1.66	8 (15%)
16	CLA	o	502	-	50,58,73	1.67	8 (16%)	58,95,113	1.63	11 (18%)
19	BCR	Y	604	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	5 (8%)
16	CLA	y	517	-	55,63,73	1.62	5 (9%)	64,101,113	1.51	9 (14%)
16	CLA	n	512	-	45,53,73	1.76	6 (13%)	52,89,113	1.71	8 (15%)
16	CLA	A	1137	-	47,55,73	1.66	9 (19%)	54,91,113	1.71	8 (14%)
16	CLA	a	1124	-	65,73,73	1.45	9 (13%)	76,113,113	1.46	10 (13%)
16	CLA	p	504	-	60,68,73	1.53	6 (10%)	70,107,113	1.50	8 (11%)
19	BCR	u	604	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	7 (12%)
16	CLA	a	1126	-	65,73,73	1.47	9 (13%)	76,113,113	1.52	11 (14%)
16	CLA	b	1240	-	50,58,73	1.69	6 (12%)	58,95,113	1.59	8 (13%)
19	BCR	w	603	-	41,41,41	1.06	2 (4%)	56,56,56	1.28	5 (8%)
16	CLA	a	1801	-	52,60,73	1.62	7 (13%)	60,97,113	1.57	8 (13%)
16	CLA	q	508	-	55,63,73	1.60	6 (10%)	64,101,113	1.54	7 (10%)
16	CLA	W	512	-	45,53,73	1.75	7 (15%)	52,89,113	1.75	8 (15%)
16	CLA	t	506	-	60,68,73	1.54	6 (10%)	70,107,113	1.49	8 (11%)
16	CLA	x	504	-	60,68,73	1.54	6 (10%)	70,107,113	1.46	8 (11%)
16	CLA	u	502	-	50,58,73	1.68	6 (12%)	58,95,113	1.61	12 (20%)
19	BCR	i	4020	-	41,41,41	1.22	3 (7%)	56,56,56	1.25	6 (10%)
16	CLA	o	511	-	65,73,73	1.44	7 (10%)	76,113,113	1.56	8 (10%)
17	PQN	G	2002	-	34,34,34	0.37	0	42,45,45	1.17	2 (4%)
16	CLA	s	512	-	45,53,73	1.73	7 (15%)	52,89,113	1.78	8 (15%)
16	CLA	Y	516	-	46,54,73	1.71	6 (13%)	53,90,113	1.68	7 (13%)
16	CLA	u	501	-	50,58,73	1.67	5 (10%)	58,95,113	1.61	10 (17%)
16	CLA	g	506	-	60,68,73	1.53	10 (16%)	70,107,113	1.57	10 (14%)
19	BCR	Y	603	-	41,41,41	1.06	2 (4%)	56,56,56	1.36	8 (14%)
16	CLA	X	513	-	50,58,73	1.66	6 (12%)	58,95,113	1.58	8 (13%)
16	CLA	g	512	-	45,53,73	1.73	5 (11%)	52,89,113	1.70	7 (13%)
16	CLA	A	1120	-	49,57,73	1.66	7 (14%)	55,93,113	1.69	9 (16%)
16	CLA	o	504	-	60,68,73	1.54	6 (10%)	70,107,113	1.47	7 (10%)
16	CLA	H	1117	-	65,73,73	1.42	7 (10%)	76,113,113	1.50	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	H	1136	-	65,73,73	1.45	8 (12%)	76,113,113	1.48	9 (11%)
16	CLA	u	512	-	45,53,73	1.72	6 (13%)	52,89,113	1.76	8 (15%)
19	BCR	n	601	-	41,41,41	1.04	2 (4%)	56,56,56	1.35	9 (16%)
16	CLA	B	1240	-	50,58,73	1.69	6 (12%)	58,95,113	1.59	8 (13%)
16	CLA	v	502	-	50,58,73	1.68	6 (12%)	58,95,113	1.55	7 (12%)
16	CLA	A	1132	-	65,73,73	1.45	9 (13%)	76,113,113	1.51	10 (13%)
16	CLA	p	503	-	46,54,73	1.75	7 (15%)	53,90,113	1.66	7 (13%)
19	BCR	u	601	-	41,41,41	1.08	2 (4%)	56,56,56	1.30	7 (12%)
16	CLA	g	516	-	46,54,73	1.75	5 (10%)	53,90,113	1.69	7 (13%)
16	CLA	W	506	-	60,68,73	1.52	7 (11%)	70,107,113	1.54	9 (12%)
16	CLA	u	516	-	46,54,73	1.75	6 (13%)	53,90,113	1.60	7 (13%)
16	CLA	G	1209	-	45,53,73	1.76	6 (13%)	52,89,113	1.66	8 (15%)
16	CLA	l	1502	-	65,73,73	1.45	9 (13%)	76,113,113	1.47	9 (11%)
16	CLA	s	511	-	65,73,73	1.48	8 (12%)	76,113,113	1.45	7 (9%)
16	CLA	b	1231	-	45,53,73	1.76	6 (13%)	52,89,113	1.78	11 (21%)
13	LHG	a	851	-	26,26,48	0.85	1 (3%)	29,32,54	1.36	3 (10%)
16	CLA	v	505	-	60,68,73	1.53	6 (10%)	70,107,113	1.46	9 (12%)
16	CLA	A	1122	-	59,67,73	1.52	8 (13%)	68,105,113	1.50	9 (13%)
14	LMG	b	848	-	43,43,55	0.80	0	51,51,63	1.32	7 (13%)
16	CLA	h	502	-	50,58,73	1.68	6 (12%)	58,95,113	1.54	7 (12%)
16	CLA	B	1230	-	45,53,73	1.70	7 (15%)	52,89,113	1.80	9 (17%)
16	CLA	v	516	-	46,54,73	1.76	5 (10%)	53,90,113	1.62	7 (13%)
16	CLA	f	1302	-	29,35,73	2.67	9 (31%)	28,60,113	1.73	6 (21%)
16	CLA	Y	513	-	50,58,73	1.68	7 (14%)	58,95,113	1.58	8 (13%)
16	CLA	x	513	-	50,58,73	1.69	6 (12%)	58,95,113	1.60	8 (13%)
16	CLA	a	1134	-	45,53,73	1.77	7 (15%)	52,89,113	1.73	9 (17%)
16	CLA	o	506	-	60,68,73	1.55	7 (11%)	70,107,113	1.47	8 (11%)
16	CLA	Z	515	-	65,73,73	1.44	6 (9%)	76,113,113	1.45	7 (9%)
16	CLA	x	515	-	65,73,73	1.46	8 (12%)	76,113,113	1.38	7 (9%)
16	CLA	b	1225	-	65,73,73	1.51	9 (13%)	76,113,113	1.45	9 (11%)
16	CLA	G	1206	-	65,73,73	1.45	8 (12%)	76,113,113	1.60	8 (10%)
16	CLA	w	513	-	50,58,73	1.67	6 (12%)	58,95,113	1.60	8 (13%)
16	CLA	h	512	-	45,53,73	1.73	6 (13%)	52,89,113	1.78	8 (15%)
16	CLA	H	1118	-	55,63,73	1.59	10 (18%)	64,101,113	1.53	7 (10%)
16	CLA	o	513	-	50,58,73	1.67	6 (12%)	58,95,113	1.59	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	a	1116	-	54,62,73	1.59	9 (16%)	62,99,113	1.61	10 (16%)
16	CLA	h	511	-	65,73,73	1.48	7 (10%)	76,113,113	1.50	9 (11%)
16	CLA	A	1107	-	50,58,73	1.63	7 (14%)	58,95,113	1.80	10 (17%)
16	CLA	b	1021	-	65,73,73	1.43	8 (12%)	76,113,113	1.57	7 (9%)
19	BCR	v	603	-	41,41,41	1.06	2 (4%)	56,56,56	1.29	7 (12%)
16	CLA	u	517	-	55,63,73	1.56	6 (10%)	64,101,113	1.74	10 (15%)
16	CLA	H	1114	-	49,57,73	1.70	6 (12%)	55,93,113	1.61	8 (14%)
19	BCR	J	4013	-	41,41,41	1.06	2 (4%)	56,56,56	1.37	6 (10%)
19	BCR	j	4015	-	41,41,41	1.13	3 (7%)	56,56,56	1.33	8 (14%)
16	CLA	G	1223	-	65,73,73	1.49	8 (12%)	76,113,113	1.44	8 (10%)
16	CLA	q	502	-	50,58,73	1.66	7 (14%)	58,95,113	1.60	8 (13%)
16	CLA	G	1235	-	62,70,73	1.47	7 (11%)	72,109,113	1.70	10 (13%)
16	CLA	B	1207	-	65,73,73	1.48	8 (12%)	76,113,113	1.47	8 (10%)
16	CLA	Y	509	-	60,68,73	1.50	7 (11%)	70,107,113	1.51	10 (14%)
16	CLA	H	1237	-	65,73,73	1.47	10 (15%)	76,113,113	1.52	10 (13%)
19	BCR	Q	4016	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	7 (12%)
16	CLA	a	1105	-	58,66,73	1.52	6 (10%)	67,104,113	1.57	8 (11%)
16	CLA	x	502	-	50,58,73	1.67	6 (12%)	58,95,113	1.54	8 (13%)
16	CLA	a	1237	-	65,73,73	1.49	10 (15%)	76,113,113	1.51	10 (13%)
16	CLA	A	1113	-	45,53,73	1.72	7 (15%)	52,89,113	1.82	8 (15%)
14	LMG	p	701	-	39,39,55	0.88	1 (2%)	47,47,63	1.24	4 (8%)
16	CLA	G	1236	-	65,73,73	1.45	7 (10%)	76,113,113	1.48	10 (13%)
16	CLA	b	1202	-	65,73,73	1.41	7 (10%)	76,113,113	1.58	9 (11%)
16	CLA	p	512	-	45,53,73	1.72	6 (13%)	52,89,113	1.76	8 (15%)
16	CLA	h	501	-	46,54,73	1.74	5 (10%)	53,90,113	1.61	7 (13%)
16	CLA	b	1201	-	54,62,73	1.59	7 (12%)	62,99,113	1.70	9 (14%)
15	CL0	H	1011	-	65,73,73	1.45	9 (13%)	76,113,113	1.66	15 (19%)
16	CLA	H	1137	-	47,55,73	1.67	9 (19%)	54,91,113	1.70	8 (14%)
16	CLA	y	509	-	60,68,73	1.51	7 (11%)	70,107,113	1.50	10 (14%)
16	CLA	g	509	-	60,68,73	1.53	6 (10%)	70,107,113	1.45	8 (11%)
16	CLA	H	1119	-	65,73,73	1.46	7 (10%)	76,113,113	1.48	8 (10%)
16	CLA	x	512	-	45,53,73	1.74	6 (13%)	52,89,113	1.72	8 (15%)
16	CLA	p	505	-	65,73,73	1.49	8 (12%)	76,113,113	1.45	8 (10%)
16	CLA	Z	502	-	50,58,73	1.70	7 (14%)	58,95,113	1.60	9 (15%)
16	CLA	X	512	-	45,53,73	1.73	6 (13%)	52,89,113	1.73	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	p	516	-	46,54,73	1.75	6 (13%)	53,90,113	1.69	7 (13%)
16	CLA	a	1132	-	65,73,73	1.45	9 (13%)	76,113,113	1.50	10 (13%)
16	CLA	Z	501	-	50,58,73	1.69	6 (12%)	58,95,113	1.56	8 (13%)
16	CLA	n	503	-	46,54,73	1.70	6 (13%)	53,90,113	1.73	7 (13%)
16	CLA	o	512	-	45,53,73	1.73	6 (13%)	52,89,113	1.76	8 (15%)
16	CLA	x	516	-	46,54,73	1.77	5 (10%)	53,90,113	1.66	7 (13%)
18	SF4	C	102	3	0,12,12	-	-	-	-	-
16	CLA	Z	512	-	45,53,73	1.73	7 (15%)	52,89,113	1.72	8 (15%)
16	CLA	U	1503	-	65,73,73	1.42	7 (10%)	76,113,113	1.49	9 (11%)
16	CLA	u	511	-	65,73,73	1.44	7 (10%)	76,113,113	1.56	8 (10%)
16	CLA	u	504	-	60,68,73	1.55	7 (11%)	70,107,113	1.47	8 (11%)
16	CLA	y	511	-	65,73,73	1.48	7 (10%)	76,113,113	1.49	8 (10%)
19	BCR	V	4021	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	5 (8%)
16	CLA	t	515	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	8 (10%)
16	CLA	X	516	-	46,54,73	1.75	6 (13%)	53,90,113	1.62	7 (13%)
16	CLA	Y	504	-	60,68,73	1.53	6 (10%)	70,107,113	1.49	8 (11%)
16	CLA	h	505	-	60,68,73	1.53	6 (10%)	70,107,113	1.47	9 (12%)
16	CLA	h	509	-	60,68,73	1.53	7 (11%)	70,107,113	1.49	8 (11%)
19	BCR	h	602	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	4 (7%)
18	SF4	N	101	3	0,12,12	-	-	-	-	-
19	BCR	R	4020	-	41,41,41	1.23	3 (7%)	56,56,56	1.25	6 (10%)
16	CLA	A	1106	-	65,73,73	1.42	9 (13%)	76,113,113	1.47	10 (13%)
16	CLA	A	1127	-	65,73,73	1.44	8 (12%)	76,113,113	1.52	7 (9%)
16	CLA	Z	510	-	60,68,73	1.51	6 (10%)	70,107,113	1.49	7 (10%)
16	CLA	q	507	-	65,73,73	1.49	8 (12%)	76,113,113	1.39	7 (9%)
16	CLA	p	510	-	65,73,73	1.44	7 (10%)	76,113,113	1.44	8 (10%)
16	CLA	b	1012	-	60,68,73	1.58	10 (16%)	70,107,113	1.51	12 (17%)
19	BCR	g	604	-	41,41,41	1.04	2 (4%)	56,56,56	1.34	9 (16%)
16	CLA	W	510	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	9 (11%)
19	BCR	H	4007	-	41,41,41	1.12	3 (7%)	56,56,56	1.35	7 (12%)
16	CLA	A	1108	-	45,53,73	1.73	7 (15%)	52,89,113	1.72	8 (15%)
19	BCR	X	601	-	41,41,41	1.10	3 (7%)	56,56,56	1.32	9 (16%)
19	BCR	w	604	-	41,41,41	1.08	2 (4%)	56,56,56	1.34	9 (16%)
16	CLA	x	507	-	65,73,73	1.47	7 (10%)	76,113,113	1.44	7 (9%)
19	BCR	q	603	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	6 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	LHG	I	103	-	43,43,48	0.65	0	46,49,54	1.26	5 (10%)
16	CLA	g	514	-	50,58,73	1.69	6 (12%)	58,95,113	1.59	8 (13%)
16	CLA	a	1101	-	65,73,73	1.43	7 (10%)	76,113,113	1.49	10 (13%)
16	CLA	n	505	-	65,73,73	1.51	7 (10%)	76,113,113	1.40	7 (9%)
16	CLA	b	1228	-	55,63,73	1.59	8 (14%)	64,101,113	1.56	9 (14%)
16	CLA	s	504	-	60,68,73	1.53	7 (11%)	70,107,113	1.49	8 (11%)
16	CLA	X	507	-	65,73,73	1.49	8 (12%)	76,113,113	1.40	7 (9%)
16	CLA	t	510	-	65,73,73	1.45	7 (10%)	76,113,113	1.40	8 (10%)
16	CLA	y	502	-	50,58,73	1.66	6 (12%)	58,95,113	1.56	7 (12%)
16	CLA	q	504	-	60,68,73	1.52	6 (10%)	70,107,113	1.48	8 (11%)
16	CLA	H	1402	-	42,49,73	1.80	7 (16%)	48,83,113	1.67	6 (12%)
19	BCR	B	4014	-	41,41,41	1.14	3 (7%)	56,56,56	1.26	5 (8%)
16	CLA	A	1130	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	9 (11%)
16	CLA	B	1224	-	60,68,73	1.47	9 (15%)	70,107,113	1.72	10 (14%)
16	CLA	b	1220	-	54,62,73	1.59	7 (12%)	62,99,113	1.67	10 (16%)
16	CLA	a	1120	-	49,57,73	1.66	7 (14%)	55,93,113	1.70	8 (14%)
16	CLA	A	1138	-	65,73,73	1.44	9 (13%)	76,113,113	1.52	10 (13%)
16	CLA	a	1127	-	65,73,73	1.43	8 (12%)	76,113,113	1.51	7 (9%)
16	CLA	w	516	-	46,54,73	1.75	6 (13%)	53,90,113	1.62	8 (15%)
18	SF4	a	3001	2,1	0,12,12	-	-	-	-	-
19	BCR	A	4007	-	41,41,41	1.12	3 (7%)	56,56,56	1.35	7 (12%)
16	CLA	B	1218	-	55,63,73	1.59	7 (12%)	64,101,113	1.54	7 (10%)
16	CLA	T	1401	-	45,53,73	1.76	8 (17%)	52,89,113	1.68	9 (17%)
14	LMG	a	4201	-	31,31,55	1.02	1 (3%)	39,39,63	1.12	3 (7%)
19	BCR	H	4008	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	8 (14%)
16	CLA	h	513	-	50,58,73	1.69	6 (12%)	58,95,113	1.56	9 (15%)
19	BCR	m	4021	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	5 (8%)
13	LHG	A	851	-	26,26,48	0.85	1 (3%)	29,32,54	1.35	3 (10%)
19	BCR	p	601	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	7 (12%)
16	CLA	q	505	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
16	CLA	b	1216	-	47,55,73	1.75	9 (19%)	54,91,113	1.58	8 (14%)
16	CLA	b	1203	-	65,73,73	1.47	7 (10%)	76,113,113	1.48	8 (10%)
16	CLA	b	1236	-	65,73,73	1.45	7 (10%)	76,113,113	1.47	9 (11%)
16	CLA	o	505	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	8 (10%)
19	BCR	a	4003	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	6 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	A	1109	-	65,73,73	1.46	8 (12%)	76,113,113	1.56	9 (11%)
16	CLA	t	505	-	65,73,73	1.49	7 (10%)	76,113,113	1.38	6 (7%)
16	CLA	L	1502	-	65,73,73	1.46	9 (13%)	76,113,113	1.47	9 (11%)
16	CLA	B	1202	-	65,73,73	1.40	7 (10%)	76,113,113	1.58	9 (11%)
16	CLA	Z	509	-	56,64,73	1.58	7 (12%)	65,102,113	1.55	10 (15%)
16	CLA	W	514	-	50,58,73	1.68	6 (12%)	58,95,113	1.59	10 (17%)
16	CLA	w	511	-	65,73,73	1.47	7 (10%)	76,113,113	1.52	9 (11%)
19	BCR	x	601	-	41,41,41	1.05	2 (4%)	56,56,56	1.30	7 (12%)
16	CLA	p	507	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
16	CLA	y	513	-	50,58,73	1.69	7 (14%)	58,95,113	1.58	10 (17%)
16	CLA	H	1101	-	65,73,73	1.44	7 (10%)	76,113,113	1.49	10 (13%)
16	CLA	G	1228	-	55,63,73	1.59	8 (14%)	64,101,113	1.57	9 (14%)
19	BCR	p	604	-	41,41,41	1.10	2 (4%)	56,56,56	1.27	6 (10%)
14	LMG	a	852	-	38,38,55	0.93	1 (2%)	46,46,63	1.24	4 (8%)
16	CLA	o	507	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
16	CLA	A	1801	-	52,60,73	1.63	7 (13%)	60,97,113	1.57	8 (13%)
16	CLA	Y	507	-	65,73,73	1.49	8 (12%)	76,113,113	1.39	7 (9%)
16	CLA	H	1140	-	65,73,73	1.45	7 (10%)	76,113,113	1.45	7 (9%)
19	BCR	x	604	-	41,41,41	1.04	2 (4%)	56,56,56	1.35	9 (16%)
16	CLA	A	1116	-	54,62,73	1.58	9 (16%)	62,99,113	1.61	9 (14%)
16	CLA	r	507	-	65,73,73	1.46	6 (9%)	76,113,113	1.44	8 (10%)
14	LMG	Y	701	-	39,39,55	0.88	1 (2%)	47,47,63	1.24	3 (6%)
14	LMG	A	4101	-	46,46,55	0.83	1 (2%)	54,54,63	1.31	6 (11%)
16	CLA	t	509	-	60,68,73	1.53	7 (11%)	70,107,113	1.47	9 (12%)
14	LMG	B	848	-	43,43,55	0.80	0	51,51,63	1.31	7 (13%)
16	CLA	A	1022	-	65,73,73	1.54	10 (15%)	76,113,113	1.44	11 (14%)
16	CLA	h	504	-	60,68,73	1.51	7 (11%)	70,107,113	1.52	8 (11%)
16	CLA	X	510	-	65,73,73	1.44	7 (10%)	76,113,113	1.44	9 (11%)
16	CLA	b	1215	-	60,68,73	1.46	7 (11%)	70,107,113	1.58	7 (10%)
19	BCR	b	4010	-	41,41,41	1.16	3 (7%)	56,56,56	1.38	11 (19%)
16	CLA	B	1204	-	65,73,73	1.42	9 (13%)	76,113,113	1.46	8 (10%)
16	CLA	g	503	-	46,54,73	1.77	6 (13%)	53,90,113	1.62	8 (15%)
16	CLA	B	1229	-	58,66,73	1.56	9 (15%)	67,104,113	1.54	10 (14%)
16	CLA	w	501	-	50,58,73	1.69	5 (10%)	58,95,113	1.55	8 (13%)
16	CLA	G	1221	-	65,73,73	1.47	8 (12%)	76,113,113	1.47	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	B	1201	-	54,62,73	1.58	7 (12%)	62,99,113	1.68	9 (14%)
16	CLA	v	514	-	50,58,73	1.69	6 (12%)	58,95,113	1.61	9 (15%)
16	CLA	h	514	-	50,58,73	1.69	6 (12%)	58,95,113	1.59	9 (15%)
16	CLA	B	1205	-	65,73,73	1.44	9 (13%)	76,113,113	1.58	10 (13%)
16	CLA	B	1232	-	45,53,73	1.79	8 (17%)	52,89,113	1.67	7 (13%)
16	CLA	b	1224	-	60,68,73	1.47	8 (13%)	70,107,113	1.73	10 (14%)
16	CLA	G	1202	-	65,73,73	1.42	7 (10%)	76,113,113	1.58	9 (11%)
19	BCR	A	4001	-	41,41,41	1.13	2 (4%)	56,56,56	1.35	9 (16%)
16	CLA	b	1213	-	55,63,73	1.57	7 (12%)	64,101,113	1.54	7 (10%)
16	CLA	G	1227	-	49,57,73	1.69	9 (18%)	55,93,113	1.64	8 (14%)
16	CLA	o	516	-	46,54,73	1.74	6 (13%)	53,90,113	1.61	7 (13%)
16	CLA	A	1237	-	65,73,73	1.48	10 (15%)	76,113,113	1.52	10 (13%)
16	CLA	p	509	-	60,68,73	1.51	7 (11%)	70,107,113	1.49	10 (14%)
19	BCR	B	4005	-	41,41,41	1.13	2 (4%)	56,56,56	1.40	7 (12%)
16	CLA	r	511	-	65,73,73	1.46	5 (7%)	76,113,113	1.48	7 (9%)
16	CLA	B	1208	-	45,53,73	1.75	6 (13%)	52,89,113	1.67	9 (17%)
16	CLA	H	1022	-	65,73,73	1.54	9 (13%)	76,113,113	1.44	11 (14%)
19	BCR	G	4004	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	4 (7%)
16	CLA	H	1134	-	45,53,73	1.77	7 (15%)	52,89,113	1.72	9 (17%)
16	CLA	Z	507	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	6 (7%)
14	LMG	a	4101	-	46,46,55	0.83	1 (2%)	54,54,63	1.32	6 (11%)
16	CLA	r	513	-	50,58,73	1.68	6 (12%)	58,95,113	1.59	8 (13%)
16	CLA	w	505	-	65,73,73	1.48	6 (9%)	76,113,113	1.44	8 (10%)
16	CLA	Y	510	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	9 (11%)
16	CLA	w	509	-	56,64,73	1.57	7 (12%)	65,102,113	1.53	10 (15%)
16	CLA	x	510	-	55,63,73	1.61	6 (10%)	64,101,113	1.48	9 (14%)
16	CLA	q	506	-	60,68,73	1.53	8 (13%)	70,107,113	1.48	8 (11%)
19	BCR	w	602	-	41,41,41	1.05	2 (4%)	56,56,56	1.25	7 (12%)
16	CLA	H	1128	-	65,73,73	1.51	10 (15%)	76,113,113	1.69	11 (14%)
19	BCR	a	4011	-	41,41,41	1.10	2 (4%)	56,56,56	1.35	8 (14%)
16	CLA	X	514	-	50,58,73	1.71	6 (12%)	58,95,113	1.57	8 (13%)
16	CLA	a	1138	-	65,73,73	1.44	9 (13%)	76,113,113	1.53	10 (13%)
16	CLA	Y	502	-	50,58,73	1.65	7 (14%)	58,95,113	1.63	11 (18%)
16	CLA	h	515	-	60,68,73	1.54	6 (10%)	70,107,113	1.50	7 (10%)
16	CLA	o	510	-	65,73,73	1.43	7 (10%)	76,113,113	1.44	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	BCR	l	4022	-	41,41,41	1.09	1 (2%)	56,56,56	1.53	12 (21%)
16	CLA	B	1223	-	65,73,73	1.49	8 (12%)	76,113,113	1.44	8 (10%)
16	CLA	B	1012	-	60,68,73	1.57	10 (16%)	70,107,113	1.51	12 (17%)
16	CLA	g	517	-	55,63,73	1.59	7 (12%)	64,101,113	1.52	8 (12%)
16	CLA	t	503	-	46,54,73	1.71	6 (13%)	53,90,113	1.72	8 (15%)
16	CLA	t	502	-	50,58,73	1.64	6 (12%)	58,95,113	1.68	11 (18%)
16	CLA	x	506	-	60,68,73	1.53	7 (11%)	70,107,113	1.53	9 (12%)
16	CLA	B	1227	-	49,57,73	1.69	9 (18%)	55,93,113	1.64	9 (16%)
19	BCR	B	4009	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	9 (16%)
16	CLA	g	510	-	55,63,73	1.60	6 (10%)	64,101,113	1.52	10 (15%)
16	CLA	a	1112	-	45,53,73	1.70	7 (15%)	52,89,113	1.80	8 (15%)
16	CLA	Y	501	-	50,58,73	1.68	5 (10%)	58,95,113	1.55	9 (15%)
19	BCR	G	4006	-	25,25,41	1.08	2 (8%)	33,33,56	1.41	6 (18%)
16	CLA	B	1220	-	54,62,73	1.59	7 (12%)	62,99,113	1.68	9 (14%)
16	CLA	b	1204	-	65,73,73	1.42	9 (13%)	76,113,113	1.46	8 (10%)
19	BCR	v	601	-	41,41,41	1.03	2 (4%)	56,56,56	1.36	8 (14%)
16	CLA	a	1123	-	65,73,73	1.47	6 (9%)	76,113,113	1.52	9 (11%)
16	CLA	Y	512	-	45,53,73	1.73	6 (13%)	52,89,113	1.77	7 (13%)
16	CLA	y	515	-	60,68,73	1.54	6 (10%)	70,107,113	1.60	9 (12%)
16	CLA	n	516	-	46,54,73	1.75	7 (15%)	53,90,113	1.63	7 (13%)
19	BCR	s	602	-	41,41,41	1.03	2 (4%)	56,56,56	1.37	8 (14%)
16	CLA	W	517	-	55,63,73	1.59	7 (12%)	64,101,113	1.59	10 (15%)
16	CLA	H	1131	-	65,73,73	1.45	8 (12%)	76,113,113	1.53	10 (13%)
16	CLA	o	501	-	50,58,73	1.67	6 (12%)	58,95,113	1.61	9 (15%)
16	CLA	q	516	-	46,54,73	1.77	5 (10%)	53,90,113	1.65	7 (13%)
16	CLA	f	1301	-	45,53,73	1.73	7 (15%)	52,89,113	1.80	8 (15%)
16	CLA	Z	514	-	50,58,73	1.69	7 (14%)	58,95,113	1.60	10 (17%)
16	CLA	g	513	-	50,58,73	1.67	6 (12%)	58,95,113	1.59	8 (13%)
19	BCR	G	4017	-	41,41,41	1.17	2 (4%)	56,56,56	1.31	7 (12%)
16	CLA	p	514	-	50,58,73	1.68	7 (14%)	58,95,113	1.58	10 (17%)
16	CLA	y	501	-	46,54,73	1.75	5 (10%)	53,90,113	1.61	7 (13%)
16	CLA	a	1118	-	55,63,73	1.60	10 (18%)	64,101,113	1.53	7 (10%)
16	CLA	G	1239	-	65,73,73	1.48	9 (13%)	76,113,113	1.47	7 (9%)
16	CLA	X	501	-	50,58,73	1.67	6 (12%)	58,95,113	1.59	9 (15%)
16	CLA	G	1210	-	65,73,73	1.41	8 (12%)	76,113,113	1.90	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	BCR	b	4005	-	41,41,41	1.12	3 (7%)	56,56,56	1.41	7 (12%)
19	BCR	a	4007	-	41,41,41	1.13	3 (7%)	56,56,56	1.35	7 (12%)
16	CLA	t	504	-	60,68,73	1.54	6 (10%)	70,107,113	1.53	9 (12%)
16	CLA	y	512	-	45,53,73	1.73	6 (13%)	52,89,113	1.78	8 (15%)
17	PQN	a	2001	-	34,34,34	0.35	0	42,45,45	1.17	4 (9%)
18	SF4	c	102	3	0,12,12	-	-	-	-	-
16	CLA	x	514	-	50,58,73	1.69	6 (12%)	58,95,113	1.63	7 (12%)
19	BCR	Z	604	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	9 (16%)
16	CLA	H	1104	-	65,73,73	1.47	8 (12%)	76,113,113	1.49	7 (9%)
16	CLA	b	1206	-	65,73,73	1.45	8 (12%)	76,113,113	1.60	8 (10%)
16	CLA	n	507	-	60,68,73	1.56	6 (10%)	70,107,113	1.46	8 (11%)
19	BCR	G	4014	-	41,41,41	1.14	3 (7%)	56,56,56	1.25	5 (8%)
19	BCR	Y	602	-	41,41,41	1.04	2 (4%)	56,56,56	1.37	8 (14%)
19	BCR	B	4006	-	25,25,41	1.08	2 (8%)	33,33,56	1.41	6 (18%)
16	CLA	b	1226	-	65,73,73	1.49	9 (13%)	76,113,113	1.64	9 (11%)
16	CLA	b	1207	-	65,73,73	1.49	8 (12%)	76,113,113	1.48	8 (10%)
16	CLA	a	1135	-	51,59,73	1.61	9 (17%)	59,96,113	1.59	8 (13%)
19	BCR	t	601	-	41,41,41	1.03	2 (4%)	56,56,56	1.33	8 (14%)
16	CLA	y	516	-	46,54,73	1.76	6 (13%)	53,90,113	1.63	7 (13%)
16	CLA	a	1108	-	45,53,73	1.73	7 (15%)	52,89,113	1.71	7 (13%)
16	CLA	a	1133	-	54,62,73	1.60	9 (16%)	62,99,113	1.56	7 (11%)
16	CLA	B	1210	-	65,73,73	1.41	8 (12%)	76,113,113	1.89	12 (15%)
16	CLA	y	508	-	55,63,73	1.62	6 (10%)	64,101,113	1.51	7 (10%)
16	CLA	Y	506	-	60,68,73	1.53	8 (13%)	70,107,113	1.50	9 (12%)
16	CLA	H	1109	-	65,73,73	1.46	8 (12%)	76,113,113	1.56	9 (11%)
19	BCR	B	4010	-	41,41,41	1.17	3 (7%)	56,56,56	1.38	10 (17%)
16	CLA	Z	508	-	55,63,73	1.60	6 (10%)	64,101,113	1.55	8 (12%)
19	BCR	y	601	-	41,41,41	1.03	2 (4%)	56,56,56	1.36	8 (14%)
16	CLA	q	515	-	65,73,73	1.45	6 (9%)	76,113,113	1.47	7 (9%)
19	BCR	y	602	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	7 (12%)
16	CLA	n	513	-	50,58,73	1.68	6 (12%)	58,95,113	1.57	9 (15%)
16	CLA	a	1102	-	56,64,73	1.55	7 (12%)	65,102,113	1.67	9 (13%)
19	BCR	A	4003	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	7 (12%)
16	CLA	p	515	-	65,73,73	1.43	6 (9%)	76,113,113	1.47	8 (10%)
16	CLA	A	1139	-	51,59,73	1.65	8 (15%)	59,96,113	1.60	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	A	1135	-	51,59,73	1.61	9 (17%)	59,96,113	1.59	8 (13%)
16	CLA	r	503	-	46,54,73	1.75	6 (13%)	53,90,113	1.62	8 (15%)
19	BCR	K	1501	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	4 (7%)
16	CLA	t	507	-	60,68,73	1.55	6 (10%)	70,107,113	1.46	8 (11%)
16	CLA	B	1209	-	45,53,73	1.76	6 (13%)	52,89,113	1.66	7 (13%)
16	CLA	X	506	-	60,68,73	1.55	8 (13%)	70,107,113	1.48	8 (11%)
16	CLA	g	515	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	8 (10%)
16	CLA	w	504	-	60,68,73	1.52	7 (11%)	70,107,113	1.48	8 (11%)
19	BCR	j	4013	-	41,41,41	1.07	2 (4%)	56,56,56	1.36	9 (16%)
16	CLA	r	504	-	60,68,73	1.54	7 (11%)	70,107,113	1.47	8 (11%)
16	CLA	b	1238	-	65,73,73	1.47	8 (12%)	76,113,113	1.49	6 (7%)
16	CLA	G	1240	-	50,58,73	1.70	6 (12%)	58,95,113	1.59	8 (13%)
16	CLA	w	514	-	50,58,73	1.70	8 (16%)	58,95,113	1.58	8 (13%)
13	LHG	R	103	-	43,43,48	0.65	1 (2%)	46,49,54	1.26	5 (10%)
16	CLA	r	512	-	45,53,73	1.74	6 (13%)	52,89,113	1.72	7 (13%)
16	CLA	H	1124	-	65,73,73	1.44	9 (13%)	76,113,113	1.46	9 (11%)
16	CLA	j	1302	-	45,53,73	1.76	6 (13%)	52,89,113	1.67	9 (17%)
16	CLA	b	1214	-	55,63,73	1.63	9 (16%)	64,101,113	1.50	10 (15%)
16	CLA	H	1126	-	65,73,73	1.47	9 (13%)	76,113,113	1.52	11 (14%)
16	CLA	G	1204	-	65,73,73	1.42	9 (13%)	76,113,113	1.47	8 (10%)
16	CLA	v	511	-	65,73,73	1.47	6 (9%)	76,113,113	1.49	9 (11%)
16	CLA	g	511	-	65,73,73	1.45	6 (9%)	76,113,113	1.53	7 (9%)
16	CLA	p	511	-	65,73,73	1.46	7 (10%)	76,113,113	1.49	7 (9%)
16	CLA	y	505	-	60,68,73	1.55	6 (10%)	70,107,113	1.46	8 (11%)
16	CLA	v	504	-	60,68,73	1.51	7 (11%)	70,107,113	1.54	8 (11%)
19	BCR	Y	601	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	8 (14%)
19	BCR	G	4009	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	9 (16%)
16	CLA	B	1217	-	45,53,73	1.75	6 (13%)	52,89,113	1.65	6 (11%)
16	CLA	X	509	-	60,68,73	1.52	7 (11%)	70,107,113	1.51	10 (14%)
19	BCR	n	603	-	41,41,41	1.09	3 (7%)	56,56,56	1.31	7 (12%)
16	CLA	u	509	-	60,68,73	1.52	6 (10%)	70,107,113	1.53	10 (14%)
16	CLA	h	507	-	65,73,73	1.48	6 (9%)	76,113,113	1.42	8 (10%)
19	BCR	g	602	-	41,41,41	1.00	2 (4%)	56,56,56	1.34	7 (12%)
19	BCR	i	4018	-	41,41,41	1.15	2 (4%)	56,56,56	1.30	7 (12%)
19	BCR	h	604	-	41,41,41	1.05	2 (4%)	56,56,56	1.34	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	LHG	H	851	-	26,26,48	0.85	1 (3%)	29,32,54	1.35	3 (10%)
16	CLA	o	509	-	60,68,73	1.52	7 (11%)	70,107,113	1.54	10 (14%)
16	CLA	H	1125	-	65,73,73	1.42	8 (12%)	76,113,113	1.55	9 (11%)
16	CLA	X	503	-	46,54,73	1.75	7 (15%)	53,90,113	1.66	8 (15%)
16	CLA	r	506	-	60,68,73	1.50	6 (10%)	70,107,113	1.57	9 (12%)
16	CLA	A	1129	-	50,58,73	1.66	9 (18%)	58,95,113	1.57	10 (17%)
16	CLA	U	1502	-	65,73,73	1.46	9 (13%)	76,113,113	1.47	9 (11%)
16	CLA	a	1109	-	65,73,73	1.45	8 (12%)	76,113,113	1.55	8 (10%)
16	CLA	H	1106	-	65,73,73	1.43	9 (13%)	76,113,113	1.47	10 (13%)
16	CLA	B	1228	-	55,63,73	1.59	8 (14%)	64,101,113	1.55	9 (14%)
16	CLA	G	1214	-	55,63,73	1.64	9 (16%)	64,101,113	1.51	10 (15%)
19	BCR	s	604	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	6 (10%)
16	CLA	w	515	-	65,73,73	1.45	7 (10%)	76,113,113	1.47	7 (9%)
16	CLA	K	1401	-	45,53,73	1.75	8 (17%)	52,89,113	1.67	9 (17%)
14	LMG	G	848	-	43,43,55	0.80	0	51,51,63	1.31	7 (13%)
16	CLA	A	1103	-	65,73,73	1.45	7 (10%)	76,113,113	1.54	8 (10%)
16	CLA	X	508	-	55,63,73	1.58	6 (10%)	64,101,113	1.61	8 (12%)
16	CLA	b	1205	-	65,73,73	1.43	9 (13%)	76,113,113	1.59	10 (13%)
16	CLA	b	1234	-	50,58,73	1.65	9 (18%)	58,95,113	1.67	9 (15%)
19	BCR	I	4018	-	41,41,41	1.13	2 (4%)	56,56,56	1.30	7 (12%)
20	LMT	l	4101	-	36,36,36	1.14	5 (13%)	47,47,47	1.06	4 (8%)
16	CLA	y	510	-	60,68,73	1.51	6 (10%)	70,107,113	1.52	9 (12%)
16	CLA	A	1126	-	65,73,73	1.48	9 (13%)	76,113,113	1.52	11 (14%)
16	CLA	s	507	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
16	CLA	Y	514	-	50,58,73	1.65	7 (14%)	58,95,113	1.65	10 (17%)
16	CLA	b	1218	-	55,63,73	1.60	7 (12%)	64,101,113	1.54	7 (10%)
16	CLA	q	514	-	50,58,73	1.69	8 (16%)	58,95,113	1.61	10 (17%)
16	CLA	y	504	-	60,68,73	1.52	6 (10%)	70,107,113	1.50	8 (11%)
19	BCR	h	601	-	41,41,41	1.03	2 (4%)	56,56,56	1.37	8 (14%)
16	CLA	B	1214	-	55,63,73	1.62	9 (16%)	64,101,113	1.50	10 (15%)
16	CLA	a	1022	-	65,73,73	1.53	10 (15%)	76,113,113	1.43	11 (14%)
16	CLA	Y	517	-	55,63,73	1.58	7 (12%)	64,101,113	1.60	7 (10%)
16	CLA	G	1215	-	60,68,73	1.46	7 (11%)	70,107,113	1.57	8 (11%)
16	CLA	H	1105	-	58,66,73	1.52	6 (10%)	67,104,113	1.57	8 (11%)
16	CLA	t	511	-	65,73,73	1.48	7 (10%)	76,113,113	1.47	7 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	x	517	-	55,63,73	1.59	7 (12%)	64,101,113	1.52	8 (12%)
16	CLA	q	509	-	56,64,73	1.58	7 (12%)	65,102,113	1.52	10 (15%)
18	SF4	H	3001	2,1	0,12,12	-	-	-		
16	CLA	A	1112	-	45,53,73	1.70	6 (13%)	52,89,113	1.80	8 (15%)
16	CLA	o	514	-	50,58,73	1.71	6 (12%)	58,95,113	1.58	8 (13%)
16	CLA	v	513	-	50,58,73	1.70	6 (12%)	58,95,113	1.56	10 (17%)
16	CLA	s	513	-	50,58,73	1.69	6 (12%)	58,95,113	1.58	8 (13%)
16	CLA	w	517	-	55,63,73	1.57	7 (12%)	64,101,113	1.67	10 (15%)
16	CLA	t	516	-	46,54,73	1.74	6 (13%)	53,90,113	1.65	6 (11%)
16	CLA	Y	503	-	46,54,73	1.74	7 (15%)	53,90,113	1.71	7 (13%)
16	CLA	H	1111	-	55,63,73	1.58	10 (18%)	64,101,113	1.54	9 (14%)
16	CLA	t	512	-	45,53,73	1.75	5 (11%)	52,89,113	1.72	7 (13%)
16	CLA	s	506	-	60,68,73	1.53	8 (13%)	70,107,113	1.50	9 (12%)
16	CLA	x	503	-	46,54,73	1.76	6 (13%)	53,90,113	1.61	8 (15%)
19	BCR	g	601	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	7 (12%)
16	CLA	u	514	-	50,58,73	1.71	6 (12%)	58,95,113	1.57	7 (12%)
19	BCR	H	4001	-	41,41,41	1.12	2 (4%)	56,56,56	1.36	9 (16%)
16	CLA	H	1133	-	54,62,73	1.60	9 (16%)	62,99,113	1.55	7 (11%)
16	CLA	u	507	-	65,73,73	1.49	7 (10%)	76,113,113	1.41	7 (9%)
18	SF4	N	102	3	0,12,12	-	-	-		
16	CLA	X	517	-	55,63,73	1.55	7 (12%)	64,101,113	1.78	10 (15%)
16	CLA	a	1140	-	65,73,73	1.44	8 (12%)	76,113,113	1.45	7 (9%)
16	CLA	Q	1302	-	29,35,73	2.67	9 (31%)	28,60,113	1.72	5 (17%)
19	BCR	s	603	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	8 (14%)
19	BCR	y	604	-	41,41,41	1.03	2 (4%)	56,56,56	1.30	5 (8%)
16	CLA	a	1128	-	65,73,73	1.52	10 (15%)	76,113,113	1.70	11 (14%)
16	CLA	Y	508	-	55,63,73	1.60	6 (10%)	64,101,113	1.53	6 (9%)
16	CLA	o	503	-	46,54,73	1.73	7 (15%)	53,90,113	1.66	8 (15%)
16	CLA	w	502	-	50,58,73	1.69	6 (12%)	58,95,113	1.61	9 (15%)
16	CLA	x	508	-	55,63,73	1.61	6 (10%)	64,101,113	1.50	7 (10%)
16	CLA	A	1118	-	55,63,73	1.60	10 (18%)	64,101,113	1.53	7 (10%)
19	BCR	S	4015	-	41,41,41	1.13	3 (7%)	56,56,56	1.32	8 (14%)
16	CLA	W	505	-	65,73,73	1.50	6 (9%)	76,113,113	1.41	7 (9%)
16	CLA	G	1021	-	65,73,73	1.43	8 (12%)	76,113,113	1.58	7 (9%)
17	PQN	A	2001	-	34,34,34	0.35	0	42,45,45	1.17	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	BCR	W	603	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	7 (12%)
16	CLA	u	508	-	55,63,73	1.58	6 (10%)	64,101,113	1.61	8 (12%)
16	CLA	Y	515	-	65,73,73	1.44	6 (9%)	76,113,113	1.48	7 (9%)
16	CLA	u	513	-	50,58,73	1.67	6 (12%)	58,95,113	1.58	8 (13%)
20	LMT	L	4101	-	36,36,36	1.15	5 (13%)	47,47,47	1.06	4 (8%)
16	CLA	H	1113	-	45,53,73	1.71	6 (13%)	52,89,113	1.82	8 (15%)
16	CLA	H	1121	-	51,59,73	1.65	7 (13%)	59,96,113	1.59	8 (13%)
16	CLA	o	508	-	55,63,73	1.57	6 (10%)	64,101,113	1.60	8 (12%)
16	CLA	w	512	-	45,53,73	1.72	7 (15%)	52,89,113	1.76	8 (15%)
16	CLA	B	1213	-	55,63,73	1.58	7 (12%)	64,101,113	1.54	7 (10%)
19	BCR	T	1501	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	4 (7%)
16	CLA	G	1222	-	55,63,73	1.58	9 (16%)	64,101,113	1.57	9 (14%)
19	BCR	q	602	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	7 (12%)
16	CLA	o	515	-	65,73,73	1.44	6 (9%)	76,113,113	1.44	6 (7%)
16	CLA	b	1221	-	65,73,73	1.46	8 (12%)	76,113,113	1.47	8 (10%)
16	CLA	a	1119	-	65,73,73	1.45	7 (10%)	76,113,113	1.48	8 (10%)
16	CLA	p	517	-	55,63,73	1.59	6 (10%)	64,101,113	1.54	7 (10%)
16	CLA	X	515	-	65,73,73	1.44	6 (9%)	76,113,113	1.45	7 (9%)
16	CLA	y	506	-	60,68,73	1.54	7 (11%)	70,107,113	1.54	8 (11%)
19	BCR	j	4012	-	41,41,41	1.14	2 (4%)	56,56,56	1.41	7 (12%)
16	CLA	A	1115	-	54,62,73	1.60	7 (12%)	62,99,113	1.60	8 (12%)
19	BCR	q	601	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	5 (8%)
16	CLA	s	503	-	46,54,73	1.73	7 (15%)	53,90,113	1.66	7 (13%)
16	CLA	W	508	-	55,63,73	1.59	6 (10%)	64,101,113	1.50	8 (12%)
19	BCR	o	601	-	41,41,41	1.08	2 (4%)	56,56,56	1.30	7 (12%)
16	CLA	h	510	-	60,68,73	1.51	6 (10%)	70,107,113	1.54	10 (14%)
16	CLA	L	1501	-	65,73,73	1.45	7 (10%)	76,113,113	1.50	9 (11%)
19	BCR	J	4015	-	41,41,41	1.13	3 (7%)	56,56,56	1.32	8 (14%)
16	CLA	G	1229	-	58,66,73	1.56	9 (15%)	67,104,113	1.54	10 (14%)
16	CLA	A	1102	-	56,64,73	1.56	7 (12%)	65,102,113	1.67	9 (13%)
14	LMG	s	701	-	39,39,55	0.87	1 (2%)	47,47,63	1.24	4 (8%)
16	CLA	a	1110	-	54,62,73	1.60	7 (12%)	62,99,113	1.57	9 (14%)
16	CLA	r	516	-	46,54,73	1.75	5 (10%)	53,90,113	1.70	7 (13%)
16	CLA	a	1129	-	50,58,73	1.66	9 (18%)	58,95,113	1.57	9 (15%)
16	CLA	v	512	-	45,53,73	1.73	6 (13%)	52,89,113	1.81	8 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	BCR	Z	601	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	8 (14%)
19	BCR	w	601	-	41,41,41	1.03	2 (4%)	56,56,56	1.30	5 (8%)
16	CLA	H	1127	-	65,73,73	1.43	8 (12%)	76,113,113	1.52	7 (9%)
16	CLA	H	1132	-	65,73,73	1.45	9 (13%)	76,113,113	1.51	10 (13%)
16	CLA	G	1230	-	45,53,73	1.70	7 (15%)	52,89,113	1.80	8 (15%)
19	BCR	r	601	-	41,41,41	1.04	2 (4%)	56,56,56	1.30	7 (12%)
16	CLA	b	1239	-	65,73,73	1.48	9 (13%)	76,113,113	1.48	7 (9%)
16	CLA	H	1115	-	54,62,73	1.59	7 (12%)	62,99,113	1.60	8 (12%)
16	CLA	u	510	-	65,73,73	1.44	7 (10%)	76,113,113	1.43	8 (10%)
16	CLA	p	513	-	50,58,73	1.69	6 (12%)	58,95,113	1.56	8 (13%)
16	CLA	U	1501	-	65,73,73	1.45	6 (9%)	76,113,113	1.50	9 (11%)
19	BCR	f	4016	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	7 (12%)
17	PQN	b	2002	-	34,34,34	0.36	0	42,45,45	1.17	2 (4%)
16	CLA	n	515	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	9 (11%)
16	CLA	B	1239	-	65,73,73	1.49	8 (12%)	76,113,113	1.48	7 (9%)
16	CLA	y	507	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	8 (10%)
16	CLA	B	1215	-	60,68,73	1.45	7 (11%)	70,107,113	1.57	8 (11%)
16	CLA	H	1120	-	49,57,73	1.65	7 (14%)	55,93,113	1.70	9 (16%)
16	CLA	h	503	-	46,54,73	1.75	6 (13%)	53,90,113	1.62	7 (13%)
16	CLA	H	1116	-	54,62,73	1.58	9 (16%)	62,99,113	1.61	10 (16%)
19	BCR	v	604	-	41,41,41	1.06	2 (4%)	56,56,56	1.23	5 (8%)
16	CLA	G	1218	-	55,63,73	1.59	7 (12%)	64,101,113	1.54	7 (10%)
16	CLA	w	507	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	7 (9%)
16	CLA	B	1236	-	65,73,73	1.44	7 (10%)	76,113,113	1.47	9 (11%)
14	LMG	H	4201	-	32,32,55	1.01	1 (3%)	40,40,63	1.12	3 (7%)
16	CLA	G	1216	-	47,55,73	1.75	10 (21%)	54,91,113	1.59	8 (14%)
19	BCR	L	4019	-	41,41,41	1.18	2 (4%)	56,56,56	1.31	6 (10%)
19	BCR	s	601	-	41,41,41	1.08	2 (4%)	56,56,56	1.36	7 (12%)
18	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
19	BCR	S	4012	-	41,41,41	1.15	2 (4%)	56,56,56	1.40	7 (12%)
16	CLA	A	1013	-	65,73,73	1.43	9 (13%)	76,113,113	1.76	13 (17%)
16	CLA	y	503	-	46,54,73	1.74	6 (13%)	53,90,113	1.64	7 (13%)
16	CLA	r	515	-	65,73,73	1.44	7 (10%)	76,113,113	1.46	8 (10%)
16	CLA	A	1136	-	65,73,73	1.45	8 (12%)	76,113,113	1.48	9 (11%)
16	CLA	F	1301	-	45,53,73	1.74	7 (15%)	52,89,113	1.83	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	BCR	I	4020	-	41,41,41	1.22	3 (7%)	56,56,56	1.25	6 (10%)
19	BCR	U	4019	-	41,41,41	1.18	2 (4%)	56,56,56	1.31	6 (10%)
16	CLA	n	517	-	55,63,73	1.58	6 (10%)	64,101,113	1.60	9 (14%)
16	CLA	A	1133	-	54,62,73	1.60	9 (16%)	62,99,113	1.55	7 (11%)
19	BCR	u	603	-	41,41,41	1.08	2 (4%)	56,56,56	1.30	7 (12%)
16	CLA	b	1235	-	62,70,73	1.47	7 (11%)	72,109,113	1.68	10 (13%)
16	CLA	b	1209	-	45,53,73	1.77	6 (13%)	52,89,113	1.66	8 (15%)
16	CLA	G	1231	-	45,53,73	1.75	7 (15%)	52,89,113	1.77	11 (21%)
16	CLA	W	503	-	46,54,73	1.73	6 (13%)	53,90,113	1.70	8 (15%)
16	CLA	v	508	-	55,63,73	1.63	5 (9%)	64,101,113	1.51	8 (12%)
16	CLA	X	511	-	65,73,73	1.44	6 (9%)	76,113,113	1.55	8 (10%)
16	CLA	a	1402	-	42,49,73	1.81	7 (16%)	48,83,113	1.68	6 (12%)
16	CLA	n	511	-	65,73,73	1.47	7 (10%)	76,113,113	1.46	7 (9%)
16	CLA	H	1013	-	65,73,73	1.43	9 (13%)	76,113,113	1.76	13 (17%)
16	CLA	G	1220	-	54,62,73	1.59	7 (12%)	62,99,113	1.67	9 (14%)
19	BCR	S	4013	-	41,41,41	1.06	2 (4%)	56,56,56	1.36	7 (12%)
16	CLA	q	503	-	46,54,73	1.73	8 (17%)	53,90,113	1.63	8 (15%)
16	CLA	n	510	-	65,73,73	1.44	7 (10%)	76,113,113	1.45	10 (13%)
16	CLA	G	1205	-	65,73,73	1.44	9 (13%)	76,113,113	1.59	10 (13%)
19	BCR	a	4008	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	8 (14%)
16	CLA	A	1121	-	51,59,73	1.65	6 (11%)	59,96,113	1.58	8 (13%)
16	CLA	G	1217	-	45,53,73	1.76	6 (13%)	52,89,113	1.63	6 (11%)
16	CLA	s	508	-	55,63,73	1.59	7 (12%)	64,101,113	1.51	7 (10%)
16	CLA	a	1114	-	49,57,73	1.69	6 (12%)	55,93,113	1.60	8 (14%)
16	CLA	u	506	-	60,68,73	1.55	8 (13%)	70,107,113	1.48	8 (11%)
16	CLA	n	502	-	50,58,73	1.66	6 (12%)	58,95,113	1.58	8 (13%)
16	CLA	h	506	-	60,68,73	1.53	6 (10%)	70,107,113	1.52	8 (11%)
14	LMG	A	852	-	38,38,55	0.92	0	46,46,63	1.24	5 (10%)
19	BCR	x	603	-	41,41,41	1.06	2 (4%)	56,56,56	1.28	8 (14%)
19	BCR	v	602	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	5 (8%)
16	CLA	a	1115	-	54,62,73	1.59	7 (12%)	62,99,113	1.61	8 (12%)
16	CLA	Q	1301	-	45,53,73	1.73	7 (15%)	52,89,113	1.81	8 (15%)
16	CLA	r	509	-	60,68,73	1.52	6 (10%)	70,107,113	1.48	10 (14%)
16	CLA	n	501	-	50,58,73	1.67	5 (10%)	58,95,113	1.56	10 (17%)
19	BCR	X	603	-	41,41,41	1.07	2 (4%)	56,56,56	1.33	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	Z	505	-	65,73,73	1.47	6 (9%)	76,113,113	1.41	7 (9%)
19	BCR	o	603	-	41,41,41	1.08	2 (4%)	56,56,56	1.30	7 (12%)
19	BCR	Z	602	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	6 (10%)
16	CLA	q	512	-	45,53,73	1.72	7 (15%)	52,89,113	1.77	8 (15%)
14	LMG	H	852	-	38,38,55	0.92	1 (2%)	46,46,63	1.24	5 (10%)
16	CLA	Z	517	-	55,63,73	1.56	7 (12%)	64,101,113	1.70	10 (15%)
19	BCR	H	4002	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	5 (8%)
16	CLA	s	516	-	46,54,73	1.74	6 (13%)	53,90,113	1.70	7 (13%)
16	CLA	l	1503	-	65,73,73	1.42	7 (10%)	76,113,113	1.49	9 (11%)
16	CLA	a	1121	-	51,59,73	1.66	6 (11%)	59,96,113	1.59	8 (13%)
16	CLA	A	1114	-	49,57,73	1.69	6 (12%)	55,93,113	1.60	8 (14%)
16	CLA	a	1013	-	65,73,73	1.43	9 (13%)	76,113,113	1.75	13 (17%)
16	CLA	a	1122	-	59,67,73	1.52	8 (13%)	68,105,113	1.50	9 (13%)
19	BCR	G	4010	-	41,41,41	1.16	3 (7%)	56,56,56	1.38	10 (17%)
16	CLA	B	1021	-	65,73,73	1.43	8 (12%)	76,113,113	1.57	7 (9%)
16	CLA	A	1128	-	65,73,73	1.52	10 (15%)	76,113,113	1.69	10 (13%)
16	CLA	B	1212	-	45,53,73	1.73	7 (15%)	52,89,113	1.71	9 (17%)
16	CLA	q	517	-	55,63,73	1.57	7 (12%)	64,101,113	1.68	10 (15%)
16	CLA	a	1130	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	9 (11%)
16	CLA	n	506	-	60,68,73	1.52	6 (10%)	70,107,113	1.47	8 (11%)
16	CLA	W	515	-	65,73,73	1.46	6 (9%)	76,113,113	1.44	9 (11%)
19	BCR	u	602	-	41,41,41	1.02	2 (4%)	56,56,56	1.35	7 (12%)
16	CLA	g	508	-	55,63,73	1.61	6 (10%)	64,101,113	1.49	7 (10%)
16	CLA	G	1224	-	60,68,73	1.48	9 (15%)	70,107,113	1.72	10 (14%)
19	BCR	p	603	-	41,41,41	1.07	2 (4%)	56,56,56	1.36	8 (14%)
16	CLA	s	515	-	65,73,73	1.44	6 (9%)	76,113,113	1.47	8 (10%)
16	CLA	H	1110	-	54,62,73	1.60	7 (12%)	62,99,113	1.58	9 (14%)
16	CLA	p	508	-	55,63,73	1.59	6 (10%)	64,101,113	1.53	8 (12%)
16	CLA	G	1023	-	65,73,73	1.45	10 (15%)	76,113,113	1.78	14 (18%)
16	CLA	a	1103	-	65,73,73	1.45	7 (10%)	76,113,113	1.54	8 (10%)
18	SF4	C	101	3	0,12,12	-	-	-	-	-
19	BCR	M	4021	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	5 (8%)
19	BCR	l	4019	-	41,41,41	1.18	2 (4%)	56,56,56	1.32	6 (10%)
16	CLA	B	1211	-	65,73,73	1.43	7 (10%)	76,113,113	1.49	8 (10%)
16	CLA	B	1222	-	55,63,73	1.58	9 (16%)	64,101,113	1.56	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	LHG	a	849	-	42,42,48	0.67	1 (2%)	45,48,54	1.24	4 (8%)
16	CLA	B	1219	-	45,53,73	1.74	6 (13%)	52,89,113	1.70	8 (15%)
16	CLA	b	1223	-	65,73,73	1.48	8 (12%)	76,113,113	1.44	8 (10%)
19	BCR	R	4018	-	41,41,41	1.15	2 (4%)	56,56,56	1.30	7 (12%)
16	CLA	w	510	-	60,68,73	1.52	6 (10%)	70,107,113	1.47	9 (12%)
19	BCR	b	4009	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	9 (16%)
16	CLA	w	503	-	46,54,73	1.74	8 (17%)	53,90,113	1.63	8 (15%)
16	CLA	t	514	-	50,58,73	1.68	5 (10%)	58,95,113	1.59	9 (15%)
16	CLA	r	510	-	55,63,73	1.60	6 (10%)	64,101,113	1.50	9 (14%)
15	CL0	A	1011	-	65,73,73	1.45	9 (13%)	76,113,113	1.67	14 (18%)
16	CLA	W	504	-	60,68,73	1.55	6 (10%)	70,107,113	1.51	9 (12%)
16	CLA	A	1119	-	65,73,73	1.45	8 (12%)	76,113,113	1.48	8 (10%)
16	CLA	g	502	-	50,58,73	1.67	6 (12%)	58,95,113	1.53	9 (15%)
16	CLA	Y	511	-	65,73,73	1.48	8 (12%)	76,113,113	1.44	8 (10%)
16	CLA	r	514	-	50,58,73	1.67	6 (12%)	58,95,113	1.64	9 (15%)
16	CLA	r	502	-	50,58,73	1.67	6 (12%)	58,95,113	1.56	9 (15%)
16	CLA	s	505	-	65,73,73	1.49	7 (10%)	76,113,113	1.46	8 (10%)
16	CLA	w	506	-	60,68,73	1.53	7 (11%)	70,107,113	1.48	8 (11%)
16	CLA	A	1110	-	54,62,73	1.58	7 (12%)	62,99,113	1.57	9 (14%)
16	CLA	h	516	-	46,54,73	1.75	6 (13%)	53,90,113	1.64	7 (13%)
16	CLA	S	1302	-	45,53,73	1.76	6 (13%)	52,89,113	1.67	9 (17%)
16	CLA	r	501	-	50,58,73	1.68	6 (12%)	58,95,113	1.58	8 (13%)
16	CLA	B	1238	-	65,73,73	1.46	8 (12%)	76,113,113	1.49	6 (7%)
16	CLA	v	510	-	60,68,73	1.51	6 (10%)	70,107,113	1.53	10 (14%)
16	CLA	s	510	-	65,73,73	1.44	7 (10%)	76,113,113	1.47	8 (10%)
16	CLA	a	1106	-	65,73,73	1.43	9 (13%)	76,113,113	1.47	10 (13%)
16	CLA	F	1302	-	29,35,73	2.66	9 (31%)	28,60,113	1.74	6 (21%)
16	CLA	B	1221	-	65,73,73	1.47	8 (12%)	76,113,113	1.47	8 (10%)
16	CLA	g	505	-	46,54,73	1.74	5 (10%)	53,90,113	1.64	8 (15%)
16	CLA	n	509	-	60,68,73	1.53	6 (10%)	70,107,113	1.47	8 (11%)
16	CLA	a	1139	-	51,59,73	1.65	8 (15%)	59,96,113	1.59	8 (13%)
16	CLA	G	1211	-	65,73,73	1.44	7 (10%)	76,113,113	1.49	8 (10%)
16	CLA	Z	503	-	46,54,73	1.74	6 (13%)	53,90,113	1.65	8 (15%)
16	CLA	W	509	-	60,68,73	1.54	6 (10%)	70,107,113	1.45	7 (10%)
16	CLA	v	506	-	60,68,73	1.53	6 (10%)	70,107,113	1.53	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	BCR	a	4002	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	5 (8%)
16	CLA	A	1111	-	55,63,73	1.58	9 (16%)	64,101,113	1.54	9 (14%)
16	CLA	v	501	-	46,54,73	1.74	6 (13%)	53,90,113	1.61	7 (13%)
16	CLA	a	1131	-	65,73,73	1.44	9 (13%)	76,113,113	1.53	10 (13%)
16	CLA	r	517	-	55,63,73	1.59	6 (10%)	64,101,113	1.56	8 (12%)
16	CLA	s	502	-	50,58,73	1.65	7 (14%)	58,95,113	1.60	10 (17%)
16	CLA	h	508	-	55,63,73	1.63	6 (10%)	64,101,113	1.50	7 (10%)
16	CLA	A	1117	-	65,73,73	1.43	7 (10%)	76,113,113	1.50	7 (9%)
16	CLA	G	1212	-	45,53,73	1.72	6 (13%)	52,89,113	1.71	9 (17%)
16	CLA	n	508	-	55,63,73	1.59	6 (10%)	64,101,113	1.51	8 (12%)
19	BCR	A	4011	-	41,41,41	1.11	2 (4%)	56,56,56	1.34	8 (14%)
16	CLA	H	1801	-	52,60,73	1.62	7 (13%)	60,97,113	1.58	8 (13%)
16	CLA	q	501	-	50,58,73	1.70	6 (12%)	58,95,113	1.54	8 (13%)
16	CLA	g	501	-	50,58,73	1.67	5 (10%)	58,95,113	1.58	8 (13%)
13	LHG	i	103	-	43,43,48	0.64	0	46,49,54	1.26	5 (10%)
16	CLA	B	1231	-	45,53,73	1.76	7 (15%)	52,89,113	1.77	11 (21%)
19	BCR	X	604	-	41,41,41	1.04	2 (4%)	56,56,56	1.33	8 (14%)
19	BCR	b	4014	-	41,41,41	1.14	3 (7%)	56,56,56	1.25	5 (8%)
16	CLA	G	1226	-	65,73,73	1.49	10 (15%)	76,113,113	1.63	9 (11%)
16	CLA	A	1125	-	65,73,73	1.42	8 (12%)	76,113,113	1.54	9 (11%)
16	CLA	G	1207	-	65,73,73	1.49	9 (13%)	76,113,113	1.46	8 (10%)
16	CLA	G	1238	-	65,73,73	1.46	7 (10%)	76,113,113	1.50	6 (7%)
16	CLA	G	1232	-	45,53,73	1.81	7 (15%)	52,89,113	1.67	7 (13%)
19	BCR	H	4003	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	7 (12%)
16	CLA	b	1230	-	45,53,73	1.71	7 (15%)	52,89,113	1.79	9 (17%)
16	CLA	H	1122	-	59,67,73	1.53	9 (15%)	68,105,113	1.51	9 (13%)
19	BCR	k	1501	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	5 (8%)
16	CLA	H	1139	-	51,59,73	1.65	8 (15%)	59,96,113	1.59	8 (13%)
19	BCR	h	603	-	41,41,41	1.06	2 (4%)	56,56,56	1.29	6 (10%)
16	CLA	g	507	-	65,73,73	1.47	7 (10%)	76,113,113	1.42	7 (9%)
16	CLA	J	1302	-	45,53,73	1.77	6 (13%)	52,89,113	1.66	9 (17%)
16	CLA	X	502	-	50,58,73	1.67	7 (14%)	58,95,113	1.61	10 (17%)
16	CLA	q	511	-	65,73,73	1.47	7 (10%)	76,113,113	1.51	9 (11%)
16	CLA	v	509	-	60,68,73	1.51	7 (11%)	70,107,113	1.51	9 (12%)
16	CLA	a	1113	-	45,53,73	1.72	7 (15%)	52,89,113	1.82	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	G	1208	-	45,53,73	1.75	6 (13%)	52,89,113	1.68	8 (15%)
19	BCR	A	4008	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	8 (14%)
19	BCR	y	603	-	41,41,41	1.08	2 (4%)	56,56,56	1.36	7 (12%)
16	CLA	b	1023	-	65,73,73	1.45	10 (15%)	76,113,113	1.79	14 (18%)
16	CLA	A	1104	-	65,73,73	1.47	7 (10%)	76,113,113	1.50	7 (9%)
16	CLA	B	1226	-	65,73,73	1.50	10 (15%)	76,113,113	1.63	9 (11%)
16	CLA	Z	516	-	46,54,73	1.75	5 (10%)	53,90,113	1.66	8 (15%)
16	CLA	a	1137	-	47,55,73	1.66	9 (19%)	54,91,113	1.70	8 (14%)
16	CLA	k	1401	-	45,53,73	1.75	8 (17%)	52,89,113	1.68	9 (17%)
16	CLA	n	514	-	50,58,73	1.69	7 (14%)	58,95,113	1.61	10 (17%)
16	CLA	x	511	-	65,73,73	1.46	7 (10%)	76,113,113	1.50	7 (9%)
19	BCR	g	603	-	41,41,41	1.07	2 (4%)	56,56,56	1.32	7 (12%)
16	CLA	t	508	-	55,63,73	1.59	6 (10%)	64,101,113	1.52	8 (12%)
16	CLA	s	514	-	50,58,73	1.67	8 (16%)	58,95,113	1.59	8 (13%)
19	BCR	Z	603	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	7 (12%)
19	BCR	q	604	-	41,41,41	1.08	2 (4%)	56,56,56	1.32	9 (16%)
16	CLA	h	517	-	55,63,73	1.63	6 (10%)	64,101,113	1.51	9 (14%)
19	BCR	o	604	-	41,41,41	1.03	2 (4%)	56,56,56	1.32	8 (14%)
16	CLA	A	1123	-	65,73,73	1.47	6 (9%)	76,113,113	1.52	9 (11%)
16	CLA	s	509	-	60,68,73	1.50	7 (11%)	70,107,113	1.50	10 (14%)
16	CLA	g	504	-	60,68,73	1.54	6 (10%)	70,107,113	1.46	9 (12%)
16	CLA	G	1234	-	50,58,73	1.65	9 (18%)	58,95,113	1.68	9 (15%)
16	CLA	A	1105	-	58,66,73	1.51	6 (10%)	67,104,113	1.57	8 (11%)
19	BCR	B	4017	-	41,41,41	1.17	2 (4%)	56,56,56	1.31	8 (14%)
16	CLA	A	1101	-	65,73,73	1.43	7 (10%)	76,113,113	1.48	10 (13%)
16	CLA	B	1216	-	47,55,73	1.75	10 (21%)	54,91,113	1.60	8 (14%)
16	CLA	B	1203	-	65,73,73	1.46	7 (10%)	76,113,113	1.49	8 (10%)
19	BCR	r	604	-	41,41,41	1.04	2 (4%)	56,56,56	1.33	9 (16%)
16	CLA	W	502	-	50,58,73	1.67	6 (12%)	58,95,113	1.55	8 (13%)
16	CLA	s	501	-	50,58,73	1.69	6 (12%)	58,95,113	1.54	9 (15%)
16	CLA	a	1107	-	50,58,73	1.64	7 (14%)	58,95,113	1.80	9 (15%)
16	CLA	p	502	-	50,58,73	1.65	6 (12%)	58,95,113	1.58	8 (13%)
16	CLA	G	1225	-	65,73,73	1.51	9 (13%)	76,113,113	1.44	9 (11%)
16	CLA	j	1303	-	38,45,73	1.86	6 (15%)	43,78,113	1.77	7 (16%)
16	CLA	A	1140	-	65,73,73	1.44	7 (10%)	76,113,113	1.45	7 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	W	501	-	50,58,73	1.66	5 (10%)	58,95,113	1.57	10 (17%)
16	CLA	a	1136	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	9 (11%)
13	LHG	H	849	-	42,42,48	0.67	1 (2%)	45,48,54	1.23	4 (8%)
16	CLA	p	501	-	50,58,73	1.69	6 (12%)	58,95,113	1.54	9 (15%)
16	CLA	y	514	-	50,58,73	1.69	6 (12%)	58,95,113	1.57	8 (13%)
16	CLA	q	510	-	60,68,73	1.52	6 (10%)	70,107,113	1.48	9 (12%)
16	CLA	t	517	-	55,63,73	1.60	6 (10%)	64,101,113	1.60	10 (15%)
18	SF4	c	101	3	0,12,12	-	-	-	-	-
19	BCR	X	602	-	41,41,41	1.03	2 (4%)	56,56,56	1.35	7 (12%)
16	CLA	S	1303	-	38,45,73	1.87	7 (18%)	43,78,113	1.77	6 (13%)
16	CLA	n	504	-	60,68,73	1.53	6 (10%)	70,107,113	1.54	8 (11%)
16	CLA	u	515	-	65,73,73	1.45	6 (9%)	76,113,113	1.46	6 (7%)
16	CLA	x	501	-	50,58,73	1.68	5 (10%)	58,95,113	1.58	8 (13%)
16	CLA	W	511	-	65,73,73	1.46	7 (10%)	76,113,113	1.53	7 (9%)
16	CLA	H	1129	-	50,58,73	1.66	9 (18%)	58,95,113	1.57	9 (15%)
16	CLA	G	1219	-	45,53,73	1.74	6 (13%)	52,89,113	1.71	9 (17%)
16	CLA	Z	504	-	60,68,73	1.53	6 (10%)	70,107,113	1.45	7 (10%)
16	CLA	b	1227	-	49,57,73	1.69	9 (18%)	55,93,113	1.63	8 (14%)
16	CLA	B	1225	-	65,73,73	1.51	9 (13%)	76,113,113	1.45	9 (11%)
16	CLA	r	508	-	55,63,73	1.60	6 (10%)	64,101,113	1.50	8 (12%)
16	CLA	W	516	-	46,54,73	1.75	6 (13%)	53,90,113	1.62	6 (11%)
16	CLA	B	1023	-	65,73,73	1.45	10 (15%)	76,113,113	1.79	14 (18%)
16	CLA	B	1234	-	50,58,73	1.65	9 (18%)	58,95,113	1.68	9 (15%)
14	LMG	H	4101	-	46,46,55	0.84	1 (2%)	54,54,63	1.32	6 (11%)
16	CLA	b	1229	-	58,66,73	1.56	9 (15%)	67,104,113	1.53	10 (14%)
16	CLA	q	513	-	50,58,73	1.68	6 (12%)	58,95,113	1.57	8 (13%)
19	BCR	b	4004	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	4 (7%)
19	BCR	A	4002	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	5 (8%)
16	CLA	H	1103	-	65,73,73	1.45	7 (10%)	76,113,113	1.55	8 (10%)
16	CLA	b	1210	-	65,73,73	1.41	8 (12%)	76,113,113	1.89	13 (17%)
16	CLA	B	1235	-	62,70,73	1.47	7 (11%)	72,109,113	1.69	10 (13%)
16	CLA	A	1124	-	65,73,73	1.44	9 (13%)	76,113,113	1.46	9 (11%)

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
16	CLA	H	1107	-	1/1/12/20	4/19/97/115	-
16	CLA	u	505	-	1/1/15/20	12/37/115/115	-
19	BCR	H	4011	-	-	16/29/63/63	0/2/2/2
13	LHG	A	849	-	-	12/47/47/53	-
19	BCR	W	601	-	-	13/29/63/63	0/2/2/2
16	CLA	H	1123	-	1/1/15/20	11/37/115/115	-
19	BCR	p	602	-	-	11/29/63/63	0/2/2/2
16	CLA	a	1117	-	1/1/15/20	15/37/115/115	-
16	CLA	W	507	-	1/1/14/20	9/31/109/115	-
16	CLA	b	1212	-	1/1/11/20	6/13/91/115	-
16	CLA	x	505	-	1/1/11/20	9/15/93/115	-
19	BCR	L	4022	-	-	10/29/63/63	0/2/2/2
16	CLA	x	509	-	1/1/14/20	11/31/109/115	-
16	CLA	o	517	-	1/1/13/20	12/25/103/115	-
16	CLA	A	1134	-	1/1/11/20	9/13/91/115	-
16	CLA	A	1402	-	1/1/9/20	0/7/81/115	-
19	BCR	o	602	-	-	11/29/63/63	0/2/2/2
19	BCR	x	602	-	-	13/29/63/63	0/2/2/2
19	BCR	G	4005	-	-	8/29/63/63	0/2/2/2
16	CLA	X	505	-	1/1/15/20	12/37/115/115	-
16	CLA	p	506	-	1/1/14/20	10/31/109/115	-
15	CL0	a	1011	-	3/3/20/25	13/37/135/135	-
16	CLA	H	1112	-	1/1/11/20	8/13/91/115	-
19	BCR	F	4016	-	-	13/29/63/63	0/2/2/2
16	CLA	b	1232	-	1/1/11/20	6/13/91/115	-
16	CLA	a	1125	-	1/1/15/20	12/37/115/115	-
19	BCR	U	4022	-	-	10/29/63/63	0/2/2/2
16	CLA	G	1213	-	1/1/13/20	5/25/103/115	-
19	BCR	b	4006	-	-	6/18/35/63	0/1/1/2
16	CLA	Z	506	-	1/1/14/20	3/31/109/115	-
16	CLA	H	1138	-	1/1/15/20	10/37/115/115	-
16	CLA	b	1211	-	1/1/15/20	9/37/115/115	-
16	CLA	b	1222	-	1/1/13/20	6/25/103/115	-
16	CLA	G	1201	-	1/1/12/20	8/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	J	1303	-	1/1/8/20	0/2/76/115	-
16	CLA	L	1503	-	1/1/15/20	15/37/115/115	-
16	CLA	b	1208	-	1/1/11/20	2/13/91/115	-
16	CLA	b	1217	-	1/1/11/20	6/13/91/115	-
16	CLA	Z	513	-	1/1/12/20	10/19/97/115	-
16	CLA	a	1104	-	1/1/15/20	9/37/115/115	-
19	BCR	J	4012	-	-	11/29/63/63	0/2/2/2
16	CLA	H	1108	-	1/1/11/20	7/13/91/115	-
16	CLA	W	513	-	1/1/12/20	6/19/97/115	-
17	PQN	H	2001	-	-	6/23/43/43	0/2/2/2
19	BCR	B	4004	-	-	9/29/63/63	0/2/2/2
16	CLA	Z	511	-	1/1/15/20	12/37/115/115	-
16	CLA	w	508	-	1/1/13/20	10/25/103/115	-
16	CLA	a	1111	-	1/1/13/20	12/25/103/115	-
16	CLA	v	517	-	1/1/13/20	7/25/103/115	-
16	CLA	s	517	-	1/1/13/20	8/25/103/115	-
19	BCR	a	4001	-	-	12/29/63/63	0/2/2/2
16	CLA	A	1131	-	1/1/15/20	8/37/115/115	-
16	CLA	v	507	-	1/1/15/20	9/37/115/115	-
19	BCR	t	603	-	-	8/29/63/63	0/2/2/2
16	CLA	H	1135	-	1/1/12/20	8/21/99/115	-
16	CLA	Y	505	-	1/1/15/20	14/37/115/115	-
16	CLA	G	1203	-	1/1/15/20	18/37/115/115	-
16	CLA	t	501	-	1/1/12/20	9/19/97/115	-
16	CLA	t	513	-	1/1/12/20	6/19/97/115	-
16	CLA	v	503	-	1/1/11/20	7/15/93/115	-
20	LMT	U	4101	-	-	8/21/61/61	0/2/2/2
16	CLA	X	504	-	1/1/14/20	11/31/109/115	-
16	CLA	H	1130	-	1/1/15/20	4/37/115/115	-
16	CLA	B	1206	-	1/1/15/20	13/37/115/115	-
16	CLA	r	505	-	1/1/11/20	10/15/93/115	-
19	BCR	r	603	-	-	7/29/63/63	0/2/2/2
17	PQN	B	2002	-	-	7/23/43/43	0/2/2/2
19	BCR	r	602	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	G	1012	-	1/1/14/20	16/31/109/115	-
16	CLA	b	1219	-	1/1/11/20	7/13/91/115	-
16	CLA	H	1102	-	1/1/13/20	9/27/105/115	-
19	BCR	b	4017	-	-	9/29/63/63	0/2/2/2
16	CLA	v	515	-	1/1/14/20	7/31/109/115	-
16	CLA	l	1501	-	1/1/15/20	20/37/115/115	-
14	LMG	A	4201	-	-	7/27/47/70	0/1/1/1
16	CLA	u	503	-	1/1/11/20	6/15/93/115	-
16	CLA	o	502	-	1/1/12/20	6/19/97/115	-
19	BCR	Y	604	-	-	11/29/63/63	0/2/2/2
16	CLA	y	517	-	1/1/13/20	6/25/103/115	-
16	CLA	n	512	-	1/1/11/20	6/13/91/115	-
16	CLA	A	1137	-	1/1/11/20	6/16/94/115	-
16	CLA	a	1124	-	1/1/15/20	9/37/115/115	-
16	CLA	p	504	-	1/1/14/20	14/31/109/115	-
19	BCR	u	604	-	-	11/29/63/63	0/2/2/2
16	CLA	a	1126	-	1/1/15/20	14/37/115/115	-
16	CLA	b	1240	-	1/1/12/20	3/19/97/115	-
19	BCR	w	603	-	-	9/29/63/63	0/2/2/2
16	CLA	a	1801	-	1/1/12/20	4/22/100/115	-
16	CLA	q	508	-	1/1/13/20	10/25/103/115	-
16	CLA	W	512	-	1/1/11/20	6/13/91/115	-
16	CLA	t	506	-	1/1/14/20	10/31/109/115	-
16	CLA	x	504	-	1/1/14/20	10/31/109/115	-
16	CLA	u	502	-	1/1/12/20	7/19/97/115	-
19	BCR	i	4020	-	-	14/29/63/63	0/2/2/2
16	CLA	o	511	-	1/1/15/20	11/37/115/115	-
17	PQN	G	2002	-	-	7/23/43/43	0/2/2/2
16	CLA	s	512	-	1/1/11/20	6/13/91/115	-
16	CLA	Y	516	-	1/1/11/20	9/15/93/115	-
16	CLA	u	501	-	1/1/12/20	9/19/97/115	-
16	CLA	g	506	-	1/1/14/20	11/31/109/115	-
19	BCR	Y	603	-	-	8/29/63/63	0/2/2/2
16	CLA	X	513	-	1/1/12/20	9/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	g	512	-	1/1/11/20	7/13/91/115	-
16	CLA	A	1120	-	1/1/11/20	13/18/96/115	-
16	CLA	o	504	-	1/1/14/20	7/31/109/115	-
16	CLA	H	1117	-	1/1/15/20	15/37/115/115	-
16	CLA	H	1136	-	1/1/15/20	5/37/115/115	-
16	CLA	u	512	-	1/1/11/20	7/13/91/115	-
19	BCR	n	601	-	-	11/29/63/63	0/2/2/2
16	CLA	B	1240	-	1/1/12/20	3/19/97/115	-
16	CLA	v	502	-	1/1/12/20	6/19/97/115	-
16	CLA	A	1132	-	1/1/15/20	9/37/115/115	-
16	CLA	p	503	-	1/1/11/20	9/15/93/115	-
19	BCR	u	601	-	-	9/29/63/63	0/2/2/2
16	CLA	g	516	-	1/1/11/20	10/15/93/115	-
16	CLA	W	506	-	1/1/14/20	13/31/109/115	-
16	CLA	u	516	-	1/1/11/20	9/15/93/115	-
16	CLA	G	1209	-	1/1/11/20	5/13/91/115	-
16	CLA	l	1502	-	1/1/15/20	12/37/115/115	-
16	CLA	s	511	-	1/1/15/20	15/37/115/115	-
16	CLA	b	1231	-	1/1/11/20	3/13/91/115	-
13	LHG	a	851	-	-	12/31/31/53	-
16	CLA	v	505	-	1/1/14/20	17/31/109/115	-
16	CLA	A	1122	-	1/1/13/20	12/30/108/115	-
14	LMG	b	848	-	-	18/38/58/70	0/1/1/1
16	CLA	h	502	-	1/1/12/20	6/19/97/115	-
16	CLA	B	1230	-	1/1/11/20	4/13/91/115	-
16	CLA	v	516	-	1/1/11/20	6/15/93/115	-
16	CLA	f	1302	-	1/1/5/20	-	-
16	CLA	Y	513	-	1/1/12/20	6/19/97/115	-
16	CLA	x	513	-	1/1/12/20	8/19/97/115	-
16	CLA	a	1134	-	1/1/11/20	9/13/91/115	-
16	CLA	o	506	-	1/1/14/20	7/31/109/115	-
16	CLA	Z	515	-	1/1/15/20	12/37/115/115	-
16	CLA	x	515	-	1/1/15/20	15/37/115/115	-
16	CLA	b	1225	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	G	1206	-	1/1/15/20	13/37/115/115	-
16	CLA	w	513	-	1/1/12/20	9/19/97/115	-
16	CLA	h	512	-	1/1/11/20	6/13/91/115	-
16	CLA	H	1118	-	1/1/13/20	6/25/103/115	-
16	CLA	o	513	-	1/1/12/20	9/19/97/115	-
16	CLA	a	1116	-	1/1/12/20	9/24/102/115	-
16	CLA	h	511	-	1/1/15/20	16/37/115/115	-
16	CLA	A	1107	-	1/1/12/20	4/19/97/115	-
16	CLA	b	1021	-	1/1/15/20	12/37/115/115	-
19	BCR	v	603	-	-	13/29/63/63	0/2/2/2
16	CLA	u	517	-	1/1/13/20	10/25/103/115	-
16	CLA	H	1114	-	1/1/11/20	7/18/96/115	-
19	BCR	J	4013	-	-	11/29/63/63	0/2/2/2
19	BCR	j	4015	-	-	12/29/63/63	0/2/2/2
16	CLA	G	1223	-	1/1/15/20	14/37/115/115	-
16	CLA	q	502	-	1/1/12/20	8/19/97/115	-
16	CLA	G	1235	-	1/1/14/20	15/34/112/115	-
16	CLA	B	1207	-	1/1/15/20	23/37/115/115	-
16	CLA	Y	509	-	1/1/14/20	15/31/109/115	-
16	CLA	H	1237	-	1/1/15/20	15/37/115/115	-
19	BCR	Q	4016	-	-	13/29/63/63	0/2/2/2
16	CLA	a	1105	-	1/1/13/20	6/29/107/115	-
16	CLA	x	502	-	1/1/12/20	3/19/97/115	-
16	CLA	a	1237	-	1/1/15/20	15/37/115/115	-
16	CLA	A	1113	-	1/1/11/20	7/13/91/115	-
14	LMG	p	701	-	-	10/34/54/70	0/1/1/1
16	CLA	G	1236	-	1/1/15/20	11/37/115/115	-
16	CLA	b	1202	-	1/1/15/20	15/37/115/115	-
16	CLA	p	512	-	1/1/11/20	6/13/91/115	-
16	CLA	h	501	-	1/1/11/20	7/15/93/115	-
16	CLA	b	1201	-	1/1/12/20	8/24/102/115	-
15	CL0	H	1011	-	3/3/20/25	13/37/135/135	-
16	CLA	H	1137	-	1/1/11/20	6/16/94/115	-
16	CLA	y	509	-	1/1/14/20	5/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	g	509	-	1/1/14/20	8/31/109/115	-
16	CLA	H	1119	-	1/1/15/20	15/37/115/115	-
16	CLA	x	512	-	1/1/11/20	7/13/91/115	-
16	CLA	p	505	-	1/1/15/20	11/37/115/115	-
16	CLA	Z	502	-	1/1/12/20	8/19/97/115	-
16	CLA	X	512	-	1/1/11/20	7/13/91/115	-
16	CLA	p	516	-	1/1/11/20	8/15/93/115	-
16	CLA	a	1132	-	1/1/15/20	9/37/115/115	-
16	CLA	Z	501	-	1/1/12/20	6/19/97/115	-
16	CLA	n	503	-	1/1/11/20	9/15/93/115	-
16	CLA	o	512	-	1/1/11/20	7/13/91/115	-
16	CLA	x	516	-	1/1/11/20	9/15/93/115	-
18	SF4	C	102	3	-	-	0/6/5/5
16	CLA	Z	512	-	1/1/11/20	7/13/91/115	-
16	CLA	U	1503	-	1/1/15/20	16/37/115/115	-
16	CLA	u	511	-	1/1/15/20	12/37/115/115	-
16	CLA	u	504	-	1/1/14/20	14/31/109/115	-
16	CLA	y	511	-	1/1/15/20	16/37/115/115	-
19	BCR	V	4021	-	-	7/29/63/63	0/2/2/2
16	CLA	t	515	-	1/1/15/20	16/37/115/115	-
16	CLA	X	516	-	1/1/11/20	9/15/93/115	-
16	CLA	Y	504	-	1/1/14/20	12/31/109/115	-
16	CLA	h	505	-	1/1/14/20	16/31/109/115	-
16	CLA	h	509	-	1/1/14/20	6/31/109/115	-
19	BCR	h	602	-	-	11/29/63/63	0/2/2/2
18	SF4	N	101	3	-	-	0/6/5/5
19	BCR	R	4020	-	-	14/29/63/63	0/2/2/2
16	CLA	A	1106	-	1/1/15/20	17/37/115/115	-
16	CLA	A	1127	-	1/1/15/20	9/37/115/115	-
16	CLA	Z	510	-	1/1/14/20	8/31/109/115	-
16	CLA	q	507	-	1/1/15/20	14/37/115/115	-
16	CLA	p	510	-	1/1/15/20	13/37/115/115	-
16	CLA	b	1012	-	1/1/14/20	16/31/109/115	-
19	BCR	g	604	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	W	510	-	1/1/15/20	10/37/115/115	-
19	BCR	H	4007	-	-	7/29/63/63	0/2/2/2
16	CLA	A	1108	-	1/1/11/20	7/13/91/115	-
19	BCR	X	601	-	-	10/29/63/63	0/2/2/2
19	BCR	w	604	-	-	15/29/63/63	0/2/2/2
16	CLA	x	507	-	1/1/15/20	15/37/115/115	-
19	BCR	q	603	-	-	9/29/63/63	0/2/2/2
13	LHG	I	103	-	-	21/48/48/53	-
16	CLA	g	514	-	1/1/12/20	8/19/97/115	-
16	CLA	a	1101	-	1/1/15/20	15/37/115/115	-
16	CLA	n	505	-	1/1/15/20	12/37/115/115	-
16	CLA	b	1228	-	1/1/13/20	5/25/103/115	-
16	CLA	s	504	-	1/1/14/20	14/31/109/115	-
16	CLA	X	507	-	1/1/15/20	13/37/115/115	-
16	CLA	t	510	-	1/1/15/20	3/37/115/115	-
16	CLA	y	502	-	1/1/12/20	7/19/97/115	-
16	CLA	q	504	-	1/1/14/20	8/31/109/115	-
16	CLA	H	1402	-	1/1/9/20	0/7/81/115	-
19	BCR	B	4014	-	-	13/29/63/63	0/2/2/2
16	CLA	A	1130	-	1/1/15/20	4/37/115/115	-
16	CLA	B	1224	-	1/1/14/20	18/31/109/115	-
16	CLA	b	1220	-	1/1/12/20	7/24/102/115	-
16	CLA	a	1120	-	1/1/11/20	13/18/96/115	-
16	CLA	A	1138	-	1/1/15/20	10/37/115/115	-
16	CLA	a	1127	-	1/1/15/20	9/37/115/115	-
16	CLA	w	516	-	1/1/11/20	8/15/93/115	-
18	SF4	a	3001	2,1	-	-	0/6/5/5
19	BCR	A	4007	-	-	7/29/63/63	0/2/2/2
16	CLA	B	1218	-	1/1/13/20	5/25/103/115	-
16	CLA	T	1401	-	1/1/11/20	3/13/91/115	-
14	LMG	a	4201	-	-	7/26/46/70	0/1/1/1
19	BCR	H	4008	-	-	12/29/63/63	0/2/2/2
16	CLA	h	513	-	1/1/12/20	5/19/97/115	-
19	BCR	m	4021	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LHG	A	851	-	-	12/31/31/53	-
19	BCR	p	601	-	-	12/29/63/63	0/2/2/2
16	CLA	q	505	-	1/1/15/20	17/37/115/115	-
16	CLA	b	1216	-	1/1/11/20	7/16/94/115	-
16	CLA	b	1203	-	1/1/15/20	18/37/115/115	-
16	CLA	b	1236	-	1/1/15/20	11/37/115/115	-
16	CLA	o	505	-	1/1/15/20	12/37/115/115	-
19	BCR	a	4003	-	-	11/29/63/63	0/2/2/2
16	CLA	A	1109	-	1/1/15/20	14/37/115/115	-
16	CLA	t	505	-	1/1/15/20	15/37/115/115	-
16	CLA	L	1502	-	1/1/15/20	12/37/115/115	-
16	CLA	B	1202	-	1/1/15/20	15/37/115/115	-
16	CLA	Z	509	-	1/1/13/20	10/27/105/115	-
16	CLA	W	514	-	1/1/12/20	7/19/97/115	-
16	CLA	w	511	-	1/1/15/20	11/37/115/115	-
19	BCR	x	601	-	-	19/29/63/63	0/2/2/2
16	CLA	p	507	-	1/1/15/20	12/37/115/115	-
16	CLA	y	513	-	1/1/12/20	4/19/97/115	-
16	CLA	H	1101	-	1/1/15/20	15/37/115/115	-
16	CLA	G	1228	-	1/1/13/20	5/25/103/115	-
19	BCR	p	604	-	-	9/29/63/63	0/2/2/2
14	LMG	a	852	-	-	17/33/53/70	0/1/1/1
16	CLA	o	507	-	1/1/15/20	12/37/115/115	-
16	CLA	A	1801	-	1/1/12/20	4/22/100/115	-
16	CLA	Y	507	-	1/1/15/20	11/37/115/115	-
16	CLA	H	1140	-	1/1/15/20	18/37/115/115	-
19	BCR	x	604	-	-	11/29/63/63	0/2/2/2
16	CLA	A	1116	-	1/1/12/20	9/24/102/115	-
16	CLA	r	507	-	1/1/15/20	15/37/115/115	-
14	LMG	Y	701	-	-	10/34/54/70	0/1/1/1
14	LMG	A	4101	-	-	18/41/61/70	0/1/1/1
16	CLA	t	509	-	1/1/14/20	8/31/109/115	-
14	LMG	B	848	-	-	18/38/58/70	0/1/1/1
16	CLA	A	1022	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	h	504	-	1/1/14/20	12/31/109/115	-
16	CLA	X	510	-	1/1/15/20	14/37/115/115	-
16	CLA	b	1215	-	1/1/14/20	17/31/109/115	-
19	BCR	b	4010	-	-	12/29/63/63	0/2/2/2
16	CLA	B	1204	-	1/1/15/20	8/37/115/115	-
16	CLA	g	503	-	1/1/11/20	9/15/93/115	-
16	CLA	B	1229	-	1/1/13/20	11/29/107/115	-
16	CLA	w	501	-	1/1/12/20	5/19/97/115	-
16	CLA	G	1221	-	1/1/15/20	10/37/115/115	-
16	CLA	B	1201	-	1/1/12/20	8/24/102/115	-
16	CLA	v	514	-	1/1/12/20	4/19/97/115	-
16	CLA	h	514	-	1/1/12/20	3/19/97/115	-
16	CLA	B	1205	-	1/1/15/20	10/37/115/115	-
16	CLA	B	1232	-	1/1/11/20	6/13/91/115	-
16	CLA	b	1224	-	1/1/14/20	18/31/109/115	-
16	CLA	G	1202	-	1/1/15/20	15/37/115/115	-
19	BCR	A	4001	-	-	12/29/63/63	0/2/2/2
16	CLA	b	1213	-	1/1/13/20	5/25/103/115	-
16	CLA	G	1227	-	1/1/11/20	10/18/96/115	-
16	CLA	o	516	-	1/1/11/20	9/15/93/115	-
16	CLA	A	1237	-	1/1/15/20	15/37/115/115	-
16	CLA	p	509	-	1/1/14/20	14/31/109/115	-
19	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
16	CLA	r	511	-	1/1/15/20	13/37/115/115	-
16	CLA	B	1208	-	1/1/11/20	2/13/91/115	-
16	CLA	H	1022	-	1/1/15/20	9/37/115/115	-
19	BCR	G	4004	-	-	9/29/63/63	0/2/2/2
16	CLA	H	1134	-	1/1/11/20	9/13/91/115	-
16	CLA	Z	507	-	1/1/15/20	13/37/115/115	-
14	LMG	a	4101	-	-	18/41/61/70	0/1/1/1
16	CLA	r	513	-	1/1/12/20	8/19/97/115	-
16	CLA	w	505	-	1/1/15/20	17/37/115/115	-
16	CLA	Y	510	-	1/1/15/20	12/37/115/115	-
16	CLA	w	509	-	1/1/13/20	12/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	x	510	-	1/1/13/20	12/25/103/115	-
16	CLA	q	506	-	1/1/14/20	5/31/109/115	-
19	BCR	w	602	-	-	9/29/63/63	0/2/2/2
16	CLA	H	1128	-	1/1/15/20	10/37/115/115	-
19	BCR	a	4011	-	-	16/29/63/63	0/2/2/2
16	CLA	X	514	-	1/1/12/20	5/19/97/115	-
16	CLA	a	1138	-	1/1/15/20	10/37/115/115	-
16	CLA	Y	502	-	1/1/12/20	5/19/97/115	-
16	CLA	h	515	-	1/1/14/20	4/31/109/115	-
16	CLA	o	510	-	1/1/15/20	13/37/115/115	-
19	BCR	l	4022	-	-	10/29/63/63	0/2/2/2
16	CLA	B	1223	-	1/1/15/20	14/37/115/115	-
16	CLA	B	1012	-	1/1/14/20	16/31/109/115	-
16	CLA	g	517	-	1/1/13/20	10/25/103/115	-
16	CLA	t	503	-	1/1/11/20	8/15/93/115	-
16	CLA	t	502	-	1/1/12/20	6/19/97/115	-
16	CLA	x	506	-	1/1/14/20	13/31/109/115	-
16	CLA	B	1227	-	1/1/11/20	10/18/96/115	-
19	BCR	B	4009	-	-	13/29/63/63	0/2/2/2
16	CLA	g	510	-	1/1/13/20	9/25/103/115	-
16	CLA	a	1112	-	1/1/11/20	8/13/91/115	-
16	CLA	Y	501	-	1/1/12/20	8/19/97/115	-
19	BCR	G	4006	-	-	6/18/35/63	0/1/1/2
16	CLA	B	1220	-	1/1/12/20	7/24/102/115	-
16	CLA	b	1204	-	1/1/15/20	8/37/115/115	-
19	BCR	v	601	-	-	12/29/63/63	0/2/2/2
16	CLA	a	1123	-	1/1/15/20	11/37/115/115	-
16	CLA	Y	512	-	1/1/11/20	6/13/91/115	-
16	CLA	y	515	-	1/1/14/20	5/31/109/115	-
16	CLA	n	516	-	1/1/11/20	9/15/93/115	-
19	BCR	s	602	-	-	11/29/63/63	0/2/2/2
16	CLA	W	517	-	1/1/13/20	13/25/103/115	-
16	CLA	H	1131	-	1/1/15/20	8/37/115/115	-
16	CLA	o	501	-	1/1/12/20	9/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	q	516	-	1/1/11/20	8/15/93/115	-
16	CLA	f	1301	-	1/1/11/20	5/13/91/115	-
16	CLA	Z	514	-	1/1/12/20	5/19/97/115	-
16	CLA	g	513	-	1/1/12/20	5/19/97/115	-
19	BCR	G	4017	-	-	9/29/63/63	0/2/2/2
16	CLA	p	514	-	1/1/12/20	2/19/97/115	-
16	CLA	y	501	-	1/1/11/20	8/15/93/115	-
16	CLA	a	1118	-	1/1/13/20	6/25/103/115	-
16	CLA	G	1239	-	1/1/15/20	14/37/115/115	-
16	CLA	X	501	-	1/1/12/20	9/19/97/115	-
16	CLA	G	1210	-	1/1/15/20	17/37/115/115	-
19	BCR	b	4005	-	-	8/29/63/63	0/2/2/2
19	BCR	a	4007	-	-	7/29/63/63	0/2/2/2
16	CLA	t	504	-	1/1/14/20	7/31/109/115	-
16	CLA	y	512	-	1/1/11/20	7/13/91/115	-
17	PQN	a	2001	-	-	6/23/43/43	0/2/2/2
19	BCR	Z	604	-	-	16/29/63/63	0/2/2/2
16	CLA	x	514	-	1/1/12/20	8/19/97/115	-
18	SF4	c	102	3	-	-	0/6/5/5
16	CLA	H	1104	-	1/1/15/20	9/37/115/115	-
16	CLA	b	1206	-	1/1/15/20	13/37/115/115	-
16	CLA	n	507	-	1/1/14/20	10/31/109/115	-
19	BCR	G	4014	-	-	13/29/63/63	0/2/2/2
19	BCR	Y	602	-	-	9/29/63/63	0/2/2/2
19	BCR	B	4006	-	-	6/18/35/63	0/1/1/2
16	CLA	b	1226	-	1/1/15/20	9/37/115/115	-
16	CLA	b	1207	-	1/1/15/20	23/37/115/115	-
16	CLA	a	1135	-	1/1/12/20	8/21/99/115	-
19	BCR	t	601	-	-	13/29/63/63	0/2/2/2
16	CLA	y	516	-	1/1/11/20	4/15/93/115	-
16	CLA	a	1108	-	1/1/11/20	7/13/91/115	-
16	CLA	a	1133	-	1/1/12/20	11/24/102/115	-
16	CLA	B	1210	-	1/1/15/20	17/37/115/115	-
16	CLA	y	508	-	1/1/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	Y	506	-	1/1/14/20	11/31/109/115	-
16	CLA	H	1109	-	1/1/15/20	14/37/115/115	-
19	BCR	B	4010	-	-	12/29/63/63	0/2/2/2
16	CLA	Z	508	-	1/1/13/20	10/25/103/115	-
19	BCR	y	601	-	-	11/29/63/63	0/2/2/2
16	CLA	q	515	-	1/1/15/20	12/37/115/115	-
19	BCR	y	602	-	-	13/29/63/63	0/2/2/2
16	CLA	n	513	-	1/1/12/20	6/19/97/115	-
16	CLA	a	1102	-	1/1/13/20	9/27/105/115	-
19	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
16	CLA	p	515	-	1/1/15/20	11/37/115/115	-
16	CLA	A	1139	-	1/1/12/20	8/21/99/115	-
16	CLA	A	1135	-	1/1/12/20	8/21/99/115	-
16	CLA	r	503	-	1/1/11/20	9/15/93/115	-
19	BCR	K	1501	-	-	11/29/63/63	0/2/2/2
16	CLA	t	507	-	1/1/14/20	11/31/109/115	-
16	CLA	B	1209	-	1/1/11/20	5/13/91/115	-
16	CLA	X	506	-	1/1/14/20	8/31/109/115	-
16	CLA	g	515	-	1/1/15/20	14/37/115/115	-
16	CLA	w	504	-	1/1/14/20	5/31/109/115	-
19	BCR	j	4013	-	-	11/29/63/63	0/2/2/2
16	CLA	r	504	-	1/1/14/20	11/31/109/115	-
16	CLA	b	1238	-	1/1/15/20	11/37/115/115	-
16	CLA	G	1240	-	1/1/12/20	3/19/97/115	-
16	CLA	w	514	-	1/1/12/20	6/19/97/115	-
13	LHG	R	103	-	-	21/48/48/53	-
16	CLA	r	512	-	1/1/11/20	7/13/91/115	-
16	CLA	H	1124	-	1/1/15/20	9/37/115/115	-
16	CLA	j	1302	-	1/1/11/20	8/13/91/115	-
16	CLA	b	1214	-	1/1/13/20	12/25/103/115	-
16	CLA	H	1126	-	1/1/15/20	14/37/115/115	-
16	CLA	G	1204	-	1/1/15/20	8/37/115/115	-
16	CLA	v	511	-	1/1/15/20	16/37/115/115	-
16	CLA	g	511	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	p	511	-	1/1/15/20	17/37/115/115	-
16	CLA	y	505	-	1/1/14/20	16/31/109/115	-
16	CLA	v	504	-	1/1/14/20	12/31/109/115	-
19	BCR	Y	601	-	-	13/29/63/63	0/2/2/2
19	BCR	G	4009	-	-	13/29/63/63	0/2/2/2
16	CLA	B	1217	-	1/1/11/20	6/13/91/115	-
16	CLA	X	509	-	1/1/14/20	8/31/109/115	-
19	BCR	n	603	-	-	8/29/63/63	0/2/2/2
16	CLA	u	509	-	1/1/14/20	8/31/109/115	-
16	CLA	h	507	-	1/1/15/20	9/37/115/115	-
19	BCR	g	602	-	-	10/29/63/63	0/2/2/2
19	BCR	i	4018	-	-	14/29/63/63	0/2/2/2
19	BCR	h	604	-	-	13/29/63/63	0/2/2/2
16	CLA	o	509	-	1/1/14/20	8/31/109/115	-
13	LHG	H	851	-	-	12/31/31/53	-
16	CLA	H	1125	-	1/1/15/20	12/37/115/115	-
16	CLA	X	503	-	1/1/11/20	7/15/93/115	-
16	CLA	r	506	-	1/1/14/20	14/31/109/115	-
16	CLA	A	1129	-	1/1/12/20	4/19/97/115	-
16	CLA	U	1502	-	1/1/15/20	12/37/115/115	-
16	CLA	a	1109	-	1/1/15/20	14/37/115/115	-
16	CLA	H	1106	-	1/1/15/20	17/37/115/115	-
16	CLA	B	1228	-	1/1/13/20	5/25/103/115	-
16	CLA	G	1214	-	1/1/13/20	12/25/103/115	-
19	BCR	s	604	-	-	8/29/63/63	0/2/2/2
16	CLA	w	515	-	1/1/15/20	12/37/115/115	-
16	CLA	K	1401	-	1/1/11/20	3/13/91/115	-
14	LMG	G	848	-	-	18/38/58/70	0/1/1/1
16	CLA	A	1103	-	1/1/15/20	17/37/115/115	-
16	CLA	X	508	-	1/1/13/20	11/25/103/115	-
16	CLA	b	1205	-	1/1/15/20	10/37/115/115	-
16	CLA	b	1234	-	1/1/12/20	8/19/97/115	-
19	BCR	I	4018	-	-	14/29/63/63	0/2/2/2
20	LMT	l	4101	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	y	510	-	1/1/14/20	12/31/109/115	-
16	CLA	A	1126	-	1/1/15/20	14/37/115/115	-
16	CLA	s	507	-	1/1/15/20	11/37/115/115	-
16	CLA	Y	514	-	1/1/12/20	3/19/97/115	-
16	CLA	b	1218	-	1/1/13/20	5/25/103/115	-
16	CLA	q	514	-	1/1/12/20	4/19/97/115	-
16	CLA	y	504	-	1/1/14/20	11/31/109/115	-
19	BCR	h	601	-	-	11/29/63/63	0/2/2/2
16	CLA	B	1214	-	1/1/13/20	12/25/103/115	-
16	CLA	a	1022	-	1/1/15/20	9/37/115/115	-
16	CLA	Y	517	-	1/1/13/20	10/25/103/115	-
16	CLA	G	1215	-	1/1/14/20	17/31/109/115	-
16	CLA	H	1105	-	1/1/13/20	6/29/107/115	-
16	CLA	t	511	-	1/1/15/20	15/37/115/115	-
16	CLA	x	517	-	1/1/13/20	9/25/103/115	-
16	CLA	q	509	-	1/1/13/20	10/27/105/115	-
18	SF4	H	3001	2,1	-	-	0/6/5/5
16	CLA	A	1112	-	1/1/11/20	8/13/91/115	-
16	CLA	o	514	-	1/1/12/20	8/19/97/115	-
16	CLA	v	513	-	1/1/12/20	5/19/97/115	-
16	CLA	s	513	-	1/1/12/20	6/19/97/115	-
16	CLA	w	517	-	1/1/13/20	9/25/103/115	-
16	CLA	t	516	-	1/1/11/20	8/15/93/115	-
16	CLA	Y	503	-	1/1/11/20	7/15/93/115	-
16	CLA	H	1111	-	1/1/13/20	12/25/103/115	-
16	CLA	t	512	-	1/1/11/20	6/13/91/115	-
16	CLA	s	506	-	1/1/14/20	12/31/109/115	-
16	CLA	x	503	-	1/1/11/20	9/15/93/115	-
19	BCR	g	601	-	-	16/29/63/63	0/2/2/2
16	CLA	u	514	-	1/1/12/20	5/19/97/115	-
19	BCR	H	4001	-	-	12/29/63/63	0/2/2/2
16	CLA	H	1133	-	1/1/12/20	11/24/102/115	-
16	CLA	u	507	-	1/1/15/20	13/37/115/115	-
18	SF4	N	102	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	X	517	-	1/1/13/20	11/25/103/115	-
16	CLA	a	1140	-	1/1/15/20	18/37/115/115	-
16	CLA	Q	1302	-	1/1/5/20	-	-
19	BCR	s	603	-	-	7/29/63/63	0/2/2/2
19	BCR	y	604	-	-	11/29/63/63	0/2/2/2
16	CLA	a	1128	-	1/1/15/20	10/37/115/115	-
16	CLA	Y	508	-	1/1/13/20	10/25/103/115	-
16	CLA	o	503	-	1/1/11/20	7/15/93/115	-
16	CLA	w	502	-	1/1/12/20	8/19/97/115	-
16	CLA	x	508	-	1/1/13/20	8/25/103/115	-
16	CLA	A	1118	-	1/1/13/20	6/25/103/115	-
19	BCR	S	4015	-	-	12/29/63/63	0/2/2/2
16	CLA	W	505	-	1/1/15/20	15/37/115/115	-
16	CLA	G	1021	-	1/1/15/20	12/37/115/115	-
17	PQN	A	2001	-	-	6/23/43/43	0/2/2/2
19	BCR	W	603	-	-	8/29/63/63	0/2/2/2
16	CLA	u	508	-	1/1/13/20	11/25/103/115	-
16	CLA	Y	515	-	1/1/15/20	12/37/115/115	-
16	CLA	u	513	-	1/1/12/20	9/19/97/115	-
20	LMT	L	4101	-	-	8/21/61/61	0/2/2/2
16	CLA	H	1113	-	1/1/11/20	7/13/91/115	-
16	CLA	H	1121	-	1/1/12/20	13/21/99/115	-
16	CLA	o	508	-	1/1/13/20	11/25/103/115	-
16	CLA	w	512	-	1/1/11/20	7/13/91/115	-
16	CLA	B	1213	-	1/1/13/20	5/25/103/115	-
19	BCR	T	1501	-	-	11/29/63/63	0/2/2/2
16	CLA	G	1222	-	1/1/13/20	6/25/103/115	-
19	BCR	q	602	-	-	8/29/63/63	0/2/2/2
16	CLA	o	515	-	1/1/15/20	10/37/115/115	-
16	CLA	b	1221	-	1/1/15/20	10/37/115/115	-
16	CLA	a	1119	-	1/1/15/20	15/37/115/115	-
16	CLA	p	517	-	1/1/13/20	8/25/103/115	-
16	CLA	X	515	-	1/1/15/20	10/37/115/115	-
16	CLA	y	506	-	1/1/14/20	10/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	j	4012	-	-	11/29/63/63	0/2/2/2
16	CLA	A	1115	-	1/1/12/20	5/24/102/115	-
19	BCR	q	601	-	-	7/29/63/63	0/2/2/2
16	CLA	s	503	-	1/1/11/20	8/15/93/115	-
16	CLA	W	508	-	1/1/13/20	12/25/103/115	-
19	BCR	o	601	-	-	8/29/63/63	0/2/2/2
16	CLA	h	510	-	1/1/14/20	15/31/109/115	-
16	CLA	L	1501	-	1/1/15/20	20/37/115/115	-
19	BCR	J	4015	-	-	12/29/63/63	0/2/2/2
16	CLA	G	1229	-	1/1/13/20	11/29/107/115	-
16	CLA	A	1102	-	1/1/13/20	9/27/105/115	-
16	CLA	r	516	-	1/1/11/20	9/15/93/115	-
16	CLA	a	1110	-	1/1/12/20	4/24/102/115	-
14	LMG	s	701	-	-	9/34/54/70	0/1/1/1
16	CLA	a	1129	-	1/1/12/20	4/19/97/115	-
16	CLA	v	512	-	1/1/11/20	7/13/91/115	-
19	BCR	Z	601	-	-	9/29/63/63	0/2/2/2
19	BCR	w	601	-	-	8/29/63/63	0/2/2/2
16	CLA	H	1127	-	1/1/15/20	9/37/115/115	-
16	CLA	H	1132	-	1/1/15/20	9/37/115/115	-
16	CLA	G	1230	-	1/1/11/20	4/13/91/115	-
19	BCR	r	601	-	-	18/29/63/63	0/2/2/2
16	CLA	b	1239	-	1/1/15/20	14/37/115/115	-
16	CLA	H	1115	-	1/1/12/20	5/24/102/115	-
16	CLA	u	510	-	1/1/15/20	13/37/115/115	-
16	CLA	p	513	-	1/1/12/20	6/19/97/115	-
16	CLA	U	1501	-	1/1/15/20	20/37/115/115	-
19	BCR	f	4016	-	-	13/29/63/63	0/2/2/2
17	PQN	b	2002	-	-	7/23/43/43	0/2/2/2
16	CLA	n	515	-	1/1/15/20	11/37/115/115	-
16	CLA	B	1239	-	1/1/15/20	14/37/115/115	-
16	CLA	y	507	-	1/1/15/20	7/37/115/115	-
16	CLA	B	1215	-	1/1/14/20	17/31/109/115	-
16	CLA	H	1120	-	1/1/11/20	13/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	h	503	-	1/1/11/20	8/15/93/115	-
16	CLA	H	1116	-	1/1/12/20	9/24/102/115	-
19	BCR	v	604	-	-	13/29/63/63	0/2/2/2
16	CLA	G	1218	-	1/1/13/20	5/25/103/115	-
16	CLA	w	507	-	1/1/15/20	14/37/115/115	-
16	CLA	B	1236	-	1/1/15/20	11/37/115/115	-
14	LMG	H	4201	-	-	8/27/47/70	0/1/1/1
16	CLA	G	1216	-	1/1/11/20	7/16/94/115	-
19	BCR	L	4019	-	-	11/29/63/63	0/2/2/2
19	BCR	s	601	-	-	13/29/63/63	0/2/2/2
18	SF4	A	3001	2,1	-	-	0/6/5/5
19	BCR	S	4012	-	-	11/29/63/63	0/2/2/2
16	CLA	A	1013	-	1/1/15/20	16/37/115/115	-
16	CLA	y	503	-	1/1/11/20	9/15/93/115	-
16	CLA	r	515	-	1/1/15/20	13/37/115/115	-
16	CLA	A	1136	-	1/1/15/20	5/37/115/115	-
16	CLA	F	1301	-	1/1/11/20	5/13/91/115	-
19	BCR	I	4020	-	-	14/29/63/63	0/2/2/2
19	BCR	U	4019	-	-	11/29/63/63	0/2/2/2
16	CLA	n	517	-	1/1/13/20	14/25/103/115	-
16	CLA	A	1133	-	1/1/12/20	11/24/102/115	-
19	BCR	u	603	-	-	11/29/63/63	0/2/2/2
16	CLA	b	1235	-	1/1/14/20	15/34/112/115	-
16	CLA	b	1209	-	1/1/11/20	5/13/91/115	-
16	CLA	G	1231	-	1/1/11/20	3/13/91/115	-
16	CLA	W	503	-	1/1/11/20	9/15/93/115	-
16	CLA	v	508	-	1/1/13/20	9/25/103/115	-
16	CLA	n	511	-	1/1/15/20	17/37/115/115	-
16	CLA	a	1402	-	1/1/9/20	0/7/81/115	-
16	CLA	X	511	-	1/1/15/20	13/37/115/115	-
16	CLA	H	1013	-	1/1/15/20	16/37/115/115	-
16	CLA	G	1220	-	1/1/12/20	7/24/102/115	-
19	BCR	S	4013	-	-	11/29/63/63	0/2/2/2
16	CLA	q	503	-	1/1/11/20	9/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	n	510	-	1/1/15/20	12/37/115/115	-
16	CLA	G	1205	-	1/1/15/20	10/37/115/115	-
19	BCR	a	4008	-	-	12/29/63/63	0/2/2/2
16	CLA	A	1121	-	1/1/12/20	13/21/99/115	-
16	CLA	G	1217	-	1/1/11/20	6/13/91/115	-
16	CLA	s	508	-	1/1/13/20	9/25/103/115	-
16	CLA	a	1114	-	1/1/11/20	7/18/96/115	-
16	CLA	u	506	-	1/1/14/20	7/31/109/115	-
16	CLA	n	502	-	1/1/12/20	6/19/97/115	-
16	CLA	h	506	-	1/1/14/20	10/31/109/115	-
14	LMG	A	852	-	-	17/33/53/70	0/1/1/1
19	BCR	x	603	-	-	9/29/63/63	0/2/2/2
19	BCR	v	602	-	-	10/29/63/63	0/2/2/2
16	CLA	a	1115	-	1/1/12/20	5/24/102/115	-
16	CLA	Q	1301	-	1/1/11/20	5/13/91/115	-
16	CLA	r	509	-	1/1/14/20	10/31/109/115	-
16	CLA	n	501	-	1/1/12/20	8/19/97/115	-
19	BCR	X	603	-	-	12/29/63/63	0/2/2/2
16	CLA	Z	505	-	1/1/15/20	18/37/115/115	-
19	BCR	o	603	-	-	12/29/63/63	0/2/2/2
19	BCR	Z	602	-	-	9/29/63/63	0/2/2/2
16	CLA	q	512	-	1/1/11/20	7/13/91/115	-
14	LMG	H	852	-	-	17/33/53/70	0/1/1/1
16	CLA	Z	517	-	1/1/13/20	11/25/103/115	-
19	BCR	H	4002	-	-	8/29/63/63	0/2/2/2
16	CLA	s	516	-	1/1/11/20	9/15/93/115	-
16	CLA	l	1503	-	1/1/15/20	16/37/115/115	-
16	CLA	a	1121	-	1/1/12/20	13/21/99/115	-
16	CLA	A	1114	-	1/1/11/20	7/18/96/115	-
16	CLA	a	1013	-	1/1/15/20	16/37/115/115	-
16	CLA	a	1122	-	1/1/13/20	12/30/108/115	-
19	BCR	G	4010	-	-	12/29/63/63	0/2/2/2
16	CLA	B	1021	-	1/1/15/20	12/37/115/115	-
16	CLA	A	1128	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	1212	-	1/1/11/20	6/13/91/115	-
16	CLA	q	517	-	1/1/13/20	9/25/103/115	-
16	CLA	a	1130	-	1/1/15/20	4/37/115/115	-
16	CLA	n	506	-	1/1/14/20	11/31/109/115	-
16	CLA	W	515	-	1/1/15/20	12/37/115/115	-
19	BCR	u	602	-	-	11/29/63/63	0/2/2/2
16	CLA	g	508	-	1/1/13/20	7/25/103/115	-
16	CLA	G	1224	-	1/1/14/20	18/31/109/115	-
19	BCR	p	603	-	-	7/29/63/63	0/2/2/2
16	CLA	s	515	-	1/1/15/20	11/37/115/115	-
16	CLA	H	1110	-	1/1/12/20	4/24/102/115	-
16	CLA	p	508	-	1/1/13/20	9/25/103/115	-
16	CLA	G	1023	-	1/1/15/20	17/37/115/115	-
16	CLA	a	1103	-	1/1/15/20	17/37/115/115	-
19	BCR	l	4019	-	-	11/29/63/63	0/2/2/2
19	BCR	M	4021	-	-	7/29/63/63	0/2/2/2
18	SF4	C	101	3	-	-	0/6/5/5
16	CLA	B	1211	-	1/1/15/20	9/37/115/115	-
16	CLA	B	1222	-	1/1/13/20	6/25/103/115	-
16	CLA	b	1223	-	1/1/15/20	14/37/115/115	-
16	CLA	B	1219	-	1/1/11/20	7/13/91/115	-
13	LHG	a	849	-	-	12/47/47/53	-
19	BCR	R	4018	-	-	14/29/63/63	0/2/2/2
16	CLA	w	510	-	1/1/14/20	5/31/109/115	-
19	BCR	b	4009	-	-	13/29/63/63	0/2/2/2
16	CLA	w	503	-	1/1/11/20	10/15/93/115	-
16	CLA	t	514	-	1/1/12/20	6/19/97/115	-
16	CLA	r	510	-	1/1/13/20	10/25/103/115	-
15	CL0	A	1011	-	3/3/20/25	13/37/135/135	-
16	CLA	W	504	-	1/1/14/20	6/31/109/115	-
16	CLA	A	1119	-	1/1/15/20	15/37/115/115	-
16	CLA	g	502	-	1/1/12/20	6/19/97/115	-
16	CLA	Y	511	-	1/1/15/20	15/37/115/115	-
16	CLA	r	514	-	1/1/12/20	8/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	r	502	-	1/1/12/20	6/19/97/115	-
16	CLA	s	505	-	1/1/15/20	10/37/115/115	-
16	CLA	w	506	-	1/1/14/20	6/31/109/115	-
16	CLA	A	1110	-	1/1/12/20	4/24/102/115	-
16	CLA	h	516	-	1/1/11/20	6/15/93/115	-
16	CLA	S	1302	-	1/1/11/20	8/13/91/115	-
16	CLA	r	501	-	1/1/12/20	6/19/97/115	-
16	CLA	B	1238	-	1/1/15/20	11/37/115/115	-
16	CLA	v	510	-	1/1/14/20	14/31/109/115	-
16	CLA	s	510	-	1/1/15/20	13/37/115/115	-
16	CLA	a	1106	-	1/1/15/20	17/37/115/115	-
16	CLA	F	1302	-	1/1/5/20	-	-
16	CLA	B	1221	-	1/1/15/20	10/37/115/115	-
16	CLA	g	505	-	1/1/11/20	9/15/93/115	-
16	CLA	n	509	-	1/1/14/20	9/31/109/115	-
16	CLA	a	1139	-	1/1/12/20	8/21/99/115	-
16	CLA	G	1211	-	1/1/15/20	8/37/115/115	-
16	CLA	Z	503	-	1/1/11/20	8/15/93/115	-
16	CLA	W	509	-	1/1/14/20	8/31/109/115	-
16	CLA	v	506	-	1/1/14/20	10/31/109/115	-
19	BCR	a	4002	-	-	8/29/63/63	0/2/2/2
16	CLA	A	1111	-	1/1/13/20	12/25/103/115	-
16	CLA	v	501	-	1/1/11/20	7/15/93/115	-
16	CLA	a	1131	-	1/1/15/20	8/37/115/115	-
16	CLA	r	517	-	1/1/13/20	9/25/103/115	-
16	CLA	s	502	-	1/1/12/20	7/19/97/115	-
16	CLA	h	508	-	1/1/13/20	7/25/103/115	-
16	CLA	A	1117	-	1/1/15/20	15/37/115/115	-
16	CLA	G	1212	-	1/1/11/20	6/13/91/115	-
16	CLA	n	508	-	1/1/13/20	12/25/103/115	-
19	BCR	A	4011	-	-	16/29/63/63	0/2/2/2
16	CLA	H	1801	-	1/1/12/20	4/22/100/115	-
16	CLA	q	501	-	1/1/12/20	5/19/97/115	-
16	CLA	g	501	-	1/1/12/20	11/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LHG	i	103	-	-	21/48/48/53	-
16	CLA	B	1231	-	1/1/11/20	3/13/91/115	-
19	BCR	X	604	-	-	14/29/63/63	0/2/2/2
19	BCR	b	4014	-	-	13/29/63/63	0/2/2/2
16	CLA	G	1226	-	1/1/15/20	9/37/115/115	-
16	CLA	A	1125	-	1/1/15/20	12/37/115/115	-
16	CLA	G	1207	-	1/1/15/20	23/37/115/115	-
16	CLA	G	1238	-	1/1/15/20	11/37/115/115	-
16	CLA	G	1232	-	1/1/11/20	6/13/91/115	-
19	BCR	H	4003	-	-	12/29/63/63	0/2/2/2
16	CLA	b	1230	-	1/1/11/20	4/13/91/115	-
16	CLA	H	1122	-	1/1/13/20	12/30/108/115	-
19	BCR	k	1501	-	-	11/29/63/63	0/2/2/2
16	CLA	H	1139	-	1/1/12/20	8/21/99/115	-
19	BCR	h	603	-	-	14/29/63/63	0/2/2/2
16	CLA	g	507	-	1/1/15/20	15/37/115/115	-
16	CLA	J	1302	-	1/1/11/20	8/13/91/115	-
16	CLA	X	502	-	1/1/12/20	5/19/97/115	-
16	CLA	q	511	-	1/1/15/20	12/37/115/115	-
16	CLA	v	509	-	1/1/14/20	7/31/109/115	-
16	CLA	a	1113	-	1/1/11/20	7/13/91/115	-
16	CLA	G	1208	-	1/1/11/20	2/13/91/115	-
19	BCR	A	4008	-	-	12/29/63/63	0/2/2/2
19	BCR	y	603	-	-	10/29/63/63	0/2/2/2
16	CLA	b	1023	-	1/1/15/20	17/37/115/115	-
16	CLA	A	1104	-	1/1/15/20	9/37/115/115	-
16	CLA	B	1226	-	1/1/15/20	9/37/115/115	-
16	CLA	Z	516	-	1/1/11/20	8/15/93/115	-
16	CLA	a	1137	-	1/1/11/20	6/16/94/115	-
16	CLA	k	1401	-	1/1/11/20	3/13/91/115	-
16	CLA	n	514	-	1/1/12/20	6/19/97/115	-
16	CLA	x	511	-	1/1/15/20	10/37/115/115	-
19	BCR	g	603	-	-	8/29/63/63	0/2/2/2
16	CLA	t	508	-	1/1/13/20	12/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	s	514	-	1/1/12/20	1/19/97/115	-
19	BCR	Z	603	-	-	10/29/63/63	0/2/2/2
19	BCR	q	604	-	-	17/29/63/63	0/2/2/2
16	CLA	h	517	-	1/1/13/20	6/25/103/115	-
19	BCR	o	604	-	-	14/29/63/63	0/2/2/2
16	CLA	A	1123	-	1/1/15/20	11/37/115/115	-
16	CLA	s	509	-	1/1/14/20	16/31/109/115	-
16	CLA	g	504	-	1/1/14/20	10/31/109/115	-
16	CLA	G	1234	-	1/1/12/20	8/19/97/115	-
16	CLA	A	1105	-	1/1/13/20	6/29/107/115	-
19	BCR	B	4017	-	-	9/29/63/63	0/2/2/2
16	CLA	A	1101	-	1/1/15/20	15/37/115/115	-
16	CLA	B	1216	-	1/1/11/20	7/16/94/115	-
16	CLA	B	1203	-	1/1/15/20	18/37/115/115	-
19	BCR	r	604	-	-	11/29/63/63	0/2/2/2
16	CLA	W	502	-	1/1/12/20	6/19/97/115	-
16	CLA	s	501	-	1/1/12/20	6/19/97/115	-
16	CLA	a	1107	-	1/1/12/20	4/19/97/115	-
16	CLA	p	502	-	1/1/12/20	4/19/97/115	-
16	CLA	G	1225	-	1/1/15/20	13/37/115/115	-
16	CLA	j	1303	-	1/1/8/20	0/2/76/115	-
16	CLA	A	1140	-	1/1/15/20	18/37/115/115	-
16	CLA	W	501	-	1/1/12/20	8/19/97/115	-
16	CLA	a	1136	-	1/1/15/20	5/37/115/115	-
13	LHG	H	849	-	-	12/47/47/53	-
16	CLA	p	501	-	1/1/12/20	6/19/97/115	-
16	CLA	y	514	-	1/1/12/20	4/19/97/115	-
16	CLA	q	510	-	1/1/14/20	5/31/109/115	-
16	CLA	t	517	-	1/1/13/20	15/25/103/115	-
19	BCR	X	602	-	-	11/29/63/63	0/2/2/2
18	SF4	c	101	3	-	-	0/6/5/5
16	CLA	S	1303	-	1/1/8/20	0/2/76/115	-
16	CLA	n	504	-	1/1/14/20	11/31/109/115	-
16	CLA	u	515	-	1/1/15/20	10/37/115/115	-
16	CLA	x	501	-	1/1/12/20	7/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	W	511	-	1/1/15/20	16/37/115/115	-
16	CLA	H	1129	-	1/1/12/20	4/19/97/115	-
16	CLA	G	1219	-	1/1/11/20	7/13/91/115	-
16	CLA	Z	504	-	1/1/14/20	6/31/109/115	-
16	CLA	b	1227	-	1/1/11/20	10/18/96/115	-
16	CLA	B	1225	-	1/1/15/20	13/37/115/115	-
16	CLA	r	508	-	1/1/13/20	9/25/103/115	-
16	CLA	W	516	-	1/1/11/20	8/15/93/115	-
16	CLA	B	1023	-	1/1/15/20	17/37/115/115	-
16	CLA	B	1234	-	1/1/12/20	8/19/97/115	-
16	CLA	q	513	-	1/1/12/20	9/19/97/115	-
16	CLA	b	1229	-	1/1/13/20	11/29/107/115	-
14	LMG	H	4101	-	-	18/41/61/70	0/1/1/1
19	BCR	b	4004	-	-	9/29/63/63	0/2/2/2
19	BCR	A	4002	-	-	8/29/63/63	0/2/2/2
16	CLA	H	1103	-	1/1/15/20	17/37/115/115	-
16	CLA	b	1210	-	1/1/15/20	17/37/115/115	-
16	CLA	B	1235	-	1/1/14/20	15/34/112/115	-
16	CLA	A	1124	-	1/1/15/20	9/37/115/115	-

The worst 5 of 4506 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Z	502	CLA	C4B-NB	7.97	1.42	1.35
16	w	502	CLA	C4B-NB	7.71	1.42	1.35
16	G	1240	CLA	C4B-NB	7.64	1.42	1.35
16	h	508	CLA	C4B-NB	7.61	1.42	1.35
16	v	508	CLA	C4B-NB	7.60	1.42	1.35

The worst 5 of 6092 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	1021	CLA	C4A-NA-C1A	9.35	110.91	106.71
16	b	1021	CLA	C4A-NA-C1A	9.33	110.90	106.71
16	B	1021	CLA	C4A-NA-C1A	9.32	110.89	106.71
16	G	1205	CLA	C4A-NA-C1A	8.51	110.53	106.71
16	b	1205	CLA	C4A-NA-C1A	8.48	110.52	106.71

5 of 597 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	A	1011	CL0	NA
15	A	1011	CL0	ND
15	A	1011	CL0	NC
15	a	1011	CL0	NA
15	a	1011	CL0	ND

5 of 7516 torsion outliers are listed below:

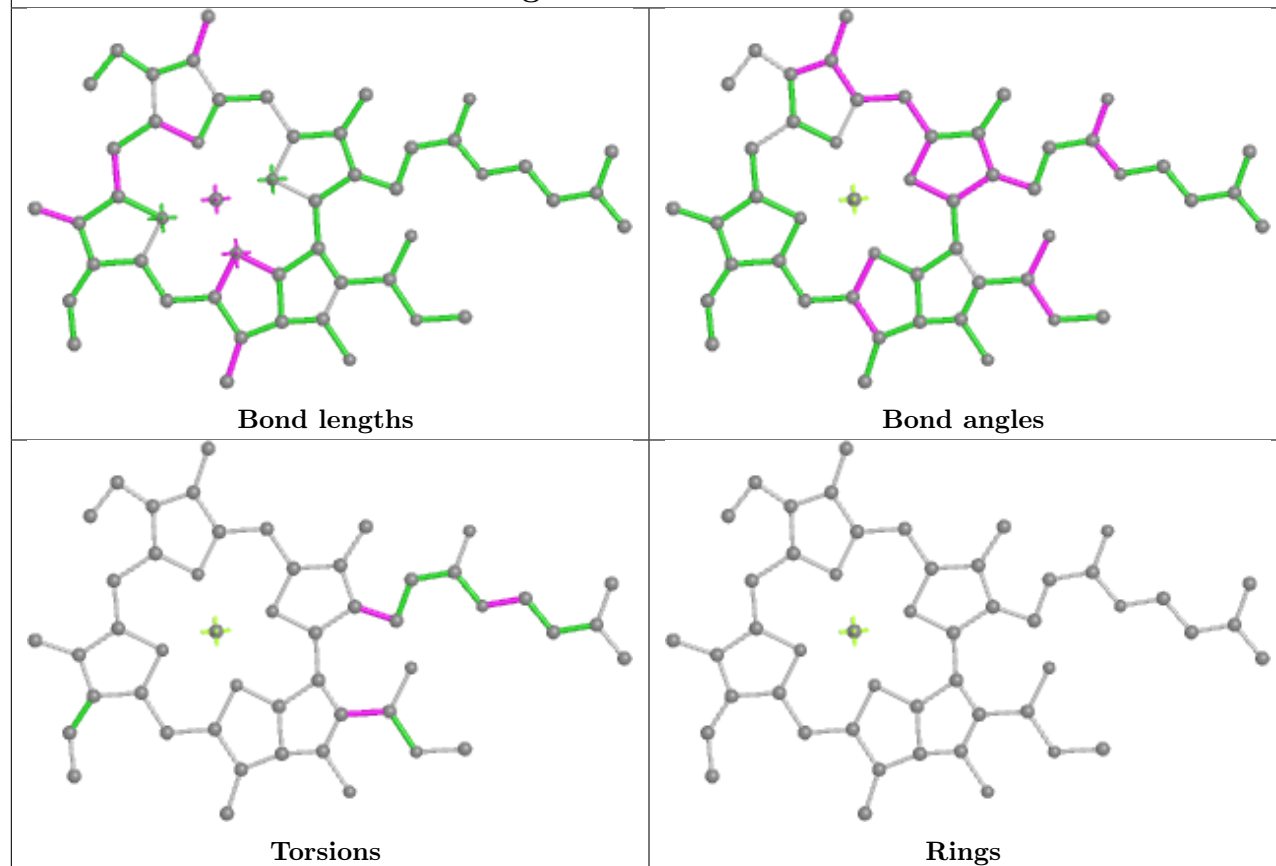
Mol	Chain	Res	Type	Atoms
13	A	849	LHG	C3-O3-P-O4
13	A	849	LHG	C3-O3-P-O6
13	A	851	LHG	O1-C1-C2-C3
13	A	851	LHG	C1-C2-C3-O3
13	A	851	LHG	C3-O3-P-O5

There are no ring outliers.

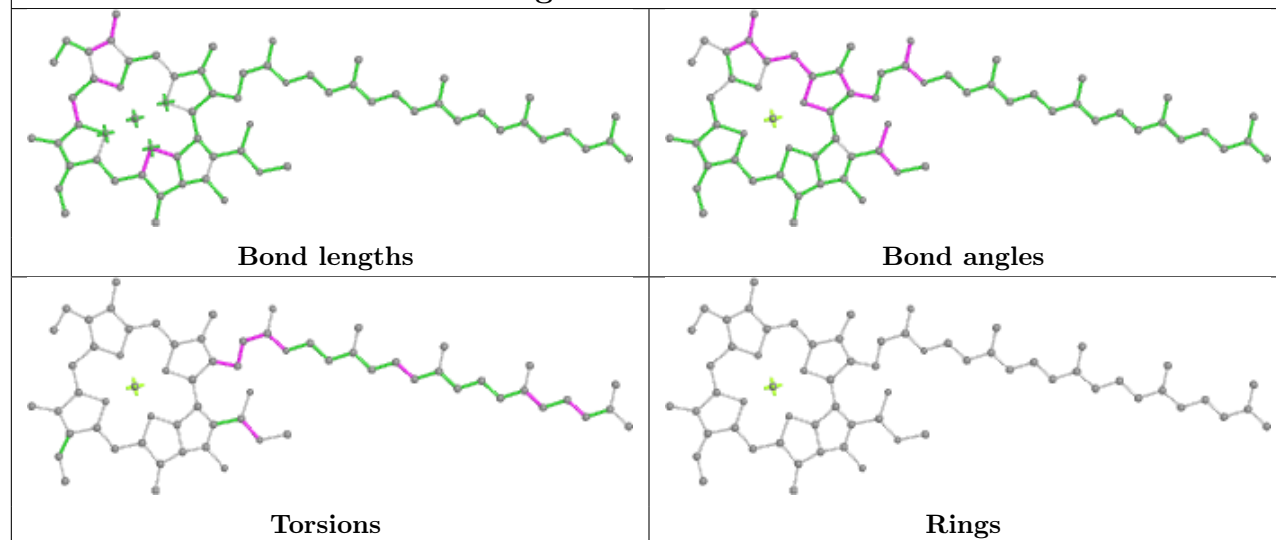
No monomer is involved in short contacts.

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

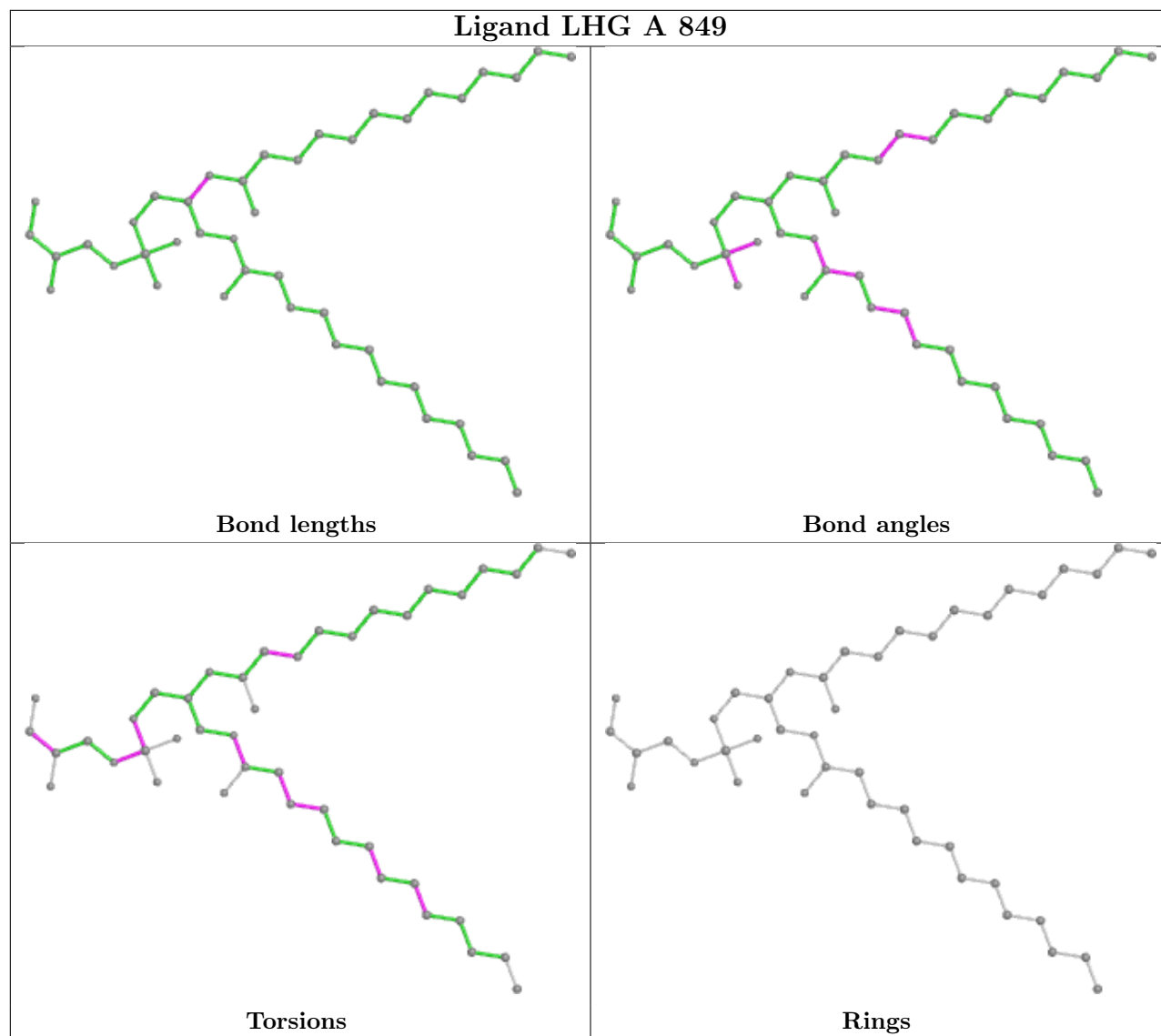
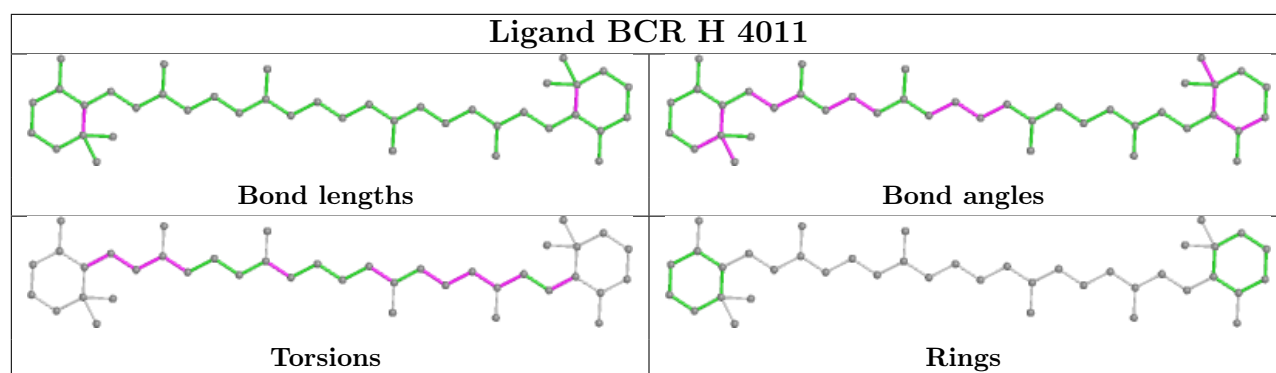
## Ligand CLA H 1107

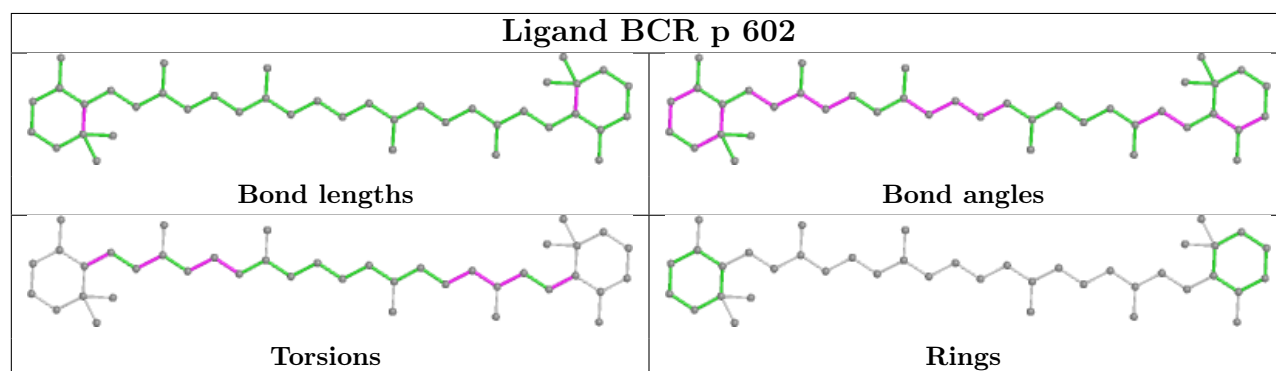
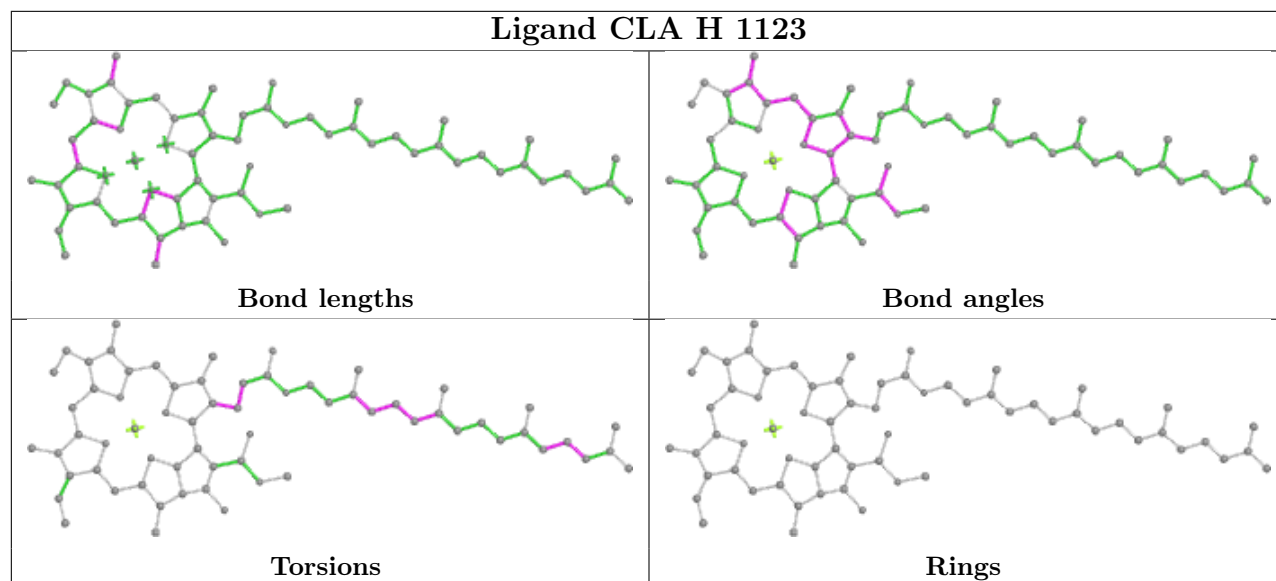
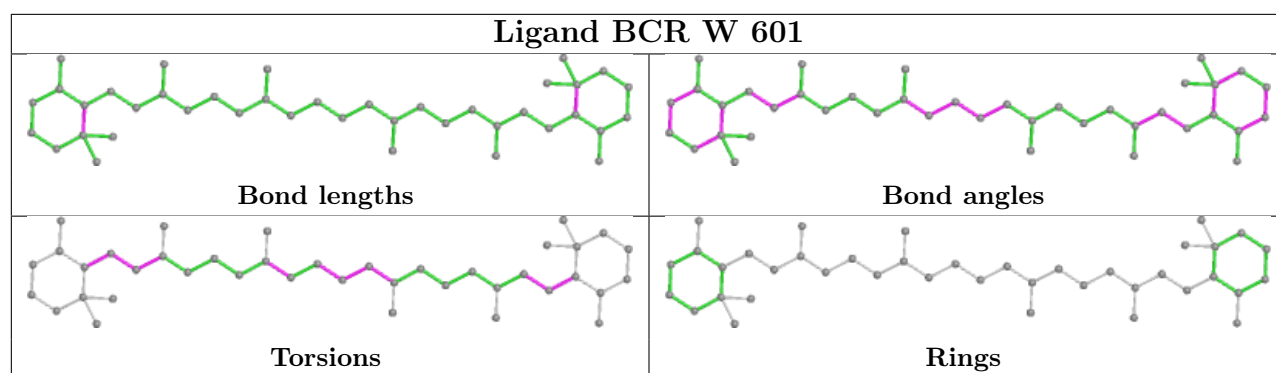


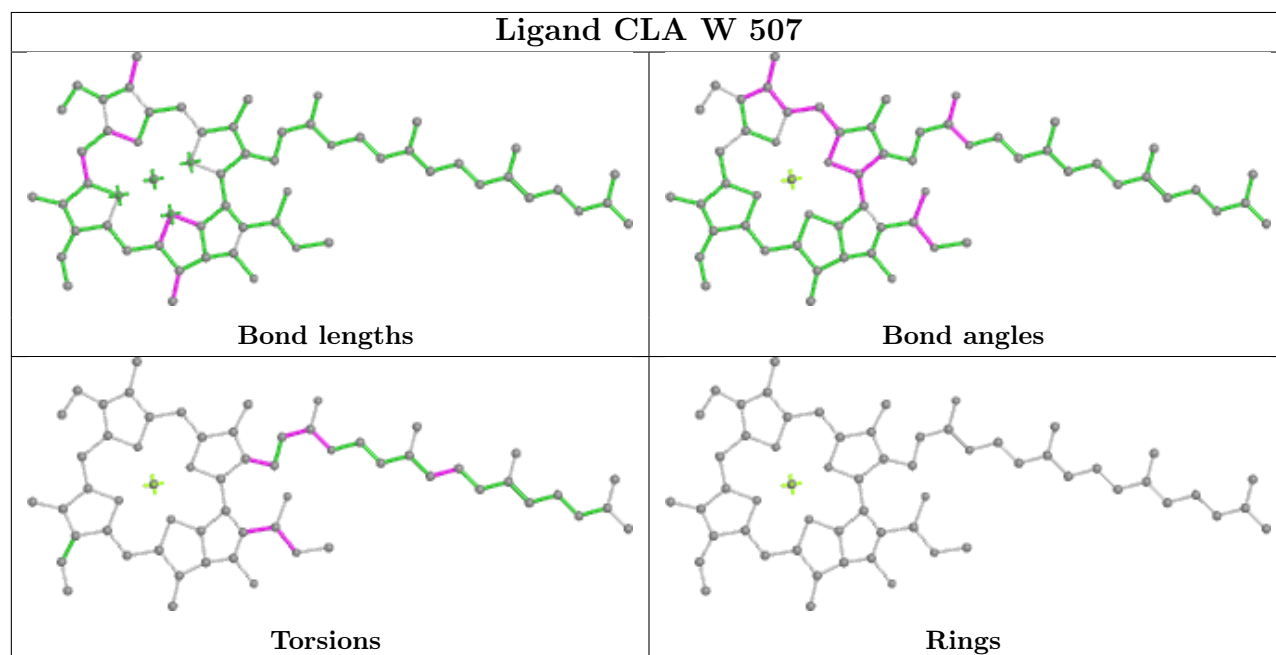
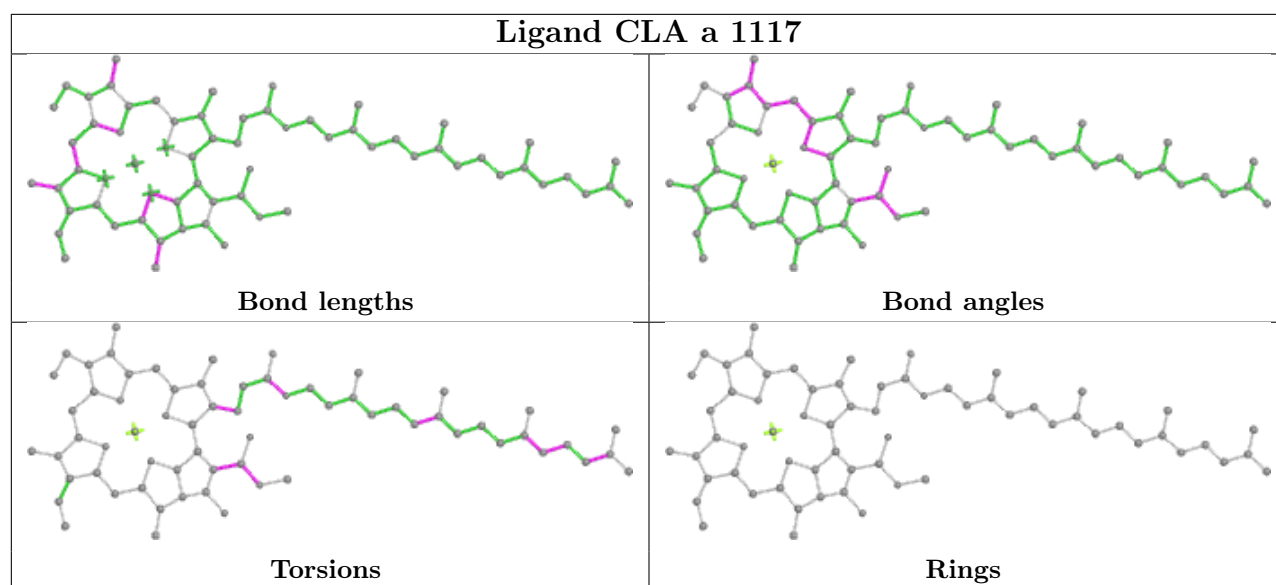
## Ligand CLA u 505

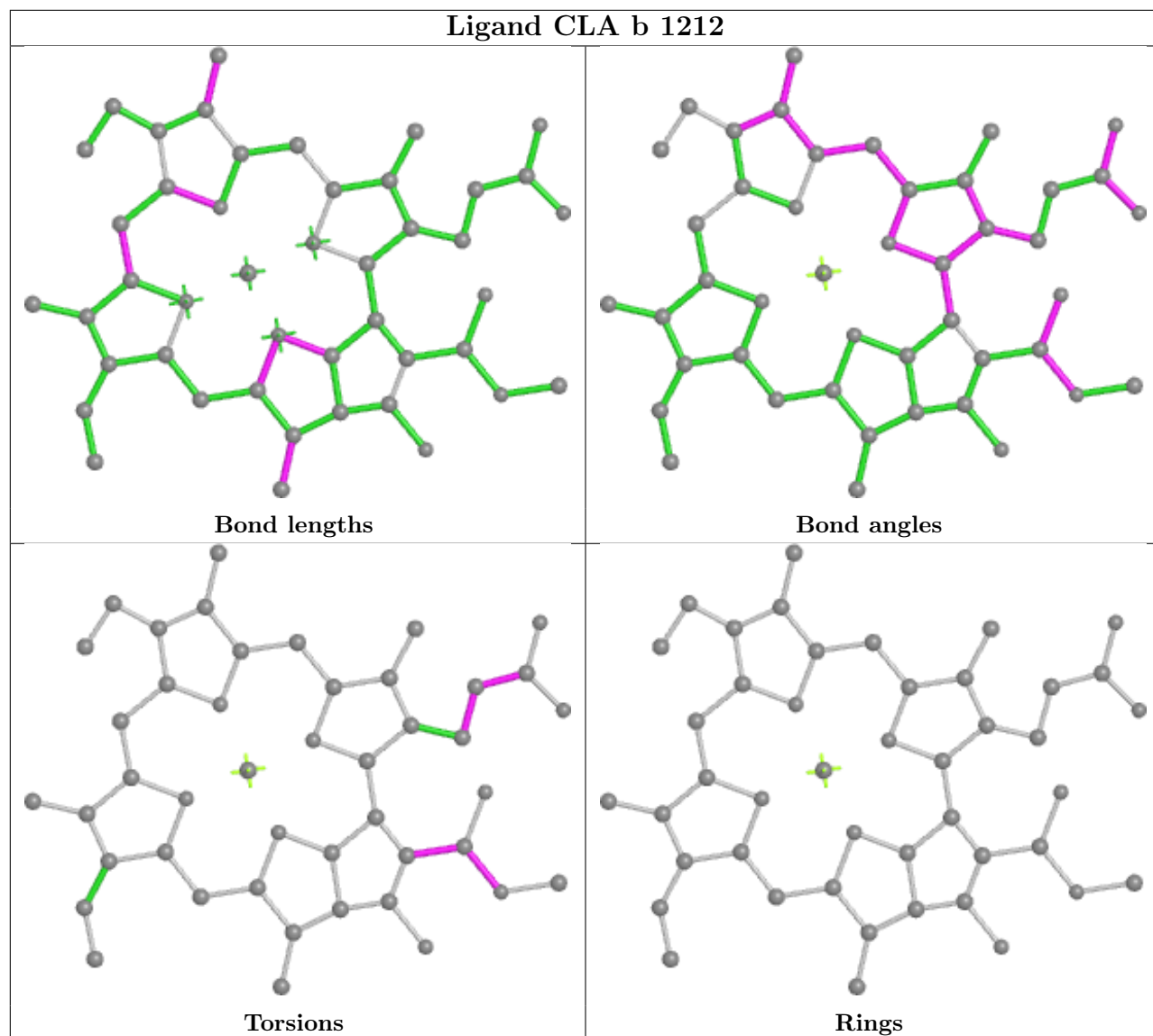




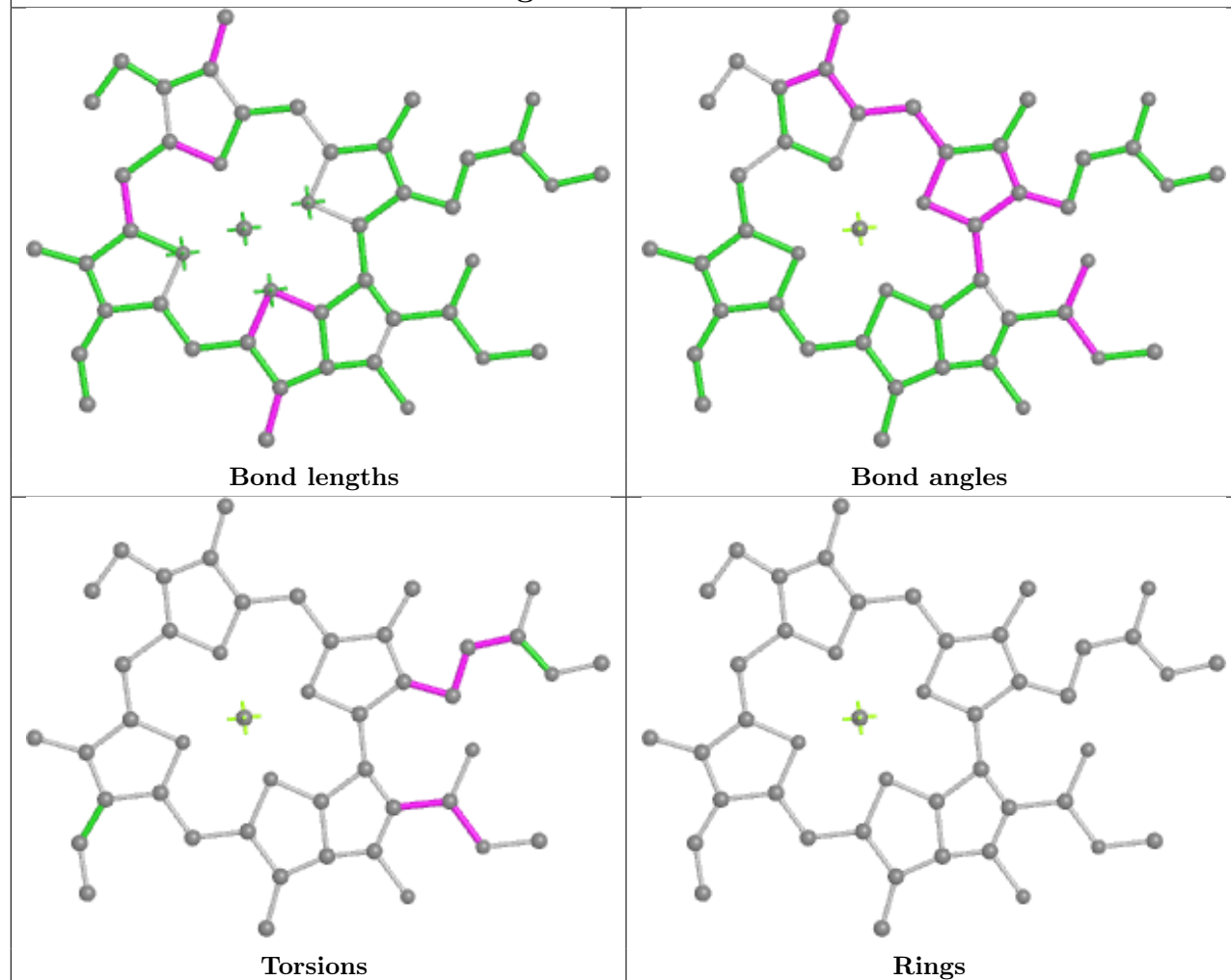




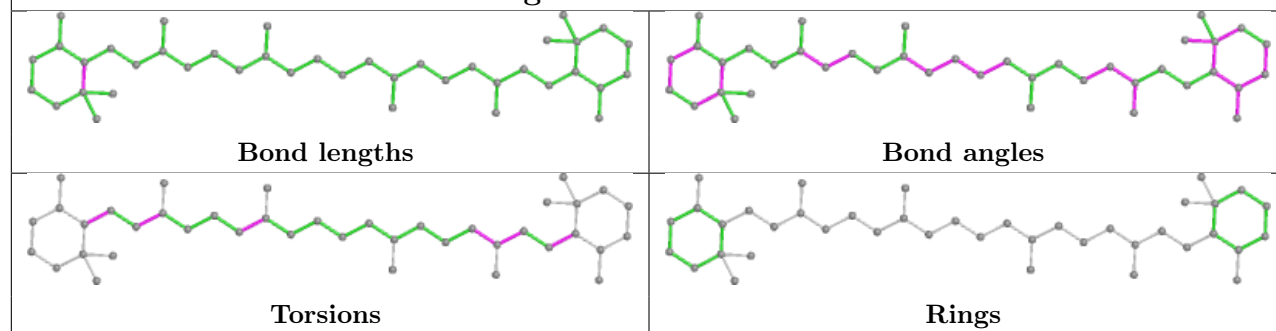




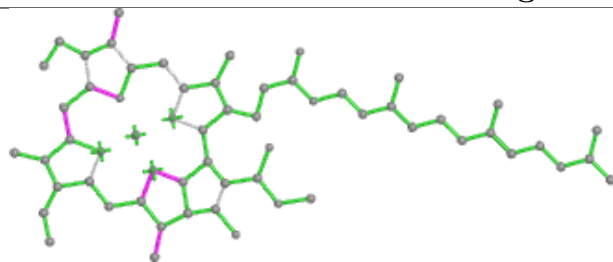
## Ligand CLA x 505



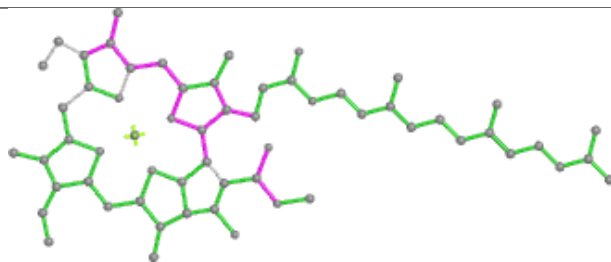
## Ligand BCR L 4022



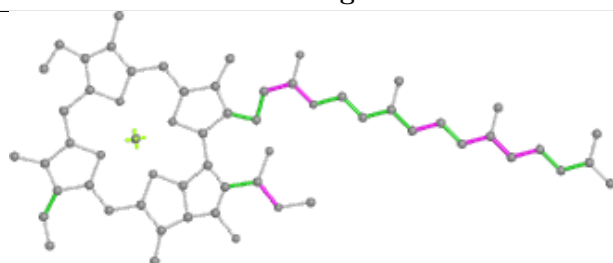
## Ligand CLA x 509



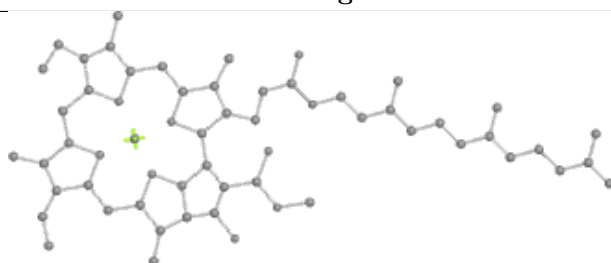
Bond lengths



Bond angles

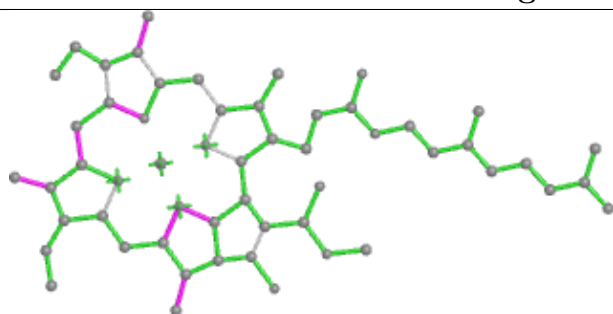


Torsions

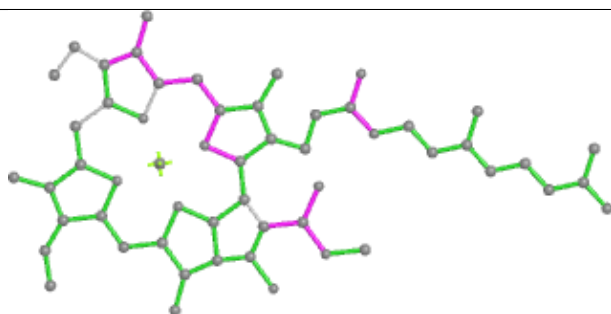


Rings

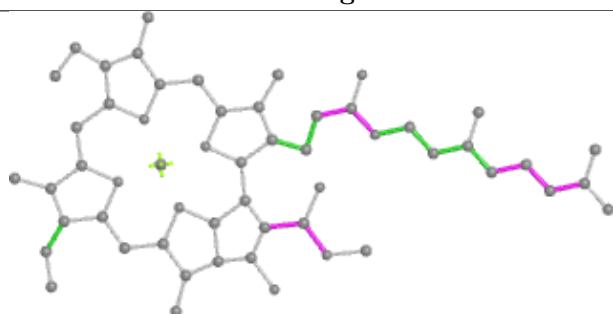
## Ligand CLA o 517



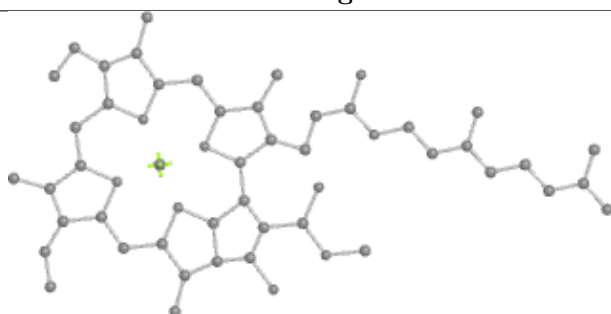
Bond lengths



Bond angles

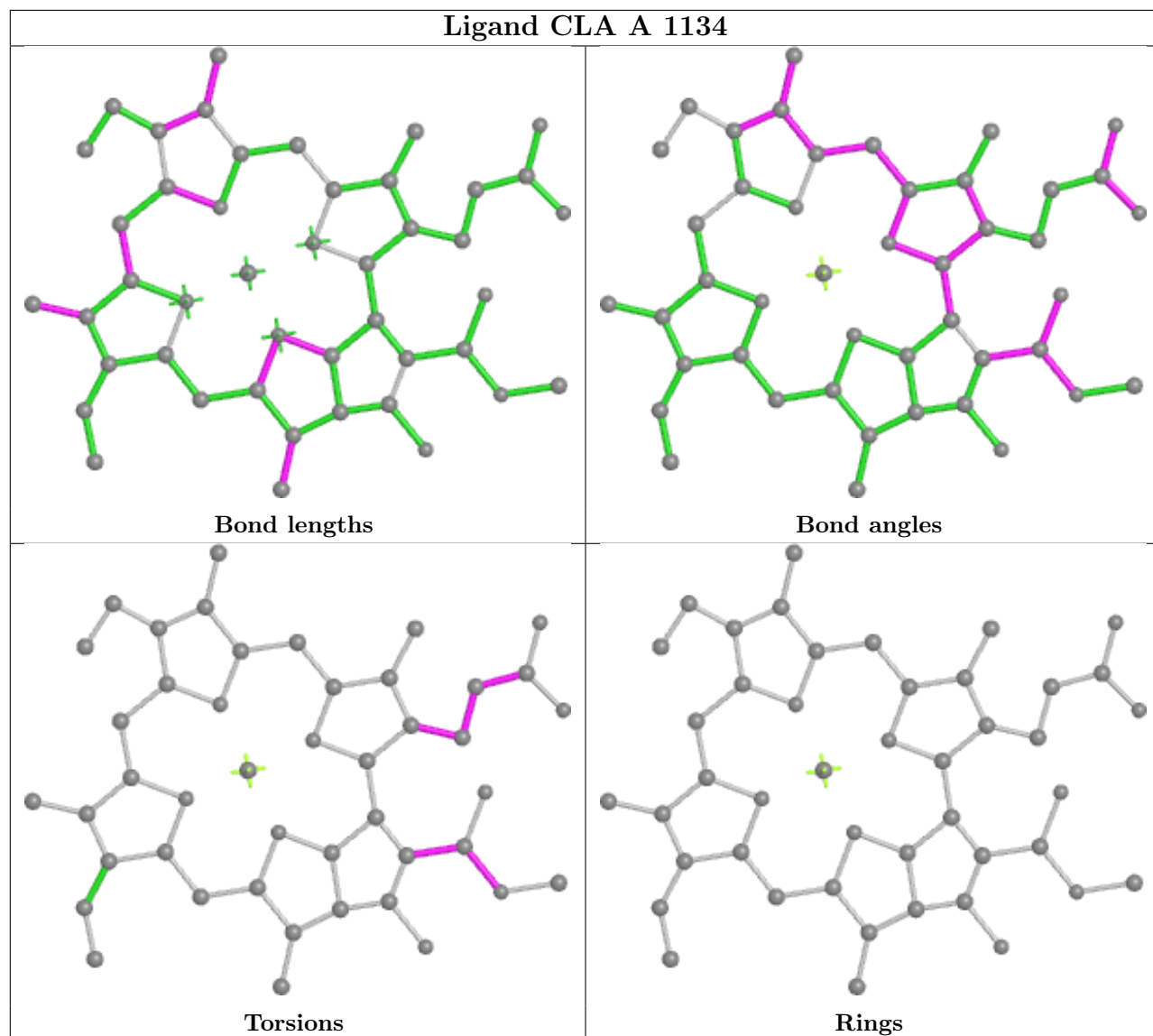


Torsions

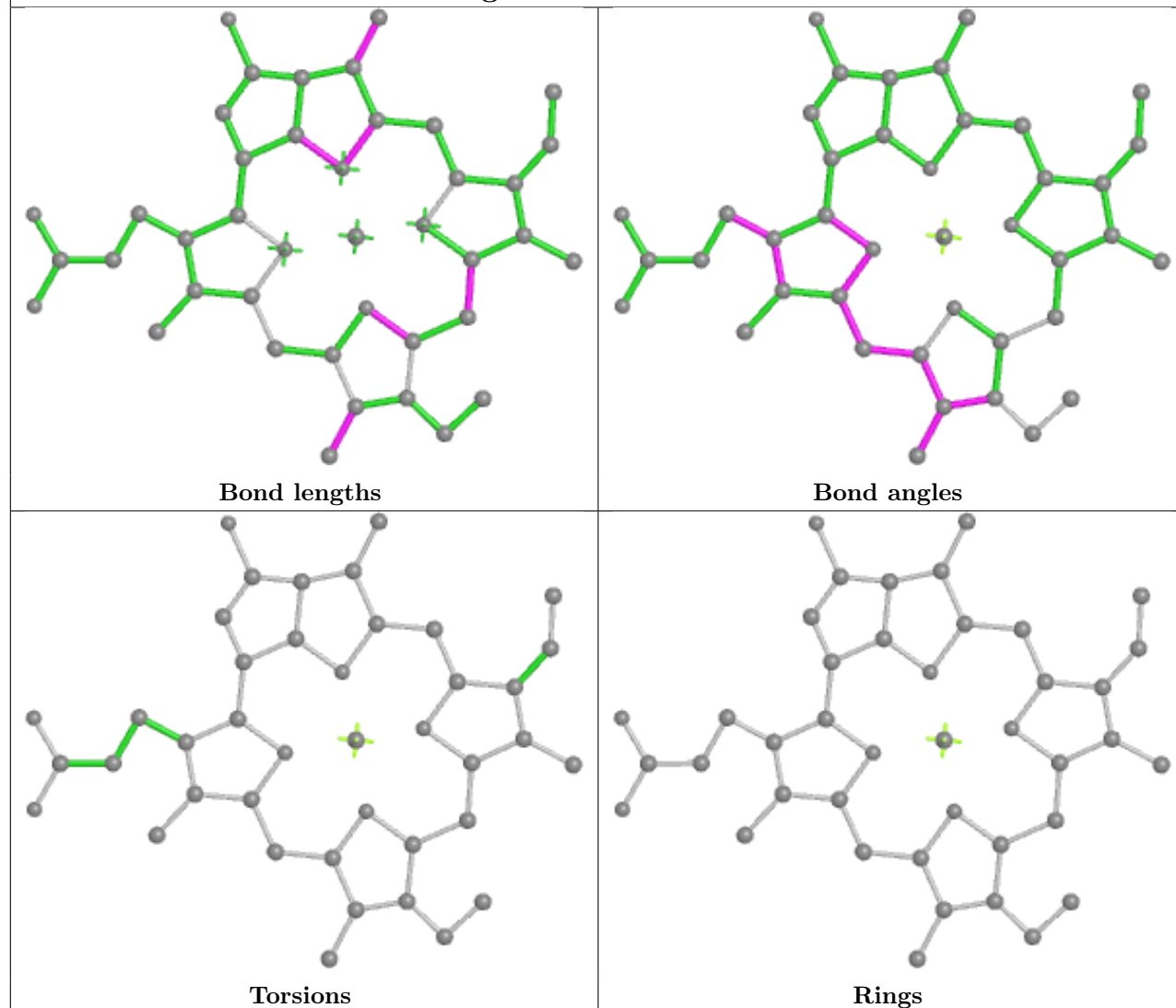


Rings

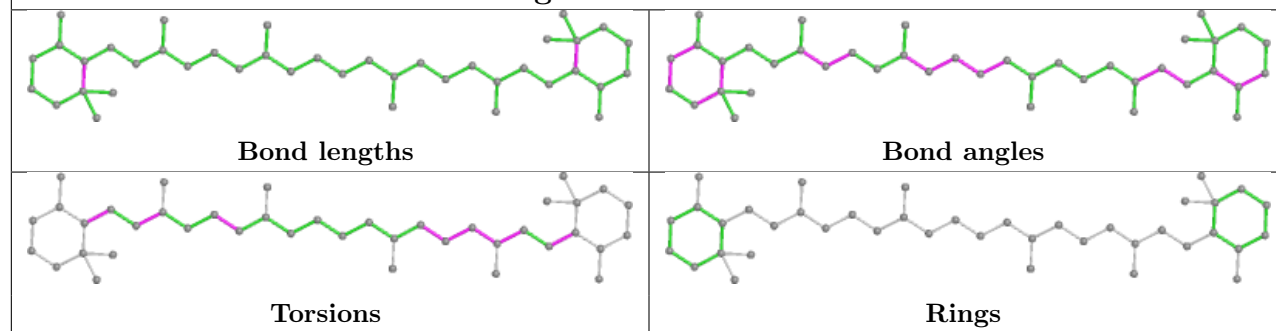
## Ligand CLA A 1134



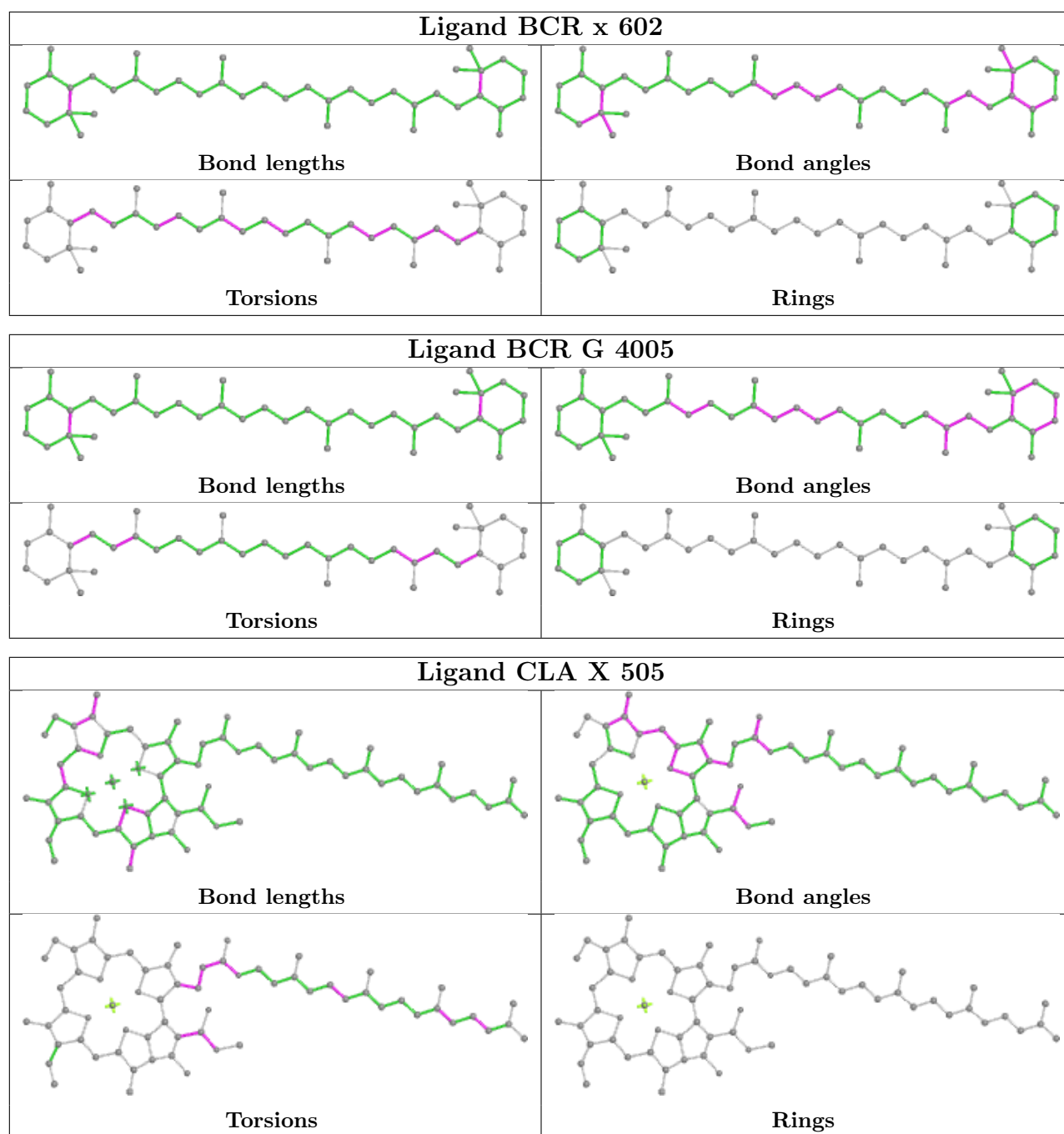
## Ligand CLA A 1402

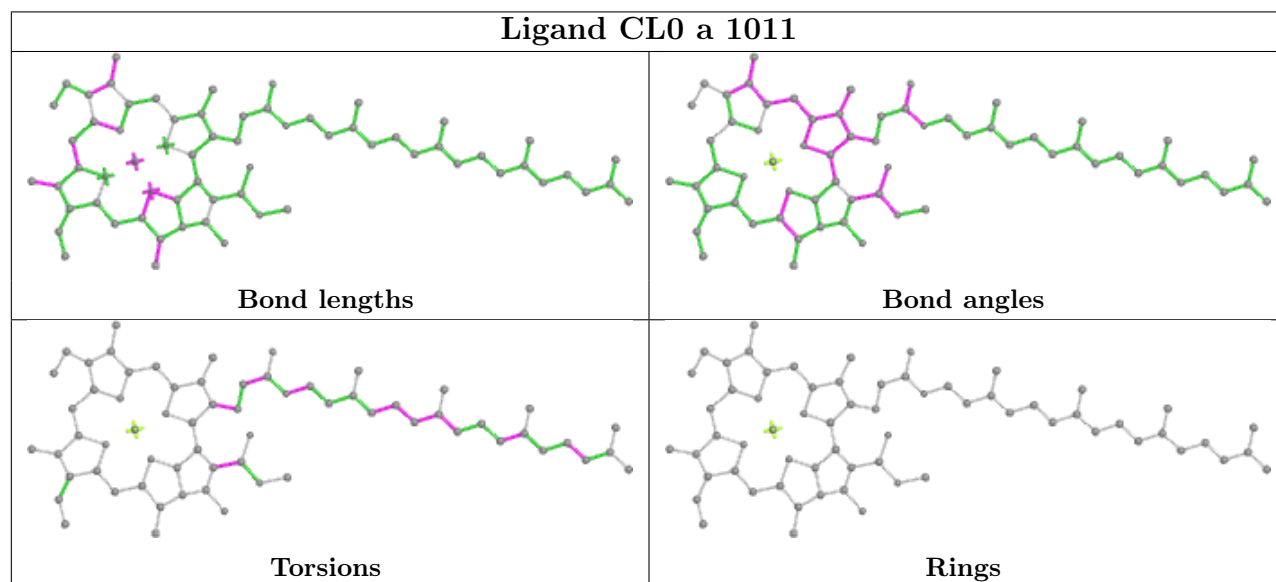
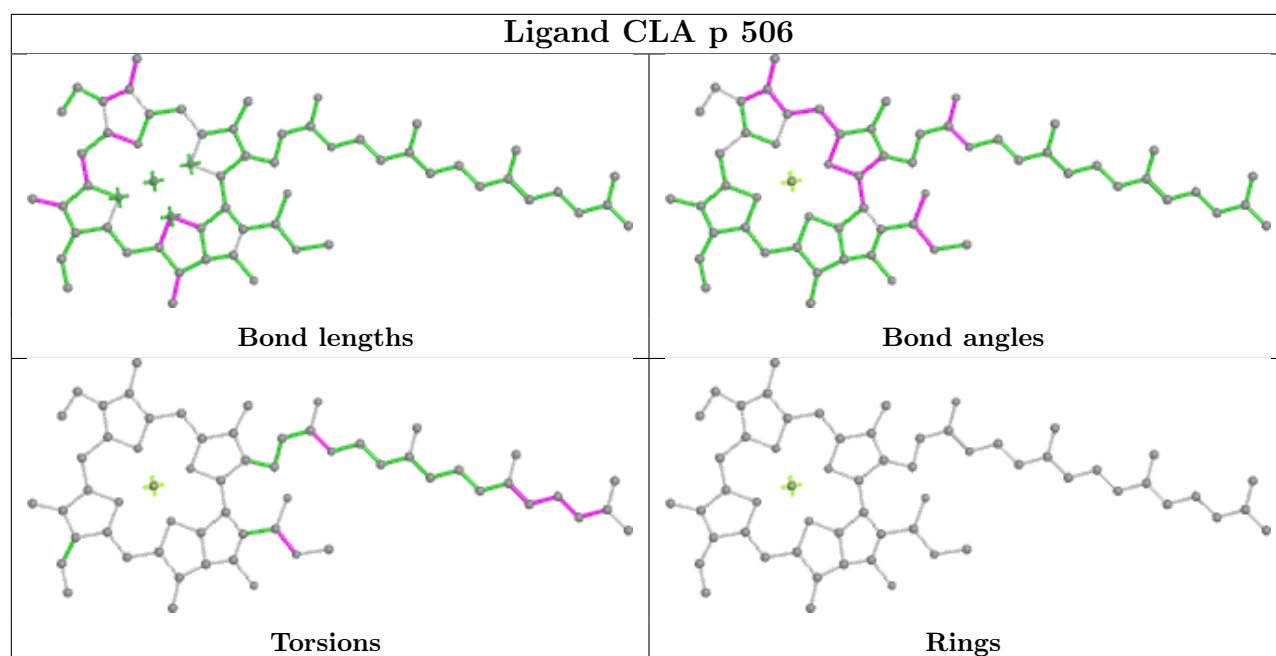


## Ligand BCR o 602

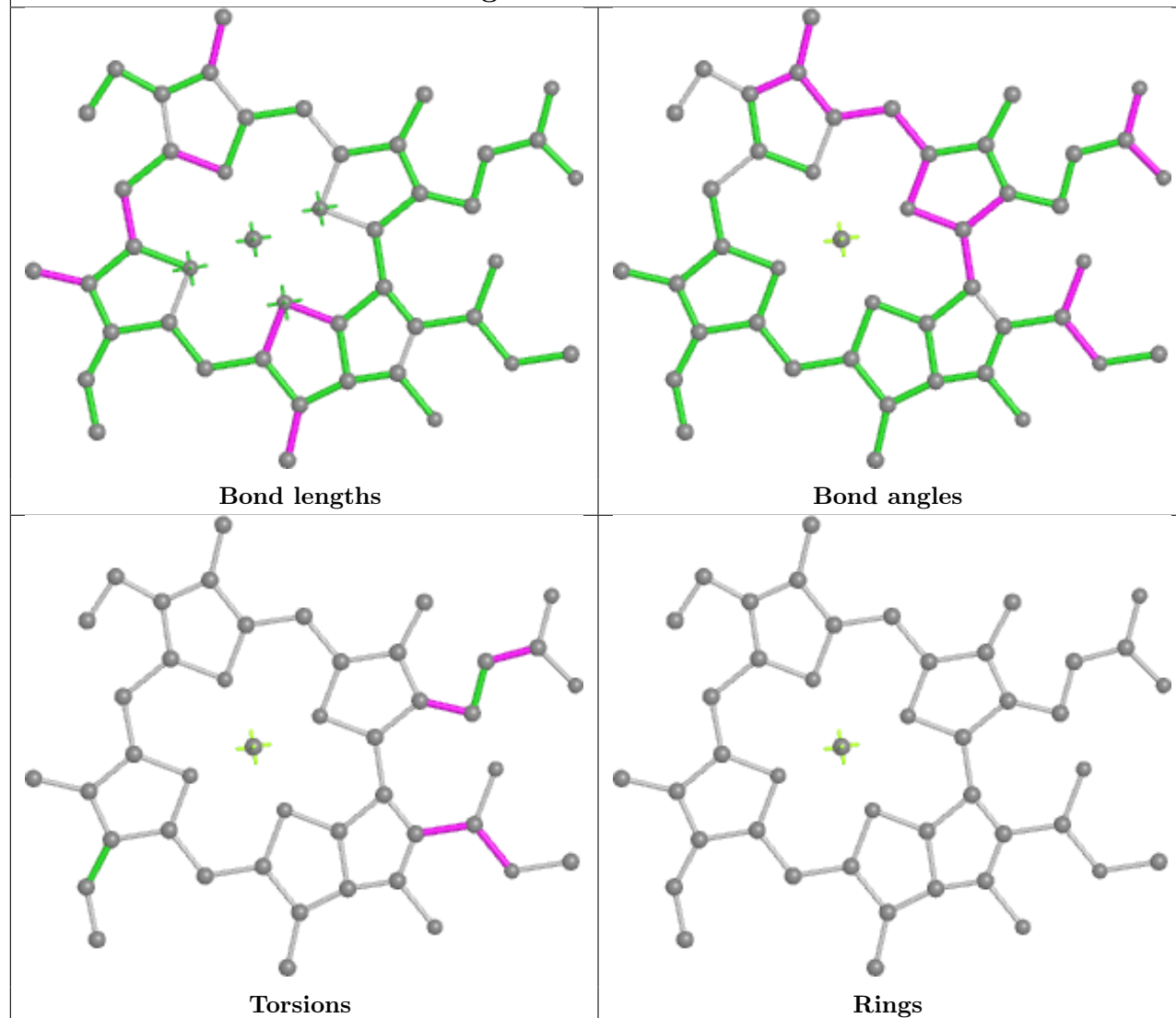




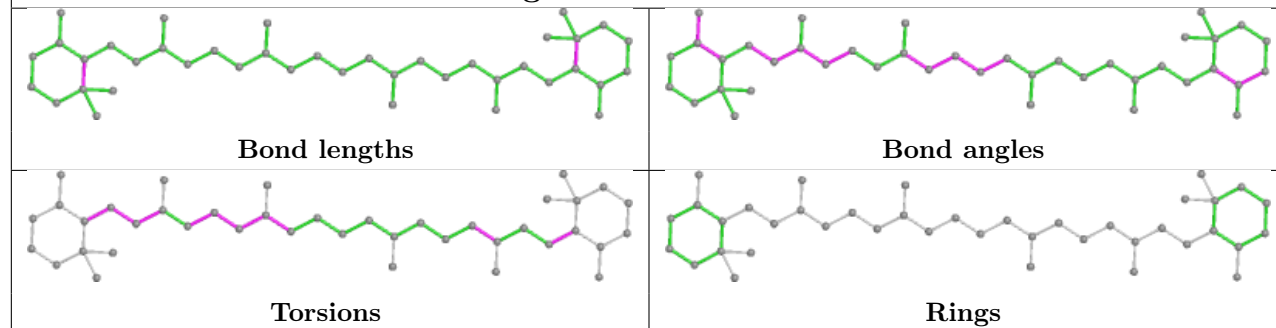


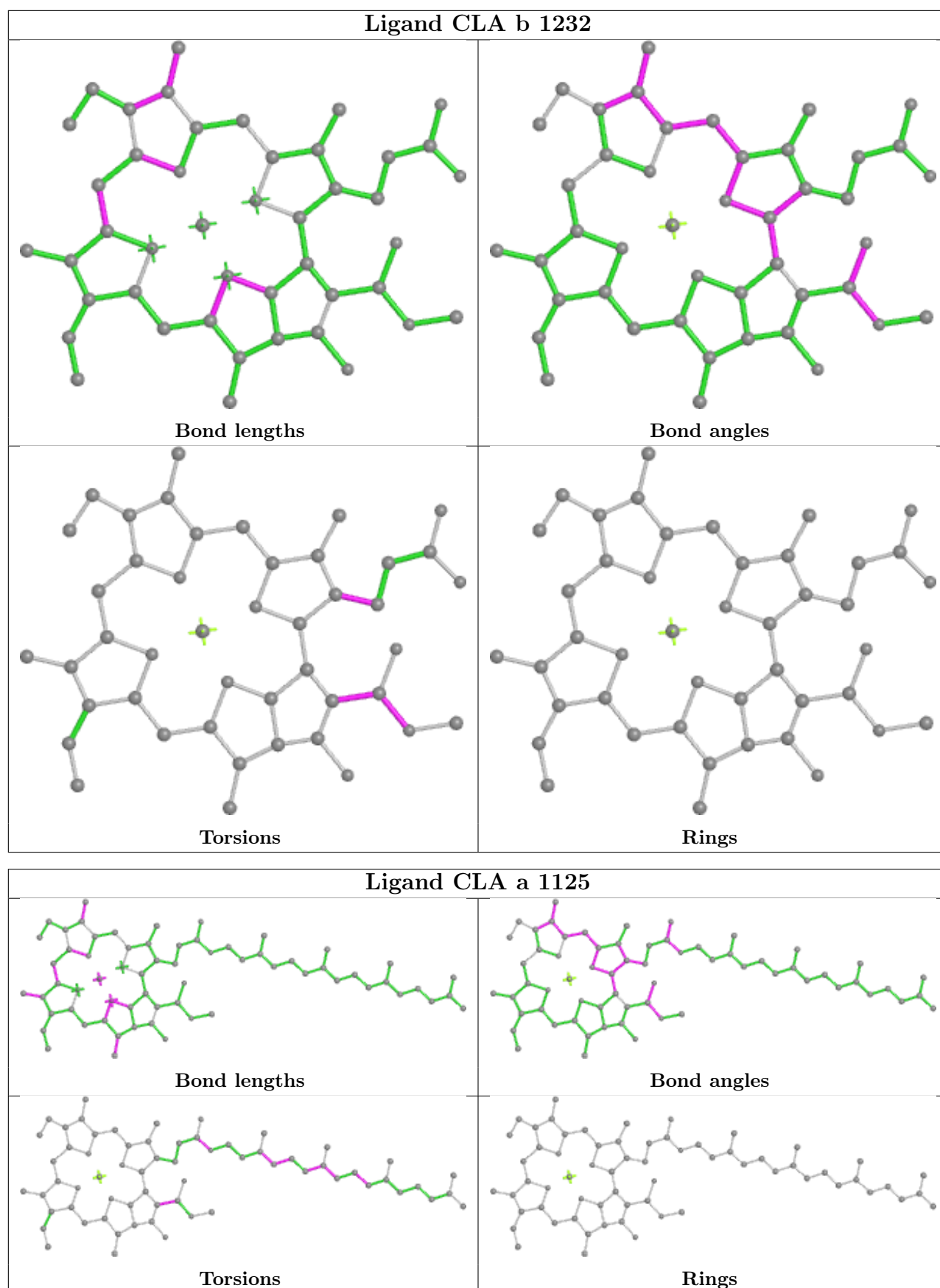


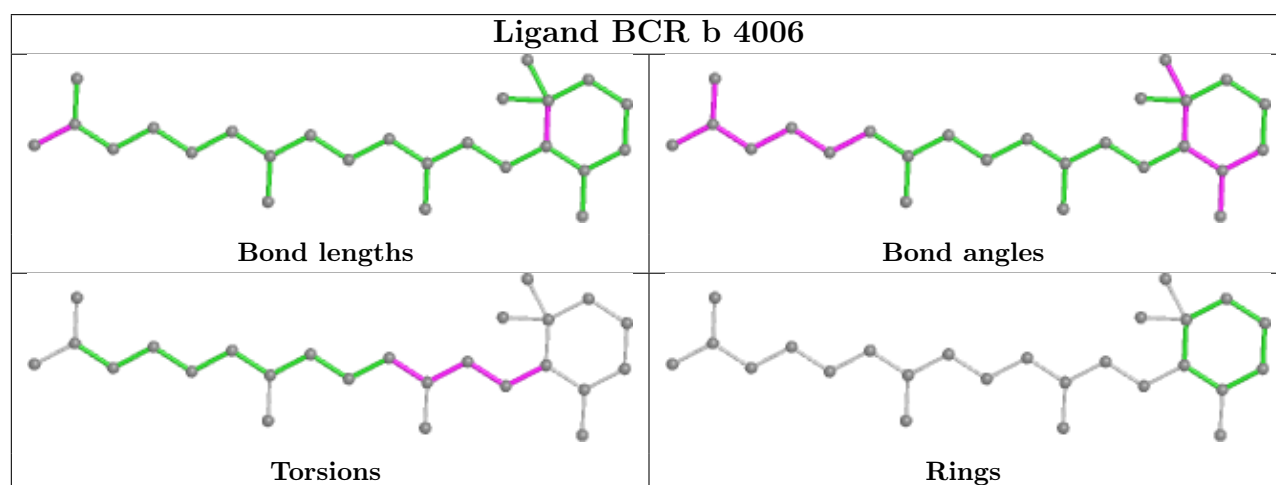
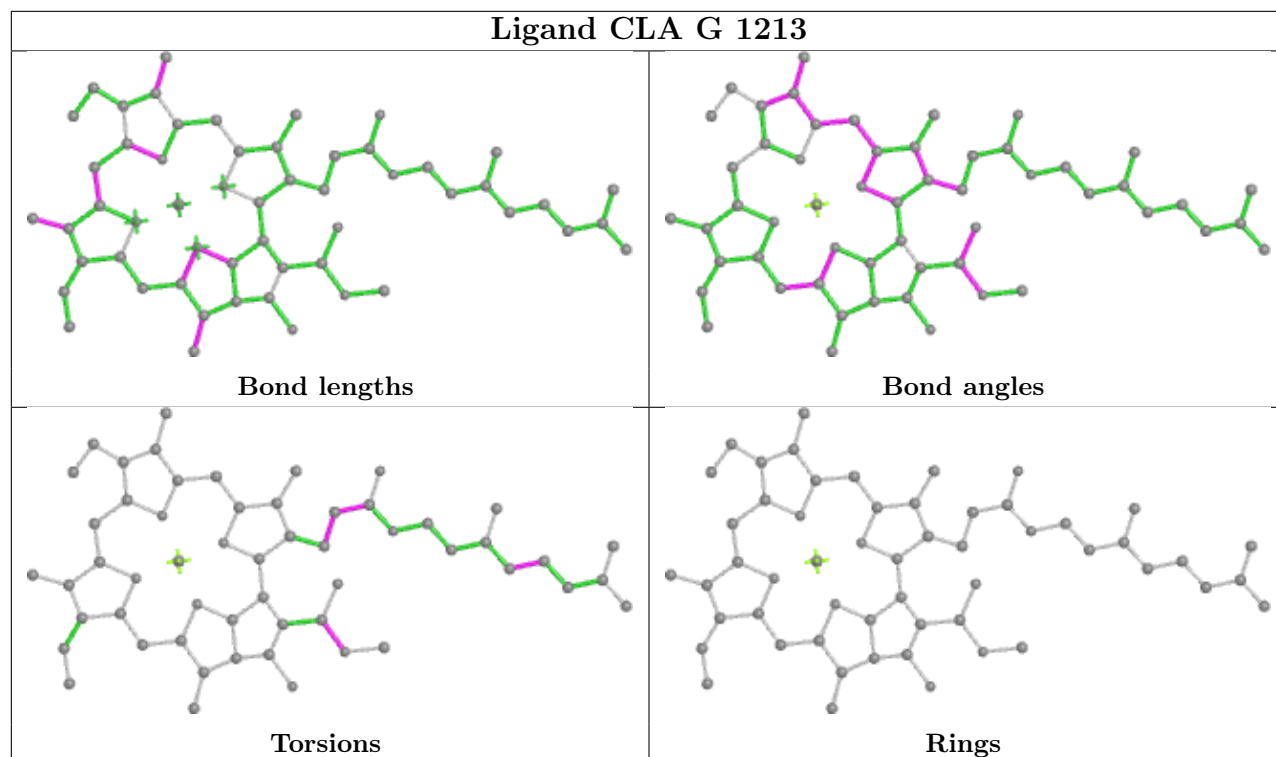
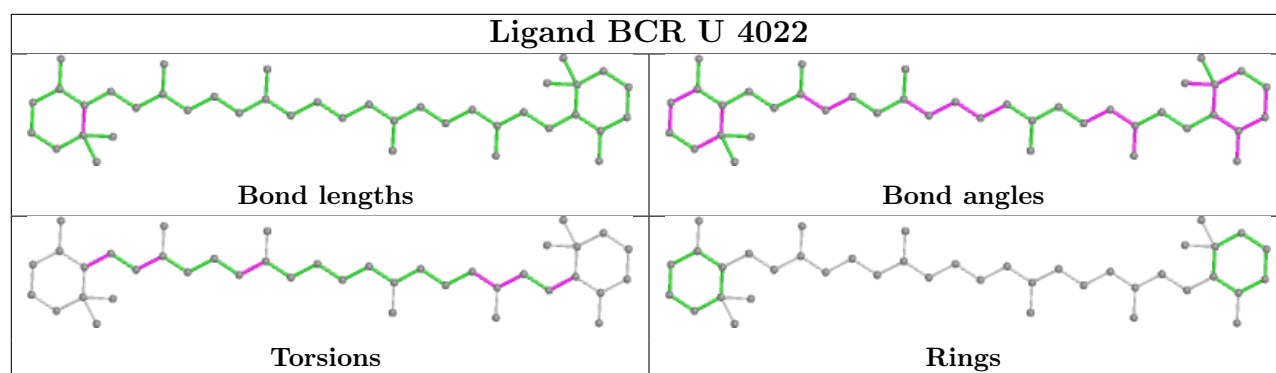
## Ligand CLA H 1112

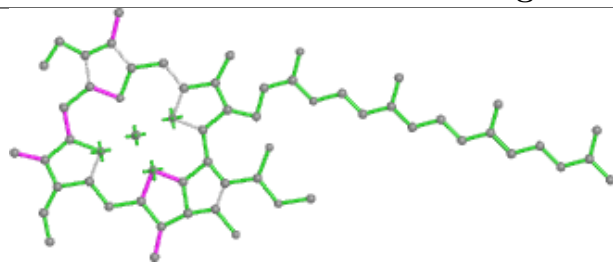


## Ligand BCR F 4016

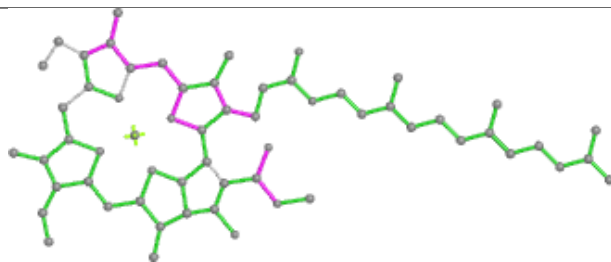




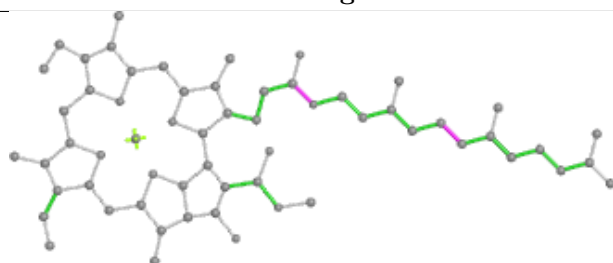


**Ligand CLA Z 506**

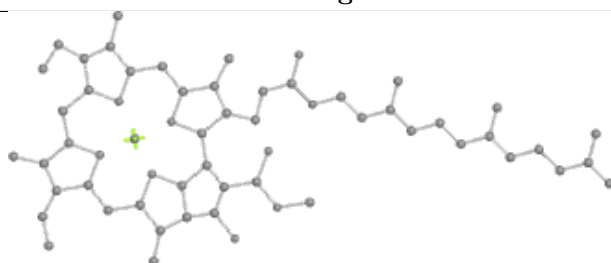
Bond lengths



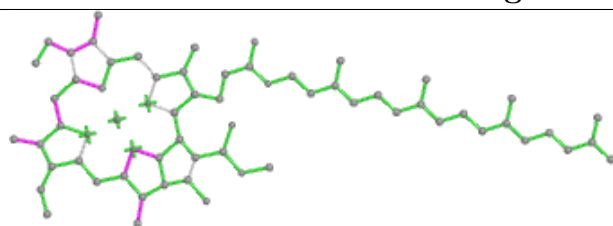
Bond angles



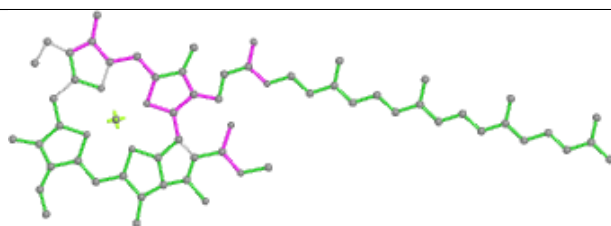
Torsions



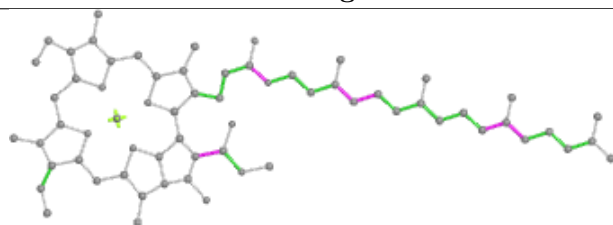
Rings

**Ligand CLA H 1138**

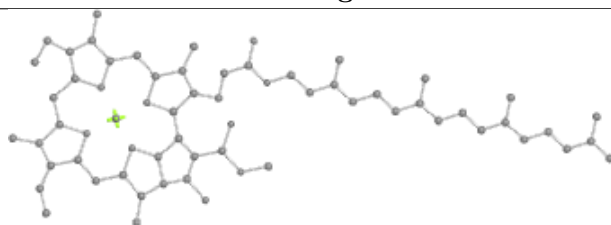
Bond lengths



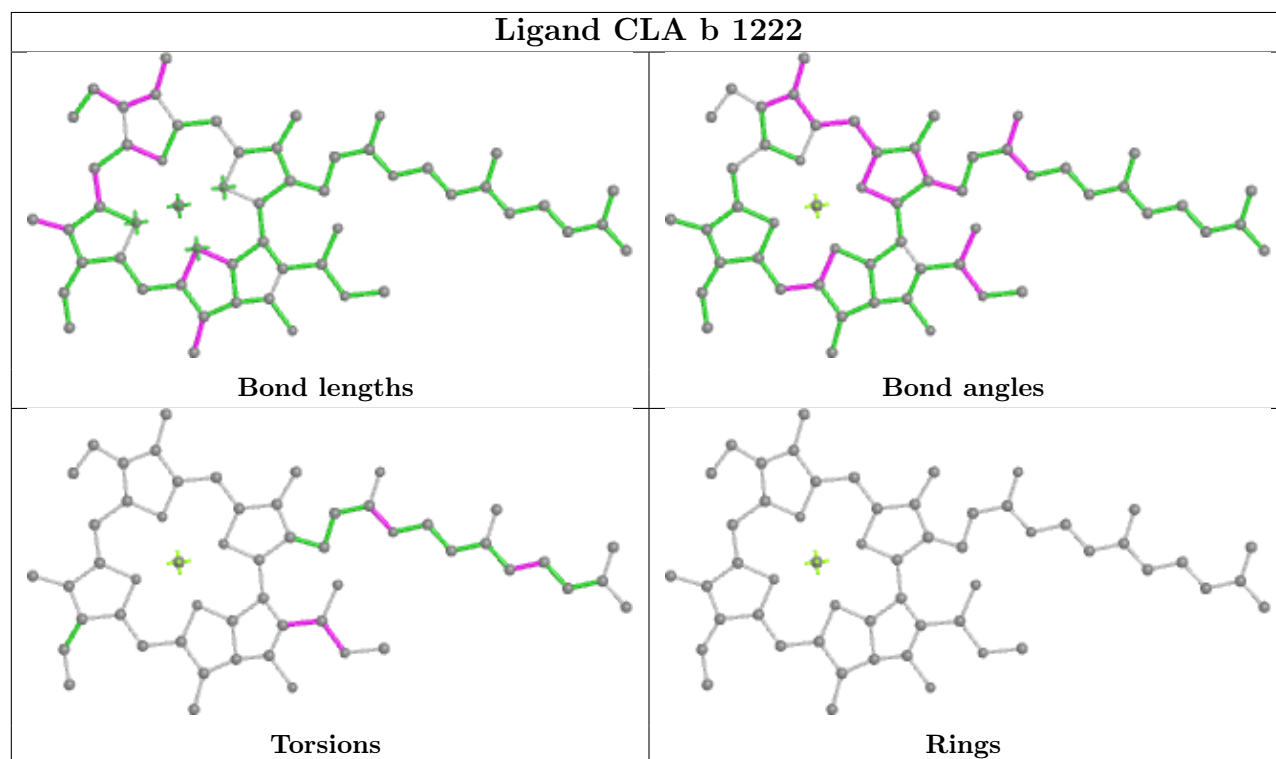
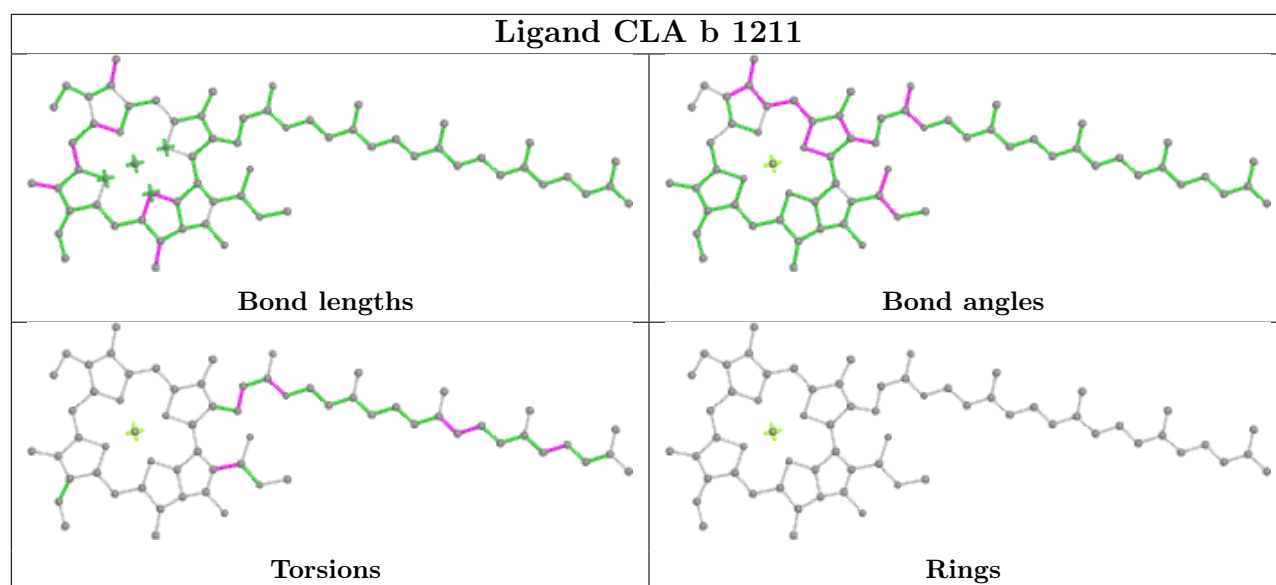
Bond angles

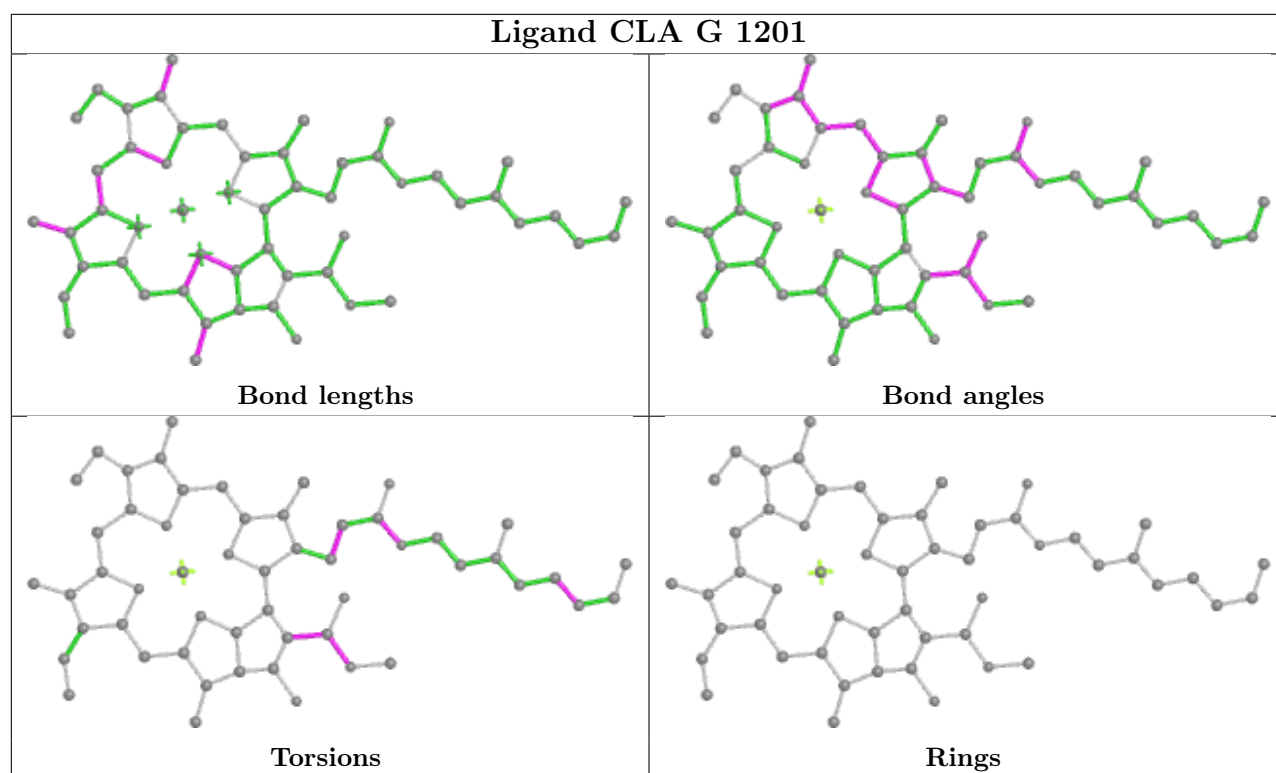


Torsions

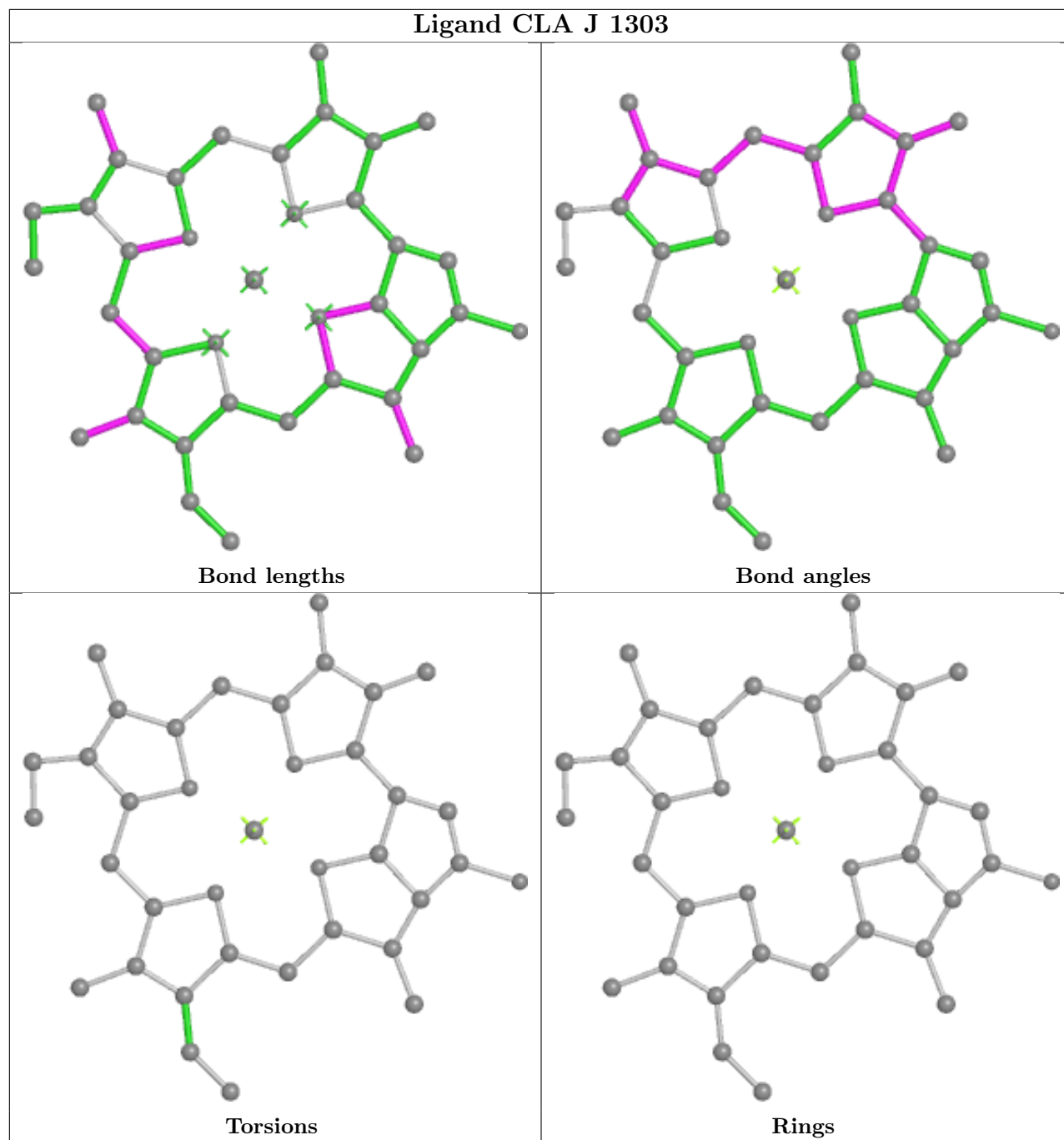


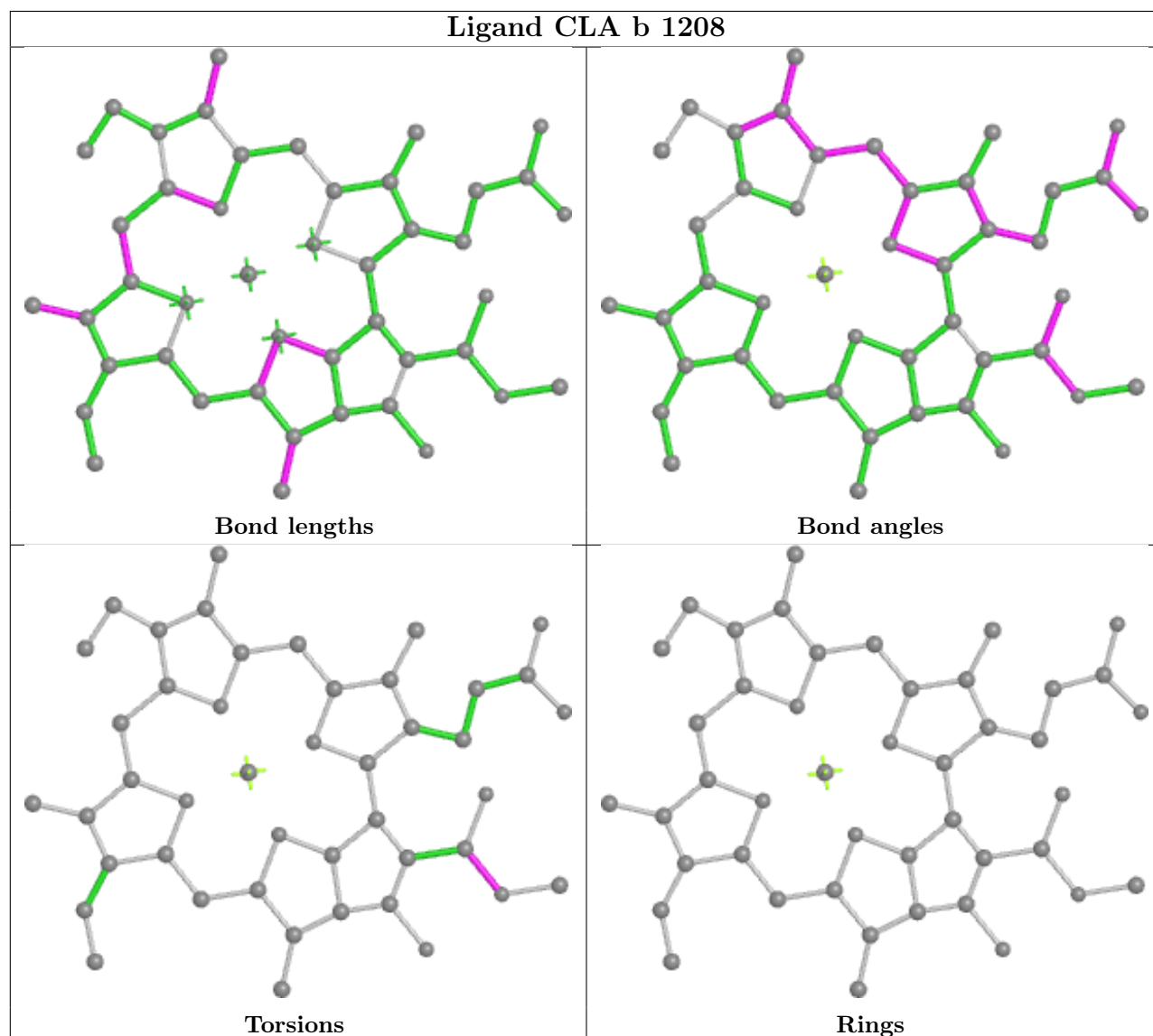
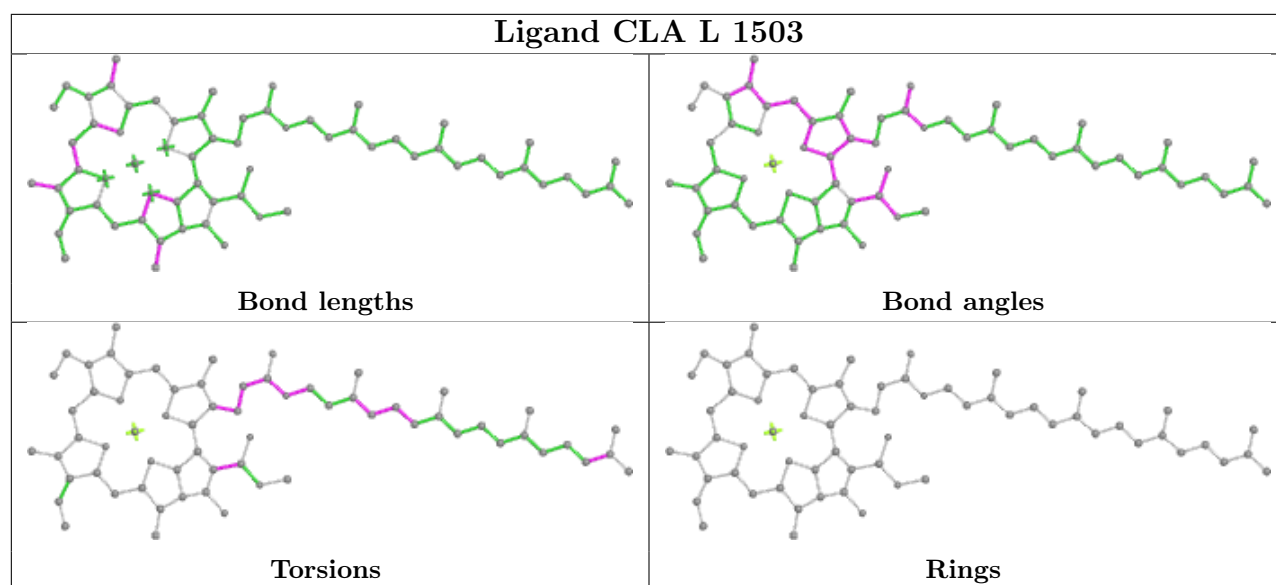
Rings

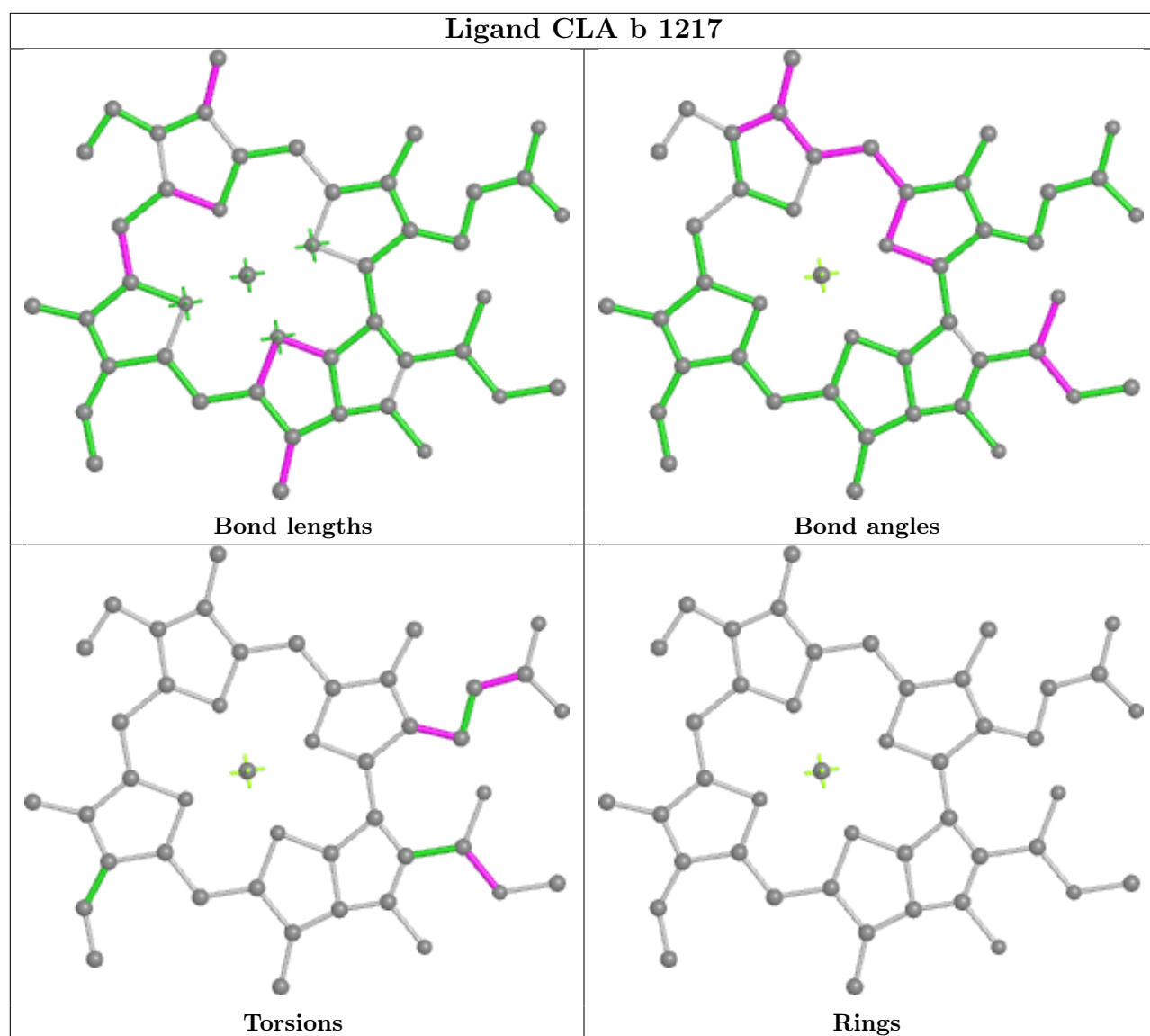




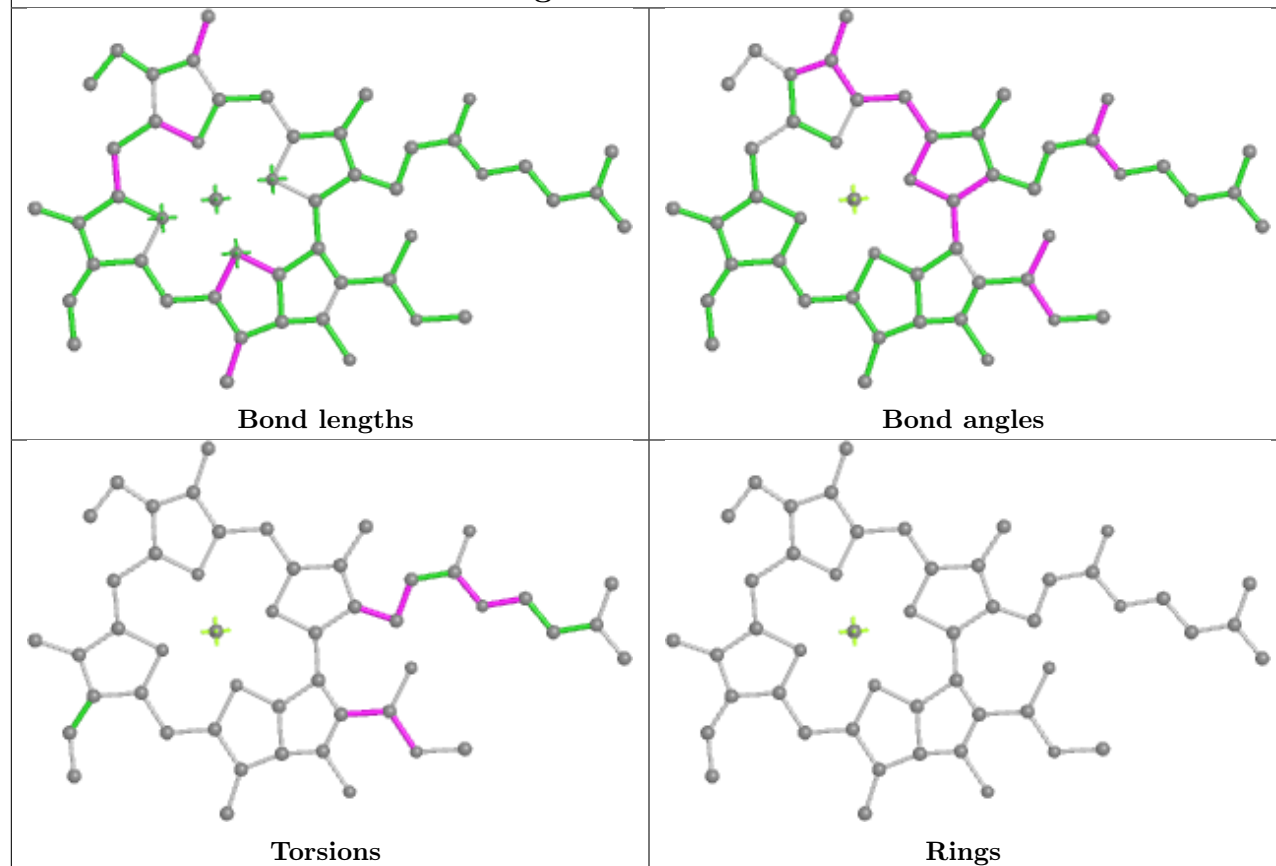




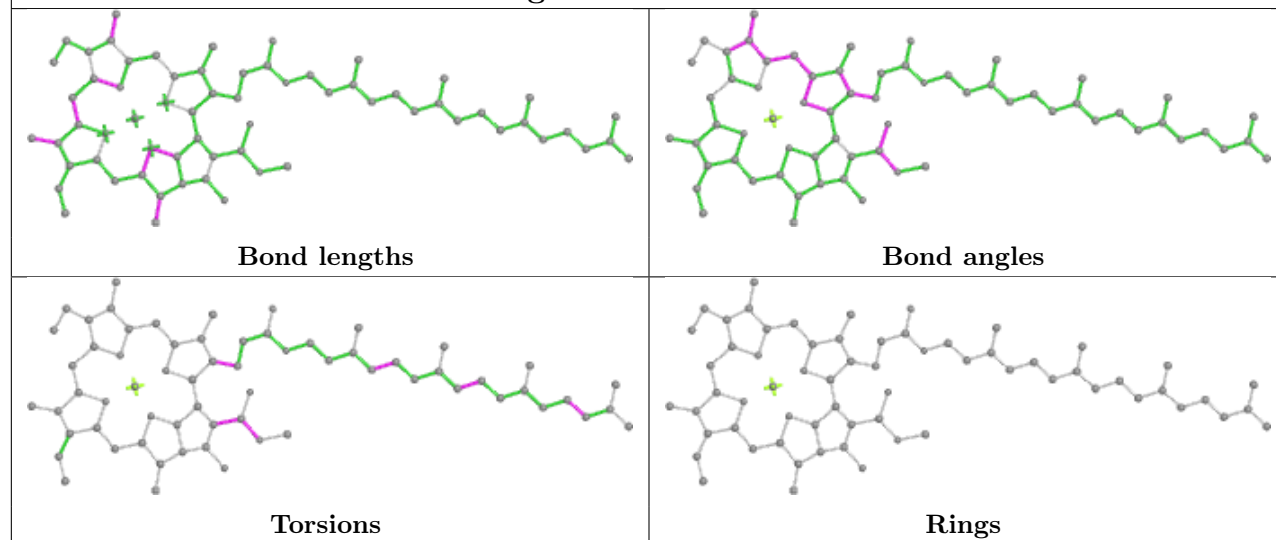


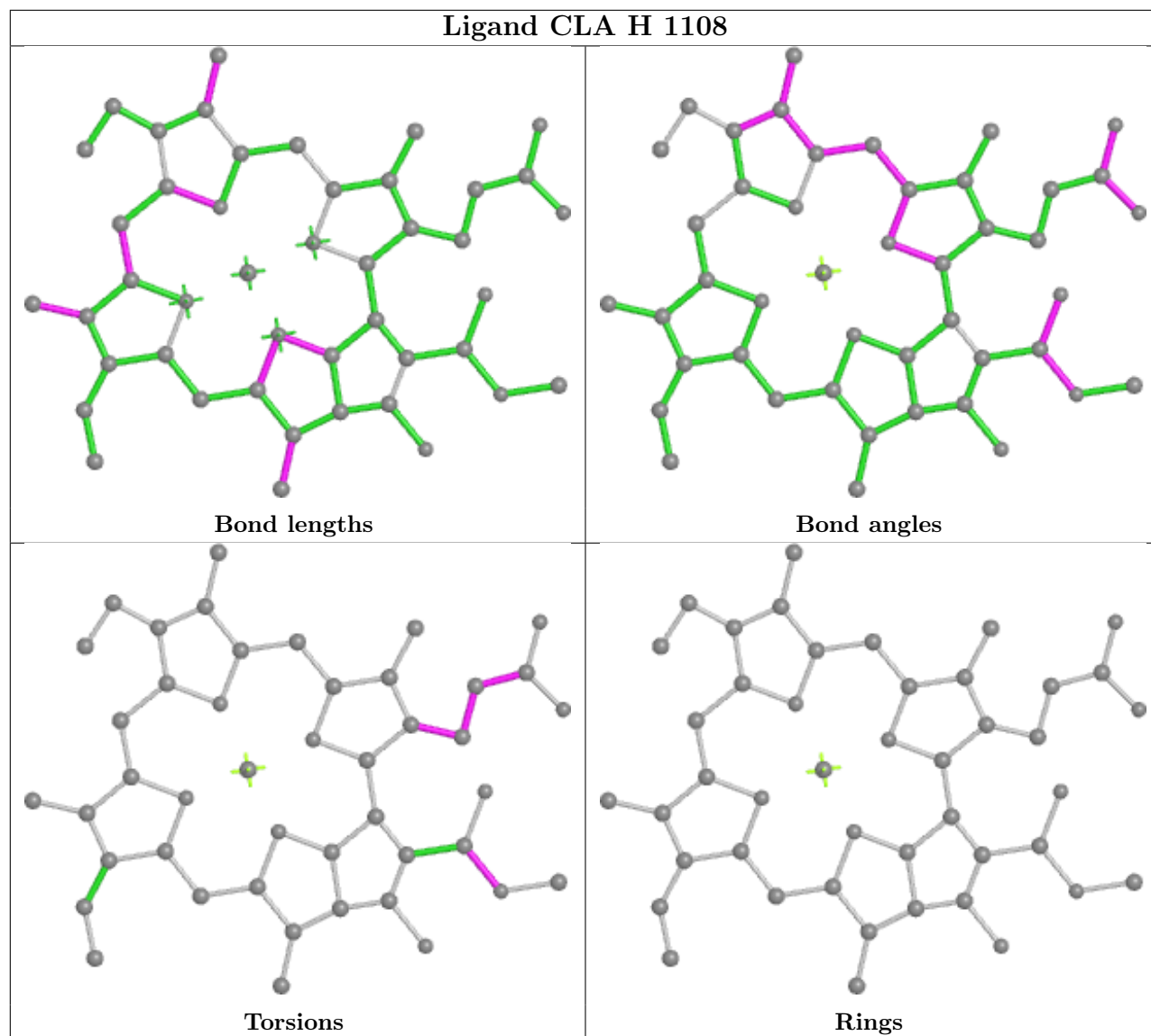
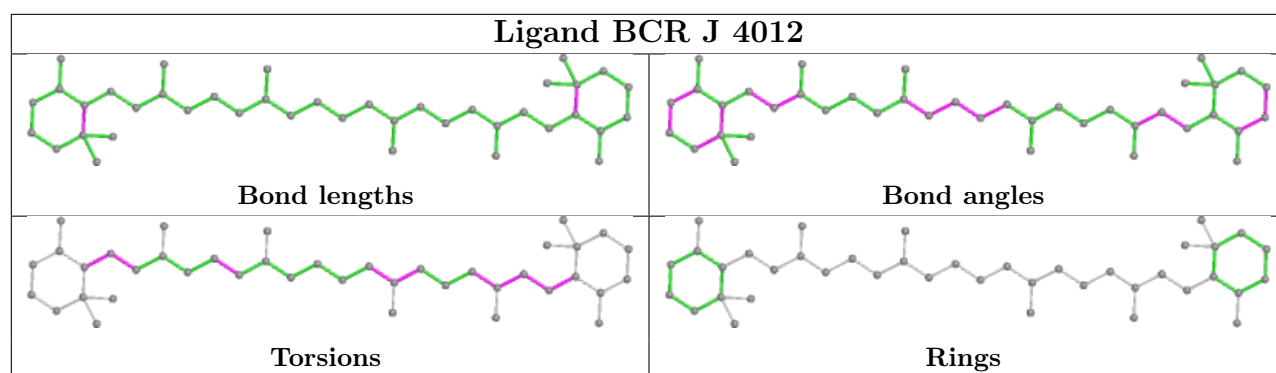


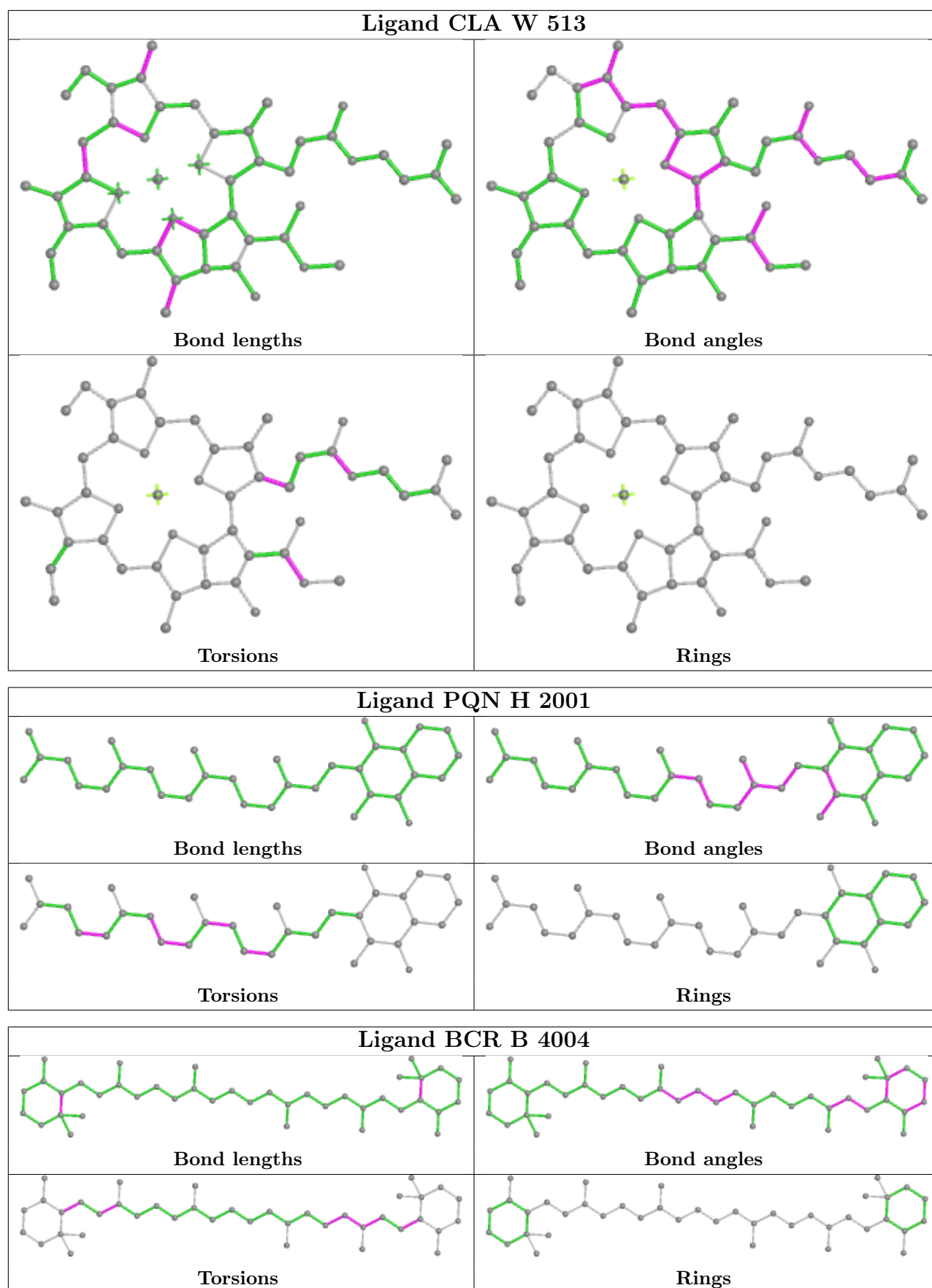
## Ligand CLA Z 513



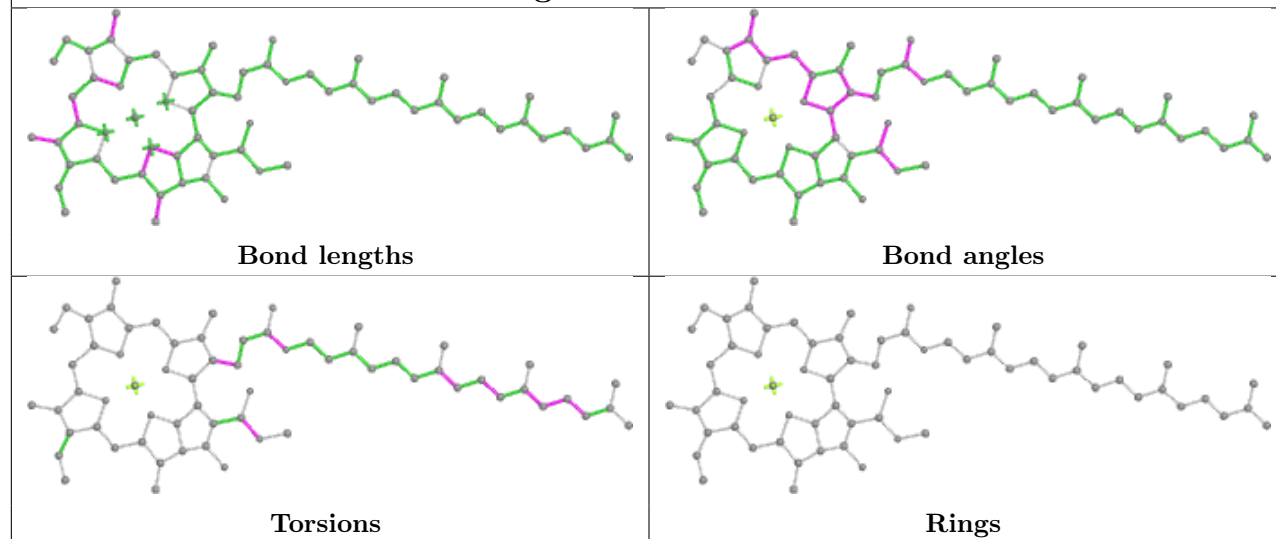
## Ligand CLA a 1104



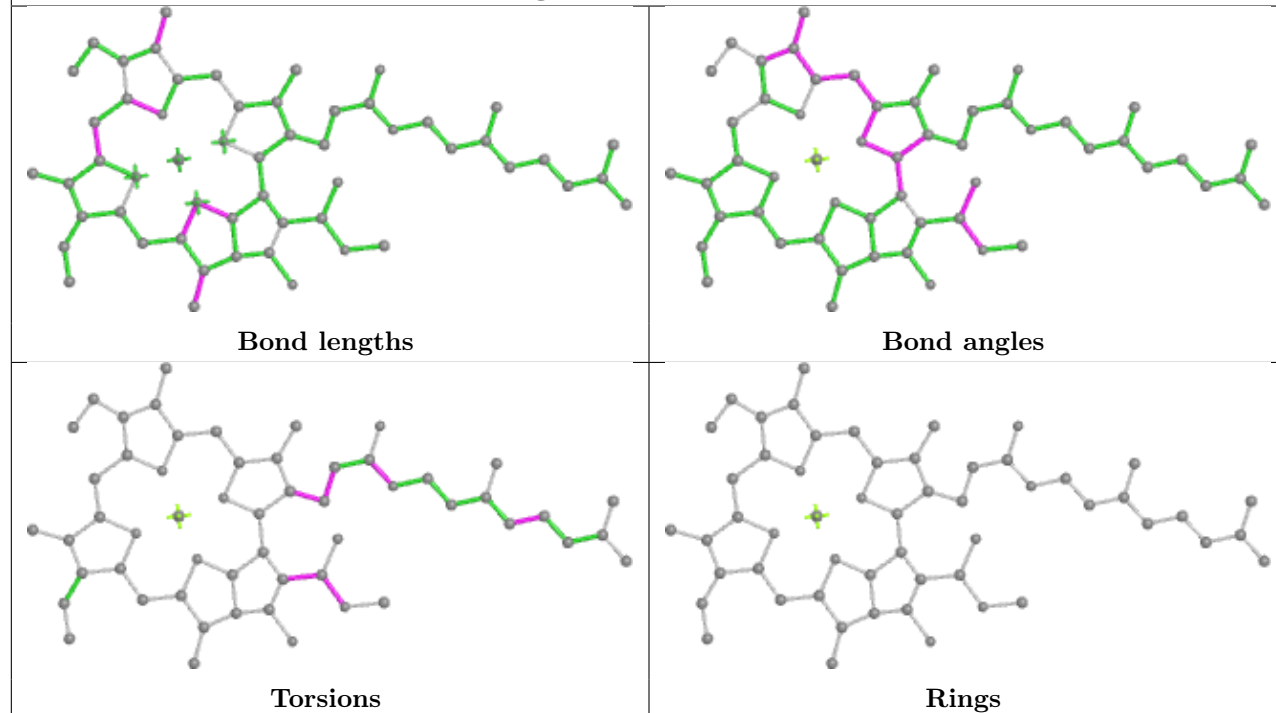


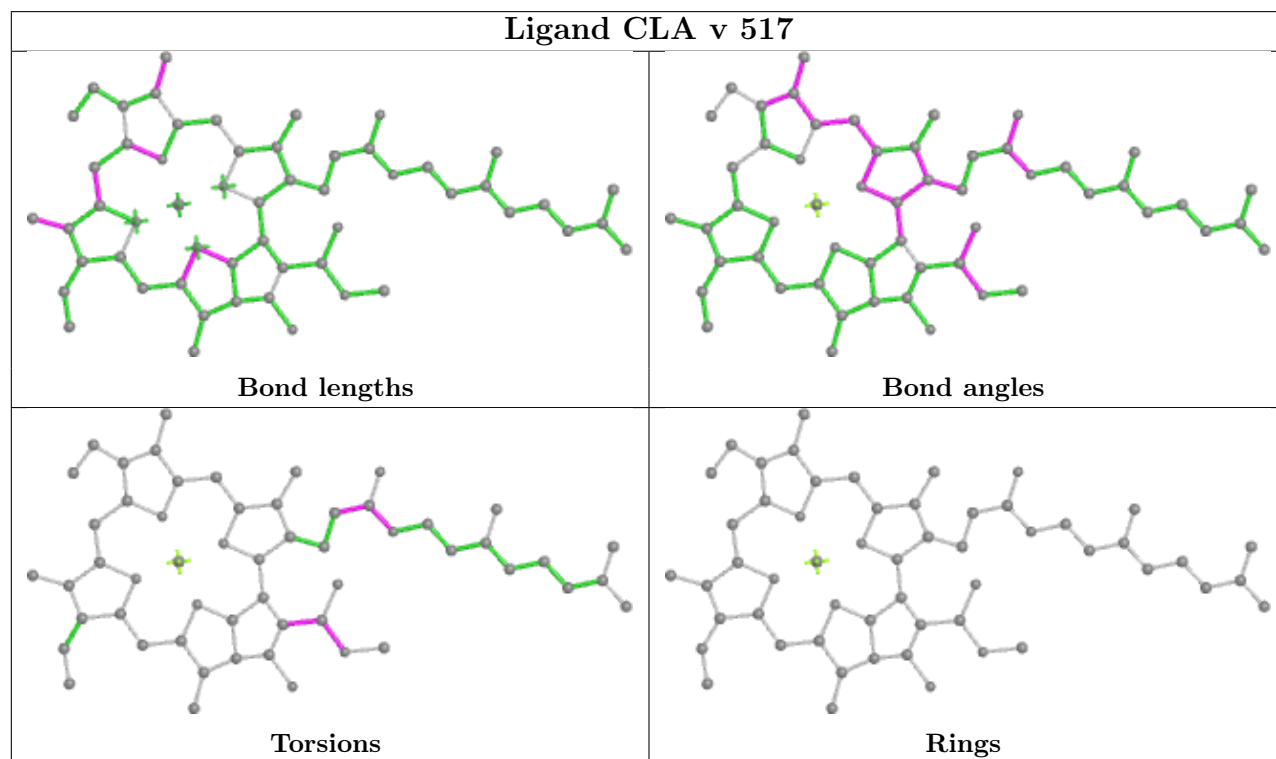
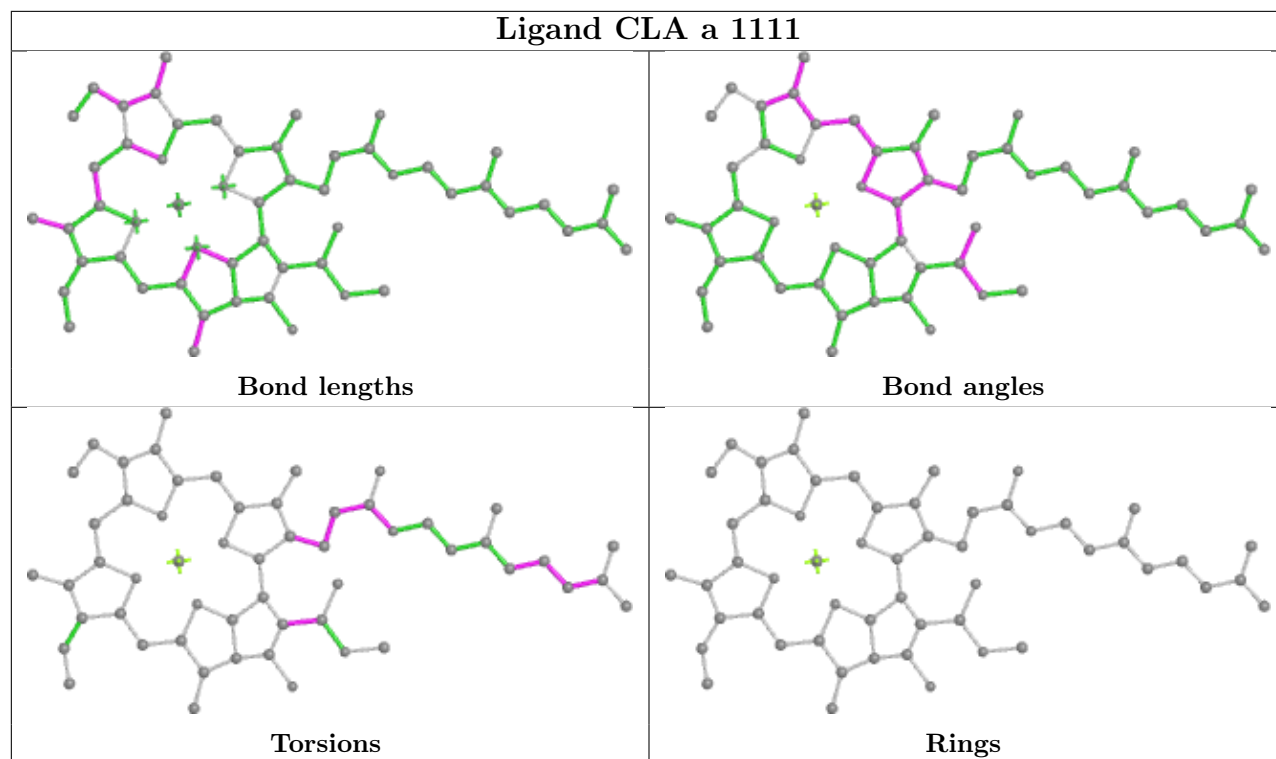


## Ligand CLA Z 511

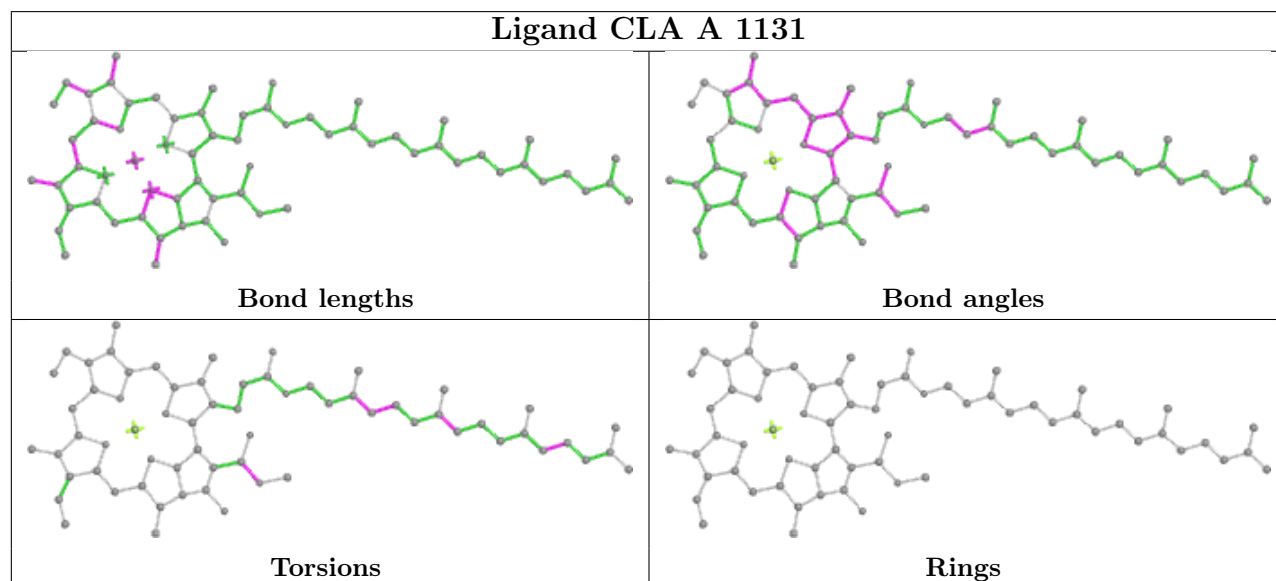
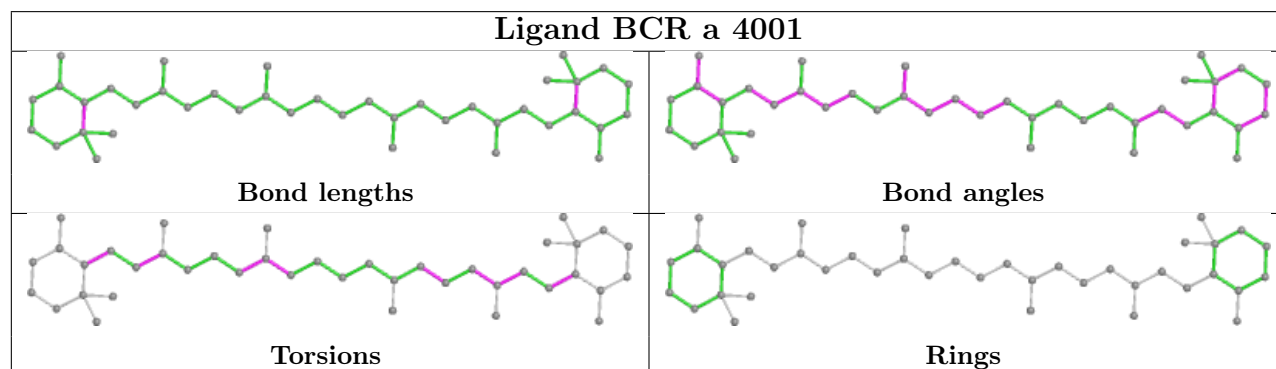
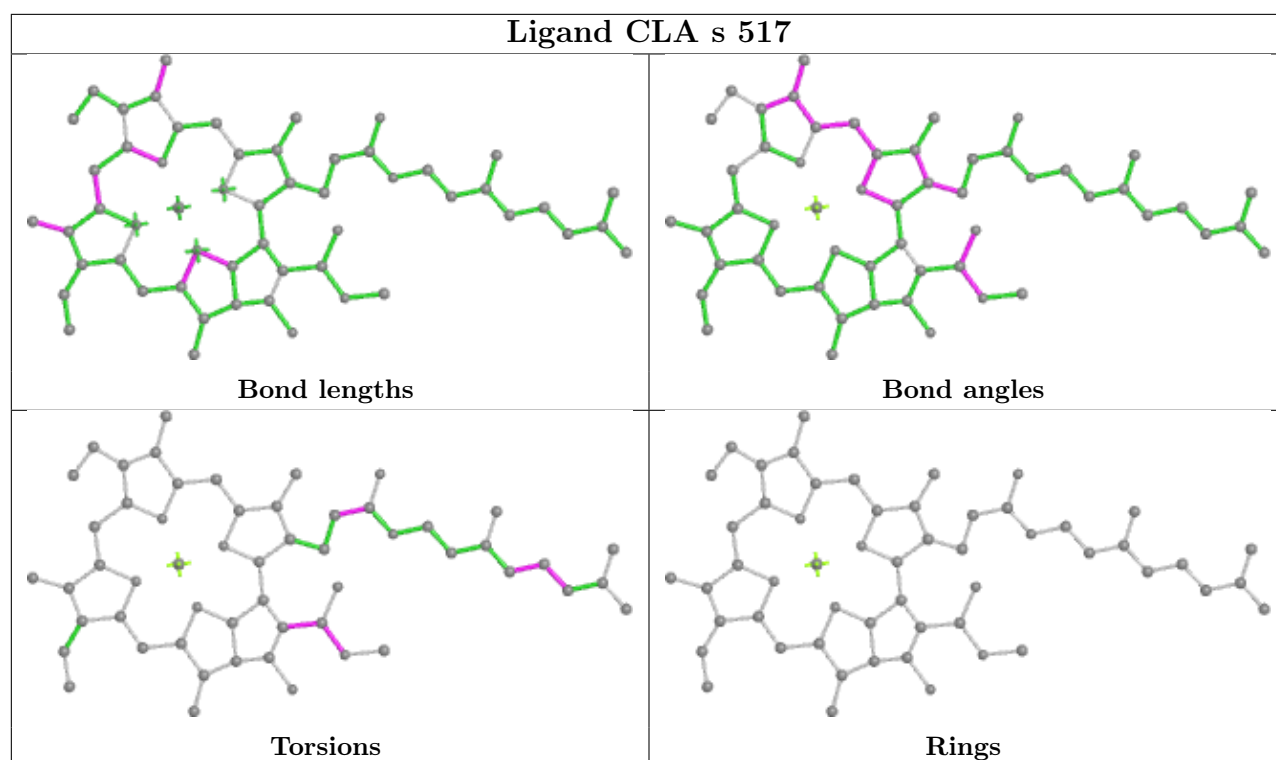


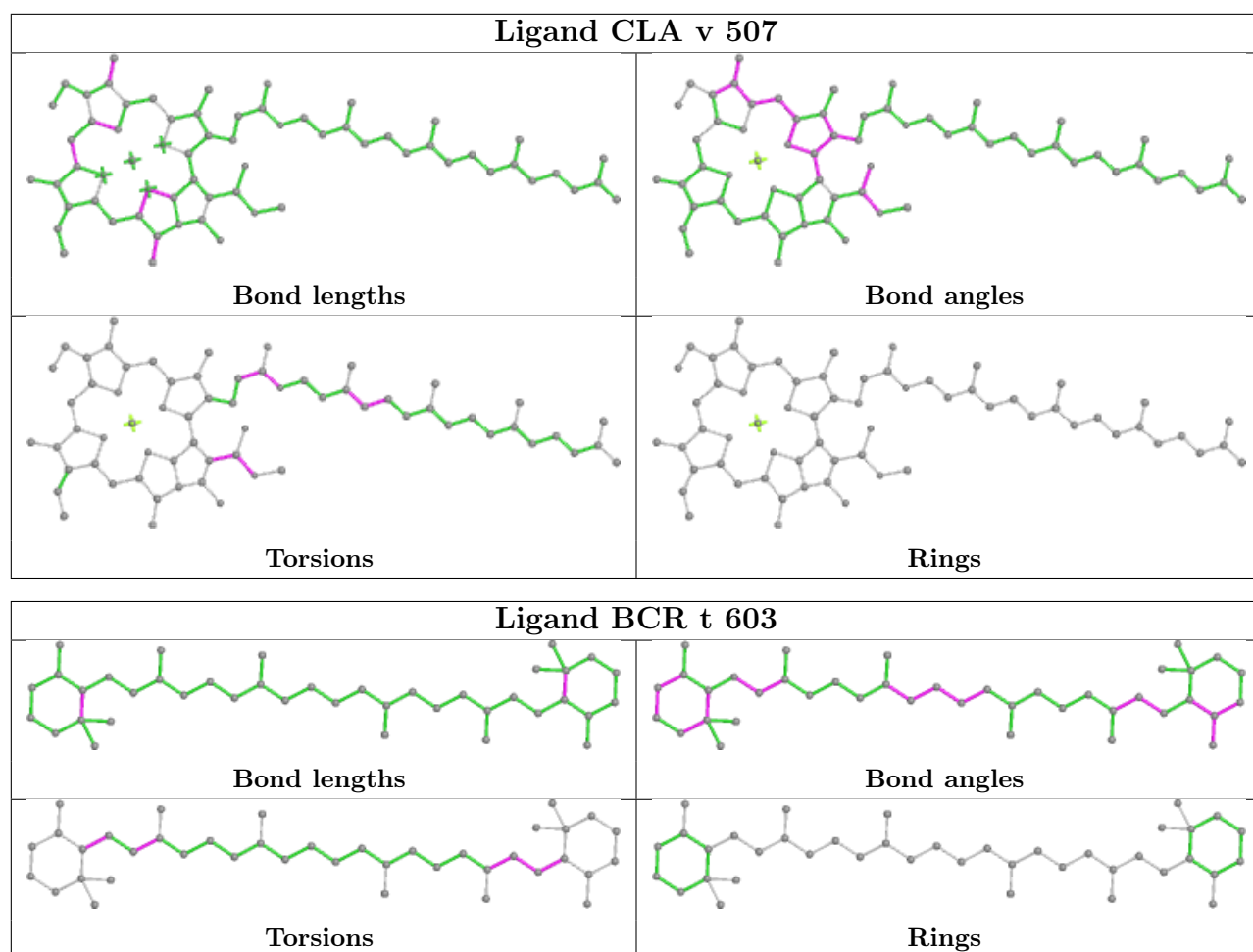
## Ligand CLA w 508



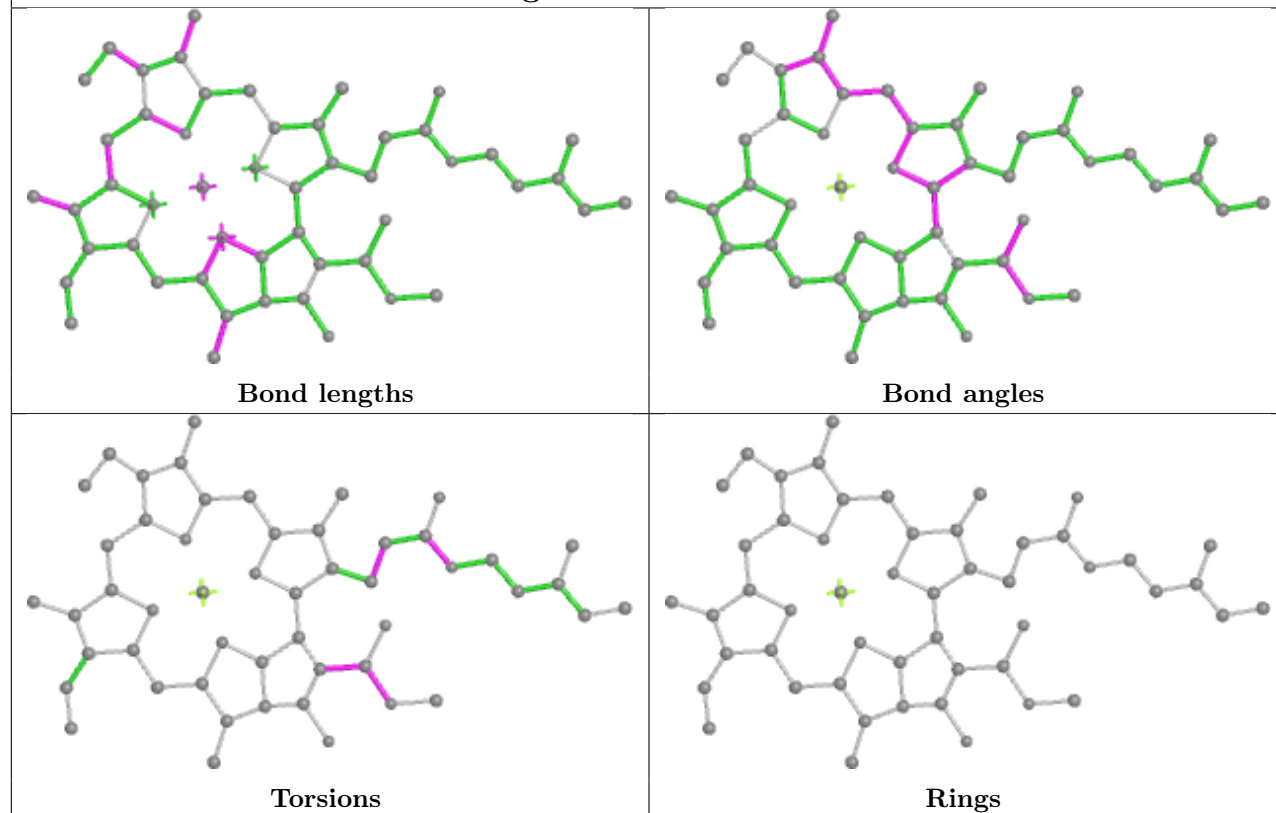




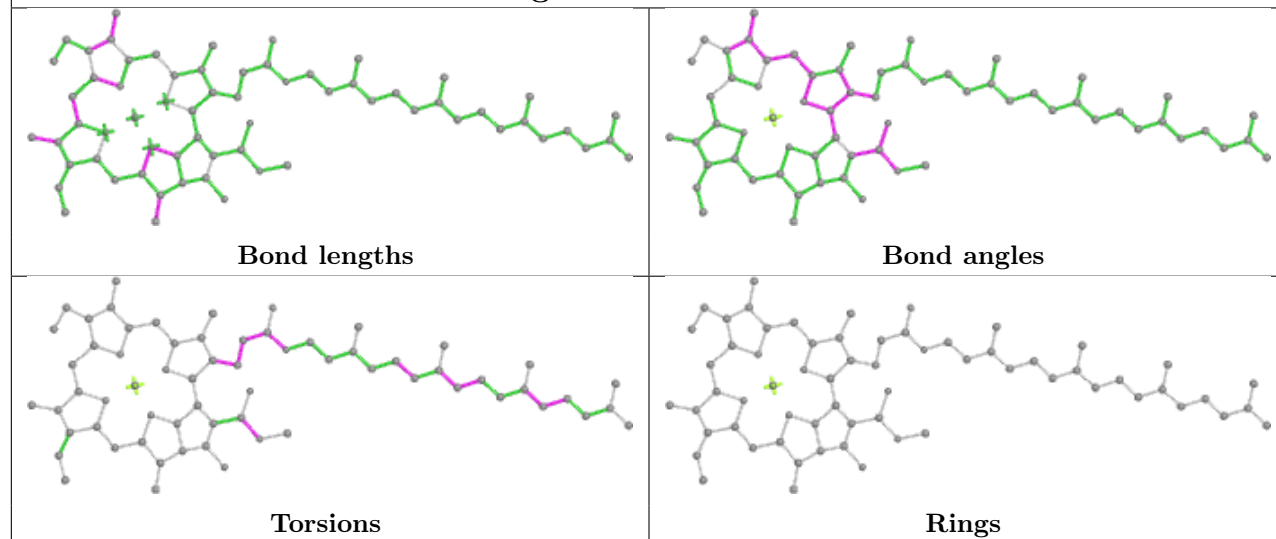




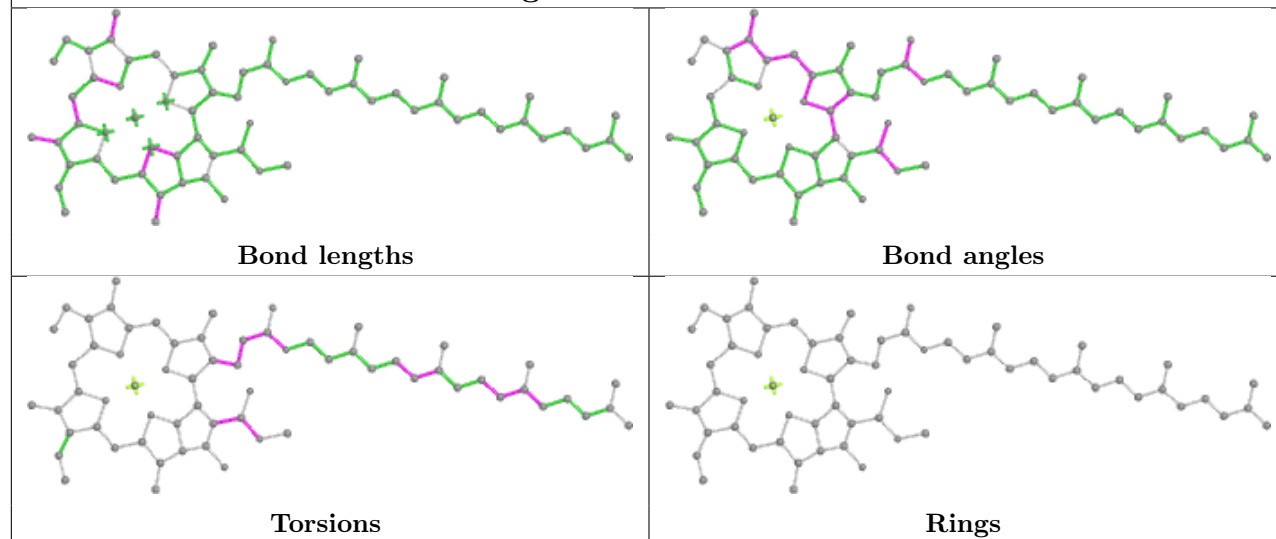
## Ligand CLA H 1135



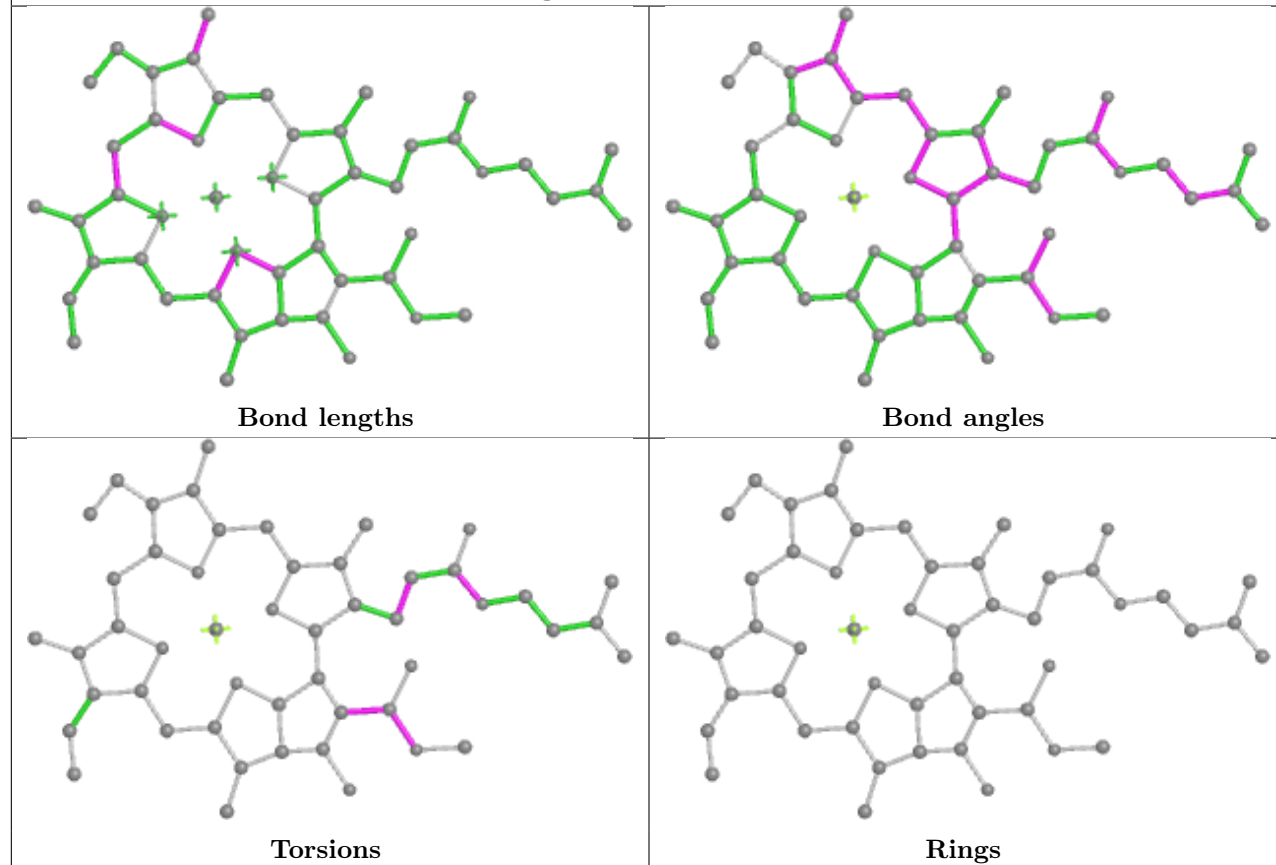
## Ligand CLA Y 505



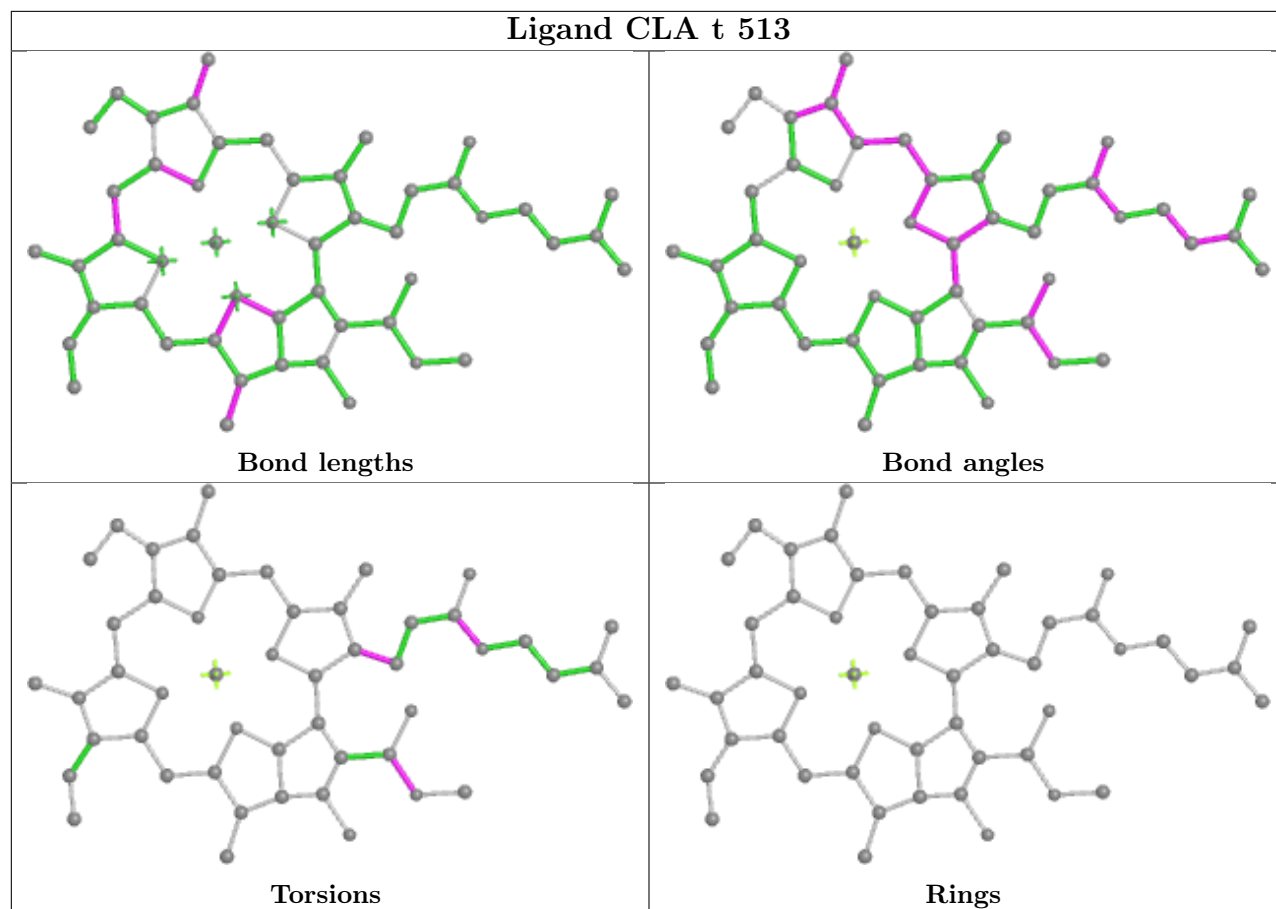
## Ligand CLA G 1203



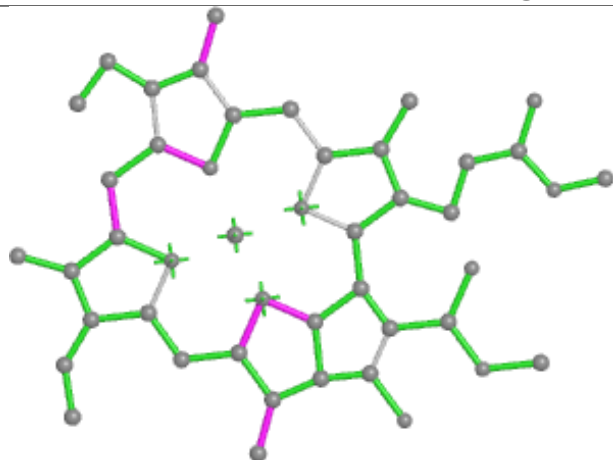
## Ligand CLA t 501



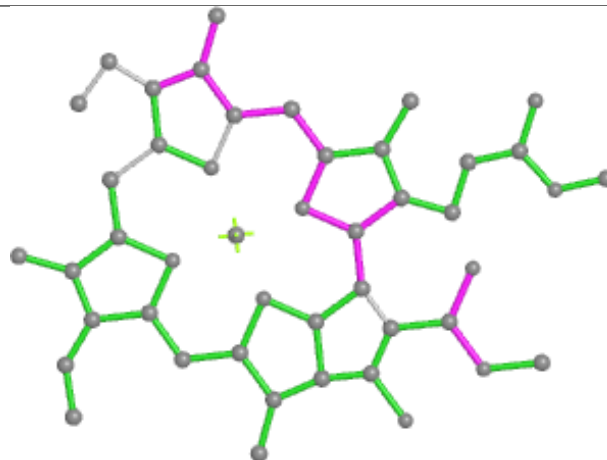
## Ligand CLA t 513



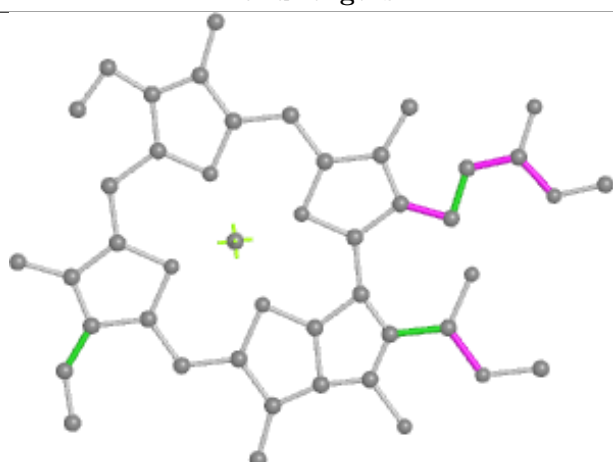
## Ligand CLA v 503



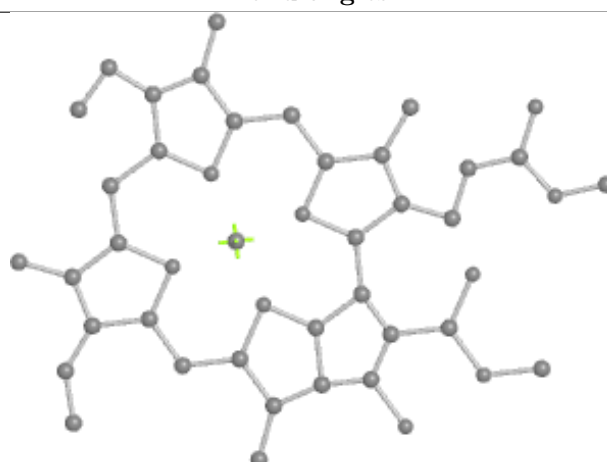
Bond lengths



Bond angles

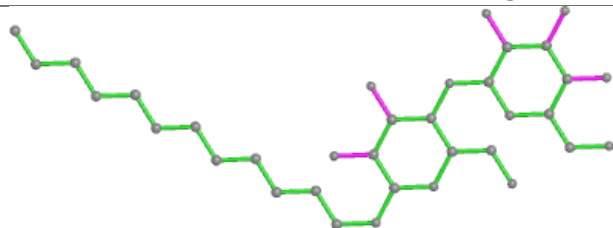


Torsions

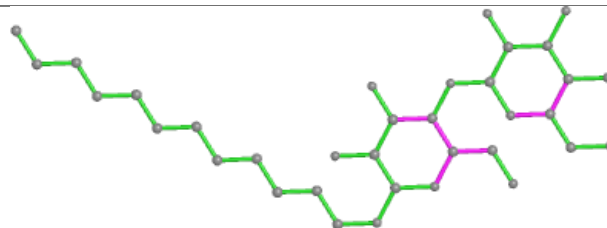


Rings

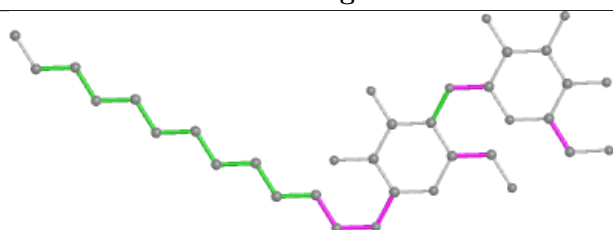
## Ligand LMT U 4101



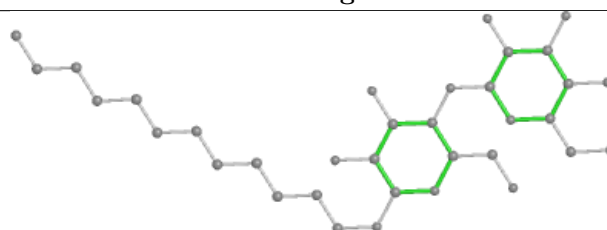
Bond lengths



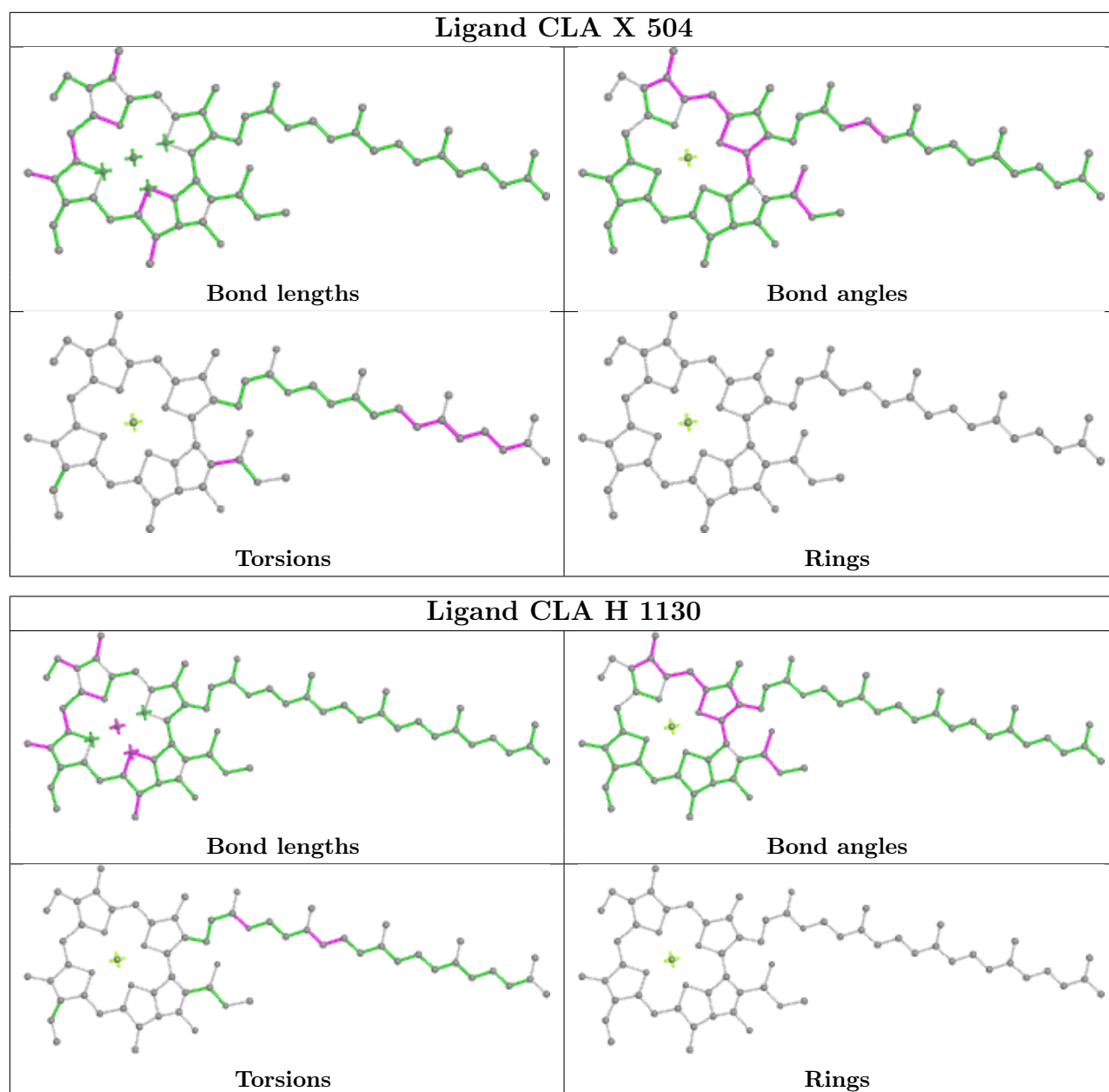
Bond angles



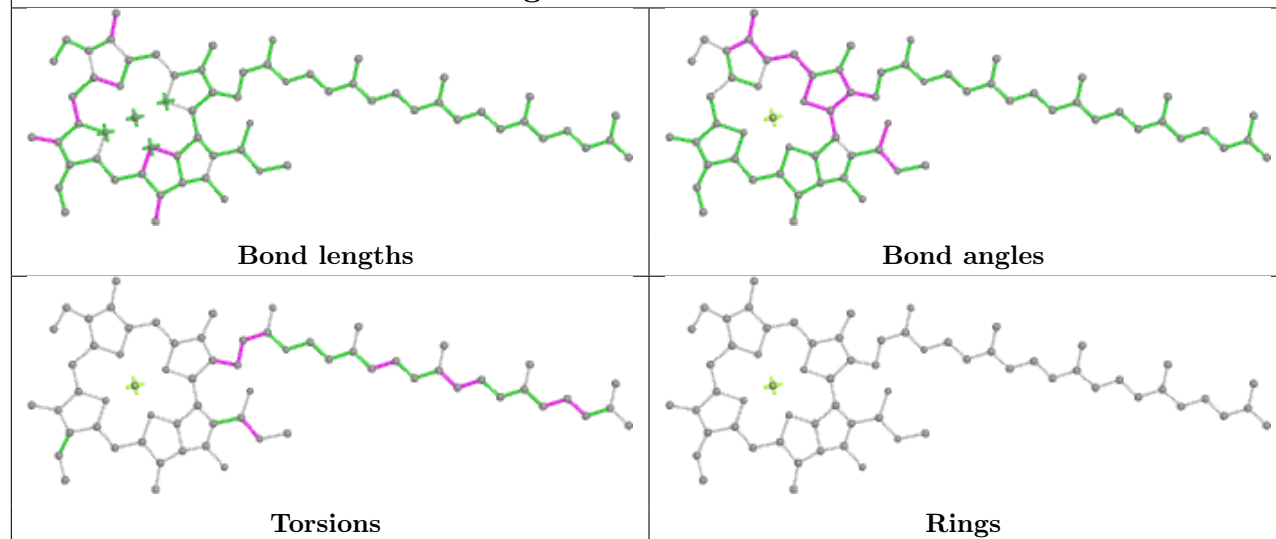
Torsions



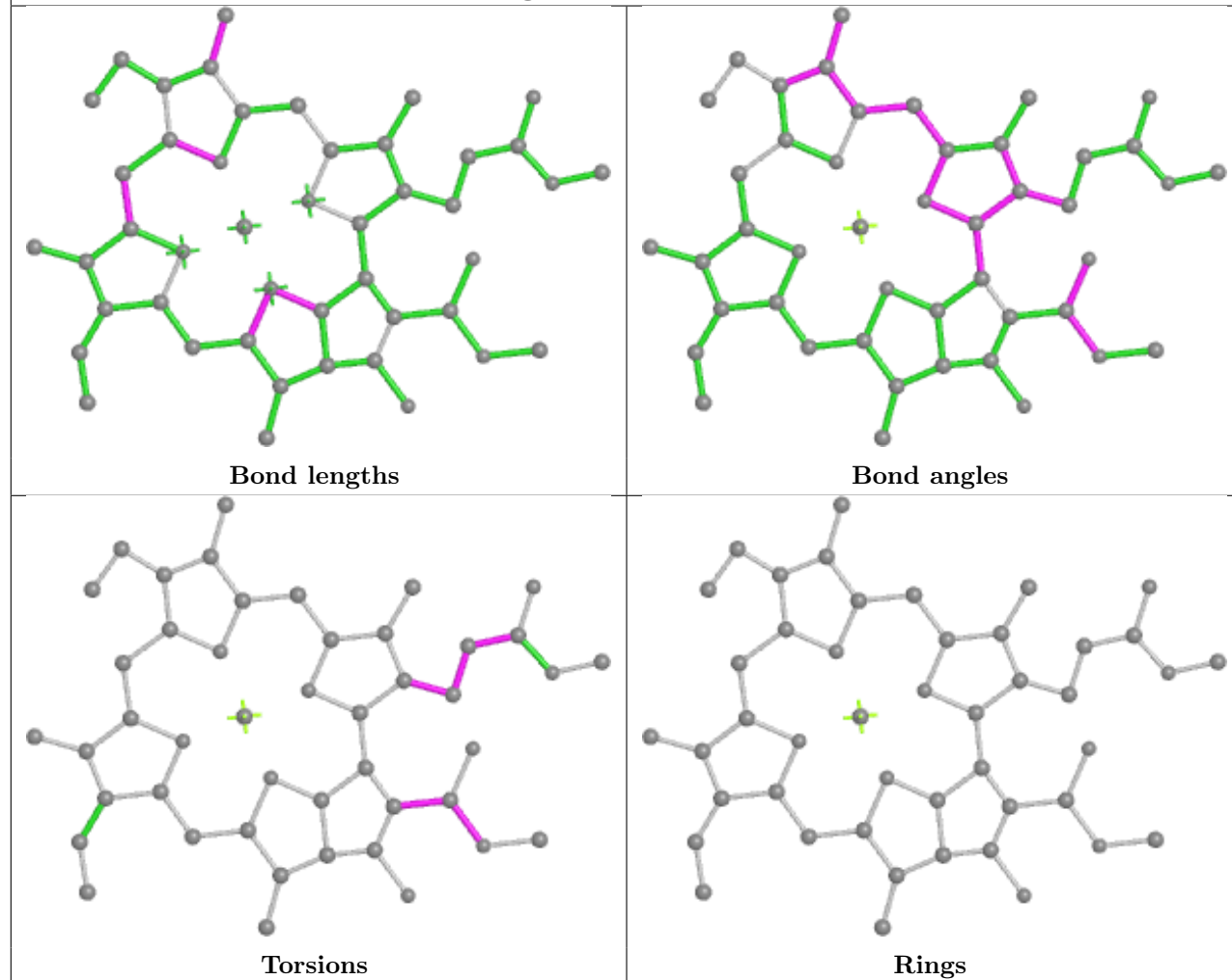
Rings



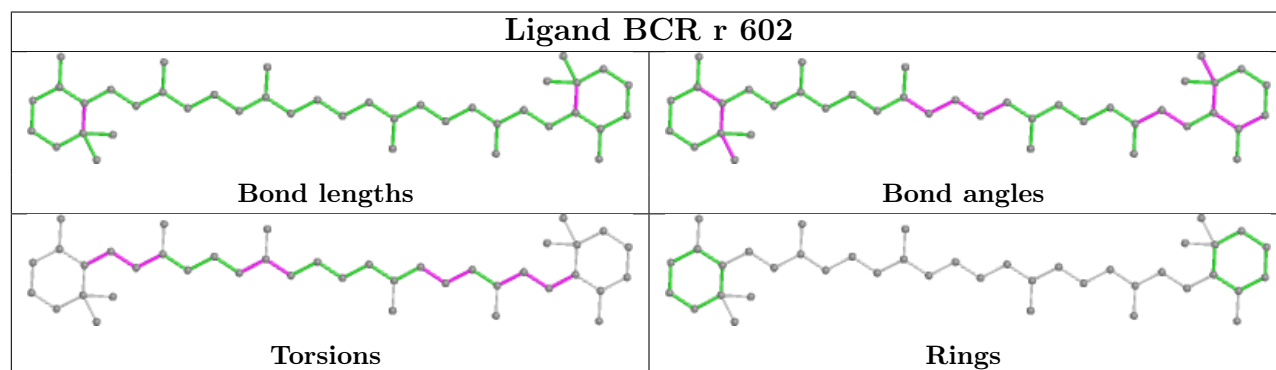
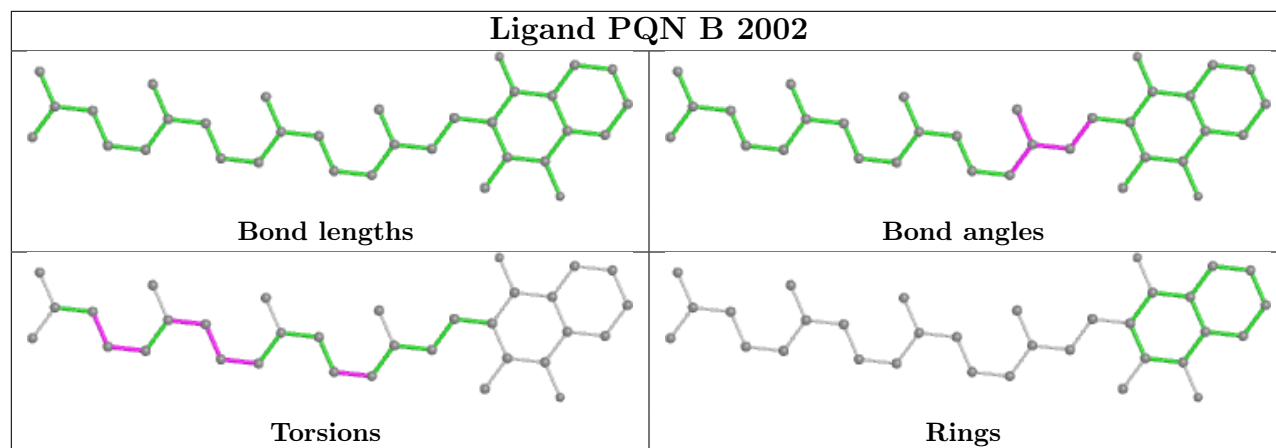
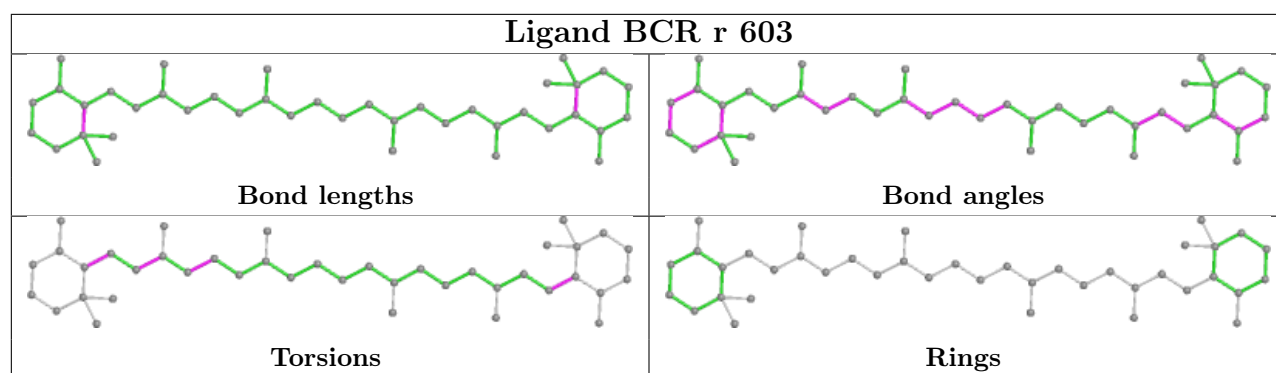
## Ligand CLA B 1206



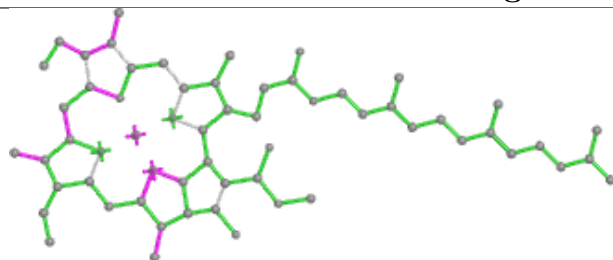
## Ligand CLA r 505



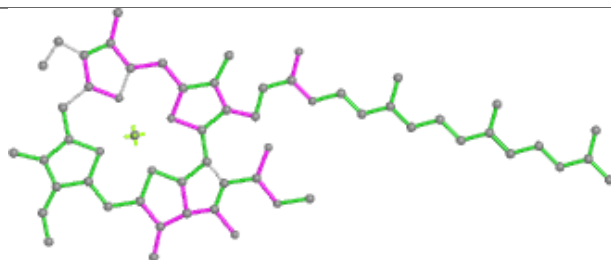




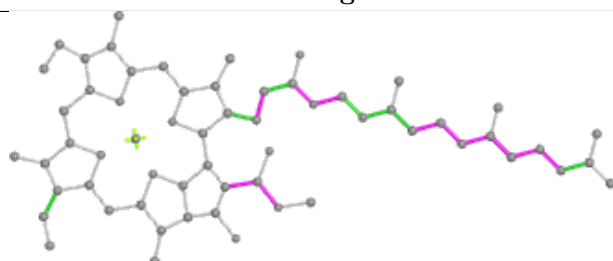
## Ligand CLA G 1012



Bond lengths



Bond angles

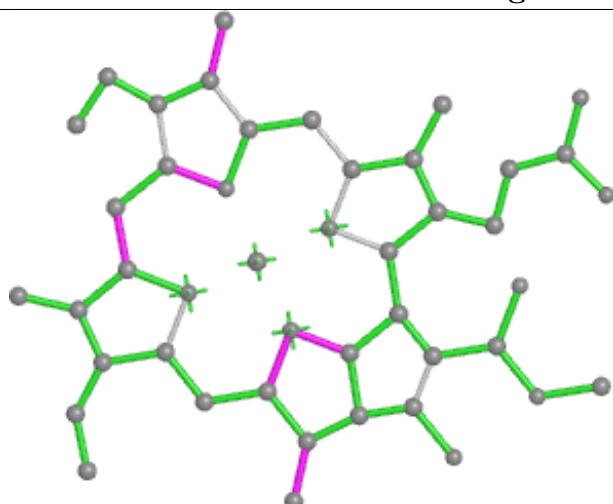


Torsions

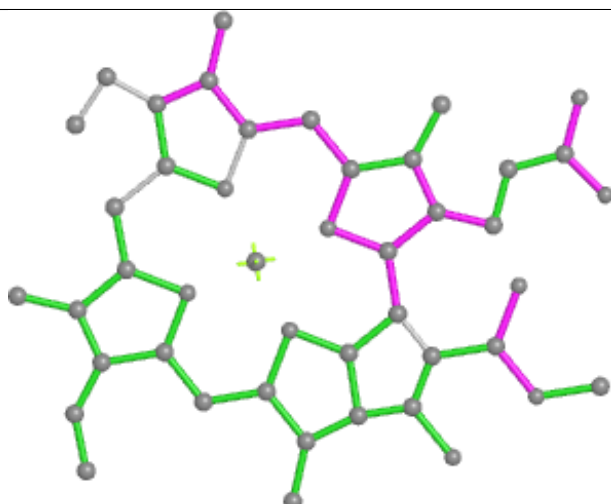


Rings

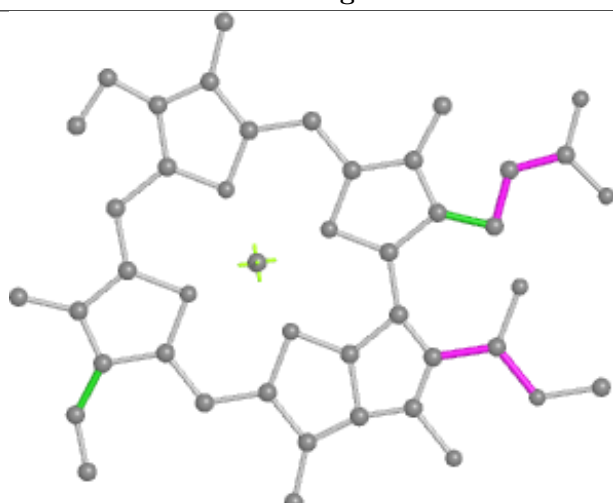
## Ligand CLA b 1219



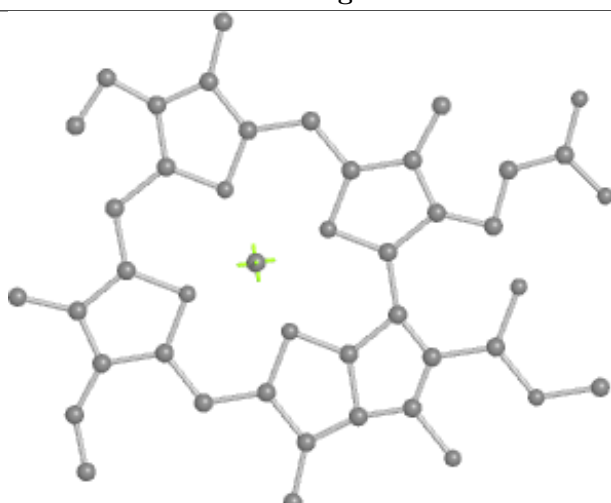
Bond lengths



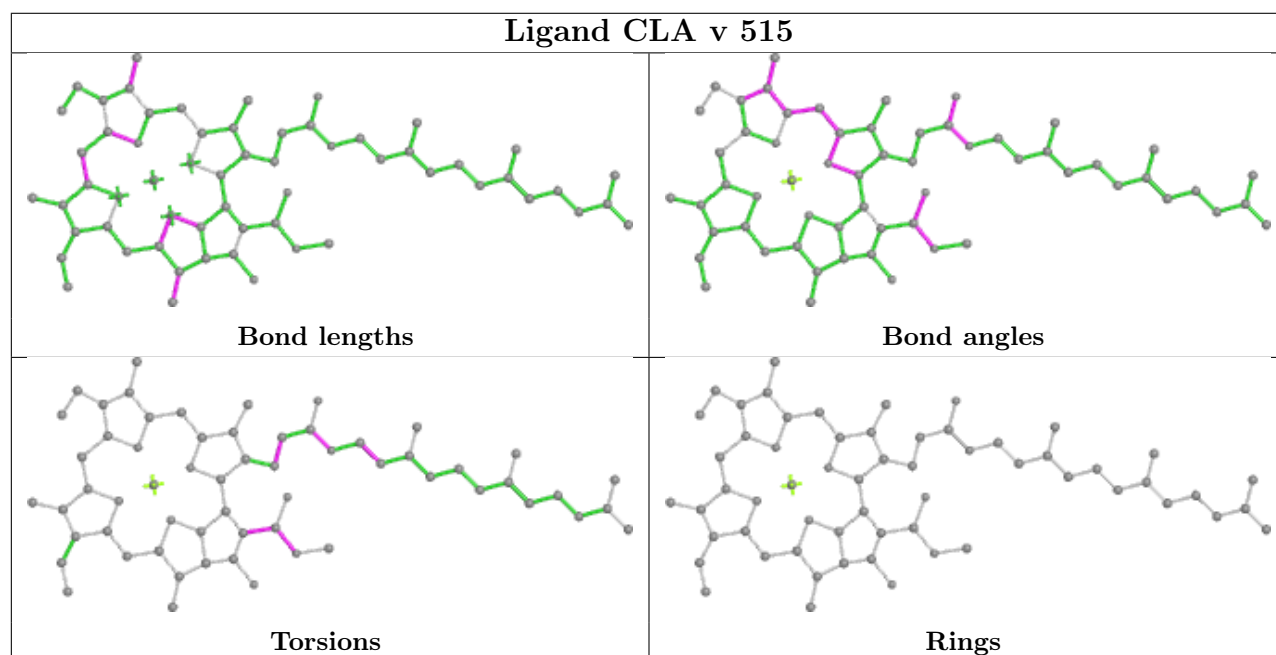
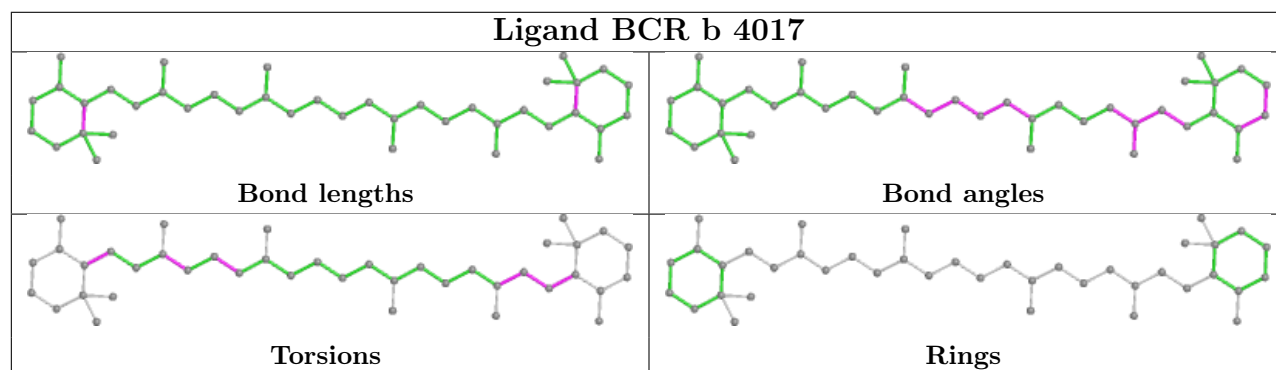
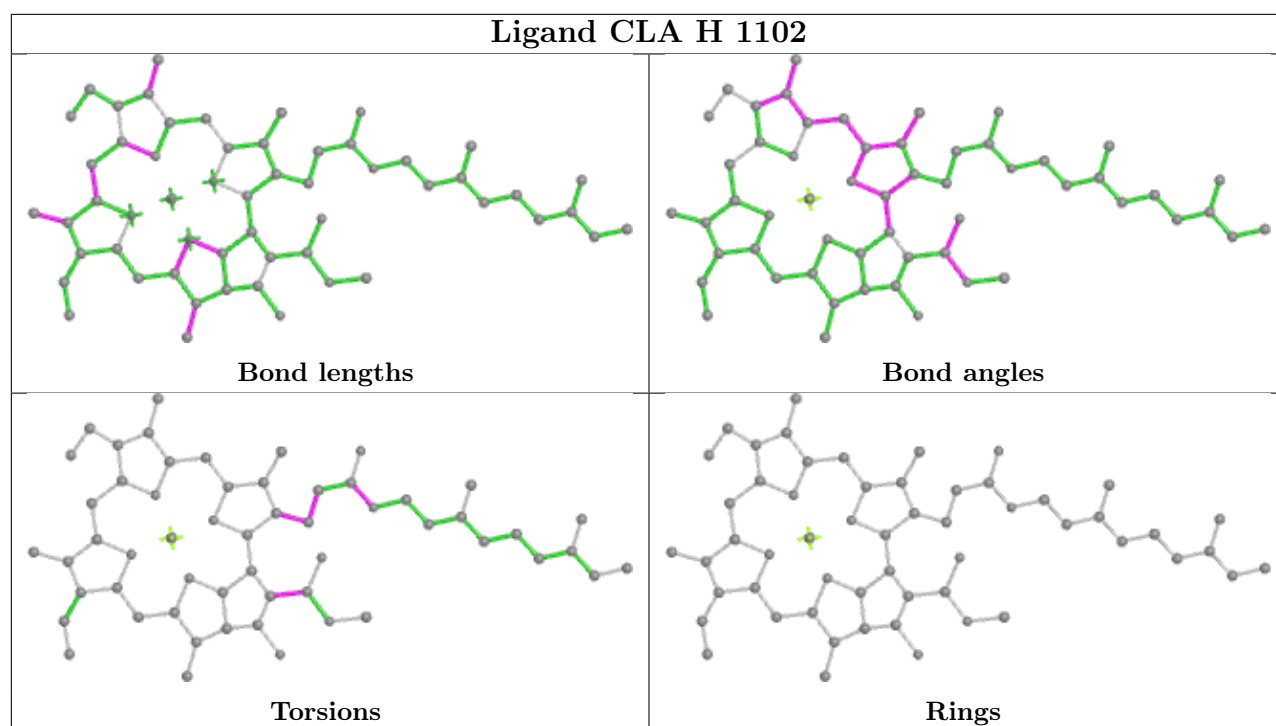
Bond angles

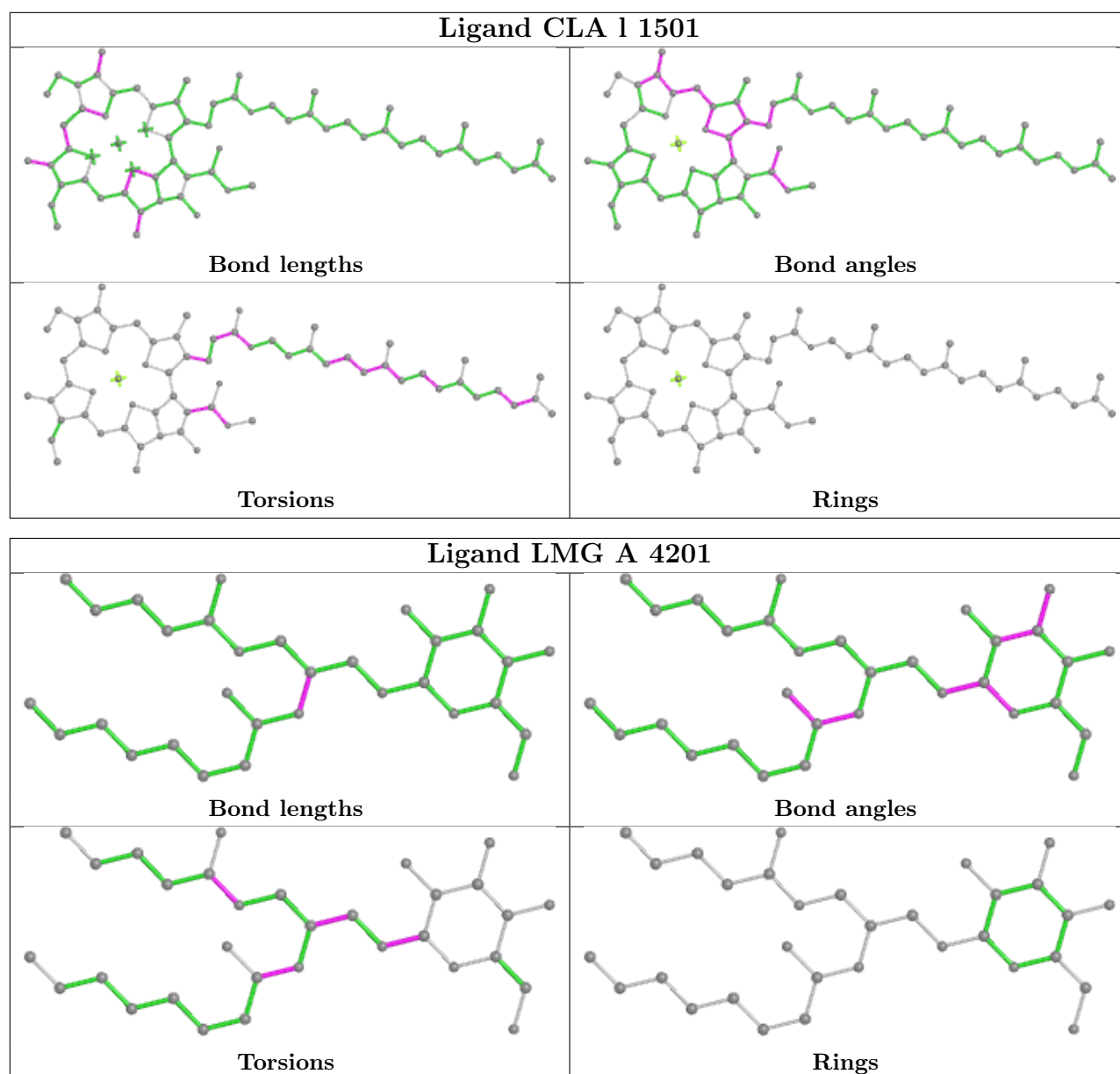


Torsions

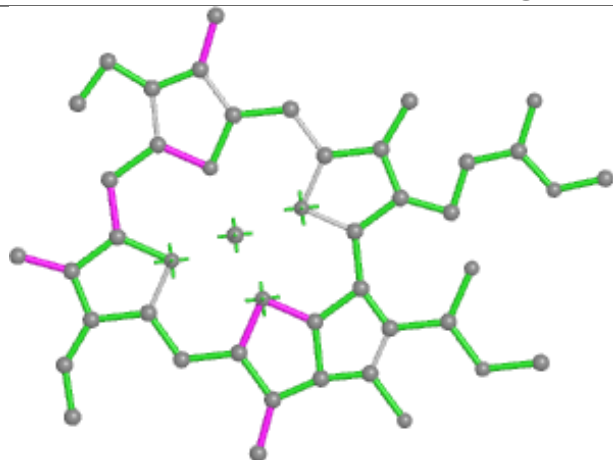


Rings

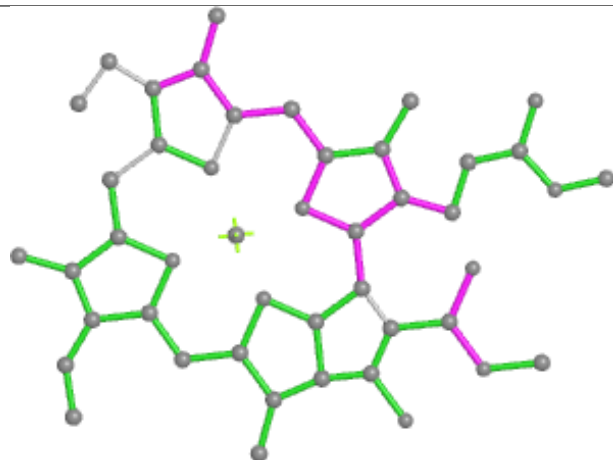




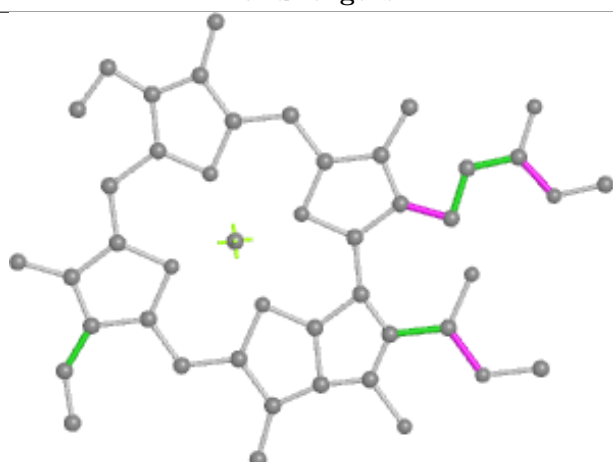
## Ligand CLA u 503



Bond lengths



Bond angles

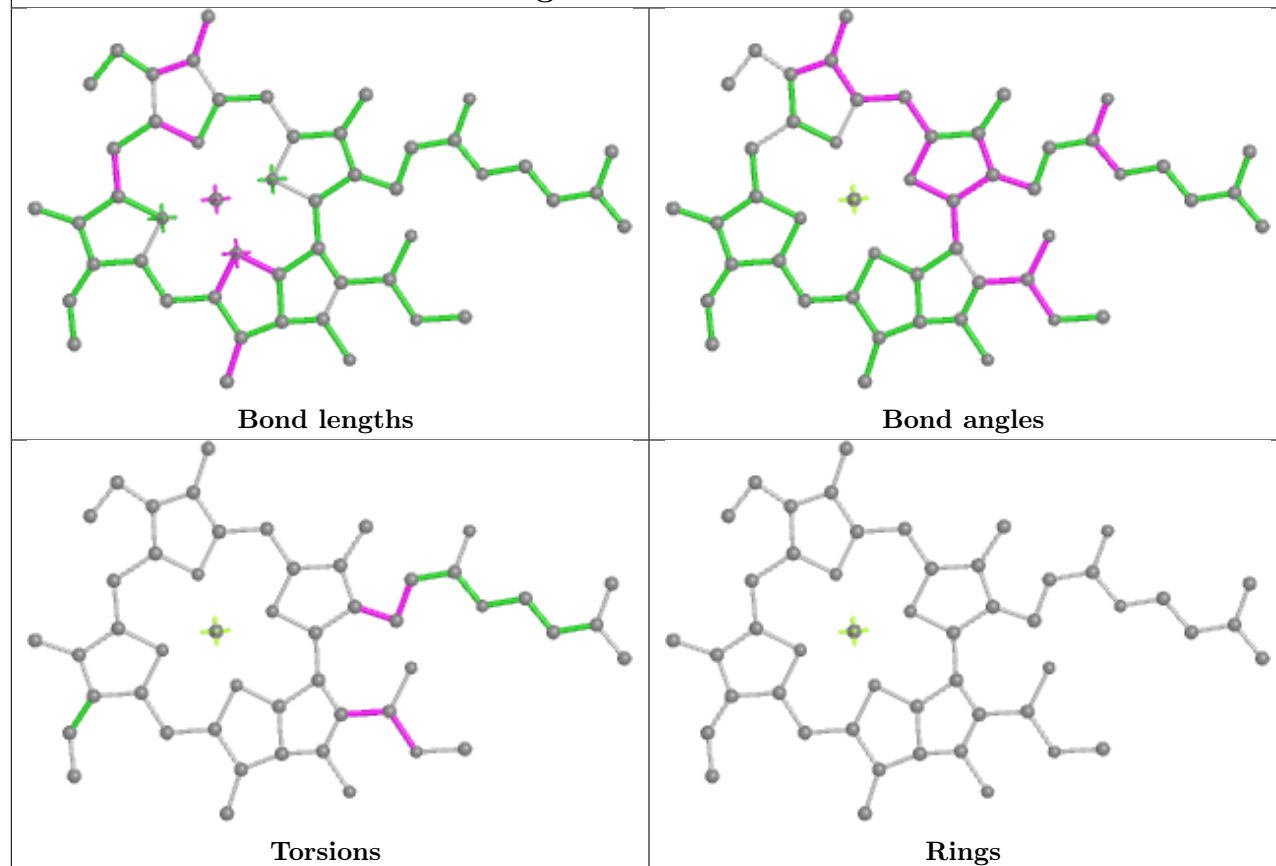


Torsions

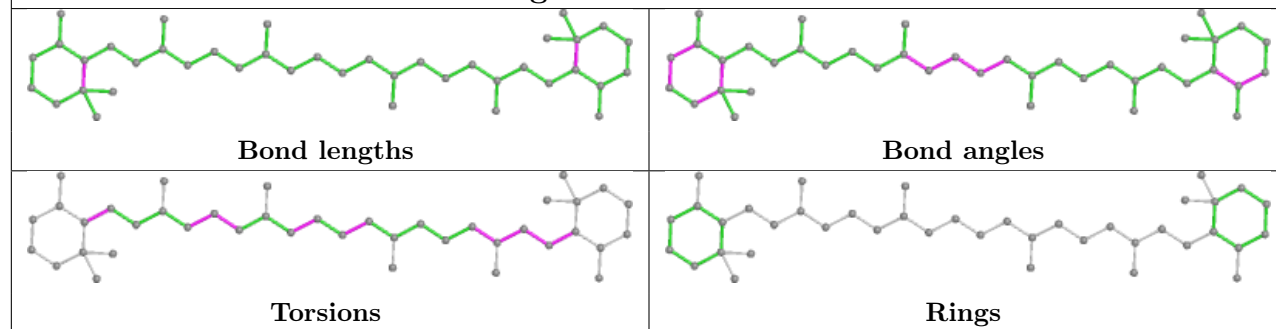


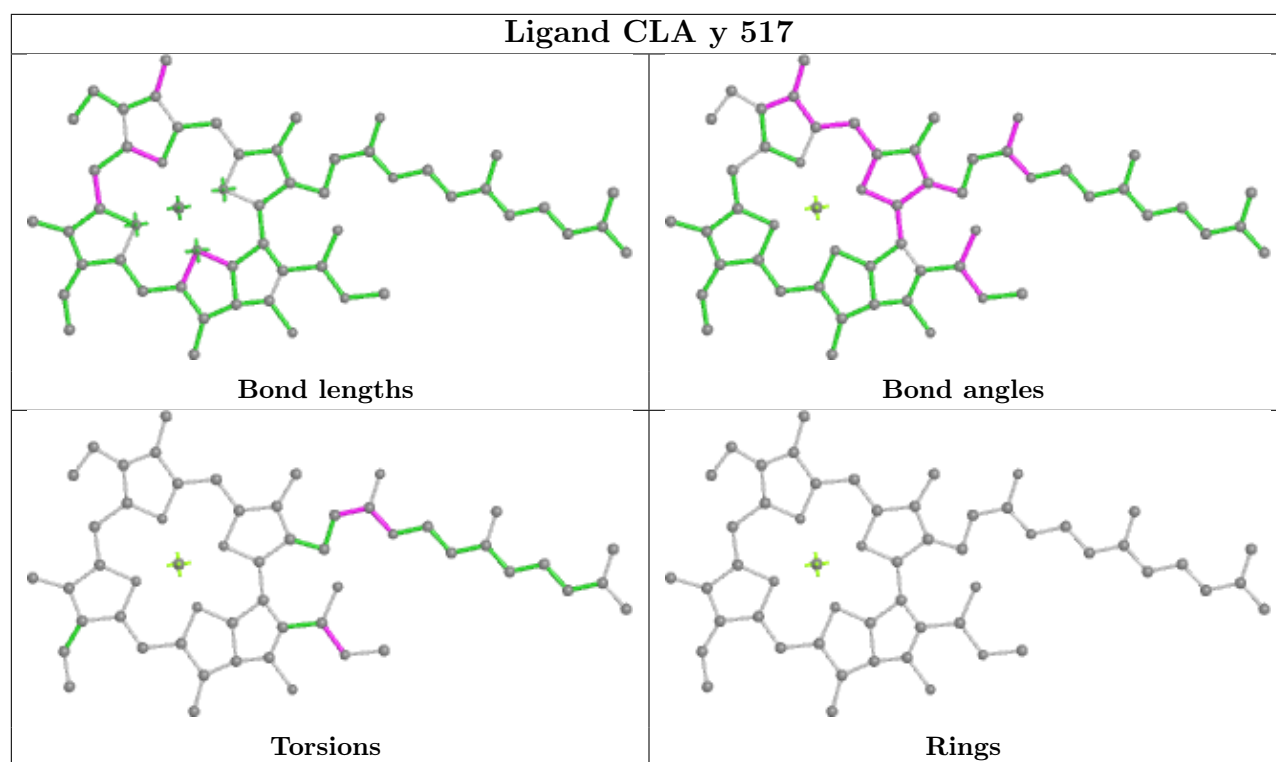
Rings

## Ligand CLA o 502

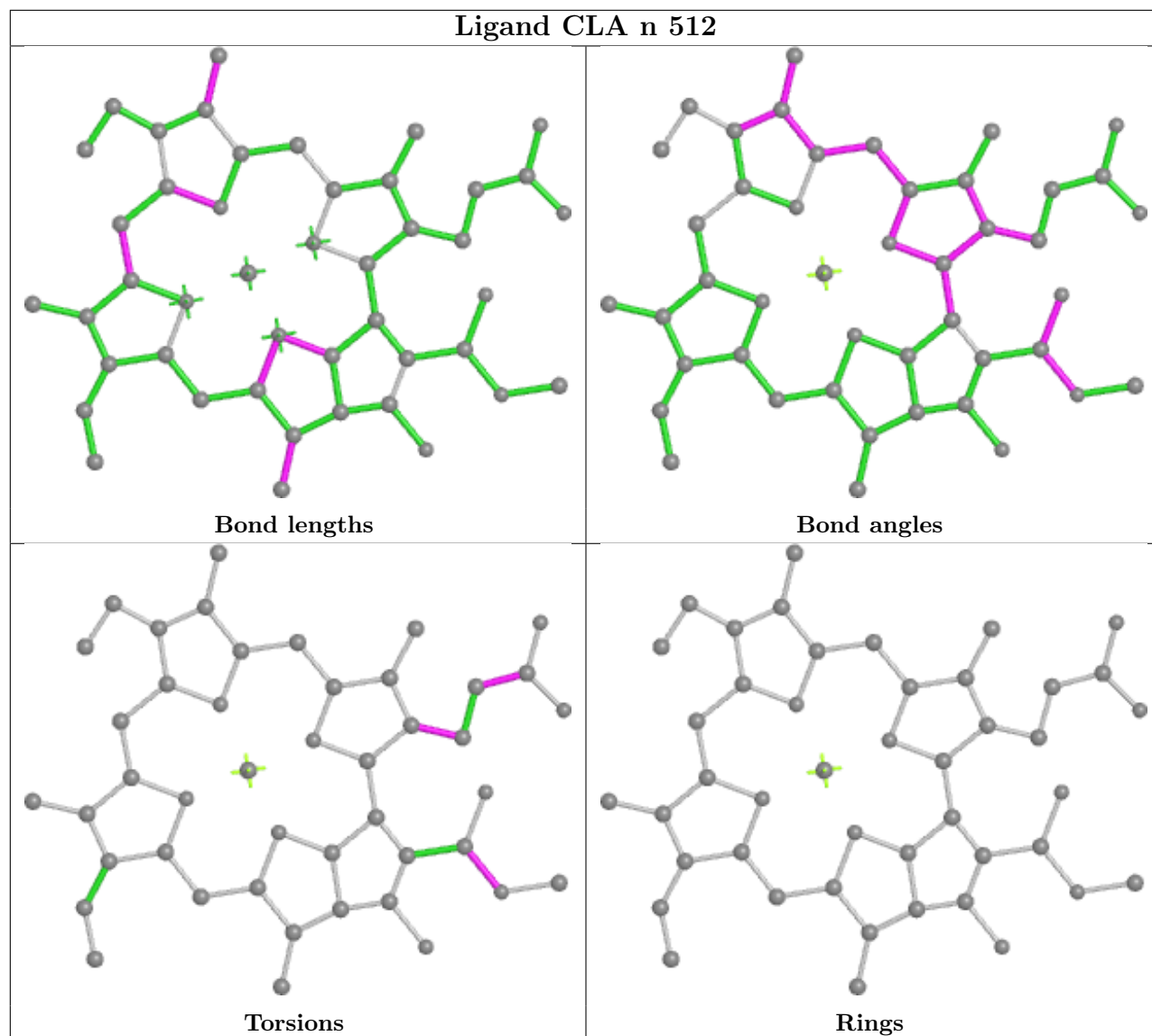


## Ligand BCR Y 604



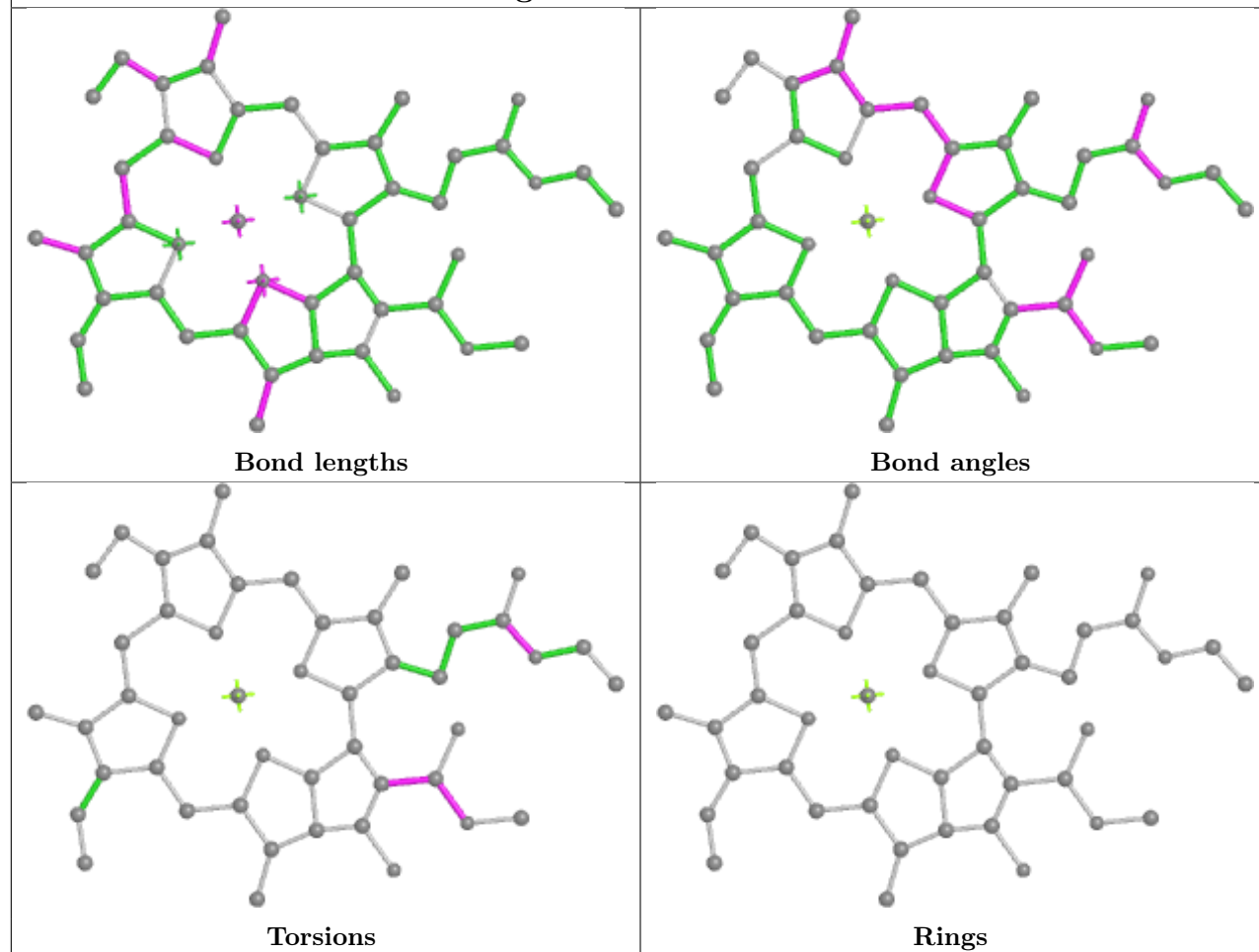


## Ligand CLA n 512

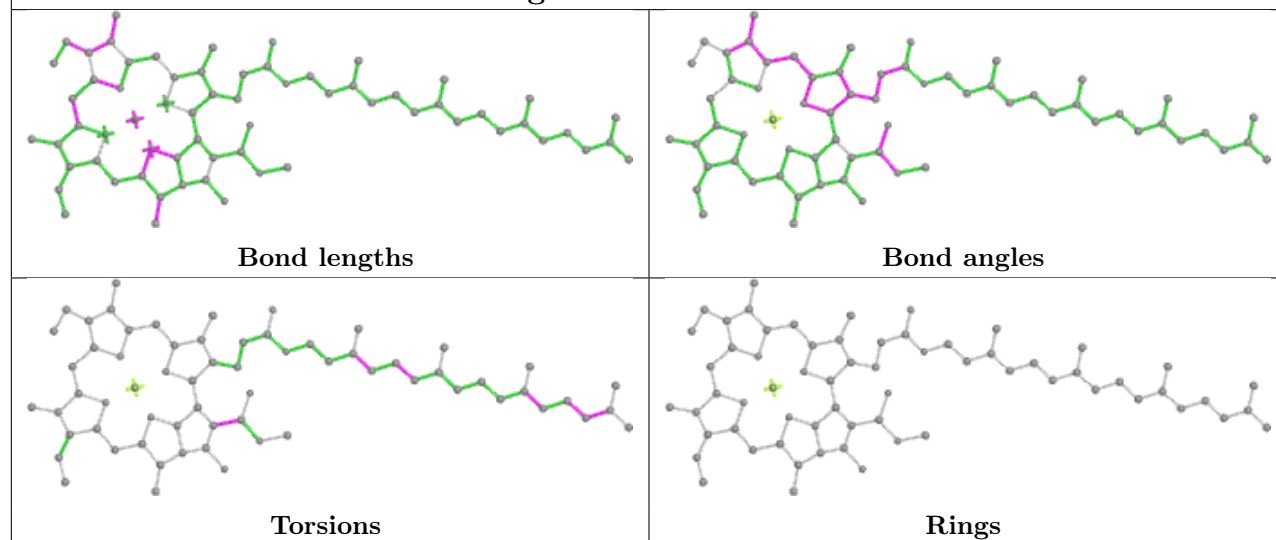




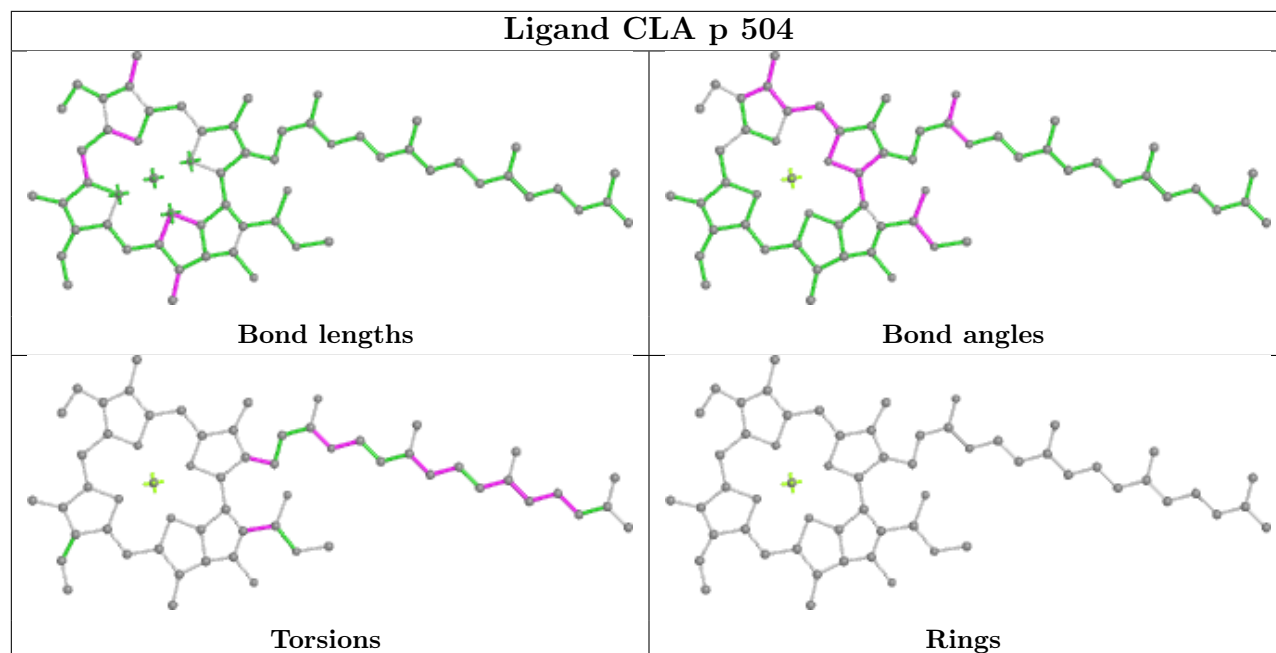
## Ligand CLA A 1137



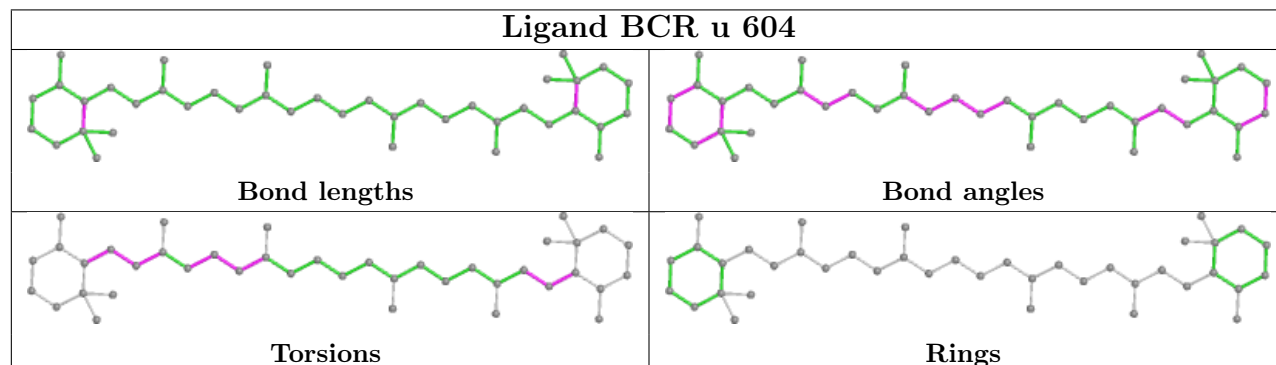
## Ligand CLA a 1124



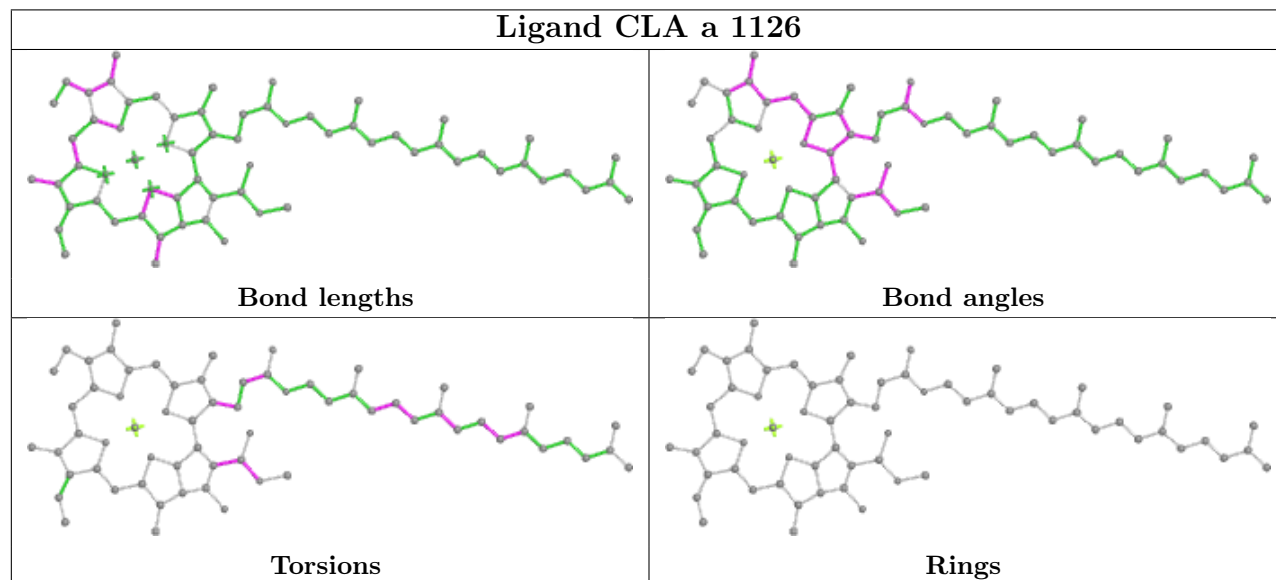
## Ligand CLA p 504

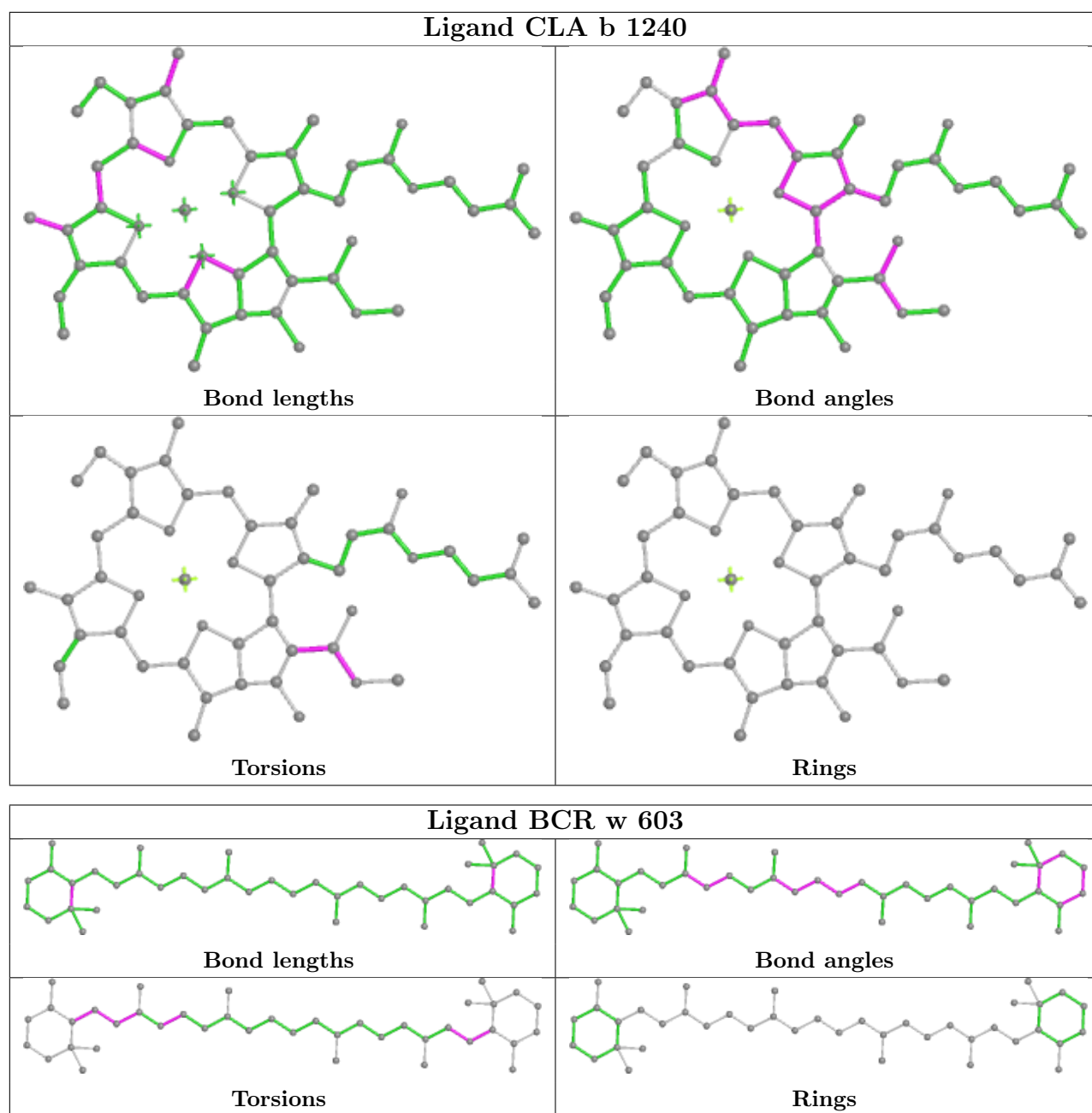


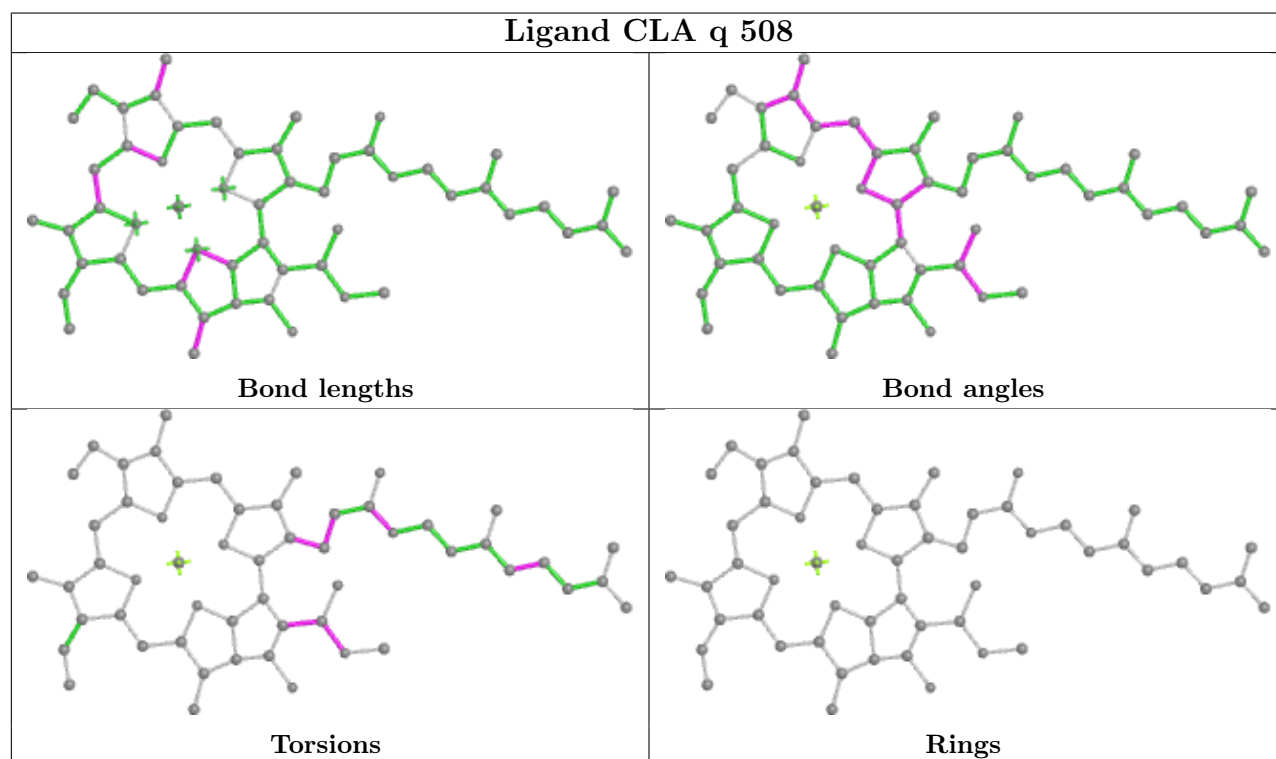
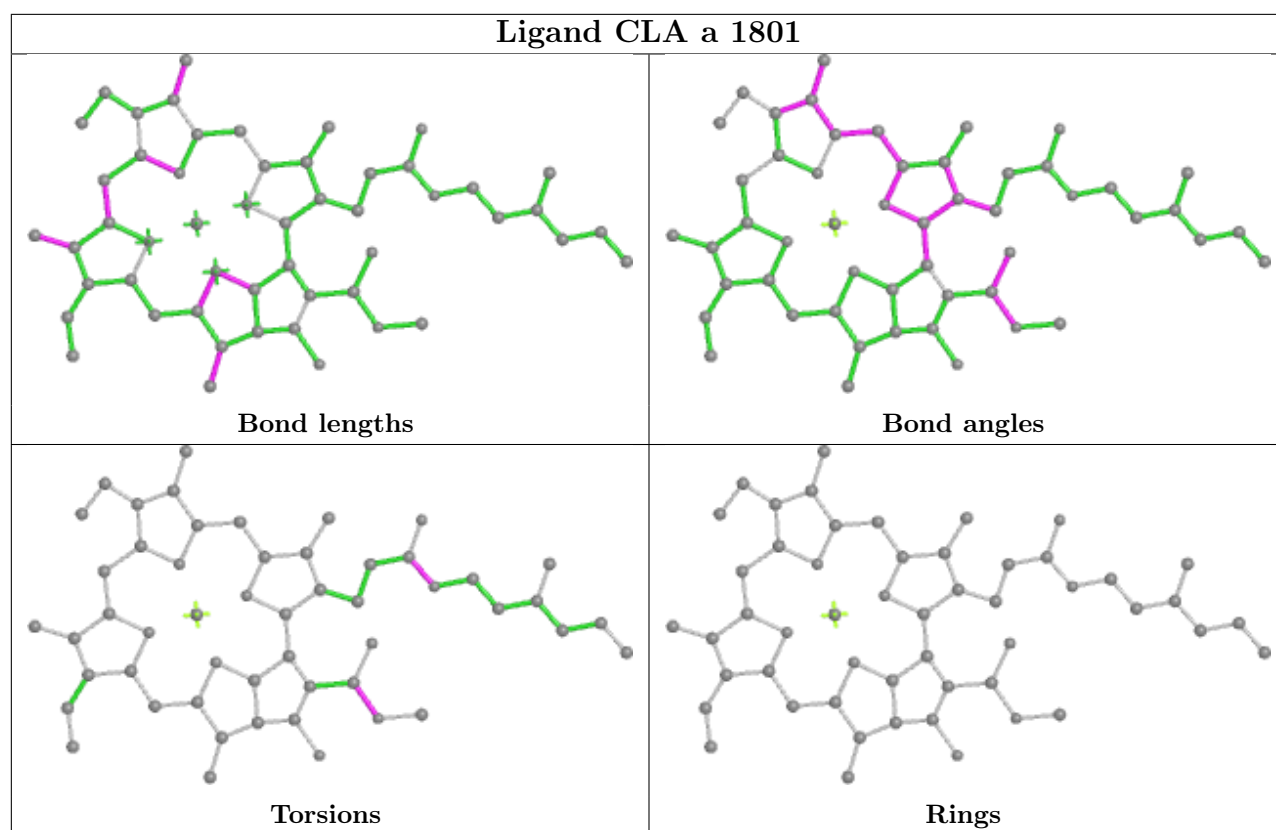
## Ligand BCR u 604

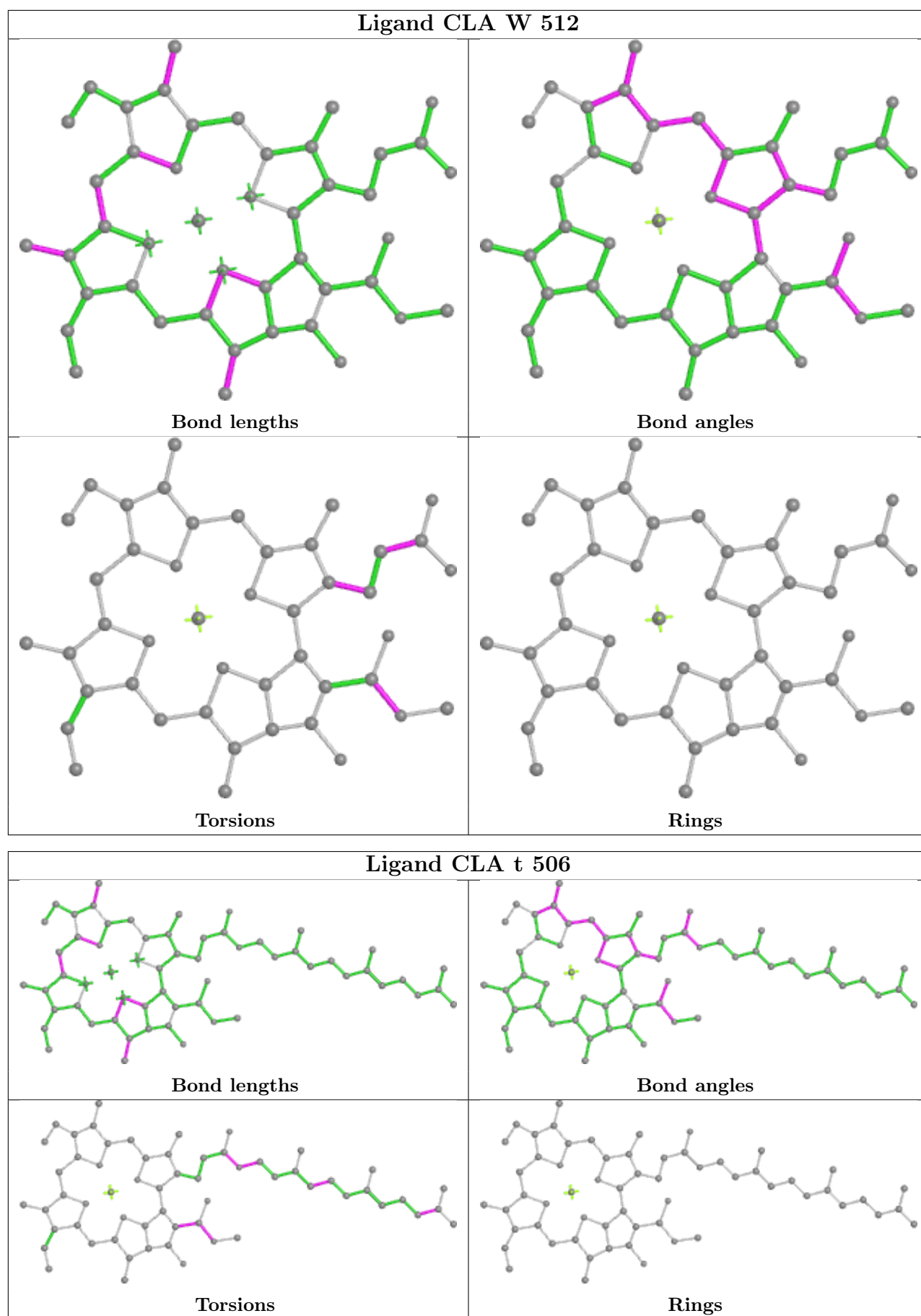


## Ligand CLA a 1126

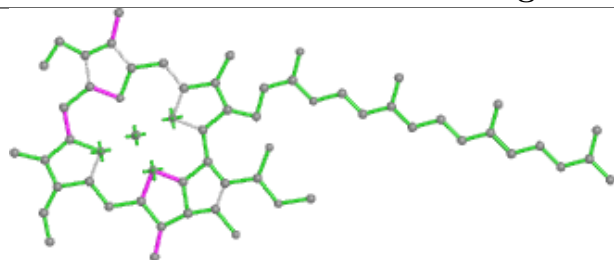




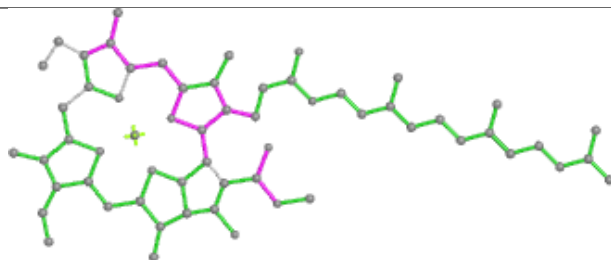




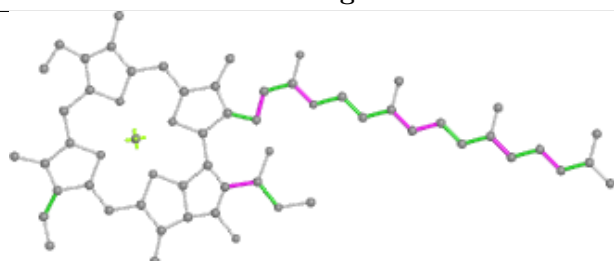
## Ligand CLA x 504



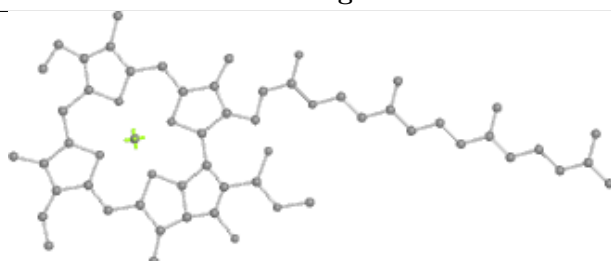
Bond lengths



Bond angles

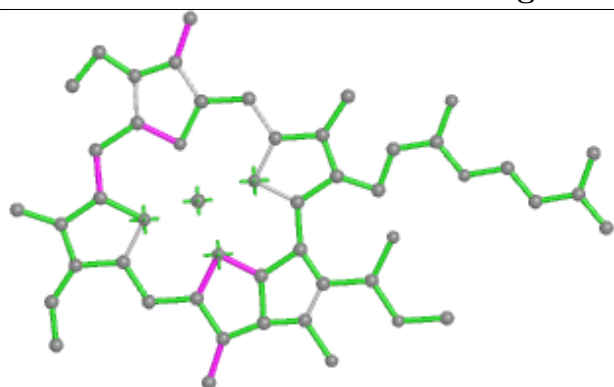


Torsions

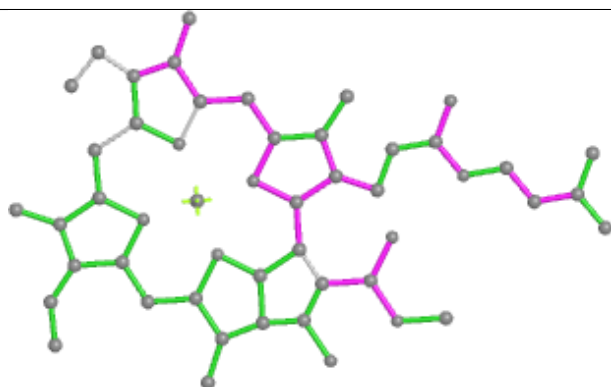


Rings

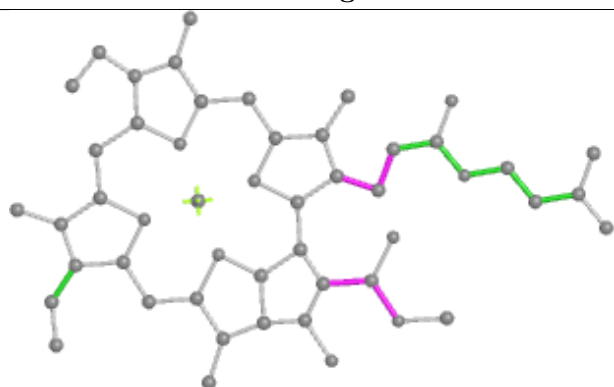
## Ligand CLA u 502



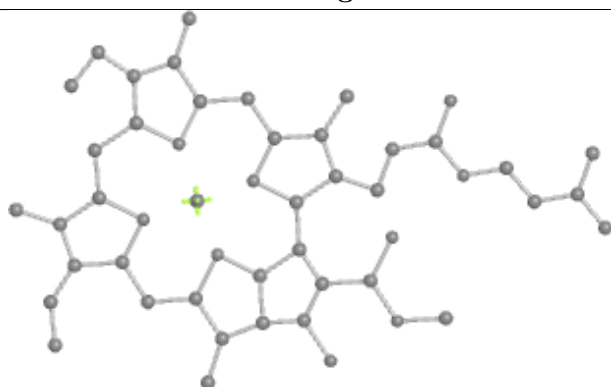
Bond lengths



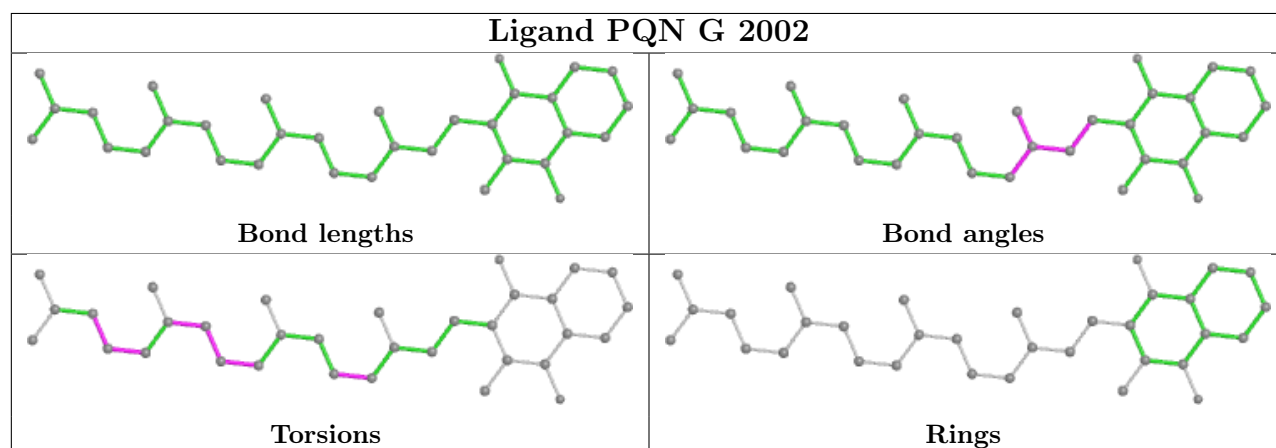
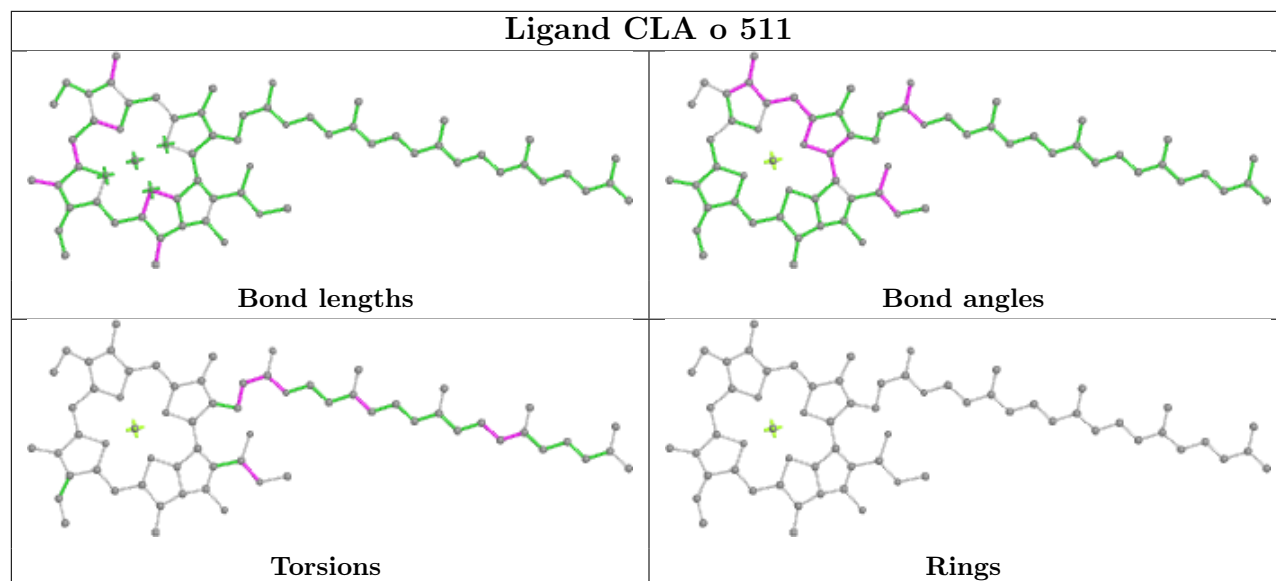
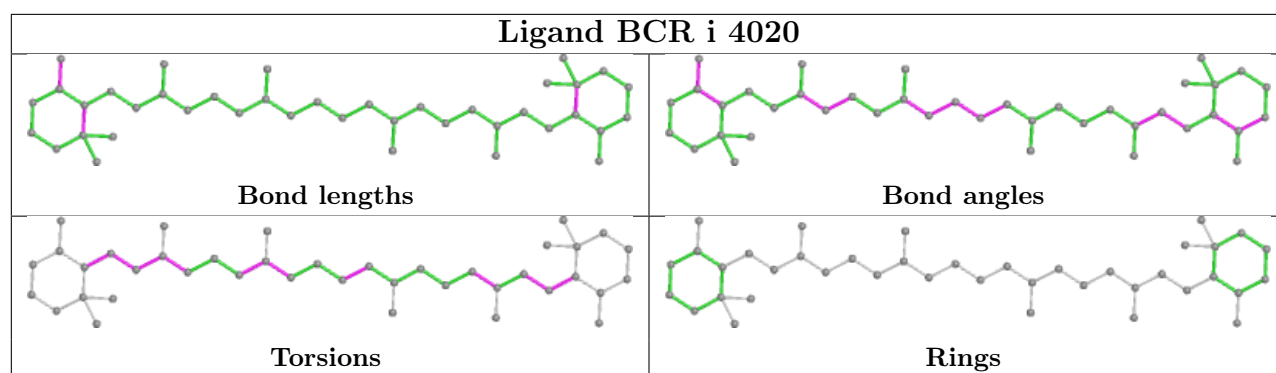
Bond angles



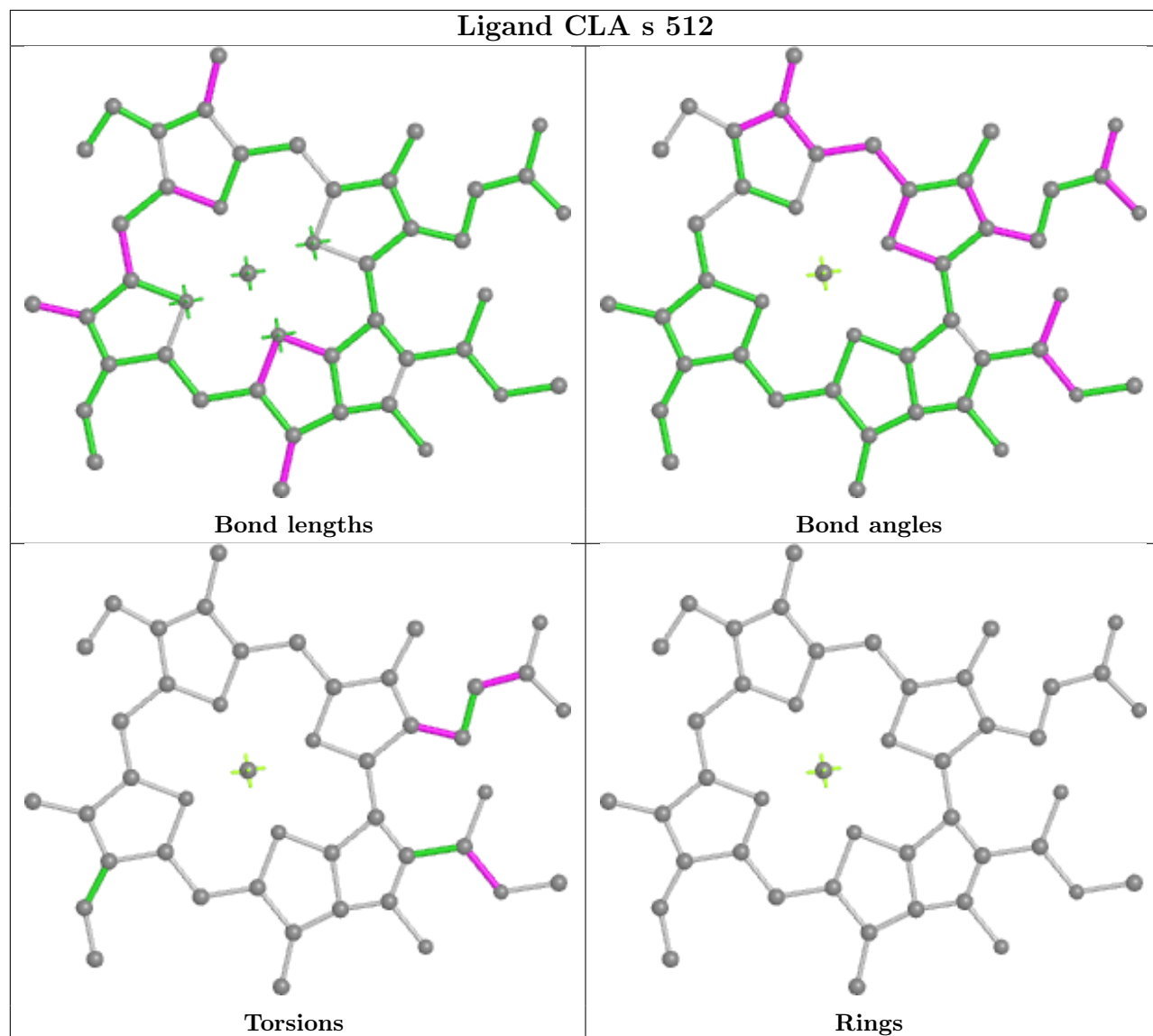
Torsions



Rings

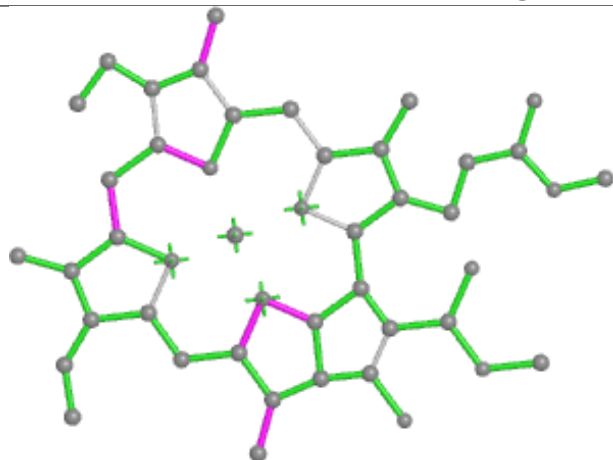


## Ligand CLA s 512

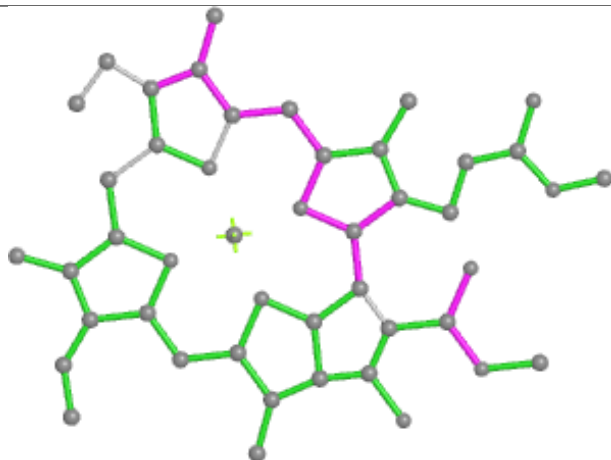




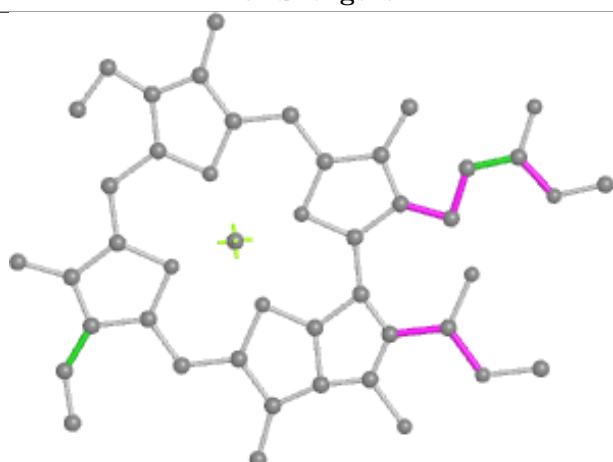
## Ligand CLA Y 516



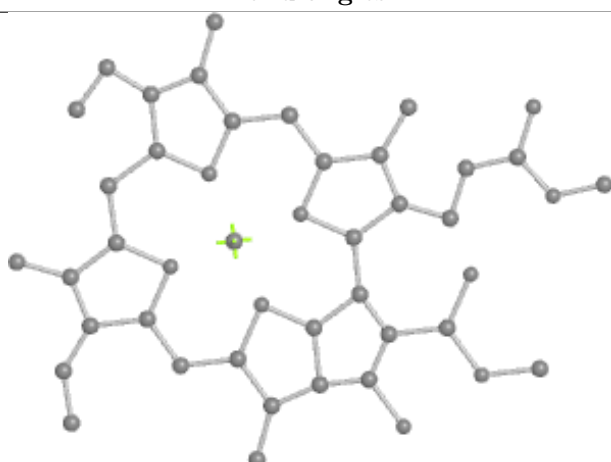
Bond lengths



Bond angles

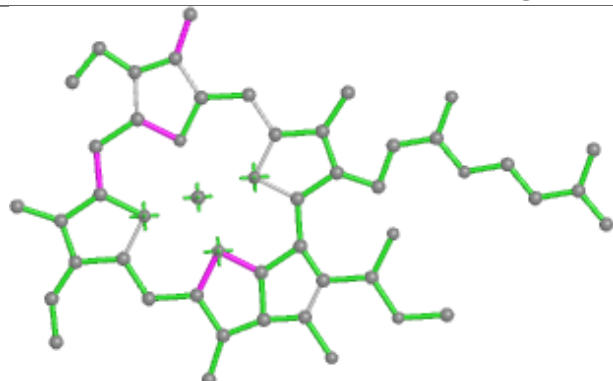


Torsions

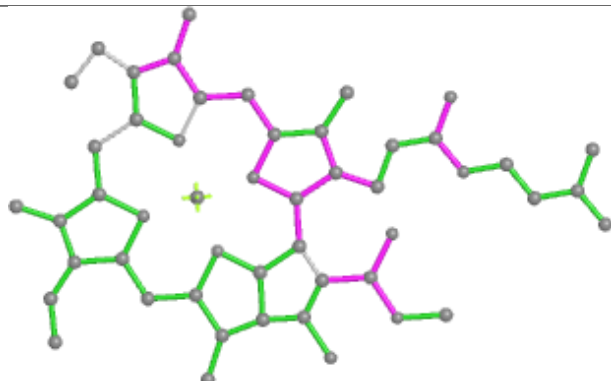


Rings

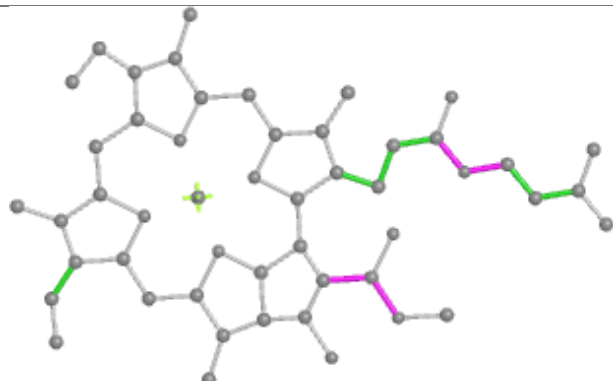
## Ligand CLA u 501



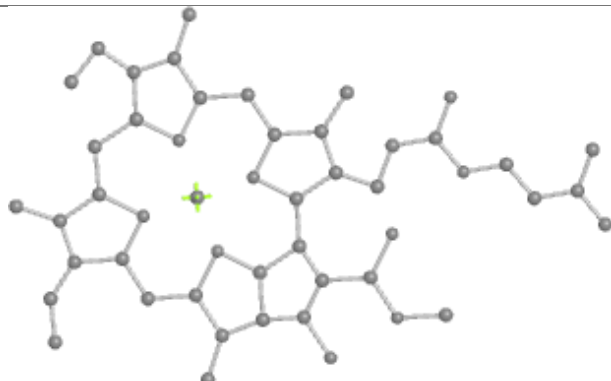
Bond lengths



Bond angles

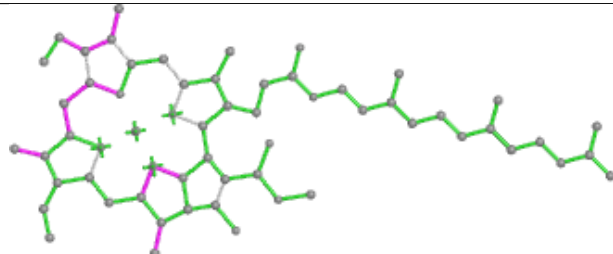


Torsions

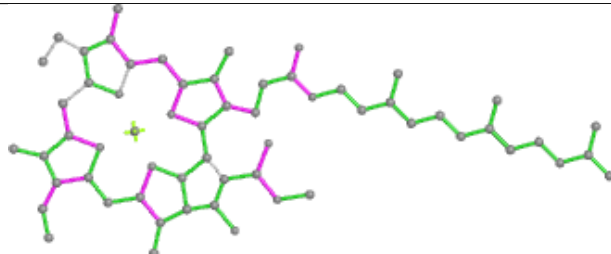


Rings

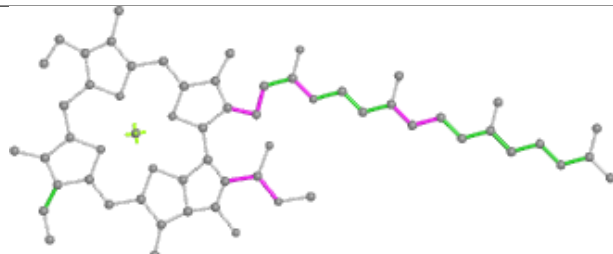
## Ligand CLA g 506



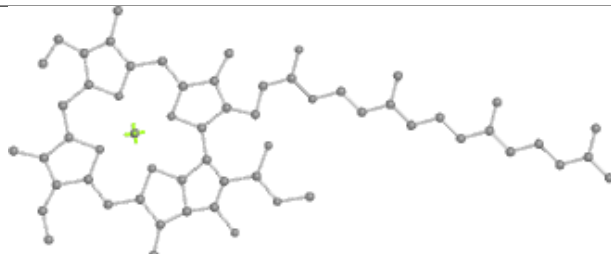
Bond lengths



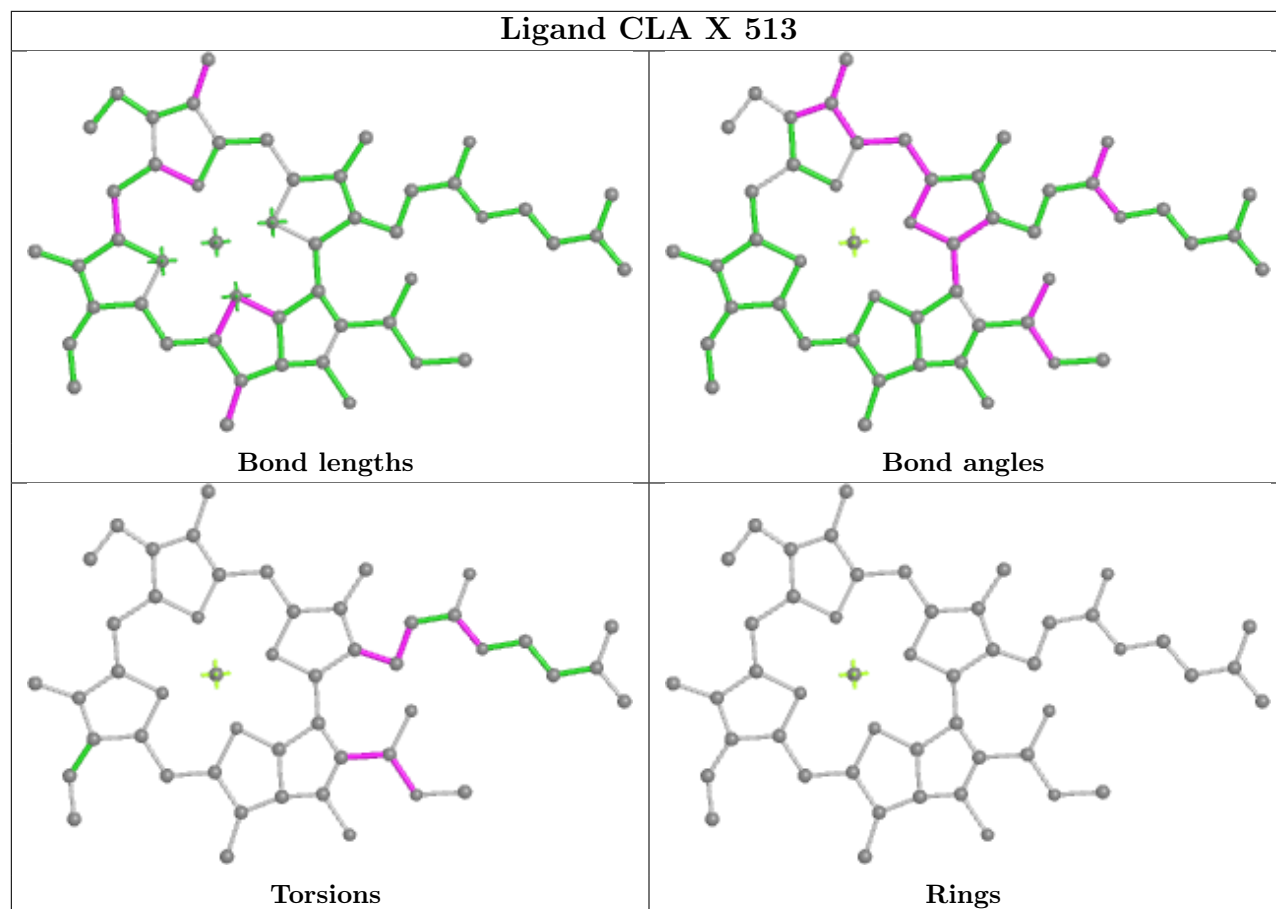
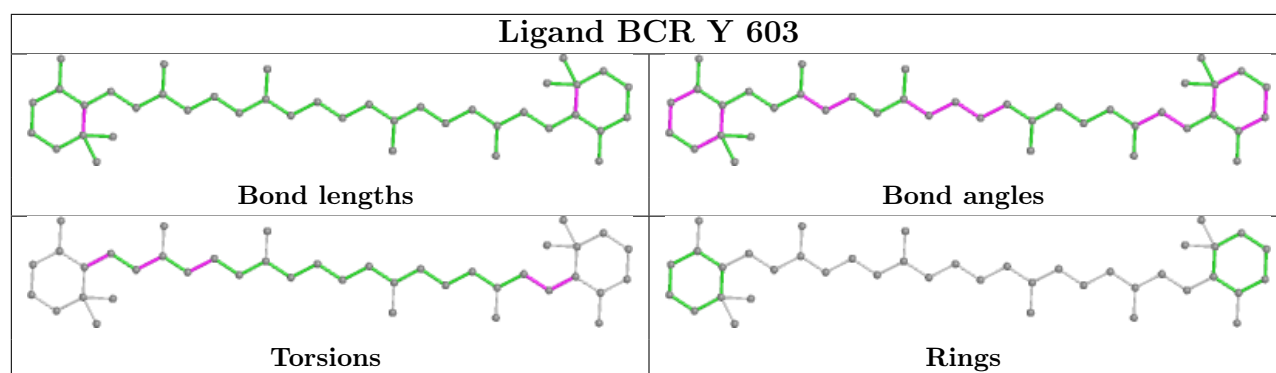
Bond angles



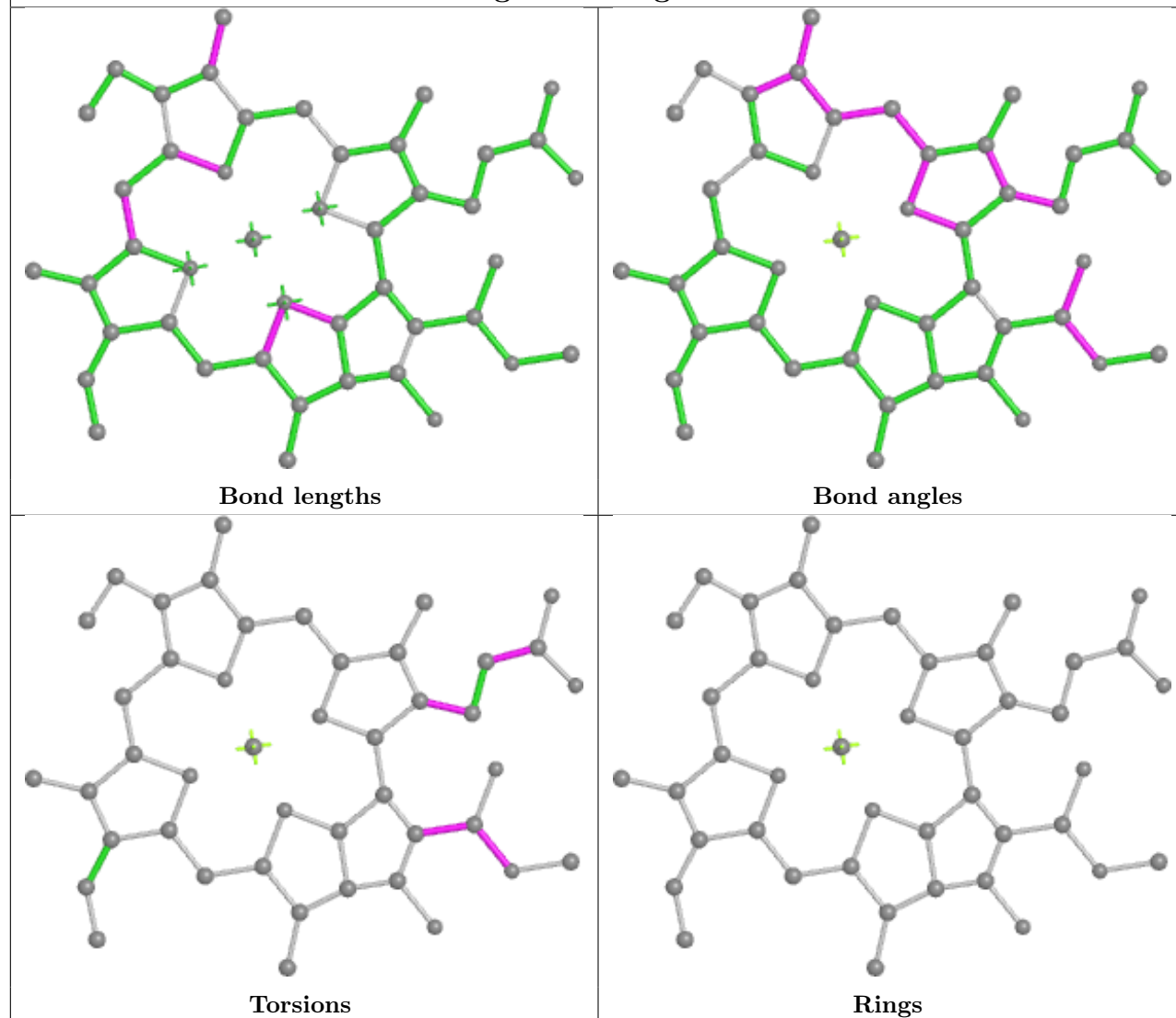
Torsions



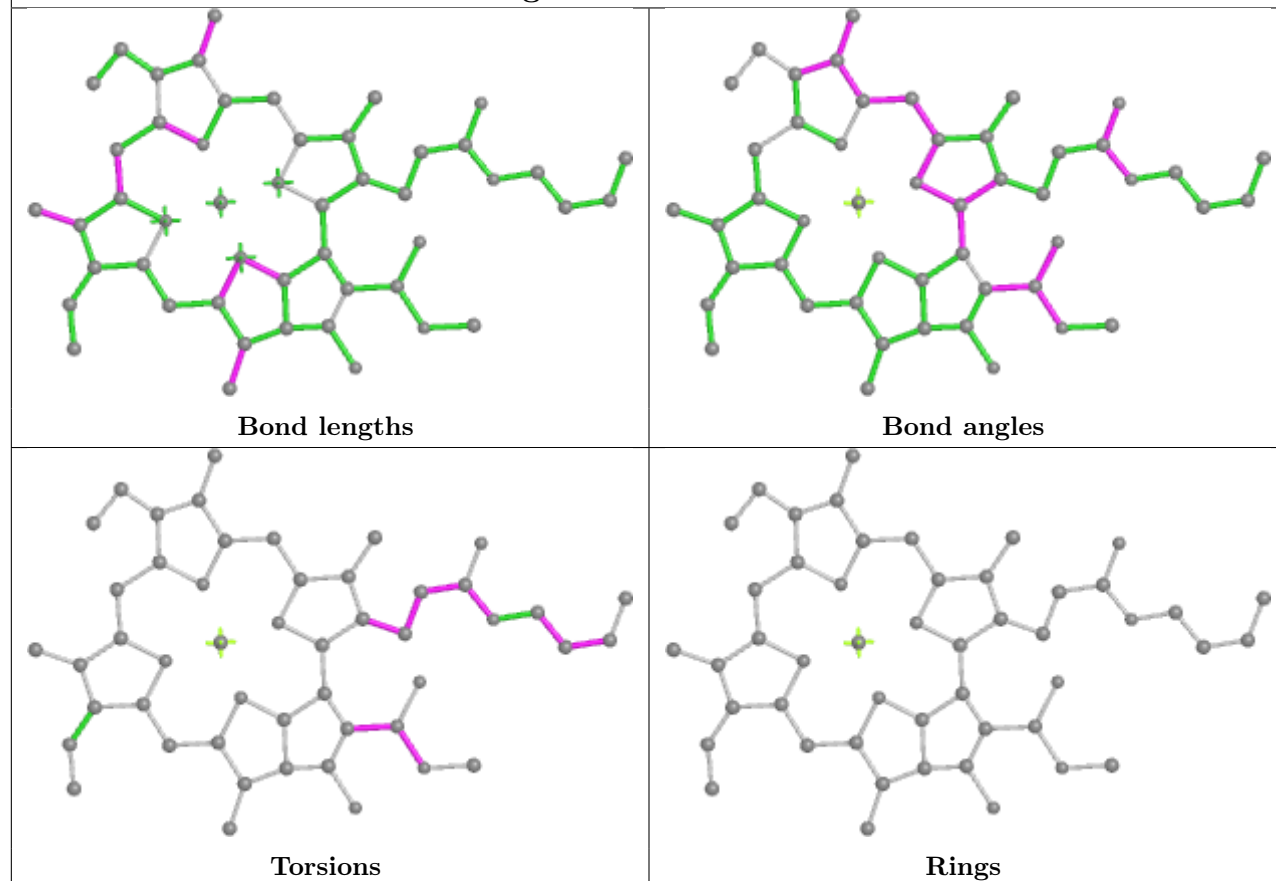
Rings



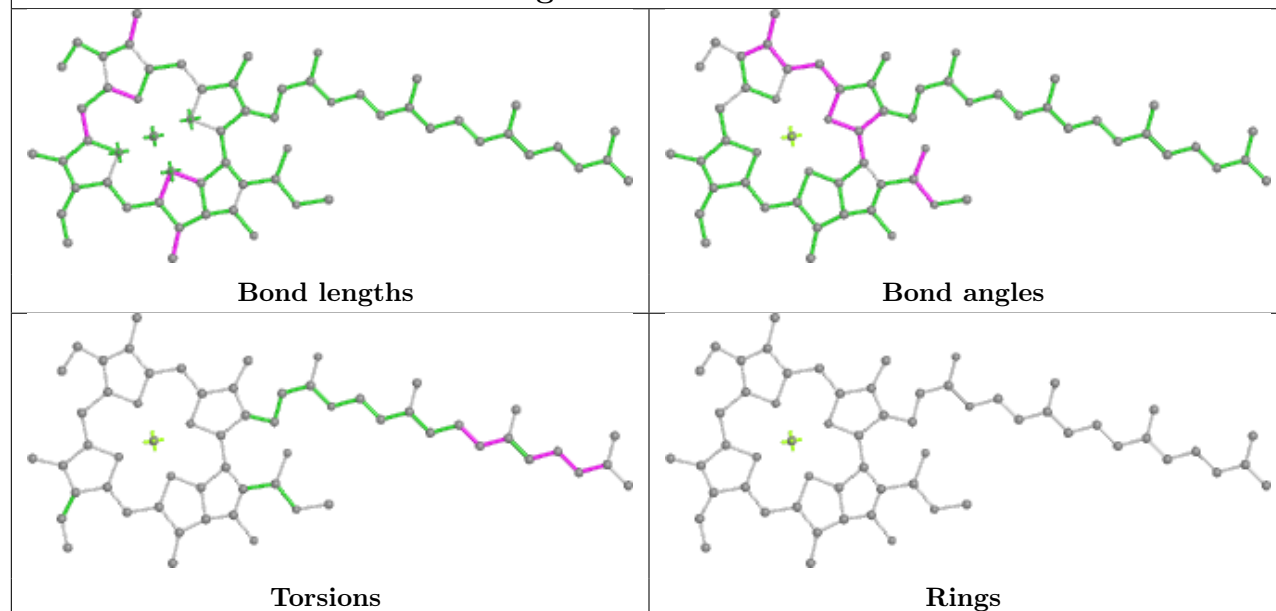
## Ligand CLA g 512

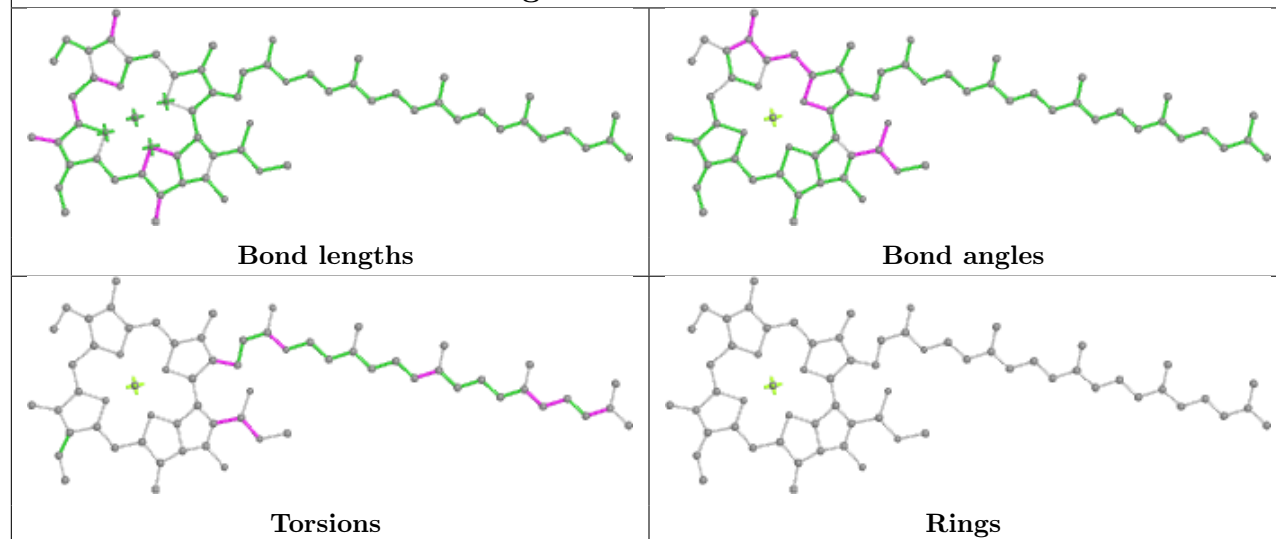
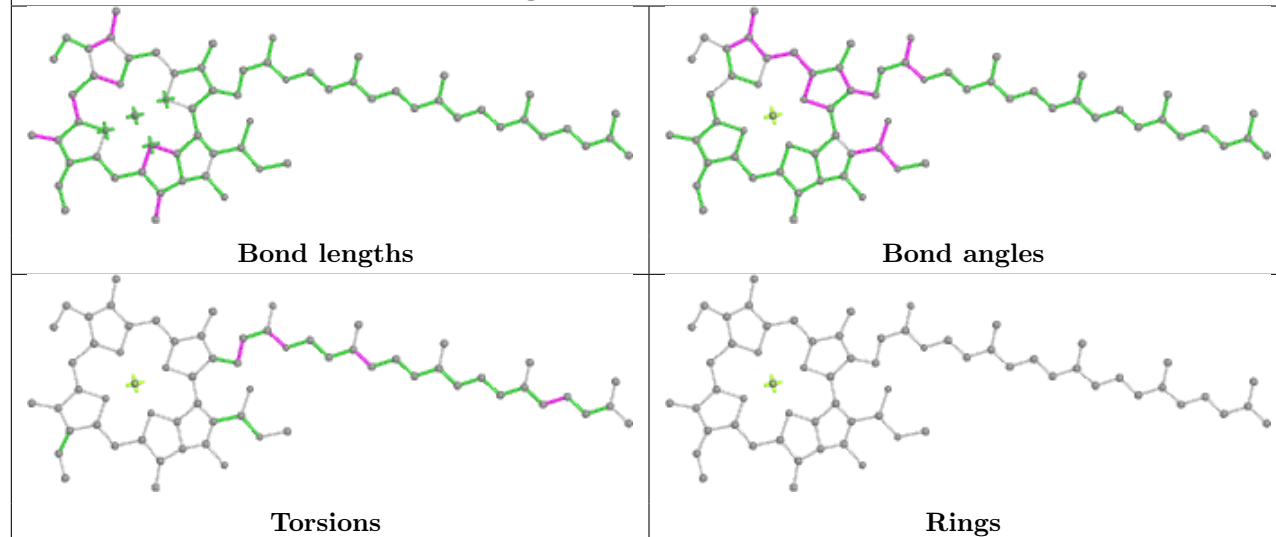


## Ligand CLA A 1120

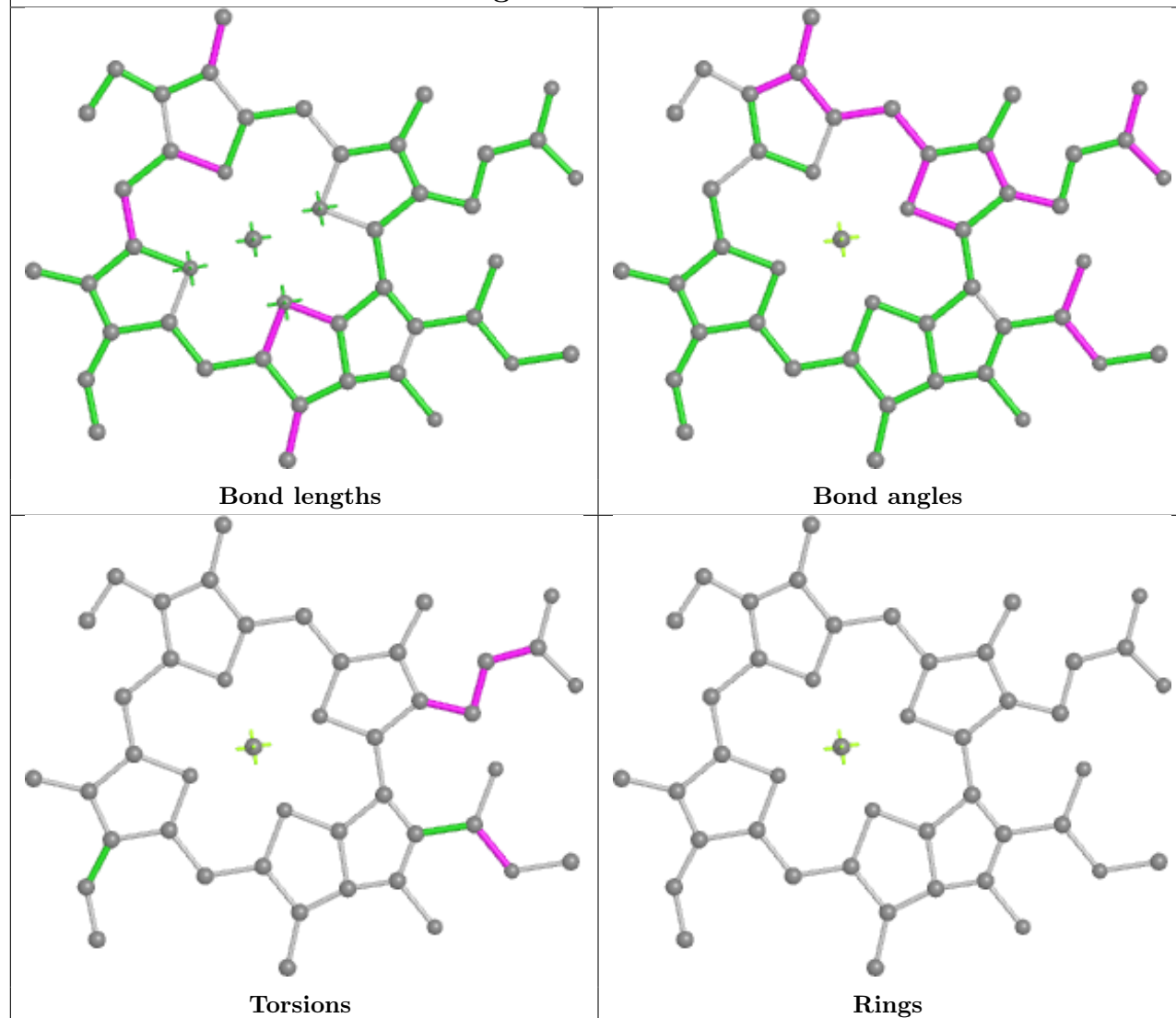


## Ligand CLA o 504

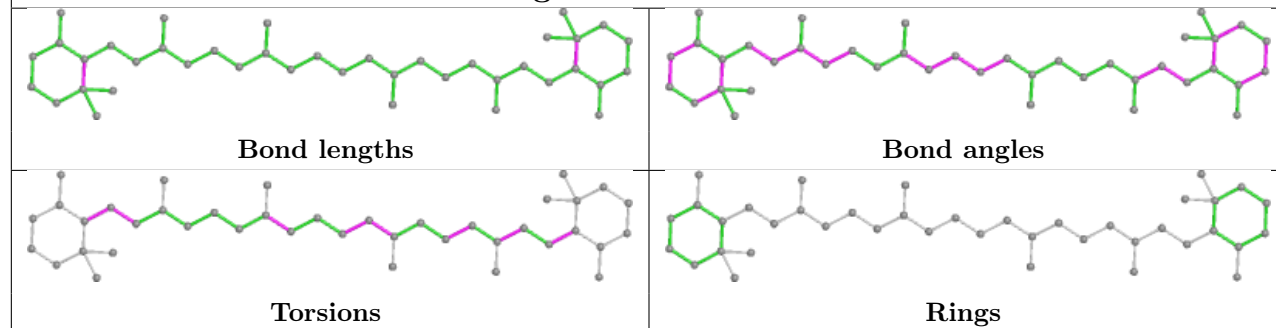


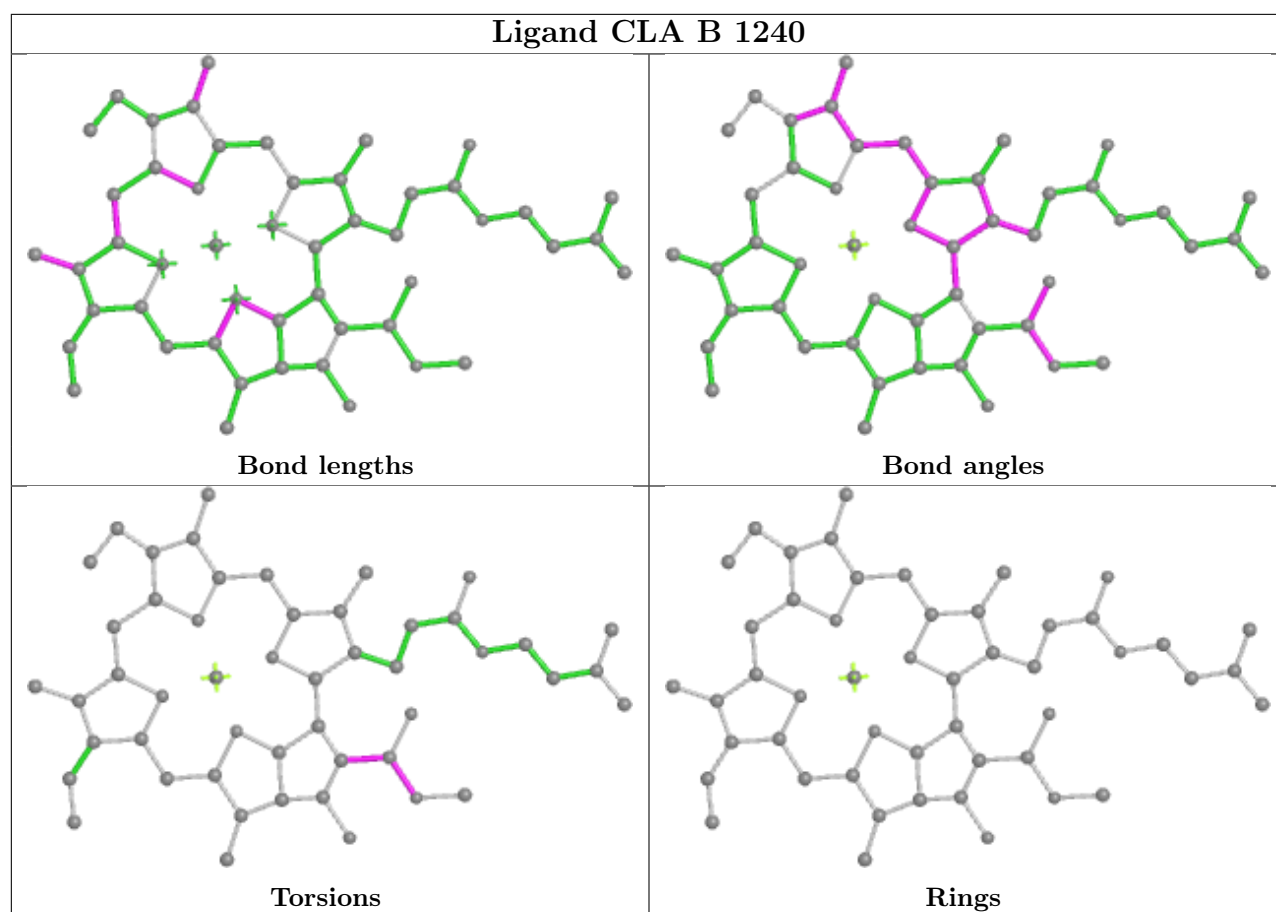
**Ligand CLA H 1117****Ligand CLA H 1136**

## Ligand CLA u 512



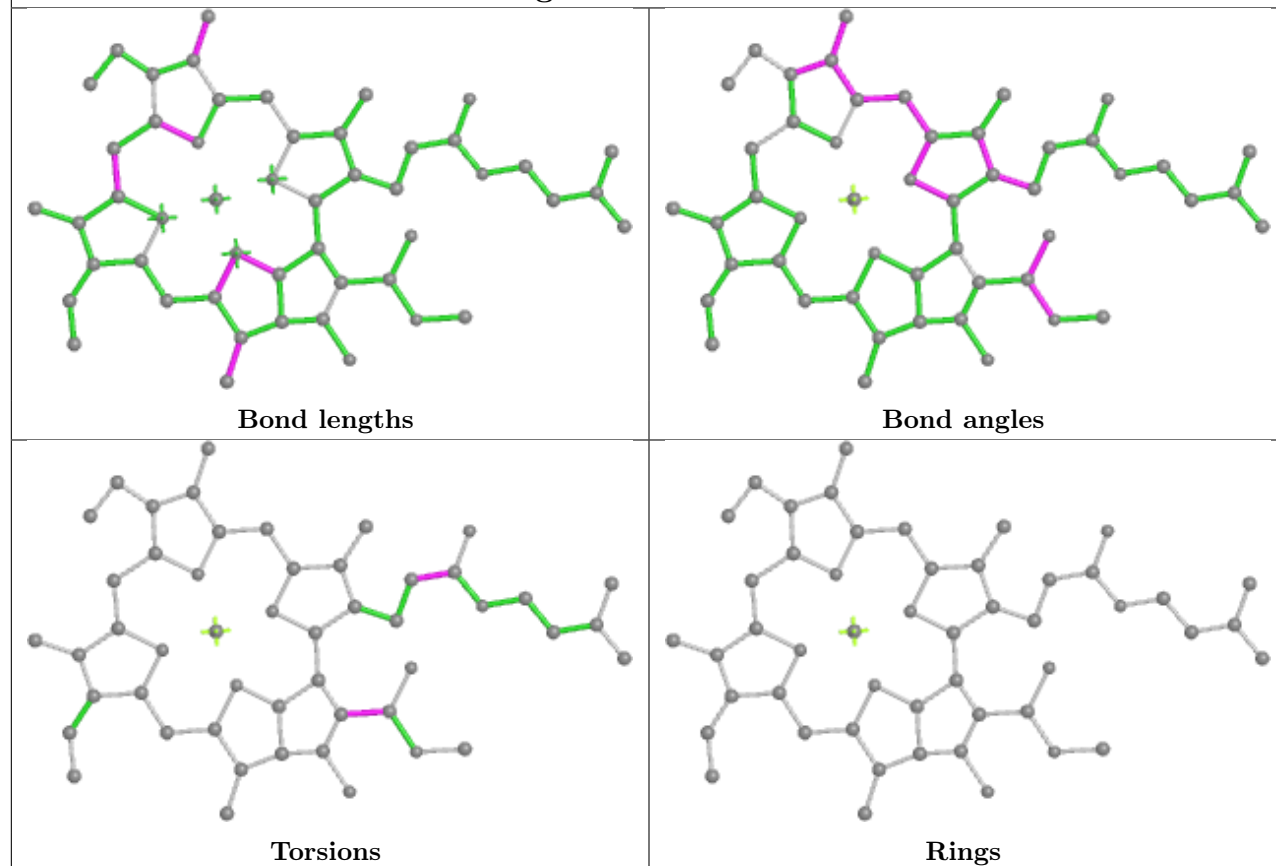
## Ligand BCR n 601



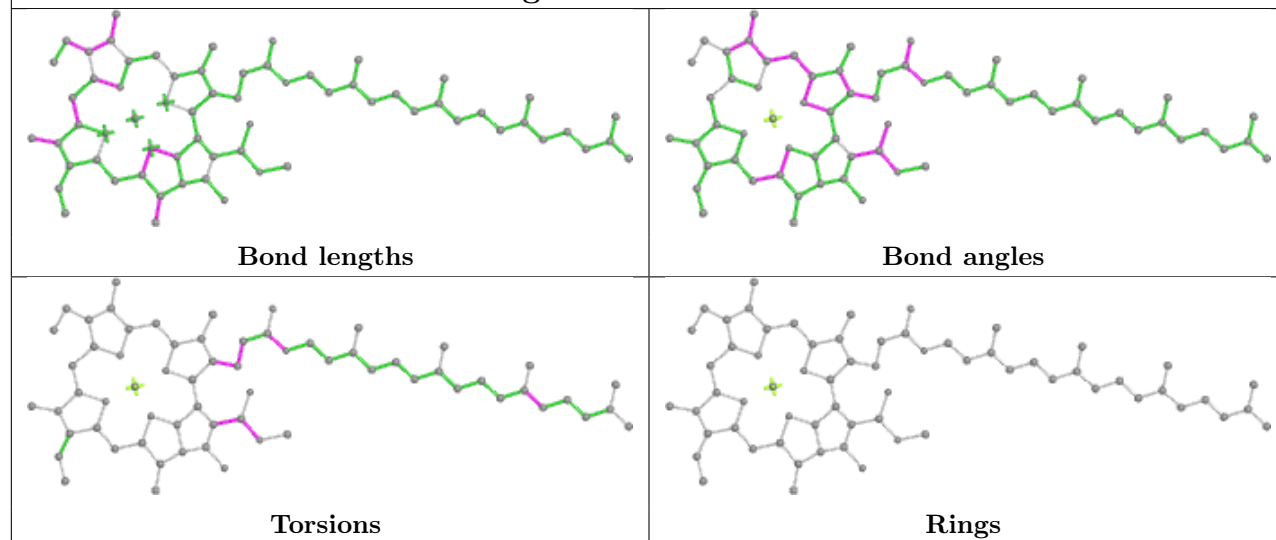




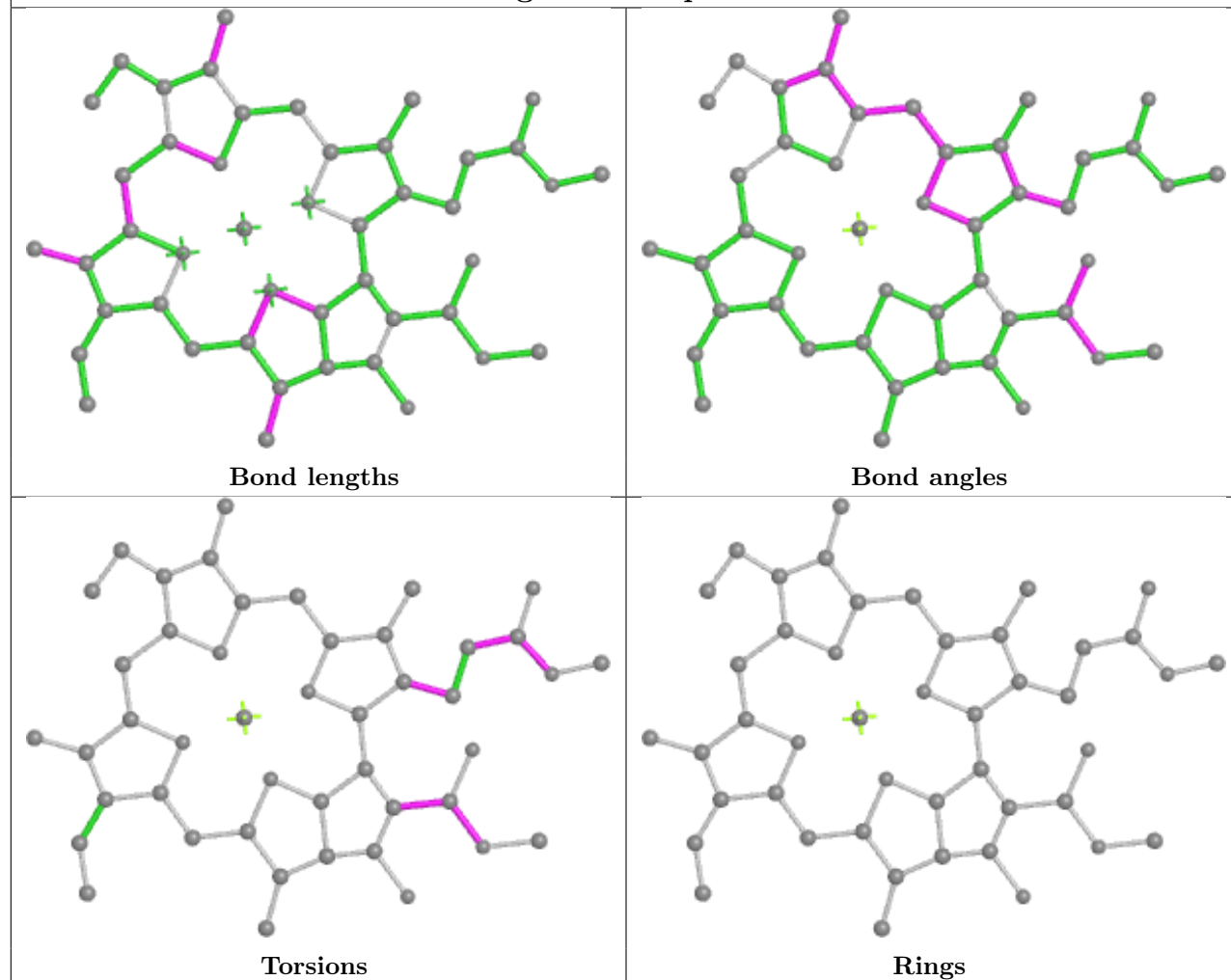
## Ligand CLA v 502



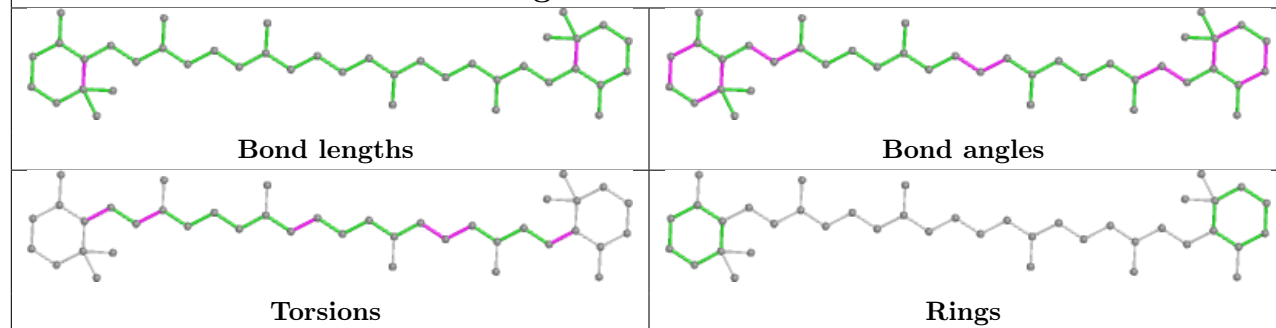
## Ligand CLA A 1132



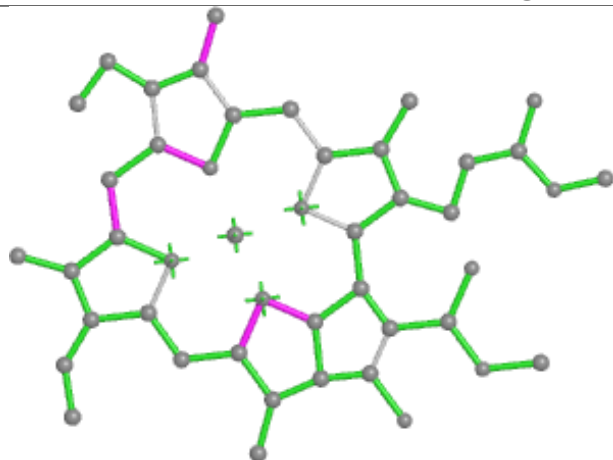
## Ligand CLA p 503



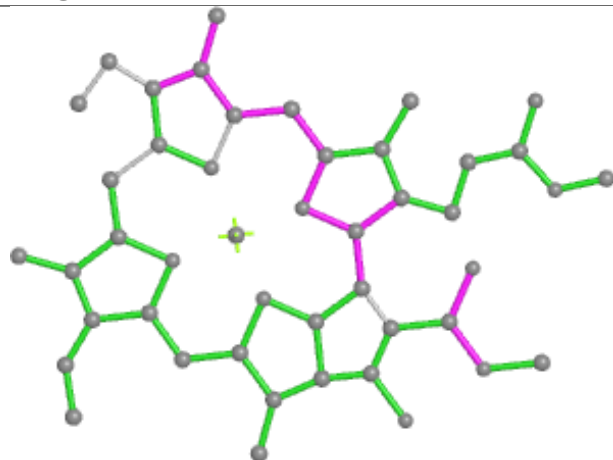
## Ligand BCR u 601



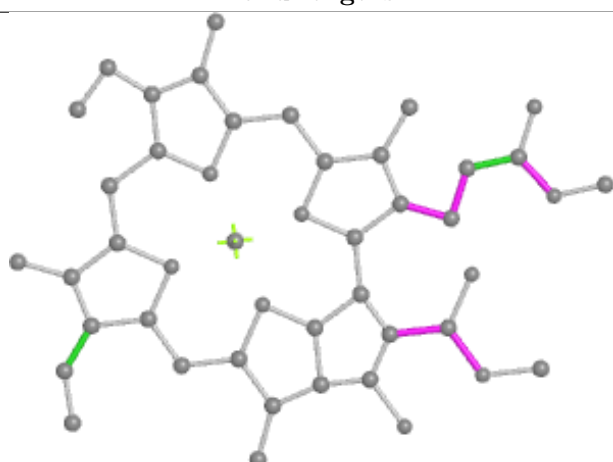
## Ligand CLA g 516



Bond lengths



Bond angles

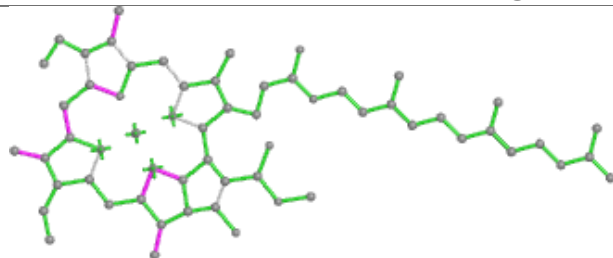


Torsions

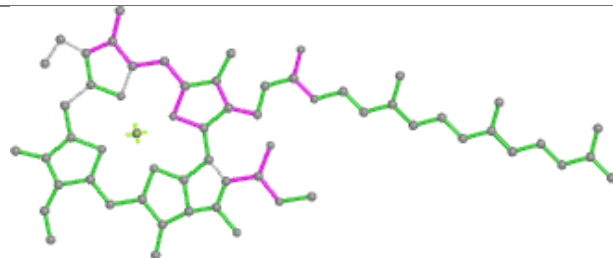


Rings

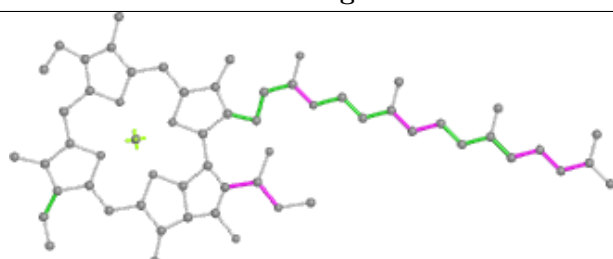
## Ligand CLA W 506



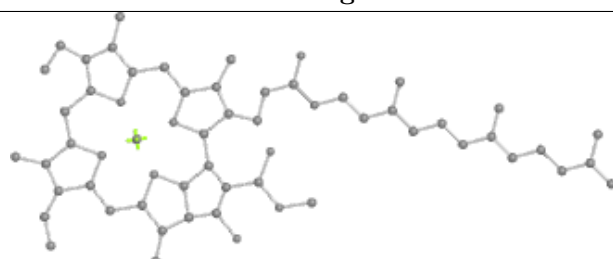
Bond lengths



Bond angles

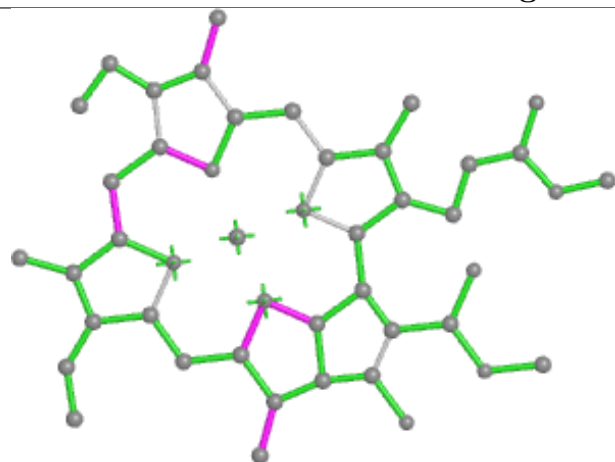


Torsions

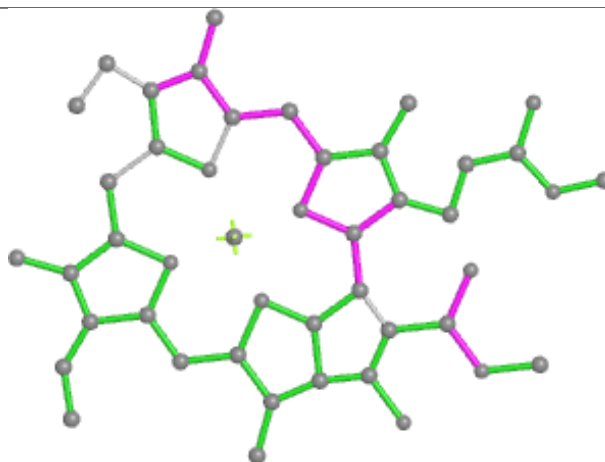


Rings

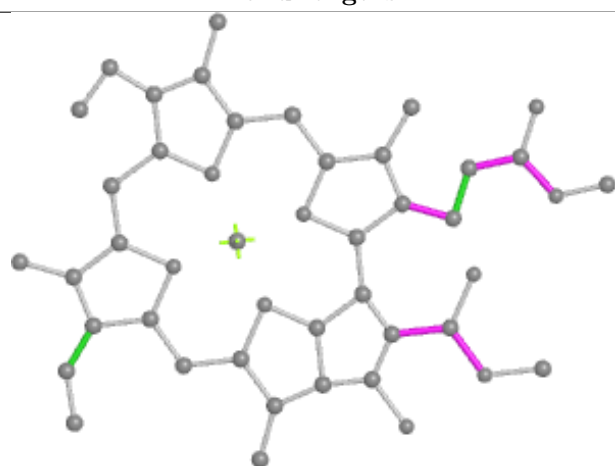
## Ligand CLA u 516



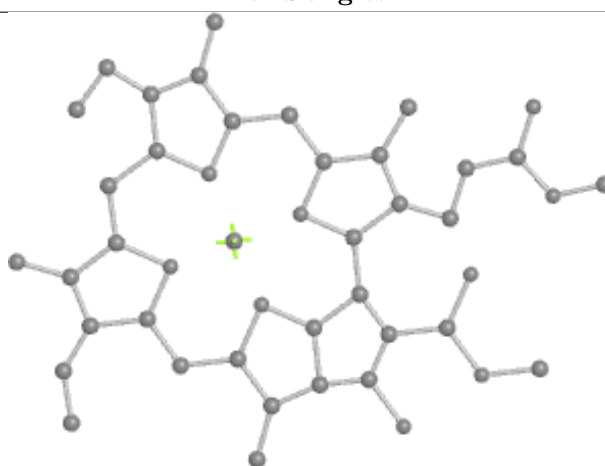
Bond lengths



Bond angles

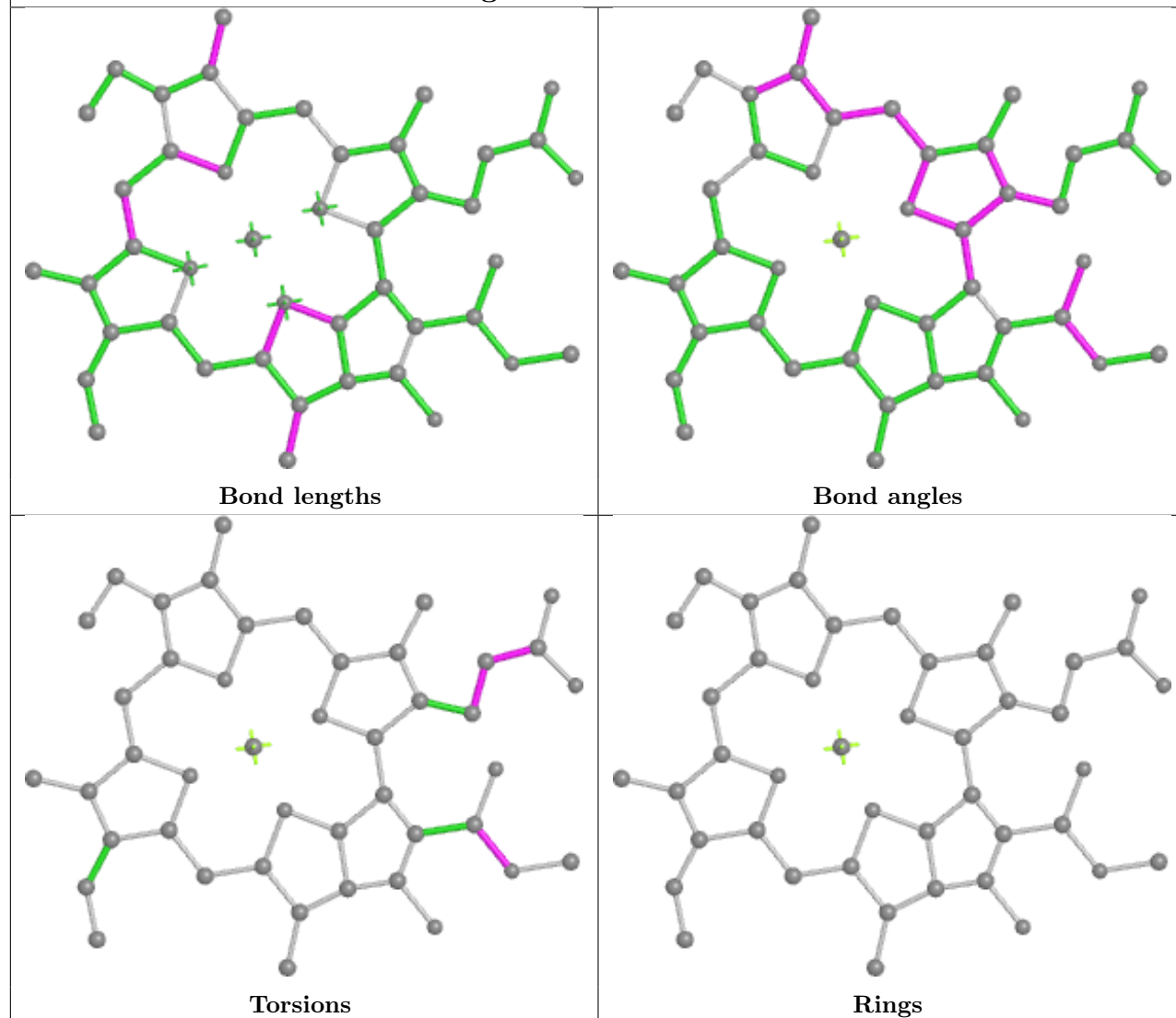


Torsions

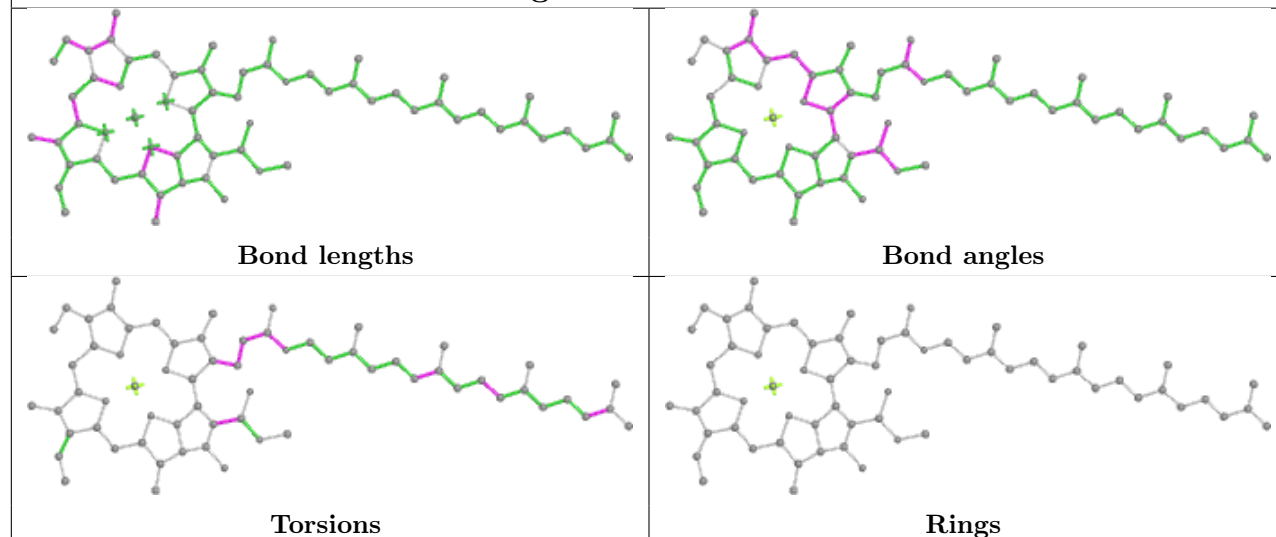


Rings

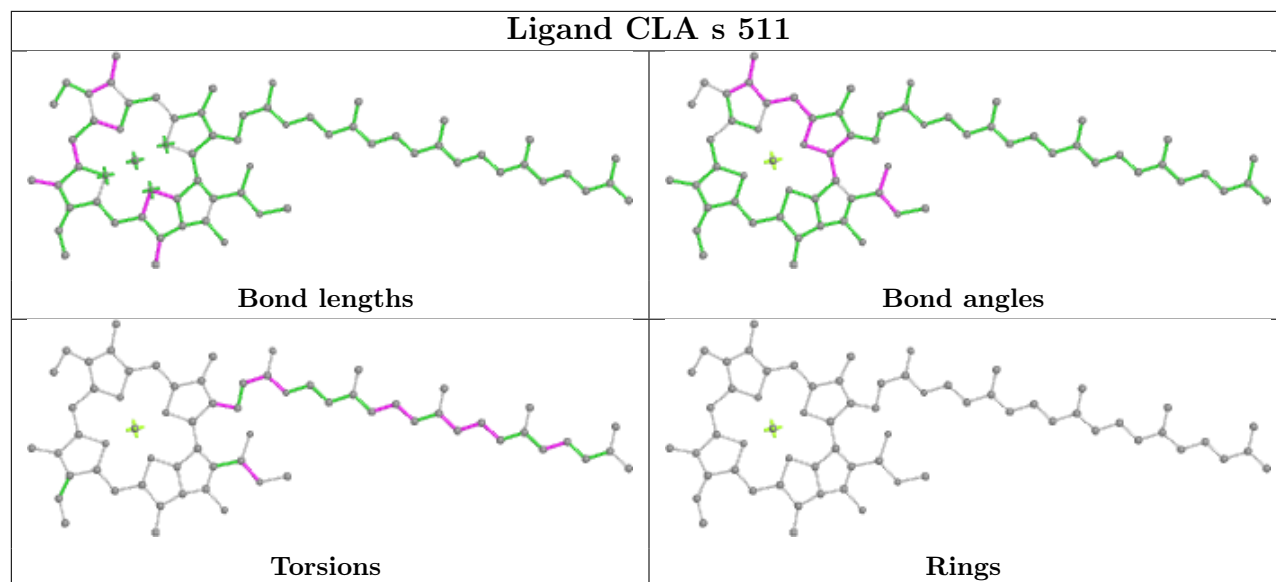
## Ligand CLA G 1209



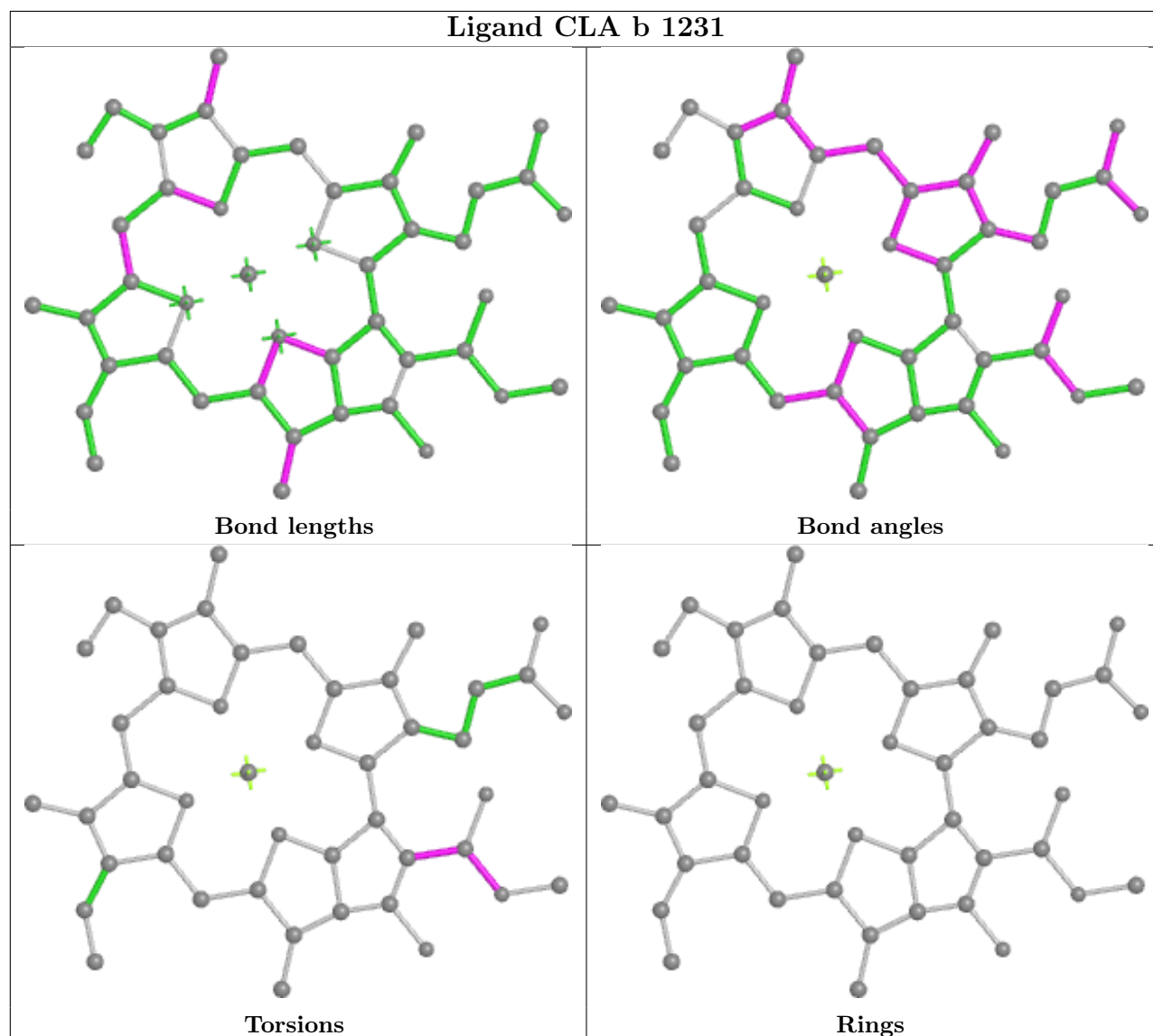
## Ligand CLA I 1502

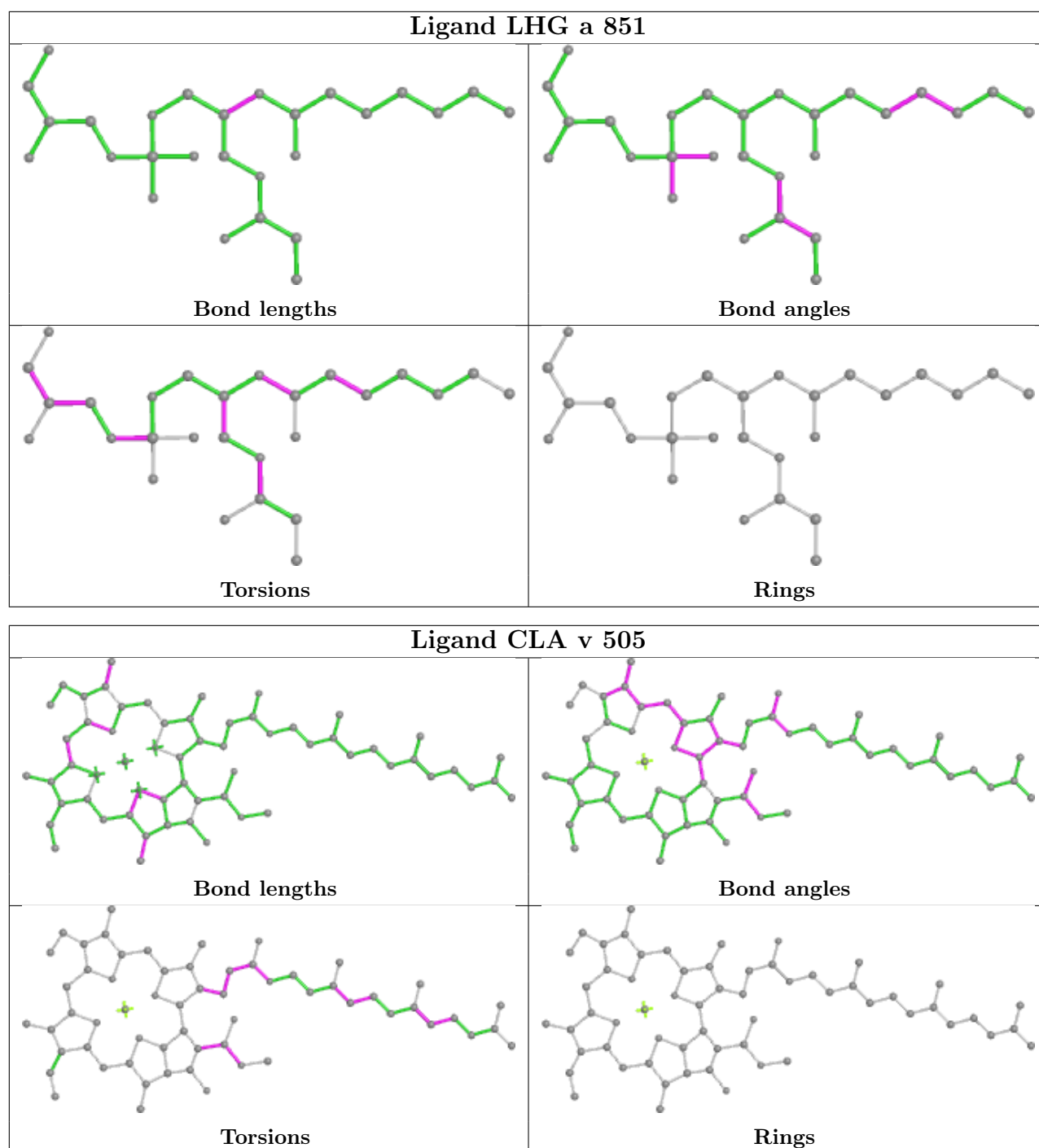


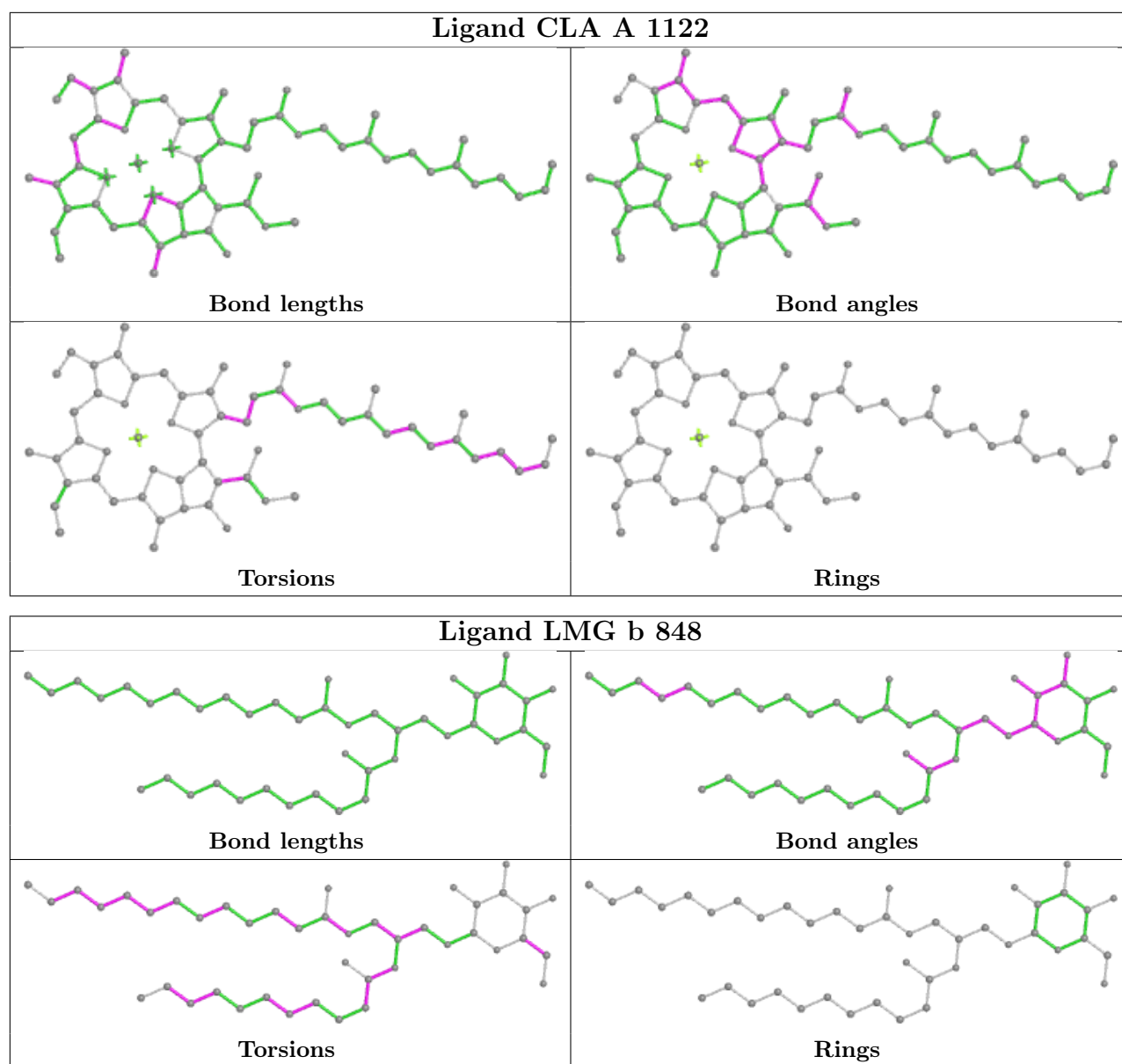
## Ligand CLA s 511



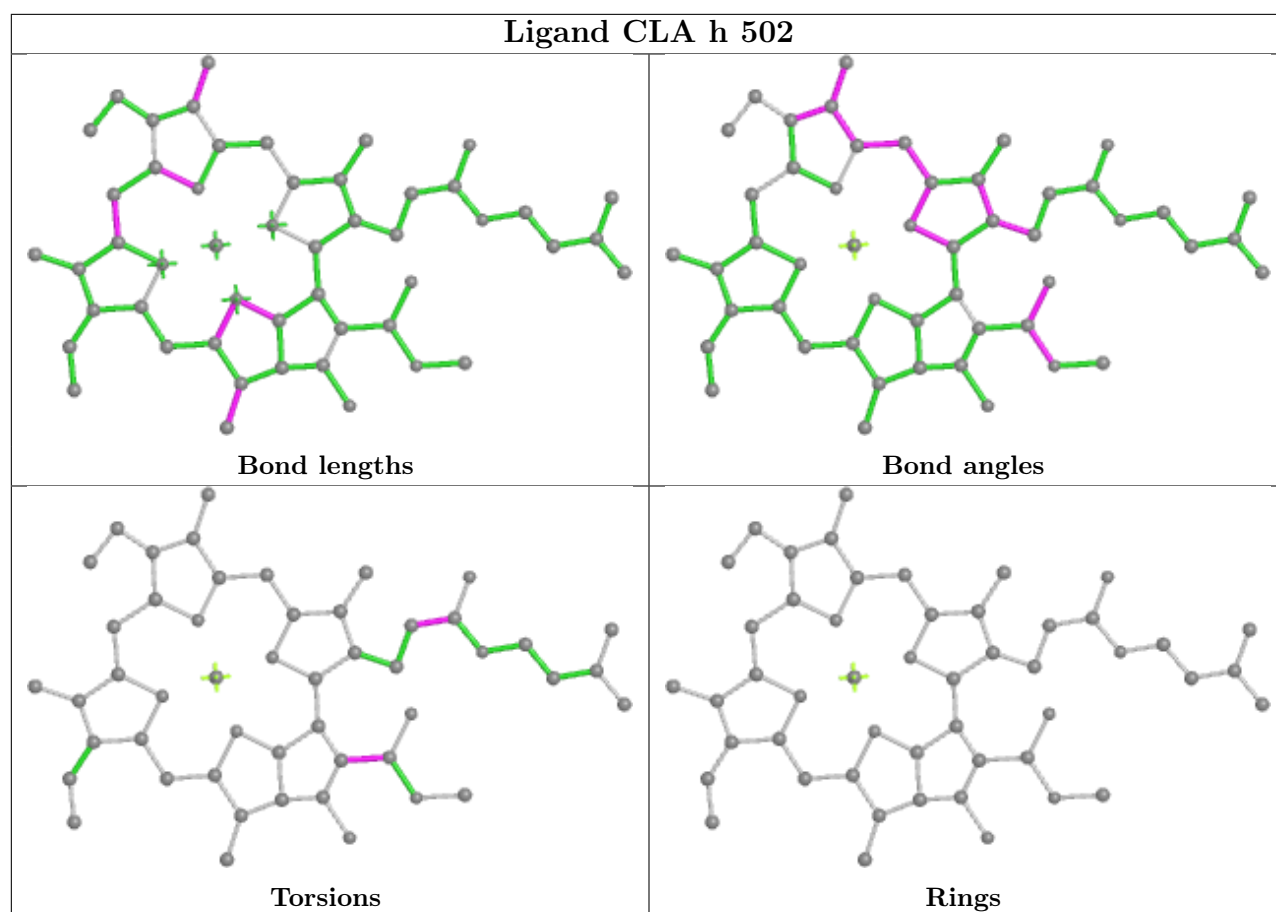
## Ligand CLA b 1231

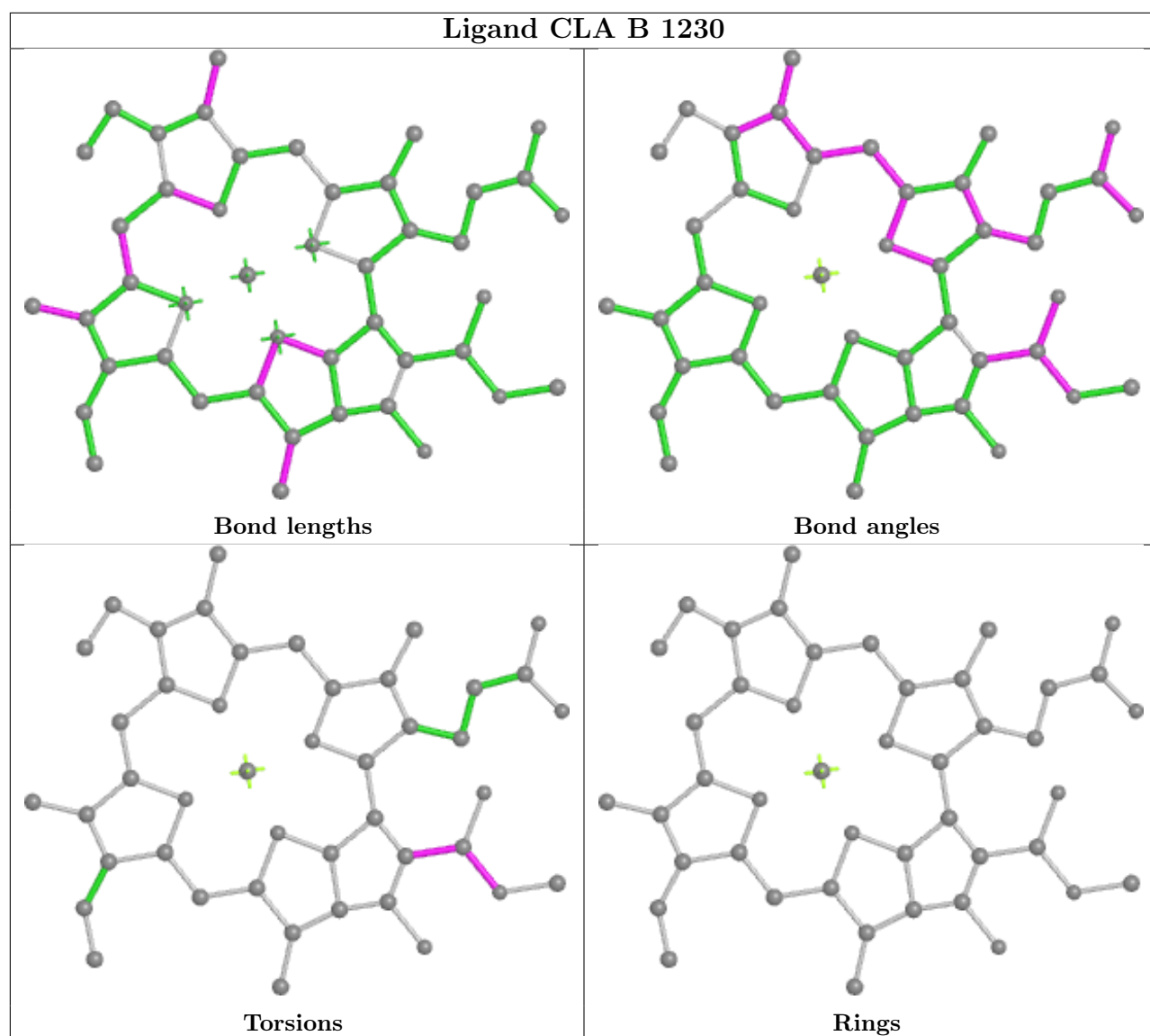




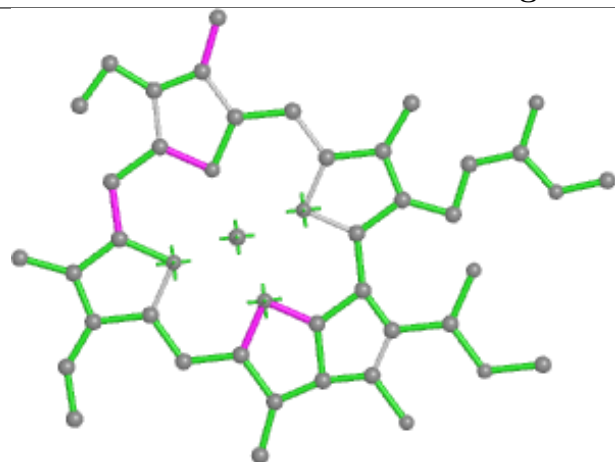




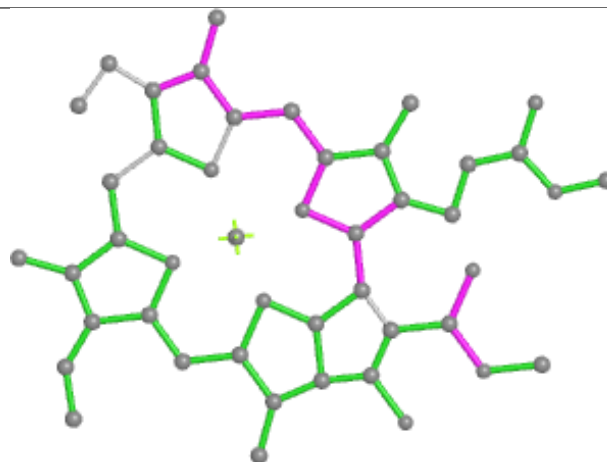




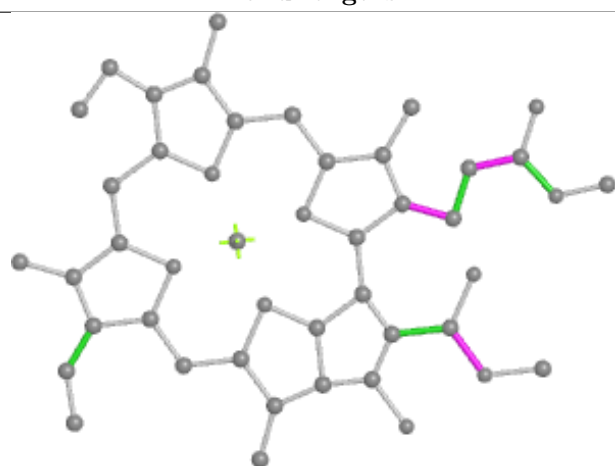
## Ligand CLA v 516



Bond lengths



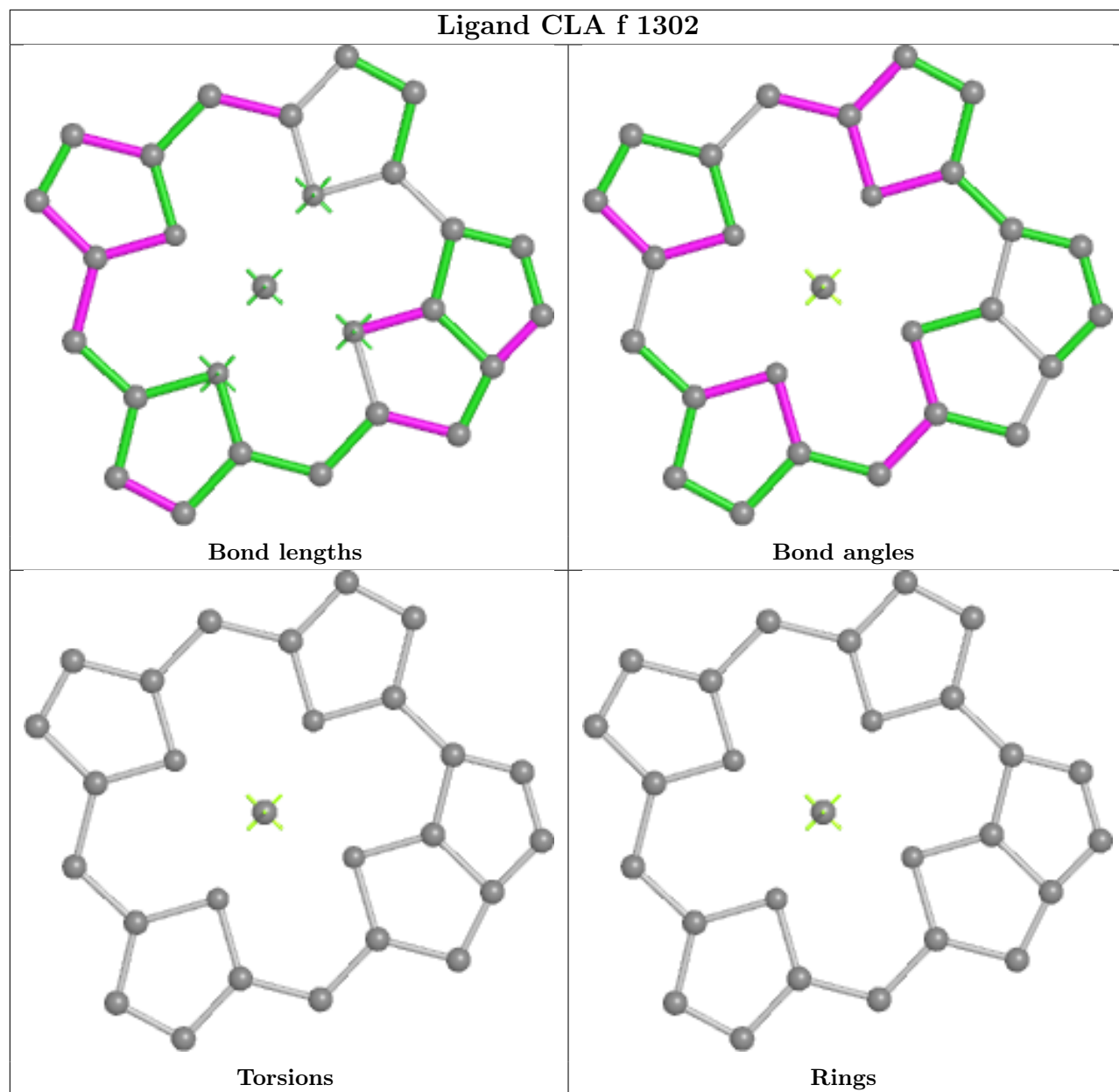
Bond angles

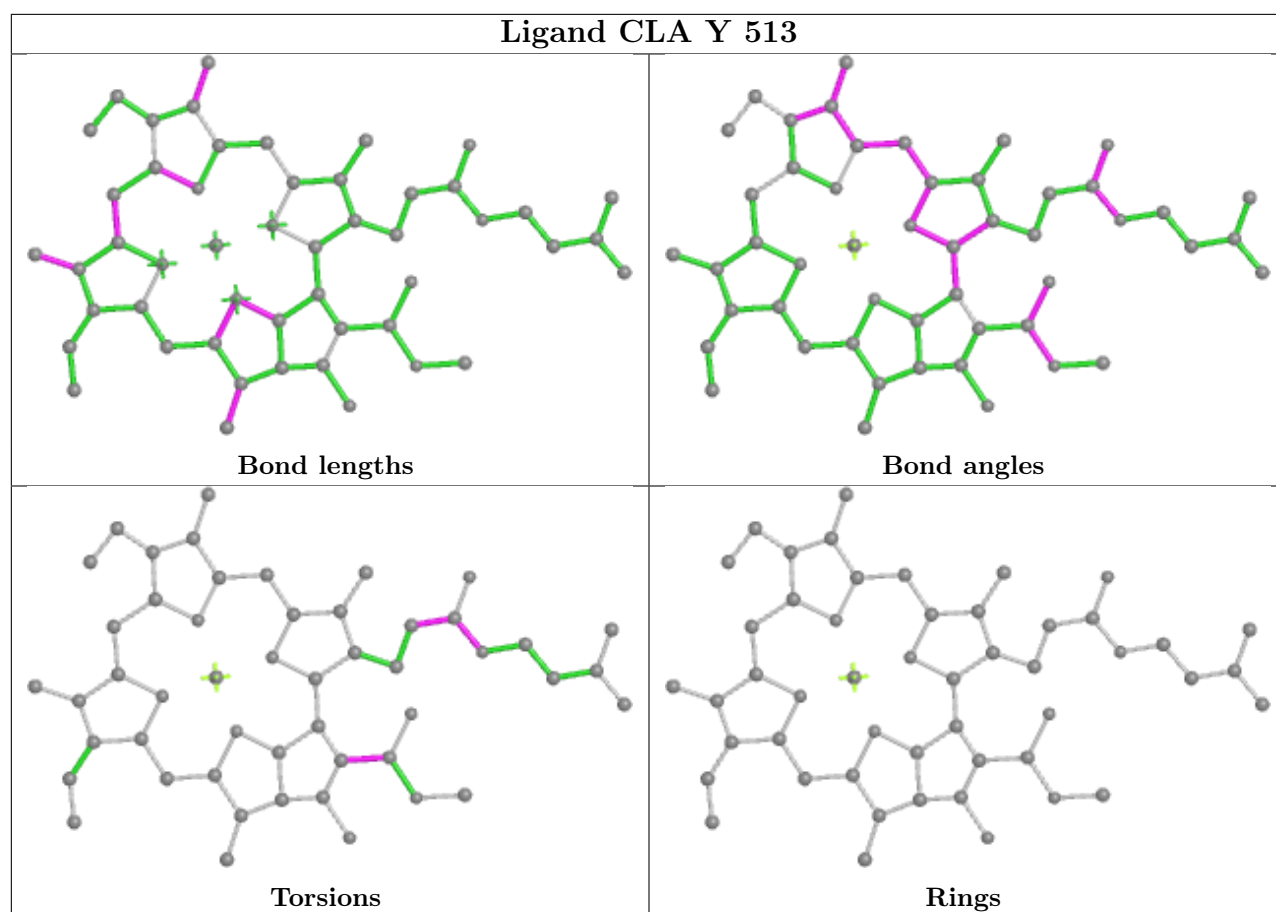


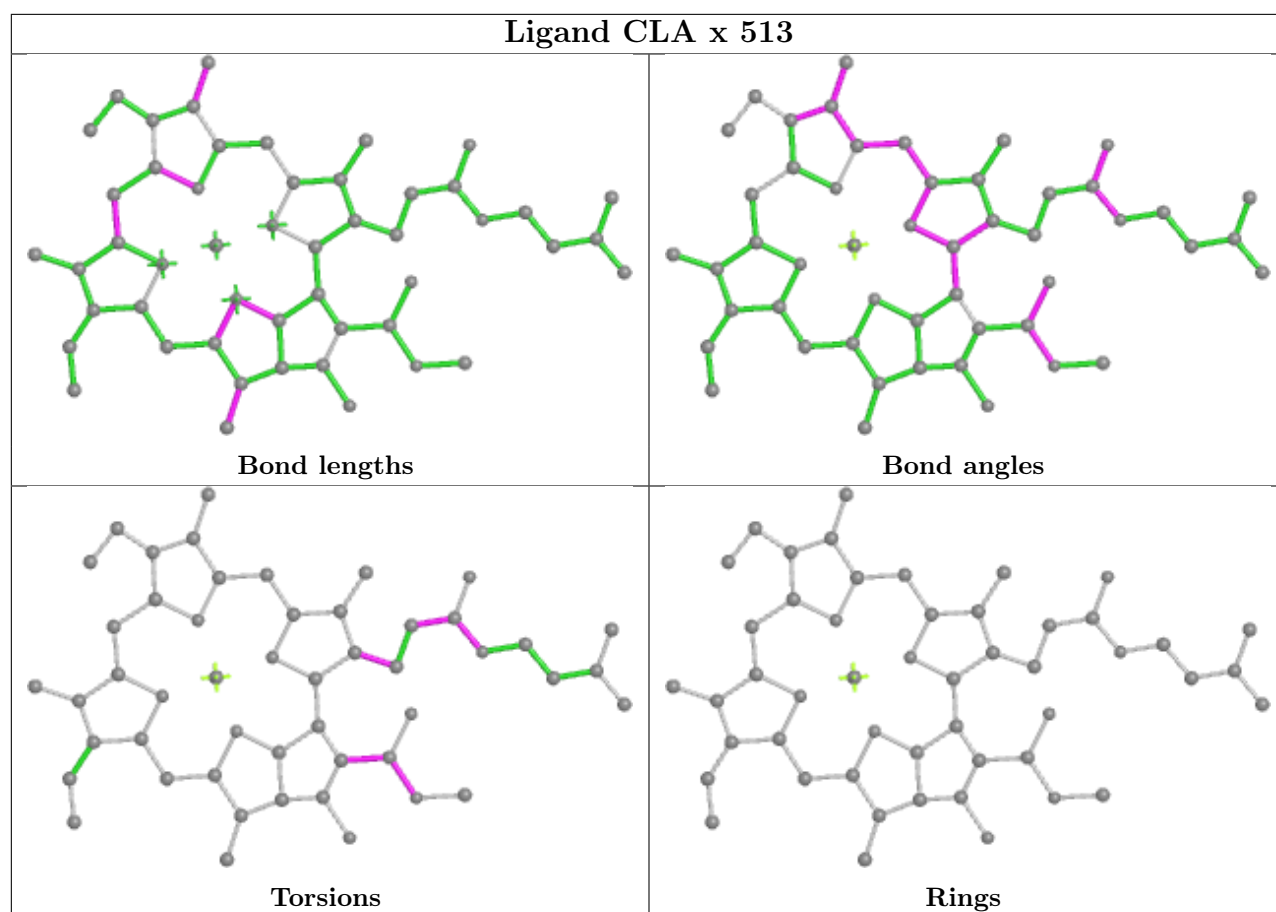
Torsions

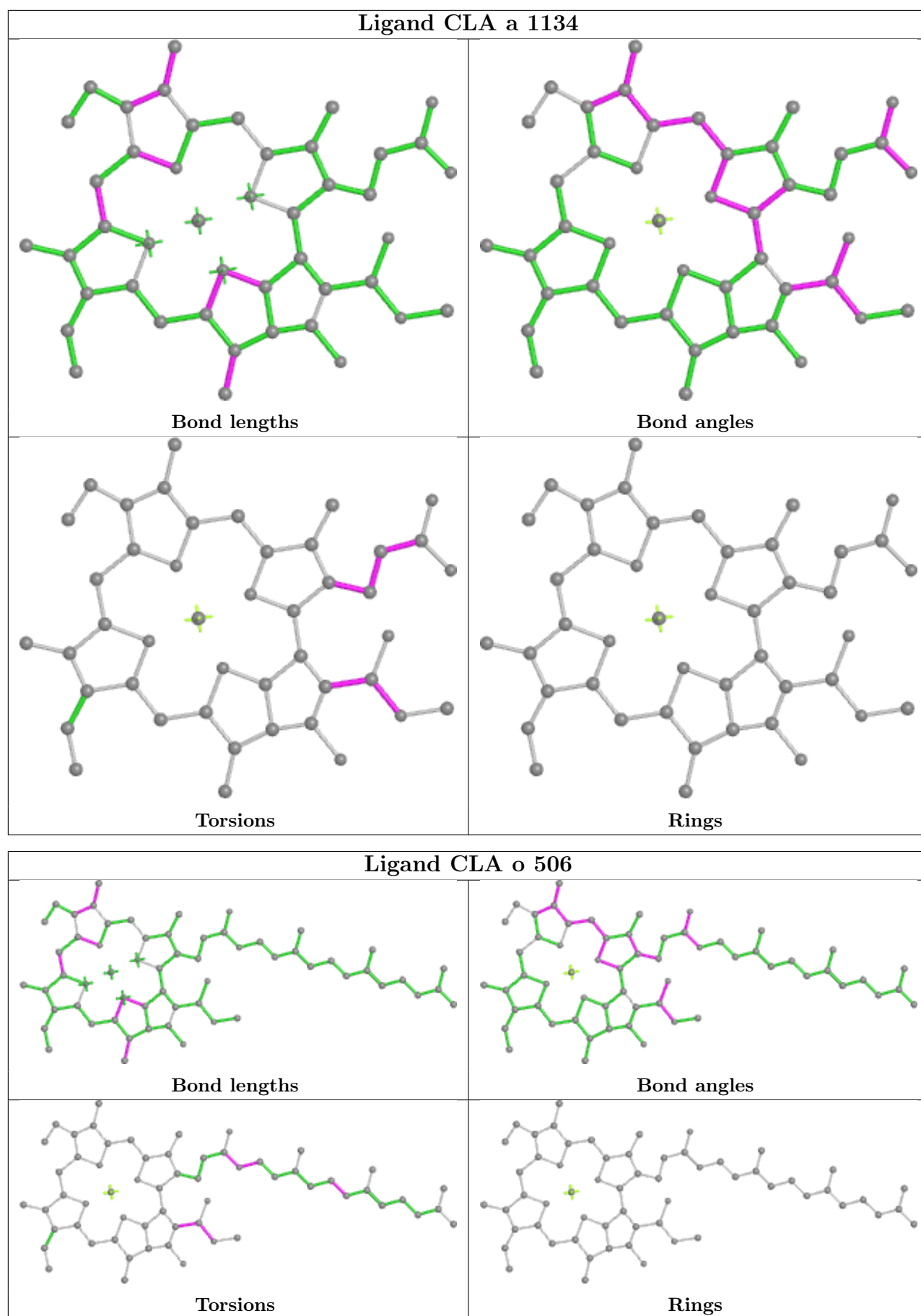


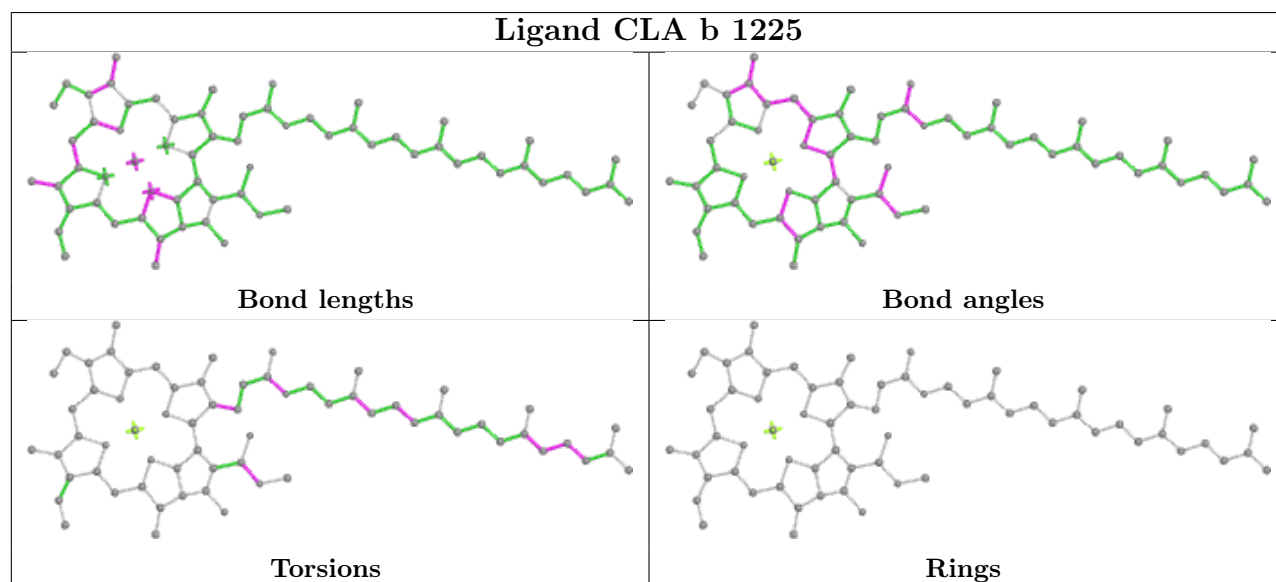
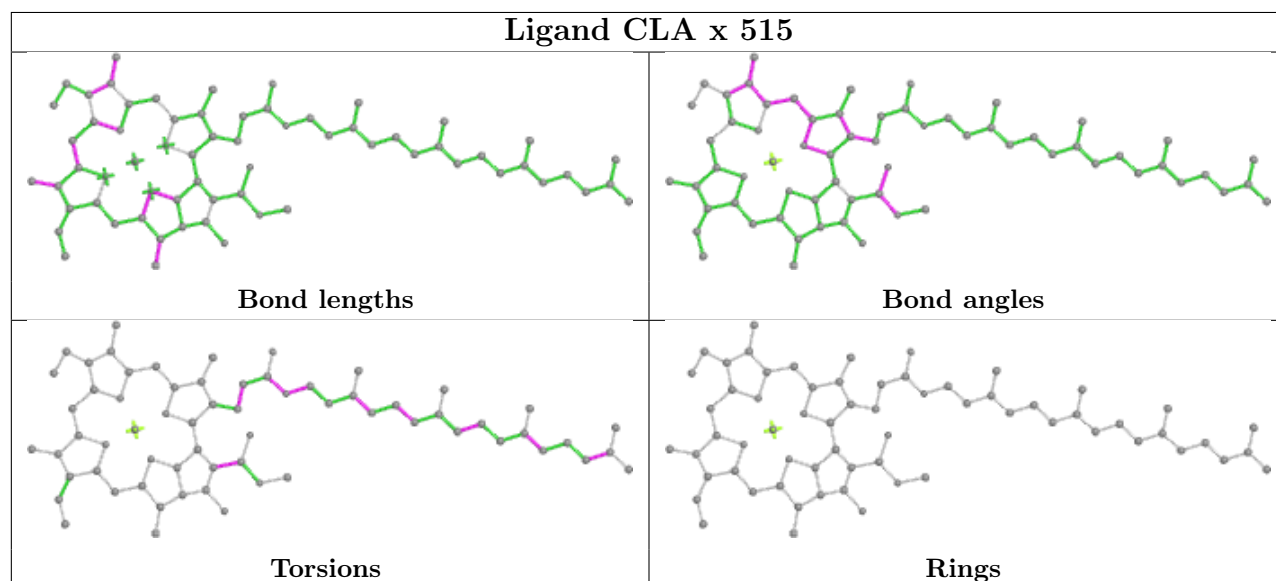
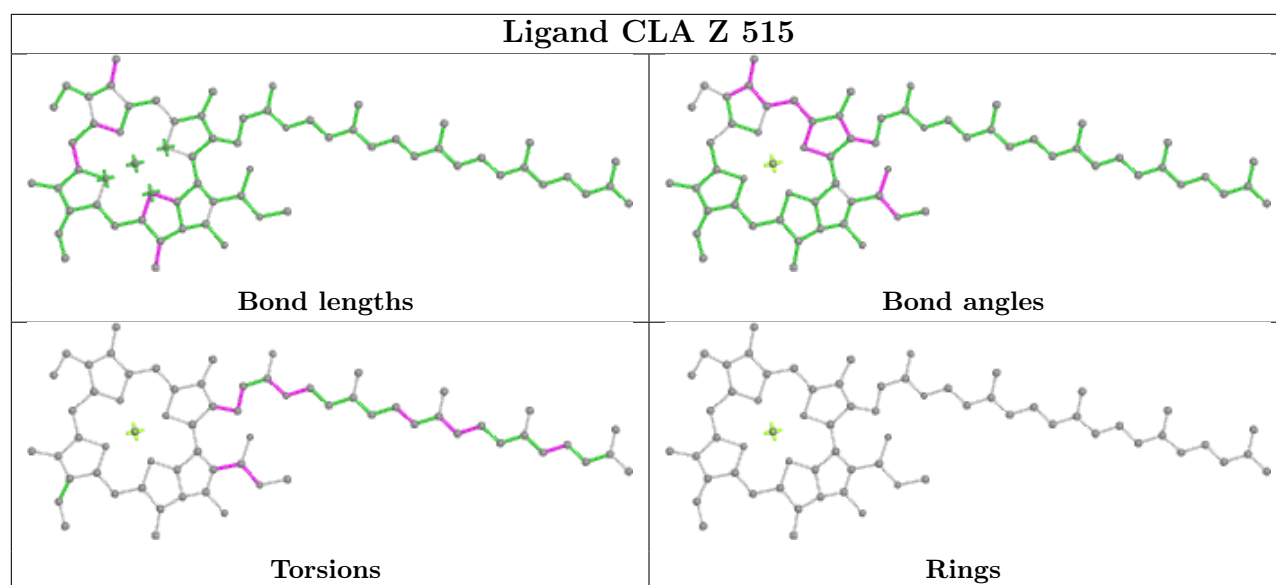
Rings





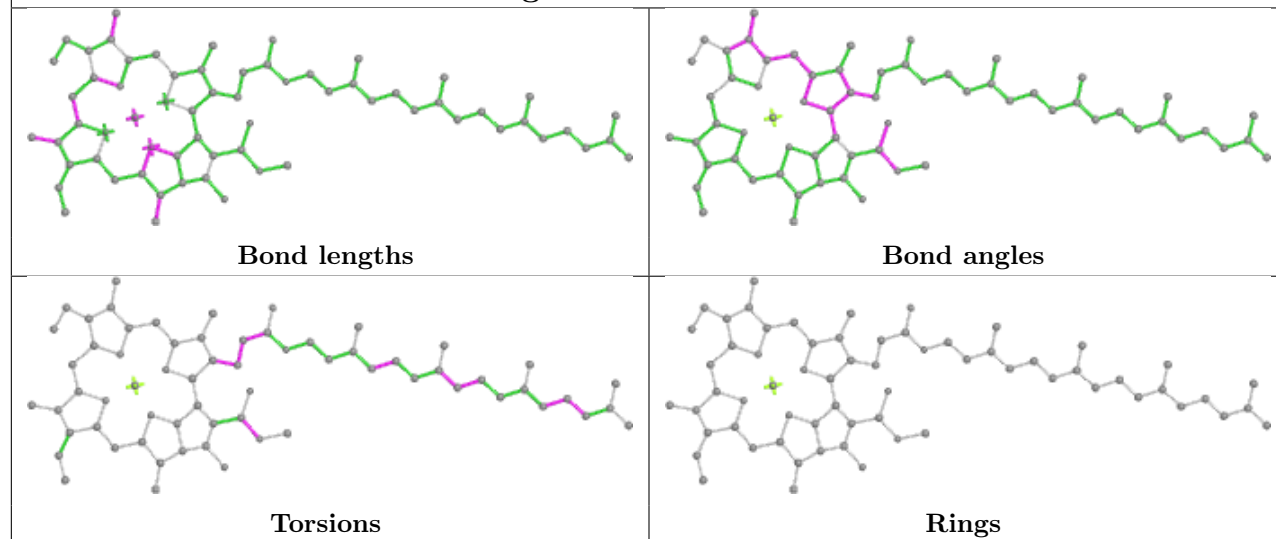




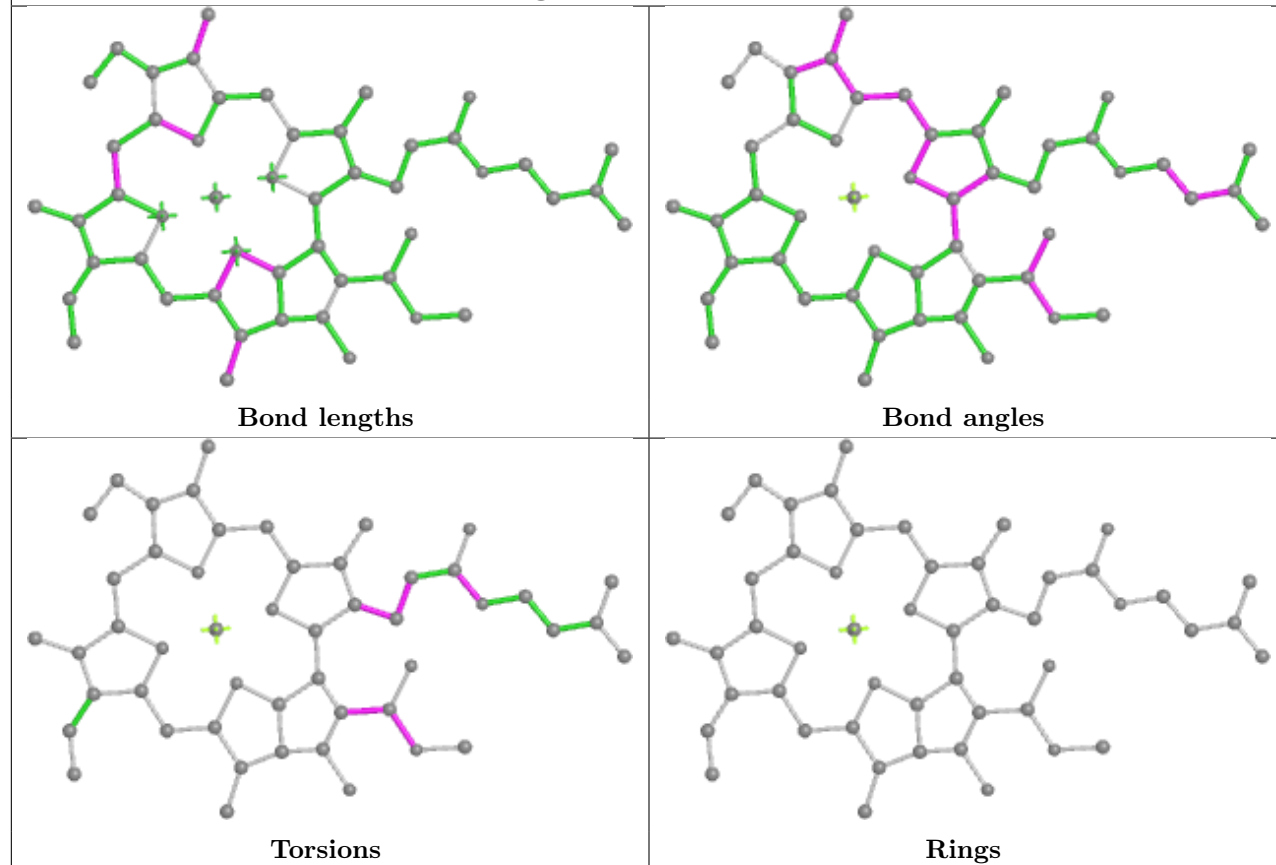




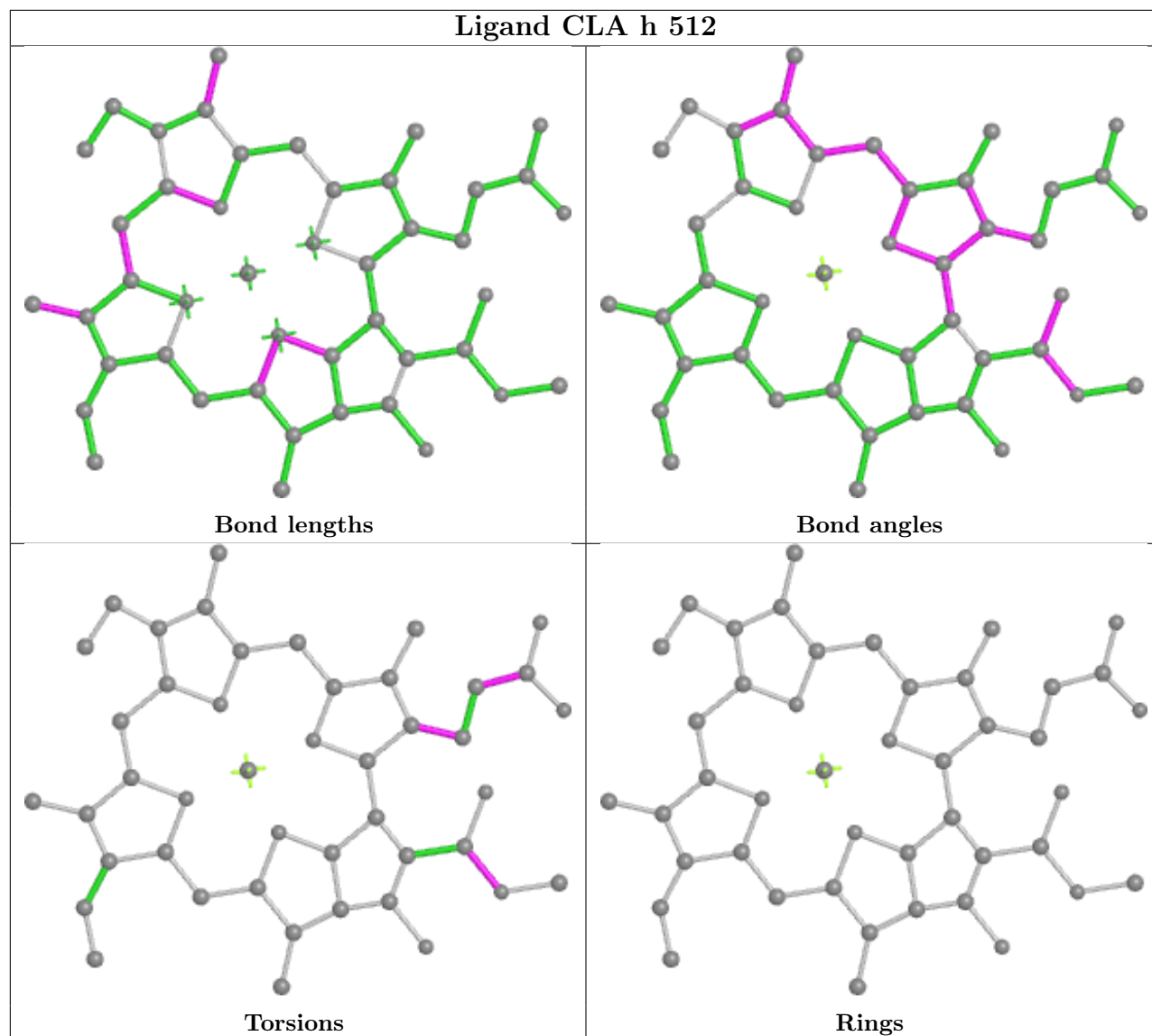
## Ligand CLA G 1206



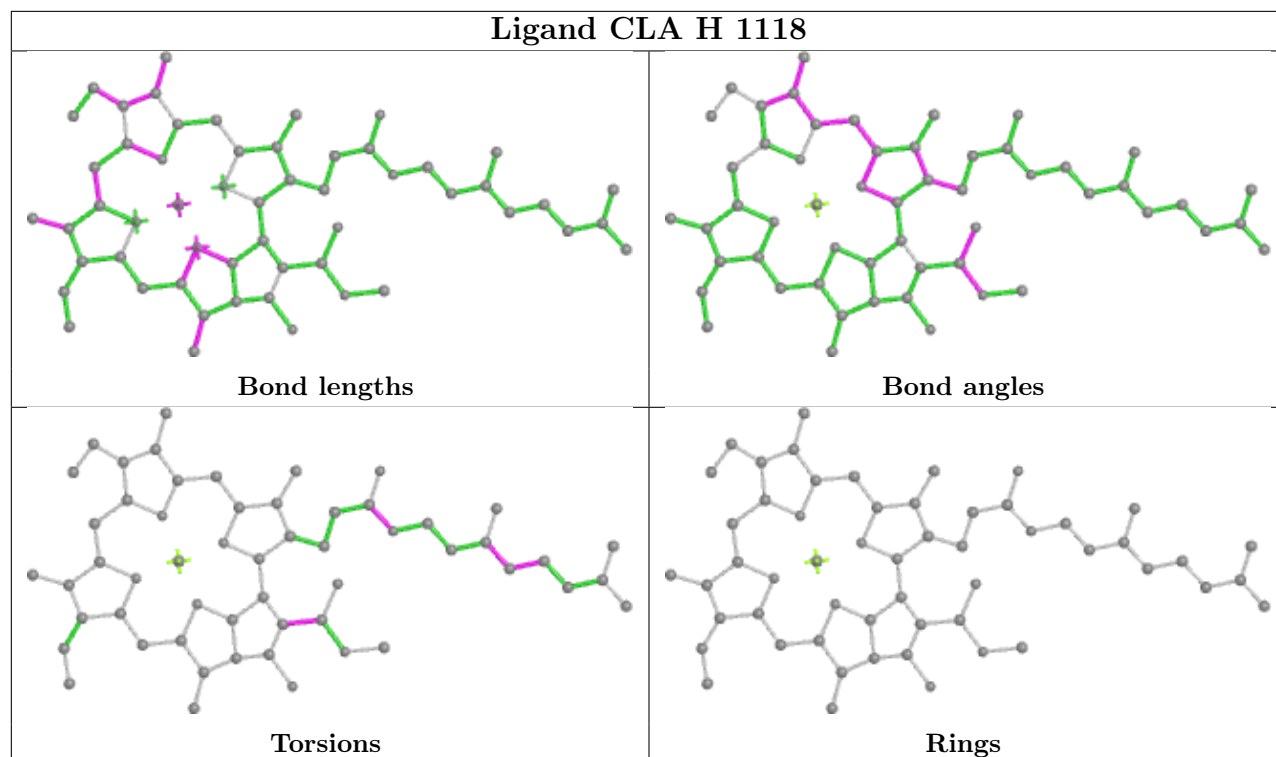
## Ligand CLA w 513



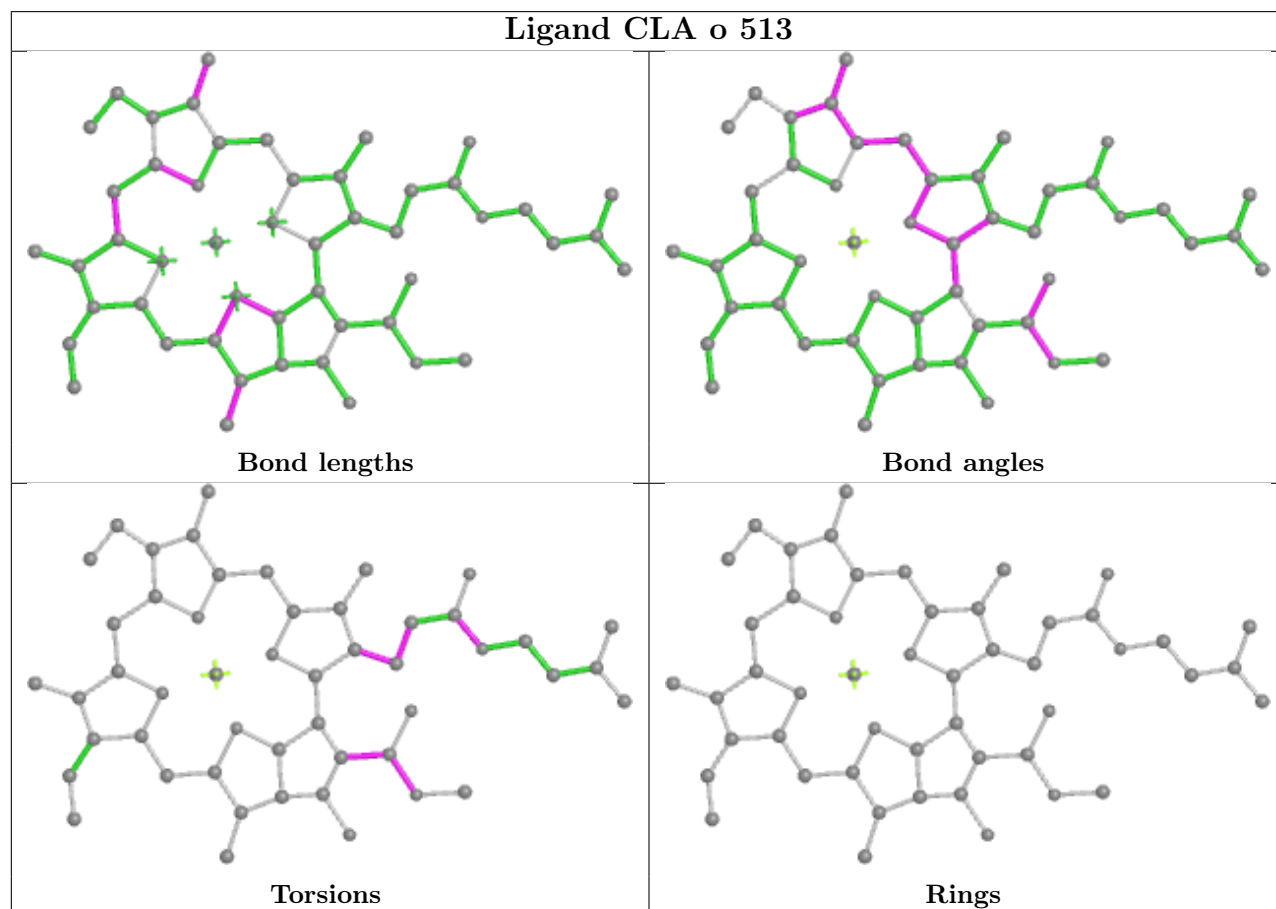
## Ligand CLA h 512

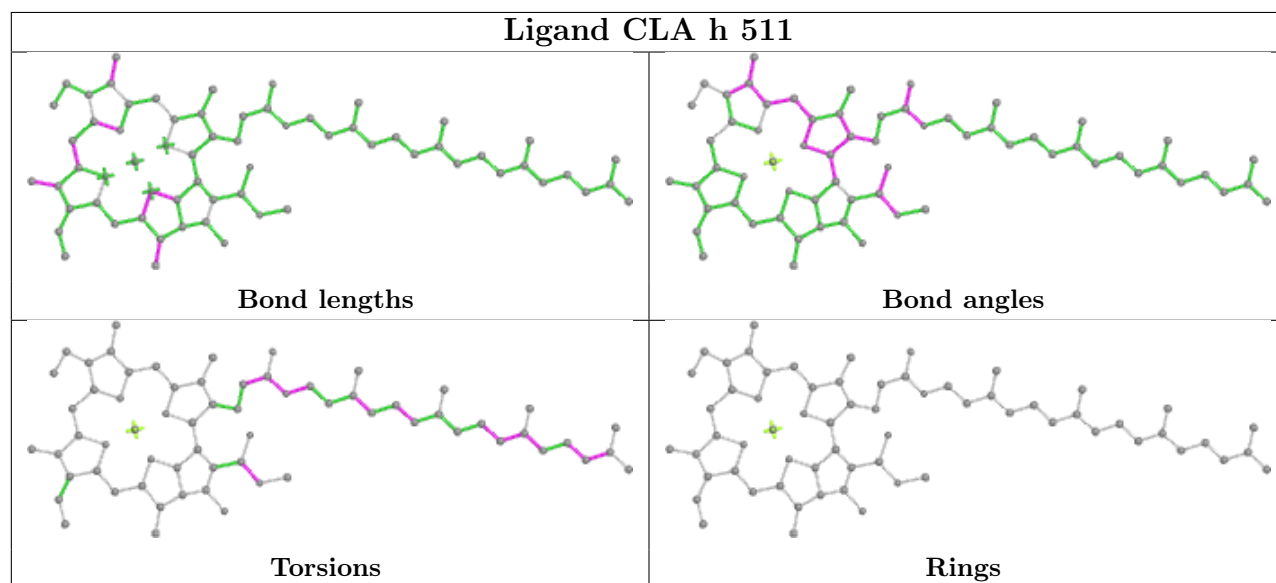
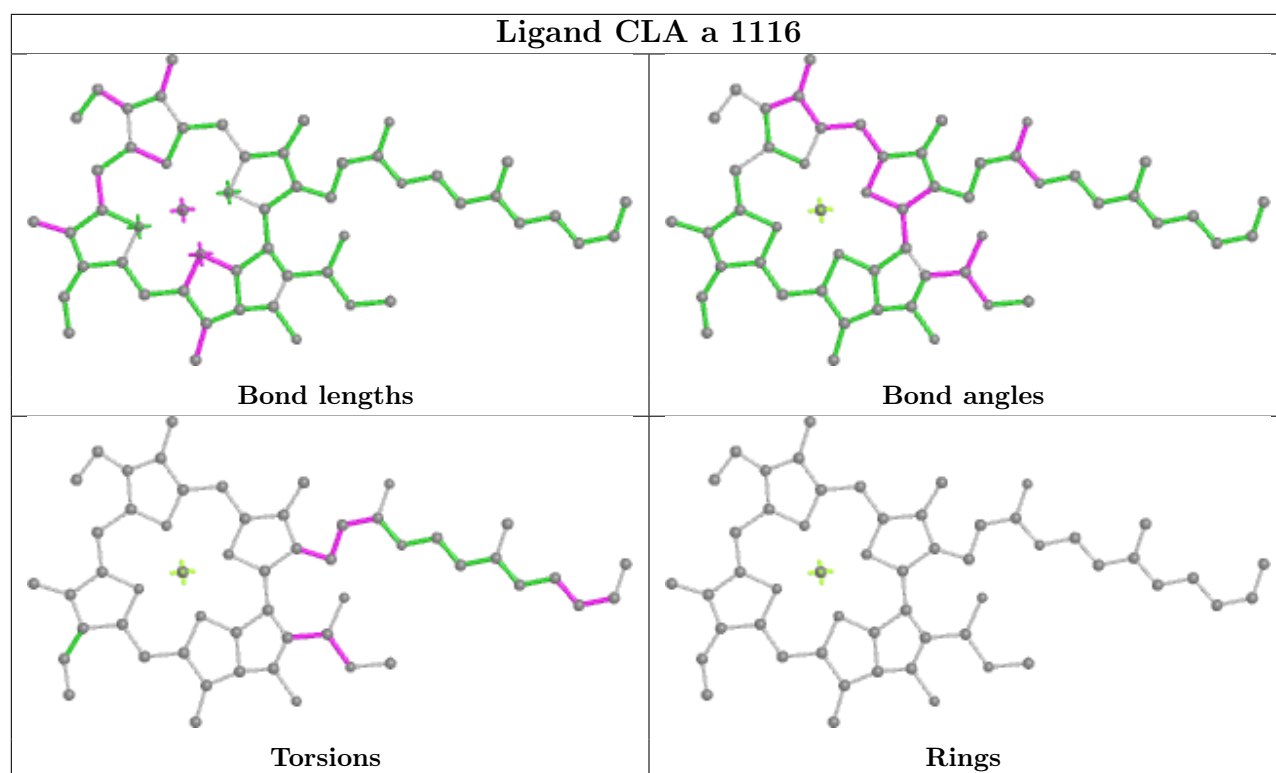


## Ligand CLA H 1118

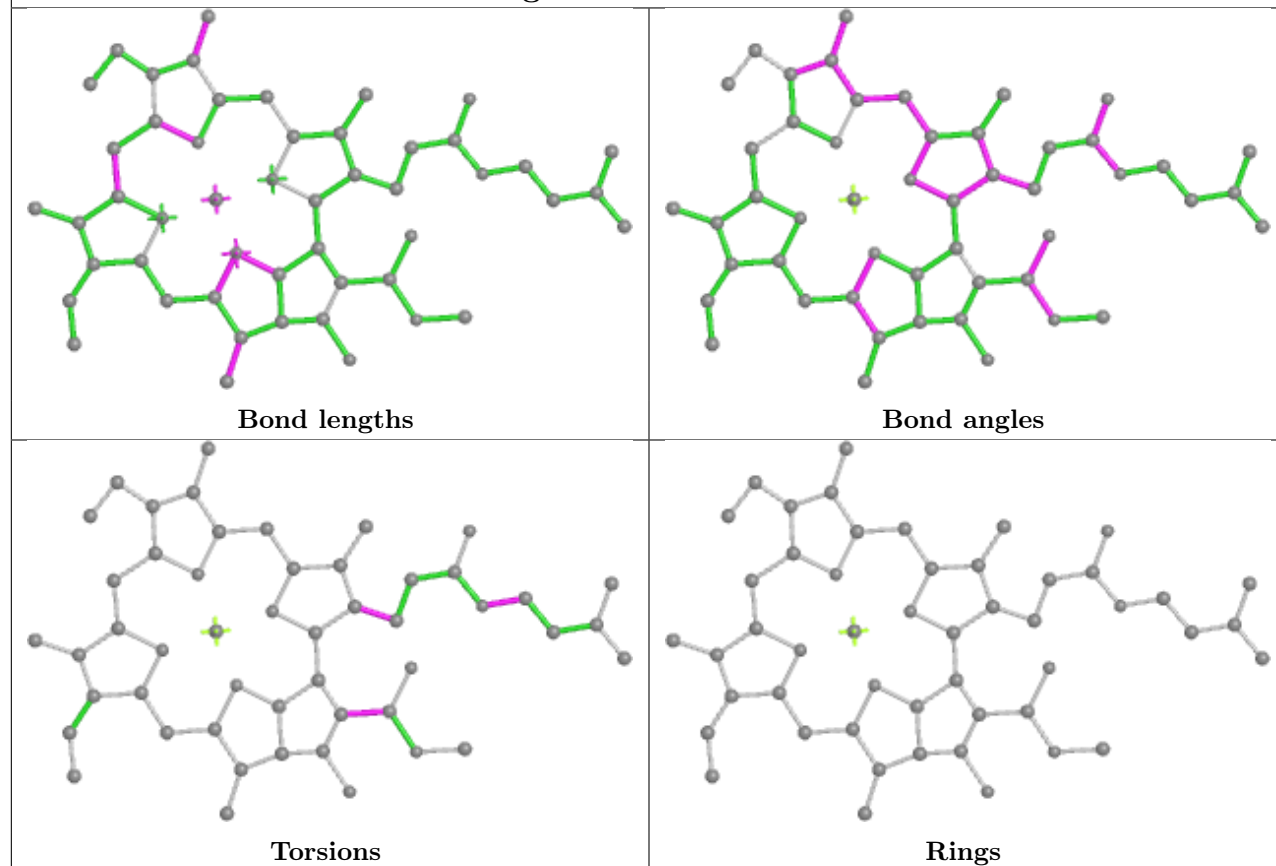


## Ligand CLA o 513

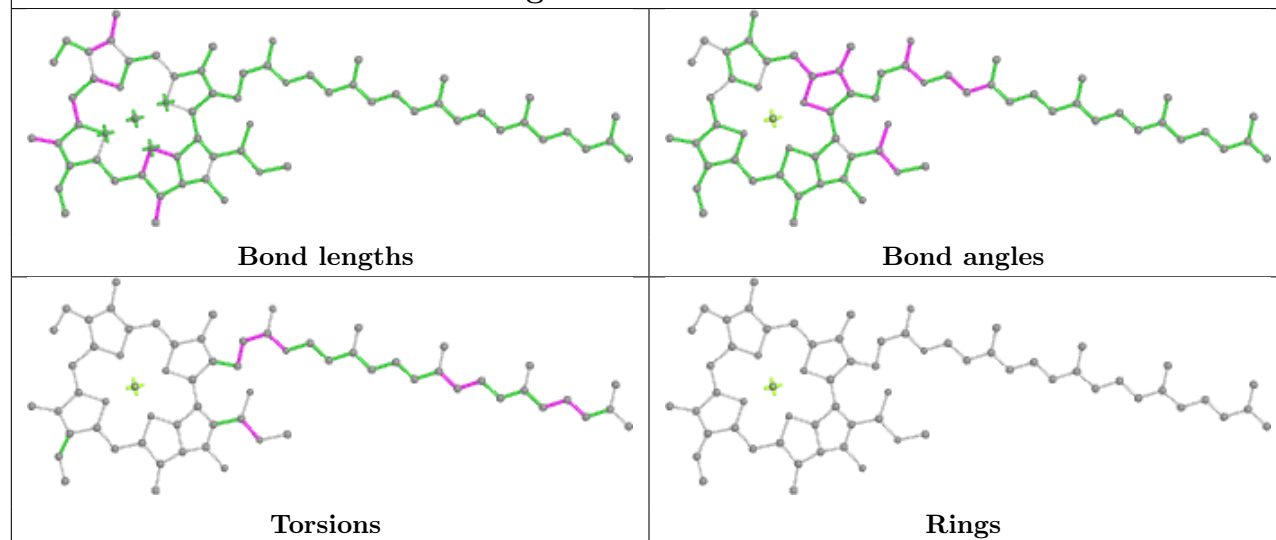


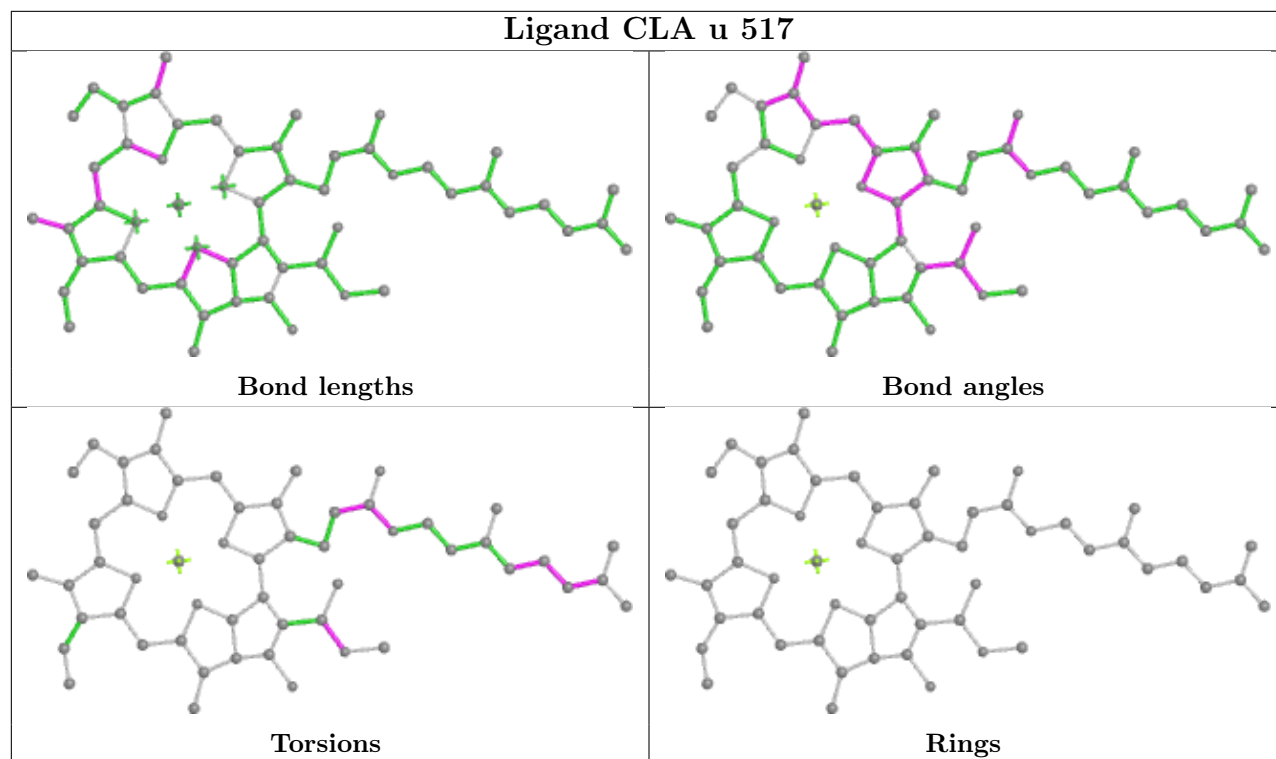
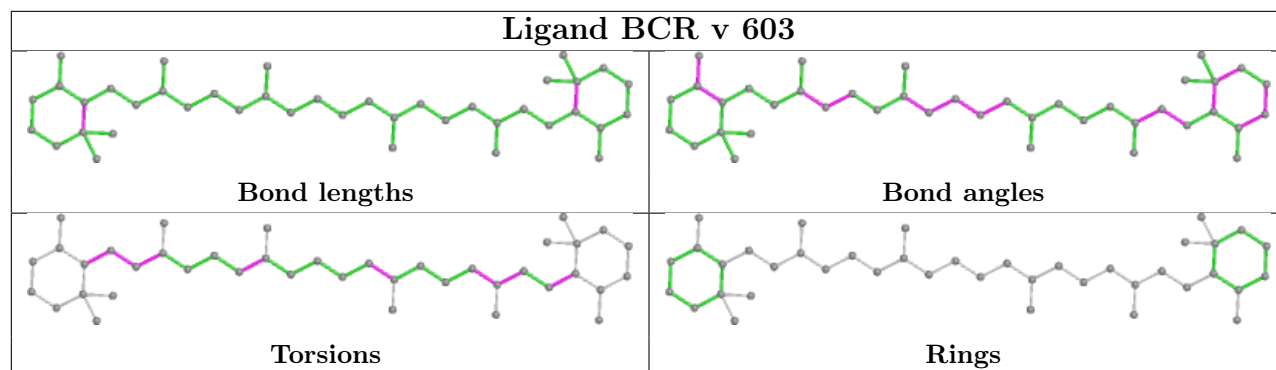


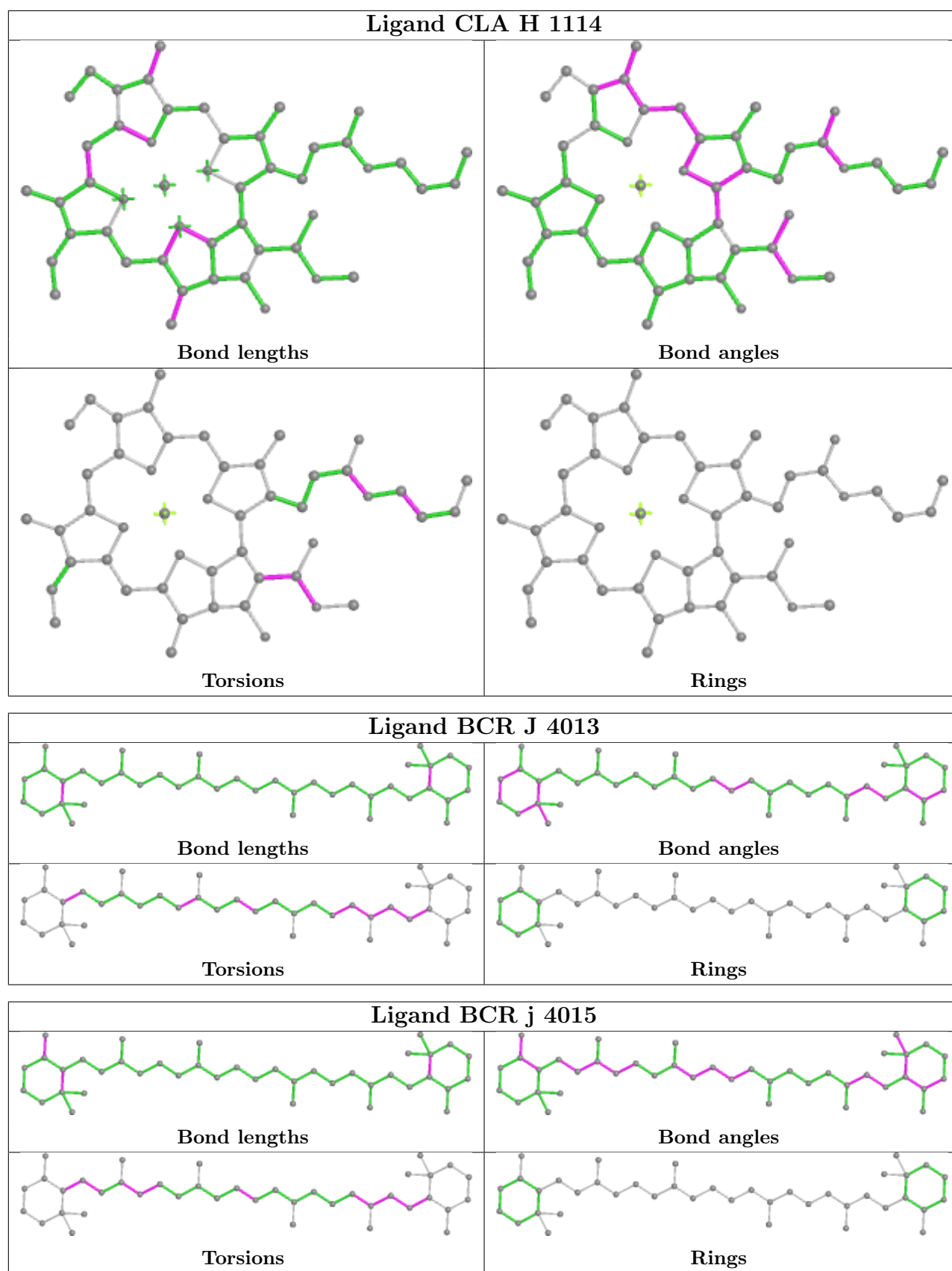
## Ligand CLA A 1107



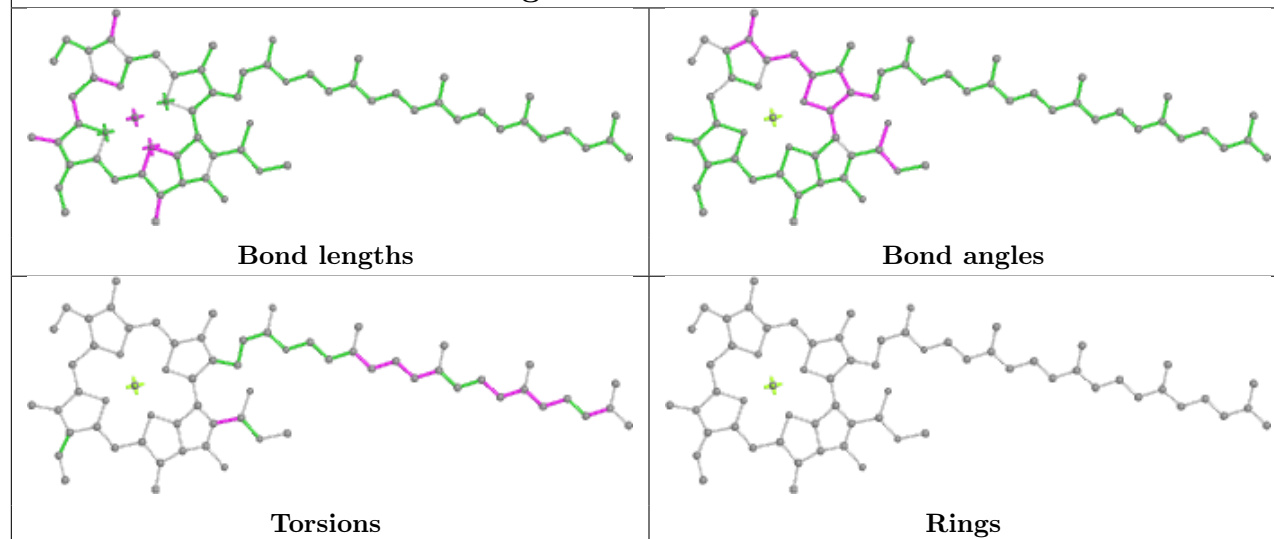
## Ligand CLA b 1021



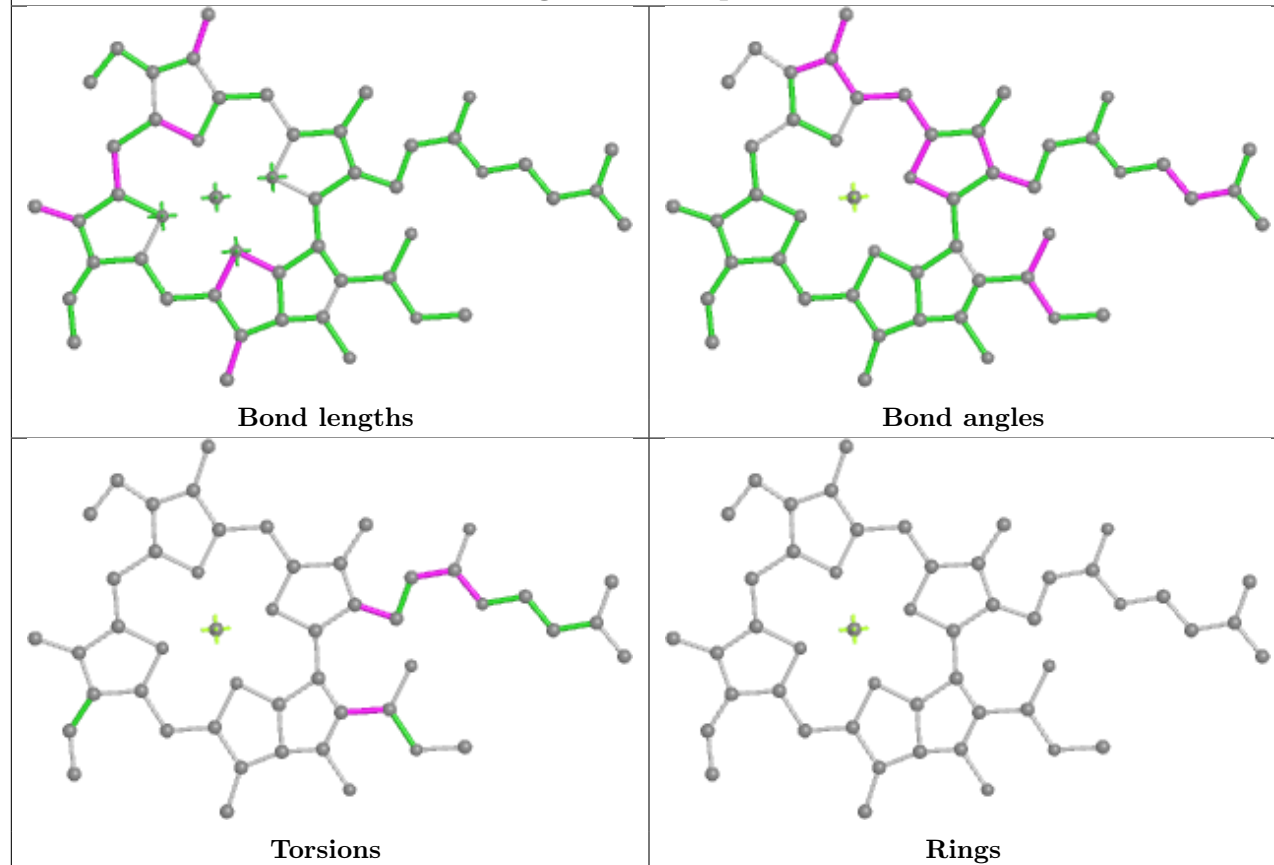




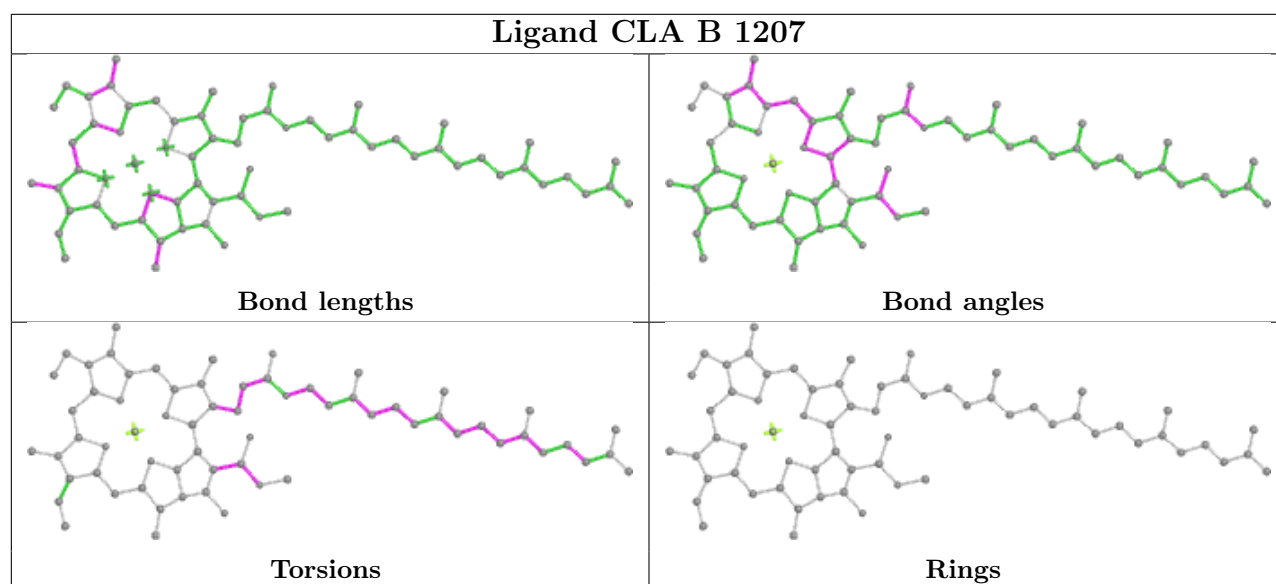
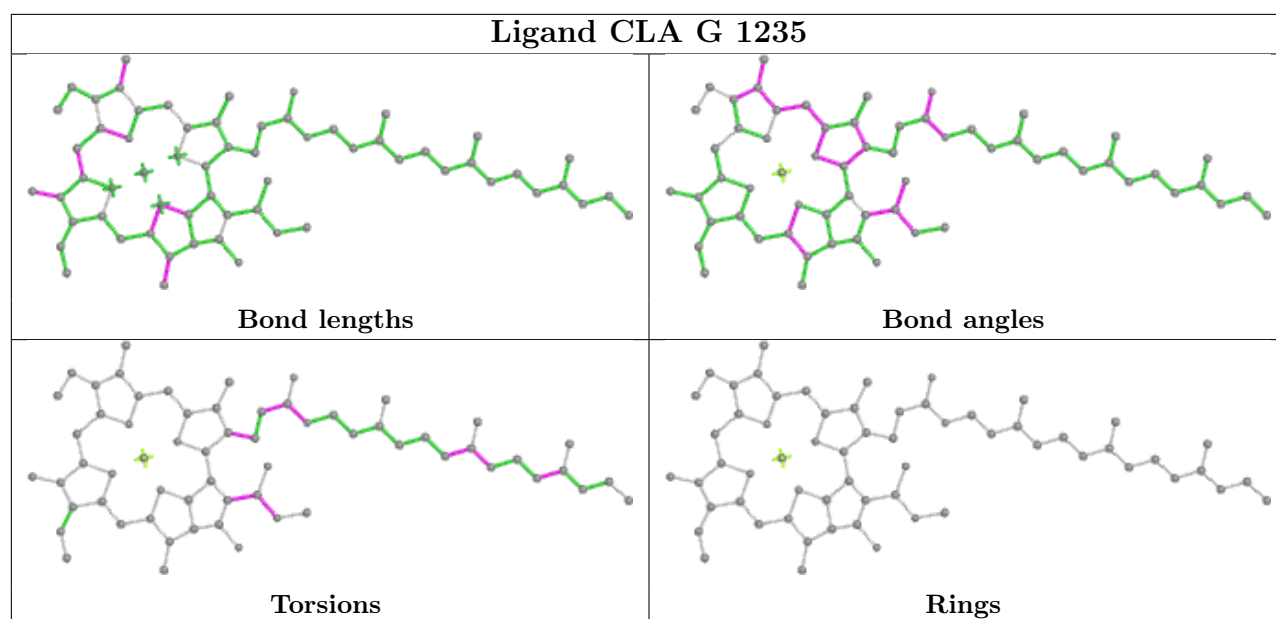
## Ligand CLA G 1223

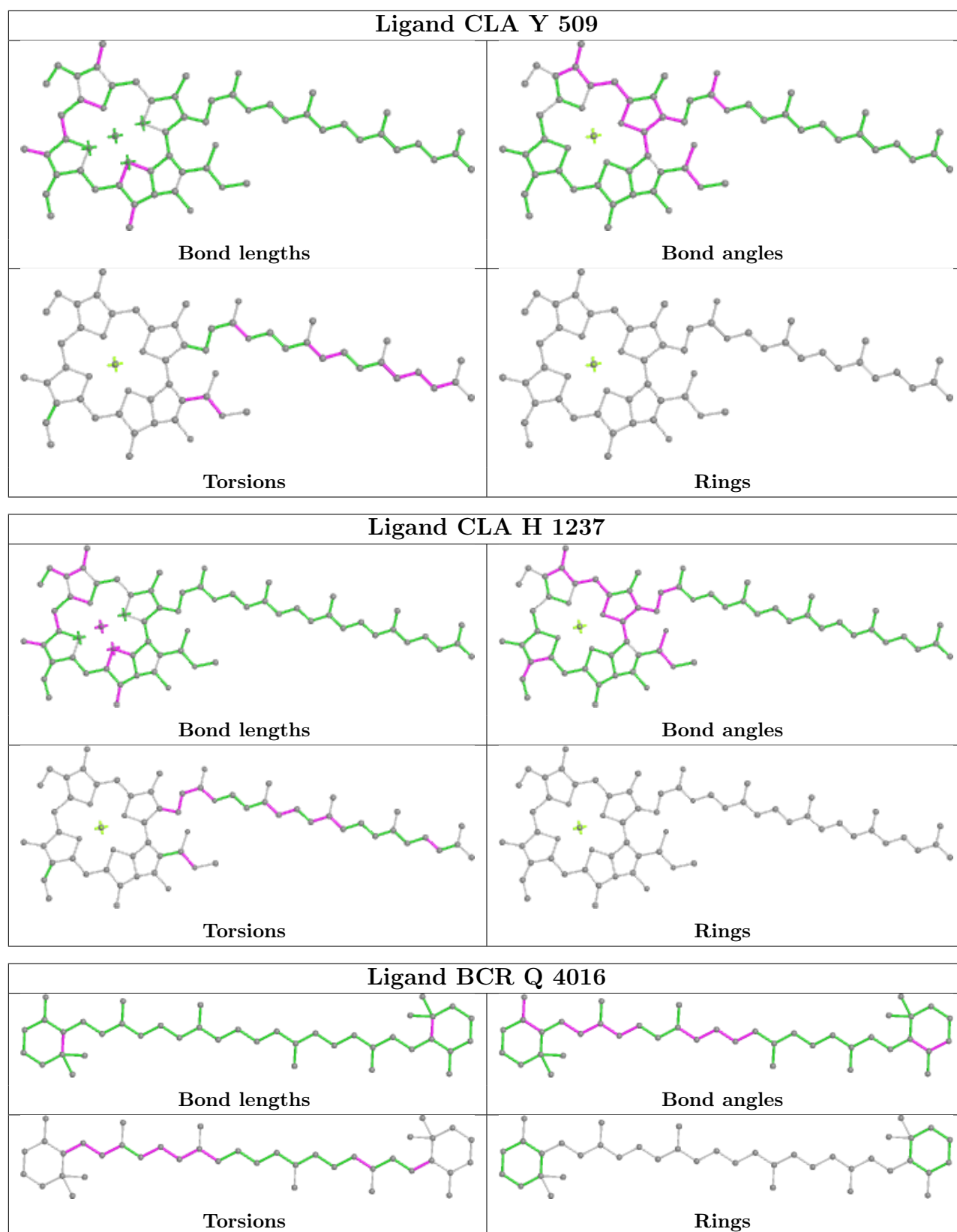


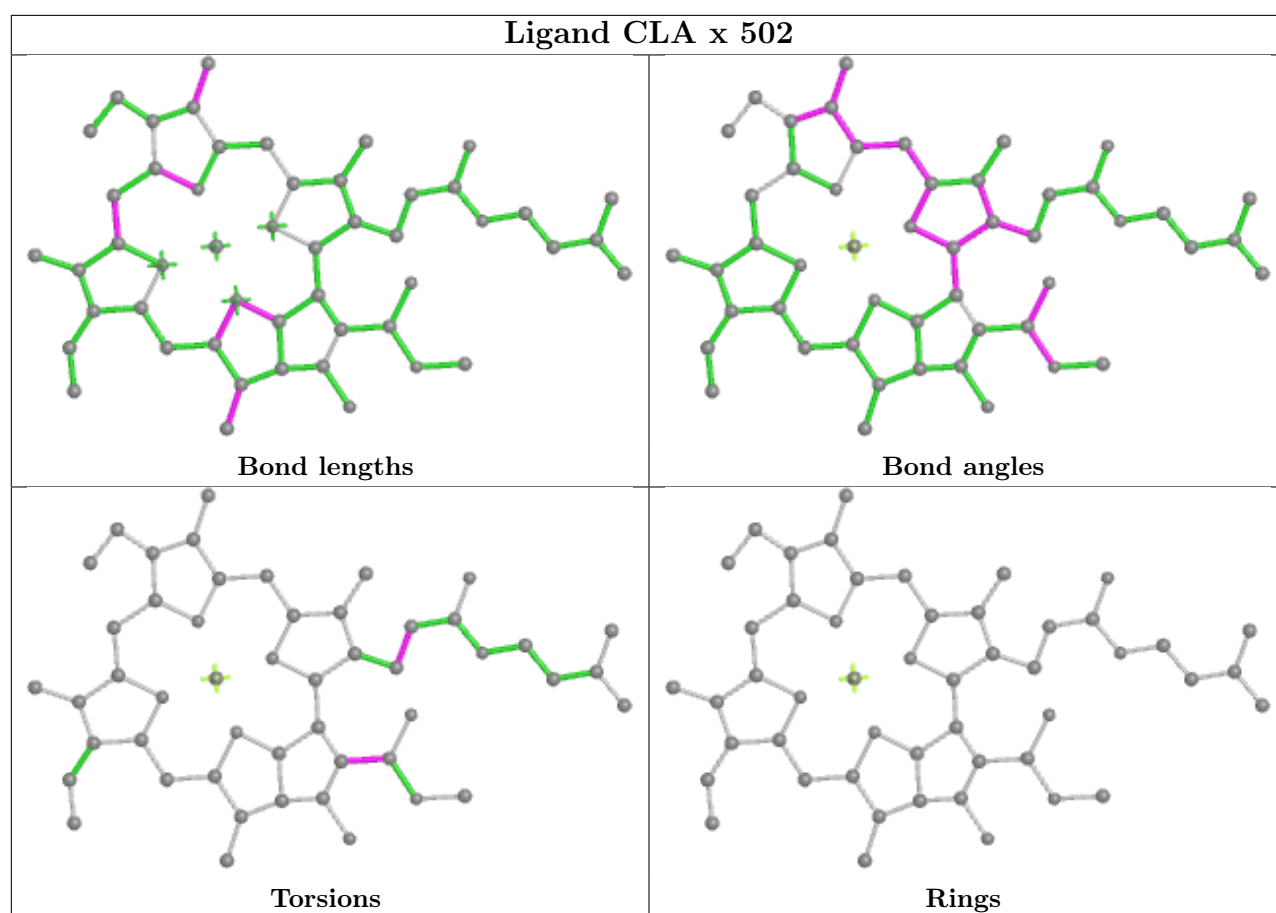
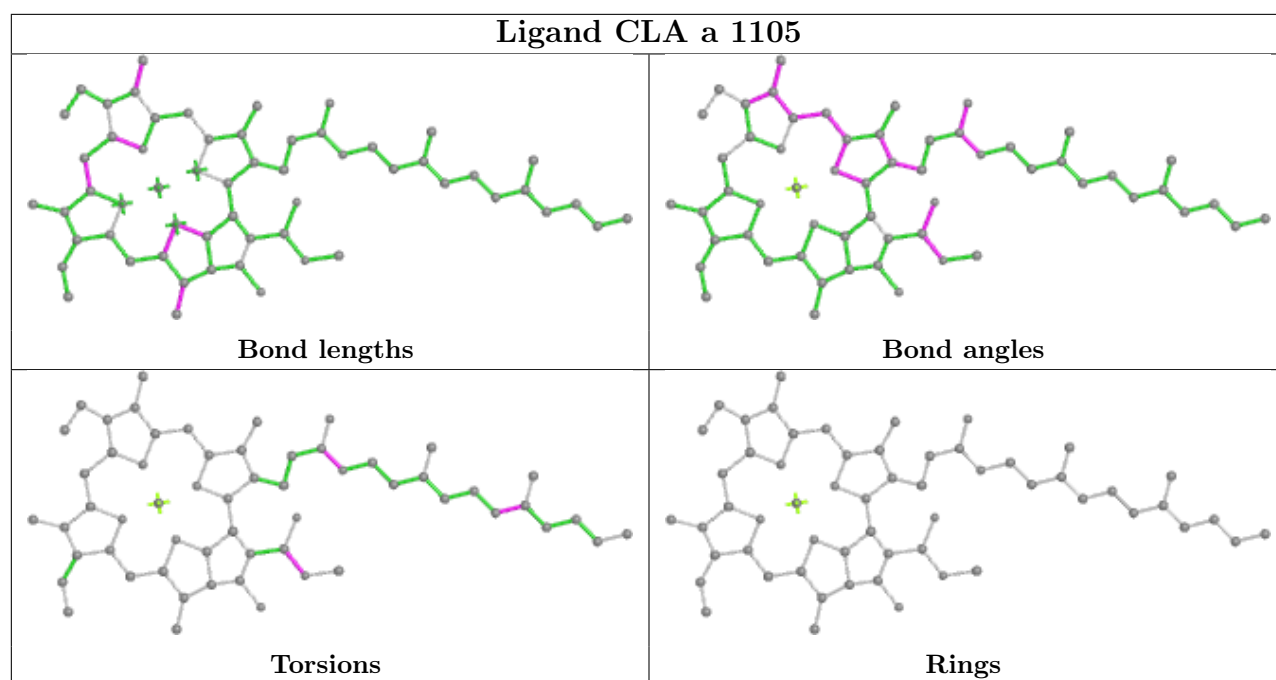
## Ligand CLA q 502

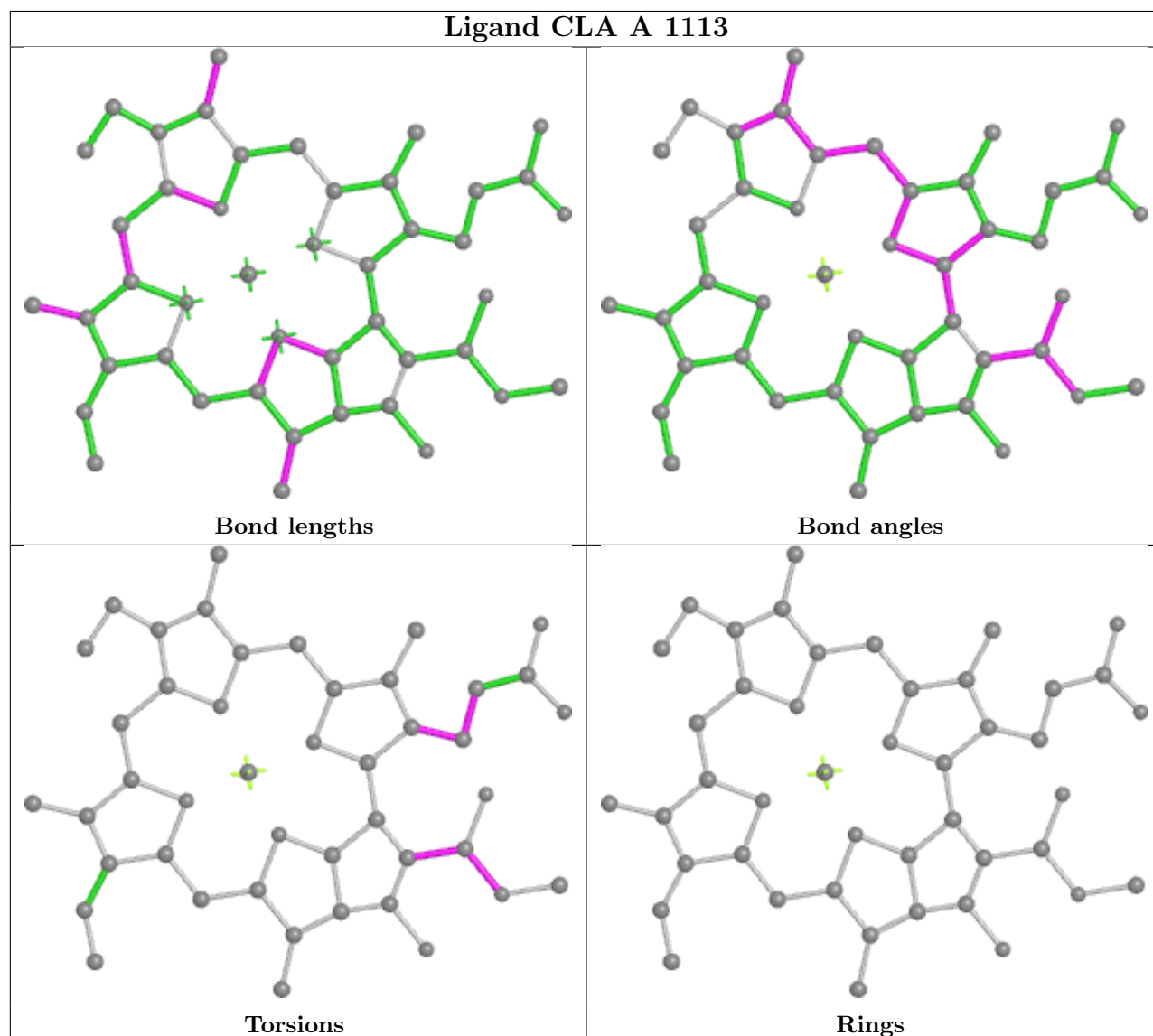
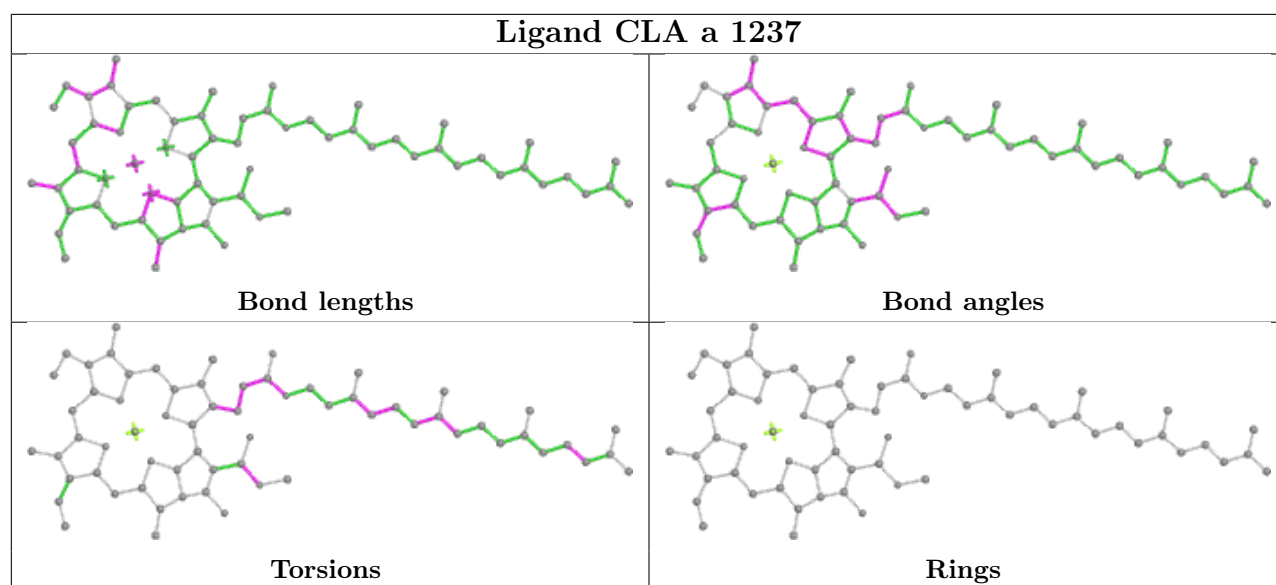


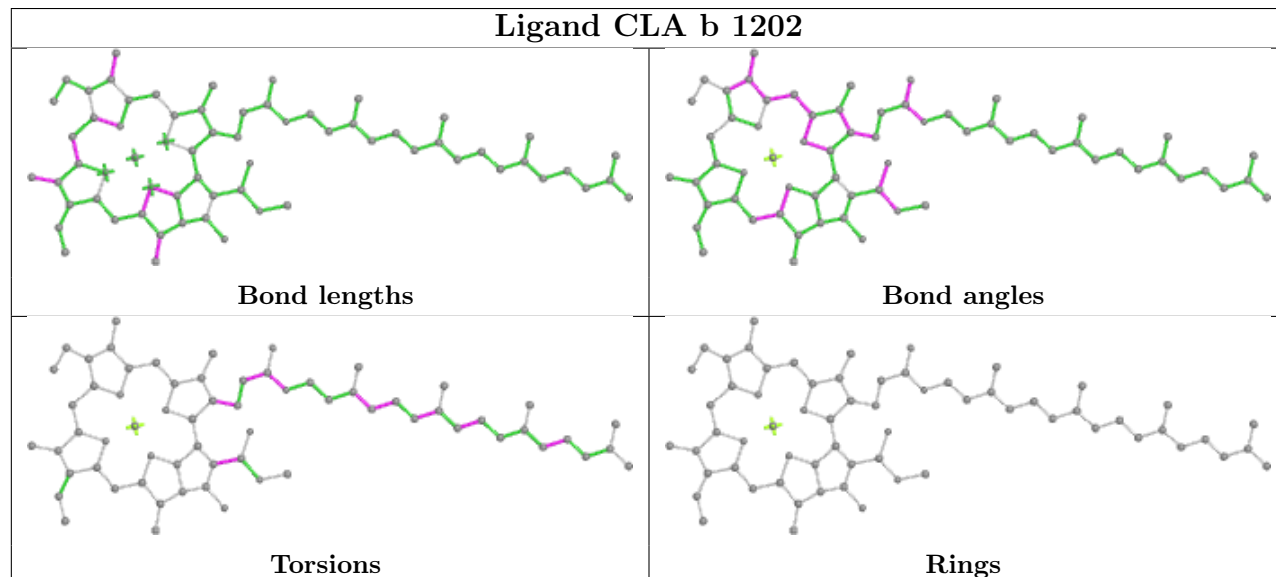
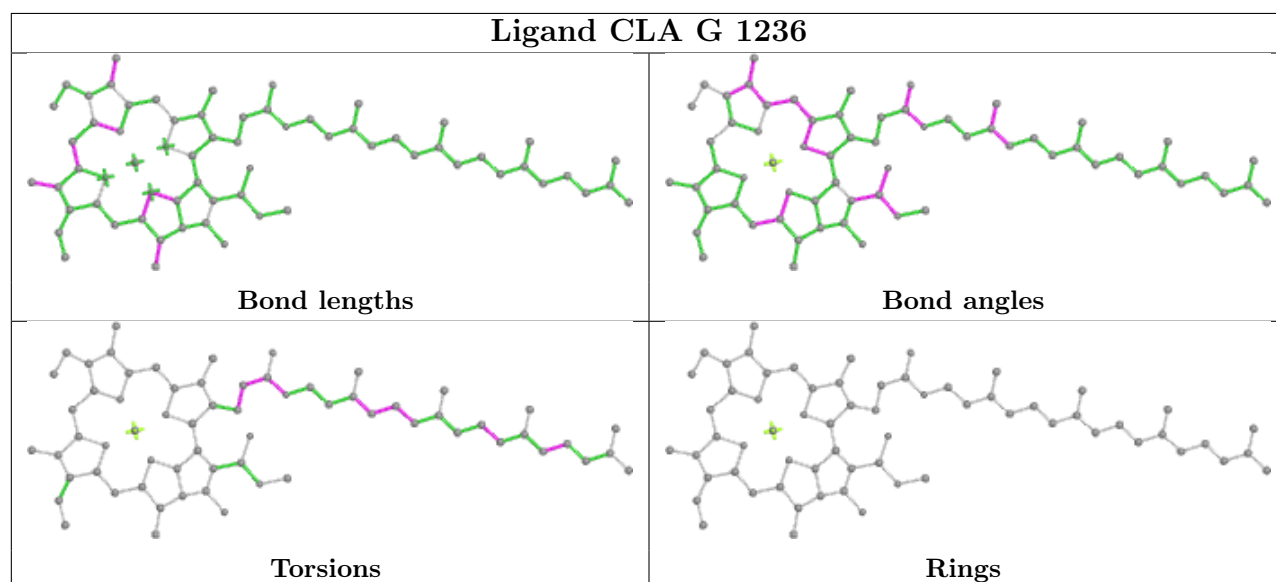
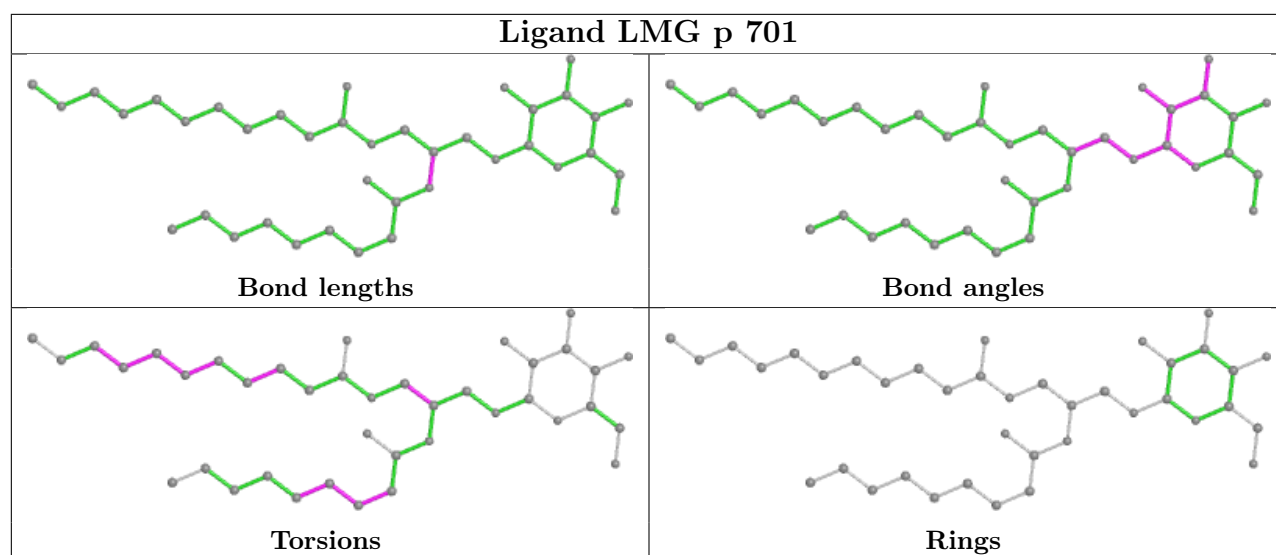




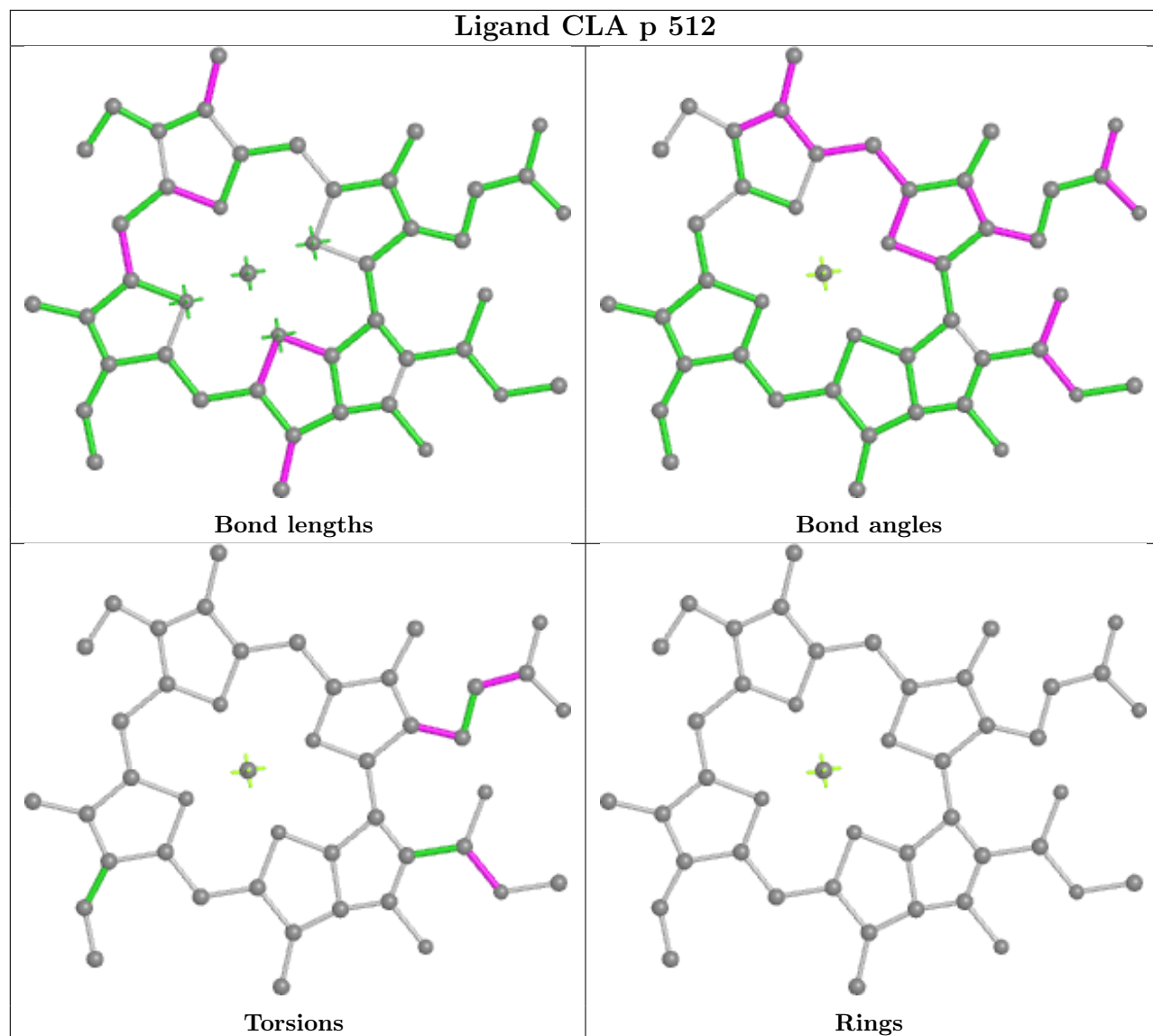




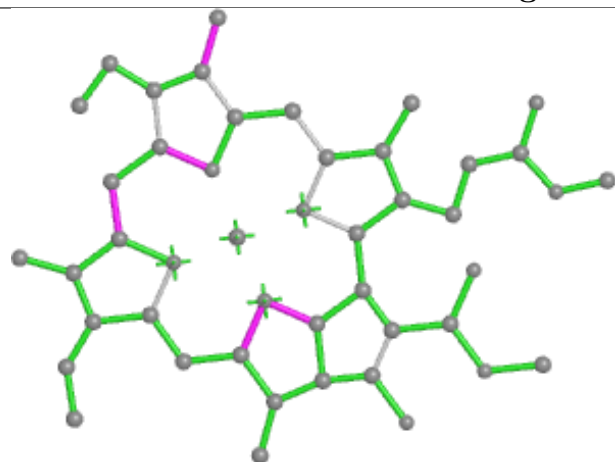




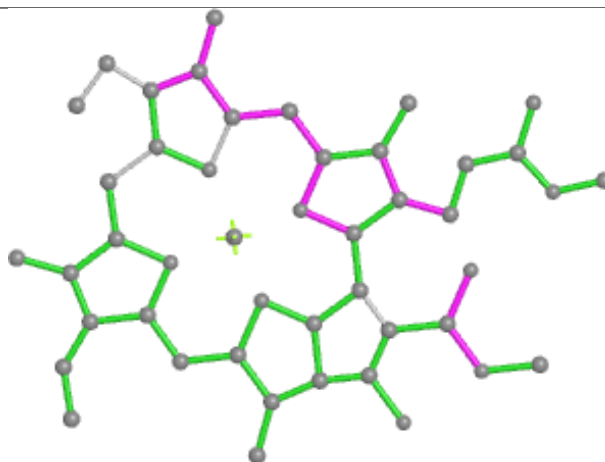
## Ligand CLA p 512



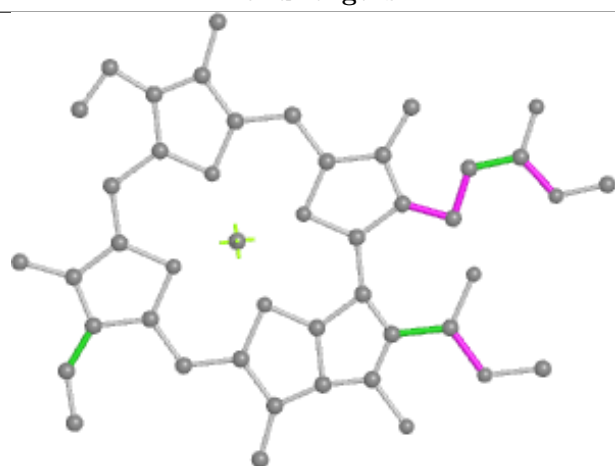
## Ligand CLA h 501



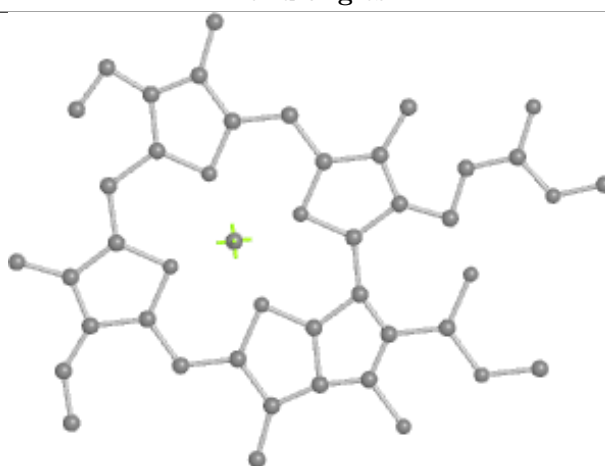
Bond lengths



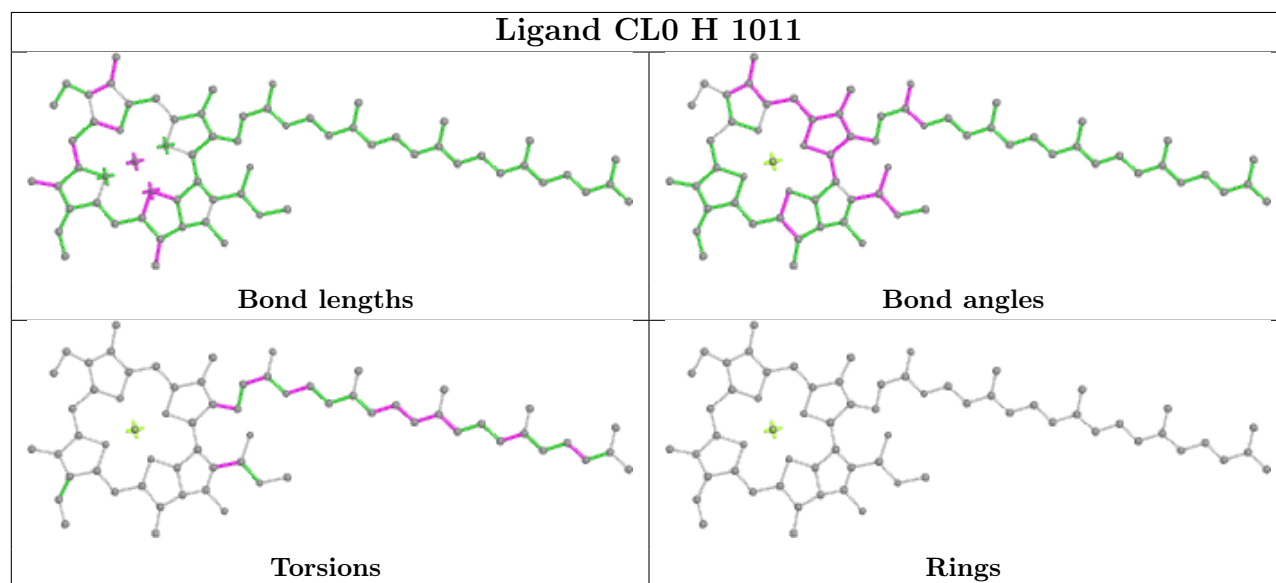
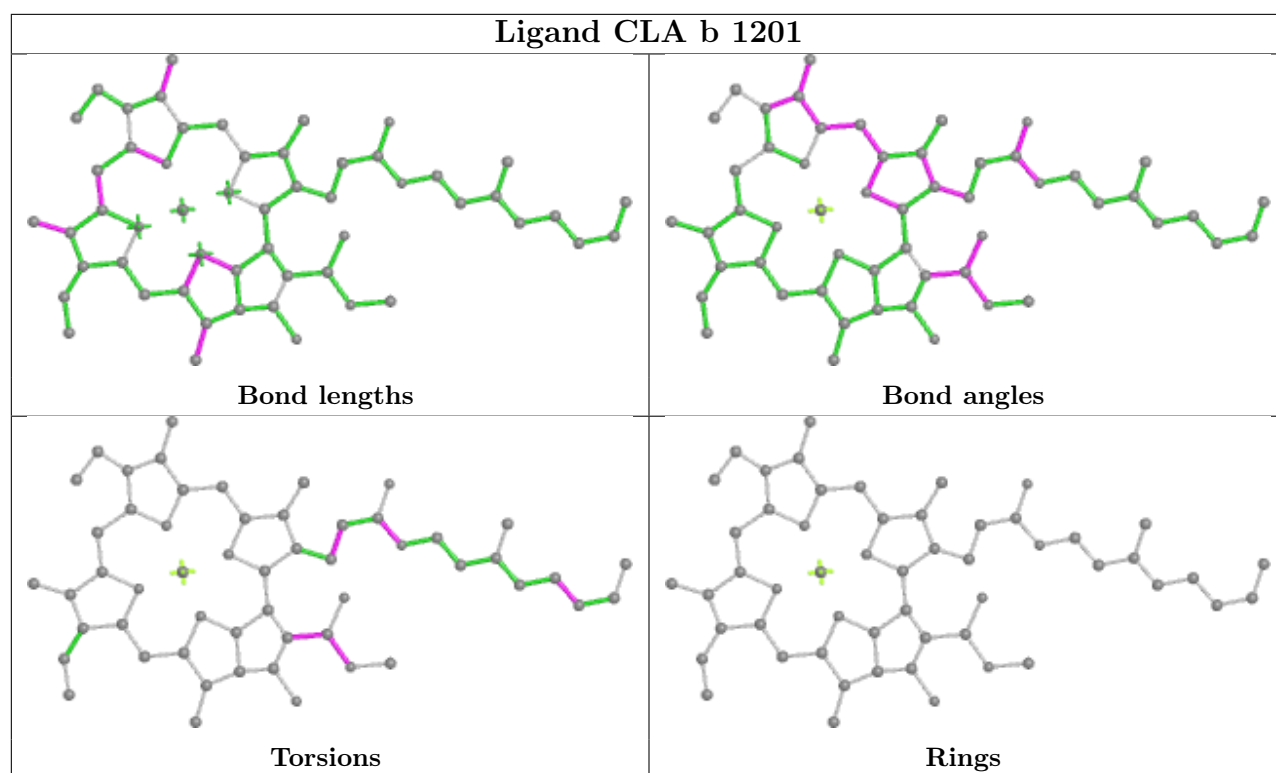
Bond angles



Torsions

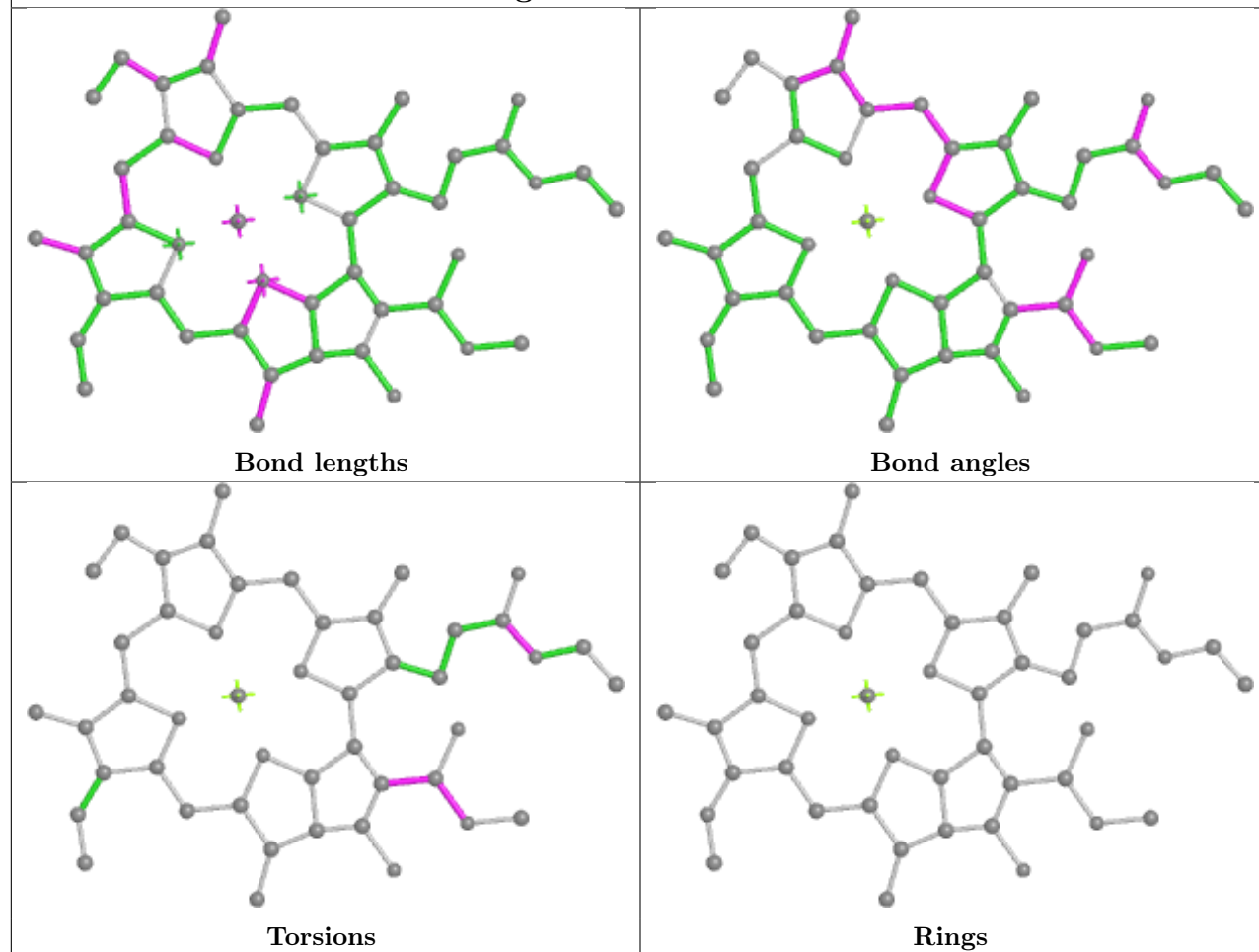


Rings

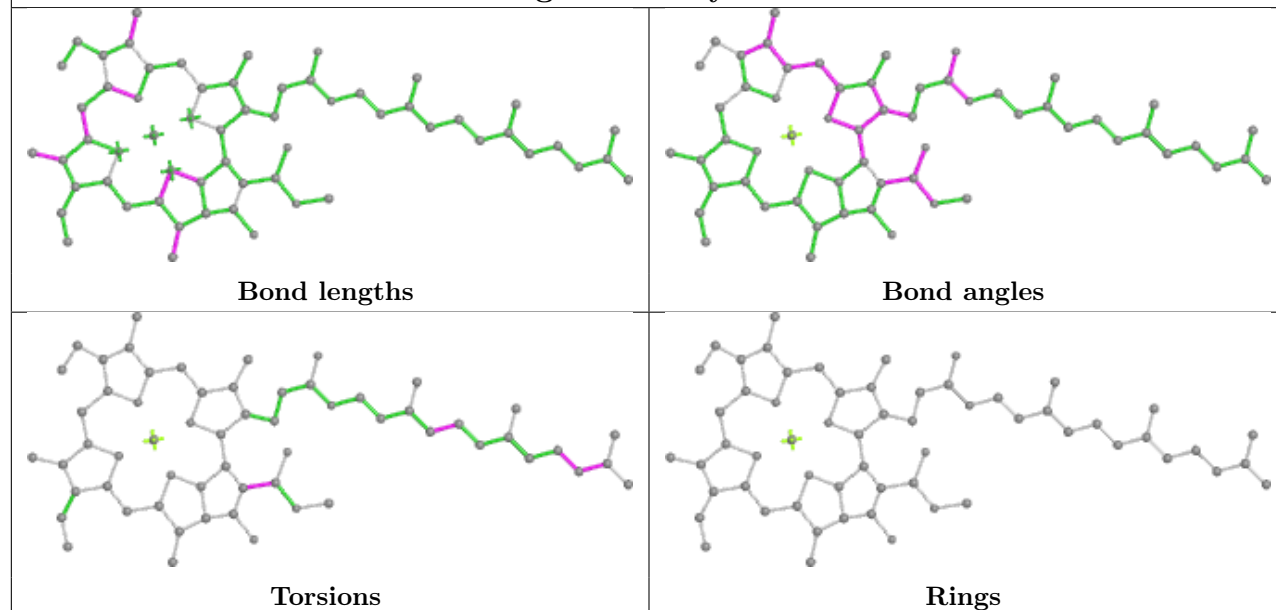


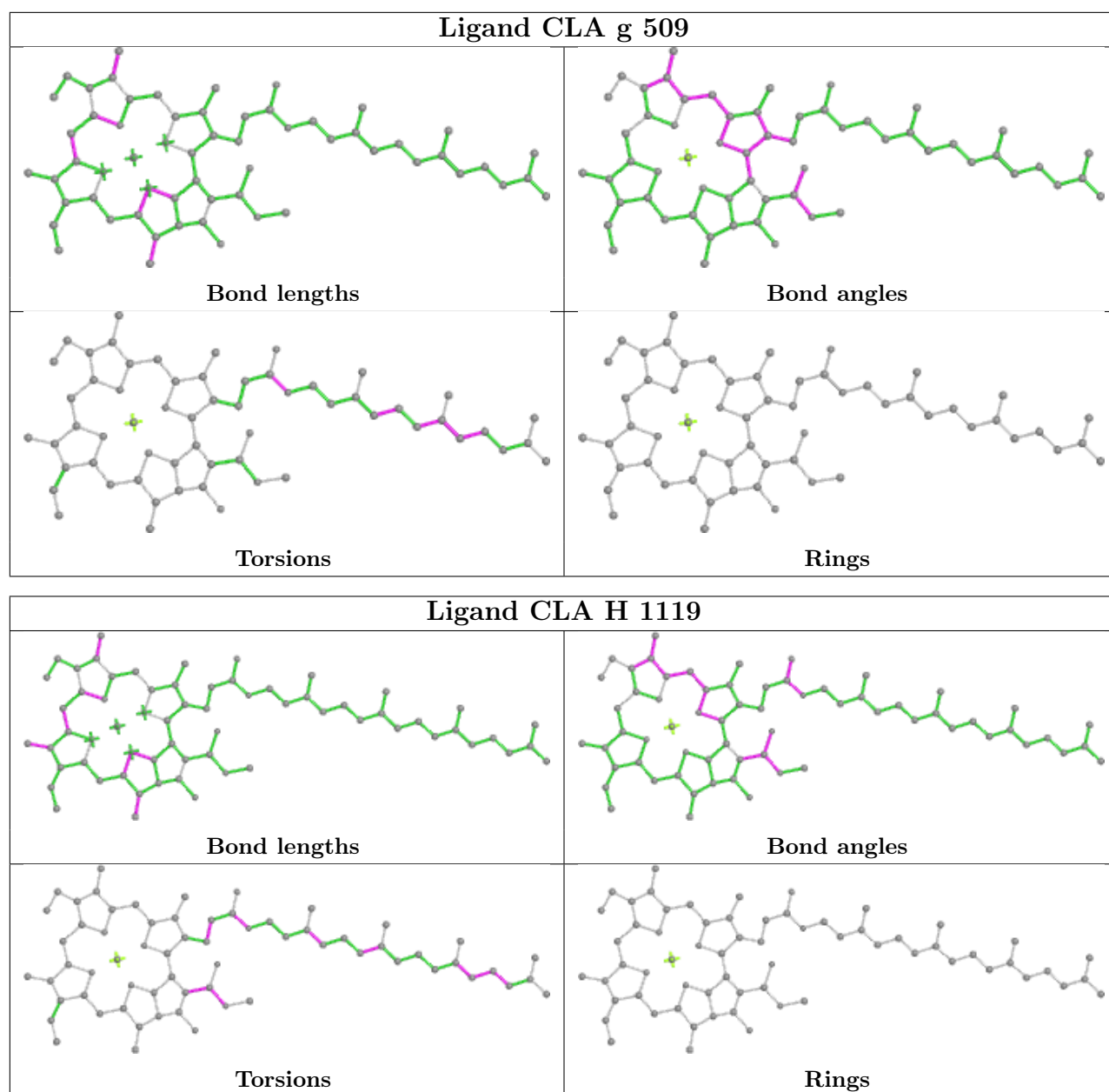


## Ligand CLA H 1137

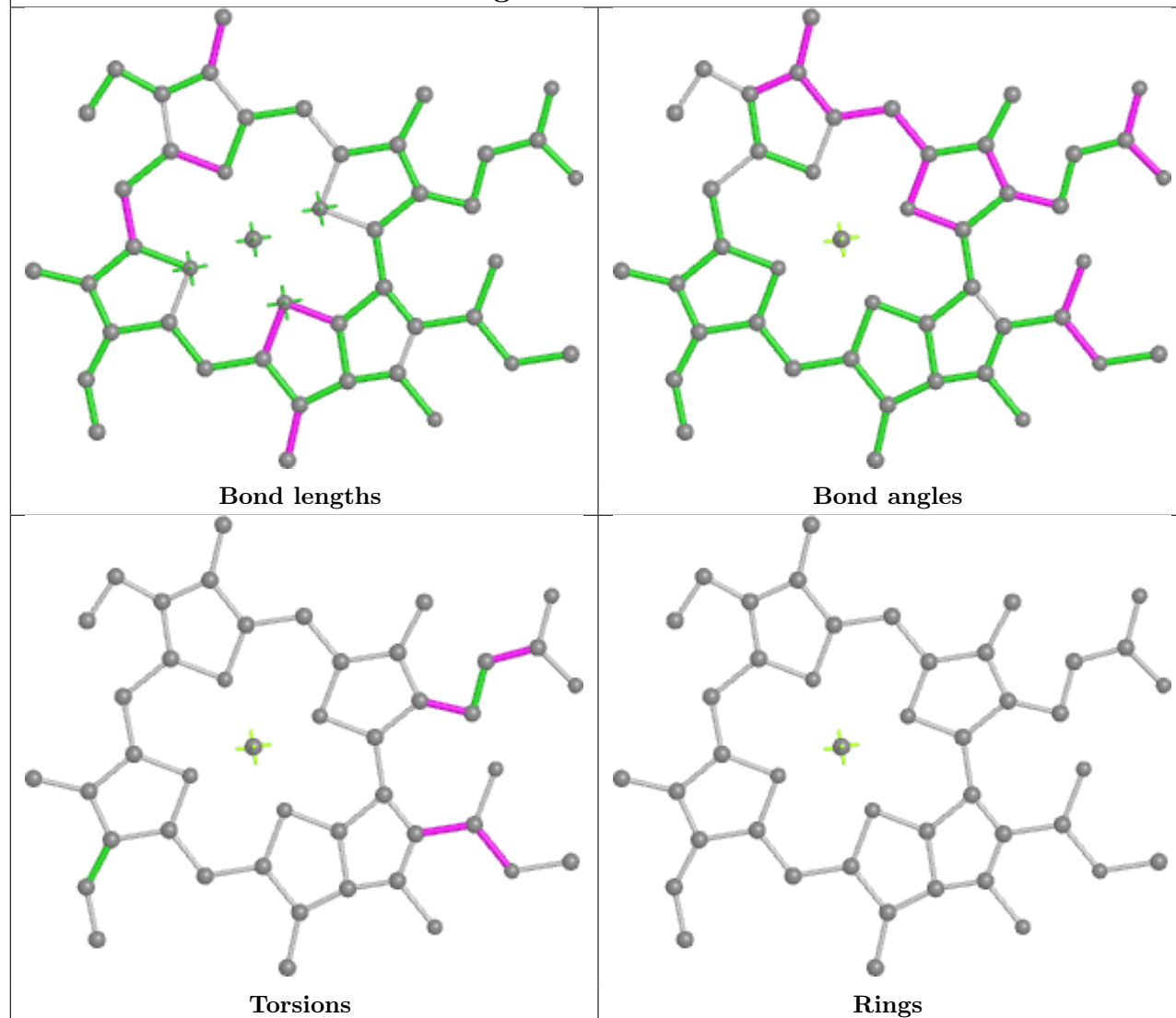


## Ligand CLA y 509

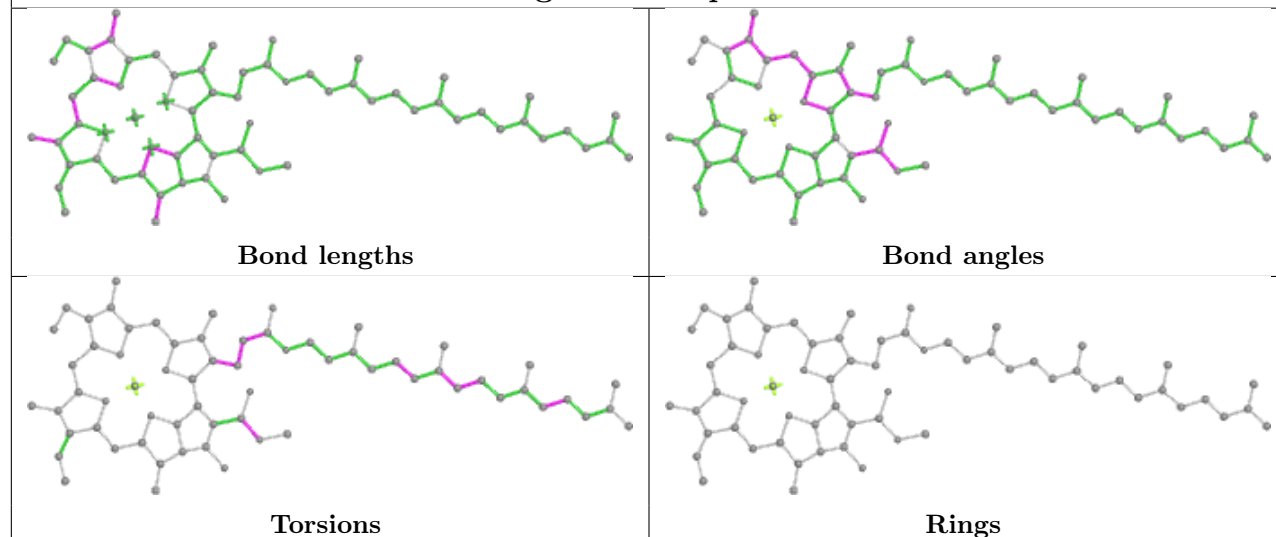


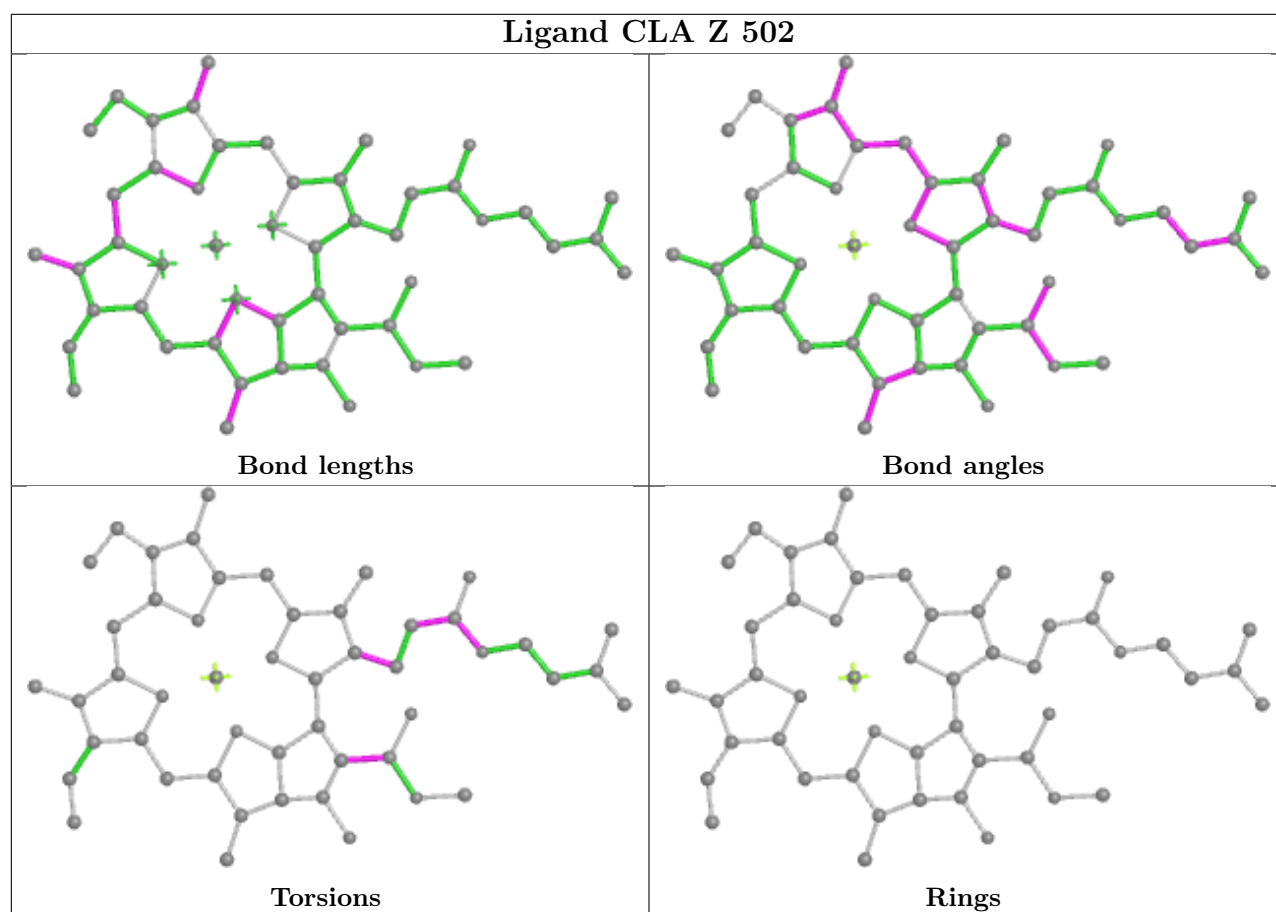


## Ligand CLA x 512

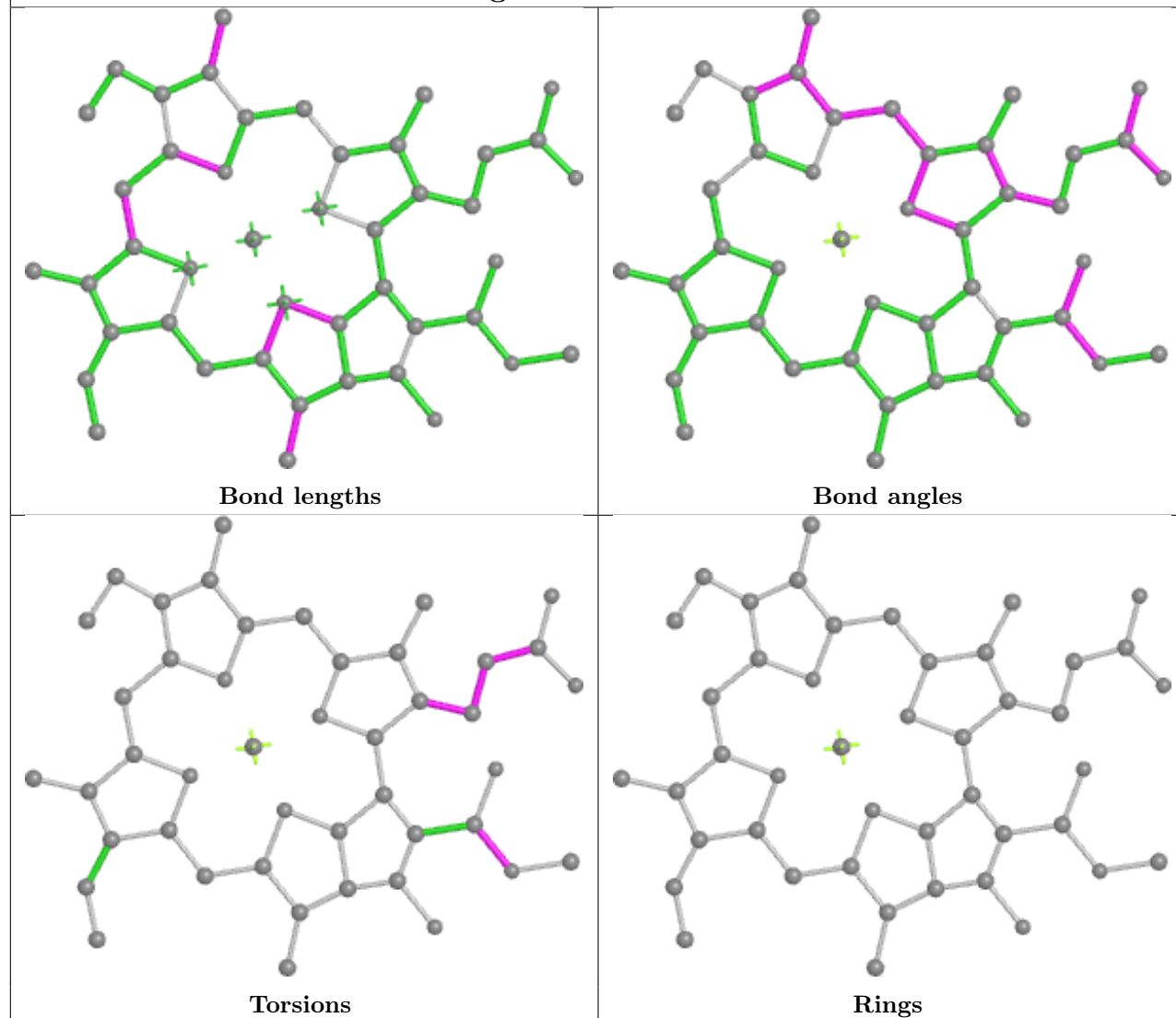


## Ligand CLA p 505

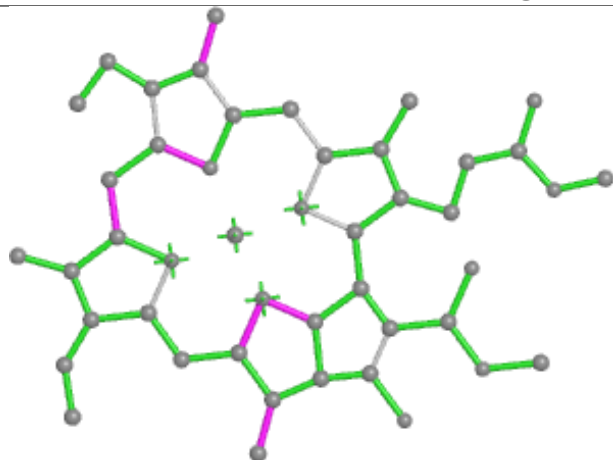




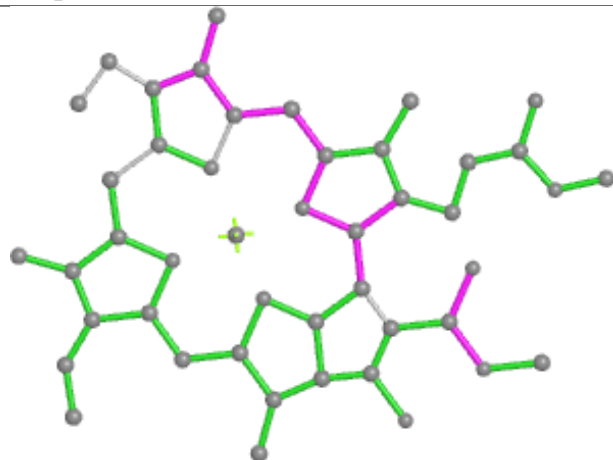
## Ligand CLA X 512



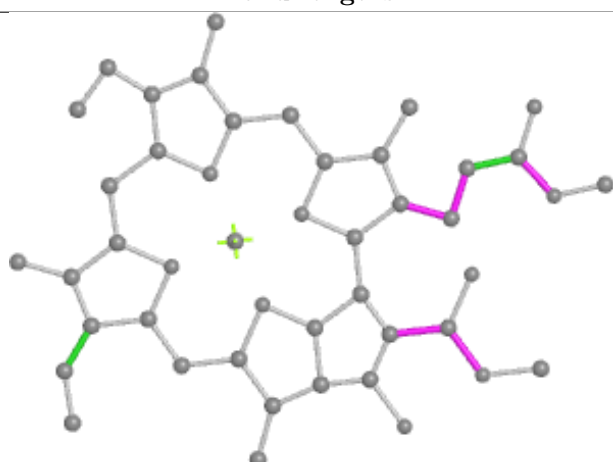
## Ligand CLA p 516



Bond lengths



Bond angles

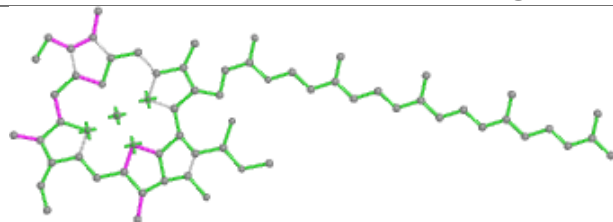


Torsions

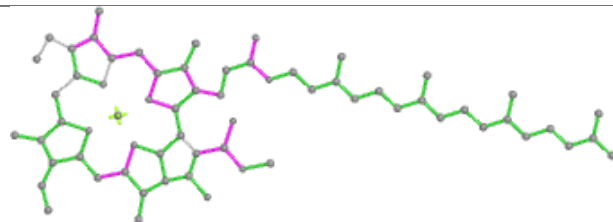


Rings

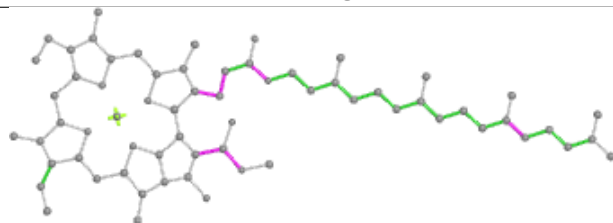
## Ligand CLA a 1132



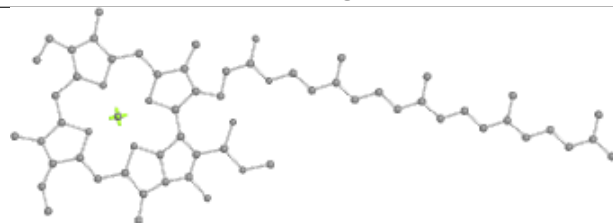
Bond lengths



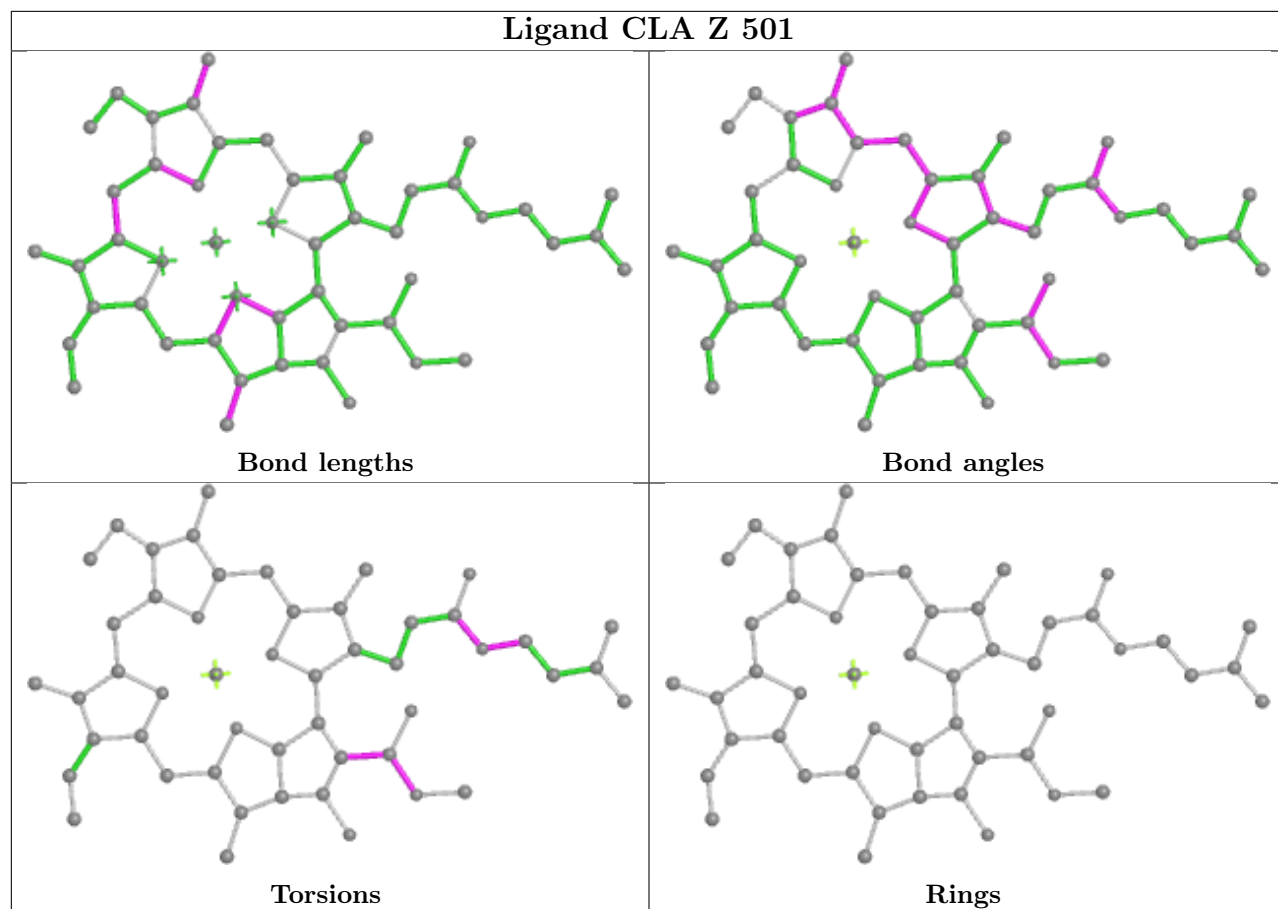
Bond angles



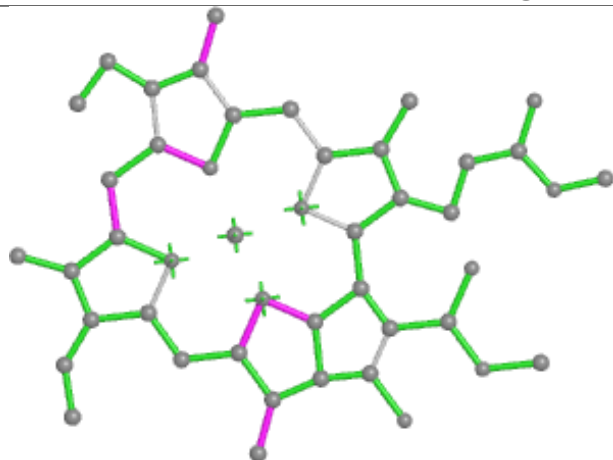
Torsions



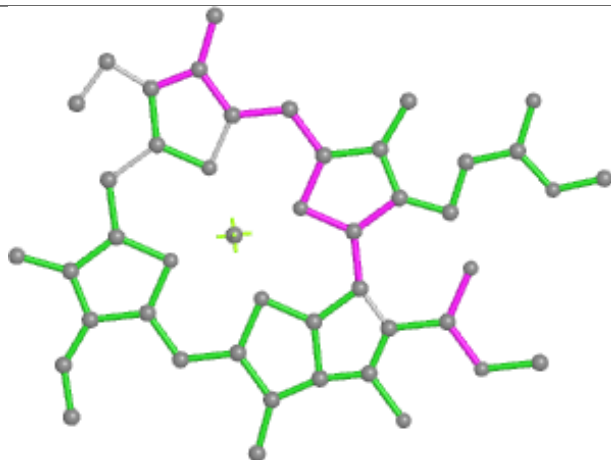
Rings



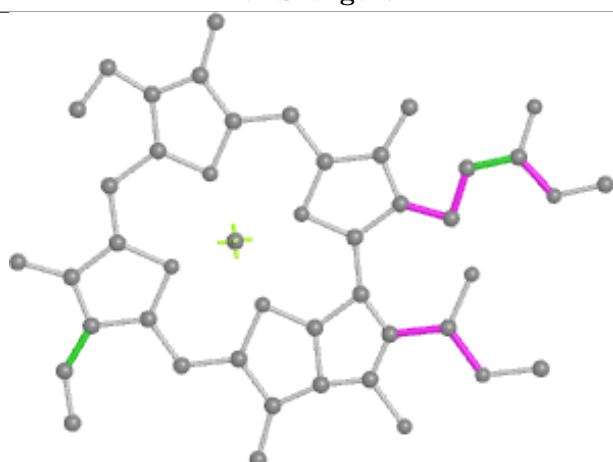
## Ligand CLA n 503



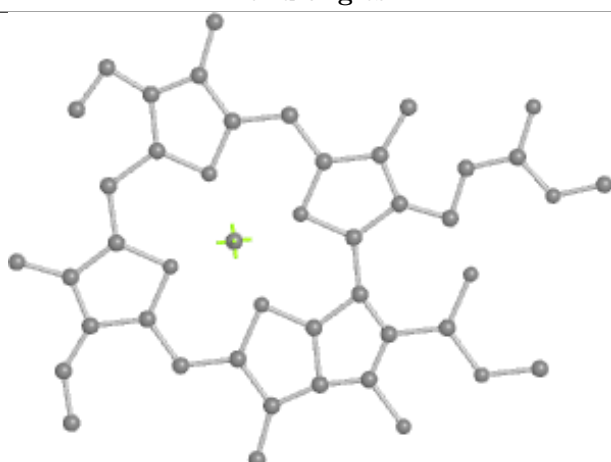
Bond lengths



Bond angles



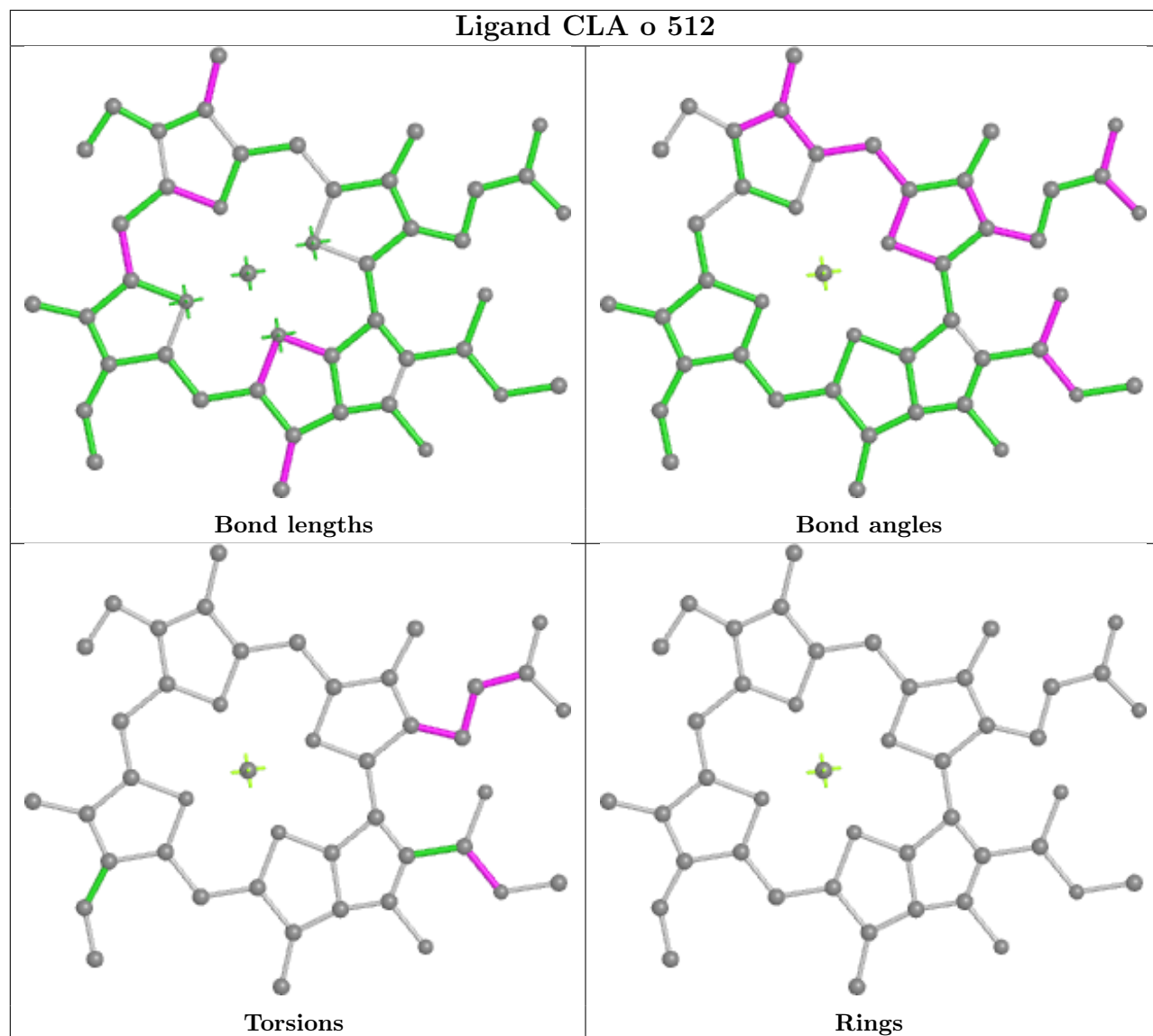
Torsions



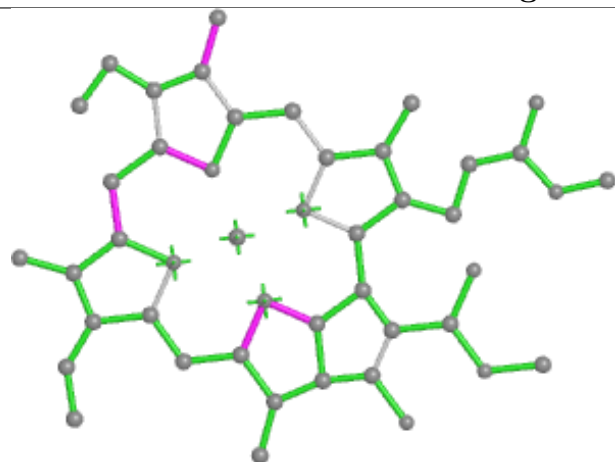
Rings



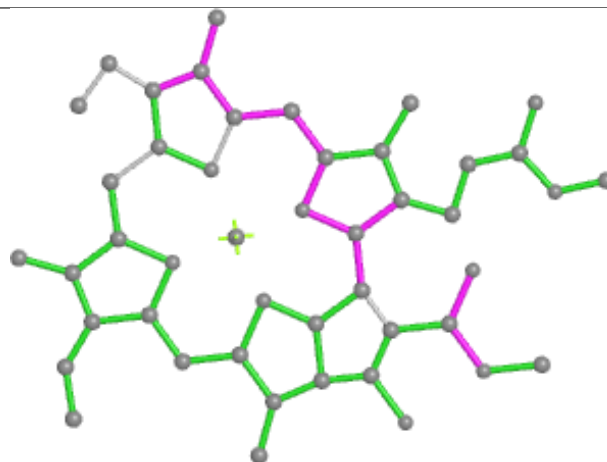
## Ligand CLA o 512



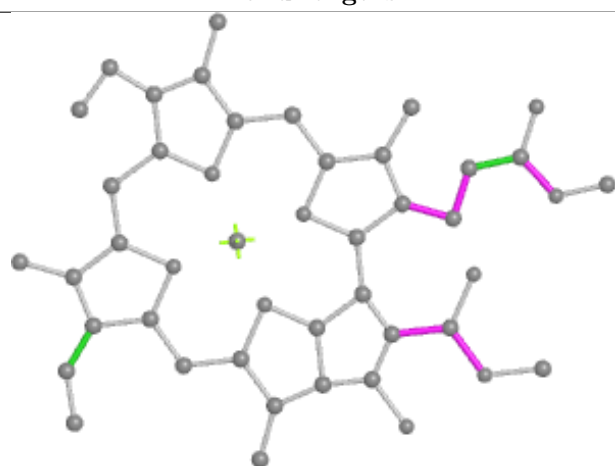
## Ligand CLA x 516



Bond lengths



Bond angles

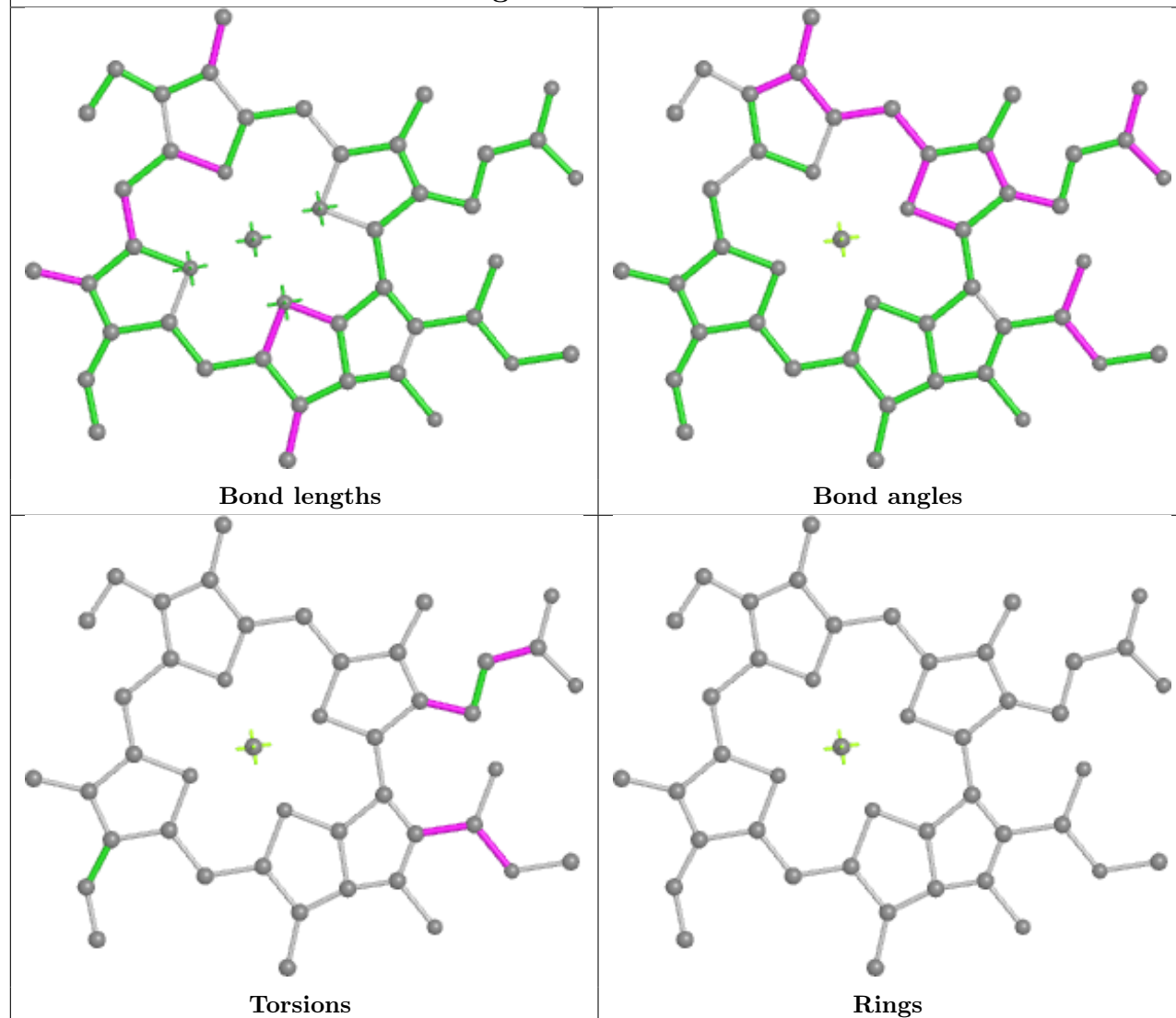


Torsions

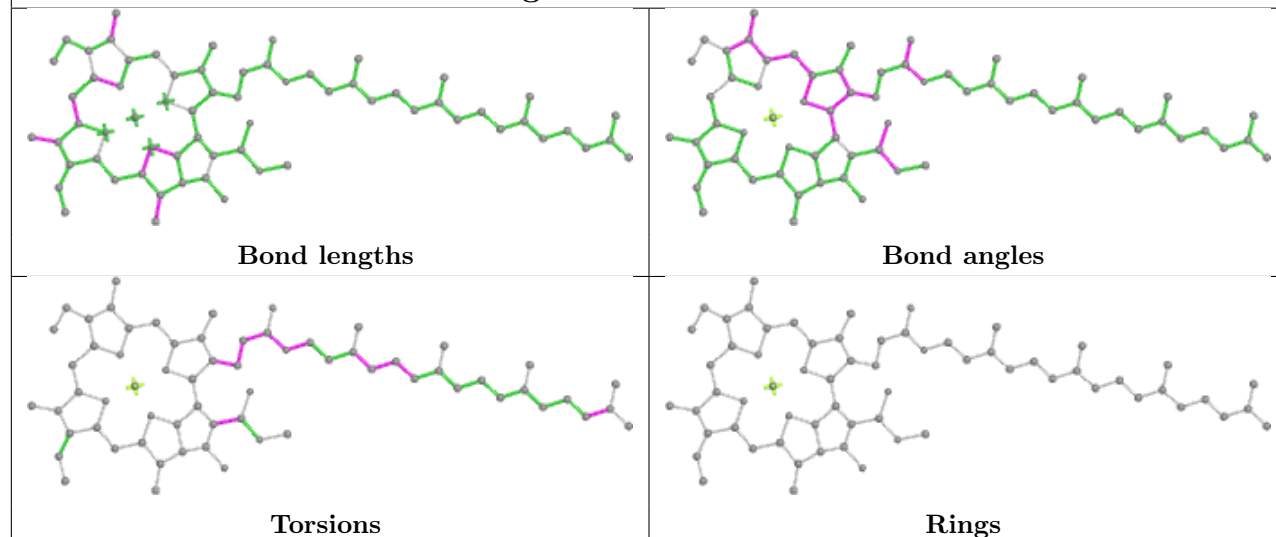


Rings

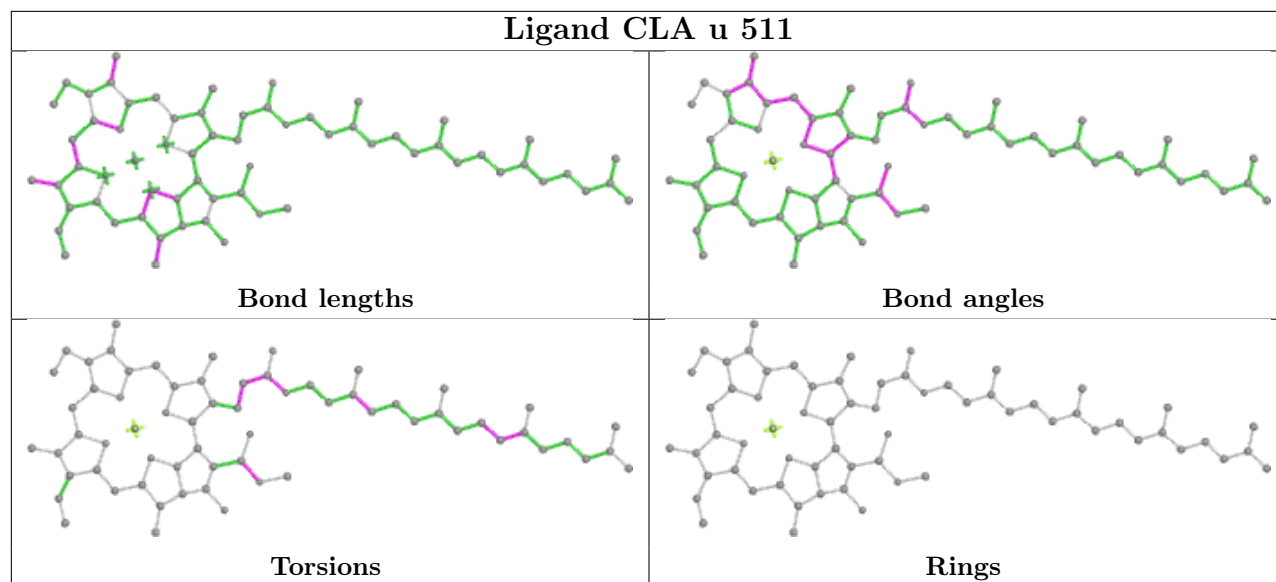
## Ligand CLA Z 512



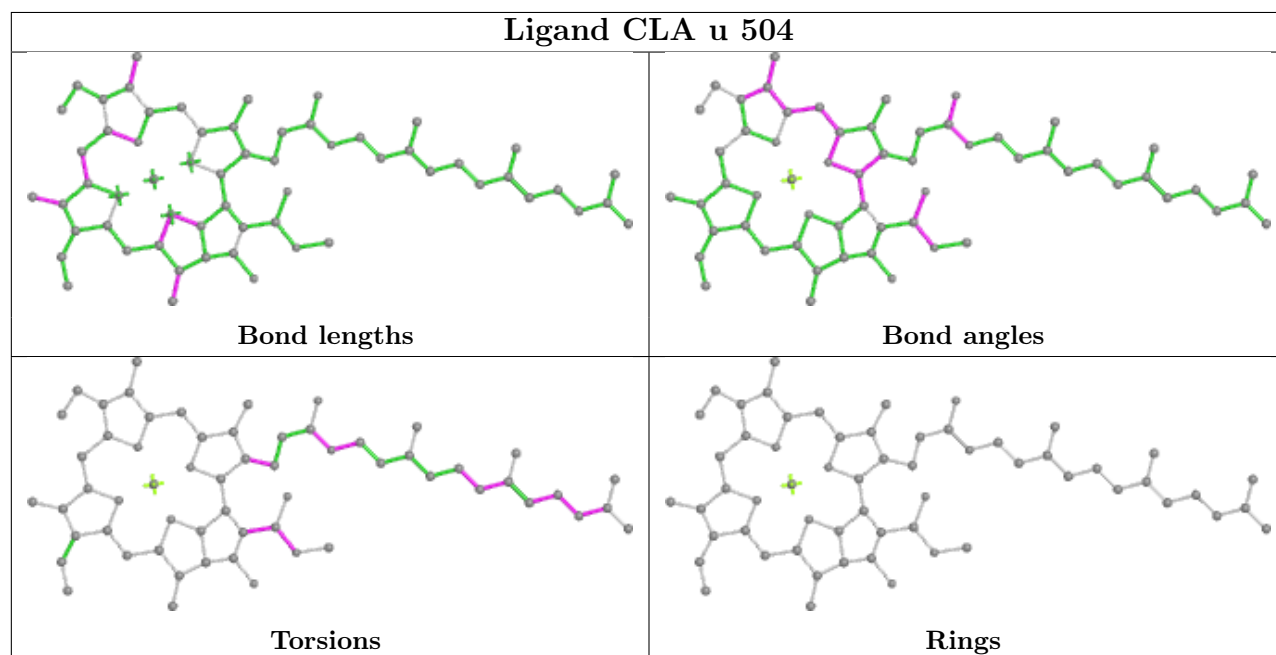
## Ligand CLA U 1503

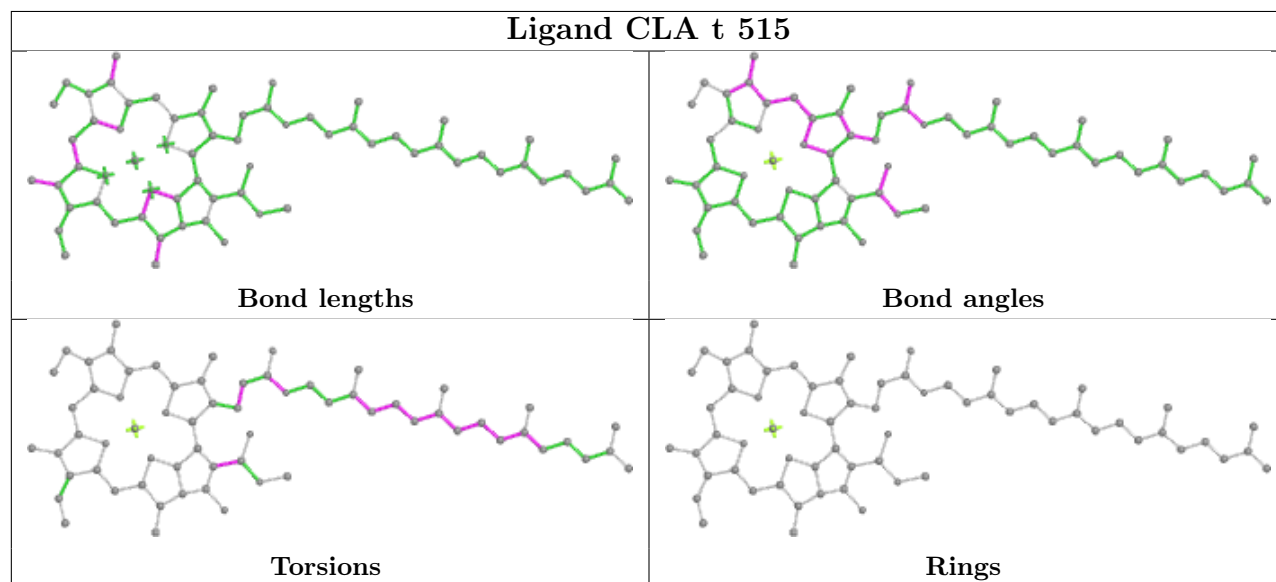
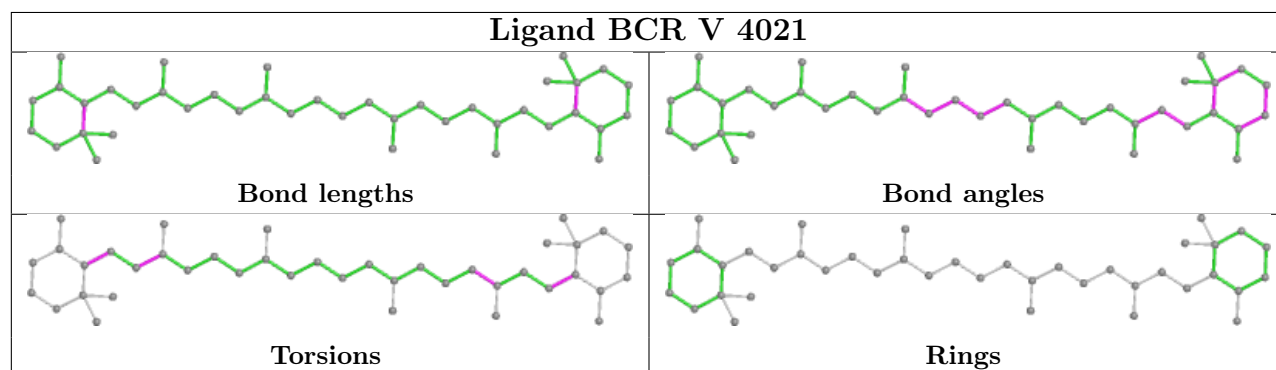
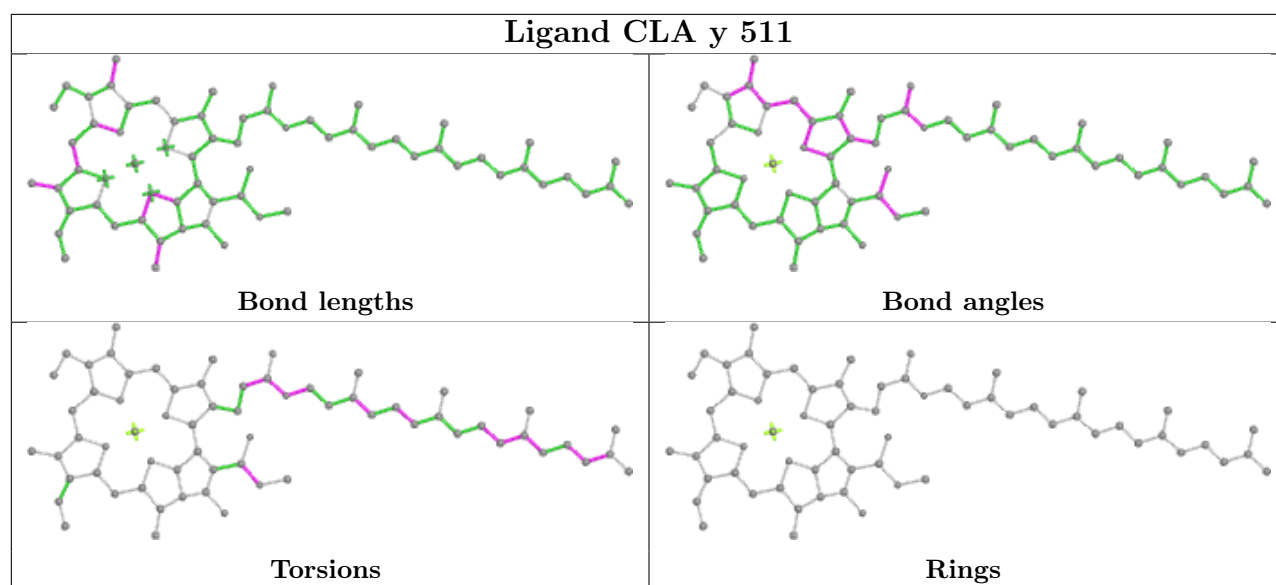


## Ligand CLA u 511

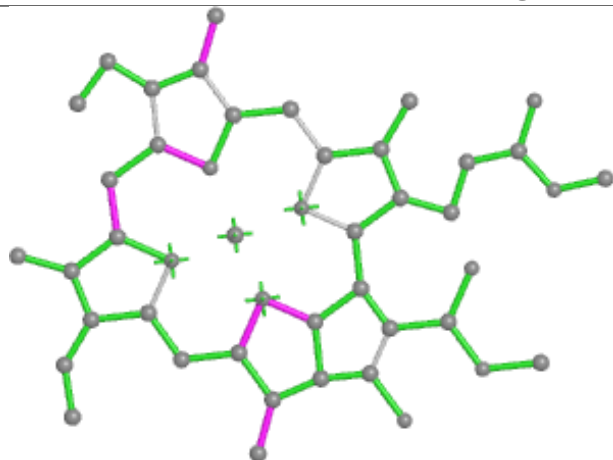


## Ligand CLA u 504

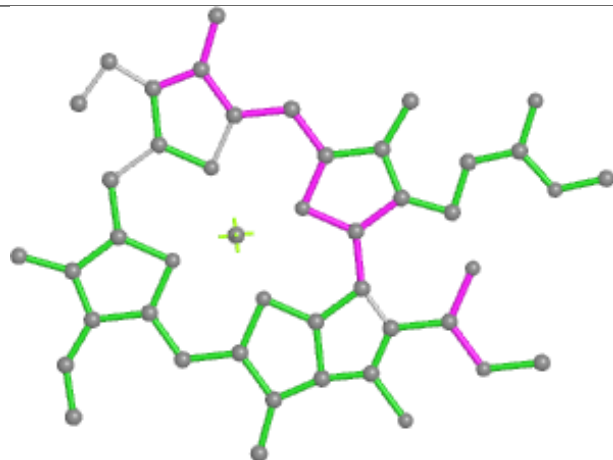




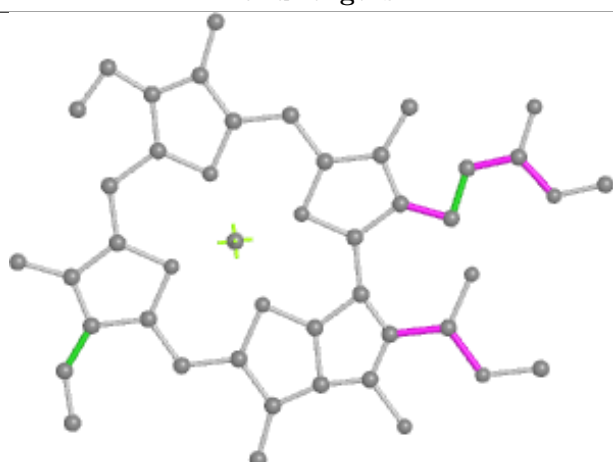
## Ligand CLA X 516



Bond lengths



Bond angles

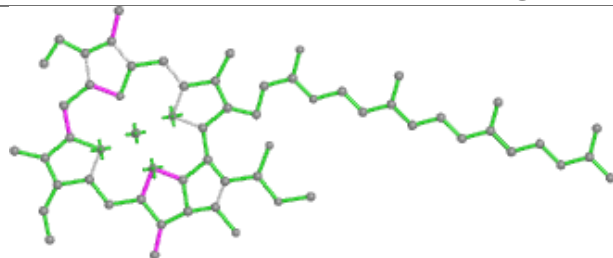


Torsions

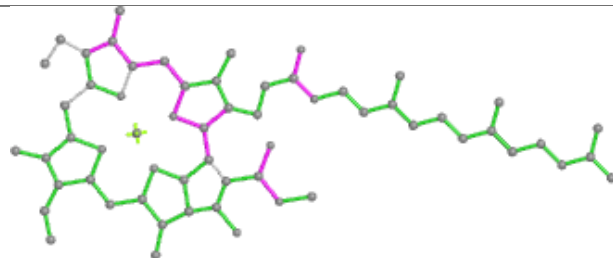


Rings

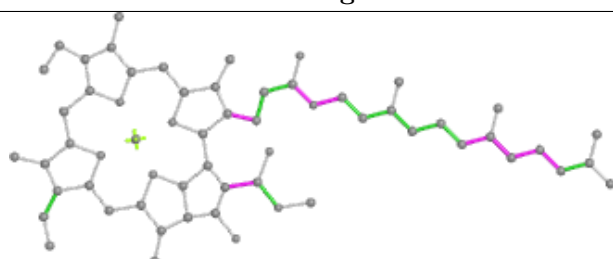
## Ligand CLA Y 504



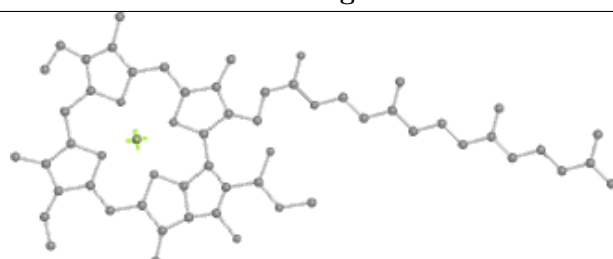
Bond lengths



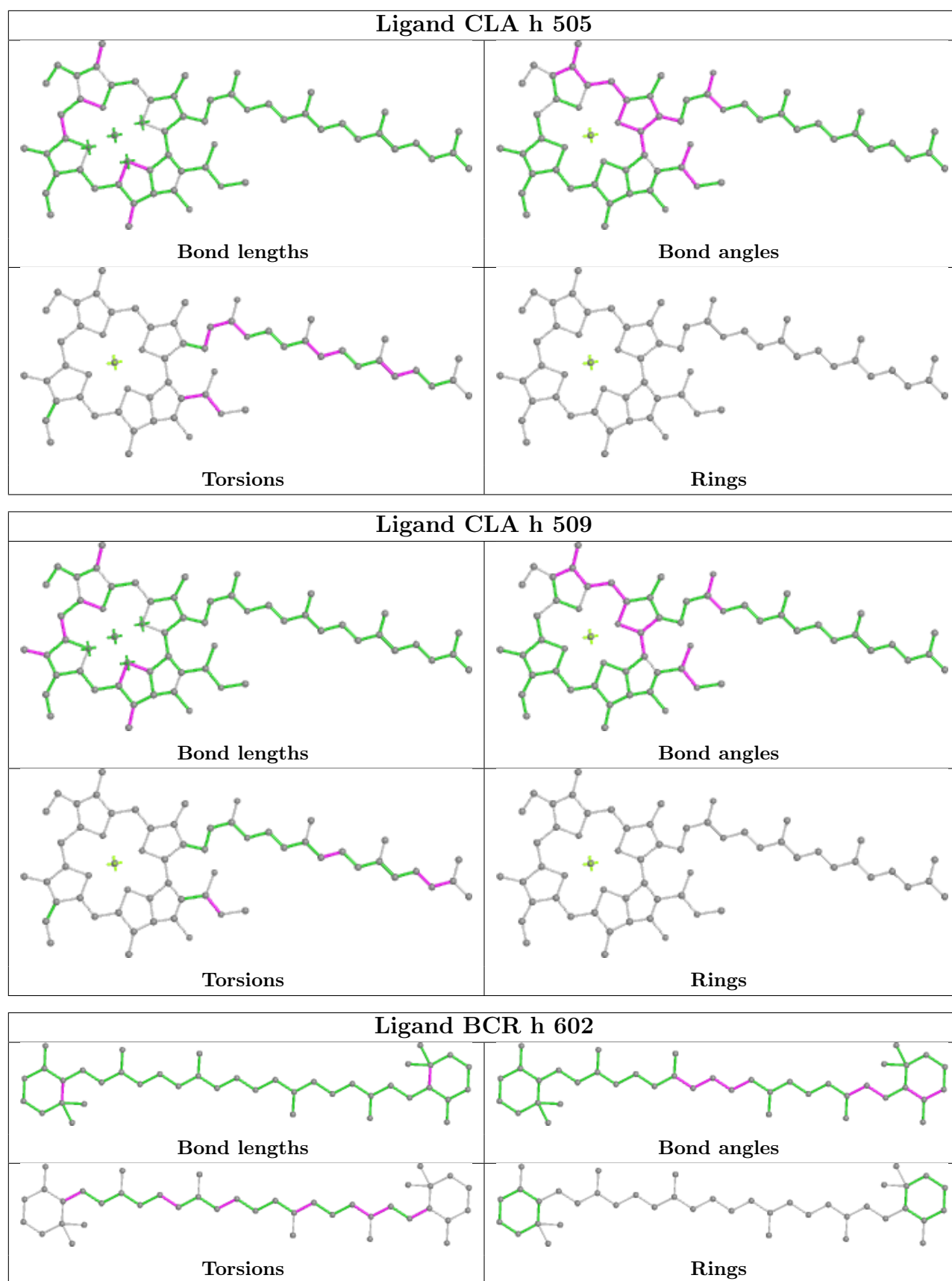
Bond angles

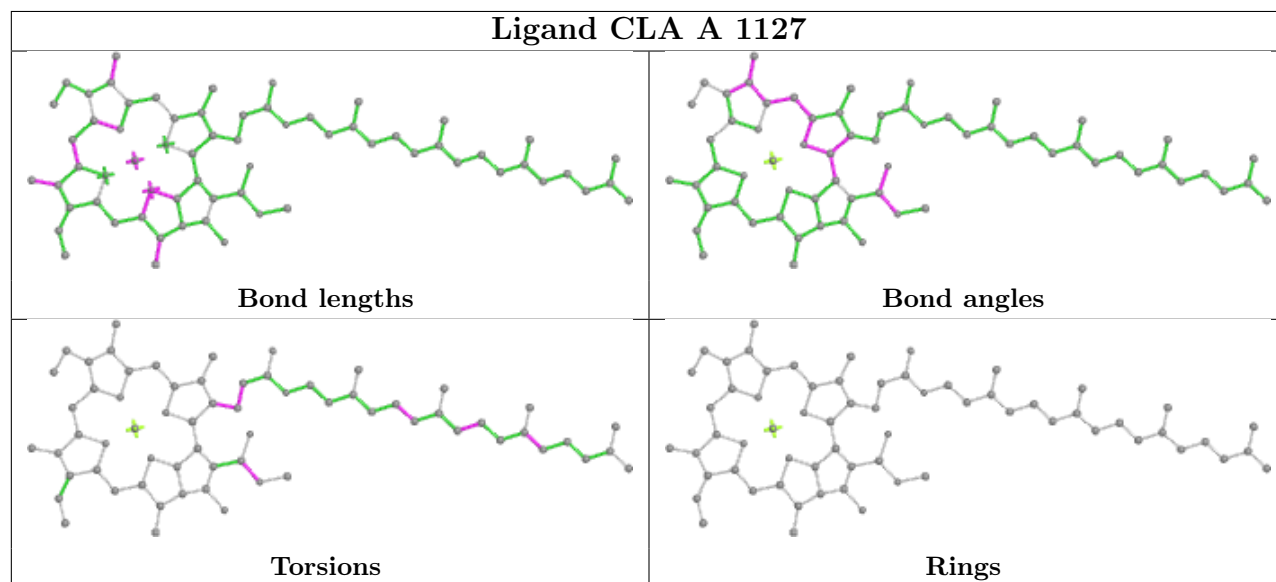
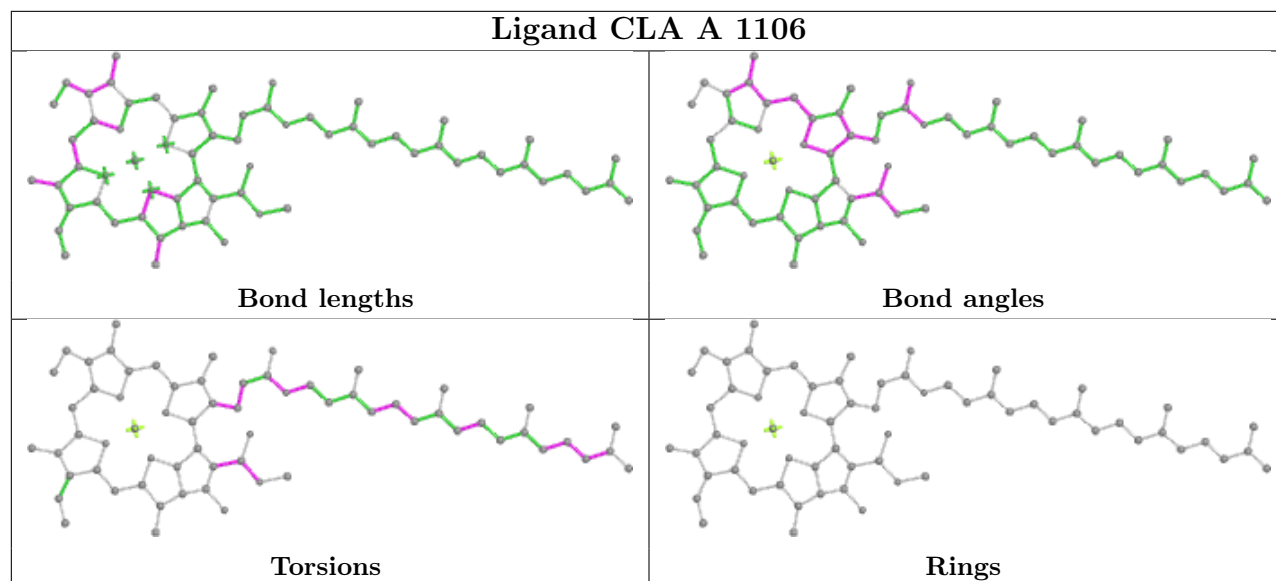
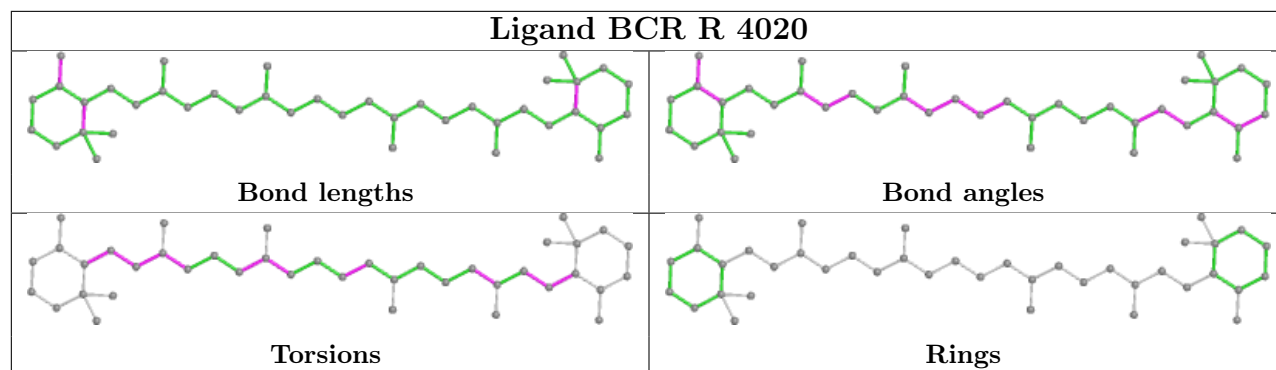


Torsions



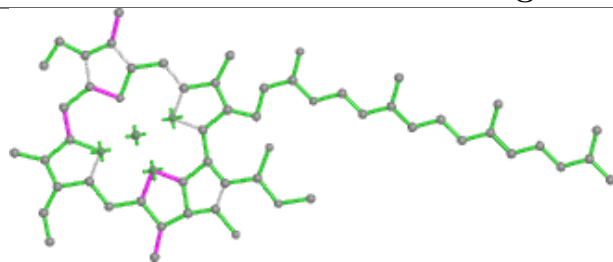
Rings



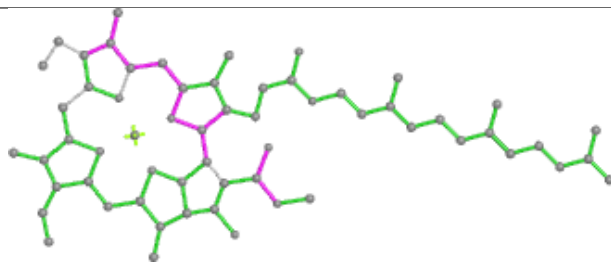




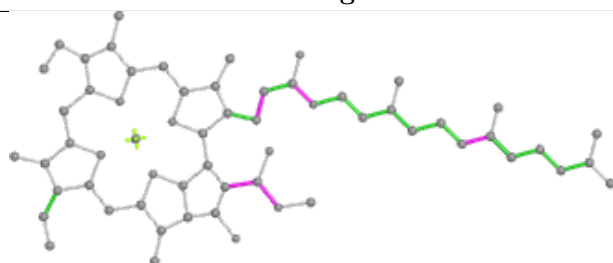
## Ligand CLA Z 510



Bond lengths



Bond angles

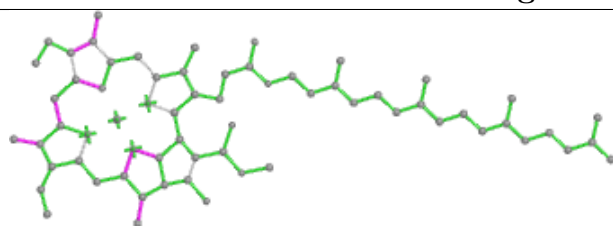


Torsions

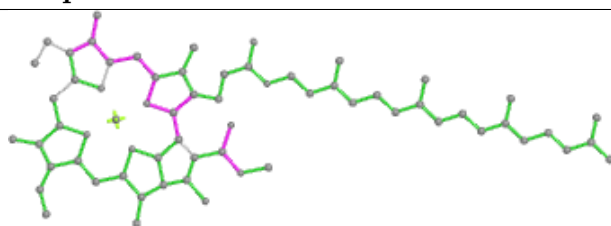


Rings

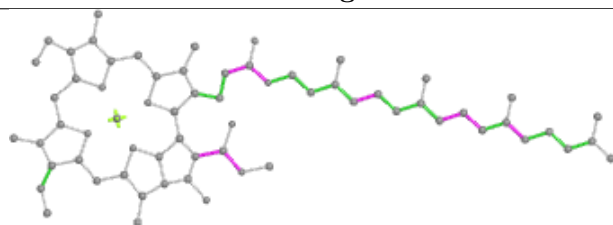
## Ligand CLA q 507



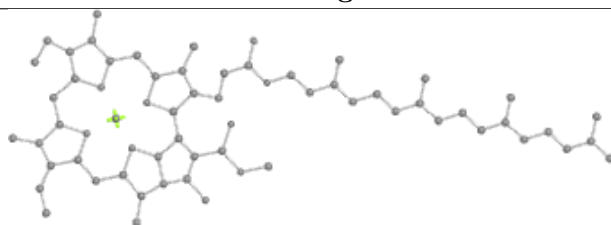
Bond lengths



Bond angles

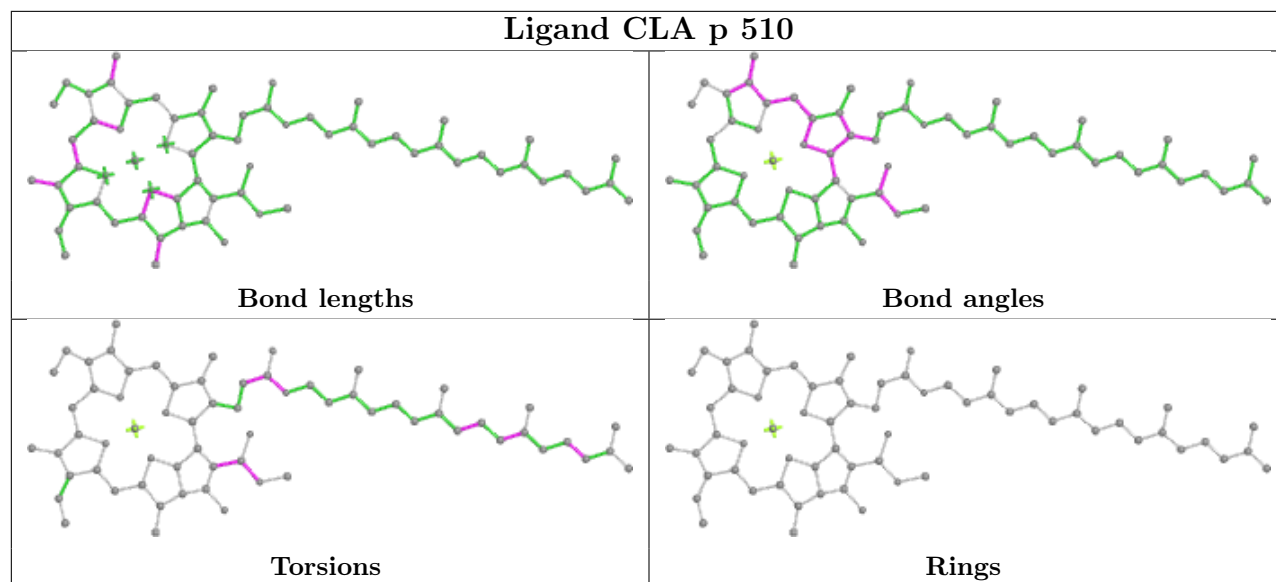


Torsions

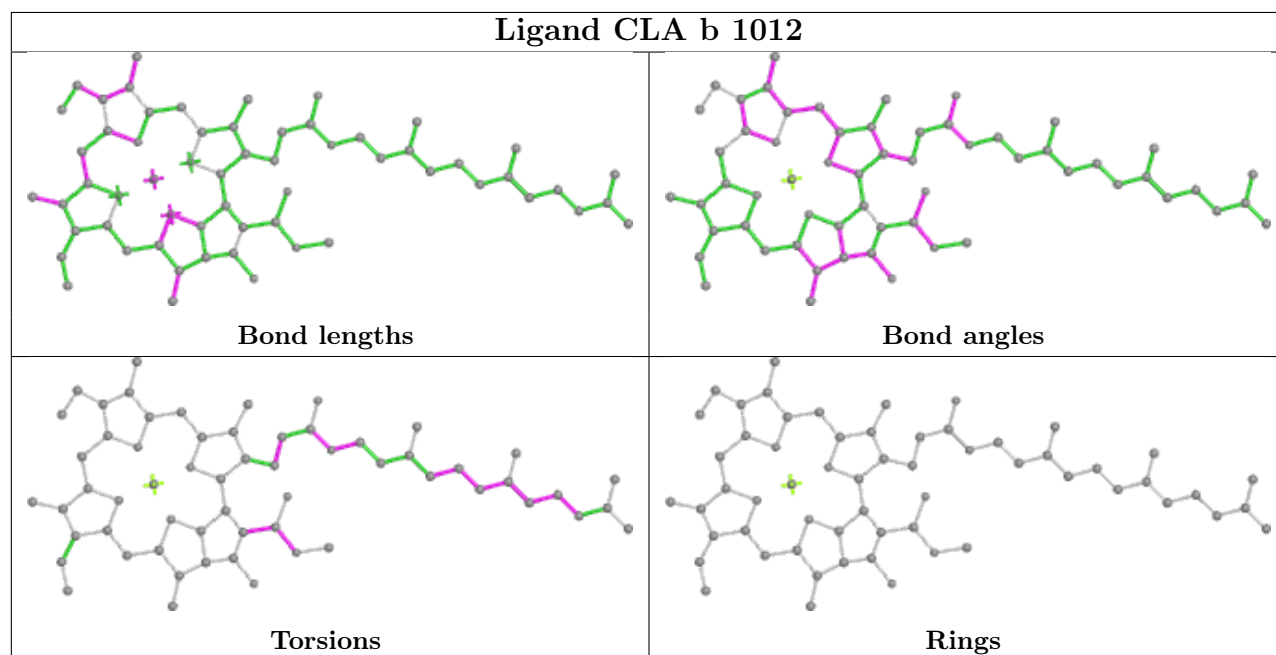


Rings

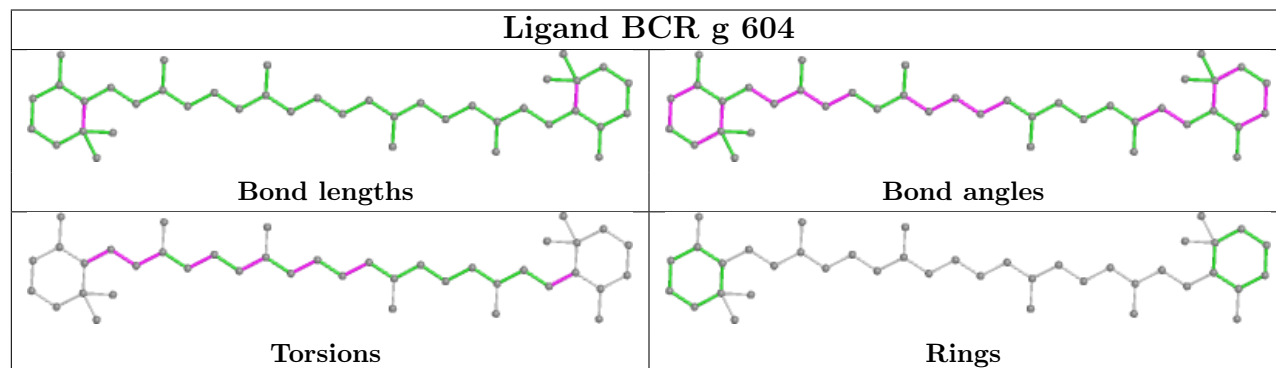
## Ligand CLA p 510

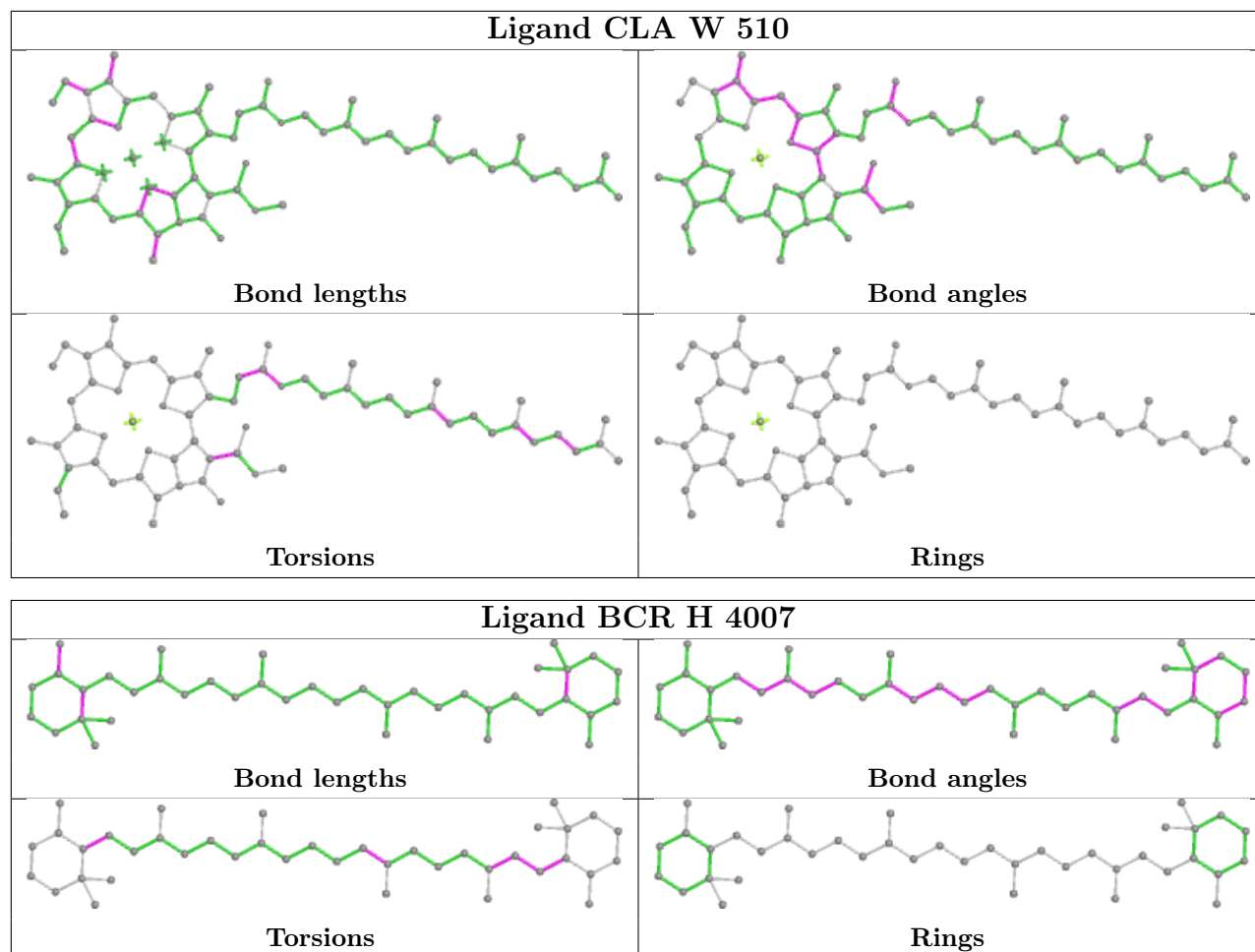


## Ligand CLA b 1012

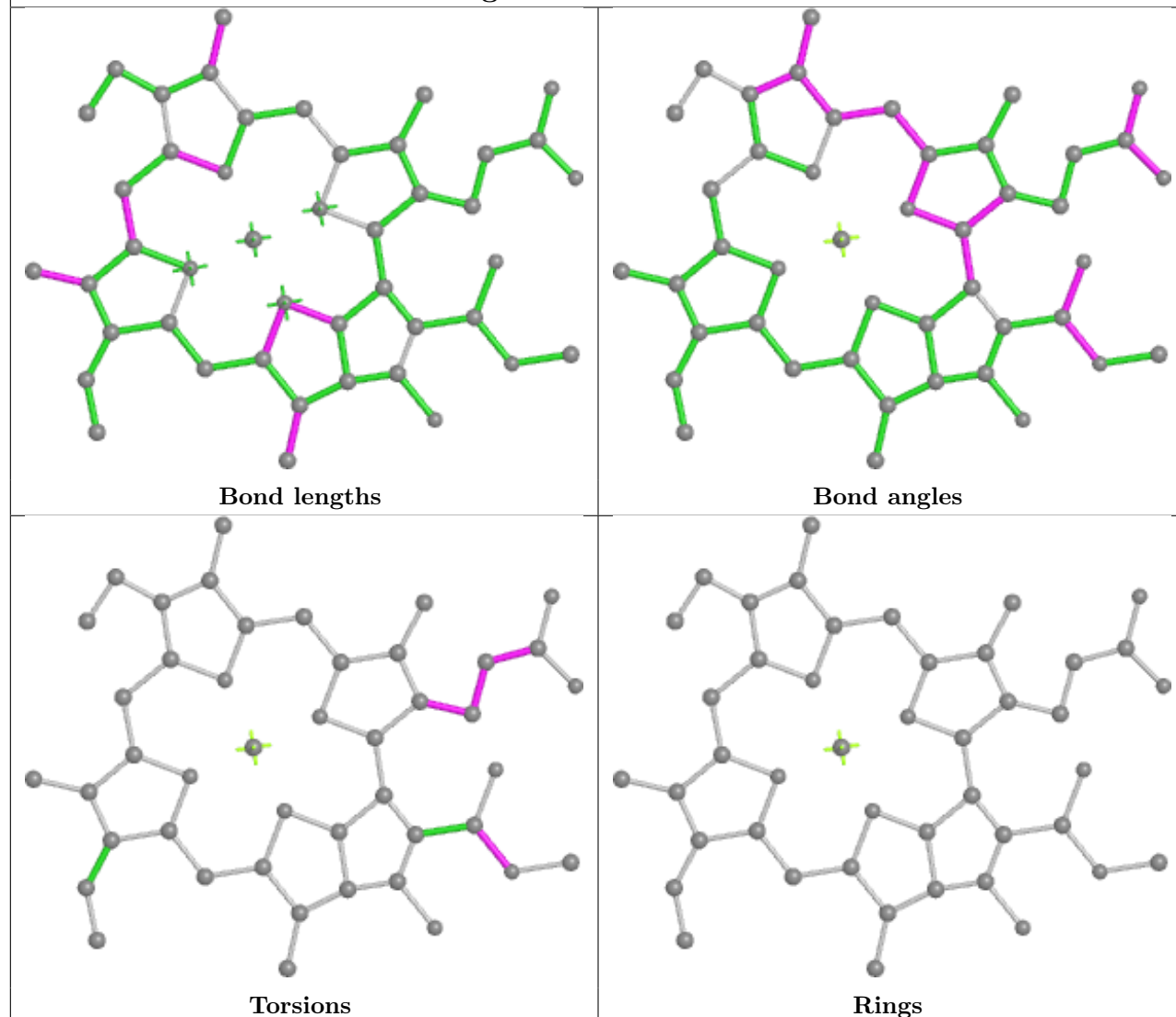


## Ligand BCR g 604

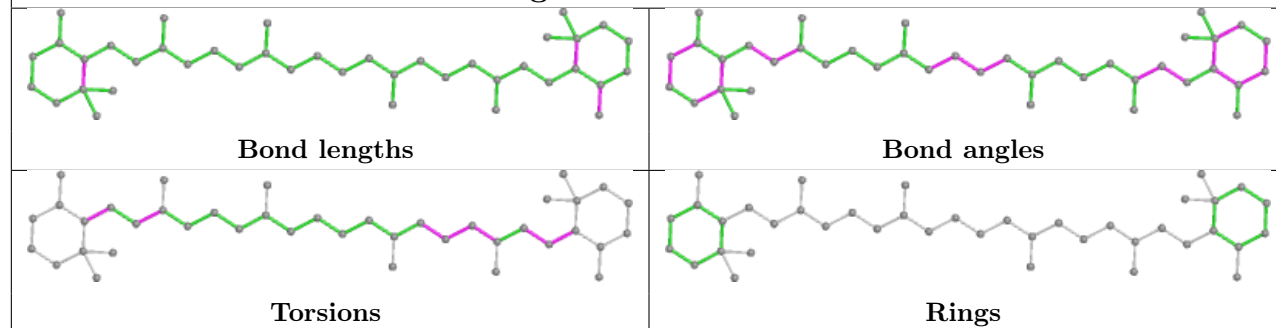


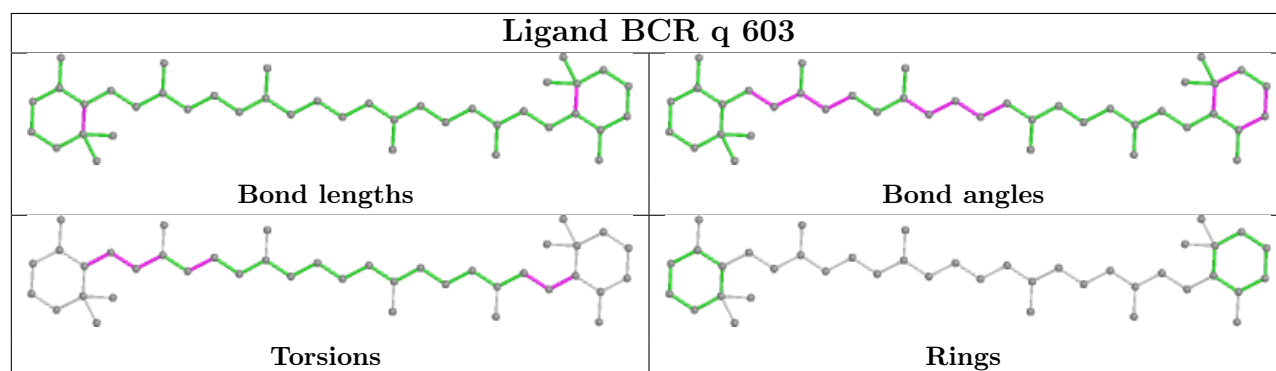
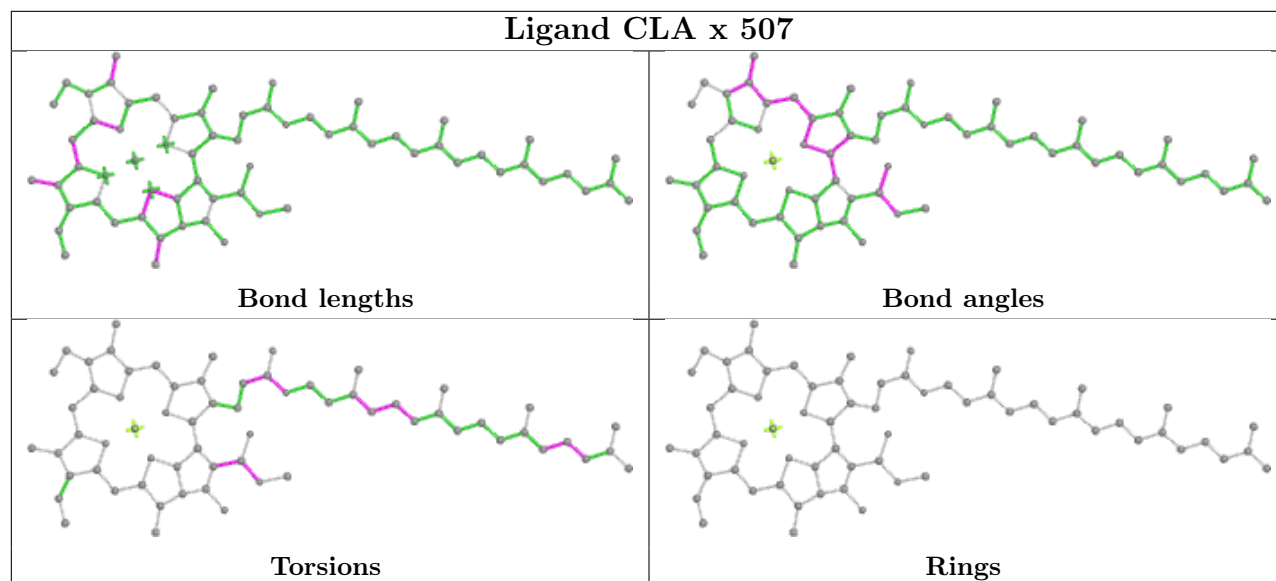
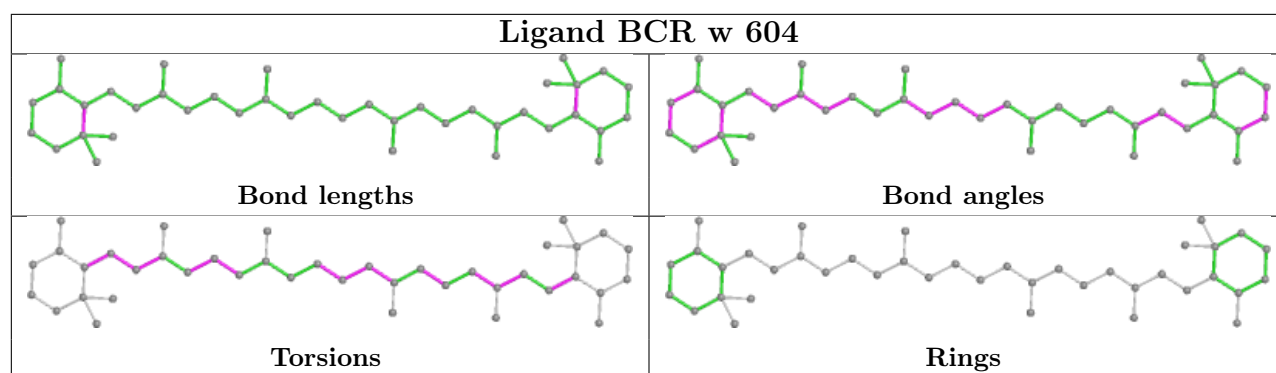


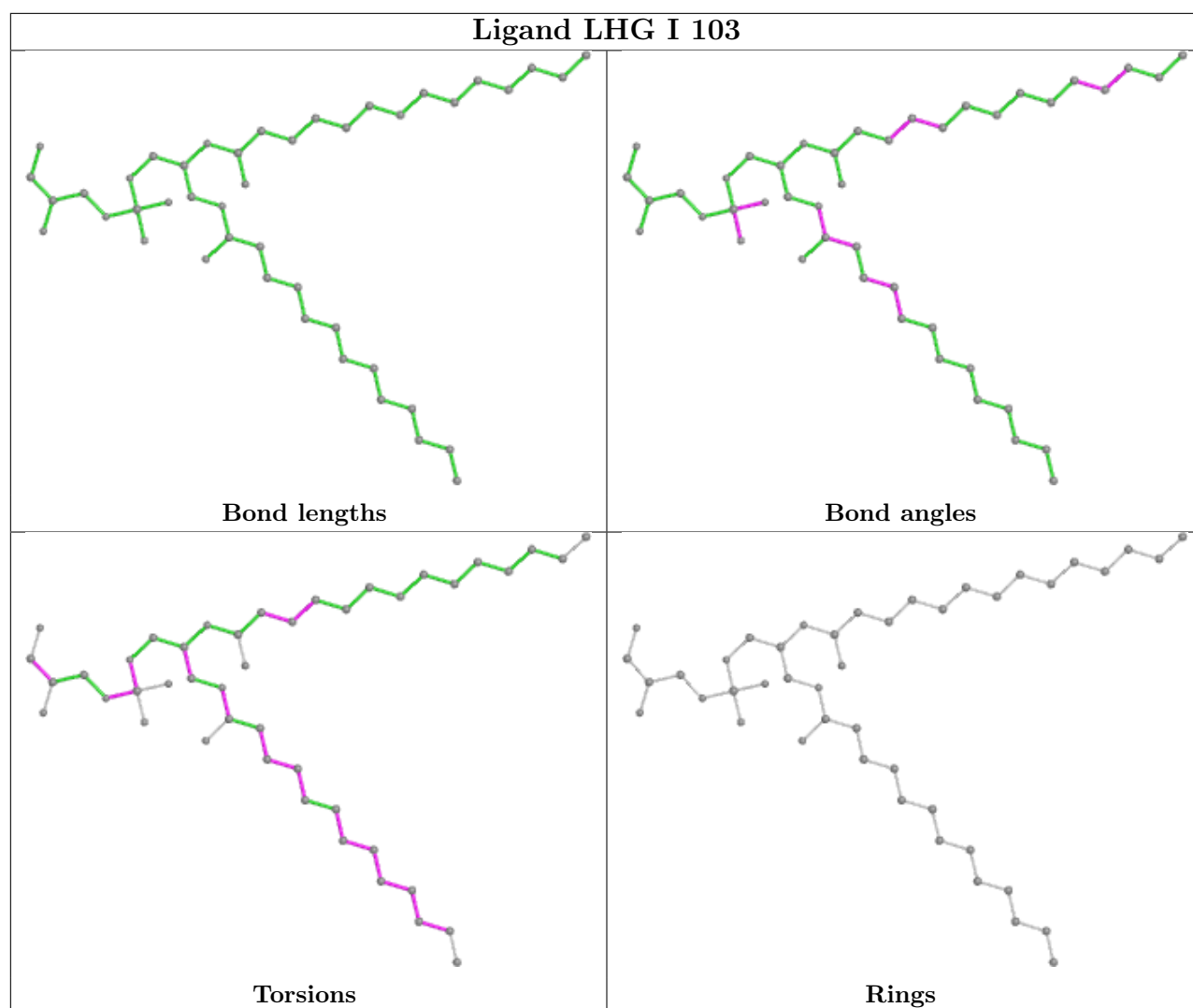
## Ligand CLA A 1108



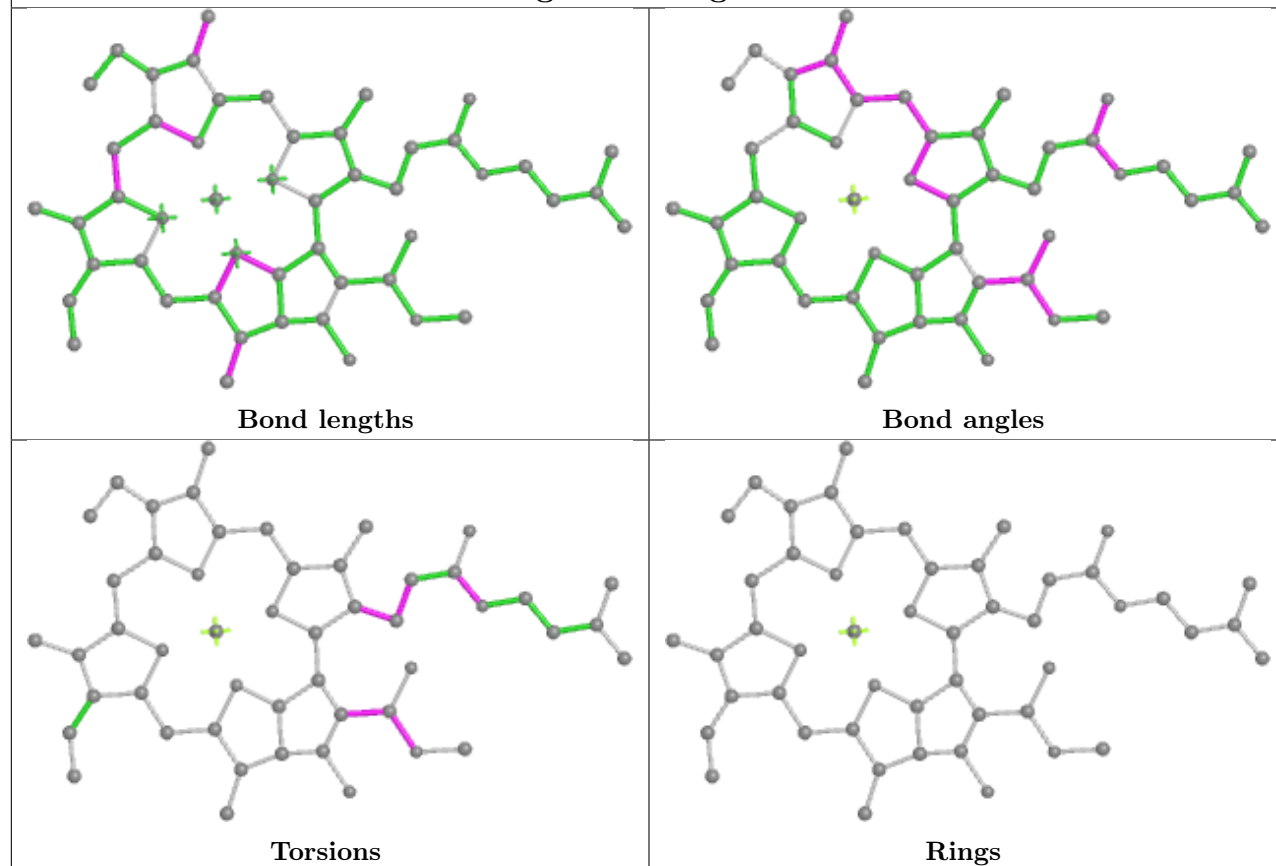
## Ligand BCR X 601



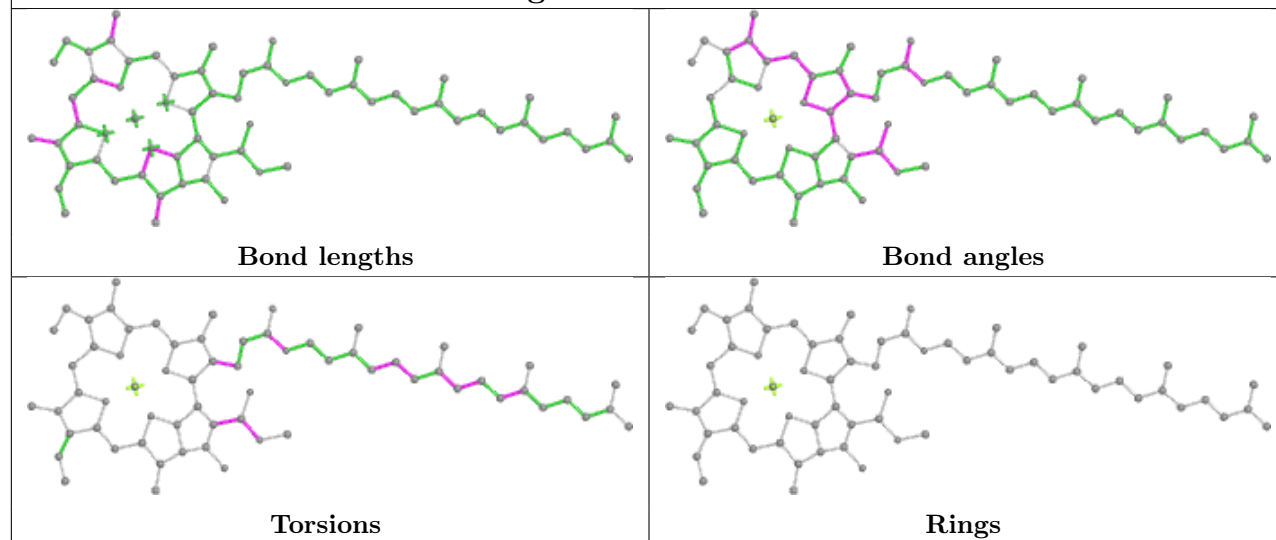


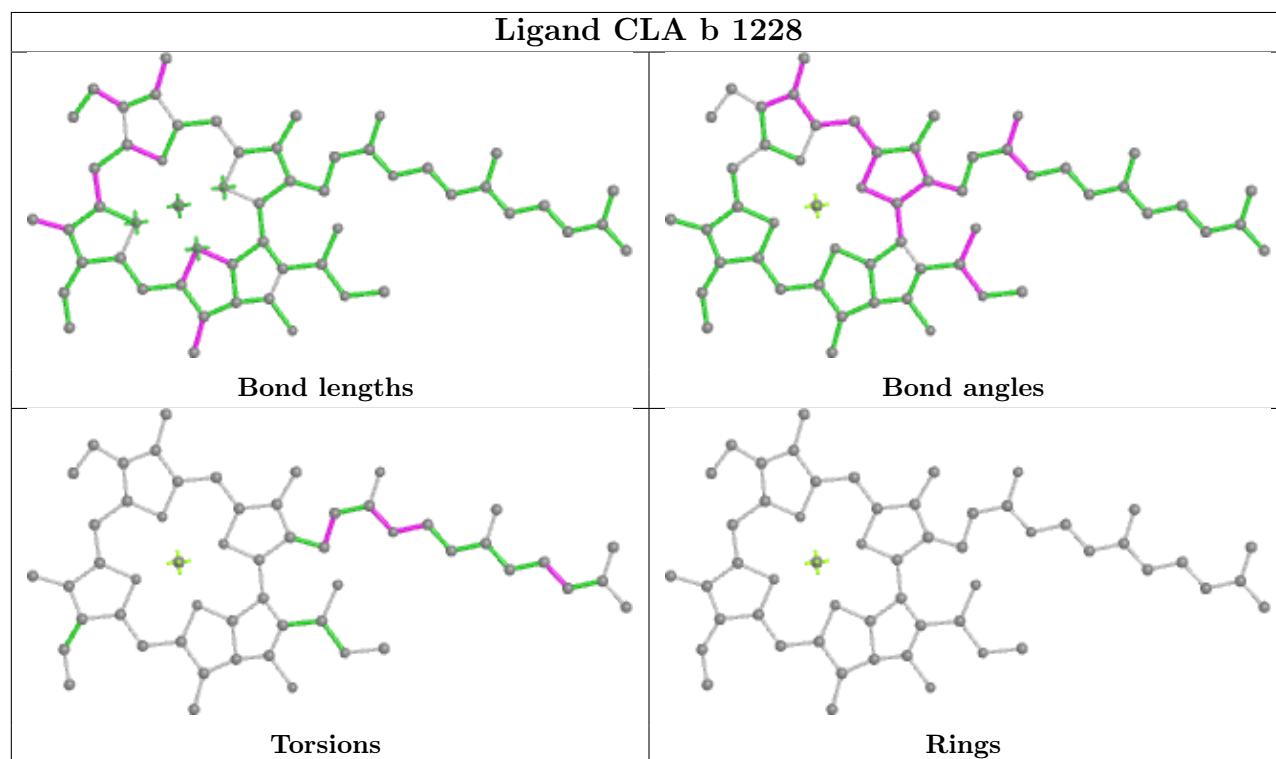
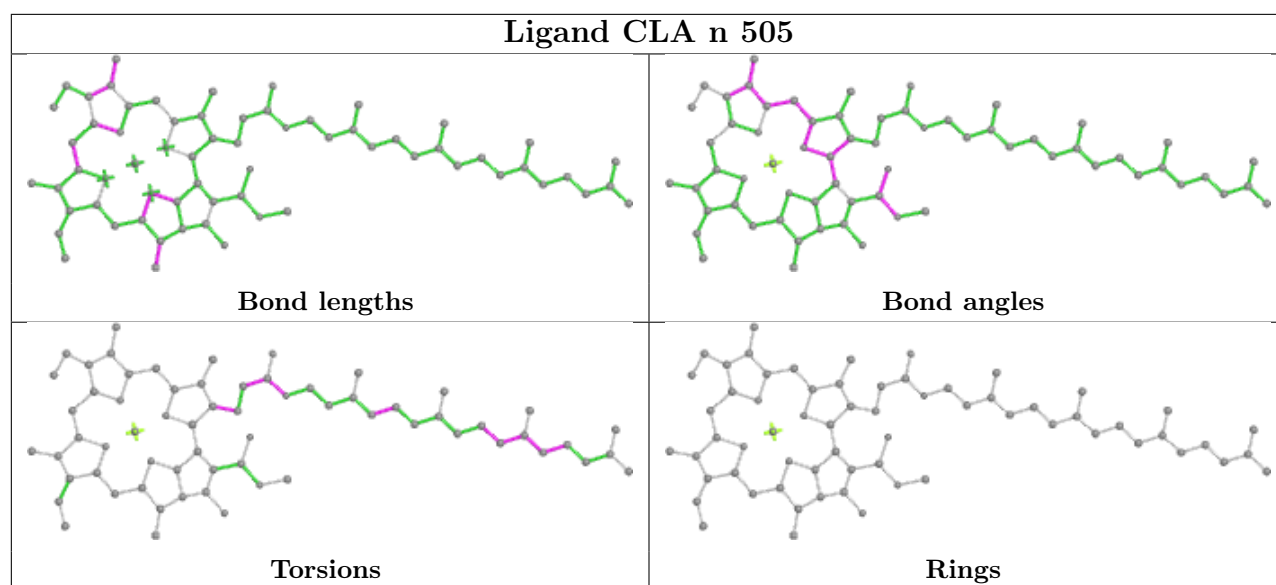


## Ligand CLA g 514



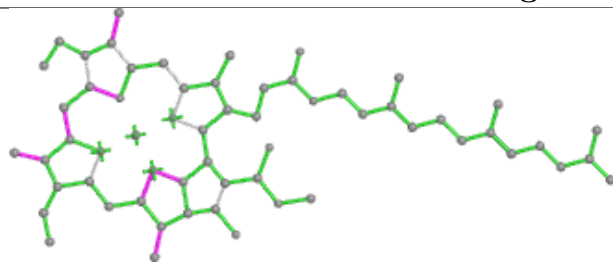
## Ligand CLA a 1101



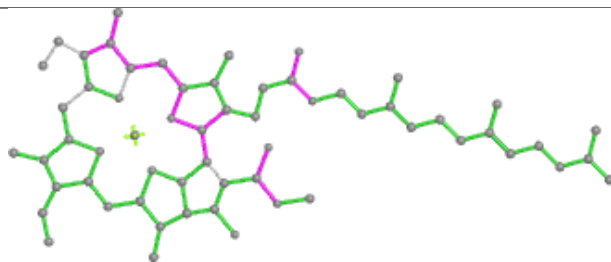




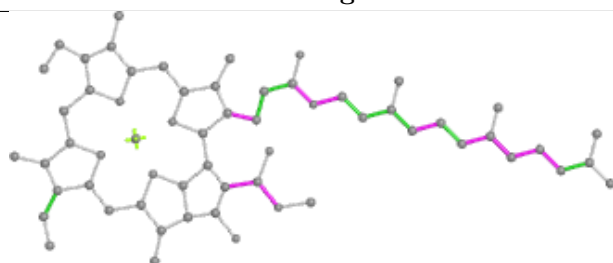
## Ligand CLA s 504



Bond lengths



Bond angles

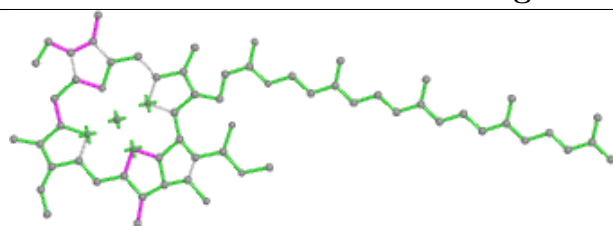


Torsions

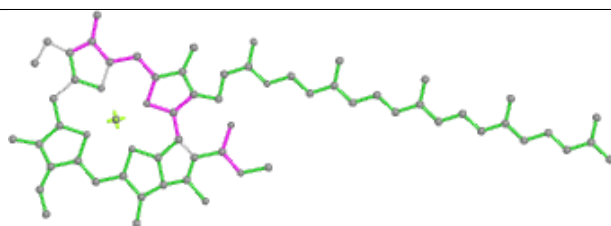


Rings

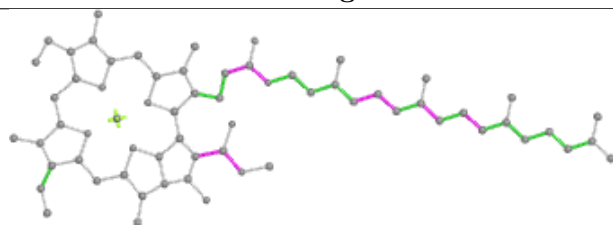
## Ligand CLA X 507



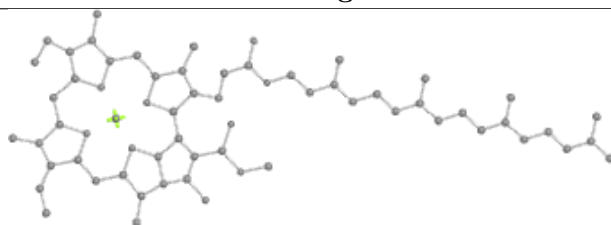
Bond lengths



Bond angles

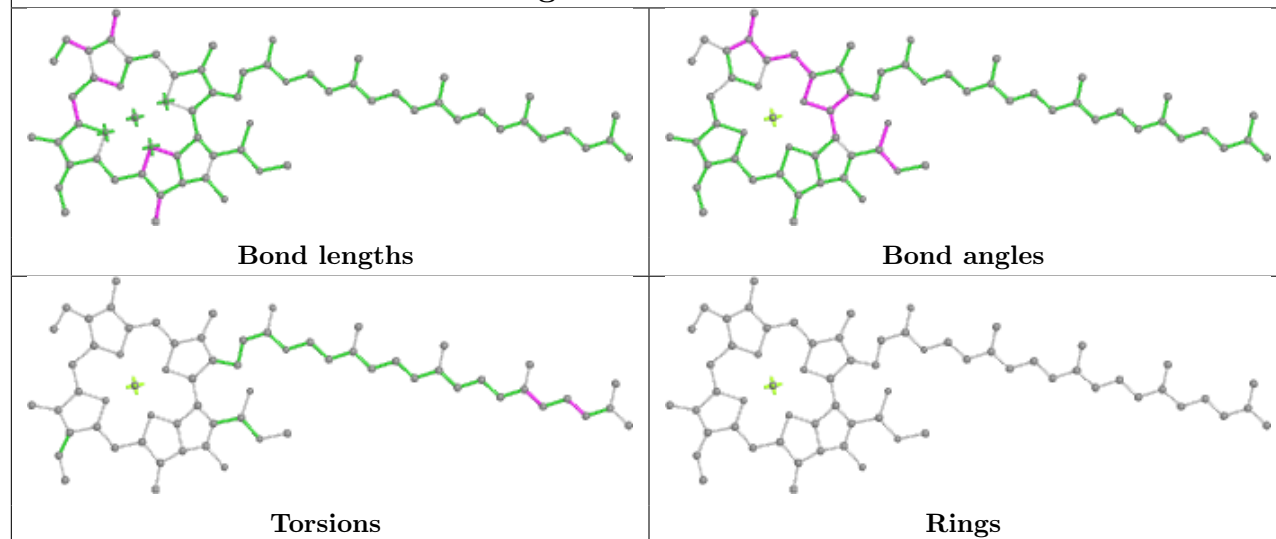


Torsions

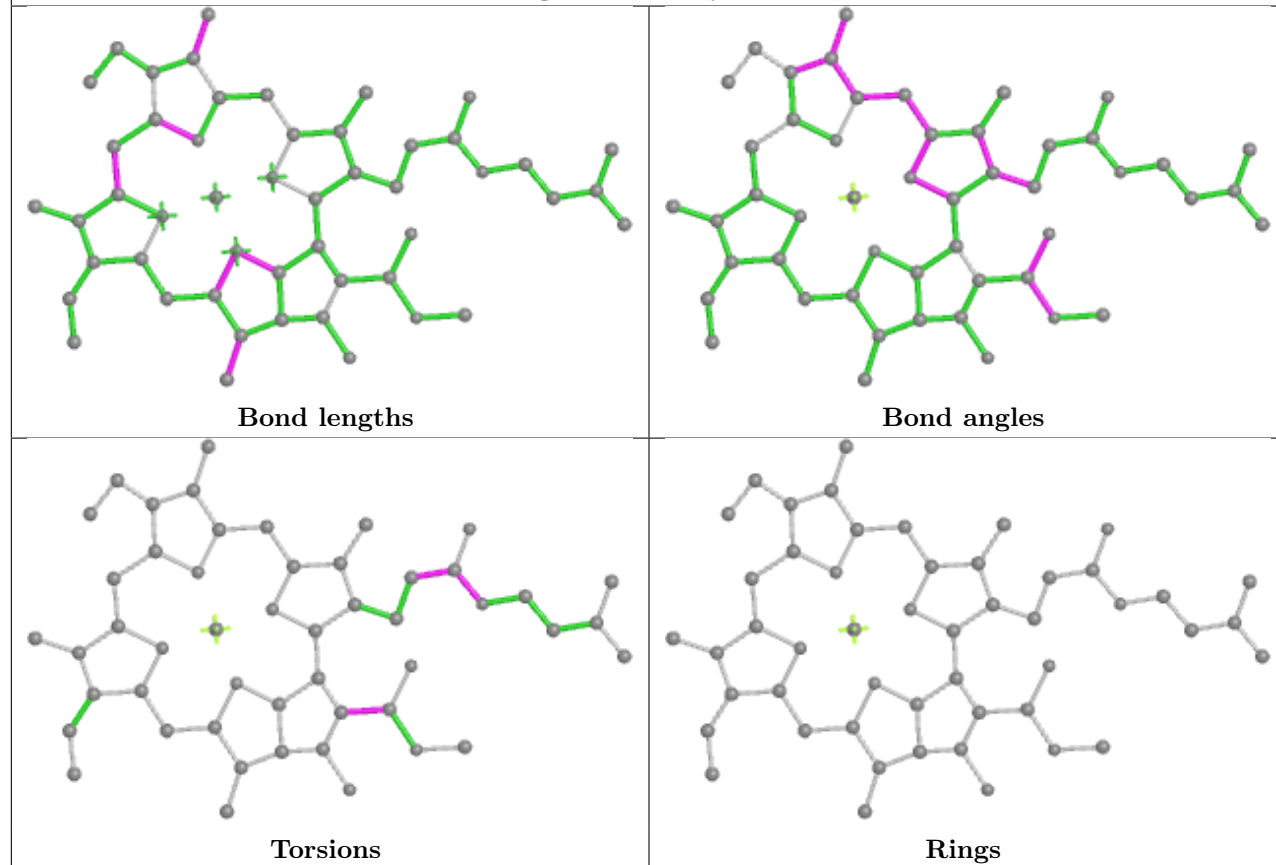


Rings

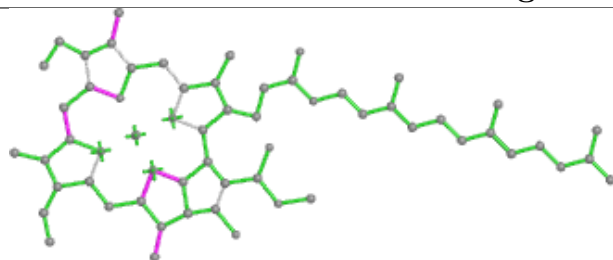
## Ligand CLA t 510



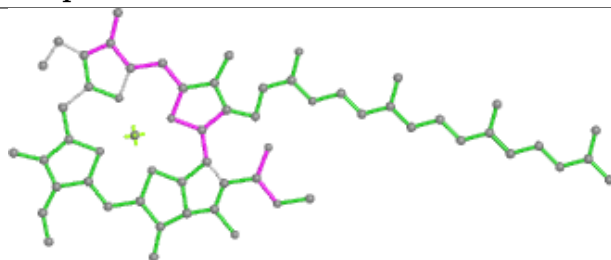
## Ligand CLA y 502



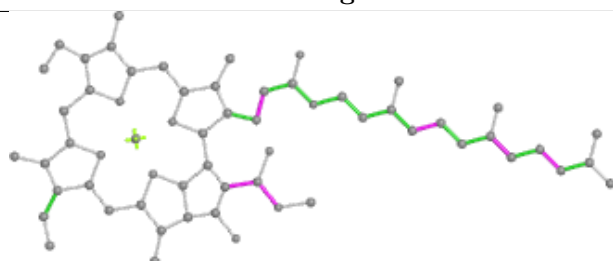
## Ligand CLA q 504



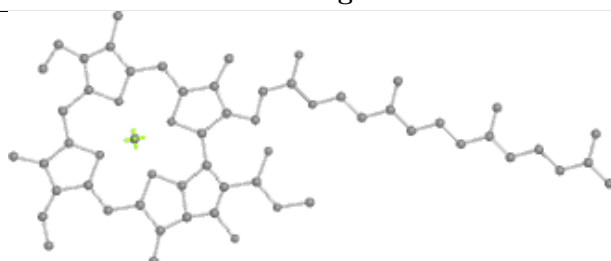
Bond lengths



Bond angles

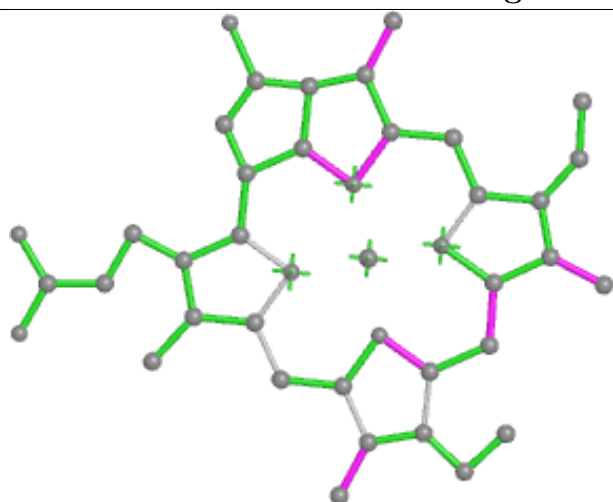


Torsions

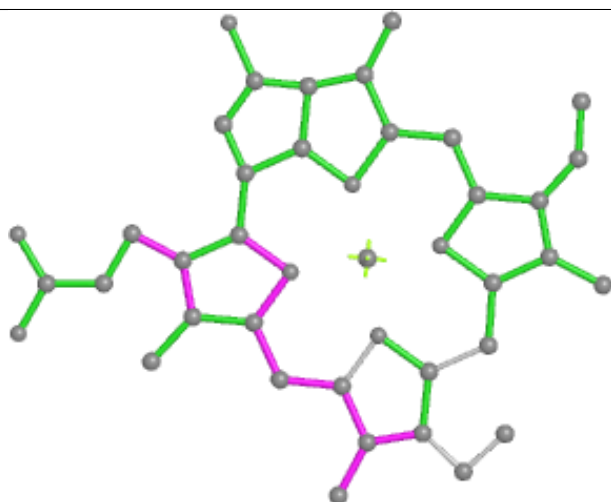


Rings

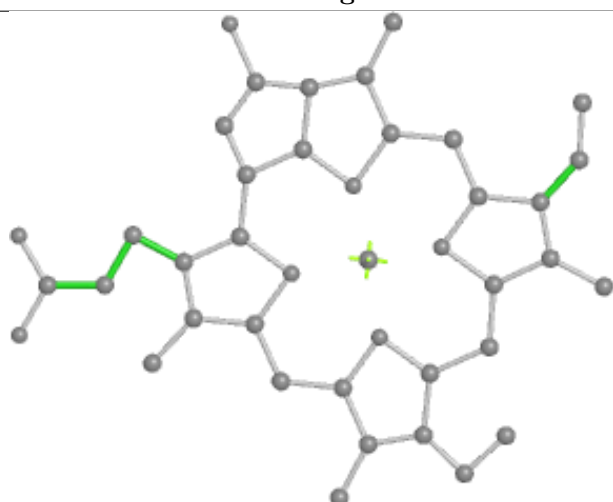
## Ligand CLA H 1402



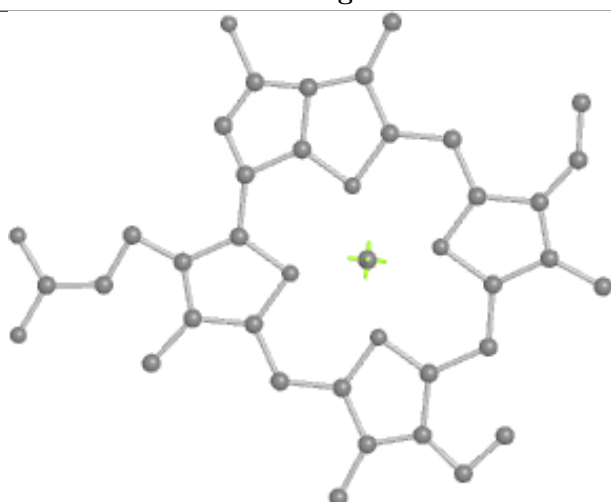
Bond lengths



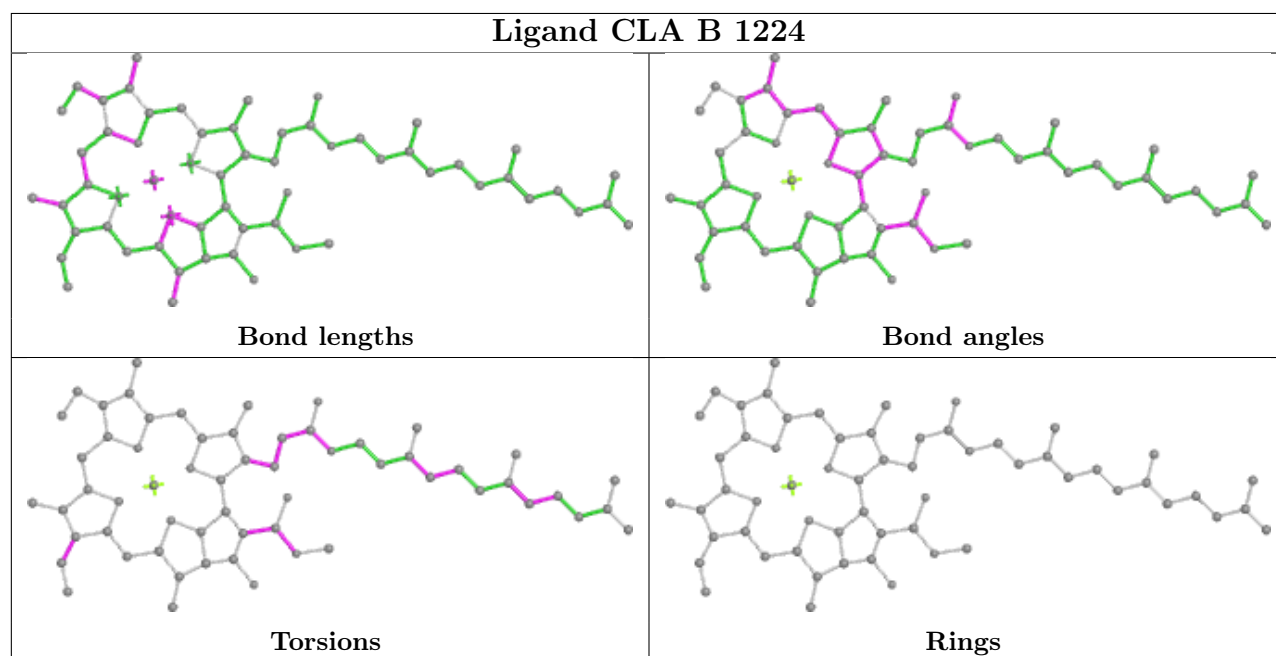
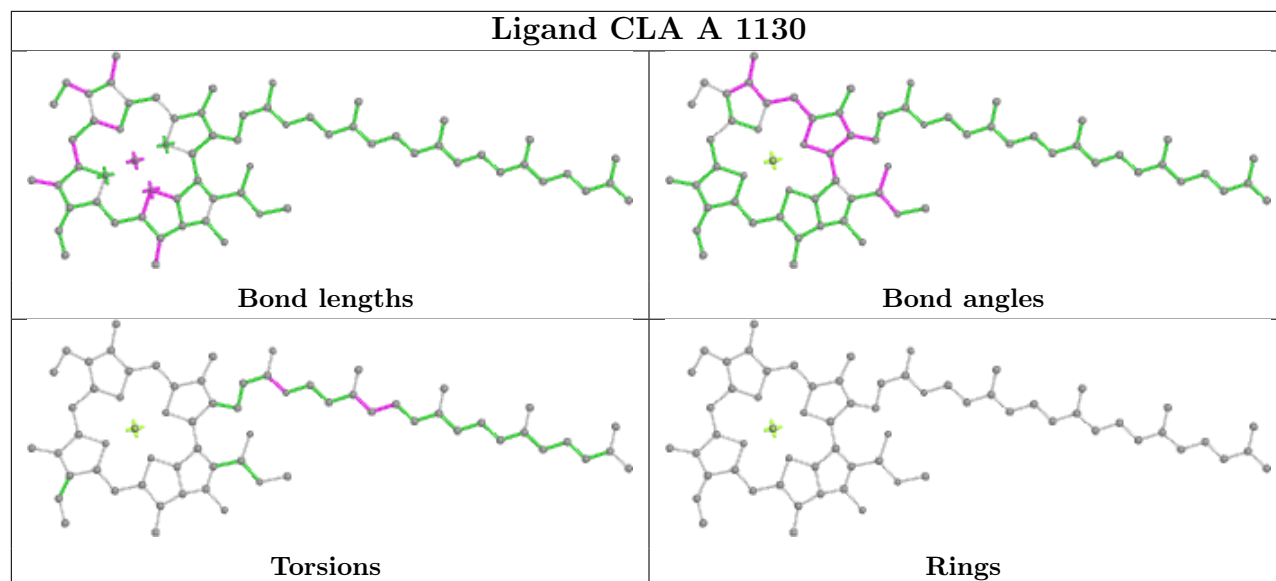
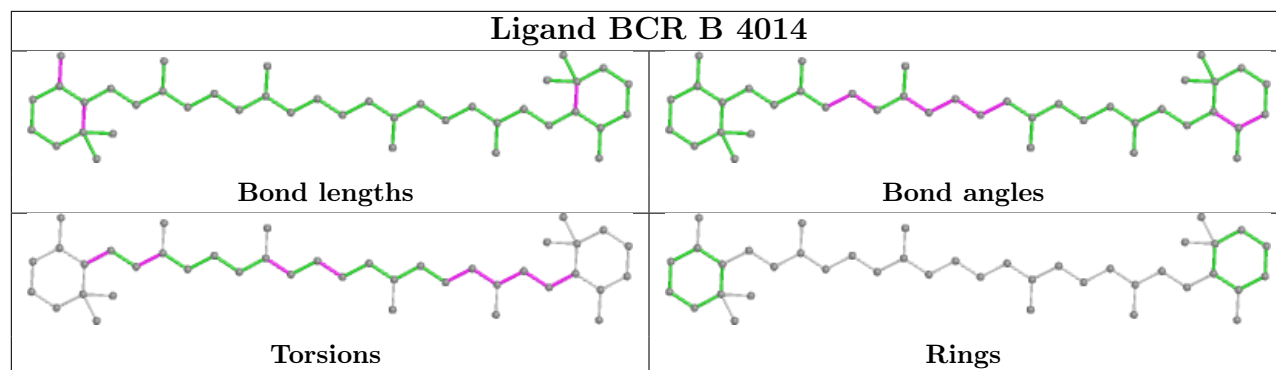
Bond angles

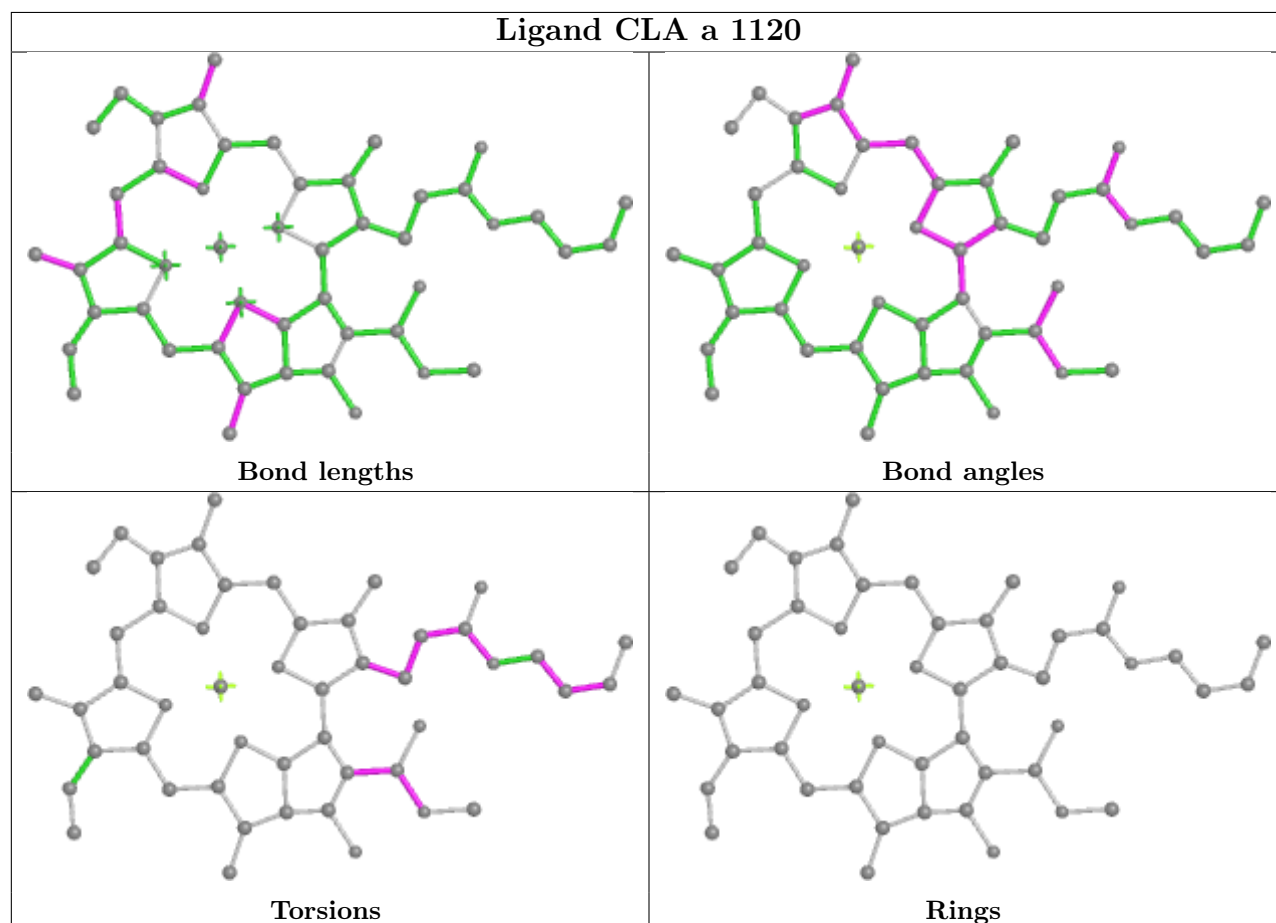
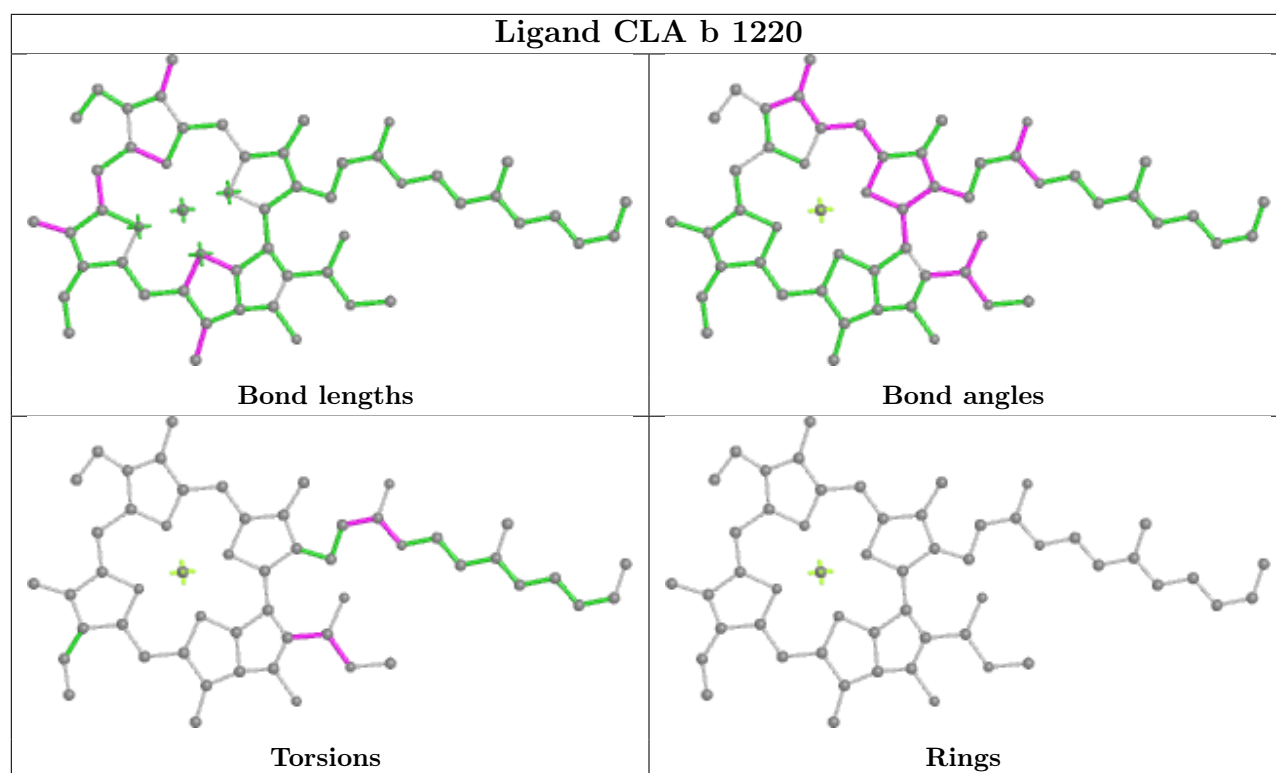


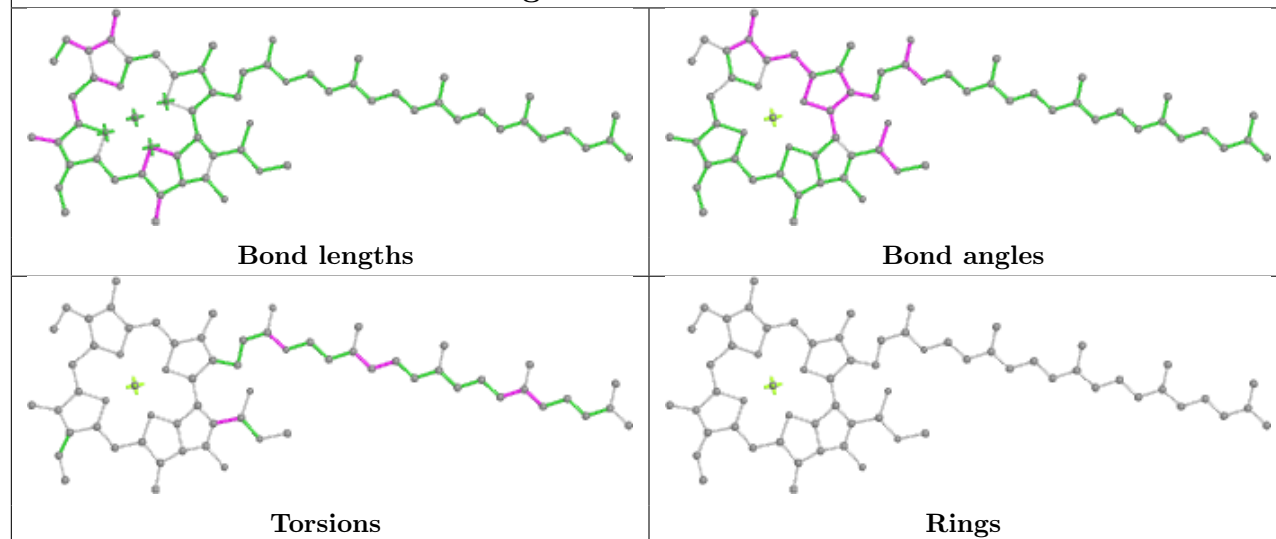
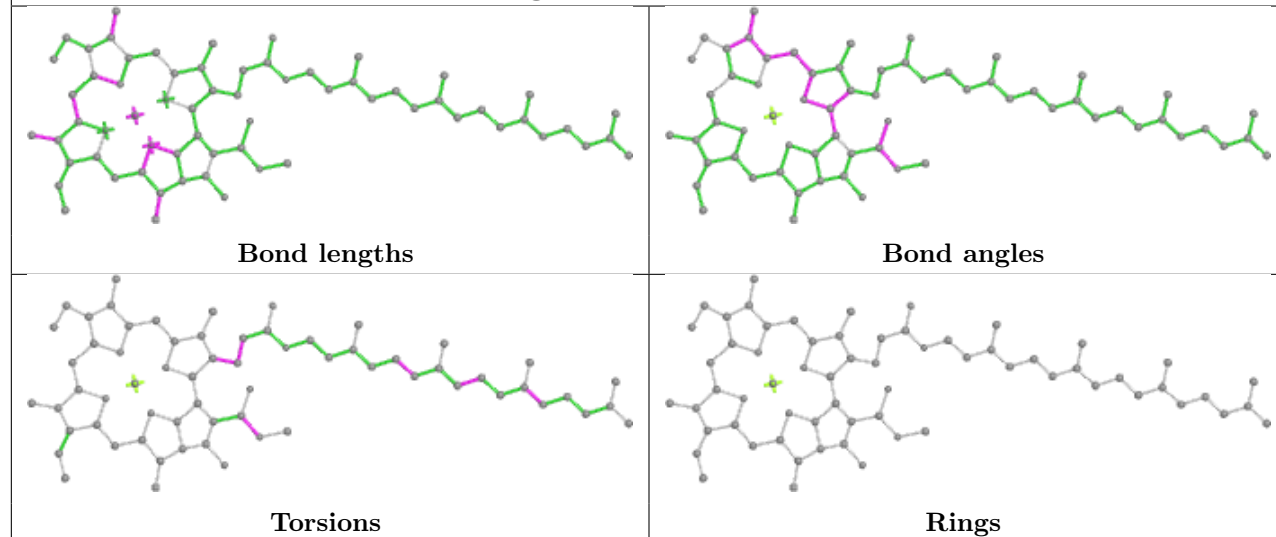
Torsions



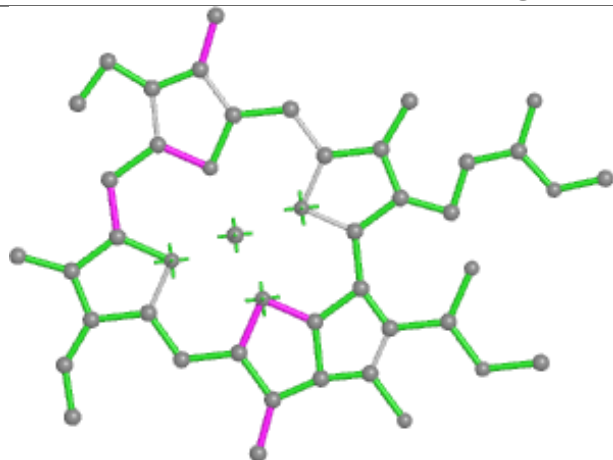
Rings



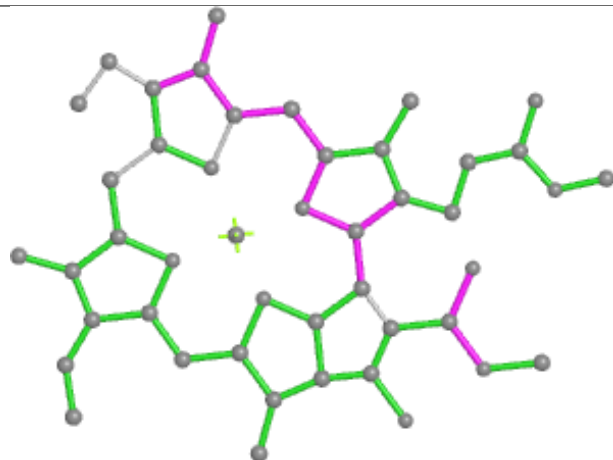


**Ligand CLA A 1138****Ligand CLA a 1127**

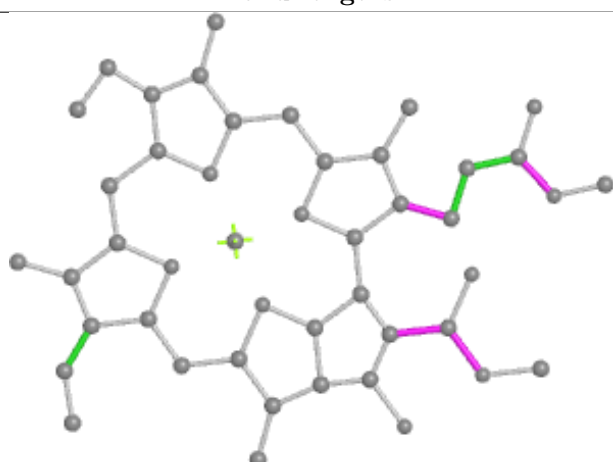
## Ligand CLA w 516



Bond lengths



Bond angles

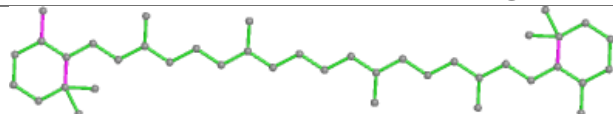


Torsions

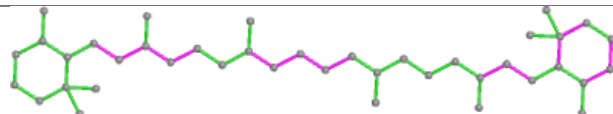


Rings

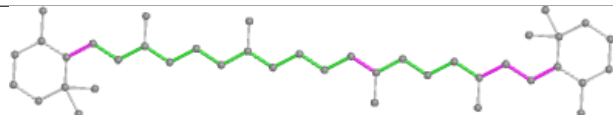
## Ligand BCR A 4007



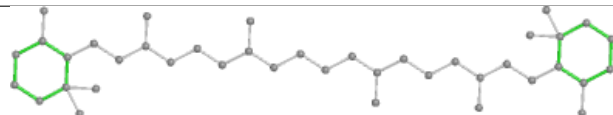
Bond lengths



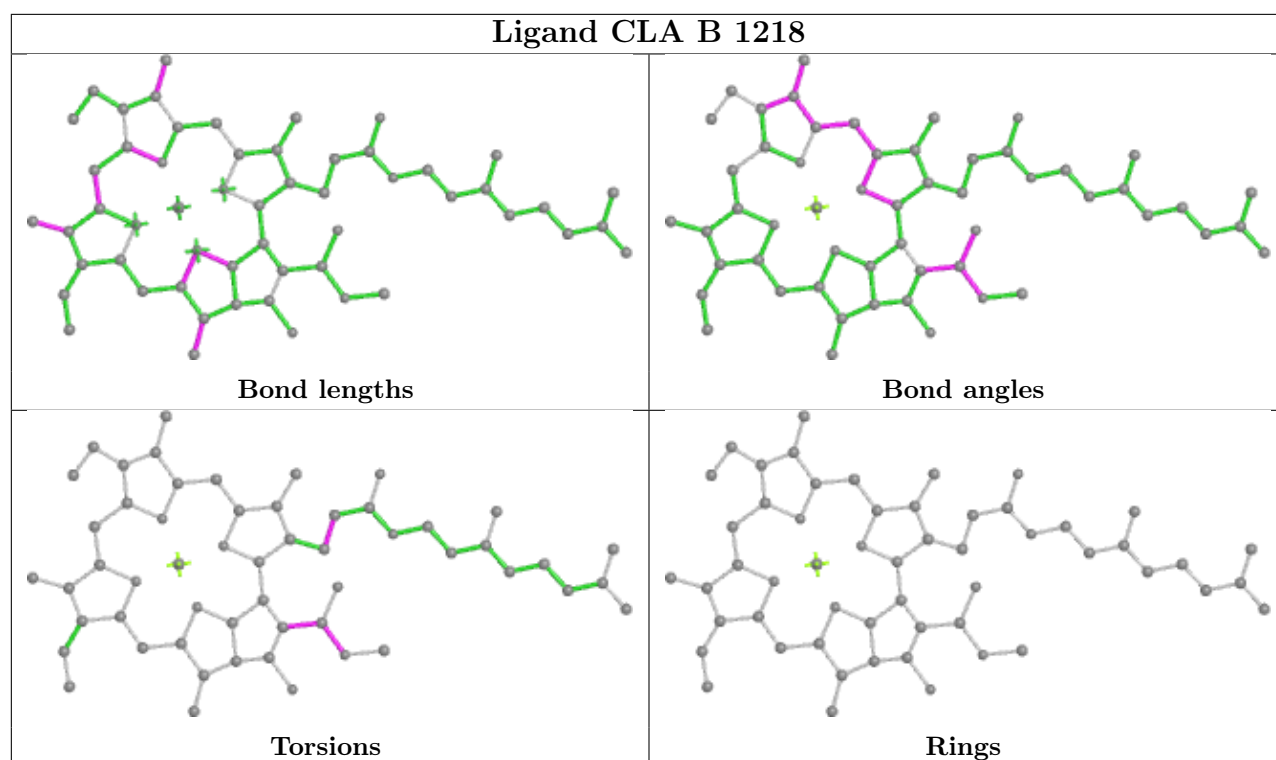
Bond angles



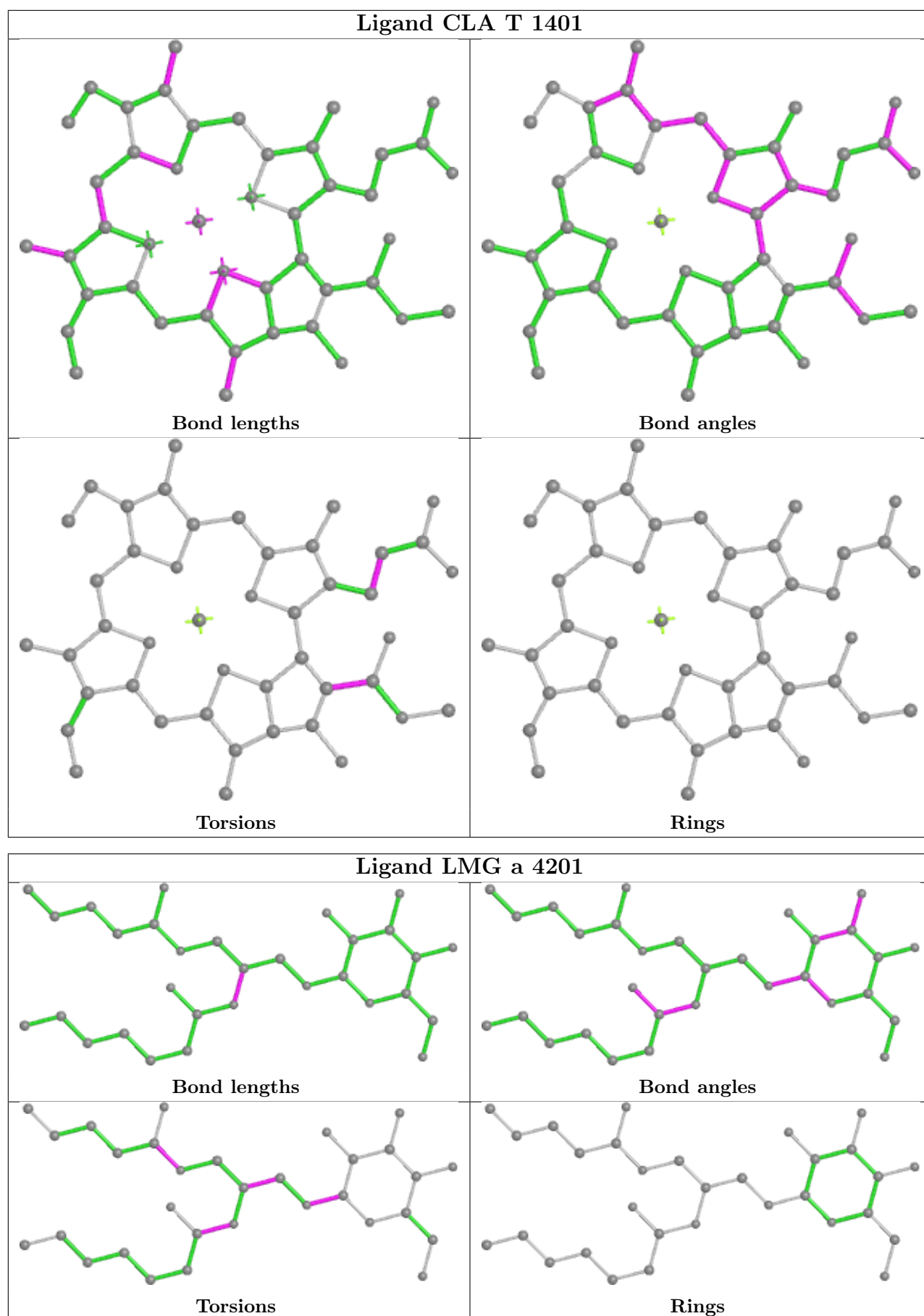
Torsions

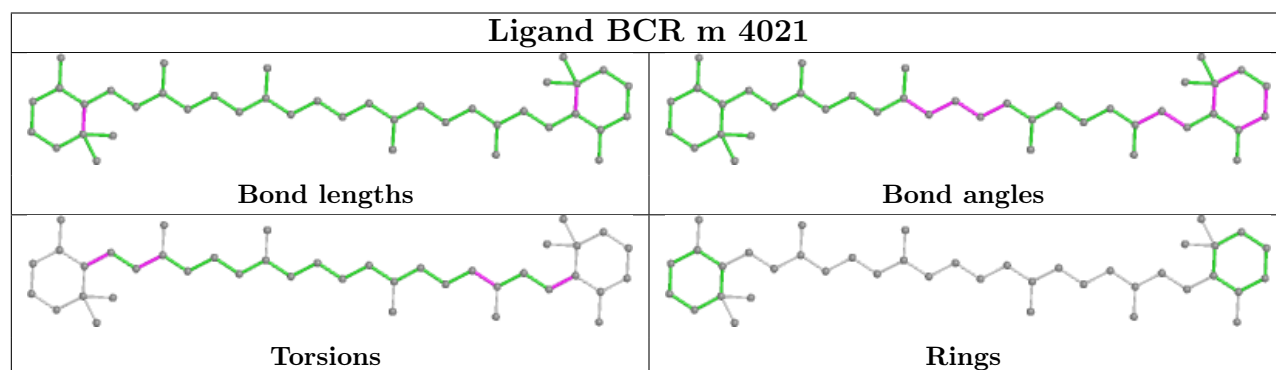
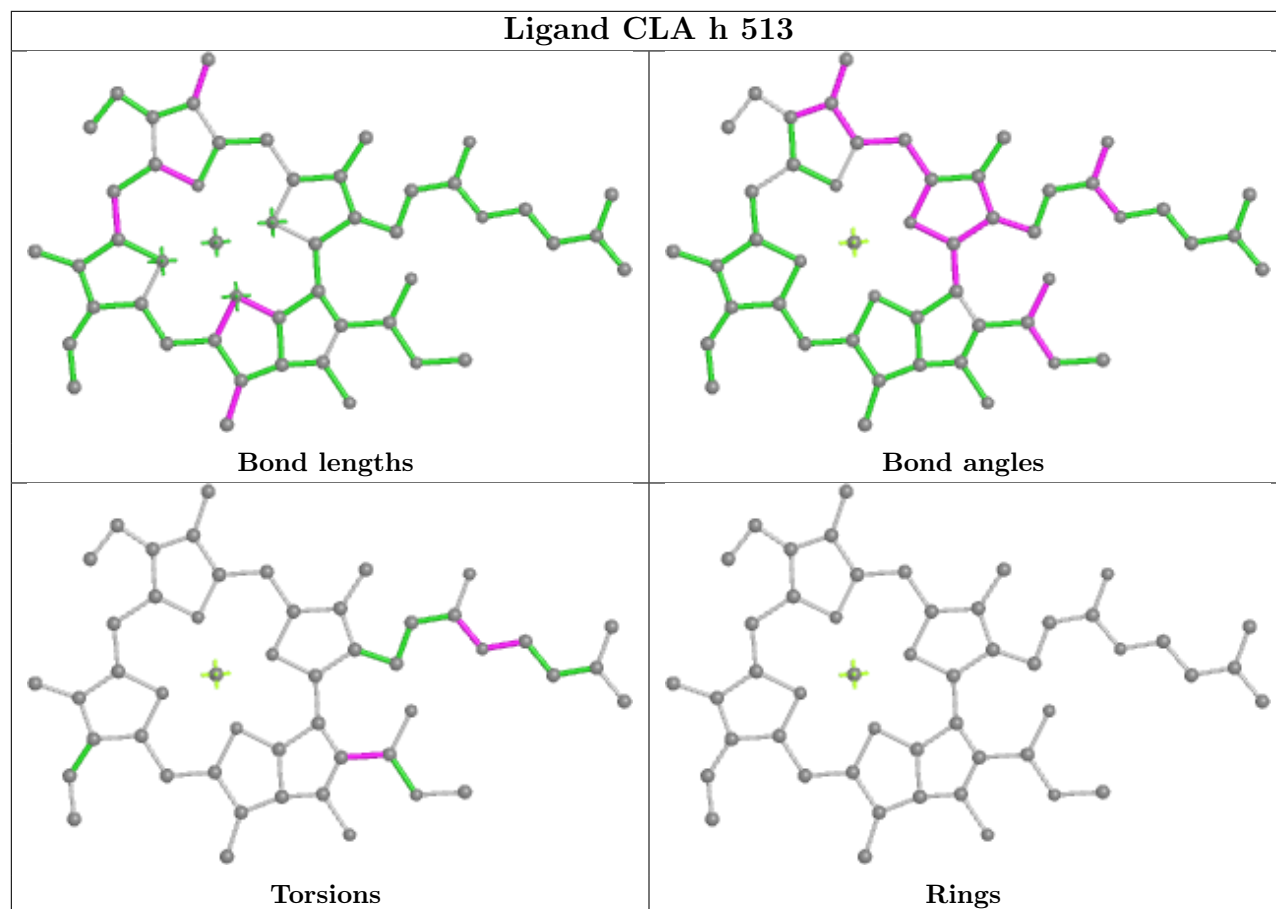
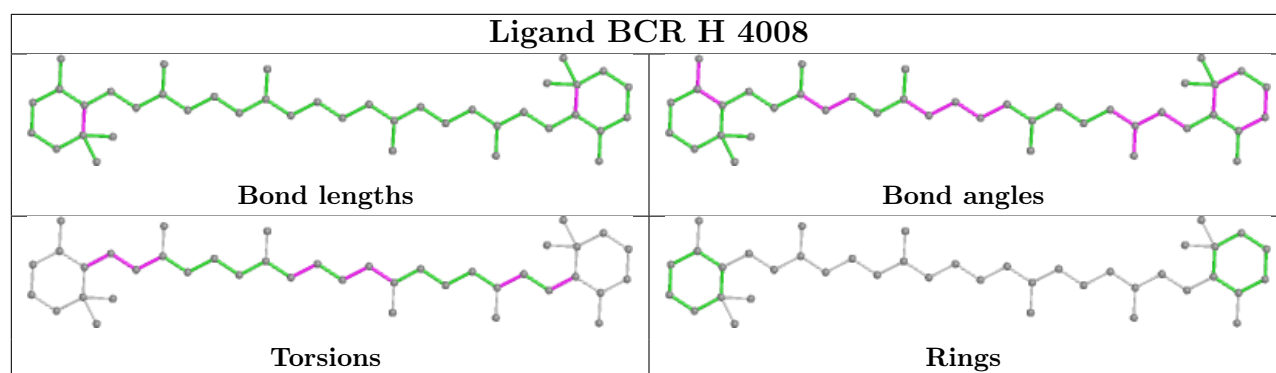


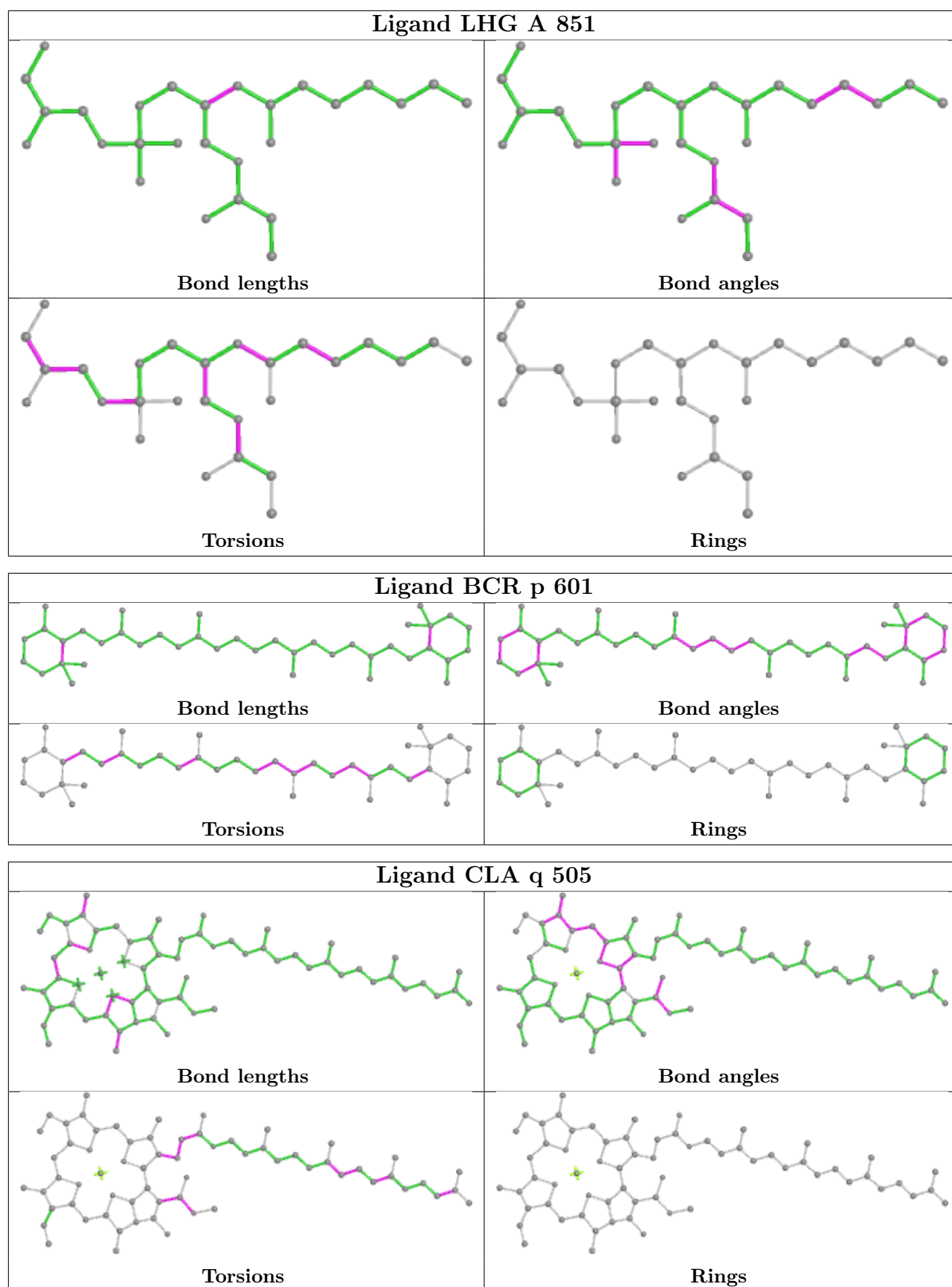
Rings

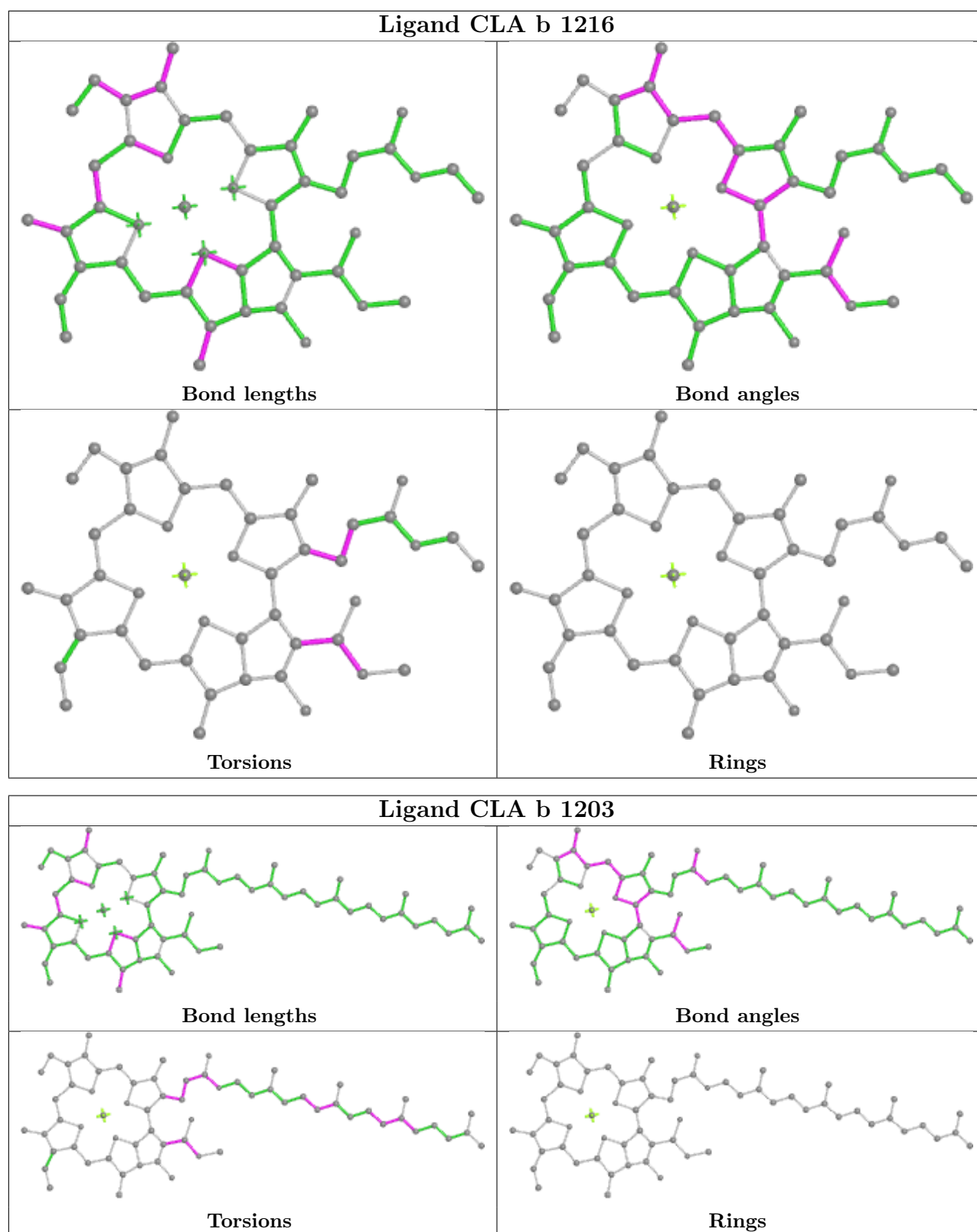


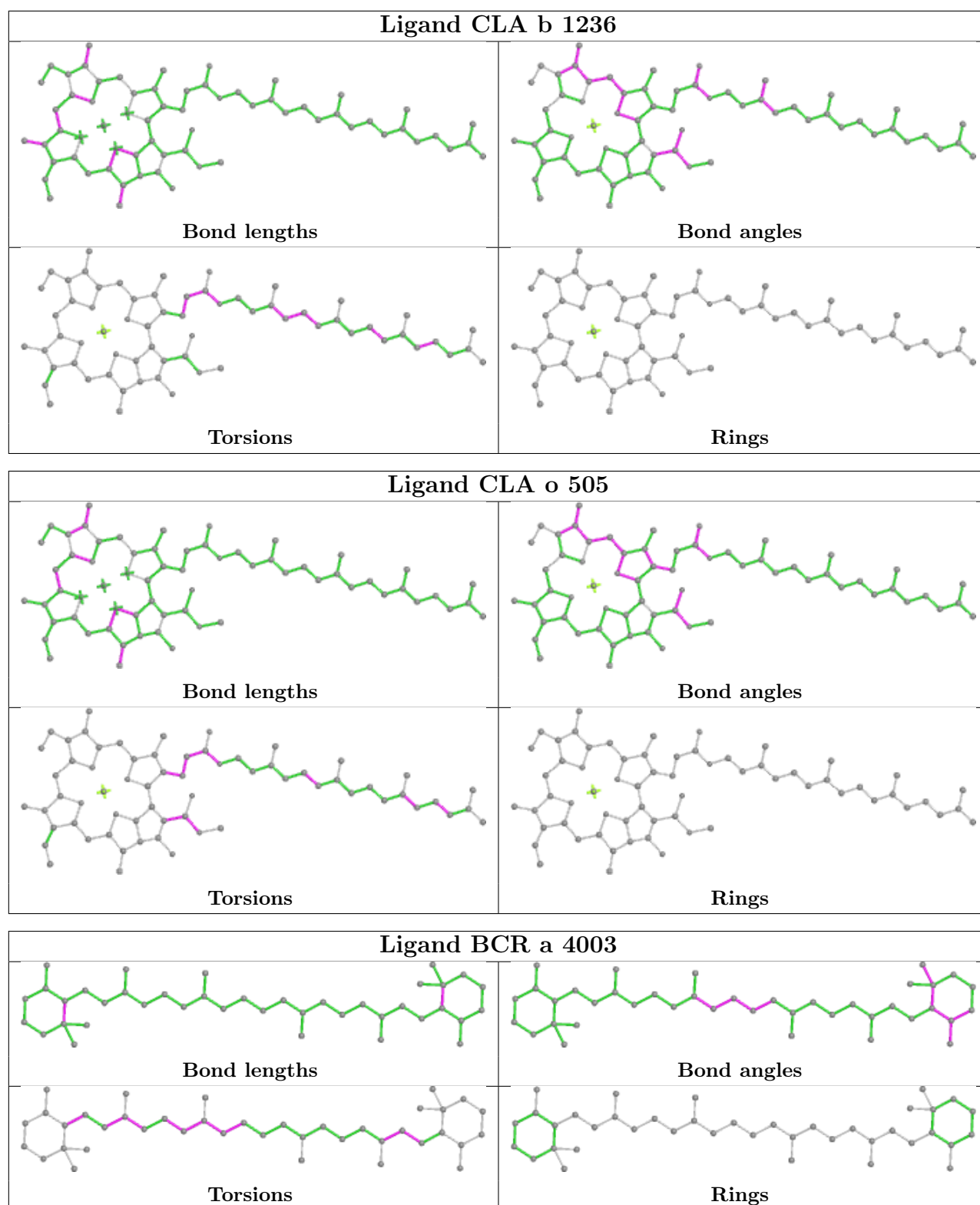




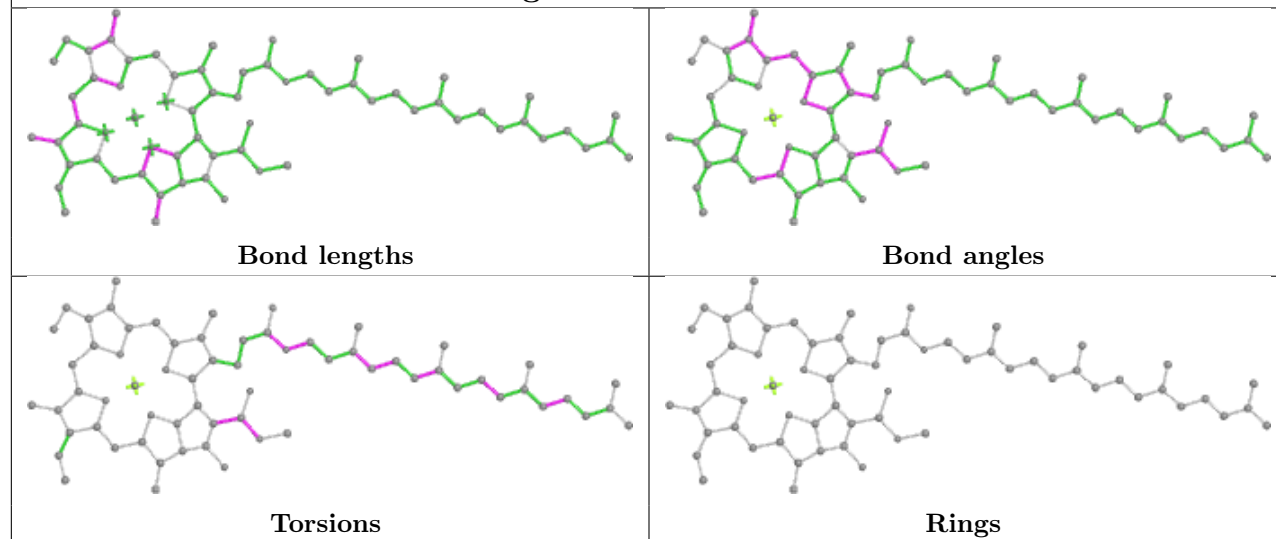




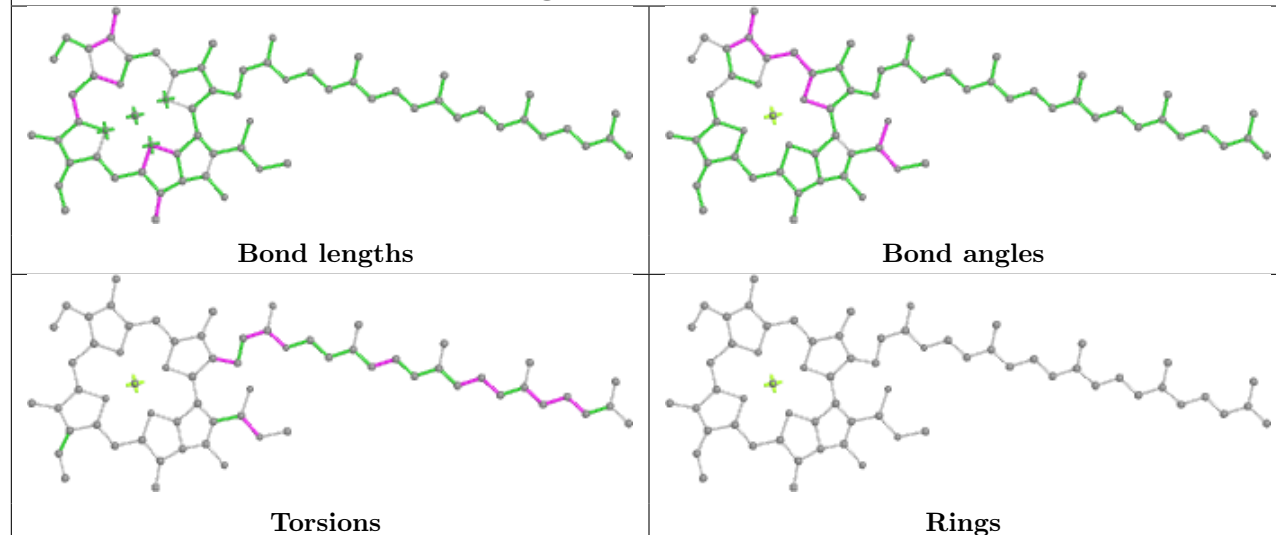




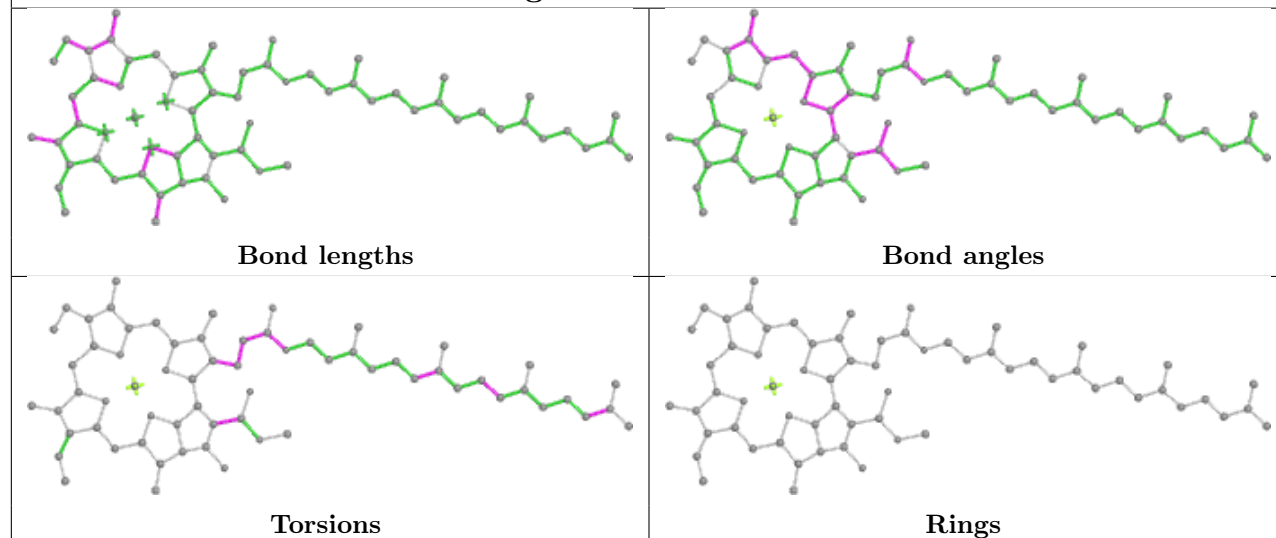
## Ligand CLA A 1109

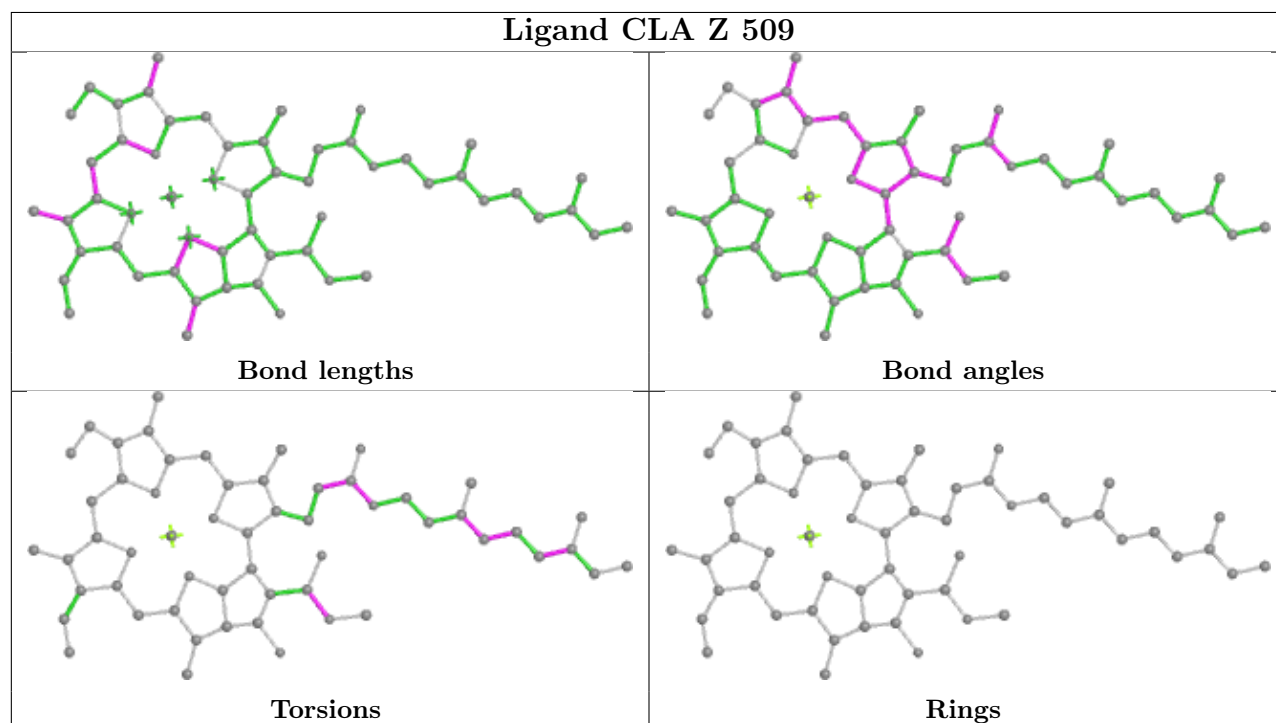
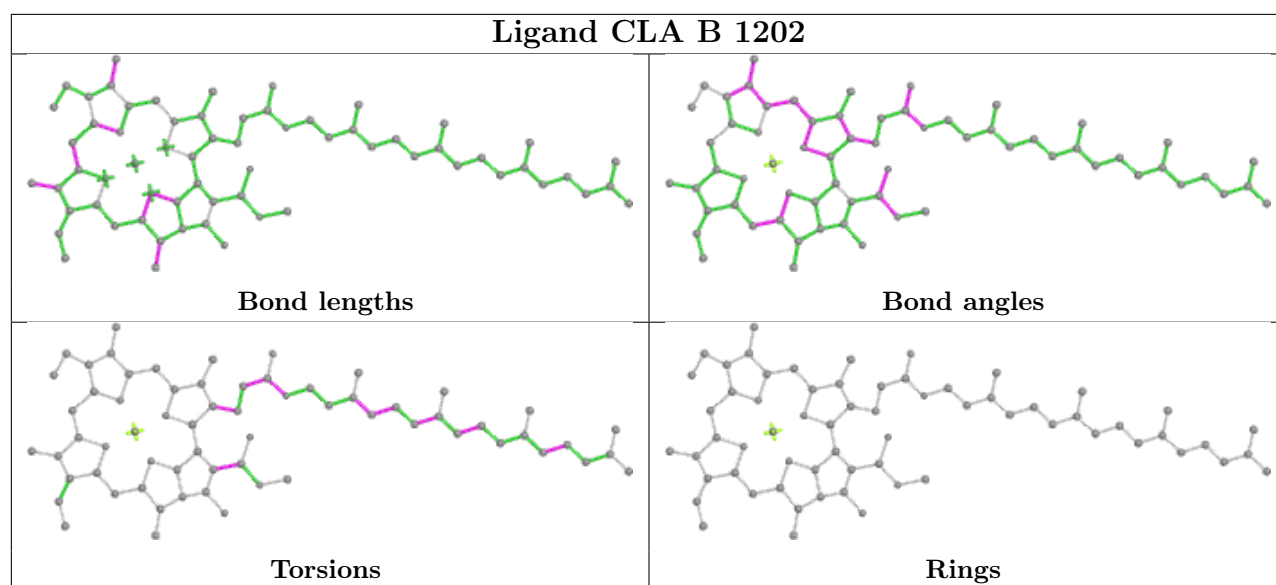


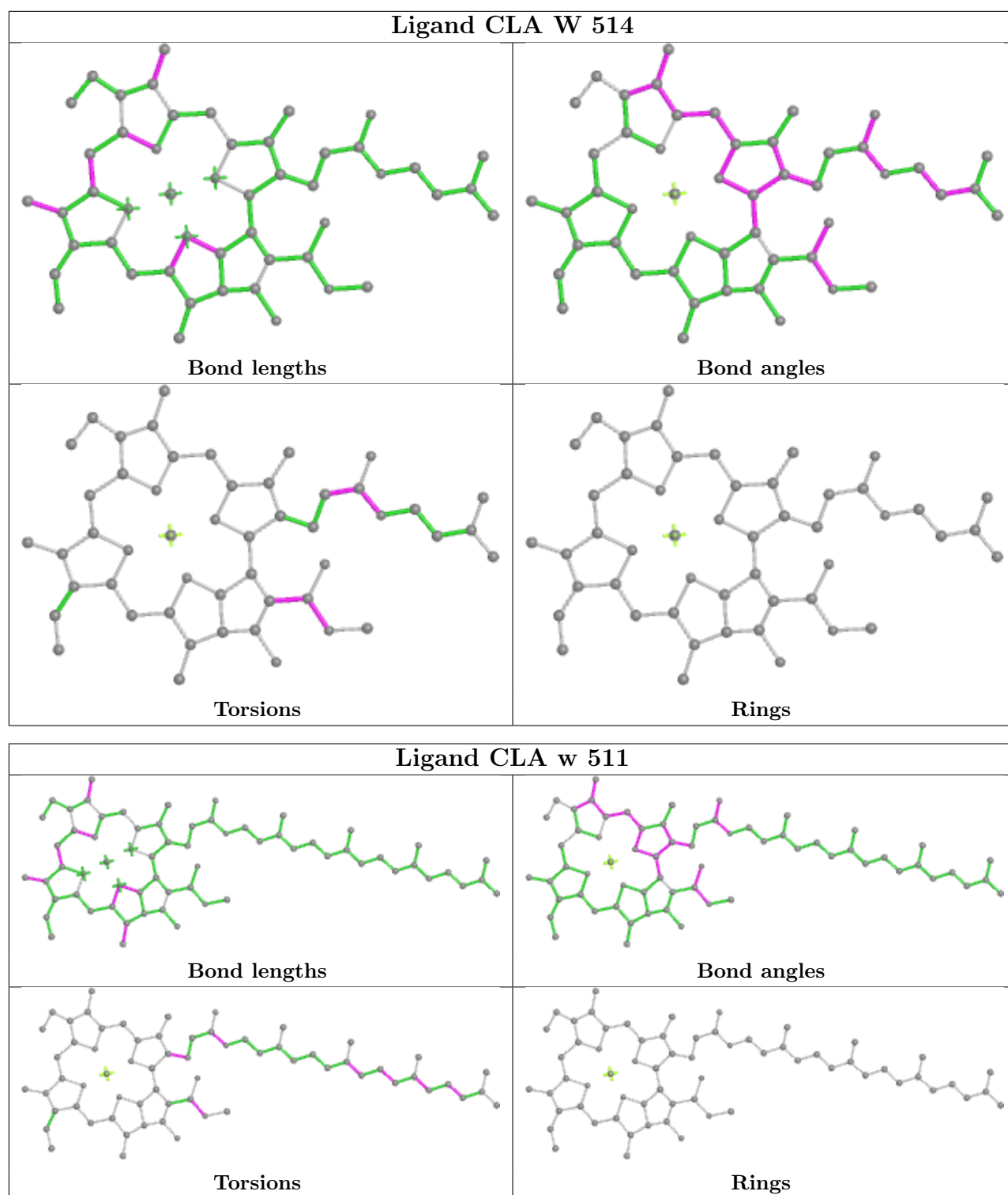
## Ligand CLA t 505



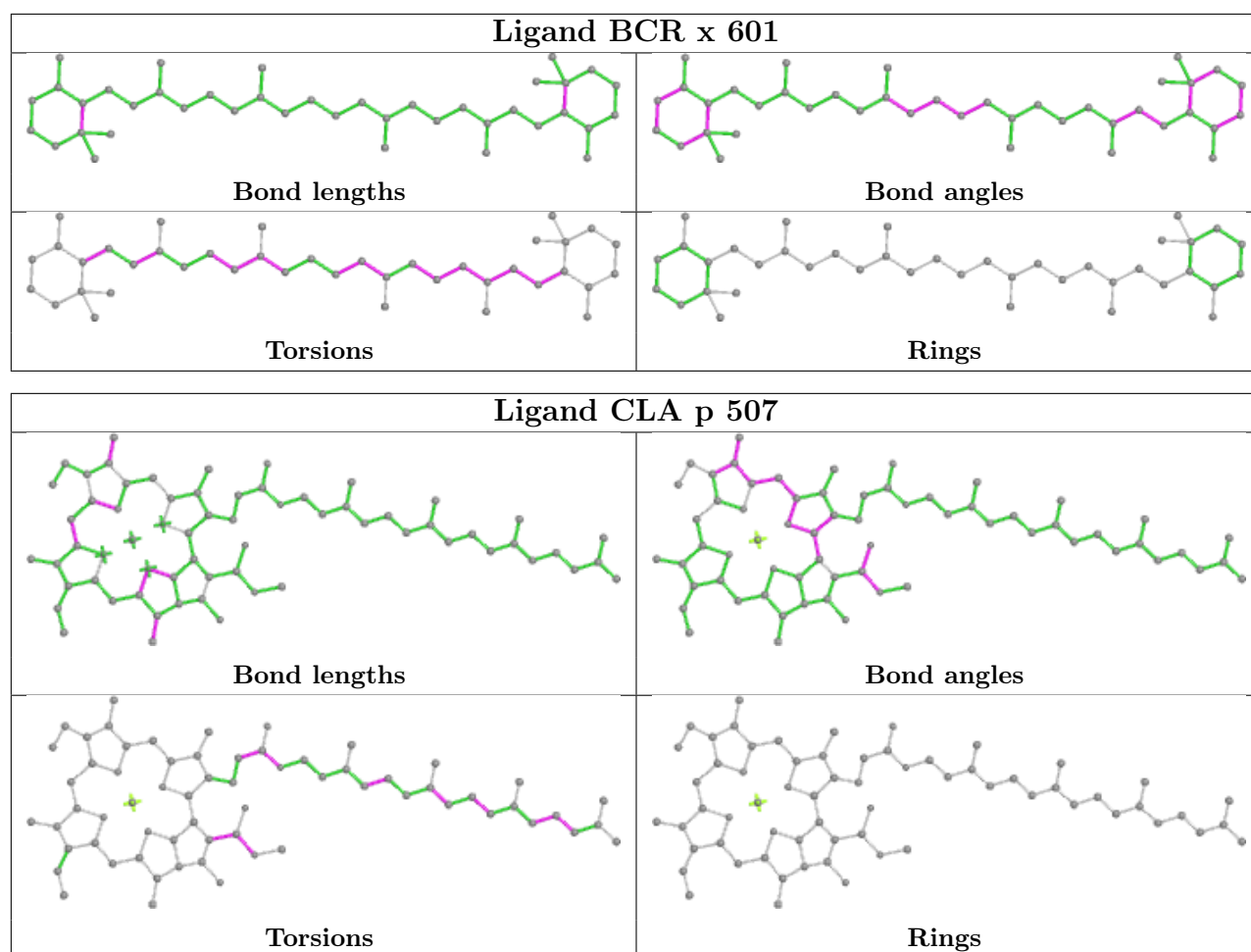
## Ligand CLA L 1502

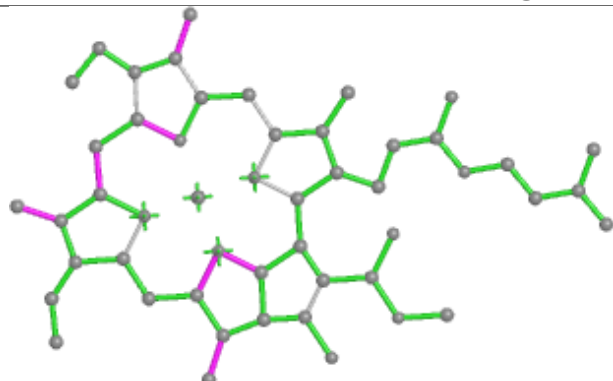




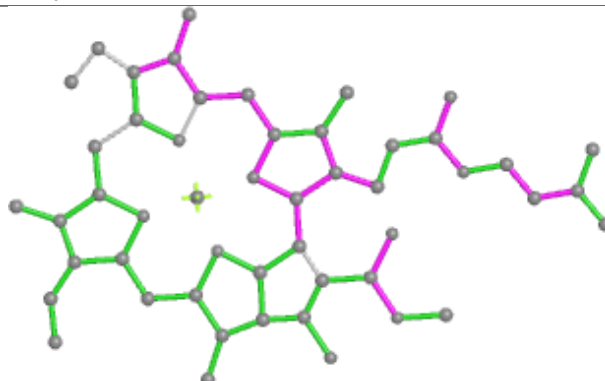




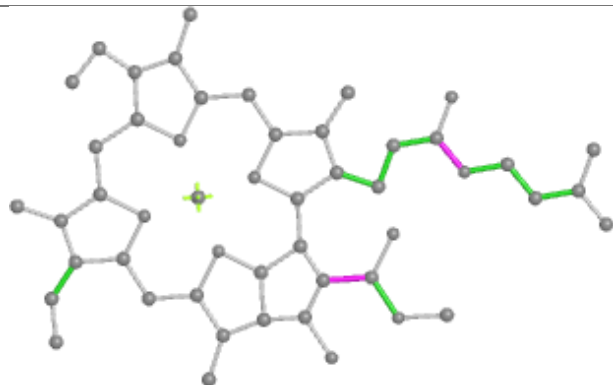


**Ligand CLA y 513**

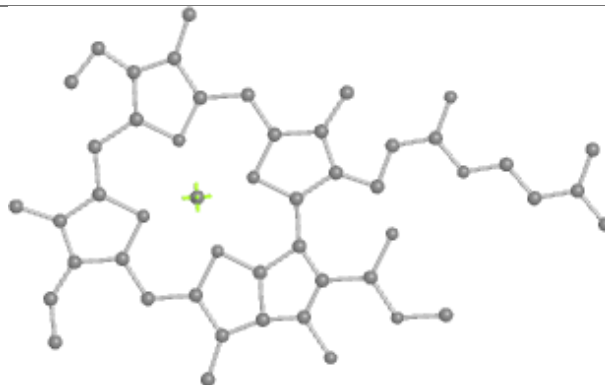
Bond lengths



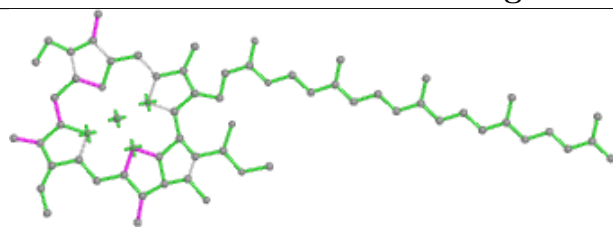
Bond angles



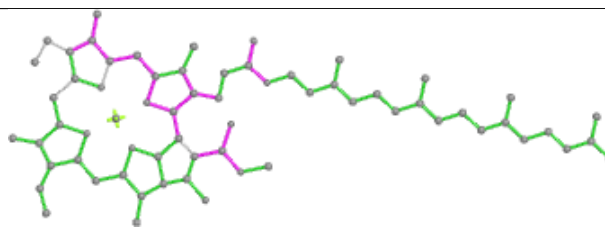
Torsions



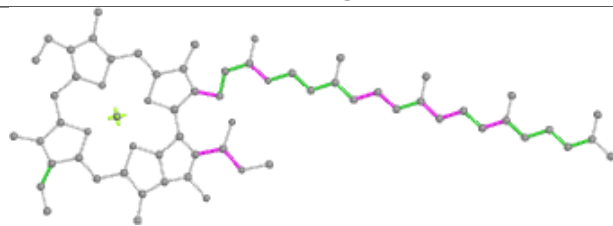
Rings

**Ligand CLA H 1101**

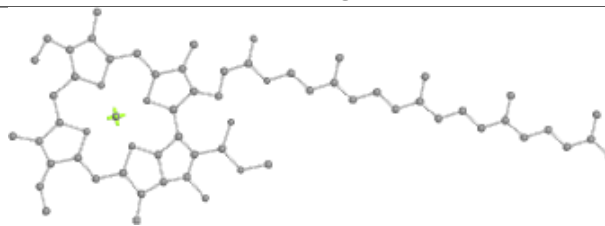
Bond lengths



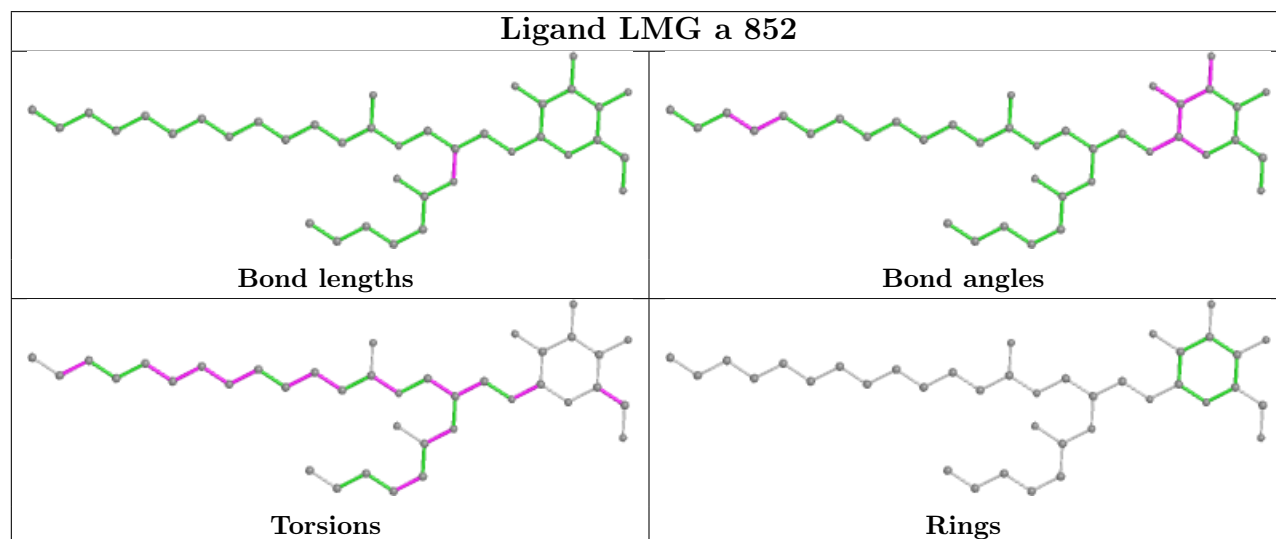
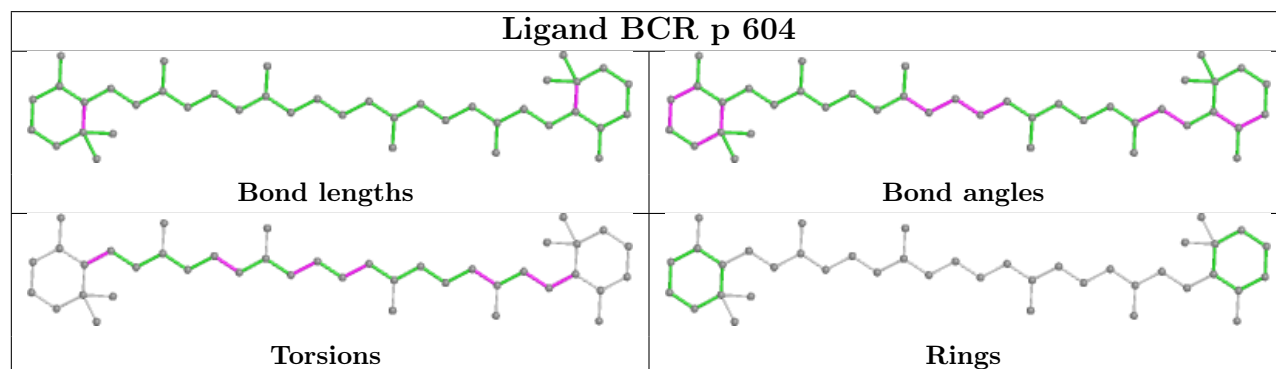
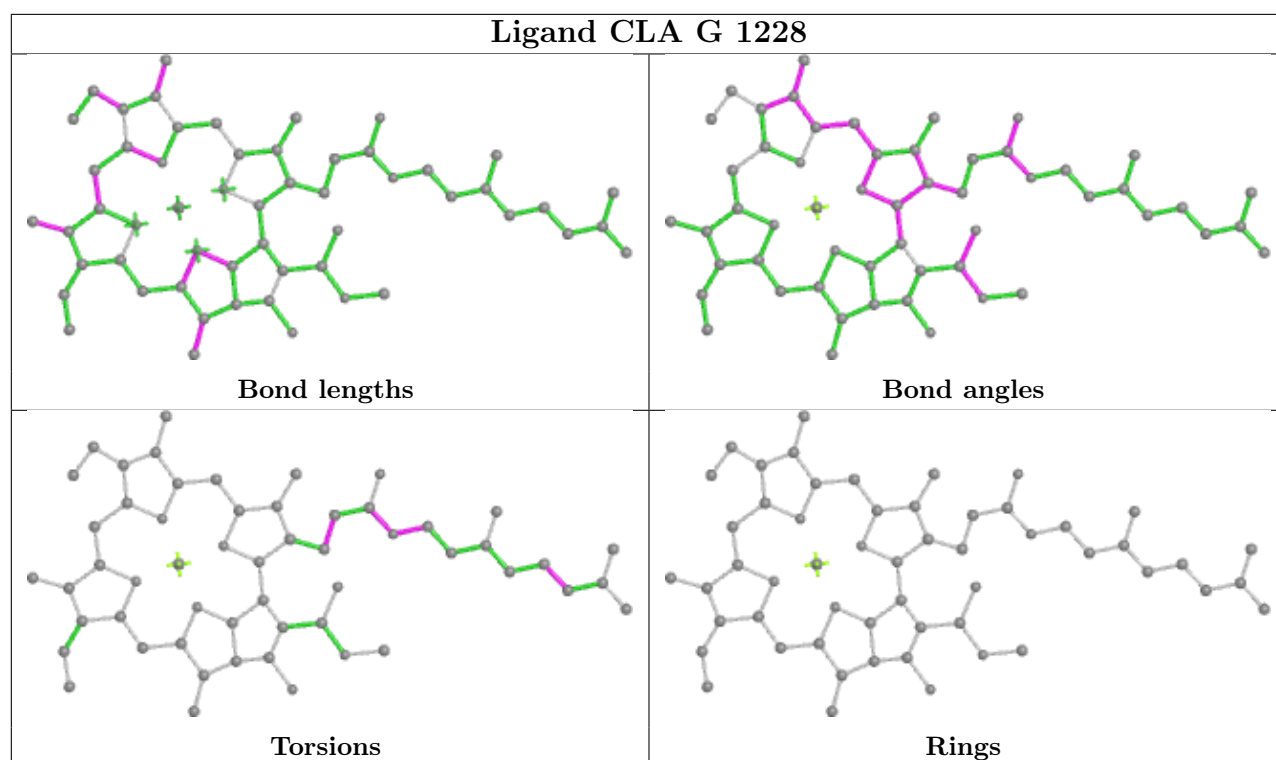
Bond angles



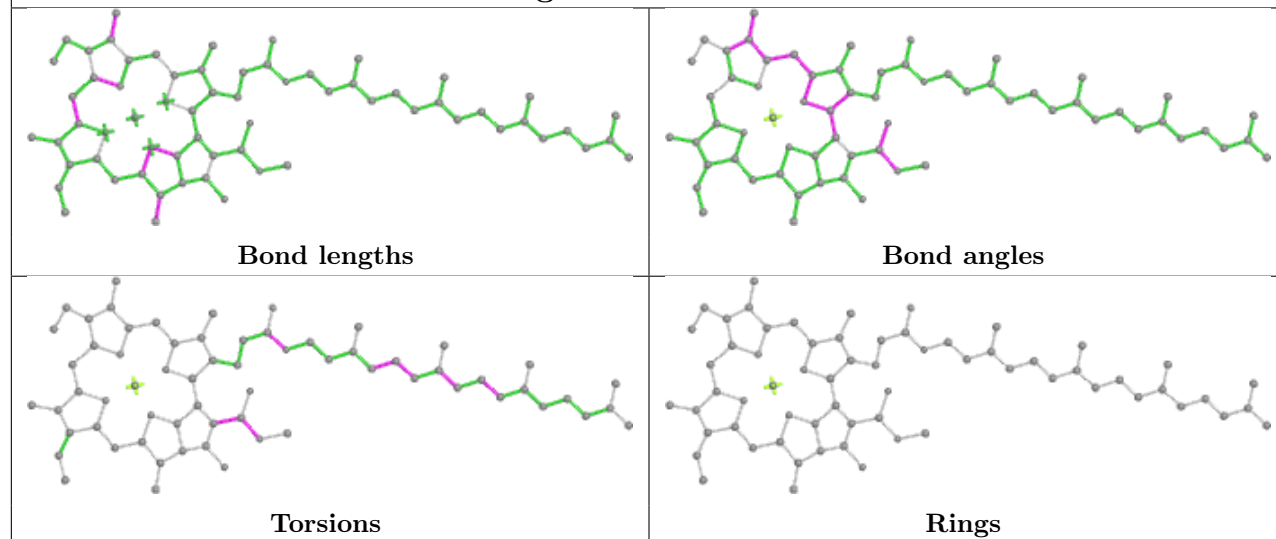
Torsions



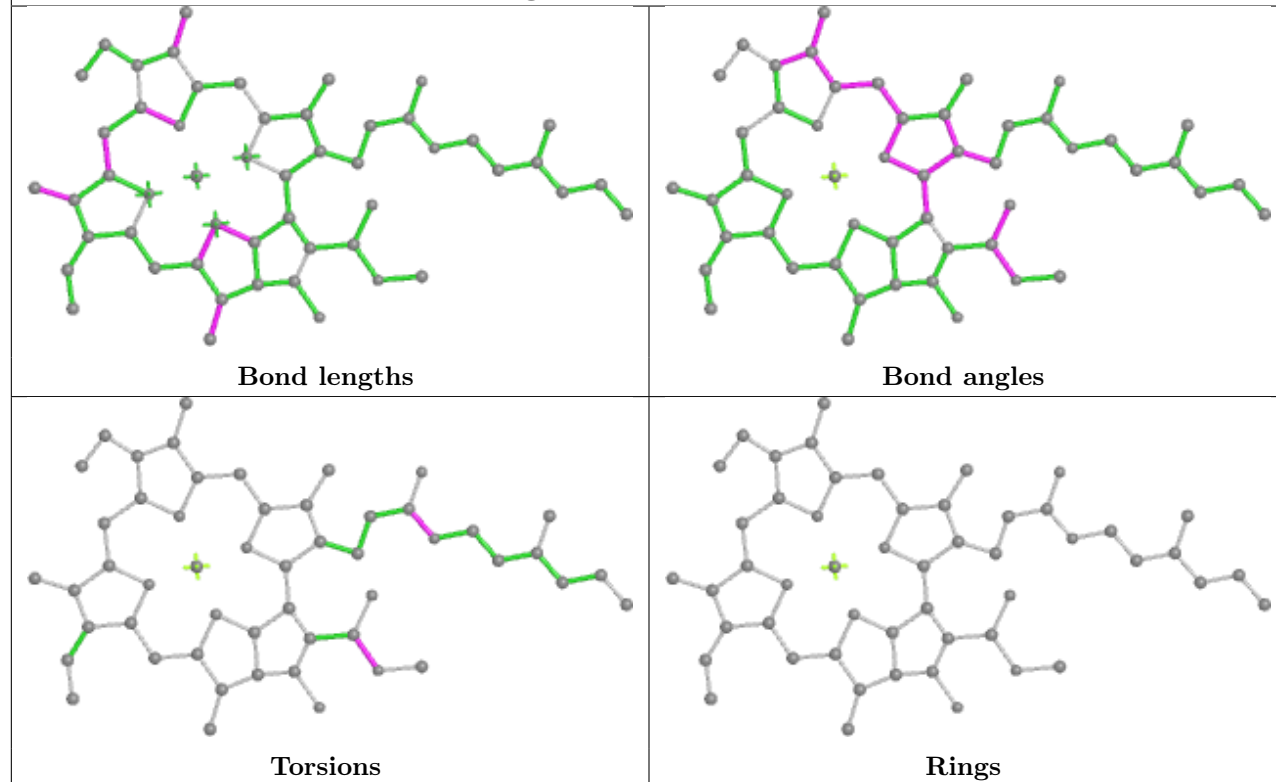
Rings



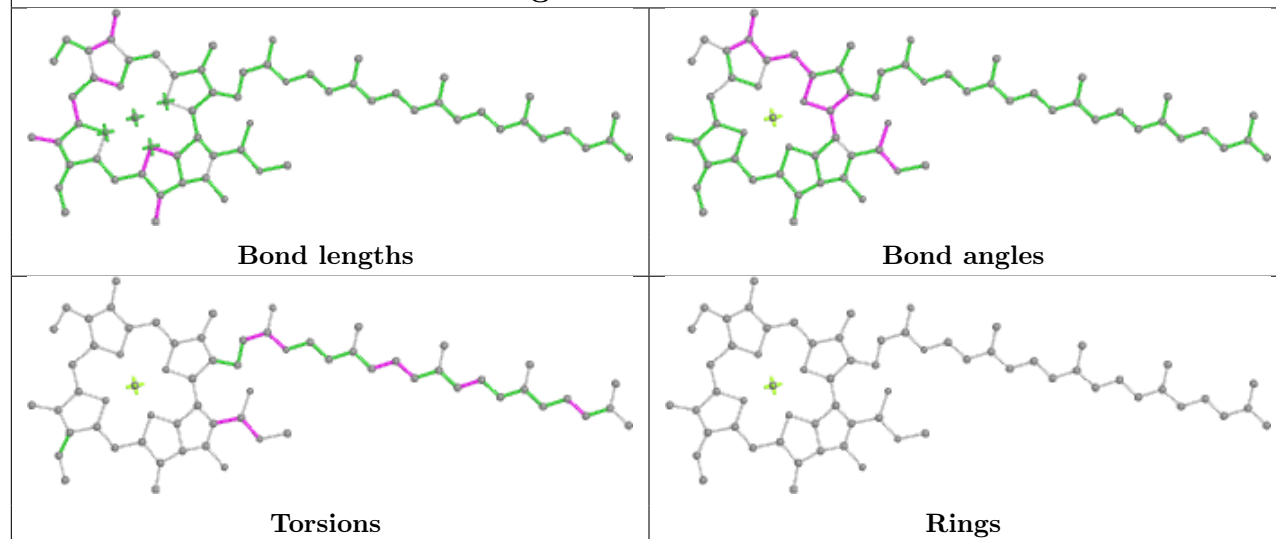
## Ligand CLA o 507



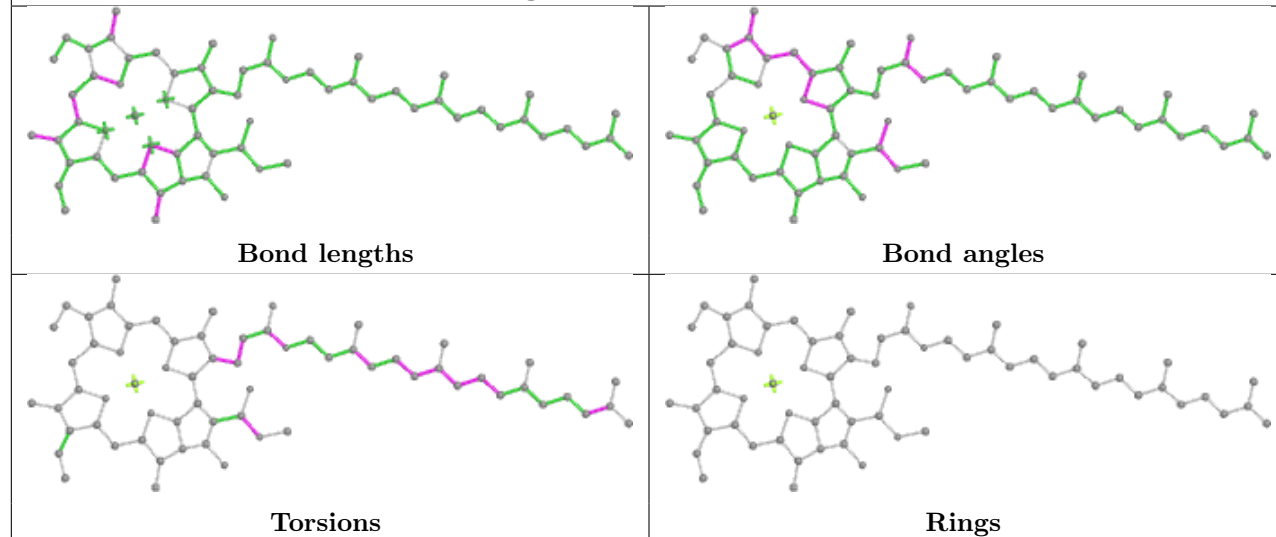
## Ligand CLA A 1801



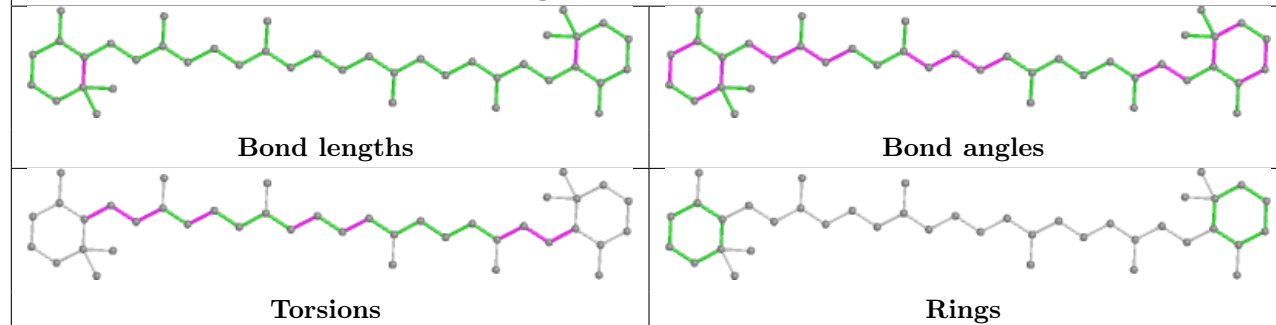
## Ligand CLA Y 507

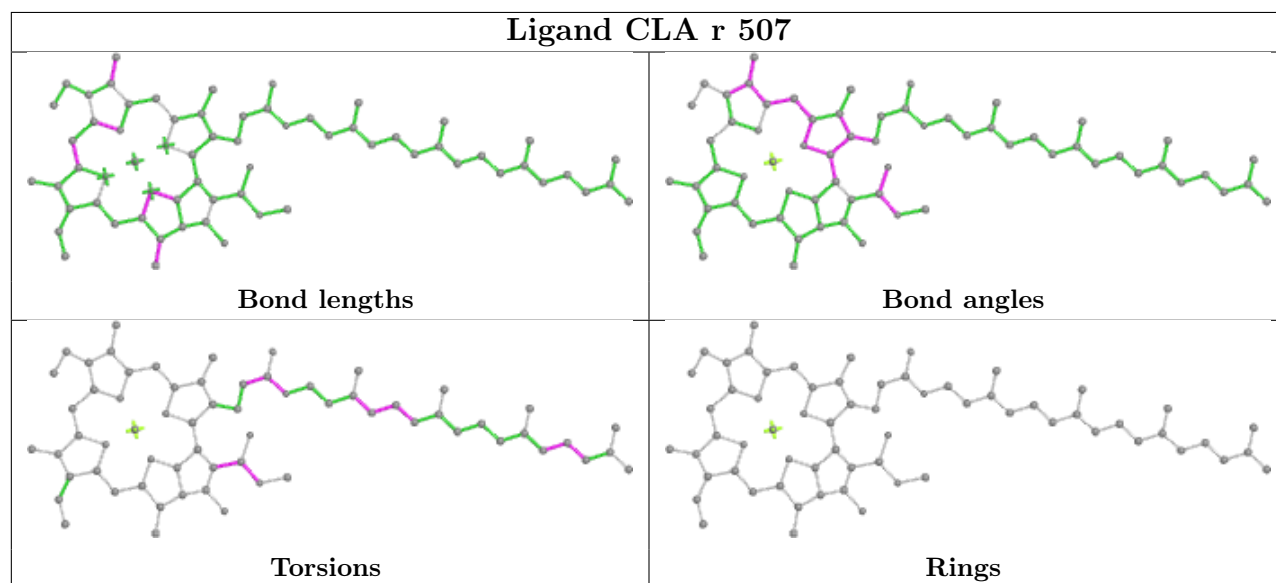
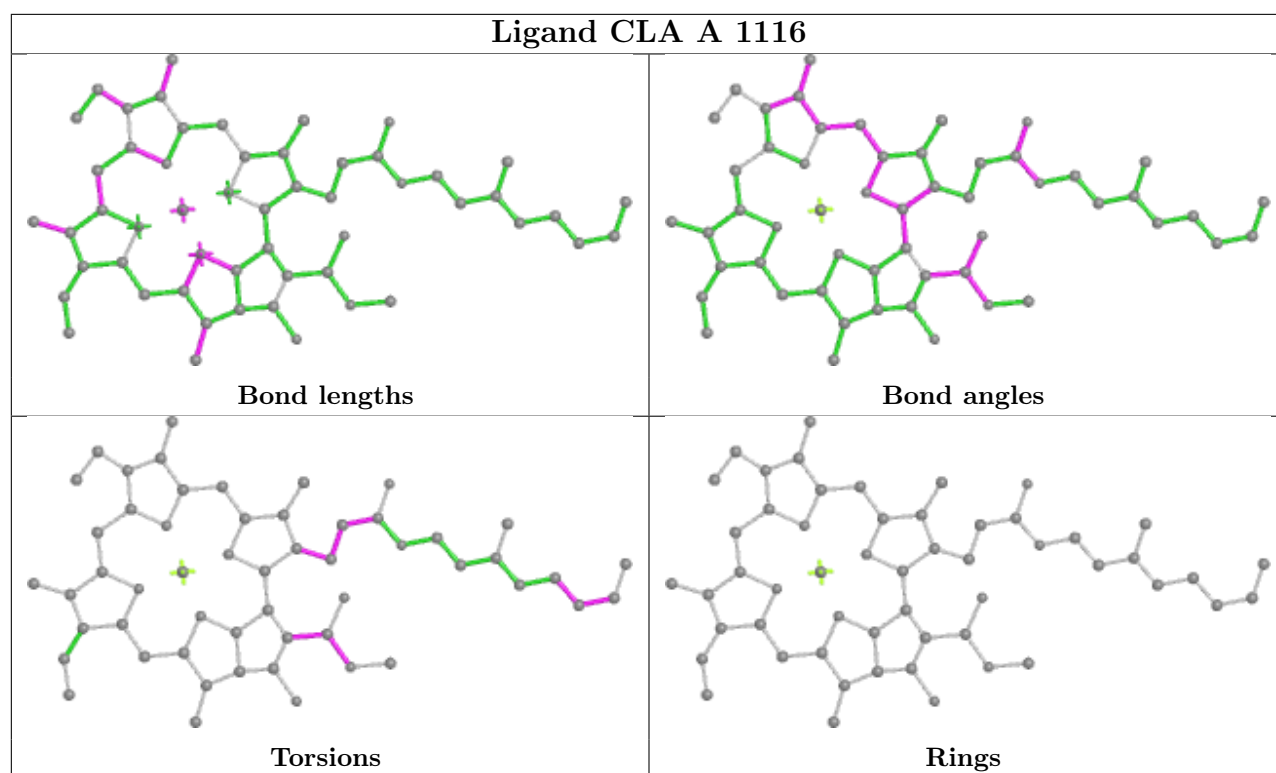


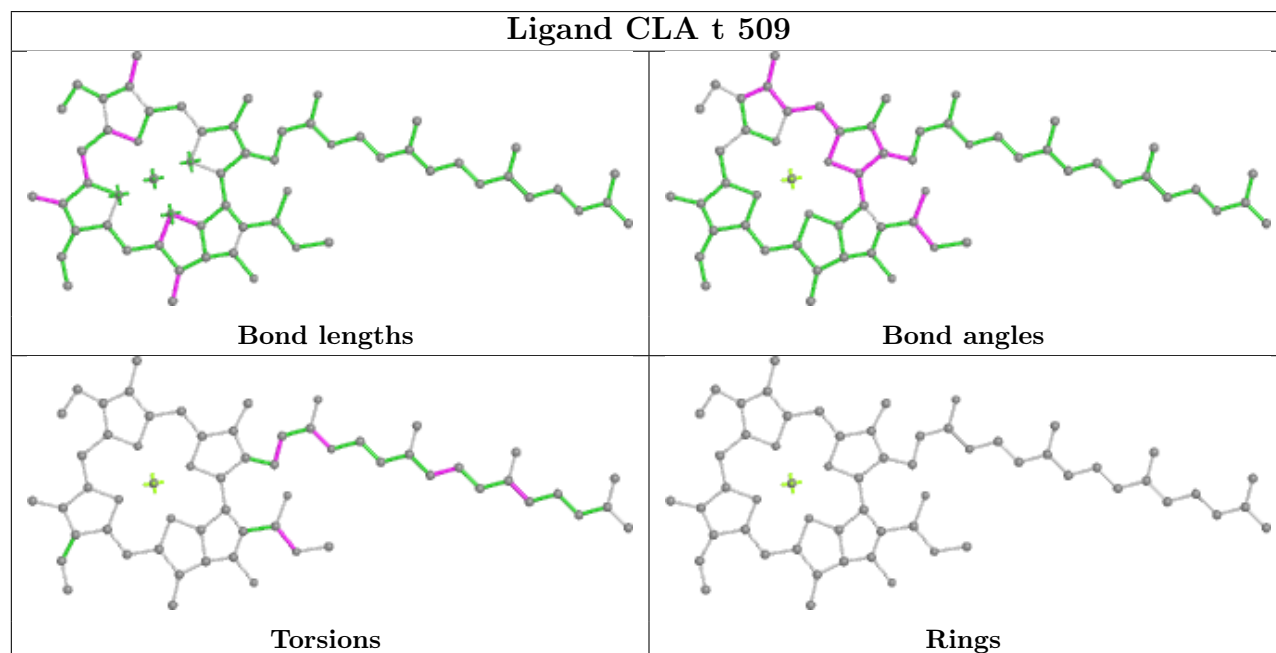
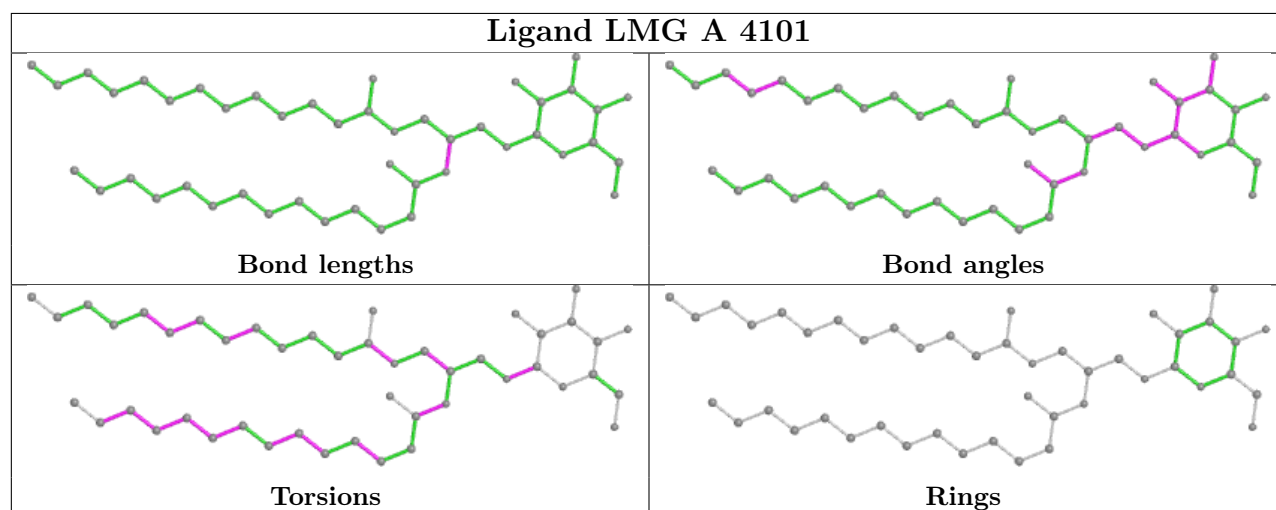
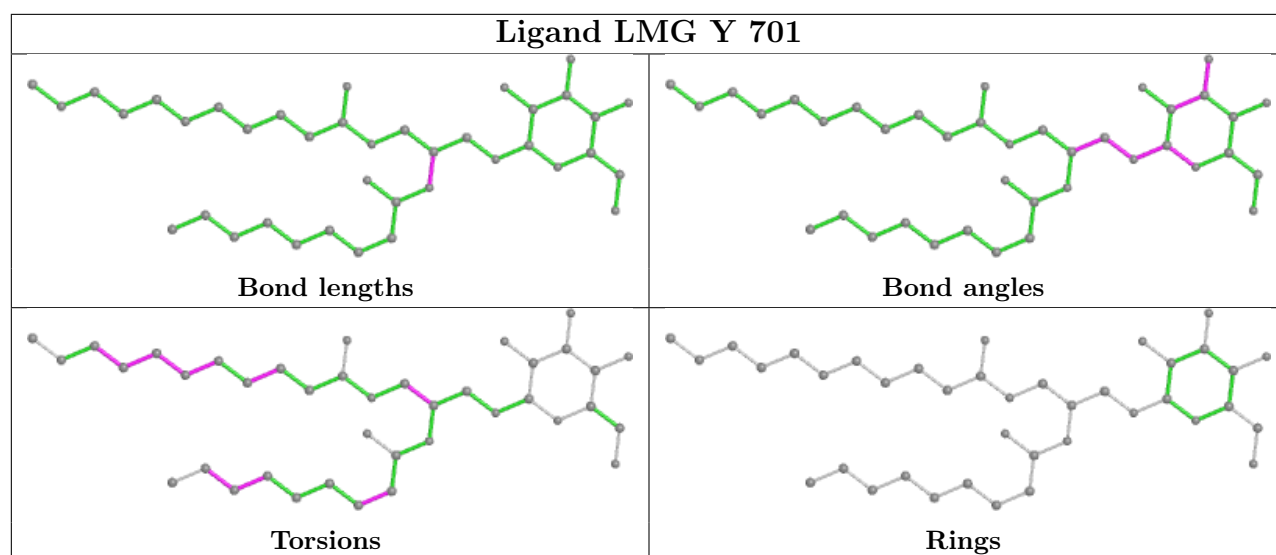
## Ligand CLA H 1140

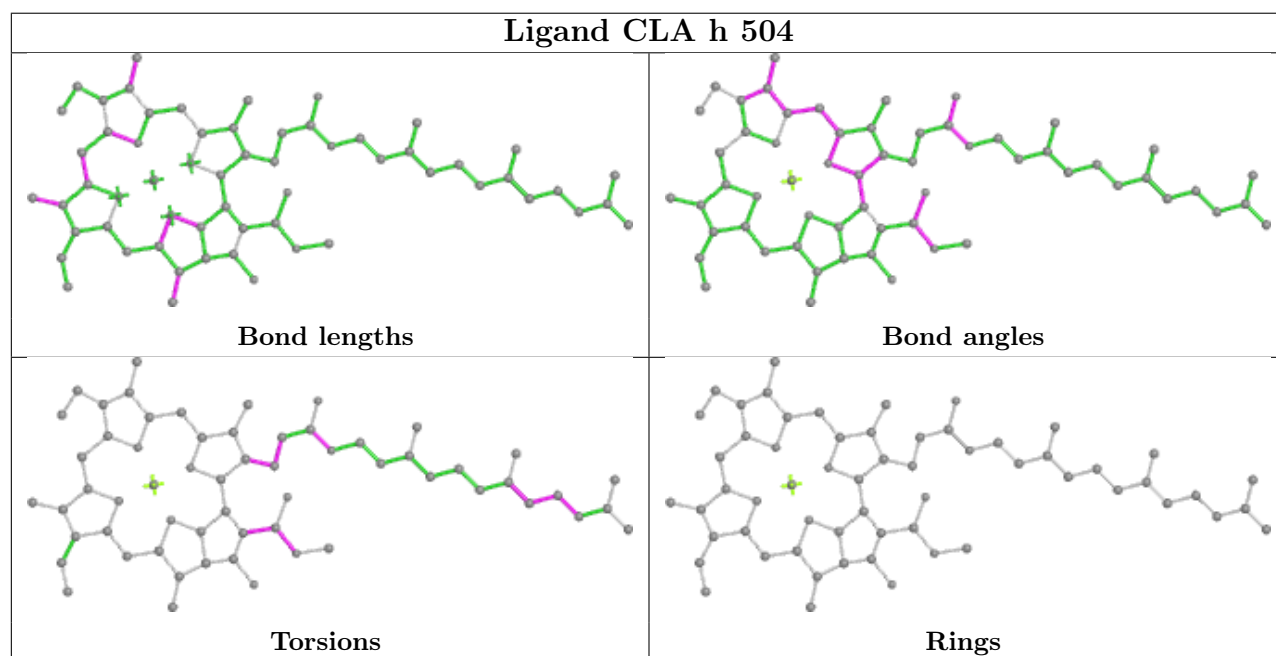
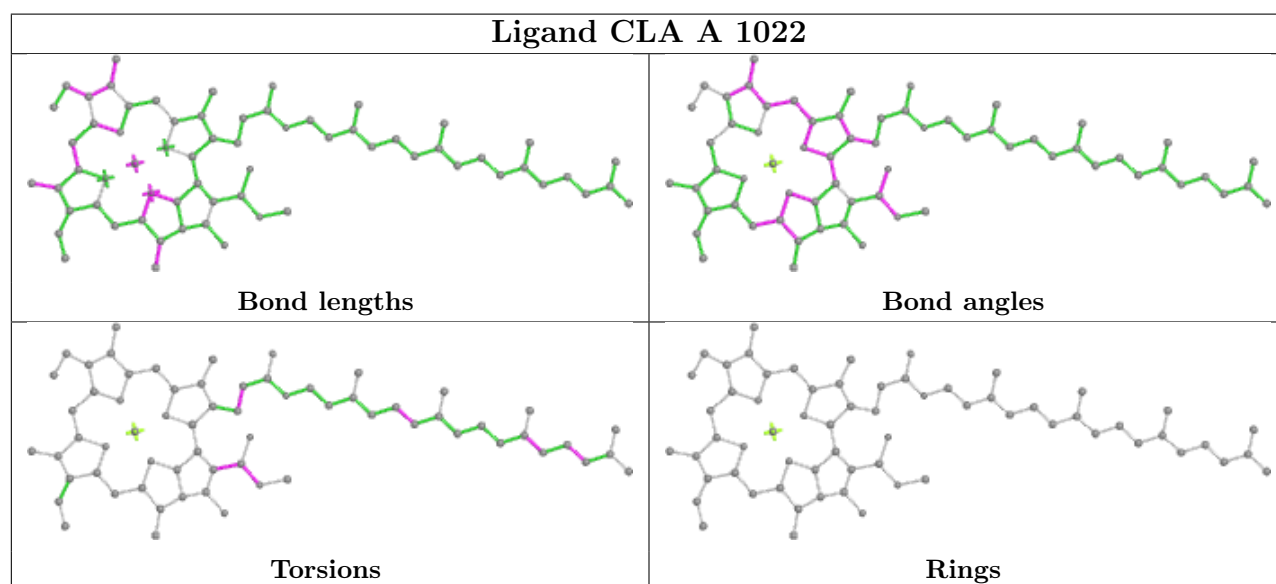
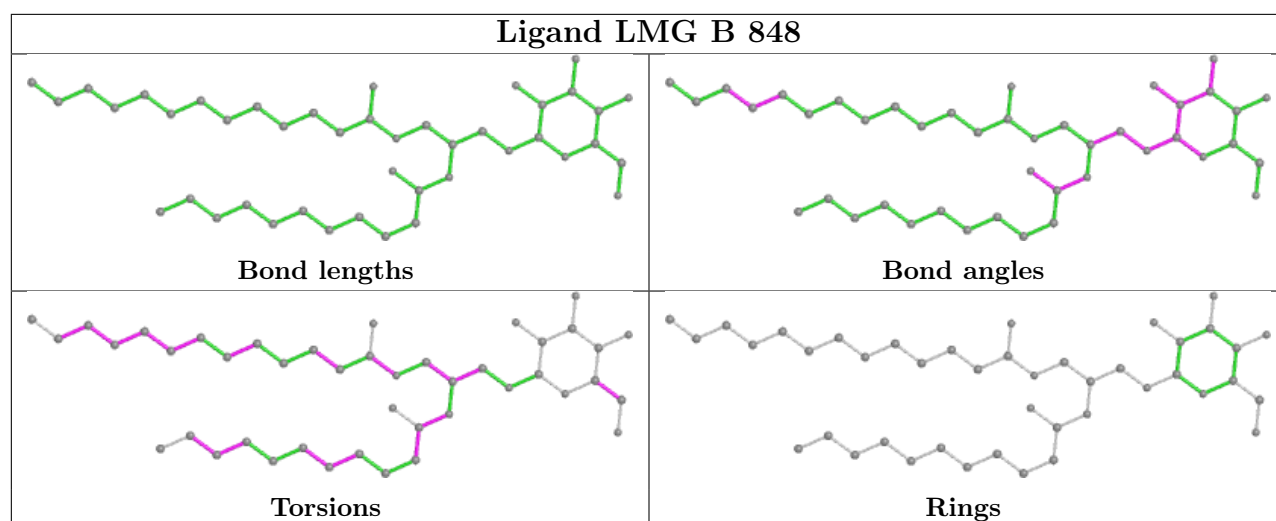


## Ligand BCR x 604

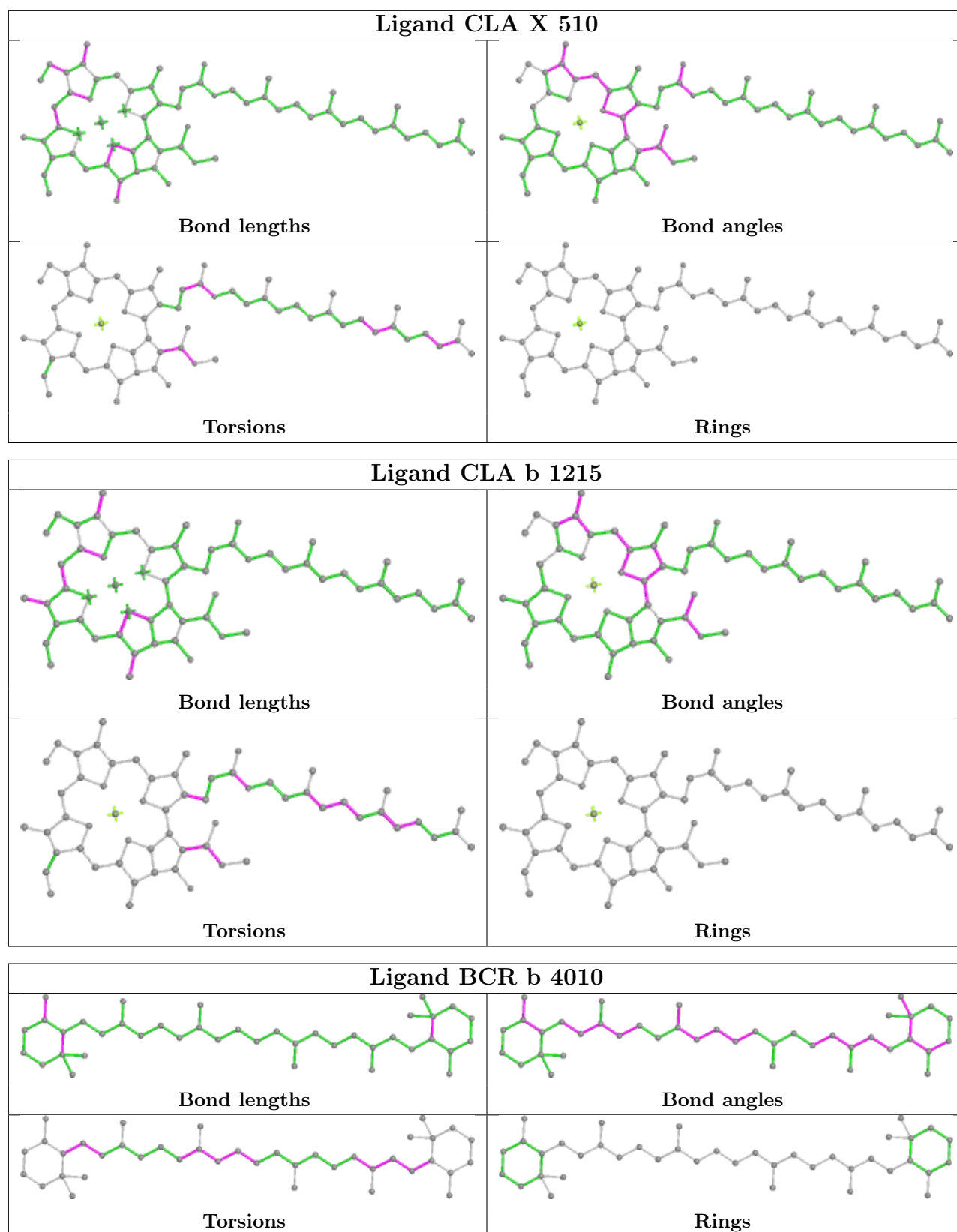




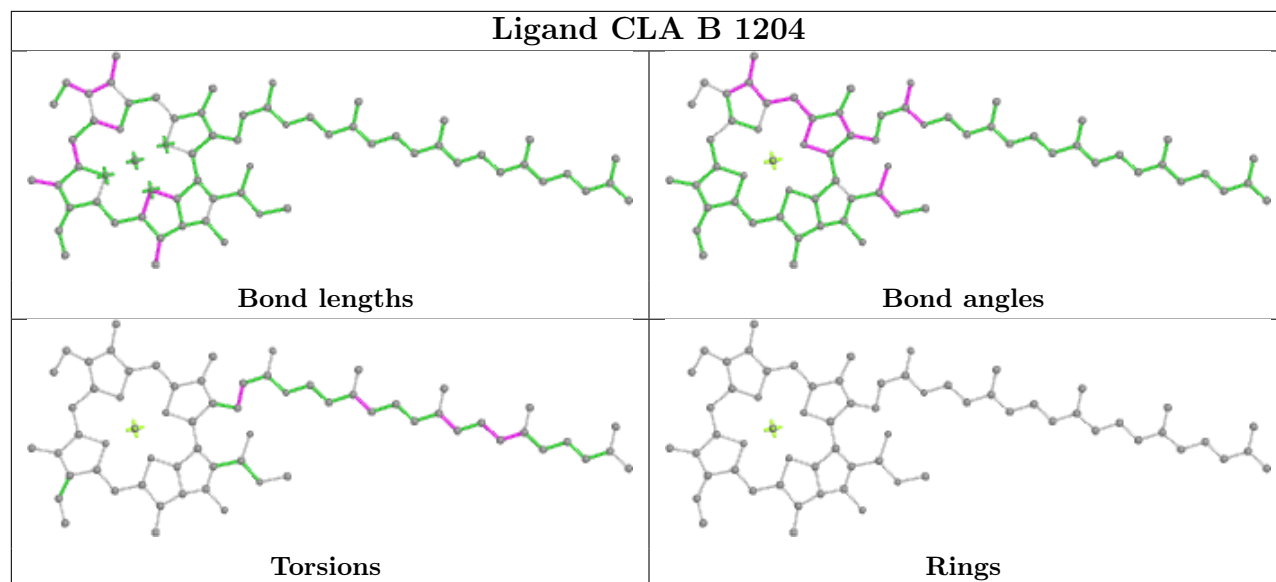




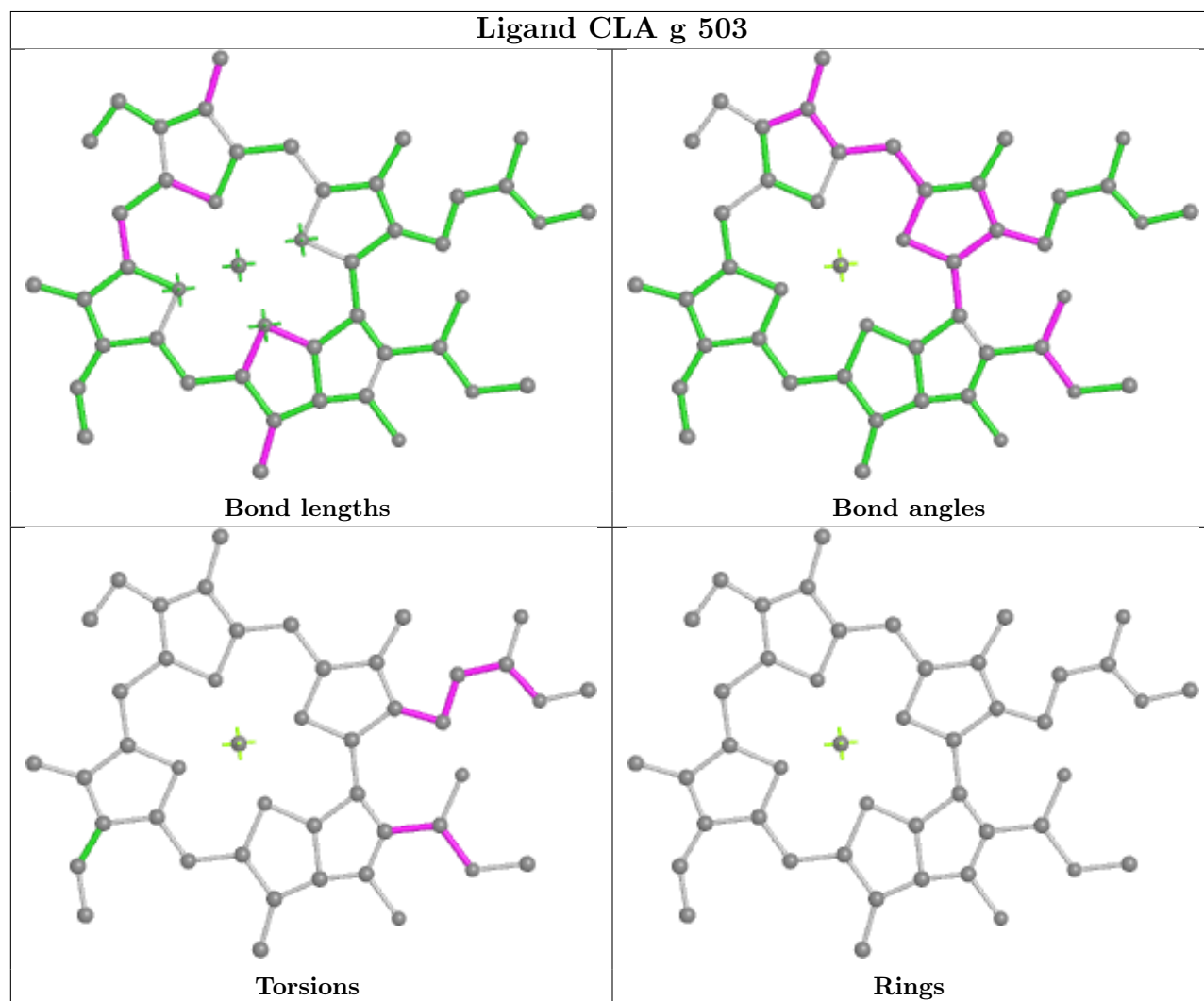




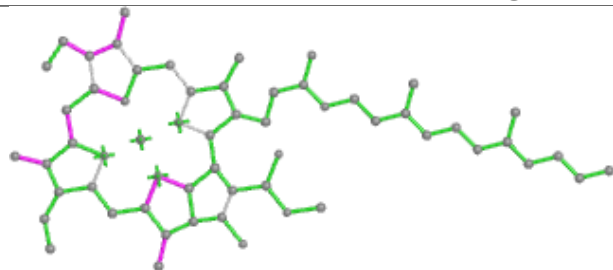
## Ligand CLA B 1204



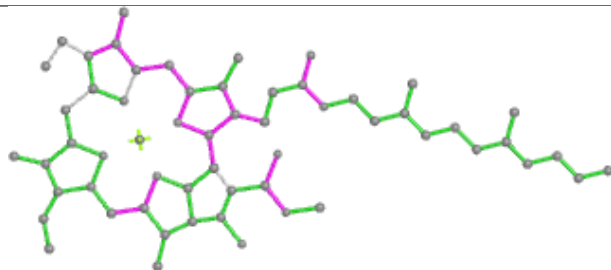
## Ligand CLA g 503



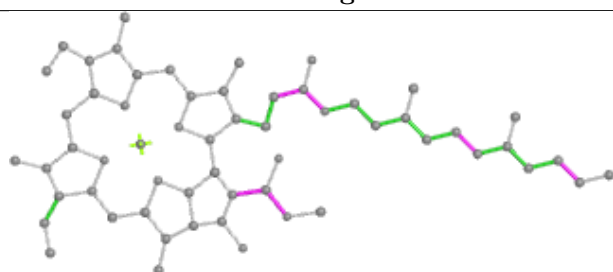
## Ligand CLA B 1229



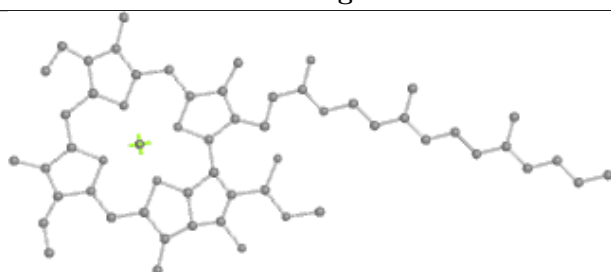
Bond lengths



Bond angles

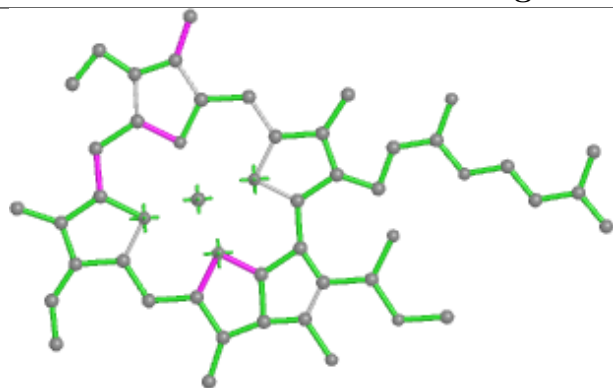


Torsions

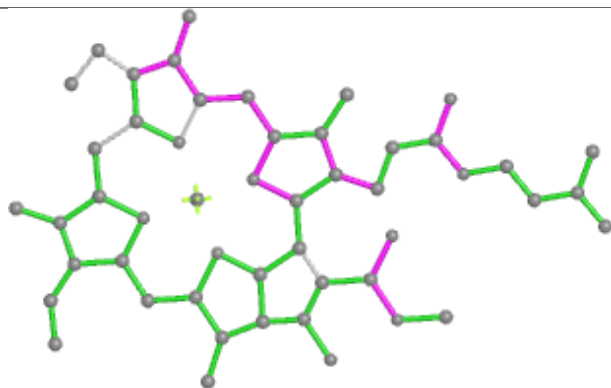


Rings

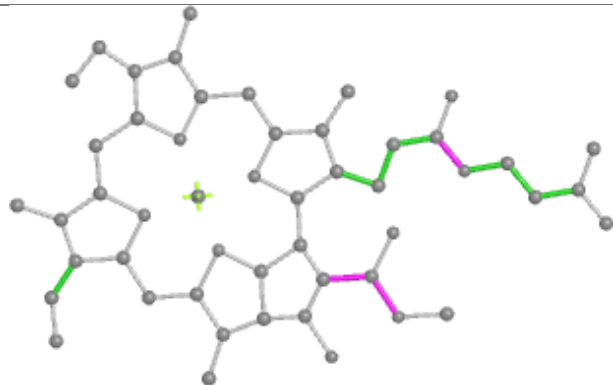
## Ligand CLA w 501



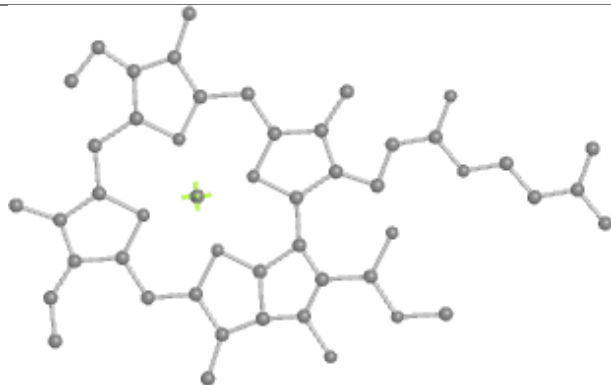
Bond lengths



Bond angles

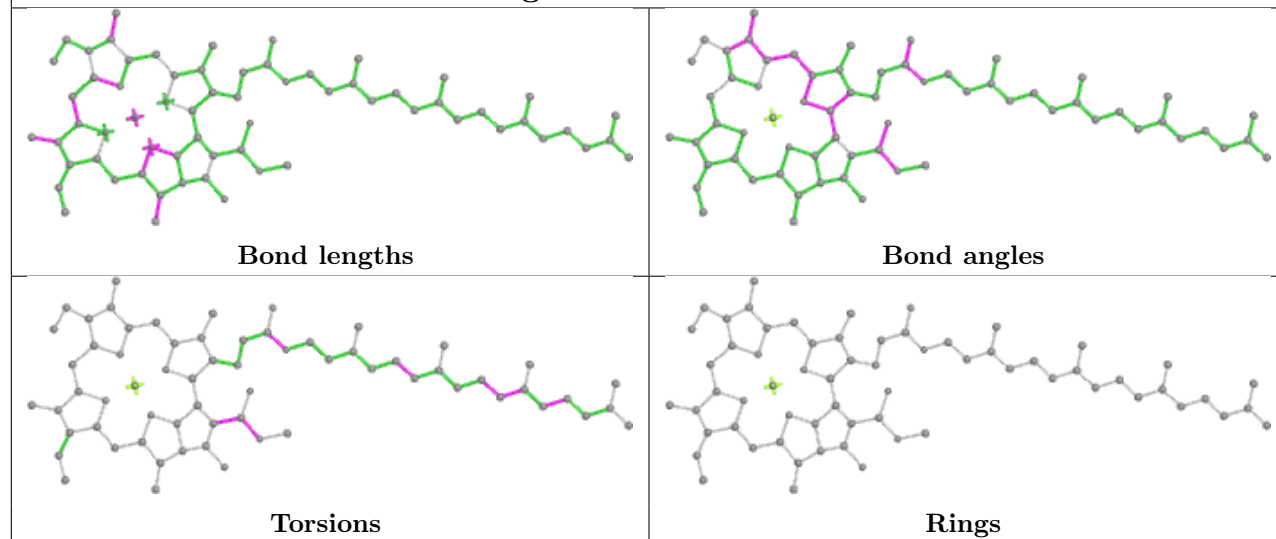


Torsions

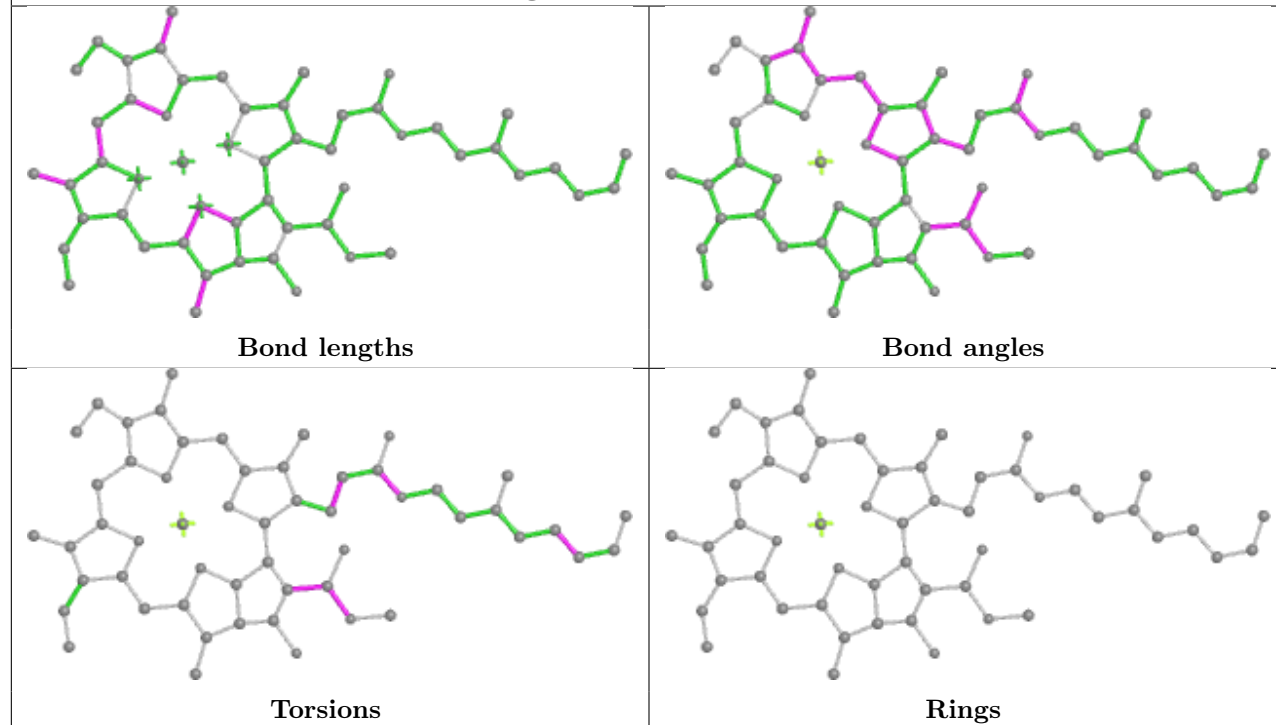


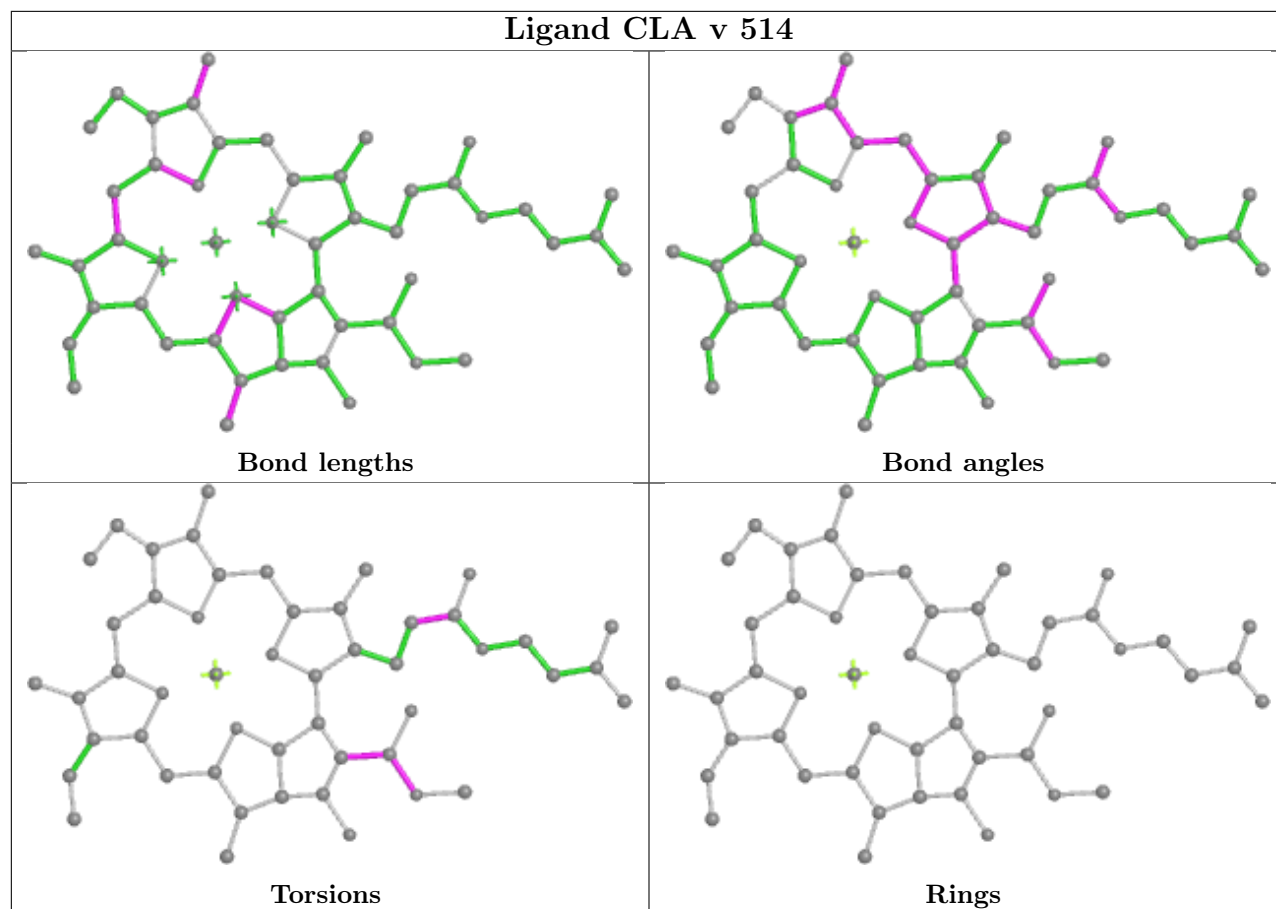
Rings

## Ligand CLA G 1221

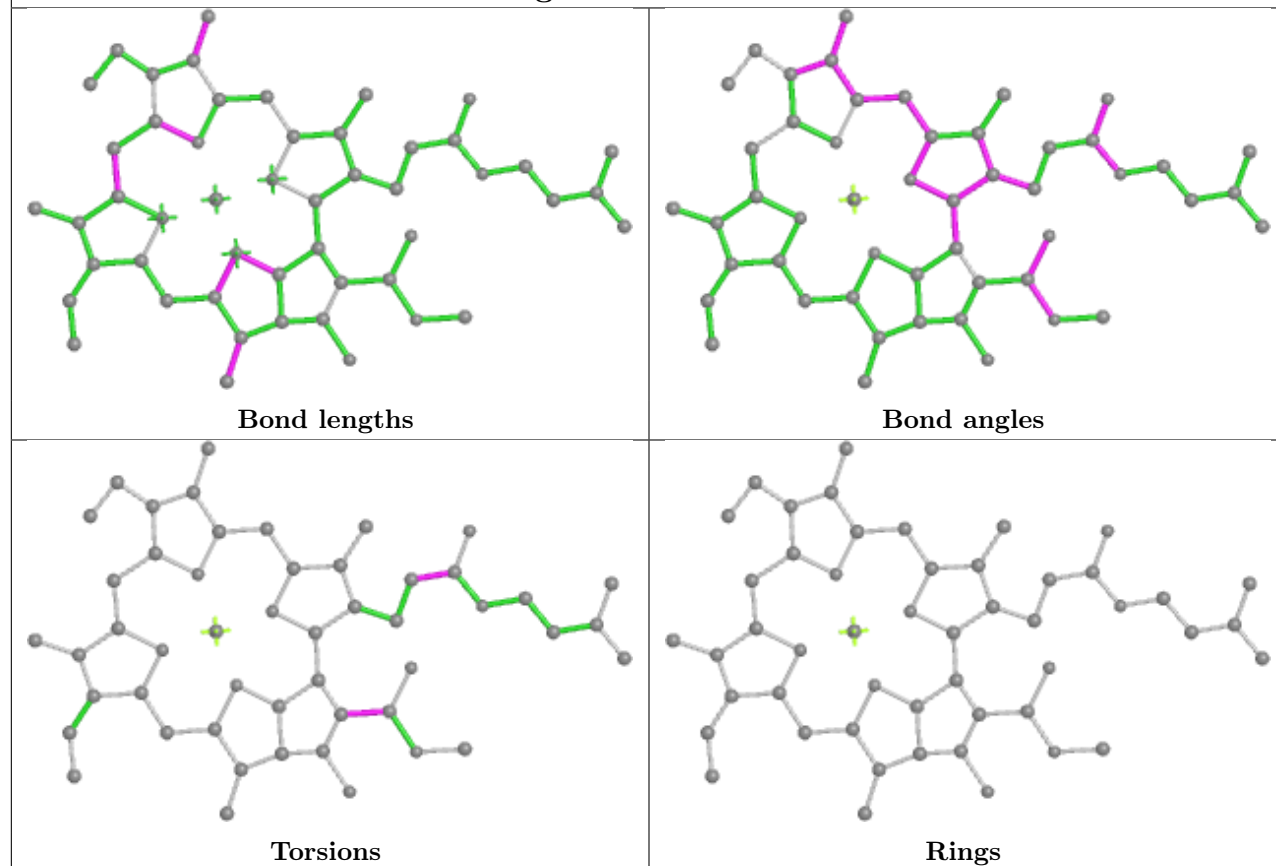


## Ligand CLA B 1201

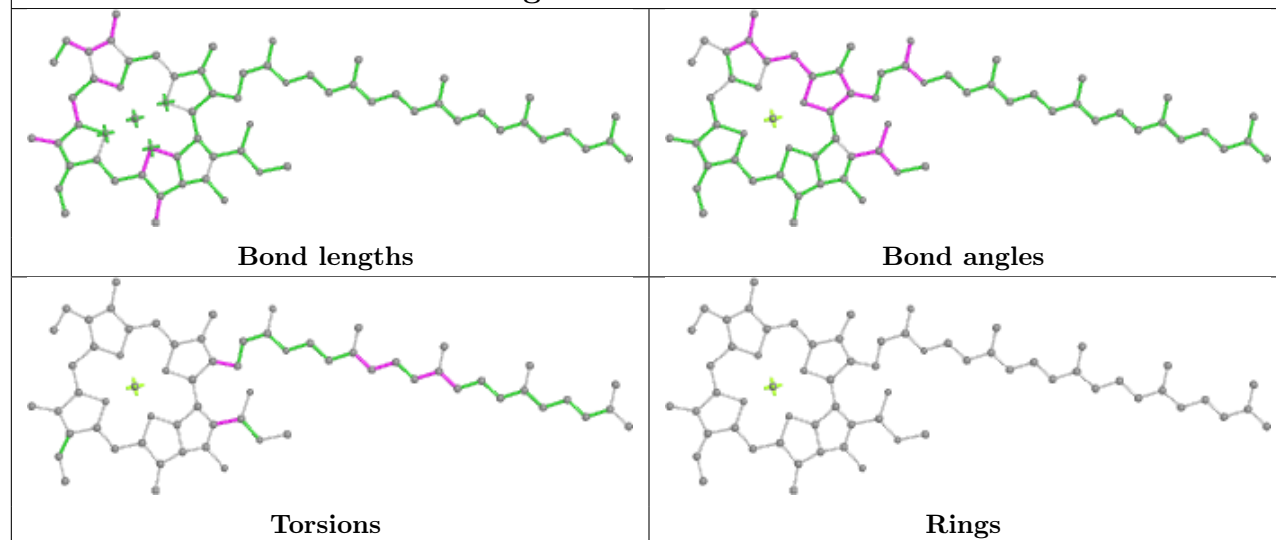




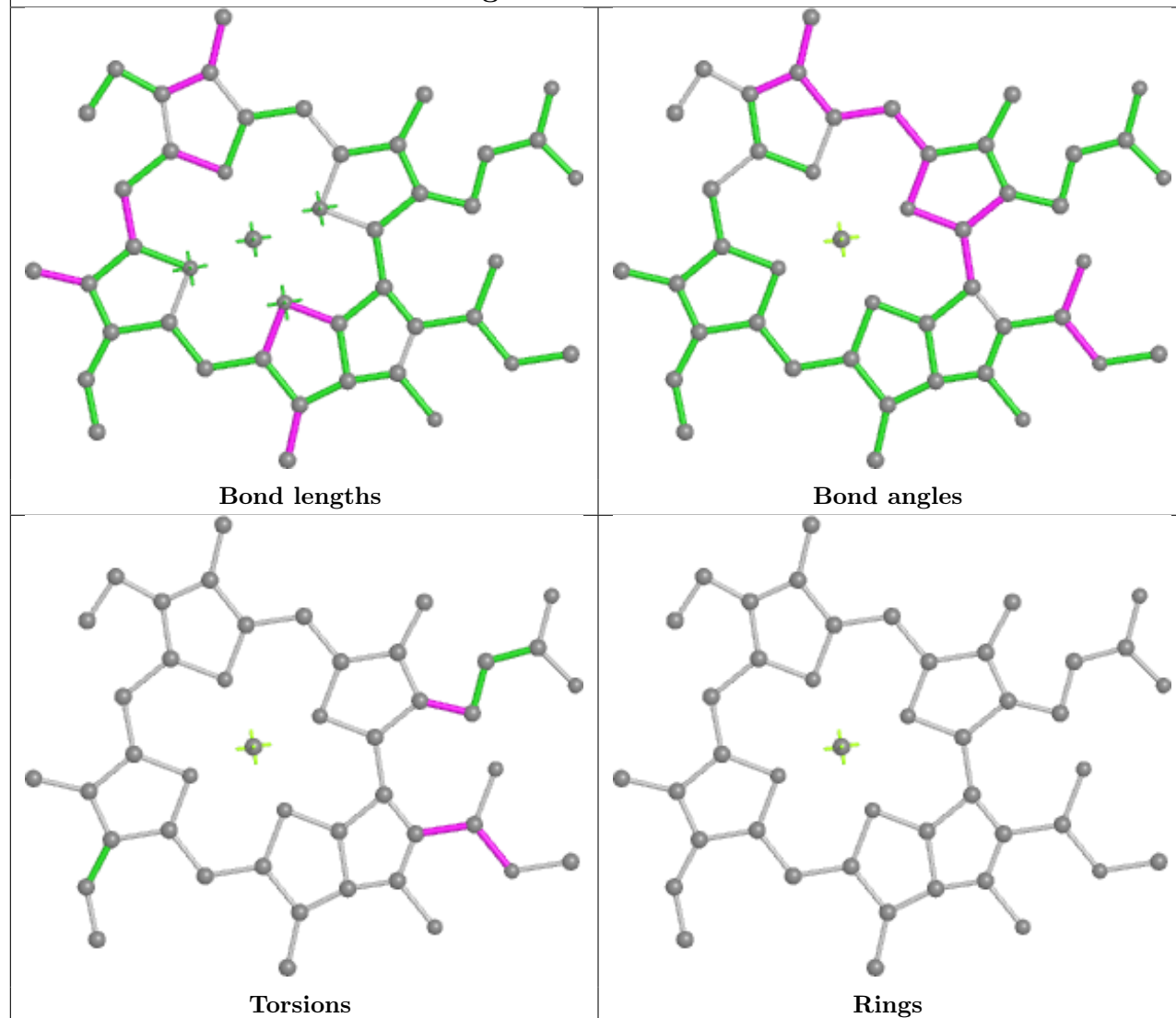
## Ligand CLA h 514



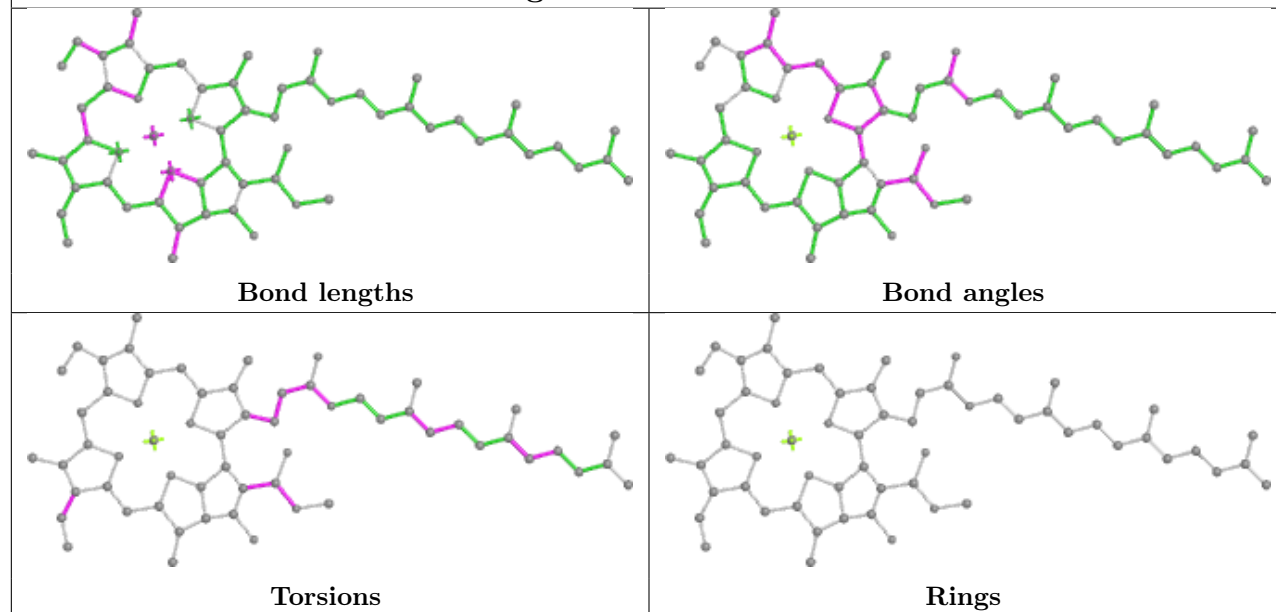
## Ligand CLA B 1205

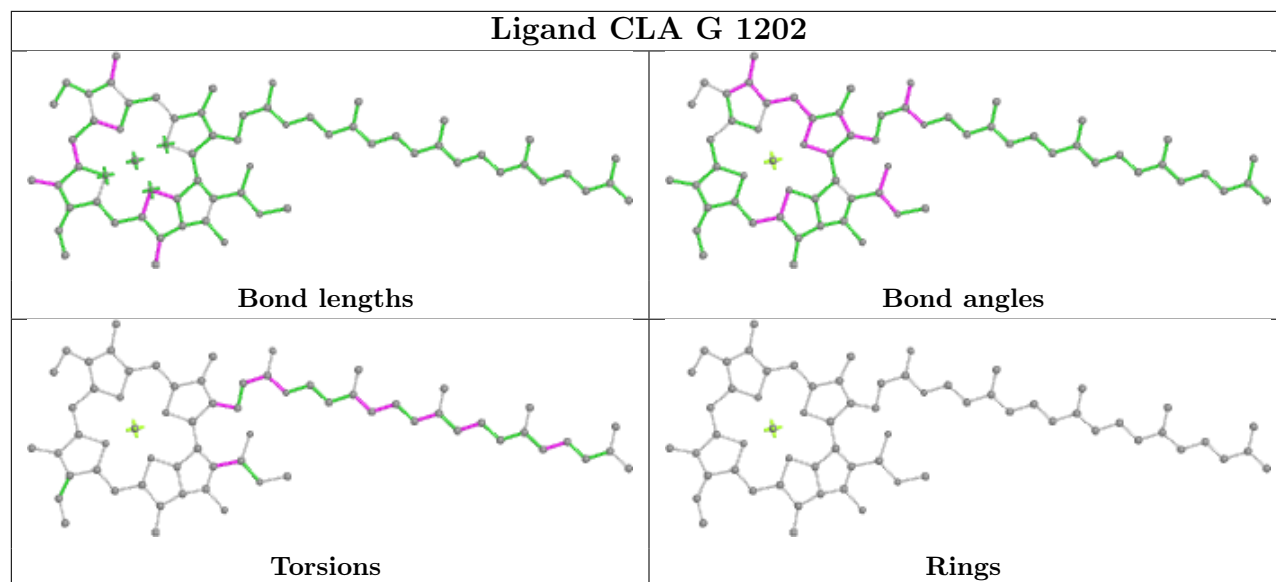
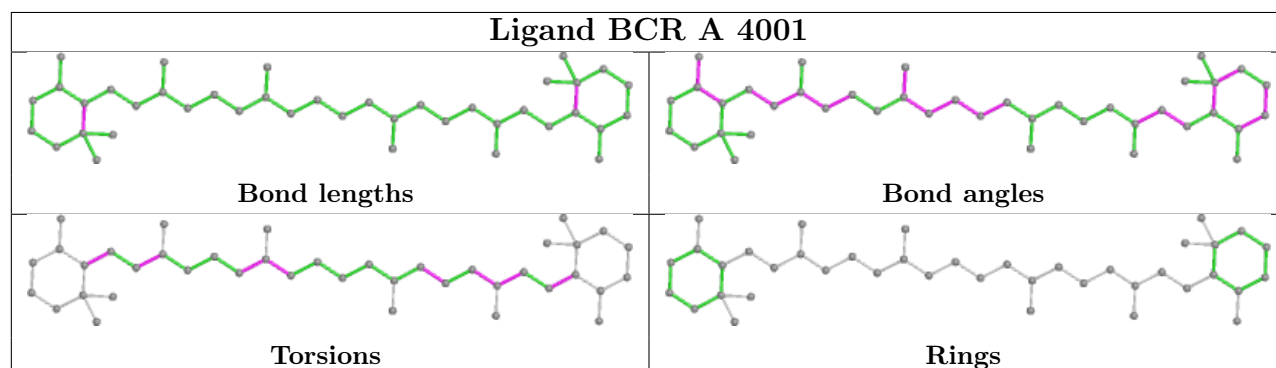
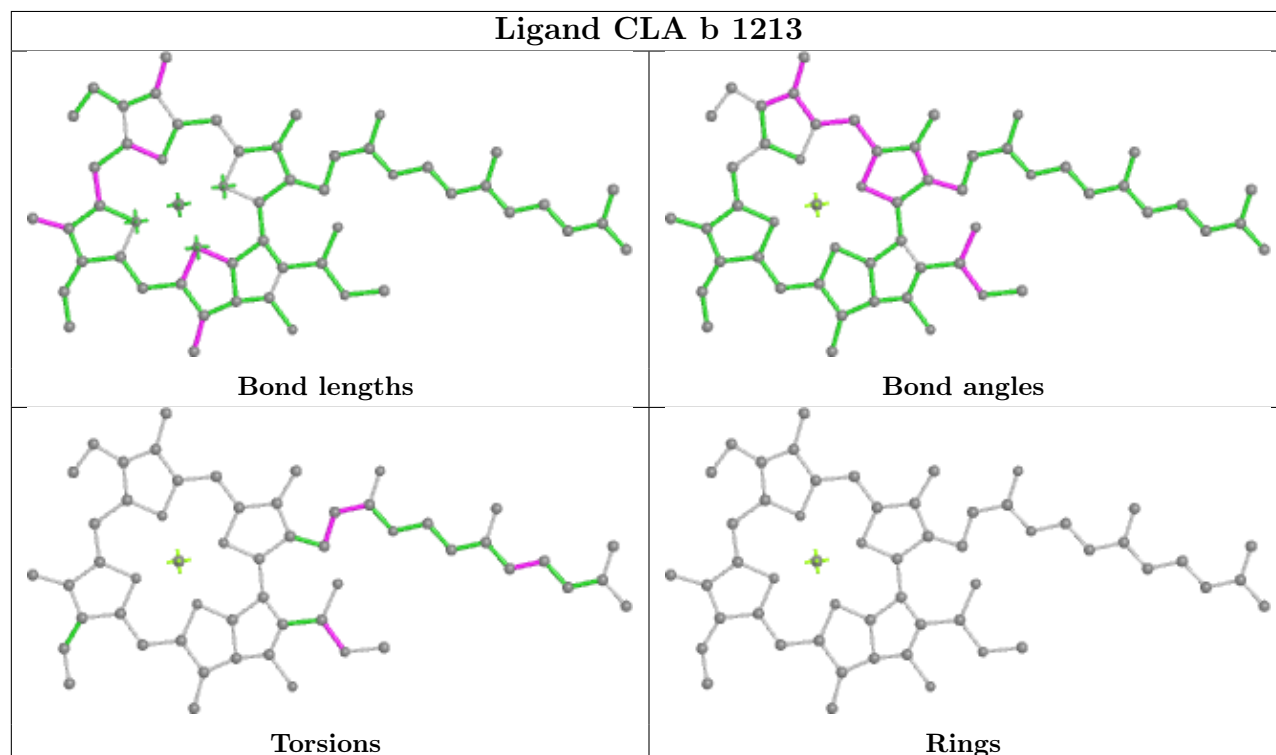


## Ligand CLA B 1232

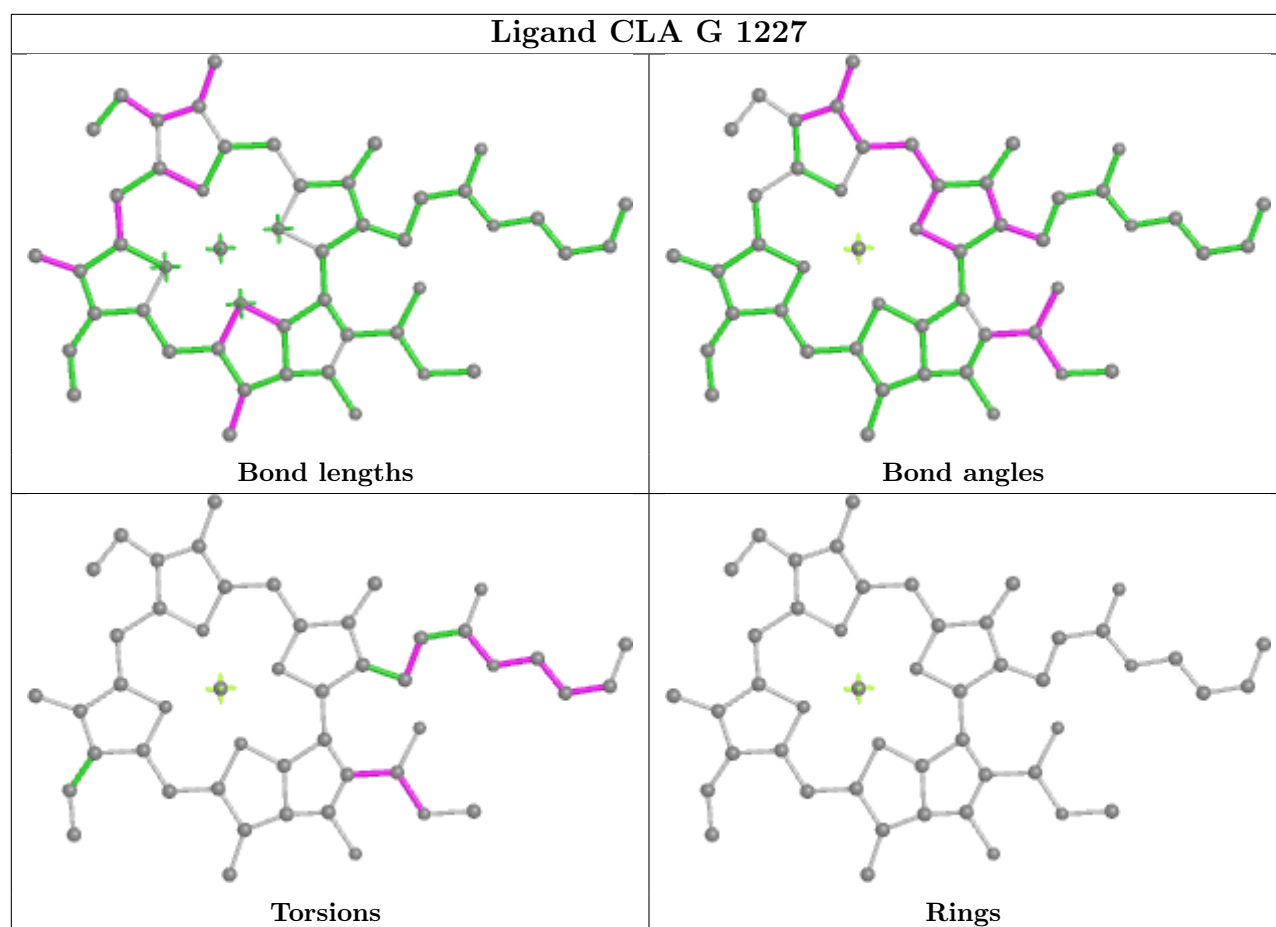


## Ligand CLA b 1224

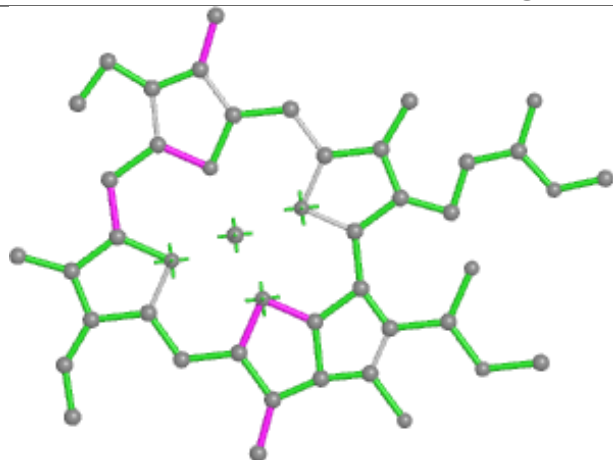


**Ligand CLA G 1202****Ligand BCR A 4001****Ligand CLA b 1213**

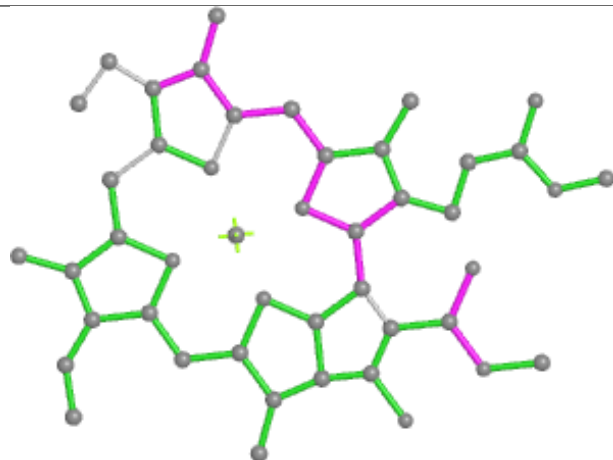




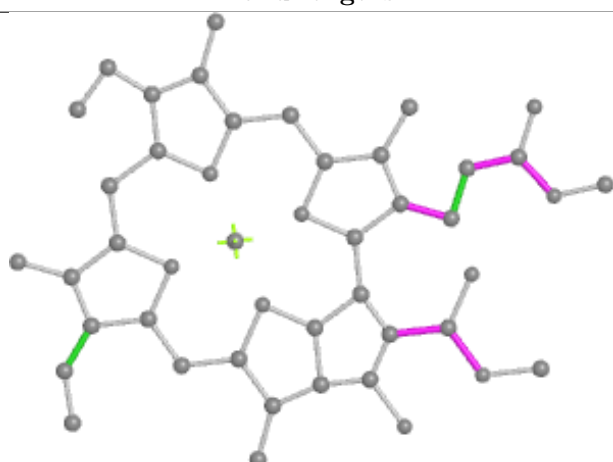
## Ligand CLA o 516



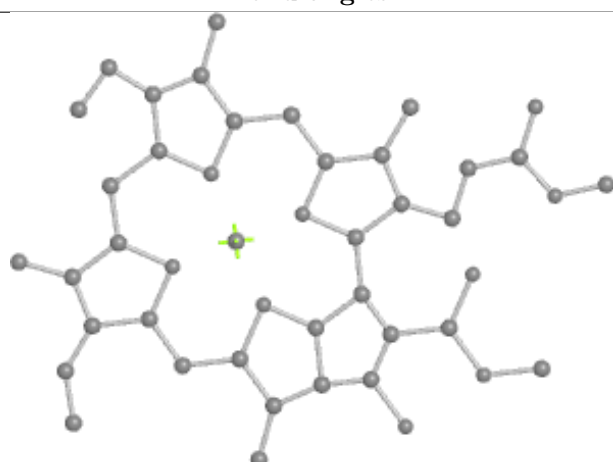
Bond lengths



Bond angles

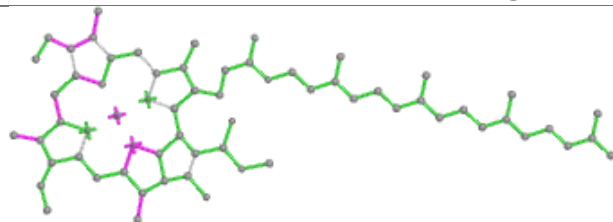


Torsions

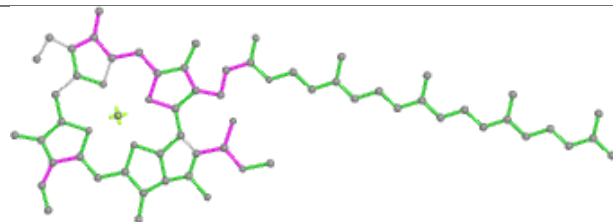


Rings

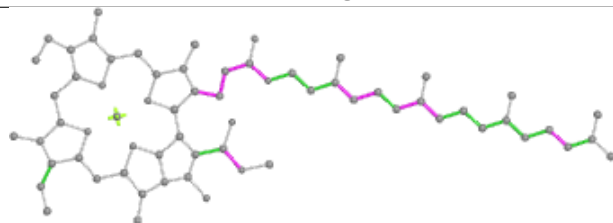
## Ligand CLA A 1237



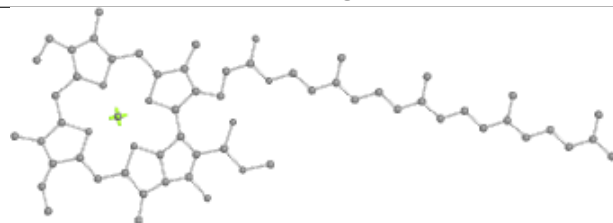
Bond lengths



Bond angles

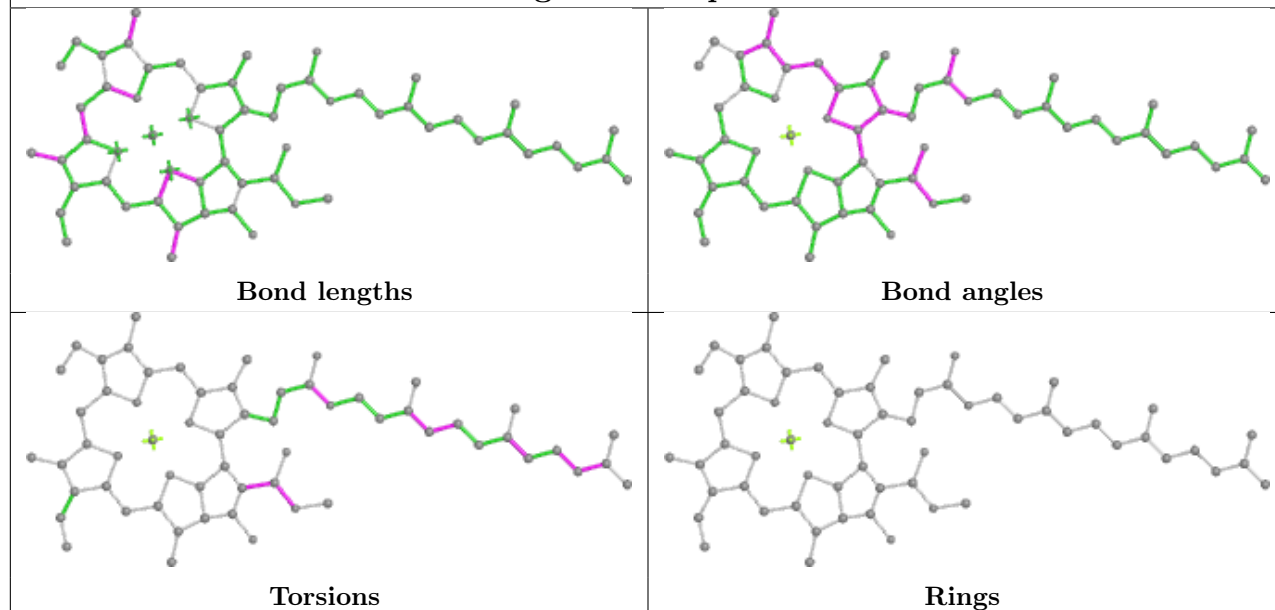


Torsions

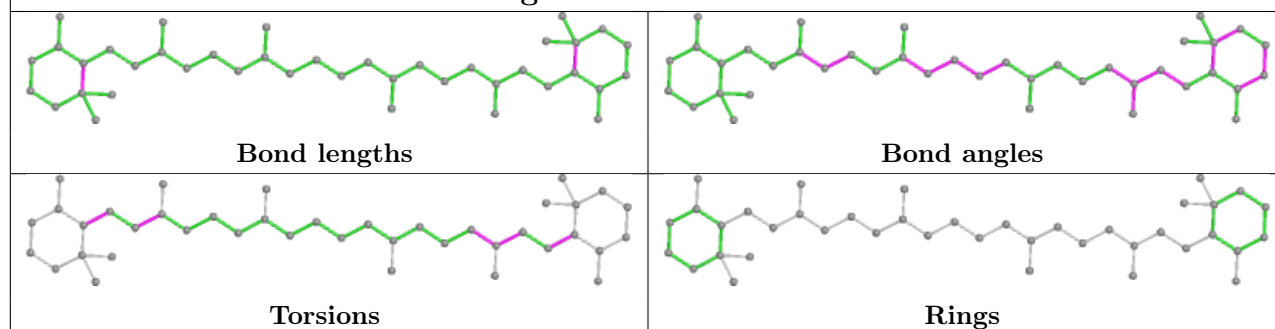


Rings

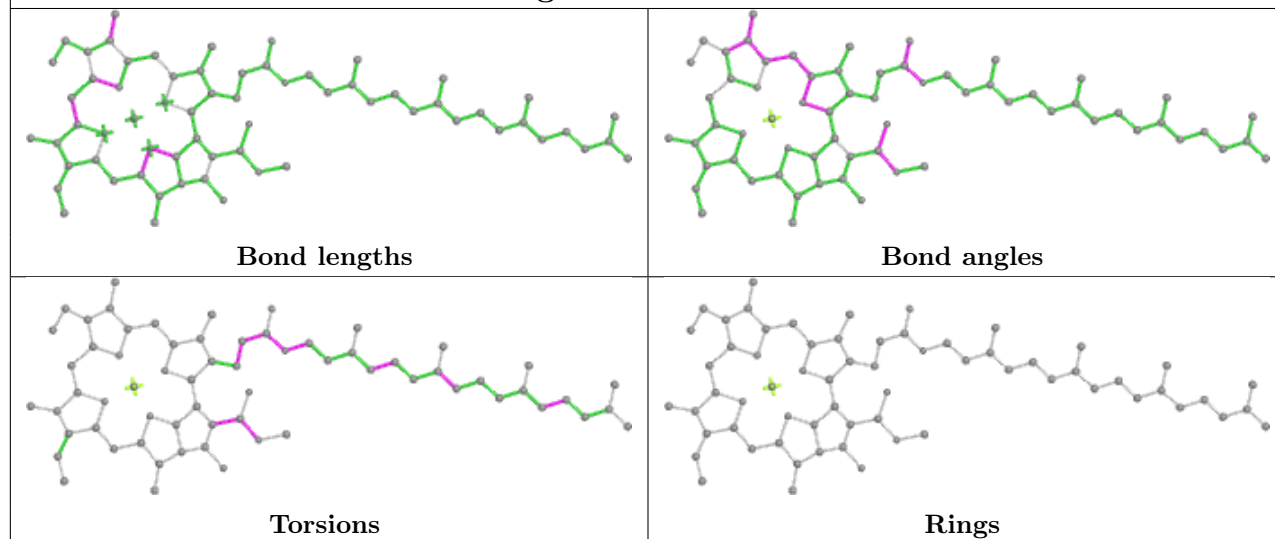
## Ligand CLA p 509



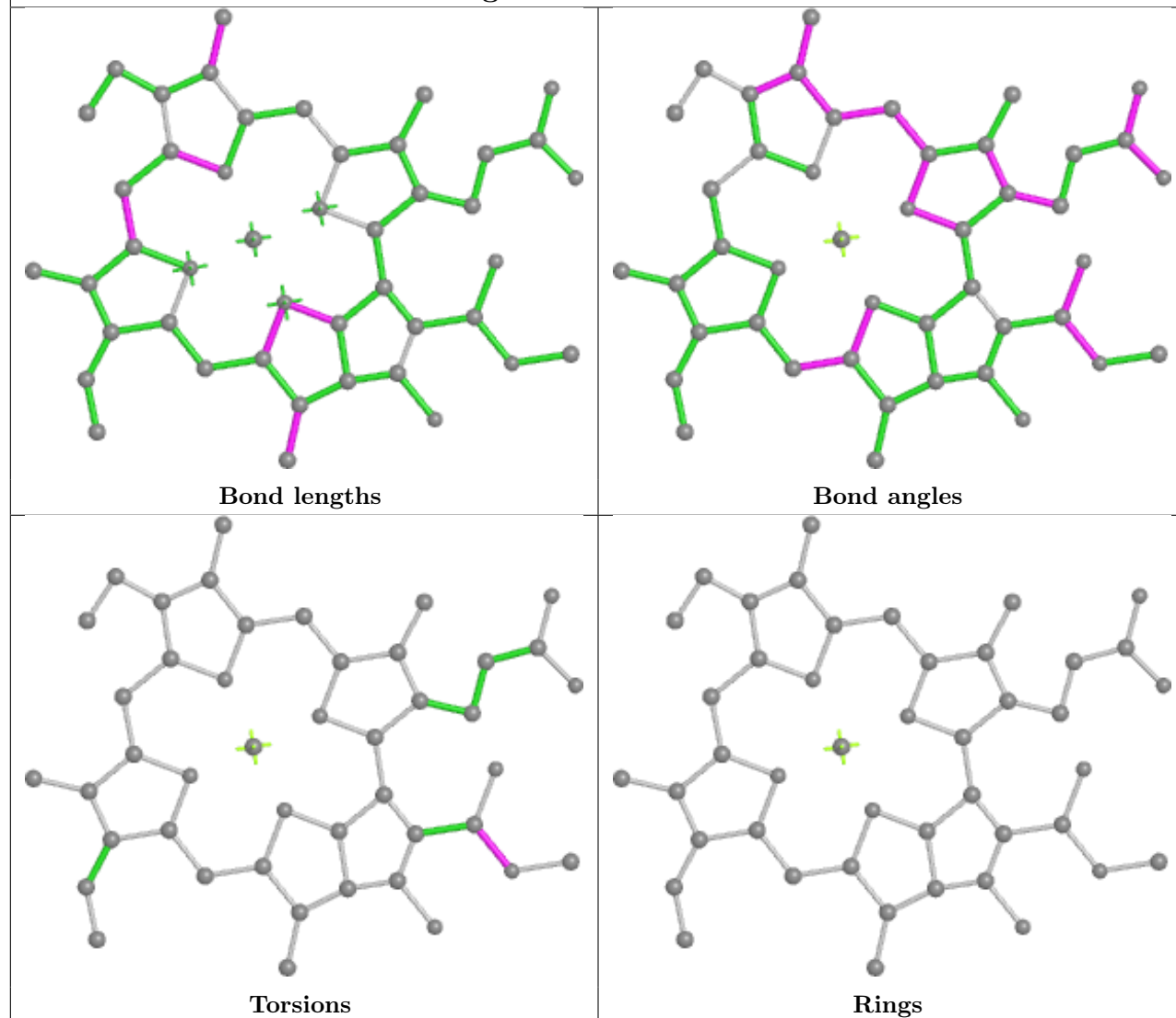
## Ligand BCR B 4005



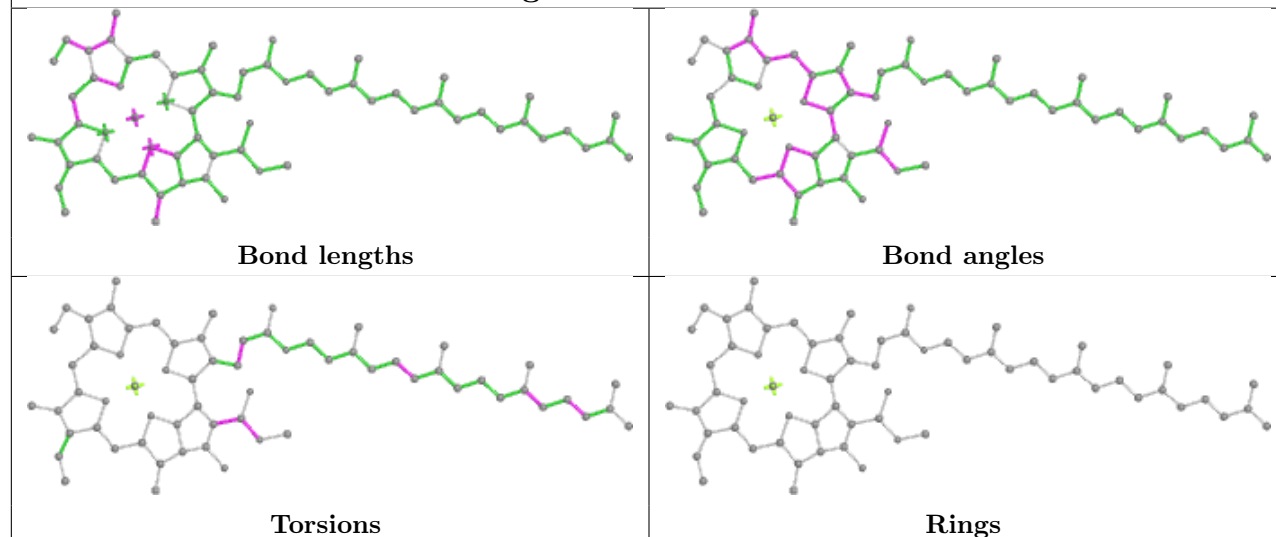
## Ligand CLA r 511

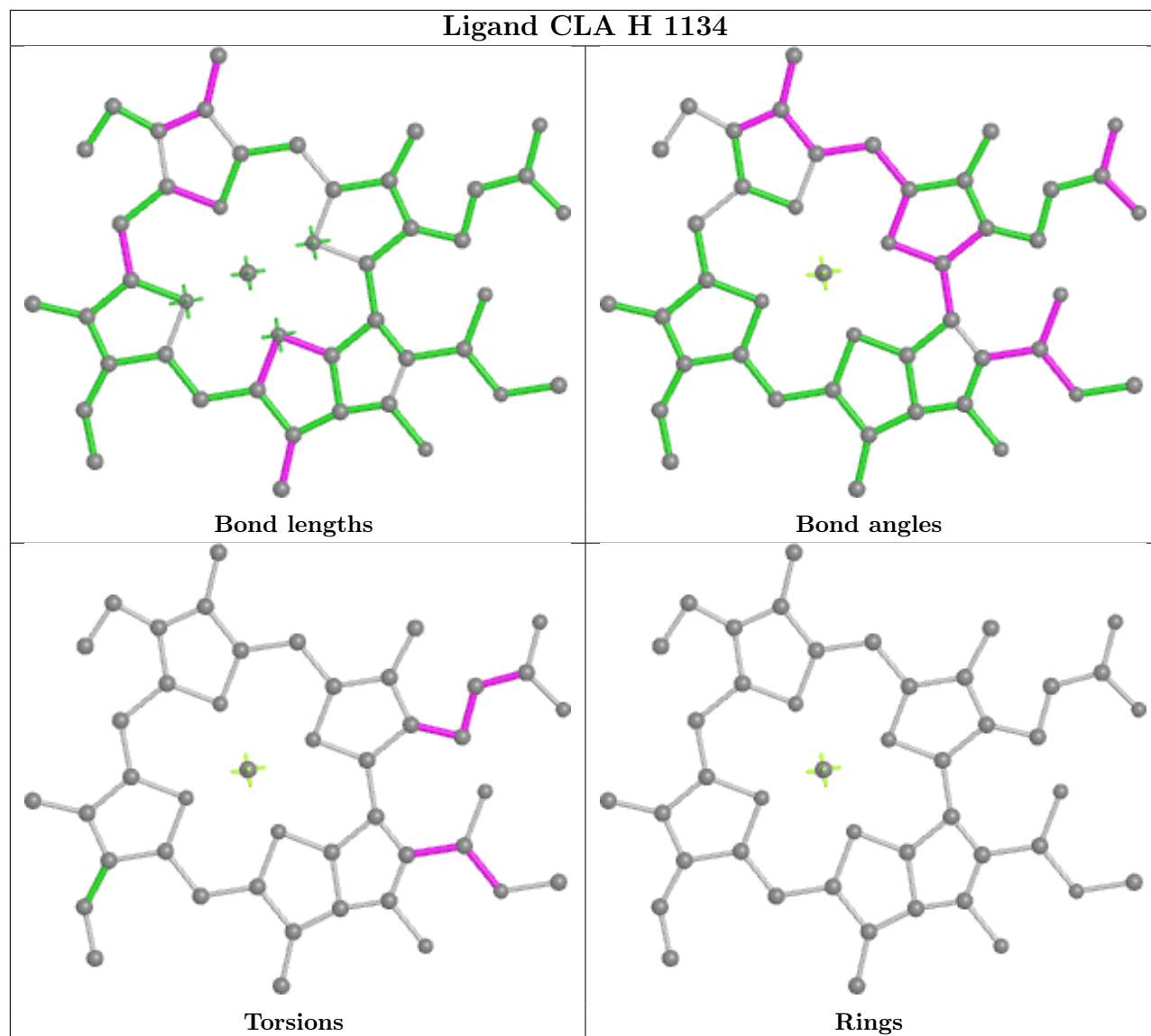
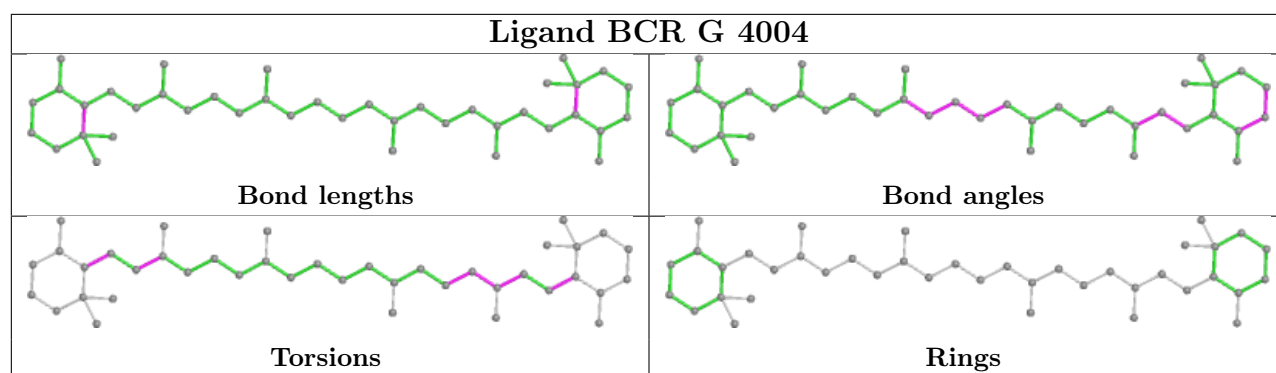


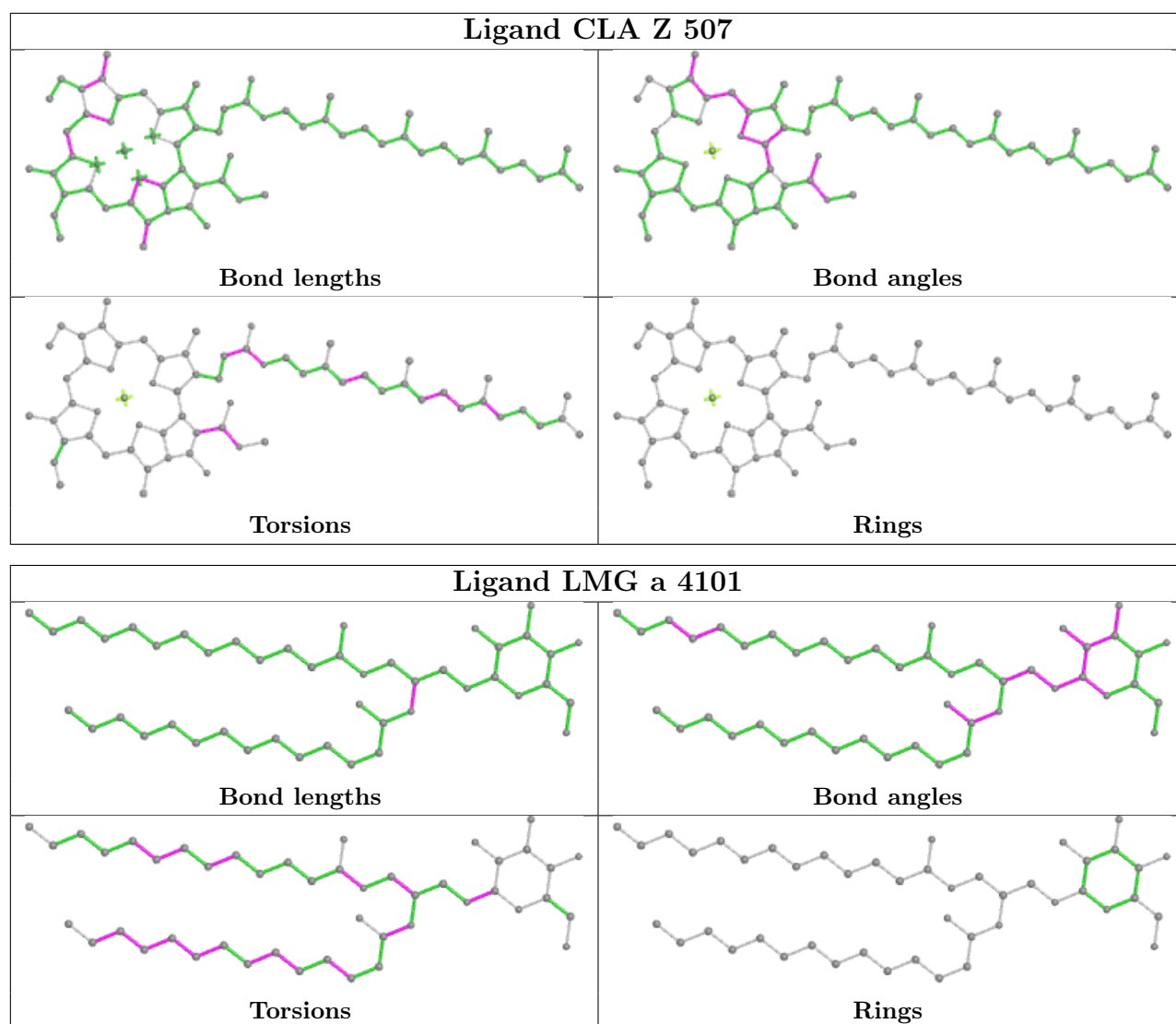
## Ligand CLA B 1208



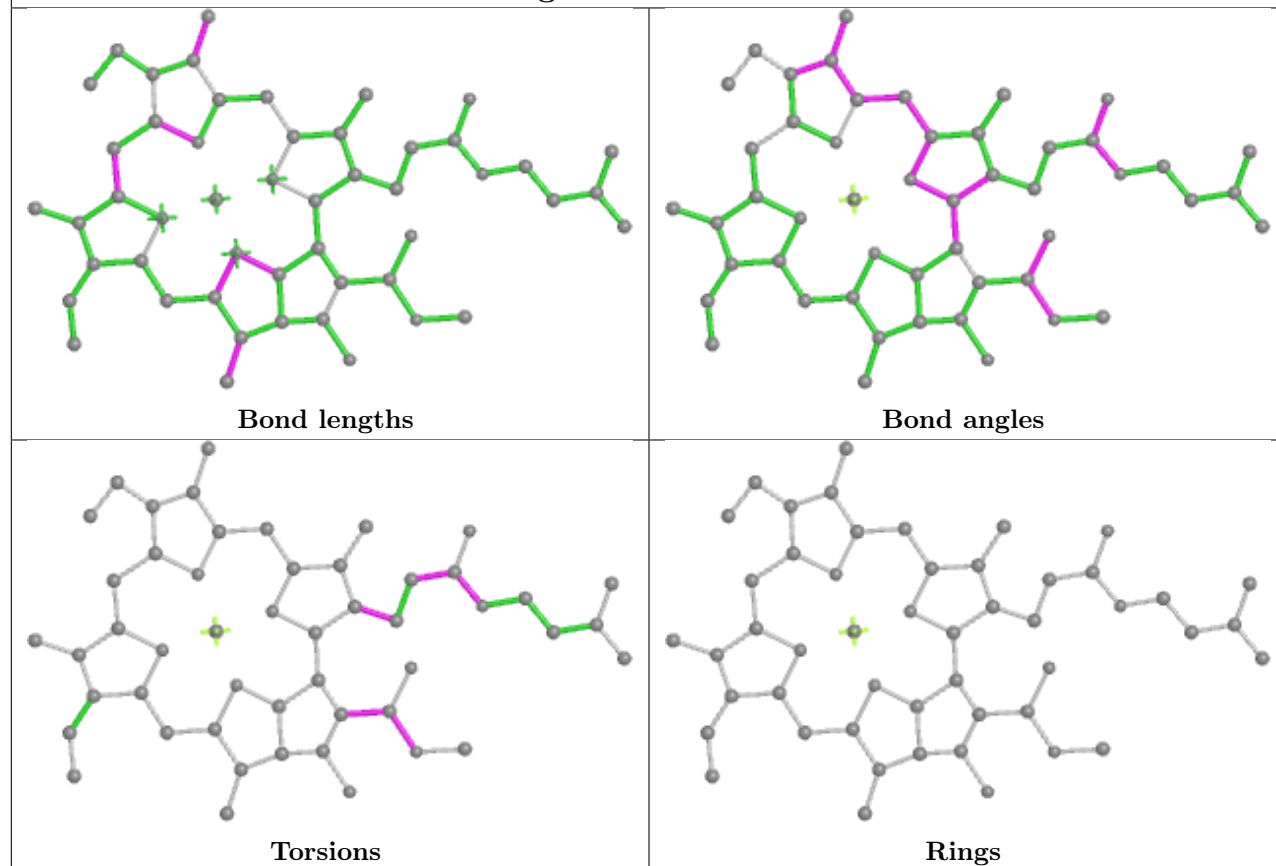
## Ligand CLA H 1022



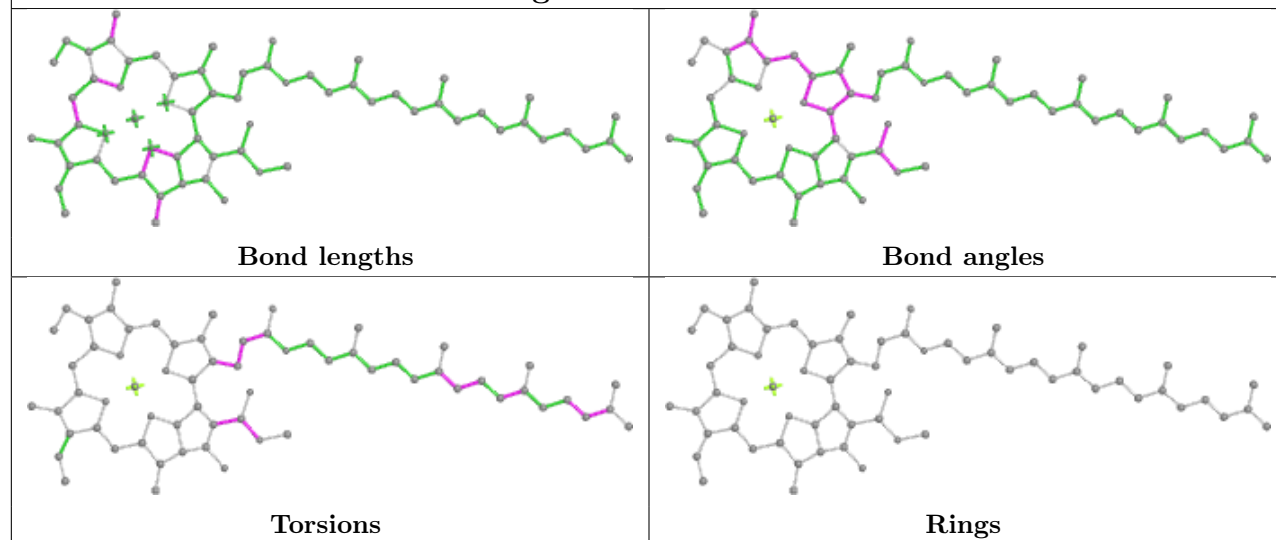


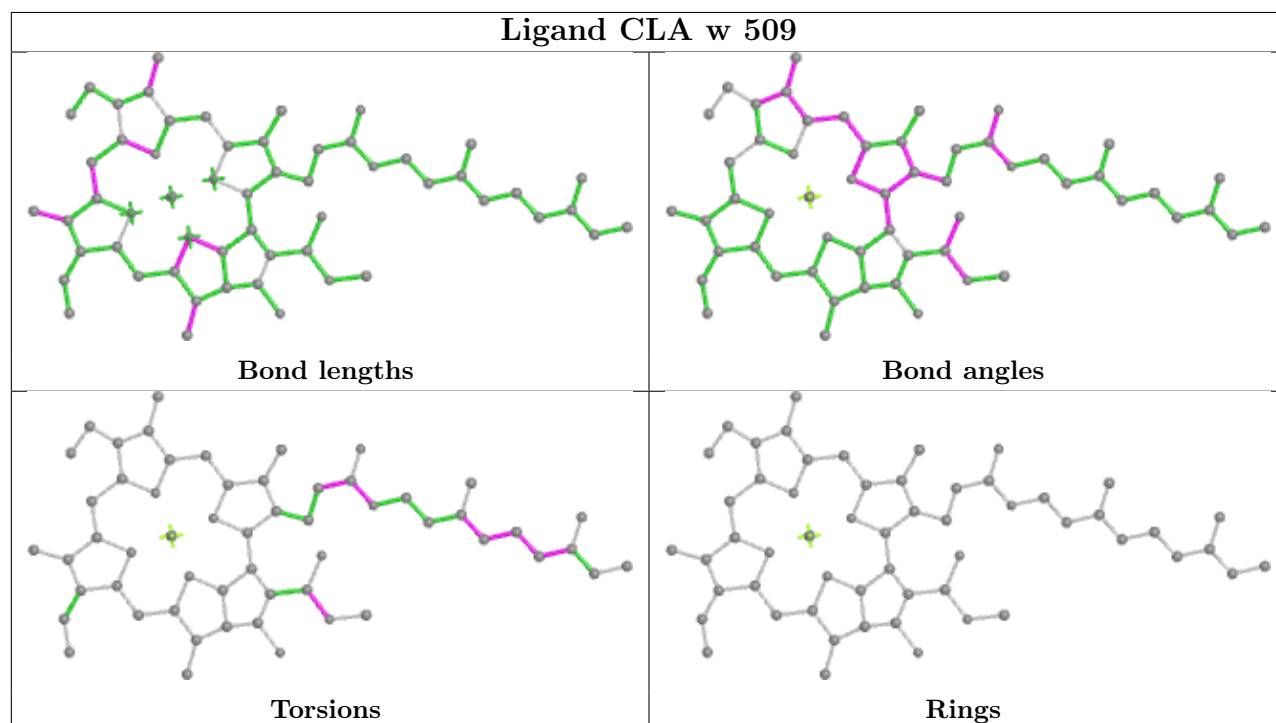
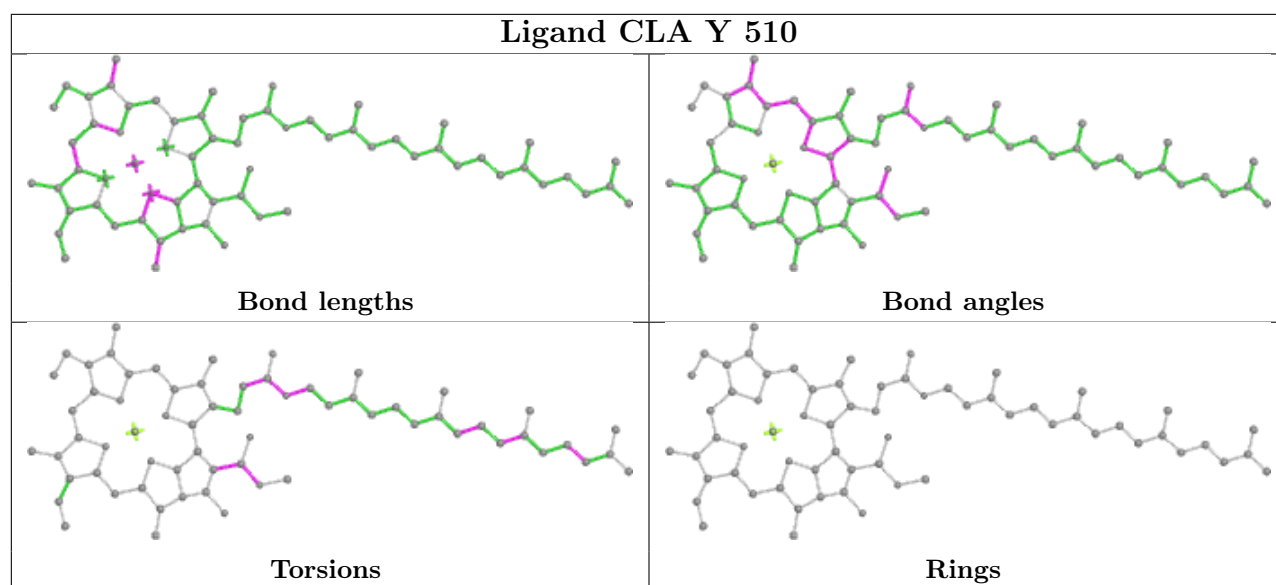


## Ligand CLA r 513

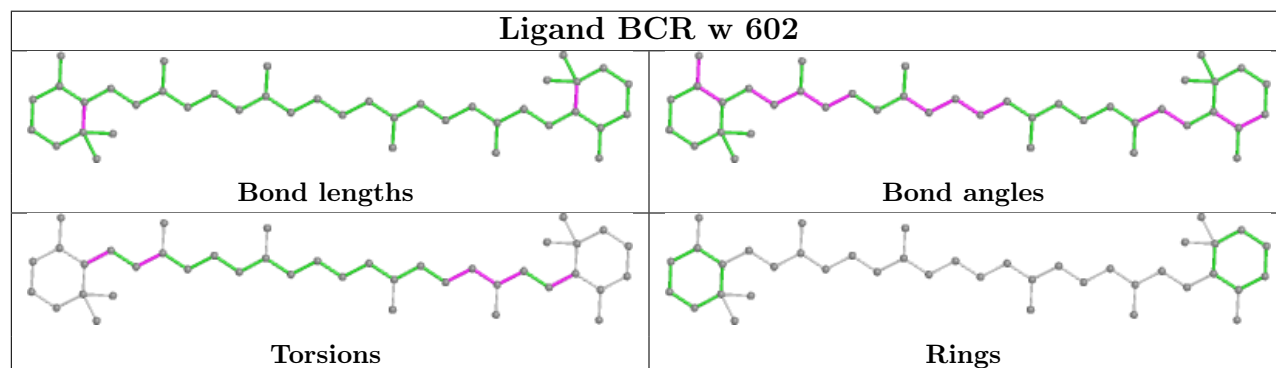
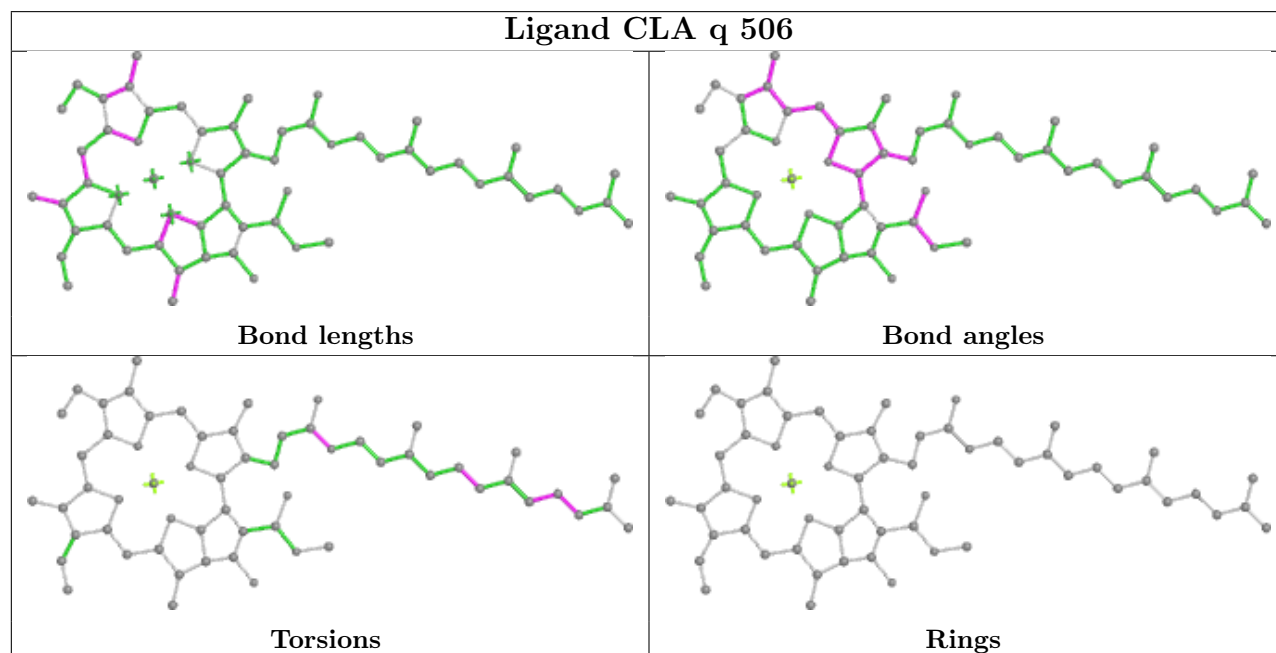
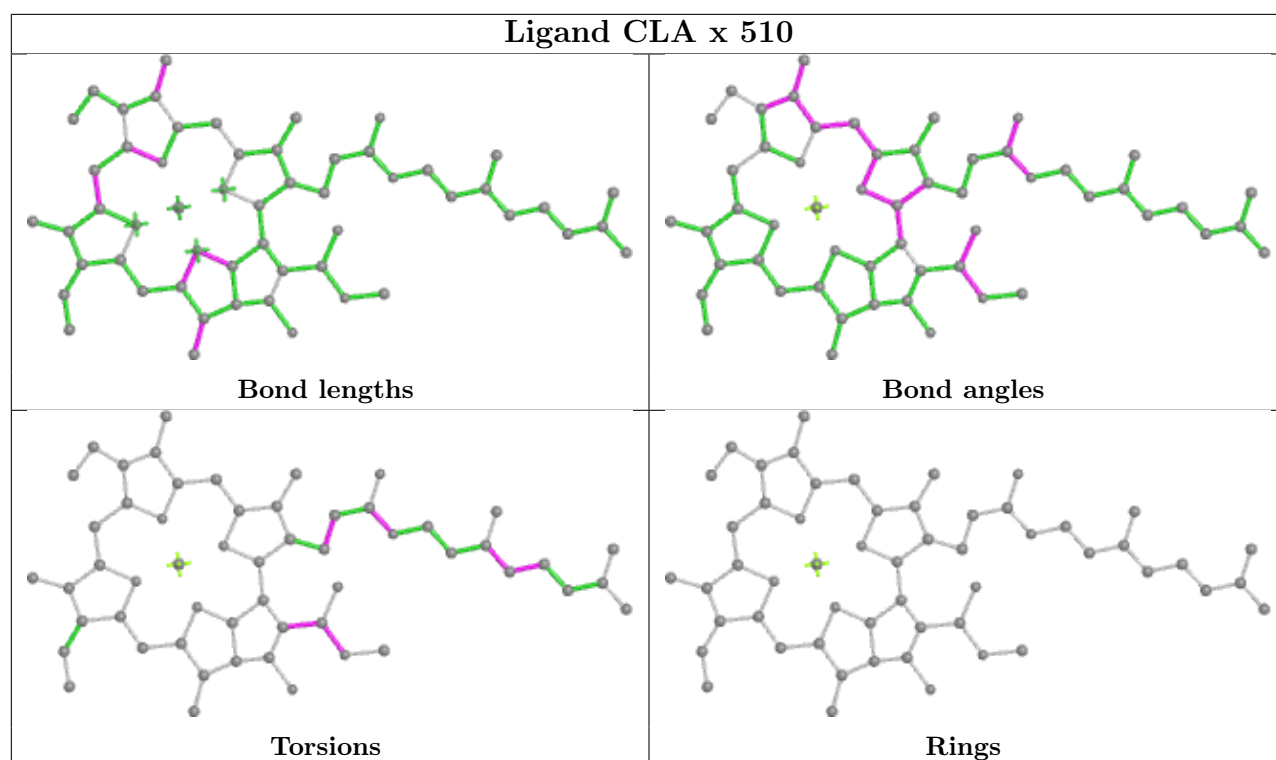


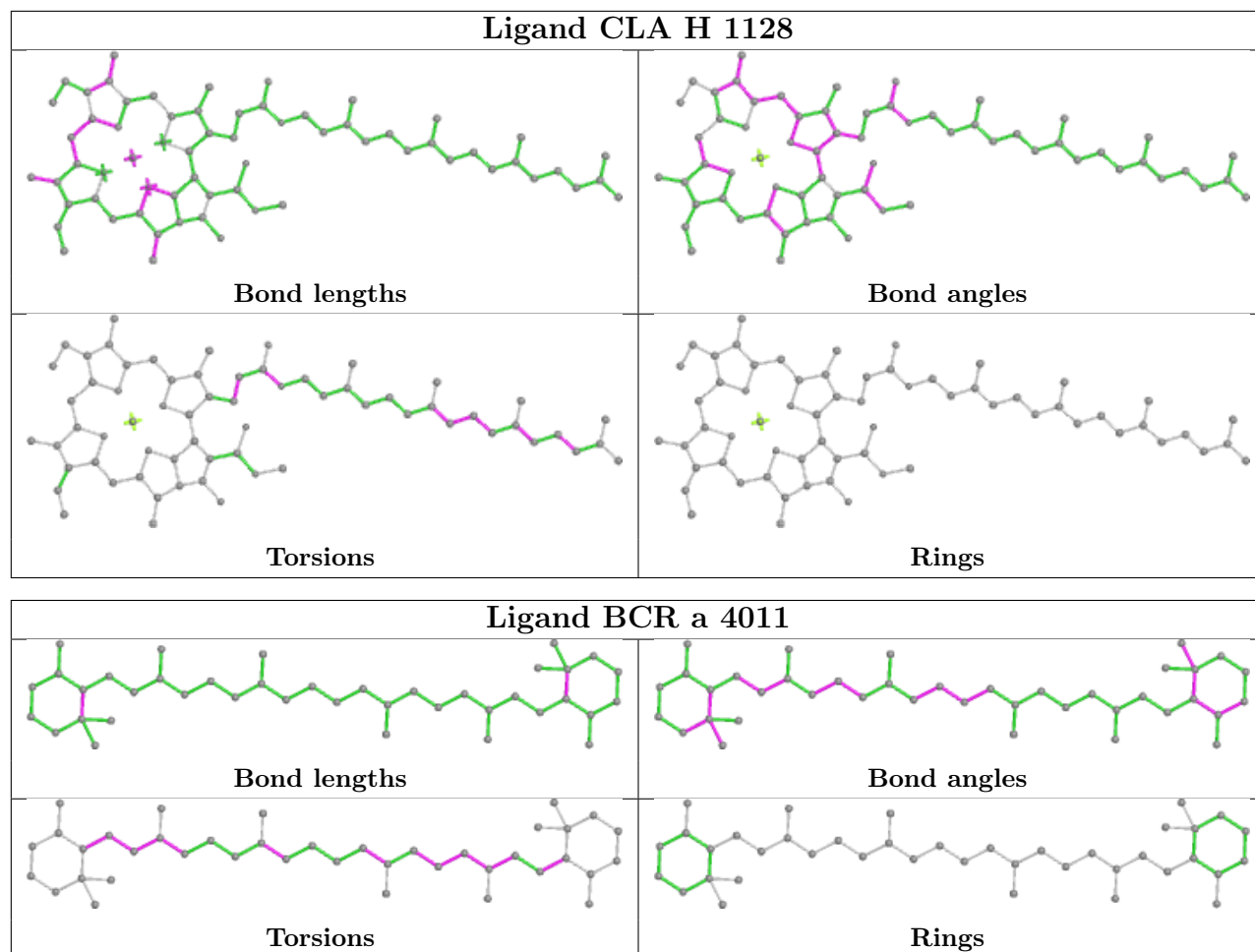
## Ligand CLA w 505



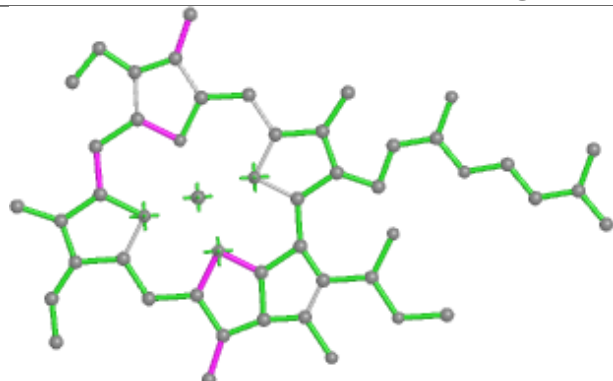




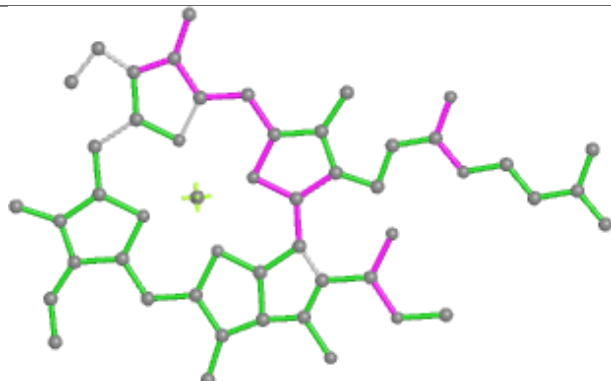




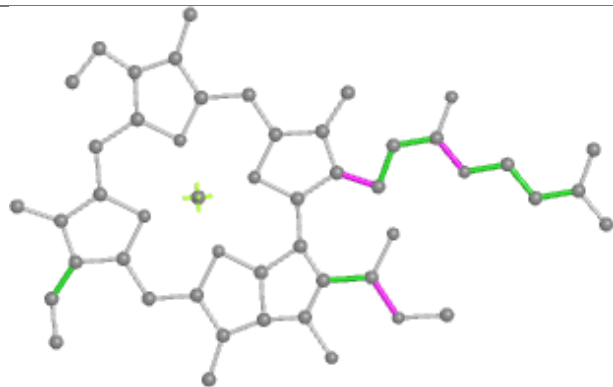
## Ligand CLA X 514



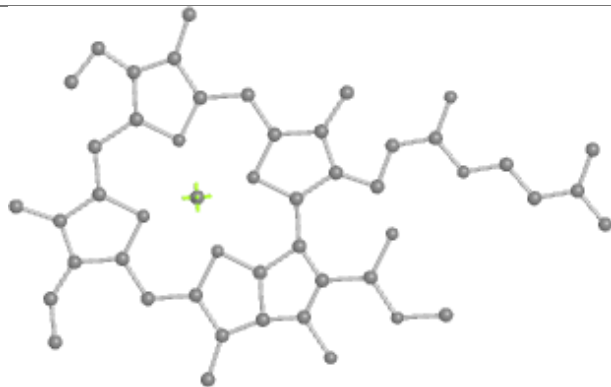
Bond lengths



Bond angles

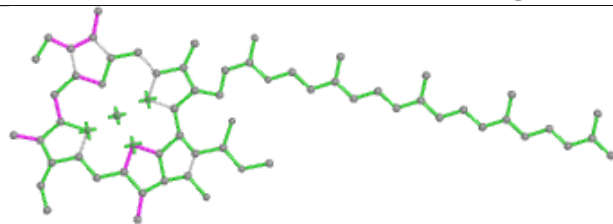


Torsions

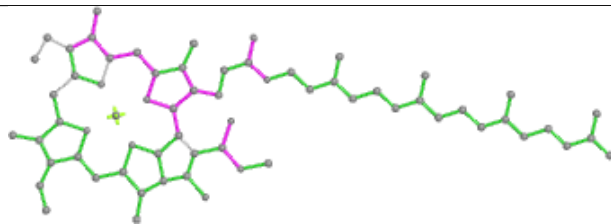


Rings

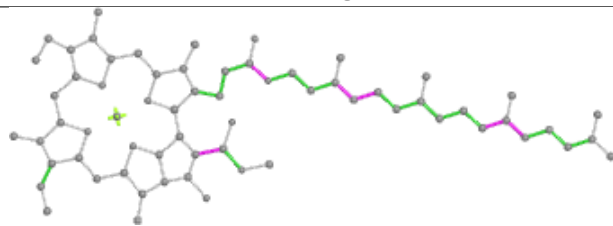
## Ligand CLA a 1138



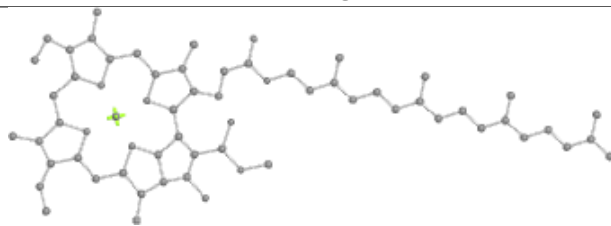
Bond lengths



Bond angles

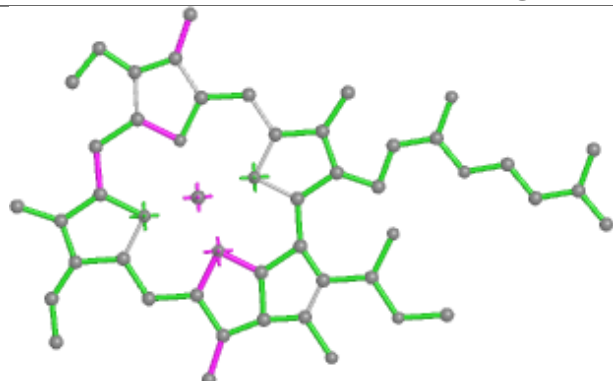


Torsions

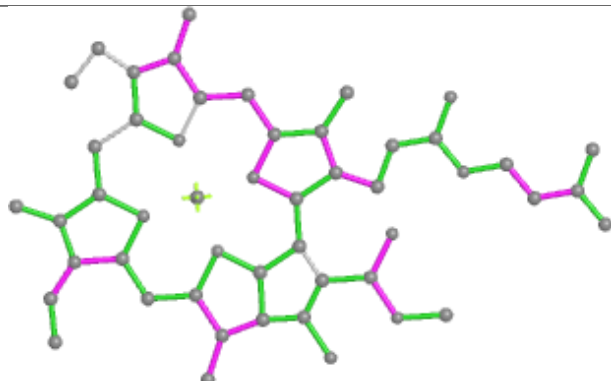


Rings

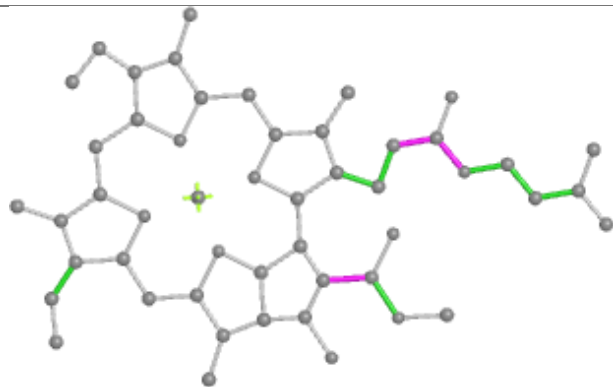
## Ligand CLA Y 502



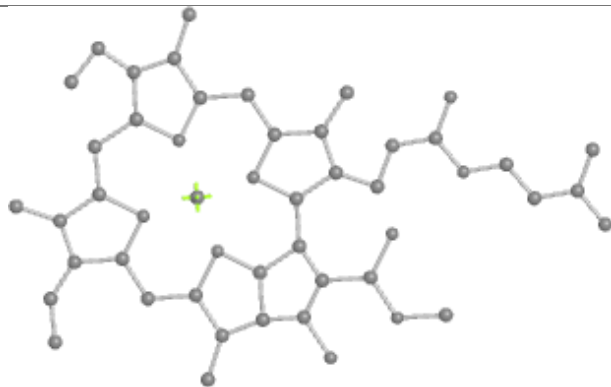
Bond lengths



Bond angles

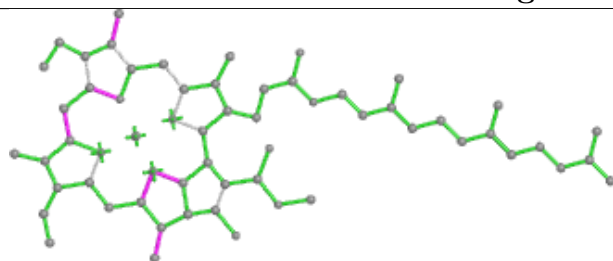


Torsions

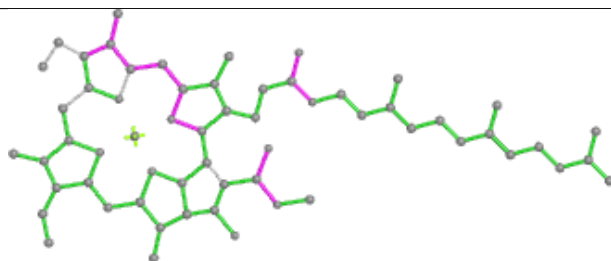


Rings

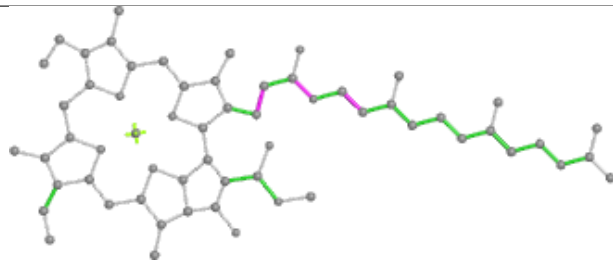
## Ligand CLA h 515



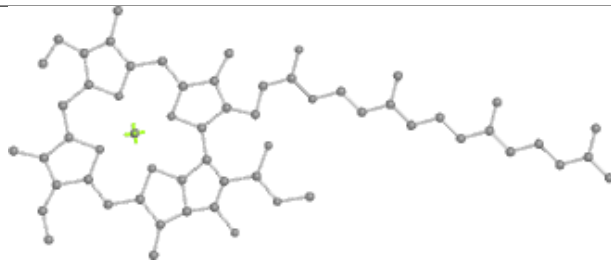
Bond lengths



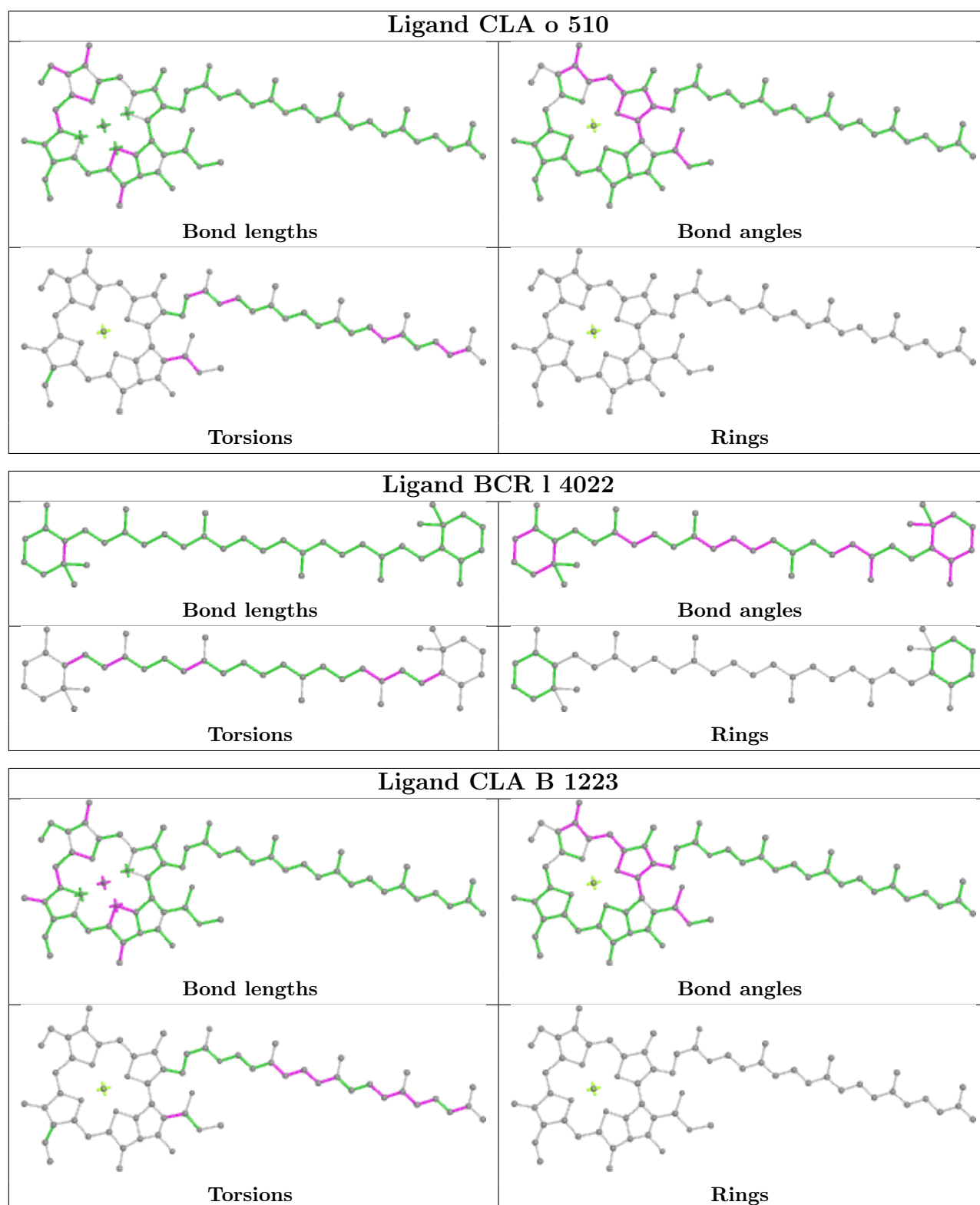
Bond angles



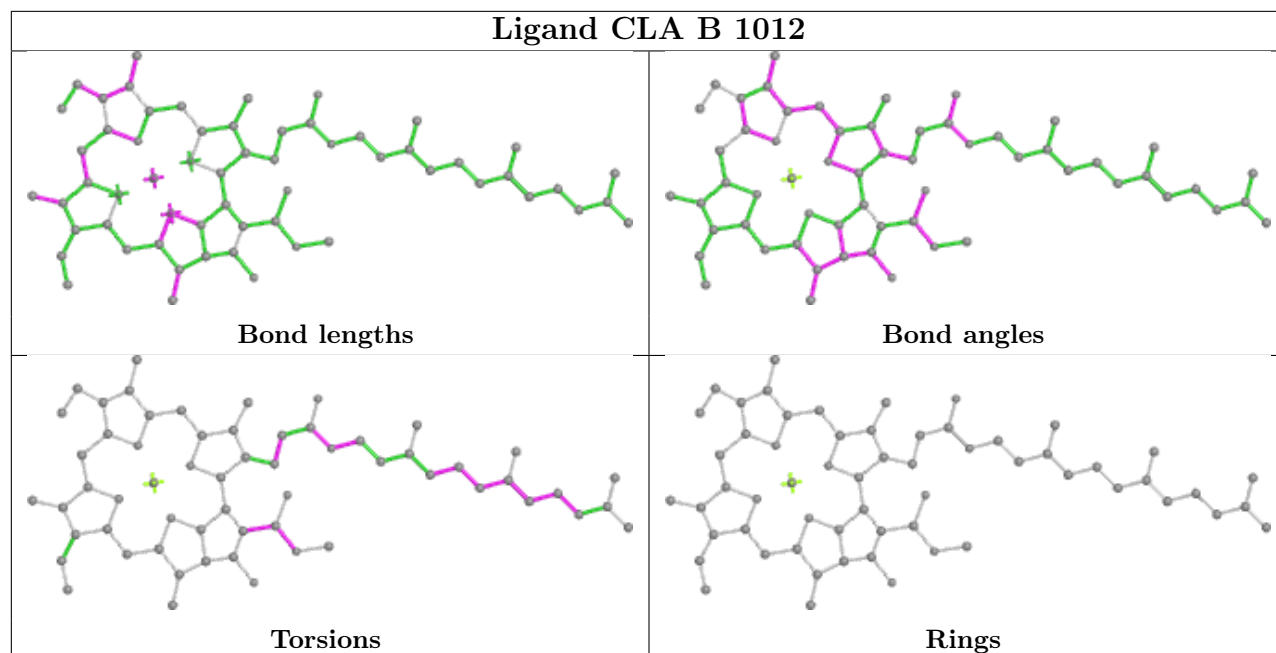
Torsions



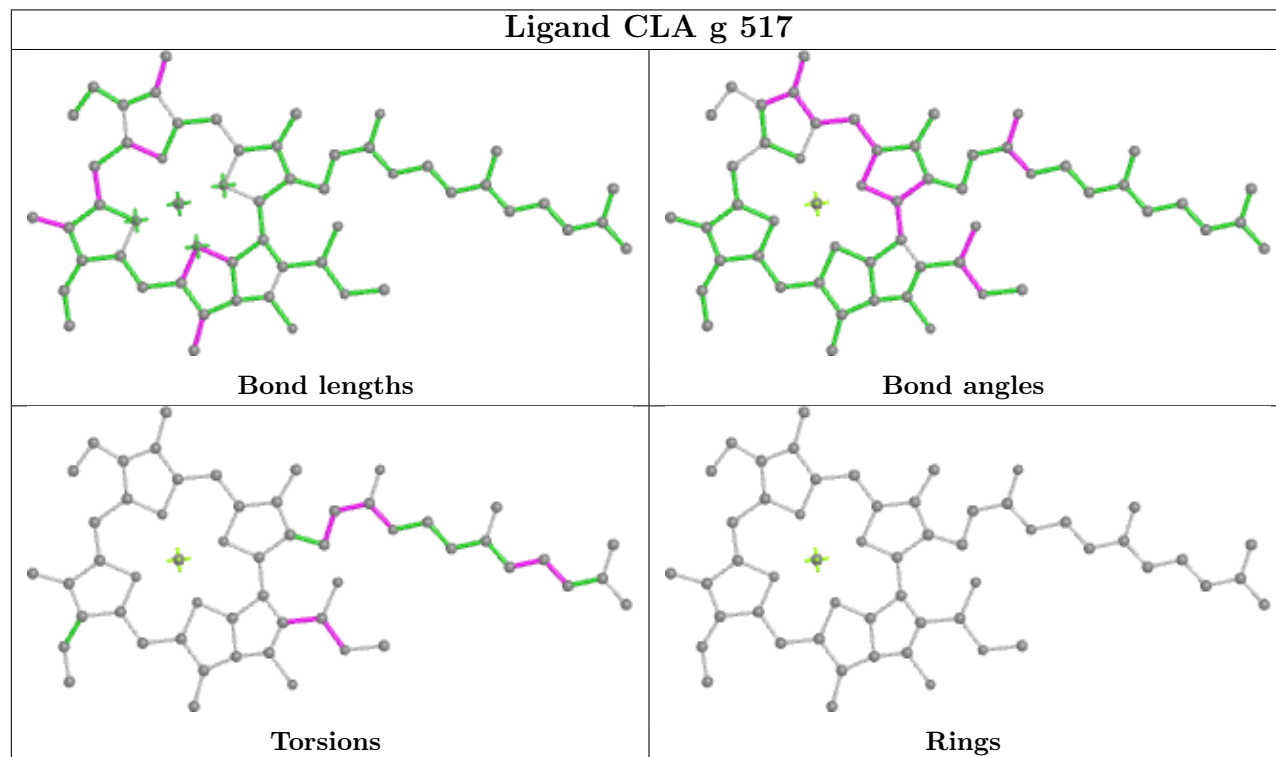
Rings



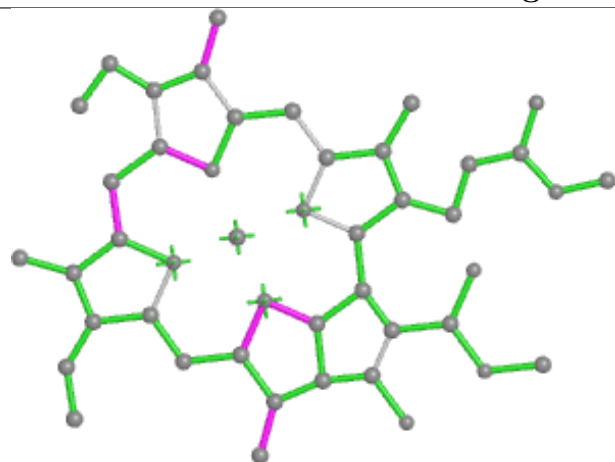
## Ligand CLA B 1012



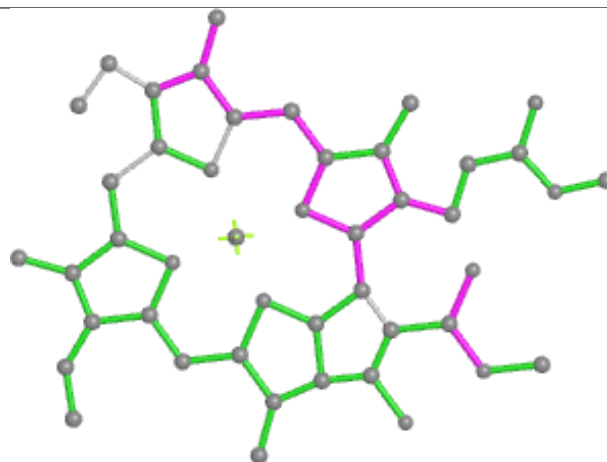
## Ligand CLA g 517



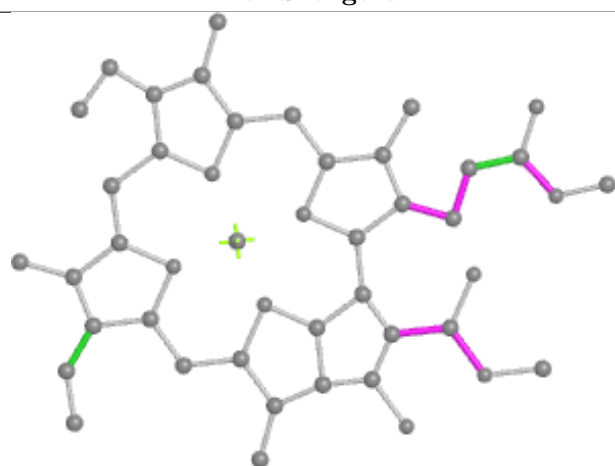
## Ligand CLA t 503



Bond lengths



Bond angles

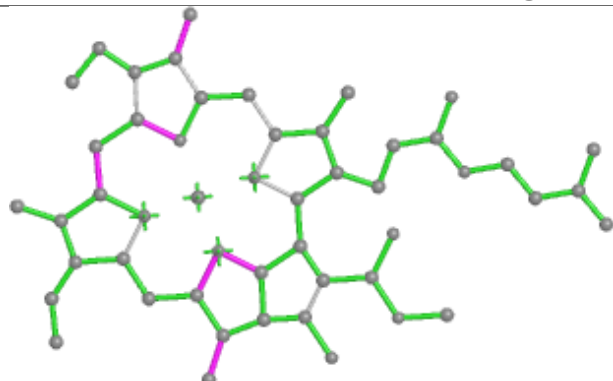


Torsions

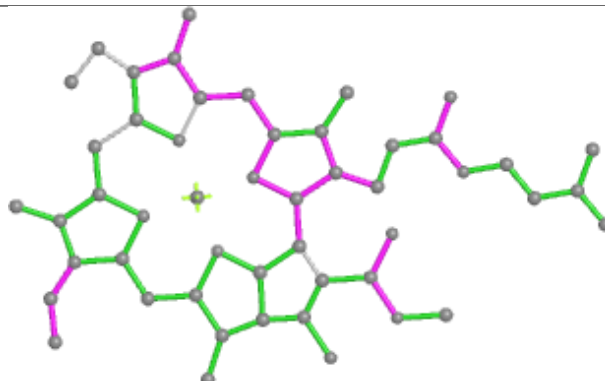


Rings

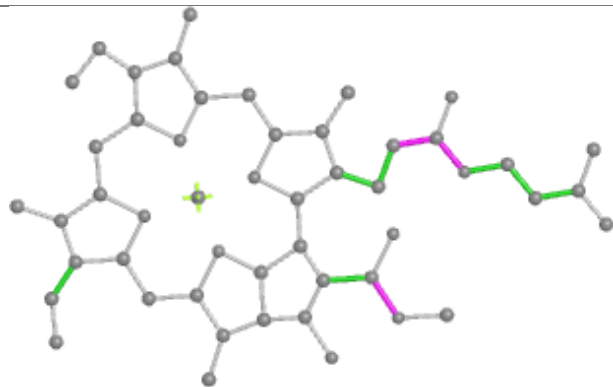
## Ligand CLA t 502



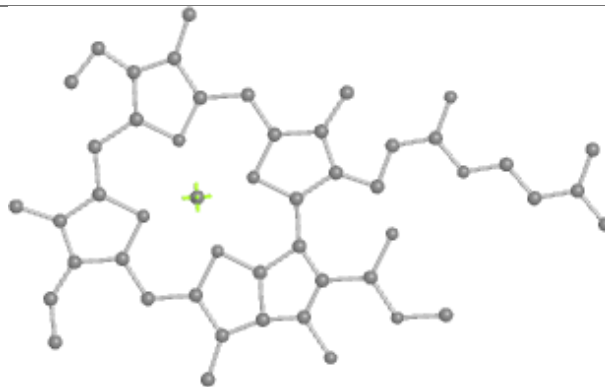
Bond lengths



Bond angles

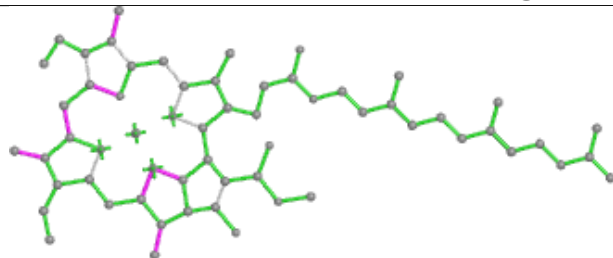


Torsions

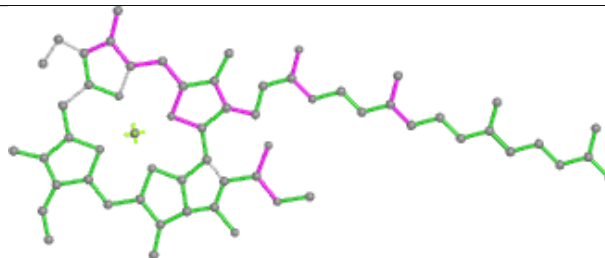


Rings

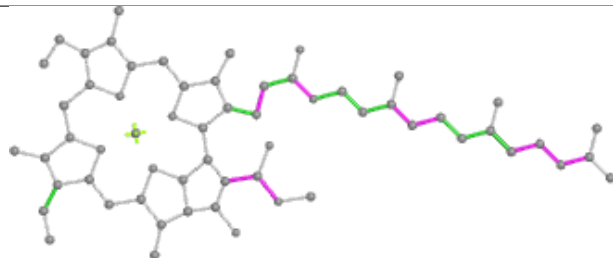
## Ligand CLA x 506



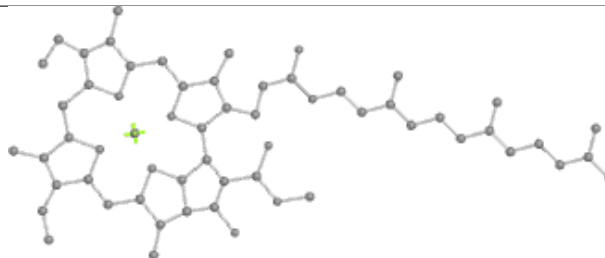
Bond lengths



Bond angles

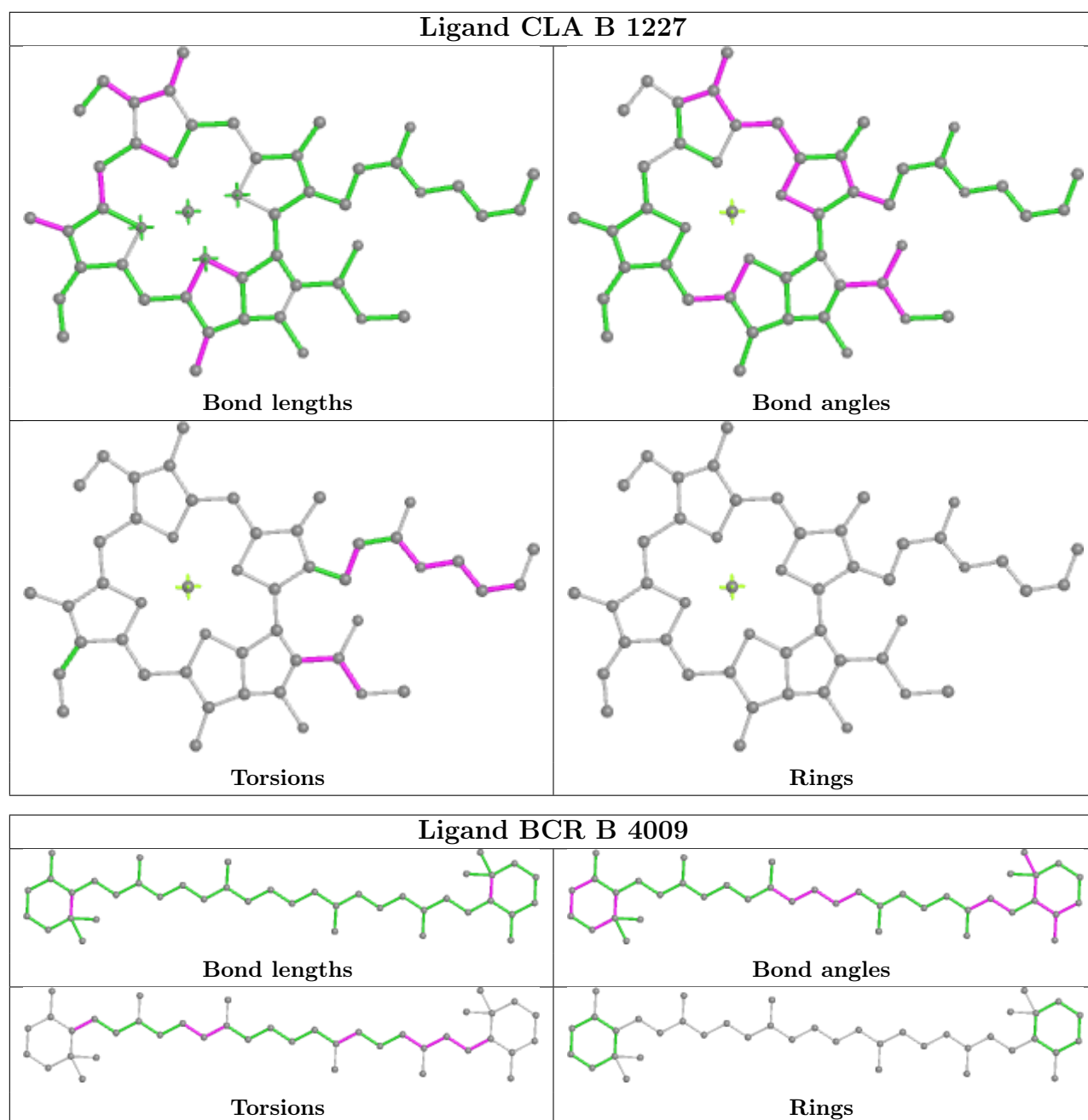


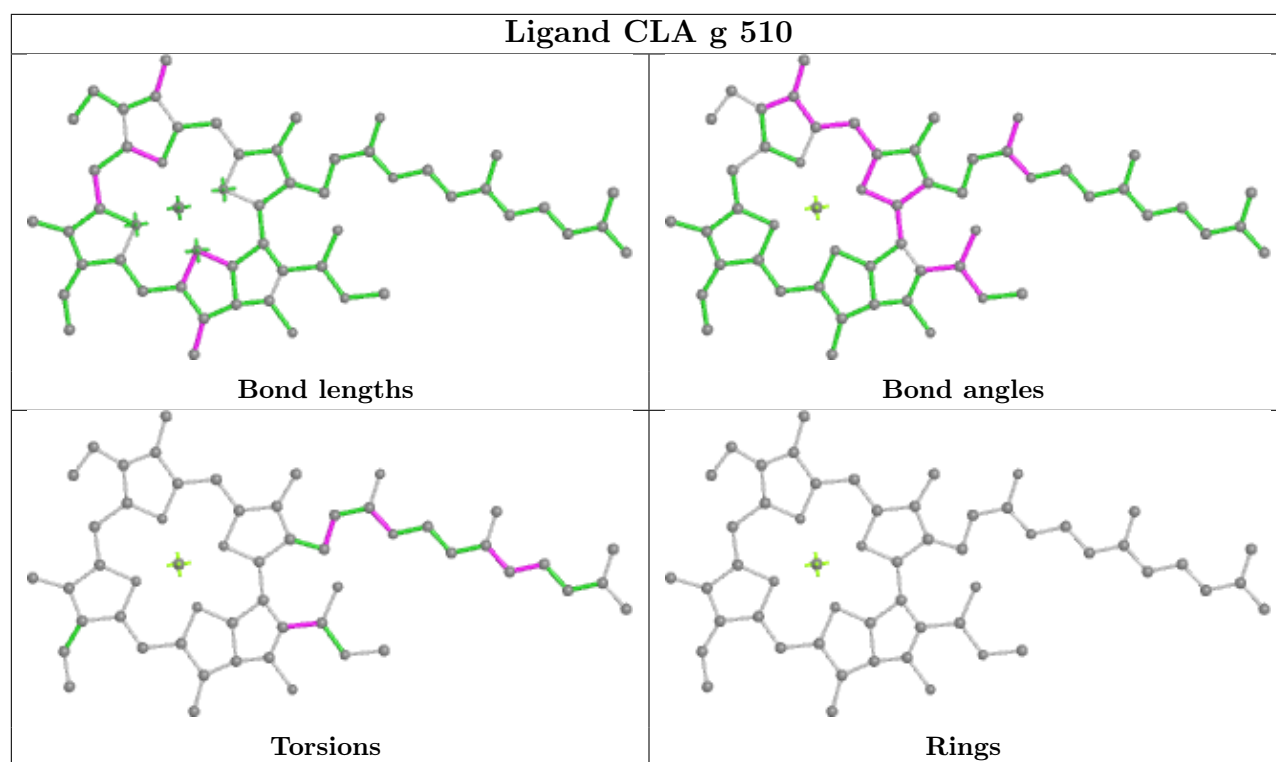
Torsions

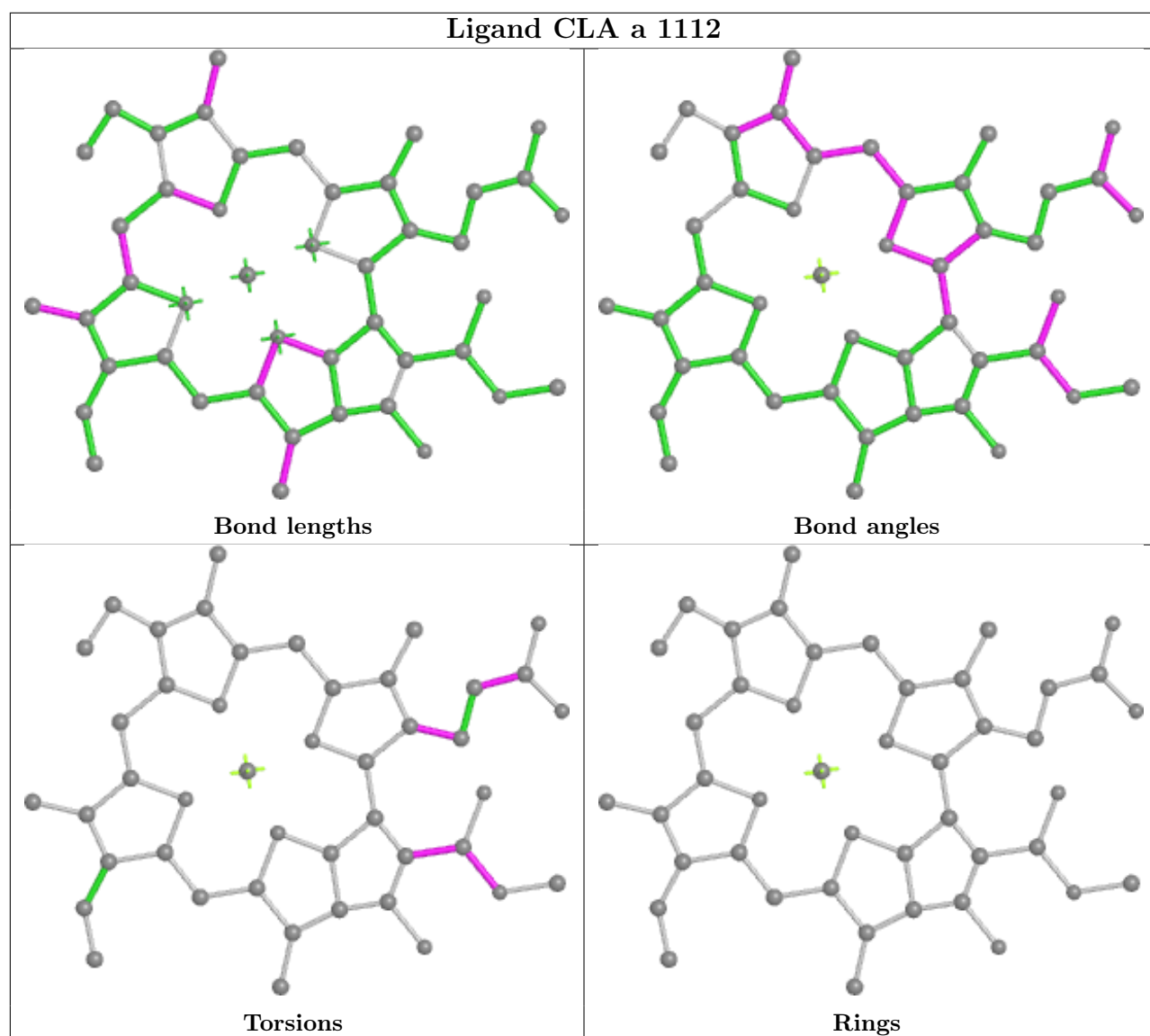


Rings

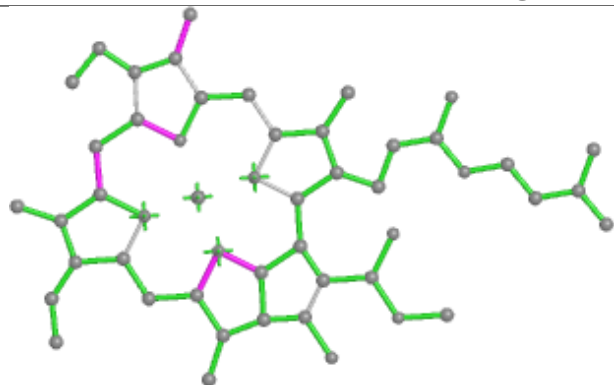




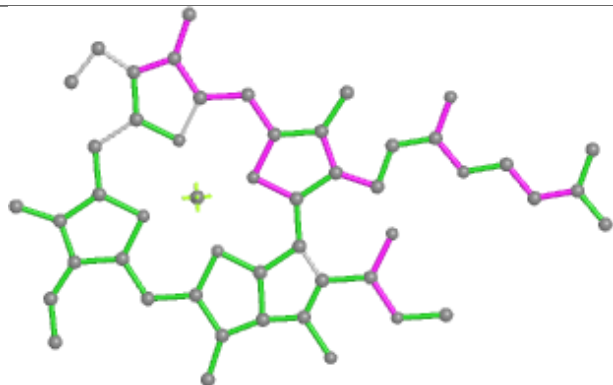




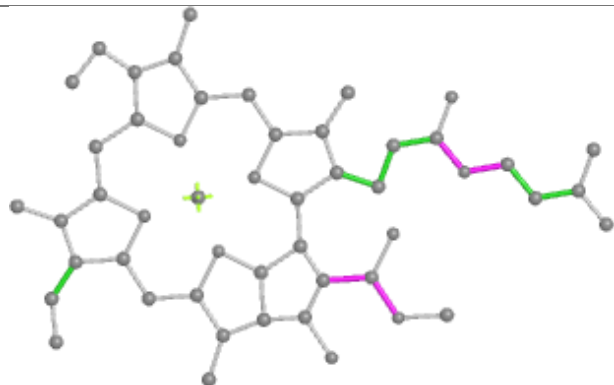
## Ligand CLA Y 501



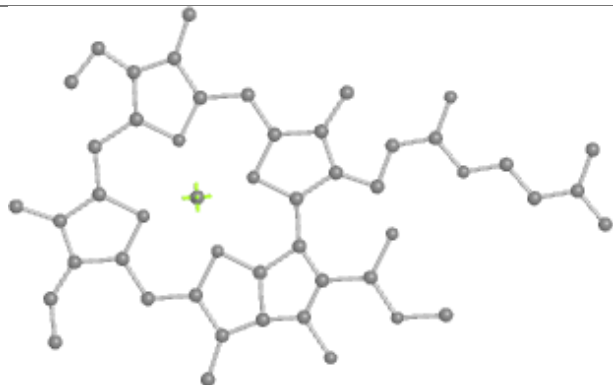
Bond lengths



Bond angles

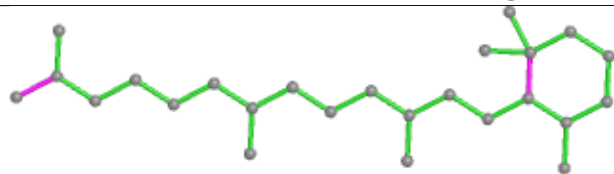


Torsions

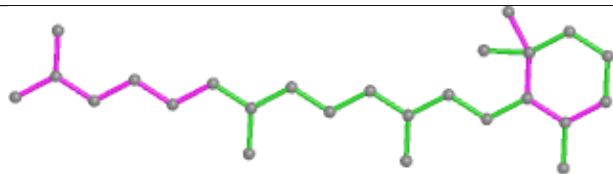


Rings

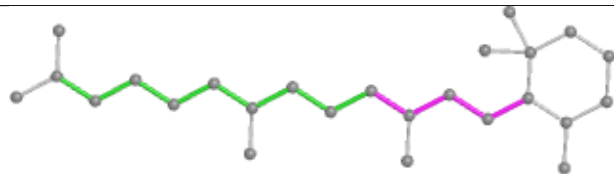
## Ligand BCR G 4006



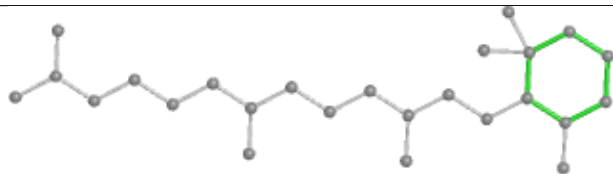
Bond lengths



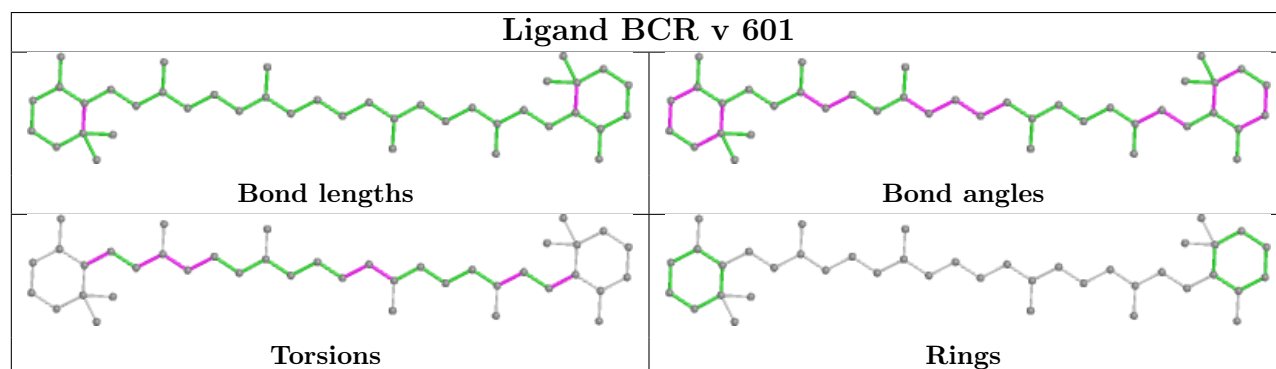
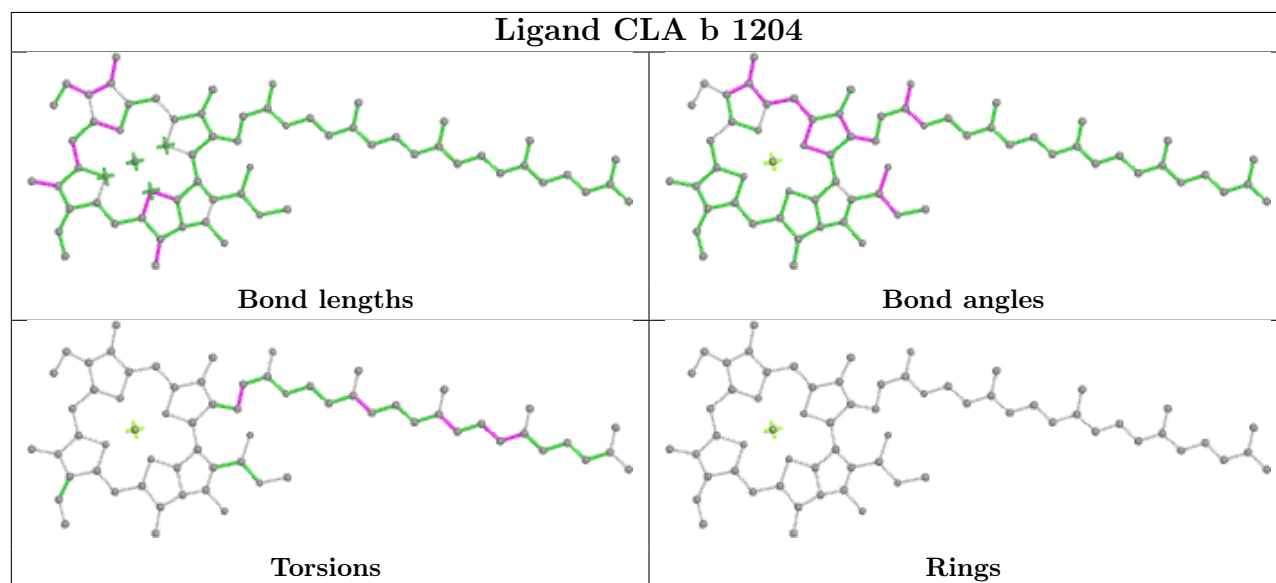
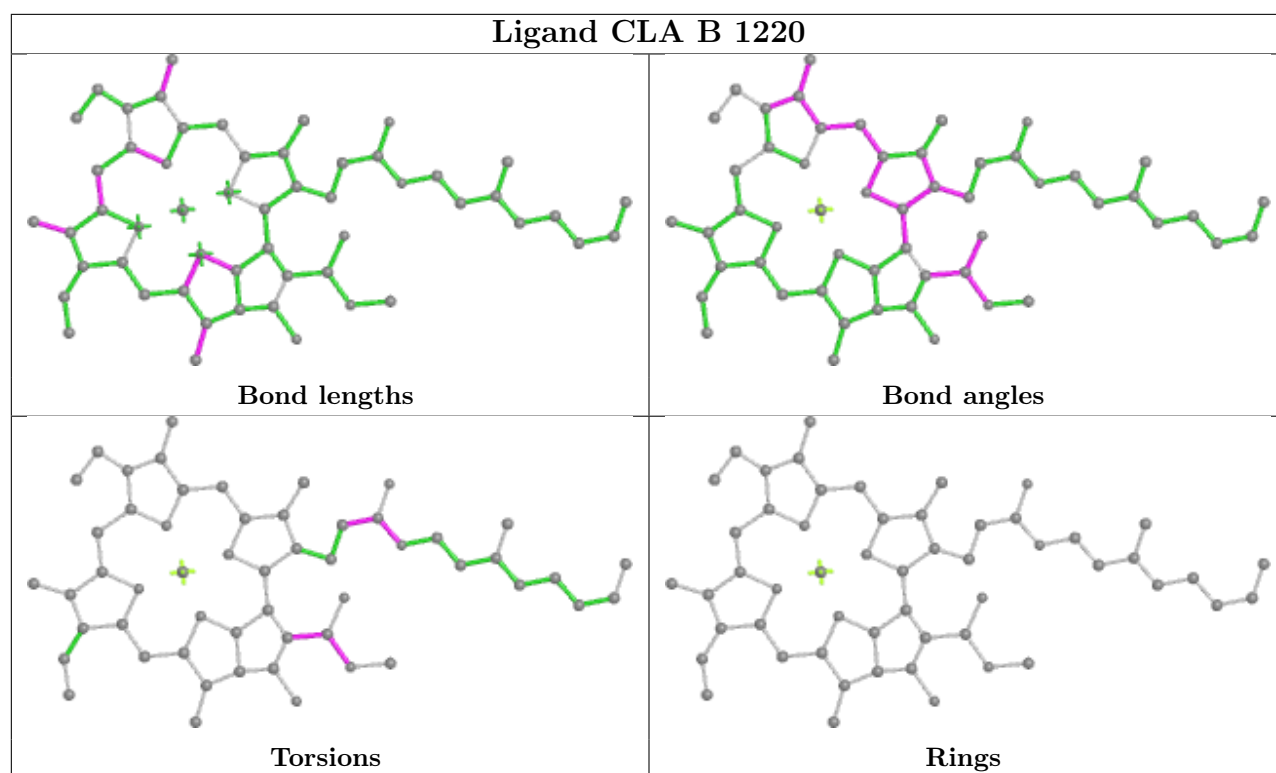
Bond angles

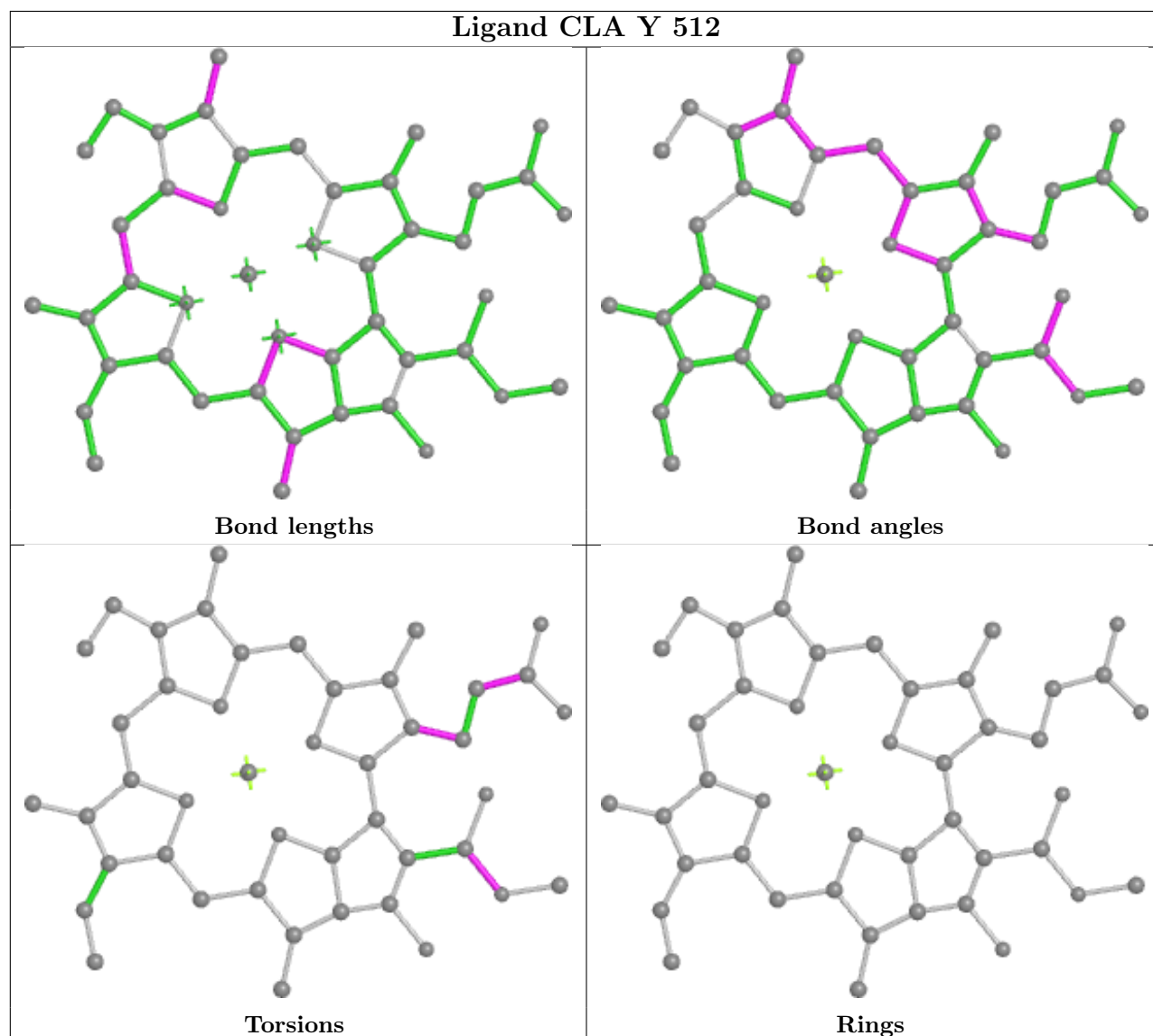
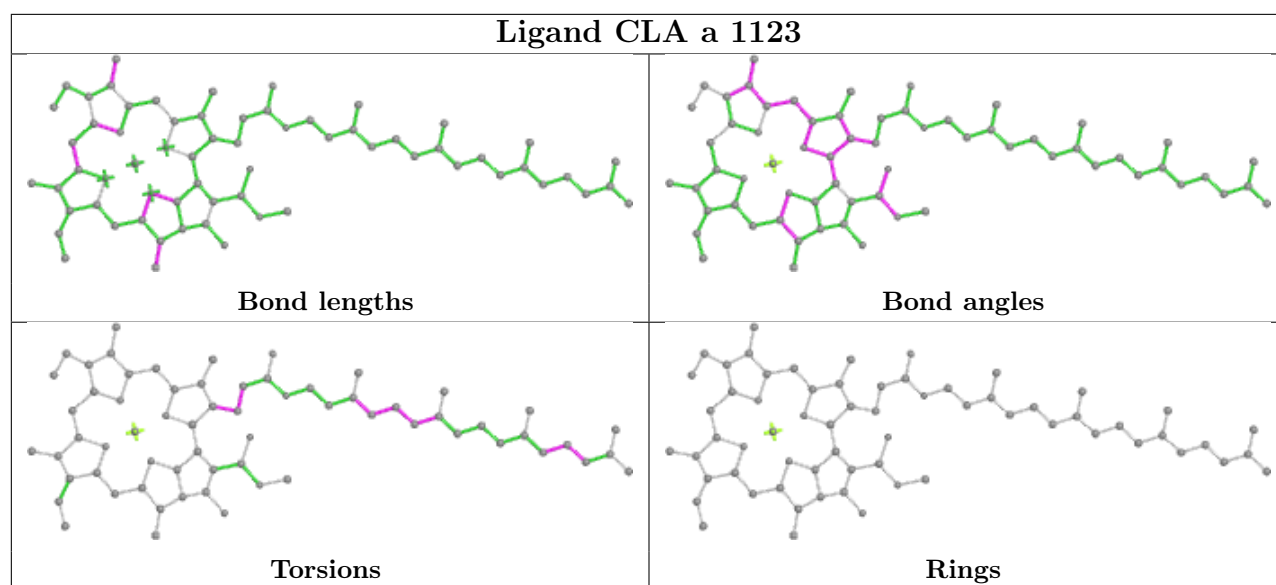


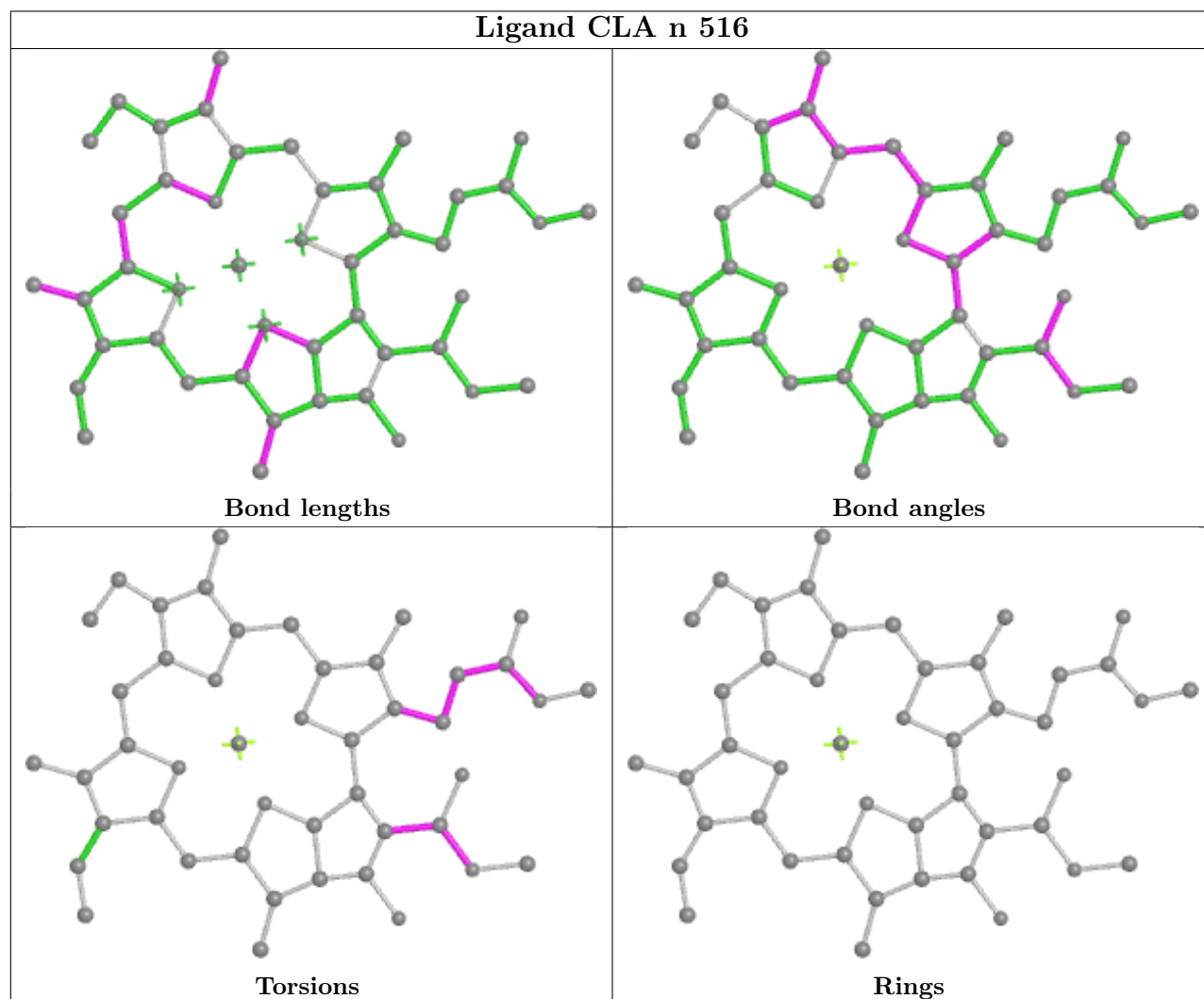
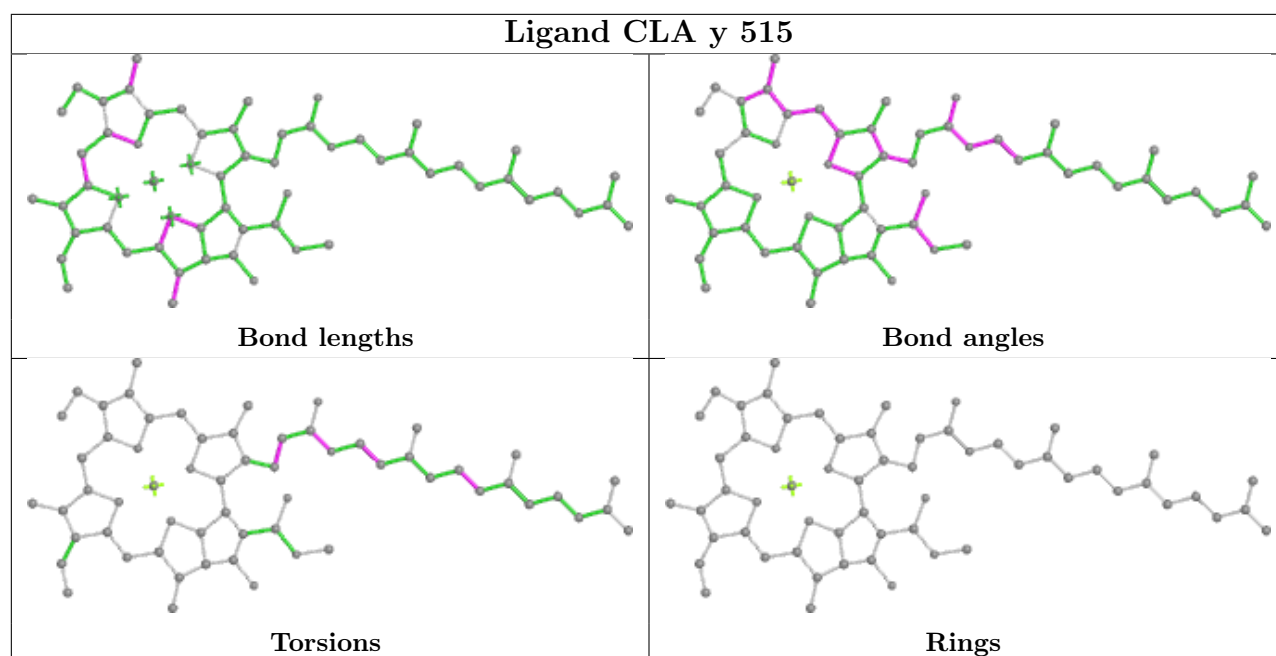
Torsions

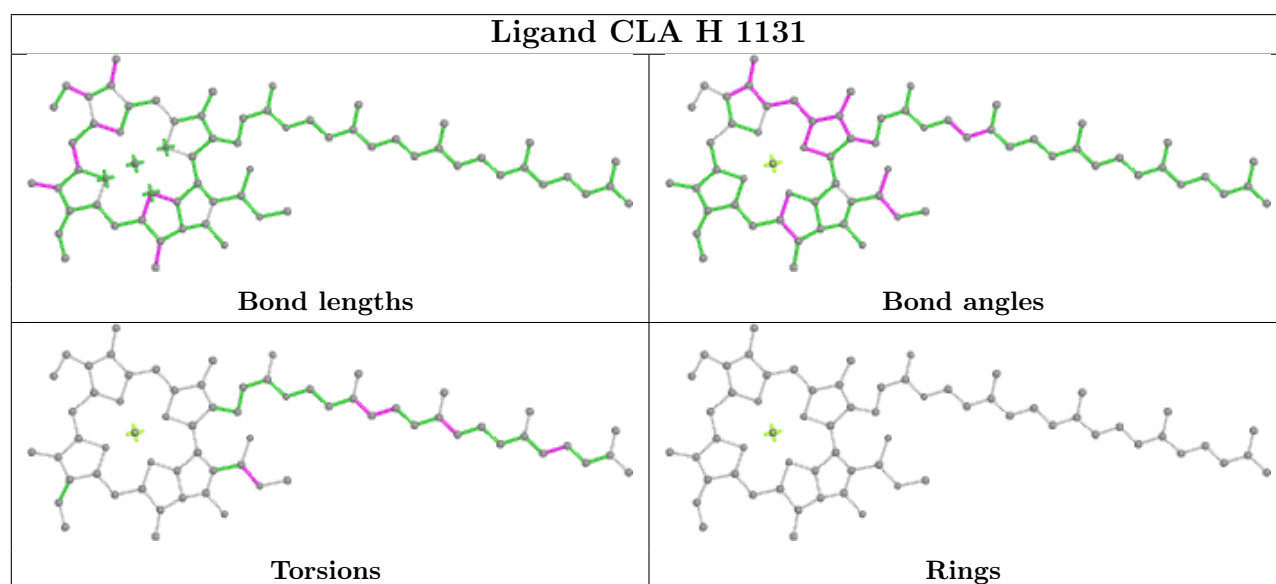
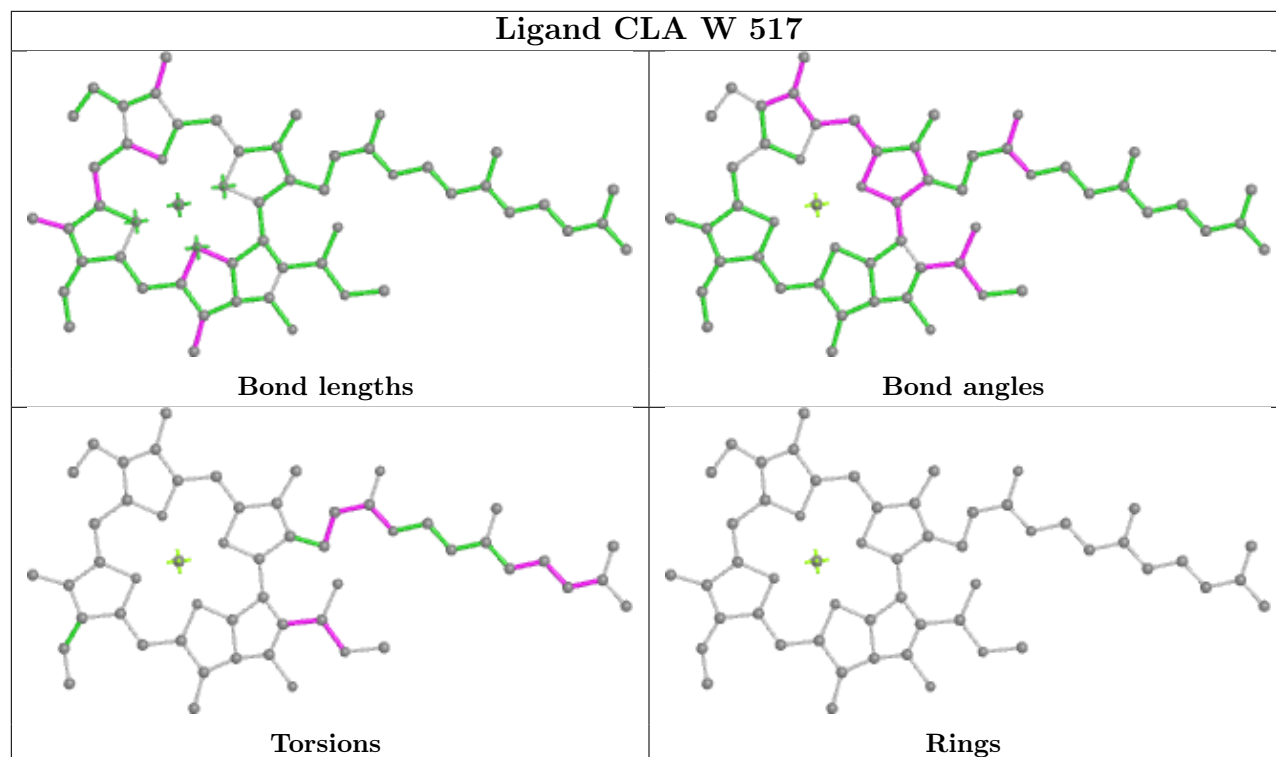
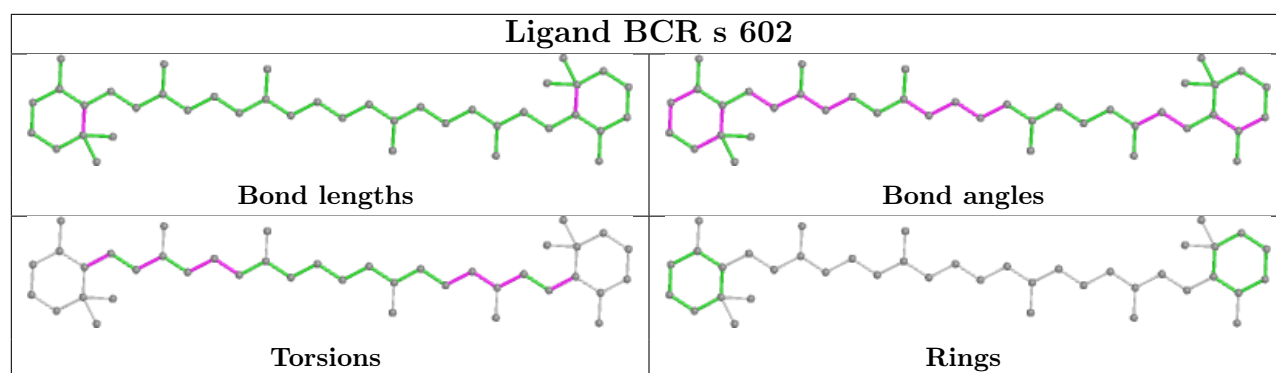


Rings



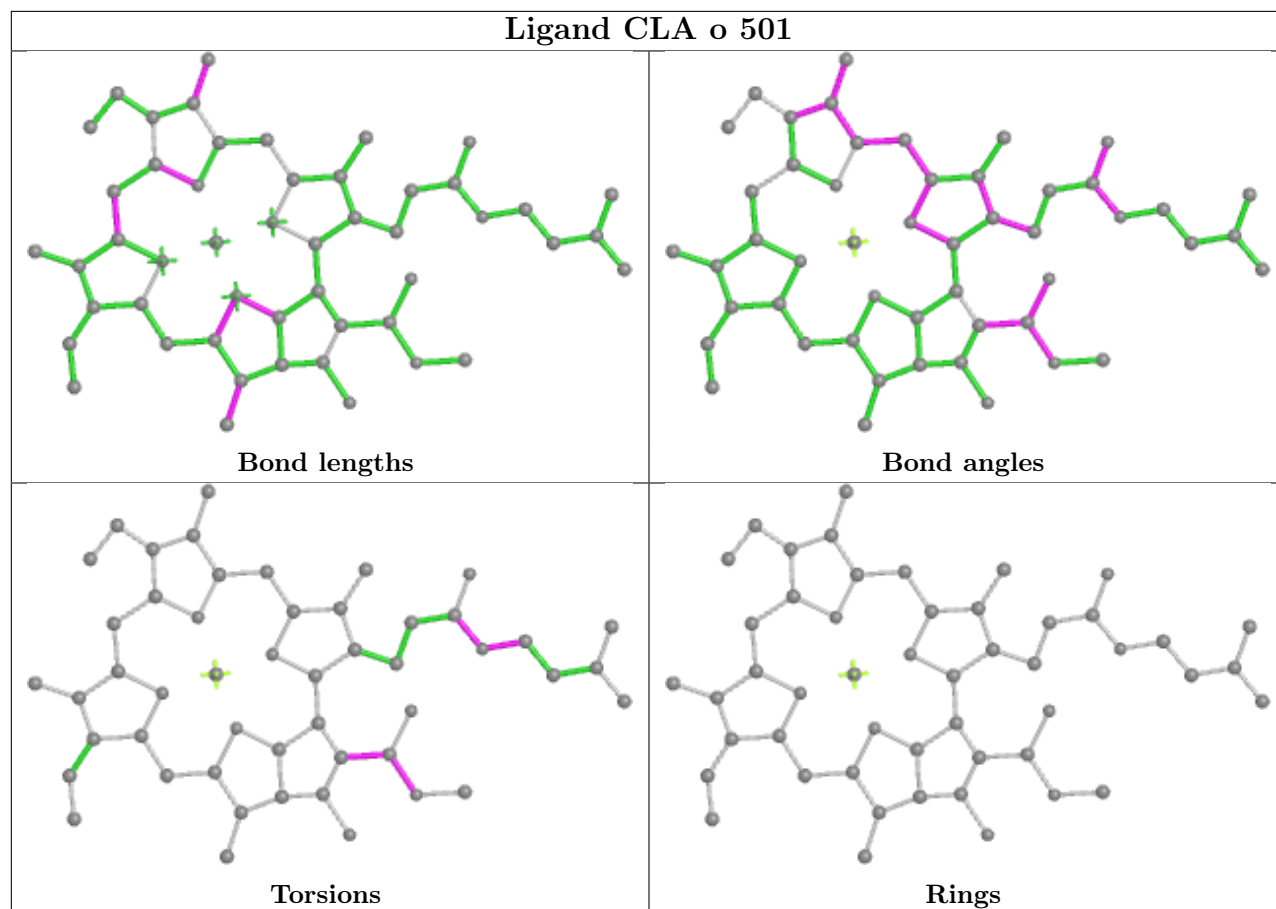




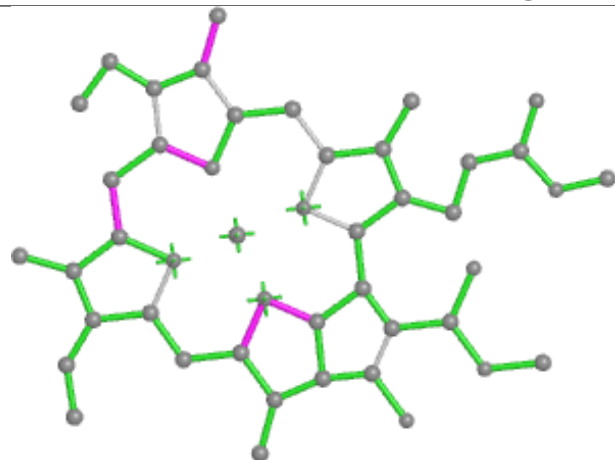




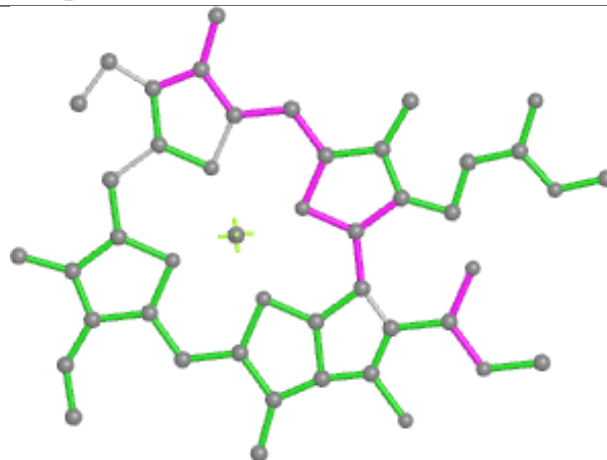
## Ligand CLA o 501



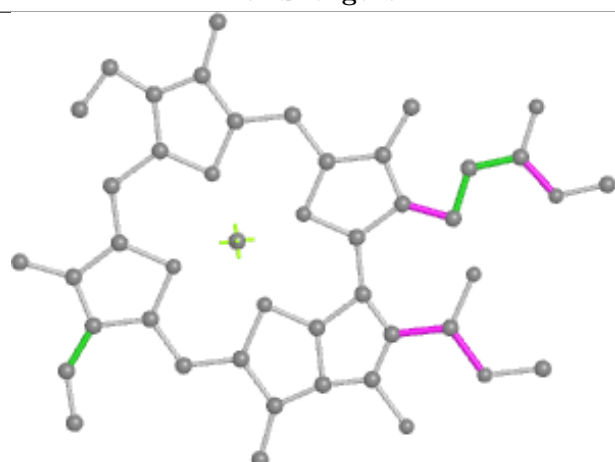
## Ligand CLA q 516



Bond lengths



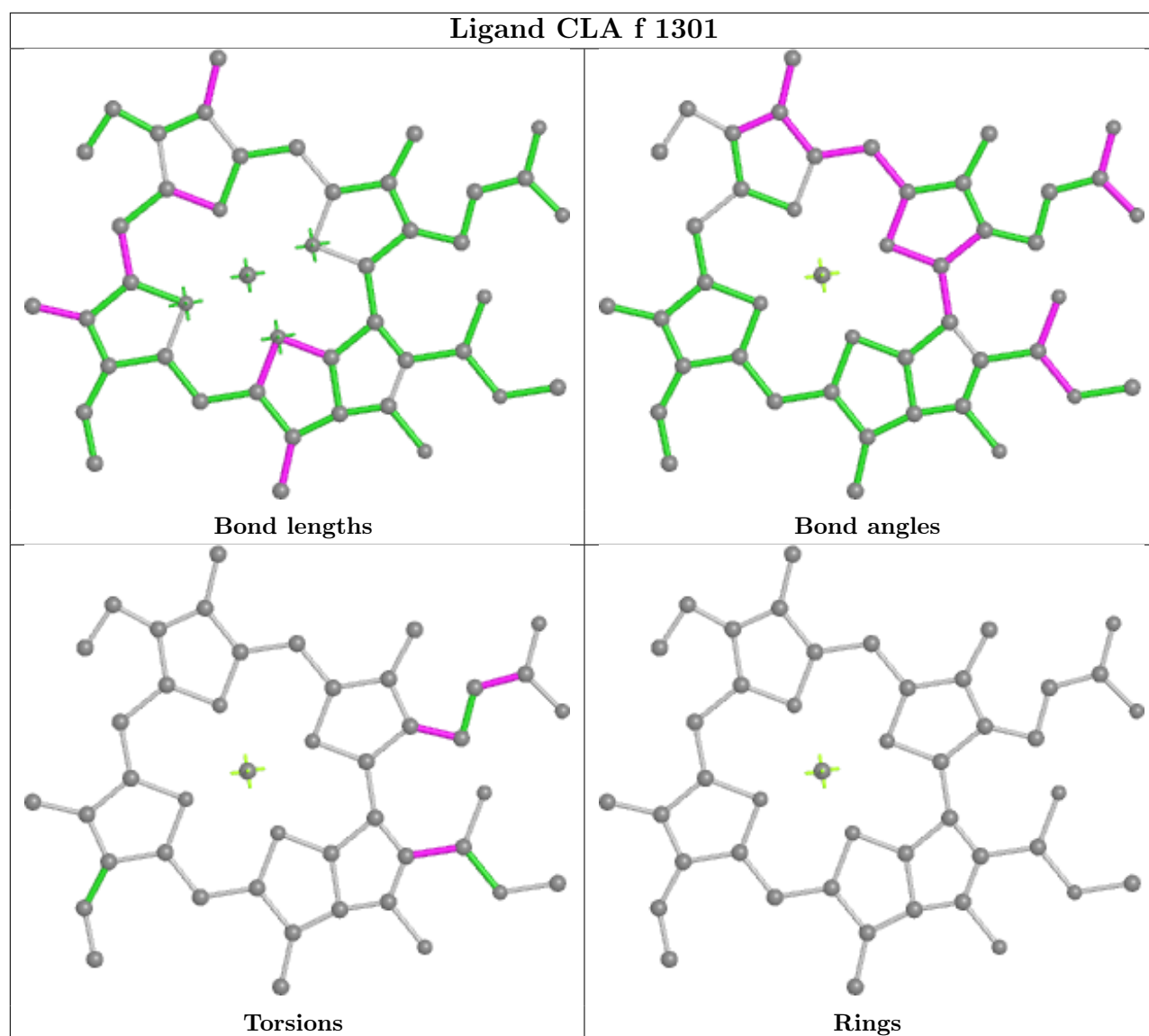
Bond angles

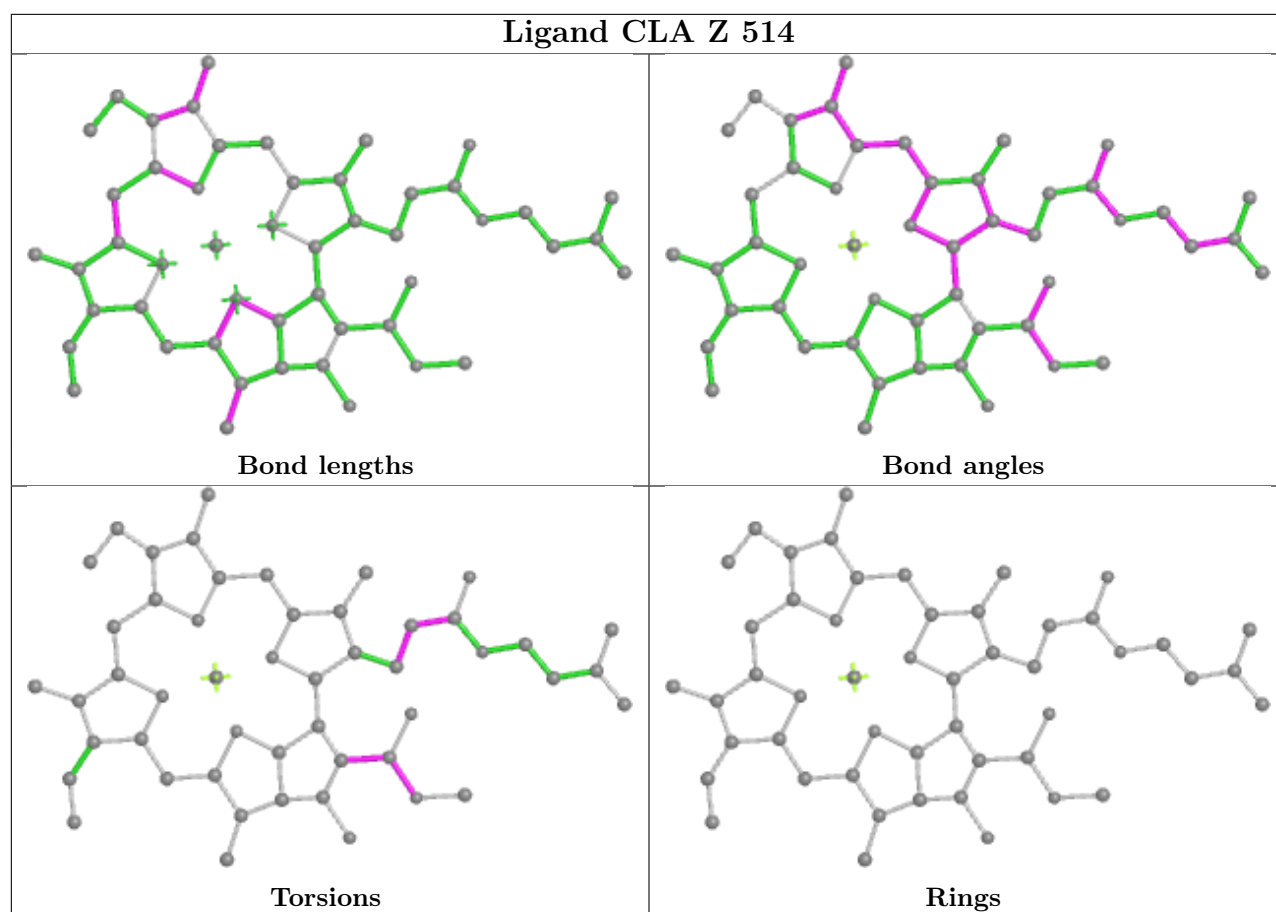


Torsions

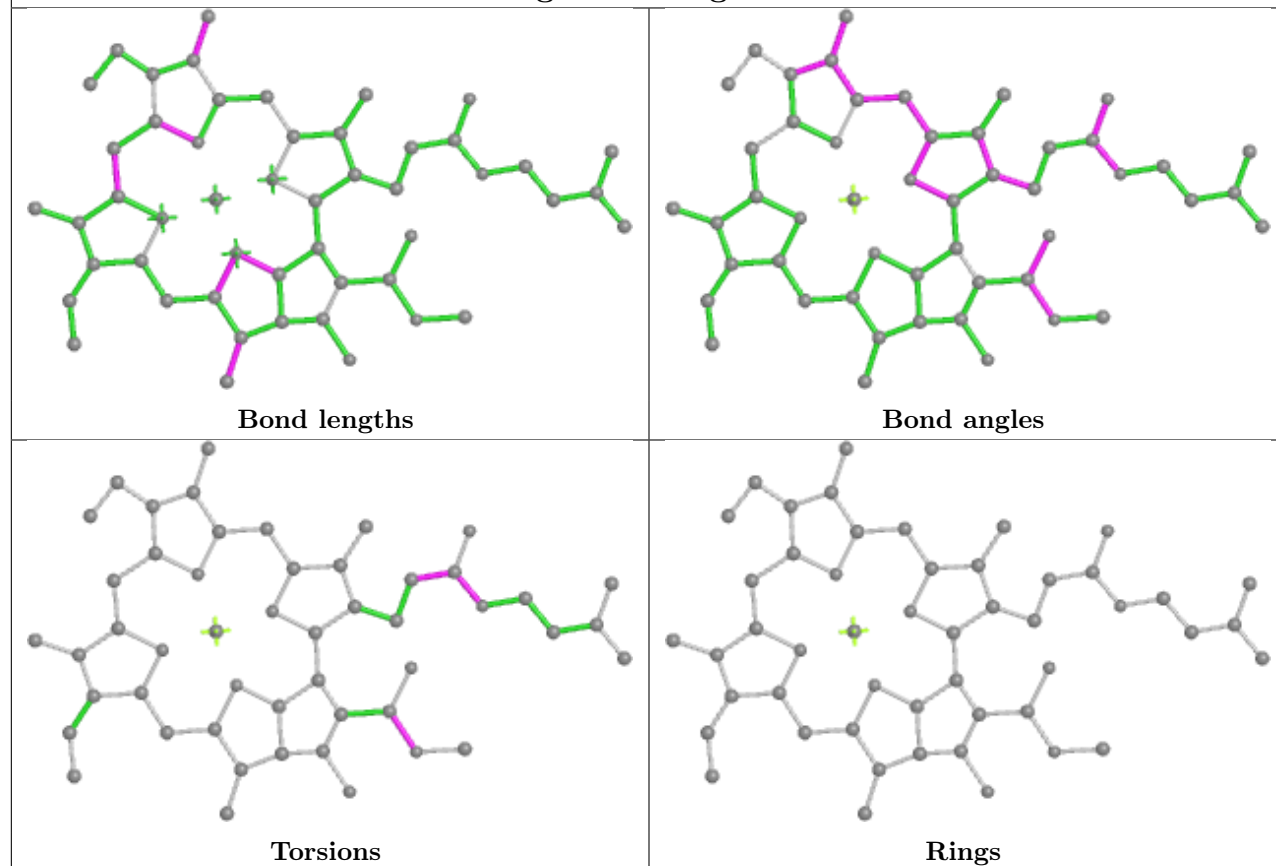


Rings

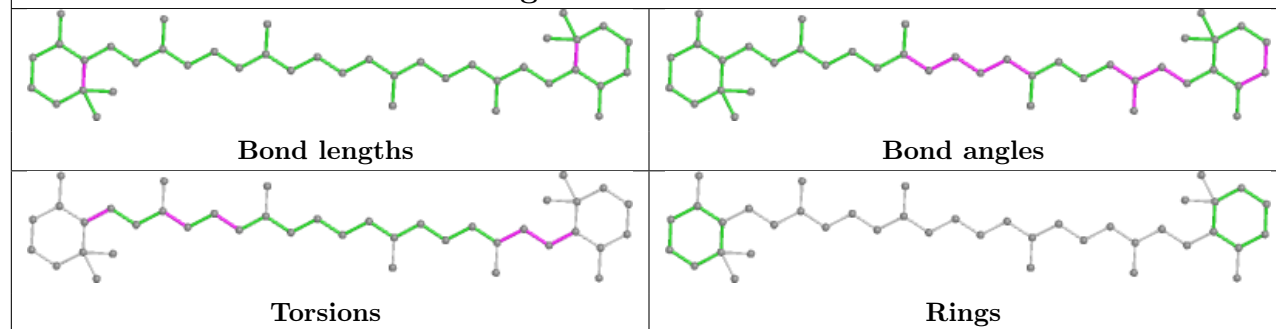


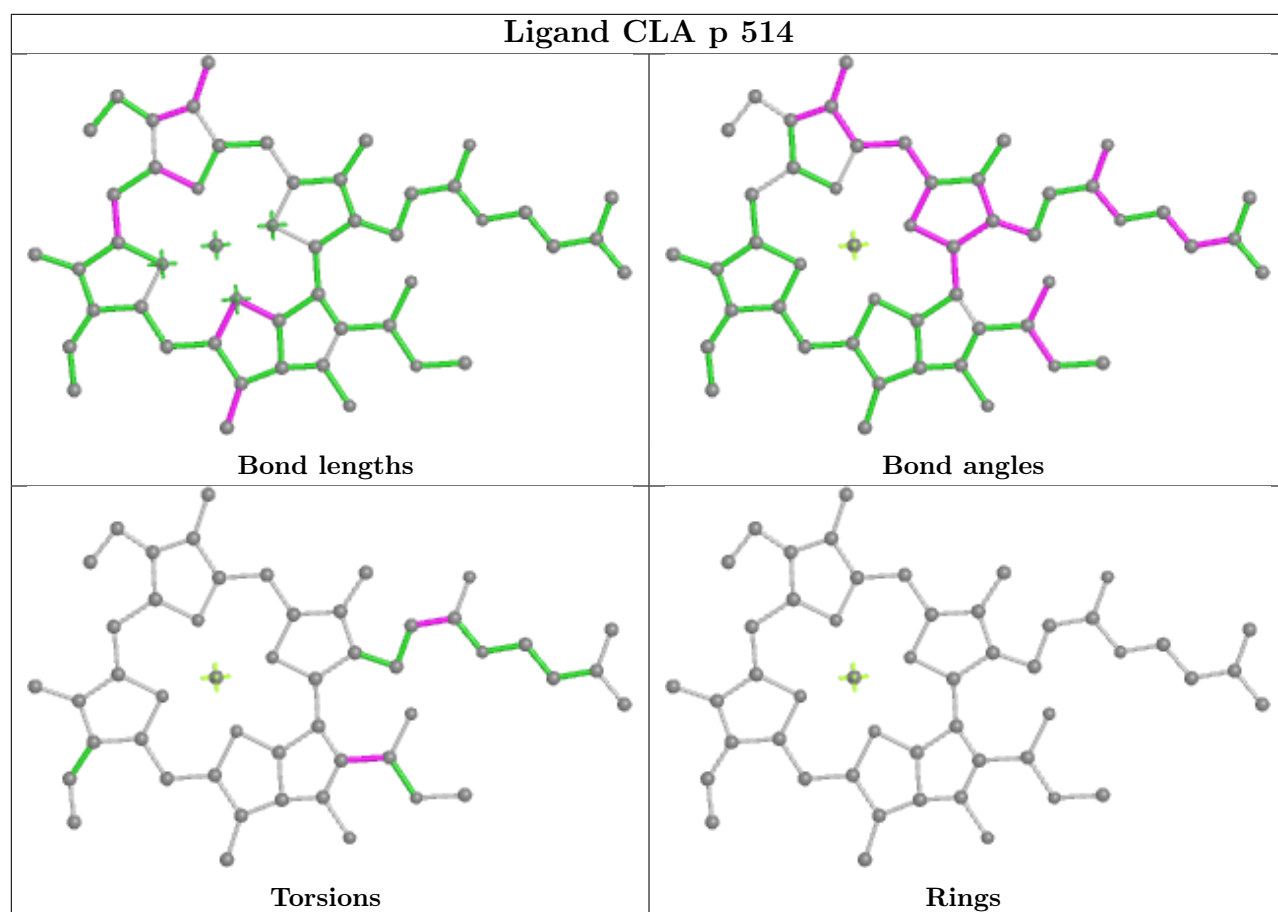


## Ligand CLA g 513

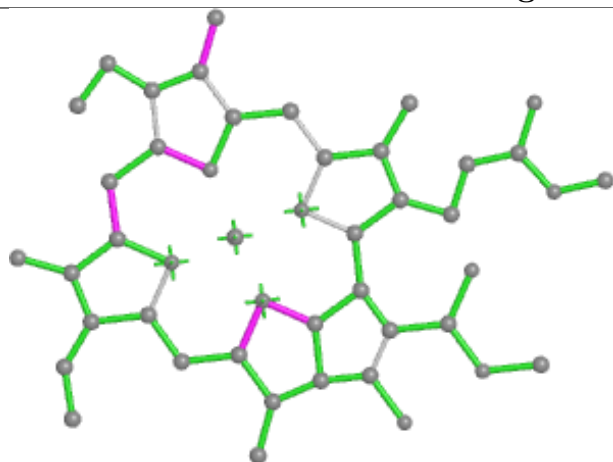


## Ligand BCR G 4017

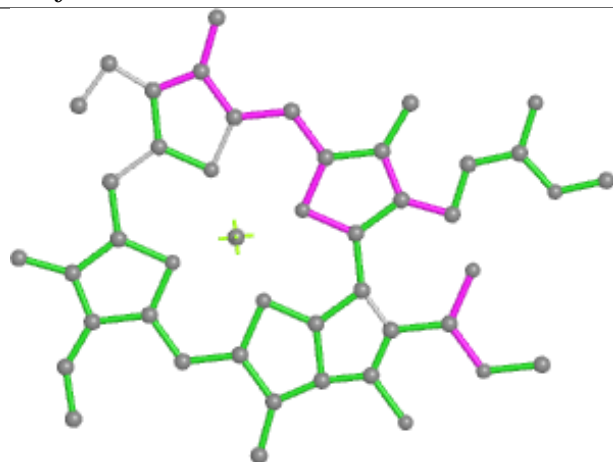




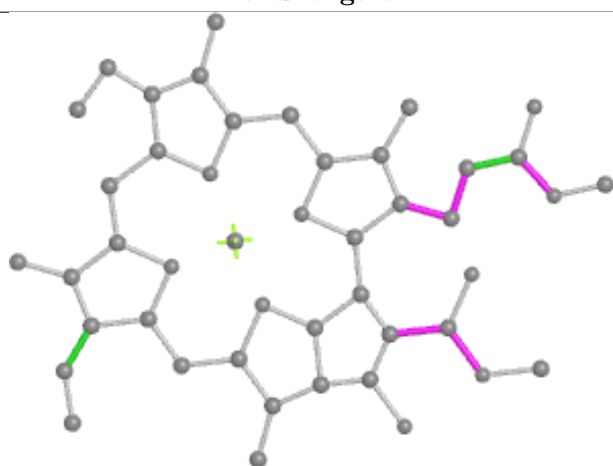
## Ligand CLA y 501



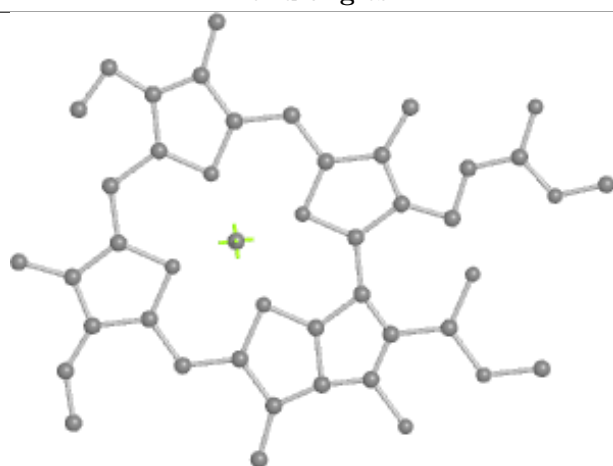
Bond lengths



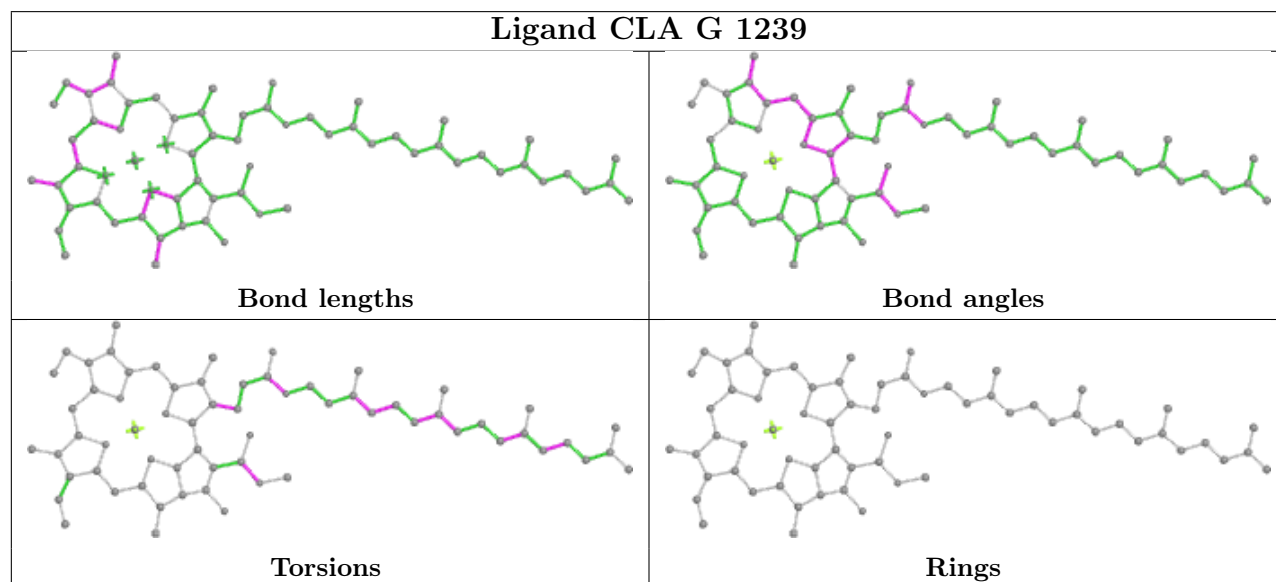
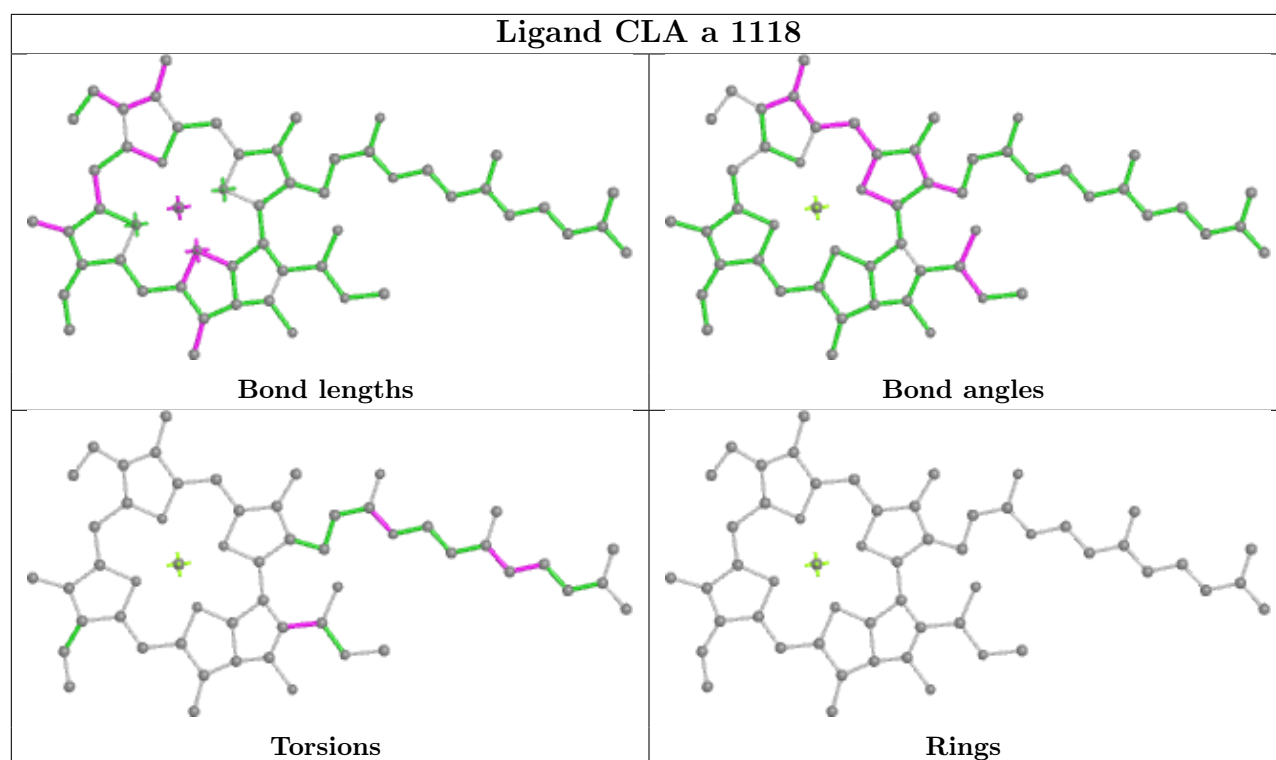
Bond angles



Torsions

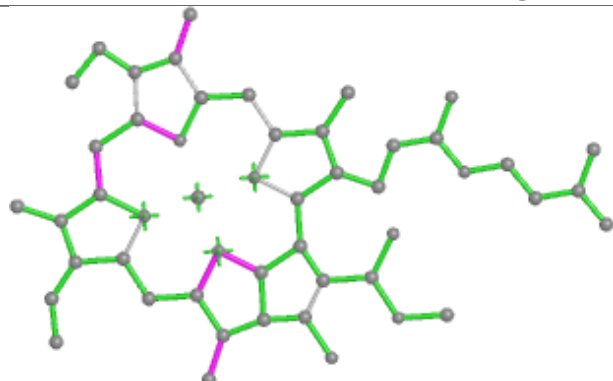


Rings

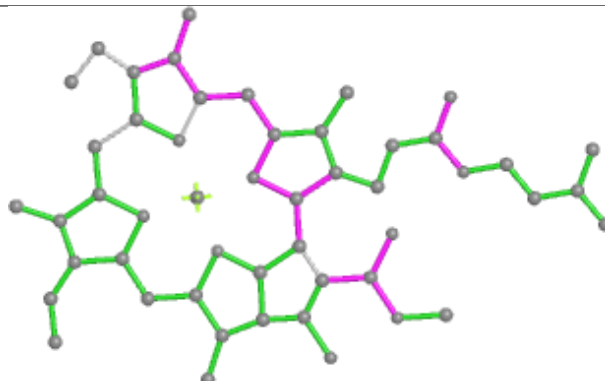




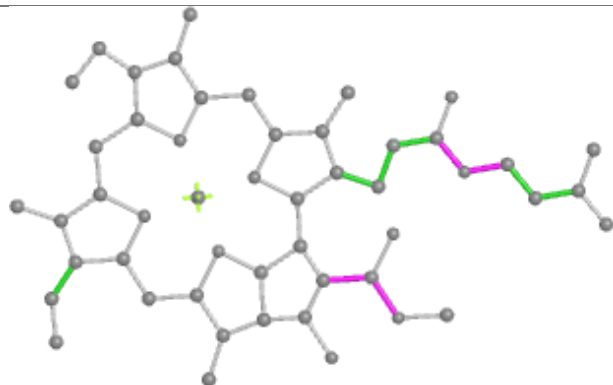
## Ligand CLA X 501



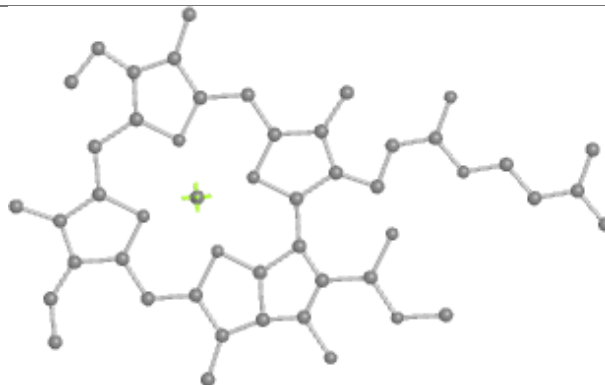
Bond lengths



Bond angles

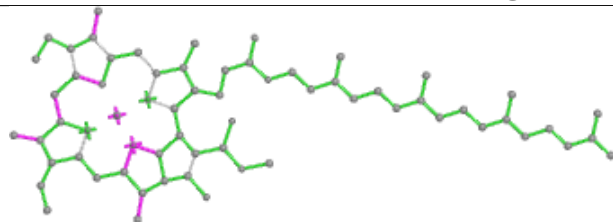


Torsions

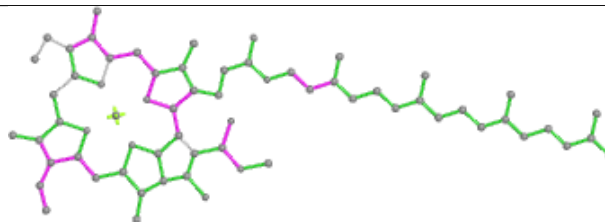


Rings

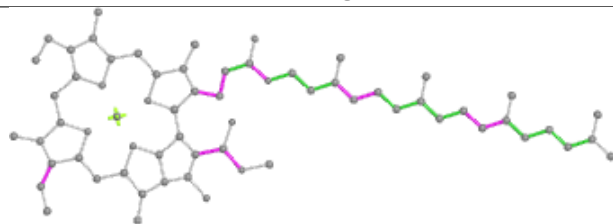
## Ligand CLA G 1210



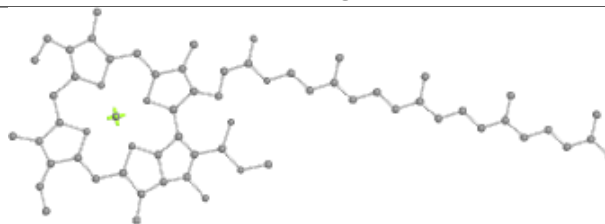
Bond lengths



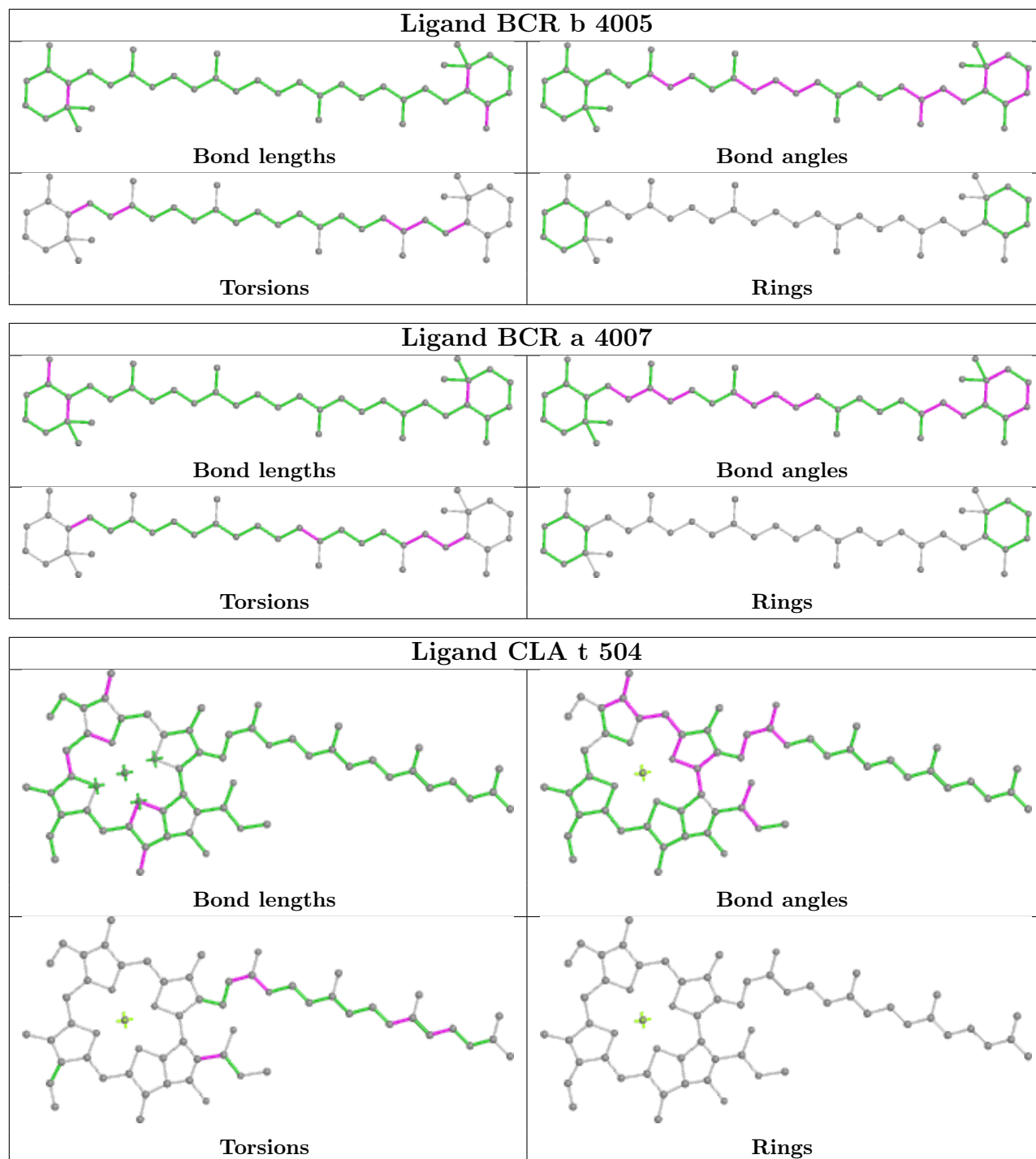
Bond angles



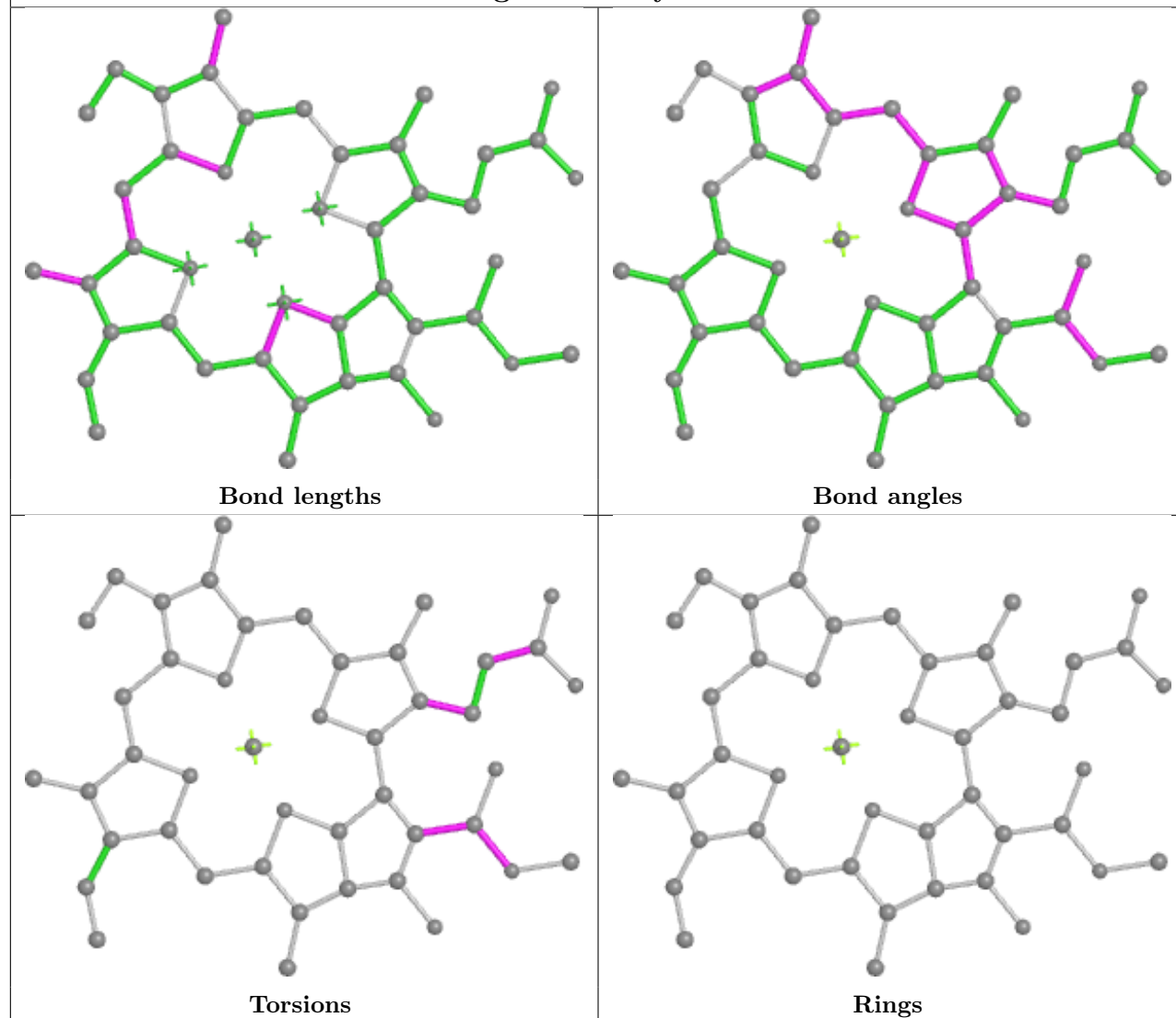
Torsions



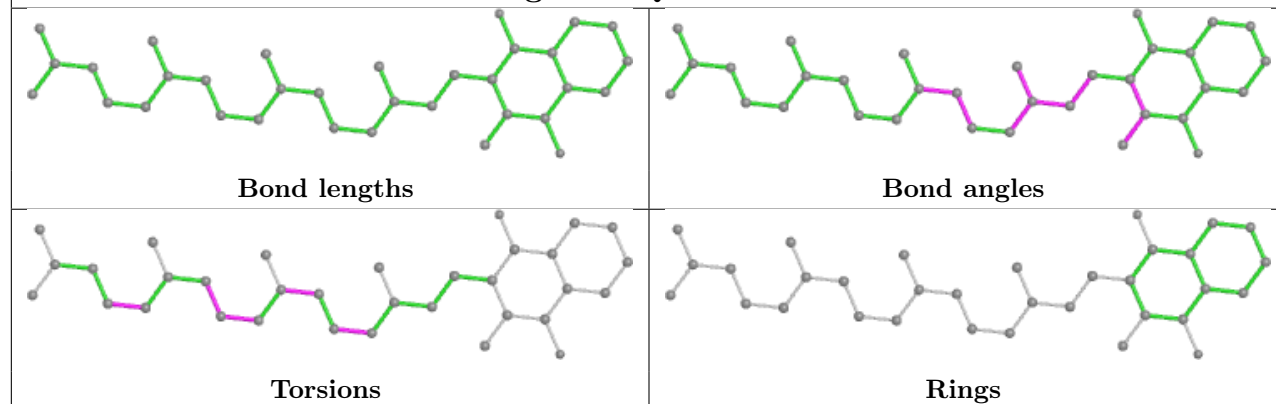
Rings

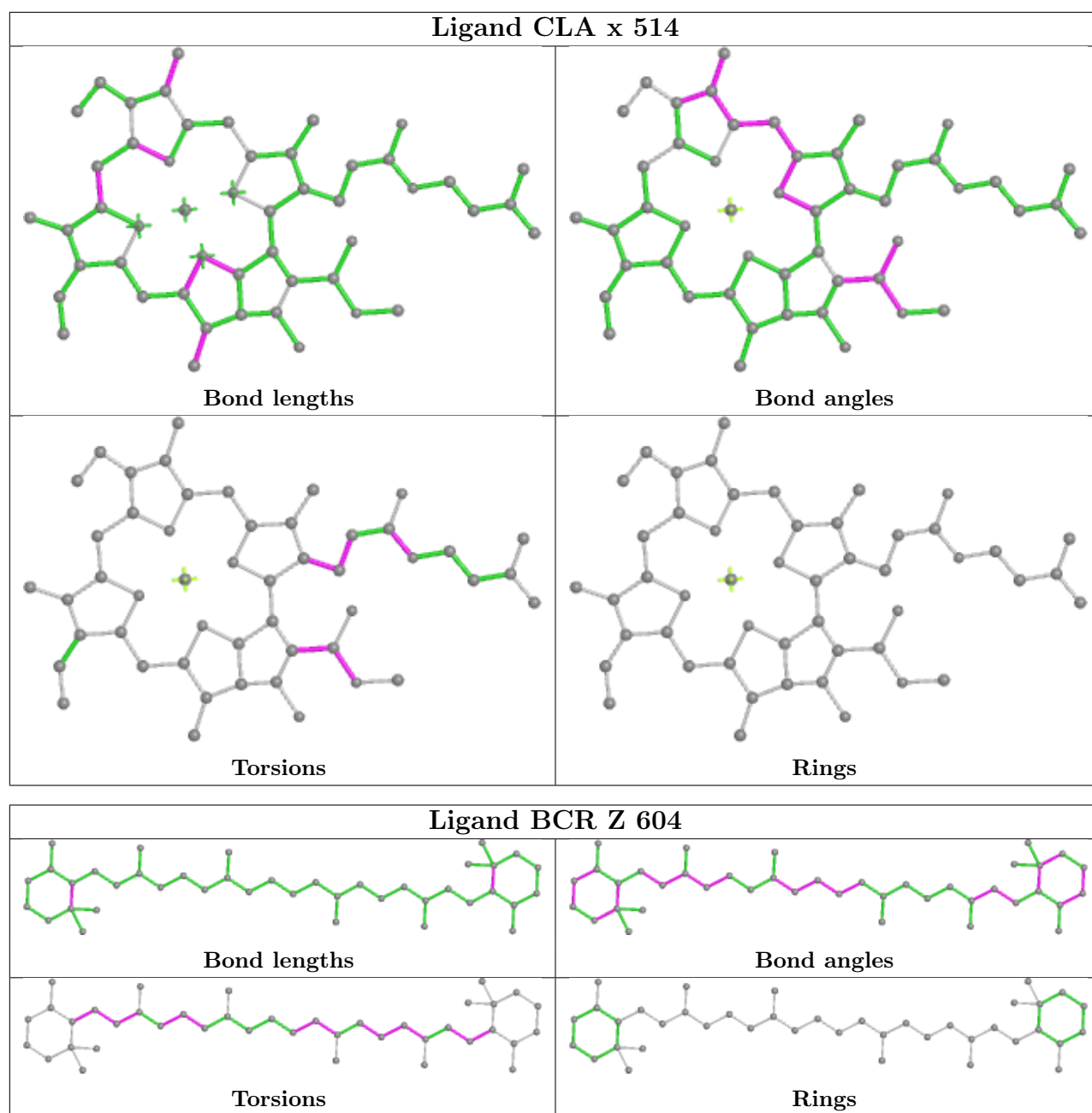


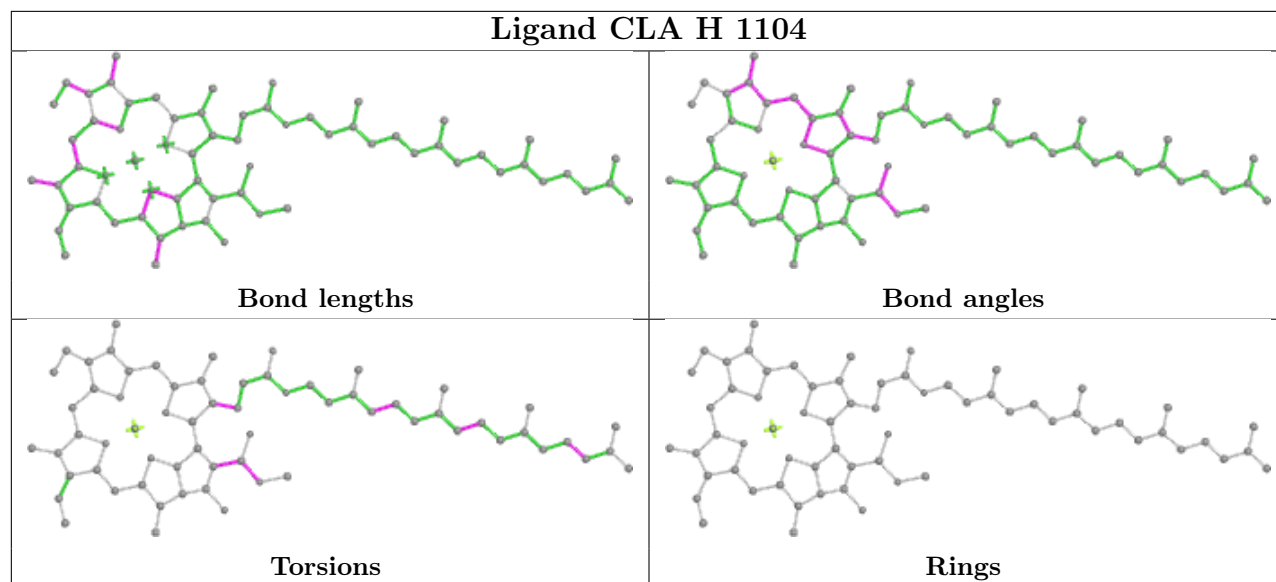
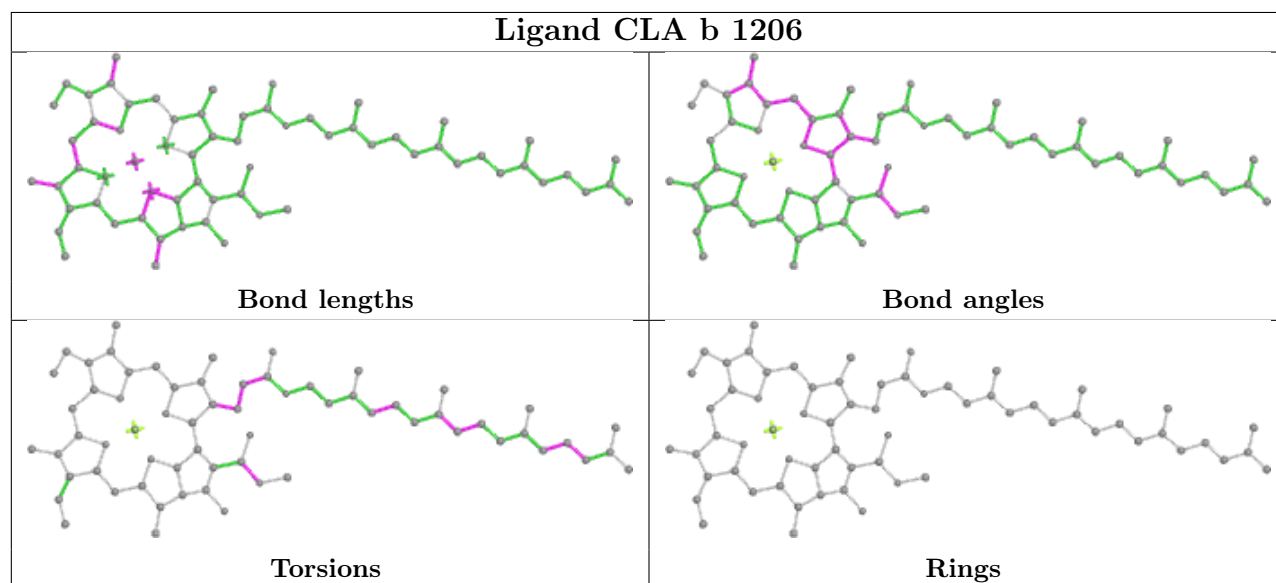
## Ligand CLA y 512

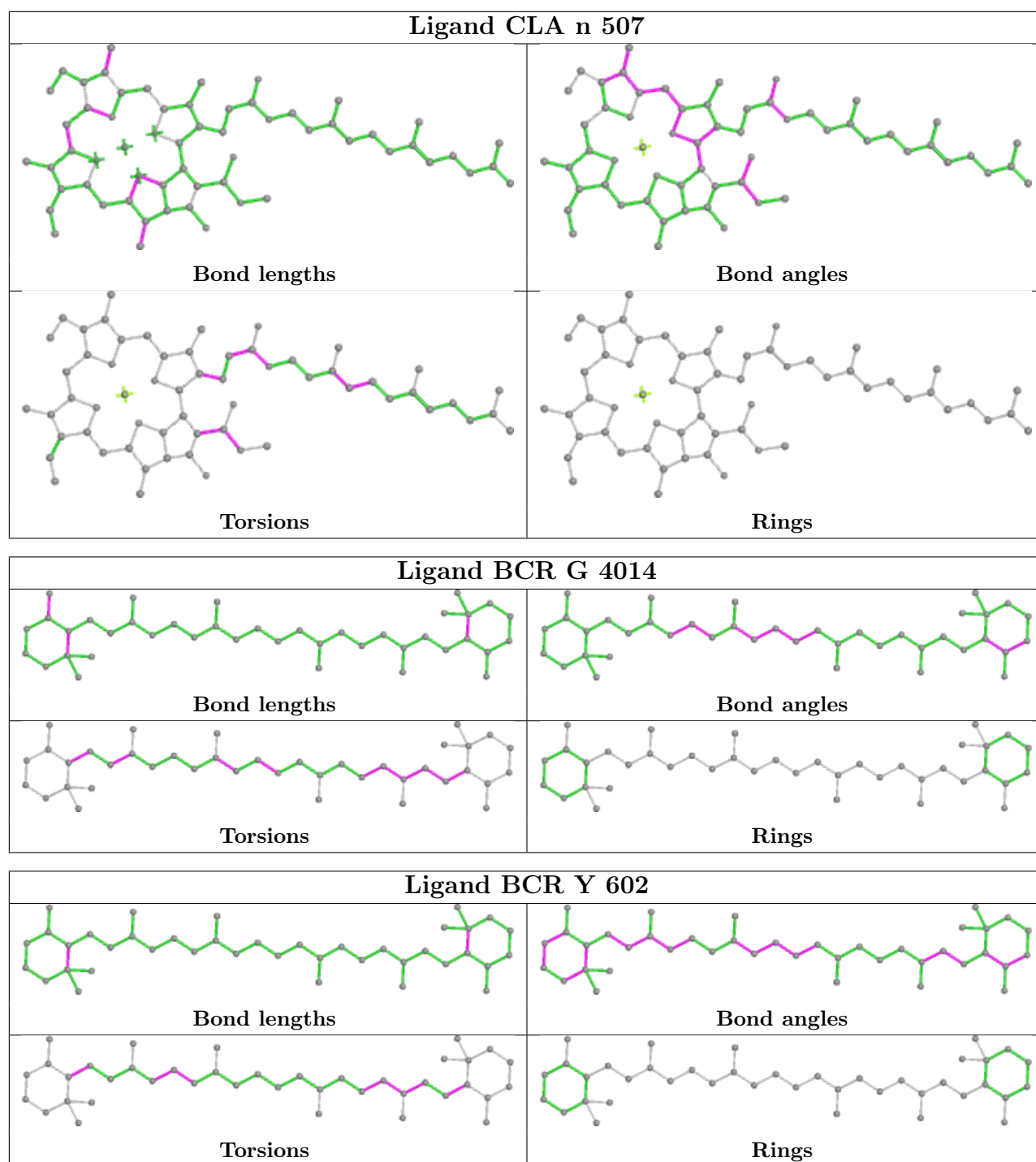


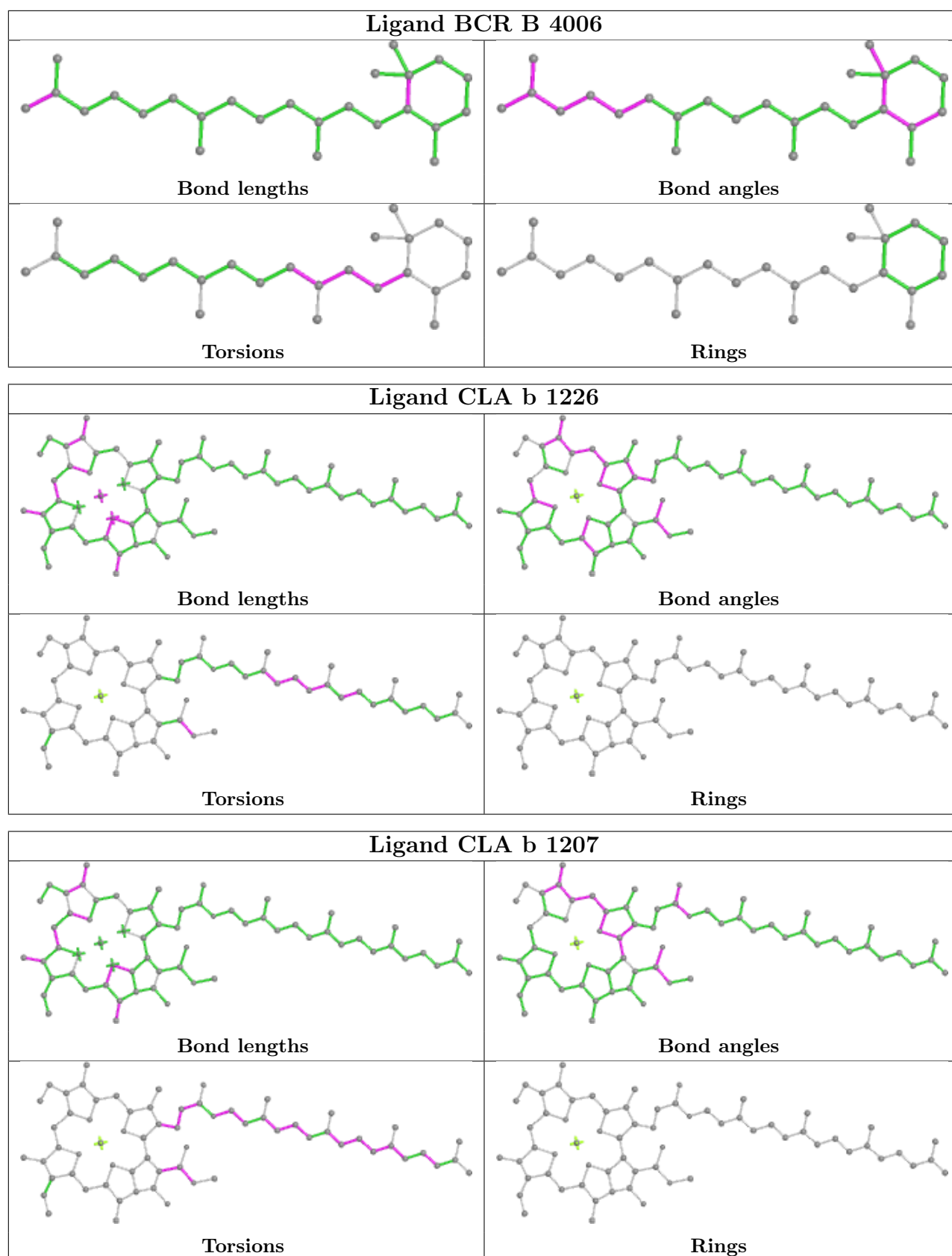
## Ligand PQN a 2001

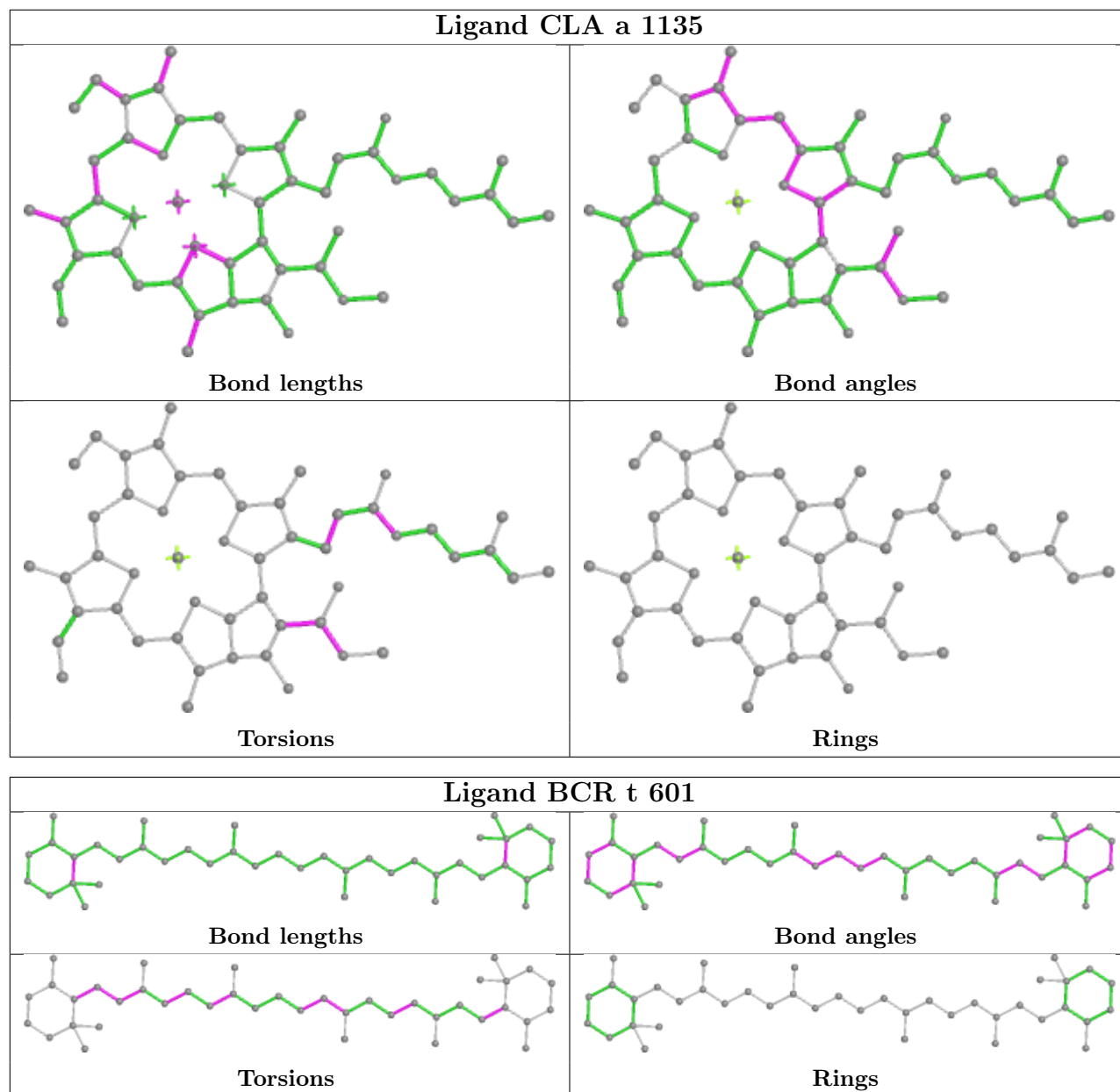




**Ligand CLA H 1104****Ligand CLA b 1206**

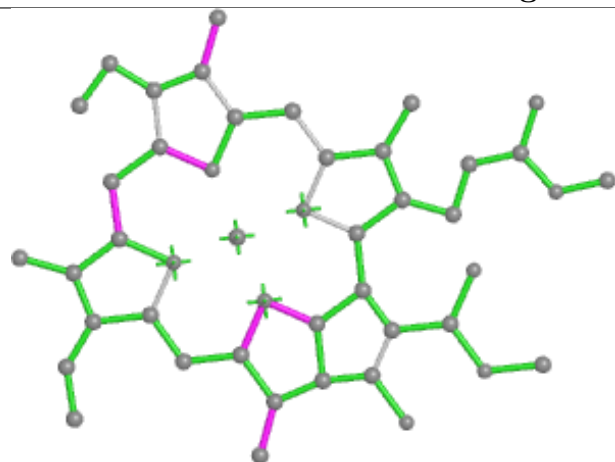




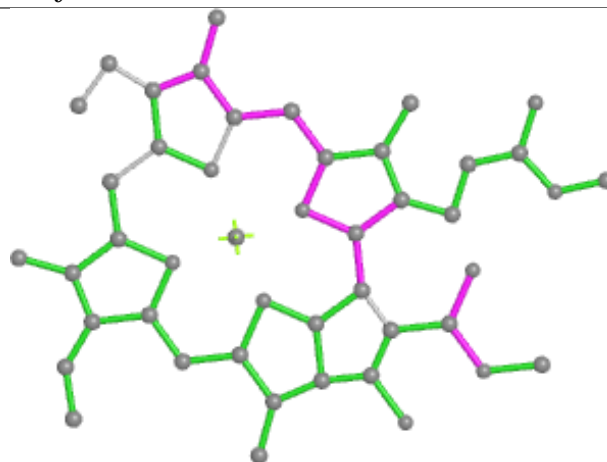




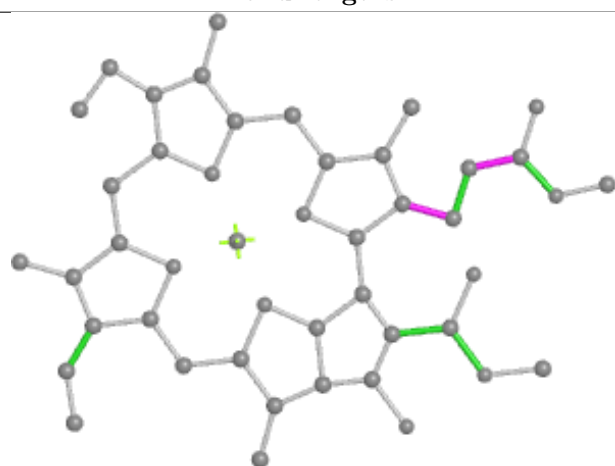
## Ligand CLA y 516



Bond lengths



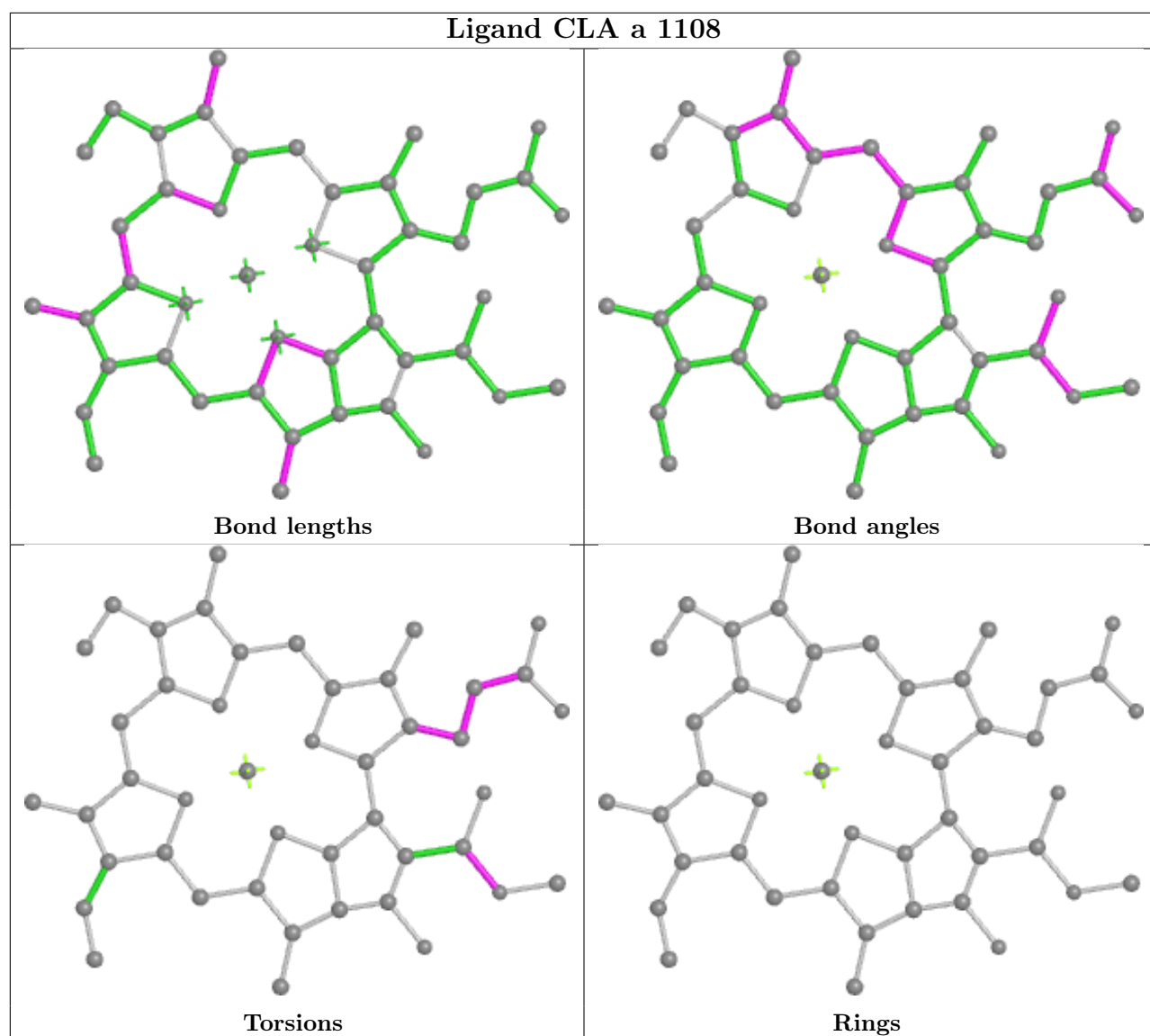
Bond angles

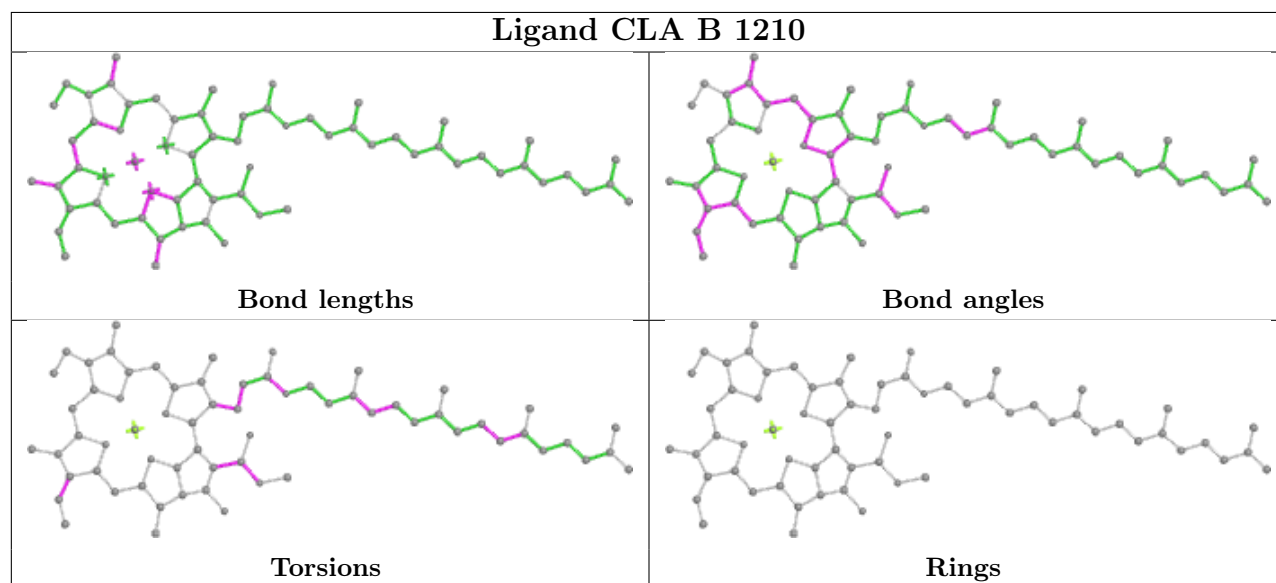
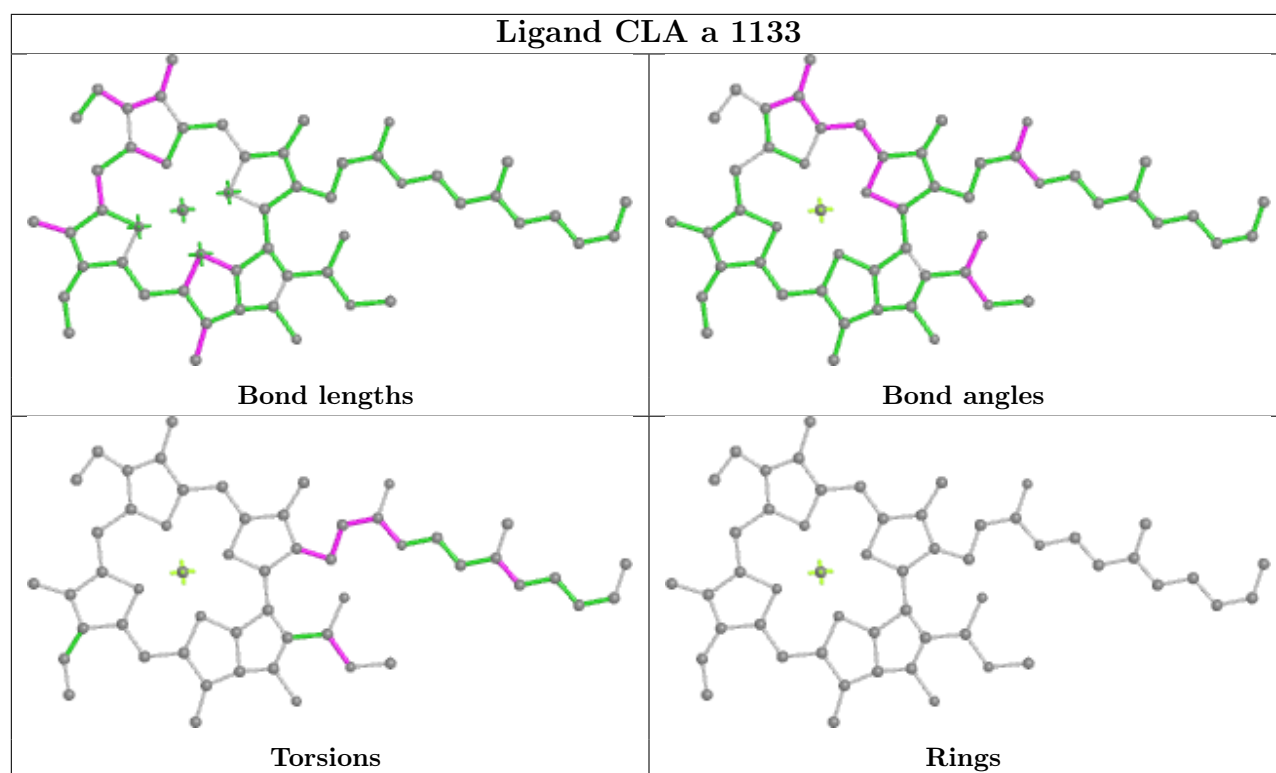


Torsions

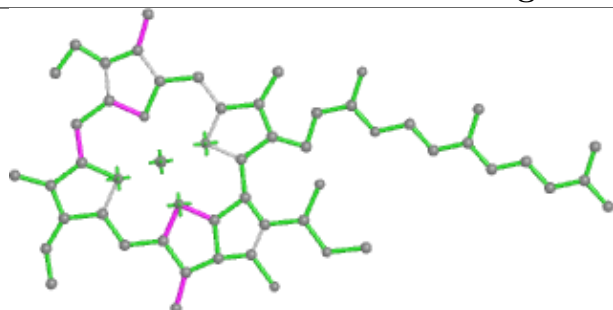


Rings

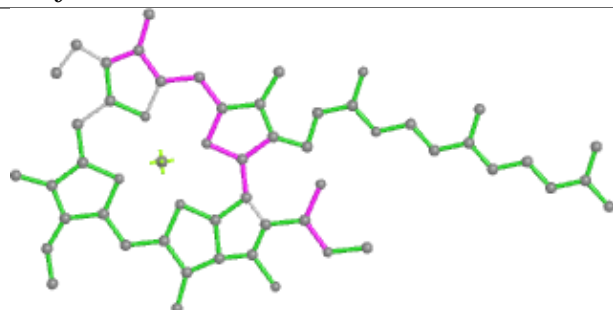




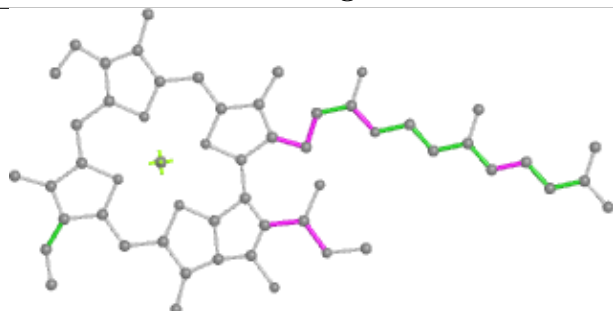
## Ligand CLA y 508



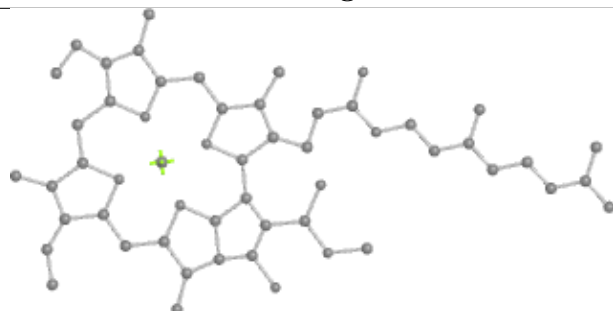
Bond lengths



Bond angles

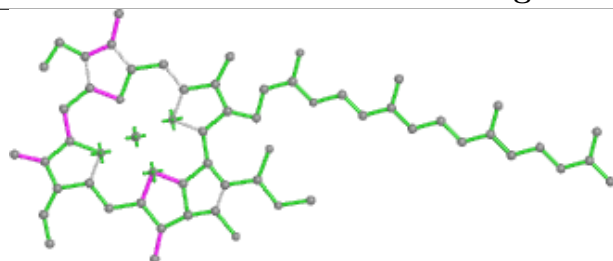


Torsions

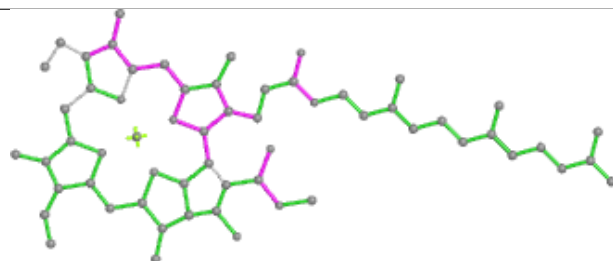


Rings

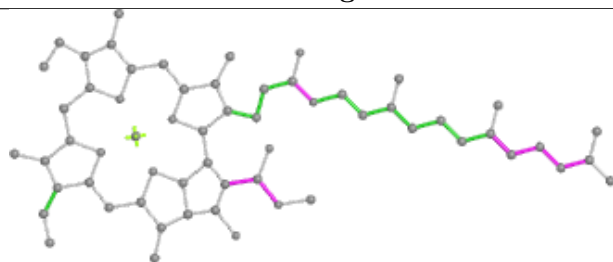
## Ligand CLA Y 506



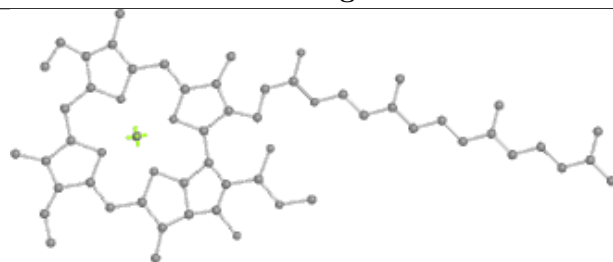
Bond lengths



Bond angles

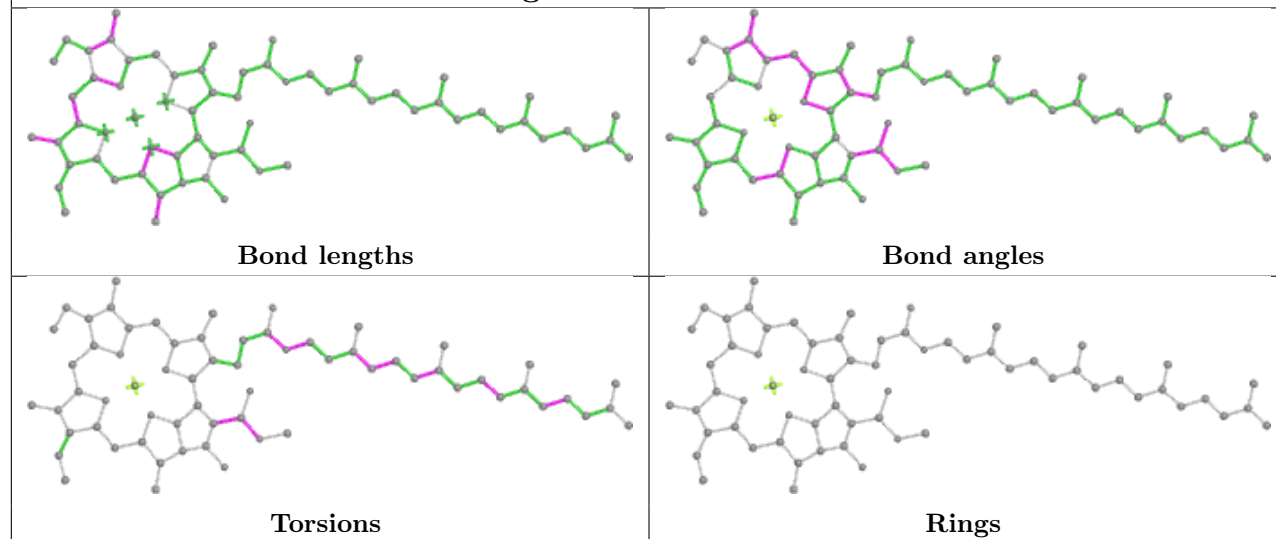


Torsions

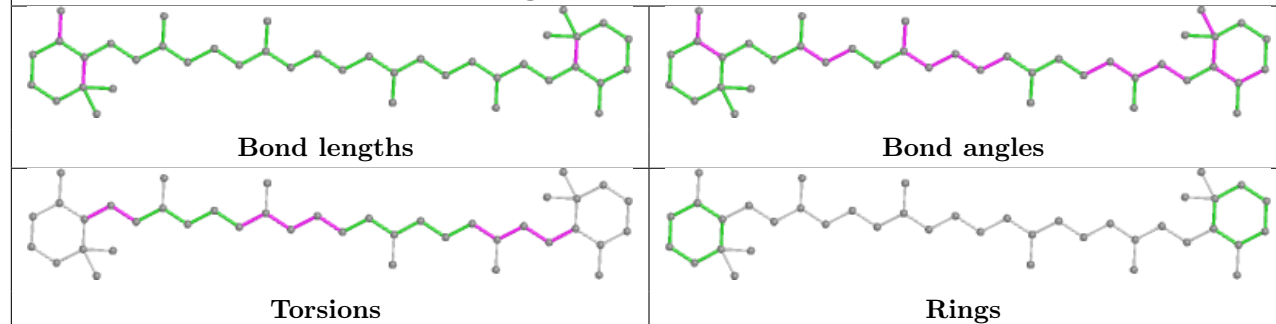


Rings

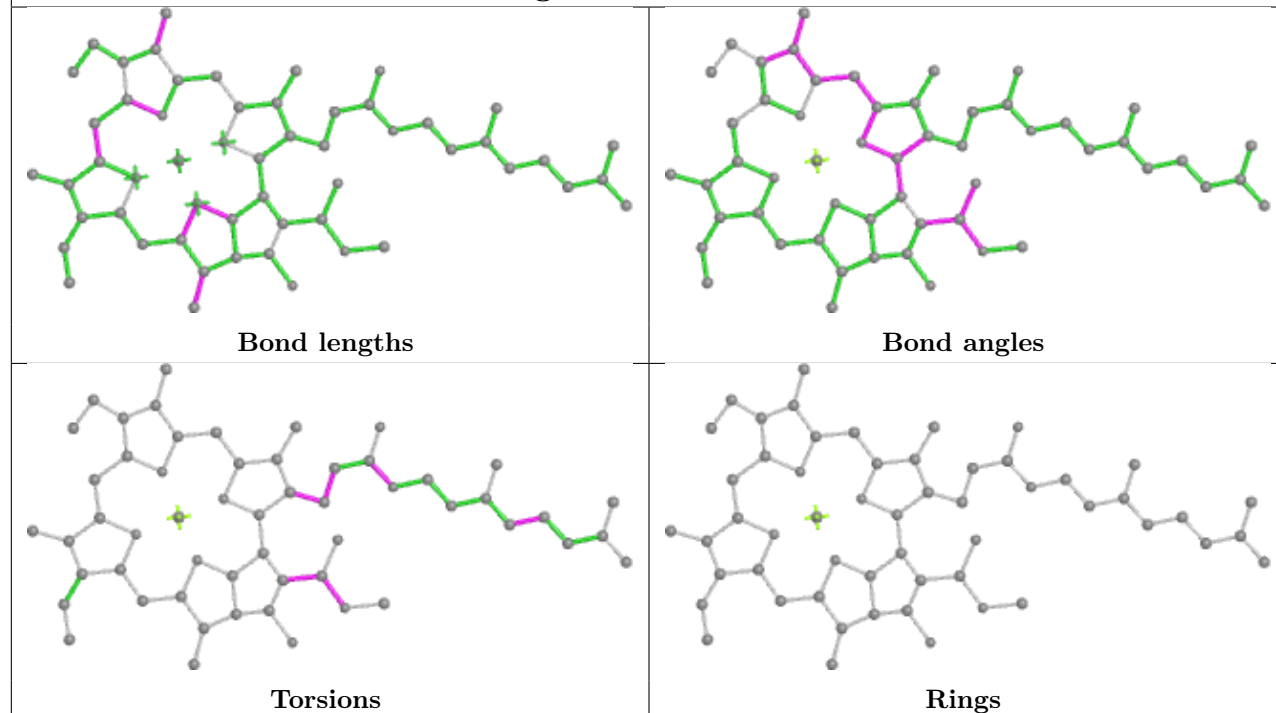
## Ligand CLA H 1109

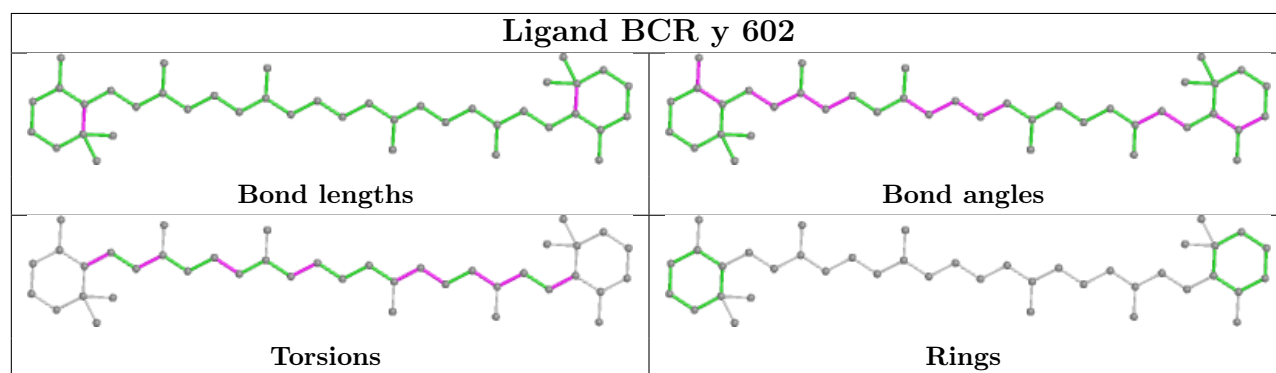
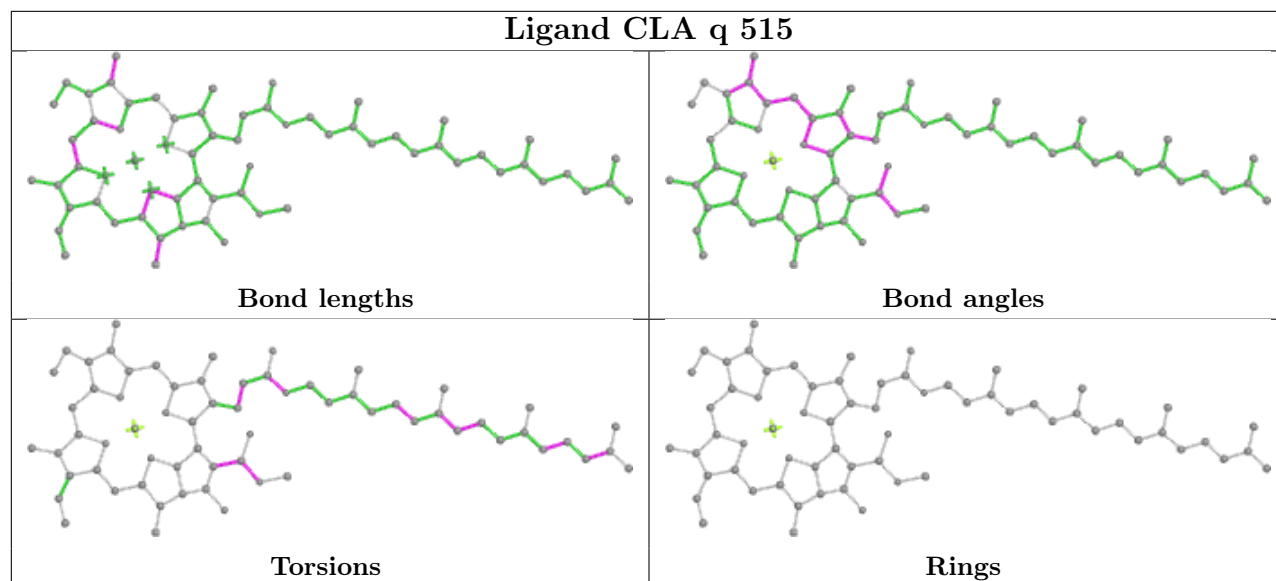
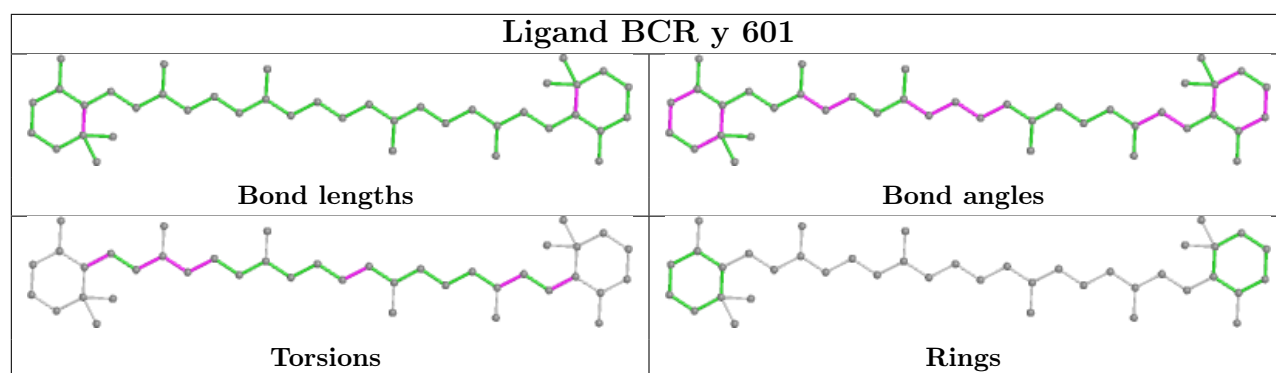


## Ligand BCR B 4010

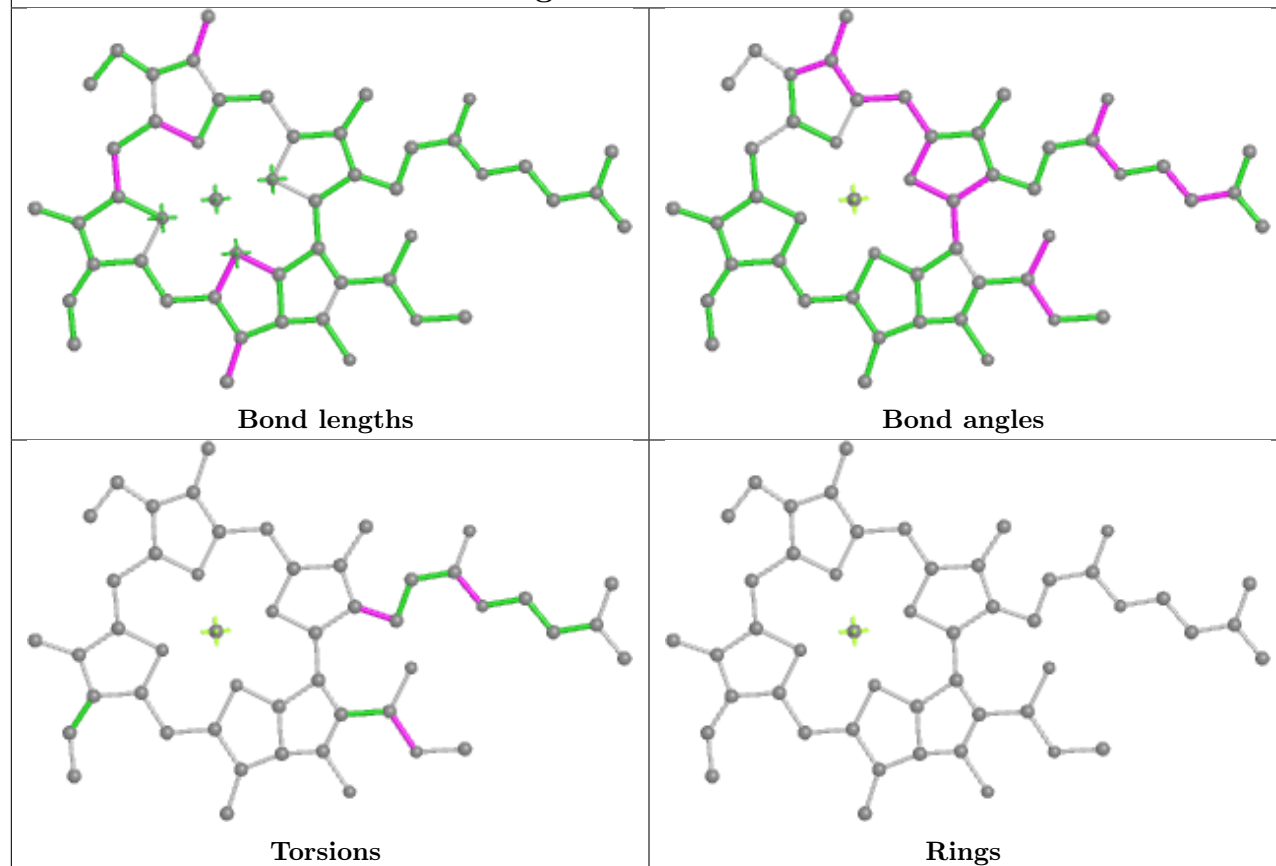


## Ligand CLA Z 508

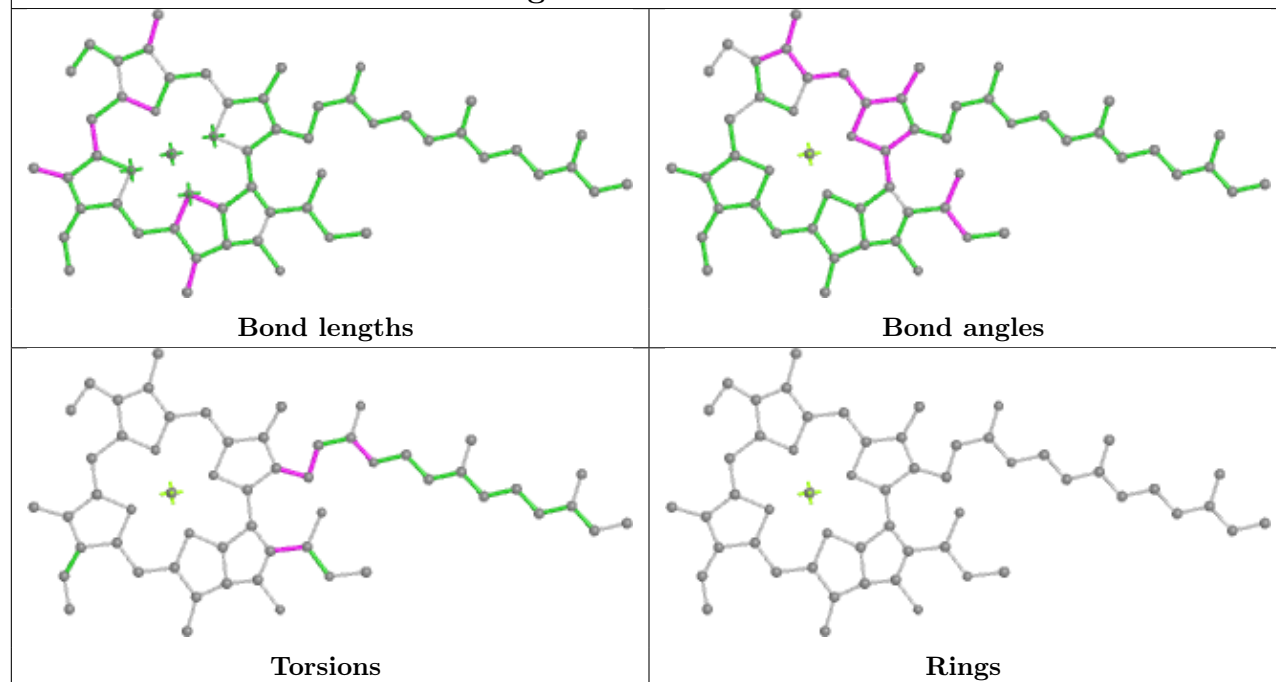


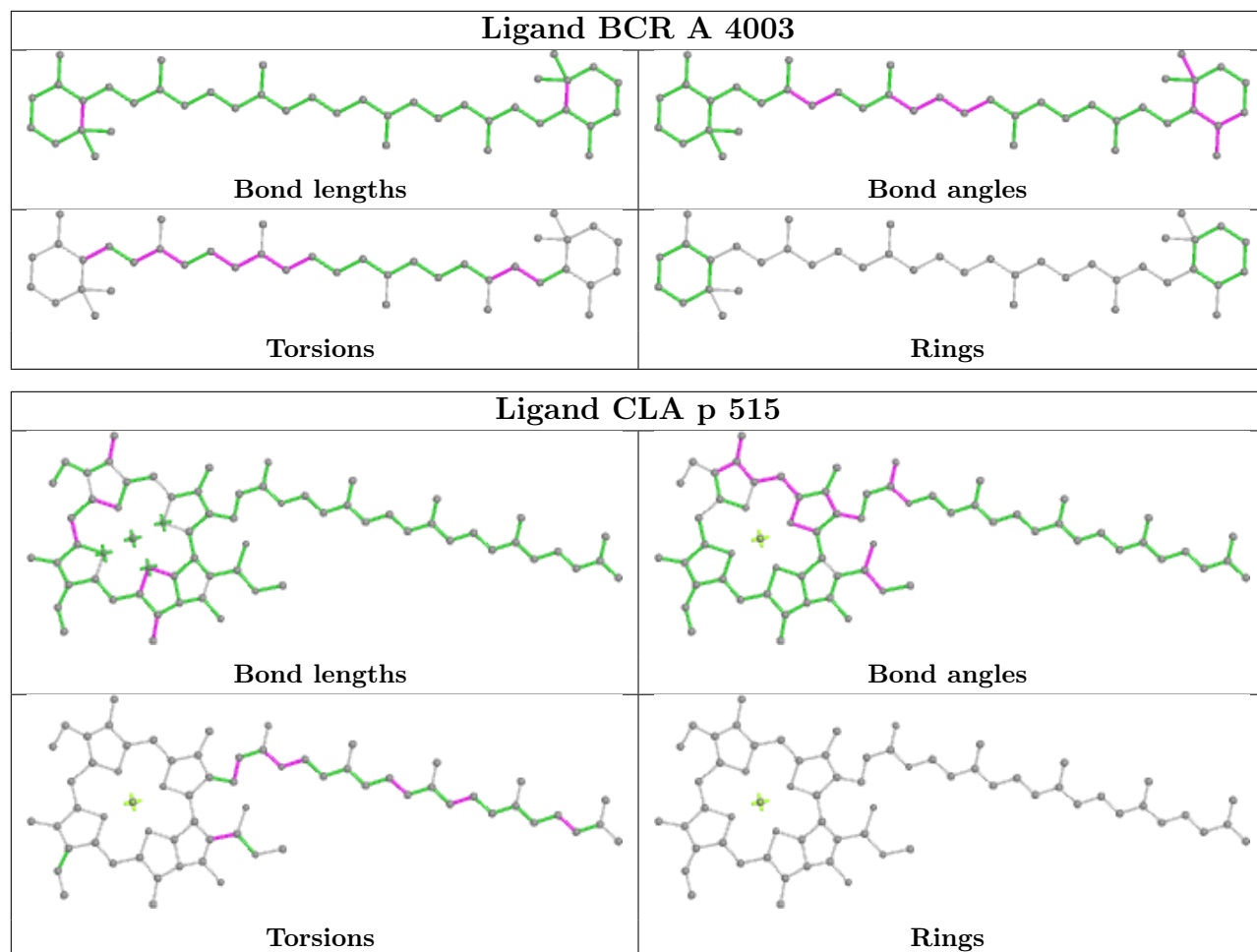


## Ligand CLA n 513



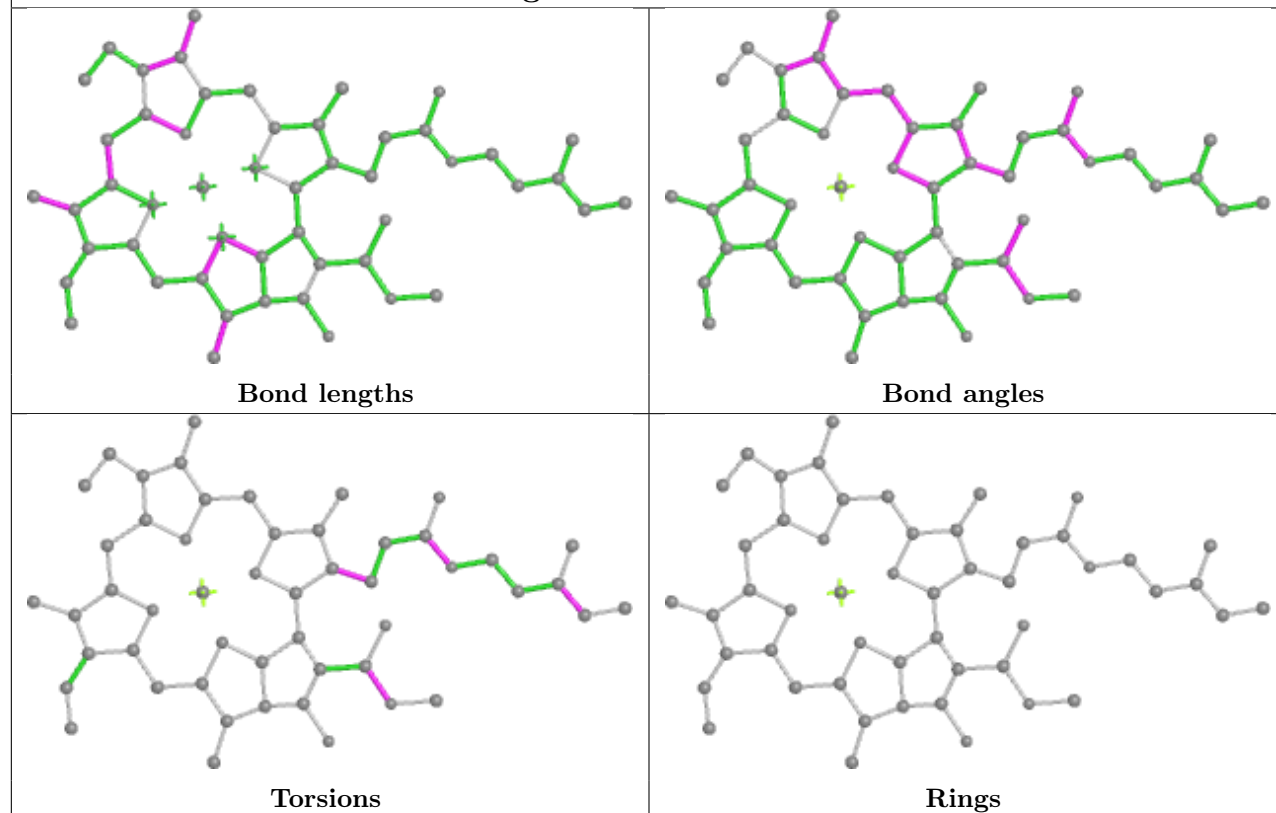
## Ligand CLA a 1102



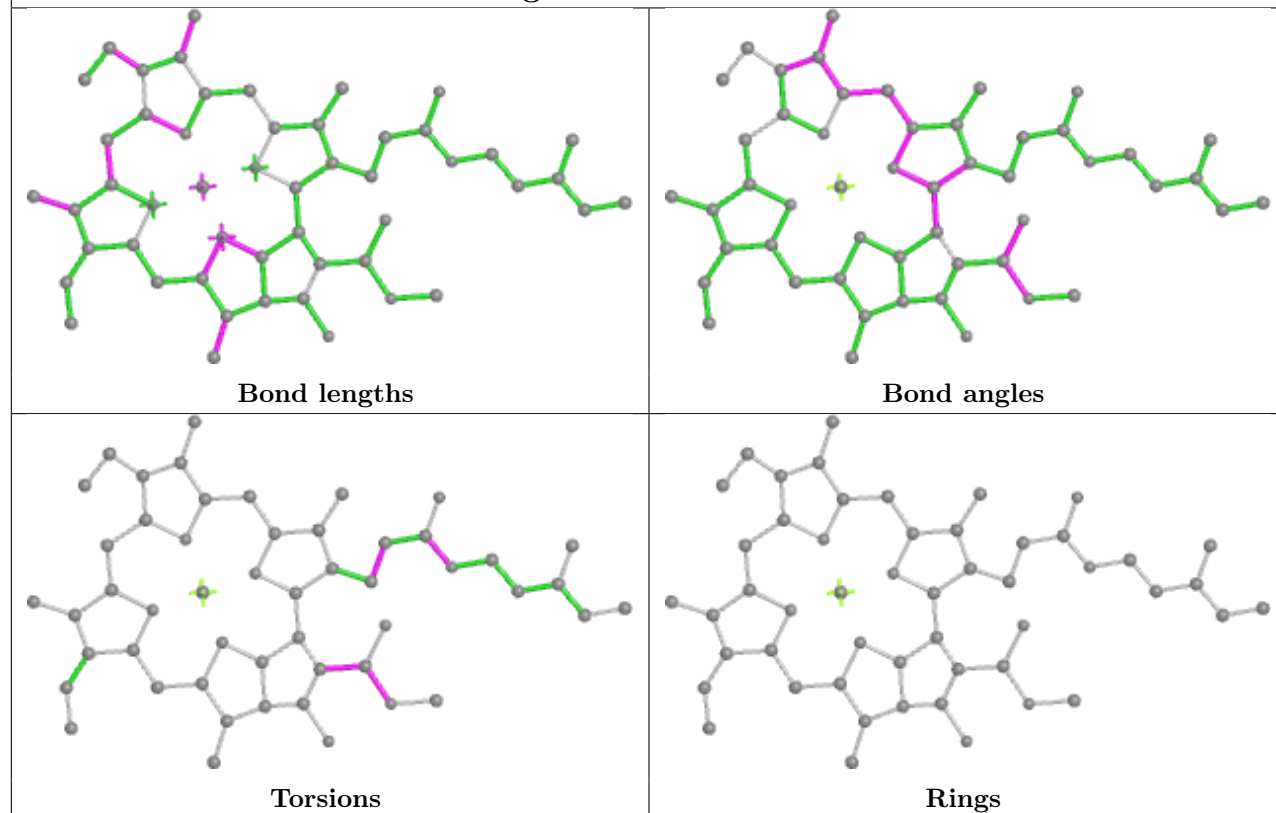




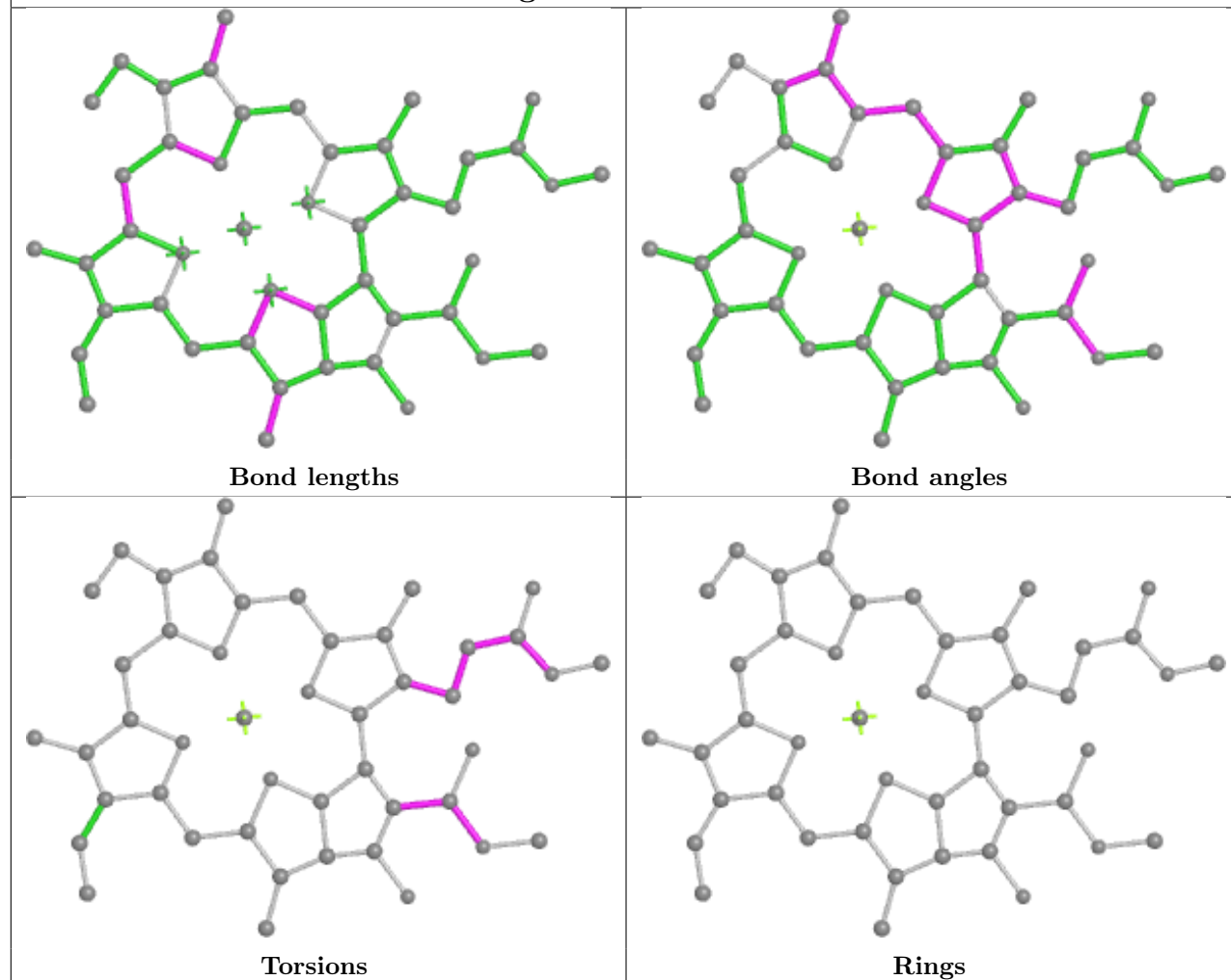
## Ligand CLA A 1139



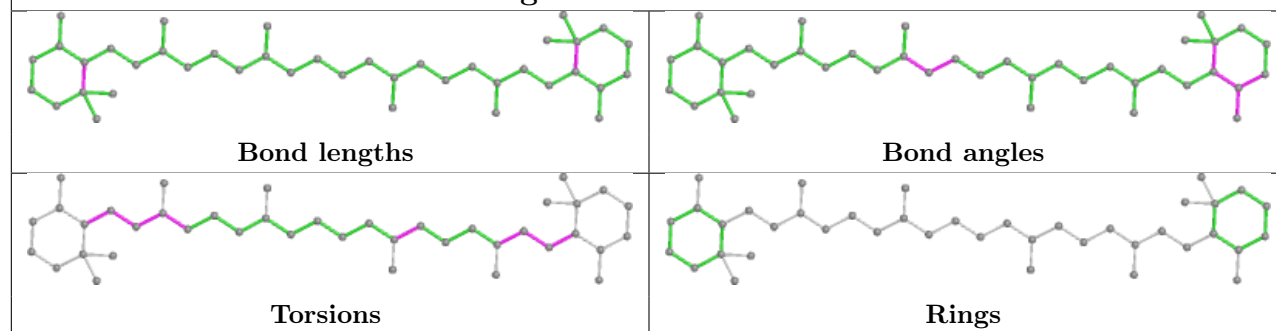
## Ligand CLA A 1135



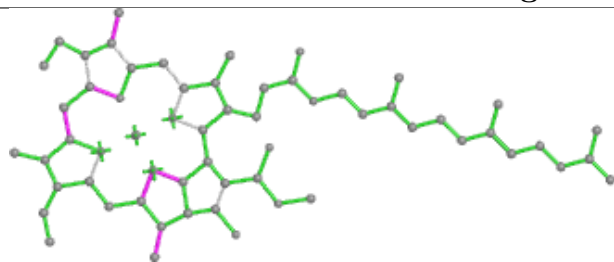
## Ligand CLA r 503



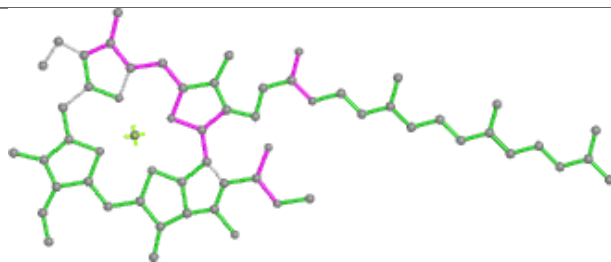
## Ligand BCR K 1501



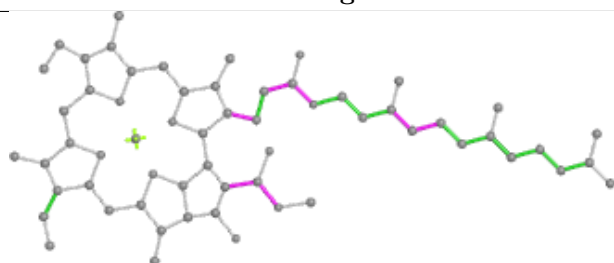
## Ligand CLA t 507



Bond lengths



Bond angles

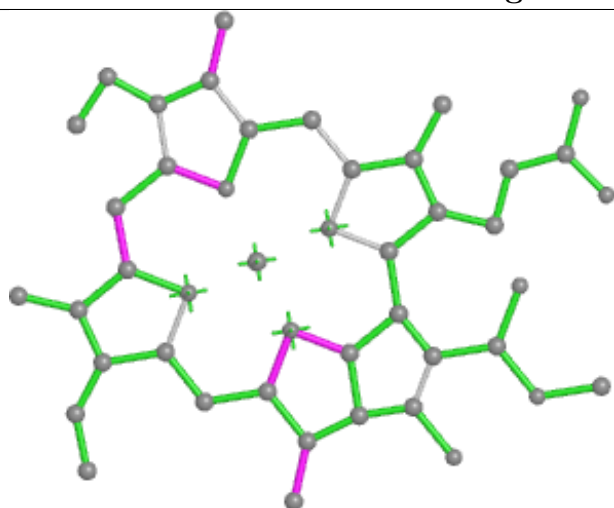


Torsions

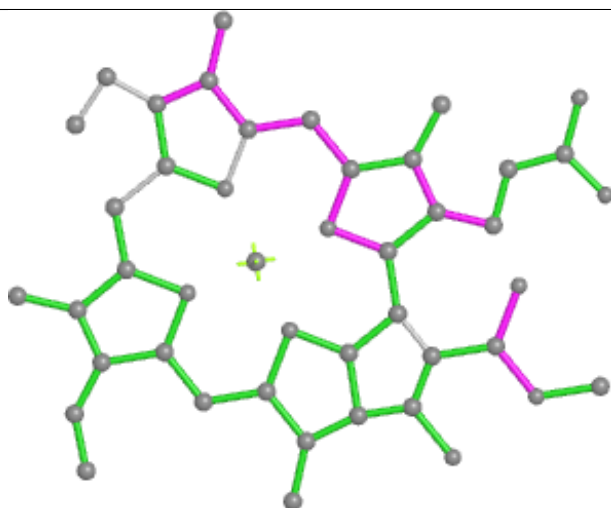


Rings

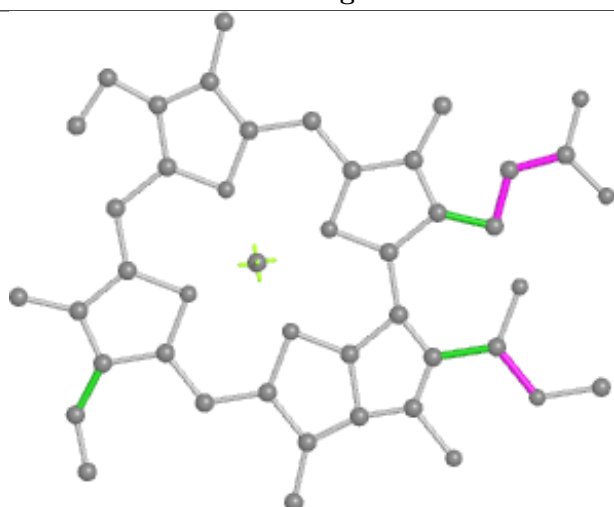
## Ligand CLA B 1209



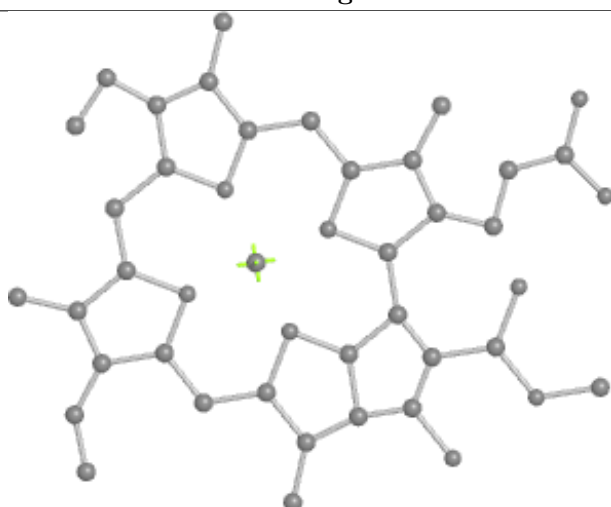
Bond lengths



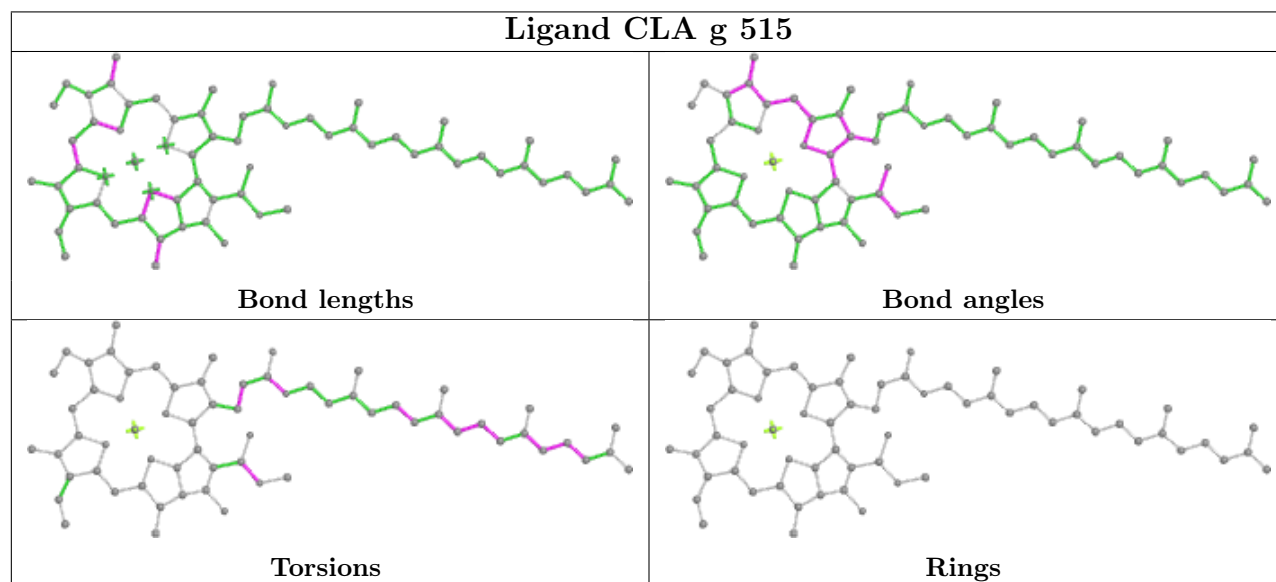
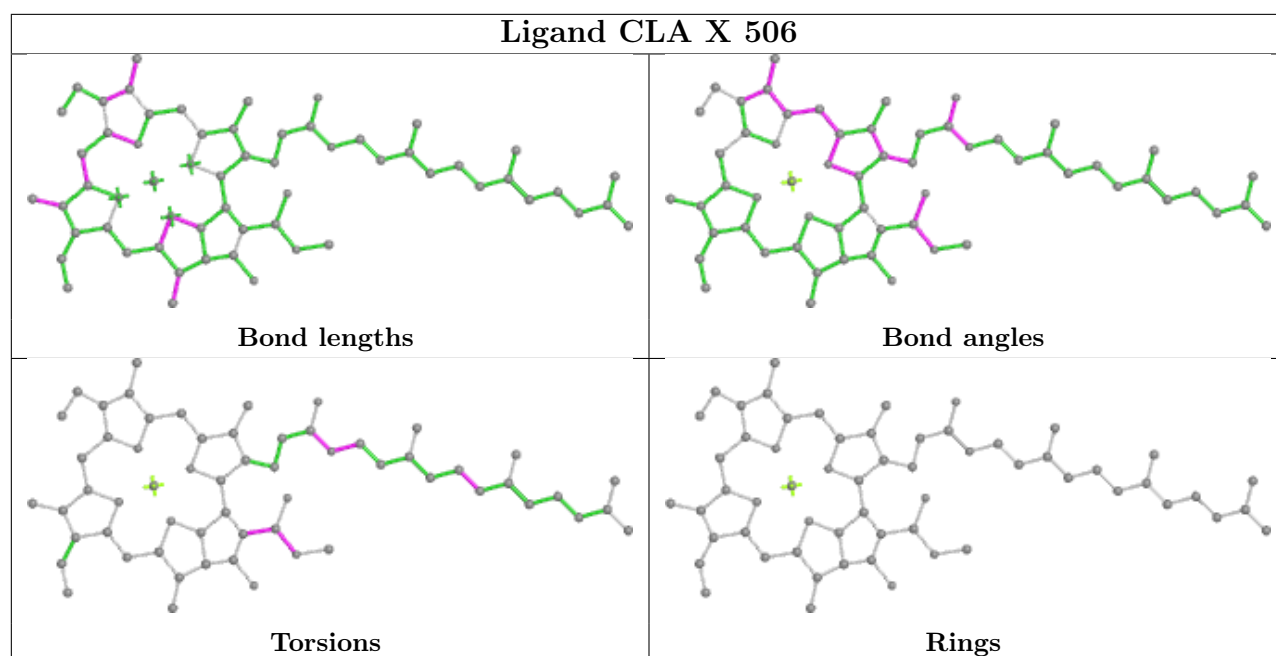
Bond angles

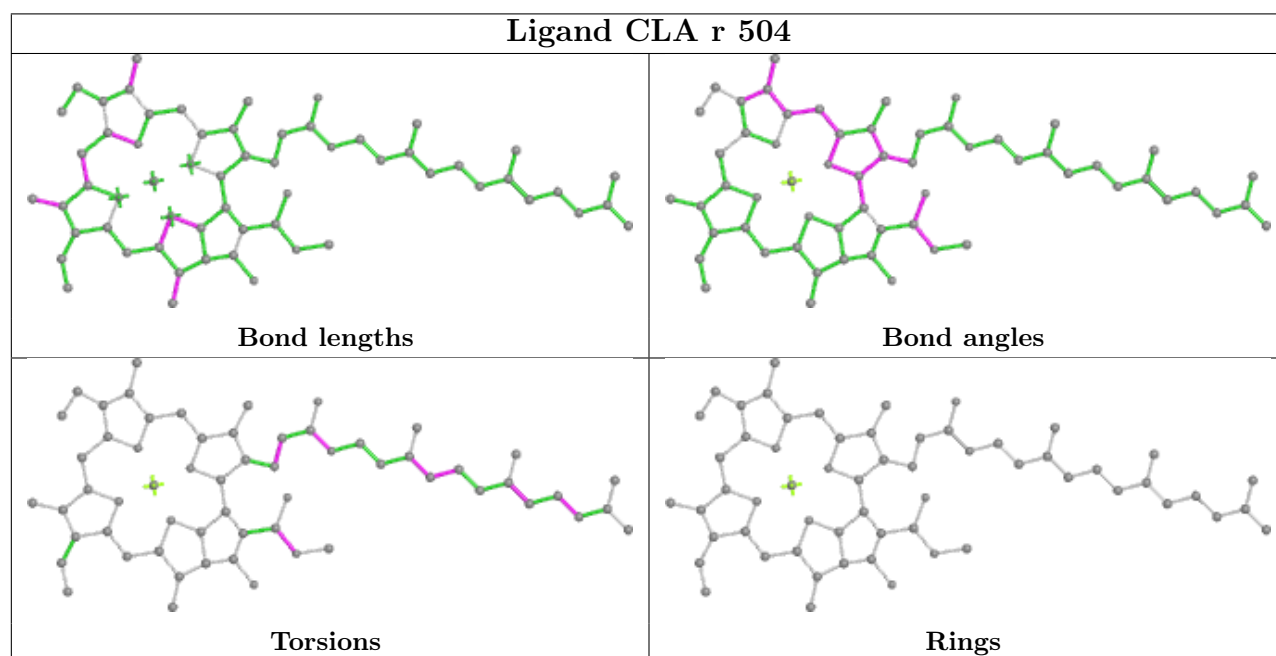
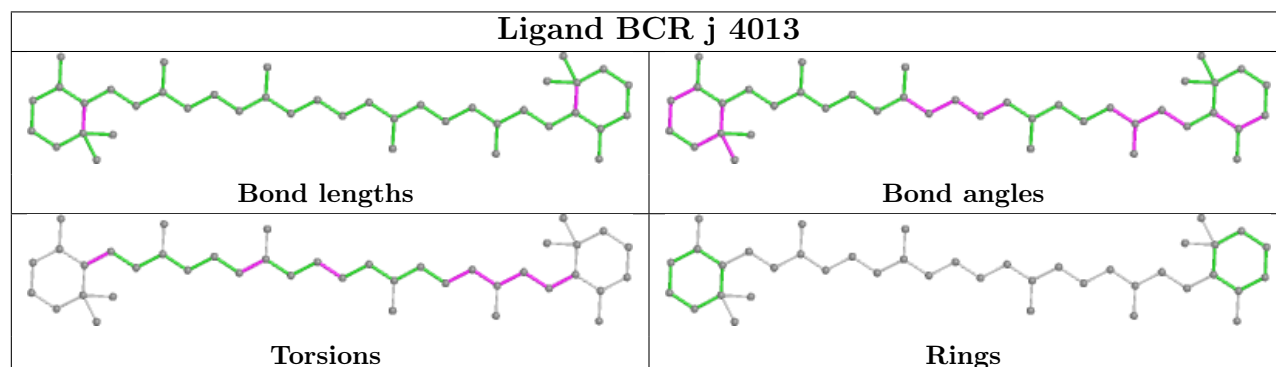
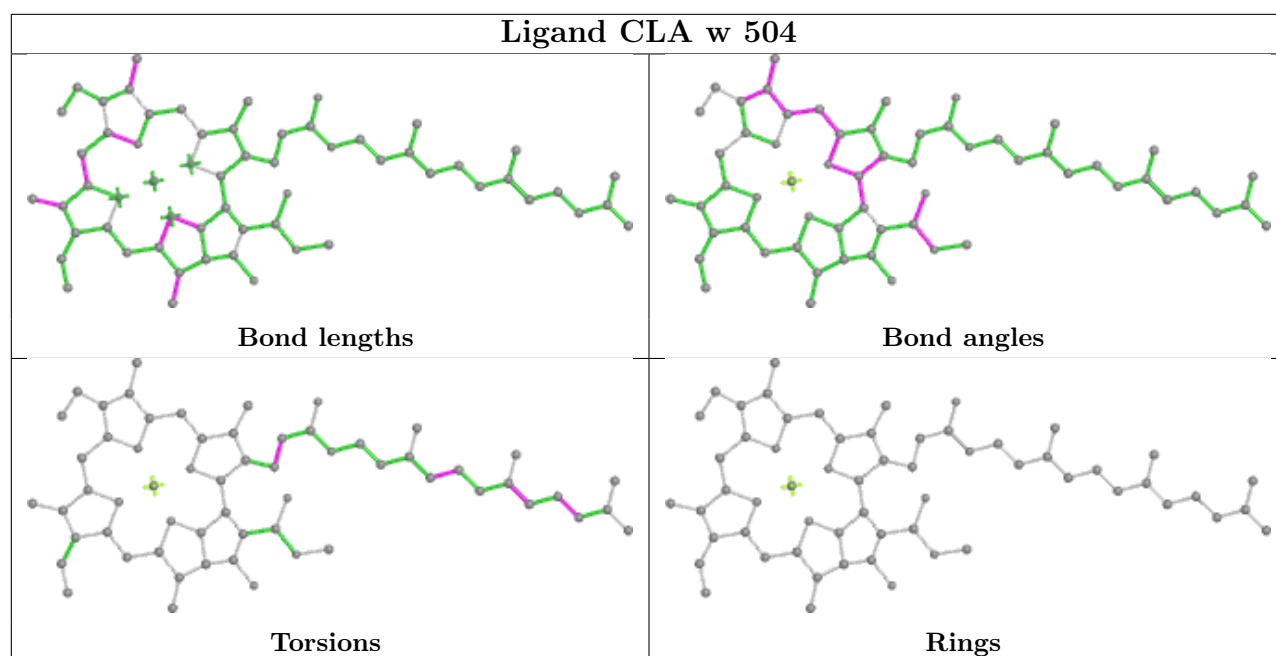


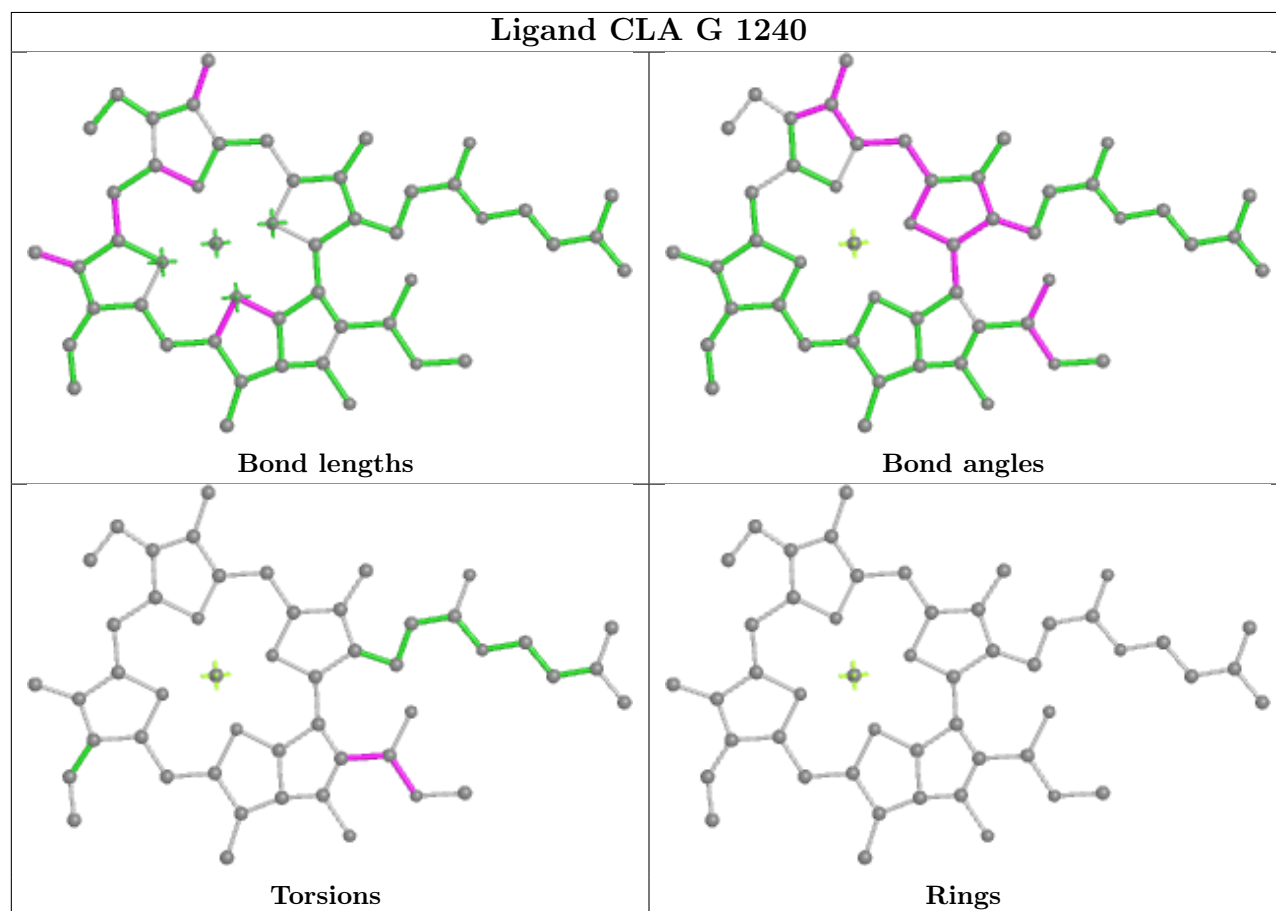
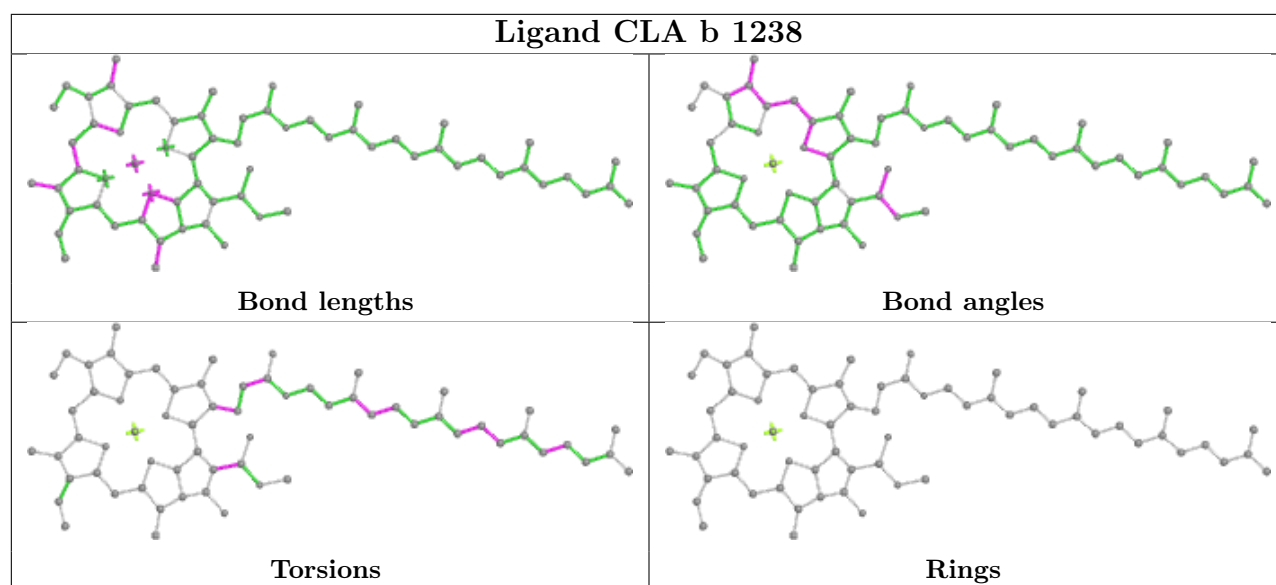
Torsions

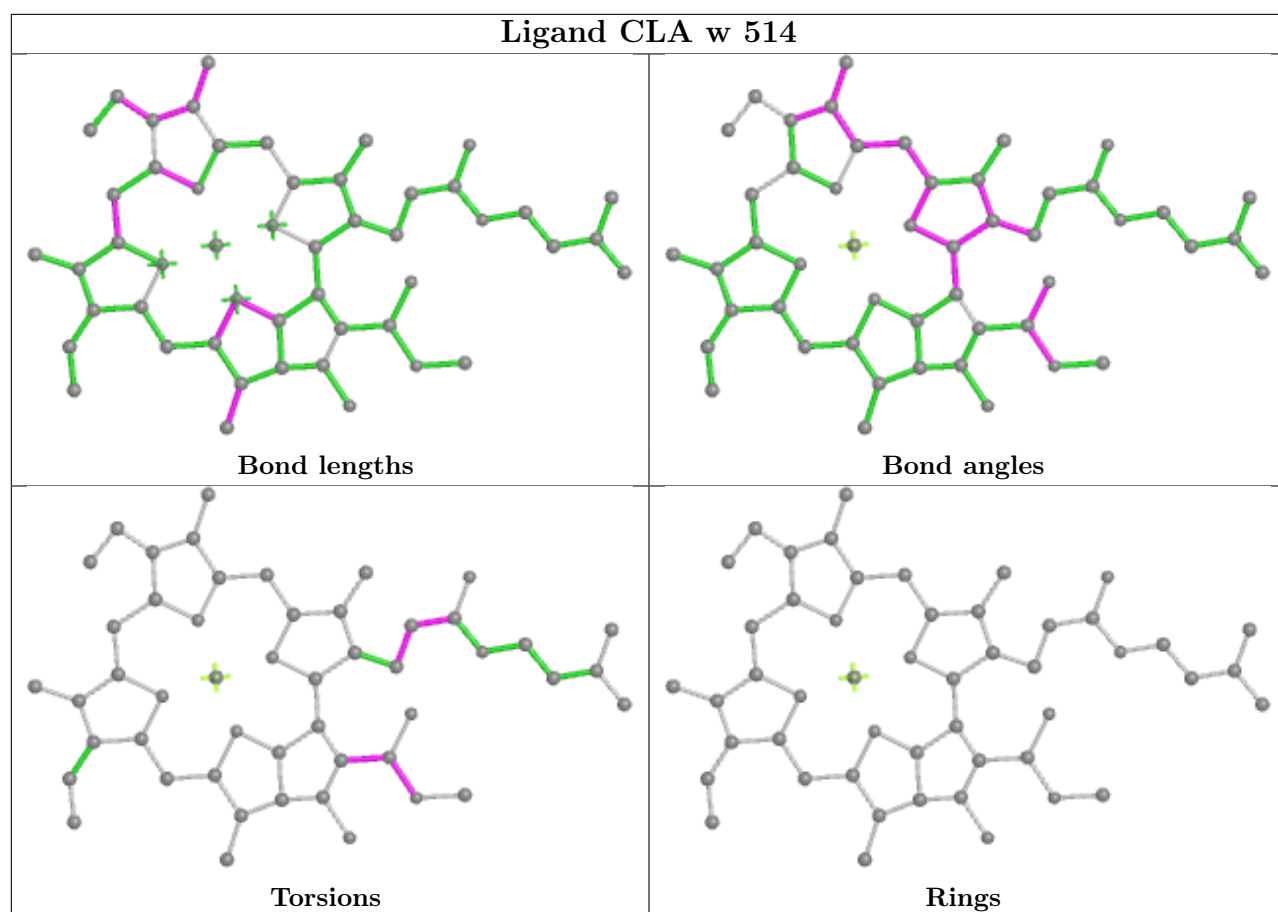


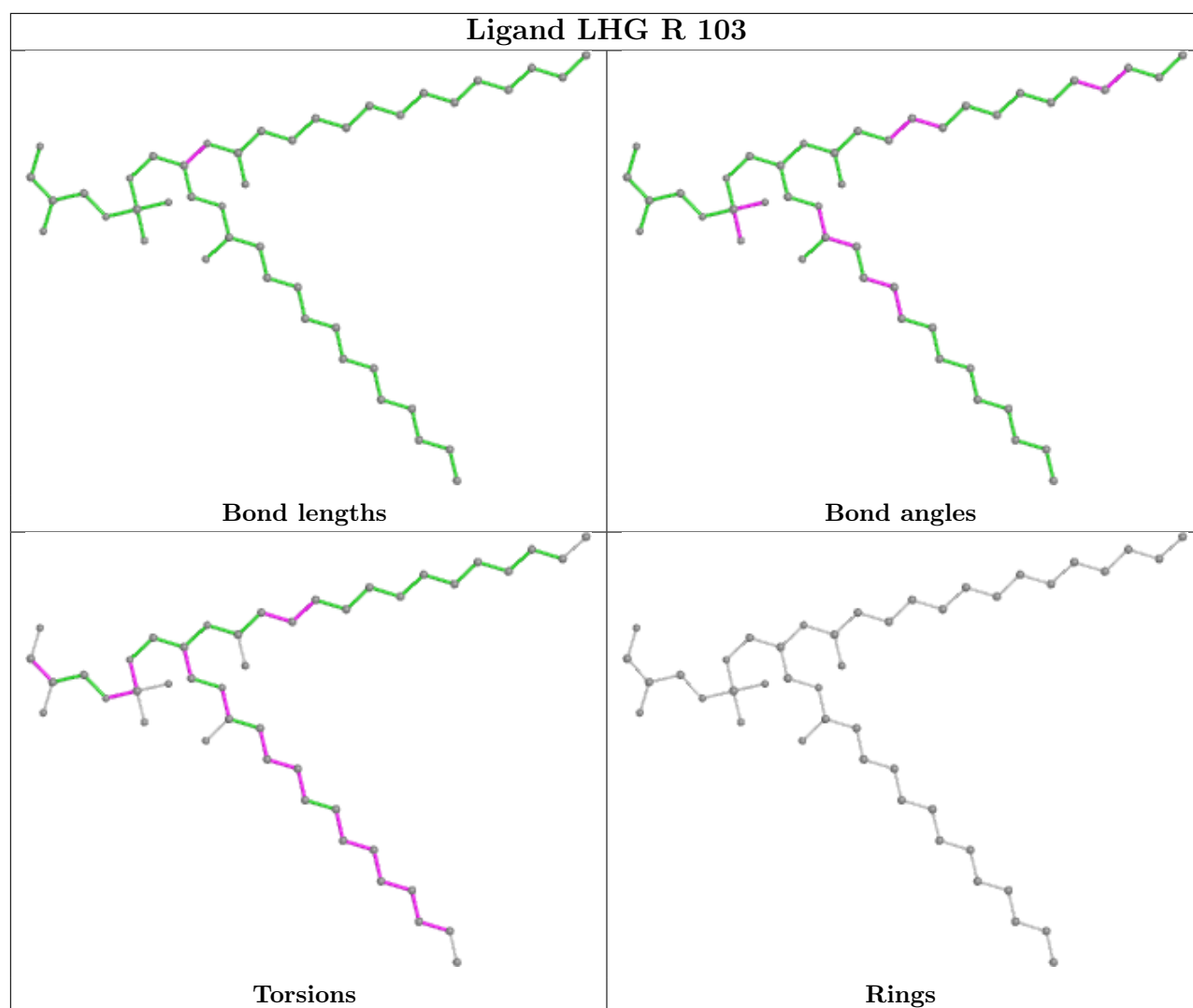
Rings





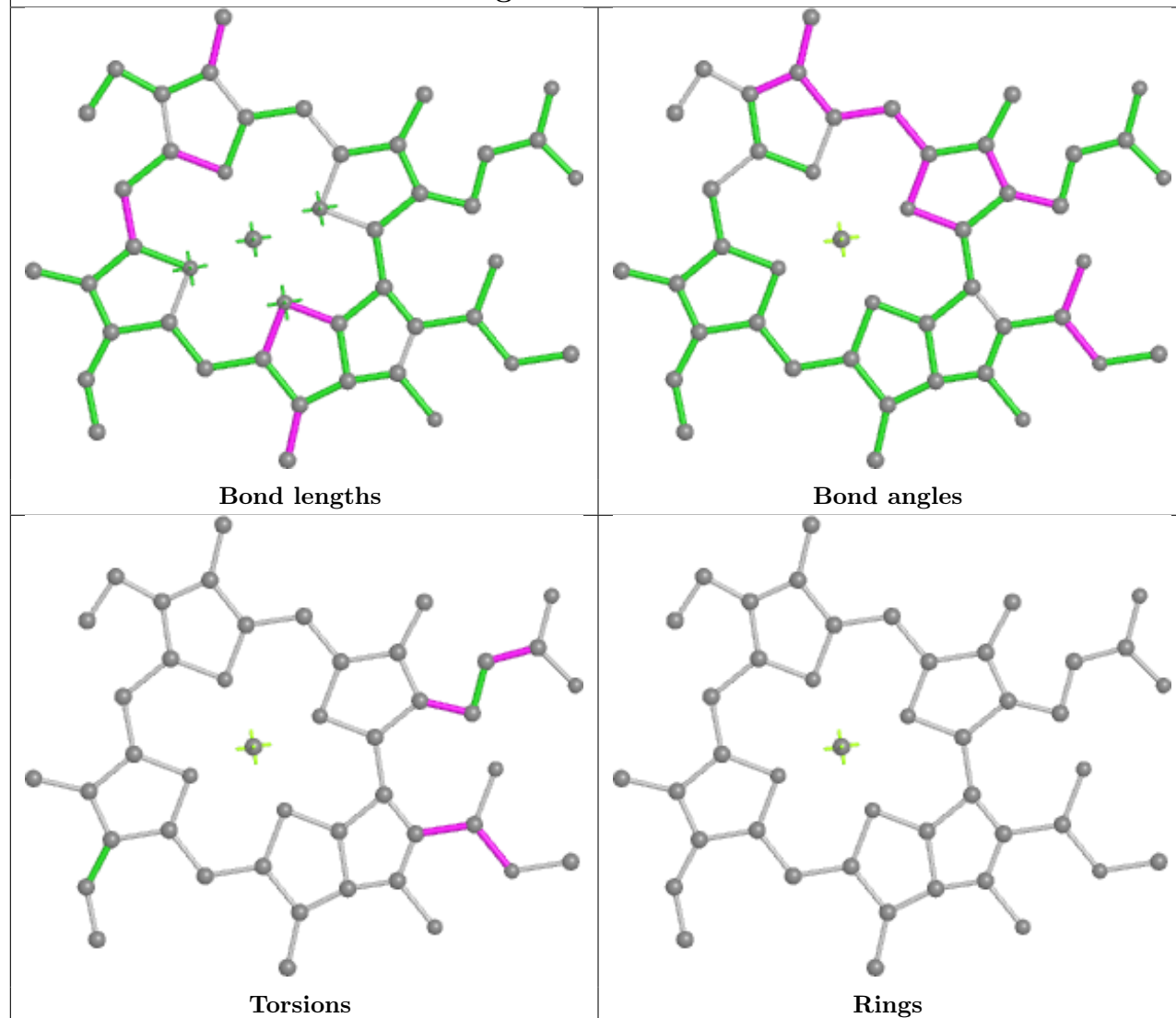




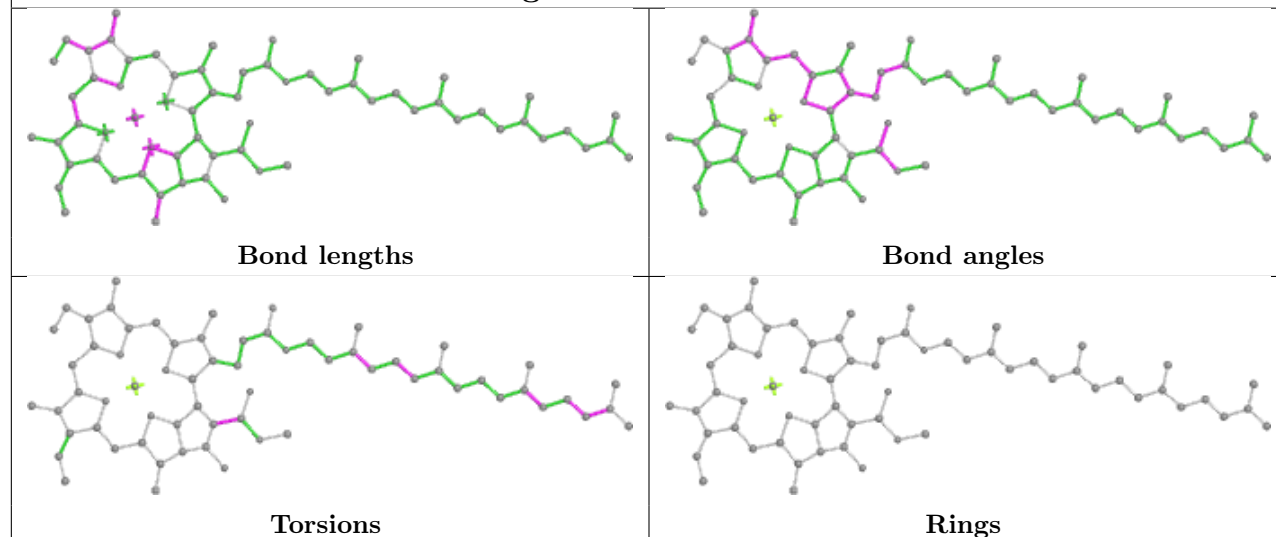


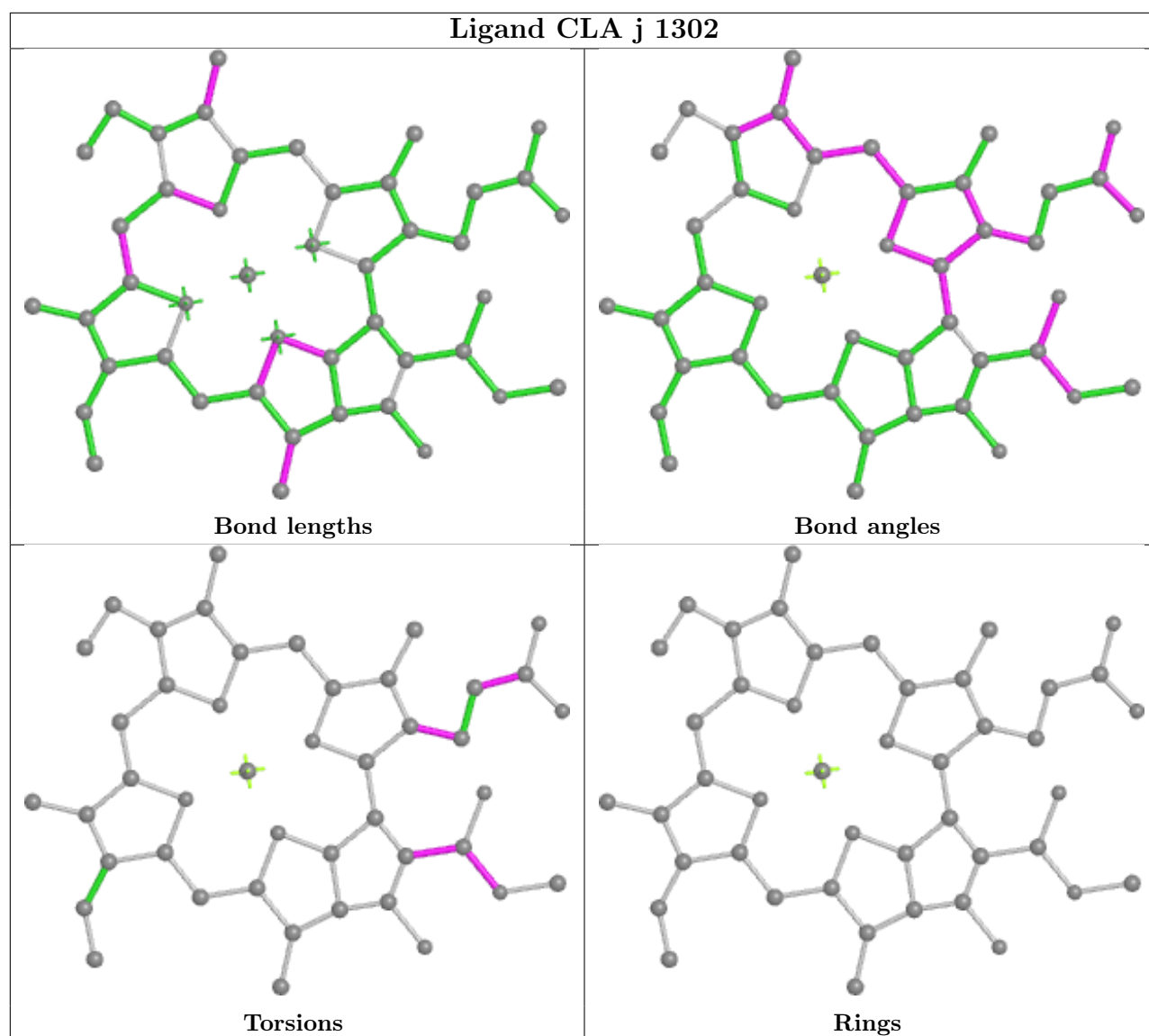


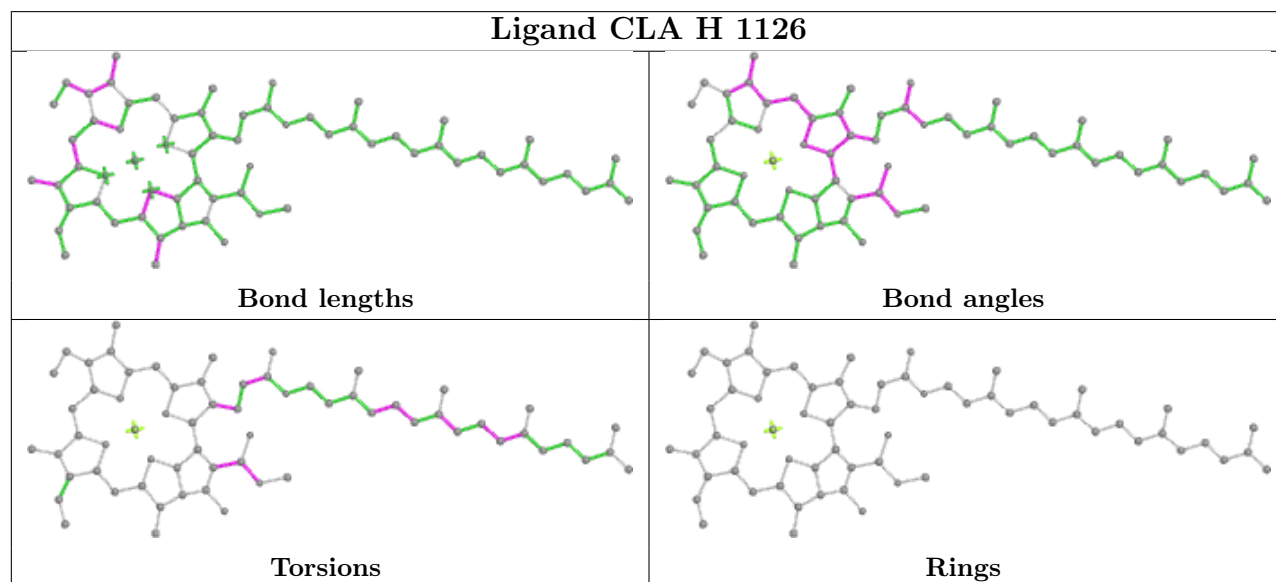
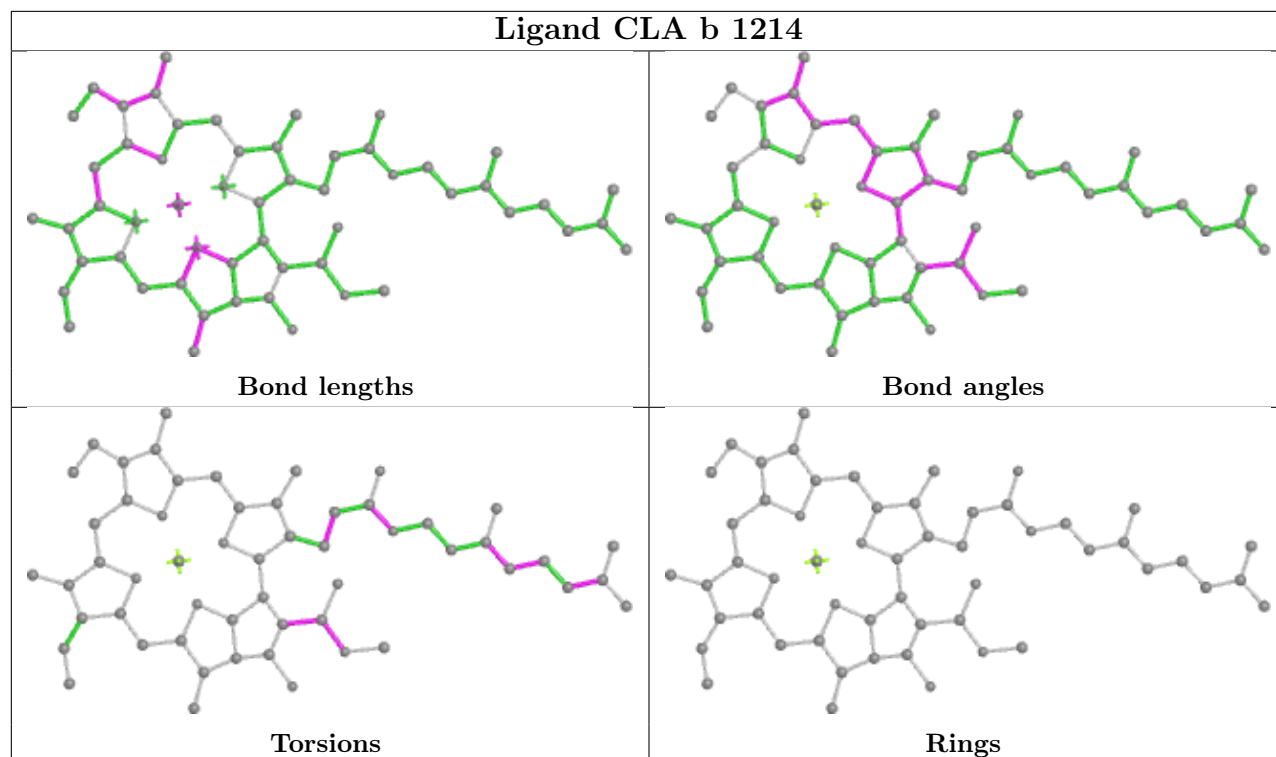
## Ligand CLA r 512

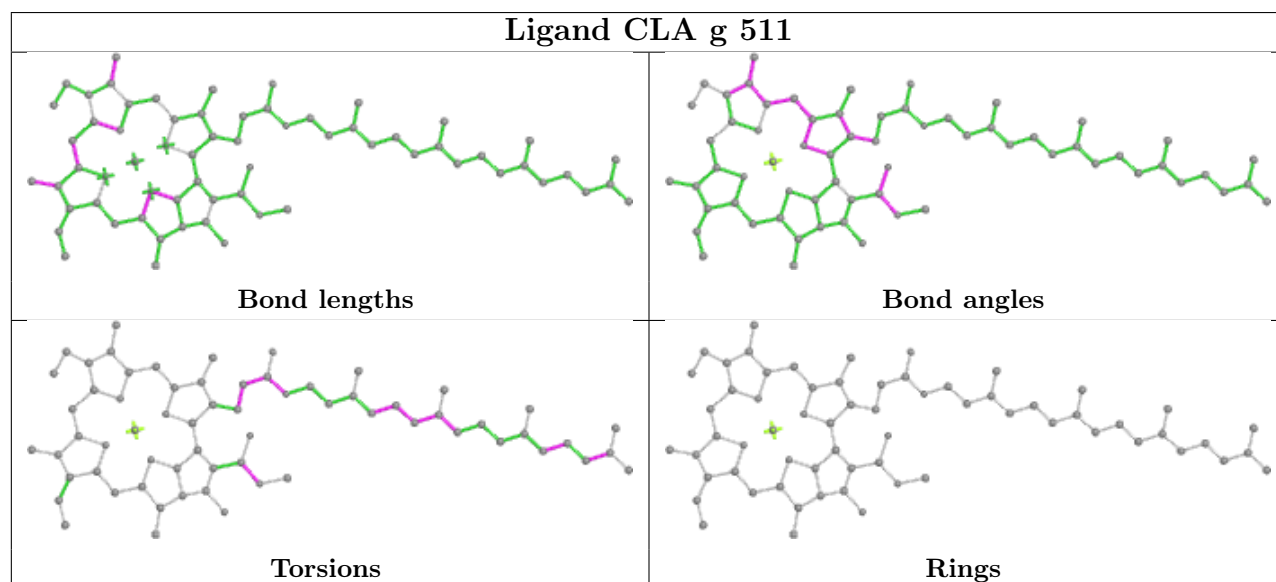
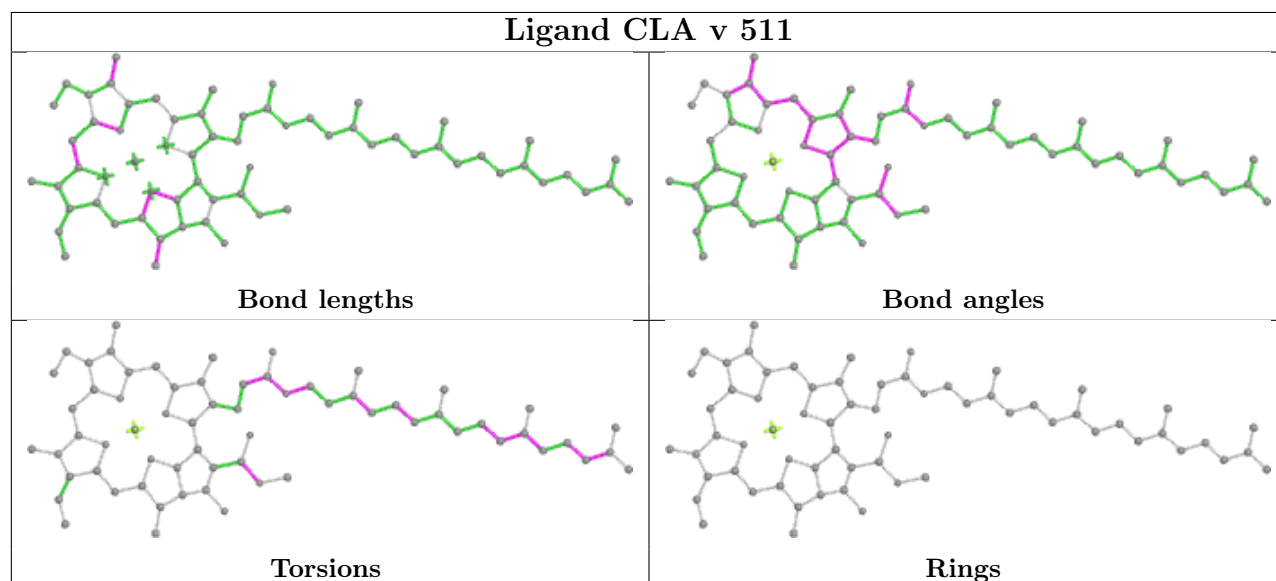
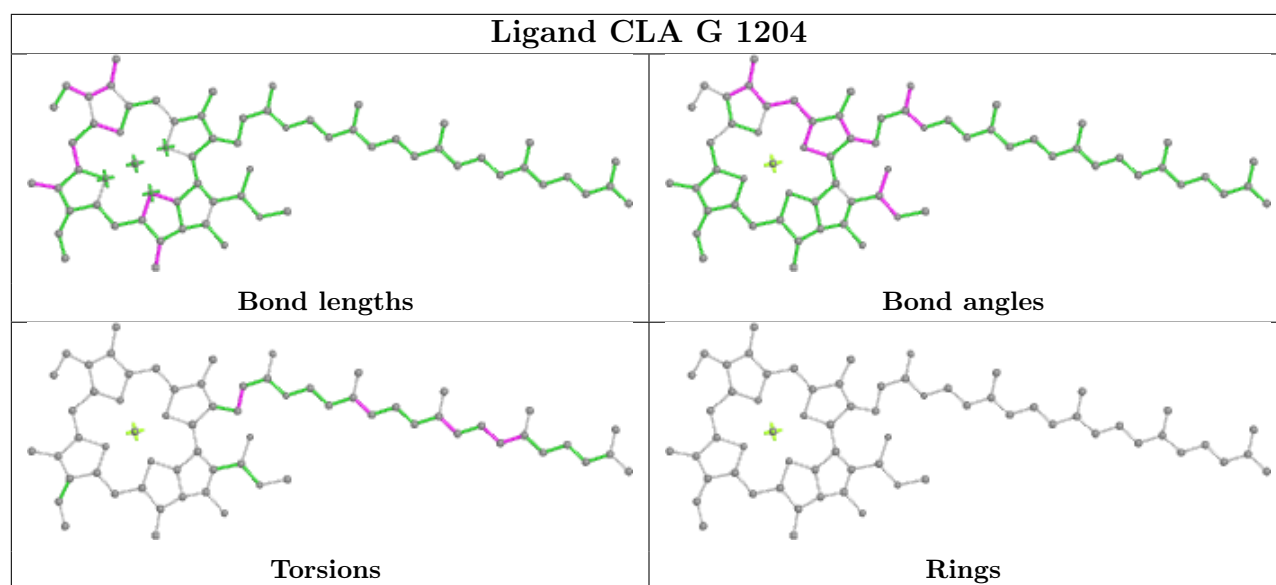


## Ligand CLA H 1124

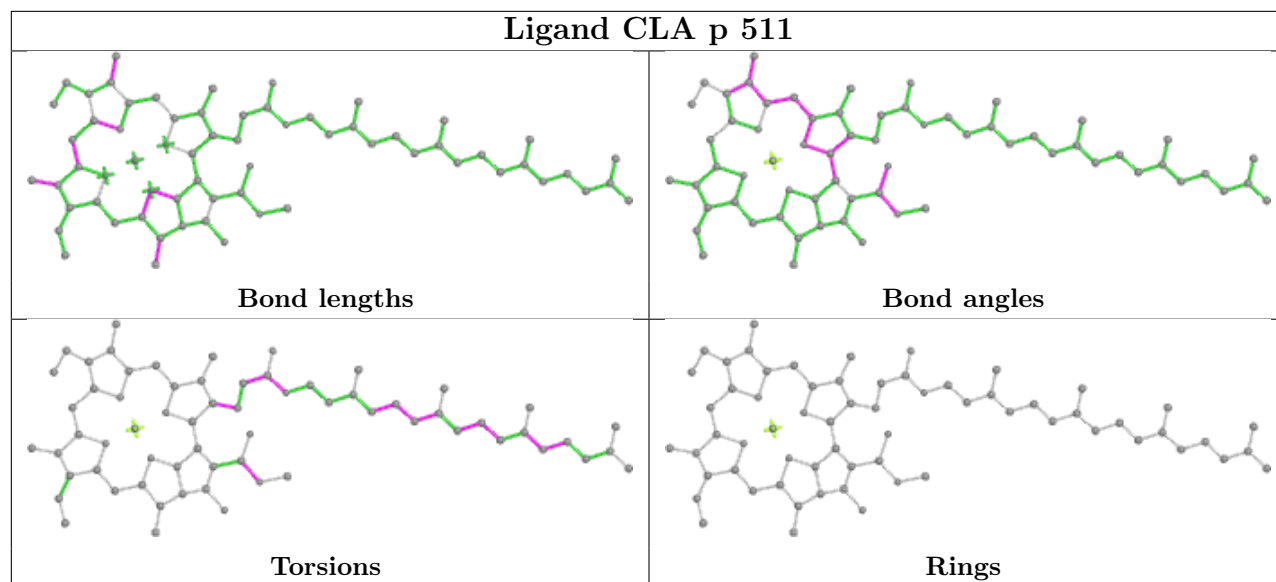




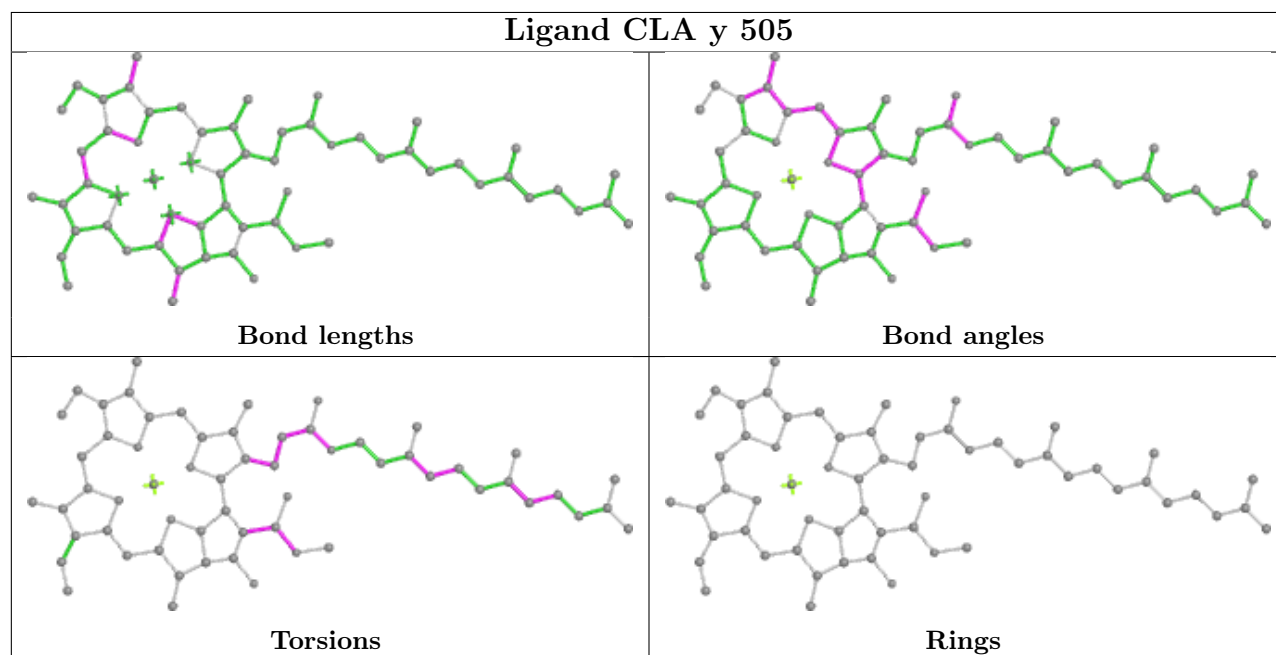


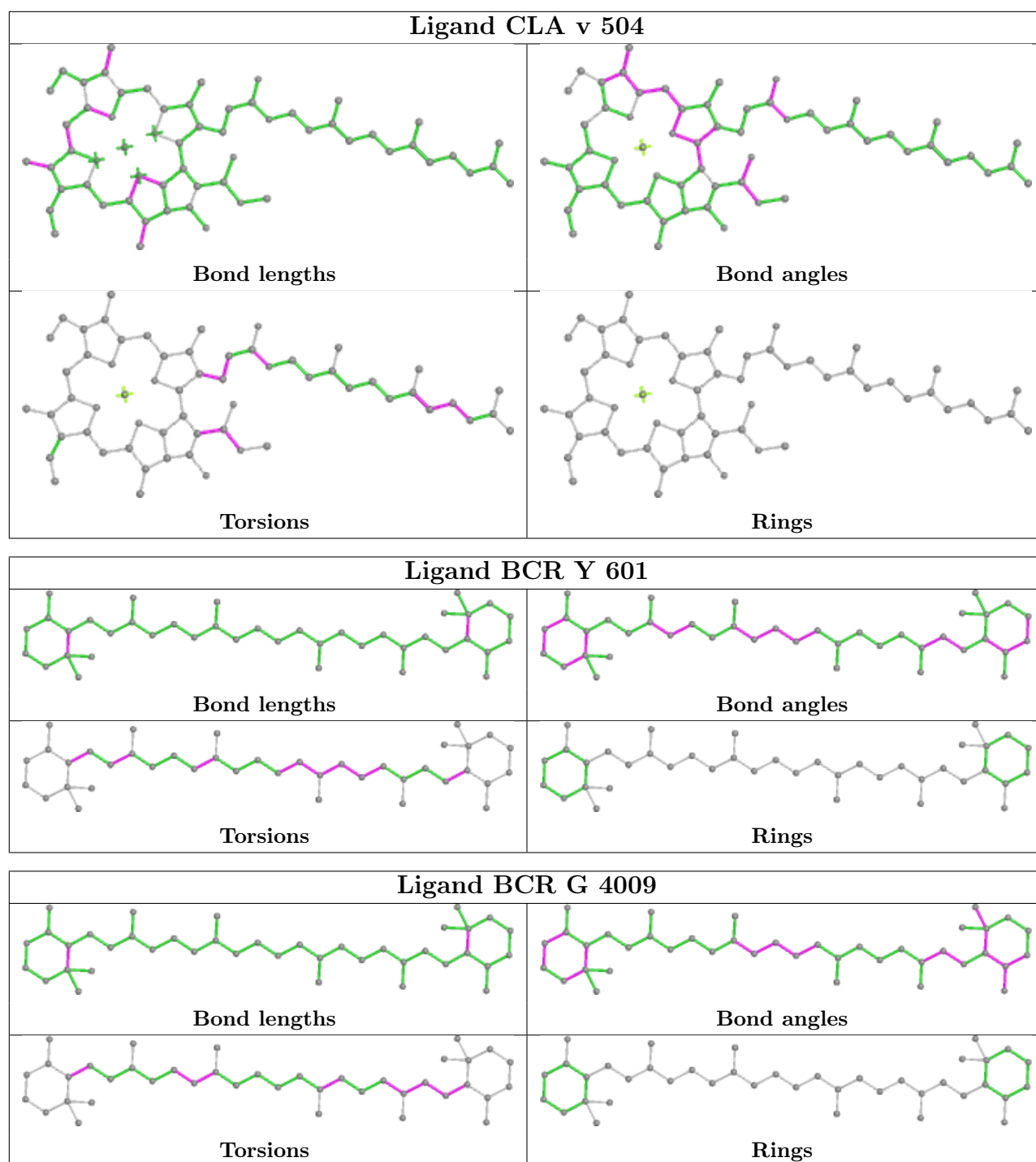


## Ligand CLA p 511

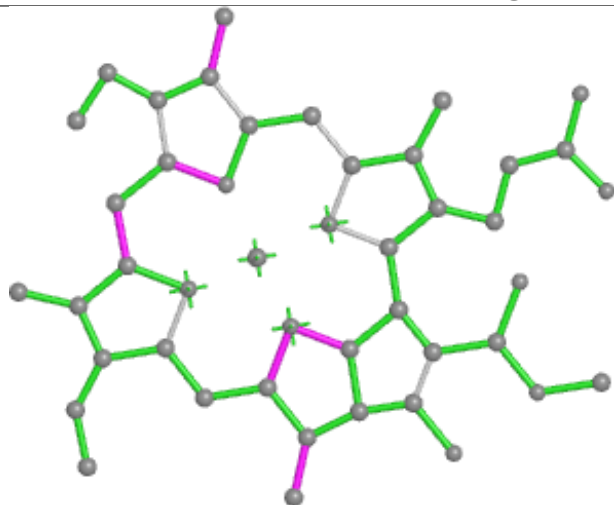


## Ligand CLA y 505

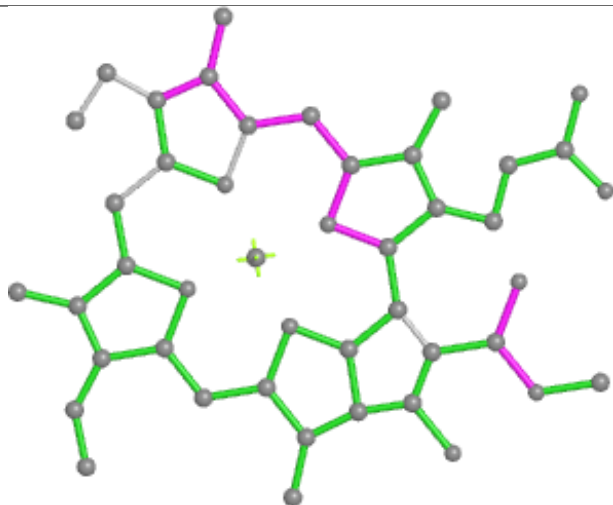




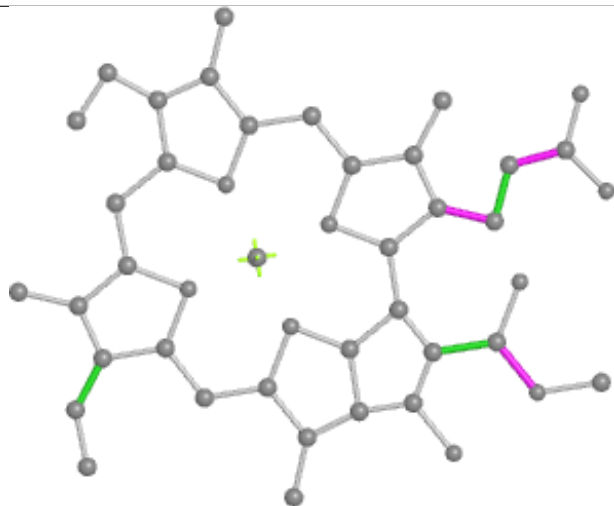
## Ligand CLA B 1217



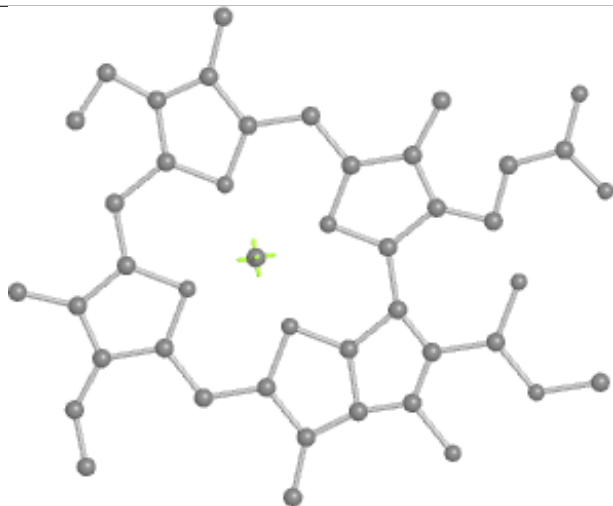
Bond lengths



Bond angles

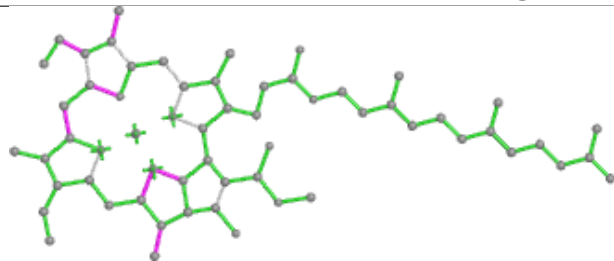


Torsions

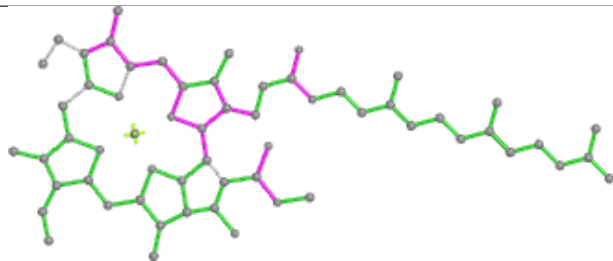


Rings

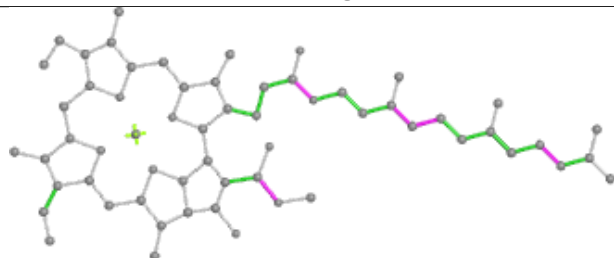
## Ligand CLA X 509



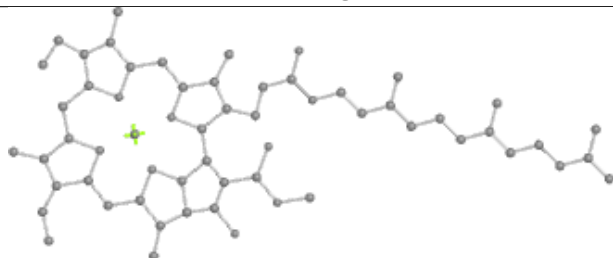
Bond lengths



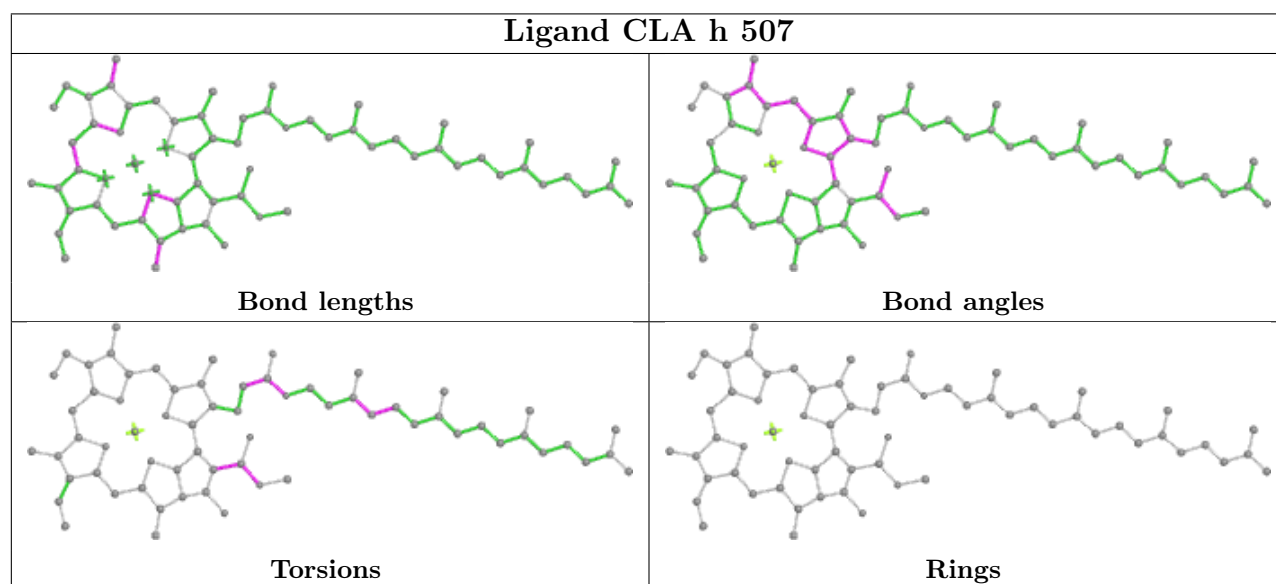
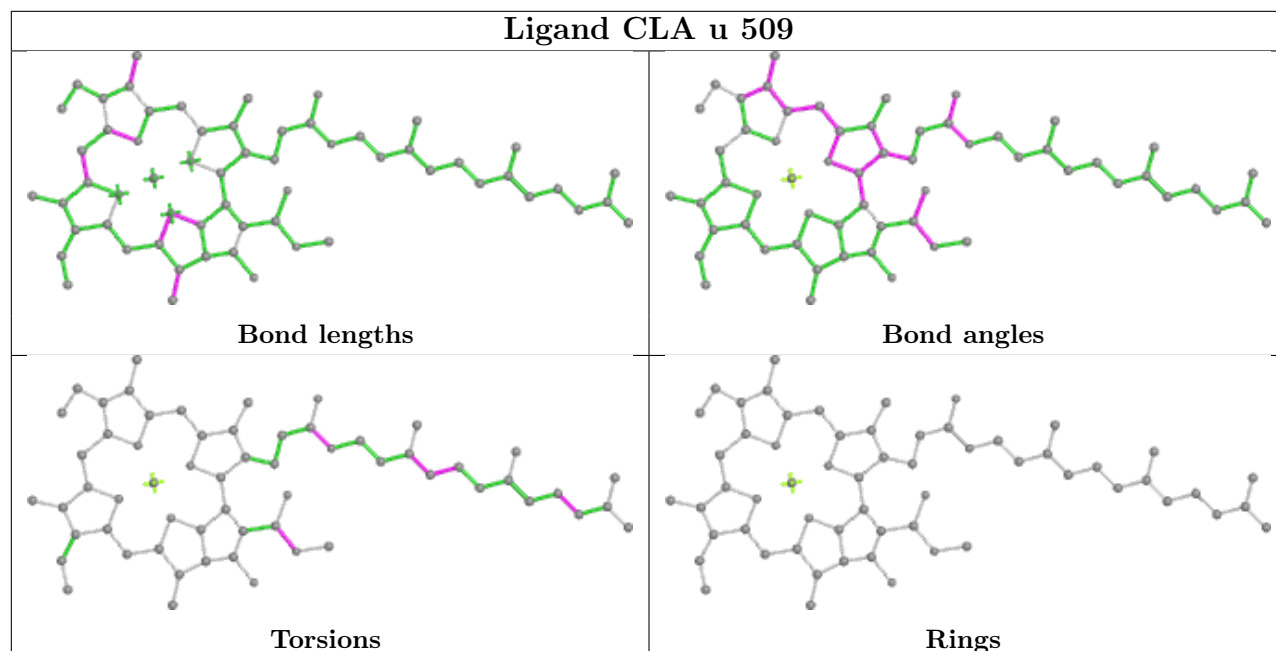
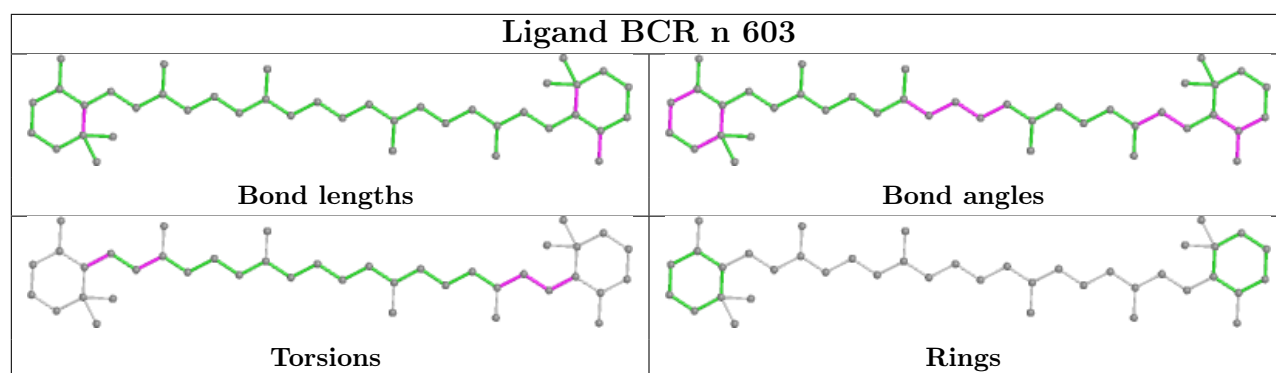
Bond angles



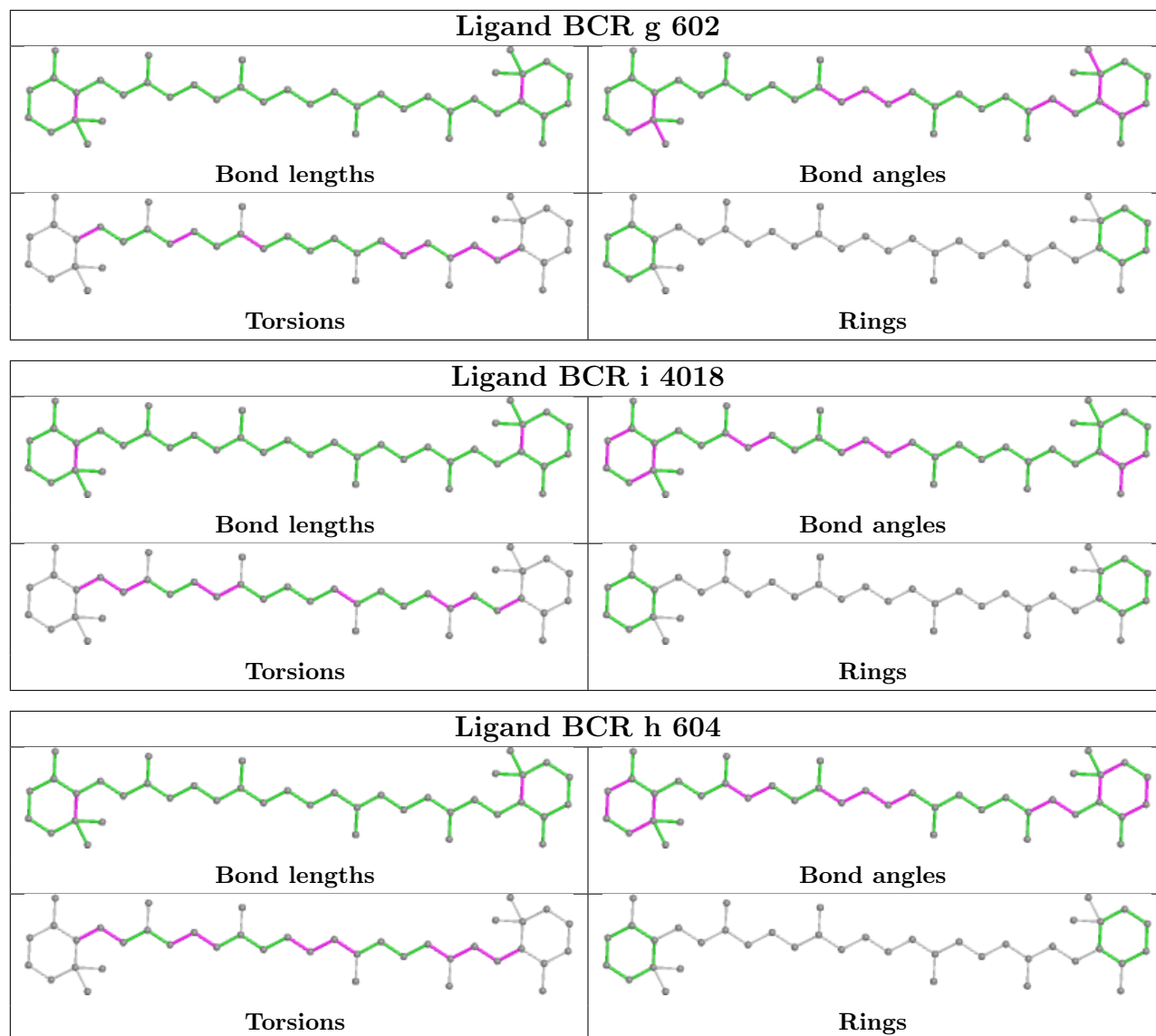
Torsions

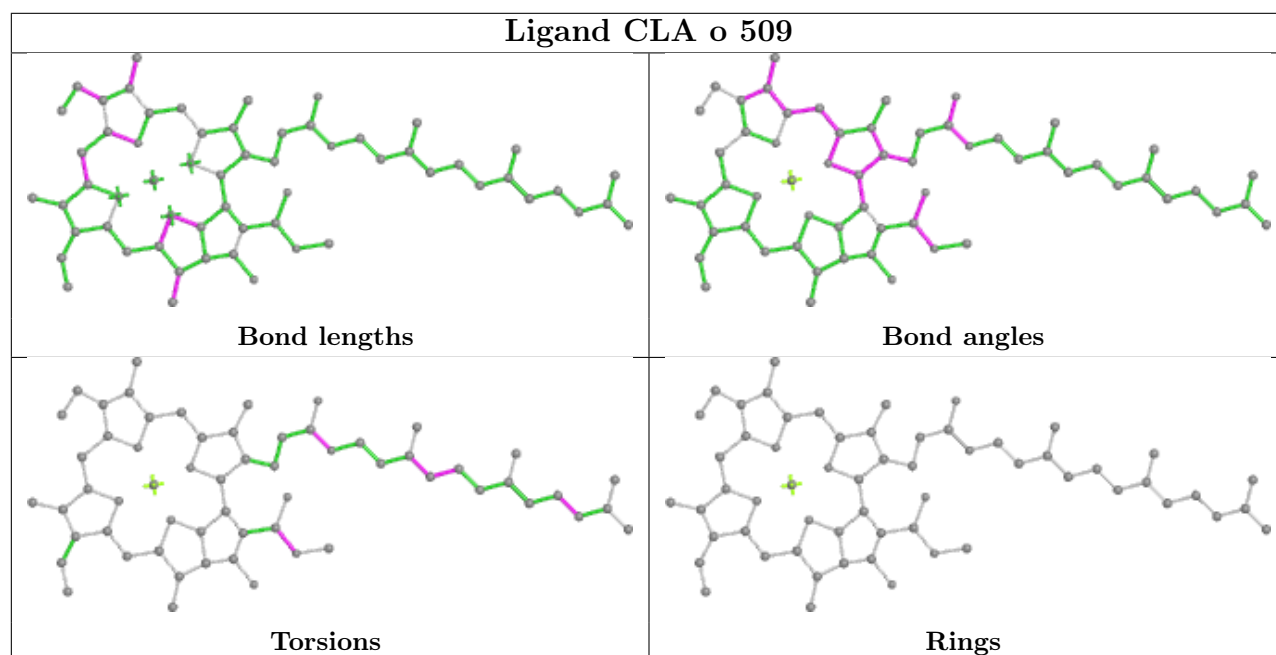
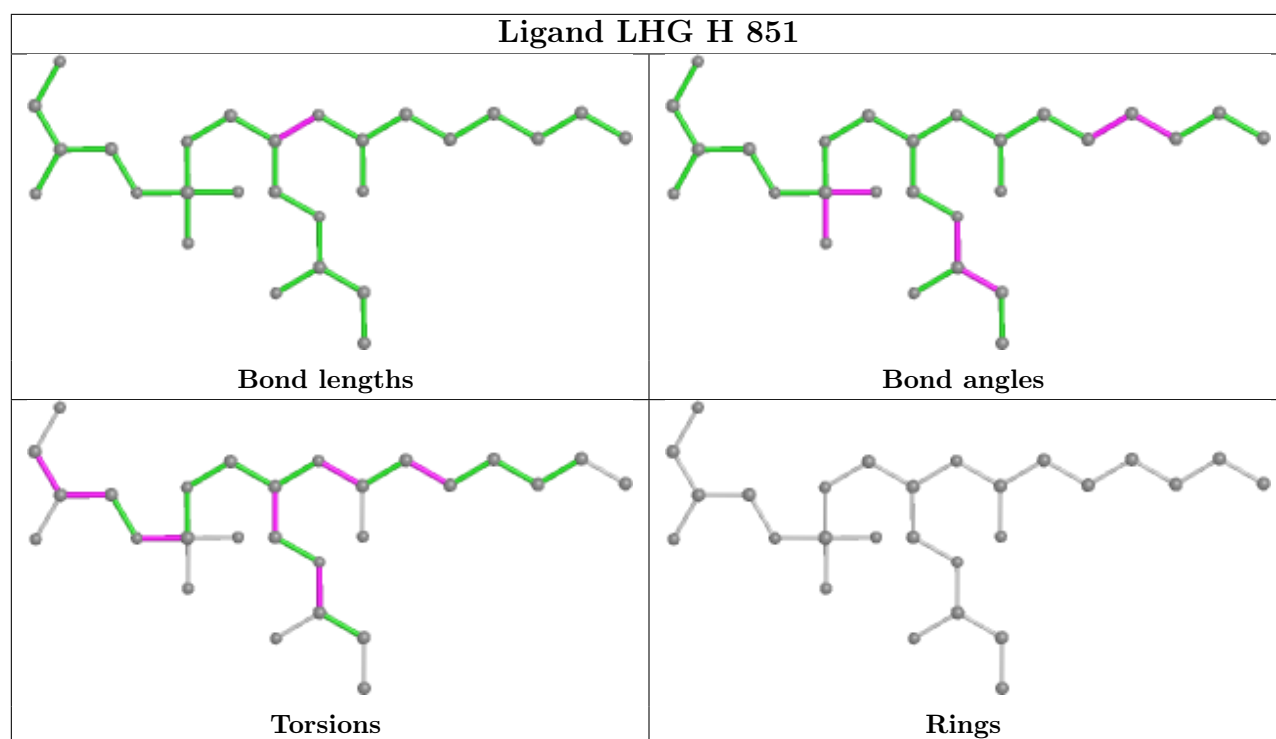


Rings

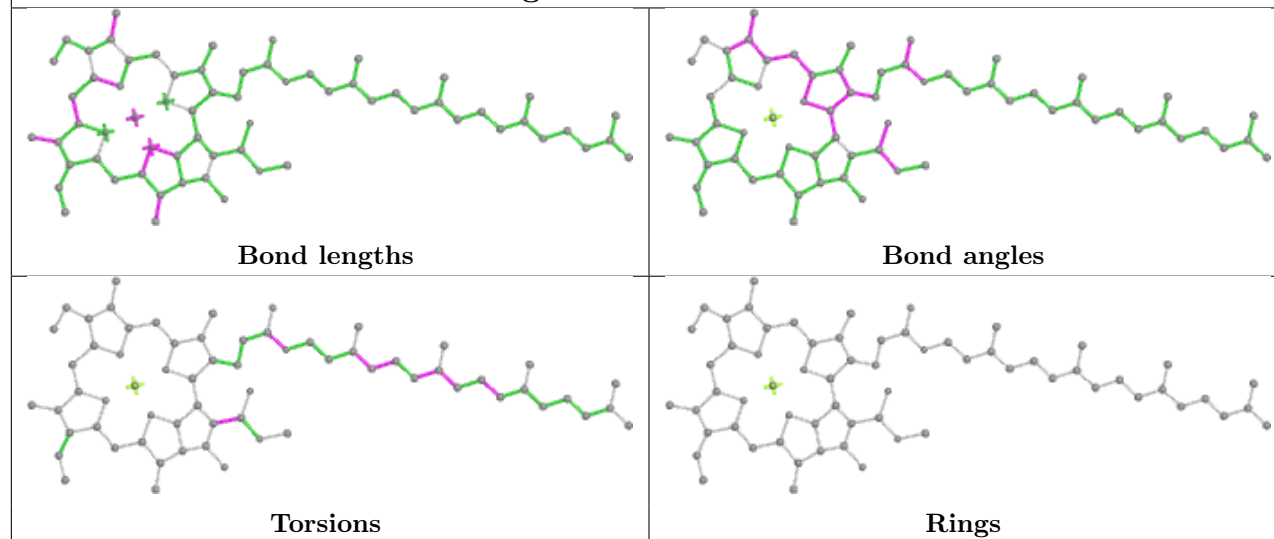




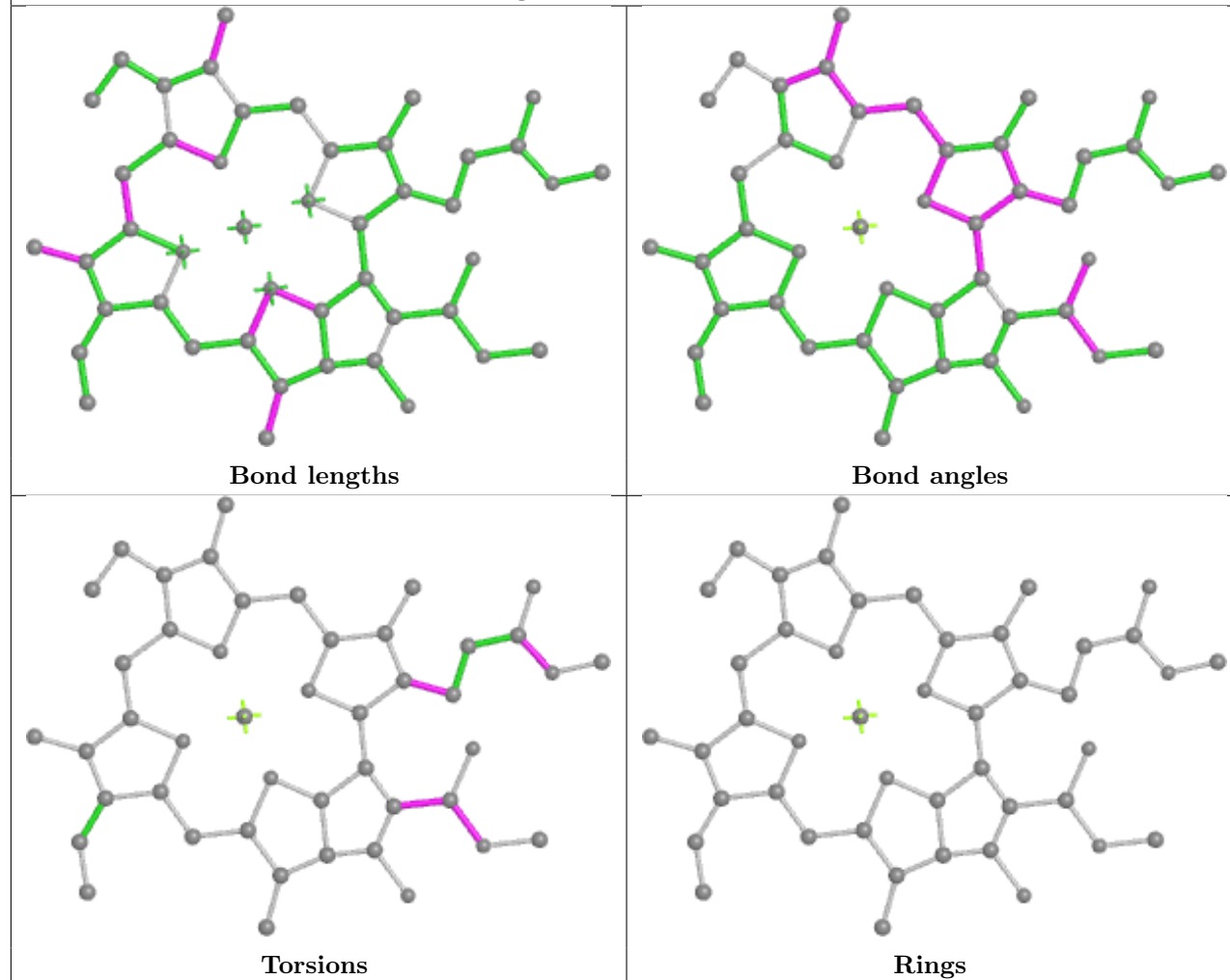




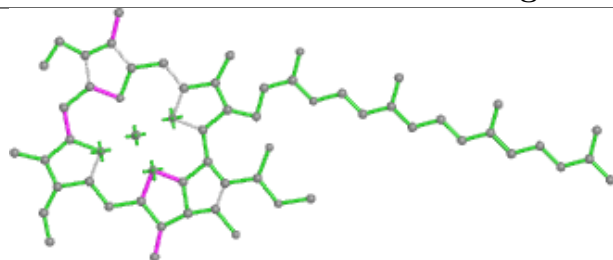
## Ligand CLA H 1125



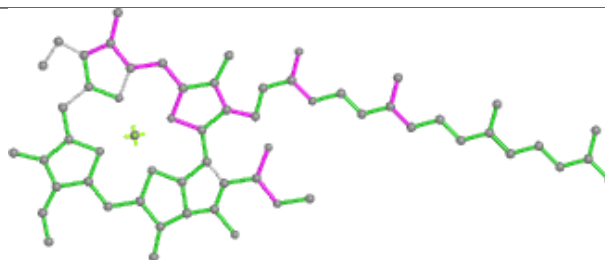
## Ligand CLA X 503



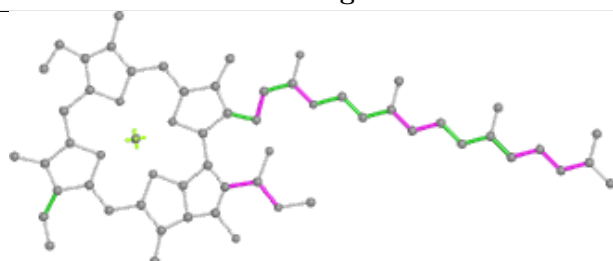
## Ligand CLA r 506



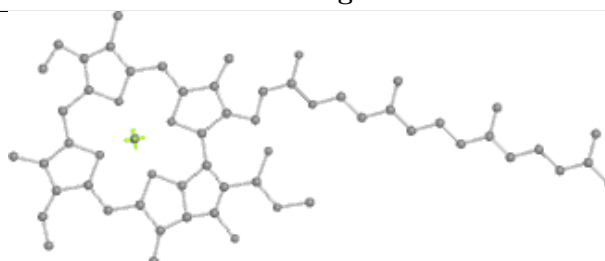
Bond lengths



Bond angles

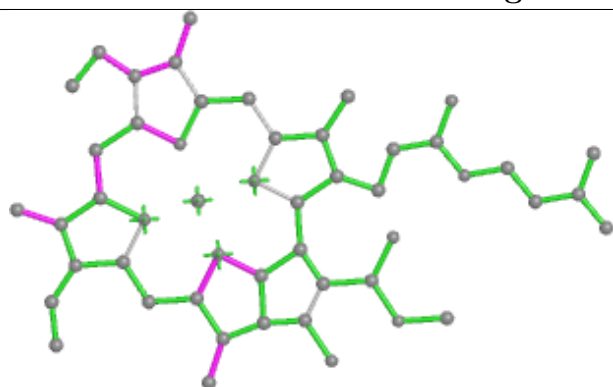


Torsions

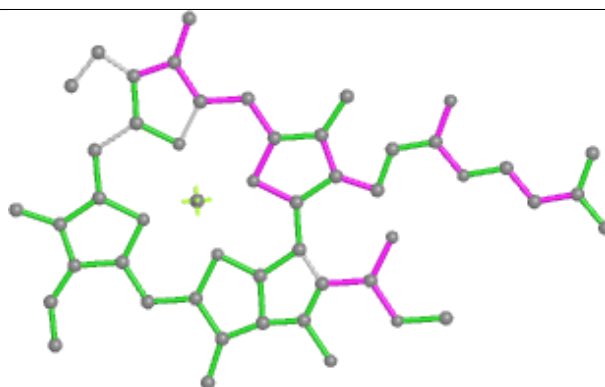


Rings

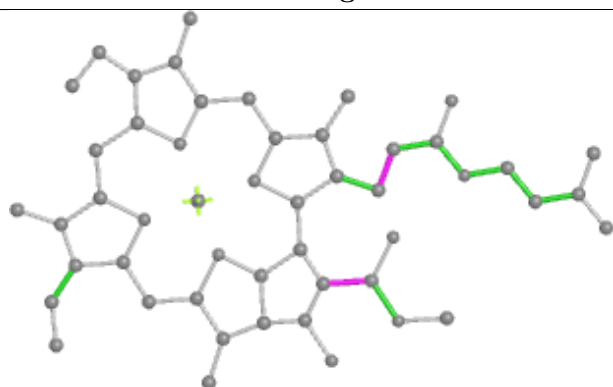
## Ligand CLA A 1129



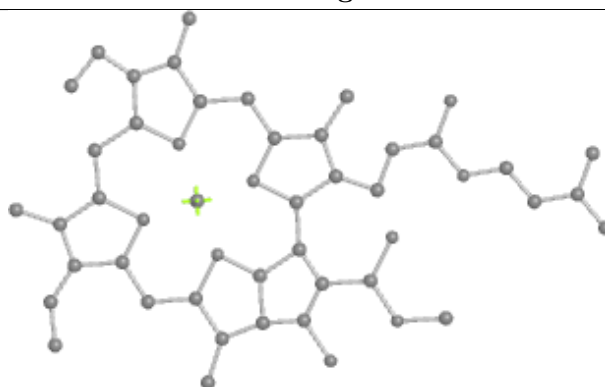
Bond lengths



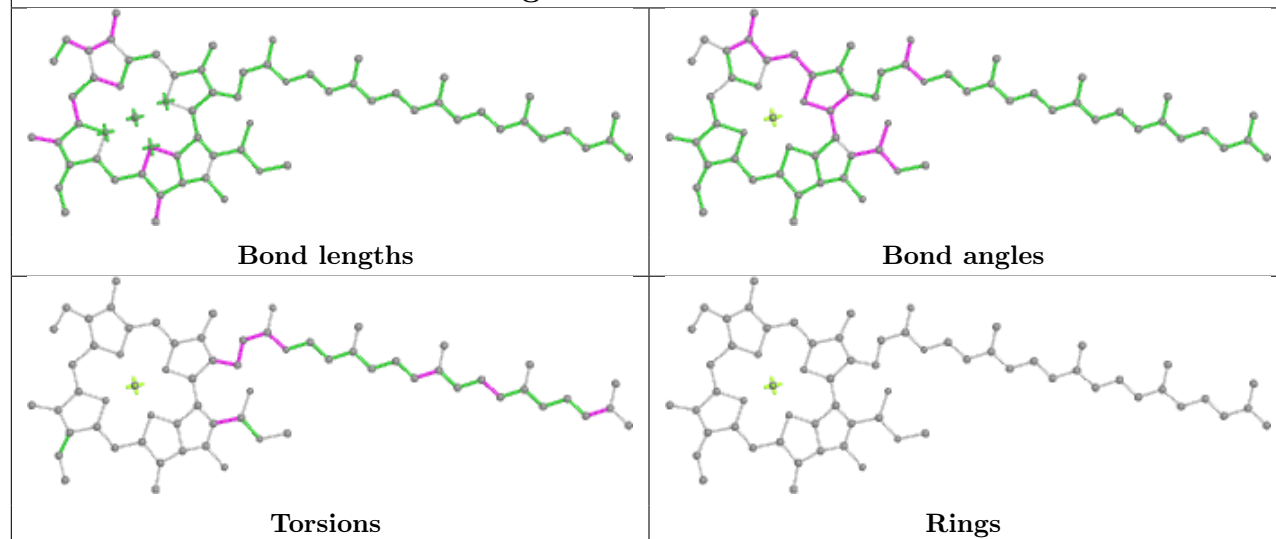
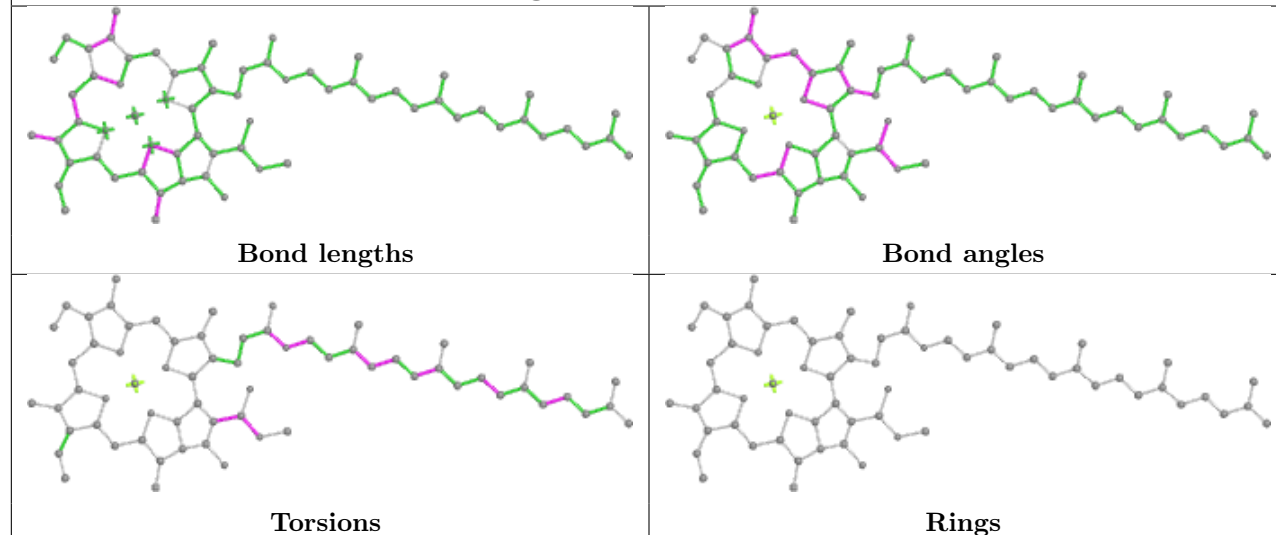
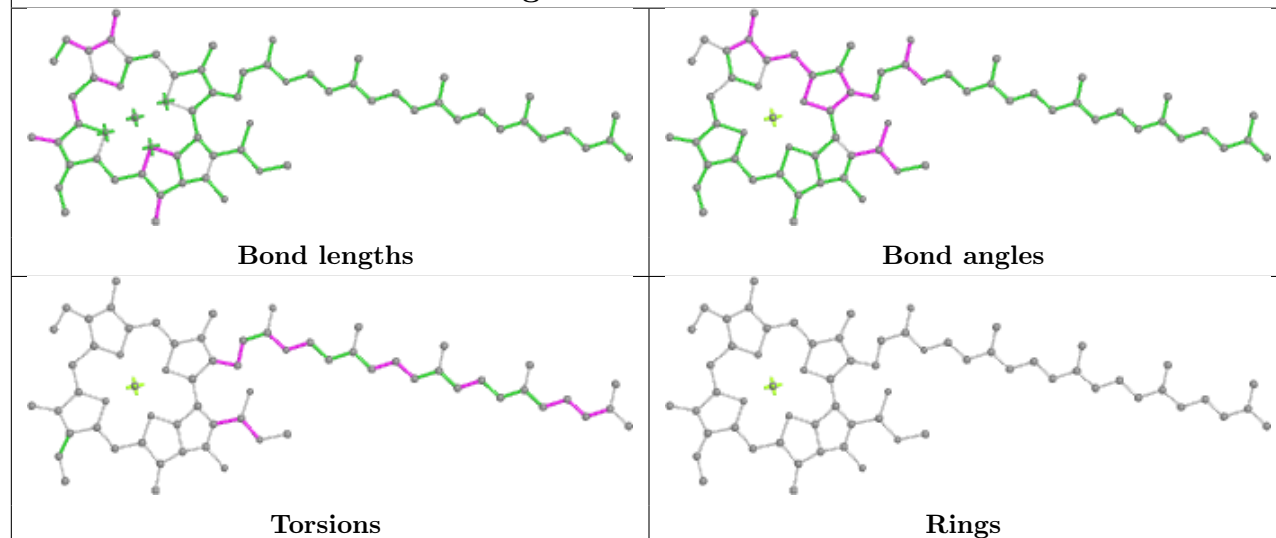
Bond angles



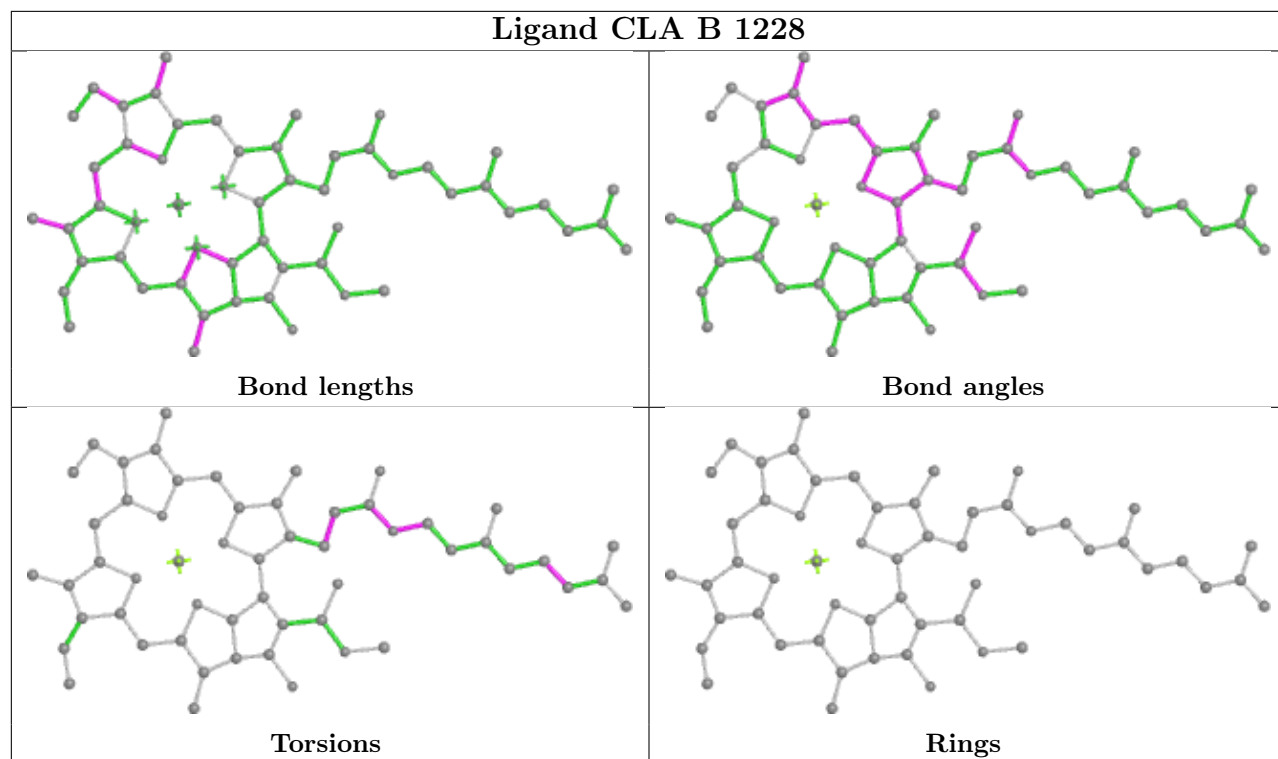
Torsions



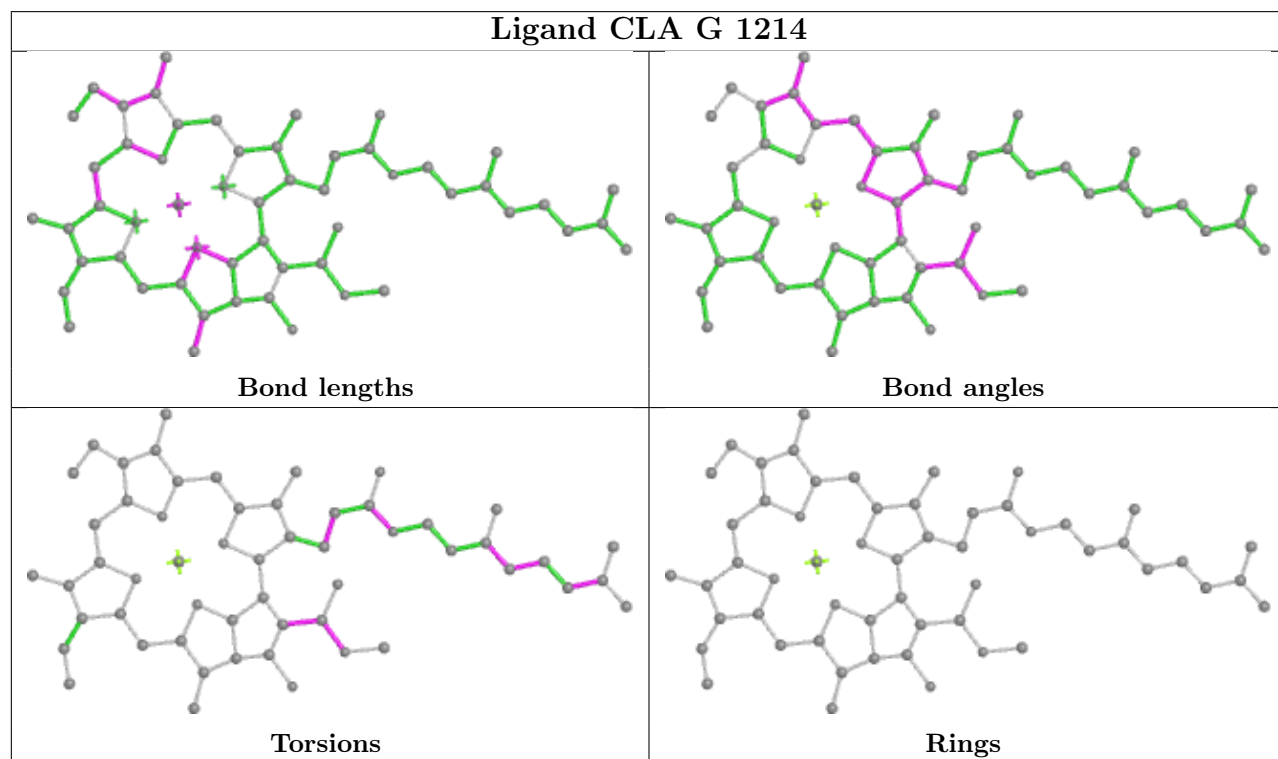
Rings

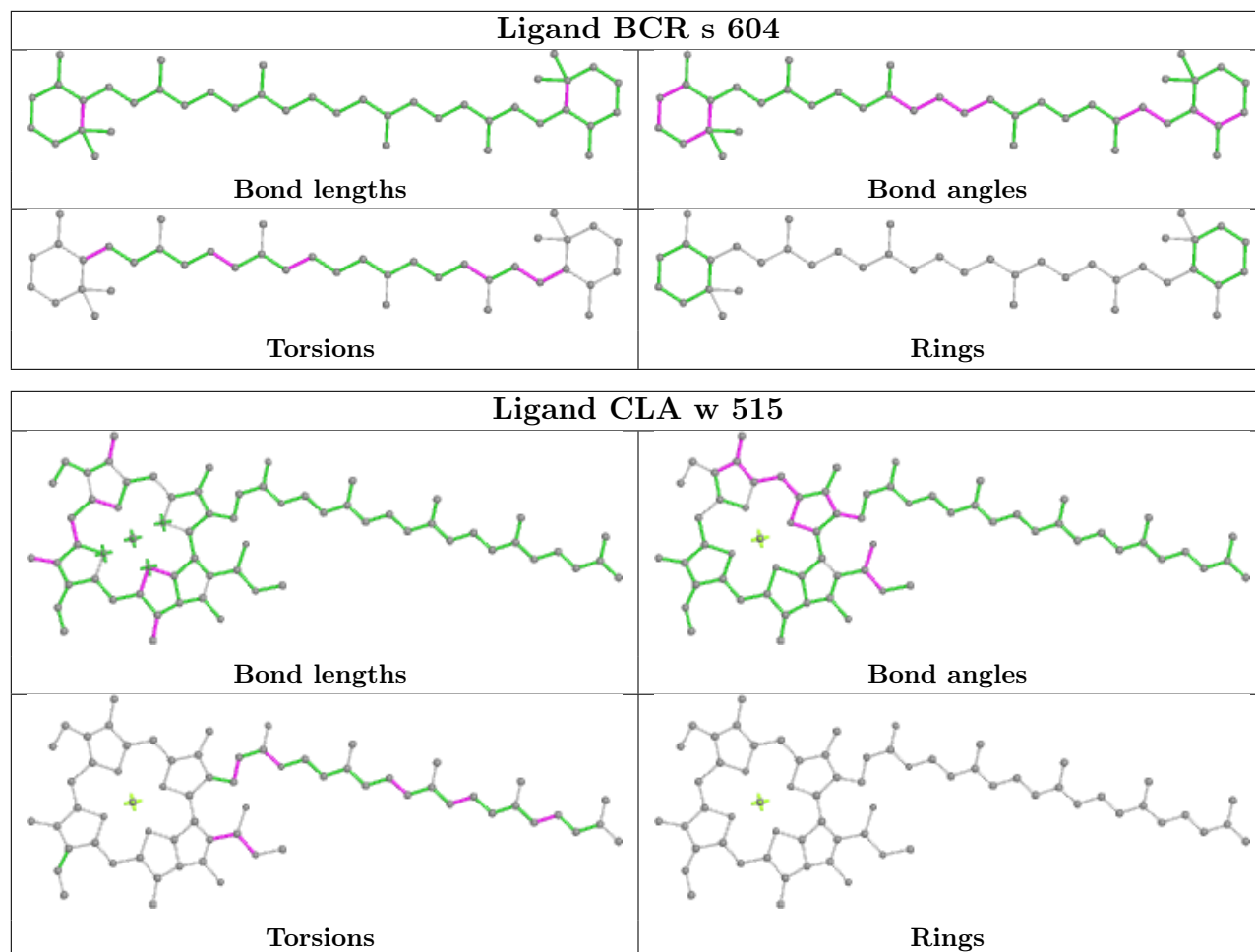
**Ligand CLA U 1502****Ligand CLA a 1109****Ligand CLA H 1106**

## Ligand CLA B 1228

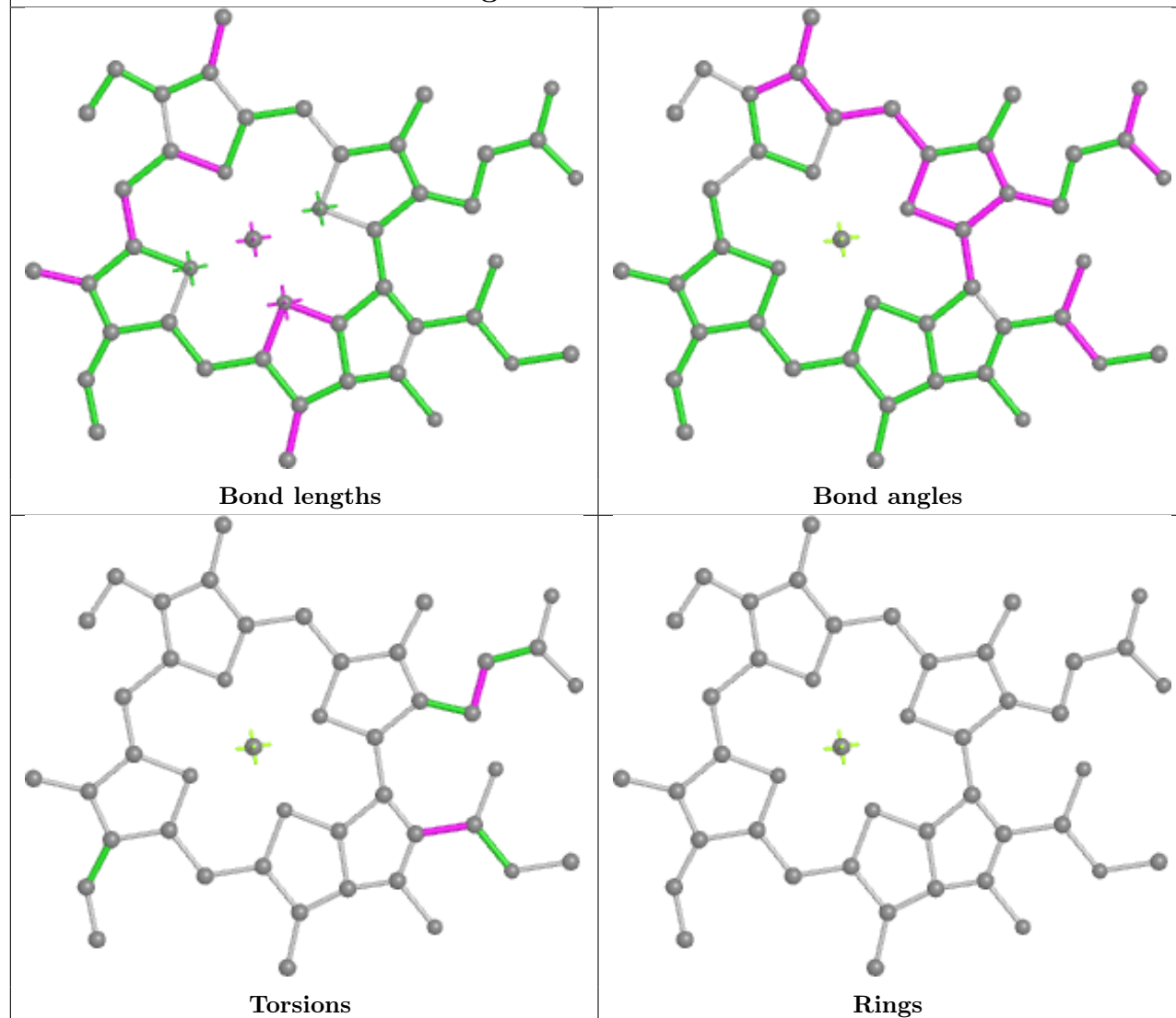


## Ligand CLA G 1214

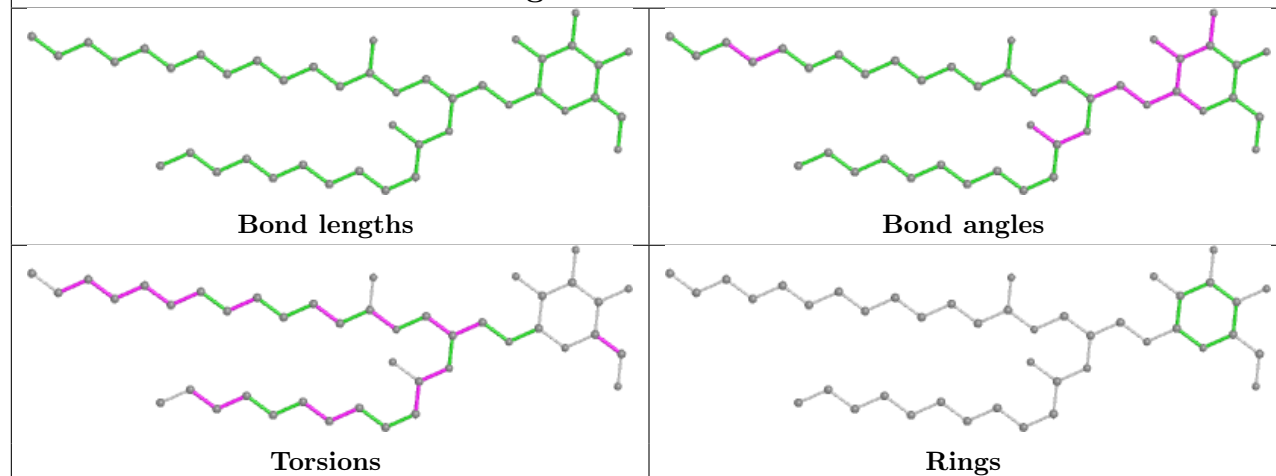




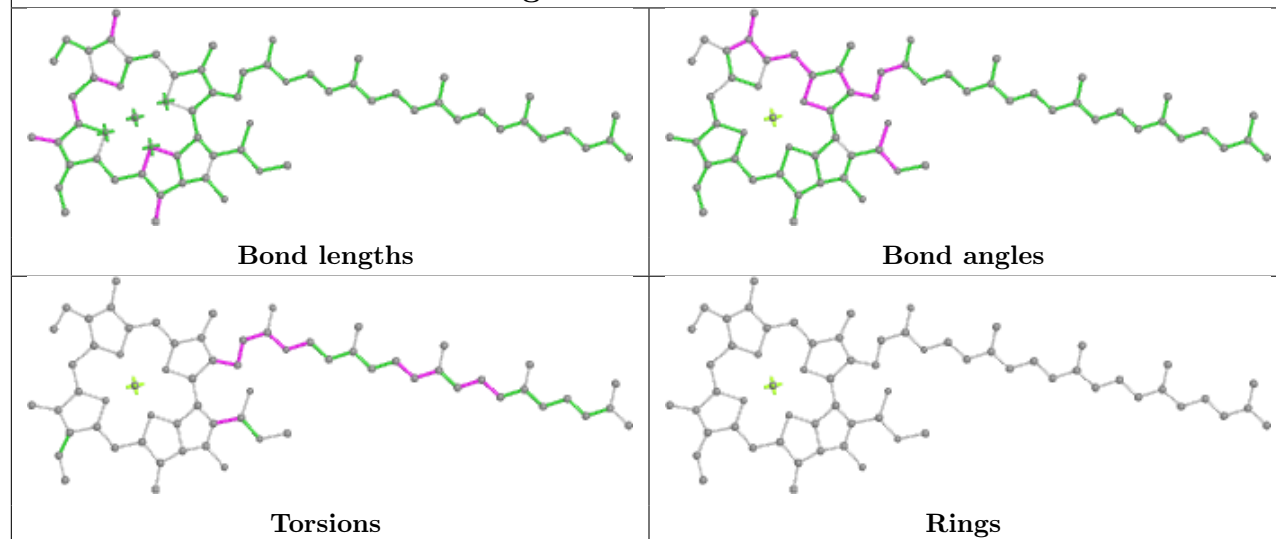
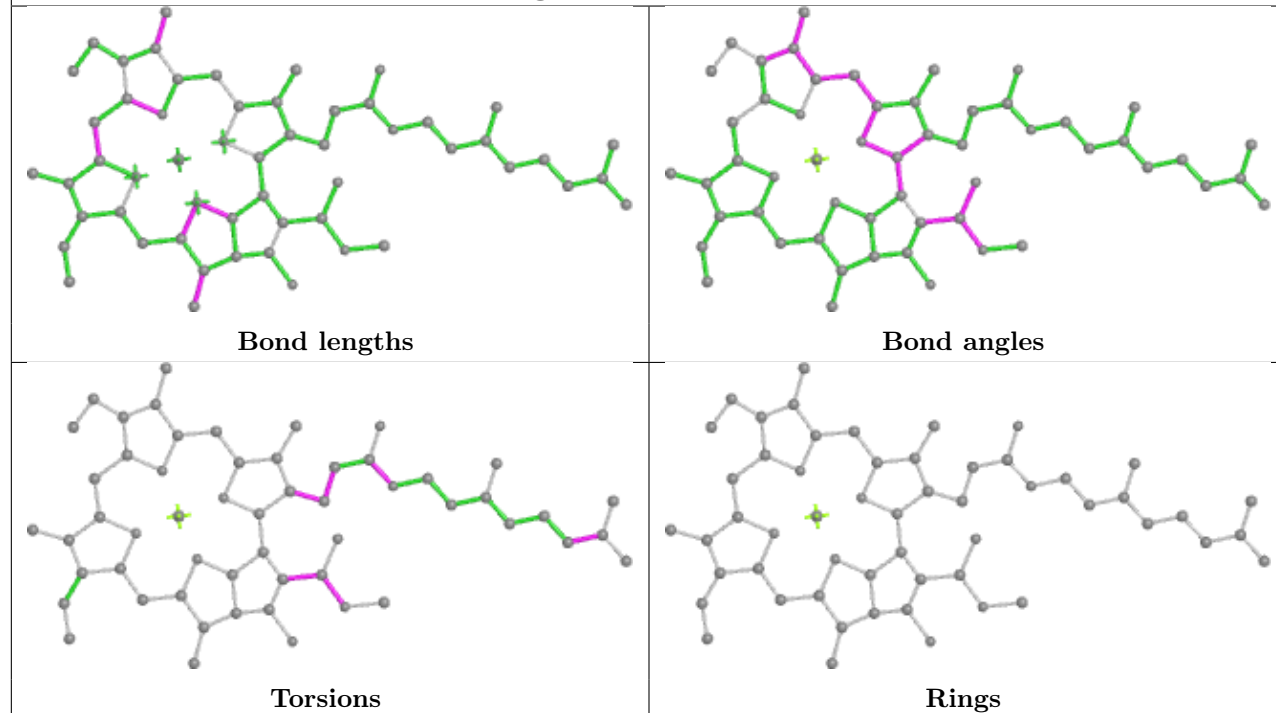
## Ligand CLA K 1401

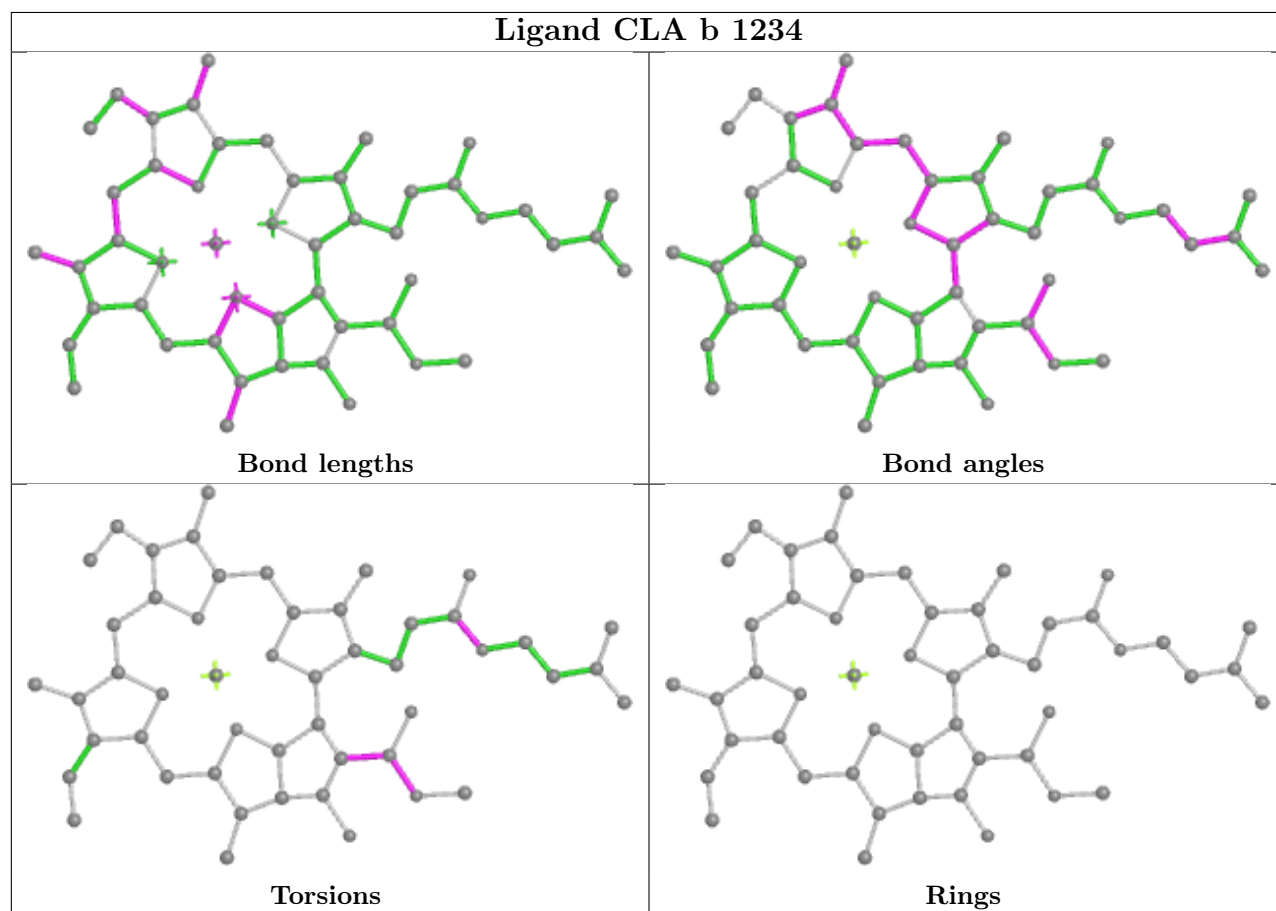
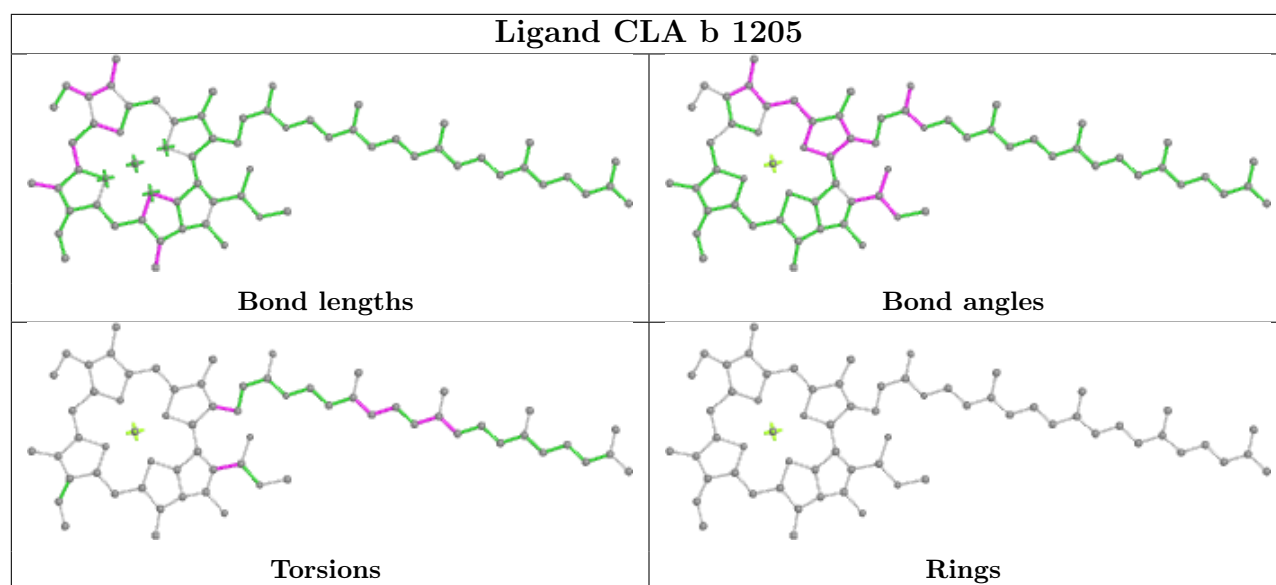


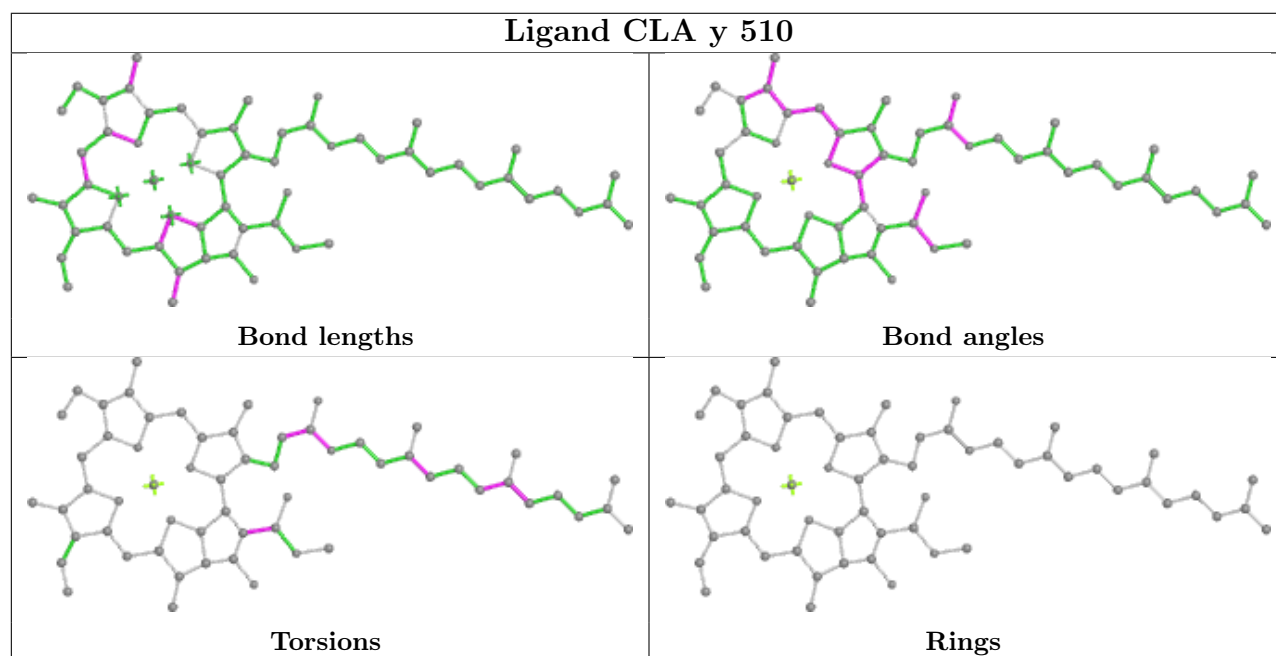
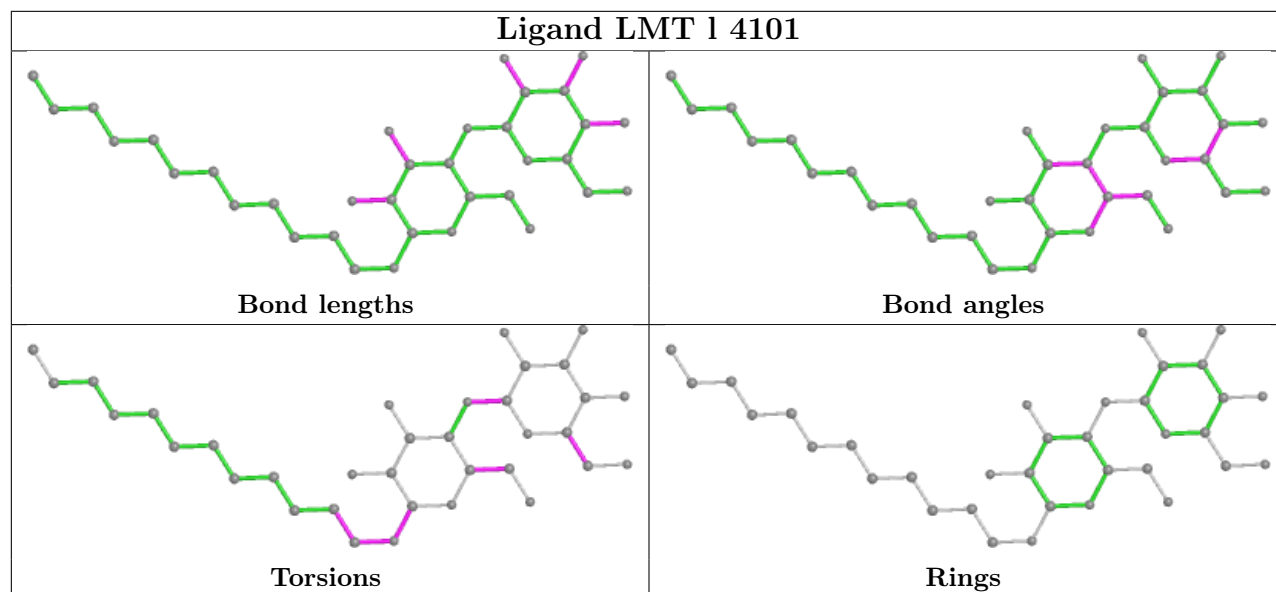
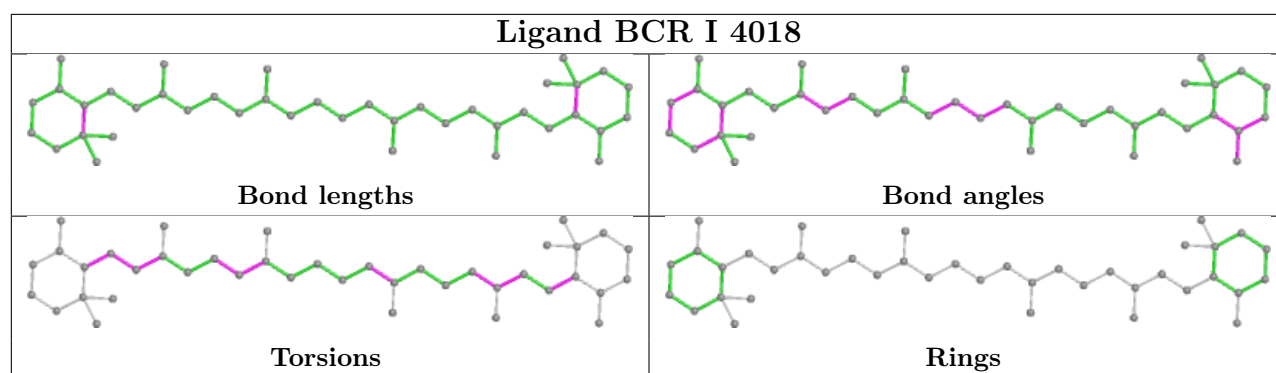
## Ligand LMG G 848

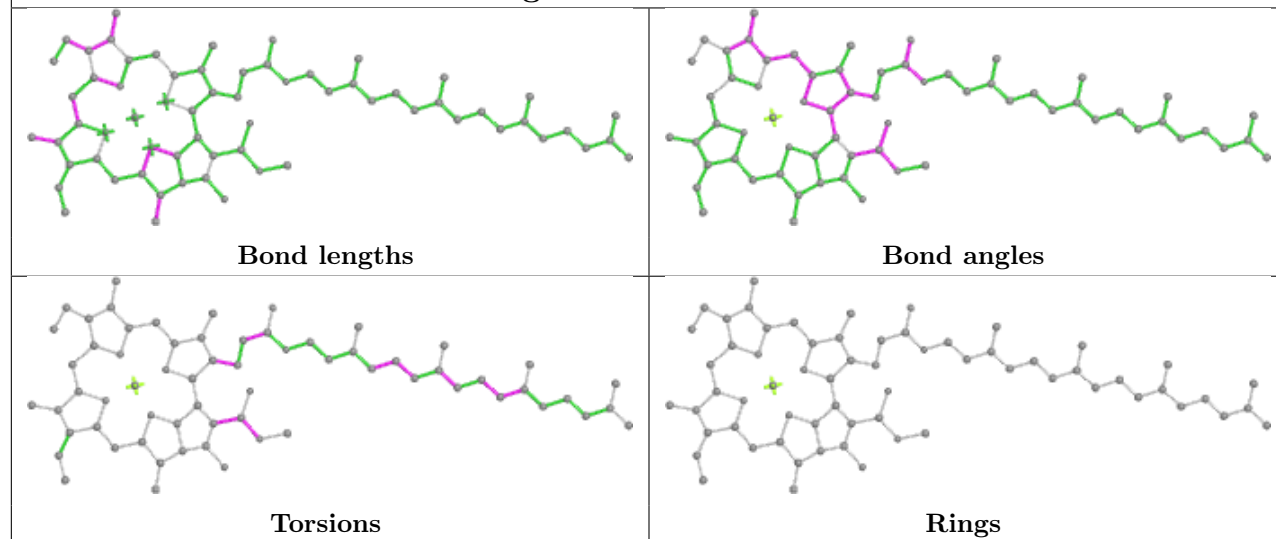
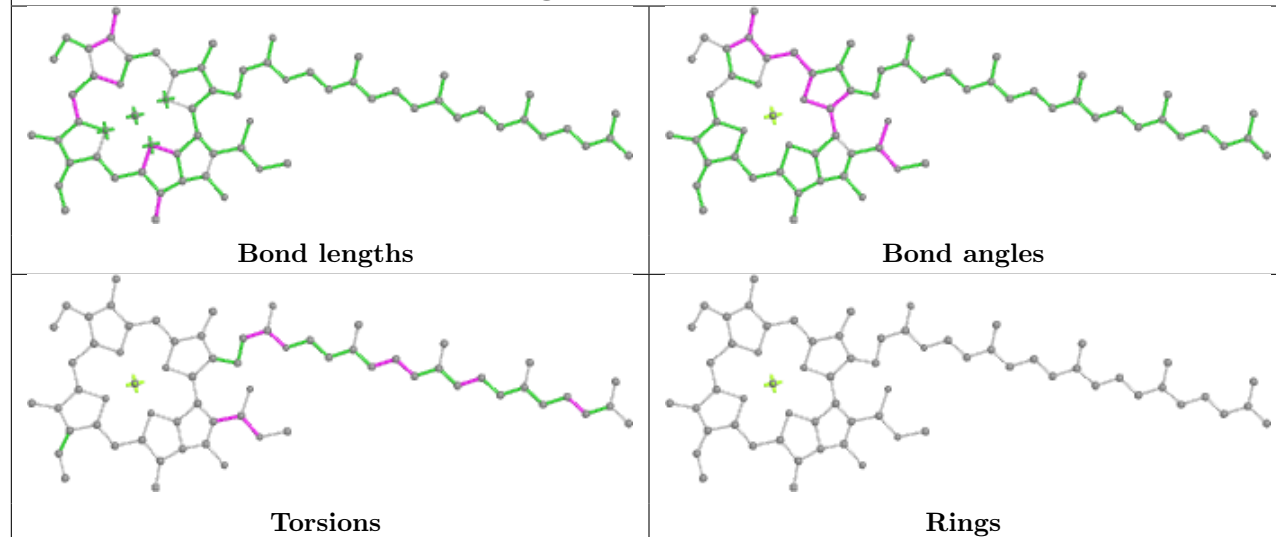




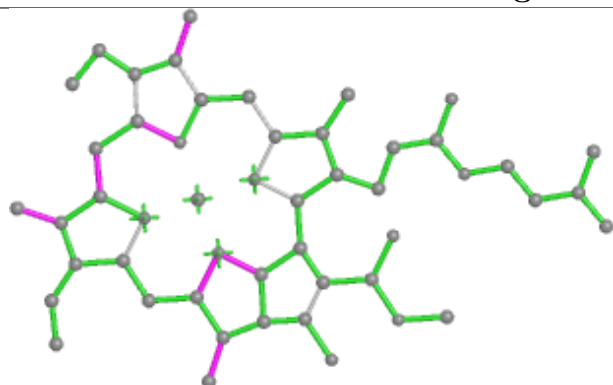
**Ligand CLA A 1103****Ligand CLA X 508**



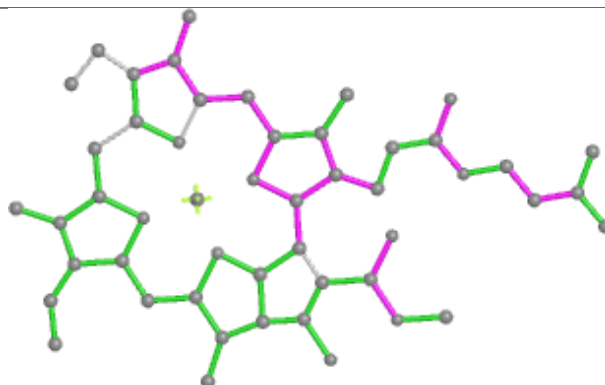


**Ligand CLA A 1126****Ligand CLA s 507**

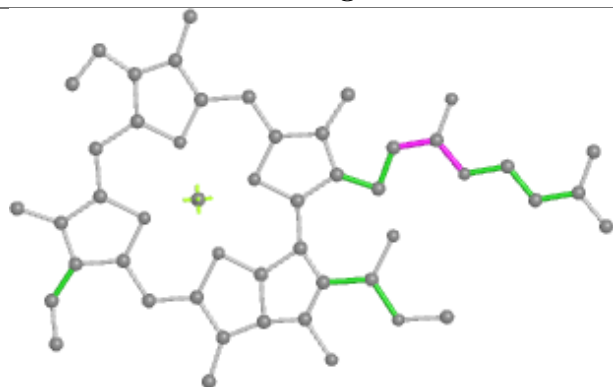
## Ligand CLA Y 514



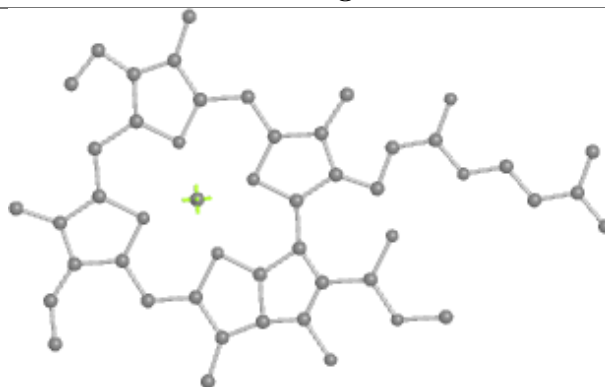
Bond lengths



Bond angles

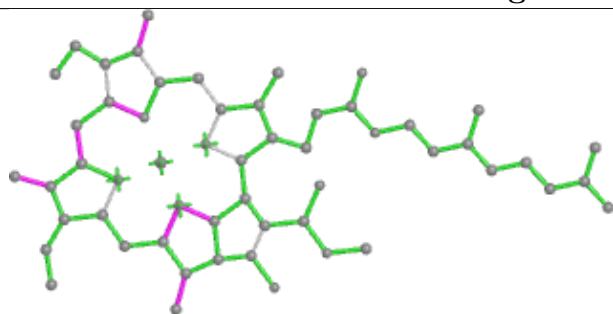


Torsions

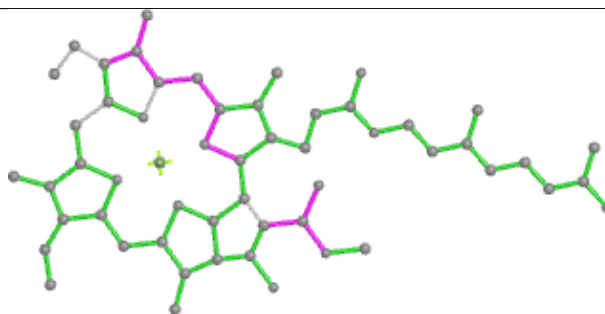


Rings

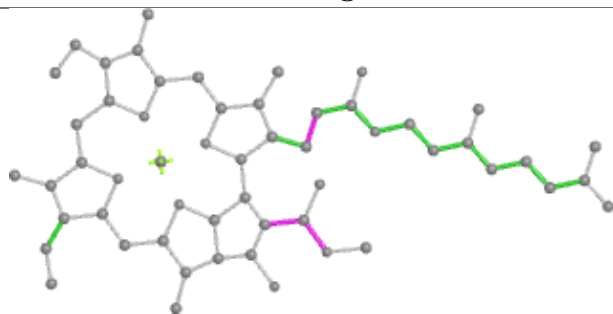
## Ligand CLA b 1218



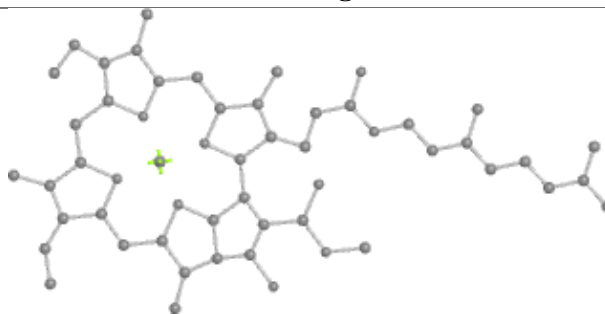
Bond lengths



Bond angles

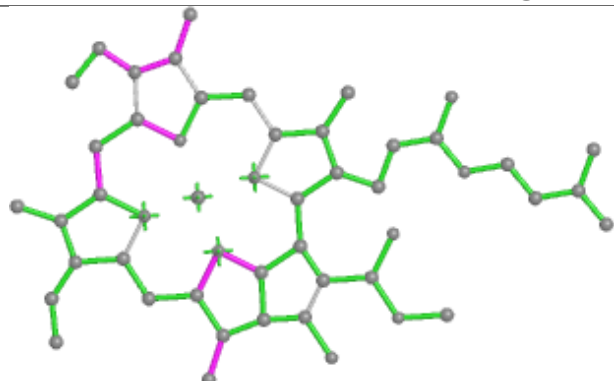


Torsions

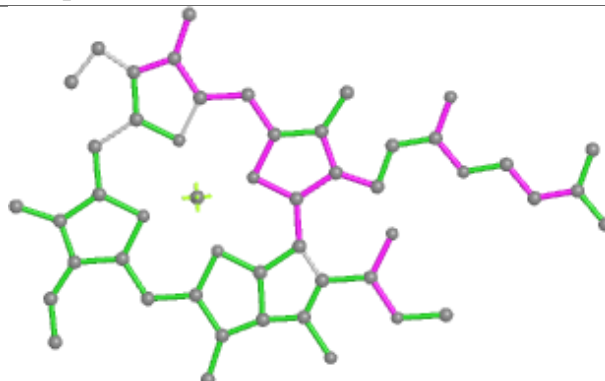


Rings

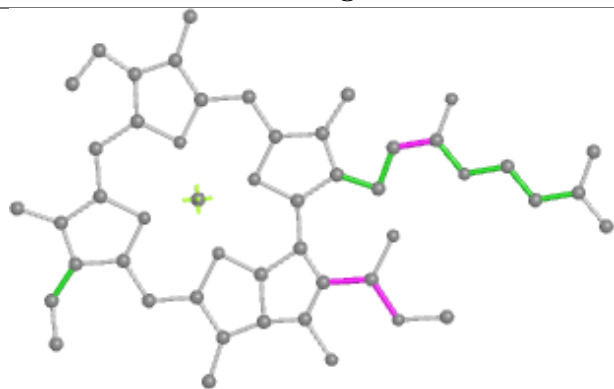
## Ligand CLA q 514



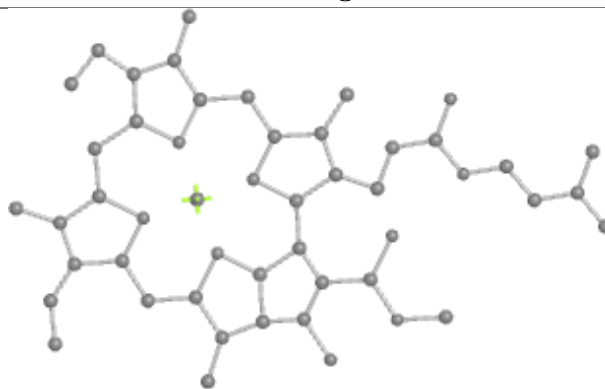
Bond lengths



Bond angles

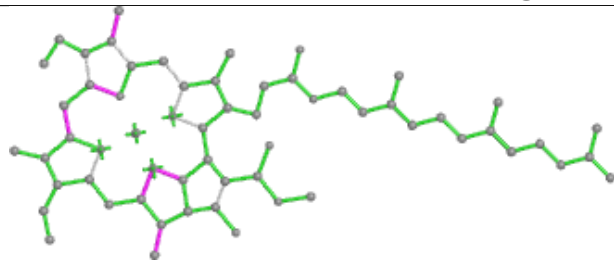


Torsions

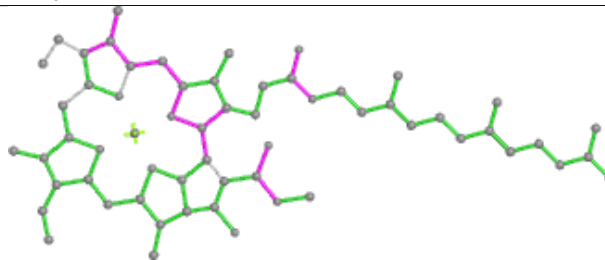


Rings

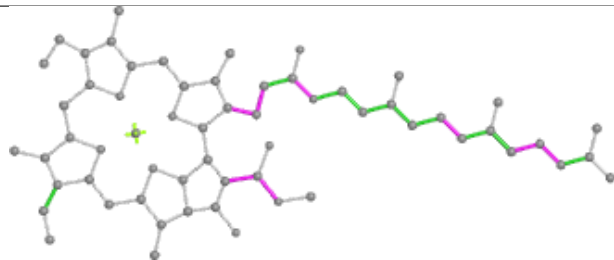
## Ligand CLA y 504



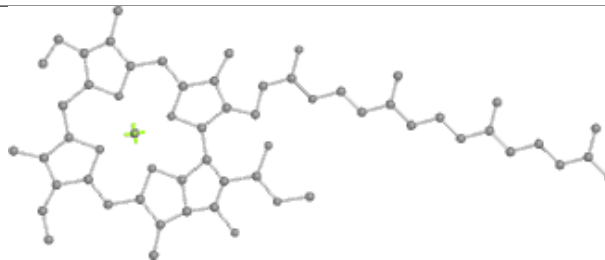
Bond lengths



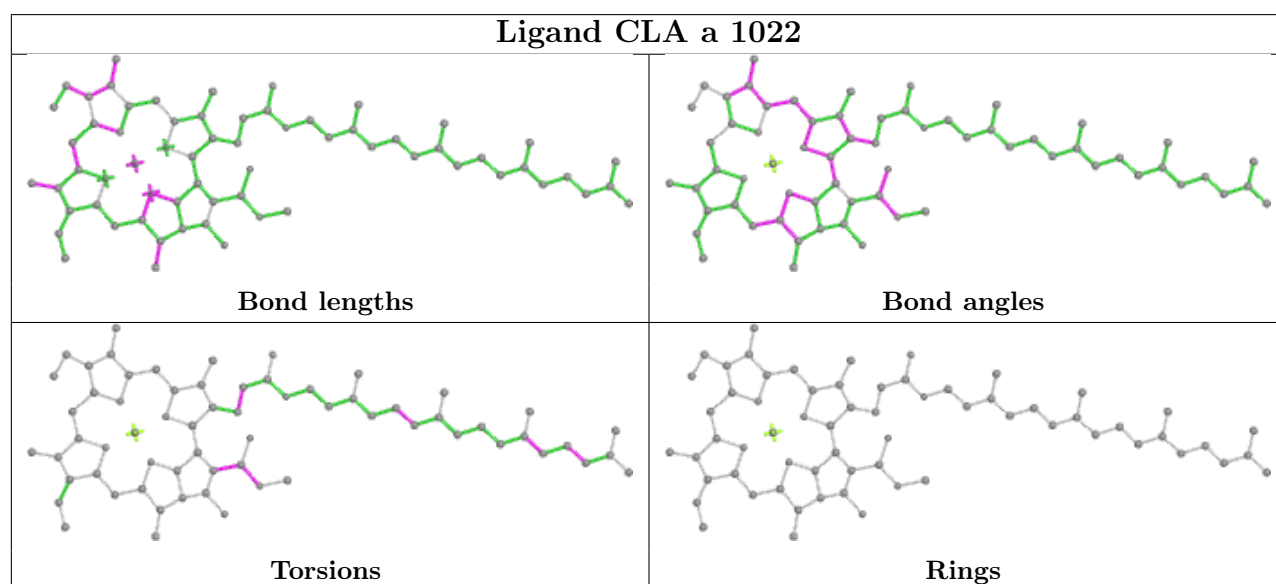
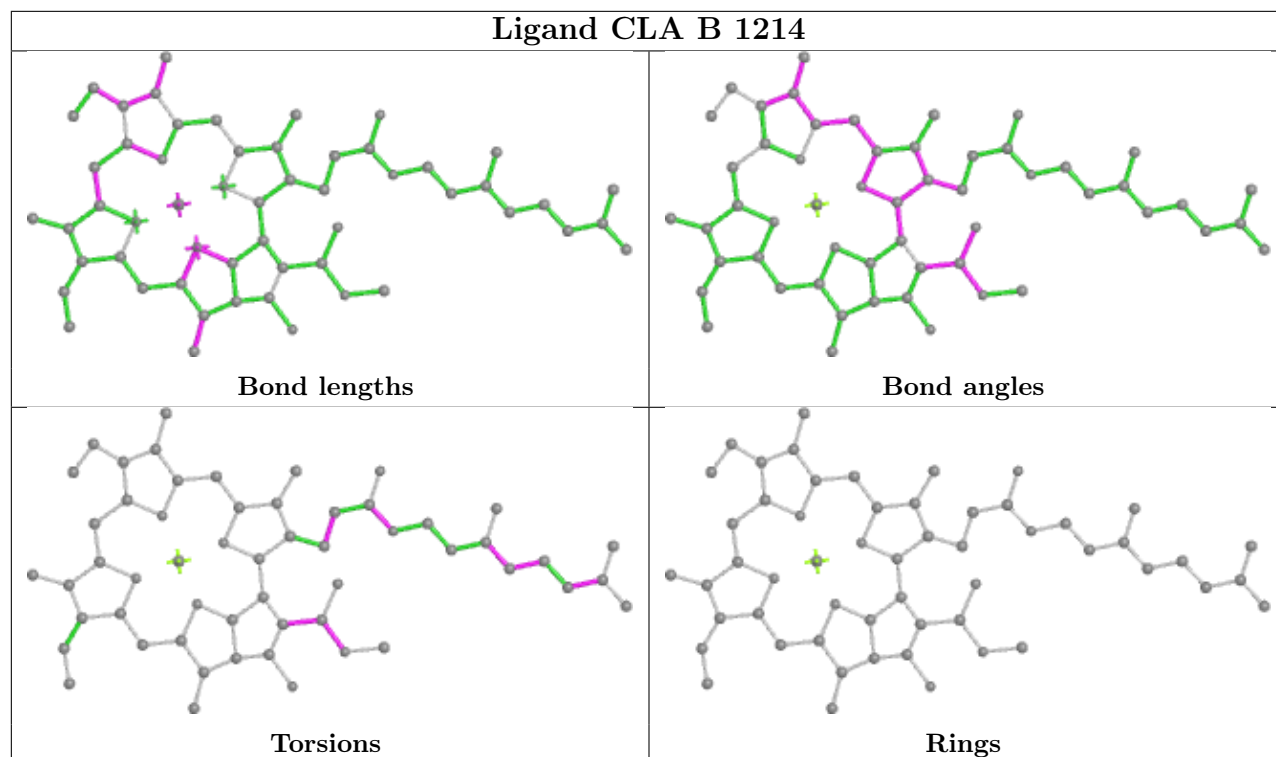
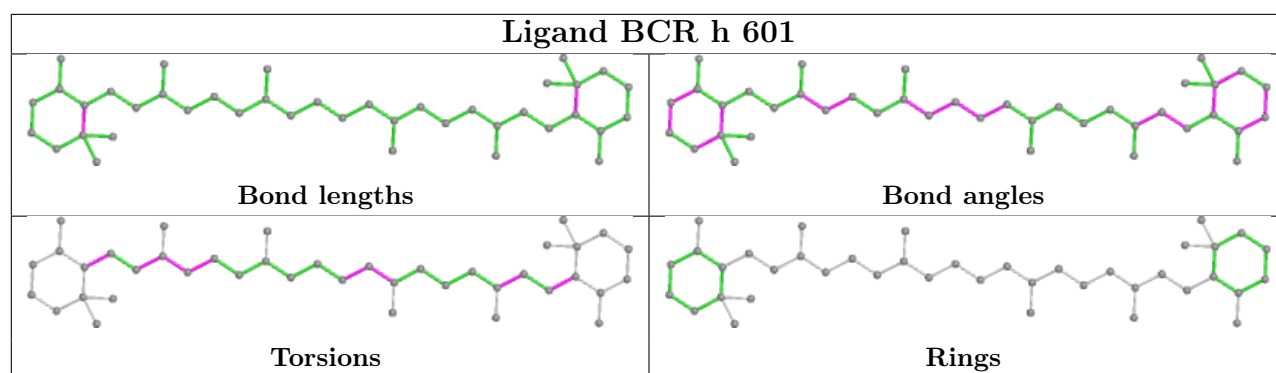
Bond angles



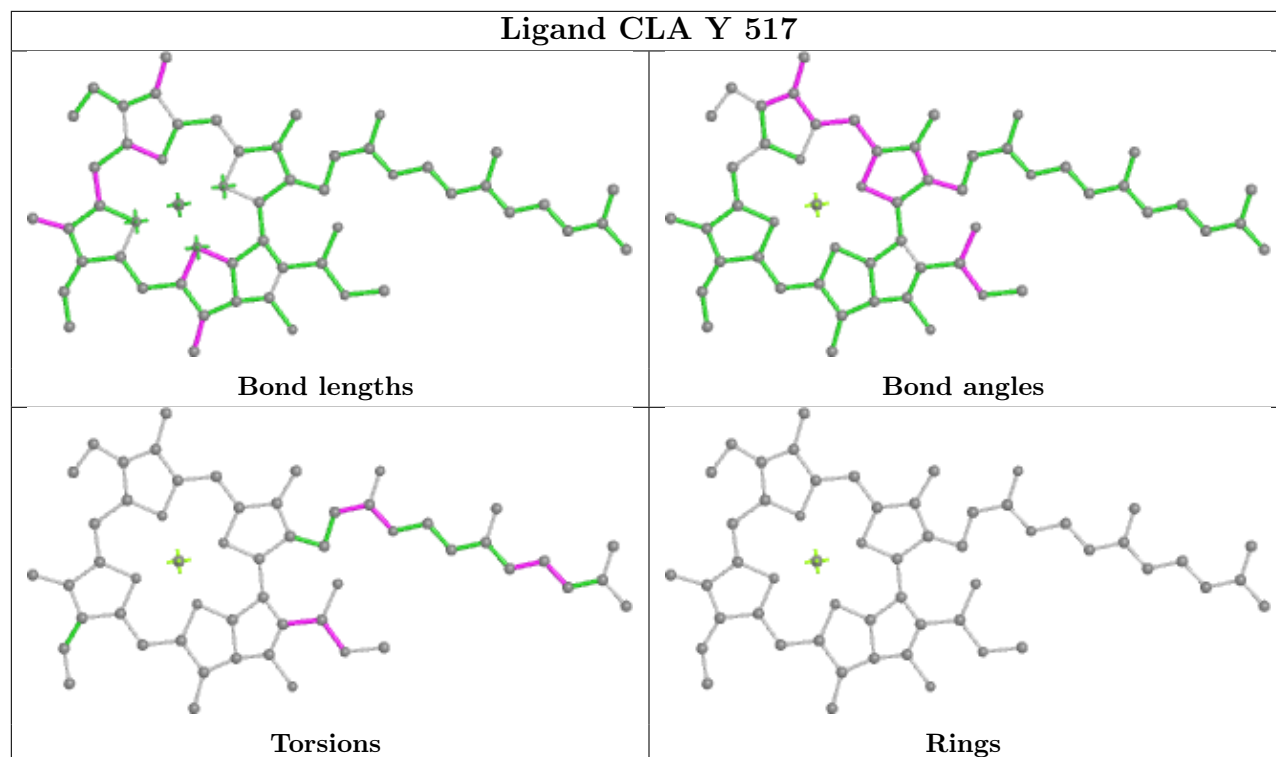
Torsions



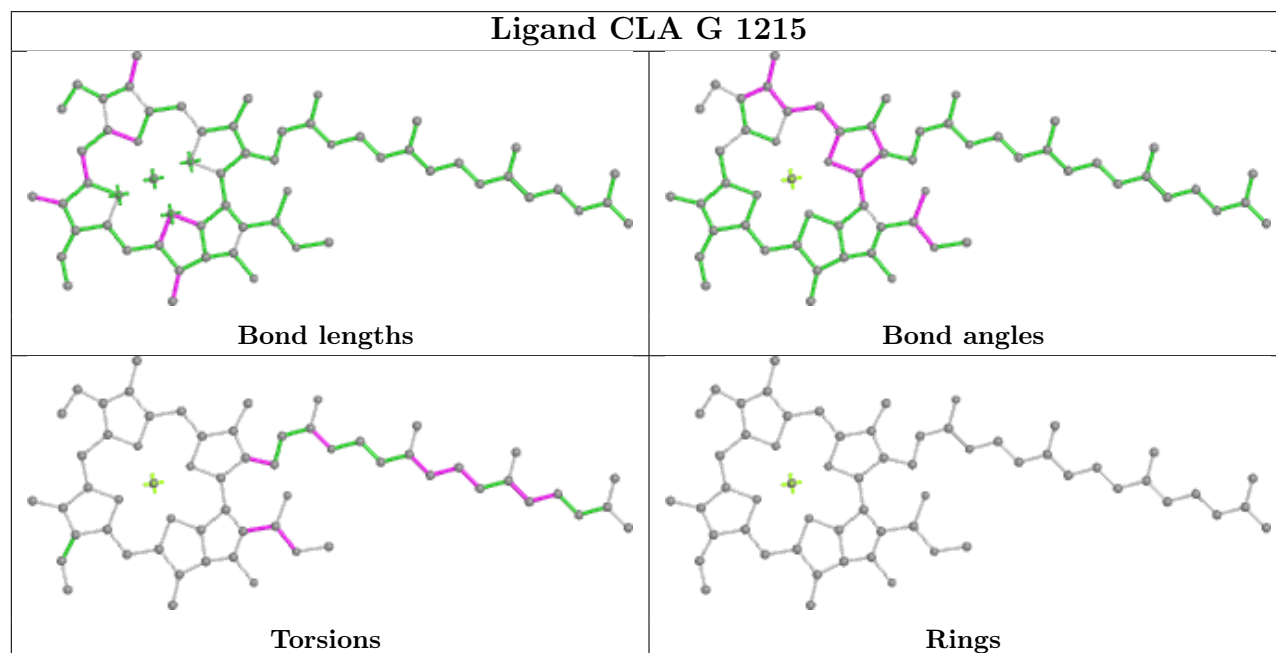
Rings



## Ligand CLA Y 517

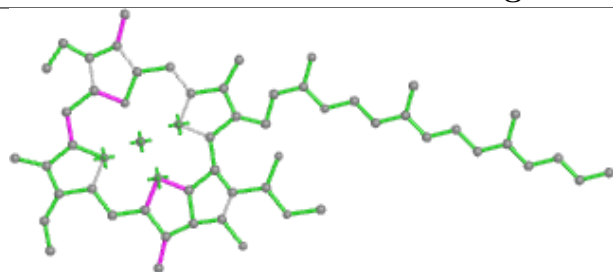


## Ligand CLA G 1215

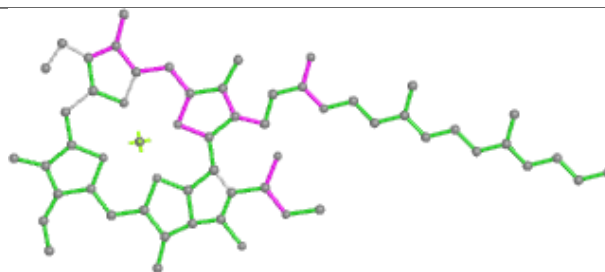




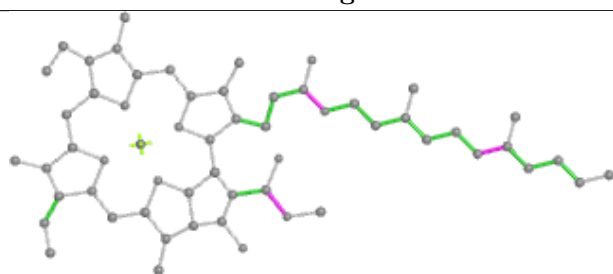
## Ligand CLA H 1105



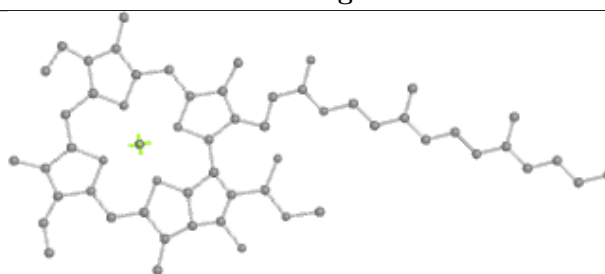
Bond lengths



Bond angles

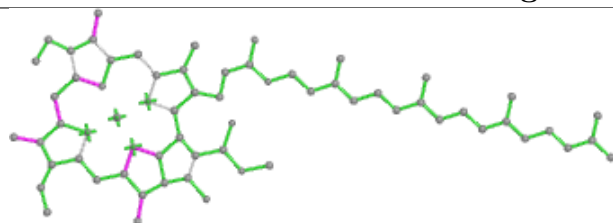


Torsions

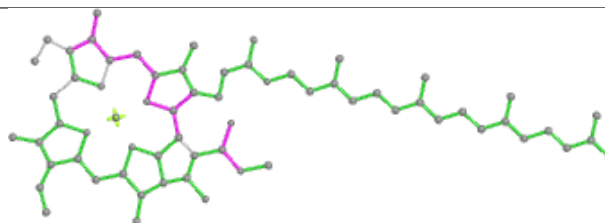


Rings

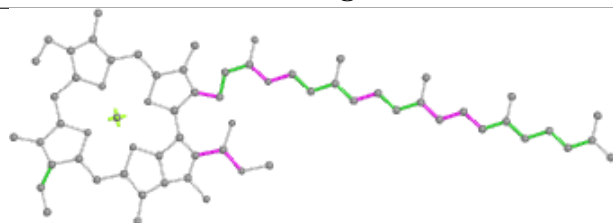
## Ligand CLA t 511



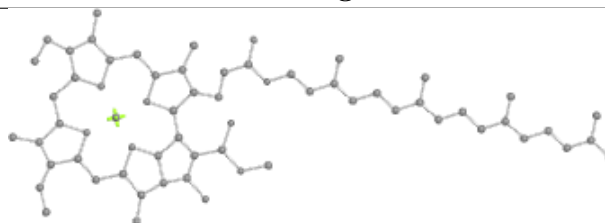
Bond lengths



Bond angles

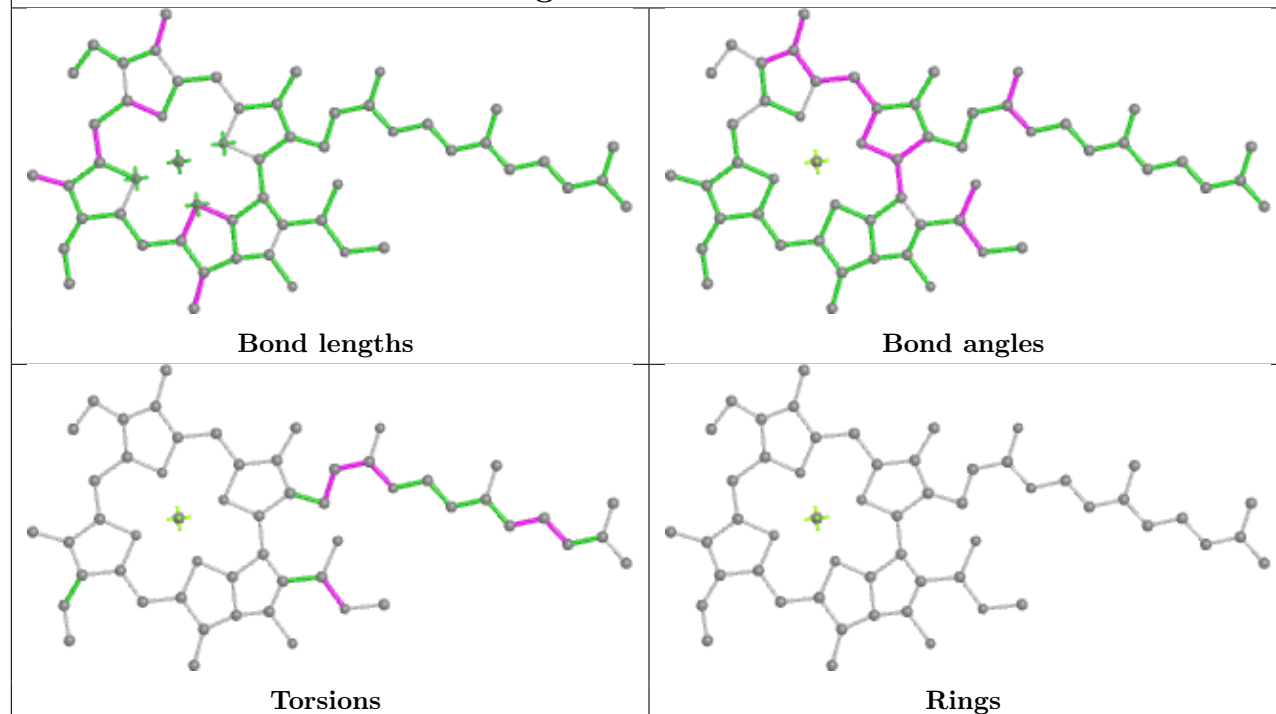


Torsions

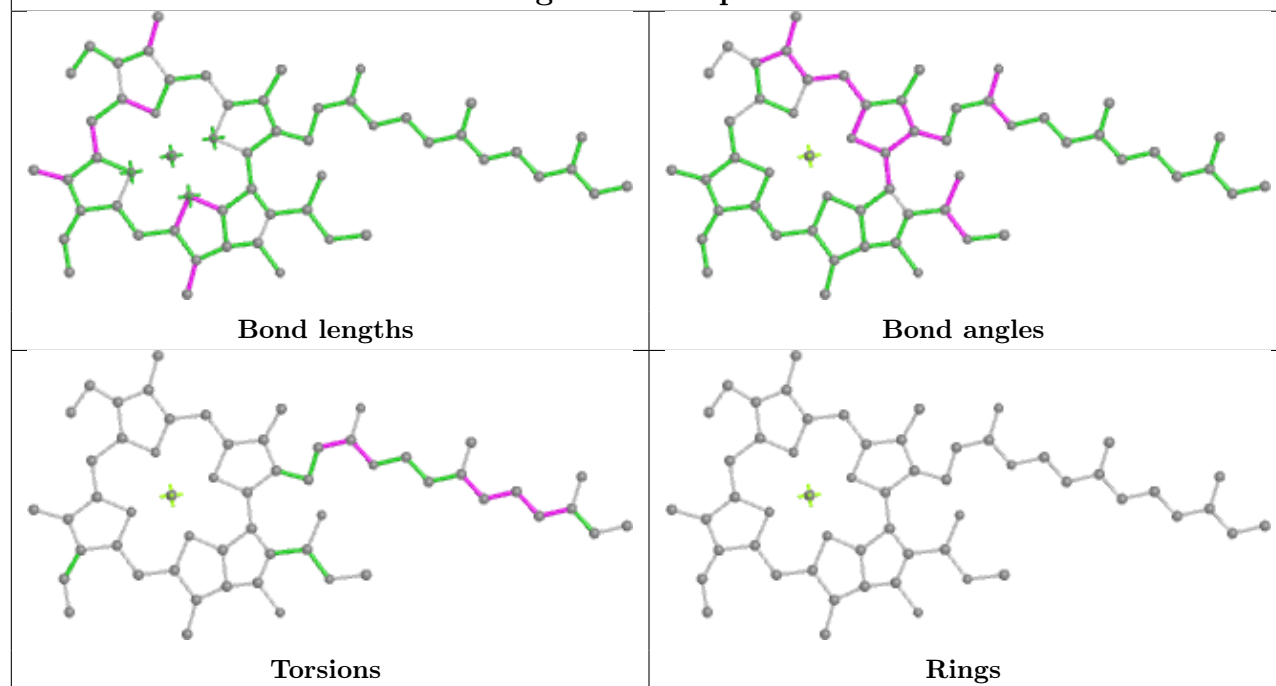


Rings

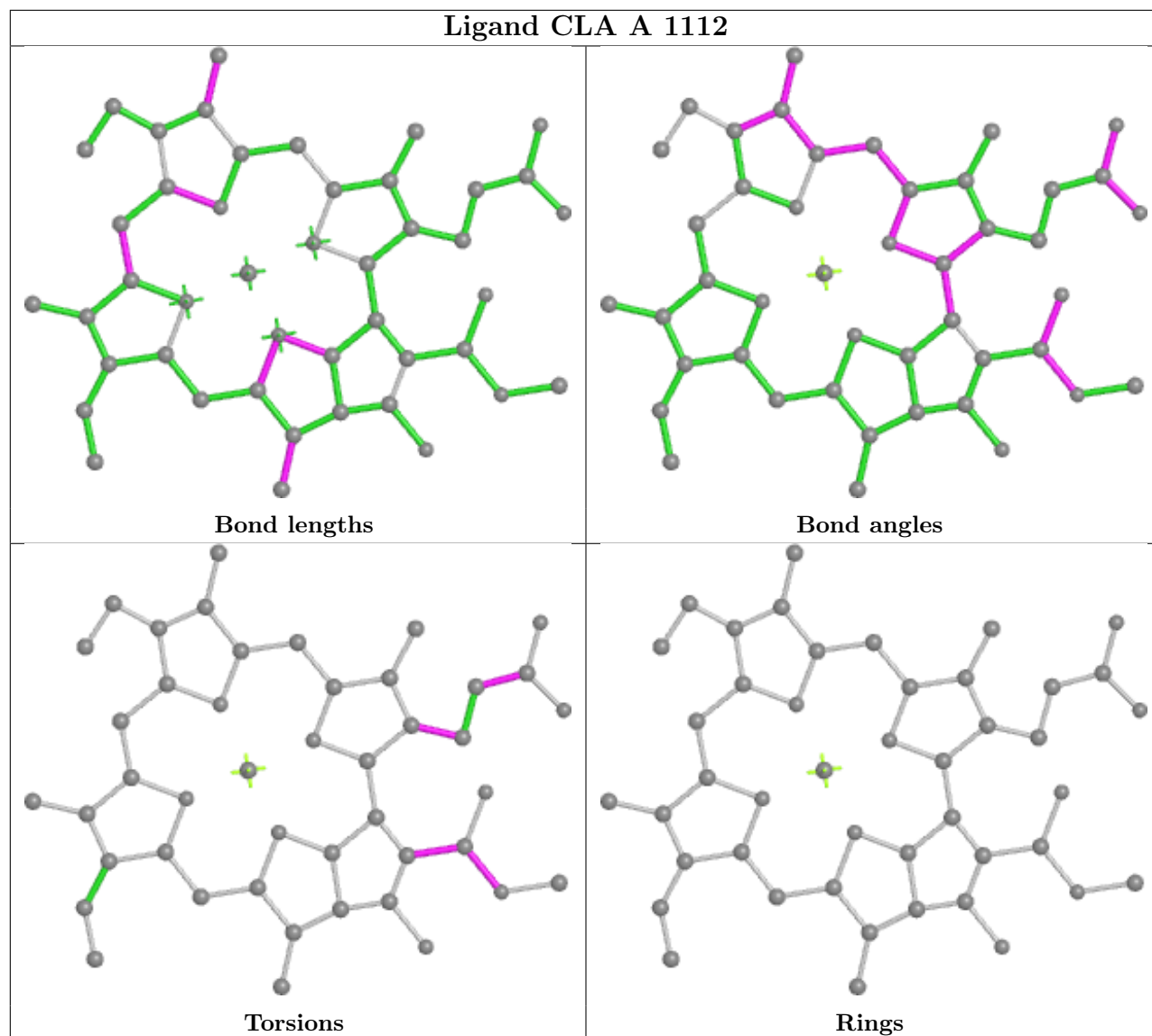
## Ligand CLA x 517

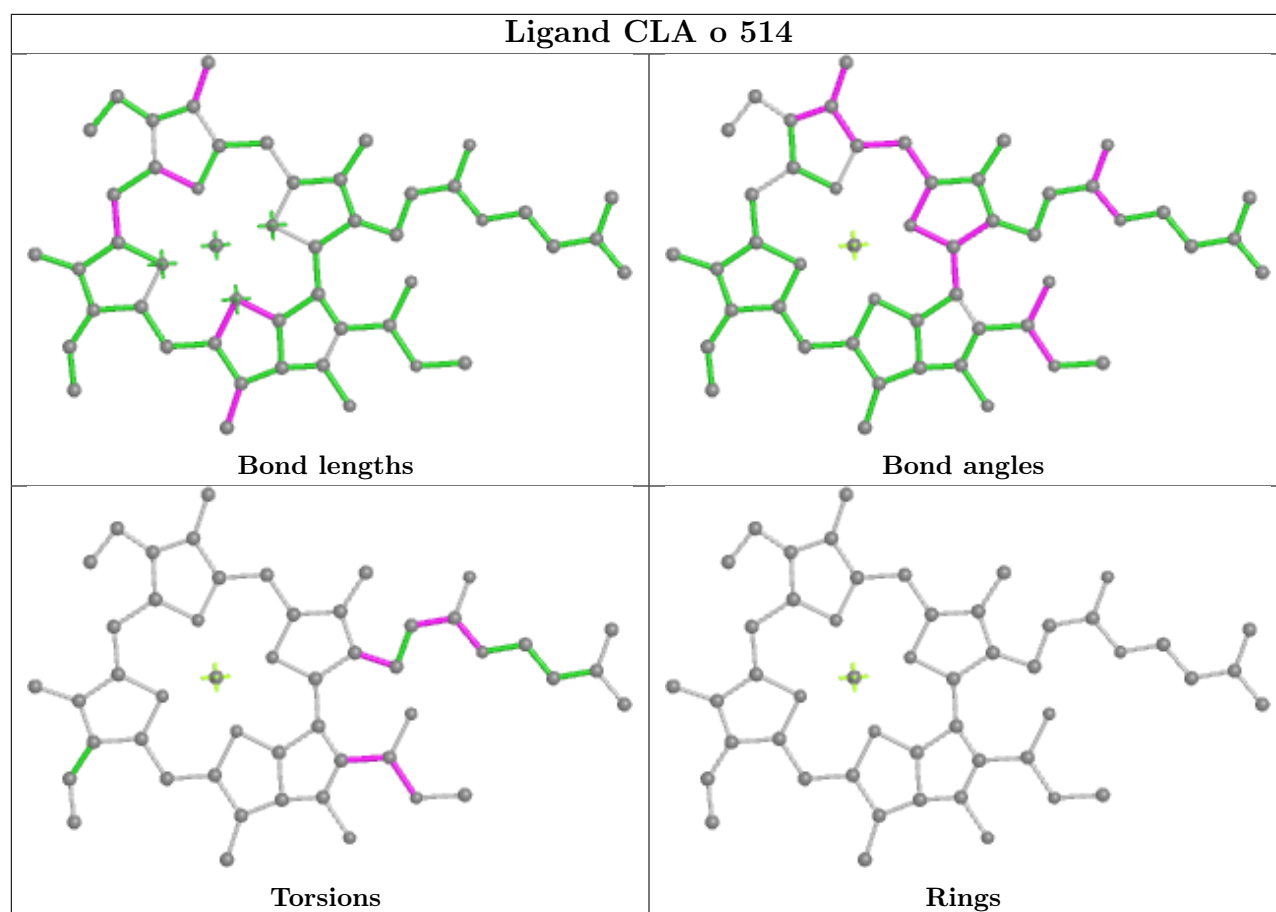


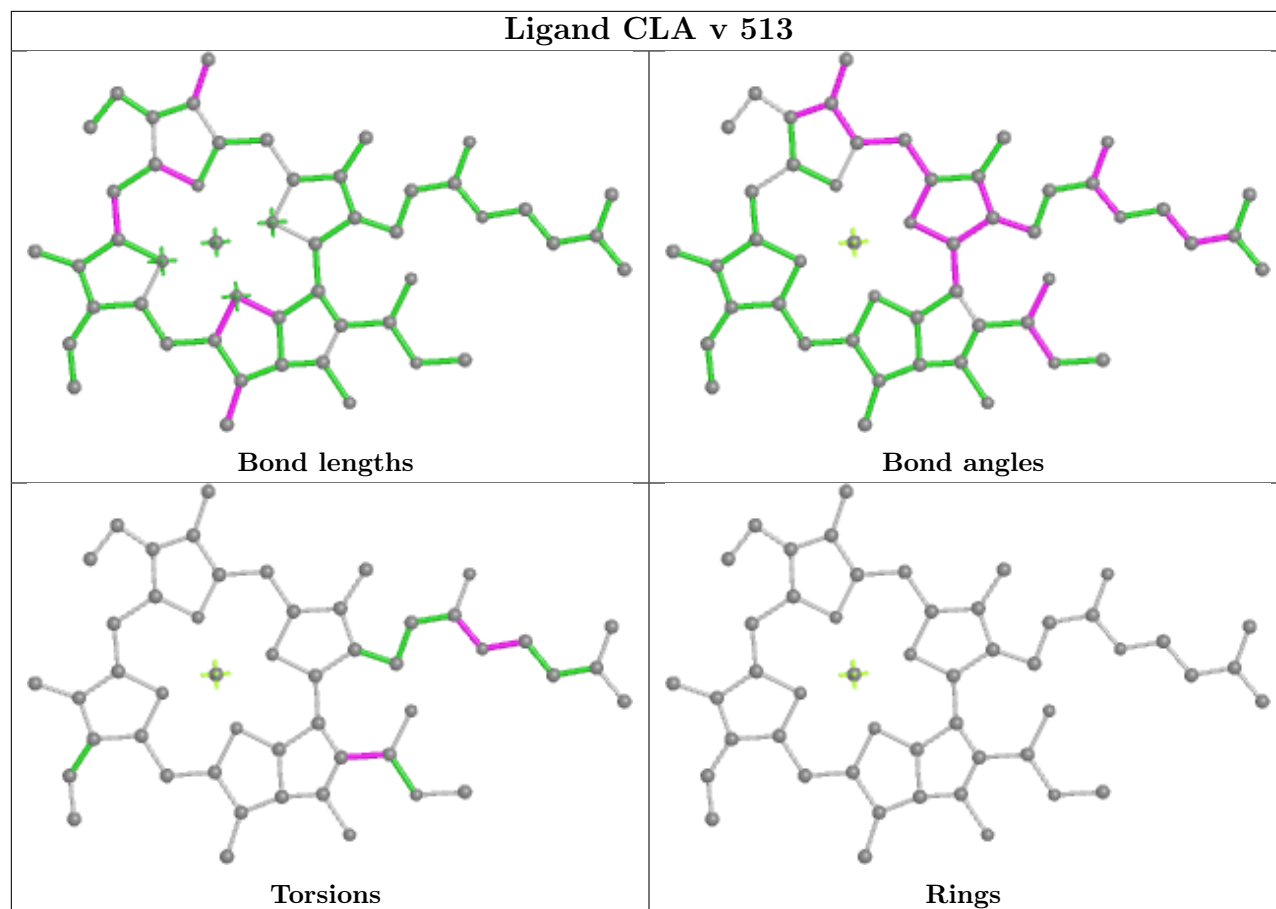
## Ligand CLA q 509



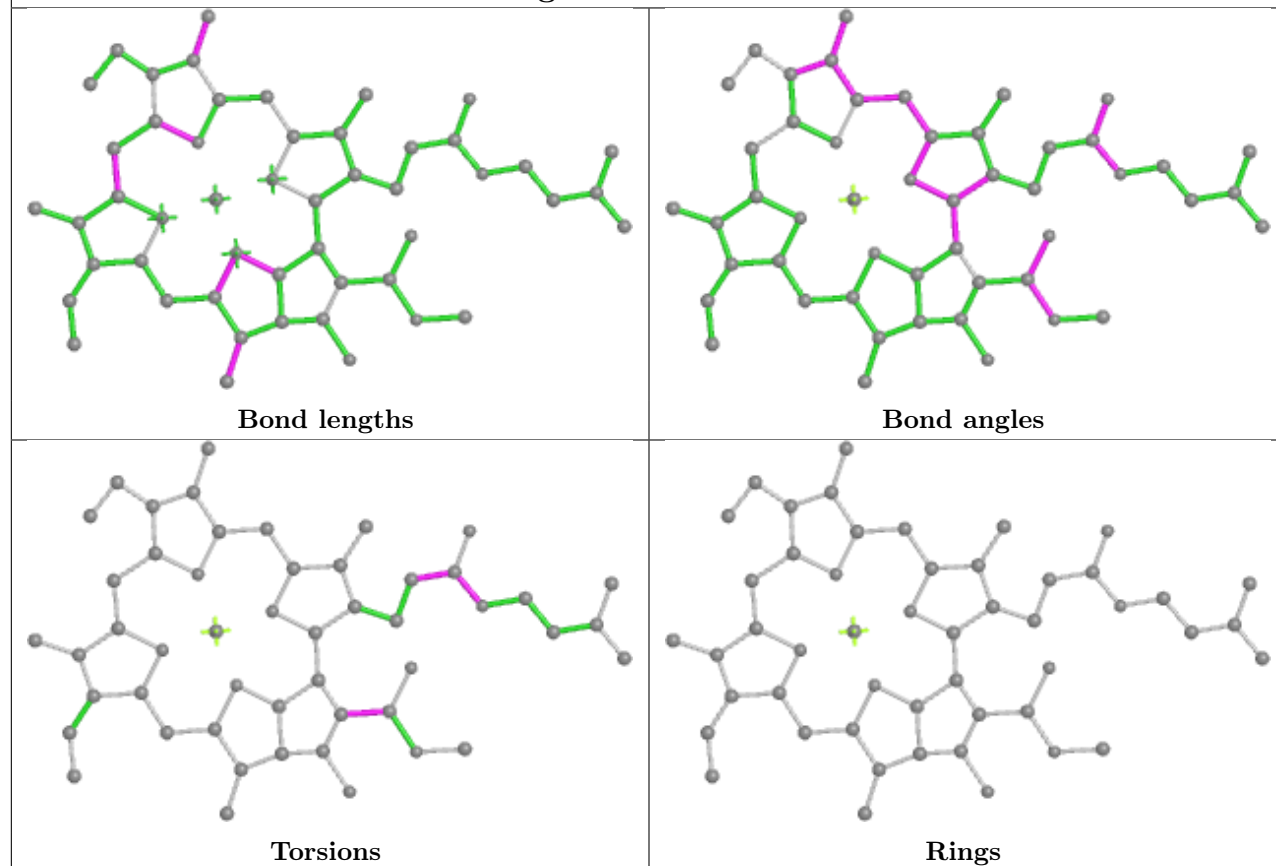
## Ligand CLA A 1112



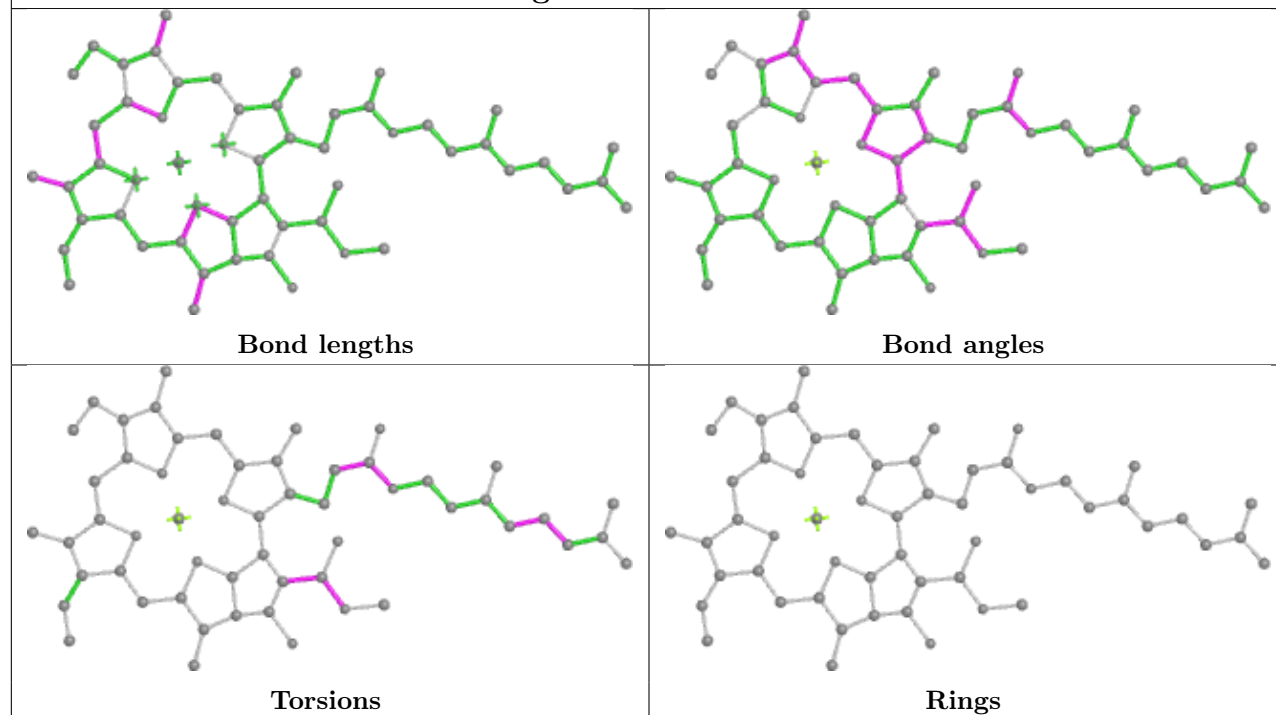




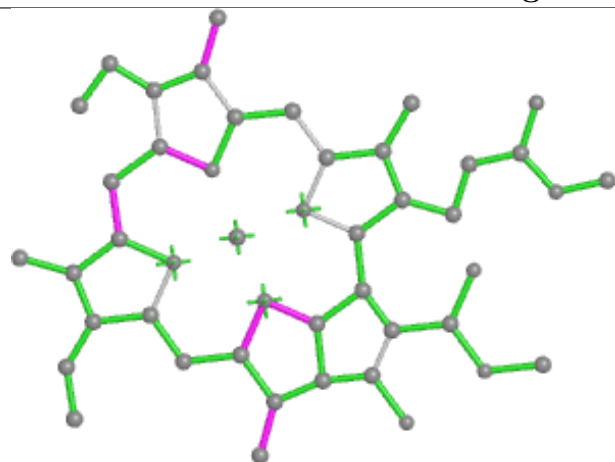
## Ligand CLA s 513



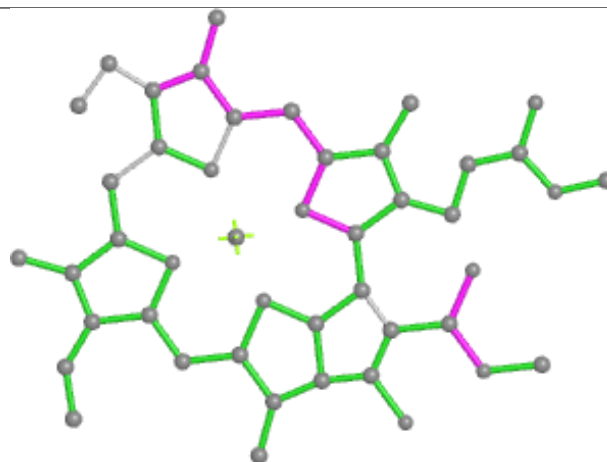
## Ligand CLA w 517



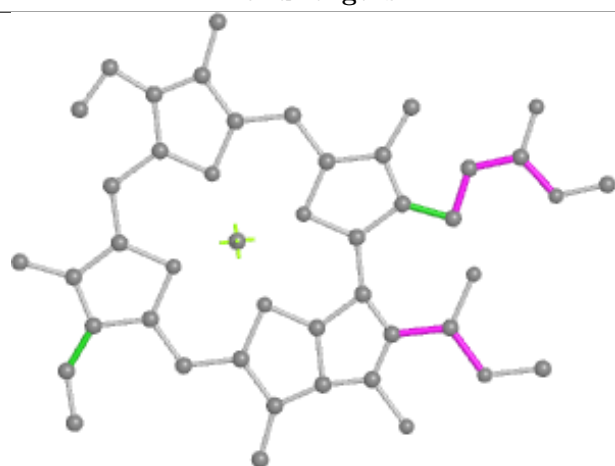
## Ligand CLA t 516



Bond lengths



Bond angles

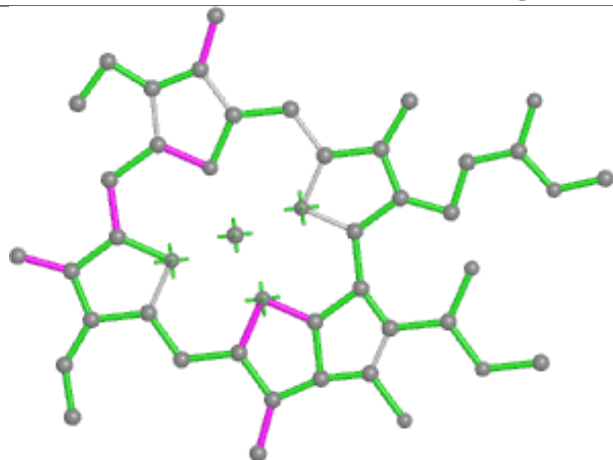


Torsions

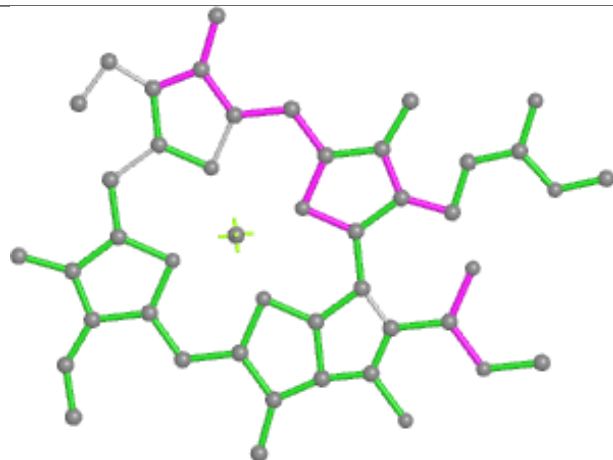


Rings

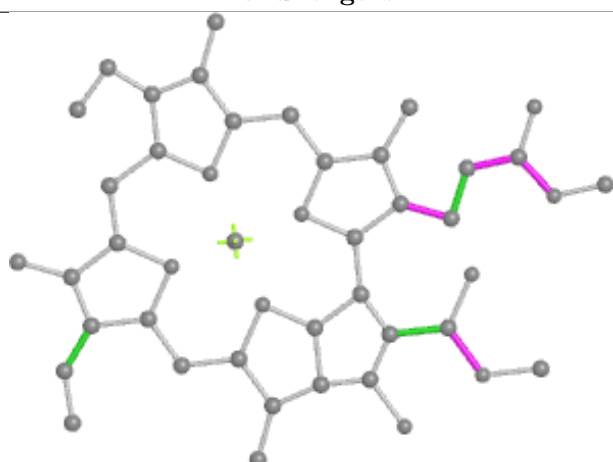
## Ligand CLA Y 503



Bond lengths



Bond angles

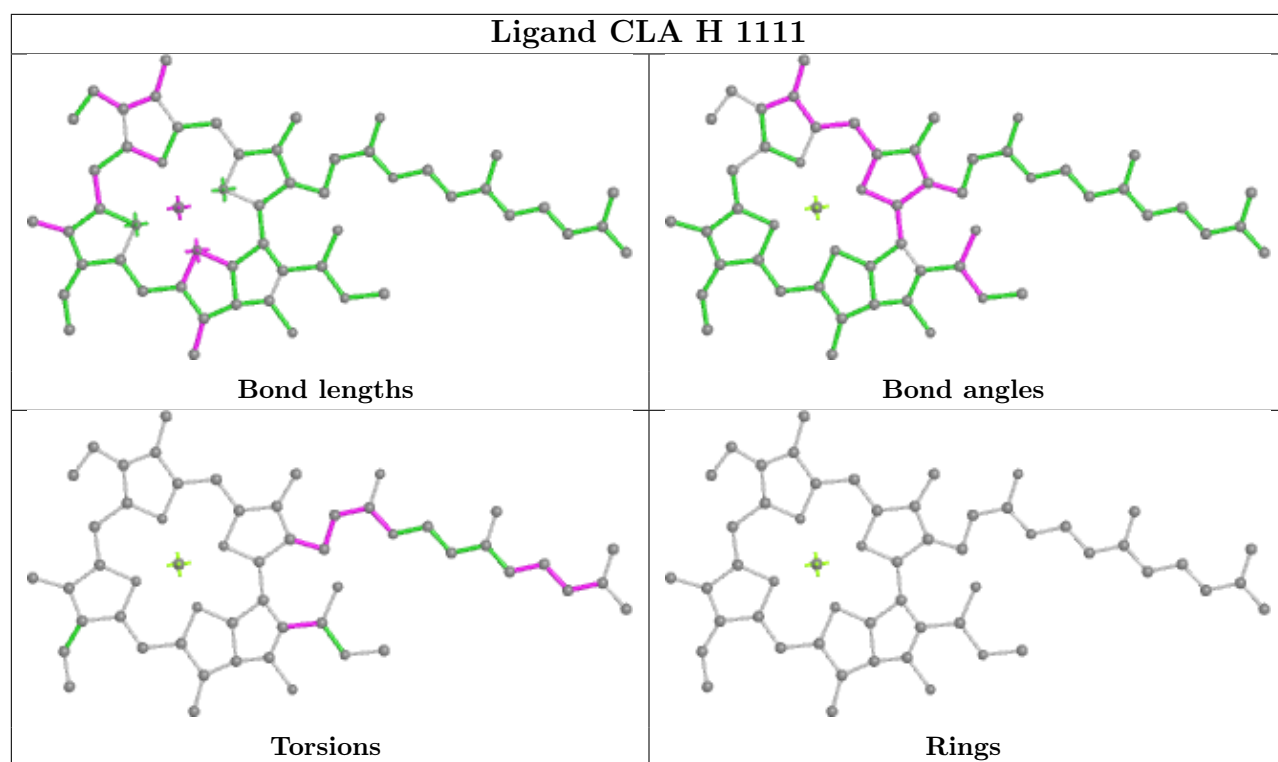


Torsions

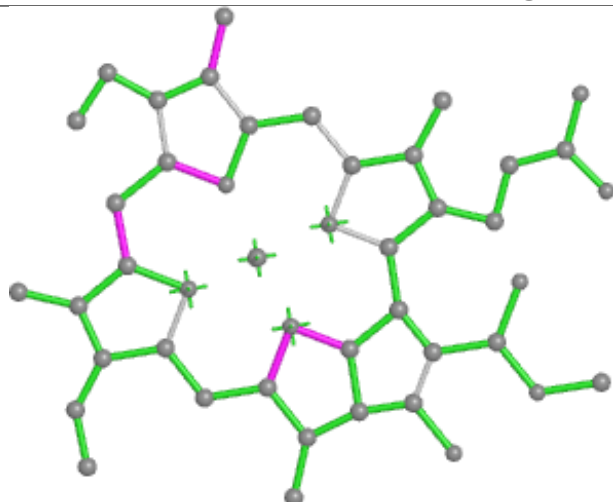


Rings

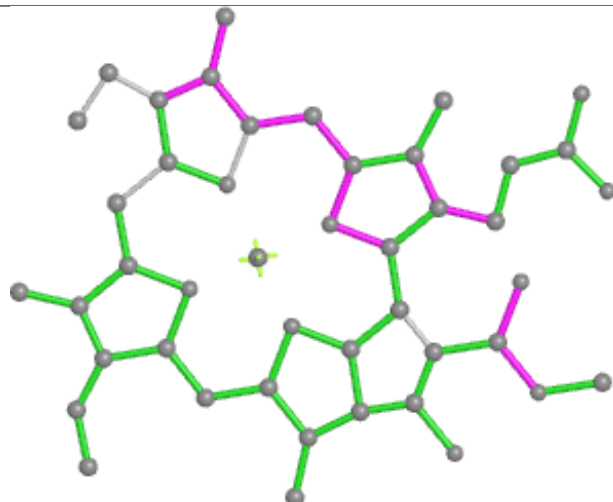




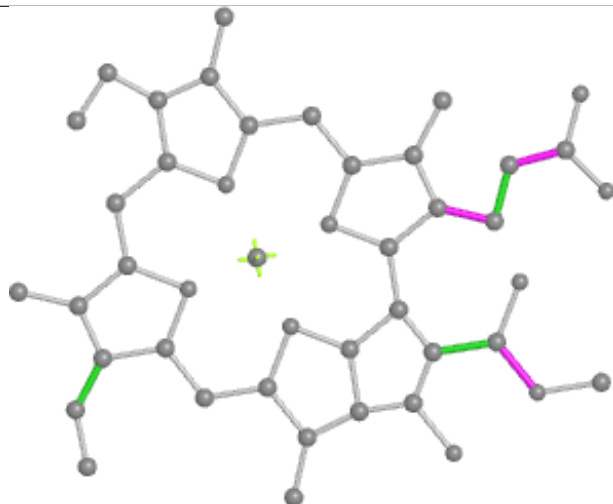
## Ligand CLA t 512



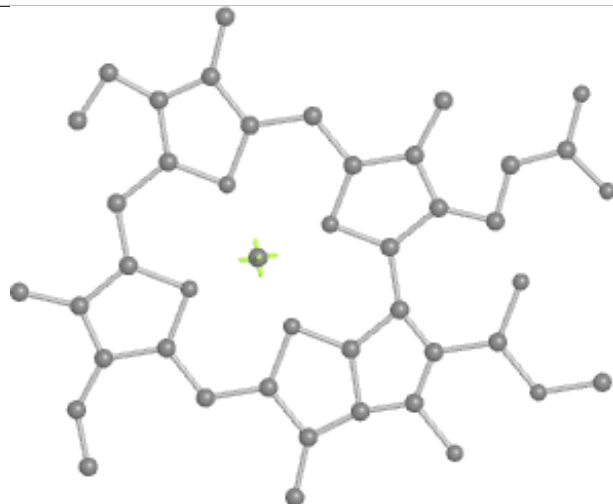
Bond lengths



Bond angles

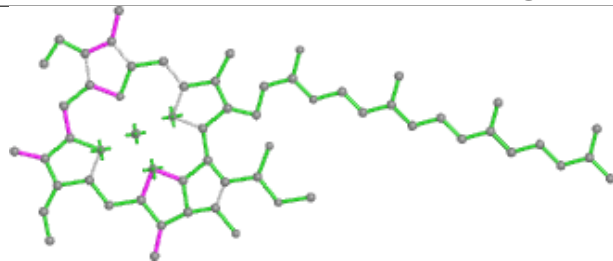


Torsions

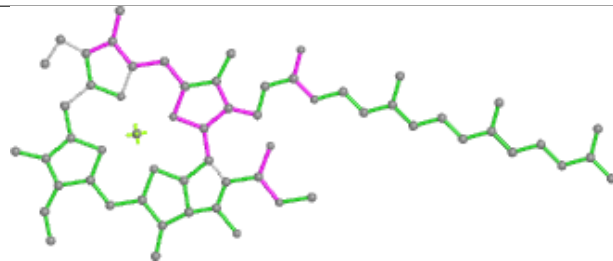


Rings

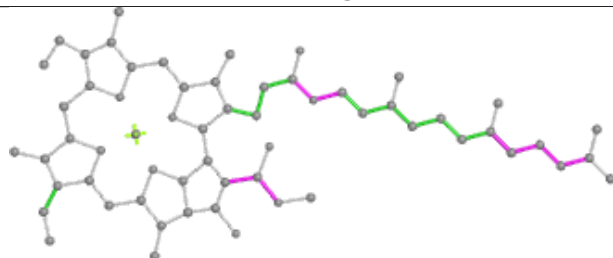
## Ligand CLA s 506



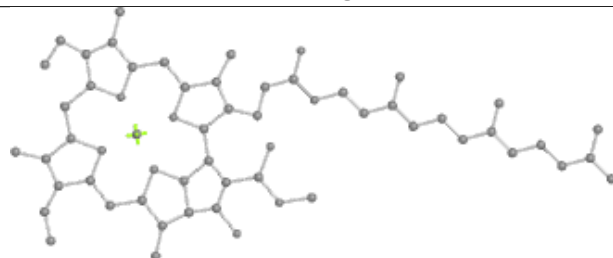
Bond lengths



Bond angles

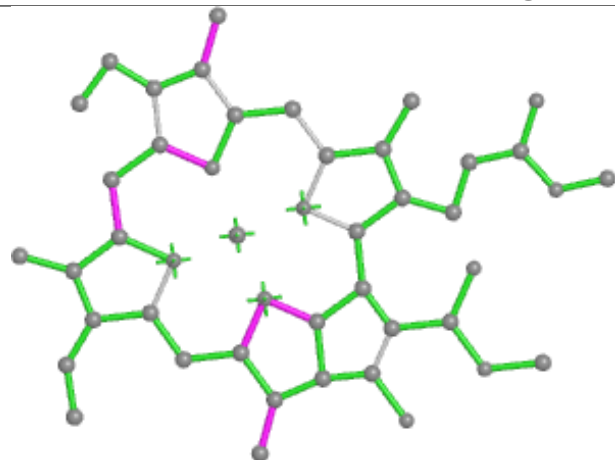


Torsions

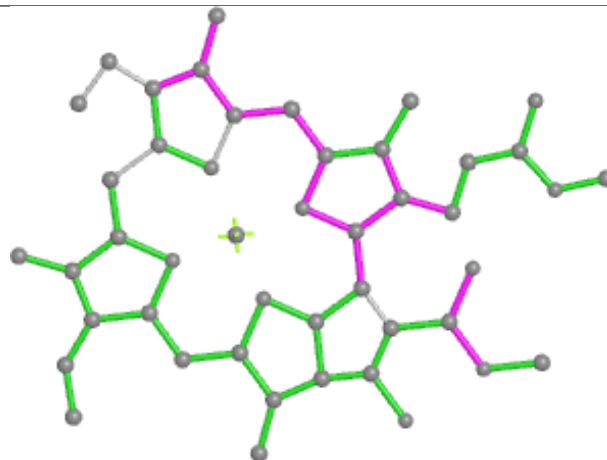


Rings

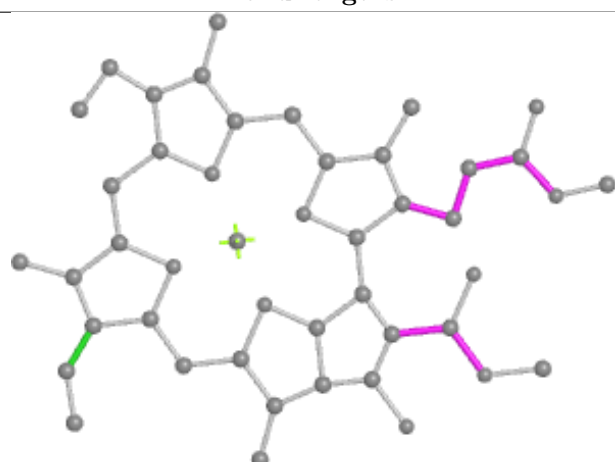
## Ligand CLA x 503



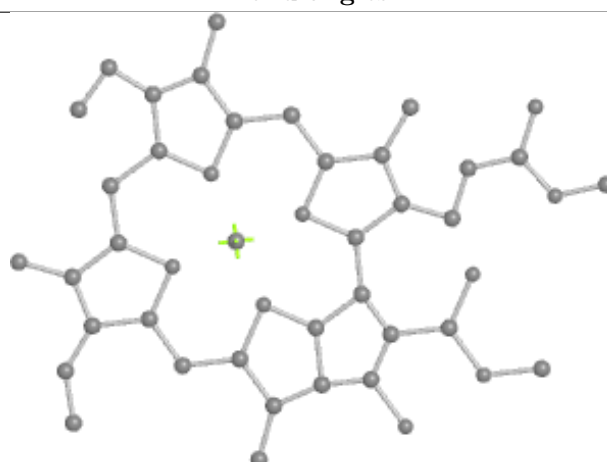
Bond lengths



Bond angles

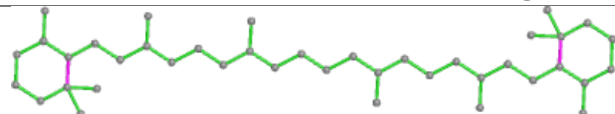


Torsions

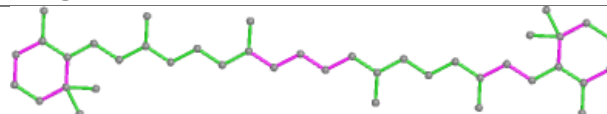


Rings

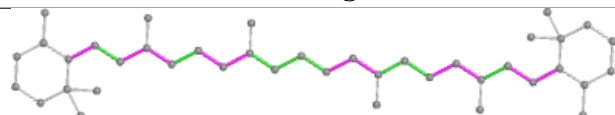
## Ligand BCR g 601



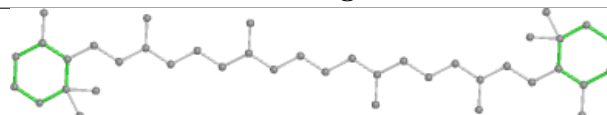
Bond lengths



Bond angles

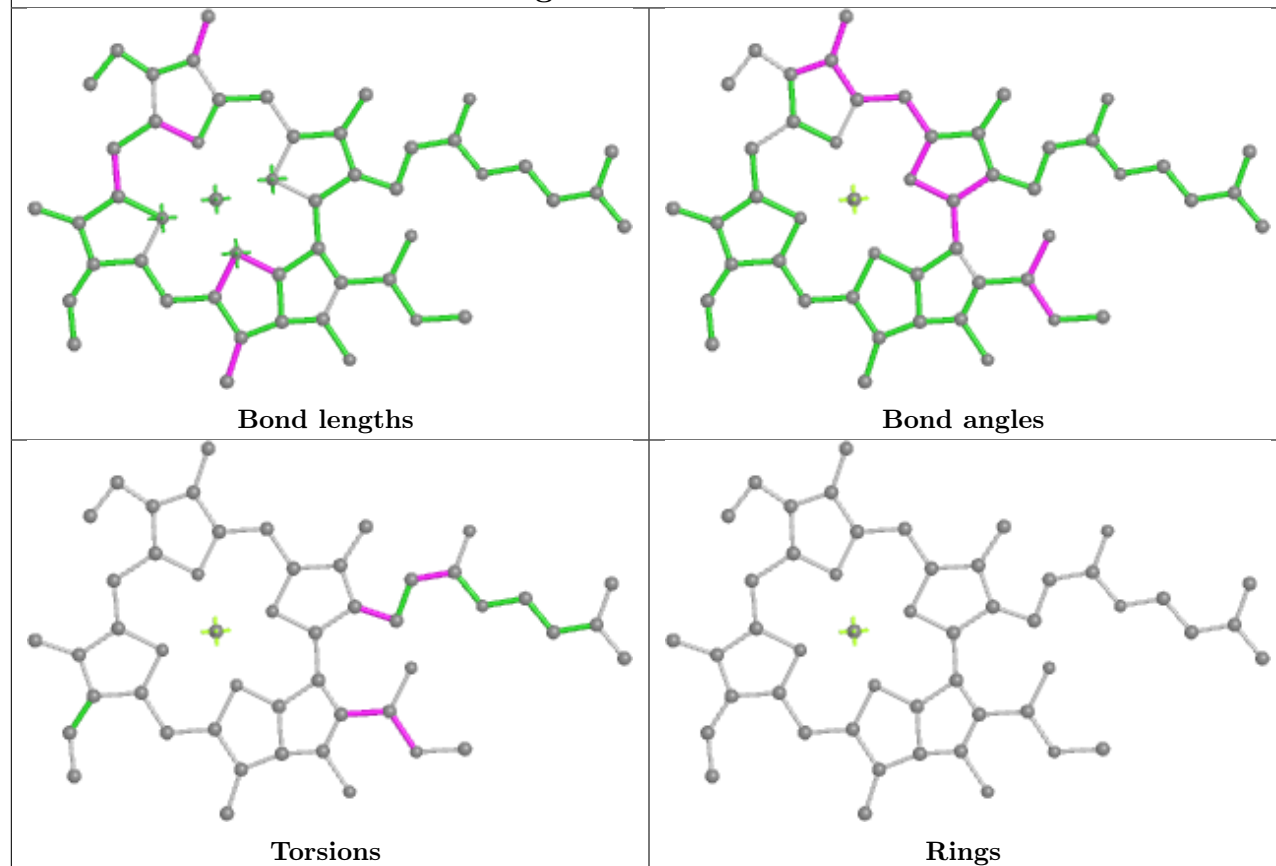


Torsions

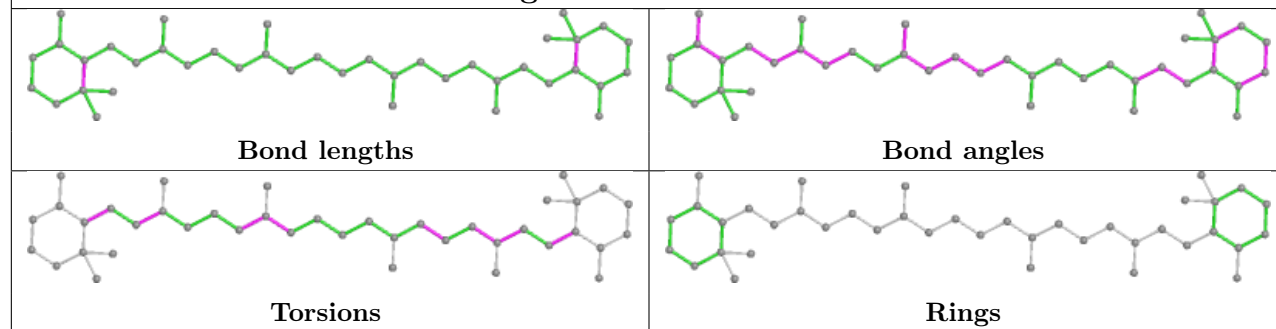


Rings

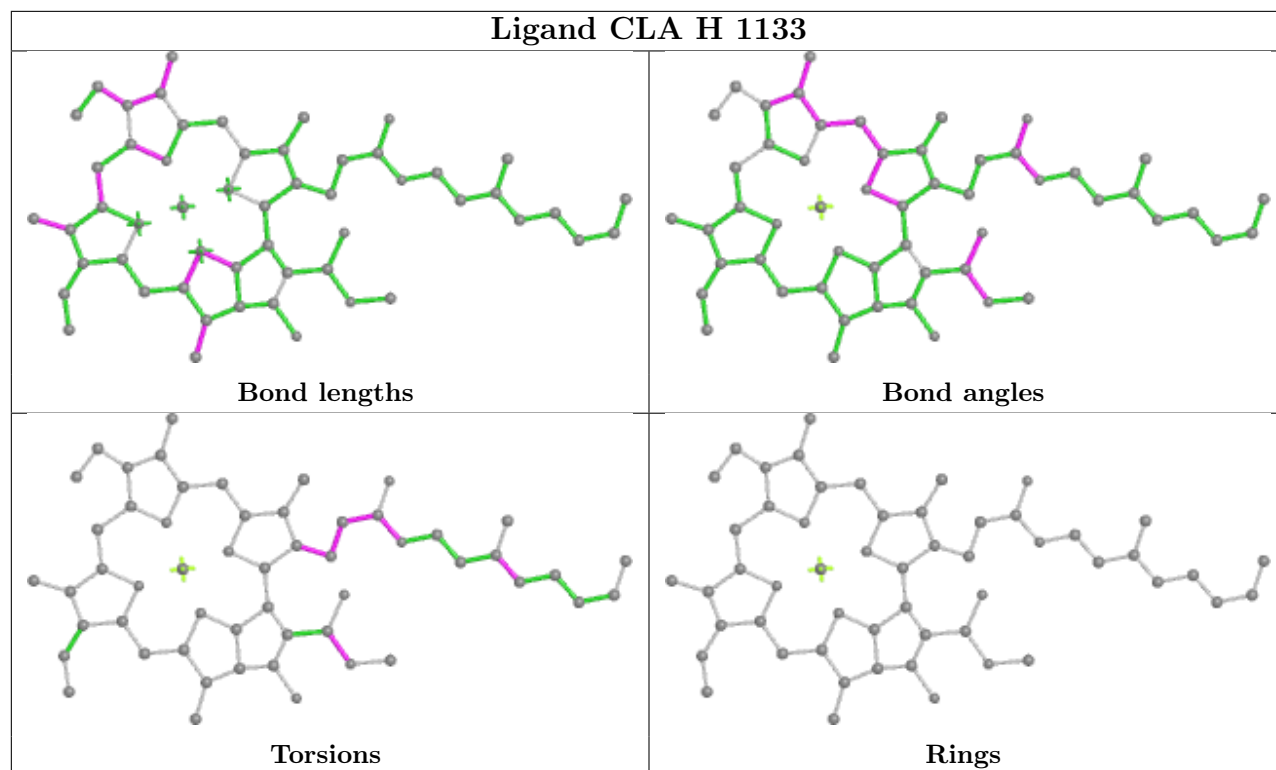
## Ligand CLA u 514



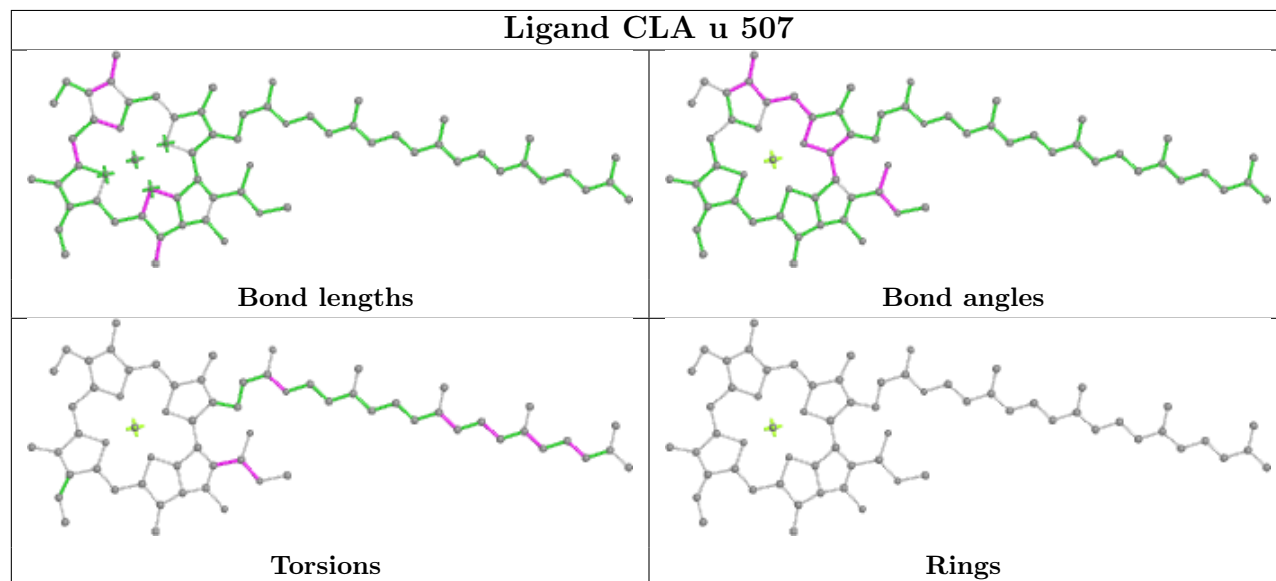
## Ligand BCR H 4001



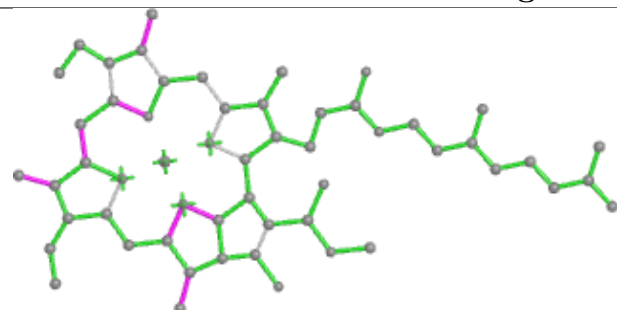
## Ligand CLA H 1133



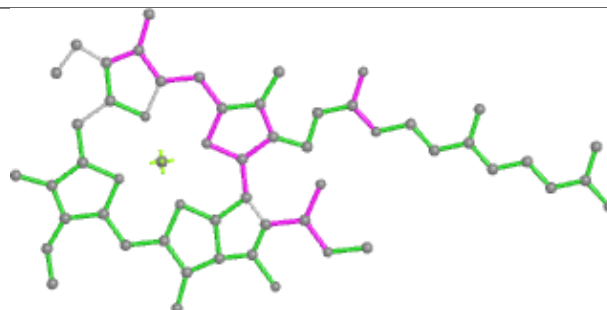
## Ligand CLA u 507



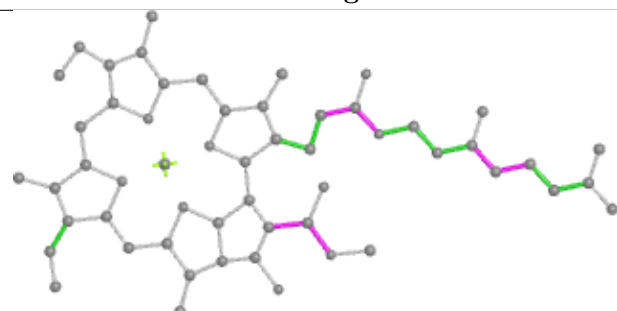
## Ligand CLA X 517



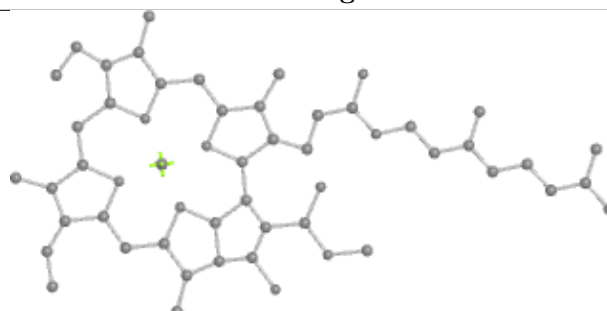
Bond lengths



Bond angles

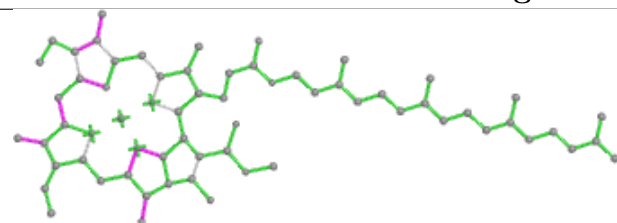


Torsions

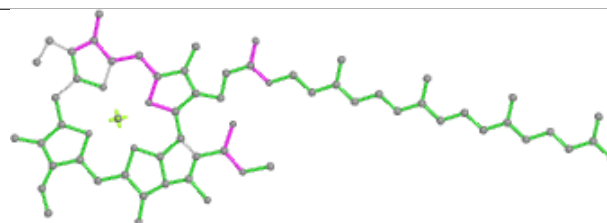


Rings

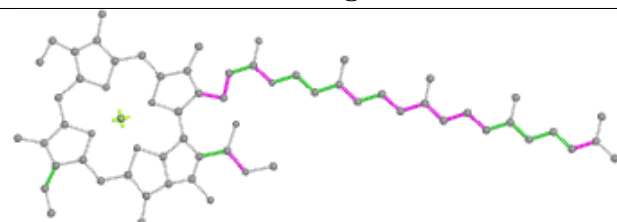
## Ligand CLA a 1140



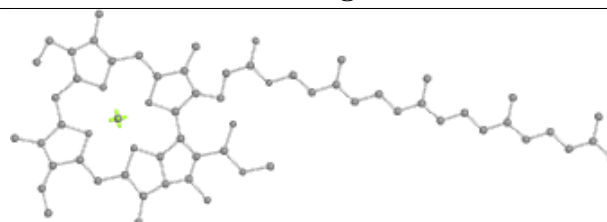
Bond lengths



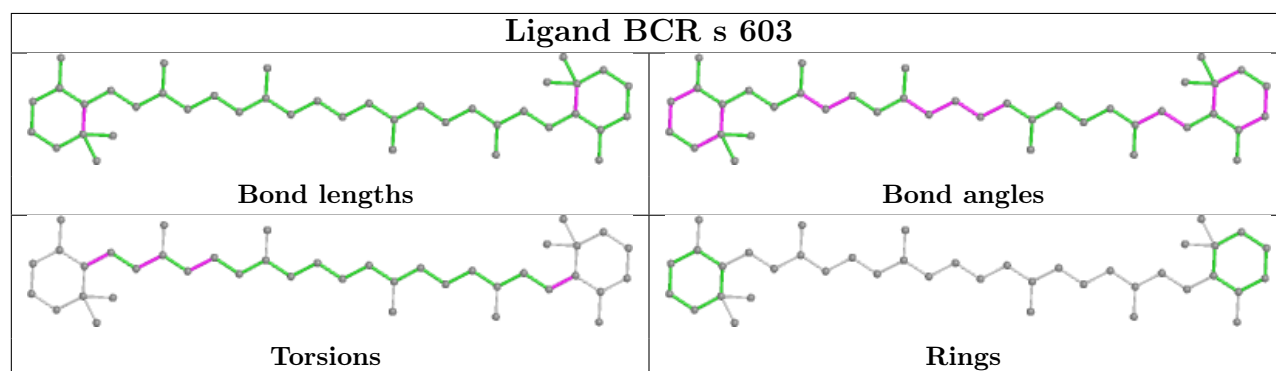
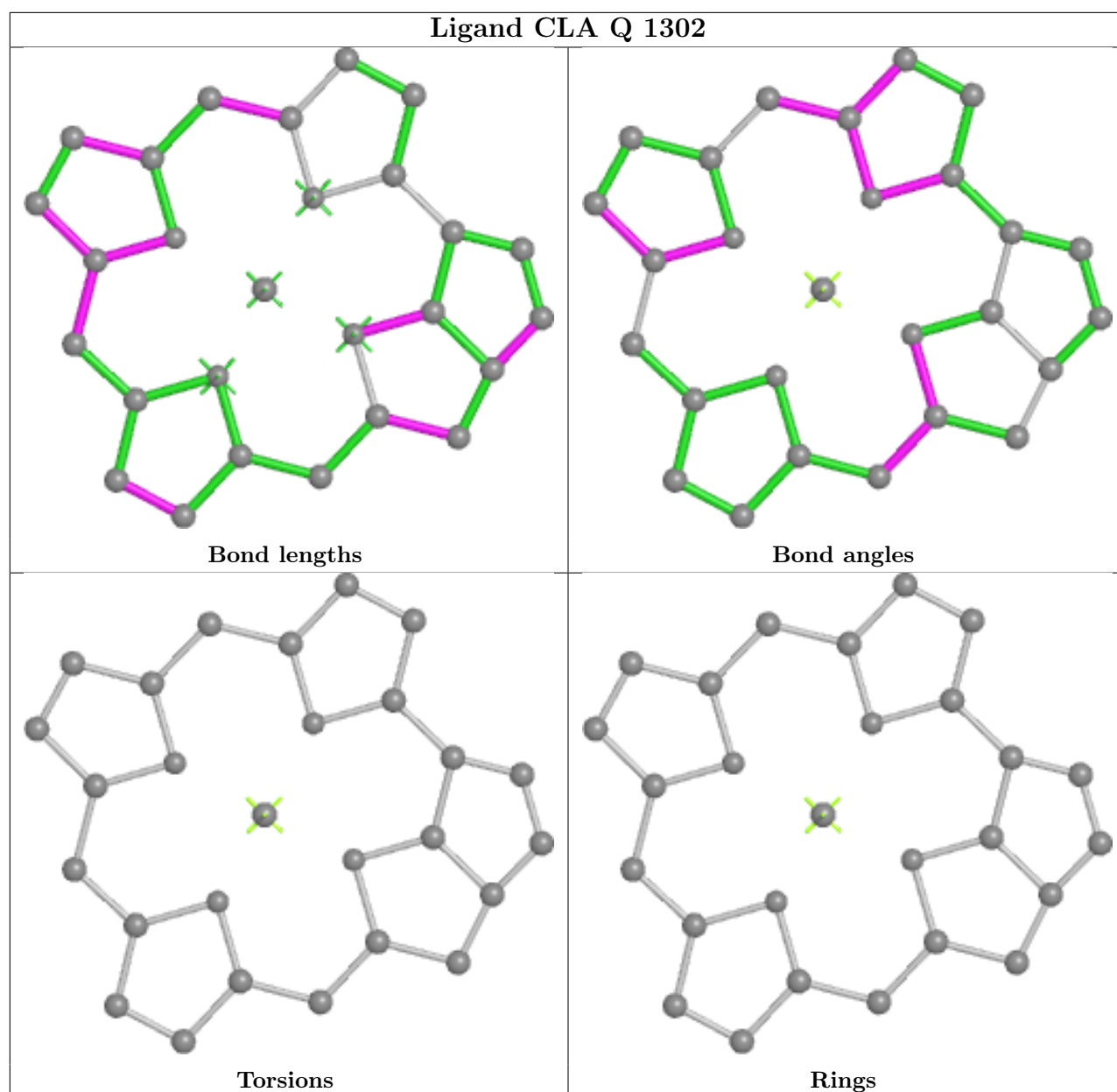
Bond angles

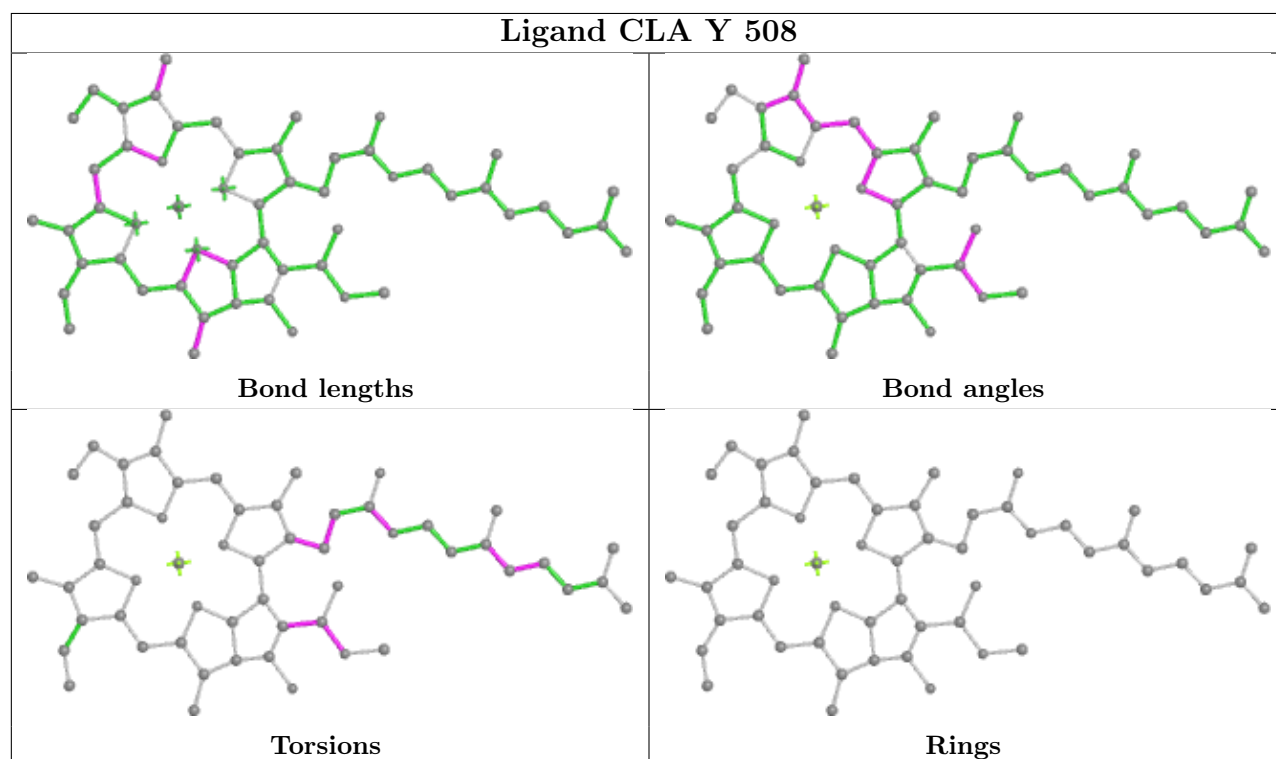
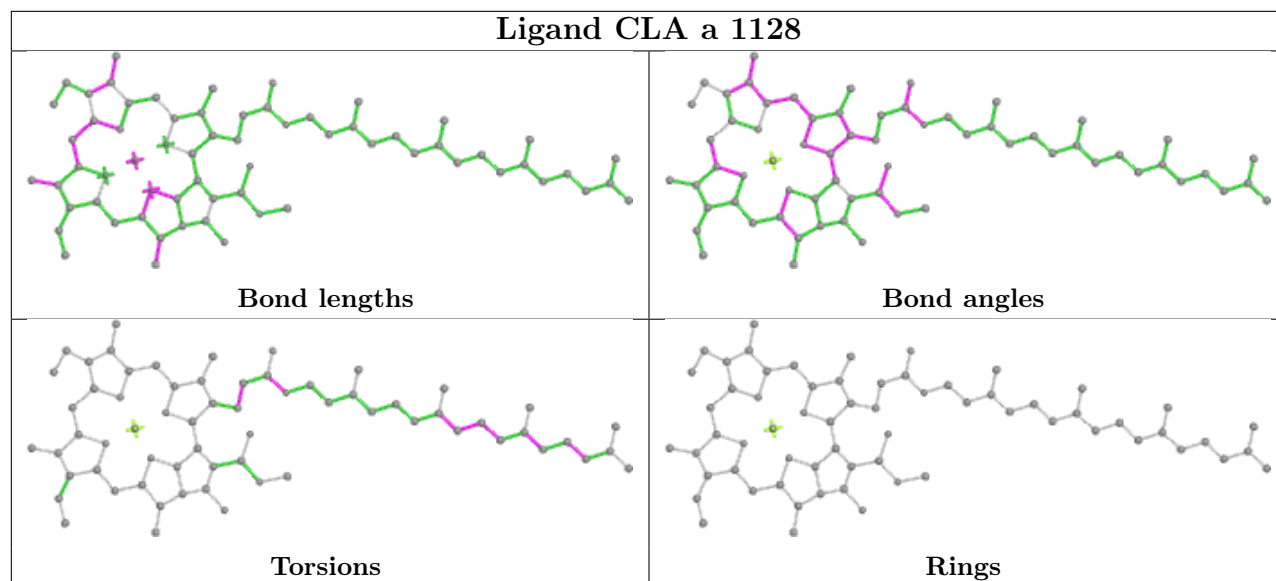
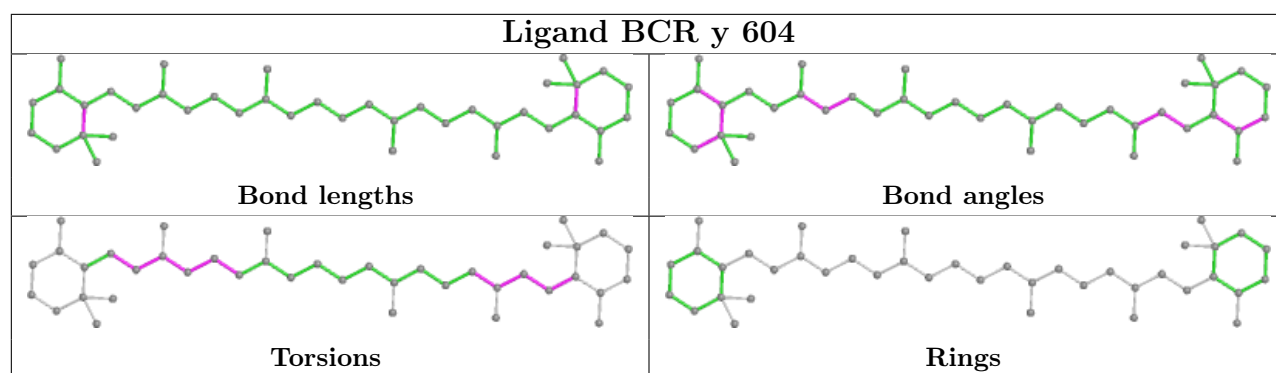


Torsions



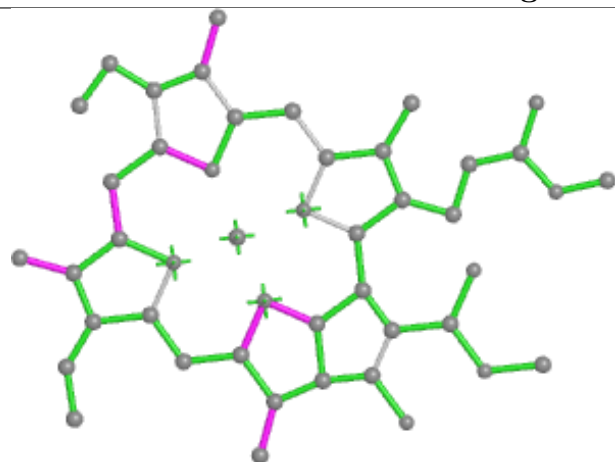
Rings



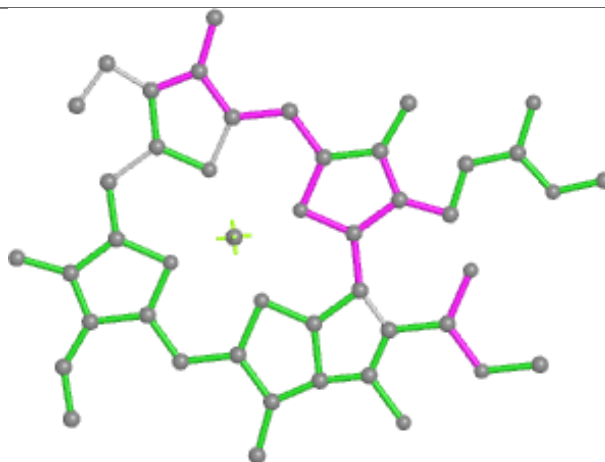




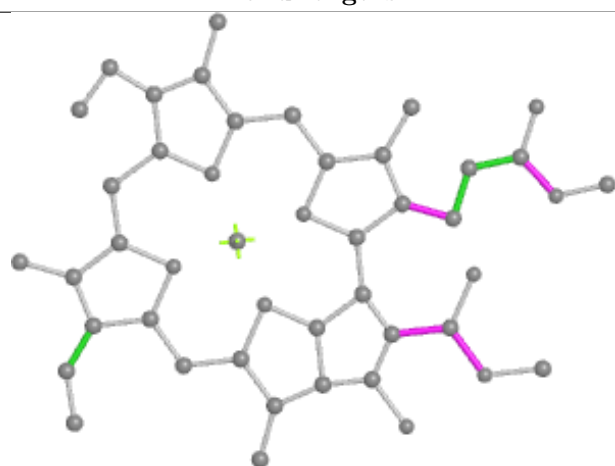
## Ligand CLA o 503



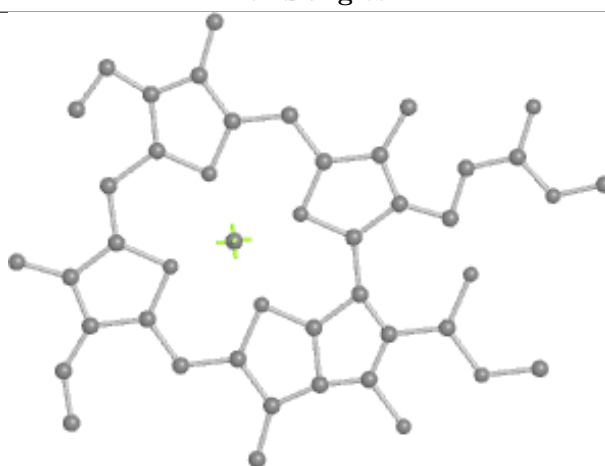
Bond lengths



Bond angles

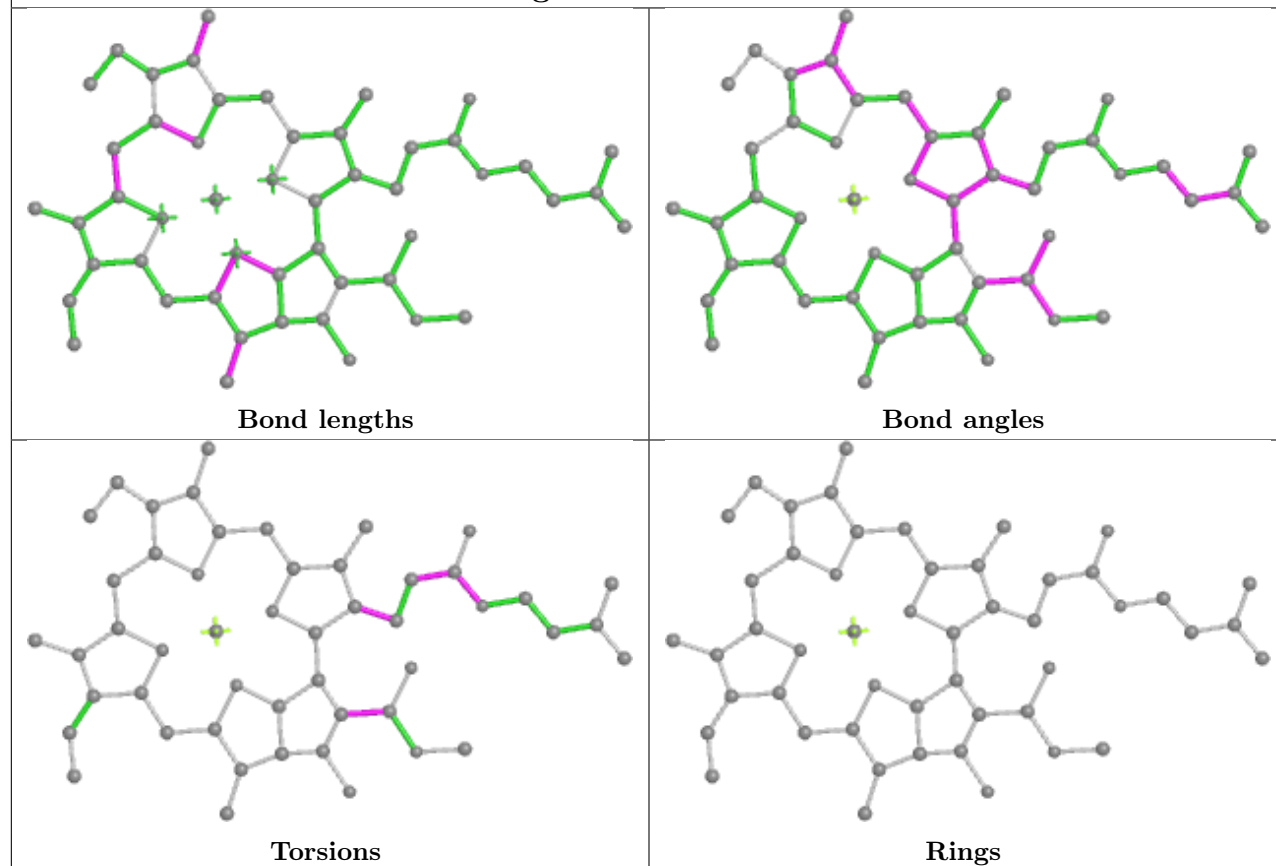


Torsions

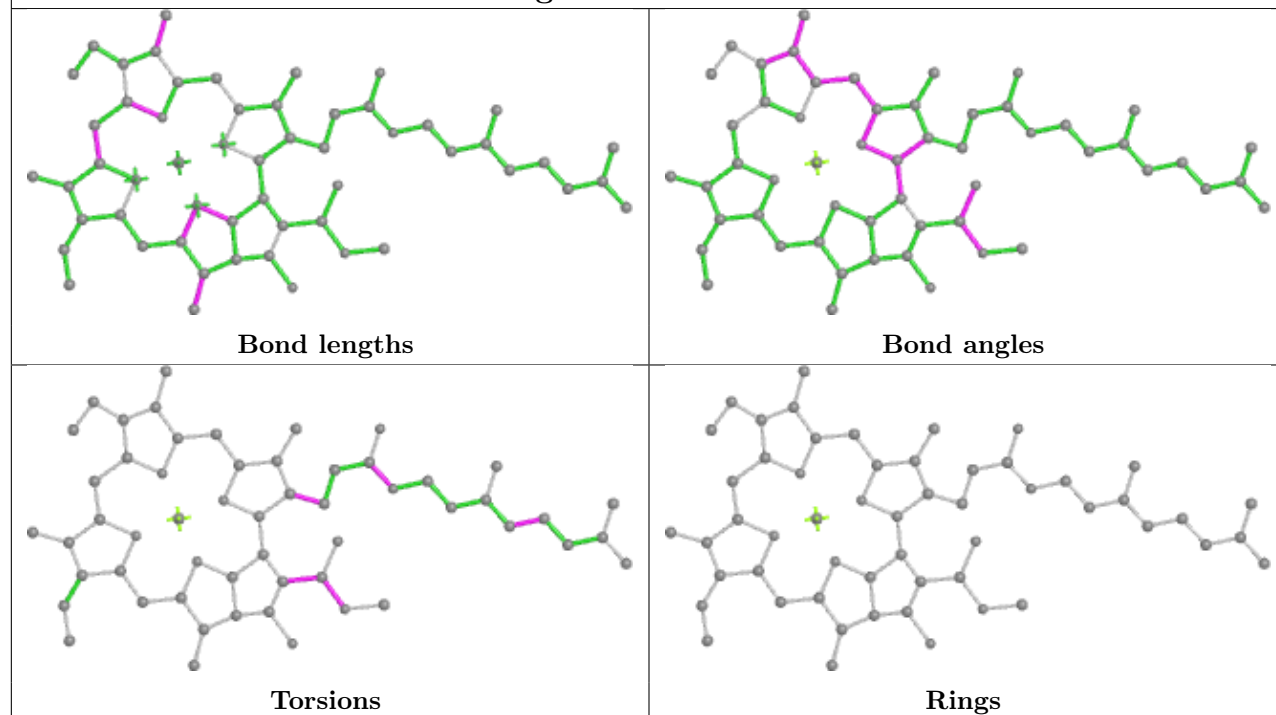


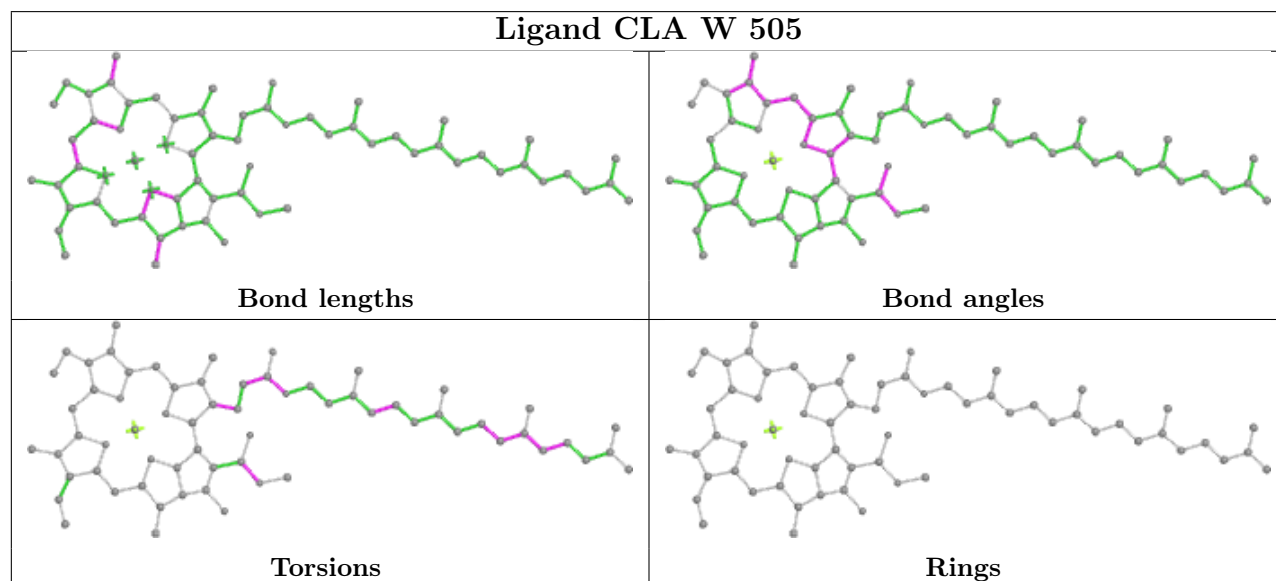
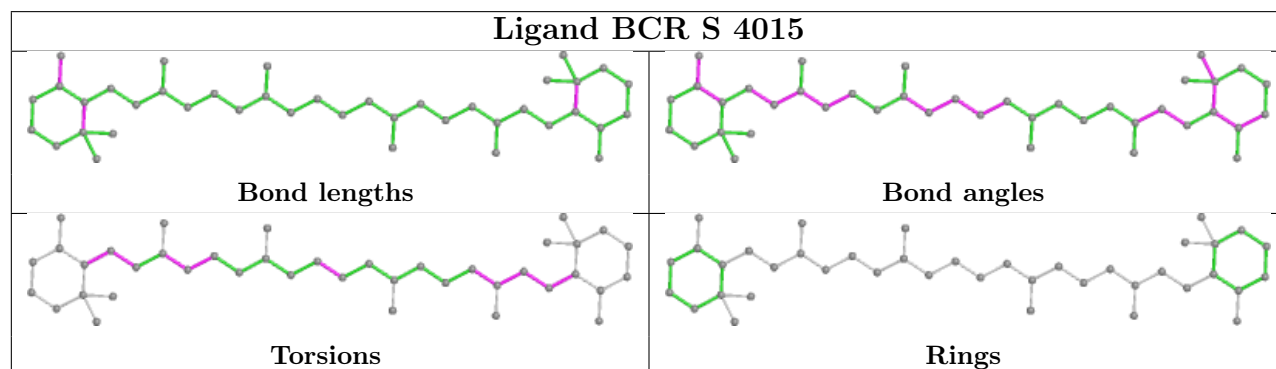
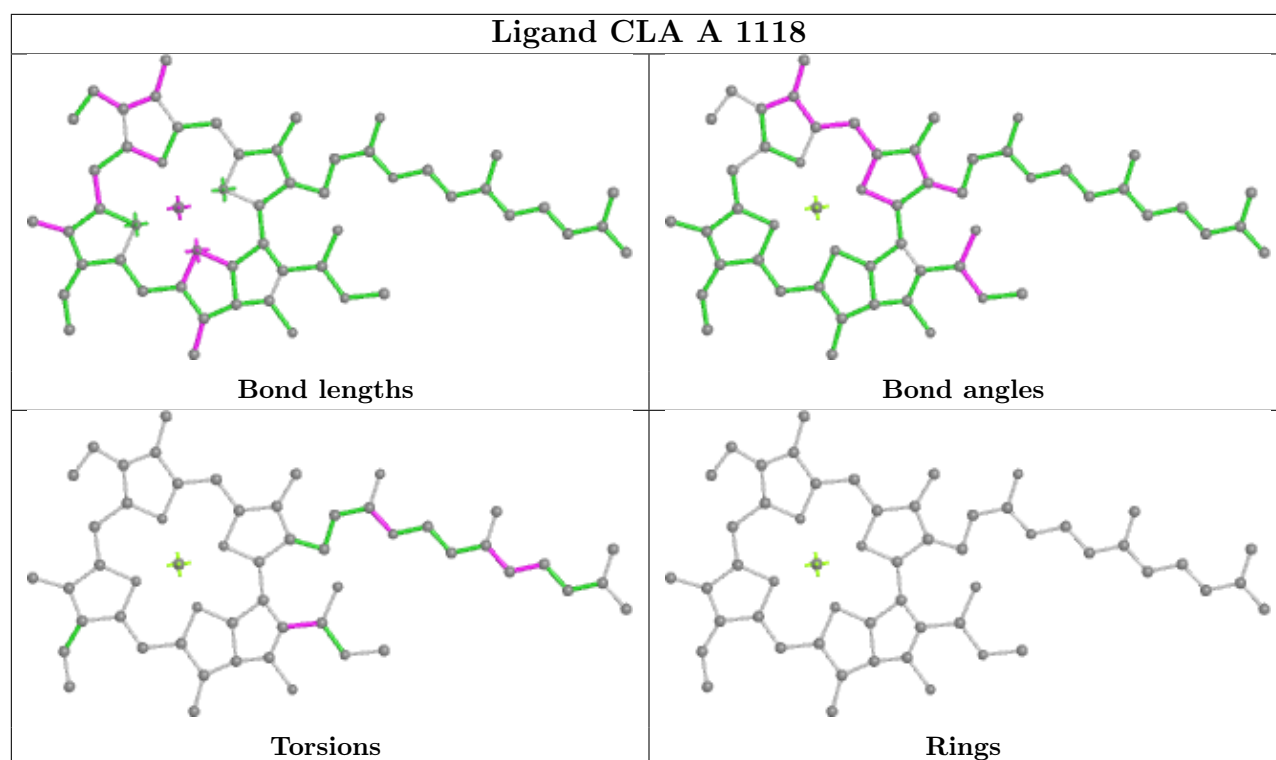
Rings

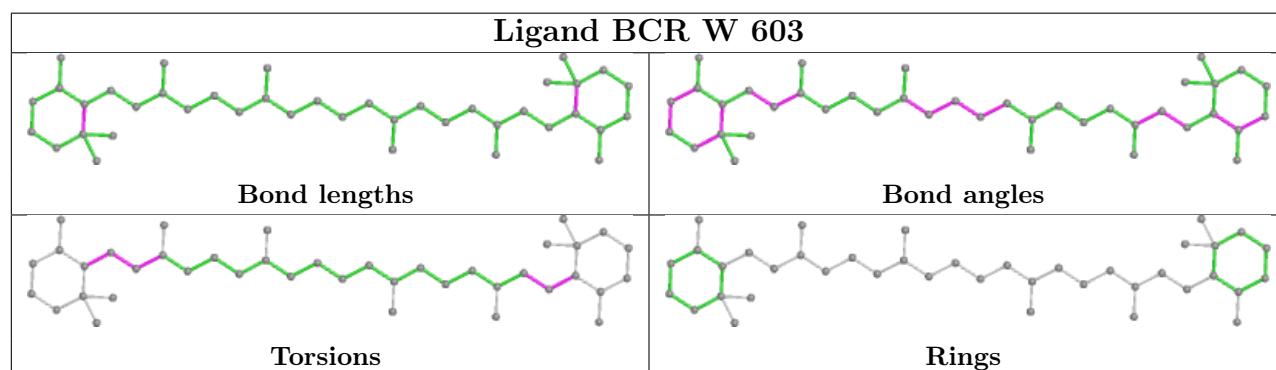
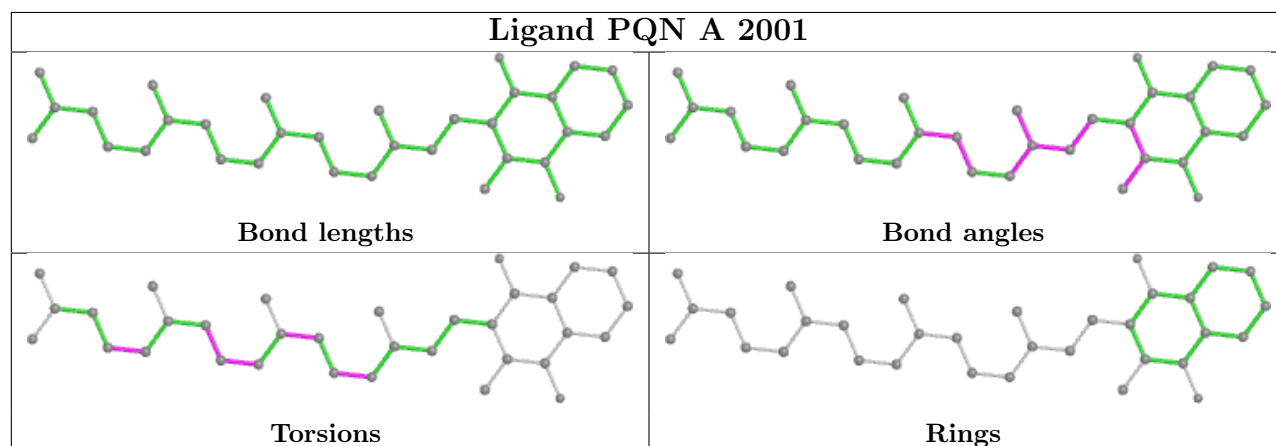
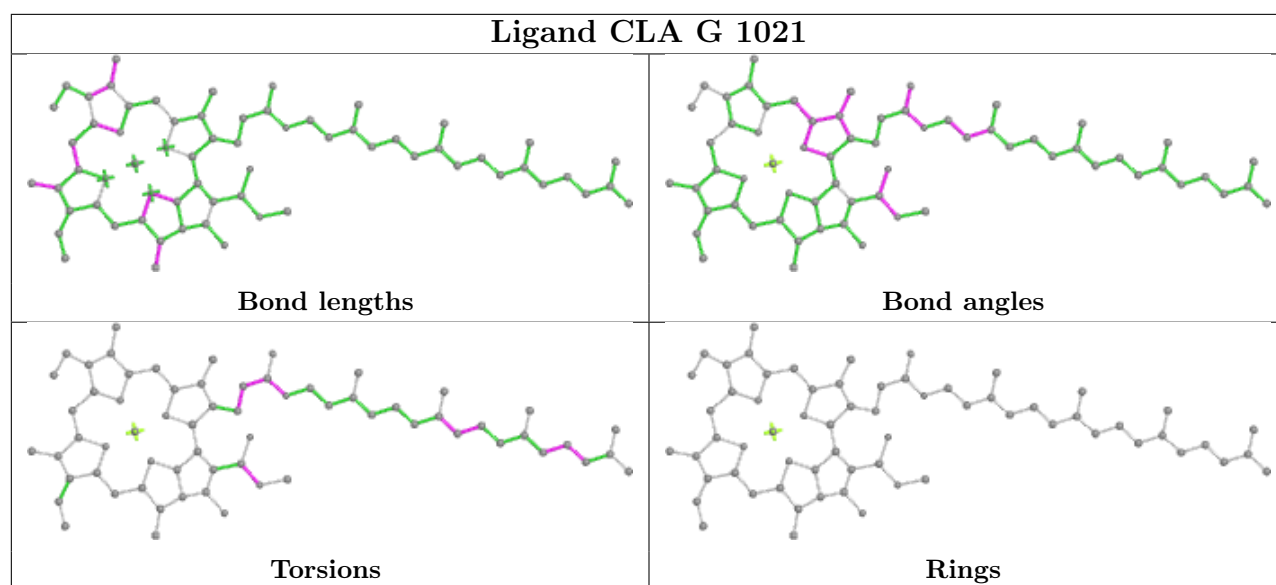
## Ligand CLA w 502



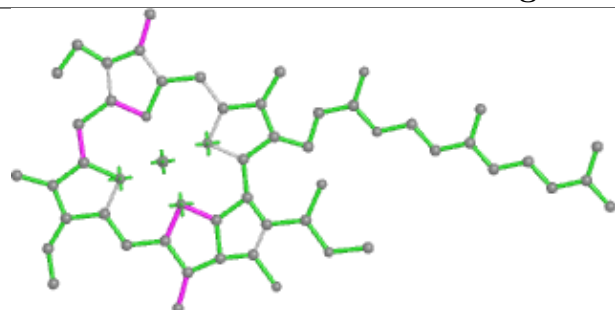
## Ligand CLA x 508



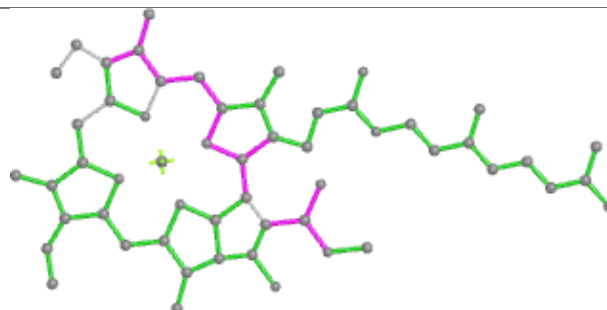




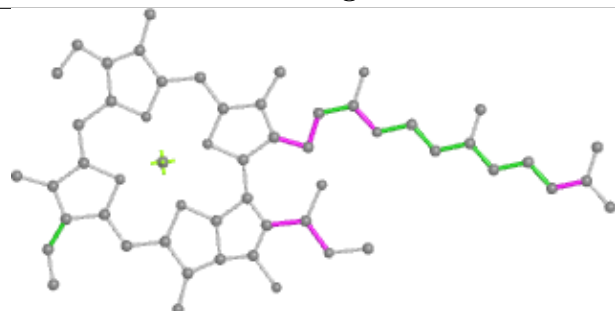
## Ligand CLA u 508



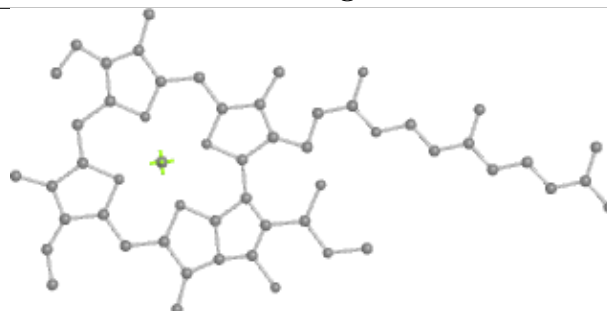
Bond lengths



Bond angles

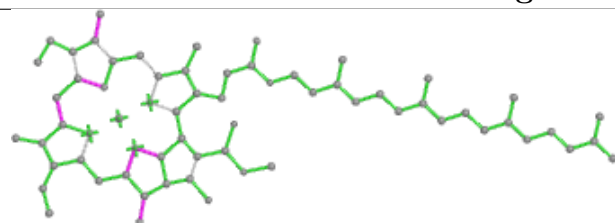


Torsions

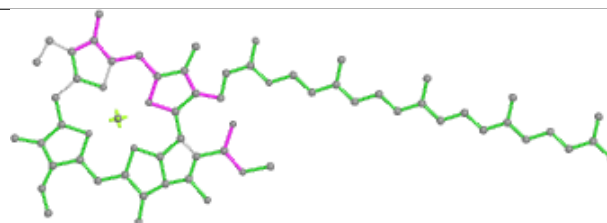


Rings

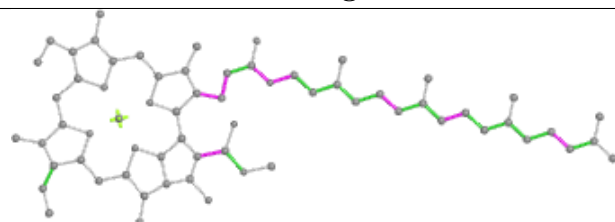
## Ligand CLA Y 515



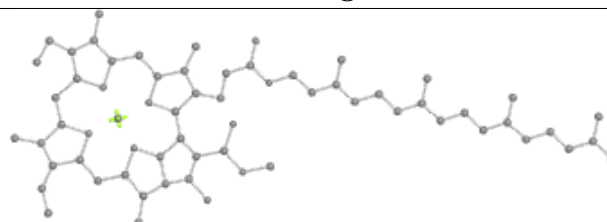
Bond lengths



Bond angles

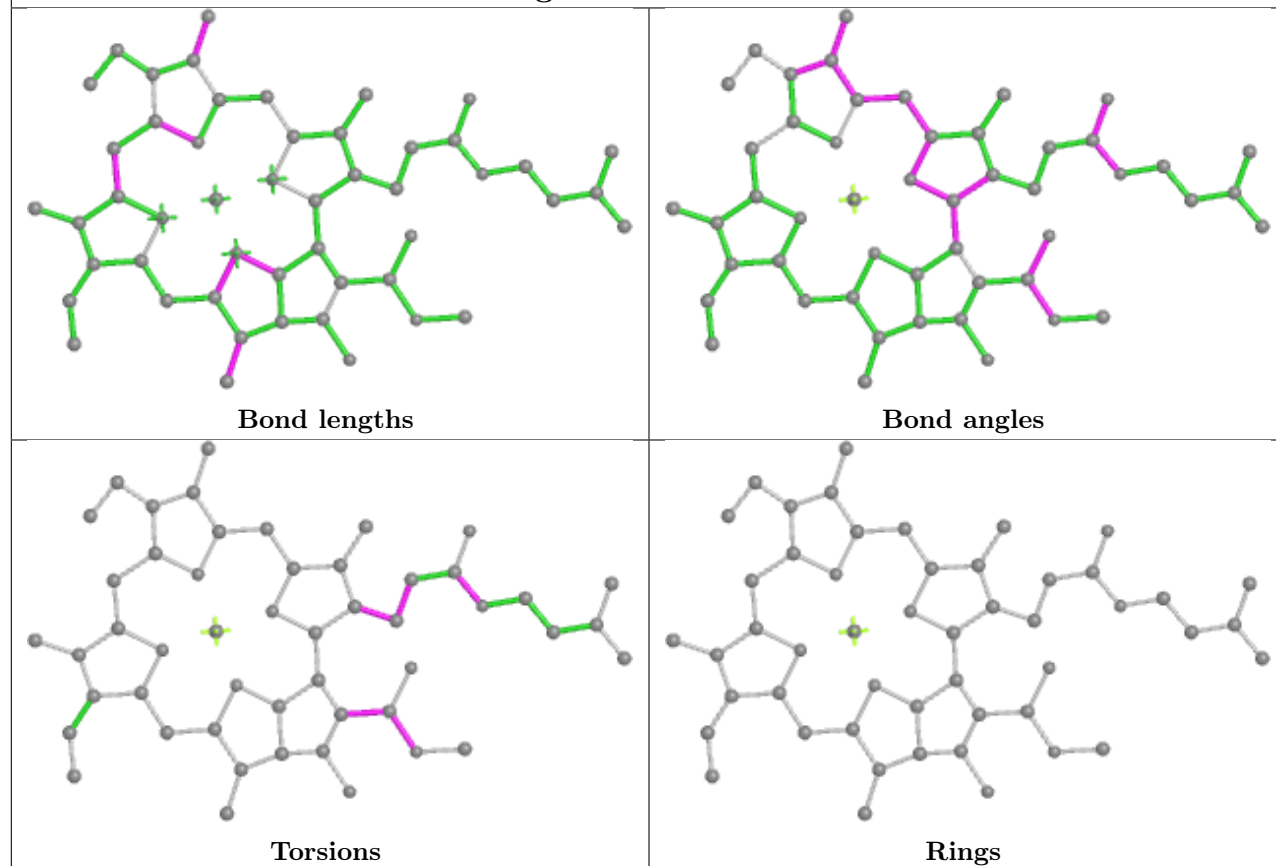


Torsions

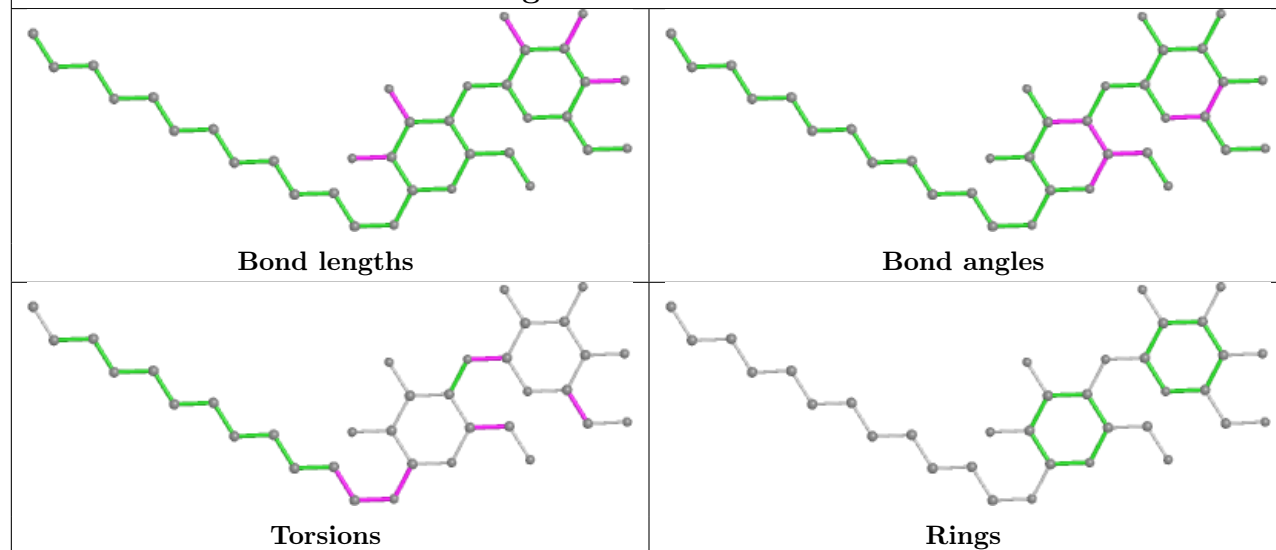


Rings

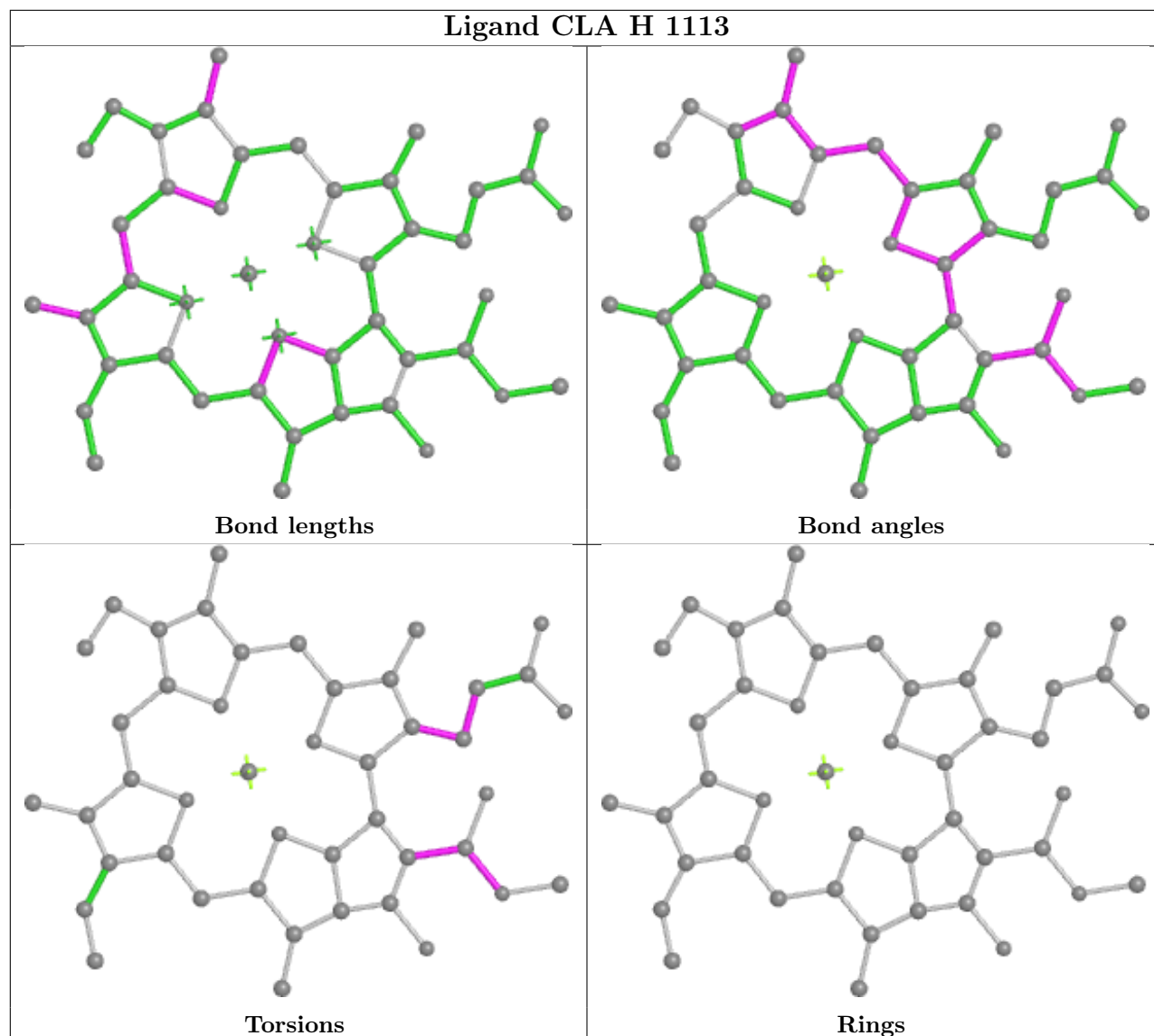
## Ligand CLA u 513



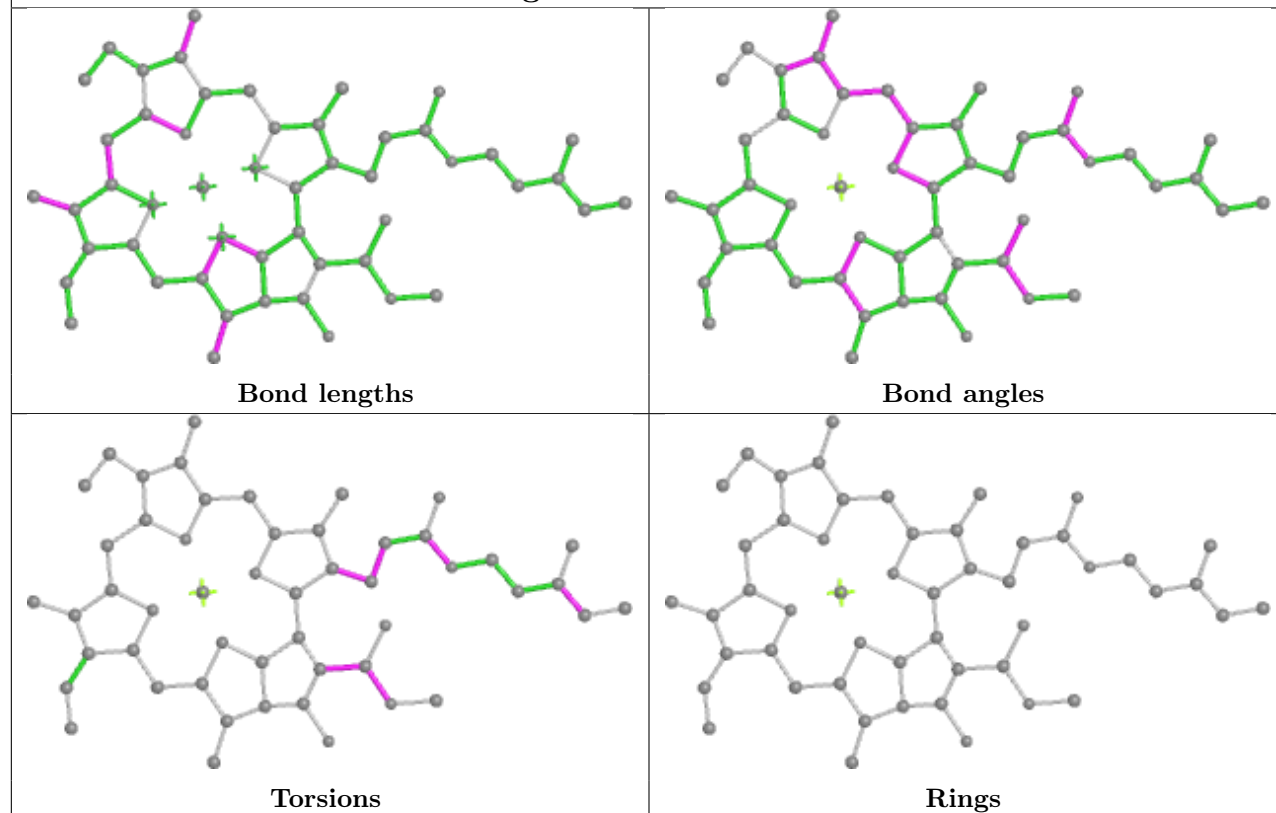
## Ligand LMT L 4101



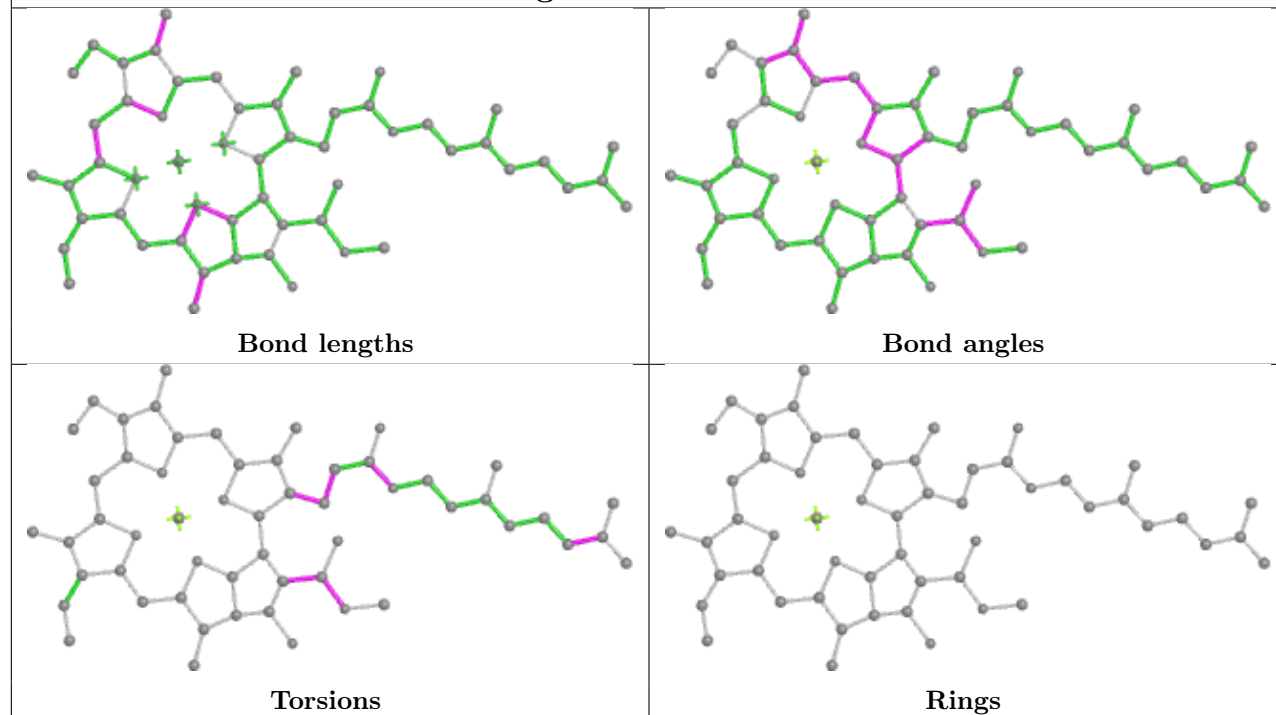
## Ligand CLA H 1113



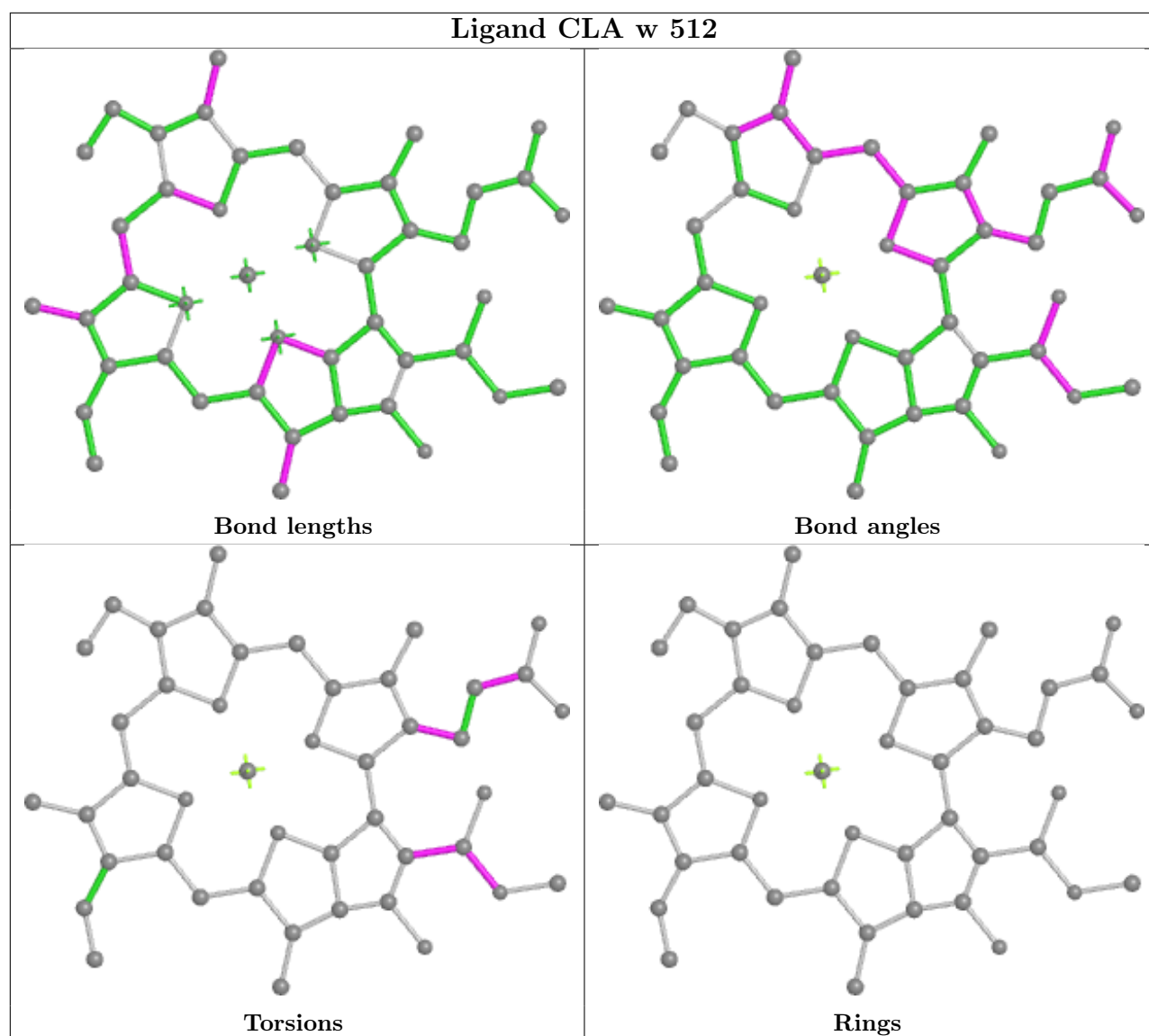
## Ligand CLA H 1121

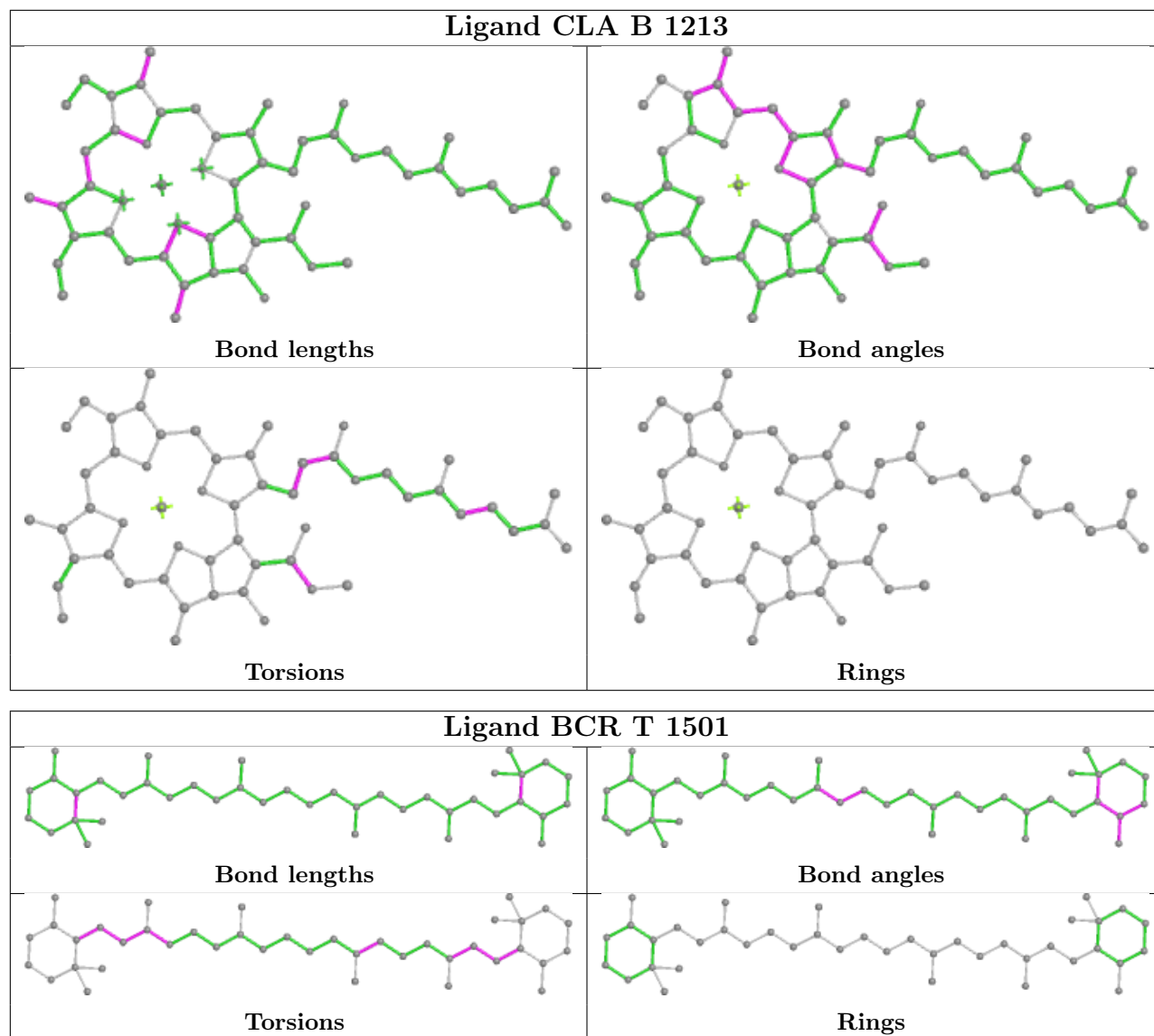


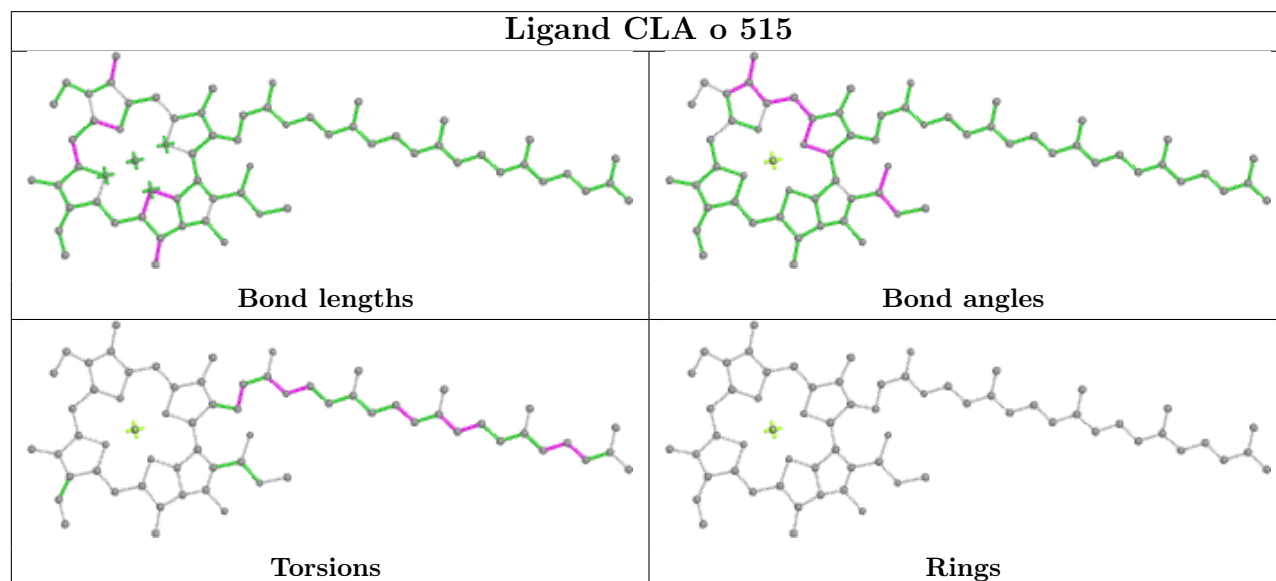
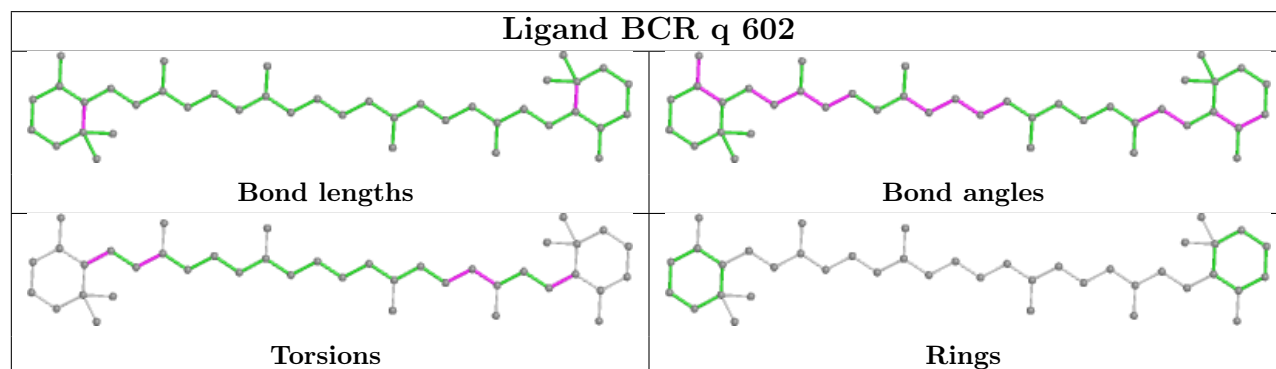
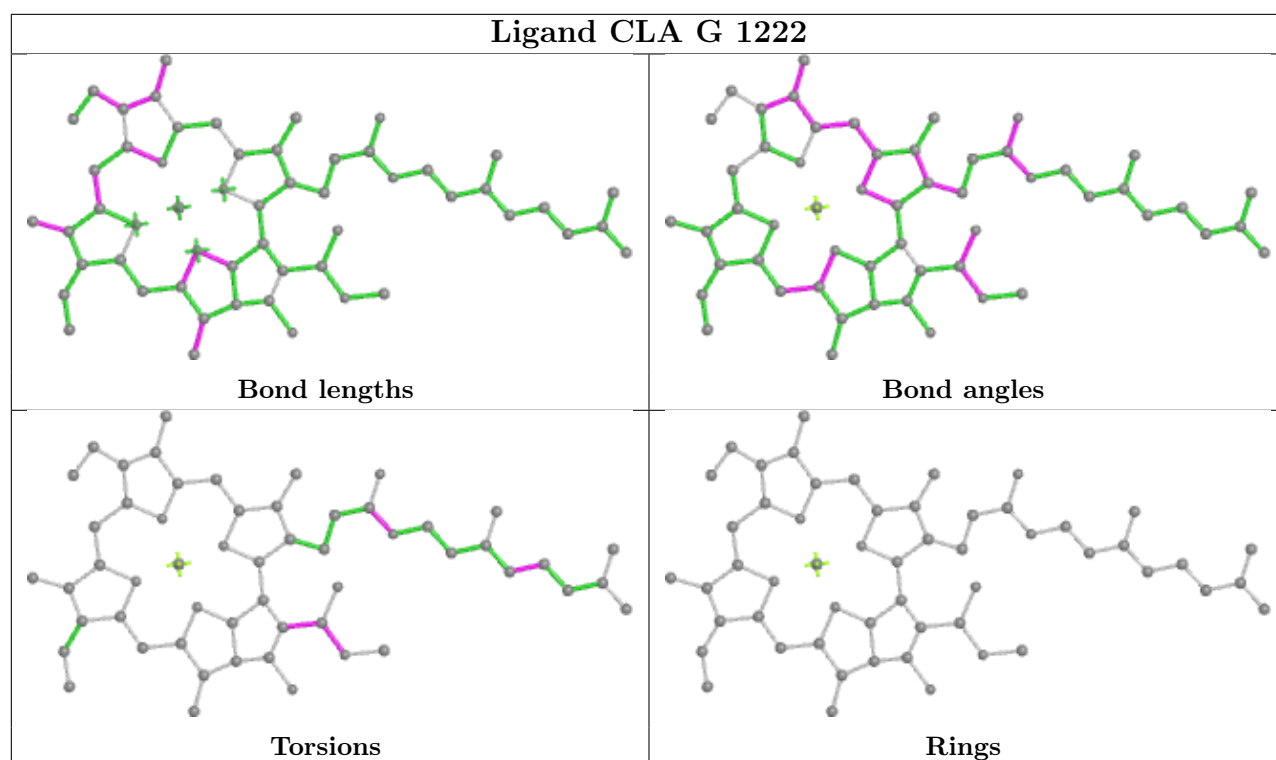
## Ligand CLA o 508

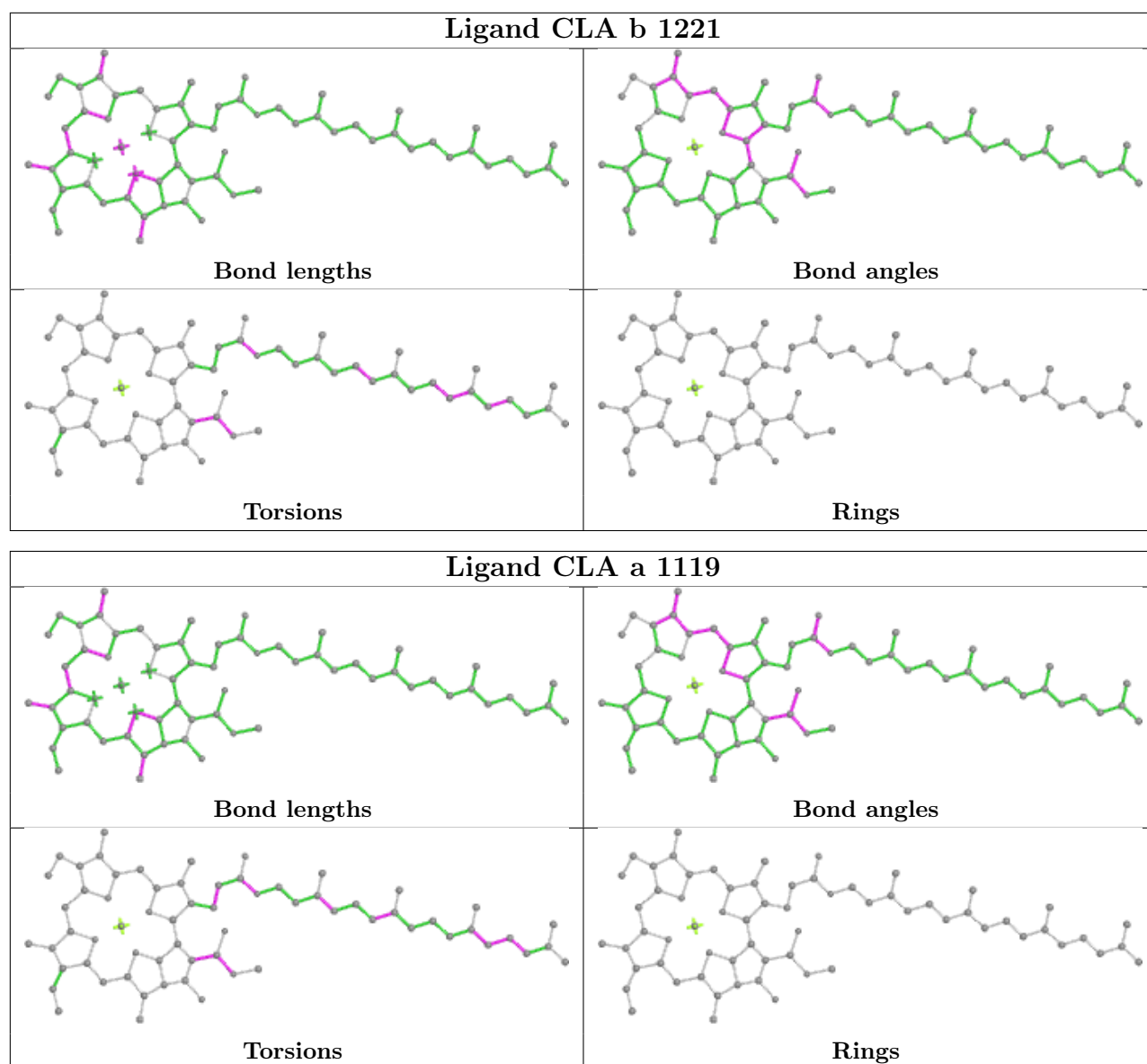




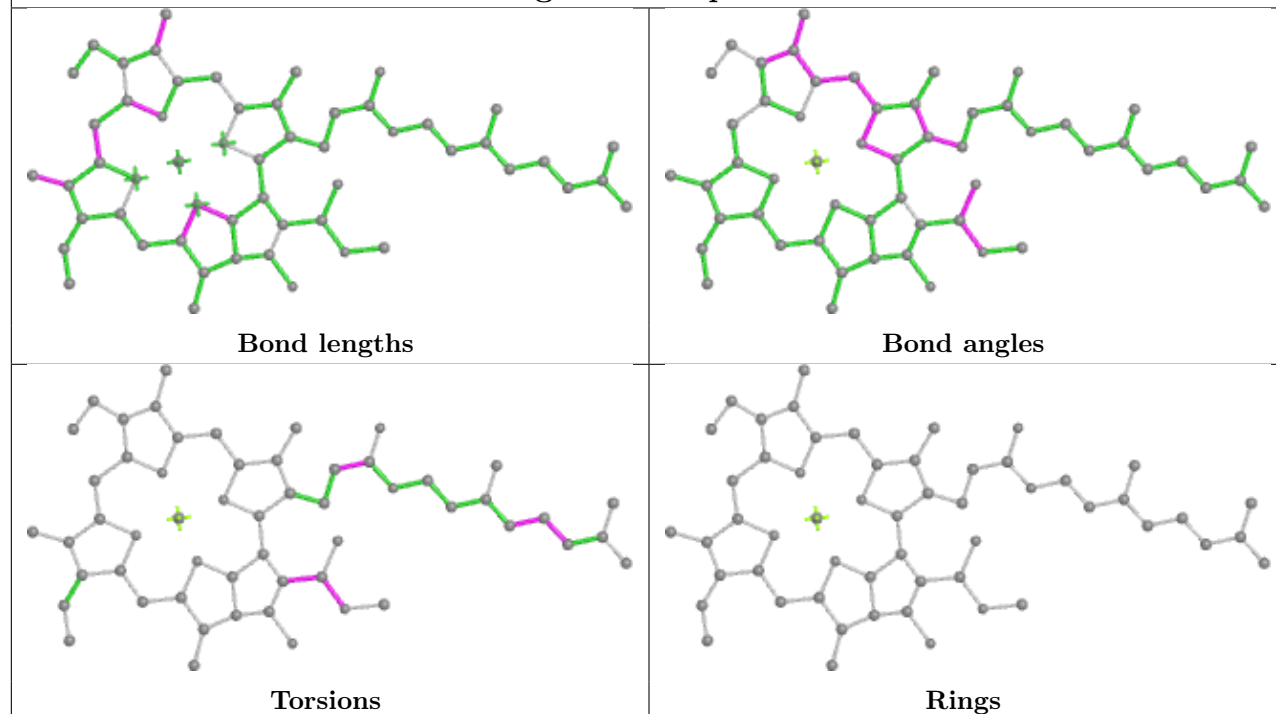




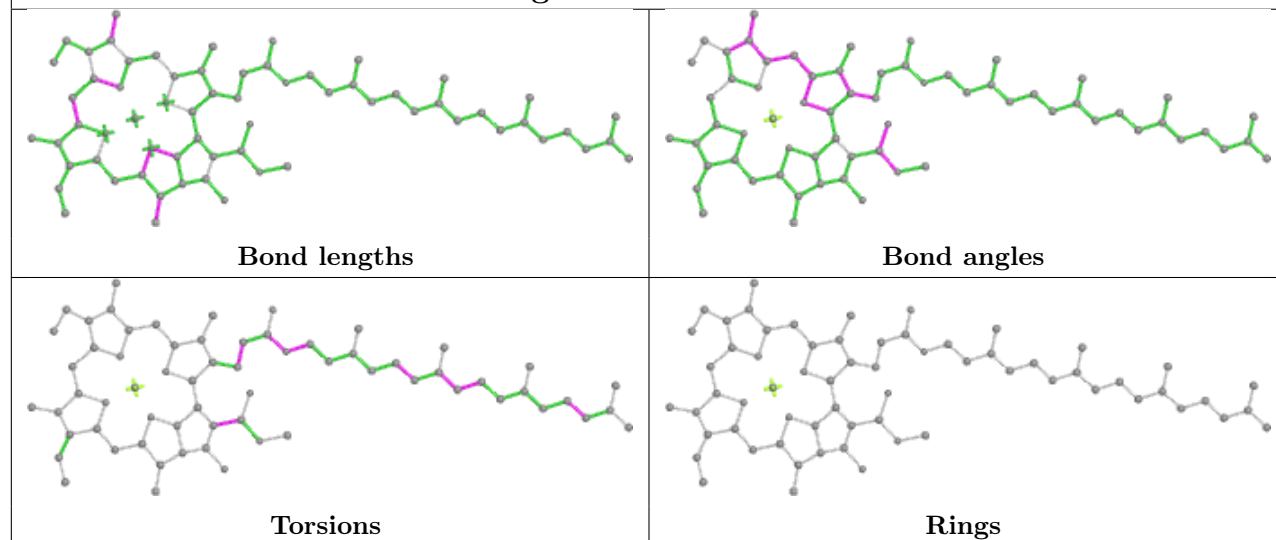


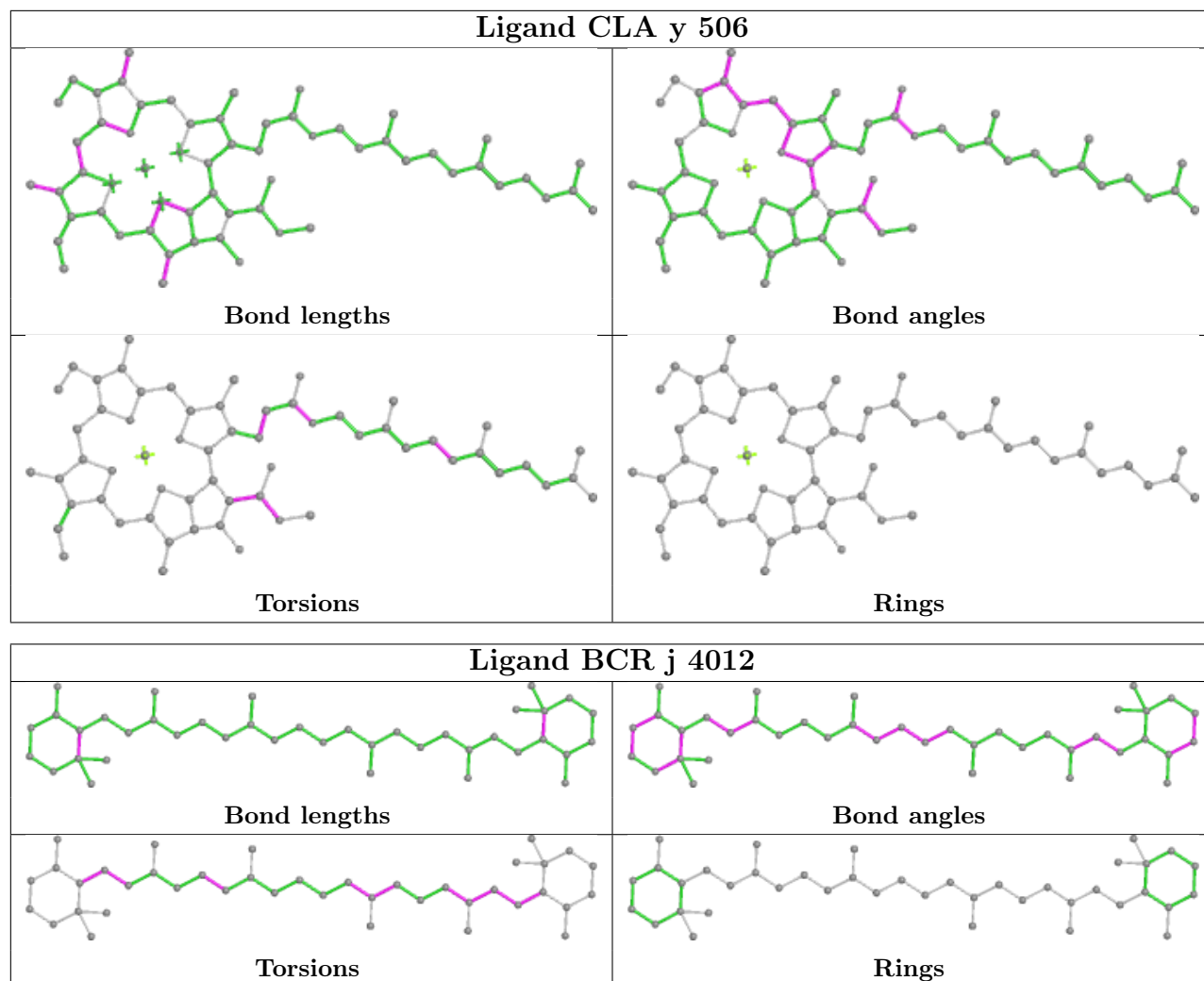


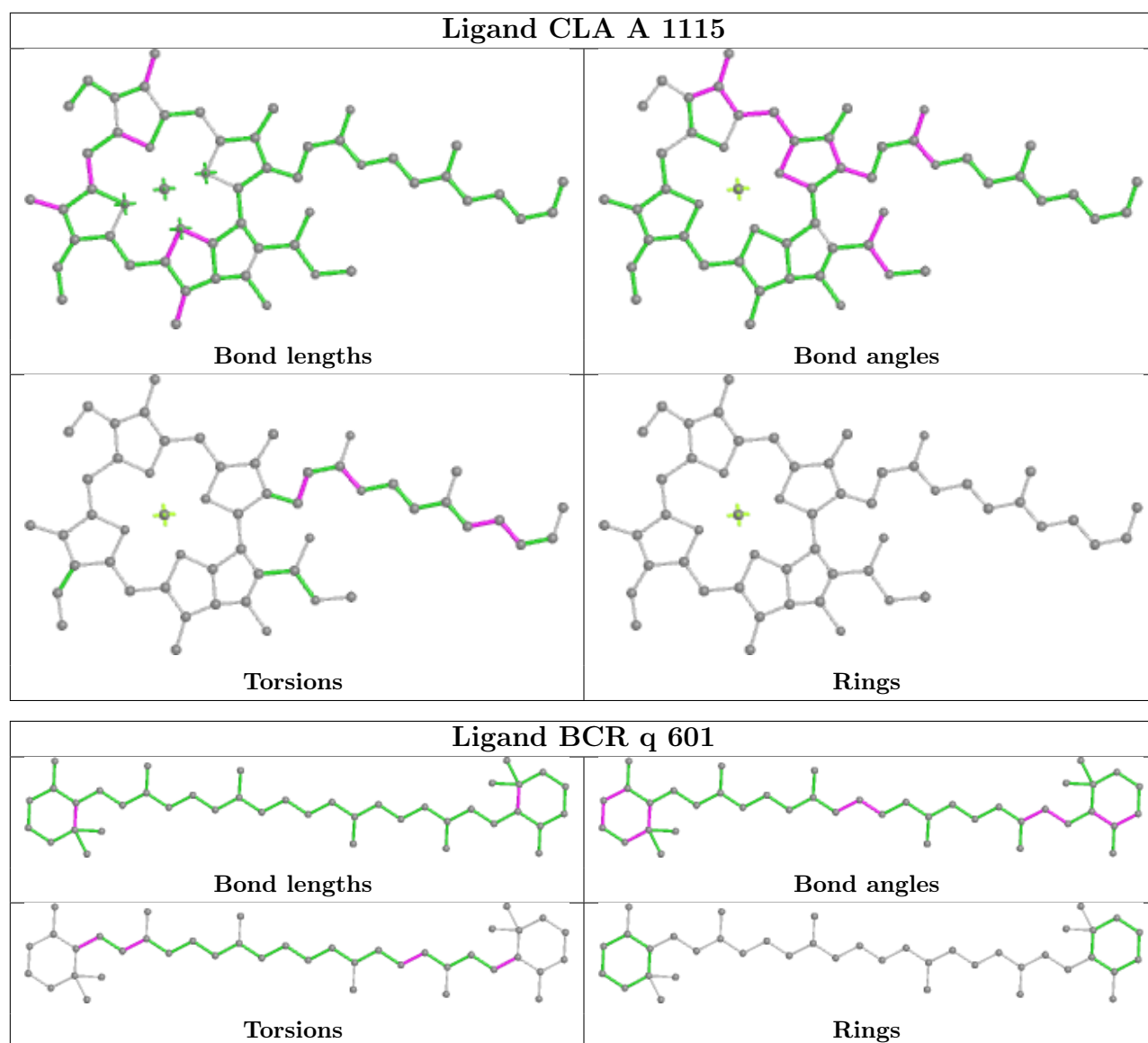
## Ligand CLA p 517



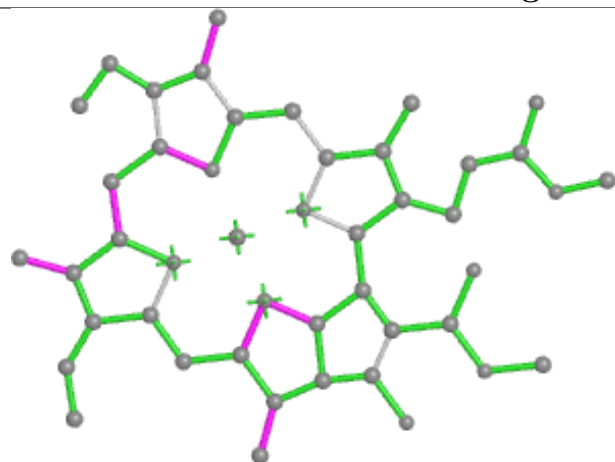
## Ligand CLA X 515



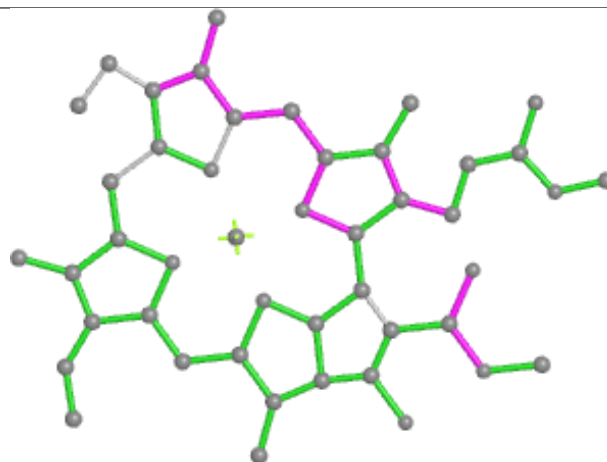




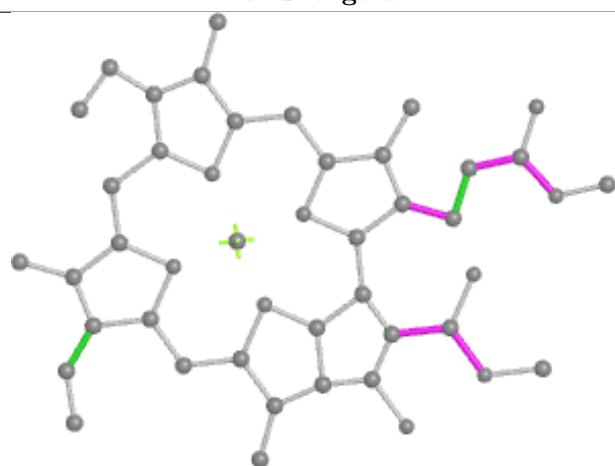
## Ligand CLA s 503



Bond lengths



Bond angles

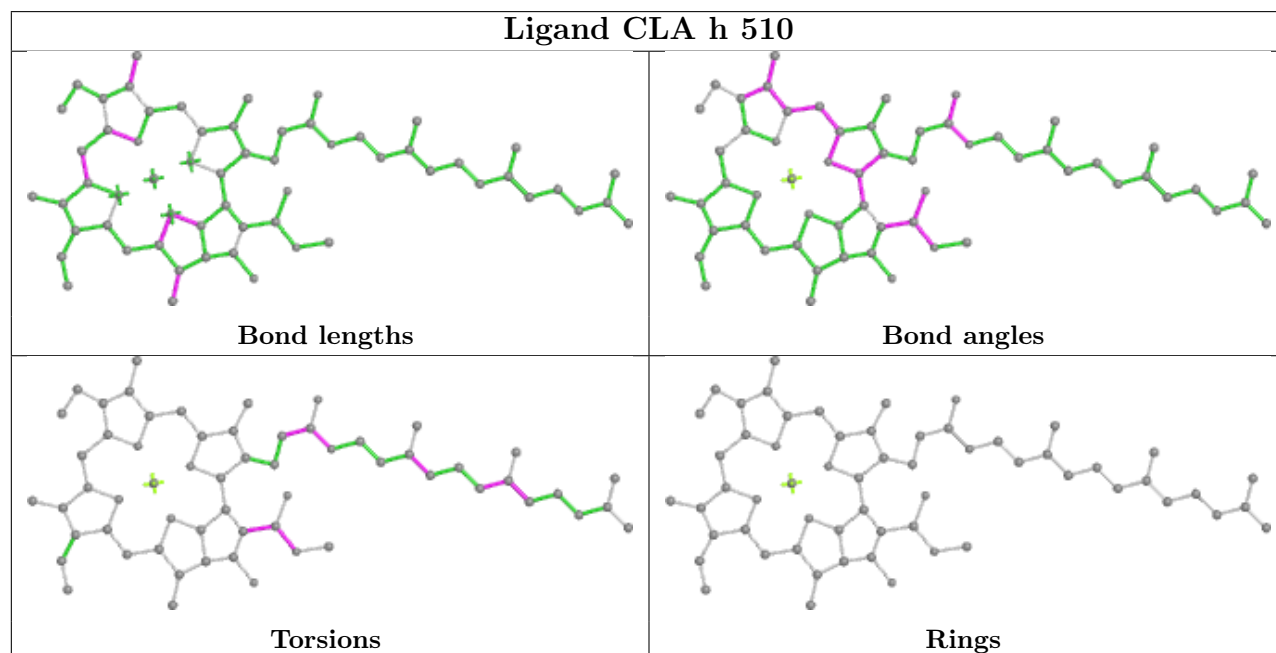
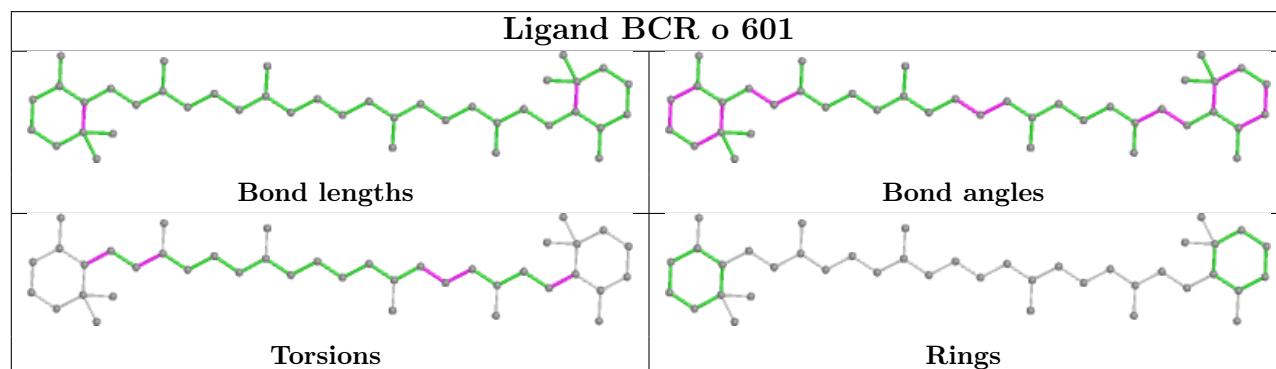
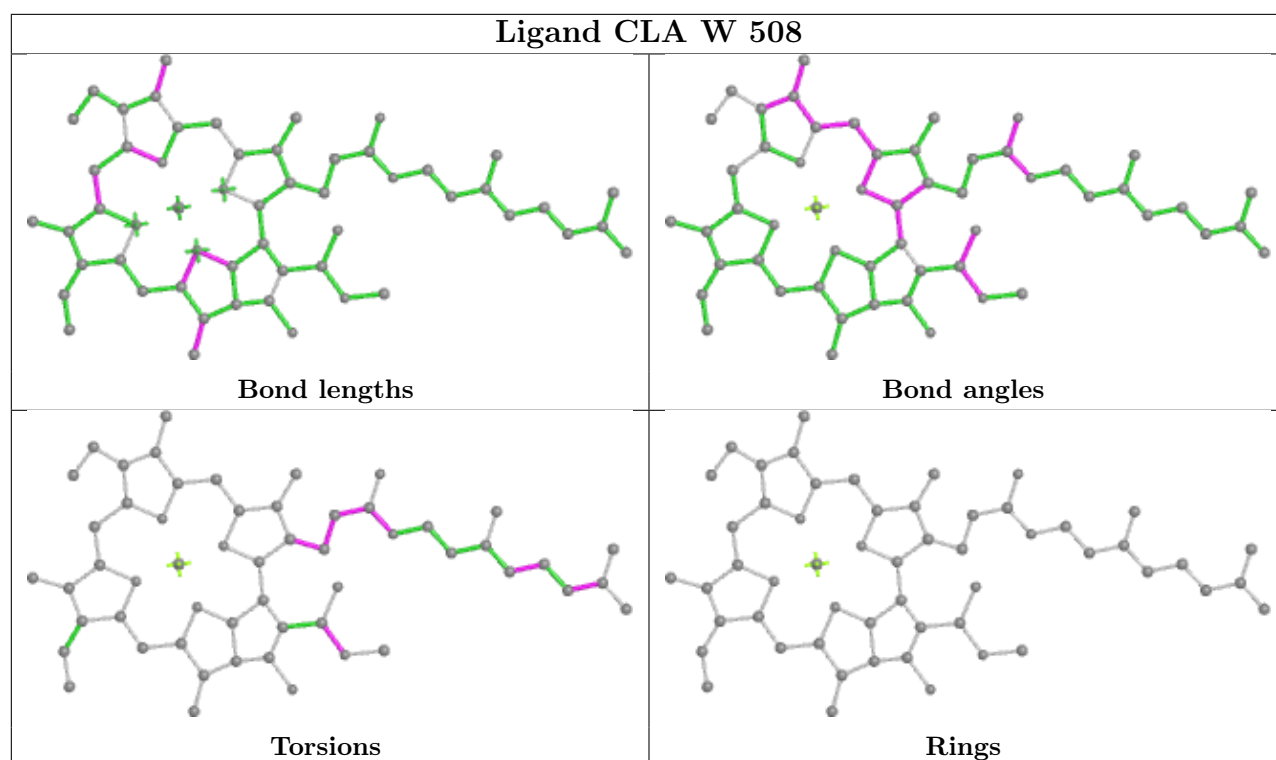


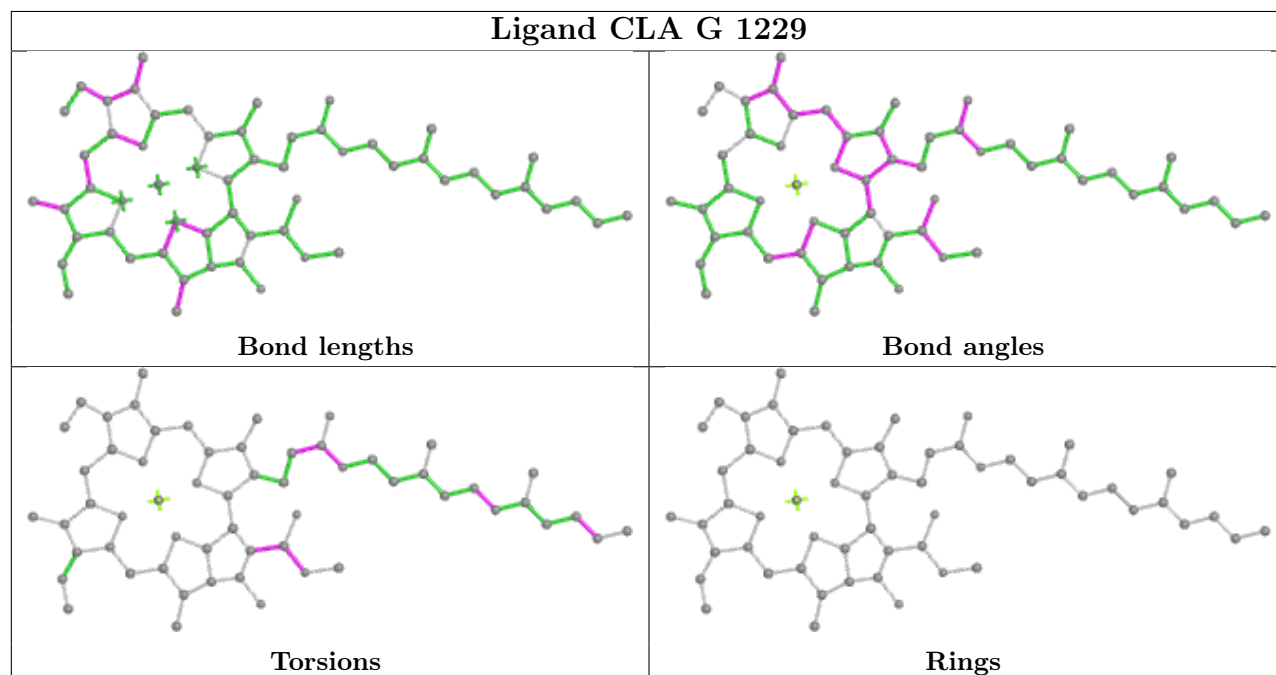
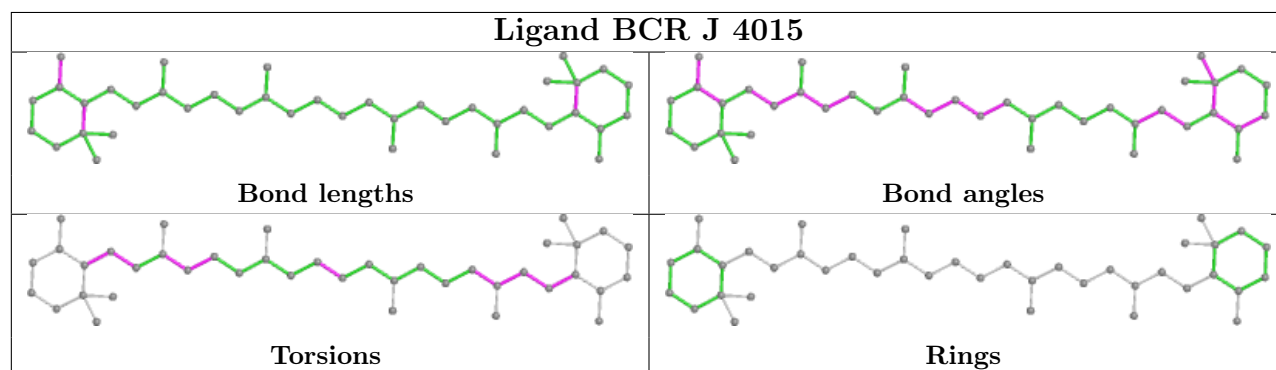
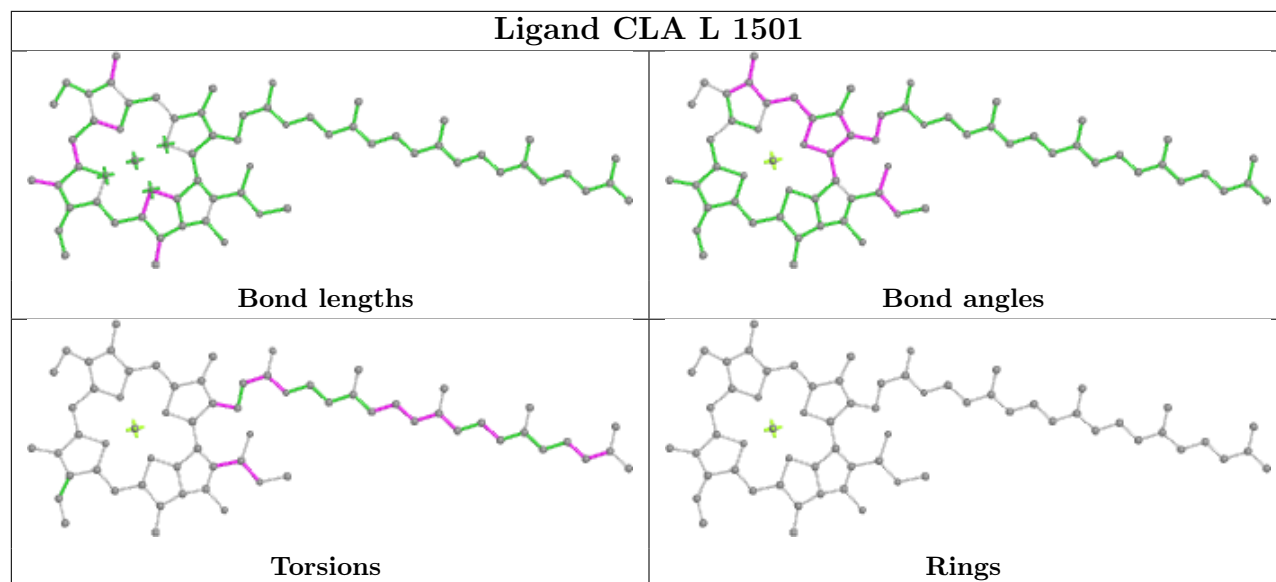
Torsions

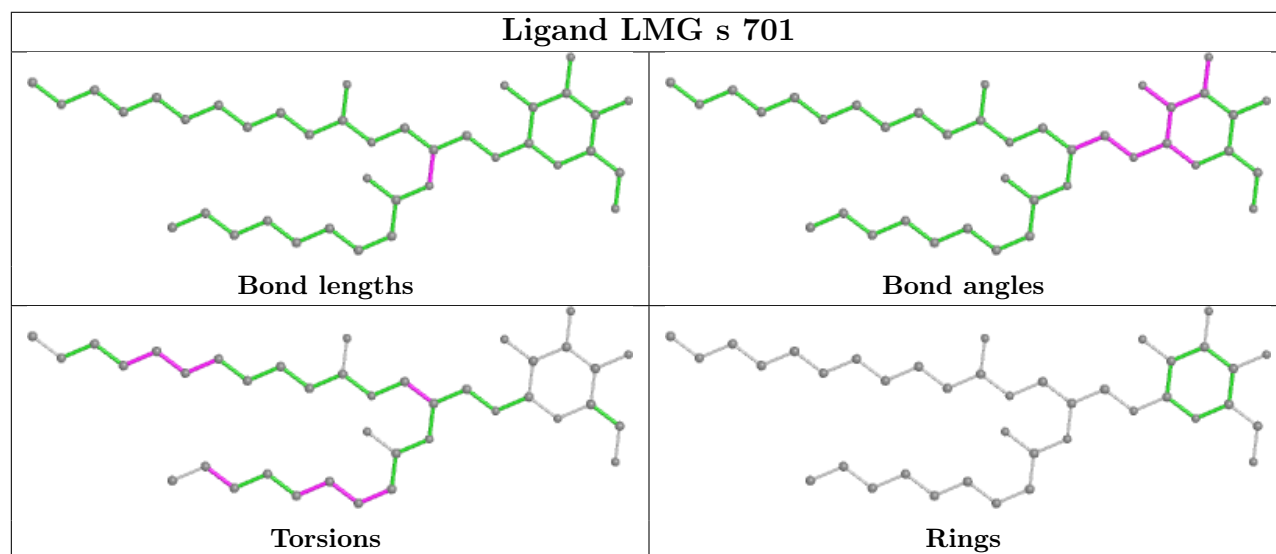
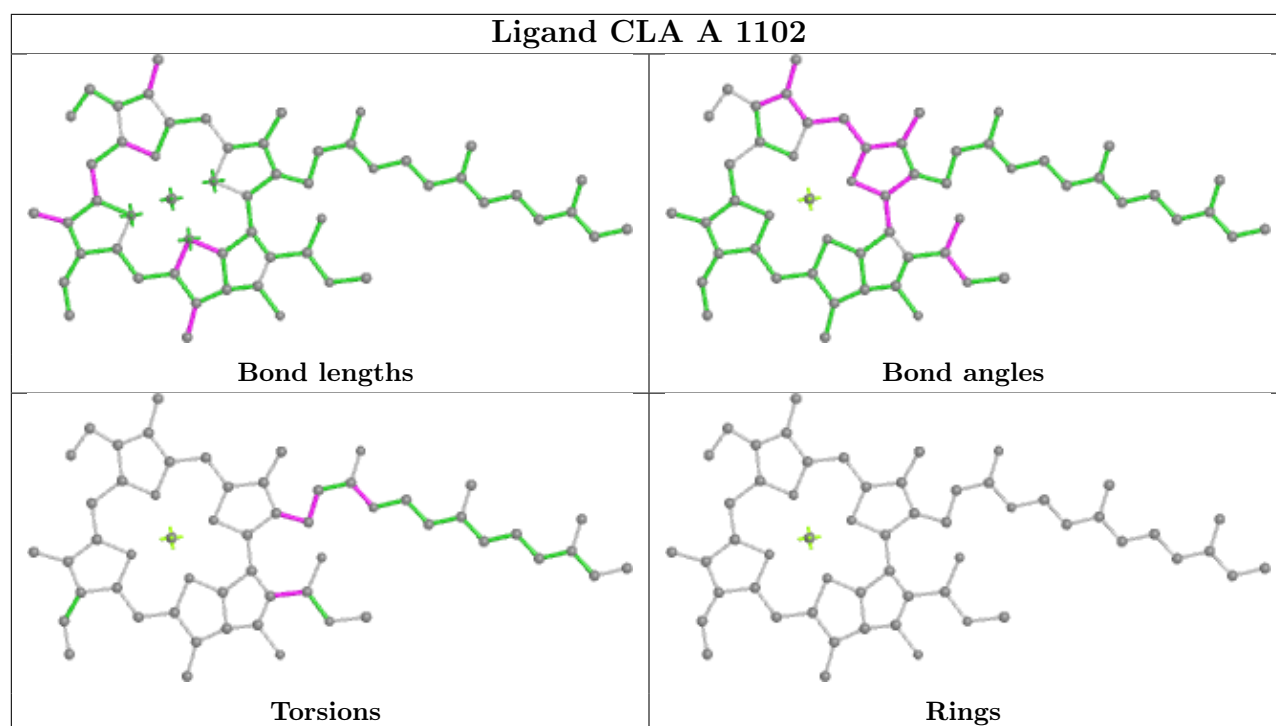


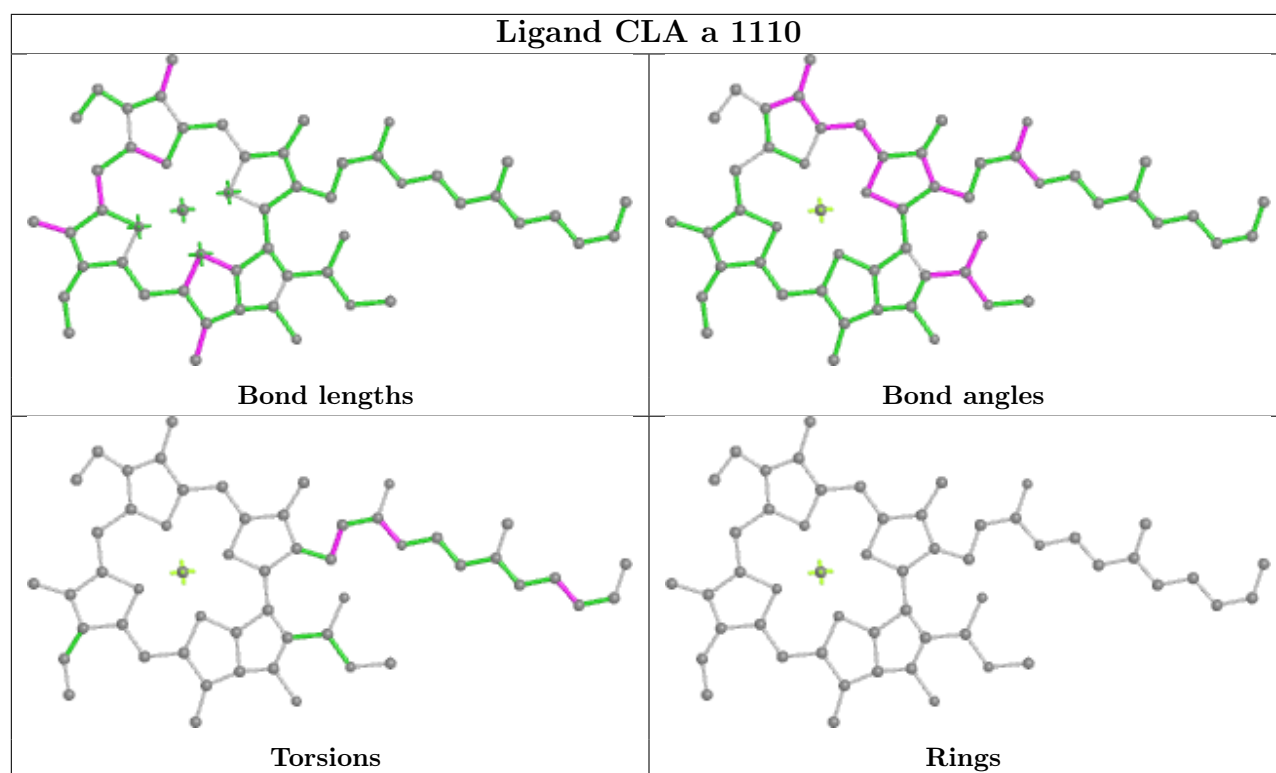
Rings



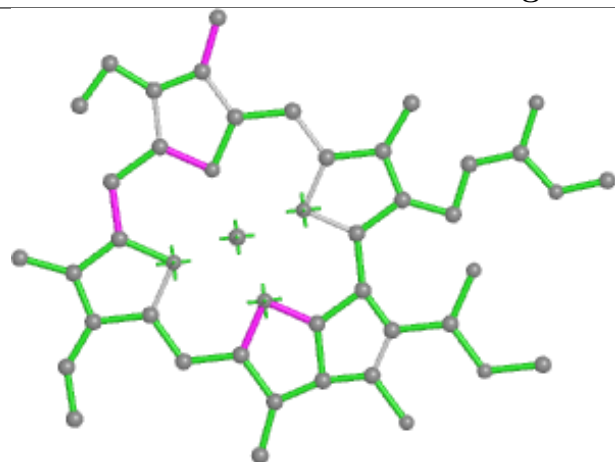




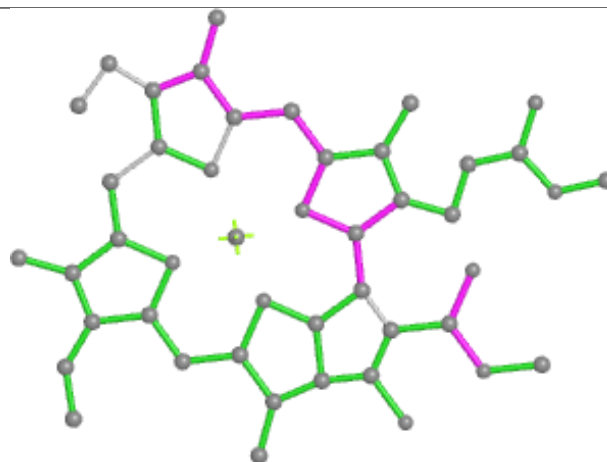




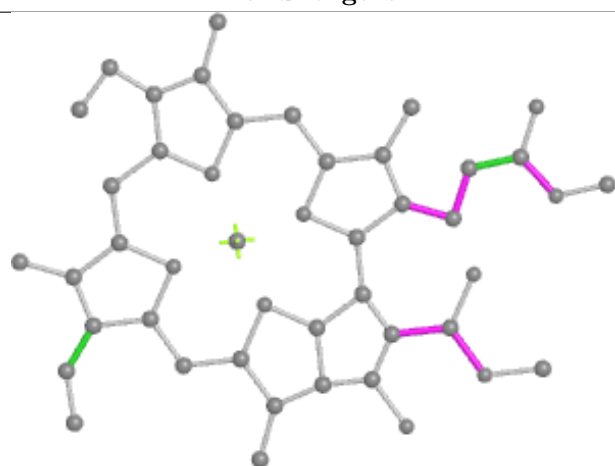
## Ligand CLA r 516



Bond lengths



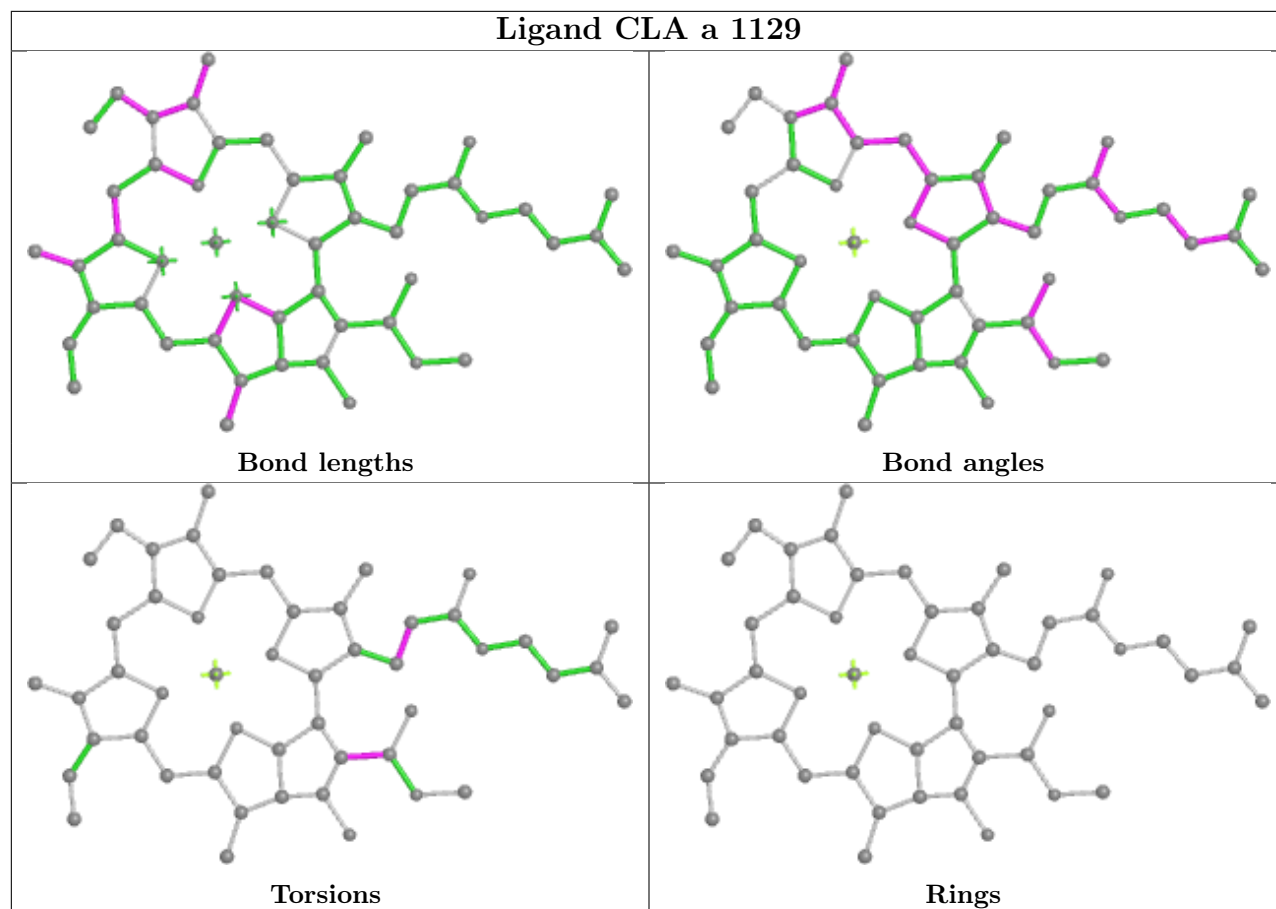
Bond angles



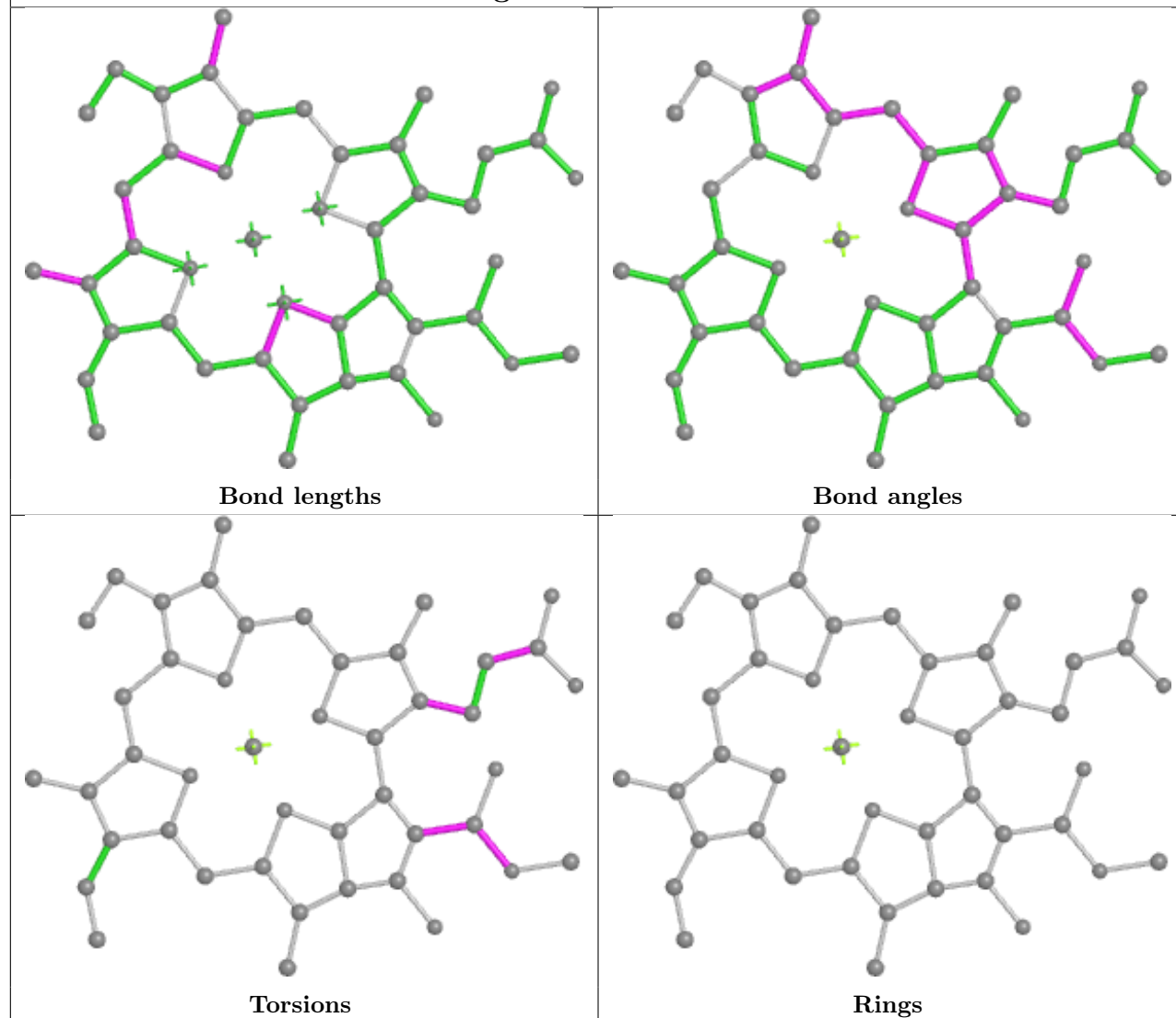
Torsions



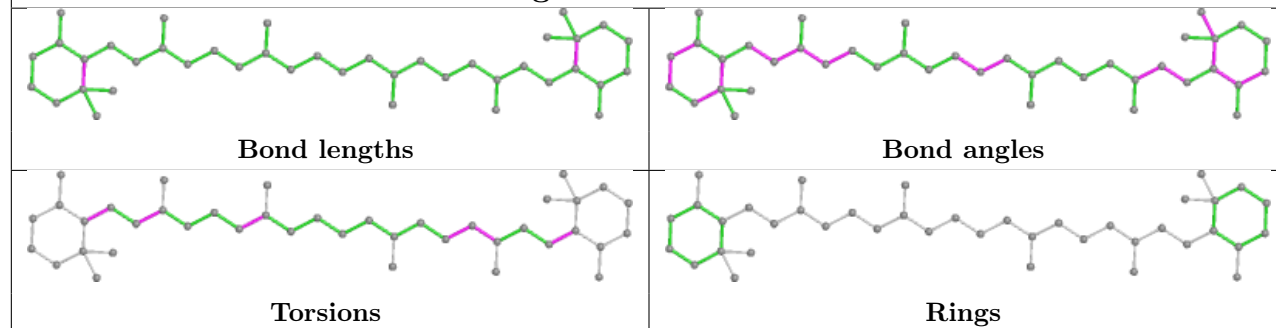
Rings

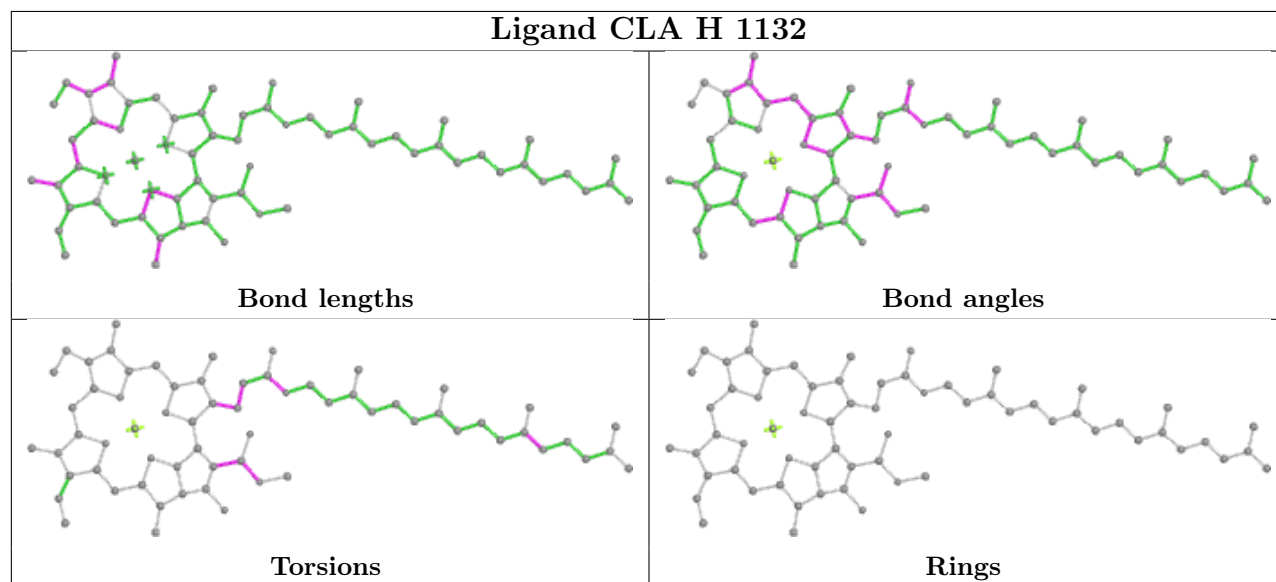
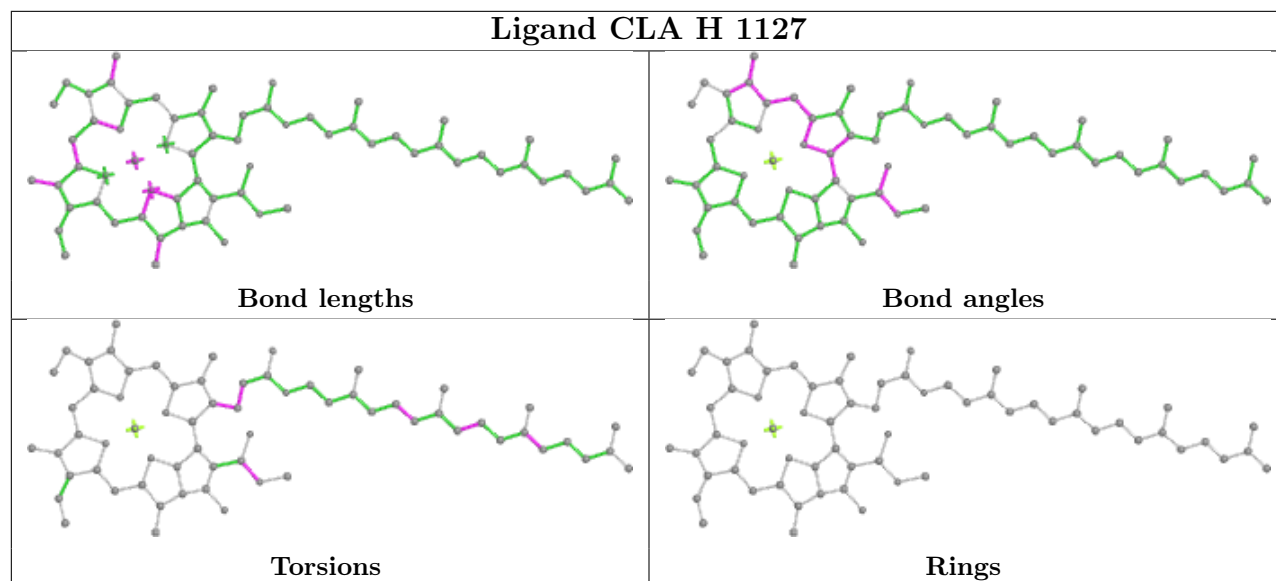
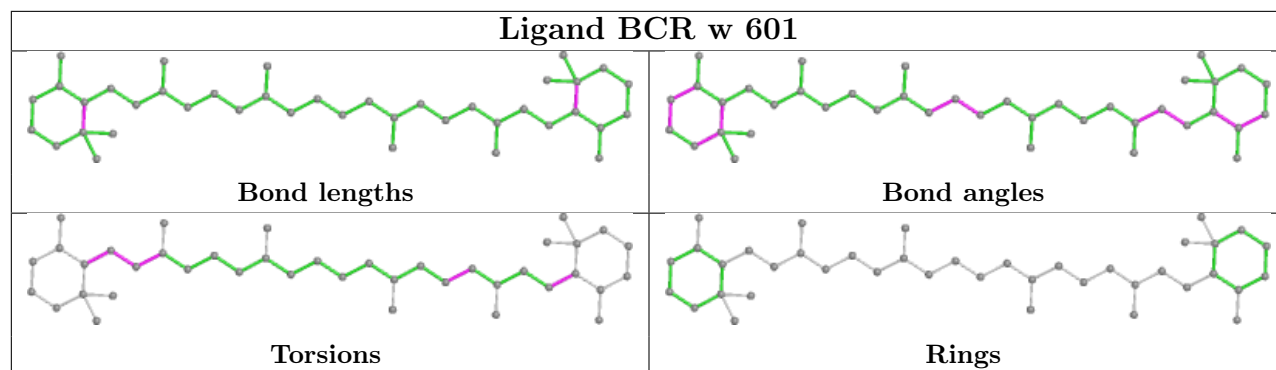


## Ligand CLA v 512



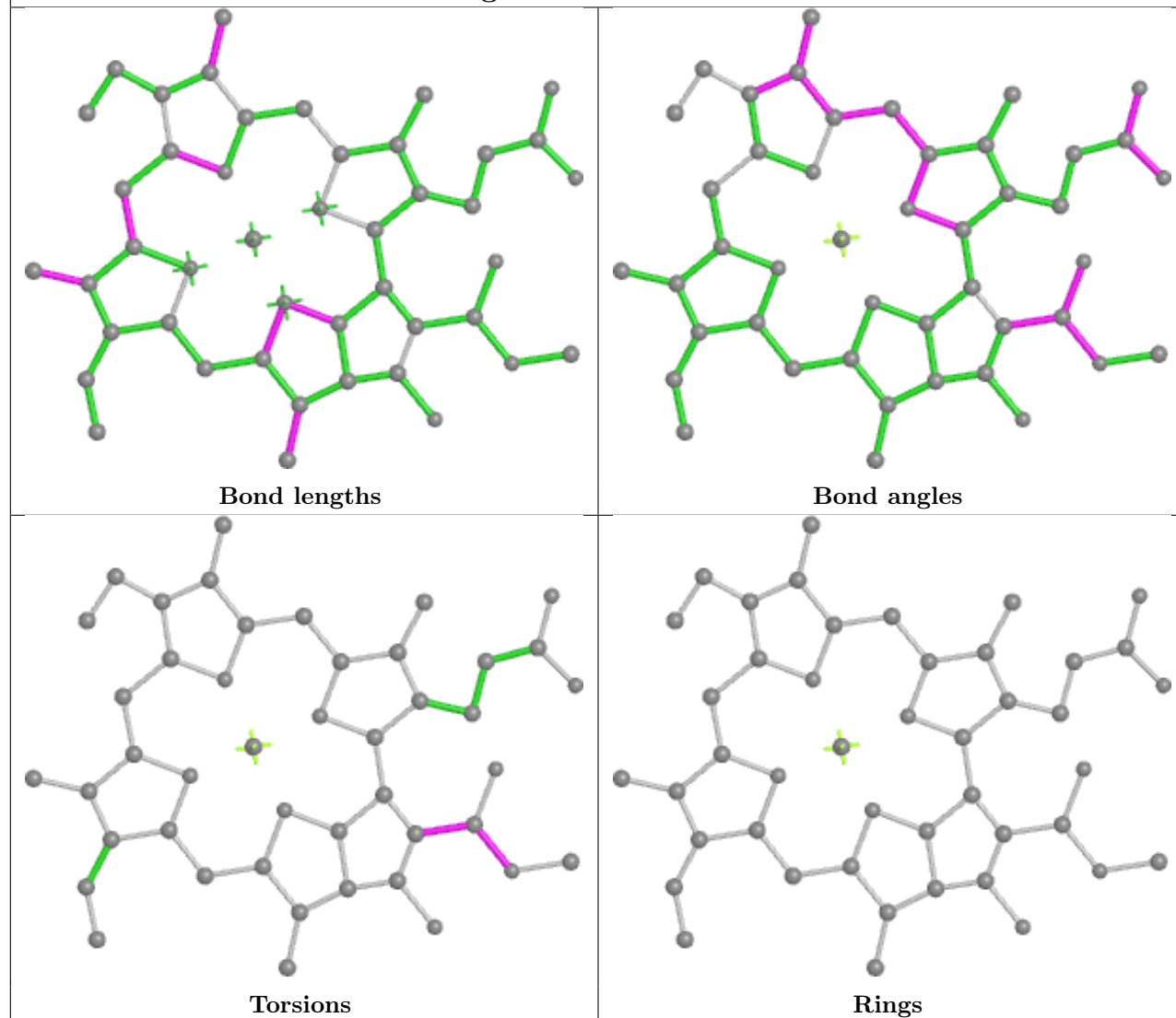
## Ligand BCR Z 601



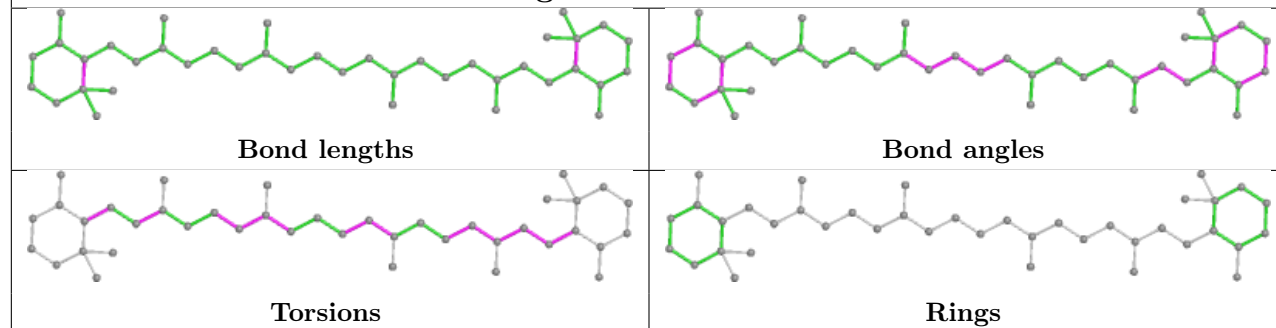


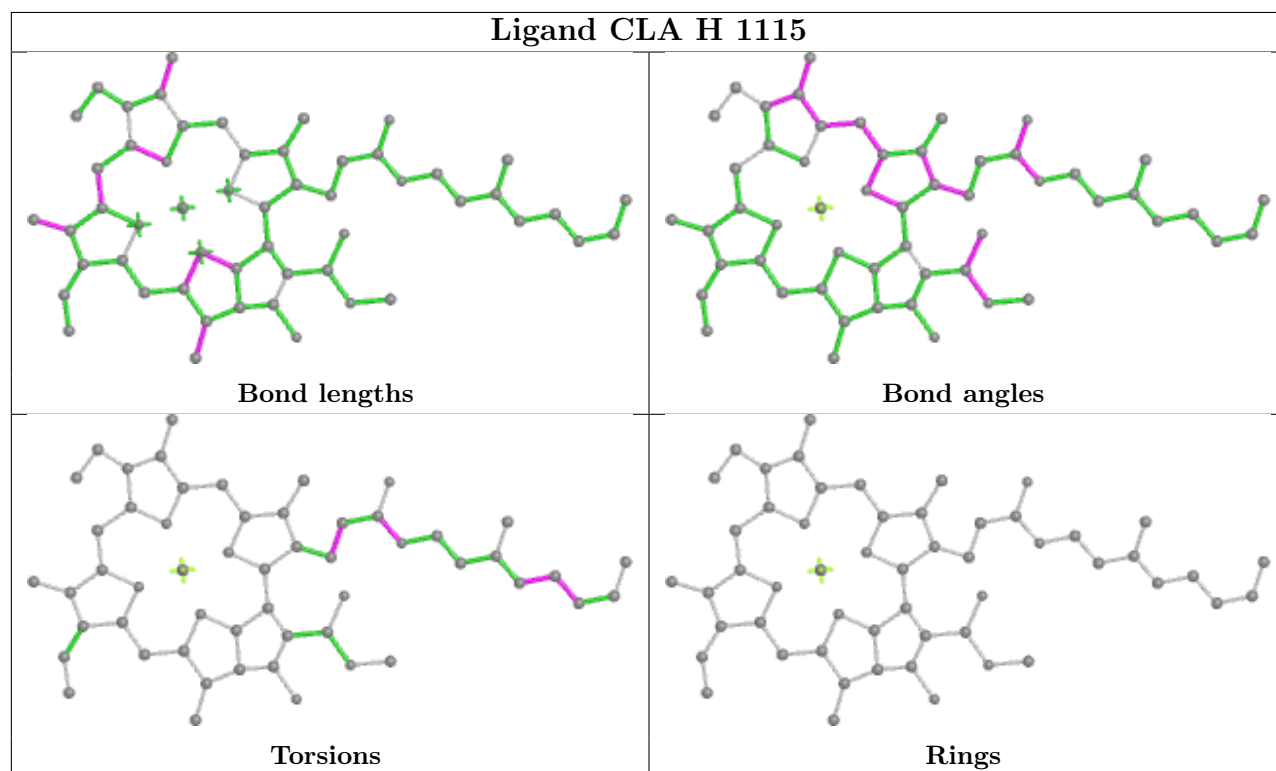
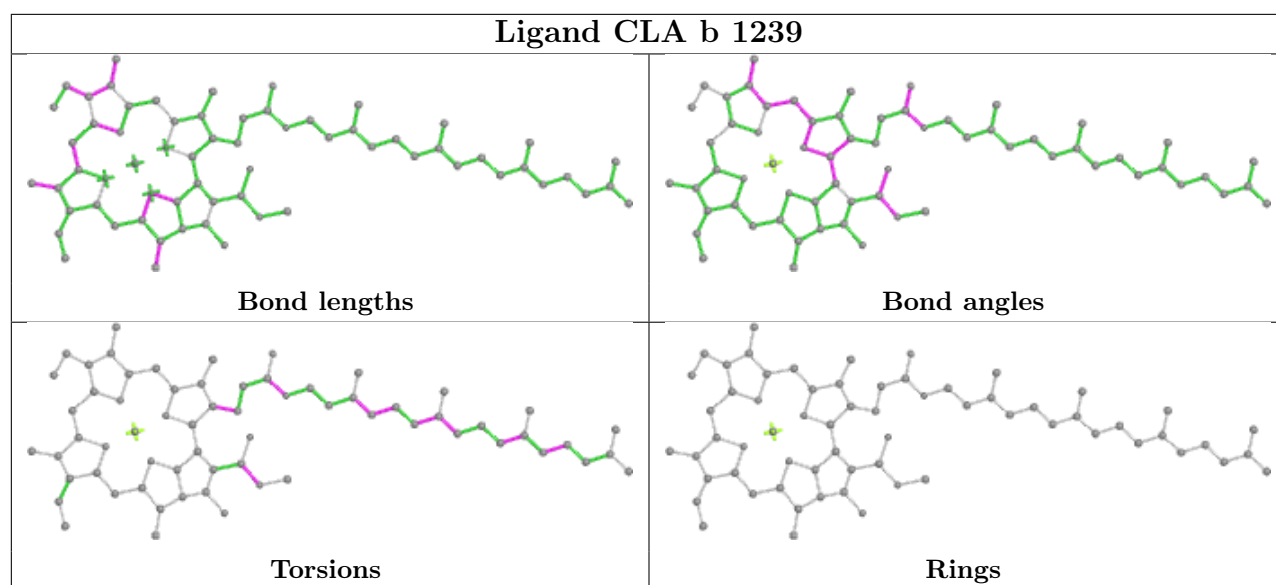


## Ligand CLA G 1230

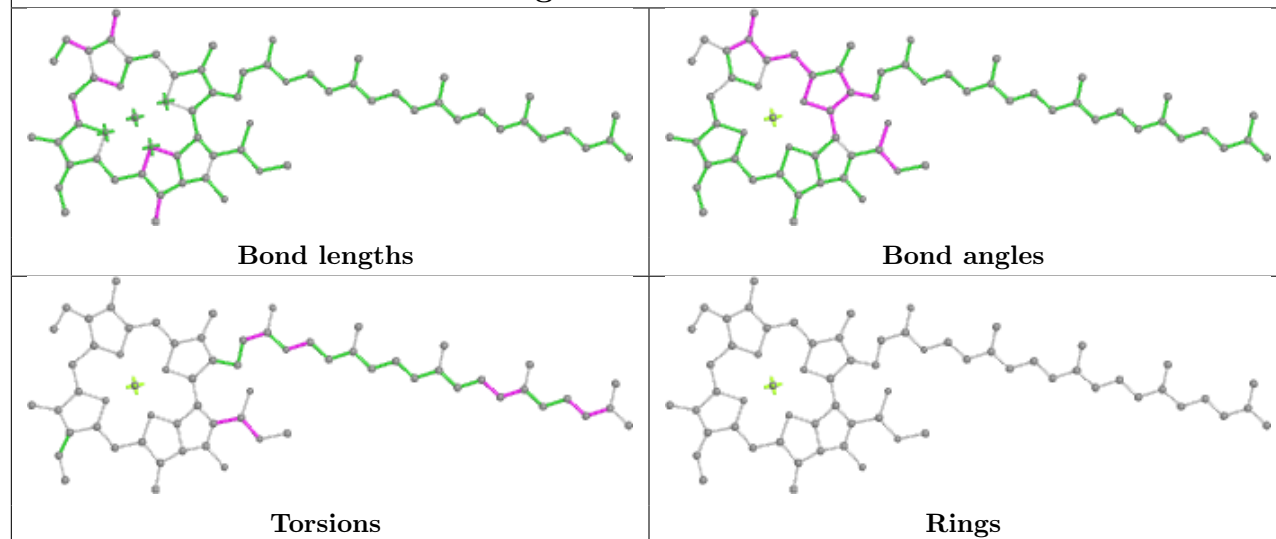


## Ligand BCR r 601

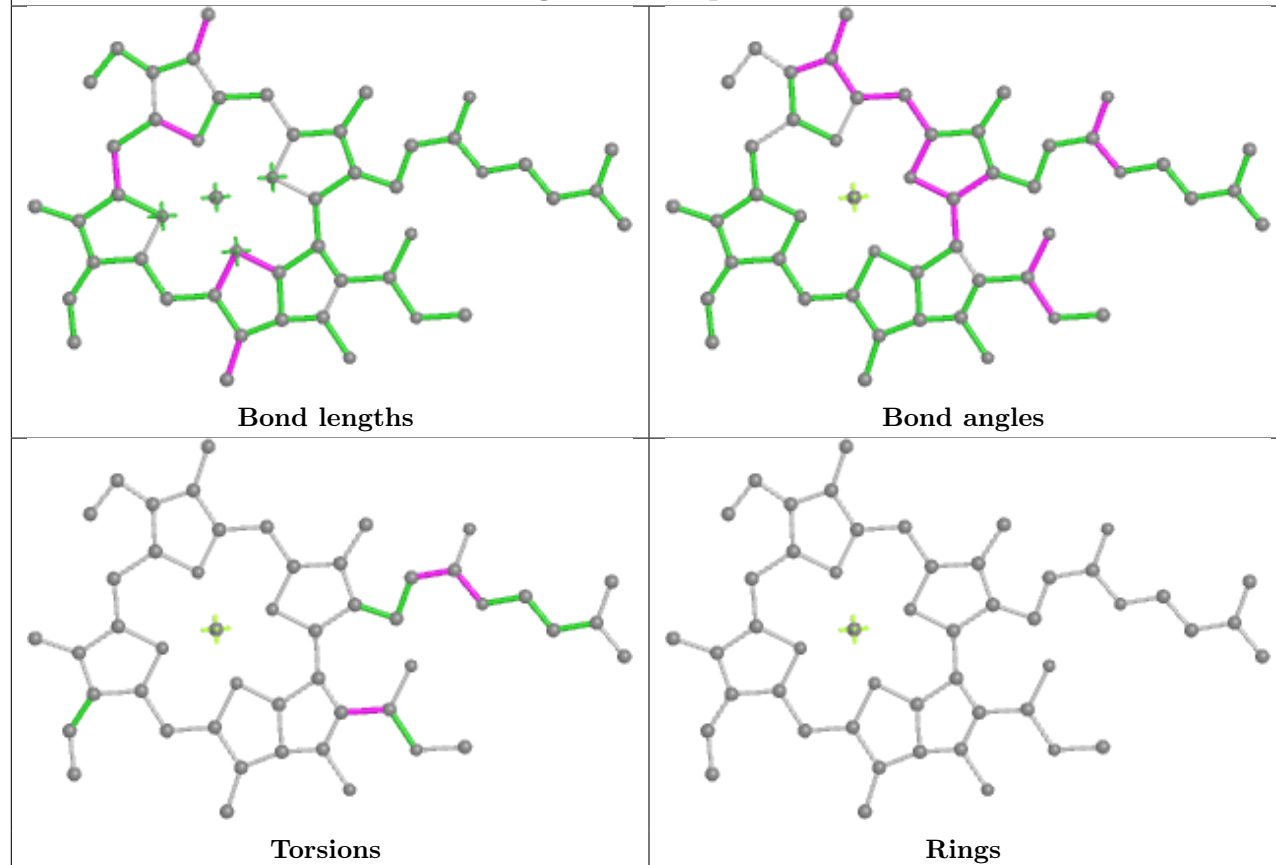


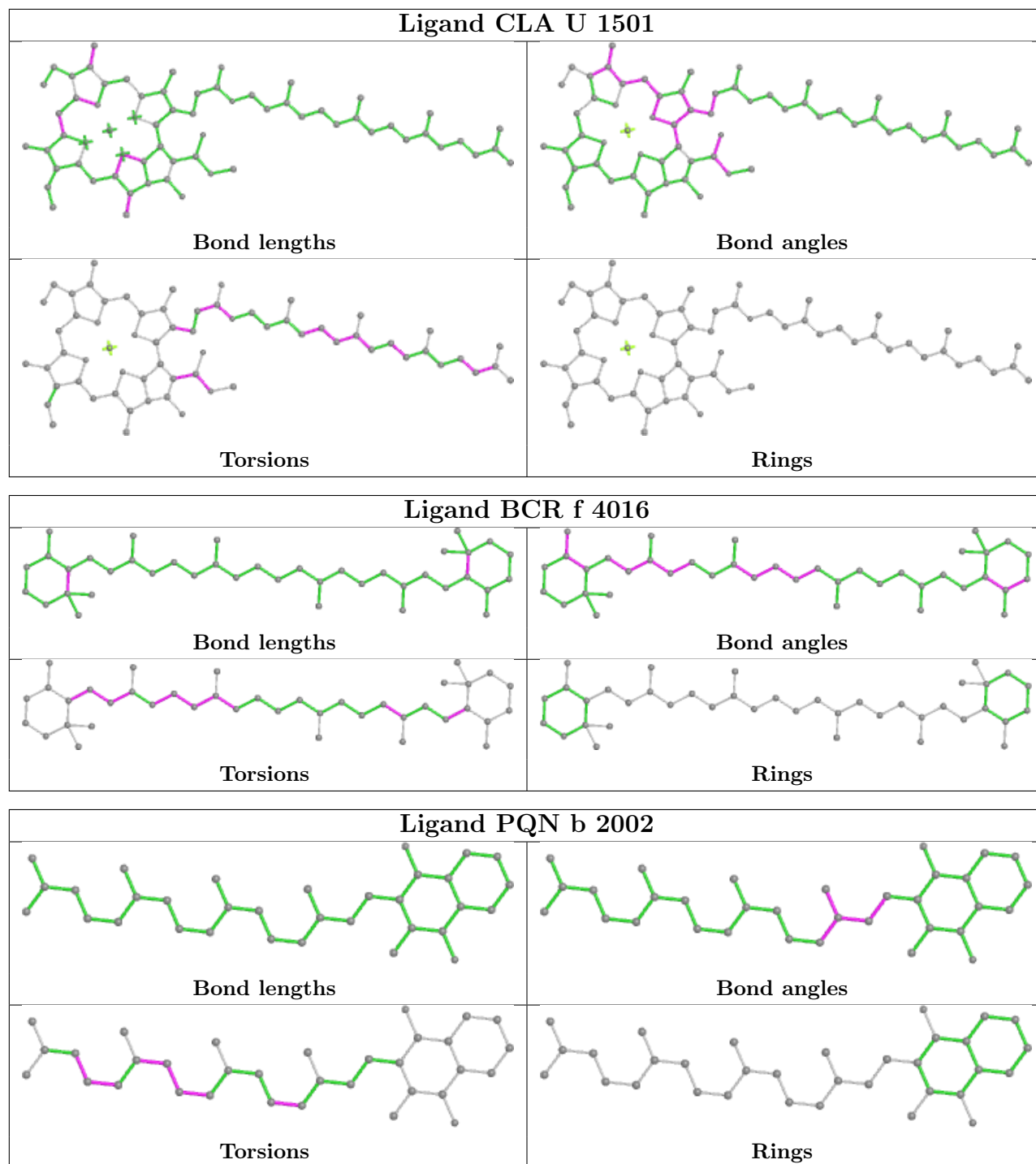


## Ligand CLA u 510

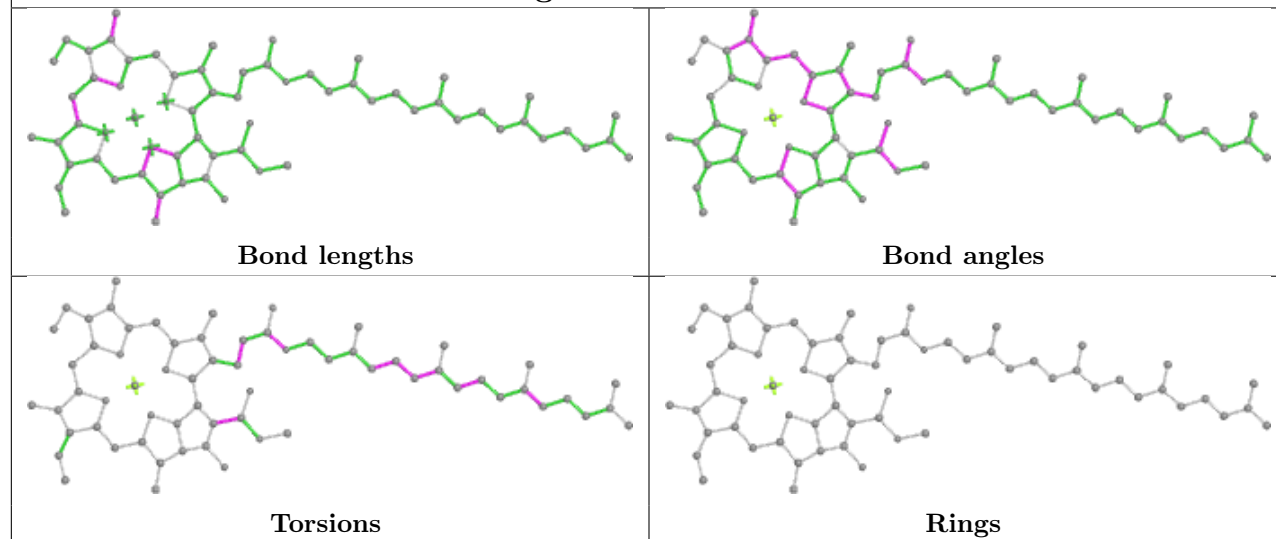


## Ligand CLA p 513

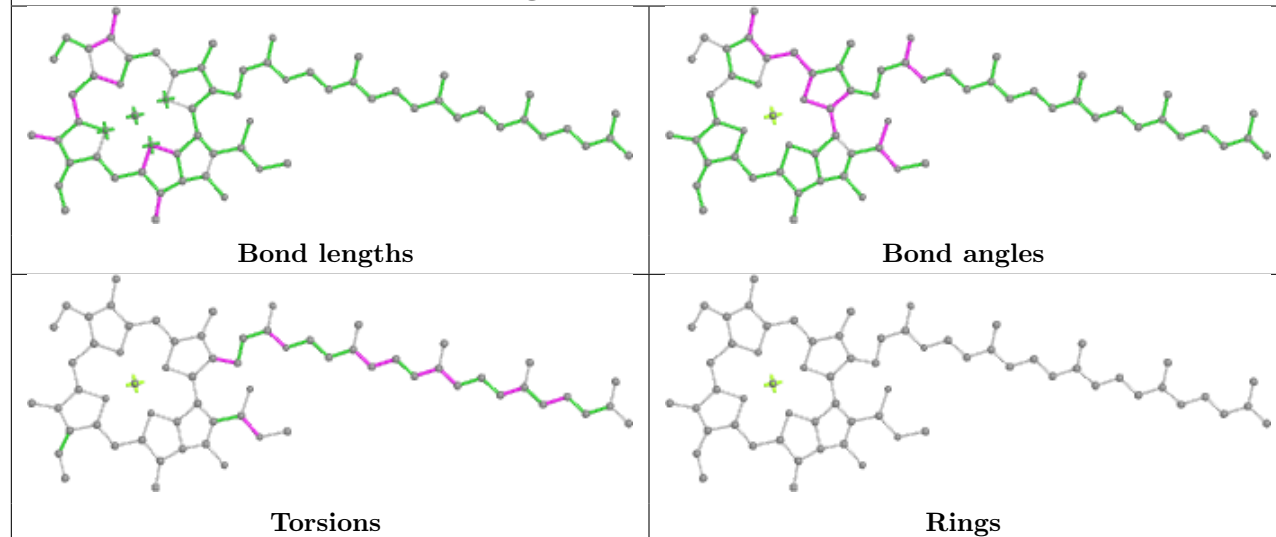




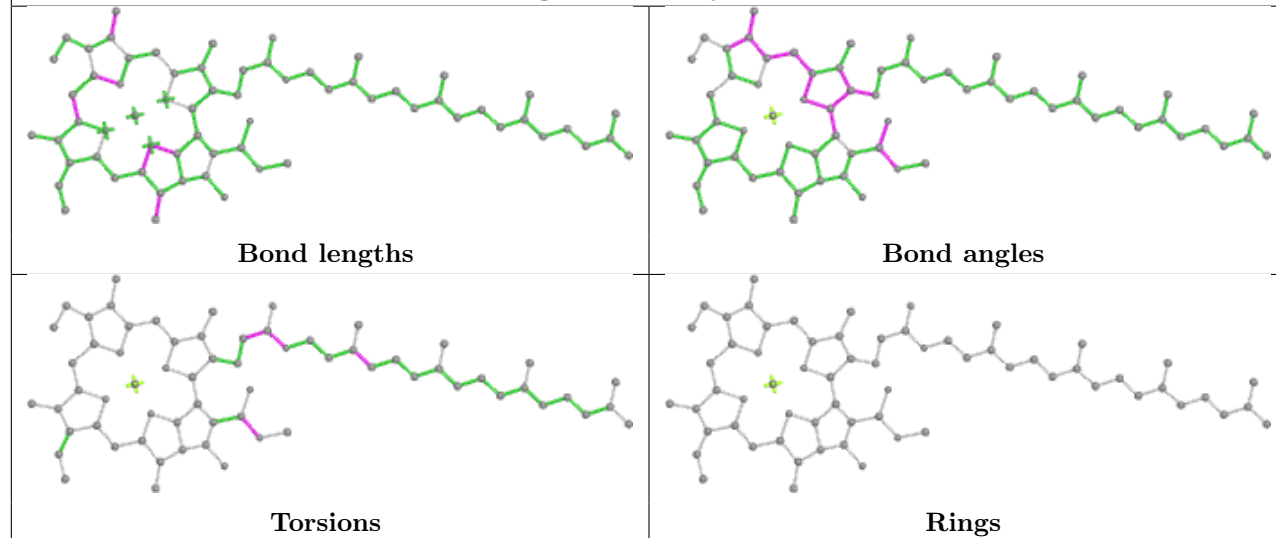
## Ligand CLA n 515



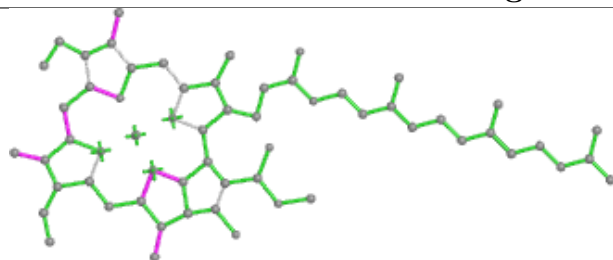
## Ligand CLA B 1239



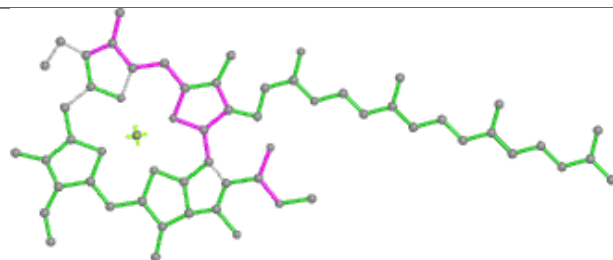
## Ligand CLA y 507



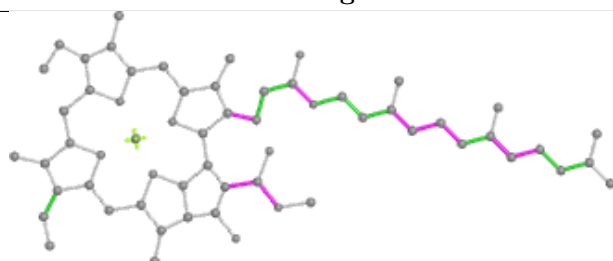
## Ligand CLA B 1215



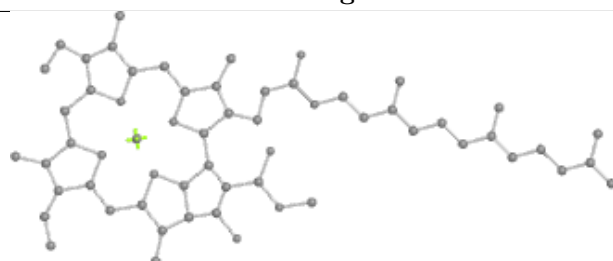
Bond lengths



Bond angles

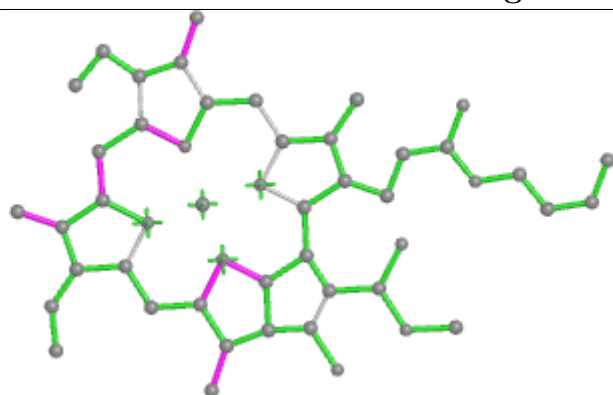


Torsions

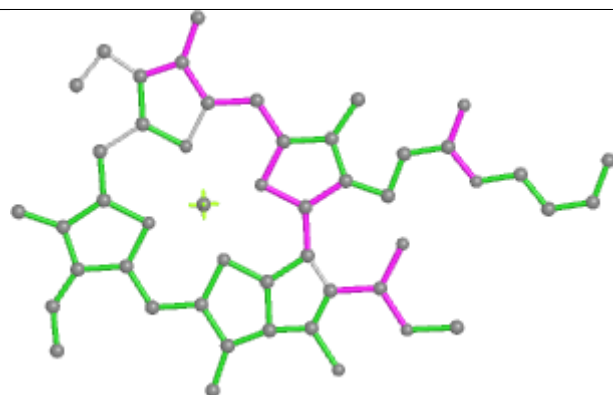


Rings

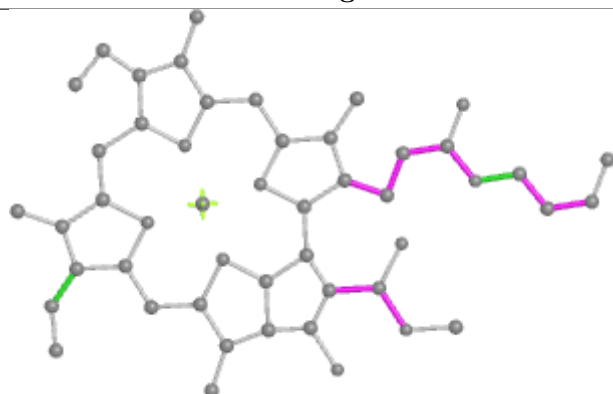
## Ligand CLA H 1120



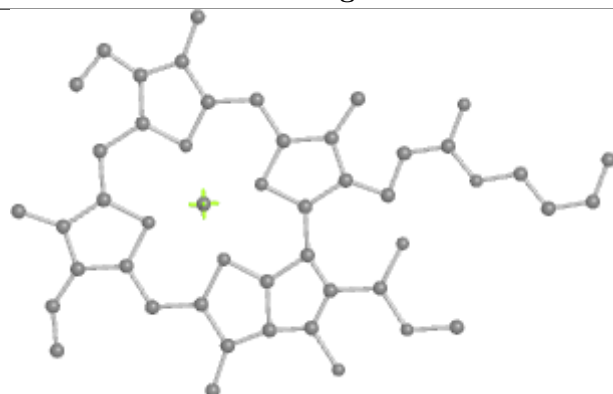
Bond lengths



Bond angles

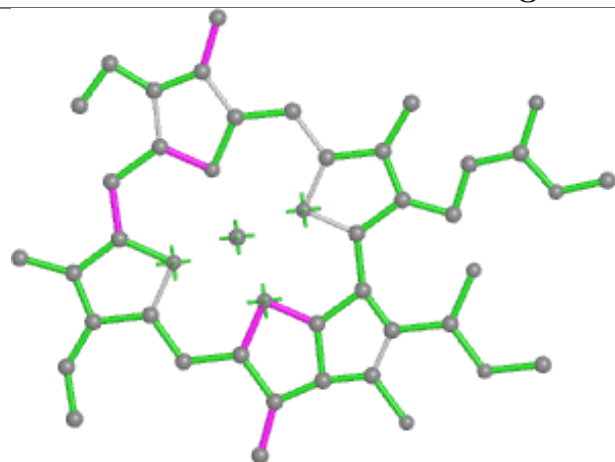


Torsions

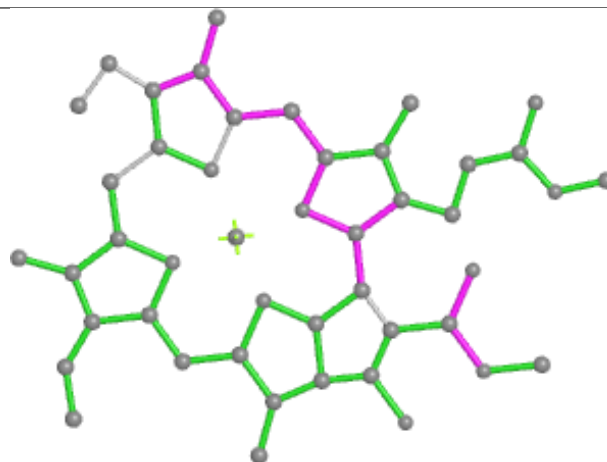


Rings

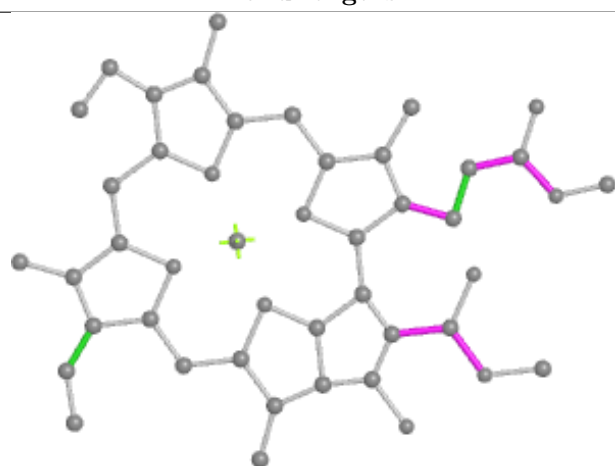
## Ligand CLA h 503



Bond lengths



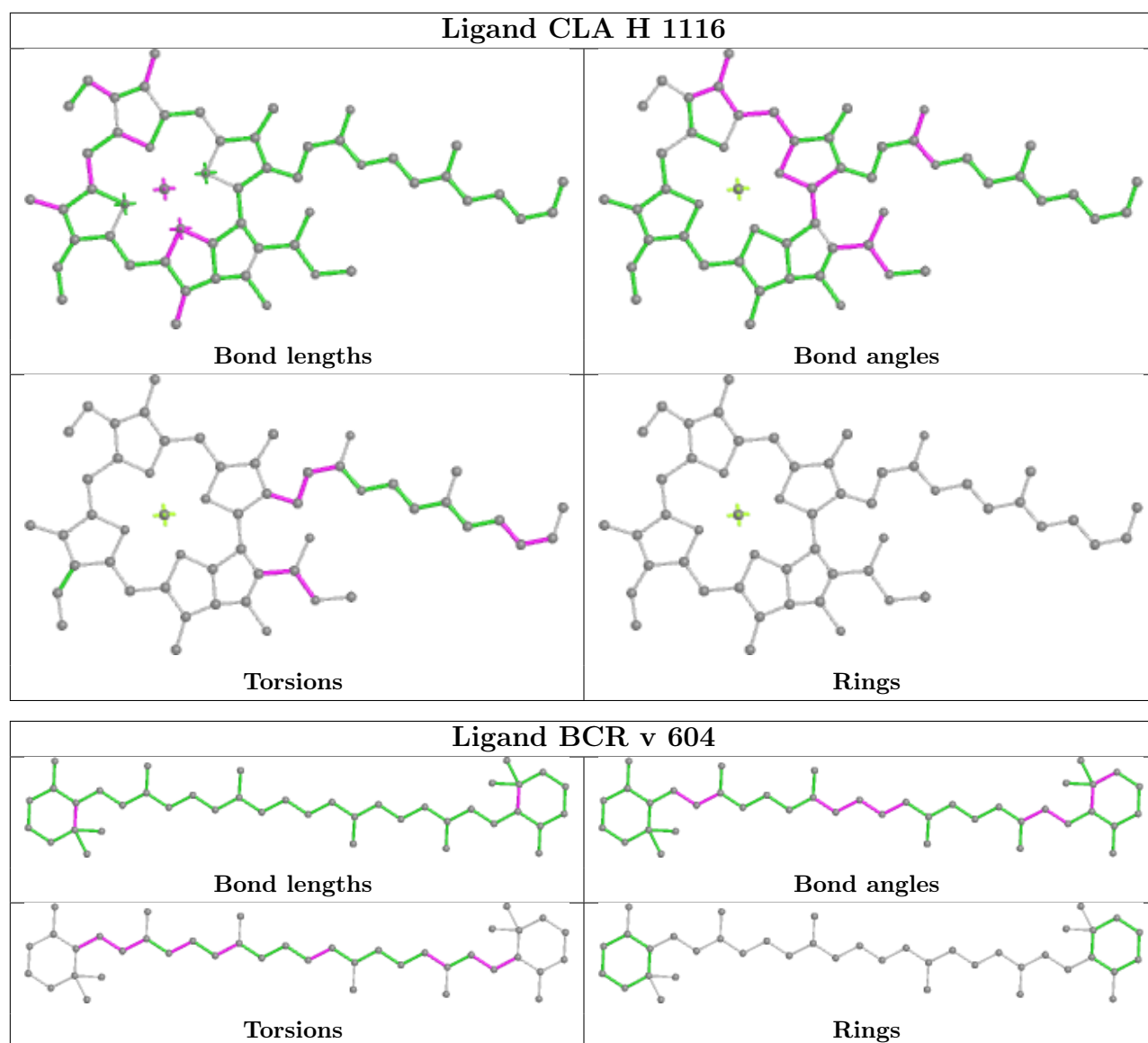
Bond angles



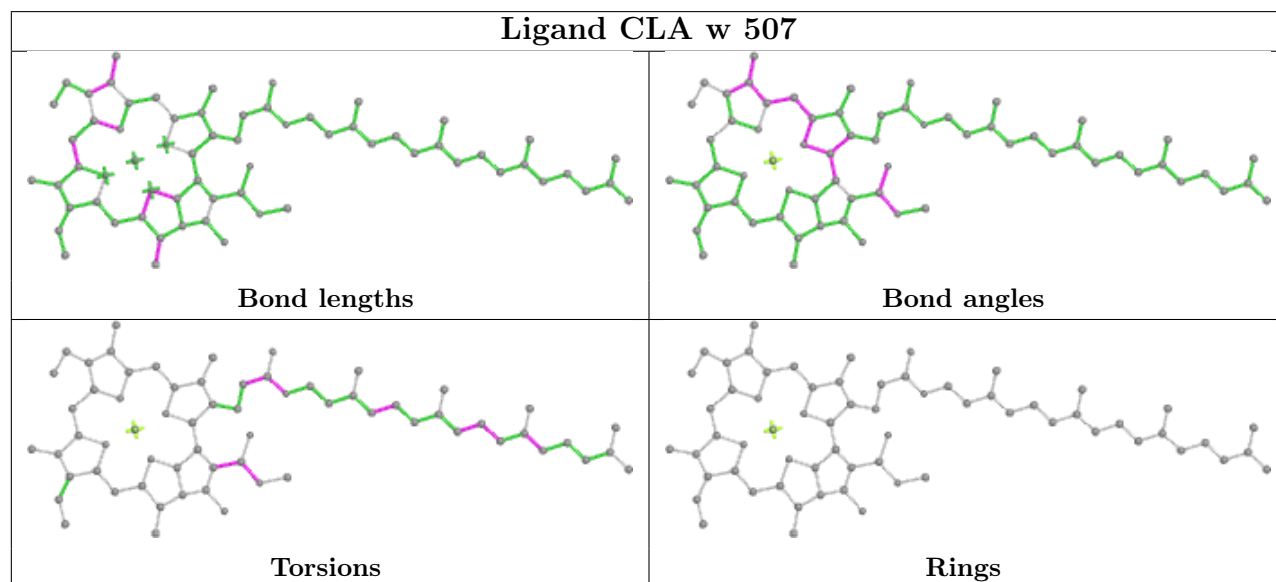
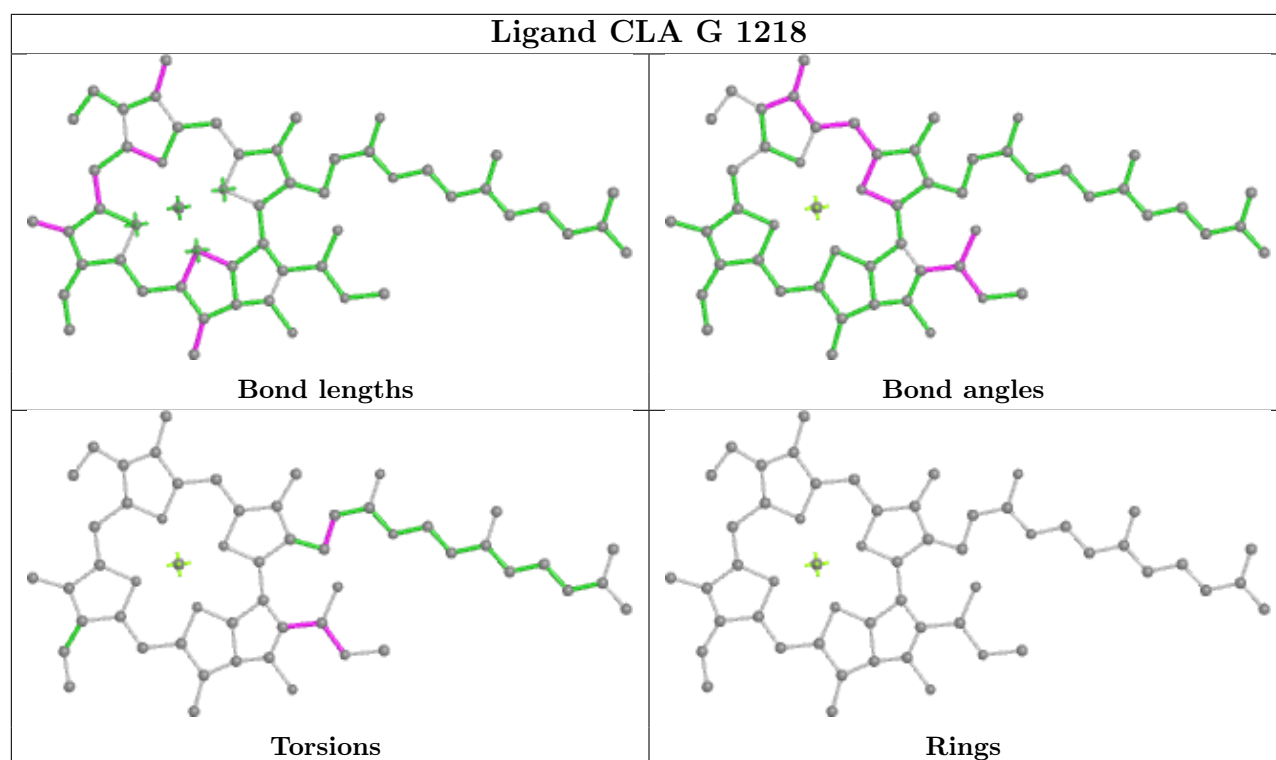
Torsions

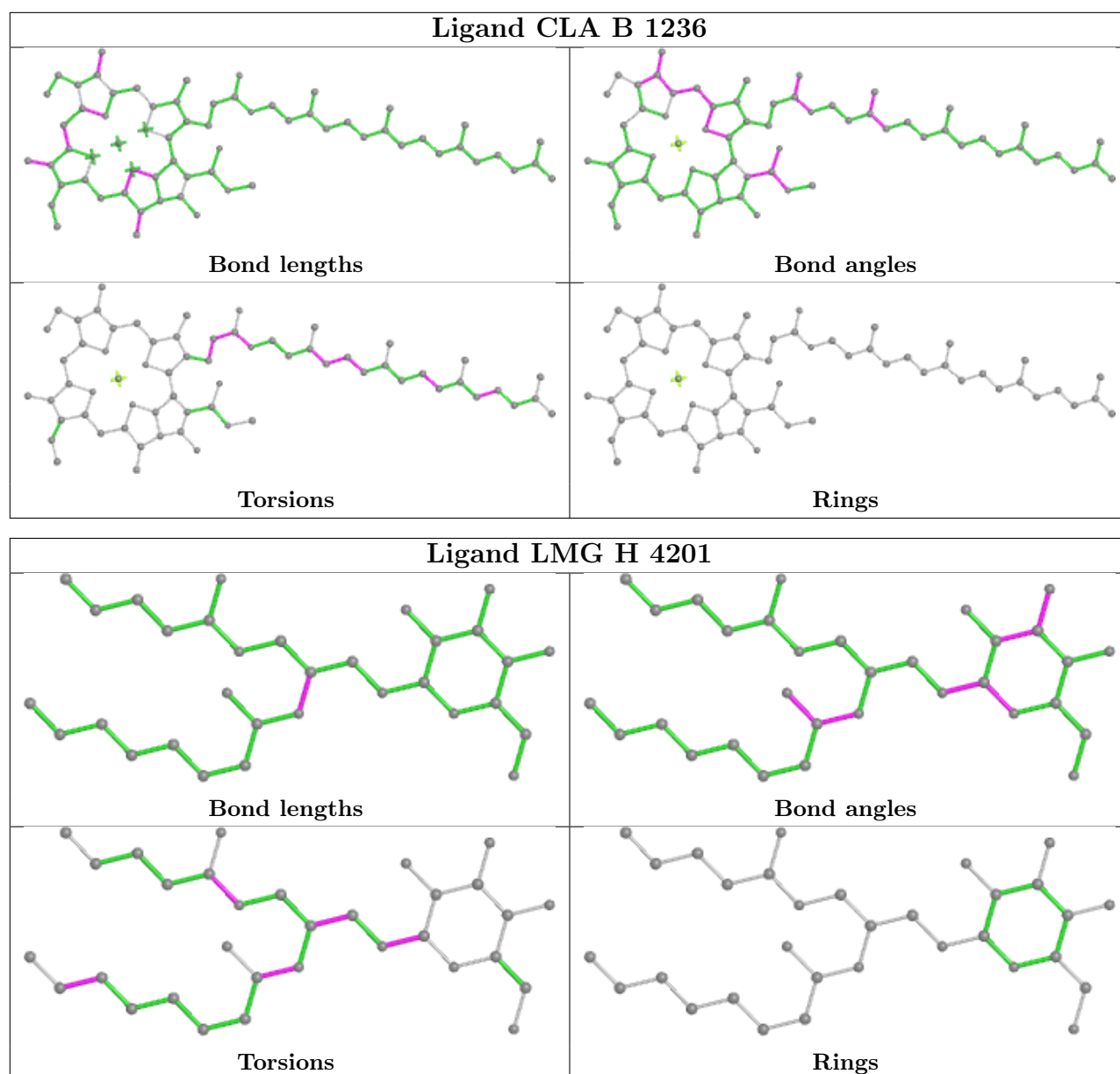


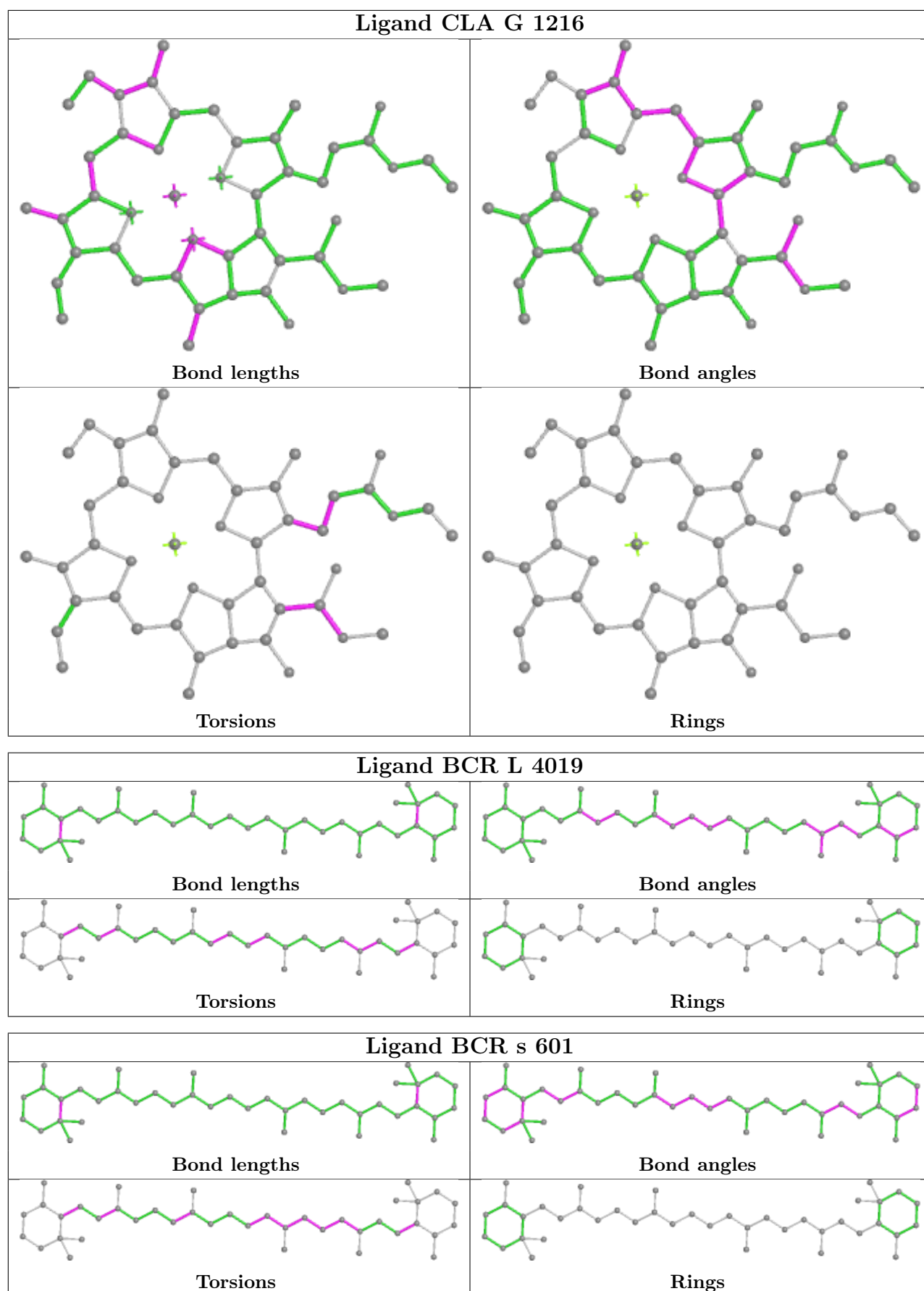
Rings

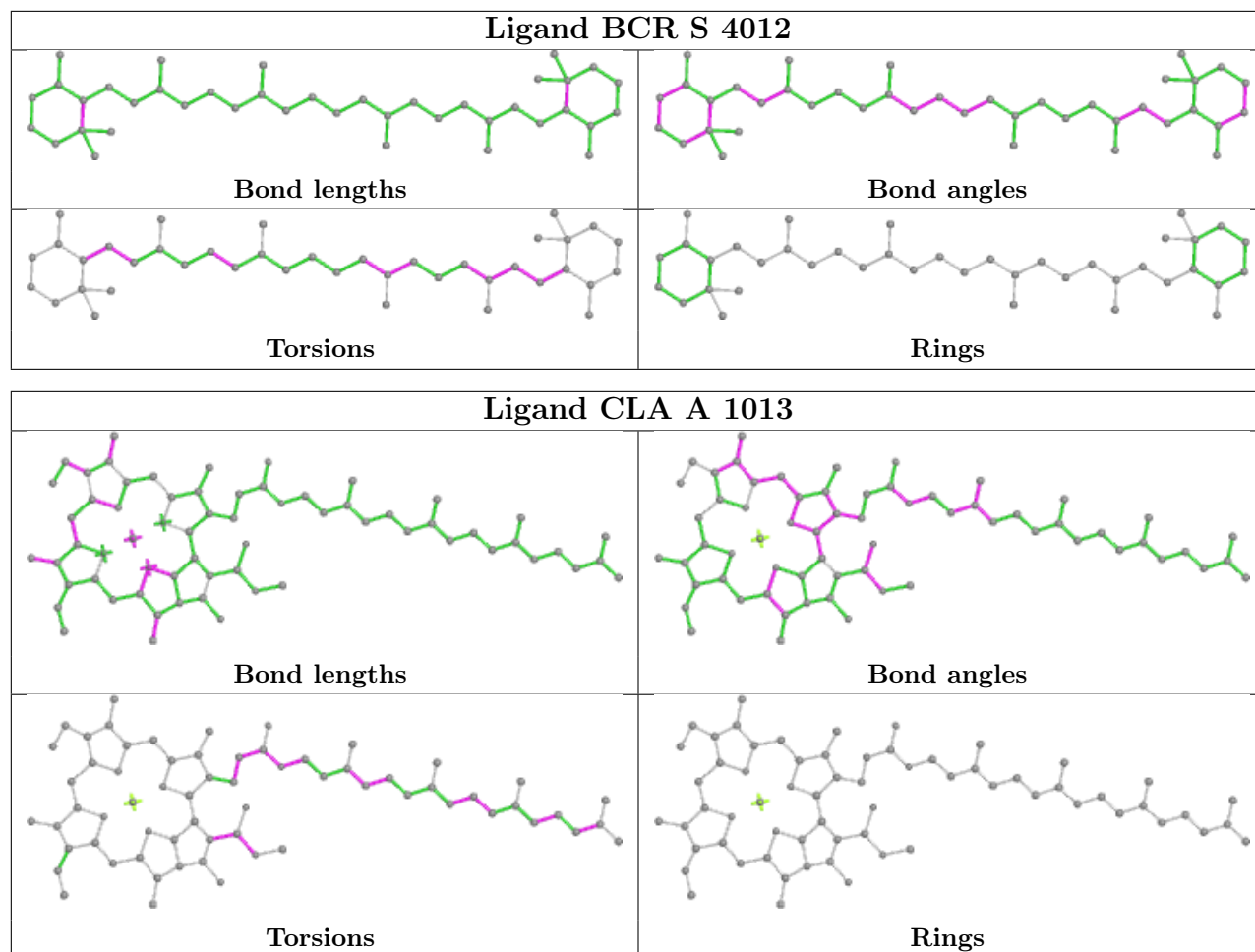




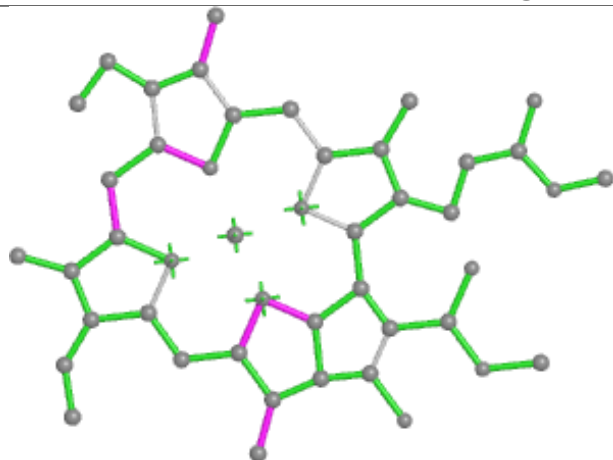




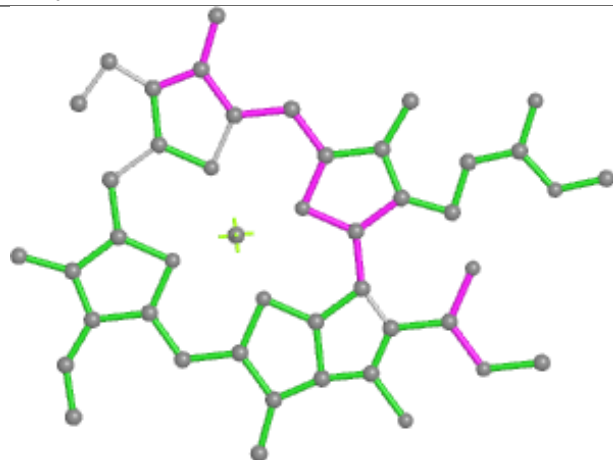




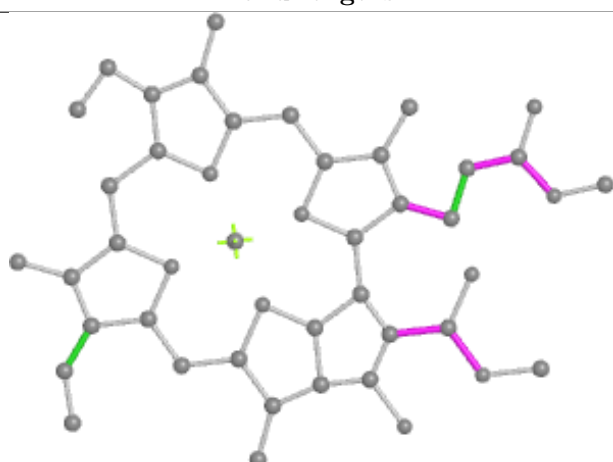
## Ligand CLA y 503



Bond lengths



Bond angles

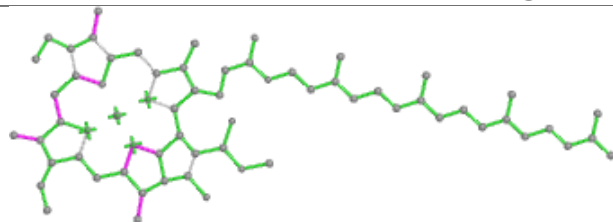


Torsions

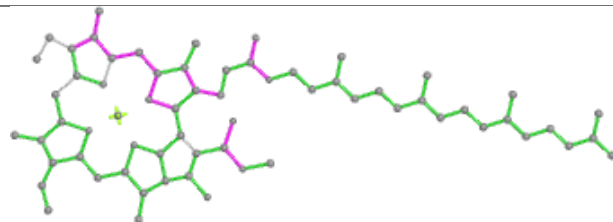


Rings

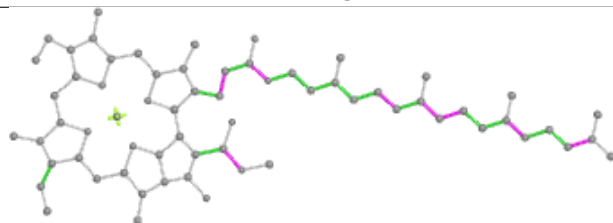
## Ligand CLA r 515



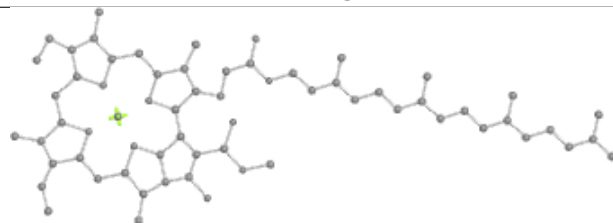
Bond lengths



Bond angles

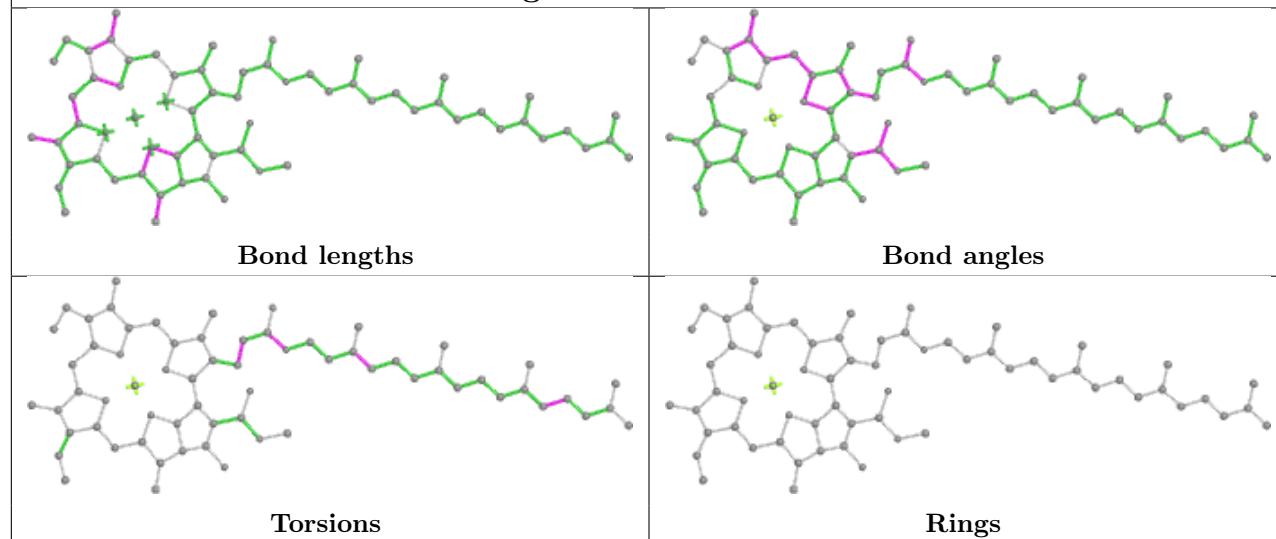


Torsions

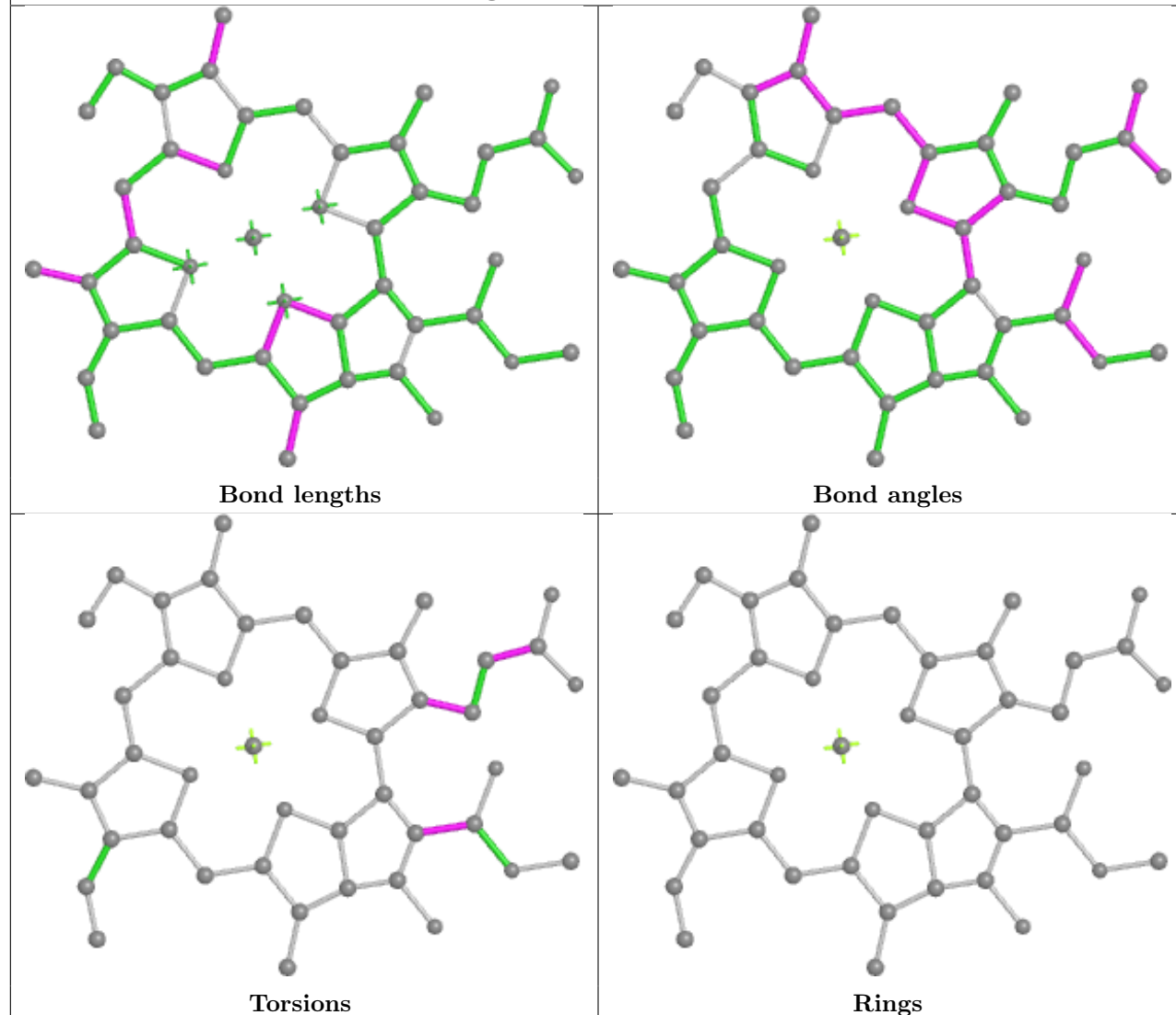


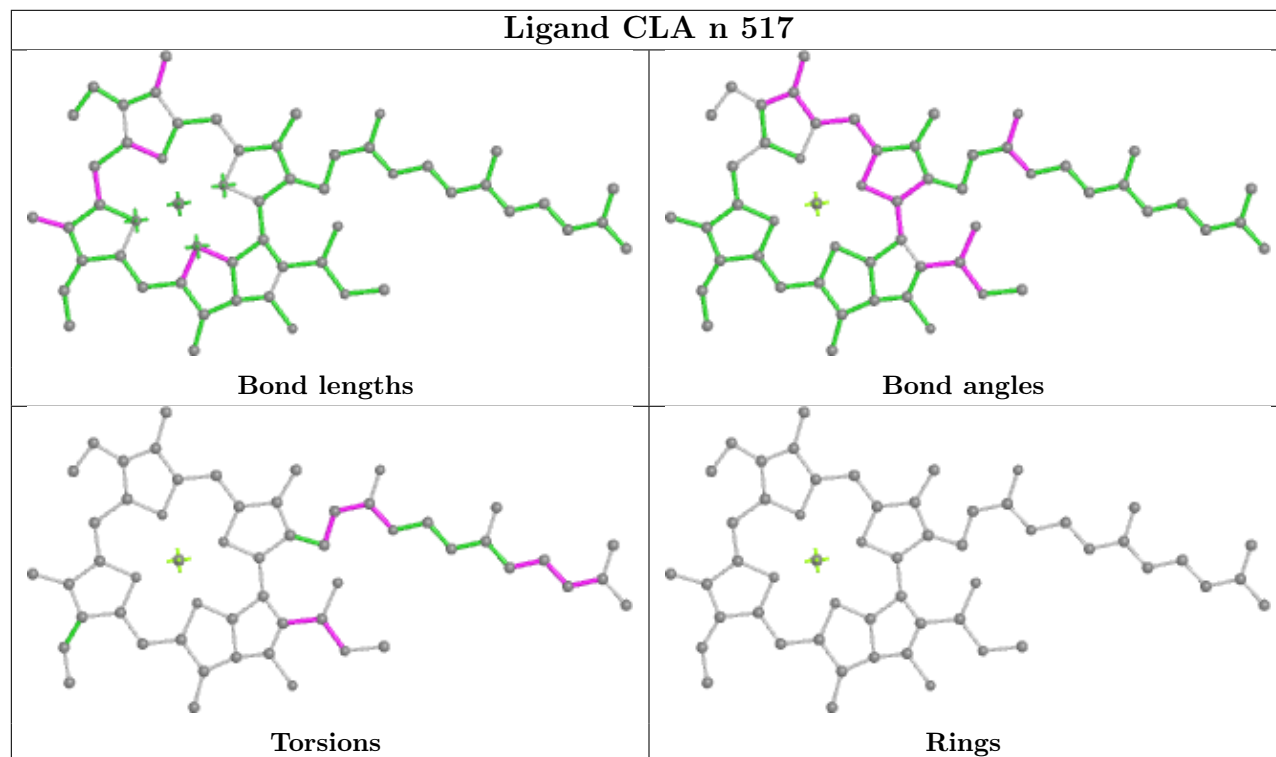
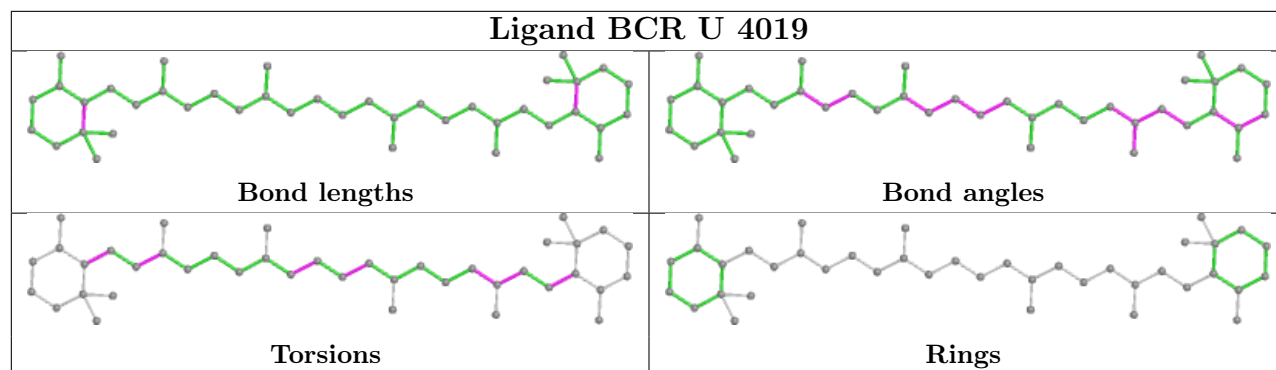
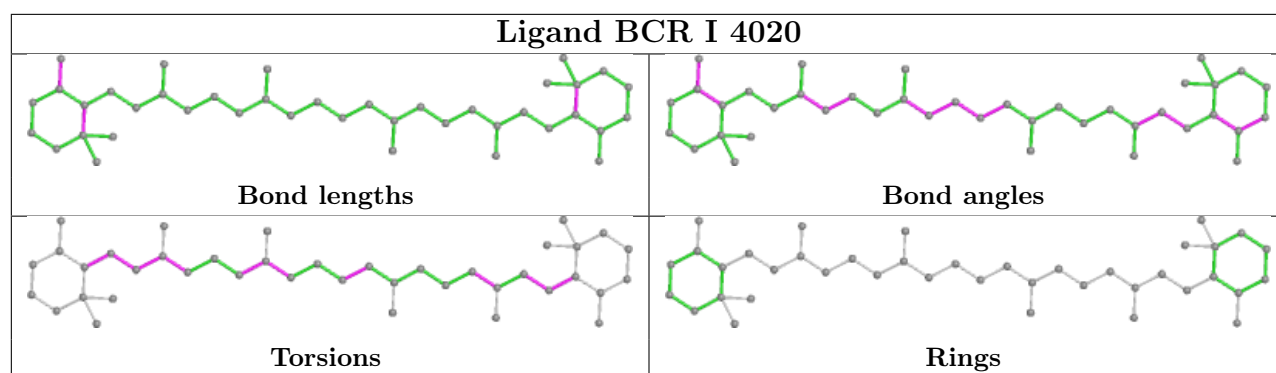
Rings

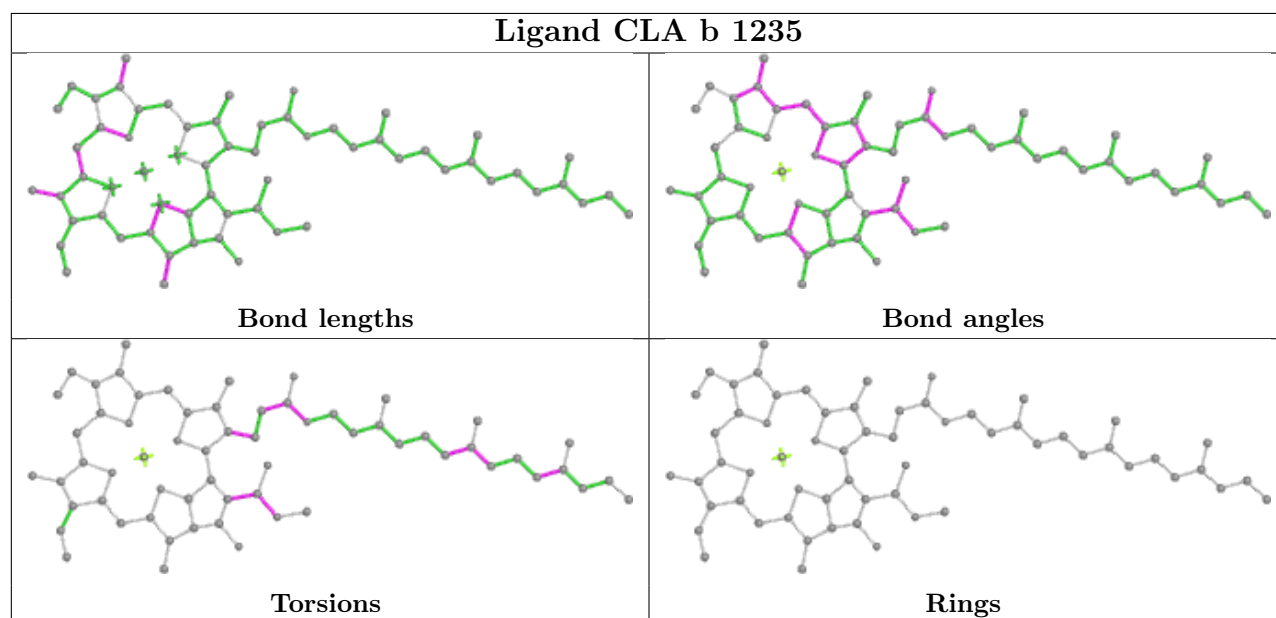
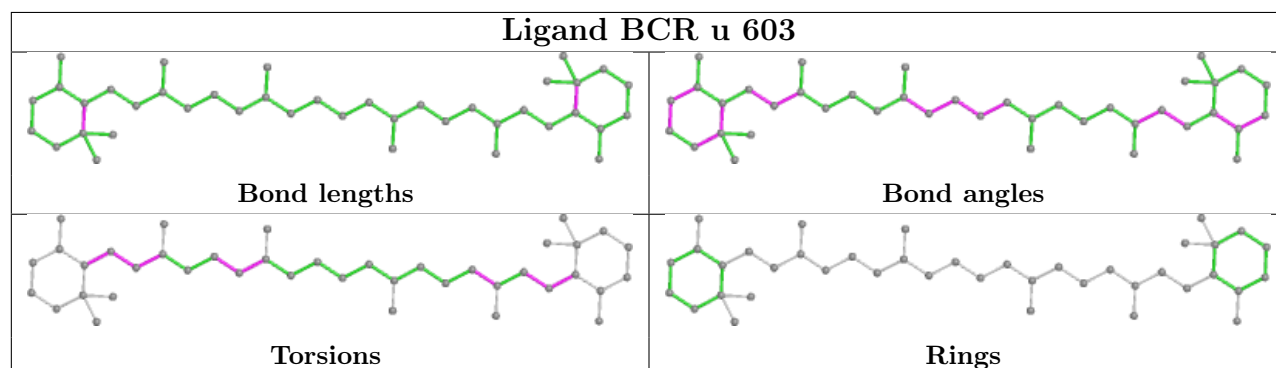
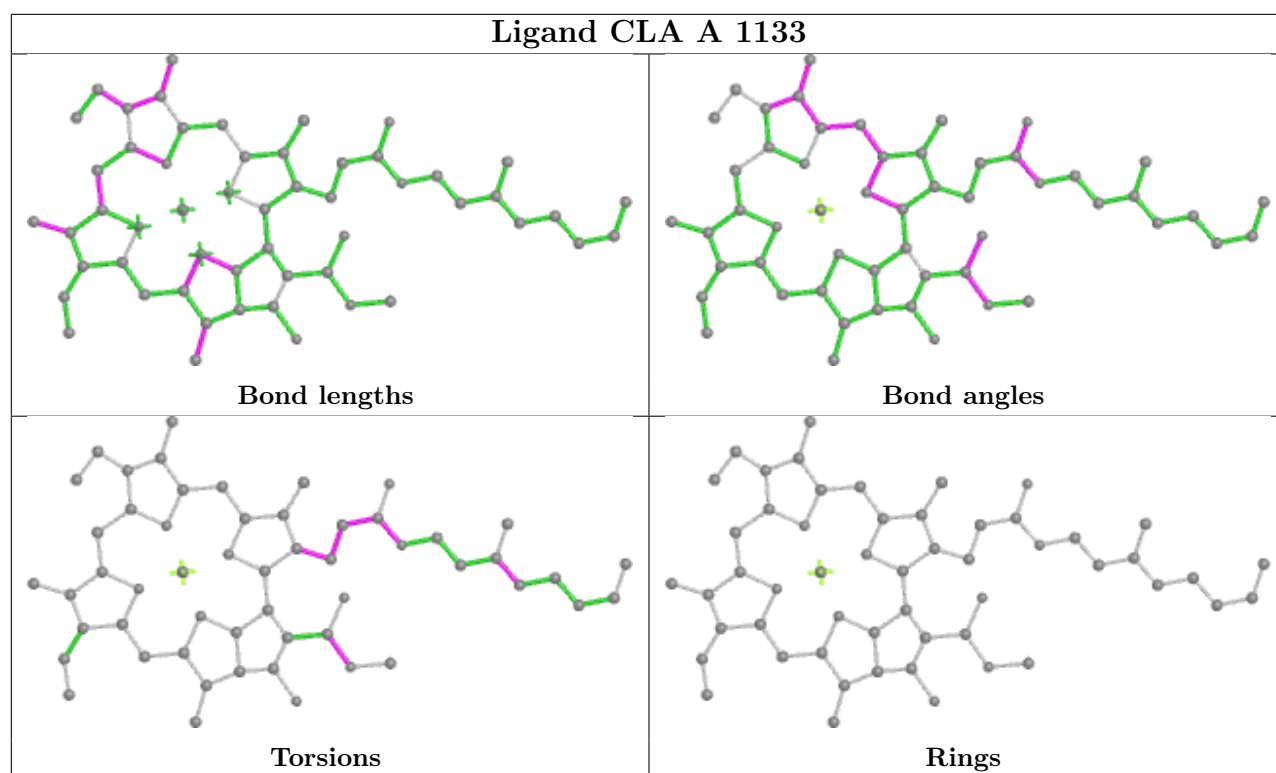
## Ligand CLA A 1136



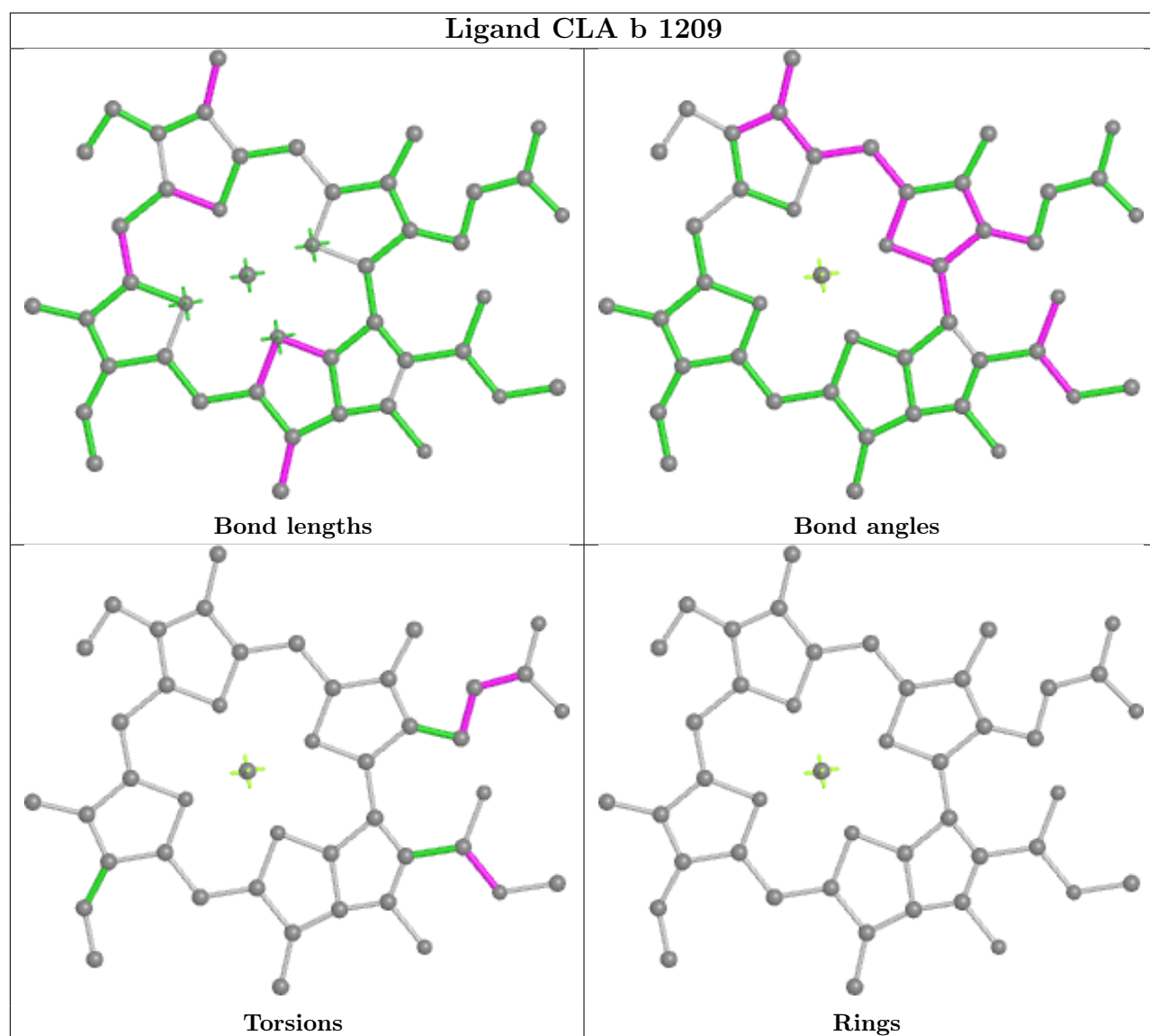
## Ligand CLA F 1301



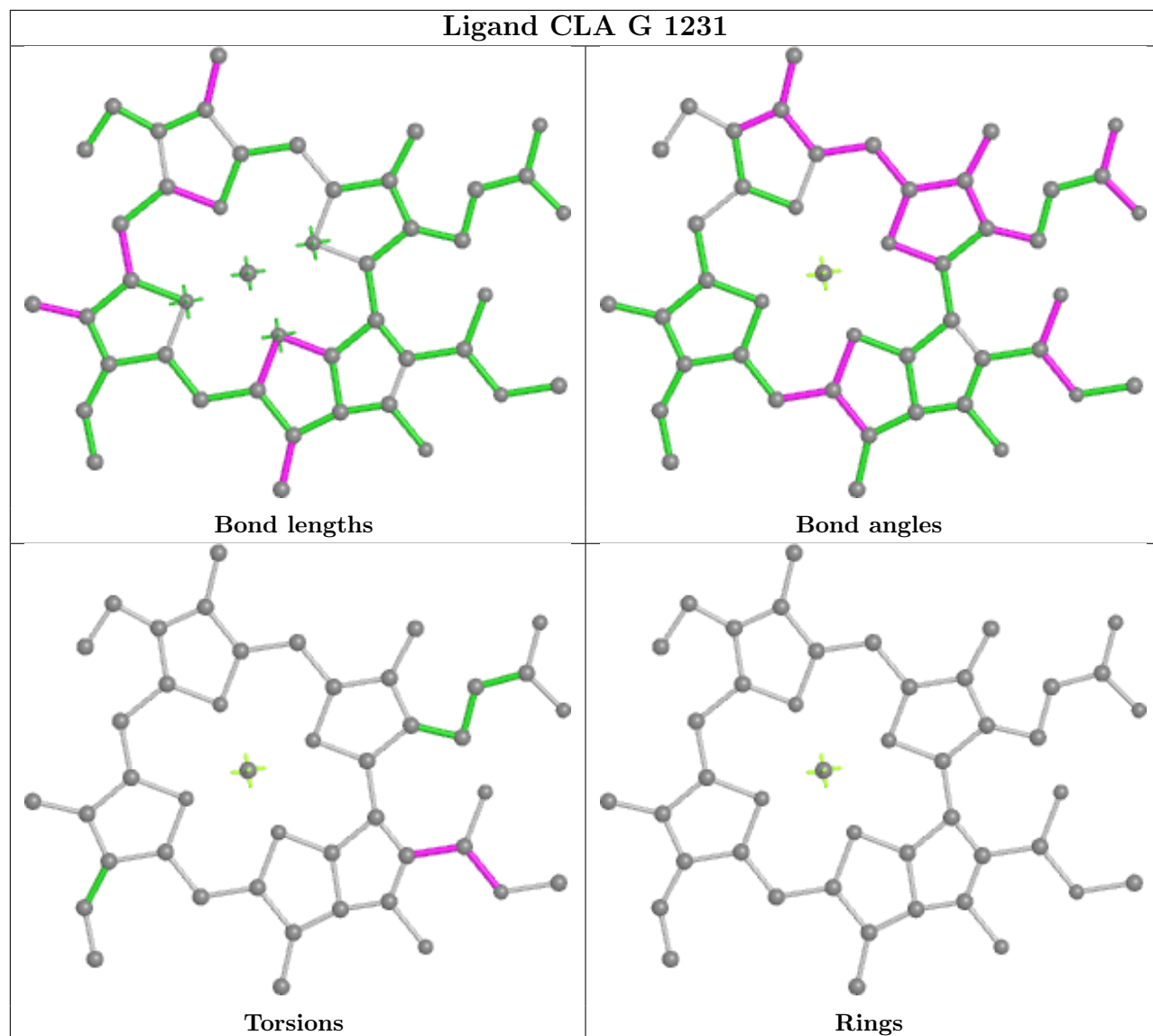


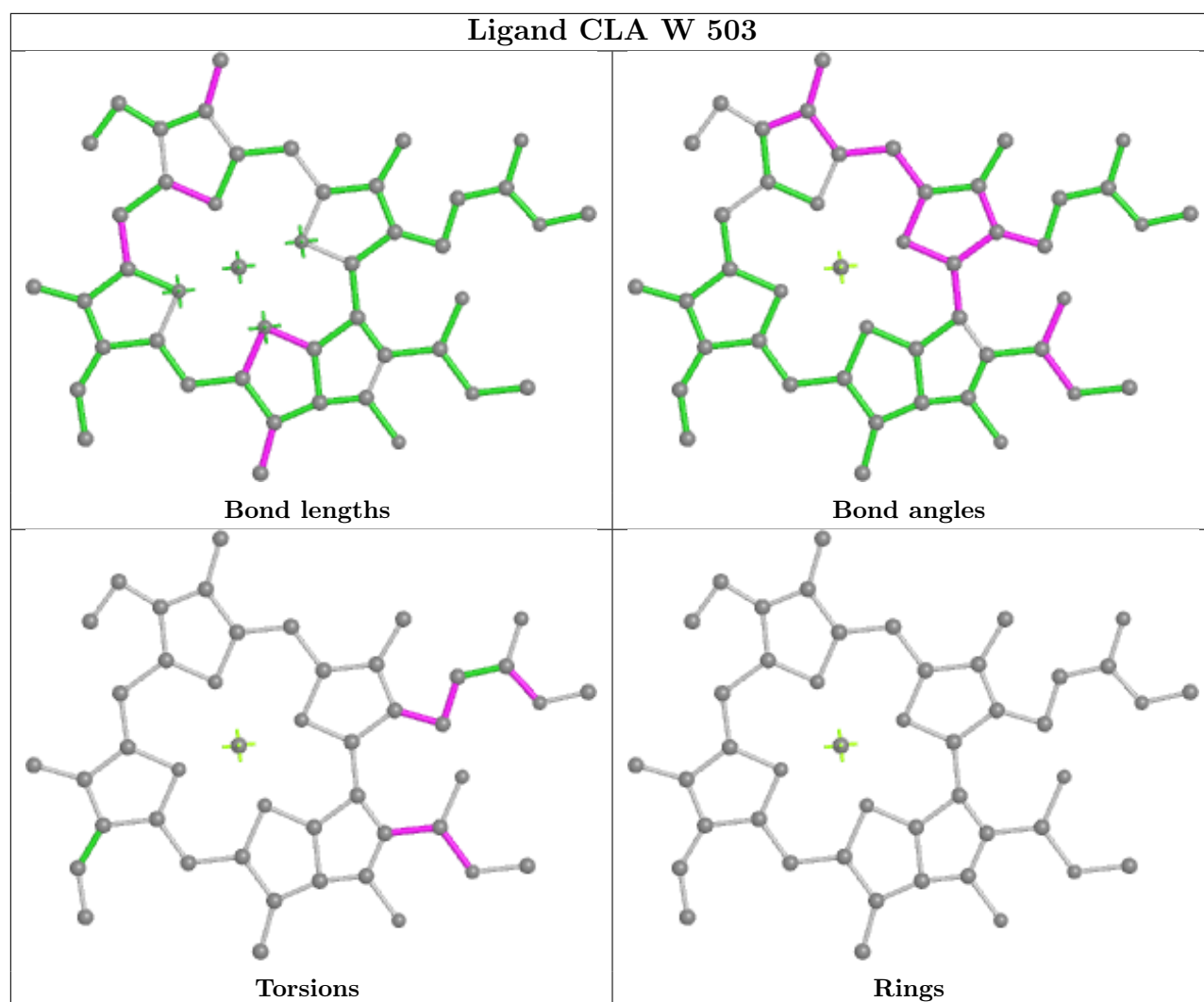




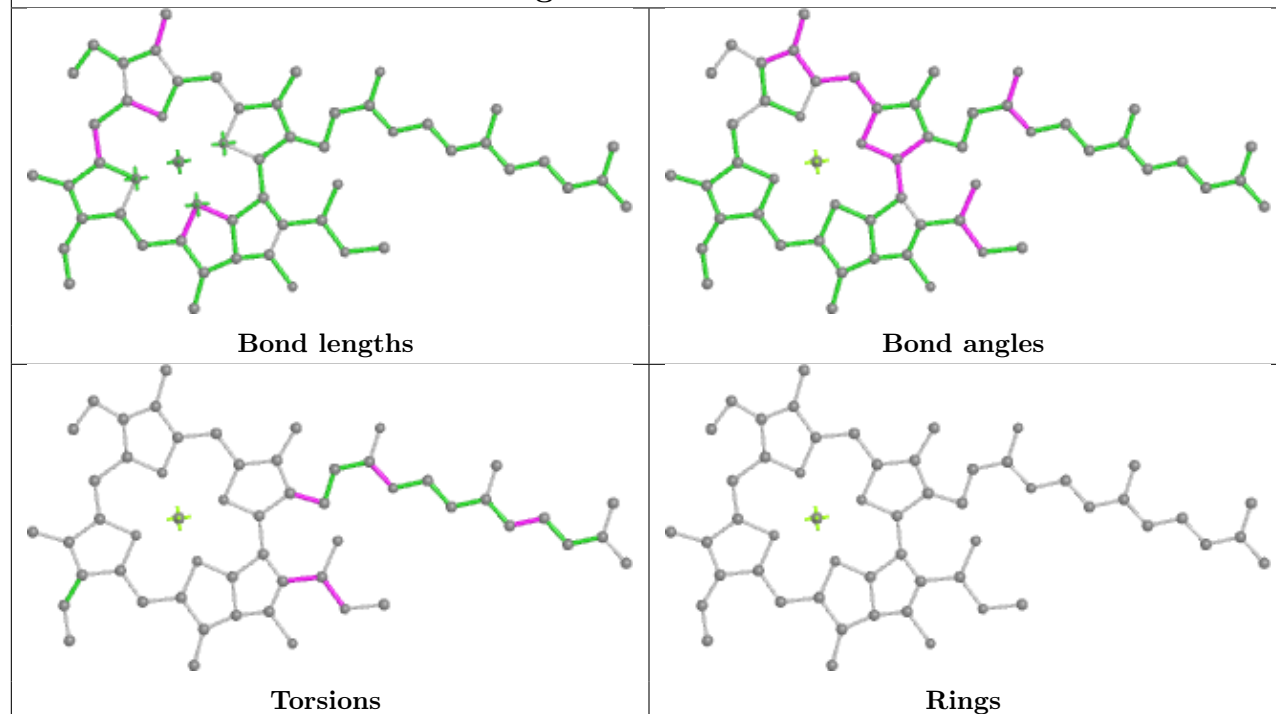


## Ligand CLA G 1231

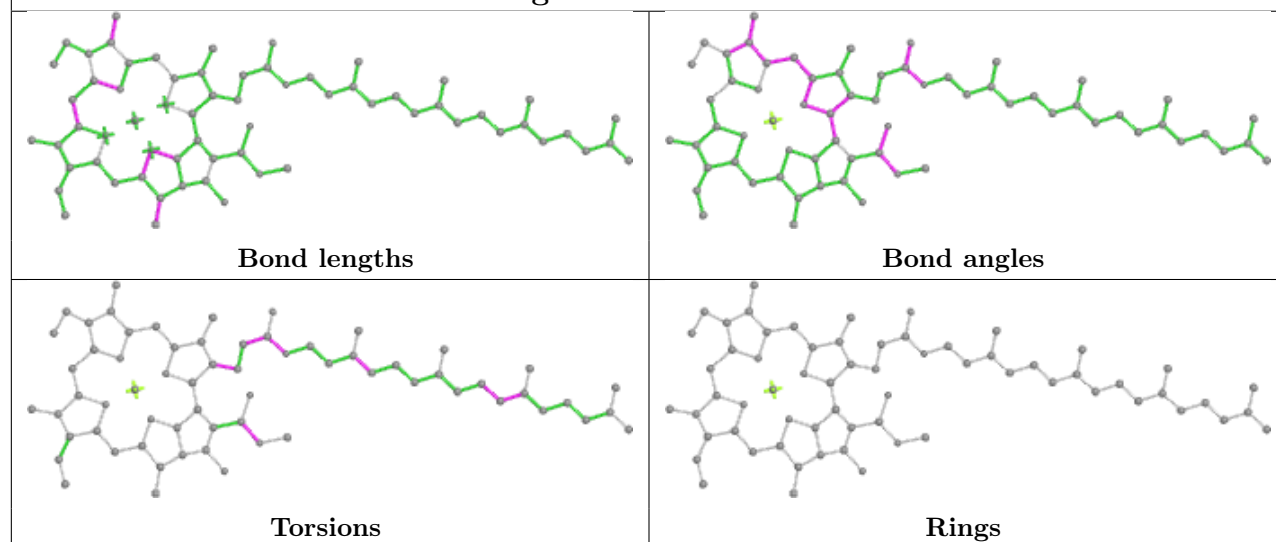


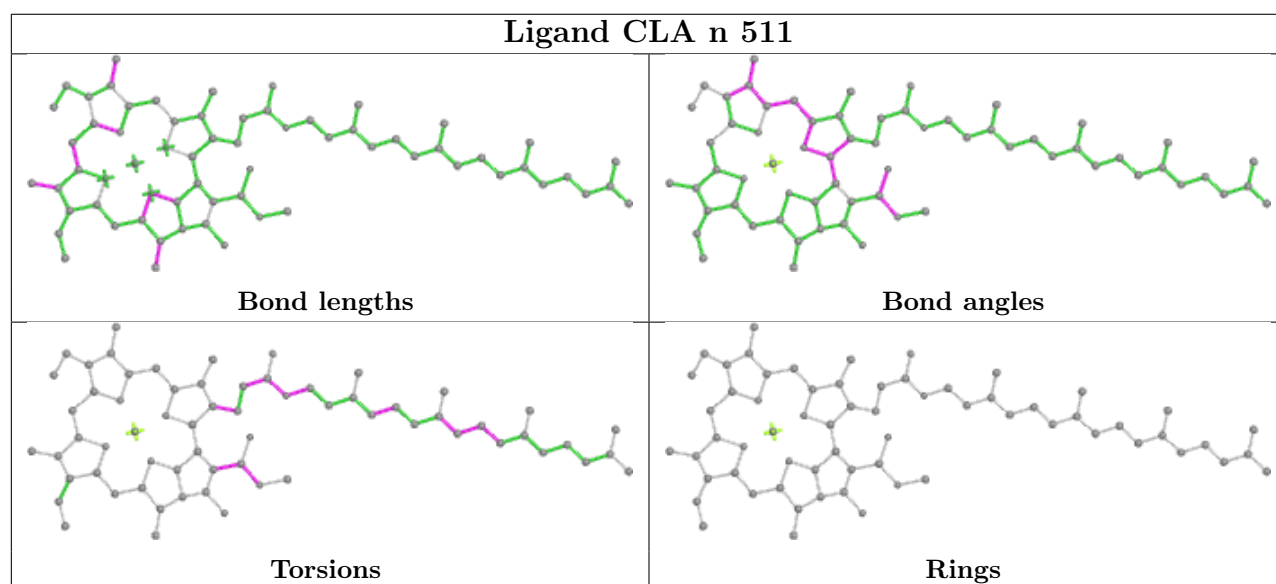
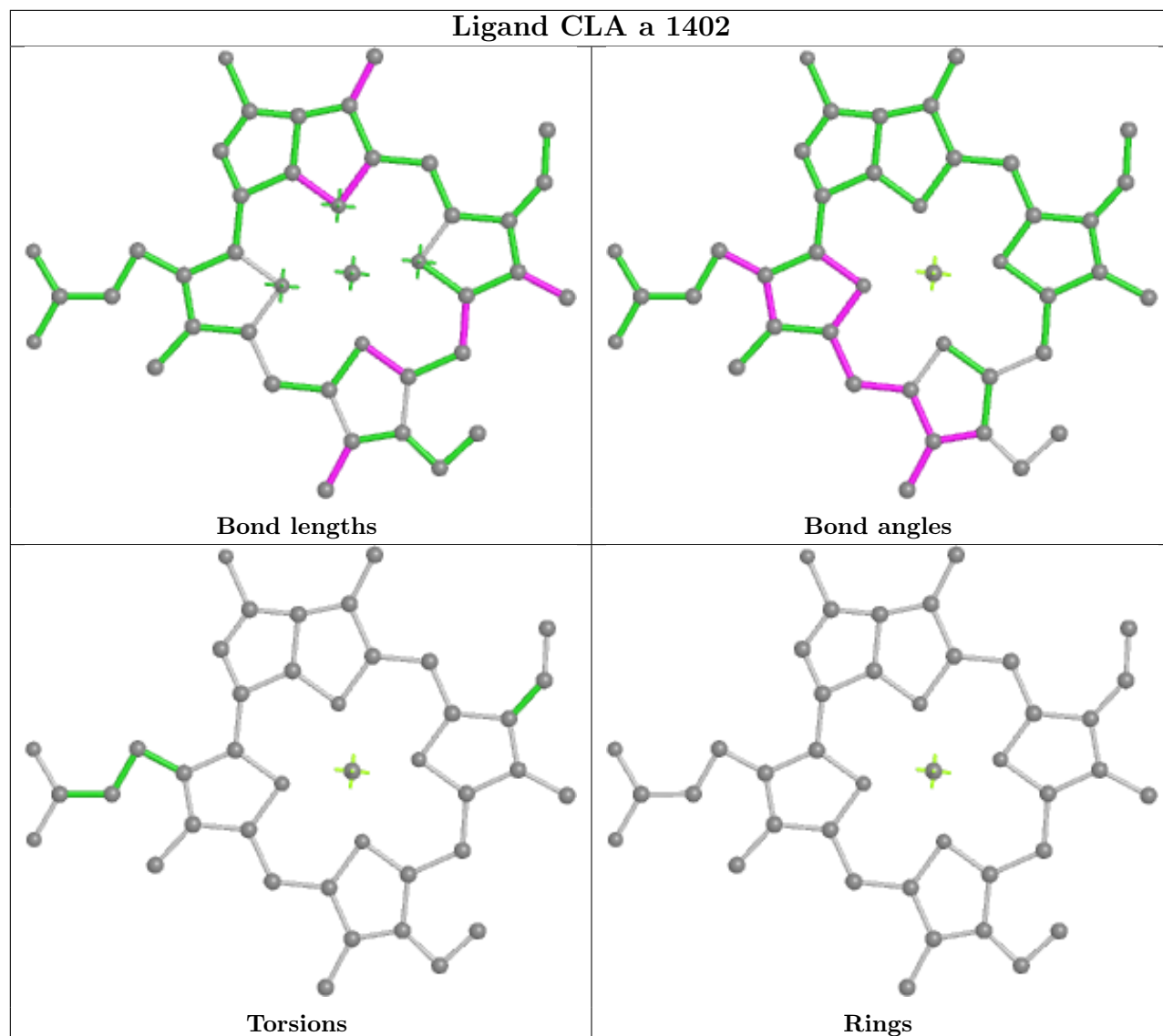


## Ligand CLA v 508

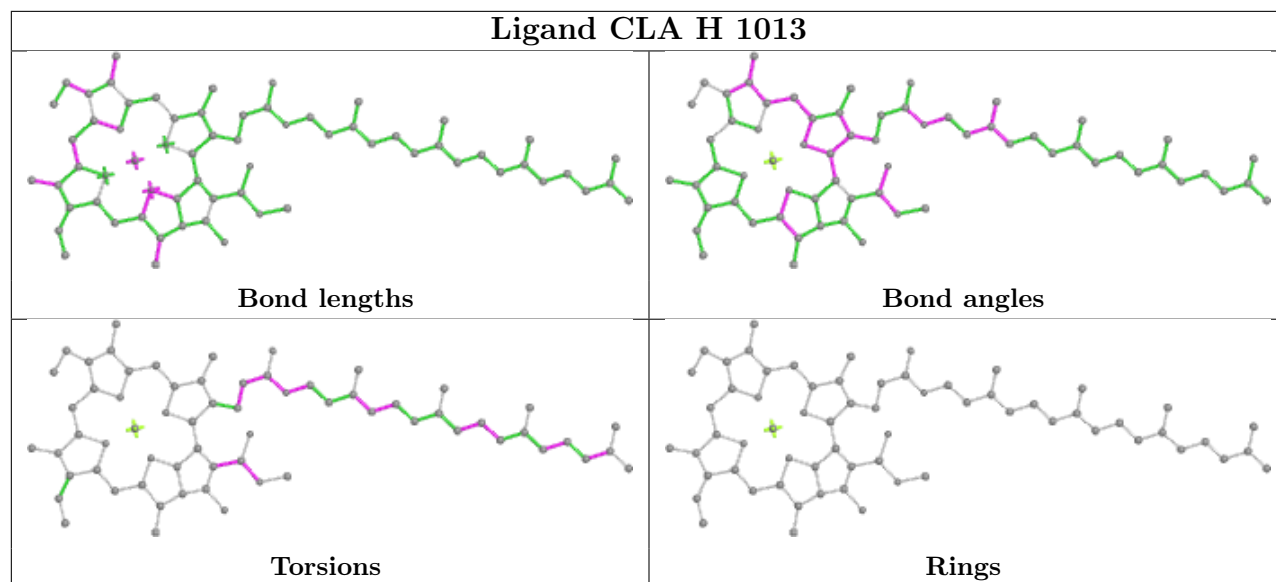


## Ligand CLA X 511

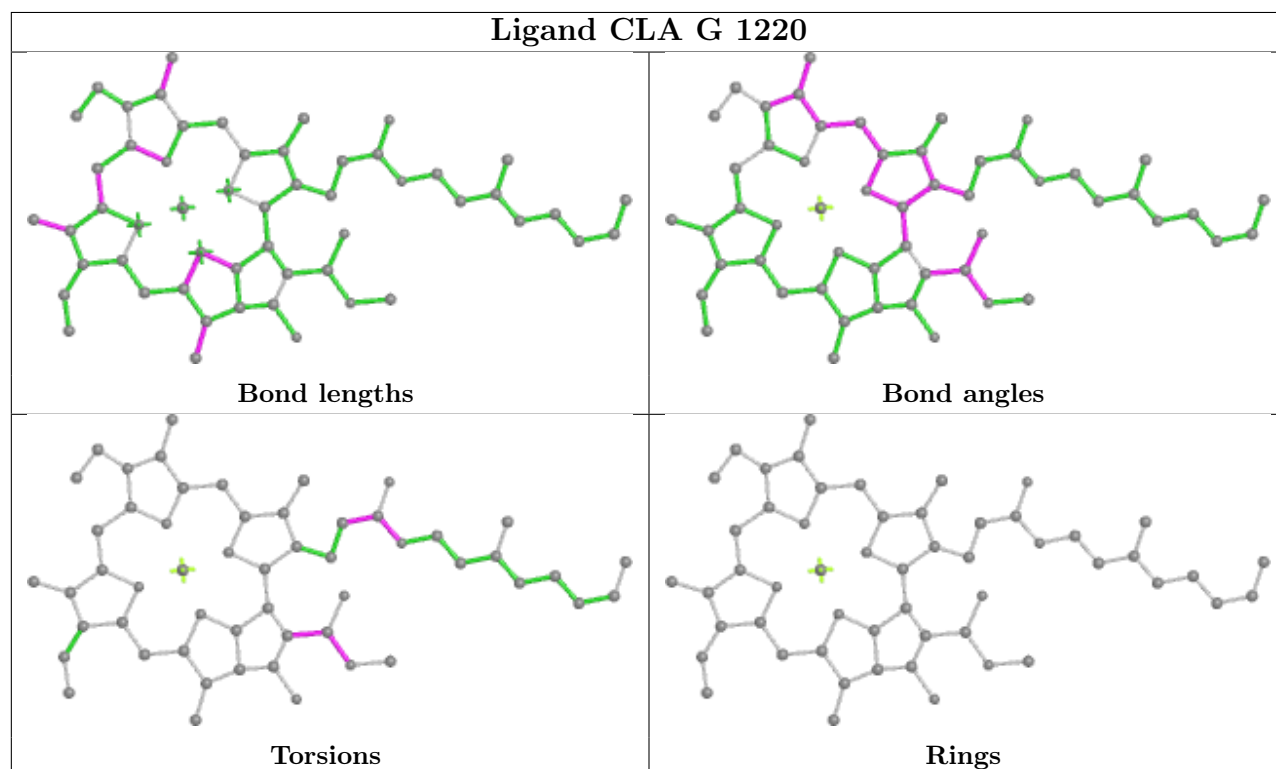




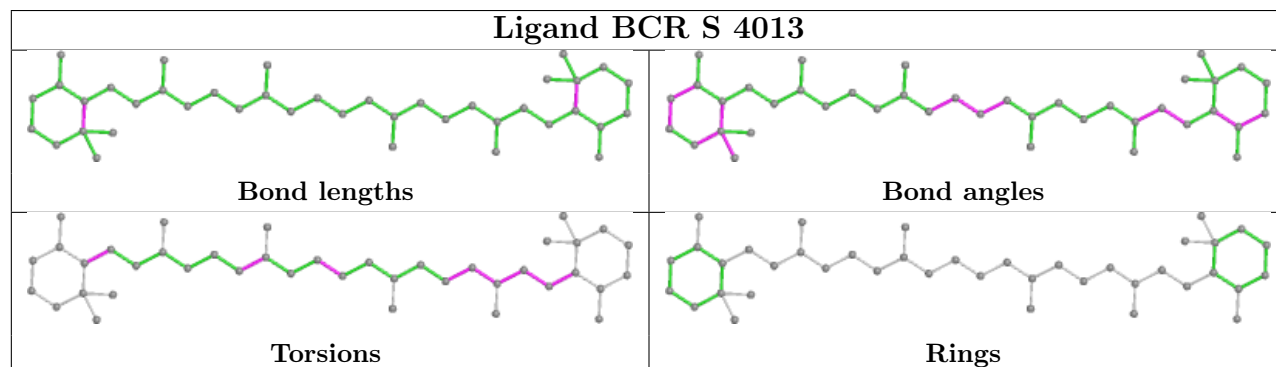
## Ligand CLA H 1013



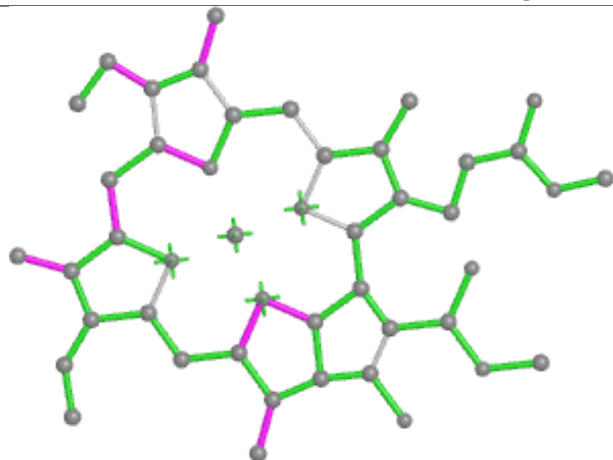
## Ligand CLA G 1220



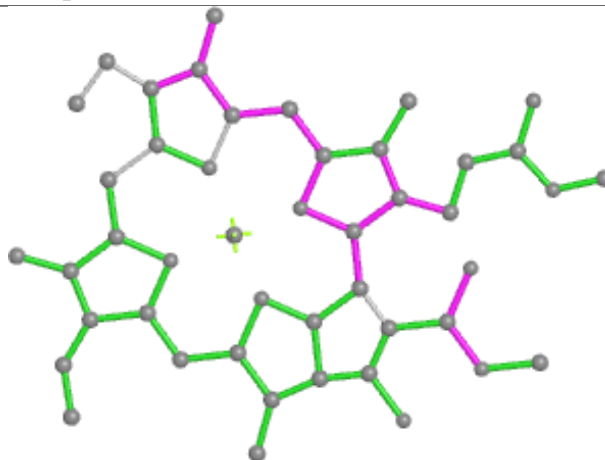
## Ligand BCR S 4013



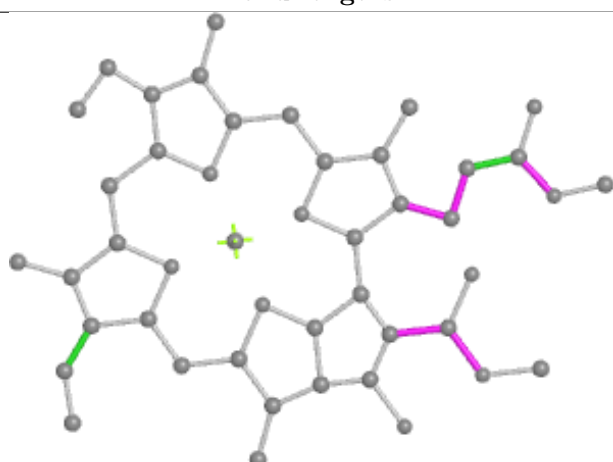
## Ligand CLA q 503



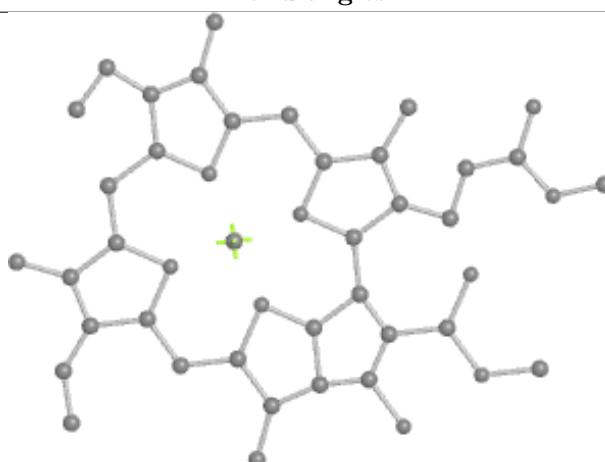
Bond lengths



Bond angles

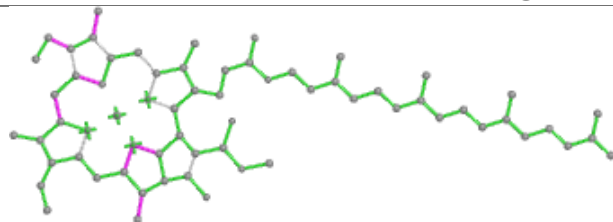


Torsions

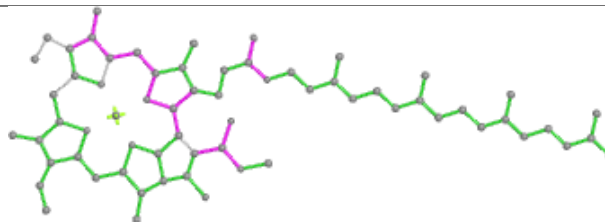


Rings

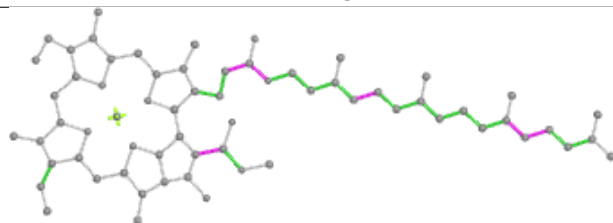
## Ligand CLA n 510



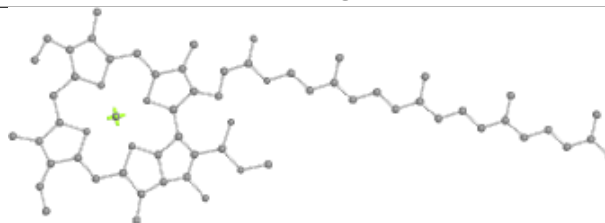
Bond lengths



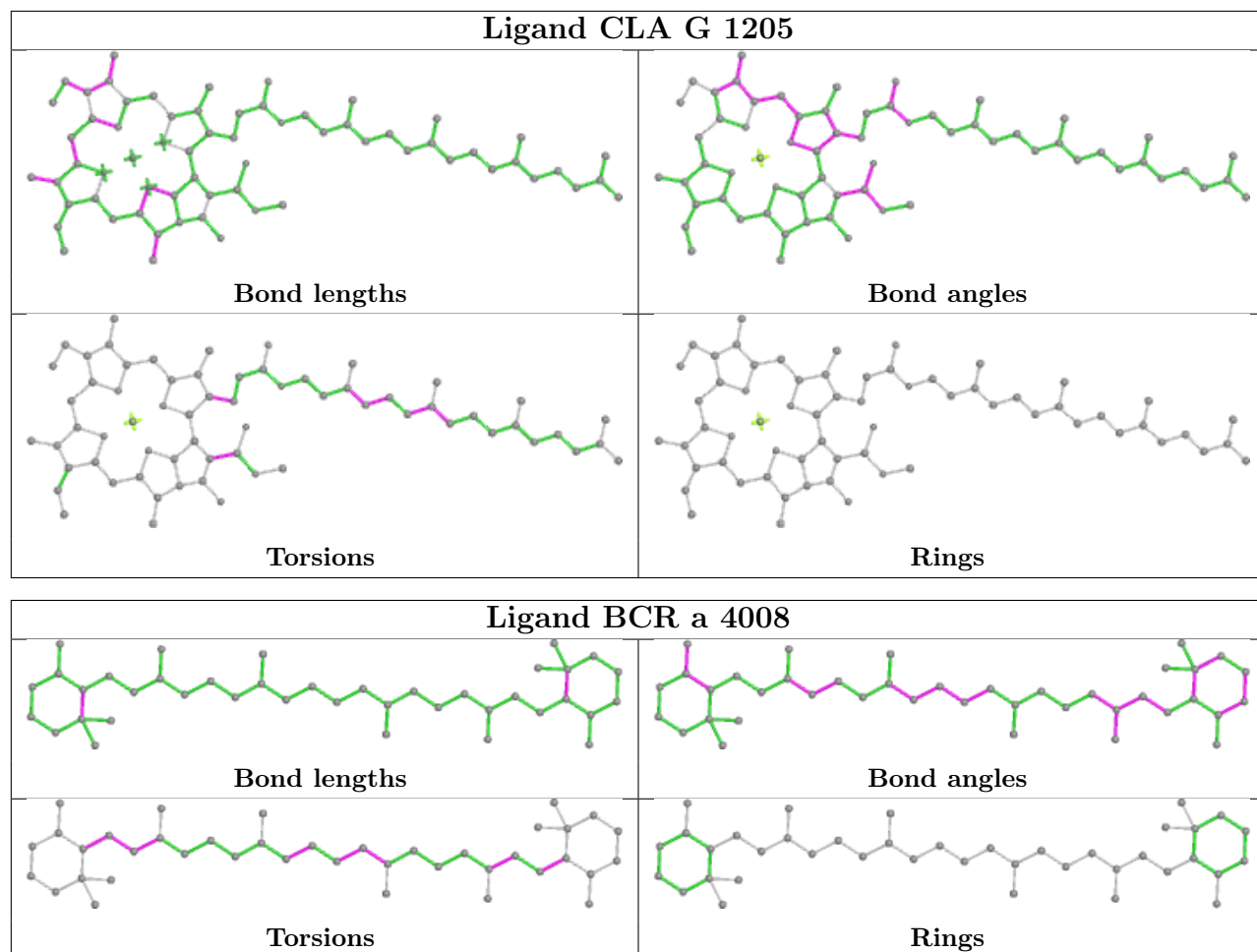
Bond angles



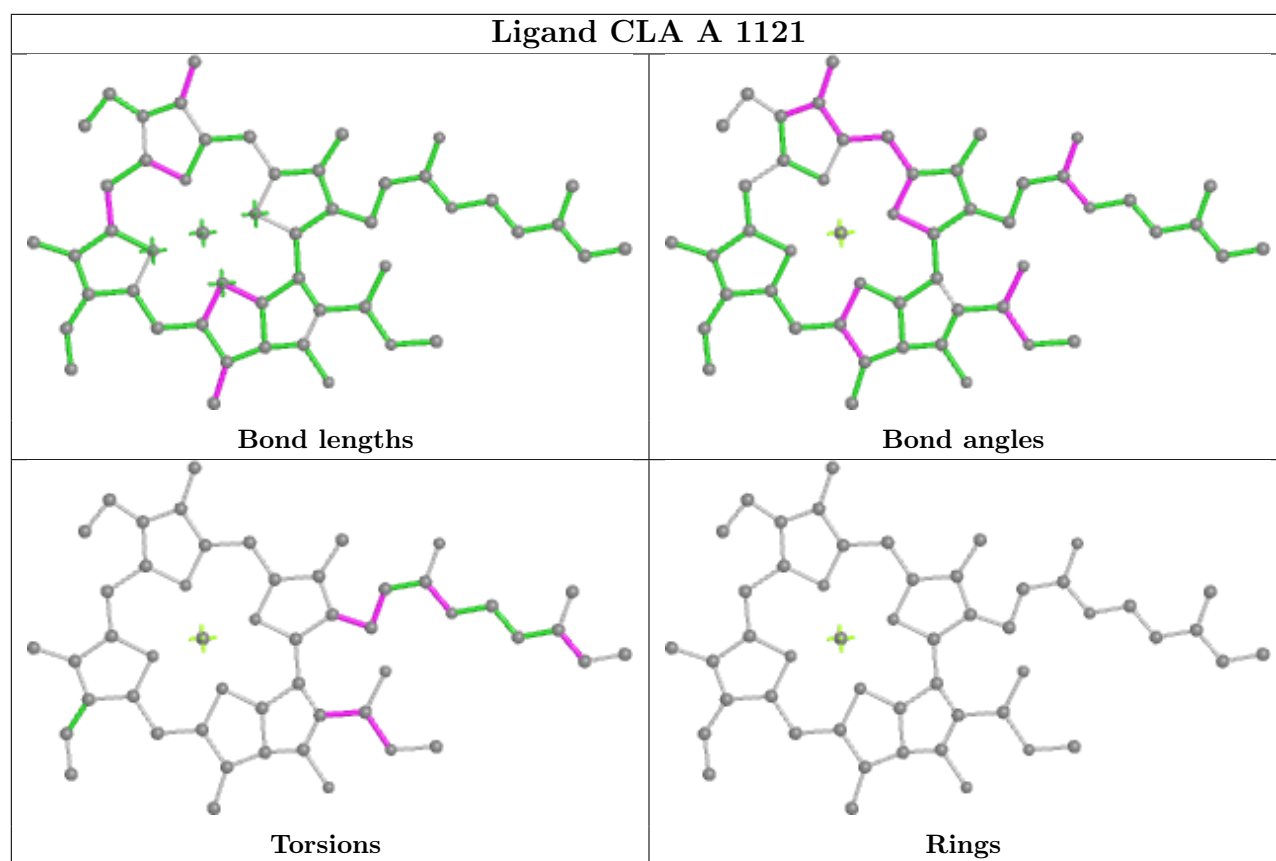
Torsions

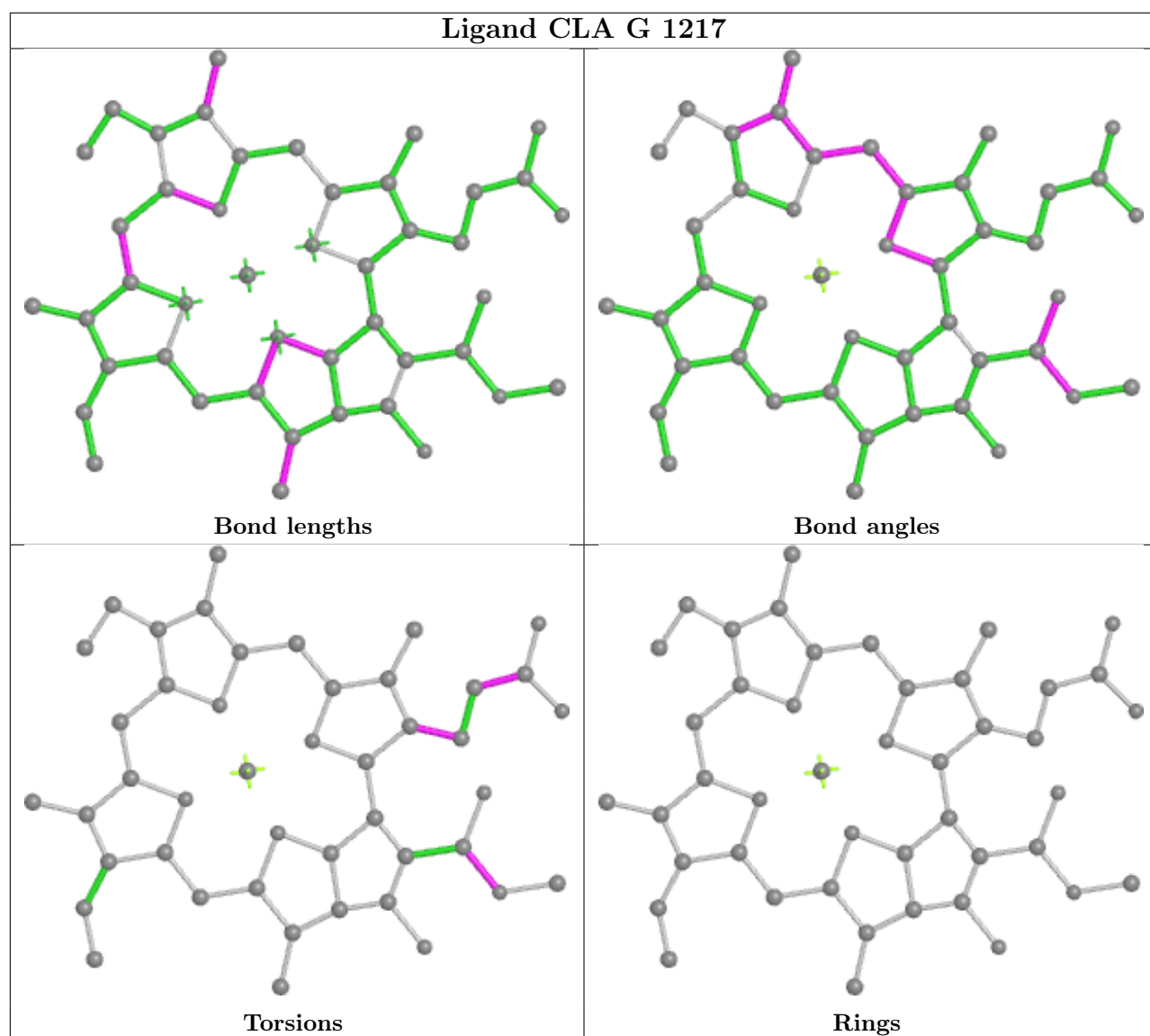


Rings

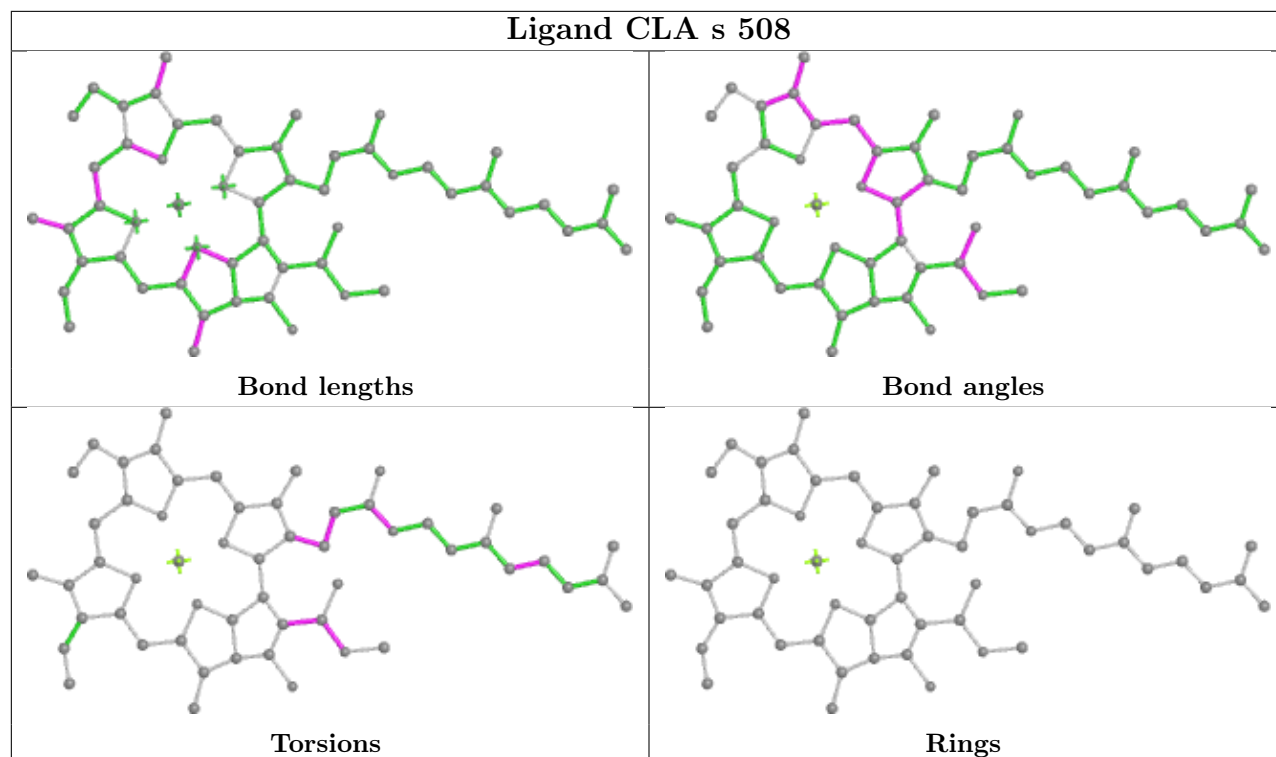




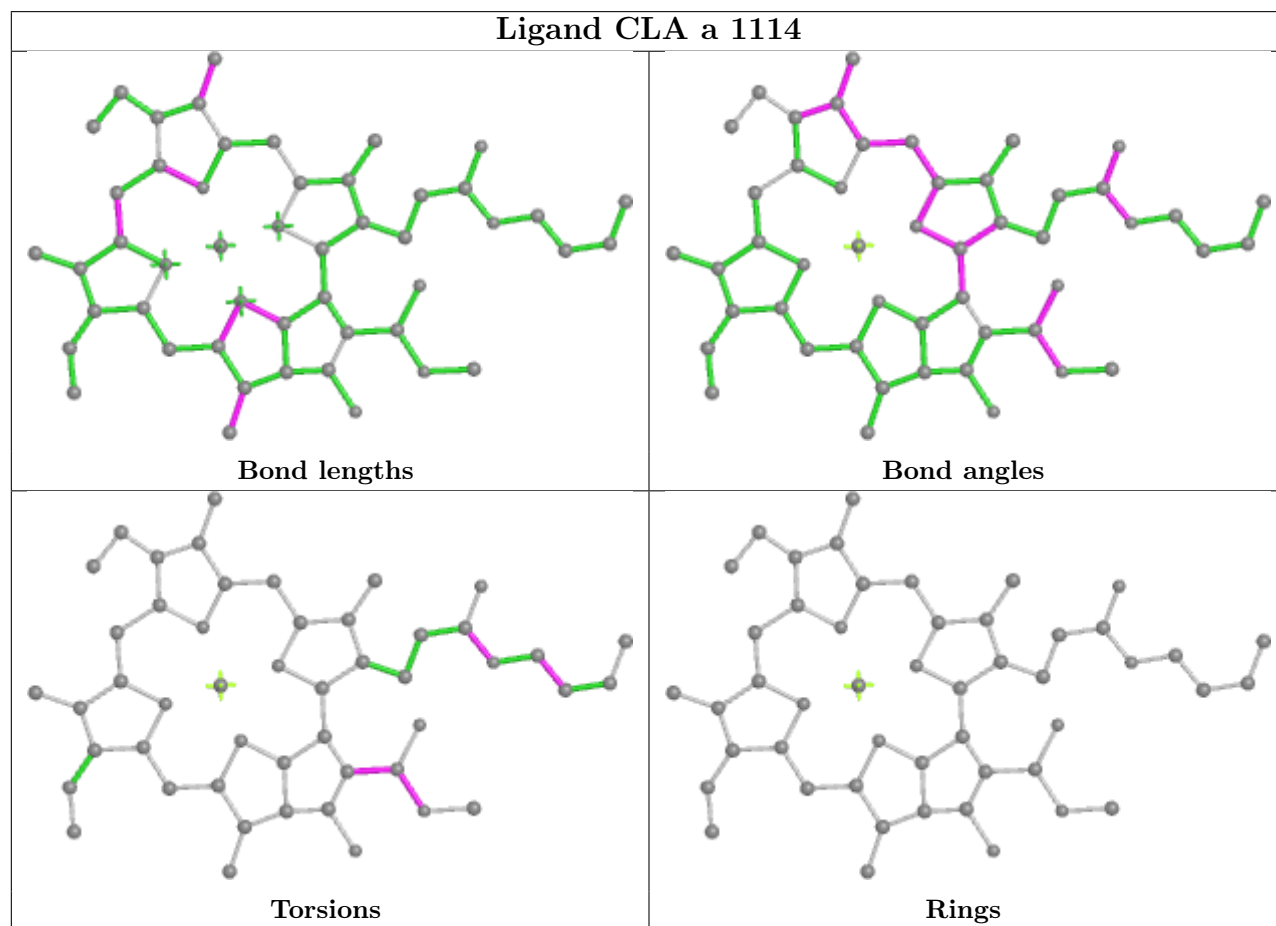




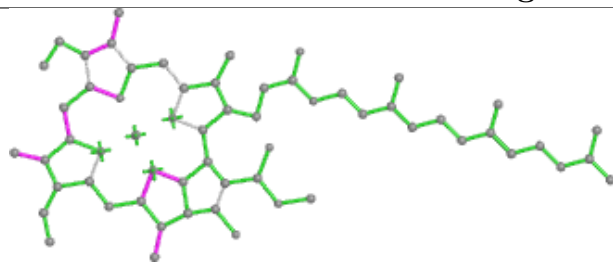
## Ligand CLA s 508



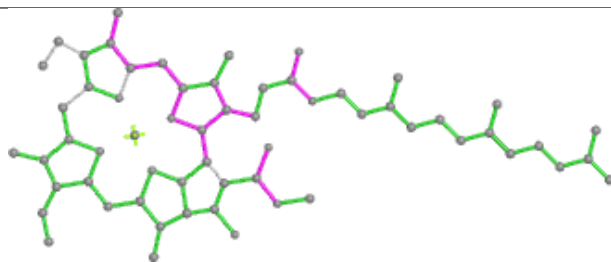
## Ligand CLA a 1114



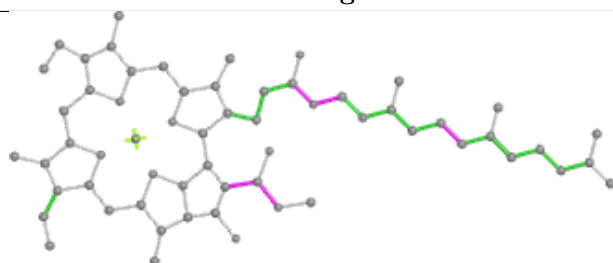
## Ligand CLA u 506



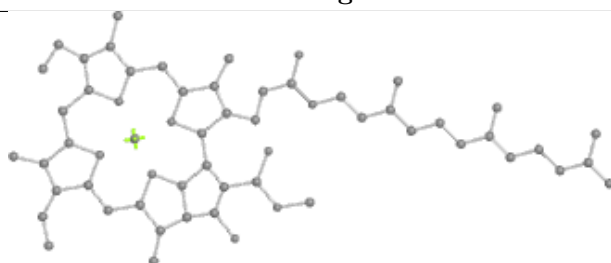
Bond lengths



Bond angles

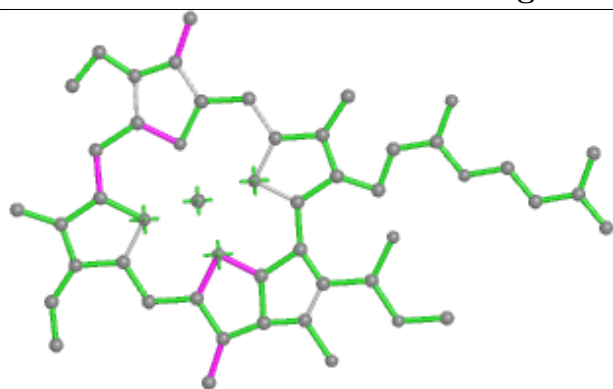


Torsions

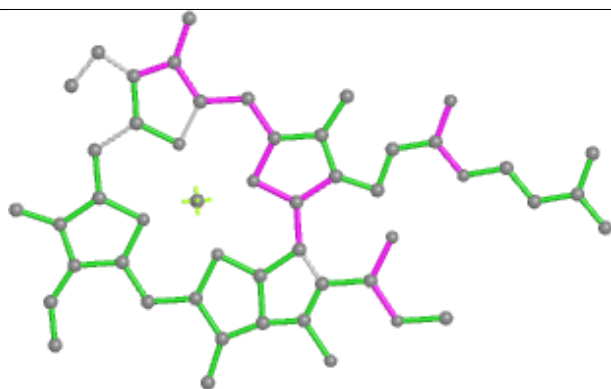


Rings

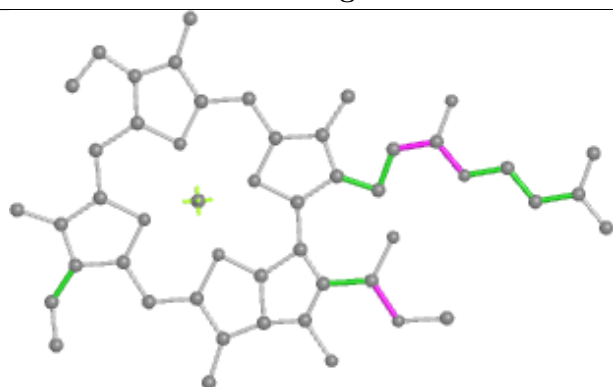
## Ligand CLA n 502



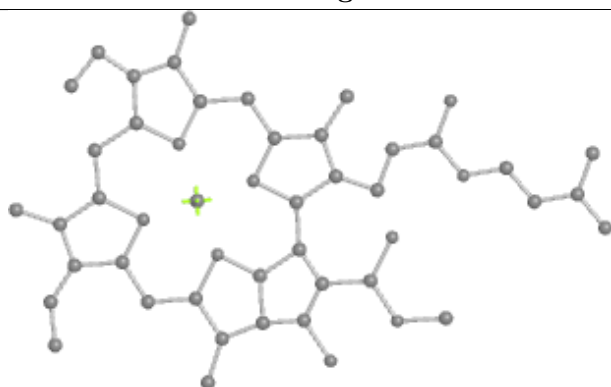
Bond lengths



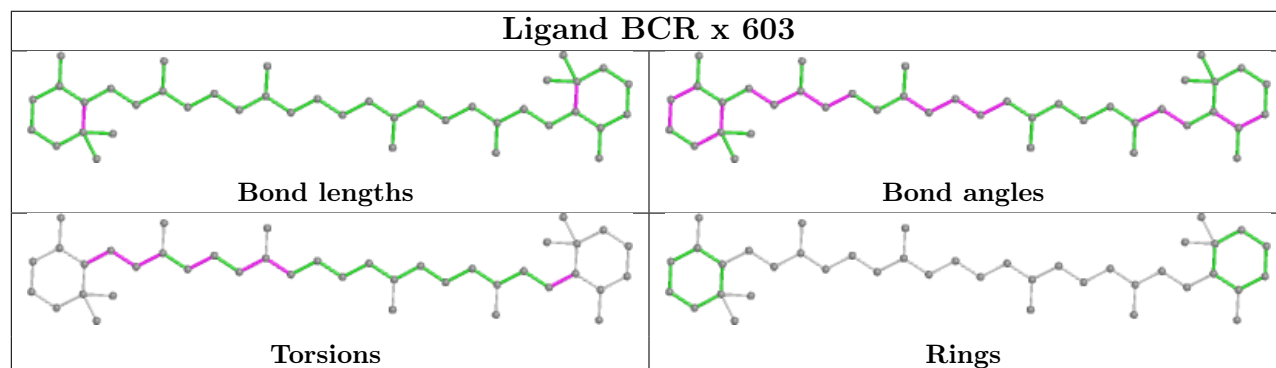
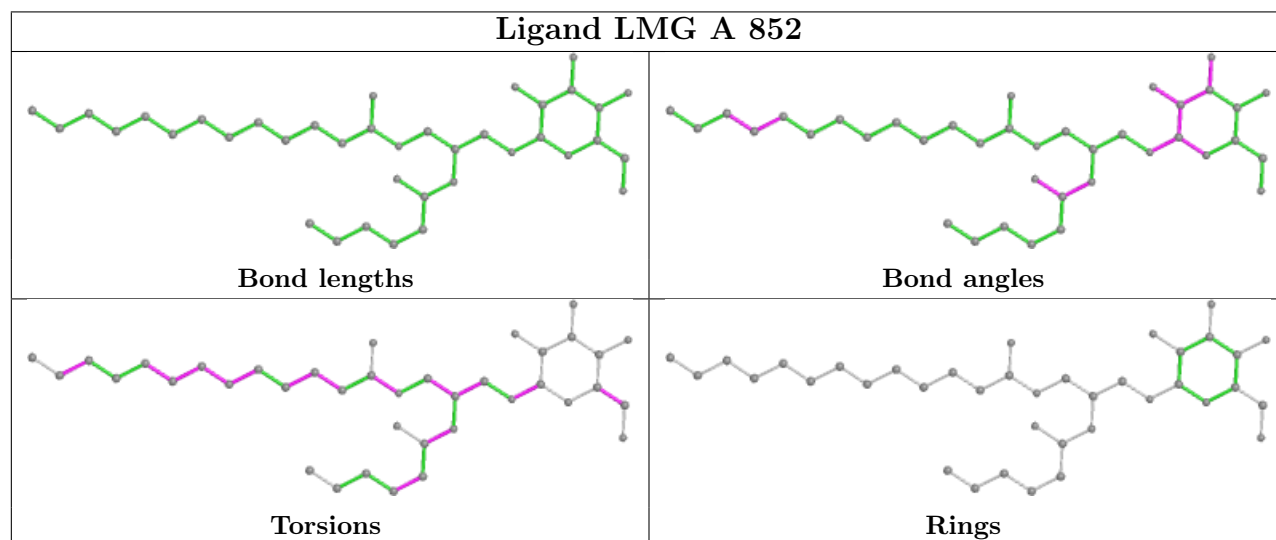
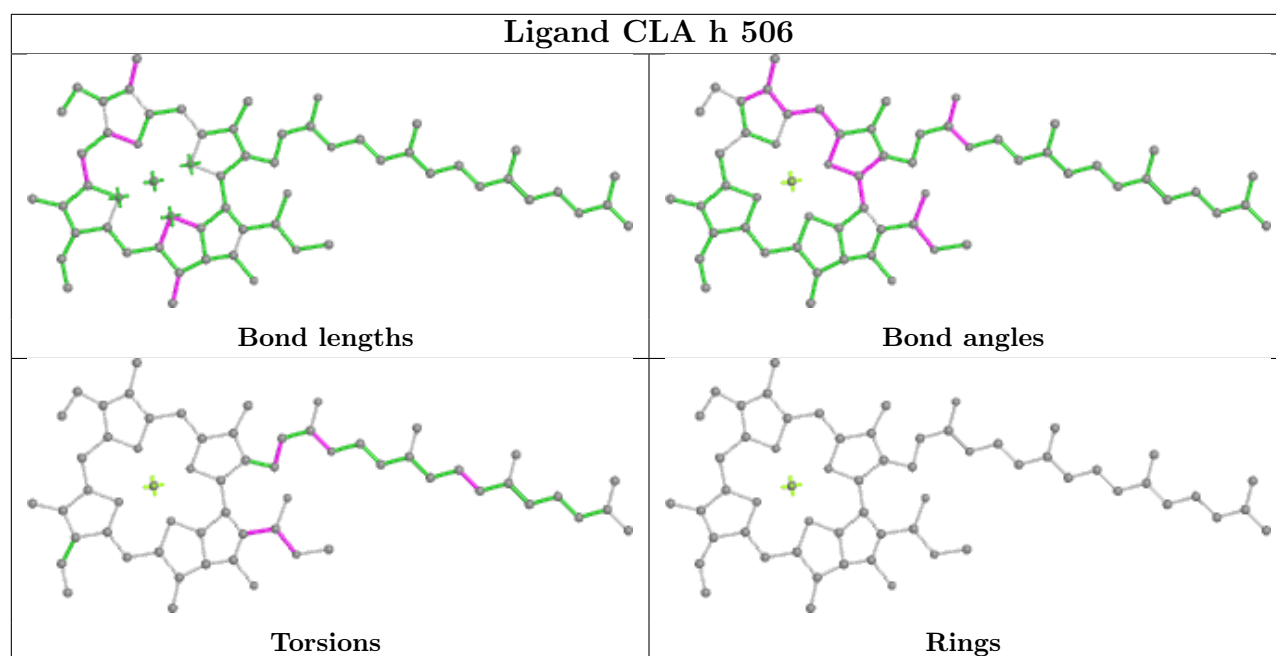
Bond angles

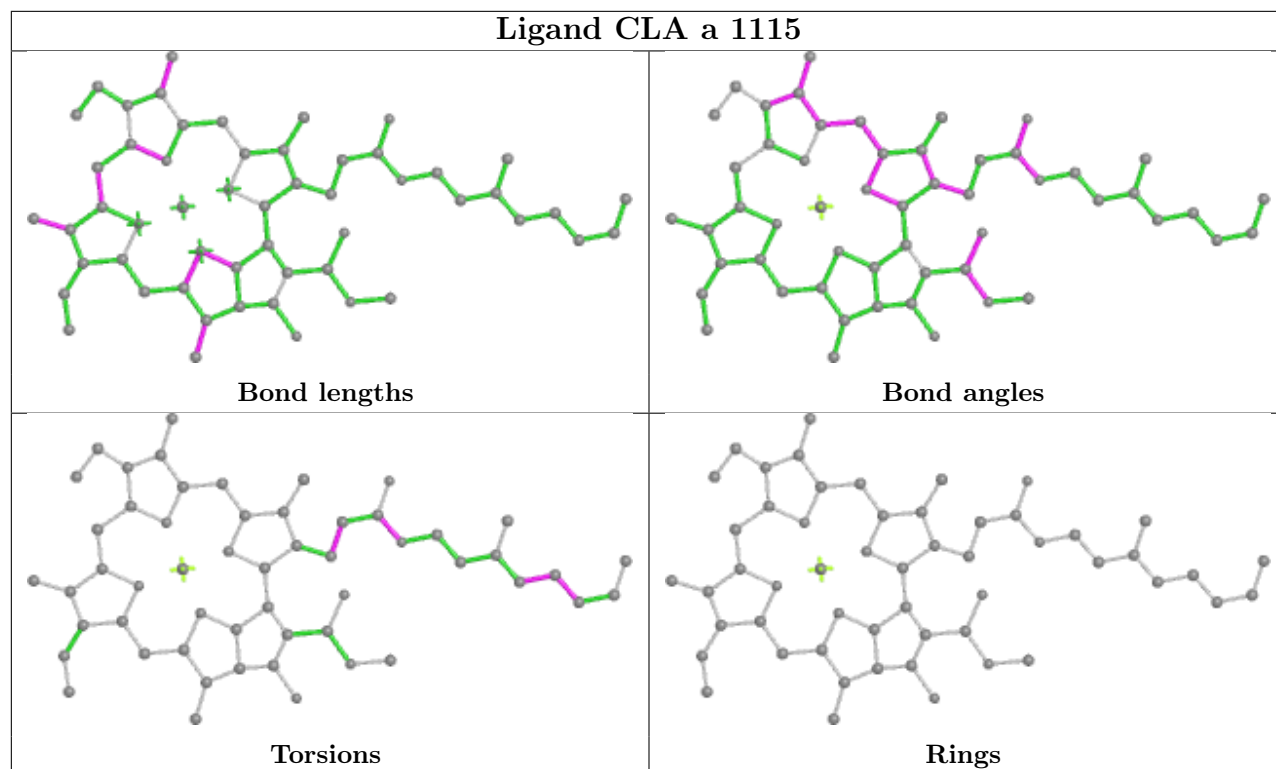
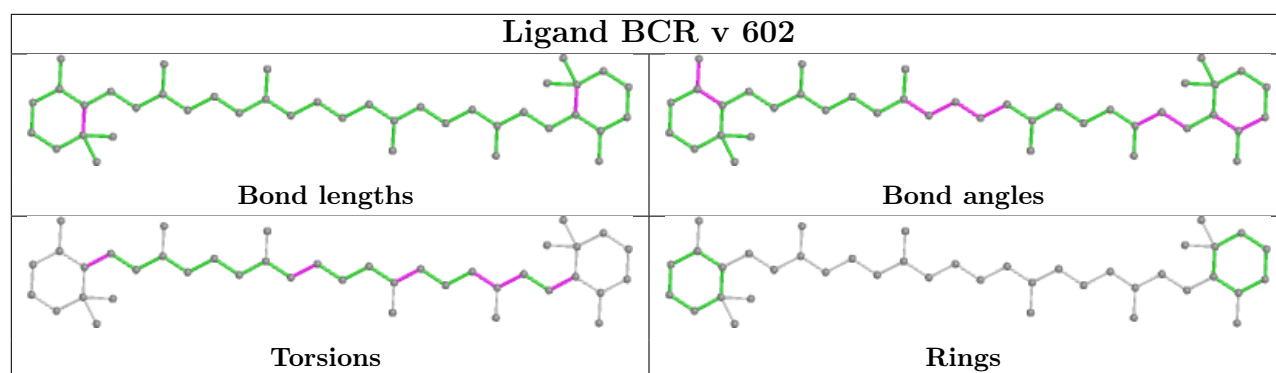


Torsions

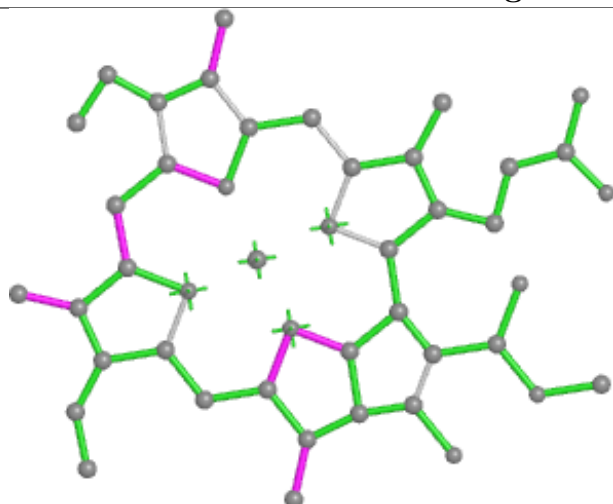


Rings

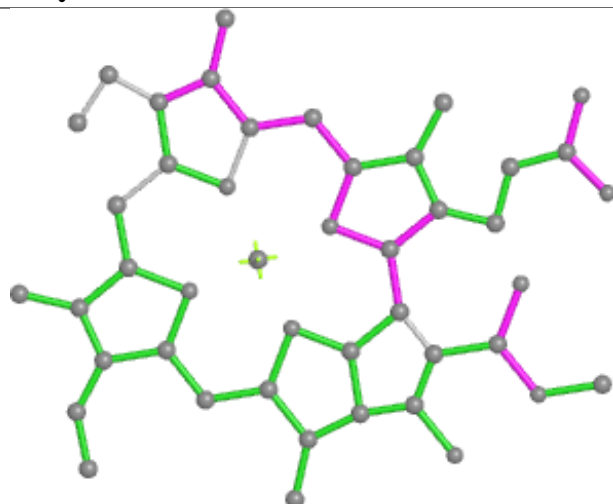




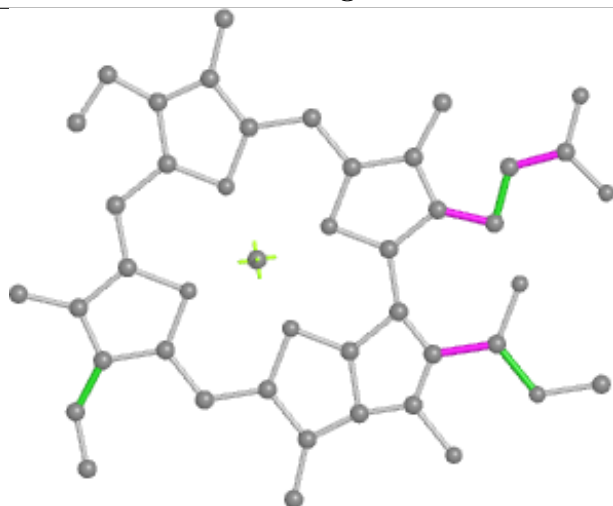
## Ligand CLA Q 1301



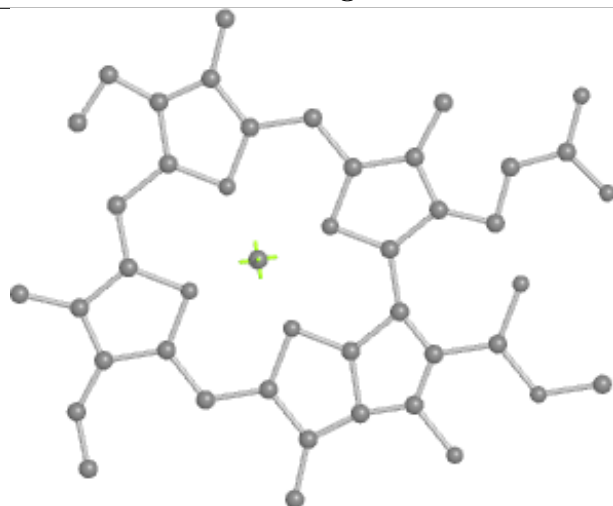
Bond lengths



Bond angles

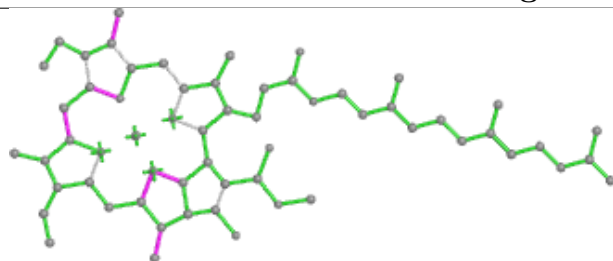


Torsions

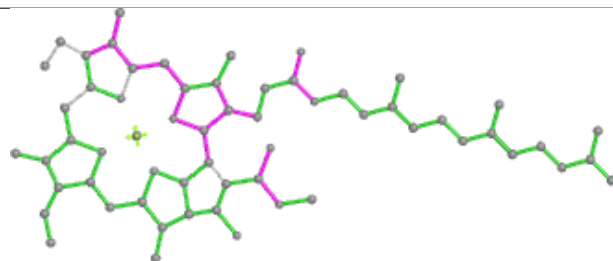


Rings

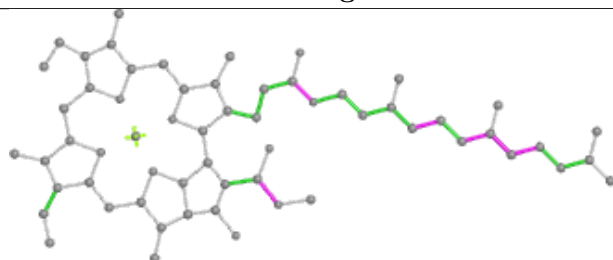
## Ligand CLA r 509



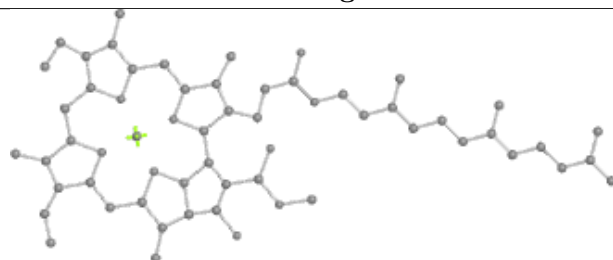
Bond lengths



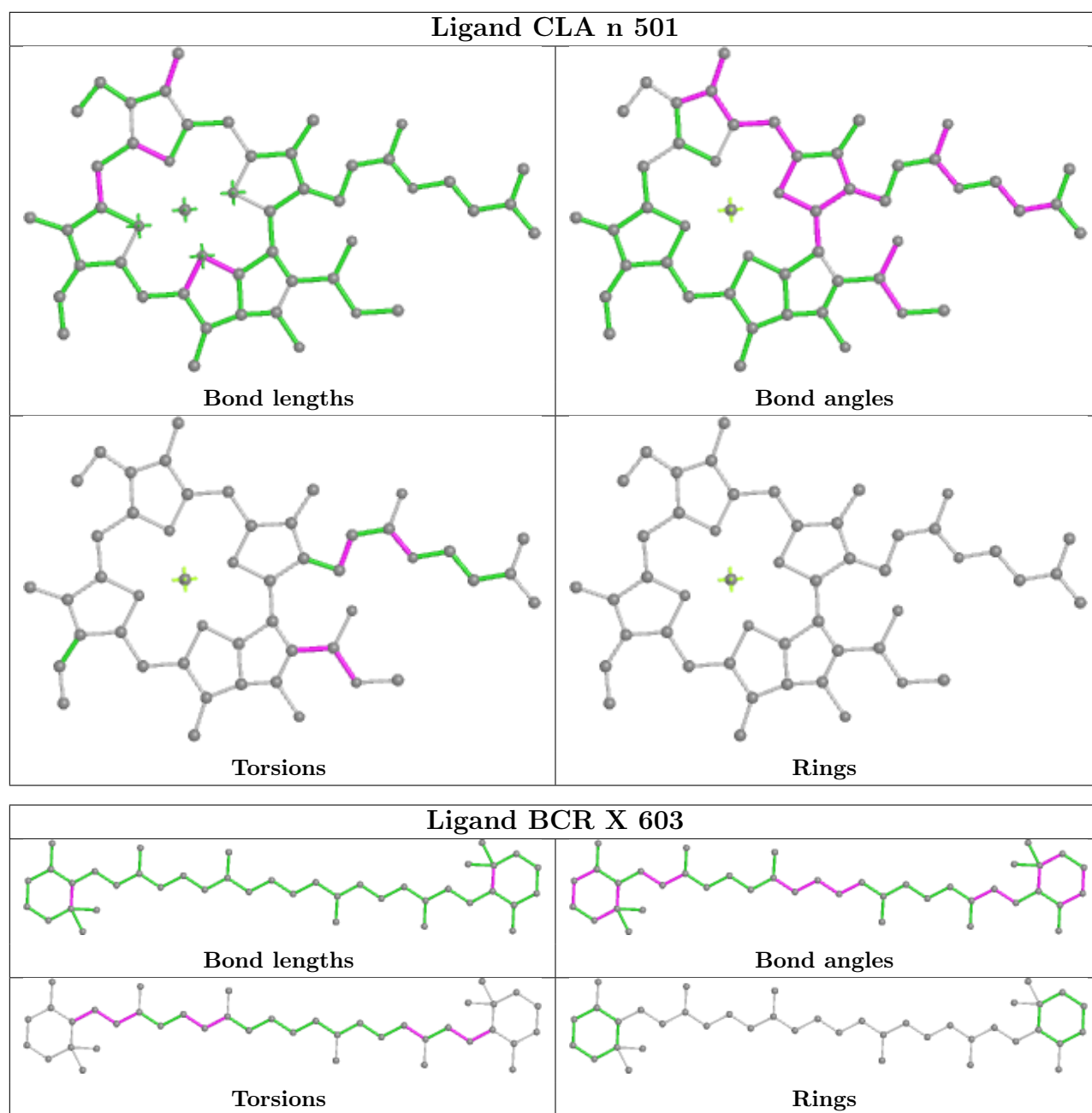
Bond angles



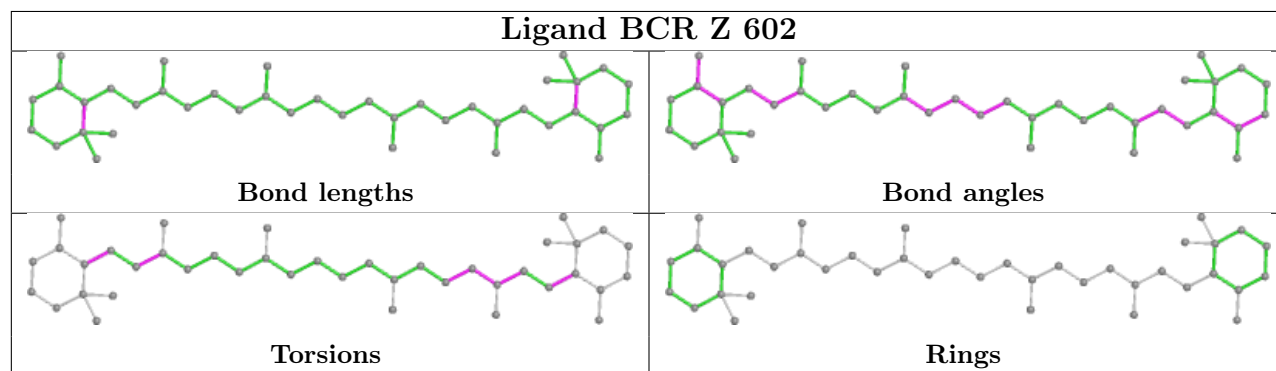
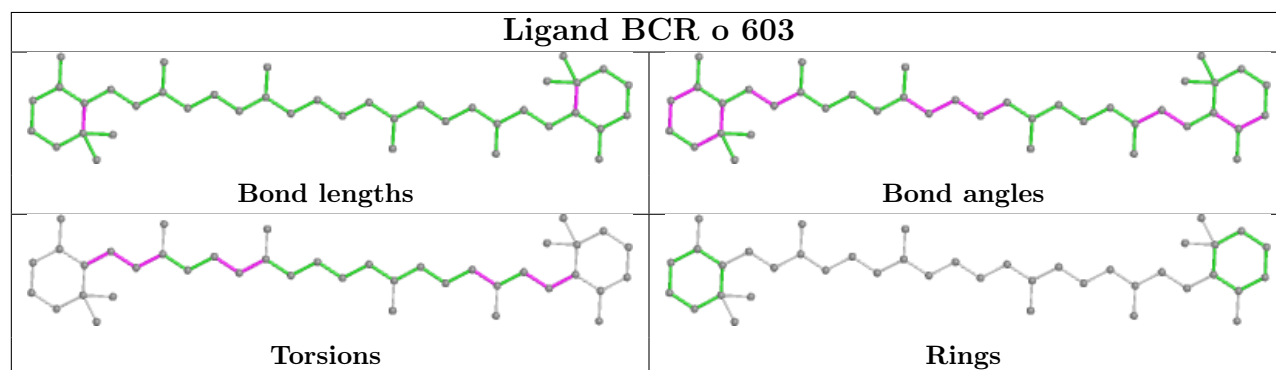
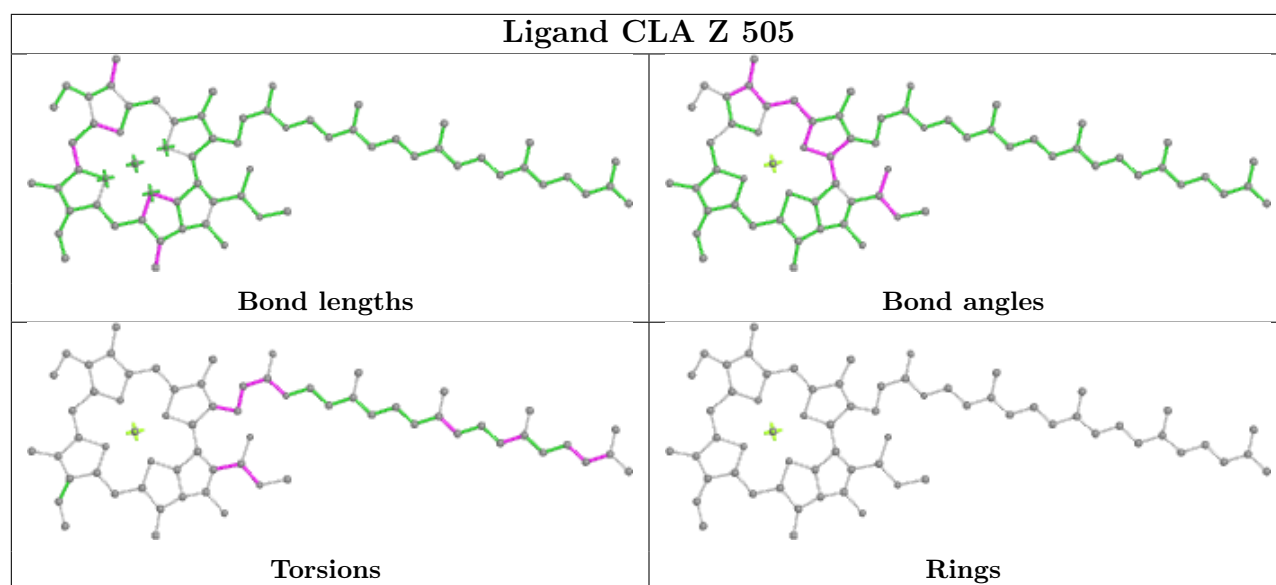
Torsions



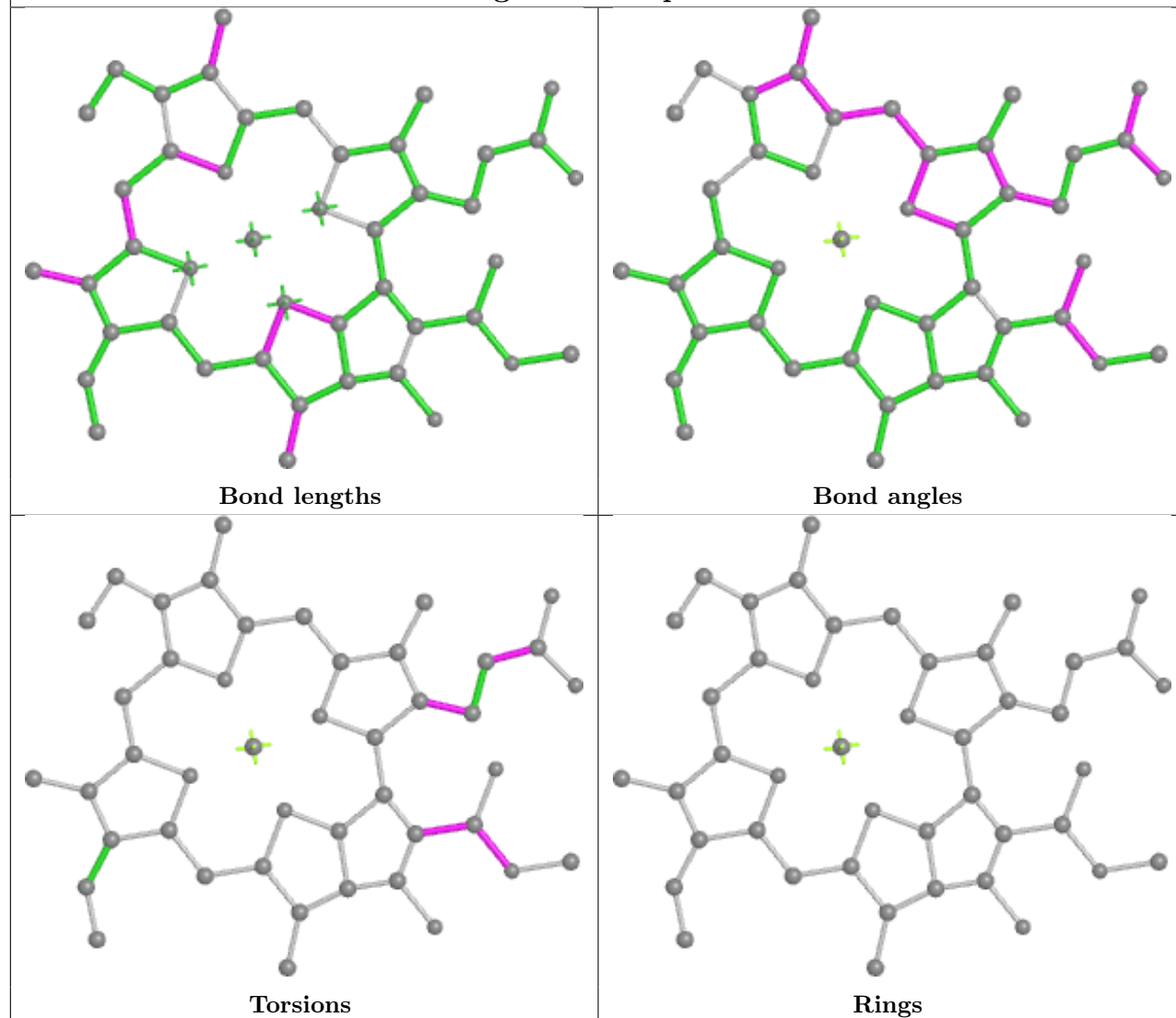
Rings



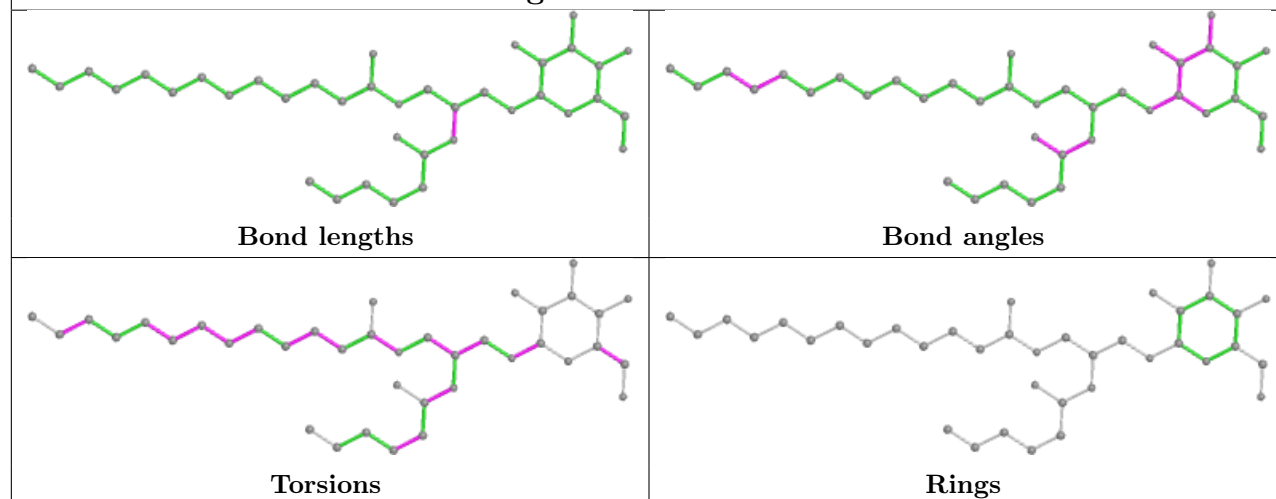


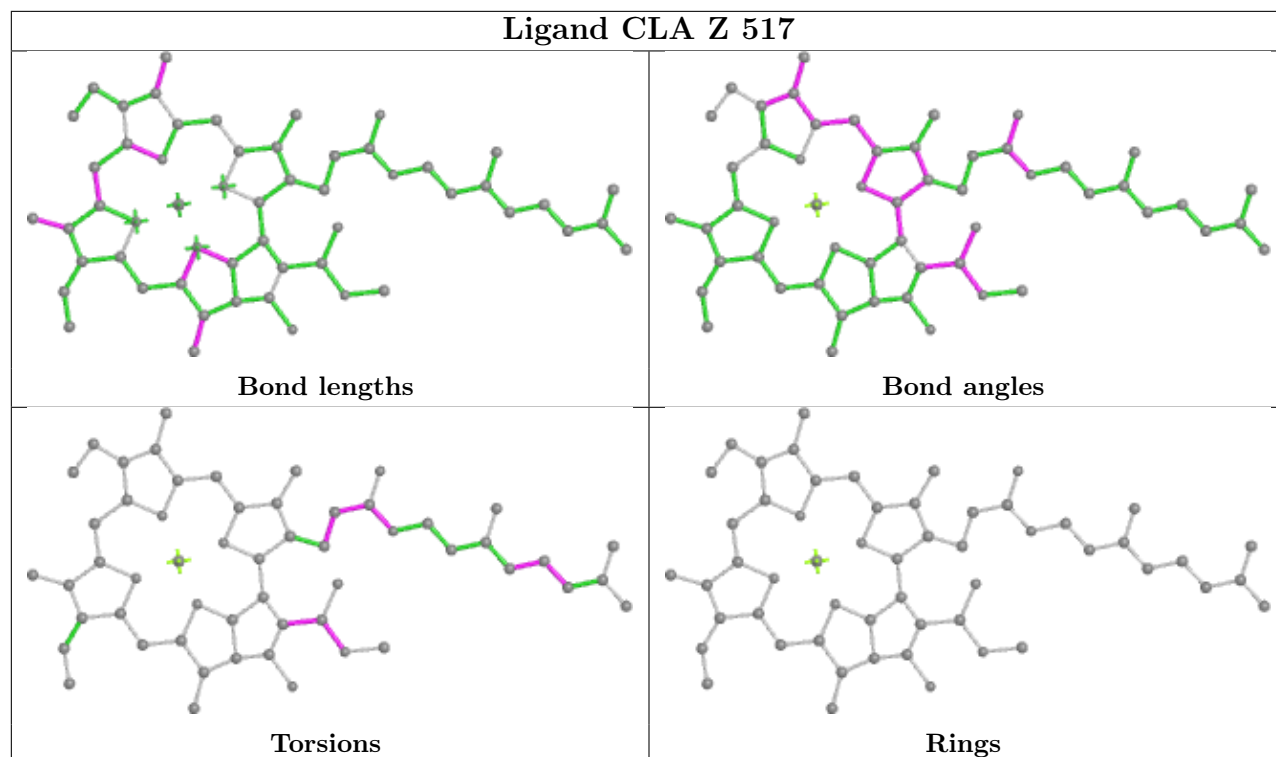
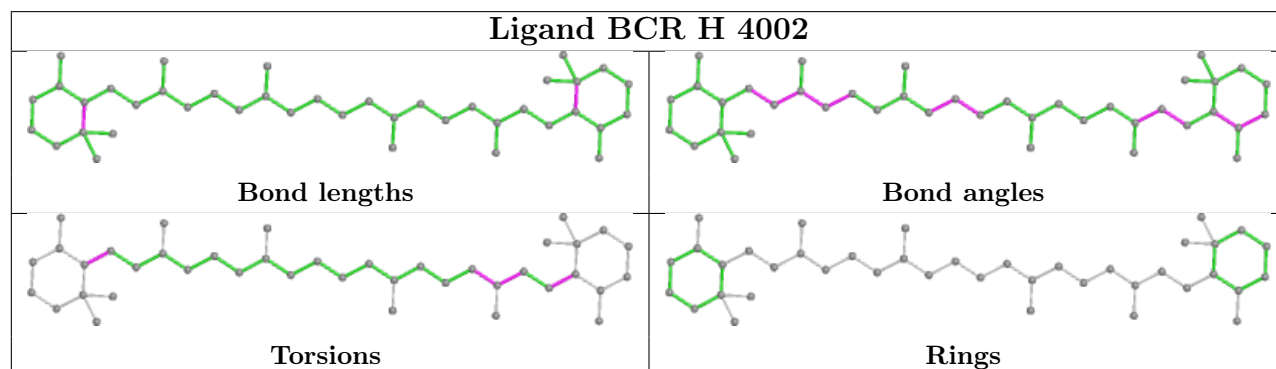


## Ligand CLA q 512

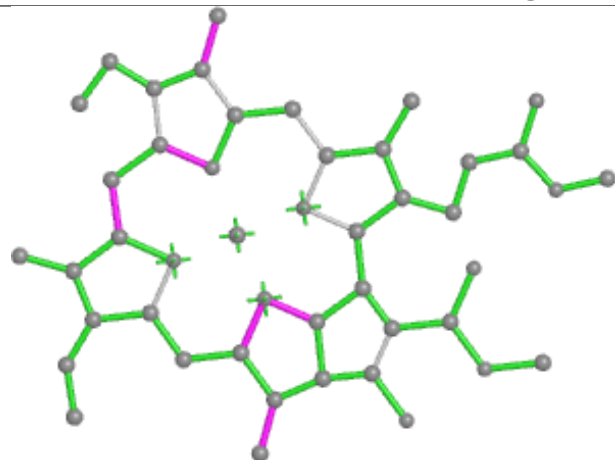


## Ligand LMG H 852

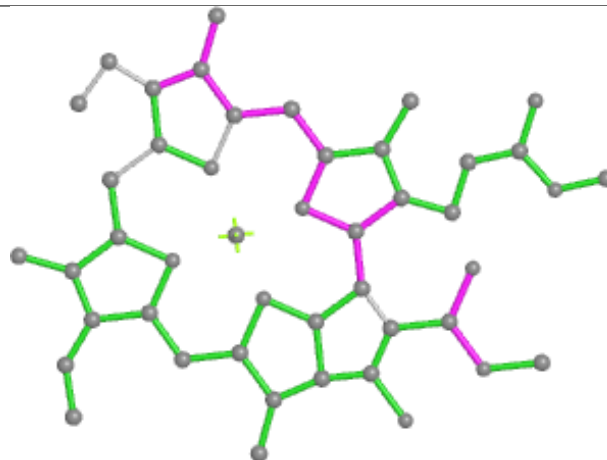


**Ligand CLA Z 517****Ligand BCR H 4002**

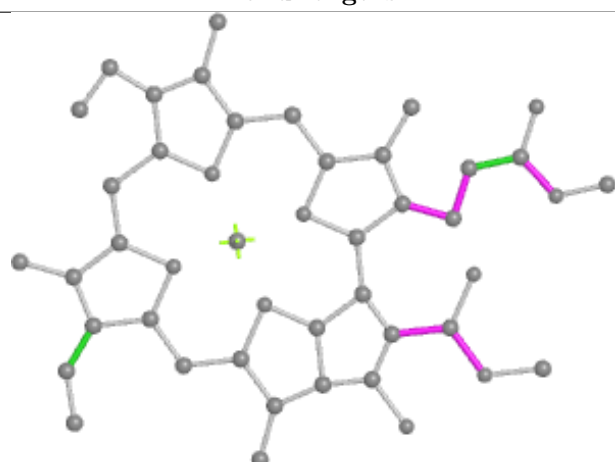
## Ligand CLA s 516



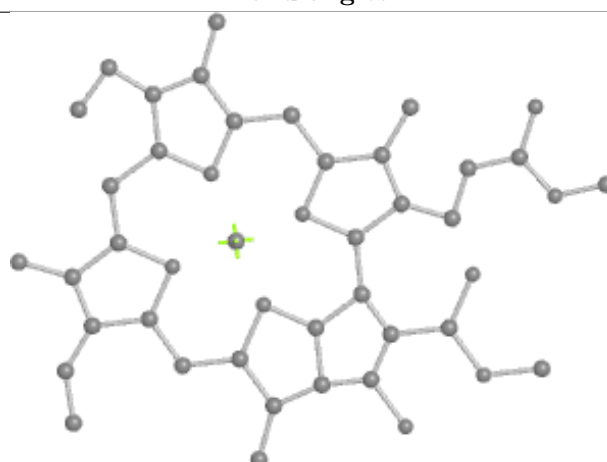
Bond lengths



Bond angles

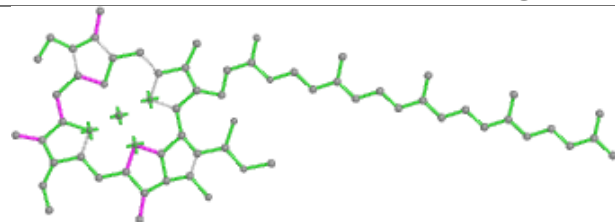


Torsions

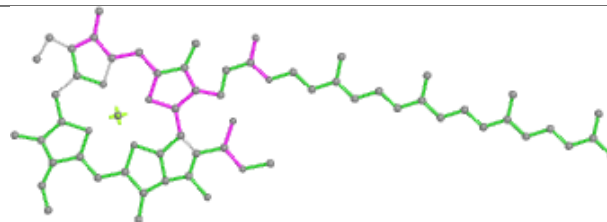


Rings

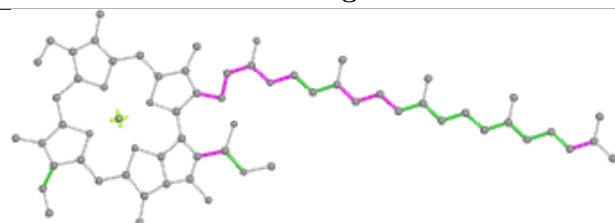
## Ligand CLA l 1503



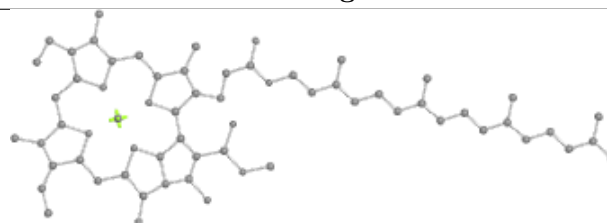
Bond lengths



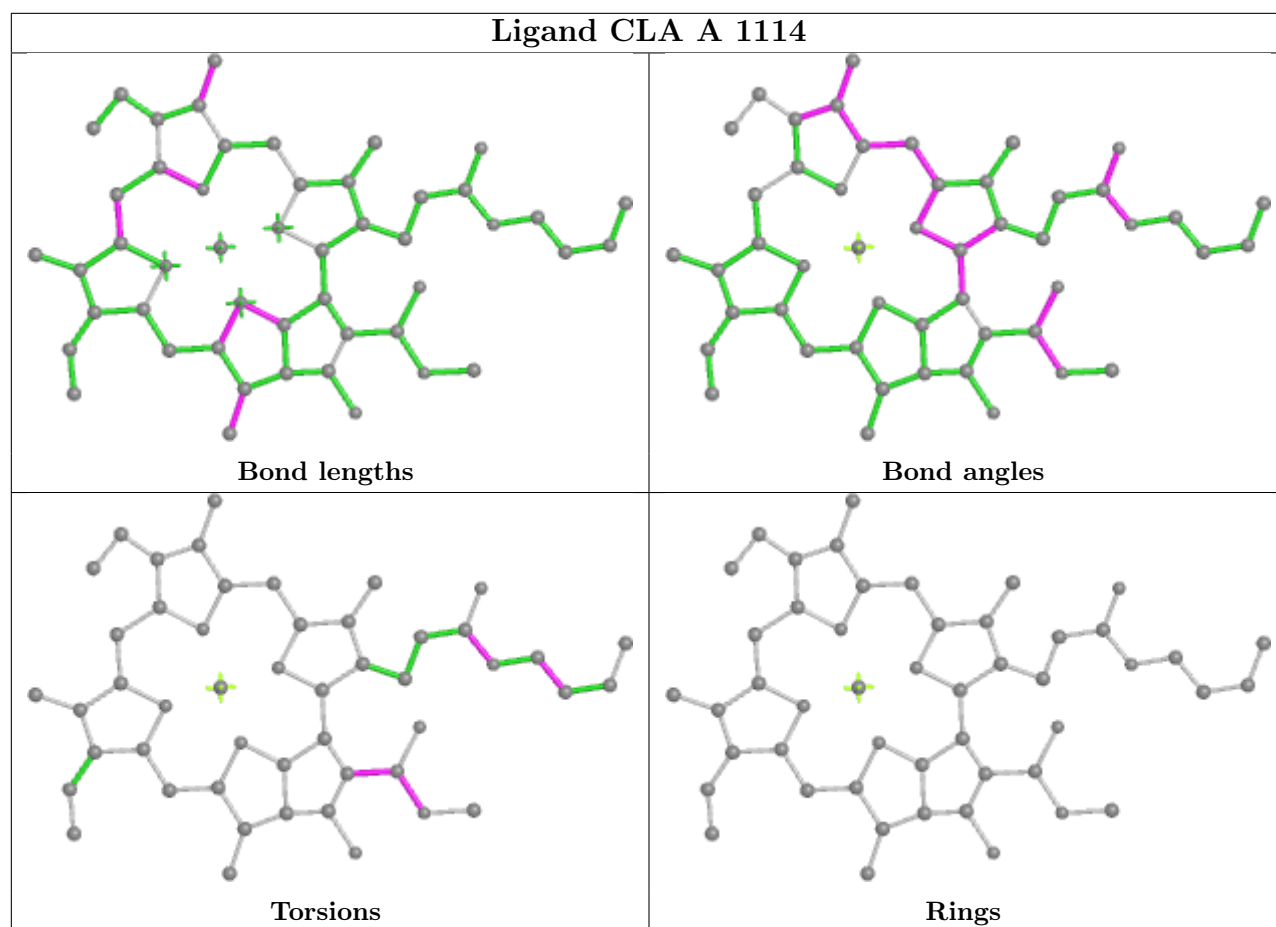
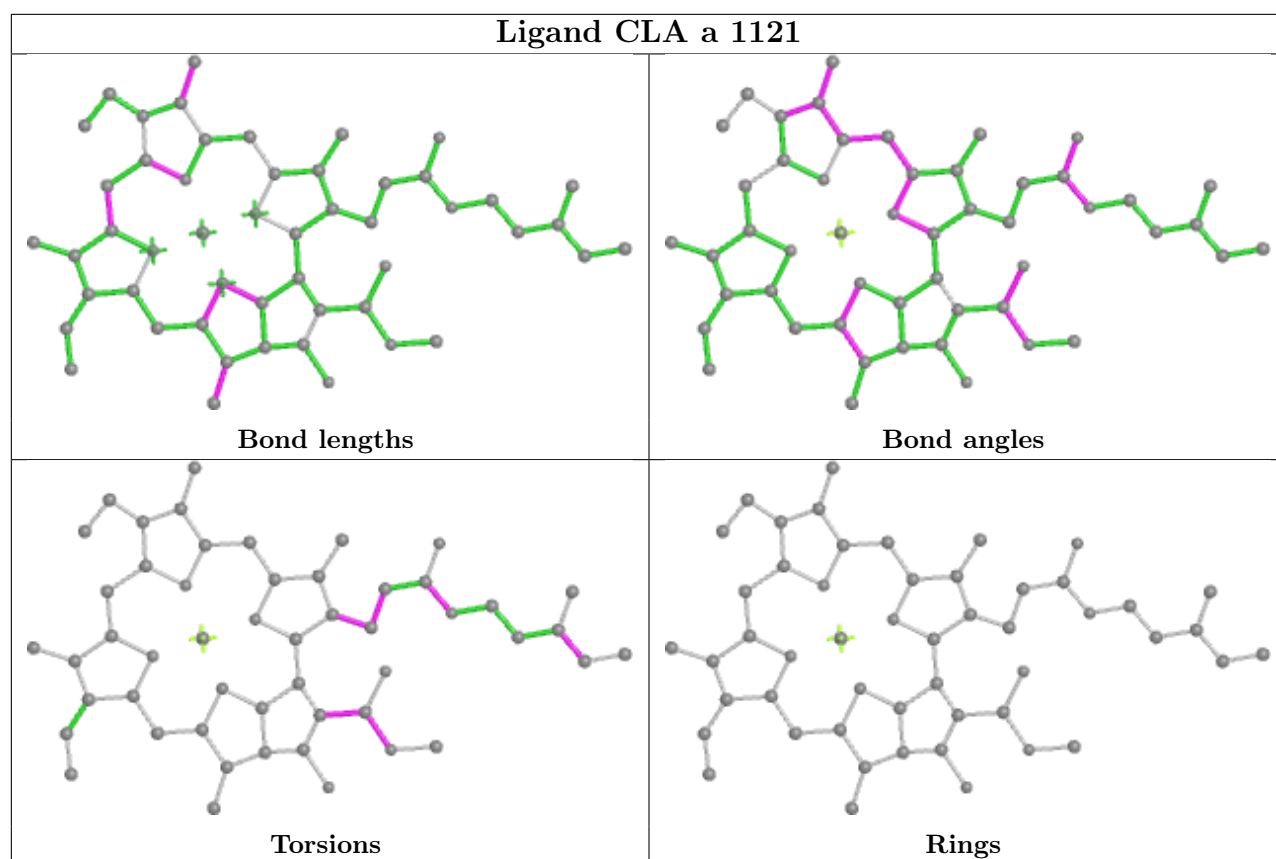
Bond angles

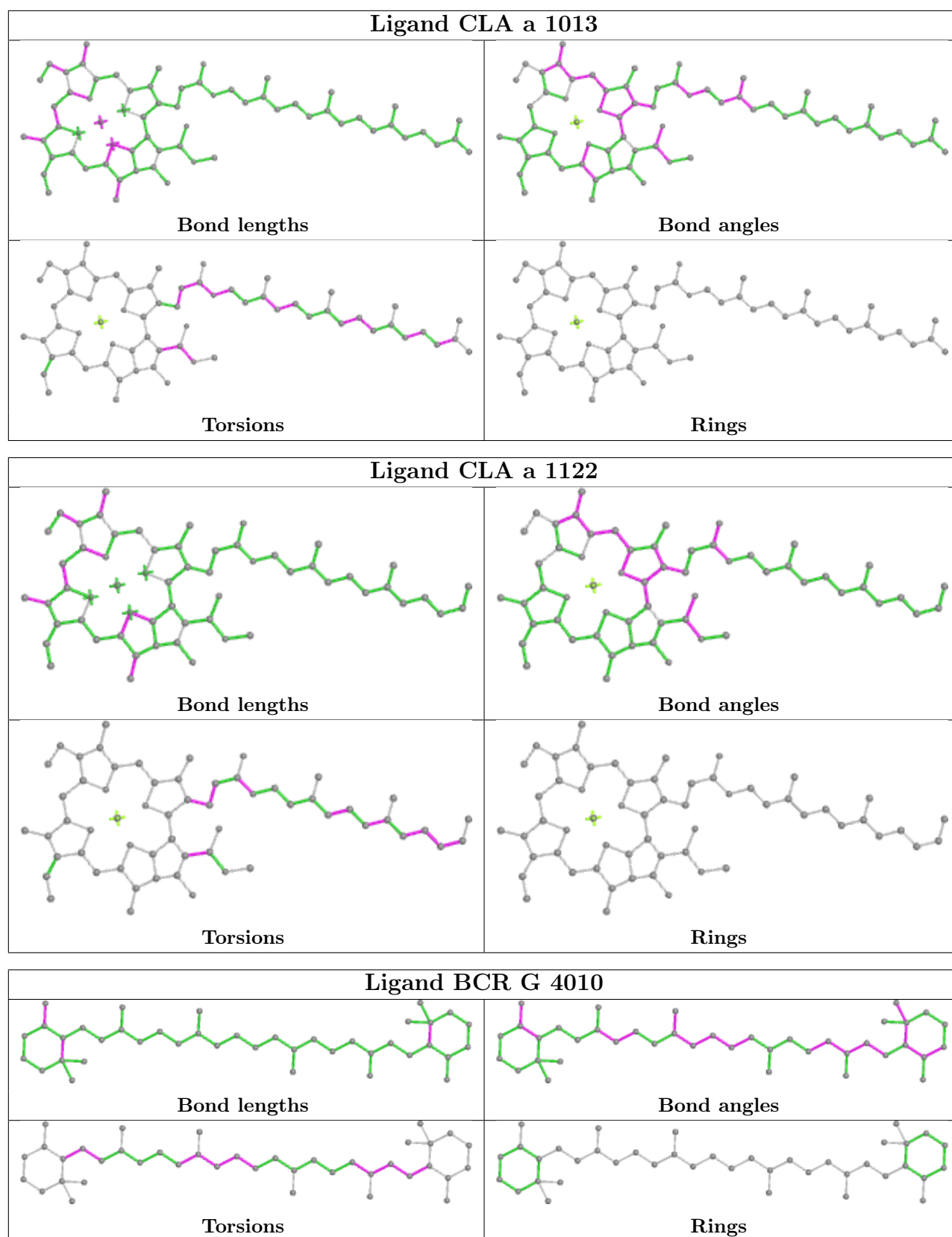


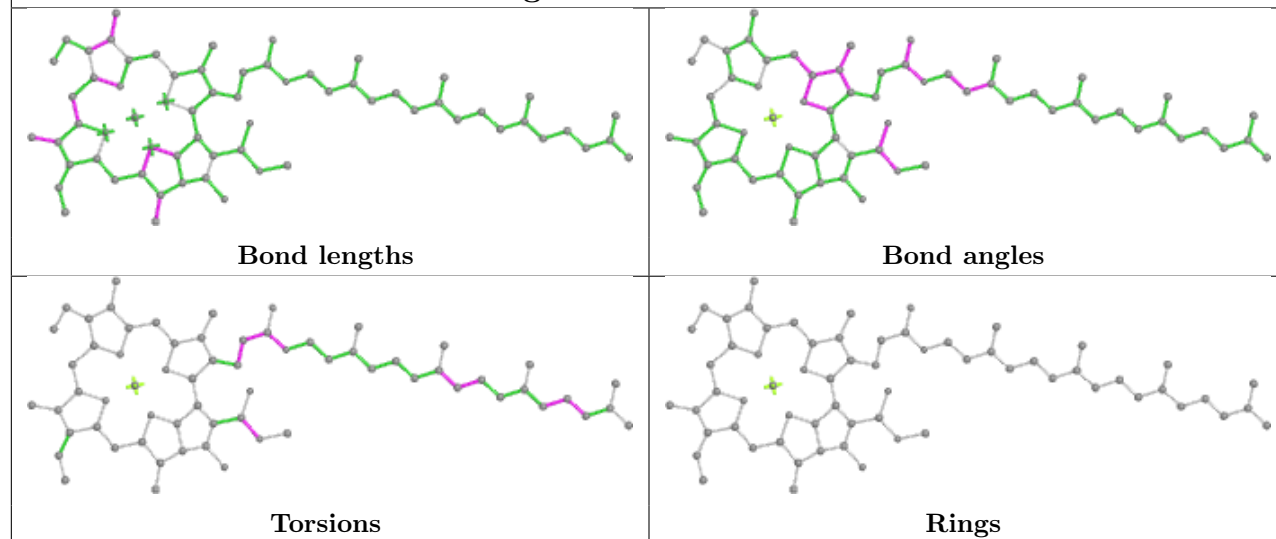
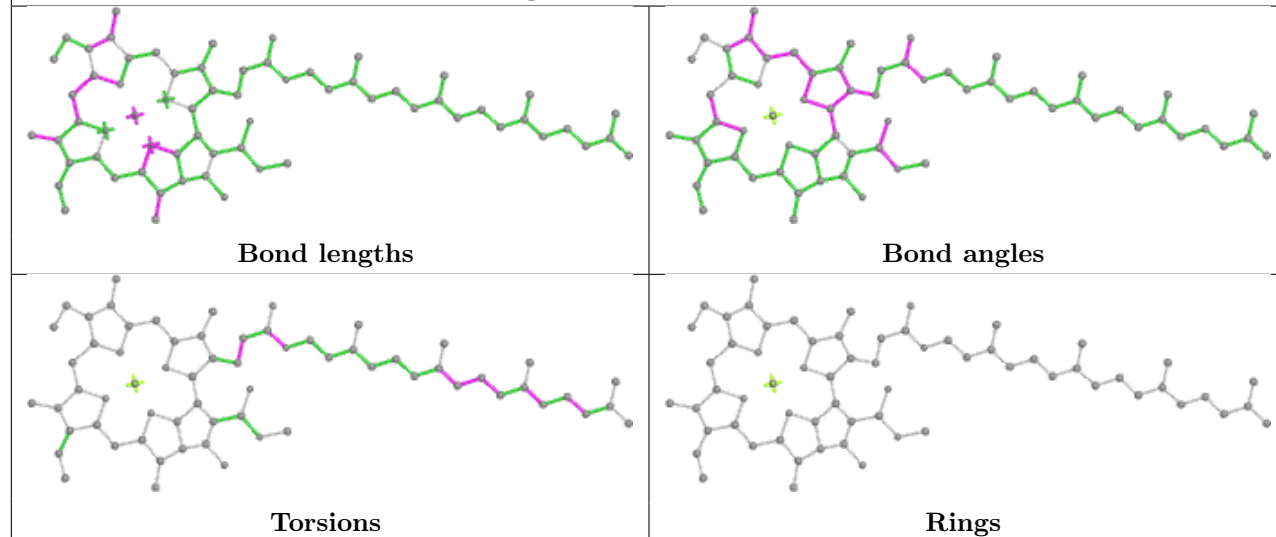
Torsions

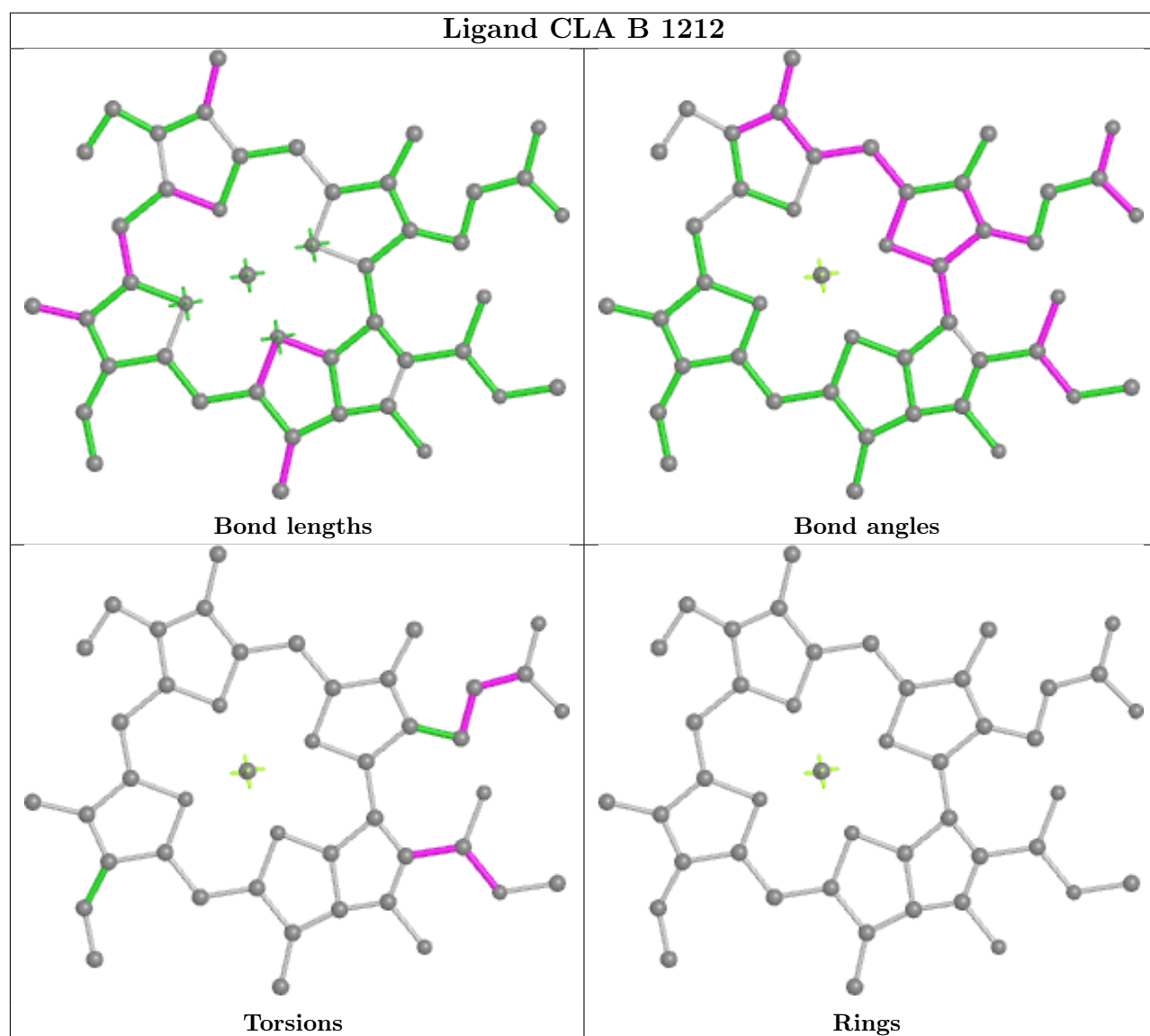


Rings



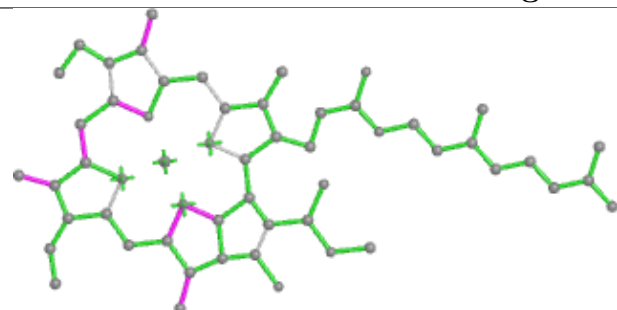


**Ligand CLA B 1021****Ligand CLA A 1128**

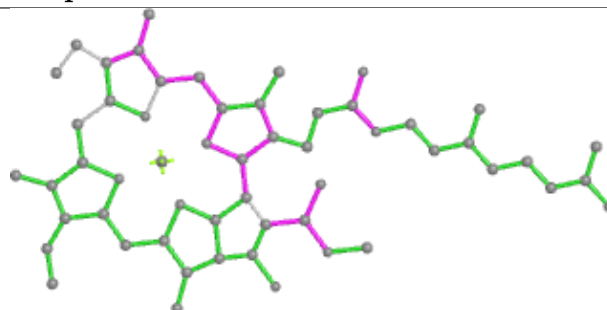




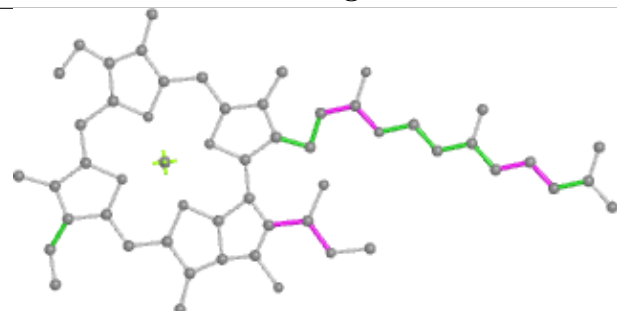
## Ligand CLA q 517



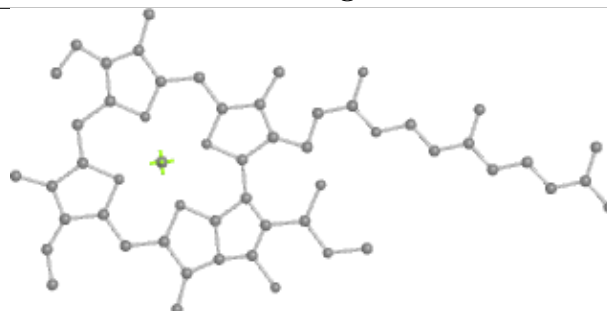
Bond lengths



Bond angles

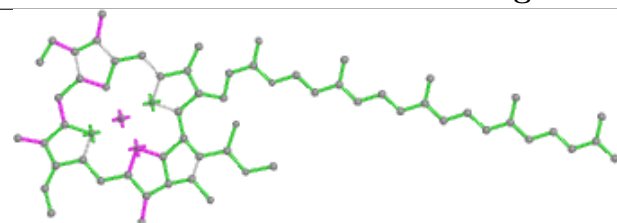


Torsions

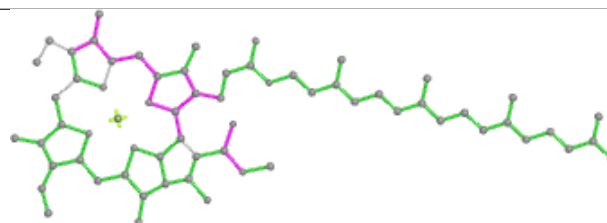


Rings

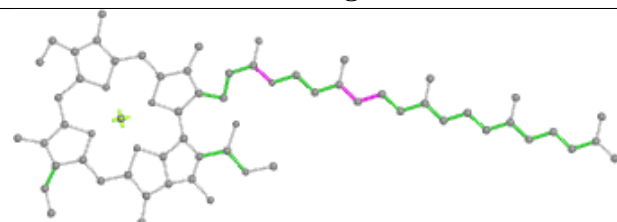
## Ligand CLA a 1130



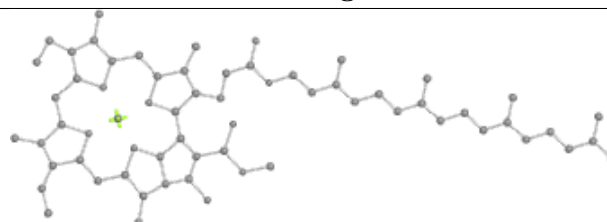
Bond lengths



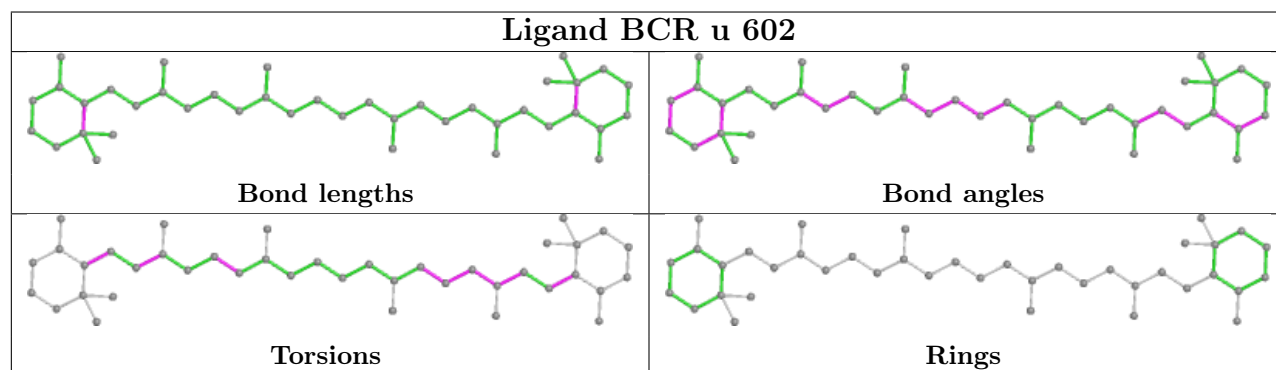
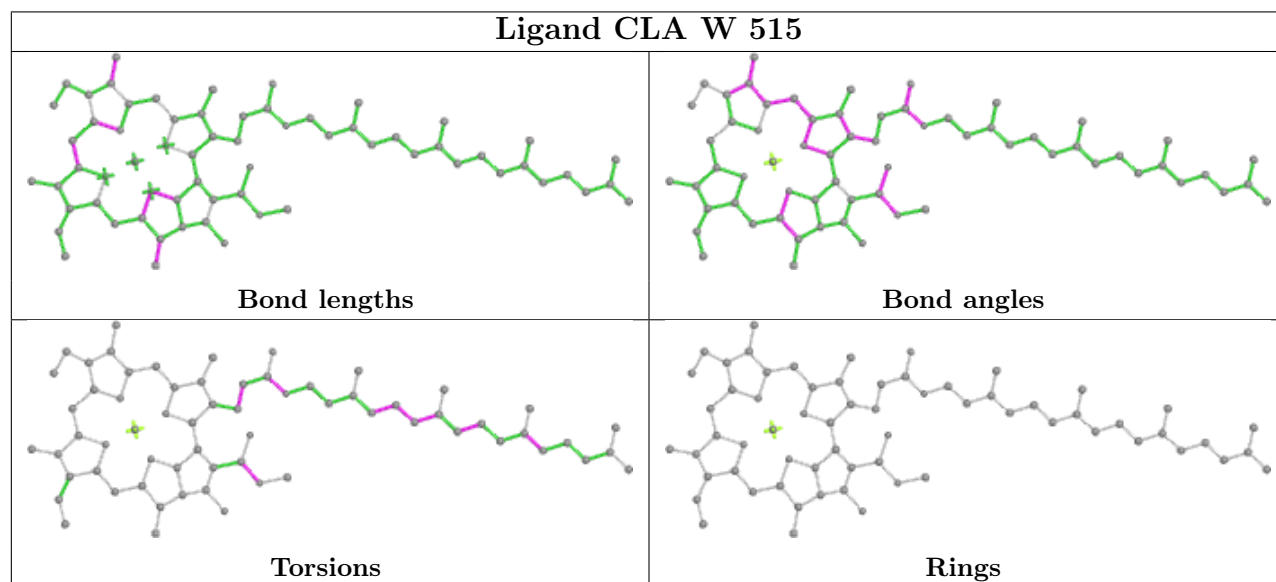
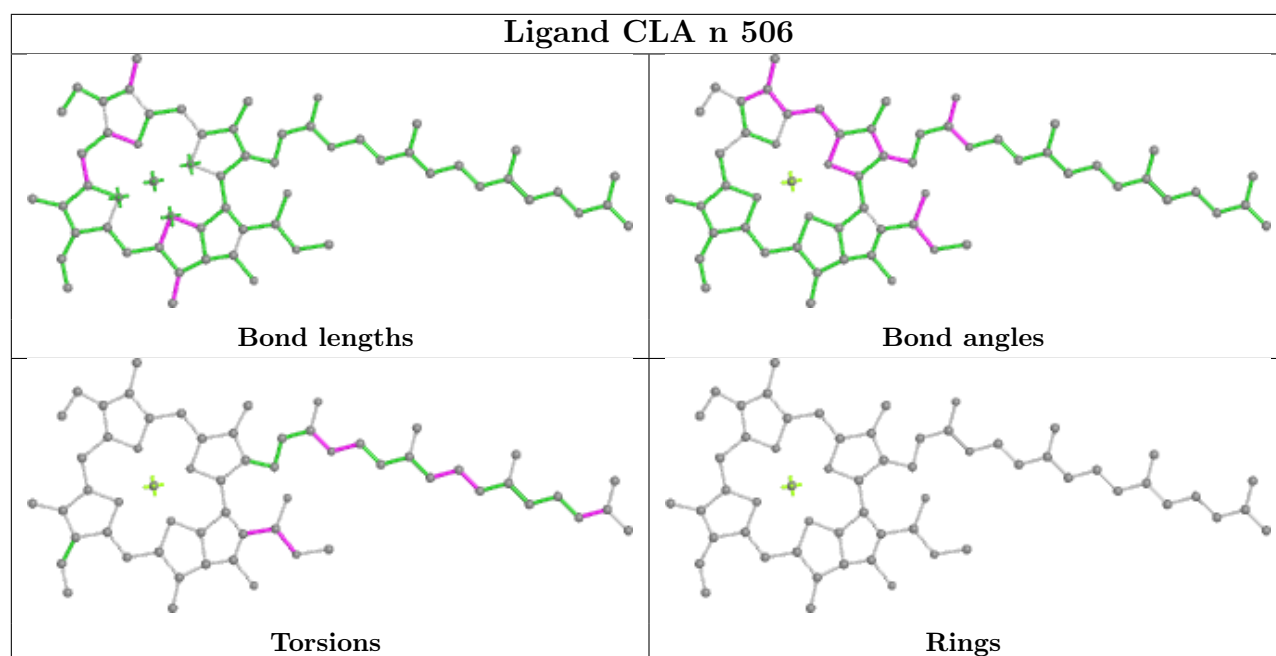
Bond angles

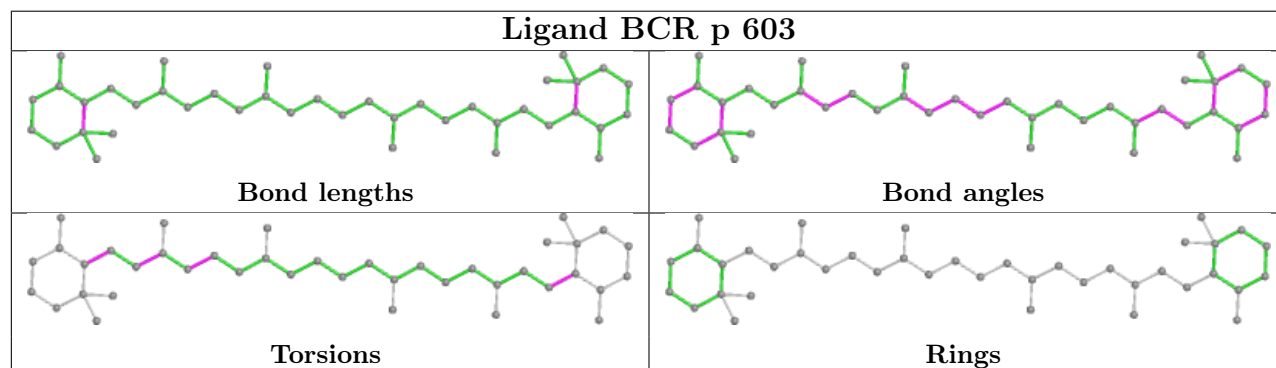
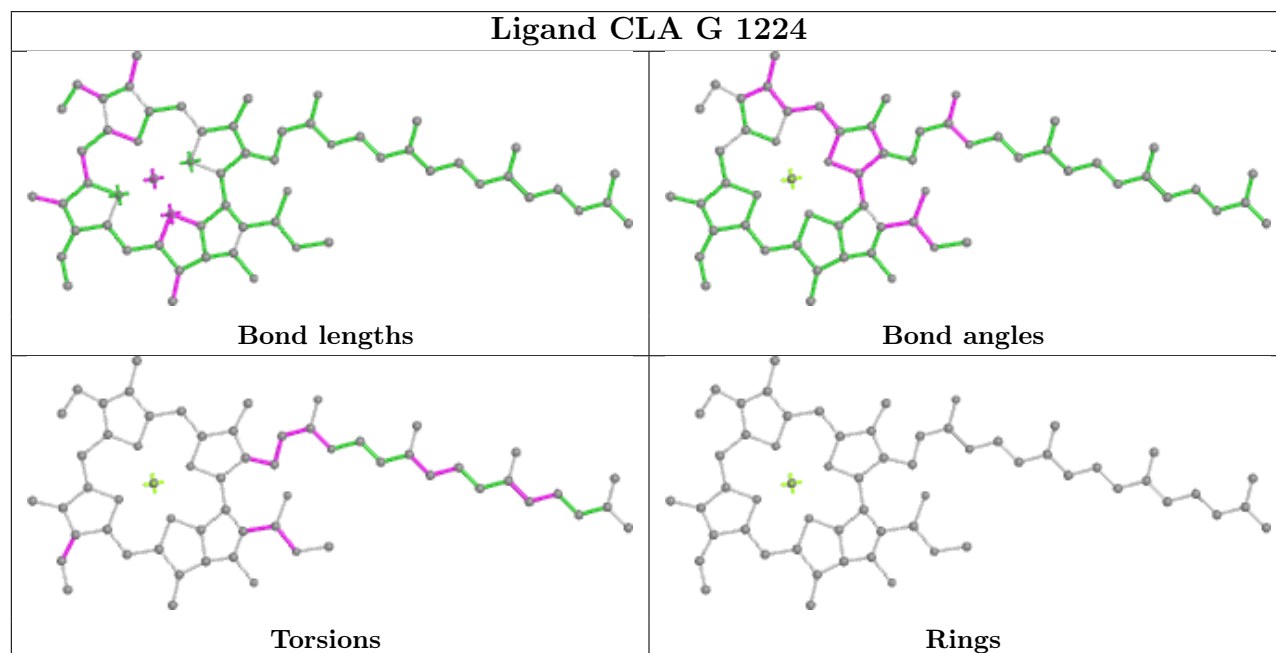
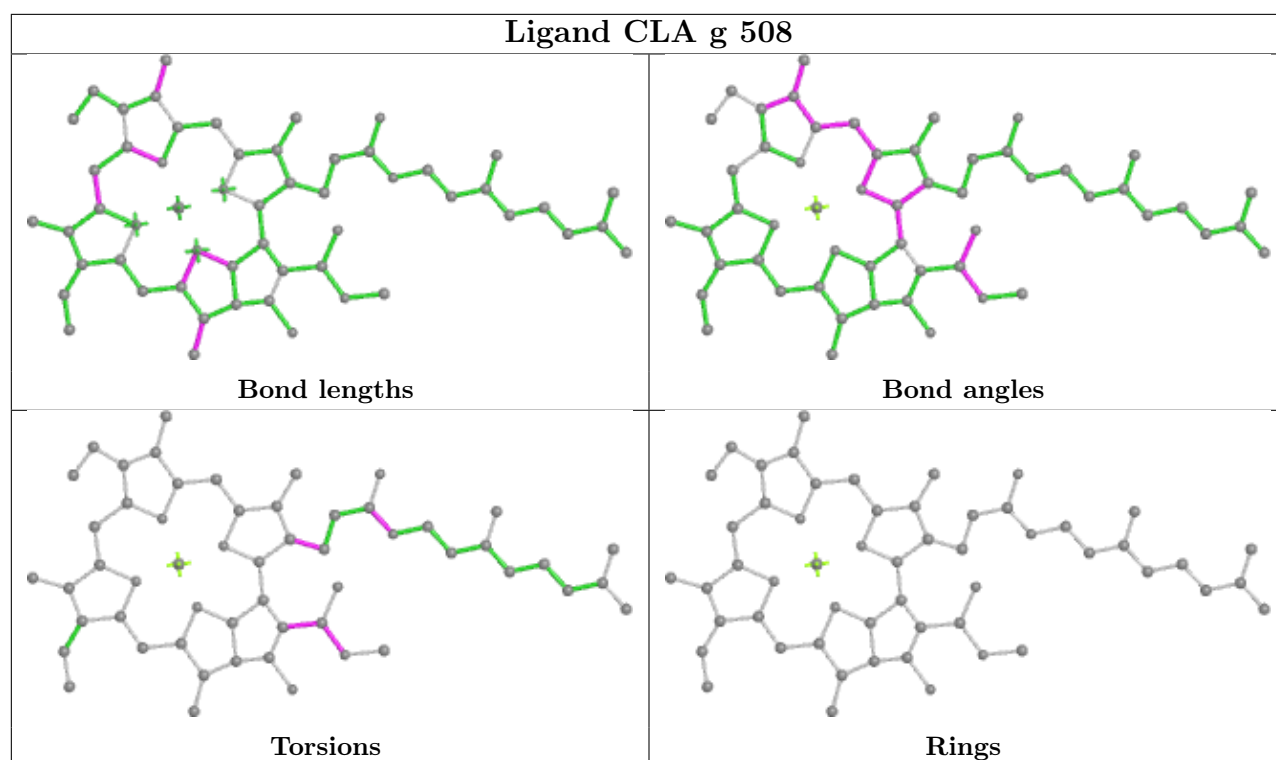


Torsions

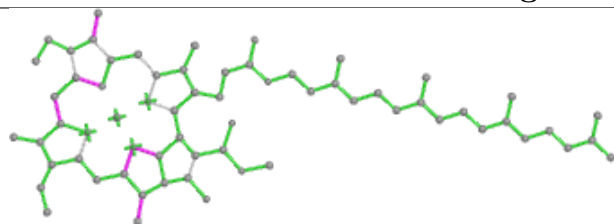


Rings

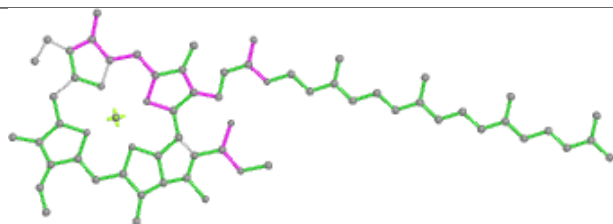




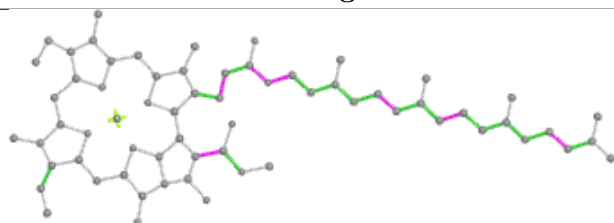
## Ligand CLA s 515



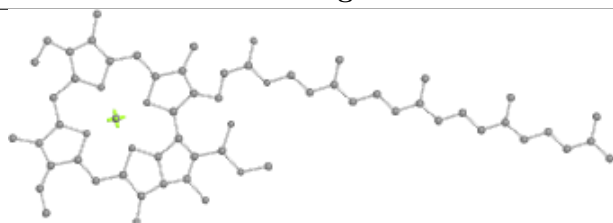
Bond lengths



Bond angles

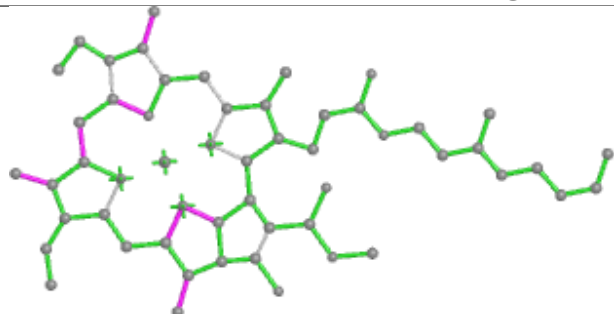


Torsions

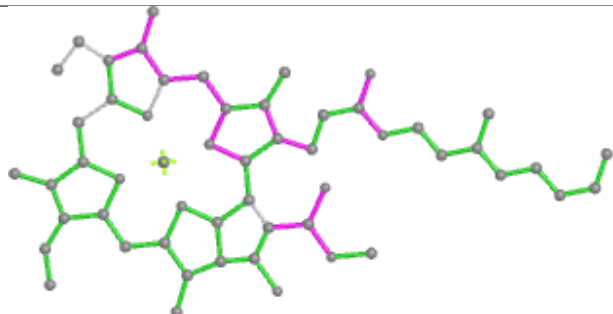


Rings

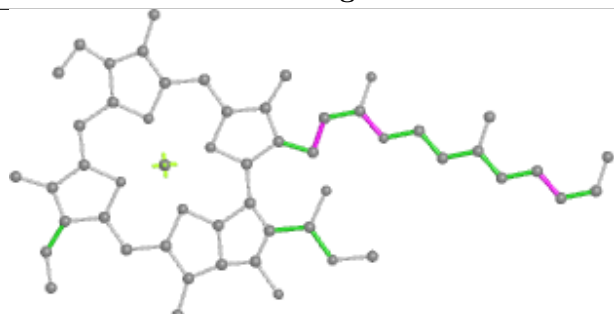
## Ligand CLA H 1110



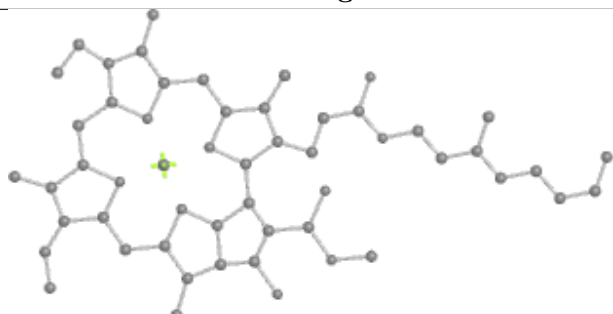
Bond lengths



Bond angles

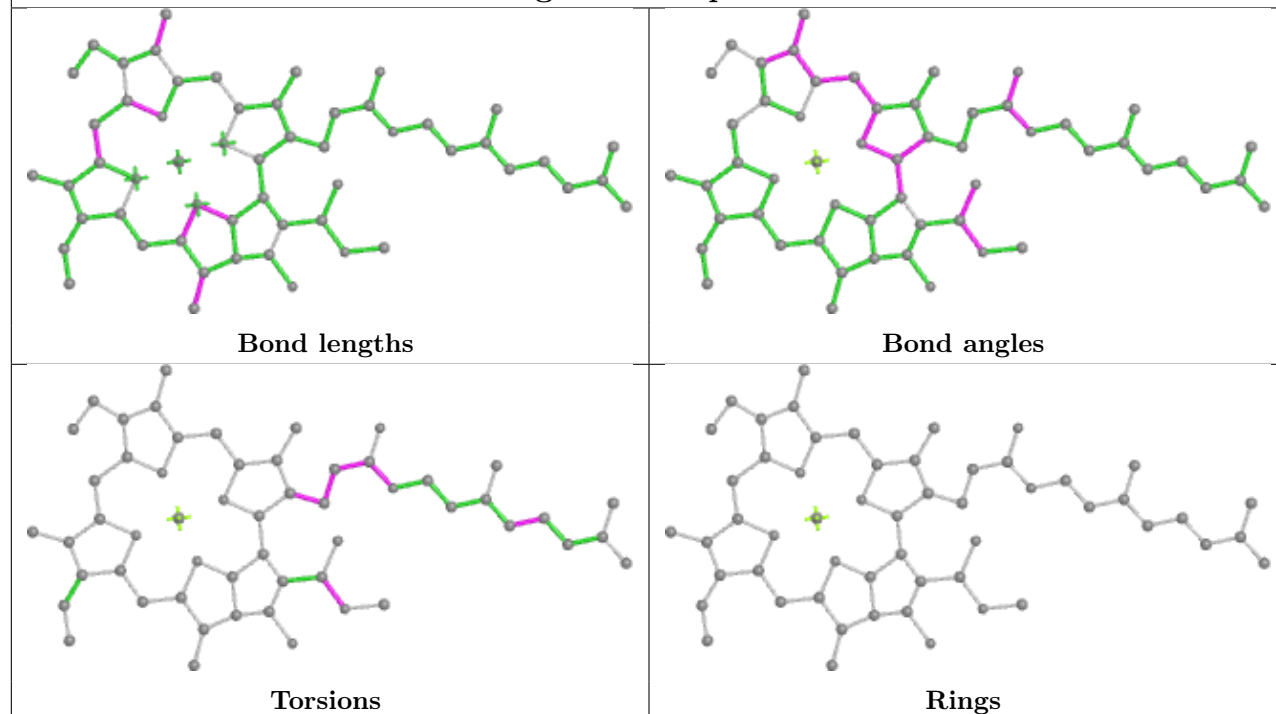


Torsions

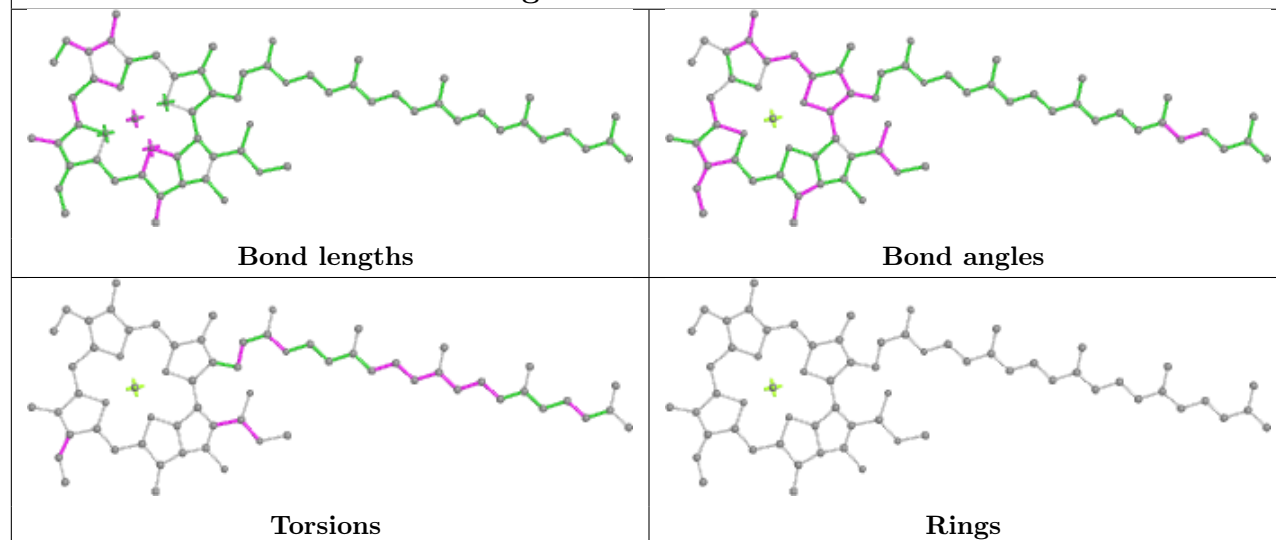


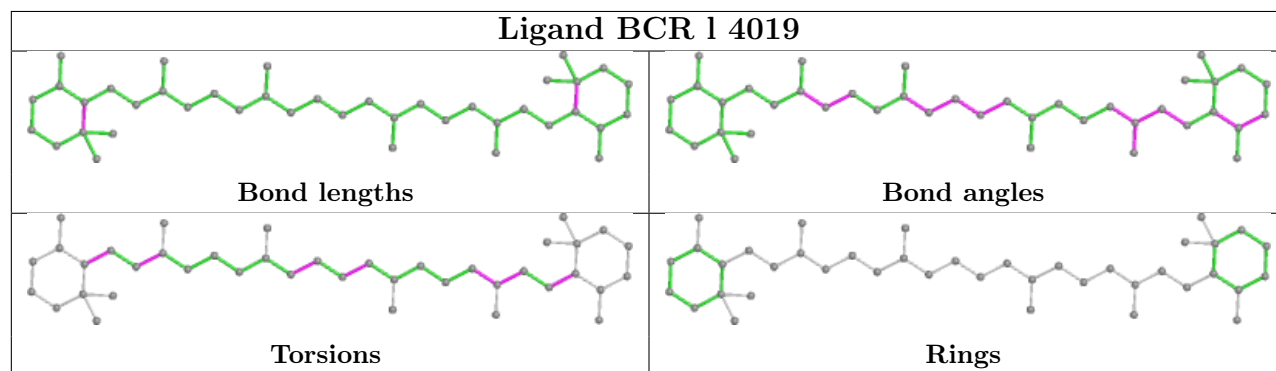
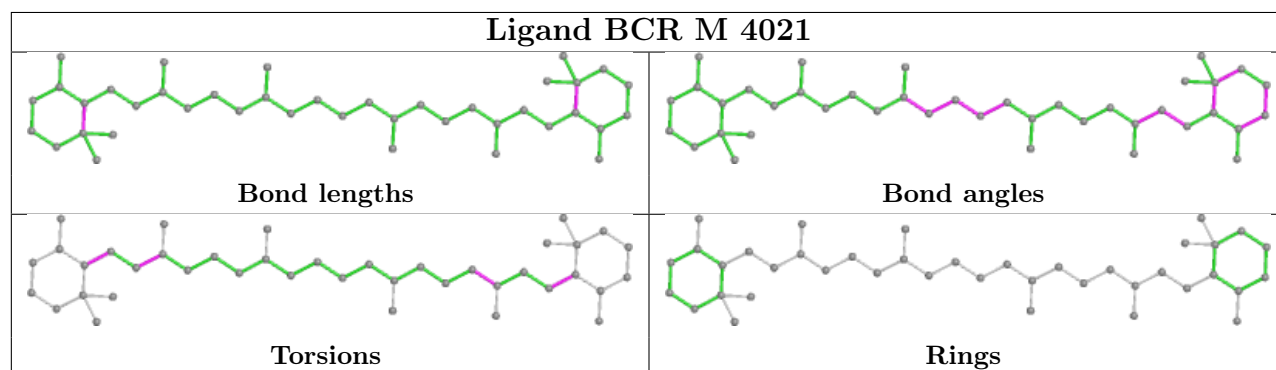
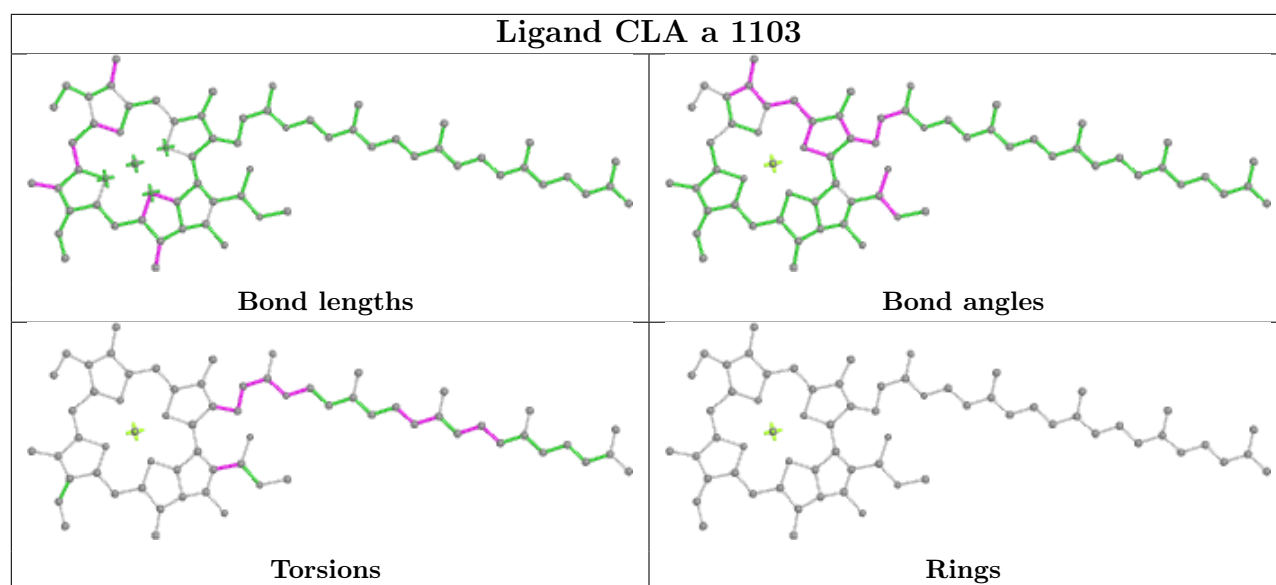
Rings

## Ligand CLA p 508

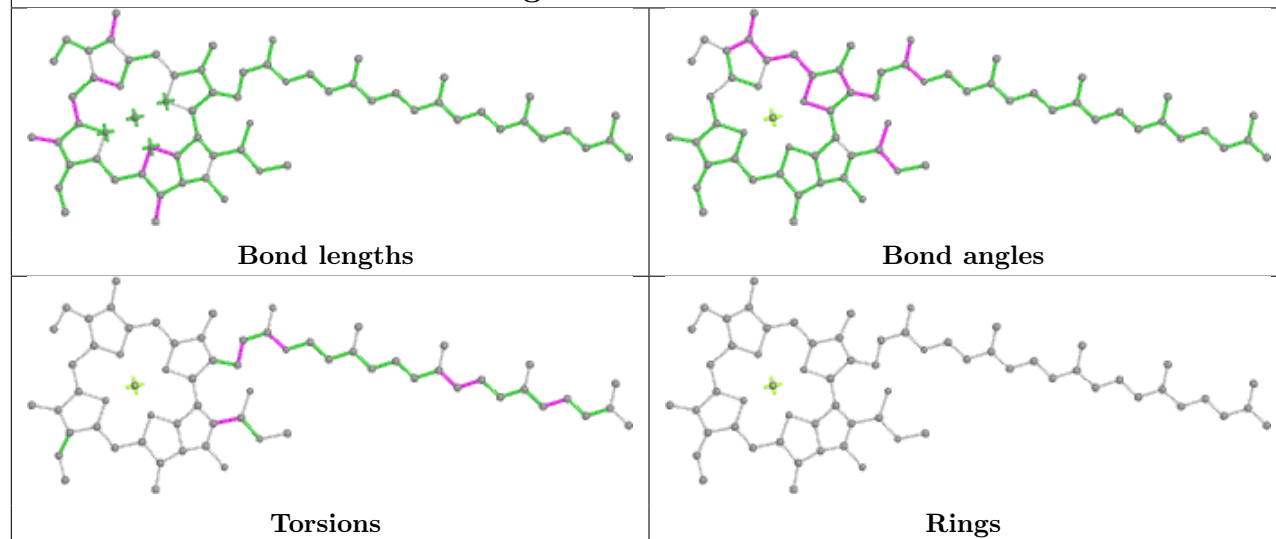


## Ligand CLA G 1023

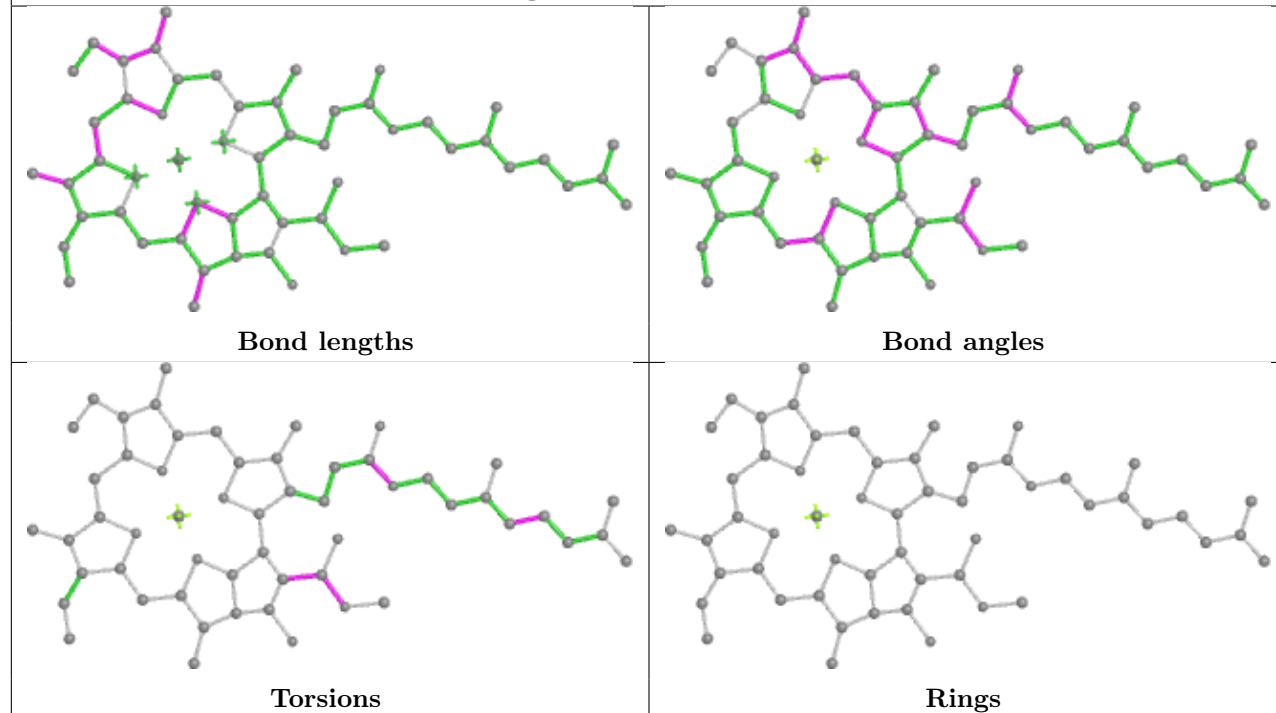


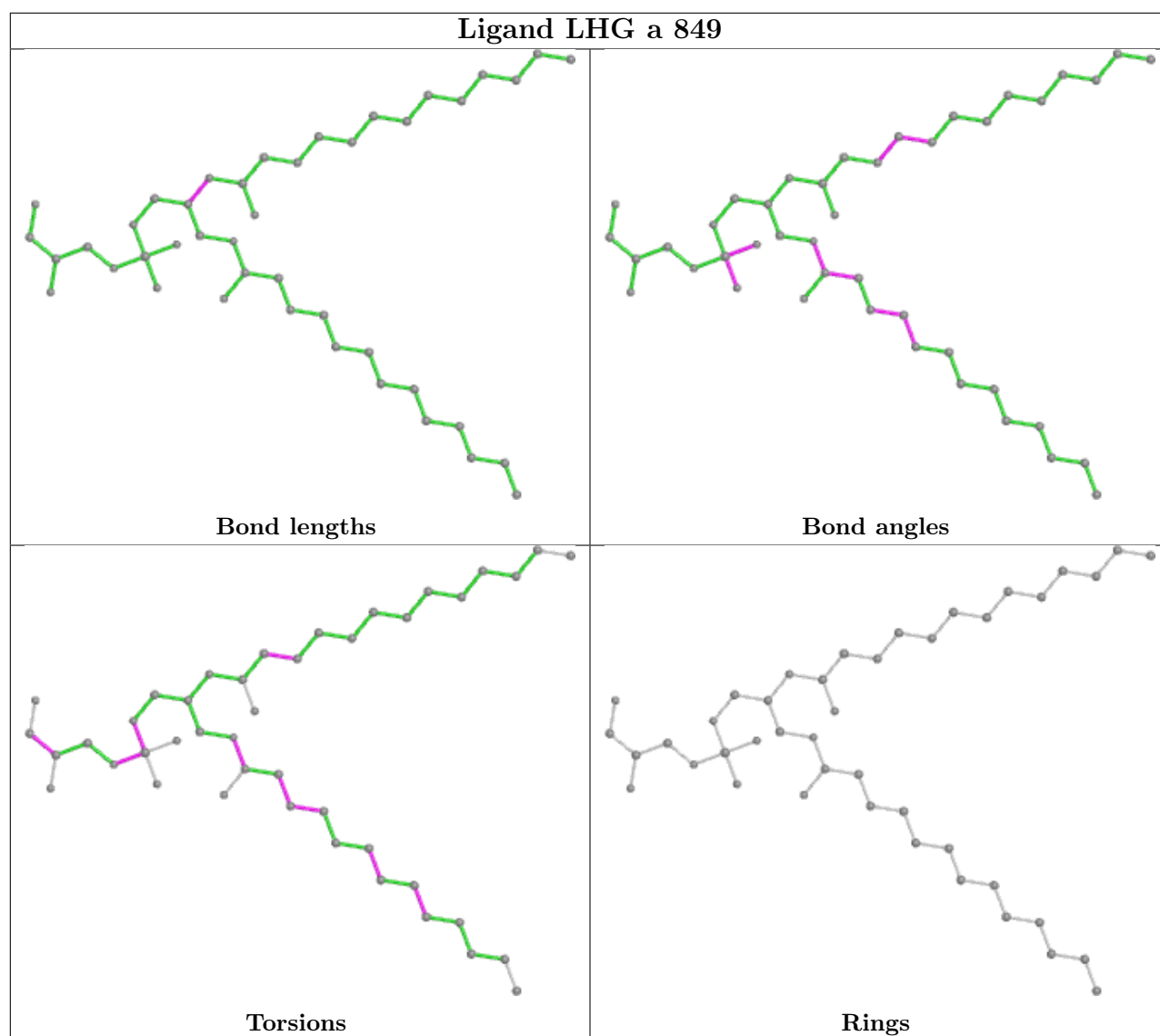


## Ligand CLA B 1211



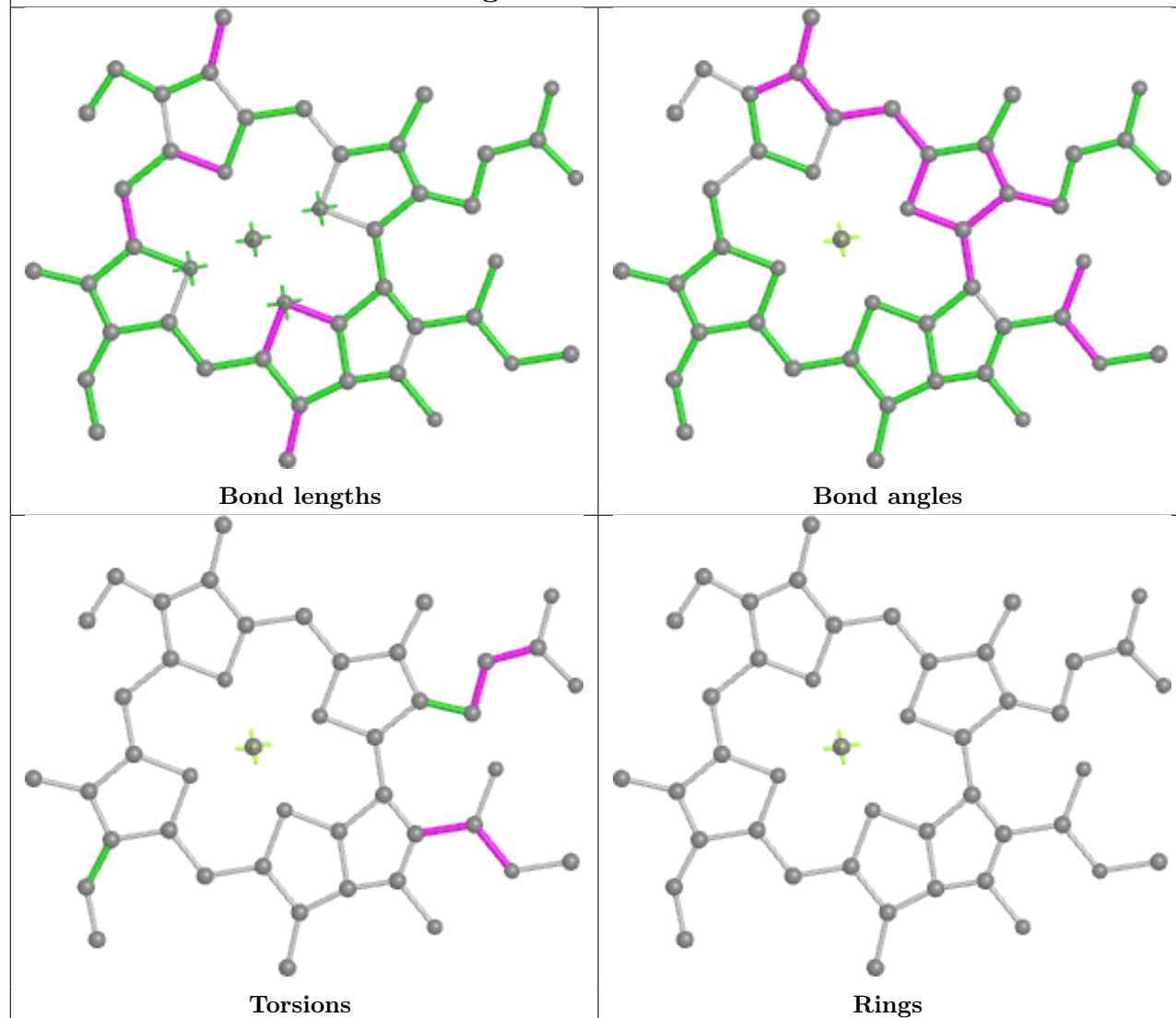
## Ligand CLA B 1222



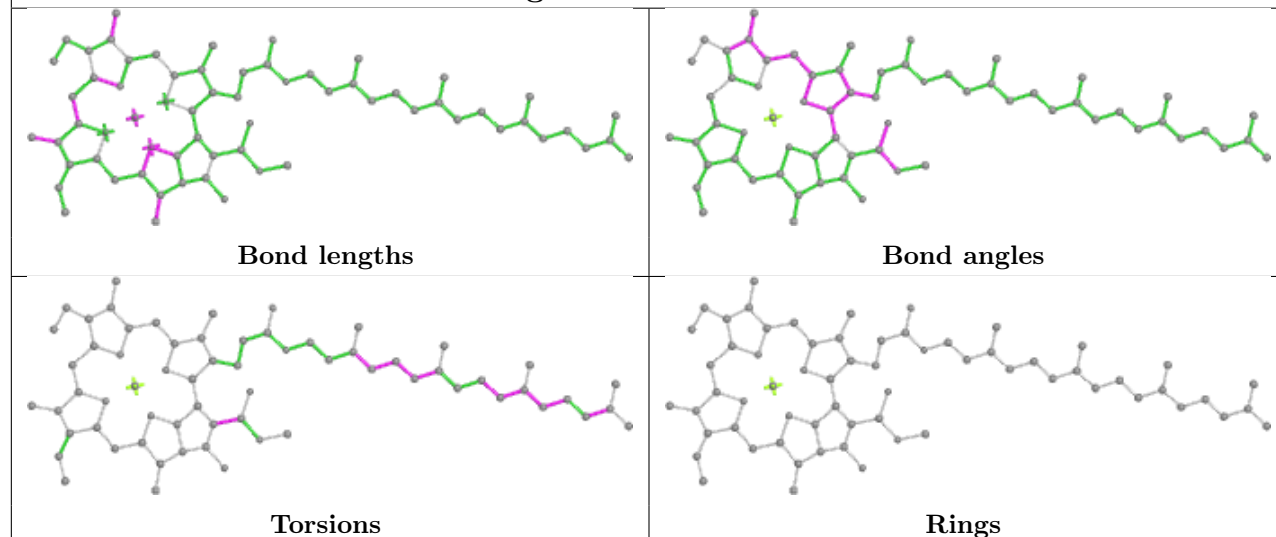


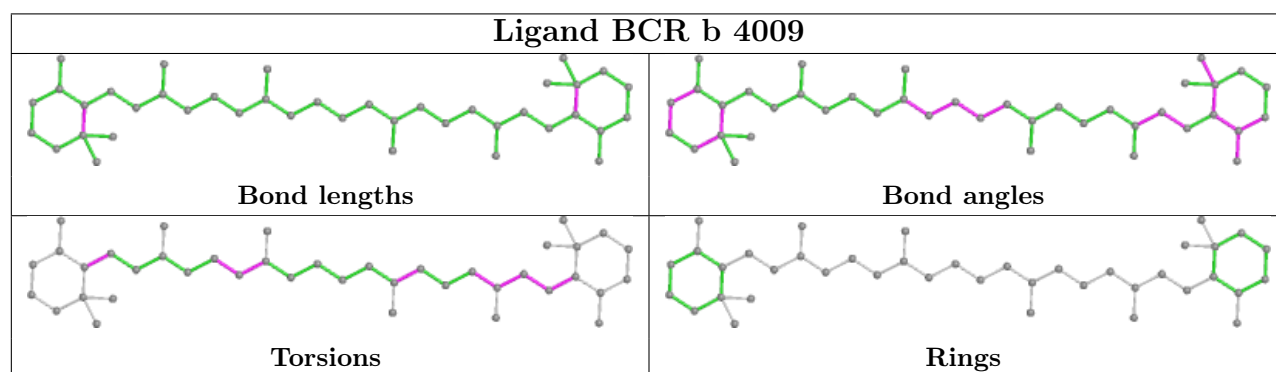
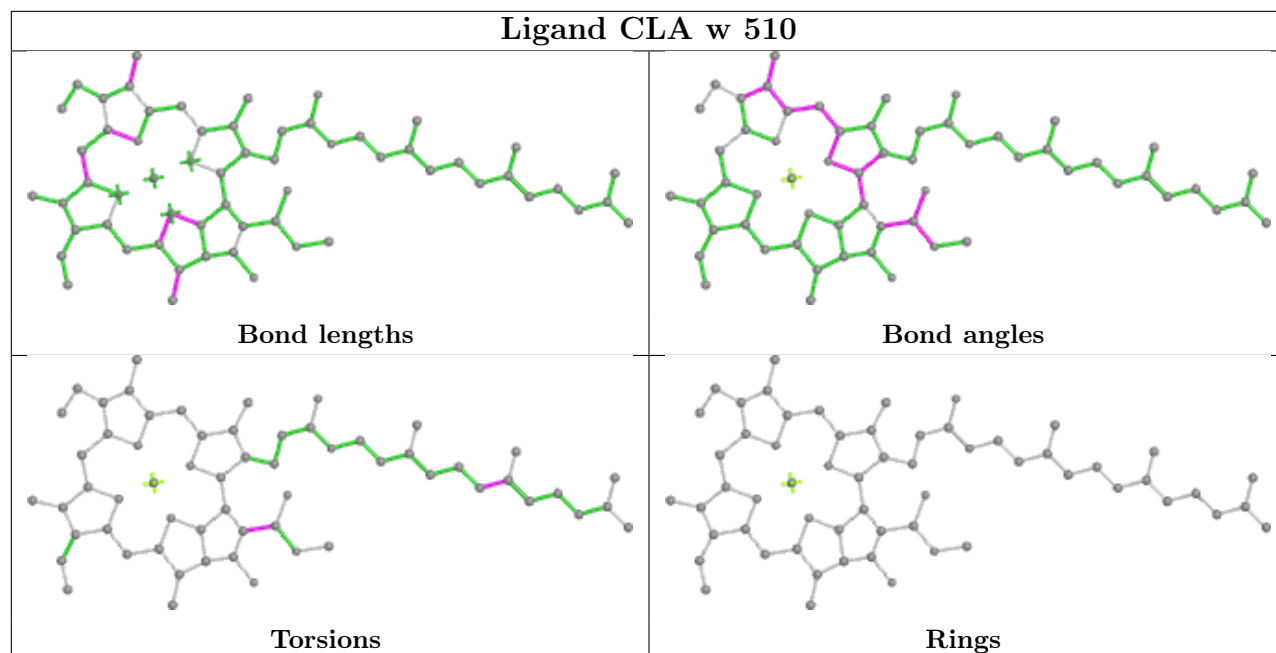
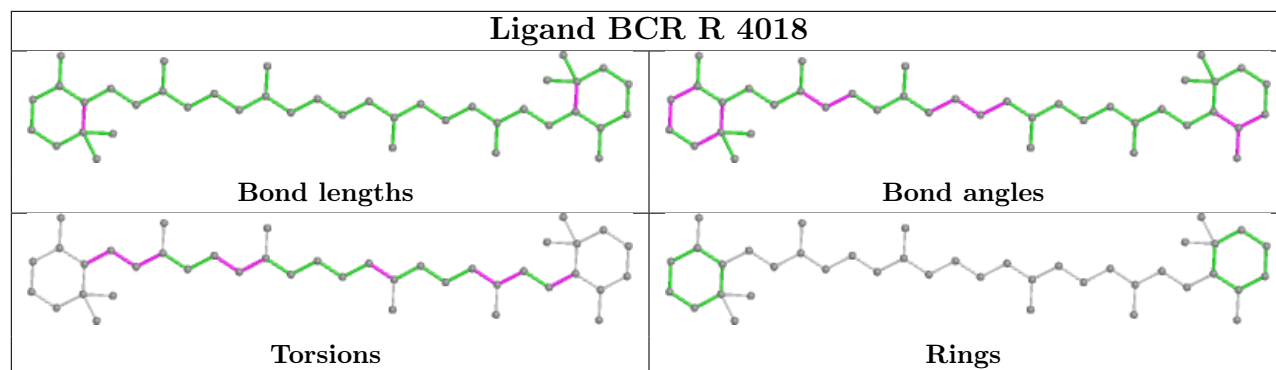


## Ligand CLA B 1219

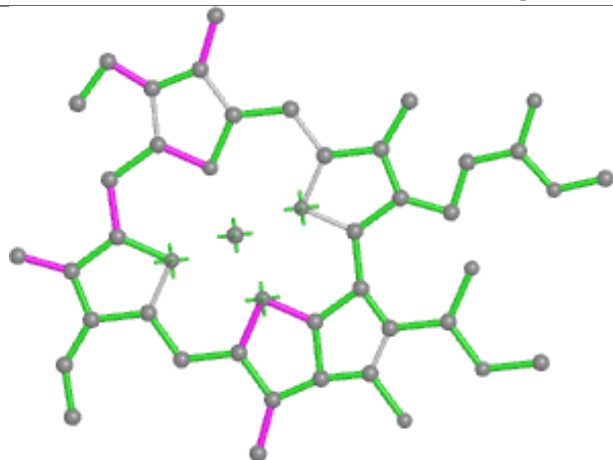


## Ligand CLA b 1223

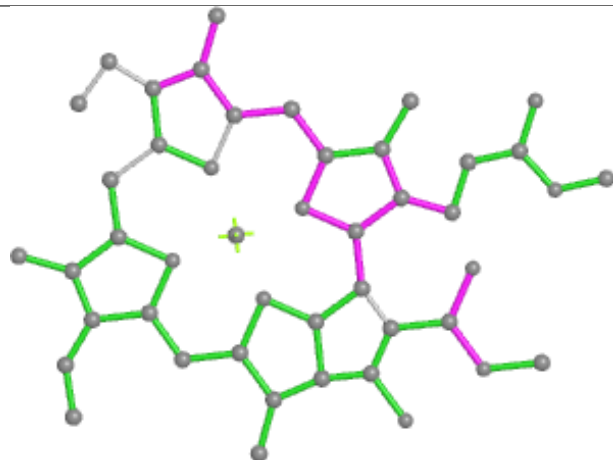




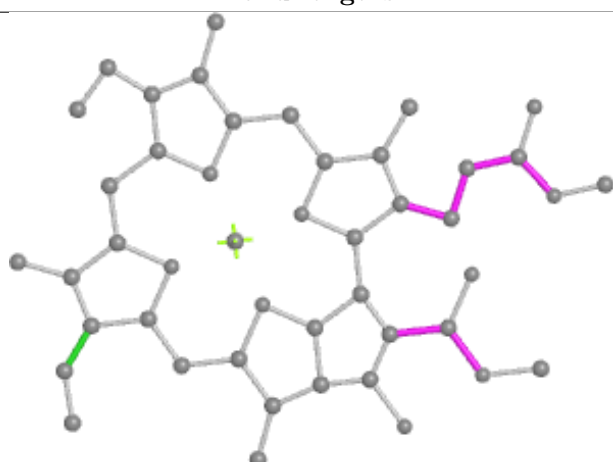
## Ligand CLA w 503



Bond lengths



Bond angles

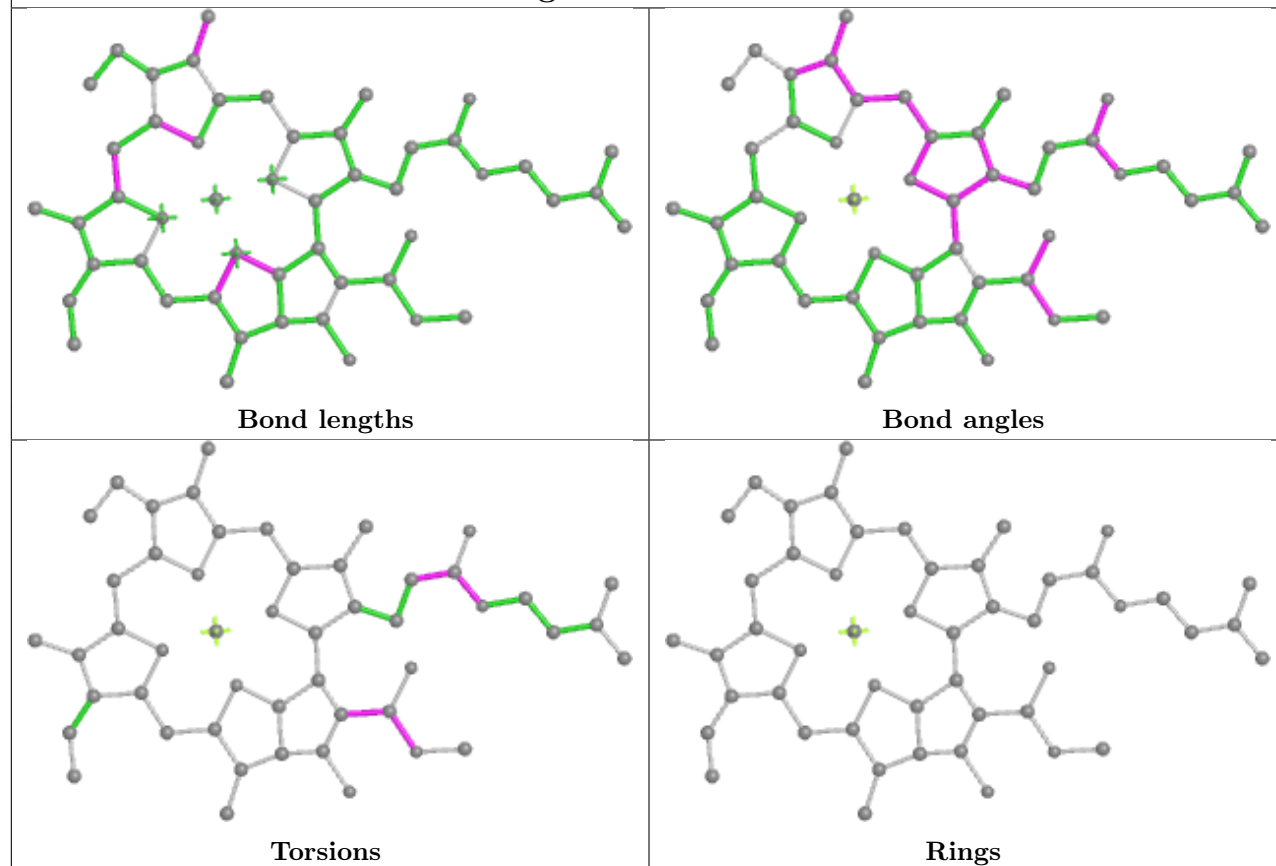


Torsions

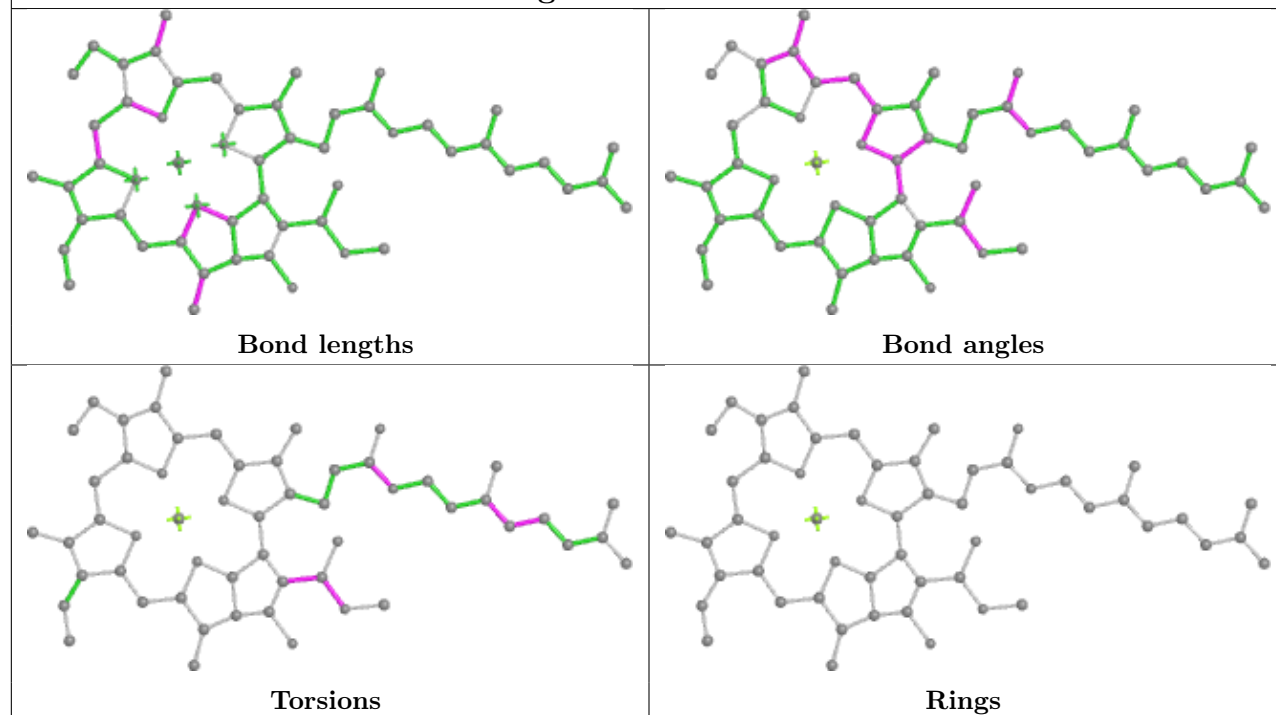


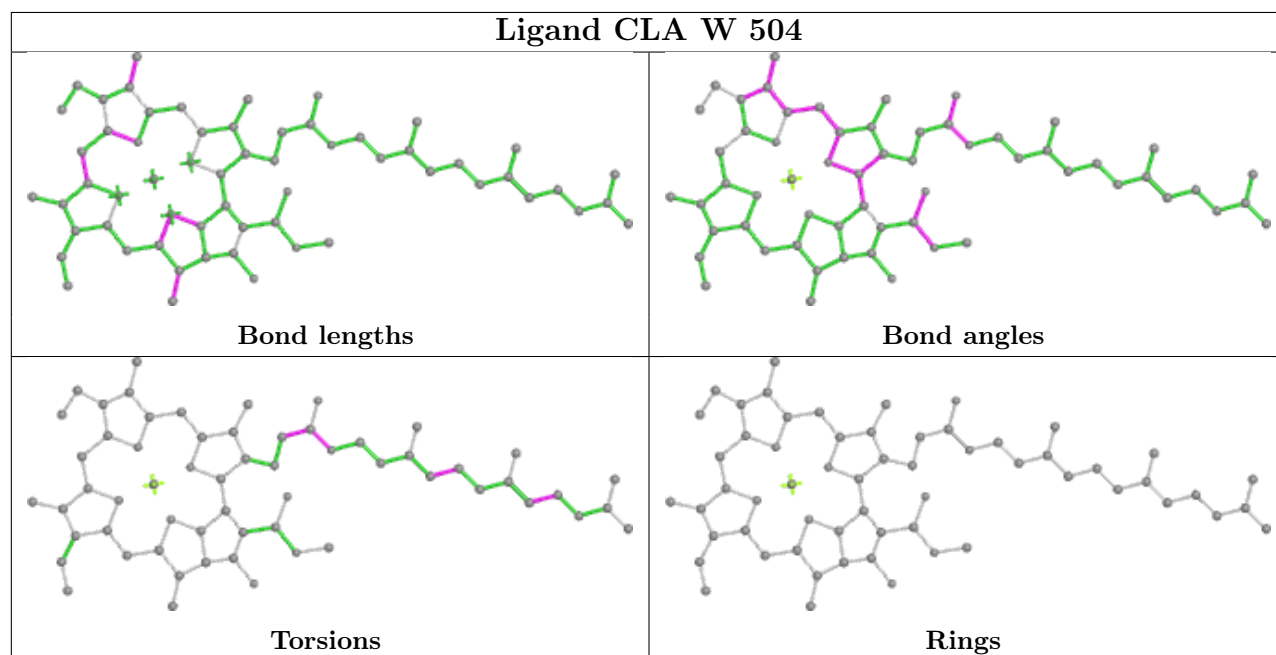
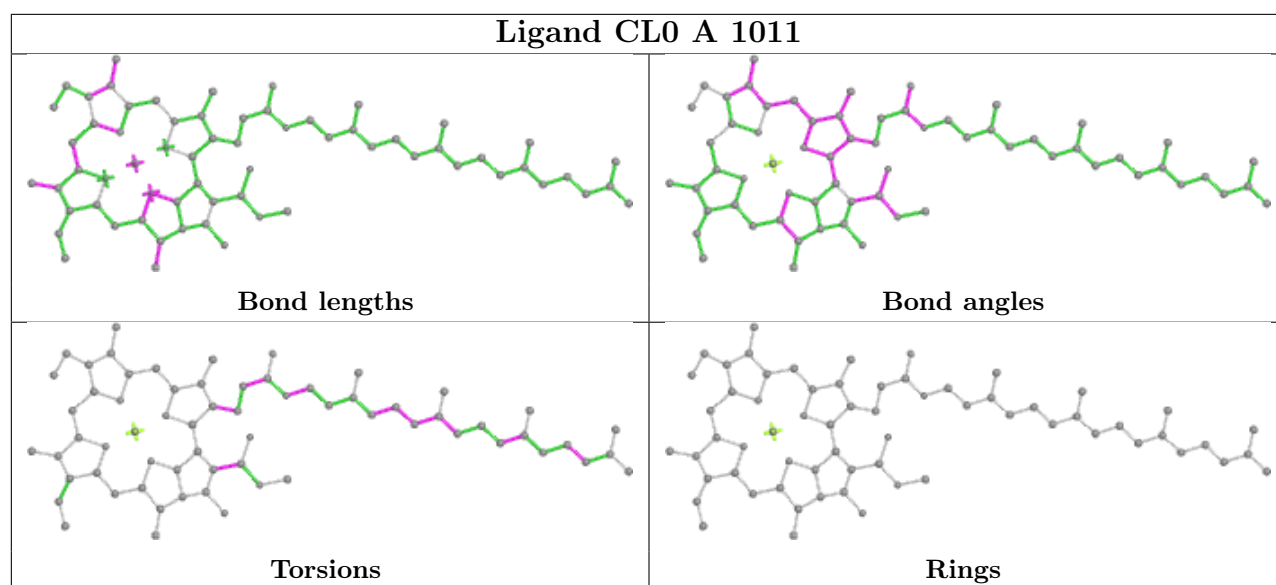
Rings

## Ligand CLA t 514

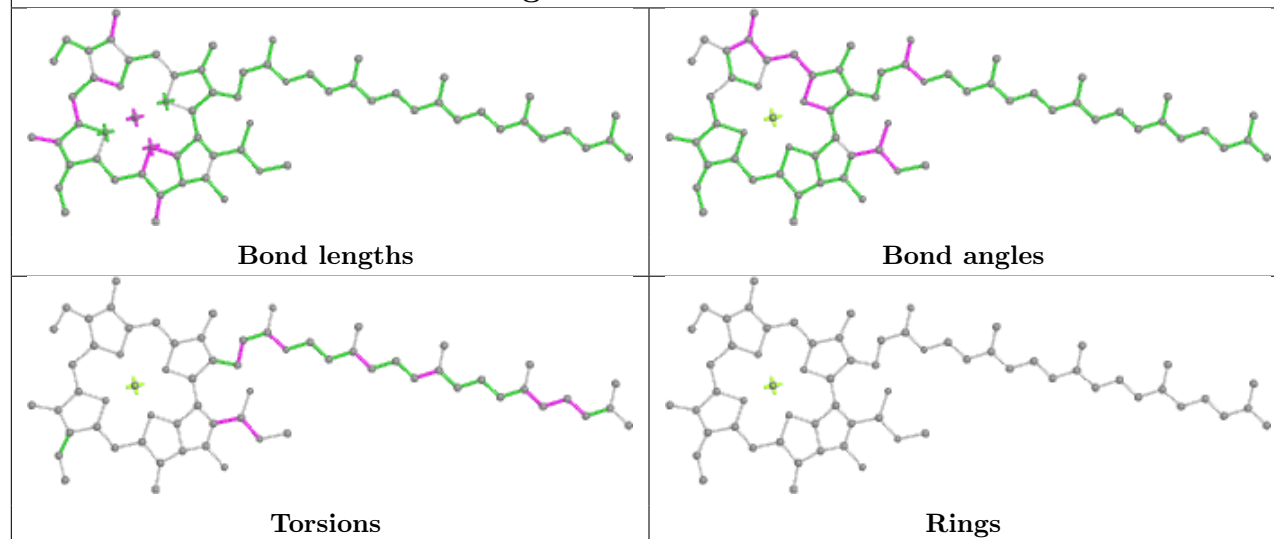


## Ligand CLA r 510

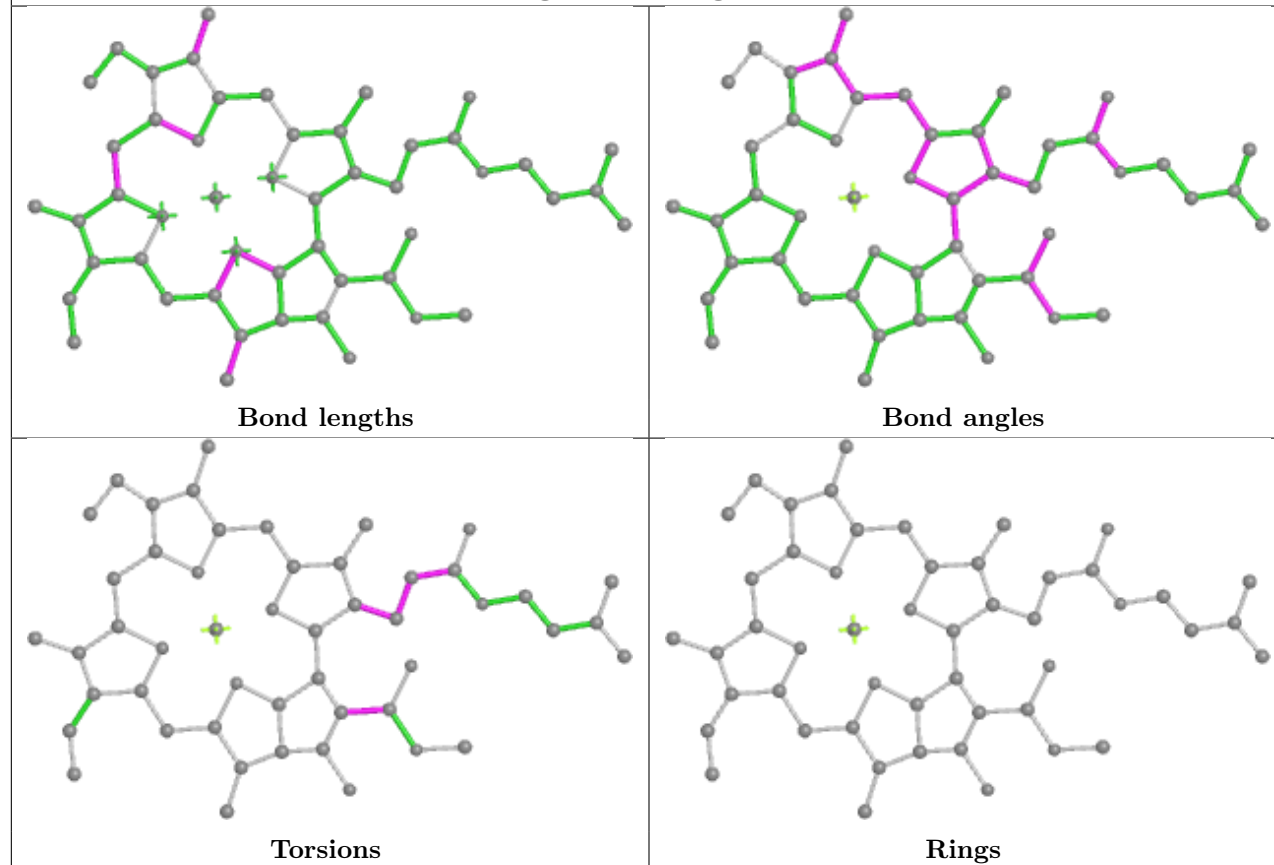




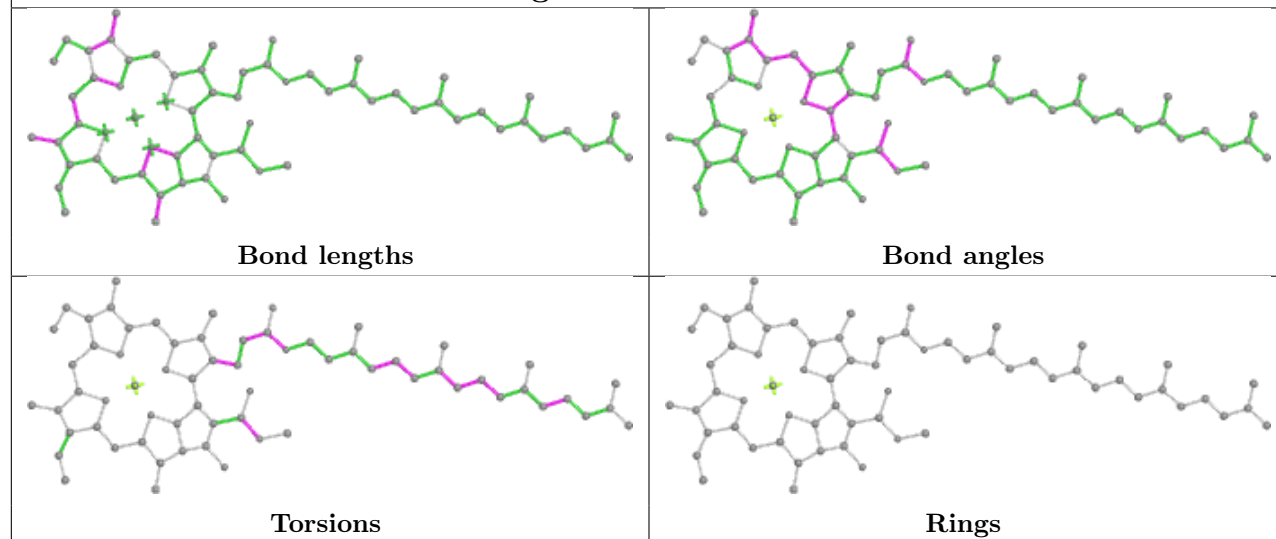
## Ligand CLA A 1119



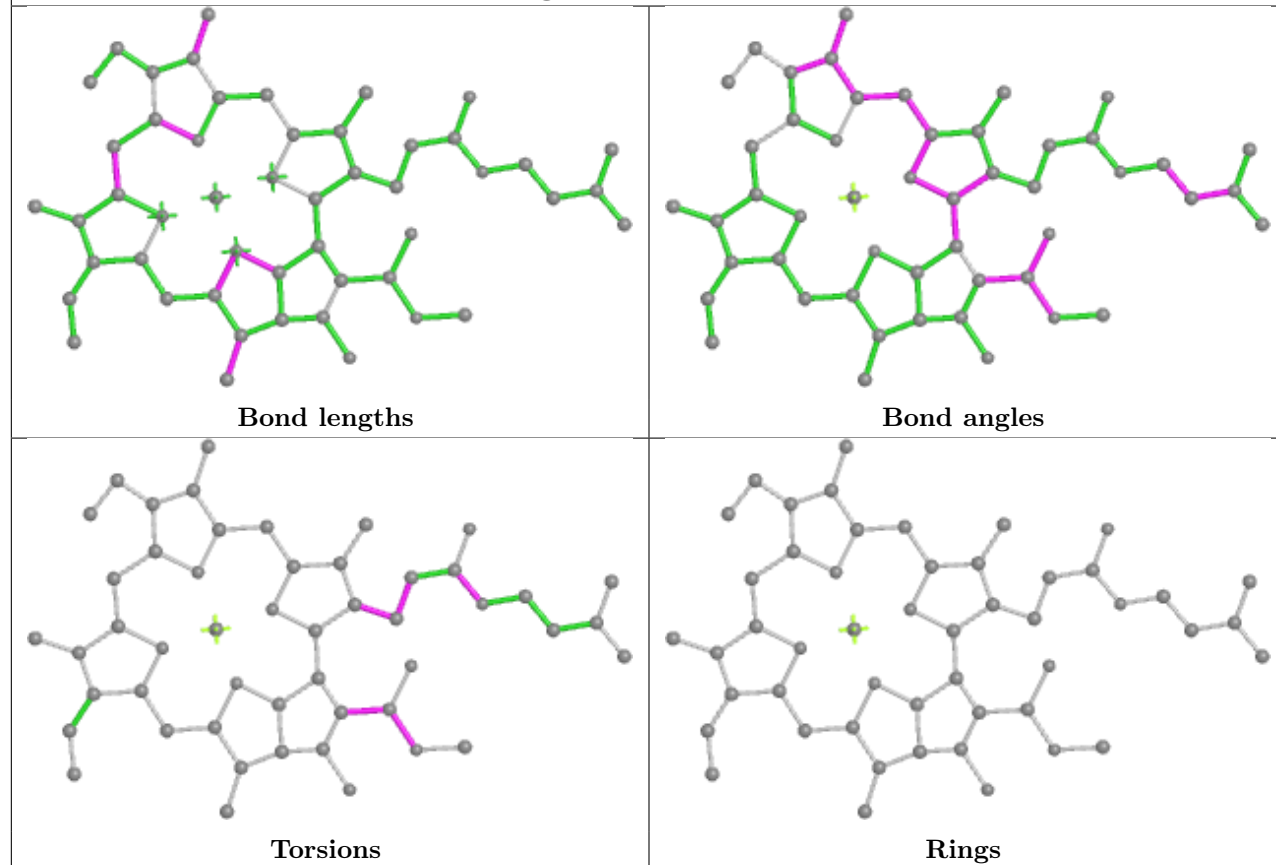
## Ligand CLA g 502



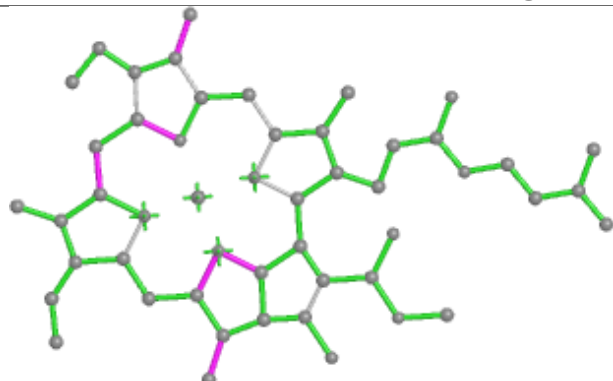
## Ligand CLA Y 511



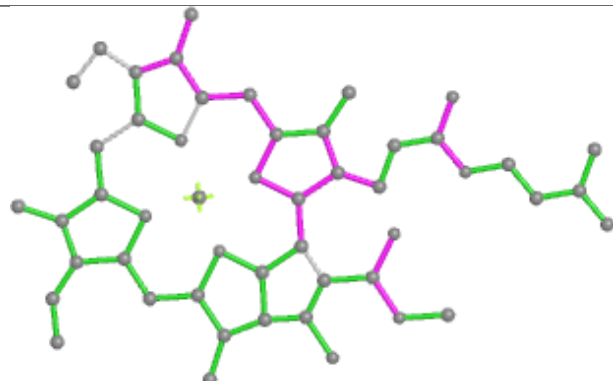
## Ligand CLA r 514



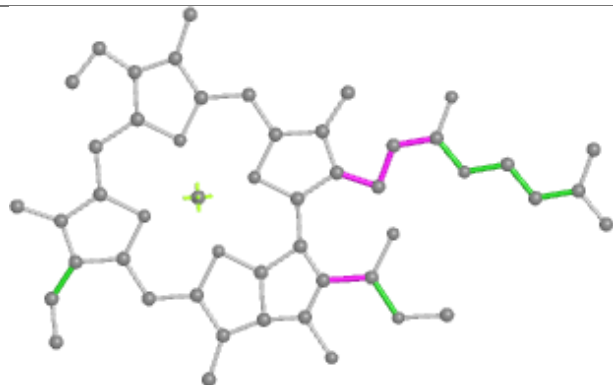
## Ligand CLA r 502



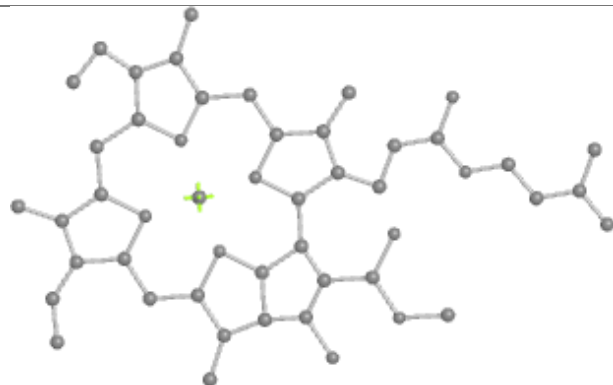
Bond lengths



Bond angles

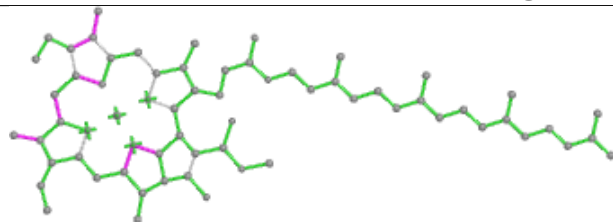


Torsions

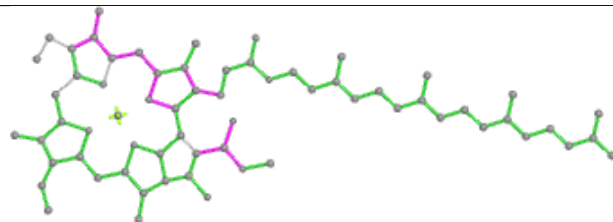


Rings

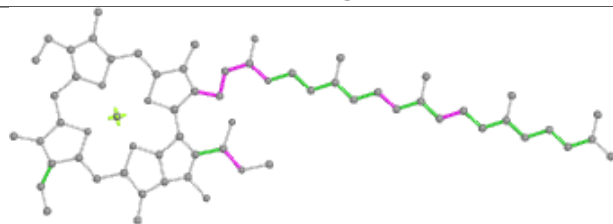
## Ligand CLA s 505



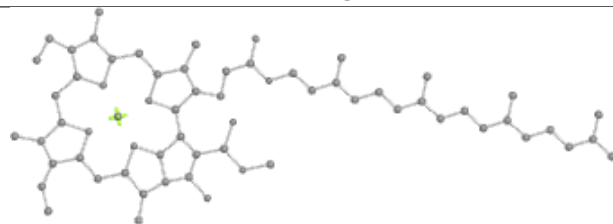
Bond lengths



Bond angles

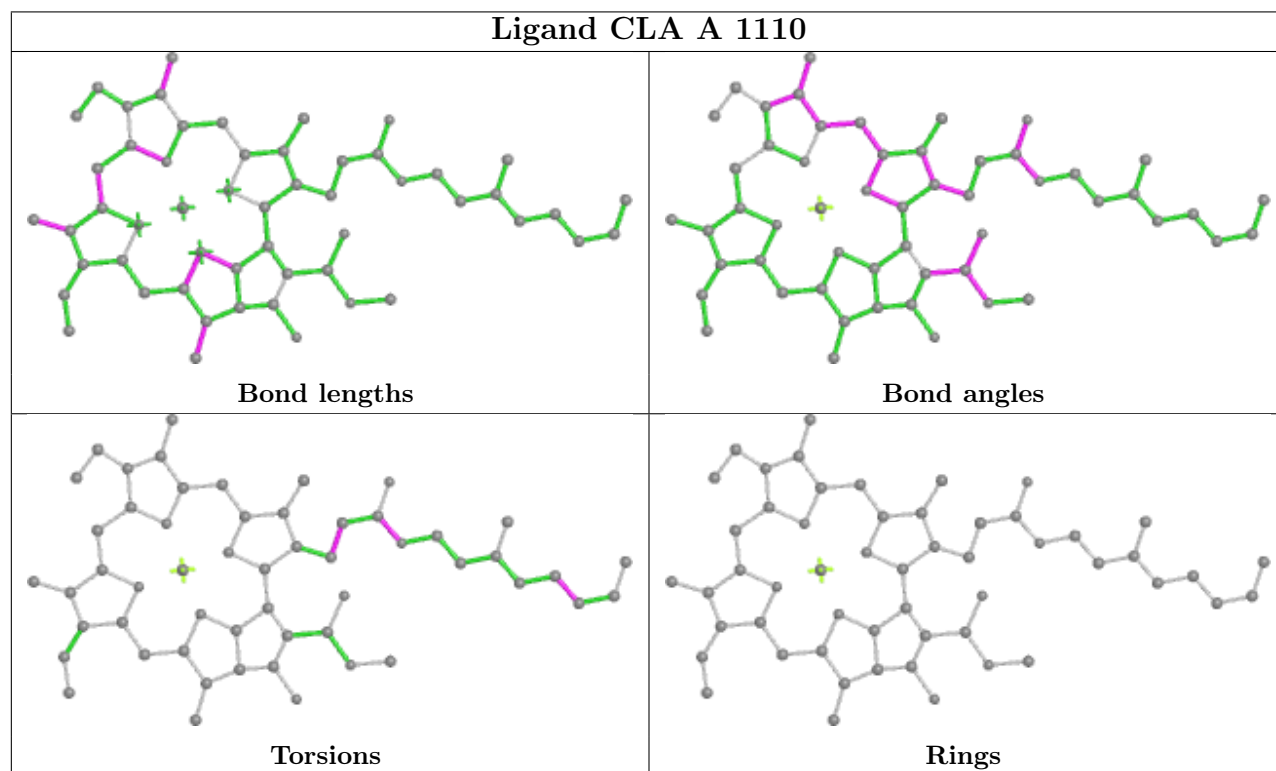
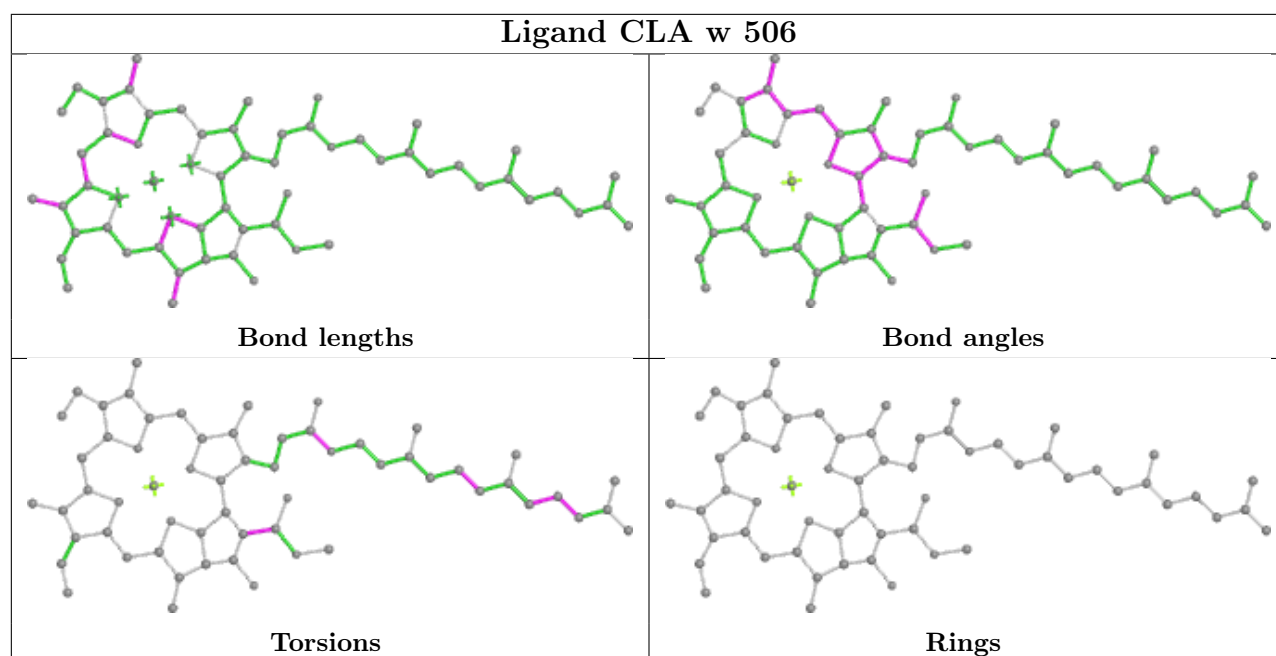


Torsions

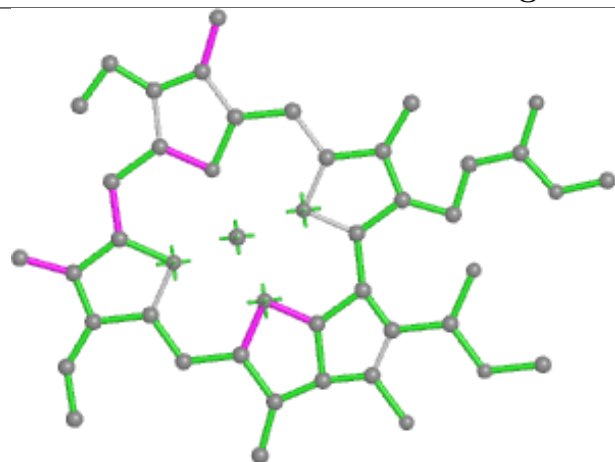


Rings

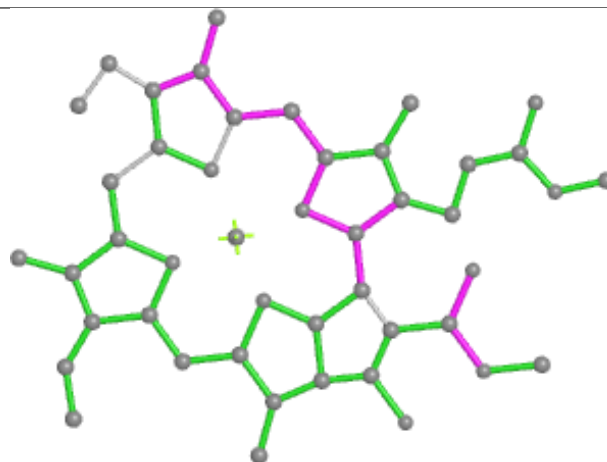




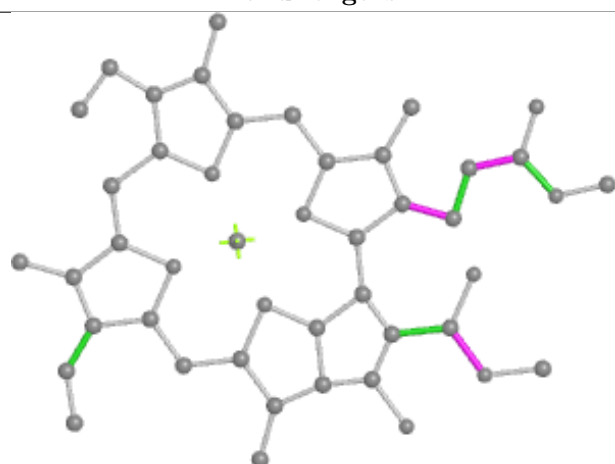
## Ligand CLA h 516



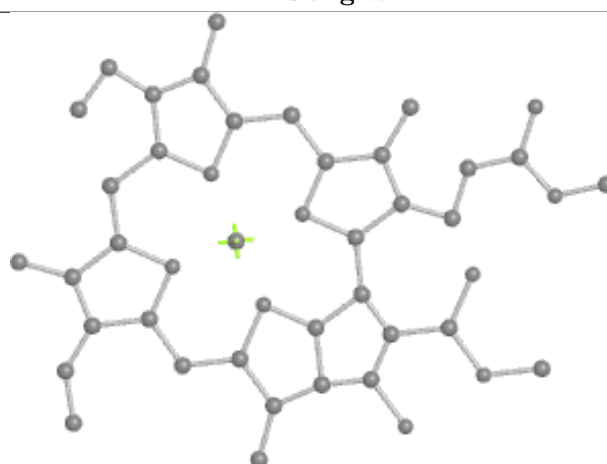
Bond lengths



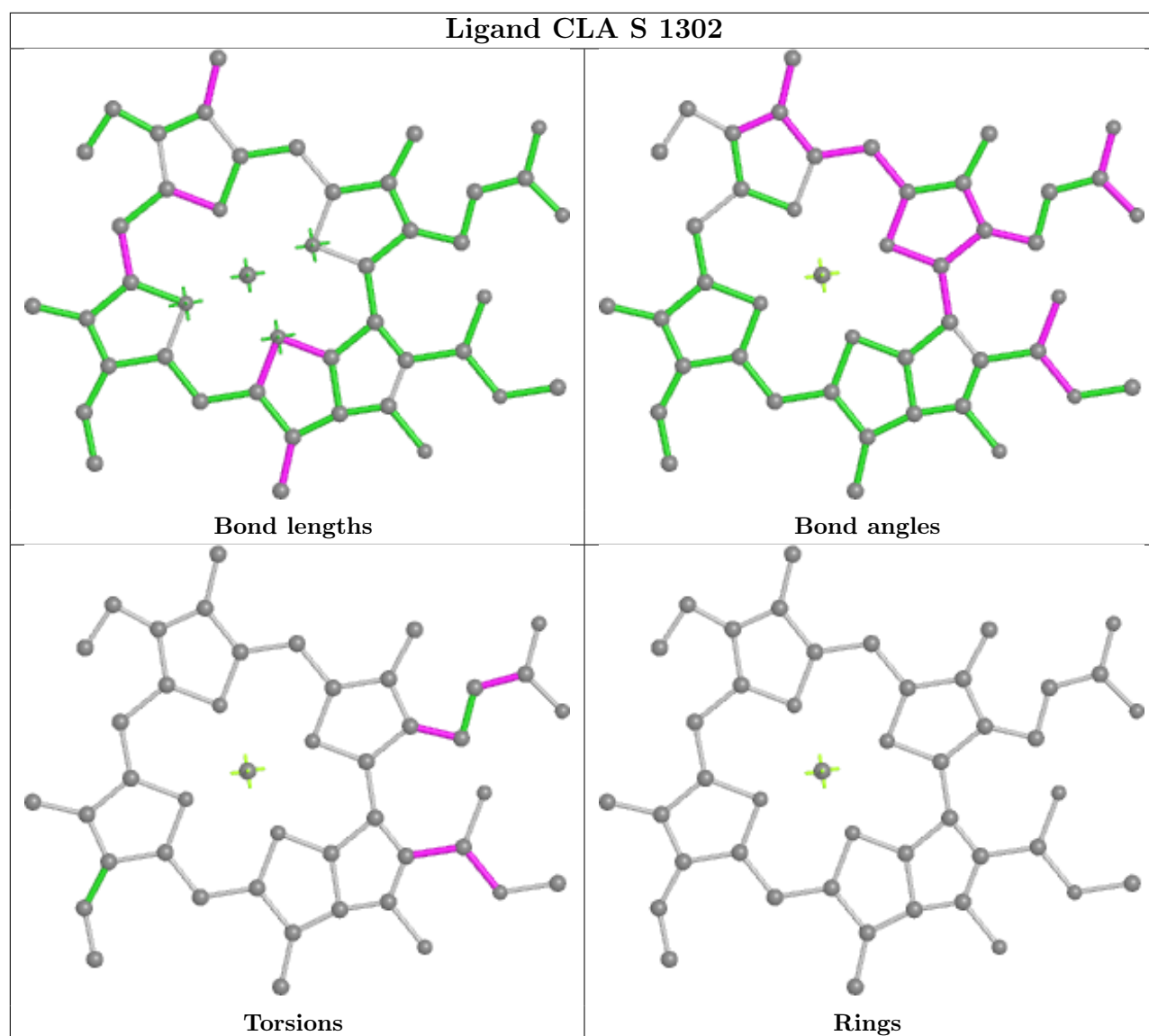
Bond angles



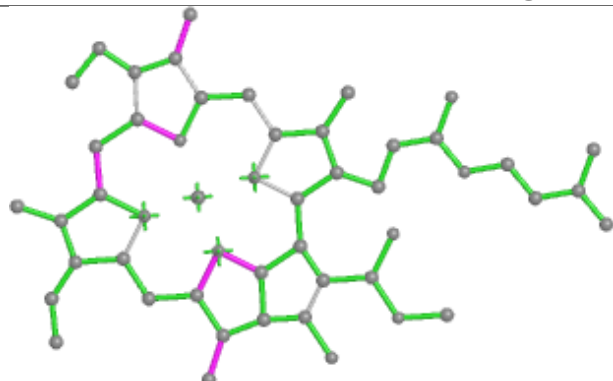
Torsions



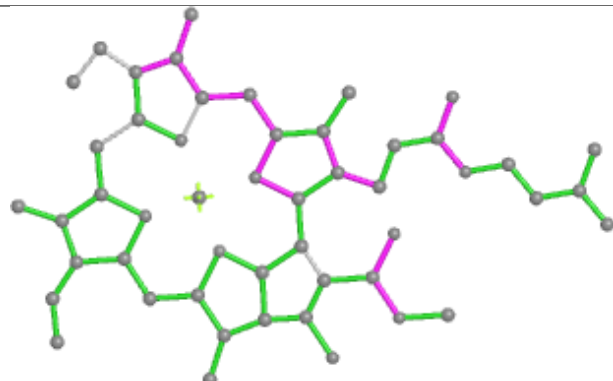
Rings



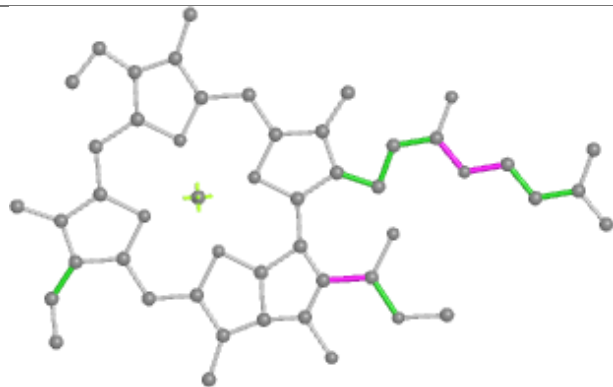
## Ligand CLA r 501



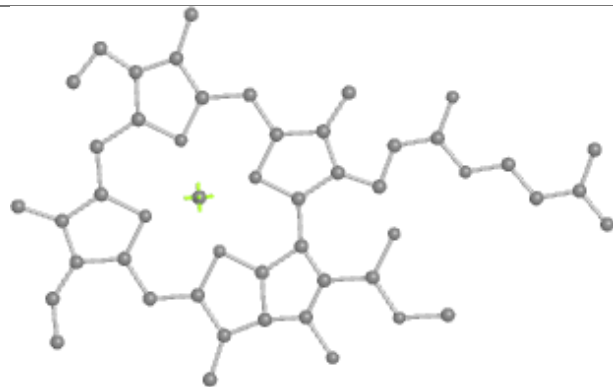
Bond lengths



Bond angles

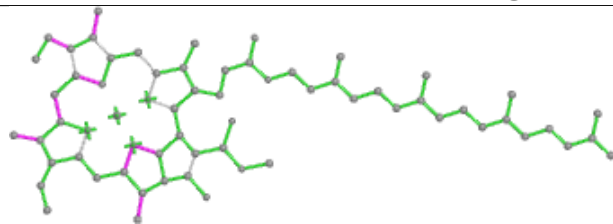


Torsions

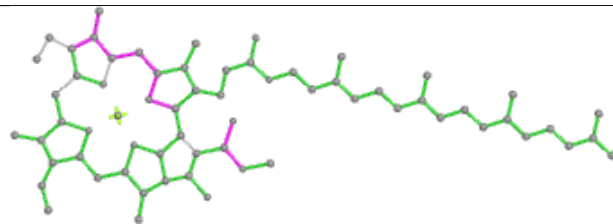


Rings

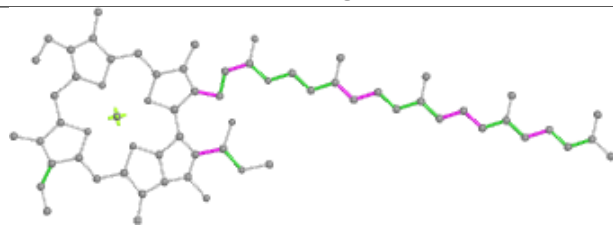
## Ligand CLA B 1238



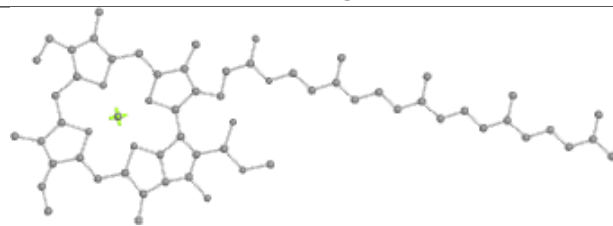
Bond lengths



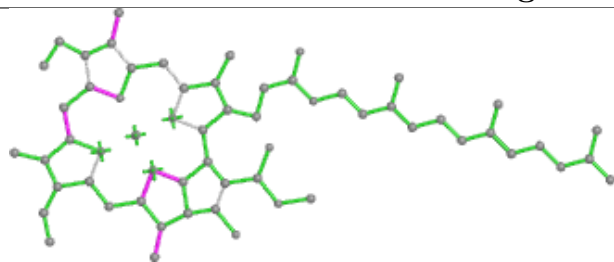
Bond angles



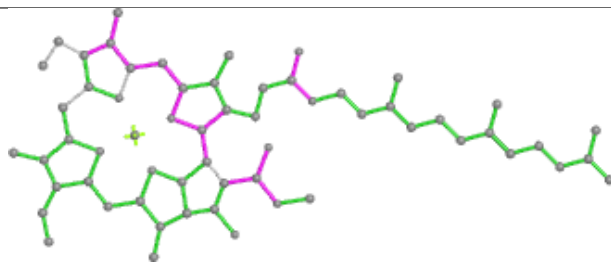
Torsions



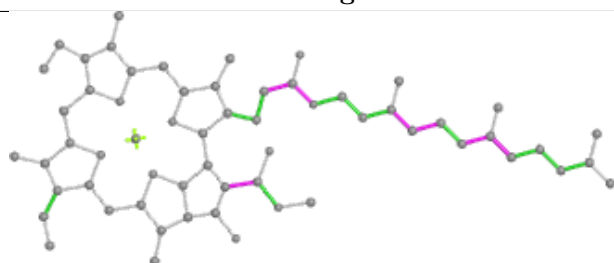
Rings

**Ligand CLA v 510**

Bond lengths



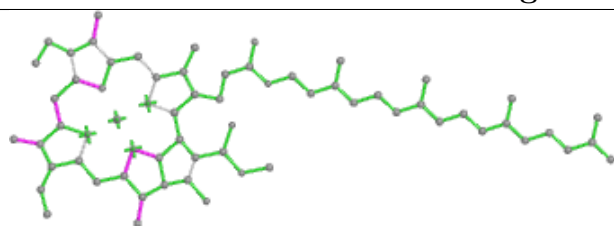
Bond angles



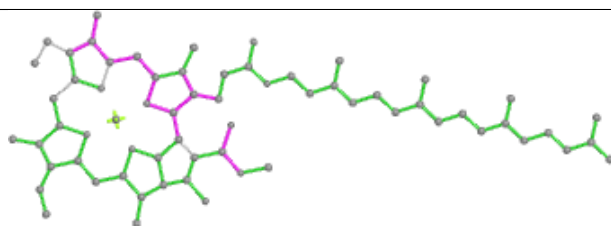
Torsions



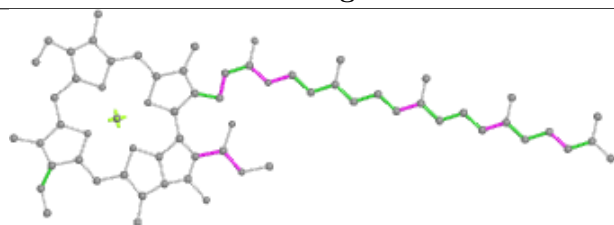
Rings

**Ligand CLA s 510**

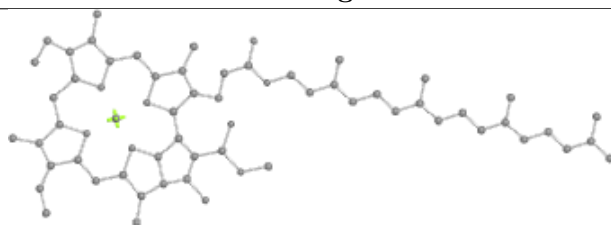
Bond lengths



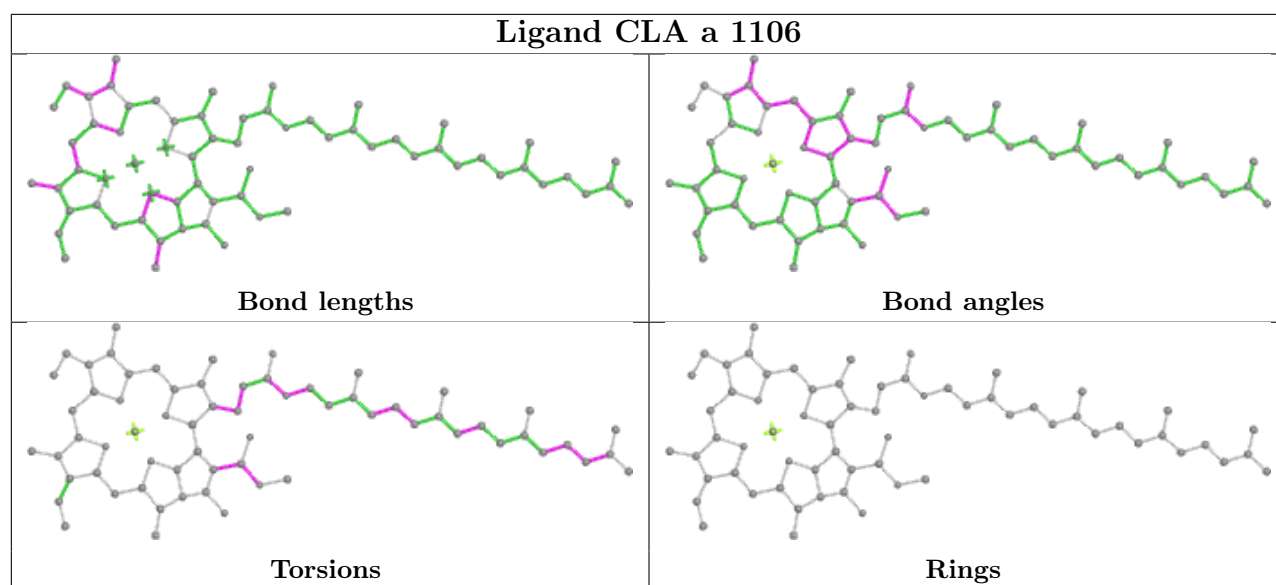
Bond angles

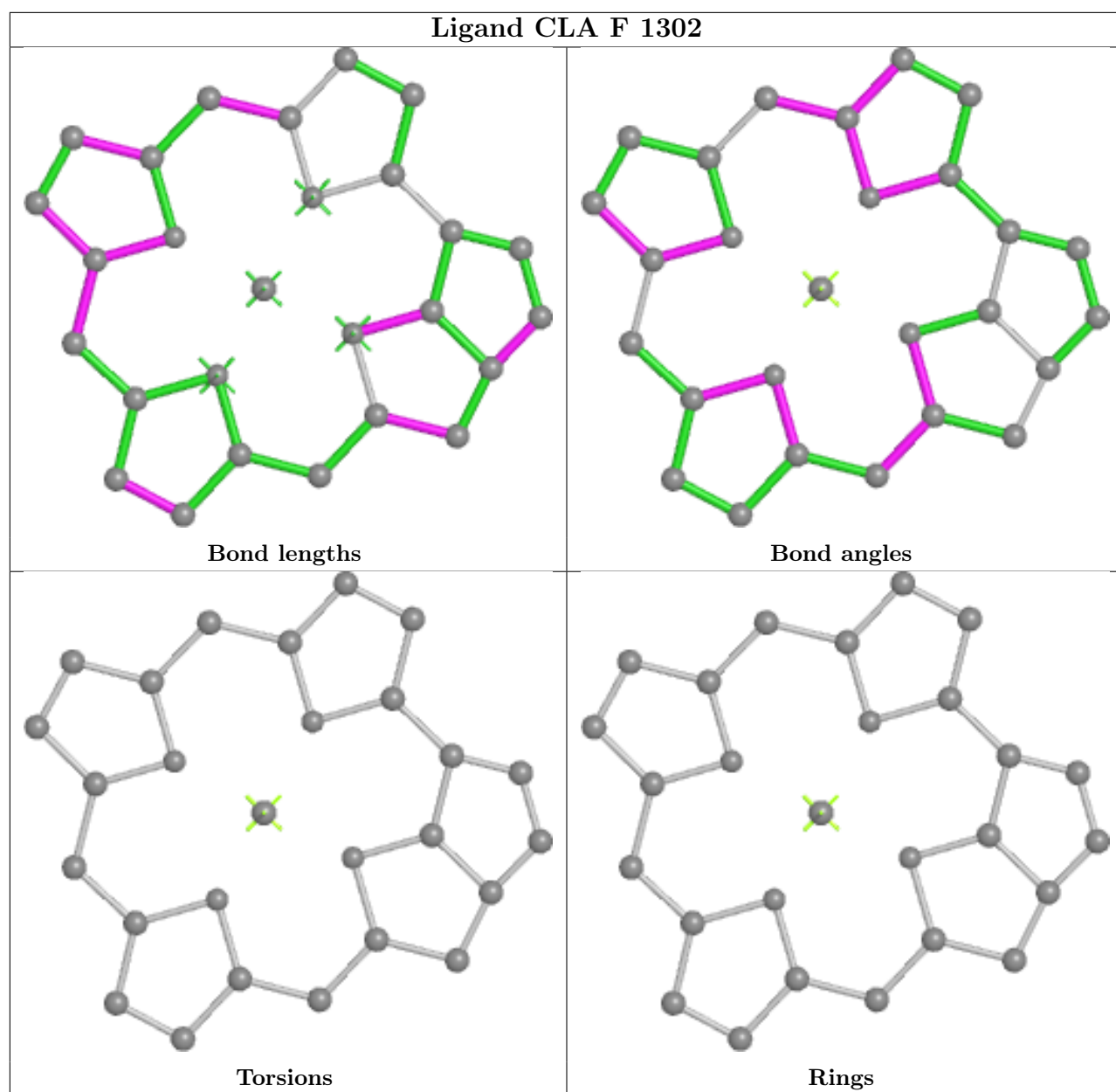


Torsions

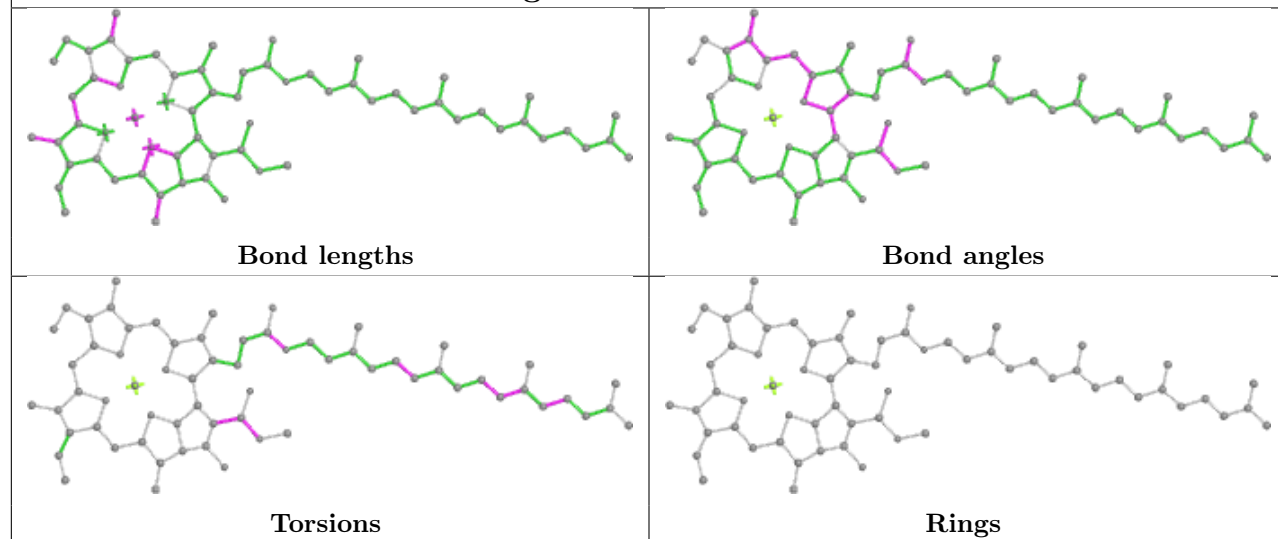


Rings

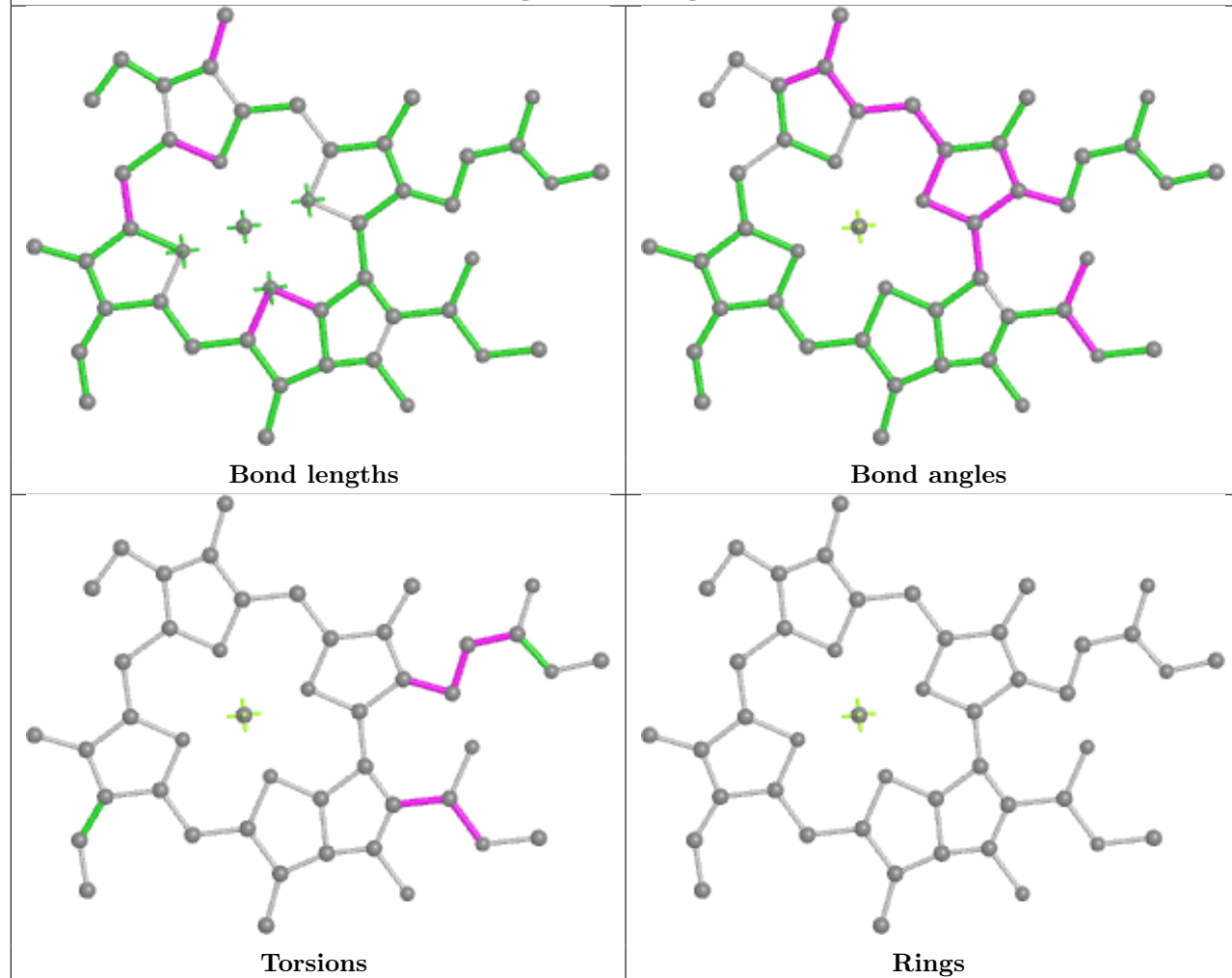




## Ligand CLA B 1221

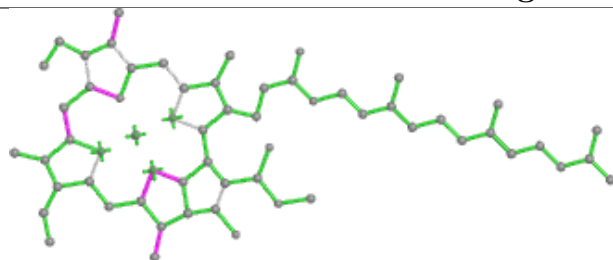


## Ligand CLA g 505

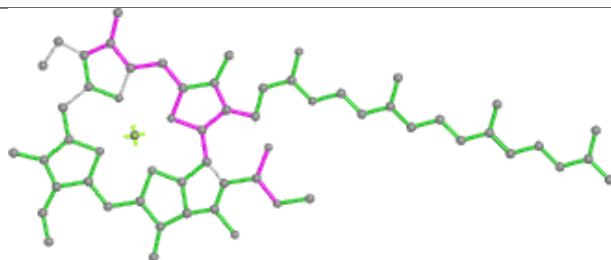




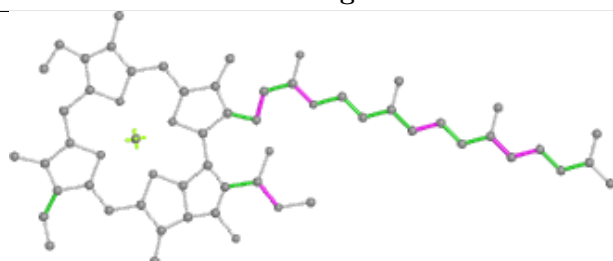
## Ligand CLA n 509



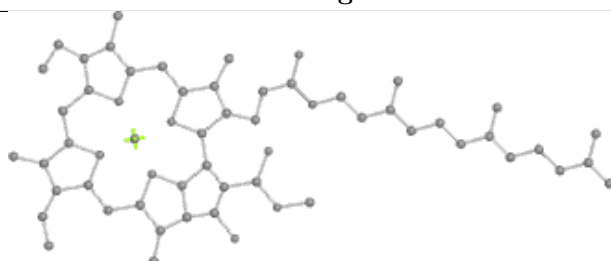
Bond lengths



Bond angles

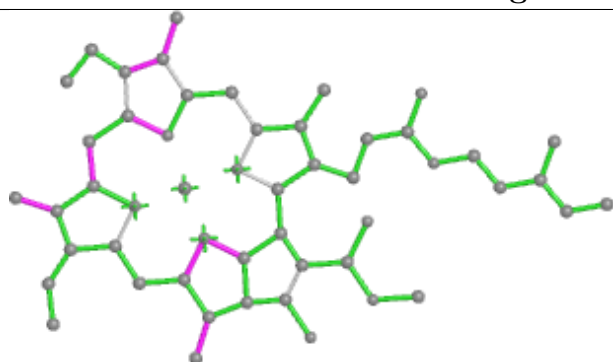


Torsions

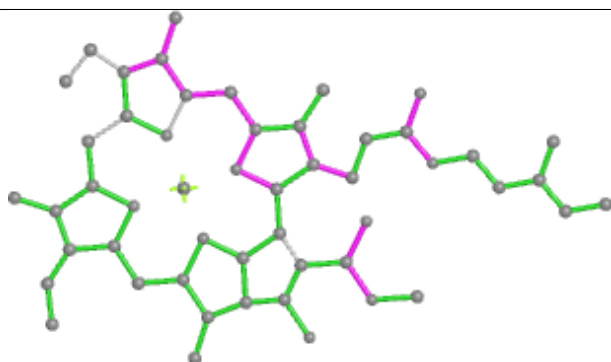


Rings

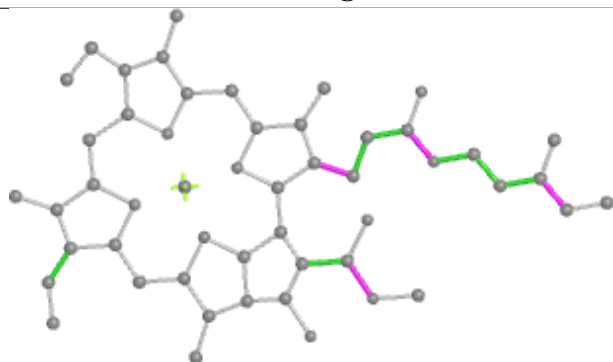
## Ligand CLA a 1139



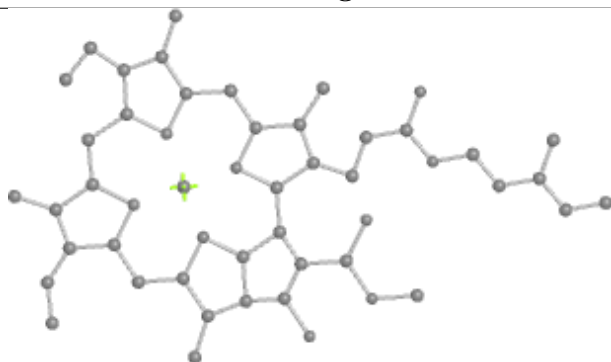
Bond lengths



Bond angles

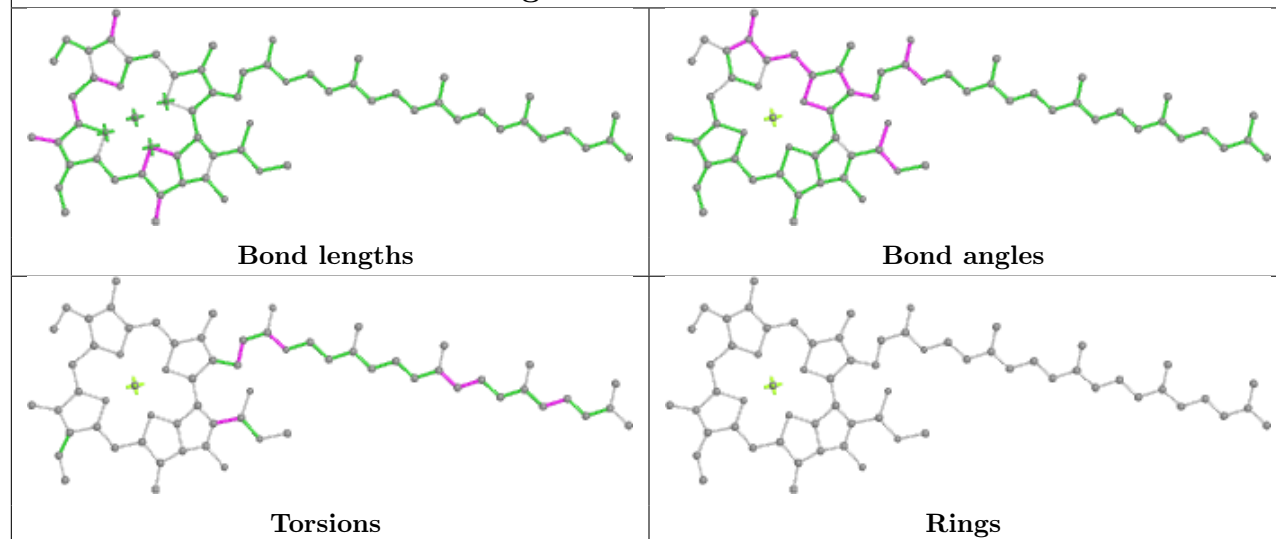


Torsions

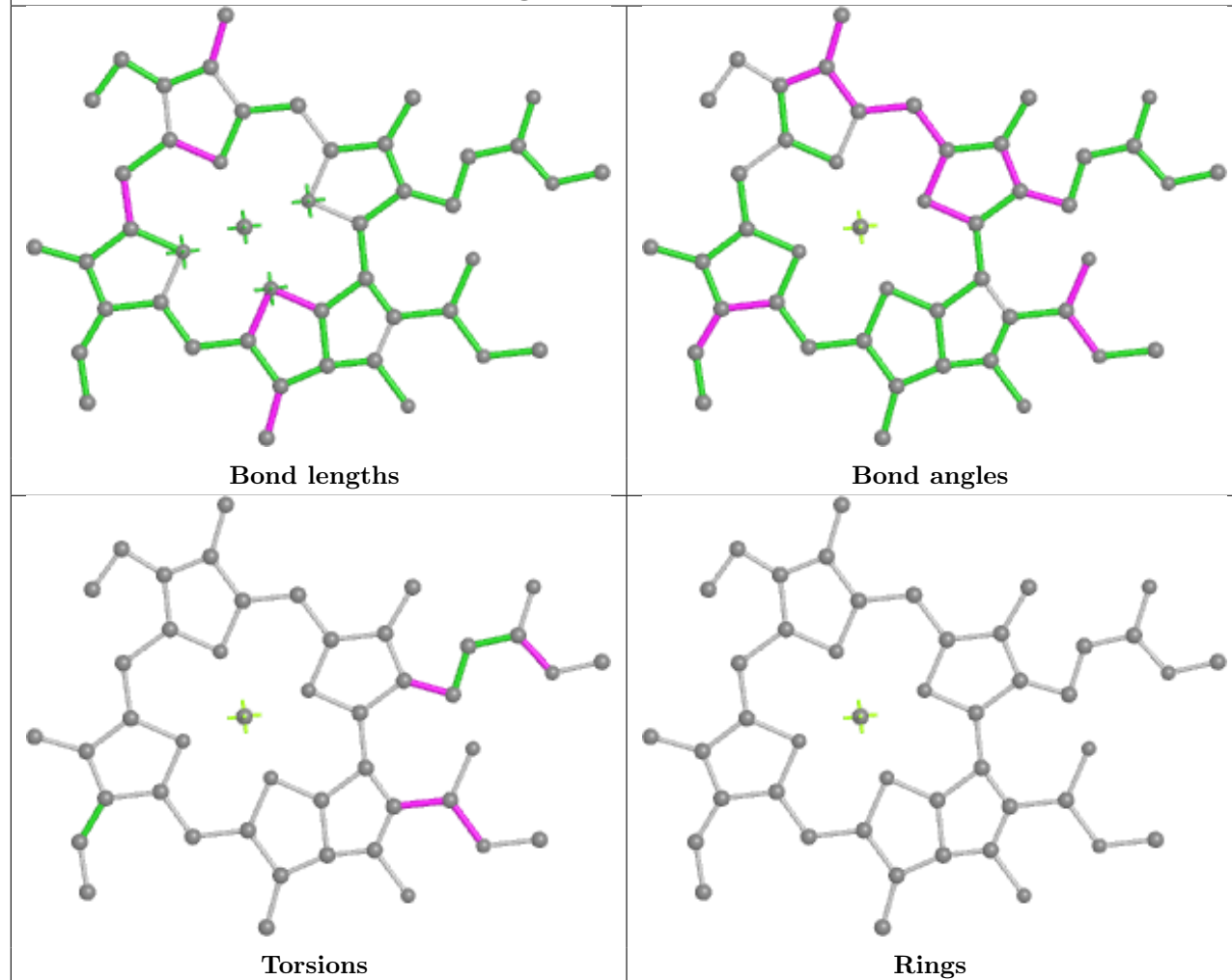


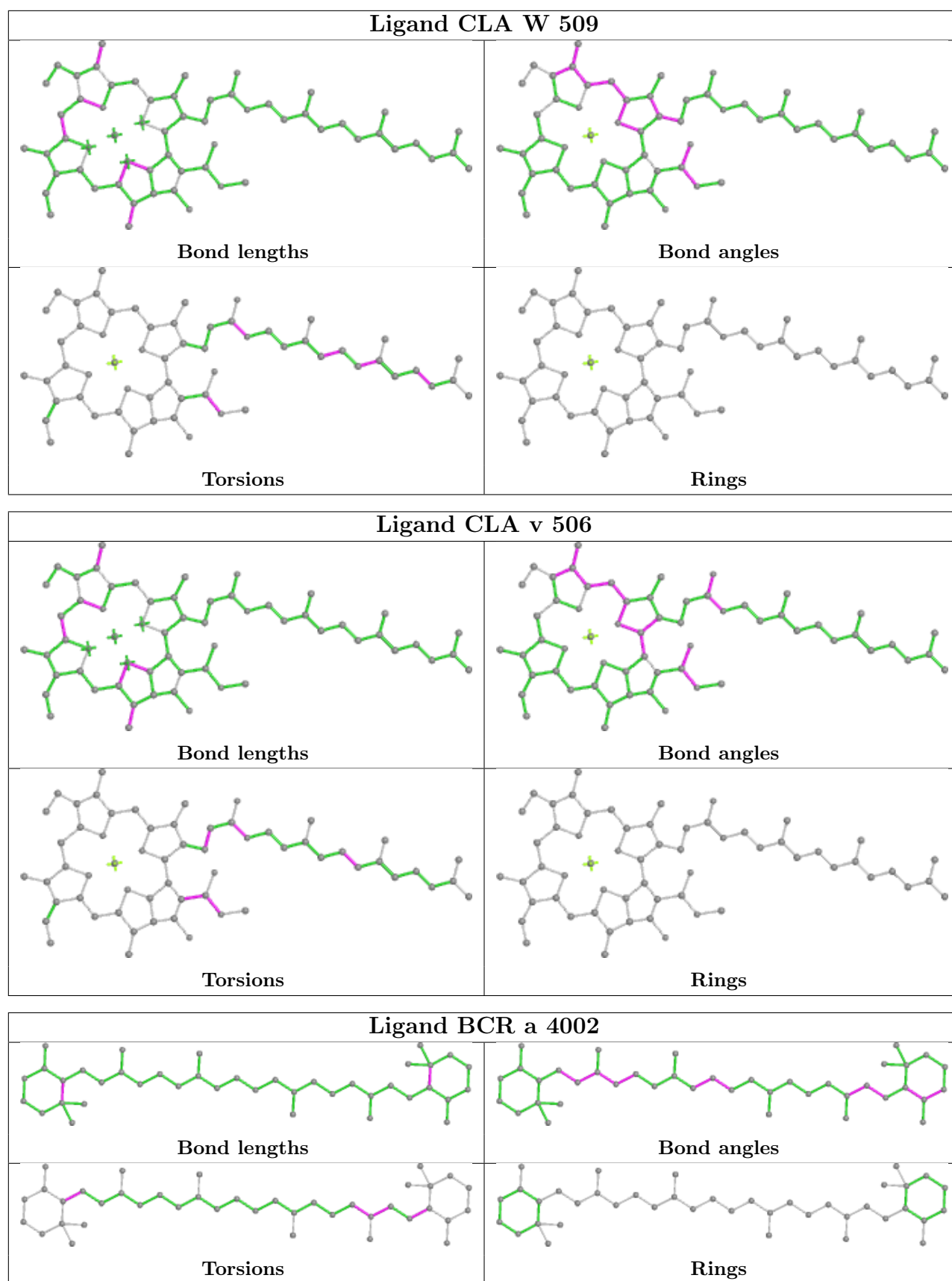
Rings

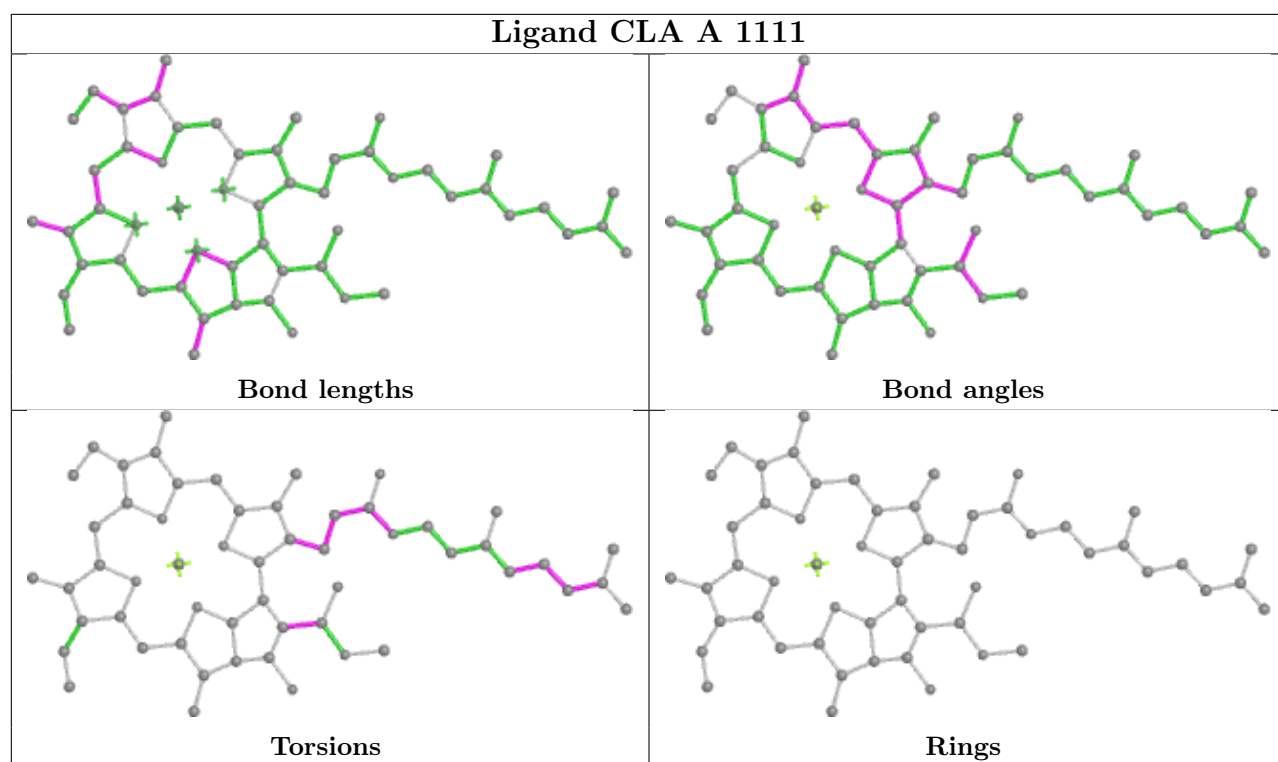
## Ligand CLA G 1211



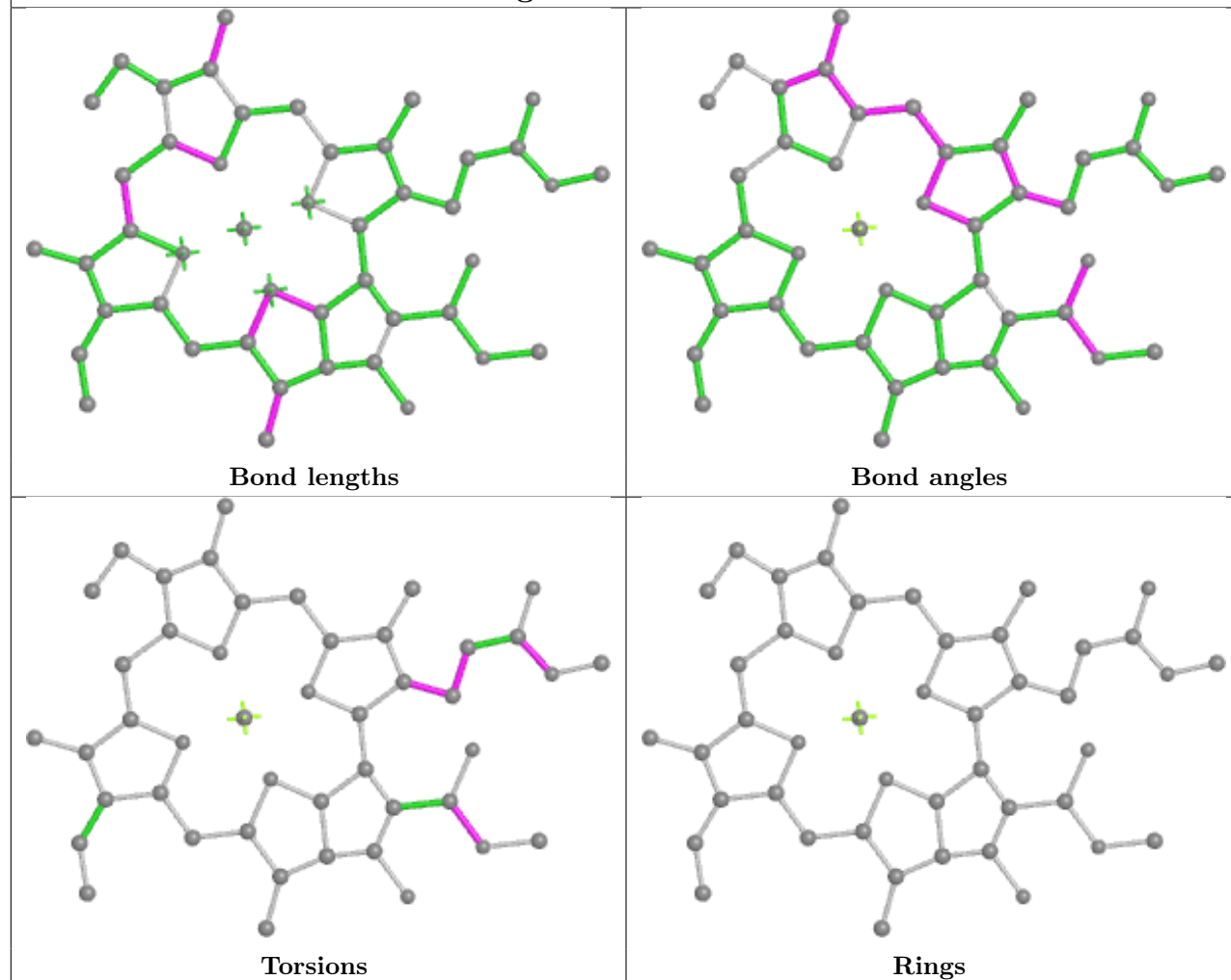
## Ligand CLA Z 503



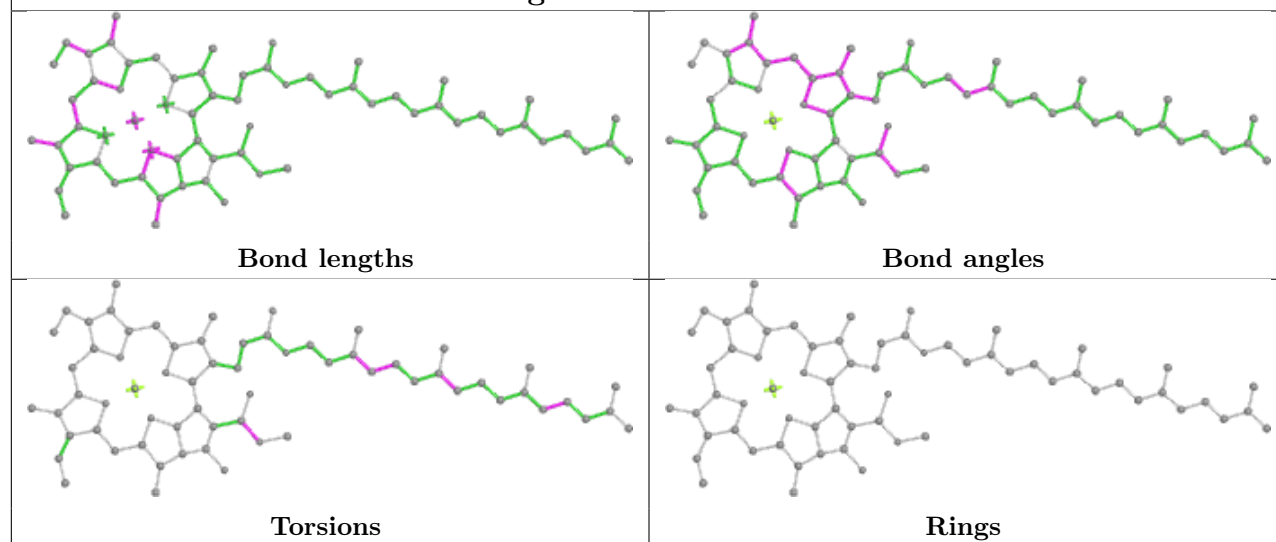




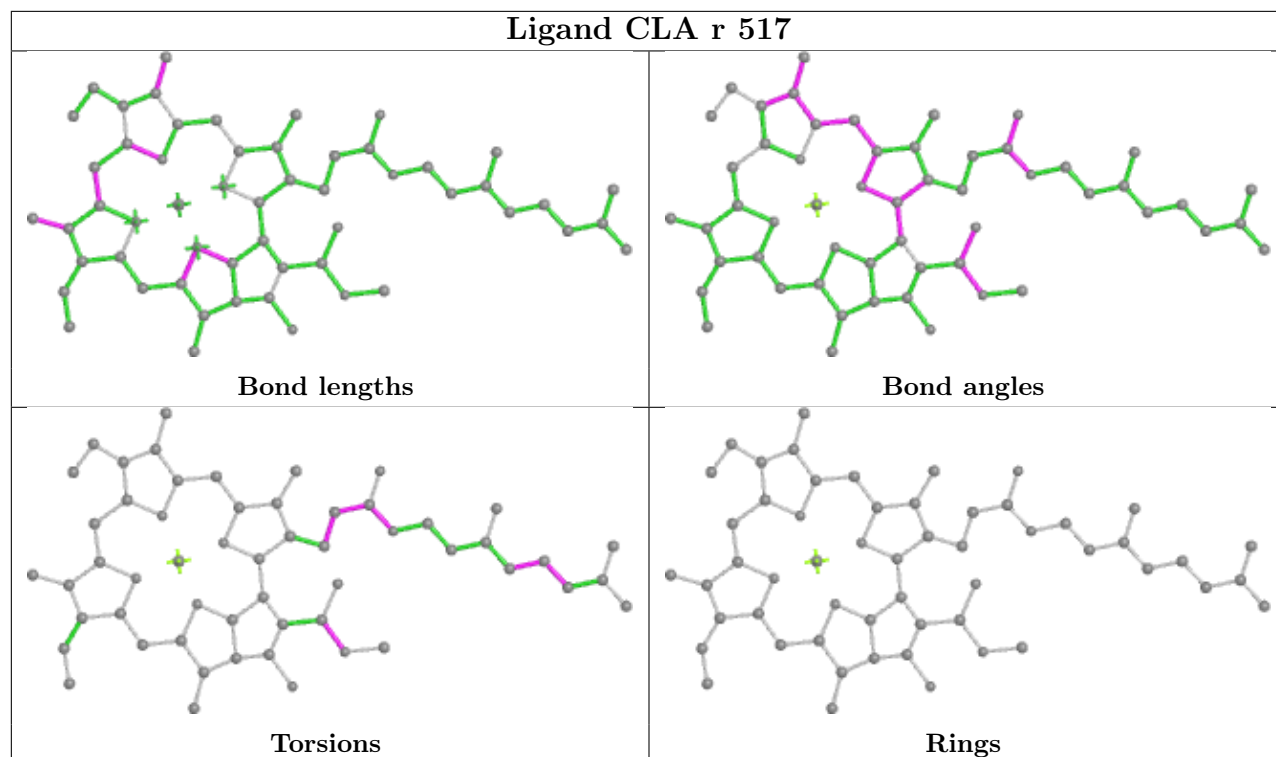
## Ligand CLA v 501



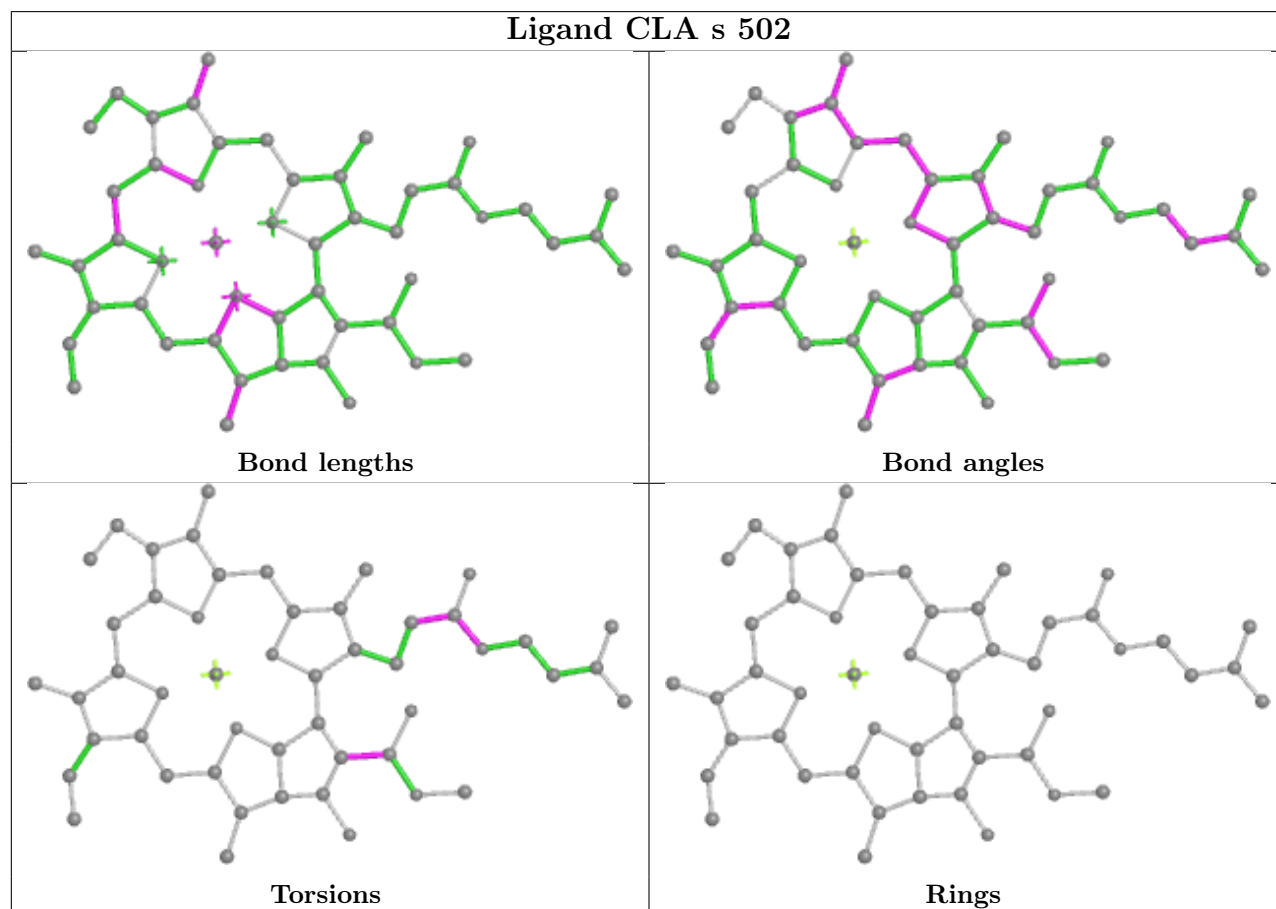
## Ligand CLA a 1131



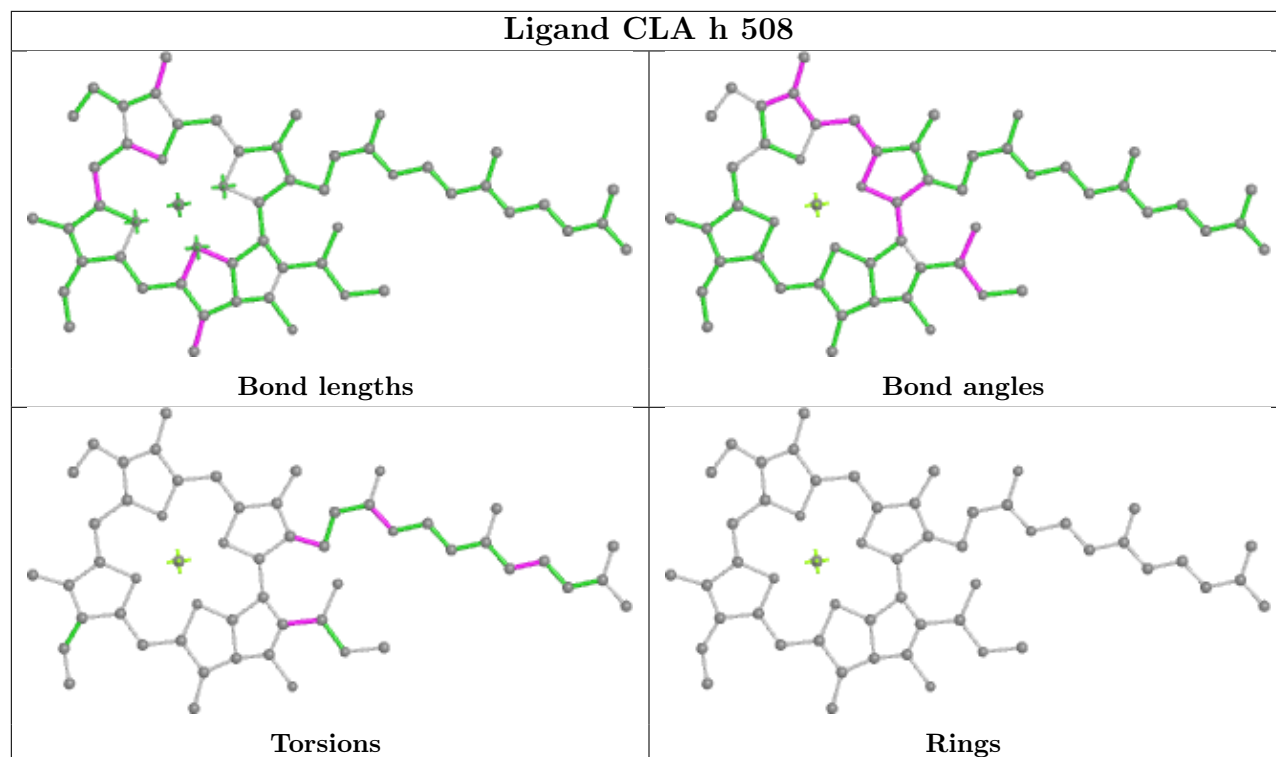
## Ligand CLA r 517



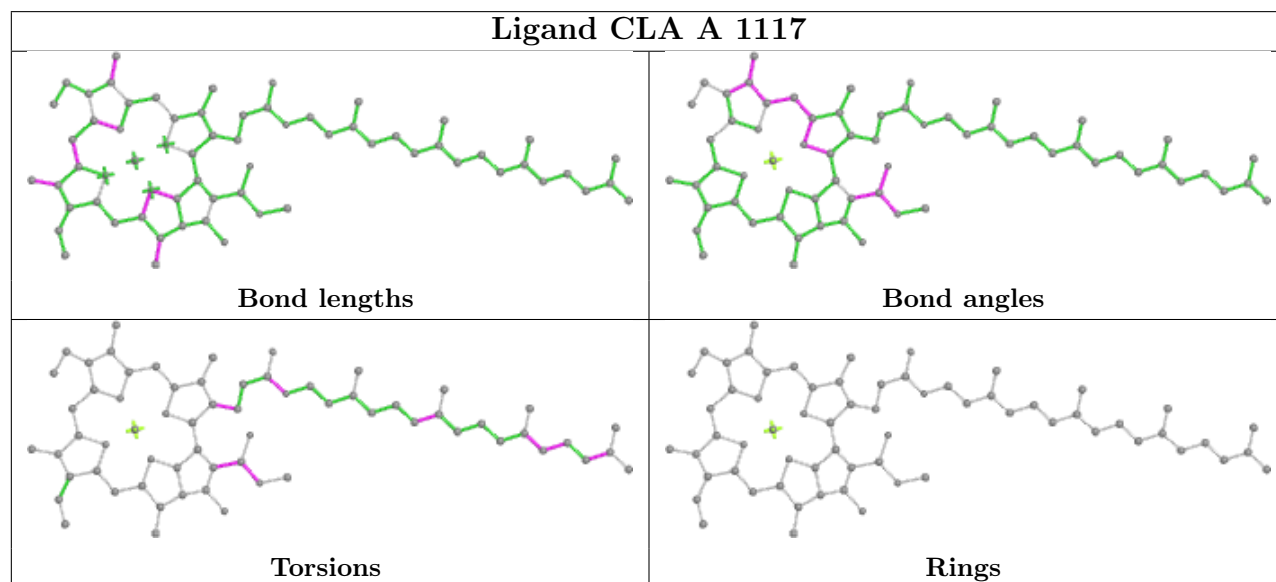
## Ligand CLA s 502



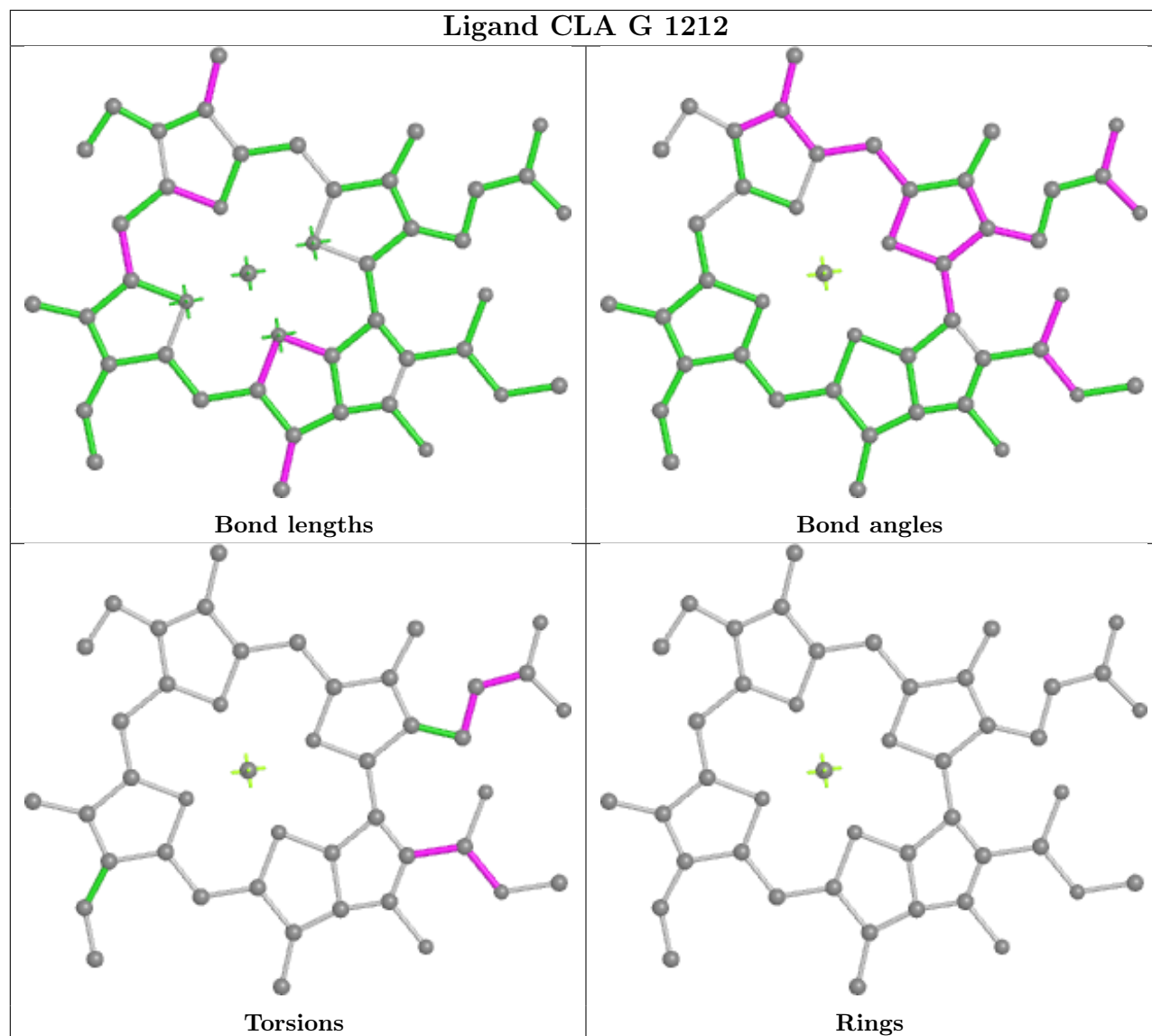
## Ligand CLA h 508



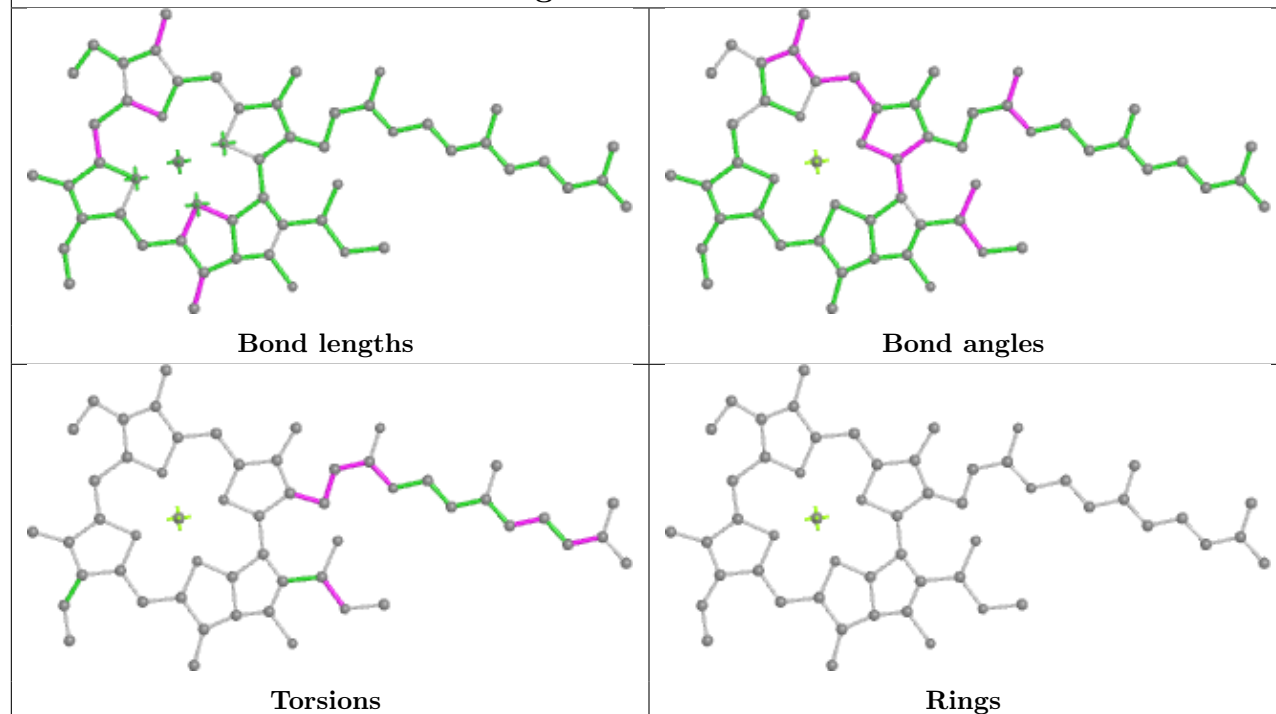
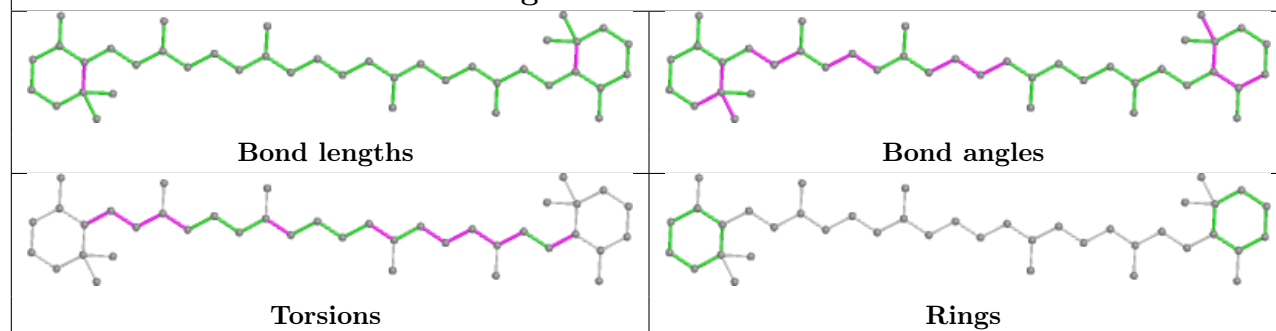
## Ligand CLA A 1117



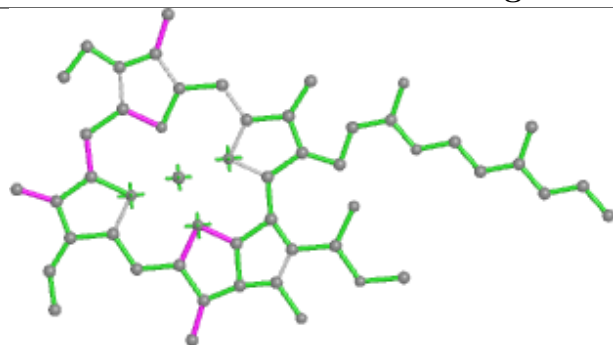
## Ligand CLA G 1212



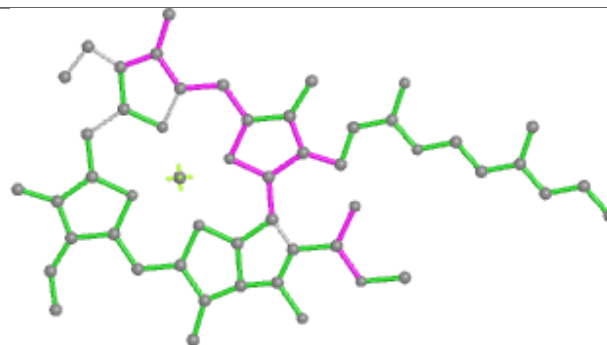


**Ligand CLA n 508****Ligand BCR A 4011**

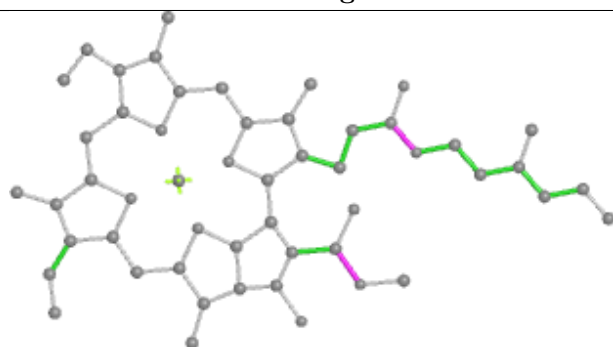
## Ligand CLA H 1801



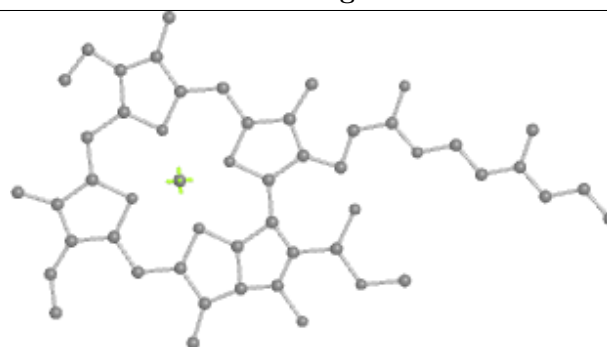
Bond lengths



Bond angles

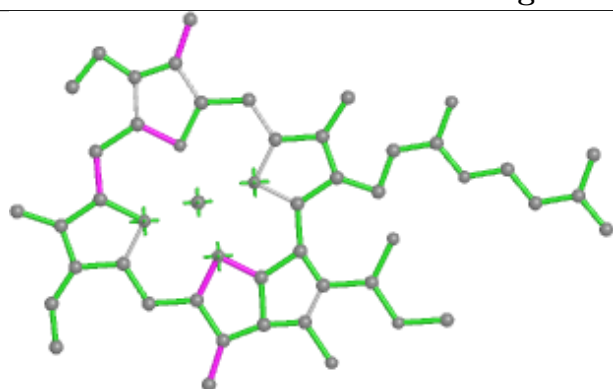


Torsions

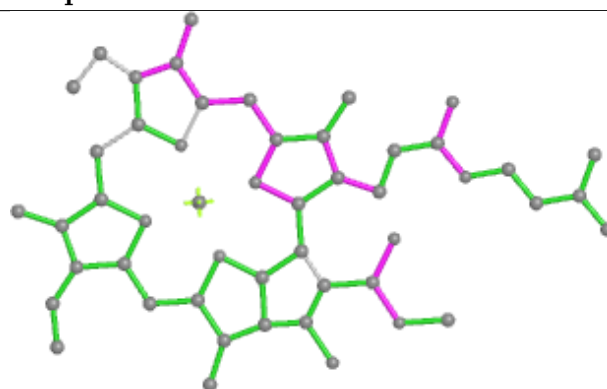


Rings

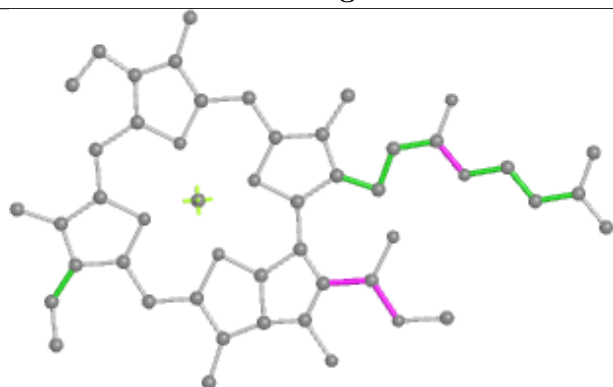
## Ligand CLA q 501



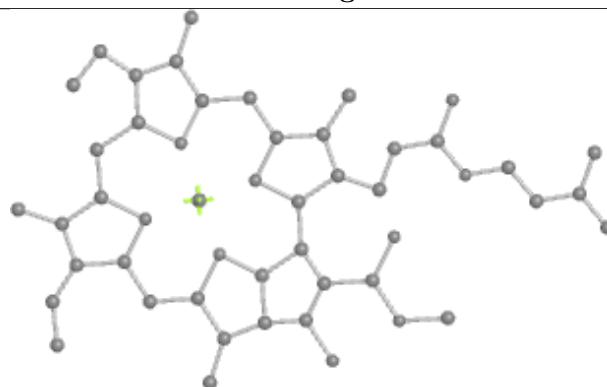
Bond lengths



Bond angles

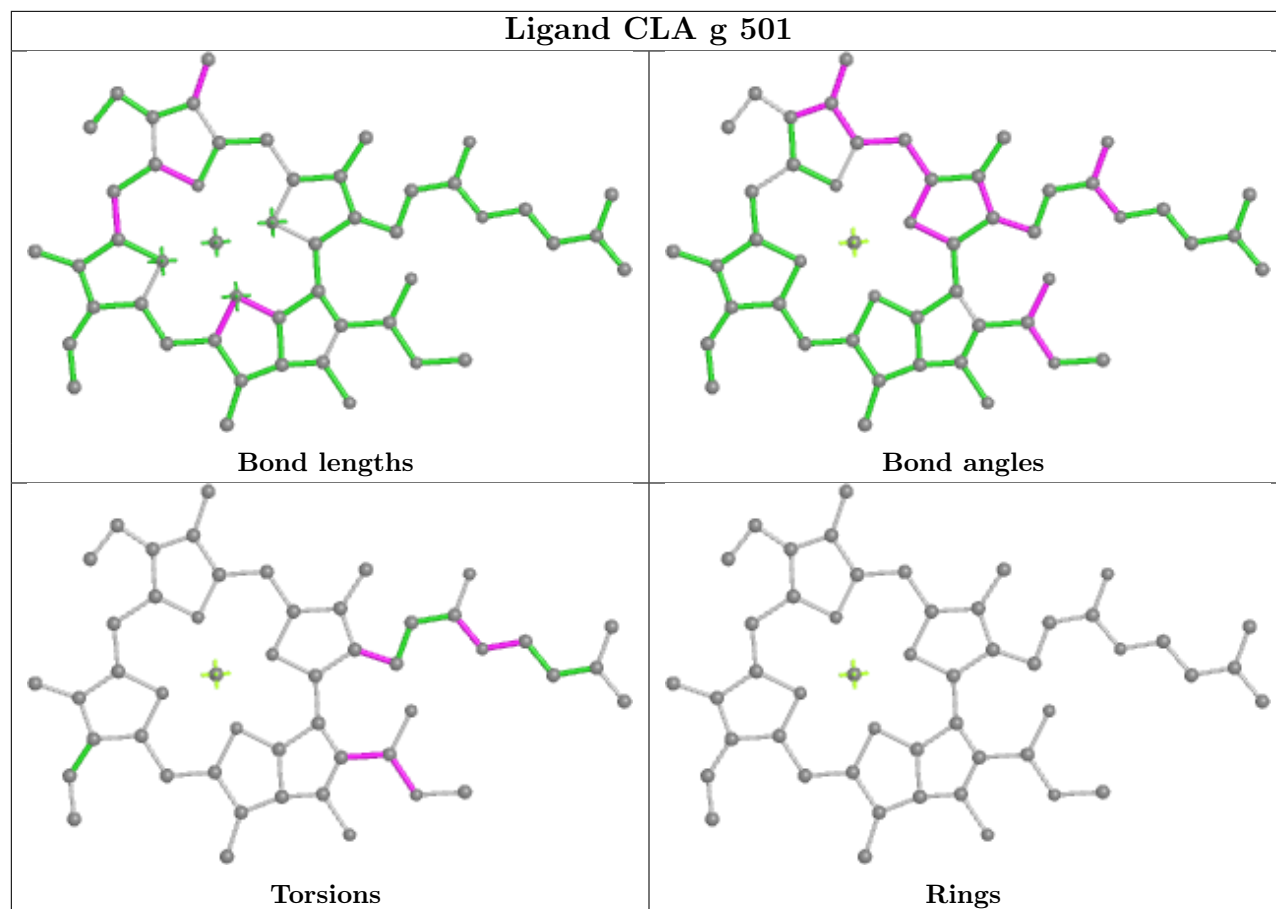


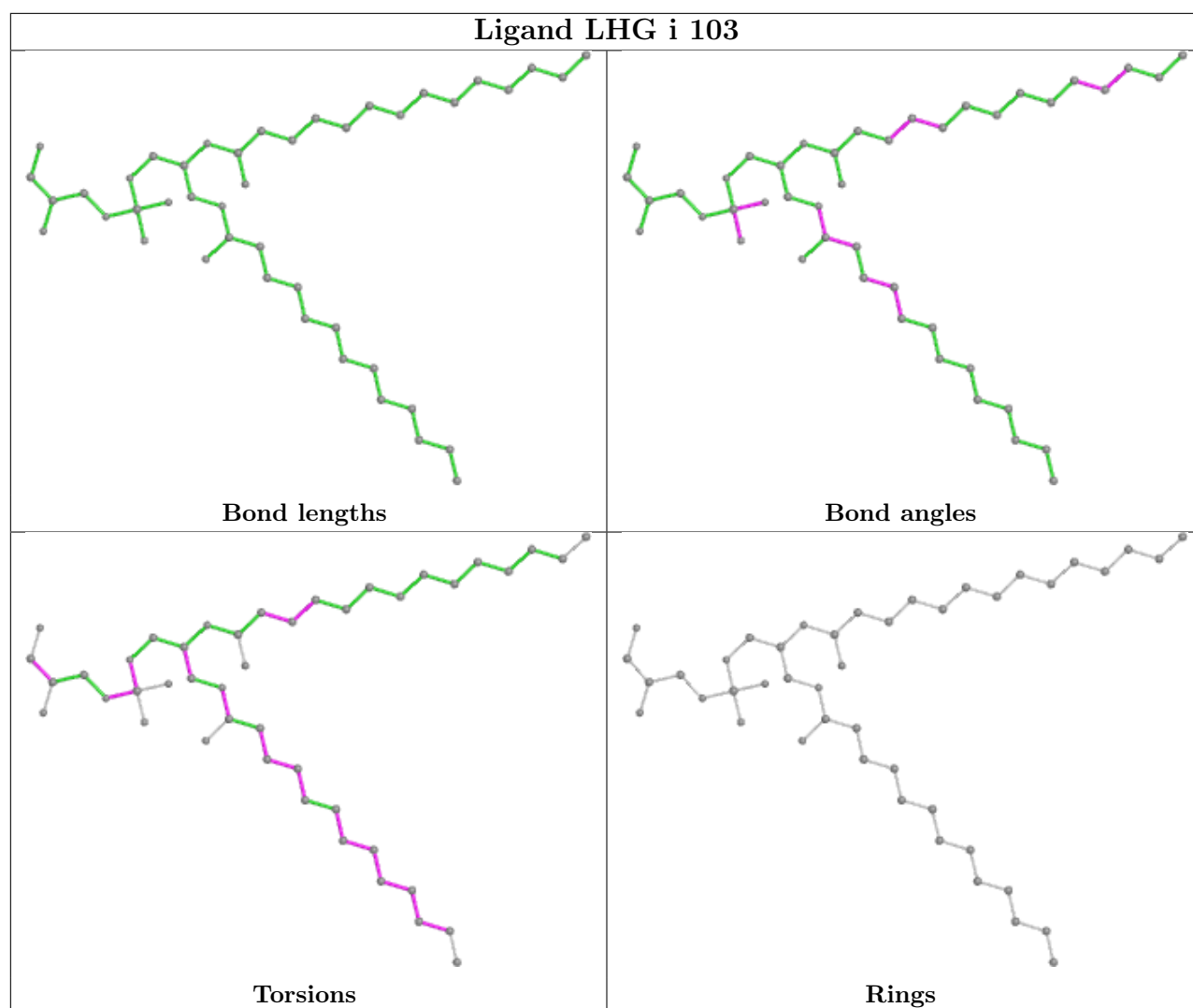
Torsions



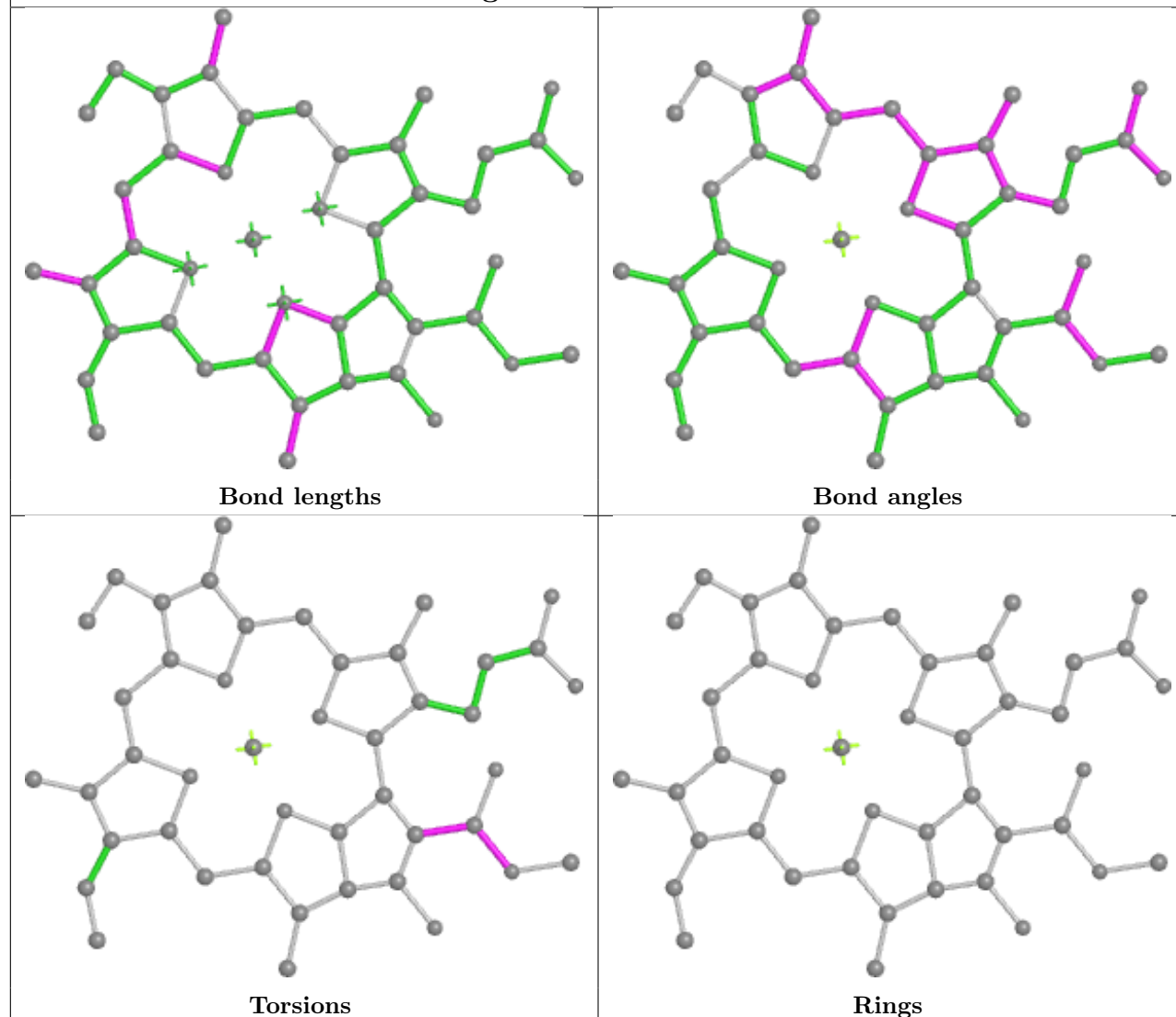
Rings

## Ligand CLA g 501

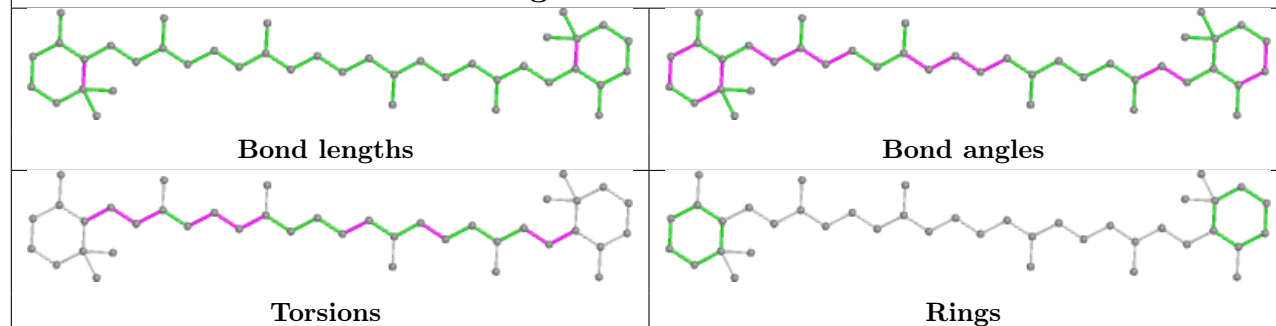


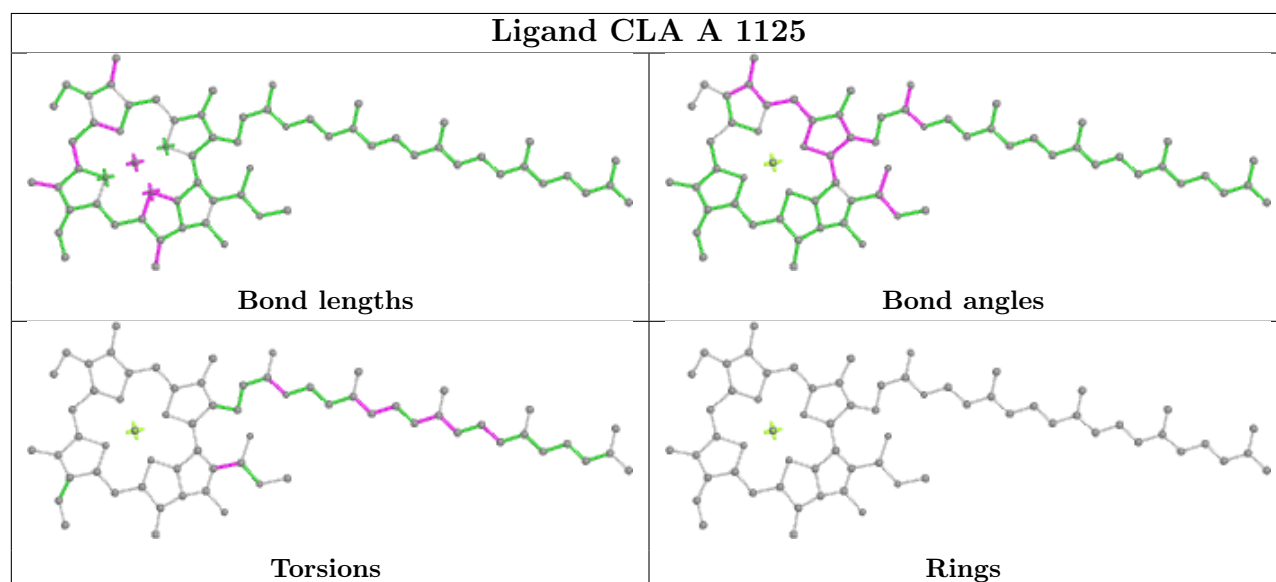
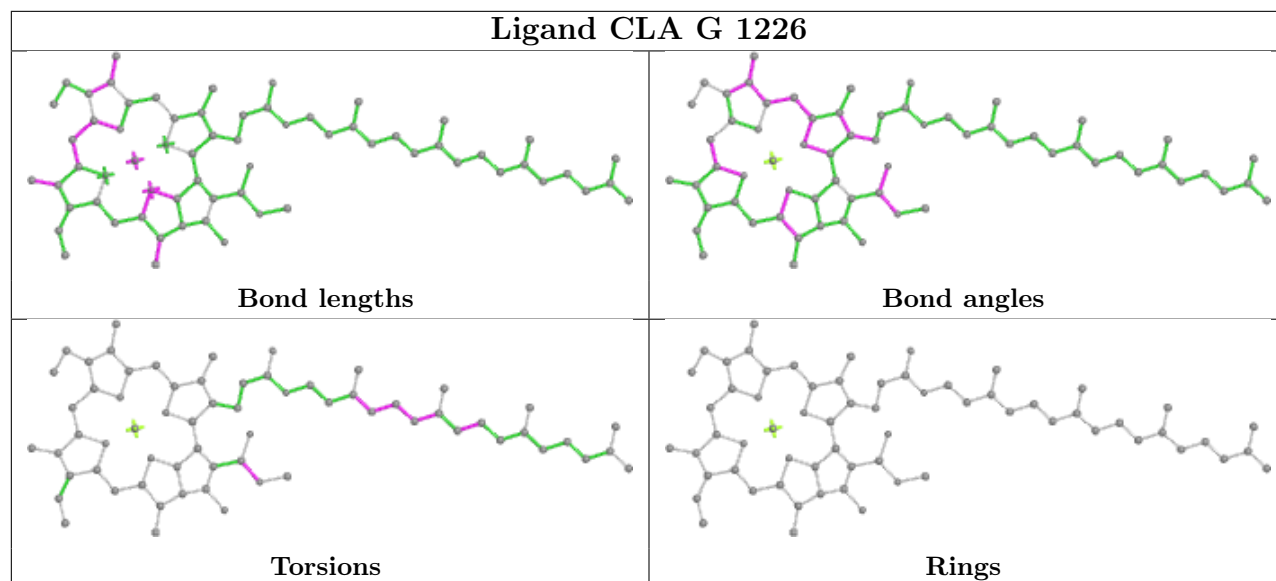
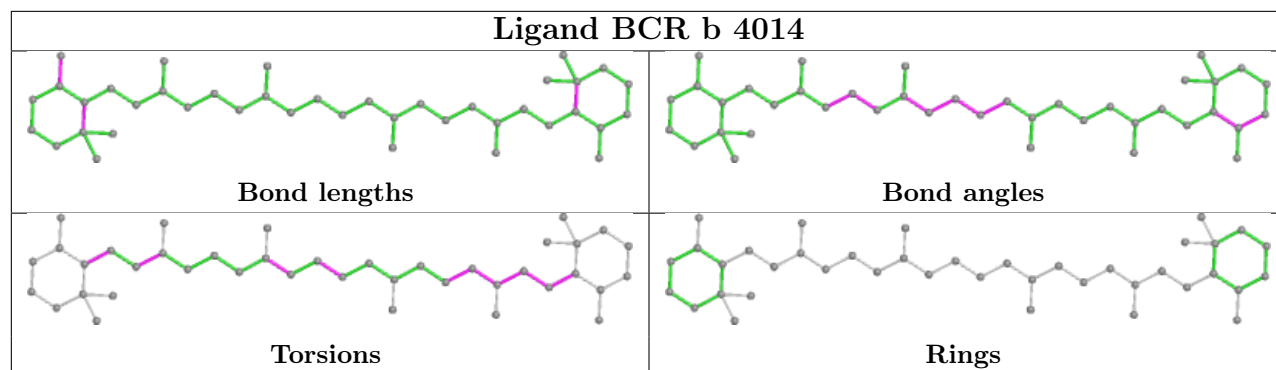


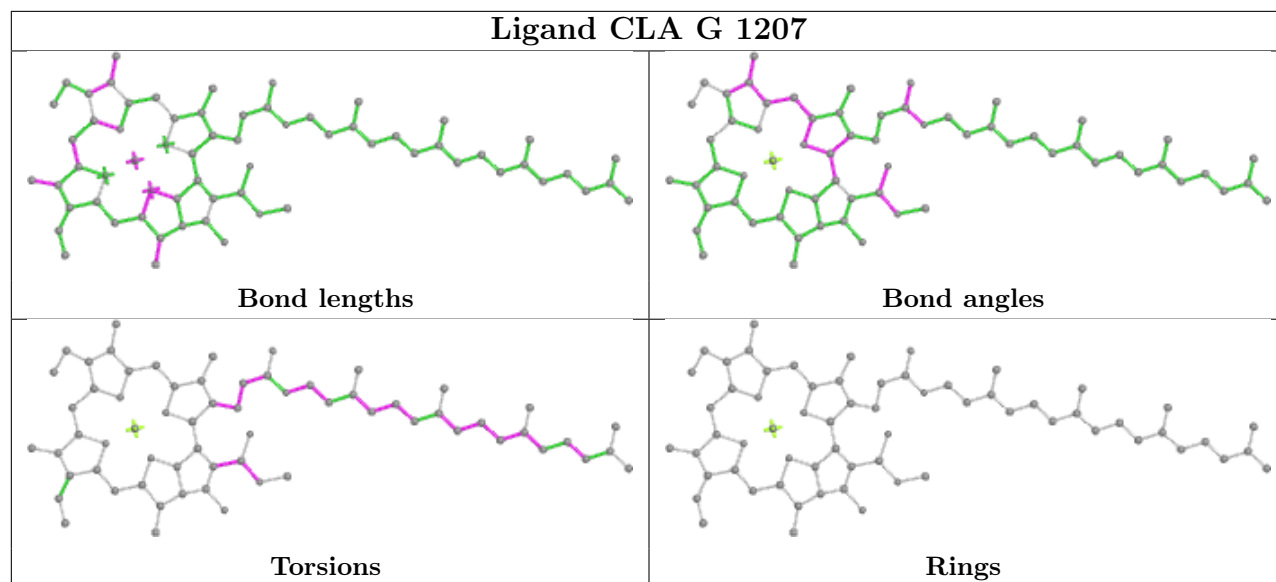
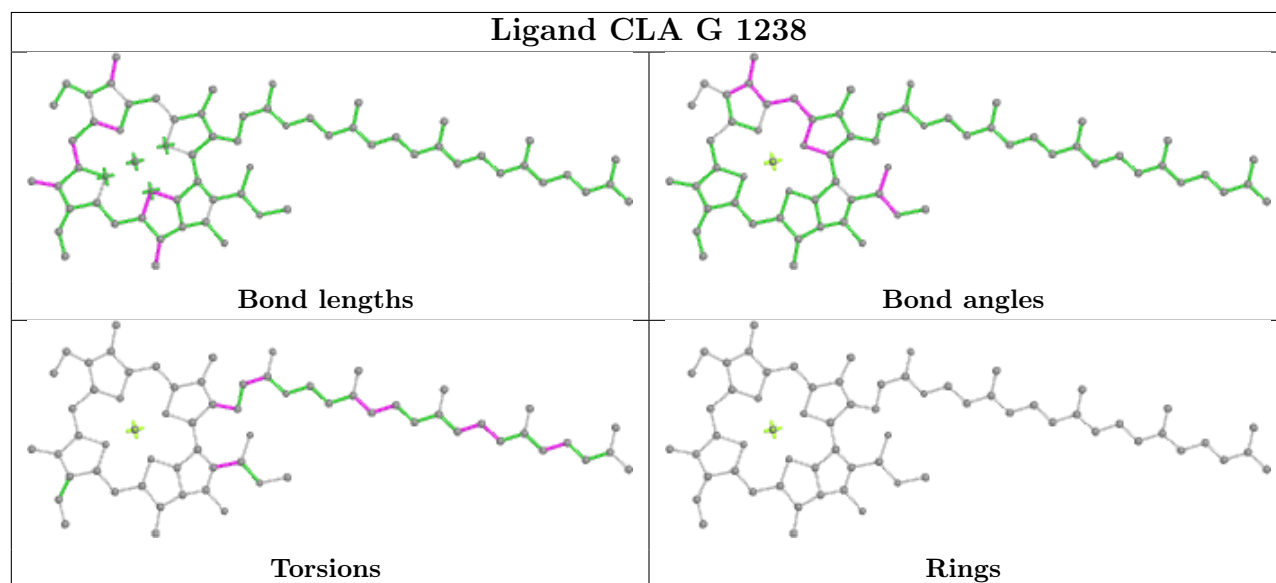
## Ligand CLA B 1231



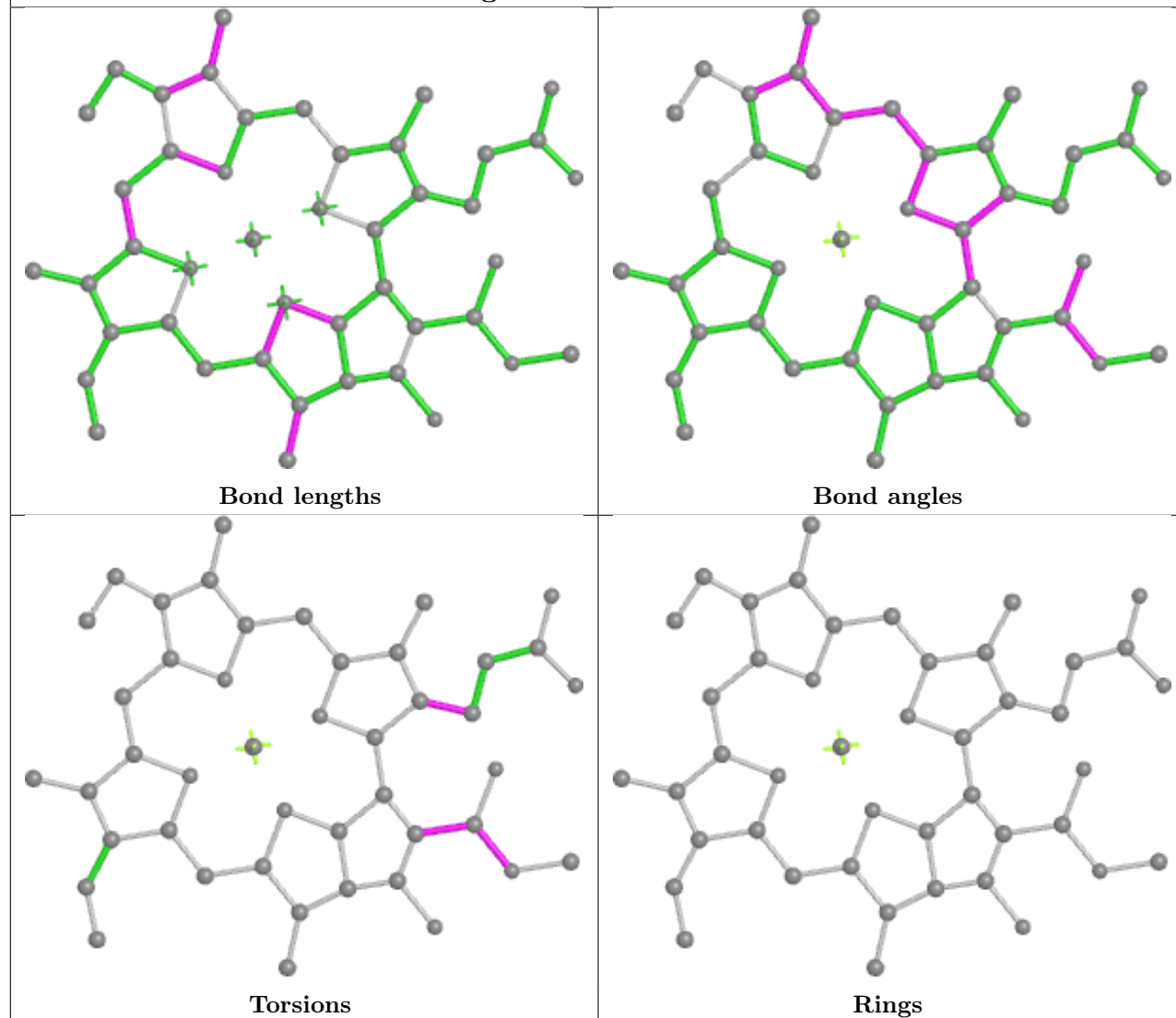
## Ligand BCR X 604



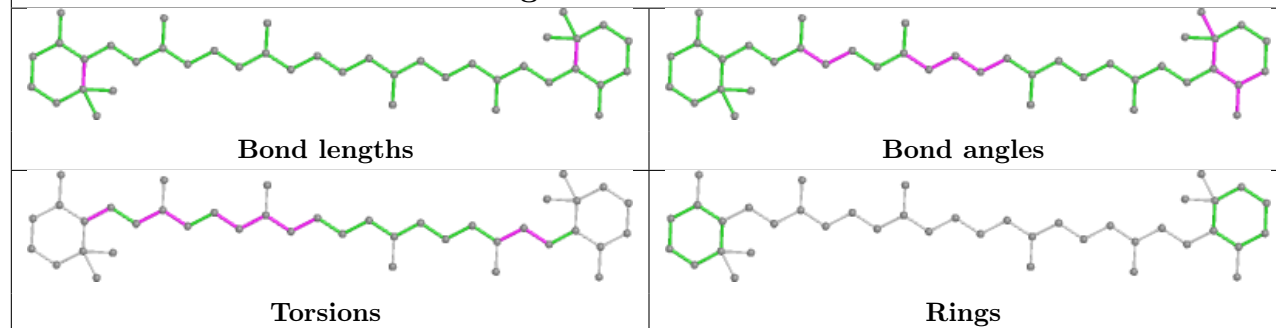


**Ligand CLA G 1207****Ligand CLA G 1238**

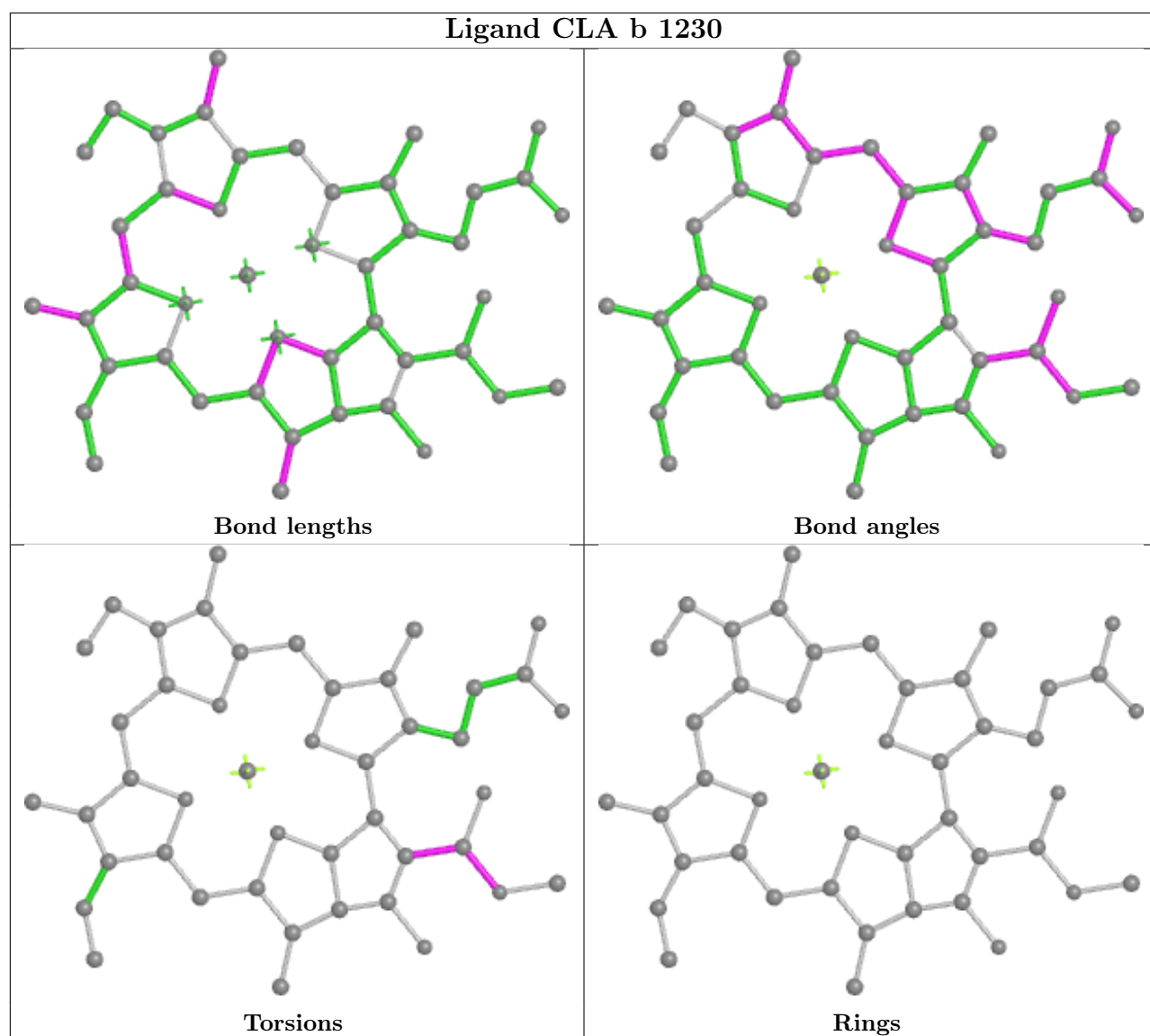
## Ligand CLA G 1232

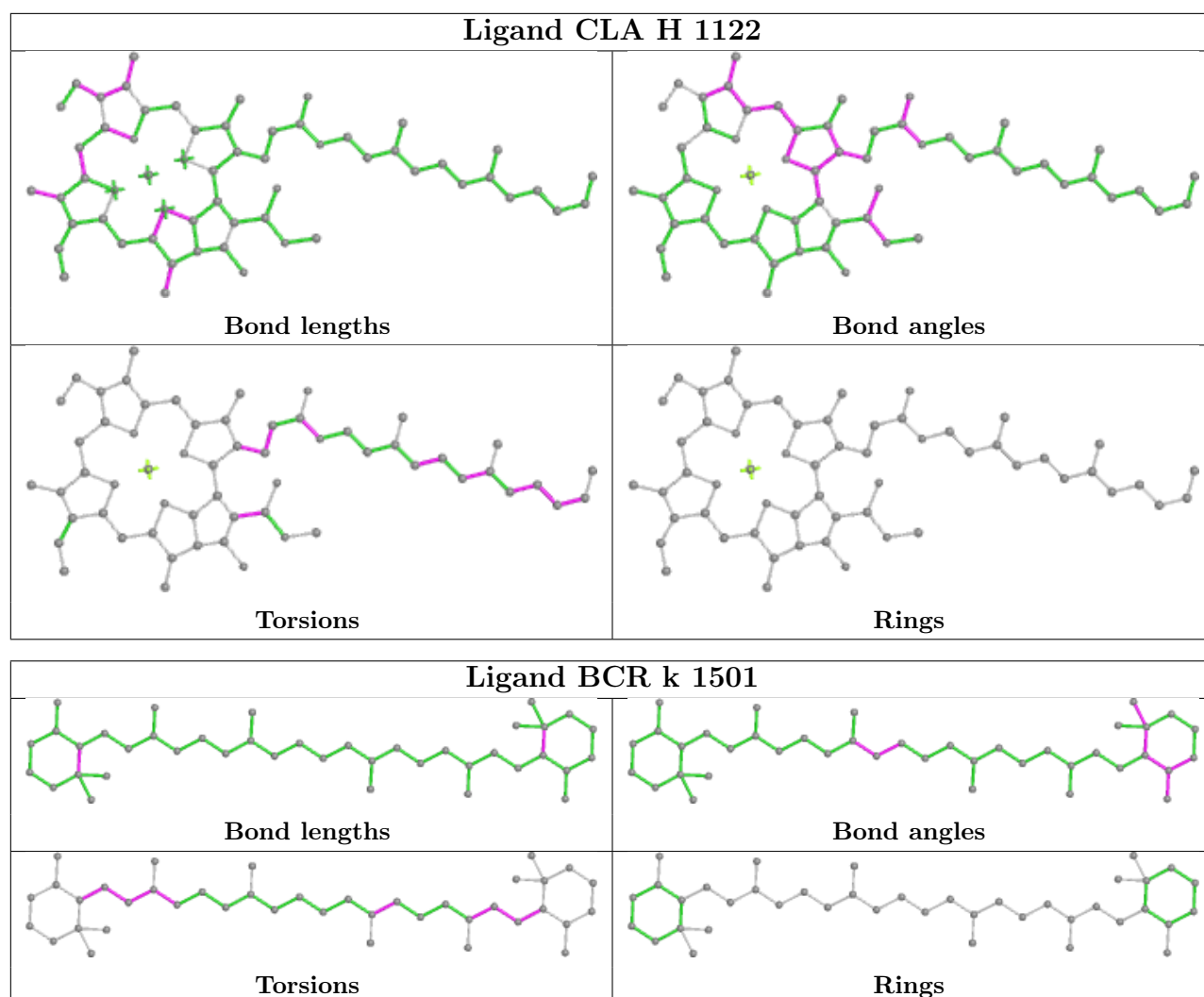


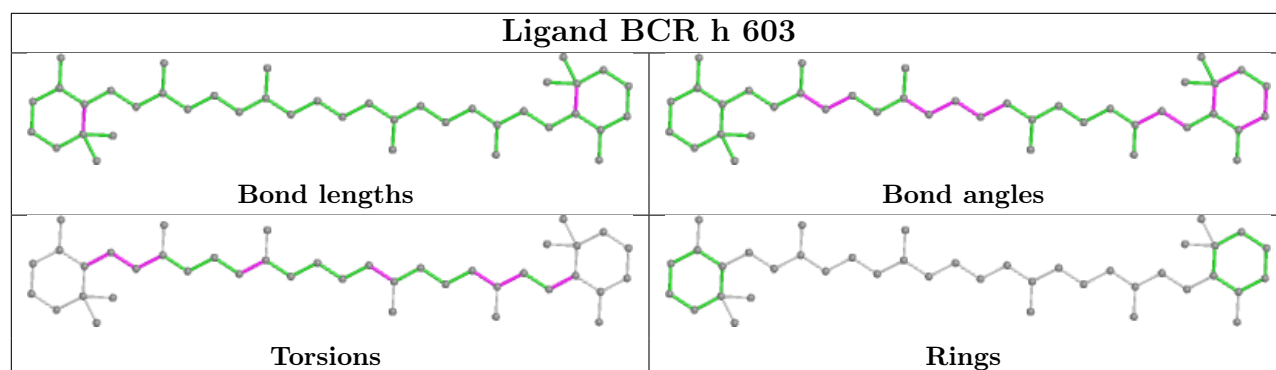
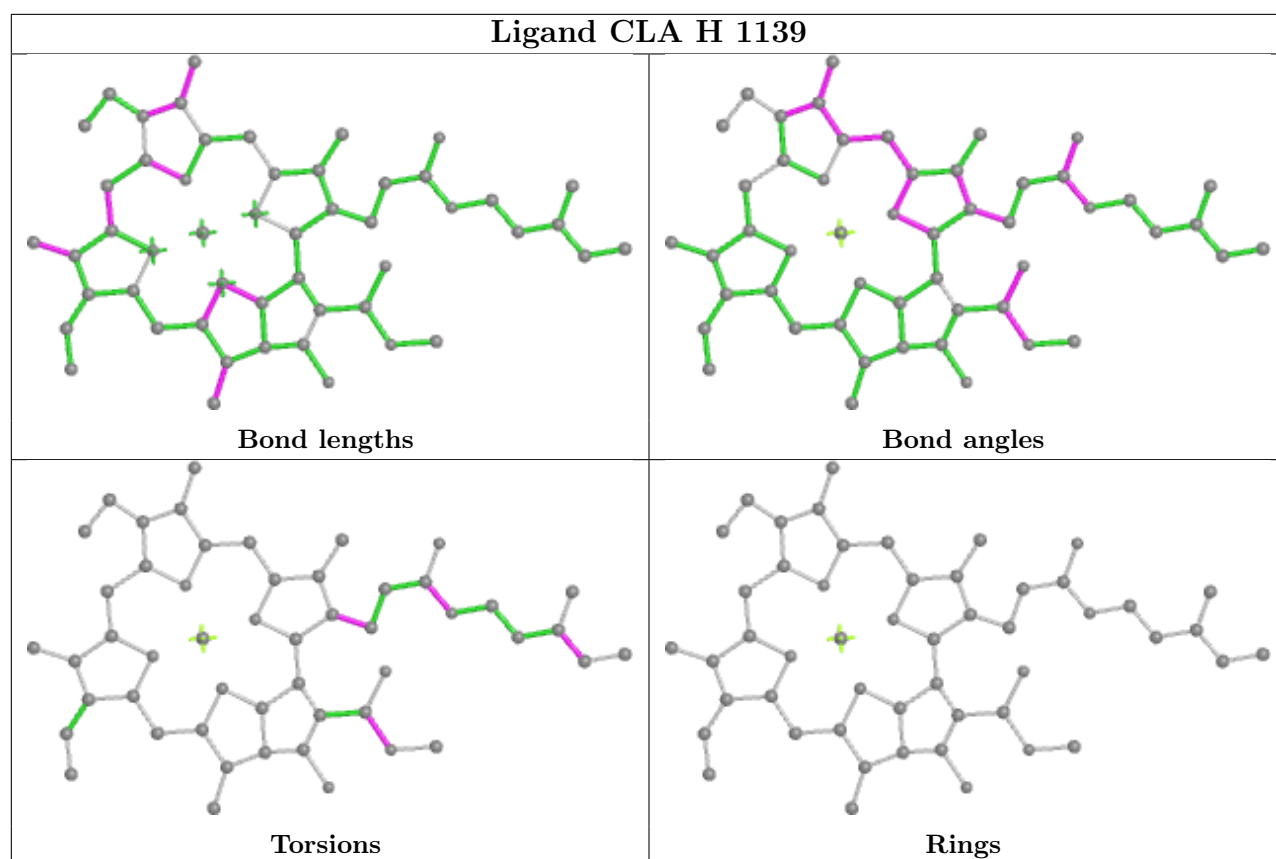
## Ligand BCR H 4003



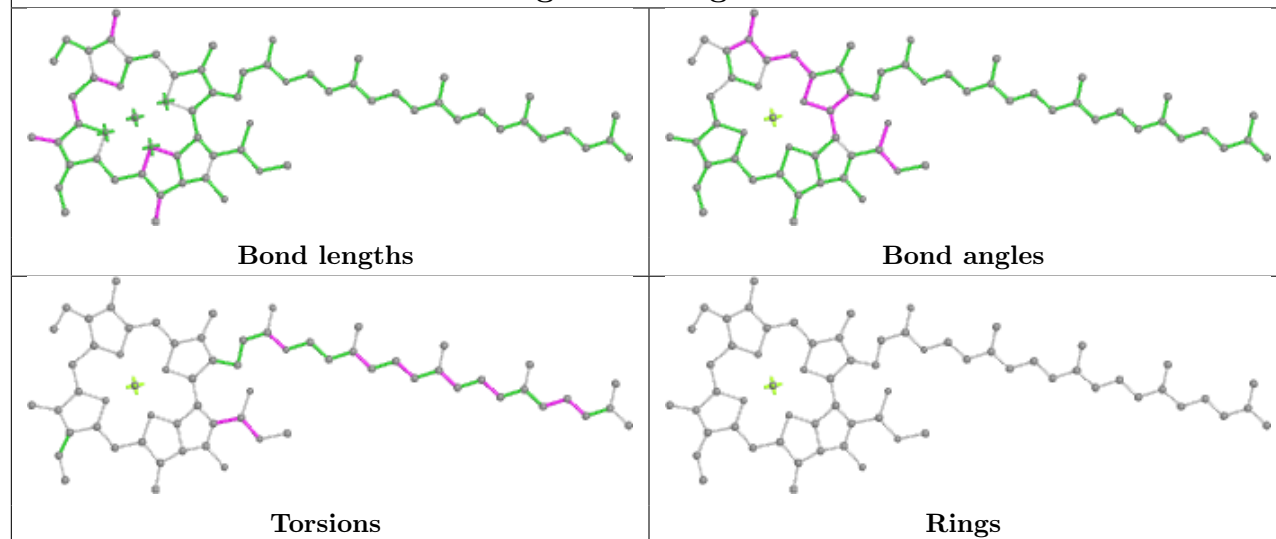




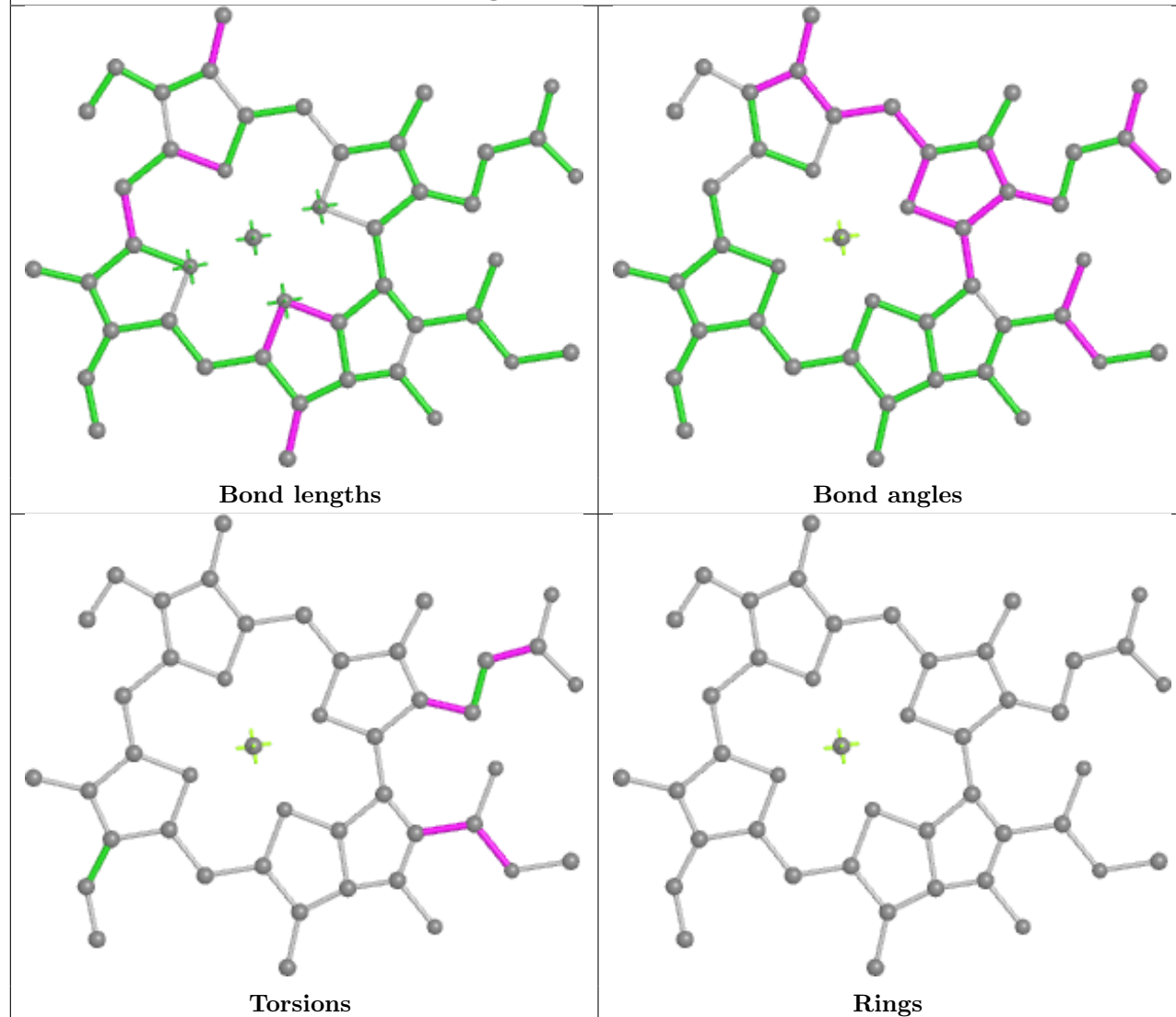




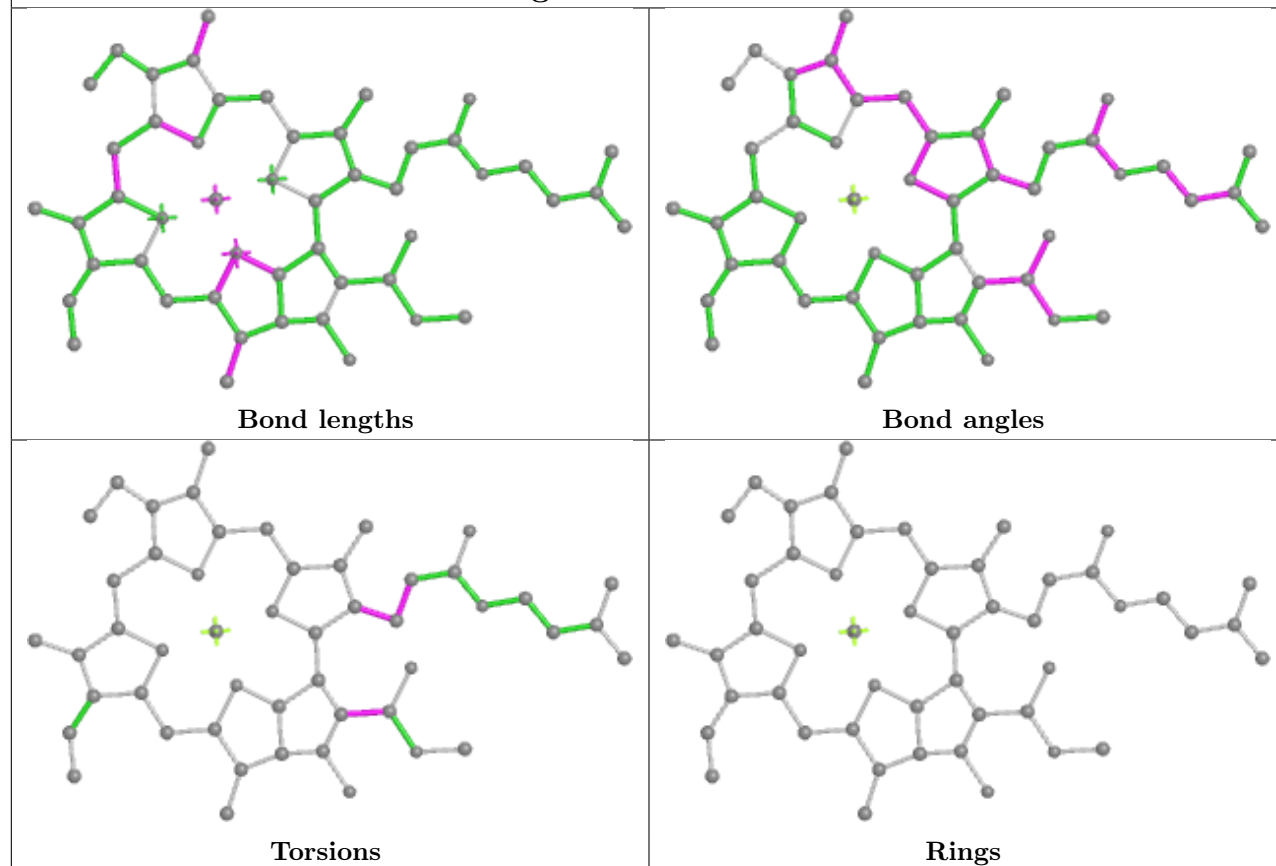
## Ligand CLA g 507



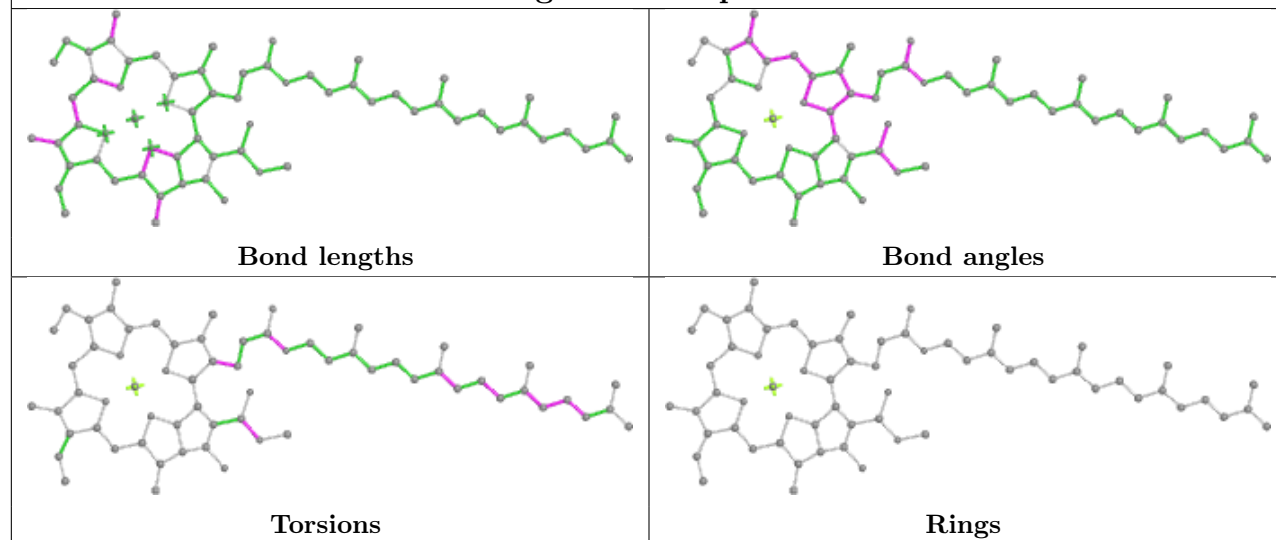
## Ligand CLA J 1302



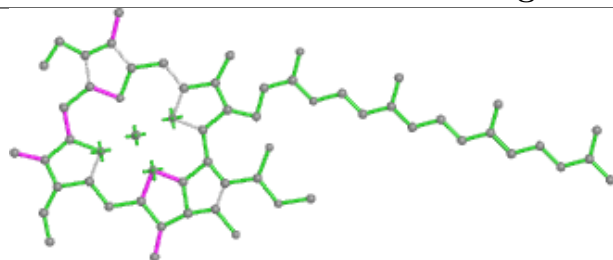
## Ligand CLA X 502



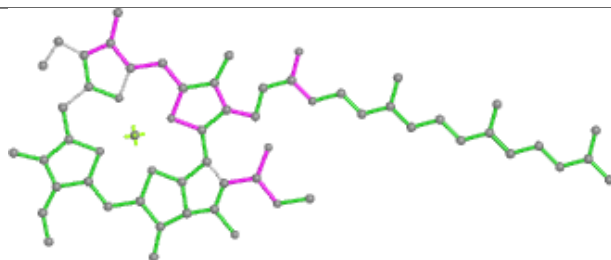
## Ligand CLA q 511



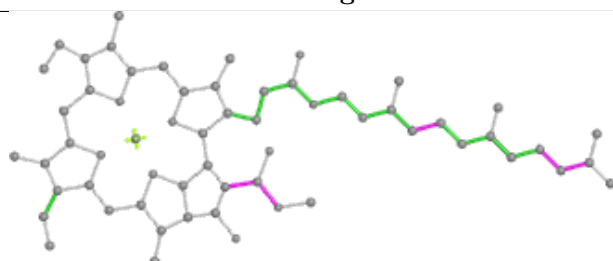
## Ligand CLA v 509



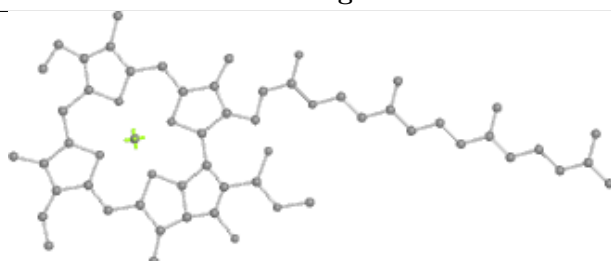
Bond lengths



Bond angles

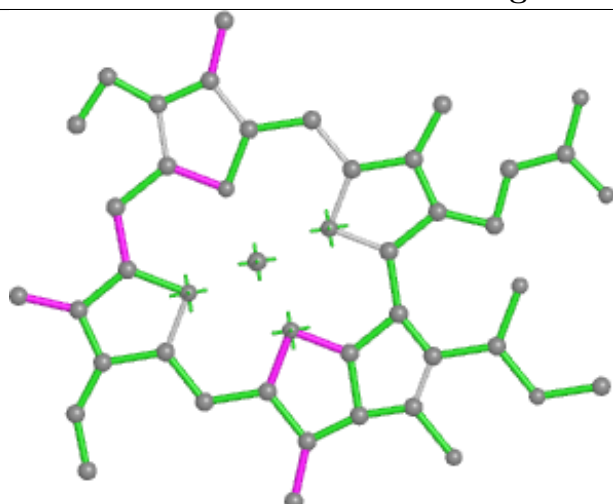


Torsions

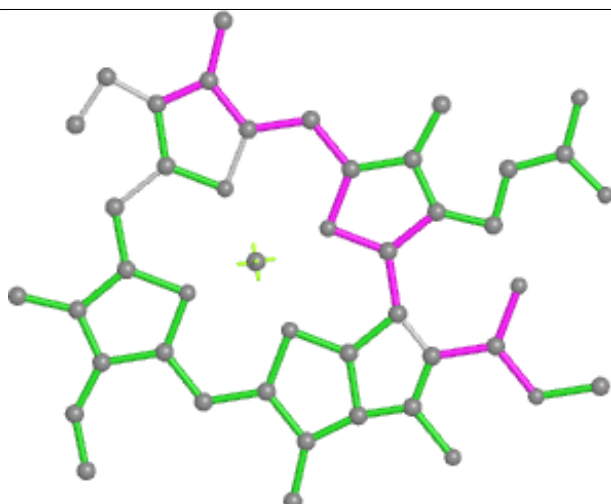


Rings

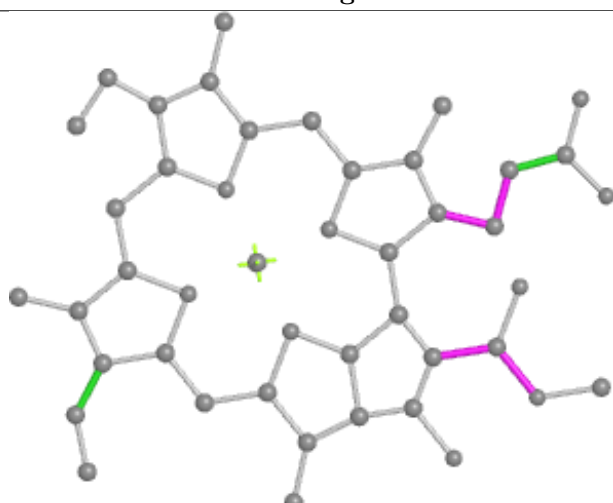
## Ligand CLA a 1113



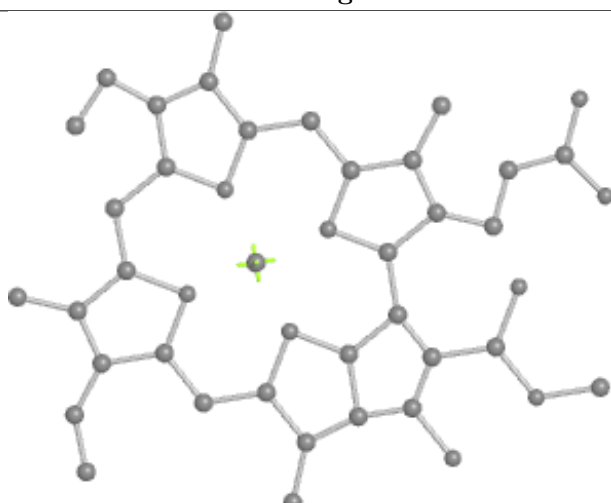
Bond lengths



Bond angles

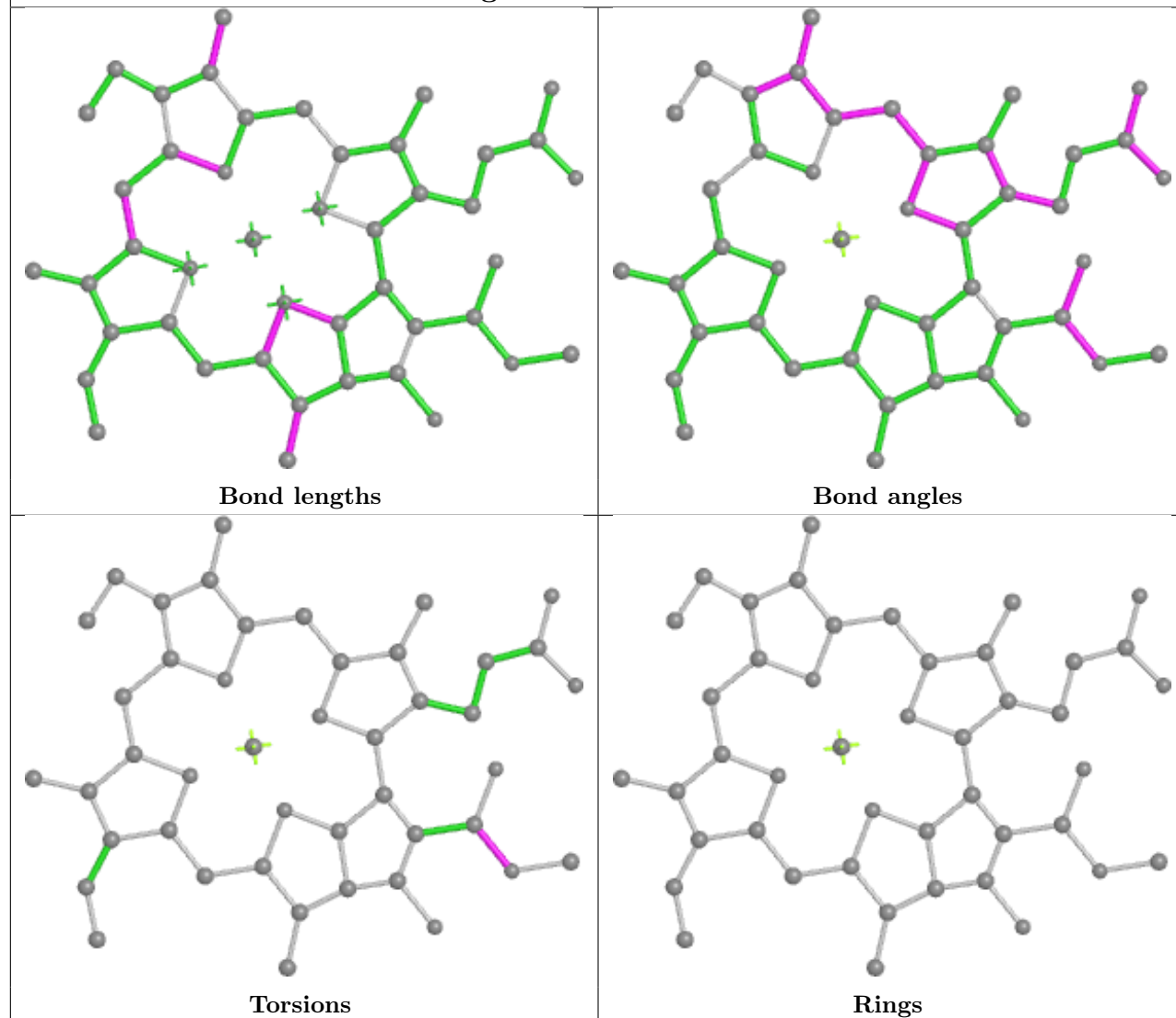


Torsions

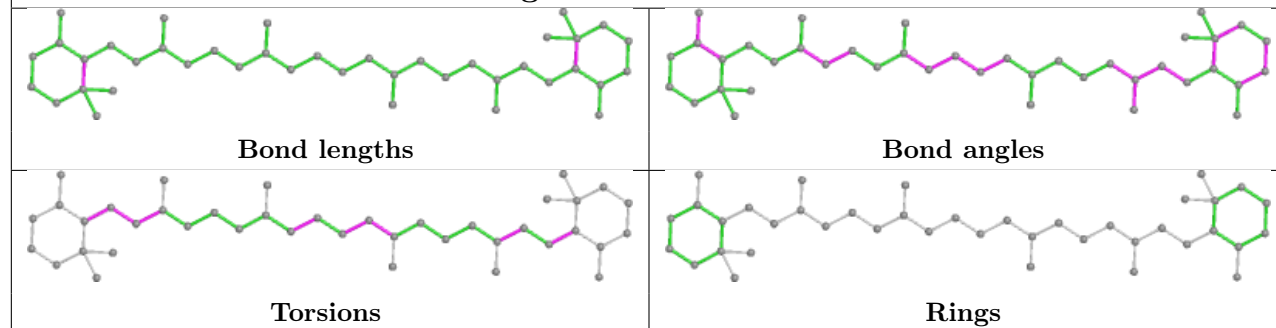


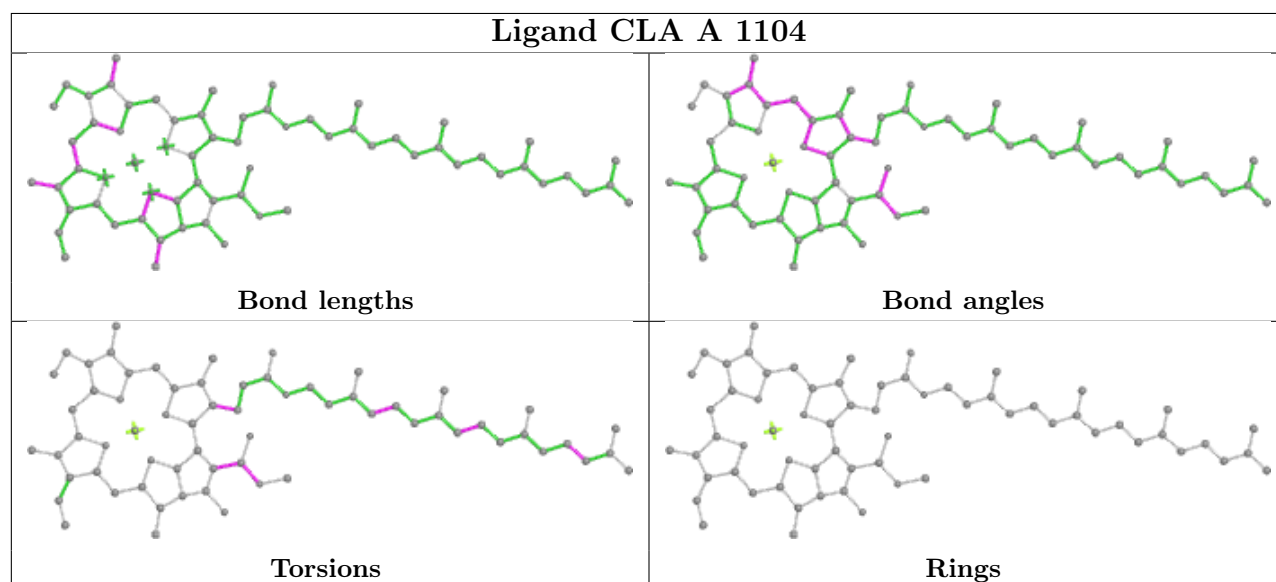
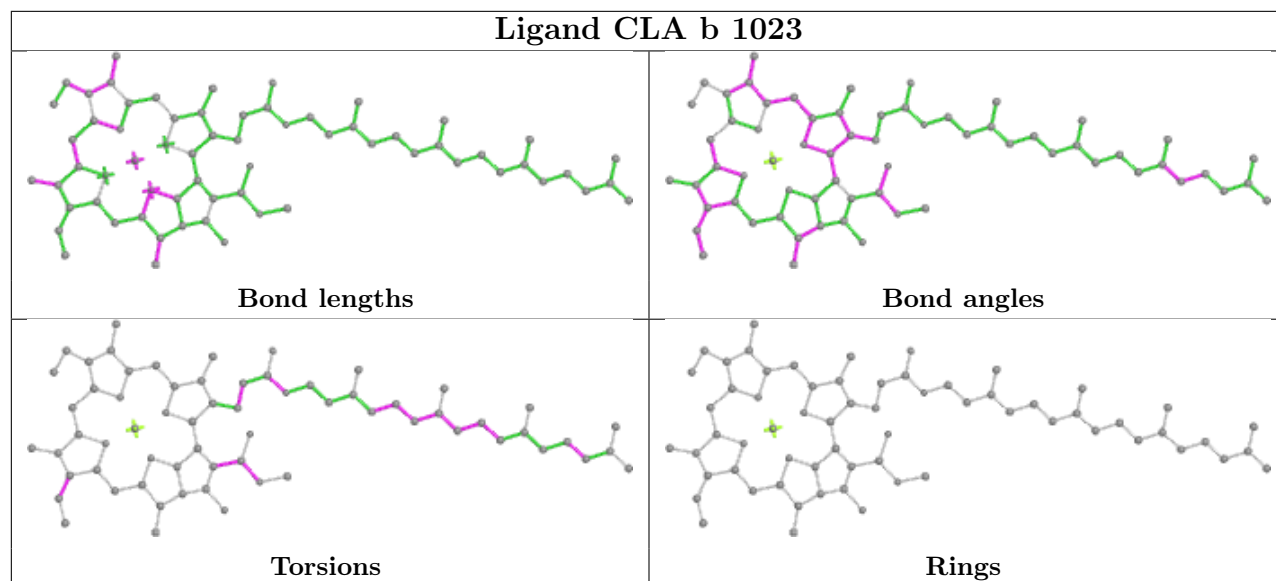
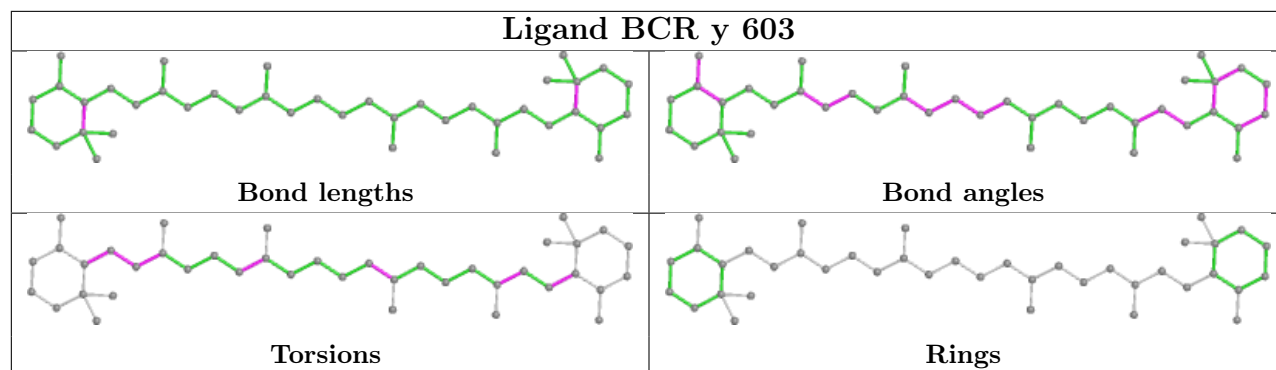
Rings

## Ligand CLA G 1208



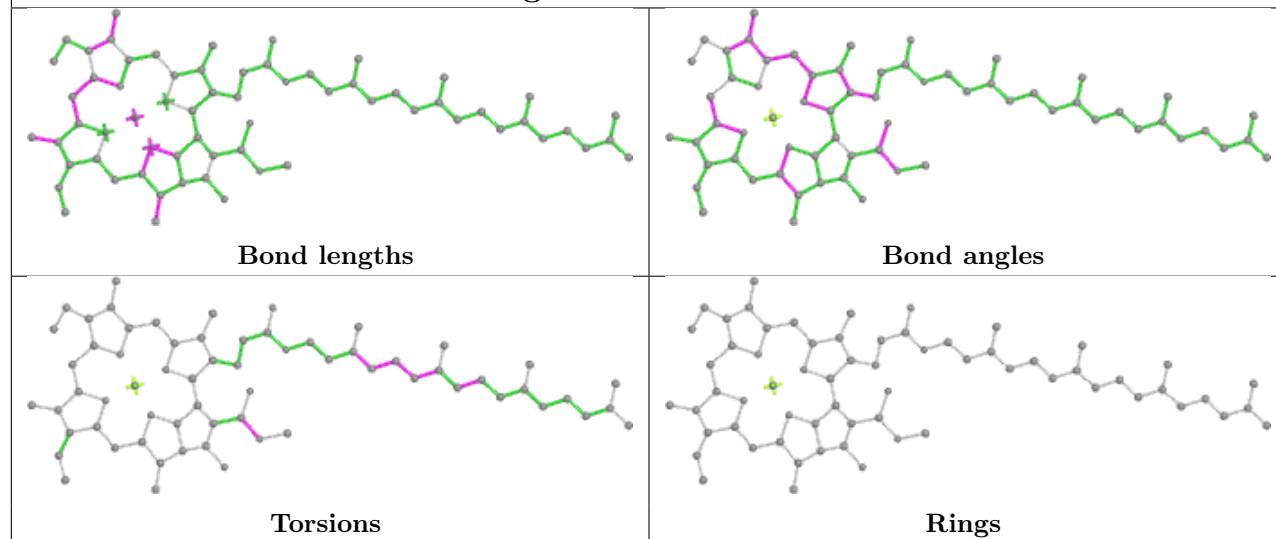
## Ligand BCR A 4008



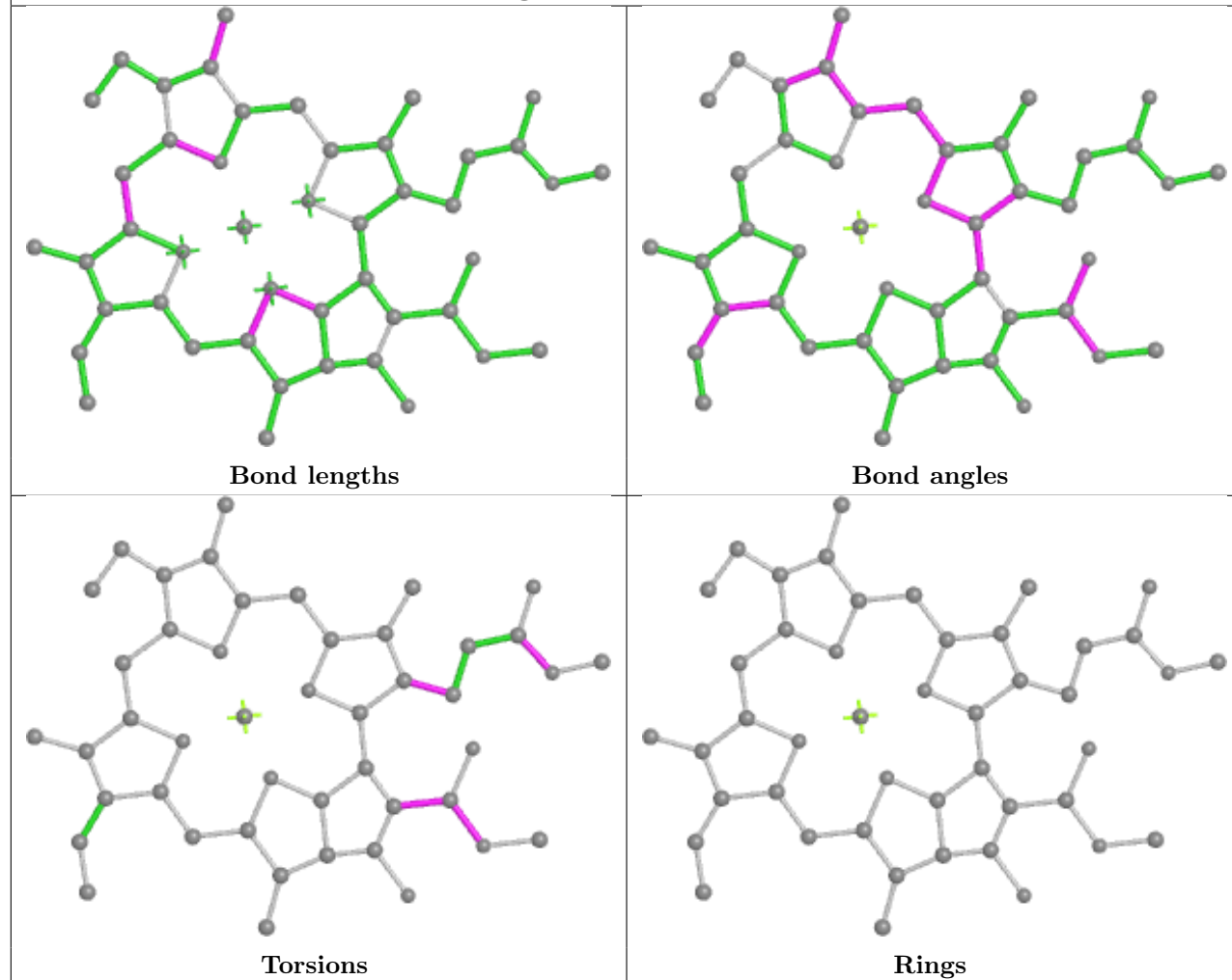


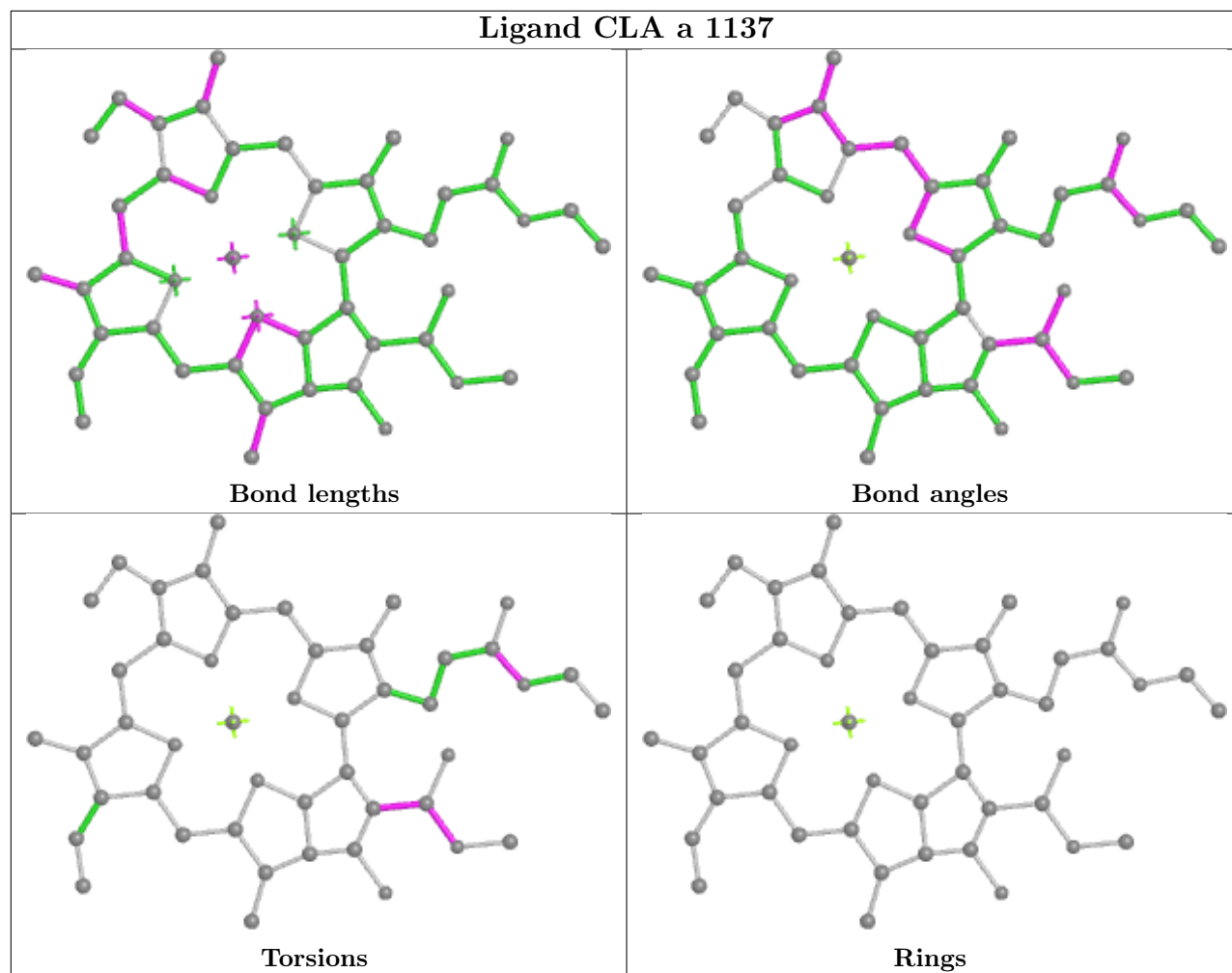


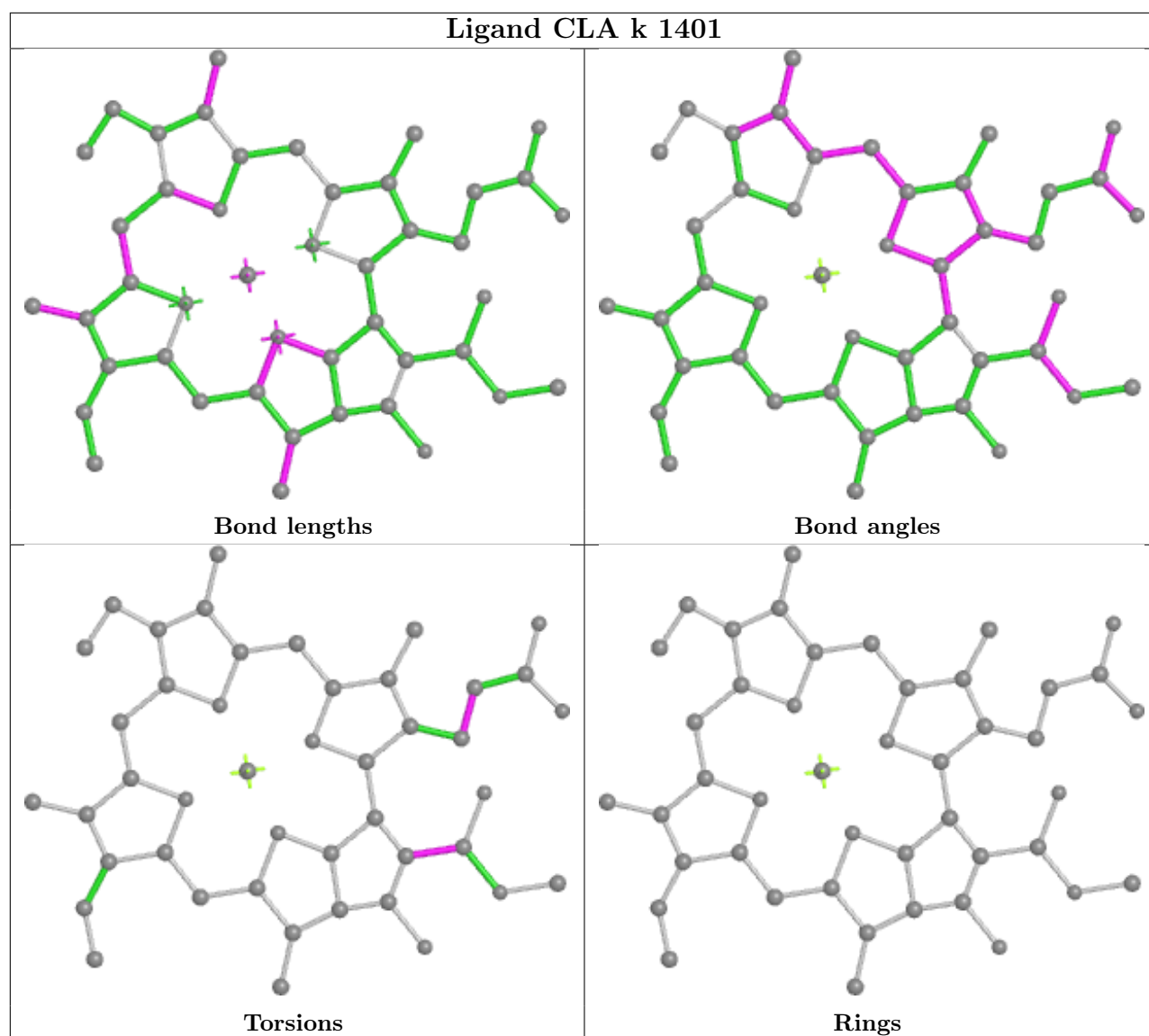
## Ligand CLA B 1226



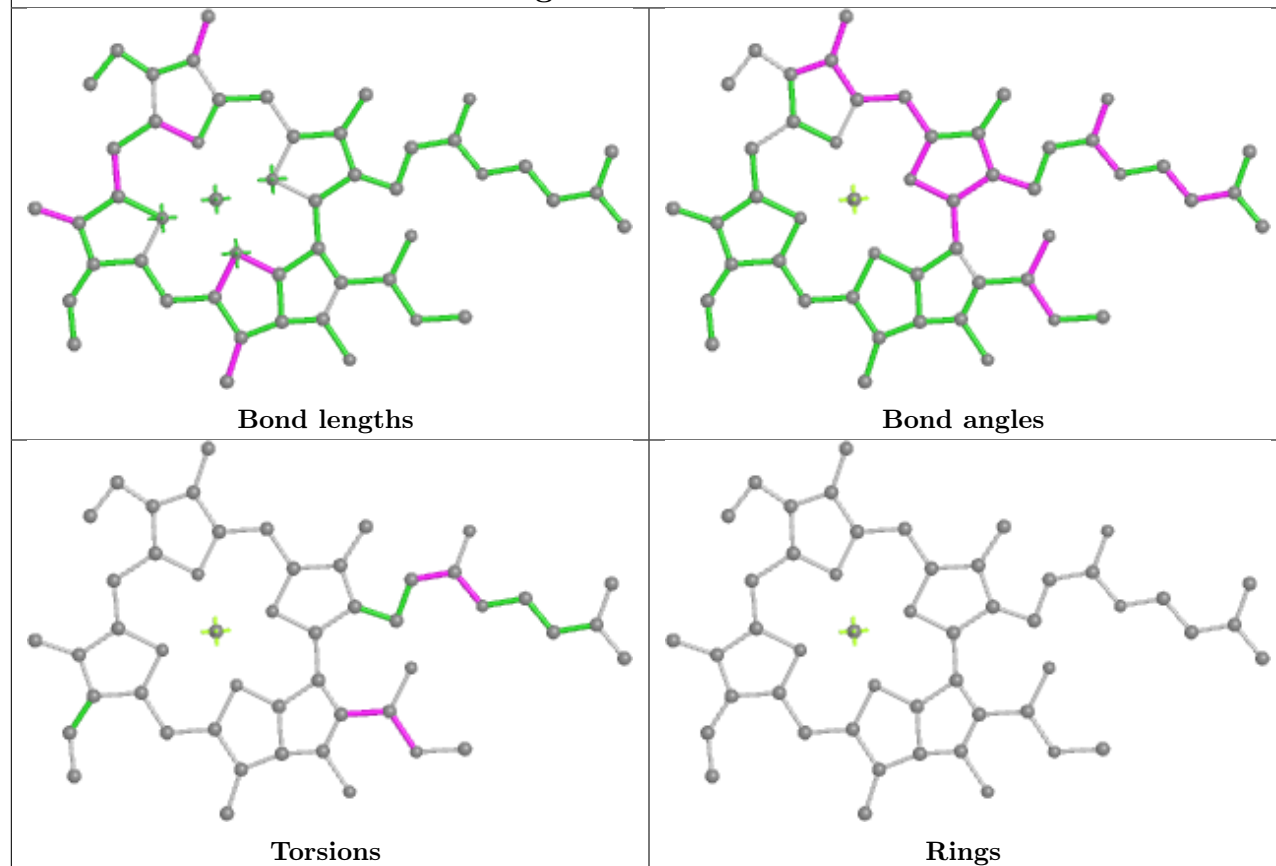
## Ligand CLA Z 516



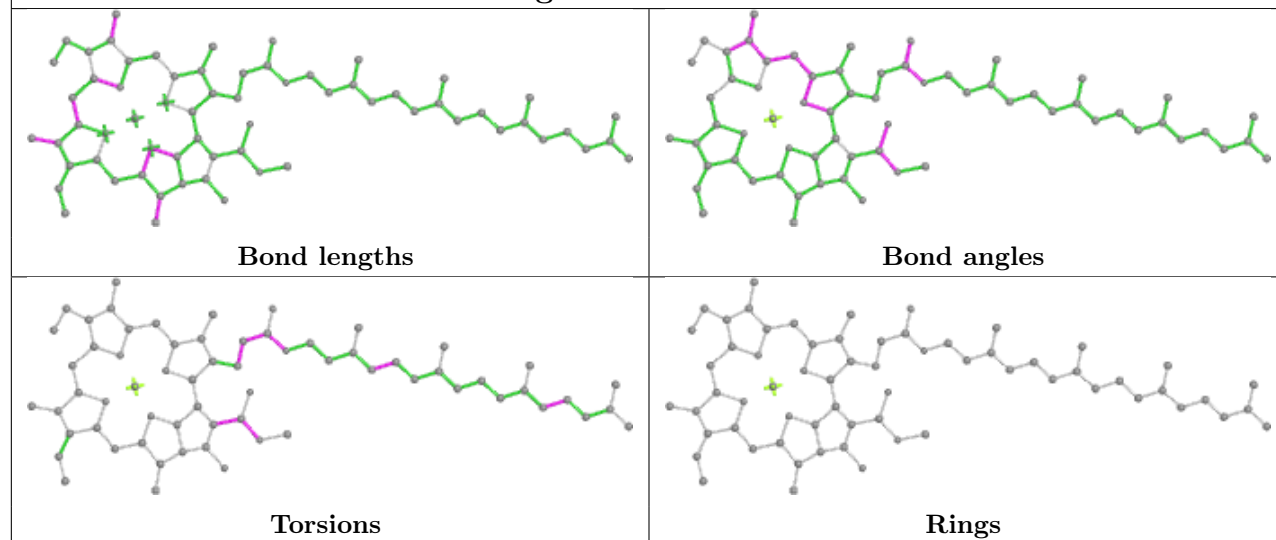


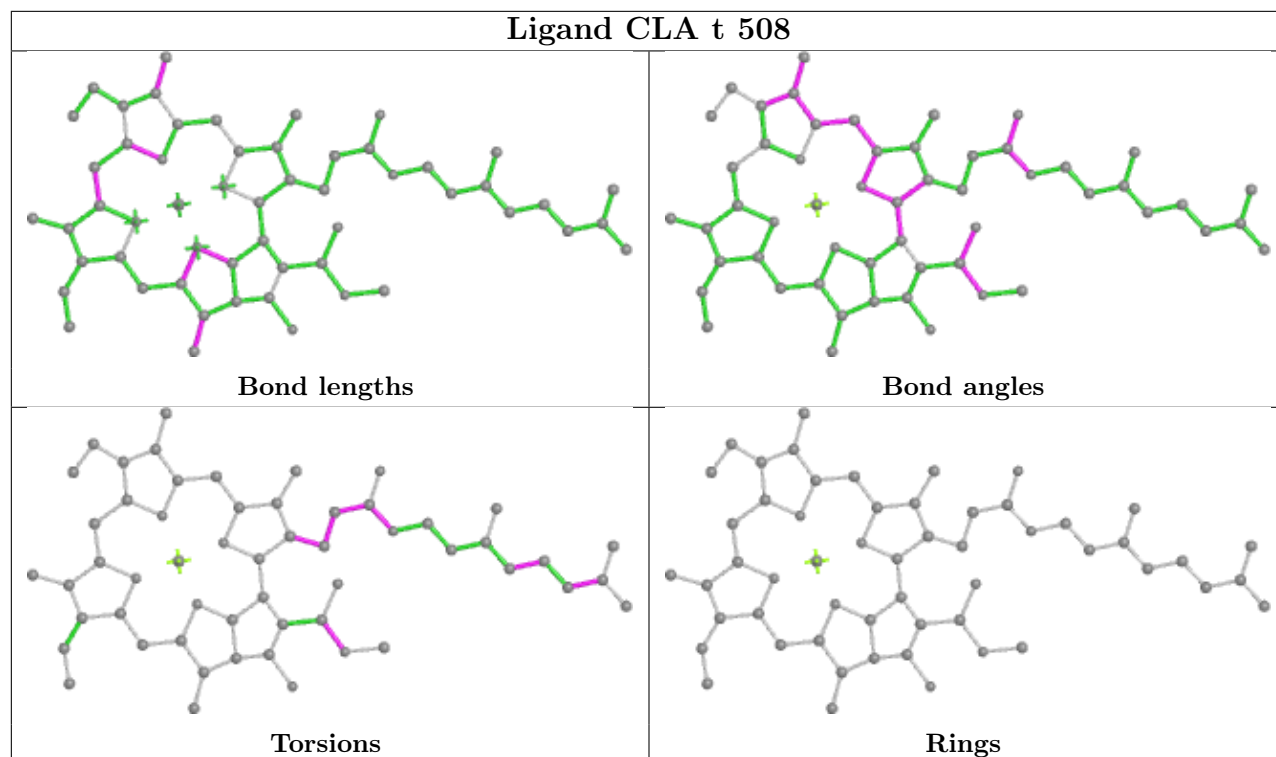
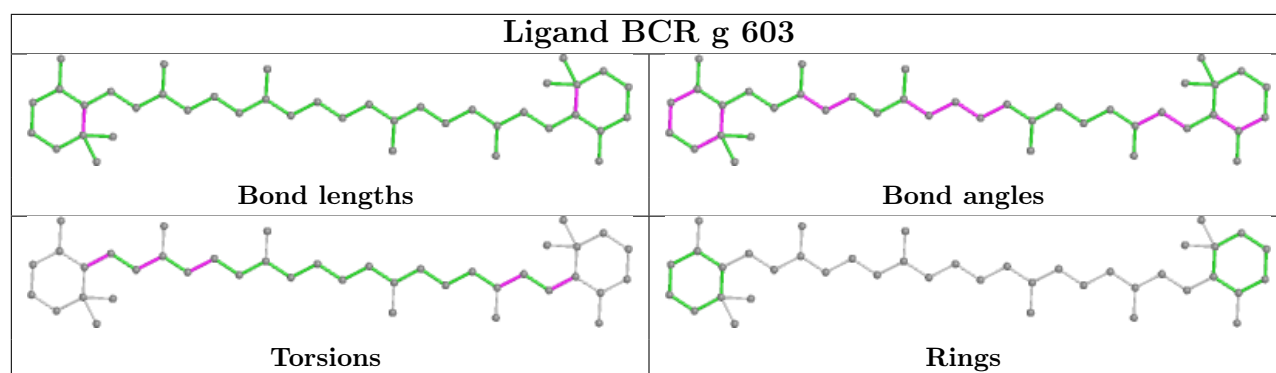


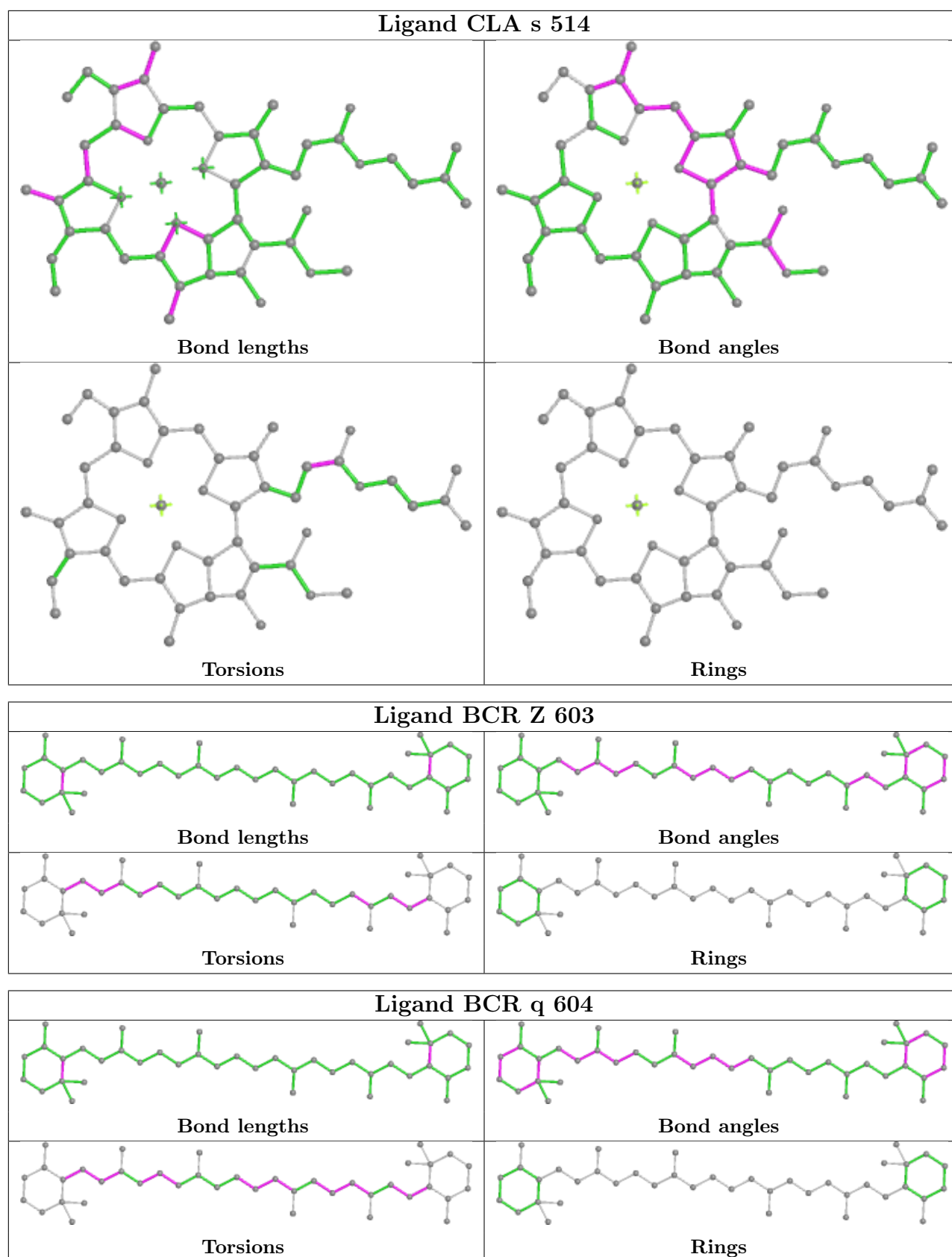
## Ligand CLA n 514

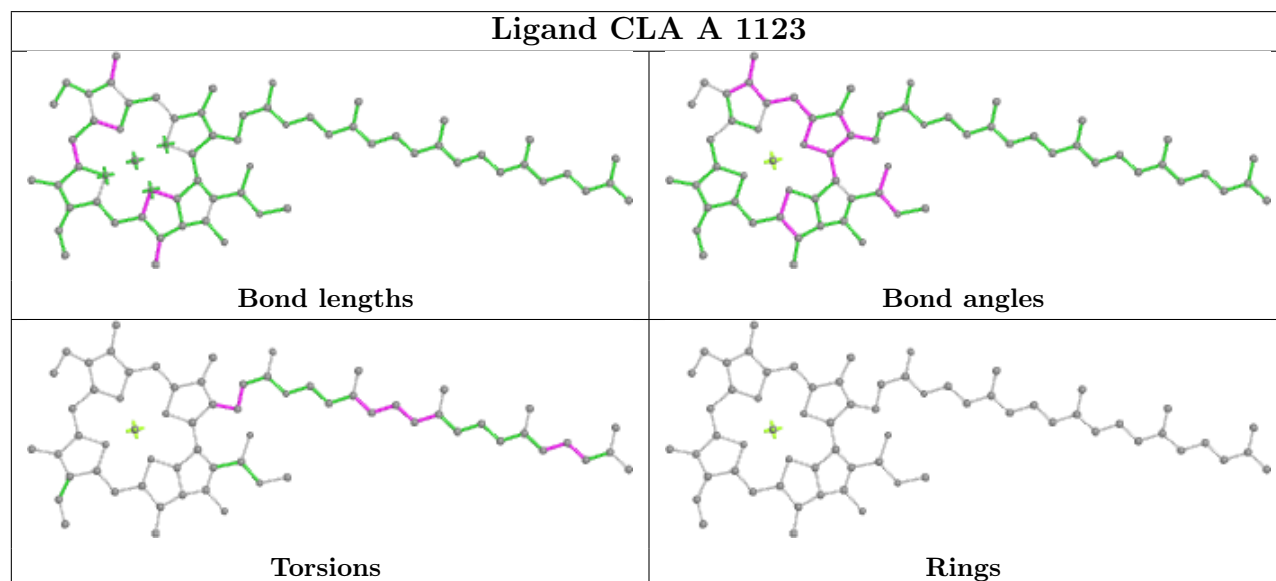
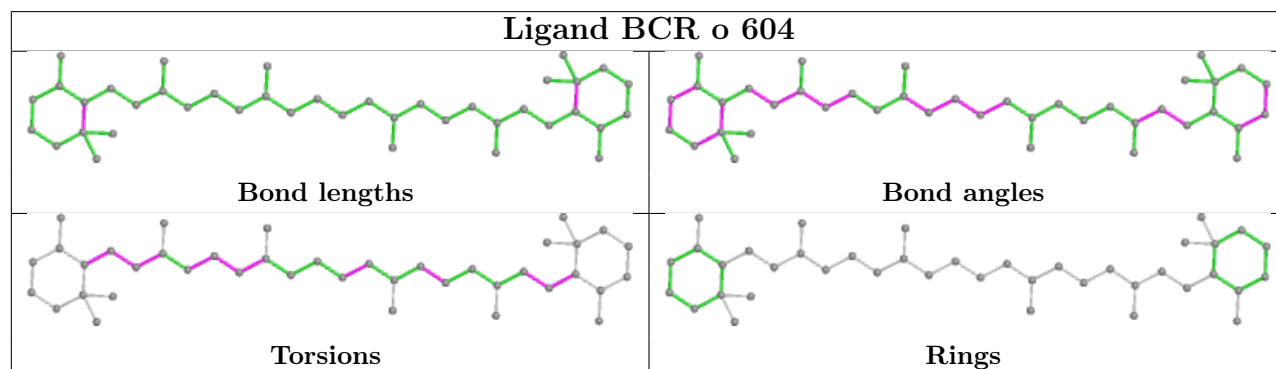
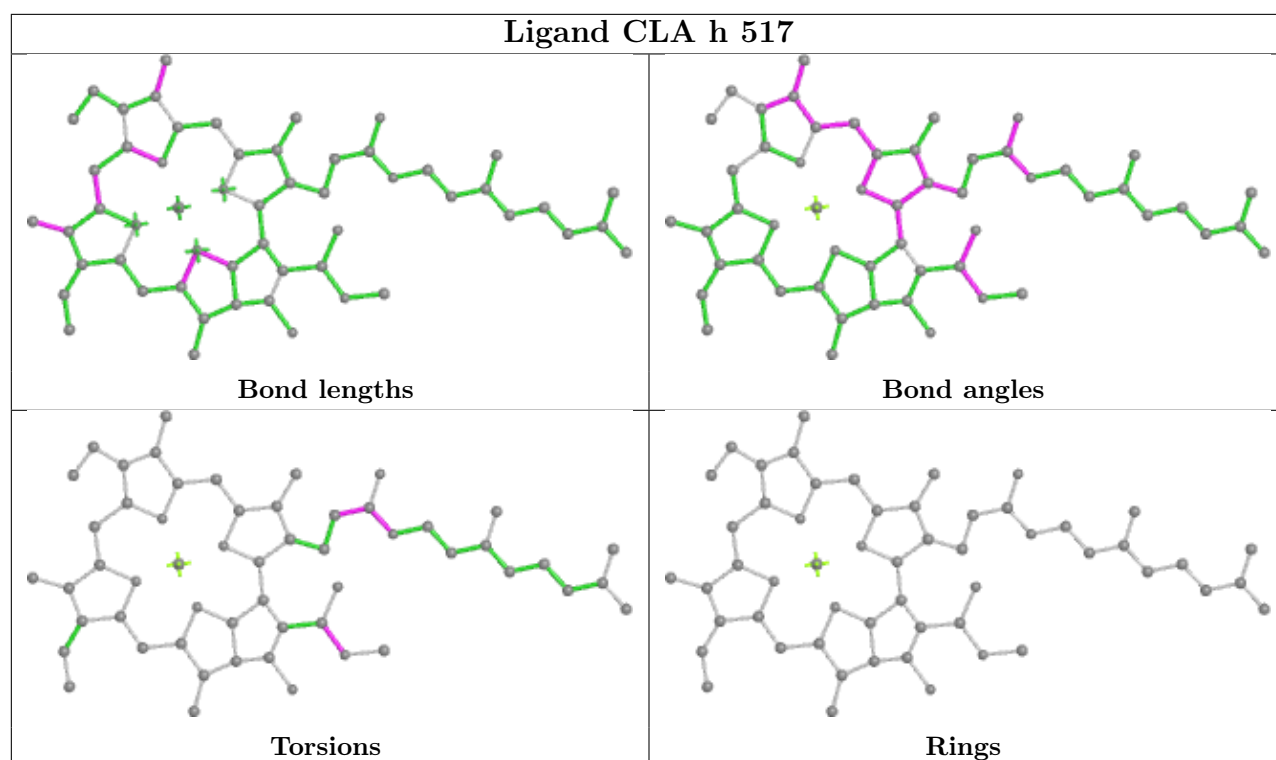


## Ligand CLA x 511

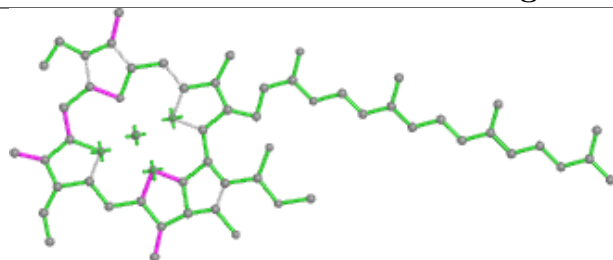




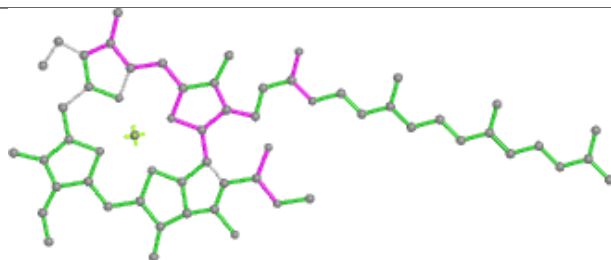




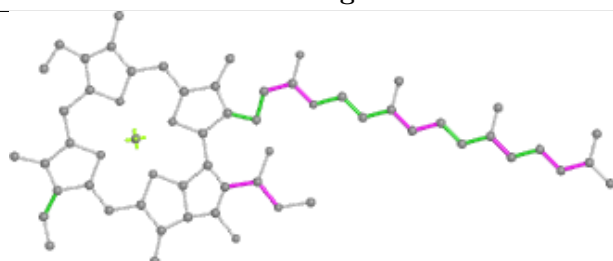
## Ligand CLA s 509



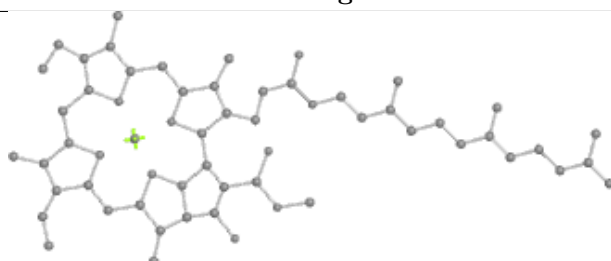
Bond lengths



Bond angles

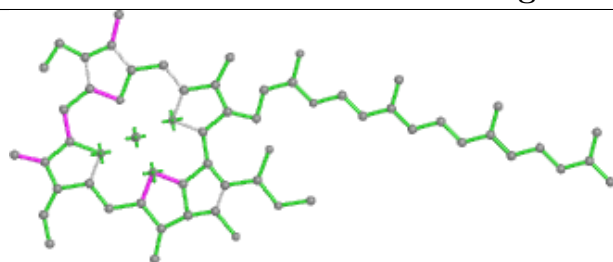


Torsions

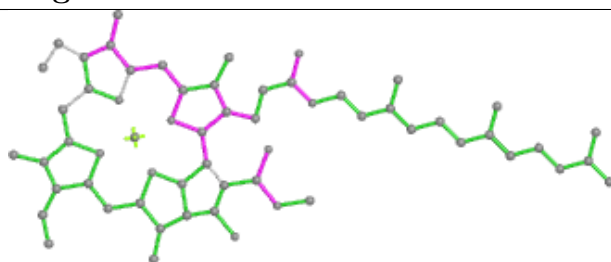


Rings

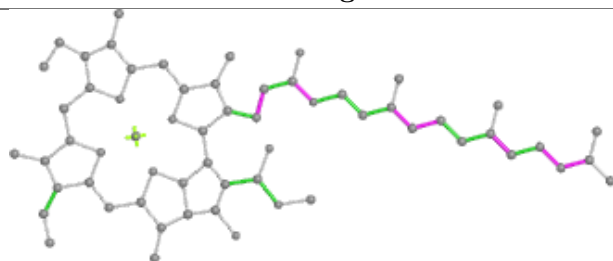
## Ligand CLA g 504



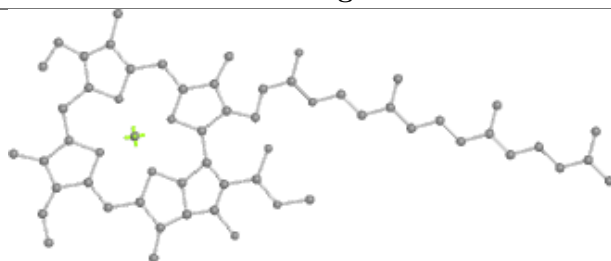
Bond lengths



Bond angles



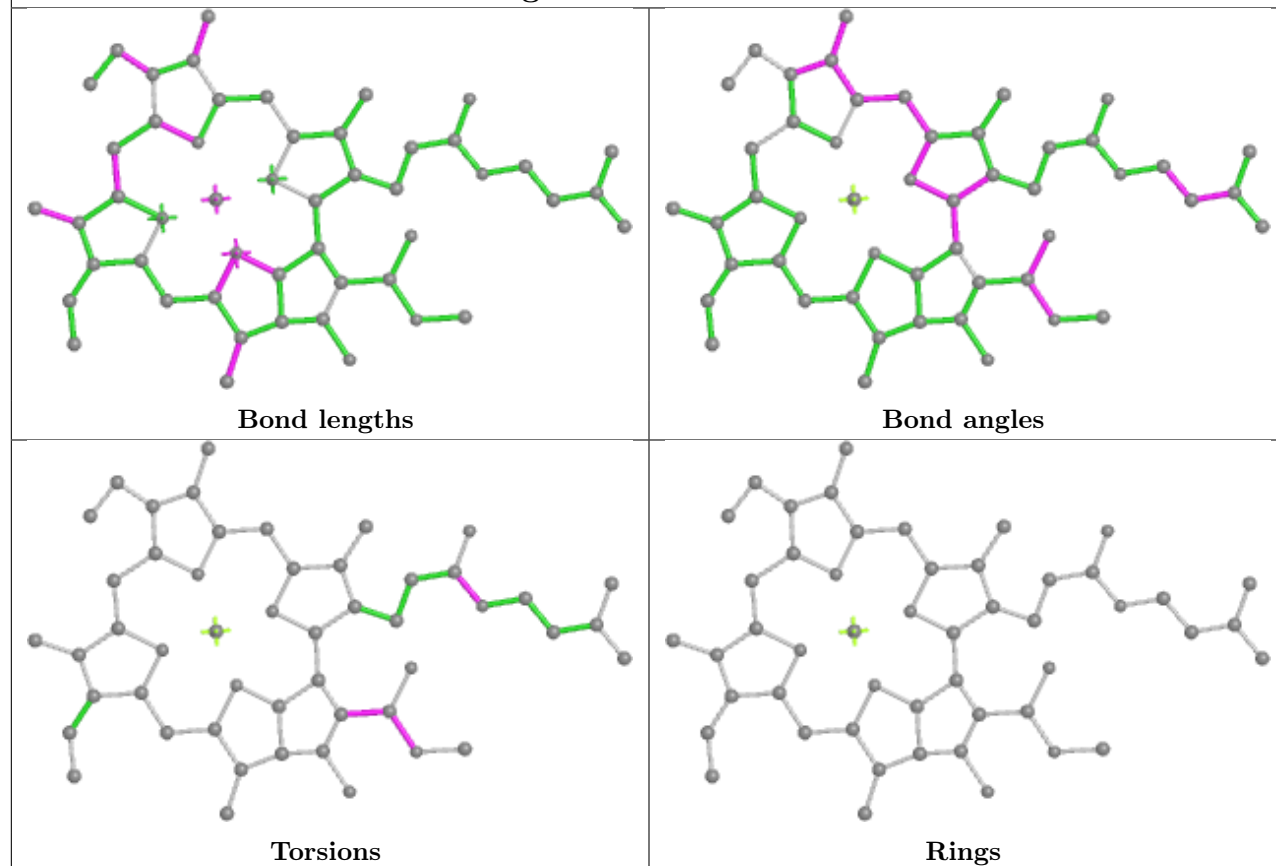
Torsions



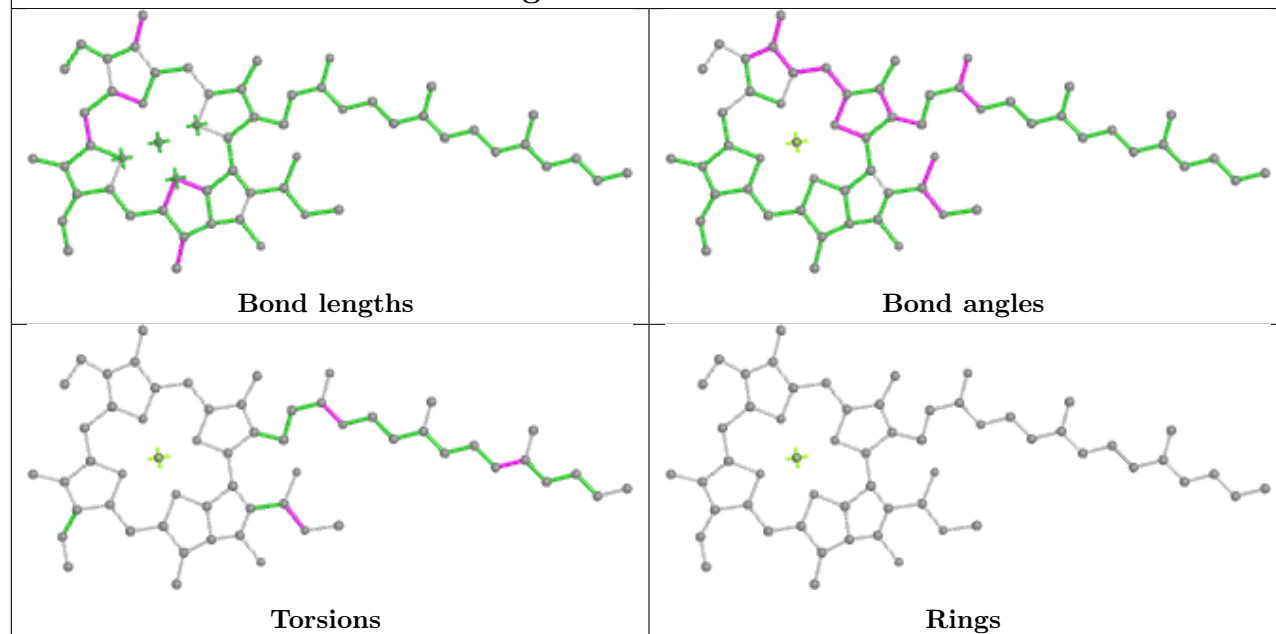
Rings

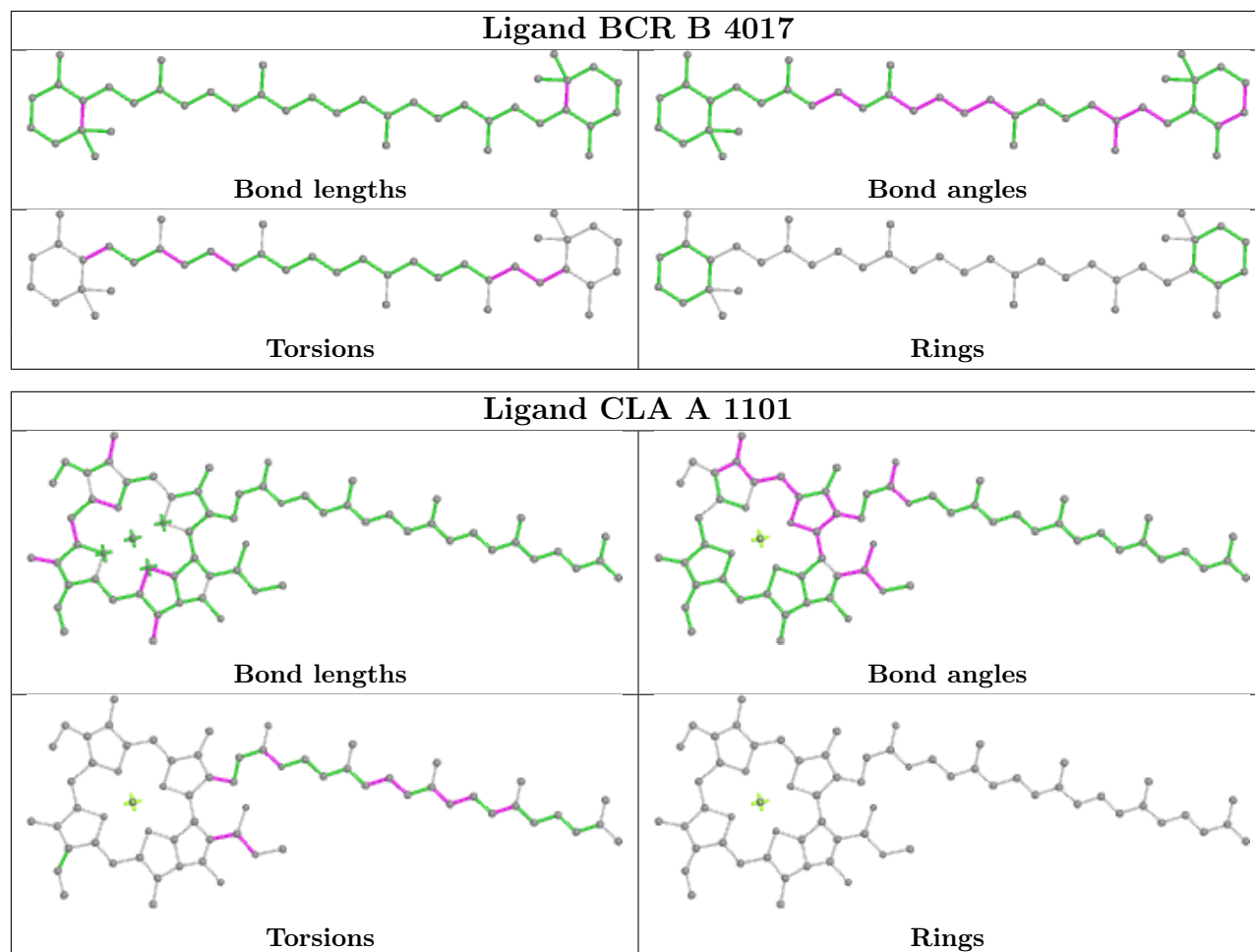


## Ligand CLA G 1234

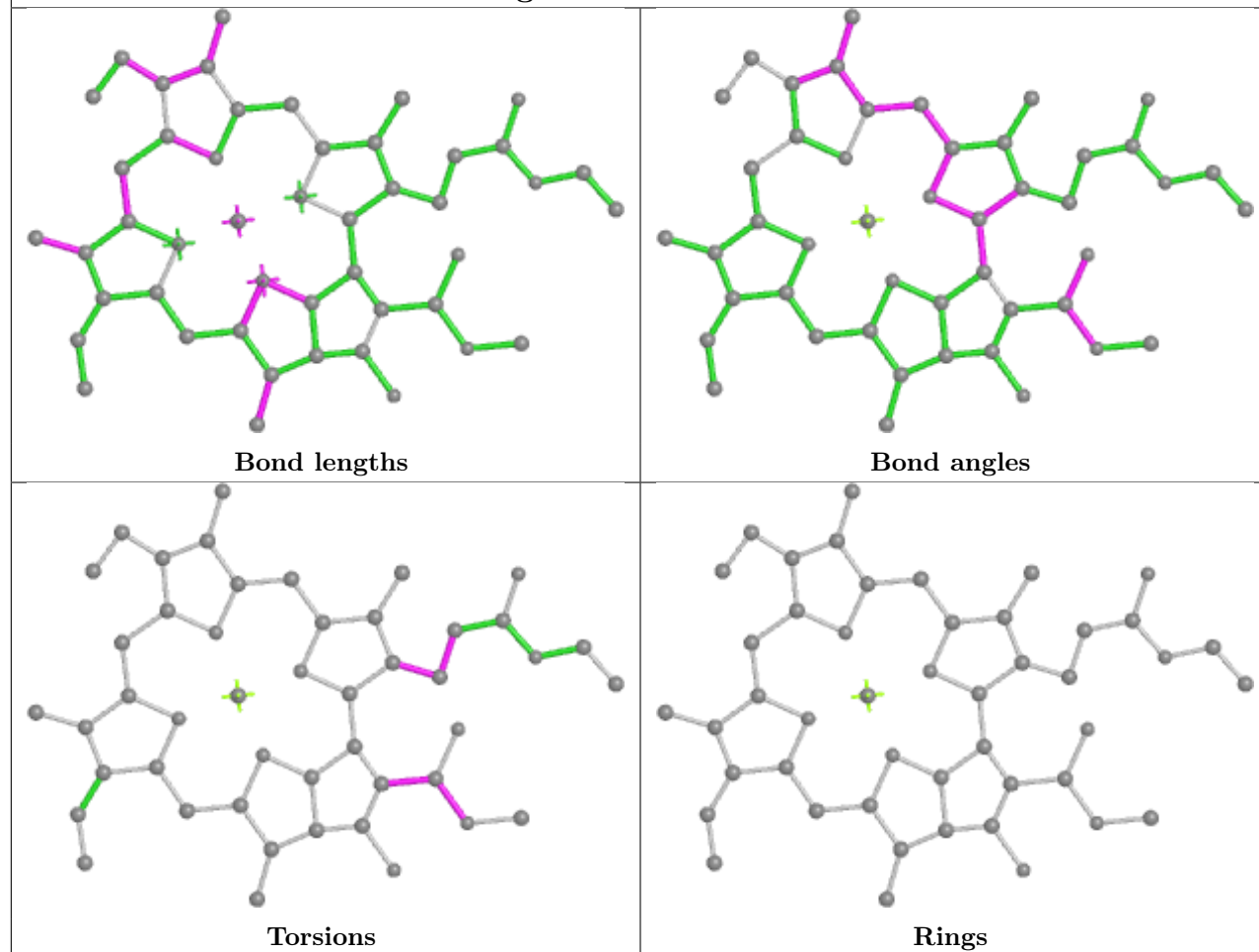


## Ligand CLA A 1105

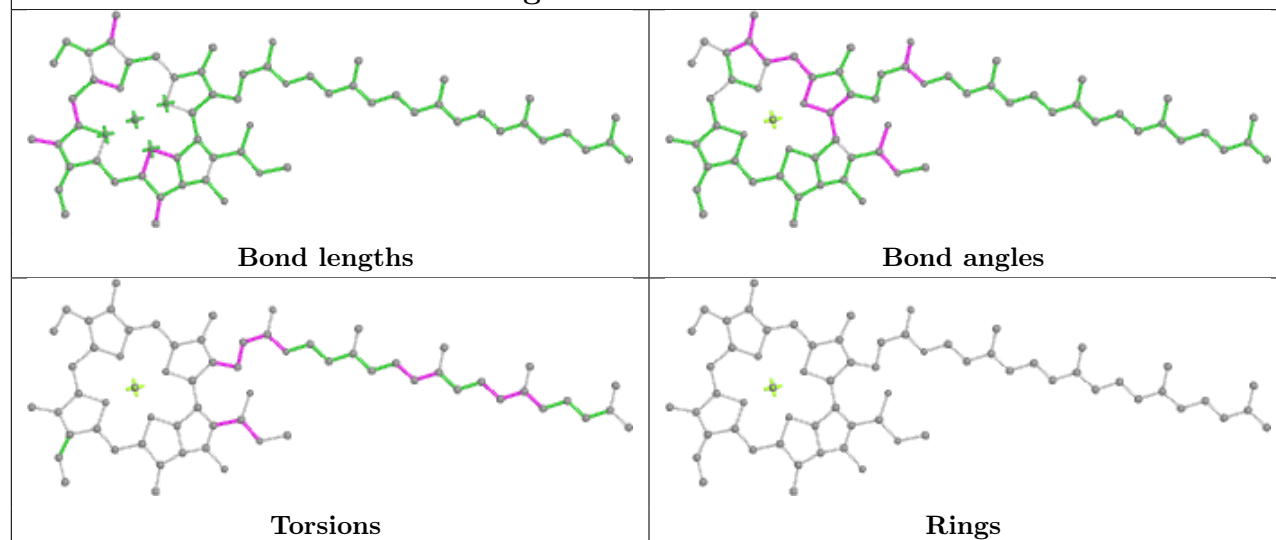


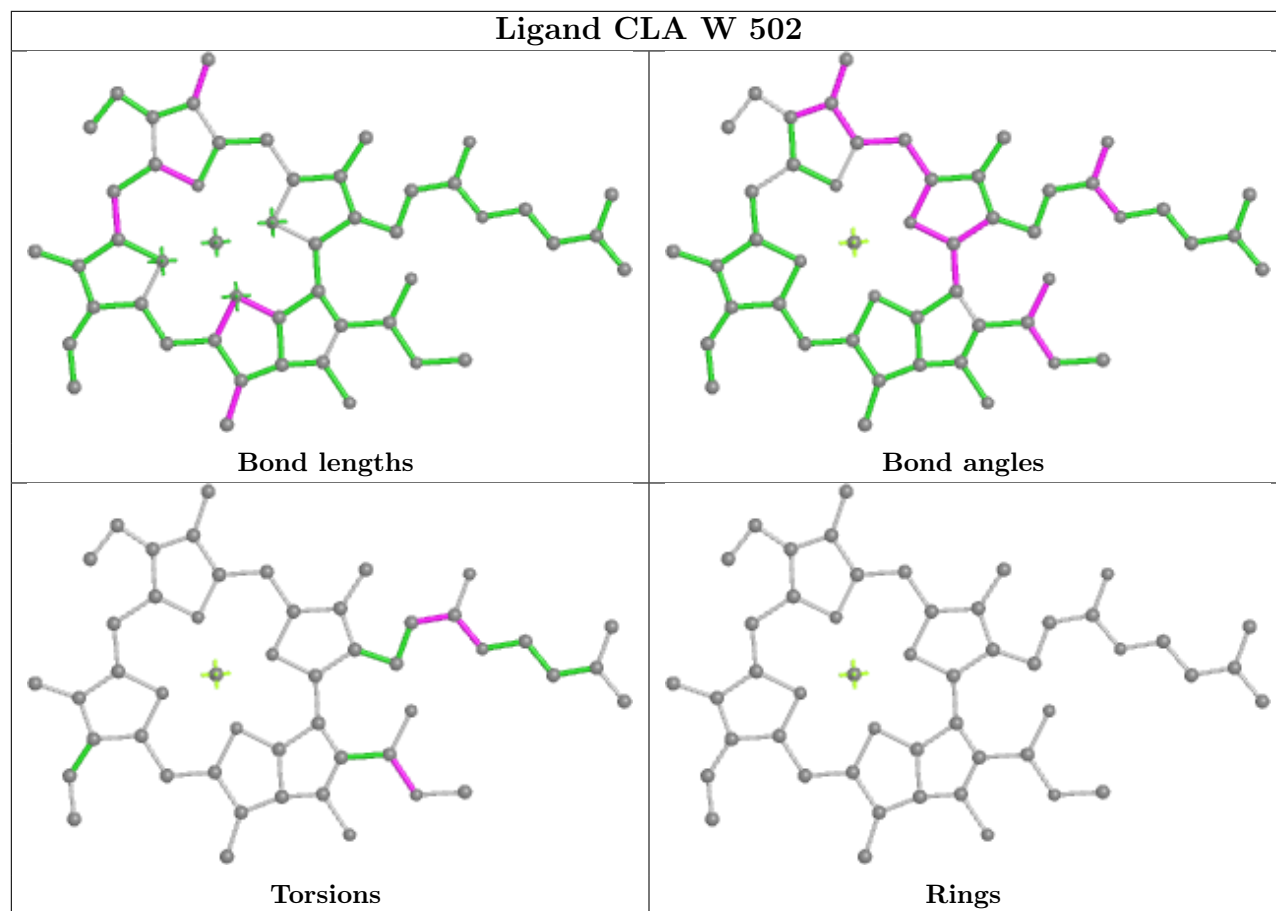
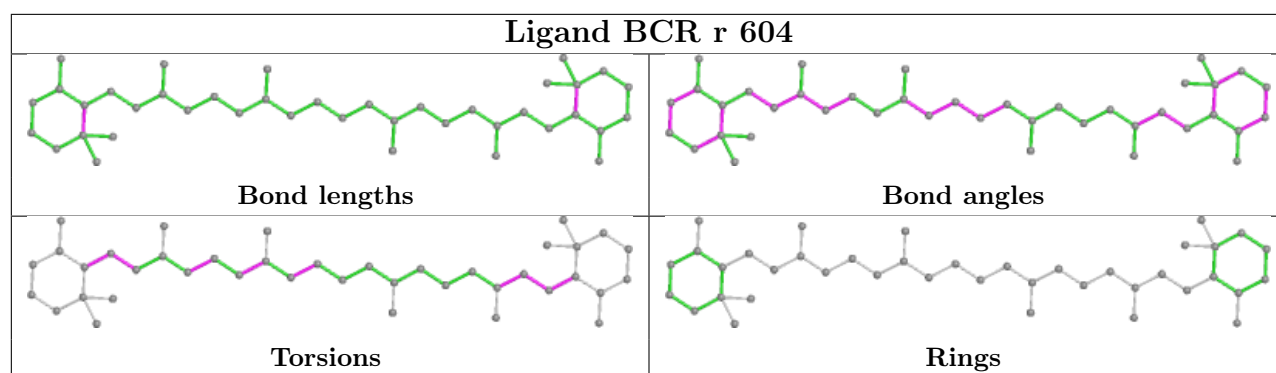


## Ligand CLA B 1216

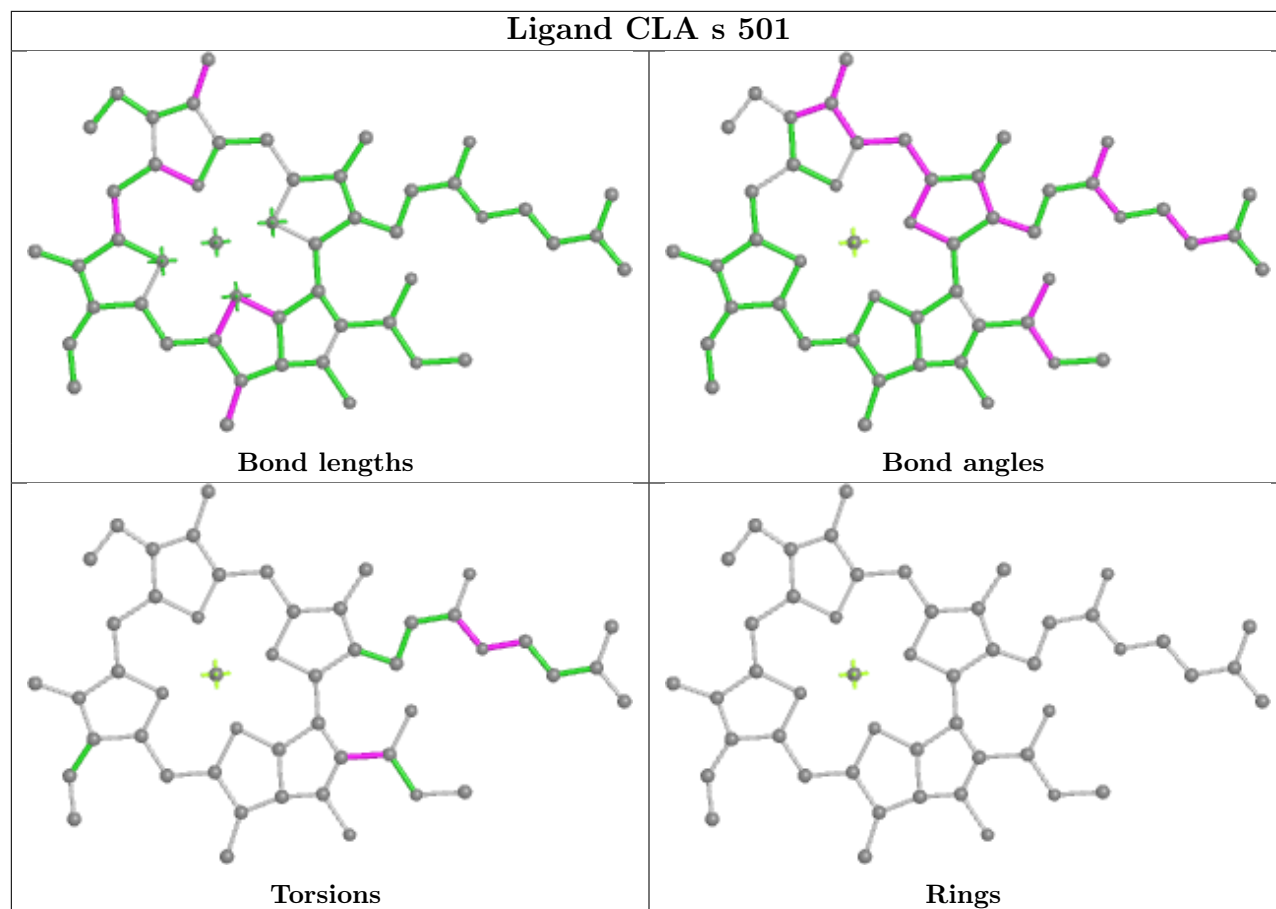


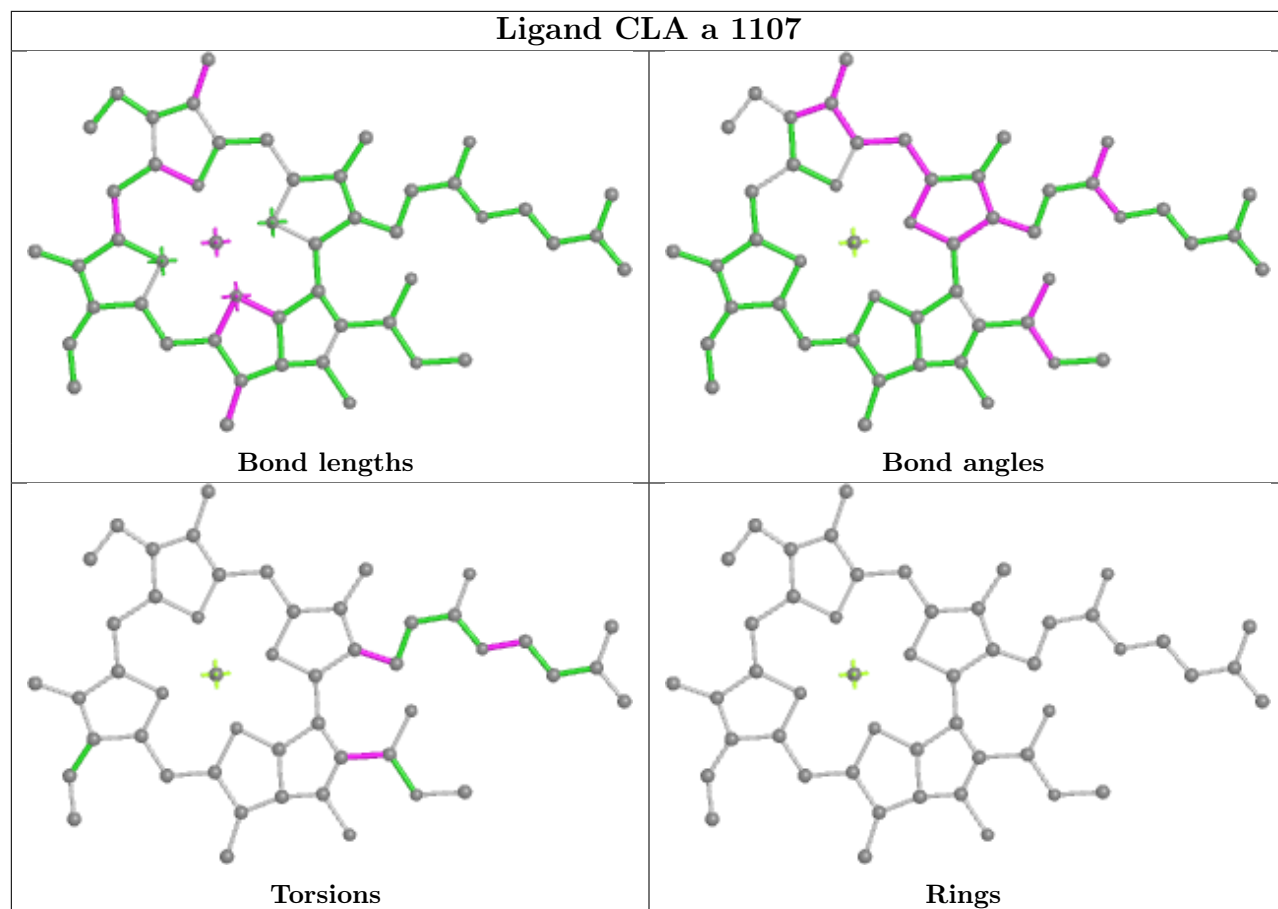
## Ligand CLA B 1203



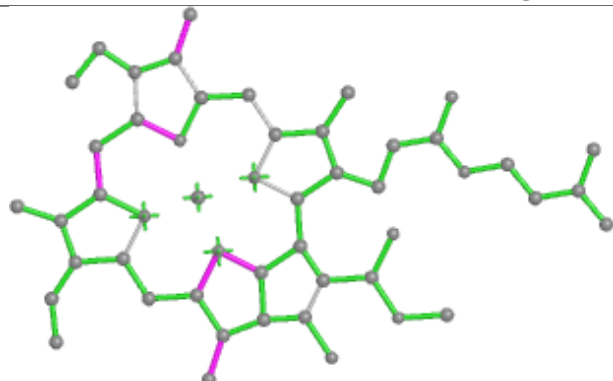


## Ligand CLA s 501

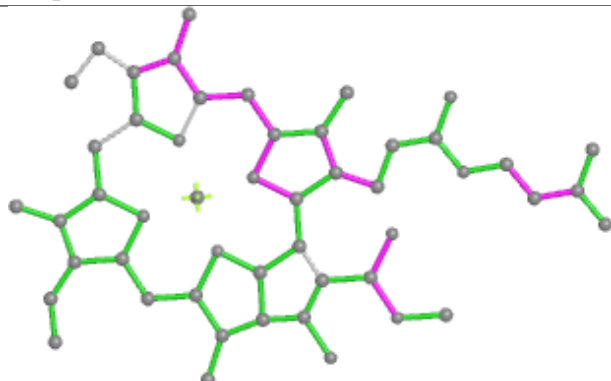




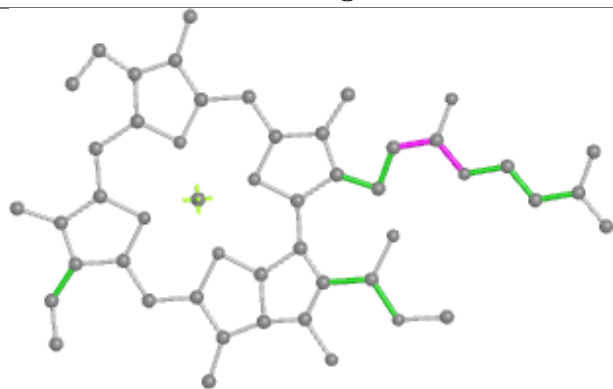
## Ligand CLA p 502



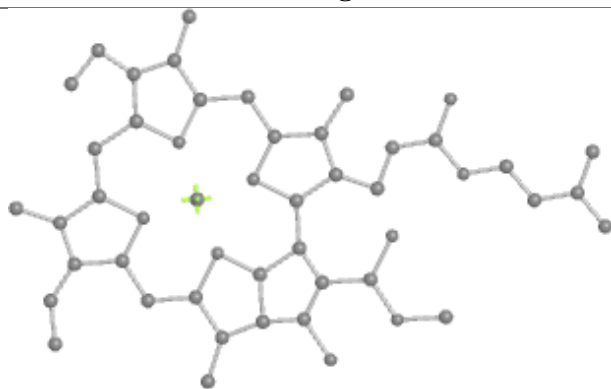
Bond lengths



Bond angles

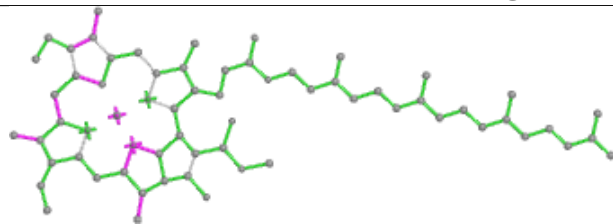


Torsions

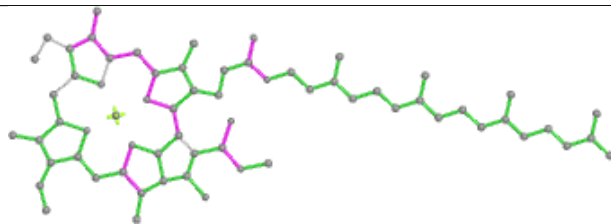


Rings

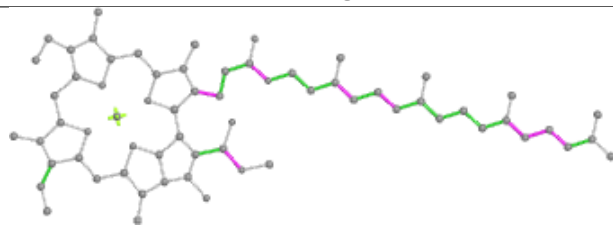
## Ligand CLA G 1225



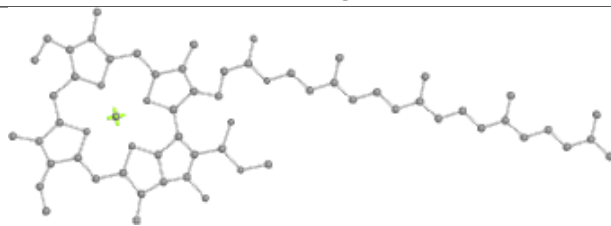
Bond lengths



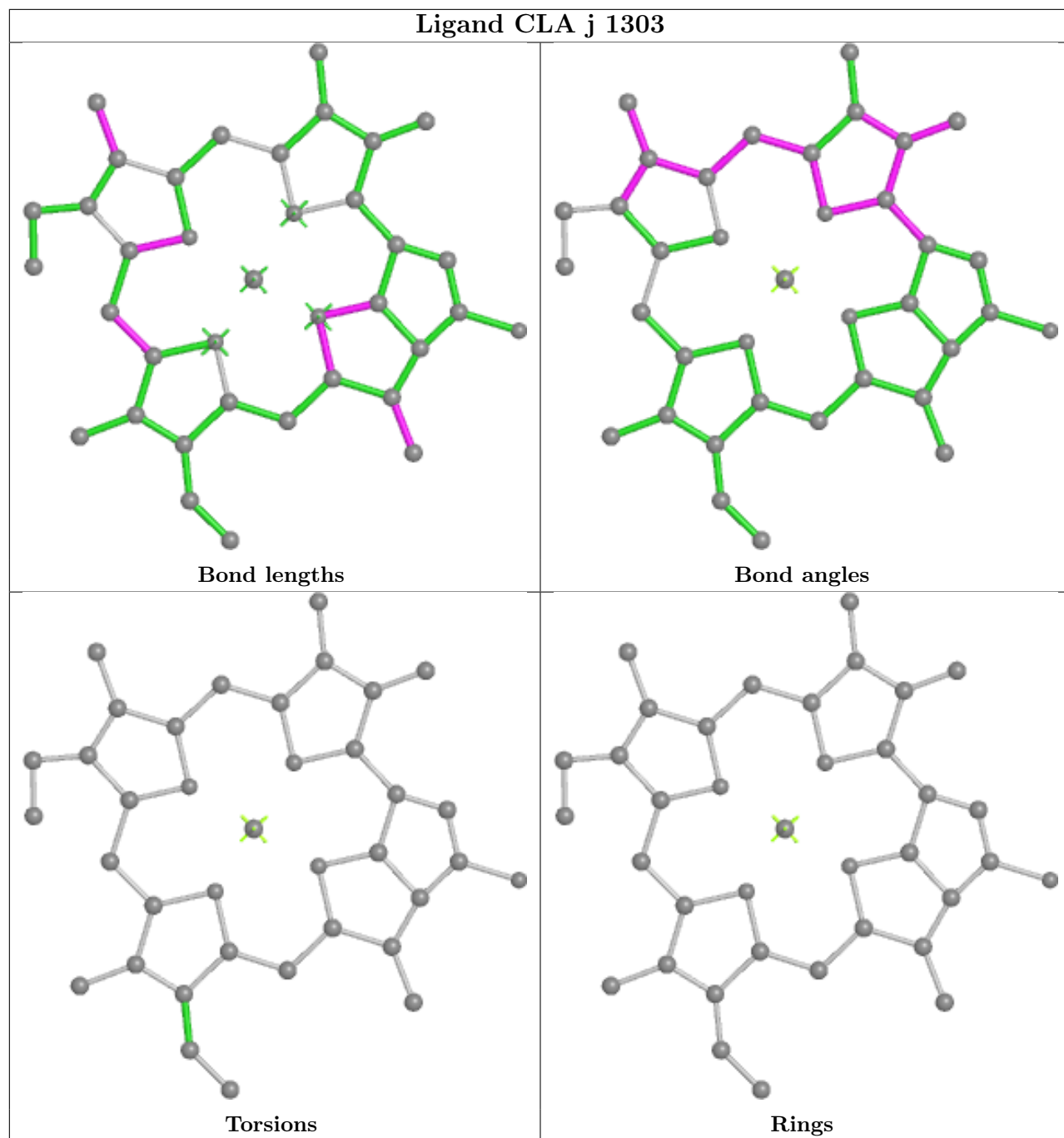
Bond angles



Torsions

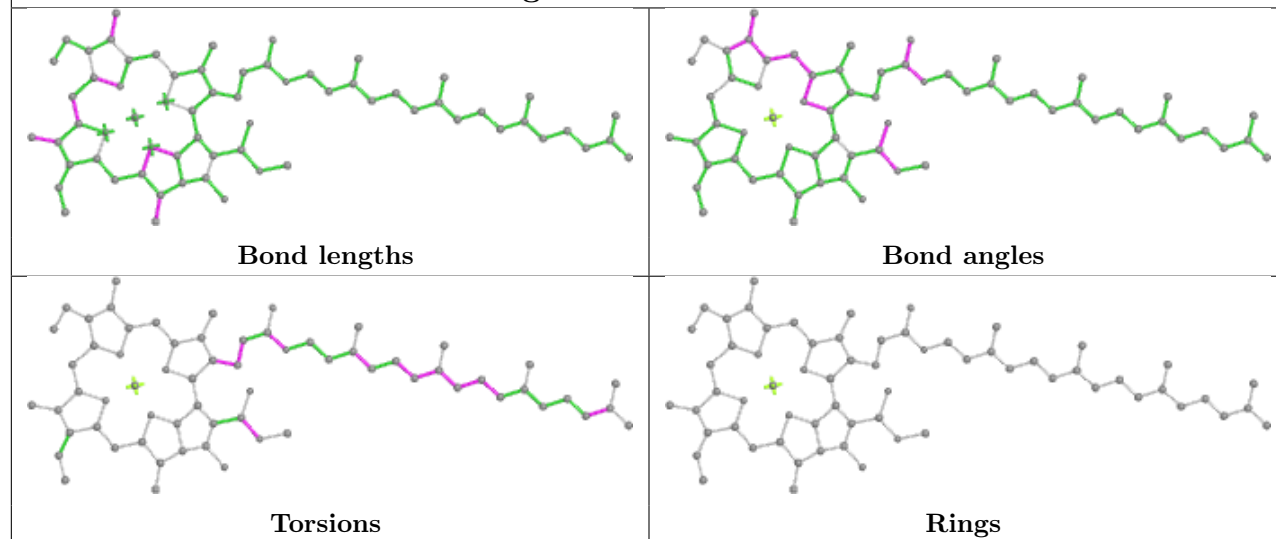


Rings

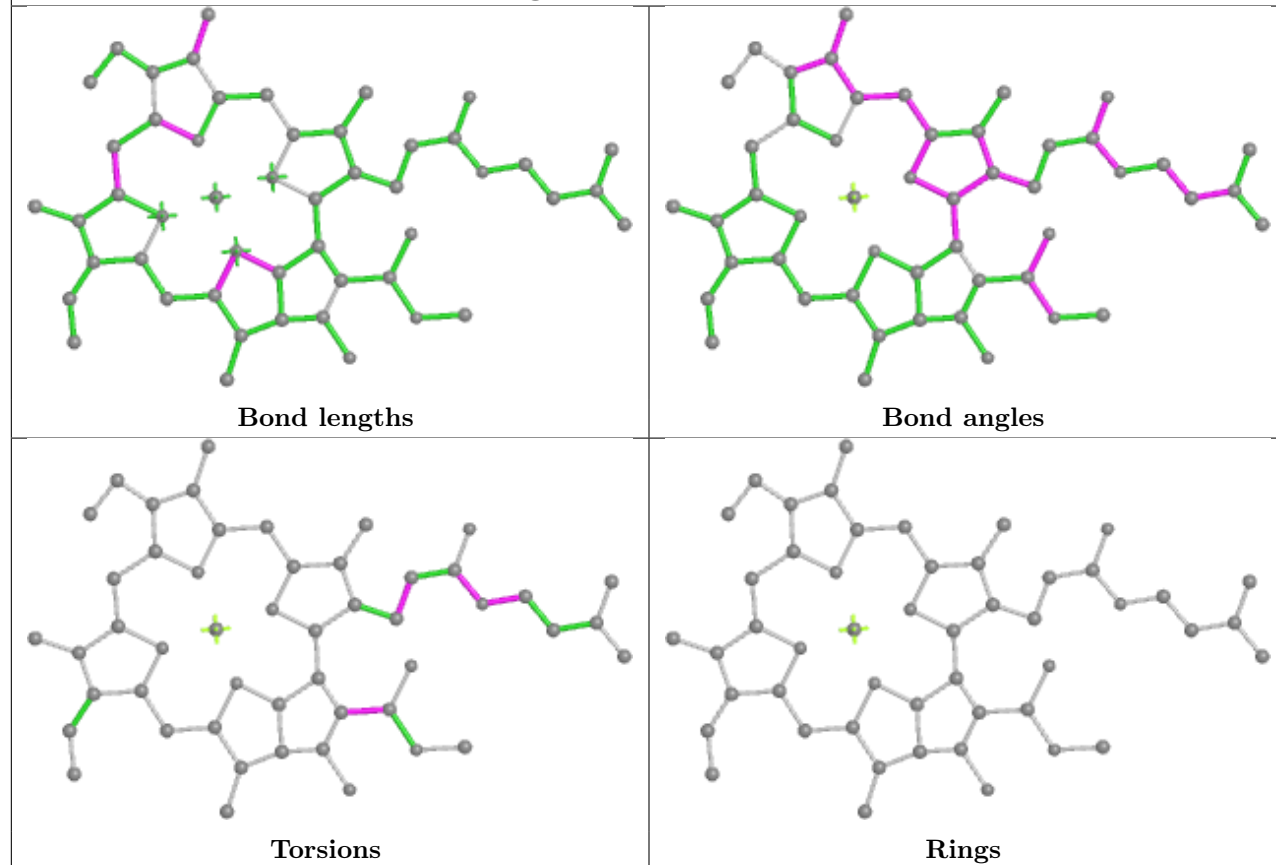


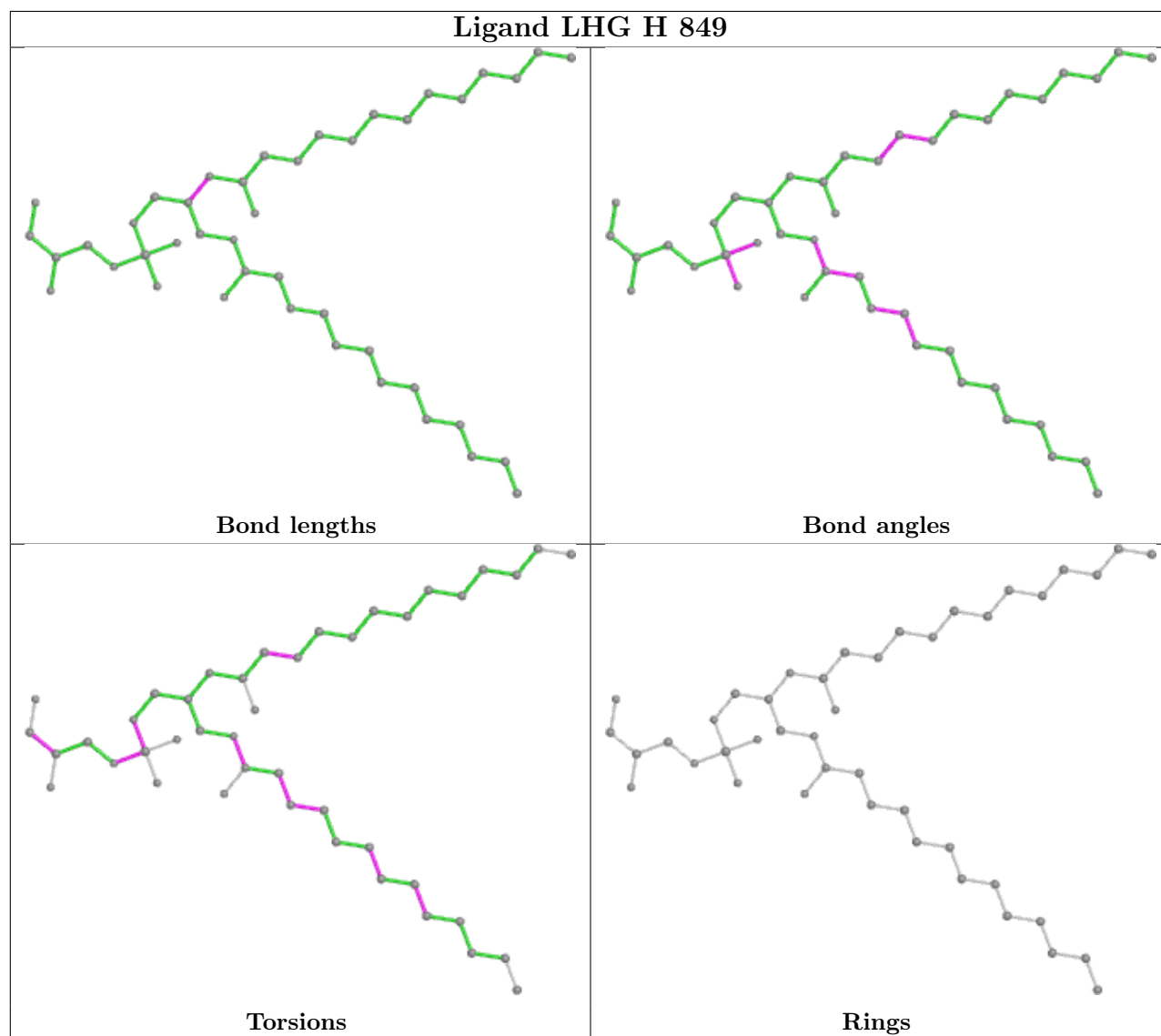
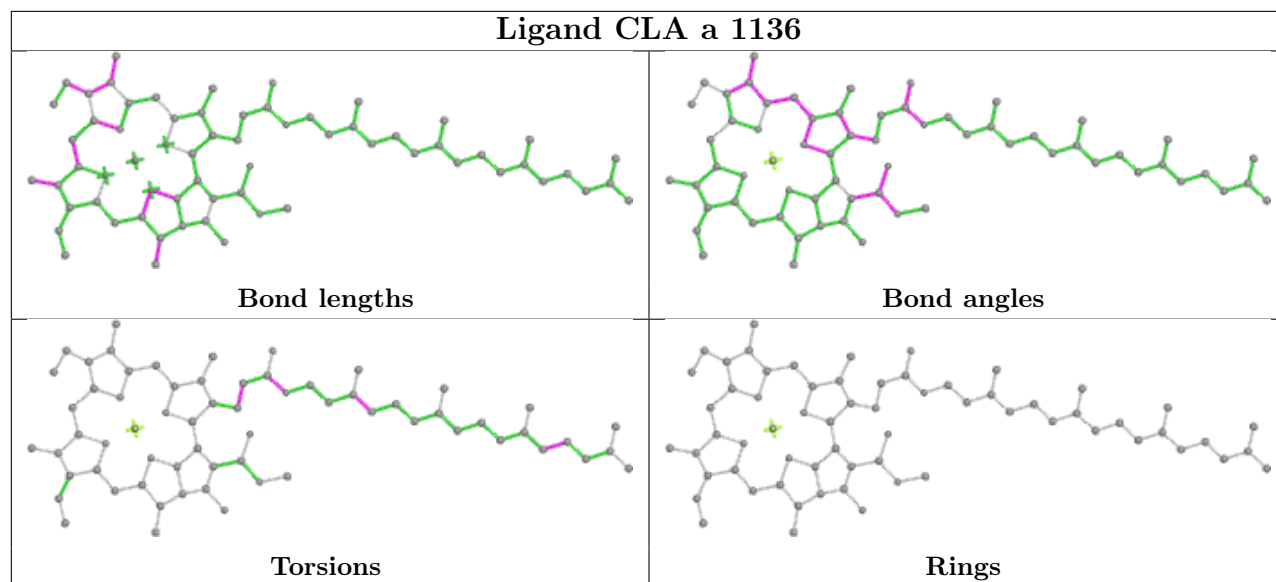


## Ligand CLA A 1140

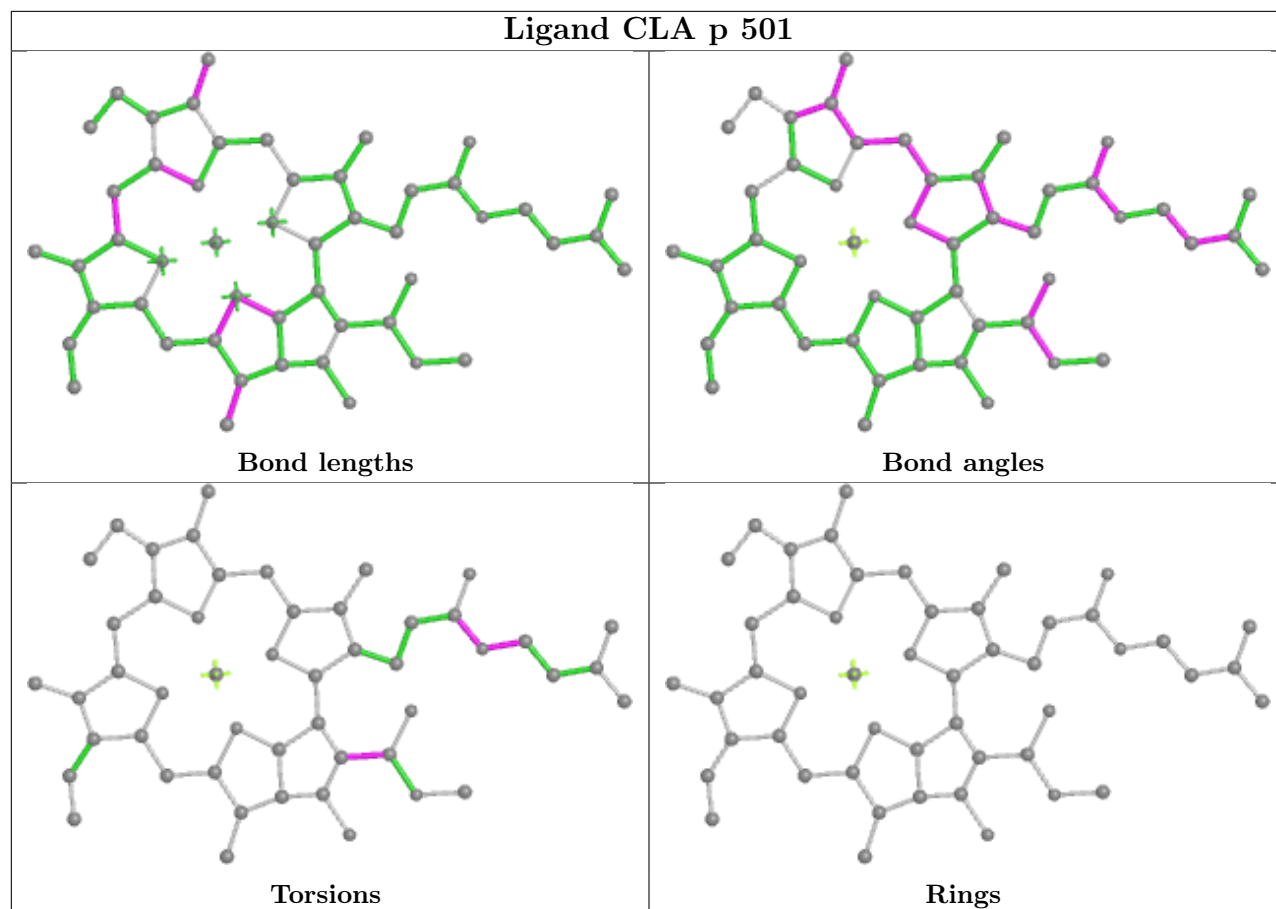


## Ligand CLA W 501

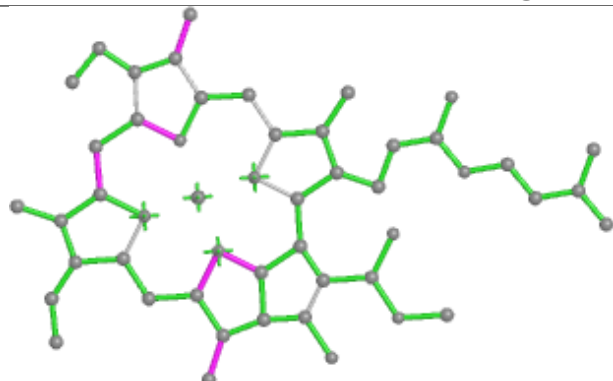




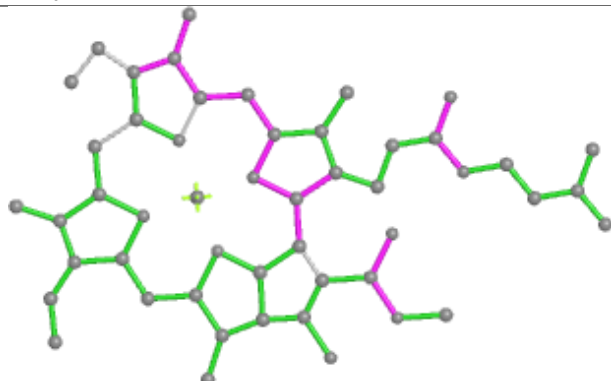
## Ligand CLA p 501



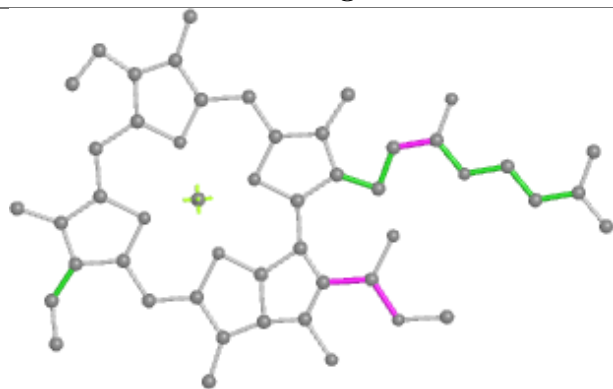
## Ligand CLA y 514



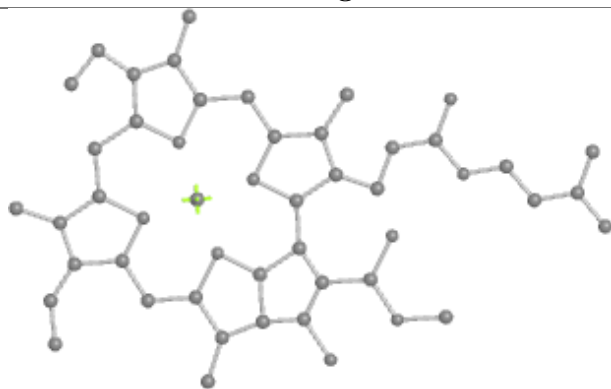
Bond lengths



Bond angles

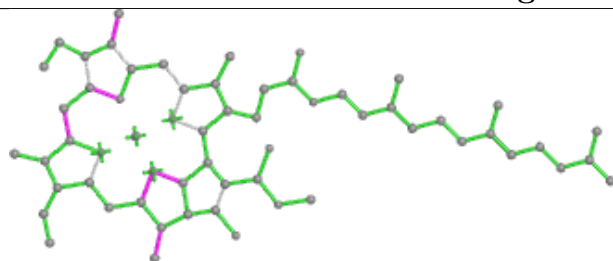


Torsions

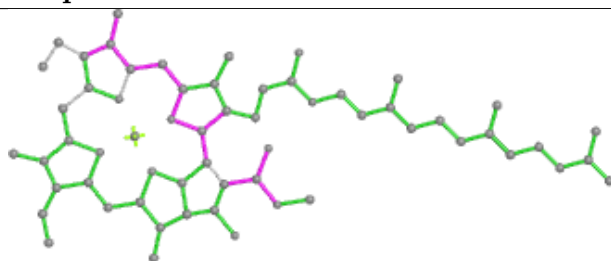


Rings

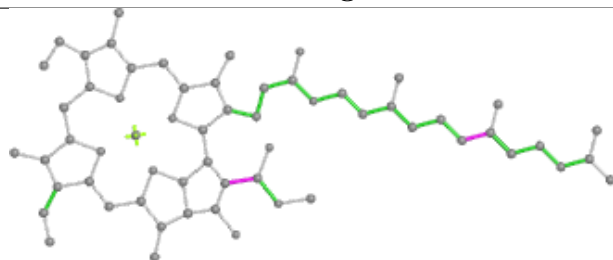
## Ligand CLA q 510



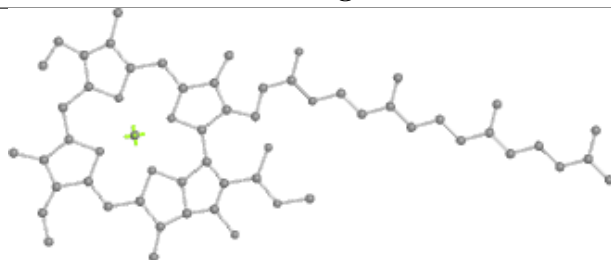
Bond lengths



Bond angles

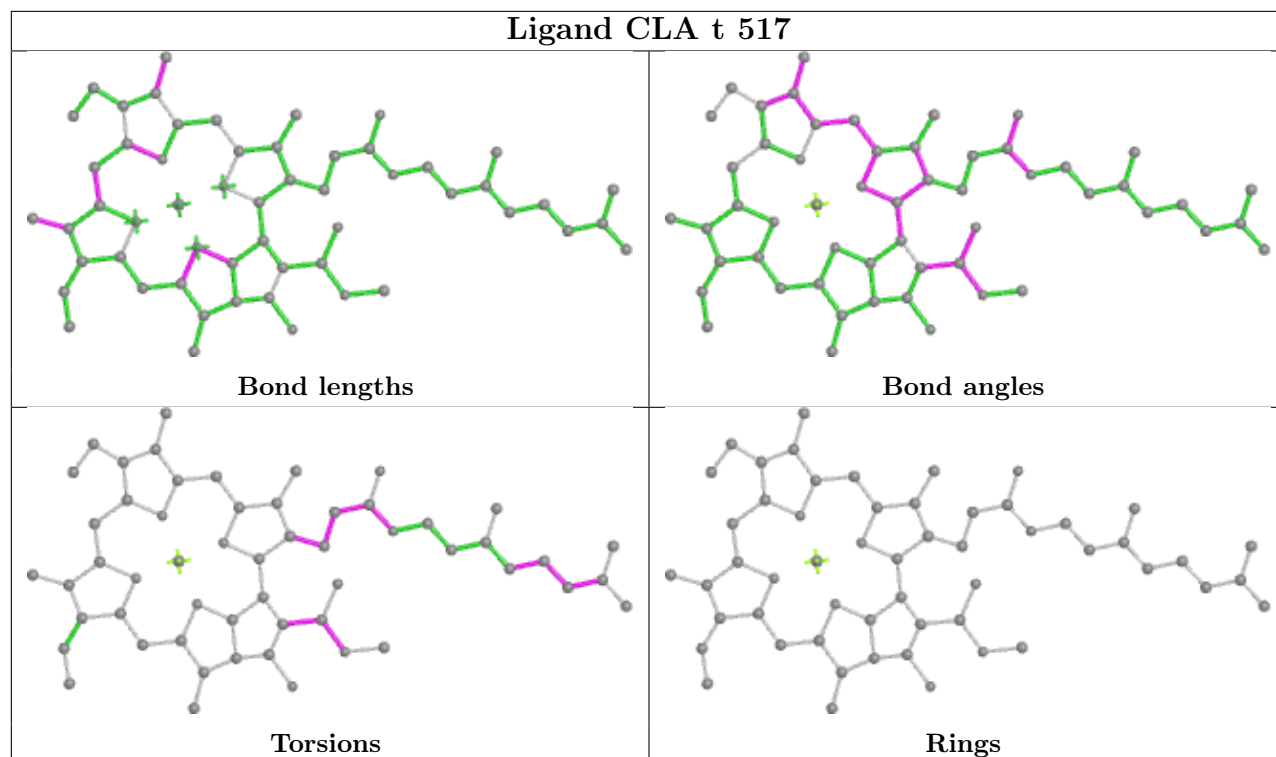


Torsions

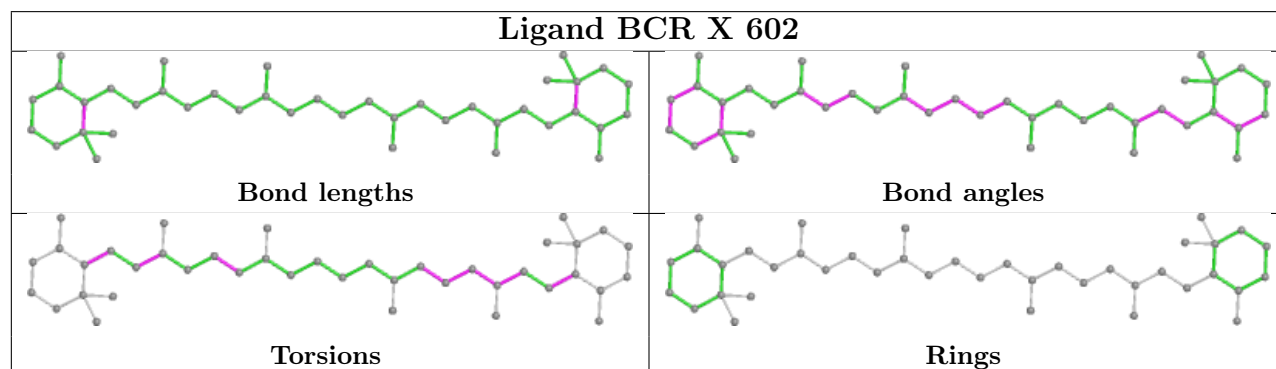


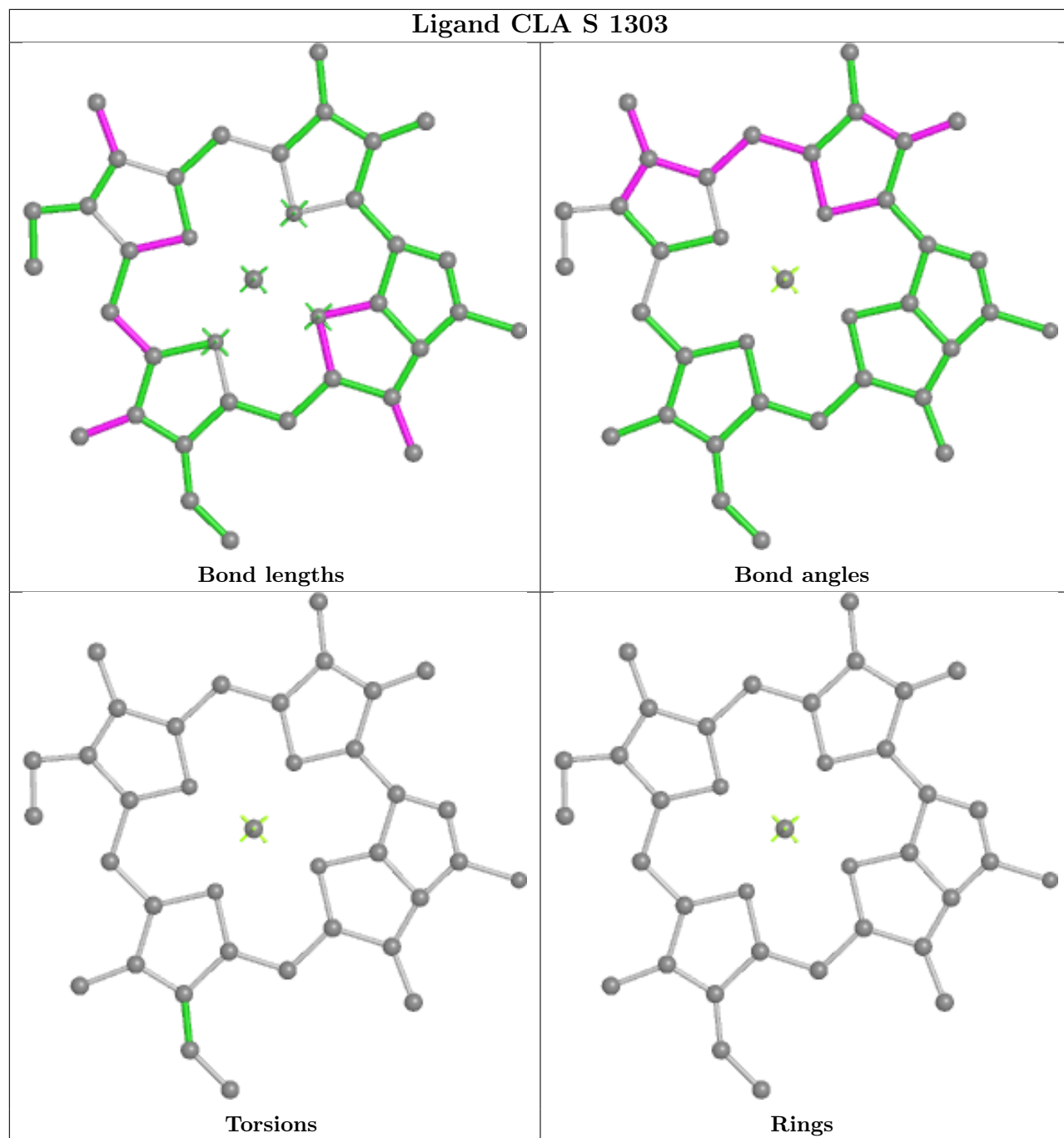
Rings

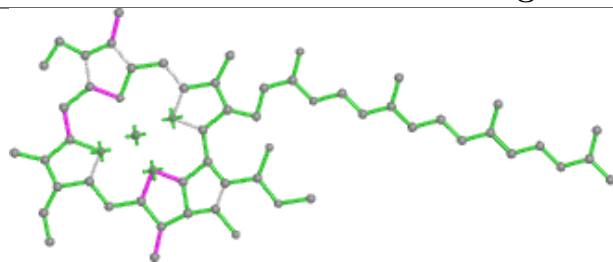
## Ligand CLA t 517



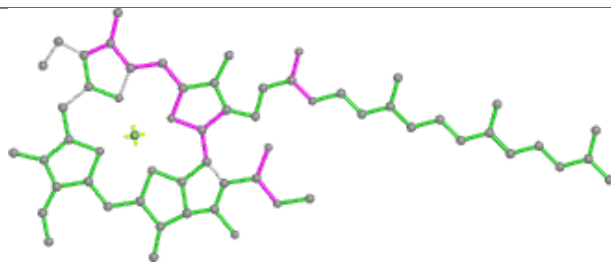
## Ligand BCR X 602



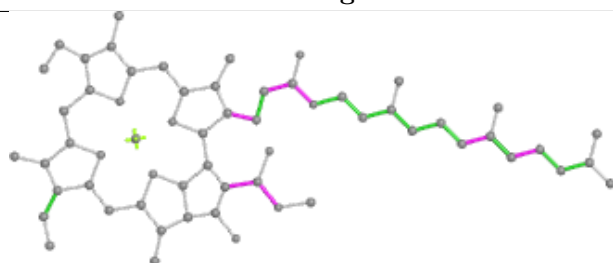


**Ligand CLA n 504**

Bond lengths



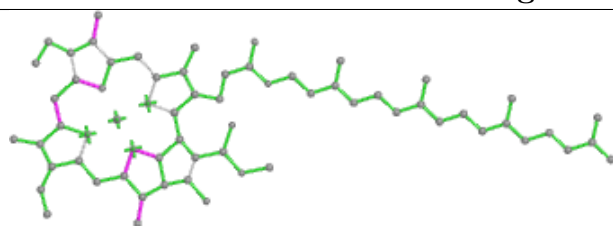
Bond angles



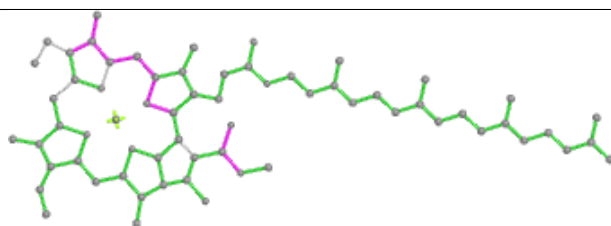
Torsions



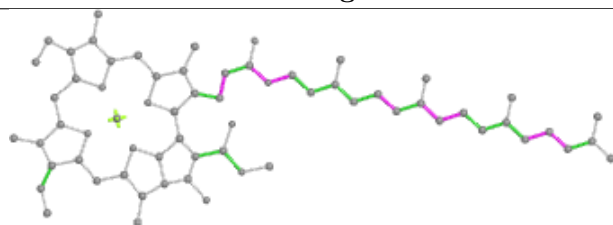
Rings

**Ligand CLA u 515**

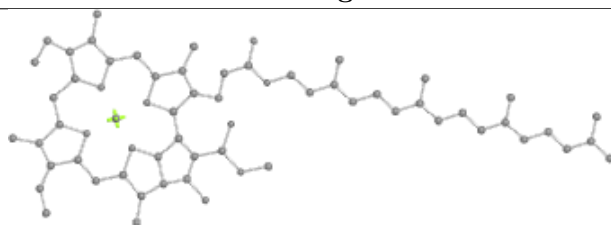
Bond lengths



Bond angles

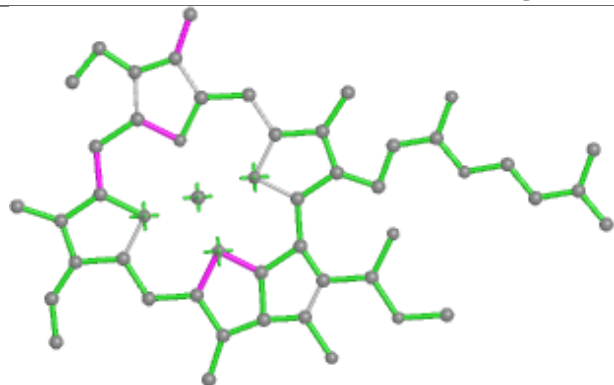


Torsions

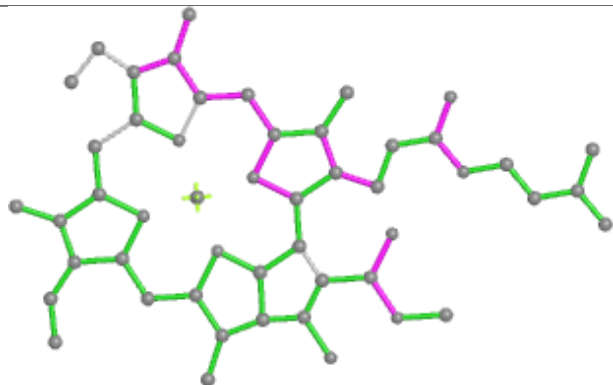


Rings

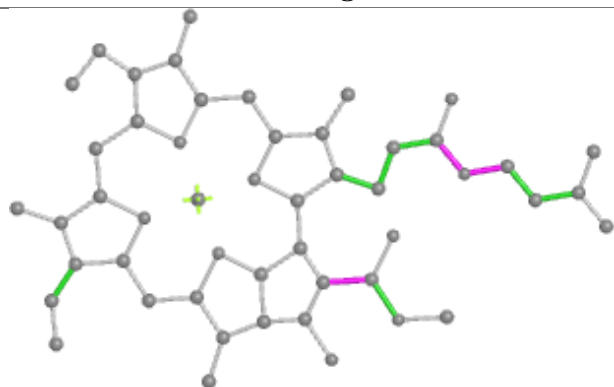
## Ligand CLA x 501



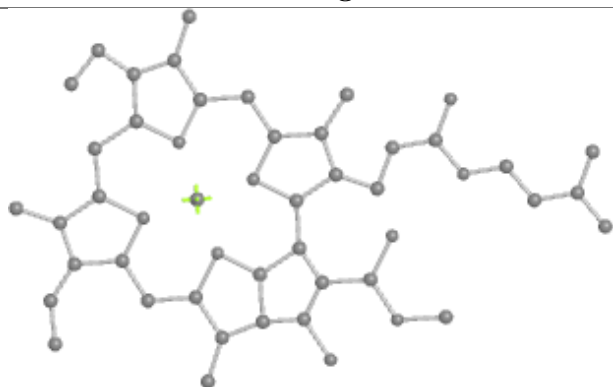
Bond lengths



Bond angles

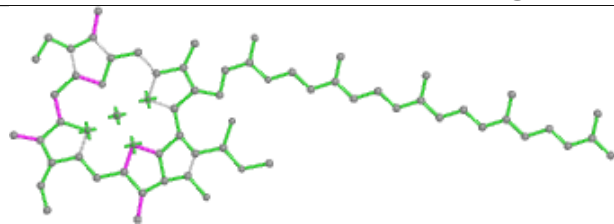


Torsions

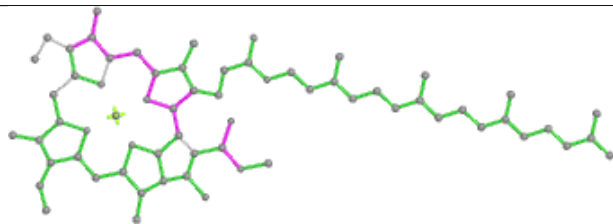


Rings

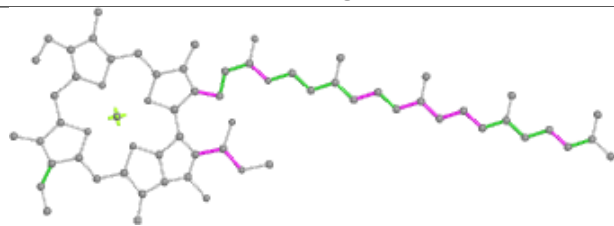
## Ligand CLA W 511



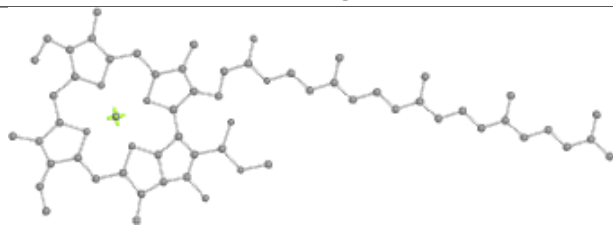
Bond lengths



Bond angles

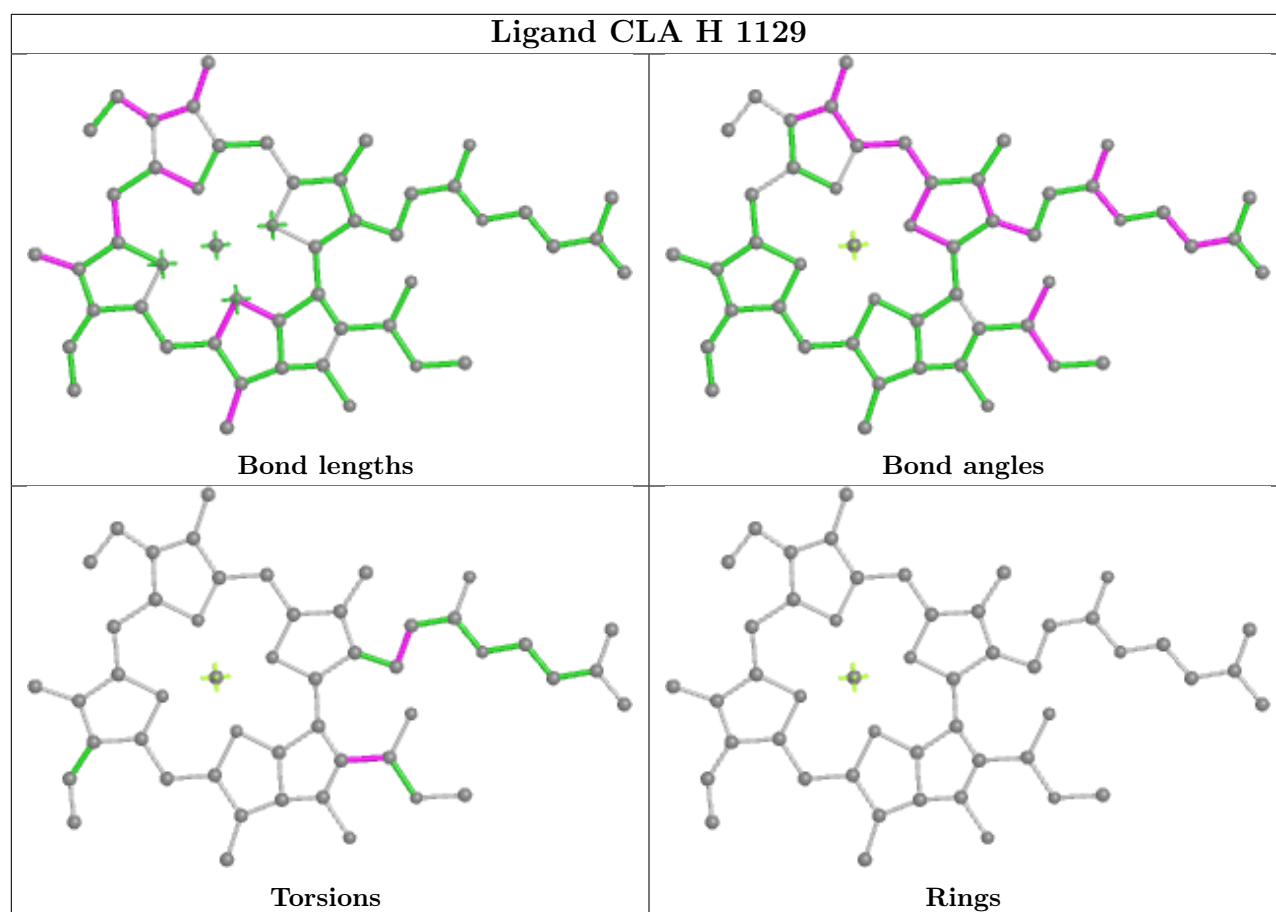


Torsions

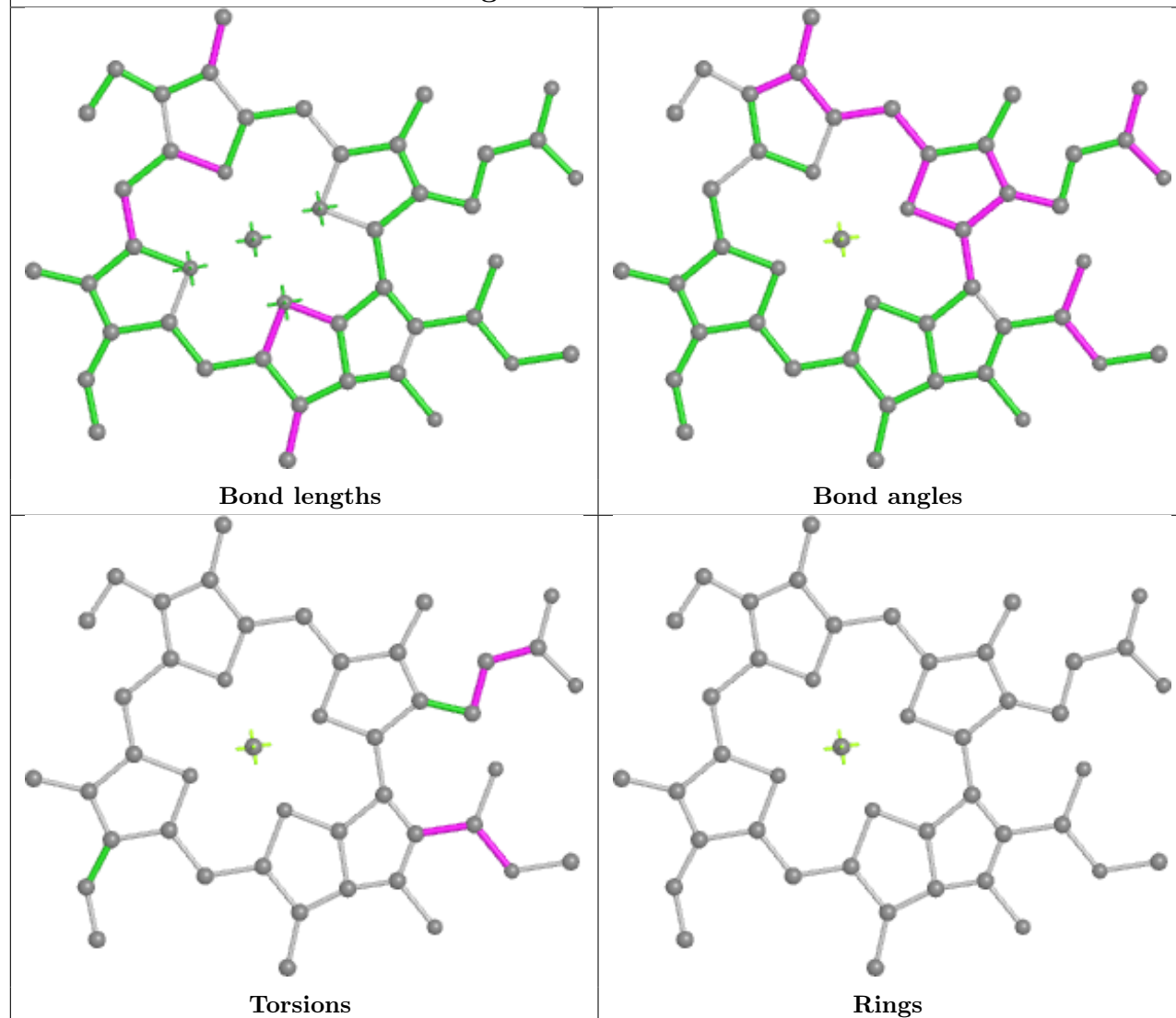


Rings

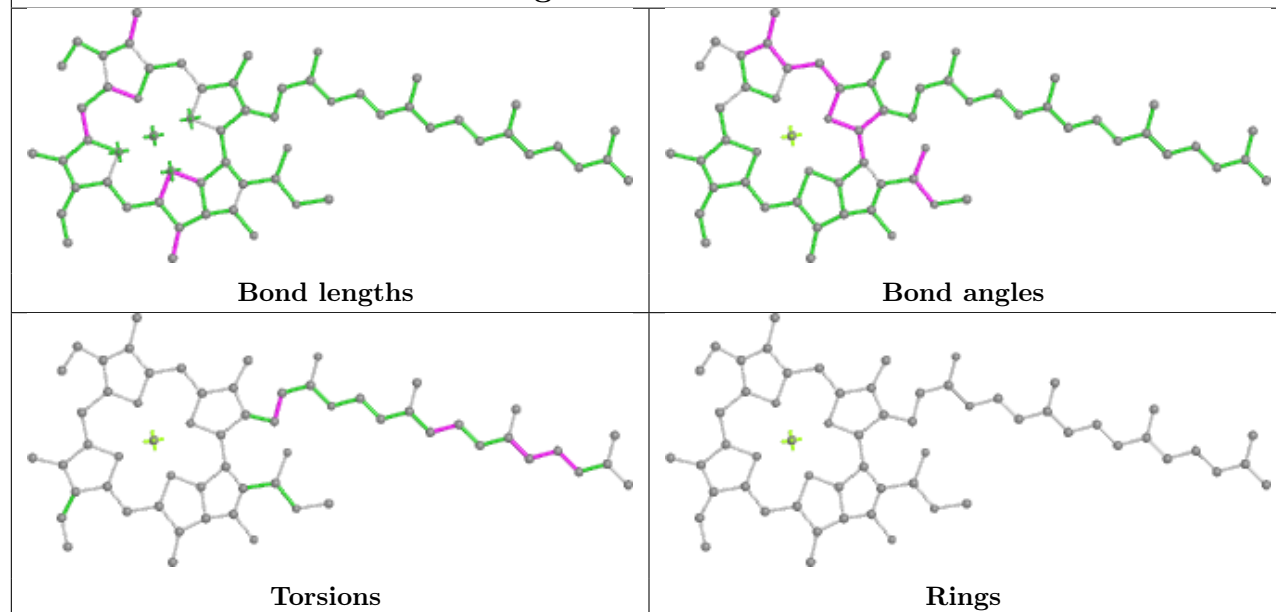


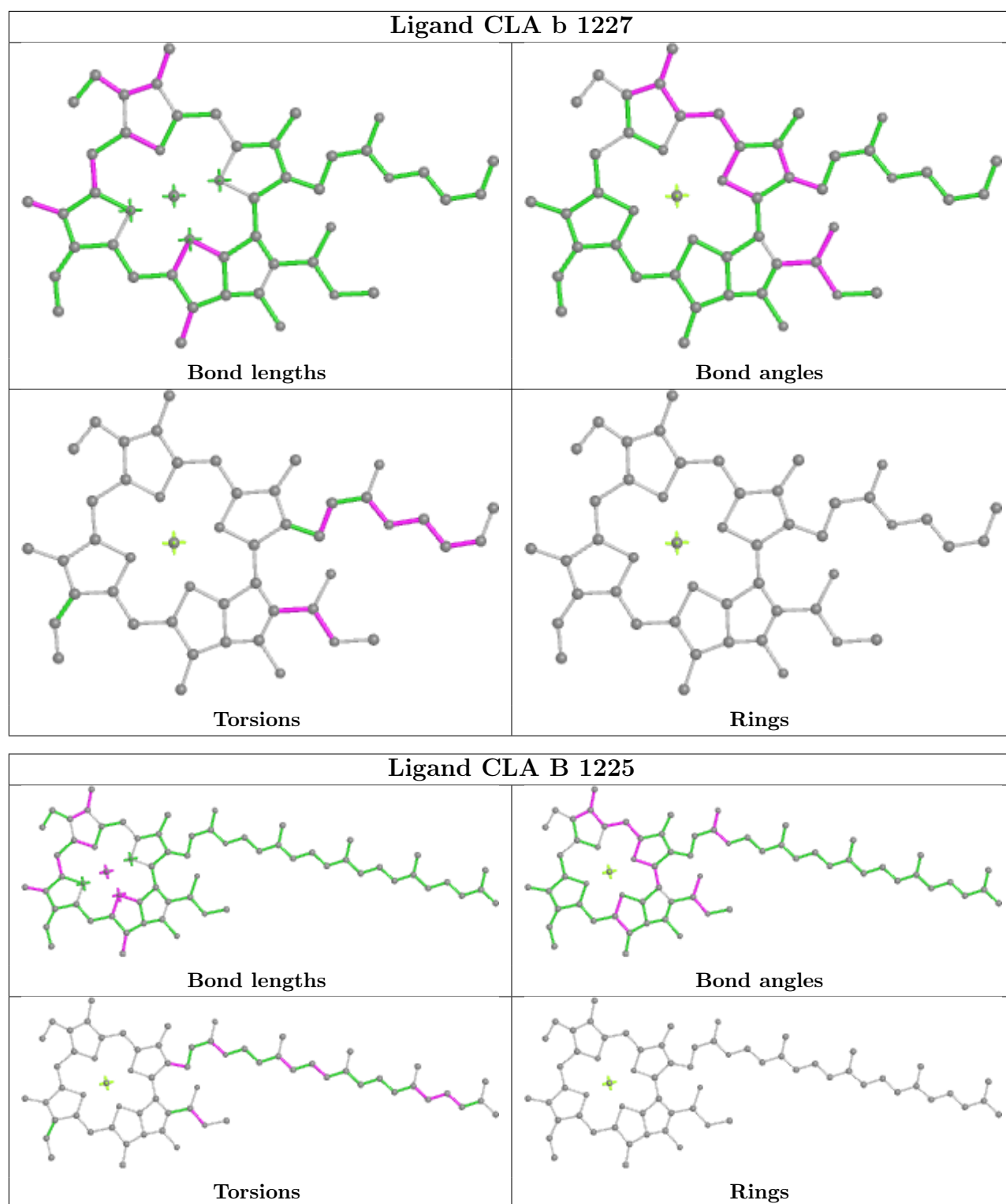


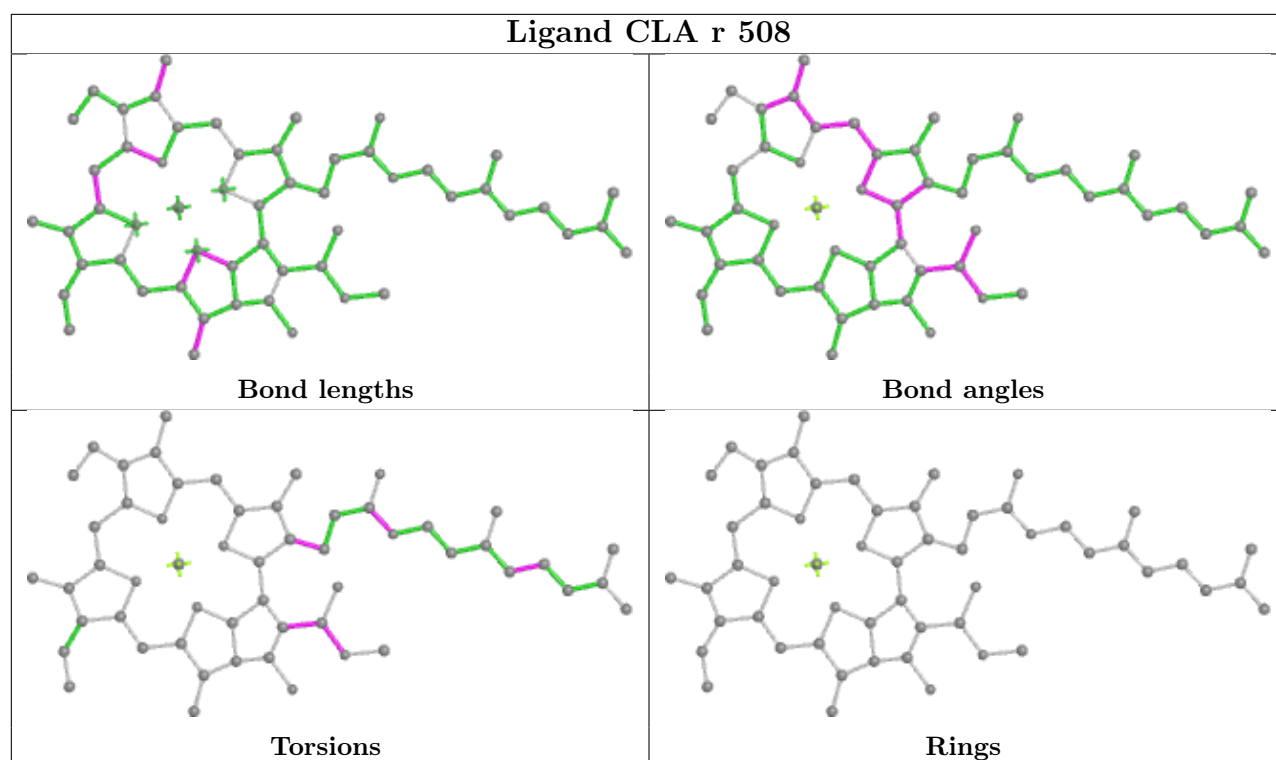
## Ligand CLA G 1219

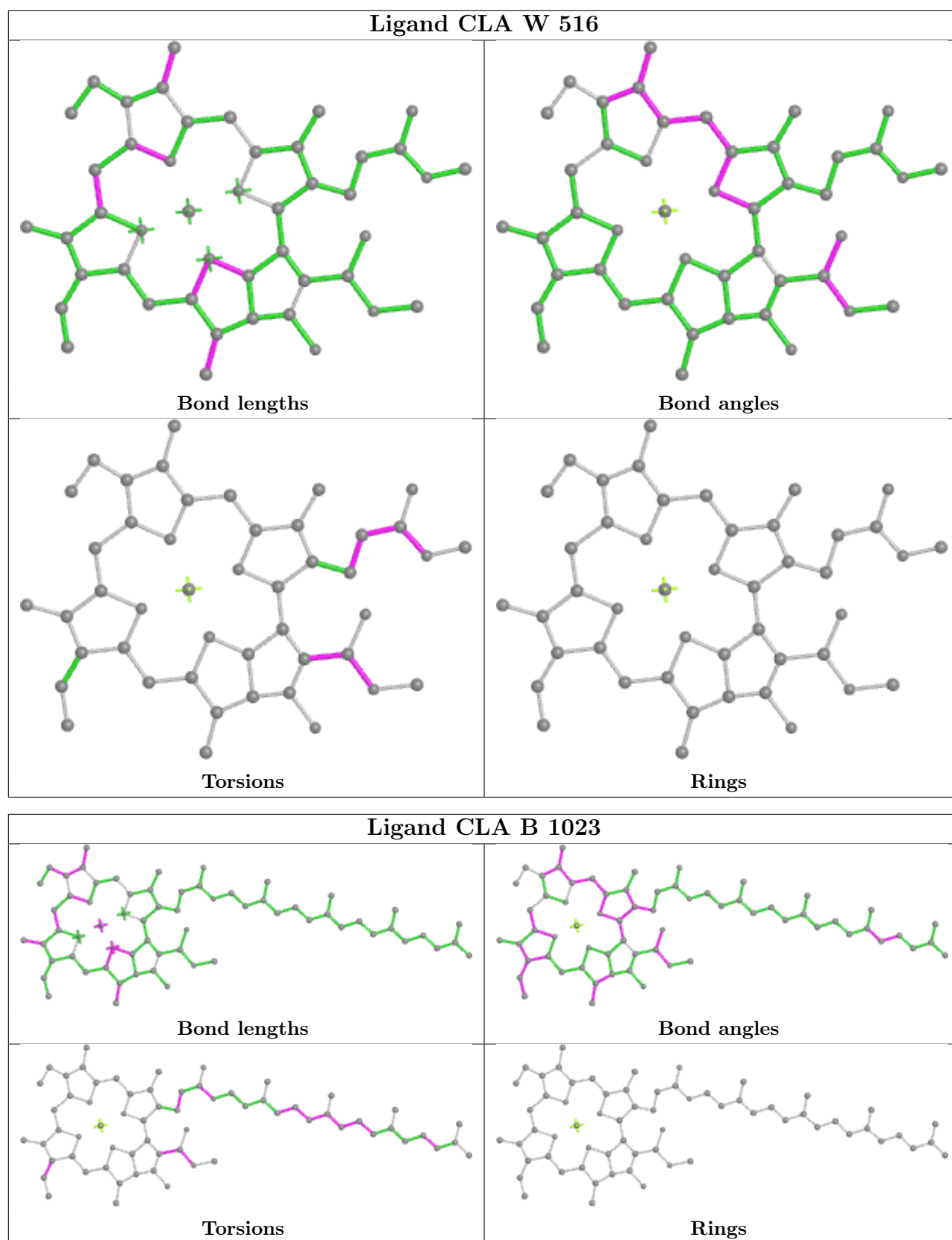


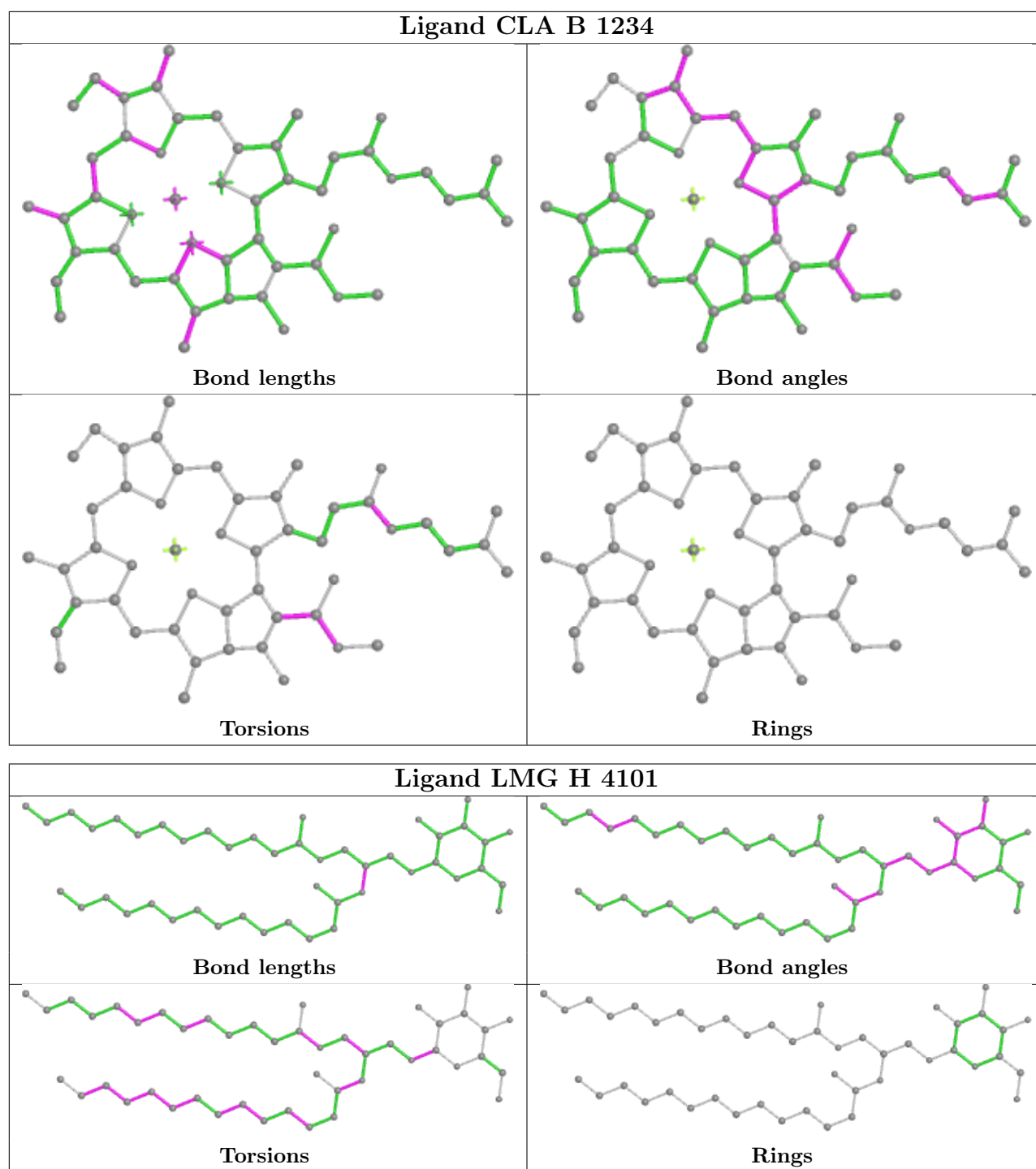
## Ligand CLA Z 504



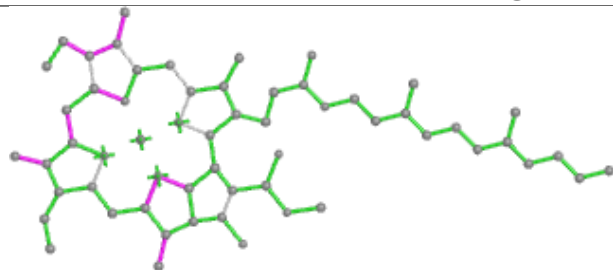




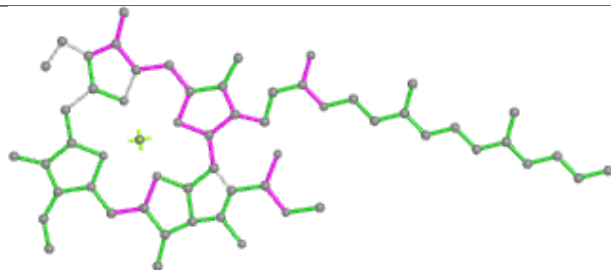




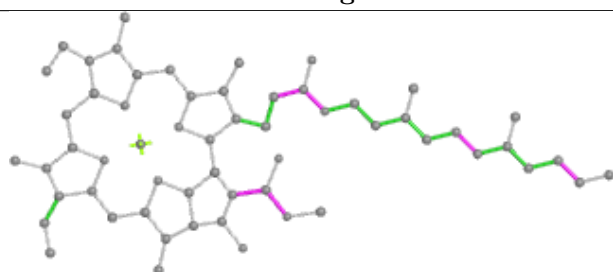
## Ligand CLA b 1229



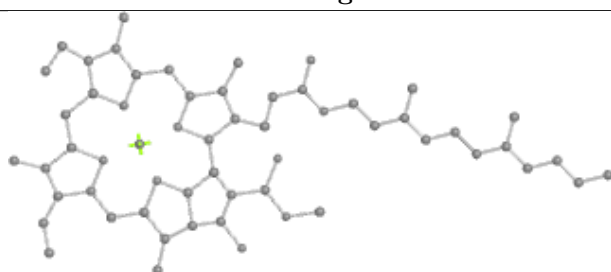
Bond lengths



Bond angles

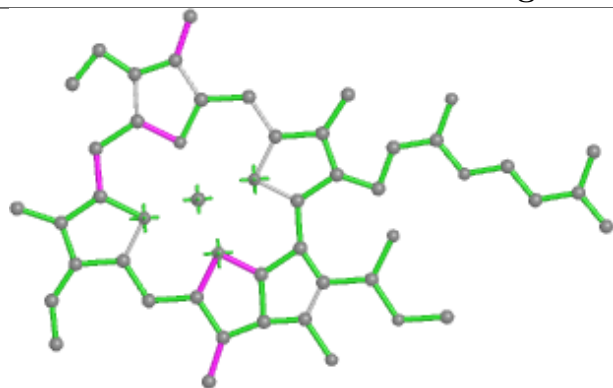


Torsions

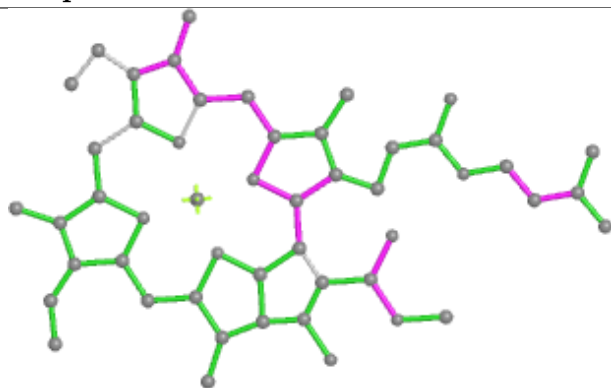


Rings

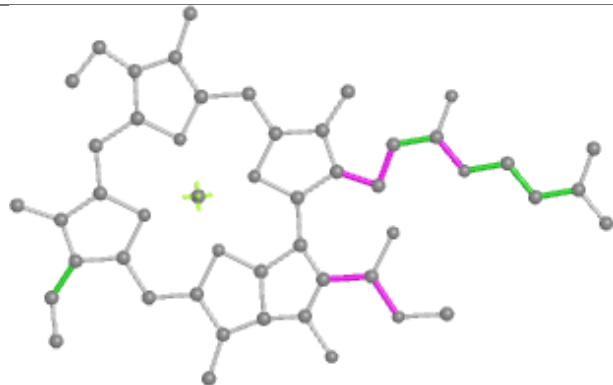
## Ligand CLA q 513



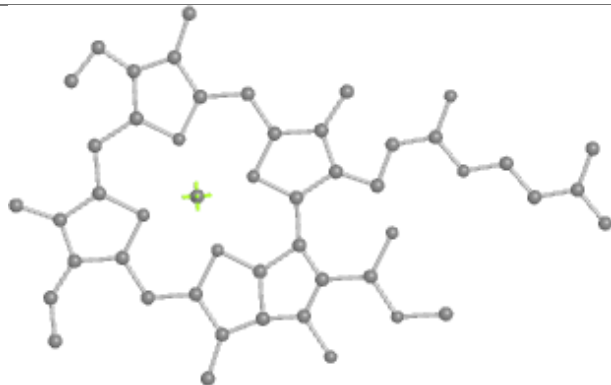
Bond lengths



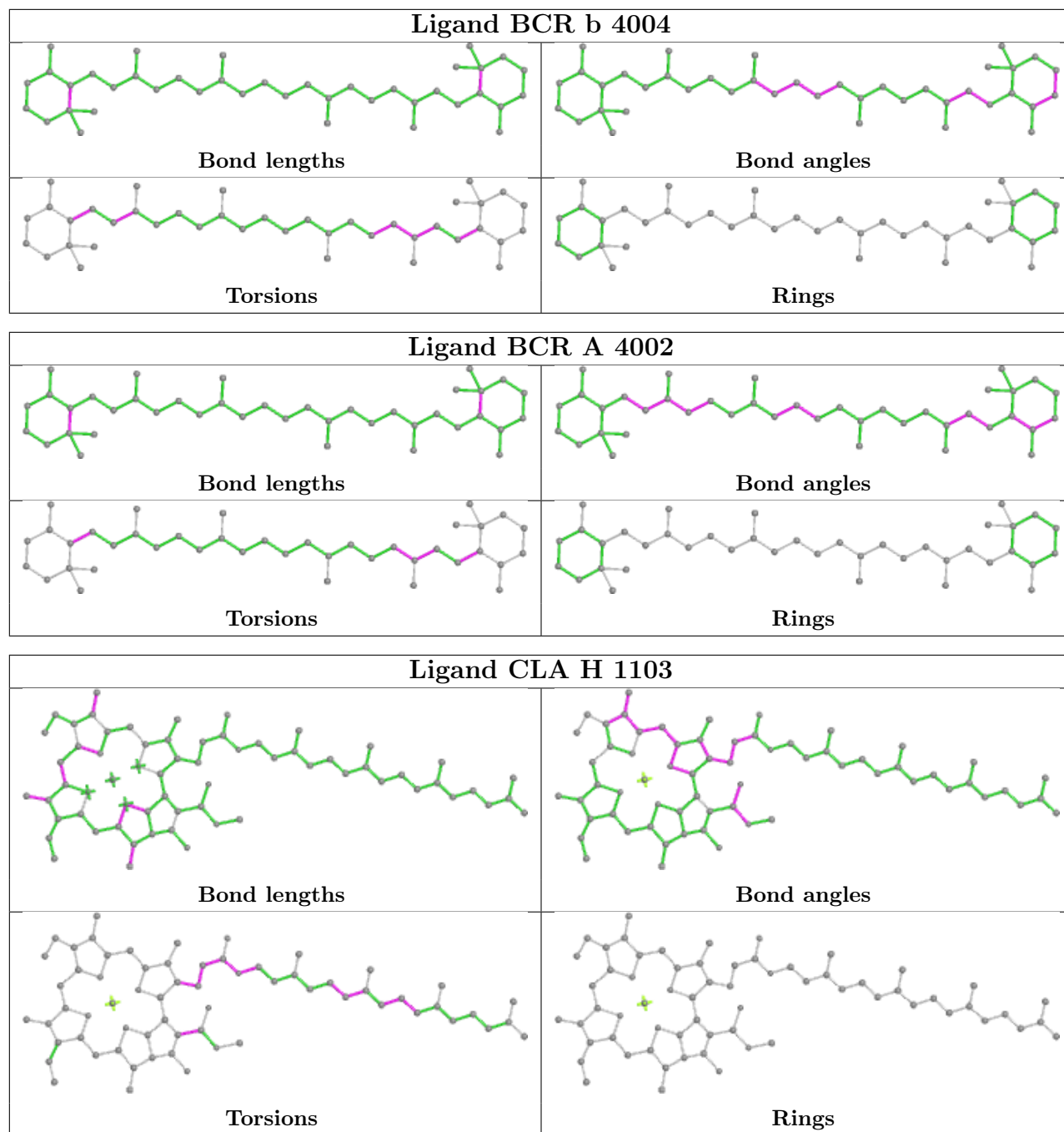
Bond angles



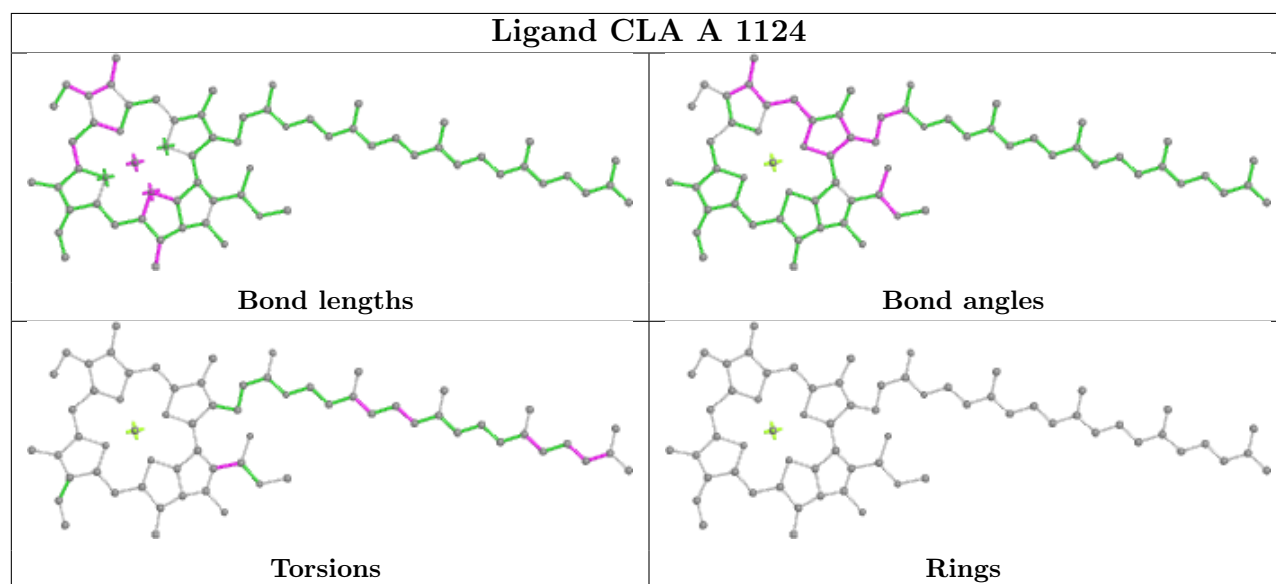
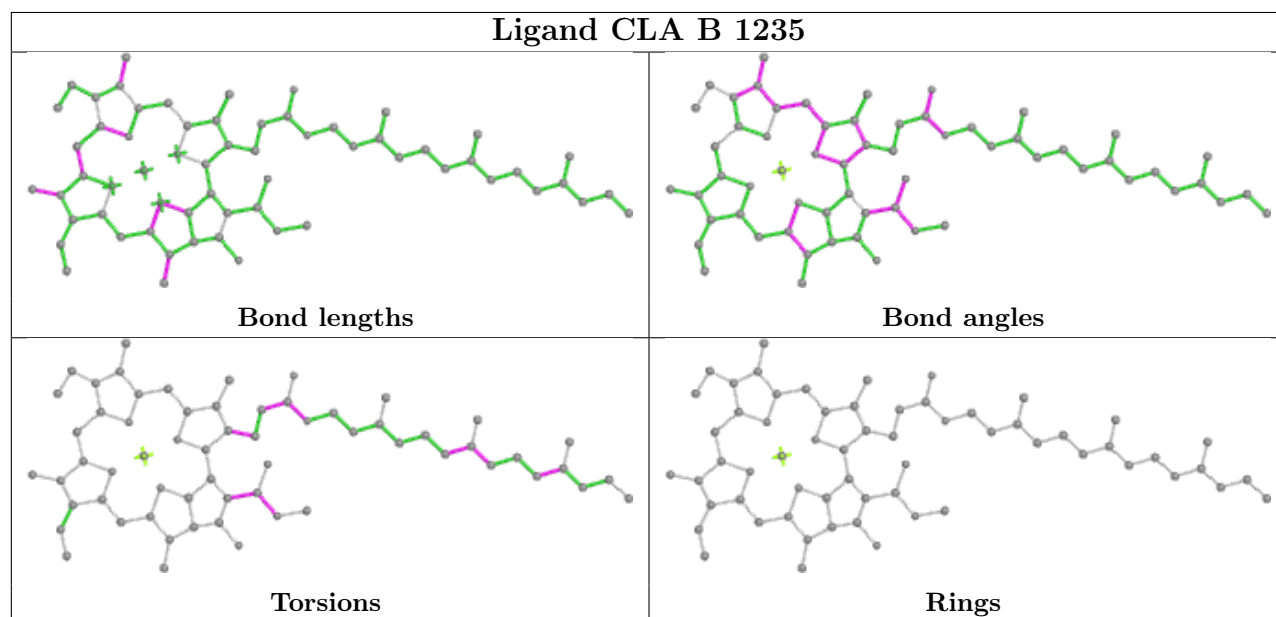
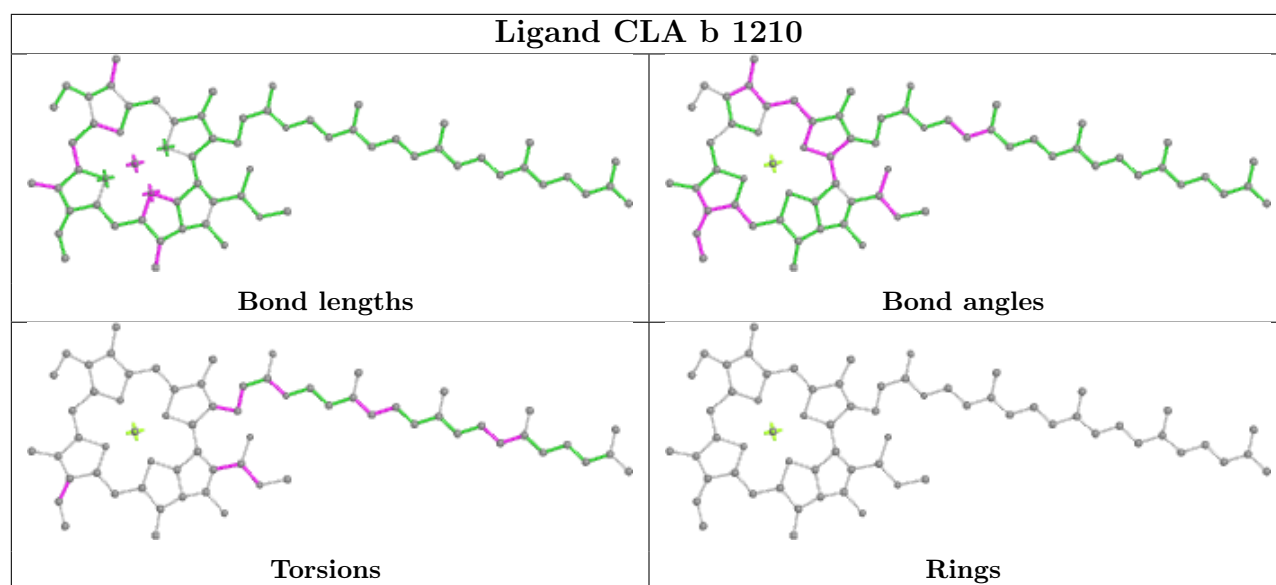
Torsions



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.

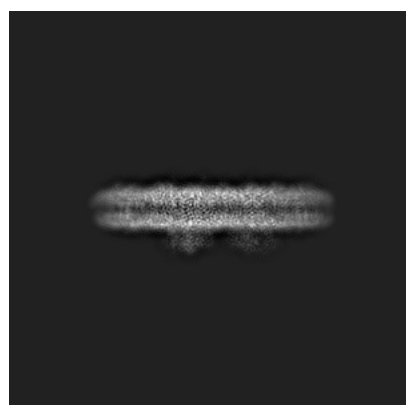
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0524. These allow visual inspection of the internal detail of the map and identification of artifacts.

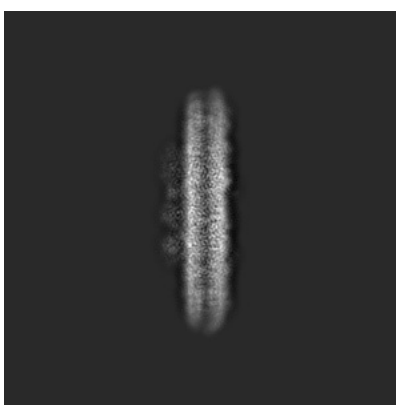
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

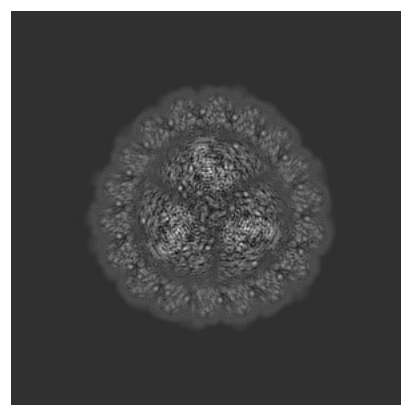
#### 6.1.1 Primary map



X



Y

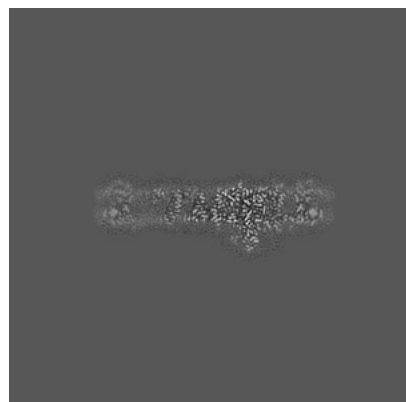


Z

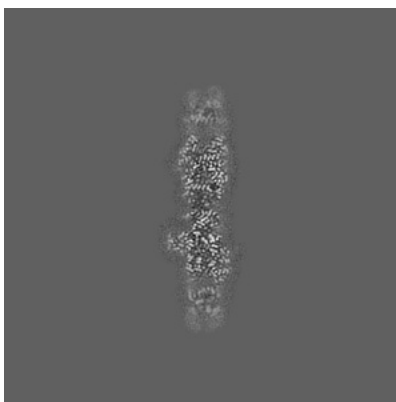
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

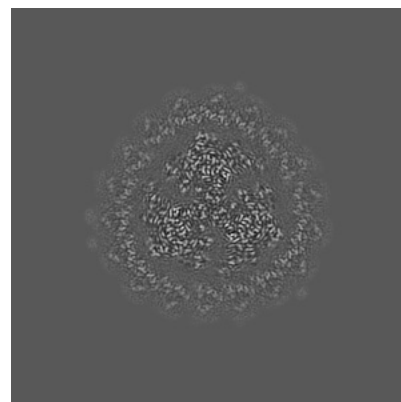
#### 6.2.1 Primary map



X Index: 250



Y Index: 250



Z Index: 250

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

## 6.3 Largest variance slices [i](#)

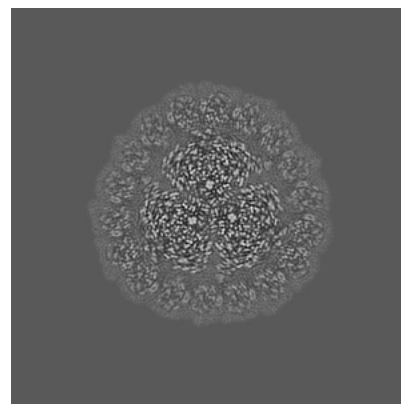
### 6.3.1 Primary map



X Index: 239



Y Index: 227

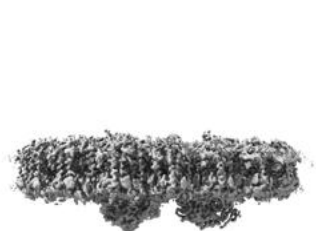


Z Index: 238

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

## 6.4 Orthogonal surface views [i](#)

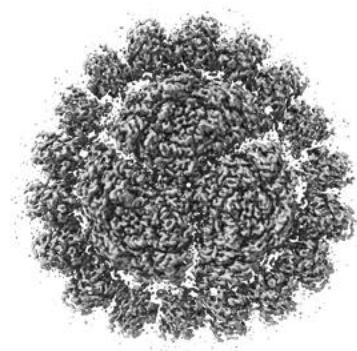
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

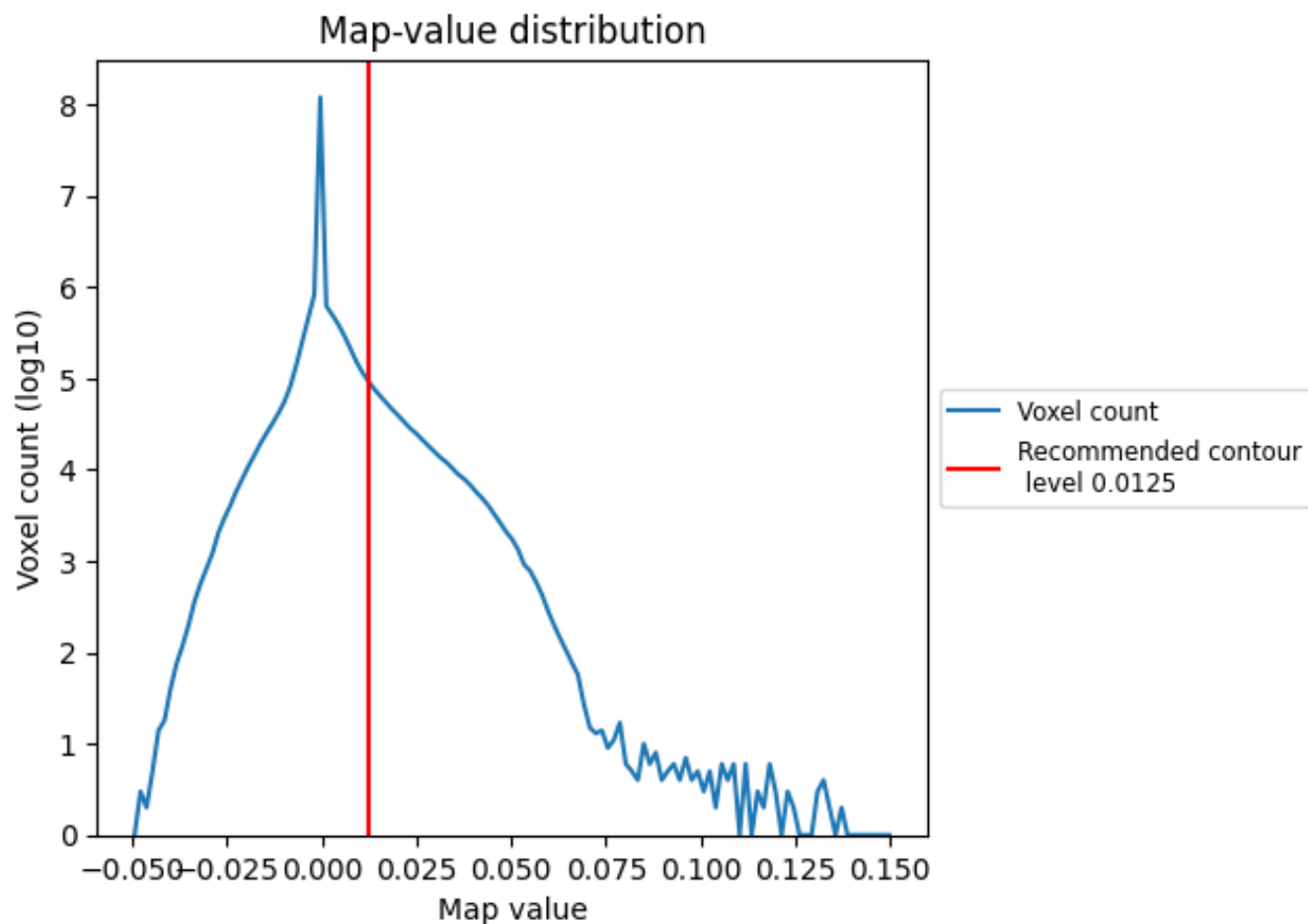
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

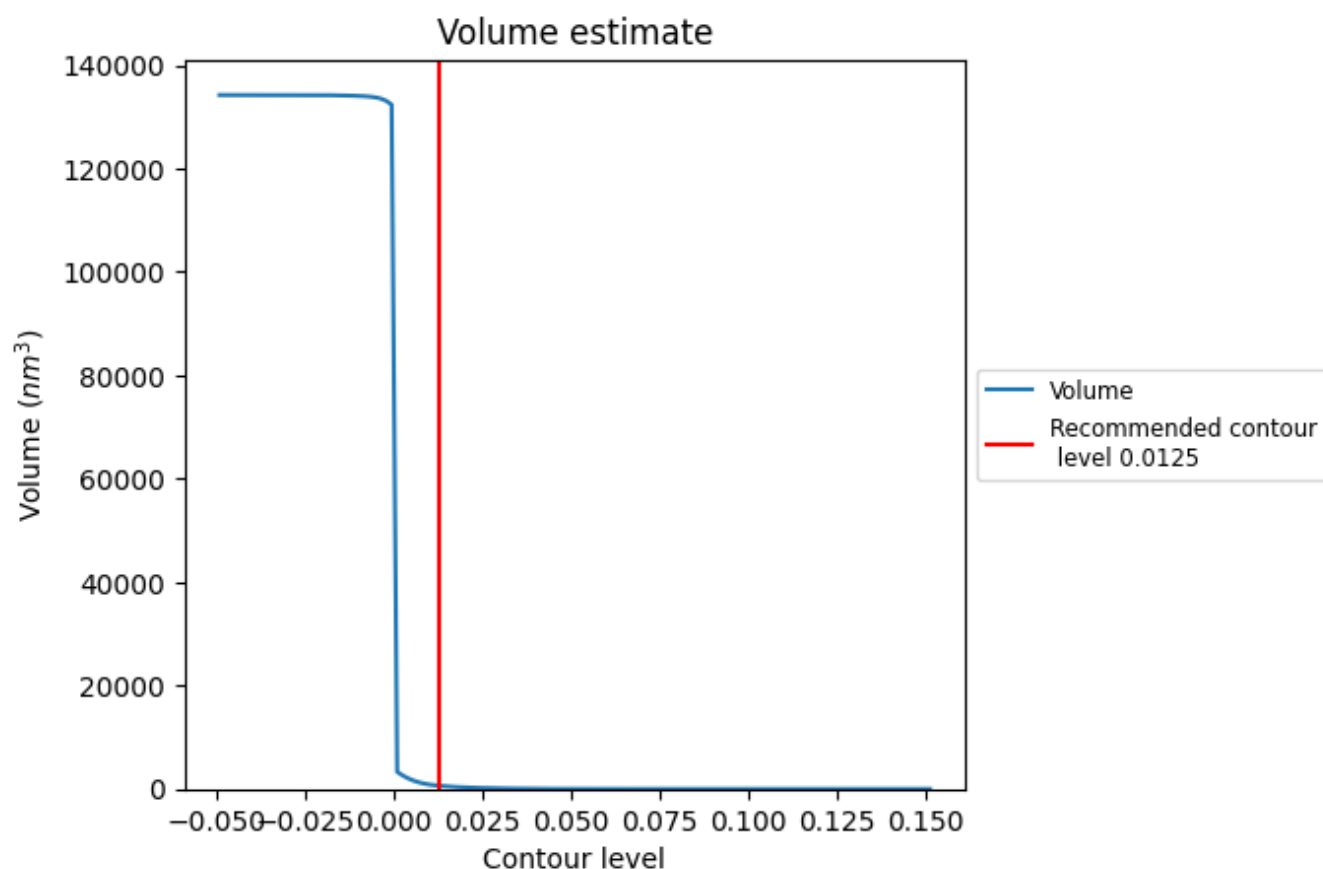
This section contains the results of statistical analysis of the map.

### 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.

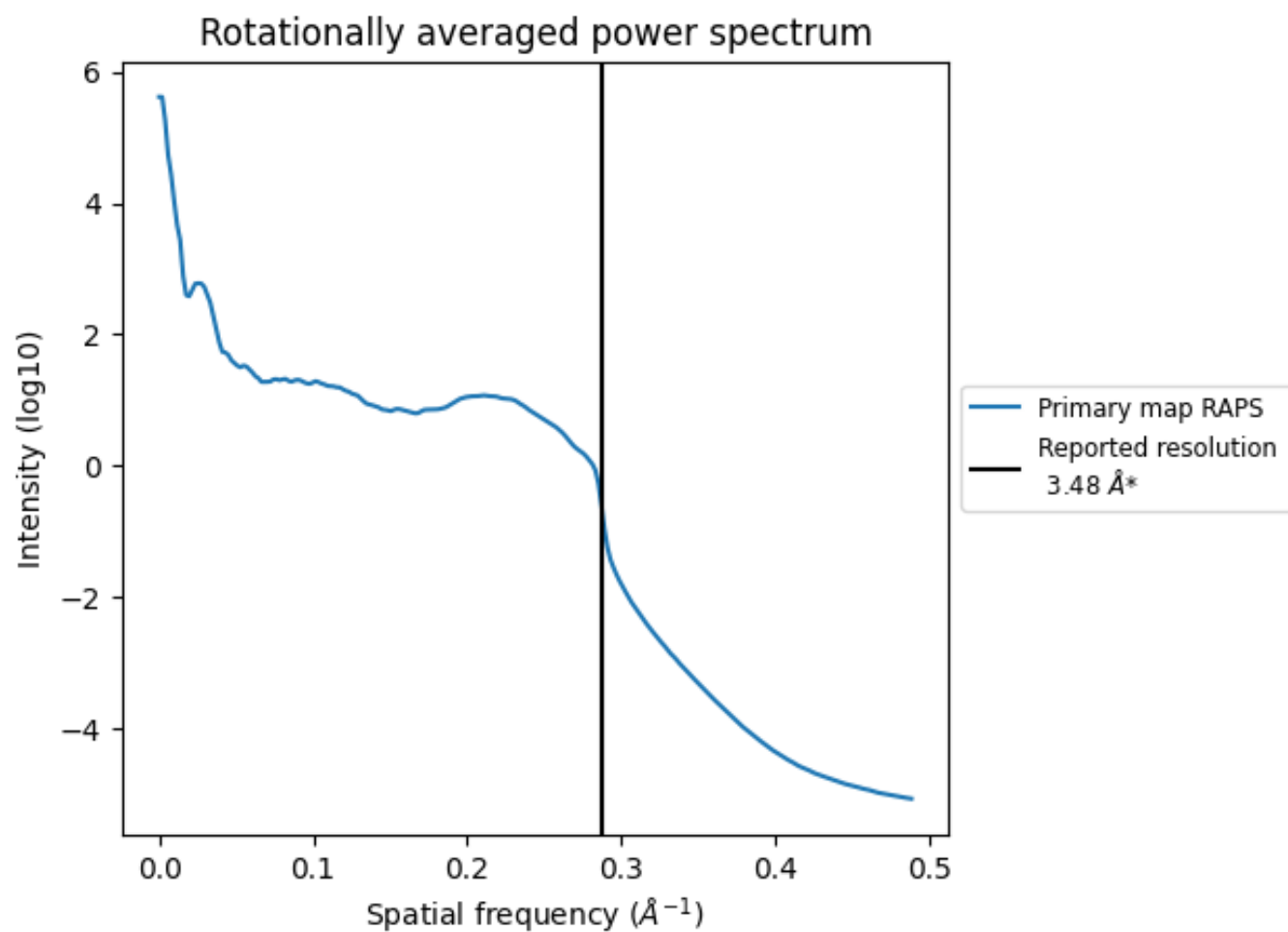
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 642  $\text{nm}^3$ ; this corresponds to an approximate mass of 580 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 ⓘ



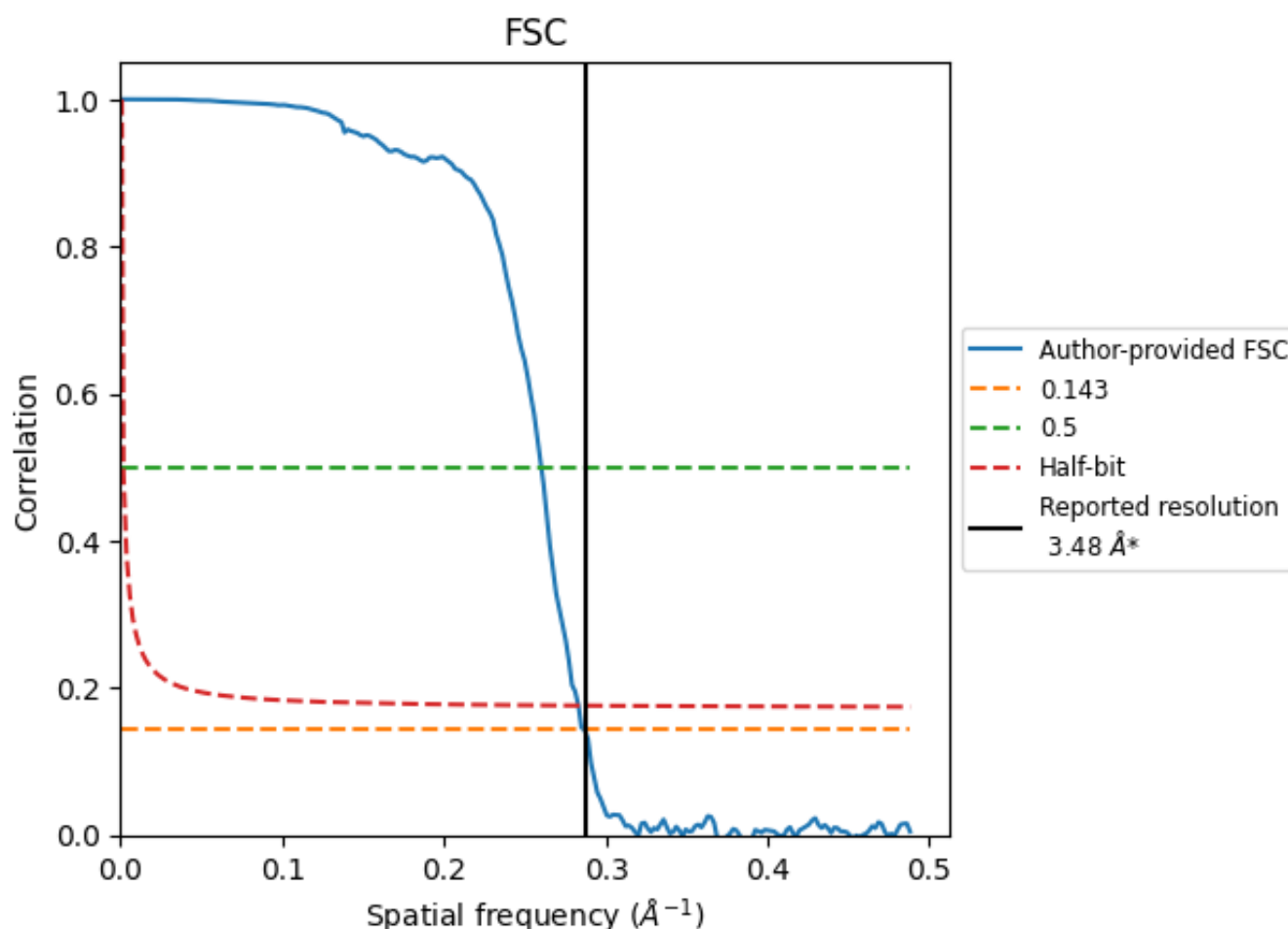
\*Reported resolution corresponds to spatial frequency of 0.287 Å<sup>-1</sup>



## 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 0.287 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

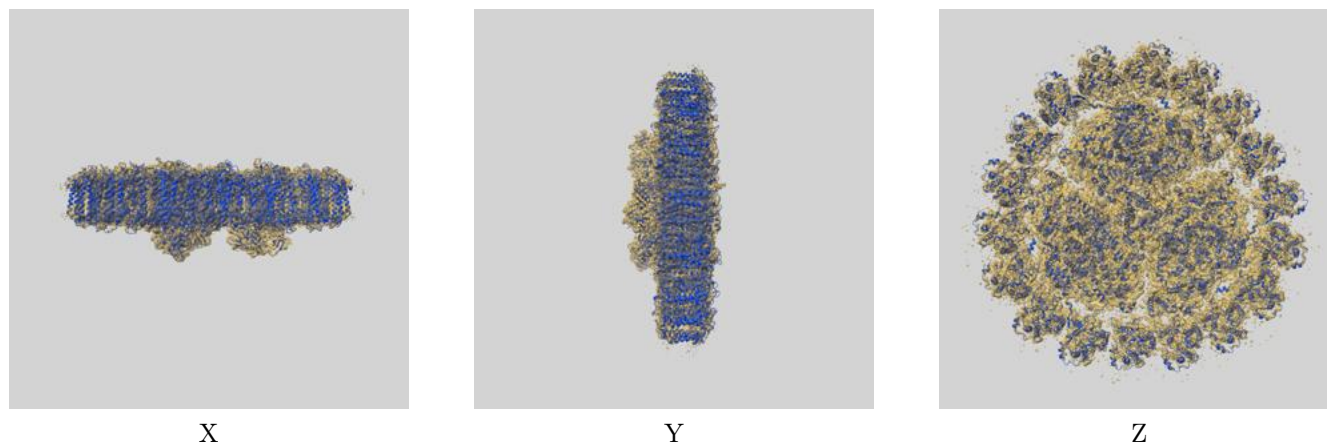
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.48	-	-
Author-provided FSC curve	3.49	3.84	3.53
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

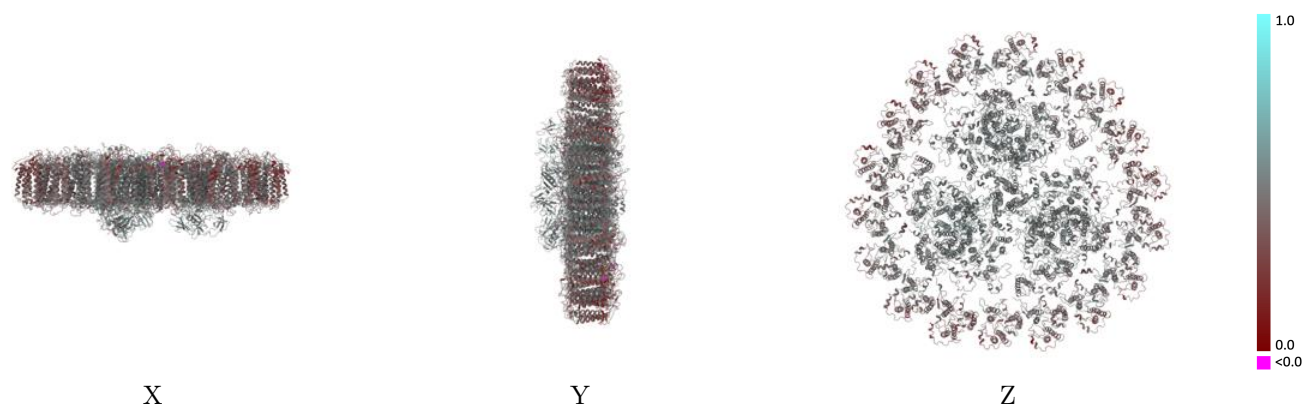
This section contains information regarding the fit between EMDB map EMD-0524 and PDB model 6NWA. Per-residue inclusion information can be found in section [3](#) on page [64](#).

### 9.1 Map-model overlay [i](#)



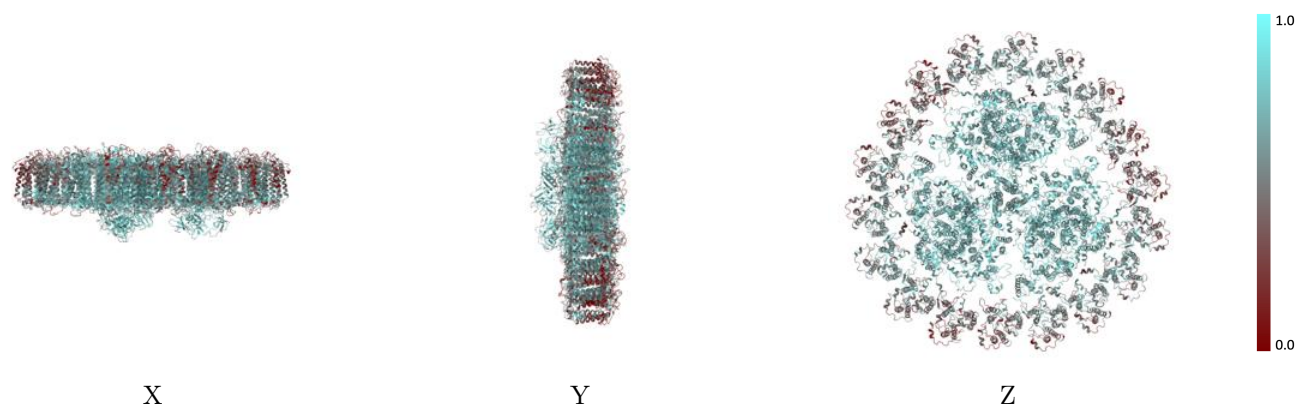
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



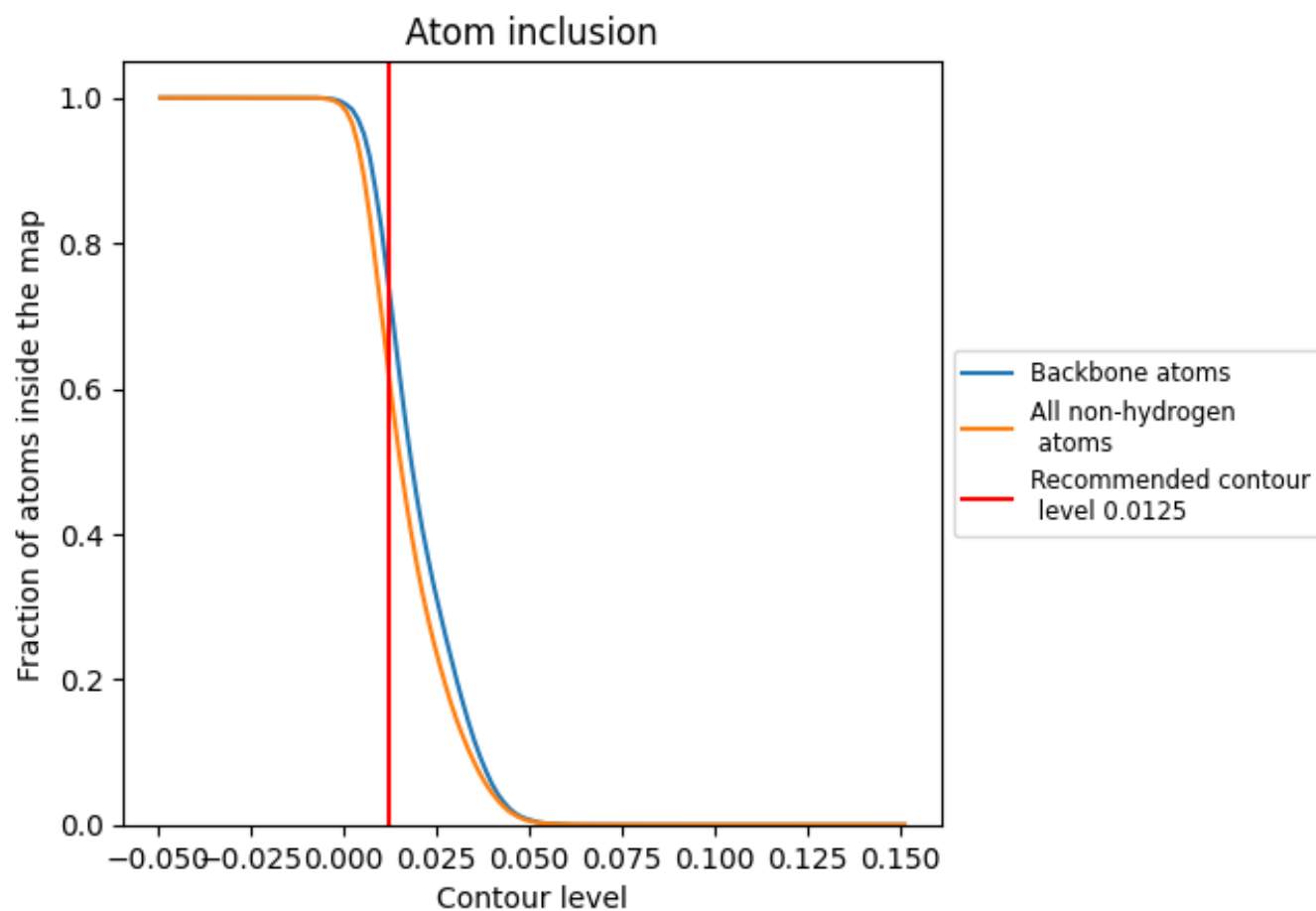
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0125).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 73% of all backbone atoms, 61% 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 (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6098	 0.4590
A	 0.7410	 0.5070
B	 0.7360	 0.5030
C	 0.7990	 0.5080
D	 0.7045	 0.5070
E	 0.7059	 0.4990
F	 0.6979	 0.4740
G	 0.7373	 0.5030
H	 0.7441	 0.5120
I	 0.7627	 0.5330
J	 0.6774	 0.4880
K	 0.6248	 0.4280
L	 0.7249	 0.5040
M	 0.6145	 0.4870
N	 0.7973	 0.5060
O	 0.6980	 0.5080
P	 0.6926	 0.5020
Q	 0.6953	 0.4790
R	 0.7724	 0.5320
S	 0.6754	 0.4990
T	 0.6035	 0.4130
U	 0.7277	 0.5080
V	 0.6400	 0.4670
W	 0.4014	 0.3750
X	 0.5100	 0.4280
Y	 0.5550	 0.4440
Z	 0.5088	 0.4170
a	 0.7465	 0.5120
b	 0.7403	 0.4980
c	 0.8123	 0.5120
d	 0.7128	 0.5070
e	 0.7116	 0.4910
f	 0.6997	 0.4690
g	 0.4621	 0.3980
h	 0.3895	 0.3840



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Chain	Atom inclusion	Q-score
i	 0.7530	 0.5260
j	 0.6814	 0.4840
k	 0.6053	 0.4380
l	 0.7263	 0.5090
m	 0.6509	 0.4870
n	 0.3997	 0.3750
o	 0.5075	 0.4270
p	 0.5639	 0.4490
q	 0.5152	 0.4220
r	 0.4655	 0.4010
s	 0.5639	 0.4540
t	 0.4102	 0.3800
u	 0.5091	 0.4350
v	 0.3933	 0.3890
w	 0.5149	 0.4210
x	 0.4690	 0.4060
y	 0.3845	 0.3830