



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 11:06 PM UTC

PDB ID : 6NWA / pdb_00006nwa
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

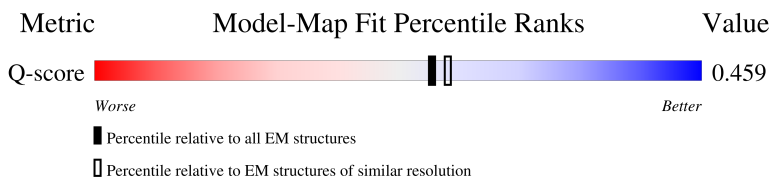
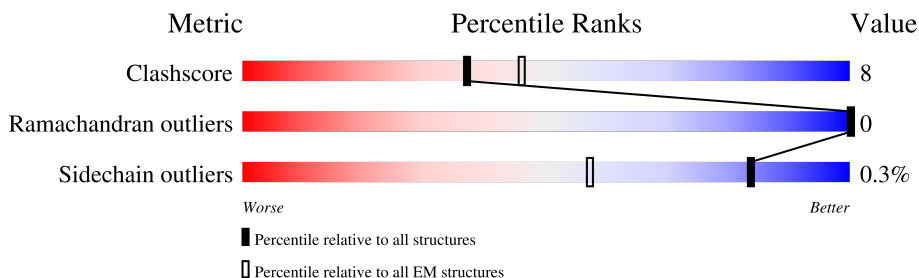
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



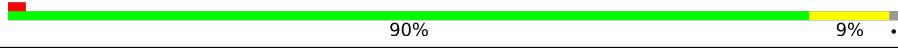
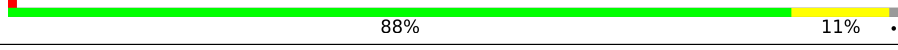
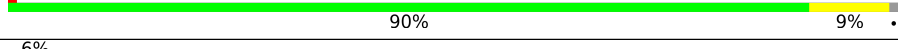
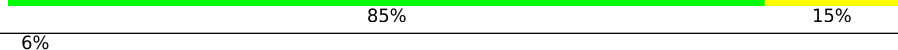
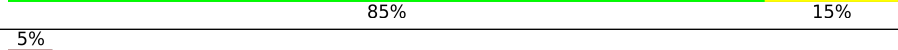
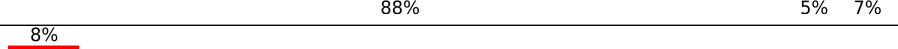
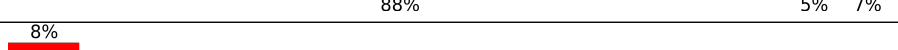
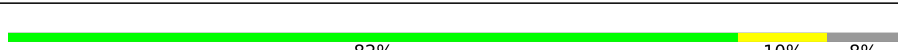
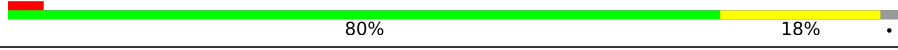
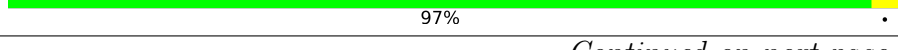
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13672 (2.98 - 3.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	
1	H	751	
1	a	751	
2	B	731	

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Mol	Chain	Length	Quality of chain
2	G	731	
2	b	731	
3	C	81	
3	N	81	
3	c	81	
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	

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Mol	Chain	Length	Quality of chain
10	m	31	
11	W	342	
11	X	342	
11	Y	342	
11	Z	342	
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	-	-	-
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	-	-	-

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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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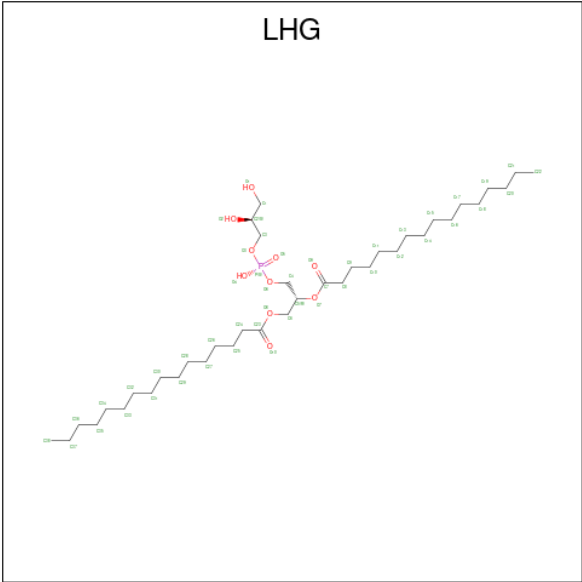
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Mol	Chain	Residues	Atoms					AltConf	Trace
11	n	329	Total	C	N	O	S	0	0
			2475	1655	401	415	4		
11	o	339	Total	C	N	O	S	0	0
			2605	1732	424	444	5		
11	p	340	Total	C	N	O	S	0	0
			2609	1735	424	445	5		
11	q	337	Total	C	N	O	S	0	0
			2582	1717	421	439	5		
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.

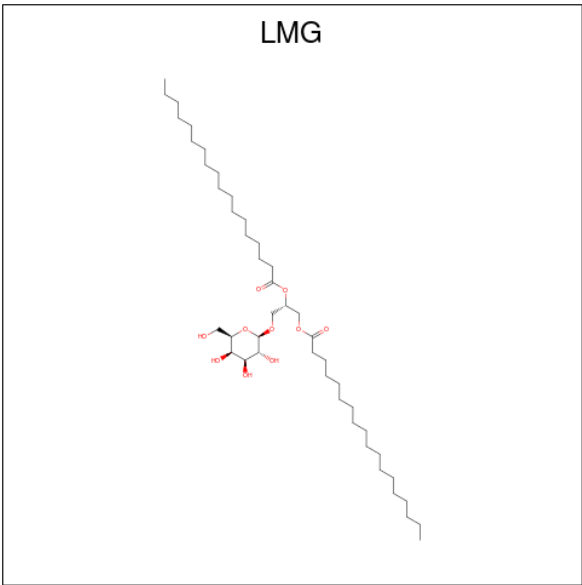
Mol	Chain	Residues	Atoms					AltConf	Trace
12	k	70	Total	C	N	O	S	0	0
			485	317	80	84	4		
12	K	70	Total	C	N	O	S	0	0
			485	317	80	84	4		
12	T	70	Total	C	N	O	S	0	0
			485	317	80	84	4		

- Molecule 13 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			43	32	10	1	
13	A	1	Total	C	O	P	0
			27	16	10	1	
13	I	1	Total	C	O	P	0
			44	33	10	1	
13	a	1	Total	C	O	P	0
			43	32	10	1	
13	a	1	Total	C	O	P	0
			27	16	10	1	
13	i	1	Total	C	O	P	0
			44	33	10	1	
13	H	1	Total	C	O	P	0
			43	32	10	1	
13	H	1	Total	C	O	P	0
			27	16	10	1	
13	R	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 14 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



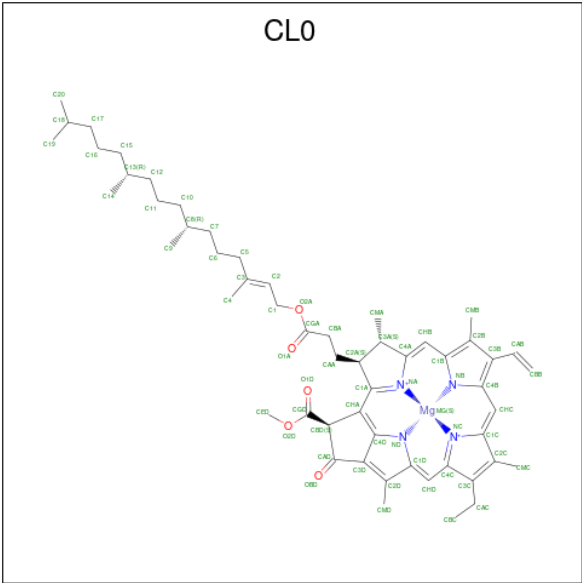
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			38	28	10	
14	A	1	Total	C	O	0
			46	36	10	
14	A	1	Total	C	O	0
			32	22	10	
14	B	1	Total	C	O	0
			43	33	10	
14	Y	1	Total	C	O	0
			39	29	10	
14	a	1	Total	C	O	0
			38	28	10	
14	a	1	Total	C	O	0
			46	36	10	
14	a	1	Total	C	O	0
			31	21	10	
14	b	1	Total	C	O	0
			43	33	10	
14	p	1	Total	C	O	0
			39	29	10	
14	H	1	Total	C	O	0
			38	28	10	
14	H	1	Total	C	O	0
			46	36	10	
14	H	1	Total	C	O	0
			32	22	10	
14	G	1	Total	C	O	0
			43	33	10	

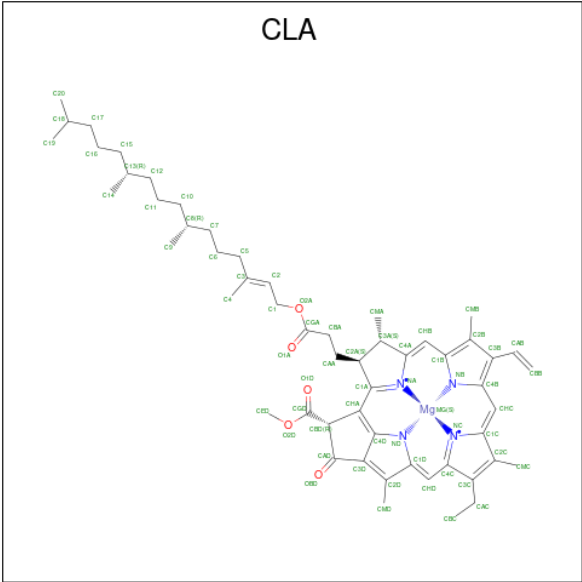
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Mol	Chain	Residues	Atoms			AltConf
14	s	1	Total	C	O	0
			39	29	10	

- Molecule 15 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).





Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
16	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
16	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
16	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
16	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	F	1	Total 27	C 22	Mg 1	N 4		0
16	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	J	1	Total 37	C 31	Mg 1	N 4	O 1	0
16	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	W	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	W	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	W	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	W	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	W	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	W	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	W	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	X	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Y	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	Z	1	Total 56	C 46	Mg 1	N 4	O 5	0
16	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	g	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	g	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	y	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	y	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	y	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	y	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	y	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	y	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 58	C 48	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 41	C 33	Mg 1	N 4	O 3	0
16	a	1	Total 52	C 42	Mg 1	N 4	O 5	0
16	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 49	C 39	Mg 1	N 4	O 5	0
16	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	n	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	n	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	o	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	o	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	o	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	o	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	o	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	o	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	p	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	q	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	q	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	q	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	q	1	Total 56	C 46	Mg 1	N 4	O 5	0
16	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	q	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	q	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	r	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	r	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	r	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	r	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	r	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	r	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	h	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	h	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	h	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	h	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	h	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	h	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	h	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 56	C 46	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	H	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
16	H	1	Total 52	C 42	Mg 1	N 4	O 5	0
16	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
16	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	G	1	Total 58	C 48	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	G	1	Total 62	C 52	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	U	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	t	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	t	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	t	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	t	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	t	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	t	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	t	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	t	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	t	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	u	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	u	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	u	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	u	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	u	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	u	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	u	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	s	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	w	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	w	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	w	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	w	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	w	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	w	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	w	1	Total 56	C 46	Mg 1	N 4	O 5	0
16	w	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	w	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	w	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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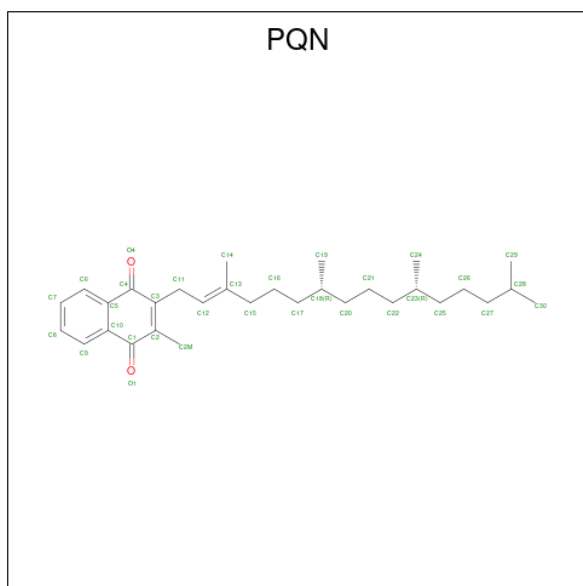
Mol	Chain	Residues	Atoms					AltConf
16	x	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	v	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	v	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	v	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	v	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	v	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	v	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	v	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	v	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	f	1	Total 27	C 22	Mg 1	N 4		0
16	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms				AltConf
16	Q	1	Total	C	Mg	N	0
			27	22	1	4	
16	j	1	Total	C	Mg	N	O
			45	35	1	4	5
16	j	1	Total	C	Mg	N	O
			37	31	1	4	1
16	S	1	Total	C	Mg	N	O
			45	35	1	4	5
16	S	1	Total	C	Mg	N	O
			37	31	1	4	1
16	K	1	Total	C	Mg	N	O
			45	35	1	4	5
16	T	1	Total	C	Mg	N	O
			45	35	1	4	5

- Molecule 17 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



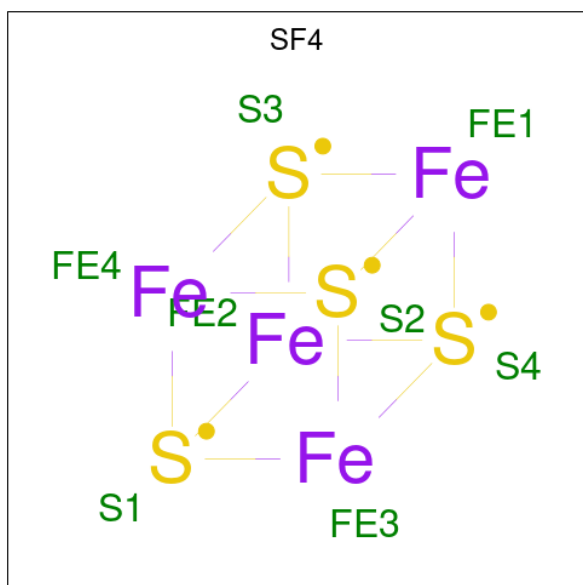
Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	C	O	0
			33	31	2	
17	B	1	Total	C	O	0
			33	31	2	
17	a	1	Total	C	O	0
			33	31	2	
17	b	1	Total	C	O	0
			33	31	2	

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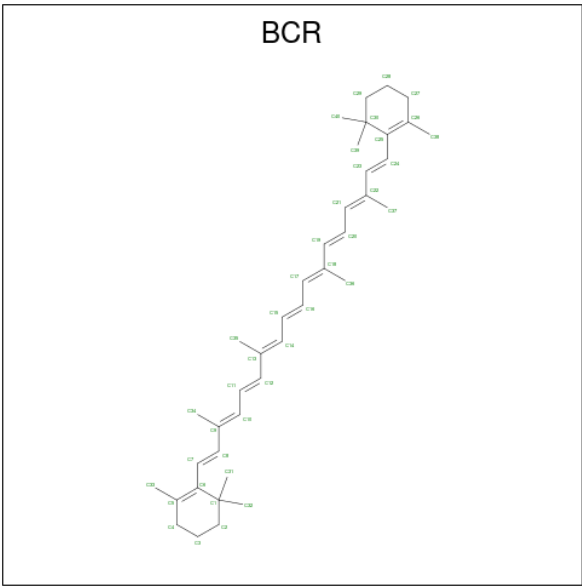
Mol	Chain	Residues	Atoms			AltConf
17	H	1	Total	C	O	0
			33	31	2	
17	G	1	Total	C	O	0
			33	31	2	

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 19 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			25	25	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	

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

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Mol	Chain	Residues	Atoms	AltConf
19	Z	1	Total C 40 40	0
19	Z	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	y	1	Total C 40 40	0
19	y	1	Total C 40 40	0
19	y	1	Total C 40 40	0
19	y	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 25 25	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0

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

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Mol	Chain	Residues	Atoms	AltConf
19	q	1	Total C 40 40	0
19	r	1	Total C 40 40	0
19	r	1	Total C 40 40	0
19	r	1	Total C 40 40	0
19	r	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	G	1	Total C 40 40	0
19	G	1	Total C 40 40	0
19	G	1	Total C 25 25	0
19	G	1	Total C 40 40	0
19	G	1	Total C 40 40	0
19	G	1	Total C 40 40	0

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

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

- Molecule 20 is DODECYL-BETA-D-MALTOSIDE (CCD ID: 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

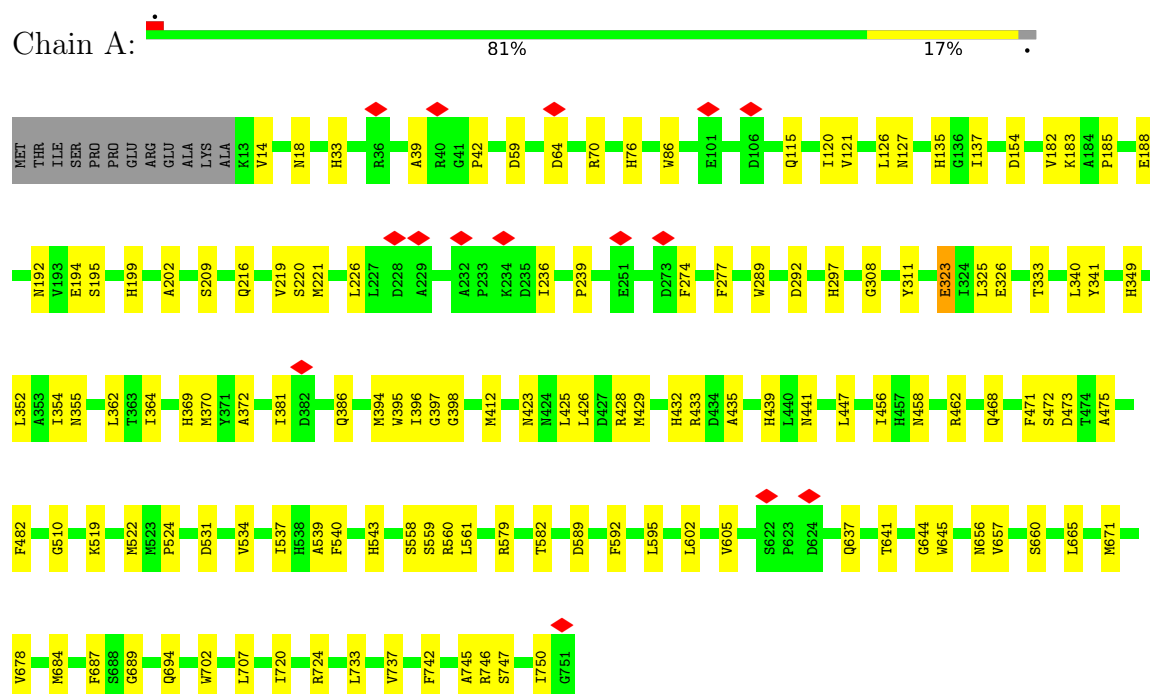
- Molecule 21 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

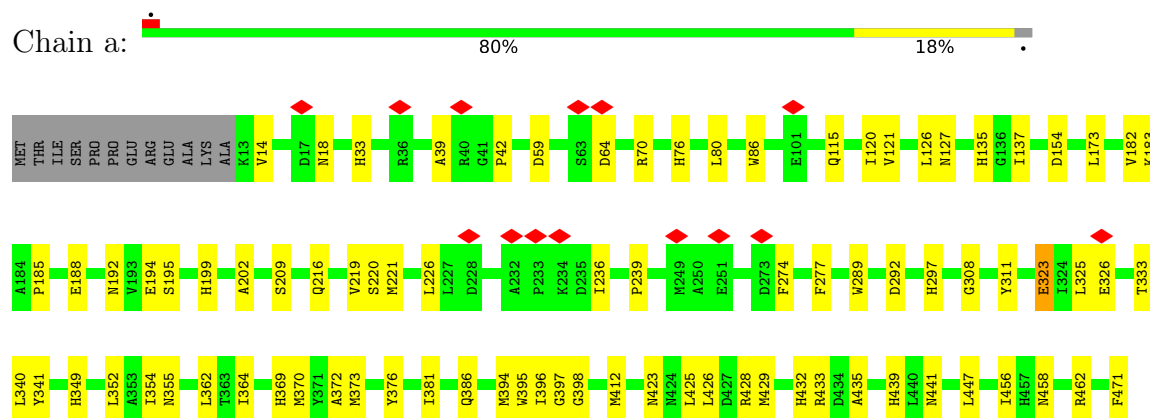
3 Residue-property plots

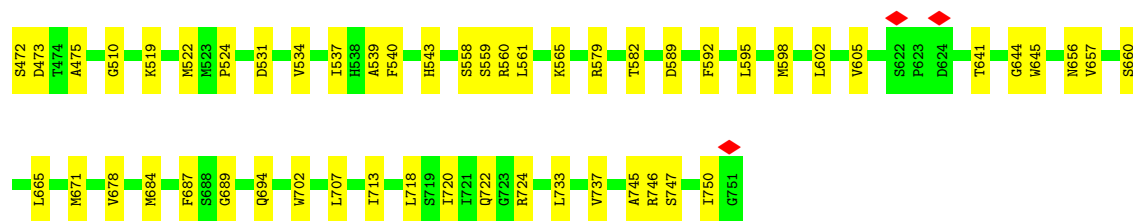
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



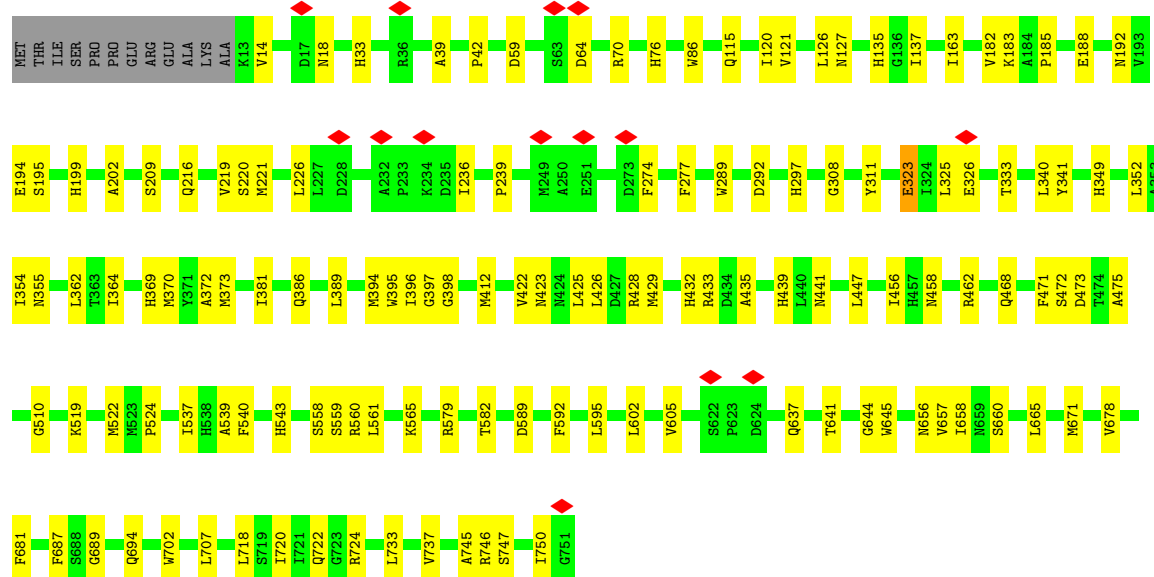
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





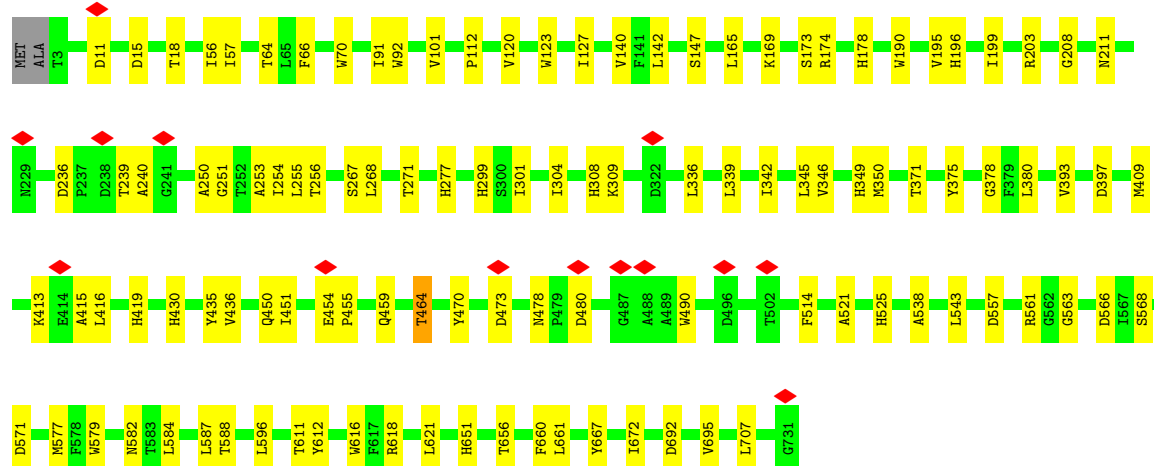
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain H: 81% 18%



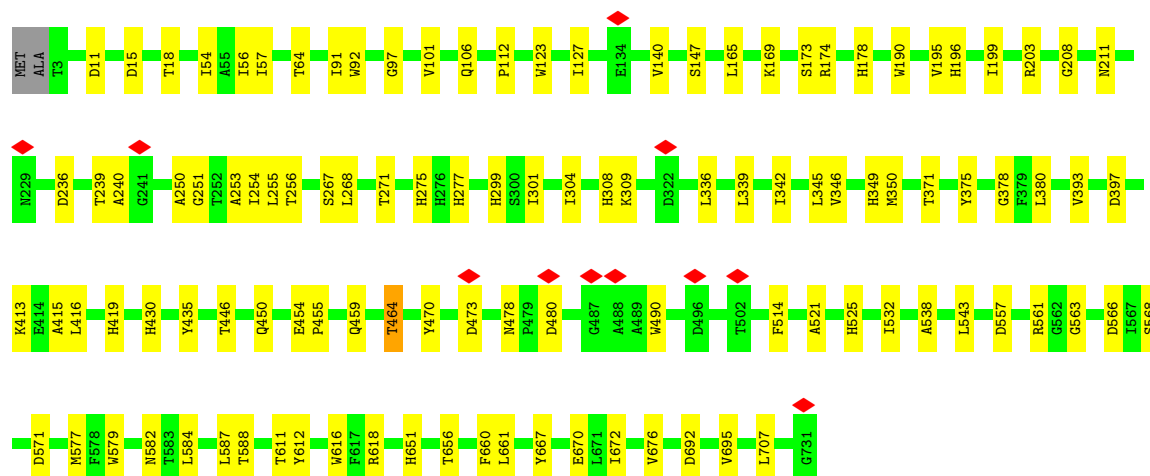
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 84% 15%

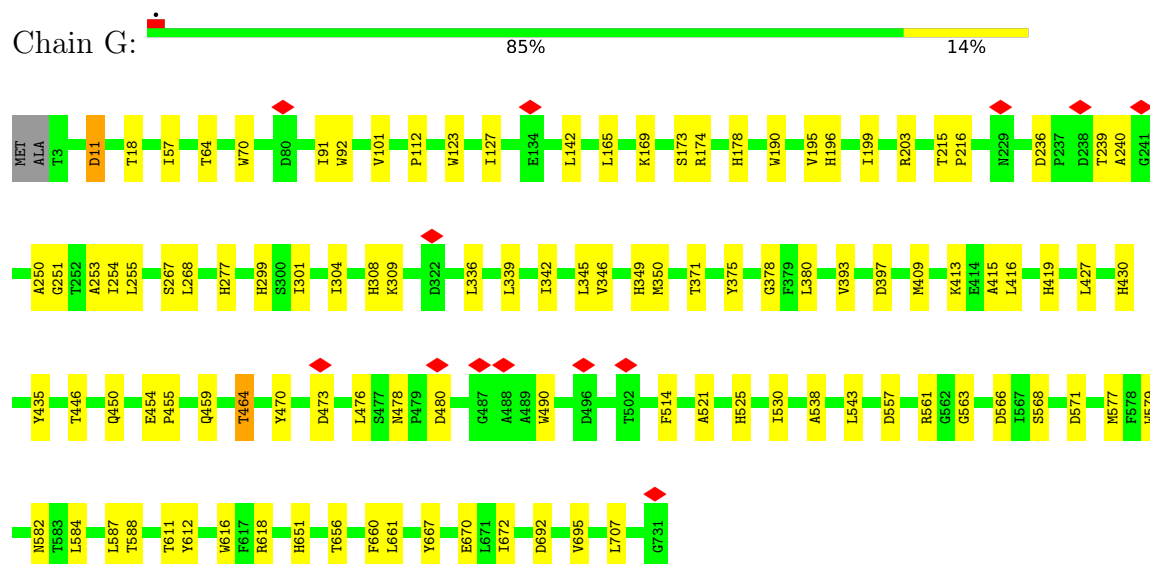


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

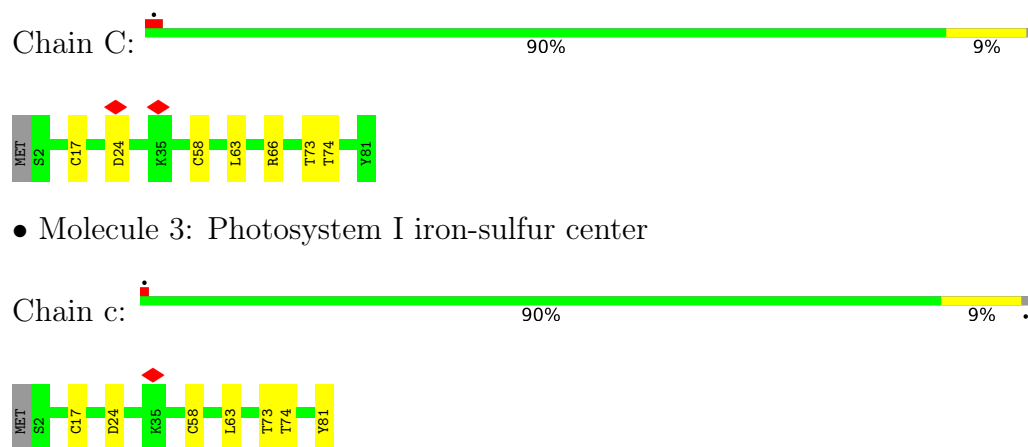
Chain b: 85% 15%



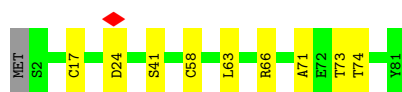
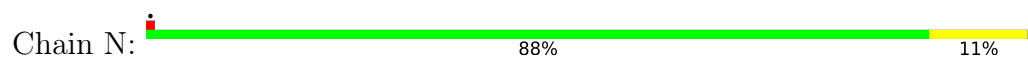
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



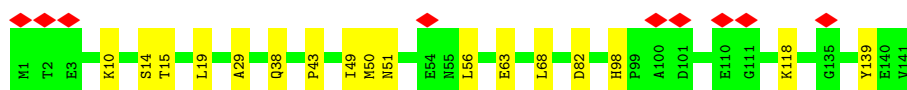
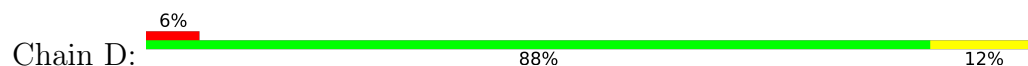
- Molecule 3: Photosystem I iron-sulfur center



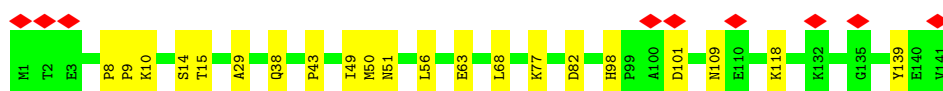
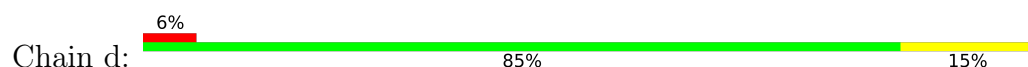
- Molecule 3: Photosystem I iron-sulfur center



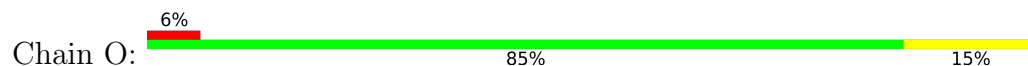
- Molecule 4: Photosystem I reaction center subunit II



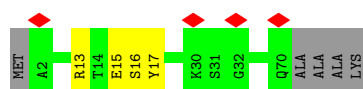
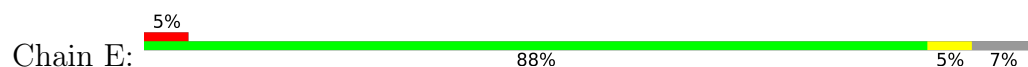
- Molecule 4: Photosystem I reaction center subunit II



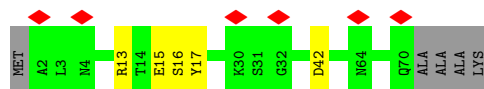
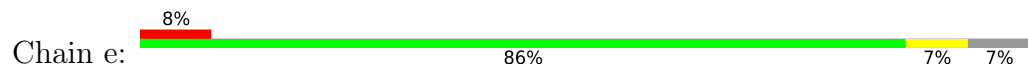
- Molecule 4: Photosystem I reaction center subunit II



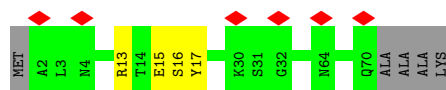
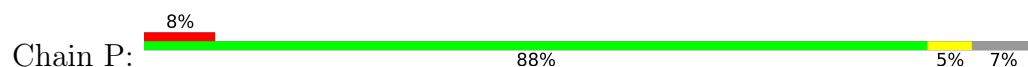
- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 5: Photosystem I reaction center subunit IV



Chain F:

5% 72% 13% 16%

1.5
1.0
0.5
0

200

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200

MET LYS HIS LEU LEU ALA LEU LEU LEU ALA THR LEU TRP PHE ASN PHE ALA PRO SER ALA SER ALA ASP ASP PHE L55 L66 L77 L88 L99 L100 L112 L124 L127 L128 L136 L137 L138 L139 L144 L148 L152 L153 L154 L159 L162 L163 L164 L170

[illegible]

Chain Q:

Chain I:

Category	Percentage
M1	80%
A6	12%
L15	8%
G19	0%
L29	0%
S36	0%
E37	0%
GLY	0%
GLY	0%
GLY	0%

Chain i: 82% 10% 8%

Residue	Color
R1	Green
I15	Yellow
G19	Yellow
L29	Green
S36	Yellow
E37	Green
GLY	Green
GLY	Grey
GLY	Grey

WORLDWIDE
PDB
PROTEIN DATA BANK

Chain R:  82% 10% 8%



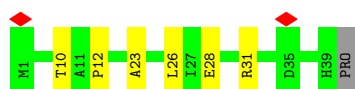
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  5% 82% 15% .



- Molecule 8: Photosystem I reaction center subunit IX

Chain j:  5% 82% 15% .



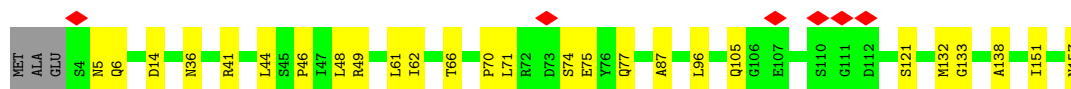
- Molecule 8: Photosystem I reaction center subunit IX

Chain S:  5% 80% 18% .



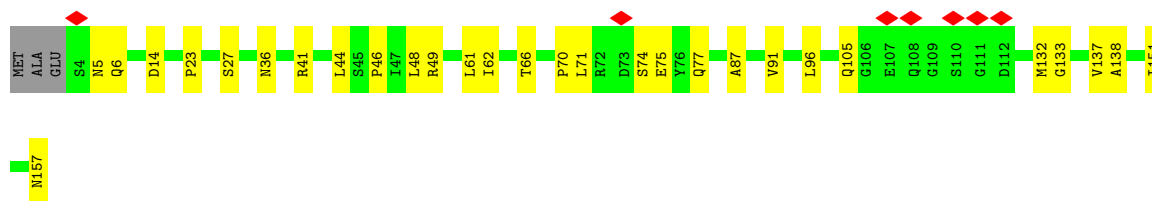
- Molecule 9: Photosystem I reaction center subunit XI

Chain L:  5% 82% 17% .



- Molecule 9: Photosystem I reaction center subunit XI

Chain l:  5% 80% 18% .



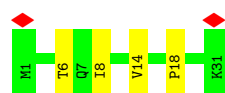
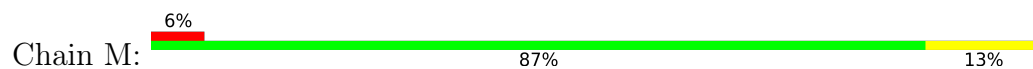
- Molecule 9: Photosystem I reaction center subunit XI

Chain U:  5% 80% 18% .





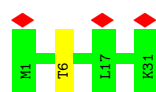
- Molecule 10: Photosystem I reaction center subunit XII



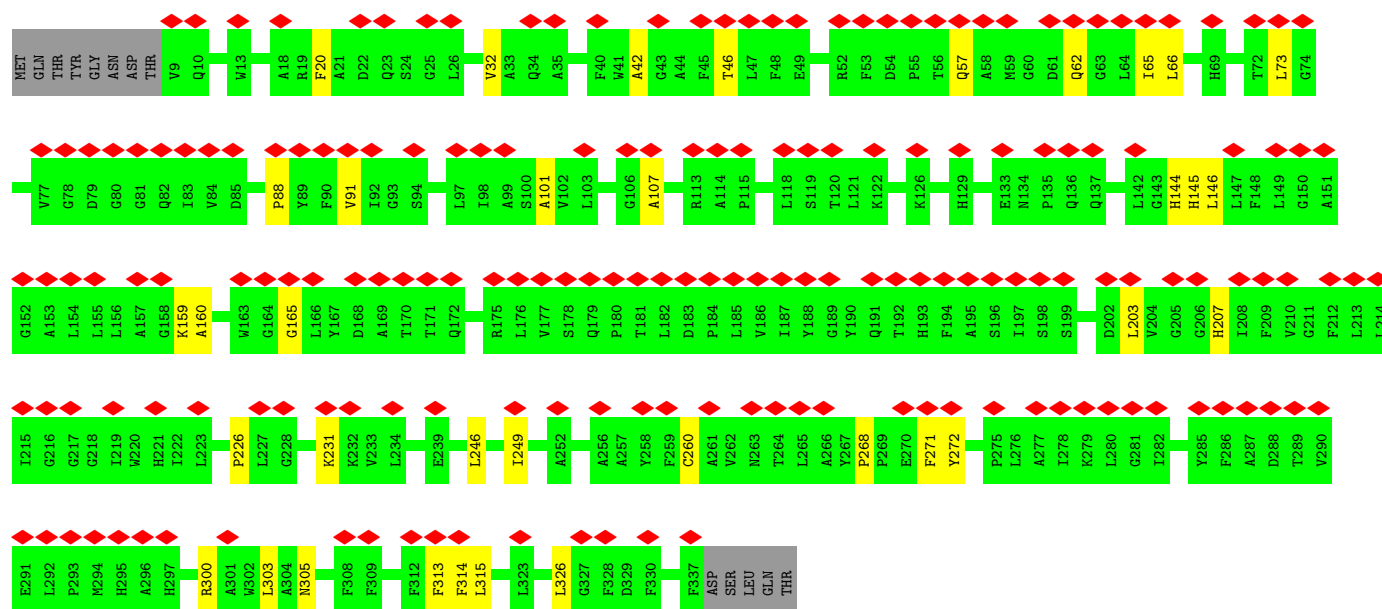
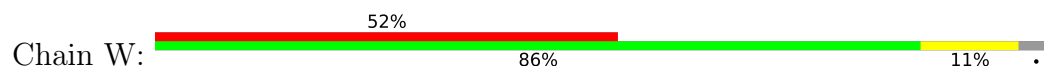
- Molecule 10: Photosystem I reaction center subunit XII



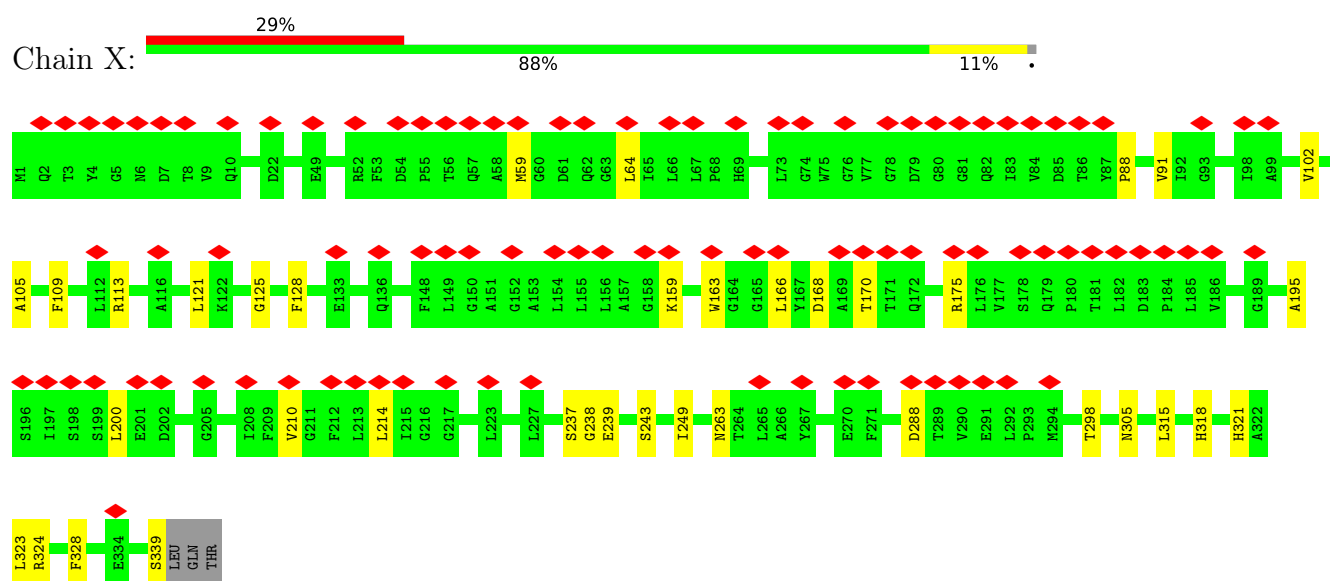
- Molecule 10: Photosystem I reaction center subunit XII



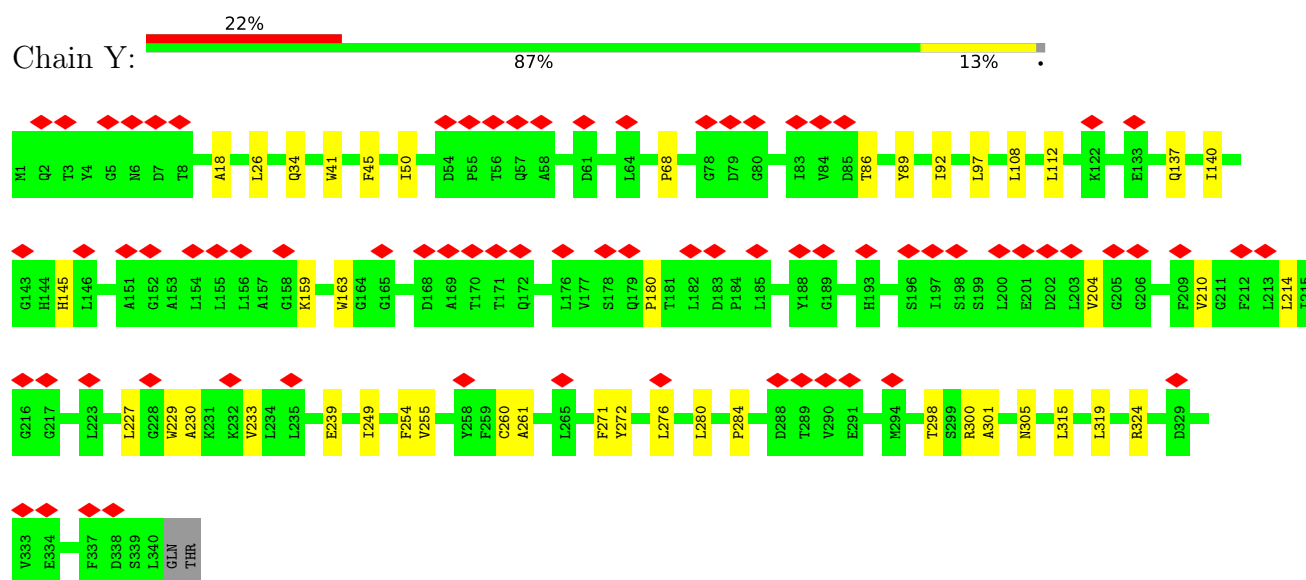
- Molecule 11: Iron stress-induced chlorophyll-binding protein



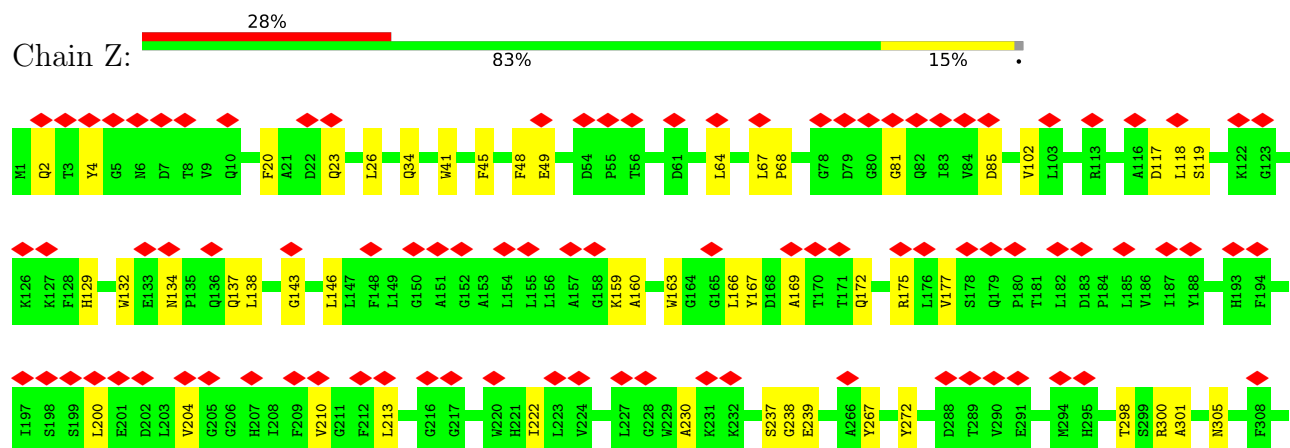
- Molecule 11: Iron stress-induced chlorophyll-binding protein

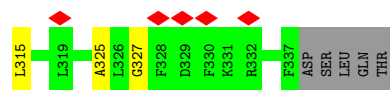


- Molecule 11: Iron stress-induced chlorophyll-binding protein

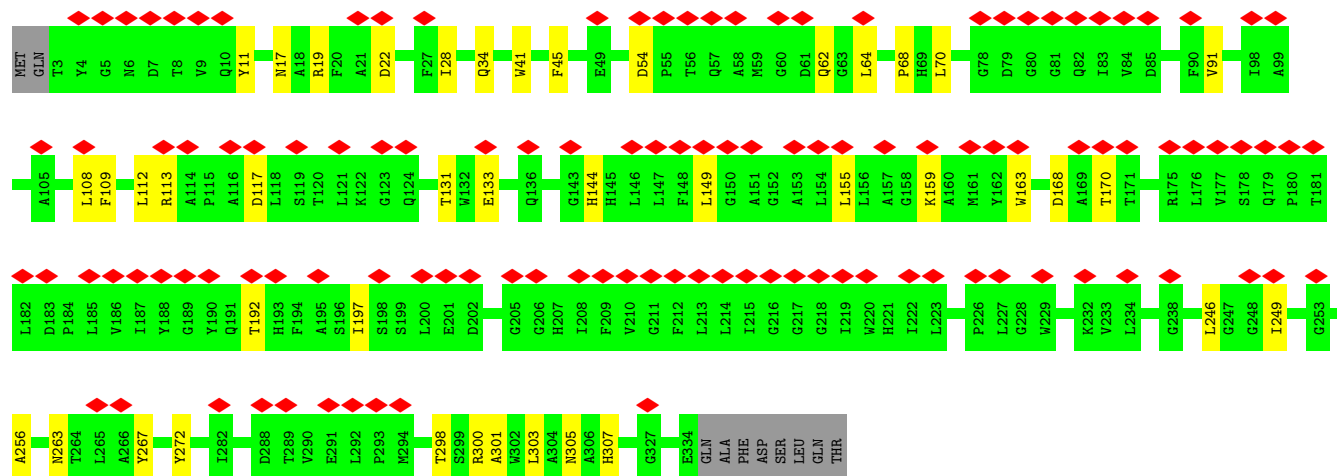
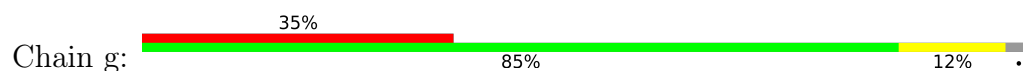


- Molecule 11: Iron stress-induced chlorophyll-binding protein

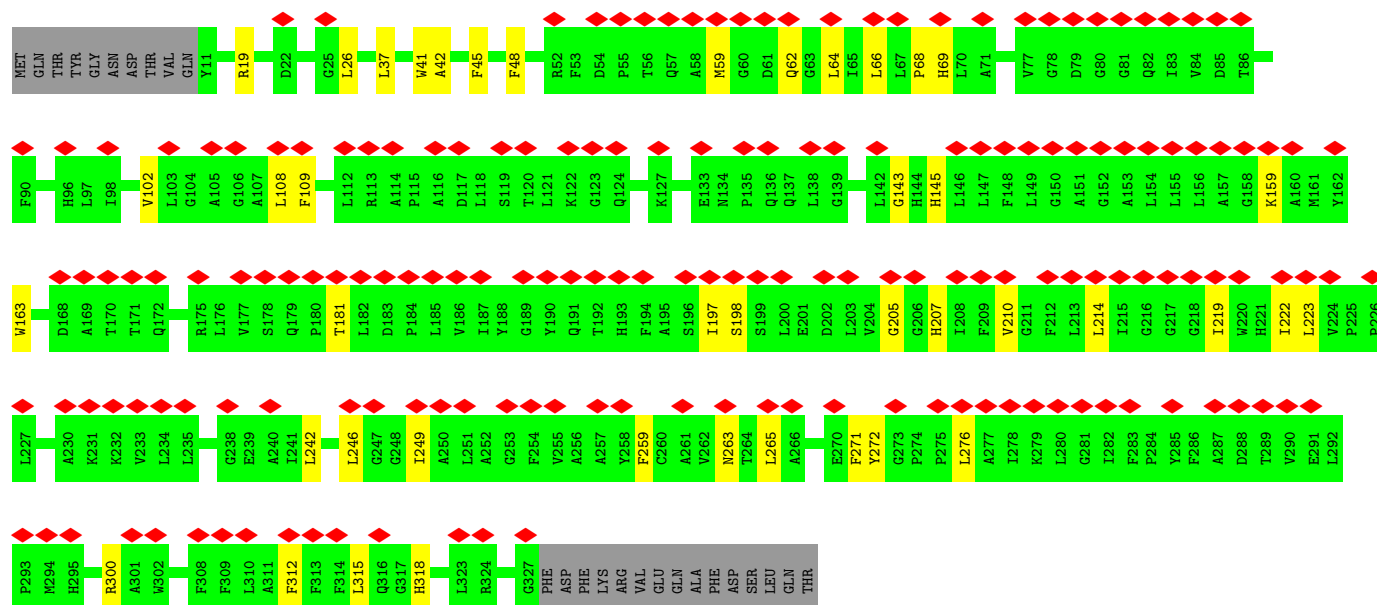
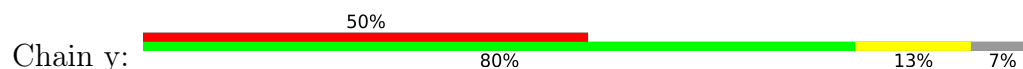




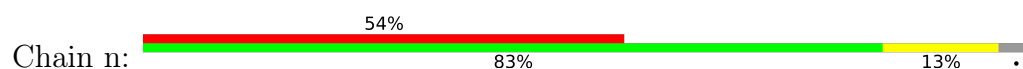
- Molecule 11: Iron stress-induced chlorophyll-binding protein

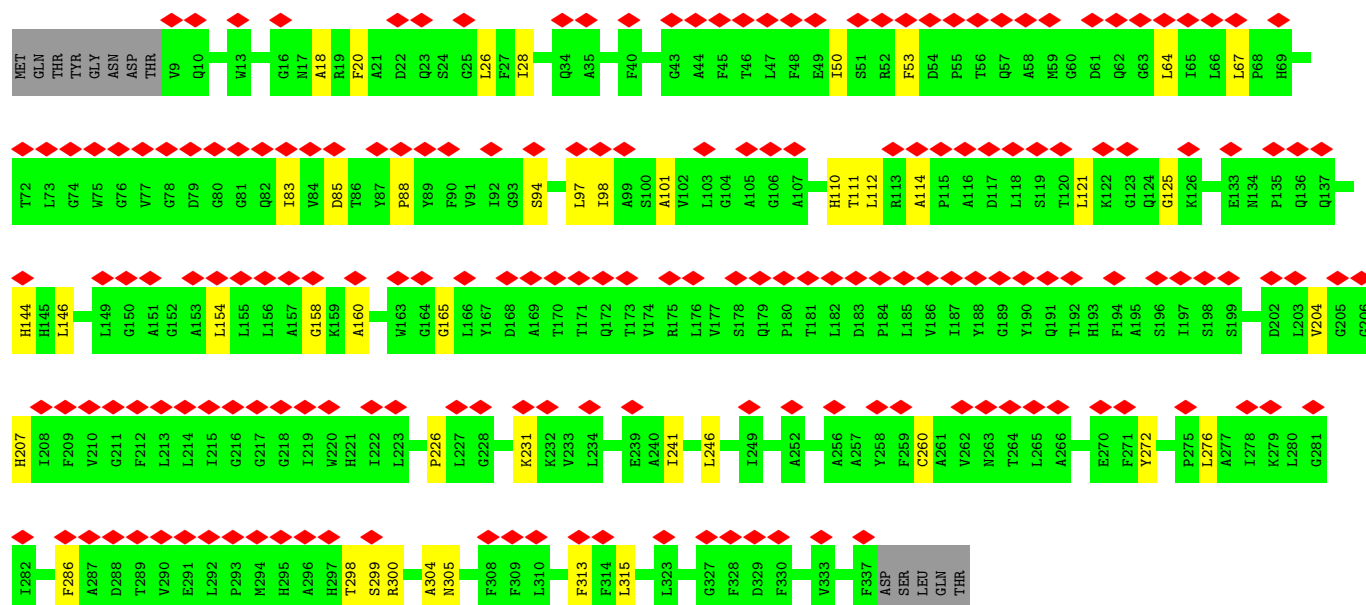


- Molecule 11: Iron stress-induced chlorophyll-binding protein



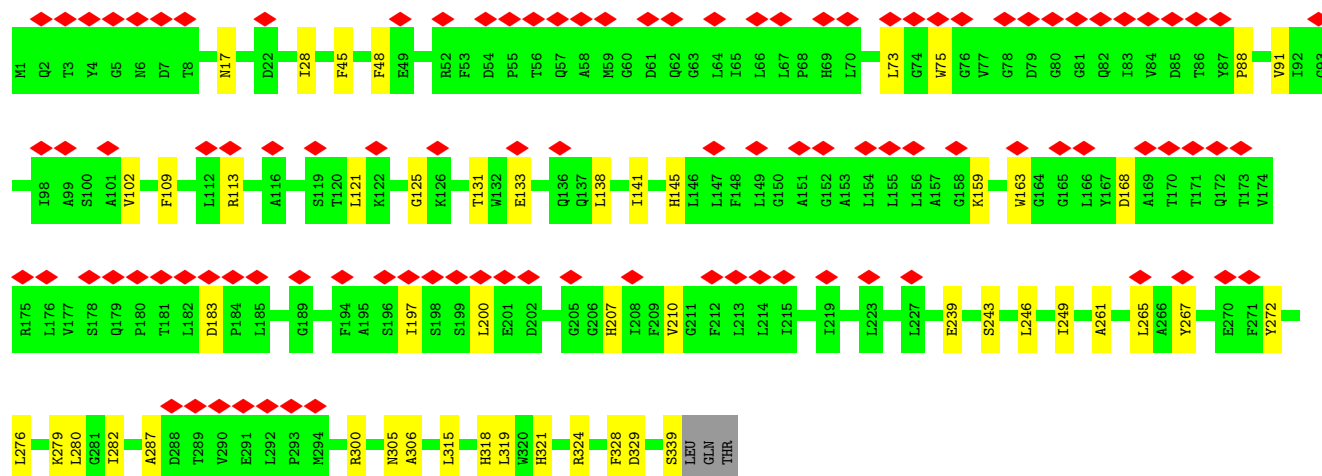
- Molecule 11: Iron stress-induced chlorophyll-binding protein





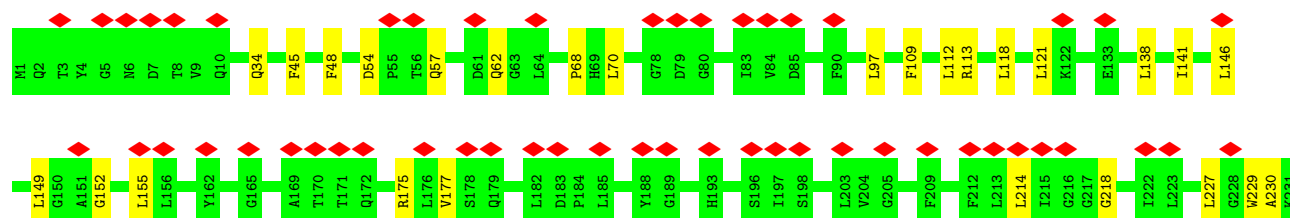
- Molecule 11: Iron stress-induced chlorophyll-binding protein

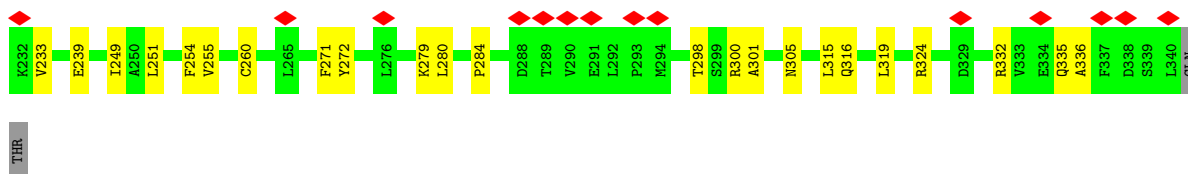
Chain o: 30% 85% 15% .



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

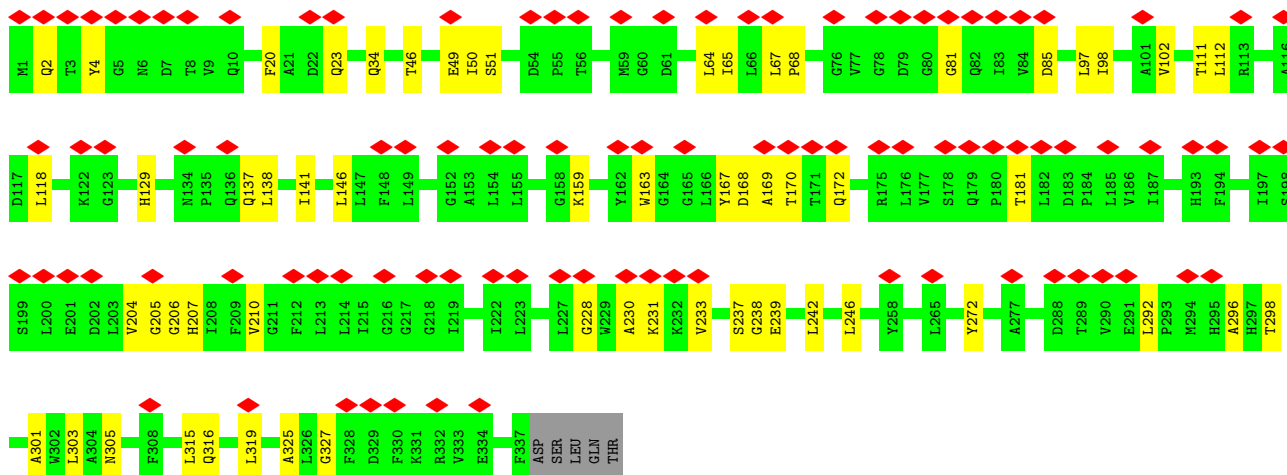
Chain p: 19% 85% 15% .





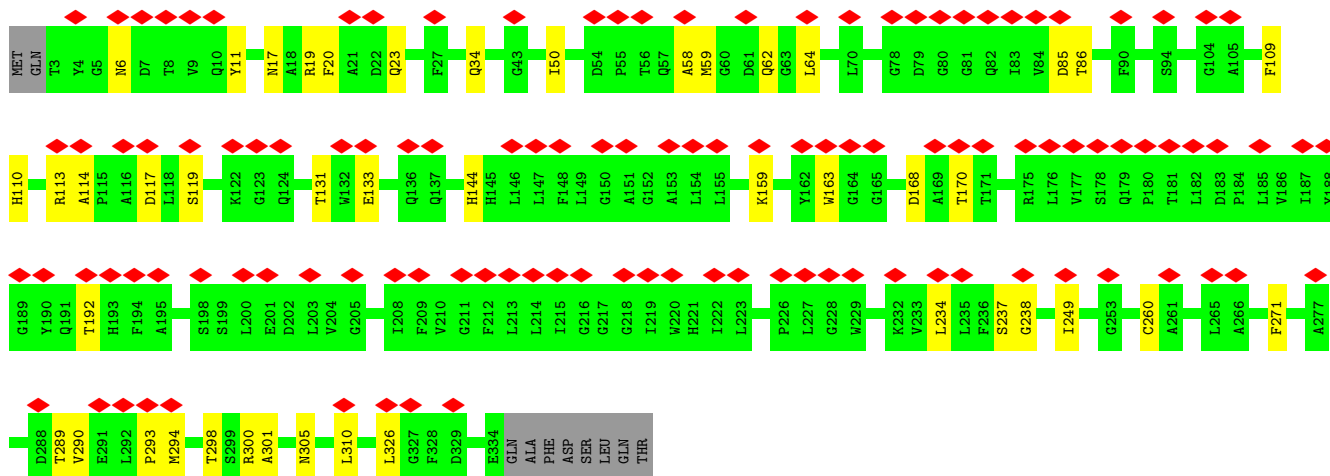
- Molecule 11: Iron stress-induced chlorophyll-binding protein

Chain q: 29% 81% 18%



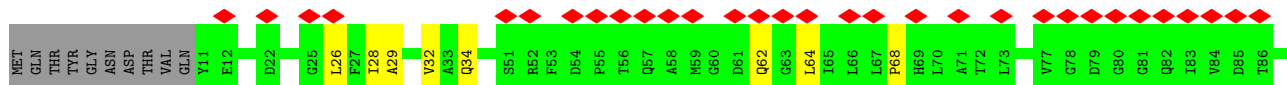
- Molecule 11: Iron stress-induced chlorophyll-binding protein

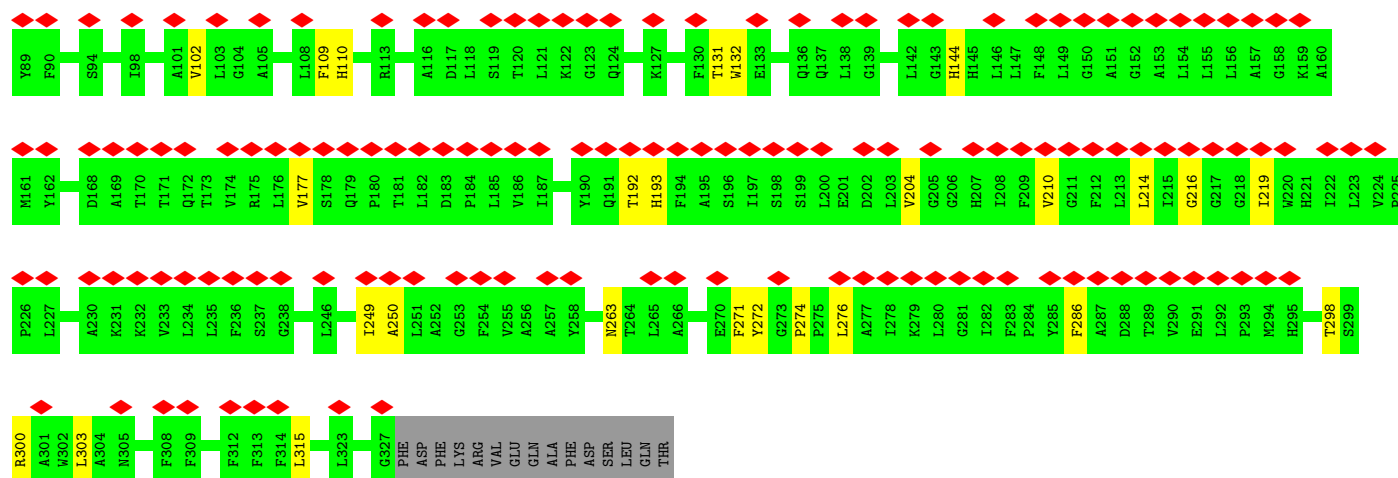
Chain r: 34% 84% 13%



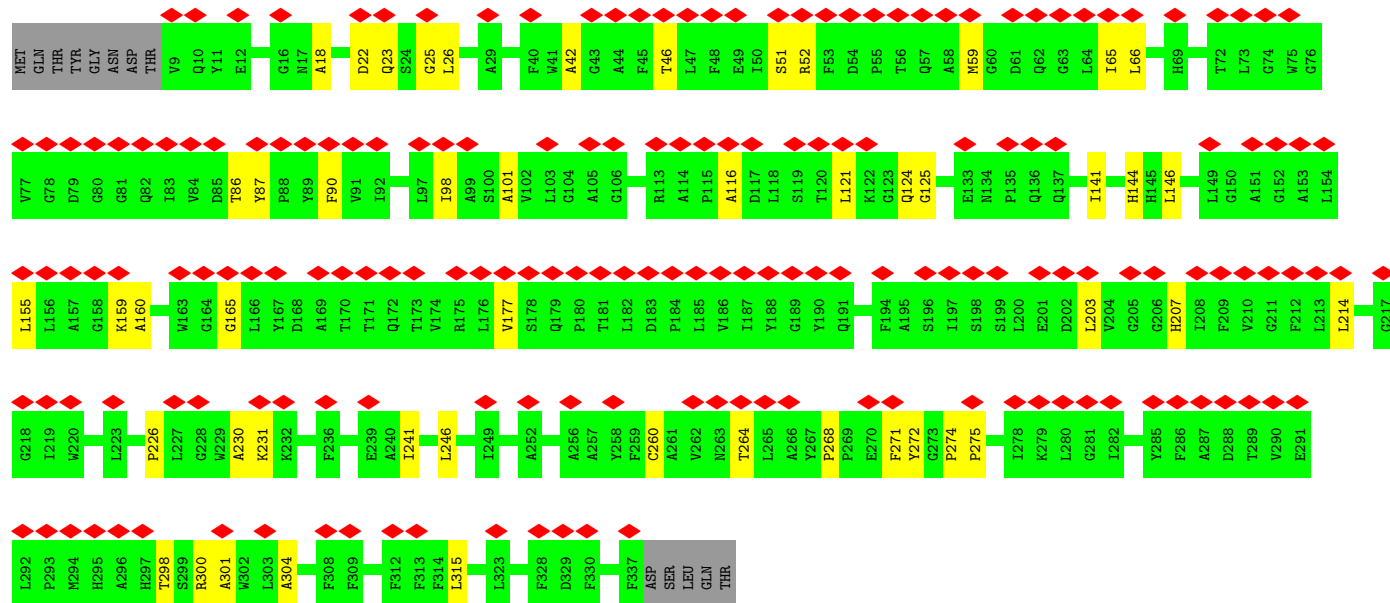
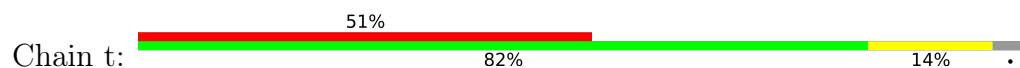
- Molecule 11: Iron stress-induced chlorophyll-binding protein

Chain h: 51% 83% 10% 7%

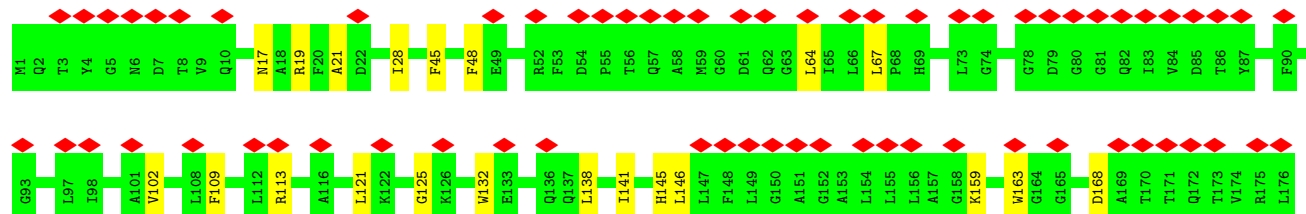
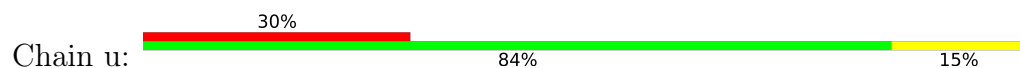


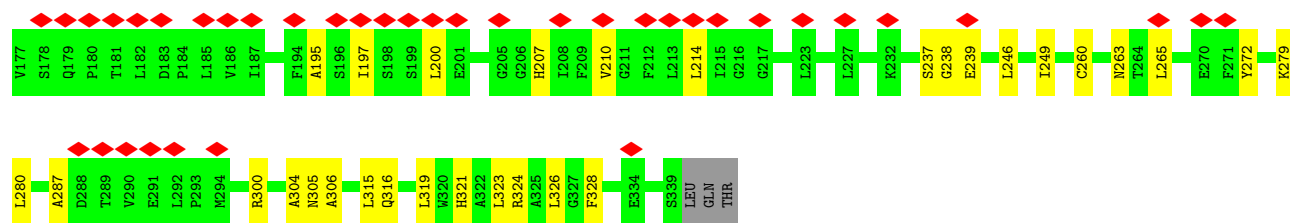


• Molecule 11: Iron stress-induced chlorophyll-binding protein



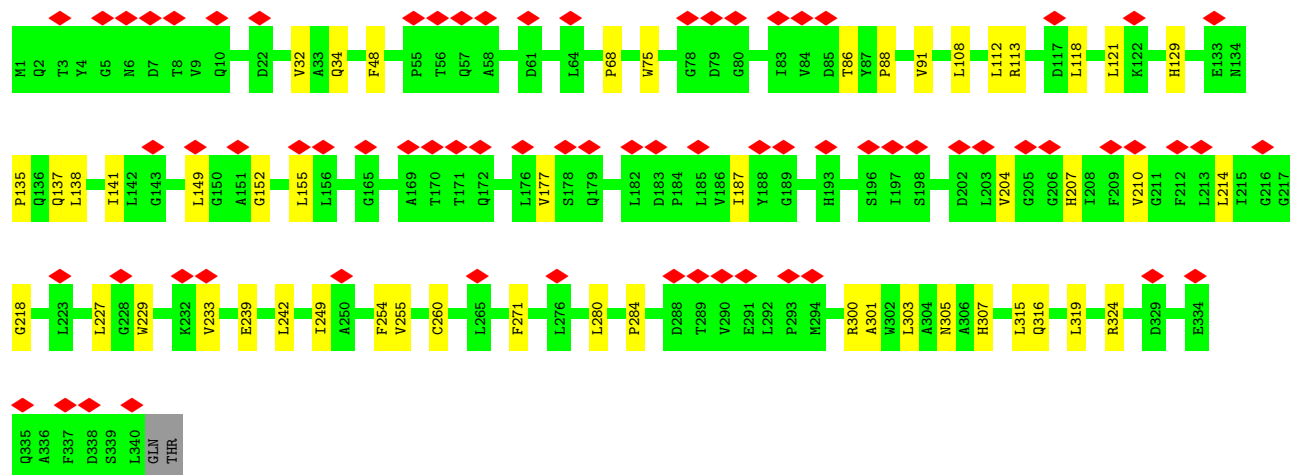
• Molecule 11: Iron stress-induced chlorophyll-binding protein





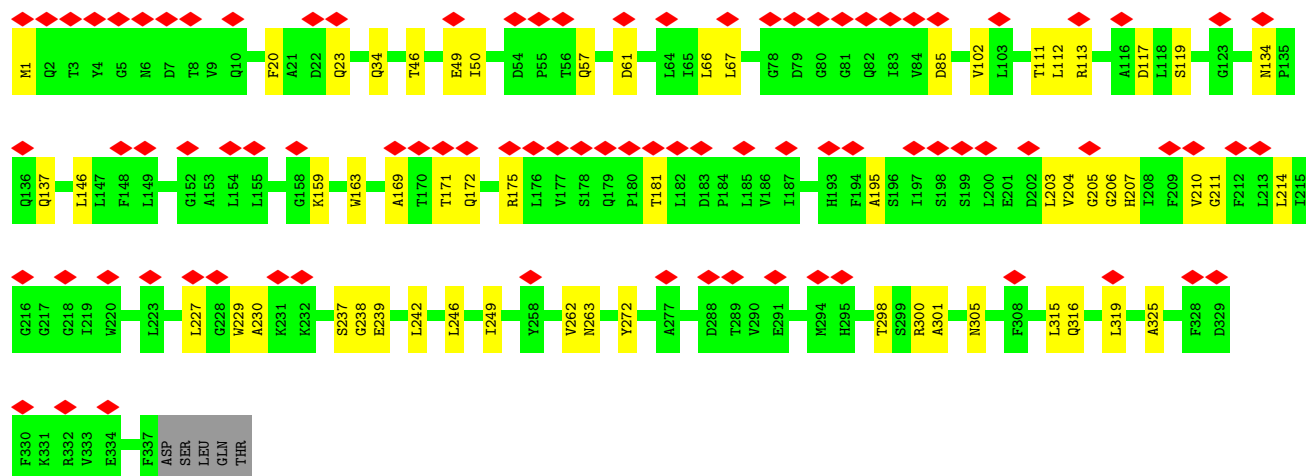
- Molecule 11: Iron stress-induced chlorophyll-binding protein

Chain s: 21% 85% 14%



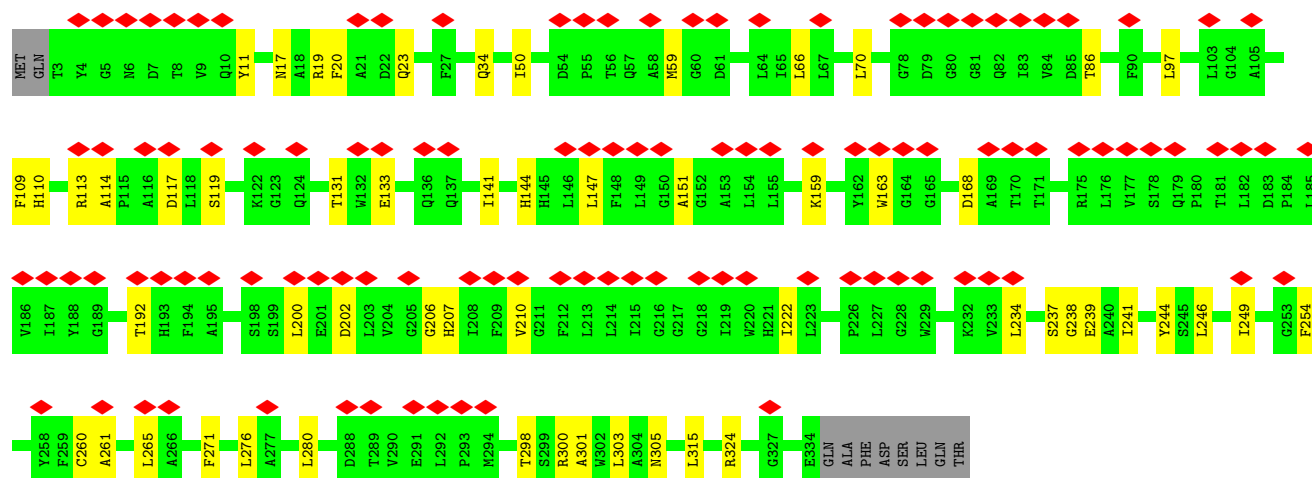
- Molecule 11: Iron stress-induced chlorophyll-binding protein

Chain w: 25% 82% 17%

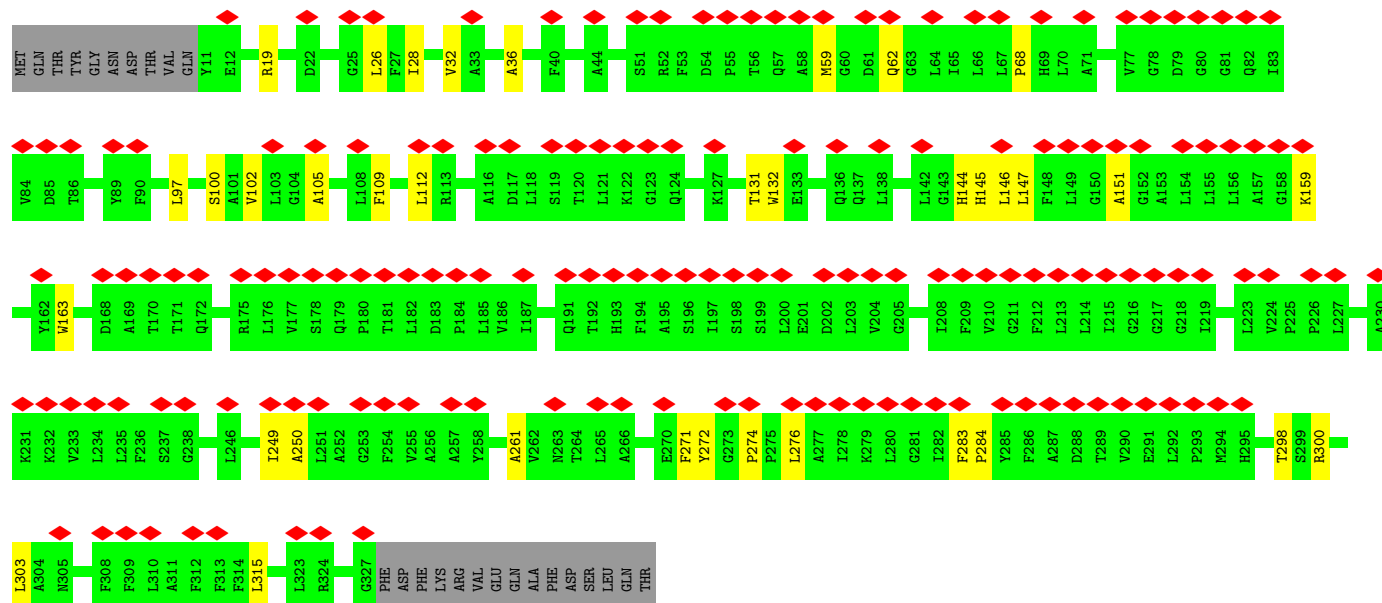
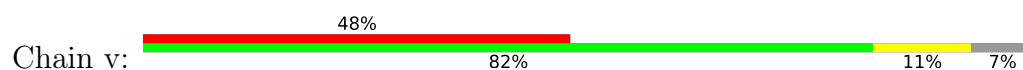


- Molecule 11: Iron stress-induced chlorophyll-binding protein

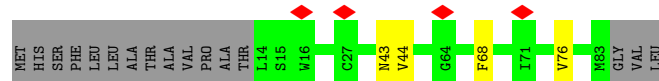
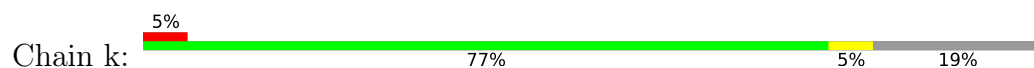
Chain x: 33% 81% 16%



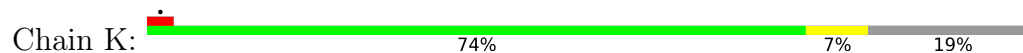
- Molecule 11: Iron stress-induced chlorophyll-binding protein

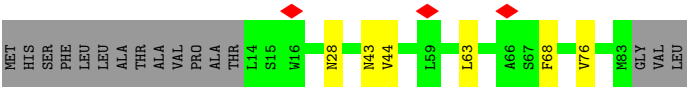


- Molecule 12: Photosystem I reaction center subunit PsaK 1

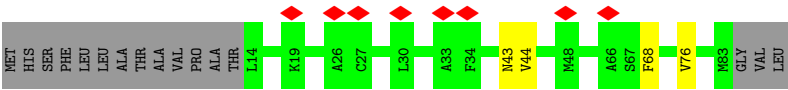
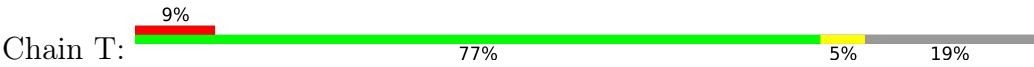


- Molecule 12: Photosystem I reaction center subunit PsaK 1





● 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 ($\text{\AA}$)	512.0, 512.0, 512.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: BCR, LHG, SF4, PQN, LMT, CLA, LMG, CL0, CA

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	0.24	0/5984	0.41	0/8157
1	H	0.24	0/5984	0.42	0/8157
1	a	0.24	0/5984	0.42	0/8157
2	B	0.24	0/5977	0.42	0/8173
2	G	0.24	0/5977	0.42	0/8173
2	b	0.24	0/5977	0.42	0/8173
3	C	0.26	0/610	0.61	0/826
3	N	0.26	0/610	0.61	0/826
3	c	0.26	0/610	0.61	0/826
4	D	0.18	0/1122	0.41	0/1513
4	O	0.18	0/1122	0.42	0/1513
4	d	0.18	0/1122	0.41	0/1513
5	E	0.17	0/551	0.37	0/745
5	P	0.17	0/551	0.37	0/745
5	e	0.17	0/551	0.37	0/745
6	F	0.20	0/1098	0.48	0/1495
6	Q	0.20	0/1098	0.48	0/1495
6	f	0.20	0/1098	0.48	0/1495
7	I	0.27	0/304	0.55	0/416
7	R	0.27	0/304	0.55	0/416
7	i	0.27	0/304	0.55	0/416
8	J	0.19	0/316	0.43	0/428
8	S	0.18	0/316	0.43	0/428
8	j	0.18	0/316	0.42	0/428
9	L	0.22	0/1186	0.47	0/1611
9	U	0.22	0/1186	0.47	0/1611
9	l	0.22	0/1186	0.47	0/1611
10	M	0.21	0/241	0.45	0/326
10	V	0.21	0/241	0.45	0/326
10	m	0.21	0/241	0.45	0/326
11	W	0.18	0/2565	0.42	0/3512
11	X	0.19	0/2695	0.43	0/3685

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	Y	0.20	0/2698	0.44	0/3691
11	Z	0.19	0/2670	0.46	0/3650
11	g	0.18	0/2618	0.43	0/3582
11	h	0.16	0/2501	0.40	0/3423
11	n	0.15	0/2562	0.37	0/3508
11	o	0.17	0/2695	0.39	0/3685
11	p	0.18	0/2699	0.40	0/3692
11	q	0.16	0/2670	0.38	0/3650
11	r	0.16	0/2618	0.39	0/3582
11	s	0.17	0/2699	0.39	0/3692
11	t	0.16	0/2565	0.40	0/3512
11	u	0.17	0/2695	0.39	0/3685
11	v	0.15	0/2501	0.39	0/3423
11	w	0.16	0/2670	0.38	0/3650
11	x	0.16	0/2618	0.39	0/3582
11	y	0.18	0/2501	0.44	0/3423
12	K	0.19	0/495	0.54	0/672
12	T	0.19	0/495	0.55	0/672
12	k	0.19	0/495	0.54	0/672
All	All	0.21	0/100892	0.42	0/137713

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5786	0	5644	89	0
1	H	5786	0	5644	92	0
1	a	5786	0	5644	94	0
2	B	5766	0	5543	86	0
2	G	5766	0	5543	82	0
2	b	5766	0	5543	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	600	0	581	5	0
3	N	600	0	581	8	0
3	c	600	0	581	5	0
4	D	1098	0	1090	11	0
4	O	1098	0	1090	16	0
4	d	1098	0	1090	13	0
5	E	542	0	525	2	0
5	P	542	0	525	3	0
5	e	542	0	525	4	0
6	F	1069	0	1051	13	0
6	Q	1069	0	1051	17	0
6	f	1069	0	1051	16	0
7	I	293	0	292	5	0
7	R	293	0	292	4	0
7	i	293	0	292	5	0
8	J	308	0	314	6	0
8	S	308	0	314	7	0
8	j	308	0	314	7	0
9	L	1156	0	1127	21	0
9	U	1156	0	1127	23	0
9	l	1156	0	1127	23	0
10	M	238	0	260	3	0
10	V	238	0	260	0	0
10	m	238	0	260	2	0
11	W	2478	0	2379	26	0
11	X	2605	0	2526	29	0
11	Y	2608	0	2523	34	0
11	Z	2582	0	2509	33	0
11	g	2531	0	2454	30	0
11	h	2416	0	2361	23	0
11	n	2475	0	2377	32	0
11	o	2605	0	2526	38	0
11	p	2609	0	2526	38	0
11	q	2582	0	2509	43	0
11	r	2531	0	2454	30	0
11	s	2609	0	2526	33	0
11	t	2478	0	2379	34	0
11	u	2605	0	2526	37	0
11	v	2416	0	2361	27	0
11	w	2582	0	2509	39	0
11	x	2531	0	2454	41	0
11	y	2416	0	2361	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	K	485	0	492	3	0
12	T	485	0	492	1	0
12	k	485	0	492	1	0
13	A	70	0	80	1	0
13	H	70	0	80	1	0
13	I	44	0	58	0	0
13	R	44	0	58	1	0
13	a	70	0	80	1	0
13	i	44	0	58	0	0
14	A	116	0	142	3	0
14	B	43	0	56	3	0
14	G	43	0	56	2	0
14	H	116	0	142	4	0
14	Y	39	0	48	1	0
14	a	115	0	140	5	0
14	b	43	0	56	2	0
14	p	39	0	48	0	0
14	s	39	0	48	0	0
15	A	65	0	72	4	0
15	H	65	0	72	3	0
15	a	65	0	72	3	0
16	A	2600	0	2556	79	0
16	B	2344	0	2276	91	0
16	F	72	0	36	2	0
16	G	2344	0	2276	91	0
16	H	2600	0	2556	86	0
16	J	82	0	58	0	0
16	K	45	0	33	0	0
16	L	195	0	216	10	0
16	Q	72	0	36	2	0
16	S	82	0	58	0	0
16	T	45	0	33	0	0
16	U	195	0	216	11	0
16	W	947	0	877	31	0
16	X	952	0	890	26	0
16	Y	952	0	890	27	0
16	Z	943	0	869	20	0
16	a	2600	0	2556	80	0
16	b	2344	0	2276	89	0
16	f	72	0	36	2	0
16	g	923	0	828	25	0
16	h	933	0	845	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	j	82	0	58	0	0
16	k	45	0	33	0	0
16	l	195	0	216	9	0
16	n	947	0	877	29	0
16	o	952	0	890	25	0
16	p	952	0	890	23	0
16	q	943	0	869	21	0
16	r	923	0	828	18	0
16	s	952	0	890	22	0
16	t	947	0	877	34	0
16	u	952	0	890	27	0
16	v	933	0	845	23	0
16	w	943	0	869	23	0
16	x	923	0	828	27	0
16	y	933	0	845	26	0
17	A	33	0	46	0	0
17	B	33	0	46	5	0
17	G	33	0	46	5	0
17	H	33	0	46	0	0
17	a	33	0	46	1	0
17	b	33	0	46	4	0
18	A	8	0	0	0	0
18	C	16	0	0	1	0
18	H	8	0	0	0	0
18	N	16	0	0	1	0
18	a	8	0	0	0	0
18	c	16	0	0	1	0
19	A	240	0	336	12	0
19	B	265	0	369	17	0
19	F	40	0	56	3	0
19	G	265	0	369	16	0
19	H	240	0	336	11	0
19	I	80	0	112	4	0
19	J	120	0	168	6	0
19	K	40	0	56	2	0
19	L	80	0	112	11	0
19	M	40	0	56	3	0
19	Q	40	0	56	3	0
19	R	80	0	112	6	0
19	S	120	0	168	8	0
19	T	40	0	56	2	0
19	U	80	0	112	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	V	40	0	56	0	0
19	W	80	0	112	6	0
19	X	160	0	224	6	0
19	Y	160	0	224	6	0
19	Z	160	0	224	9	0
19	a	240	0	336	13	0
19	b	265	0	369	18	0
19	f	40	0	56	4	0
19	g	160	0	224	9	0
19	h	160	0	224	4	0
19	i	80	0	112	7	0
19	j	120	0	168	8	0
19	k	40	0	56	2	0
19	l	80	0	112	7	0
19	m	40	0	56	3	0
19	n	80	0	112	4	0
19	o	160	0	224	9	0
19	p	160	0	224	7	0
19	q	160	0	224	10	0
19	r	160	0	224	8	0
19	s	160	0	224	6	0
19	t	80	0	112	5	0
19	u	160	0	224	8	0
19	v	160	0	224	6	0
19	w	160	0	224	9	0
19	x	160	0	224	7	0
19	y	160	0	224	9	0
20	L	35	0	45	0	0
20	U	35	0	45	0	0
20	l	35	0	45	0	0
21	L	1	0	0	0	0
21	U	1	0	0	0	0
21	l	1	0	0	0	0
All	All	137509	0	135407	2074	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 2074 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:b:4009:BCR:H24C	19:b:4010:BCR:HC8	1.61	0.81
19:B:4009:BCR:H24C	19:B:4010:BCR:HC8	1.62	0.80
19:G:4009:BCR:H24C	19:G:4010:BCR:HC8	1.62	0.80
19:a:4001:BCR:H23C	12:k:68:PHE:HB2	1.64	0.79
2:G:587:LEU:HD22	16:G:1234:CLA:HBB2	1.67	0.77

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	592 (100%)	1 (0%)	87	84
1	H	593/603 (98%)	592 (100%)	1 (0%)	87	84
1	a	593/603 (98%)	592 (100%)	1 (0%)	87	84
2	B	581/583 (100%)	579 (100%)	2 (0%)	86	83
2	G	581/583 (100%)	579 (100%)	2 (0%)	86	83
2	b	581/583 (100%)	579 (100%)	2 (0%)	86	83
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%)	70	75
6	Q	112/137 (82%)	111 (99%)	1 (1%)	70	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	112/137 (82%)	111 (99%)	1 (1%)	70	75
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
9	l	116/118 (98%)	116 (100%)	0	100	100
10	M	25/25 (100%)	24 (96%)	1 (4%)	28	54
10	V	25/25 (100%)	24 (96%)	1 (4%)	28	54
10	m	25/25 (100%)	24 (96%)	1 (4%)	28	54
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%)	84	81
11	s	252/260 (97%)	251 (100%)	1 (0%)	84	81
11	t	232/260 (89%)	231 (100%)	1 (0%)	84	81
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	48/62 (77%)	45 (94%)	3 (6%)	16	43
12	T	48/62 (77%)	45 (94%)	3 (6%)	16	43
12	k	48/62 (77%)	45 (94%)	3 (6%)	16	43
All	All	9715/10200 (95%)	9688 (100%)	27 (0%)	84	83

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	11	ASP
11	t	86	THR
12	T	43	ASN
10	V	6	THR
11	s	86	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
11	s	221	HIS
11	w	305	ASN
12	T	28	ASN
1	a	79	HIS
1	a	54	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	n	506	-	64,68,73	1.21	9 (14%)	76,107,113	1.37	6 (7%)
16	CLA	r	510	-	59,63,73	1.26	9 (15%)	70,101,113	1.39	7 (10%)
16	CLA	H	1101	-	69,73,73	1.15	9 (13%)	82,113,113	1.37	9 (10%)
19	BCR	q	603	-	41,41,41	1.06	2 (4%)	56,56,56	1.30	6 (10%)
16	CLA	H	1130	-	69,73,73	1.16	10 (14%)	82,113,113	1.35	10 (12%)
16	CLA	A	1106	-	69,73,73	1.14	9 (13%)	82,113,113	1.37	8 (9%)
16	CLA	B	1210	-	69,73,73	1.16	10 (14%)	82,113,113	1.74	13 (15%)
16	CLA	n	513	-	54,58,73	1.31	8 (14%)	64,95,113	1.44	8 (12%)
16	CLA	q	504	-	64,68,73	1.21	8 (12%)	76,107,113	1.36	6 (7%)
16	CLA	p	505	-	69,73,73	1.17	9 (13%)	82,113,113	1.36	6 (7%)
16	CLA	w	503	-	50,54,73	1.36	9 (18%)	59,90,113	1.51	6 (10%)
16	CLA	l	1503	-	69,73,73	1.15	8 (11%)	82,113,113	1.34	10 (12%)
16	CLA	a	1133	-	58,62,73	1.25	9 (15%)	68,99,113	1.44	6 (8%)
16	CLA	a	1112	-	49,53,73	1.36	9 (18%)	58,89,113	1.57	9 (15%)
16	CLA	A	1801	-	56,60,73	1.28	9 (16%)	65,97,113	1.44	7 (10%)
16	CLA	A	1112	-	49,53,73	1.36	10 (20%)	58,89,113	1.57	9 (15%)
16	CLA	A	1101	-	69,73,73	1.14	9 (13%)	82,113,113	1.36	9 (10%)
16	CLA	U	1502	-	69,73,73	1.15	9 (13%)	82,113,113	1.38	7 (8%)
16	CLA	B	1240	-	54,58,73	1.31	8 (14%)	64,95,113	1.45	6 (9%)
16	CLA	b	1227	-	53,57,73	1.31	9 (16%)	61,93,113	1.50	7 (11%)
19	BCR	Z	604	-	41,41,41	1.07	2 (4%)	56,56,56	1.38	9 (16%)
16	CLA	H	1131	-	69,73,73	1.16	9 (13%)	82,113,113	1.42	9 (10%)
16	CLA	n	503	-	50,54,73	1.34	7 (14%)	59,90,113	1.54	8 (13%)
16	CLA	H	1102	-	60,64,73	1.24	9 (15%)	71,102,113	1.51	9 (12%)
19	BCR	H	4002	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	5 (8%)
16	CLA	Z	507	-	69,73,73	1.17	8 (11%)	82,113,113	1.32	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	BCR	J	4015	-	41,41,41	1.12	3 (7%)	56,56,56	1.34	8 (14%)
19	BCR	S	4012	-	41,41,41	1.14	2 (4%)	56,56,56	1.43	9 (16%)
14	LMG	A	4201	-	32,32,55	1.00	1 (3%)	40,40,63	1.13	4 (10%)
16	CLA	v	516	-	50,54,73	1.36	8 (16%)	59,90,113	1.47	5 (8%)
16	CLA	H	1125	-	69,73,73	1.16	10 (14%)	82,113,113	1.39	9 (10%)
16	CLA	a	1402	-	45,49,73	1.41	9 (20%)	54,83,113	1.51	4 (7%)
16	CLA	t	517	-	59,63,73	1.26	9 (15%)	70,101,113	1.48	8 (11%)
16	CLA	h	504	-	64,68,73	1.21	9 (14%)	76,107,113	1.40	6 (7%)
16	CLA	Y	502	-	54,58,73	1.29	9 (16%)	64,95,113	1.51	10 (15%)
19	BCR	K	1501	-	41,41,41	1.10	2 (4%)	56,56,56	1.27	5 (8%)
16	CLA	p	501	-	54,58,73	1.31	9 (16%)	64,95,113	1.44	7 (10%)
16	CLA	H	1127	-	69,73,73	1.17	10 (14%)	82,113,113	1.39	7 (8%)
16	CLA	a	1120	-	53,57,73	1.31	8 (15%)	61,93,113	1.54	7 (11%)
17	PQN	A	2001	-	34,34,34	0.37	0	43,45,45	1.19	5 (11%)
16	CLA	W	510	-	69,73,73	1.17	7 (10%)	82,113,113	1.33	9 (10%)
16	CLA	H	1022	-	69,73,73	1.22	8 (11%)	82,113,113	1.42	9 (10%)
16	CLA	u	508	-	59,63,73	1.25	9 (15%)	70,101,113	1.49	6 (8%)
16	CLA	G	1226	-	69,73,73	1.22	9 (13%)	82,113,113	1.48	10 (12%)
16	CLA	t	509	-	64,68,73	1.21	9 (14%)	76,107,113	1.35	7 (9%)
19	BCR	r	601	-	41,41,41	1.05	2 (4%)	56,56,56	1.32	7 (12%)
16	CLA	G	1238	-	69,73,73	1.17	9 (13%)	82,113,113	1.40	7 (8%)
19	BCR	W	601	-	41,41,41	1.04	2 (4%)	56,56,56	1.36	9 (16%)
16	CLA	s	512	-	49,53,73	1.37	9 (18%)	58,89,113	1.57	7 (12%)
16	CLA	g	506	-	64,68,73	1.22	7 (10%)	76,107,113	1.51	10 (13%)
16	CLA	h	505	-	64,68,73	1.22	9 (14%)	76,107,113	1.36	7 (9%)
16	CLA	X	514	-	54,58,73	1.33	8 (14%)	64,95,113	1.45	6 (9%)
16	CLA	b	1012	-	64,68,73	1.24	10 (15%)	76,107,113	1.51	11 (14%)
16	CLA	b	1021	-	69,73,73	1.16	7 (10%)	82,113,113	1.52	8 (9%)
19	BCR	n	601	-	41,41,41	1.04	2 (4%)	56,56,56	1.37	10 (17%)
16	CLA	G	1204	-	69,73,73	1.13	8 (11%)	82,113,113	1.38	6 (7%)
16	CLA	G	1214	-	59,63,73	1.28	10 (16%)	70,101,113	1.41	11 (15%)
16	CLA	G	1219	-	49,53,73	1.38	8 (16%)	58,89,113	1.55	6 (10%)
16	CLA	x	506	-	64,68,73	1.22	9 (14%)	76,107,113	1.41	7 (9%)
16	CLA	o	504	-	64,68,73	1.22	9 (14%)	76,107,113	1.34	5 (6%)
16	CLA	H	1801	-	56,60,73	1.27	9 (16%)	65,97,113	1.44	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	f	1301	-	49,53,73	1.38	10 (20%)	58,89,113	1.57	9 (15%)
13	LHG	A	849	-	42,42,48	0.68	1 (2%)	45,48,54	1.26	4 (8%)
14	LMG	G	848	-	43,43,55	0.80	1 (2%)	51,51,63	1.32	7 (13%)
16	CLA	h	506	-	64,68,73	1.21	9 (14%)	76,107,113	1.41	7 (9%)
16	CLA	G	1207	-	69,73,73	1.17	9 (13%)	82,113,113	1.37	6 (7%)
16	CLA	H	1013	-	69,73,73	1.18	10 (14%)	82,113,113	1.61	12 (14%)
16	CLA	G	1232	-	49,53,73	1.40	9 (18%)	58,89,113	1.52	5 (8%)
16	CLA	b	1231	-	49,53,73	1.39	9 (18%)	58,89,113	1.58	8 (13%)
16	CLA	Q	1301	-	49,53,73	1.38	9 (18%)	58,89,113	1.58	9 (15%)
16	CLA	W	504	-	64,68,73	1.24	8 (12%)	76,107,113	1.39	8 (10%)
16	CLA	v	517	-	59,63,73	1.28	9 (15%)	70,101,113	1.40	7 (10%)
16	CLA	Y	503	-	50,54,73	1.35	8 (16%)	59,90,113	1.55	5 (8%)
16	CLA	b	1220	-	58,62,73	1.26	9 (15%)	68,99,113	1.51	10 (14%)
16	CLA	v	505	-	64,68,73	1.21	8 (12%)	76,107,113	1.36	7 (9%)
16	CLA	n	515	-	69,73,73	1.17	9 (13%)	82,113,113	1.32	6 (7%)
16	CLA	v	509	-	64,68,73	1.20	9 (14%)	76,107,113	1.38	9 (11%)
16	CLA	a	1125	-	69,73,73	1.16	10 (14%)	82,113,113	1.39	9 (10%)
16	CLA	x	511	-	69,73,73	1.16	9 (13%)	82,113,113	1.36	8 (9%)
20	LMT	L	4101	-	36,36,36	1.12	5 (13%)	47,47,47	1.08	4 (8%)
16	CLA	t	512	-	49,53,73	1.38	9 (18%)	58,89,113	1.54	6 (10%)
19	BCR	p	603	-	41,41,41	1.08	3 (7%)	56,56,56	1.39	8 (14%)
16	CLA	h	501	-	50,54,73	1.35	8 (16%)	59,90,113	1.47	5 (8%)
16	CLA	s	503	-	50,54,73	1.35	8 (16%)	59,90,113	1.51	5 (8%)
19	BCR	w	601	-	41,41,41	1.04	2 (4%)	56,56,56	1.33	6 (10%)
16	CLA	Y	516	-	50,54,73	1.34	9 (18%)	59,90,113	1.51	6 (10%)
16	CLA	g	515	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	7 (8%)
16	CLA	a	1013	-	69,73,73	1.18	10 (14%)	82,113,113	1.60	12 (14%)
19	BCR	b	4017	-	41,41,41	1.17	3 (7%)	56,56,56	1.32	9 (16%)
16	CLA	B	1229	-	62,66,73	1.23	9 (14%)	73,104,113	1.44	7 (9%)
16	CLA	Y	507	-	69,73,73	1.18	8 (11%)	82,113,113	1.31	6 (7%)
16	CLA	H	1106	-	69,73,73	1.14	9 (13%)	82,113,113	1.37	8 (9%)
19	BCR	q	601	-	41,41,41	1.05	2 (4%)	56,56,56	1.33	6 (10%)
16	CLA	b	1206	-	69,73,73	1.18	10 (14%)	82,113,113	1.44	9 (10%)
16	CLA	H	1116	-	58,62,73	1.25	10 (17%)	68,99,113	1.47	11 (16%)
16	CLA	h	503	-	50,54,73	1.37	8 (16%)	59,90,113	1.48	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	H	1115	-	58,62,73	1.25	9 (15%)	68,99,113	1.46	7 (10%)
16	CLA	x	509	-	64,68,73	1.22	9 (14%)	76,107,113	1.34	9 (11%)
16	CLA	T	1401	-	49,53,73	1.37	10 (20%)	58,89,113	1.55	7 (12%)
16	CLA	H	1107	-	54,58,73	1.31	9 (16%)	64,95,113	1.65	8 (12%)
16	CLA	b	1217	-	49,53,73	1.38	9 (18%)	58,89,113	1.50	4 (6%)
19	BCR	H	4003	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	7 (12%)
19	BCR	a	4002	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	6 (10%)
19	BCR	s	601	-	41,41,41	1.08	2 (4%)	56,56,56	1.38	10 (17%)
16	CLA	t	511	-	69,73,73	1.18	9 (13%)	82,113,113	1.33	7 (8%)
16	CLA	H	1113	-	49,53,73	1.36	9 (18%)	58,89,113	1.60	8 (13%)
15	CL0	H	1011	-	58,73,73	2.13	14 (24%)	60,113,113	1.95	17 (28%)
16	CLA	a	1139	-	55,59,73	1.30	9 (16%)	64,96,113	1.48	6 (9%)
16	CLA	t	506	-	64,68,73	1.21	9 (14%)	76,107,113	1.40	7 (9%)
16	CLA	S	1303	-	41,45,73	1.45	9 (21%)	50,78,113	1.60	5 (10%)
19	BCR	S	4013	-	41,41,41	1.05	2 (4%)	56,56,56	1.38	7 (12%)
19	BCR	H	4011	-	41,41,41	1.10	2 (4%)	56,56,56	1.38	8 (14%)
16	CLA	s	502	-	54,58,73	1.29	8 (14%)	64,95,113	1.48	9 (14%)
16	CLA	U	1501	-	69,73,73	1.15	9 (13%)	82,113,113	1.40	8 (9%)
16	CLA	a	1801	-	56,60,73	1.27	9 (16%)	65,97,113	1.44	6 (9%)
16	CLA	h	512	-	49,53,73	1.37	7 (14%)	58,89,113	1.56	8 (13%)
16	CLA	w	517	-	59,63,73	1.25	8 (13%)	70,101,113	1.52	10 (14%)
19	BCR	b	4010	-	41,41,41	1.15	3 (7%)	56,56,56	1.39	10 (17%)
19	BCR	u	602	-	41,41,41	1.03	2 (4%)	56,56,56	1.37	7 (12%)
16	CLA	H	1134	-	49,53,73	1.37	9 (18%)	58,89,113	1.58	7 (12%)
19	BCR	B	4005	-	41,41,41	1.13	3 (7%)	56,56,56	1.40	7 (12%)
16	CLA	o	514	-	54,58,73	1.33	8 (14%)	64,95,113	1.45	6 (9%)
16	CLA	X	503	-	50,54,73	1.37	8 (16%)	59,90,113	1.53	6 (10%)
16	CLA	B	1231	-	49,53,73	1.39	9 (18%)	58,89,113	1.57	8 (13%)
16	CLA	x	508	-	59,63,73	1.27	8 (13%)	70,101,113	1.38	5 (7%)
16	CLA	b	1230	-	49,53,73	1.36	9 (18%)	58,89,113	1.61	9 (15%)
16	CLA	Z	509	-	60,64,73	1.26	9 (15%)	71,102,113	1.40	10 (14%)
19	BCR	h	601	-	41,41,41	1.03	2 (4%)	56,56,56	1.39	8 (14%)
19	BCR	a	4007	-	41,41,41	1.12	3 (7%)	56,56,56	1.36	7 (12%)
16	CLA	A	1140	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
16	CLA	G	1239	-	69,73,73	1.17	8 (11%)	82,113,113	1.40	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	SF4	c	102	3	0,12,12	-	-	-		
16	CLA	W	507	-	64,68,73	1.23	8 (12%)	76,107,113	1.34	7 (9%)
16	CLA	o	505	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	6 (7%)
16	CLA	X	512	-	49,53,73	1.37	9 (18%)	58,89,113	1.55	7 (12%)
16	CLA	h	513	-	54,58,73	1.32	8 (14%)	64,95,113	1.44	8 (12%)
16	CLA	k	1401	-	49,53,73	1.38	10 (20%)	58,89,113	1.56	7 (12%)
16	CLA	h	517	-	59,63,73	1.28	9 (15%)	70,101,113	1.39	7 (10%)
16	CLA	u	502	-	54,58,73	1.32	7 (12%)	64,95,113	1.49	10 (15%)
16	CLA	y	512	-	49,53,73	1.37	8 (16%)	58,89,113	1.56	8 (13%)
16	CLA	u	504	-	64,68,73	1.23	9 (14%)	76,107,113	1.36	6 (7%)
16	CLA	A	1237	-	69,73,73	1.18	8 (11%)	82,113,113	1.44	9 (10%)
16	CLA	Y	509	-	64,68,73	1.20	9 (14%)	76,107,113	1.37	10 (13%)
16	CLA	t	503	-	50,54,73	1.35	7 (14%)	59,90,113	1.52	8 (13%)
19	BCR	B	4006	-	25,25,41	1.08	2 (8%)	33,33,56	1.43	6 (18%)
16	CLA	g	505	-	50,54,73	1.35	9 (18%)	59,90,113	1.50	6 (10%)
16	CLA	h	509	-	64,68,73	1.21	9 (14%)	76,107,113	1.36	7 (9%)
16	CLA	A	1111	-	59,63,73	1.25	9 (15%)	70,101,113	1.44	8 (11%)
16	CLA	A	1013	-	69,73,73	1.18	10 (14%)	82,113,113	1.61	12 (14%)
16	CLA	y	503	-	50,54,73	1.36	8 (16%)	59,90,113	1.50	6 (10%)
16	CLA	w	507	-	69,73,73	1.17	9 (13%)	82,113,113	1.32	5 (6%)
19	BCR	Y	602	-	41,41,41	1.04	2 (4%)	56,56,56	1.39	9 (16%)
16	CLA	Z	506	-	64,68,73	1.22	9 (14%)	76,107,113	1.38	5 (6%)
16	CLA	A	1110	-	58,62,73	1.25	9 (15%)	68,99,113	1.44	7 (10%)
19	BCR	L	4019	-	41,41,41	1.18	2 (4%)	56,56,56	1.33	5 (8%)
16	CLA	y	515	-	64,68,73	1.22	8 (12%)	76,107,113	1.47	6 (7%)
16	CLA	Z	508	-	59,63,73	1.26	8 (13%)	70,101,113	1.43	6 (8%)
16	CLA	G	1236	-	69,73,73	1.15	9 (13%)	82,113,113	1.36	10 (12%)
16	CLA	o	502	-	54,58,73	1.32	8 (14%)	64,95,113	1.51	9 (14%)
16	CLA	H	1132	-	69,73,73	1.14	9 (13%)	82,113,113	1.41	7 (8%)
16	CLA	o	516	-	50,54,73	1.35	8 (16%)	59,90,113	1.46	5 (8%)
16	CLA	G	1227	-	53,57,73	1.32	9 (16%)	61,93,113	1.52	6 (9%)
16	CLA	B	1219	-	49,53,73	1.38	8 (16%)	58,89,113	1.54	6 (10%)
16	CLA	o	501	-	54,58,73	1.32	8 (14%)	64,95,113	1.47	7 (10%)
16	CLA	A	1113	-	49,53,73	1.37	8 (16%)	58,89,113	1.60	8 (13%)
16	CLA	X	509	-	64,68,73	1.21	9 (14%)	76,107,113	1.39	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	f	1302	-	27,35,73	1.84	6 (22%)	32,60,113	1.63	5 (15%)
16	CLA	b	1212	-	49,53,73	1.36	9 (18%)	58,89,113	1.54	7 (12%)
16	CLA	A	1121	-	55,59,73	1.30	8 (14%)	64,96,113	1.46	5 (7%)
16	CLA	o	511	-	69,73,73	1.16	10 (14%)	82,113,113	1.39	9 (10%)
16	CLA	Z	511	-	69,73,73	1.16	9 (13%)	82,113,113	1.41	9 (10%)
19	BCR	R	4018	-	41,41,41	1.14	2 (4%)	56,56,56	1.32	6 (10%)
16	CLA	A	1116	-	58,62,73	1.25	10 (17%)	68,99,113	1.47	11 (16%)
16	CLA	B	1218	-	59,63,73	1.25	9 (15%)	70,101,113	1.43	5 (7%)
16	CLA	Z	503	-	50,54,73	1.36	8 (16%)	59,90,113	1.53	6 (10%)
16	CLA	G	1222	-	59,63,73	1.26	9 (15%)	70,101,113	1.45	6 (8%)
16	CLA	p	507	-	69,73,73	1.18	9 (13%)	82,113,113	1.30	6 (7%)
16	CLA	a	1103	-	69,73,73	1.16	8 (11%)	82,113,113	1.42	6 (7%)
16	CLA	q	505	-	69,73,73	1.17	8 (11%)	82,113,113	1.34	6 (7%)
16	CLA	H	1117	-	69,73,73	1.14	9 (13%)	82,113,113	1.37	8 (9%)
16	CLA	A	1130	-	69,73,73	1.17	11 (15%)	82,113,113	1.36	10 (12%)
16	CLA	Z	512	-	49,53,73	1.37	9 (18%)	58,89,113	1.54	7 (12%)
16	CLA	u	501	-	54,58,73	1.31	8 (14%)	64,95,113	1.47	8 (12%)
18	SF4	C	102	3	0,12,12	-	-	-	-	-
19	BCR	A	4011	-	41,41,41	1.11	2 (4%)	56,56,56	1.37	8 (14%)
16	CLA	B	1239	-	69,73,73	1.17	8 (11%)	82,113,113	1.41	6 (7%)
19	BCR	Z	601	-	41,41,41	1.05	2 (4%)	56,56,56	1.33	8 (14%)
16	CLA	s	511	-	69,73,73	1.18	9 (13%)	82,113,113	1.33	6 (7%)
16	CLA	a	1121	-	55,59,73	1.31	8 (14%)	64,96,113	1.47	5 (7%)
16	CLA	l	1501	-	69,73,73	1.16	9 (13%)	82,113,113	1.40	8 (9%)
19	BCR	X	601	-	41,41,41	1.11	3 (7%)	56,56,56	1.35	9 (16%)
16	CLA	x	504	-	64,68,73	1.22	9 (14%)	76,107,113	1.36	7 (9%)
16	CLA	H	1114	-	53,57,73	1.32	8 (15%)	61,93,113	1.47	7 (11%)
16	CLA	h	515	-	64,68,73	1.22	8 (12%)	76,107,113	1.38	6 (7%)
16	CLA	G	1215	-	64,68,73	1.18	9 (14%)	76,107,113	1.43	8 (10%)
16	CLA	y	505	-	64,68,73	1.22	8 (12%)	76,107,113	1.37	7 (9%)
19	BCR	t	603	-	41,41,41	1.10	3 (7%)	56,56,56	1.33	8 (14%)
16	CLA	H	1124	-	69,73,73	1.15	9 (13%)	82,113,113	1.39	7 (8%)
16	CLA	p	517	-	59,63,73	1.25	9 (15%)	70,101,113	1.41	5 (7%)
19	BCR	H	4007	-	41,41,41	1.12	3 (7%)	56,56,56	1.36	7 (12%)
16	CLA	Y	508	-	59,63,73	1.26	9 (15%)	70,101,113	1.41	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	t	504	-	64,68,73	1.23	9 (14%)	76,107,113	1.40	7 (9%)
16	CLA	A	1104	-	69,73,73	1.16	9 (13%)	82,113,113	1.40	5 (6%)
16	CLA	a	1129	-	54,58,73	1.30	9 (16%)	64,95,113	1.46	8 (12%)
16	CLA	B	1224	-	64,68,73	1.19	11 (17%)	76,107,113	1.59	10 (13%)
16	CLA	a	1122	-	63,67,73	1.20	9 (14%)	74,105,113	1.38	7 (9%)
16	CLA	L	1503	-	69,73,73	1.15	8 (11%)	82,113,113	1.35	10 (12%)
16	CLA	H	1112	-	49,53,73	1.36	8 (16%)	58,89,113	1.57	9 (15%)
17	PQN	a	2001	-	34,34,34	0.37	0	43,45,45	1.19	5 (11%)
16	CLA	a	1136	-	69,73,73	1.16	9 (13%)	82,113,113	1.37	9 (10%)
16	CLA	p	515	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	9 (10%)
16	CLA	b	1214	-	59,63,73	1.27	9 (15%)	70,101,113	1.41	9 (12%)
19	BCR	W	603	-	41,41,41	1.09	2 (4%)	56,56,56	1.32	7 (12%)
19	BCR	r	602	-	41,41,41	0.99	2 (4%)	56,56,56	1.34	8 (14%)
16	CLA	B	1021	-	69,73,73	1.16	7 (10%)	82,113,113	1.52	7 (8%)
16	CLA	b	1210	-	69,73,73	1.16	9 (13%)	82,113,113	1.74	12 (14%)
16	CLA	Z	515	-	69,73,73	1.15	8 (11%)	82,113,113	1.35	6 (7%)
16	CLA	A	1129	-	54,58,73	1.30	9 (16%)	64,95,113	1.46	8 (12%)
16	CLA	G	1221	-	69,73,73	1.17	10 (14%)	82,113,113	1.36	9 (10%)
16	CLA	Y	514	-	54,58,73	1.30	9 (16%)	64,95,113	1.49	10 (15%)
16	CLA	b	1234	-	54,58,73	1.30	8 (14%)	64,95,113	1.52	7 (10%)
19	BCR	m	4021	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	6 (10%)
16	CLA	A	1109	-	69,73,73	1.15	9 (13%)	82,113,113	1.44	7 (8%)
16	CLA	A	1107	-	54,58,73	1.31	9 (16%)	64,95,113	1.64	8 (12%)
16	CLA	Y	517	-	59,63,73	1.26	8 (13%)	70,101,113	1.42	7 (10%)
14	LMG	s	701	-	39,39,55	0.87	1 (2%)	47,47,63	1.25	4 (8%)
16	CLA	Y	515	-	69,73,73	1.16	8 (11%)	82,113,113	1.36	6 (7%)
16	CLA	q	503	-	50,54,73	1.36	9 (18%)	59,90,113	1.51	6 (10%)
16	CLA	b	1236	-	69,73,73	1.14	9 (13%)	82,113,113	1.35	8 (9%)
17	PQN	H	2001	-	34,34,34	0.37	0	43,45,45	1.19	5 (11%)
14	LMG	b	848	-	43,43,55	0.79	1 (2%)	51,51,63	1.32	7 (13%)
16	CLA	X	505	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	6 (7%)
16	CLA	q	510	-	64,68,73	1.22	8 (12%)	76,107,113	1.36	7 (9%)
16	CLA	r	511	-	69,73,73	1.16	9 (13%)	82,113,113	1.35	8 (9%)
16	CLA	W	511	-	69,73,73	1.17	9 (13%)	82,113,113	1.36	7 (8%)
16	CLA	B	1205	-	69,73,73	1.15	8 (11%)	82,113,113	1.51	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	BCR	J	4012	-	41,41,41	1.14	2 (4%)	56,56,56	1.42	9 (16%)
16	CLA	q	508	-	59,63,73	1.26	8 (13%)	70,101,113	1.42	5 (7%)
16	CLA	W	506	-	64,68,73	1.21	9 (14%)	76,107,113	1.44	8 (10%)
19	BCR	x	604	-	41,41,41	1.04	2 (4%)	56,56,56	1.37	9 (16%)
19	BCR	B	4009	-	41,41,41	1.05	2 (4%)	56,56,56	1.38	9 (16%)
16	CLA	A	1123	-	69,73,73	1.18	8 (11%)	82,113,113	1.37	7 (8%)
16	CLA	A	1138	-	69,73,73	1.14	9 (13%)	82,113,113	1.43	9 (10%)
16	CLA	F	1301	-	49,53,73	1.39	10 (20%)	58,89,113	1.60	9 (15%)
16	CLA	X	508	-	59,63,73	1.25	9 (15%)	70,101,113	1.49	6 (8%)
16	CLA	y	501	-	50,54,73	1.36	8 (16%)	59,90,113	1.47	5 (8%)
19	BCR	U	4019	-	41,41,41	1.19	2 (4%)	56,56,56	1.33	5 (8%)
19	BCR	w	602	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	7 (12%)
16	CLA	q	512	-	49,53,73	1.37	9 (18%)	58,89,113	1.56	7 (12%)
19	BCR	h	604	-	41,41,41	1.05	2 (4%)	56,56,56	1.36	8 (14%)
19	BCR	a	4011	-	41,41,41	1.10	2 (4%)	56,56,56	1.38	8 (14%)
16	CLA	w	510	-	64,68,73	1.21	8 (12%)	76,107,113	1.35	7 (9%)
16	CLA	q	514	-	54,58,73	1.31	9 (16%)	64,95,113	1.48	8 (12%)
16	CLA	h	507	-	69,73,73	1.18	8 (11%)	82,113,113	1.32	6 (7%)
19	BCR	q	602	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	8 (14%)
16	CLA	a	1102	-	60,64,73	1.24	10 (16%)	71,102,113	1.50	9 (12%)
19	BCR	G	4009	-	41,41,41	1.05	2 (4%)	56,56,56	1.38	9 (16%)
16	CLA	u	512	-	49,53,73	1.37	9 (18%)	58,89,113	1.57	8 (13%)
16	CLA	u	510	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	6 (7%)
16	CLA	H	1119	-	69,73,73	1.16	9 (13%)	82,113,113	1.36	8 (9%)
19	BCR	s	602	-	41,41,41	1.03	2 (4%)	56,56,56	1.39	8 (14%)
19	BCR	u	601	-	41,41,41	1.09	2 (4%)	56,56,56	1.33	8 (14%)
16	CLA	K	1401	-	49,53,73	1.37	10 (20%)	58,89,113	1.55	7 (12%)
16	CLA	A	1114	-	53,57,73	1.33	8 (15%)	61,93,113	1.46	6 (9%)
16	CLA	q	502	-	54,58,73	1.30	9 (16%)	64,95,113	1.49	8 (12%)
19	BCR	Q	4016	-	41,41,41	1.10	2 (4%)	56,56,56	1.31	8 (14%)
14	LMG	B	848	-	43,43,55	0.80	1 (2%)	51,51,63	1.32	7 (13%)
16	CLA	r	501	-	54,58,73	1.31	8 (14%)	64,95,113	1.45	6 (9%)
19	BCR	A	4007	-	41,41,41	1.12	3 (7%)	56,56,56	1.36	7 (12%)
16	CLA	W	501	-	54,58,73	1.30	8 (14%)	64,95,113	1.44	8 (12%)
16	CLA	F	1302	-	27,35,73	1.84	7 (25%)	32,60,113	1.64	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	p	511	-	69,73,73	1.17	9 (13%)	82,113,113	1.34	7 (8%)
16	CLA	p	510	-	69,73,73	1.16	8 (11%)	82,113,113	1.33	6 (7%)
16	CLA	a	1114	-	53,57,73	1.32	8 (15%)	61,93,113	1.46	6 (9%)
19	BCR	x	603	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	8 (14%)
16	CLA	G	1203	-	69,73,73	1.16	8 (11%)	82,113,113	1.38	6 (7%)
19	BCR	v	604	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	6 (10%)
16	CLA	x	513	-	54,58,73	1.33	8 (14%)	64,95,113	1.46	6 (9%)
16	CLA	p	506	-	64,68,73	1.22	8 (12%)	76,107,113	1.40	7 (9%)
16	CLA	t	508	-	59,63,73	1.26	8 (13%)	70,101,113	1.40	7 (10%)
16	CLA	s	501	-	54,58,73	1.32	8 (14%)	64,95,113	1.43	7 (10%)
16	CLA	x	515	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	5 (6%)
16	CLA	s	505	-	69,73,73	1.17	8 (11%)	82,113,113	1.37	6 (7%)
16	CLA	A	1120	-	53,57,73	1.30	8 (15%)	61,93,113	1.53	7 (11%)
16	CLA	l	1502	-	69,73,73	1.15	9 (13%)	82,113,113	1.39	7 (8%)
16	CLA	u	514	-	54,58,73	1.33	8 (14%)	64,95,113	1.44	6 (9%)
19	BCR	F	4016	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	8 (14%)
16	CLA	u	505	-	69,73,73	1.16	9 (13%)	82,113,113	1.35	7 (8%)
16	CLA	G	1216	-	51,55,73	1.36	9 (17%)	60,91,113	1.48	6 (10%)
16	CLA	A	1124	-	69,73,73	1.15	9 (13%)	82,113,113	1.38	7 (8%)
16	CLA	y	509	-	64,68,73	1.20	9 (14%)	76,107,113	1.37	10 (13%)
16	CLA	g	502	-	54,58,73	1.31	9 (16%)	64,95,113	1.42	7 (10%)
19	BCR	G	4014	-	41,41,41	1.14	3 (7%)	56,56,56	1.27	6 (10%)
16	CLA	B	1215	-	64,68,73	1.17	8 (12%)	76,107,113	1.43	8 (10%)
16	CLA	H	1139	-	55,59,73	1.30	9 (16%)	64,96,113	1.48	6 (9%)
16	CLA	n	502	-	54,58,73	1.30	8 (14%)	64,95,113	1.46	6 (9%)
19	BCR	X	602	-	41,41,41	1.03	2 (4%)	56,56,56	1.37	8 (14%)
16	CLA	a	1134	-	49,53,73	1.38	9 (18%)	58,89,113	1.59	7 (12%)
16	CLA	y	514	-	54,58,73	1.32	8 (14%)	64,95,113	1.45	7 (10%)
16	CLA	p	513	-	54,58,73	1.32	9 (16%)	64,95,113	1.43	7 (10%)
16	CLA	p	503	-	50,54,73	1.36	8 (16%)	59,90,113	1.51	5 (8%)
16	CLA	w	512	-	49,53,73	1.37	9 (18%)	58,89,113	1.55	8 (13%)
16	CLA	G	1210	-	69,73,73	1.16	10 (14%)	82,113,113	1.75	12 (14%)
16	CLA	G	1223	-	69,73,73	1.18	9 (13%)	82,113,113	1.35	7 (8%)
16	CLA	B	1217	-	49,53,73	1.37	8 (16%)	58,89,113	1.50	4 (6%)
19	BCR	I	4020	-	41,41,41	1.22	3 (7%)	56,56,56	1.26	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	PQN	B	2002	-	34,34,34	0.38	0	43,45,45	1.18	2 (4%)
16	CLA	X	502	-	54,58,73	1.31	9 (16%)	64,95,113	1.50	8 (12%)
16	CLA	t	516	-	50,54,73	1.36	9 (18%)	59,90,113	1.49	4 (6%)
16	CLA	J	1303	-	41,45,73	1.44	9 (21%)	50,78,113	1.60	6 (12%)
16	CLA	G	1206	-	69,73,73	1.18	9 (13%)	82,113,113	1.45	9 (10%)
16	CLA	X	504	-	64,68,73	1.23	9 (14%)	76,107,113	1.34	6 (7%)
16	CLA	B	1202	-	69,73,73	1.13	8 (11%)	82,113,113	1.41	8 (9%)
16	CLA	t	507	-	64,68,73	1.23	8 (12%)	76,107,113	1.36	6 (7%)
19	BCR	l	4019	-	41,41,41	1.18	2 (4%)	56,56,56	1.33	5 (8%)
16	CLA	B	1209	-	49,53,73	1.38	9 (18%)	58,89,113	1.51	5 (8%)
16	CLA	X	511	-	69,73,73	1.16	10 (14%)	82,113,113	1.38	8 (9%)
16	CLA	A	1125	-	69,73,73	1.15	10 (14%)	82,113,113	1.39	9 (10%)
14	LMG	H	4101	-	46,46,55	0.84	1 (2%)	54,54,63	1.32	6 (11%)
16	CLA	v	515	-	64,68,73	1.21	8 (12%)	76,107,113	1.39	6 (7%)
19	BCR	a	4003	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	6 (10%)
16	CLA	s	513	-	54,58,73	1.32	9 (16%)	64,95,113	1.45	7 (10%)
16	CLA	w	514	-	54,58,73	1.32	9 (16%)	64,95,113	1.46	7 (10%)
19	BCR	o	604	-	41,41,41	1.04	2 (4%)	56,56,56	1.34	10 (17%)
19	BCR	p	601	-	41,41,41	1.09	2 (4%)	56,56,56	1.37	8 (14%)
16	CLA	r	512	-	49,53,73	1.37	9 (18%)	58,89,113	1.54	6 (10%)
19	BCR	h	602	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	4 (7%)
16	CLA	b	1222	-	59,63,73	1.26	9 (15%)	70,101,113	1.44	6 (8%)
16	CLA	r	514	-	54,58,73	1.31	8 (14%)	64,95,113	1.48	10 (15%)
16	CLA	v	514	-	54,58,73	1.33	8 (14%)	64,95,113	1.46	7 (10%)
16	CLA	A	1119	-	69,73,73	1.16	10 (14%)	82,113,113	1.36	8 (9%)
16	CLA	H	1121	-	55,59,73	1.30	9 (16%)	64,96,113	1.46	5 (7%)
16	CLA	W	516	-	50,54,73	1.36	8 (16%)	59,90,113	1.47	4 (6%)
16	CLA	b	1216	-	51,55,73	1.36	8 (15%)	60,91,113	1.47	6 (10%)
16	CLA	g	508	-	59,63,73	1.27	8 (13%)	70,101,113	1.38	5 (7%)
16	CLA	n	514	-	54,58,73	1.33	9 (16%)	64,95,113	1.47	8 (12%)
16	CLA	H	1123	-	69,73,73	1.18	7 (10%)	82,113,113	1.38	7 (8%)
19	BCR	j	4013	-	41,41,41	1.06	2 (4%)	56,56,56	1.38	8 (14%)
19	BCR	y	602	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	7 (12%)
16	CLA	A	1131	-	69,73,73	1.15	10 (14%)	82,113,113	1.41	10 (12%)
16	CLA	r	502	-	54,58,73	1.31	8 (14%)	64,95,113	1.44	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	b	1207	-	69,73,73	1.18	8 (11%)	82,113,113	1.38	6 (7%)
16	CLA	G	1205	-	69,73,73	1.15	7 (10%)	82,113,113	1.51	9 (10%)
19	BCR	Z	602	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	6 (10%)
19	BCR	T	1501	-	41,41,41	1.09	3 (7%)	56,56,56	1.27	5 (8%)
17	PQN	G	2002	-	34,34,34	0.39	0	43,45,45	1.18	2 (4%)
16	CLA	j	1302	-	49,53,73	1.37	9 (18%)	58,89,113	1.52	6 (10%)
16	CLA	a	1115	-	58,62,73	1.25	9 (15%)	68,99,113	1.46	7 (10%)
16	CLA	A	1139	-	55,59,73	1.30	9 (16%)	64,96,113	1.48	6 (9%)
16	CLA	A	1137	-	51,55,73	1.31	10 (19%)	60,91,113	1.55	7 (11%)
16	CLA	g	516	-	50,54,73	1.37	8 (16%)	59,90,113	1.50	7 (11%)
19	BCR	o	603	-	41,41,41	1.09	2 (4%)	56,56,56	1.33	7 (12%)
16	CLA	A	1115	-	58,62,73	1.26	9 (15%)	68,99,113	1.45	7 (10%)
16	CLA	o	513	-	54,58,73	1.31	8 (14%)	64,95,113	1.46	6 (9%)
16	CLA	u	506	-	64,68,73	1.22	8 (12%)	76,107,113	1.39	7 (9%)
16	CLA	y	516	-	50,54,73	1.36	8 (16%)	59,90,113	1.48	6 (10%)
19	BCR	G	4010	-	41,41,41	1.15	3 (7%)	56,56,56	1.39	11 (19%)
16	CLA	y	507	-	69,73,73	1.18	9 (13%)	82,113,113	1.31	6 (7%)
19	BCR	j	4015	-	41,41,41	1.12	3 (7%)	56,56,56	1.35	8 (14%)
16	CLA	u	517	-	59,63,73	1.25	8 (13%)	70,101,113	1.59	10 (14%)
14	LMG	p	701	-	39,39,55	0.88	1 (2%)	47,47,63	1.24	4 (8%)
16	CLA	a	1137	-	51,55,73	1.31	10 (19%)	60,91,113	1.55	6 (10%)
16	CLA	B	1221	-	69,73,73	1.18	11 (15%)	82,113,113	1.36	8 (9%)
19	BCR	V	4021	-	41,41,41	1.10	2 (4%)	56,56,56	1.27	7 (12%)
16	CLA	G	1240	-	54,58,73	1.32	8 (14%)	64,95,113	1.46	6 (9%)
16	CLA	H	1104	-	69,73,73	1.16	9 (13%)	82,113,113	1.39	5 (6%)
16	CLA	B	1023	-	69,73,73	1.16	10 (14%)	82,113,113	1.68	13 (15%)
16	CLA	x	510	-	59,63,73	1.27	9 (15%)	70,101,113	1.37	7 (10%)
16	CLA	W	503	-	50,54,73	1.35	7 (14%)	59,90,113	1.52	8 (13%)
19	BCR	k	1501	-	41,41,41	1.10	3 (7%)	56,56,56	1.27	5 (8%)
16	CLA	S	1302	-	49,53,73	1.38	8 (16%)	58,89,113	1.52	6 (10%)
13	LHG	A	851	-	26,26,48	0.87	1 (3%)	29,32,54	1.36	3 (10%)
16	CLA	X	516	-	50,54,73	1.36	8 (16%)	59,90,113	1.47	5 (8%)
16	CLA	b	1232	-	49,53,73	1.40	9 (18%)	58,89,113	1.52	5 (8%)
16	CLA	B	1236	-	69,73,73	1.14	9 (13%)	82,113,113	1.36	8 (9%)
16	CLA	Z	505	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	o	506	-	64,68,73	1.22	9 (14%)	76,107,113	1.38	6 (7%)
19	BCR	b	4004	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	5 (8%)
16	CLA	W	502	-	54,58,73	1.31	8 (14%)	64,95,113	1.44	6 (9%)
16	CLA	H	1129	-	54,58,73	1.30	9 (16%)	64,95,113	1.45	8 (12%)
19	BCR	R	4020	-	41,41,41	1.22	3 (7%)	56,56,56	1.26	6 (10%)
16	CLA	r	516	-	50,54,73	1.37	8 (16%)	59,90,113	1.51	7 (11%)
16	CLA	B	1203	-	69,73,73	1.16	8 (11%)	82,113,113	1.39	6 (7%)
16	CLA	Y	505	-	69,73,73	1.17	9 (13%)	82,113,113	1.39	7 (8%)
16	CLA	H	1103	-	69,73,73	1.16	8 (11%)	82,113,113	1.42	6 (7%)
16	CLA	a	1105	-	62,66,73	1.20	9 (14%)	73,104,113	1.43	7 (9%)
16	CLA	x	503	-	50,54,73	1.37	8 (16%)	59,90,113	1.48	6 (10%)
19	BCR	Y	604	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	6 (10%)
16	CLA	g	509	-	64,68,73	1.21	9 (14%)	76,107,113	1.34	7 (9%)
16	CLA	X	513	-	54,58,73	1.31	8 (14%)	64,95,113	1.45	6 (9%)
16	CLA	a	1106	-	69,73,73	1.14	9 (13%)	82,113,113	1.37	8 (9%)
16	CLA	v	510	-	64,68,73	1.21	8 (12%)	76,107,113	1.39	11 (14%)
16	CLA	Z	510	-	64,68,73	1.21	8 (12%)	76,107,113	1.37	5 (6%)
16	CLA	H	1109	-	69,73,73	1.15	9 (13%)	82,113,113	1.44	7 (8%)
19	BCR	M	4021	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	7 (12%)
16	CLA	H	1128	-	69,73,73	1.21	9 (13%)	82,113,113	1.54	11 (13%)
16	CLA	H	1138	-	69,73,73	1.14	9 (13%)	82,113,113	1.44	9 (10%)
16	CLA	B	1223	-	69,73,73	1.18	9 (13%)	82,113,113	1.36	7 (8%)
16	CLA	B	1238	-	69,73,73	1.17	9 (13%)	82,113,113	1.38	7 (8%)
16	CLA	v	512	-	49,53,73	1.37	9 (18%)	58,89,113	1.58	8 (13%)
19	BCR	v	603	-	41,41,41	1.06	2 (4%)	56,56,56	1.31	7 (12%)
16	CLA	b	1224	-	64,68,73	1.19	11 (17%)	76,107,113	1.59	10 (13%)
13	LHG	H	851	-	26,26,48	0.87	1 (3%)	29,32,54	1.36	3 (10%)
19	BCR	J	4013	-	41,41,41	1.05	2 (4%)	56,56,56	1.39	7 (12%)
15	CL0	a	1011	-	58,73,73	2.12	14 (24%)	60,113,113	1.95	17 (28%)
16	CLA	q	511	-	69,73,73	1.17	9 (13%)	82,113,113	1.38	8 (9%)
16	CLA	x	514	-	54,58,73	1.33	9 (16%)	64,95,113	1.47	7 (10%)
16	CLA	A	1108	-	49,53,73	1.36	8 (16%)	58,89,113	1.54	7 (12%)
16	CLA	B	1230	-	49,53,73	1.36	8 (16%)	58,89,113	1.62	9 (15%)
16	CLA	n	509	-	64,68,73	1.21	9 (14%)	76,107,113	1.34	6 (7%)
16	CLA	Y	501	-	54,58,73	1.31	8 (14%)	64,95,113	1.44	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	BCR	v	601	-	41,41,41	1.03	2 (4%)	56,56,56	1.38	8 (14%)
16	CLA	t	510	-	69,73,73	1.16	6 (8%)	82,113,113	1.30	6 (7%)
16	CLA	W	513	-	54,58,73	1.32	8 (14%)	64,95,113	1.44	7 (10%)
16	CLA	Z	516	-	50,54,73	1.36	9 (18%)	59,90,113	1.51	7 (11%)
16	CLA	W	508	-	59,63,73	1.26	8 (13%)	70,101,113	1.38	8 (11%)
16	CLA	r	508	-	59,63,73	1.26	8 (13%)	70,101,113	1.39	6 (8%)
16	CLA	B	1201	-	58,62,73	1.25	9 (15%)	68,99,113	1.51	9 (13%)
16	CLA	p	516	-	50,54,73	1.36	9 (18%)	59,90,113	1.52	6 (10%)
13	LHG	a	849	-	42,42,48	0.69	1 (2%)	45,48,54	1.26	4 (8%)
16	CLA	v	513	-	54,58,73	1.32	8 (14%)	64,95,113	1.44	8 (12%)
19	BCR	B	4017	-	41,41,41	1.17	3 (7%)	56,56,56	1.33	9 (16%)
16	CLA	x	512	-	49,53,73	1.37	9 (18%)	58,89,113	1.53	6 (10%)
16	CLA	a	1111	-	59,63,73	1.25	9 (15%)	70,101,113	1.44	8 (11%)
16	CLA	A	1105	-	62,66,73	1.20	9 (14%)	73,104,113	1.43	7 (9%)
16	CLA	v	502	-	54,58,73	1.31	8 (14%)	64,95,113	1.43	6 (9%)
16	CLA	W	509	-	64,68,73	1.22	9 (14%)	76,107,113	1.33	5 (6%)
19	BCR	y	601	-	41,41,41	1.03	2 (4%)	56,56,56	1.39	8 (14%)
19	BCR	x	602	-	41,41,41	1.00	2 (4%)	56,56,56	1.35	7 (12%)
16	CLA	G	1229	-	62,66,73	1.22	9 (14%)	73,104,113	1.43	7 (9%)
16	CLA	q	506	-	64,68,73	1.22	9 (14%)	76,107,113	1.38	7 (9%)
16	CLA	b	1205	-	69,73,73	1.14	7 (10%)	82,113,113	1.51	9 (10%)
16	CLA	t	514	-	54,58,73	1.33	9 (16%)	64,95,113	1.46	7 (10%)
16	CLA	b	1203	-	69,73,73	1.16	9 (13%)	82,113,113	1.38	6 (7%)
16	CLA	y	502	-	54,58,73	1.30	8 (14%)	64,95,113	1.44	6 (9%)
16	CLA	n	504	-	64,68,73	1.22	8 (12%)	76,107,113	1.41	6 (7%)
16	CLA	H	1108	-	49,53,73	1.37	9 (18%)	58,89,113	1.54	8 (13%)
16	CLA	u	507	-	69,73,73	1.18	9 (13%)	82,113,113	1.32	7 (8%)
16	CLA	a	1104	-	69,73,73	1.16	9 (13%)	82,113,113	1.40	5 (6%)
16	CLA	u	511	-	69,73,73	1.16	10 (14%)	82,113,113	1.38	9 (10%)
16	CLA	Q	1302	-	27,35,73	1.84	7 (25%)	32,60,113	1.62	4 (12%)
16	CLA	x	502	-	54,58,73	1.31	9 (16%)	64,95,113	1.43	6 (9%)
16	CLA	s	508	-	59,63,73	1.25	9 (15%)	70,101,113	1.40	6 (8%)
19	BCR	j	4012	-	41,41,41	1.14	2 (4%)	56,56,56	1.43	9 (16%)
16	CLA	b	1213	-	59,63,73	1.24	9 (15%)	70,101,113	1.41	5 (7%)
16	CLA	r	506	-	64,68,73	1.21	7 (10%)	76,107,113	1.45	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	Y	510	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	9 (10%)
16	CLA	G	1217	-	49,53,73	1.38	9 (18%)	58,89,113	1.49	4 (6%)
19	BCR	H	4008	-	41,41,41	1.17	3 (7%)	56,56,56	1.41	7 (12%)
16	CLA	q	501	-	54,58,73	1.31	8 (14%)	64,95,113	1.42	6 (9%)
16	CLA	G	1208	-	49,53,73	1.37	8 (16%)	58,89,113	1.54	5 (8%)
16	CLA	t	502	-	54,58,73	1.29	7 (12%)	64,95,113	1.56	9 (14%)
16	CLA	h	510	-	64,68,73	1.21	8 (12%)	76,107,113	1.40	11 (14%)
16	CLA	b	1215	-	64,68,73	1.18	8 (12%)	76,107,113	1.43	8 (10%)
16	CLA	A	1135	-	55,59,73	1.28	9 (16%)	64,96,113	1.47	8 (12%)
16	CLA	G	1209	-	49,53,73	1.37	9 (18%)	58,89,113	1.52	6 (10%)
16	CLA	B	1212	-	49,53,73	1.37	8 (16%)	58,89,113	1.54	7 (12%)
19	BCR	G	4005	-	41,41,41	1.12	2 (4%)	56,56,56	1.41	7 (12%)
13	LHG	H	849	-	42,42,48	0.69	1 (2%)	45,48,54	1.26	4 (8%)
16	CLA	b	1219	-	49,53,73	1.38	8 (16%)	58,89,113	1.55	6 (10%)
16	CLA	A	1103	-	69,73,73	1.16	9 (13%)	82,113,113	1.42	6 (7%)
16	CLA	B	1234	-	54,58,73	1.31	8 (14%)	64,95,113	1.54	7 (10%)
18	SF4	N	101	3	0,12,12	-	-	-	-	-
16	CLA	w	504	-	64,68,73	1.22	9 (14%)	76,107,113	1.36	6 (7%)
18	SF4	H	3001	2,1	0,12,12	-	-	-	-	-
19	BCR	v	602	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
19	BCR	p	604	-	41,41,41	1.10	2 (4%)	56,56,56	1.30	6 (10%)
16	CLA	Z	514	-	54,58,73	1.31	9 (16%)	64,95,113	1.47	8 (12%)
16	CLA	B	1204	-	69,73,73	1.13	8 (11%)	82,113,113	1.37	6 (7%)
16	CLA	G	1228	-	59,63,73	1.26	9 (15%)	70,101,113	1.43	8 (11%)
16	CLA	w	515	-	69,73,73	1.16	8 (11%)	82,113,113	1.36	5 (6%)
16	CLA	Z	502	-	54,58,73	1.32	9 (16%)	64,95,113	1.50	8 (12%)
16	CLA	b	1208	-	49,53,73	1.37	9 (18%)	58,89,113	1.52	5 (8%)
16	CLA	a	1109	-	69,73,73	1.15	9 (13%)	82,113,113	1.43	7 (8%)
16	CLA	B	1222	-	59,63,73	1.25	9 (15%)	70,101,113	1.45	6 (8%)
16	CLA	b	1238	-	69,73,73	1.17	10 (14%)	82,113,113	1.38	7 (8%)
16	CLA	s	509	-	64,68,73	1.21	9 (14%)	76,107,113	1.36	10 (13%)
16	CLA	a	1117	-	69,73,73	1.15	9 (13%)	82,113,113	1.38	7 (8%)
19	BCR	p	602	-	41,41,41	1.04	2 (4%)	56,56,56	1.39	8 (14%)
16	CLA	a	1128	-	69,73,73	1.22	9 (13%)	82,113,113	1.55	11 (13%)
16	CLA	X	506	-	64,68,73	1.22	8 (12%)	76,107,113	1.39	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	u	515	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	6 (7%)
16	CLA	b	1235	-	66,70,73	1.20	9 (13%)	78,109,113	1.52	9 (11%)
16	CLA	n	516	-	50,54,73	1.36	9 (18%)	59,90,113	1.47	5 (8%)
16	CLA	B	1213	-	59,63,73	1.25	9 (15%)	70,101,113	1.41	5 (7%)
16	CLA	n	501	-	54,58,73	1.31	8 (14%)	64,95,113	1.43	8 (12%)
16	CLA	B	1206	-	69,73,73	1.18	8 (11%)	82,113,113	1.45	9 (10%)
16	CLA	r	509	-	64,68,73	1.22	9 (14%)	76,107,113	1.34	10 (13%)
16	CLA	H	1402	-	45,49,73	1.41	9 (20%)	54,83,113	1.51	4 (7%)
16	CLA	G	1225	-	69,73,73	1.21	10 (14%)	82,113,113	1.34	7 (8%)
16	CLA	r	504	-	64,68,73	1.21	9 (14%)	76,107,113	1.36	7 (9%)
16	CLA	h	502	-	54,58,73	1.31	8 (14%)	64,95,113	1.43	6 (9%)
18	SF4	a	3001	2,1	0,12,12	-	-	-	-	-
16	CLA	A	1132	-	69,73,73	1.14	9 (13%)	82,113,113	1.41	7 (8%)
16	CLA	G	1201	-	58,62,73	1.25	9 (15%)	68,99,113	1.52	9 (13%)
16	CLA	X	510	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	8 (9%)
16	CLA	g	504	-	64,68,73	1.22	9 (14%)	76,107,113	1.34	7 (9%)
19	BCR	f	4016	-	41,41,41	1.10	2 (4%)	56,56,56	1.30	8 (14%)
16	CLA	B	1207	-	69,73,73	1.17	8 (11%)	82,113,113	1.38	6 (7%)
16	CLA	g	514	-	54,58,73	1.32	8 (14%)	64,95,113	1.46	6 (9%)
16	CLA	q	517	-	59,63,73	1.25	8 (13%)	70,101,113	1.52	10 (14%)
16	CLA	X	501	-	54,58,73	1.32	8 (14%)	64,95,113	1.46	8 (12%)
14	LMG	A	852	-	38,38,55	0.92	1 (2%)	46,46,63	1.25	5 (10%)
16	CLA	H	1122	-	63,67,73	1.21	9 (14%)	74,105,113	1.40	7 (9%)
16	CLA	B	1226	-	69,73,73	1.22	9 (13%)	82,113,113	1.48	10 (12%)
16	CLA	u	516	-	50,54,73	1.36	9 (18%)	59,90,113	1.46	5 (8%)
16	CLA	H	1140	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	6 (7%)
16	CLA	a	1124	-	69,73,73	1.16	9 (13%)	82,113,113	1.38	8 (9%)
16	CLA	n	508	-	59,63,73	1.25	8 (13%)	70,101,113	1.39	7 (10%)
16	CLA	o	515	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	5 (6%)
16	CLA	G	1224	-	64,68,73	1.19	11 (17%)	76,107,113	1.59	10 (13%)
16	CLA	n	505	-	69,73,73	1.18	9 (13%)	82,113,113	1.32	5 (6%)
19	BCR	Y	601	-	41,41,41	1.08	2 (4%)	56,56,56	1.37	9 (16%)
19	BCR	x	601	-	41,41,41	1.07	2 (4%)	56,56,56	1.32	7 (12%)
16	CLA	A	1133	-	58,62,73	1.26	8 (13%)	68,99,113	1.43	6 (8%)
19	BCR	u	603	-	41,41,41	1.09	2 (4%)	56,56,56	1.33	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	J	1302	-	49,53,73	1.38	9 (18%)	58,89,113	1.51	6 (10%)
16	CLA	y	508	-	59,63,73	1.27	9 (15%)	70,101,113	1.39	5 (7%)
16	CLA	a	1140	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
19	BCR	A	4008	-	41,41,41	1.17	2 (4%)	56,56,56	1.41	7 (12%)
18	SF4	C	101	3	0,12,12	-	-	-	-	-
16	CLA	B	1214	-	59,63,73	1.27	9 (15%)	70,101,113	1.41	10 (14%)
16	CLA	n	517	-	59,63,73	1.25	9 (15%)	70,101,113	1.46	9 (12%)
16	CLA	b	1239	-	69,73,73	1.17	8 (11%)	82,113,113	1.41	6 (7%)
16	CLA	v	504	-	64,68,73	1.21	8 (12%)	76,107,113	1.41	7 (9%)
16	CLA	b	1202	-	69,73,73	1.14	8 (11%)	82,113,113	1.41	8 (9%)
16	CLA	w	511	-	69,73,73	1.17	9 (13%)	82,113,113	1.38	8 (9%)
16	CLA	v	507	-	69,73,73	1.17	8 (11%)	82,113,113	1.32	6 (7%)
16	CLA	A	1128	-	69,73,73	1.22	9 (13%)	82,113,113	1.54	11 (13%)
16	CLA	s	510	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	6 (7%)
16	CLA	a	1126	-	69,73,73	1.16	9 (13%)	82,113,113	1.44	11 (13%)
19	BCR	a	4008	-	41,41,41	1.17	3 (7%)	56,56,56	1.41	7 (12%)
16	CLA	w	505	-	69,73,73	1.17	8 (11%)	82,113,113	1.34	6 (7%)
16	CLA	o	512	-	49,53,73	1.37	8 (16%)	58,89,113	1.57	8 (13%)
19	BCR	g	604	-	41,41,41	1.04	2 (4%)	56,56,56	1.37	9 (16%)
16	CLA	t	513	-	54,58,73	1.30	8 (14%)	64,95,113	1.43	7 (10%)
18	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
16	CLA	A	1402	-	45,49,73	1.41	9 (20%)	54,83,113	1.51	4 (7%)
14	LMG	Y	701	-	39,39,55	0.87	1 (2%)	47,47,63	1.25	4 (8%)
16	CLA	s	504	-	64,68,73	1.22	9 (14%)	76,107,113	1.38	6 (7%)
19	BCR	g	603	-	41,41,41	1.08	2 (4%)	56,56,56	1.34	7 (12%)
16	CLA	X	517	-	59,63,73	1.24	8 (13%)	70,101,113	1.61	10 (14%)
16	CLA	b	1221	-	69,73,73	1.17	10 (14%)	82,113,113	1.36	8 (9%)
19	BCR	o	601	-	41,41,41	1.08	2 (4%)	56,56,56	1.33	8 (14%)
16	CLA	y	517	-	59,63,73	1.28	9 (15%)	70,101,113	1.39	7 (10%)
16	CLA	t	515	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
16	CLA	o	508	-	59,63,73	1.25	9 (15%)	70,101,113	1.49	6 (8%)
16	CLA	g	511	-	69,73,73	1.16	9 (13%)	82,113,113	1.39	7 (8%)
16	CLA	U	1503	-	69,73,73	1.15	8 (11%)	82,113,113	1.34	10 (12%)
19	BCR	w	603	-	41,41,41	1.05	2 (4%)	56,56,56	1.30	7 (12%)
16	CLA	y	504	-	64,68,73	1.21	9 (14%)	76,107,113	1.38	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	w	513	-	54,58,73	1.31	8 (14%)	64,95,113	1.47	7 (10%)
16	CLA	y	511	-	69,73,73	1.17	9 (13%)	82,113,113	1.34	8 (9%)
16	CLA	b	1226	-	69,73,73	1.22	9 (13%)	82,113,113	1.49	10 (12%)
18	SF4	c	101	3	0,12,12	-	-	-	-	-
16	CLA	w	501	-	54,58,73	1.31	8 (14%)	64,95,113	1.43	6 (9%)
16	CLA	v	508	-	59,63,73	1.28	9 (15%)	70,101,113	1.39	6 (8%)
19	BCR	n	603	-	41,41,41	1.11	3 (7%)	56,56,56	1.34	8 (14%)
16	CLA	o	503	-	50,54,73	1.35	8 (16%)	59,90,113	1.52	6 (10%)
16	CLA	q	516	-	50,54,73	1.38	8 (16%)	59,90,113	1.50	6 (10%)
19	BCR	G	4017	-	41,41,41	1.17	3 (7%)	56,56,56	1.32	9 (16%)
16	CLA	G	1234	-	54,58,73	1.30	8 (14%)	64,95,113	1.53	7 (10%)
19	BCR	r	603	-	41,41,41	1.08	2 (4%)	56,56,56	1.33	7 (12%)
16	CLA	B	1232	-	49,53,73	1.39	9 (18%)	58,89,113	1.51	5 (8%)
16	CLA	r	513	-	54,58,73	1.32	8 (14%)	64,95,113	1.45	6 (9%)
16	CLA	B	1220	-	58,62,73	1.26	9 (15%)	68,99,113	1.52	10 (14%)
19	BCR	q	604	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	9 (16%)
13	LHG	I	103	-	43,43,48	0.66	2 (4%)	46,49,54	1.28	5 (10%)
16	CLA	q	507	-	69,73,73	1.18	8 (11%)	82,113,113	1.32	6 (7%)
16	CLA	W	515	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	6 (7%)
14	LMG	A	4101	-	46,46,55	0.83	1 (2%)	54,54,63	1.32	6 (11%)
16	CLA	a	1127	-	69,73,73	1.17	9 (13%)	82,113,113	1.38	8 (9%)
19	BCR	u	604	-	41,41,41	1.04	2 (4%)	56,56,56	1.33	9 (16%)
16	CLA	L	1502	-	69,73,73	1.15	9 (13%)	82,113,113	1.38	7 (8%)
16	CLA	o	507	-	69,73,73	1.17	9 (13%)	82,113,113	1.31	7 (8%)
13	LHG	a	851	-	26,26,48	0.87	1 (3%)	29,32,54	1.36	3 (10%)
16	CLA	u	503	-	50,54,73	1.36	8 (16%)	59,90,113	1.52	6 (10%)
19	BCR	S	4015	-	41,41,41	1.12	3 (7%)	56,56,56	1.34	8 (14%)
16	CLA	A	1126	-	69,73,73	1.16	9 (13%)	82,113,113	1.44	10 (12%)
16	CLA	g	501	-	54,58,73	1.31	8 (14%)	64,95,113	1.45	7 (10%)
16	CLA	H	1237	-	69,73,73	1.18	8 (11%)	82,113,113	1.44	9 (10%)
16	CLA	x	505	-	50,54,73	1.35	9 (18%)	59,90,113	1.49	6 (10%)
16	CLA	a	1123	-	69,73,73	1.18	7 (10%)	82,113,113	1.38	7 (8%)
19	BCR	L	4022	-	41,41,41	1.08	1 (2%)	56,56,56	1.55	11 (19%)
19	BCR	I	4018	-	41,41,41	1.13	2 (4%)	56,56,56	1.32	6 (10%)
19	BCR	A	4002	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	g	507	-	69,73,73	1.17	9 (13%)	82,113,113	1.32	6 (7%)
16	CLA	v	506	-	64,68,73	1.21	7 (10%)	76,107,113	1.41	8 (10%)
16	CLA	p	514	-	54,58,73	1.31	9 (16%)	64,95,113	1.46	8 (12%)
16	CLA	G	1021	-	69,73,73	1.17	7 (10%)	82,113,113	1.52	7 (8%)
16	CLA	B	1012	-	64,68,73	1.23	10 (15%)	76,107,113	1.51	10 (13%)
16	CLA	y	510	-	64,68,73	1.20	8 (12%)	76,107,113	1.38	9 (11%)
16	CLA	p	502	-	54,58,73	1.30	7 (12%)	64,95,113	1.45	7 (10%)
16	CLA	H	1118	-	59,63,73	1.26	10 (16%)	70,101,113	1.43	5 (7%)
19	BCR	A	4001	-	41,41,41	1.13	3 (7%)	56,56,56	1.36	9 (16%)
19	BCR	Y	603	-	41,41,41	1.06	2 (4%)	56,56,56	1.39	8 (14%)
16	CLA	t	505	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	4 (4%)
19	BCR	a	4001	-	41,41,41	1.13	3 (7%)	56,56,56	1.36	9 (16%)
16	CLA	A	1136	-	69,73,73	1.15	9 (13%)	82,113,113	1.37	9 (10%)
14	LMG	H	852	-	38,38,55	0.92	1 (2%)	46,46,63	1.25	5 (10%)
16	CLA	o	517	-	59,63,73	1.25	8 (13%)	70,101,113	1.49	9 (12%)
16	CLA	Y	504	-	64,68,73	1.21	9 (14%)	76,107,113	1.38	6 (7%)
16	CLA	q	515	-	69,73,73	1.16	9 (13%)	82,113,113	1.36	6 (7%)
16	CLA	a	1131	-	69,73,73	1.15	10 (14%)	82,113,113	1.42	10 (12%)
16	CLA	B	1227	-	53,57,73	1.32	9 (16%)	61,93,113	1.52	6 (9%)
17	PQN	b	2002	-	34,34,34	0.38	0	43,45,45	1.18	2 (4%)
19	BCR	X	604	-	41,41,41	1.04	2 (4%)	56,56,56	1.35	10 (17%)
16	CLA	Z	504	-	64,68,73	1.22	9 (14%)	76,107,113	1.33	5 (6%)
19	BCR	i	4020	-	41,41,41	1.22	3 (7%)	56,56,56	1.26	6 (10%)
16	CLA	G	1202	-	69,73,73	1.15	8 (11%)	82,113,113	1.41	8 (9%)
13	LHG	i	103	-	43,43,48	0.66	2 (4%)	46,49,54	1.29	5 (10%)
16	CLA	X	507	-	69,73,73	1.18	8 (11%)	82,113,113	1.33	7 (8%)
16	CLA	h	508	-	59,63,73	1.28	9 (15%)	70,101,113	1.38	5 (7%)
19	BCR	s	603	-	41,41,41	1.08	3 (7%)	56,56,56	1.38	8 (14%)
16	CLA	a	1022	-	69,73,73	1.22	8 (11%)	82,113,113	1.41	9 (10%)
19	BCR	b	4005	-	41,41,41	1.12	3 (7%)	56,56,56	1.41	7 (12%)
16	CLA	H	1126	-	69,73,73	1.15	9 (13%)	82,113,113	1.44	10 (12%)
16	CLA	s	517	-	59,63,73	1.25	9 (15%)	70,101,113	1.40	5 (7%)
19	BCR	G	4004	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	5 (8%)
16	CLA	b	1240	-	54,58,73	1.32	9 (16%)	64,95,113	1.45	6 (9%)
16	CLA	B	1208	-	49,53,73	1.37	8 (16%)	58,89,113	1.52	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMG	a	4101	-	46,46,55	0.83	1 (2%)	54,54,63	1.32	6 (11%)
16	CLA	a	1118	-	59,63,73	1.26	9 (15%)	70,101,113	1.43	5 (7%)
16	CLA	s	514	-	54,58,73	1.31	9 (16%)	64,95,113	1.46	8 (12%)
16	CLA	v	503	-	50,54,73	1.37	8 (16%)	59,90,113	1.48	5 (8%)
16	CLA	A	1127	-	69,73,73	1.17	10 (14%)	82,113,113	1.39	8 (9%)
16	CLA	y	506	-	64,68,73	1.22	8 (12%)	76,107,113	1.43	7 (9%)
19	BCR	o	602	-	41,41,41	1.03	2 (4%)	56,56,56	1.37	7 (12%)
16	CLA	x	501	-	54,58,73	1.32	8 (14%)	64,95,113	1.46	6 (9%)
16	CLA	A	1022	-	69,73,73	1.22	9 (13%)	82,113,113	1.41	9 (10%)
16	CLA	B	1235	-	66,70,73	1.20	9 (13%)	78,109,113	1.52	9 (11%)
16	CLA	g	517	-	59,63,73	1.26	9 (15%)	70,101,113	1.40	6 (8%)
16	CLA	b	1228	-	59,63,73	1.26	9 (15%)	70,101,113	1.43	8 (11%)
16	CLA	h	514	-	54,58,73	1.33	8 (14%)	64,95,113	1.44	7 (10%)
16	CLA	H	1111	-	59,63,73	1.25	10 (16%)	70,101,113	1.44	7 (10%)
16	CLA	w	502	-	54,58,73	1.32	8 (14%)	64,95,113	1.49	8 (12%)
16	CLA	y	513	-	54,58,73	1.32	9 (16%)	64,95,113	1.45	8 (12%)
16	CLA	j	1303	-	41,45,73	1.44	8 (19%)	50,78,113	1.60	6 (12%)
16	CLA	H	1135	-	55,59,73	1.28	8 (14%)	64,96,113	1.47	8 (12%)
16	CLA	h	516	-	50,54,73	1.36	8 (16%)	59,90,113	1.49	5 (8%)
16	CLA	G	1212	-	49,53,73	1.36	8 (16%)	58,89,113	1.53	7 (12%)
16	CLA	t	501	-	54,58,73	1.31	8 (14%)	64,95,113	1.42	8 (12%)
19	BCR	U	4022	-	41,41,41	1.08	2 (4%)	56,56,56	1.55	10 (17%)
16	CLA	a	1237	-	69,73,73	1.19	8 (11%)	82,113,113	1.43	9 (10%)
16	CLA	n	507	-	64,68,73	1.23	9 (14%)	76,107,113	1.36	7 (9%)
16	CLA	G	1211	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	8 (9%)
16	CLA	B	1216	-	51,55,73	1.36	10 (19%)	60,91,113	1.49	6 (10%)
16	CLA	b	1225	-	69,73,73	1.21	10 (14%)	82,113,113	1.34	7 (8%)
16	CLA	p	508	-	59,63,73	1.25	9 (15%)	70,101,113	1.41	6 (8%)
13	LHG	R	103	-	43,43,48	0.66	2 (4%)	46,49,54	1.28	5 (10%)
19	BCR	r	604	-	41,41,41	1.05	2 (4%)	56,56,56	1.36	9 (16%)
16	CLA	s	506	-	64,68,73	1.22	7 (10%)	76,107,113	1.40	7 (9%)
16	CLA	r	507	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	6 (7%)
16	CLA	H	1136	-	69,73,73	1.15	9 (13%)	82,113,113	1.37	9 (10%)
19	BCR	X	603	-	41,41,41	1.07	2 (4%)	56,56,56	1.36	8 (14%)
16	CLA	a	1110	-	58,62,73	1.26	9 (15%)	68,99,113	1.44	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	a	1108	-	49,53,73	1.37	8 (16%)	58,89,113	1.52	6 (10%)
16	CLA	a	1135	-	55,59,73	1.28	8 (14%)	64,96,113	1.46	8 (12%)
16	CLA	G	1231	-	49,53,73	1.38	9 (18%)	58,89,113	1.57	8 (13%)
16	CLA	X	515	-	69,73,73	1.15	8 (11%)	82,113,113	1.34	5 (6%)
16	CLA	Z	501	-	54,58,73	1.32	8 (14%)	64,95,113	1.44	6 (9%)
14	LMG	H	4201	-	32,32,55	1.00	1 (3%)	40,40,63	1.13	4 (10%)
19	BCR	b	4006	-	25,25,41	1.09	2 (8%)	33,33,56	1.44	6 (18%)
16	CLA	b	1223	-	69,73,73	1.18	9 (13%)	82,113,113	1.36	8 (9%)
16	CLA	b	1218	-	59,63,73	1.26	9 (15%)	70,101,113	1.43	5 (7%)
16	CLA	G	1213	-	59,63,73	1.25	9 (15%)	70,101,113	1.40	5 (7%)
16	CLA	q	509	-	60,64,73	1.25	9 (15%)	71,102,113	1.37	10 (14%)
19	BCR	B	4010	-	41,41,41	1.16	3 (7%)	56,56,56	1.39	10 (17%)
16	CLA	W	512	-	49,53,73	1.38	9 (18%)	58,89,113	1.57	7 (12%)
20	LMT	U	4101	-	36,36,36	1.12	5 (13%)	47,47,47	1.08	4 (8%)
16	CLA	v	501	-	50,54,73	1.35	8 (16%)	59,90,113	1.47	5 (8%)
16	CLA	a	1113	-	49,53,73	1.36	9 (18%)	58,89,113	1.61	8 (13%)
16	CLA	a	1119	-	69,73,73	1.15	9 (13%)	82,113,113	1.36	8 (9%)
19	BCR	b	4009	-	41,41,41	1.06	2 (4%)	56,56,56	1.38	9 (16%)
16	CLA	W	514	-	54,58,73	1.32	9 (16%)	64,95,113	1.47	8 (12%)
16	CLA	x	517	-	59,63,73	1.26	9 (15%)	70,101,113	1.39	6 (8%)
16	CLA	H	1133	-	58,62,73	1.26	9 (15%)	68,99,113	1.44	6 (8%)
16	CLA	A	1118	-	59,63,73	1.26	9 (15%)	70,101,113	1.43	5 (7%)
16	CLA	a	1116	-	58,62,73	1.25	10 (17%)	68,99,113	1.47	11 (16%)
16	CLA	G	1220	-	58,62,73	1.26	9 (15%)	68,99,113	1.51	10 (14%)
16	CLA	b	1201	-	58,62,73	1.25	9 (15%)	68,99,113	1.52	9 (13%)
16	CLA	w	516	-	50,54,73	1.37	9 (18%)	59,90,113	1.48	6 (10%)
19	BCR	t	601	-	41,41,41	1.04	2 (4%)	56,56,56	1.35	9 (16%)
16	CLA	s	516	-	50,54,73	1.36	9 (18%)	59,90,113	1.52	7 (11%)
16	CLA	r	517	-	59,63,73	1.25	8 (13%)	70,101,113	1.41	8 (11%)
19	BCR	h	603	-	41,41,41	1.06	2 (4%)	56,56,56	1.31	7 (12%)
16	CLA	W	517	-	59,63,73	1.26	9 (15%)	70,101,113	1.47	8 (11%)
19	BCR	w	604	-	41,41,41	1.08	2 (4%)	56,56,56	1.37	11 (19%)
16	CLA	B	1225	-	69,73,73	1.21	10 (14%)	82,113,113	1.34	7 (8%)
16	CLA	a	1130	-	69,73,73	1.17	11 (15%)	82,113,113	1.35	10 (12%)
16	CLA	B	1228	-	59,63,73	1.26	9 (15%)	70,101,113	1.42	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	BCR	A	4003	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	7 (12%)
19	BCR	s	604	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	6 (10%)
16	CLA	Y	511	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	7 (8%)
16	CLA	x	507	-	69,73,73	1.17	9 (13%)	82,113,113	1.34	6 (7%)
16	CLA	o	510	-	69,73,73	1.15	8 (11%)	82,113,113	1.35	6 (7%)
16	CLA	b	1229	-	62,66,73	1.22	9 (14%)	73,104,113	1.43	7 (9%)
16	CLA	r	515	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
20	LMT	l	4101	-	36,36,36	1.11	5 (13%)	47,47,47	1.07	4 (8%)
16	CLA	B	1211	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	8 (9%)
16	CLA	p	512	-	49,53,73	1.36	9 (18%)	58,89,113	1.55	8 (13%)
16	CLA	h	511	-	69,73,73	1.18	9 (13%)	82,113,113	1.35	9 (10%)
16	CLA	Y	506	-	64,68,73	1.23	7 (10%)	76,107,113	1.41	7 (9%)
16	CLA	H	1137	-	51,55,73	1.31	10 (19%)	60,91,113	1.55	7 (11%)
19	BCR	i	4018	-	41,41,41	1.14	2 (4%)	56,56,56	1.32	6 (10%)
19	BCR	B	4004	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	5 (8%)
19	BCR	y	603	-	41,41,41	1.08	2 (4%)	56,56,56	1.38	7 (12%)
16	CLA	r	503	-	50,54,73	1.36	9 (18%)	59,90,113	1.49	6 (10%)
16	CLA	G	1235	-	66,70,73	1.20	9 (13%)	78,109,113	1.53	9 (11%)
16	CLA	A	1102	-	60,64,73	1.24	10 (16%)	71,102,113	1.51	9 (12%)
19	BCR	Z	603	-	41,41,41	1.06	2 (4%)	56,56,56	1.32	7 (12%)
16	CLA	A	1134	-	49,53,73	1.38	9 (18%)	58,89,113	1.59	8 (13%)
16	CLA	Z	513	-	54,58,73	1.31	8 (14%)	64,95,113	1.45	7 (10%)
16	CLA	g	503	-	50,54,73	1.37	8 (16%)	59,90,113	1.49	6 (10%)
16	CLA	Z	517	-	59,63,73	1.25	8 (13%)	70,101,113	1.52	11 (15%)
16	CLA	G	1218	-	59,63,73	1.26	9 (15%)	70,101,113	1.43	5 (7%)
16	CLA	s	507	-	69,73,73	1.18	8 (11%)	82,113,113	1.31	7 (8%)
15	CL0	A	1011	-	58,73,73	2.12	14 (24%)	60,113,113	1.95	17 (28%)
14	LMG	a	852	-	38,38,55	0.92	1 (2%)	46,46,63	1.25	5 (10%)
16	CLA	p	509	-	64,68,73	1.21	9 (14%)	76,107,113	1.36	10 (13%)
16	CLA	g	510	-	59,63,73	1.27	8 (13%)	70,101,113	1.40	8 (11%)
16	CLA	G	1230	-	49,53,73	1.35	9 (18%)	58,89,113	1.62	9 (15%)
16	CLA	G	1023	-	69,73,73	1.16	10 (14%)	82,113,113	1.68	13 (15%)
16	CLA	Y	513	-	54,58,73	1.32	9 (16%)	64,95,113	1.45	7 (10%)
16	CLA	s	515	-	69,73,73	1.16	8 (11%)	82,113,113	1.36	6 (7%)
16	CLA	a	1138	-	69,73,73	1.14	9 (13%)	82,113,113	1.44	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	G	1012	-	64,68,73	1.24	10 (15%)	76,107,113	1.51	10 (13%)
19	BCR	b	4014	-	41,41,41	1.14	3 (7%)	56,56,56	1.27	6 (10%)
19	BCR	l	4022	-	41,41,41	1.08	2 (4%)	56,56,56	1.55	11 (19%)
16	CLA	o	509	-	64,68,73	1.21	9 (14%)	76,107,113	1.41	10 (13%)
16	CLA	H	1105	-	62,66,73	1.21	9 (14%)	73,104,113	1.43	7 (9%)
16	CLA	b	1204	-	69,73,73	1.13	8 (11%)	82,113,113	1.38	6 (7%)
16	CLA	q	513	-	54,58,73	1.31	8 (14%)	64,95,113	1.45	7 (10%)
16	CLA	a	1132	-	69,73,73	1.15	9 (13%)	82,113,113	1.40	7 (8%)
16	CLA	Y	512	-	49,53,73	1.37	9 (18%)	58,89,113	1.57	7 (12%)
16	CLA	a	1101	-	69,73,73	1.15	9 (13%)	82,113,113	1.37	9 (10%)
16	CLA	w	509	-	60,64,73	1.25	9 (15%)	71,102,113	1.39	10 (14%)
16	CLA	g	512	-	49,53,73	1.37	8 (16%)	58,89,113	1.52	7 (12%)
16	CLA	a	1107	-	54,58,73	1.31	9 (16%)	64,95,113	1.64	9 (14%)
16	CLA	H	1120	-	53,57,73	1.30	9 (16%)	61,93,113	1.54	7 (11%)
16	CLA	v	511	-	69,73,73	1.17	9 (13%)	82,113,113	1.35	9 (10%)
16	CLA	u	513	-	54,58,73	1.31	8 (14%)	64,95,113	1.45	6 (9%)
19	BCR	g	602	-	41,41,41	1.00	2 (4%)	56,56,56	1.36	7 (12%)
16	CLA	b	1209	-	49,53,73	1.38	9 (18%)	58,89,113	1.51	6 (10%)
16	CLA	b	1023	-	69,73,73	1.16	10 (14%)	82,113,113	1.68	13 (15%)
19	BCR	g	601	-	41,41,41	1.05	2 (4%)	56,56,56	1.34	7 (12%)
14	LMG	a	4201	-	31,31,55	1.01	1 (3%)	39,39,63	1.13	4 (10%)
16	CLA	u	509	-	64,68,73	1.21	9 (14%)	76,107,113	1.40	10 (13%)
16	CLA	n	511	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	6 (7%)
16	CLA	L	1501	-	69,73,73	1.16	9 (13%)	82,113,113	1.39	8 (9%)
16	CLA	r	505	-	50,54,73	1.36	8 (16%)	59,90,113	1.49	6 (10%)
16	CLA	W	505	-	69,73,73	1.18	8 (11%)	82,113,113	1.33	5 (6%)
16	CLA	g	513	-	54,58,73	1.32	8 (14%)	64,95,113	1.46	6 (9%)
16	CLA	A	1117	-	69,73,73	1.15	9 (13%)	82,113,113	1.37	7 (8%)
16	CLA	b	1211	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	8 (9%)
16	CLA	w	506	-	64,68,73	1.22	9 (14%)	76,107,113	1.36	6 (7%)
18	SF4	N	102	3	0,12,12	-	-	-	-	-
19	BCR	H	4001	-	41,41,41	1.13	2 (4%)	56,56,56	1.37	9 (16%)
16	CLA	H	1110	-	58,62,73	1.27	9 (15%)	68,99,113	1.45	7 (10%)
16	CLA	x	516	-	50,54,73	1.38	8 (16%)	59,90,113	1.49	6 (10%)
19	BCR	y	604	-	41,41,41	1.03	2 (4%)	56,56,56	1.31	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	n	512	-	49,53,73	1.39	9 (18%)	58,89,113	1.53	7 (12%)
16	CLA	w	508	-	59,63,73	1.26	8 (13%)	70,101,113	1.42	5 (7%)
19	BCR	B	4014	-	41,41,41	1.14	3 (7%)	56,56,56	1.28	6 (10%)
16	CLA	p	504	-	64,68,73	1.21	9 (14%)	76,107,113	1.39	6 (7%)
16	CLA	n	510	-	69,73,73	1.17	6 (8%)	82,113,113	1.34	8 (9%)
19	BCR	G	4006	-	25,25,41	1.09	2 (8%)	33,33,56	1.43	6 (18%)
16	CLA	A	1122	-	63,67,73	1.21	9 (14%)	74,105,113	1.38	7 (9%)

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	n	506	-	1/1/14/20	13/33/109/115	-
16	CLA	r	510	-	1/1/13/20	11/27/103/115	-
16	CLA	H	1101	-	1/1/15/20	15/39/115/115	-
19	BCR	q	603	-	-	9/29/63/63	0/2/2/2
16	CLA	H	1130	-	1/1/15/20	6/39/115/115	-
16	CLA	A	1106	-	1/1/15/20	19/39/115/115	-
16	CLA	B	1210	-	1/1/15/20	15/39/115/115	-
16	CLA	n	513	-	1/1/12/20	8/21/97/115	-
16	CLA	q	504	-	1/1/14/20	9/33/109/115	-
16	CLA	p	505	-	1/1/15/20	13/39/115/115	-
16	CLA	w	503	-	1/1/11/20	12/17/93/115	-
16	CLA	l	1503	-	1/1/15/20	15/39/115/115	-
16	CLA	a	1133	-	1/1/12/20	11/26/102/115	-
16	CLA	a	1112	-	1/1/11/20	6/15/91/115	-
16	CLA	A	1801	-	1/1/12/20	6/24/100/115	-
16	CLA	A	1112	-	1/1/11/20	6/15/91/115	-
16	CLA	A	1101	-	1/1/15/20	15/39/115/115	-
16	CLA	U	1502	-	1/1/15/20	12/39/115/115	-
16	CLA	B	1240	-	1/1/12/20	4/21/97/115	-
16	CLA	b	1227	-	1/1/11/20	9/20/96/115	-
19	BCR	Z	604	-	-	16/29/63/63	0/2/2/2
16	CLA	H	1131	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	n	503	-	1/1/11/20	9/17/93/115	-
16	CLA	H	1102	-	1/1/13/20	7/29/105/115	-
19	BCR	H	4002	-	-	8/29/63/63	0/2/2/2
16	CLA	Z	507	-	1/1/15/20	14/39/115/115	-
19	BCR	J	4015	-	-	11/29/63/63	0/2/2/2
19	BCR	S	4012	-	-	10/29/63/63	0/2/2/2
14	LMG	A	4201	-	-	7/27/47/70	0/1/1/1
16	CLA	v	516	-	1/1/11/20	8/17/93/115	-
16	CLA	H	1125	-	1/1/15/20	10/39/115/115	-
16	CLA	a	1402	-	1/1/9/20	2/9/81/115	-
16	CLA	t	517	-	1/1/13/20	15/27/103/115	-
16	CLA	h	504	-	1/1/14/20	14/33/109/115	-
16	CLA	Y	502	-	1/1/12/20	6/21/97/115	-
19	BCR	K	1501	-	-	10/29/63/63	0/2/2/2
16	CLA	p	501	-	1/1/12/20	7/21/97/115	-
16	CLA	H	1127	-	1/1/15/20	10/39/115/115	-
16	CLA	a	1120	-	1/1/11/20	11/20/96/115	-
17	PQN	A	2001	-	-	6/23/43/43	0/2/2/2
16	CLA	W	510	-	1/1/15/20	11/39/115/115	-
16	CLA	H	1022	-	1/1/15/20	9/39/115/115	-
16	CLA	u	508	-	1/1/13/20	11/27/103/115	-
16	CLA	G	1226	-	1/1/15/20	9/39/115/115	-
16	CLA	t	509	-	1/1/14/20	10/33/109/115	-
19	BCR	r	601	-	-	18/29/63/63	0/2/2/2
16	CLA	G	1238	-	1/1/15/20	12/39/115/115	-
19	BCR	W	601	-	-	13/29/63/63	0/2/2/2
16	CLA	s	512	-	1/1/11/20	6/15/91/115	-
16	CLA	g	506	-	1/1/14/20	13/33/109/115	-
16	CLA	h	505	-	1/1/14/20	17/33/109/115	-
16	CLA	X	514	-	1/1/12/20	10/21/97/115	-
16	CLA	b	1012	-	1/1/14/20	16/33/109/115	-
16	CLA	b	1021	-	1/1/15/20	14/39/115/115	-
19	BCR	n	601	-	-	11/29/63/63	0/2/2/2
16	CLA	G	1204	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	G	1214	-	1/1/13/20	12/27/103/115	-
16	CLA	G	1219	-	1/1/11/20	7/15/91/115	-
16	CLA	x	506	-	1/1/14/20	16/33/109/115	-
16	CLA	o	504	-	1/1/14/20	7/33/109/115	-
16	CLA	H	1801	-	1/1/12/20	6/24/100/115	-
16	CLA	f	1301	-	1/1/11/20	4/15/91/115	-
13	LHG	A	849	-	-	11/47/47/53	-
14	LMG	G	848	-	-	18/38/58/70	0/1/1/1
16	CLA	h	506	-	1/1/14/20	10/33/109/115	-
16	CLA	G	1207	-	1/1/15/20	23/39/115/115	-
16	CLA	H	1013	-	1/1/15/20	16/39/115/115	-
16	CLA	G	1232	-	1/1/11/20	6/15/91/115	-
16	CLA	b	1231	-	1/1/11/20	4/15/91/115	-
16	CLA	Q	1301	-	1/1/11/20	4/15/91/115	-
16	CLA	W	504	-	1/1/14/20	8/33/109/115	-
16	CLA	v	517	-	1/1/13/20	9/27/103/115	-
16	CLA	Y	503	-	1/1/11/20	10/17/93/115	-
16	CLA	b	1220	-	1/1/12/20	5/26/102/115	-
16	CLA	v	505	-	1/1/14/20	18/33/109/115	-
16	CLA	n	515	-	1/1/15/20	13/39/115/115	-
16	CLA	v	509	-	1/1/14/20	8/33/109/115	-
16	CLA	a	1125	-	1/1/15/20	10/39/115/115	-
16	CLA	x	511	-	1/1/15/20	9/39/115/115	-
20	LMT	L	4101	-	-	7/21/61/61	0/2/2/2
16	CLA	t	512	-	1/1/11/20	6/15/91/115	-
19	BCR	p	603	-	-	7/29/63/63	0/2/2/2
16	CLA	h	501	-	1/1/11/20	9/17/93/115	-
16	CLA	s	503	-	1/1/11/20	11/17/93/115	-
19	BCR	w	601	-	-	8/29/63/63	0/2/2/2
16	CLA	Y	516	-	1/1/11/20	9/17/93/115	-
16	CLA	g	515	-	1/1/15/20	16/39/115/115	-
16	CLA	a	1013	-	1/1/15/20	16/39/115/115	-
19	BCR	b	4017	-	-	9/29/63/63	0/2/2/2
16	CLA	B	1229	-	1/1/13/20	11/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	Y	507	-	1/1/15/20	12/39/115/115	-
16	CLA	H	1106	-	1/1/15/20	19/39/115/115	-
19	BCR	q	601	-	-	7/29/63/63	0/2/2/2
16	CLA	b	1206	-	1/1/15/20	13/39/115/115	-
16	CLA	H	1116	-	1/1/12/20	10/26/102/115	-
16	CLA	h	503	-	1/1/11/20	11/17/93/115	-
16	CLA	H	1115	-	1/1/12/20	7/26/102/115	-
16	CLA	x	509	-	1/1/14/20	12/33/109/115	-
16	CLA	T	1401	-	1/1/11/20	3/15/91/115	-
16	CLA	H	1107	-	1/1/12/20	3/21/97/115	-
16	CLA	b	1217	-	1/1/11/20	8/15/91/115	-
19	BCR	H	4003	-	-	11/29/63/63	0/2/2/2
19	BCR	a	4002	-	-	8/29/63/63	0/2/2/2
19	BCR	s	601	-	-	13/29/63/63	0/2/2/2
16	CLA	t	511	-	1/1/15/20	11/39/115/115	-
16	CLA	H	1113	-	1/1/11/20	5/15/91/115	-
15	CL0	H	1011	-	3/3/20/25	12/37/135/135	-
16	CLA	a	1139	-	1/1/12/20	10/23/99/115	-
16	CLA	t	506	-	1/1/14/20	12/33/109/115	-
16	CLA	S	1303	-	1/1/8/20	2/4/76/115	-
19	BCR	S	4013	-	-	11/29/63/63	0/2/2/2
19	BCR	H	4011	-	-	15/29/63/63	0/2/2/2
16	CLA	s	502	-	1/1/12/20	7/21/97/115	-
16	CLA	U	1501	-	1/1/15/20	19/39/115/115	-
16	CLA	a	1801	-	1/1/12/20	6/24/100/115	-
16	CLA	h	512	-	1/1/11/20	6/15/91/115	-
16	CLA	w	517	-	1/1/13/20	8/27/103/115	-
19	BCR	b	4010	-	-	12/29/63/63	0/2/2/2
19	BCR	u	602	-	-	10/29/63/63	0/2/2/2
16	CLA	H	1134	-	1/1/11/20	11/15/91/115	-
19	BCR	B	4005	-	-	7/29/63/63	0/2/2/2
16	CLA	o	514	-	1/1/12/20	10/21/97/115	-
16	CLA	X	503	-	1/1/11/20	10/17/93/115	-
16	CLA	B	1231	-	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	x	508	-	1/1/13/20	11/27/103/115	-
16	CLA	b	1230	-	1/1/11/20	4/15/91/115	-
16	CLA	Z	509	-	1/1/13/20	10/29/105/115	-
19	BCR	h	601	-	-	11/29/63/63	0/2/2/2
19	BCR	a	4007	-	-	7/29/63/63	0/2/2/2
16	CLA	A	1140	-	1/1/15/20	21/39/115/115	-
16	CLA	G	1239	-	1/1/15/20	17/39/115/115	-
18	SF4	c	102	3	-	-	0/6/5/5
16	CLA	W	507	-	1/1/14/20	12/33/109/115	-
16	CLA	o	505	-	1/1/15/20	13/39/115/115	-
16	CLA	X	512	-	1/1/11/20	7/15/91/115	-
16	CLA	h	513	-	1/1/12/20	4/21/97/115	-
16	CLA	k	1401	-	1/1/11/20	3/15/91/115	-
16	CLA	h	517	-	1/1/13/20	10/27/103/115	-
16	CLA	u	502	-	1/1/12/20	9/21/97/115	-
16	CLA	y	512	-	1/1/11/20	6/15/91/115	-
16	CLA	u	504	-	1/1/14/20	16/33/109/115	-
16	CLA	A	1237	-	1/1/15/20	15/39/115/115	-
16	CLA	Y	509	-	1/1/14/20	14/33/109/115	-
16	CLA	t	503	-	1/1/11/20	9/17/93/115	-
19	BCR	B	4006	-	-	5/18/35/63	0/1/1/2
16	CLA	g	505	-	1/1/11/20	10/17/93/115	-
16	CLA	h	509	-	1/1/14/20	8/33/109/115	-
16	CLA	A	1111	-	1/1/13/20	11/27/103/115	-
16	CLA	A	1013	-	1/1/15/20	16/39/115/115	-
16	CLA	y	503	-	1/1/11/20	12/17/93/115	-
16	CLA	w	507	-	1/1/15/20	14/39/115/115	-
19	BCR	Y	602	-	-	10/29/63/63	0/2/2/2
16	CLA	Z	506	-	1/1/14/20	7/33/109/115	-
16	CLA	A	1110	-	1/1/12/20	6/26/102/115	-
19	BCR	L	4019	-	-	11/29/63/63	0/2/2/2
16	CLA	y	515	-	1/1/14/20	6/33/109/115	-
16	CLA	Z	508	-	1/1/13/20	10/27/103/115	-
16	CLA	G	1236	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	o	502	-	1/1/12/20	9/21/97/115	-
16	CLA	H	1132	-	1/1/15/20	11/39/115/115	-
16	CLA	o	516	-	1/1/11/20	10/17/93/115	-
16	CLA	G	1227	-	1/1/11/20	9/20/96/115	-
16	CLA	B	1219	-	1/1/11/20	7/15/91/115	-
16	CLA	o	501	-	1/1/12/20	9/21/97/115	-
16	CLA	A	1113	-	1/1/11/20	5/15/91/115	-
16	CLA	X	509	-	1/1/14/20	10/33/109/115	-
16	CLA	f	1302	-	1/1/5/20	-	-
16	CLA	b	1212	-	1/1/11/20	6/15/91/115	-
16	CLA	A	1121	-	1/1/12/20	13/23/99/115	-
16	CLA	o	511	-	1/1/15/20	12/39/115/115	-
16	CLA	Z	511	-	1/1/15/20	12/39/115/115	-
19	BCR	R	4018	-	-	14/29/63/63	0/2/2/2
16	CLA	A	1116	-	1/1/12/20	10/26/102/115	-
16	CLA	B	1218	-	1/1/13/20	8/27/103/115	-
16	CLA	Z	503	-	1/1/11/20	10/17/93/115	-
16	CLA	G	1222	-	1/1/13/20	7/27/103/115	-
16	CLA	p	507	-	1/1/15/20	14/39/115/115	-
16	CLA	a	1103	-	1/1/15/20	15/39/115/115	-
16	CLA	q	505	-	1/1/15/20	17/39/115/115	-
16	CLA	H	1117	-	1/1/15/20	14/39/115/115	-
16	CLA	A	1130	-	1/1/15/20	6/39/115/115	-
16	CLA	Z	512	-	1/1/11/20	6/15/91/115	-
16	CLA	u	501	-	1/1/12/20	9/21/97/115	-
18	SF4	C	102	3	-	-	0/6/5/5
19	BCR	A	4011	-	-	15/29/63/63	0/2/2/2
16	CLA	B	1239	-	1/1/15/20	17/39/115/115	-
19	BCR	Z	601	-	-	9/29/63/63	0/2/2/2
16	CLA	s	511	-	1/1/15/20	17/39/115/115	-
16	CLA	a	1121	-	1/1/12/20	13/23/99/115	-
16	CLA	l	1501	-	1/1/15/20	19/39/115/115	-
19	BCR	X	601	-	-	10/29/63/63	0/2/2/2
16	CLA	x	504	-	1/1/14/20	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	1114	-	1/1/11/20	7/20/96/115	-
16	CLA	h	515	-	1/1/14/20	5/33/109/115	-
16	CLA	G	1215	-	1/1/14/20	15/33/109/115	-
16	CLA	y	505	-	1/1/14/20	16/33/109/115	-
19	BCR	t	603	-	-	8/29/63/63	0/2/2/2
16	CLA	H	1124	-	1/1/15/20	10/39/115/115	-
16	CLA	p	517	-	1/1/13/20	10/27/103/115	-
19	BCR	H	4007	-	-	7/29/63/63	0/2/2/2
16	CLA	Y	508	-	1/1/13/20	11/27/103/115	-
16	CLA	t	504	-	1/1/14/20	9/33/109/115	-
16	CLA	A	1104	-	1/1/15/20	9/39/115/115	-
16	CLA	a	1129	-	1/1/12/20	5/21/97/115	-
16	CLA	B	1224	-	1/1/14/20	20/33/109/115	-
16	CLA	a	1122	-	1/1/13/20	12/32/108/115	-
16	CLA	L	1503	-	1/1/15/20	15/39/115/115	-
16	CLA	H	1112	-	1/1/11/20	6/15/91/115	-
17	PQN	a	2001	-	-	6/23/43/43	0/2/2/2
16	CLA	a	1136	-	1/1/15/20	8/39/115/115	-
16	CLA	p	515	-	1/1/15/20	9/39/115/115	-
16	CLA	b	1214	-	1/1/13/20	12/27/103/115	-
19	BCR	W	603	-	-	8/29/63/63	0/2/2/2
19	BCR	r	602	-	-	11/29/63/63	0/2/2/2
16	CLA	B	1021	-	1/1/15/20	14/39/115/115	-
16	CLA	b	1210	-	1/1/15/20	15/39/115/115	-
16	CLA	Z	515	-	1/1/15/20	12/39/115/115	-
16	CLA	A	1129	-	1/1/12/20	5/21/97/115	-
16	CLA	G	1221	-	1/1/15/20	12/39/115/115	-
16	CLA	Y	514	-	1/1/12/20	6/21/97/115	-
16	CLA	b	1234	-	1/1/12/20	6/21/97/115	-
19	BCR	m	4021	-	-	7/29/63/63	0/2/2/2
16	CLA	A	1109	-	1/1/15/20	14/39/115/115	-
16	CLA	A	1107	-	1/1/12/20	3/21/97/115	-
16	CLA	Y	517	-	1/1/13/20	10/27/103/115	-
14	LMG	s	701	-	-	9/34/54/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	Y	515	-	1/1/15/20	10/39/115/115	-
16	CLA	q	503	-	1/1/11/20	11/17/93/115	-
16	CLA	b	1236	-	1/1/15/20	13/39/115/115	-
17	PQN	H	2001	-	-	6/23/43/43	0/2/2/2
16	CLA	X	505	-	1/1/15/20	15/39/115/115	-
14	LMG	b	848	-	-	18/38/58/70	0/1/1/1
16	CLA	q	510	-	1/1/14/20	5/33/109/115	-
16	CLA	r	511	-	1/1/15/20	10/39/115/115	-
16	CLA	W	511	-	1/1/15/20	14/39/115/115	-
16	CLA	B	1205	-	1/1/15/20	10/39/115/115	-
19	BCR	J	4012	-	-	10/29/63/63	0/2/2/2
16	CLA	q	508	-	1/1/13/20	10/27/103/115	-
16	CLA	W	506	-	1/1/14/20	15/33/109/115	-
19	BCR	x	604	-	-	11/29/63/63	0/2/2/2
19	BCR	B	4009	-	-	13/29/63/63	0/2/2/2
16	CLA	A	1123	-	1/1/15/20	11/39/115/115	-
16	CLA	A	1138	-	1/1/15/20	10/39/115/115	-
16	CLA	F	1301	-	1/1/11/20	4/15/91/115	-
16	CLA	X	508	-	1/1/13/20	11/27/103/115	-
16	CLA	y	501	-	1/1/11/20	9/17/93/115	-
19	BCR	U	4019	-	-	11/29/63/63	0/2/2/2
19	BCR	w	602	-	-	8/29/63/63	0/2/2/2
16	CLA	q	512	-	1/1/11/20	6/15/91/115	-
19	BCR	h	604	-	-	13/29/63/63	0/2/2/2
19	BCR	a	4011	-	-	15/29/63/63	0/2/2/2
16	CLA	w	510	-	1/1/14/20	4/33/109/115	-
16	CLA	q	514	-	1/1/12/20	5/21/97/115	-
16	CLA	h	507	-	1/1/15/20	10/39/115/115	-
19	BCR	q	602	-	-	8/29/63/63	0/2/2/2
16	CLA	a	1102	-	1/1/13/20	7/29/105/115	-
19	BCR	G	4009	-	-	13/29/63/63	0/2/2/2
16	CLA	u	512	-	1/1/11/20	6/15/91/115	-
16	CLA	u	510	-	1/1/15/20	15/39/115/115	-
16	CLA	H	1119	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	s	602	-	-	9/29/63/63	0/2/2/2
19	BCR	u	601	-	-	9/29/63/63	0/2/2/2
16	CLA	K	1401	-	1/1/11/20	3/15/91/115	-
16	CLA	A	1114	-	1/1/11/20	7/20/96/115	-
16	CLA	q	502	-	1/1/12/20	10/21/97/115	-
19	BCR	Q	4016	-	-	13/29/63/63	0/2/2/2
14	LMG	B	848	-	-	18/38/58/70	0/1/1/1
16	CLA	r	501	-	1/1/12/20	7/21/97/115	-
19	BCR	A	4007	-	-	7/29/63/63	0/2/2/2
16	CLA	W	501	-	1/1/12/20	8/21/97/115	-
16	CLA	F	1302	-	1/1/5/20	-	-
16	CLA	p	511	-	1/1/15/20	17/39/115/115	-
16	CLA	p	510	-	1/1/15/20	11/39/115/115	-
16	CLA	a	1114	-	1/1/11/20	7/20/96/115	-
19	BCR	x	603	-	-	9/29/63/63	0/2/2/2
16	CLA	G	1203	-	1/1/15/20	18/39/115/115	-
19	BCR	v	604	-	-	13/29/63/63	0/2/2/2
16	CLA	x	513	-	1/1/12/20	8/21/97/115	-
16	CLA	p	506	-	1/1/14/20	10/33/109/115	-
16	CLA	t	508	-	1/1/13/20	14/27/103/115	-
16	CLA	s	501	-	1/1/12/20	7/21/97/115	-
16	CLA	x	515	-	1/1/15/20	16/39/115/115	-
16	CLA	s	505	-	1/1/15/20	12/39/115/115	-
16	CLA	A	1120	-	1/1/11/20	11/20/96/115	-
16	CLA	l	1502	-	1/1/15/20	12/39/115/115	-
16	CLA	u	514	-	1/1/12/20	8/21/97/115	-
19	BCR	F	4016	-	-	13/29/63/63	0/2/2/2
16	CLA	u	505	-	1/1/15/20	13/39/115/115	-
16	CLA	G	1216	-	1/1/11/20	7/18/94/115	-
16	CLA	A	1124	-	1/1/15/20	10/39/115/115	-
16	CLA	y	509	-	1/1/14/20	7/33/109/115	-
16	CLA	g	502	-	1/1/12/20	6/21/97/115	-
19	BCR	G	4014	-	-	13/29/63/63	0/2/2/2
16	CLA	B	1215	-	1/1/14/20	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	1139	-	1/1/12/20	10/23/99/115	-
16	CLA	n	502	-	1/1/12/20	9/21/97/115	-
19	BCR	X	602	-	-	11/29/63/63	0/2/2/2
16	CLA	a	1134	-	1/1/11/20	11/15/91/115	-
16	CLA	y	514	-	1/1/12/20	7/21/97/115	-
16	CLA	p	513	-	1/1/12/20	6/21/97/115	-
16	CLA	p	503	-	1/1/11/20	10/17/93/115	-
16	CLA	w	512	-	1/1/11/20	6/15/91/115	-
16	CLA	G	1210	-	1/1/15/20	15/39/115/115	-
16	CLA	G	1223	-	1/1/15/20	14/39/115/115	-
16	CLA	B	1217	-	1/1/11/20	8/15/91/115	-
19	BCR	I	4020	-	-	14/29/63/63	0/2/2/2
17	PQN	B	2002	-	-	5/23/43/43	0/2/2/2
16	CLA	X	502	-	1/1/12/20	7/21/97/115	-
16	CLA	t	516	-	1/1/11/20	9/17/93/115	-
16	CLA	J	1303	-	1/1/8/20	2/4/76/115	-
16	CLA	G	1206	-	1/1/15/20	13/39/115/115	-
16	CLA	X	504	-	1/1/14/20	11/33/109/115	-
16	CLA	B	1202	-	1/1/15/20	13/39/115/115	-
16	CLA	t	507	-	1/1/14/20	14/33/109/115	-
19	BCR	l	4019	-	-	11/29/63/63	0/2/2/2
16	CLA	B	1209	-	1/1/11/20	8/15/91/115	-
16	CLA	X	511	-	1/1/15/20	13/39/115/115	-
16	CLA	A	1125	-	1/1/15/20	10/39/115/115	-
16	CLA	v	515	-	1/1/14/20	9/33/109/115	-
14	LMG	H	4101	-	-	17/41/61/70	0/1/1/1
19	BCR	a	4003	-	-	11/29/63/63	0/2/2/2
16	CLA	s	513	-	1/1/12/20	6/21/97/115	-
16	CLA	w	514	-	1/1/12/20	6/21/97/115	-
19	BCR	o	604	-	-	14/29/63/63	0/2/2/2
19	BCR	p	601	-	-	12/29/63/63	0/2/2/2
16	CLA	r	512	-	1/1/11/20	6/15/91/115	-
19	BCR	h	602	-	-	11/29/63/63	0/2/2/2
16	CLA	b	1222	-	1/1/13/20	7/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	r	514	-	1/1/12/20	9/21/97/115	-
16	CLA	v	514	-	1/1/12/20	7/21/97/115	-
16	CLA	A	1119	-	1/1/15/20	17/39/115/115	-
16	CLA	H	1121	-	1/1/12/20	13/23/99/115	-
16	CLA	W	516	-	1/1/11/20	9/17/93/115	-
16	CLA	b	1216	-	1/1/11/20	7/18/94/115	-
16	CLA	g	508	-	1/1/13/20	8/27/103/115	-
16	CLA	n	514	-	1/1/12/20	9/21/97/115	-
16	CLA	H	1123	-	1/1/15/20	11/39/115/115	-
19	BCR	j	4013	-	-	11/29/63/63	0/2/2/2
19	BCR	y	602	-	-	13/29/63/63	0/2/2/2
16	CLA	A	1131	-	1/1/15/20	11/39/115/115	-
16	CLA	r	502	-	1/1/12/20	8/21/97/115	-
16	CLA	b	1207	-	1/1/15/20	23/39/115/115	-
16	CLA	G	1205	-	1/1/15/20	10/39/115/115	-
19	BCR	Z	602	-	-	9/29/63/63	0/2/2/2
19	BCR	T	1501	-	-	10/29/63/63	0/2/2/2
17	PQN	G	2002	-	-	5/23/43/43	0/2/2/2
16	CLA	j	1302	-	1/1/11/20	8/15/91/115	-
16	CLA	a	1115	-	1/1/12/20	7/26/102/115	-
16	CLA	A	1139	-	1/1/12/20	10/23/99/115	-
16	CLA	A	1137	-	1/1/11/20	8/18/94/115	-
16	CLA	g	516	-	1/1/11/20	7/17/93/115	-
19	BCR	o	603	-	-	12/29/63/63	0/2/2/2
16	CLA	A	1115	-	1/1/12/20	7/26/102/115	-
16	CLA	o	513	-	1/1/12/20	9/21/97/115	-
16	CLA	u	506	-	1/1/14/20	10/33/109/115	-
16	CLA	y	516	-	1/1/11/20	6/17/93/115	-
19	BCR	G	4010	-	-	12/29/63/63	0/2/2/2
16	CLA	y	507	-	1/1/15/20	11/39/115/115	-
19	BCR	j	4015	-	-	11/29/63/63	0/2/2/2
16	CLA	u	517	-	1/1/13/20	10/27/103/115	-
16	CLA	a	1137	-	1/1/11/20	8/18/94/115	-
14	LMG	p	701	-	-	10/34/54/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	1221	-	1/1/15/20	12/39/115/115	-
19	BCR	V	4021	-	-	7/29/63/63	0/2/2/2
16	CLA	G	1240	-	1/1/12/20	4/21/97/115	-
16	CLA	H	1104	-	1/1/15/20	9/39/115/115	-
16	CLA	B	1023	-	1/1/15/20	18/39/115/115	-
16	CLA	x	510	-	1/1/13/20	12/27/103/115	-
16	CLA	W	503	-	1/1/11/20	9/17/93/115	-
19	BCR	k	1501	-	-	10/29/63/63	0/2/2/2
16	CLA	S	1302	-	1/1/11/20	8/15/91/115	-
13	LHG	A	851	-	-	11/31/31/53	-
16	CLA	X	516	-	1/1/11/20	10/17/93/115	-
16	CLA	b	1232	-	1/1/11/20	6/15/91/115	-
16	CLA	B	1236	-	1/1/15/20	13/39/115/115	-
16	CLA	Z	505	-	1/1/15/20	18/39/115/115	-
16	CLA	o	506	-	1/1/14/20	10/33/109/115	-
19	BCR	b	4004	-	-	9/29/63/63	0/2/2/2
16	CLA	W	502	-	1/1/12/20	8/21/97/115	-
16	CLA	H	1129	-	1/1/12/20	5/21/97/115	-
19	BCR	R	4020	-	-	14/29/63/63	0/2/2/2
16	CLA	r	516	-	1/1/11/20	8/17/93/115	-
16	CLA	B	1203	-	1/1/15/20	18/39/115/115	-
16	CLA	Y	505	-	1/1/15/20	16/39/115/115	-
16	CLA	H	1103	-	1/1/15/20	15/39/115/115	-
16	CLA	a	1105	-	1/1/13/20	9/31/107/115	-
16	CLA	x	503	-	1/1/11/20	10/17/93/115	-
19	BCR	Y	604	-	-	11/29/63/63	0/2/2/2
16	CLA	g	509	-	1/1/14/20	10/33/109/115	-
16	CLA	X	513	-	1/1/12/20	9/21/97/115	-
16	CLA	a	1106	-	1/1/15/20	19/39/115/115	-
16	CLA	v	510	-	1/1/14/20	14/33/109/115	-
16	CLA	Z	510	-	1/1/14/20	11/33/109/115	-
16	CLA	H	1109	-	1/1/15/20	14/39/115/115	-
19	BCR	M	4021	-	-	7/29/63/63	0/2/2/2
16	CLA	H	1128	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	1138	-	1/1/15/20	10/39/115/115	-
16	CLA	B	1223	-	1/1/15/20	14/39/115/115	-
16	CLA	B	1238	-	1/1/15/20	12/39/115/115	-
16	CLA	v	512	-	1/1/11/20	6/15/91/115	-
19	BCR	v	603	-	-	13/29/63/63	0/2/2/2
16	CLA	b	1224	-	1/1/14/20	20/33/109/115	-
13	LHG	H	851	-	-	11/31/31/53	-
19	BCR	J	4013	-	-	11/29/63/63	0/2/2/2
15	CL0	a	1011	-	3/3/20/25	12/37/135/135	-
16	CLA	q	511	-	1/1/15/20	12/39/115/115	-
16	CLA	x	514	-	1/1/12/20	10/21/97/115	-
16	CLA	A	1108	-	1/1/11/20	7/15/91/115	-
16	CLA	B	1230	-	1/1/11/20	4/15/91/115	-
16	CLA	n	509	-	1/1/14/20	11/33/109/115	-
16	CLA	Y	501	-	1/1/12/20	9/21/97/115	-
19	BCR	v	601	-	-	12/29/63/63	0/2/2/2
16	CLA	t	510	-	1/1/15/20	5/39/115/115	-
16	CLA	W	513	-	1/1/12/20	8/21/97/115	-
16	CLA	Z	516	-	1/1/11/20	8/17/93/115	-
16	CLA	W	508	-	1/1/13/20	14/27/103/115	-
16	CLA	r	508	-	1/1/13/20	11/27/103/115	-
16	CLA	B	1201	-	1/1/12/20	8/26/102/115	-
16	CLA	p	516	-	1/1/11/20	8/17/93/115	-
16	CLA	v	513	-	1/1/12/20	5/21/97/115	-
13	LHG	a	849	-	-	11/47/47/53	-
19	BCR	B	4017	-	-	9/29/63/63	0/2/2/2
16	CLA	x	512	-	1/1/11/20	6/15/91/115	-
16	CLA	a	1111	-	1/1/13/20	11/27/103/115	-
16	CLA	A	1105	-	1/1/13/20	9/31/107/115	-
16	CLA	v	502	-	1/1/12/20	6/21/97/115	-
16	CLA	W	509	-	1/1/14/20	10/33/109/115	-
19	BCR	y	601	-	-	11/29/63/63	0/2/2/2
19	BCR	x	602	-	-	13/29/63/63	0/2/2/2
16	CLA	G	1229	-	1/1/13/20	11/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	q	506	-	1/1/14/20	7/33/109/115	-
16	CLA	b	1205	-	1/1/15/20	10/39/115/115	-
16	CLA	t	514	-	1/1/12/20	9/21/97/115	-
16	CLA	b	1203	-	1/1/15/20	18/39/115/115	-
16	CLA	y	502	-	1/1/12/20	7/21/97/115	-
16	CLA	n	504	-	1/1/14/20	11/33/109/115	-
16	CLA	H	1108	-	1/1/11/20	7/15/91/115	-
16	CLA	u	507	-	1/1/15/20	14/39/115/115	-
16	CLA	a	1104	-	1/1/15/20	9/39/115/115	-
16	CLA	u	511	-	1/1/15/20	12/39/115/115	-
16	CLA	Q	1302	-	1/1/5/20	-	-
16	CLA	x	502	-	1/1/12/20	5/21/97/115	-
16	CLA	s	508	-	1/1/13/20	10/27/103/115	-
19	BCR	j	4012	-	-	10/29/63/63	0/2/2/2
16	CLA	b	1213	-	1/1/13/20	7/27/103/115	-
16	CLA	r	506	-	1/1/14/20	14/33/109/115	-
16	CLA	Y	510	-	1/1/15/20	11/39/115/115	-
16	CLA	G	1217	-	1/1/11/20	8/15/91/115	-
19	BCR	H	4008	-	-	12/29/63/63	0/2/2/2
16	CLA	q	501	-	1/1/12/20	6/21/97/115	-
16	CLA	G	1208	-	1/1/11/20	4/15/91/115	-
16	CLA	t	502	-	1/1/12/20	9/21/97/115	-
16	CLA	h	510	-	1/1/14/20	15/33/109/115	-
16	CLA	b	1215	-	1/1/14/20	15/33/109/115	-
16	CLA	A	1135	-	1/1/12/20	9/23/99/115	-
16	CLA	G	1209	-	1/1/11/20	8/15/91/115	-
16	CLA	B	1212	-	1/1/11/20	6/15/91/115	-
19	BCR	G	4005	-	-	7/29/63/63	0/2/2/2
13	LHG	H	849	-	-	11/47/47/53	-
16	CLA	b	1219	-	1/1/11/20	7/15/91/115	-
16	CLA	A	1103	-	1/1/15/20	15/39/115/115	-
16	CLA	B	1234	-	1/1/12/20	6/21/97/115	-
18	SF4	N	101	3	-	-	0/6/5/5
16	CLA	w	504	-	1/1/14/20	8/33/109/115	-
18	SF4	H	3001	2,1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	v	602	-	-	10/29/63/63	0/2/2/2
19	BCR	p	604	-	-	9/29/63/63	0/2/2/2
16	CLA	Z	514	-	1/1/12/20	6/21/97/115	-
16	CLA	B	1204	-	1/1/15/20	10/39/115/115	-
16	CLA	G	1228	-	1/1/13/20	8/27/103/115	-
16	CLA	w	515	-	1/1/15/20	12/39/115/115	-
16	CLA	Z	502	-	1/1/12/20	8/21/97/115	-
16	CLA	b	1208	-	1/1/11/20	4/15/91/115	-
16	CLA	a	1109	-	1/1/15/20	14/39/115/115	-
16	CLA	B	1222	-	1/1/13/20	7/27/103/115	-
16	CLA	b	1238	-	1/1/15/20	12/39/115/115	-
16	CLA	s	509	-	1/1/14/20	15/33/109/115	-
16	CLA	a	1117	-	1/1/15/20	14/39/115/115	-
19	BCR	p	602	-	-	10/29/63/63	0/2/2/2
16	CLA	a	1128	-	1/1/15/20	11/39/115/115	-
16	CLA	X	506	-	1/1/14/20	10/33/109/115	-
16	CLA	u	515	-	1/1/15/20	10/39/115/115	-
16	CLA	b	1235	-	1/1/14/20	12/36/112/115	-
16	CLA	n	516	-	1/1/11/20	10/17/93/115	-
16	CLA	B	1213	-	1/1/13/20	7/27/103/115	-
16	CLA	n	501	-	1/1/12/20	9/21/97/115	-
16	CLA	B	1206	-	1/1/15/20	13/39/115/115	-
16	CLA	r	509	-	1/1/14/20	9/33/109/115	-
16	CLA	H	1402	-	1/1/9/20	2/9/81/115	-
16	CLA	G	1225	-	1/1/15/20	14/39/115/115	-
16	CLA	r	504	-	1/1/14/20	15/33/109/115	-
16	CLA	h	502	-	1/1/12/20	6/21/97/115	-
18	SF4	a	3001	2,1	-	-	0/6/5/5
16	CLA	A	1132	-	1/1/15/20	11/39/115/115	-
16	CLA	G	1201	-	1/1/12/20	8/26/102/115	-
16	CLA	X	510	-	1/1/15/20	16/39/115/115	-
16	CLA	g	504	-	1/1/14/20	12/33/109/115	-
19	BCR	f	4016	-	-	13/29/63/63	0/2/2/2
16	CLA	B	1207	-	1/1/15/20	23/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	g	514	-	1/1/12/20	10/21/97/115	-
16	CLA	q	517	-	1/1/13/20	7/27/103/115	-
16	CLA	X	501	-	1/1/12/20	9/21/97/115	-
14	LMG	A	852	-	-	17/33/53/70	0/1/1/1
16	CLA	H	1122	-	1/1/13/20	12/32/108/115	-
16	CLA	B	1226	-	1/1/15/20	9/39/115/115	-
16	CLA	u	516	-	1/1/11/20	10/17/93/115	-
16	CLA	H	1140	-	1/1/15/20	21/39/115/115	-
16	CLA	a	1124	-	1/1/15/20	10/39/115/115	-
16	CLA	n	508	-	1/1/13/20	14/27/103/115	-
16	CLA	o	515	-	1/1/15/20	9/39/115/115	-
16	CLA	G	1224	-	1/1/14/20	20/33/109/115	-
16	CLA	n	505	-	1/1/15/20	13/39/115/115	-
19	BCR	Y	601	-	-	12/29/63/63	0/2/2/2
19	BCR	x	601	-	-	18/29/63/63	0/2/2/2
16	CLA	A	1133	-	1/1/12/20	11/26/102/115	-
19	BCR	u	603	-	-	11/29/63/63	0/2/2/2
16	CLA	J	1302	-	1/1/11/20	8/15/91/115	-
16	CLA	y	508	-	1/1/13/20	10/27/103/115	-
16	CLA	a	1140	-	1/1/15/20	21/39/115/115	-
19	BCR	A	4008	-	-	12/29/63/63	0/2/2/2
18	SF4	C	101	3	-	-	0/6/5/5
16	CLA	B	1214	-	1/1/13/20	12/27/103/115	-
16	CLA	n	517	-	1/1/13/20	13/27/103/115	-
16	CLA	b	1239	-	1/1/15/20	17/39/115/115	-
16	CLA	v	504	-	1/1/14/20	14/33/109/115	-
16	CLA	b	1202	-	1/1/15/20	13/39/115/115	-
16	CLA	w	511	-	1/1/15/20	11/39/115/115	-
16	CLA	v	507	-	1/1/15/20	10/39/115/115	-
16	CLA	A	1128	-	1/1/15/20	11/39/115/115	-
16	CLA	s	510	-	1/1/15/20	15/39/115/115	-
16	CLA	a	1126	-	1/1/15/20	15/39/115/115	-
19	BCR	a	4008	-	-	12/29/63/63	0/2/2/2
16	CLA	w	505	-	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	o	512	-	1/1/11/20	6/15/91/115	-
19	BCR	g	604	-	-	10/29/63/63	0/2/2/2
16	CLA	t	513	-	1/1/12/20	8/21/97/115	-
18	SF4	A	3001	2,1	-	-	0/6/5/5
16	CLA	A	1402	-	1/1/9/20	2/9/81/115	-
16	CLA	s	504	-	1/1/14/20	16/33/109/115	-
14	LMG	Y	701	-	-	9/34/54/70	0/1/1/1
19	BCR	g	603	-	-	8/29/63/63	0/2/2/2
16	CLA	X	517	-	1/1/13/20	9/27/103/115	-
16	CLA	b	1221	-	1/1/15/20	12/39/115/115	-
19	BCR	o	601	-	-	8/29/63/63	0/2/2/2
16	CLA	y	517	-	1/1/13/20	10/27/103/115	-
16	CLA	t	515	-	1/1/15/20	17/39/115/115	-
16	CLA	o	508	-	1/1/13/20	11/27/103/115	-
16	CLA	g	511	-	1/1/15/20	13/39/115/115	-
16	CLA	U	1503	-	1/1/15/20	15/39/115/115	-
19	BCR	w	603	-	-	9/29/63/63	0/2/2/2
16	CLA	y	504	-	1/1/14/20	13/33/109/115	-
16	CLA	w	513	-	1/1/12/20	11/21/97/115	-
16	CLA	y	511	-	1/1/15/20	15/39/115/115	-
16	CLA	b	1226	-	1/1/15/20	9/39/115/115	-
18	SF4	c	101	3	-	-	0/6/5/5
16	CLA	w	501	-	1/1/12/20	6/21/97/115	-
16	CLA	v	508	-	1/1/13/20	9/27/103/115	-
19	BCR	n	603	-	-	8/29/63/63	0/2/2/2
16	CLA	o	503	-	1/1/11/20	8/17/93/115	-
16	CLA	q	516	-	1/1/11/20	8/17/93/115	-
19	BCR	G	4017	-	-	9/29/63/63	0/2/2/2
16	CLA	G	1234	-	1/1/12/20	6/21/97/115	-
19	BCR	r	603	-	-	7/29/63/63	0/2/2/2
16	CLA	B	1232	-	1/1/11/20	6/15/91/115	-
16	CLA	r	513	-	1/1/12/20	8/21/97/115	-
16	CLA	B	1220	-	1/1/12/20	5/26/102/115	-
19	BCR	q	604	-	-	17/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LHG	I	103	-	-	21/48/48/53	-
16	CLA	q	507	-	1/1/15/20	13/39/115/115	-
16	CLA	W	515	-	1/1/15/20	16/39/115/115	-
14	LMG	A	4101	-	-	17/41/61/70	0/1/1/1
16	CLA	a	1127	-	1/1/15/20	9/39/115/115	-
19	BCR	u	604	-	-	11/29/63/63	0/2/2/2
16	CLA	L	1502	-	1/1/15/20	12/39/115/115	-
16	CLA	o	507	-	1/1/15/20	13/39/115/115	-
13	LHG	a	851	-	-	11/31/31/53	-
16	CLA	u	503	-	1/1/11/20	8/17/93/115	-
19	BCR	S	4015	-	-	11/29/63/63	0/2/2/2
16	CLA	A	1126	-	1/1/15/20	15/39/115/115	-
16	CLA	g	501	-	1/1/12/20	11/21/97/115	-
16	CLA	H	1237	-	1/1/15/20	15/39/115/115	-
16	CLA	x	505	-	1/1/11/20	10/17/93/115	-
16	CLA	a	1123	-	1/1/15/20	11/39/115/115	-
19	BCR	L	4022	-	-	9/29/63/63	0/2/2/2
19	BCR	I	4018	-	-	14/29/63/63	0/2/2/2
19	BCR	A	4002	-	-	8/29/63/63	0/2/2/2
16	CLA	g	507	-	1/1/15/20	16/39/115/115	-
16	CLA	v	506	-	1/1/14/20	10/33/109/115	-
16	CLA	p	514	-	1/1/12/20	5/21/97/115	-
16	CLA	G	1021	-	1/1/15/20	14/39/115/115	-
16	CLA	B	1012	-	1/1/14/20	16/33/109/115	-
16	CLA	y	510	-	1/1/14/20	13/33/109/115	-
16	CLA	p	502	-	1/1/12/20	6/21/97/115	-
16	CLA	H	1118	-	1/1/13/20	6/27/103/115	-
19	BCR	A	4001	-	-	12/29/63/63	0/2/2/2
19	BCR	Y	603	-	-	8/29/63/63	0/2/2/2
16	CLA	t	505	-	1/1/15/20	17/39/115/115	-
19	BCR	a	4001	-	-	12/29/63/63	0/2/2/2
16	CLA	A	1136	-	1/1/15/20	8/39/115/115	-
16	CLA	o	517	-	1/1/13/20	12/27/103/115	-
14	LMG	H	852	-	-	17/33/53/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	Y	504	-	1/1/14/20	14/33/109/115	-
16	CLA	q	515	-	1/1/15/20	11/39/115/115	-
16	CLA	a	1131	-	1/1/15/20	11/39/115/115	-
16	CLA	B	1227	-	1/1/11/20	9/20/96/115	-
17	PQN	b	2002	-	-	5/23/43/43	0/2/2/2
19	BCR	X	604	-	-	14/29/63/63	0/2/2/2
16	CLA	Z	504	-	1/1/14/20	8/33/109/115	-
19	BCR	i	4020	-	-	14/29/63/63	0/2/2/2
16	CLA	G	1202	-	1/1/15/20	13/39/115/115	-
13	LHG	i	103	-	-	21/48/48/53	-
16	CLA	X	507	-	1/1/15/20	13/39/115/115	-
16	CLA	h	508	-	1/1/13/20	7/27/103/115	-
19	BCR	s	603	-	-	7/29/63/63	0/2/2/2
16	CLA	a	1022	-	1/1/15/20	9/39/115/115	-
19	BCR	b	4005	-	-	7/29/63/63	0/2/2/2
16	CLA	H	1126	-	1/1/15/20	15/39/115/115	-
16	CLA	s	517	-	1/1/13/20	10/27/103/115	-
19	BCR	G	4004	-	-	9/29/63/63	0/2/2/2
16	CLA	b	1240	-	1/1/12/20	4/21/97/115	-
16	CLA	B	1208	-	1/1/11/20	4/15/91/115	-
14	LMG	a	4101	-	-	17/41/61/70	0/1/1/1
16	CLA	a	1118	-	1/1/13/20	6/27/103/115	-
16	CLA	s	514	-	1/1/12/20	5/21/97/115	-
16	CLA	v	503	-	1/1/11/20	11/17/93/115	-
16	CLA	A	1127	-	1/1/15/20	10/39/115/115	-
16	CLA	y	506	-	1/1/14/20	10/33/109/115	-
19	BCR	o	602	-	-	11/29/63/63	0/2/2/2
16	CLA	x	501	-	1/1/12/20	7/21/97/115	-
16	CLA	A	1022	-	1/1/15/20	9/39/115/115	-
16	CLA	B	1235	-	1/1/14/20	12/36/112/115	-
16	CLA	g	517	-	1/1/13/20	12/27/103/115	-
16	CLA	b	1228	-	1/1/13/20	8/27/103/115	-
16	CLA	h	514	-	1/1/12/20	5/21/97/115	-
16	CLA	H	1111	-	1/1/13/20	11/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	w	502	-	1/1/12/20	8/21/97/115	-
16	CLA	y	513	-	1/1/12/20	4/21/97/115	-
16	CLA	j	1303	-	1/1/8/20	2/4/76/115	-
16	CLA	H	1135	-	1/1/12/20	9/23/99/115	-
16	CLA	h	516	-	1/1/11/20	8/17/93/115	-
16	CLA	G	1212	-	1/1/11/20	6/15/91/115	-
16	CLA	t	501	-	1/1/12/20	9/21/97/115	-
19	BCR	U	4022	-	-	9/29/63/63	0/2/2/2
16	CLA	a	1237	-	1/1/15/20	15/39/115/115	-
16	CLA	n	507	-	1/1/14/20	13/33/109/115	-
16	CLA	G	1211	-	1/1/15/20	9/39/115/115	-
16	CLA	B	1216	-	1/1/11/20	7/18/94/115	-
16	CLA	b	1225	-	1/1/15/20	14/39/115/115	-
16	CLA	p	508	-	1/1/13/20	11/27/103/115	-
13	LHG	R	103	-	-	21/48/48/53	-
19	BCR	r	604	-	-	11/29/63/63	0/2/2/2
16	CLA	s	506	-	1/1/14/20	13/33/109/115	-
16	CLA	r	507	-	1/1/15/20	16/39/115/115	-
16	CLA	H	1136	-	1/1/15/20	8/39/115/115	-
19	BCR	X	603	-	-	12/29/63/63	0/2/2/2
16	CLA	a	1110	-	1/1/12/20	6/26/102/115	-
16	CLA	a	1108	-	1/1/11/20	7/15/91/115	-
16	CLA	a	1135	-	1/1/12/20	9/23/99/115	-
16	CLA	G	1231	-	1/1/11/20	4/15/91/115	-
16	CLA	X	515	-	1/1/15/20	11/39/115/115	-
16	CLA	Z	501	-	1/1/12/20	7/21/97/115	-
14	LMG	H	4201	-	-	8/27/47/70	0/1/1/1
19	BCR	b	4006	-	-	5/18/35/63	0/1/1/2
16	CLA	b	1223	-	1/1/15/20	14/39/115/115	-
16	CLA	b	1218	-	1/1/13/20	8/27/103/115	-
16	CLA	G	1213	-	1/1/13/20	7/27/103/115	-
16	CLA	q	509	-	1/1/13/20	11/29/105/115	-
19	BCR	B	4010	-	-	12/29/63/63	0/2/2/2
16	CLA	W	512	-	1/1/11/20	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMT	U	4101	-	-	7/21/61/61	0/2/2/2
16	CLA	v	501	-	1/1/11/20	9/17/93/115	-
16	CLA	a	1113	-	1/1/11/20	5/15/91/115	-
16	CLA	a	1119	-	1/1/15/20	17/39/115/115	-
19	BCR	b	4009	-	-	13/29/63/63	0/2/2/2
16	CLA	W	514	-	1/1/12/20	9/21/97/115	-
16	CLA	x	517	-	1/1/13/20	12/27/103/115	-
16	CLA	H	1133	-	1/1/12/20	11/26/102/115	-
16	CLA	A	1118	-	1/1/13/20	6/27/103/115	-
16	CLA	a	1116	-	1/1/12/20	10/26/102/115	-
16	CLA	G	1220	-	1/1/12/20	5/26/102/115	-
16	CLA	b	1201	-	1/1/12/20	8/26/102/115	-
16	CLA	w	516	-	1/1/11/20	8/17/93/115	-
19	BCR	t	601	-	-	13/29/63/63	0/2/2/2
16	CLA	s	516	-	1/1/11/20	9/17/93/115	-
16	CLA	r	517	-	1/1/13/20	9/27/103/115	-
19	BCR	h	603	-	-	14/29/63/63	0/2/2/2
16	CLA	W	517	-	1/1/13/20	13/27/103/115	-
19	BCR	w	604	-	-	15/29/63/63	0/2/2/2
16	CLA	B	1225	-	1/1/15/20	14/39/115/115	-
16	CLA	a	1130	-	1/1/15/20	6/39/115/115	-
16	CLA	B	1228	-	1/1/13/20	8/27/103/115	-
19	BCR	A	4003	-	-	11/29/63/63	0/2/2/2
19	BCR	s	604	-	-	8/29/63/63	0/2/2/2
16	CLA	Y	511	-	1/1/15/20	17/39/115/115	-
16	CLA	x	507	-	1/1/15/20	15/39/115/115	-
16	CLA	o	510	-	1/1/15/20	14/39/115/115	-
16	CLA	b	1229	-	1/1/13/20	11/31/107/115	-
16	CLA	r	515	-	1/1/15/20	13/39/115/115	-
20	LMT	l	4101	-	-	7/21/61/61	0/2/2/2
16	CLA	B	1211	-	1/1/15/20	9/39/115/115	-
16	CLA	p	512	-	1/1/11/20	7/15/91/115	-
16	CLA	h	511	-	1/1/15/20	16/39/115/115	-
16	CLA	Y	506	-	1/1/14/20	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	1137	-	1/1/11/20	8/18/94/115	-
19	BCR	i	4018	-	-	14/29/63/63	0/2/2/2
19	BCR	B	4004	-	-	9/29/63/63	0/2/2/2
19	BCR	y	603	-	-	10/29/63/63	0/2/2/2
16	CLA	r	503	-	1/1/11/20	10/17/93/115	-
16	CLA	G	1235	-	1/1/14/20	12/36/112/115	-
16	CLA	A	1102	-	1/1/13/20	7/29/105/115	-
19	BCR	Z	603	-	-	10/29/63/63	0/2/2/2
16	CLA	A	1134	-	1/1/11/20	11/15/91/115	-
16	CLA	Z	513	-	1/1/12/20	12/21/97/115	-
16	CLA	g	503	-	1/1/11/20	10/17/93/115	-
16	CLA	Z	517	-	1/1/13/20	8/27/103/115	-
16	CLA	G	1218	-	1/1/13/20	8/27/103/115	-
16	CLA	s	507	-	1/1/15/20	11/39/115/115	-
15	CL0	A	1011	-	3/3/20/25	12/37/135/135	-
14	LMG	a	852	-	-	17/33/53/70	0/1/1/1
16	CLA	p	509	-	1/1/14/20	13/33/109/115	-
16	CLA	g	510	-	1/1/13/20	10/27/103/115	-
16	CLA	G	1230	-	1/1/11/20	4/15/91/115	-
16	CLA	G	1023	-	1/1/15/20	18/39/115/115	-
16	CLA	Y	513	-	1/1/12/20	6/21/97/115	-
16	CLA	s	515	-	1/1/15/20	9/39/115/115	-
16	CLA	a	1138	-	1/1/15/20	10/39/115/115	-
16	CLA	G	1012	-	1/1/14/20	16/33/109/115	-
19	BCR	b	4014	-	-	13/29/63/63	0/2/2/2
19	BCR	l	4022	-	-	9/29/63/63	0/2/2/2
16	CLA	o	509	-	1/1/14/20	10/33/109/115	-
16	CLA	H	1105	-	1/1/13/20	9/31/107/115	-
16	CLA	b	1204	-	1/1/15/20	10/39/115/115	-
16	CLA	q	513	-	1/1/12/20	11/21/97/115	-
16	CLA	a	1132	-	1/1/15/20	11/39/115/115	-
16	CLA	Y	512	-	1/1/11/20	7/15/91/115	-
16	CLA	a	1101	-	1/1/15/20	15/39/115/115	-
16	CLA	w	509	-	1/1/13/20	14/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	g	512	-	1/1/11/20	6/15/91/115	-
16	CLA	a	1107	-	1/1/12/20	3/21/97/115	-
16	CLA	H	1120	-	1/1/11/20	11/20/96/115	-
16	CLA	v	511	-	1/1/15/20	16/39/115/115	-
16	CLA	u	513	-	1/1/12/20	9/21/97/115	-
19	BCR	g	602	-	-	10/29/63/63	0/2/2/2
16	CLA	b	1209	-	1/1/11/20	8/15/91/115	-
16	CLA	b	1023	-	1/1/15/20	18/39/115/115	-
19	BCR	g	601	-	-	16/29/63/63	0/2/2/2
16	CLA	u	509	-	1/1/14/20	10/33/109/115	-
14	LMG	a	4201	-	-	7/26/46/70	0/1/1/1
16	CLA	n	511	-	1/1/15/20	14/39/115/115	-
16	CLA	L	1501	-	1/1/15/20	19/39/115/115	-
16	CLA	r	505	-	1/1/11/20	10/17/93/115	-
16	CLA	W	505	-	1/1/15/20	18/39/115/115	-
16	CLA	g	513	-	1/1/12/20	8/21/97/115	-
16	CLA	A	1117	-	1/1/15/20	14/39/115/115	-
16	CLA	b	1211	-	1/1/15/20	9/39/115/115	-
16	CLA	w	506	-	1/1/14/20	8/33/109/115	-
19	BCR	H	4001	-	-	12/29/63/63	0/2/2/2
18	SF4	N	102	3	-	-	0/6/5/5
16	CLA	H	1110	-	1/1/12/20	6/26/102/115	-
16	CLA	x	516	-	1/1/11/20	9/17/93/115	-
19	BCR	y	604	-	-	12/29/63/63	0/2/2/2
16	CLA	n	512	-	1/1/11/20	8/15/91/115	-
16	CLA	w	508	-	1/1/13/20	10/27/103/115	-
19	BCR	B	4014	-	-	13/29/63/63	0/2/2/2
16	CLA	p	504	-	1/1/14/20	16/33/109/115	-
16	CLA	n	510	-	1/1/15/20	13/39/115/115	-
19	BCR	G	4006	-	-	5/18/35/63	0/1/1/2
16	CLA	A	1122	-	1/1/13/20	12/32/108/115	-

The worst 5 of 5486 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	1011	CL0	C1B-C2B	7.74	1.48	1.39
15	A	1011	CL0	C1B-C2B	7.72	1.48	1.39
15	a	1011	CL0	C1B-C2B	7.70	1.48	1.39
15	H	1011	CL0	C3B-C4B	7.66	1.48	1.41
15	a	1011	CL0	C3B-C4B	7.63	1.48	1.41

The worst 5 of 5458 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	1021	CLA	C4A-NA-C1A	9.27	110.91	106.68
16	b	1021	CLA	C4A-NA-C1A	9.25	110.90	106.68
16	B	1021	CLA	C4A-NA-C1A	9.24	110.89	106.68
16	G	1205	CLA	C4A-NA-C1A	8.44	110.53	106.68
16	b	1205	CLA	C4A-NA-C1A	8.41	110.52	106.68

5 of 597 chirality outliers are listed below:

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

5 of 7890 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.

607 monomers are involved in 1204 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	r	510	CLA	1	0
16	H	1101	CLA	5	0
19	q	603	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	H	1130	CLA	5	0
16	A	1106	CLA	3	0
16	B	1210	CLA	6	0
16	n	513	CLA	1	0
16	p	505	CLA	2	0
16	w	503	CLA	1	0
16	l	1503	CLA	4	0
16	a	1133	CLA	1	0
16	A	1112	CLA	1	0
16	A	1101	CLA	4	0
16	U	1502	CLA	4	0
16	B	1240	CLA	2	0
16	b	1227	CLA	2	0
16	H	1131	CLA	5	0
16	H	1102	CLA	1	0
19	H	4002	BCR	1	0
16	Z	507	CLA	2	0
19	J	4015	BCR	4	0
19	S	4012	BCR	2	0
14	A	4201	LMG	2	0
16	v	516	CLA	2	0
16	t	517	CLA	1	0
16	h	504	CLA	2	0
19	K	1501	BCR	2	0
16	H	1127	CLA	5	0
16	a	1120	CLA	1	0
16	W	510	CLA	2	0
16	H	1022	CLA	4	0
16	u	508	CLA	1	0
16	G	1226	CLA	1	0
16	t	509	CLA	2	0
19	r	601	BCR	2	0
16	G	1238	CLA	6	0
19	W	601	BCR	3	0
16	g	506	CLA	4	0
16	X	514	CLA	1	0
16	b	1012	CLA	3	0
16	b	1021	CLA	6	0
19	n	601	BCR	2	0
16	G	1204	CLA	2	0
16	G	1214	CLA	2	0
16	G	1219	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	x	506	CLA	1	0
16	o	504	CLA	2	0
16	f	1301	CLA	2	0
13	A	849	LHG	1	0
14	G	848	LMG	2	0
16	h	506	CLA	5	0
16	G	1207	CLA	4	0
16	H	1013	CLA	5	0
16	G	1232	CLA	1	0
16	b	1231	CLA	1	0
16	Q	1301	CLA	2	0
16	W	504	CLA	1	0
16	v	517	CLA	2	0
16	b	1220	CLA	2	0
16	v	505	CLA	1	0
16	n	515	CLA	7	0
16	v	509	CLA	1	0
16	a	1125	CLA	1	0
16	x	511	CLA	2	0
16	t	512	CLA	1	0
19	p	603	BCR	3	0
19	w	601	BCR	4	0
16	Y	516	CLA	2	0
16	g	515	CLA	3	0
16	a	1013	CLA	3	0
19	b	4017	BCR	4	0
16	B	1229	CLA	2	0
16	Y	507	CLA	4	0
16	H	1106	CLA	4	0
19	q	601	BCR	5	0
16	b	1206	CLA	3	0
16	H	1116	CLA	4	0
16	h	503	CLA	1	0
16	x	509	CLA	1	0
16	H	1107	CLA	1	0
16	b	1217	CLA	1	0
19	H	4003	BCR	1	0
19	a	4002	BCR	1	0
19	s	601	BCR	1	0
16	t	511	CLA	4	0
16	H	1113	CLA	1	0
15	H	1011	CL0	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	a	1139	CLA	1	0
16	t	506	CLA	1	0
19	S	4013	BCR	1	0
19	H	4011	BCR	4	0
16	s	502	CLA	3	0
16	U	1501	CLA	3	0
16	h	512	CLA	1	0
16	w	517	CLA	1	0
19	b	4010	BCR	2	0
19	u	602	BCR	1	0
16	H	1134	CLA	1	0
19	B	4005	BCR	2	0
16	X	503	CLA	3	0
16	B	1231	CLA	1	0
16	x	508	CLA	1	0
16	b	1230	CLA	5	0
16	Z	509	CLA	2	0
19	h	601	BCR	1	0
19	a	4007	BCR	3	0
16	A	1140	CLA	4	0
16	G	1239	CLA	3	0
18	c	102	SF4	1	0
16	W	507	CLA	3	0
16	o	505	CLA	4	0
16	h	513	CLA	1	0
16	h	517	CLA	2	0
16	u	502	CLA	1	0
16	y	512	CLA	2	0
16	u	504	CLA	3	0
16	A	1237	CLA	3	0
16	Y	509	CLA	3	0
16	t	503	CLA	1	0
19	B	4006	BCR	5	0
16	g	505	CLA	1	0
16	h	509	CLA	2	0
16	A	1111	CLA	2	0
16	A	1013	CLA	4	0
16	w	507	CLA	2	0
19	Y	602	BCR	1	0
16	Z	506	CLA	2	0
19	L	4019	BCR	4	0
16	y	515	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Z	508	CLA	2	0
16	G	1236	CLA	2	0
16	H	1132	CLA	3	0
16	o	516	CLA	1	0
16	G	1227	CLA	2	0
16	B	1219	CLA	1	0
16	A	1113	CLA	1	0
16	X	509	CLA	1	0
16	A	1121	CLA	2	0
16	o	511	CLA	4	0
16	Z	511	CLA	1	0
19	R	4018	BCR	3	0
16	A	1116	CLA	3	0
16	Z	503	CLA	1	0
16	G	1222	CLA	2	0
16	p	507	CLA	2	0
16	a	1103	CLA	4	0
16	q	505	CLA	2	0
16	H	1117	CLA	3	0
16	A	1130	CLA	3	0
16	Z	512	CLA	1	0
18	C	102	SF4	1	0
19	A	4011	BCR	4	0
16	B	1239	CLA	3	0
19	Z	601	BCR	5	0
16	s	511	CLA	6	0
16	a	1121	CLA	1	0
16	l	1501	CLA	2	0
19	X	601	BCR	2	0
16	x	504	CLA	2	0
16	h	515	CLA	1	0
16	G	1215	CLA	3	0
16	H	1124	CLA	2	0
16	p	517	CLA	1	0
19	H	4007	BCR	1	0
16	Y	508	CLA	2	0
16	t	504	CLA	1	0
16	A	1104	CLA	5	0
16	B	1224	CLA	3	0
16	a	1122	CLA	1	0
16	L	1503	CLA	2	0
16	H	1112	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	a	2001	PQN	1	0
16	a	1136	CLA	3	0
16	p	515	CLA	2	0
16	b	1214	CLA	2	0
19	W	603	BCR	3	0
19	r	602	BCR	3	0
16	B	1021	CLA	5	0
16	b	1210	CLA	6	0
16	Z	515	CLA	2	0
16	G	1221	CLA	6	0
16	b	1234	CLA	2	0
19	m	4021	BCR	3	0
16	A	1109	CLA	2	0
16	A	1107	CLA	2	0
16	Y	515	CLA	3	0
16	q	503	CLA	1	0
16	b	1236	CLA	3	0
14	b	848	LMG	2	0
16	X	505	CLA	3	0
16	q	510	CLA	2	0
16	r	511	CLA	2	0
16	W	511	CLA	3	0
16	B	1205	CLA	6	0
19	J	4012	BCR	1	0
16	q	508	CLA	2	0
16	W	506	CLA	3	0
19	B	4009	BCR	2	0
16	A	1123	CLA	1	0
16	A	1138	CLA	4	0
16	F	1301	CLA	2	0
16	X	508	CLA	1	0
19	U	4019	BCR	2	0
19	w	602	BCR	2	0
19	a	4011	BCR	4	0
16	w	510	CLA	2	0
16	h	507	CLA	3	0
19	G	4009	BCR	2	0
16	u	512	CLA	1	0
16	u	510	CLA	4	0
16	H	1119	CLA	1	0
19	s	602	BCR	2	0
19	u	601	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	q	502	CLA	1	0
19	Q	4016	BCR	3	0
14	B	848	LMG	3	0
19	A	4007	BCR	2	0
16	p	511	CLA	2	0
16	p	510	CLA	5	0
19	x	603	BCR	3	0
16	G	1203	CLA	6	0
19	v	604	BCR	2	0
16	x	513	CLA	2	0
16	p	506	CLA	1	0
16	x	515	CLA	10	0
16	s	505	CLA	1	0
16	A	1120	CLA	1	0
16	l	1502	CLA	3	0
19	F	4016	BCR	3	0
16	u	505	CLA	3	0
16	G	1216	CLA	3	0
16	A	1124	CLA	2	0
16	y	509	CLA	3	0
16	g	502	CLA	2	0
19	G	4014	BCR	1	0
16	B	1215	CLA	2	0
16	H	1139	CLA	1	0
16	n	502	CLA	2	0
19	X	602	BCR	3	0
16	a	1134	CLA	1	0
16	G	1210	CLA	5	0
16	G	1223	CLA	1	0
16	B	1217	CLA	1	0
19	I	4020	BCR	3	0
17	B	2002	PQN	5	0
16	X	502	CLA	3	0
16	t	516	CLA	2	0
16	G	1206	CLA	3	0
16	X	504	CLA	3	0
16	B	1202	CLA	2	0
16	t	507	CLA	3	0
19	l	4019	BCR	3	0
16	B	1209	CLA	1	0
16	X	511	CLA	3	0
16	A	1125	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	4101	LMG	2	0
16	v	515	CLA	2	0
19	a	4003	BCR	1	0
19	o	604	BCR	1	0
19	p	601	BCR	2	0
16	r	512	CLA	1	0
19	h	602	BCR	2	0
16	b	1222	CLA	2	0
16	A	1119	CLA	2	0
16	H	1121	CLA	1	0
16	W	516	CLA	1	0
16	b	1216	CLA	3	0
16	g	508	CLA	2	0
16	n	514	CLA	1	0
16	H	1123	CLA	3	0
19	j	4013	BCR	1	0
19	y	602	BCR	2	0
16	A	1131	CLA	4	0
16	r	502	CLA	2	0
16	b	1207	CLA	5	0
16	G	1205	CLA	6	0
19	Z	602	BCR	2	0
19	T	1501	BCR	2	0
17	G	2002	PQN	5	0
16	A	1137	CLA	1	0
16	g	516	CLA	1	0
19	o	603	BCR	3	0
16	o	513	CLA	1	0
16	u	506	CLA	5	0
16	y	516	CLA	2	0
19	G	4010	BCR	2	0
16	y	507	CLA	3	0
19	j	4015	BCR	5	0
16	a	1137	CLA	1	0
16	B	1221	CLA	4	0
16	G	1240	CLA	2	0
16	H	1104	CLA	4	0
16	B	1023	CLA	9	0
16	x	510	CLA	1	0
19	k	1501	BCR	2	0
16	X	516	CLA	1	0
16	b	1232	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1236	CLA	2	0
16	Z	505	CLA	1	0
16	o	506	CLA	3	0
16	W	502	CLA	1	0
19	R	4020	BCR	4	0
16	r	516	CLA	1	0
16	B	1203	CLA	4	0
16	Y	505	CLA	2	0
16	H	1103	CLA	4	0
16	a	1105	CLA	1	0
16	g	509	CLA	1	0
16	X	513	CLA	1	0
16	a	1106	CLA	3	0
16	Z	510	CLA	1	0
19	M	4021	BCR	3	0
16	H	1128	CLA	3	0
16	H	1138	CLA	4	0
16	B	1223	CLA	1	0
16	B	1238	CLA	4	0
16	v	512	CLA	2	0
19	v	603	BCR	1	0
16	b	1224	CLA	2	0
19	J	4013	BCR	1	0
15	a	1011	CL0	3	0
16	q	511	CLA	2	0
16	A	1108	CLA	1	0
16	B	1230	CLA	7	0
16	n	509	CLA	4	0
19	v	601	BCR	1	0
16	t	510	CLA	7	0
16	W	513	CLA	1	0
16	Z	516	CLA	3	0
16	W	508	CLA	2	0
16	r	508	CLA	3	0
16	p	516	CLA	3	0
13	a	849	LHG	1	0
16	v	513	CLA	2	0
19	B	4017	BCR	4	0
16	a	1111	CLA	3	0
16	A	1105	CLA	1	0
16	v	502	CLA	3	0
16	W	509	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	x	602	BCR	2	0
16	G	1229	CLA	2	0
16	b	1205	CLA	5	0
16	t	514	CLA	1	0
16	b	1203	CLA	5	0
16	y	502	CLA	1	0
16	n	504	CLA	1	0
16	H	1108	CLA	2	0
16	u	507	CLA	5	0
16	a	1104	CLA	5	0
16	u	511	CLA	4	0
16	x	502	CLA	3	0
19	j	4012	BCR	2	0
16	b	1213	CLA	1	0
16	r	506	CLA	1	0
16	Y	510	CLA	3	0
19	H	4008	BCR	2	0
16	t	502	CLA	2	0
16	h	510	CLA	2	0
16	b	1215	CLA	2	0
16	A	1135	CLA	1	0
16	G	1209	CLA	1	0
19	G	4005	BCR	4	0
13	H	849	LHG	1	0
16	b	1219	CLA	1	0
16	A	1103	CLA	4	0
16	B	1234	CLA	2	0
16	w	504	CLA	1	0
19	v	602	BCR	2	0
16	Z	514	CLA	1	0
16	B	1204	CLA	3	0
16	G	1228	CLA	3	0
16	w	515	CLA	2	0
16	Z	502	CLA	1	0
16	a	1109	CLA	2	0
16	B	1222	CLA	1	0
16	b	1238	CLA	5	0
16	s	509	CLA	4	0
16	a	1117	CLA	3	0
19	p	602	BCR	2	0
16	a	1128	CLA	4	0
16	X	506	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	u	515	CLA	1	0
16	b	1235	CLA	2	0
16	n	516	CLA	1	0
16	B	1213	CLA	1	0
16	B	1206	CLA	2	0
16	r	509	CLA	2	0
16	G	1225	CLA	6	0
16	h	502	CLA	3	0
16	A	1132	CLA	3	0
16	X	510	CLA	3	0
16	g	504	CLA	2	0
19	f	4016	BCR	4	0
16	B	1207	CLA	5	0
16	q	517	CLA	1	0
14	A	852	LMG	1	0
16	H	1122	CLA	1	0
16	B	1226	CLA	2	0
16	u	516	CLA	2	0
16	H	1140	CLA	6	0
16	a	1124	CLA	2	0
16	n	508	CLA	2	0
16	o	515	CLA	2	0
16	G	1224	CLA	2	0
16	n	505	CLA	3	0
19	Y	601	BCR	4	0
19	x	601	BCR	2	0
16	A	1133	CLA	1	0
19	u	603	BCR	1	0
16	y	508	CLA	2	0
16	a	1140	CLA	3	0
19	A	4008	BCR	3	0
16	B	1214	CLA	2	0
16	b	1239	CLA	3	0
16	v	504	CLA	1	0
16	b	1202	CLA	2	0
16	w	511	CLA	2	0
16	v	507	CLA	4	0
16	A	1128	CLA	3	0
16	s	510	CLA	3	0
16	a	1126	CLA	4	0
19	a	4008	BCR	2	0
16	w	505	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	1402	CLA	1	0
14	Y	701	LMG	1	0
16	s	504	CLA	1	0
19	g	603	BCR	4	0
16	X	517	CLA	1	0
16	b	1221	CLA	4	0
19	o	601	BCR	4	0
16	y	517	CLA	2	0
16	t	515	CLA	6	0
16	o	508	CLA	1	0
16	g	511	CLA	3	0
16	U	1503	CLA	4	0
19	w	603	BCR	3	0
16	y	504	CLA	3	0
16	w	513	CLA	2	0
16	y	511	CLA	2	0
16	b	1226	CLA	1	0
16	v	508	CLA	2	0
19	n	603	BCR	2	0
16	o	503	CLA	3	0
16	q	516	CLA	3	0
19	G	4017	BCR	4	0
16	G	1234	CLA	2	0
19	r	603	BCR	3	0
16	B	1232	CLA	2	0
16	B	1220	CLA	2	0
16	q	507	CLA	1	0
16	W	515	CLA	8	0
14	A	4101	LMG	1	0
16	a	1127	CLA	5	0
19	u	604	BCR	1	0
16	L	1502	CLA	5	0
16	o	507	CLA	3	0
16	u	503	CLA	3	0
19	S	4015	BCR	5	0
16	A	1126	CLA	4	0
16	H	1237	CLA	3	0
16	a	1123	CLA	2	0
19	L	4022	BCR	7	0
19	I	4018	BCR	2	0
16	g	507	CLA	4	0
16	v	506	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	1021	CLA	5	0
16	B	1012	CLA	3	0
16	y	510	CLA	4	0
16	p	502	CLA	1	0
19	A	4001	BCR	2	0
19	Y	603	BCR	1	0
16	t	505	CLA	7	0
19	a	4001	BCR	2	0
16	A	1136	CLA	3	0
14	H	852	LMG	1	0
16	o	517	CLA	1	0
16	Y	504	CLA	2	0
16	q	515	CLA	3	0
16	a	1131	CLA	4	0
16	B	1227	CLA	2	0
17	b	2002	PQN	4	0
19	i	4020	BCR	5	0
16	G	1202	CLA	2	0
16	X	507	CLA	2	0
16	h	508	CLA	2	0
19	s	603	BCR	2	0
16	a	1022	CLA	4	0
19	b	4005	BCR	3	0
16	H	1126	CLA	4	0
16	s	517	CLA	1	0
19	G	4004	BCR	1	0
16	b	1240	CLA	2	0
14	a	4101	LMG	2	0
16	v	503	CLA	1	0
16	A	1127	CLA	5	0
16	y	506	CLA	5	0
19	o	602	BCR	1	0
16	A	1022	CLA	3	0
16	B	1235	CLA	3	0
16	g	517	CLA	2	0
16	b	1228	CLA	3	0
16	H	1111	CLA	2	0
16	w	502	CLA	1	0
16	y	513	CLA	2	0
16	h	516	CLA	2	0
19	U	4022	BCR	8	0
16	a	1237	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	n	507	CLA	2	0
16	G	1211	CLA	3	0
16	B	1216	CLA	3	0
16	b	1225	CLA	6	0
16	p	508	CLA	1	0
13	R	103	LHG	1	0
16	r	507	CLA	1	0
16	H	1136	CLA	4	0
19	X	603	BCR	1	0
16	a	1108	CLA	1	0
16	G	1231	CLA	1	0
16	X	515	CLA	2	0
14	H	4201	LMG	2	0
19	b	4006	BCR	5	0
16	b	1218	CLA	1	0
16	G	1213	CLA	1	0
16	q	509	CLA	2	0
19	B	4010	BCR	2	0
16	W	512	CLA	1	0
16	a	1113	CLA	1	0
16	a	1119	CLA	2	0
19	b	4009	BCR	4	0
16	W	514	CLA	1	0
16	x	517	CLA	1	0
16	H	1133	CLA	1	0
16	a	1116	CLA	4	0
16	G	1220	CLA	2	0
16	w	516	CLA	3	0
19	t	601	BCR	5	0
16	s	516	CLA	3	0
16	r	517	CLA	1	0
19	h	603	BCR	1	0
16	B	1225	CLA	6	0
16	a	1130	CLA	4	0
16	B	1228	CLA	3	0
19	A	4003	BCR	1	0
19	s	604	BCR	1	0
16	Y	511	CLA	7	0
16	x	507	CLA	4	0
16	o	510	CLA	3	0
16	b	1229	CLA	2	0
16	r	515	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1211	CLA	3	0
16	h	511	CLA	1	0
16	Y	506	CLA	3	0
16	H	1137	CLA	1	0
19	i	4018	BCR	3	0
19	B	4004	BCR	1	0
19	y	603	BCR	1	0
16	G	1235	CLA	4	0
16	A	1102	CLA	1	0
19	Z	603	BCR	2	0
16	A	1134	CLA	2	0
16	Z	513	CLA	2	0
16	g	503	CLA	1	0
16	s	507	CLA	4	0
15	A	1011	CL0	4	0
14	a	852	LMG	2	0
16	p	509	CLA	3	0
16	g	510	CLA	1	0
16	G	1230	CLA	4	0
16	G	1023	CLA	9	0
16	a	1138	CLA	3	0
16	G	1012	CLA	3	0
19	b	4014	BCR	1	0
19	l	4022	BCR	4	0
16	o	509	CLA	2	0
16	H	1105	CLA	1	0
16	b	1204	CLA	2	0
16	q	513	CLA	2	0
16	a	1132	CLA	3	0
16	Y	512	CLA	2	0
16	a	1101	CLA	5	0
16	w	509	CLA	3	0
16	g	512	CLA	1	0
16	a	1107	CLA	2	0
16	v	511	CLA	1	0
19	g	602	BCR	3	0
16	b	1209	CLA	1	0
16	b	1023	CLA	8	0
19	g	601	BCR	2	0
14	a	4201	LMG	2	0
16	u	509	CLA	3	0
16	n	511	CLA	5	0

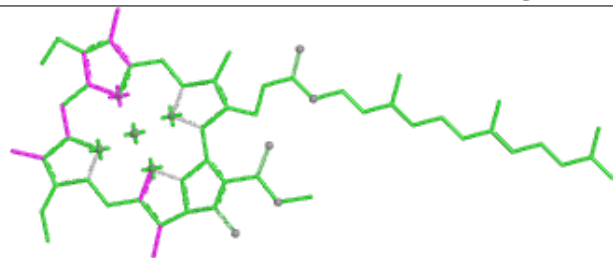
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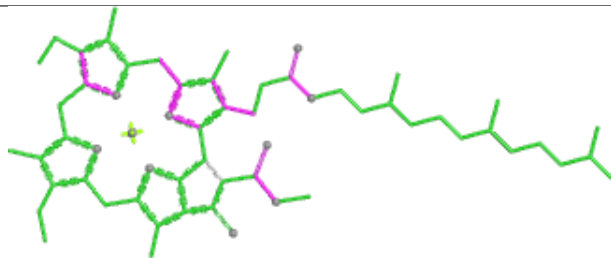
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	L	1501	CLA	3	0
16	W	505	CLA	2	0
16	A	1117	CLA	2	0
16	b	1211	CLA	3	0
16	w	506	CLA	1	0
18	N	102	SF4	1	0
19	H	4001	BCR	2	0
16	x	516	CLA	1	0
19	y	604	BCR	6	0
16	n	512	CLA	1	0
16	w	508	CLA	2	0
19	B	4014	BCR	2	0
16	p	504	CLA	2	0
16	n	510	CLA	3	0
19	G	4006	BCR	3	0
16	A	1122	CLA	2	0

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

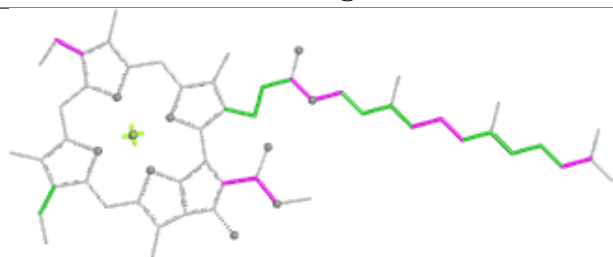
Ligand CLA n 506



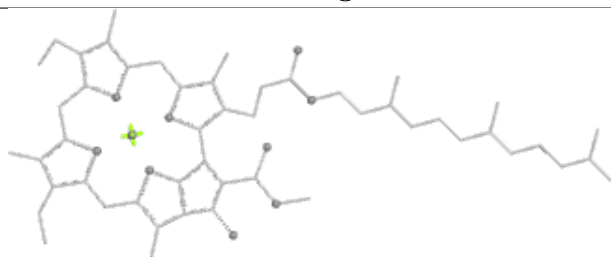
Bond lengths



Bond angles

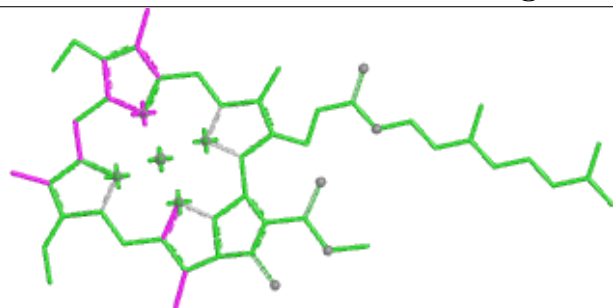


Torsions

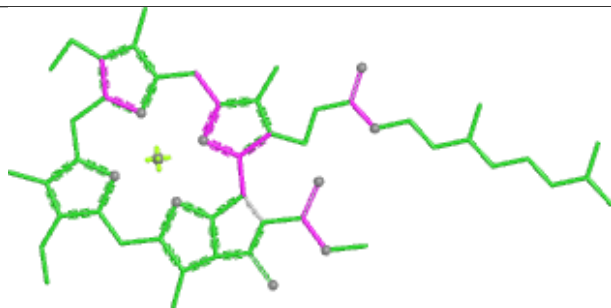


Rings

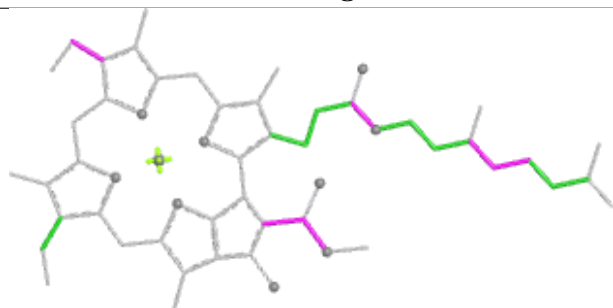
Ligand CLA r 510



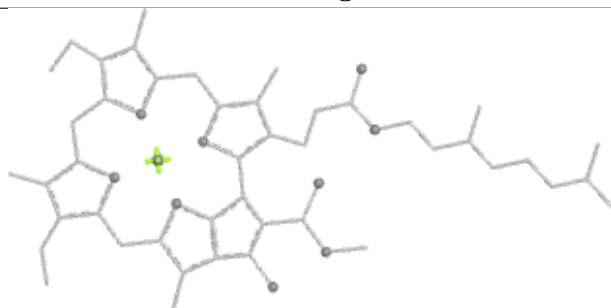
Bond lengths



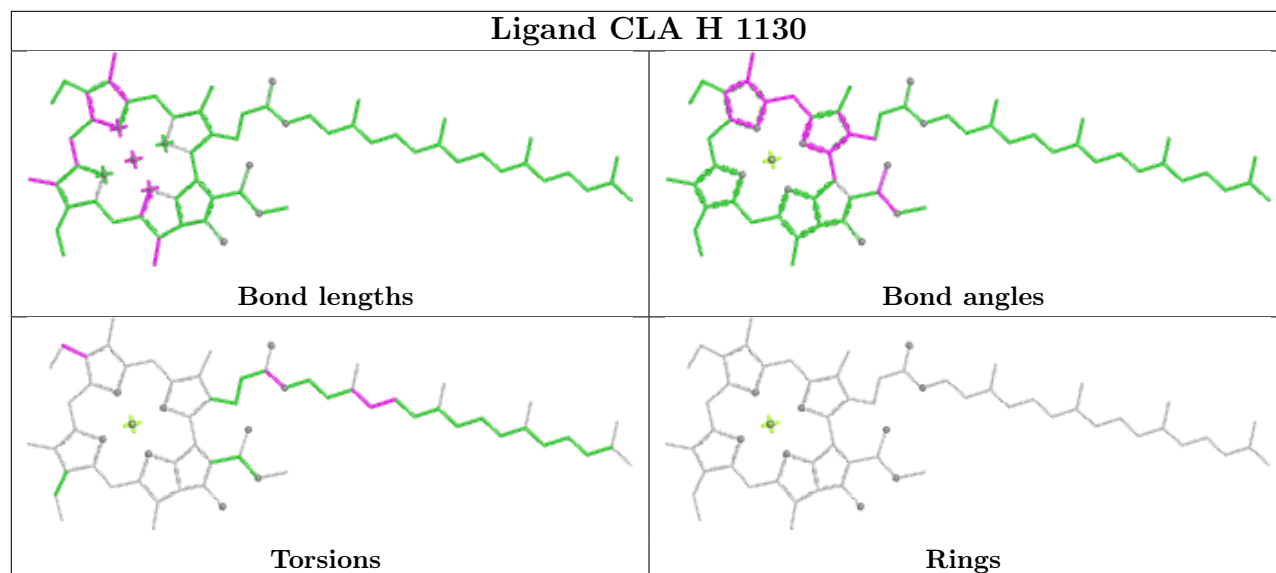
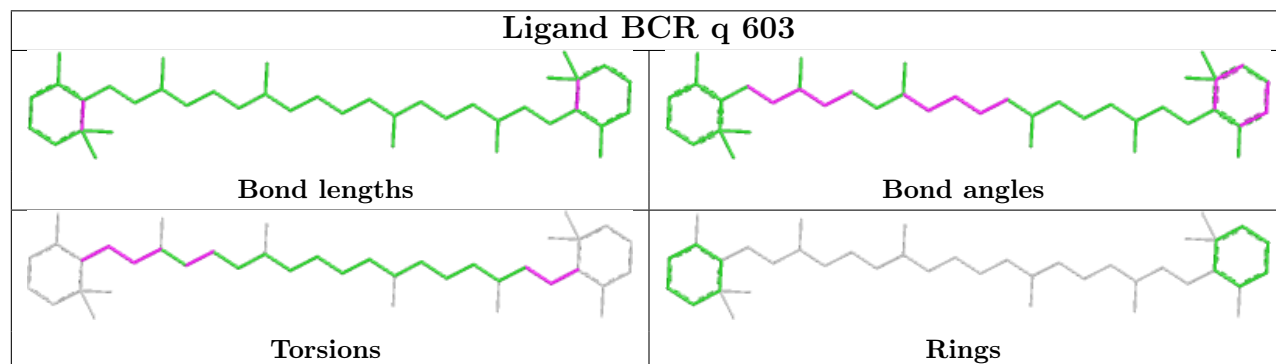
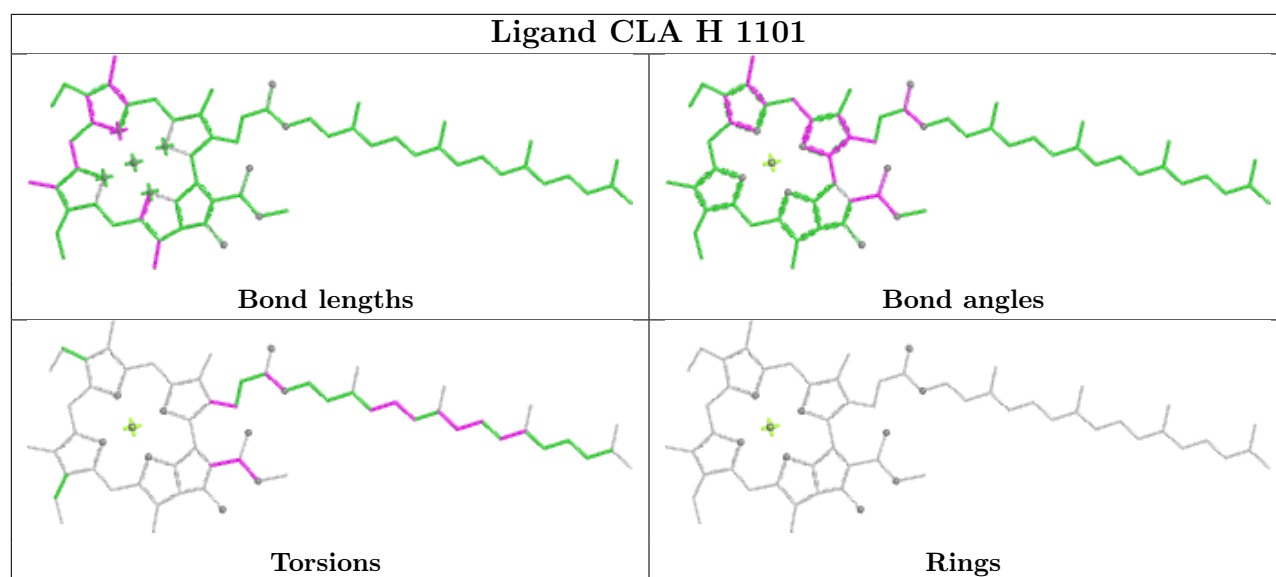
Bond angles

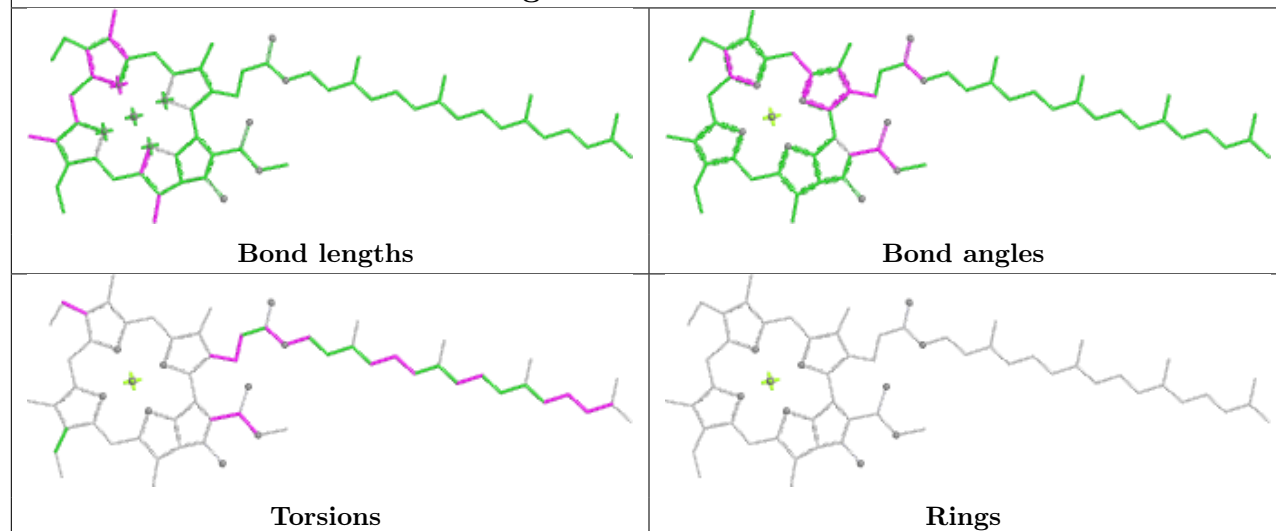
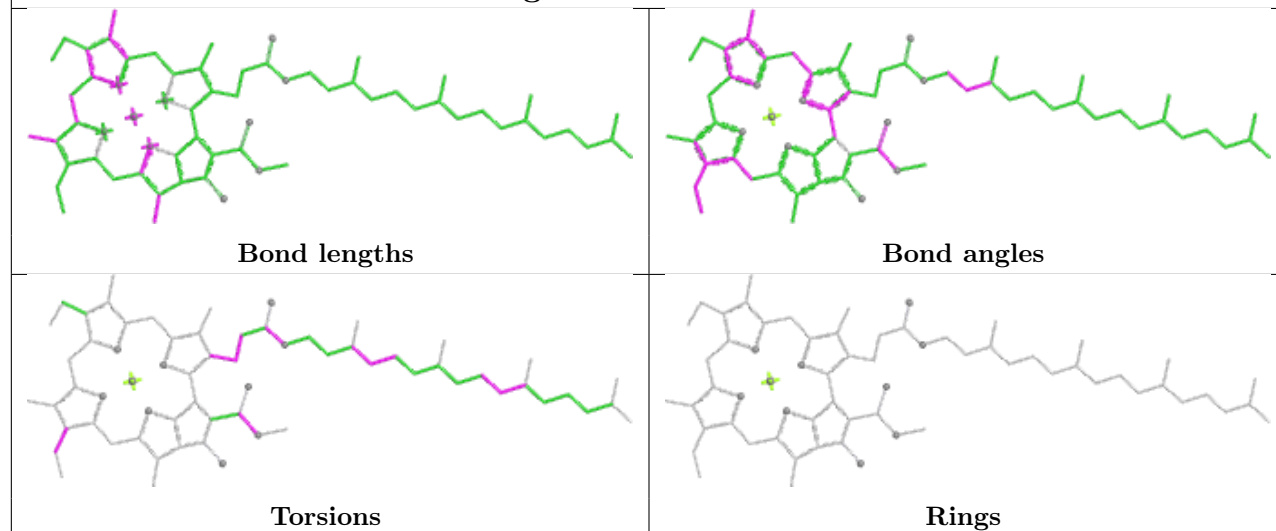


Torsions

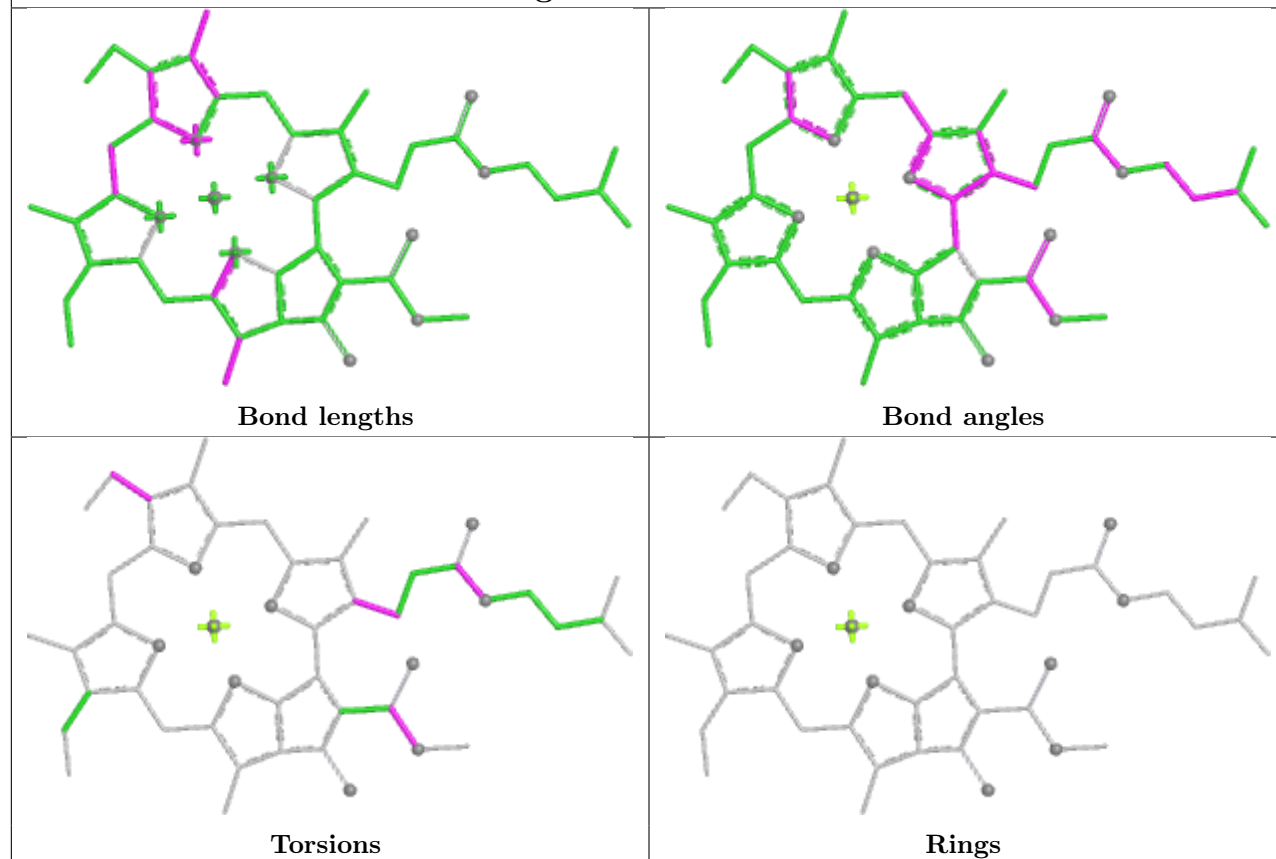


Rings

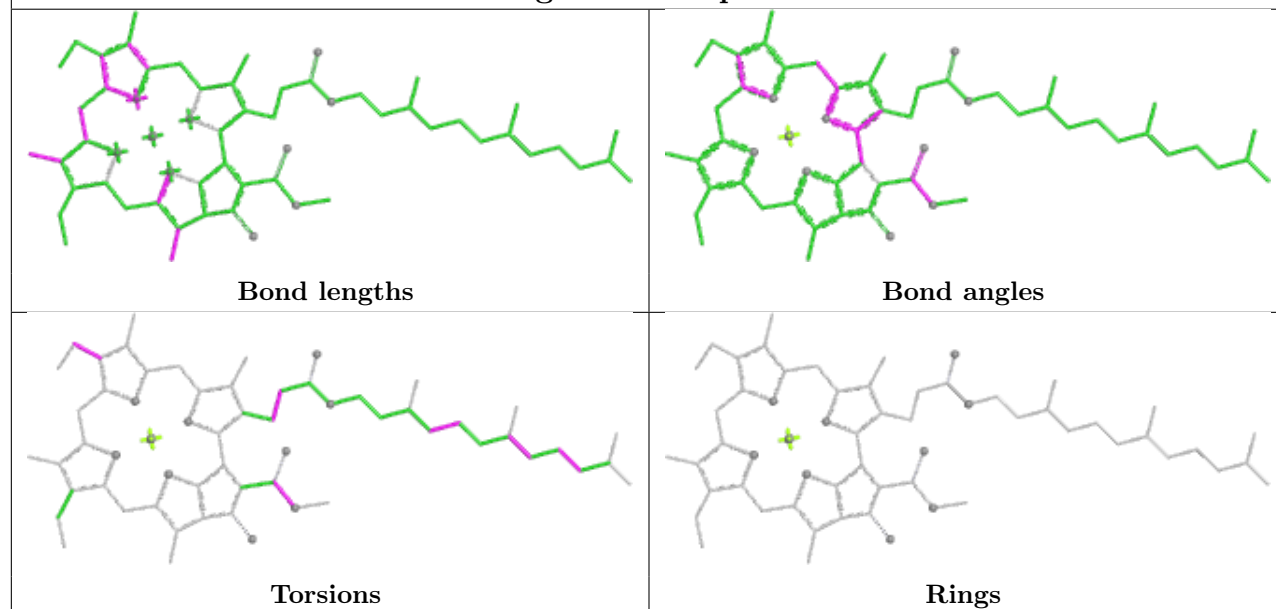


Ligand CLA A 1106**Ligand CLA B 1210**

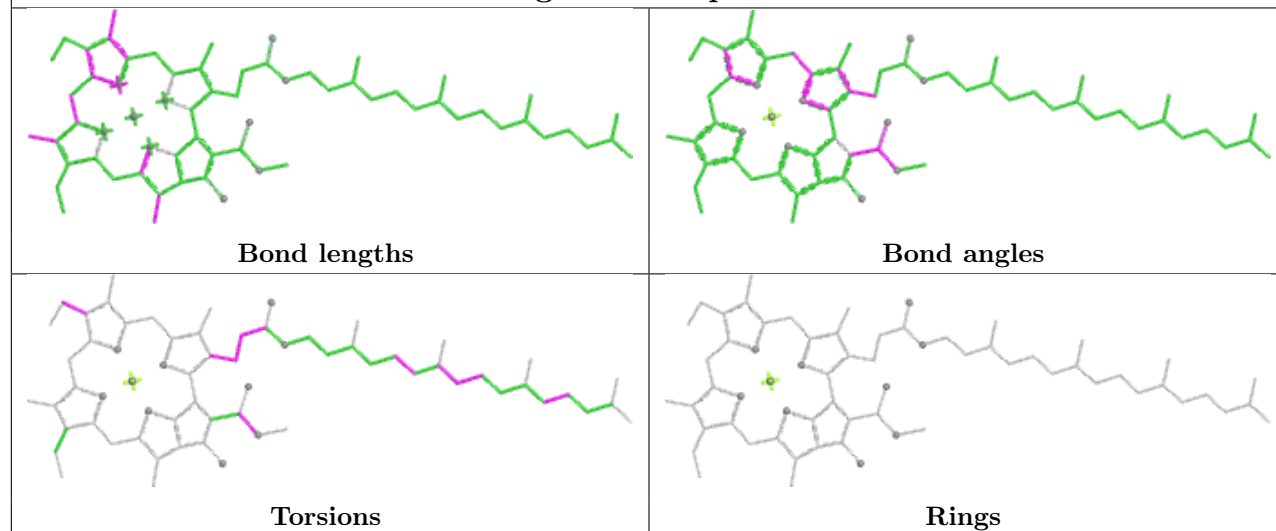
Ligand CLA n 513



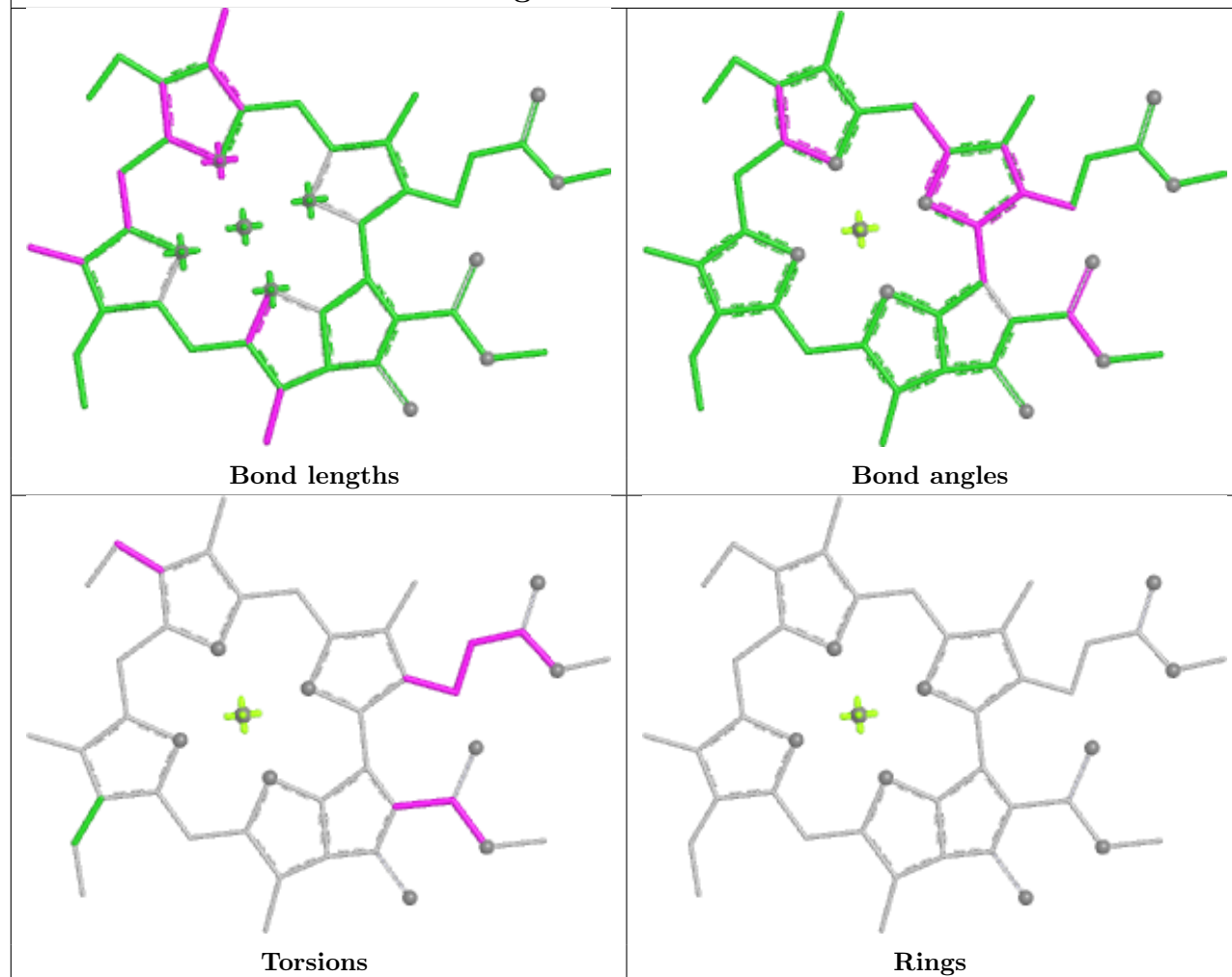
Ligand CLA q 504

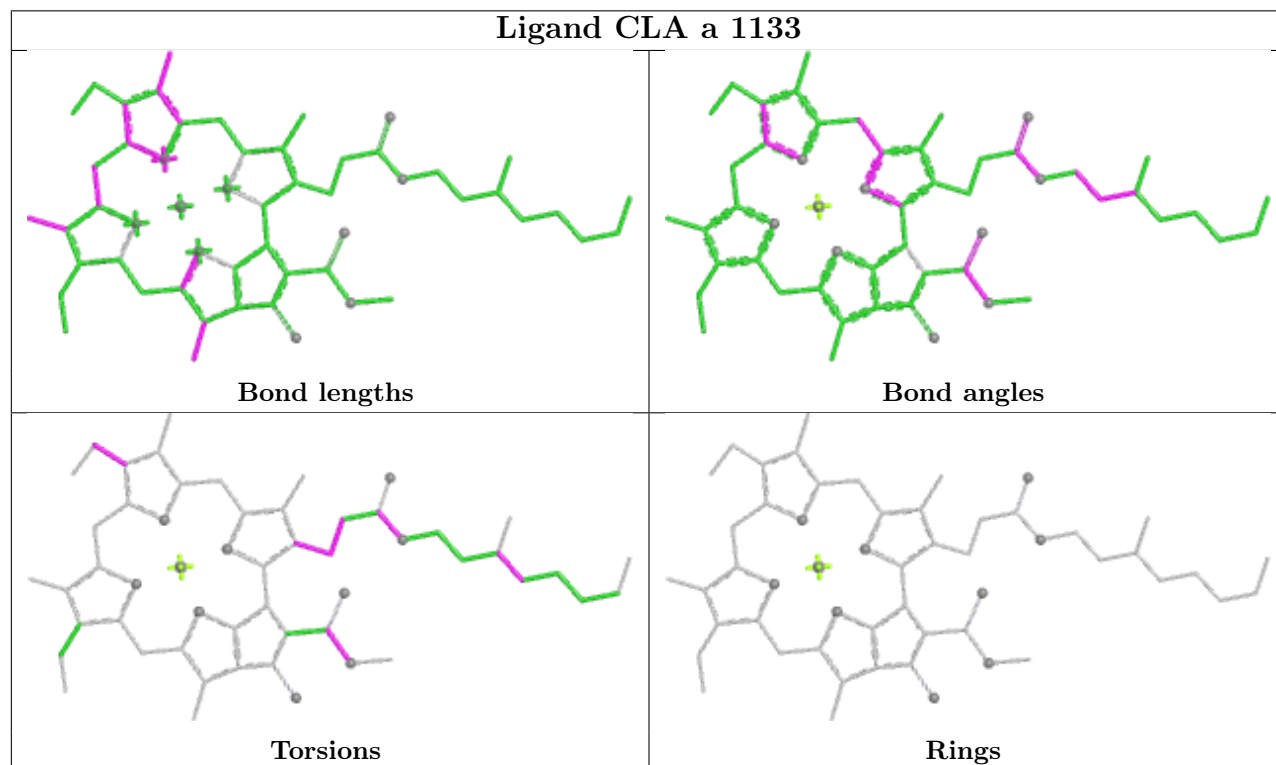
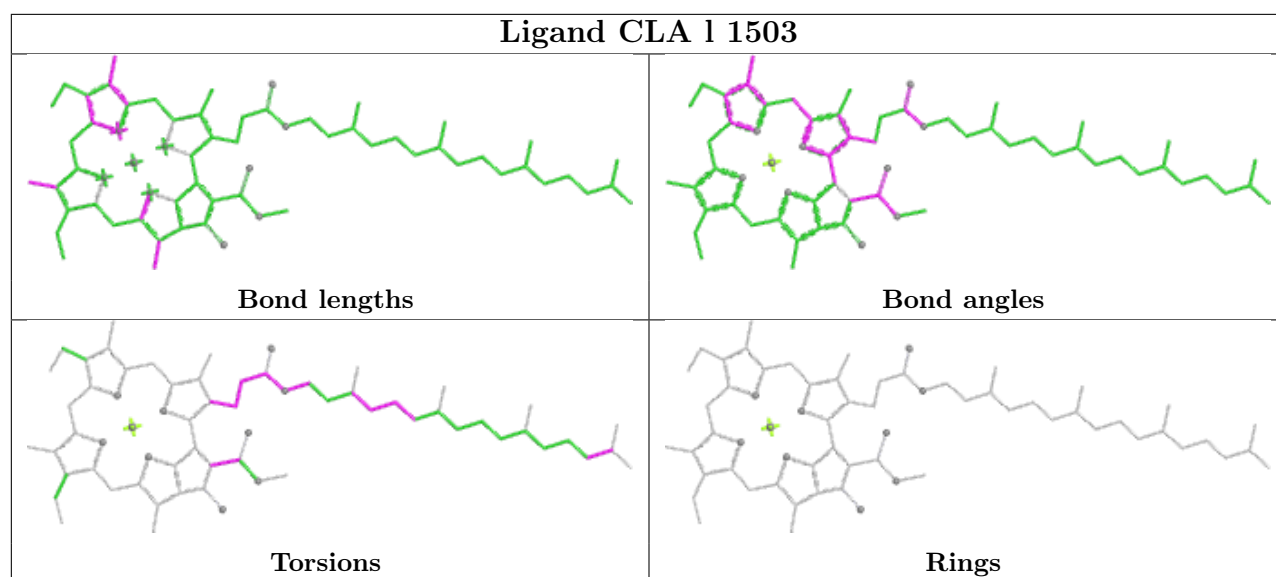


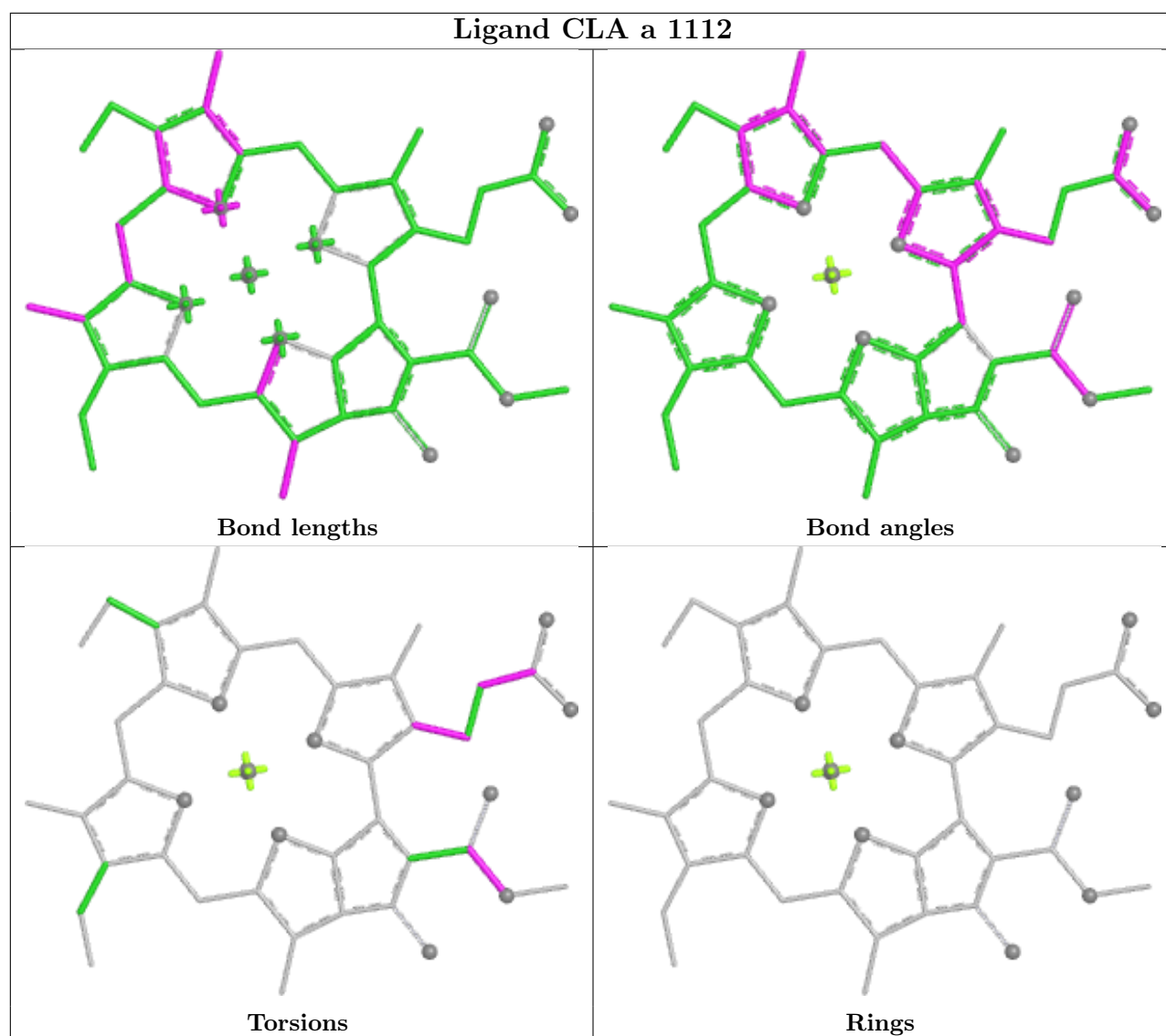
Ligand CLA p 505

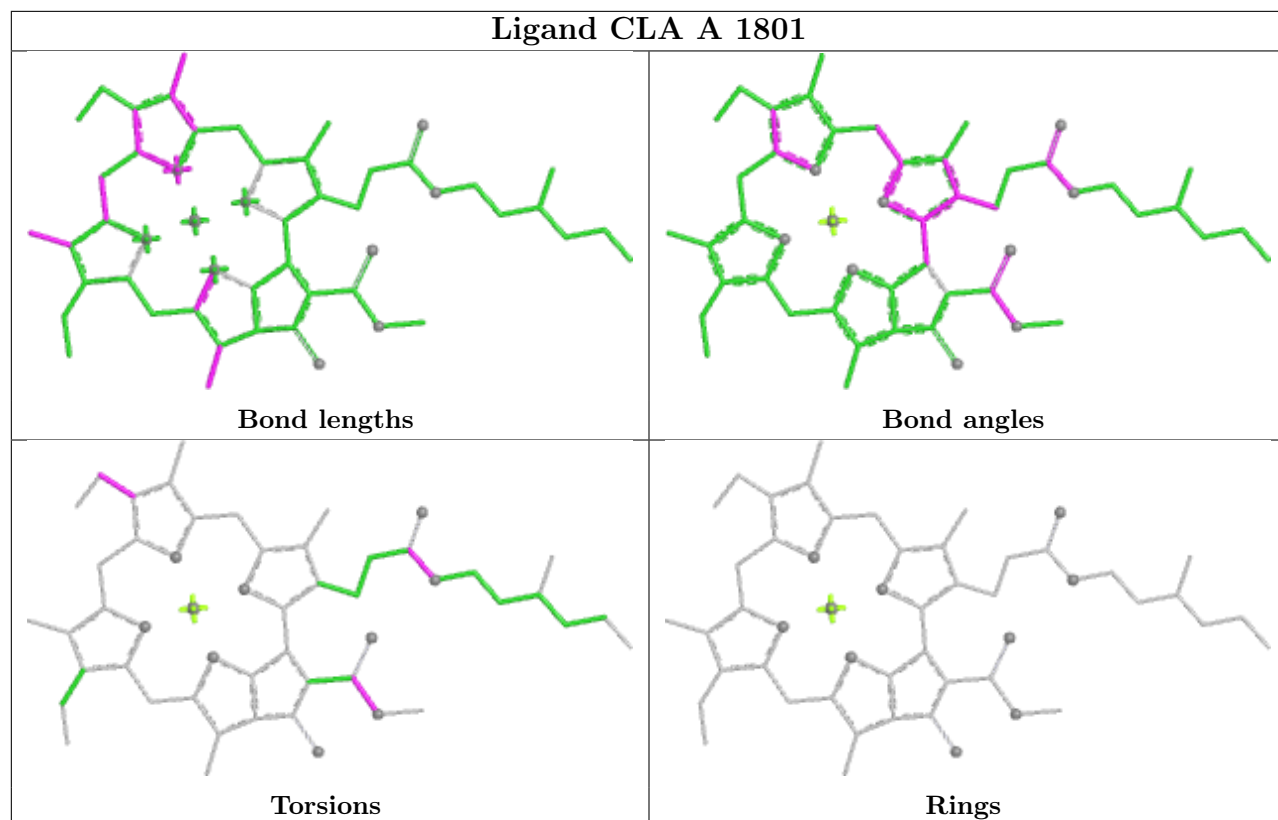


Ligand CLA w 503

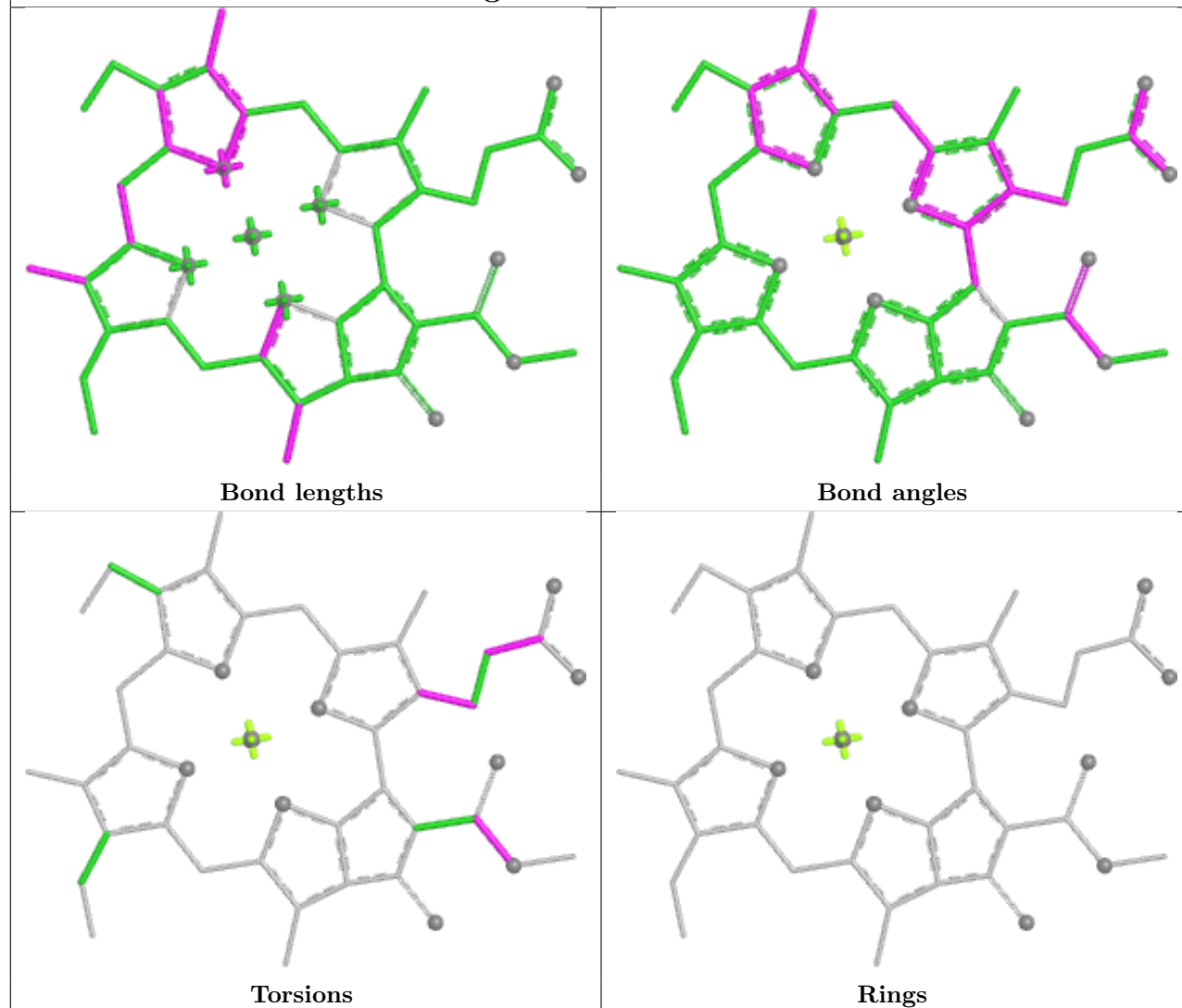




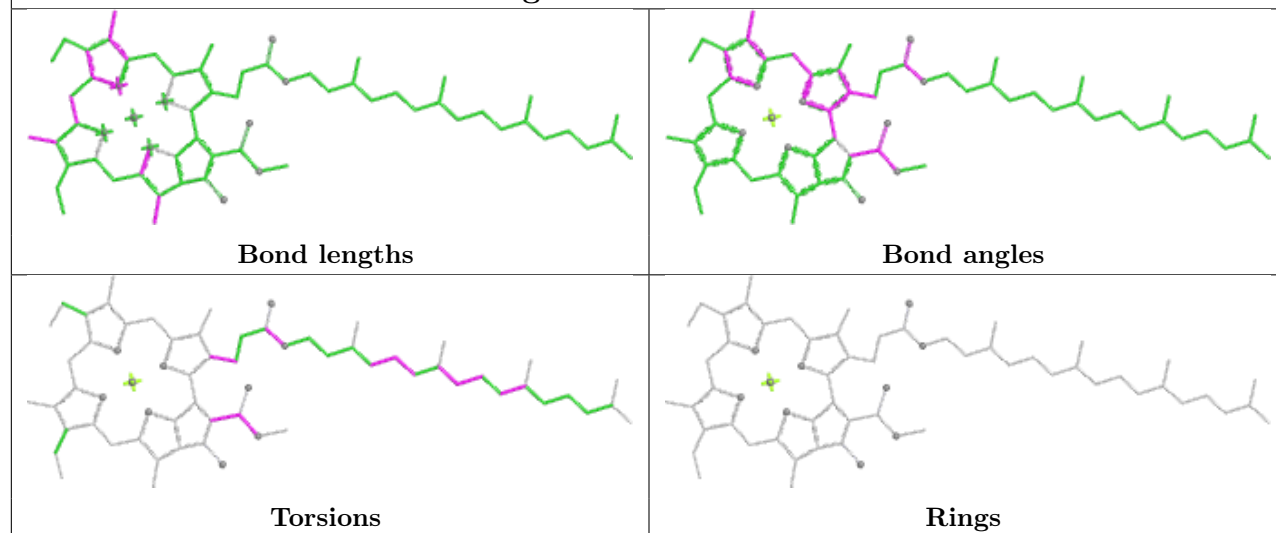


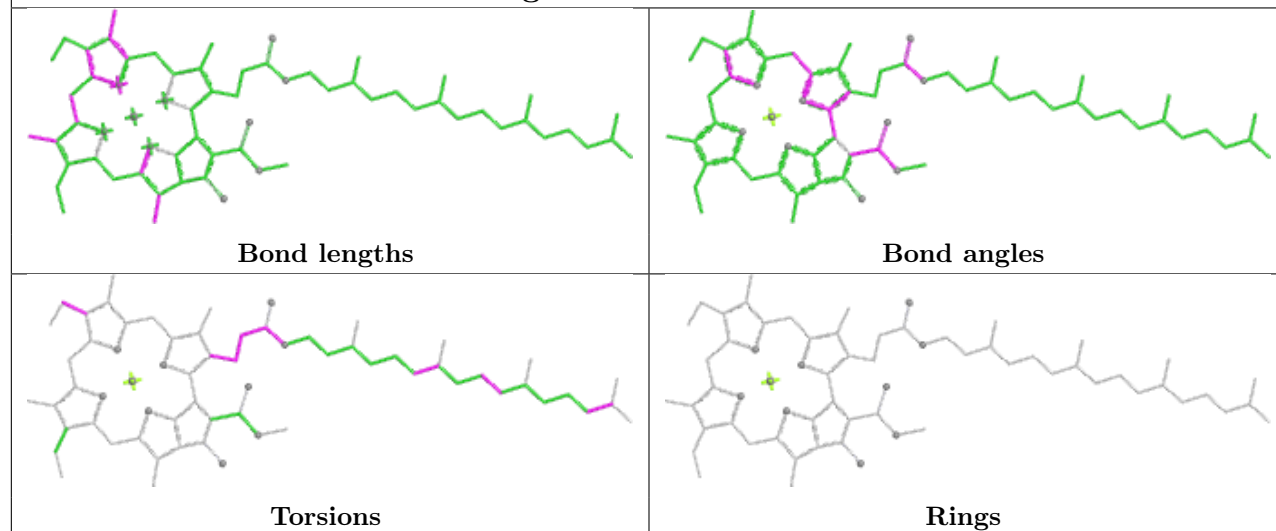
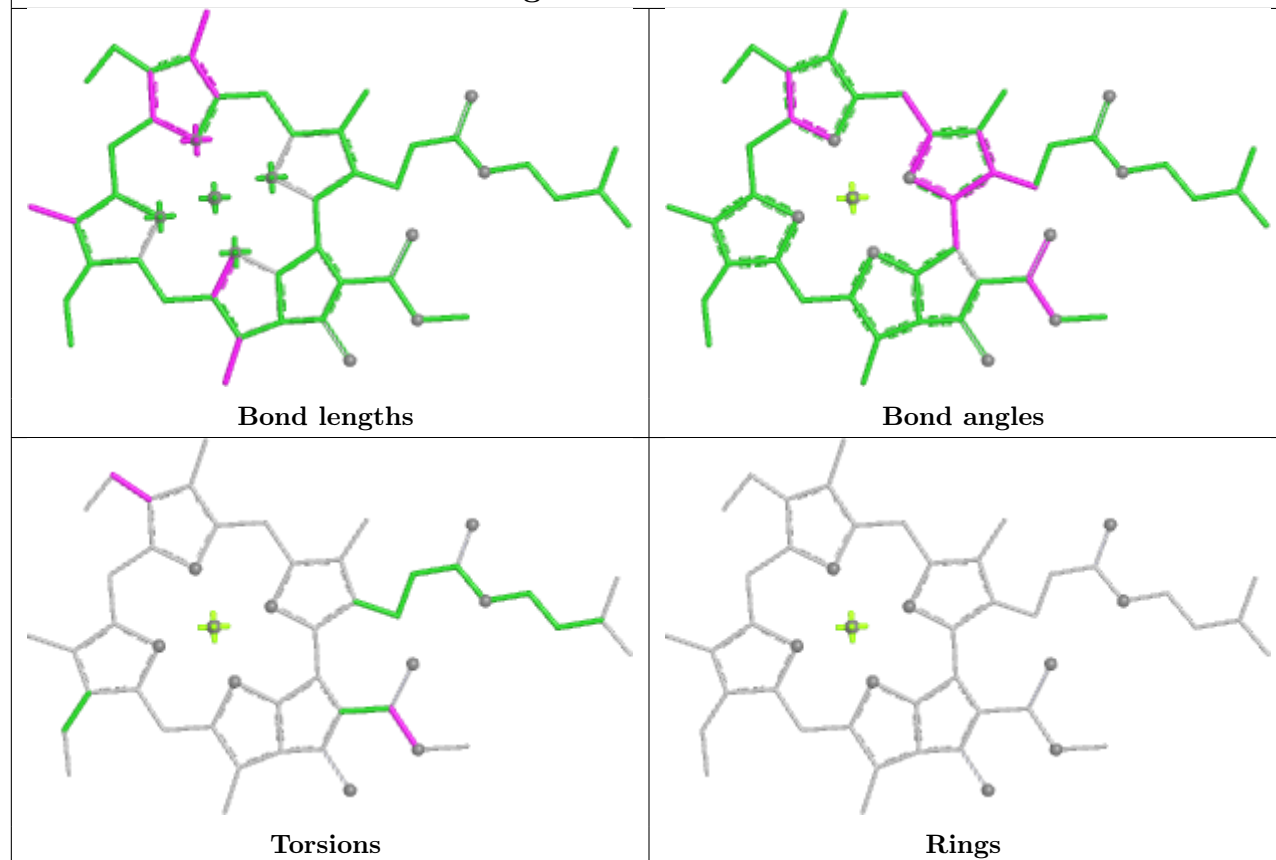


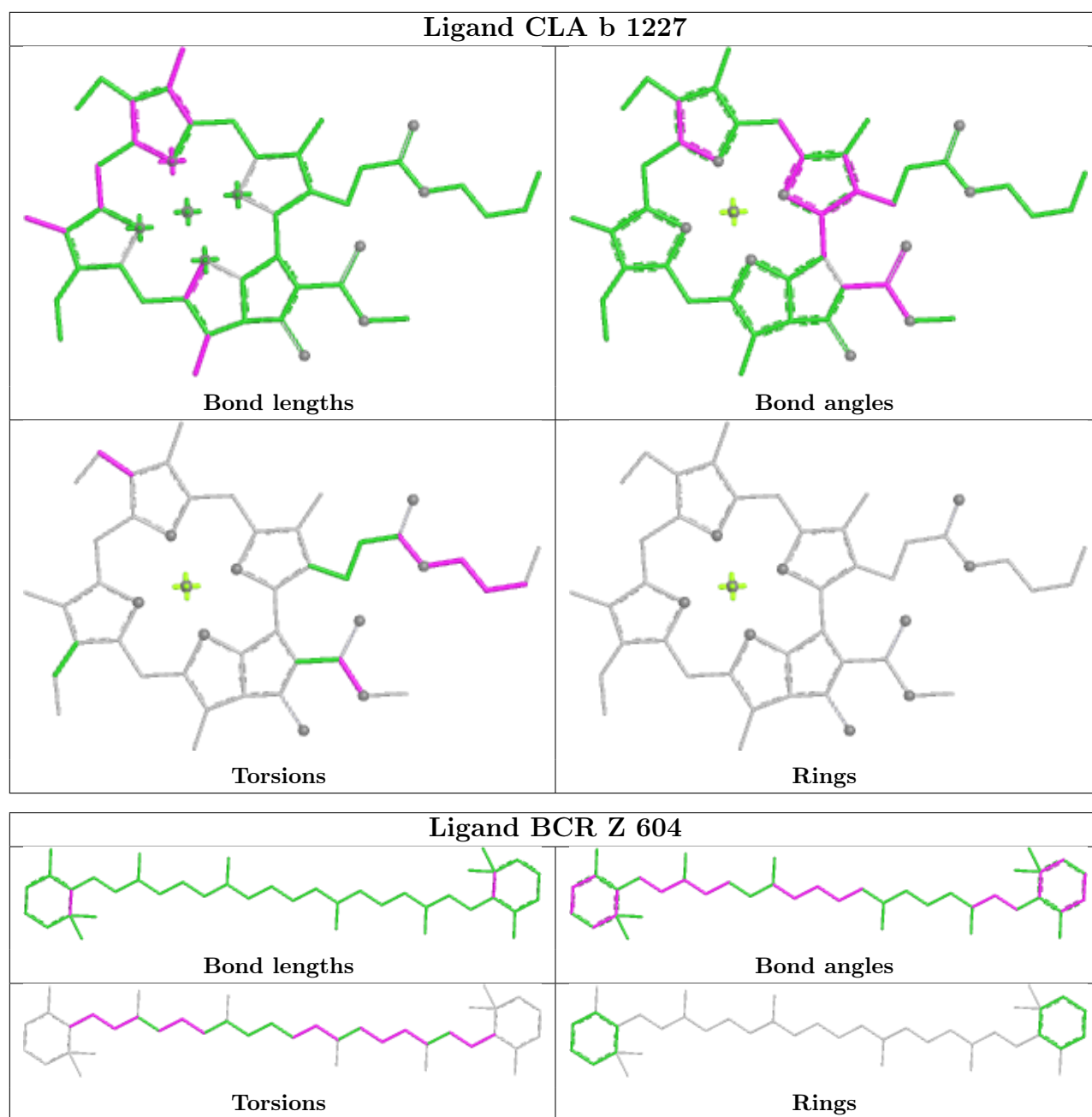
Ligand CLA A 1112



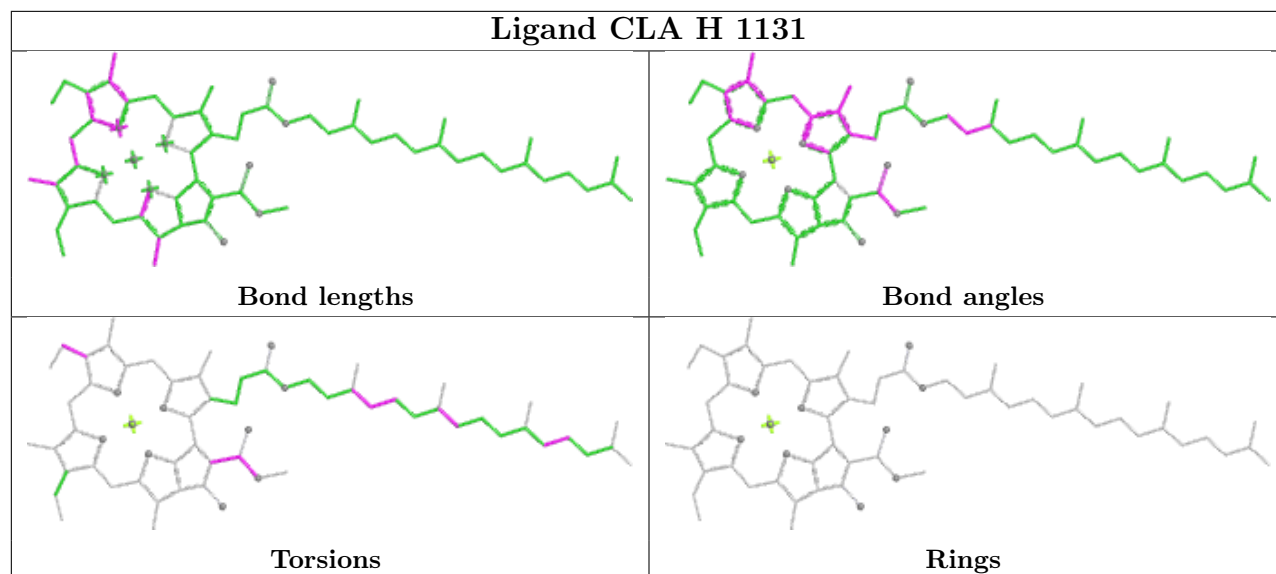
Ligand CLA A 1101



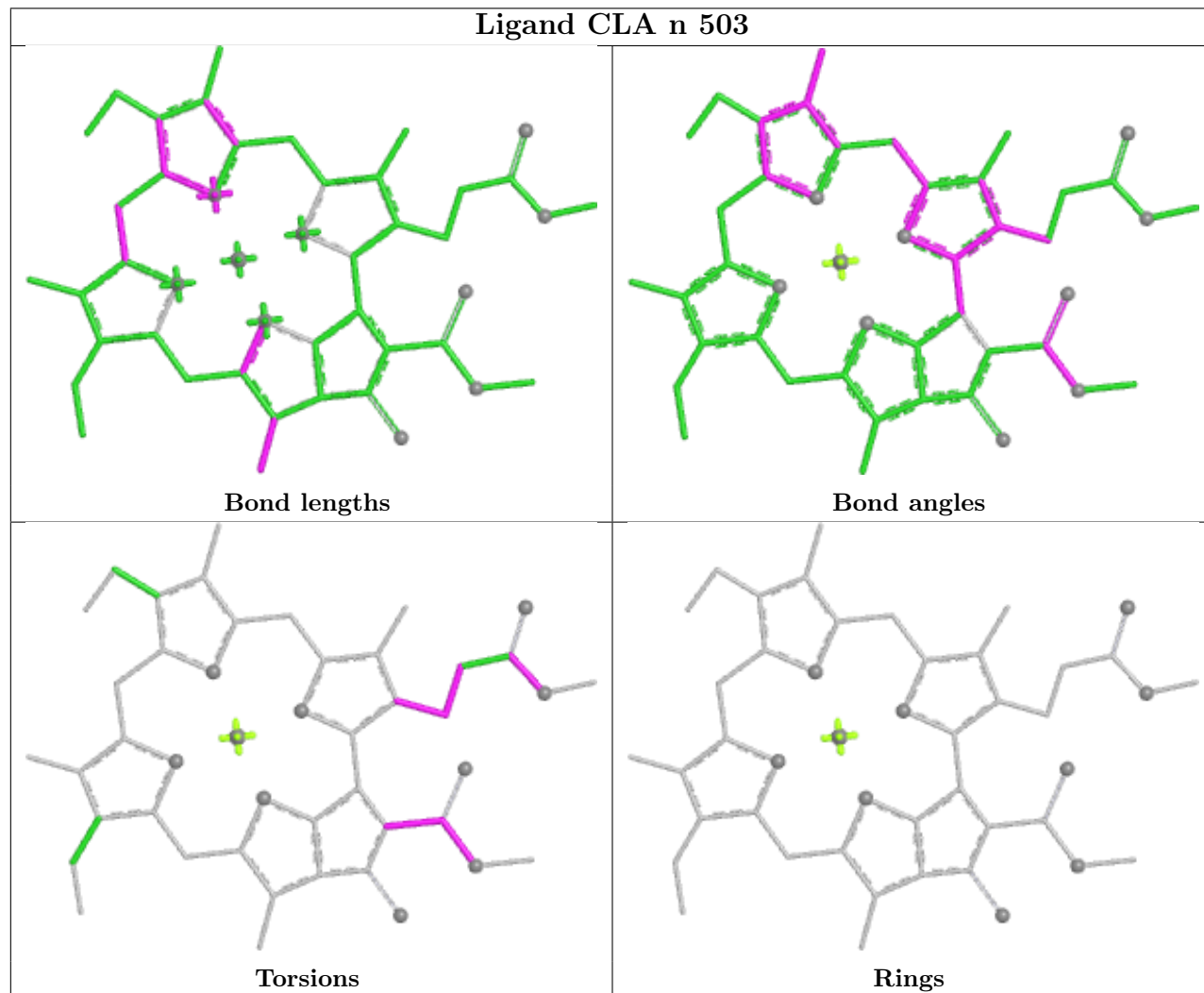
Ligand CLA U 1502**Ligand CLA B 1240**

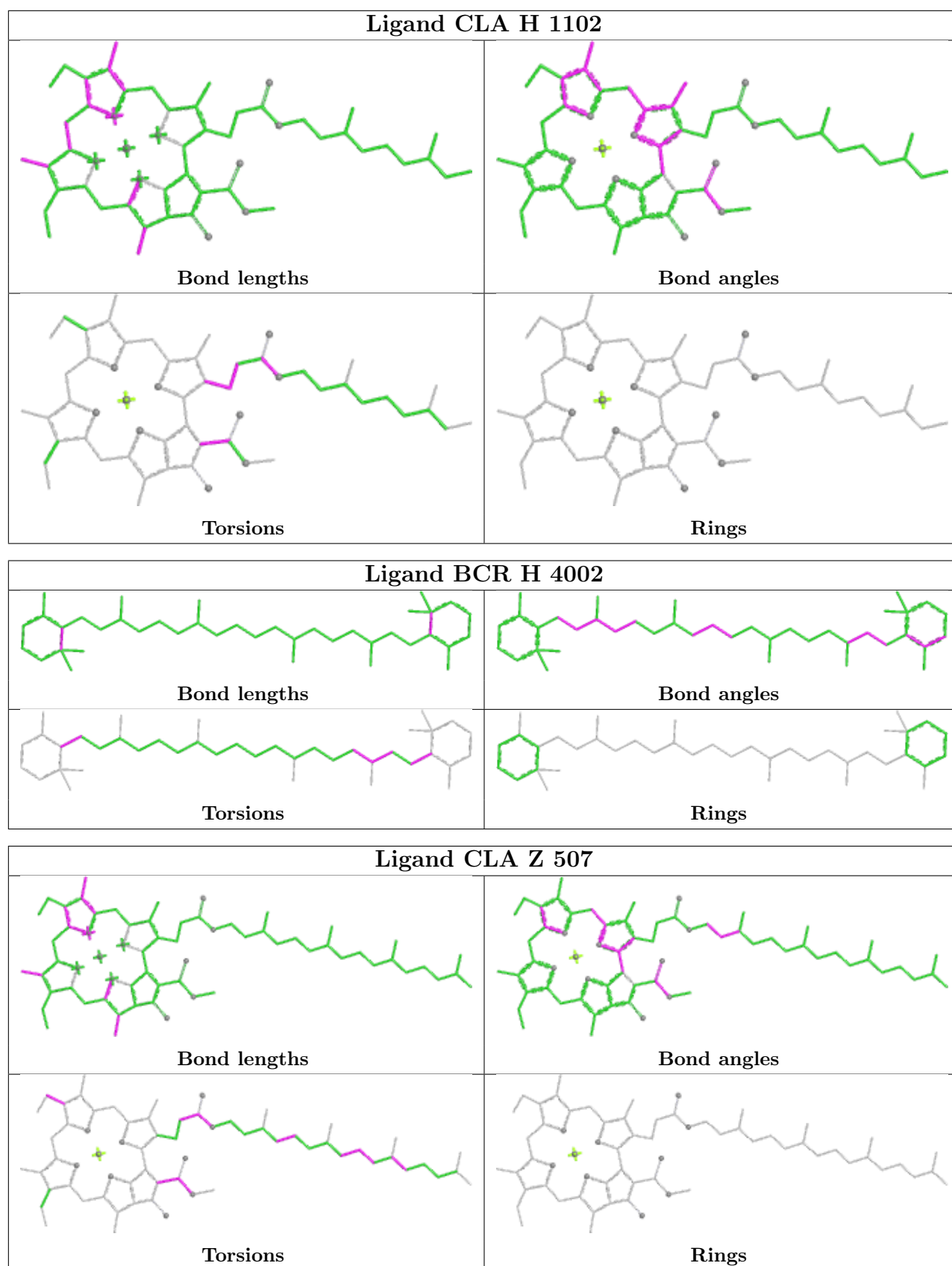


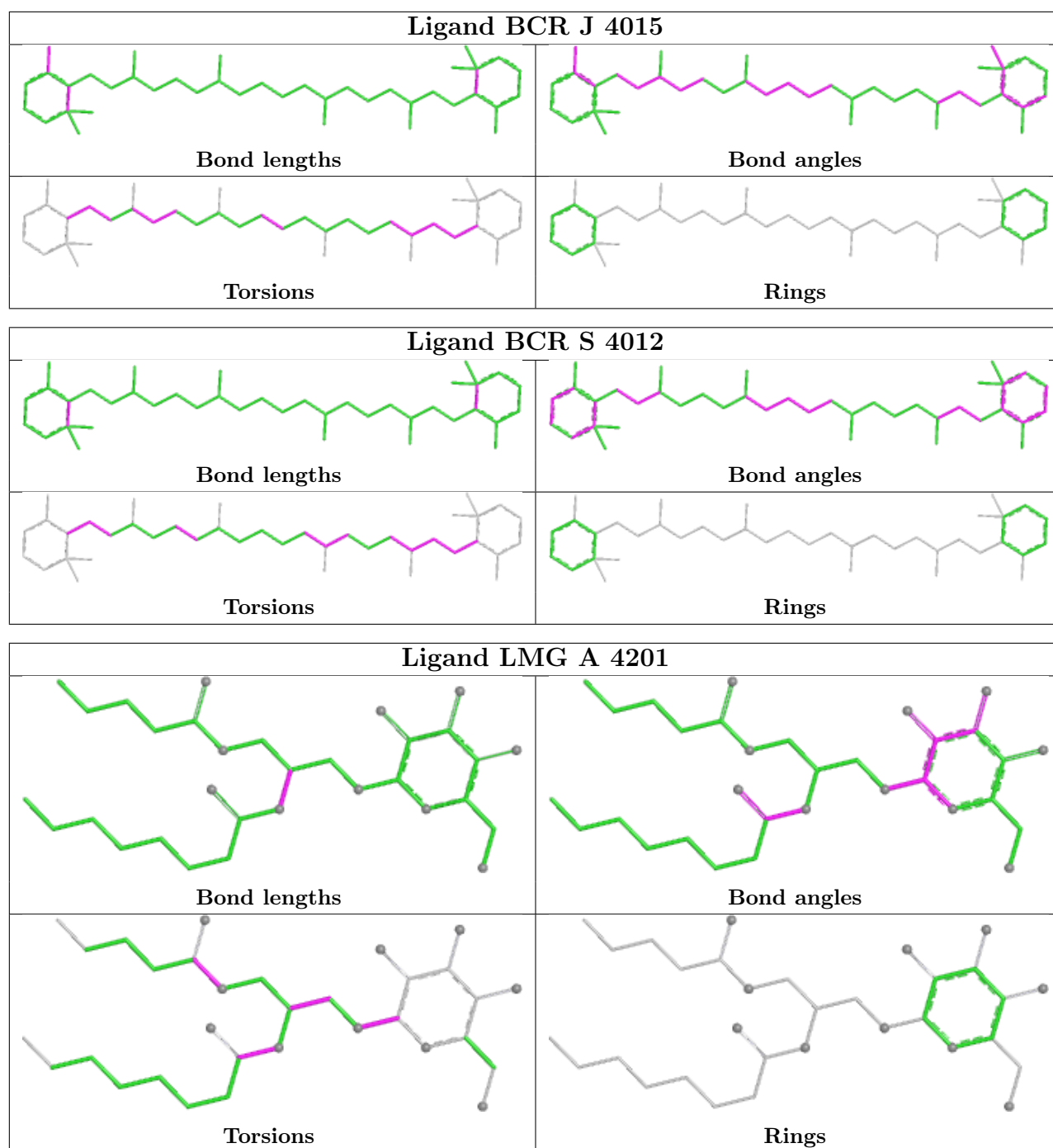
Ligand CLA H 1131



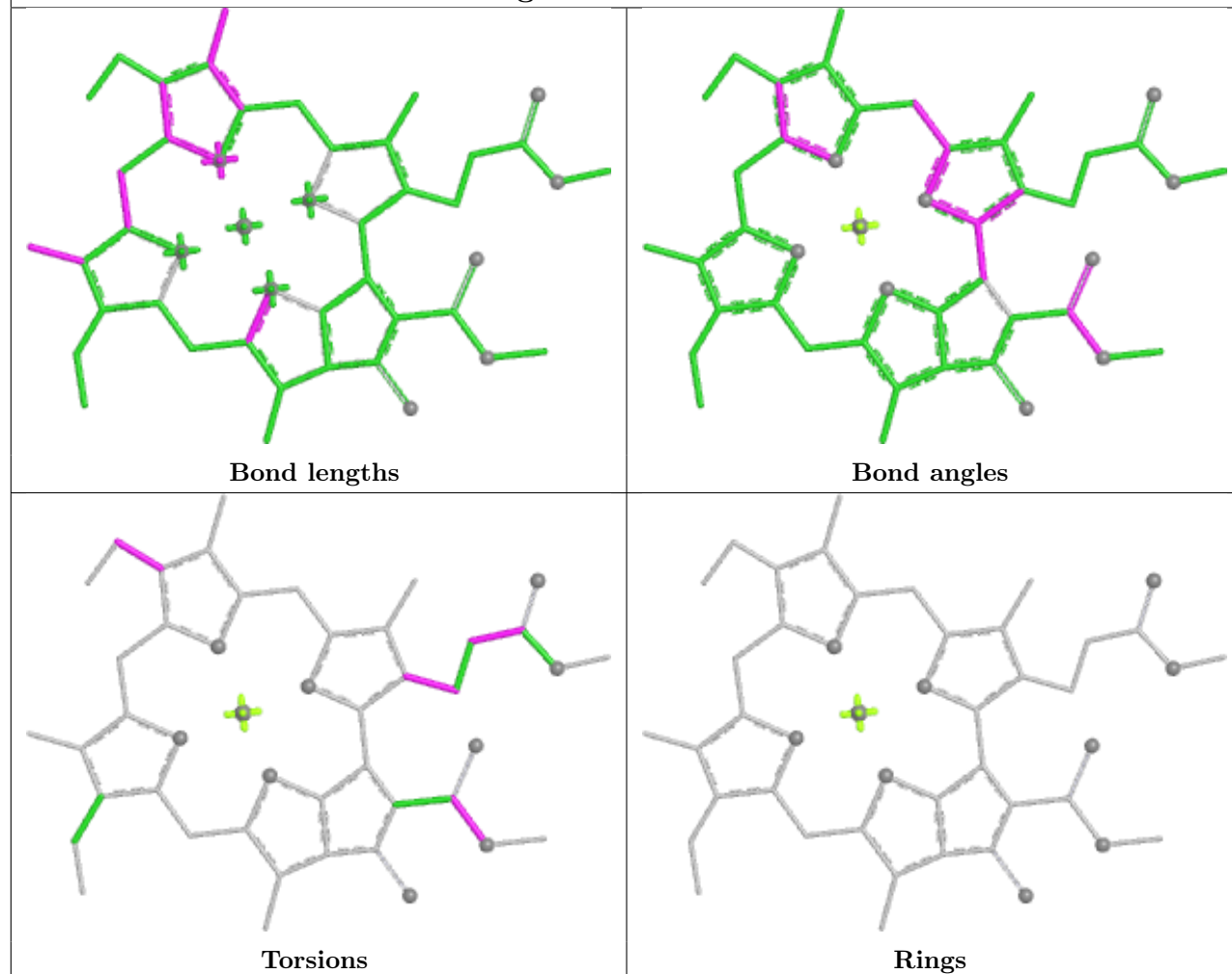
Ligand CLA n 503



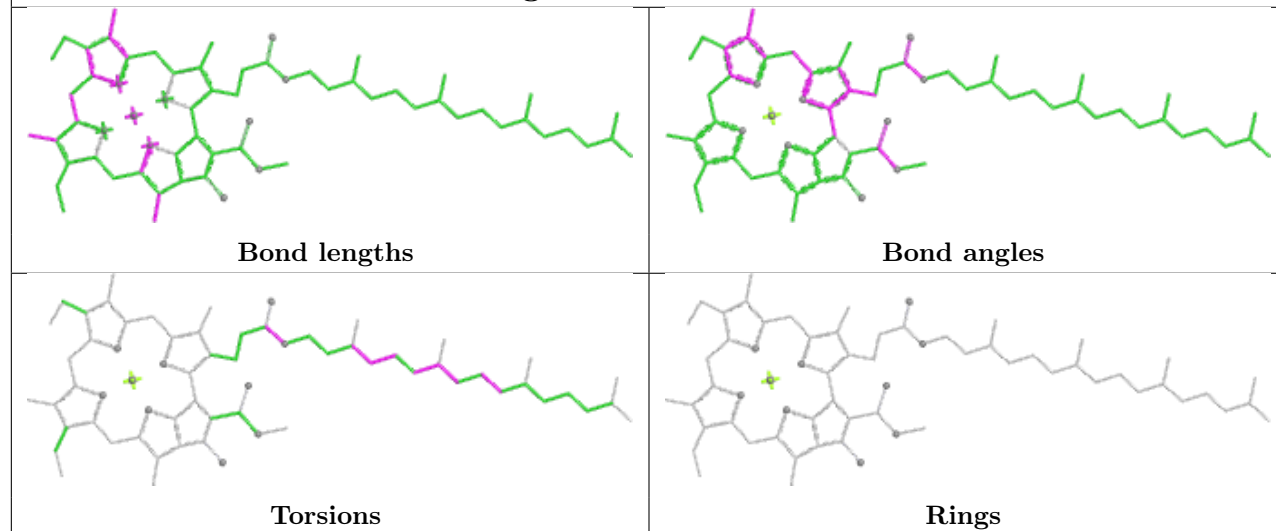


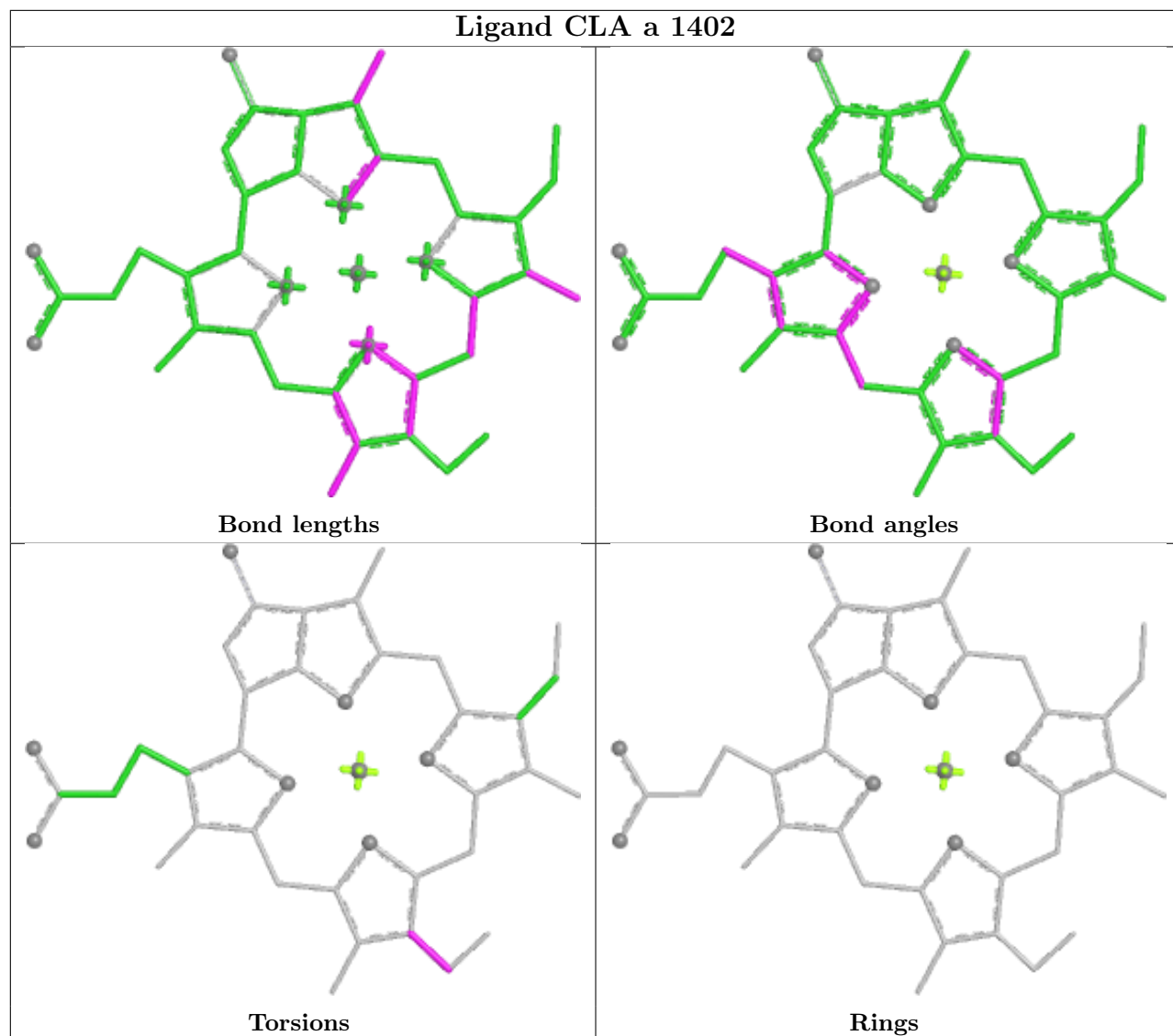


Ligand CLA v 516

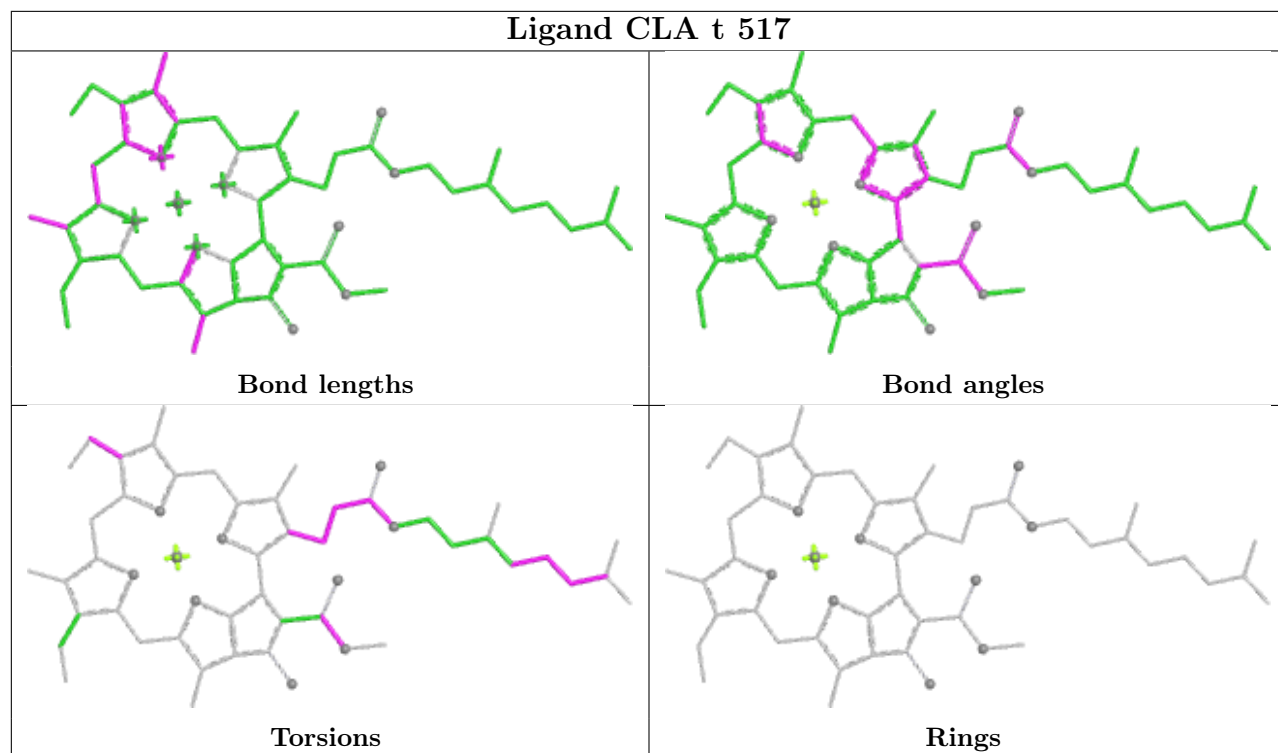


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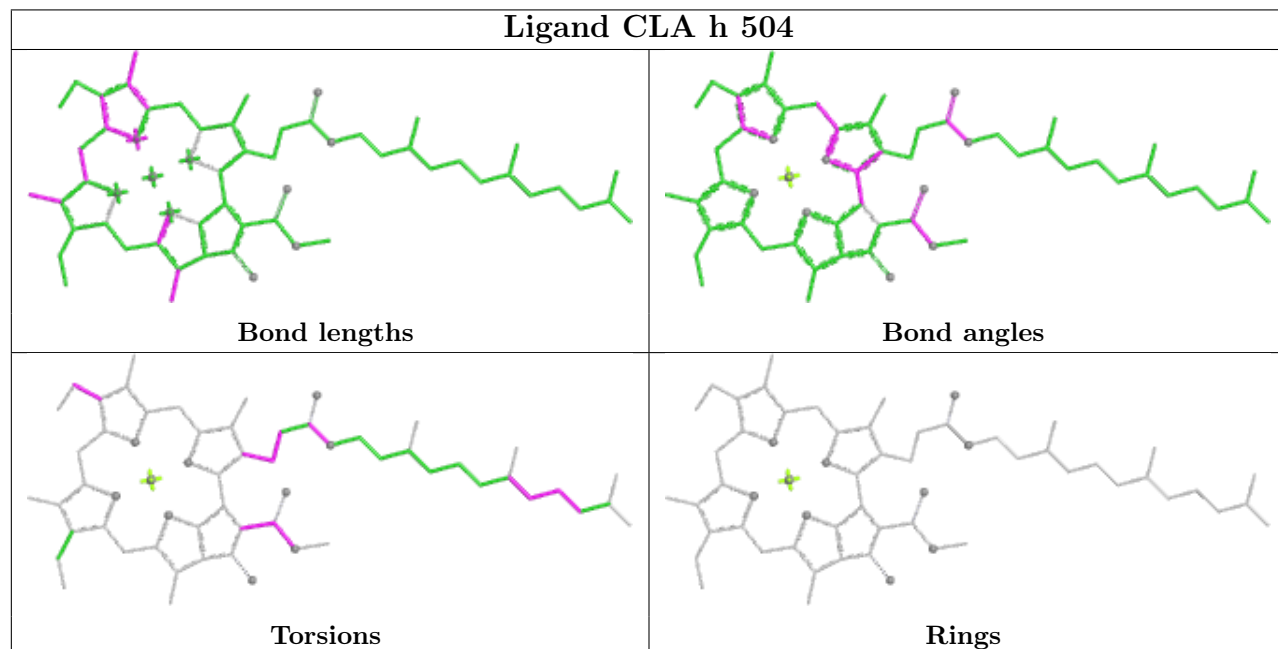


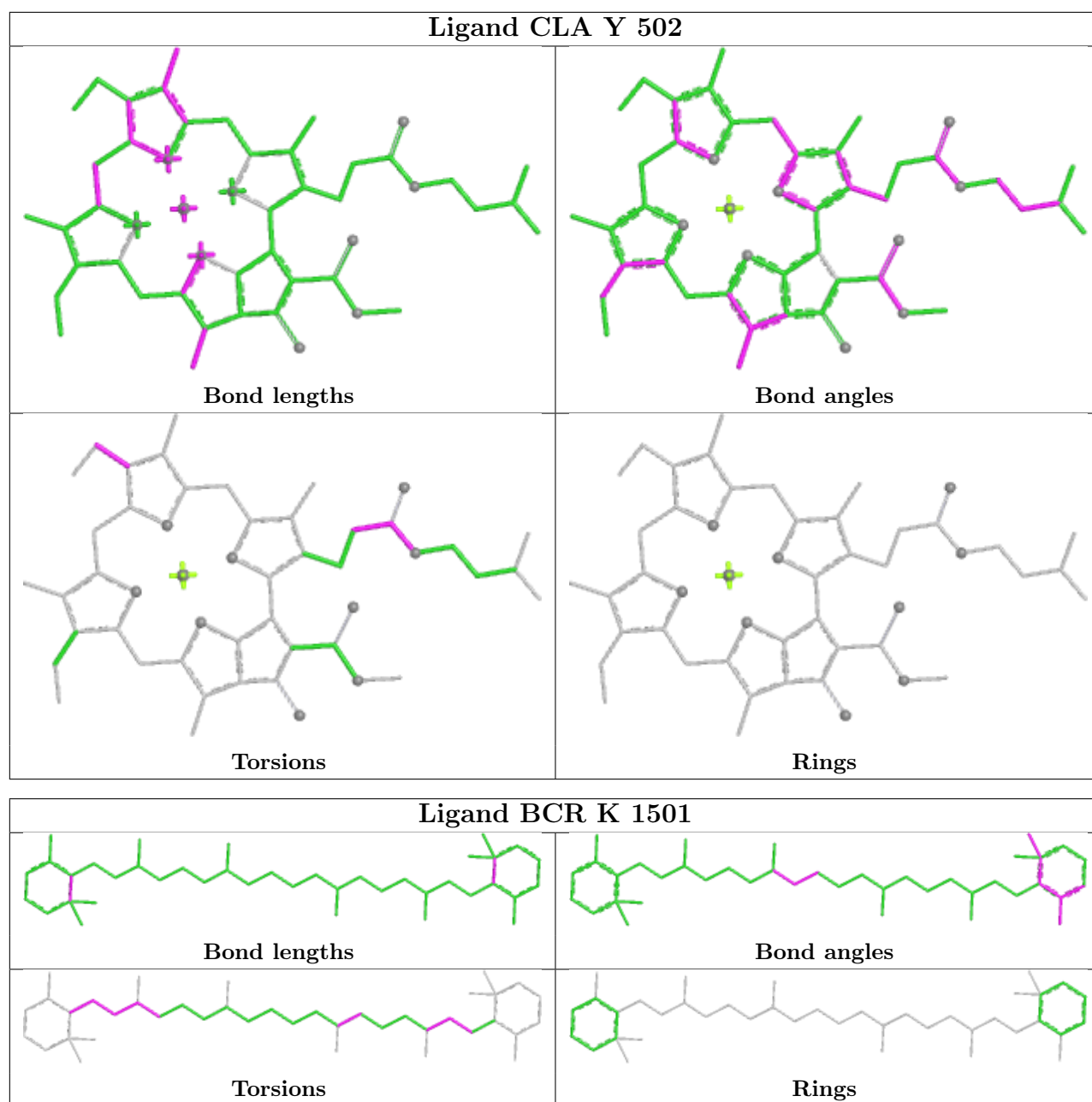


Ligand CLA t 517

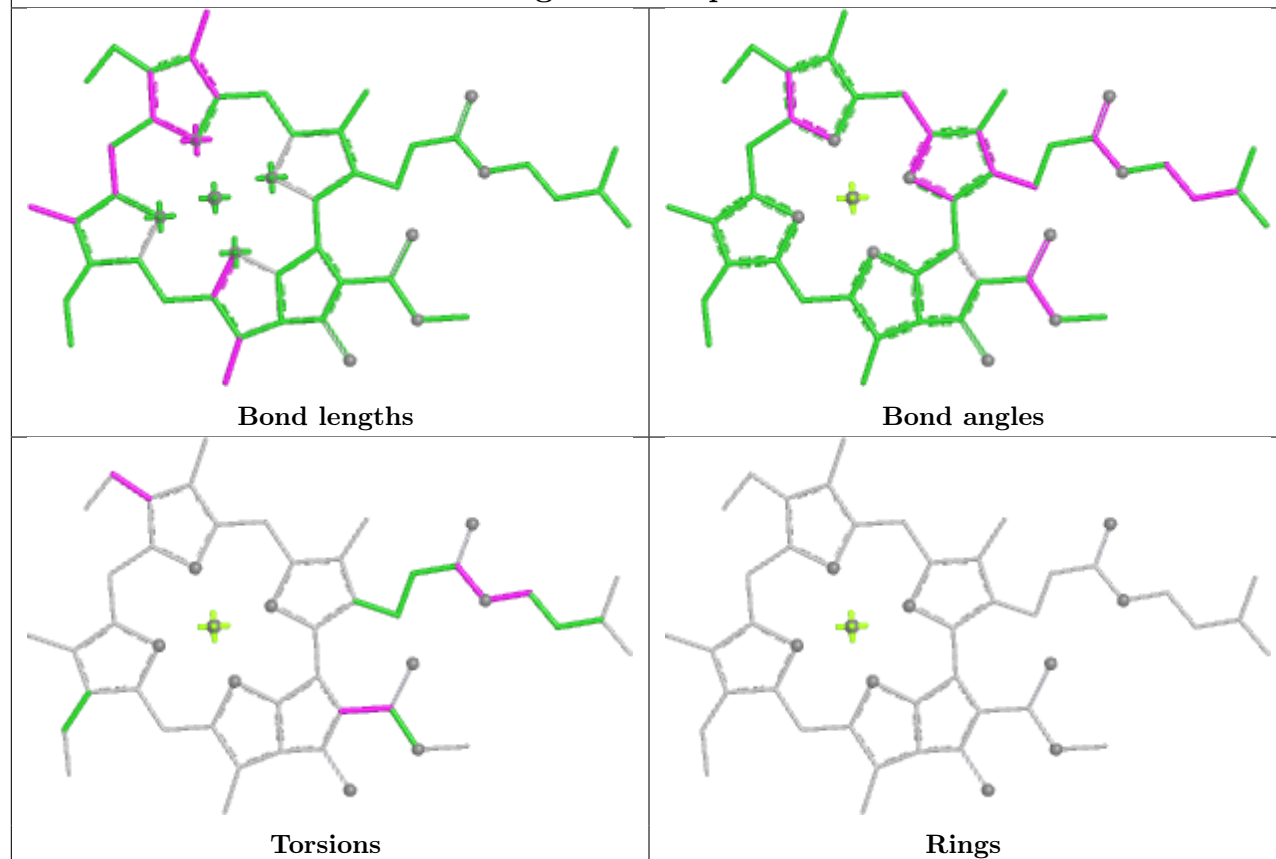


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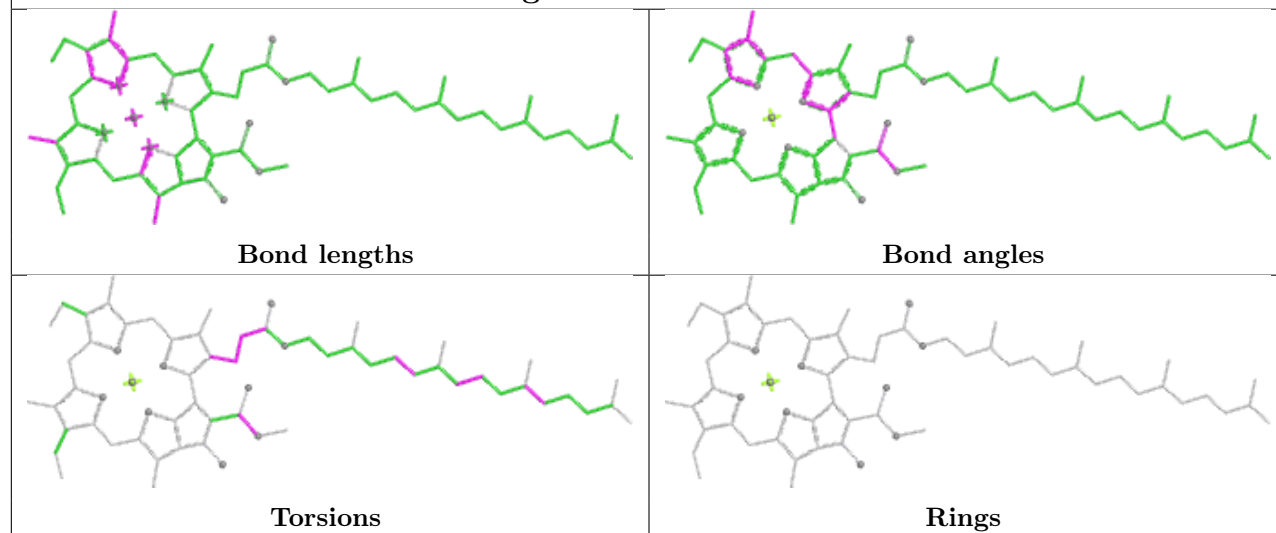


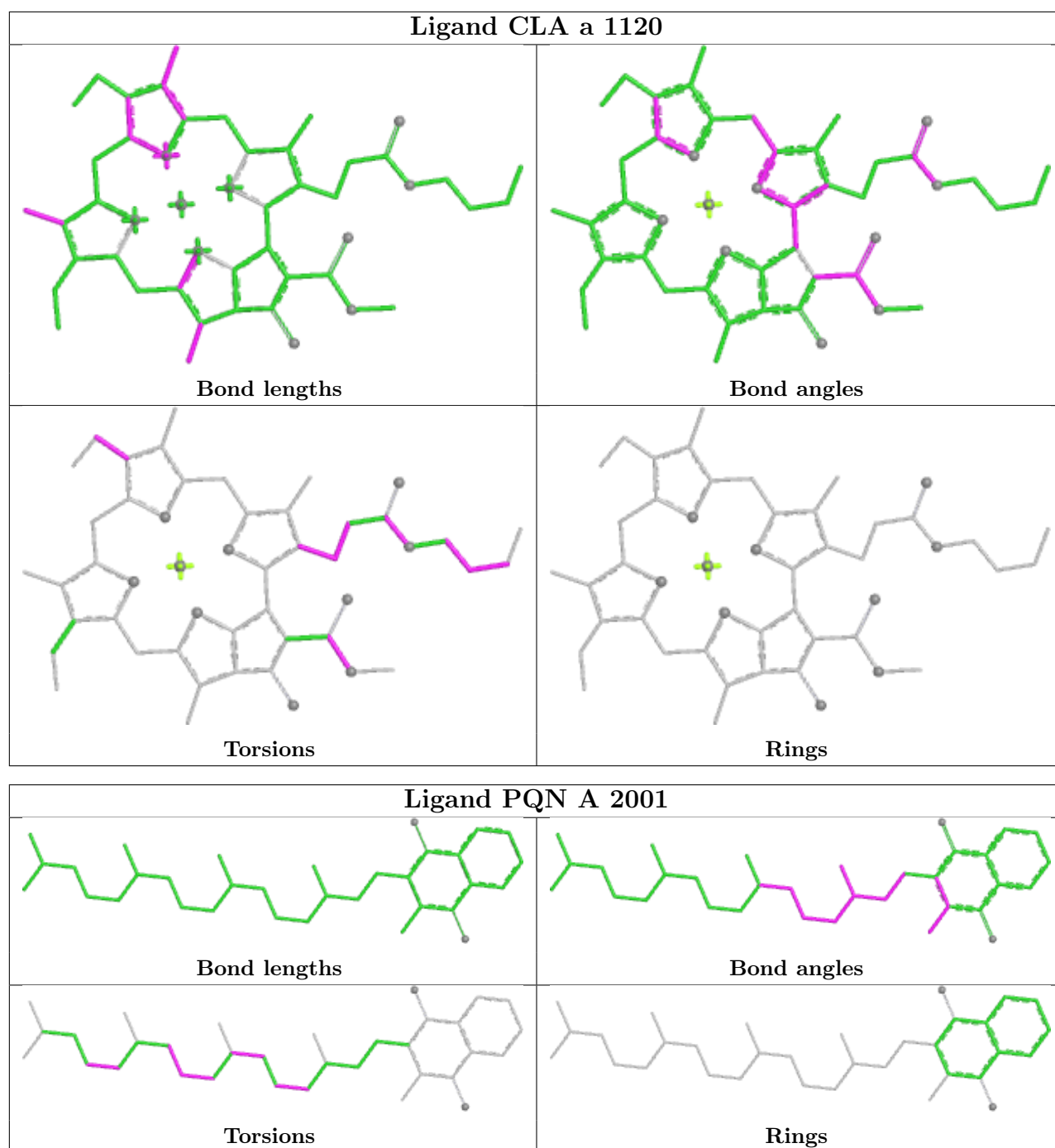


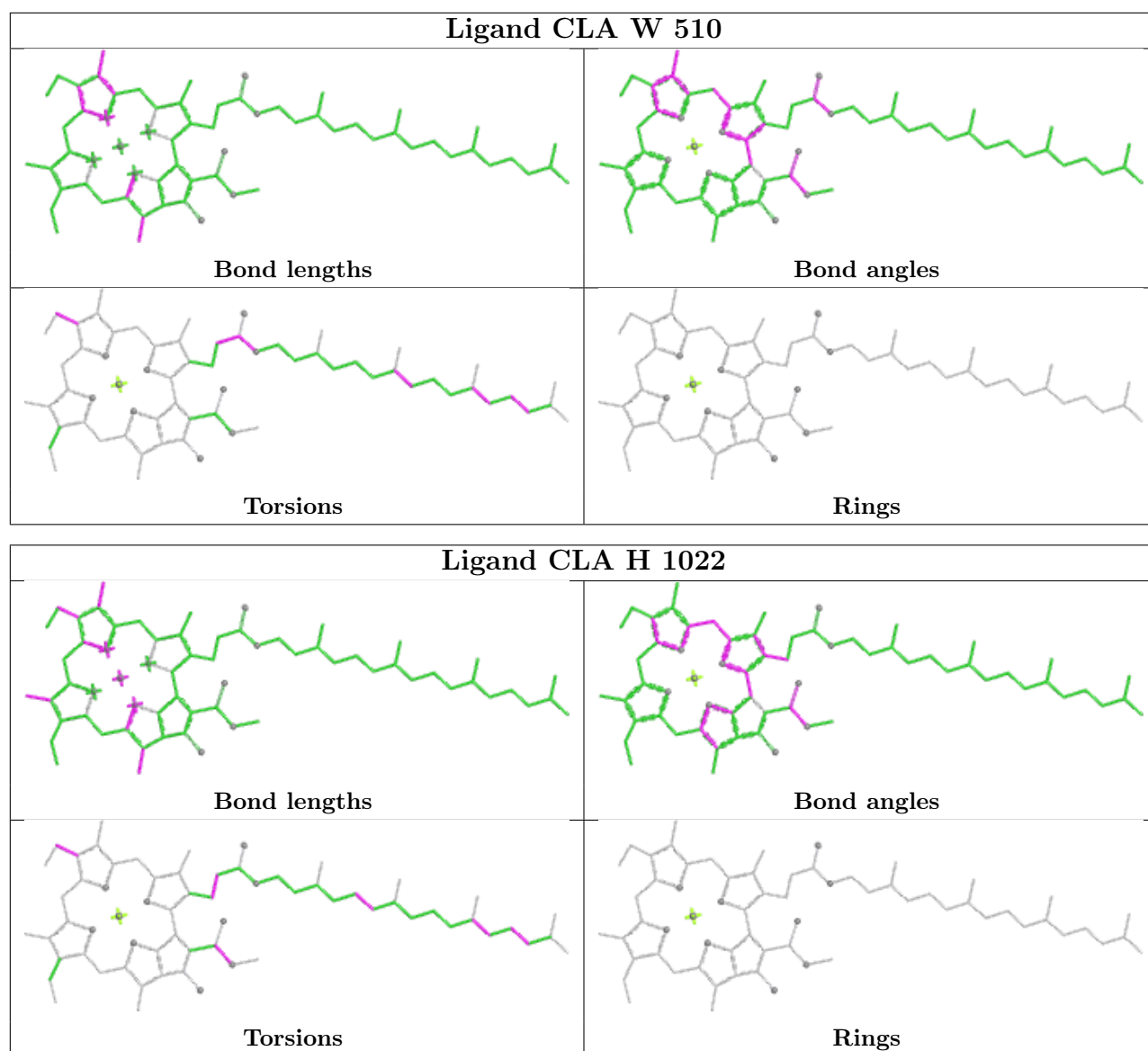
Ligand CLA p 501



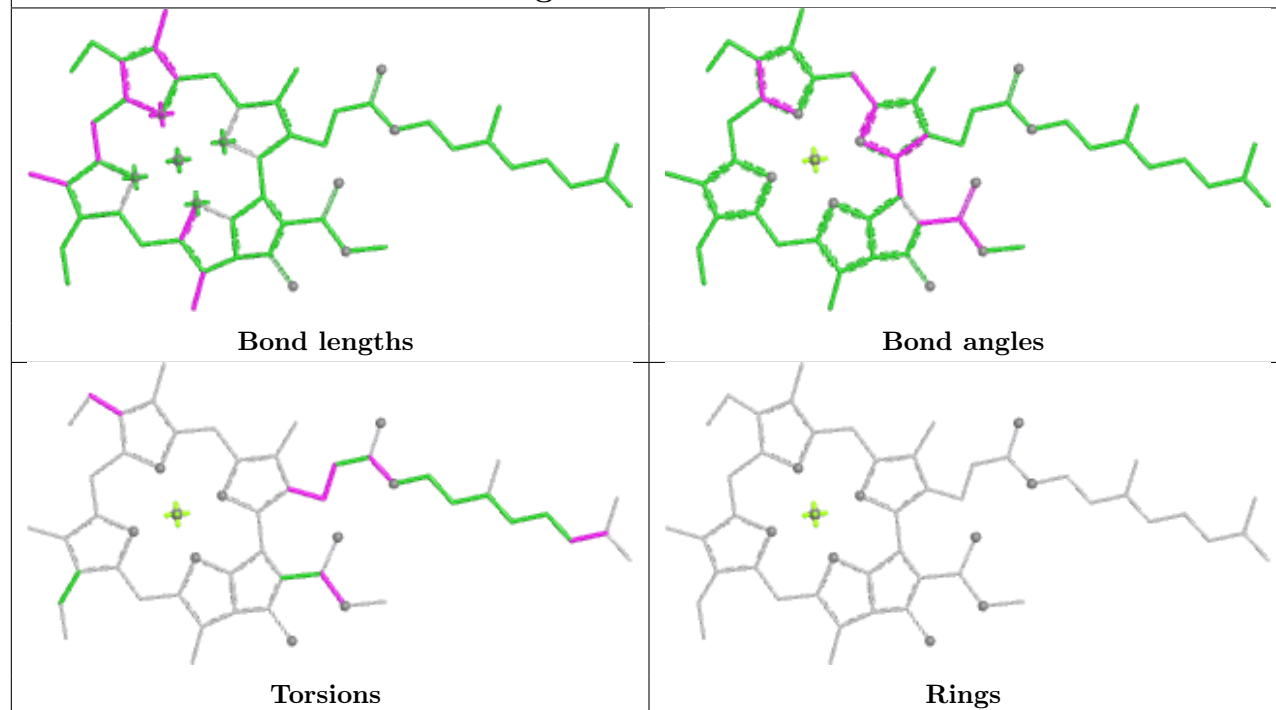
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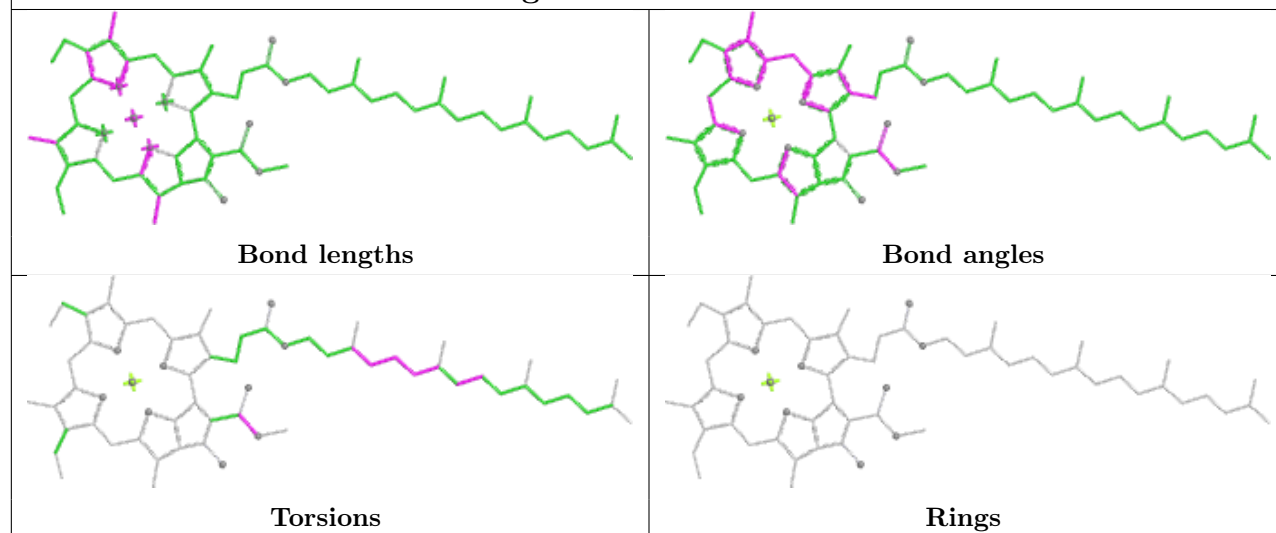


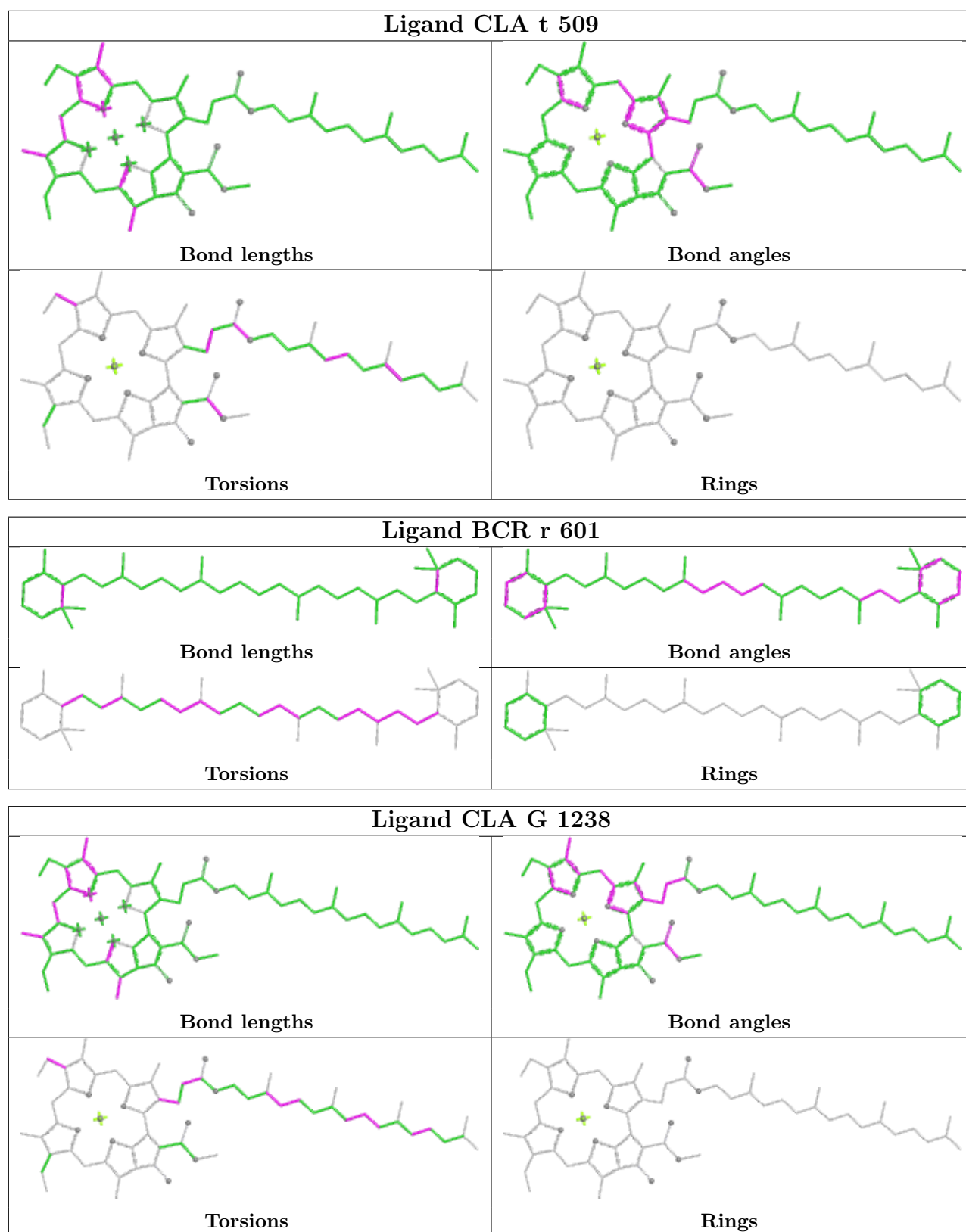


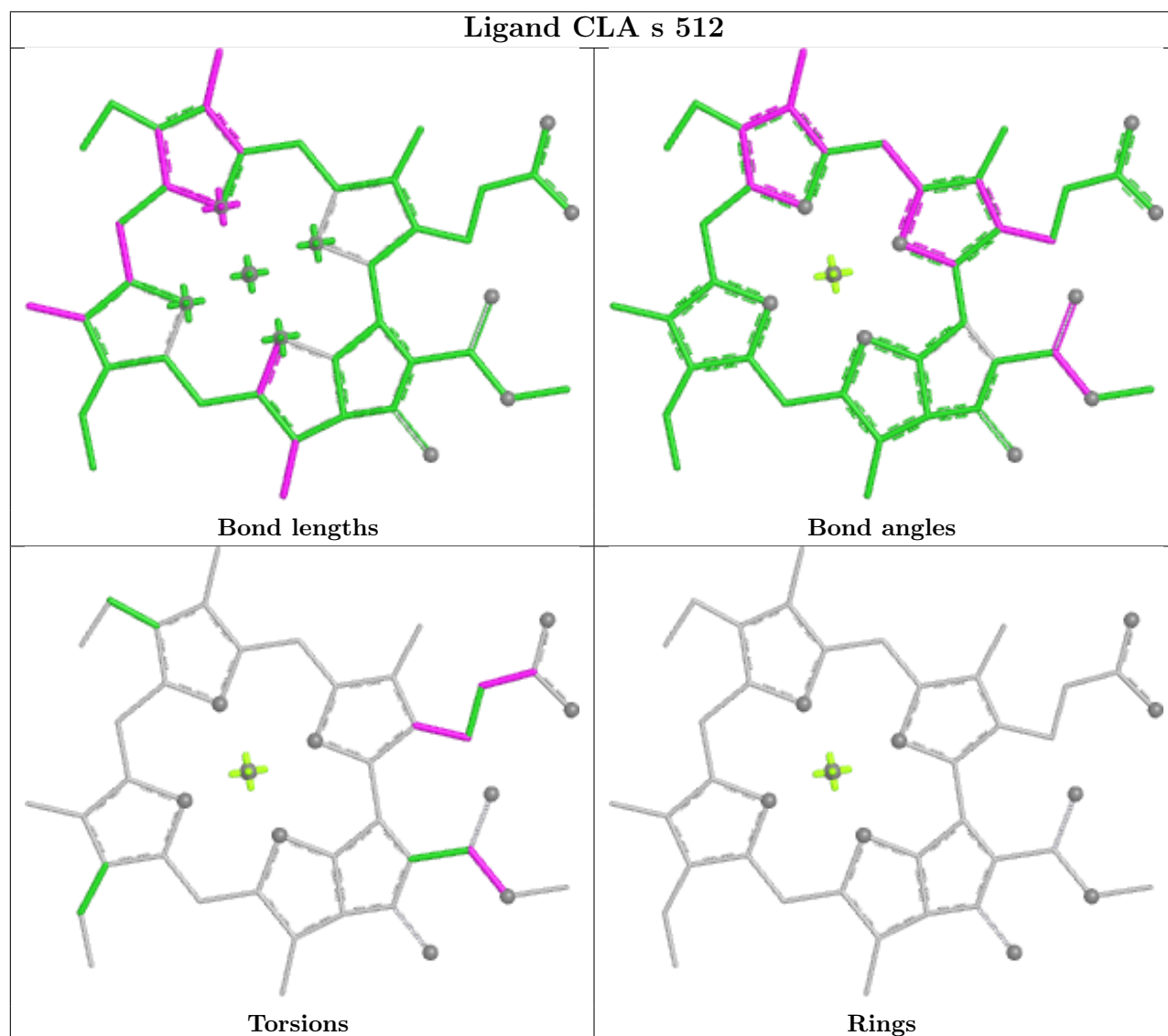
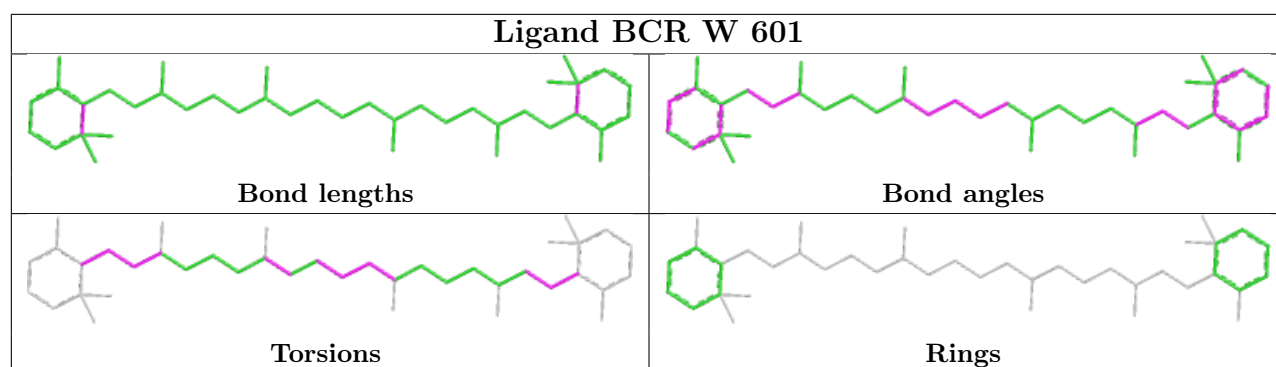
Ligand CLA u 508



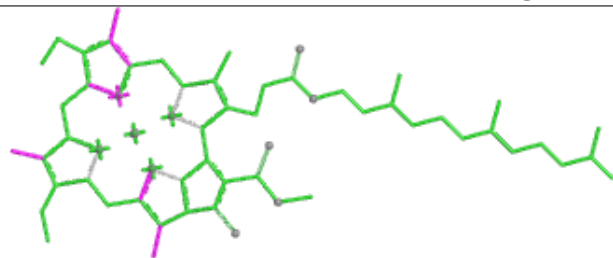
Ligand CLA G 1226



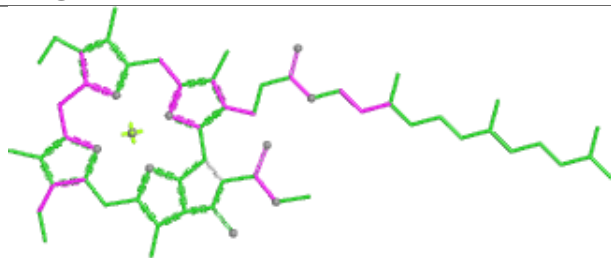




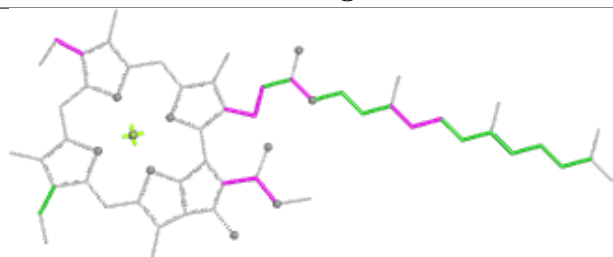
Ligand CLA g 506



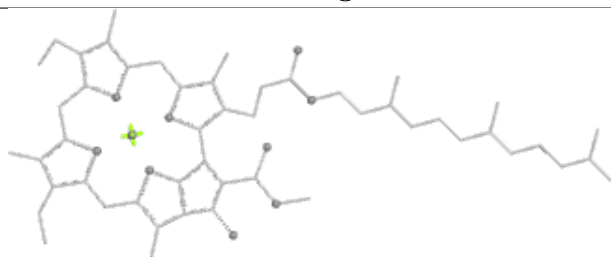
Bond lengths



Bond angles

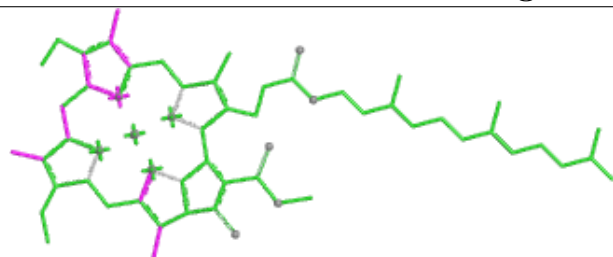


Torsions

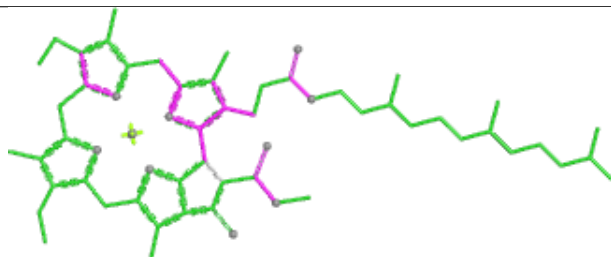


Rings

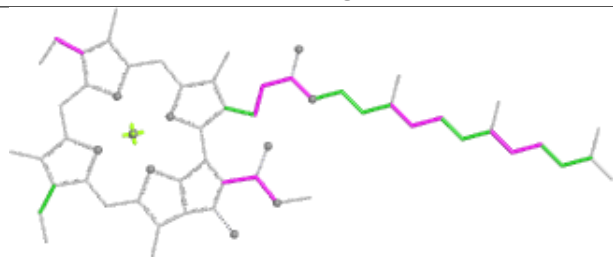
Ligand CLA h 505



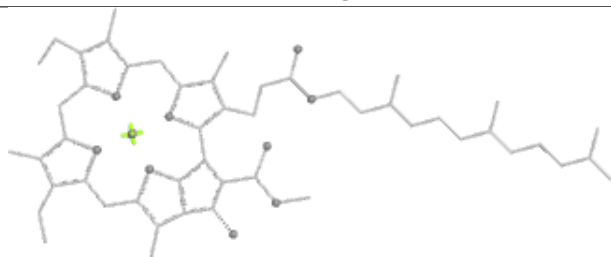
Bond lengths



Bond angles

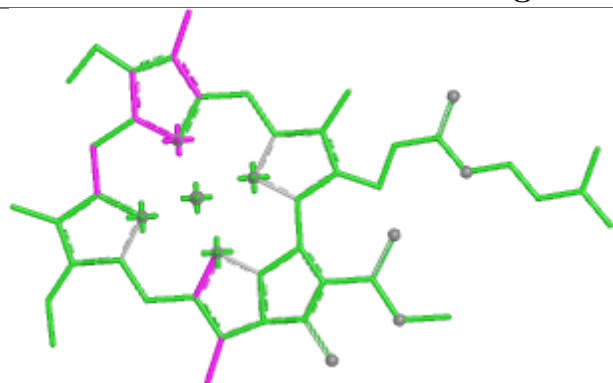


Torsions

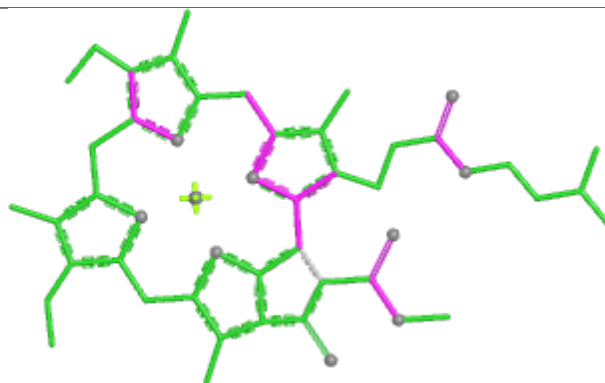


Rings

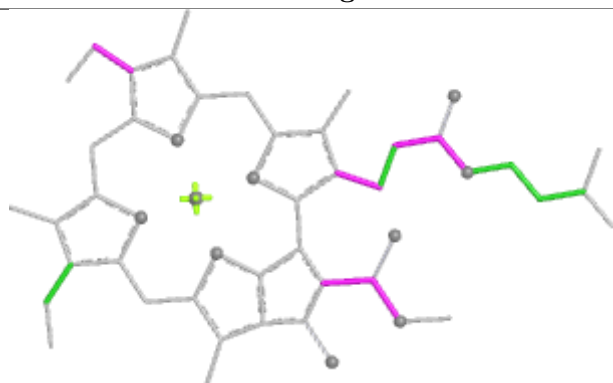
Ligand CLA X 514



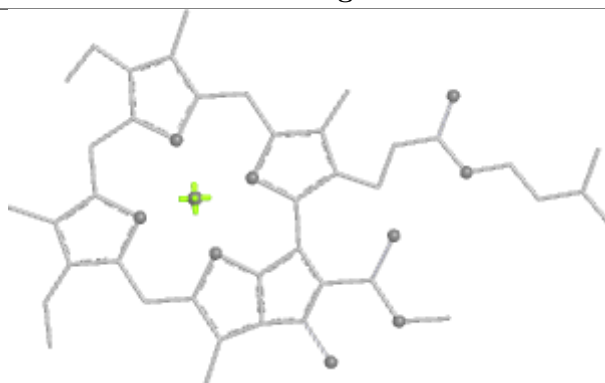
Bond lengths



Bond angles

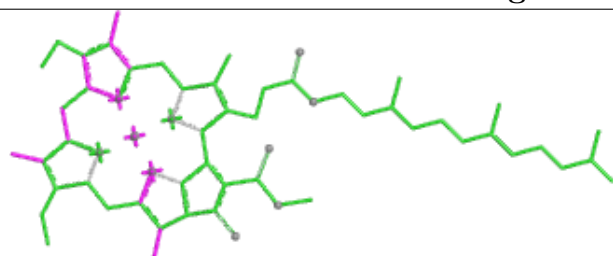


Torsions

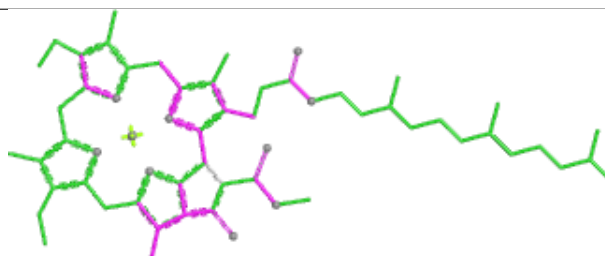


Rings

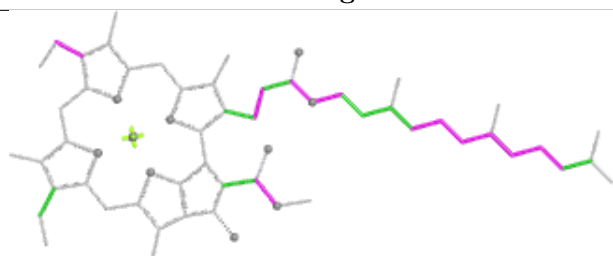
Ligand CLA b 1012



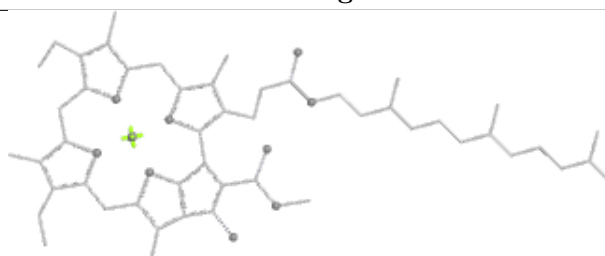
Bond lengths



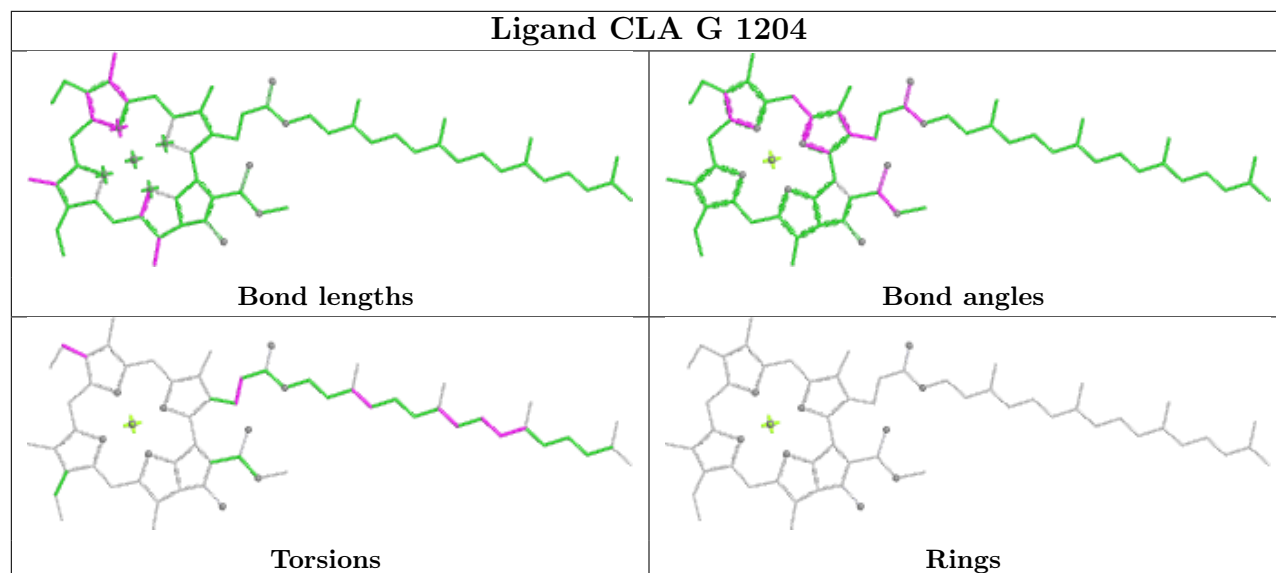
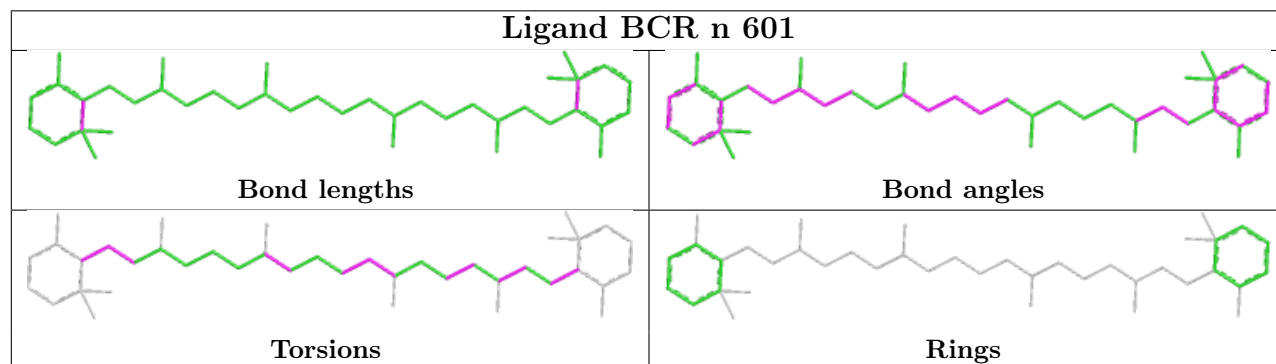
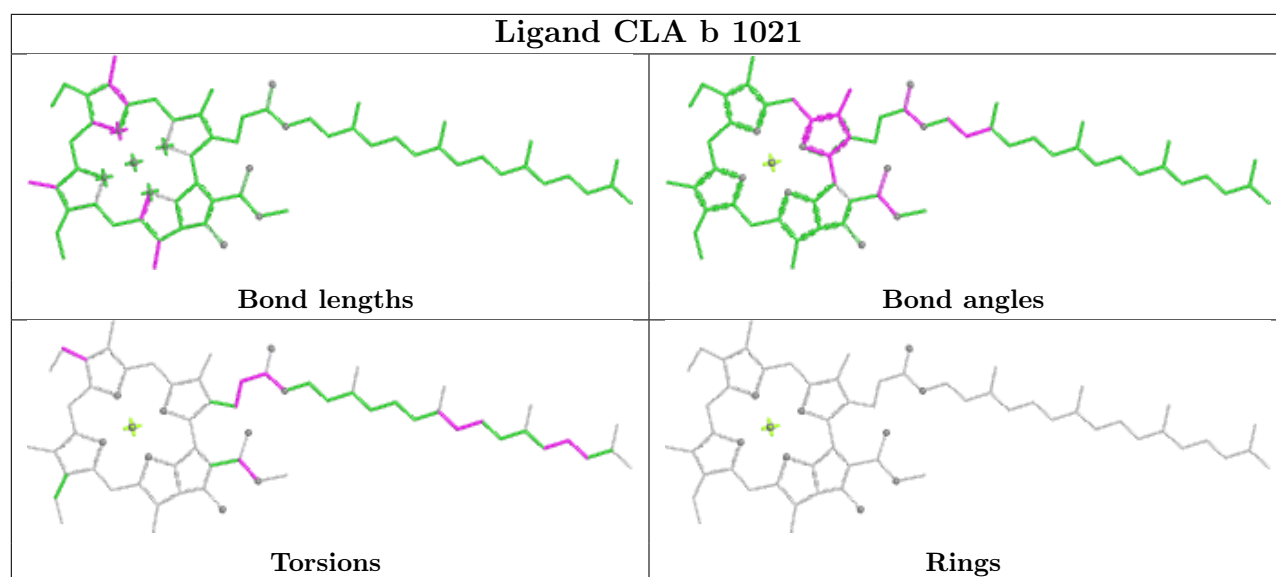
Bond angles

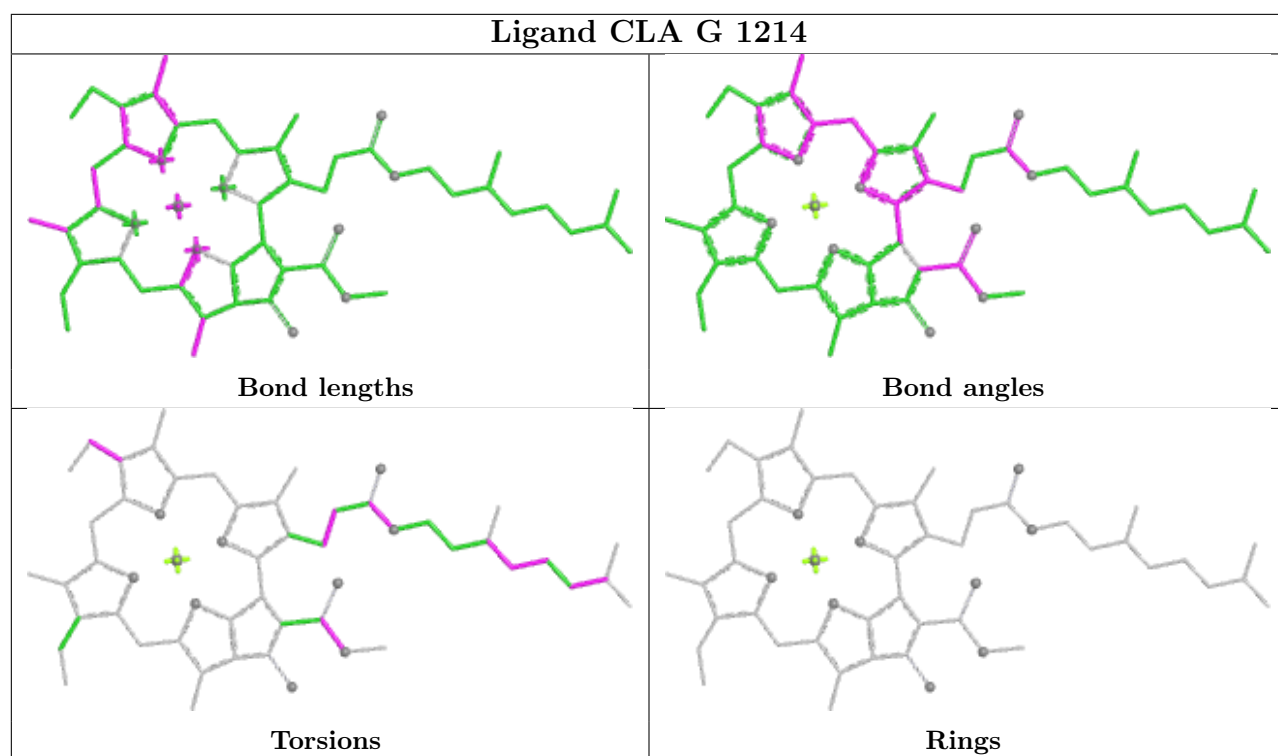


Torsions

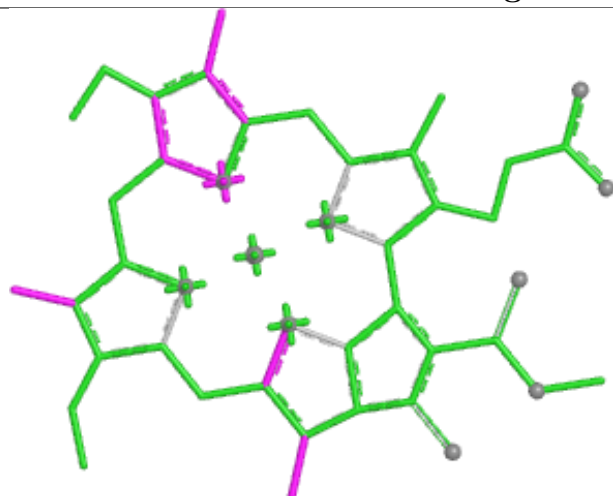


Rings

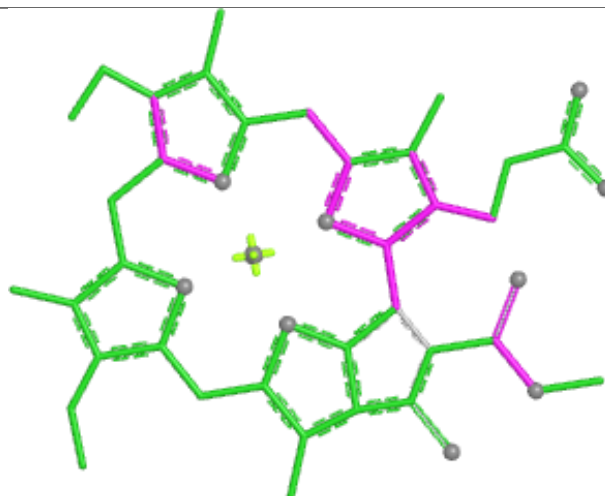




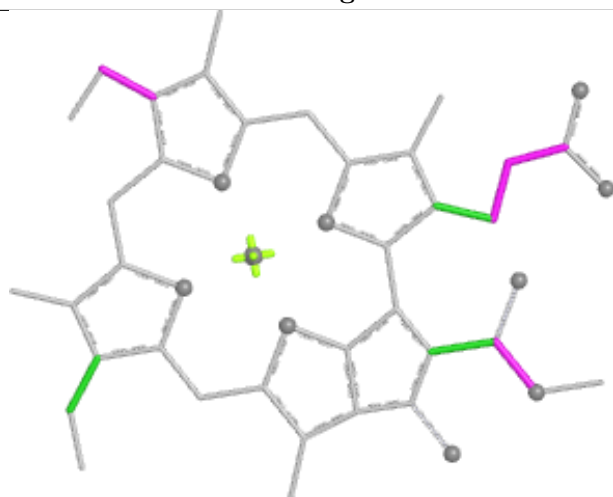
Ligand CLA G 1219



Bond lengths



Bond angles

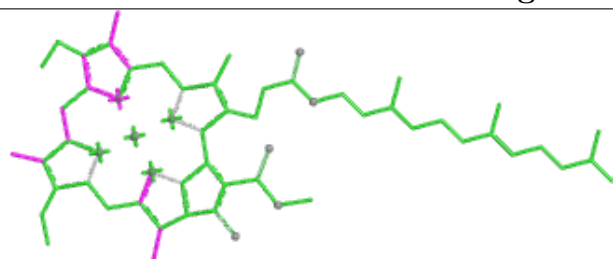


Torsions

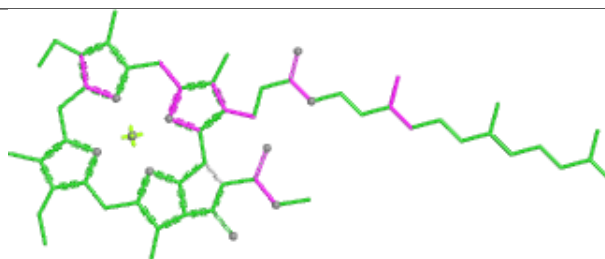


Rings

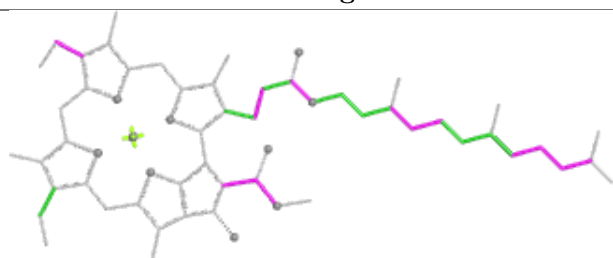
Ligand CLA x 506



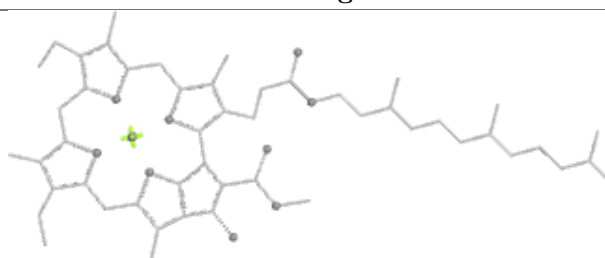
Bond lengths



Bond angles

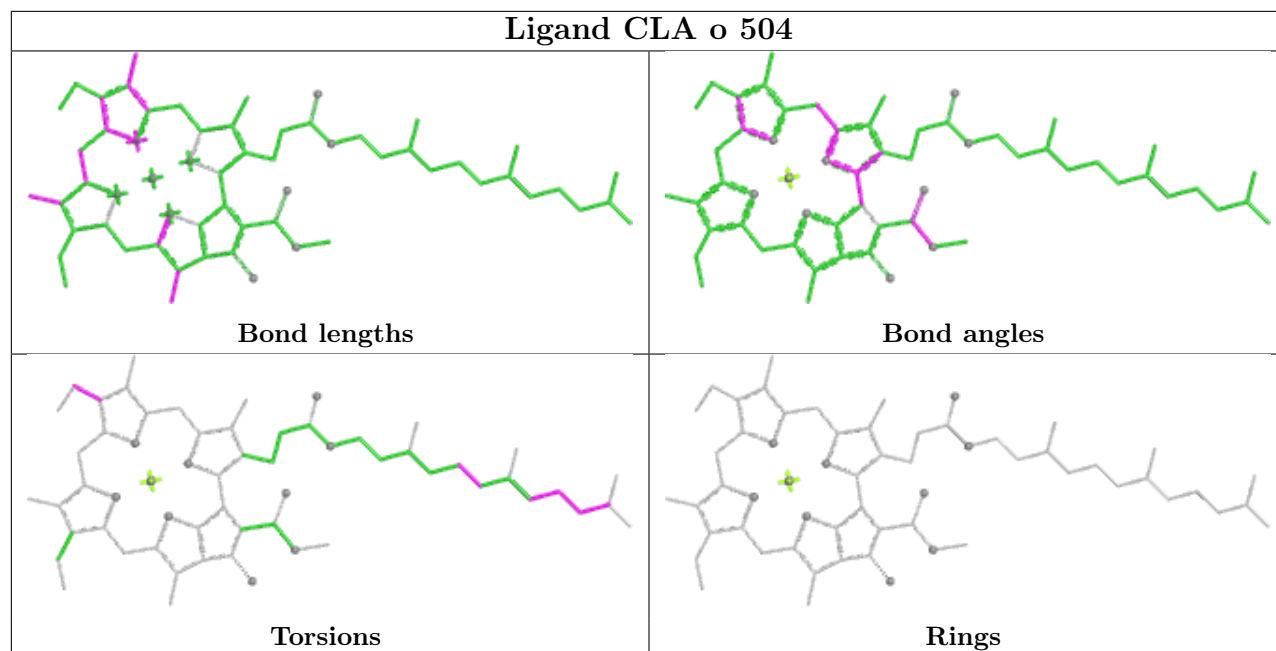


Torsions

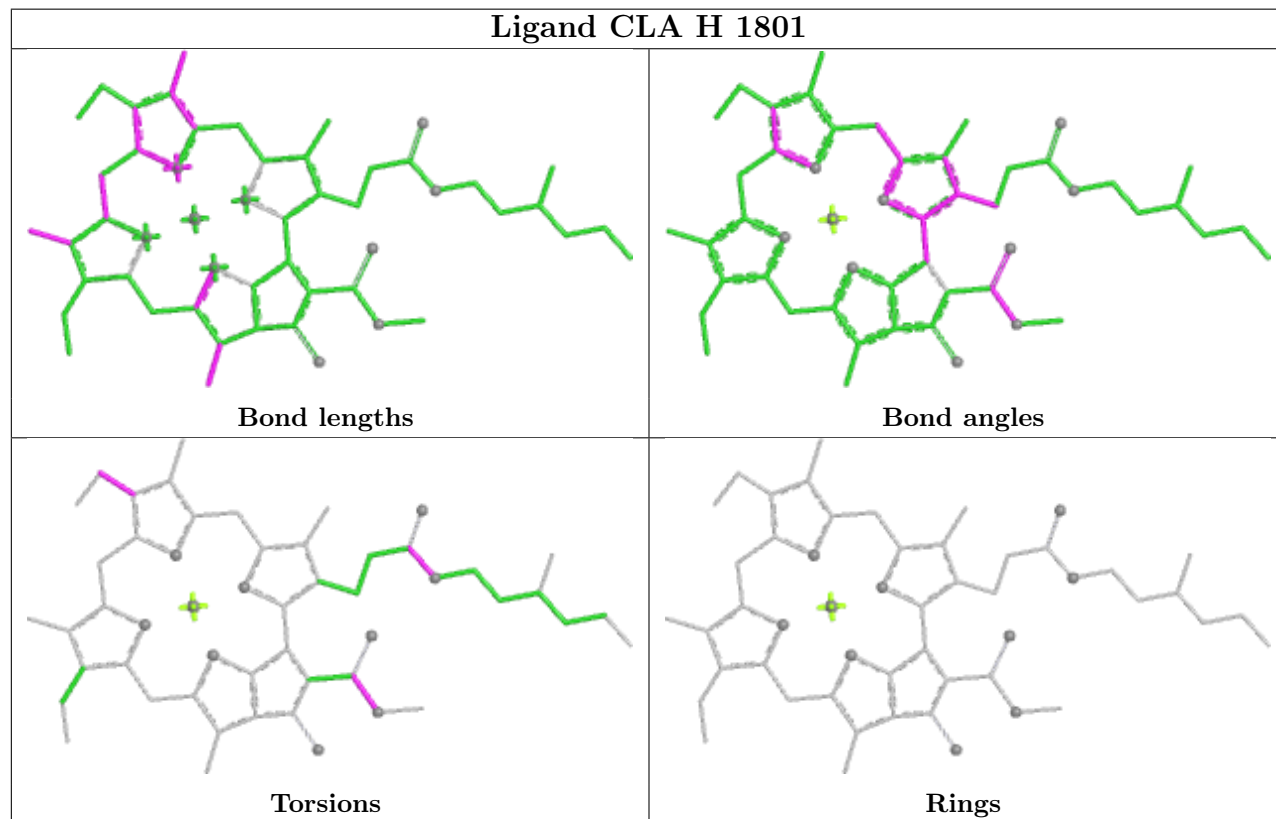


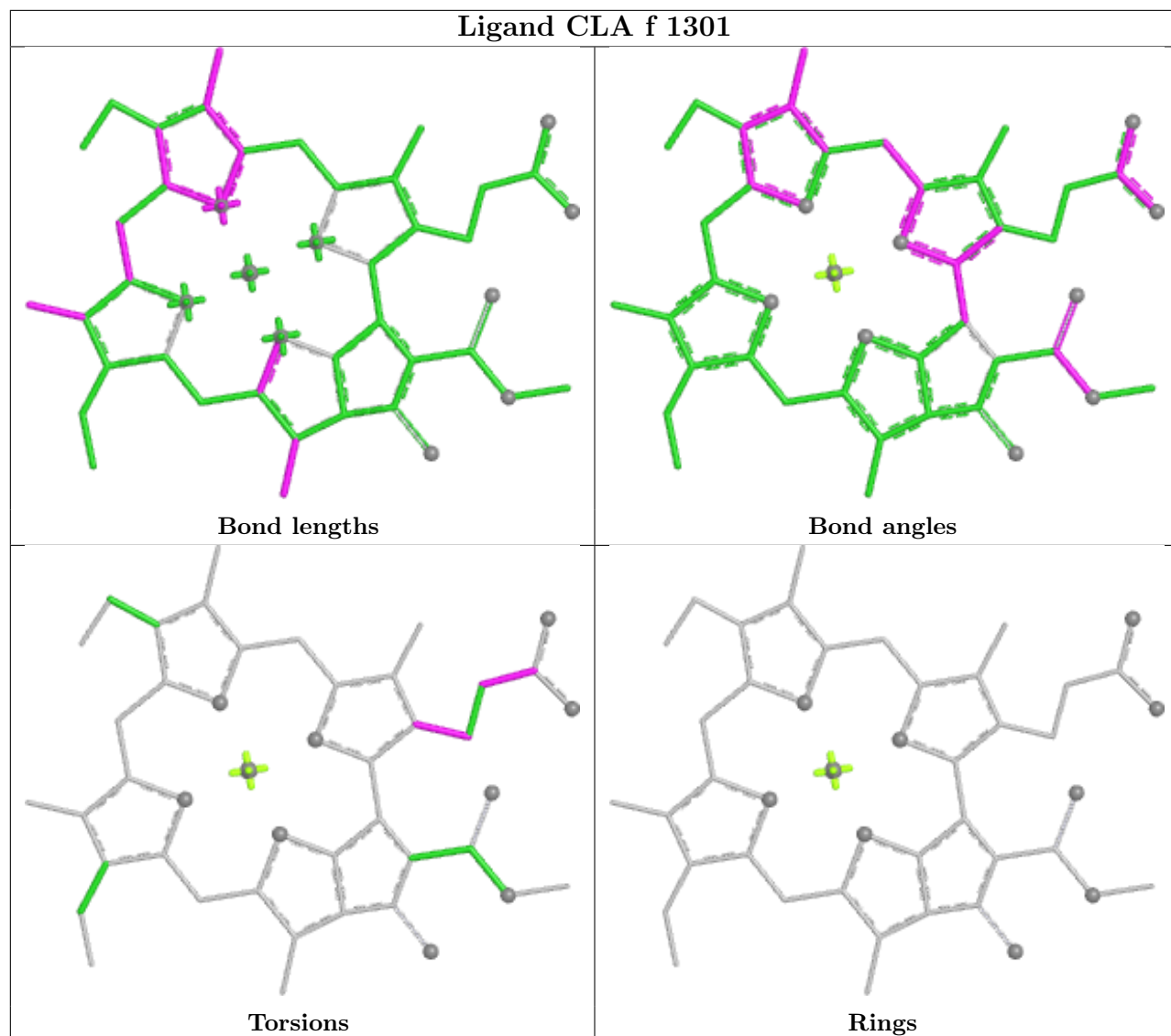
Rings

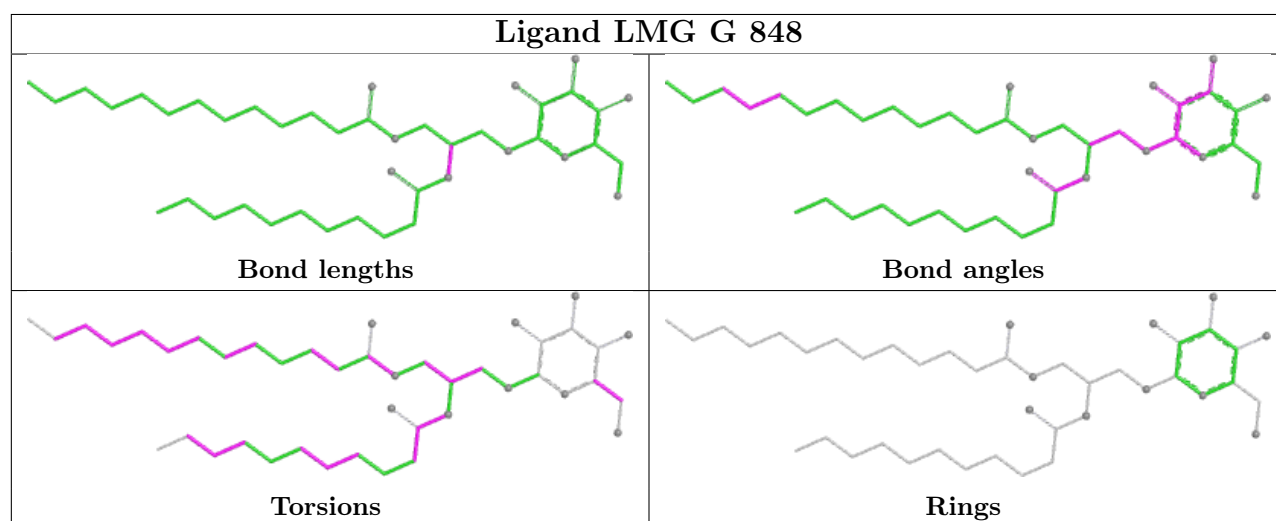
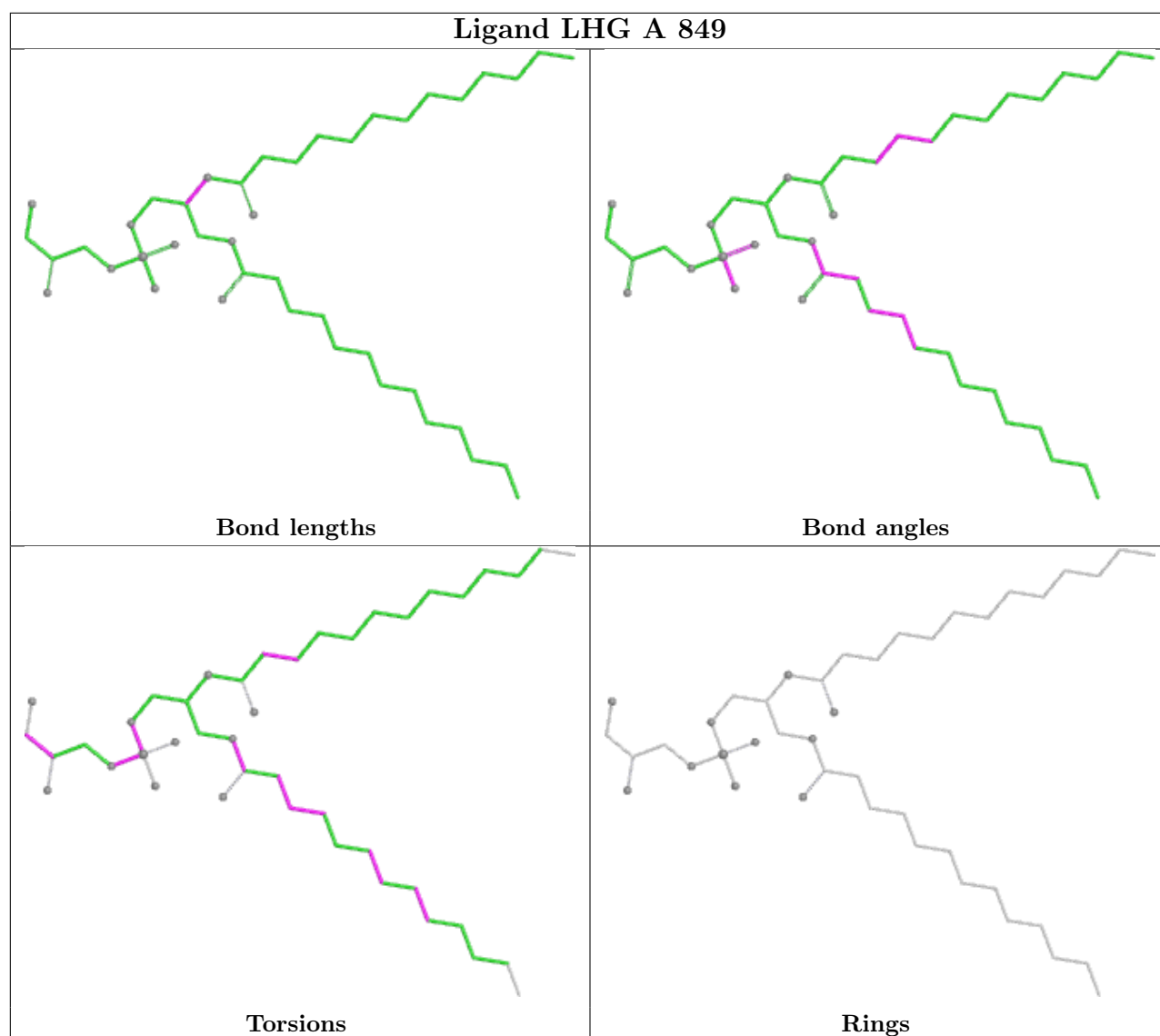
Ligand CLA o 504

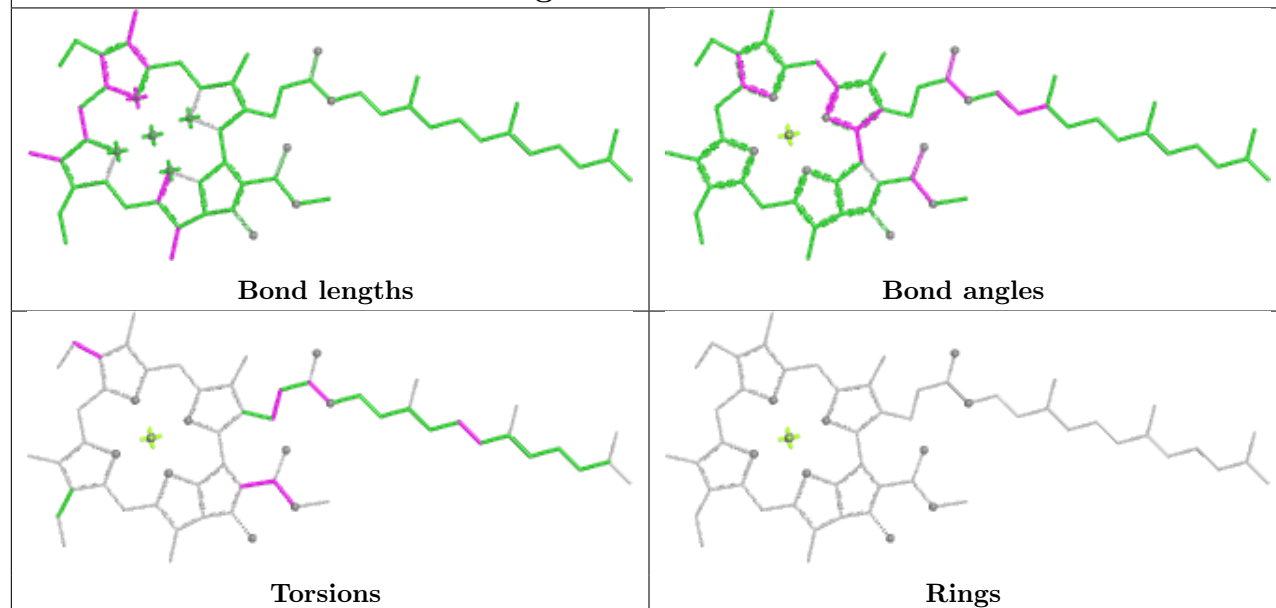
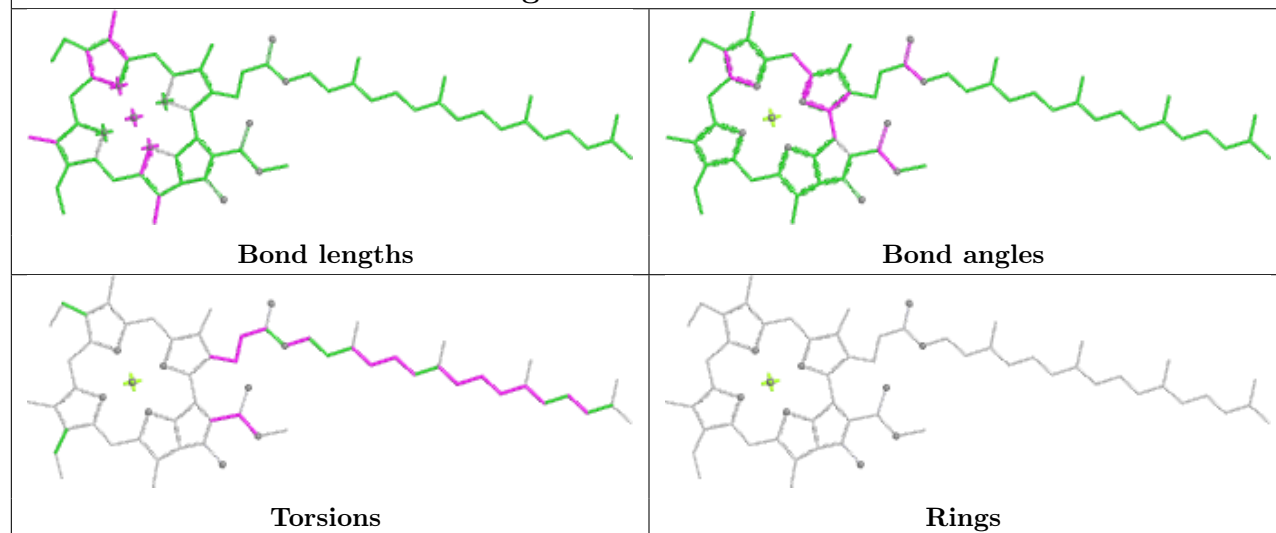


Ligand CLA H 1801

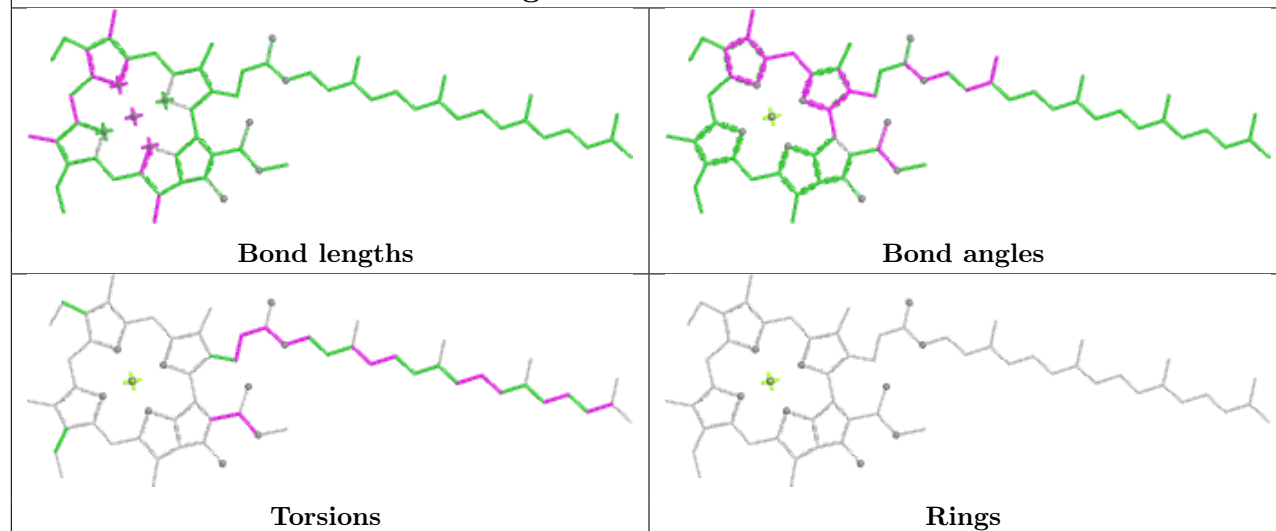




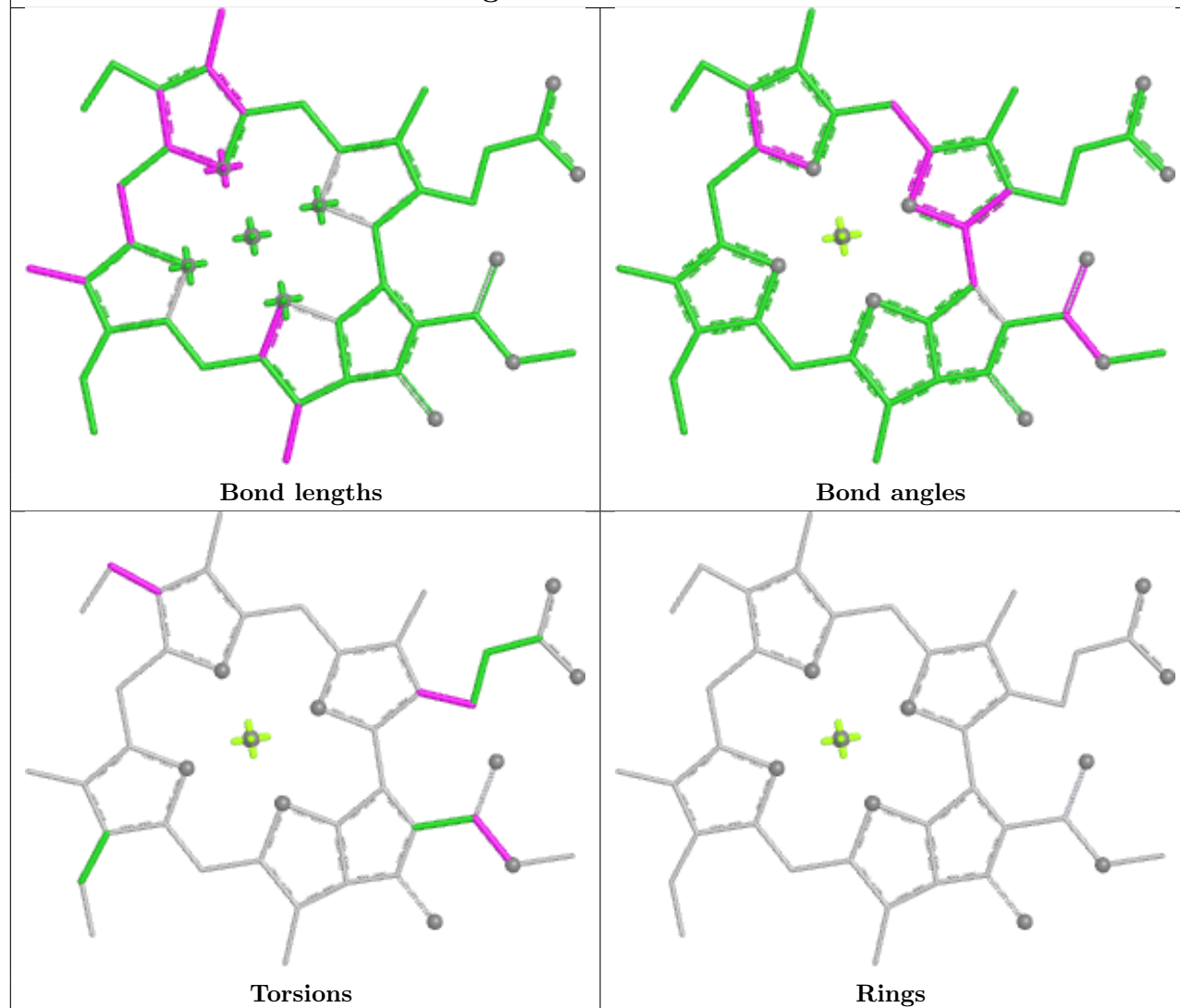


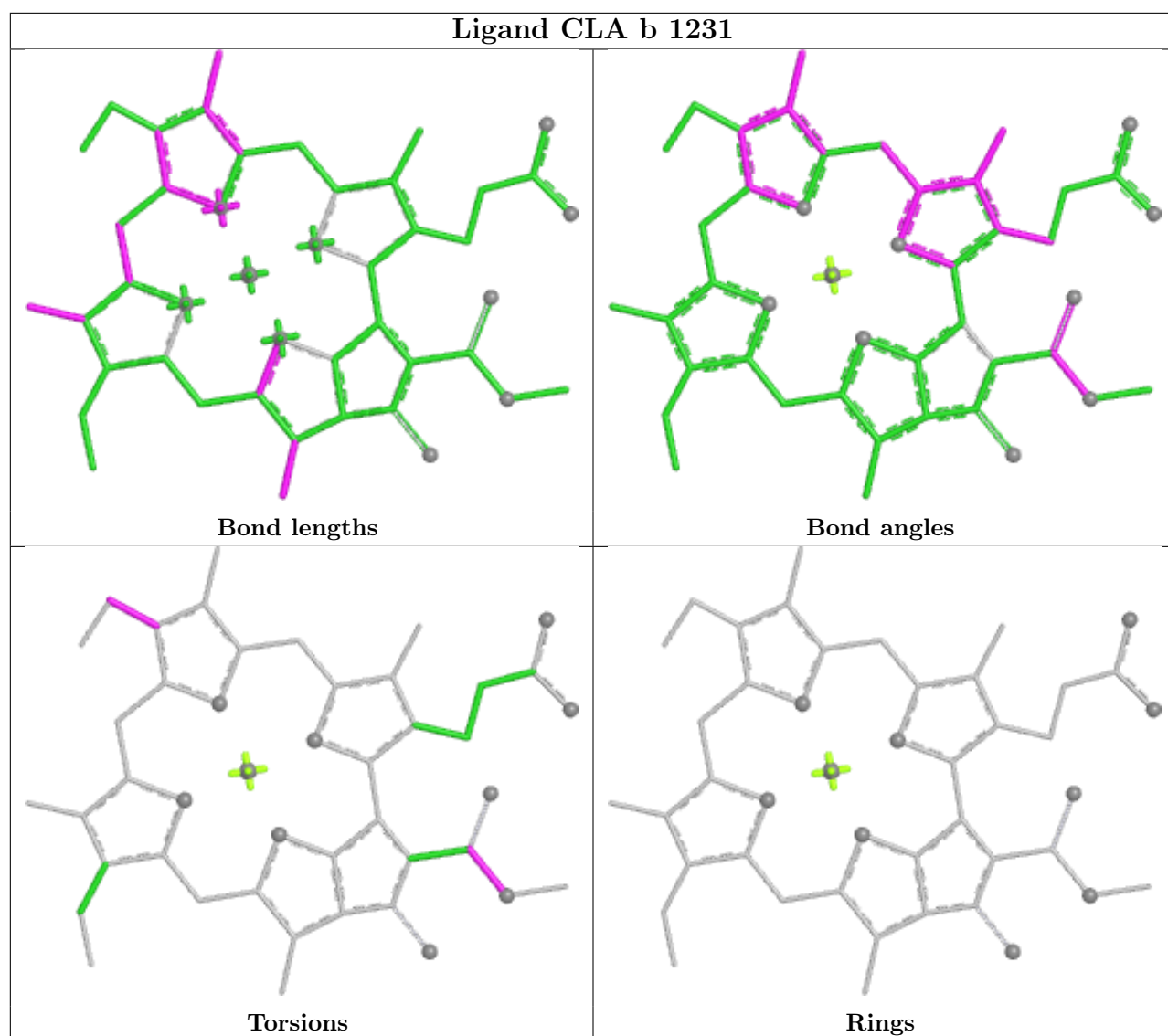
Ligand CLA h 506**Ligand CLA G 1207**

Ligand CLA H 1013

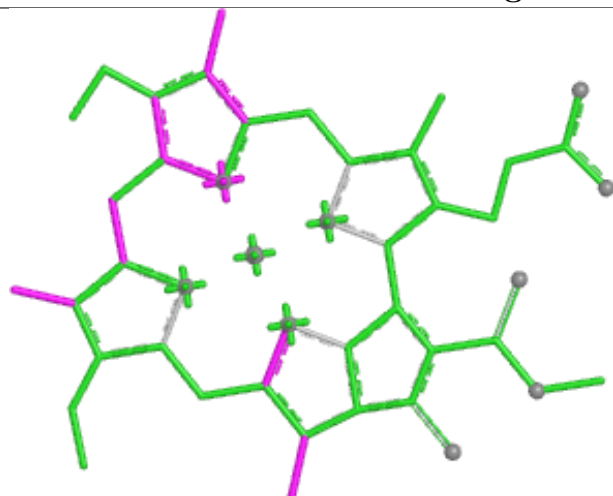


Ligand CLA G 1232

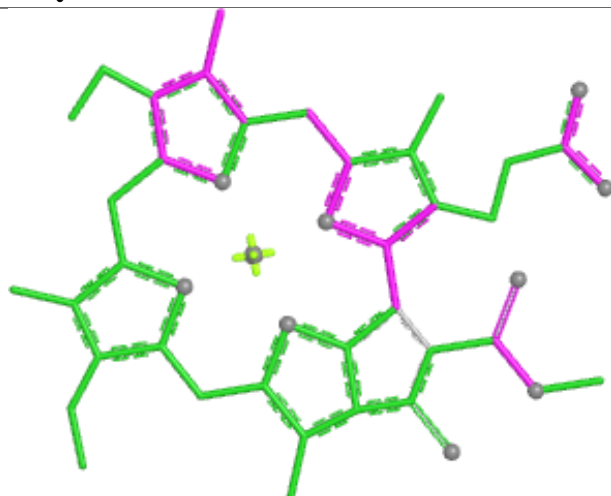




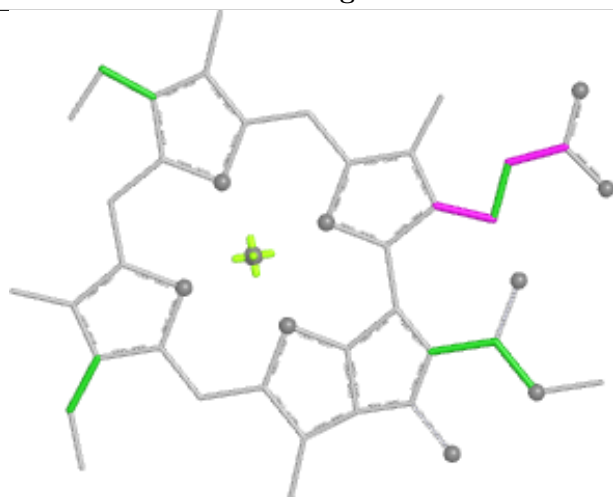
Ligand CLA Q 1301



Bond lengths



Bond angles

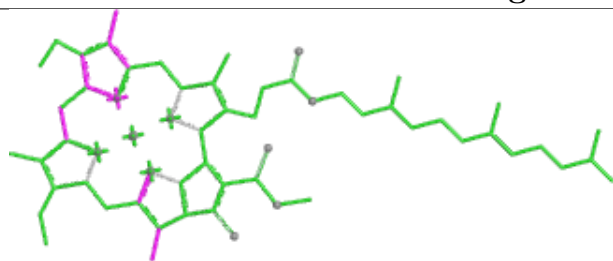


Torsions

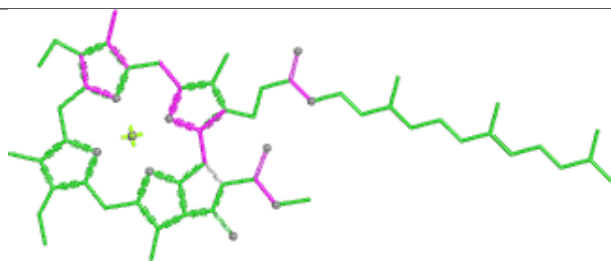


Rings

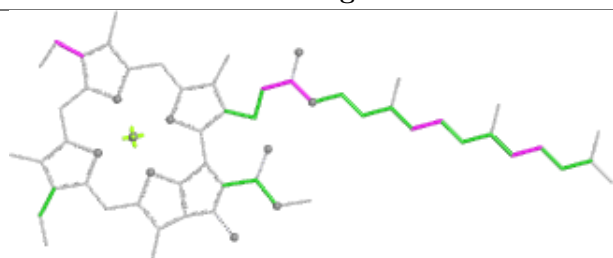
Ligand CLA W 504



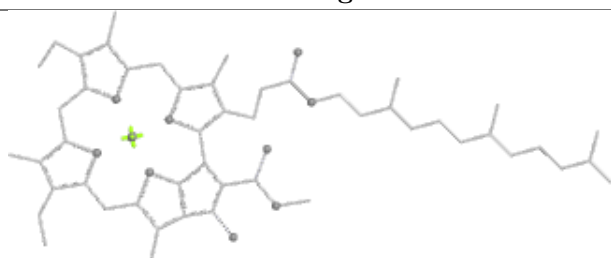
Bond lengths



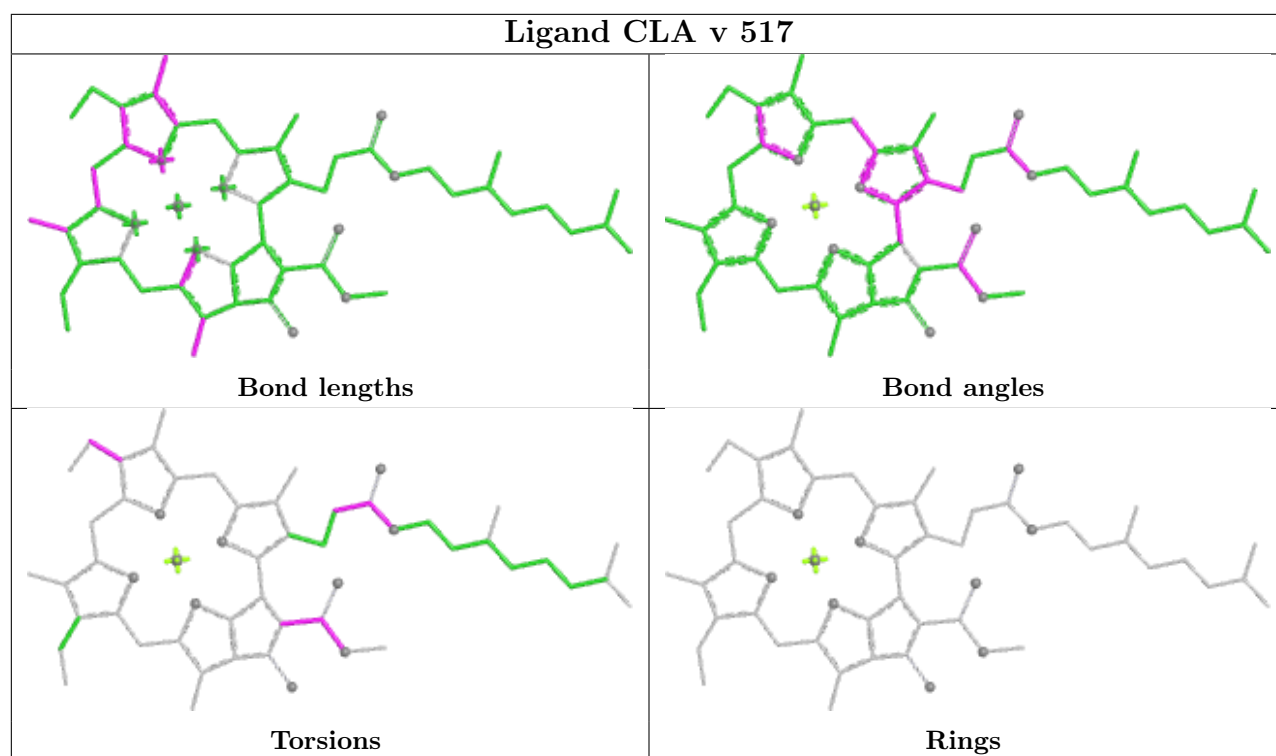
Bond angles



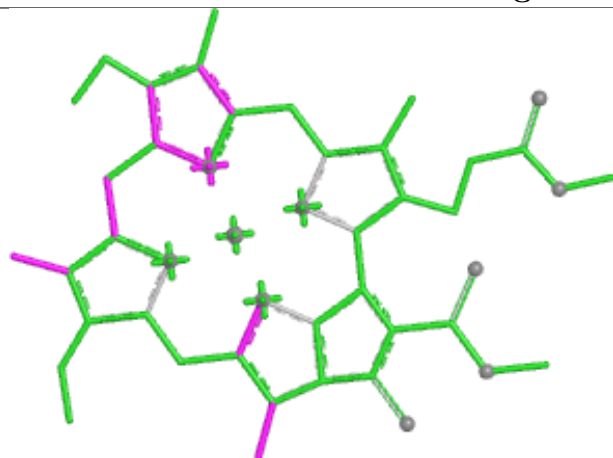
Torsions



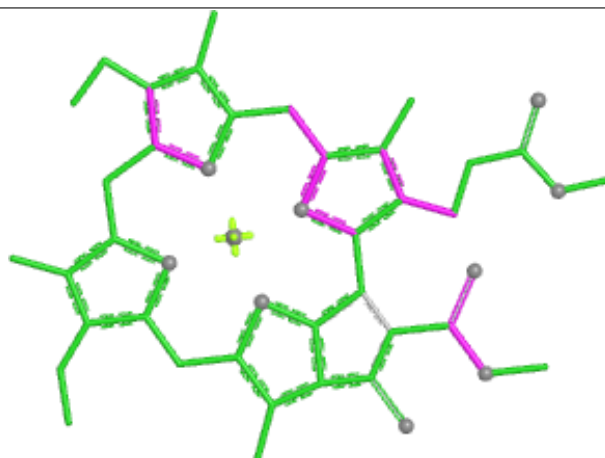
Rings



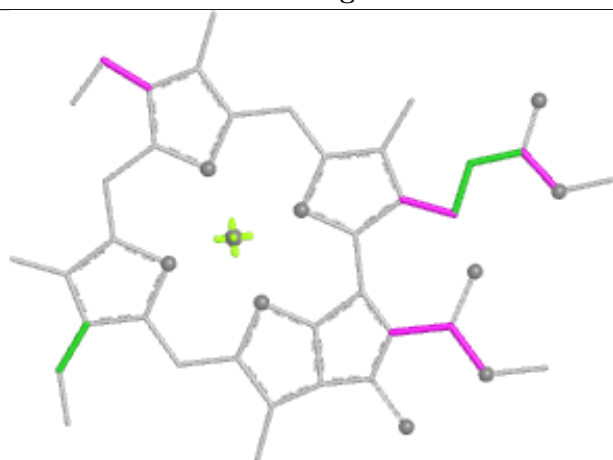
Ligand CLA Y 503



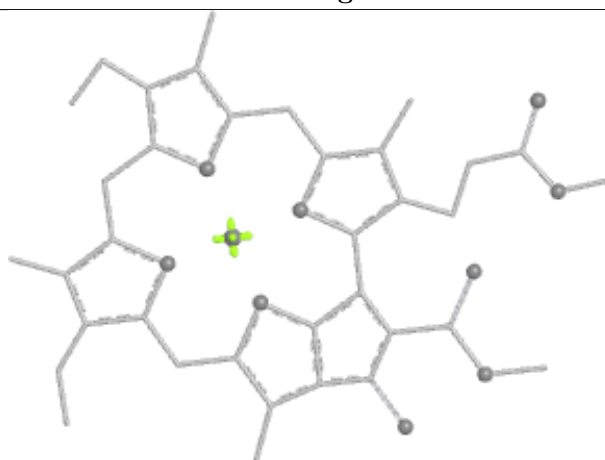
Bond lengths



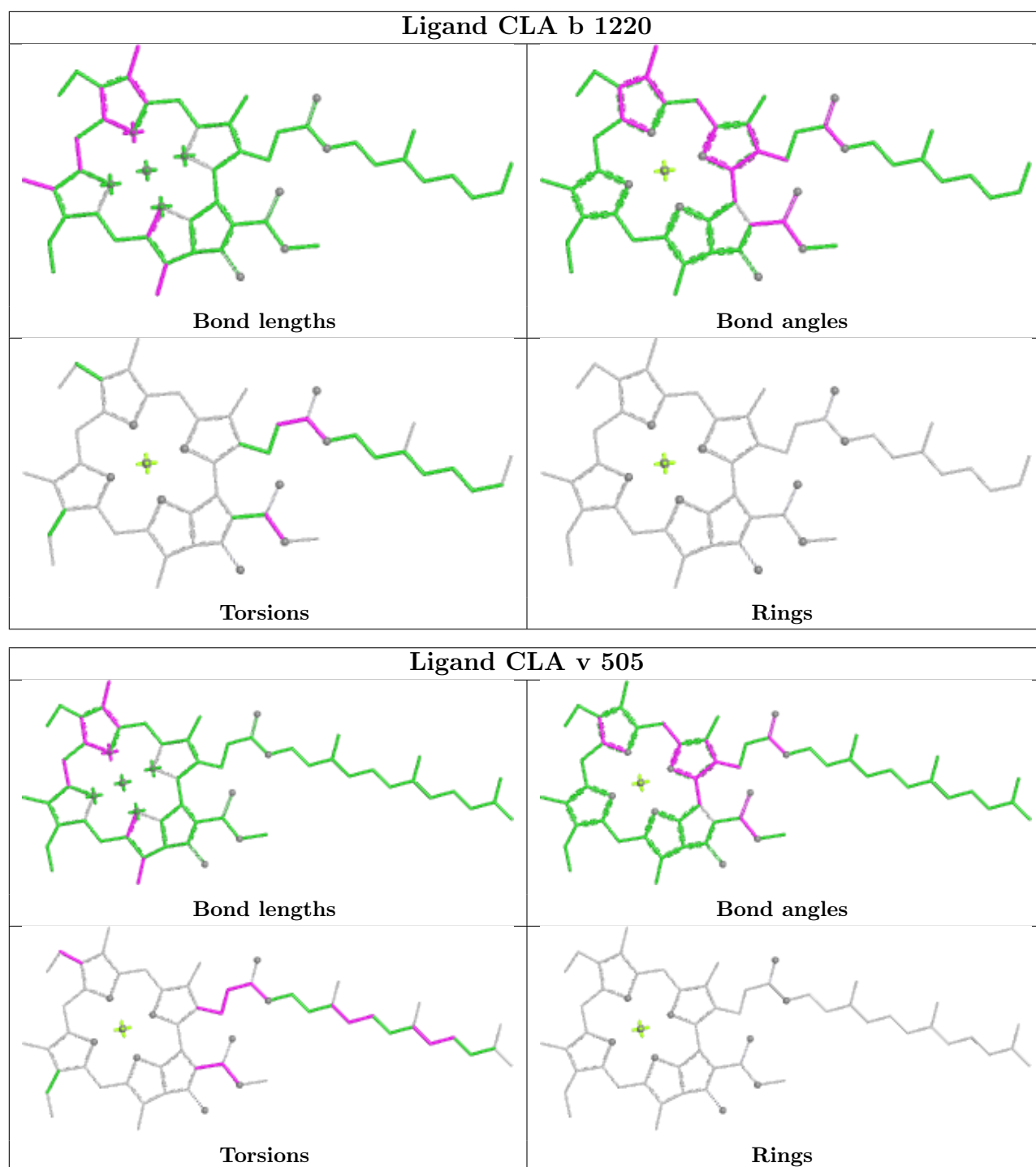
Bond angles

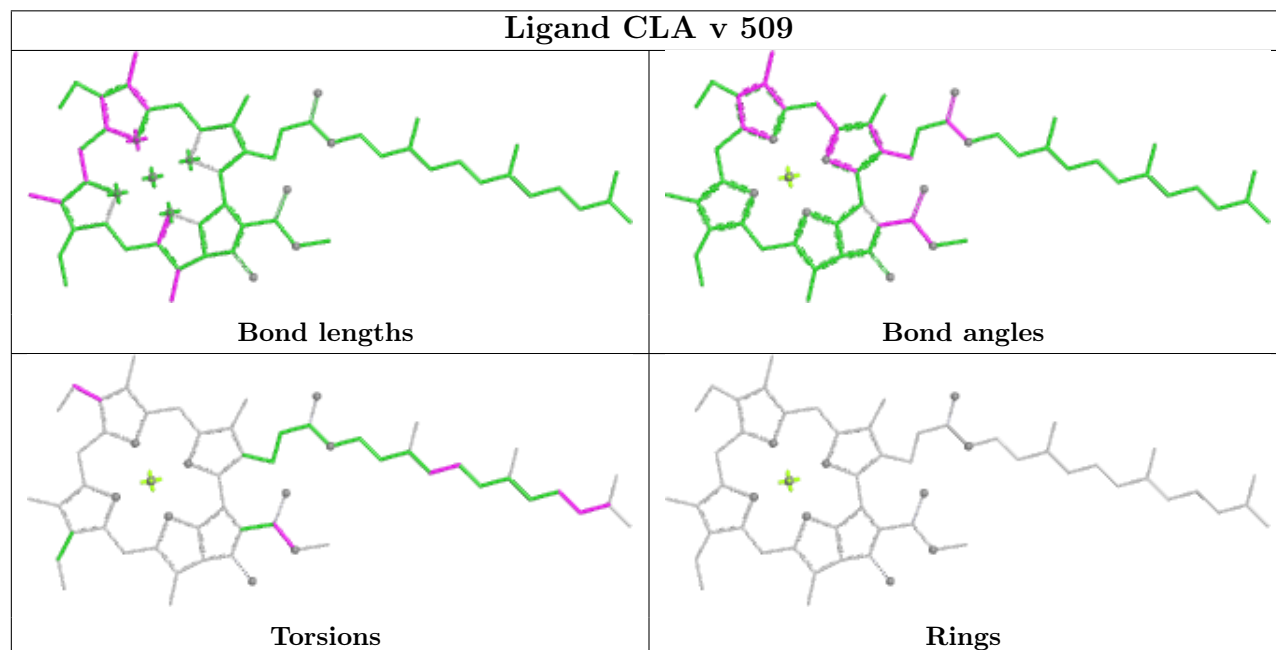
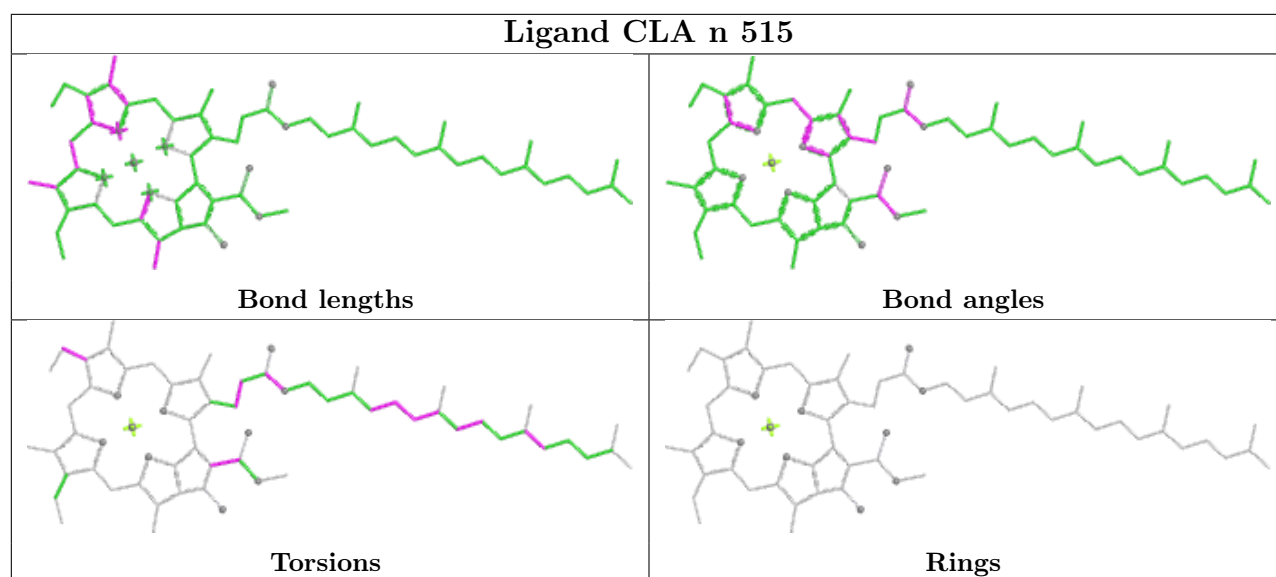


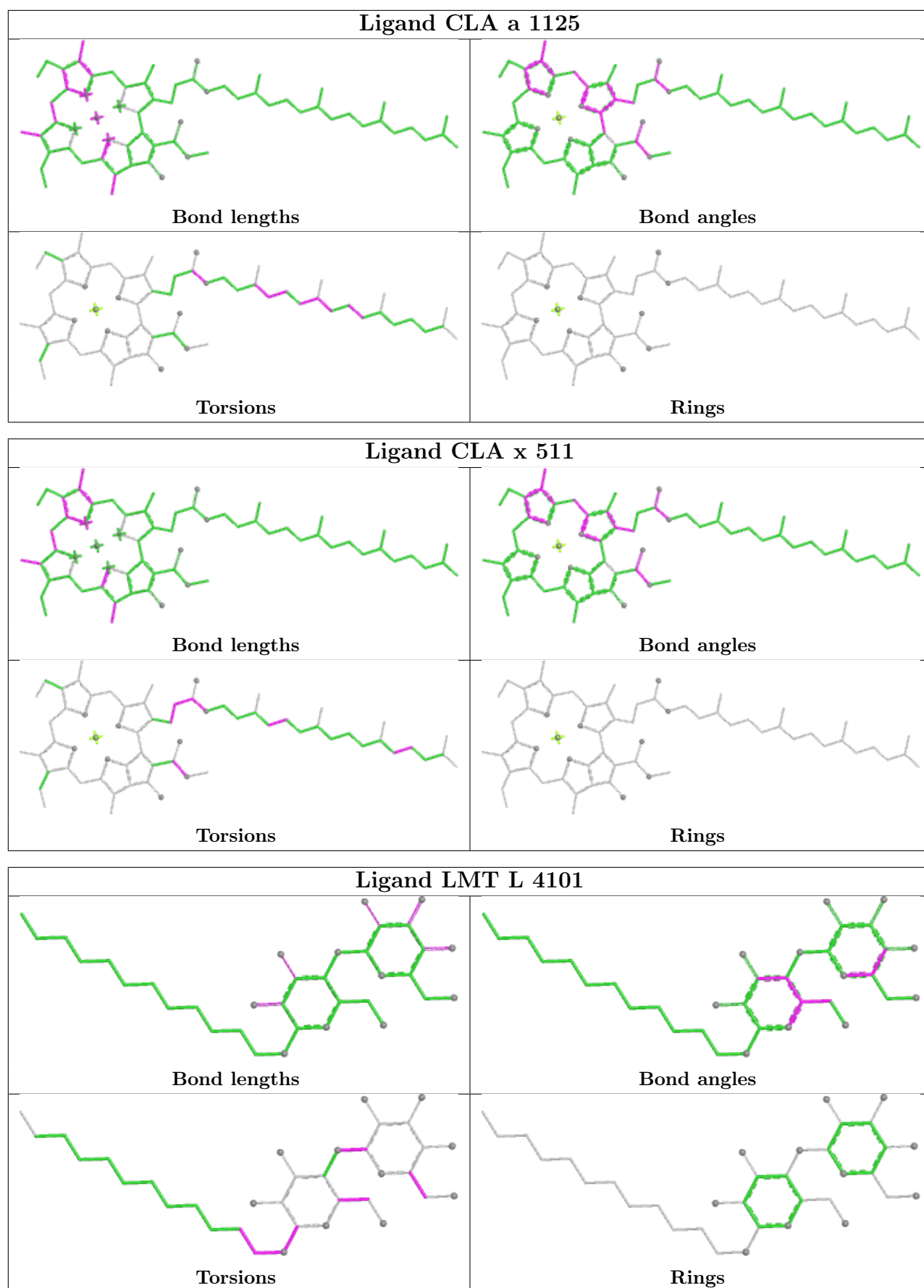
Torsions



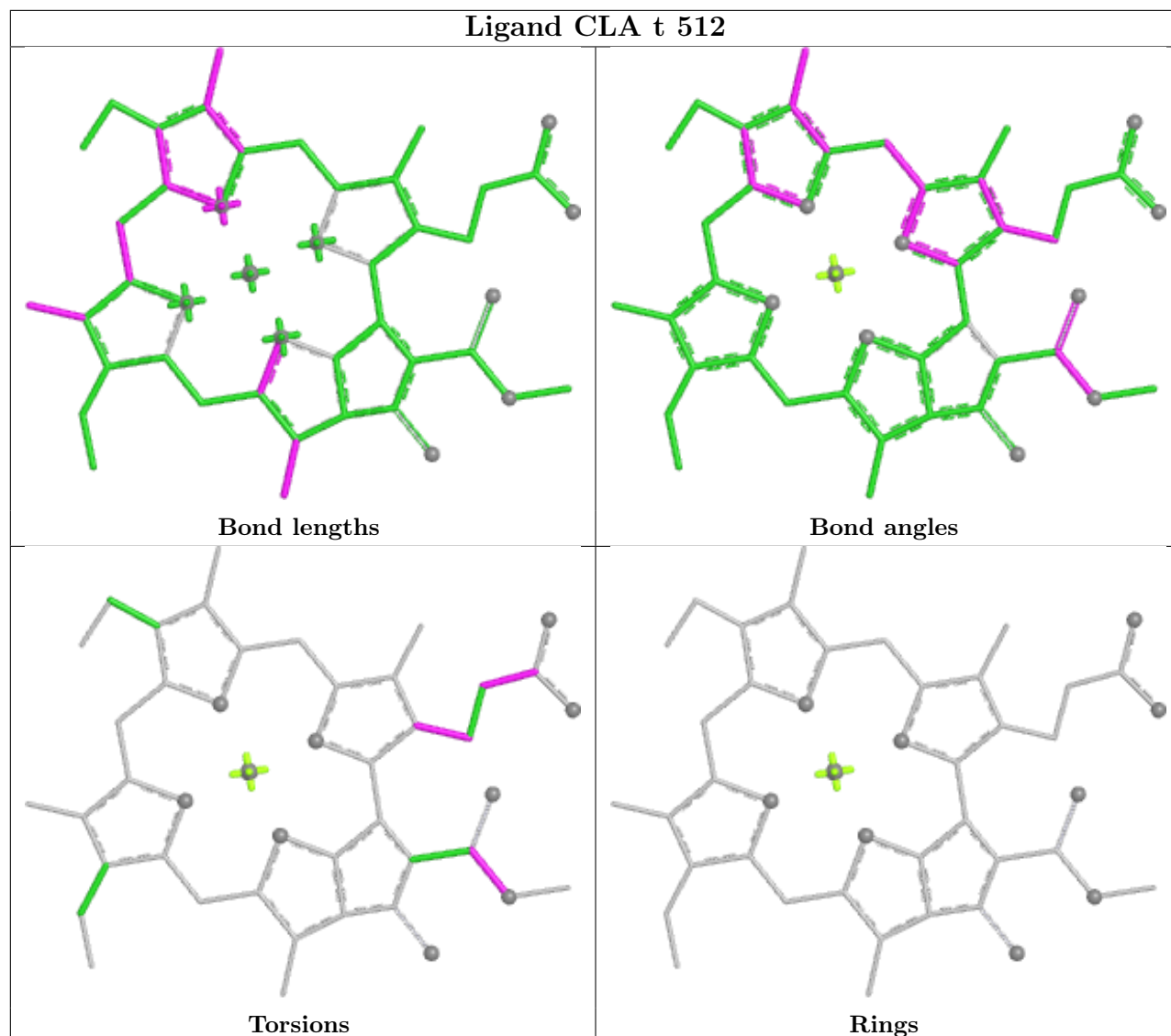
Rings



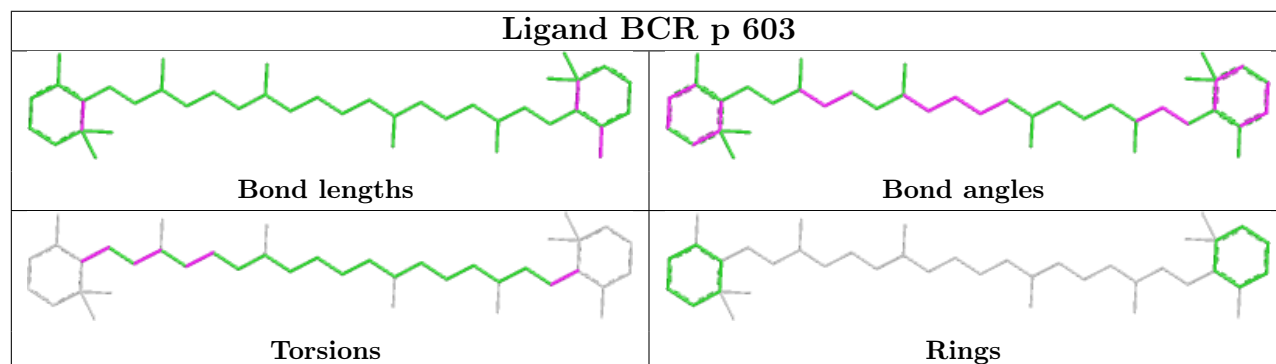




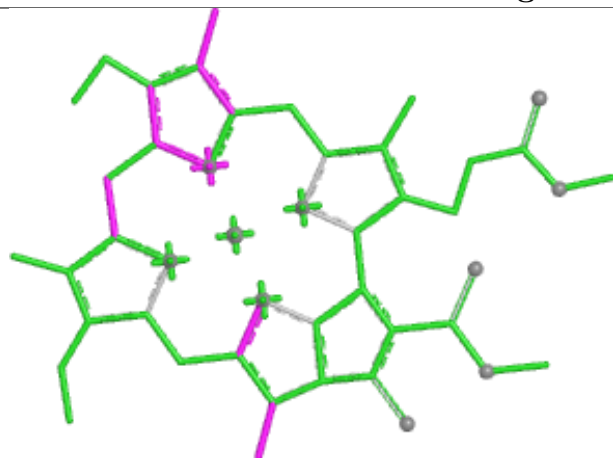
Ligand CLA t 512



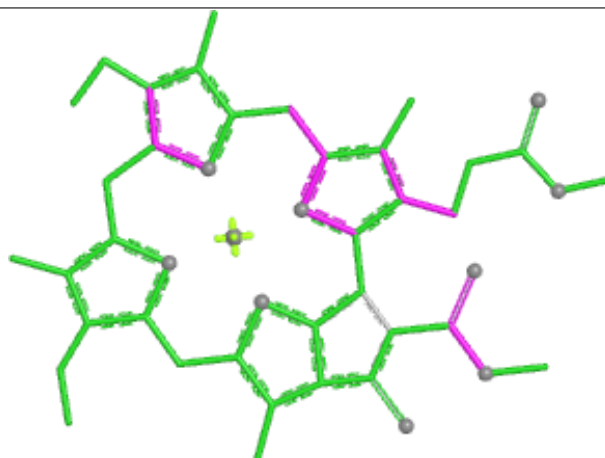
Ligand BCR p 603



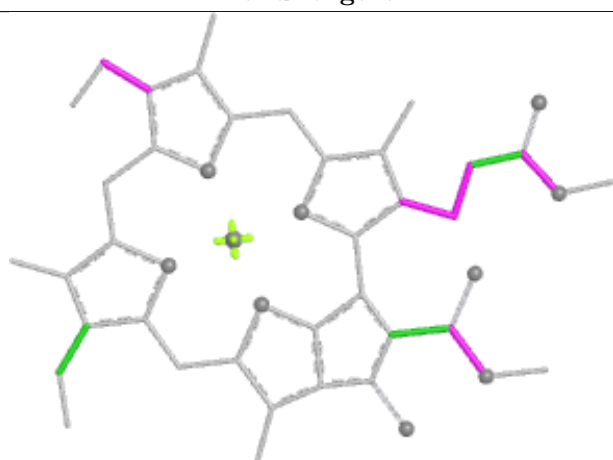
Ligand CLA h 501



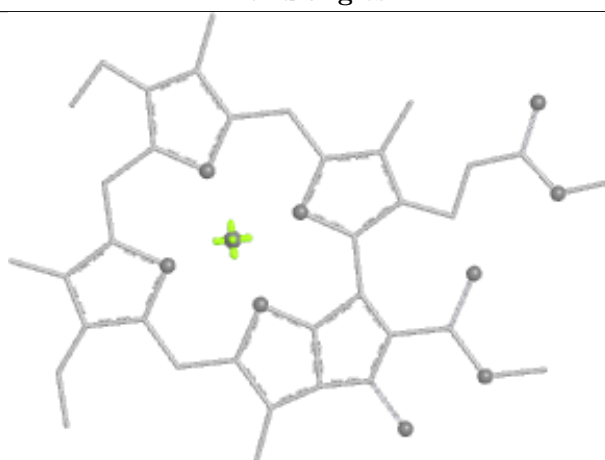
Bond lengths



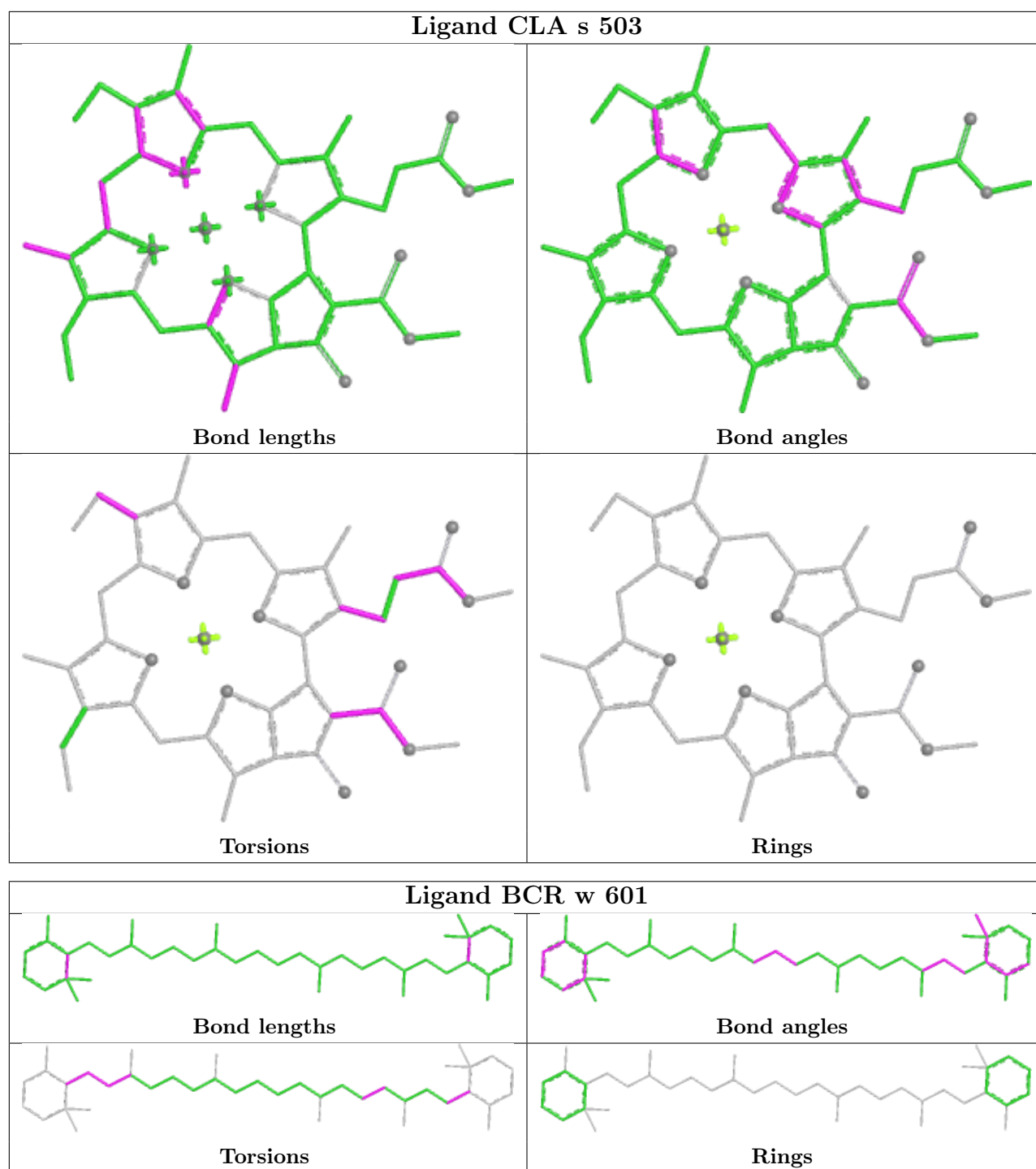
Bond angles



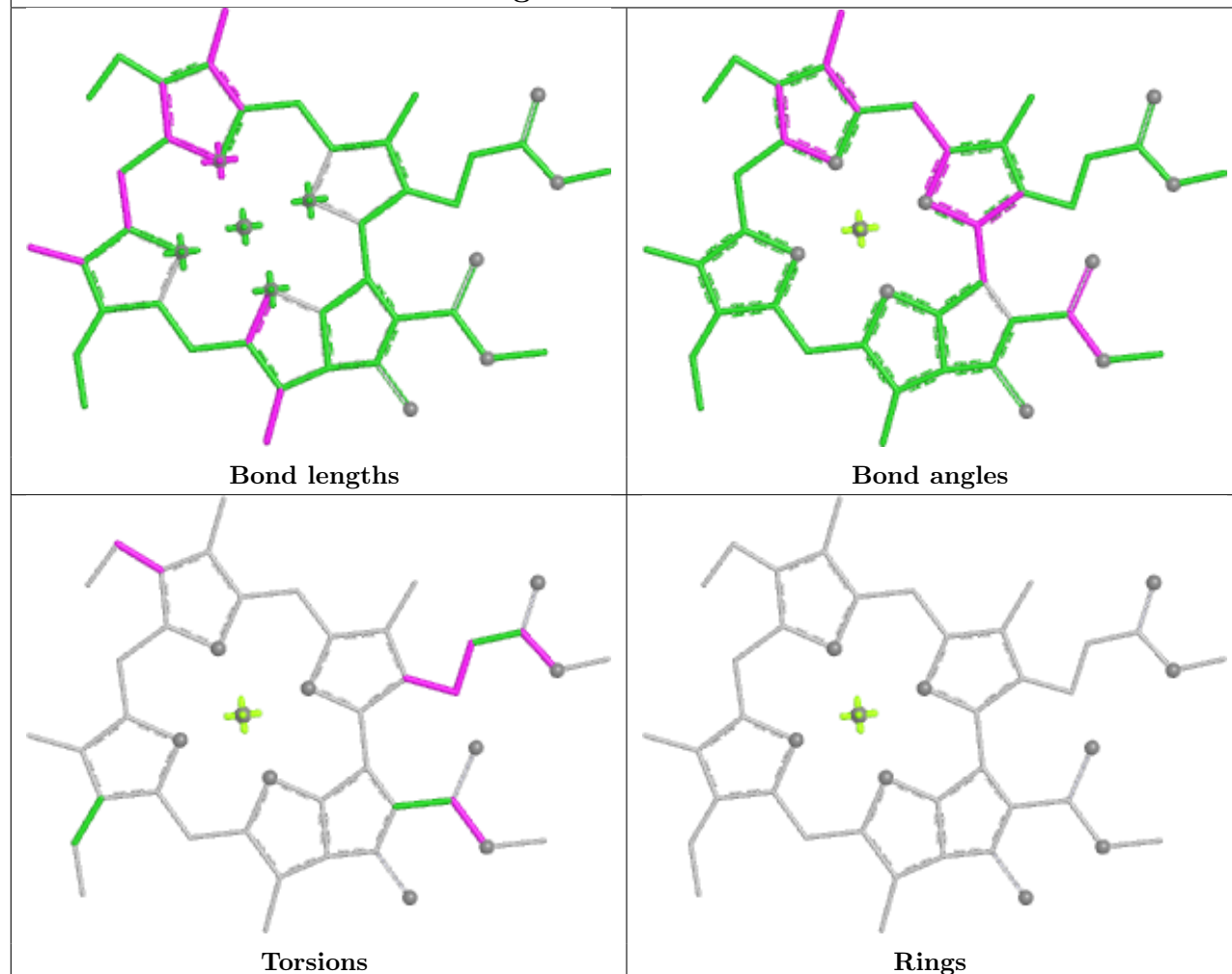
Torsions



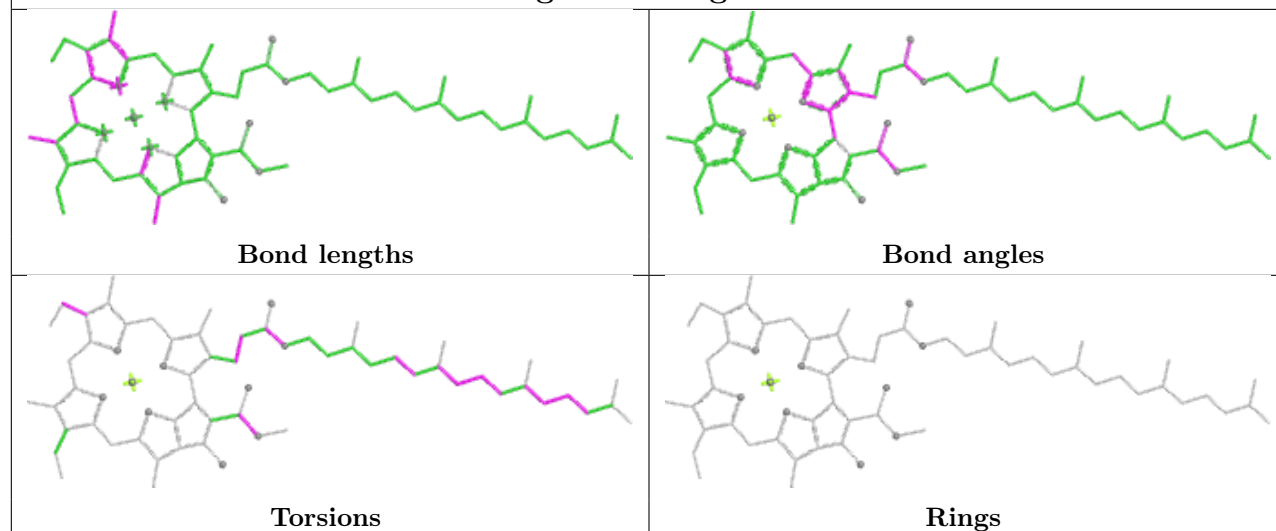
Rings

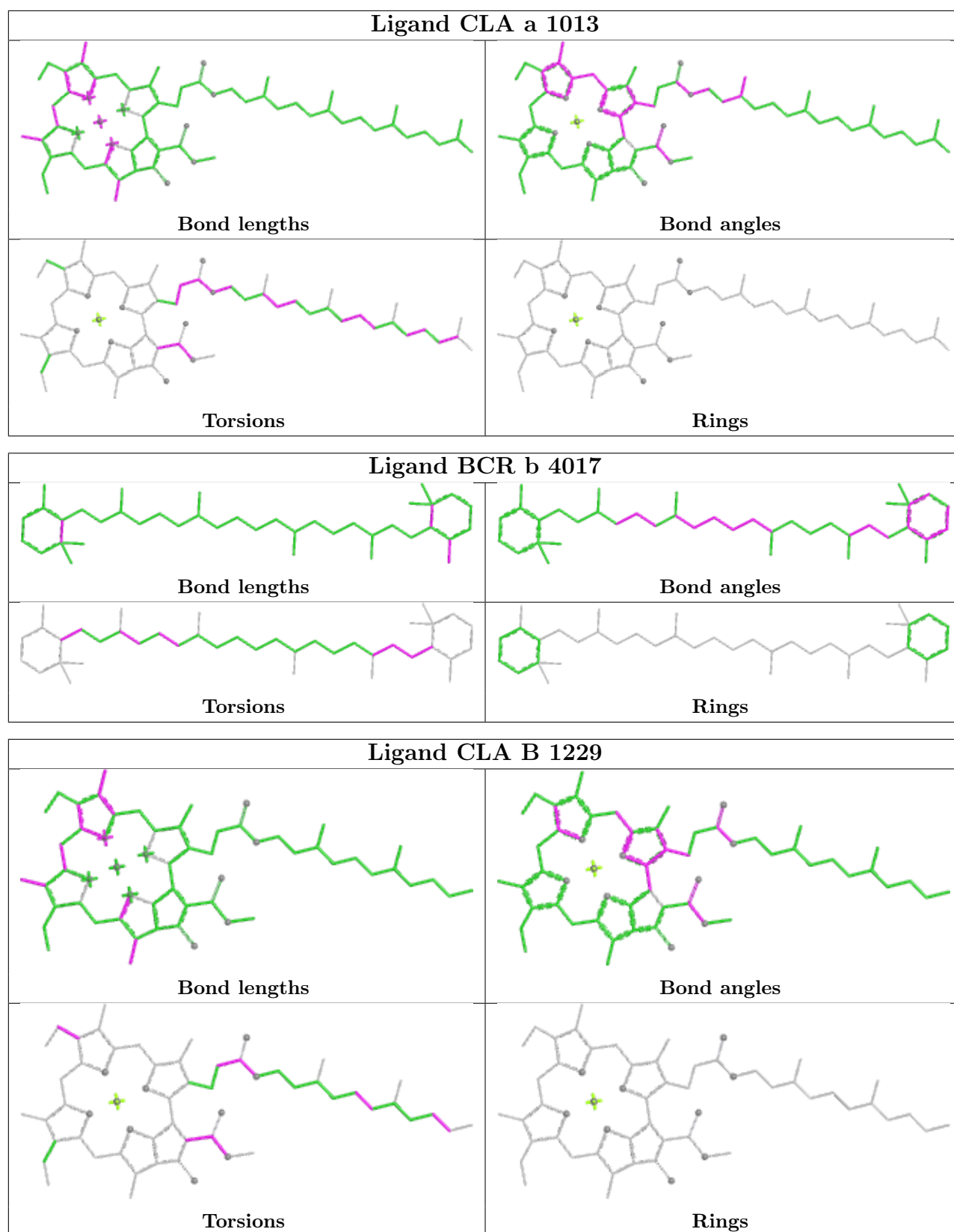


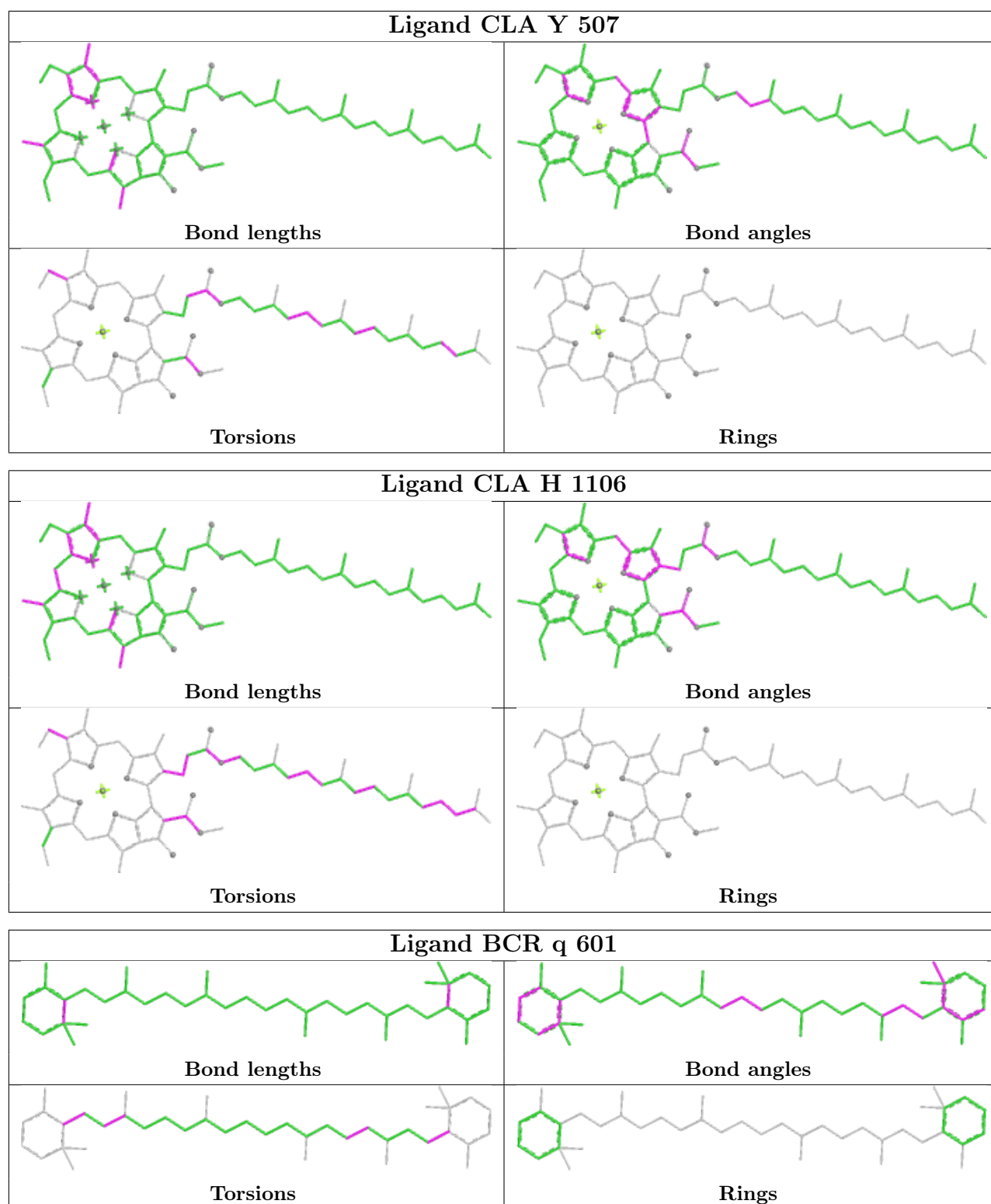
Ligand CLA Y 516

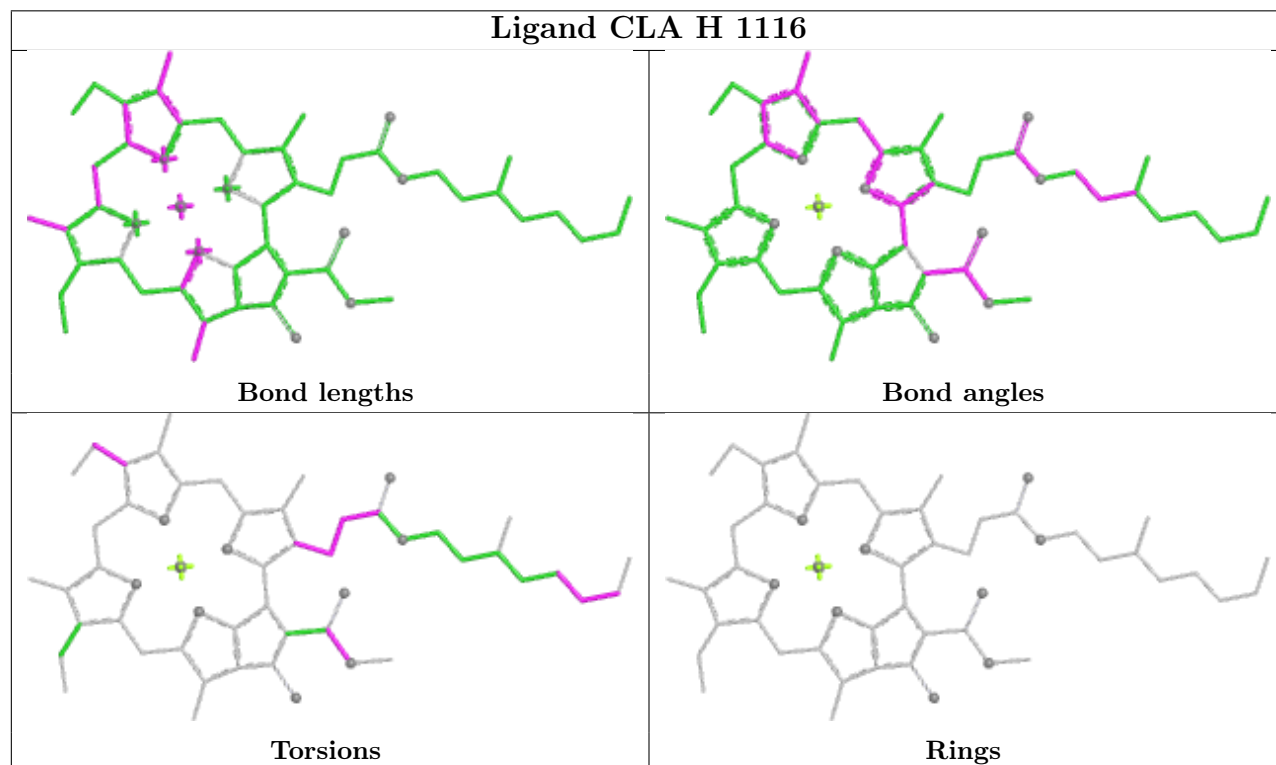
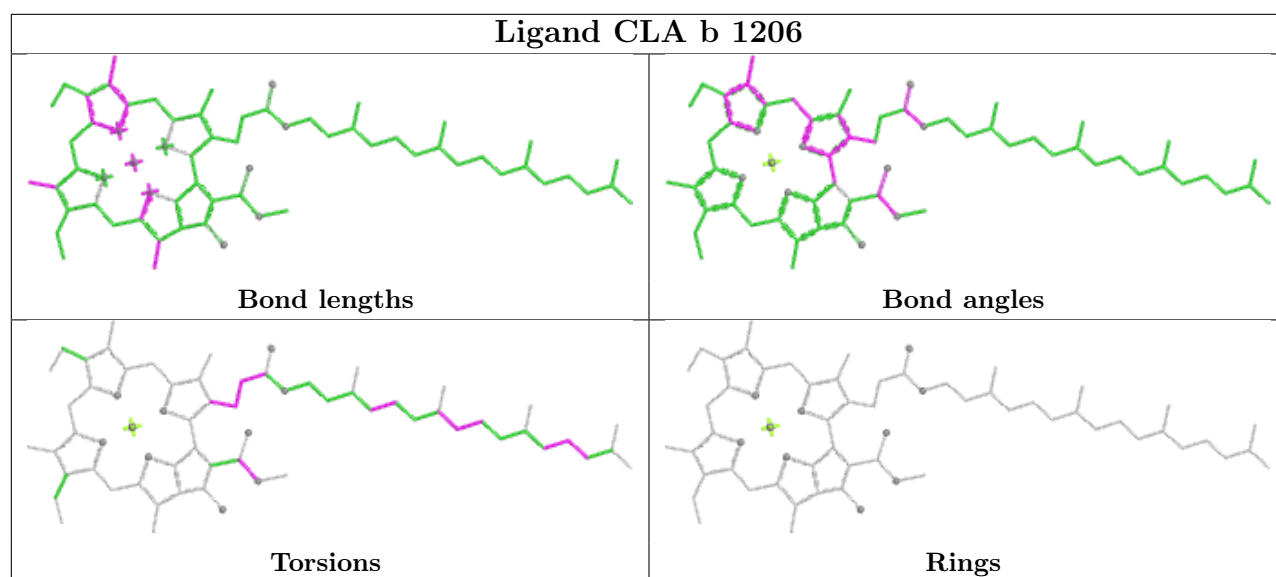


Ligand CLA g 515

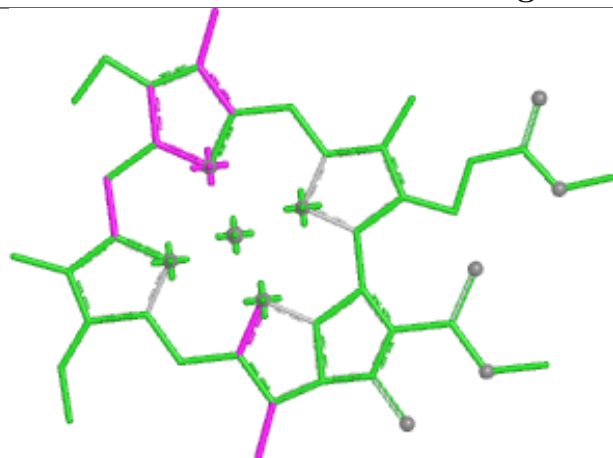




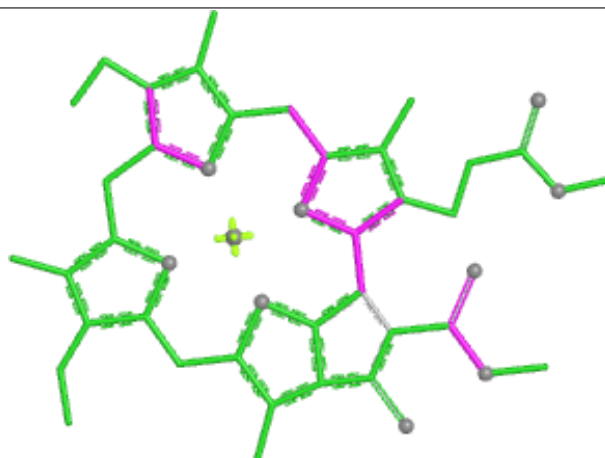




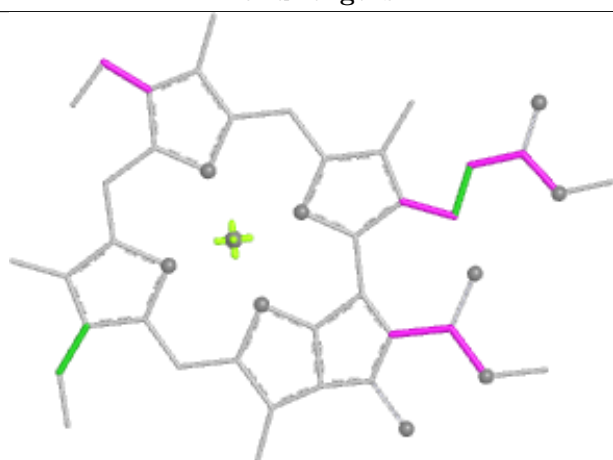
Ligand CLA h 503



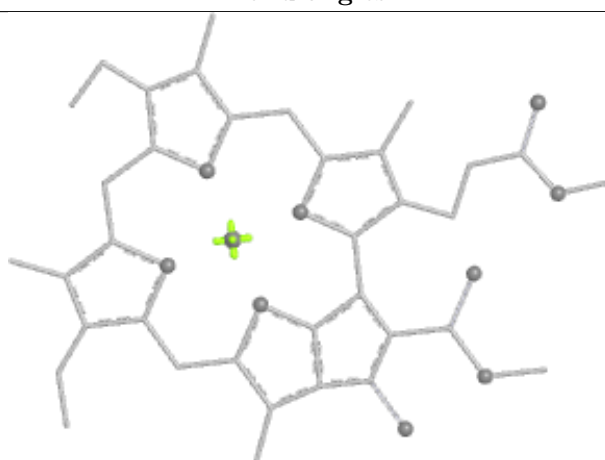
Bond lengths



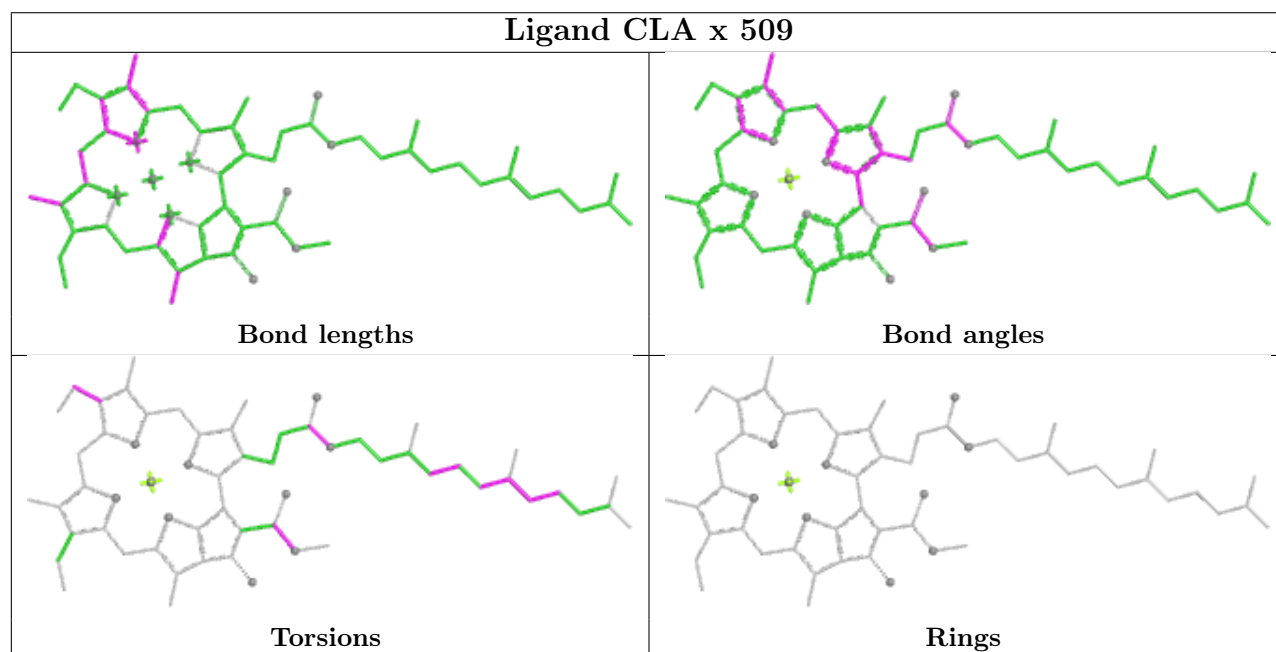
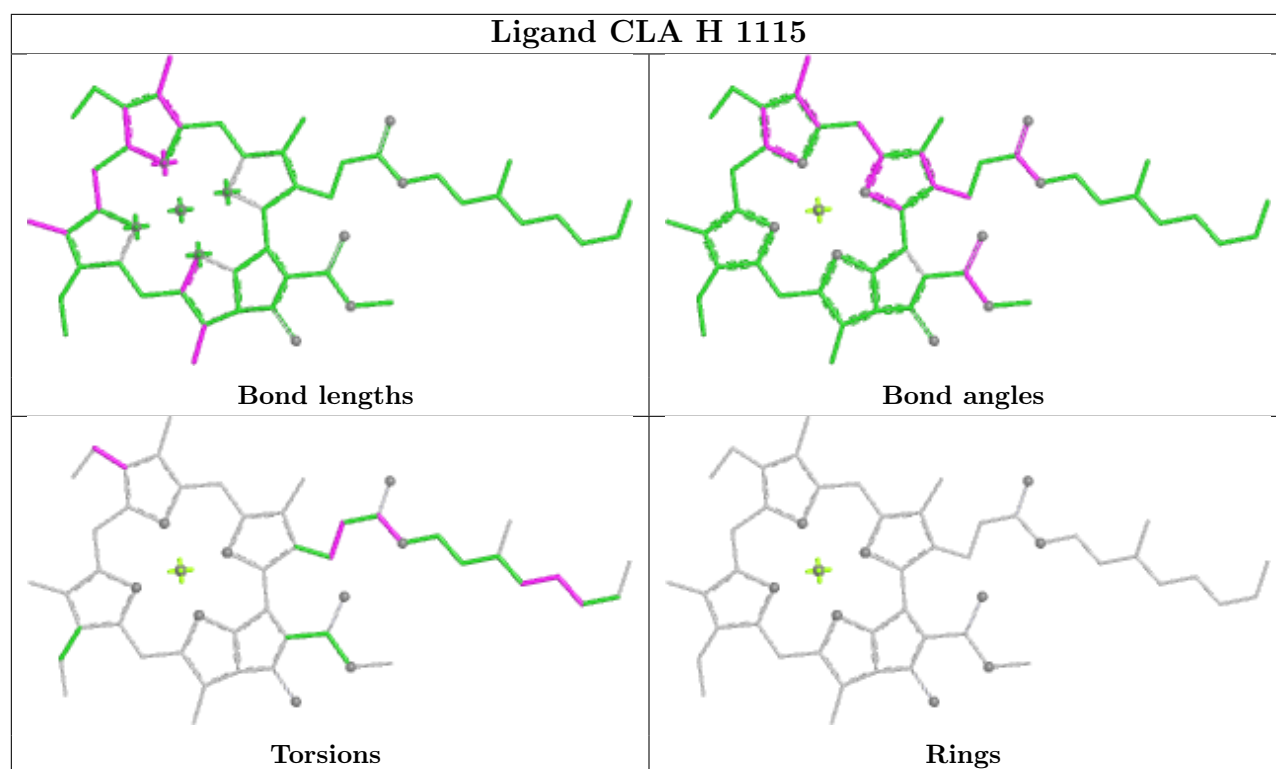
Bond angles

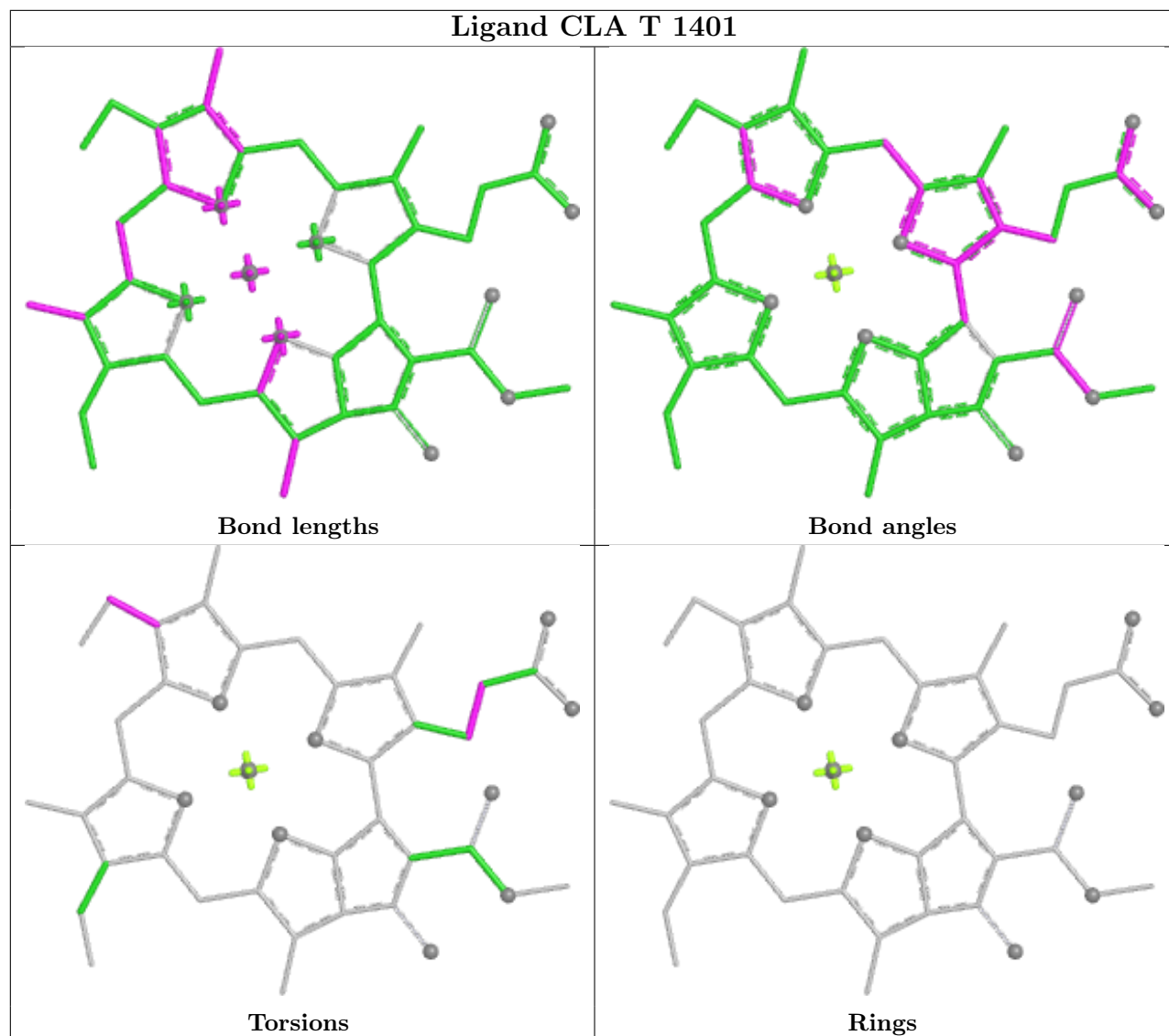


Torsions

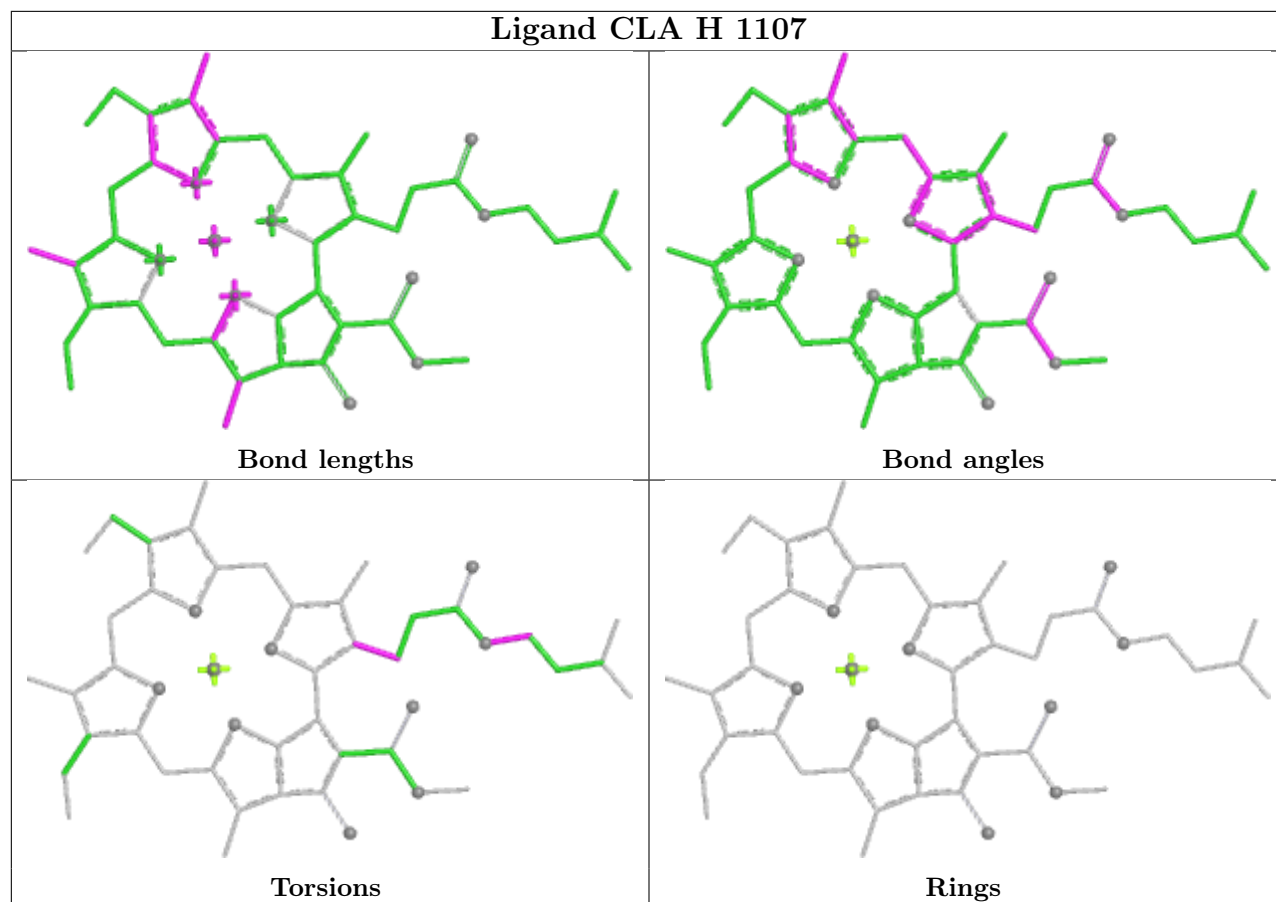


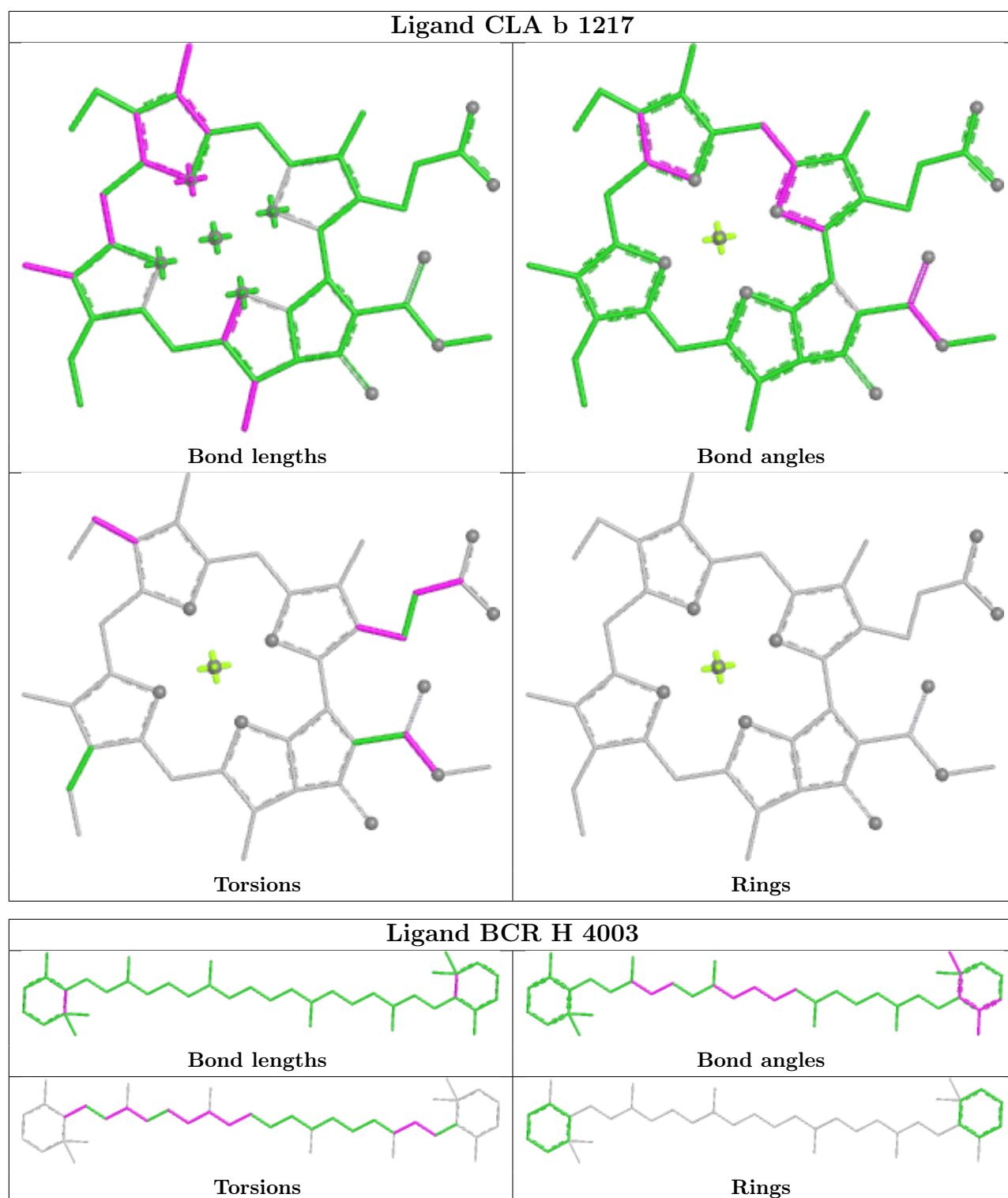
Rings

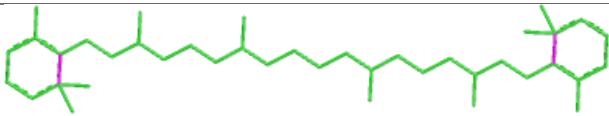
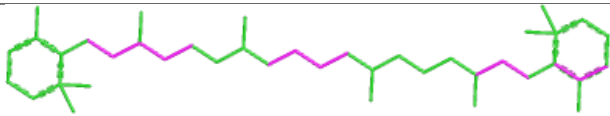
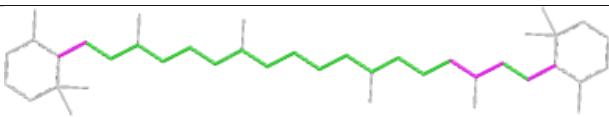
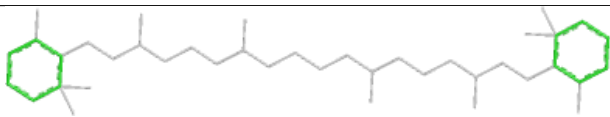


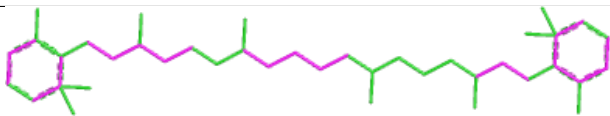
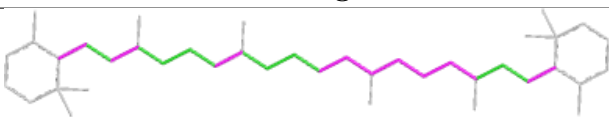
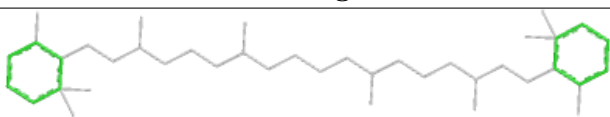


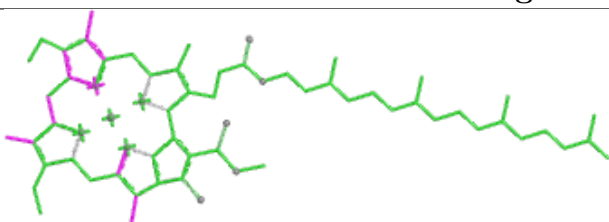
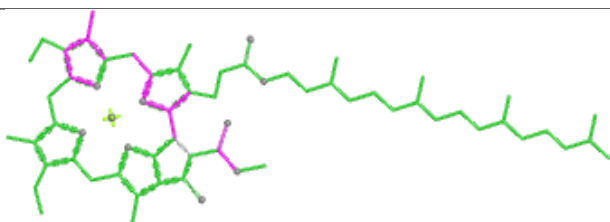
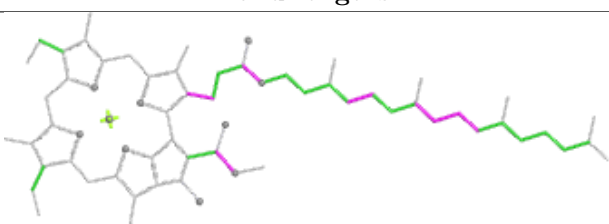
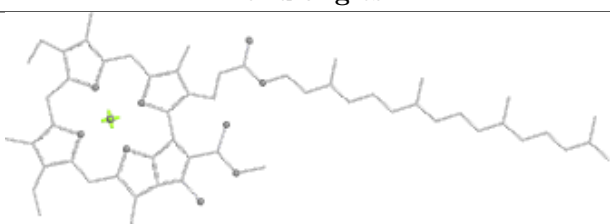
Ligand CLA H 1107



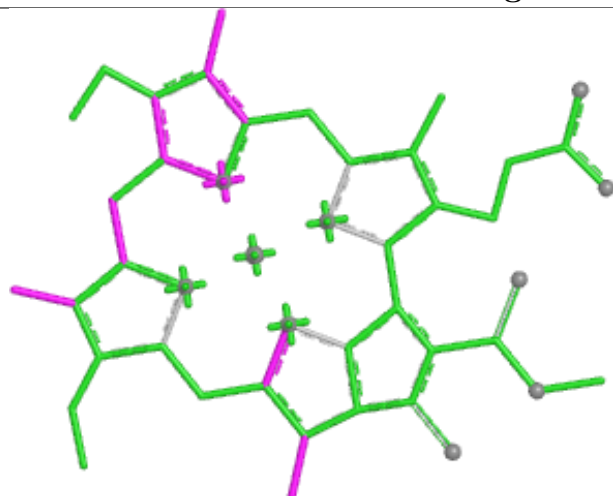


Ligand BCR a 4002	
	
Bond lengths	Bond angles
	
Torsions	Rings

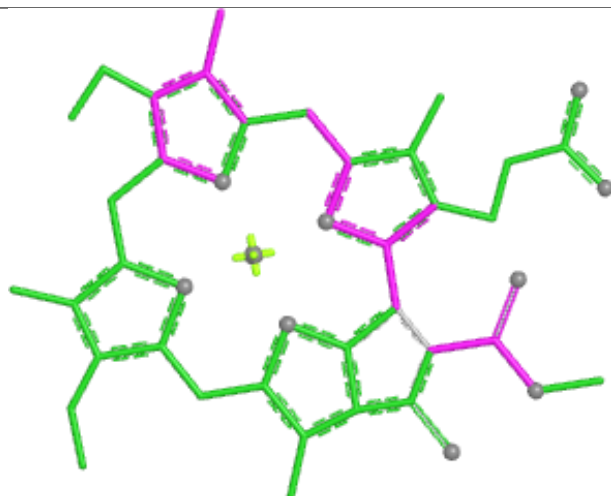
Ligand BCR s 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA t 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

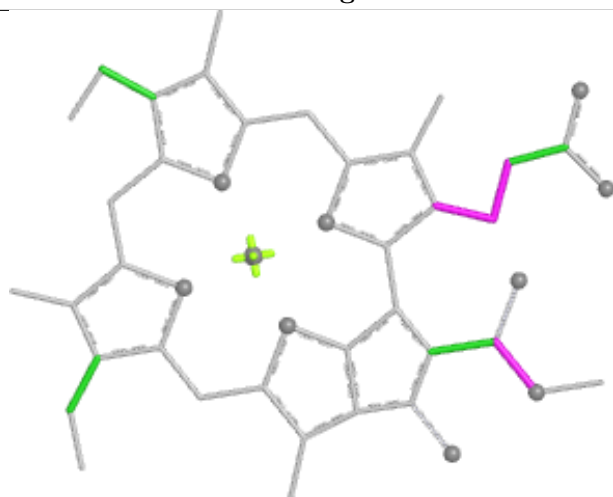
Ligand CLA H 1113



Bond lengths



Bond angles

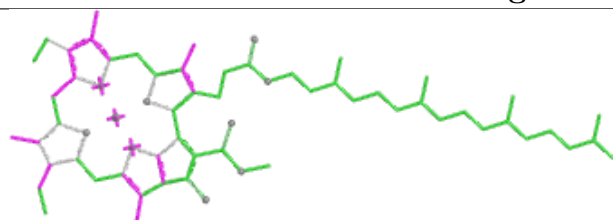


Torsions

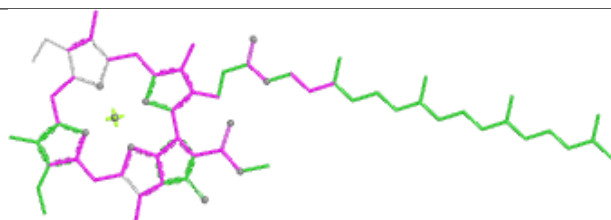


Rings

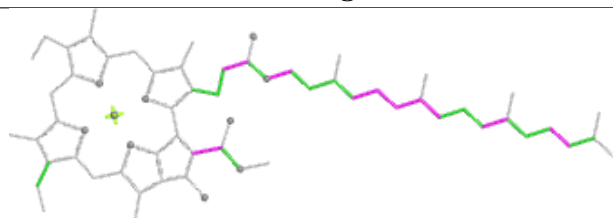
Ligand CL0 H 1011



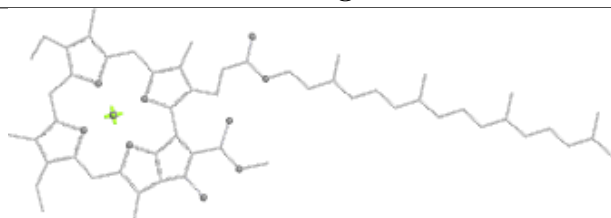
Bond lengths



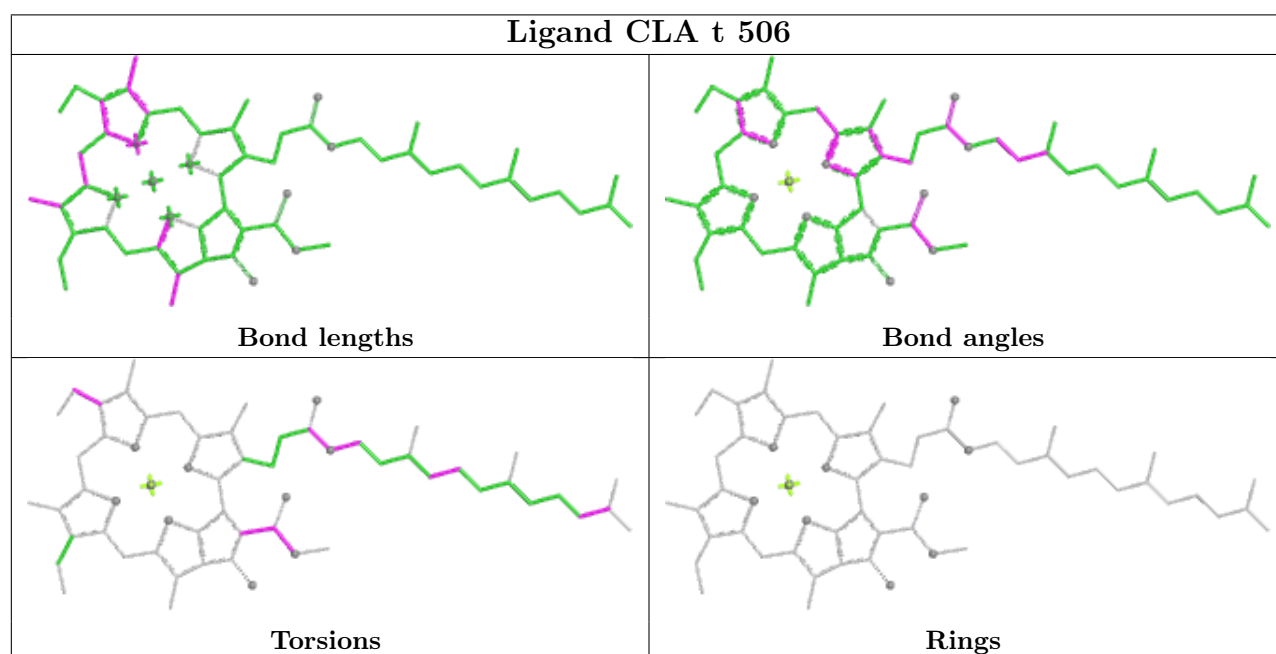
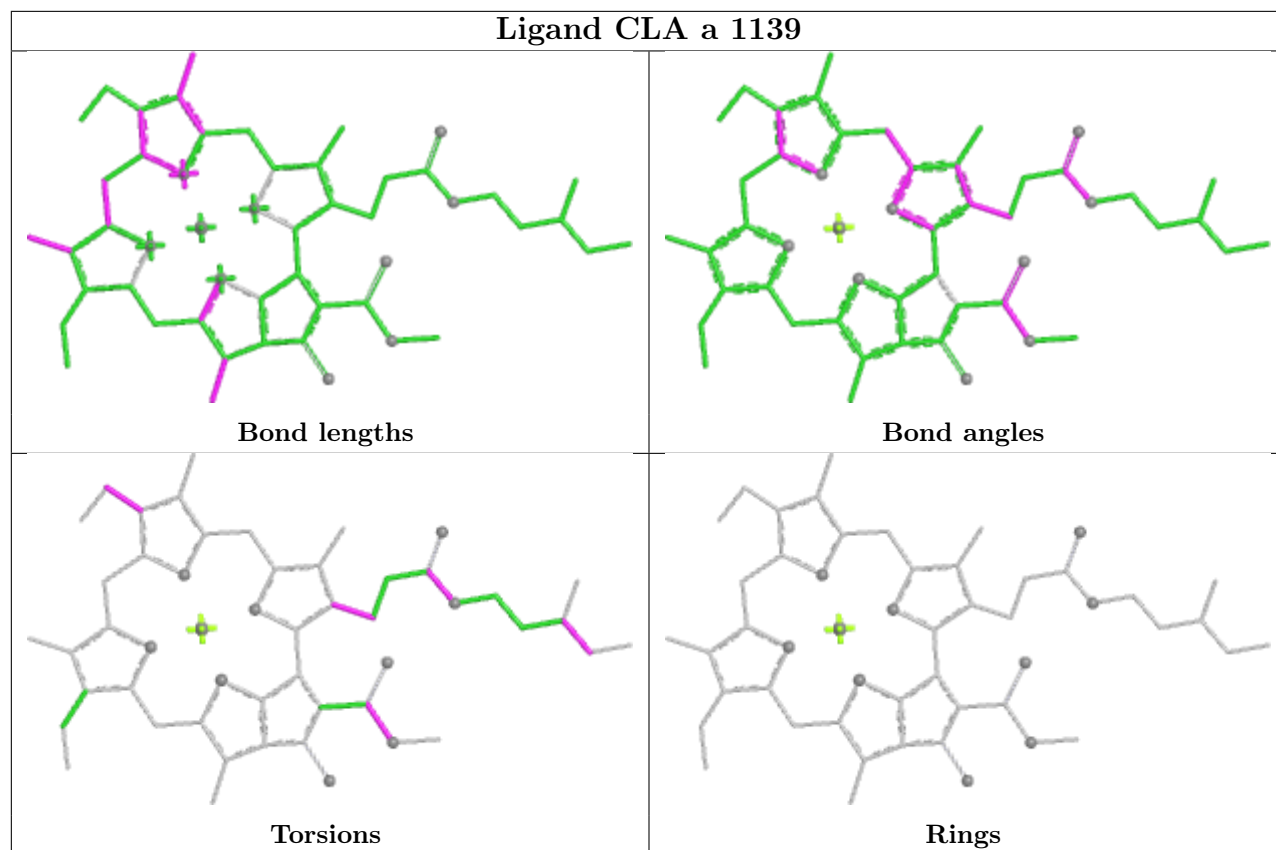
Bond angles

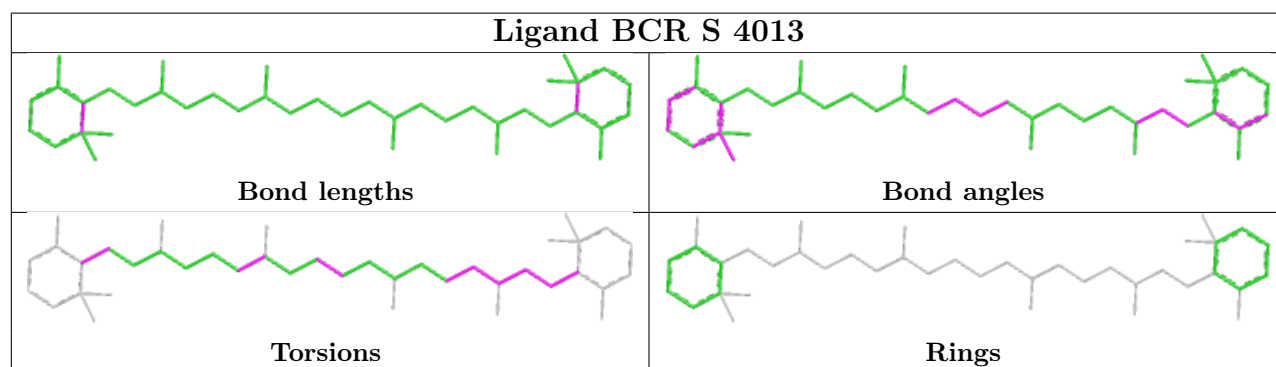
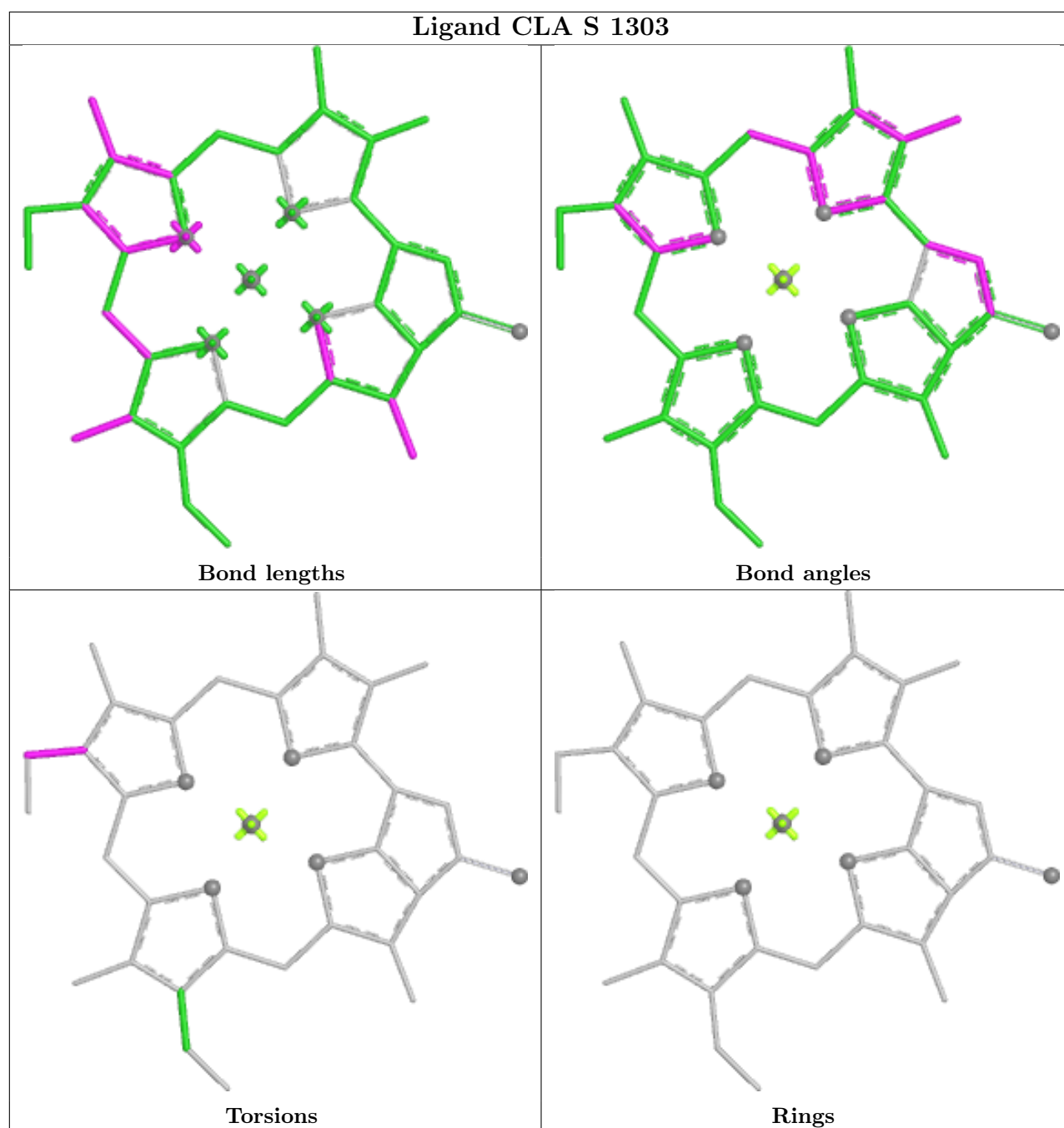


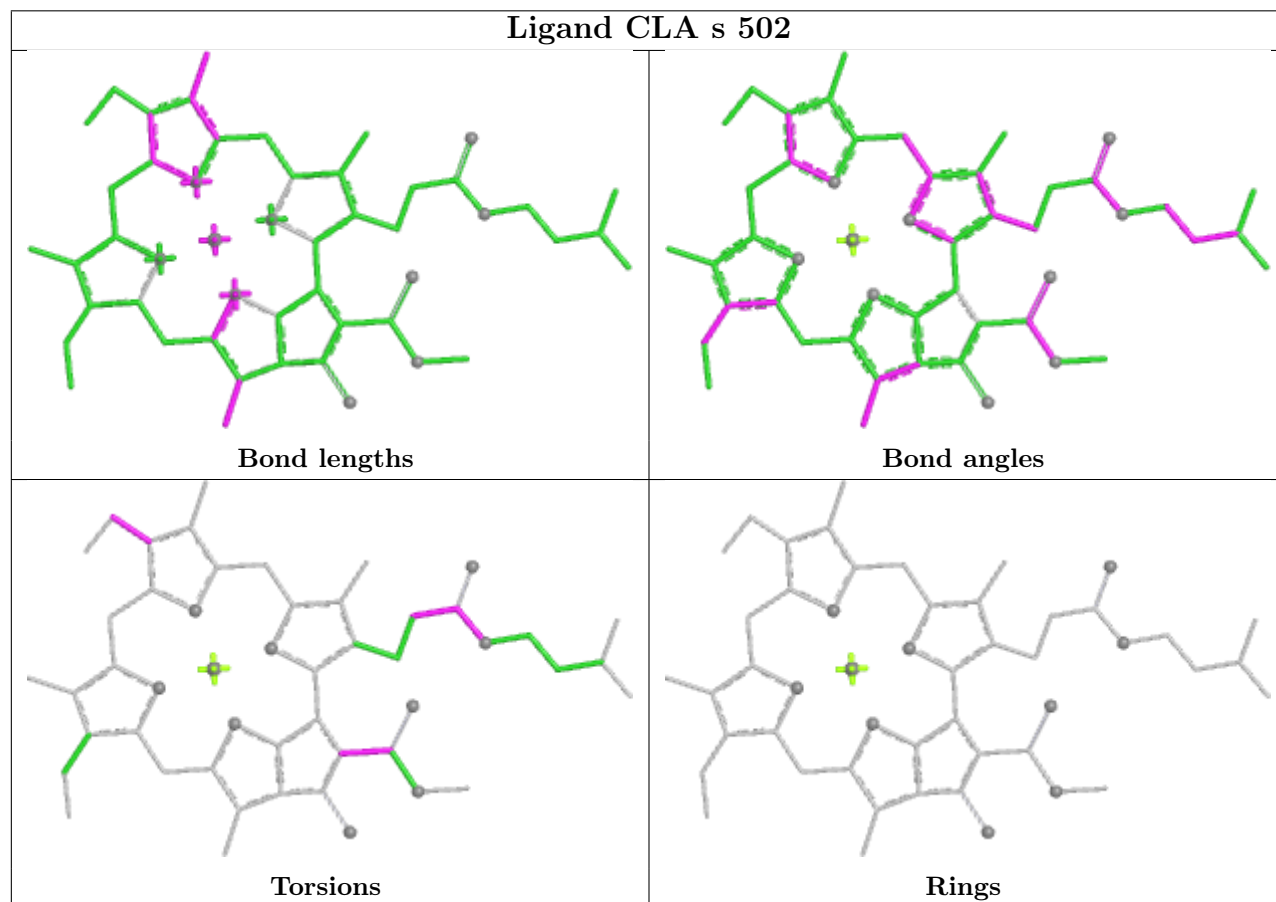
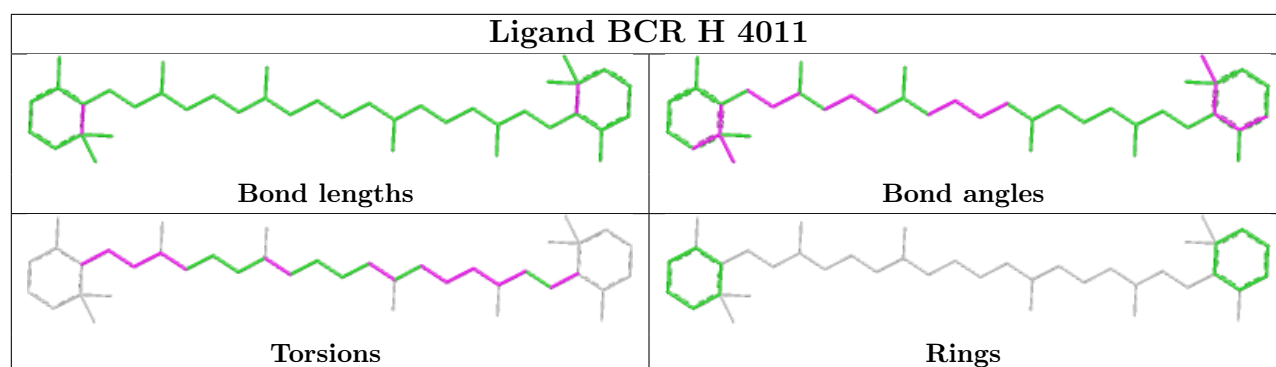
Torsions

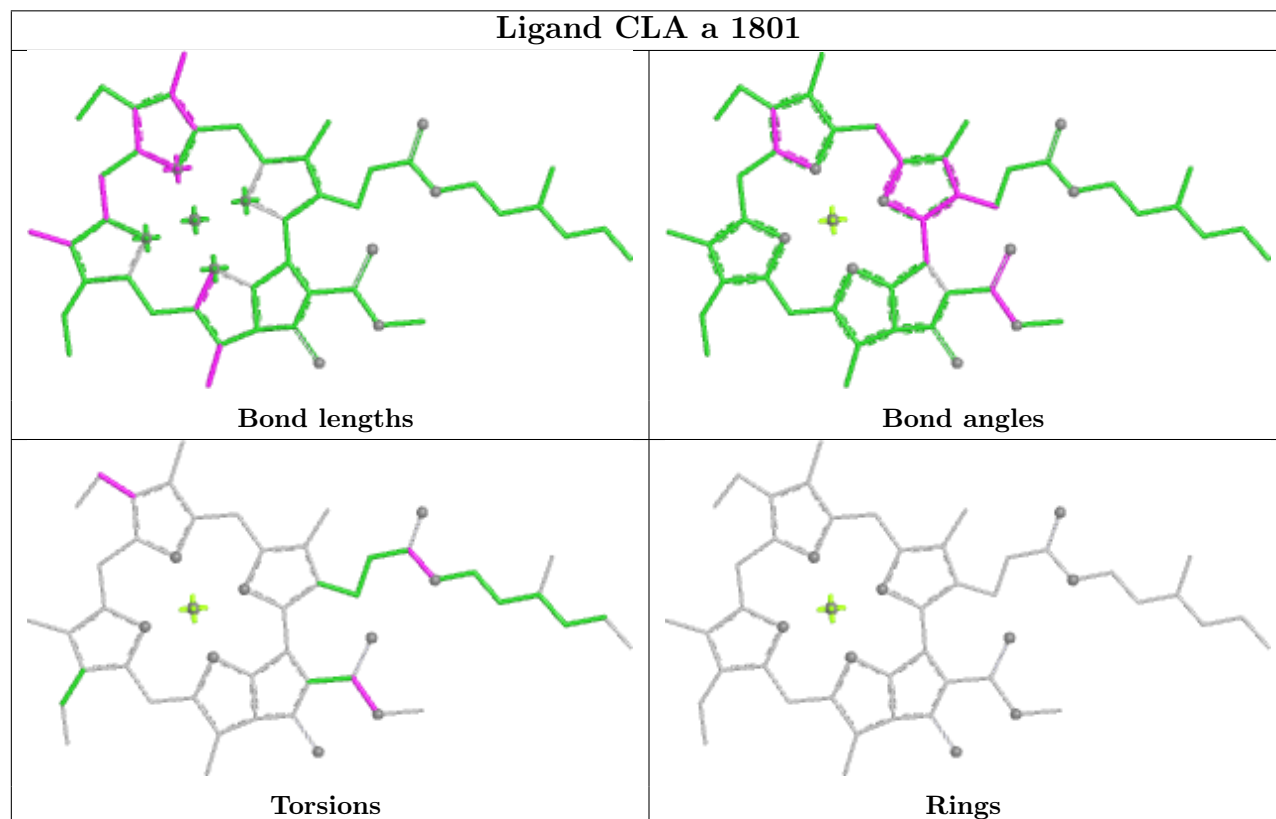
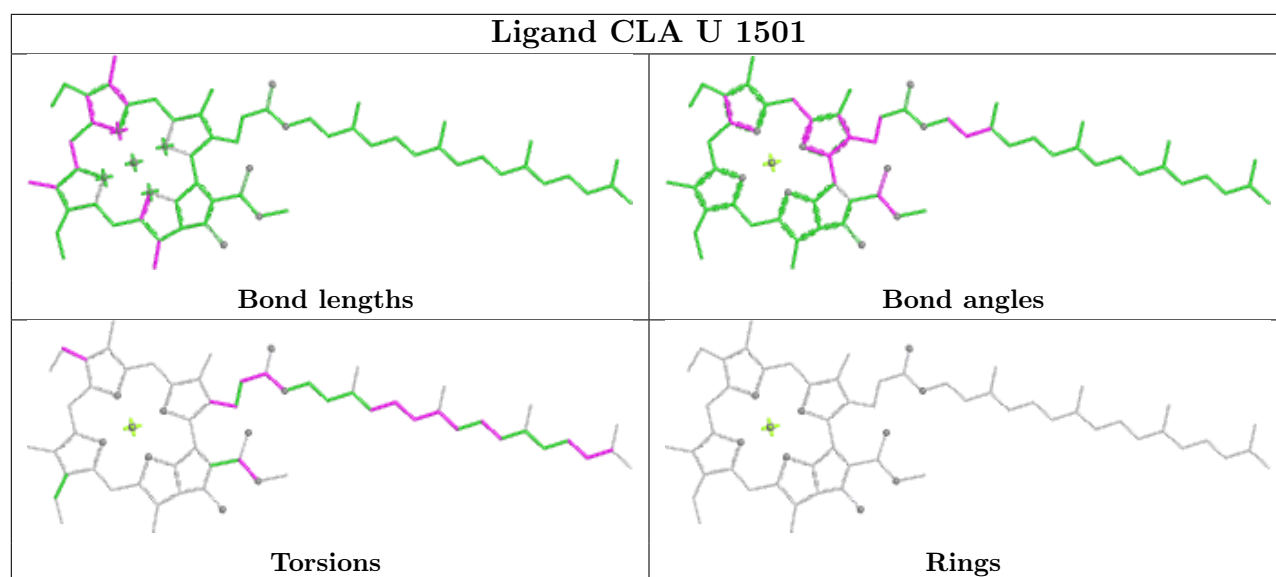


Rings

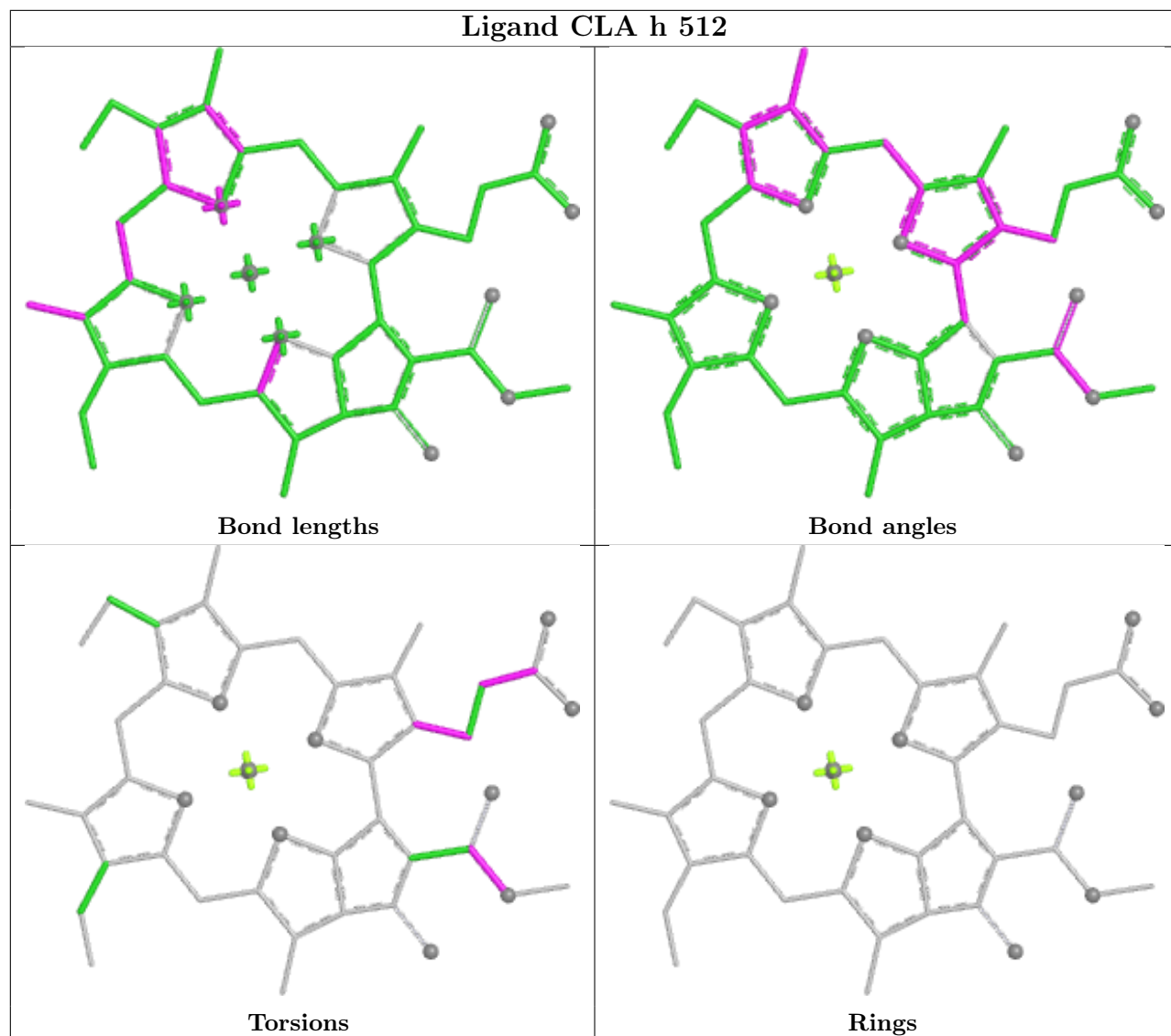


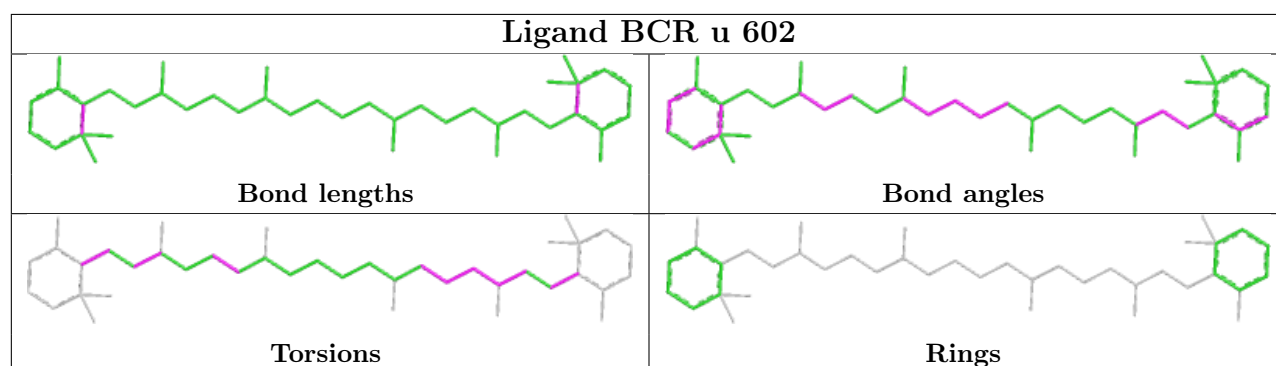
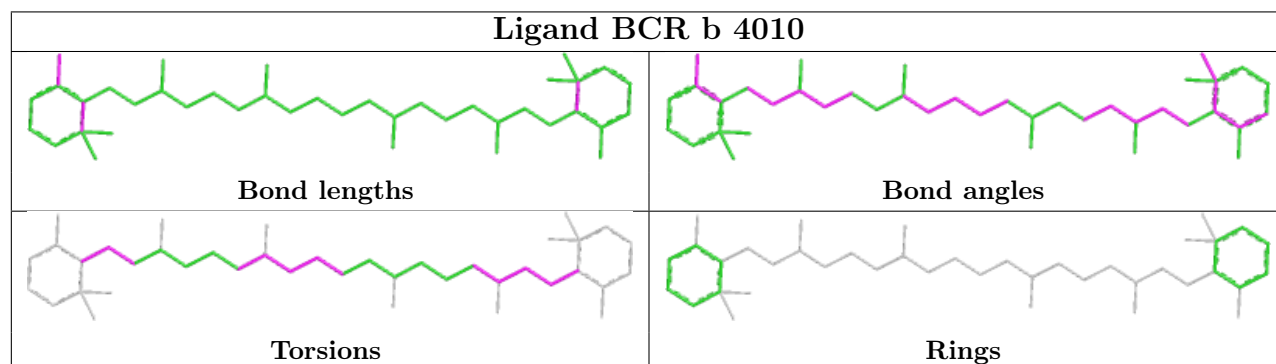
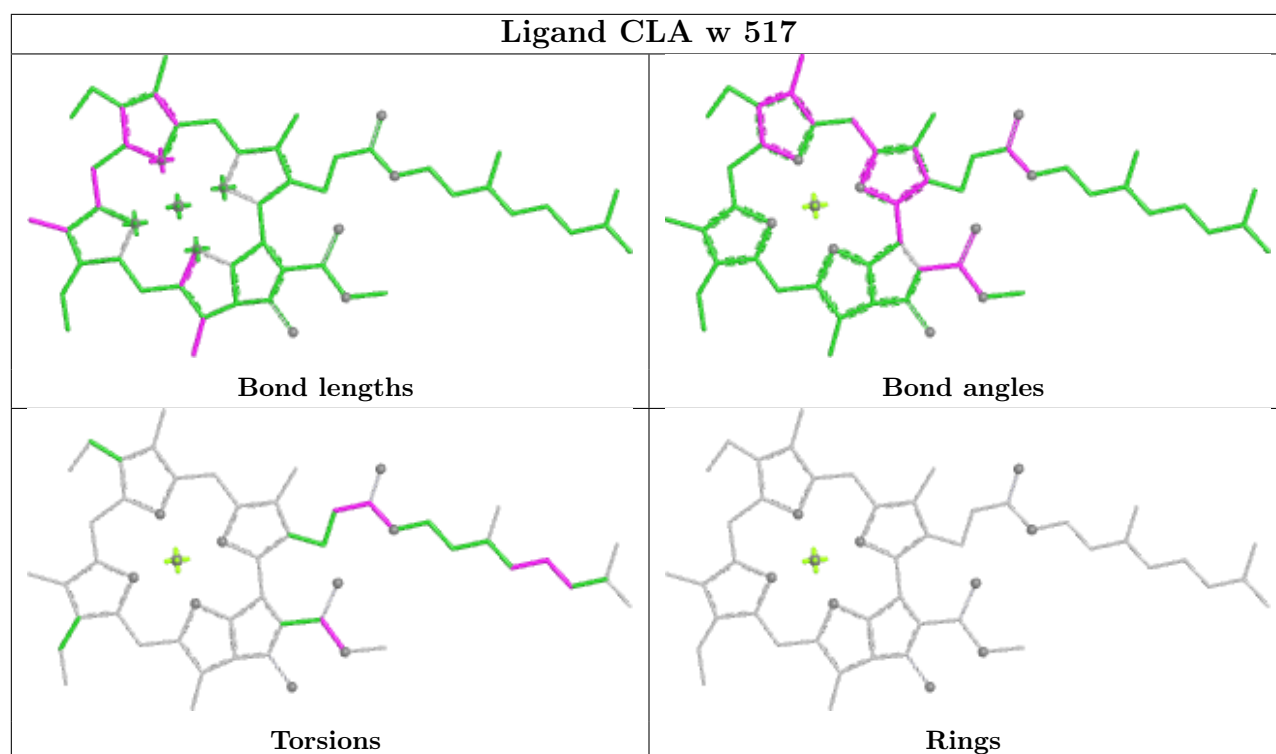




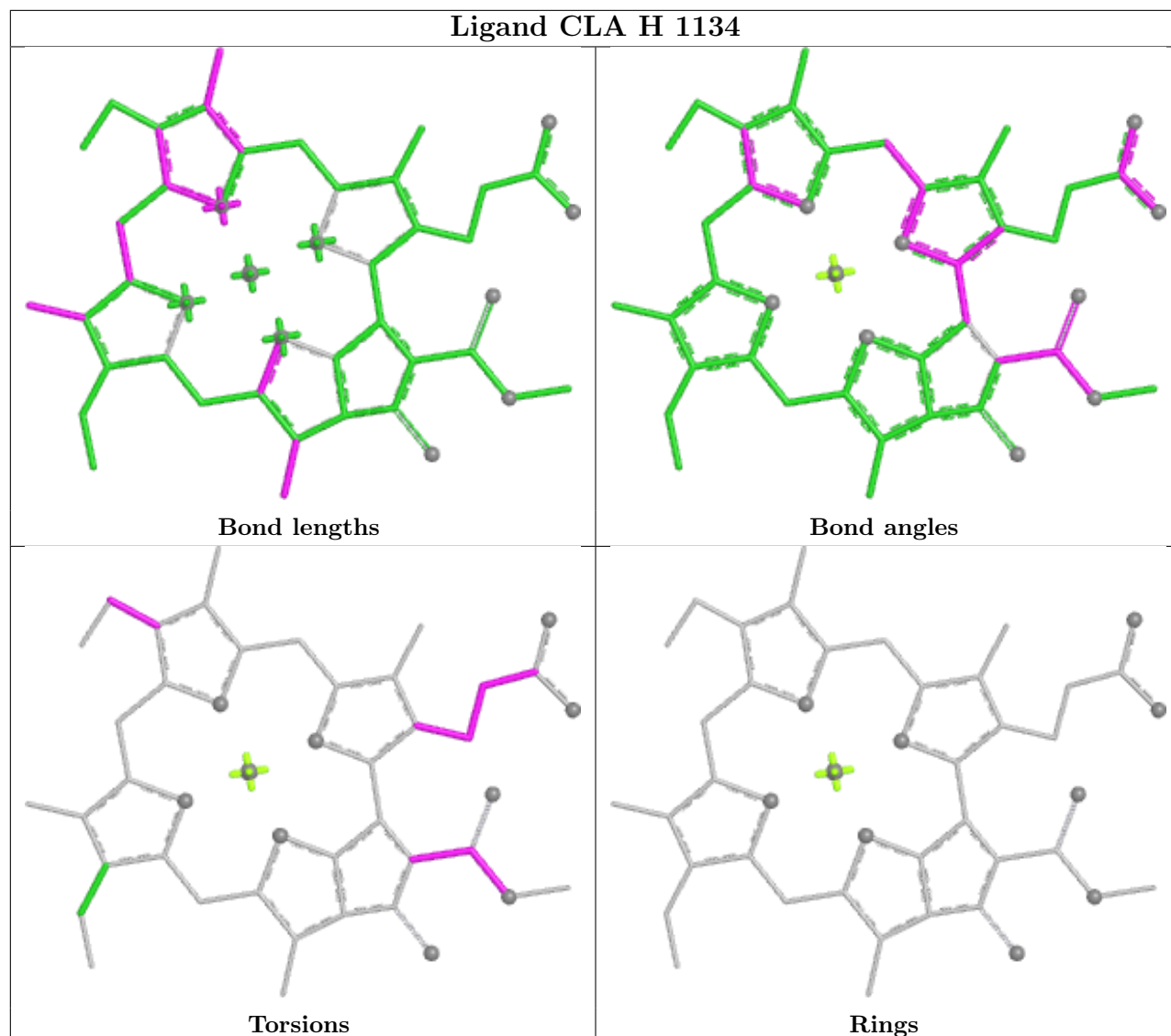


Ligand CLA h 512

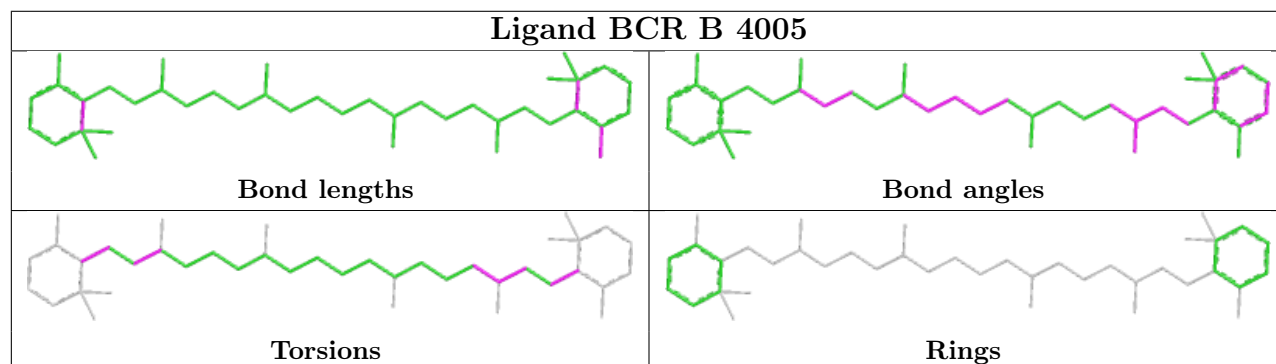




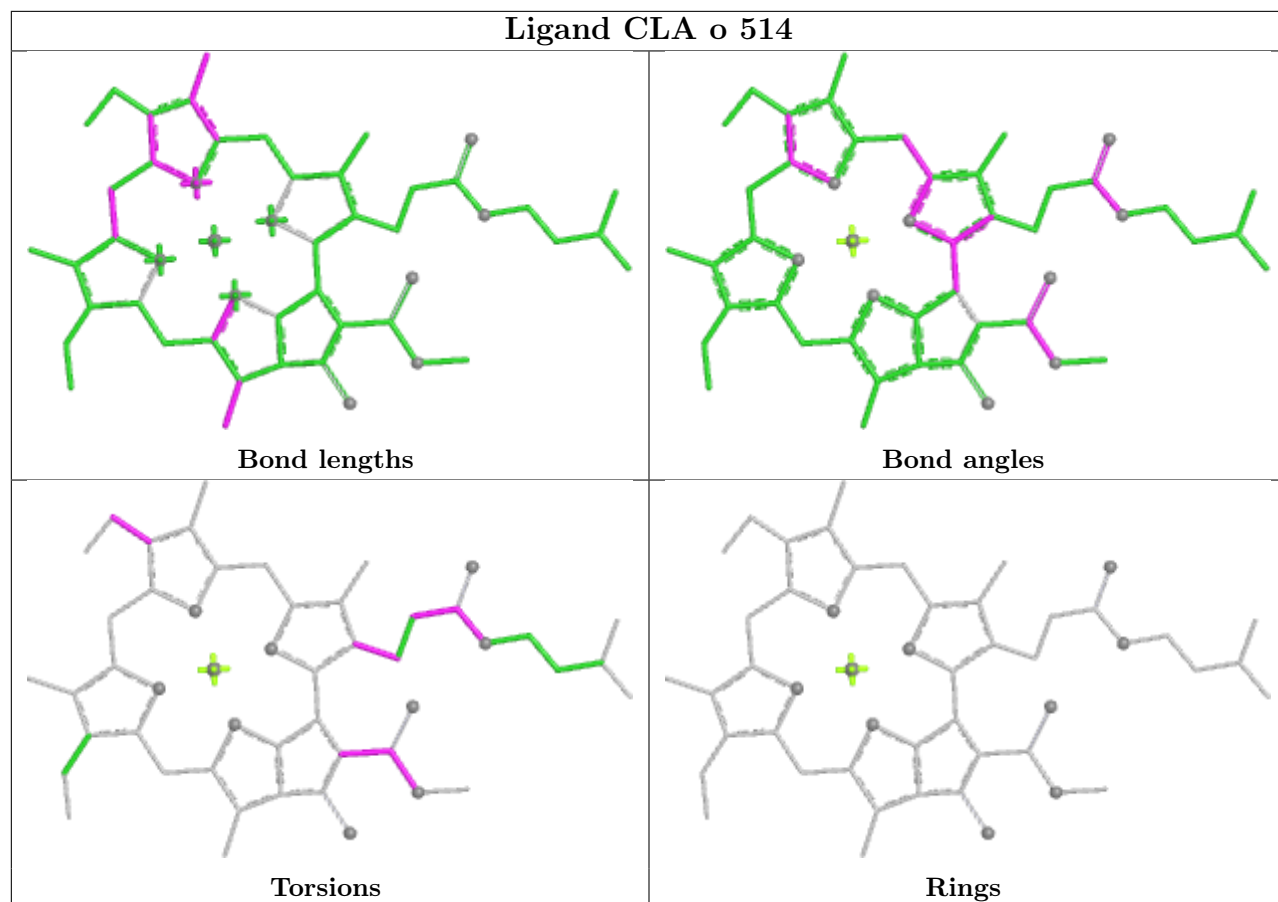
Ligand CLA H 1134



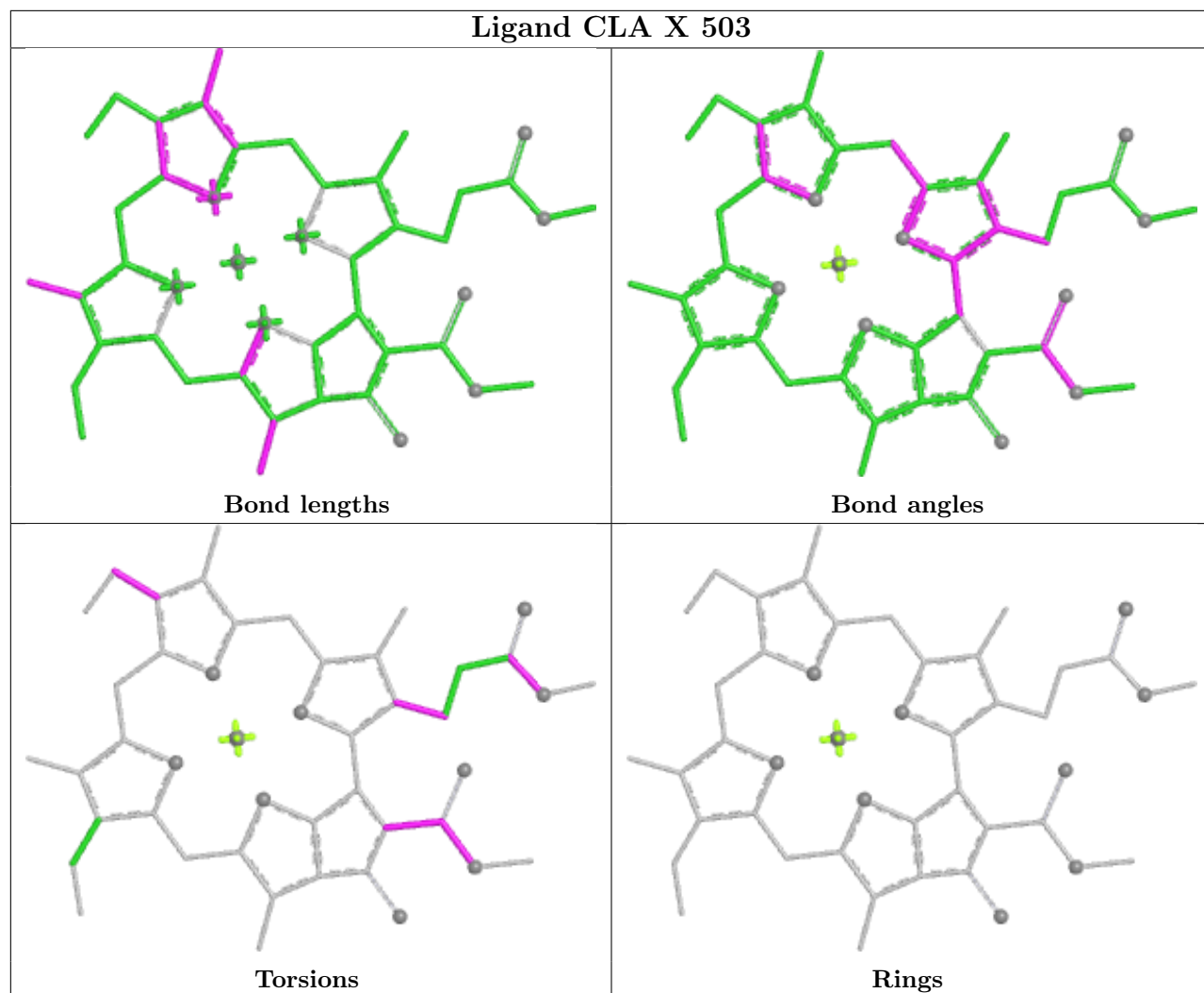
Ligand BCR B 4005



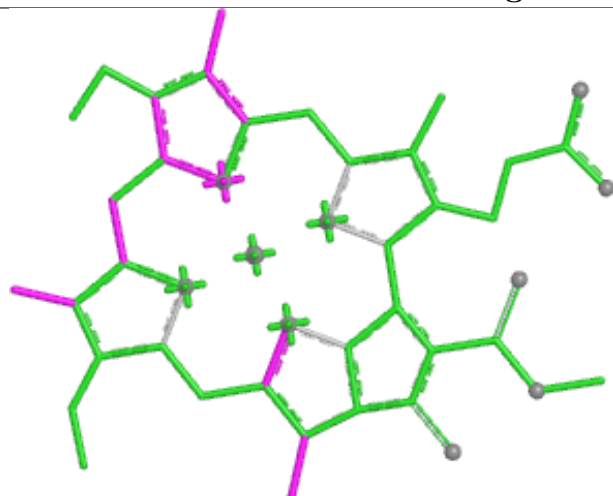
Ligand CLA o 514



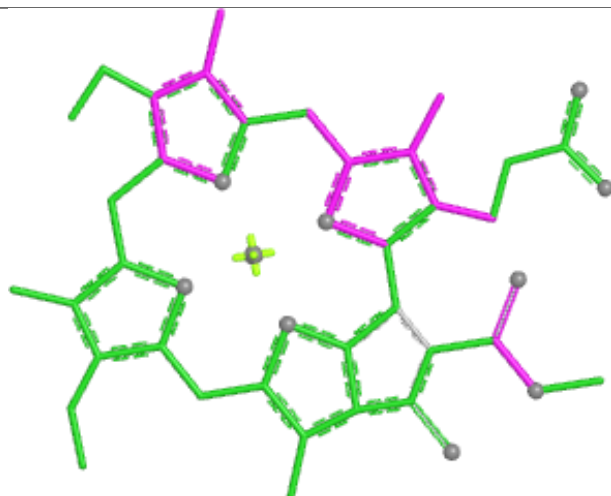
Ligand CLA X 503



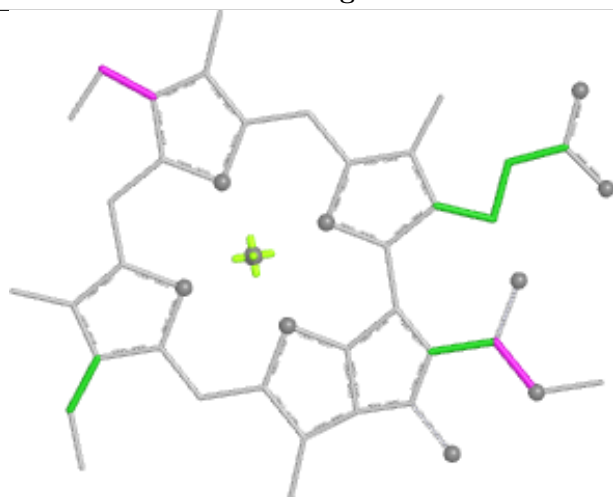
Ligand CLA B 1231



Bond lengths



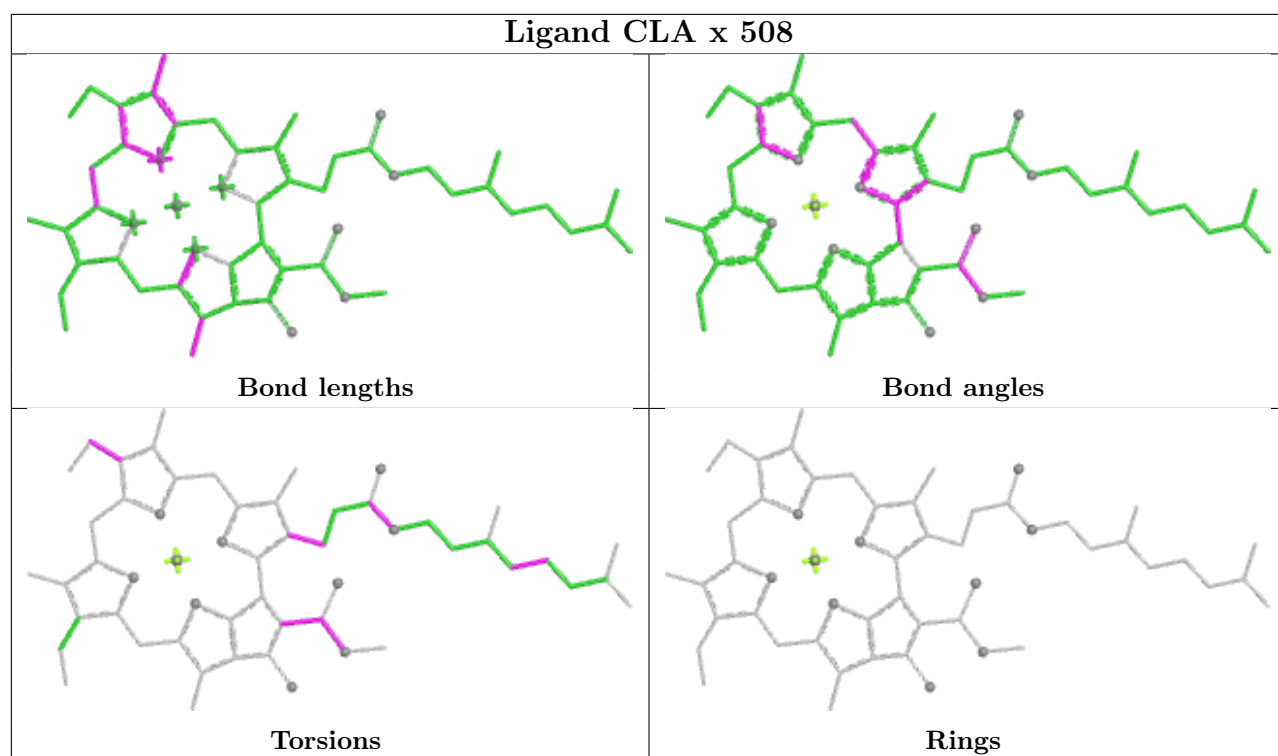
Bond angles

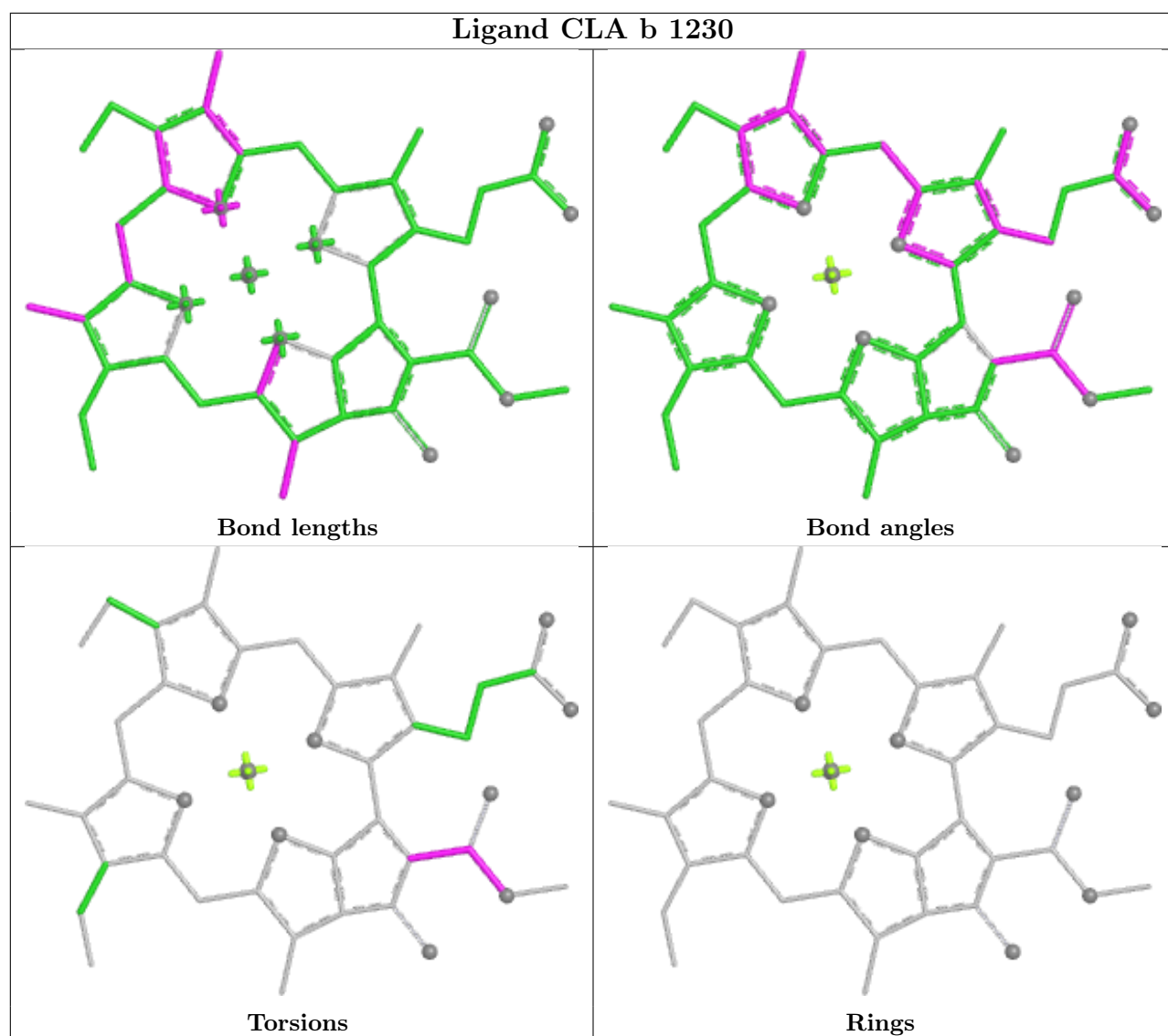


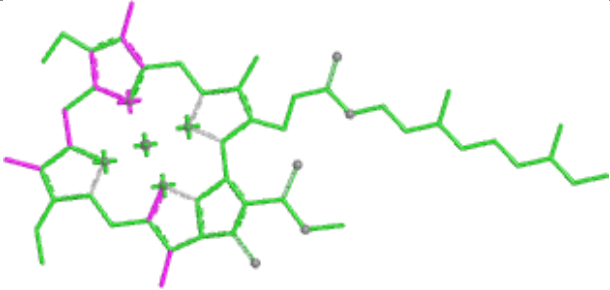
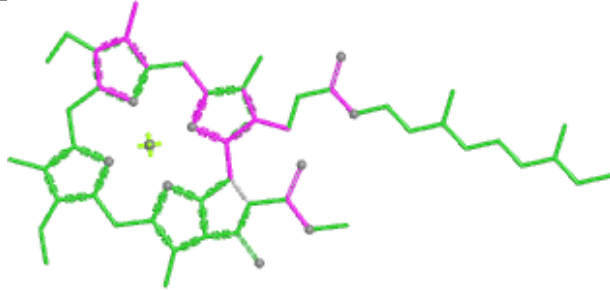
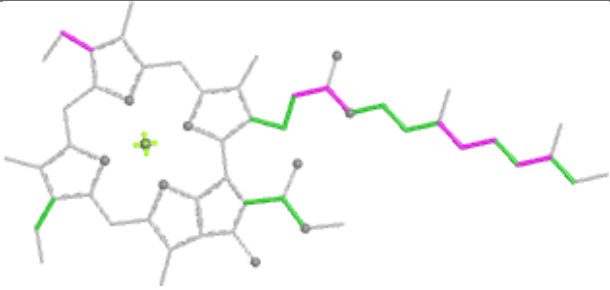
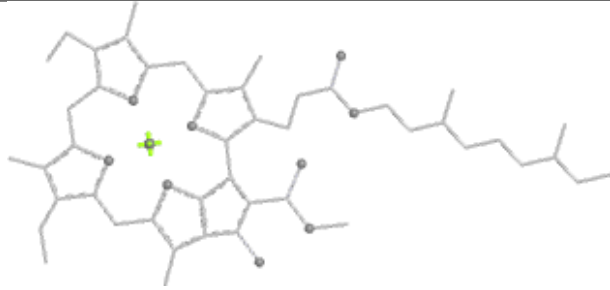
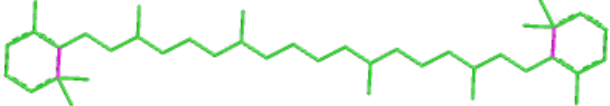
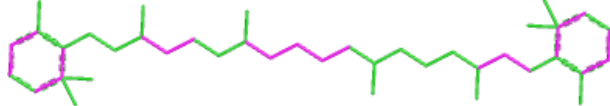
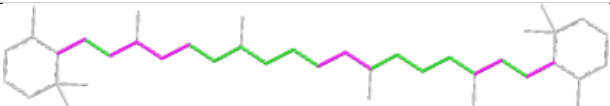
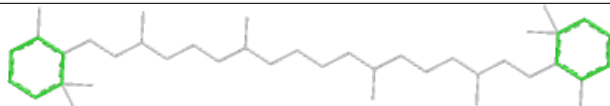
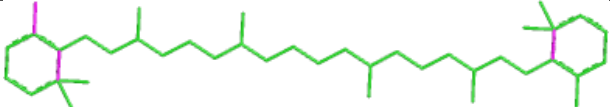
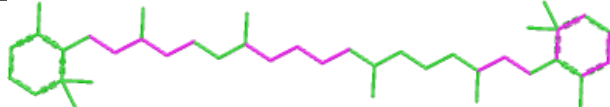
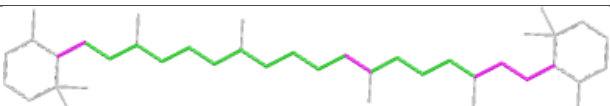
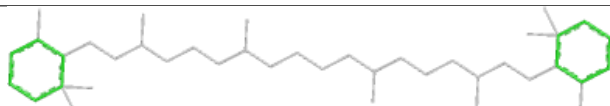
Torsions

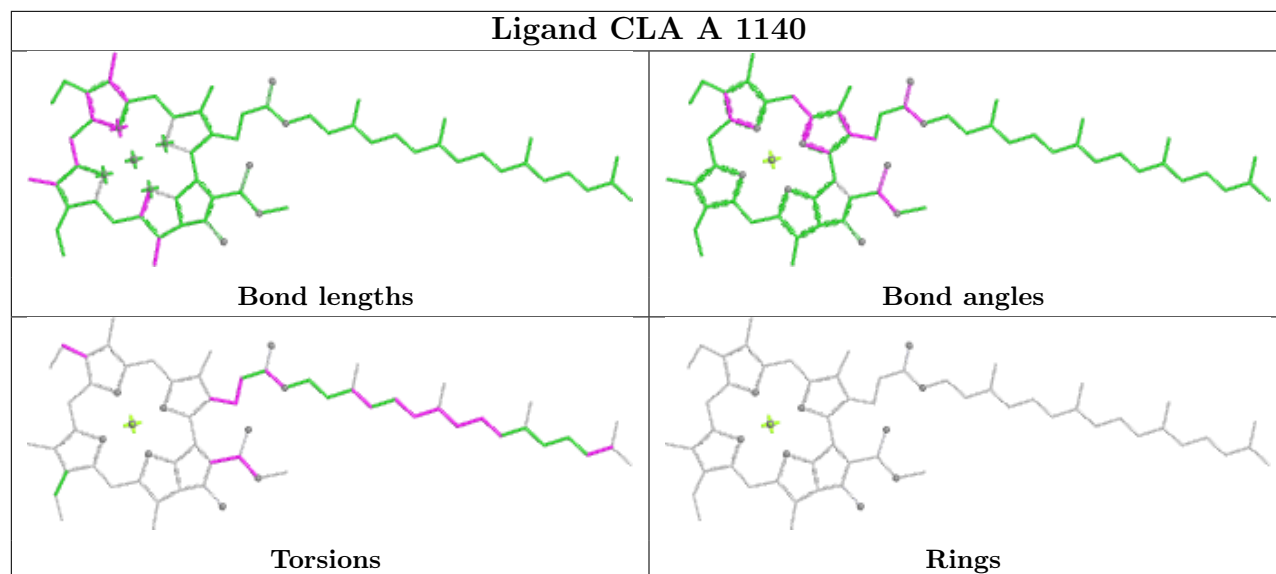
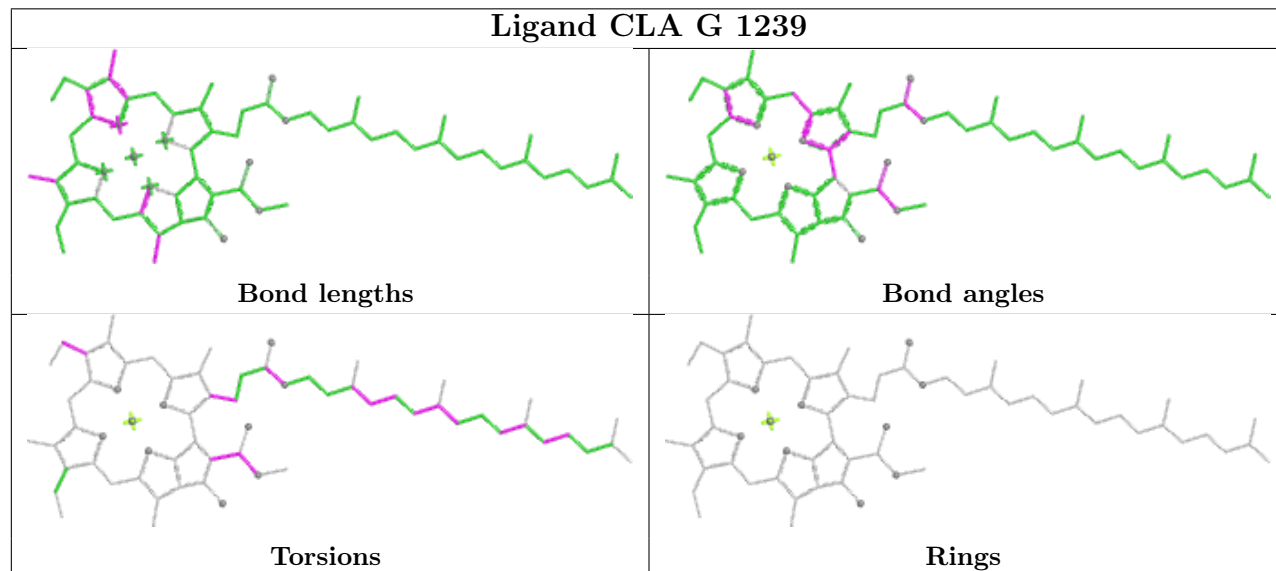


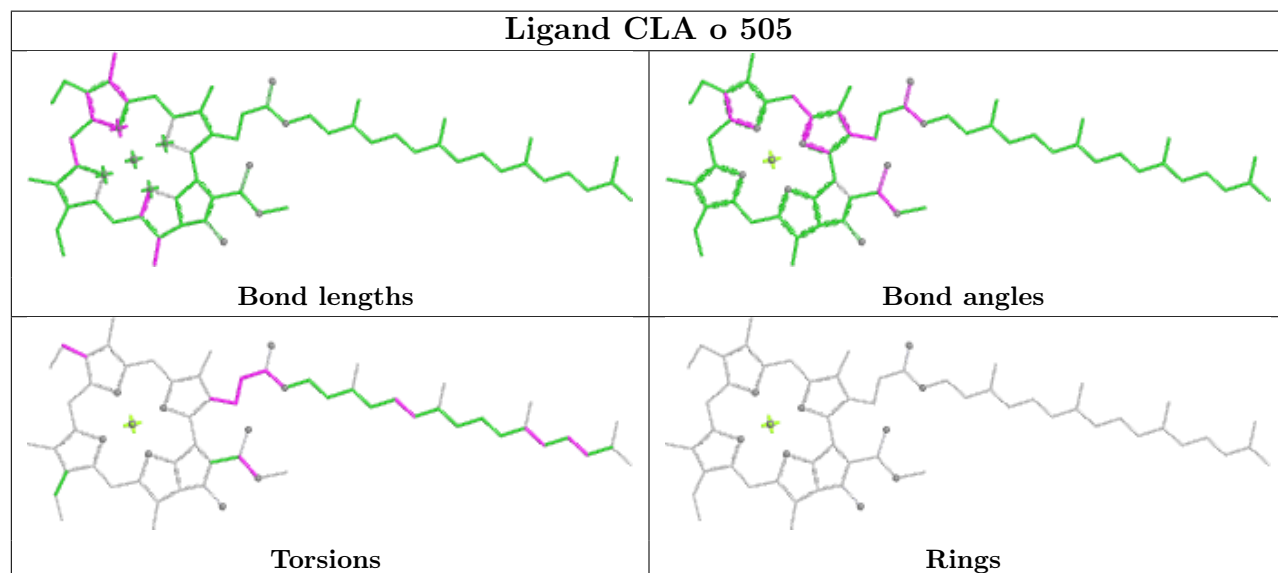
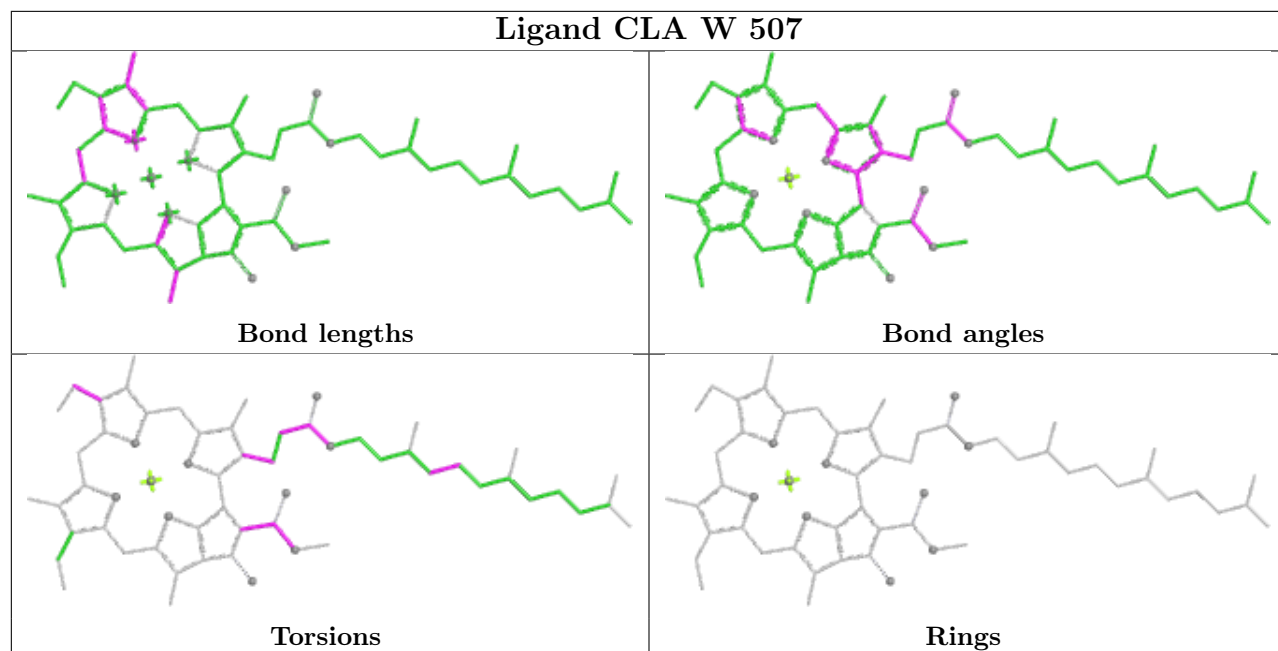
Rings

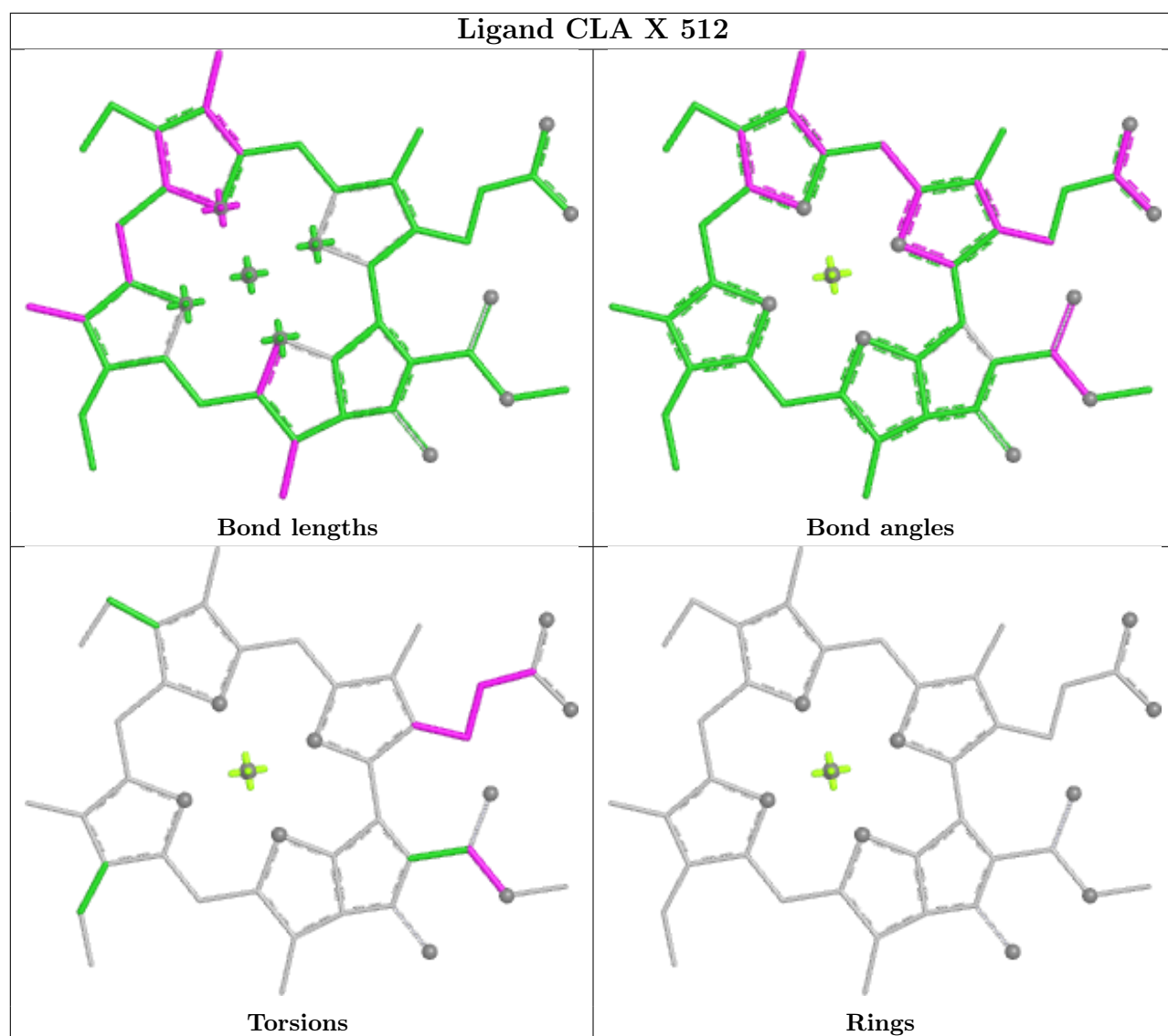




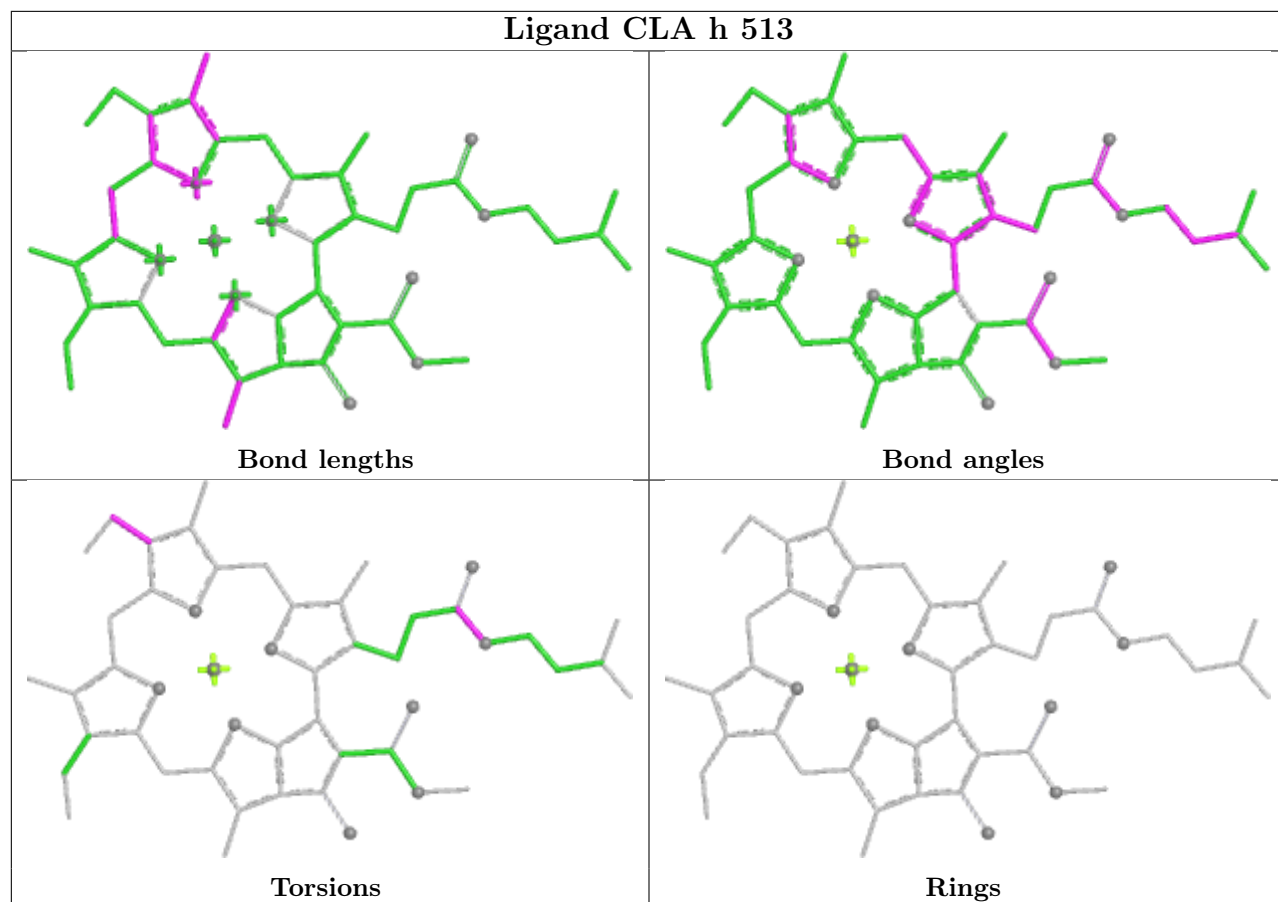
Ligand CLA Z 509	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR h 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR a 4007	
 Bond lengths	 Bond angles
 Torsions	 Rings

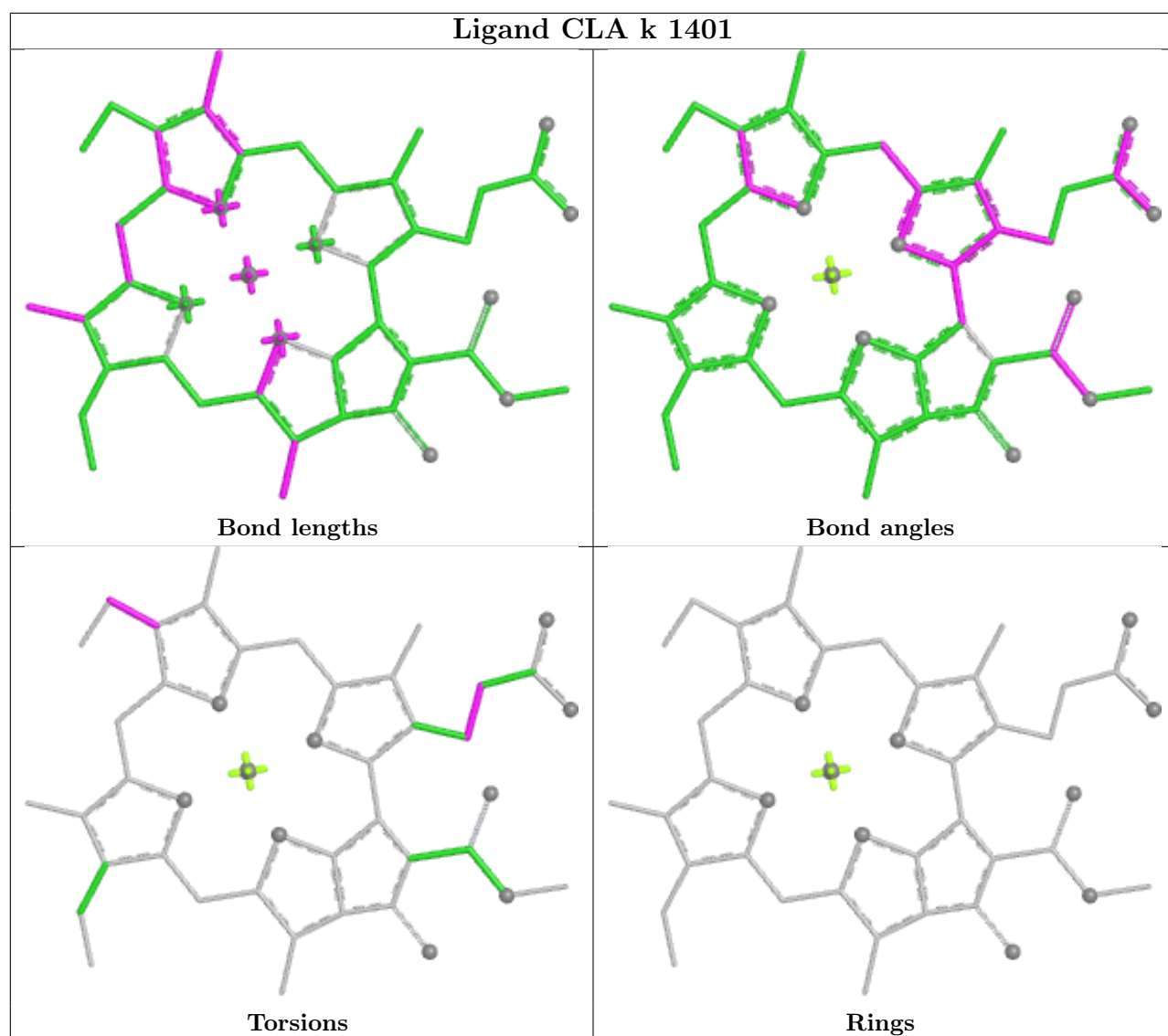
Ligand CLA A 1140**Ligand CLA G 1239**



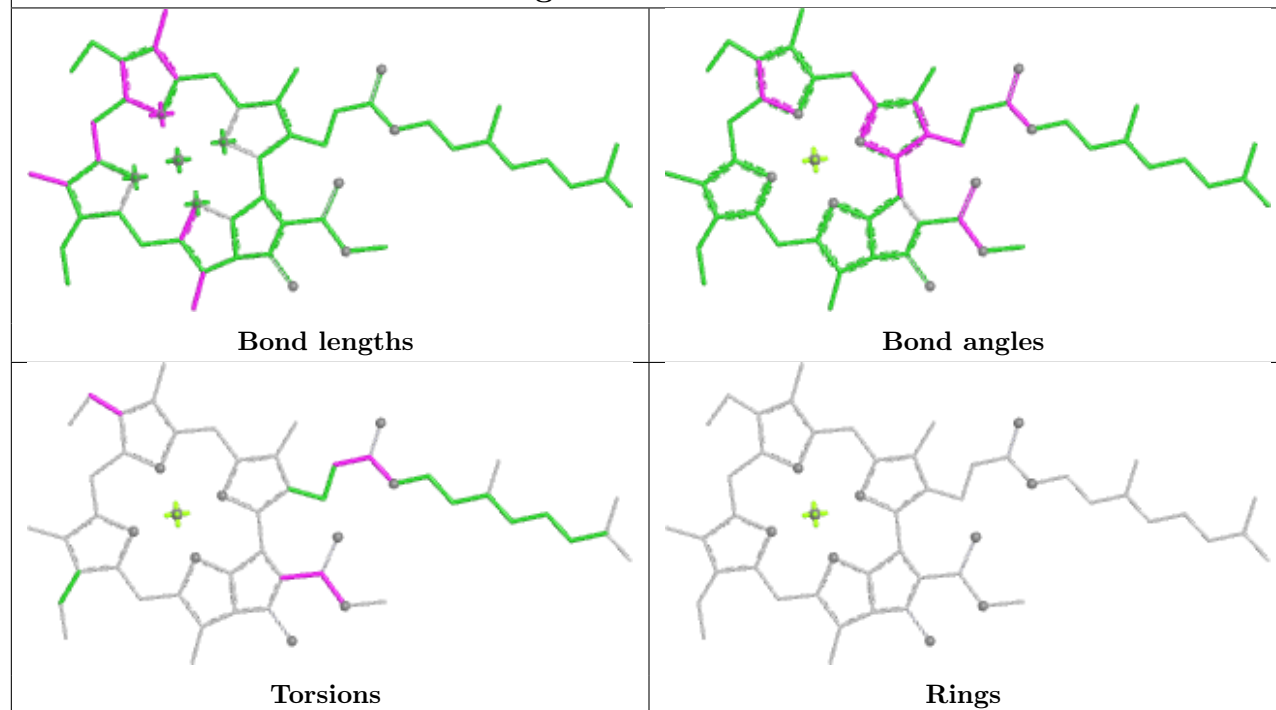


Ligand CLA h 513

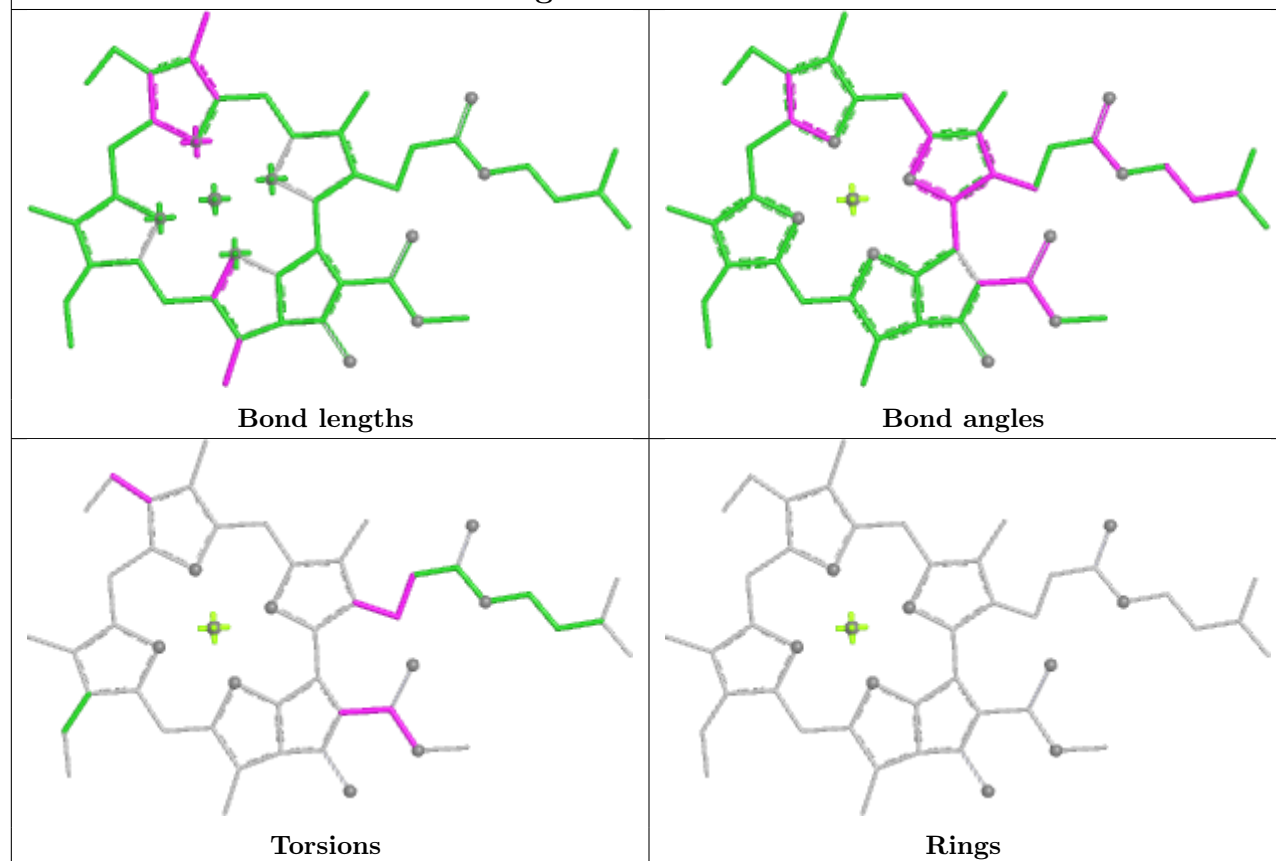




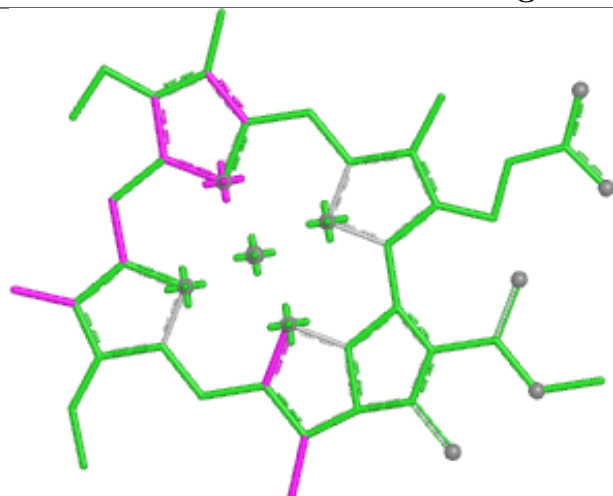
Ligand CLA h 517



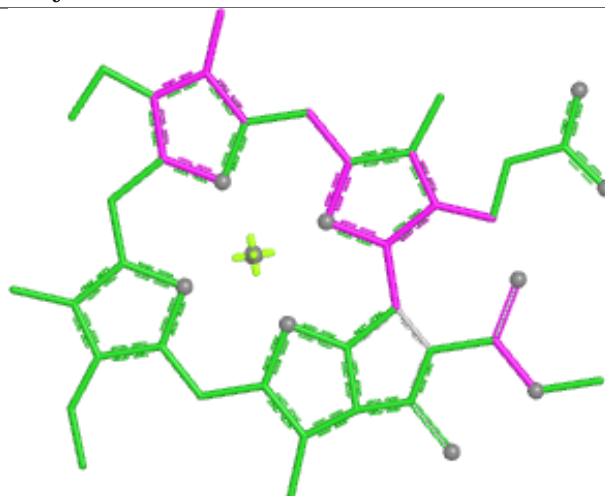
Ligand CLA u 502



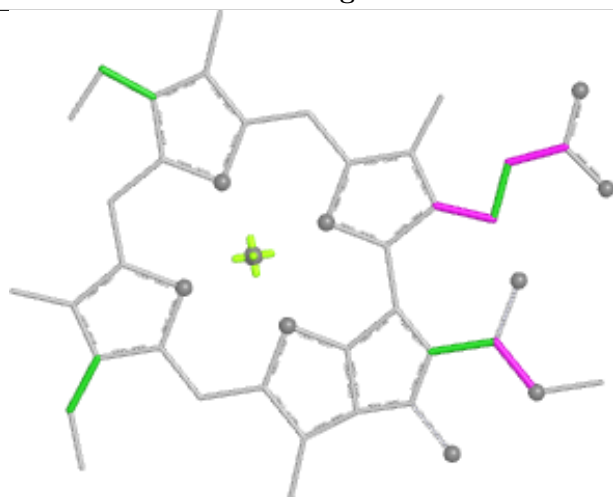
Ligand CLA y 512



Bond lengths



Bond angles

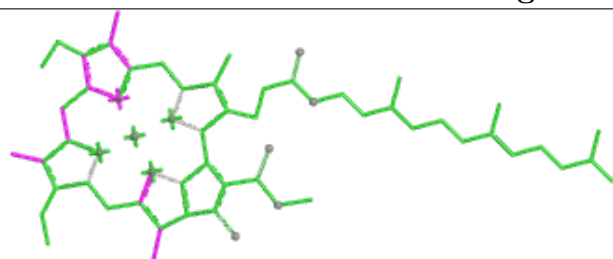


Torsions

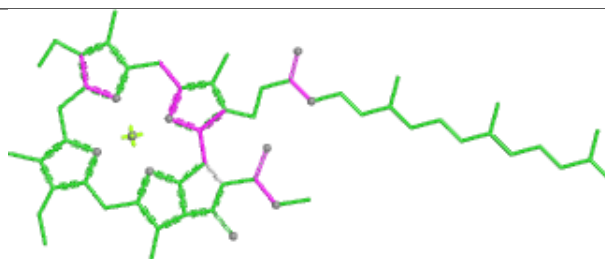


Rings

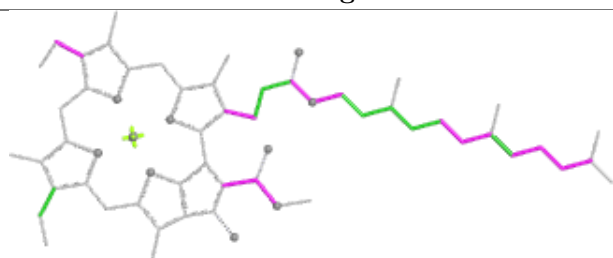
Ligand CLA u 504



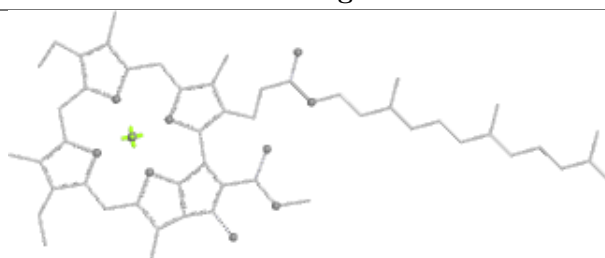
Bond lengths



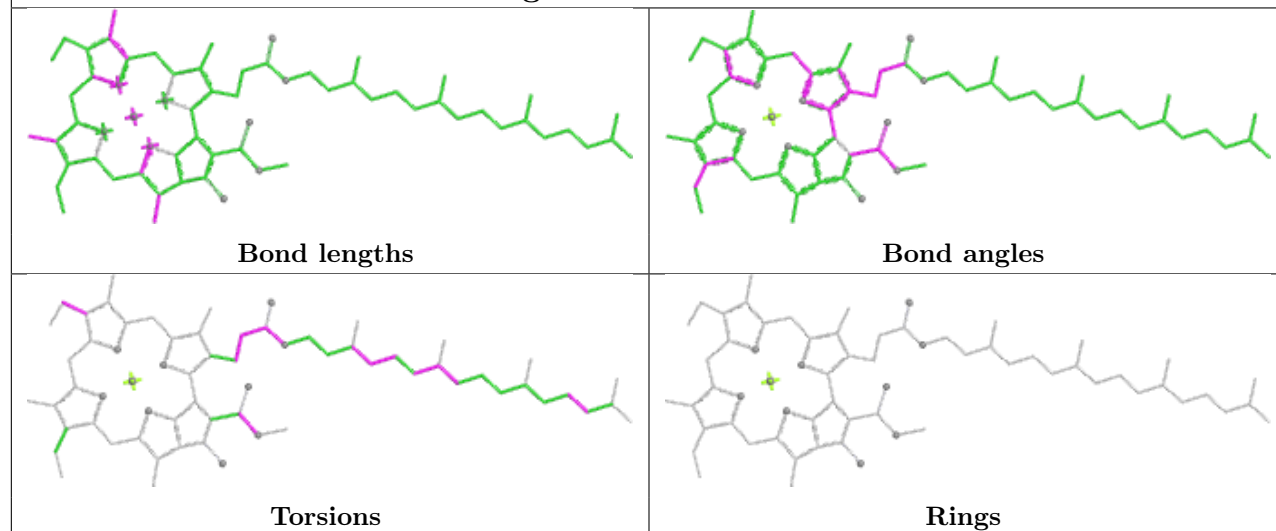
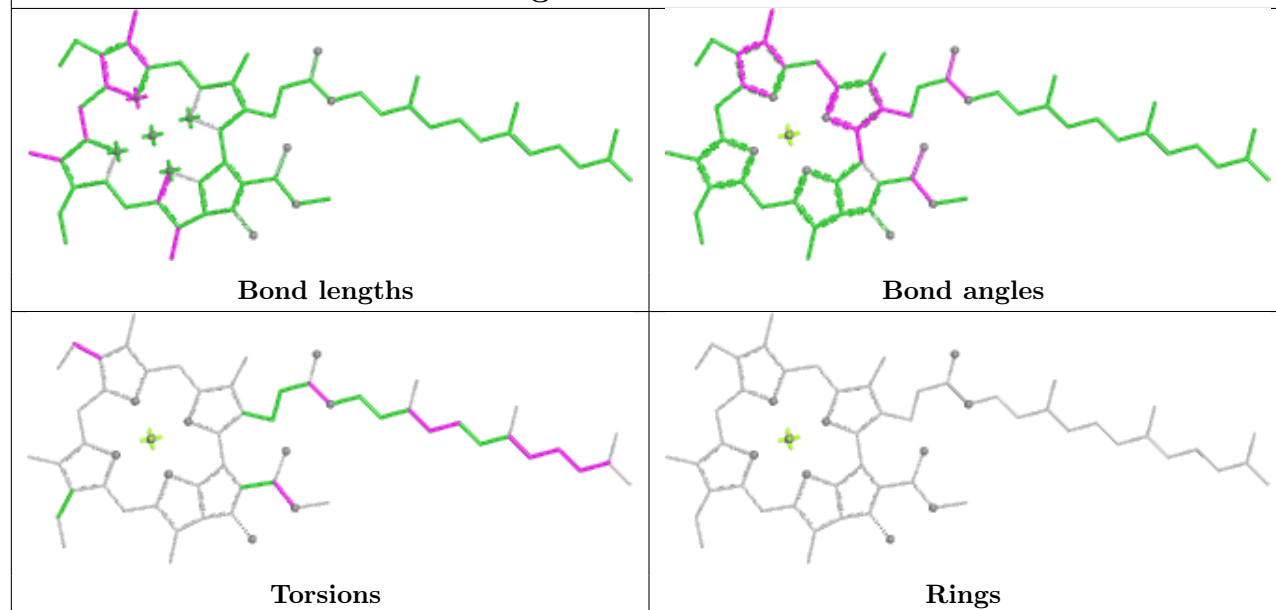
Bond angles



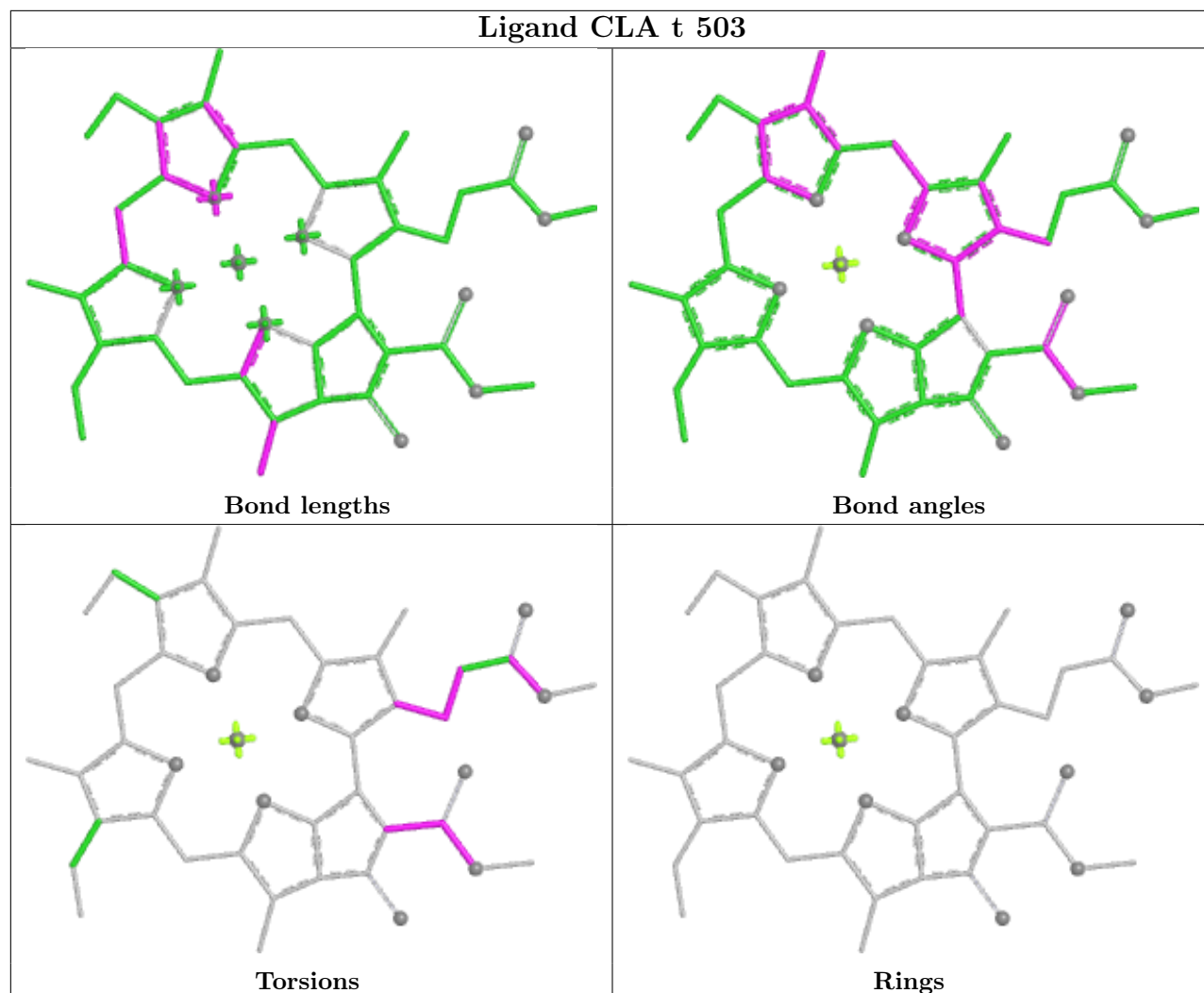
Torsions



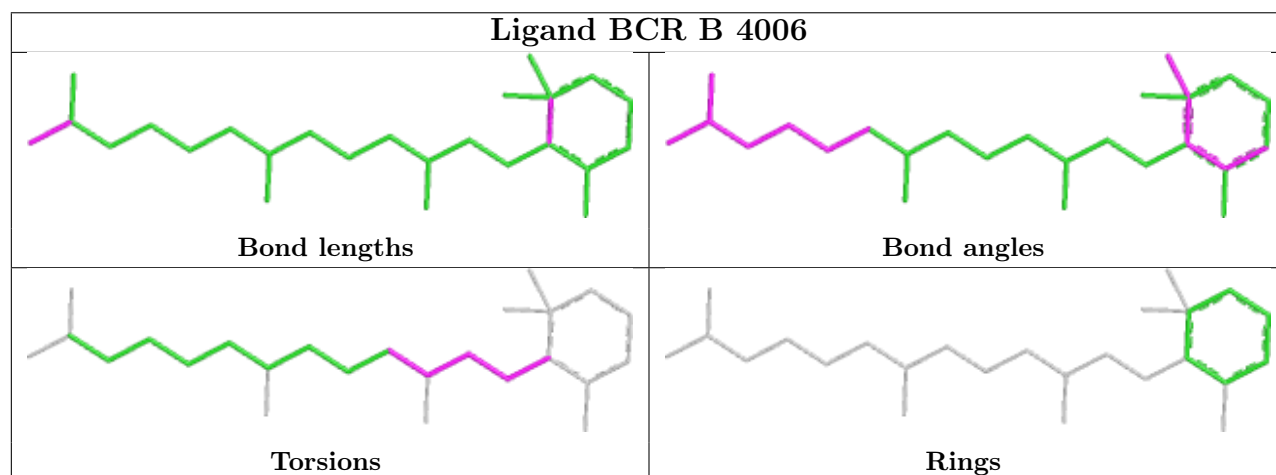
Rings

Ligand CLA A 1237**Ligand CLA Y 509**

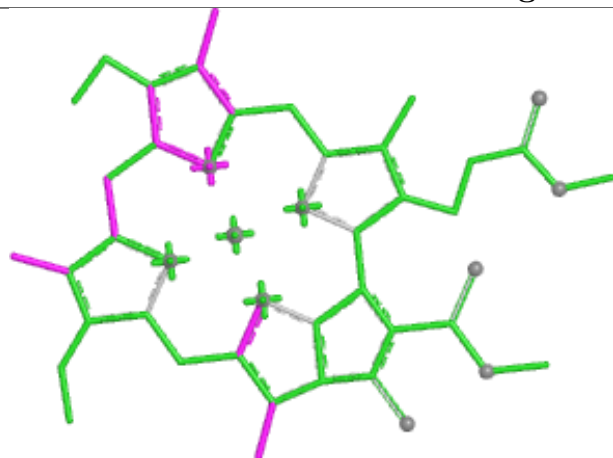
Ligand CLA t 503



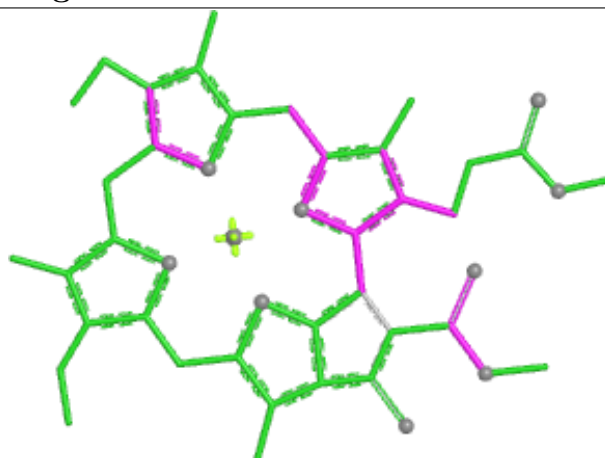
Ligand BCR B 4006



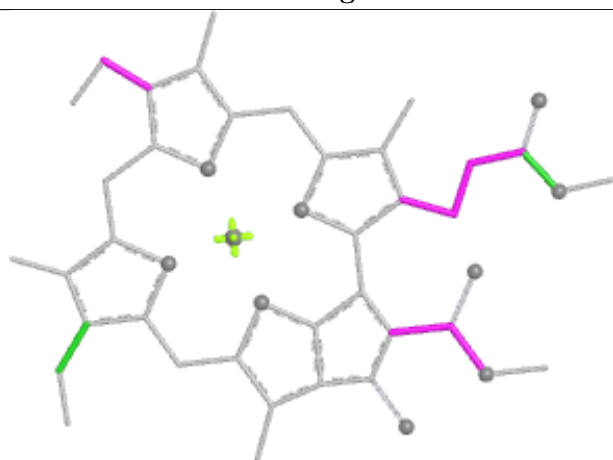
Ligand CLA g 505



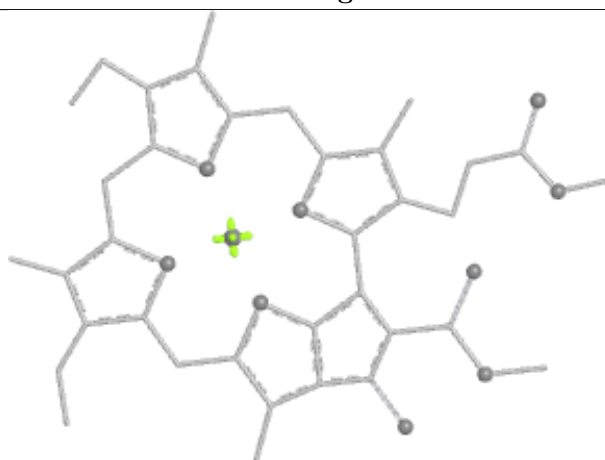
Bond lengths



Bond angles

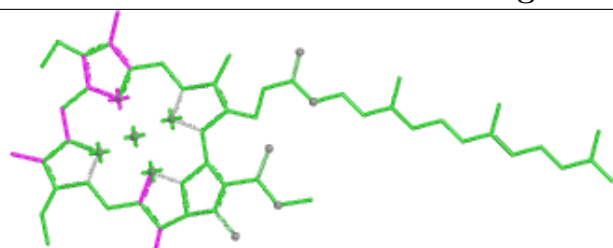


Torsions

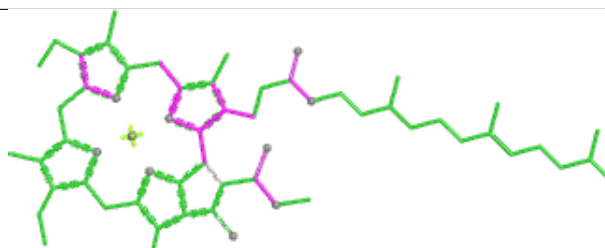


Rings

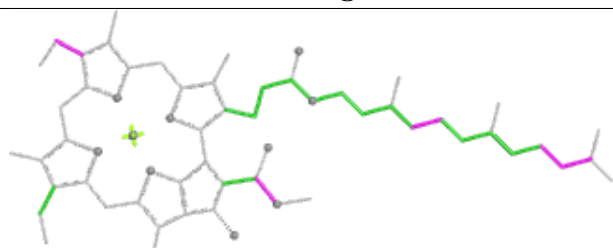
Ligand CLA h 509



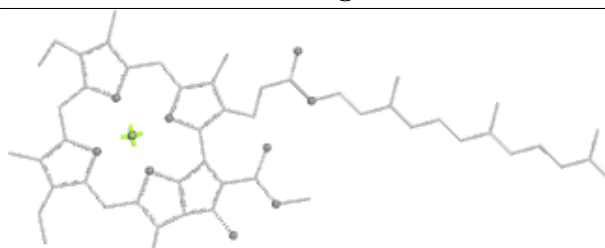
Bond lengths



Bond angles

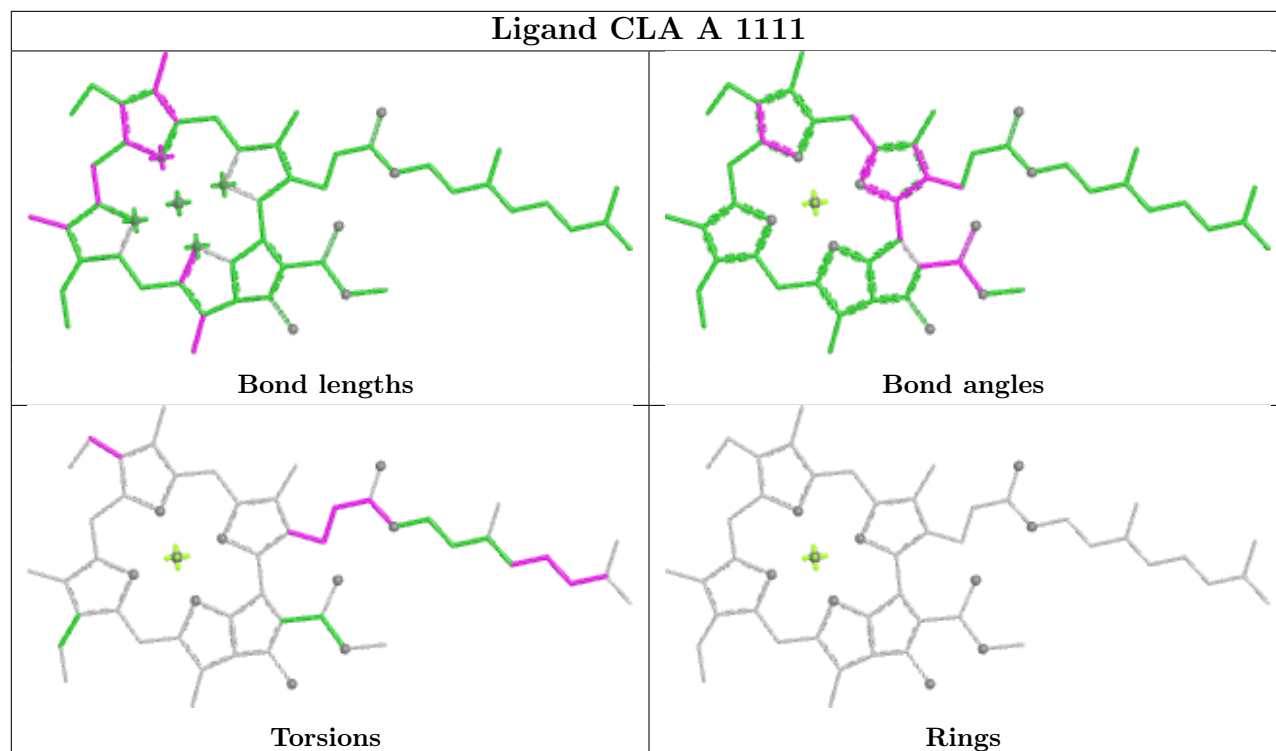


Torsions

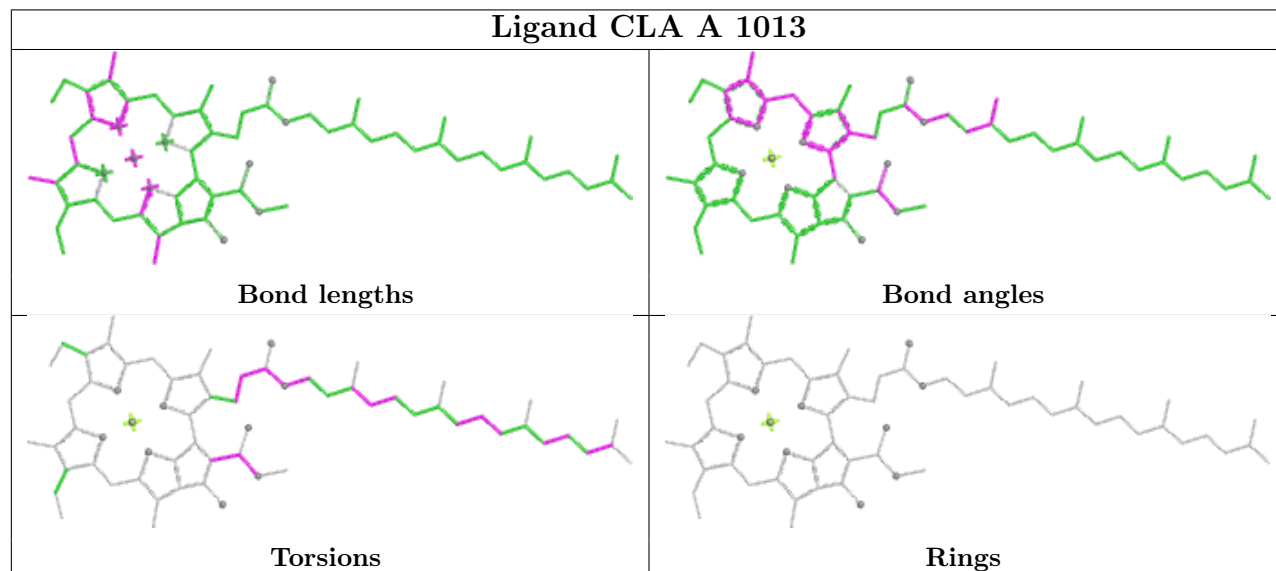


Rings

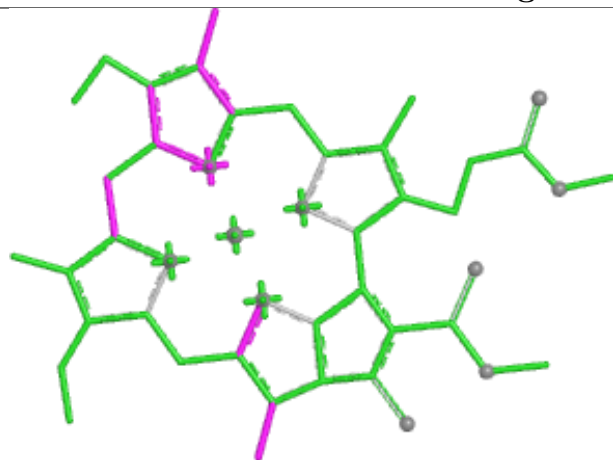
Ligand CLA A 1111



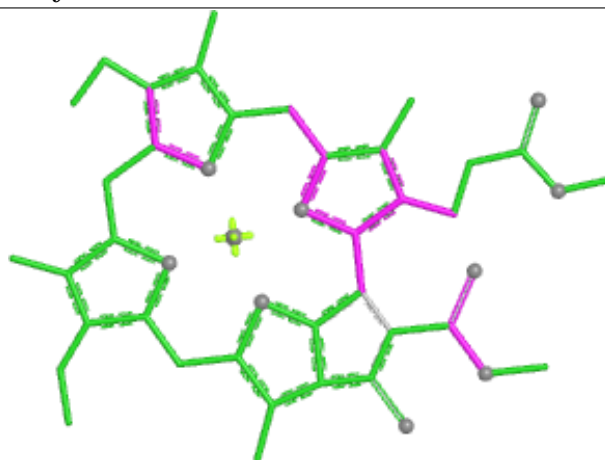
Ligand CLA A 1013



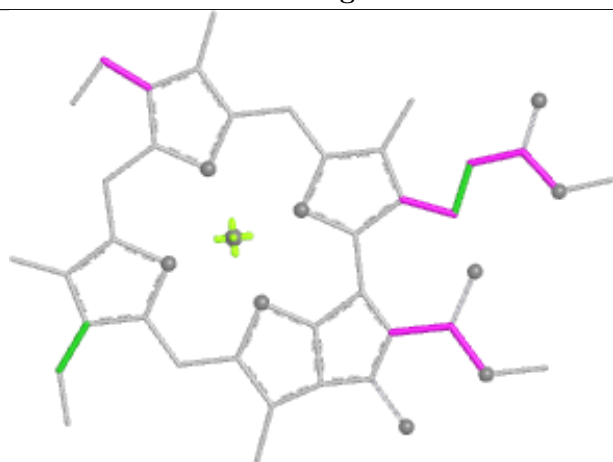
Ligand CLA y 503



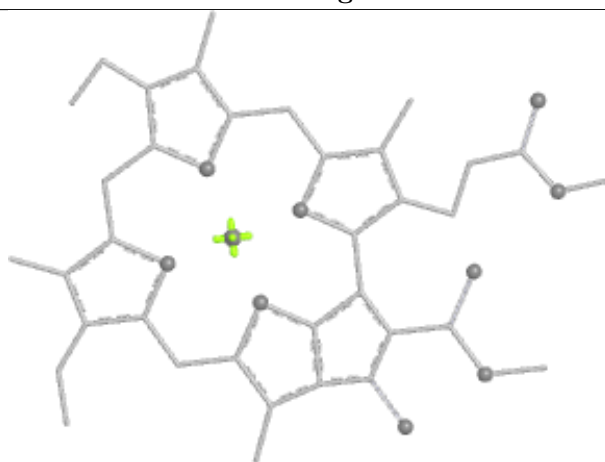
Bond lengths



Bond angles

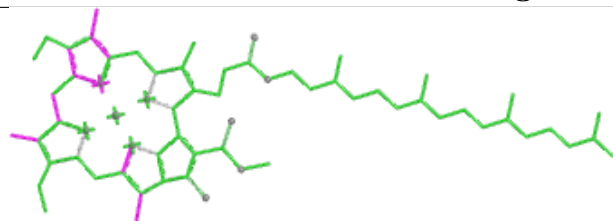


Torsions

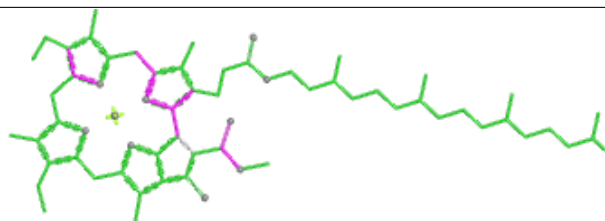


Rings

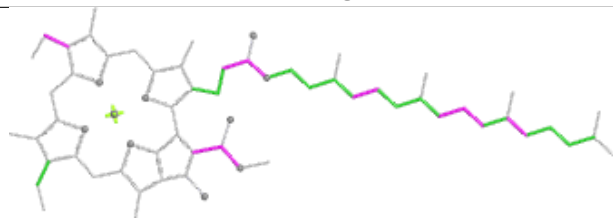
Ligand CLA w 507



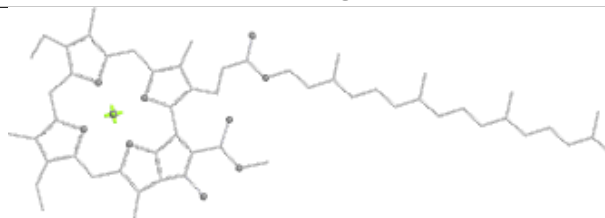
Bond lengths



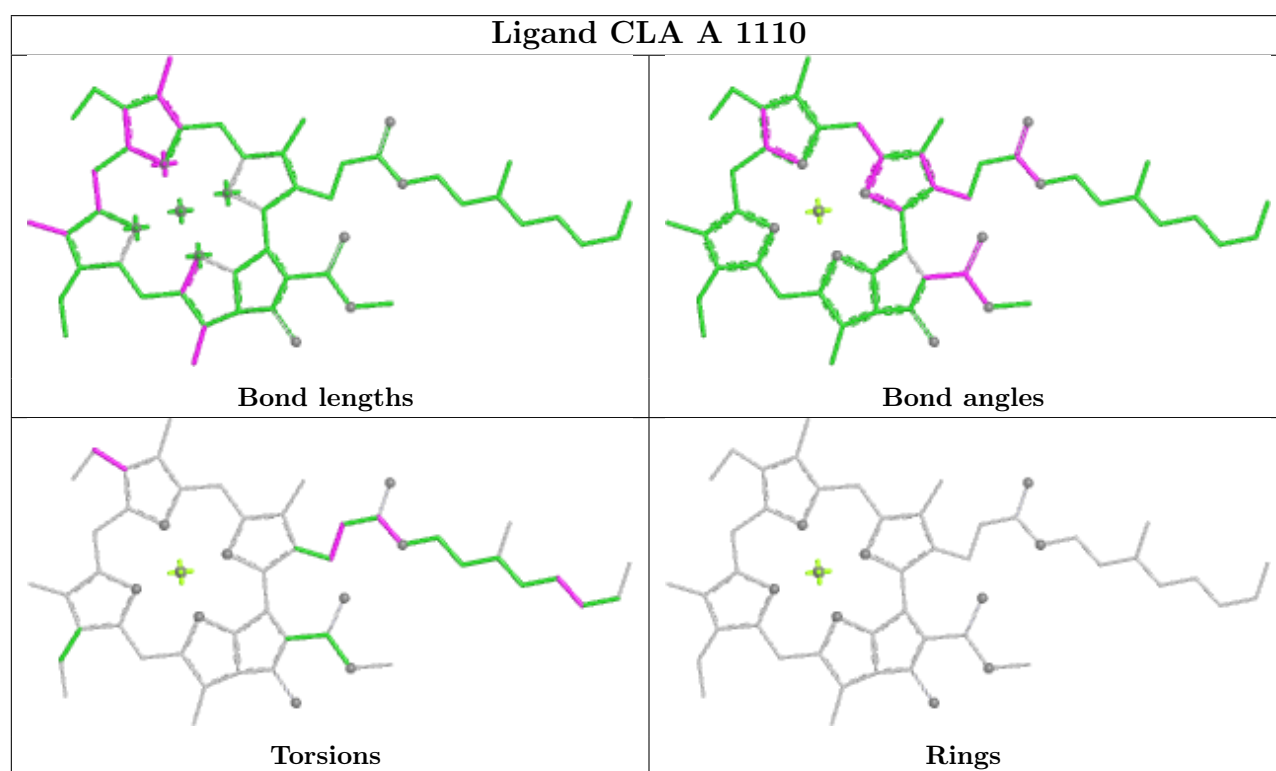
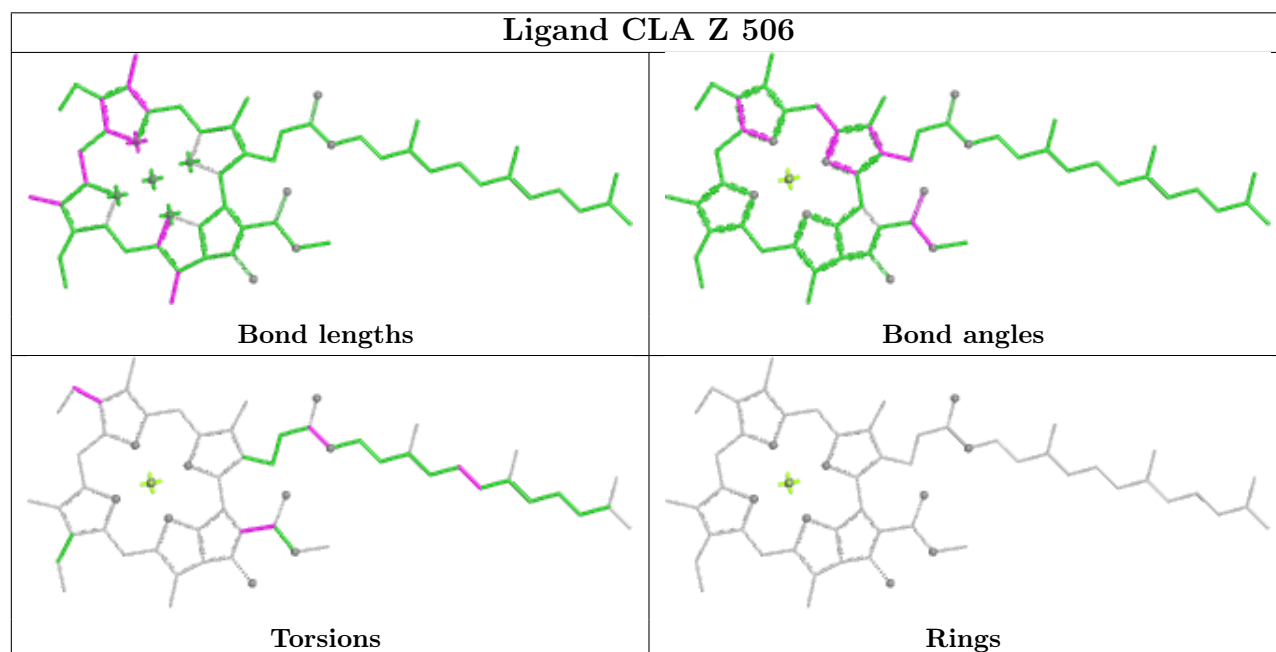
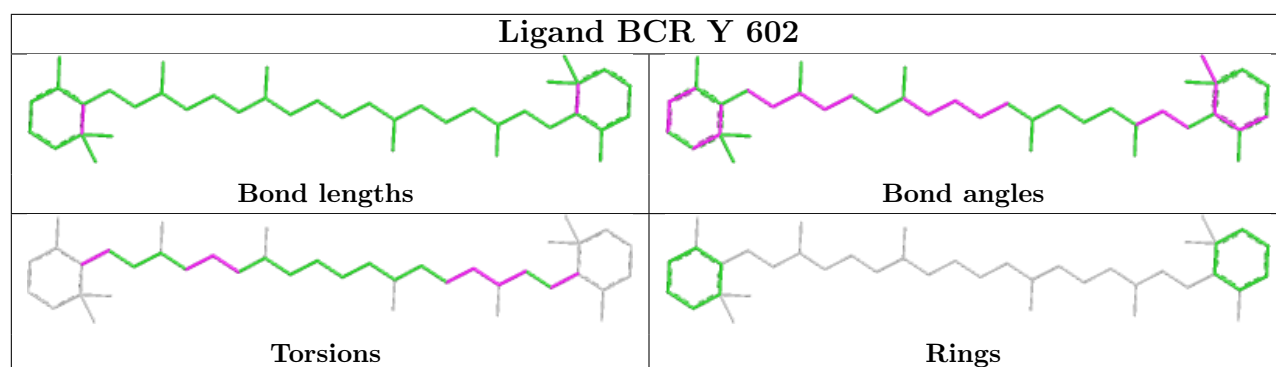
Bond angles

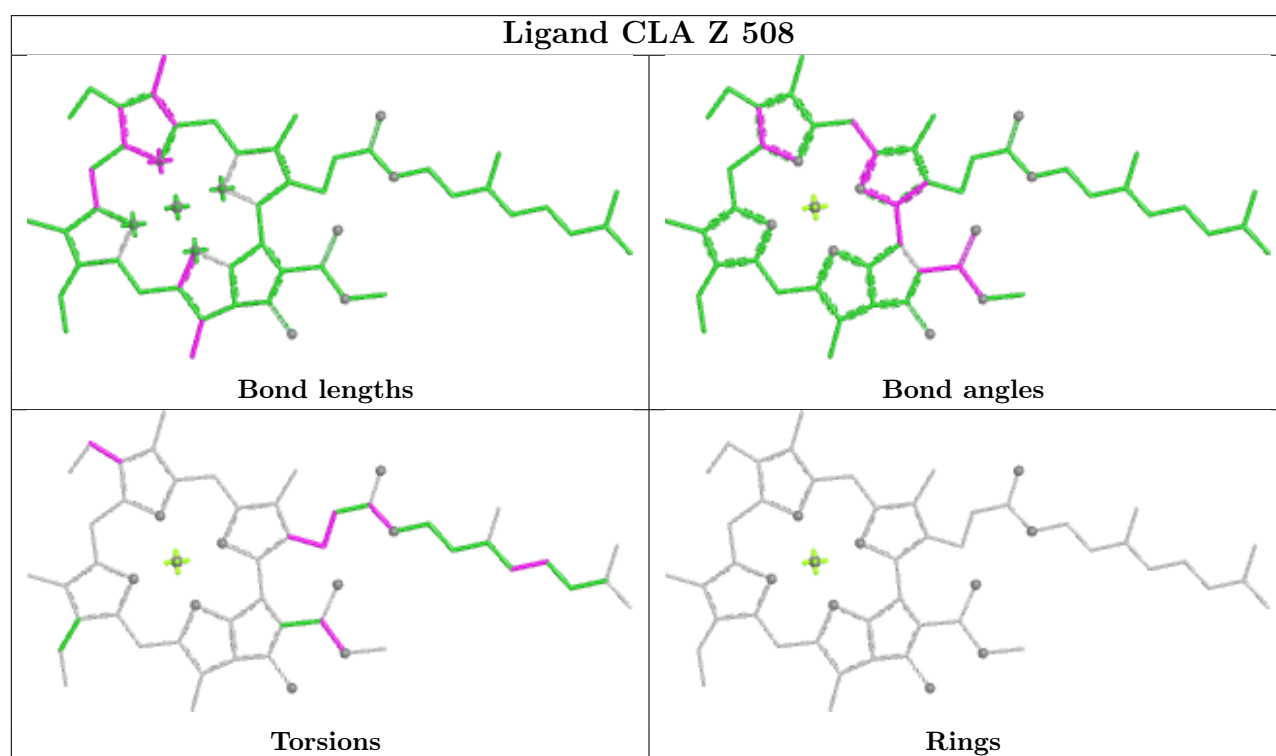
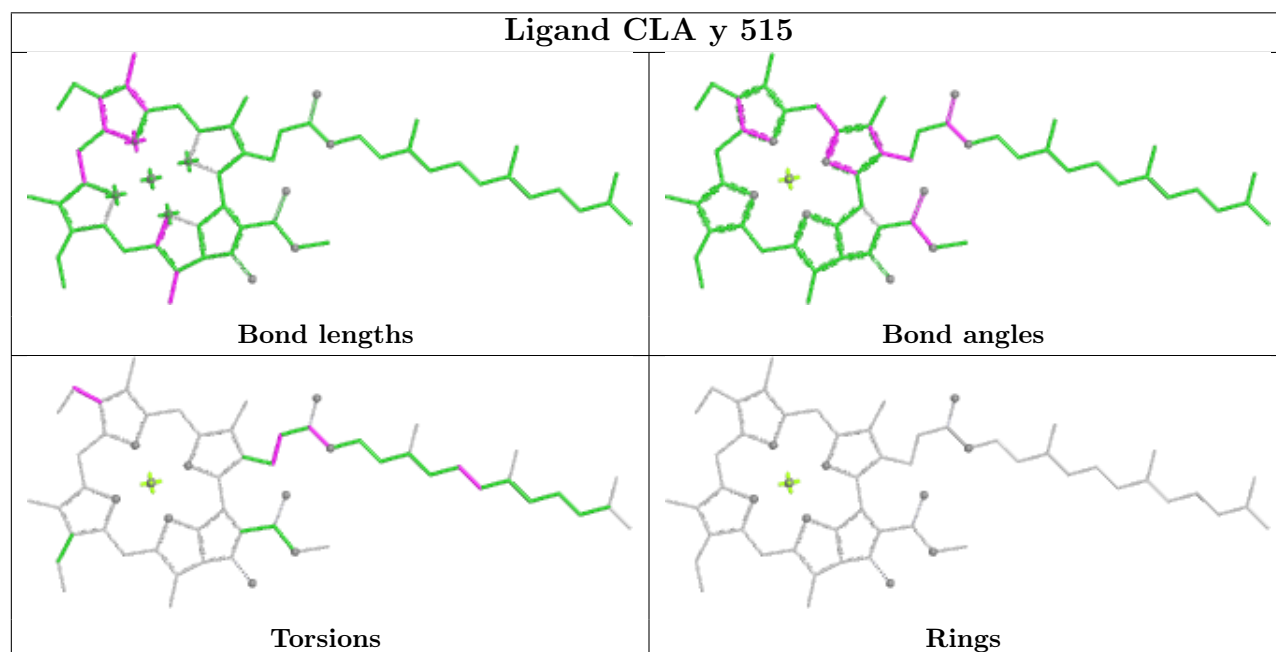
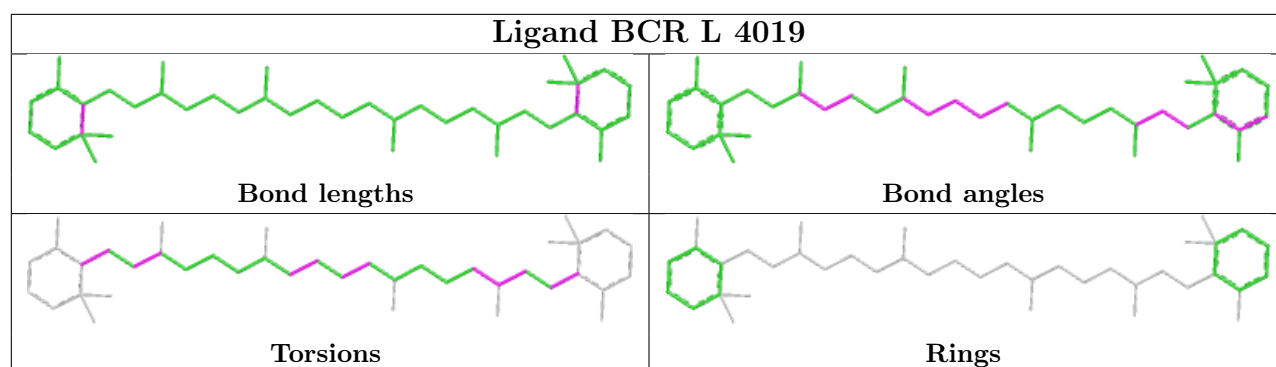


Torsions

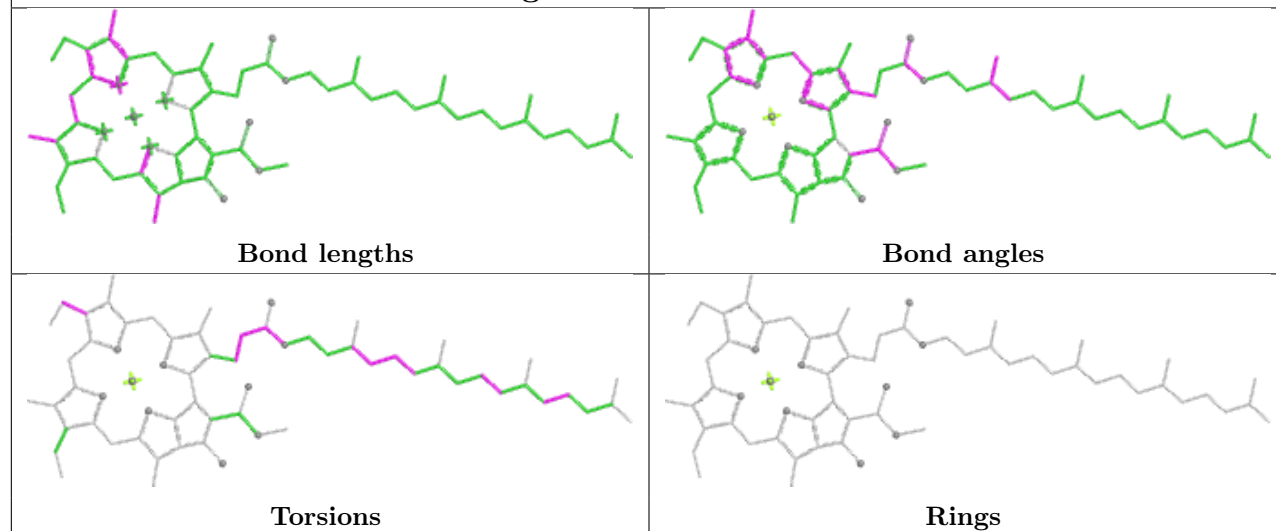


Rings

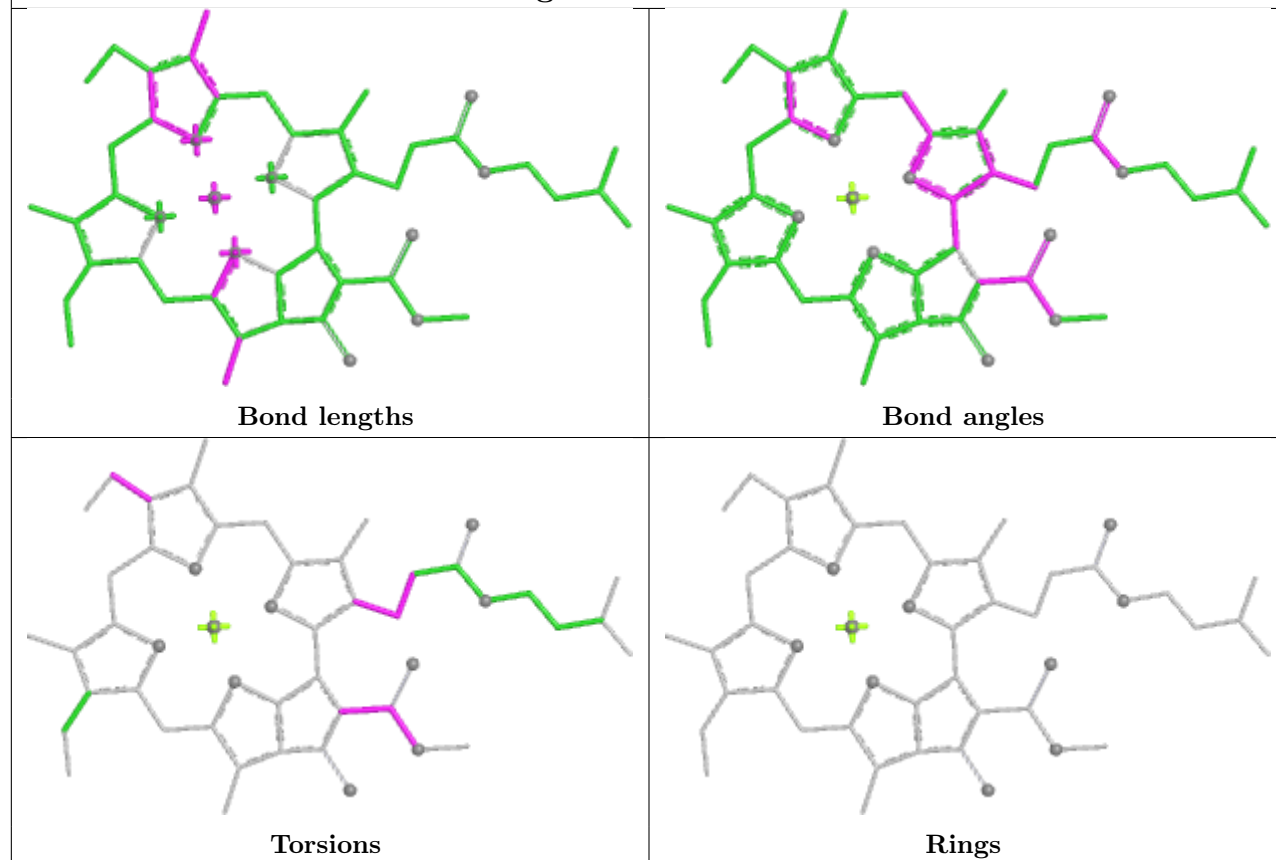




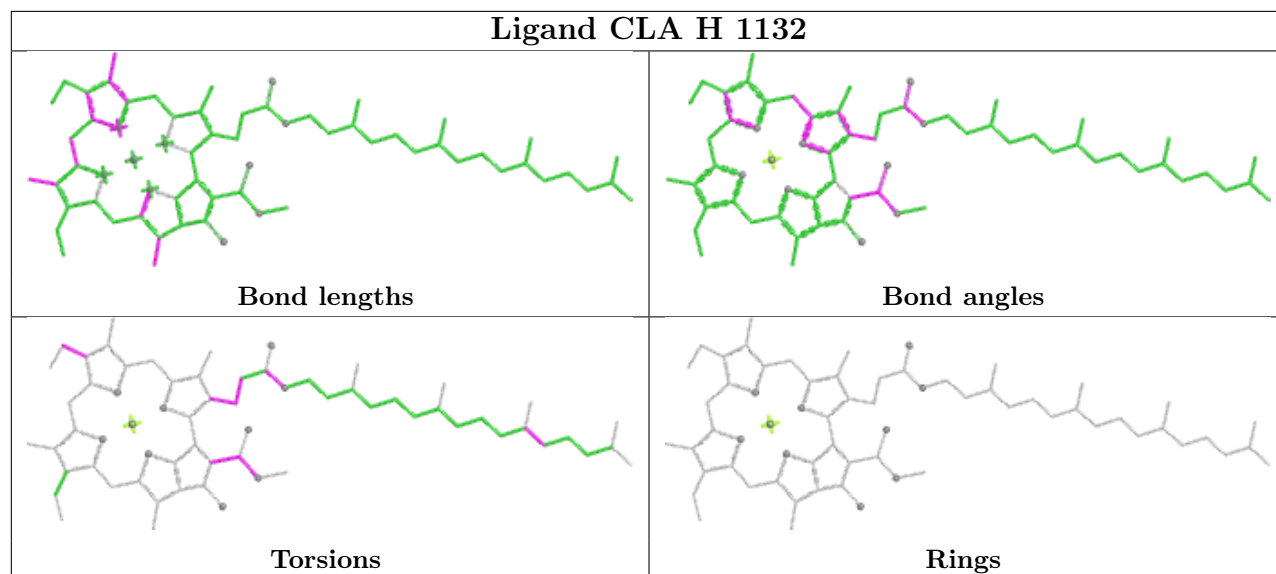
Ligand CLA G 1236



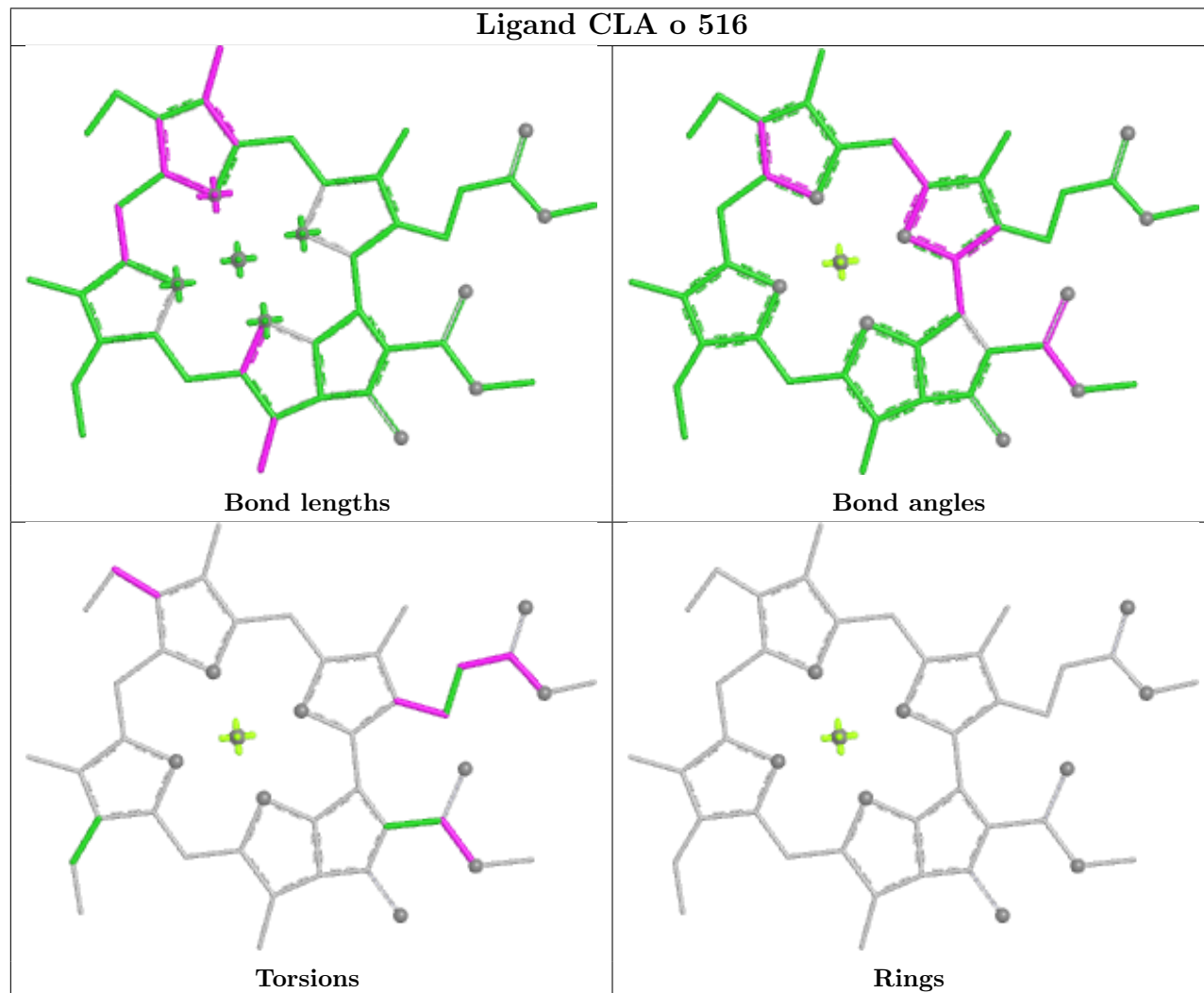
Ligand CLA o 502

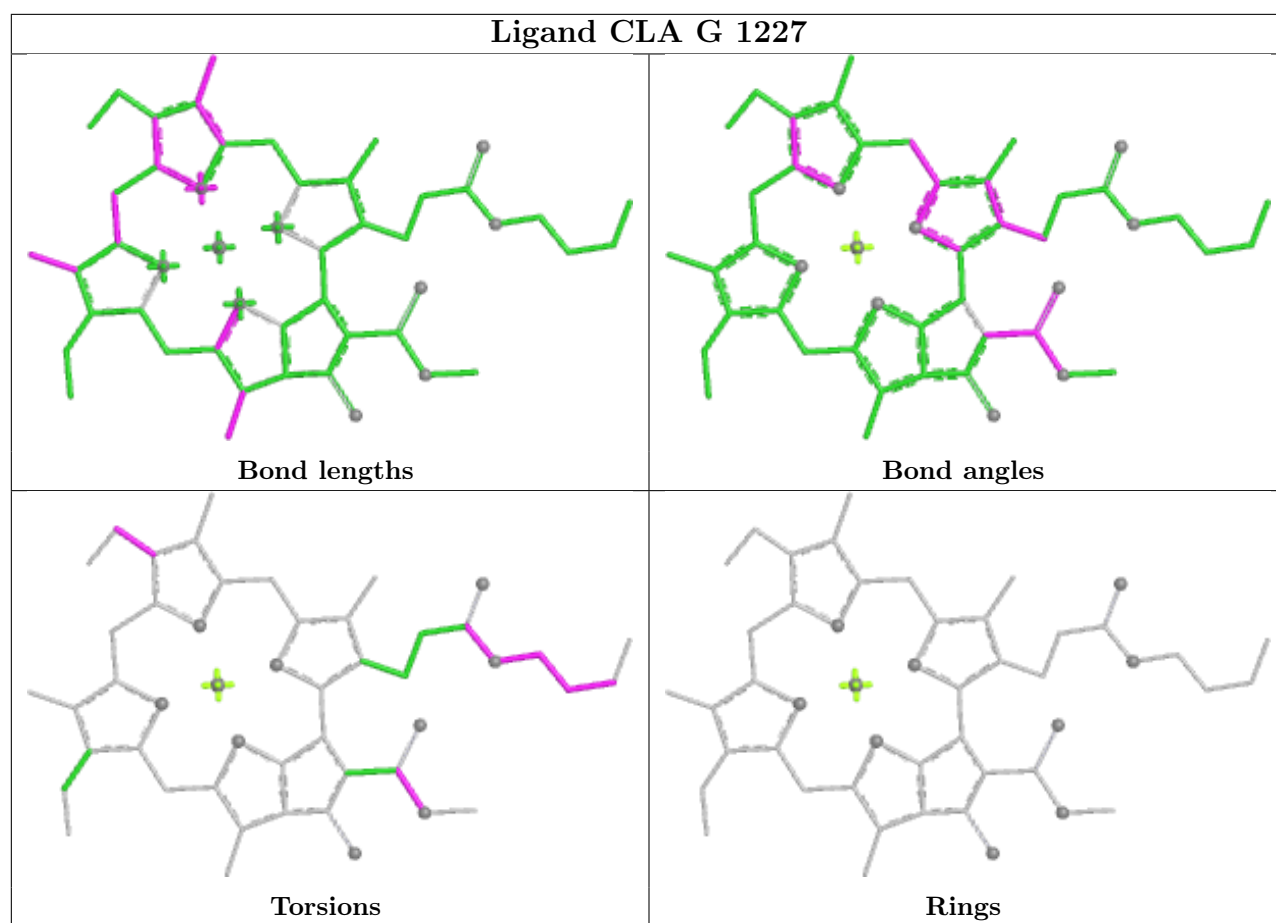


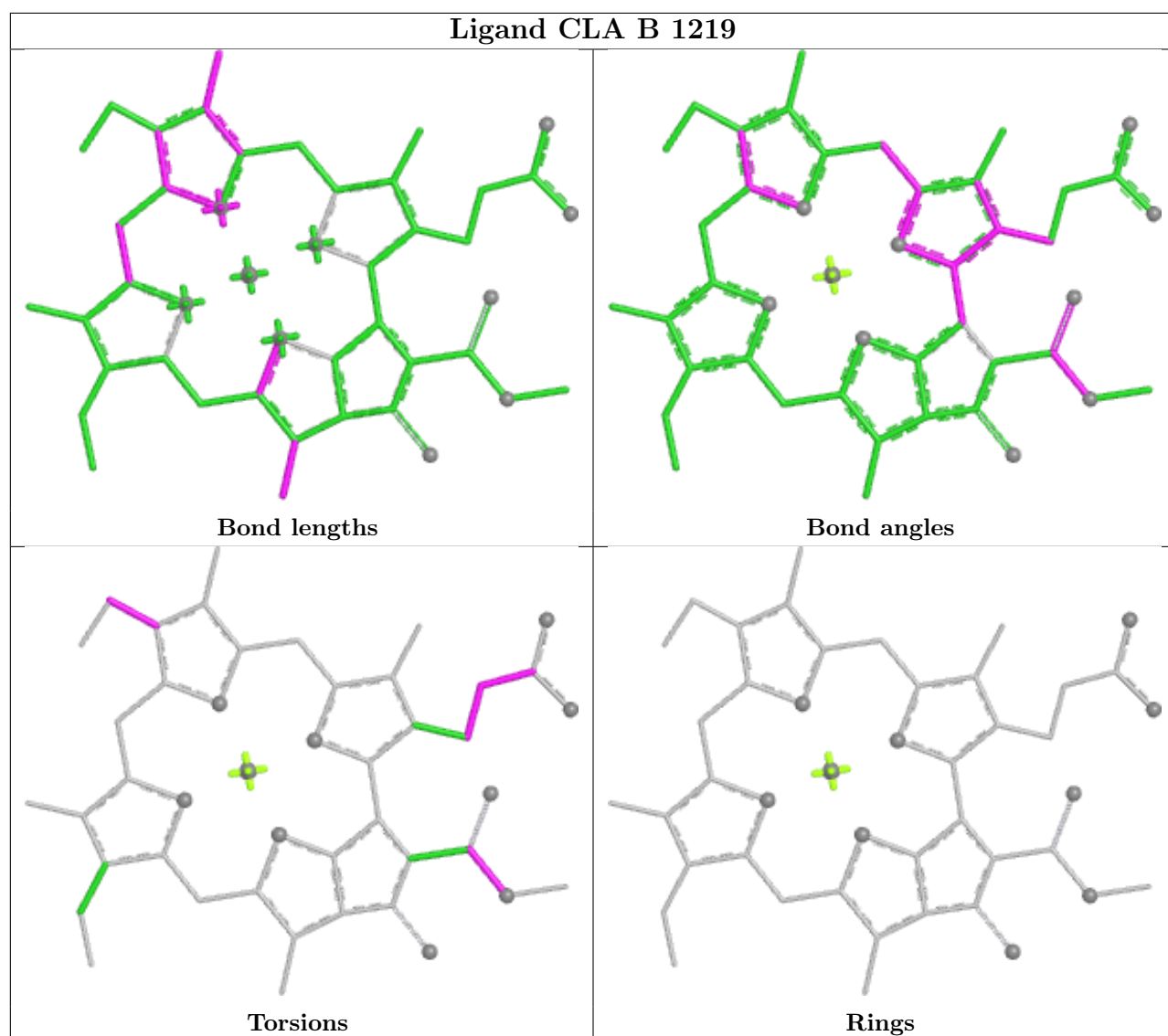
Ligand CLA H 1132



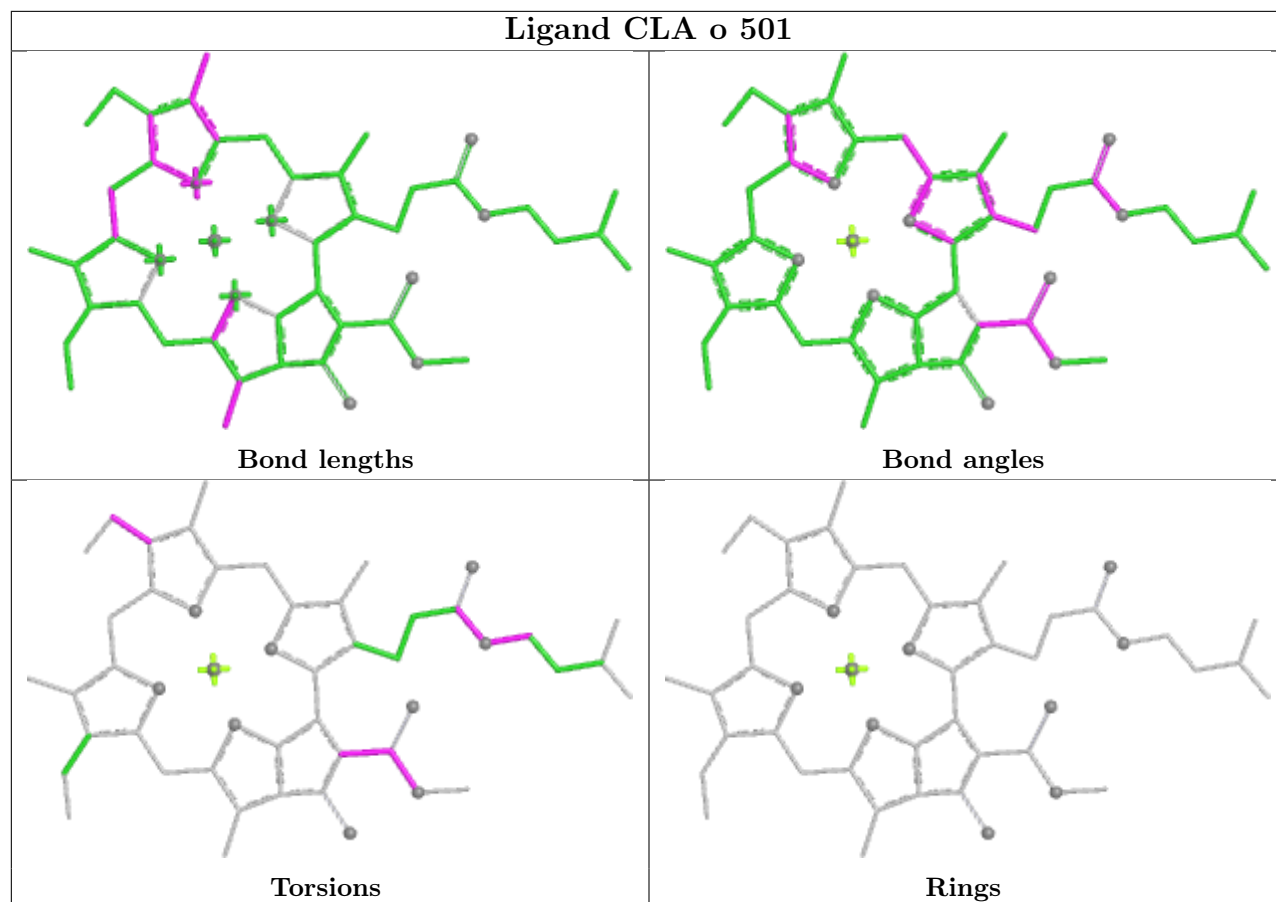
Ligand CLA o 516



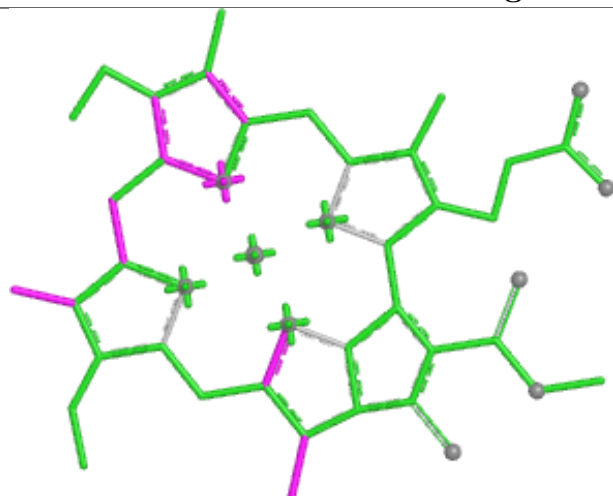




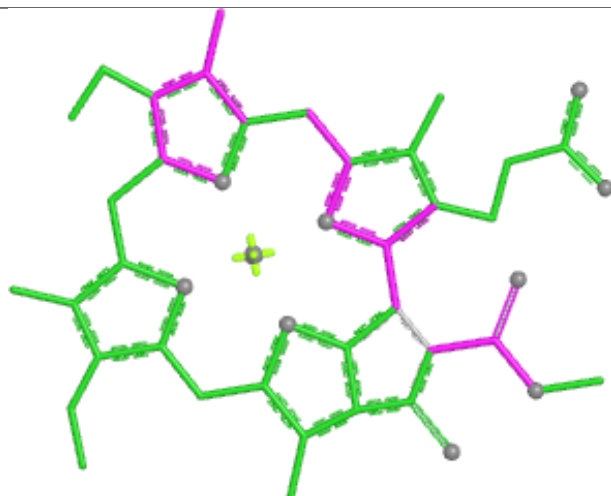
Ligand CLA o 501



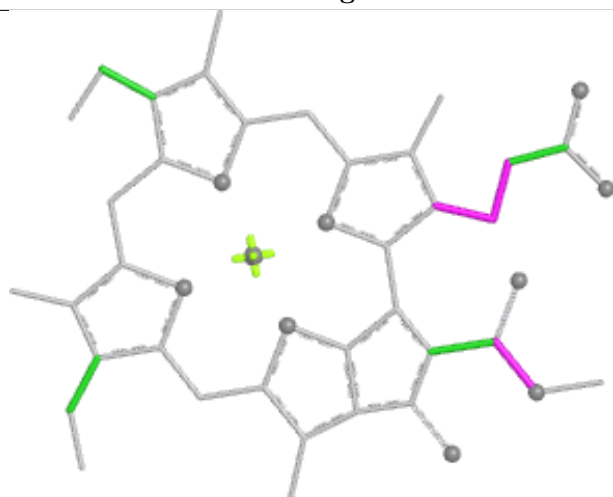
Ligand CLA A 1113



Bond lengths



Bond angles

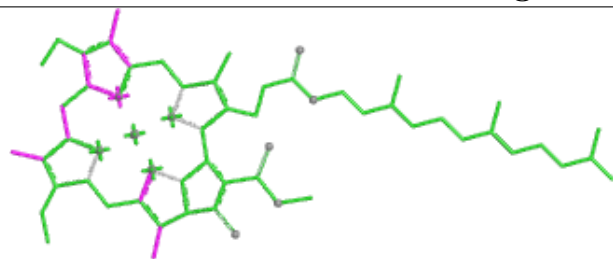


Torsions

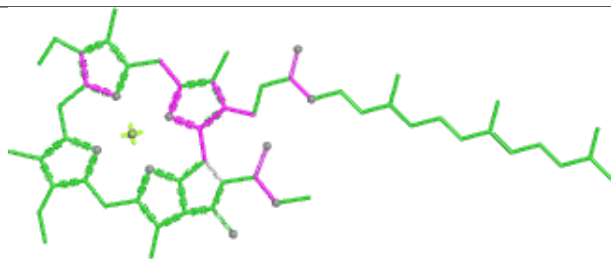


Rings

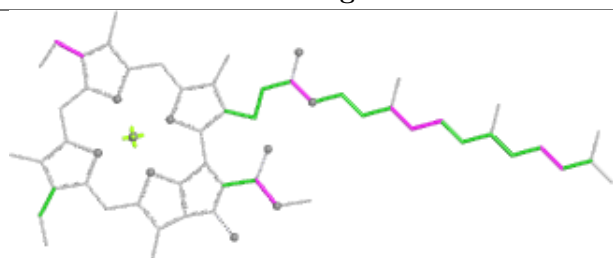
Ligand CLA X 509



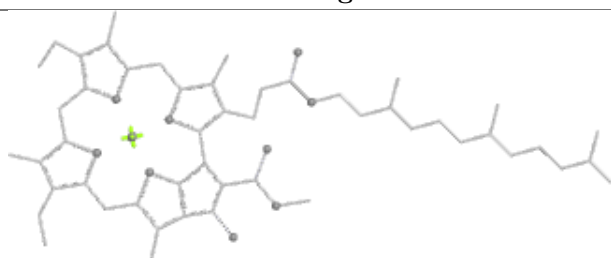
Bond lengths



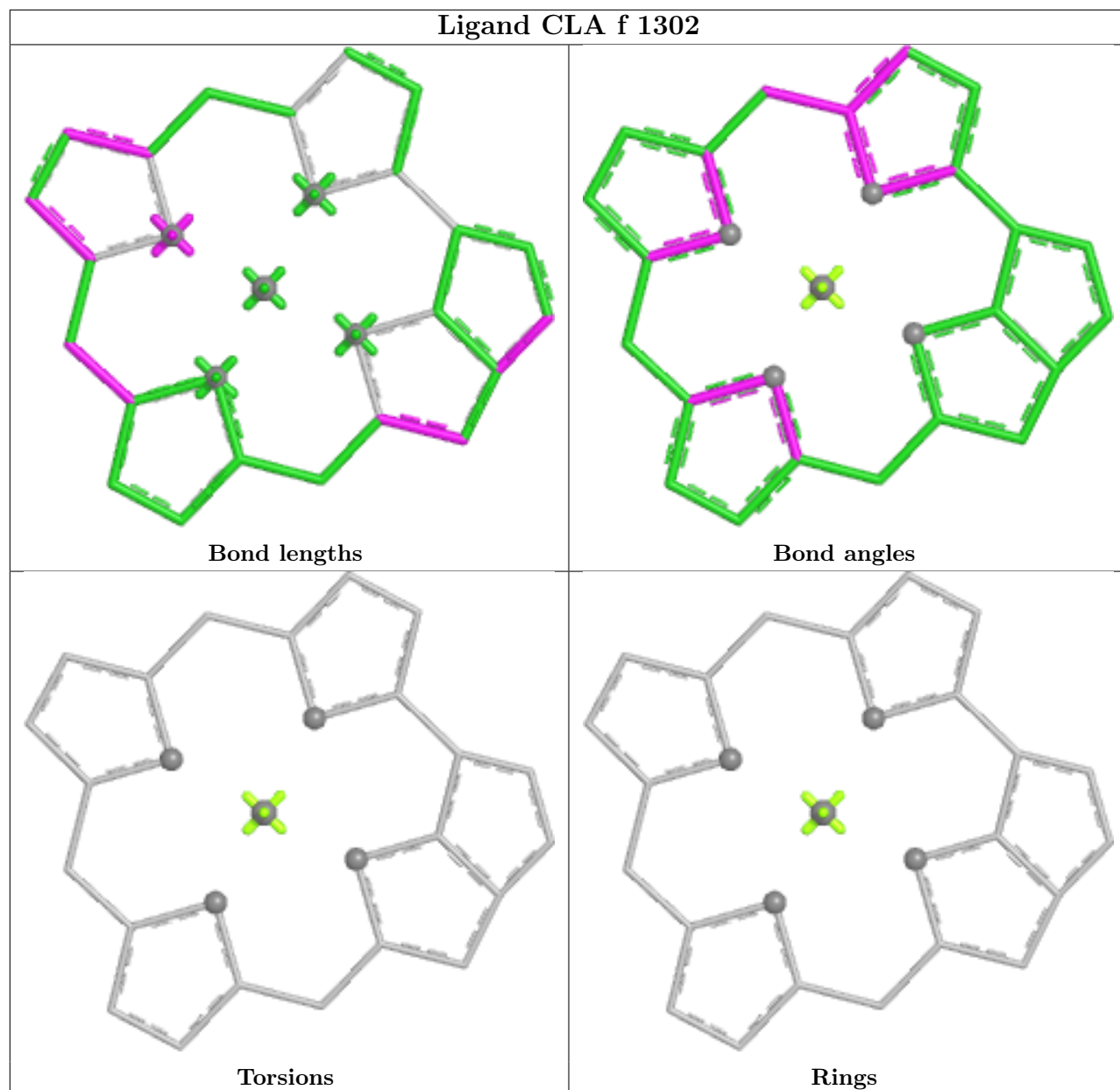
Bond angles

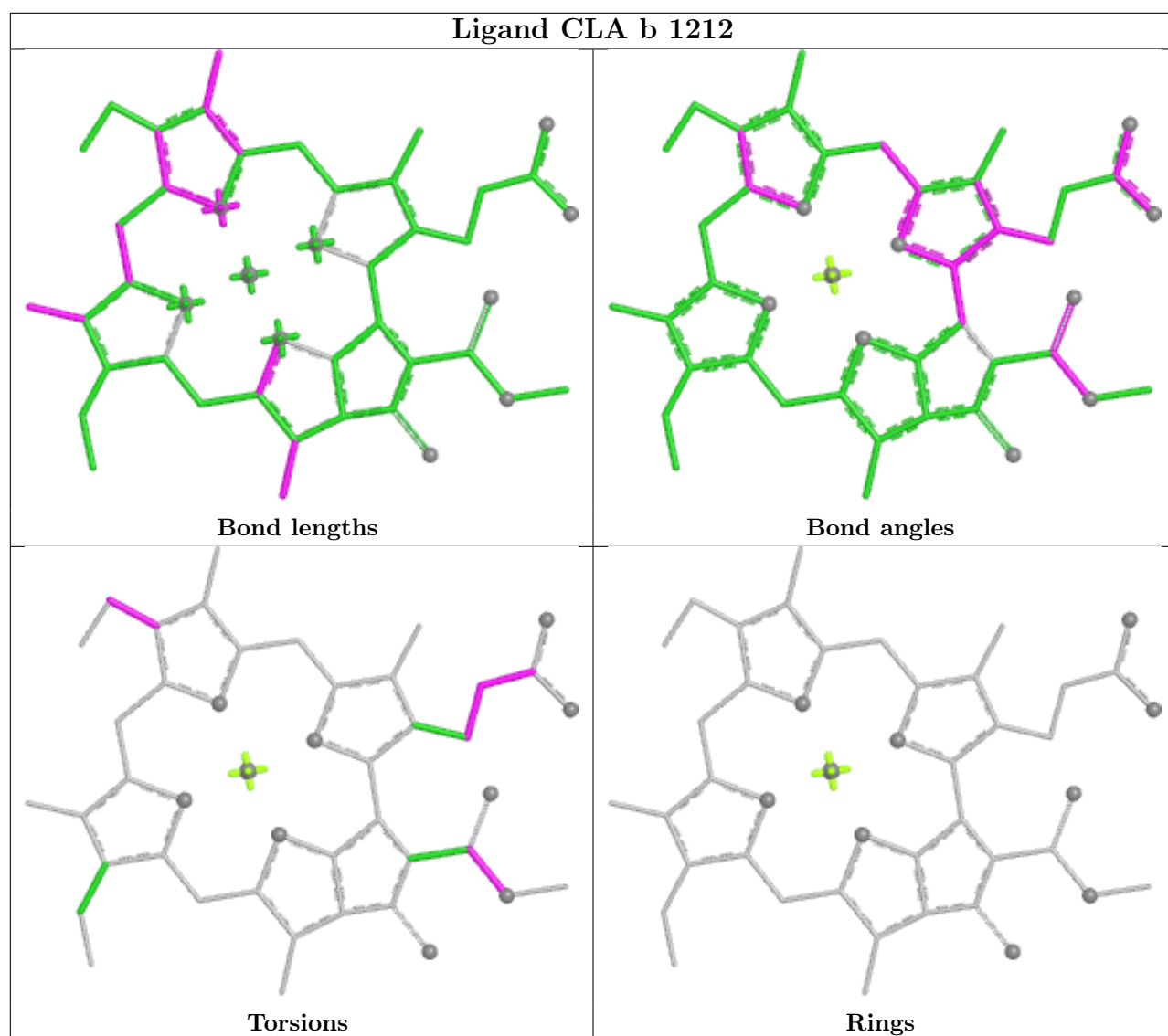


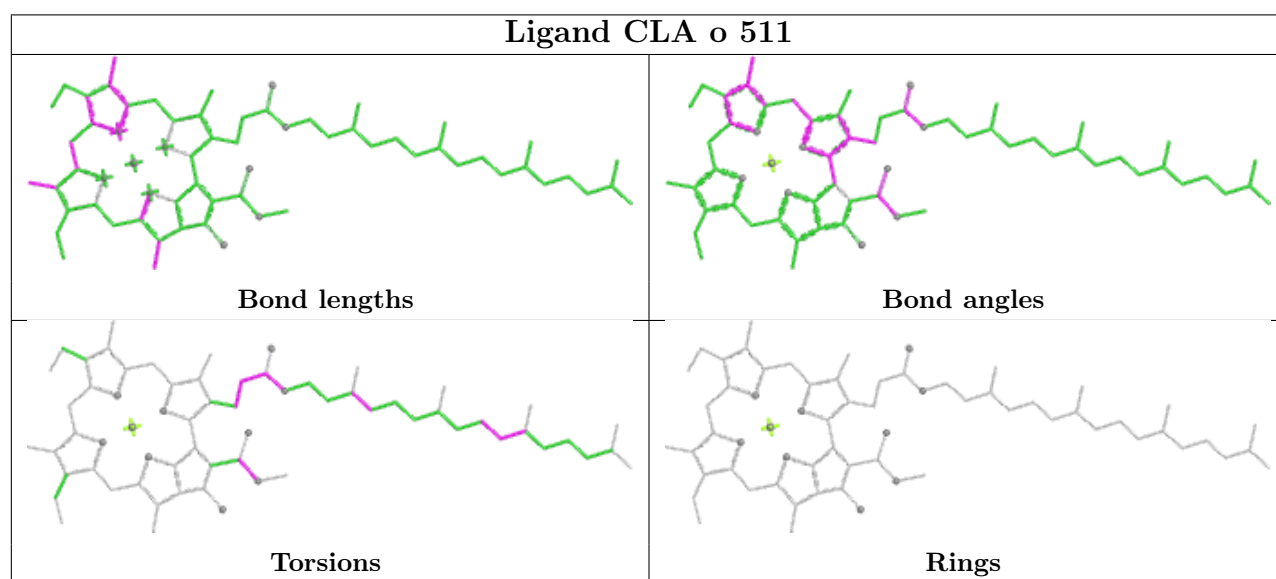
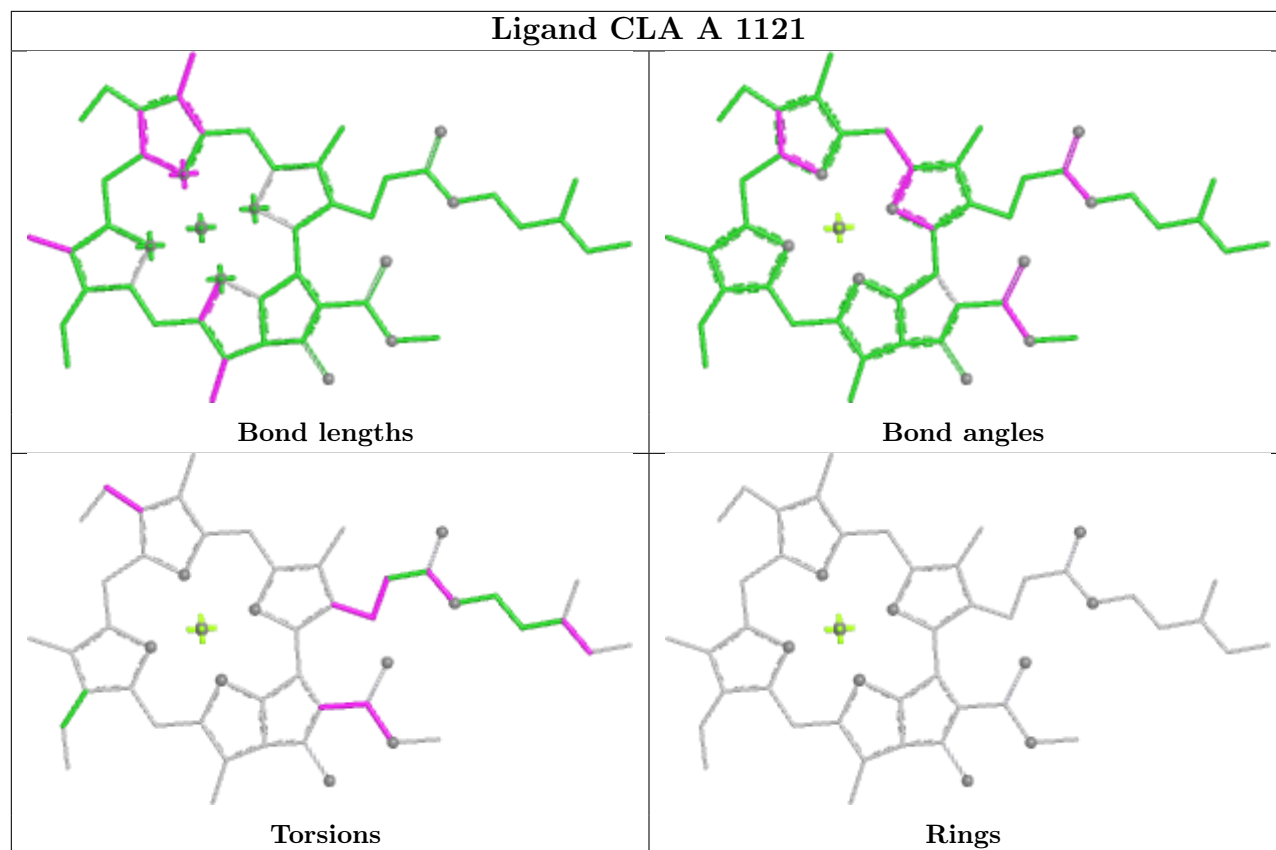
Torsions

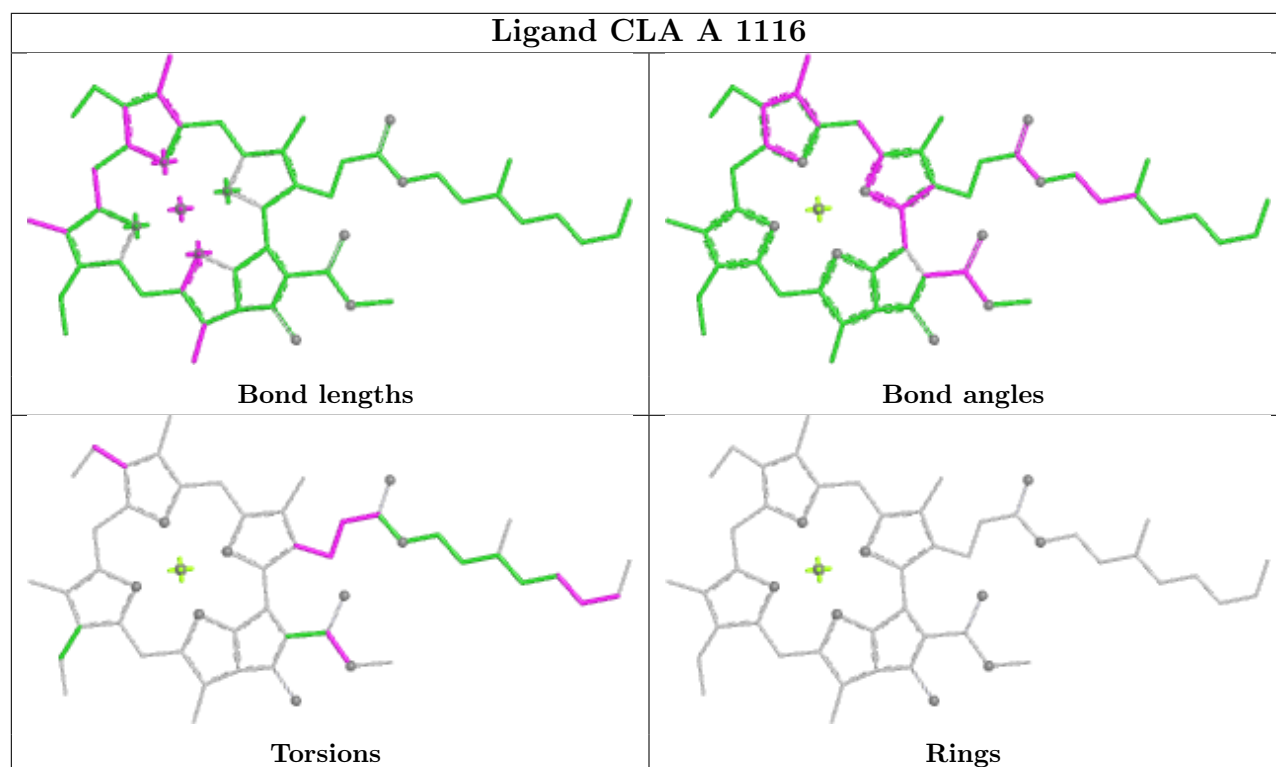
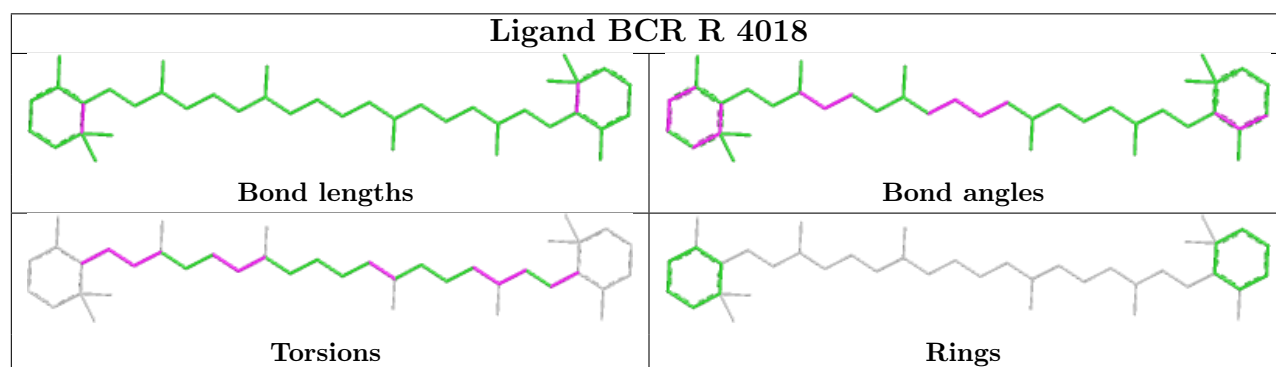
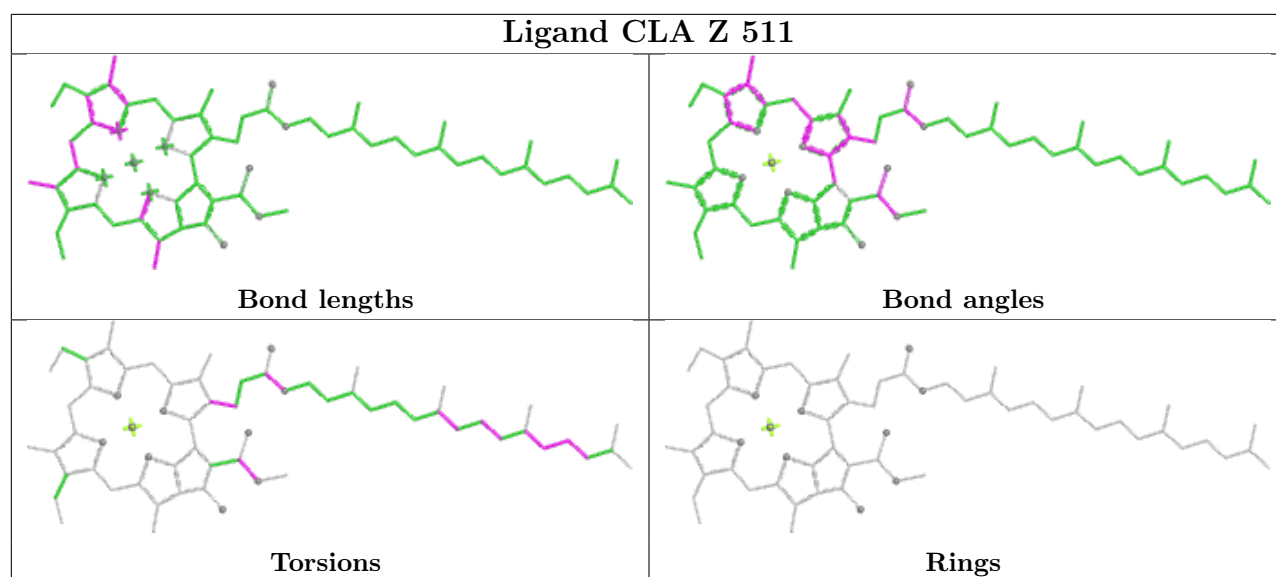


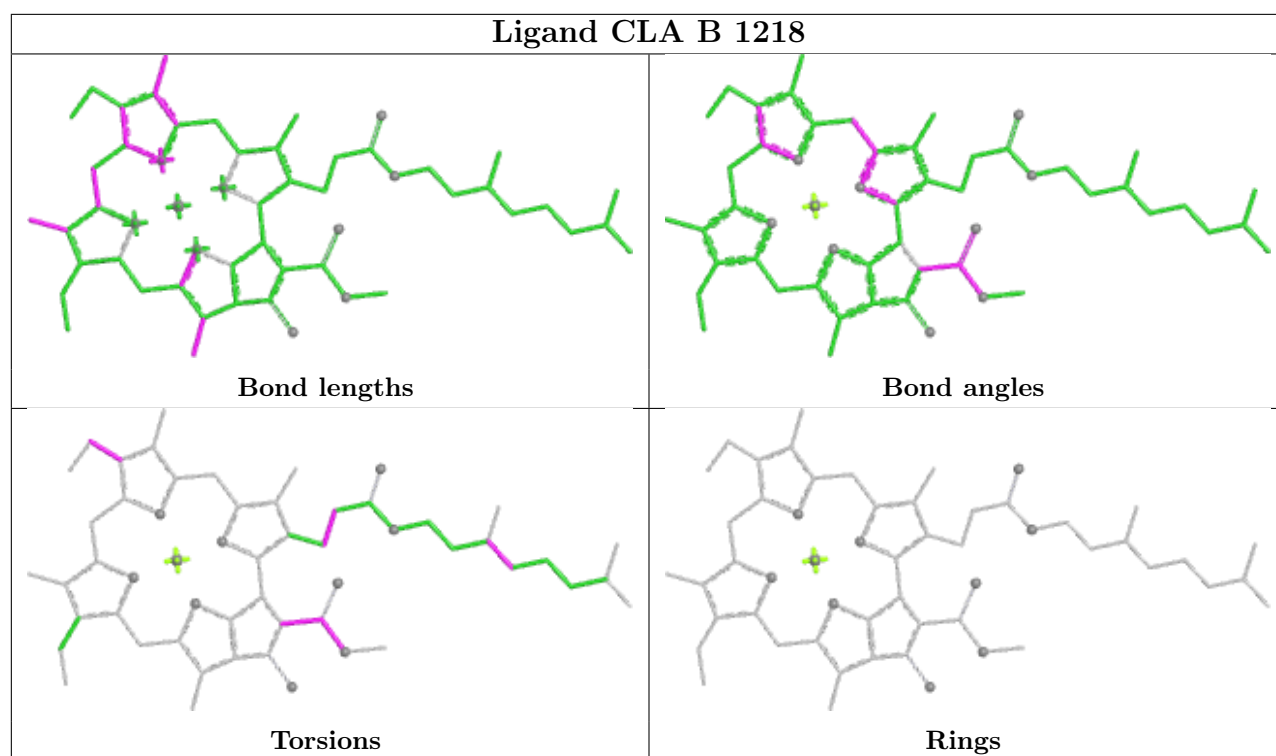
Rings



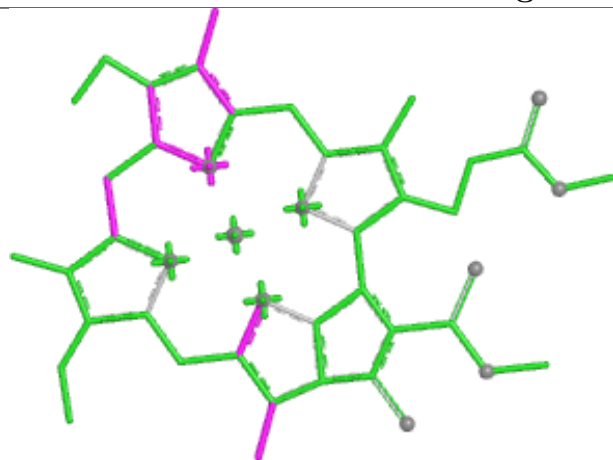




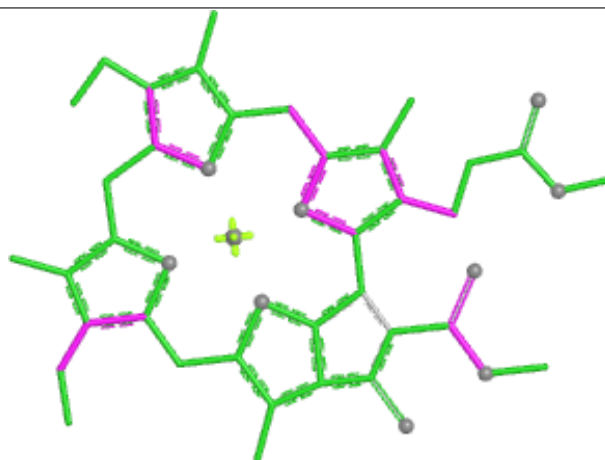




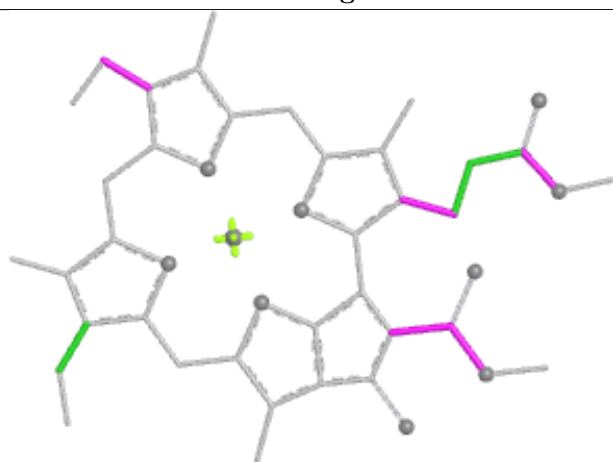
Ligand CLA Z 503



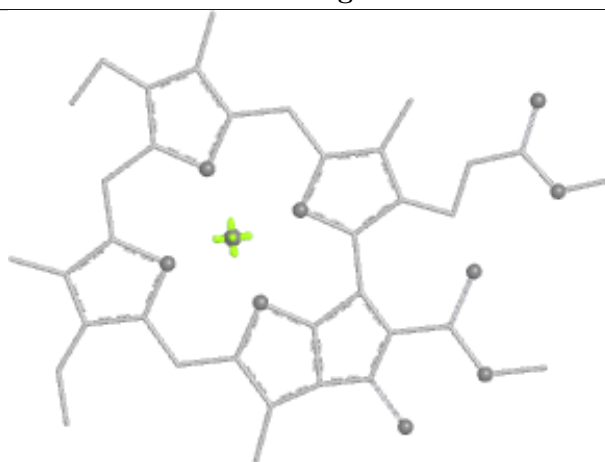
Bond lengths



Bond angles

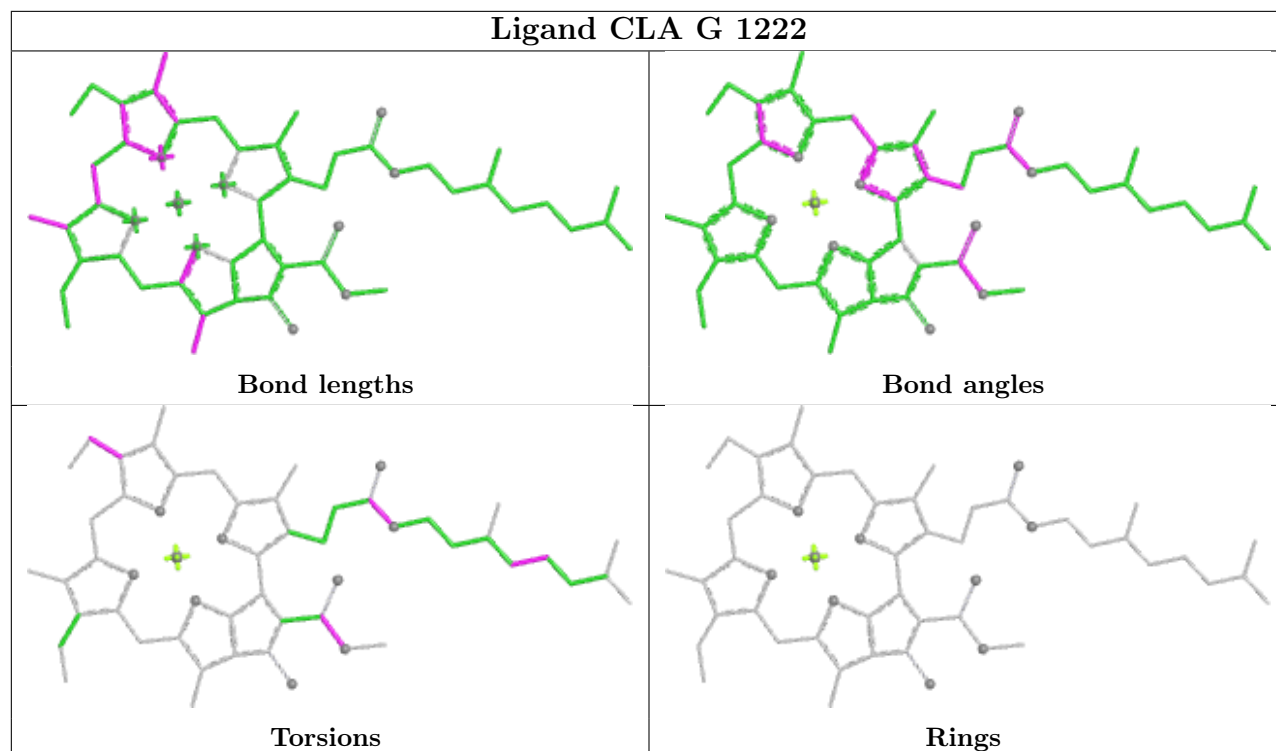


Torsions

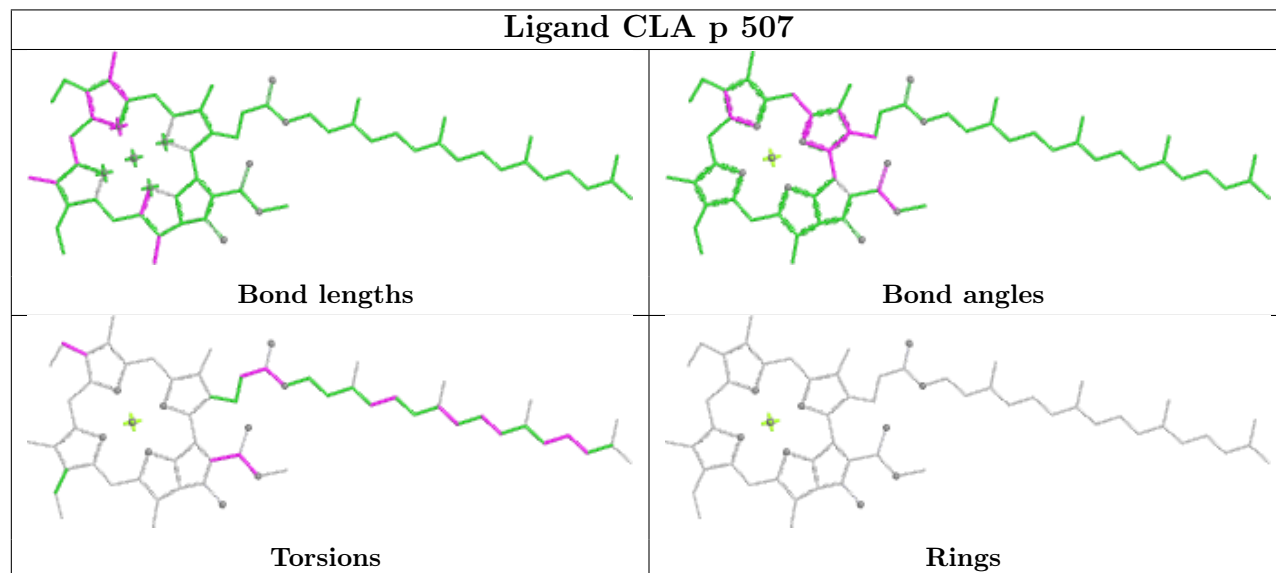


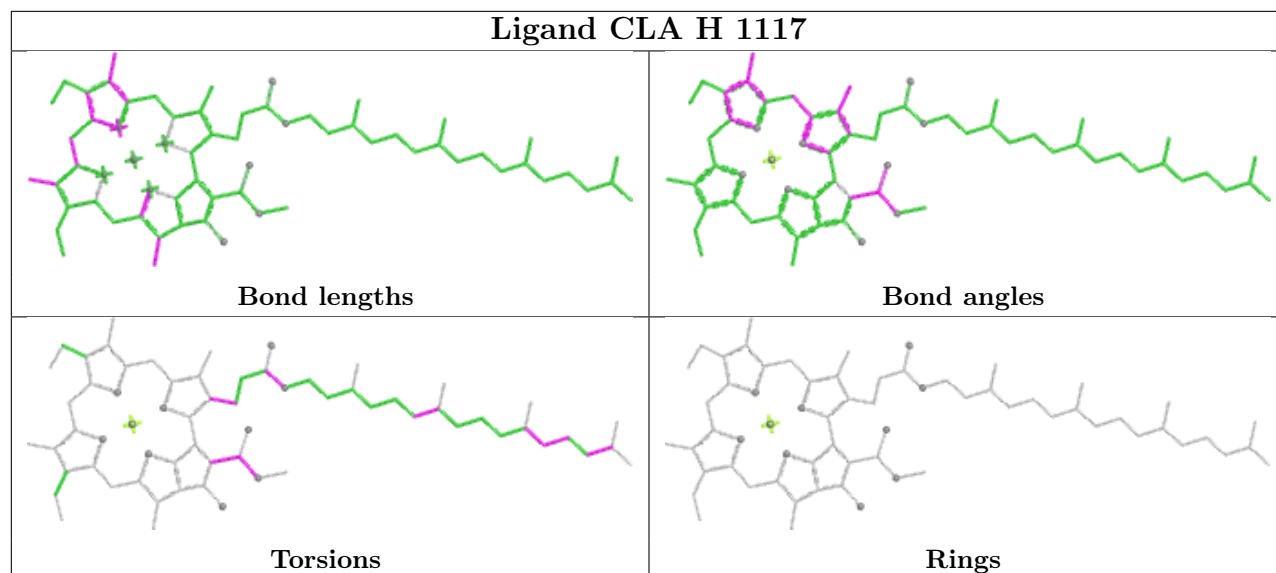
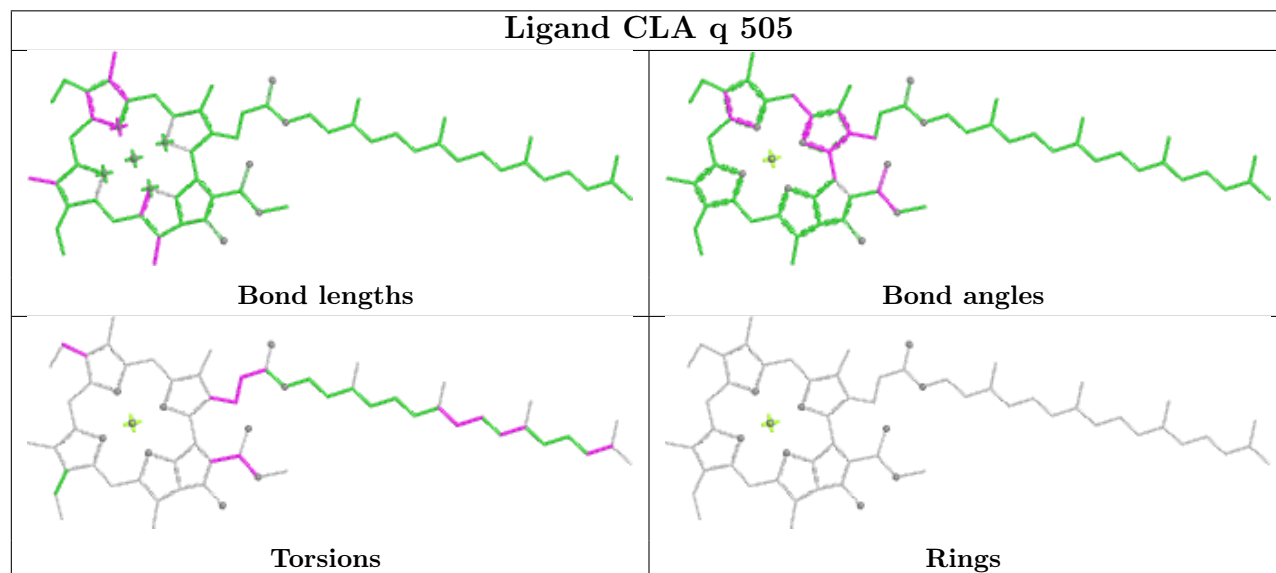
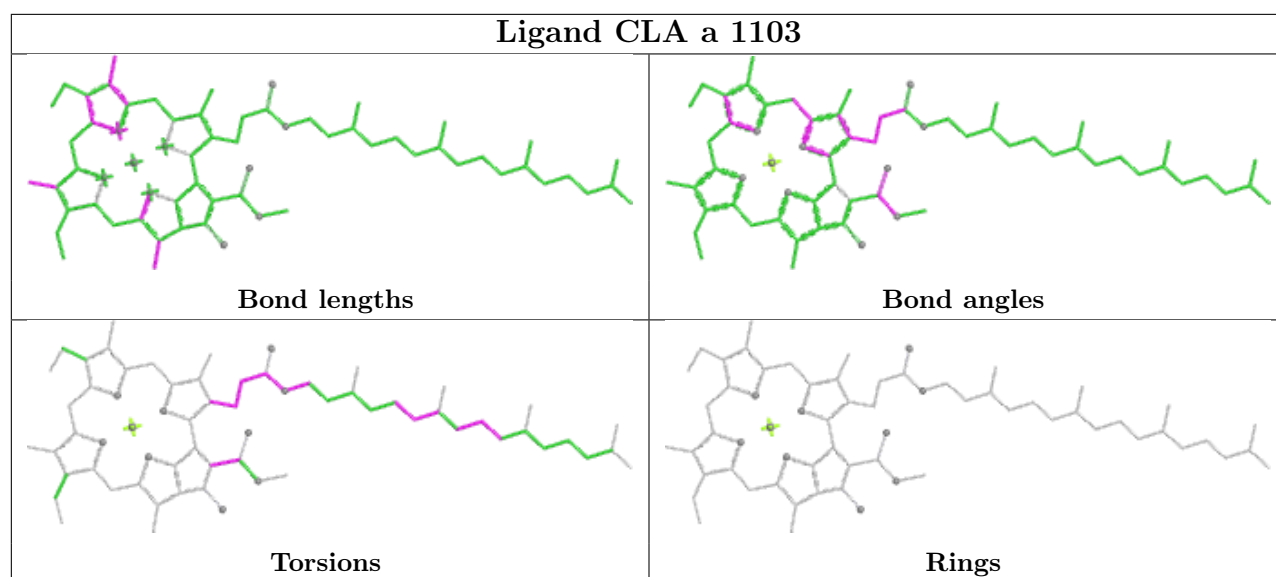
Rings

Ligand CLA G 1222

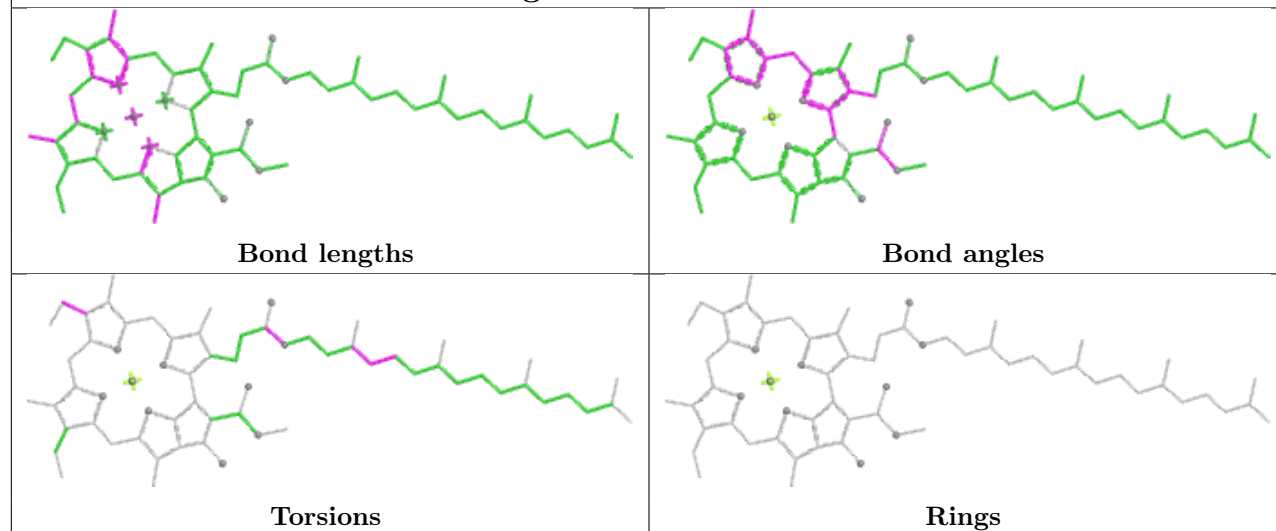


Ligand CLA p 507

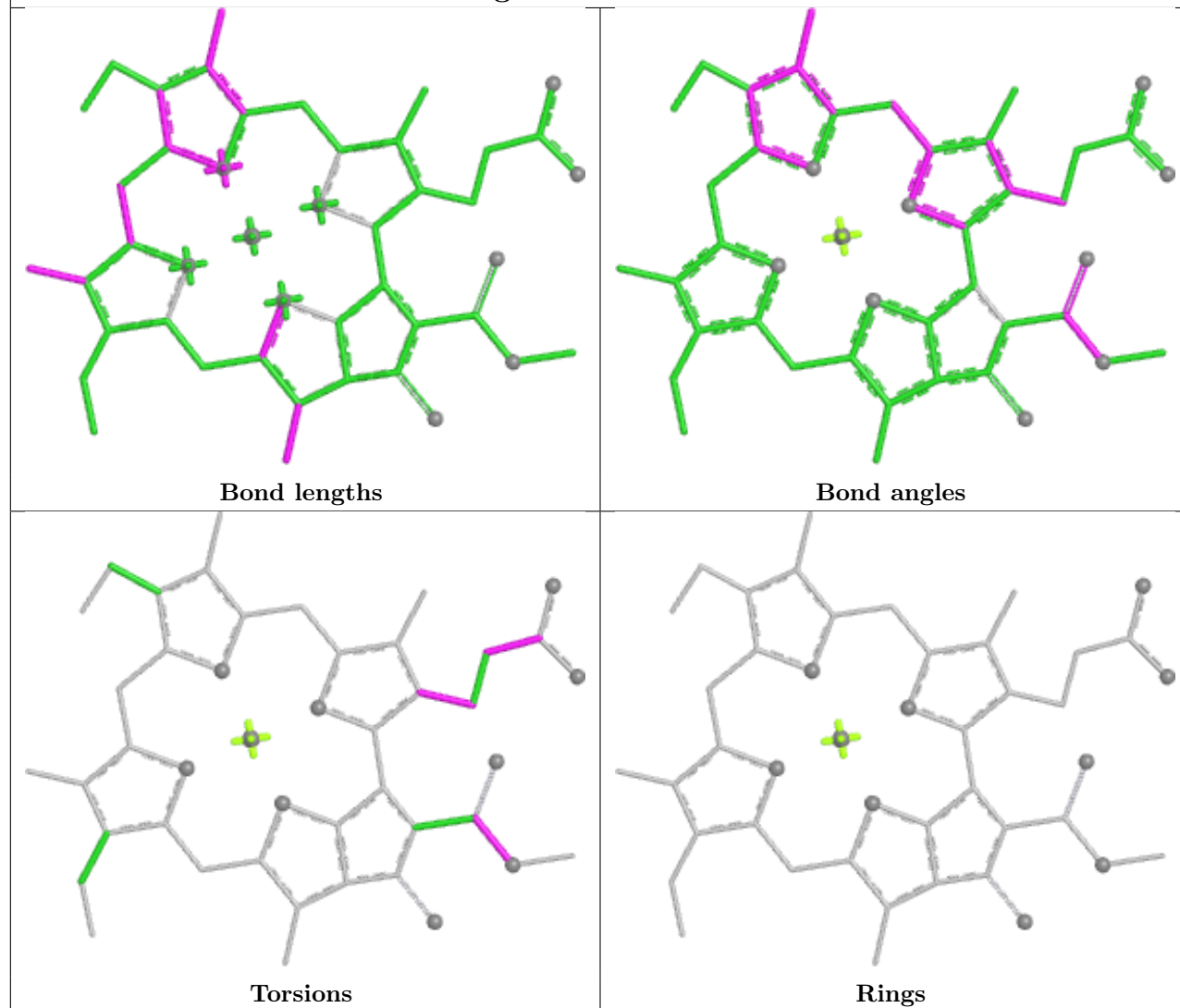




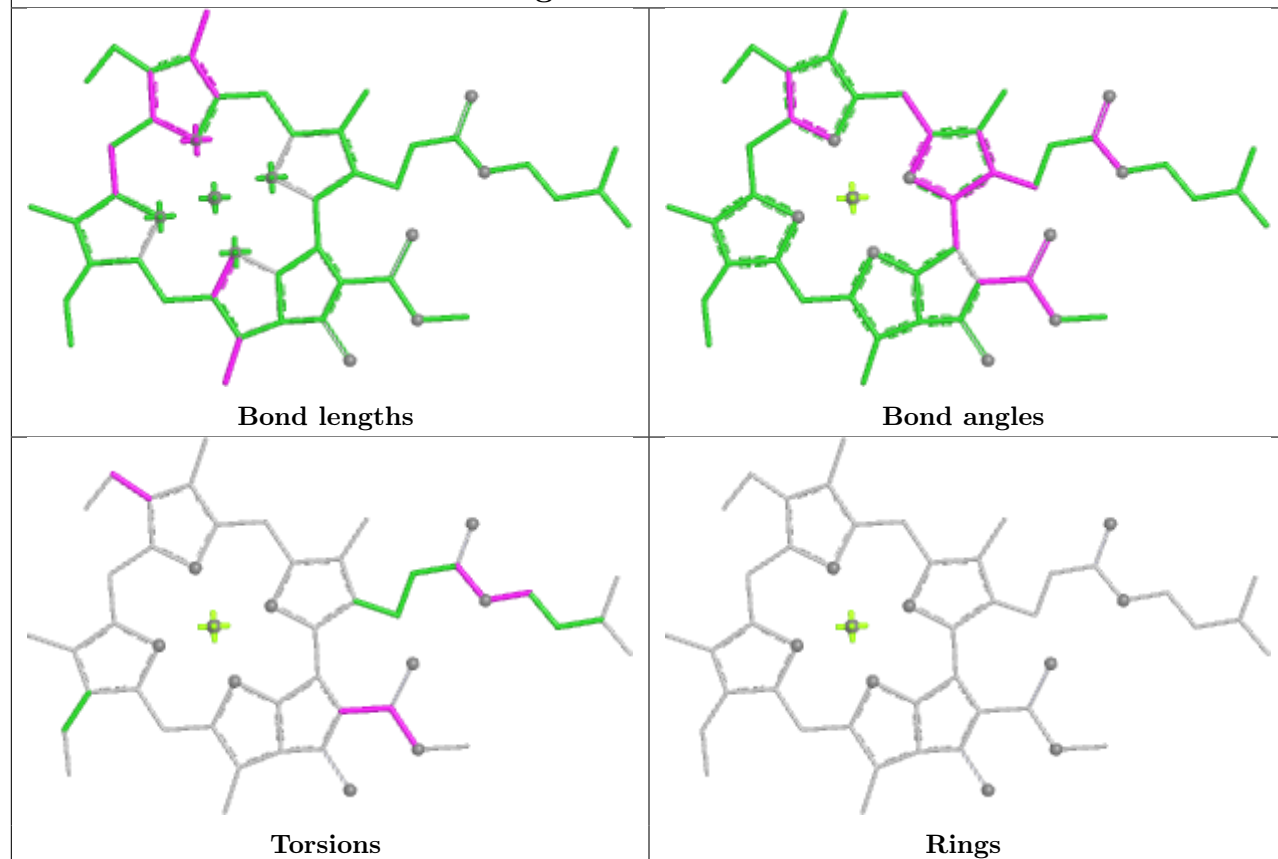
Ligand CLA A 1130



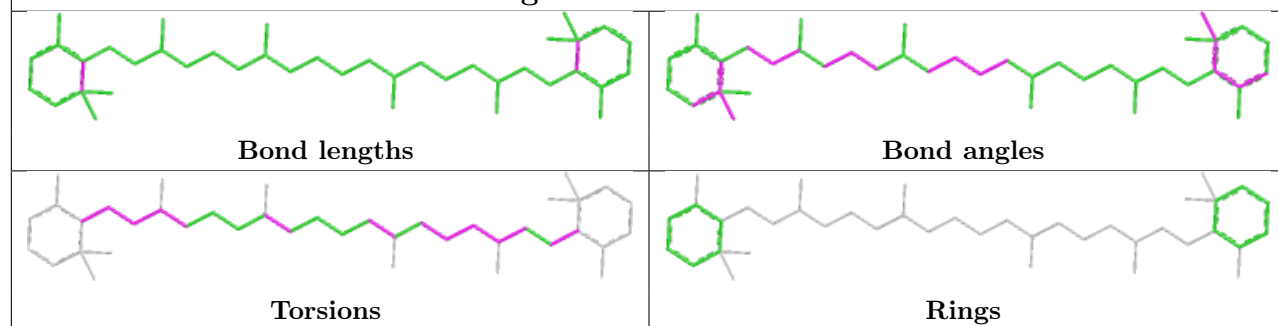
Ligand CLA Z 512

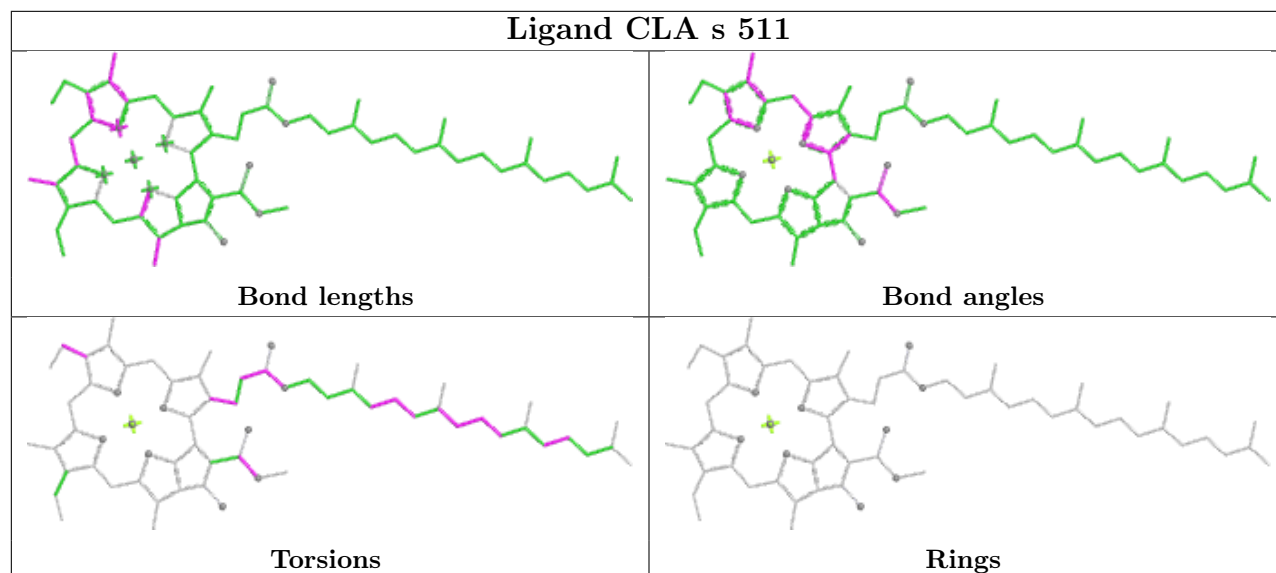
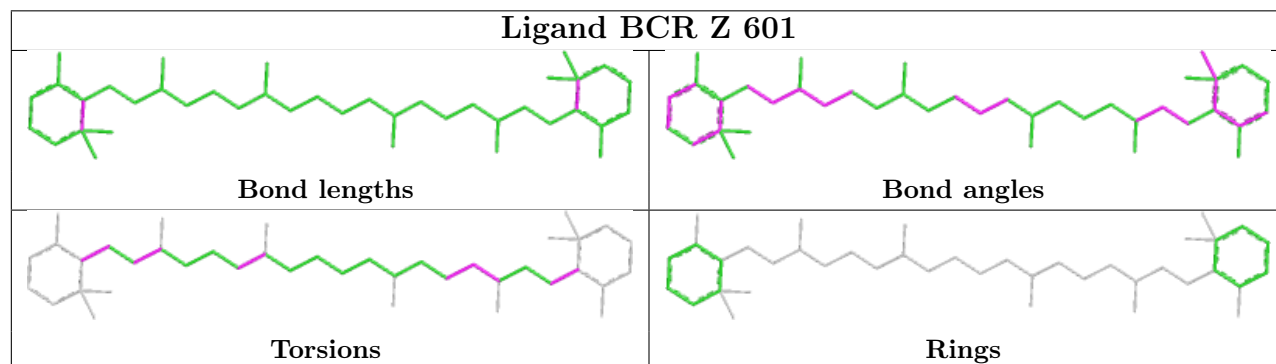
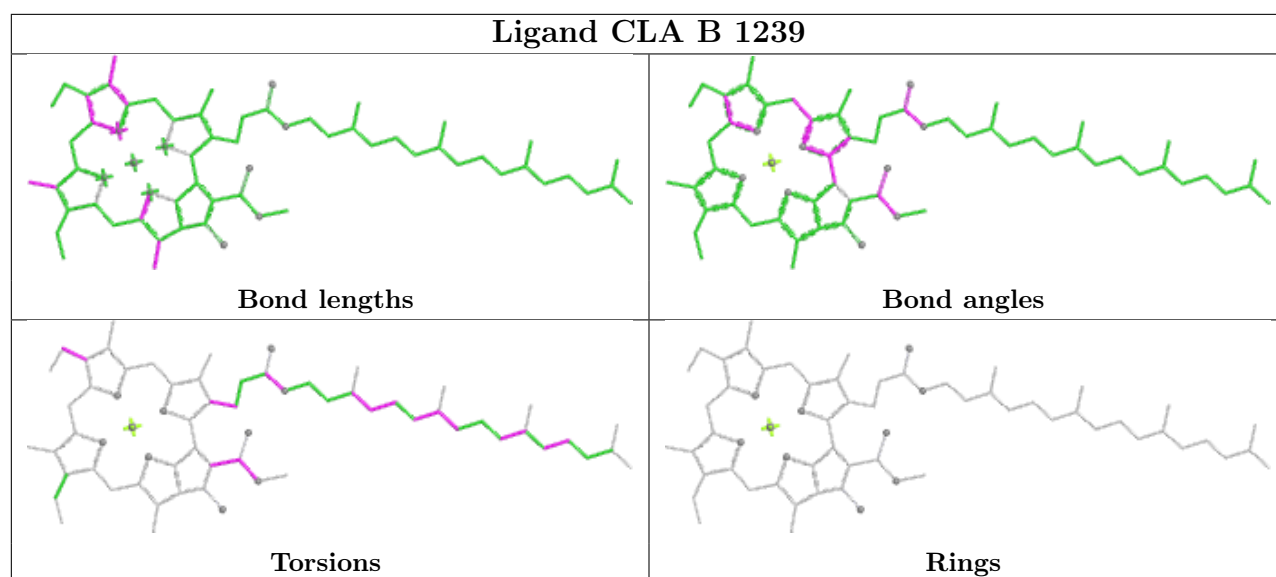


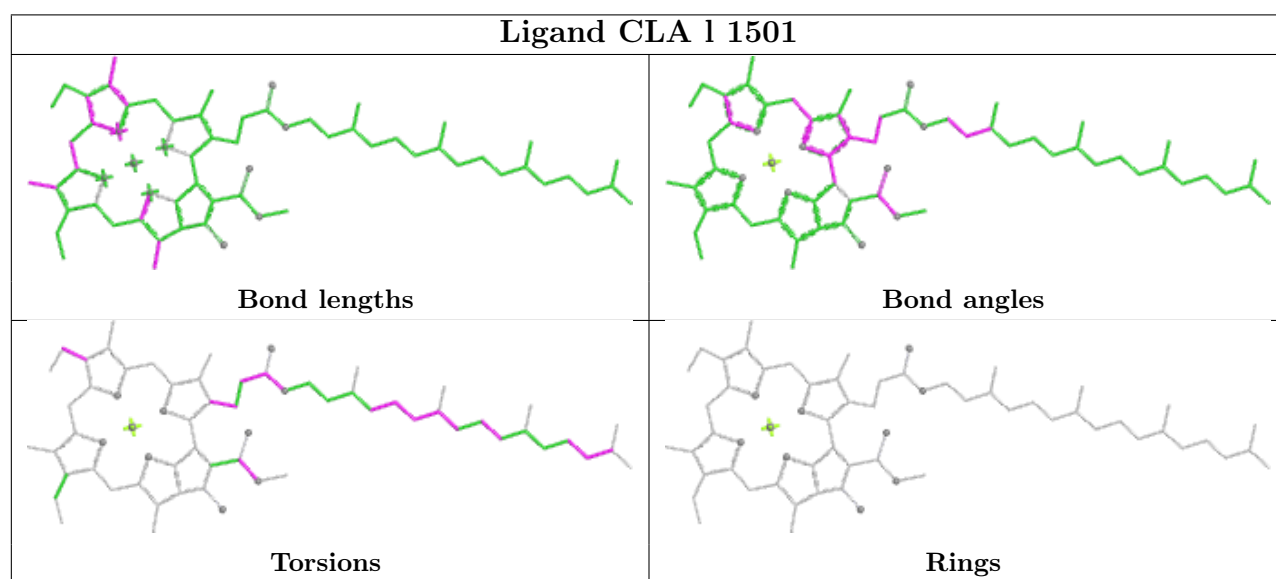
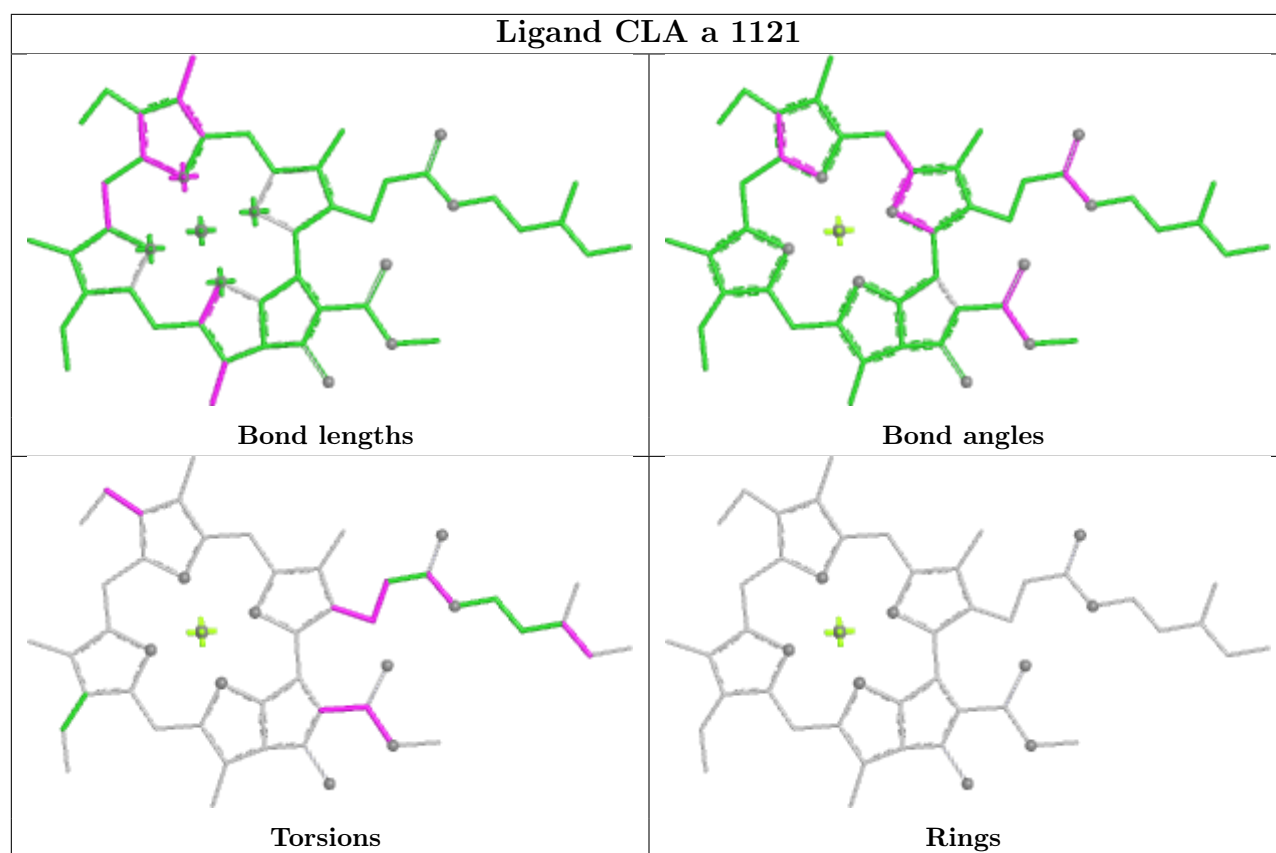
Ligand CLA u 501

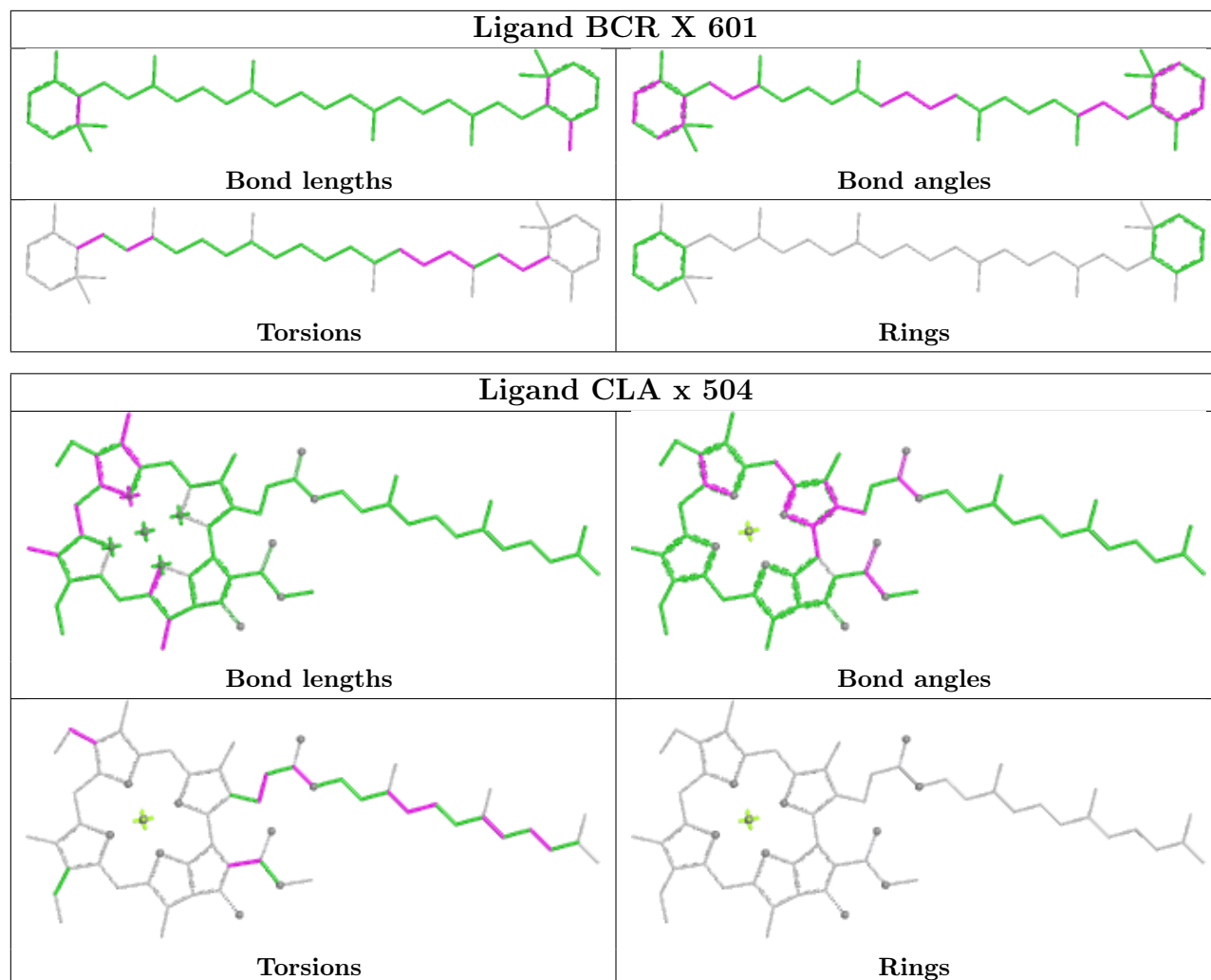


Ligand BCR A 4011

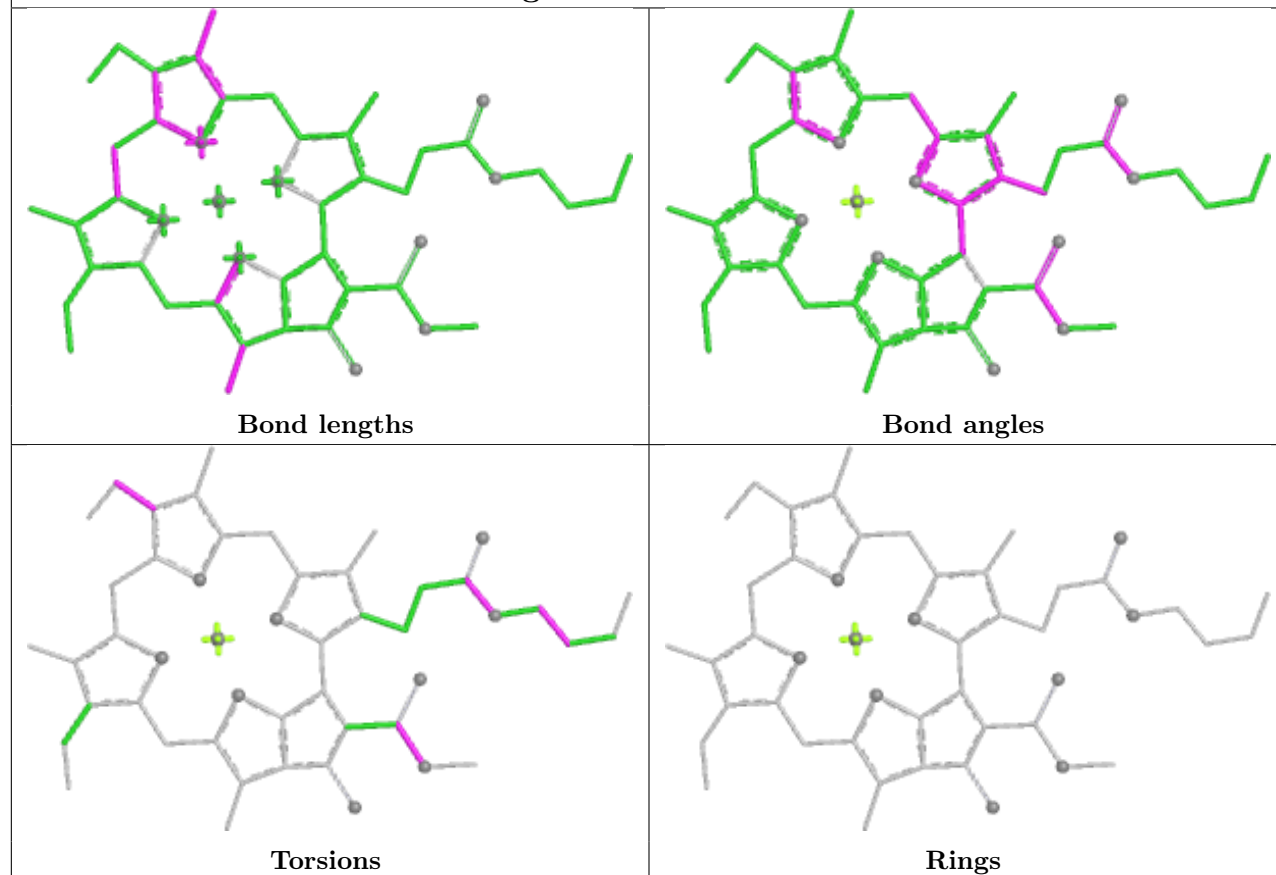




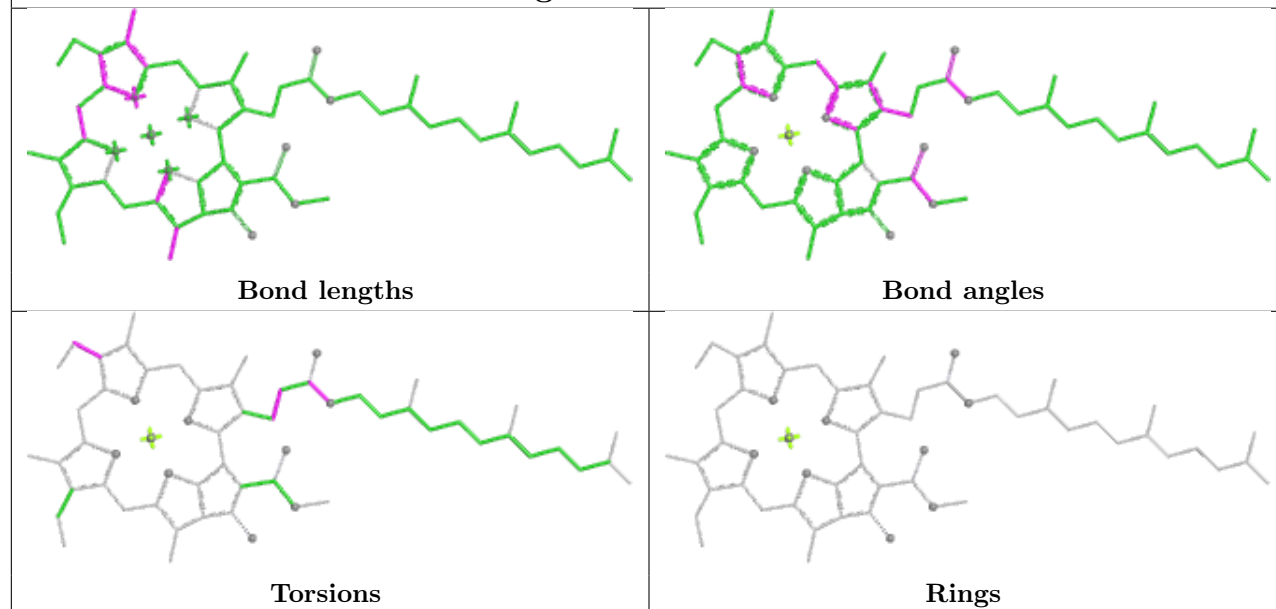


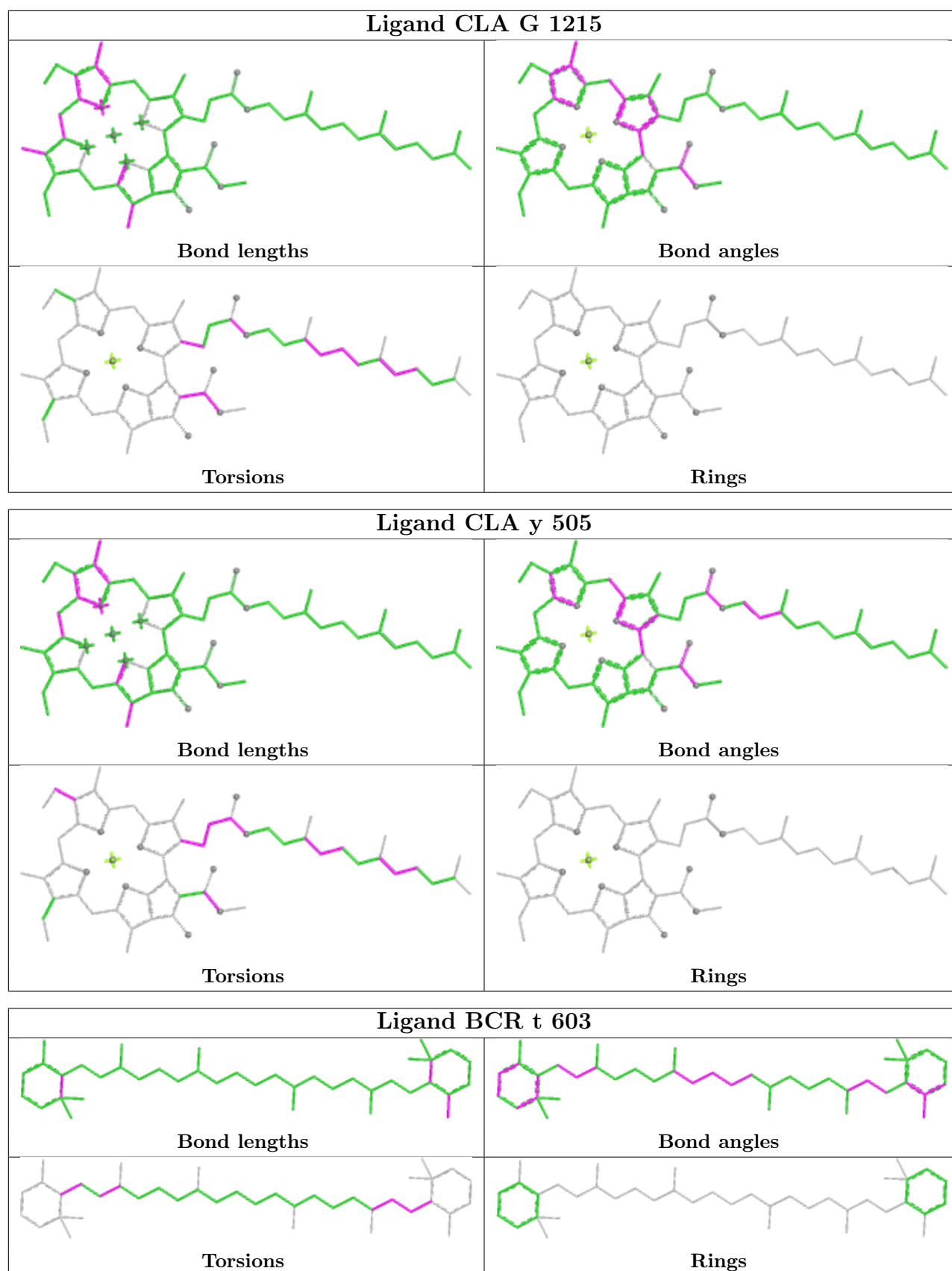


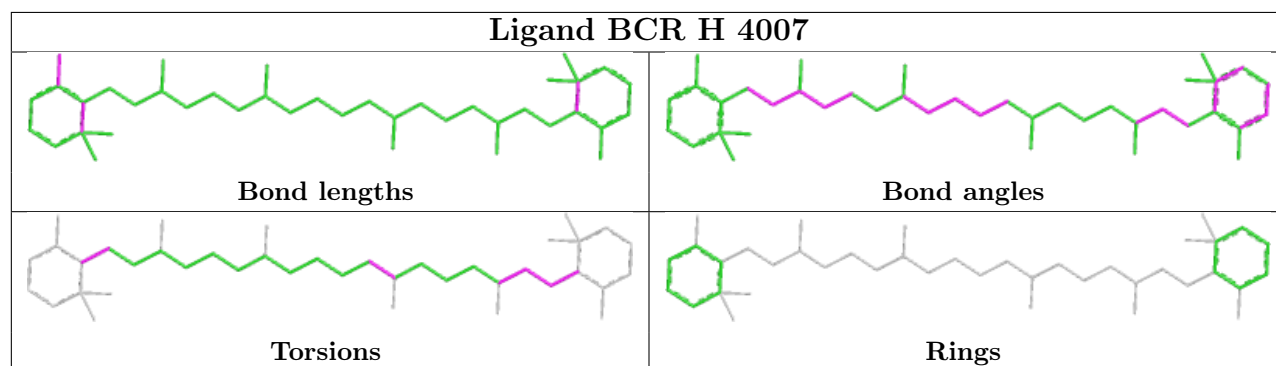
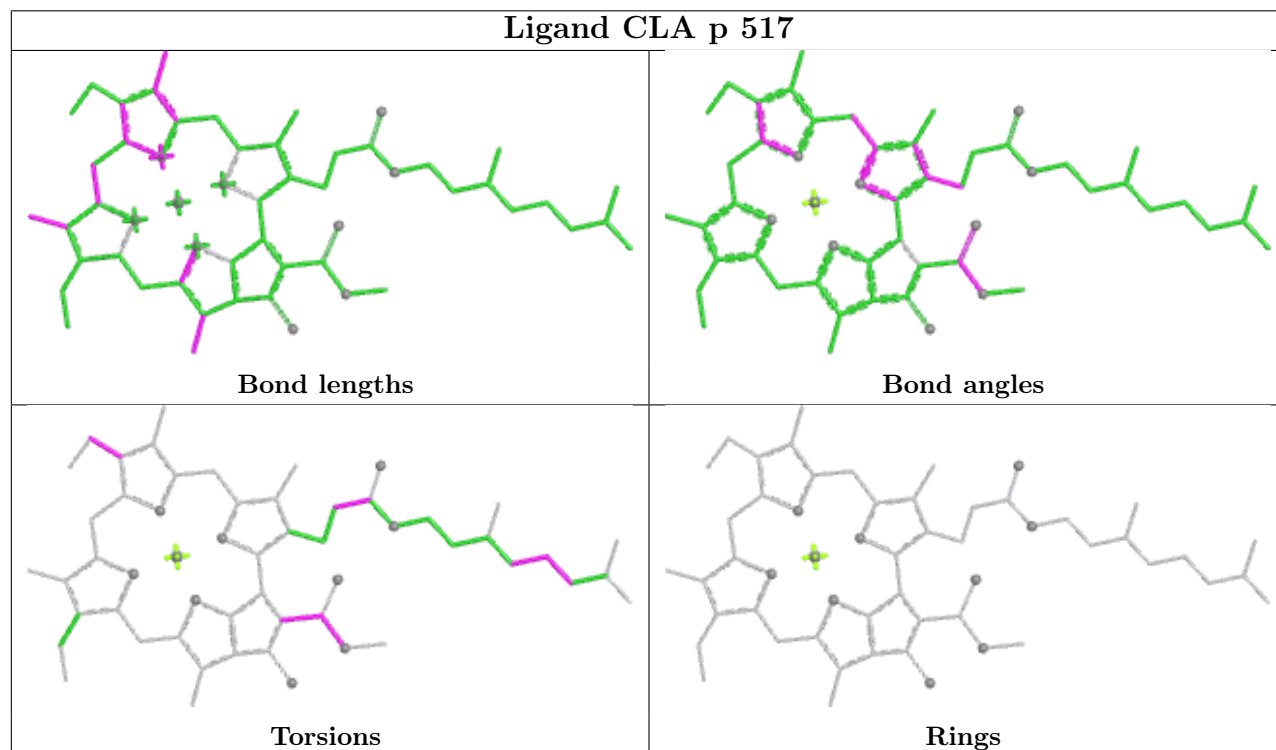
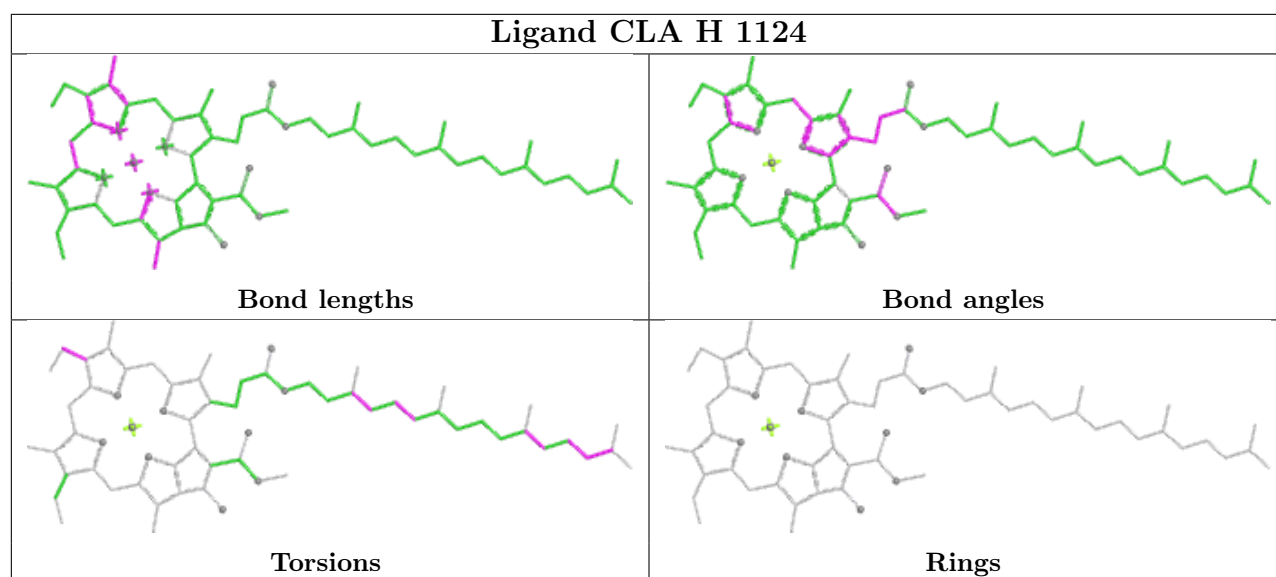
Ligand CLA H 1114



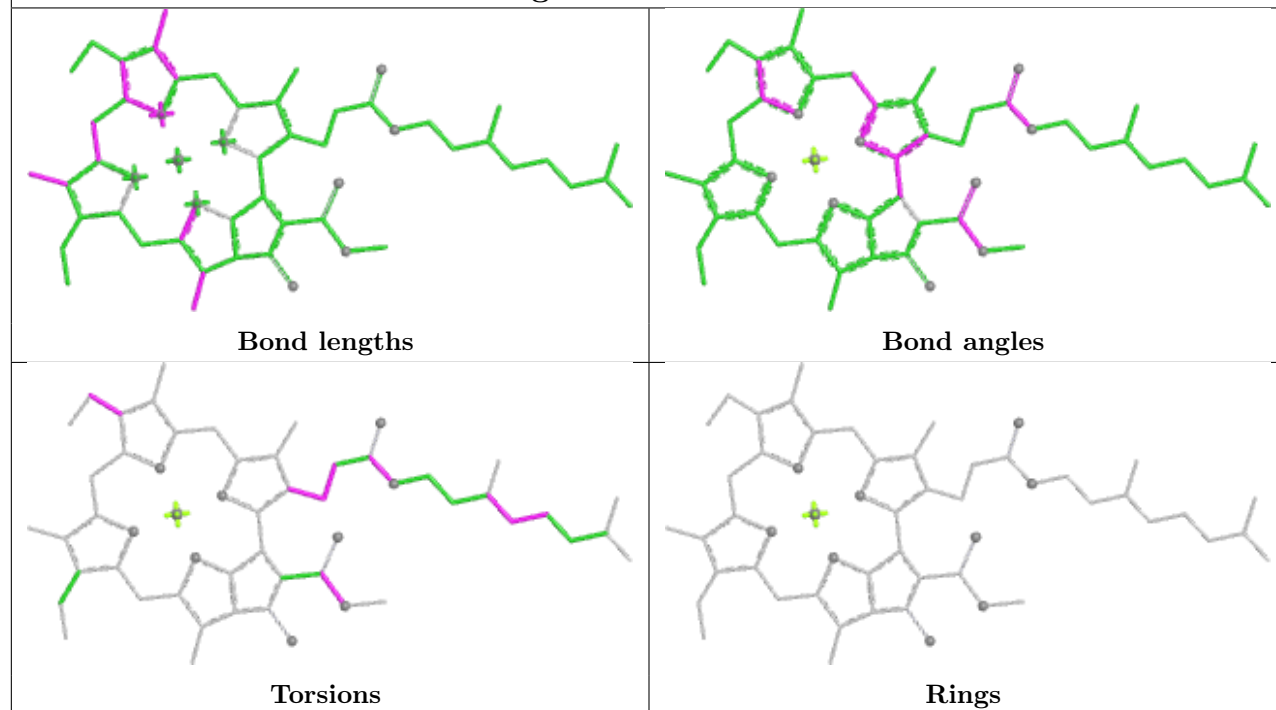
Ligand CLA h 515



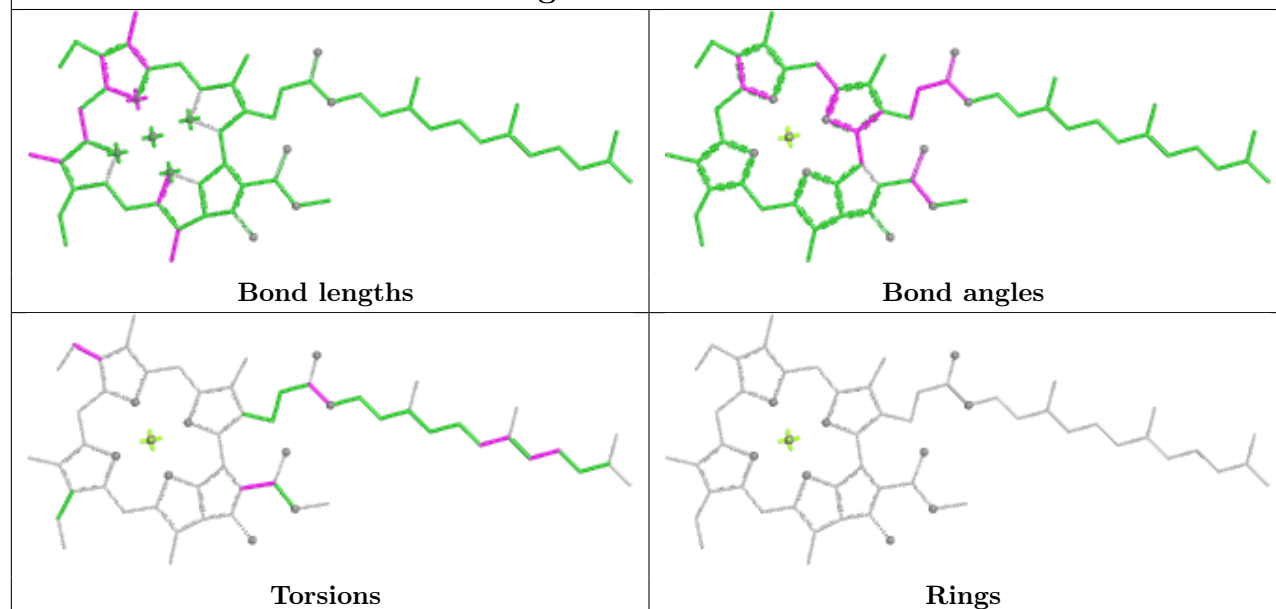




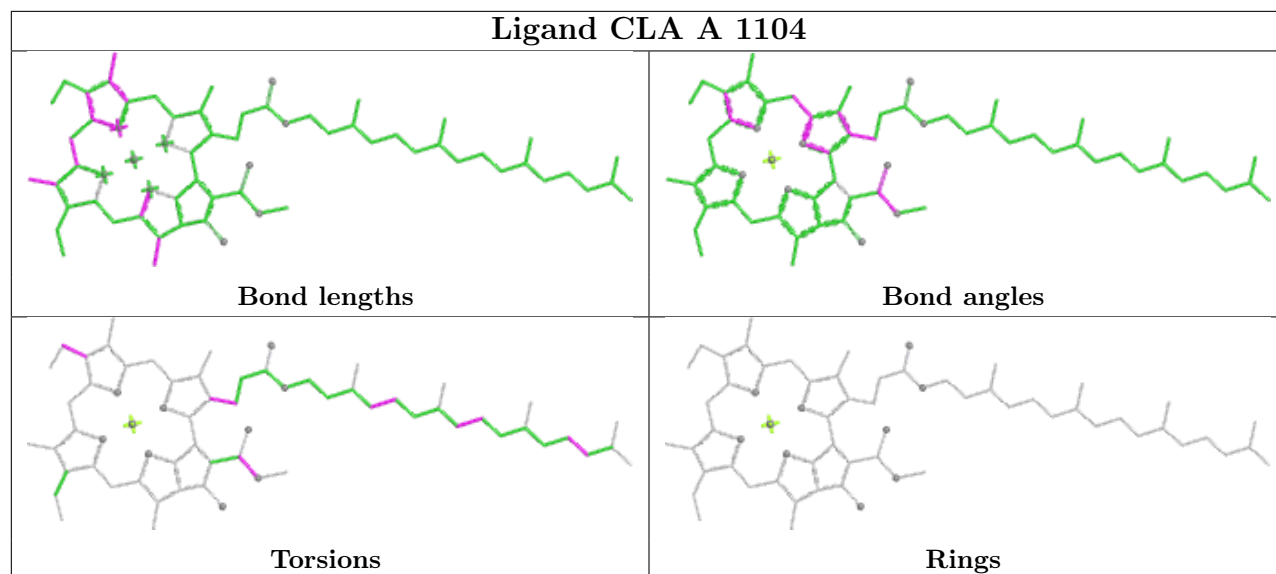
Ligand CLA Y 508



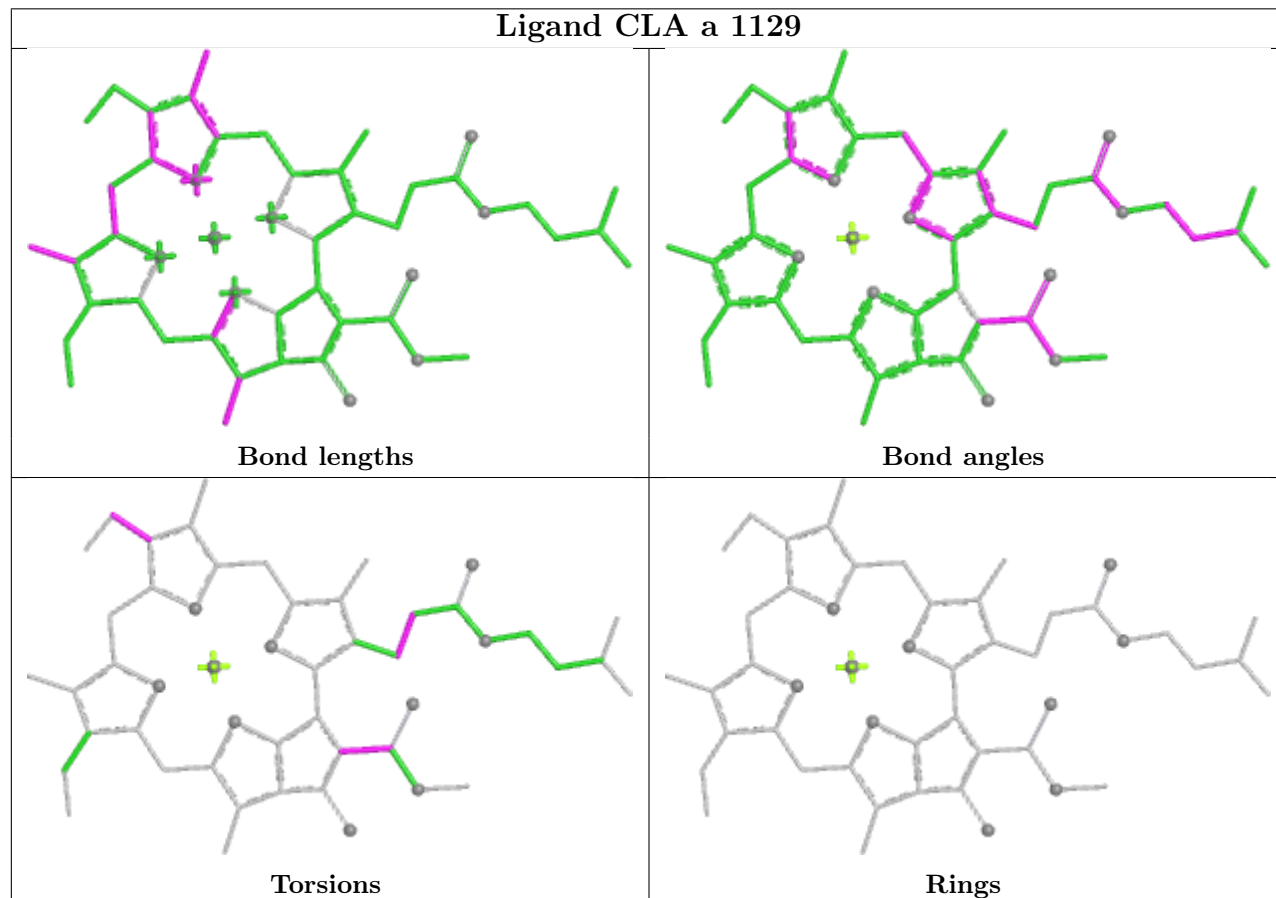
Ligand CLA t 504

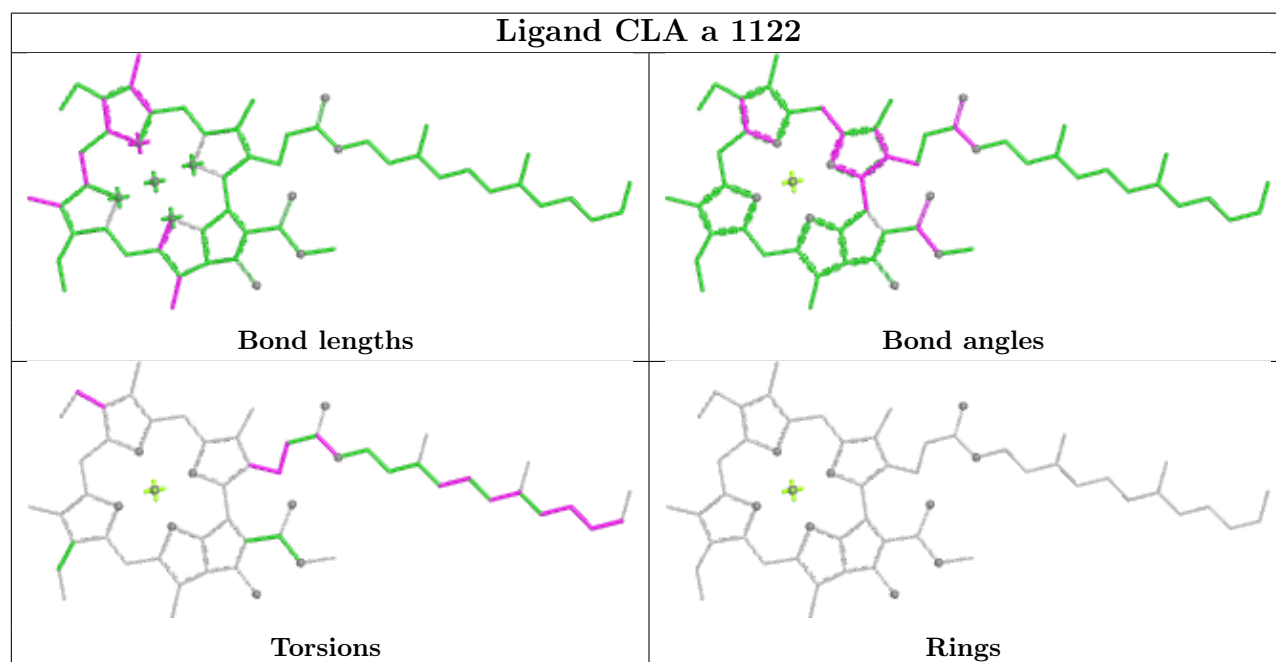
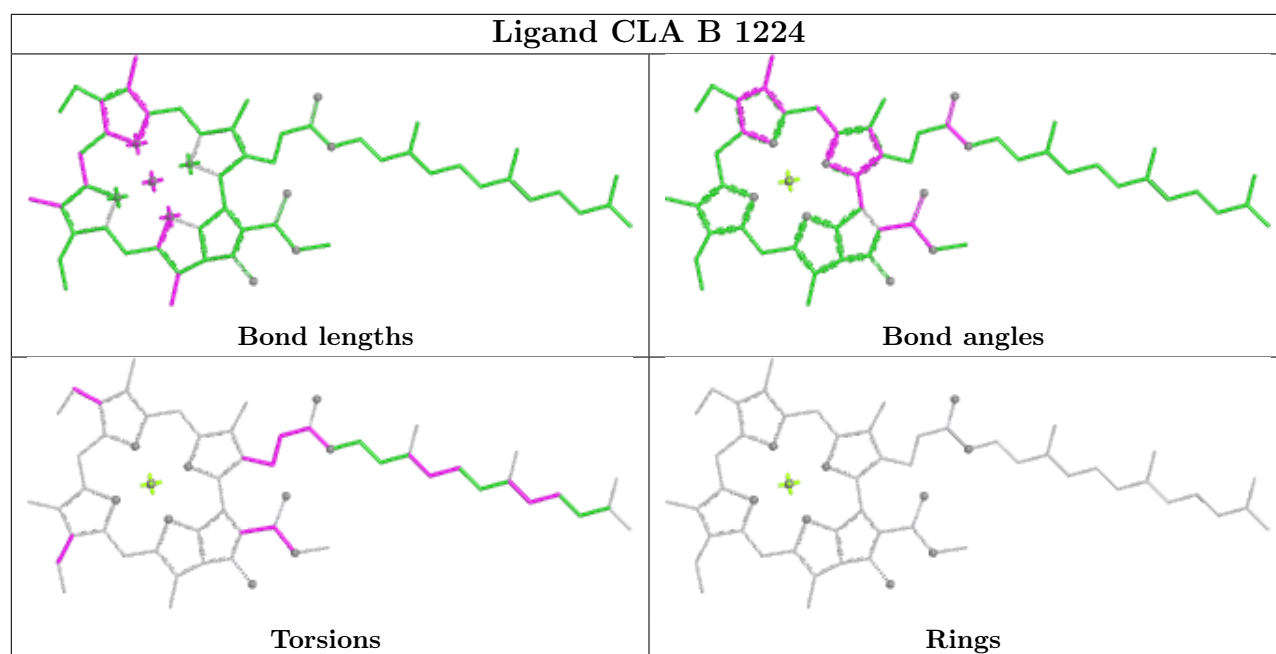


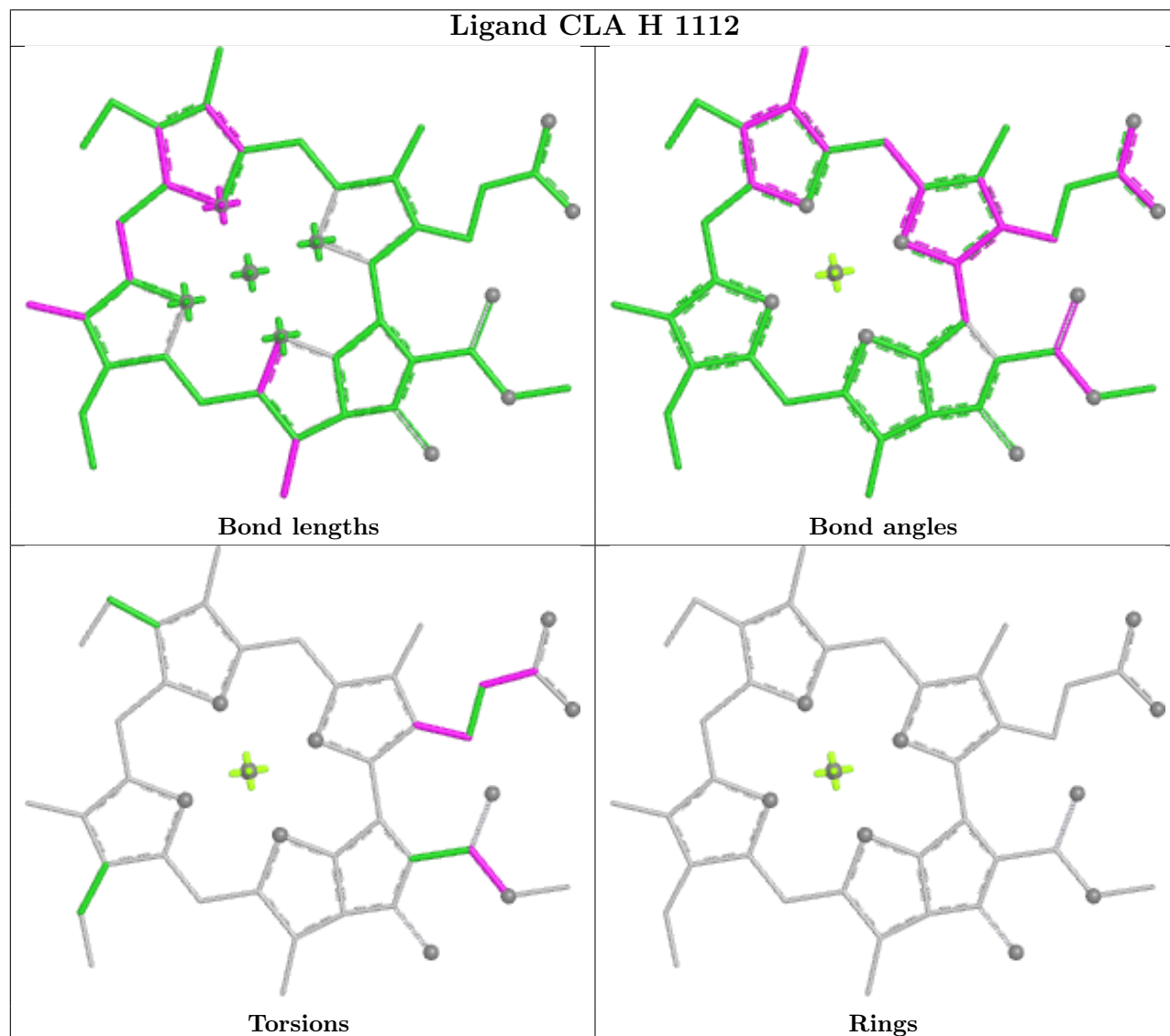
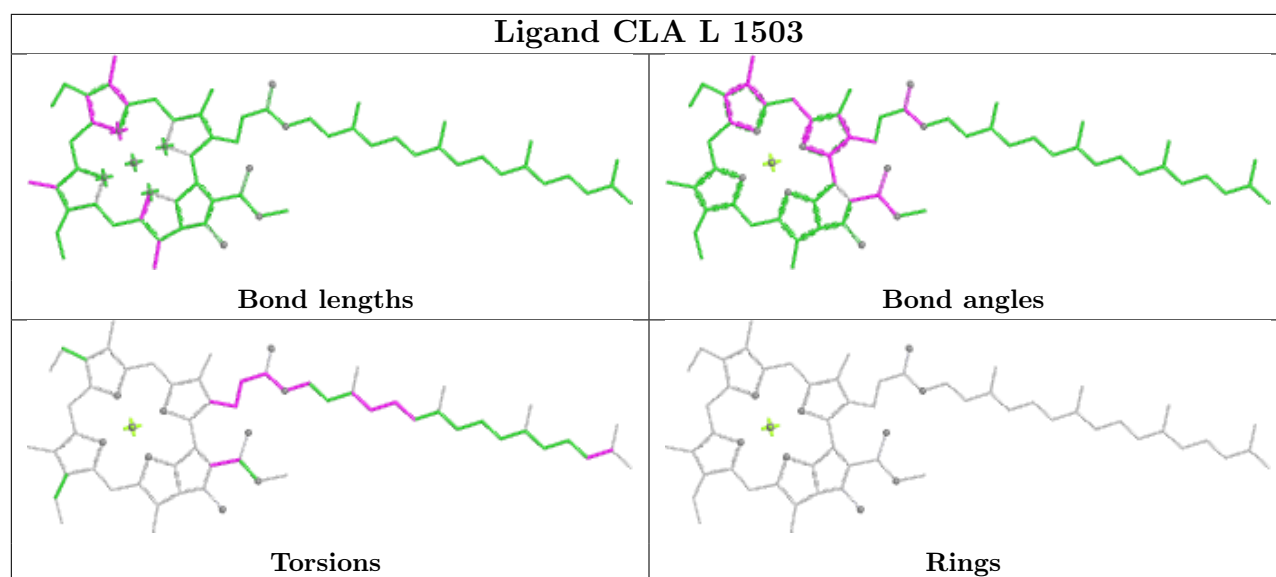
Ligand CLA A 1104

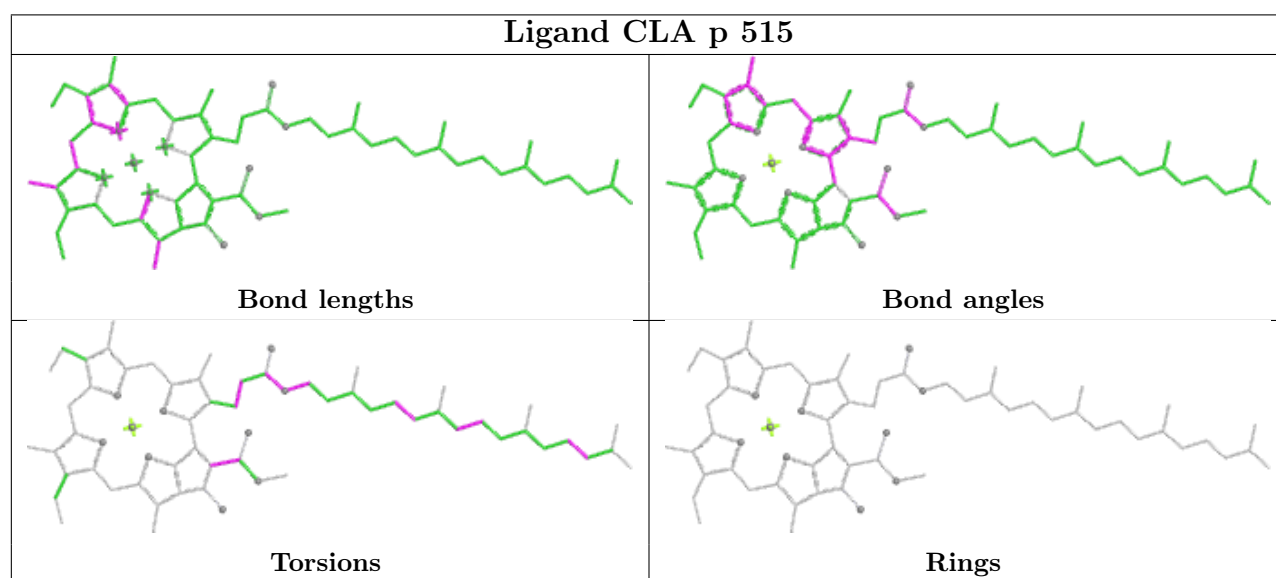
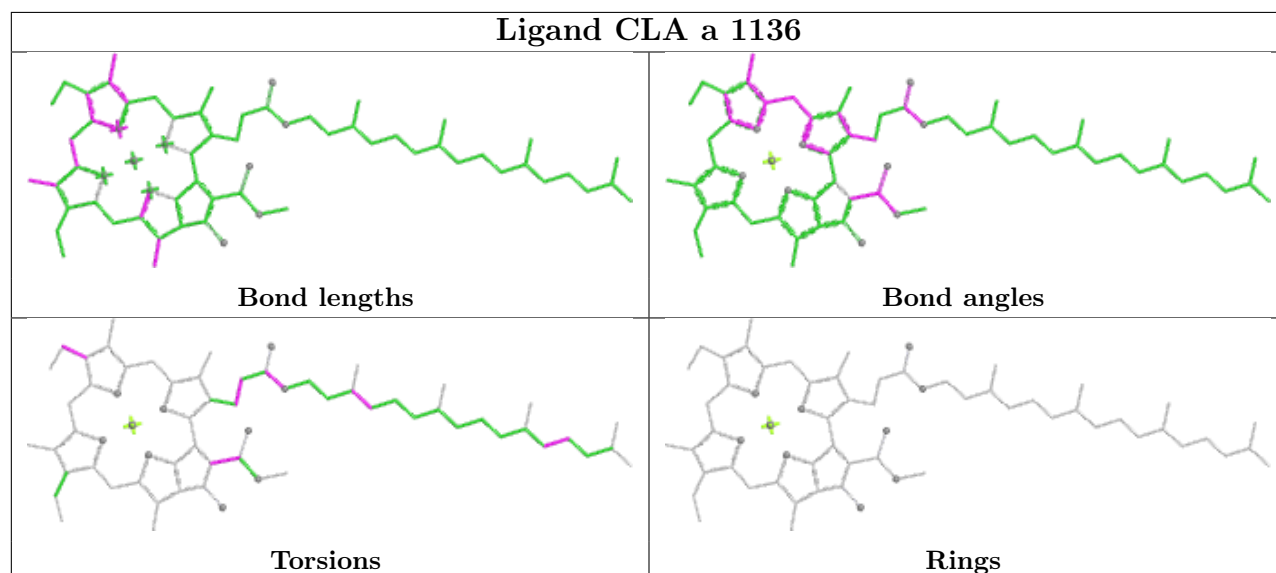
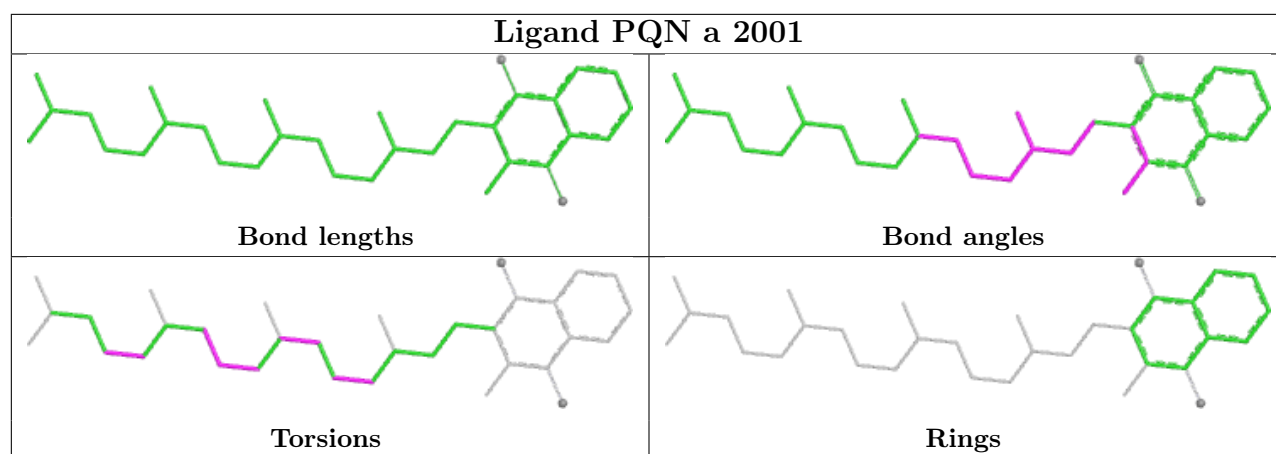


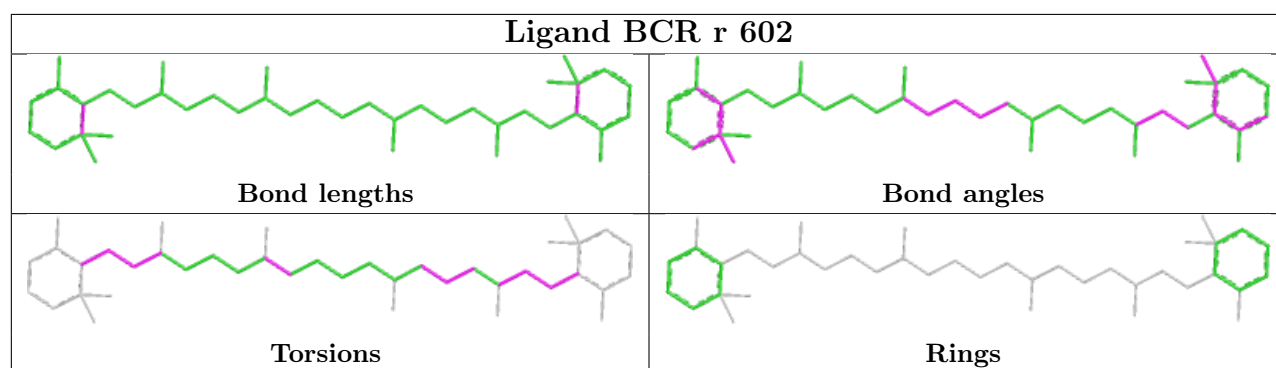
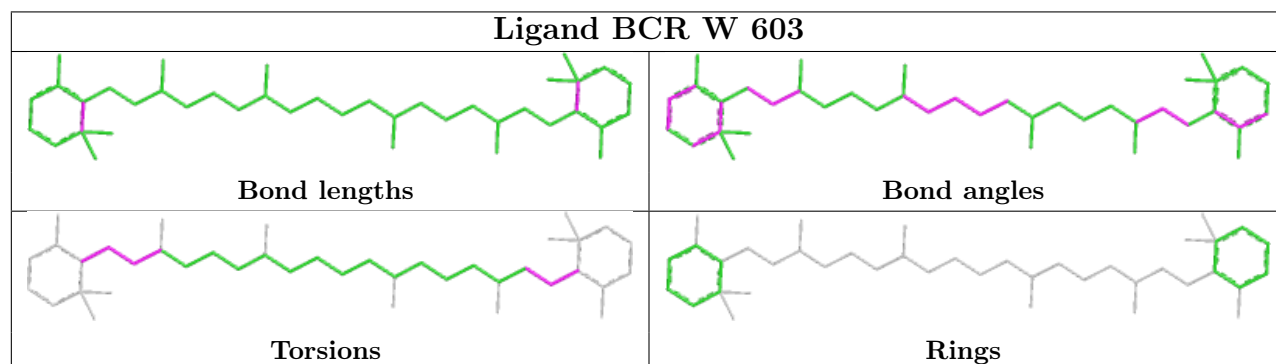
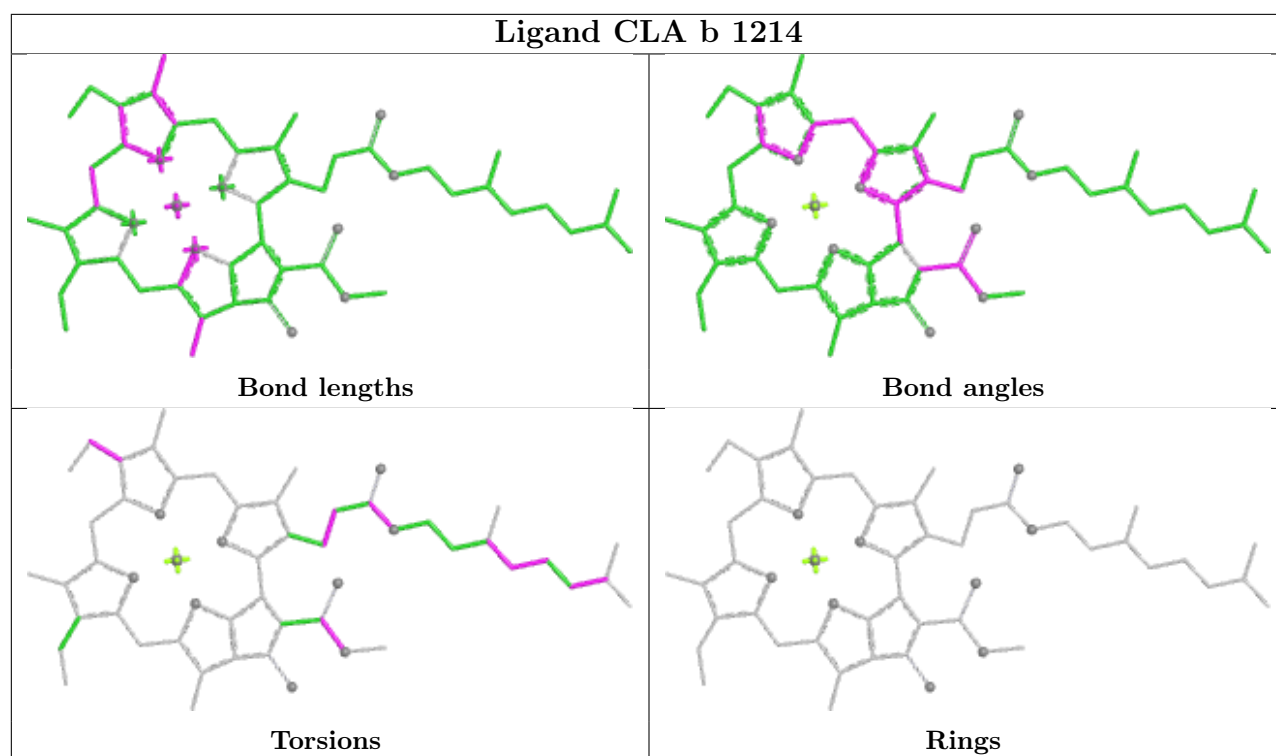
Ligand CLA a 1129

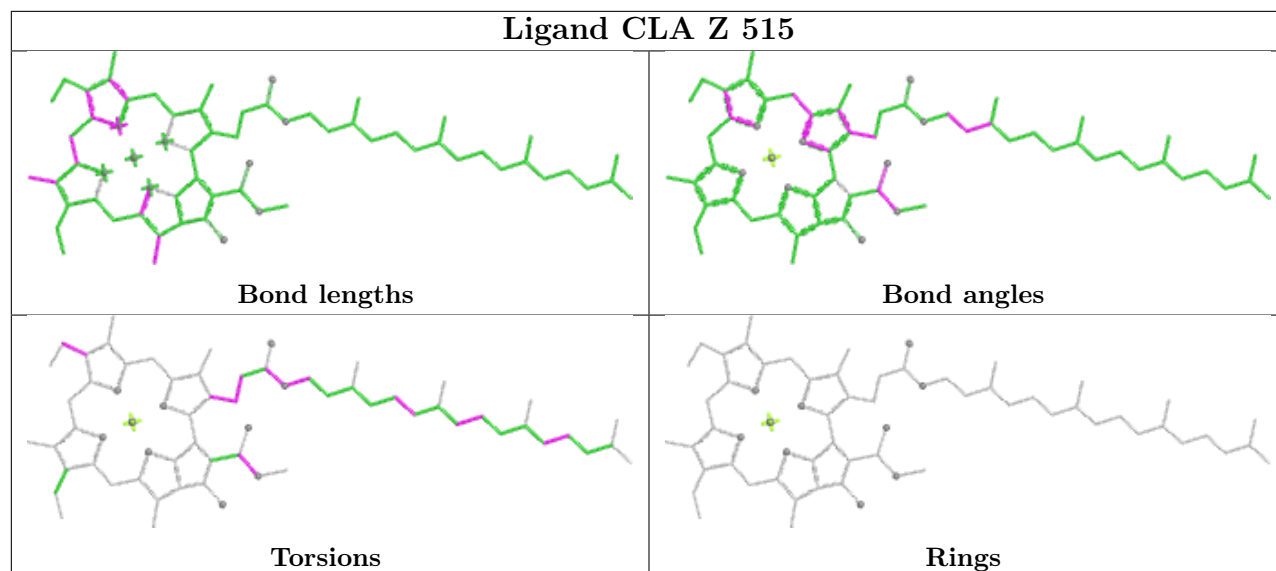
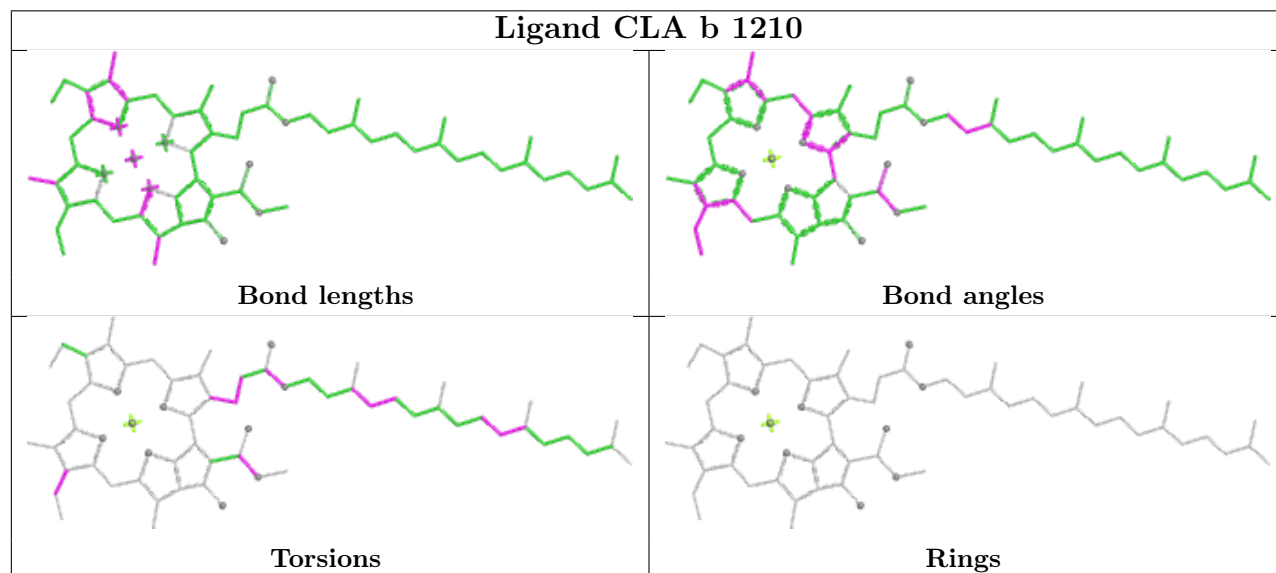
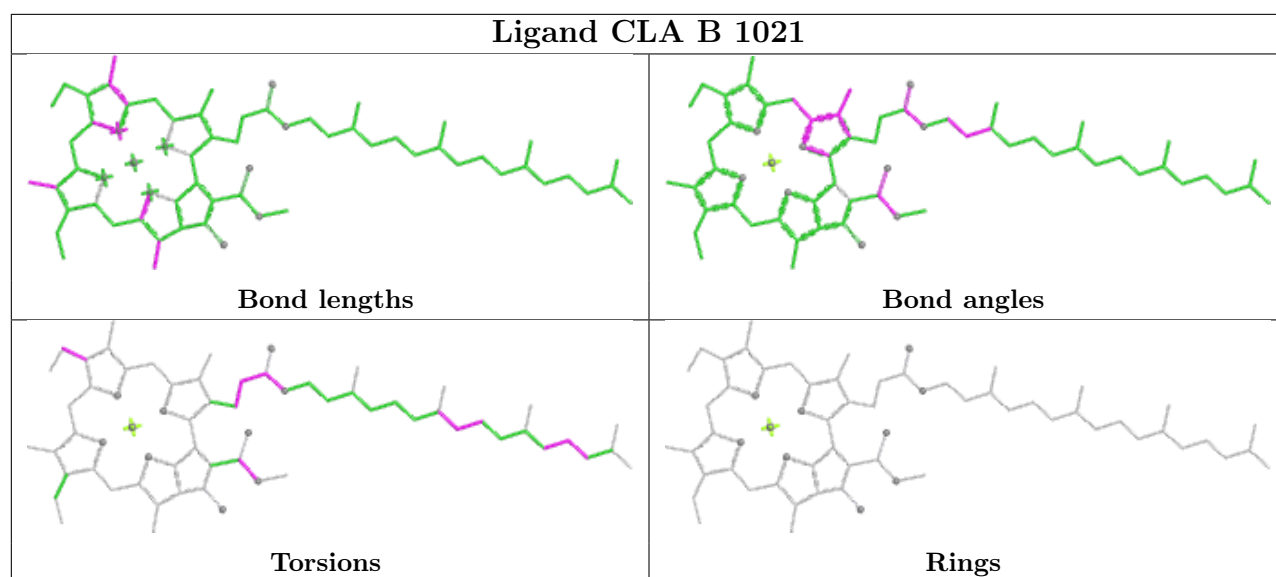




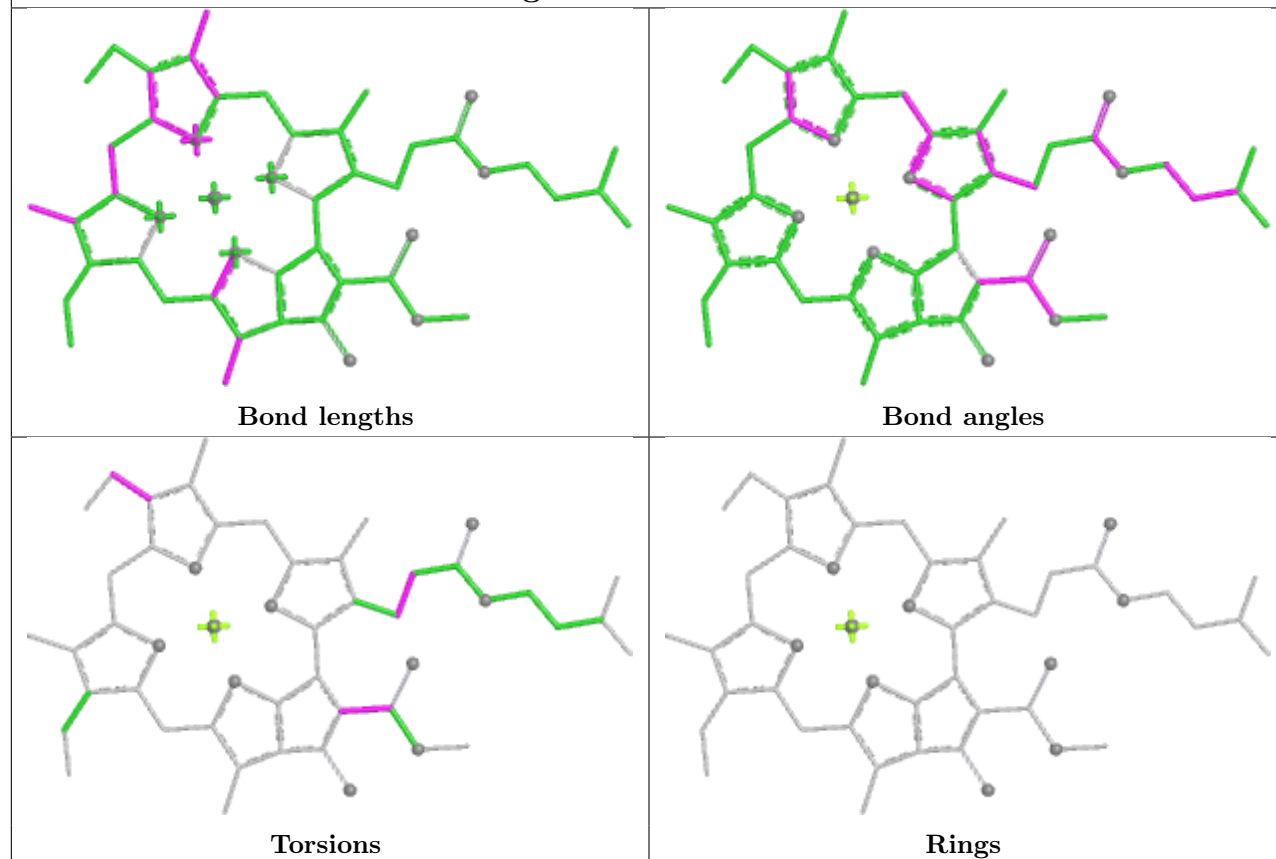




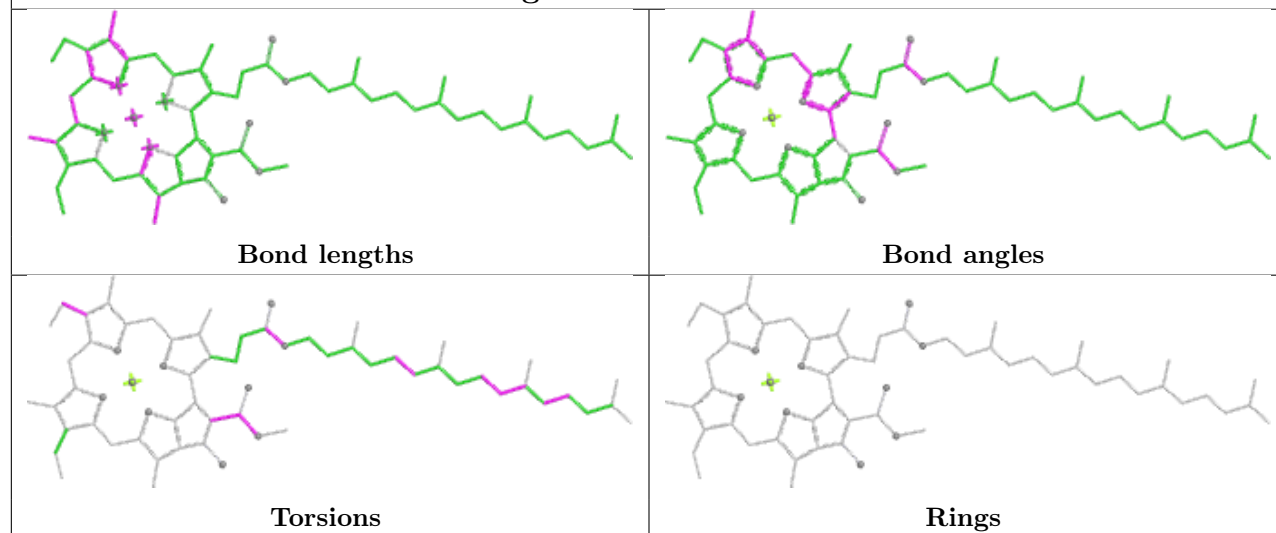


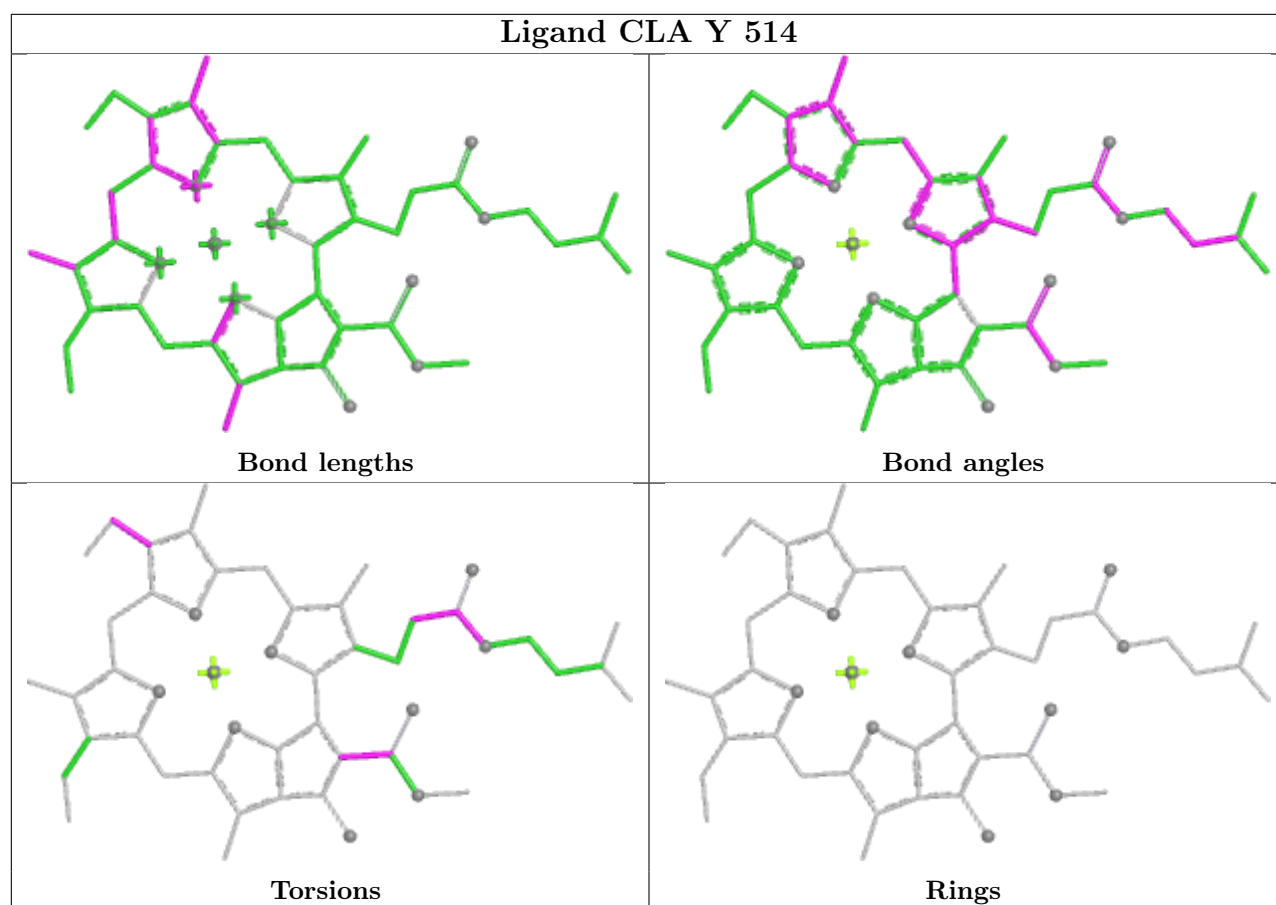


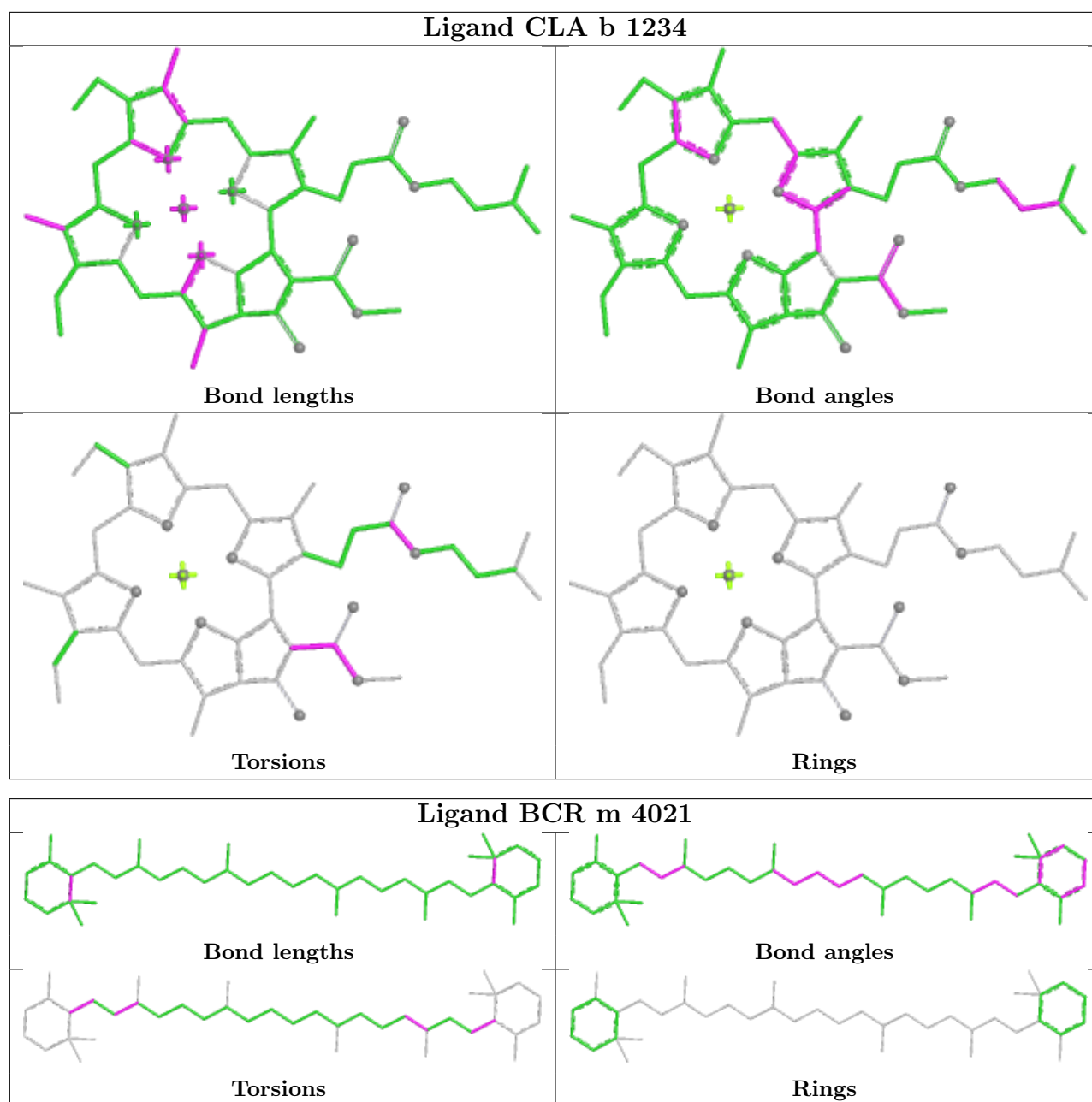
Ligand CLA A 1129



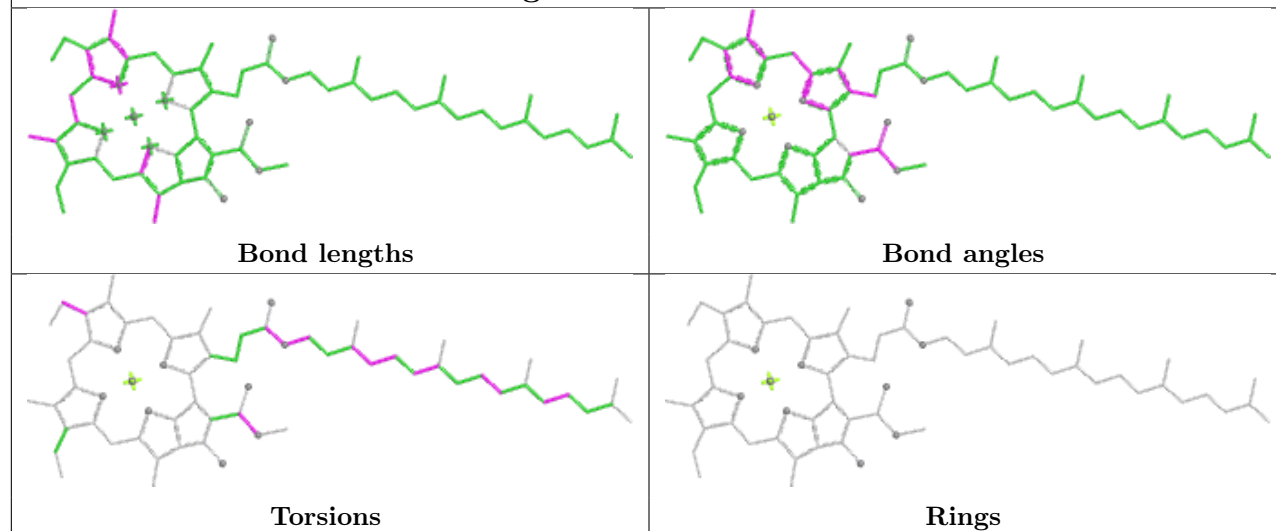
Ligand CLA G 1221



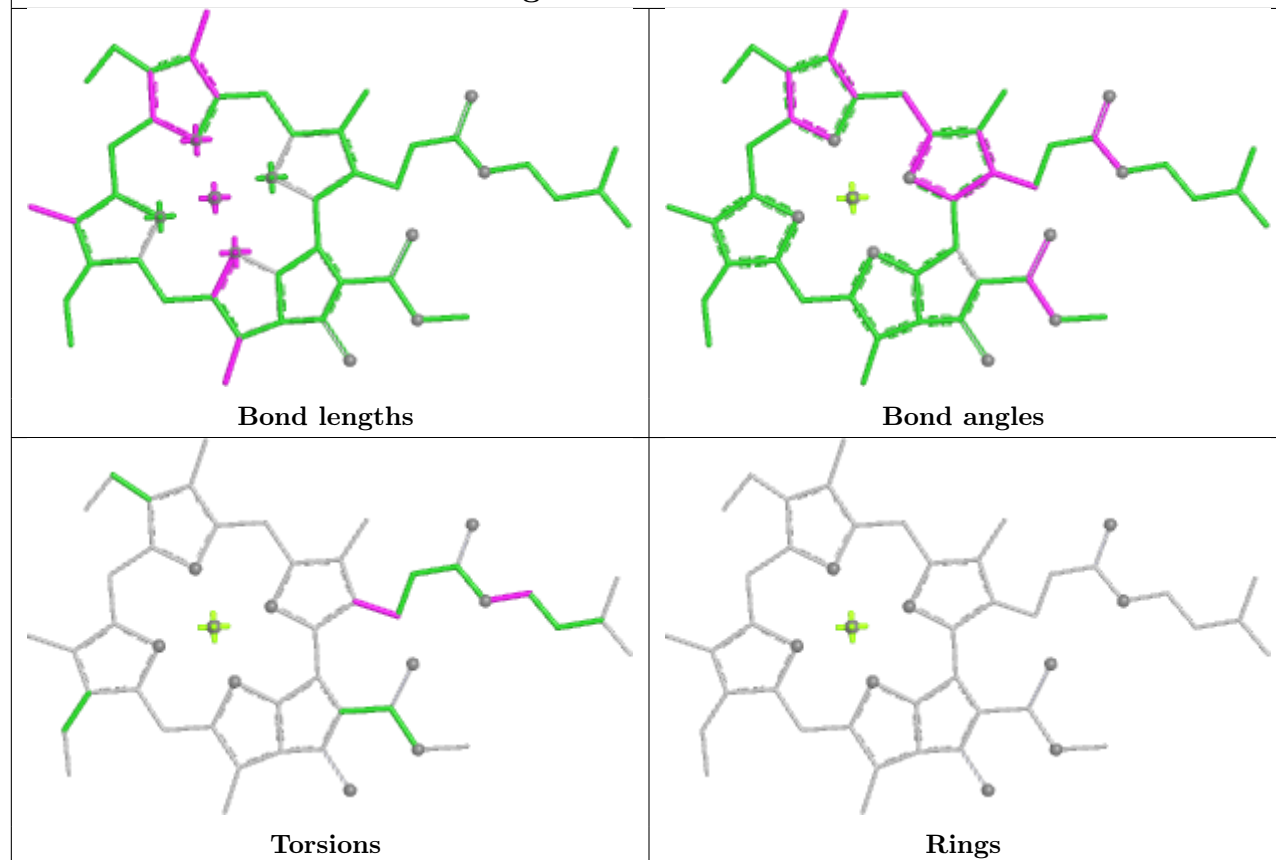


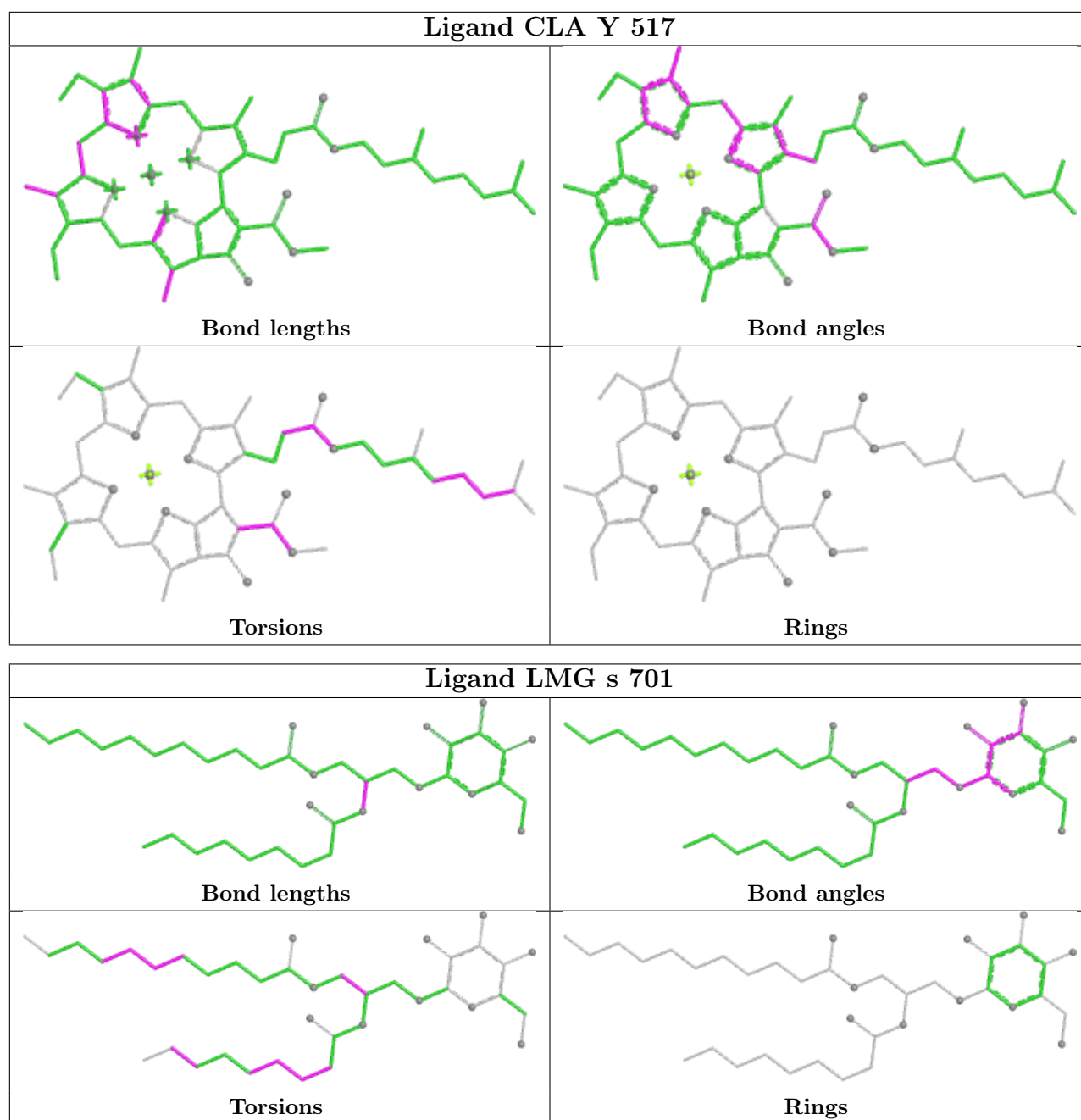


Ligand CLA A 1109

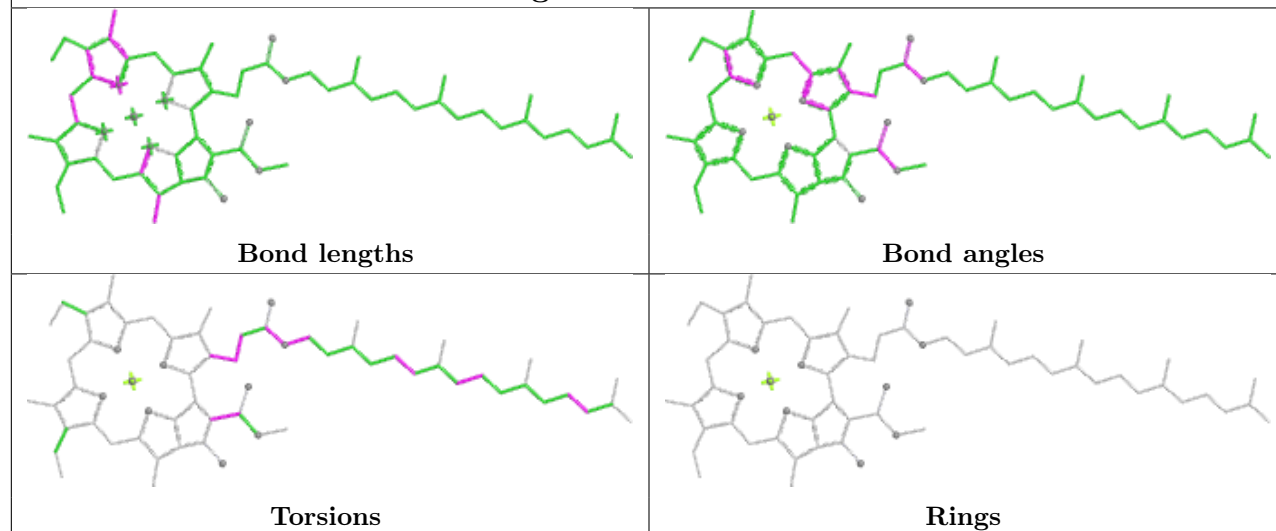


Ligand CLA A 1107

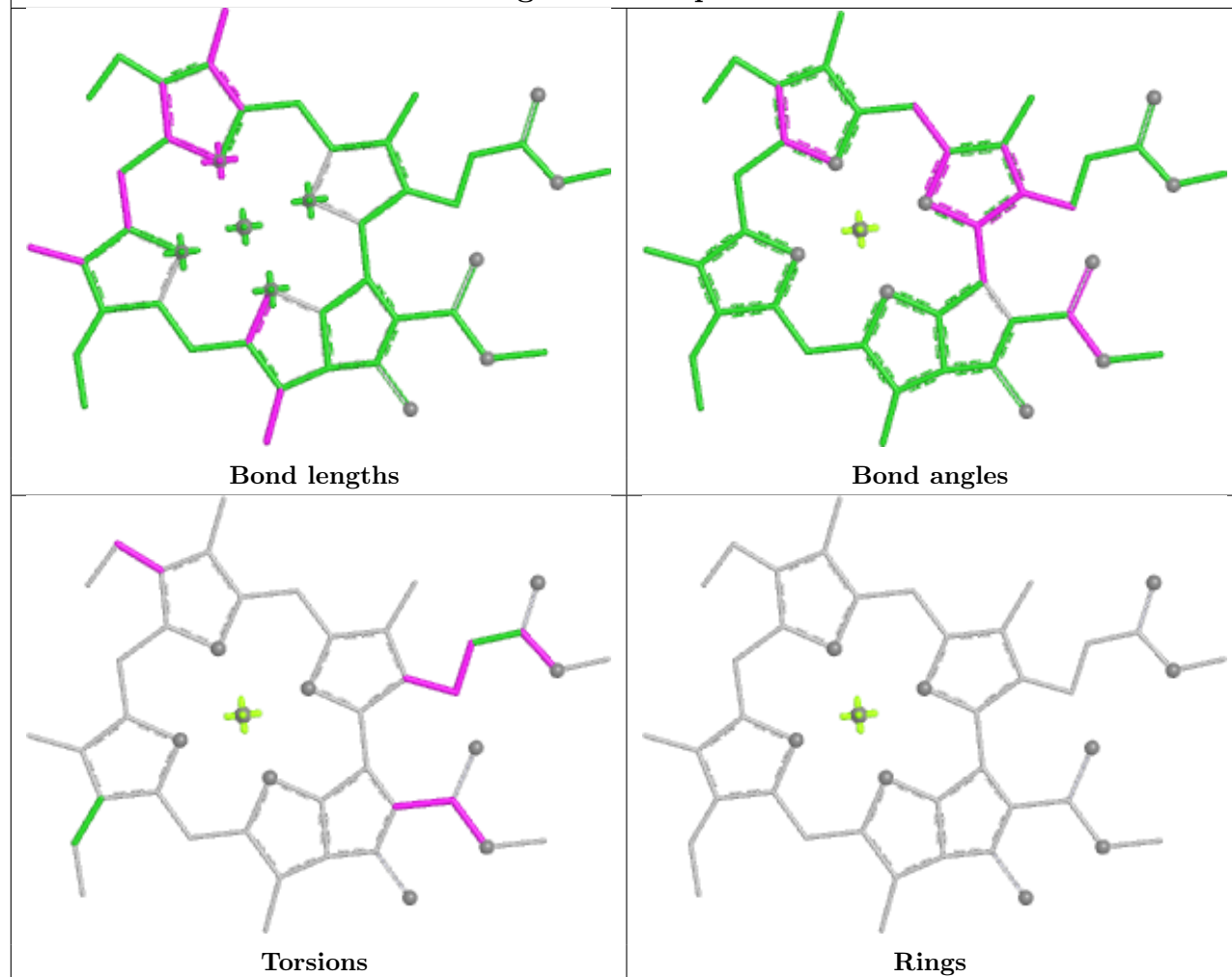


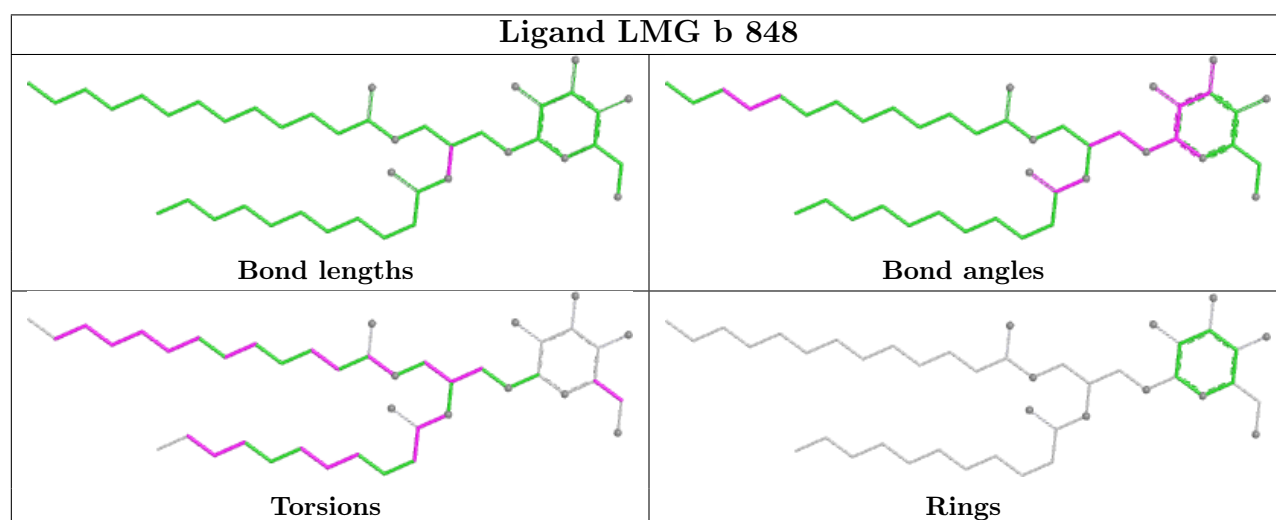
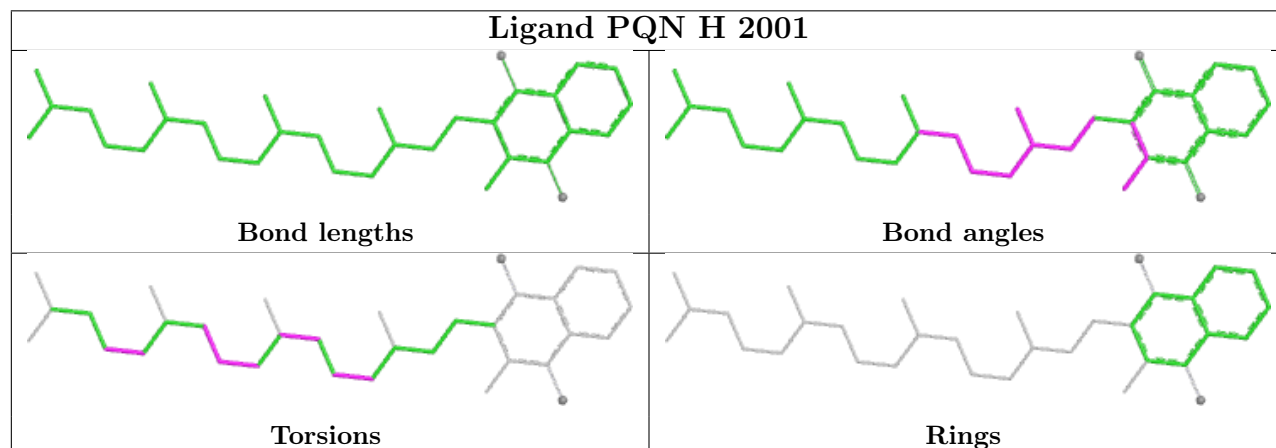
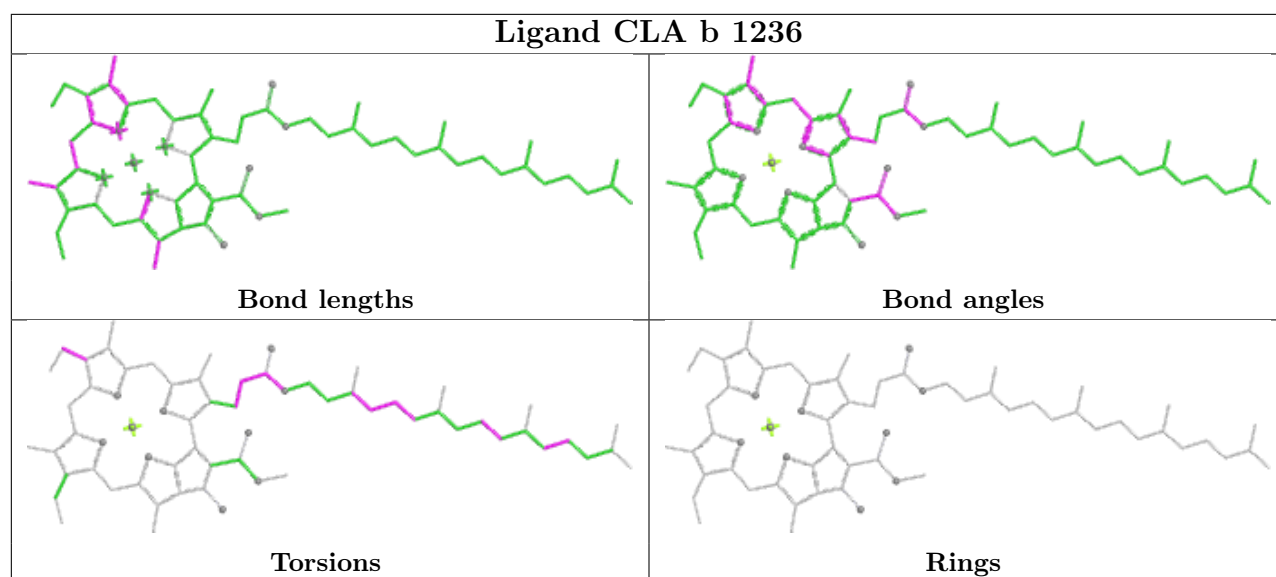


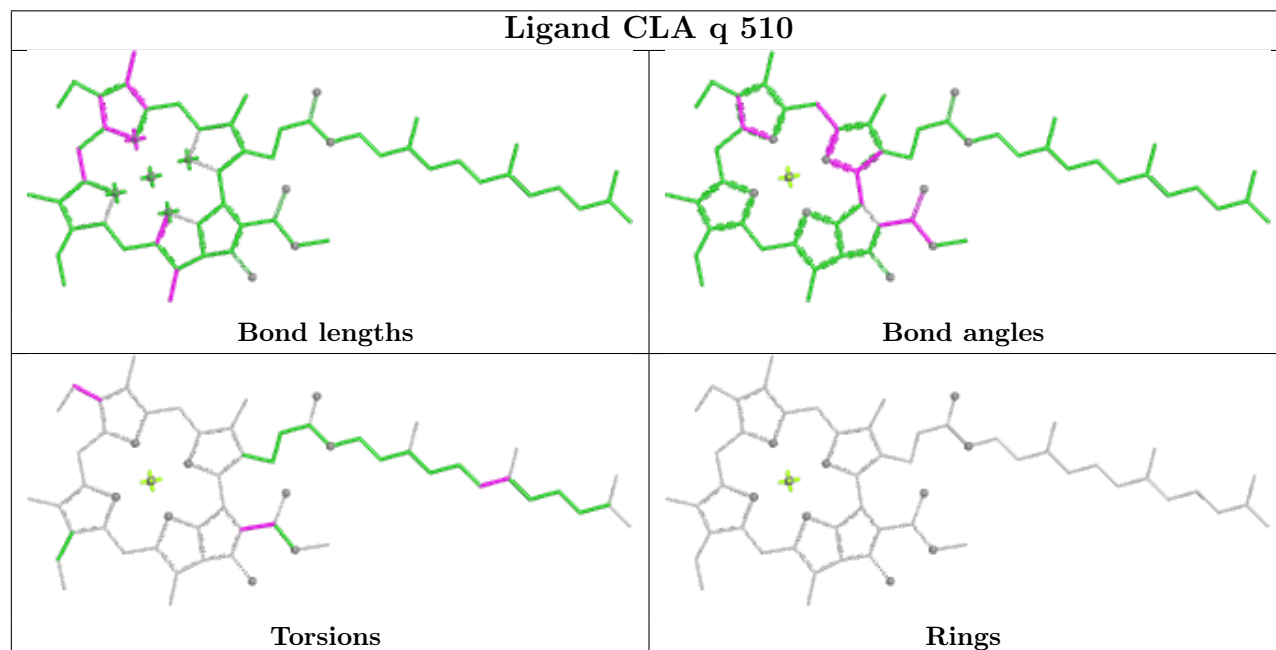
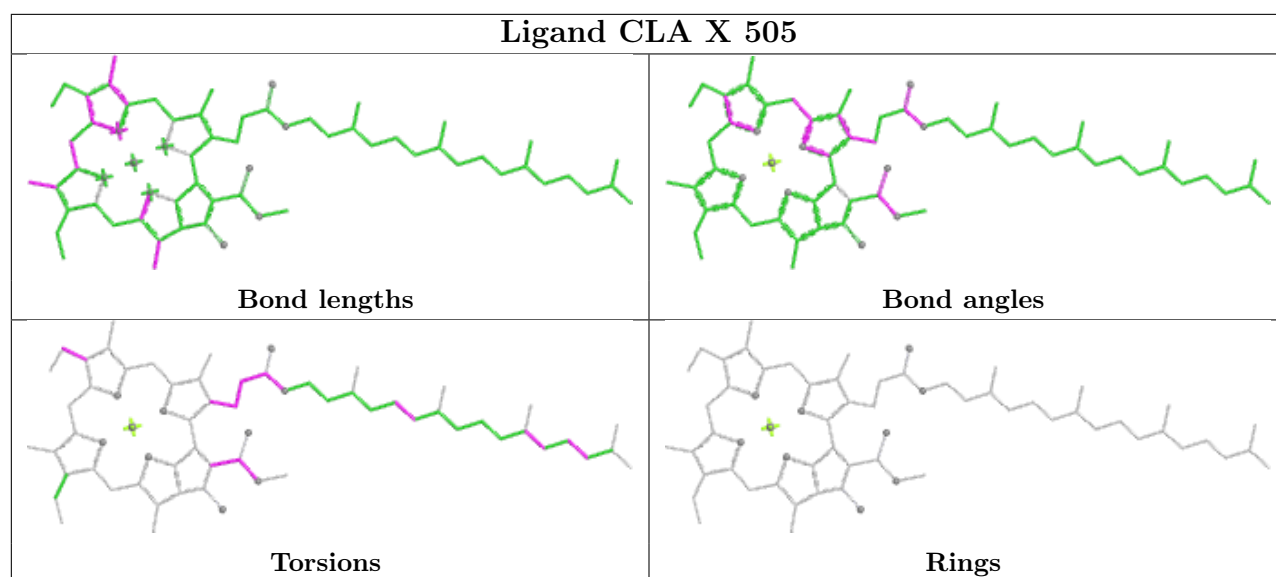
Ligand CLA Y 515

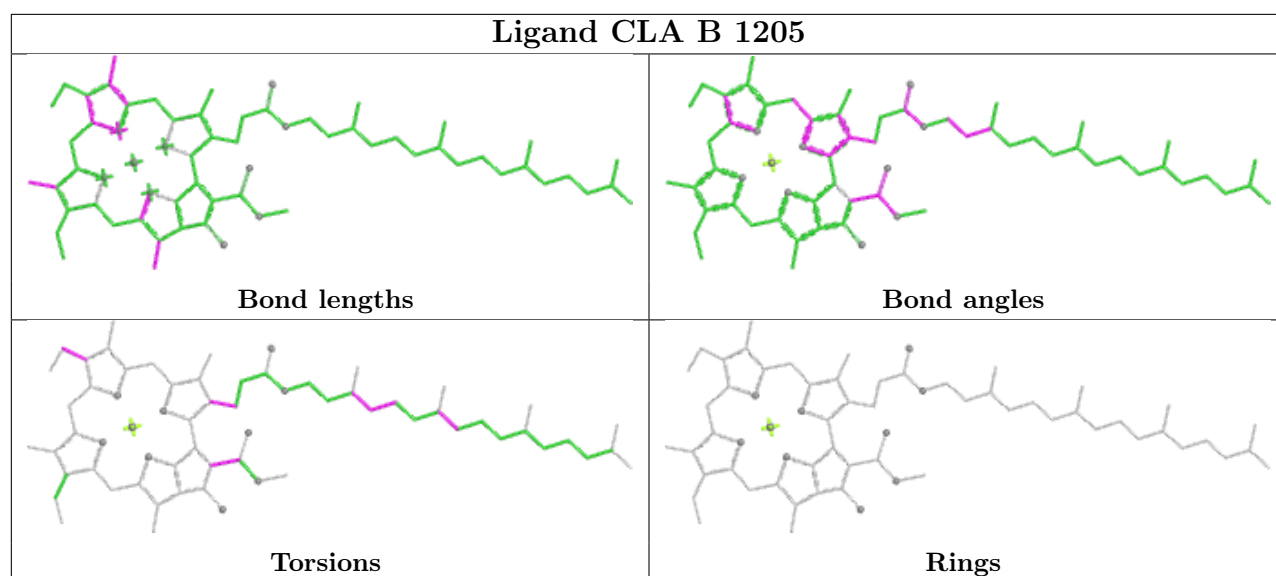
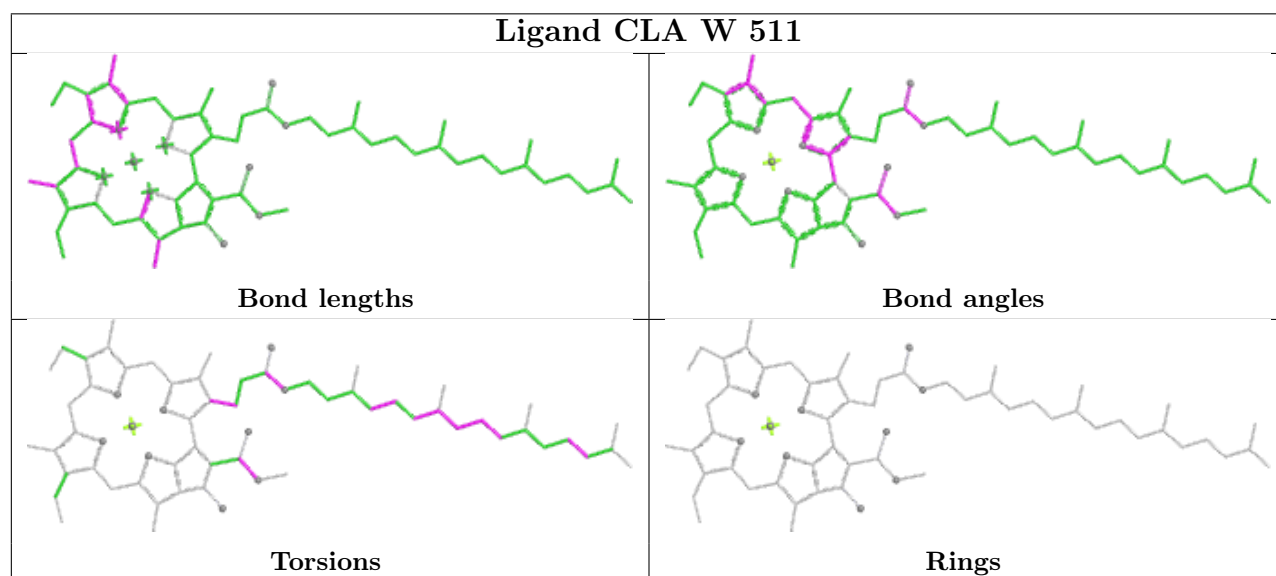
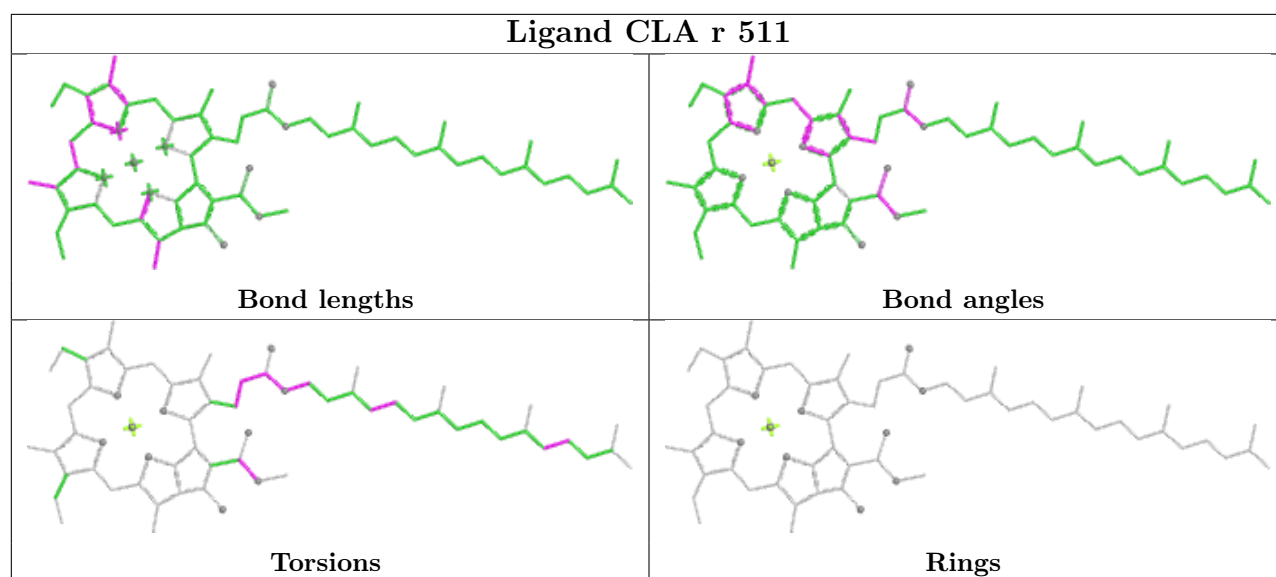


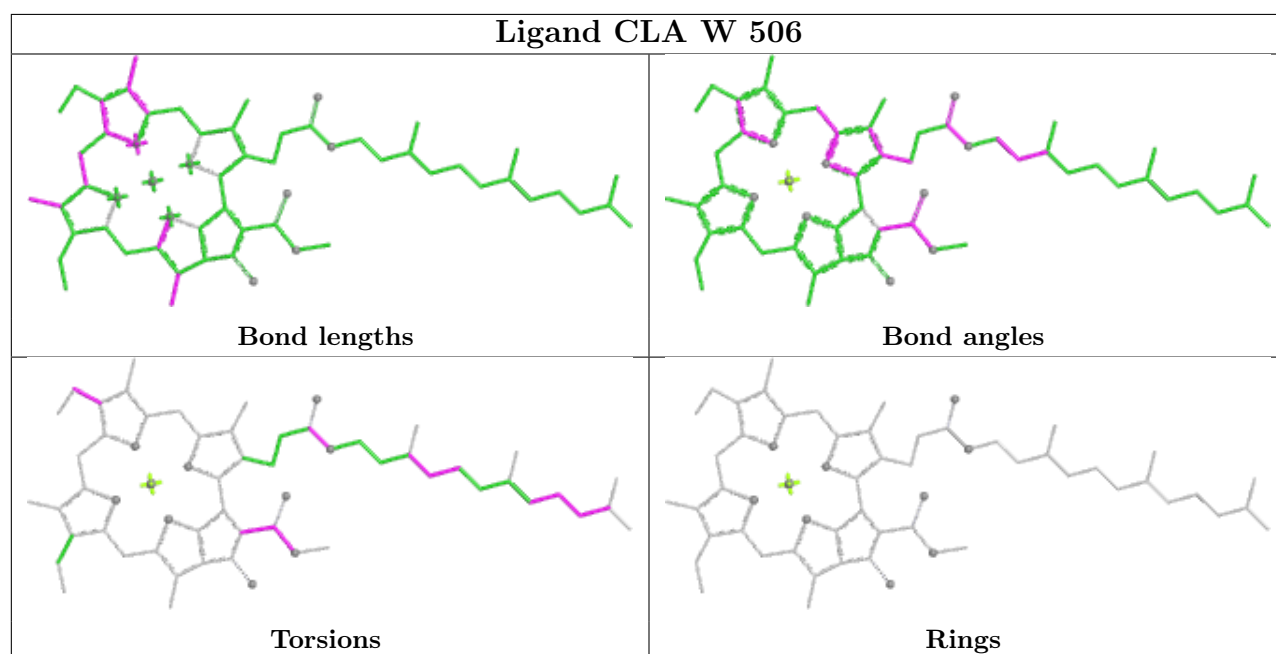
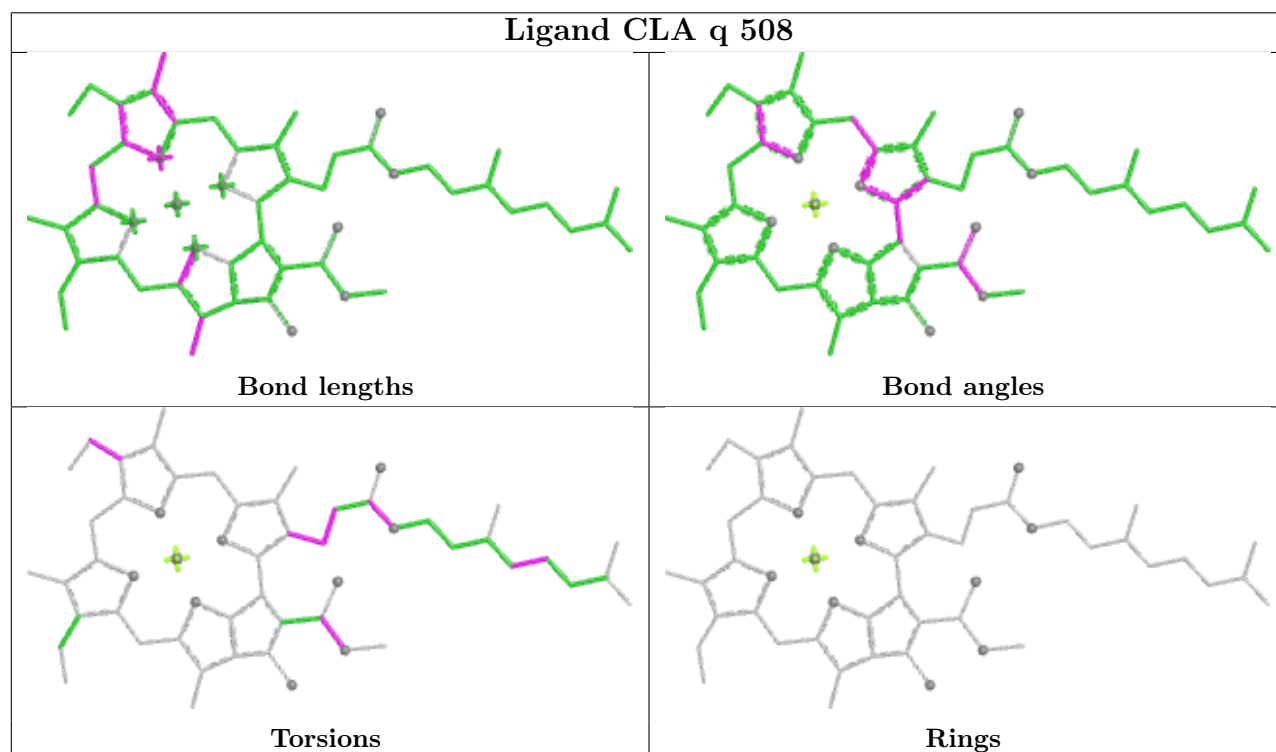
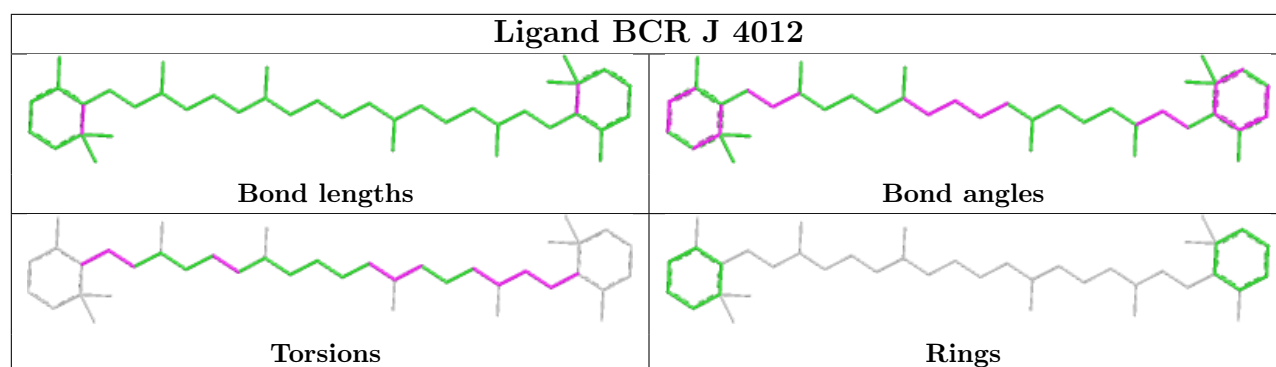
Ligand CLA q 503

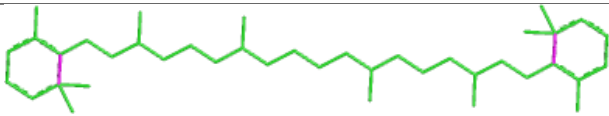
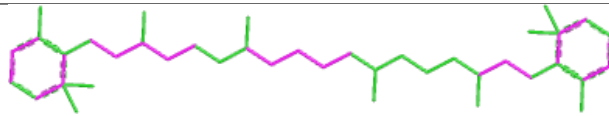
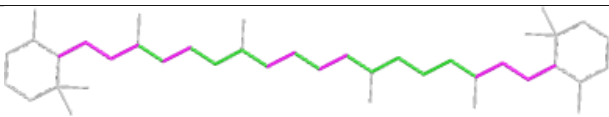
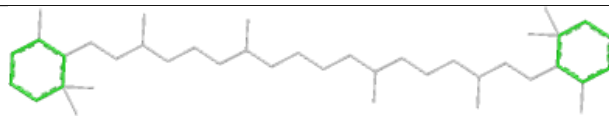


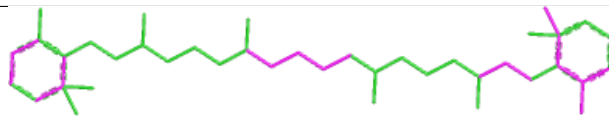
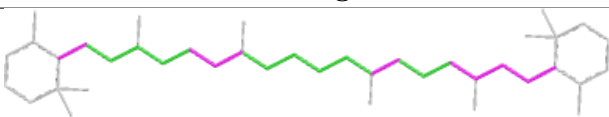
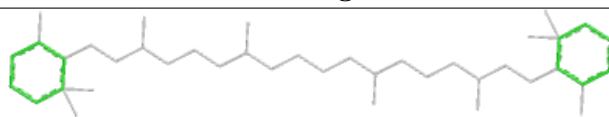


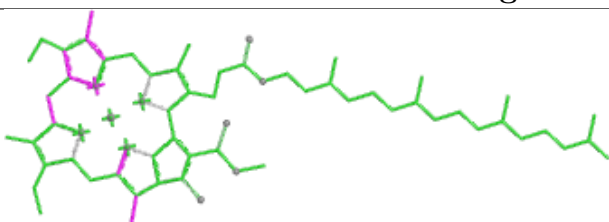
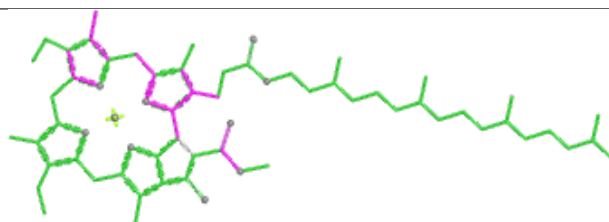
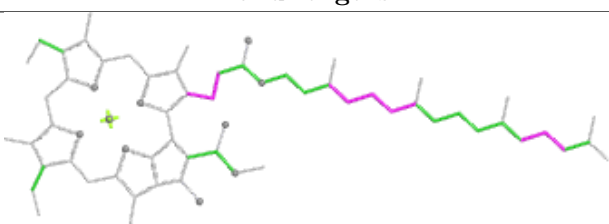
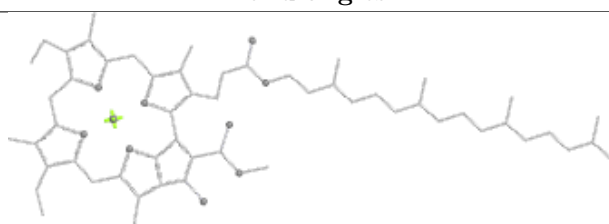




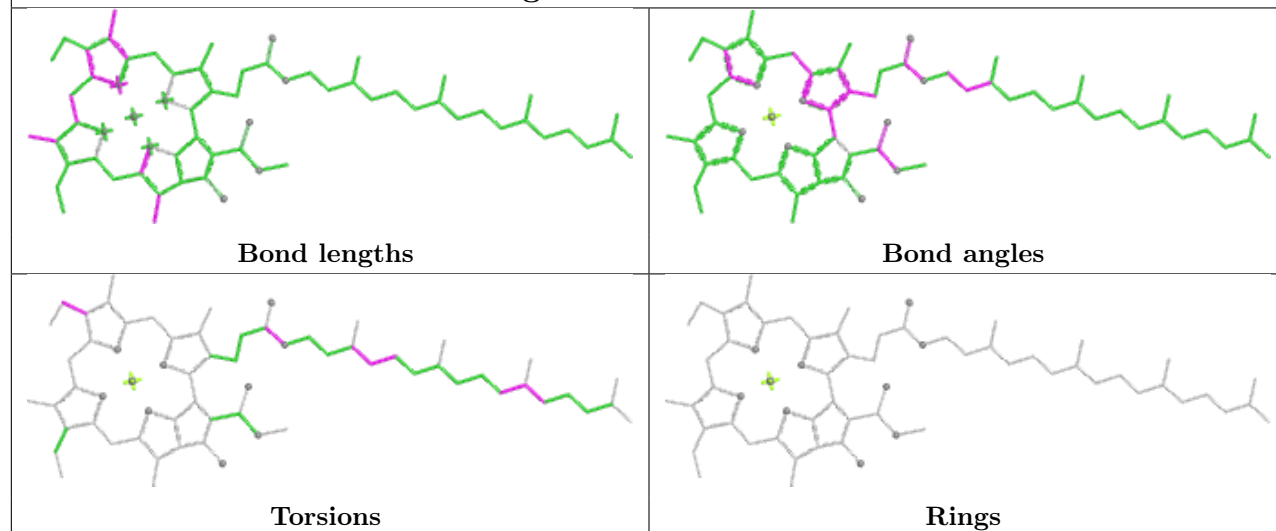


Ligand BCR x 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

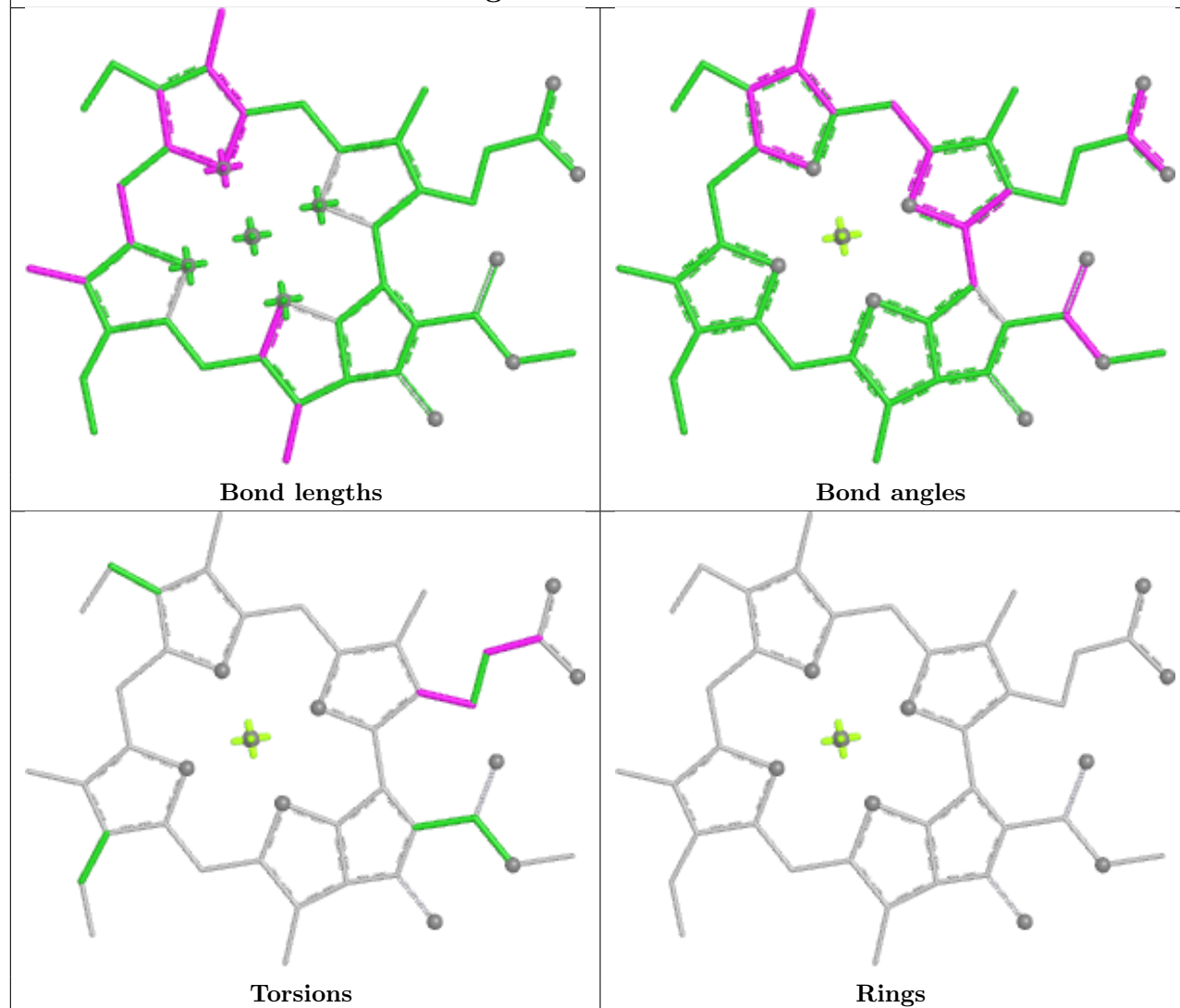
Ligand BCR B 4009	
	
Bond lengths	Bond angles
	
Torsions	Rings

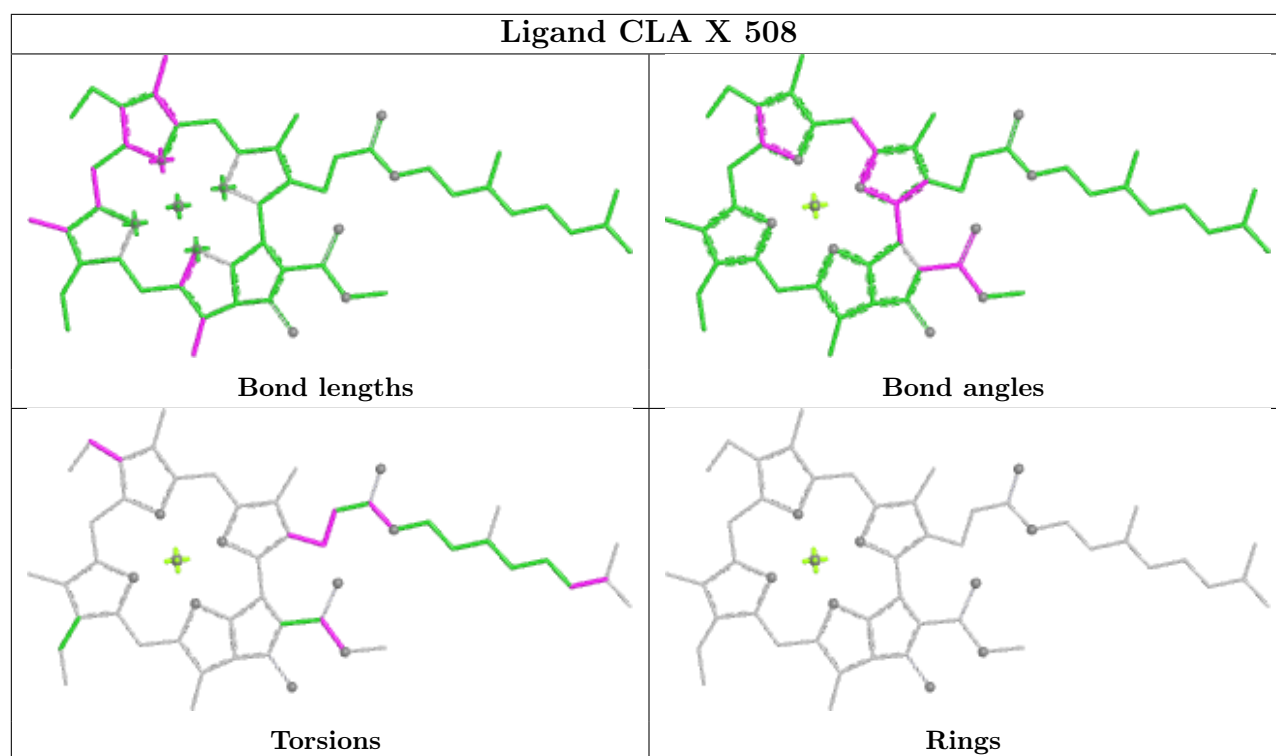
Ligand CLA A 1123	
	
Bond lengths	Bond angles
	
Torsions	Rings

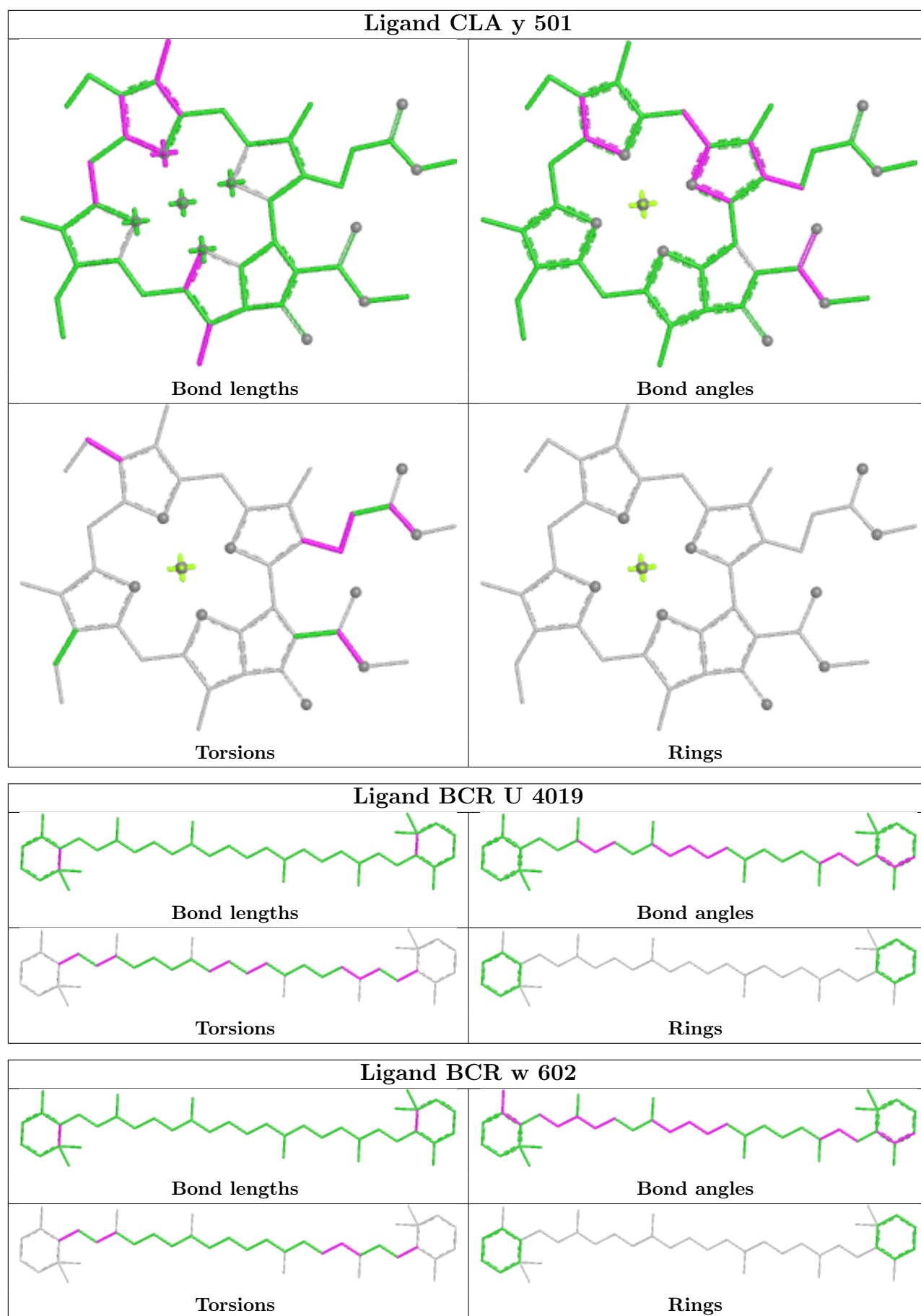
Ligand CLA A 1138



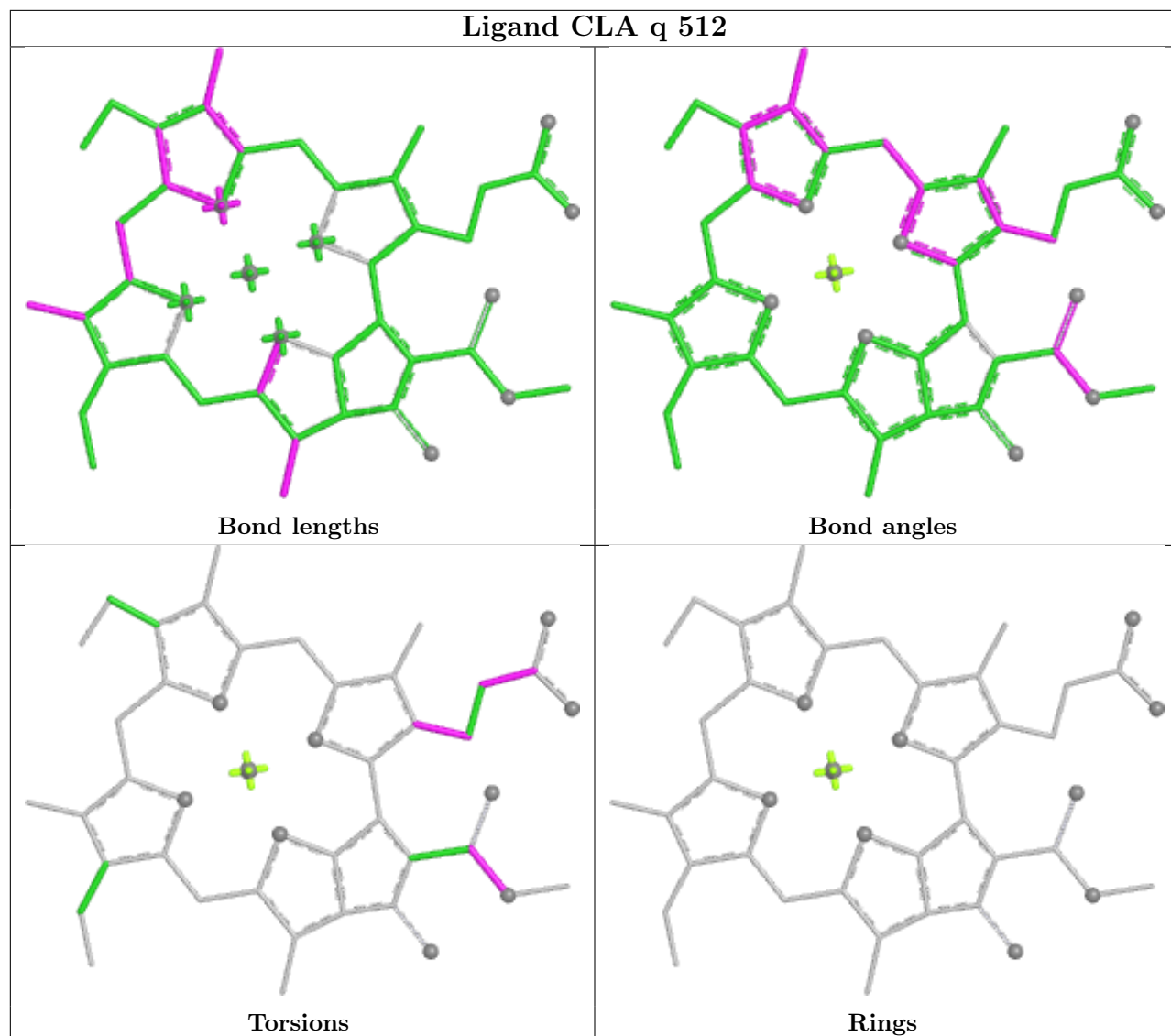
Ligand CLA F 1301



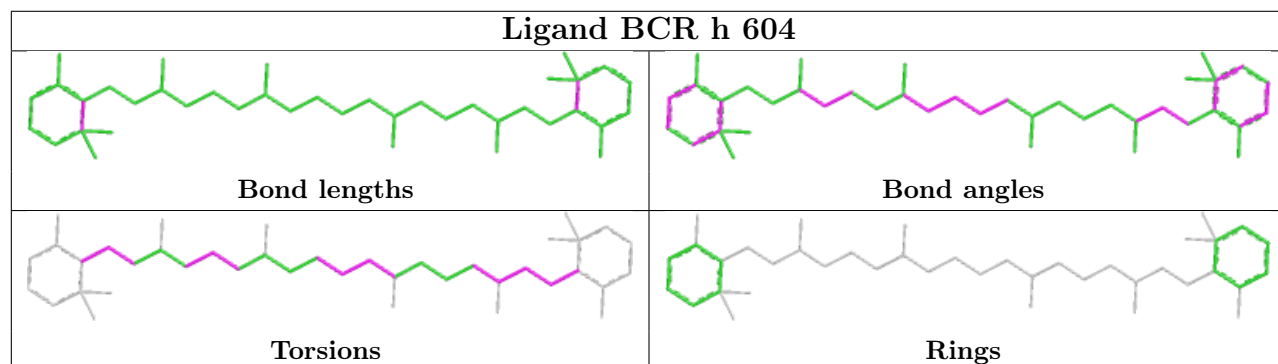


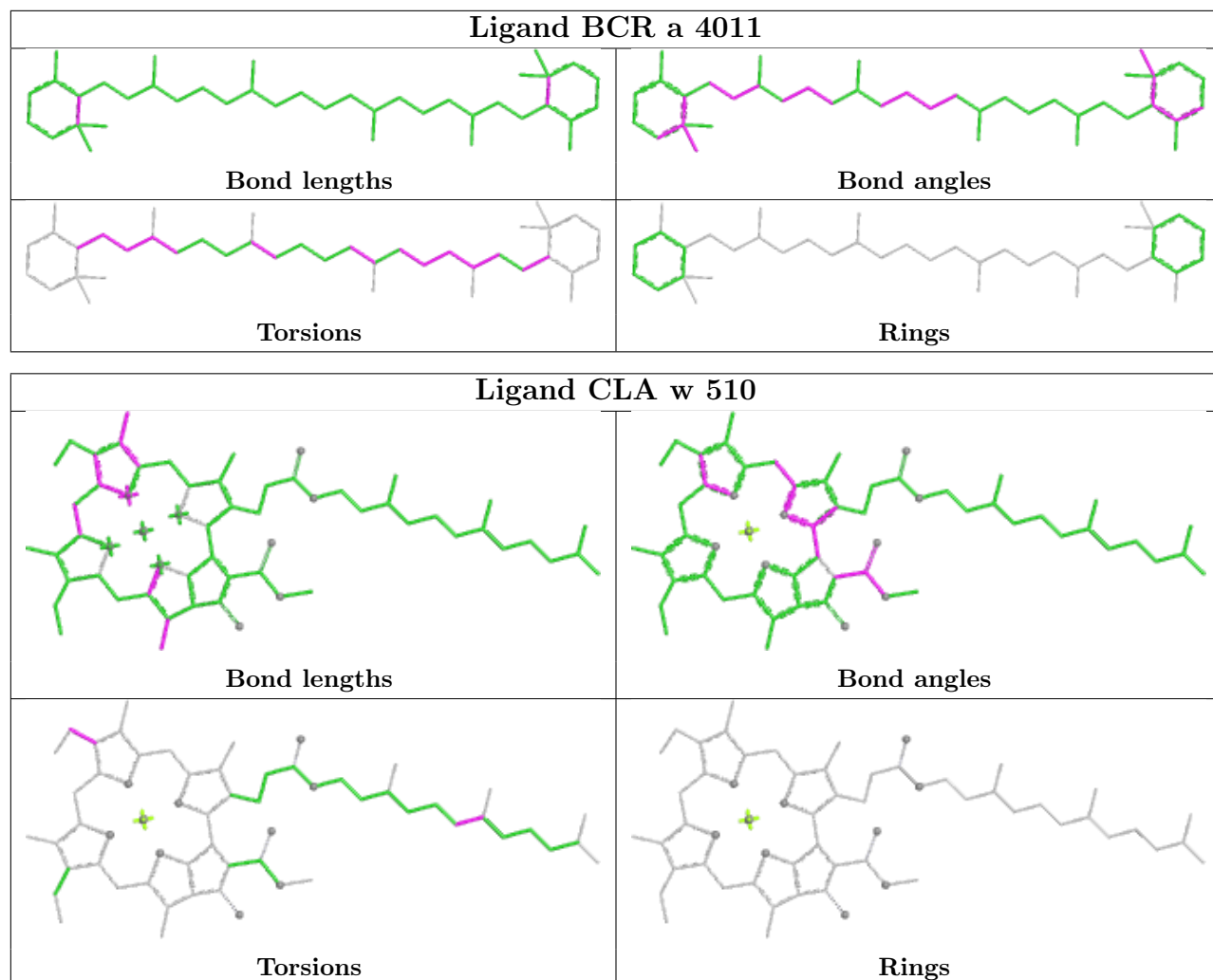


Ligand CLA q 512

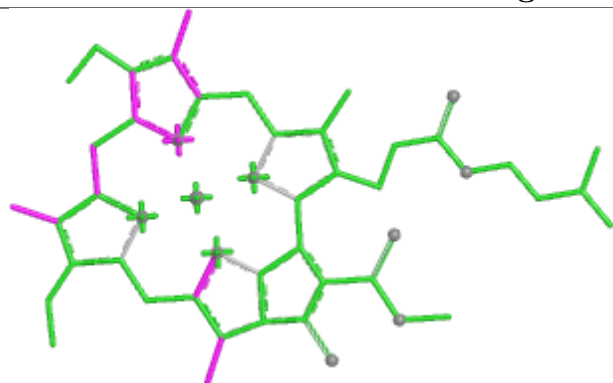


Ligand BCR h 604

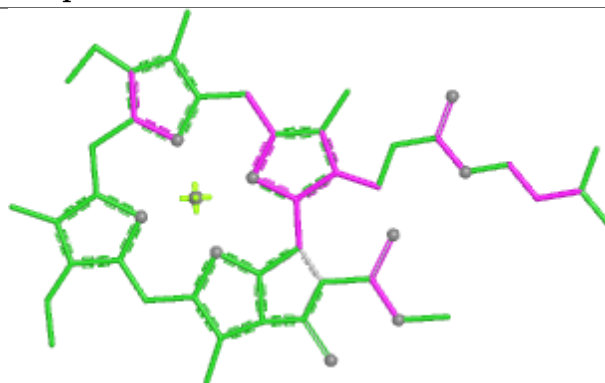




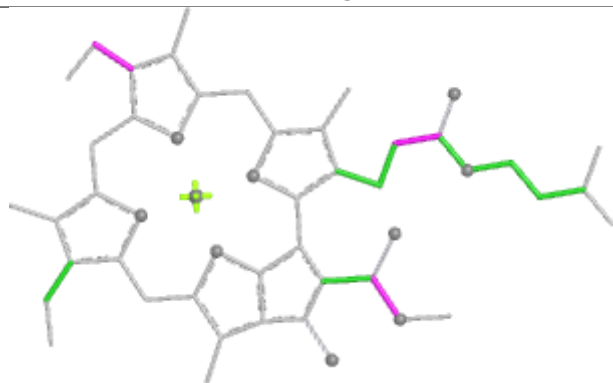
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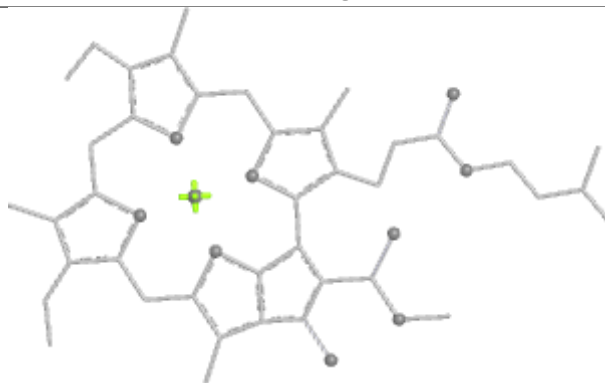
Bond lengths



Bond angles

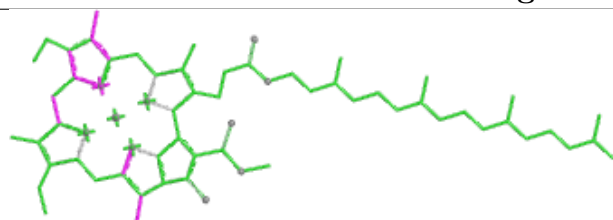


Torsions

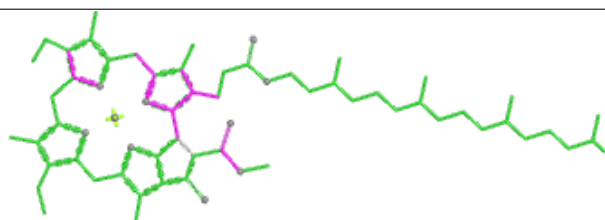


Rings

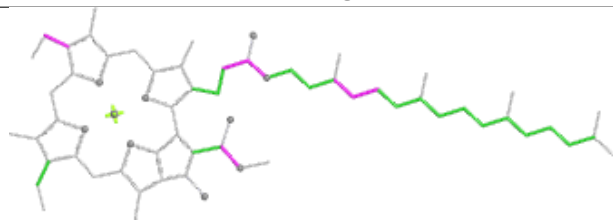
Ligand CLA h 507



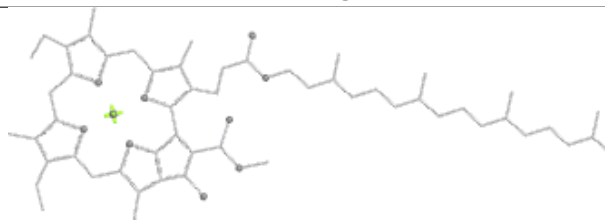
Bond lengths



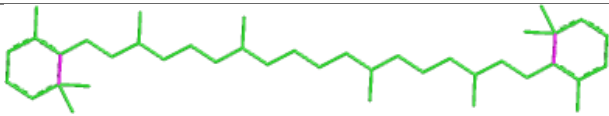
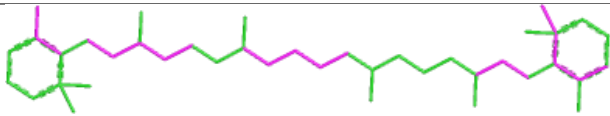
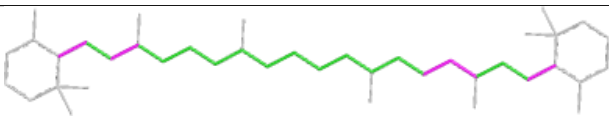
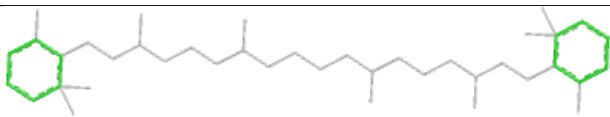
Bond angles

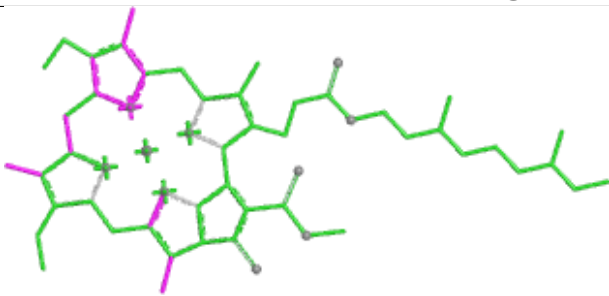
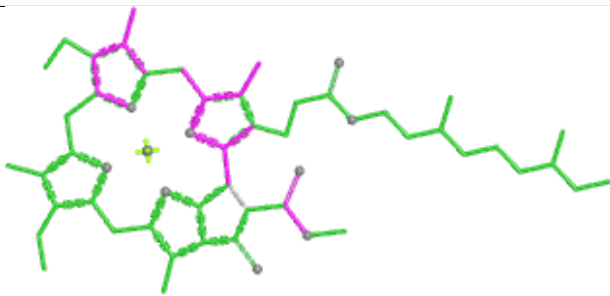
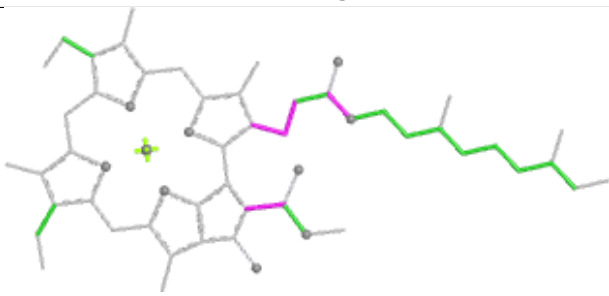
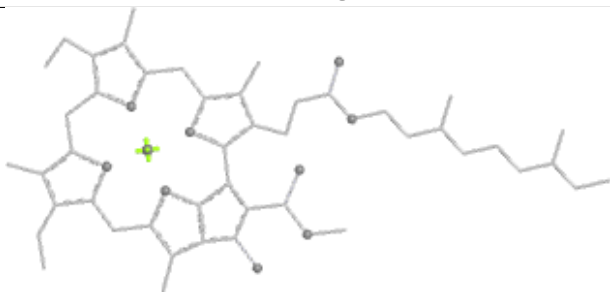


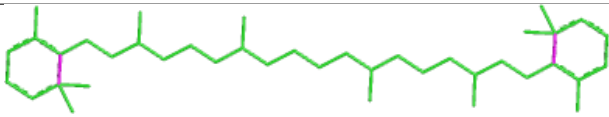
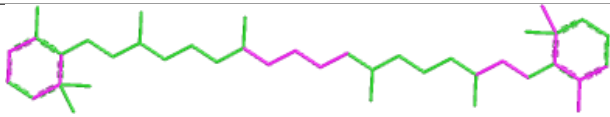
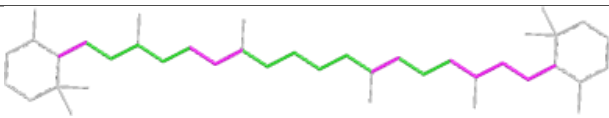
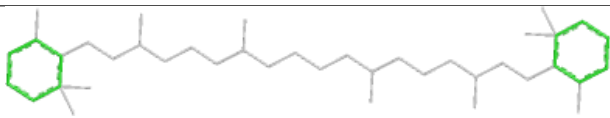
Torsions



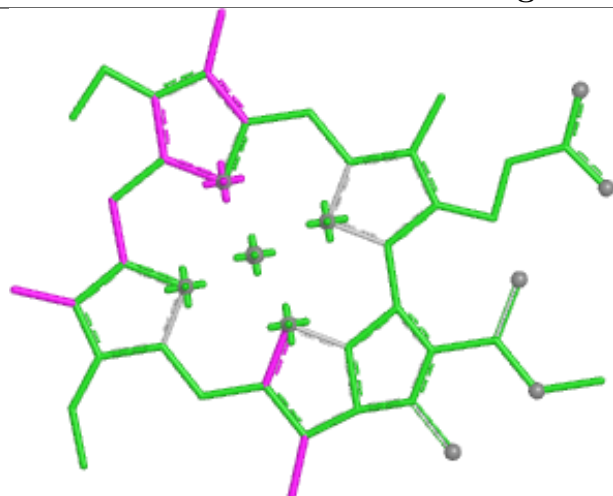
Rings

Ligand BCR q 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

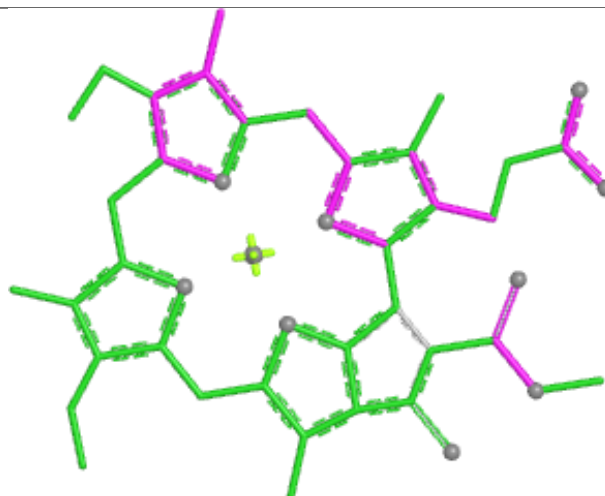
Ligand CLA a 1102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR G 4009	
	
Bond lengths	Bond angles
	
Torsions	Rings

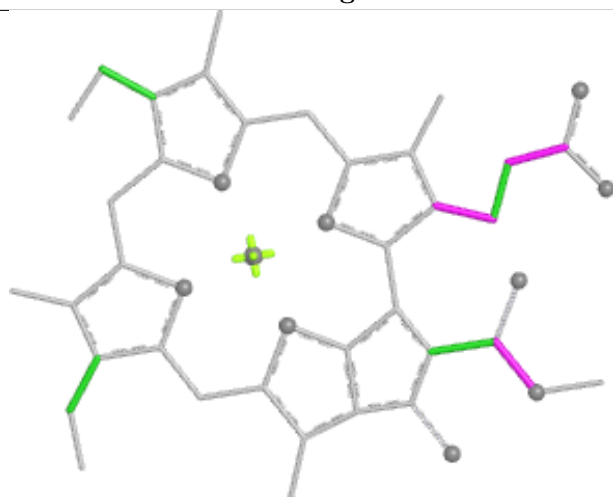
Ligand CLA u 512



Bond lengths



Bond angles

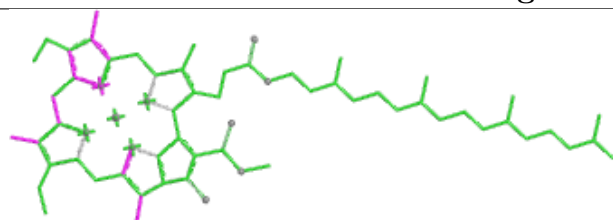


Torsions

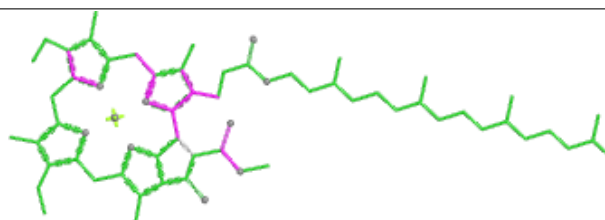


Rings

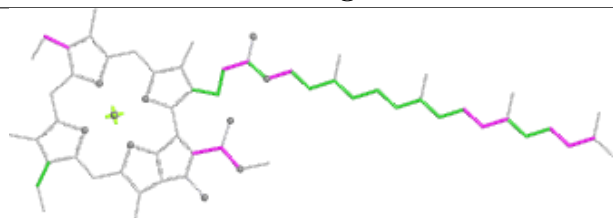
Ligand CLA u 510



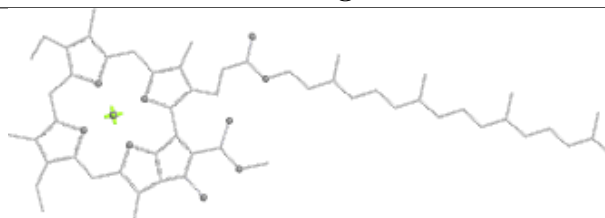
Bond lengths



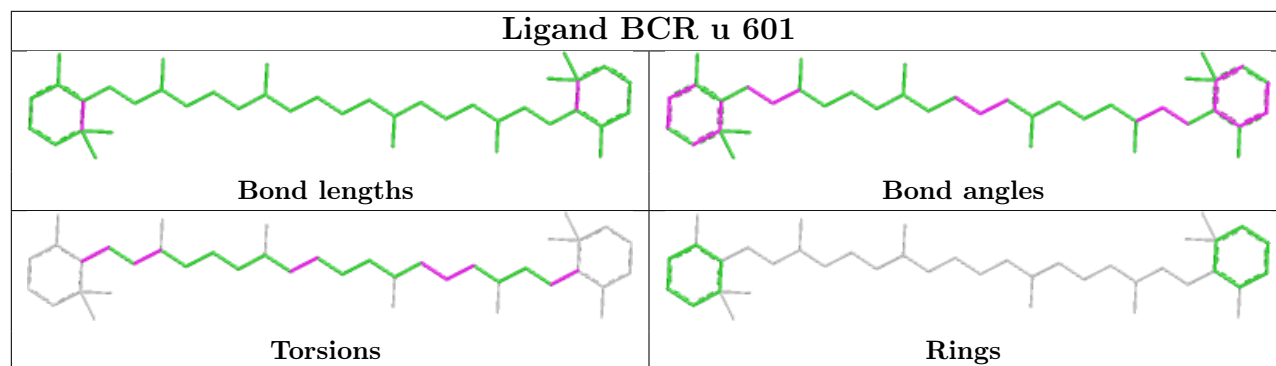
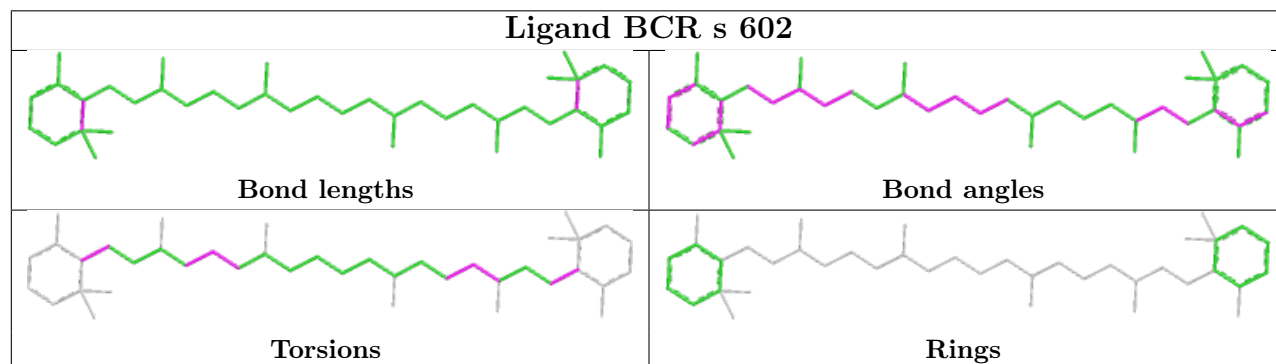
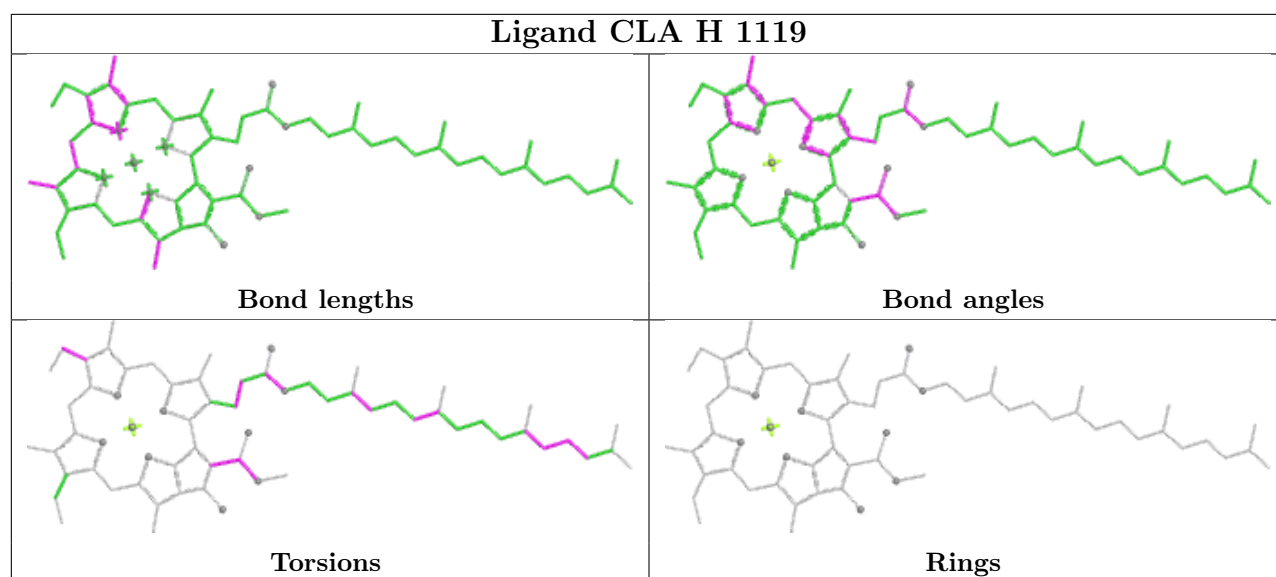
Bond angles



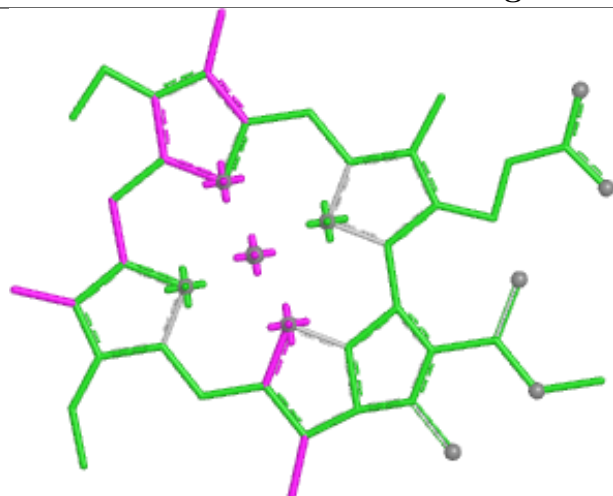
Torsions



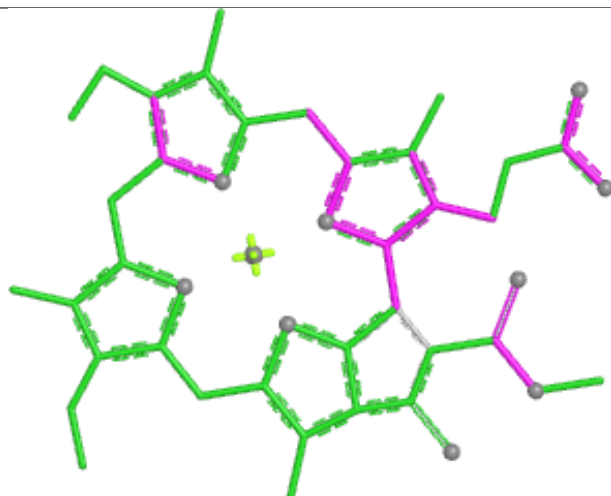
Rings



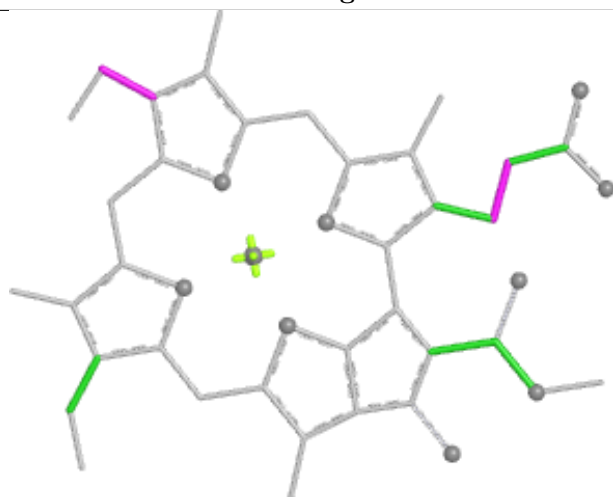
Ligand CLA K 1401



Bond lengths



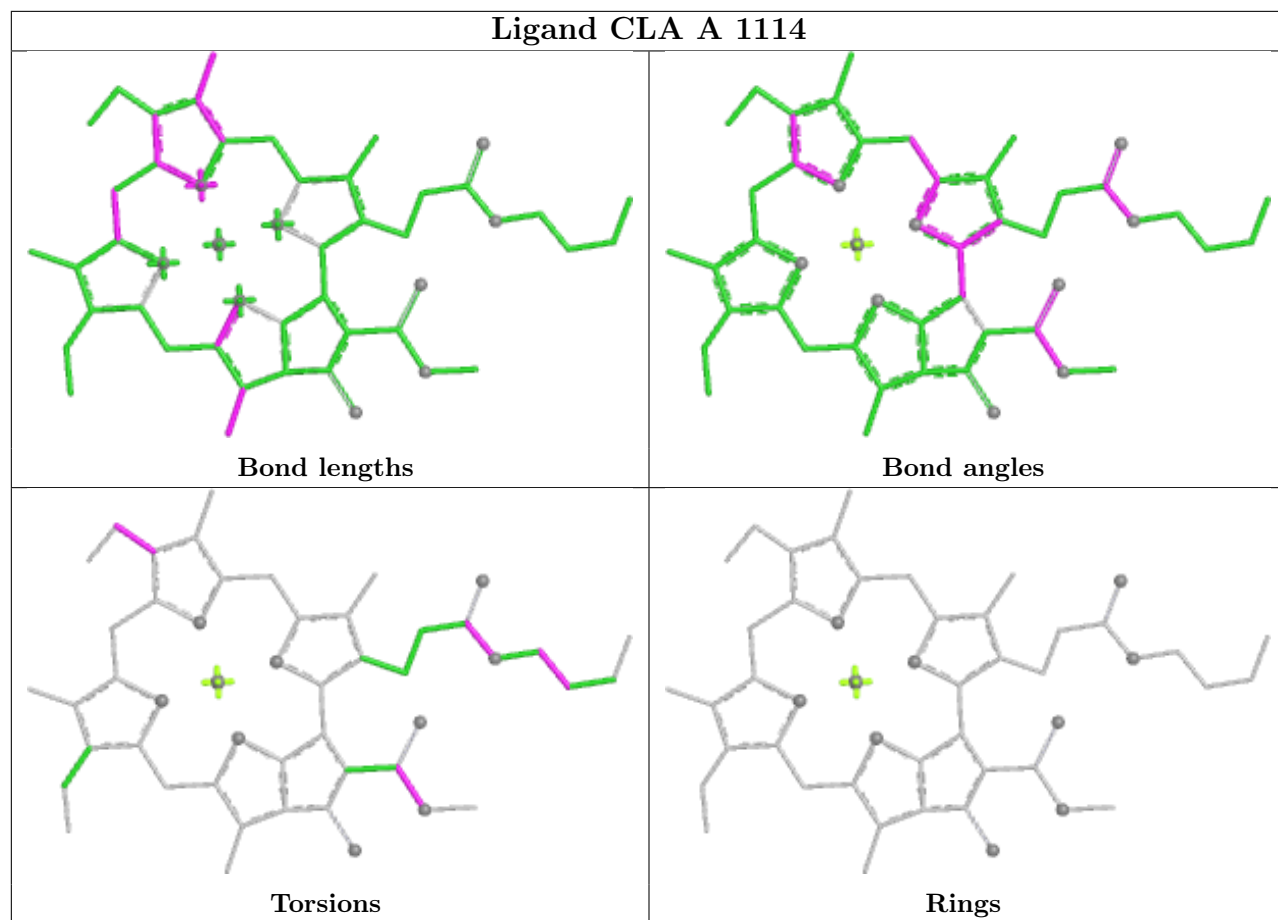
Bond angles



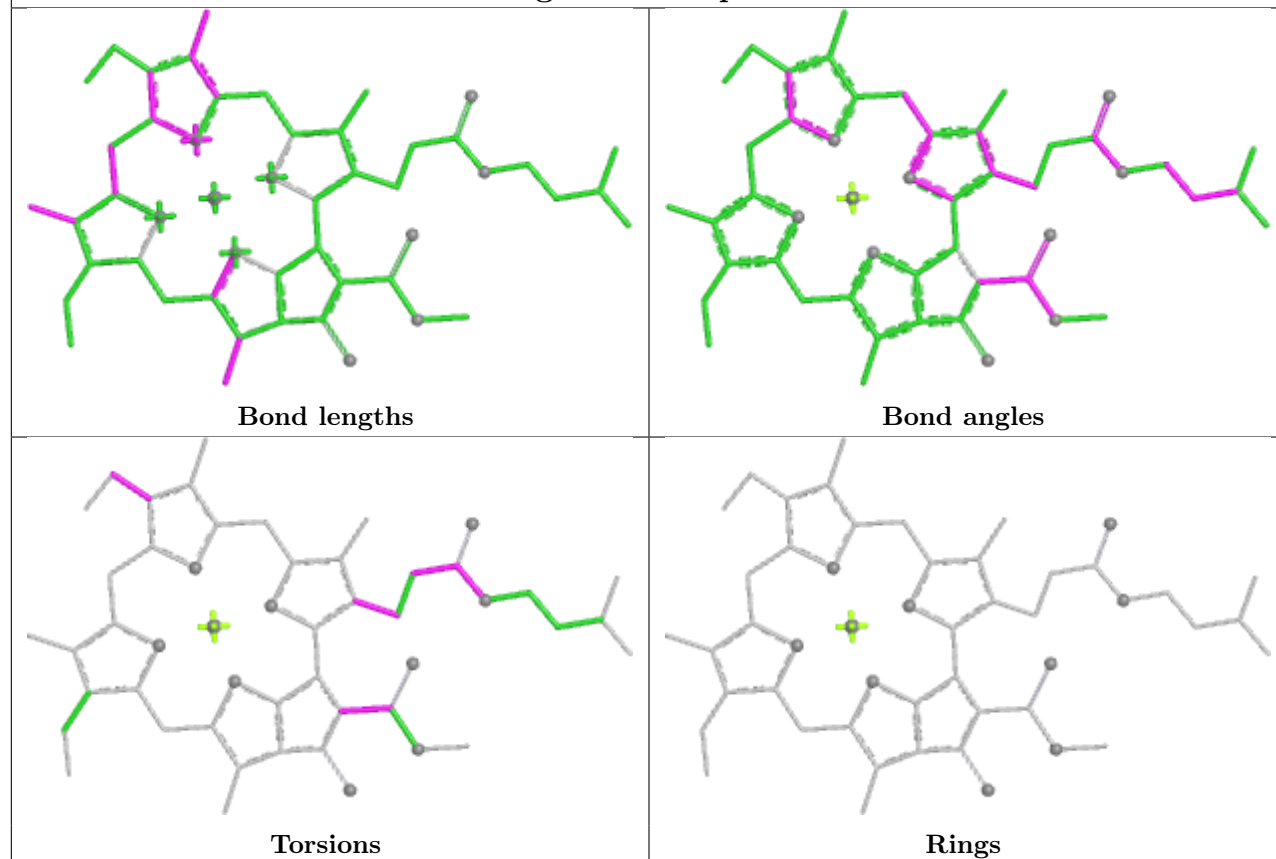
Torsions



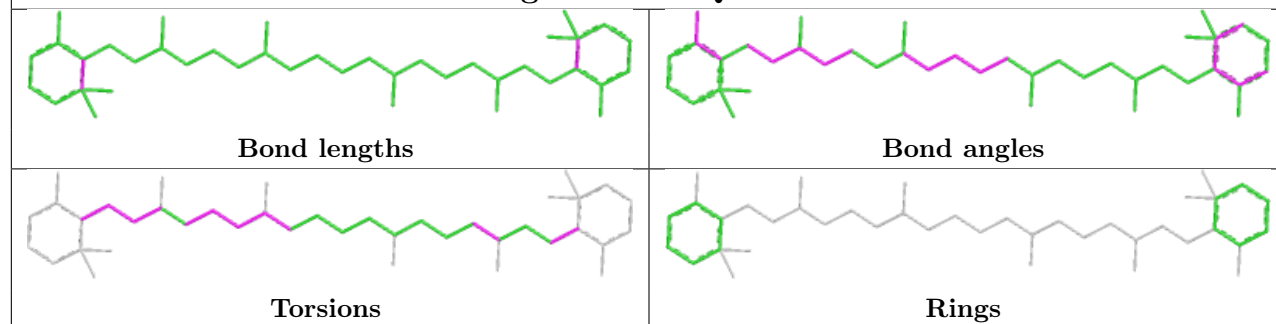
Rings

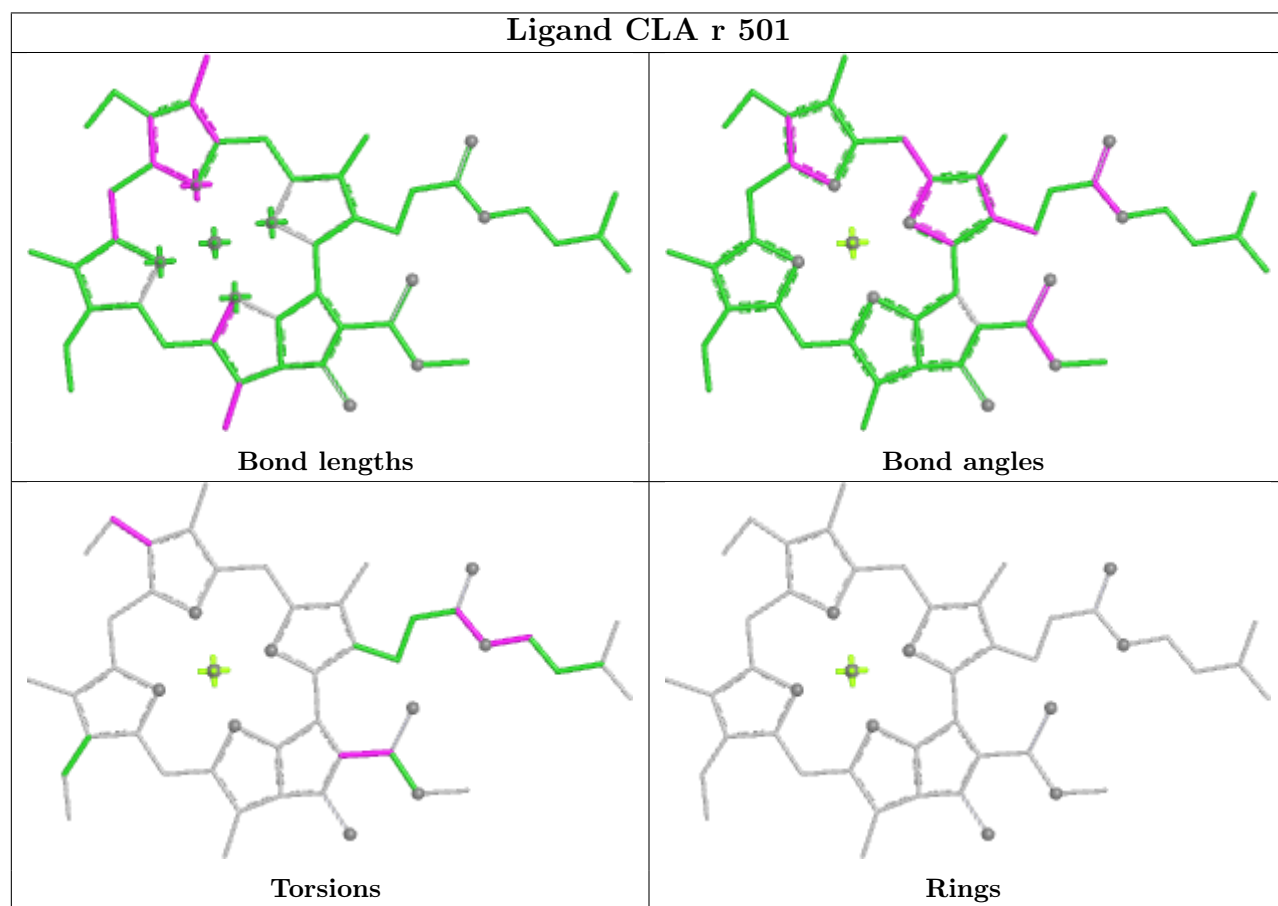
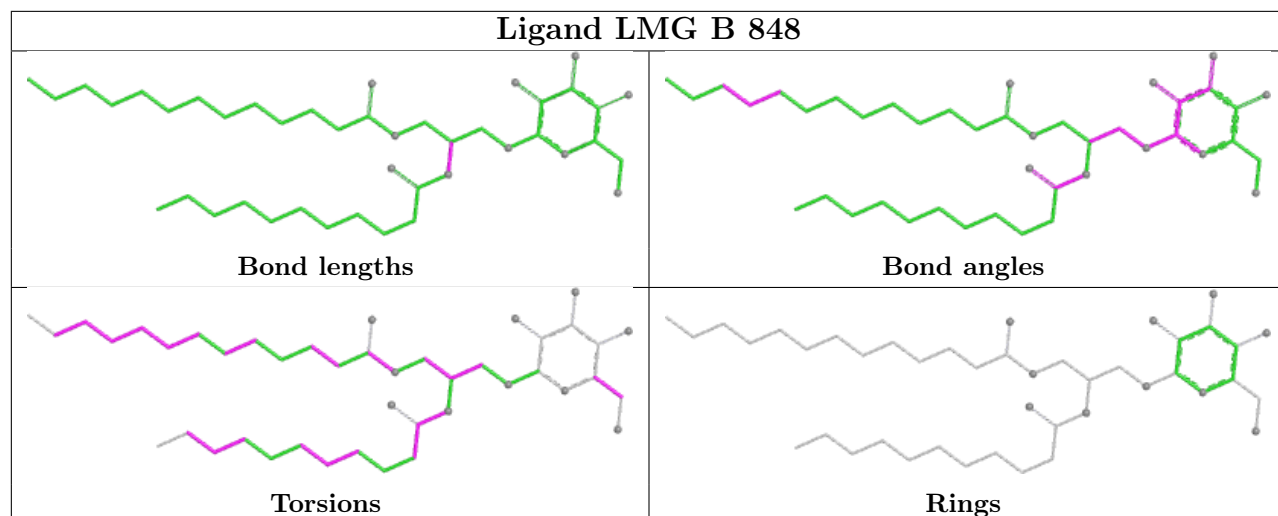


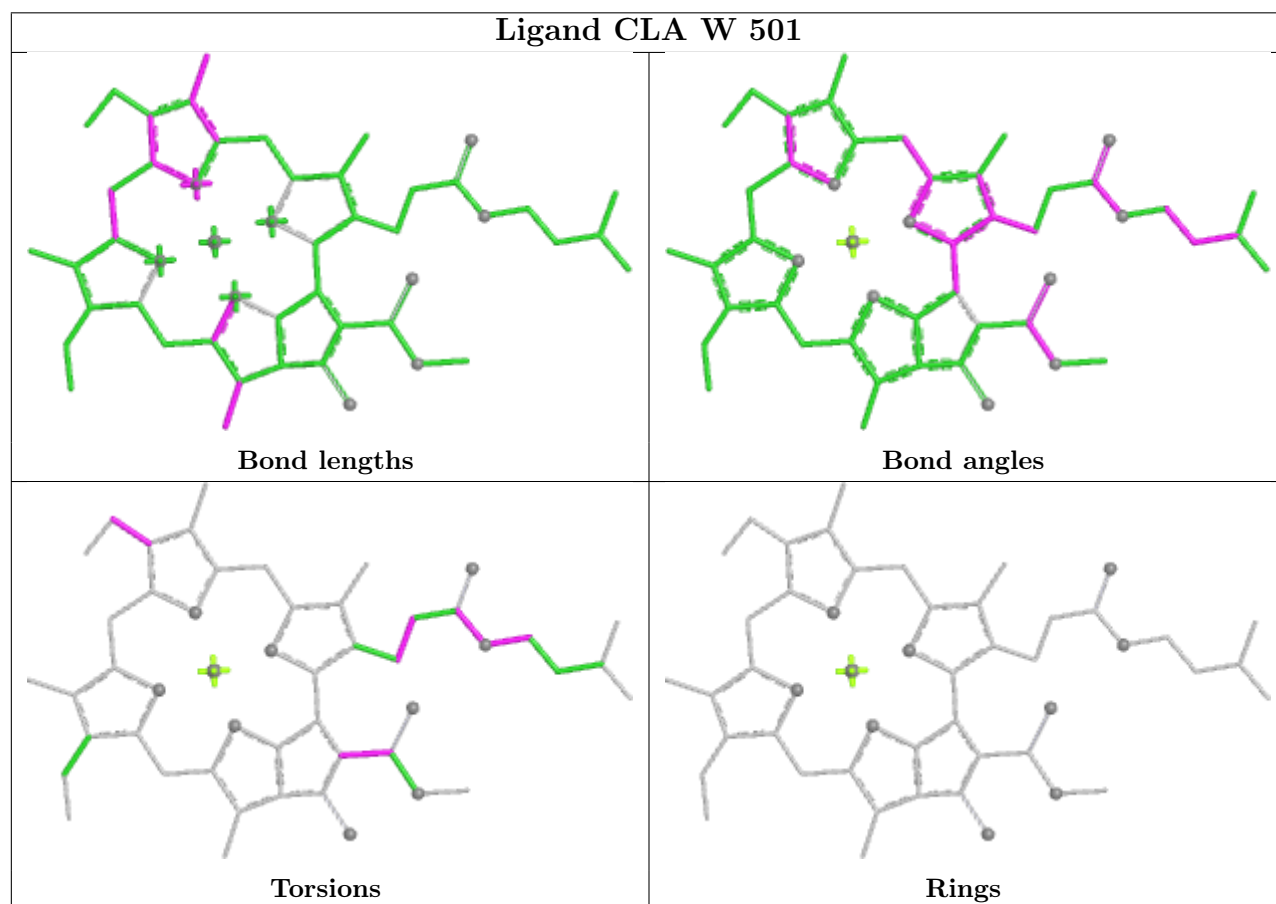
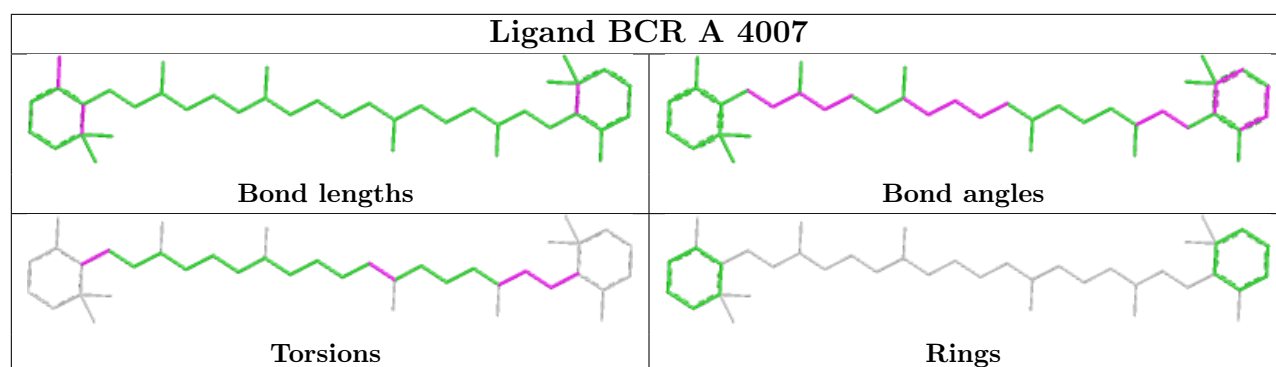
Ligand CLA q 502

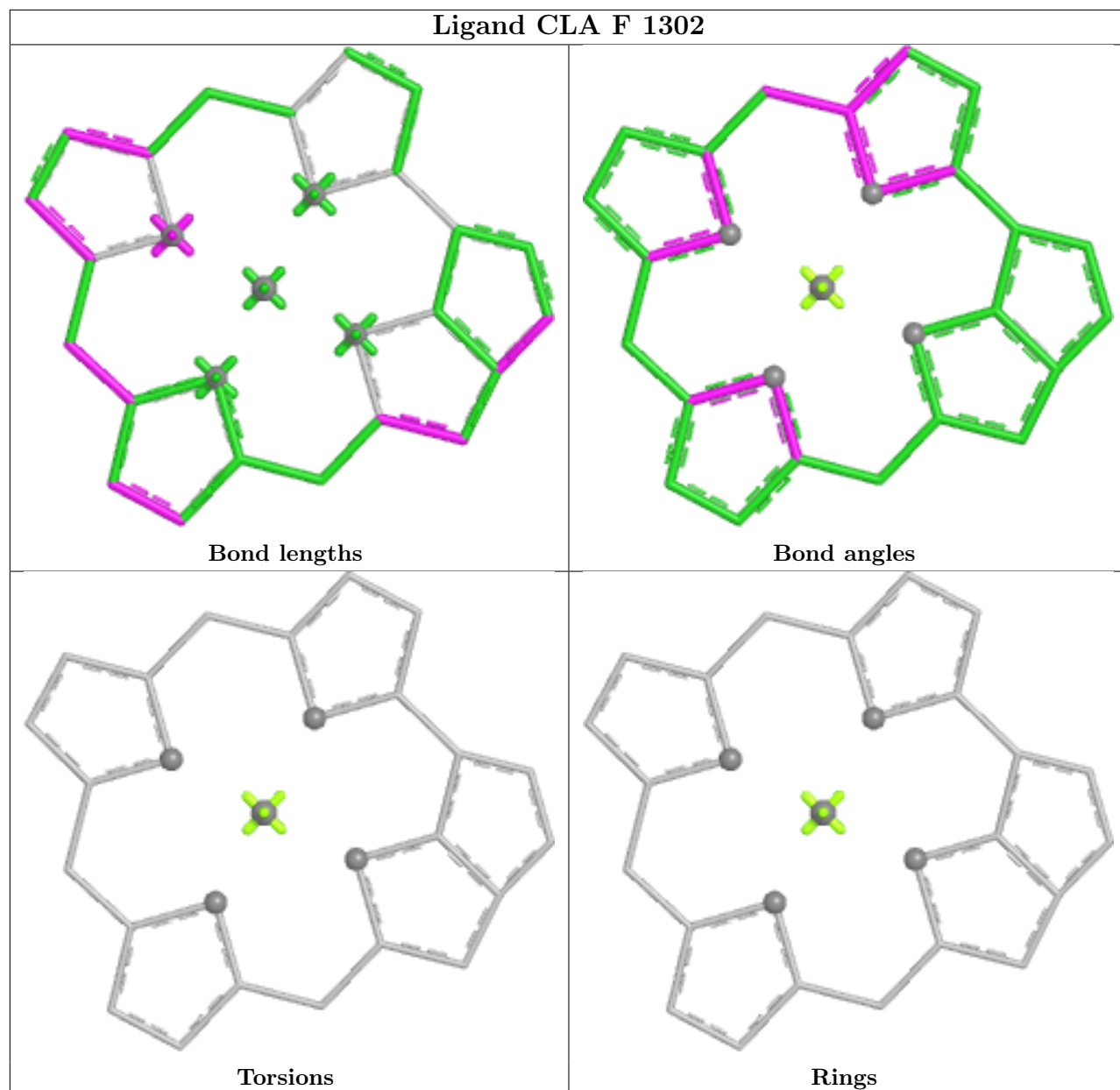


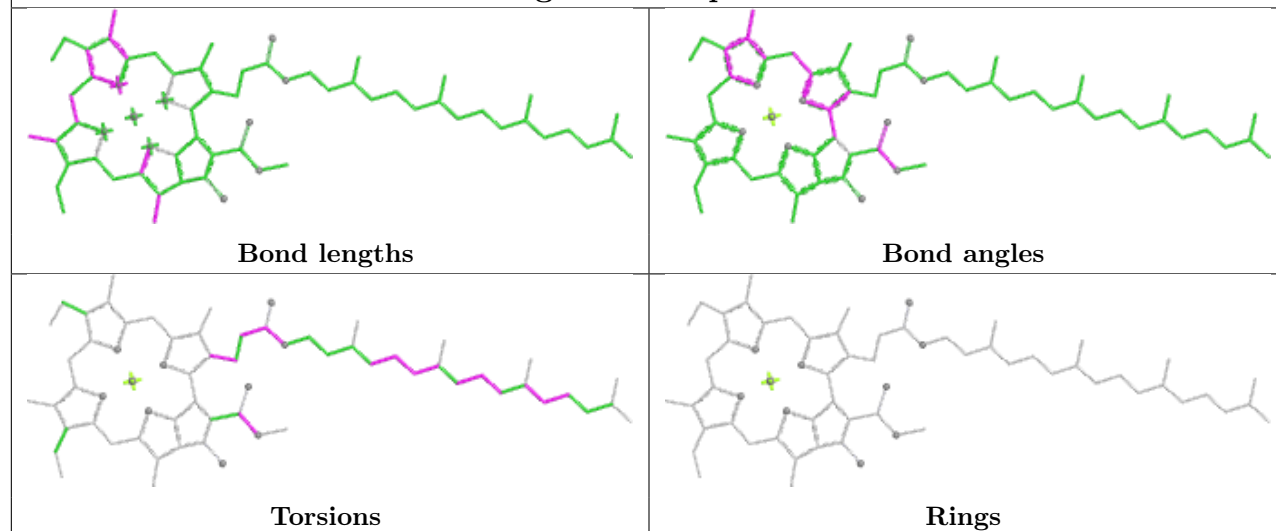
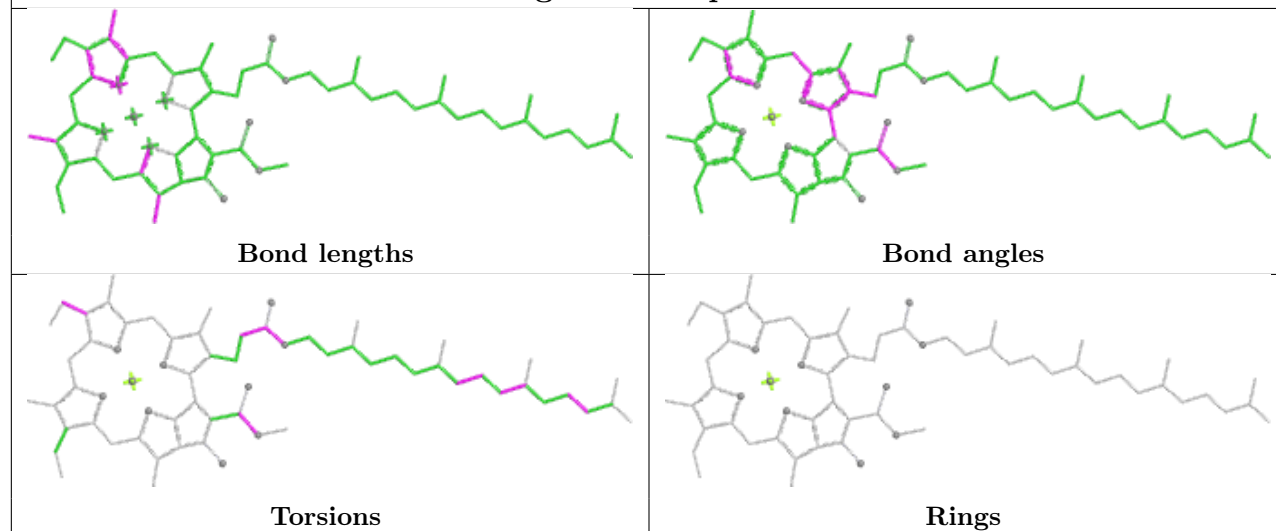
Ligand BCR Q 4016

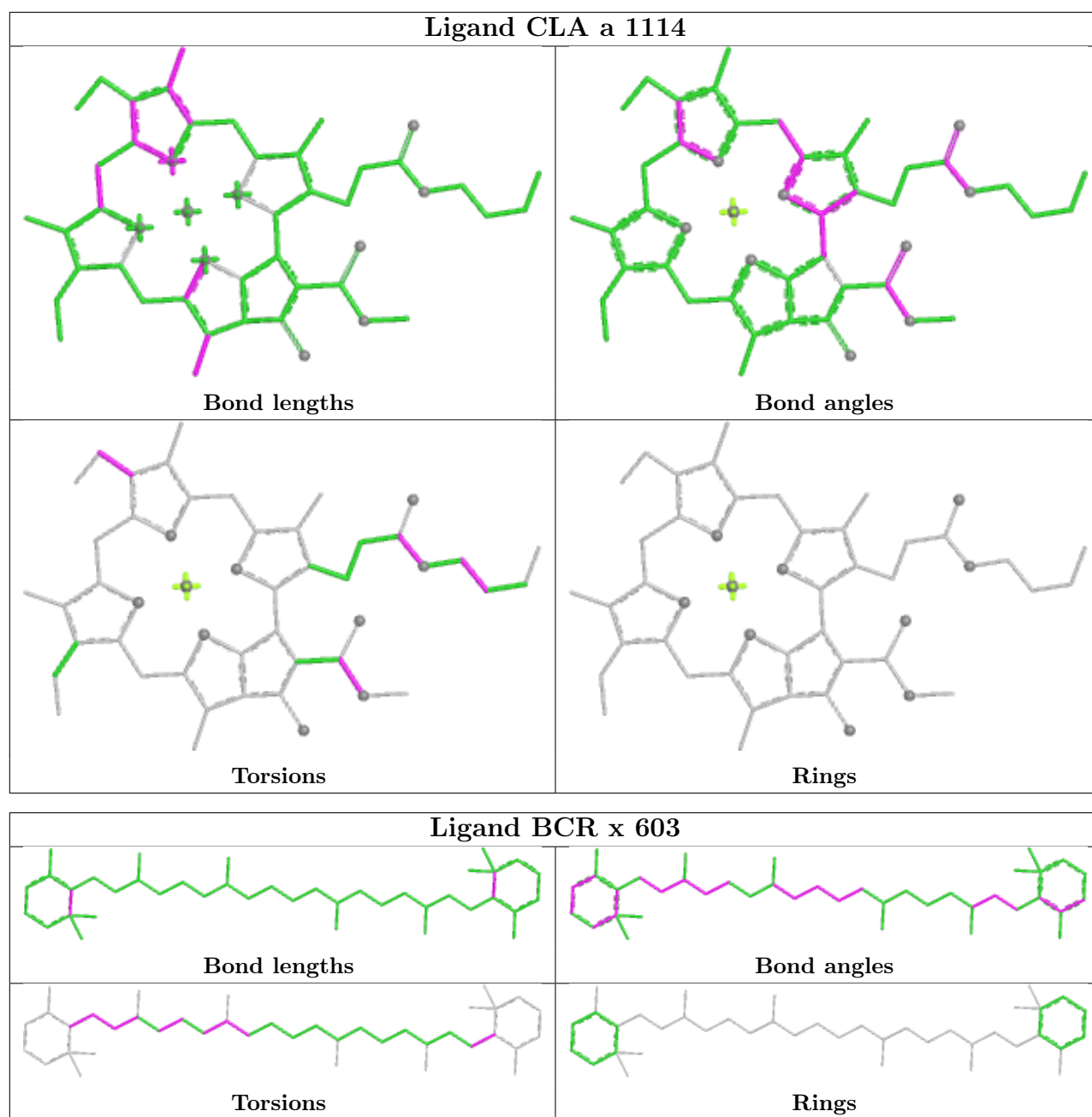


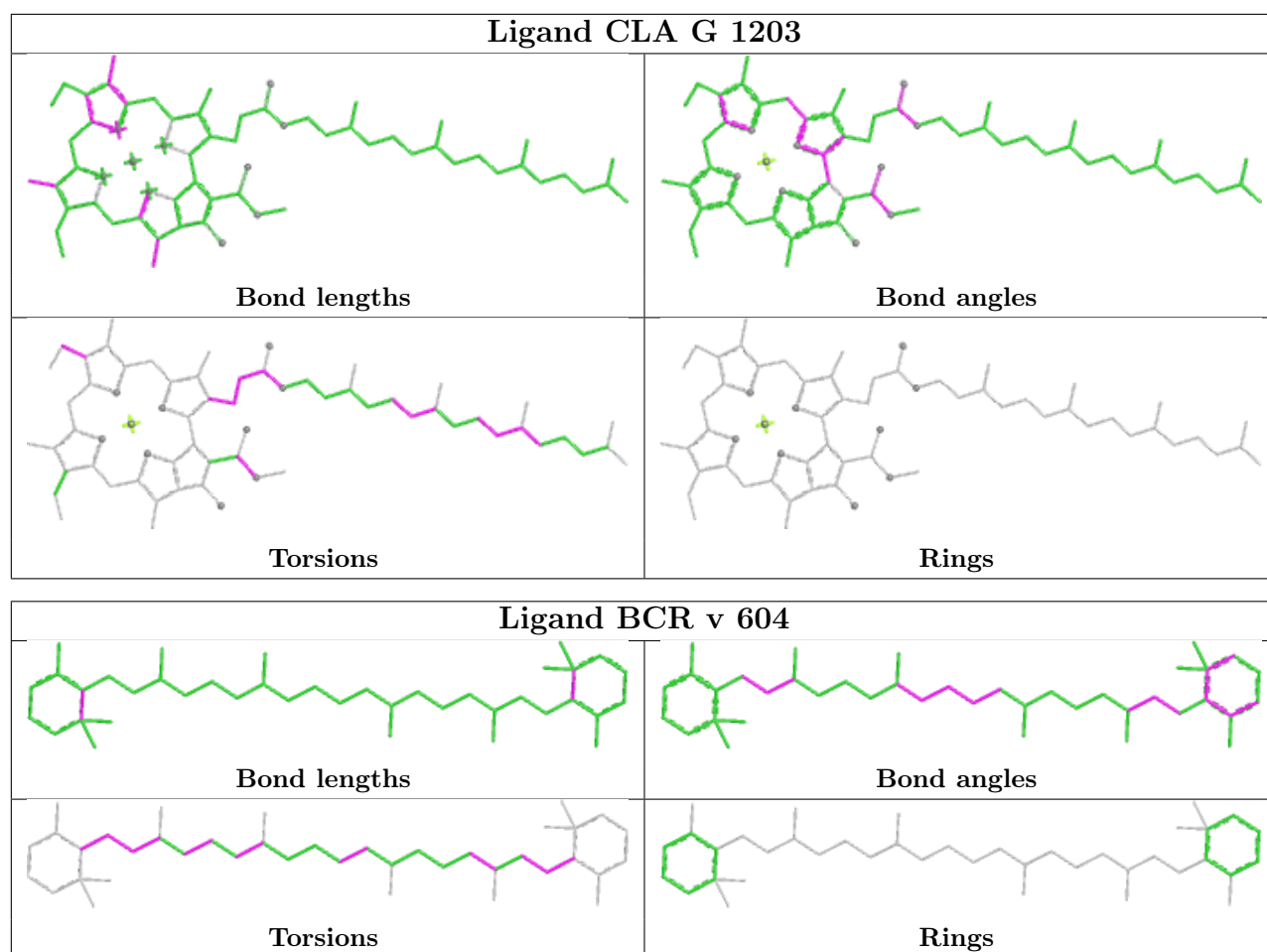




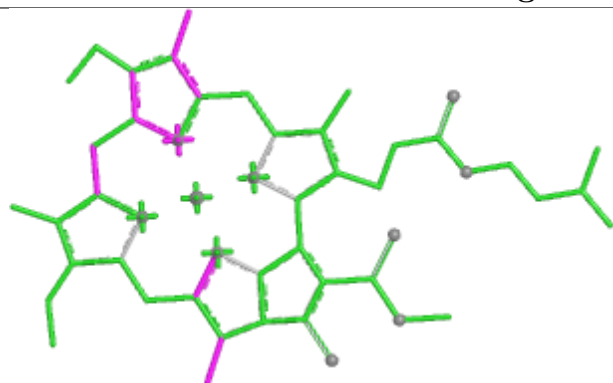


Ligand CLA p 511**Ligand CLA p 510**

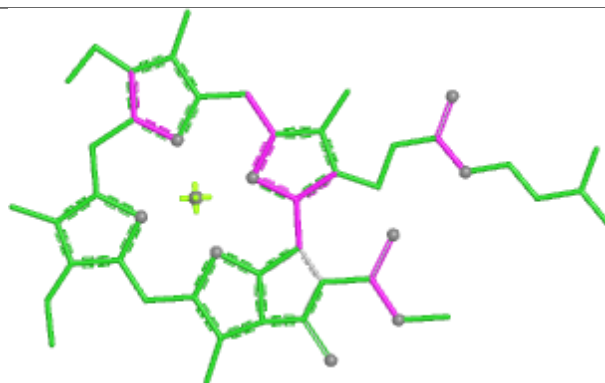




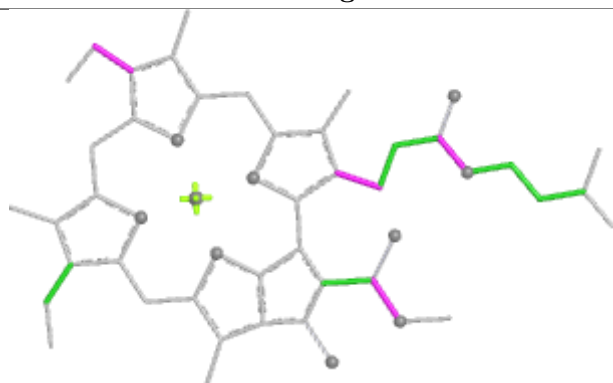
Ligand CLA x 513



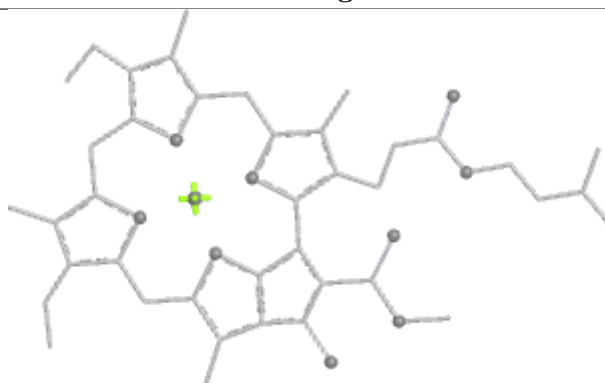
Bond lengths



Bond angles

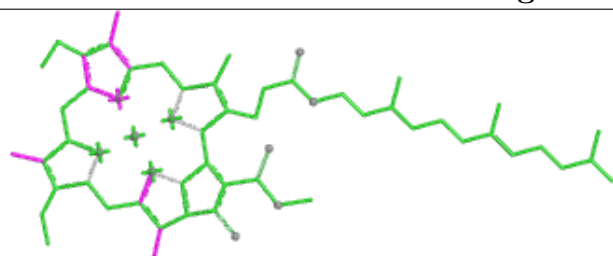


Torsions

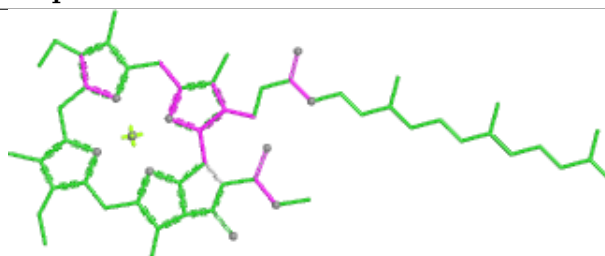


Rings

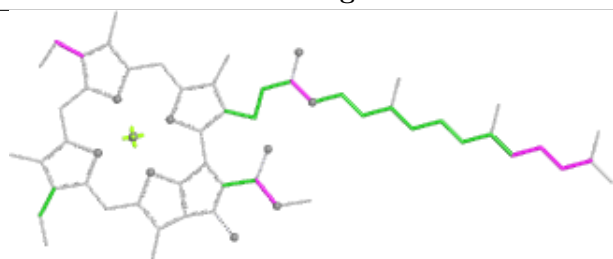
Ligand CLA p 506



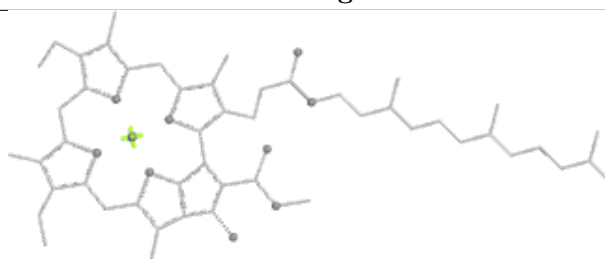
Bond lengths



Bond angles

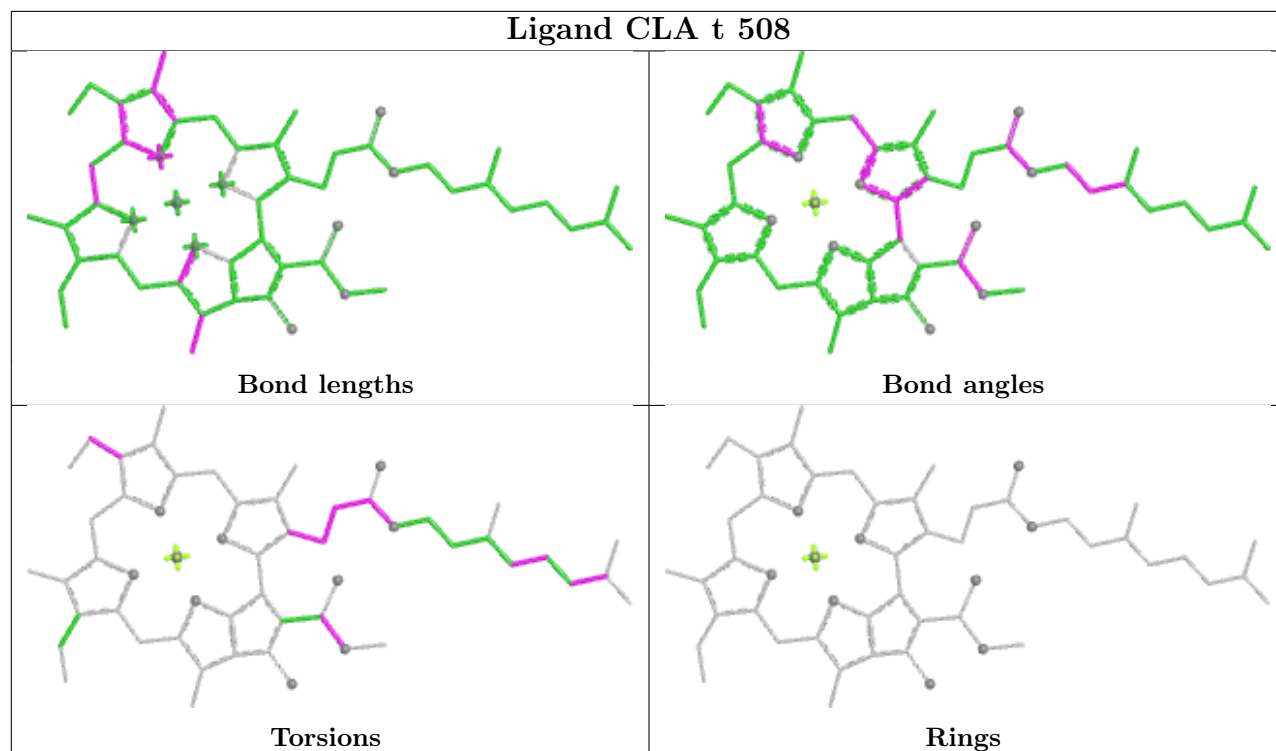


Torsions

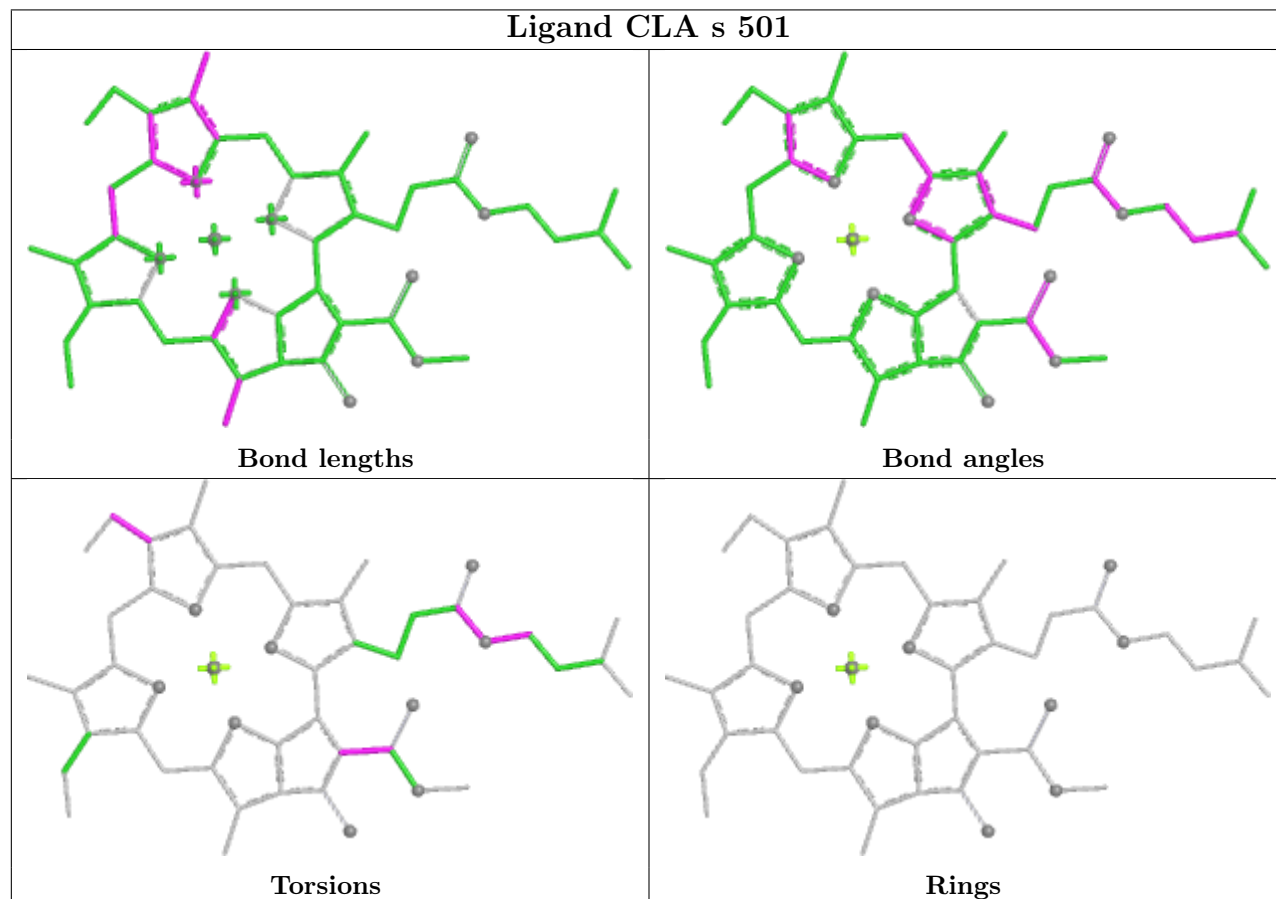


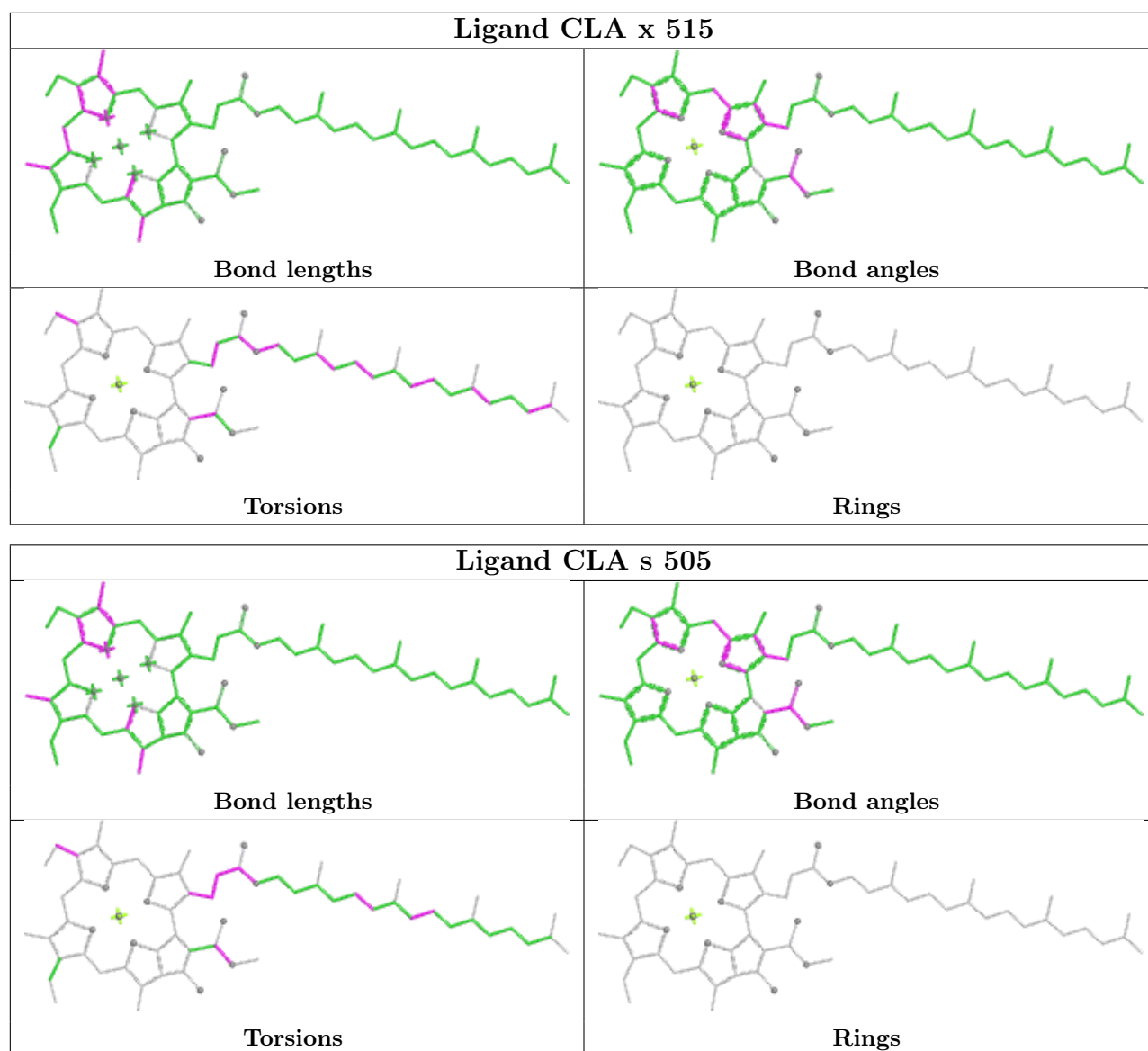
Rings

Ligand CLA t 508

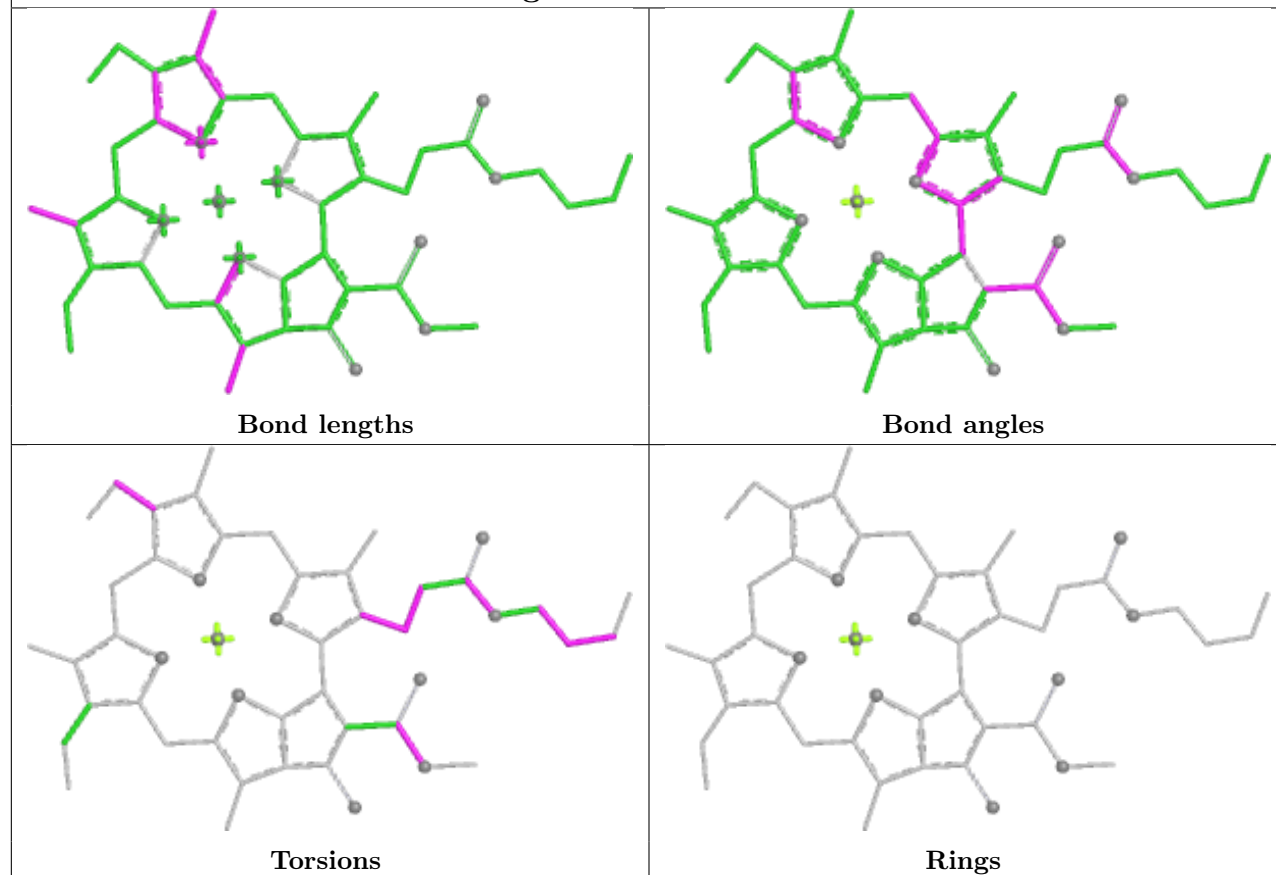


Ligand CLA s 501

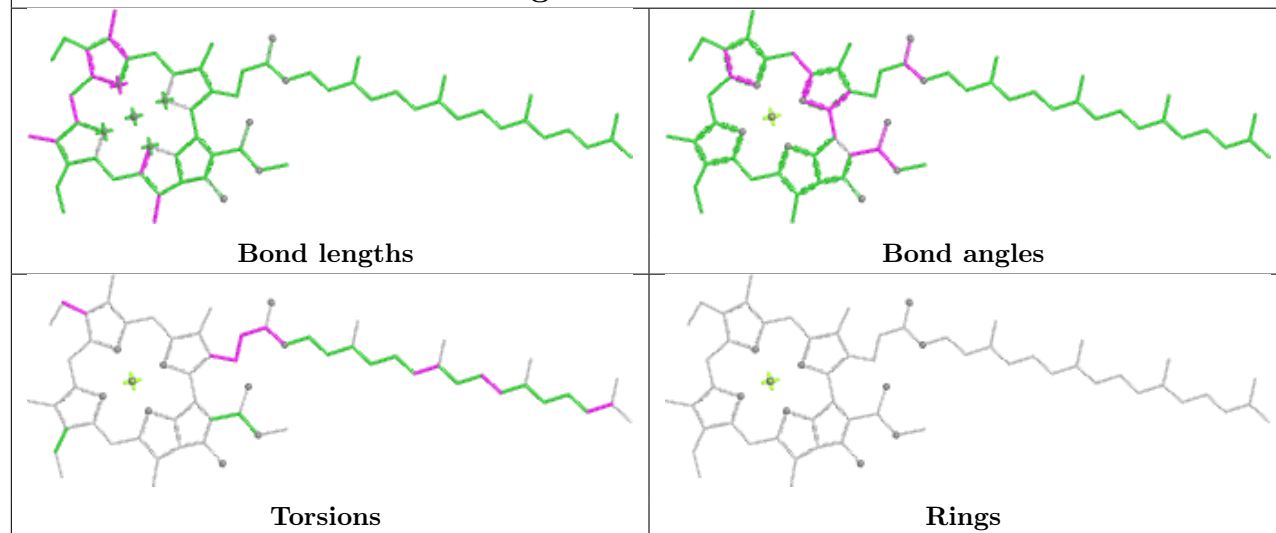




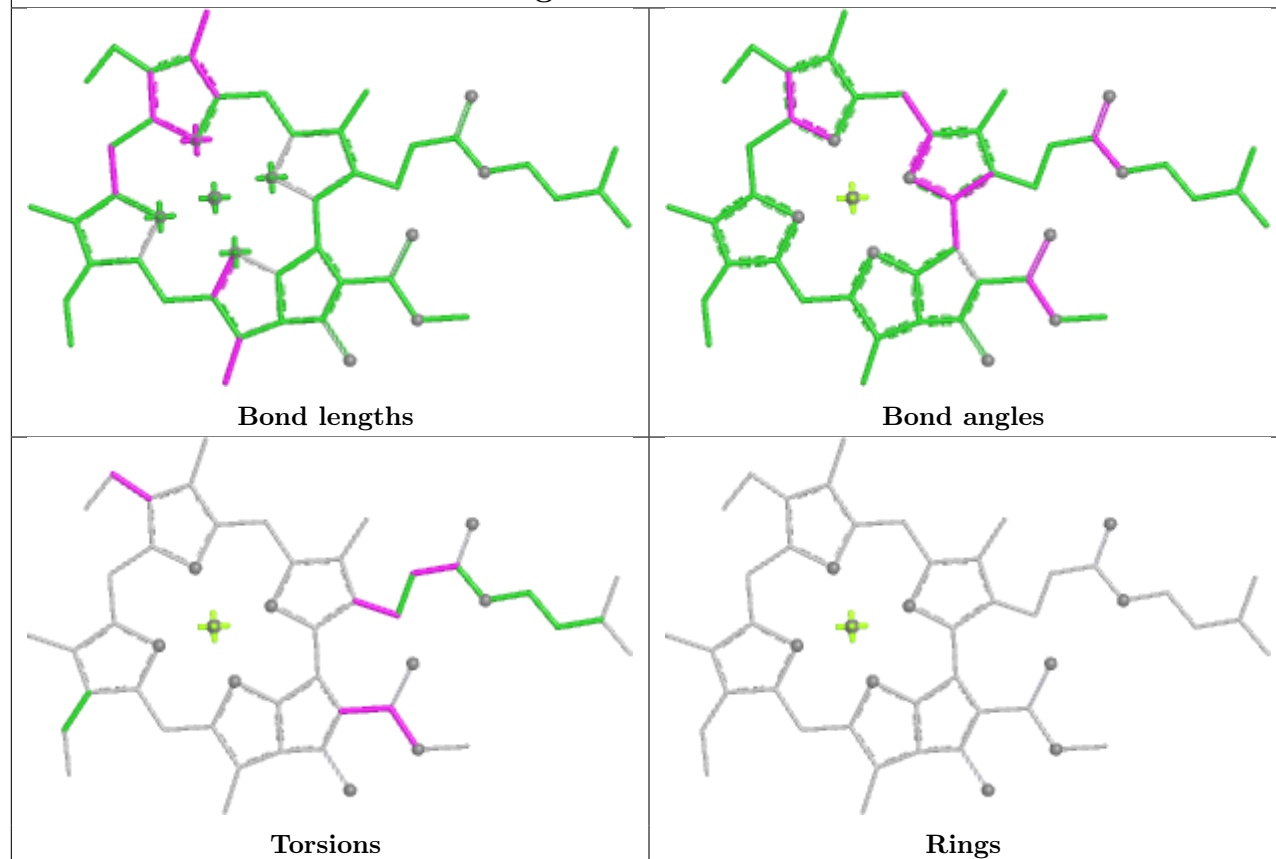
Ligand CLA A 1120



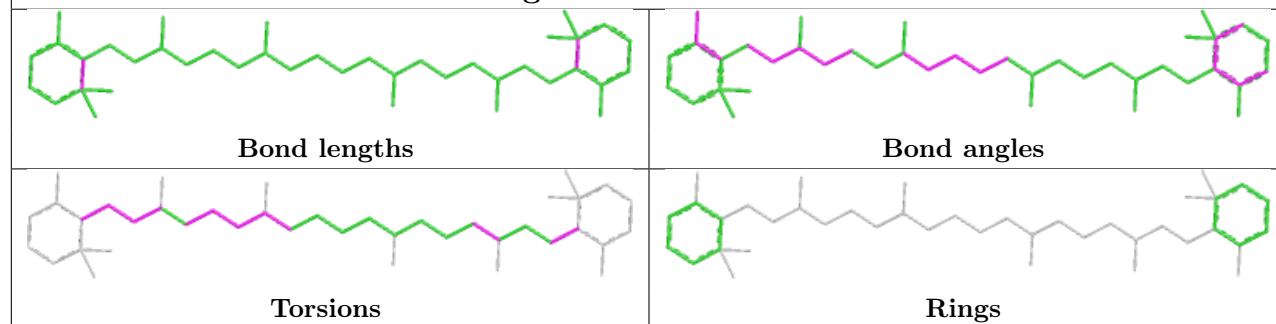
Ligand CLA 1 1502



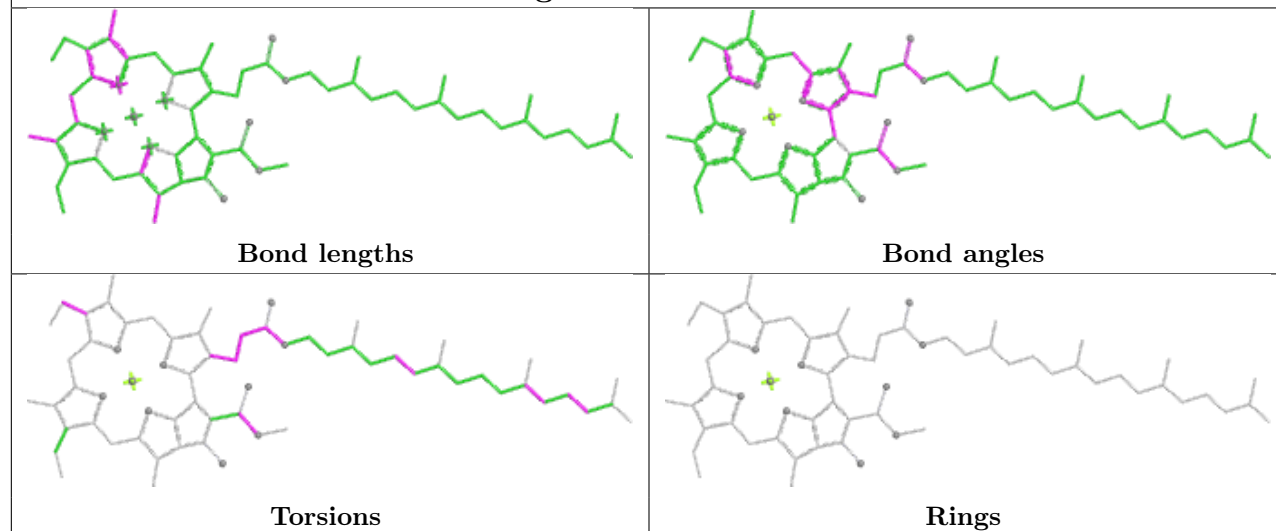
Ligand CLA u 514



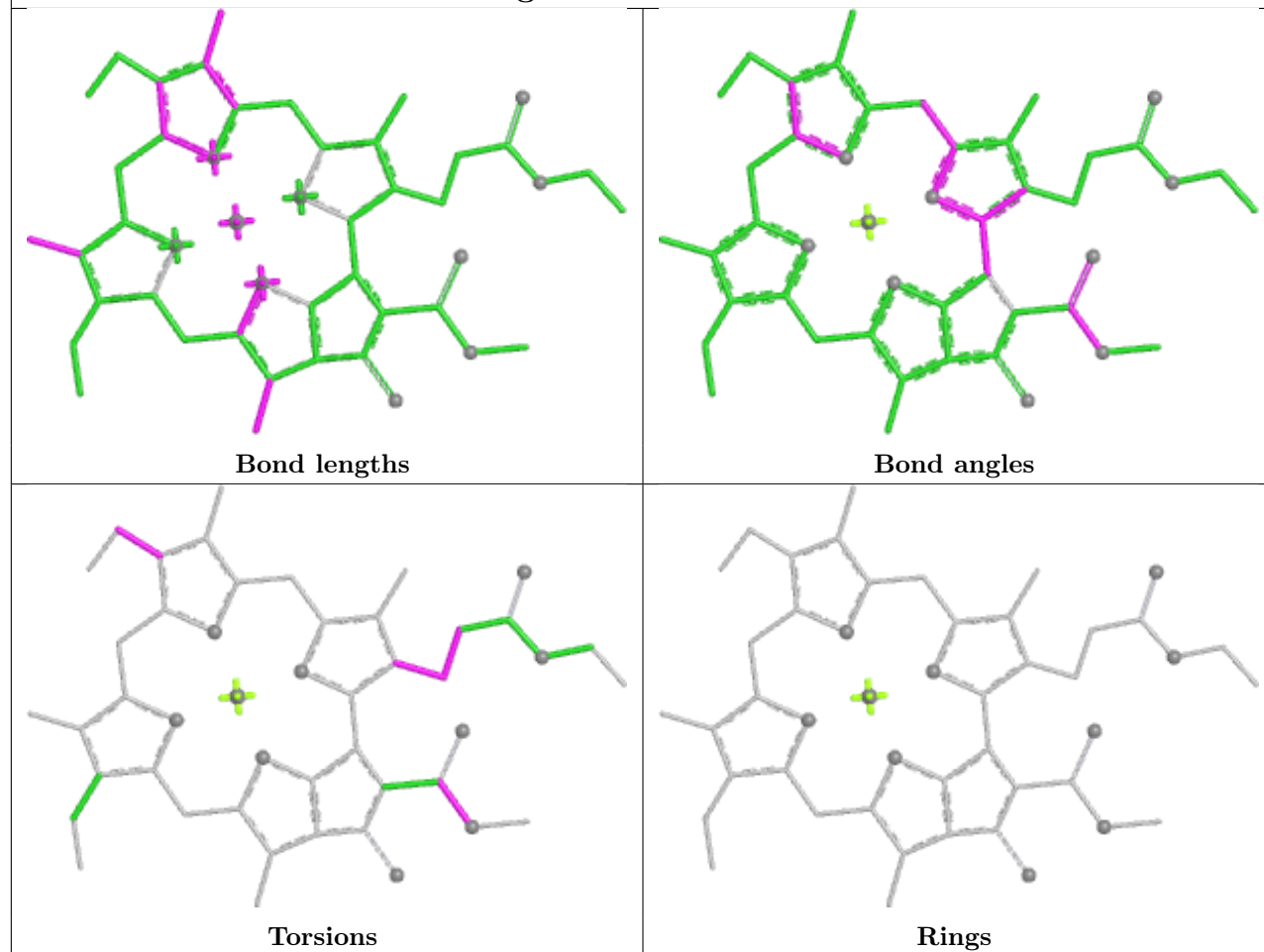
Ligand BCR F 4016

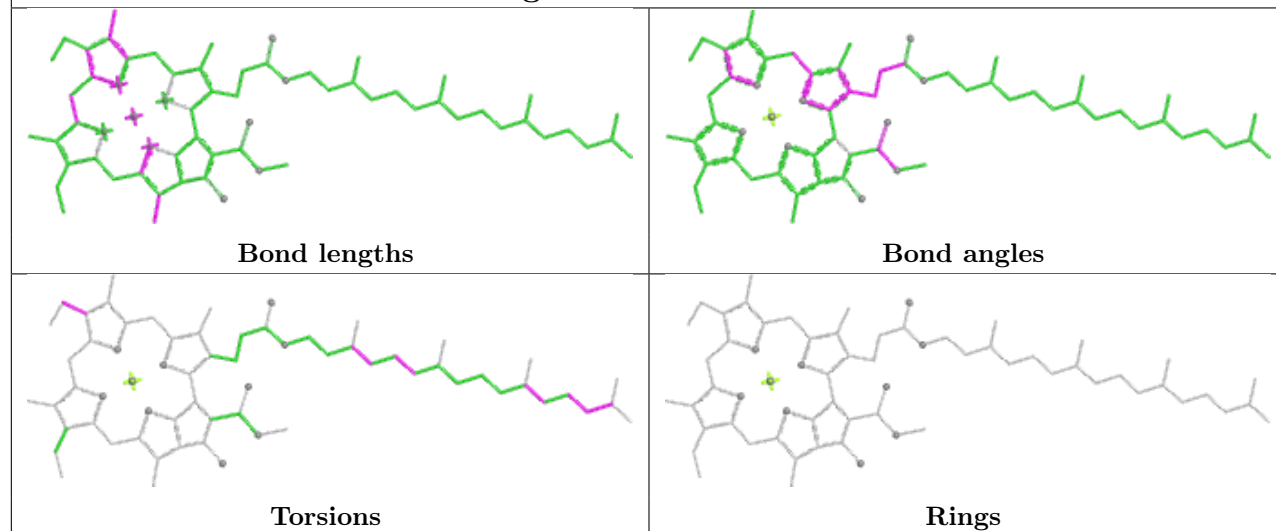
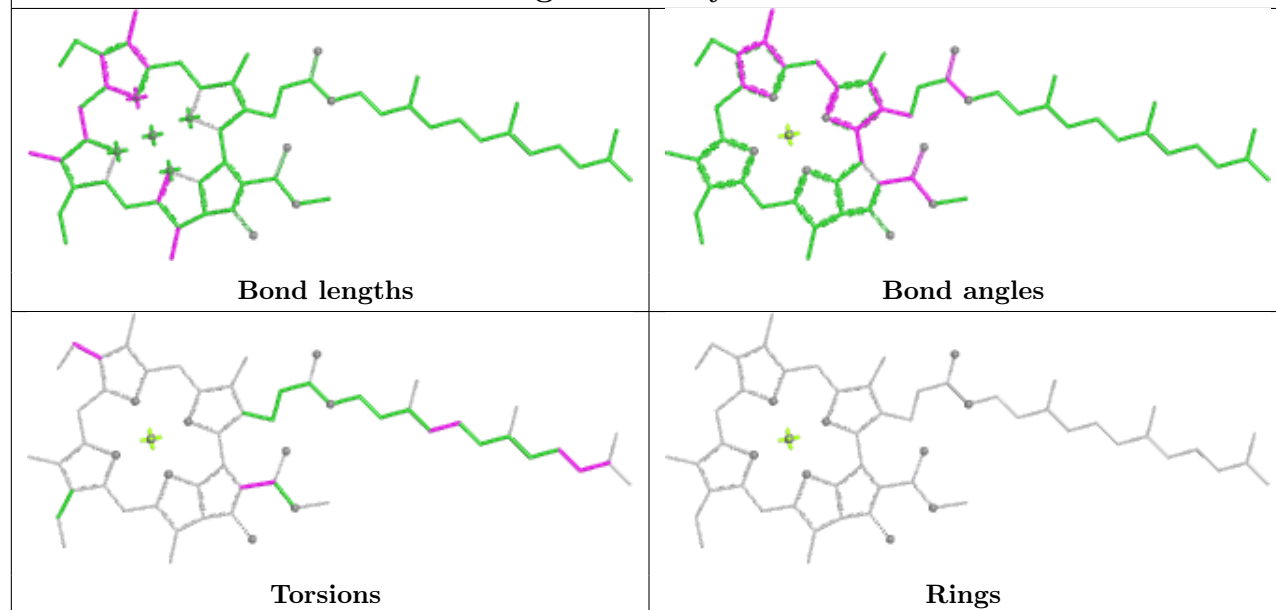


Ligand CLA u 505

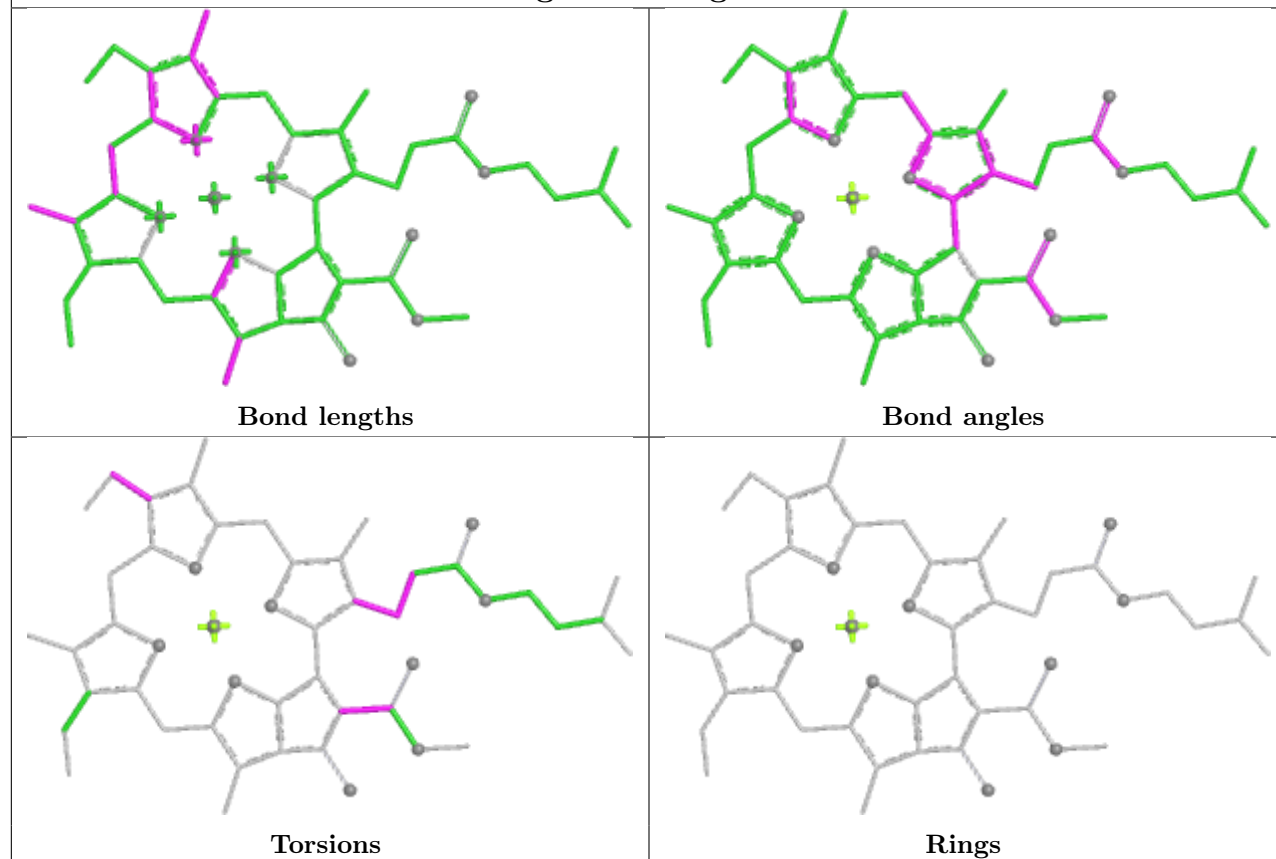


Ligand CLA G 1216

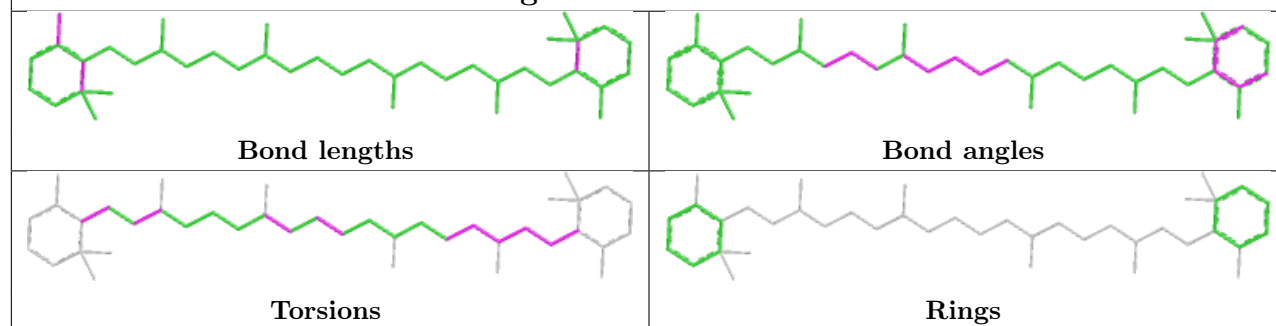


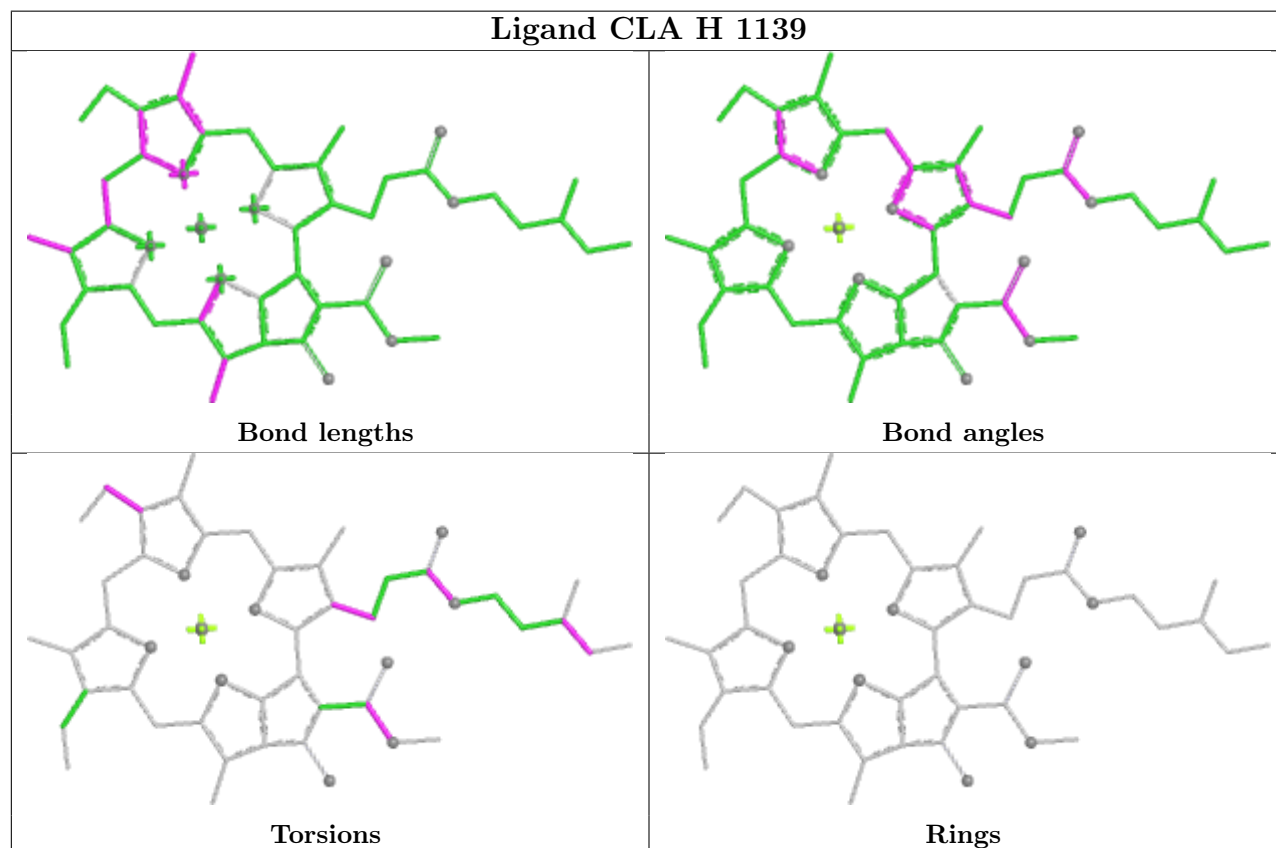
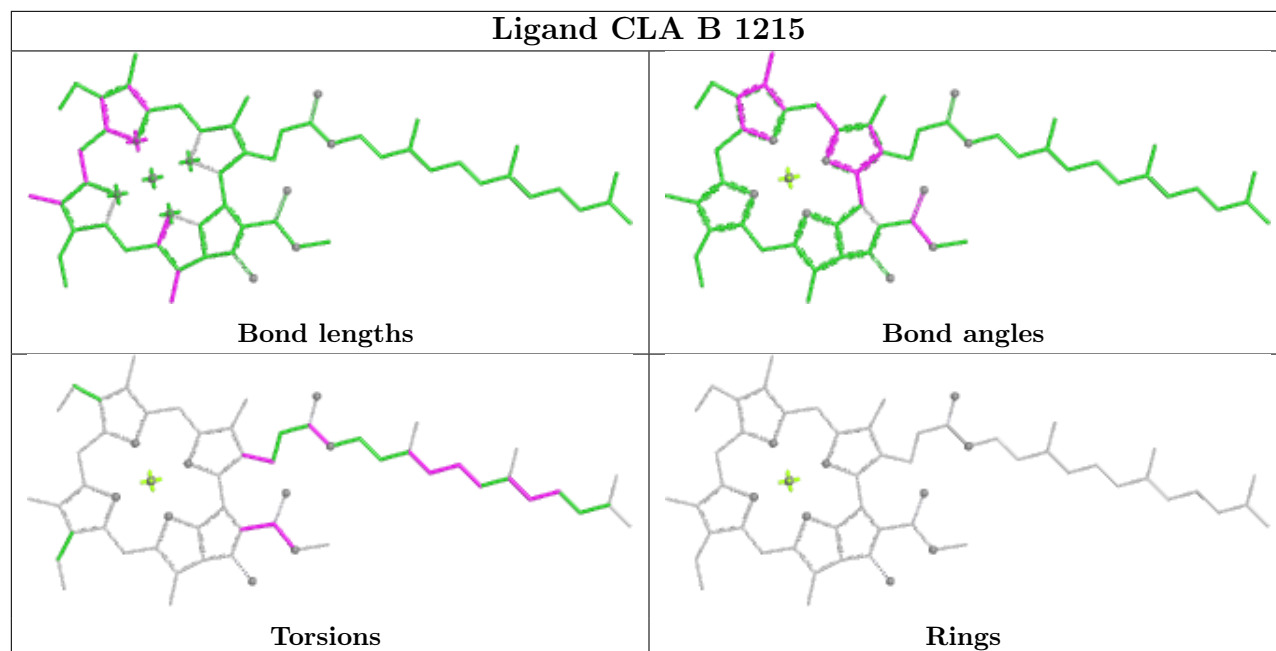
Ligand CLA A 1124**Ligand CLA y 509**

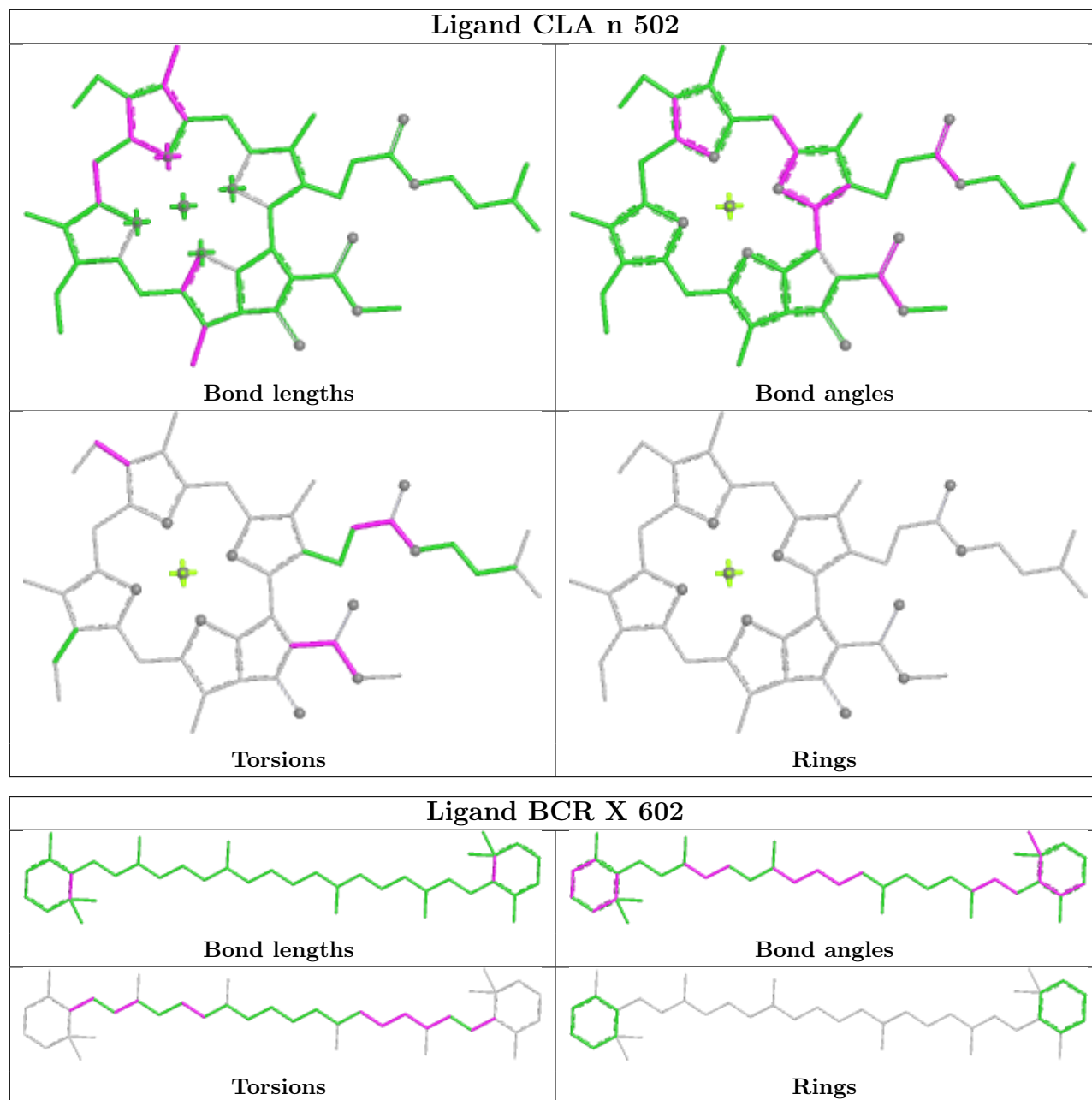
Ligand CLA g 502

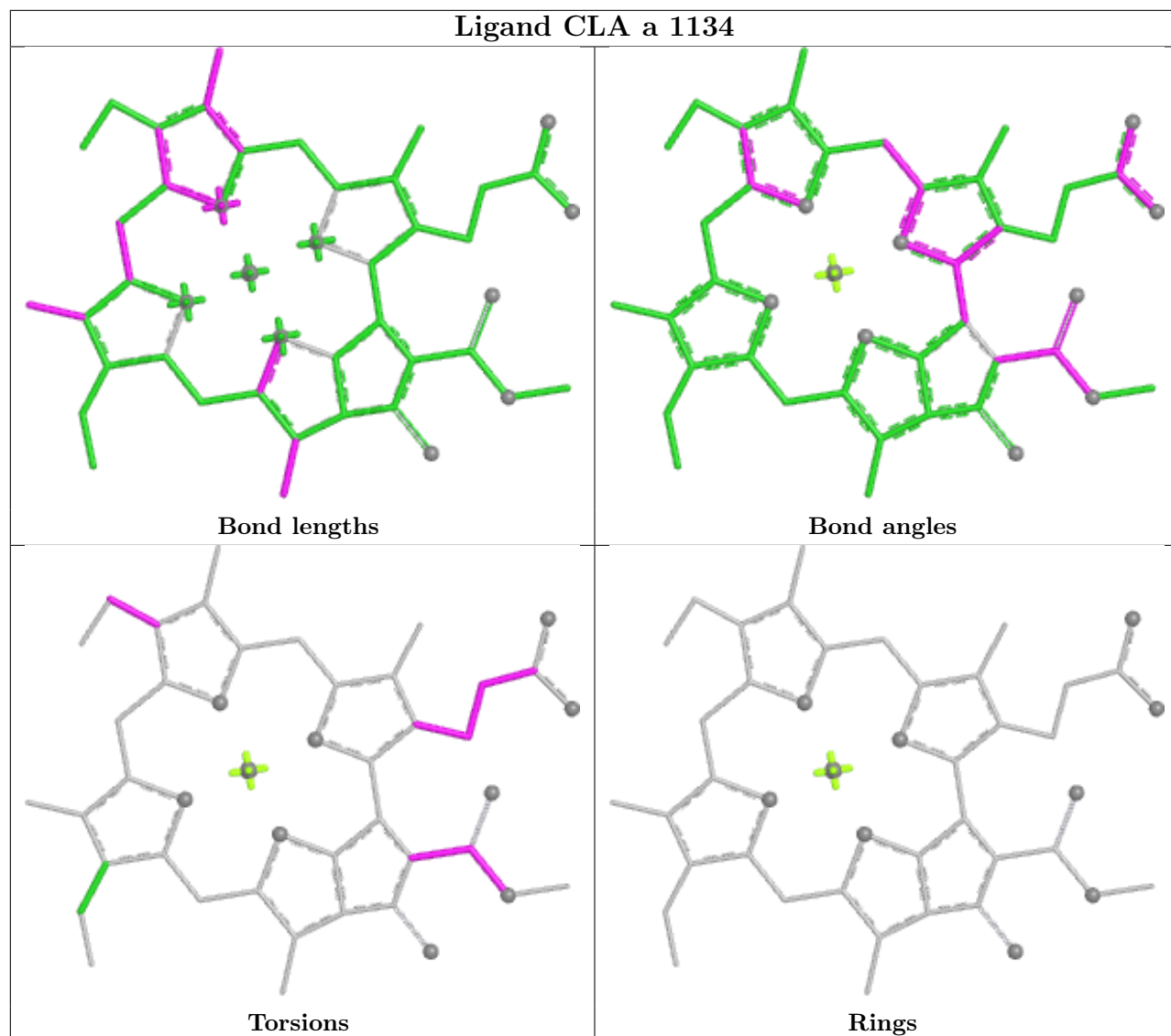


Ligand BCR G 4014

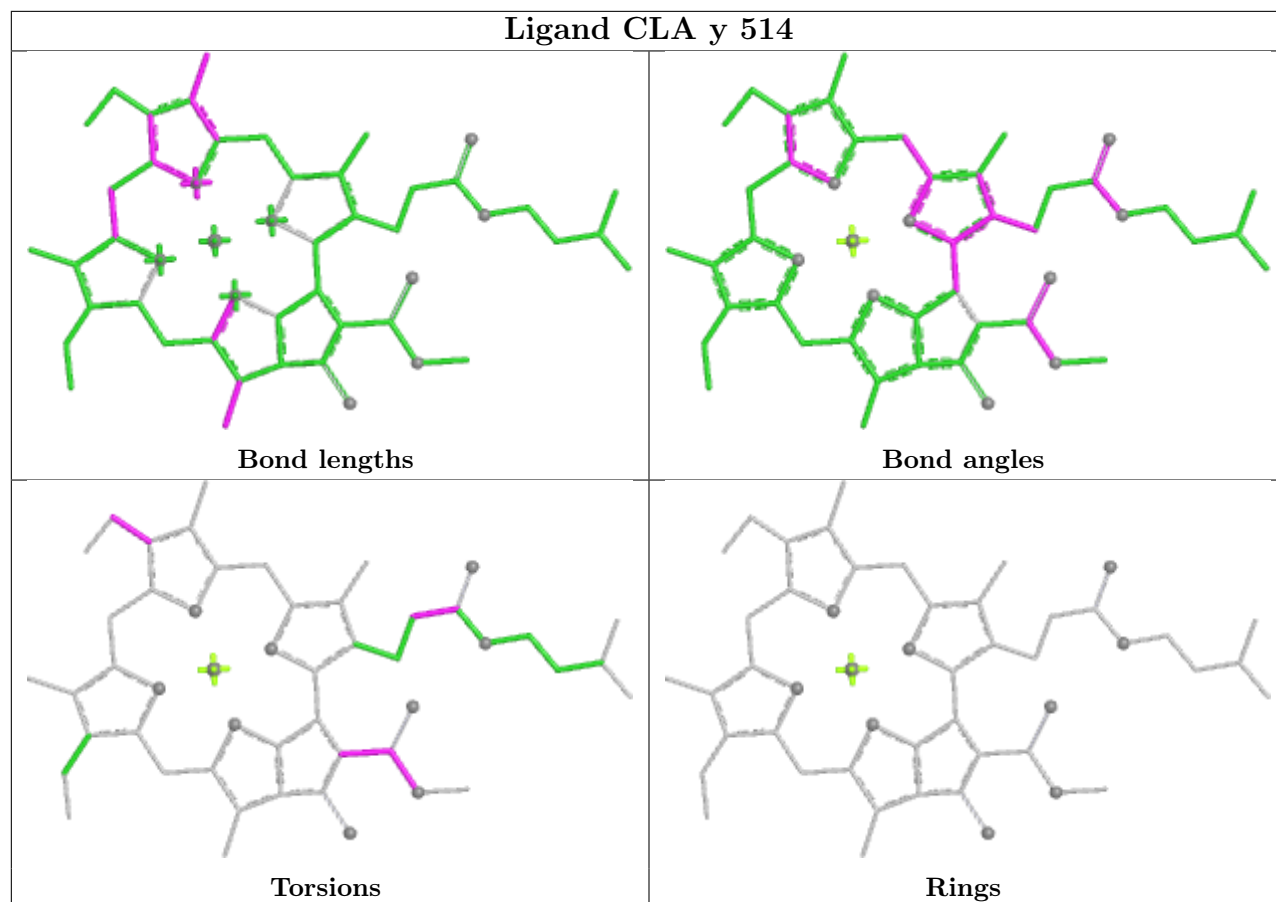




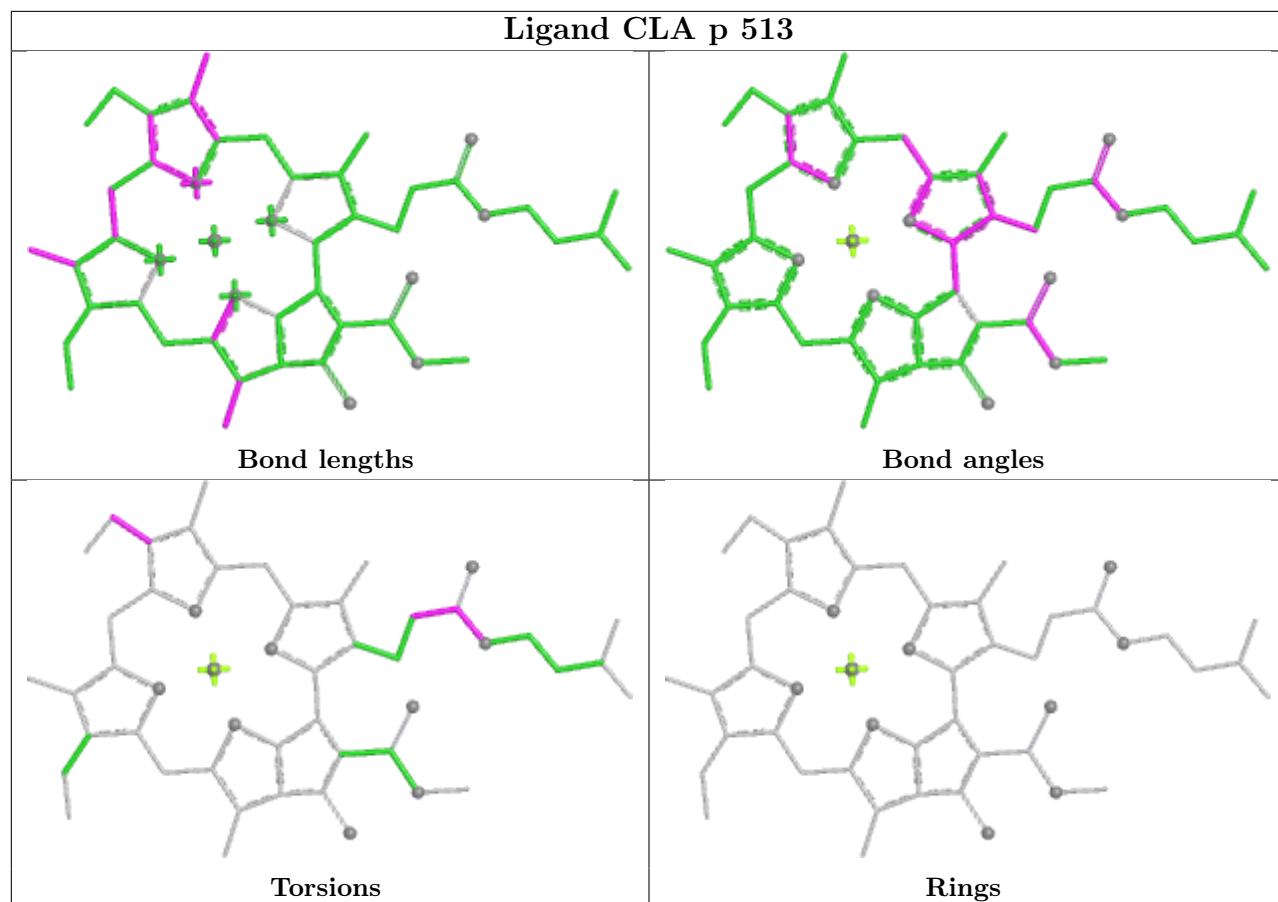




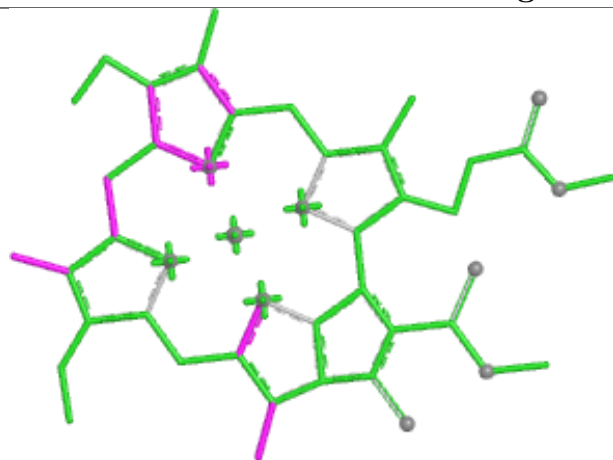
Ligand CLA y 514



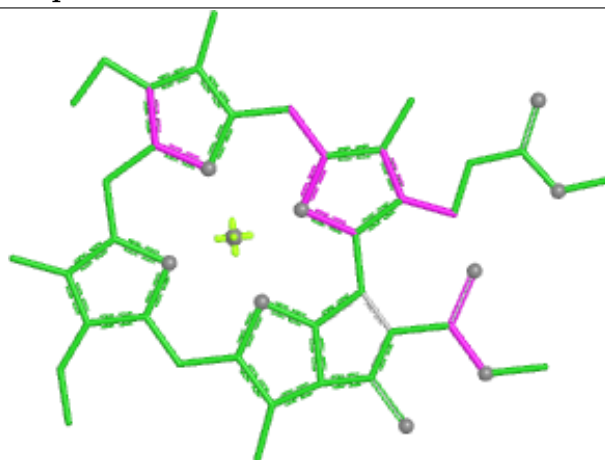
Ligand CLA p 513



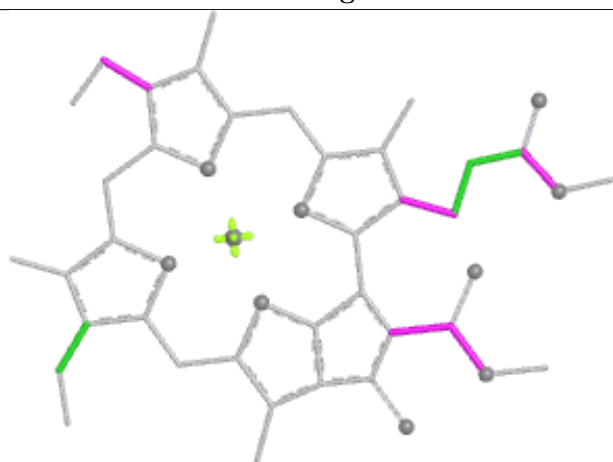
Ligand CLA p 503



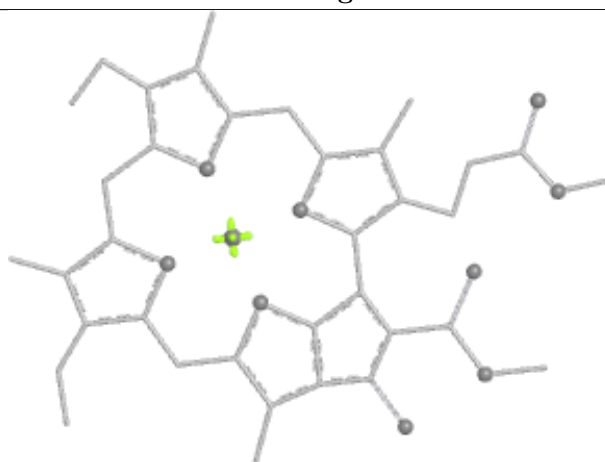
Bond lengths



Bond angles

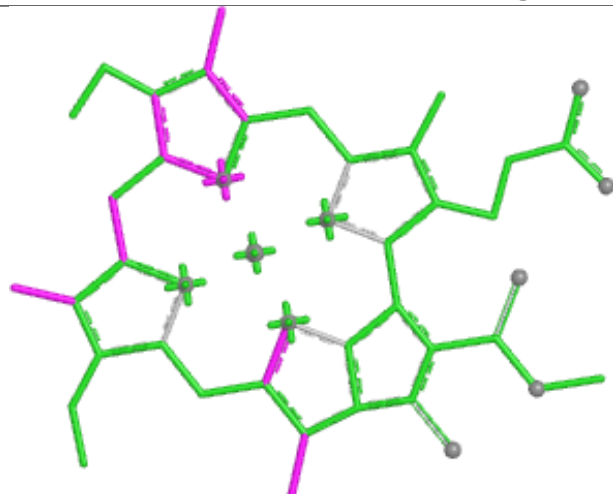


Torsions

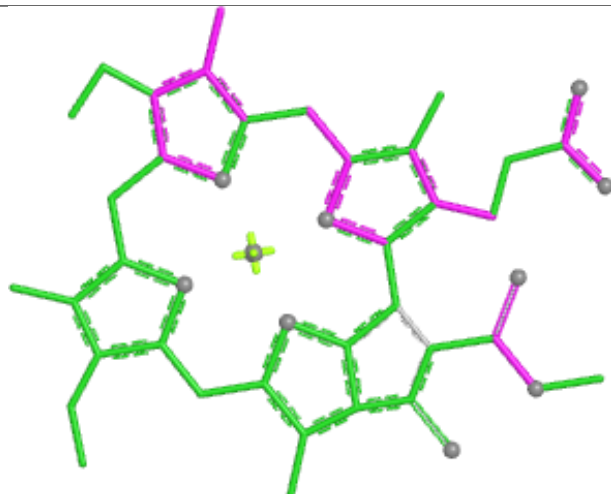


Rings

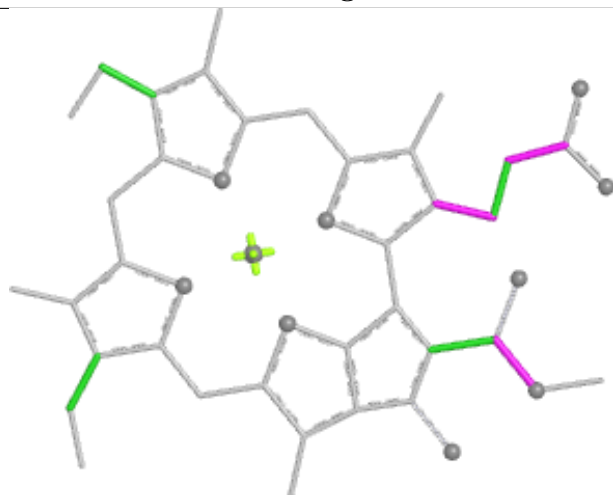
Ligand CLA w 512



Bond lengths



Bond angles

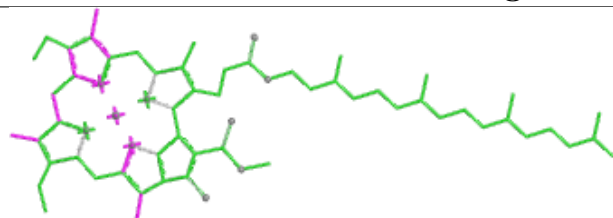


Torsions

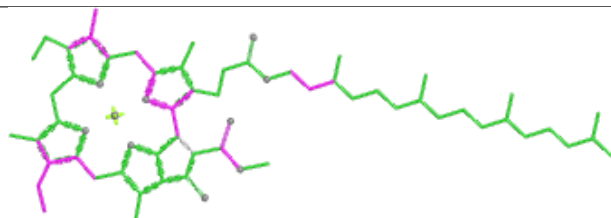


Rings

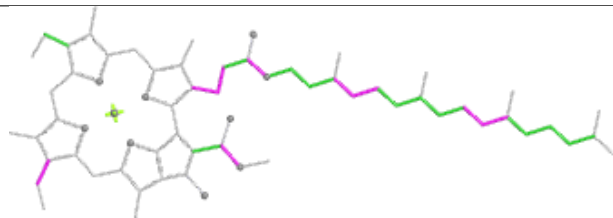
Ligand CLA G 1210



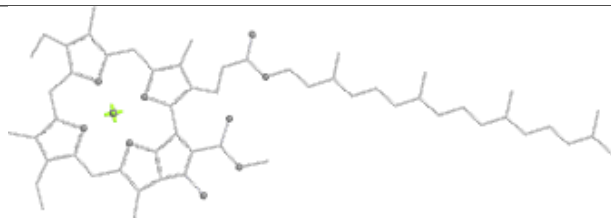
Bond lengths



Bond angles

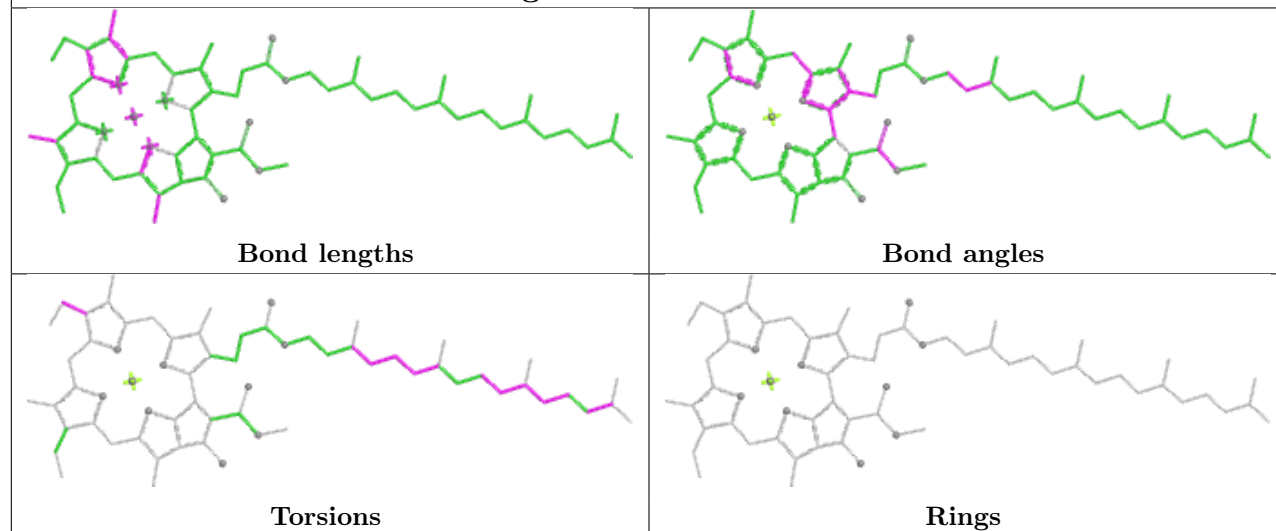


Torsions

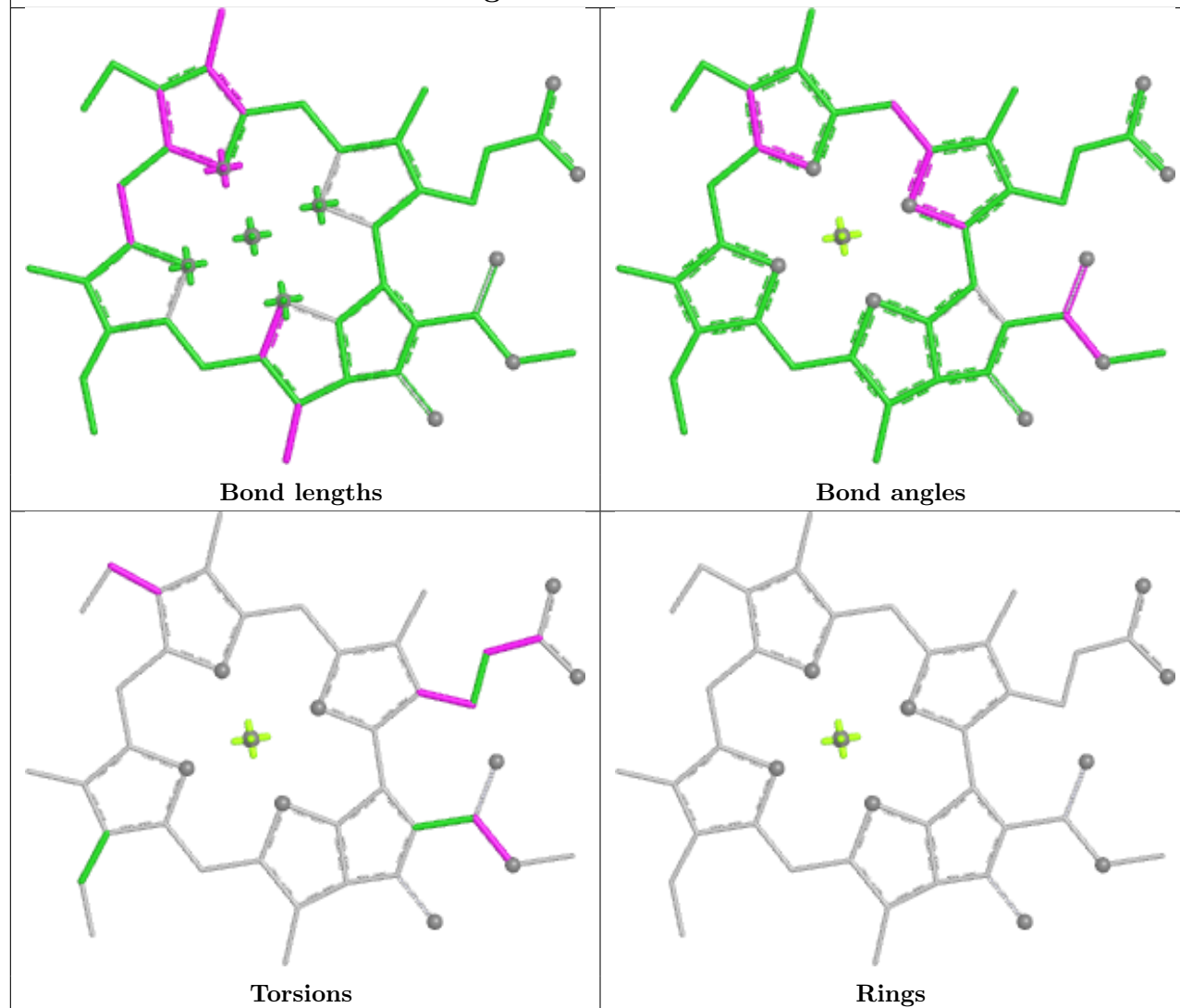


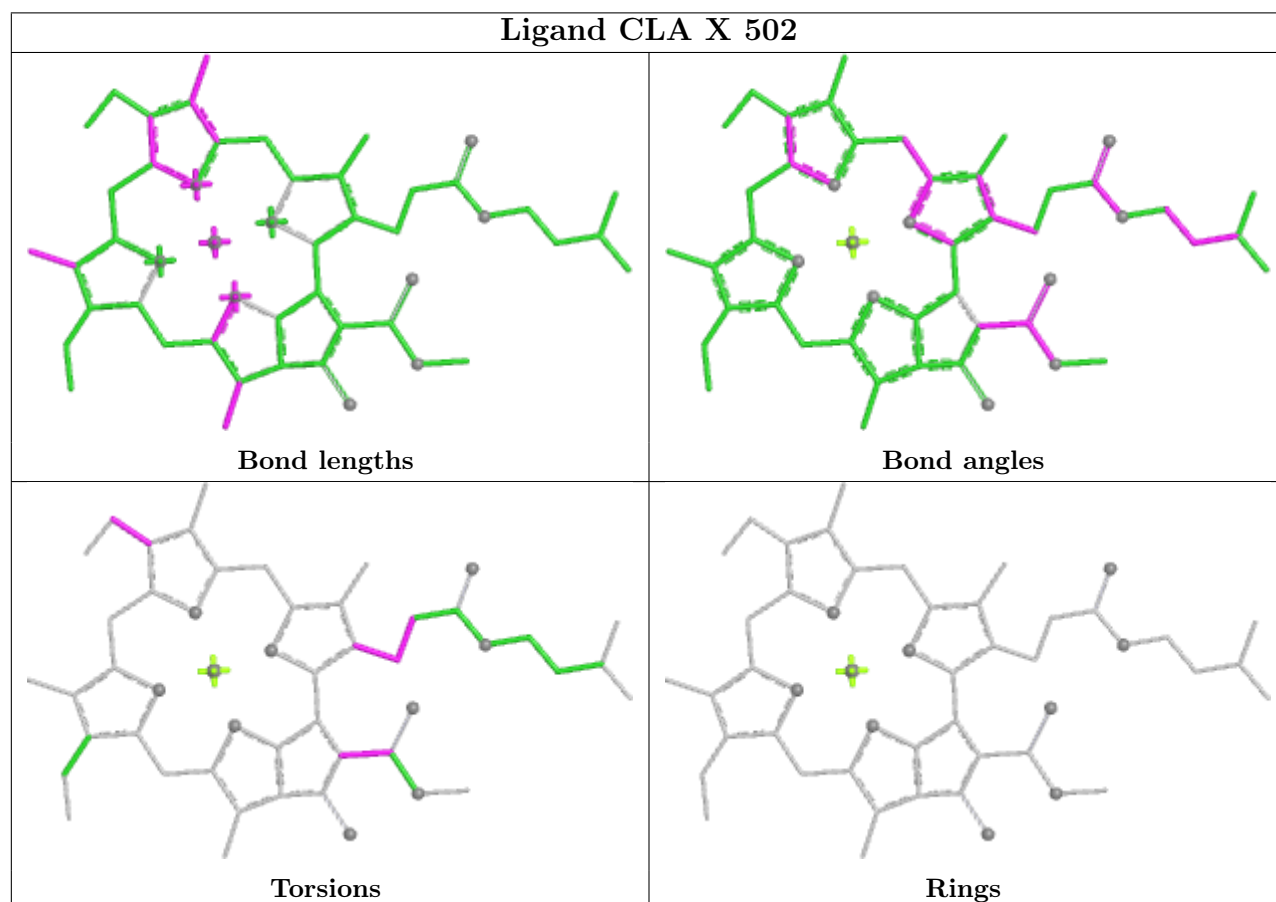
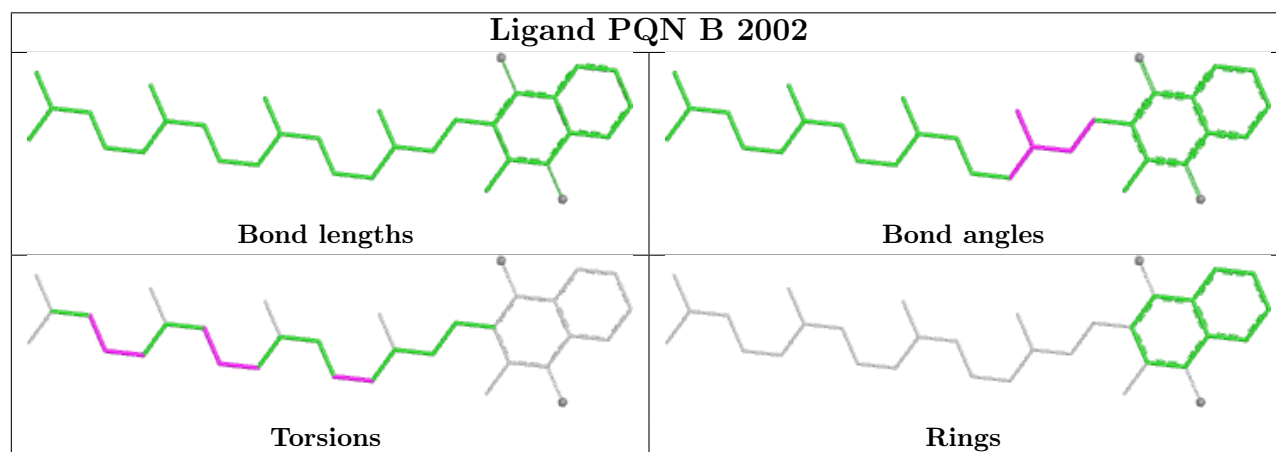
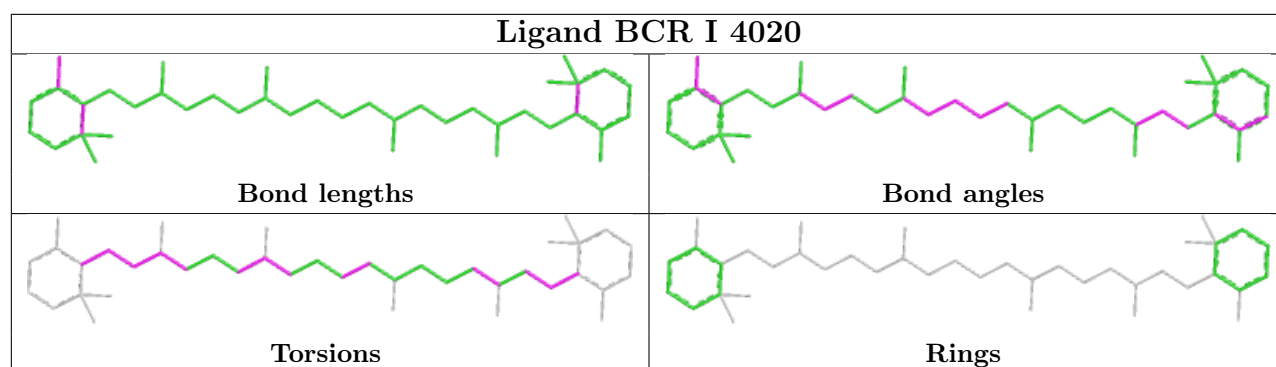
Rings

Ligand CLA G 1223

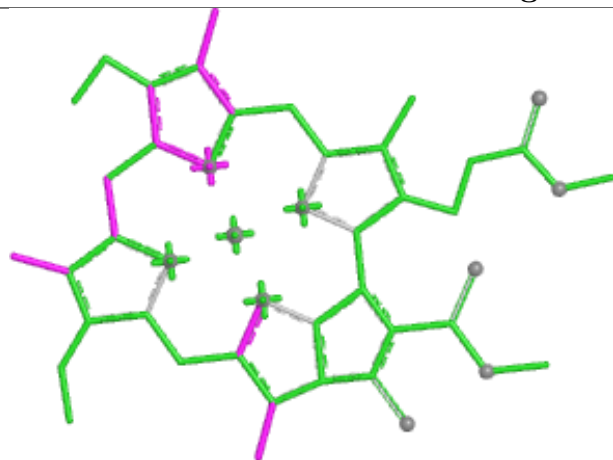


Ligand CLA B 1217

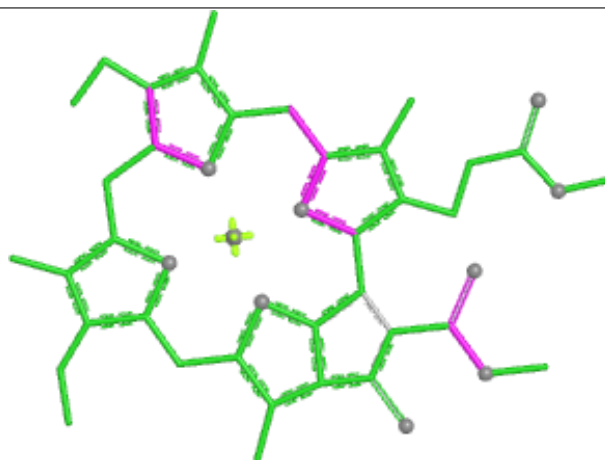




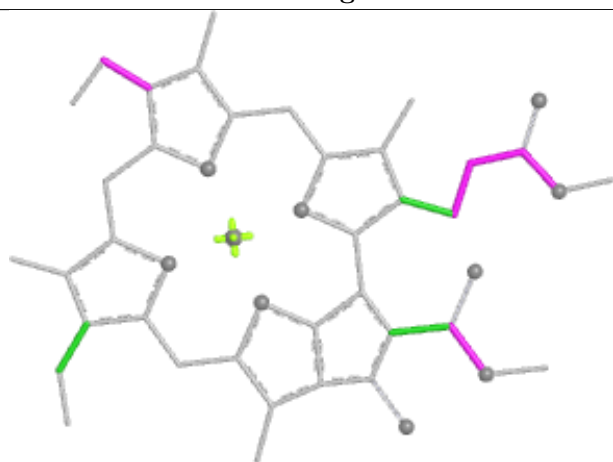
Ligand CLA t 516



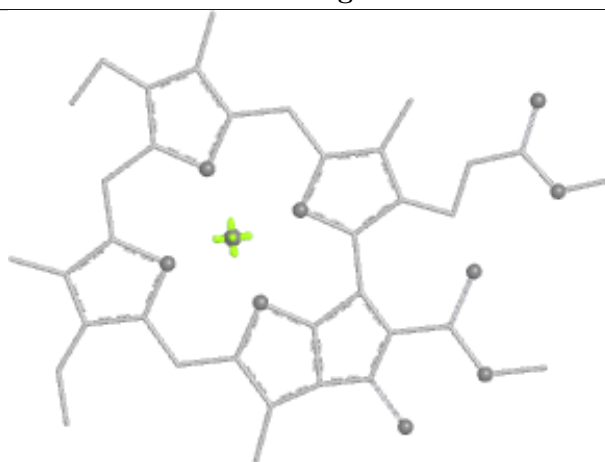
Bond lengths



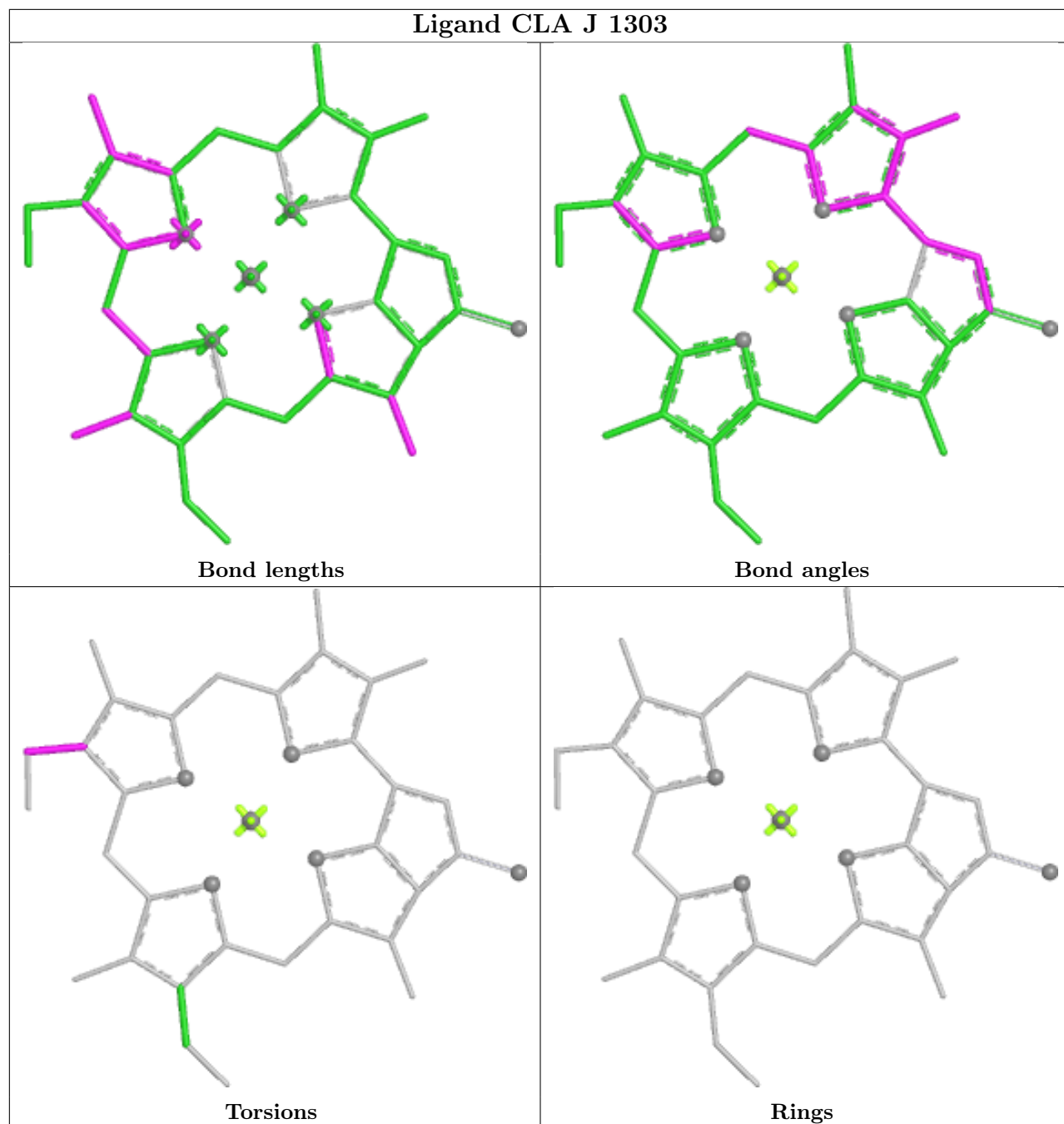
Bond angles

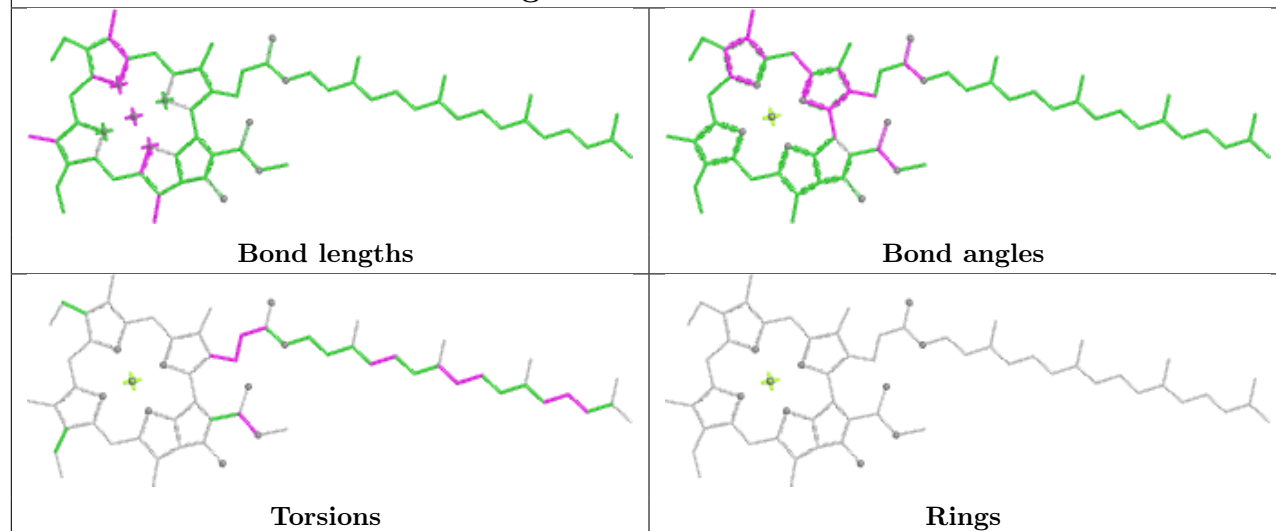
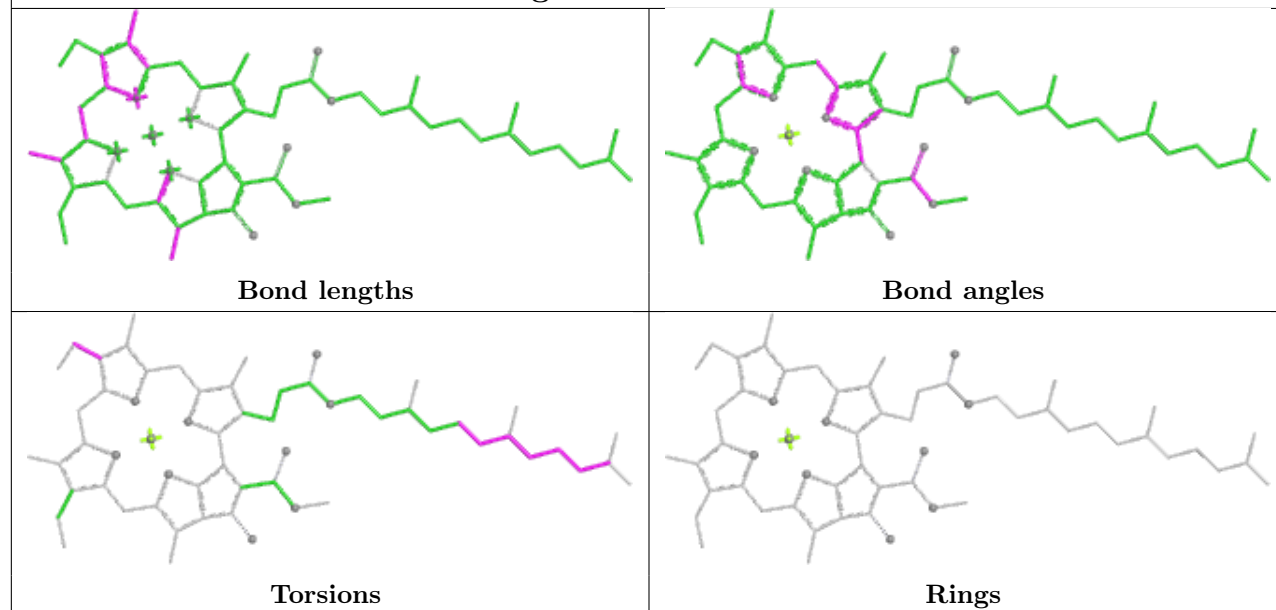


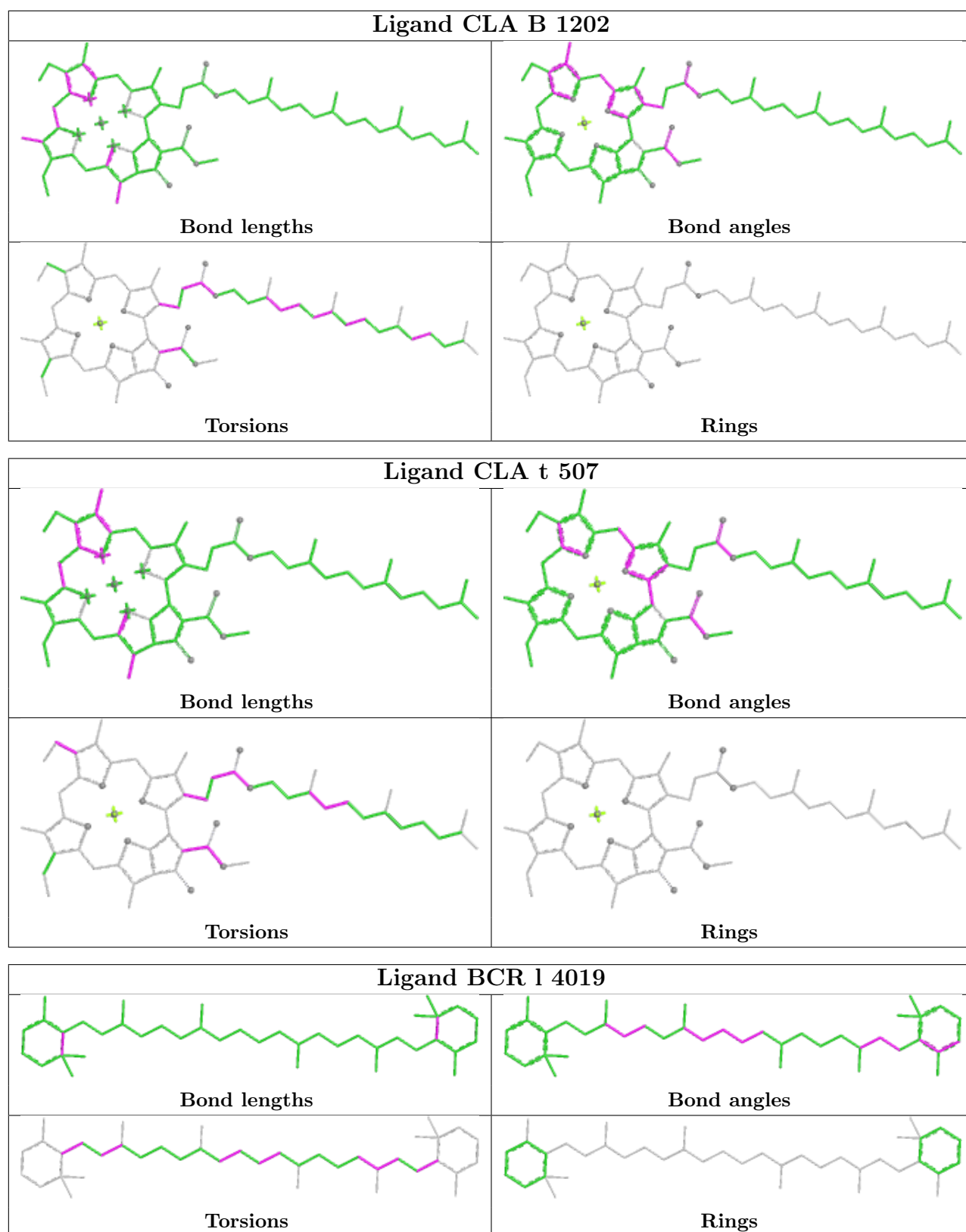
Torsions

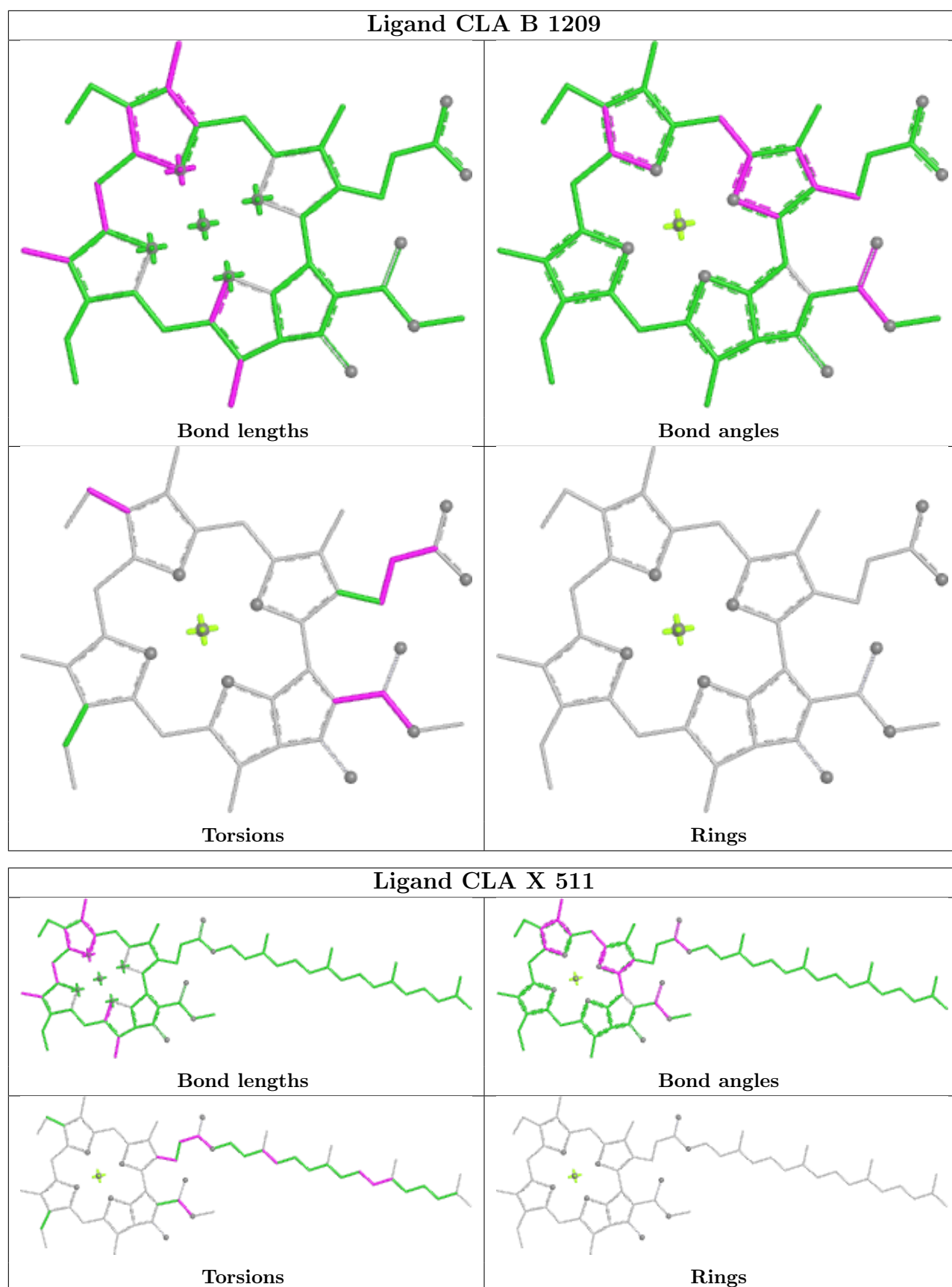


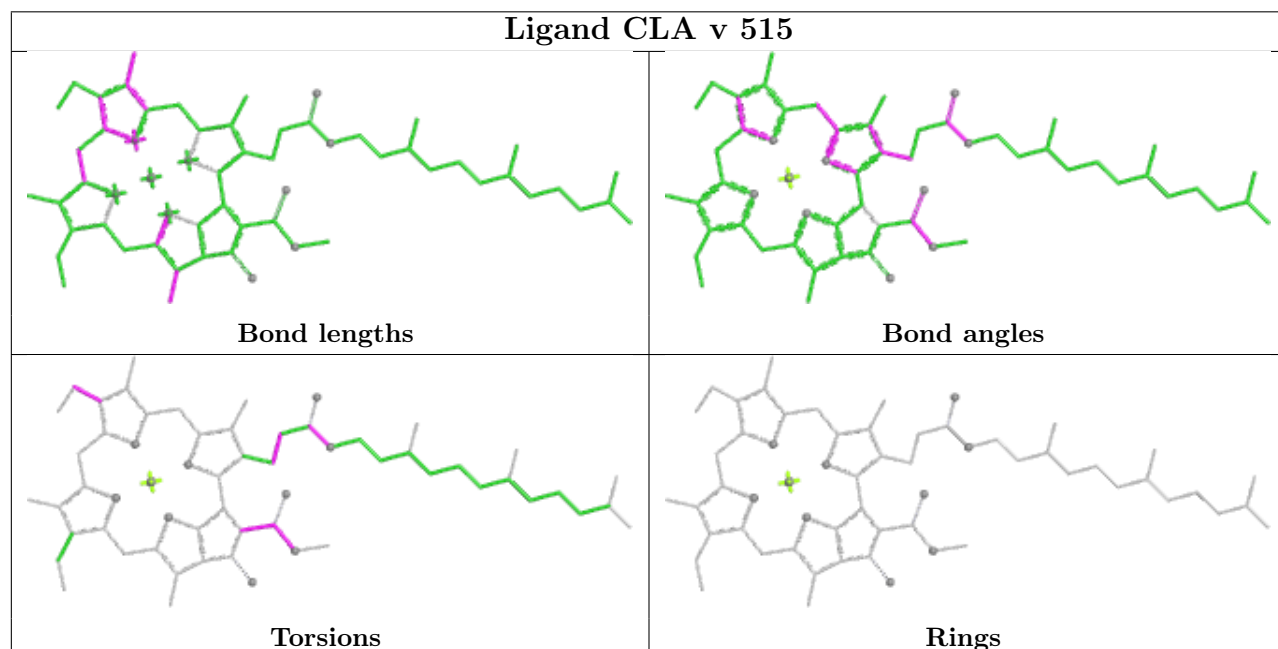
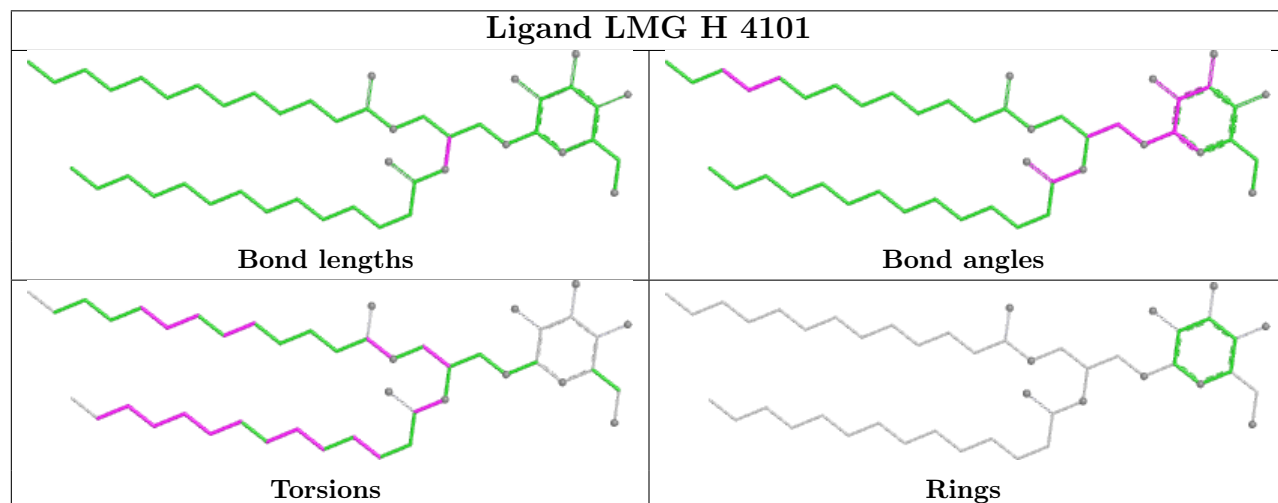
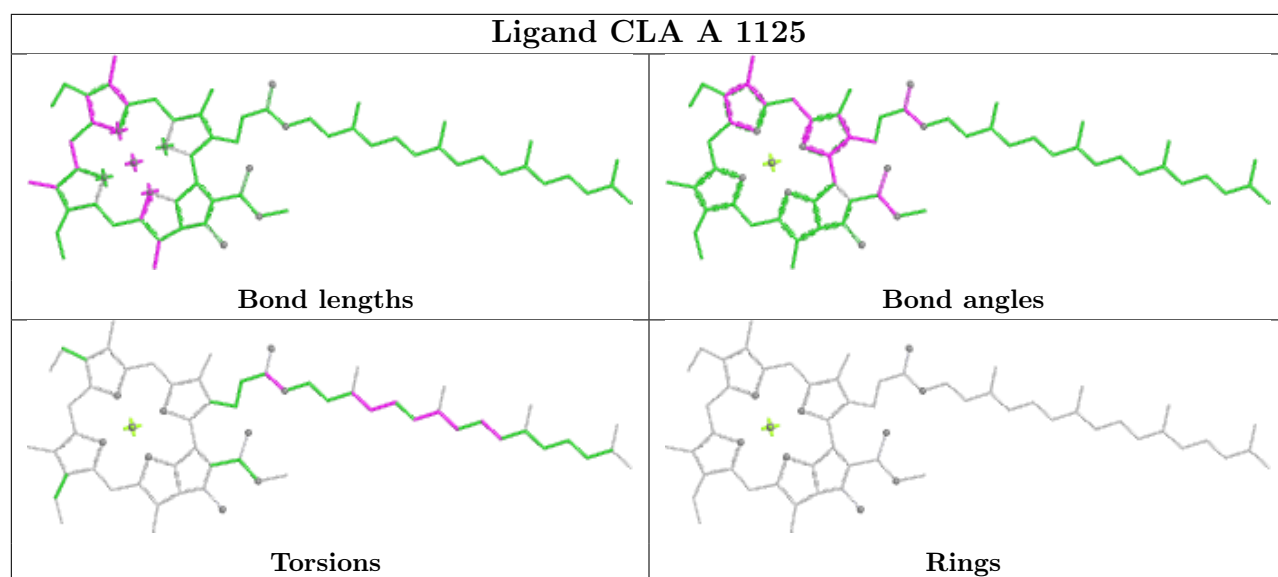
Rings

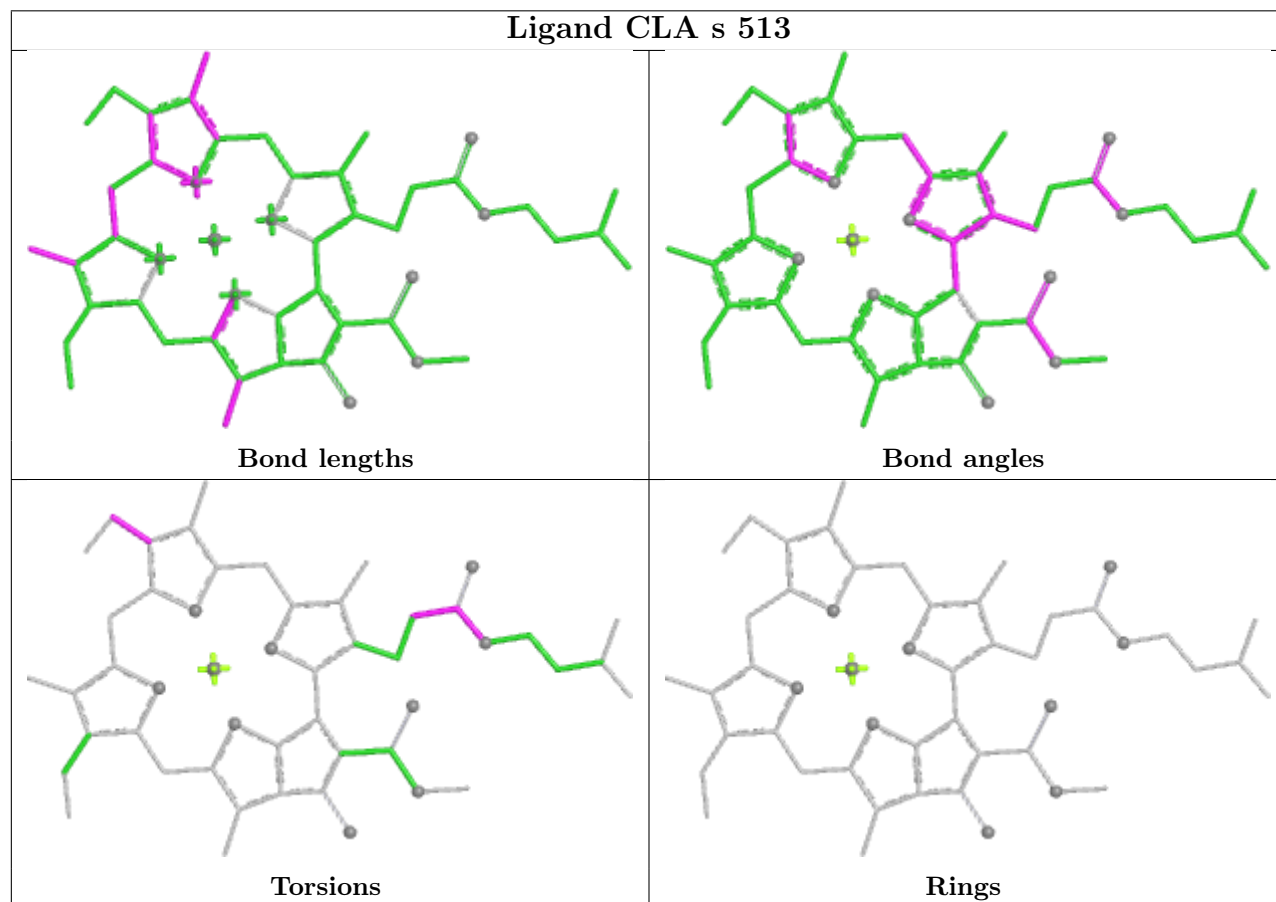
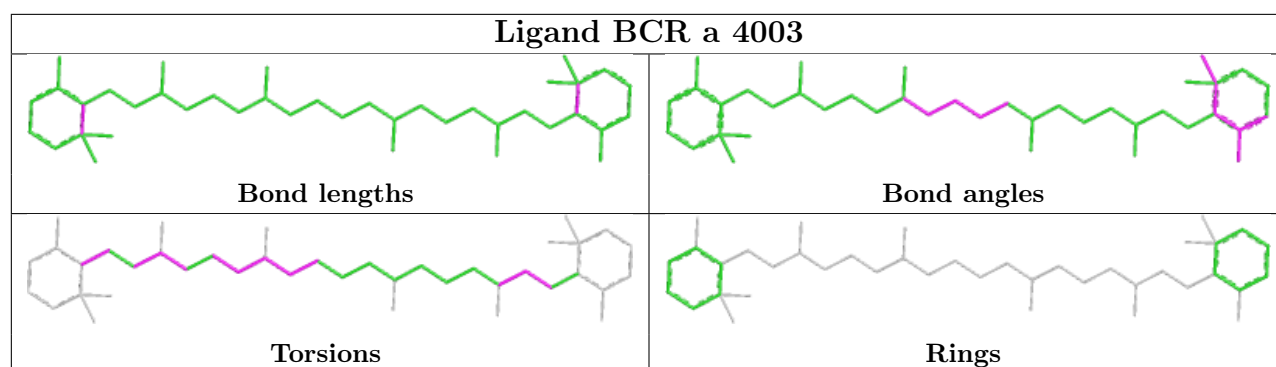


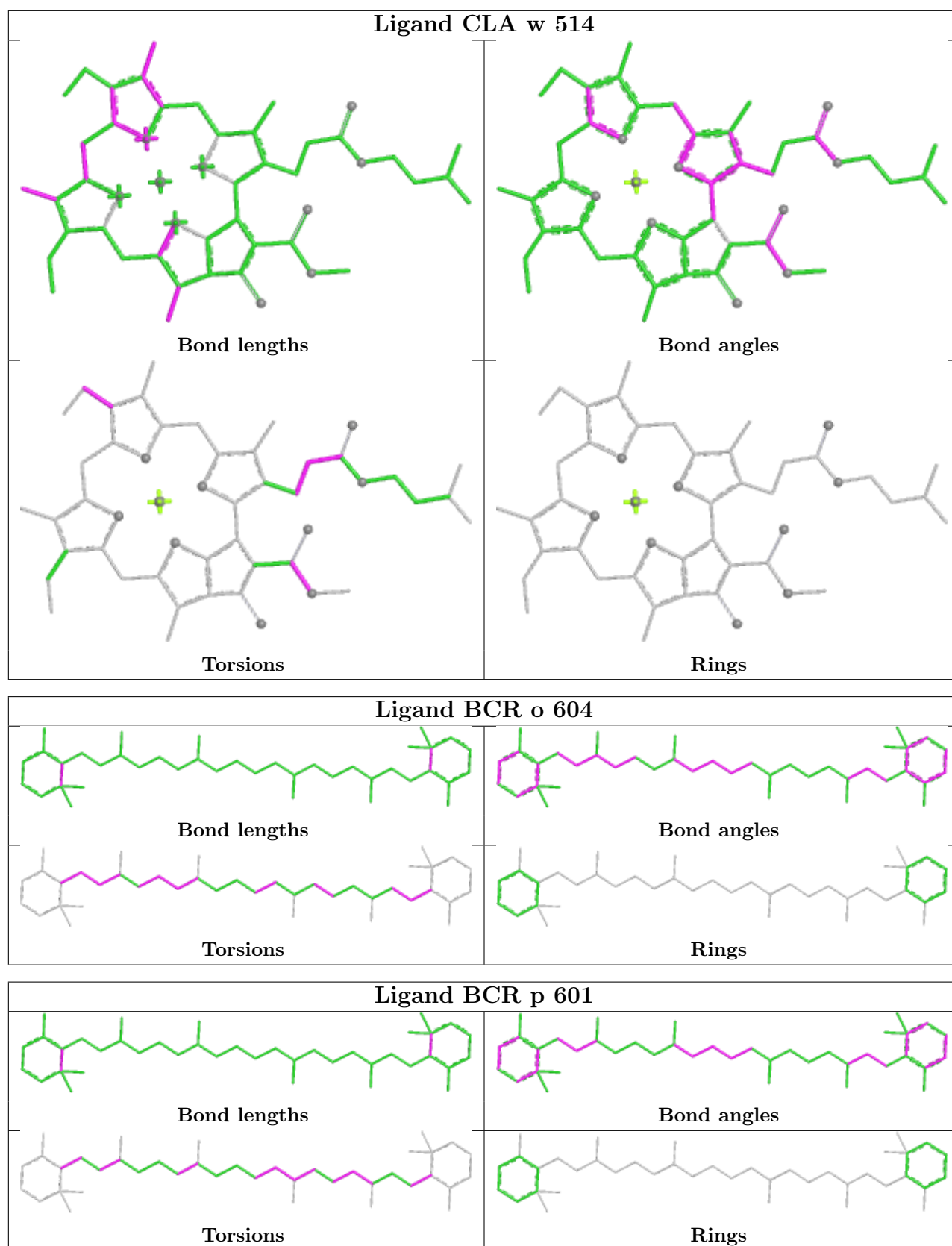
Ligand CLA G 1206**Ligand CLA X 504**



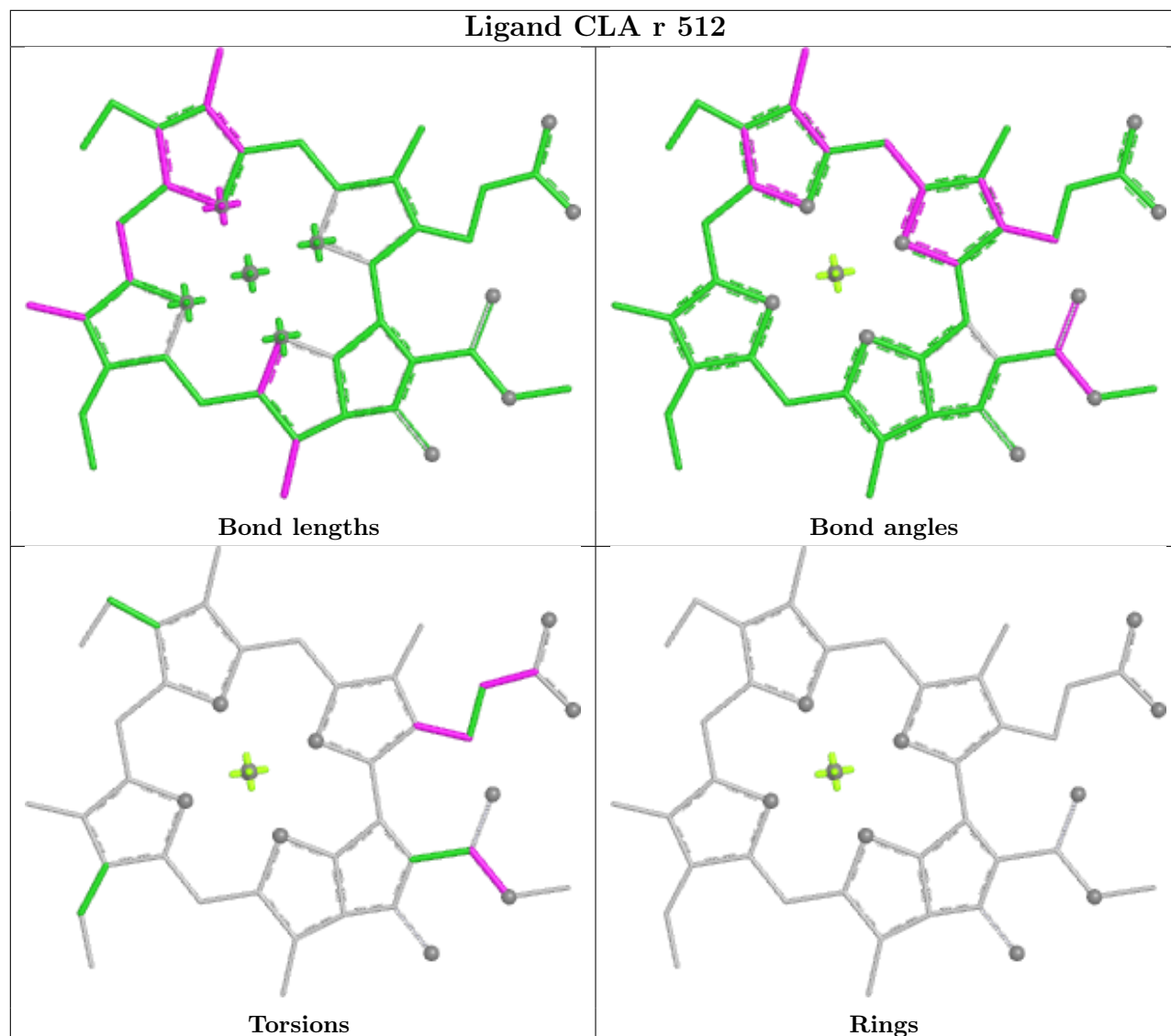




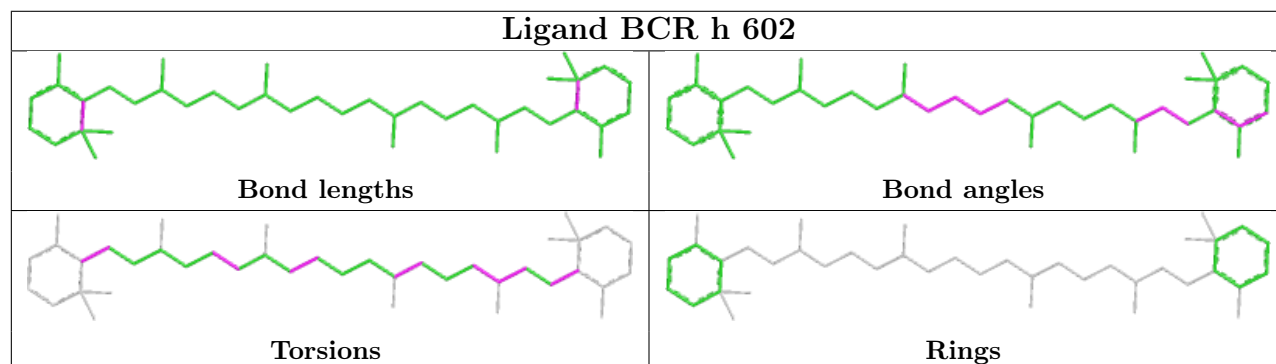


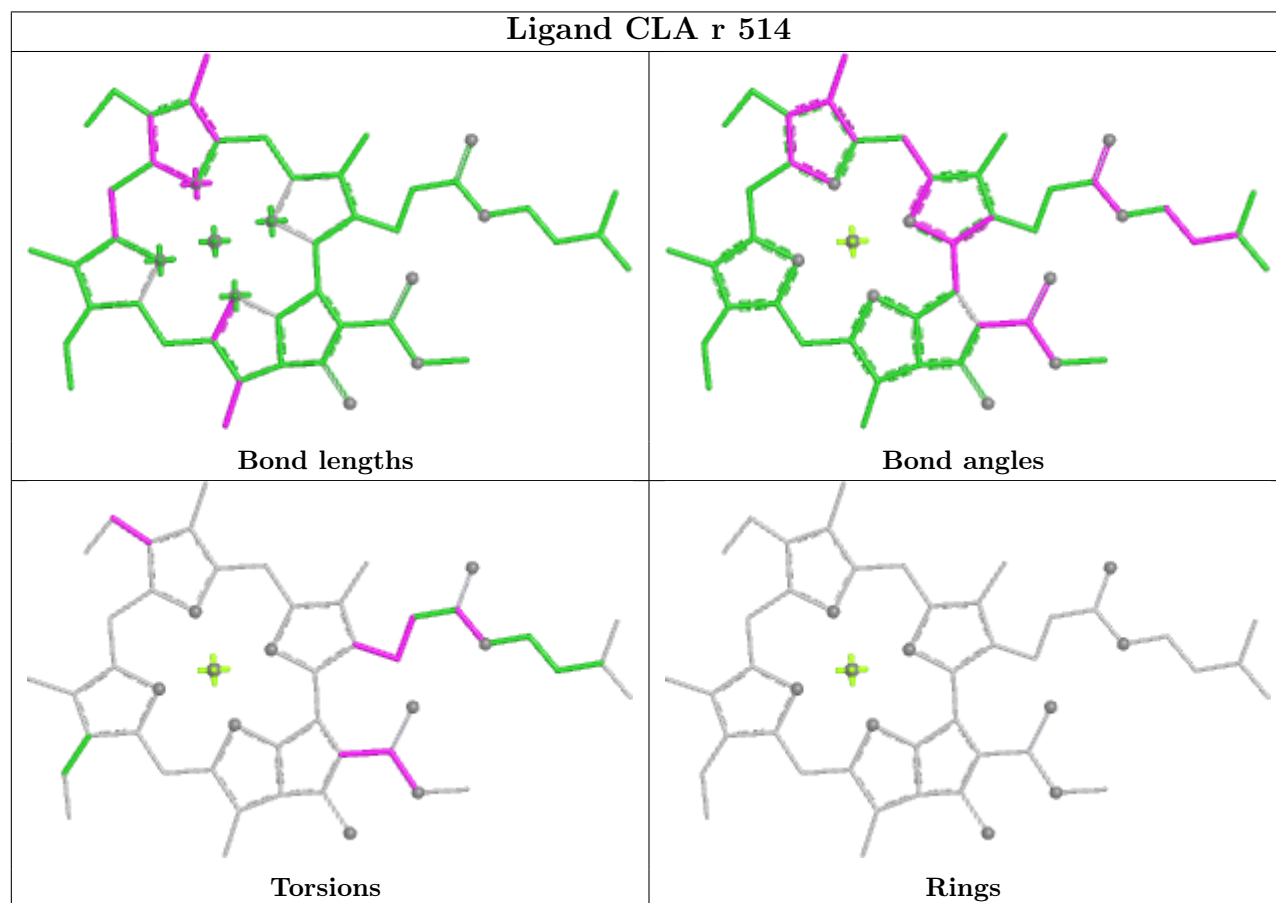
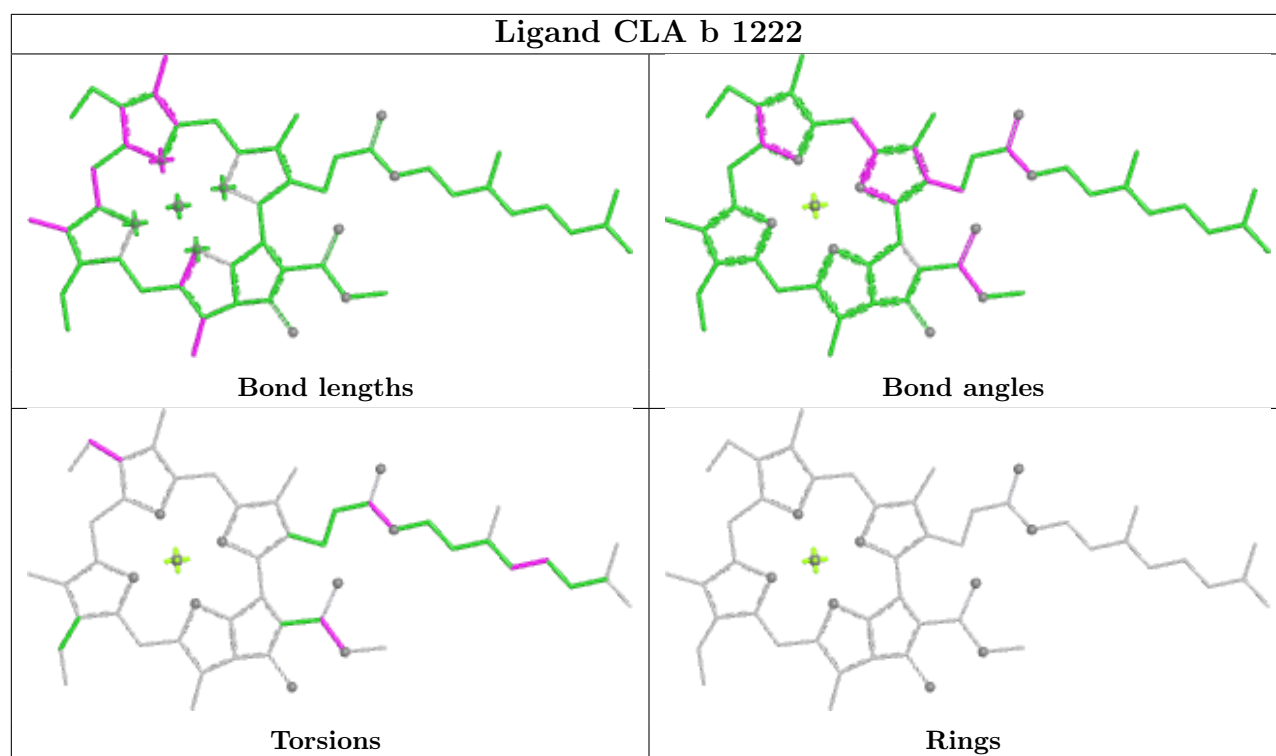


Ligand CLA r 512

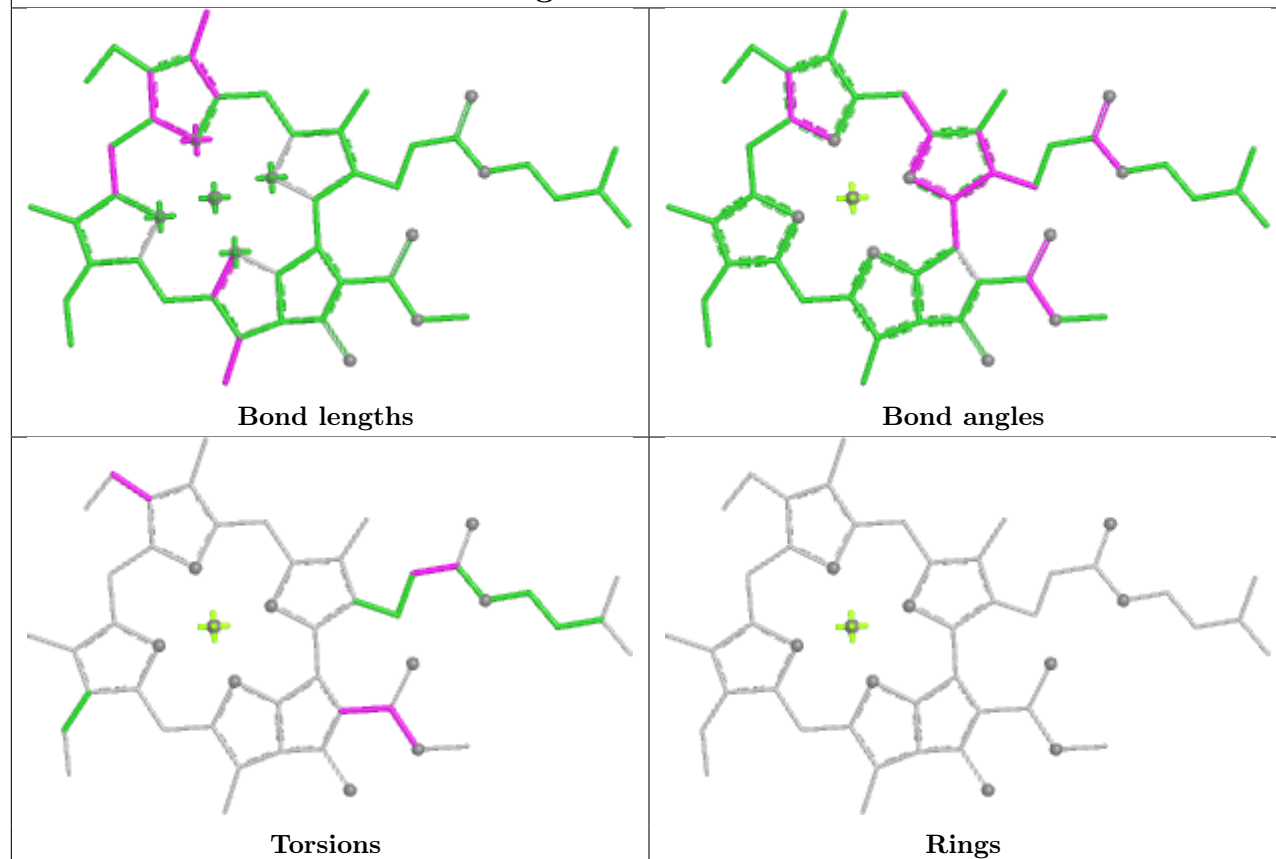


Ligand BCR h 602

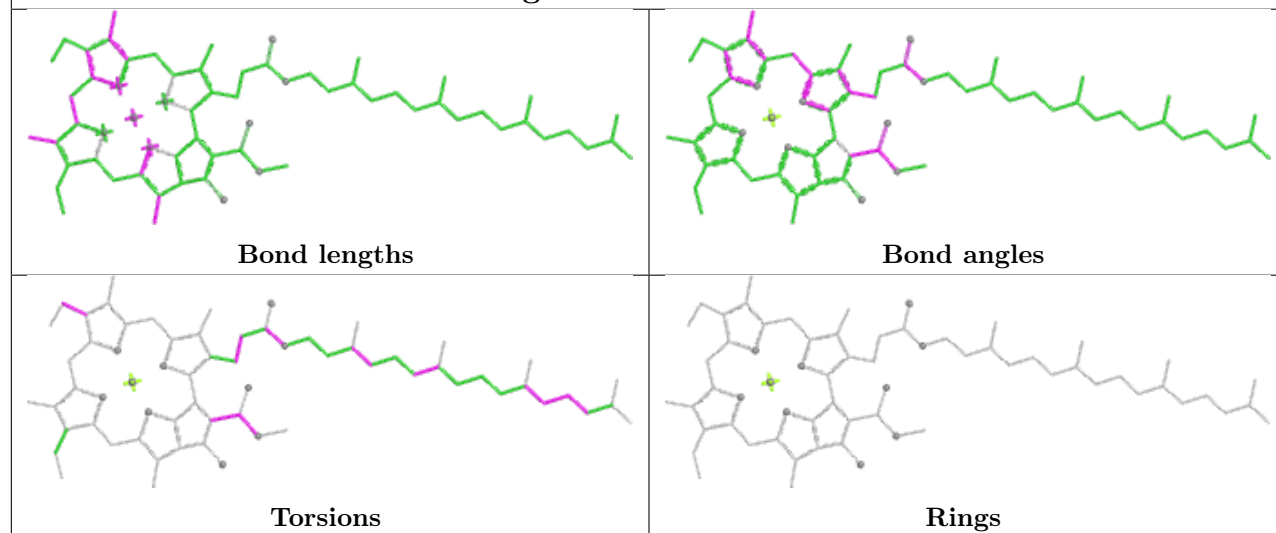


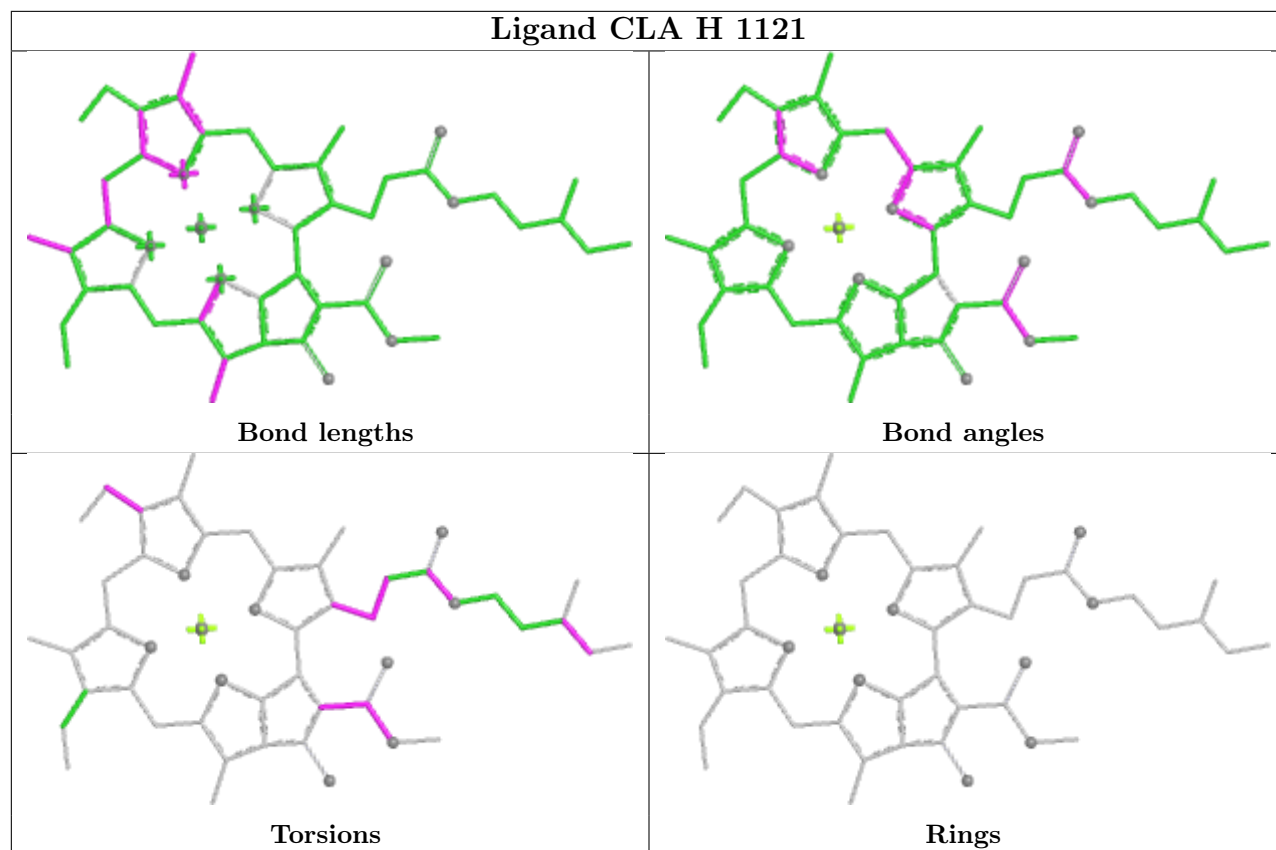


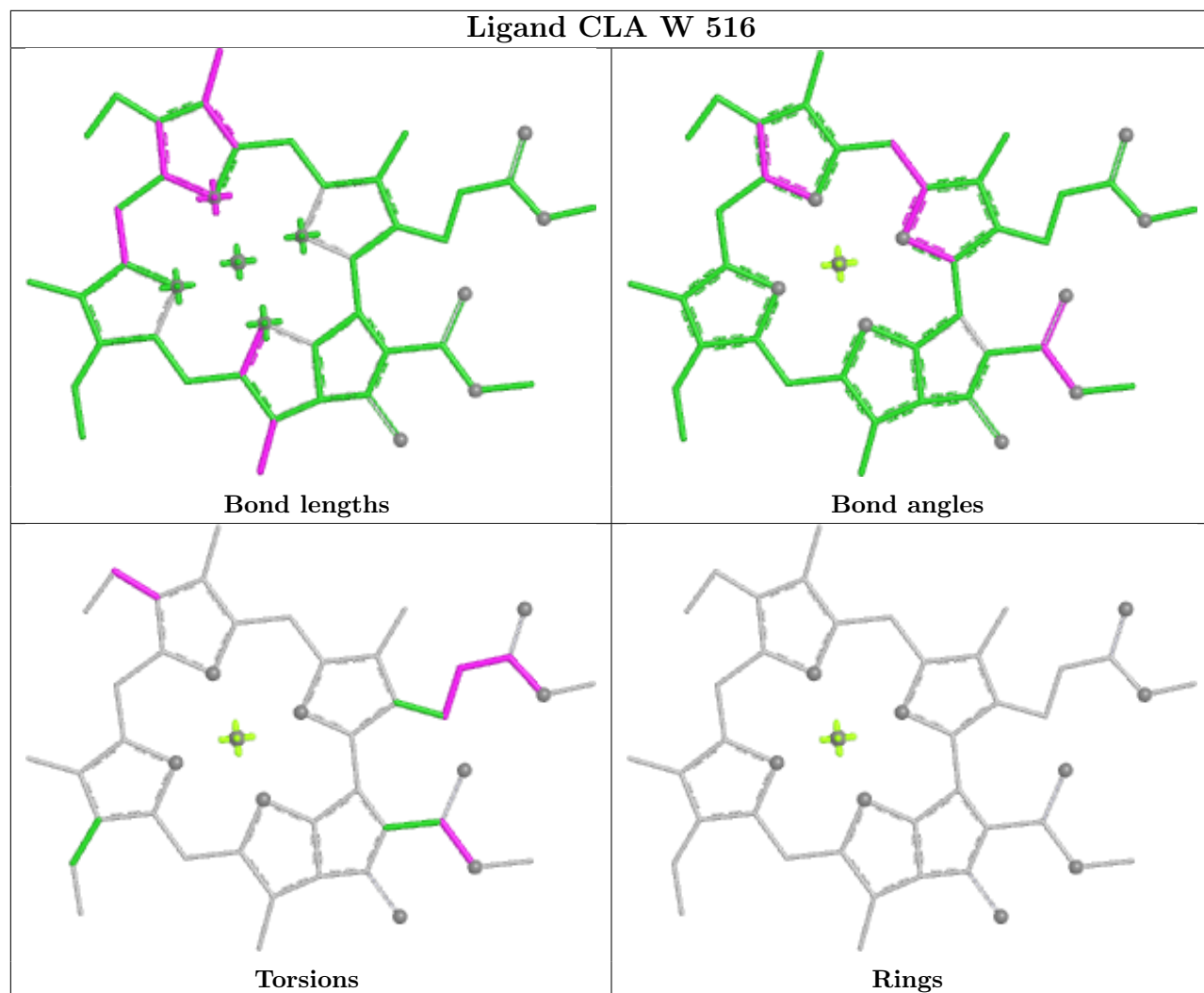
Ligand CLA v 514

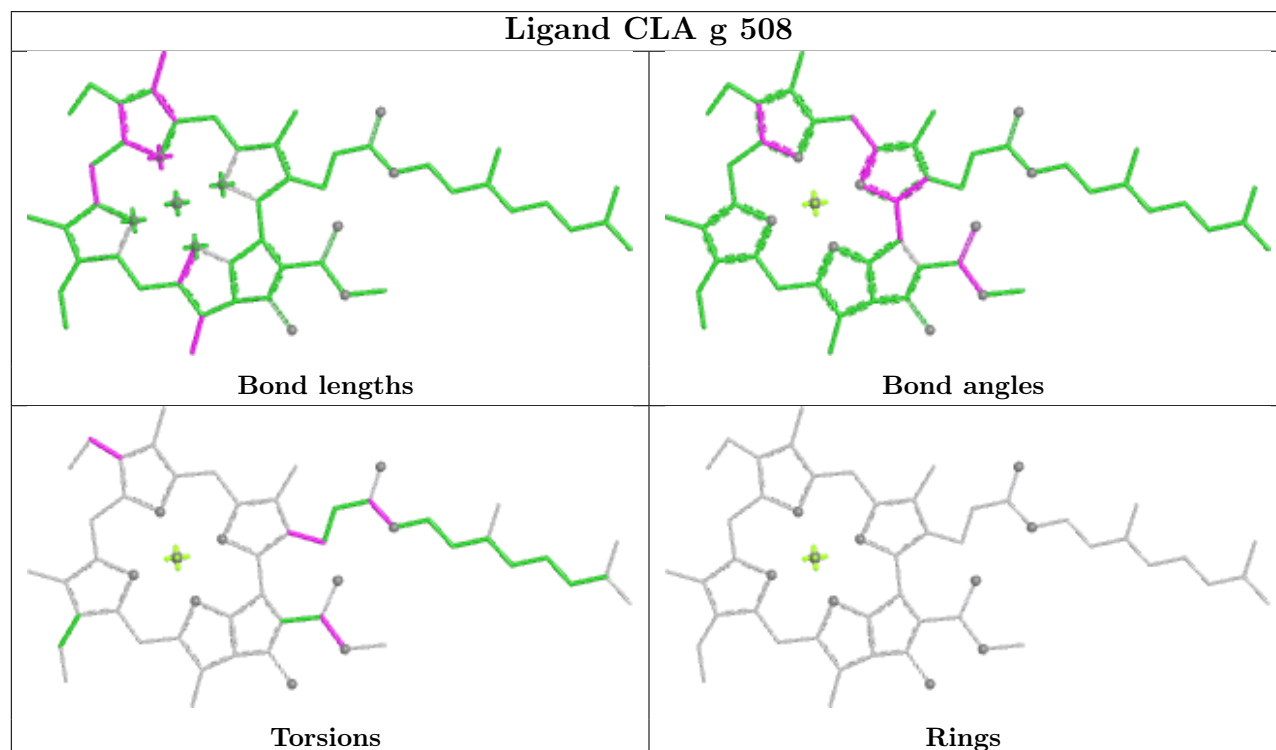
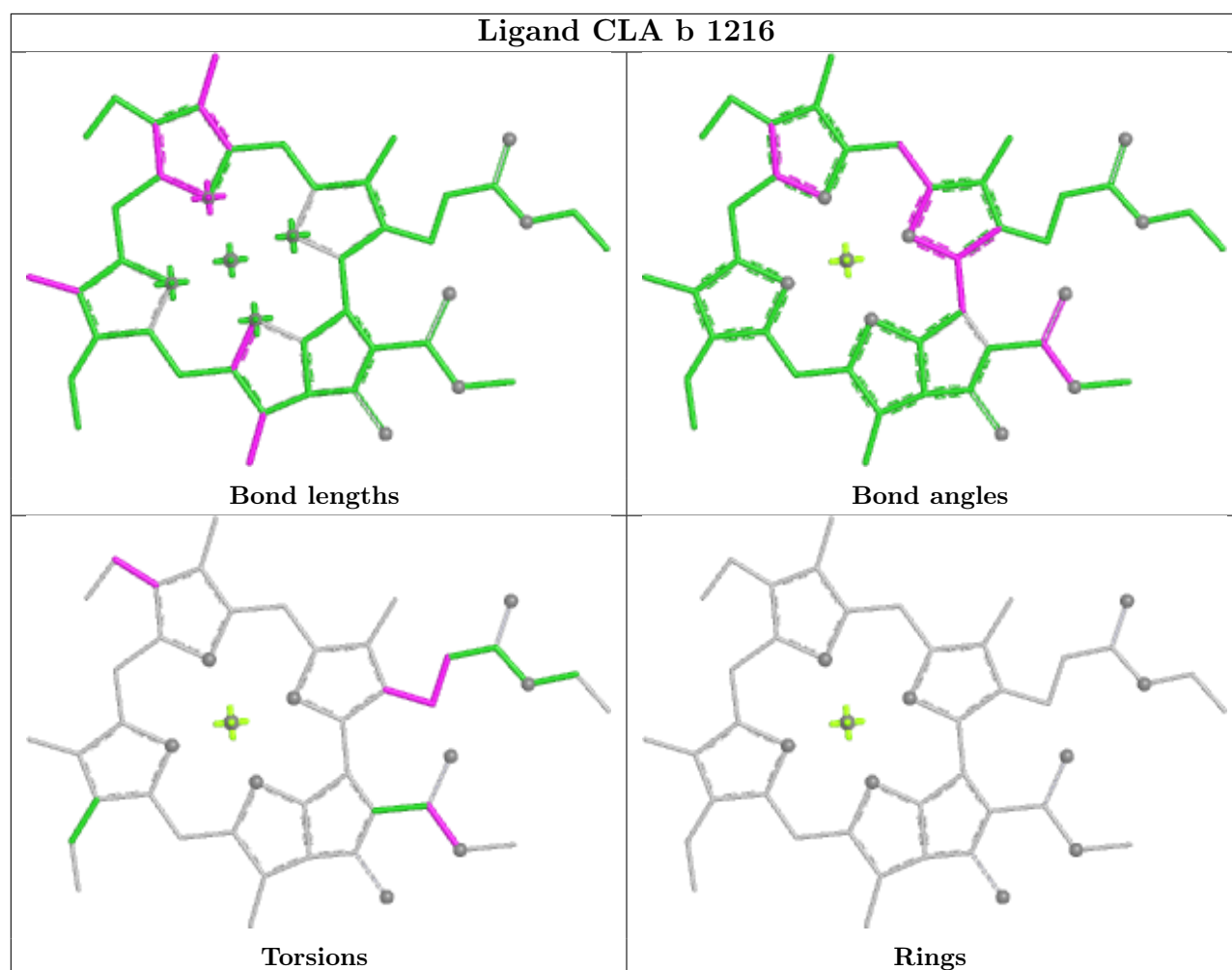


Ligand CLA A 1119

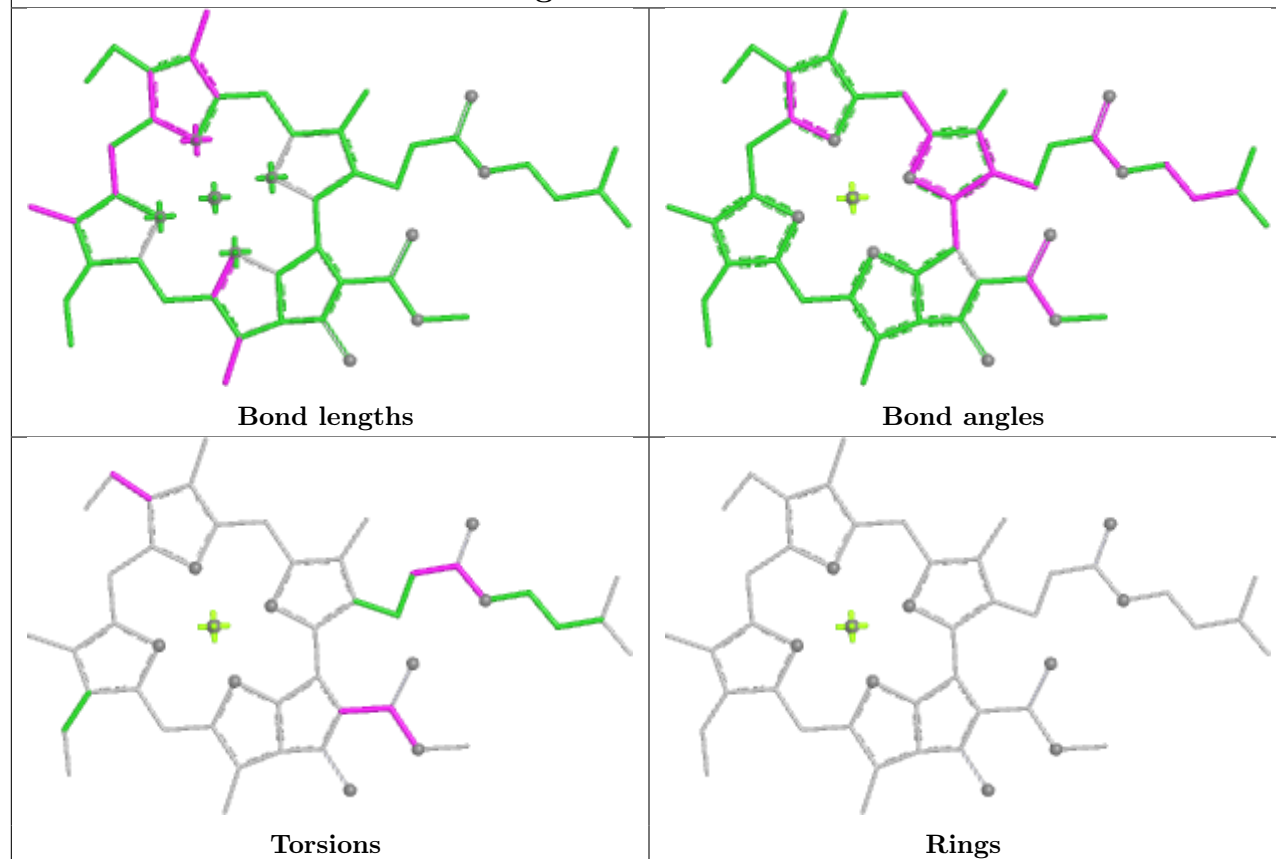




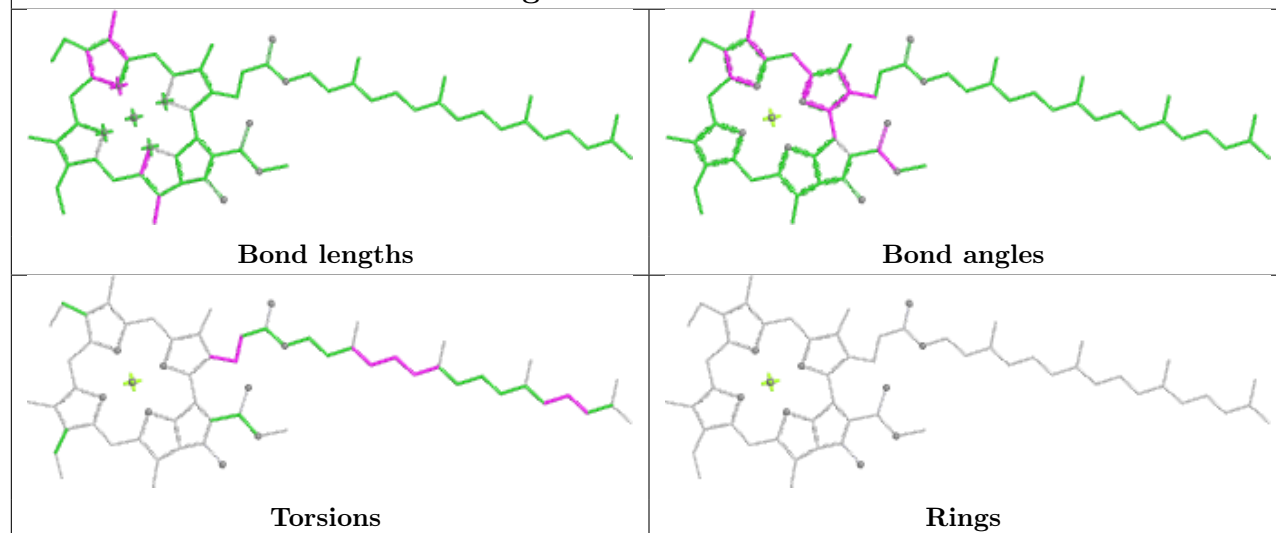


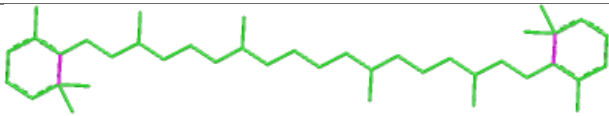
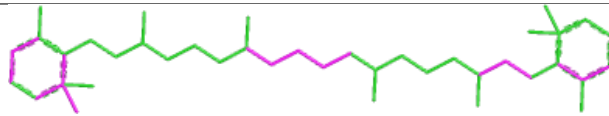
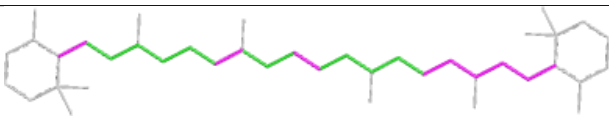
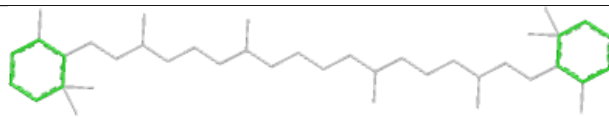


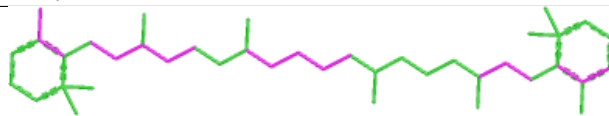
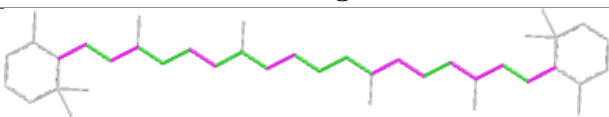
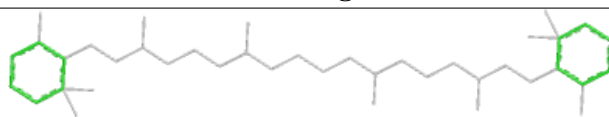
Ligand CLA n 514

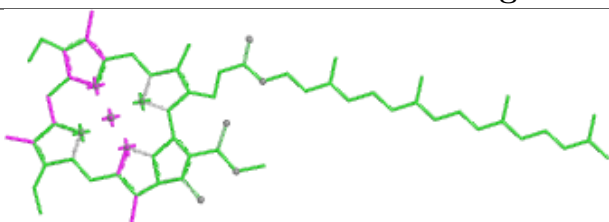
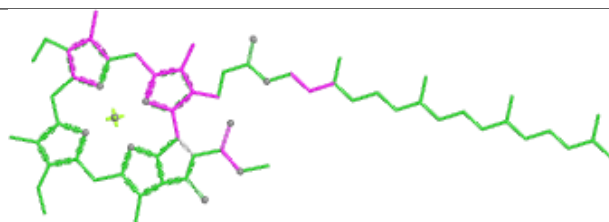
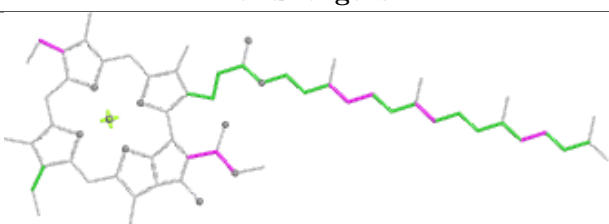
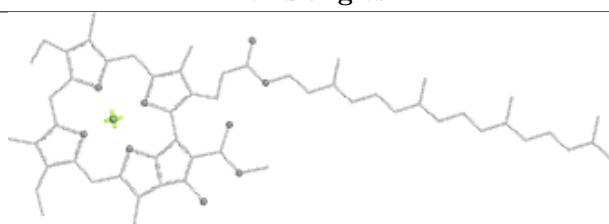


Ligand CLA H 1123

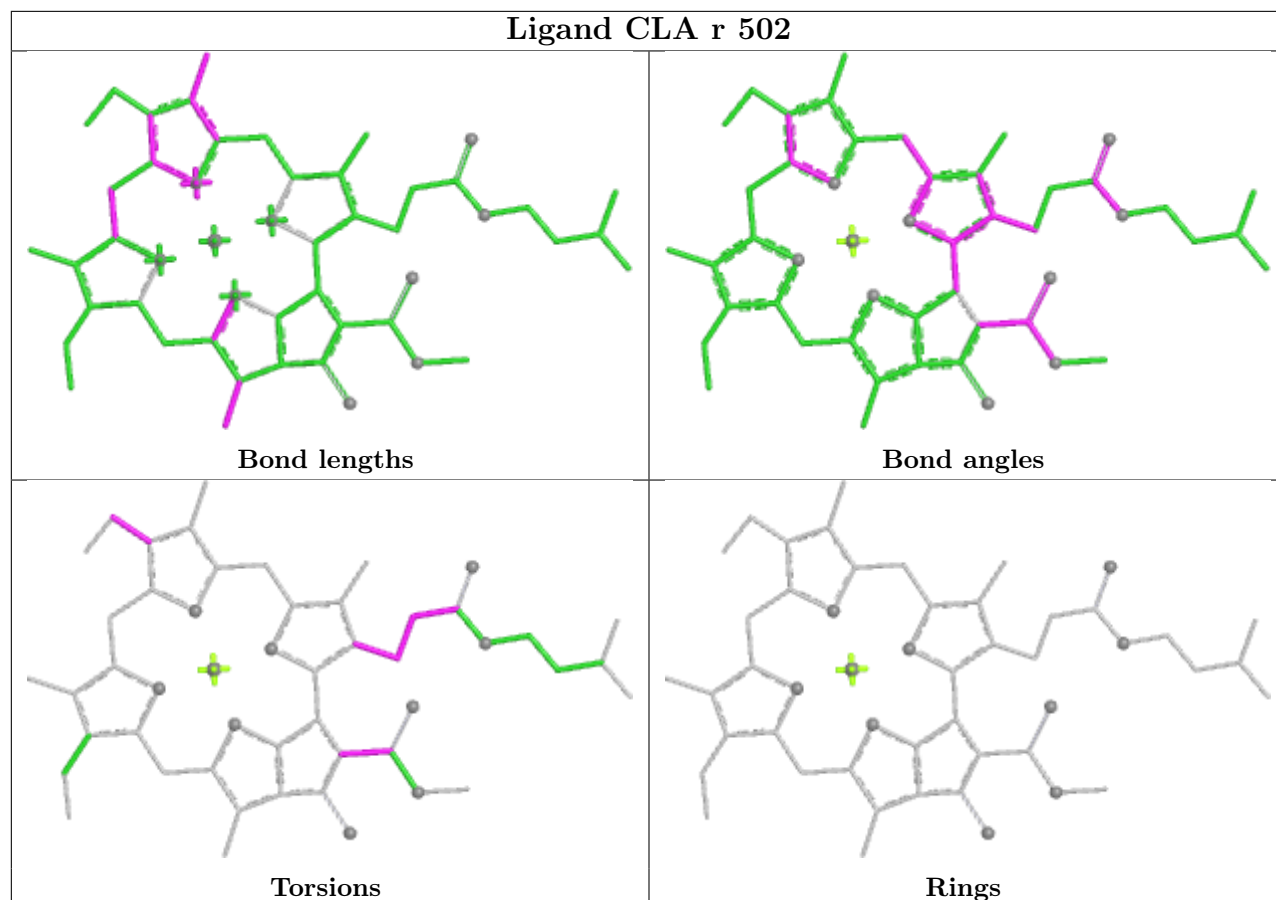


Ligand BCR j 4013	
	
Bond lengths	Bond angles
	
Torsions	Rings

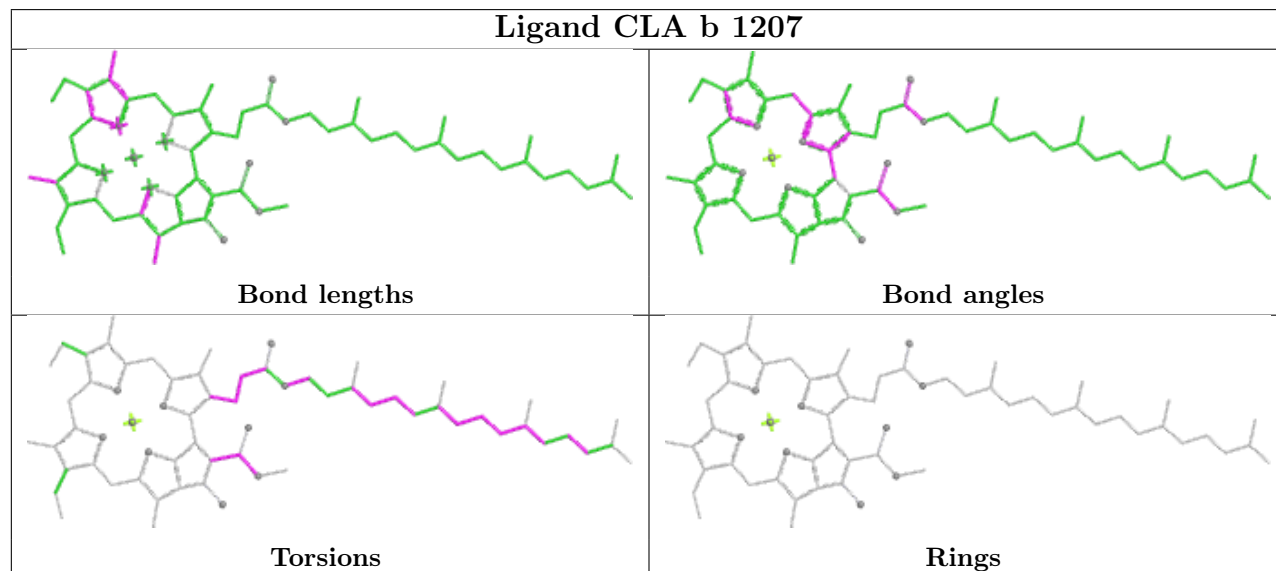
Ligand BCR y 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

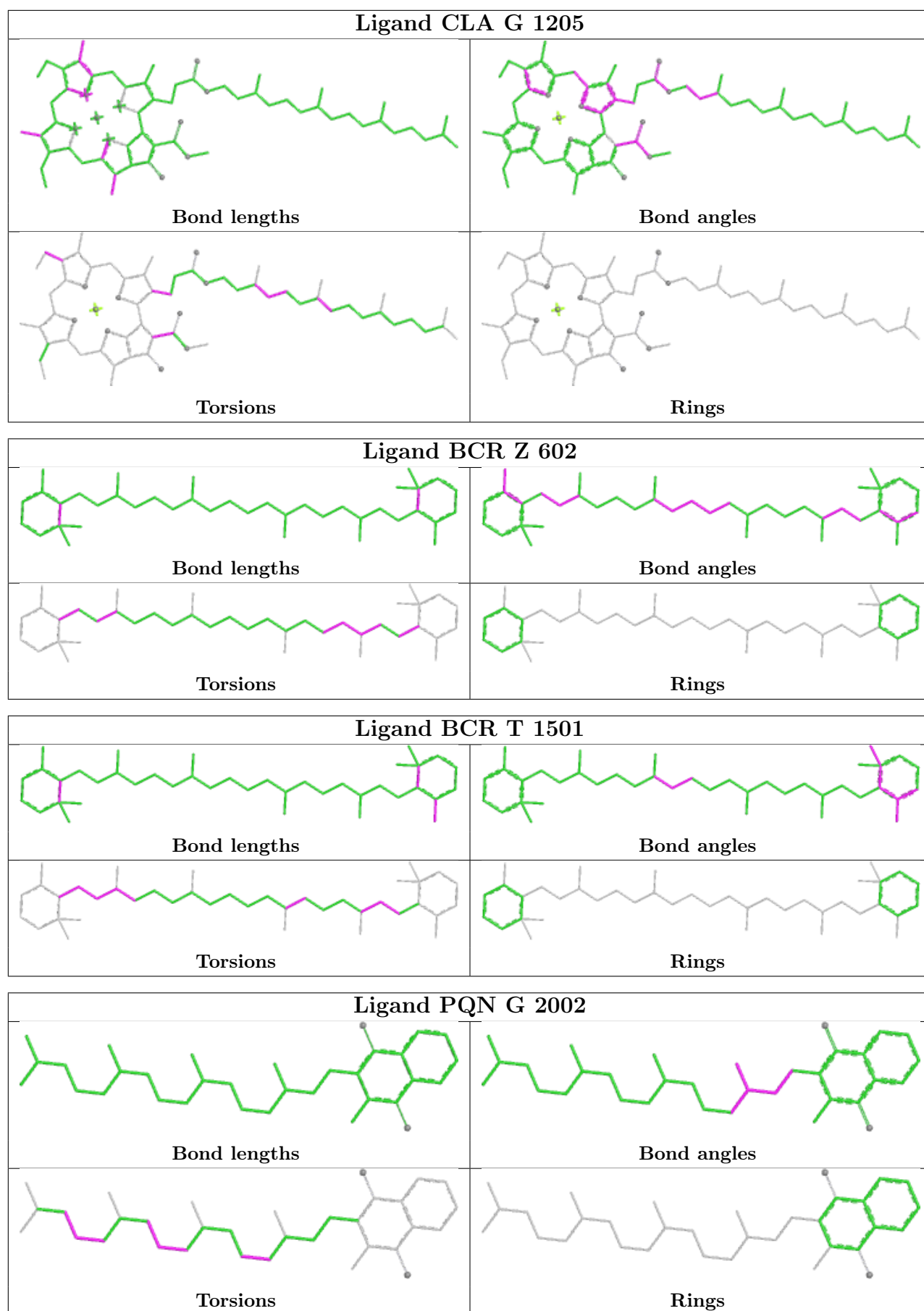
Ligand CLA A 1131	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA r 502

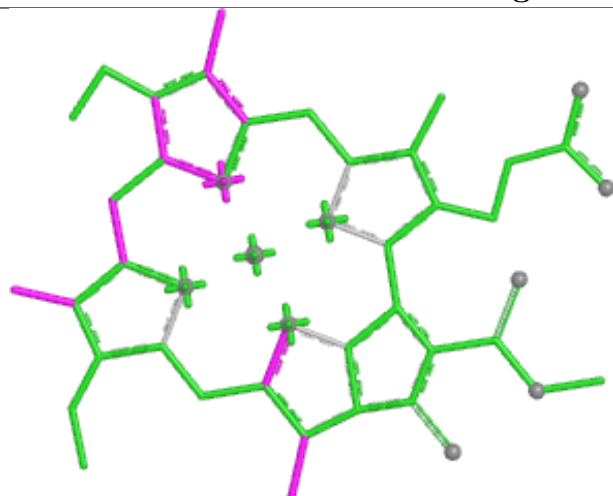


Ligand CLA b 1207

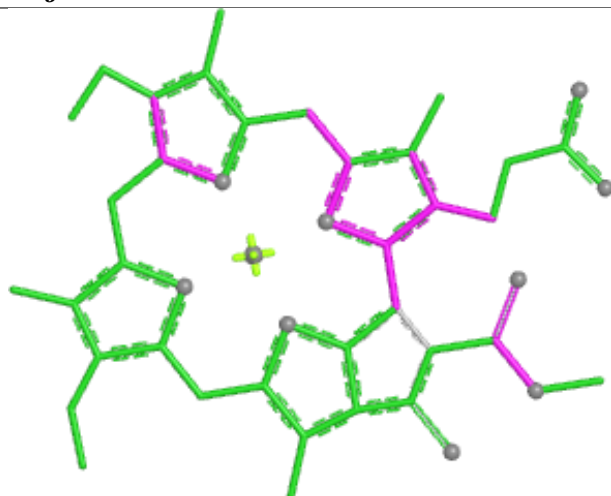




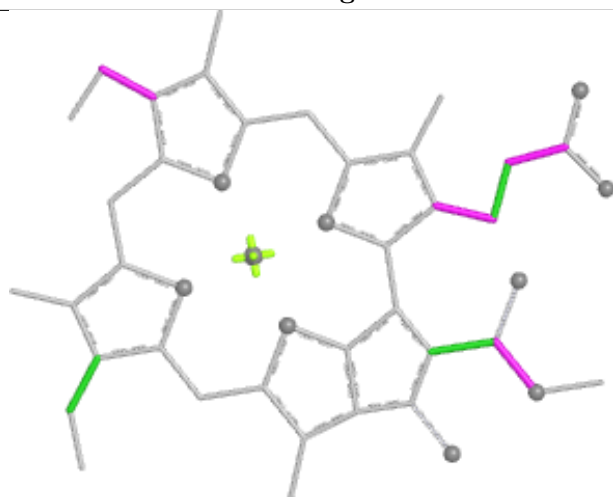
Ligand CLA j 1302



Bond lengths



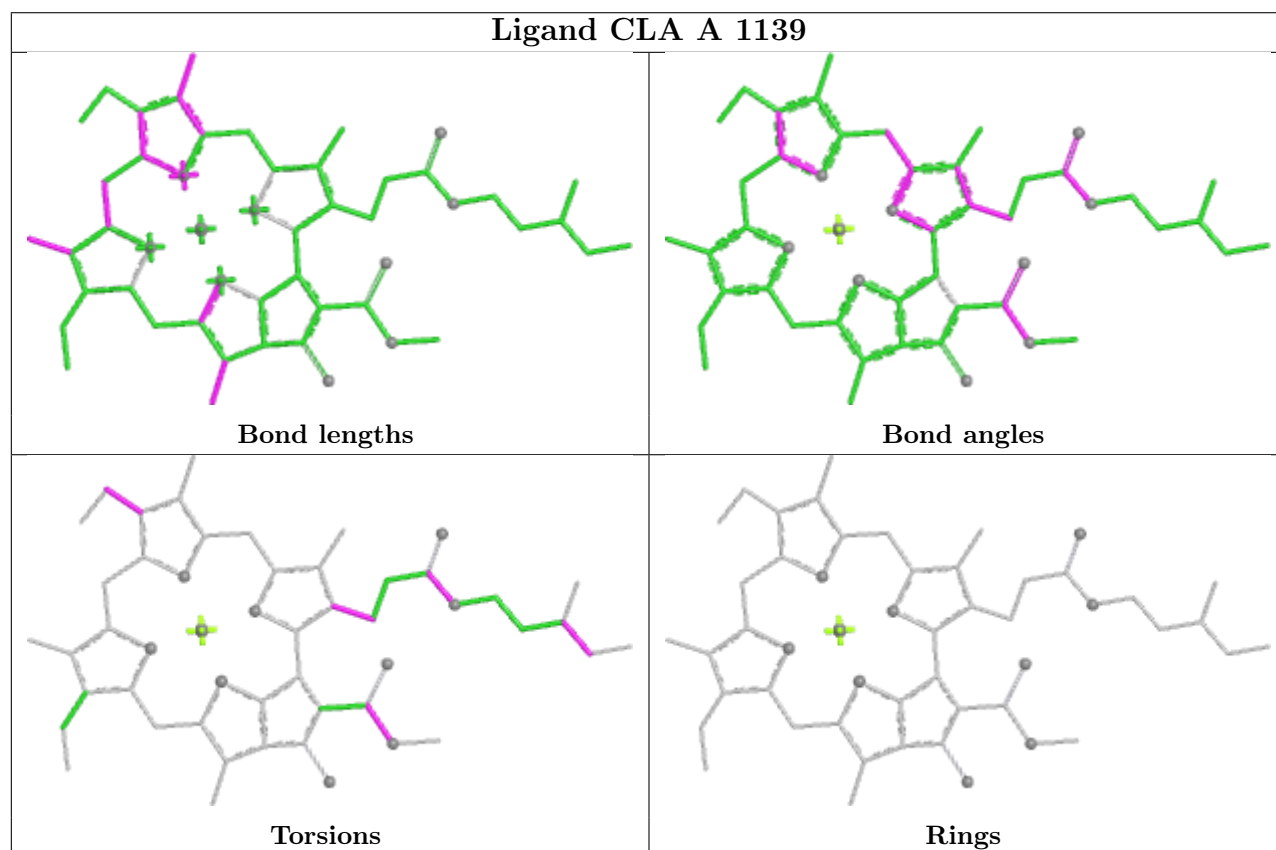
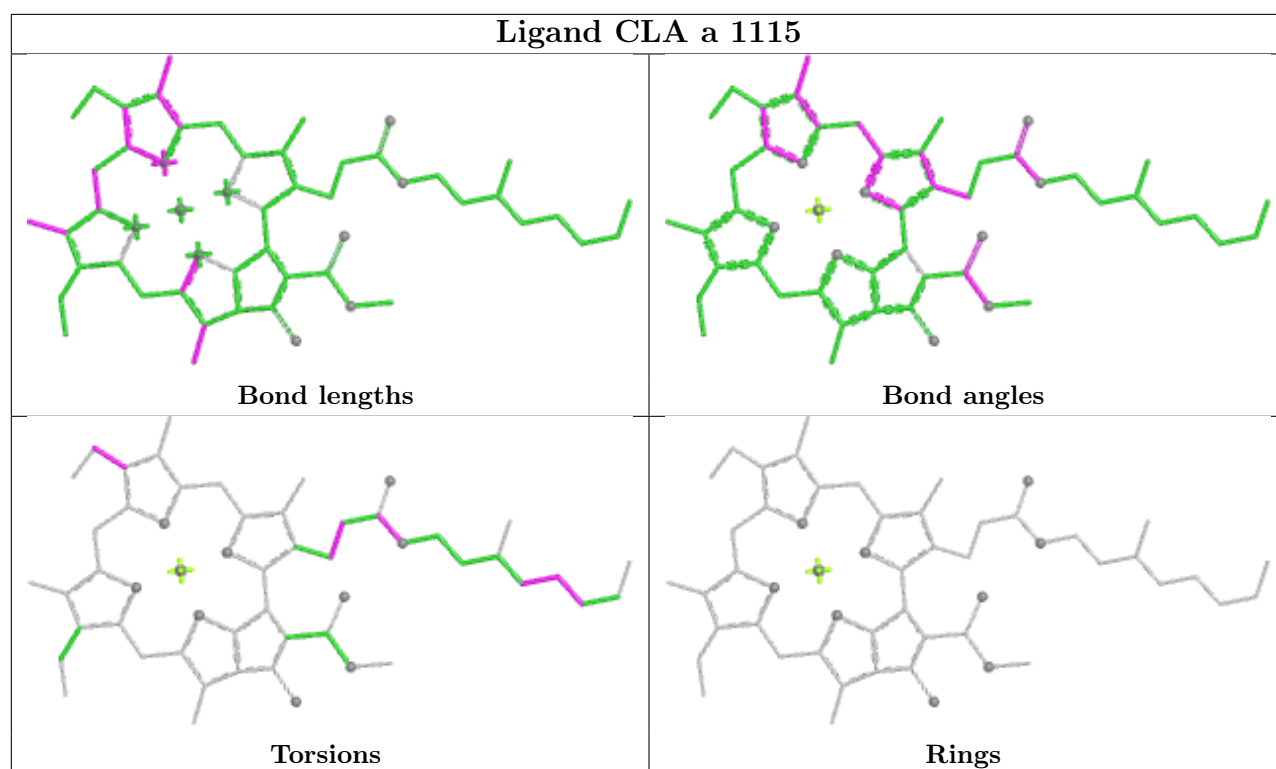
Bond angles



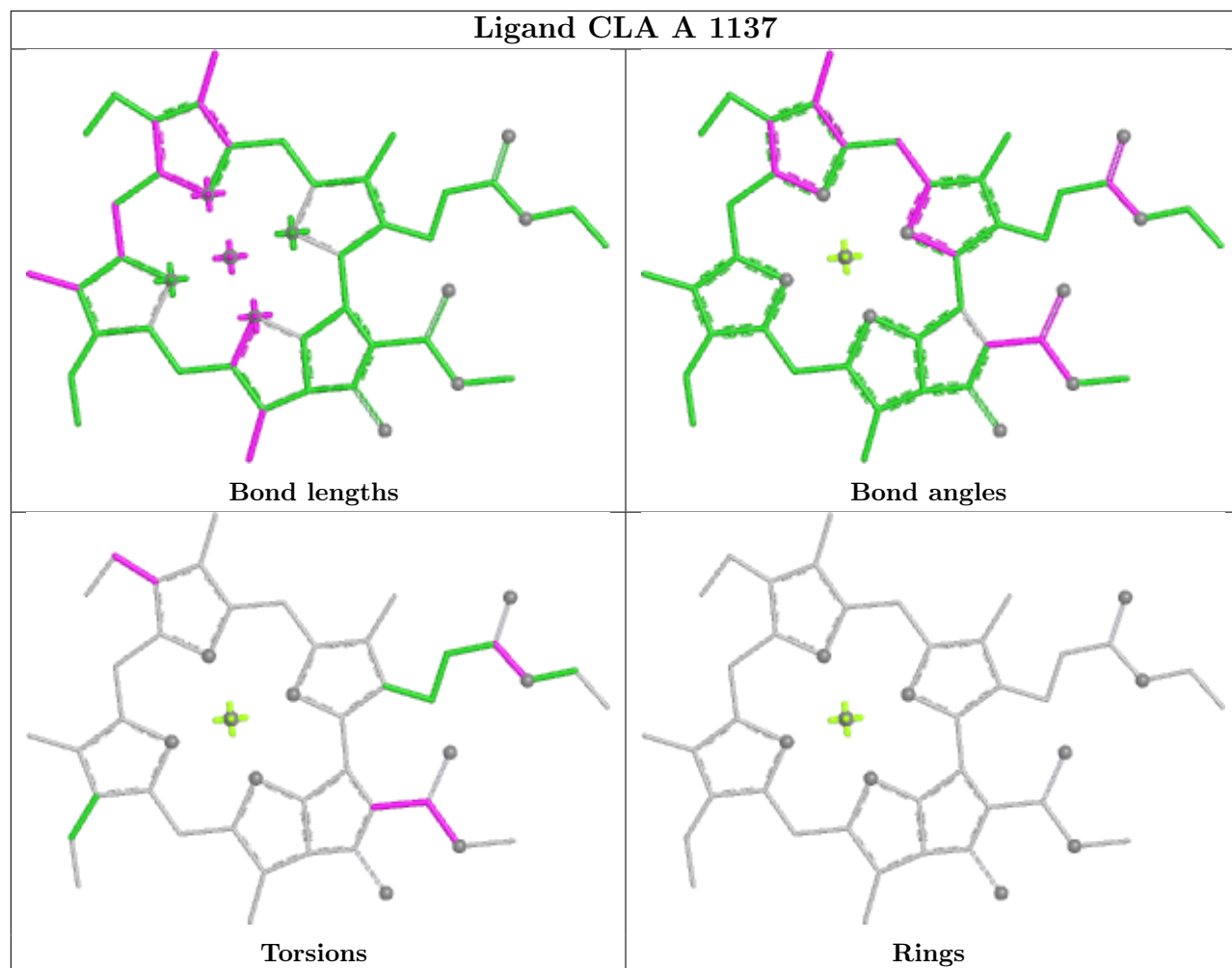
Torsions



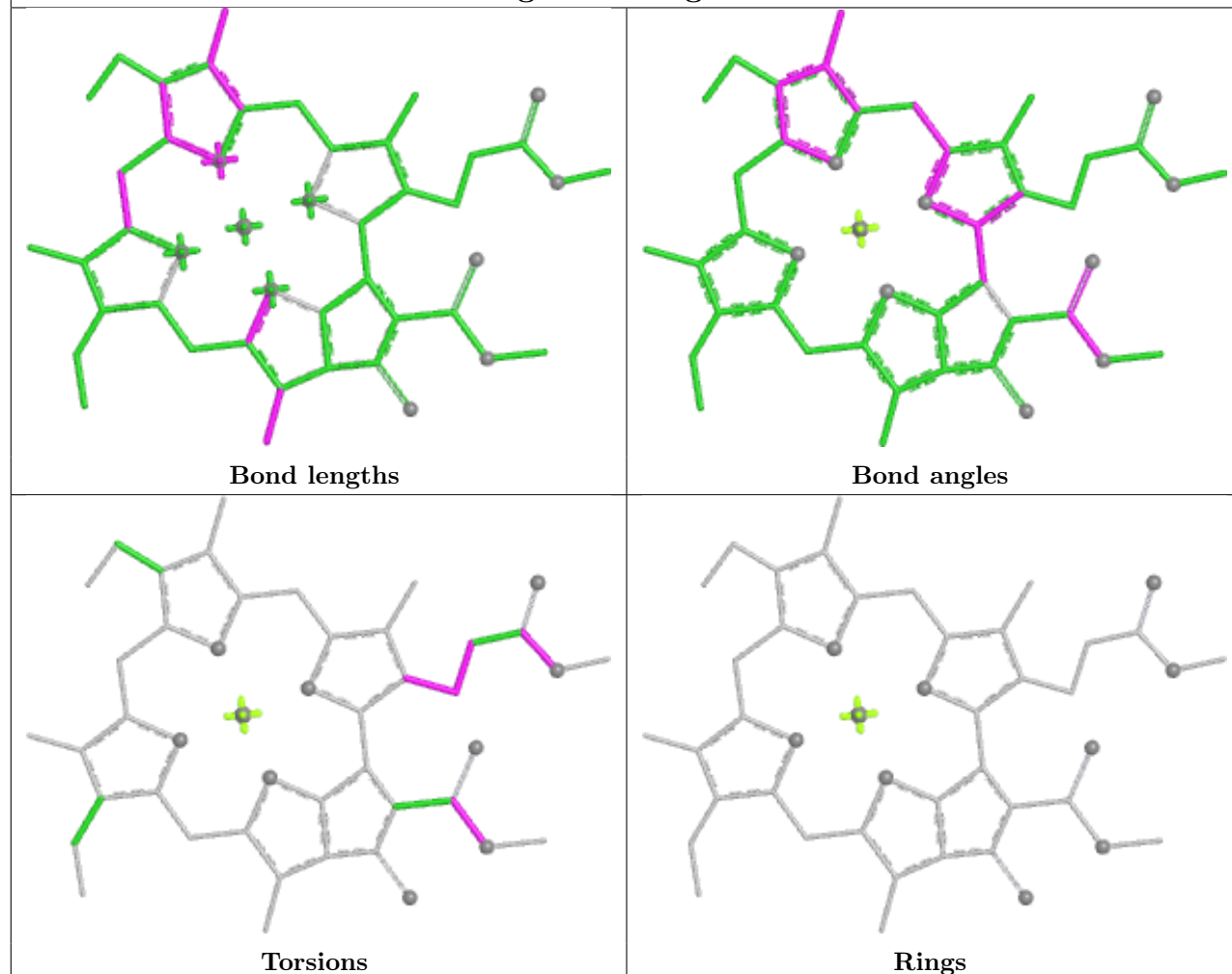
Rings



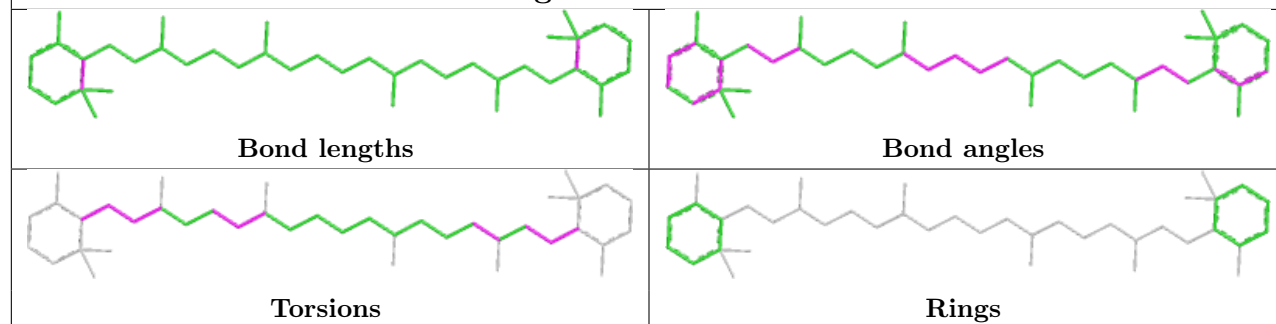
Ligand CLA A 1137



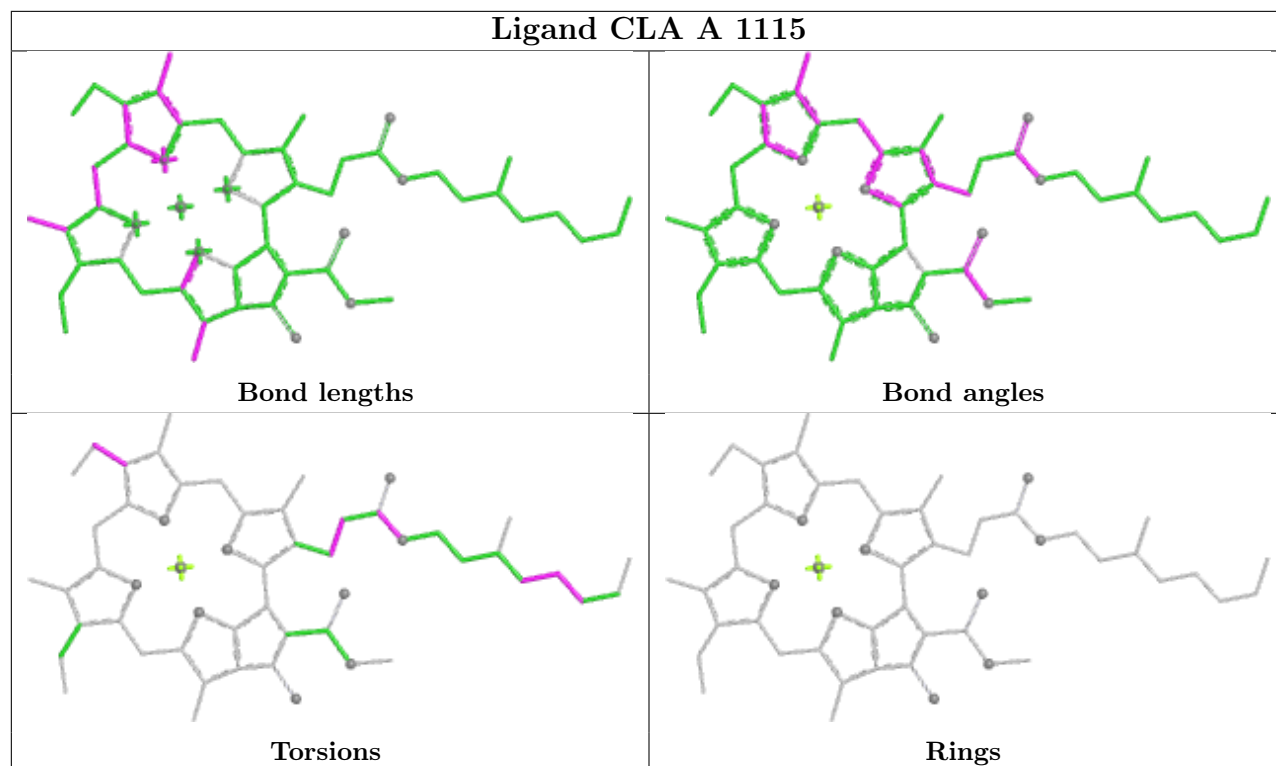
Ligand CLA g 516



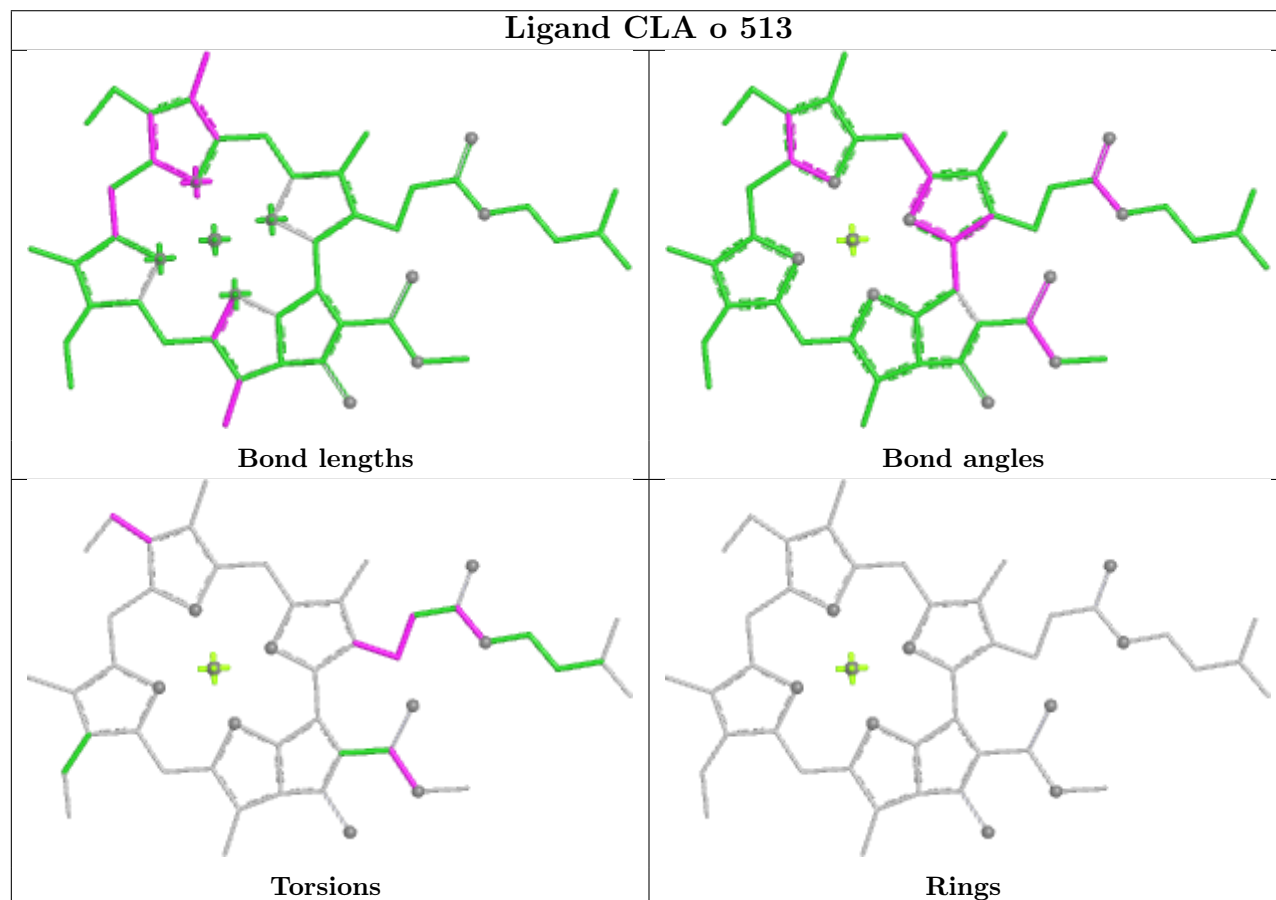
Ligand BCR o 603



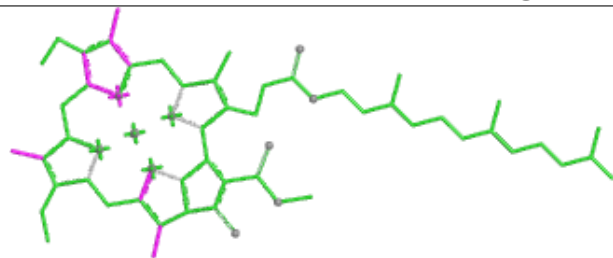
Ligand CLA A 1115



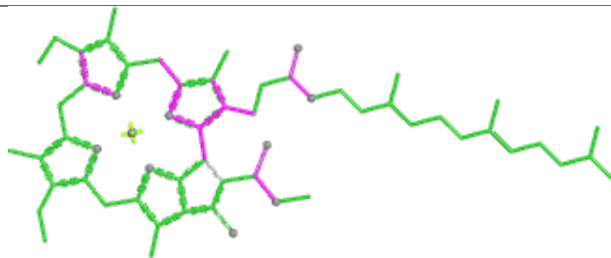
Ligand CLA o 513



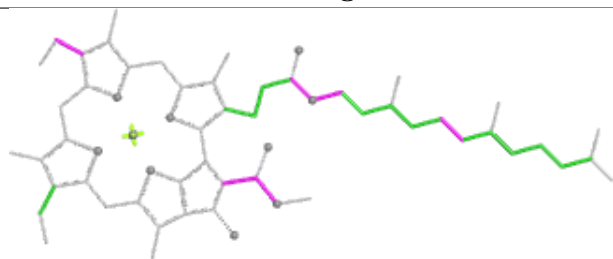
Ligand CLA u 506



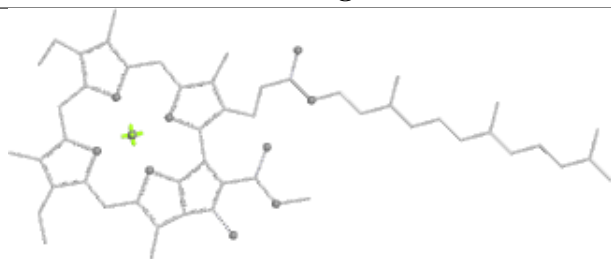
Bond lengths



Bond angles

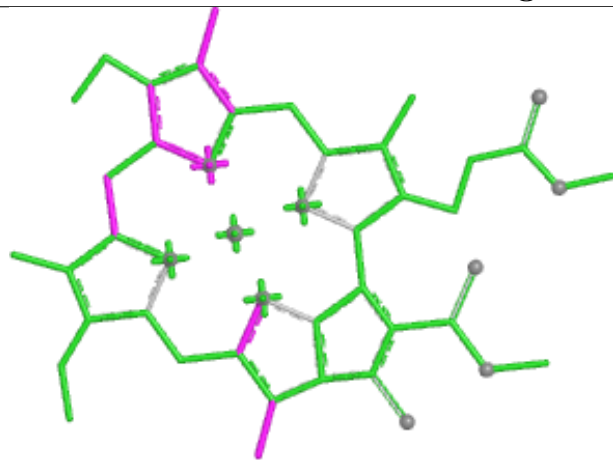


Torsions

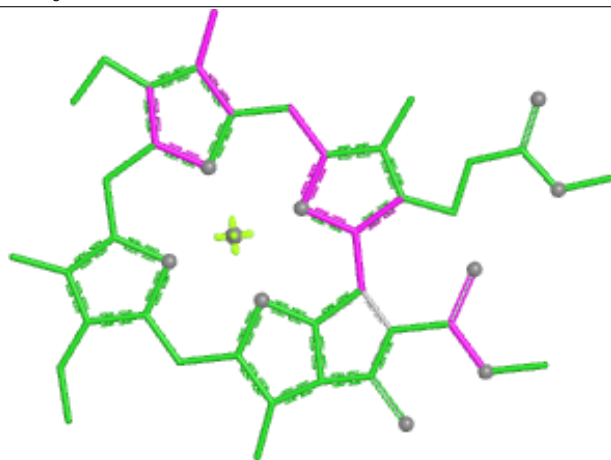


Rings

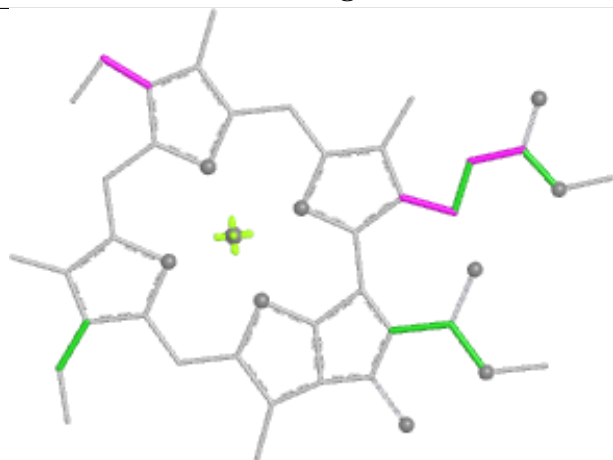
Ligand CLA y 516



Bond lengths



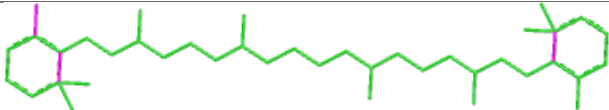
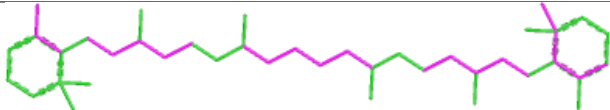
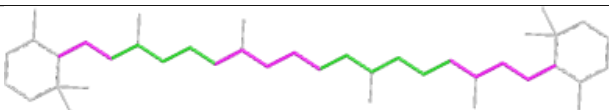
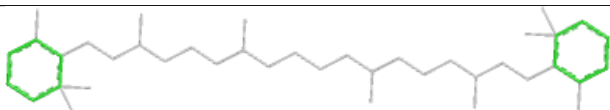
Bond angles

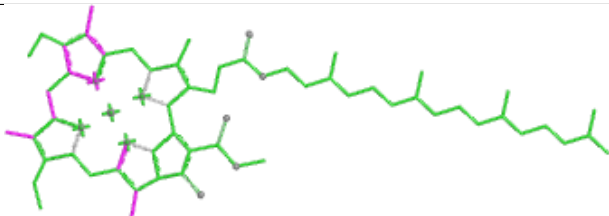
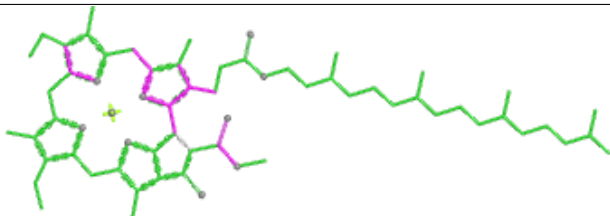
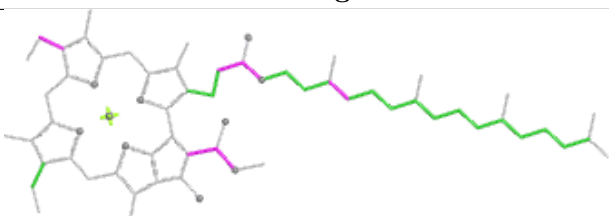
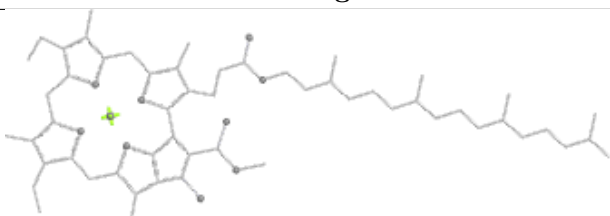


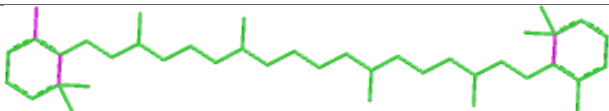
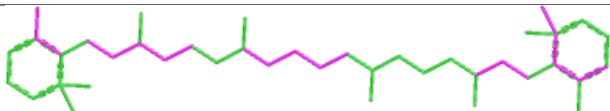
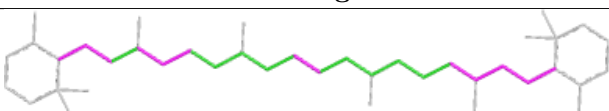
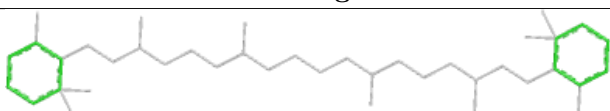
Torsions



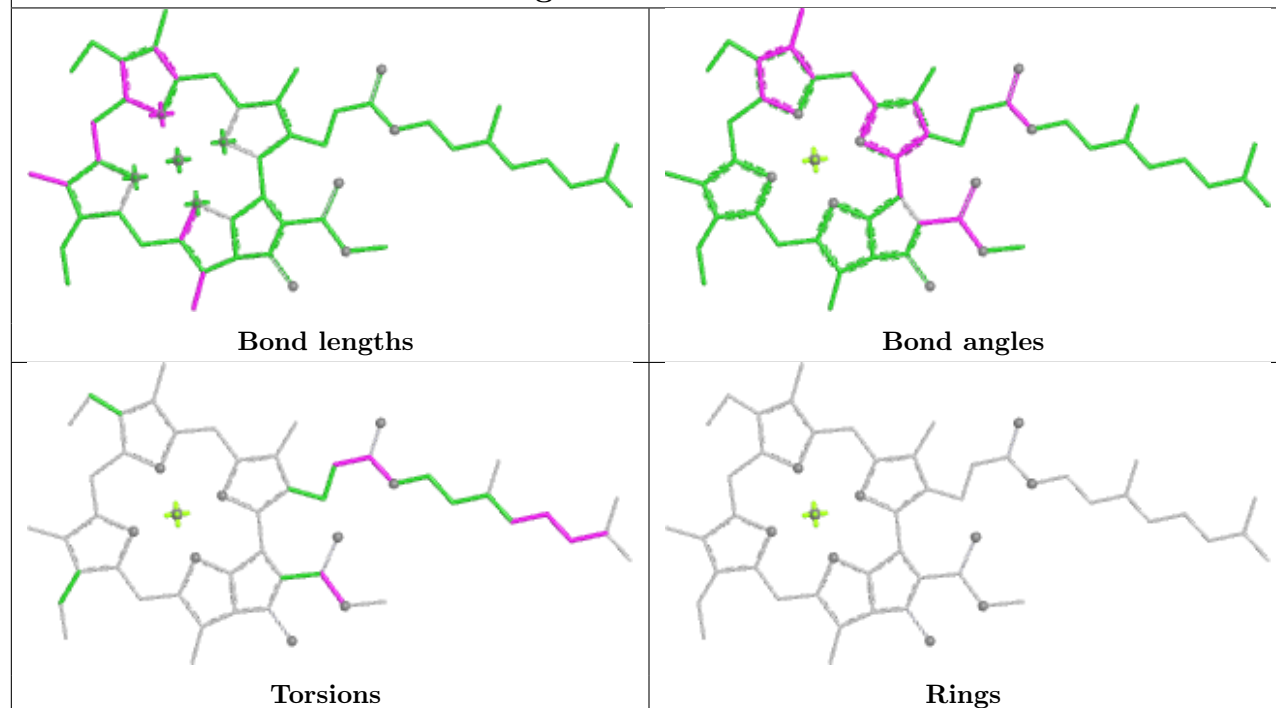
Rings

Ligand BCR G 4010	
	
Bond lengths	Bond angles
	
Torsions	Rings

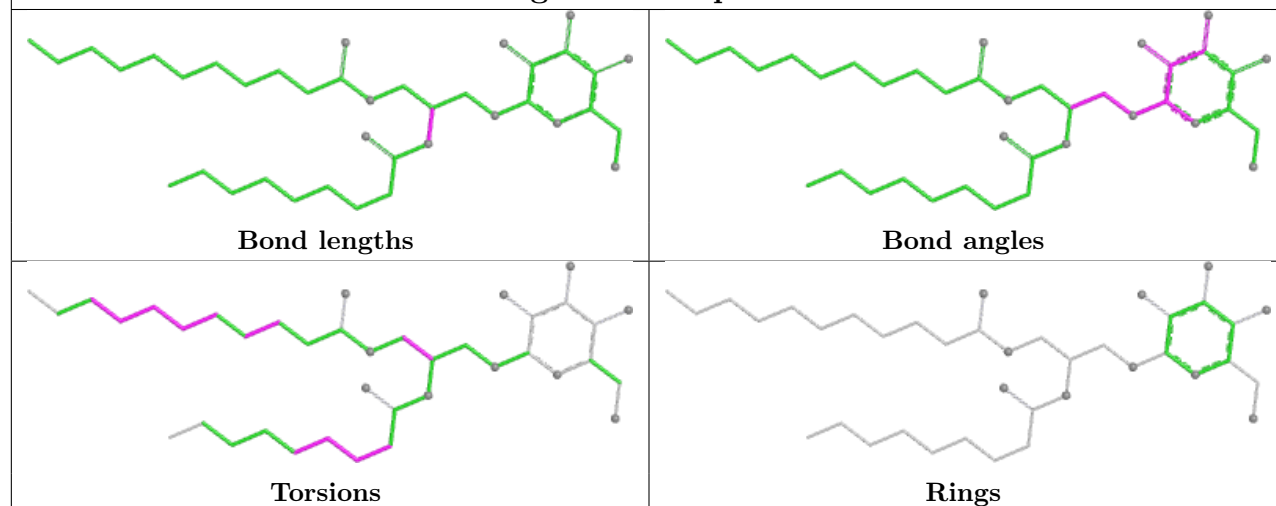
Ligand CLA y 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

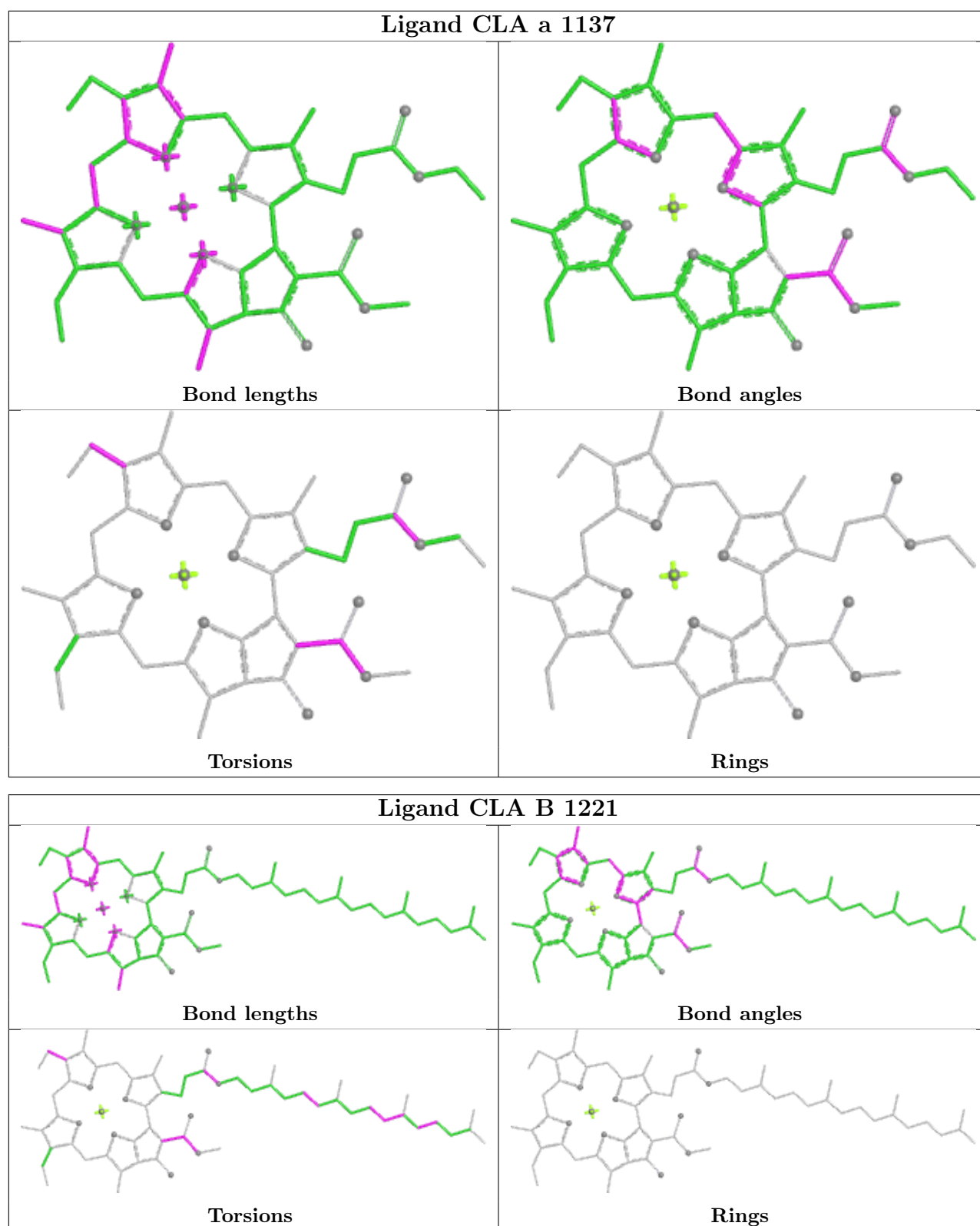
Ligand BCR j 4015	
	
Bond lengths	Bond angles
	
Torsions	Rings

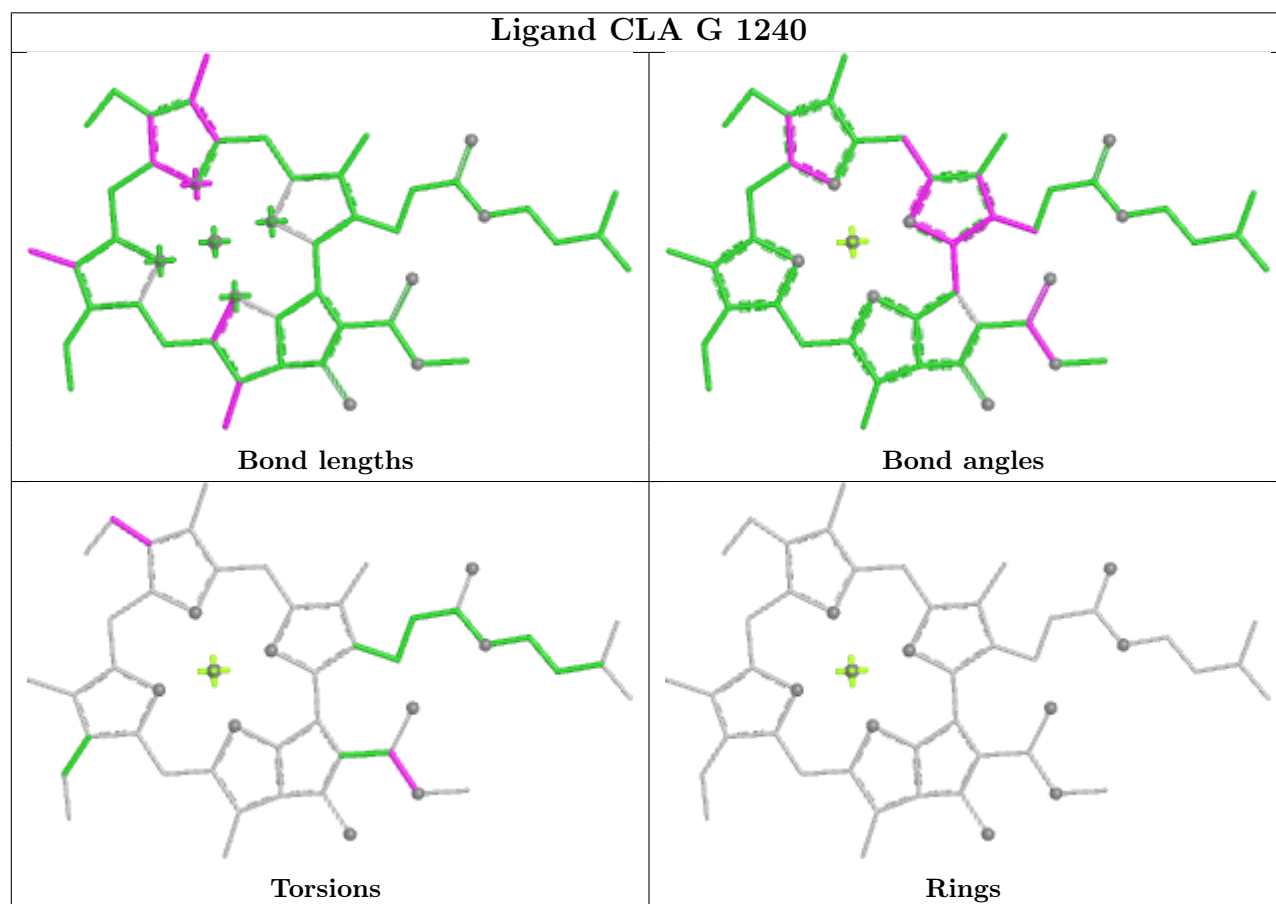
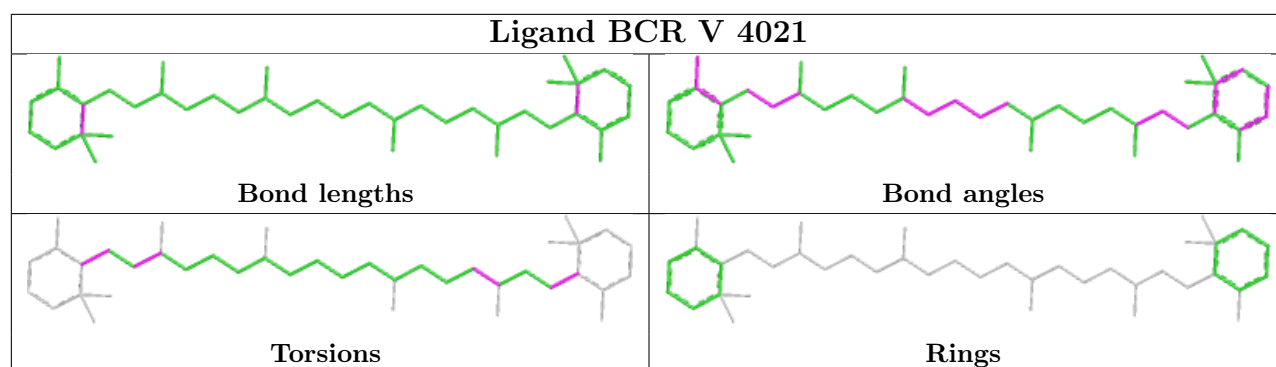
Ligand CLA u 517

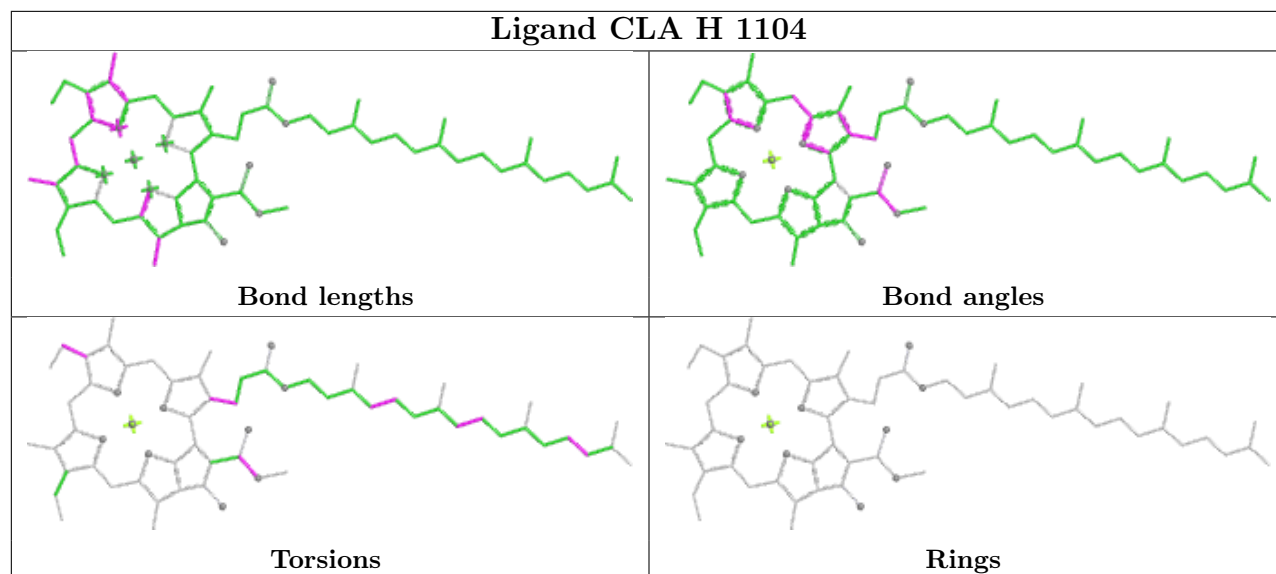
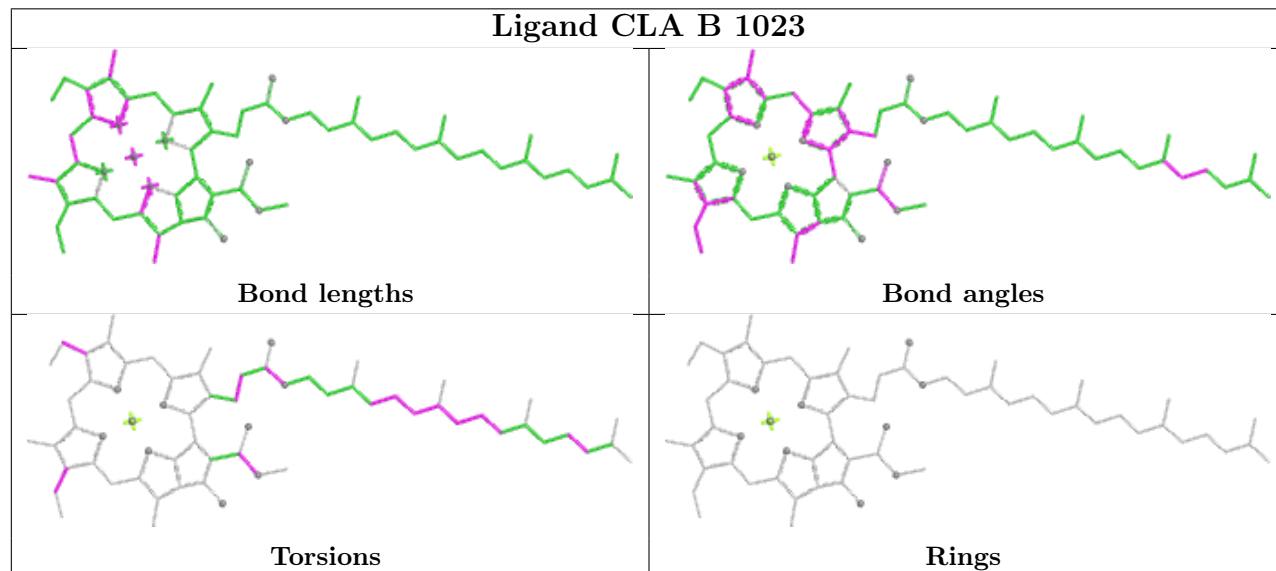


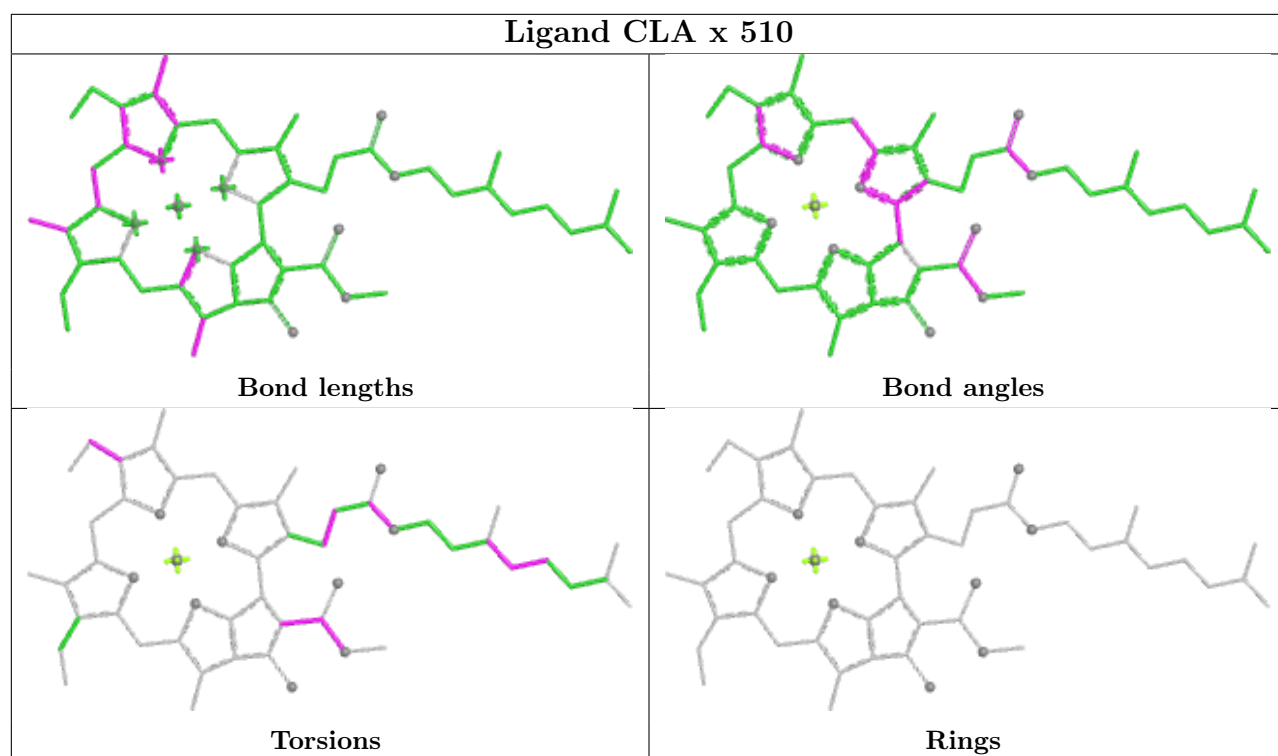
Ligand LMG p 701

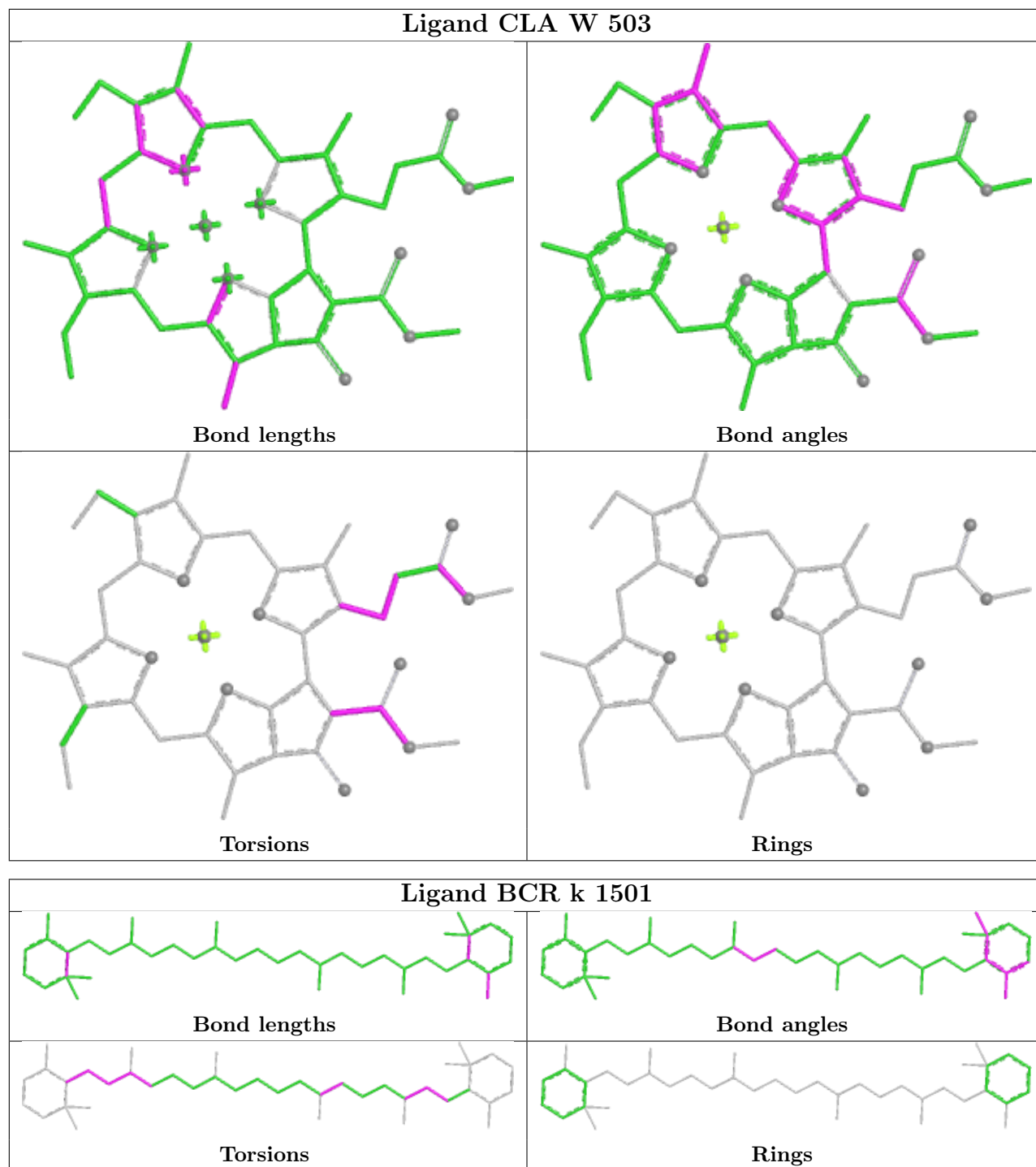


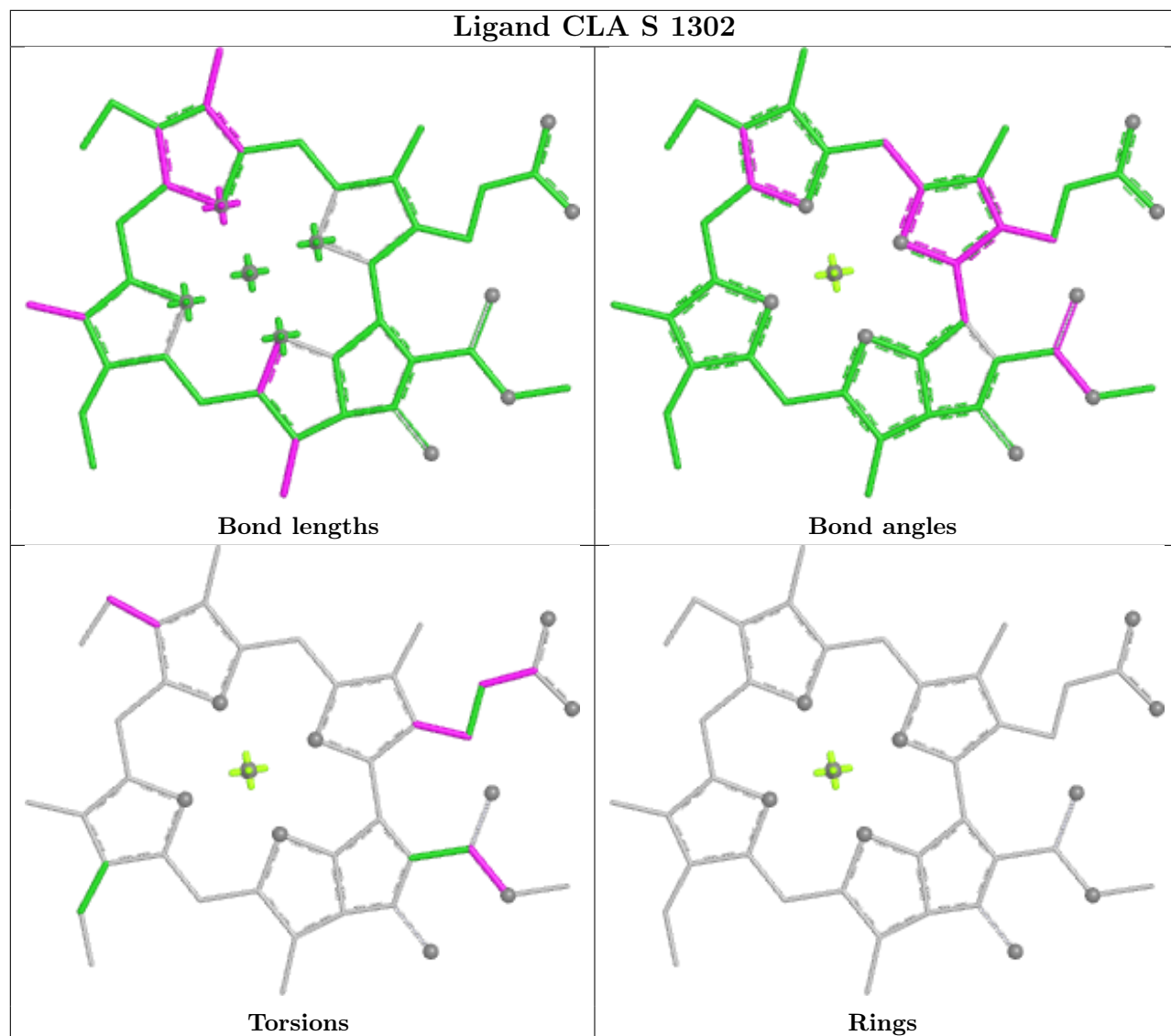


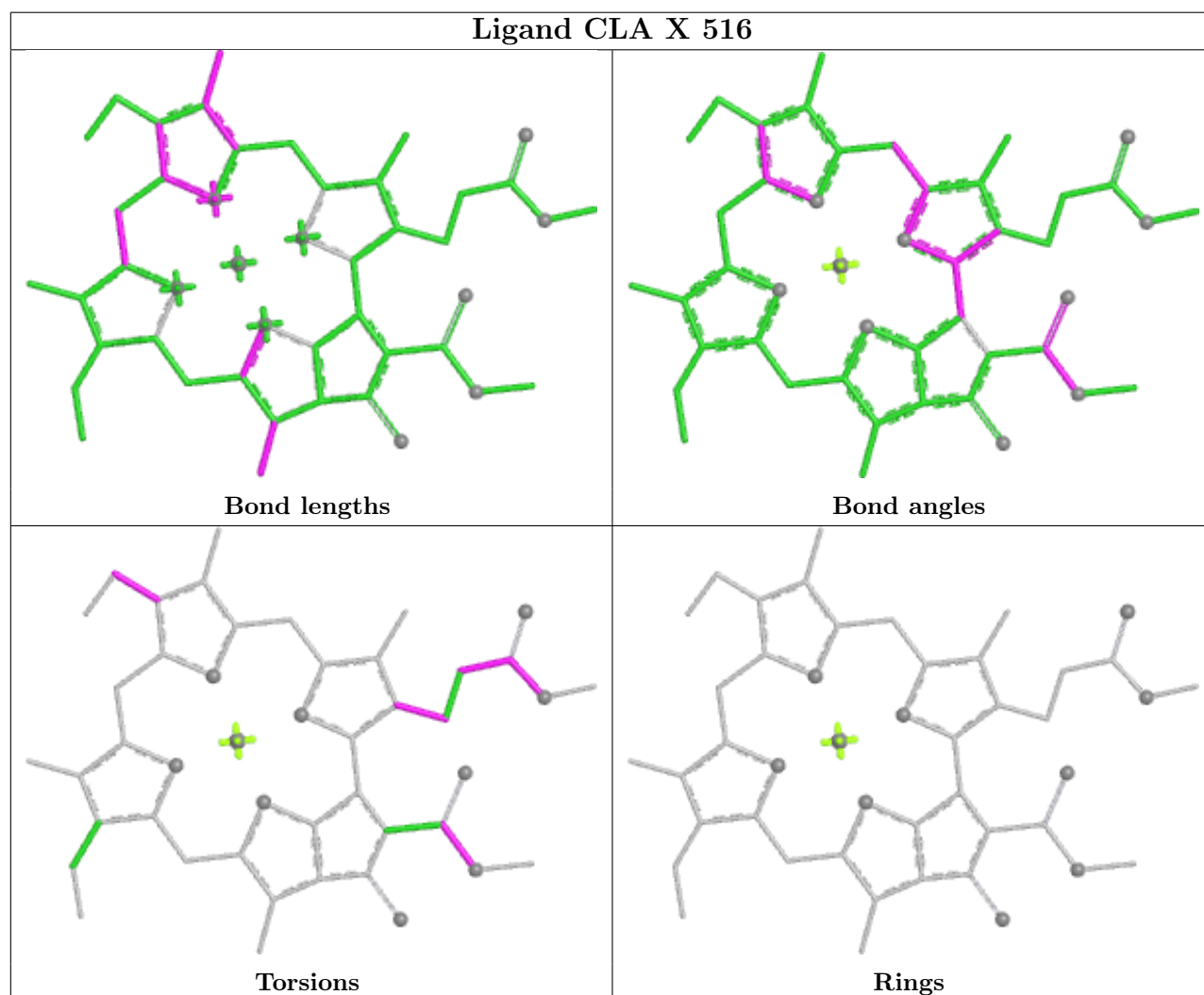
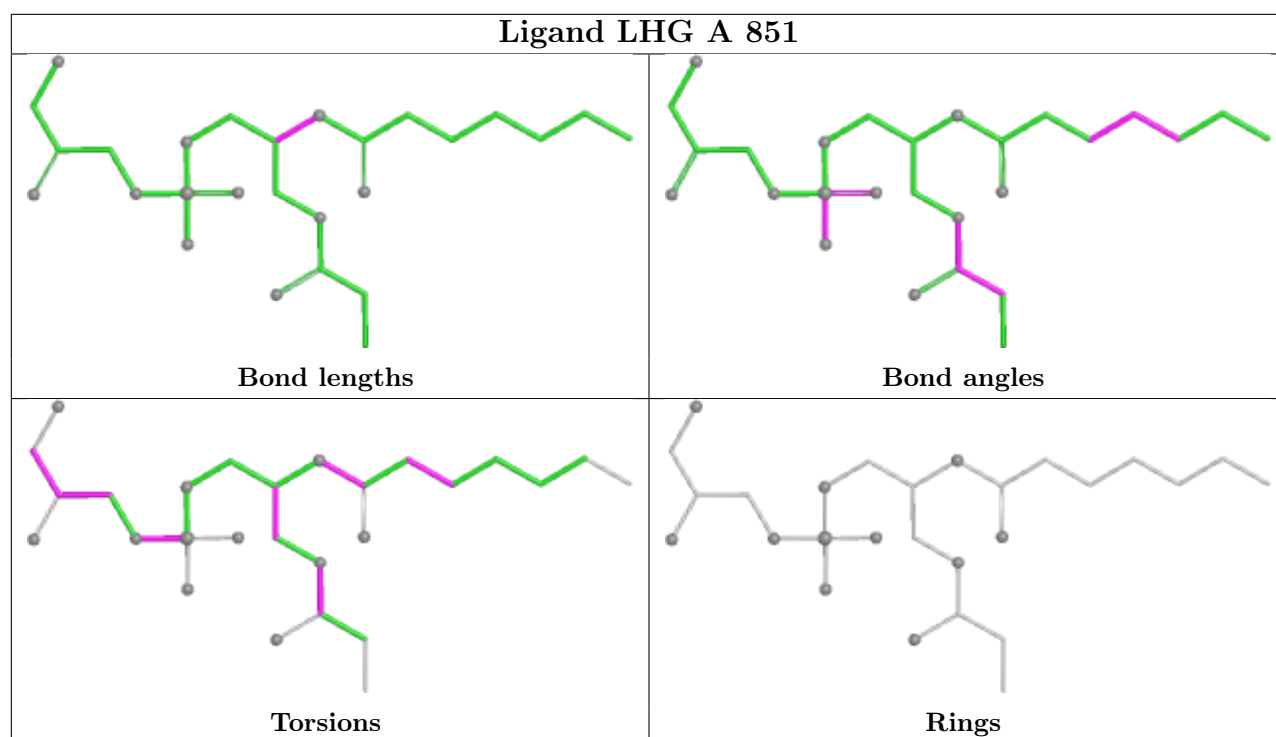


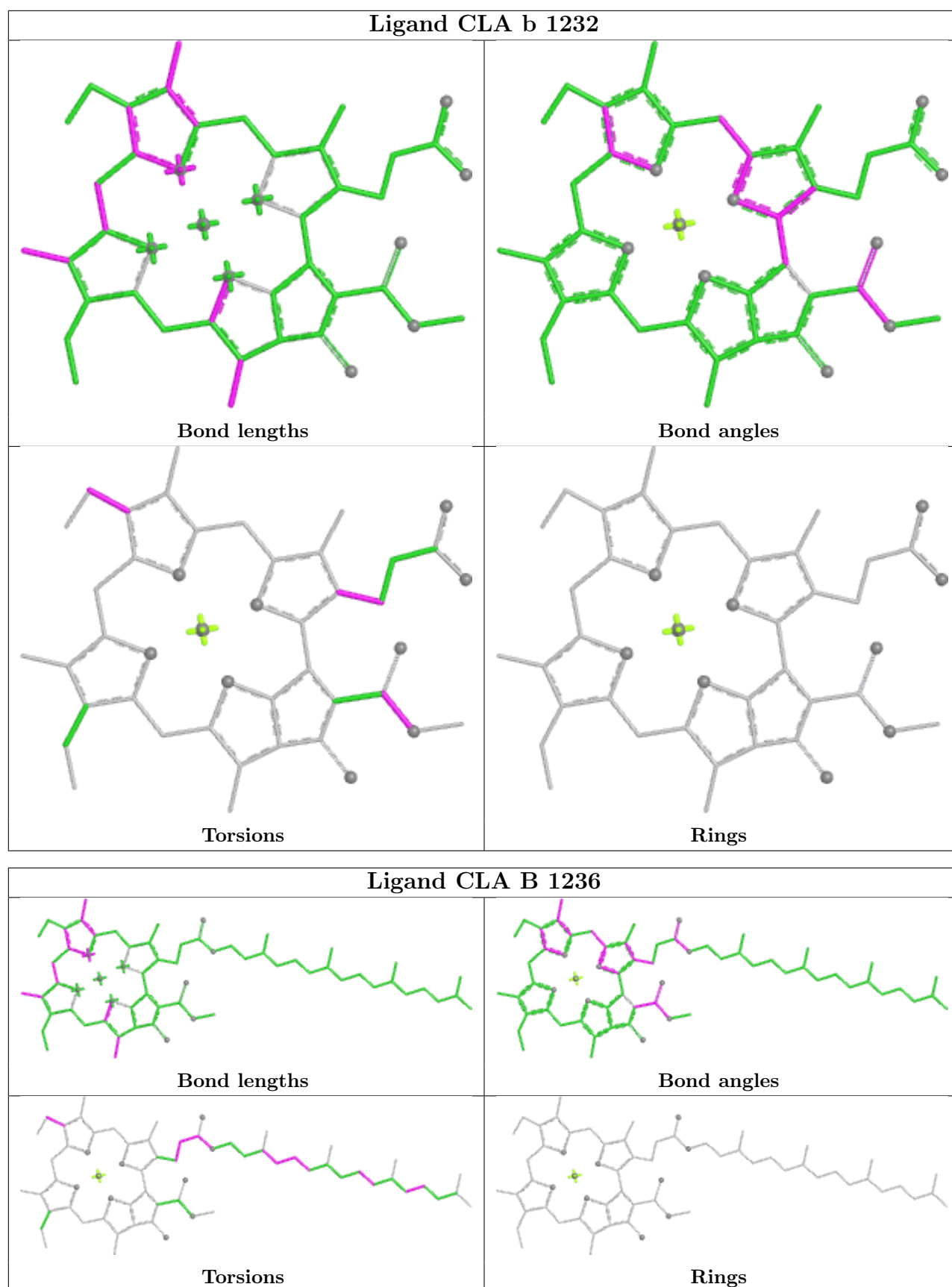
Ligand CLA H 1104**Ligand CLA B 1023**

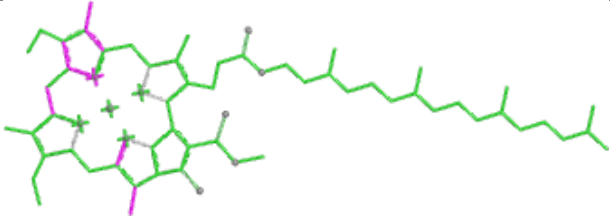
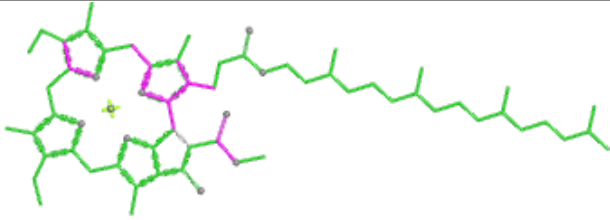
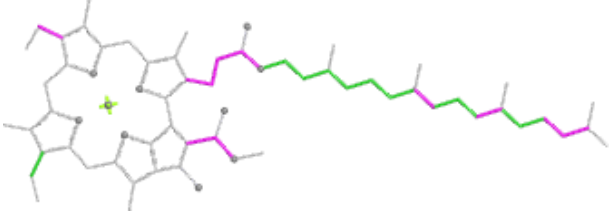
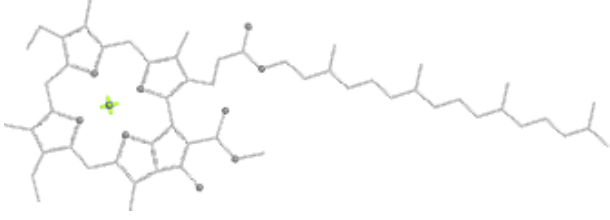
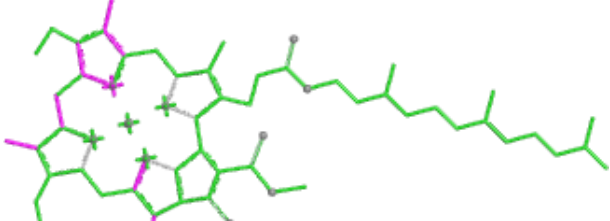
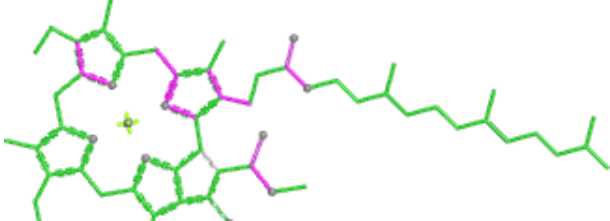
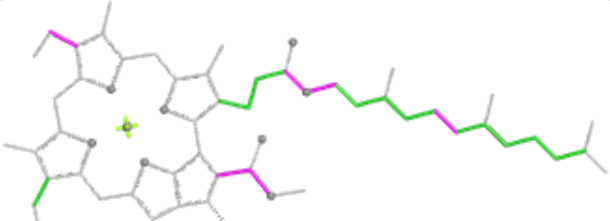
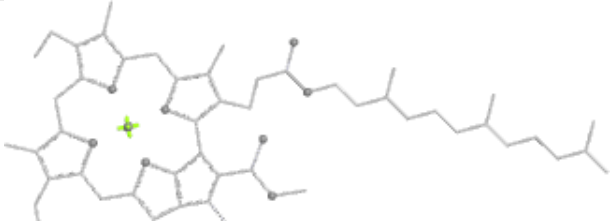
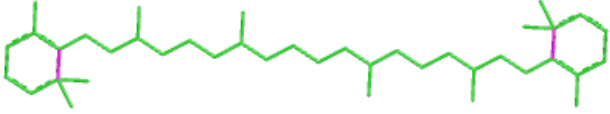
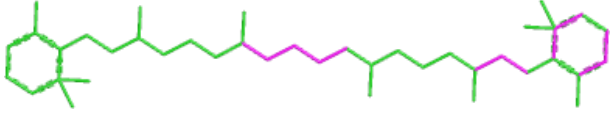
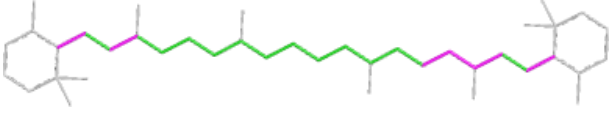
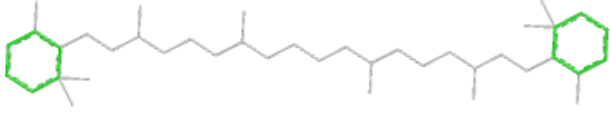


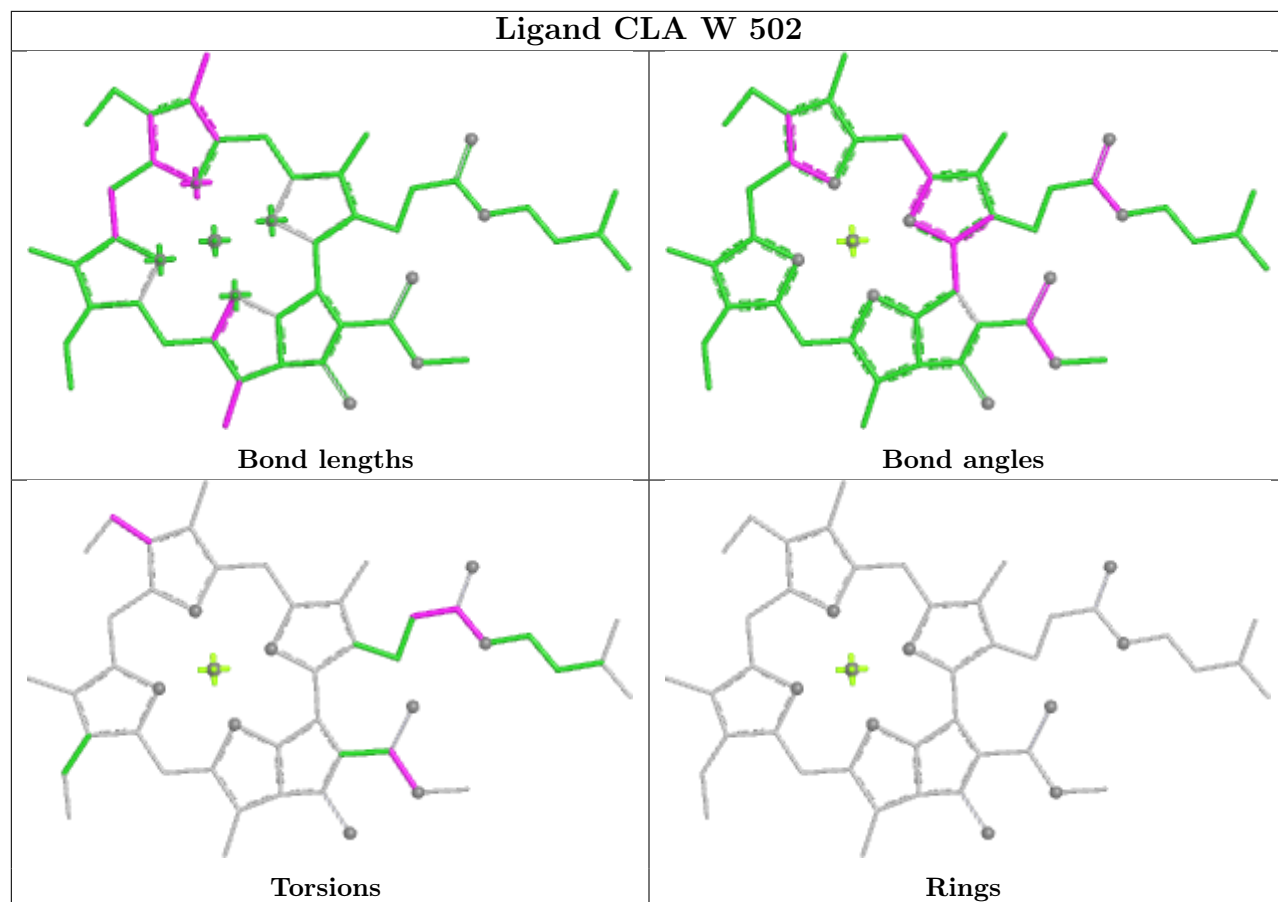




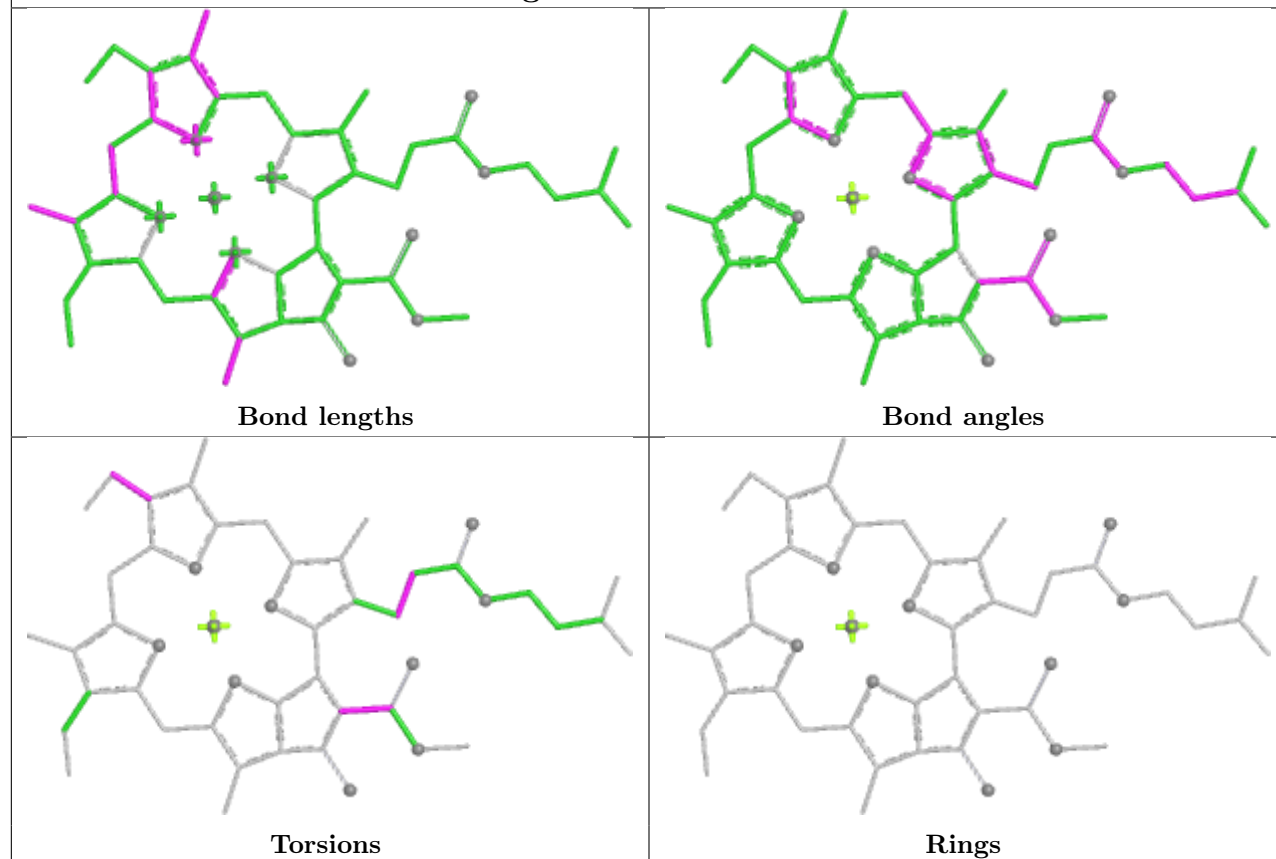




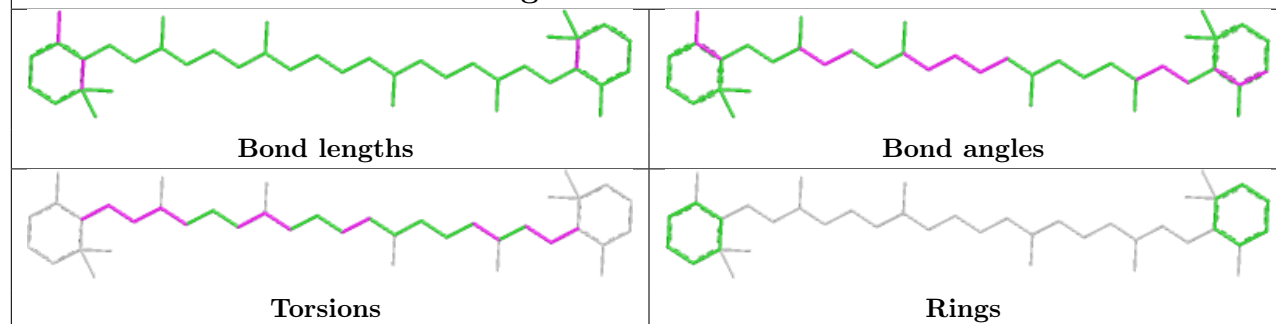
Ligand CLA Z 505	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA o 506	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 4004	
 Bond lengths	 Bond angles
 Torsions	 Rings



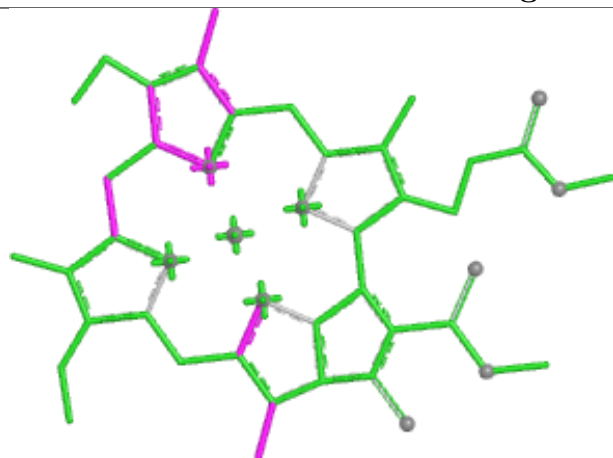
Ligand CLA H 1129



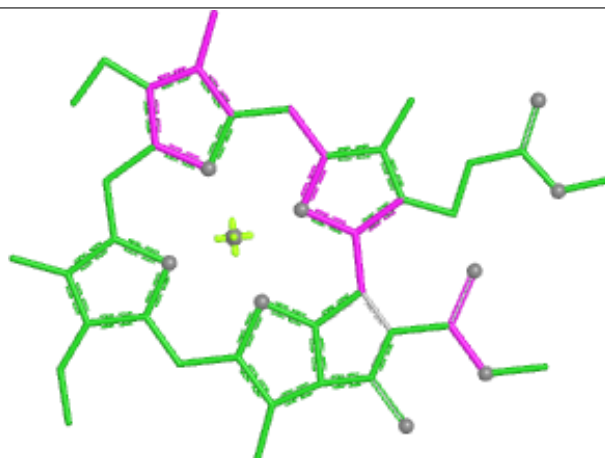
Ligand BCR R 4020



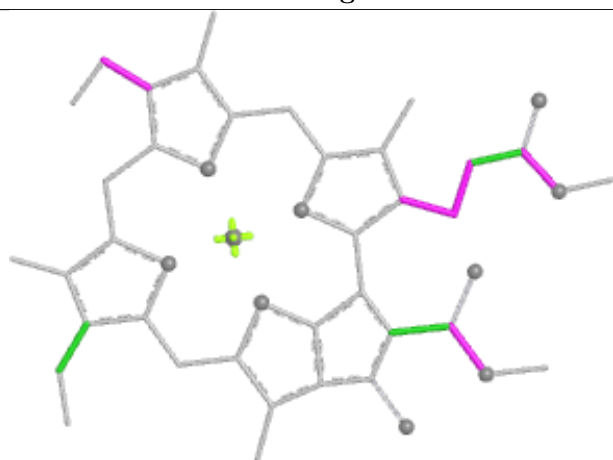
Ligand CLA r 516



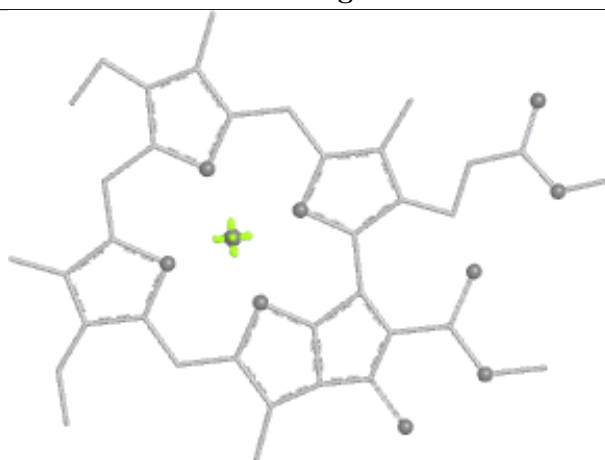
Bond lengths



Bond angles

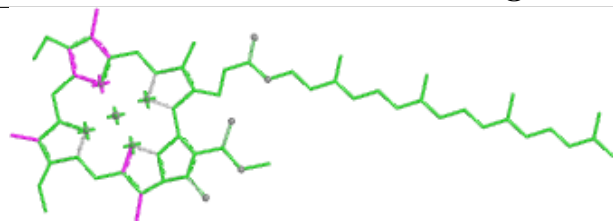


Torsions

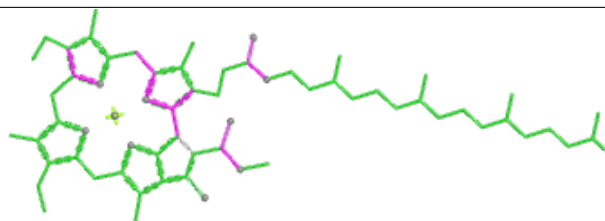


Rings

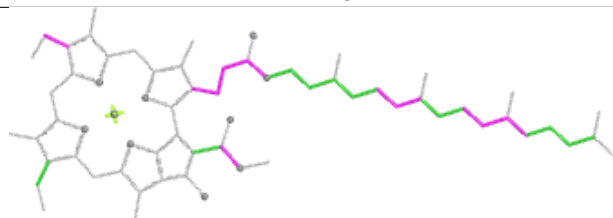
Ligand CLA B 1203



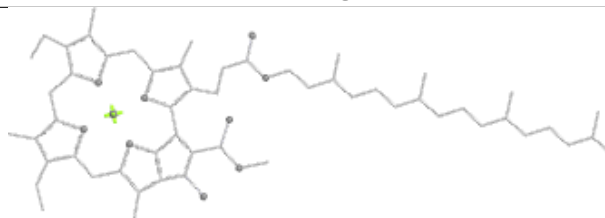
Bond lengths



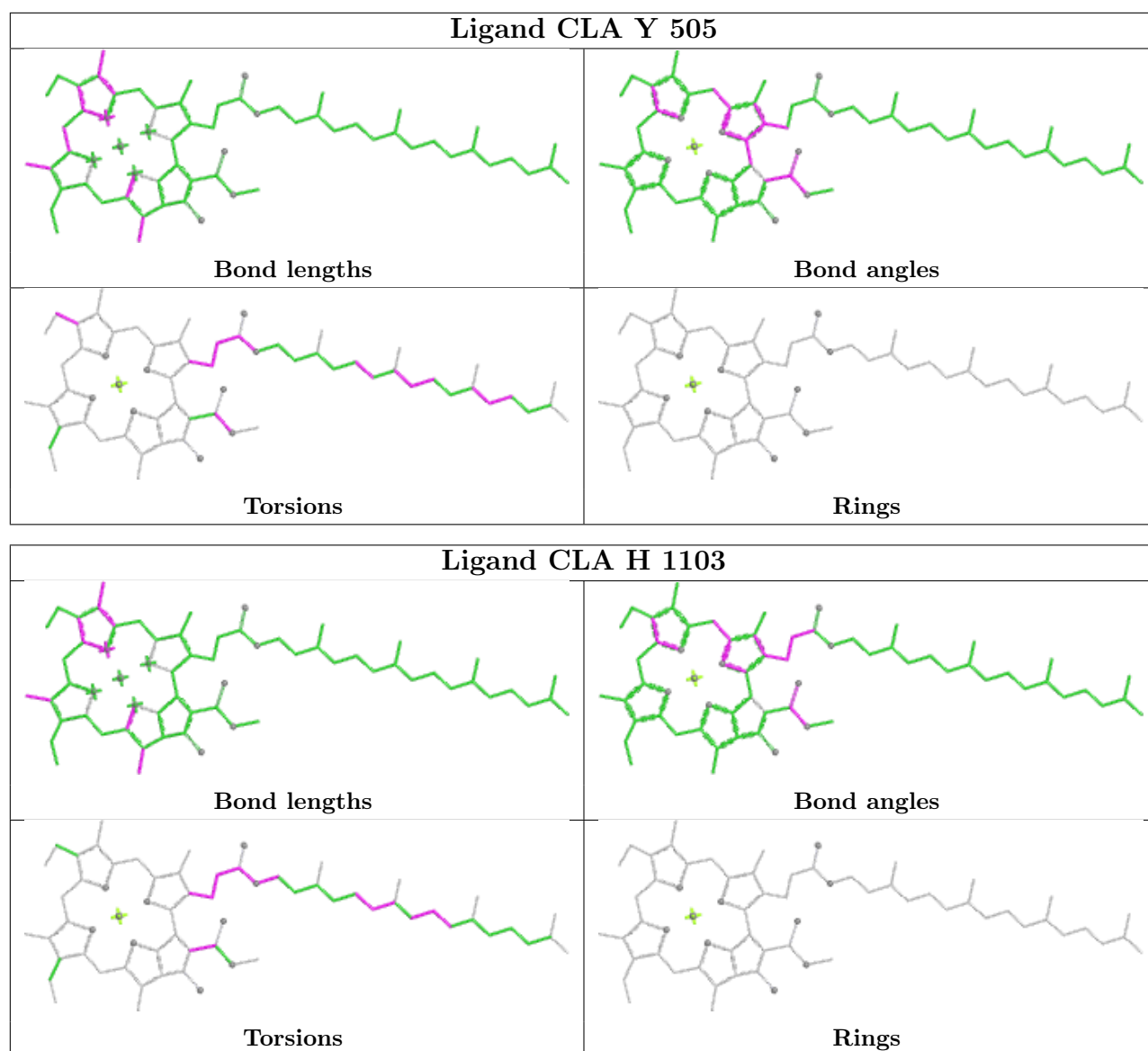
Bond angles

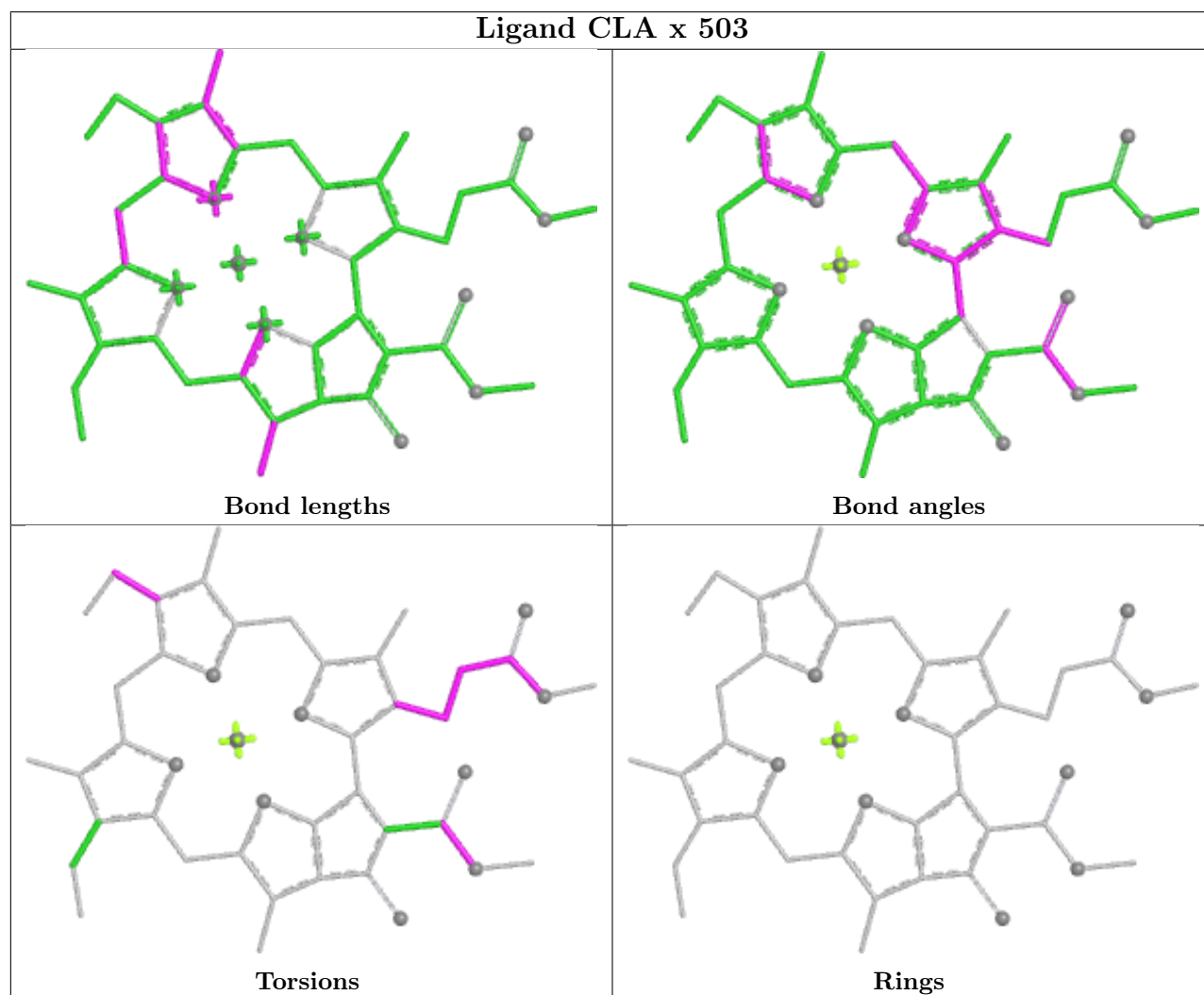
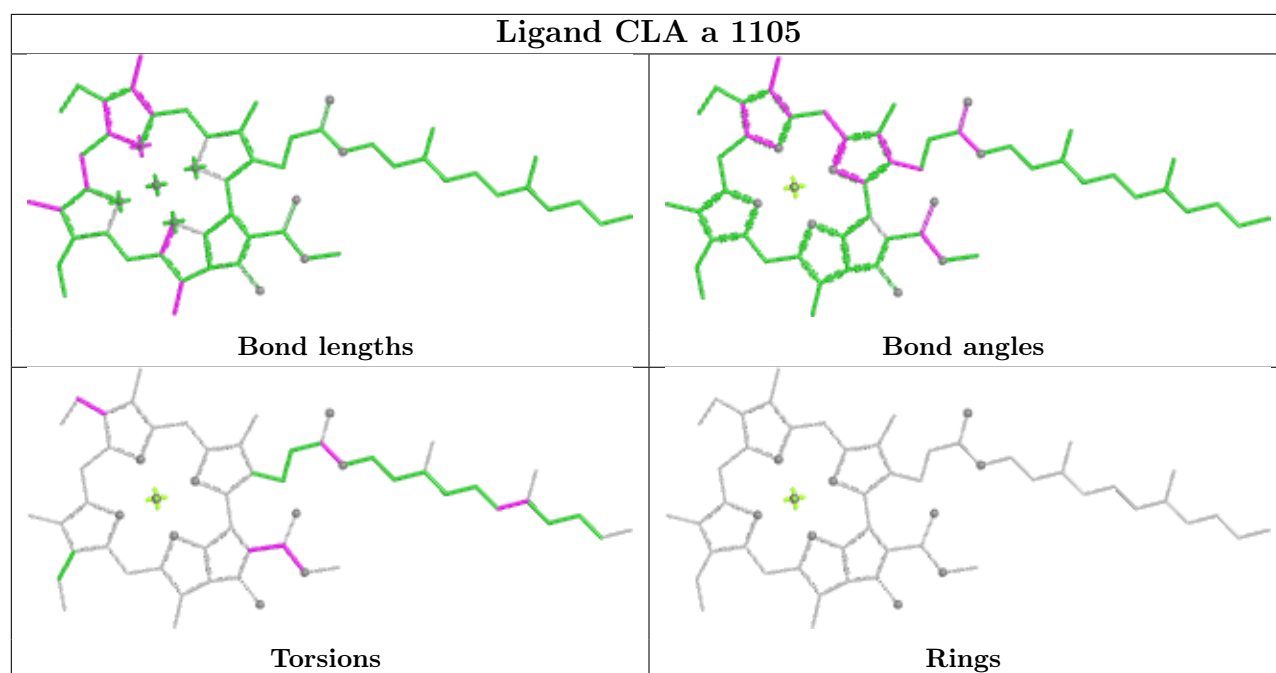


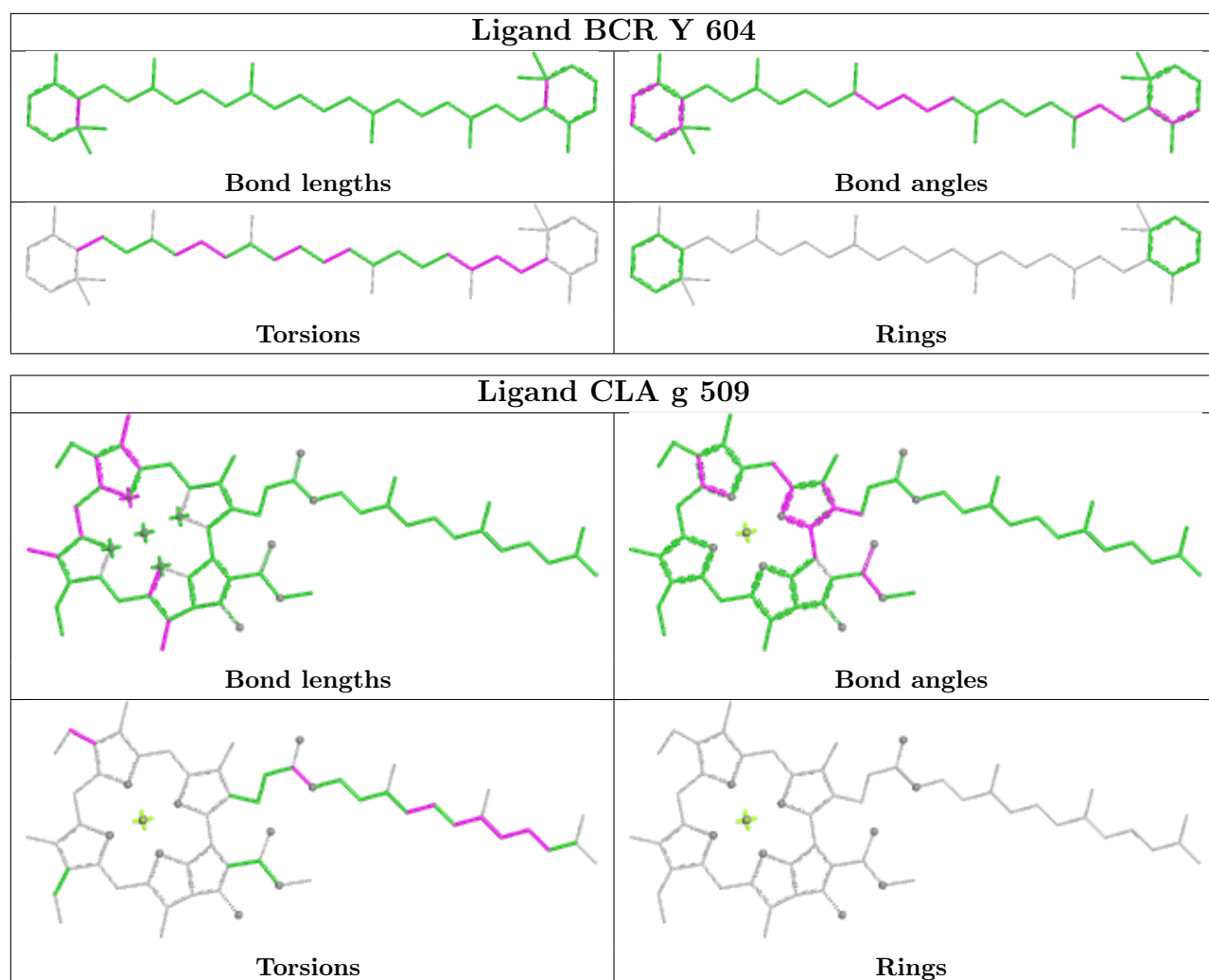
Torsions



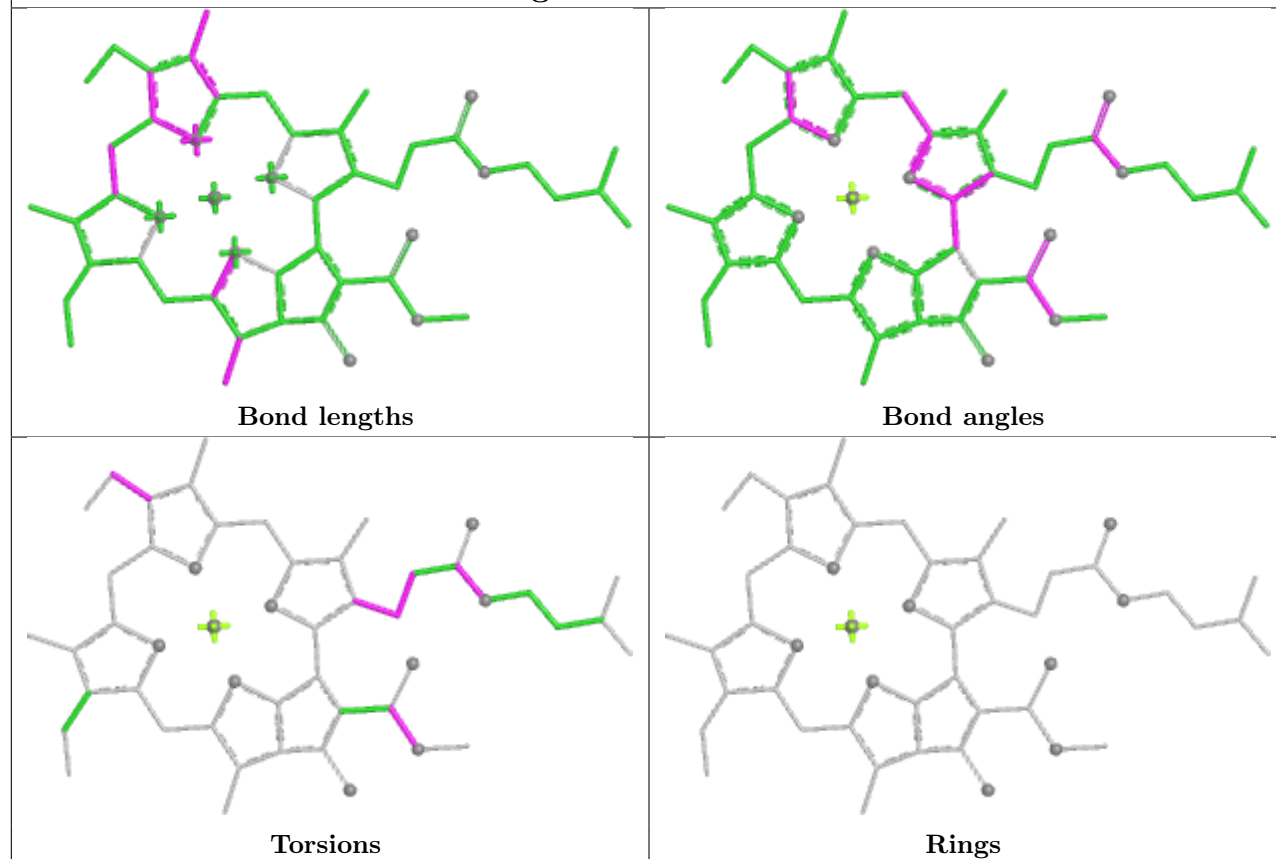
Rings



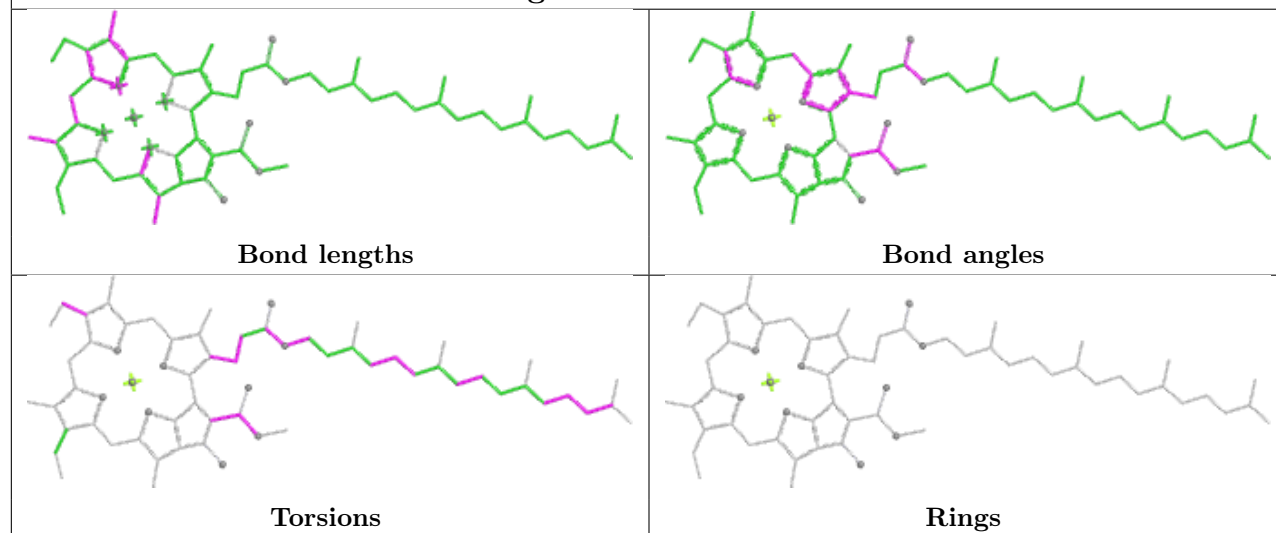




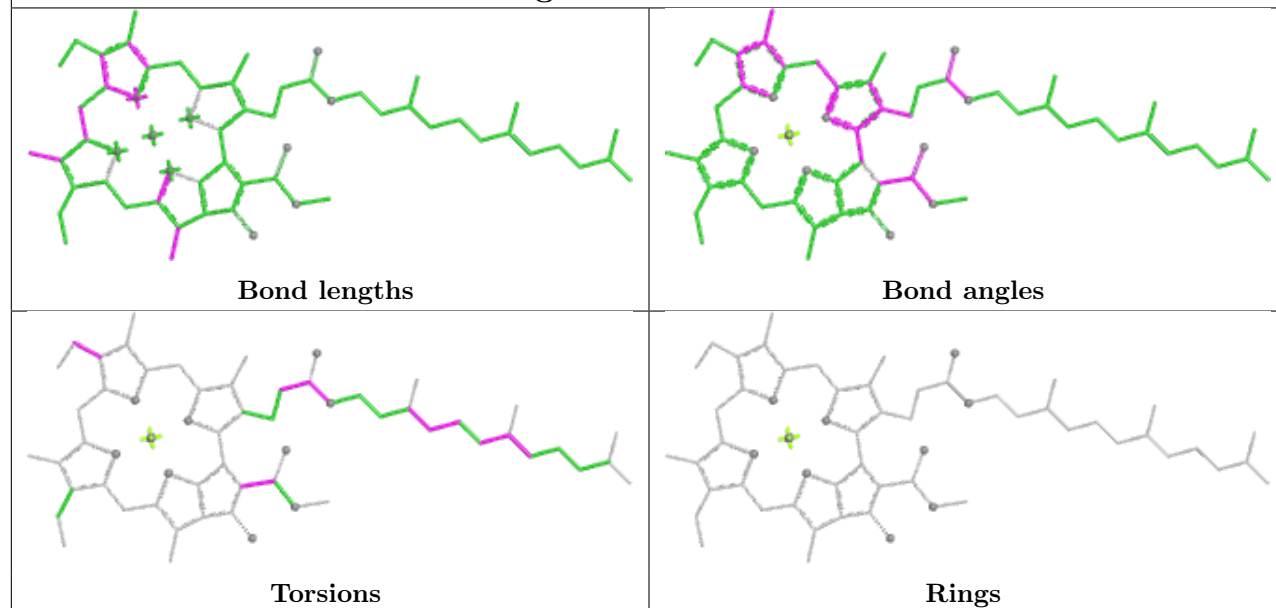
Ligand CLA X 513



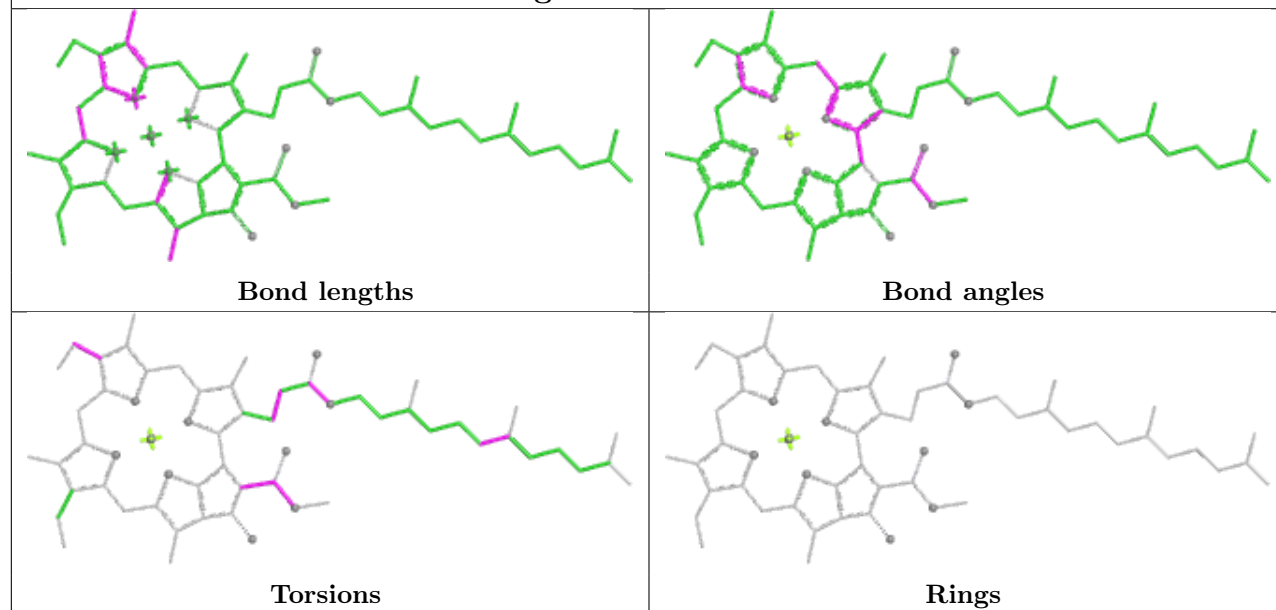
Ligand CLA a 1106

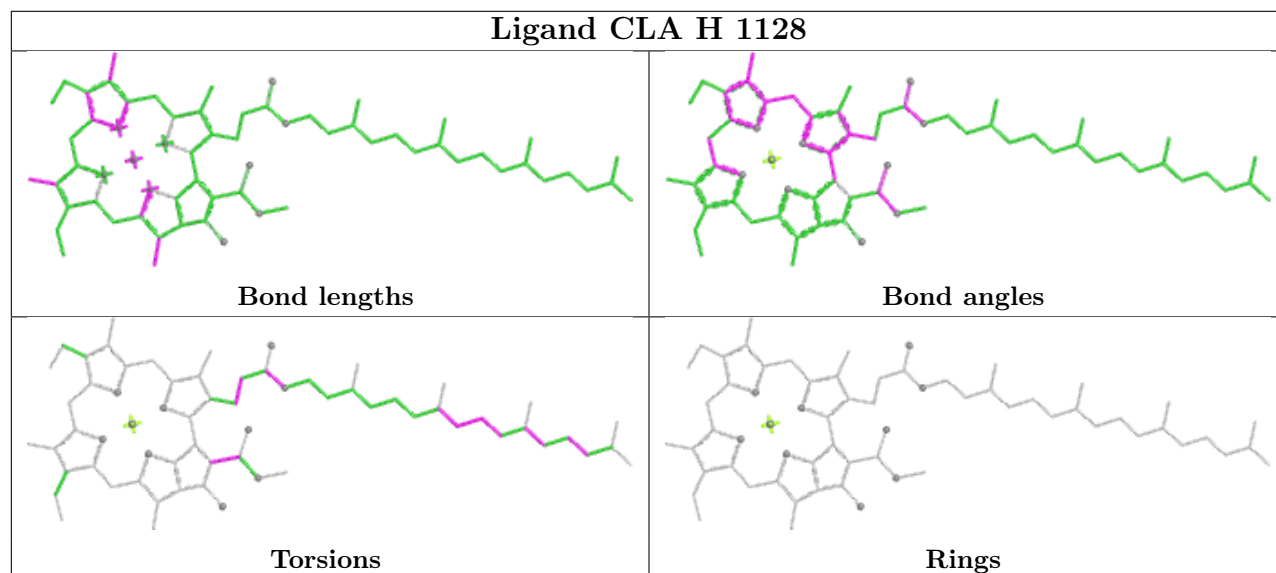
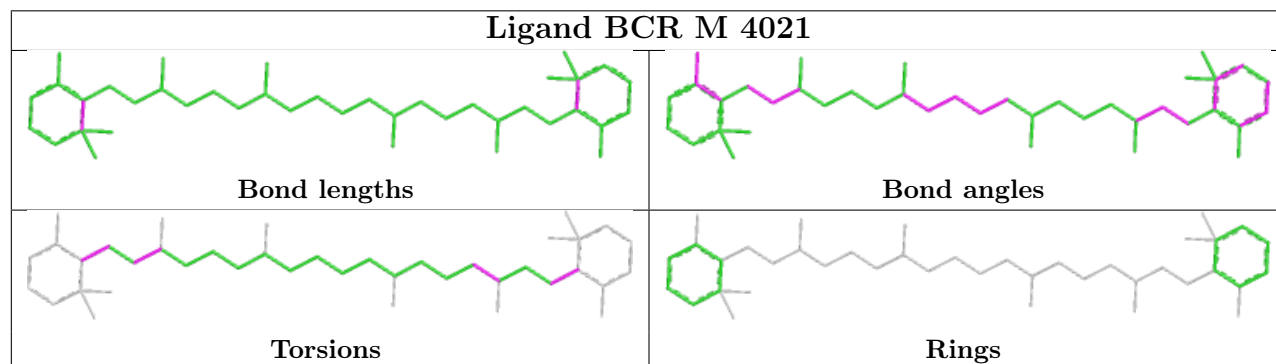
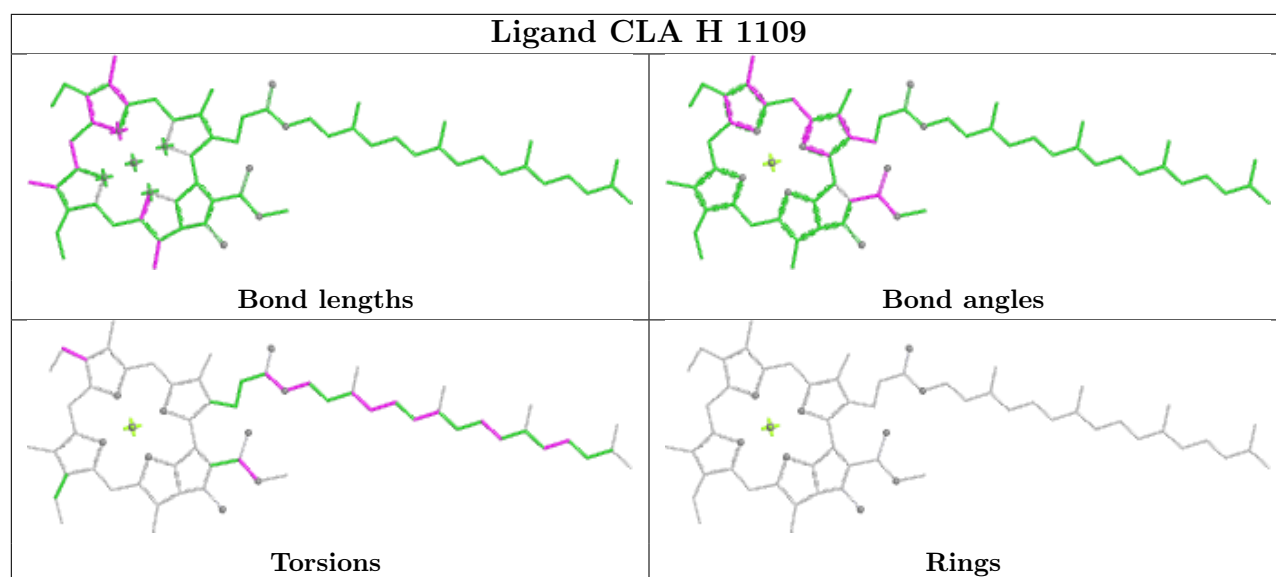


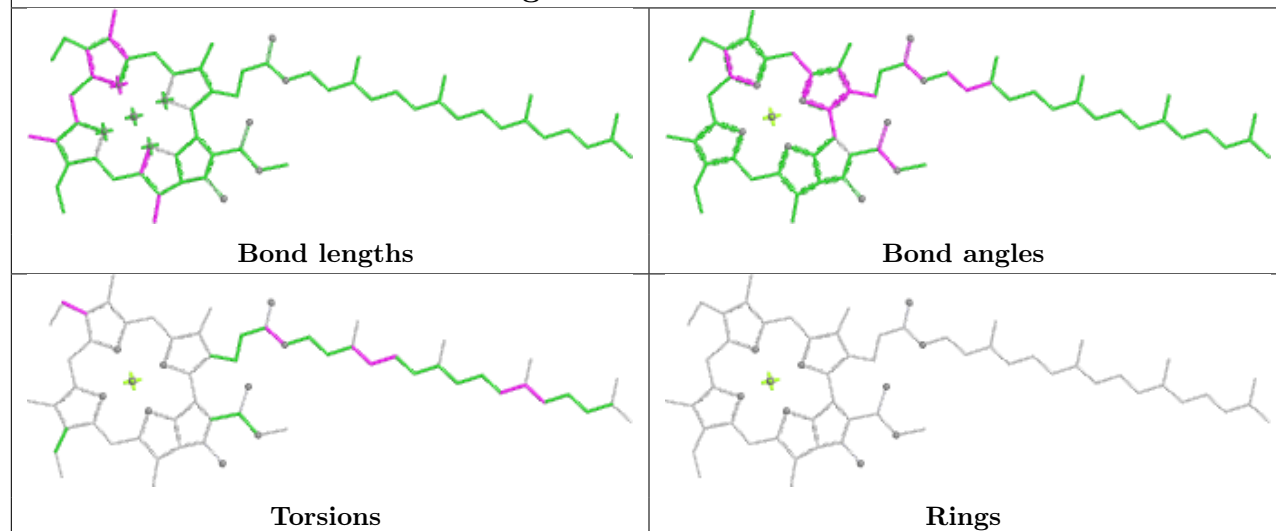
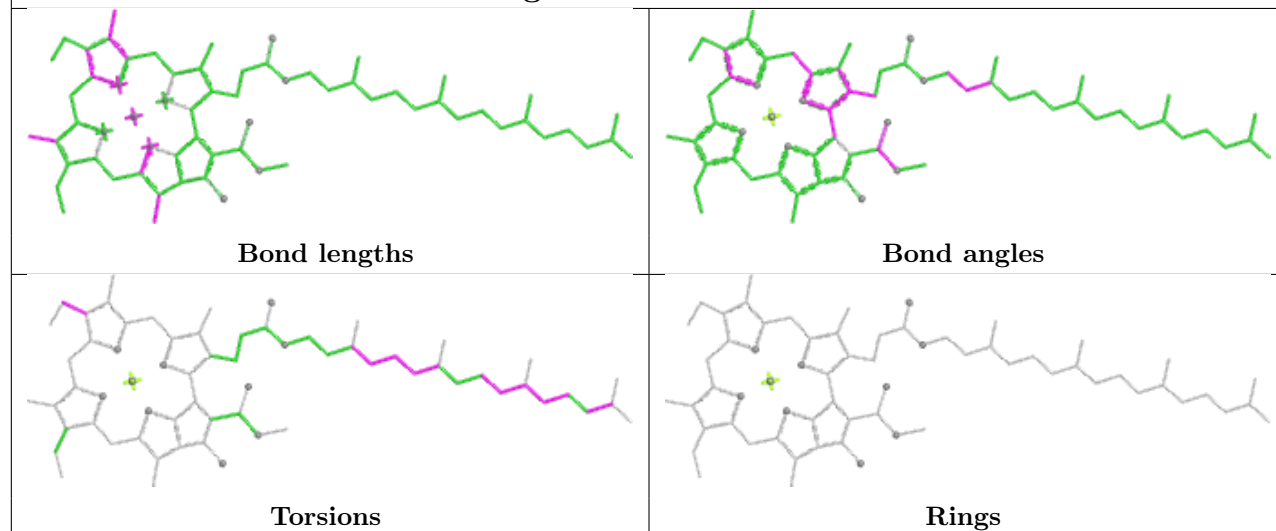
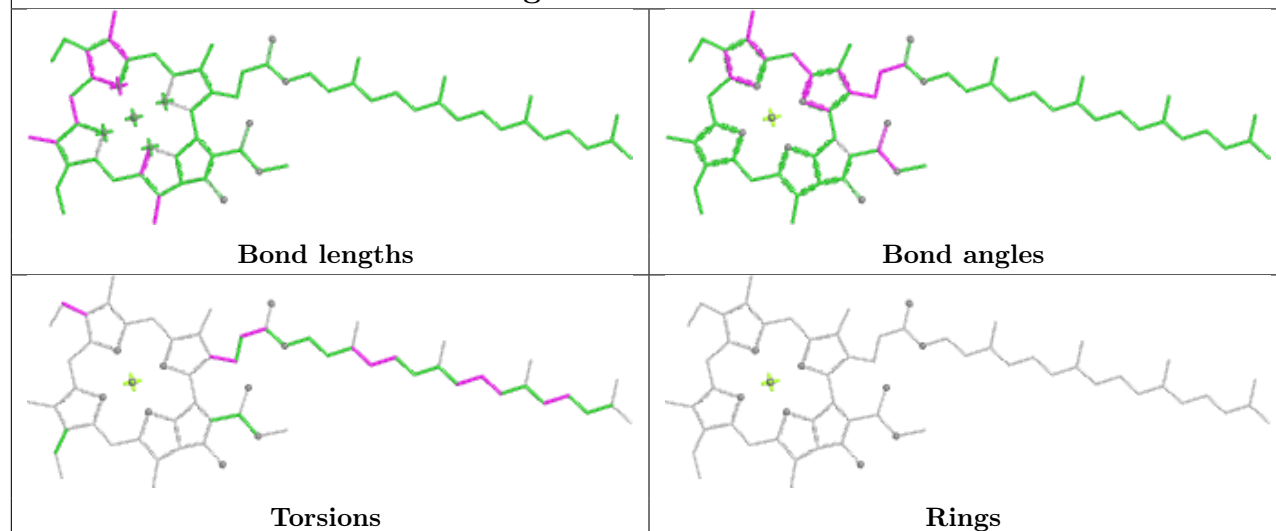
Ligand CLA v 510



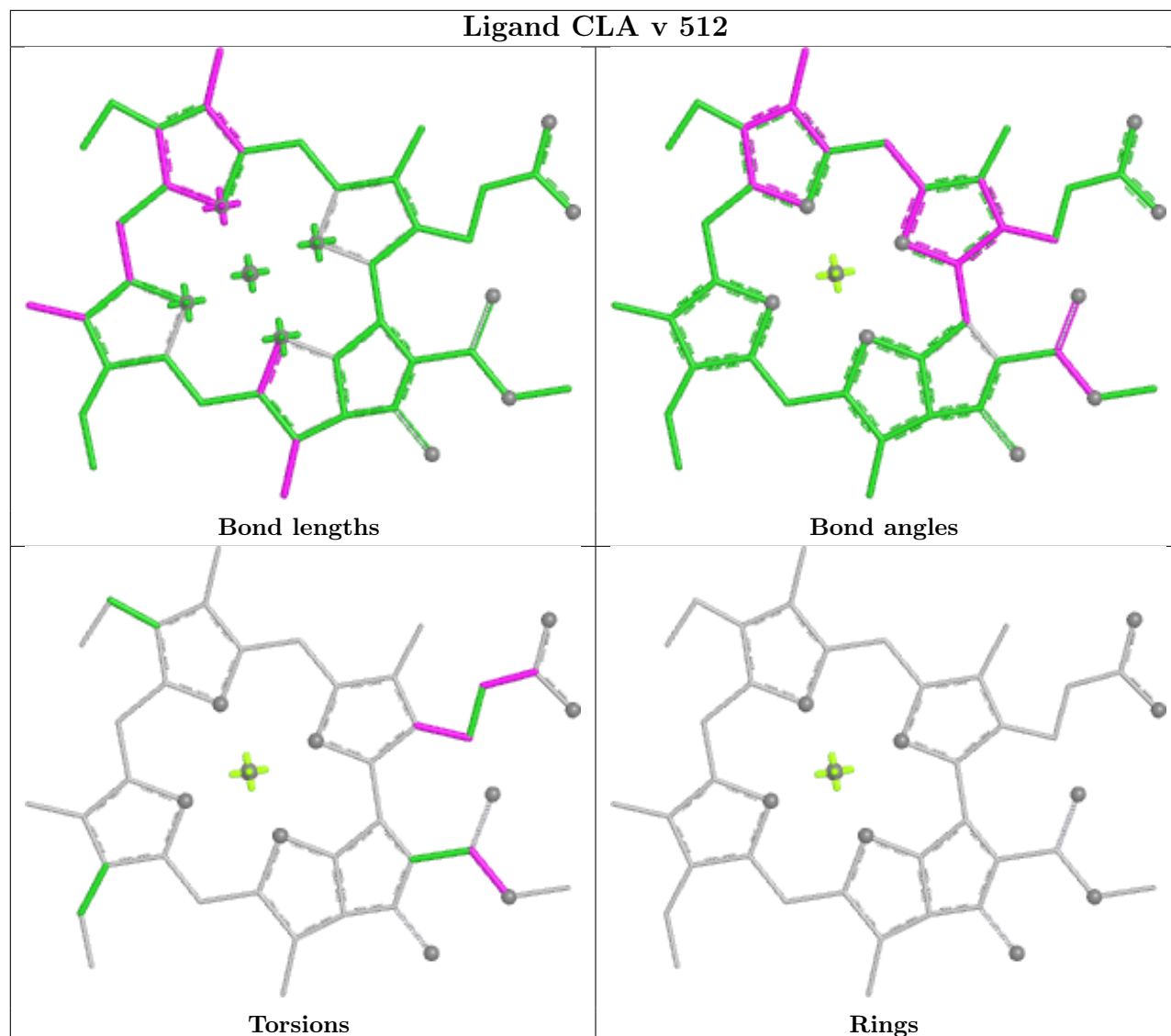
Ligand CLA Z 510



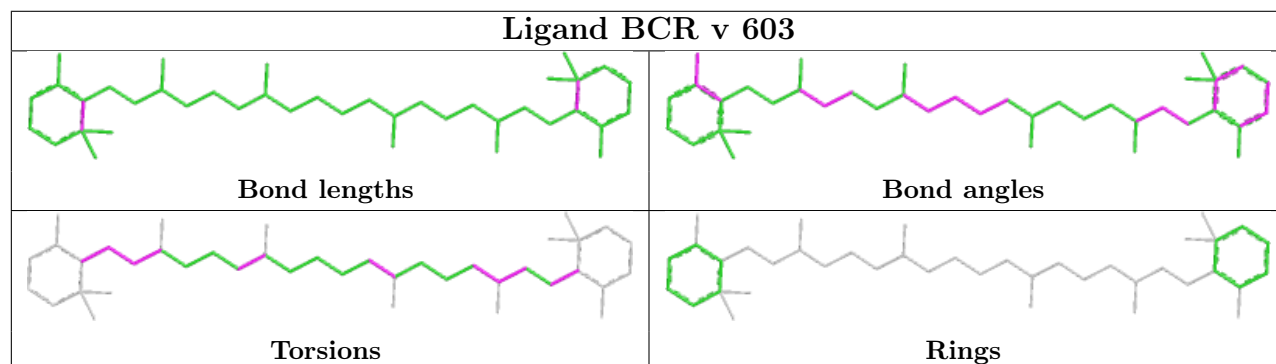


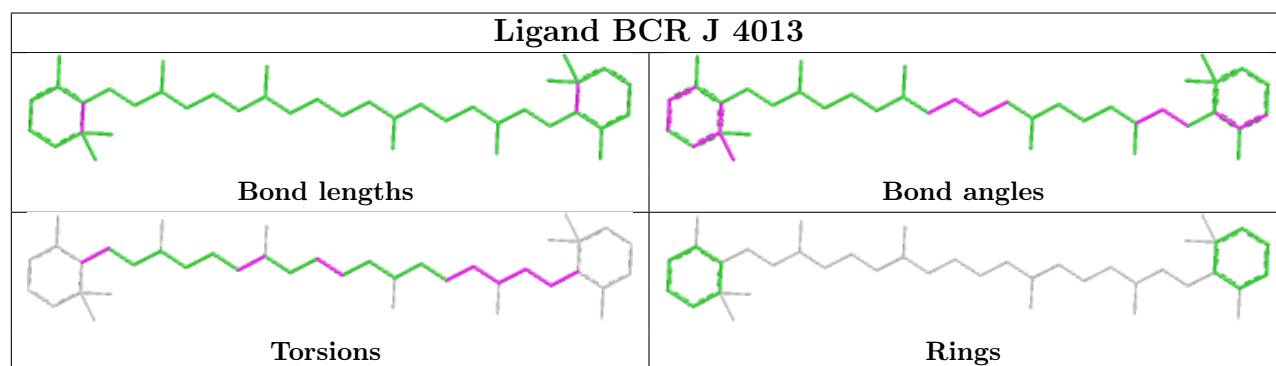
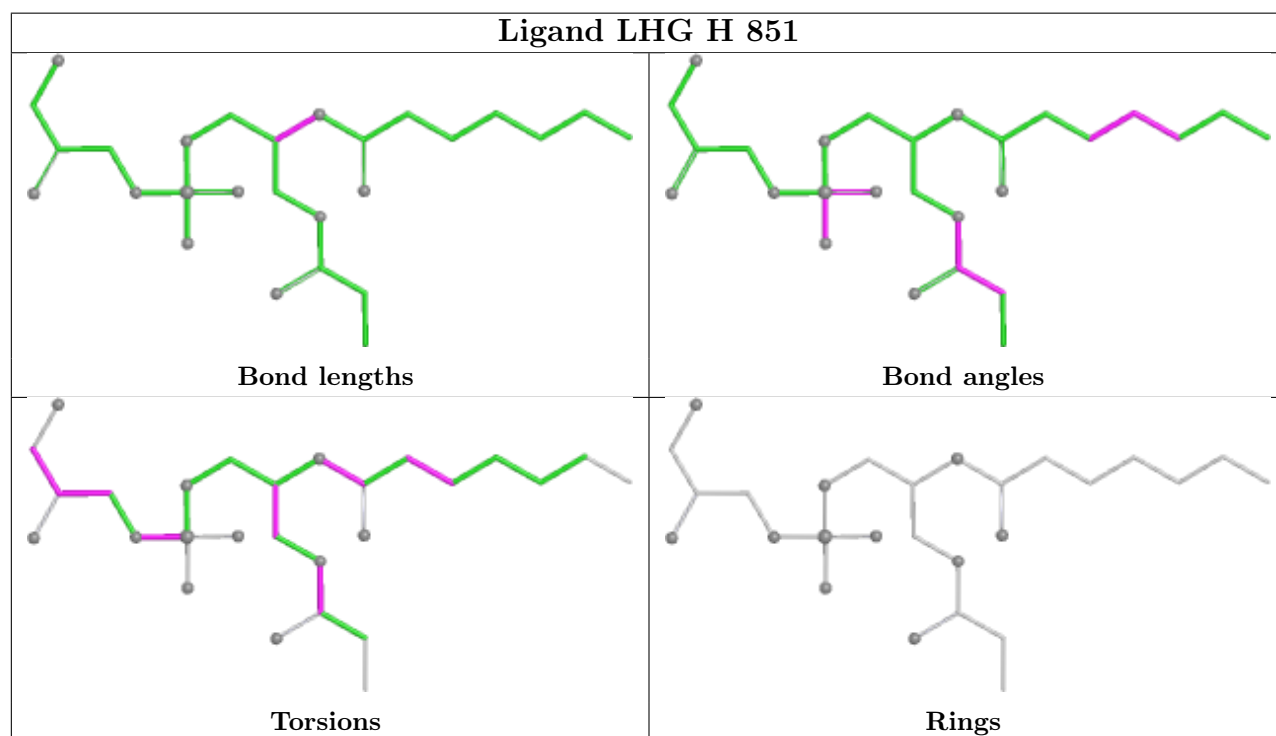
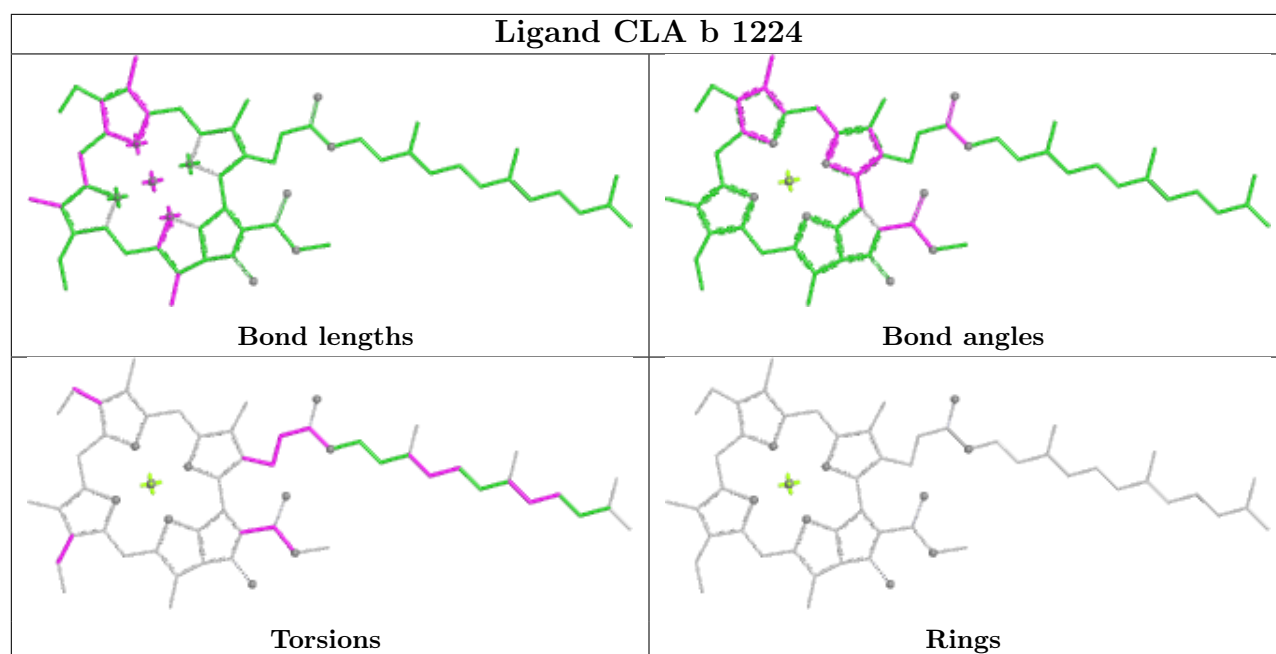
Ligand CLA H 1138**Ligand CLA B 1223****Ligand CLA B 1238**

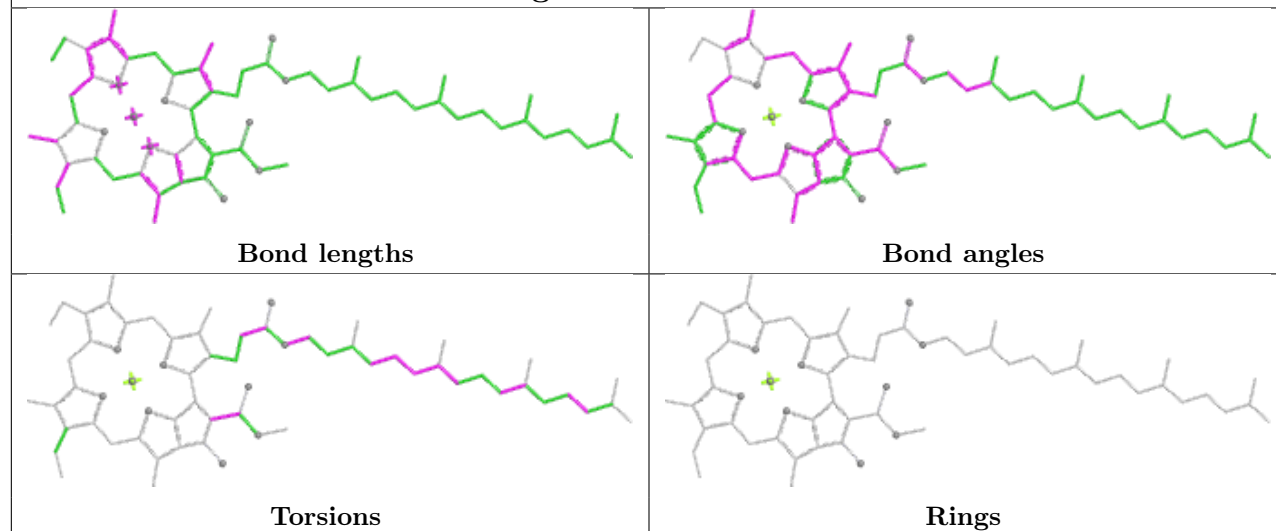
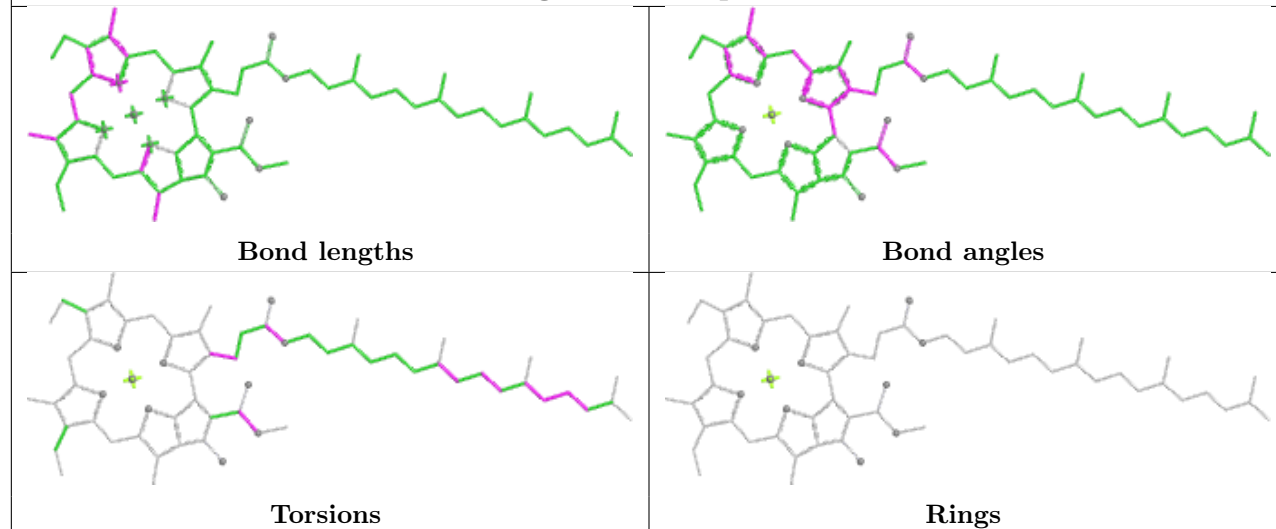
Ligand CLA v 512

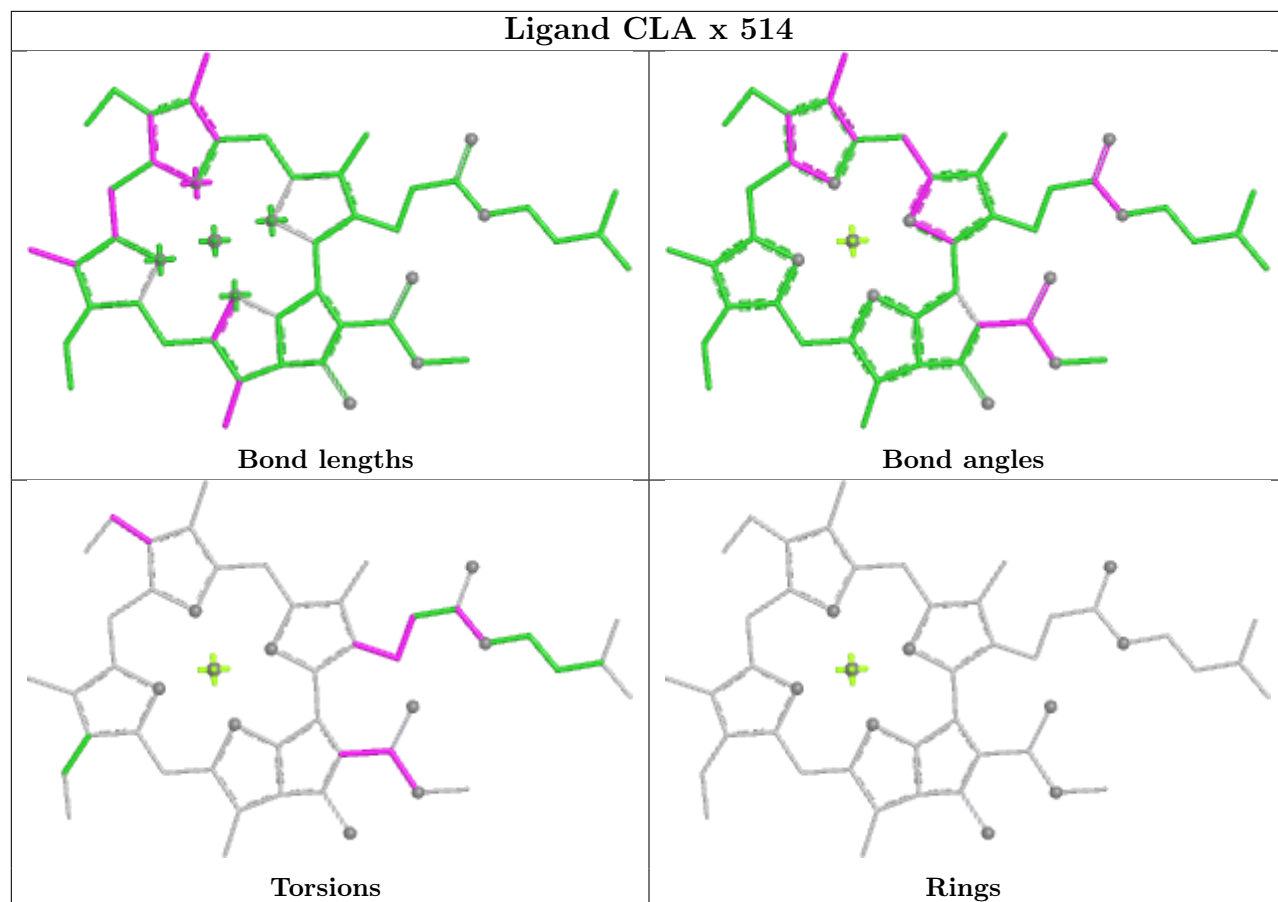


Ligand BCR v 603

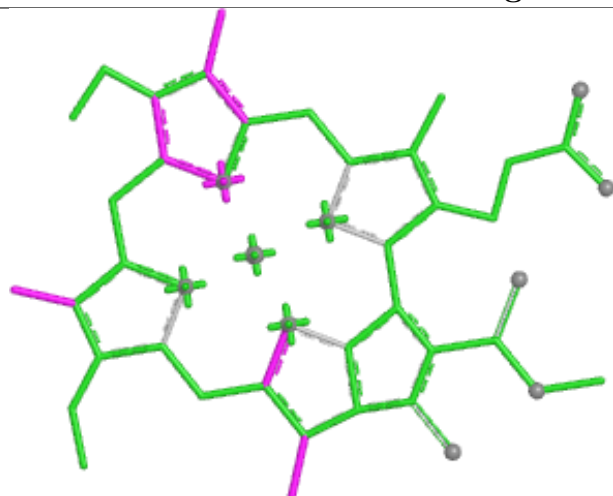




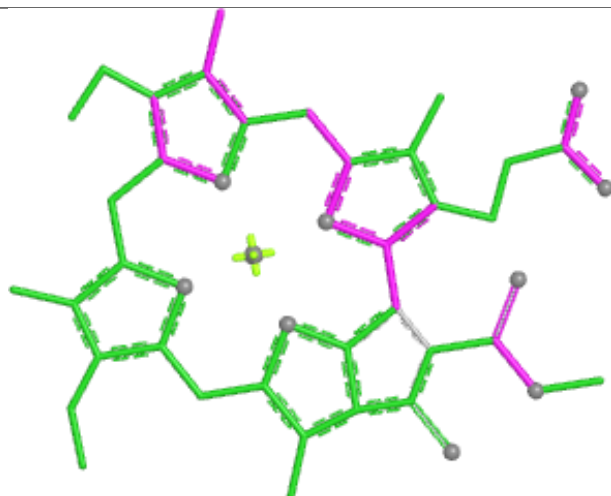
Ligand CL0 a 1011**Ligand CLA q 511**



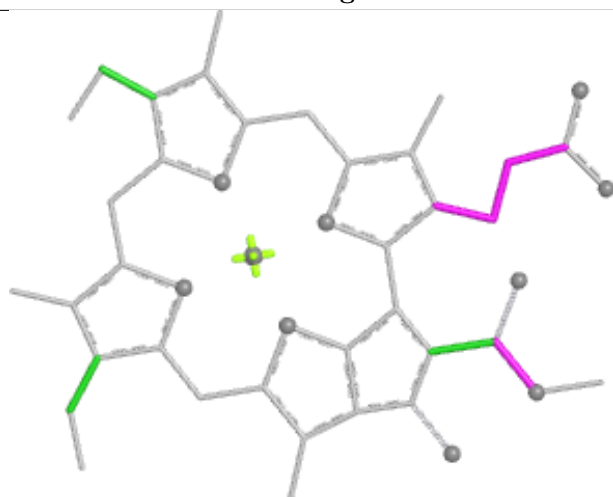
Ligand CLA A 1108



Bond lengths



Bond angles

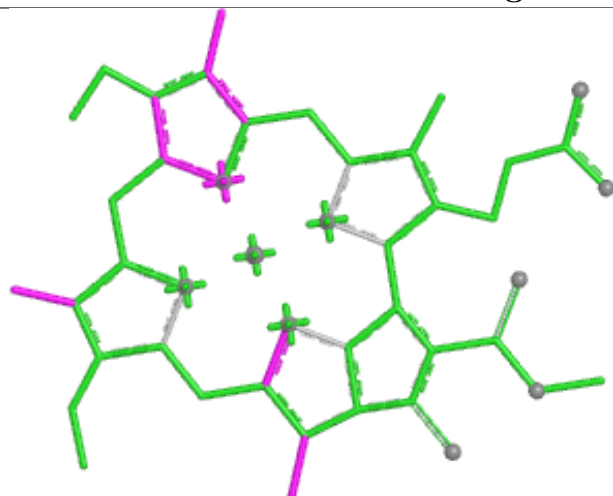


Torsions

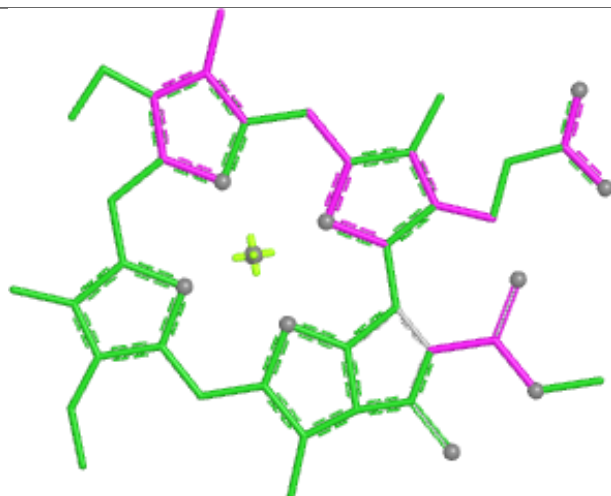


Rings

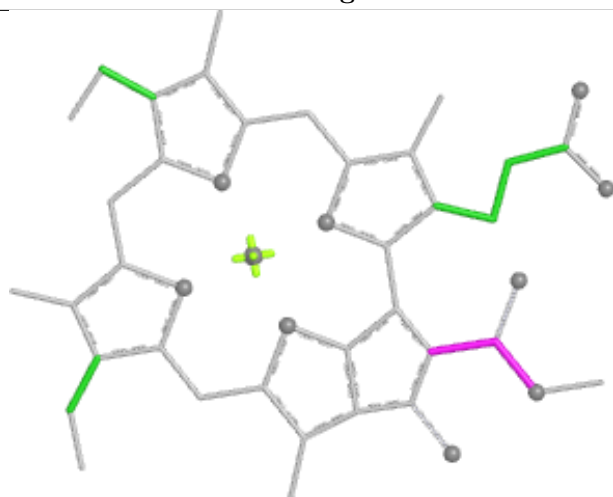
Ligand CLA B 1230



Bond lengths



Bond angles

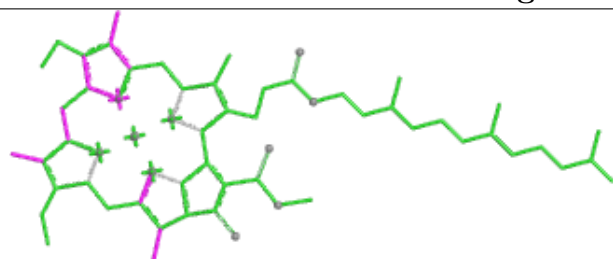


Torsions

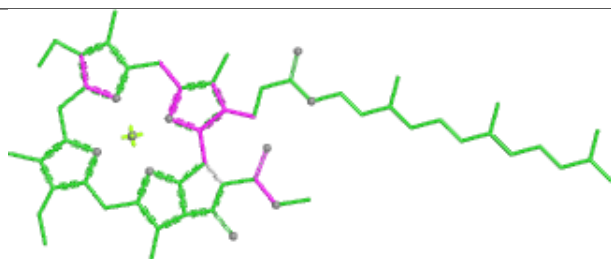


Rings

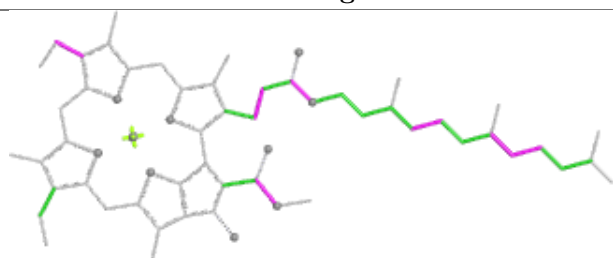
Ligand CLA n 509



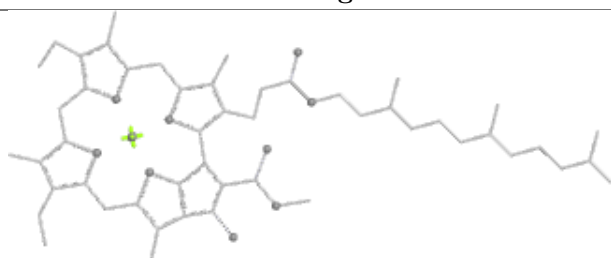
Bond lengths



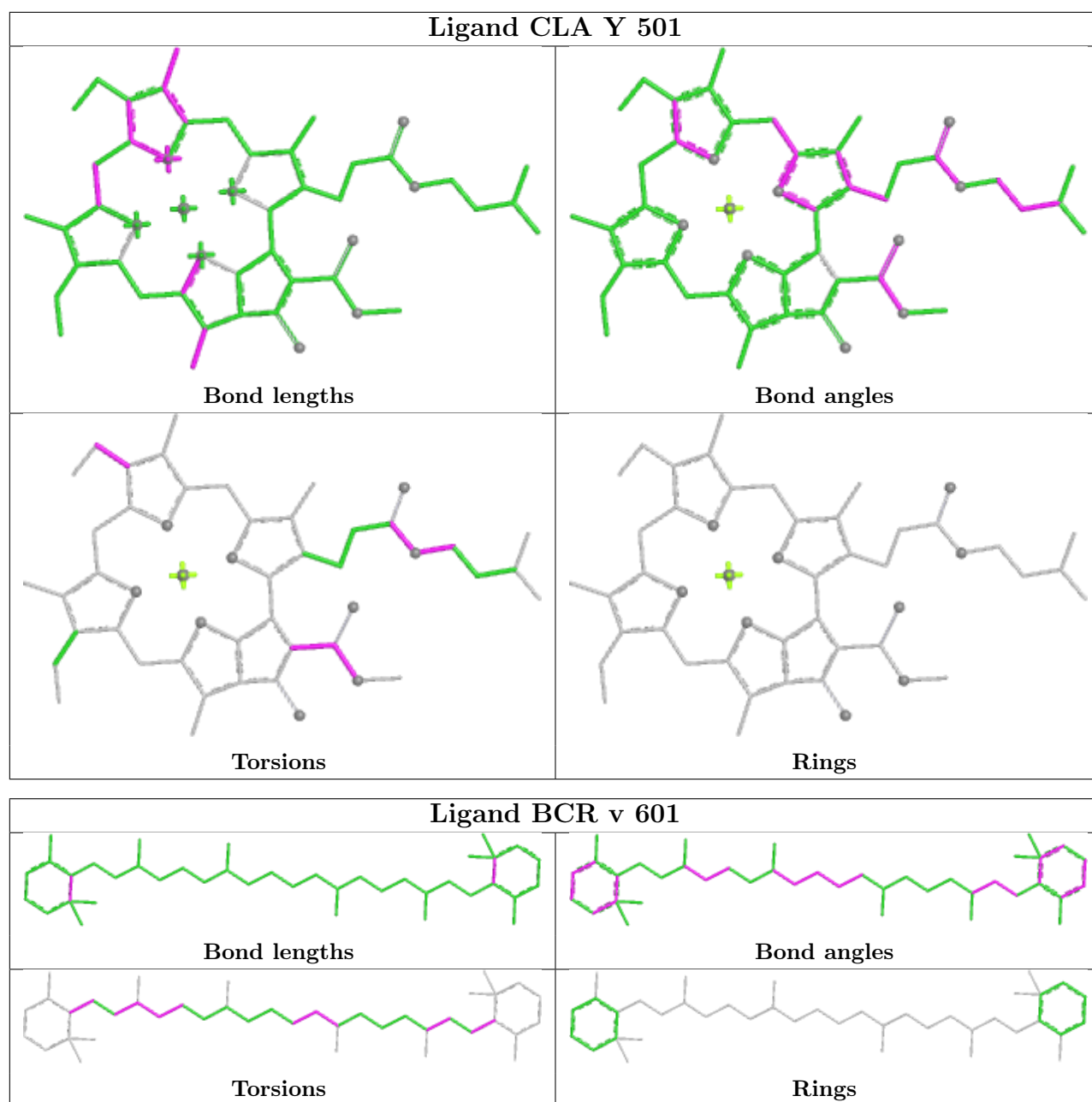
Bond angles



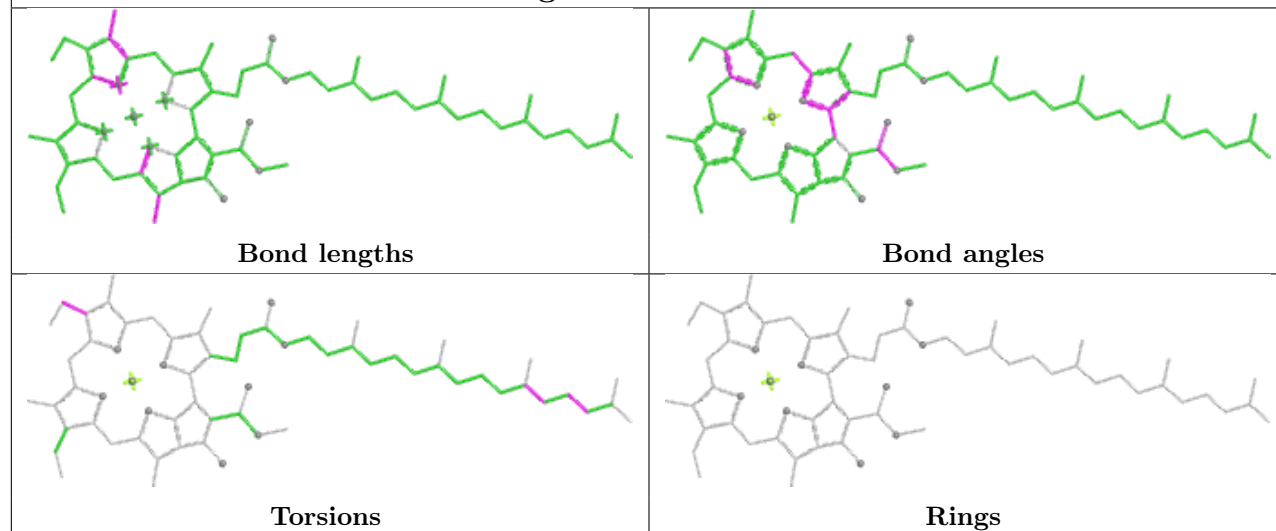
Torsions



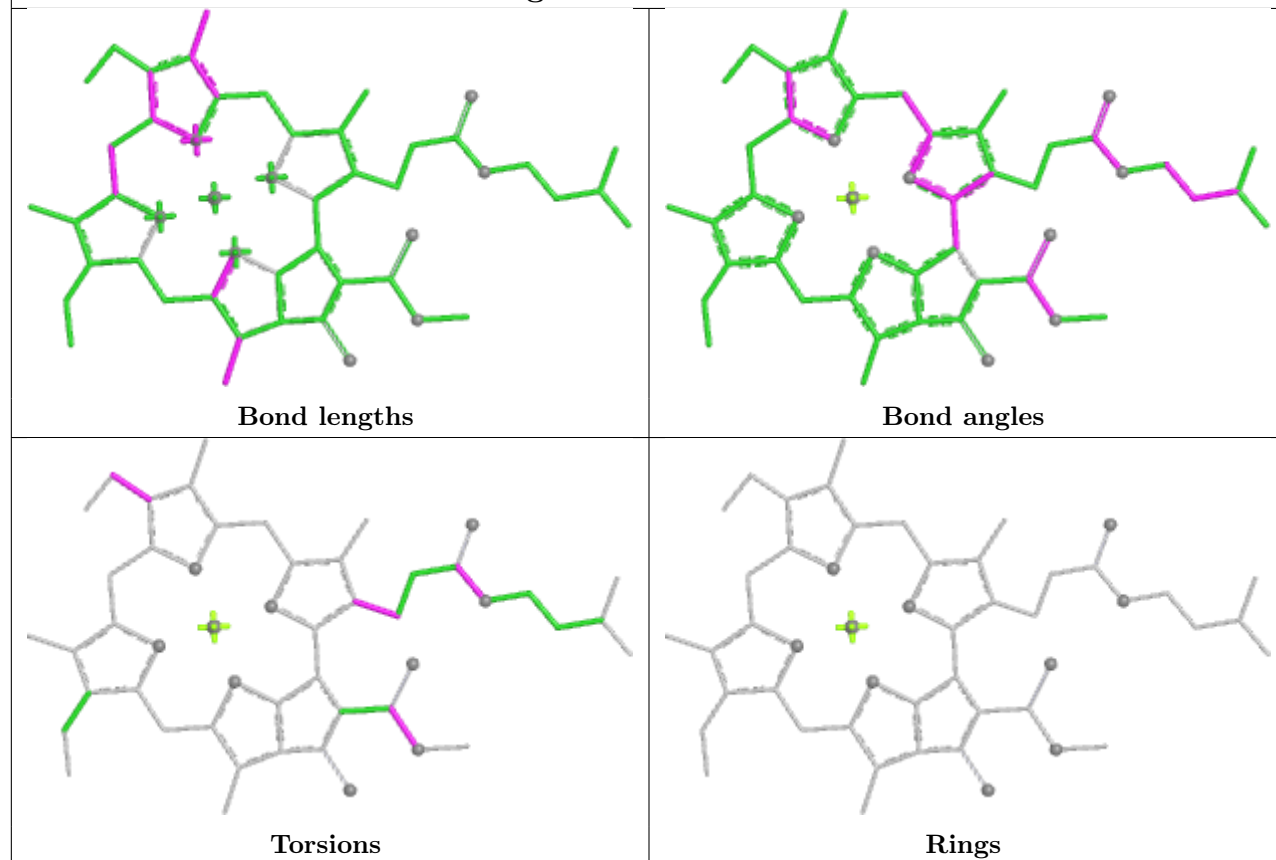
Rings



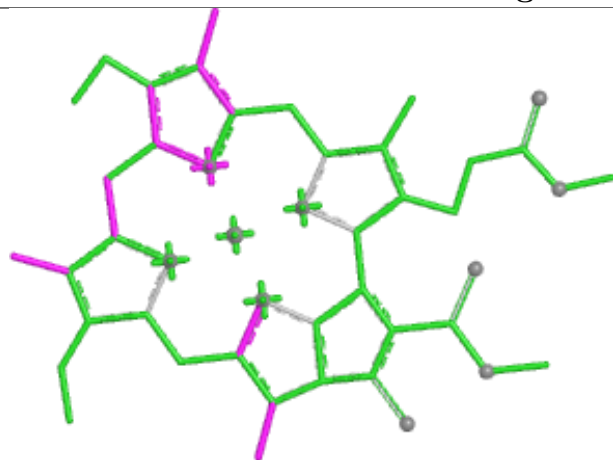
Ligand CLA t 510



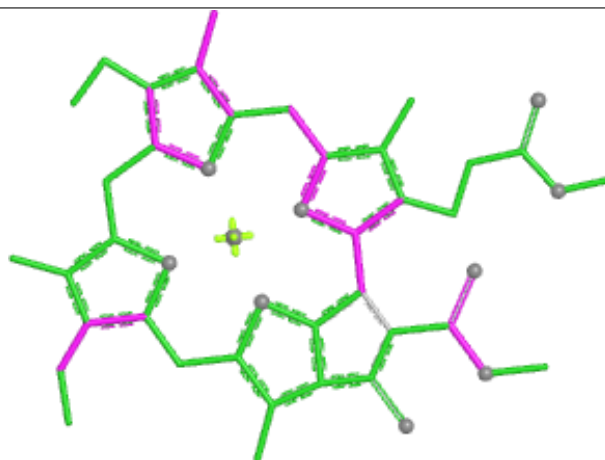
Ligand CLA W 513



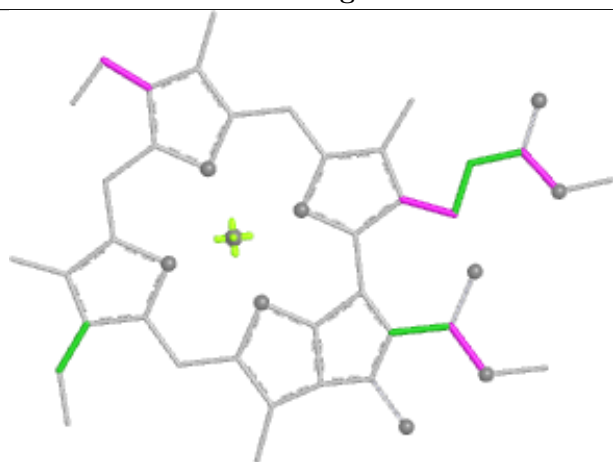
Ligand CLA Z 516



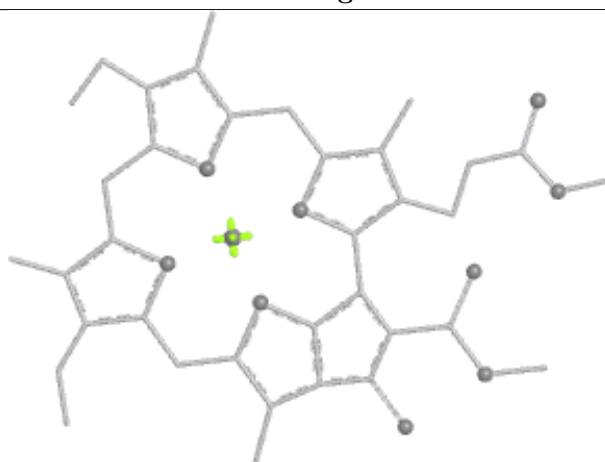
Bond lengths



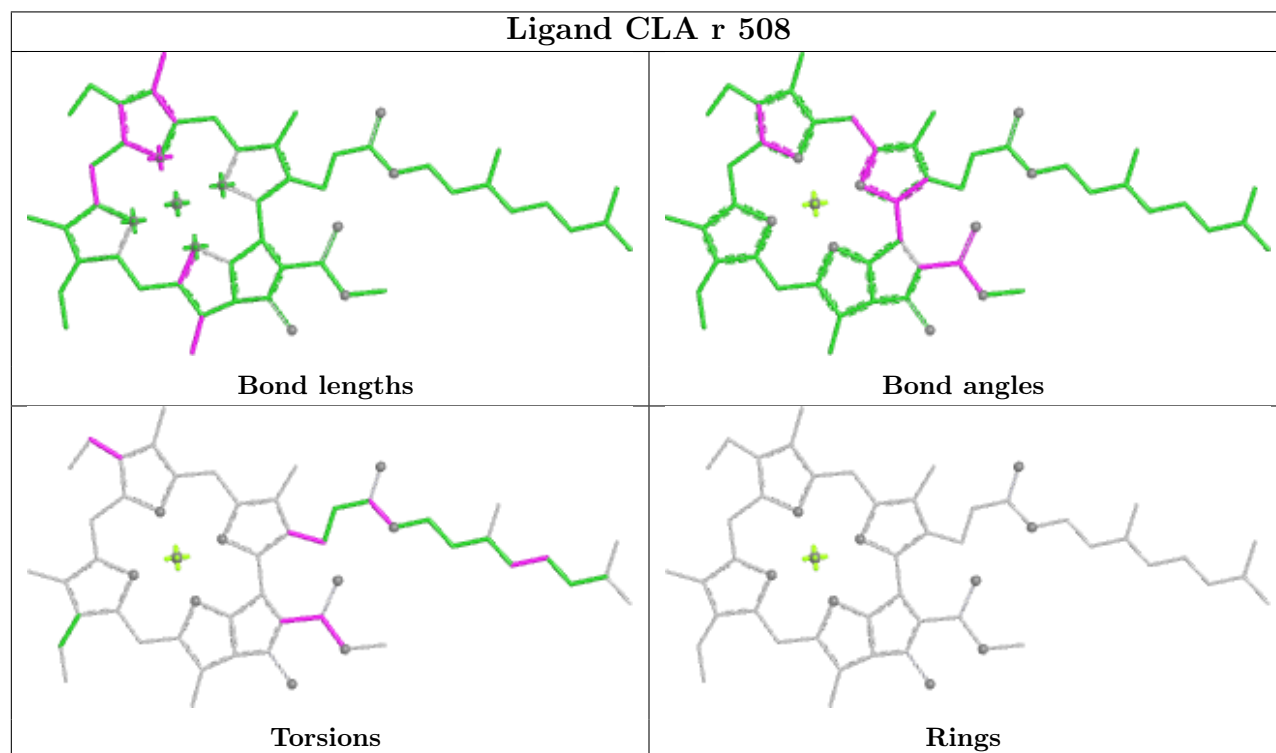
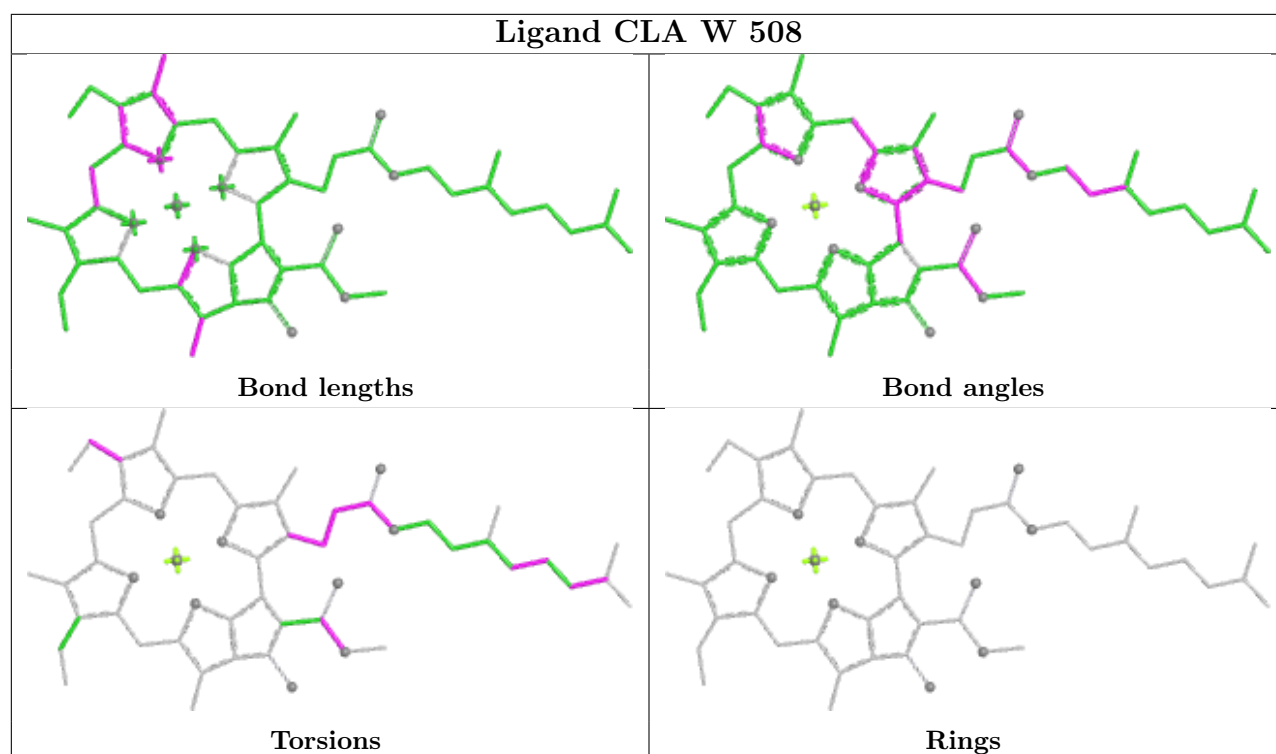
Bond angles

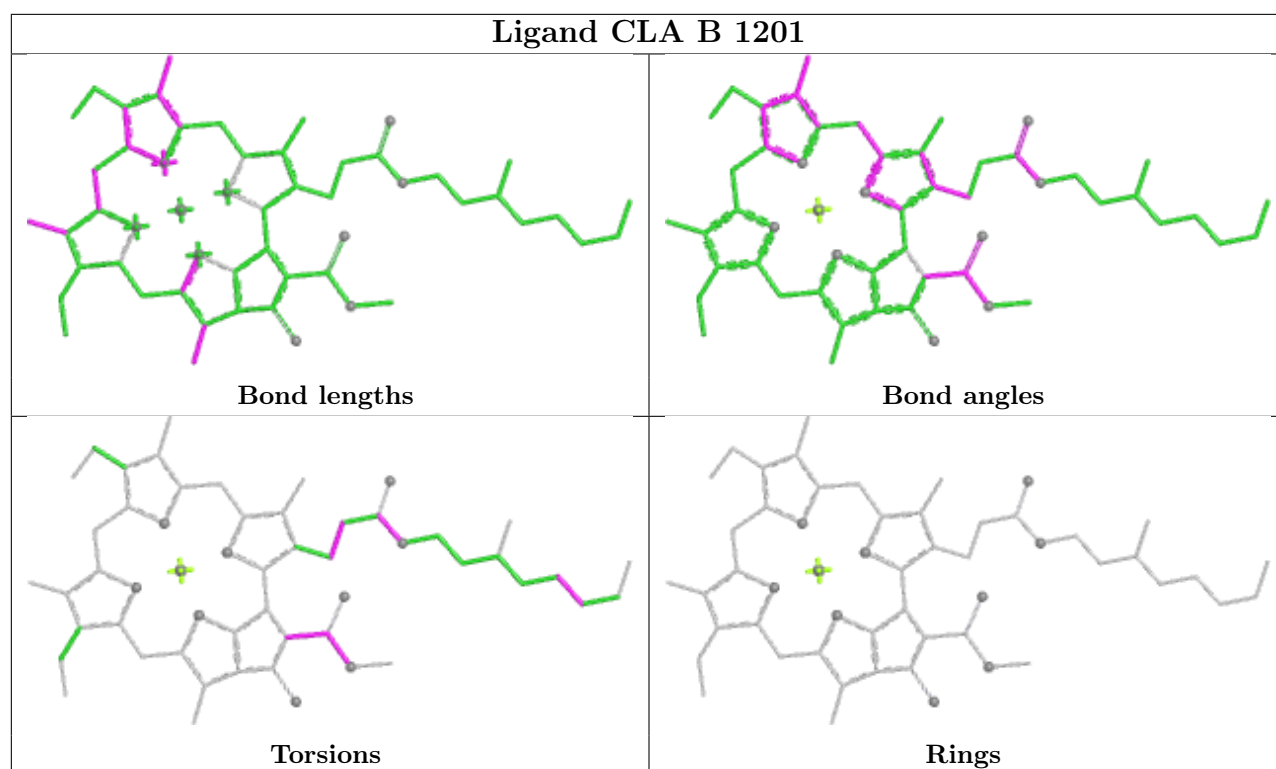


Torsions

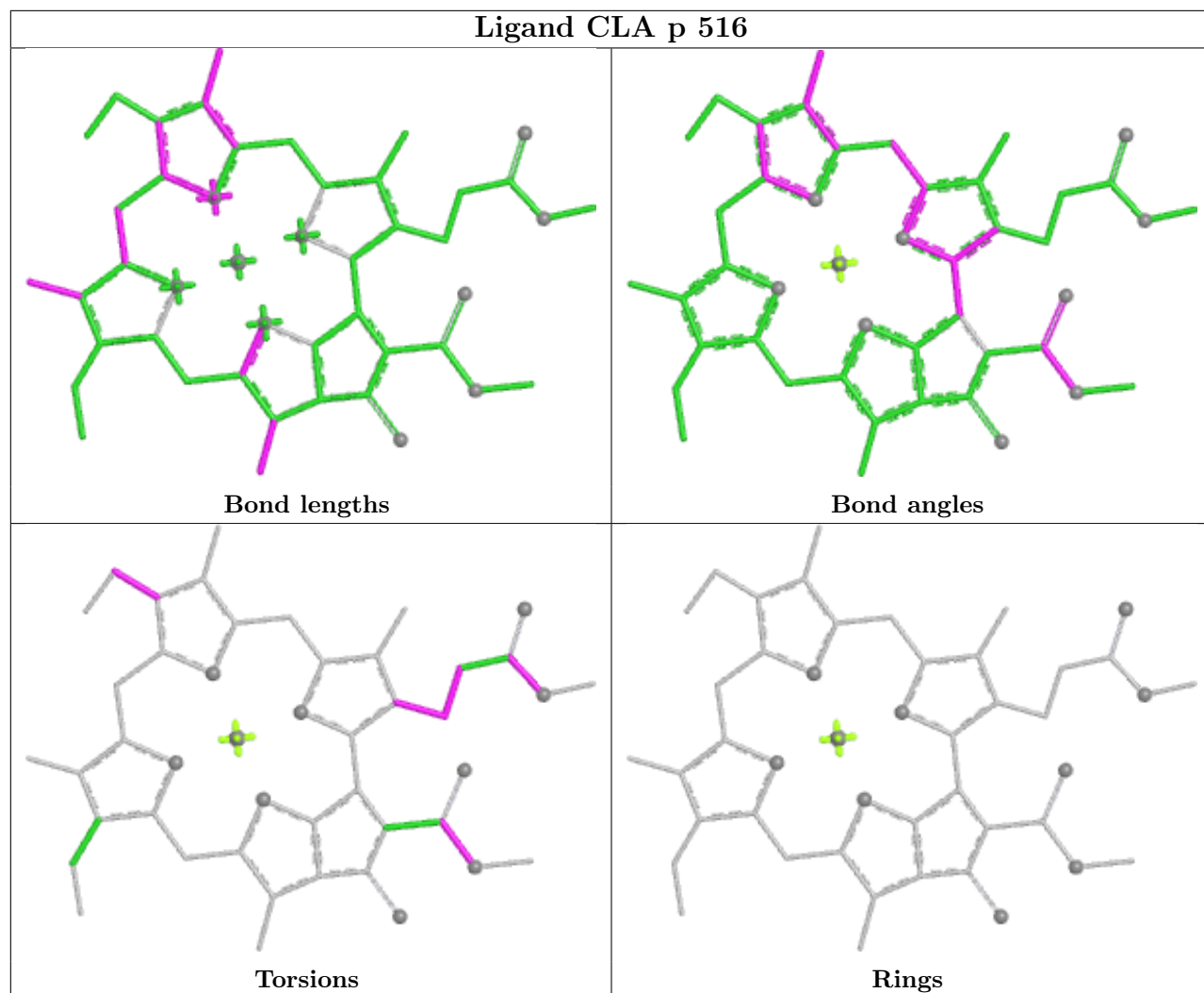


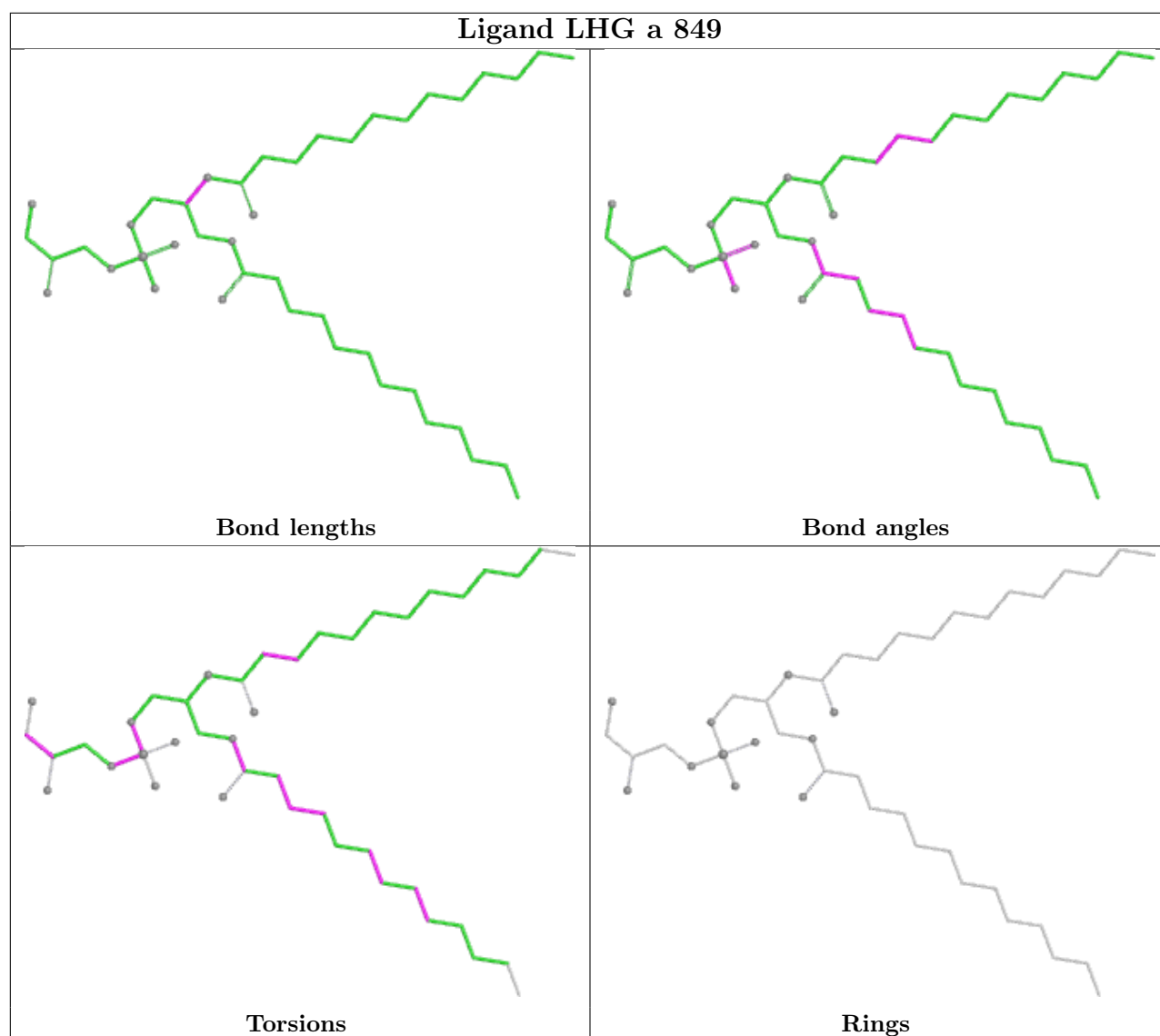
Rings



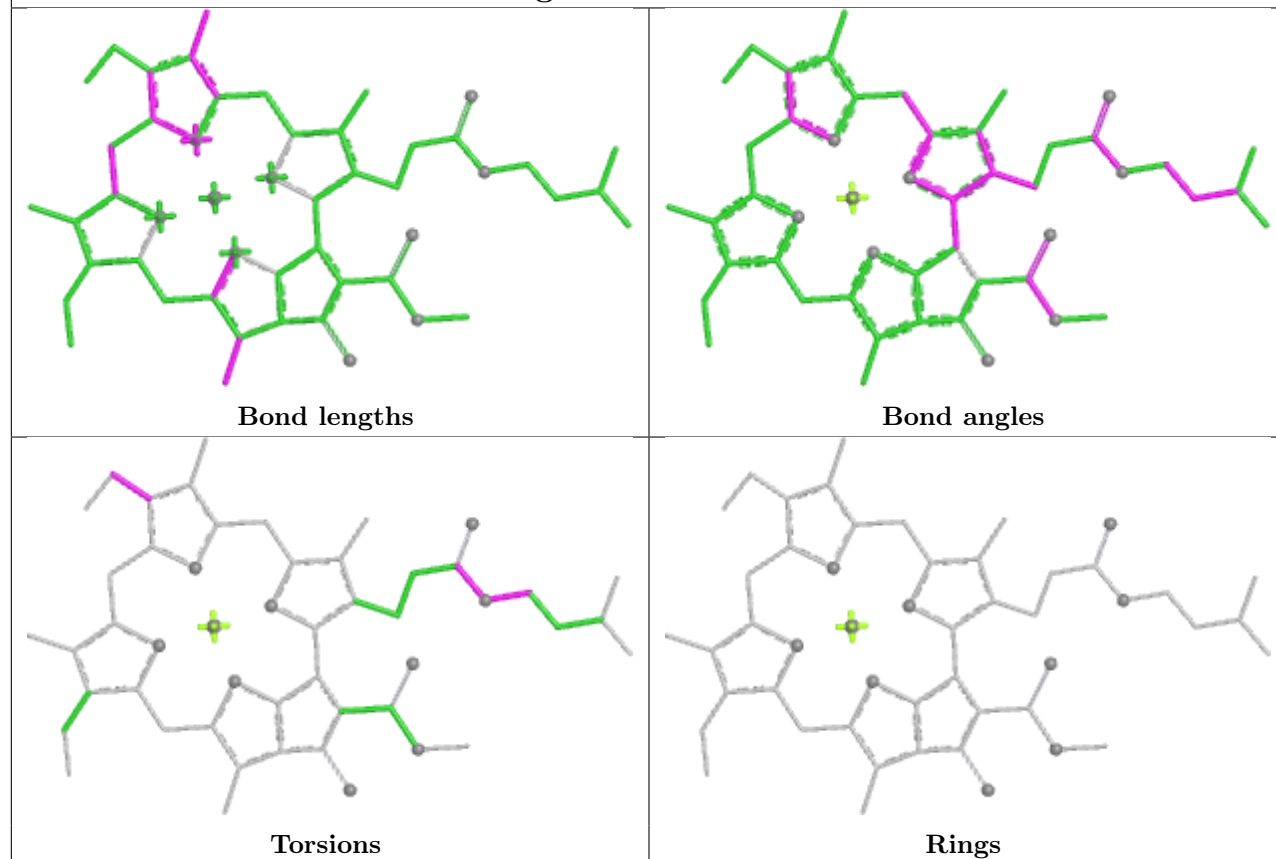


Ligand CLA p 516

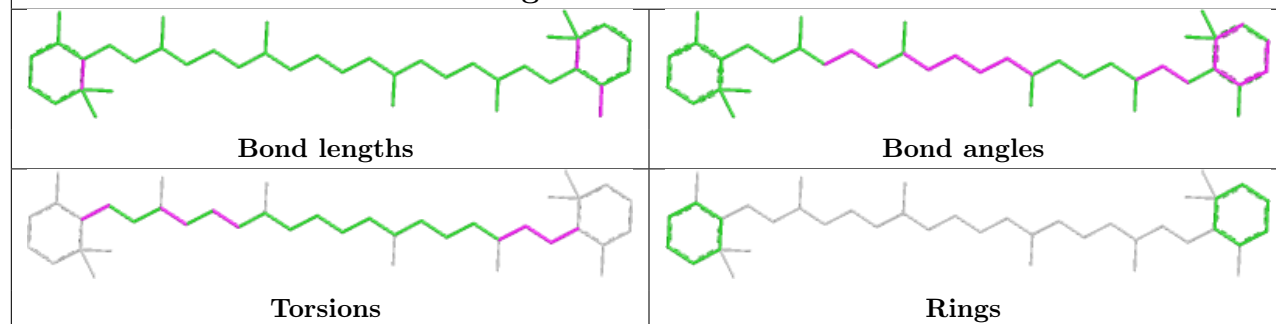




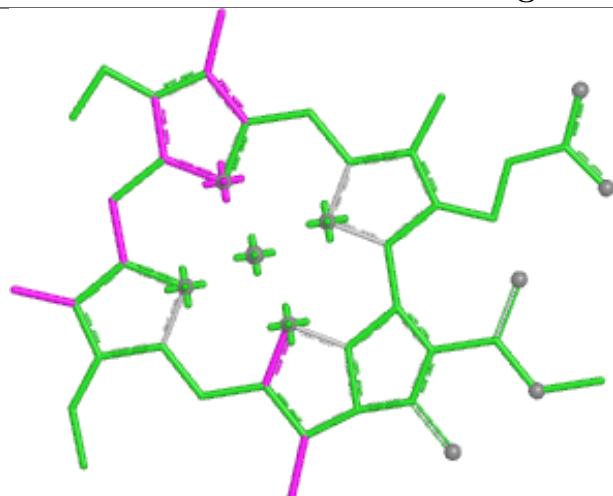
Ligand CLA v 513



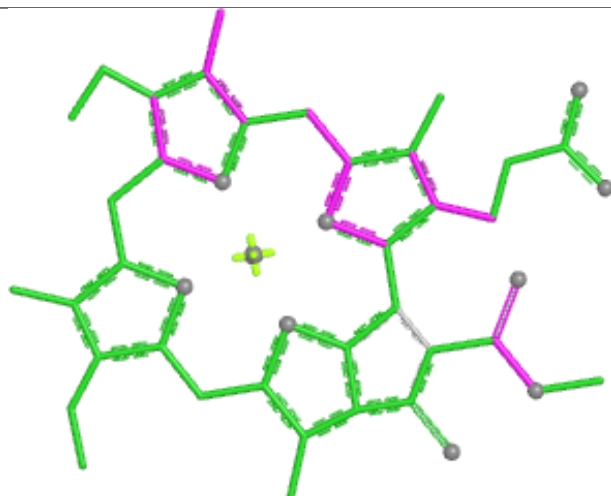
Ligand BCR B 4017



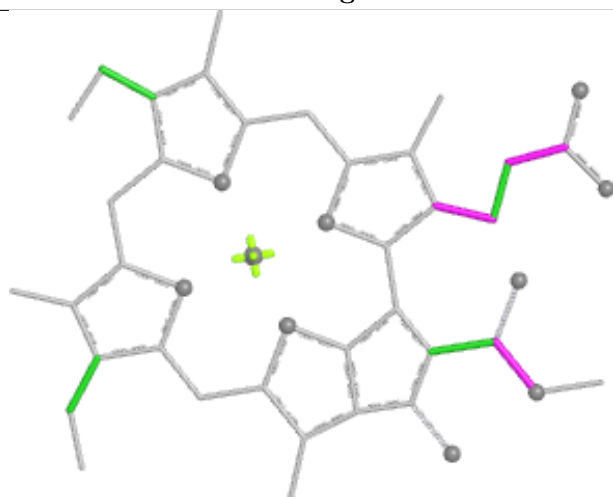
Ligand CLA x 512



Bond lengths



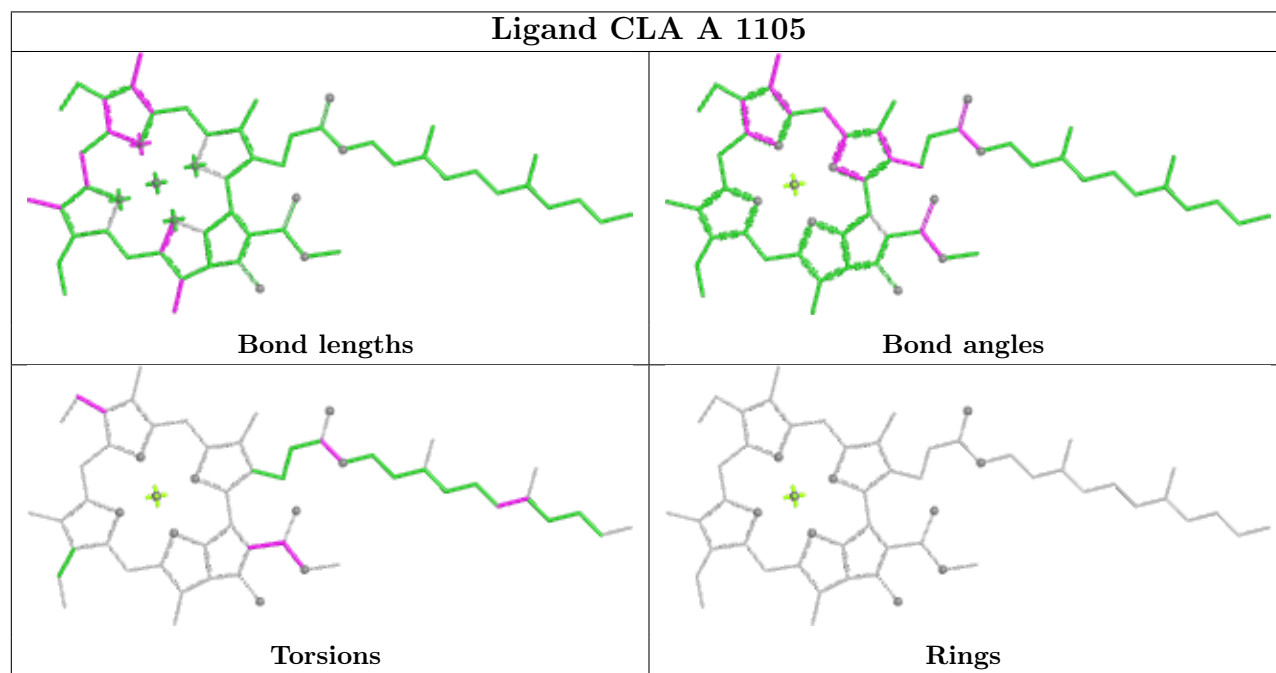
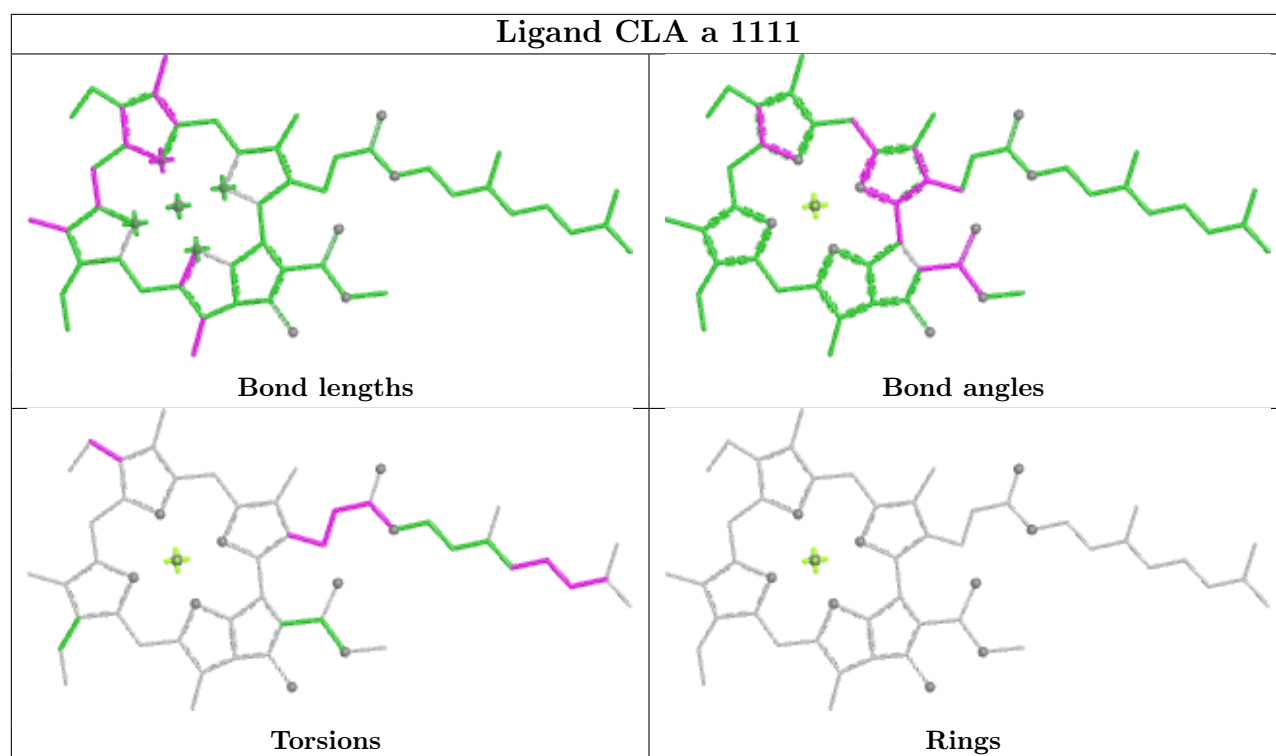
Bond angles



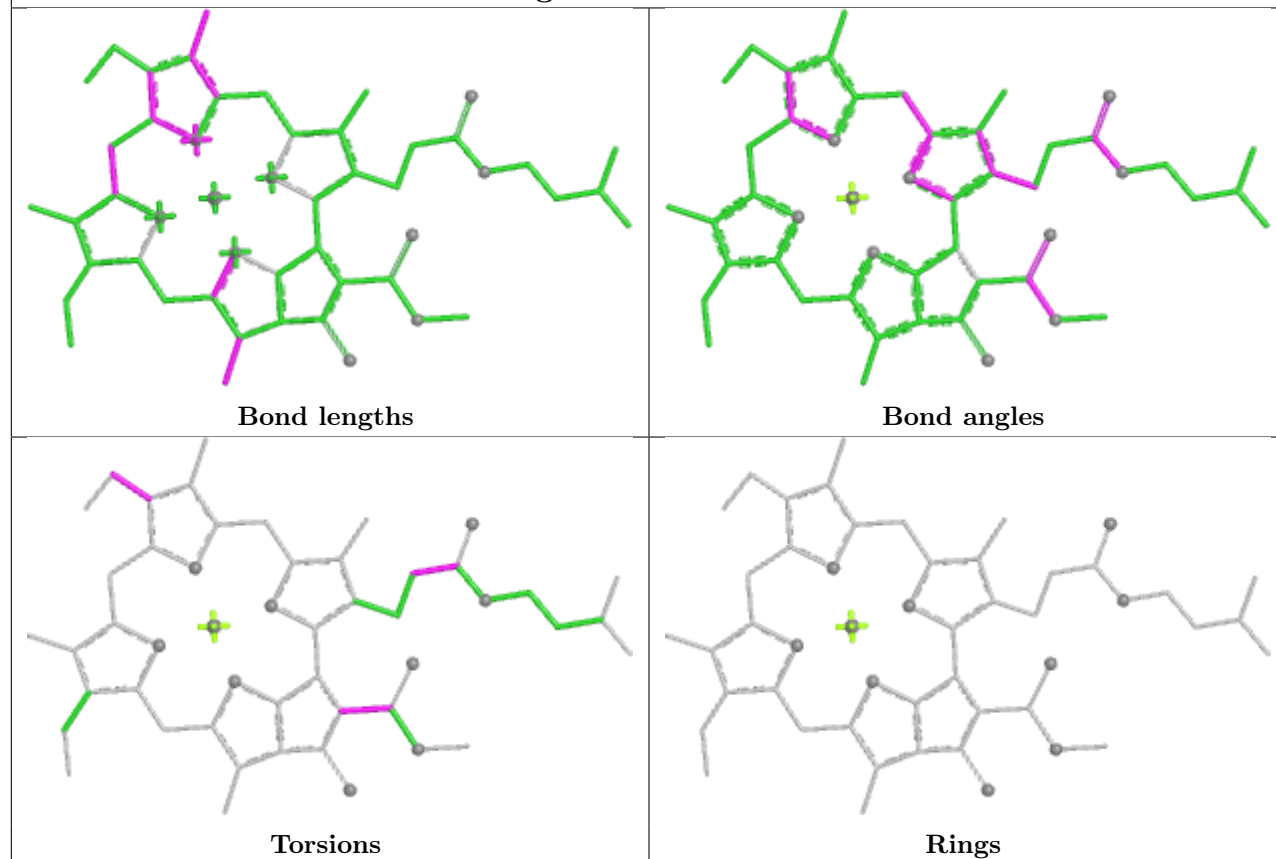
Torsions



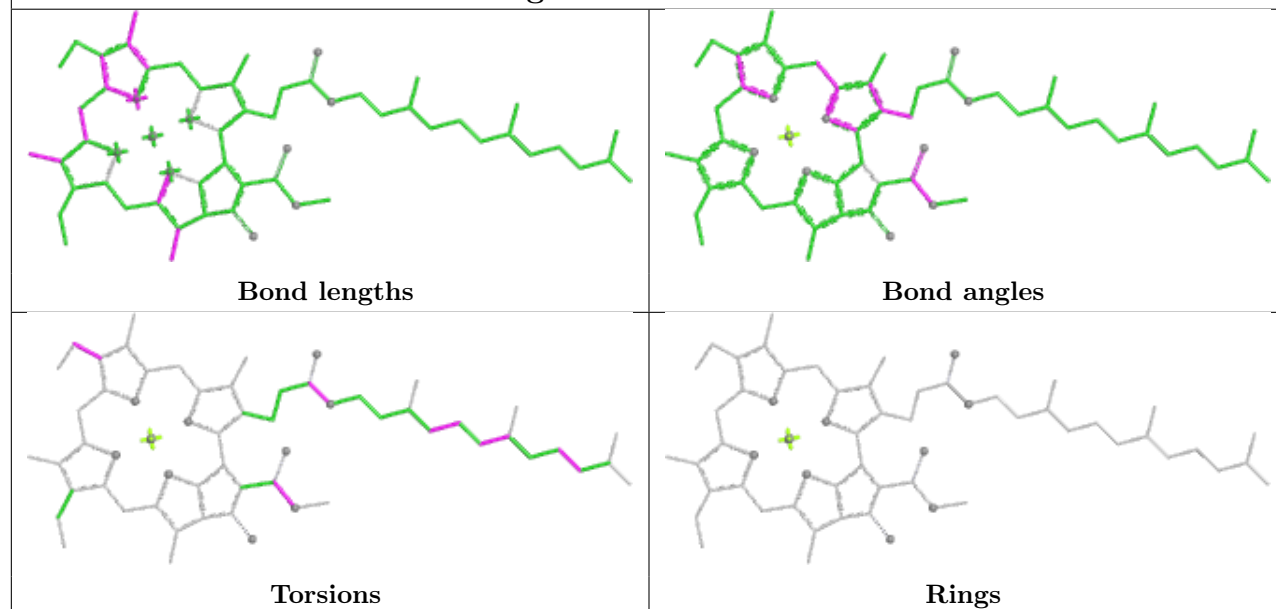
Rings

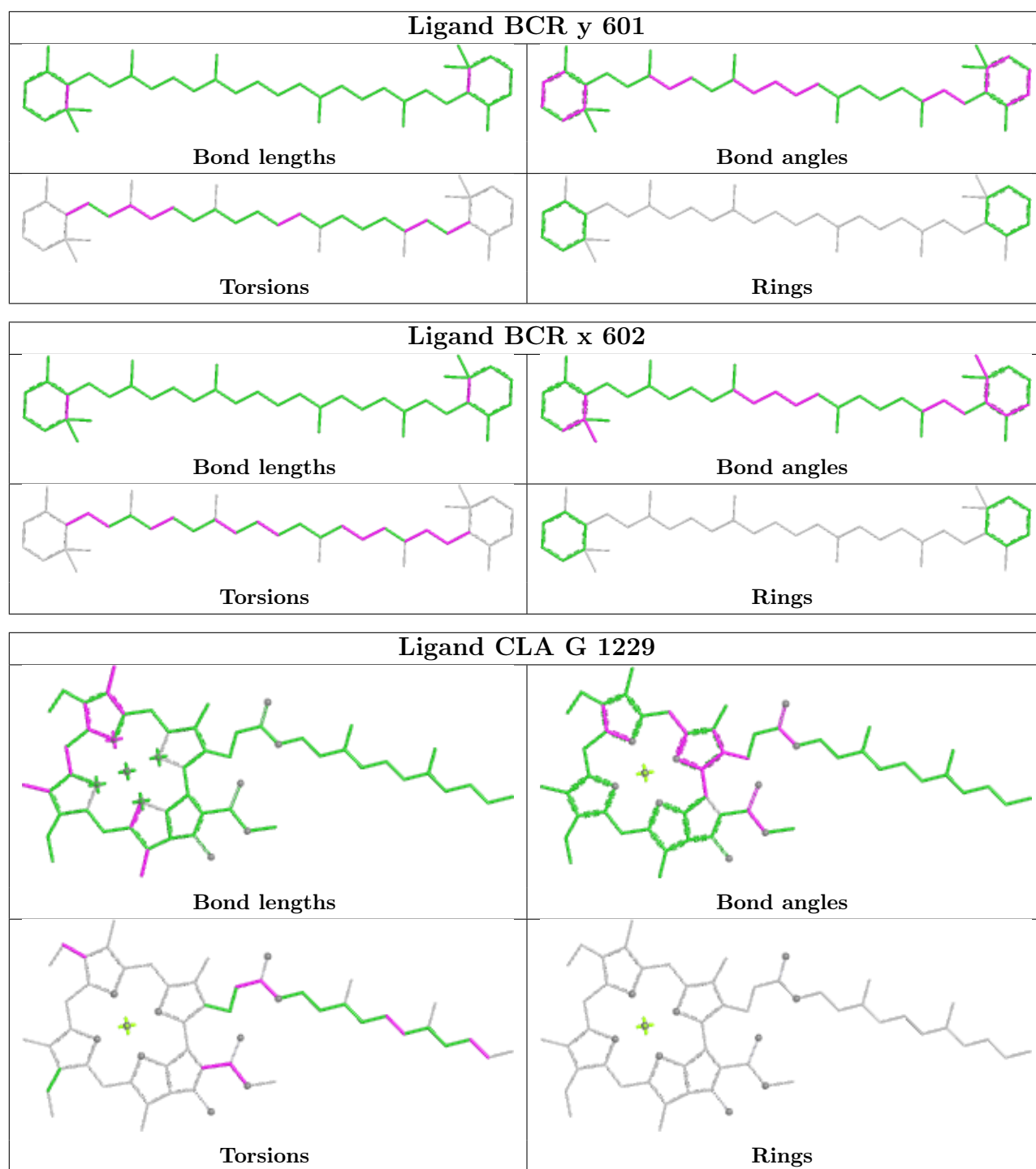


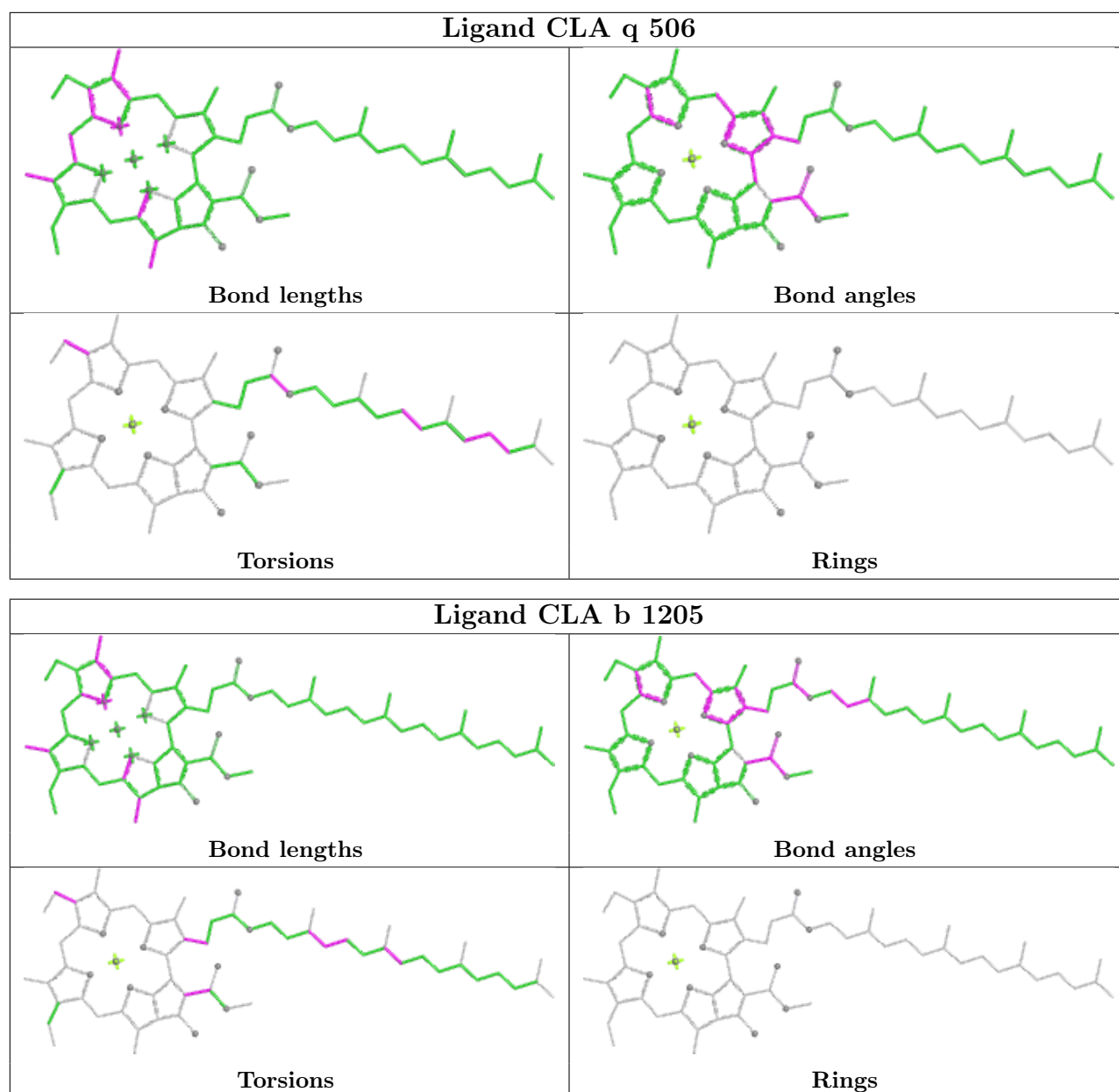
Ligand CLA v 502



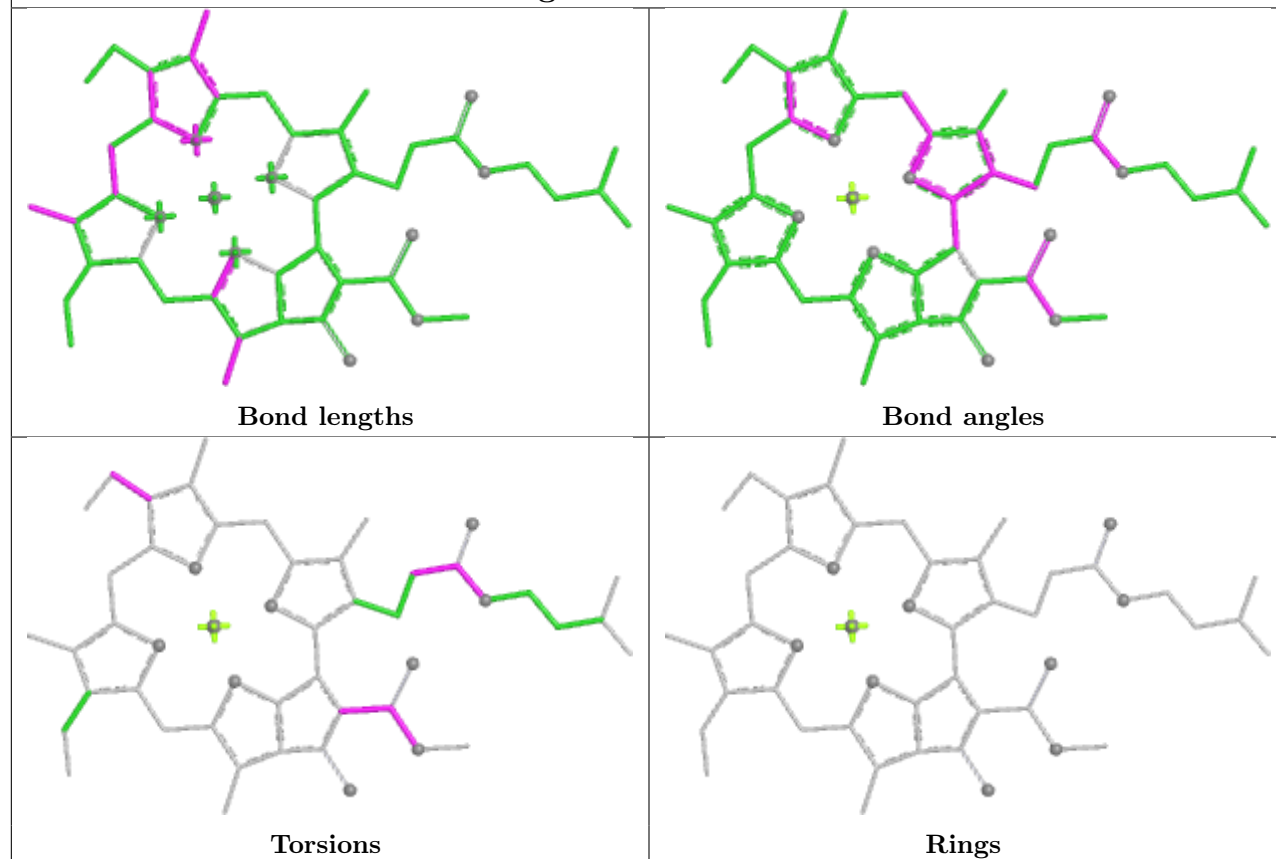
Ligand CLA W 509



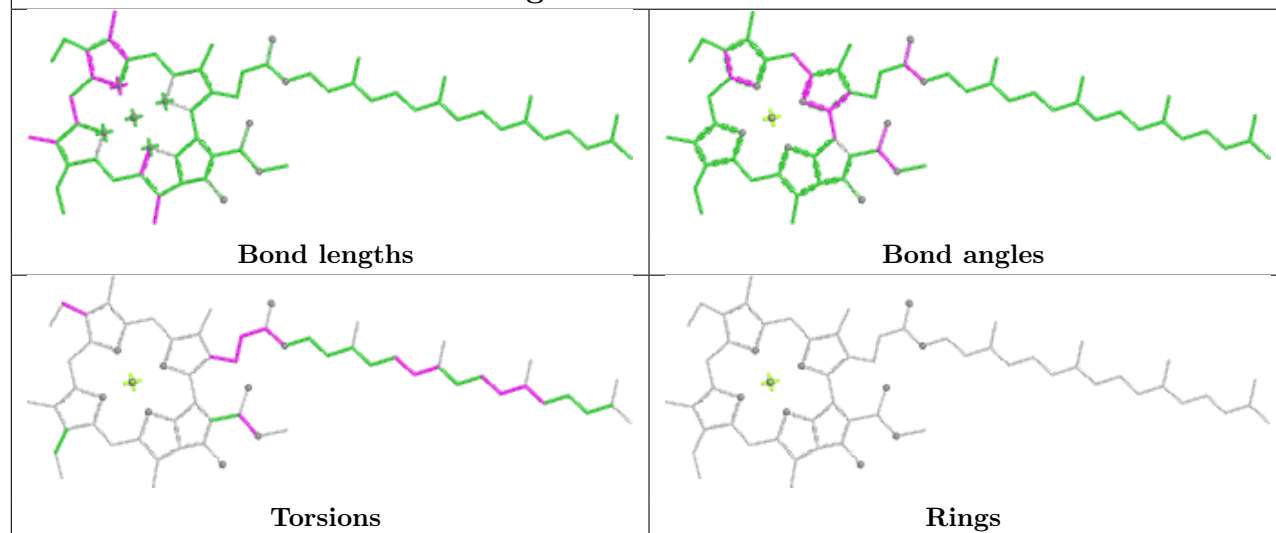




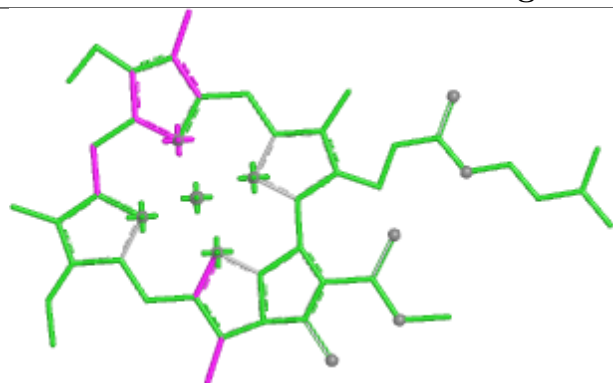
Ligand CLA t 514



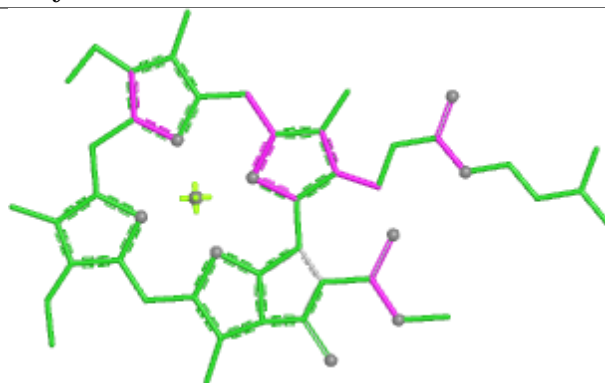
Ligand CLA b 1203



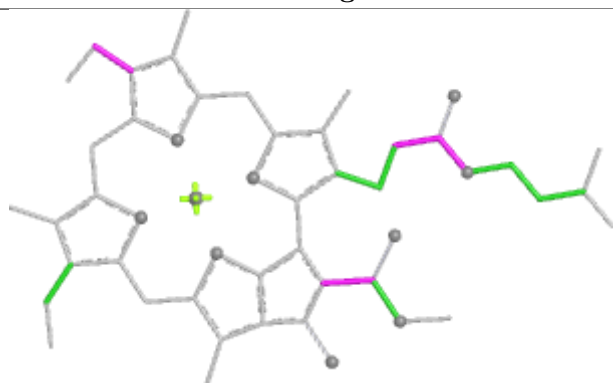
Ligand CLA y 502



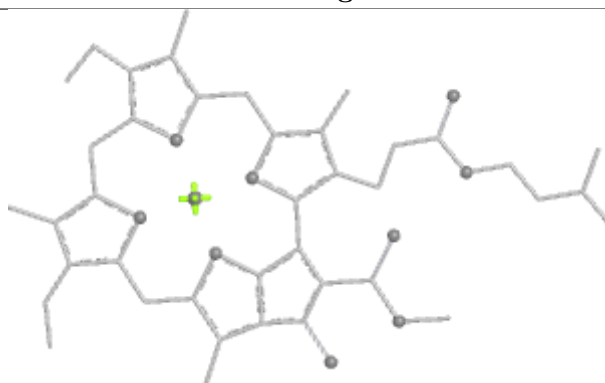
Bond lengths



Bond angles

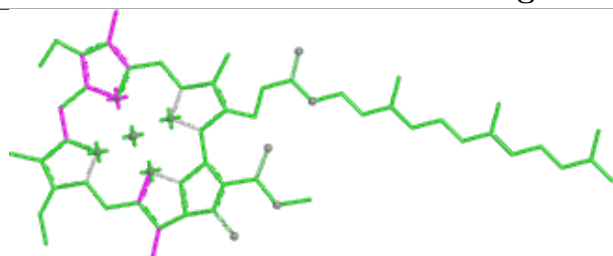


Torsions

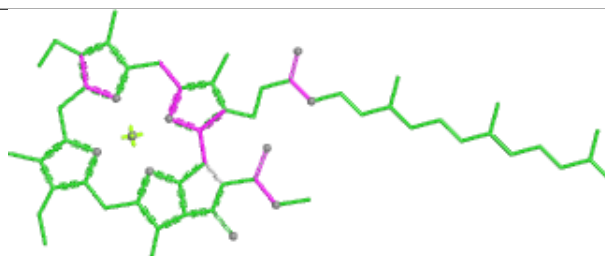


Rings

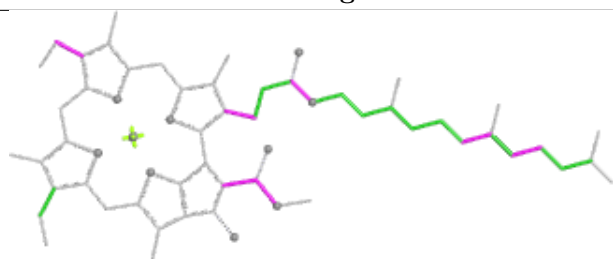
Ligand CLA n 504



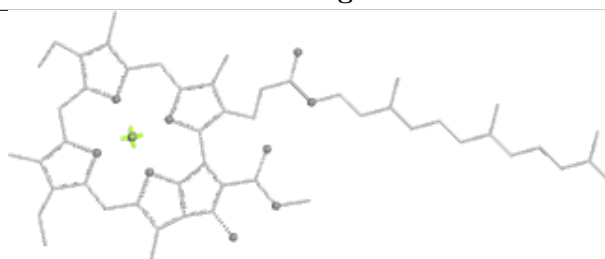
Bond lengths



Bond angles

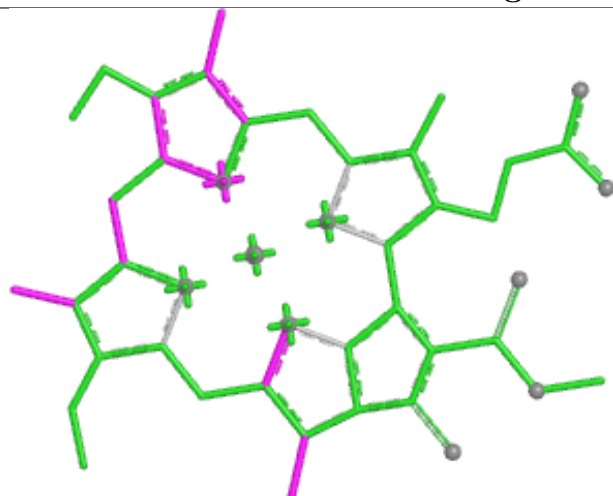


Torsions

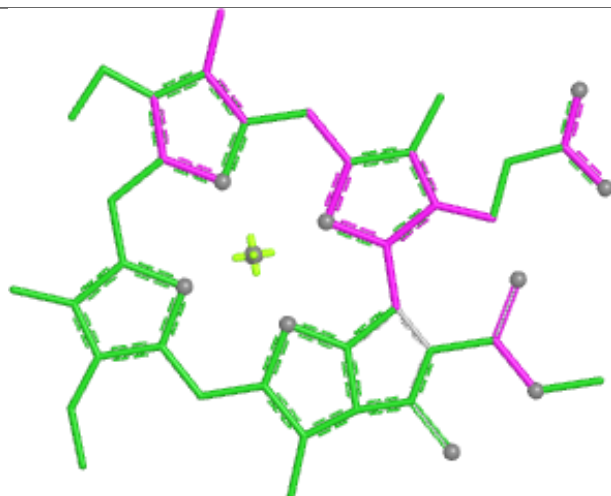


Rings

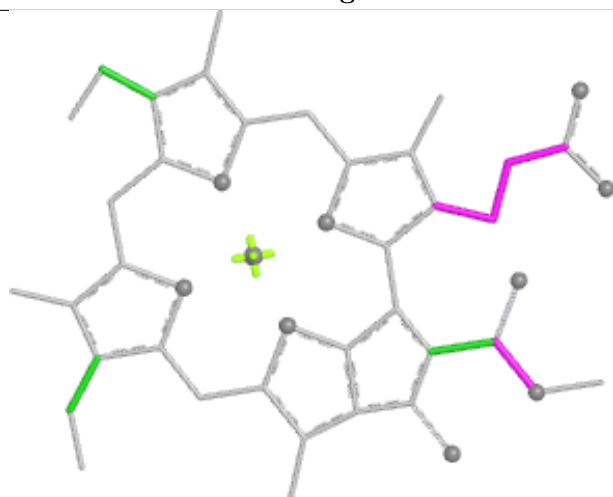
Ligand CLA H 1108



Bond lengths



Bond angles

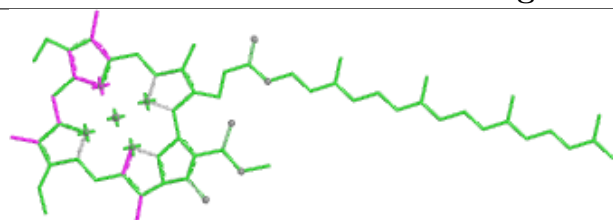


Torsions

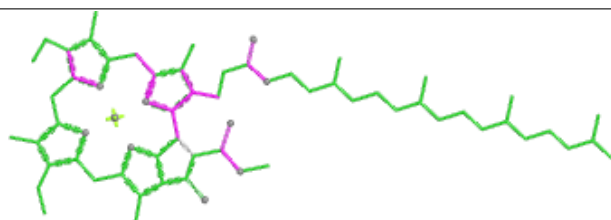


Rings

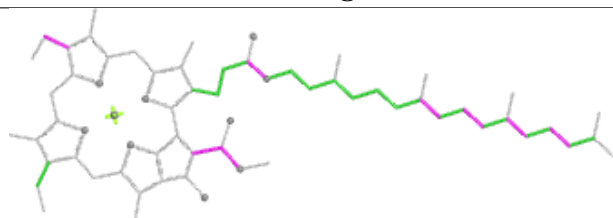
Ligand CLA u 507



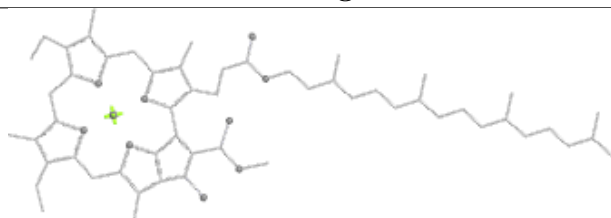
Bond lengths



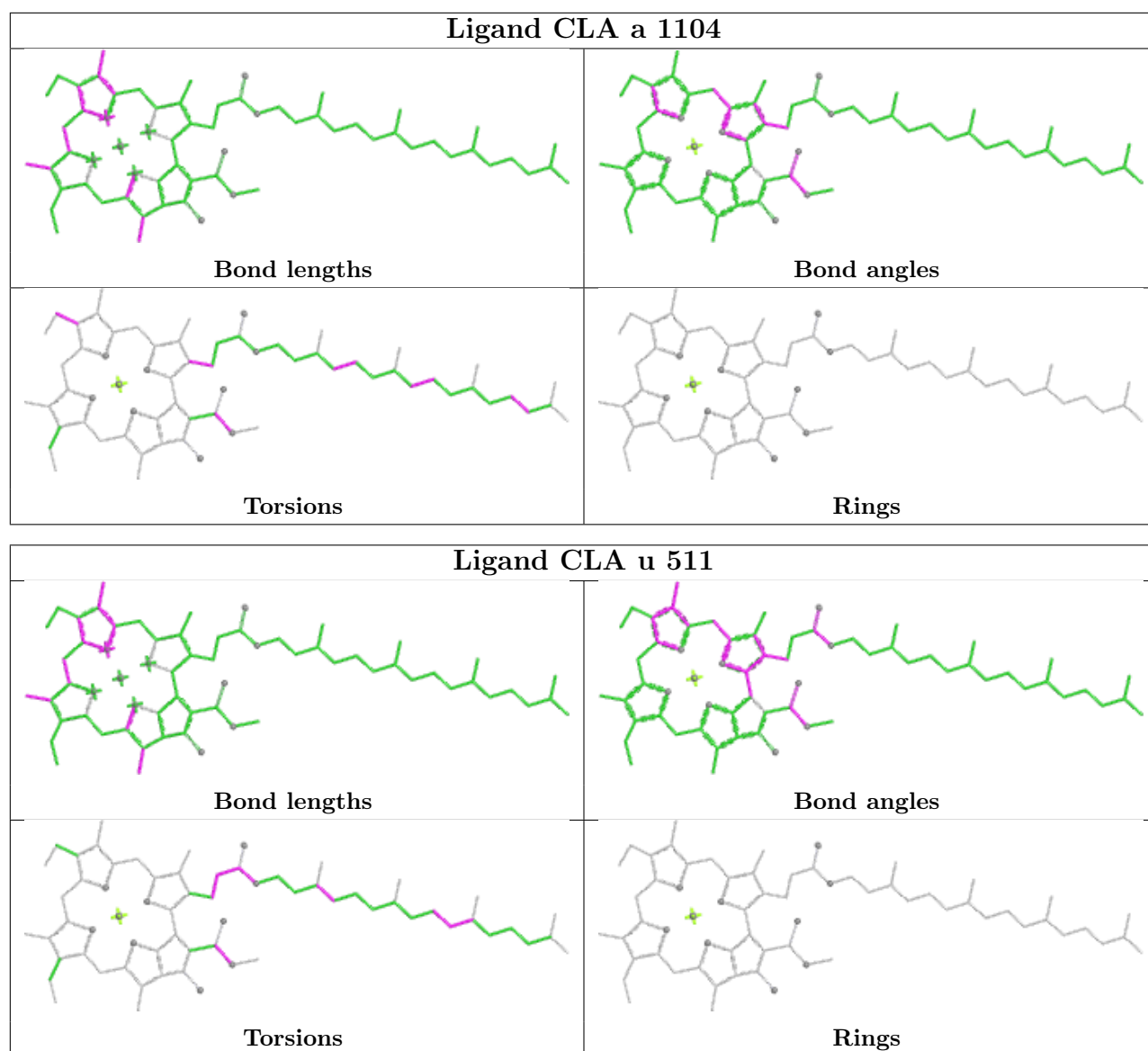
Bond angles



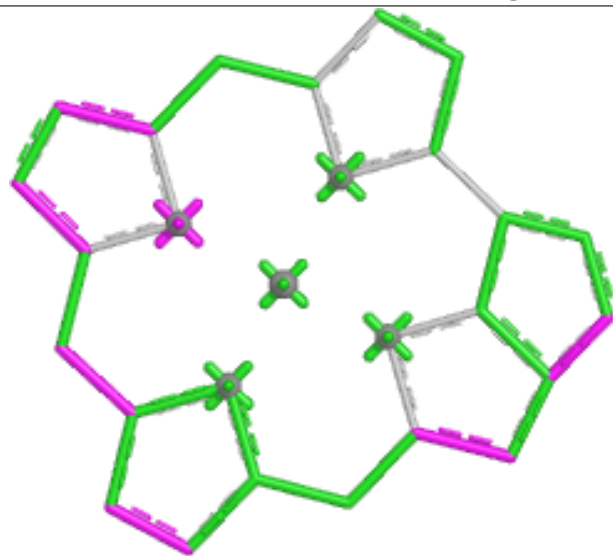
Torsions



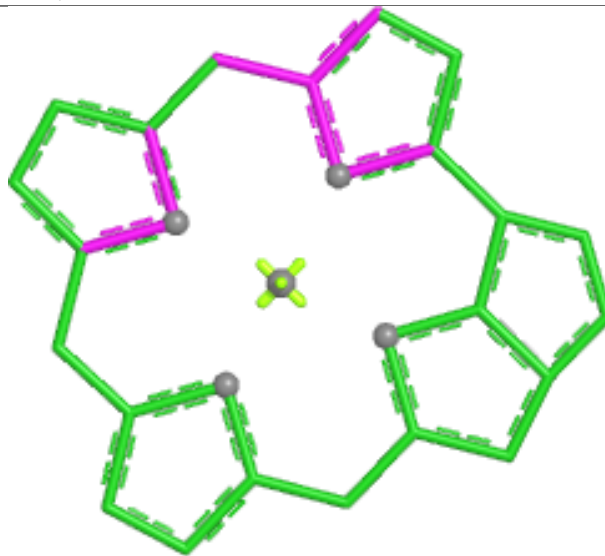
Rings



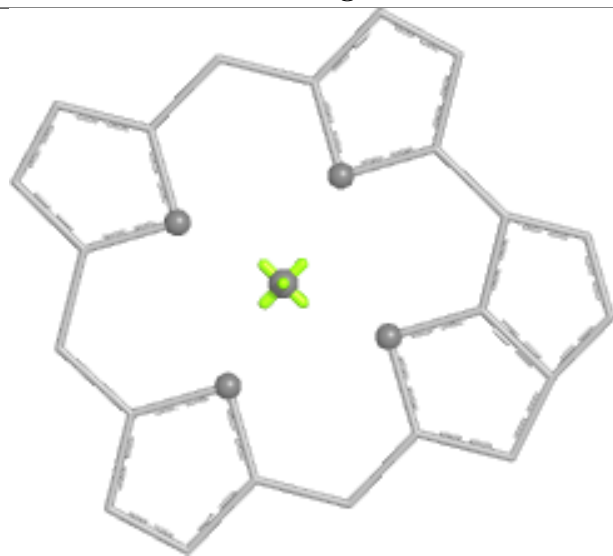
Ligand CLA Q 1302



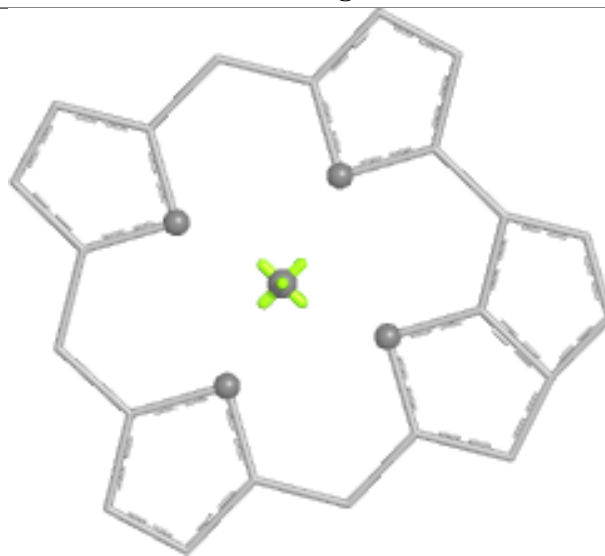
Bond lengths



Bond angles

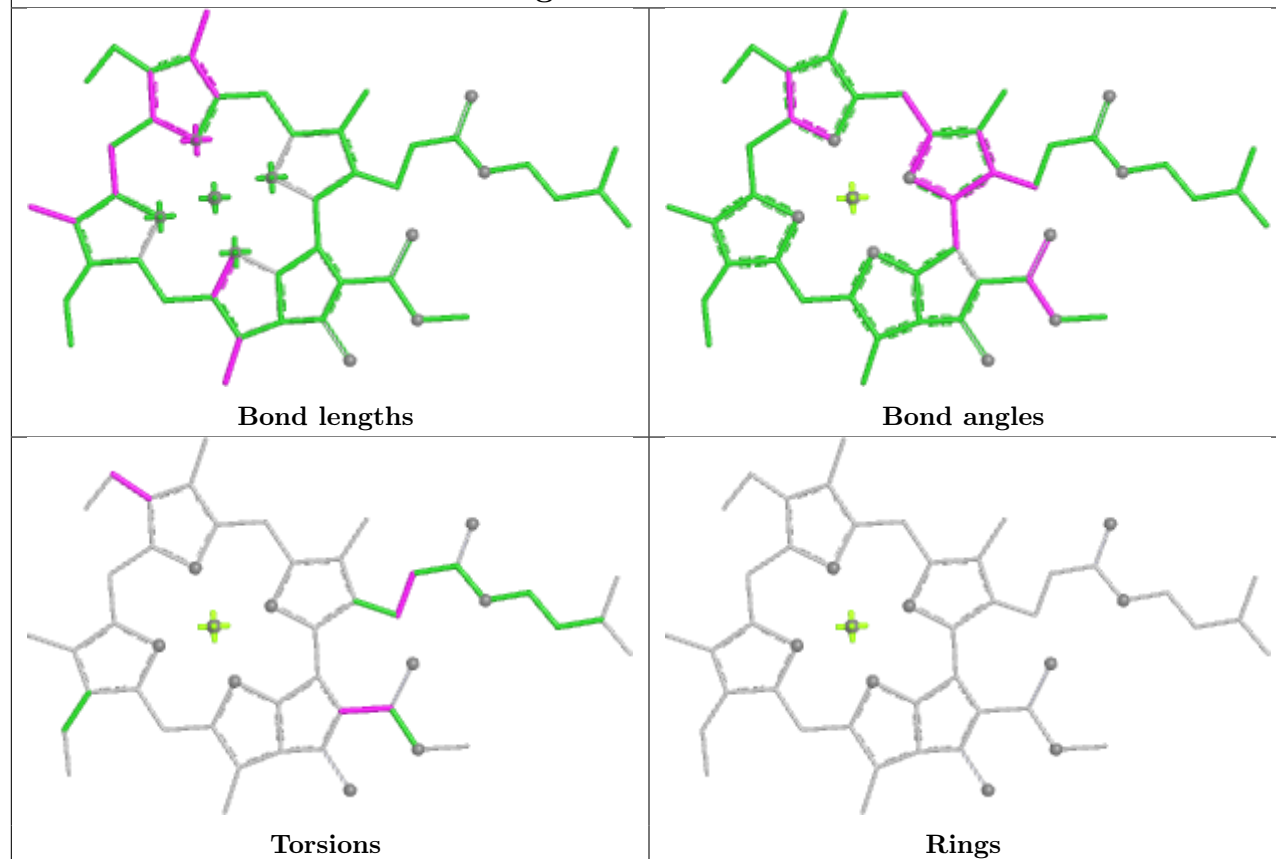


Torsions

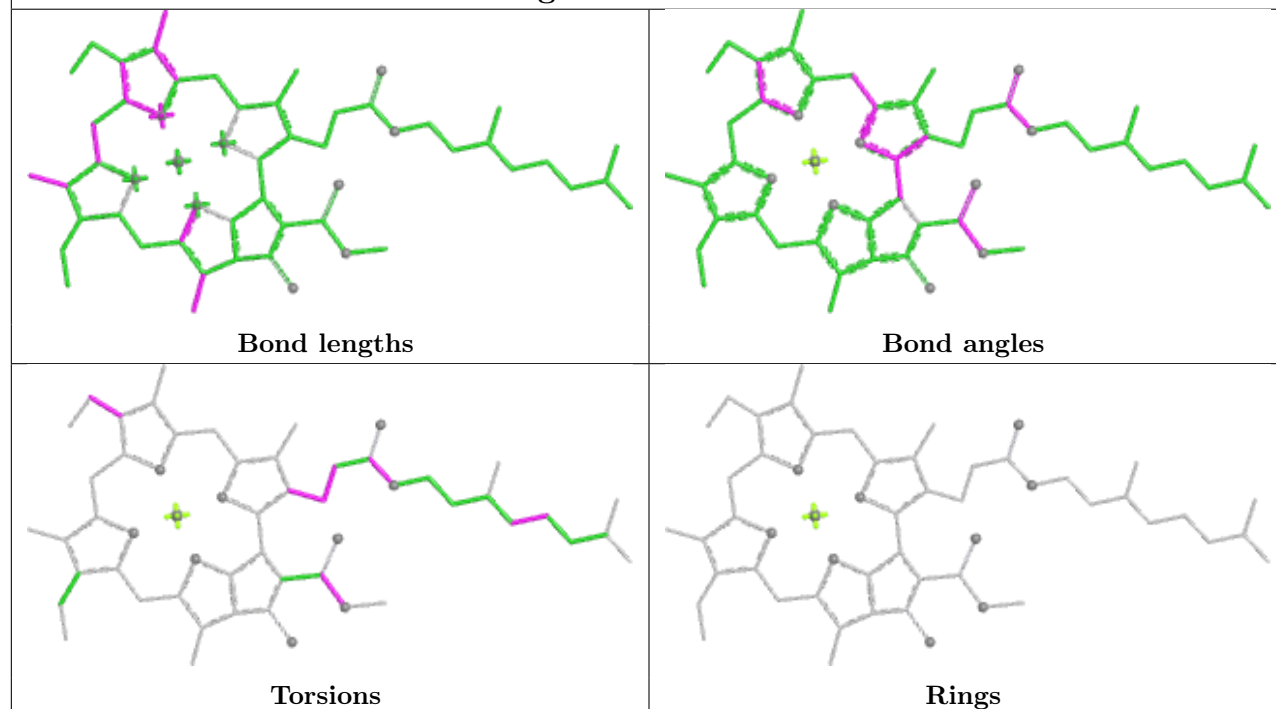


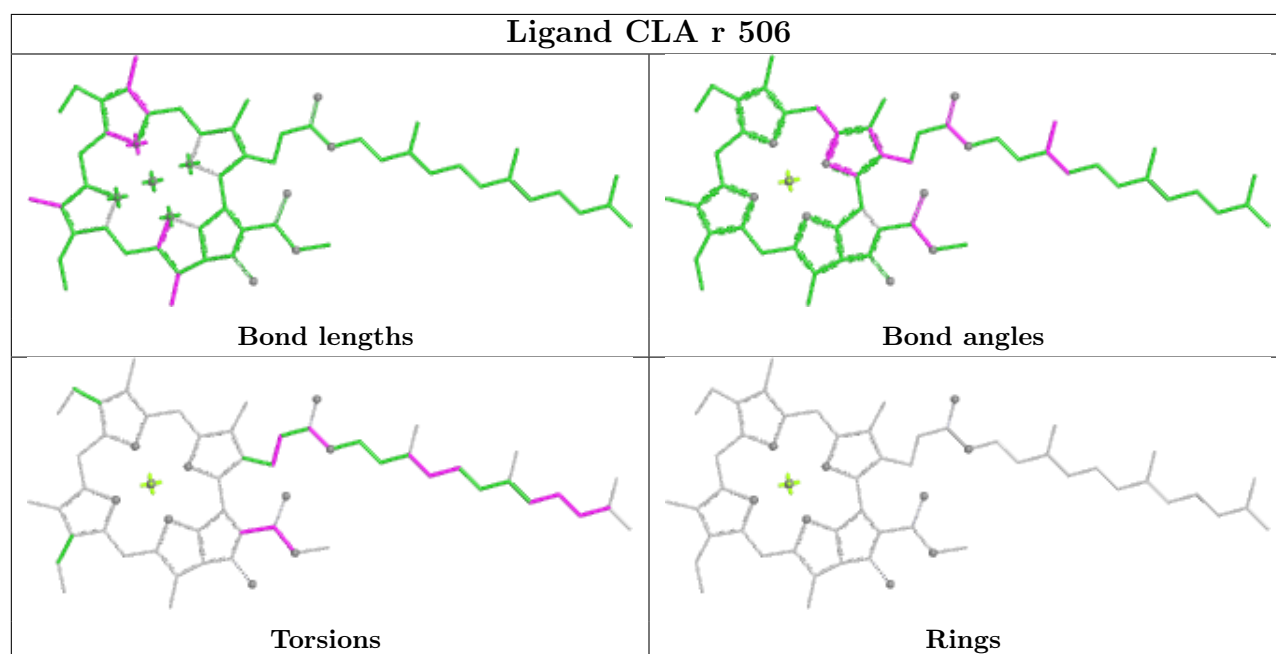
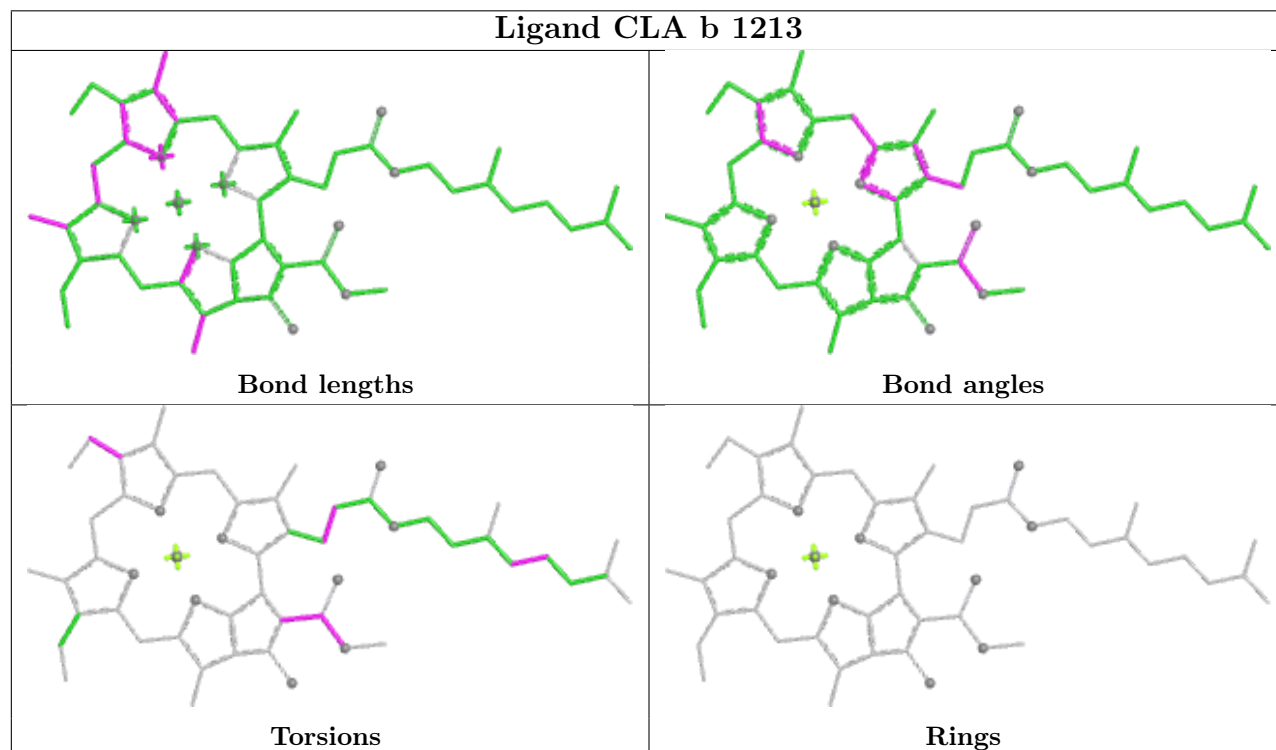
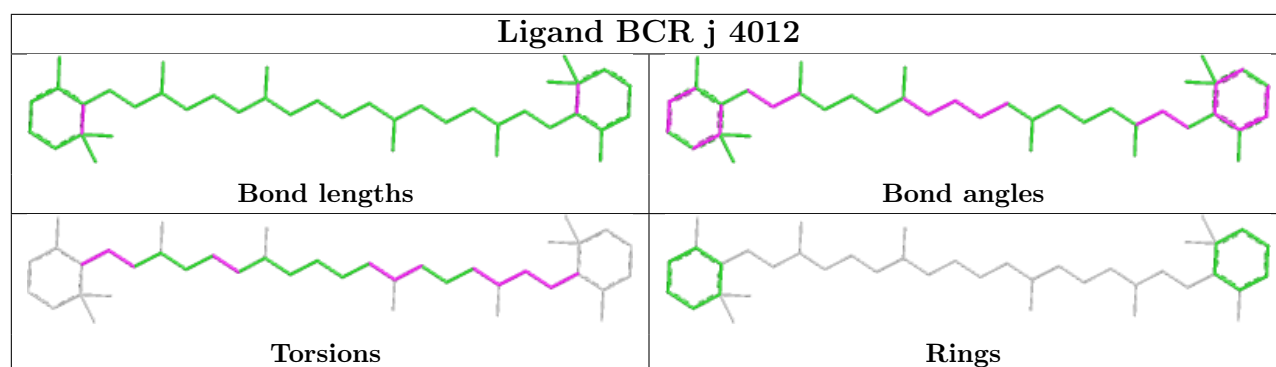
Rings

Ligand CLA x 502

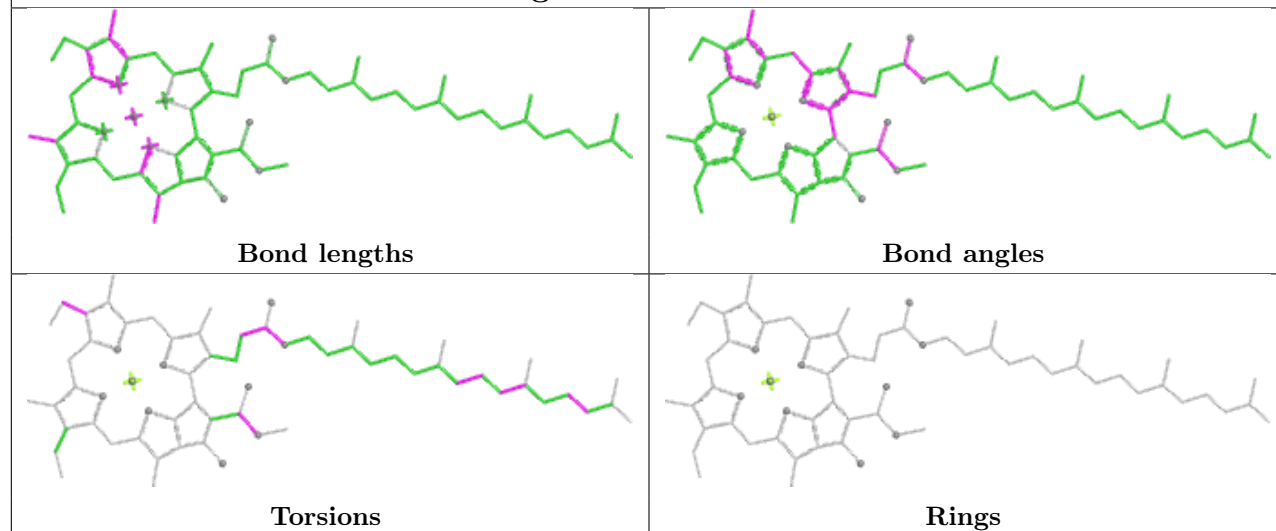


Ligand CLA s 508

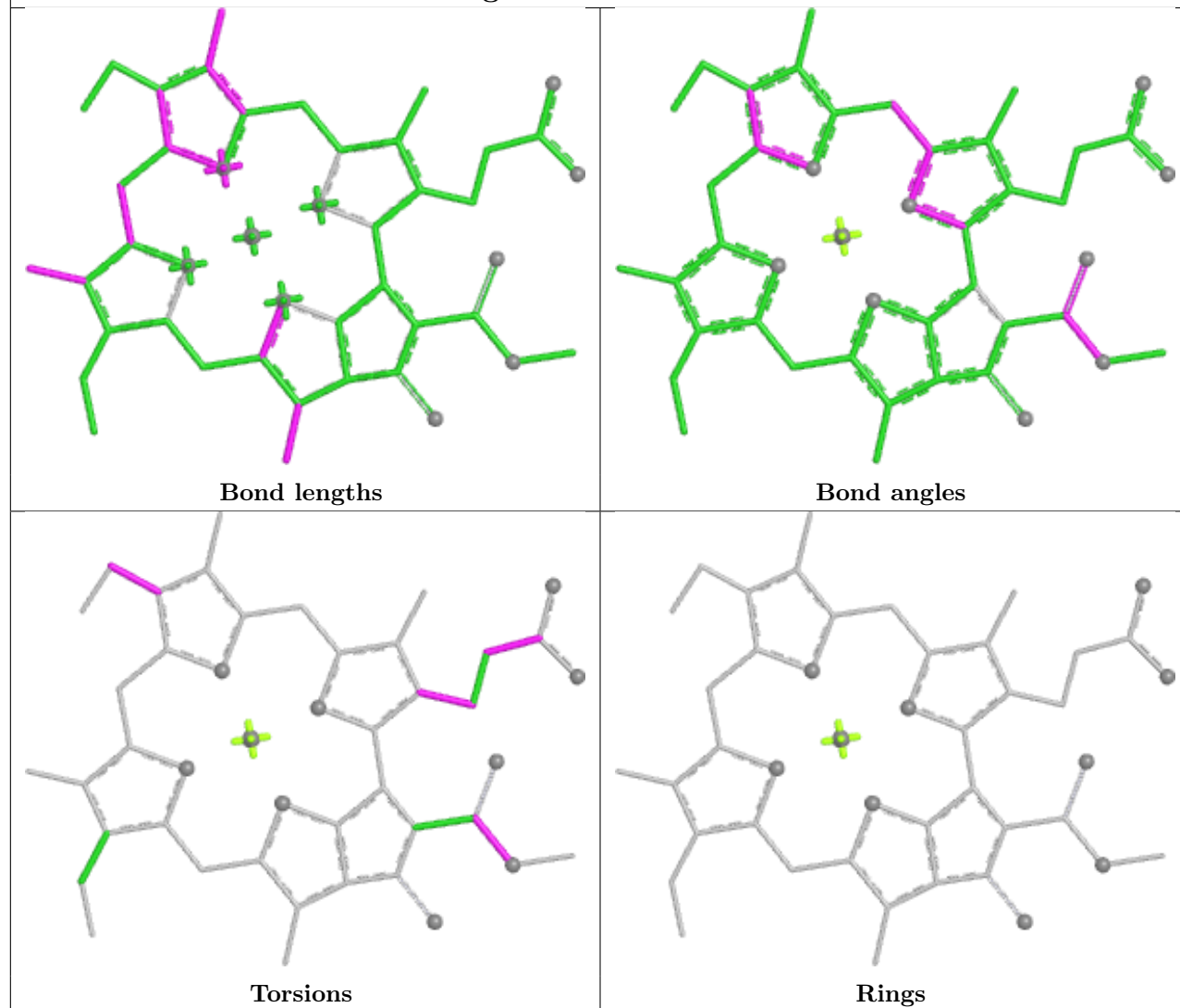


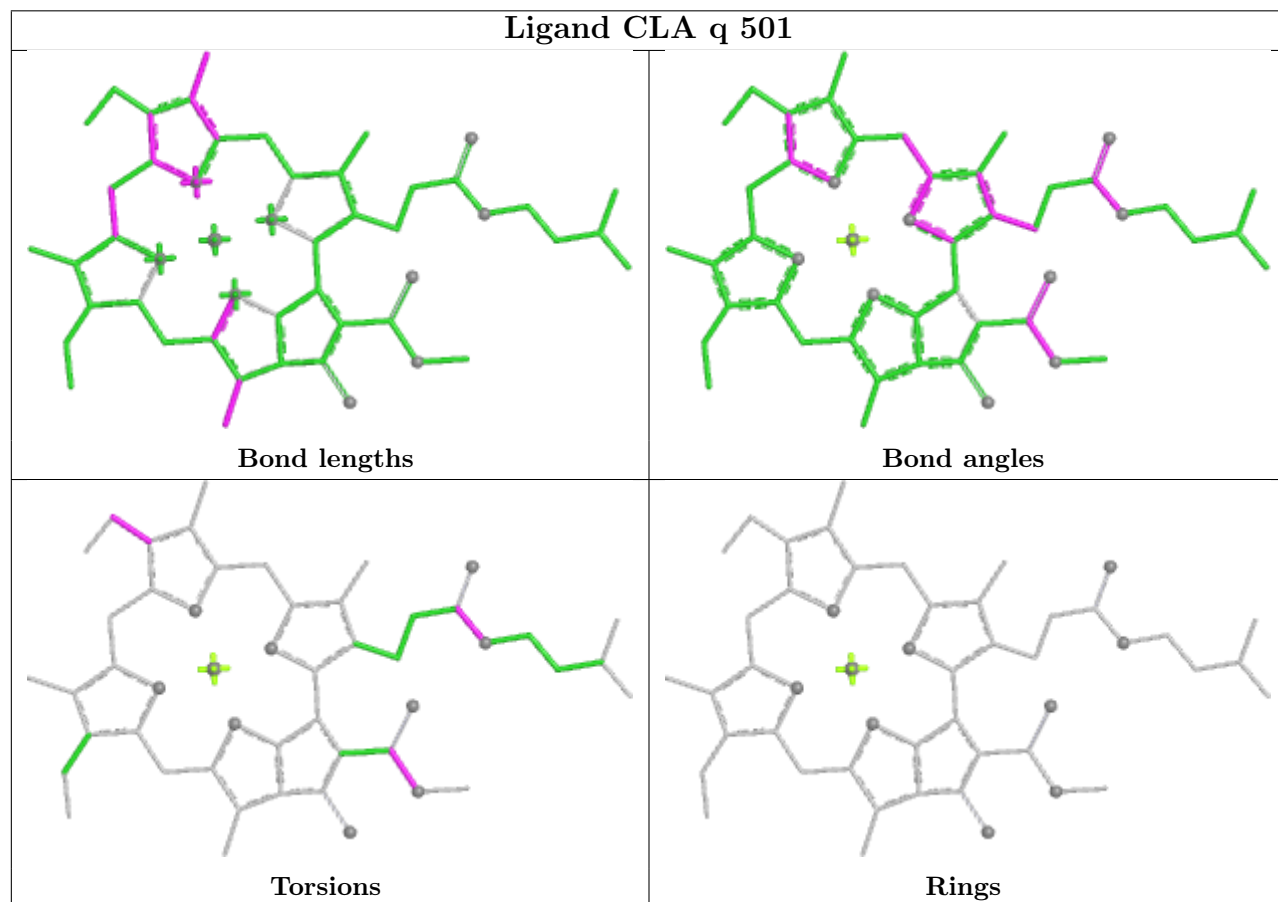
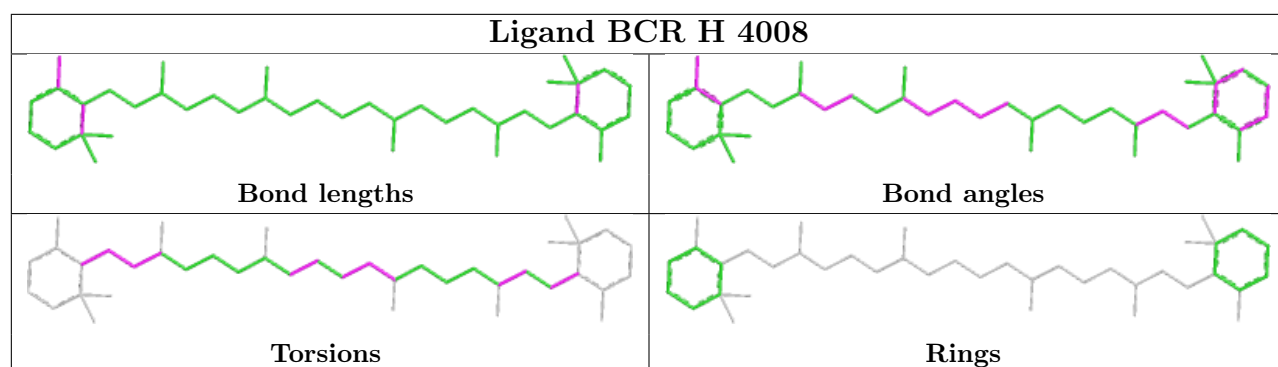


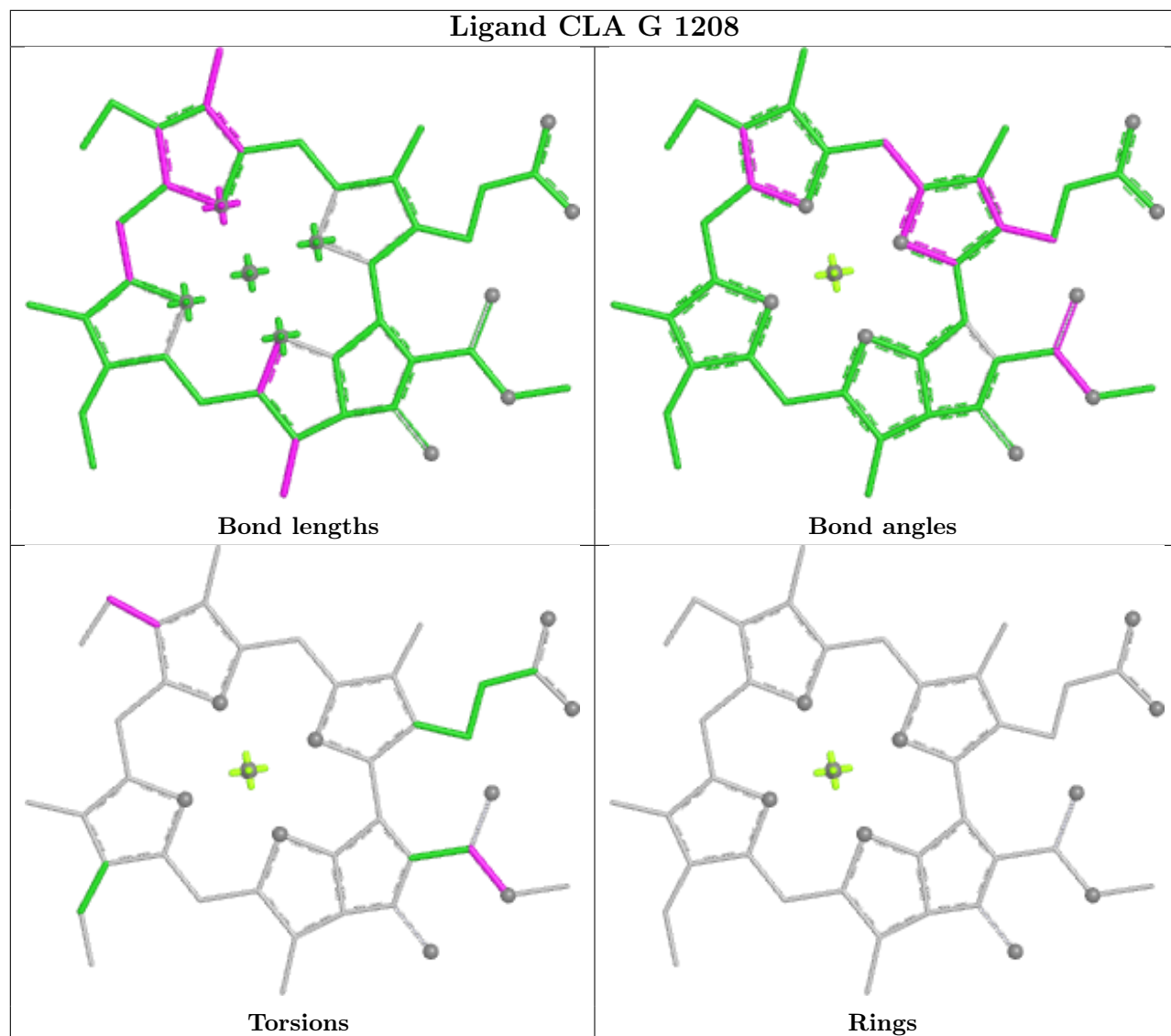
Ligand CLA Y 510



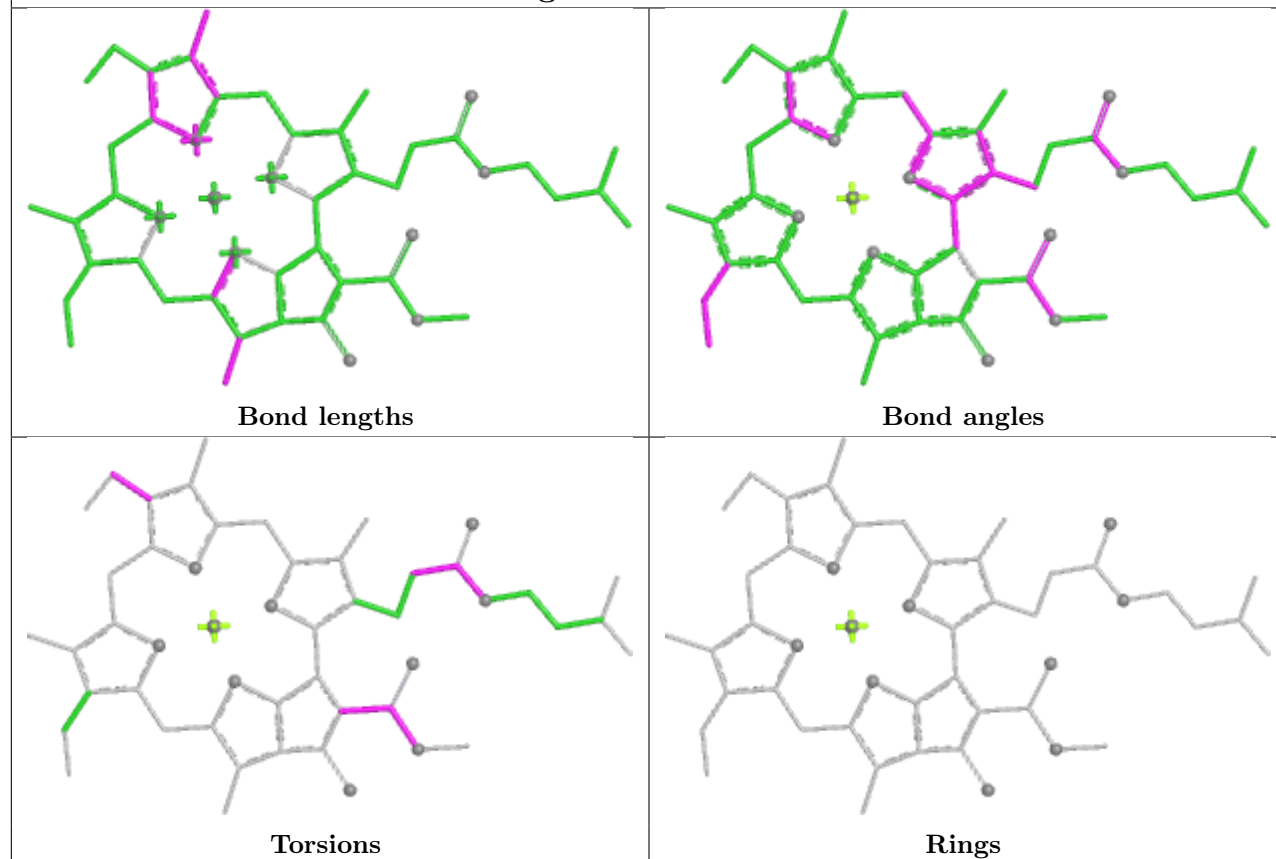
Ligand CLA G 1217



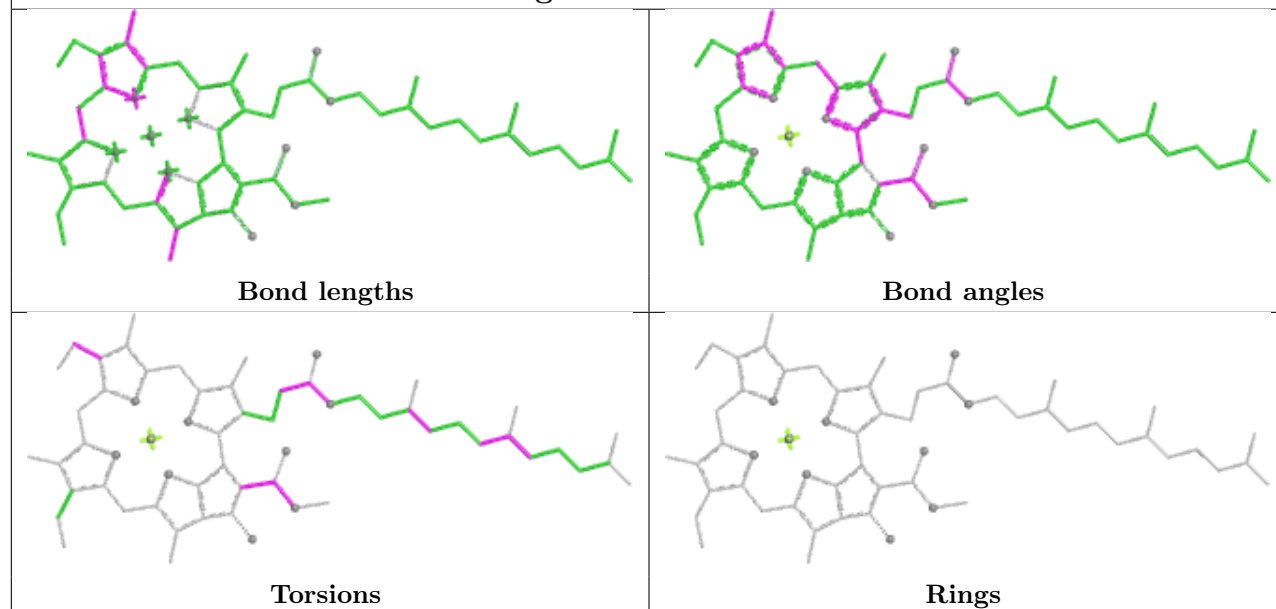


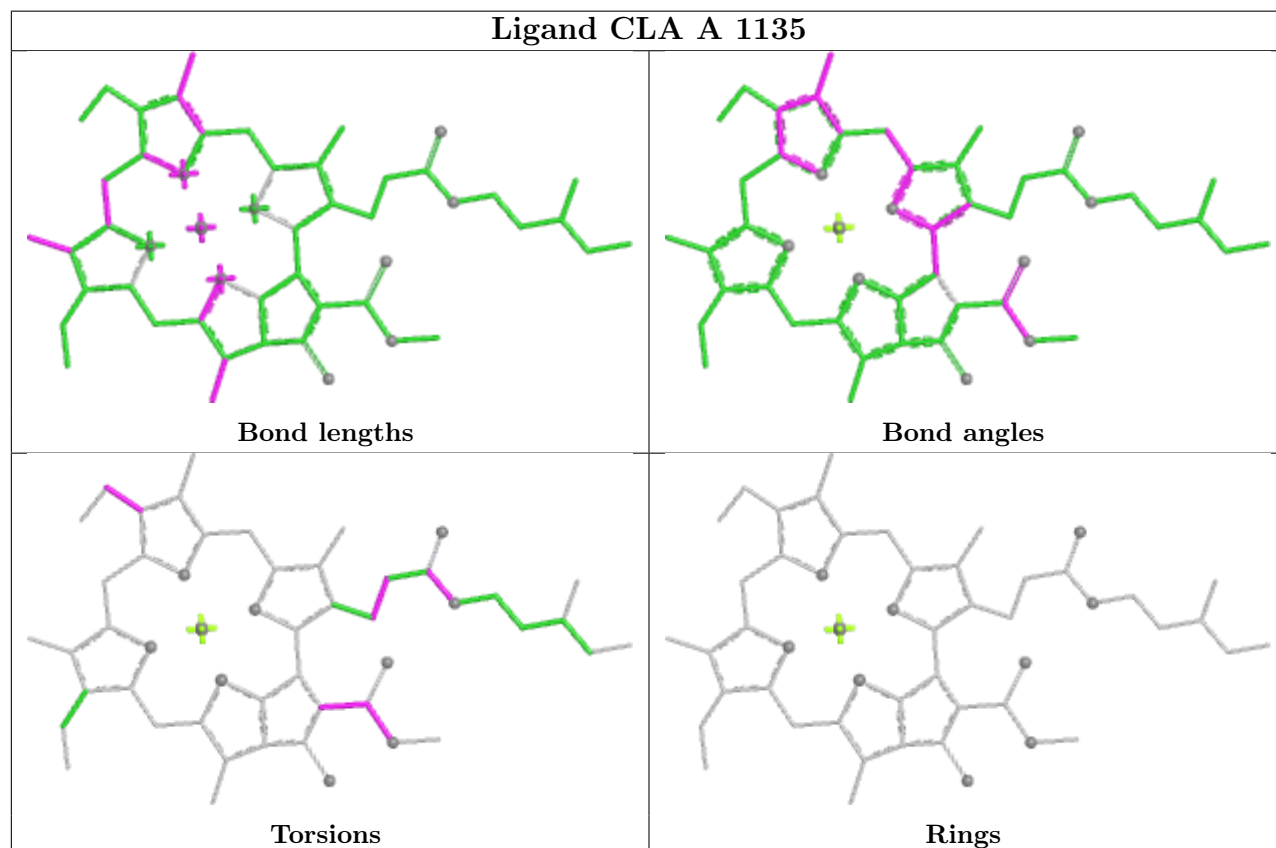
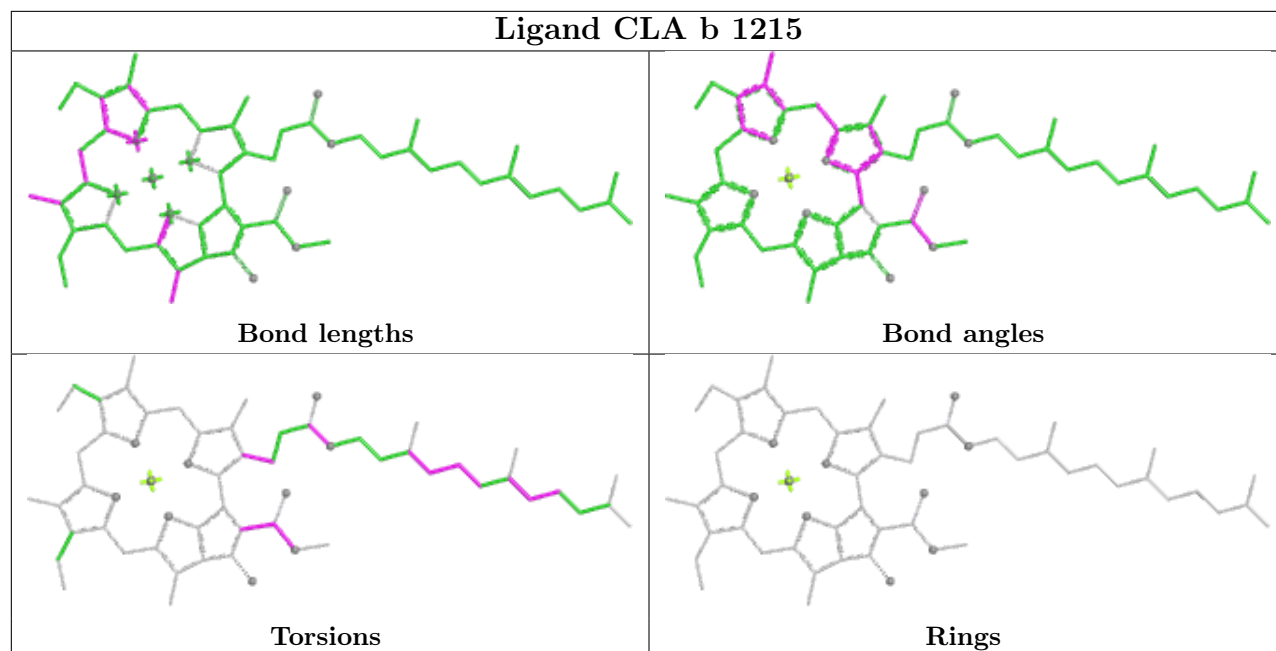


Ligand CLA t 502

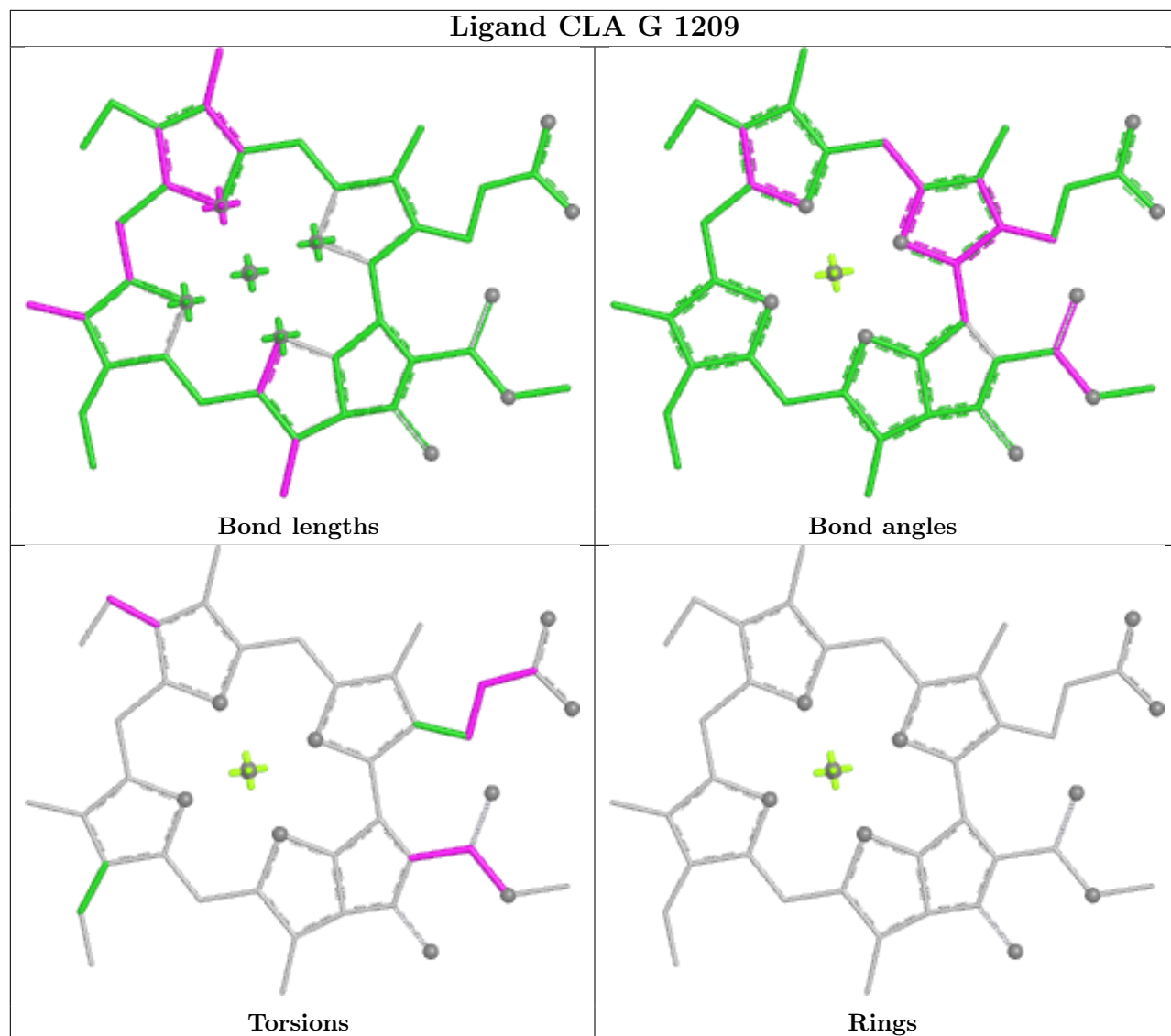


Ligand CLA h 510

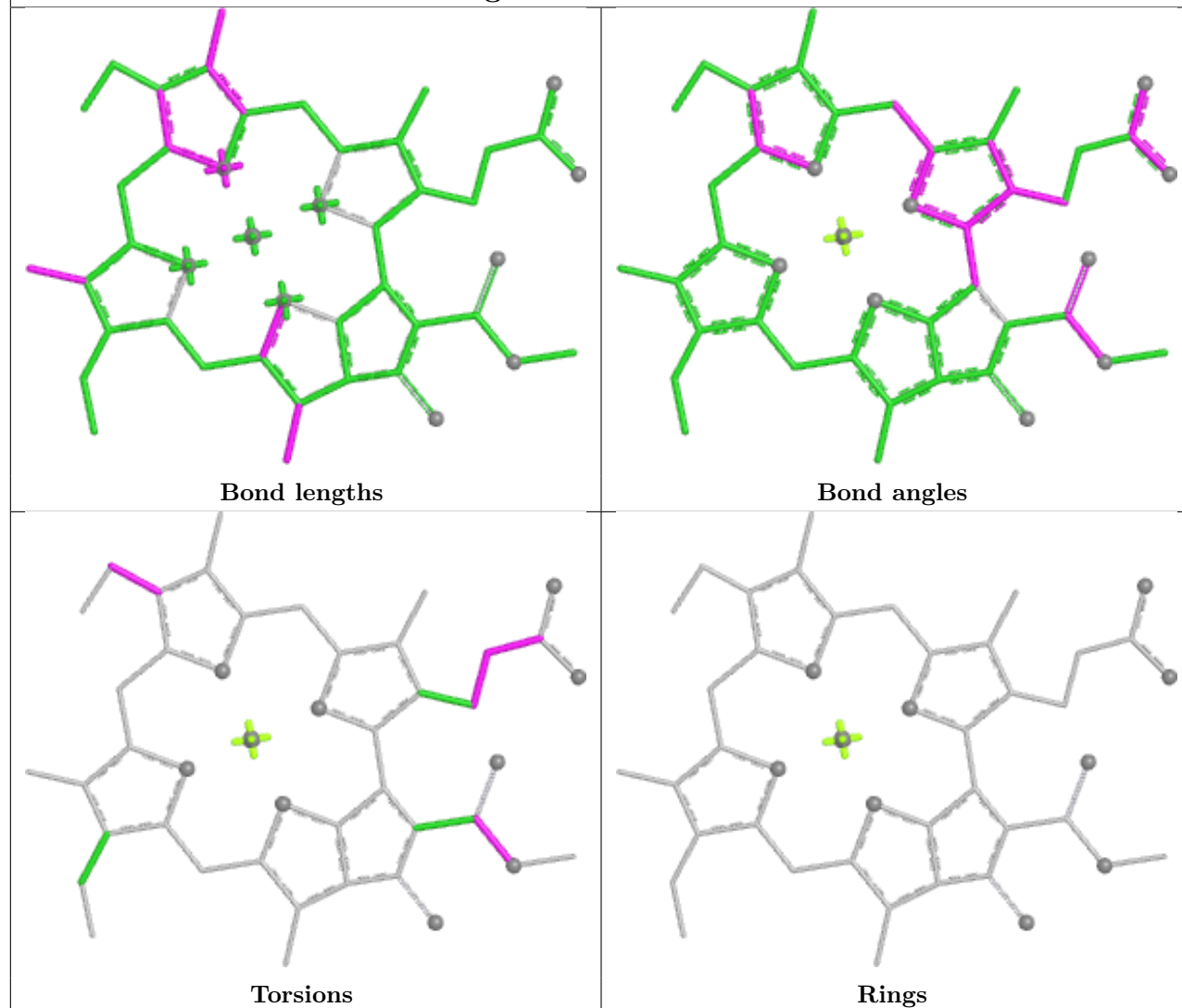




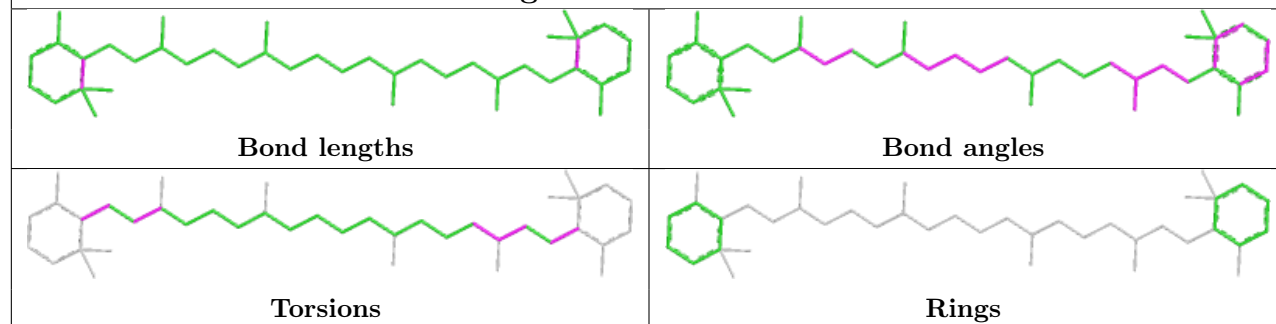
Ligand CLA G 1209

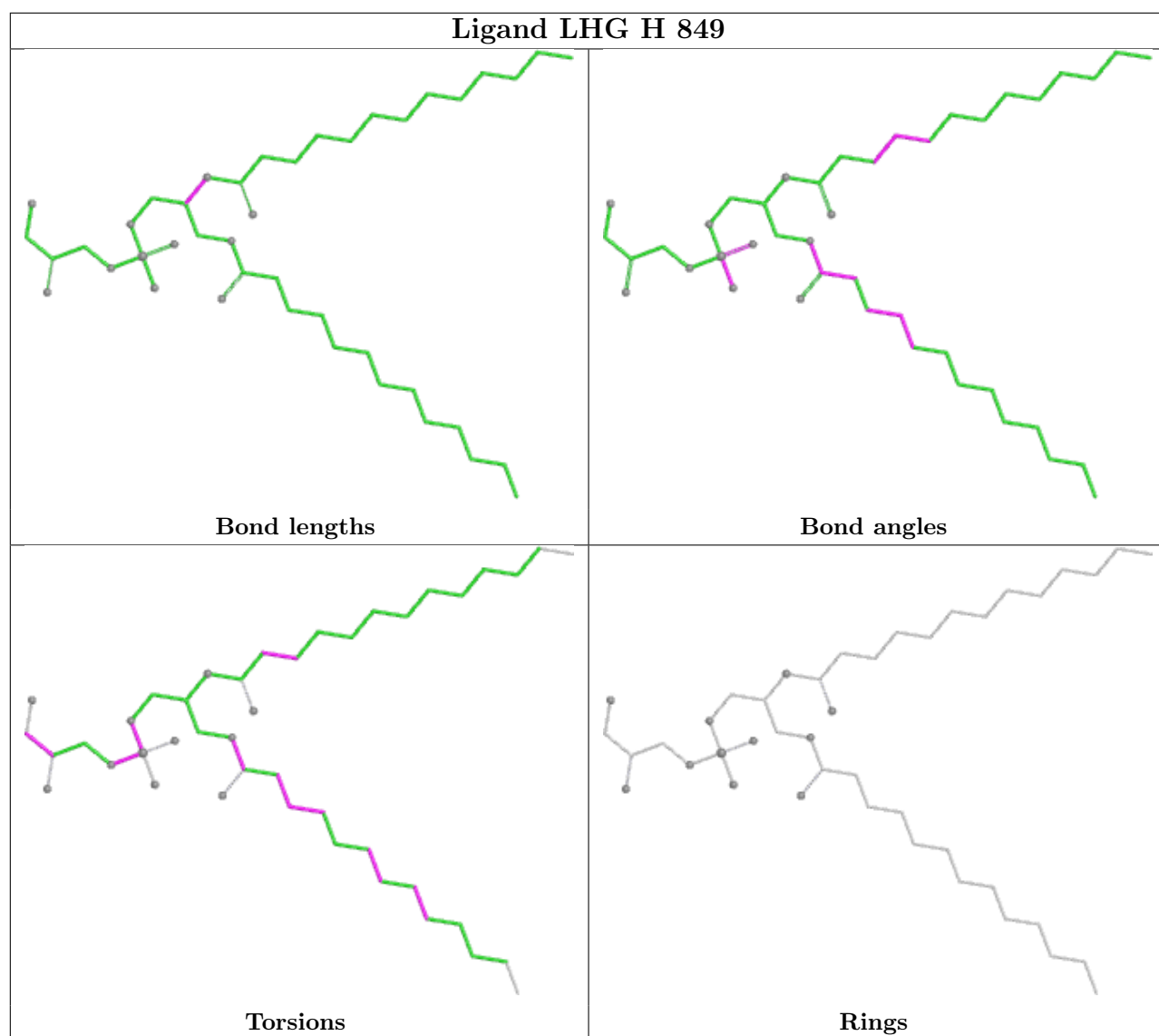


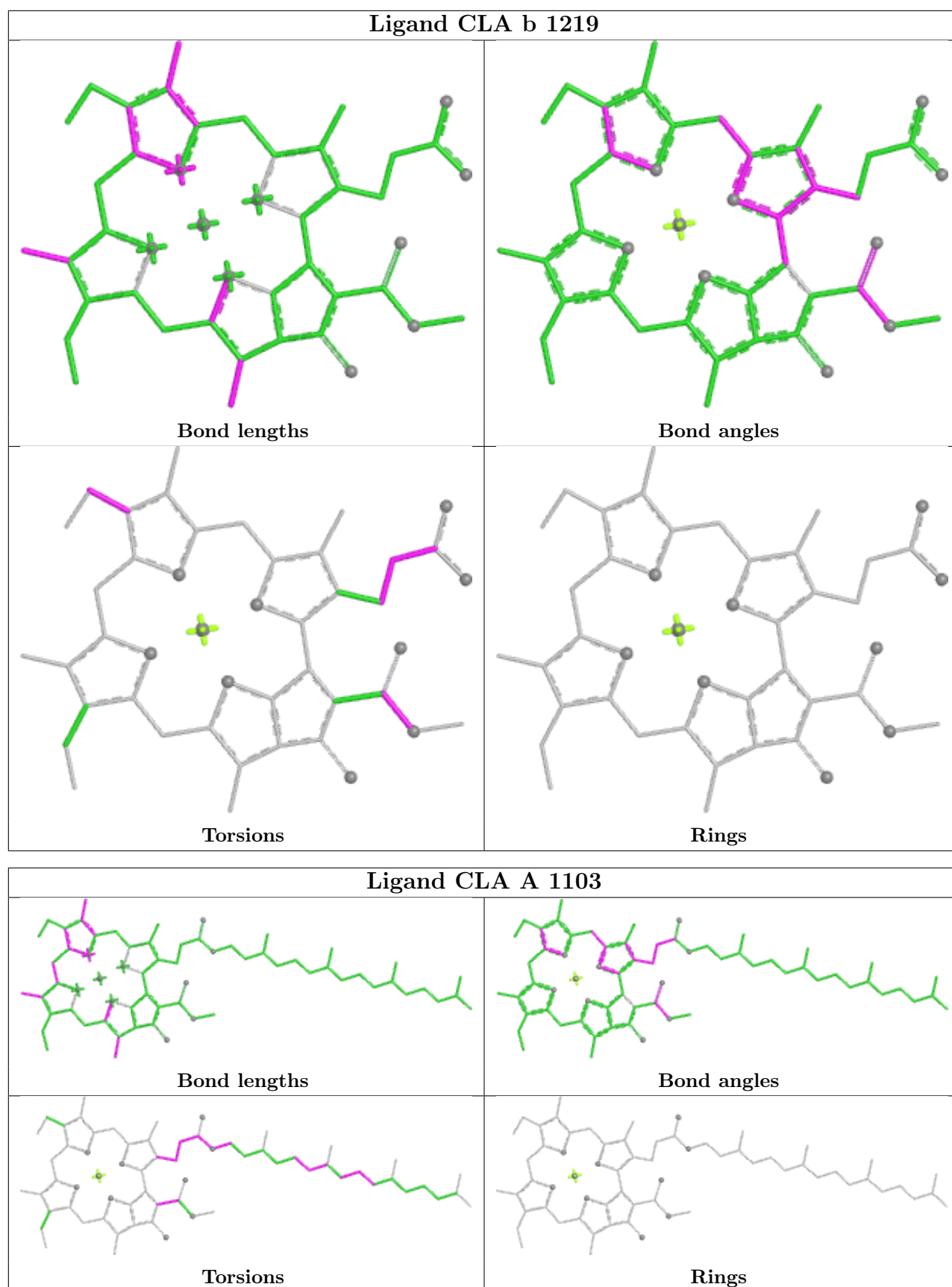
Ligand CLA B 1212

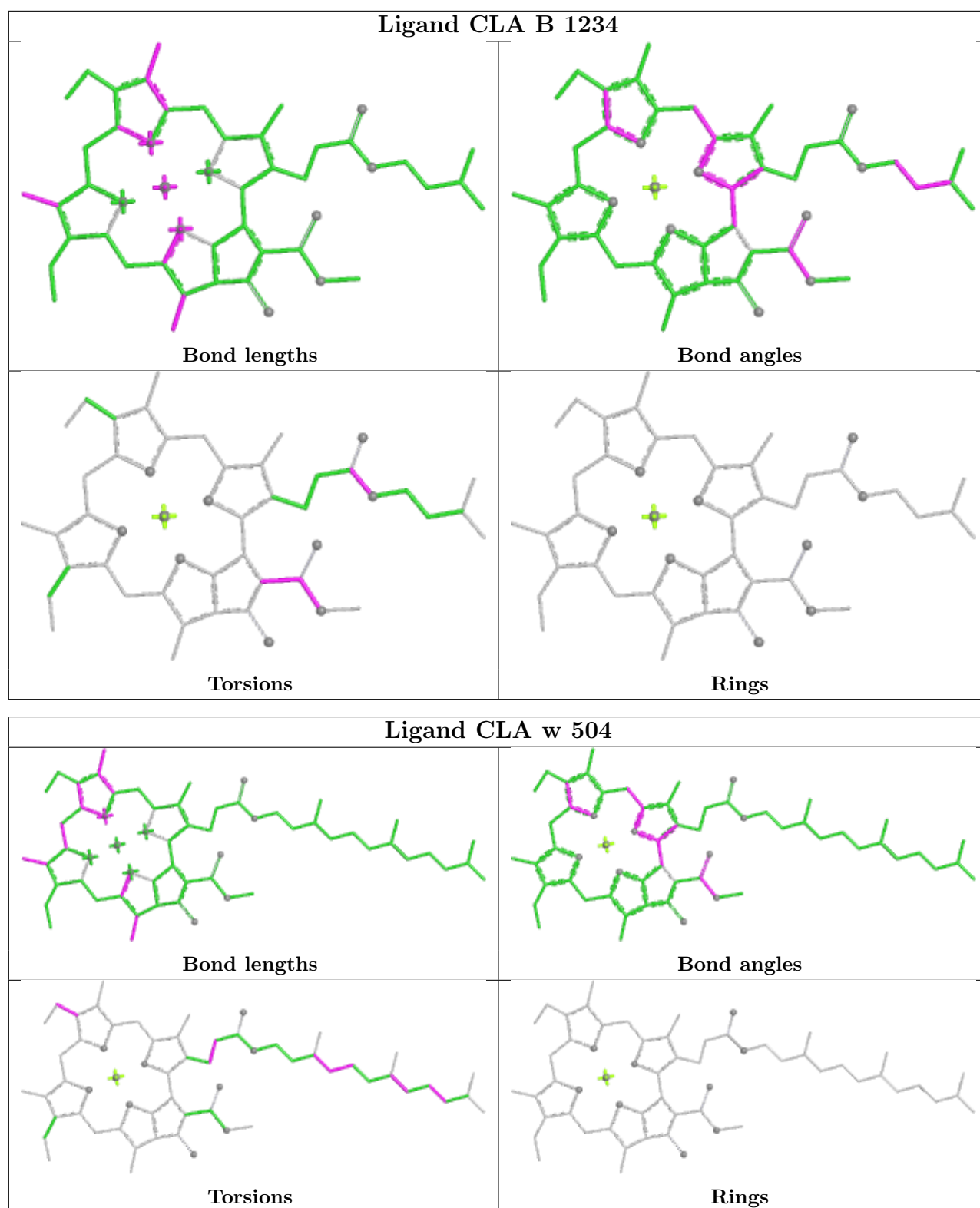


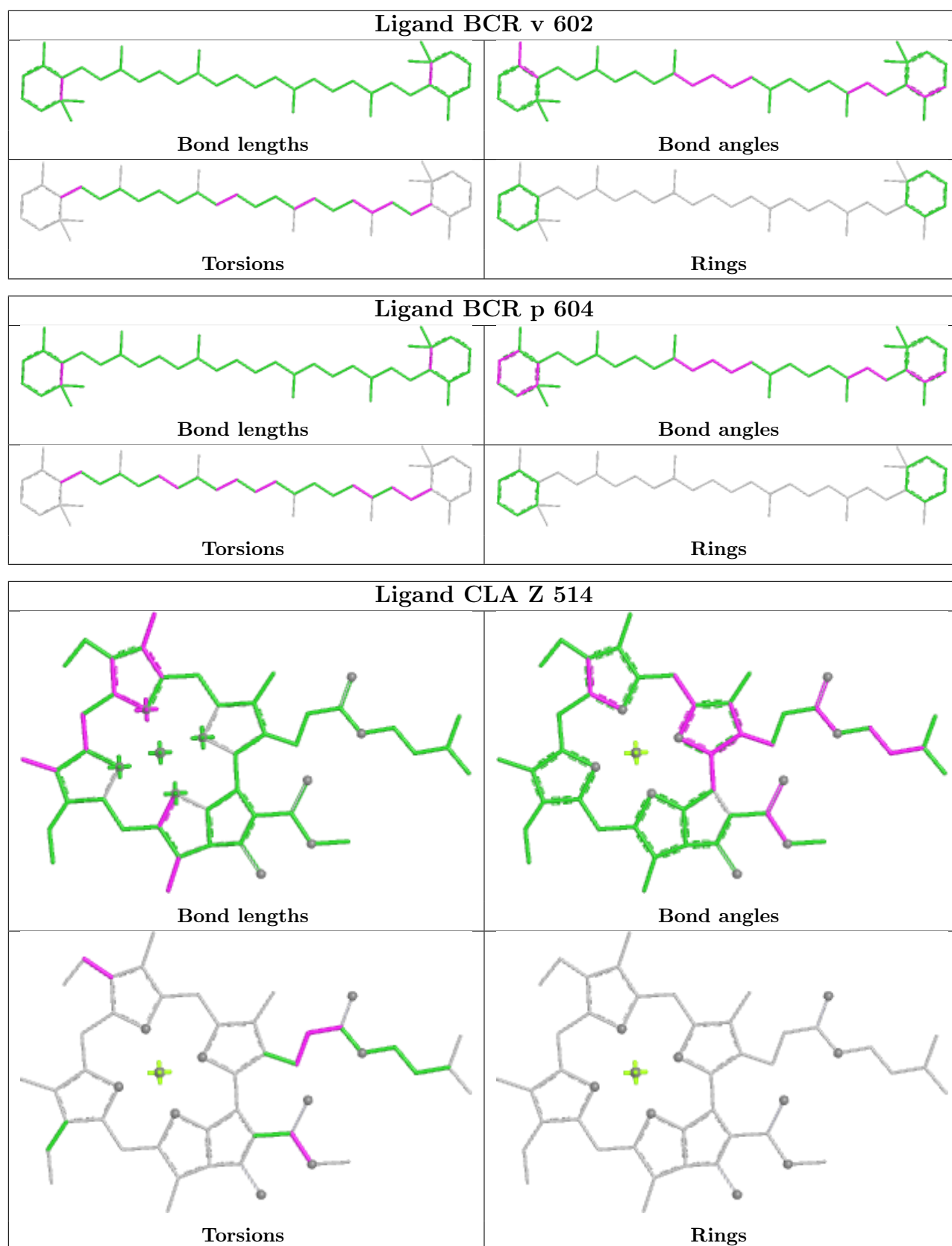
Ligand BCR G 4005

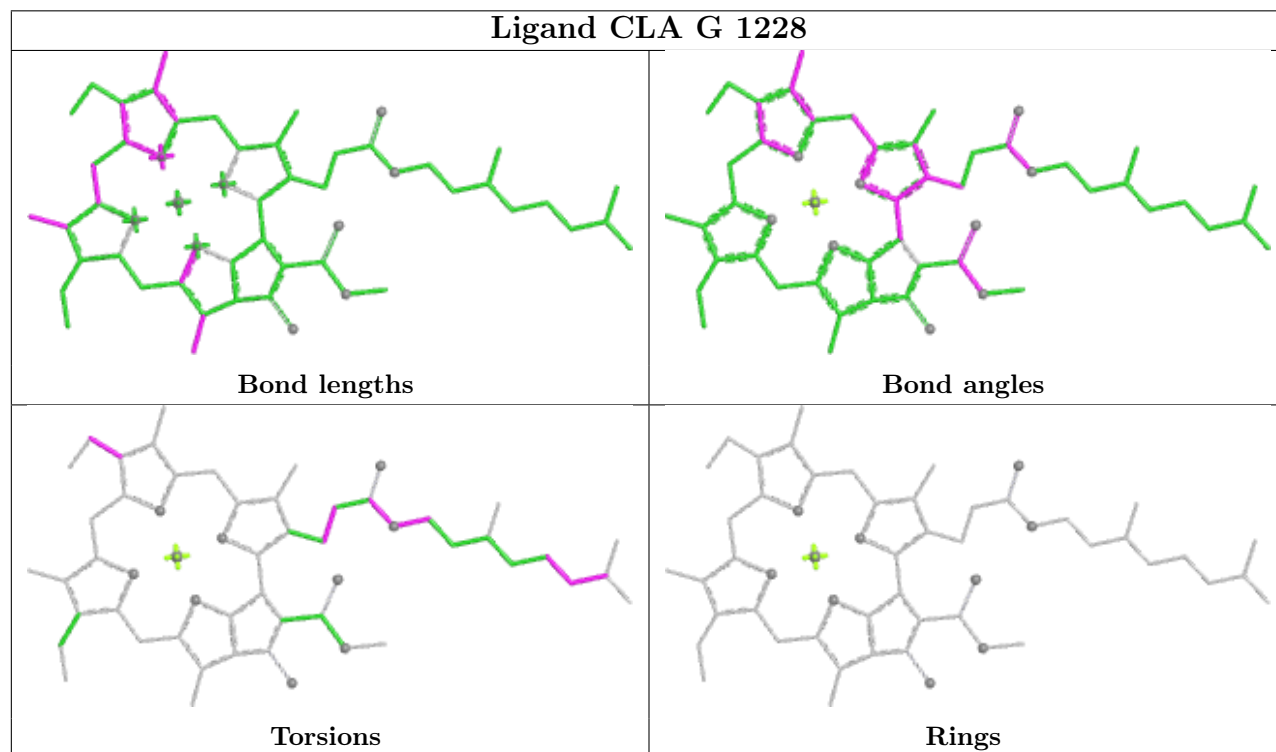
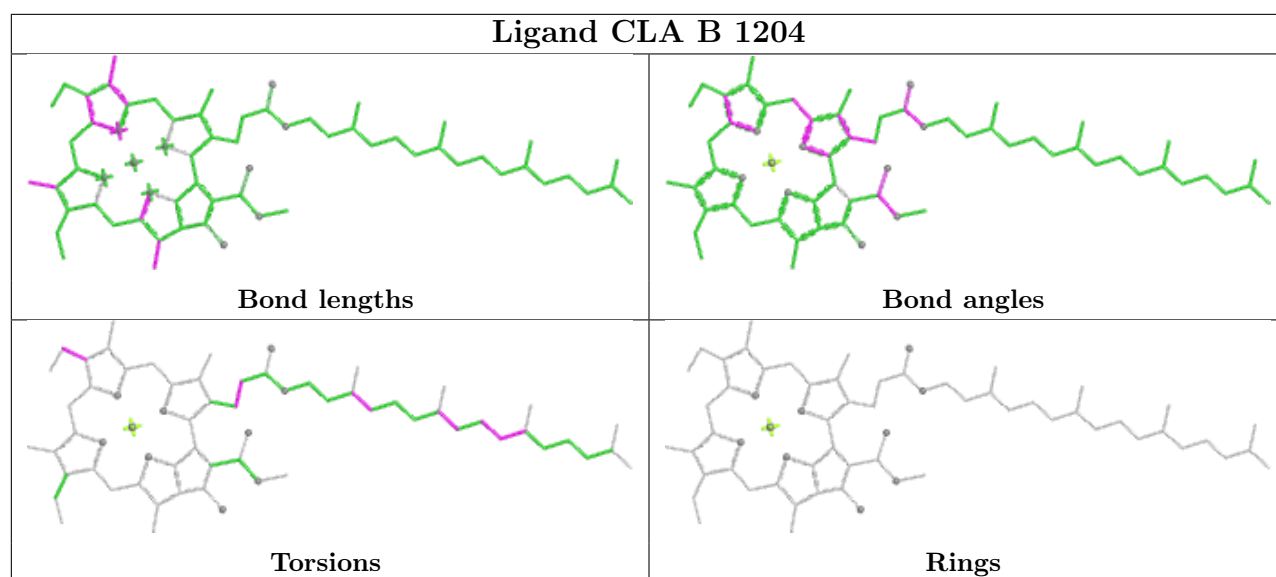


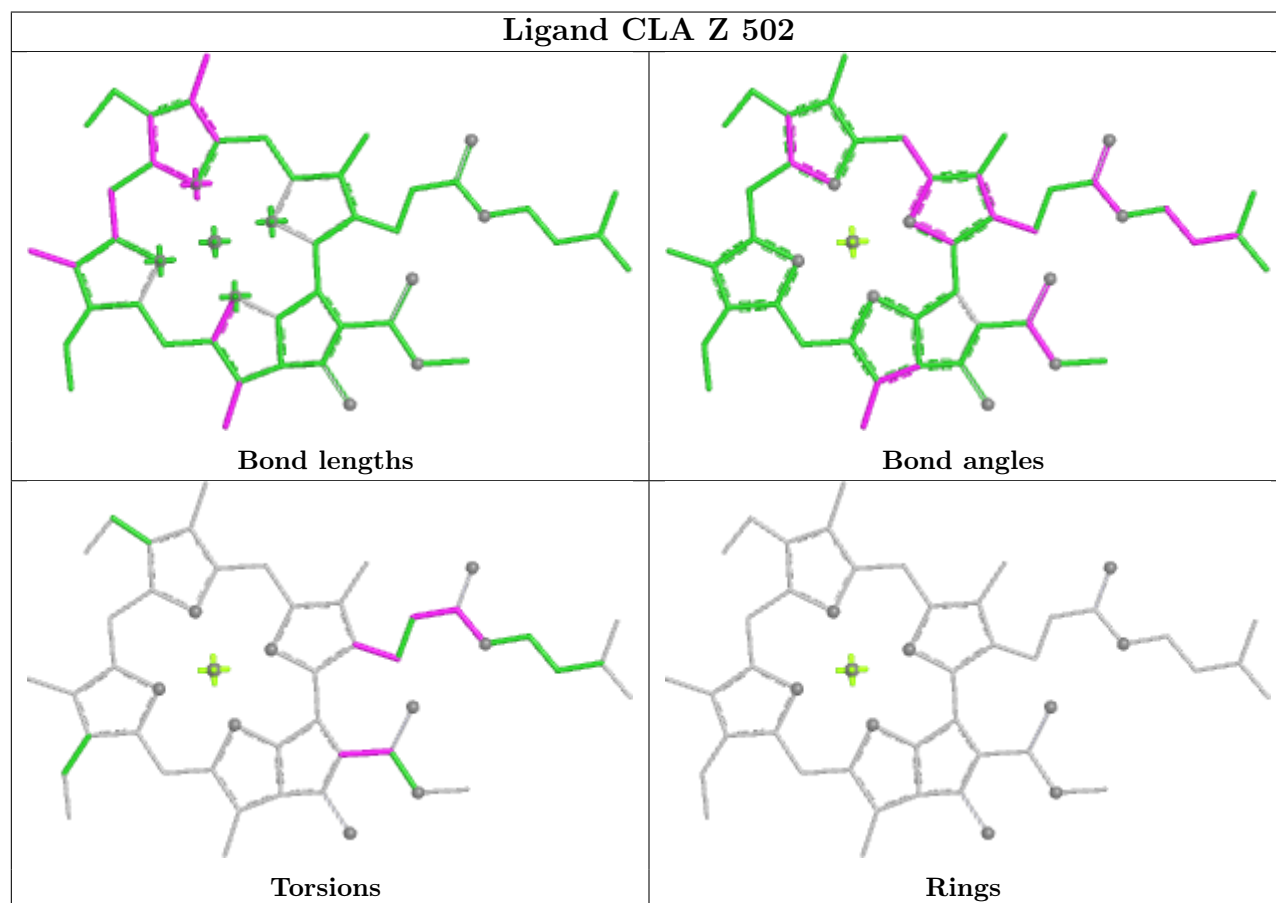
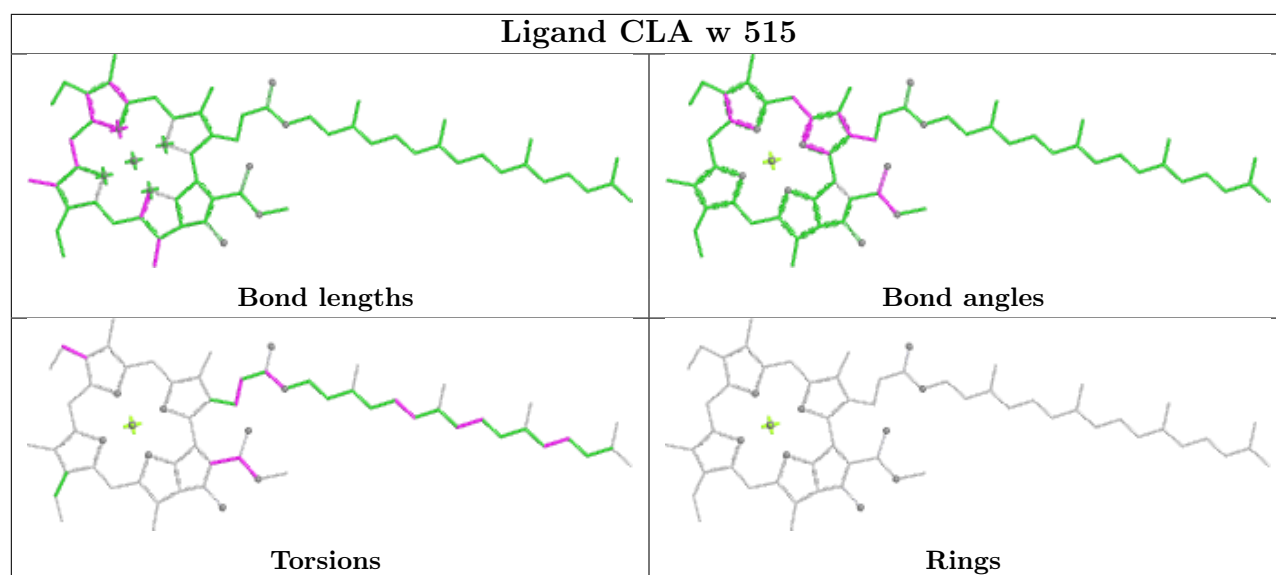


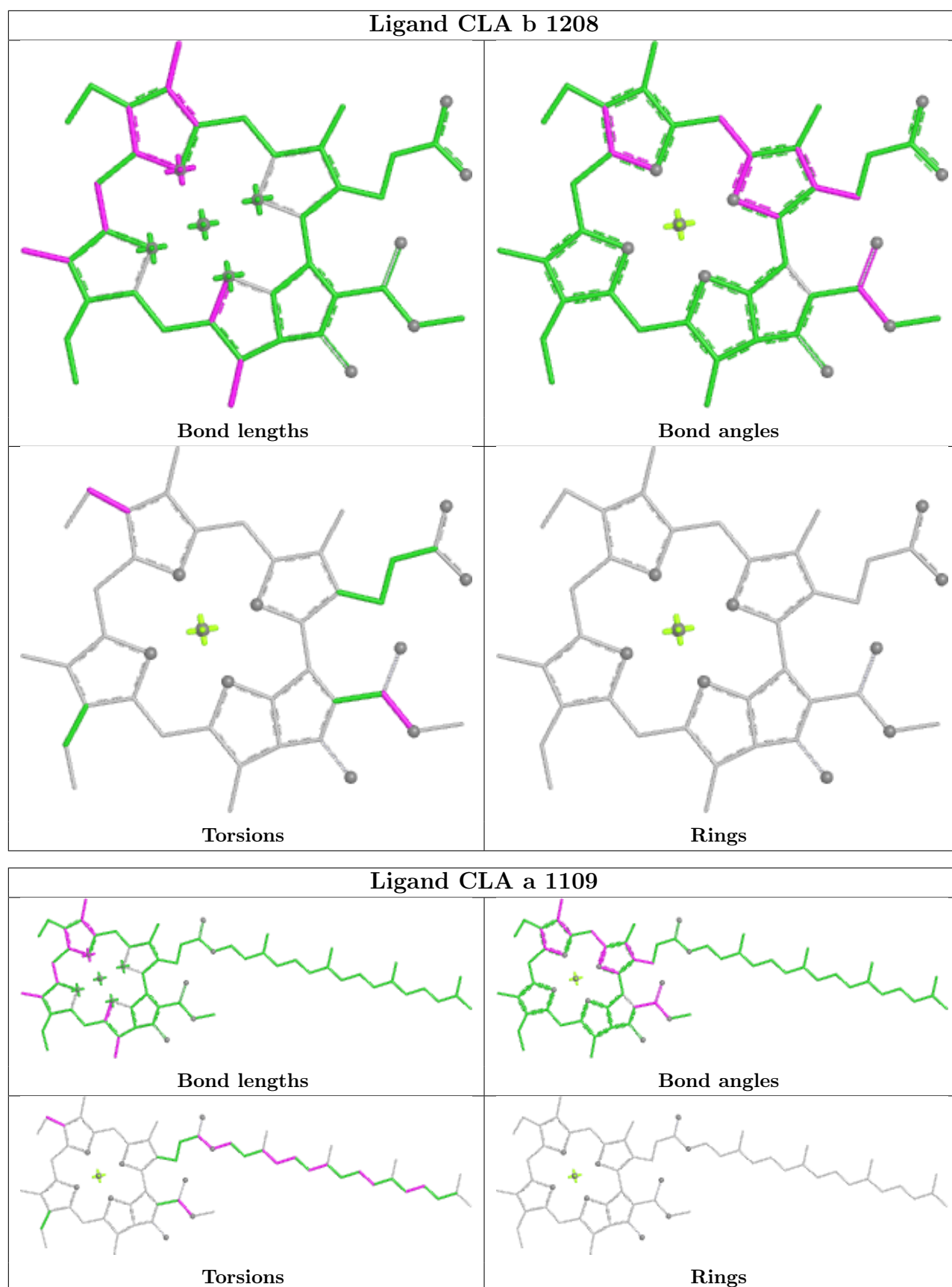


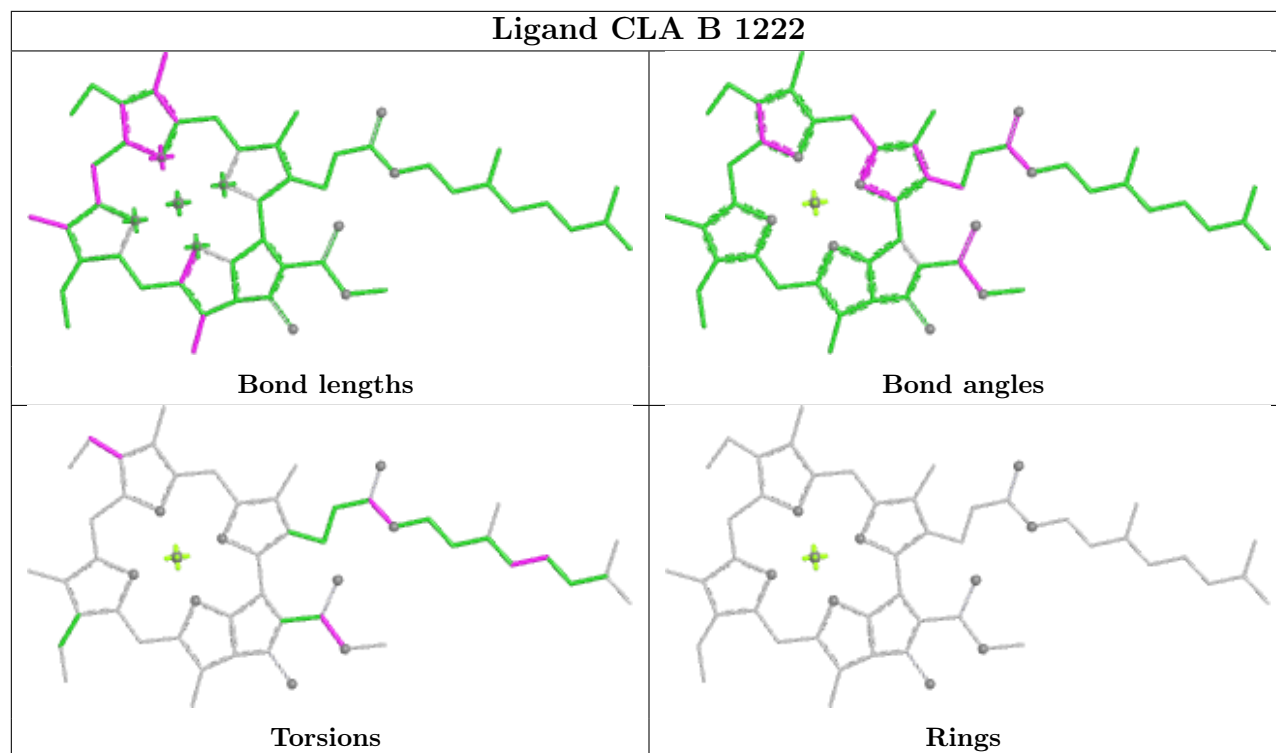
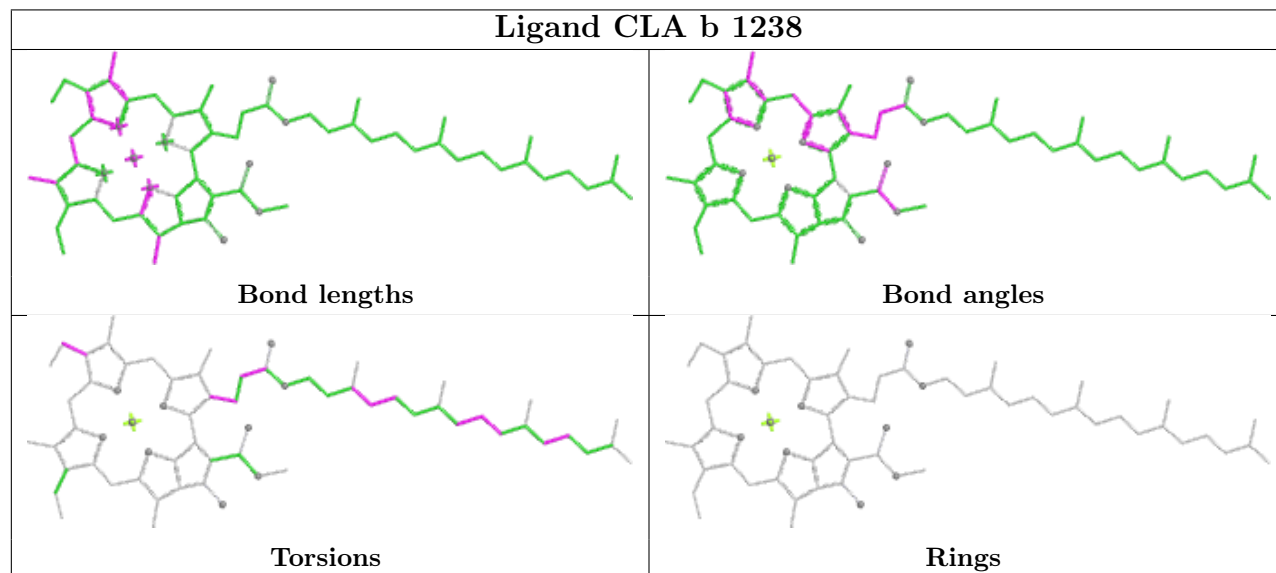


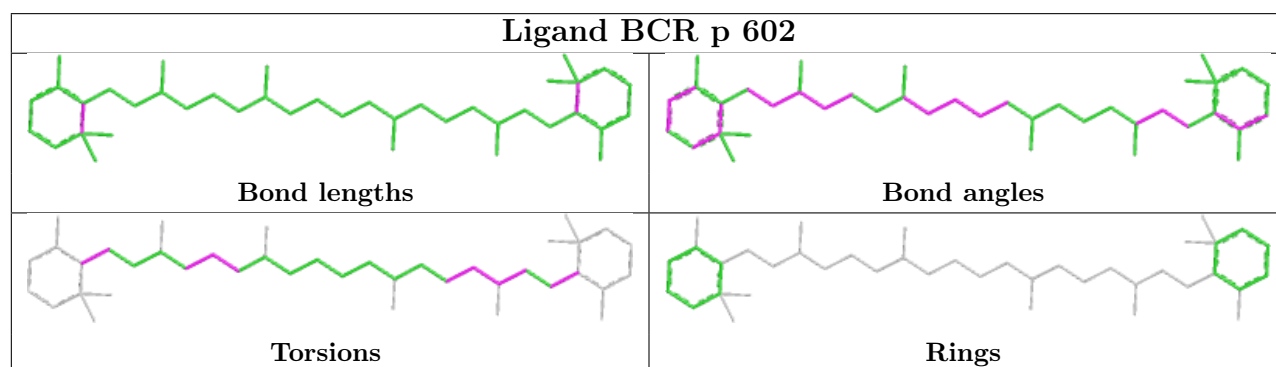
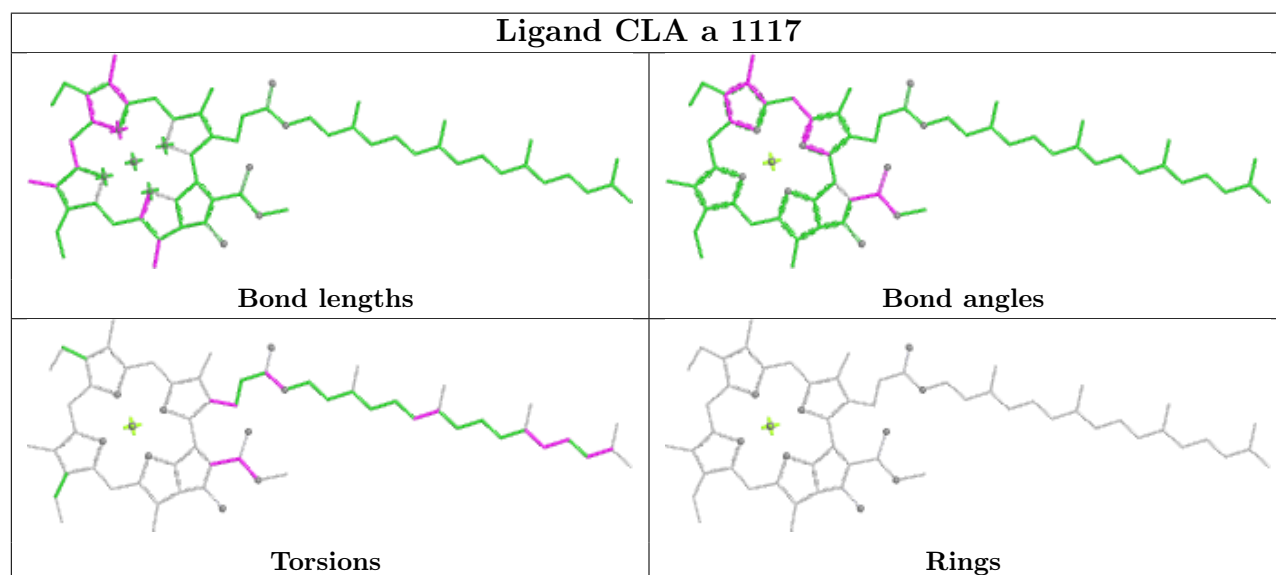
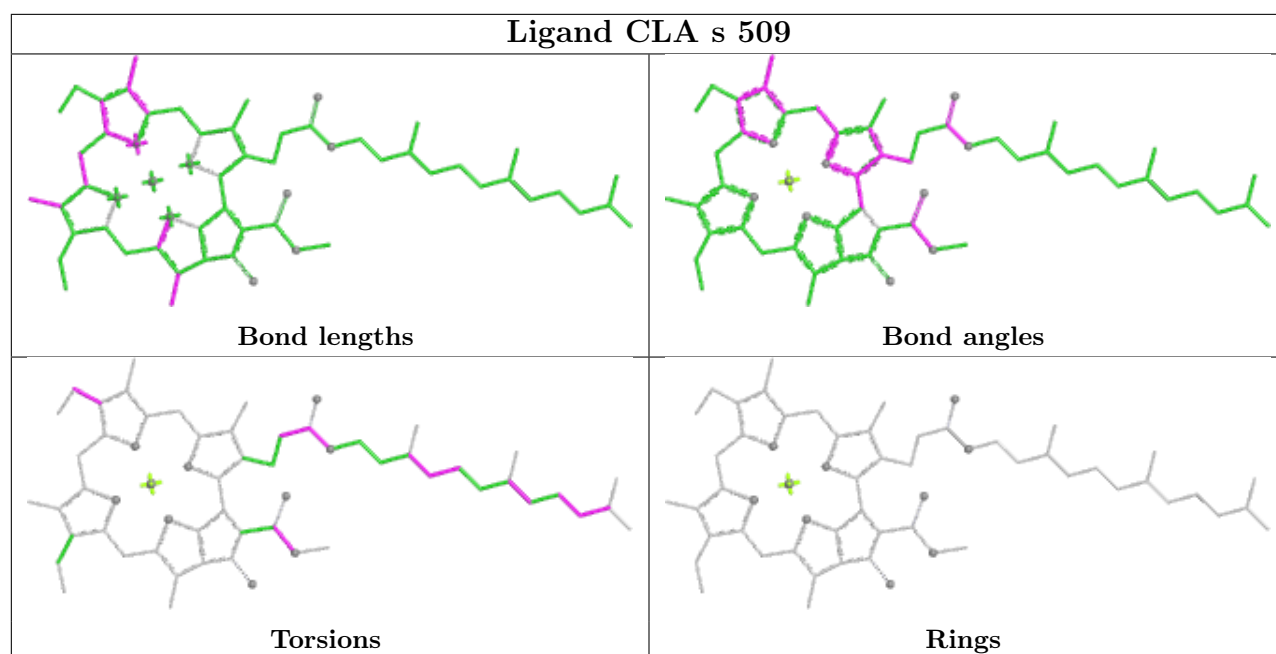


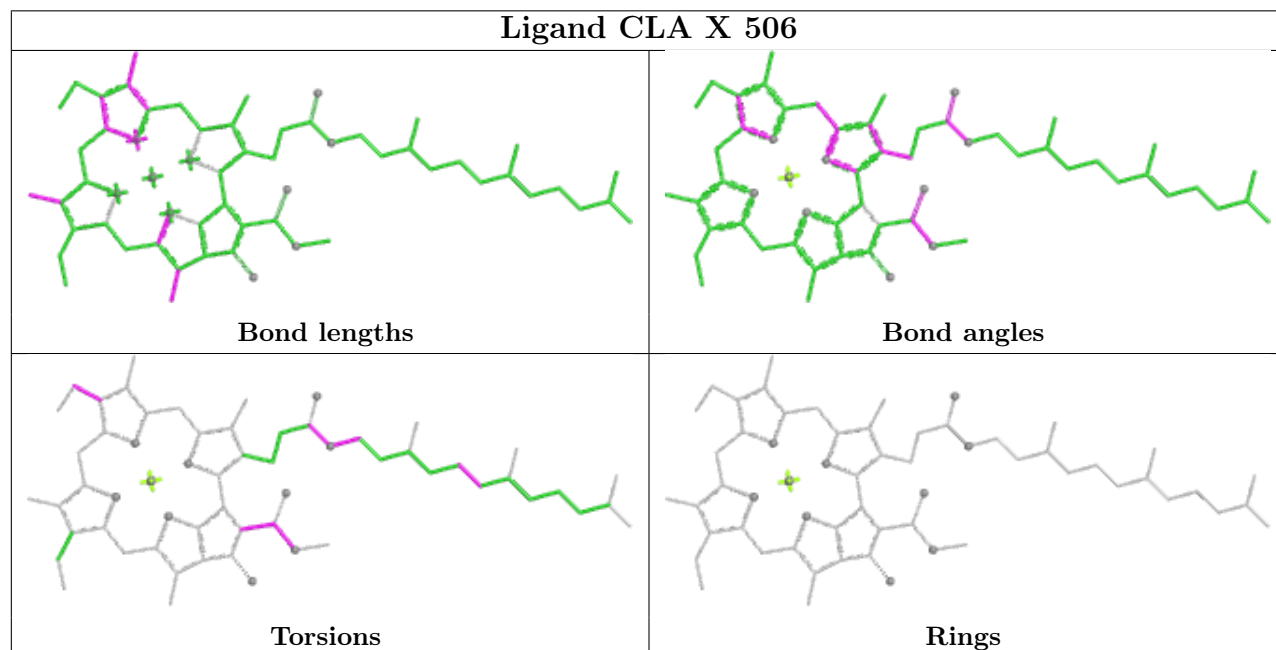
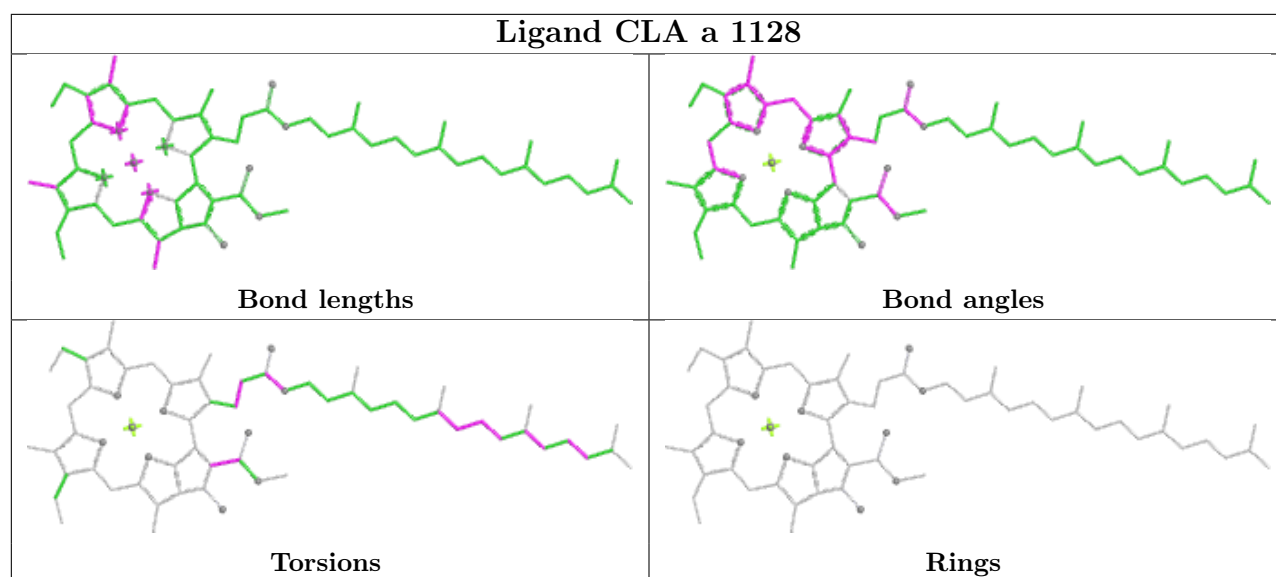


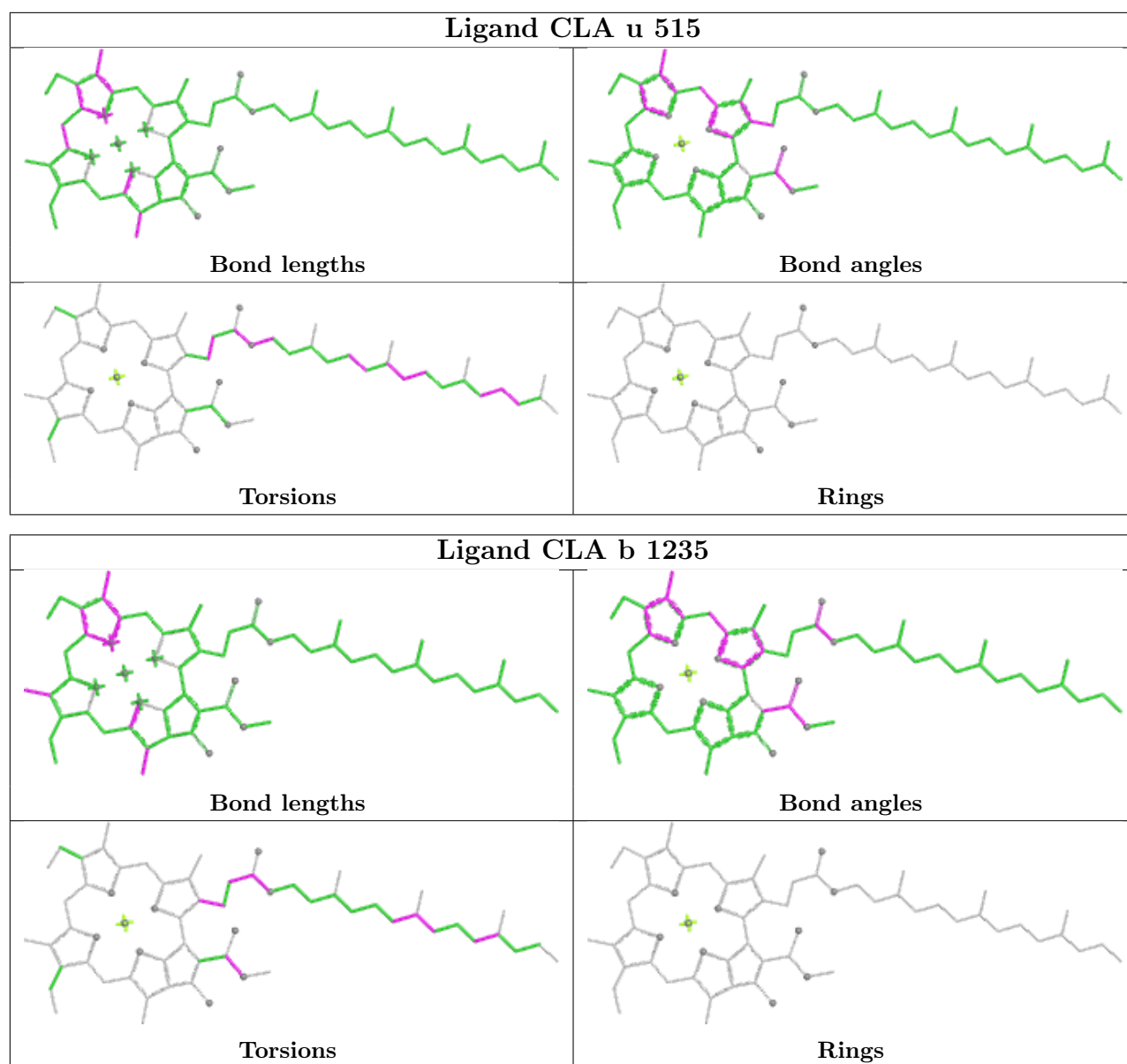




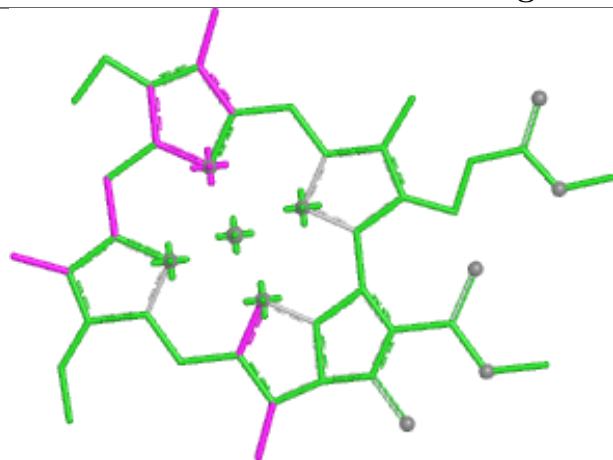
Ligand CLA B 1222**Ligand CLA b 1238**



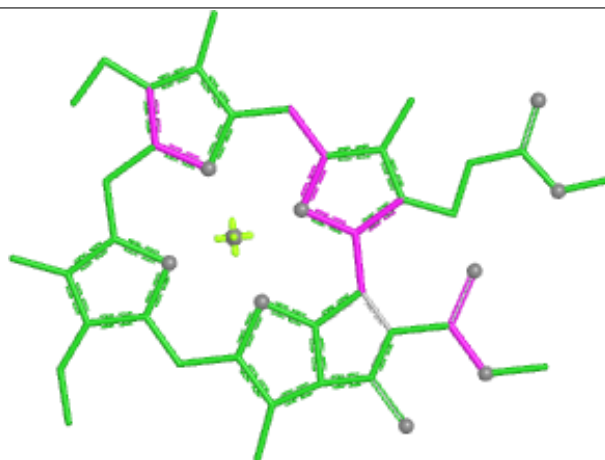




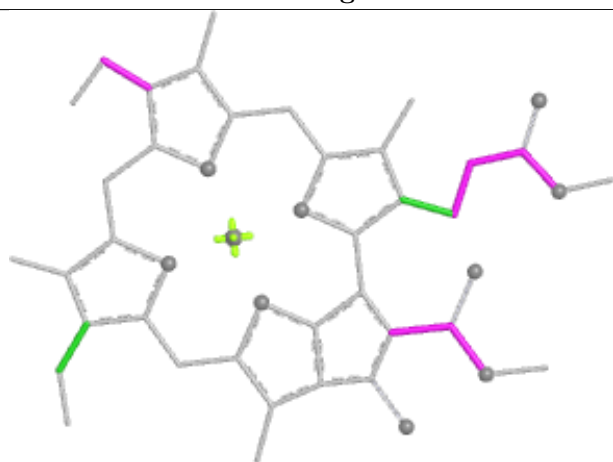
Ligand CLA n 516



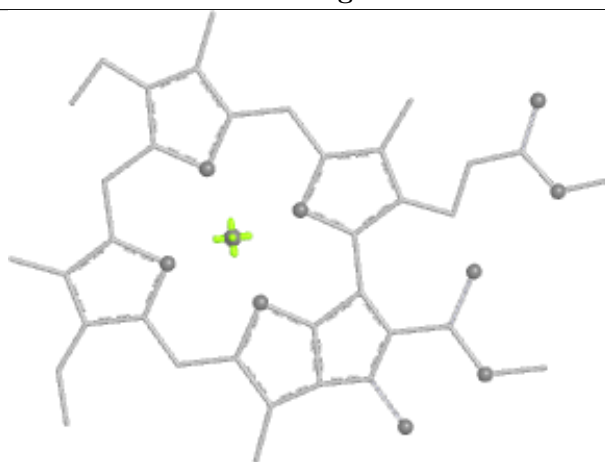
Bond lengths



Bond angles

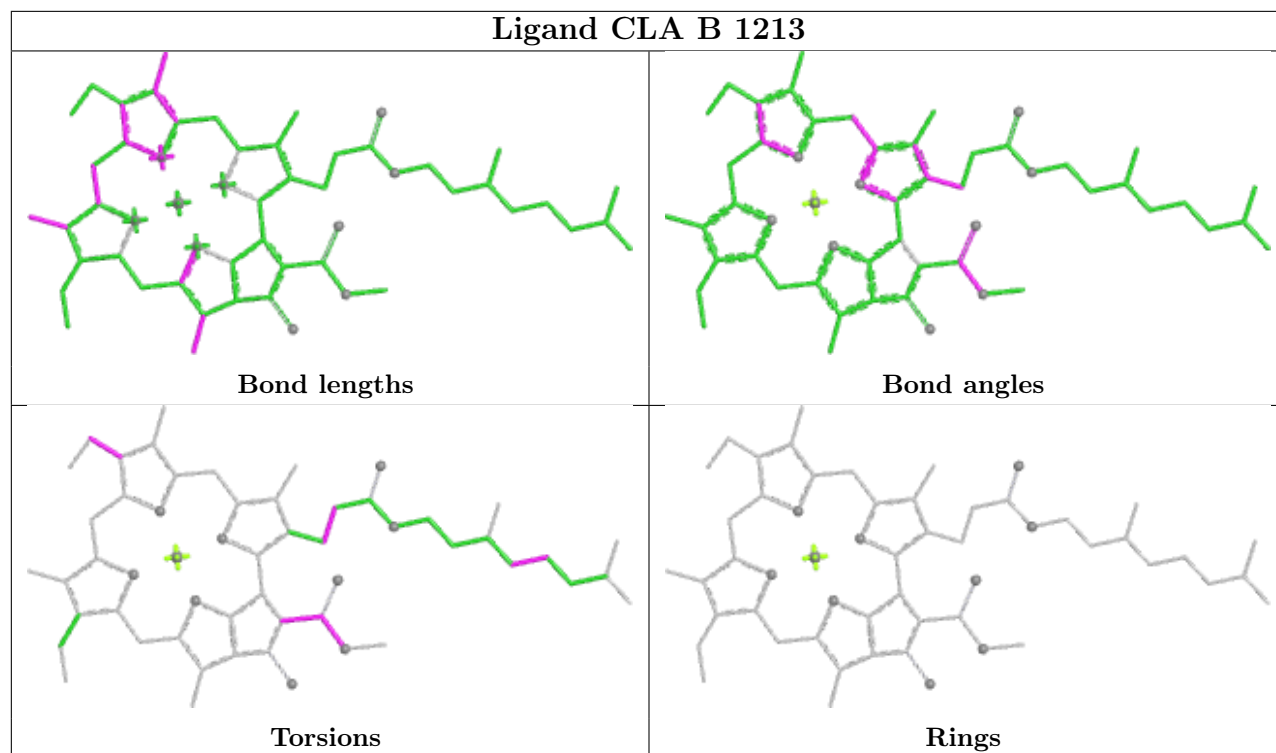


Torsions

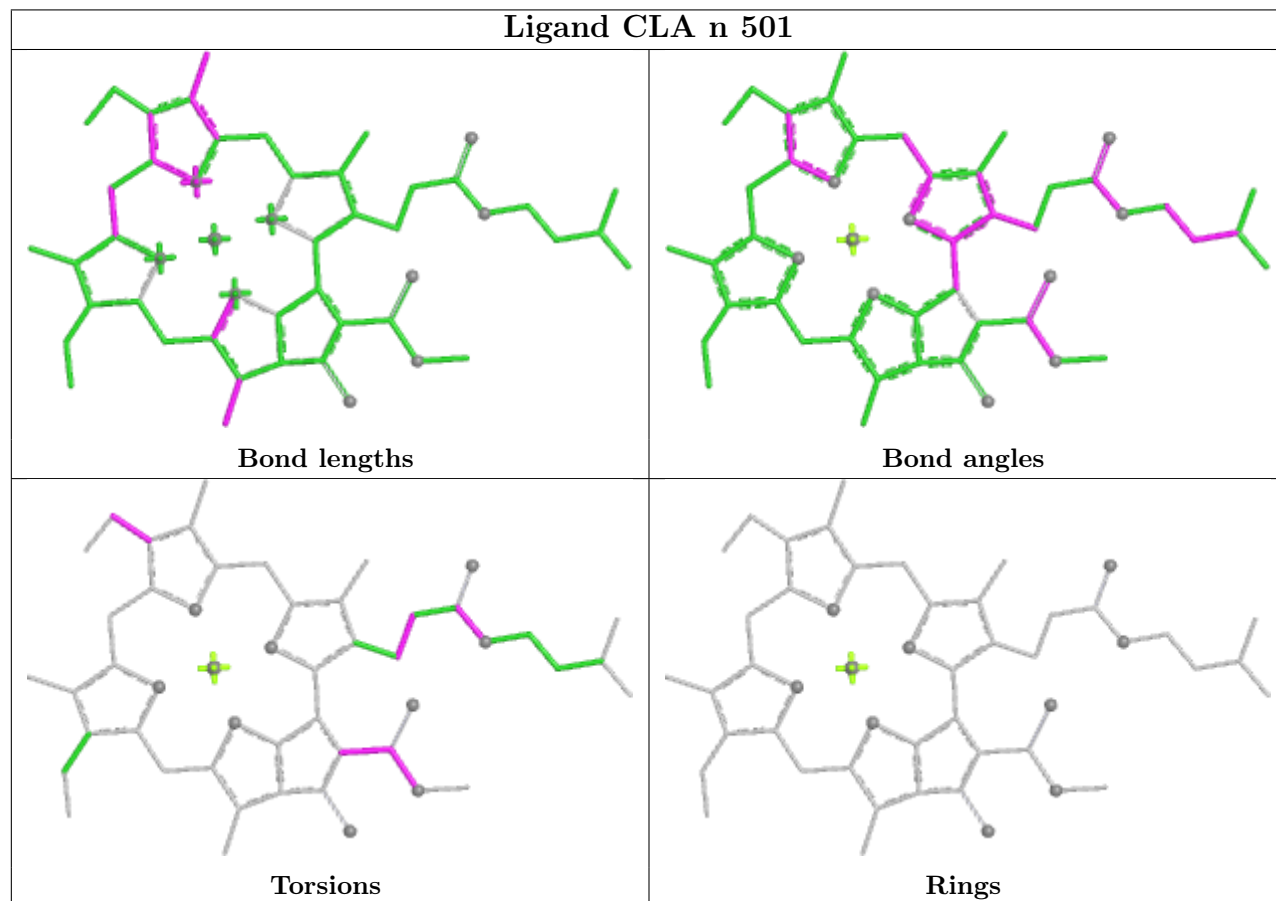


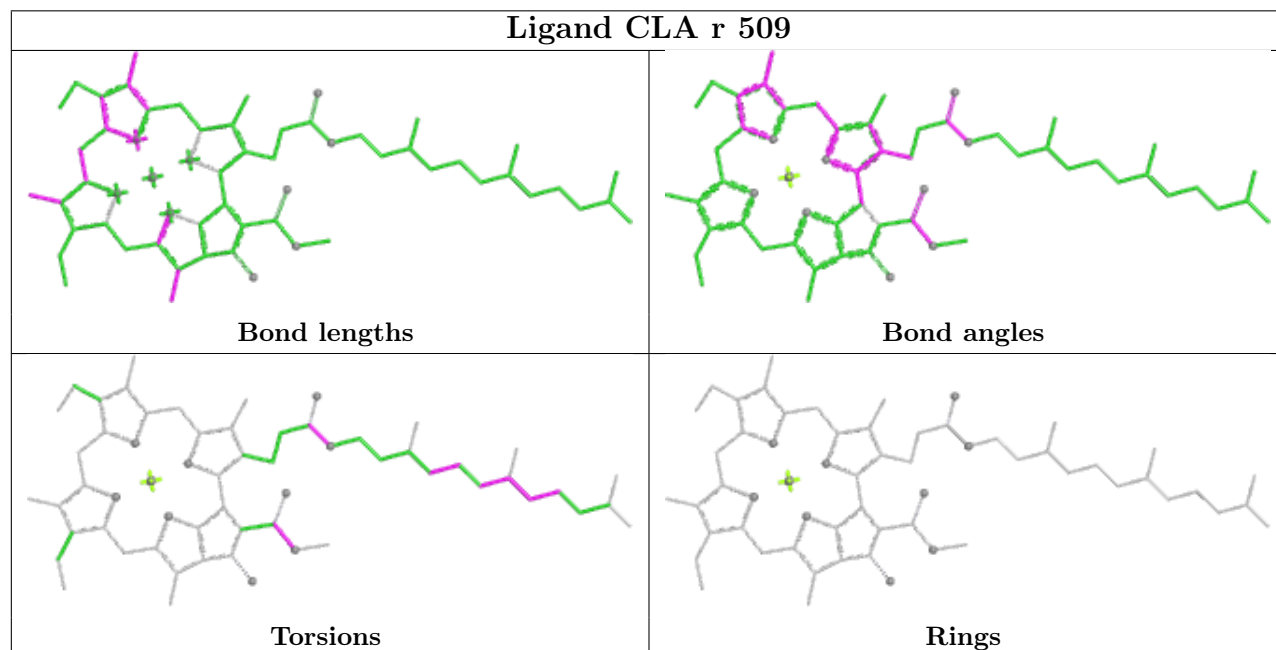
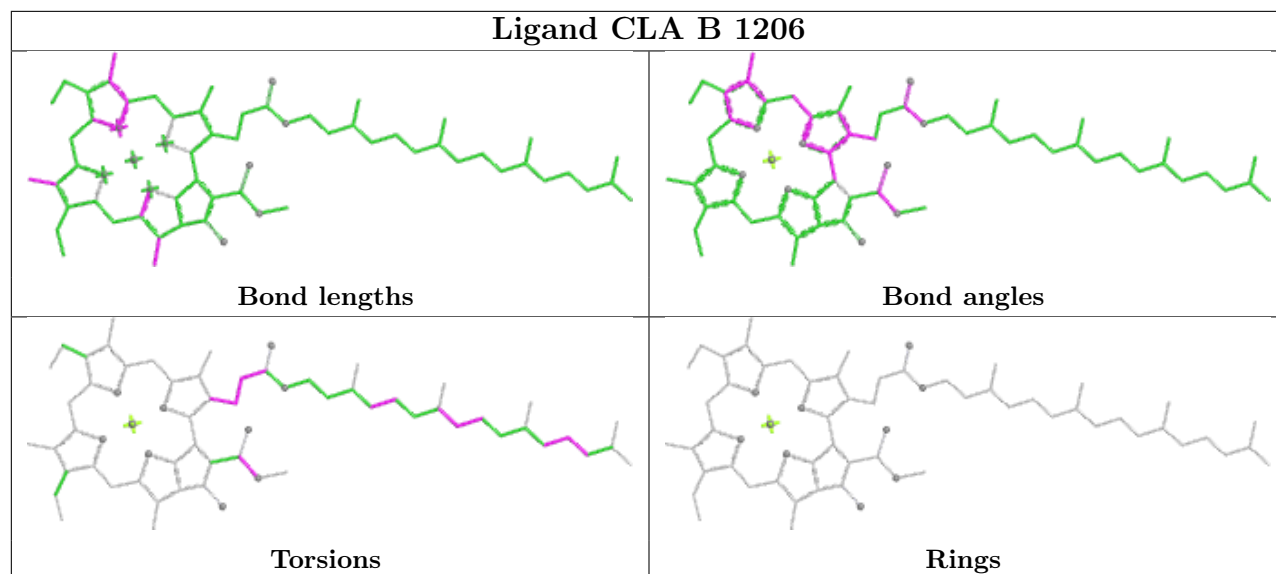
Rings

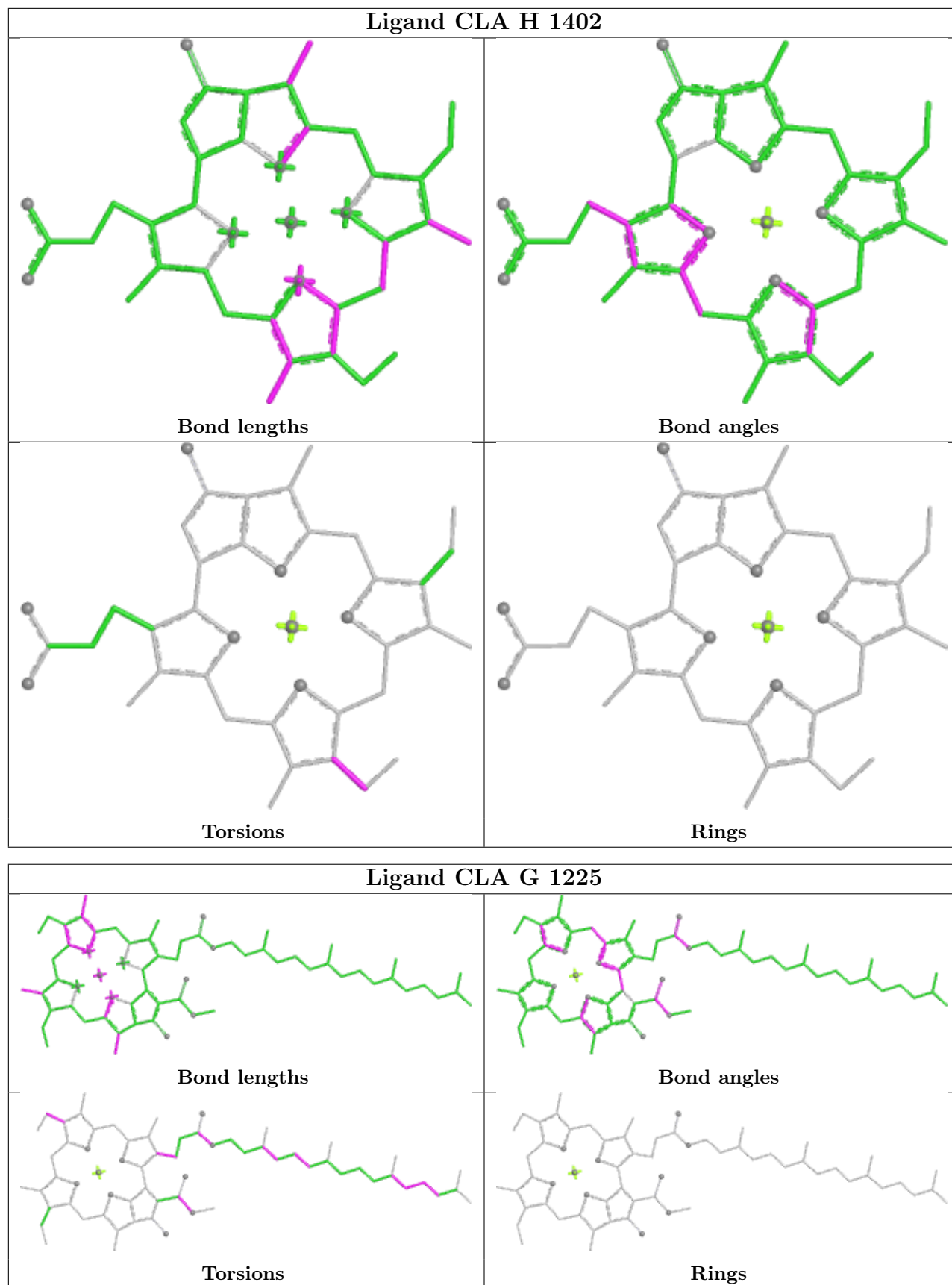
Ligand CLA B 1213



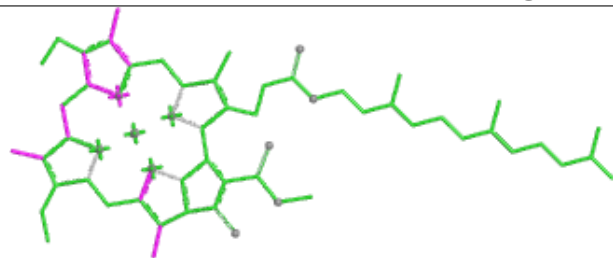
Ligand CLA n 501



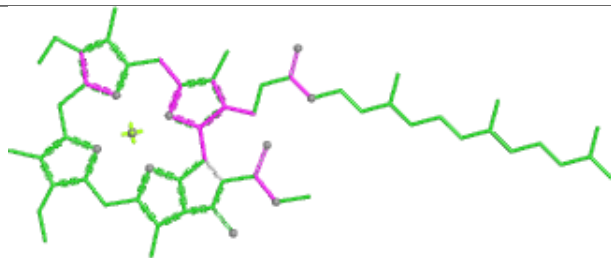




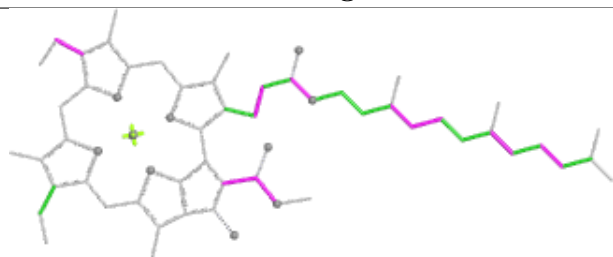
Ligand CLA r 504



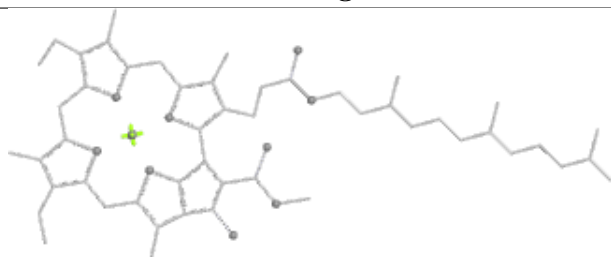
Bond lengths



Bond angles

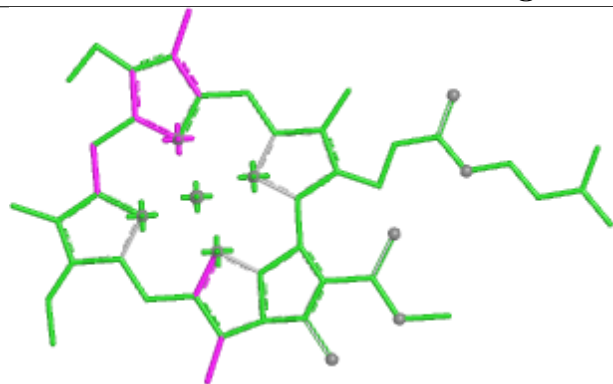


Torsions

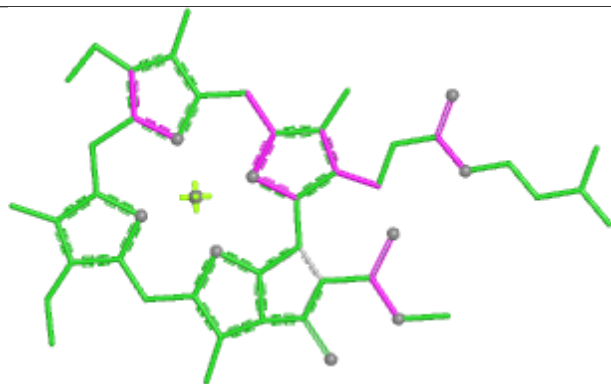


Rings

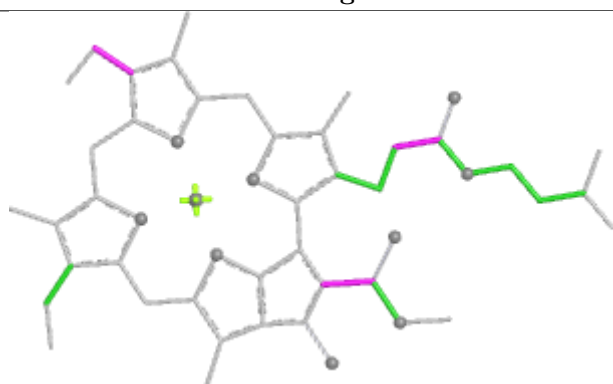
Ligand CLA h 502



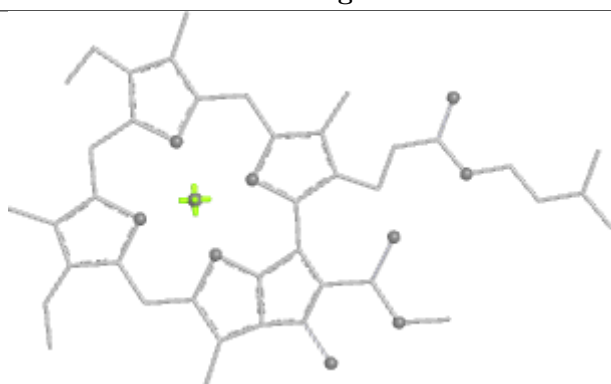
Bond lengths



Bond angles

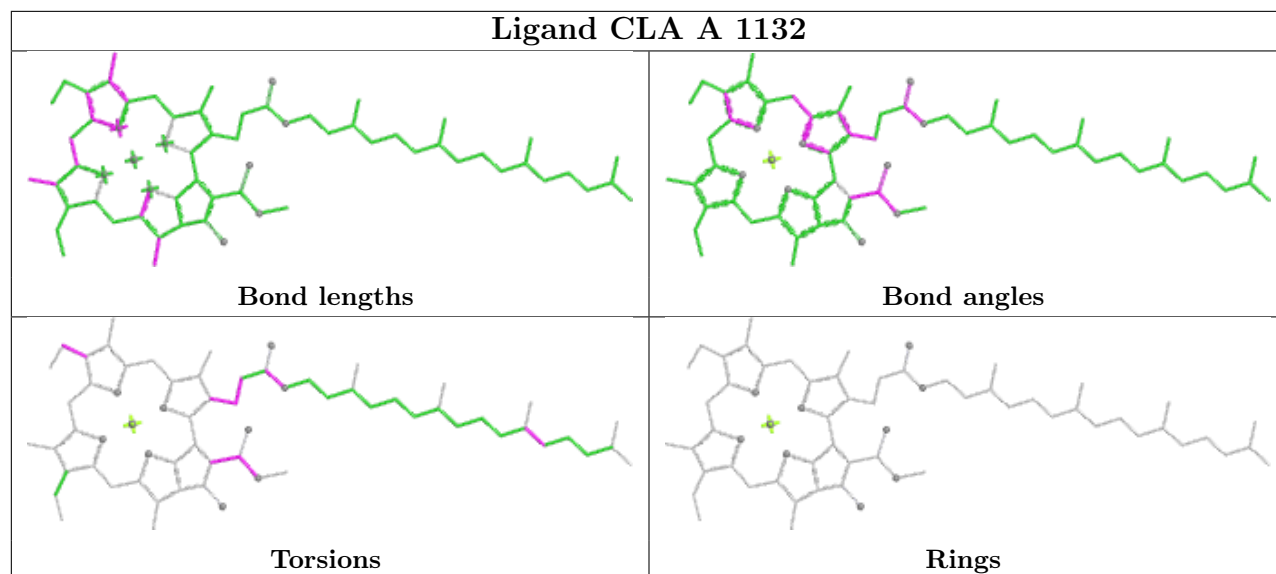


Torsions

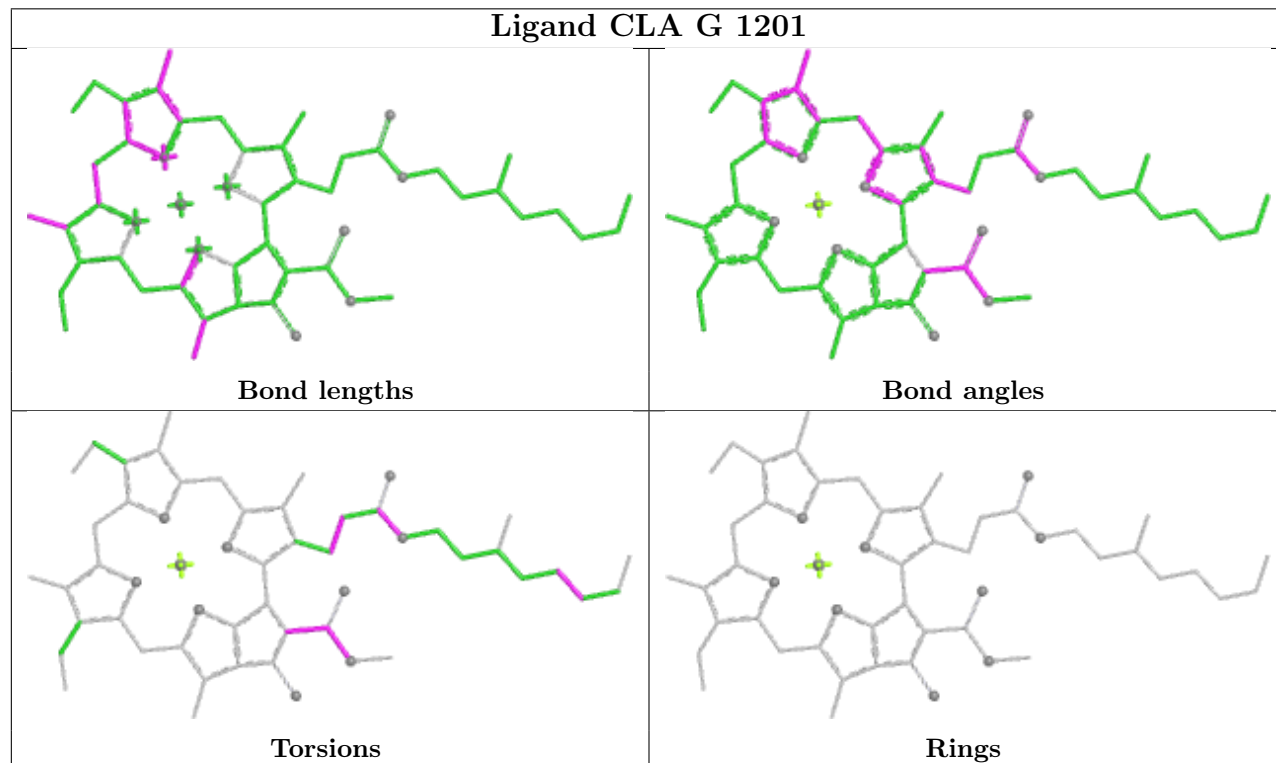


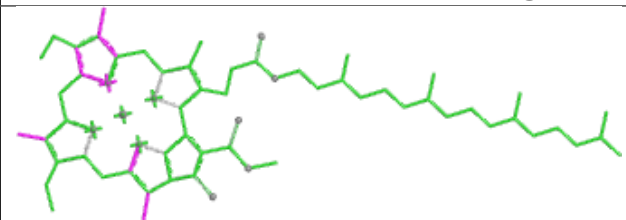
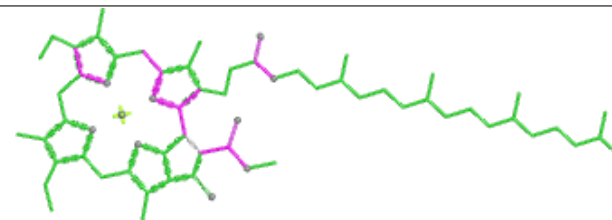
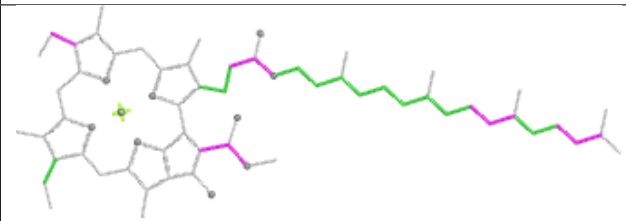
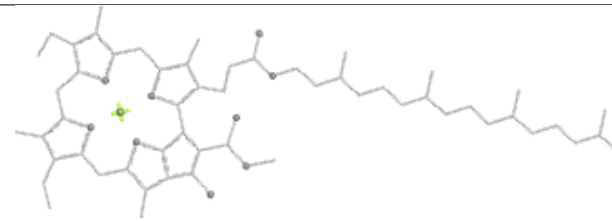
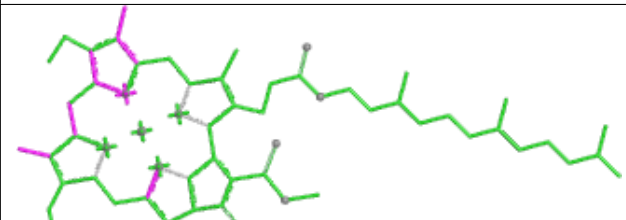
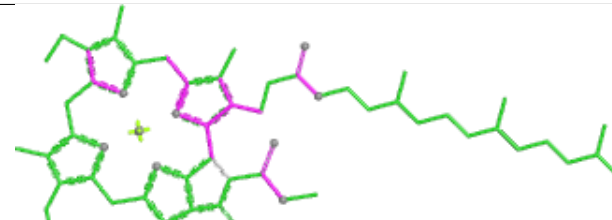
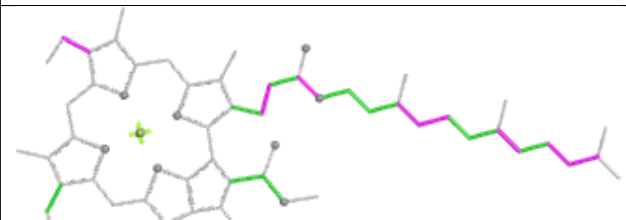
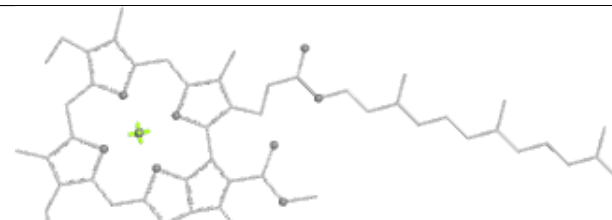
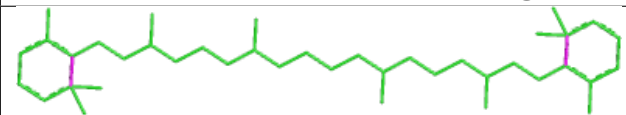
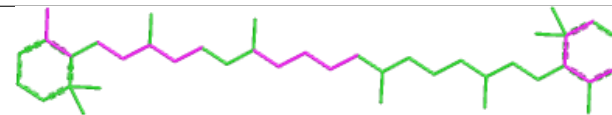
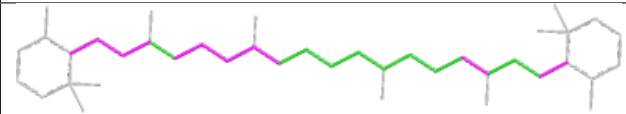
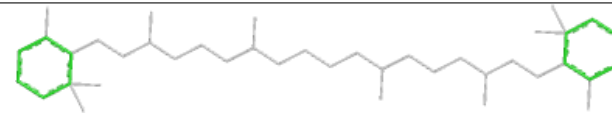
Rings

Ligand CLA A 1132

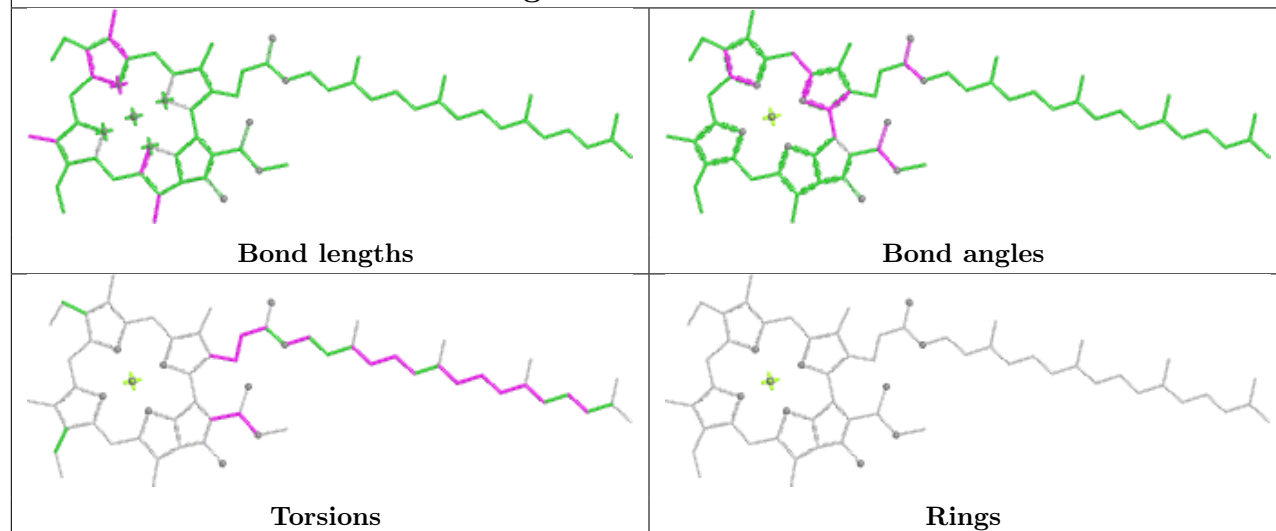


Ligand CLA G 1201

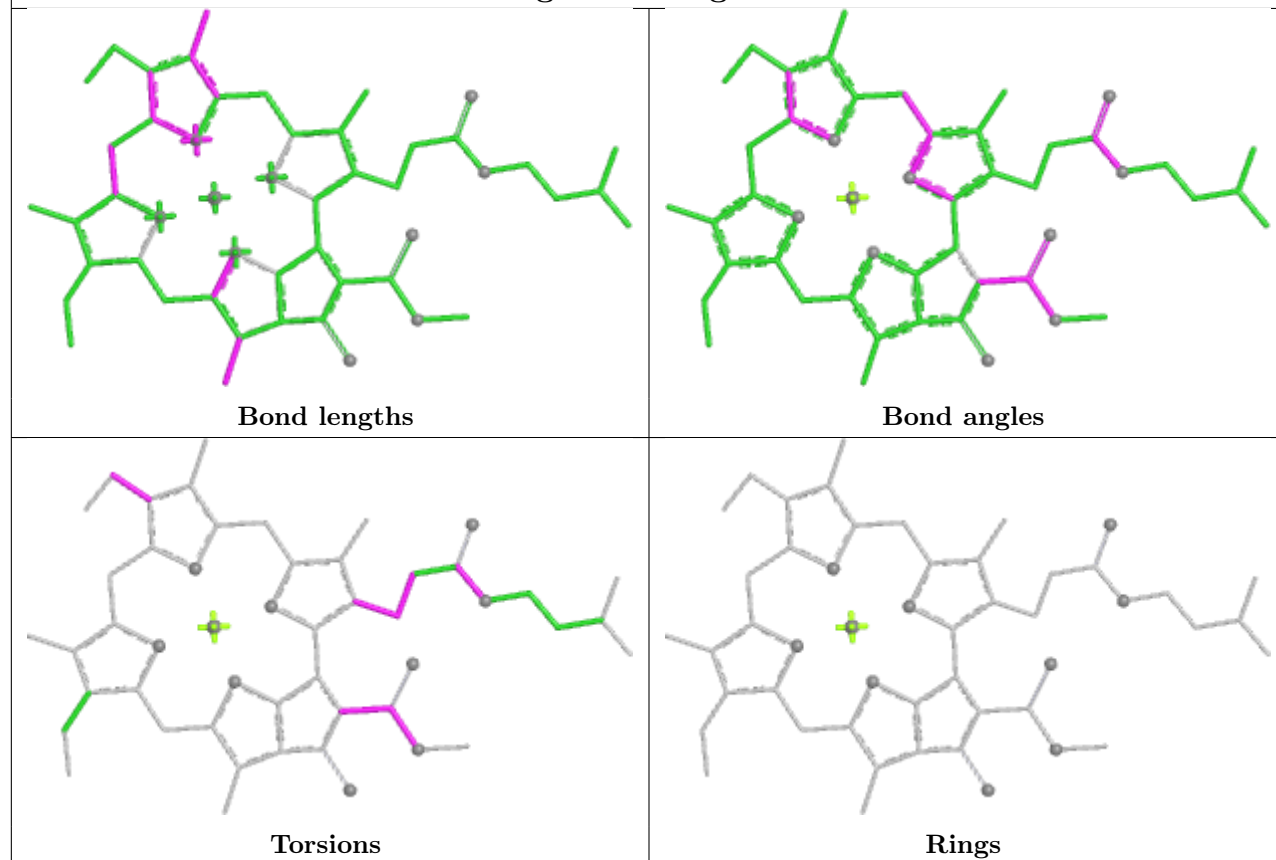


Ligand CLA X 510	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA g 504	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR f 4016	
	
Bond lengths	Bond angles
	
Torsions	Rings

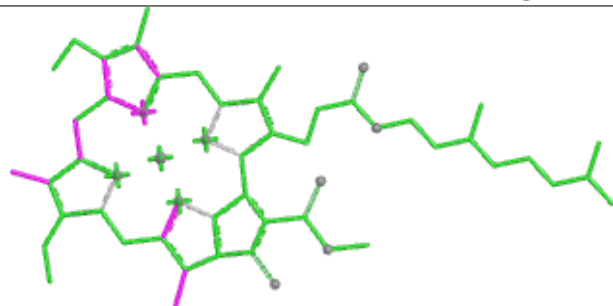
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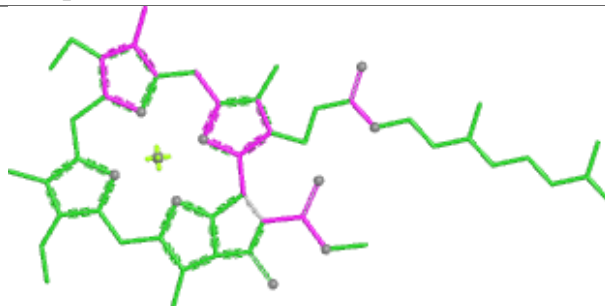
Ligand CLA g 514



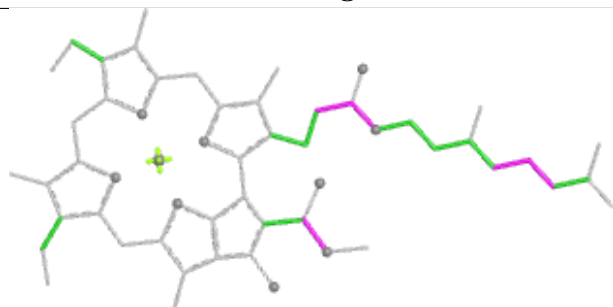
Ligand CLA q 517



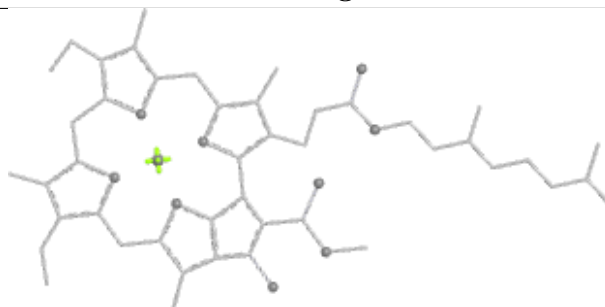
Bond lengths



Bond angles

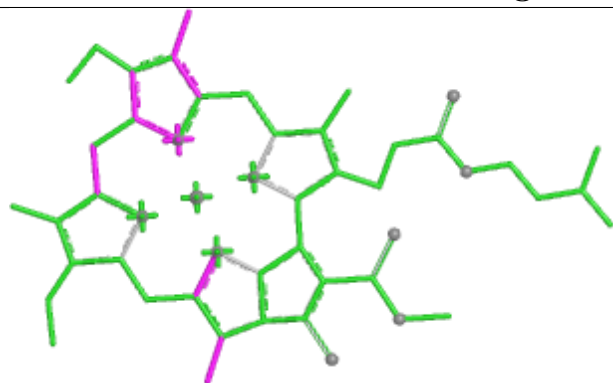


Torsions

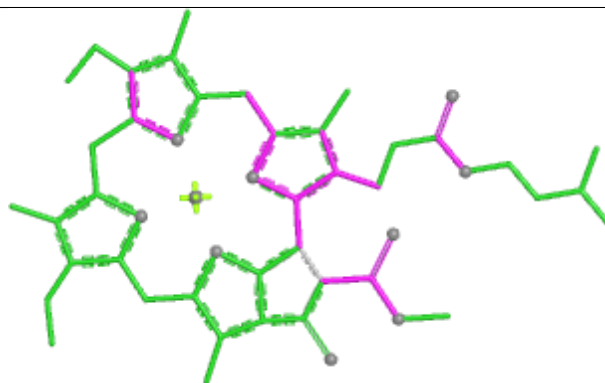


Rings

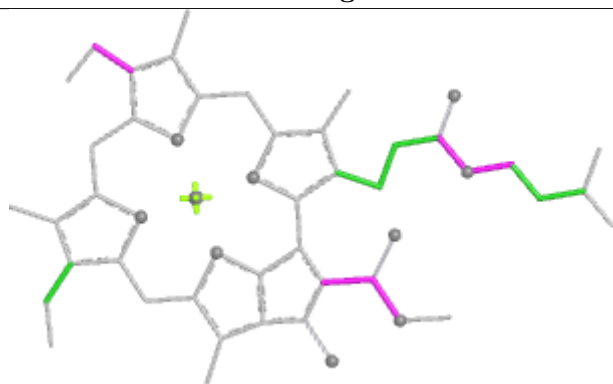
Ligand CLA X 501



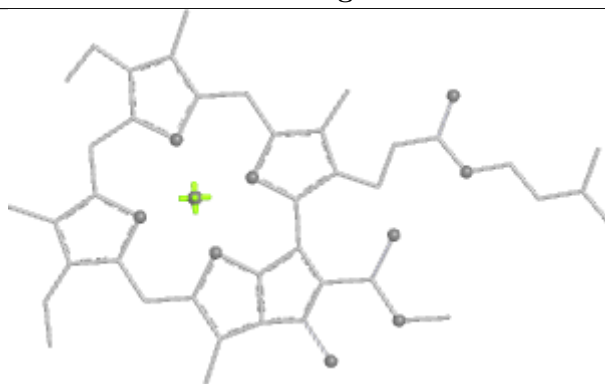
Bond lengths



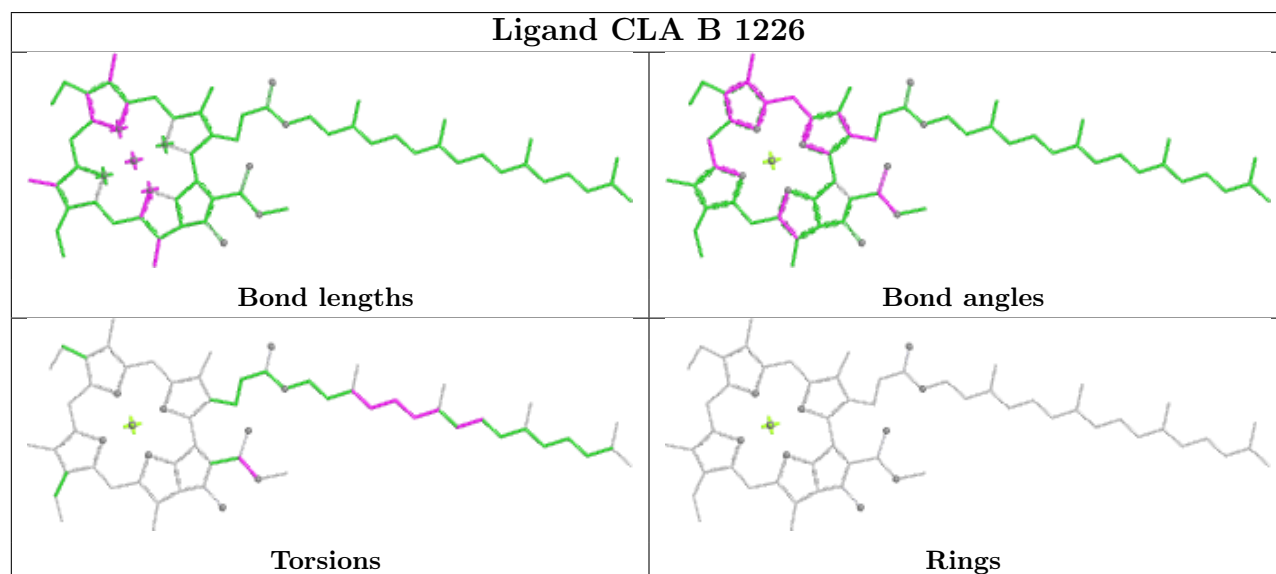
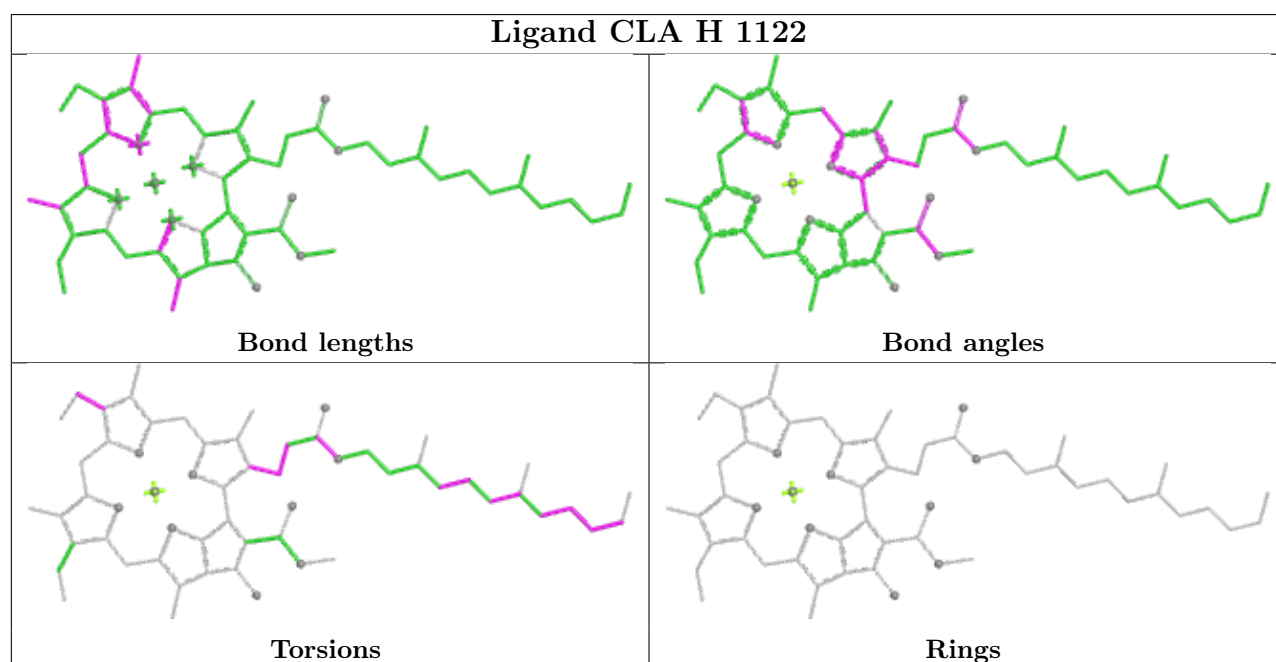
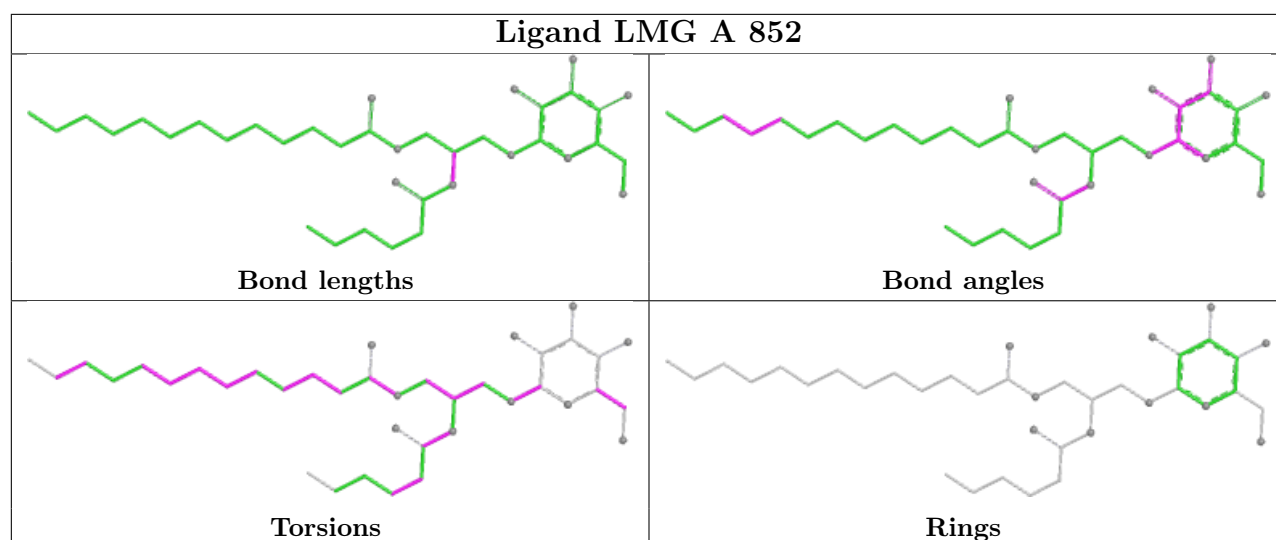
Bond angles



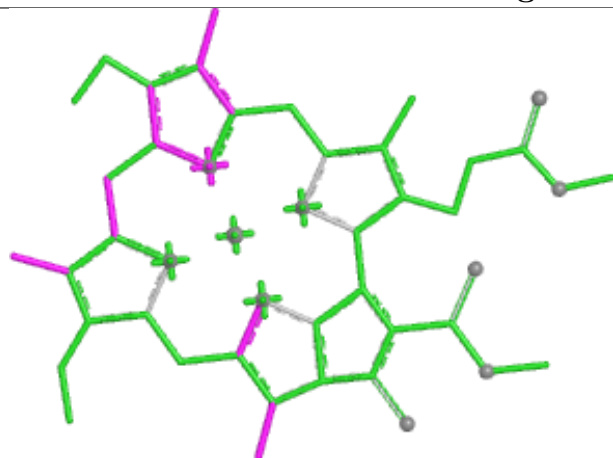
Torsions



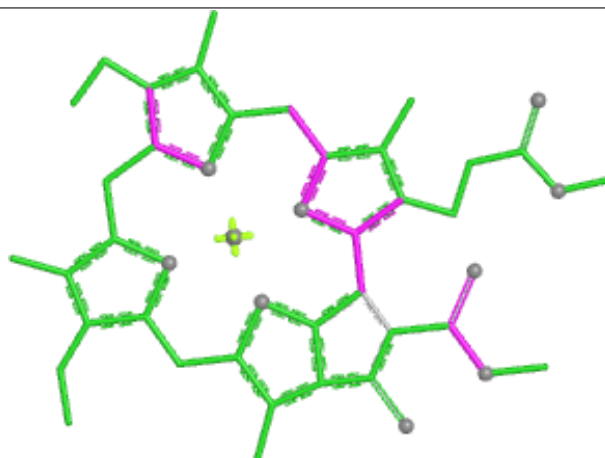
Rings



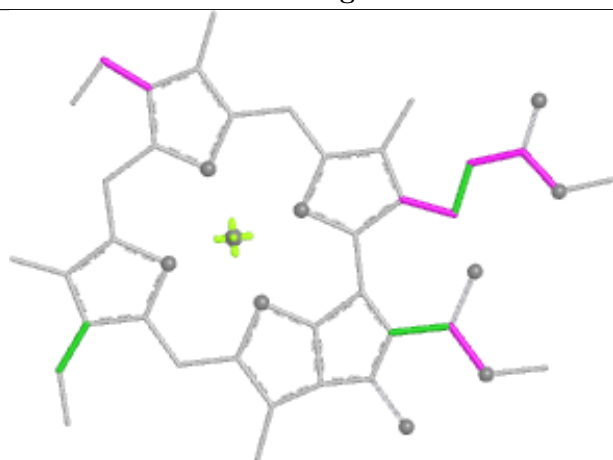
Ligand CLA u 516



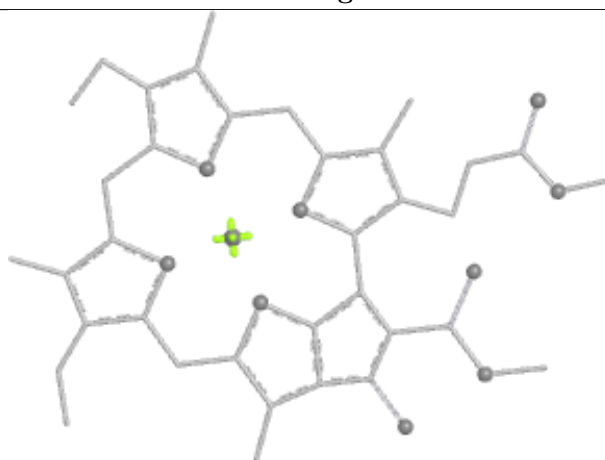
Bond lengths



Bond angles

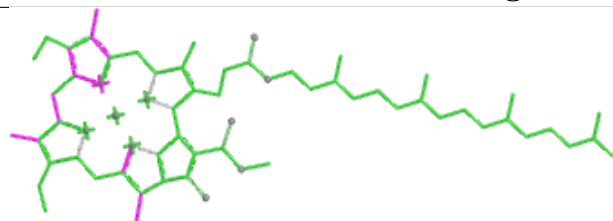


Torsions

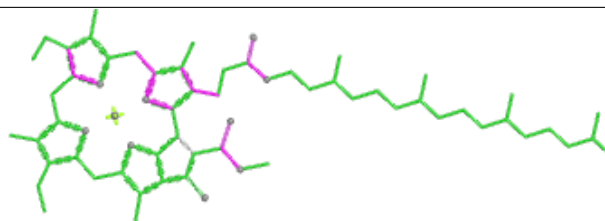


Rings

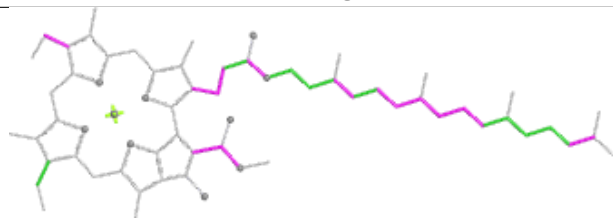
Ligand CLA H 1140



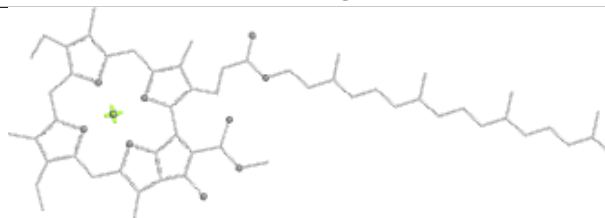
Bond lengths



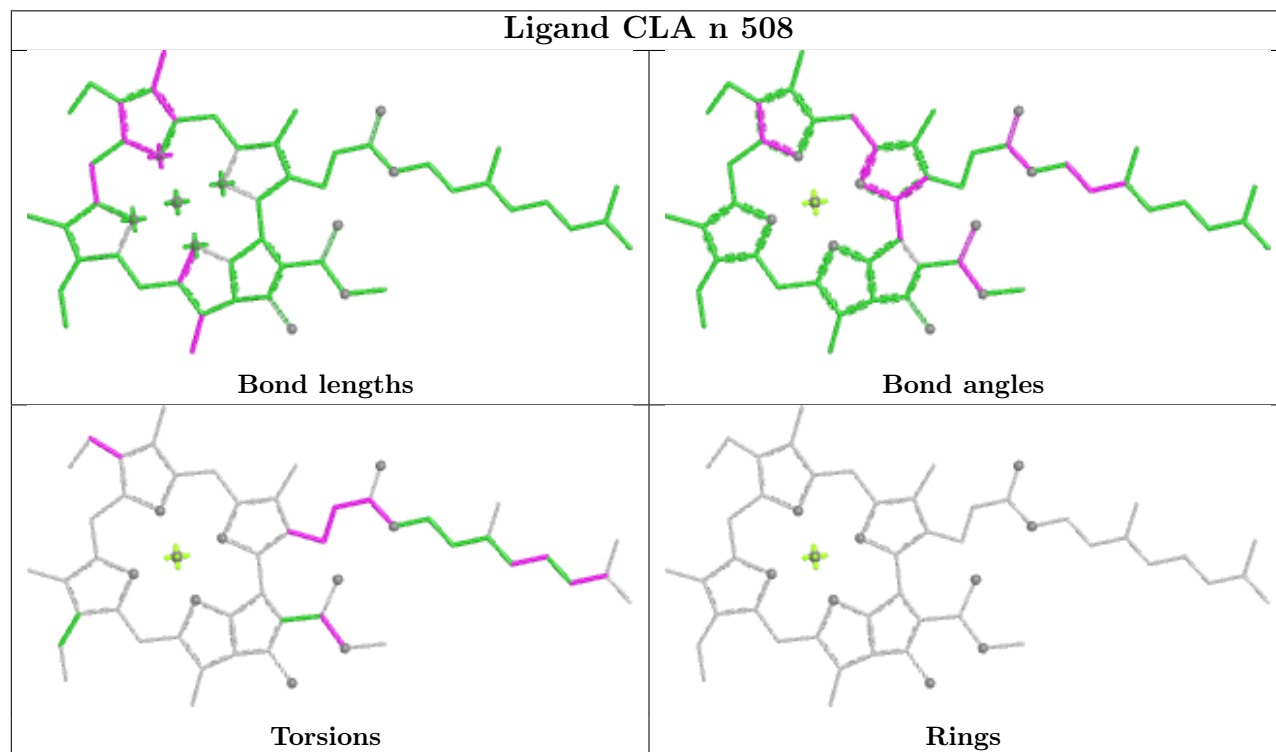
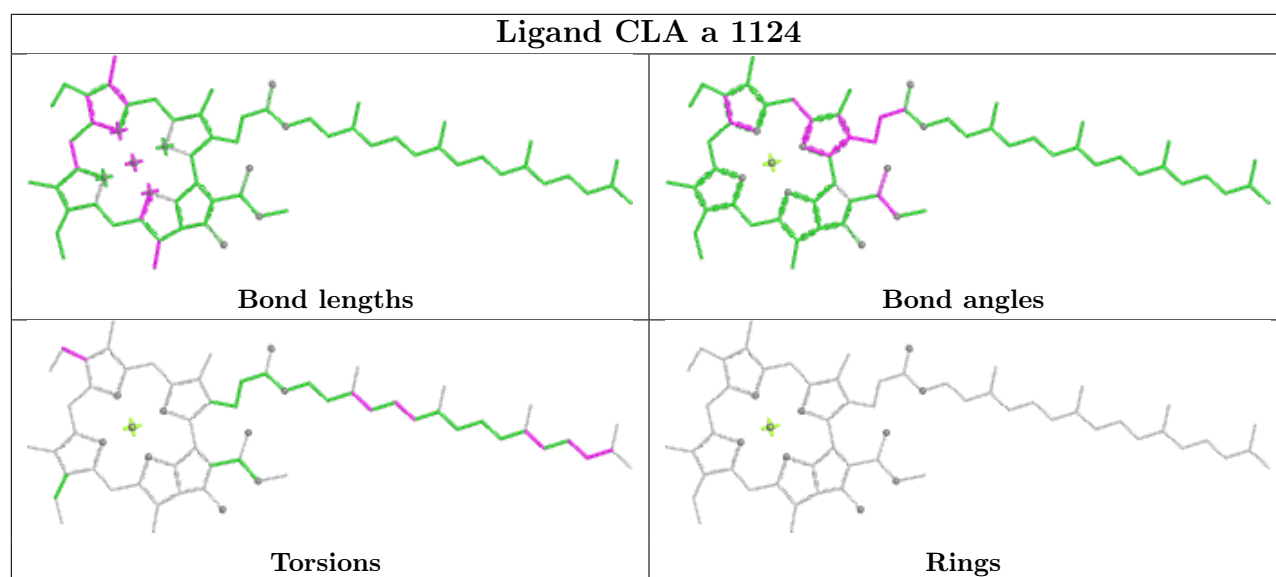
Bond angles

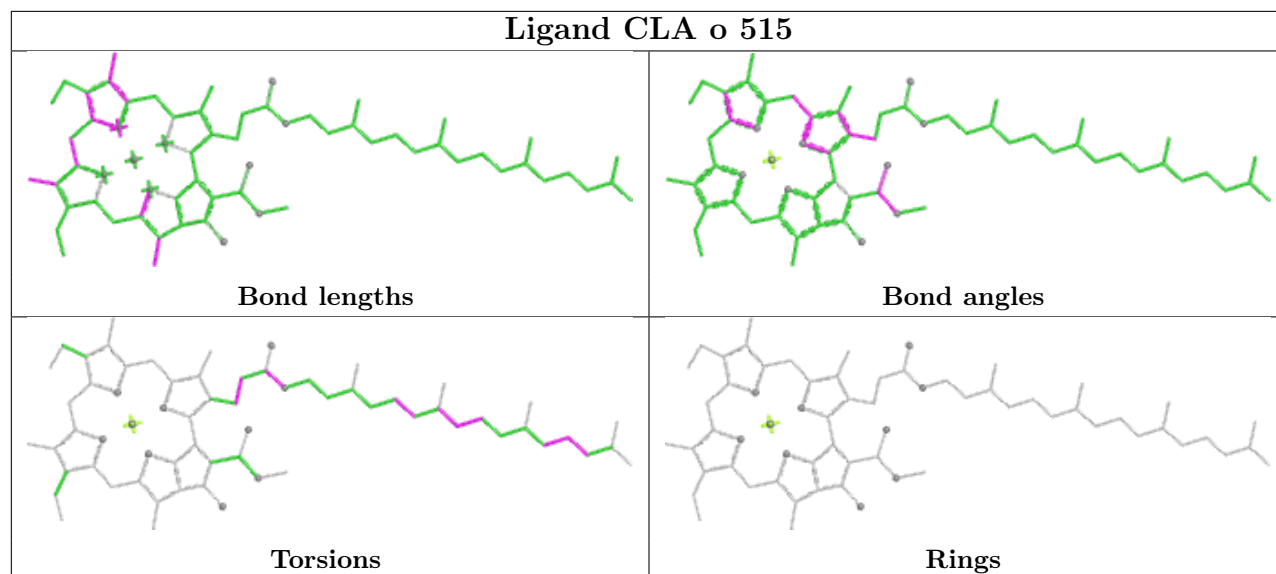
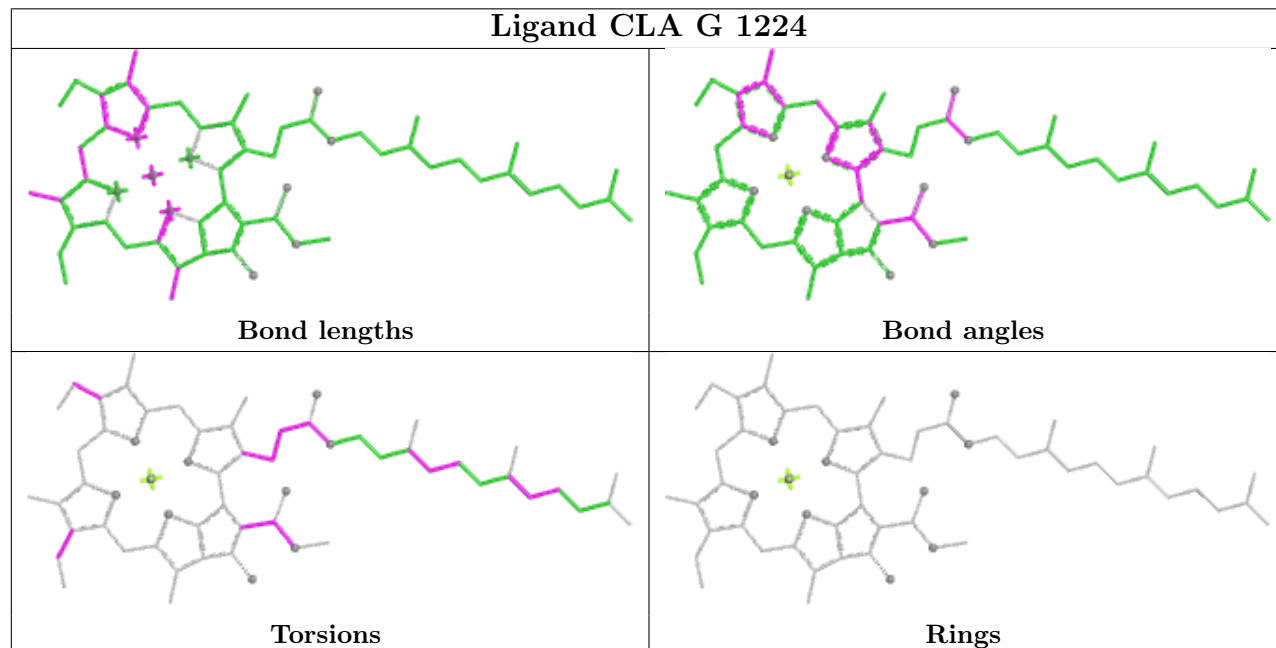


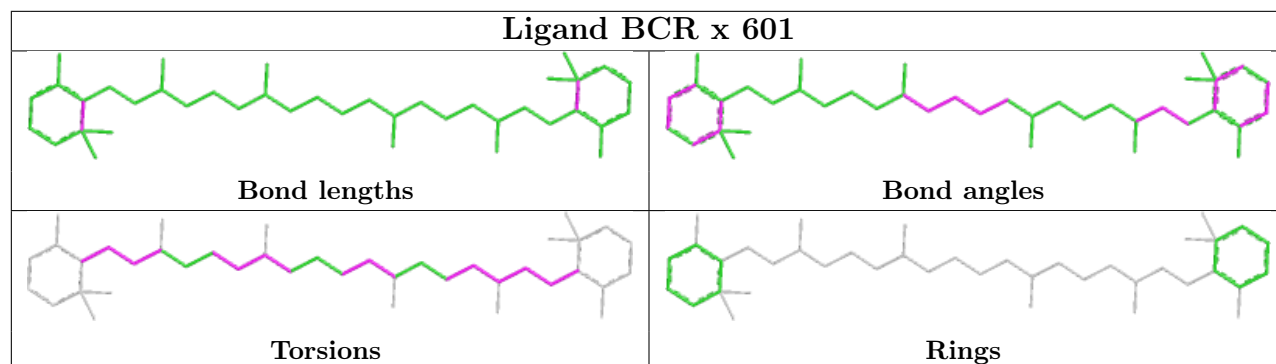
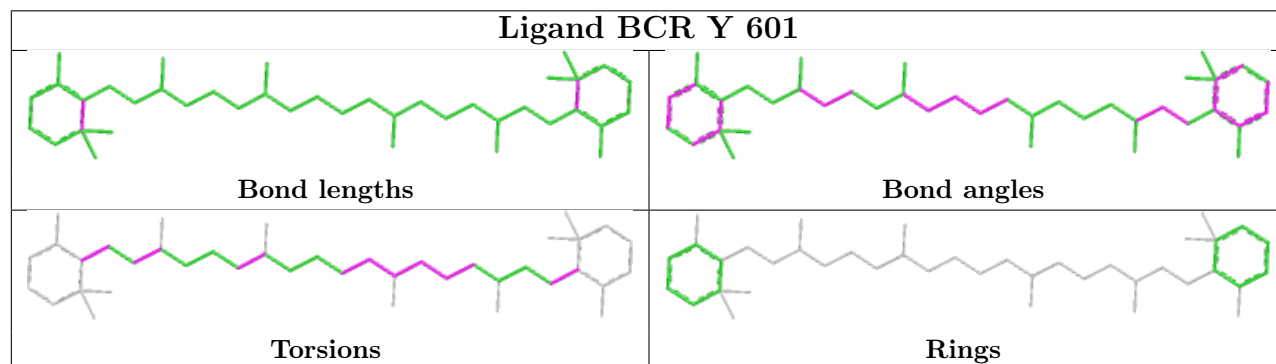
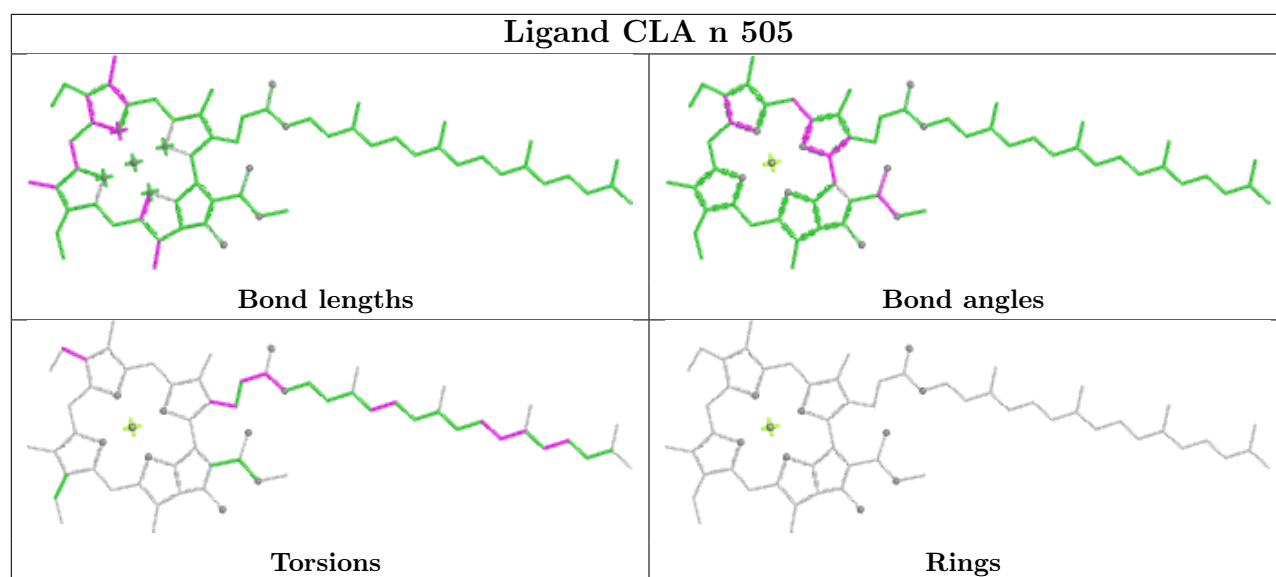
Torsions

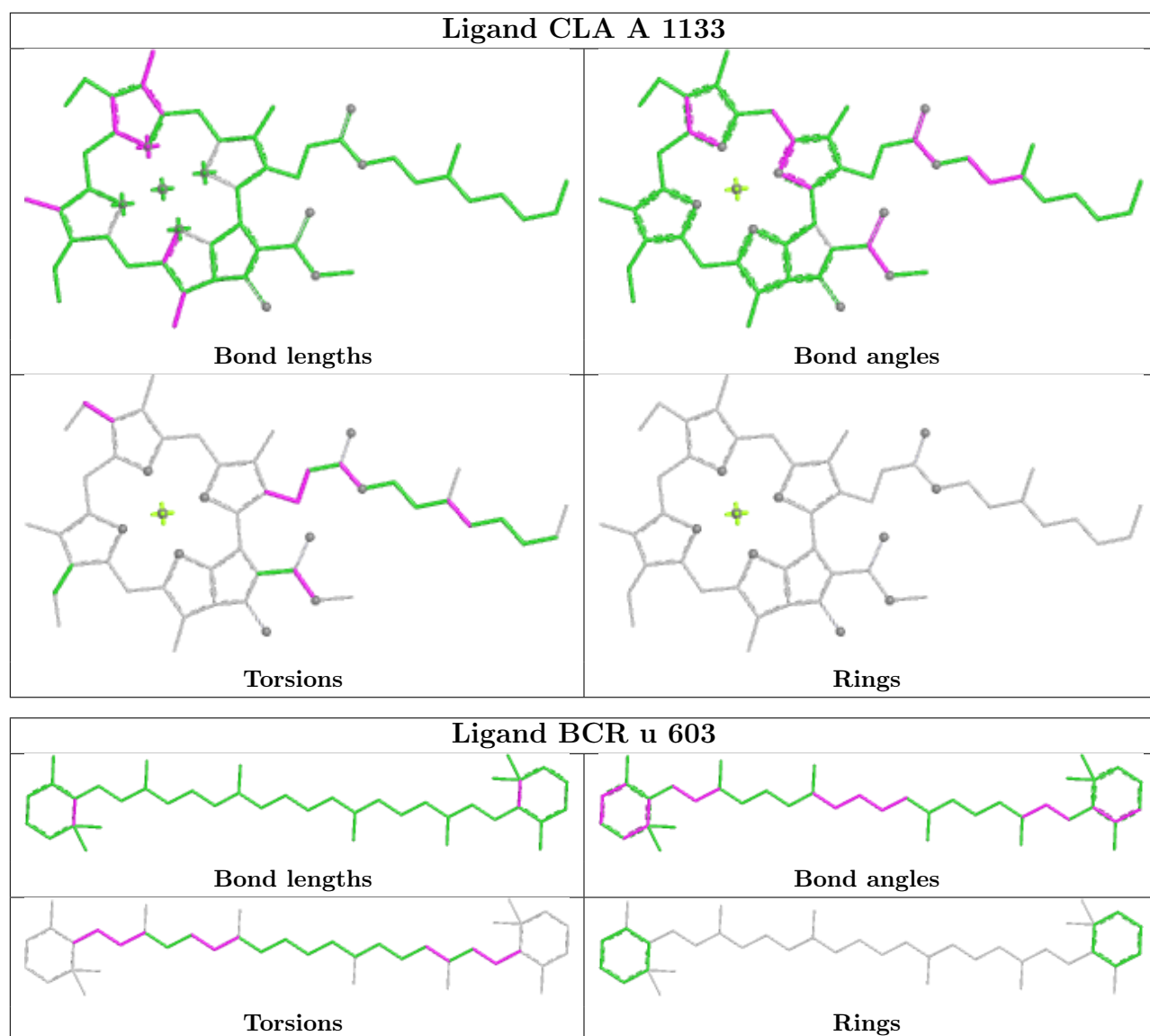


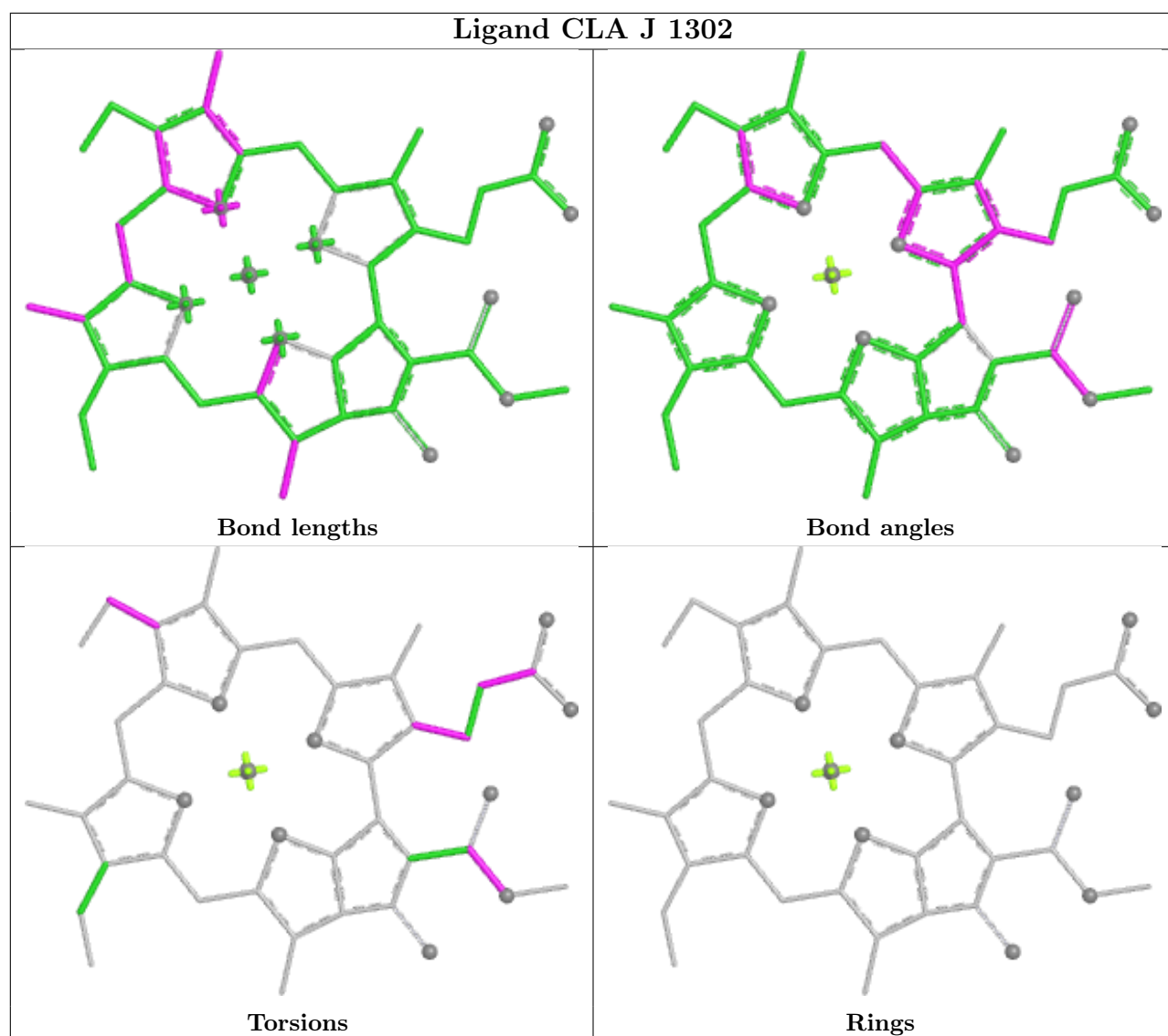
Rings

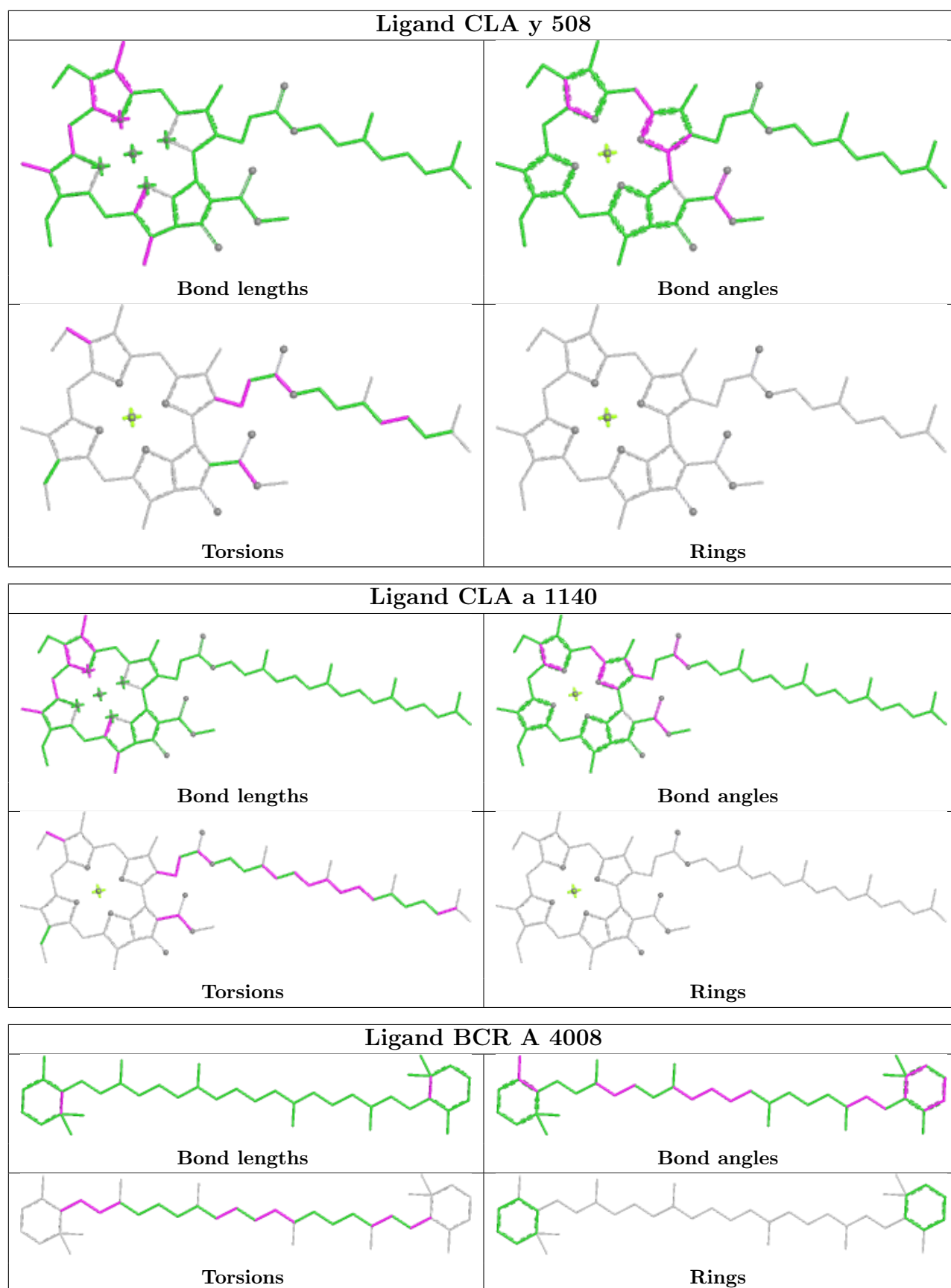


Ligand CLA o 515**Ligand CLA G 1224**

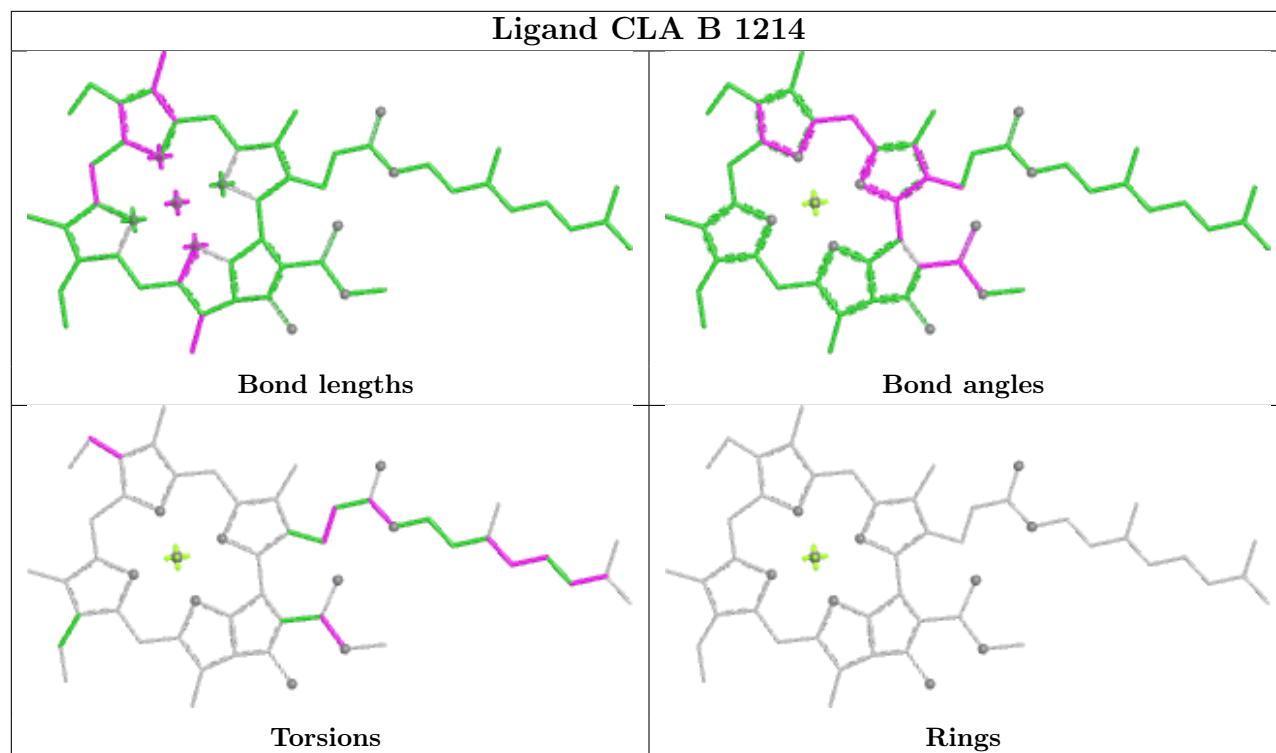




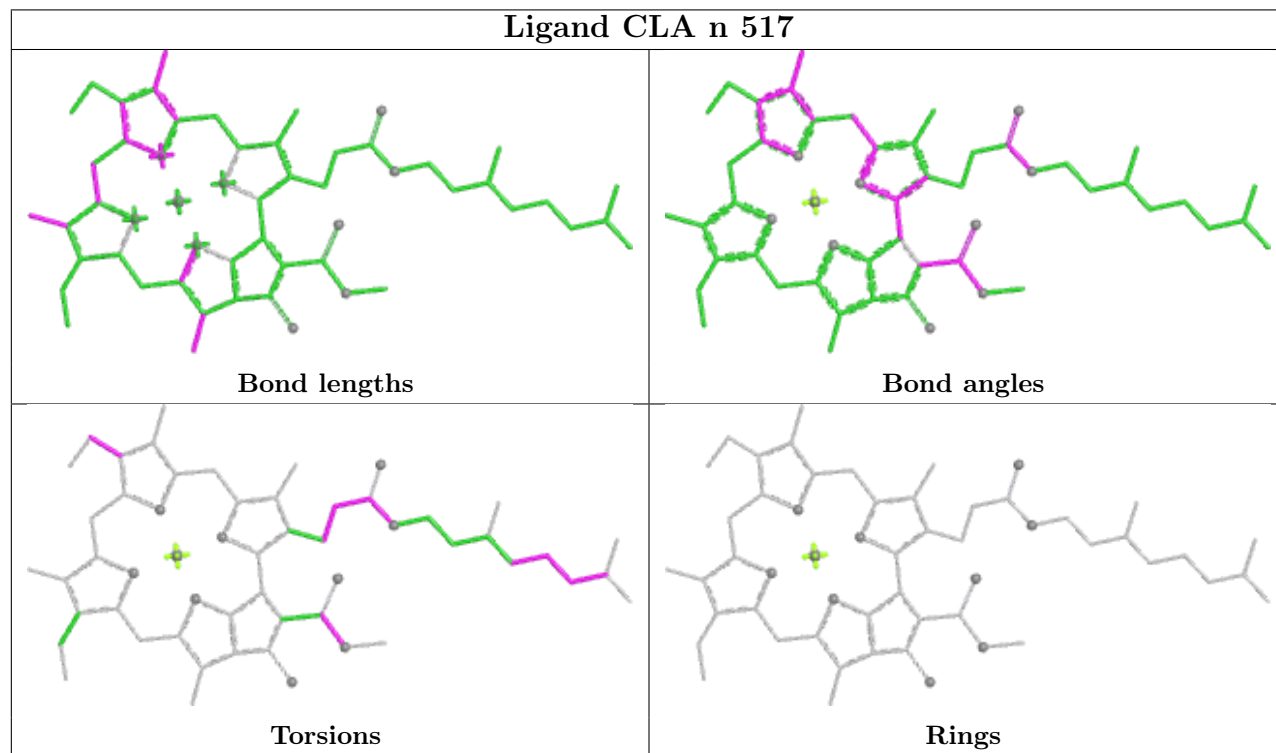


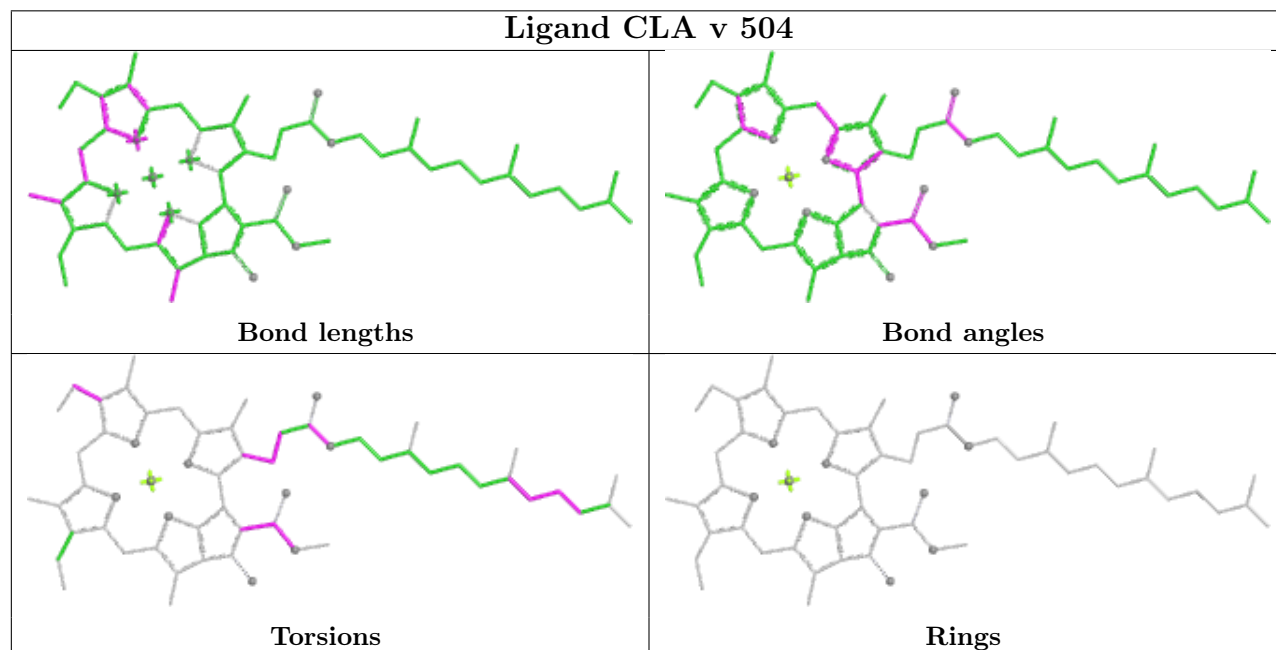
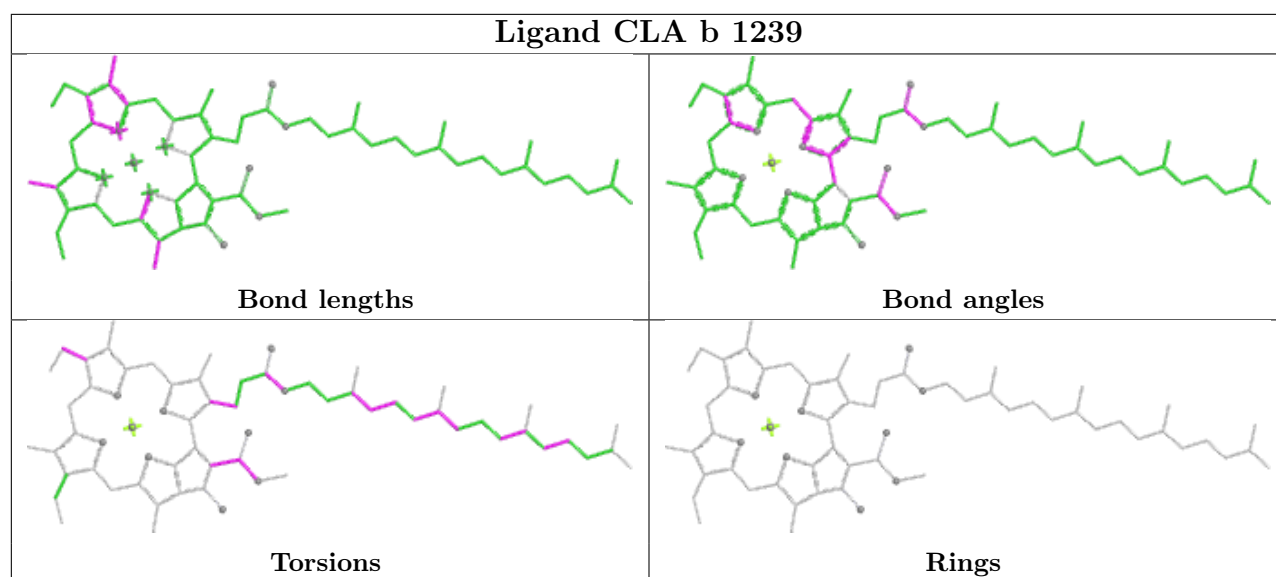


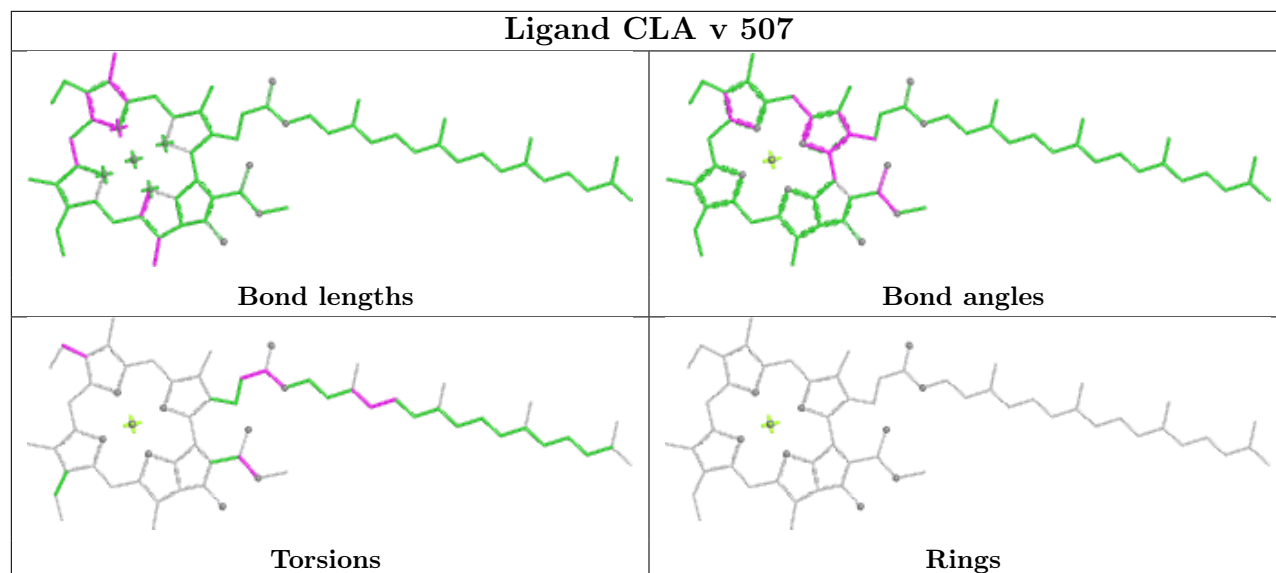
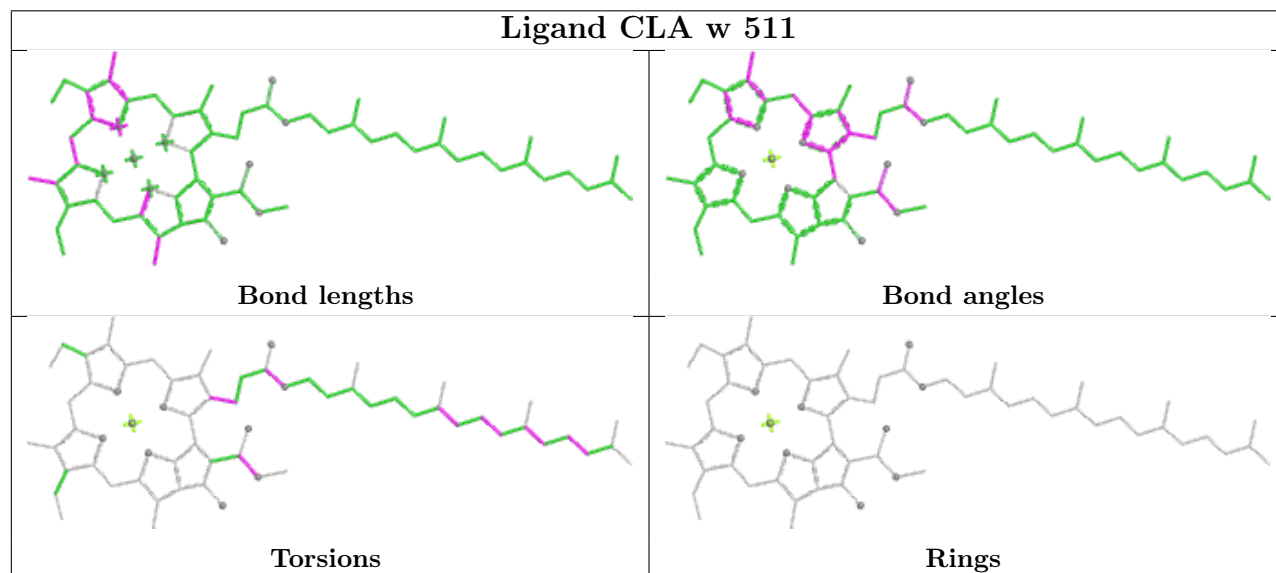
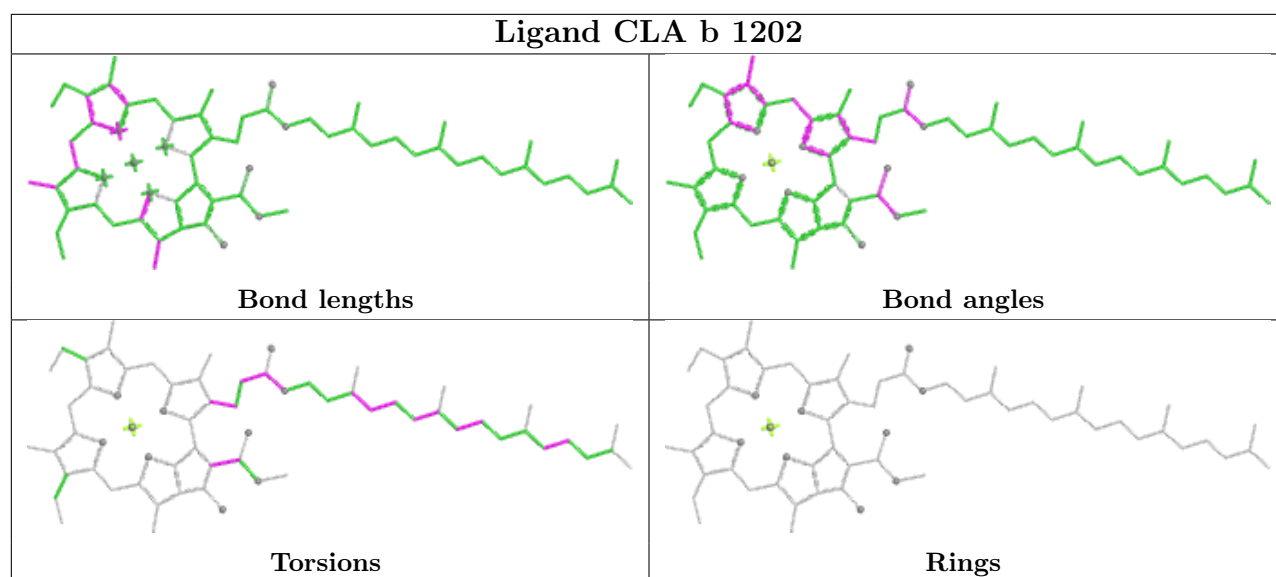
Ligand CLA B 1214

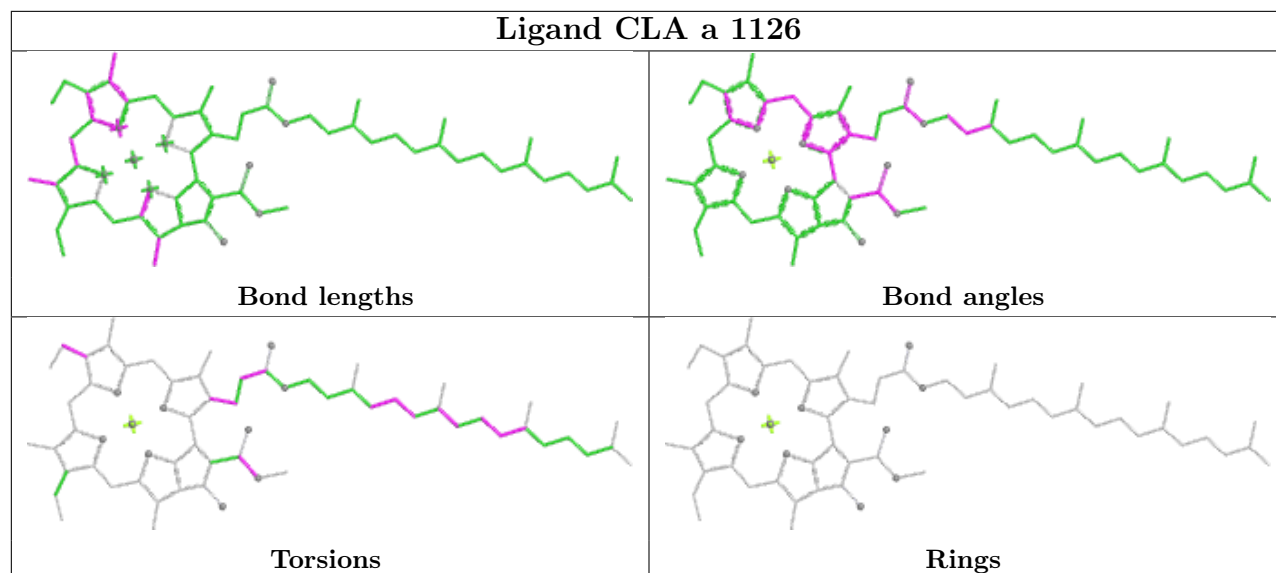
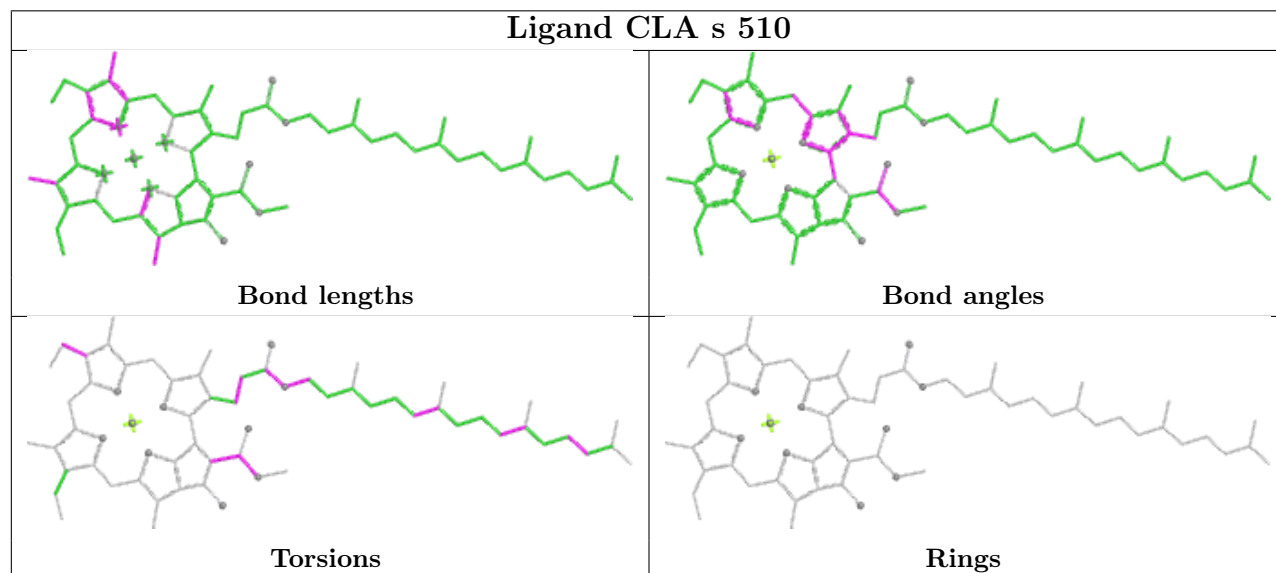
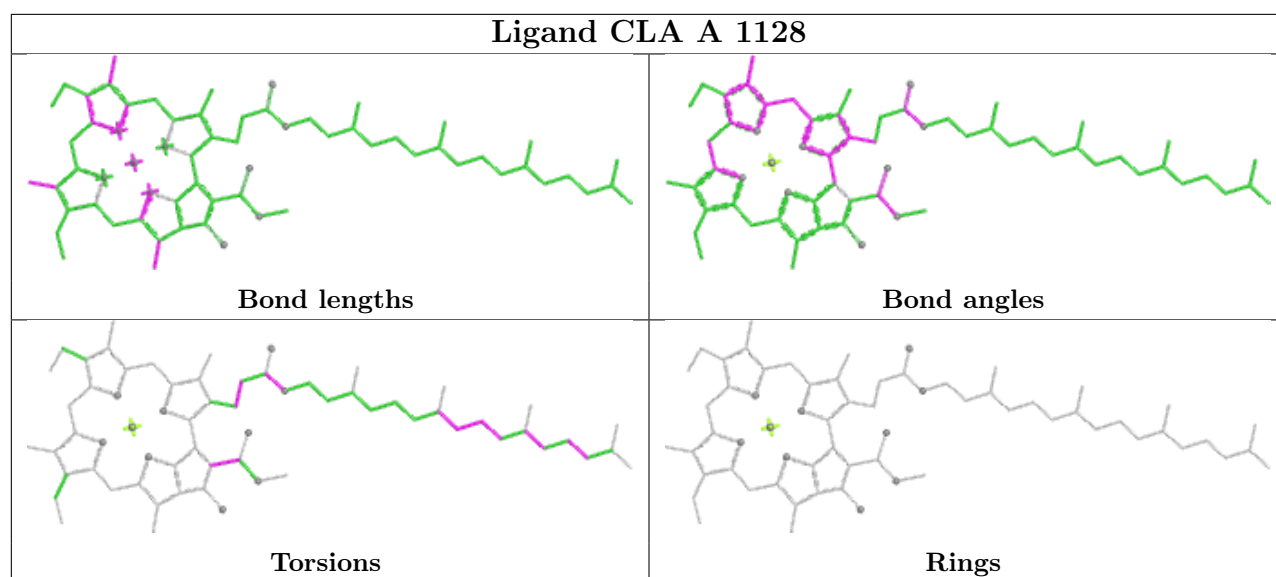


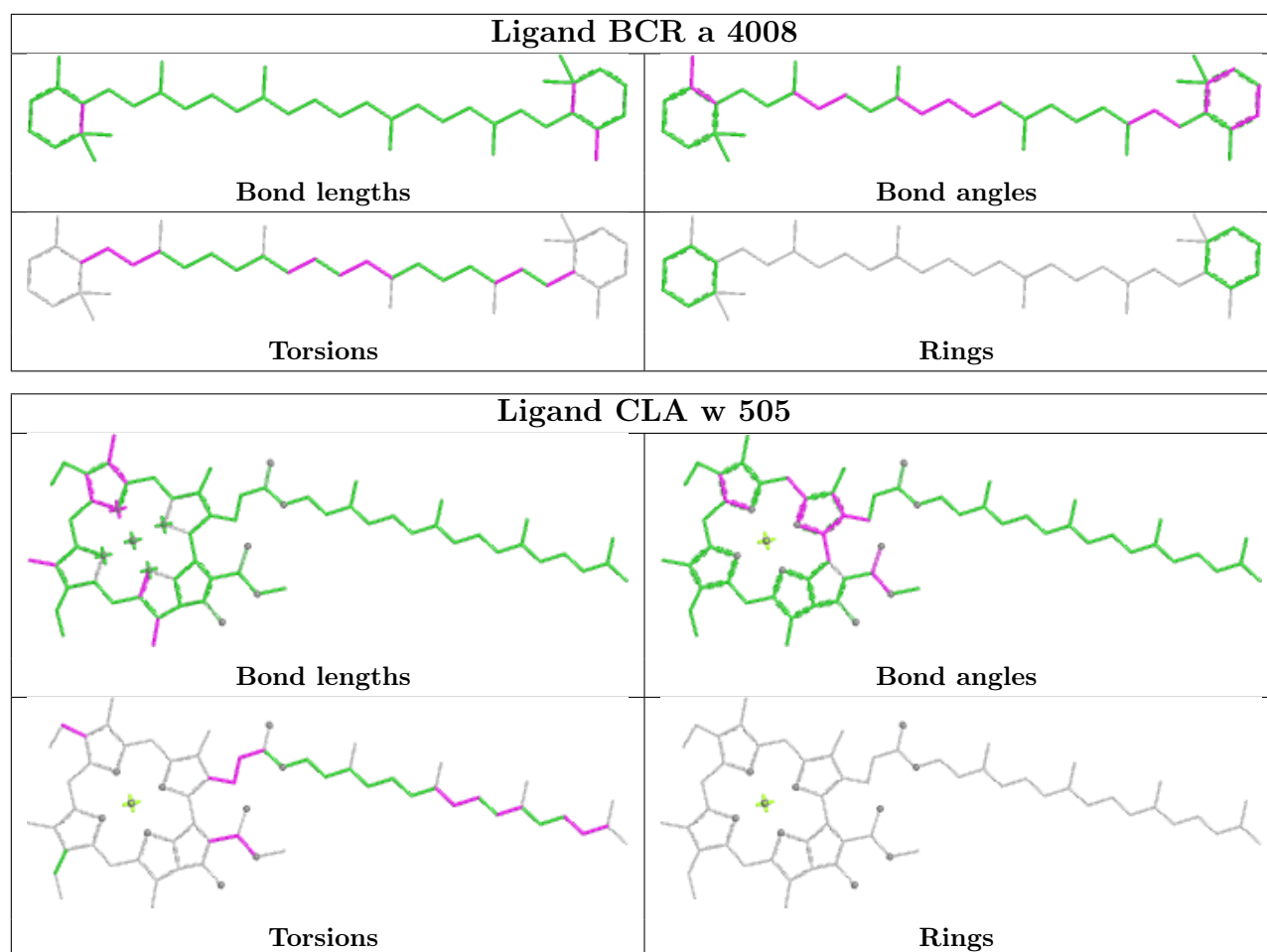
Ligand CLA n 517



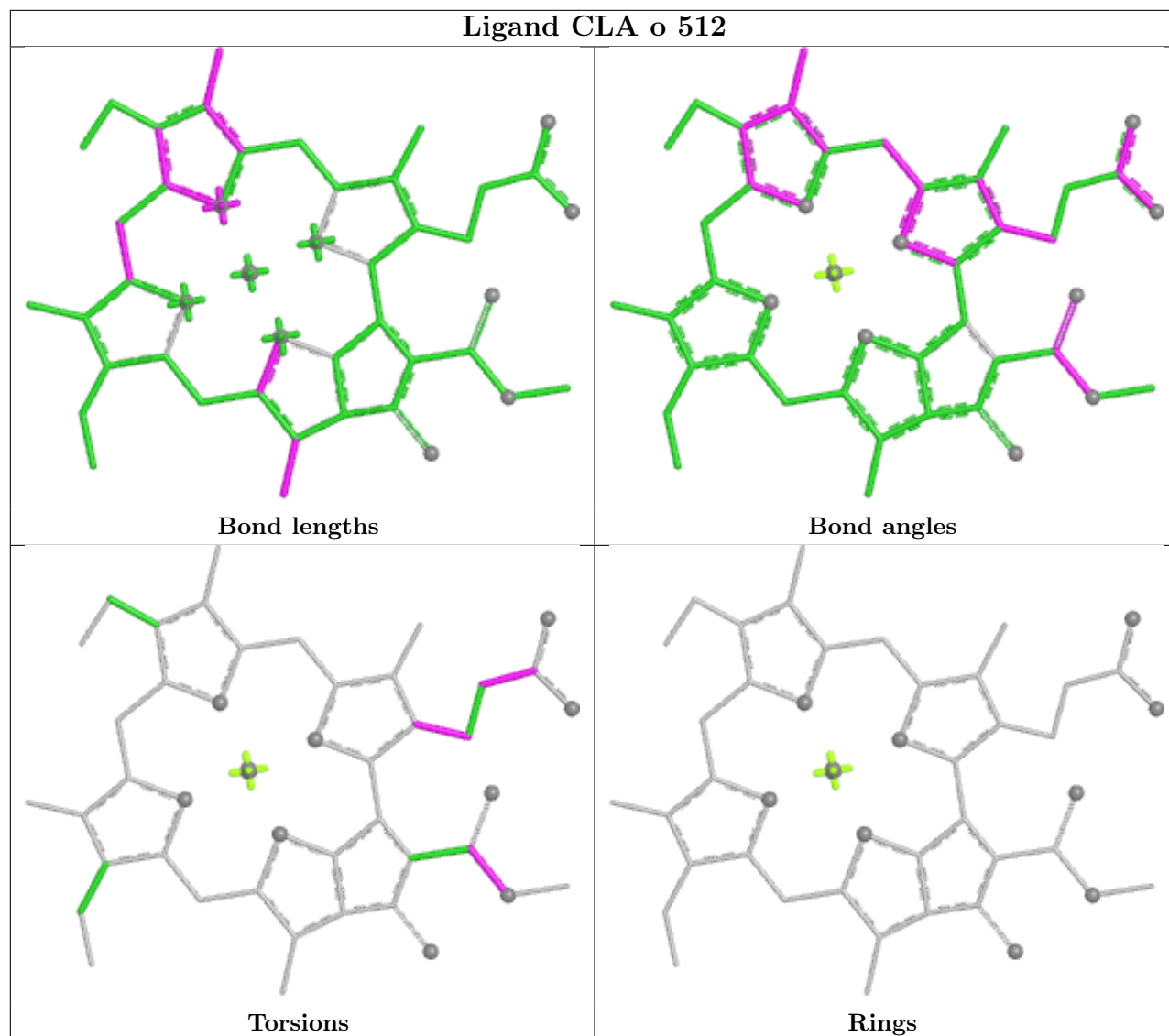




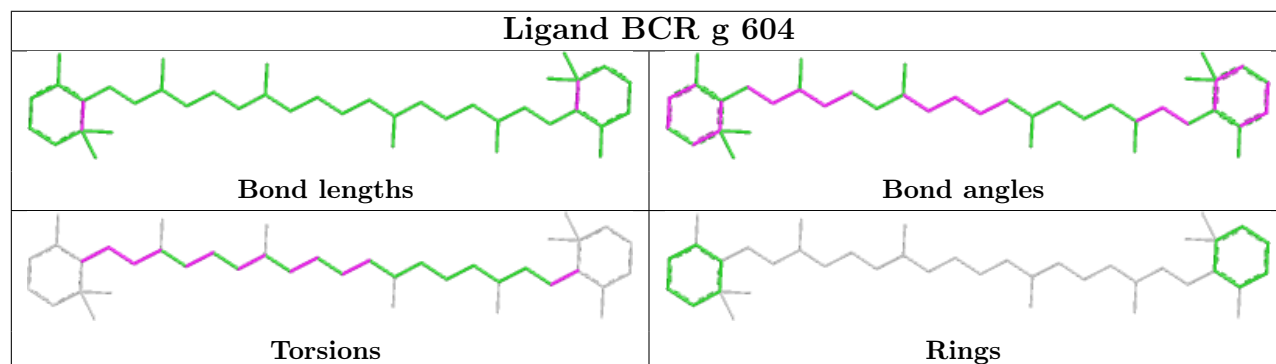




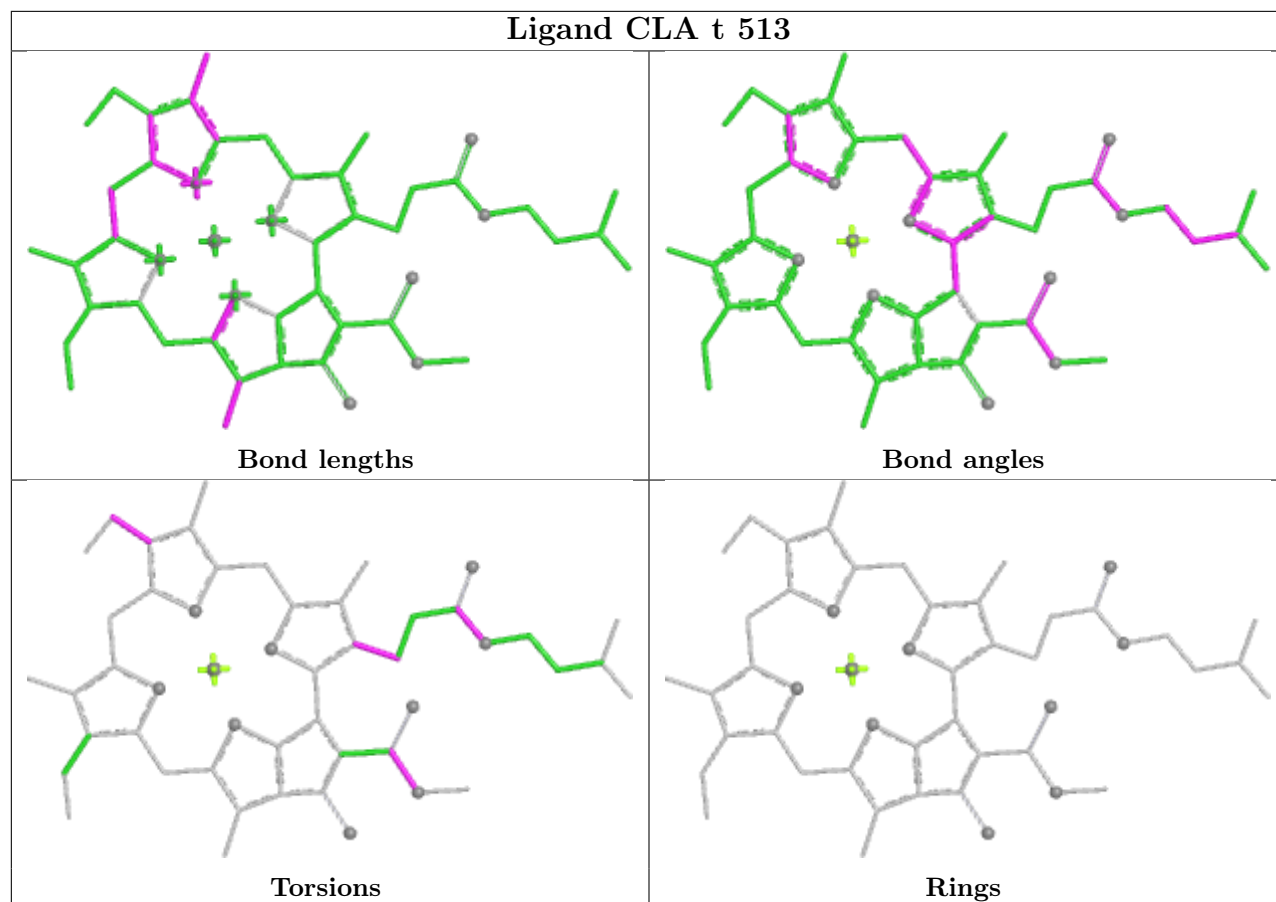
Ligand CLA o 512

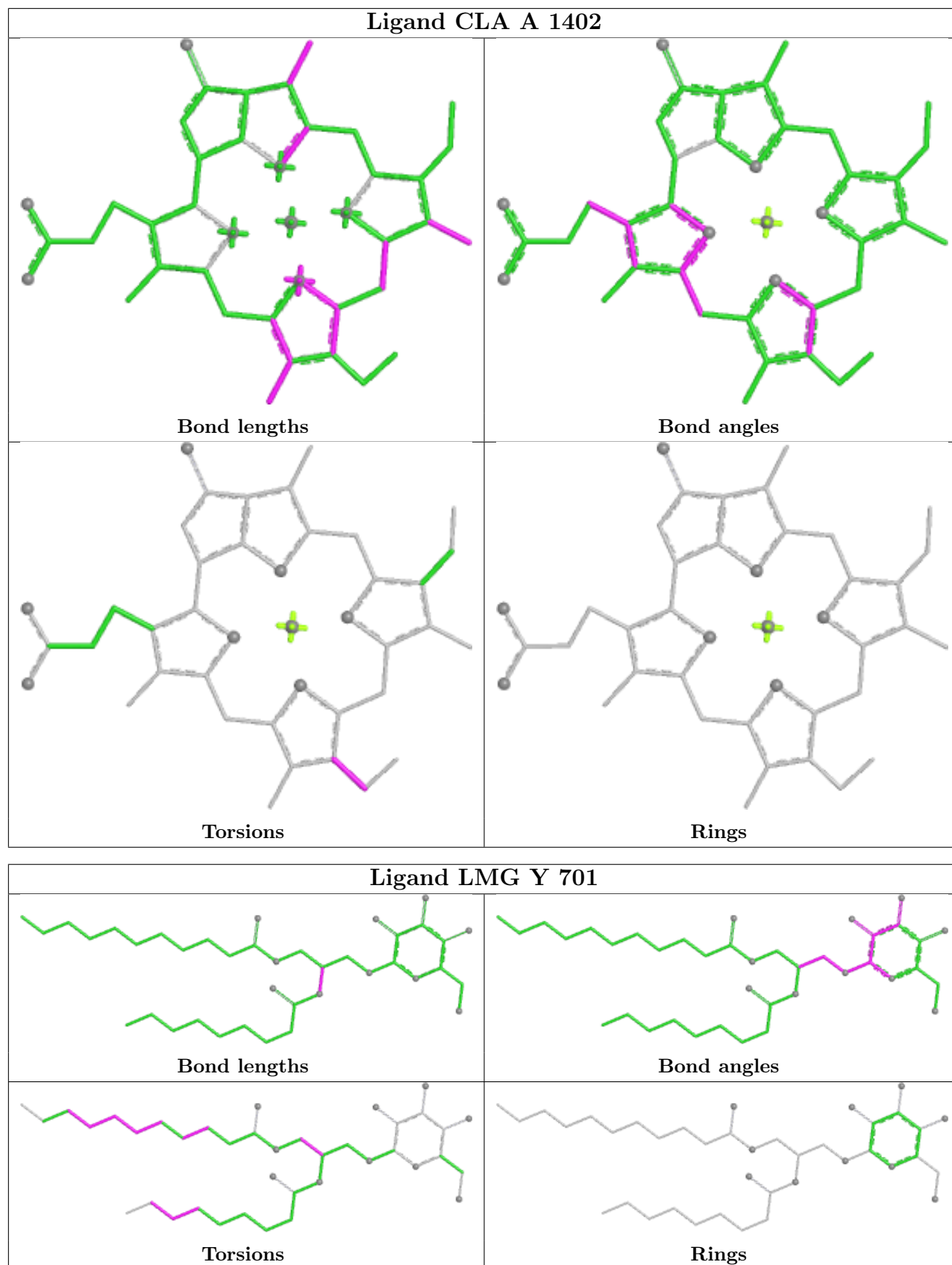


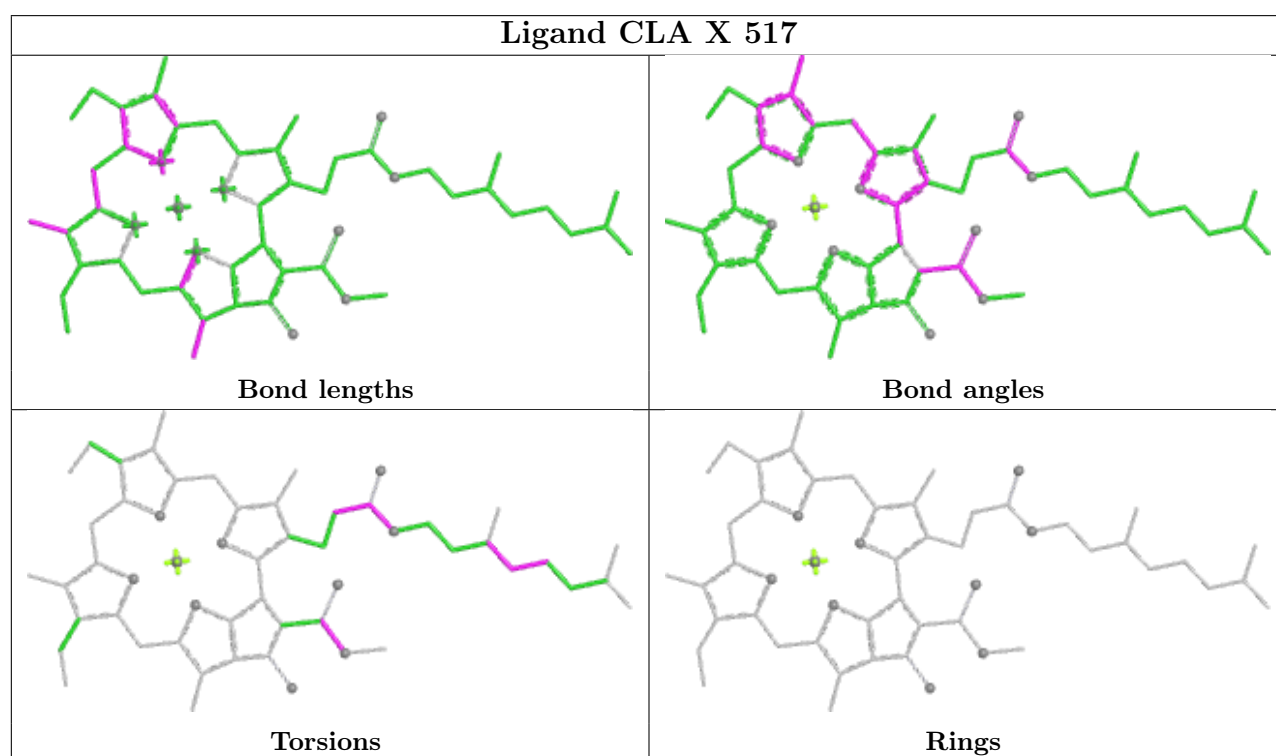
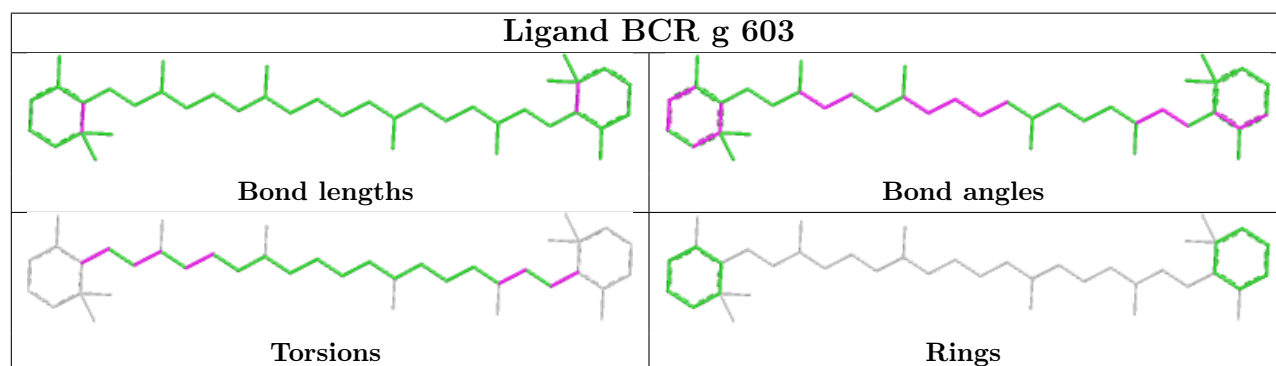
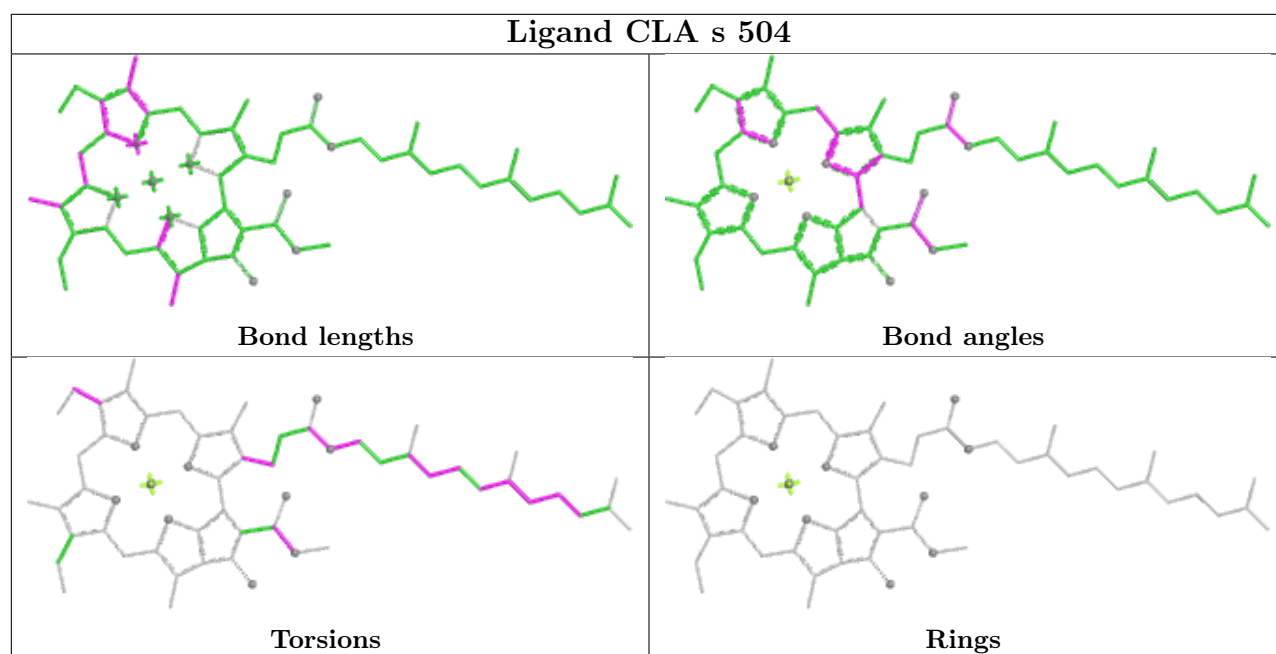
Ligand BCR g 604

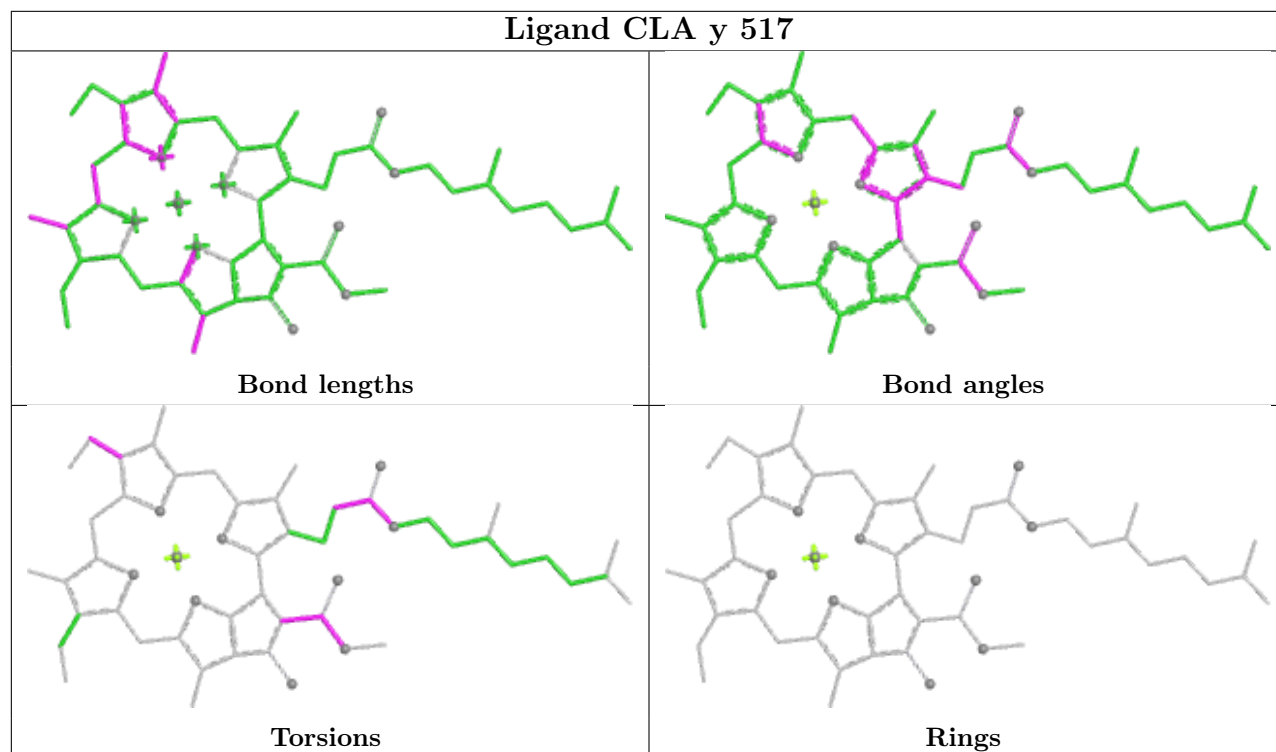
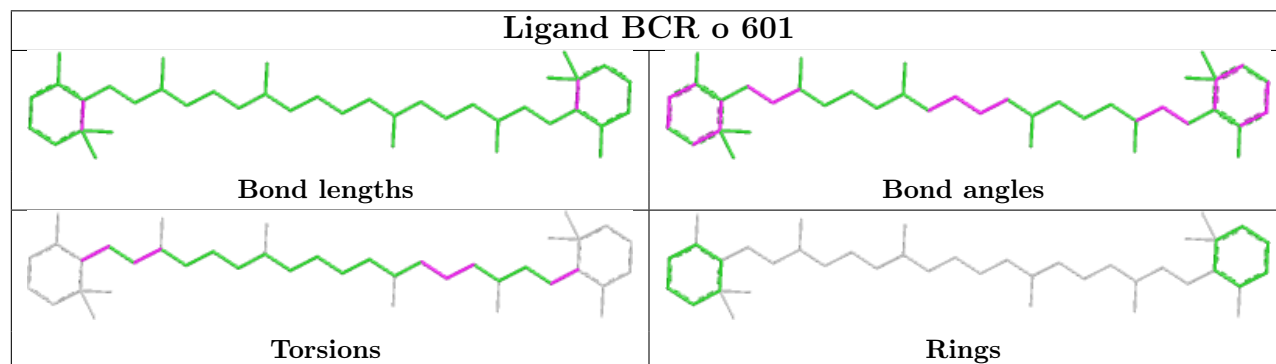
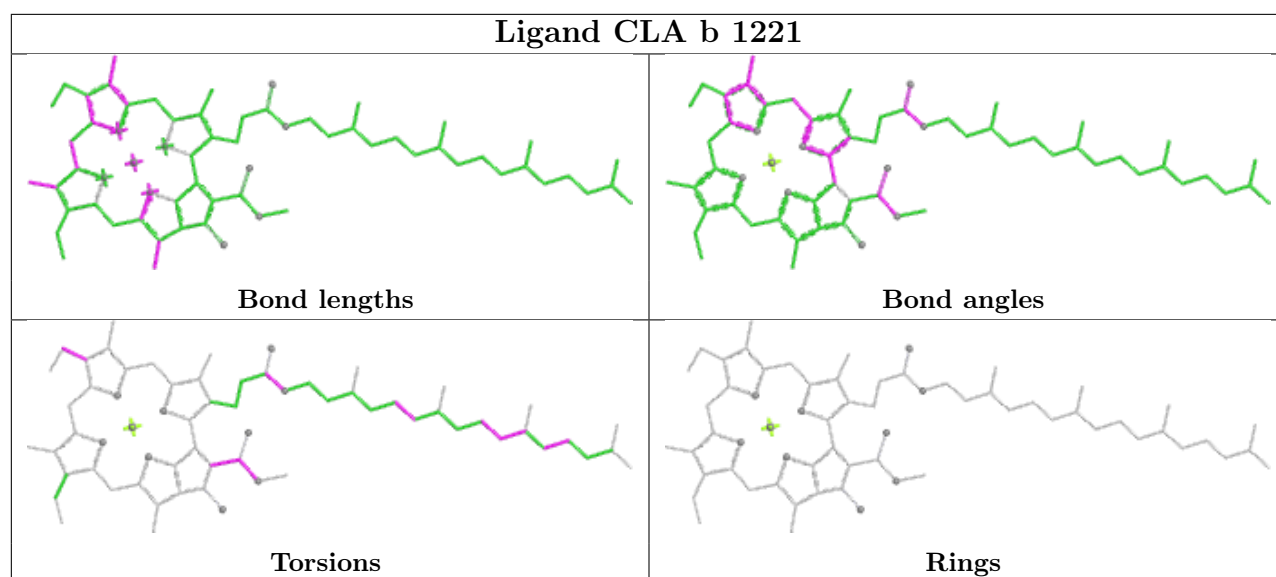


Ligand CLA t 513

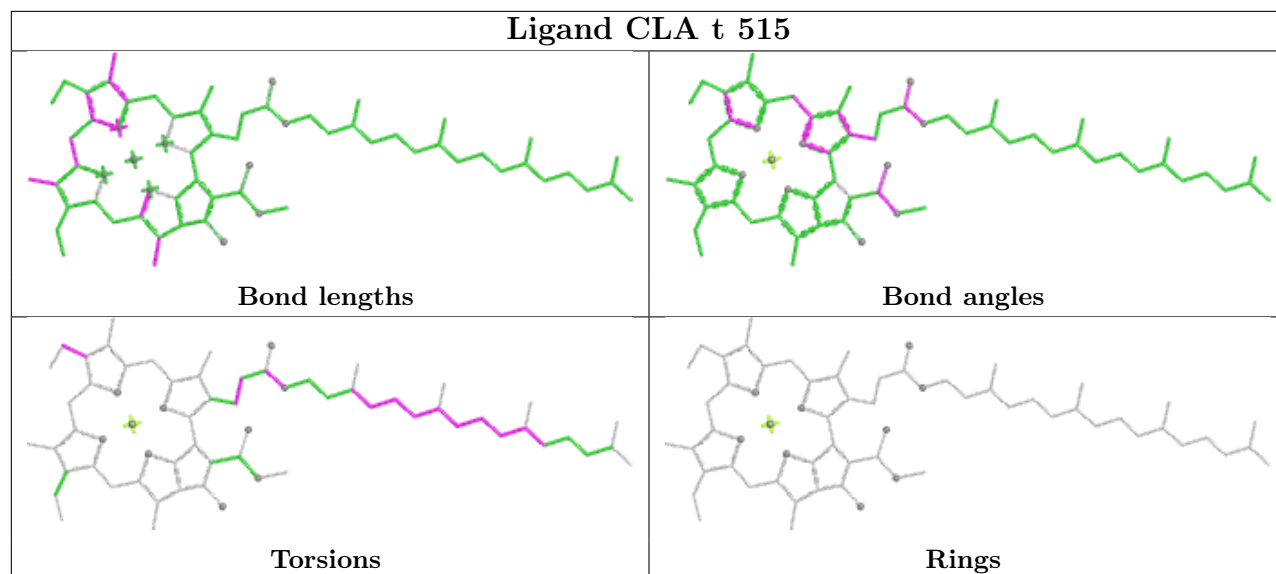




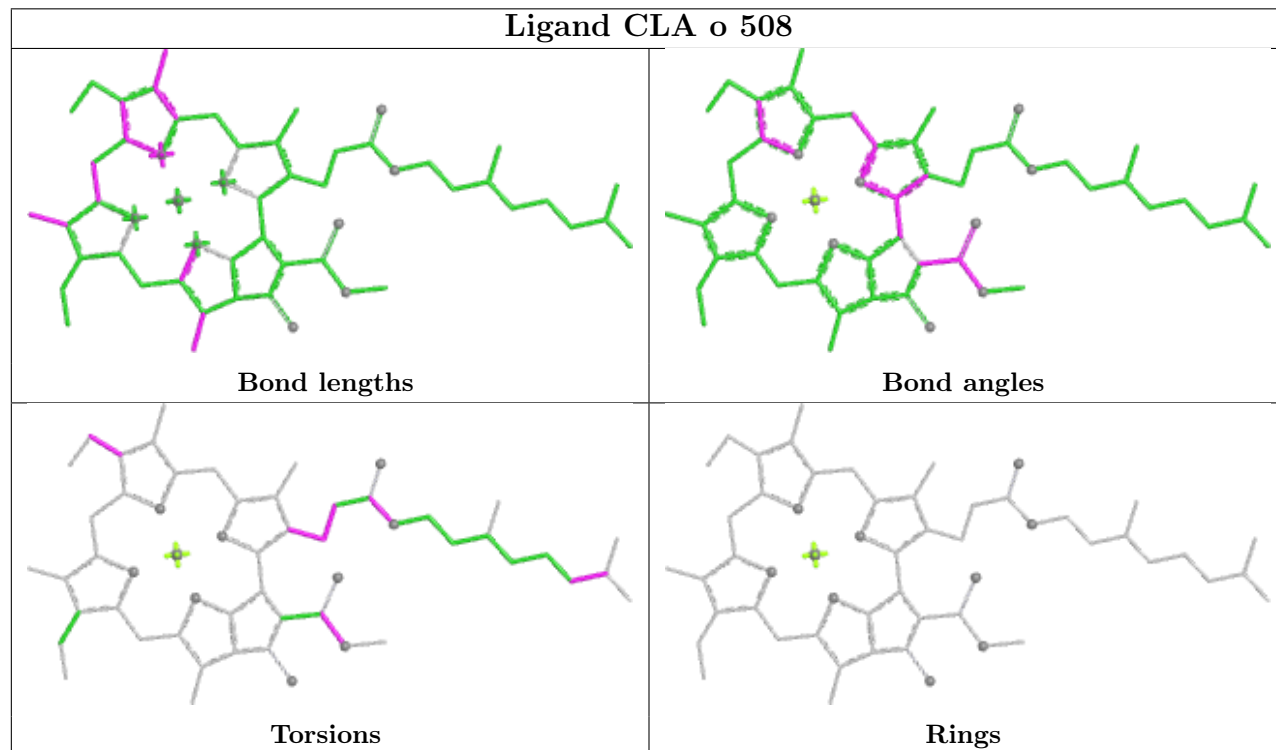


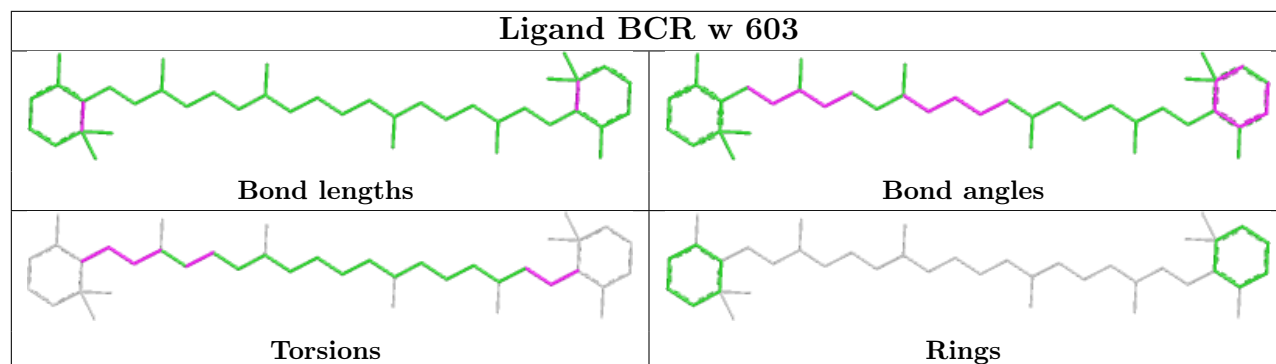
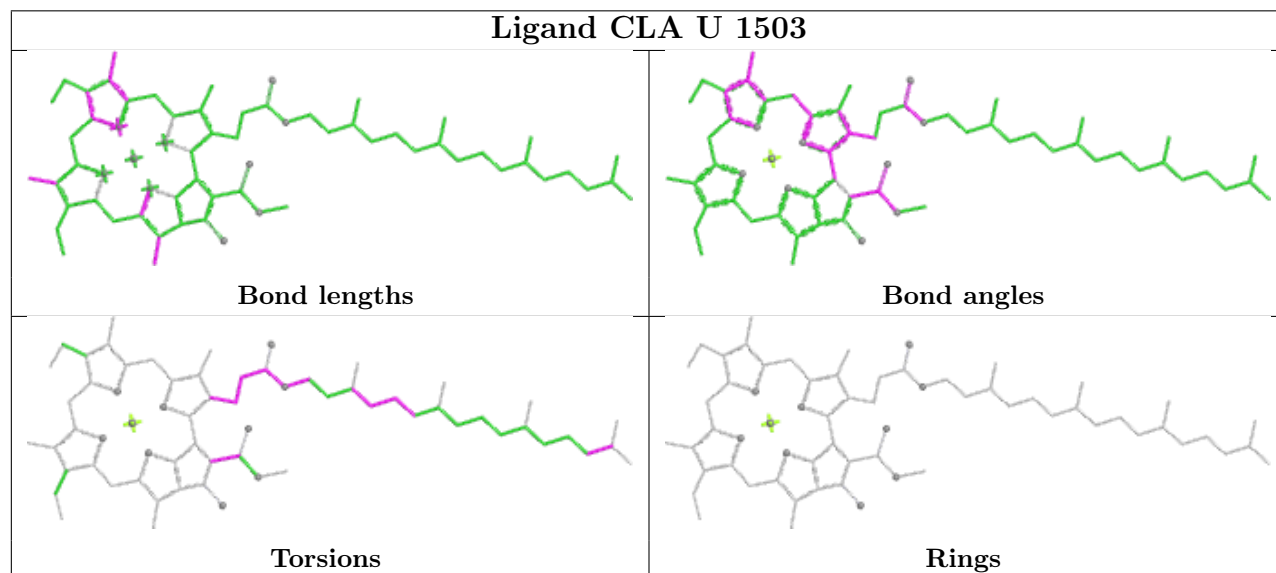
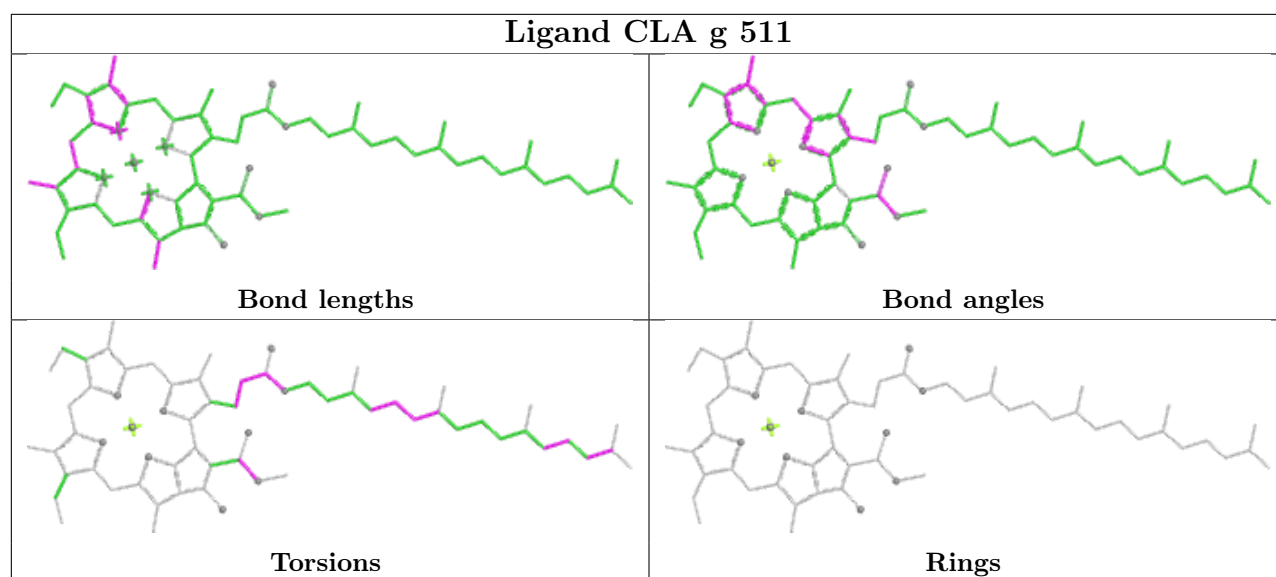


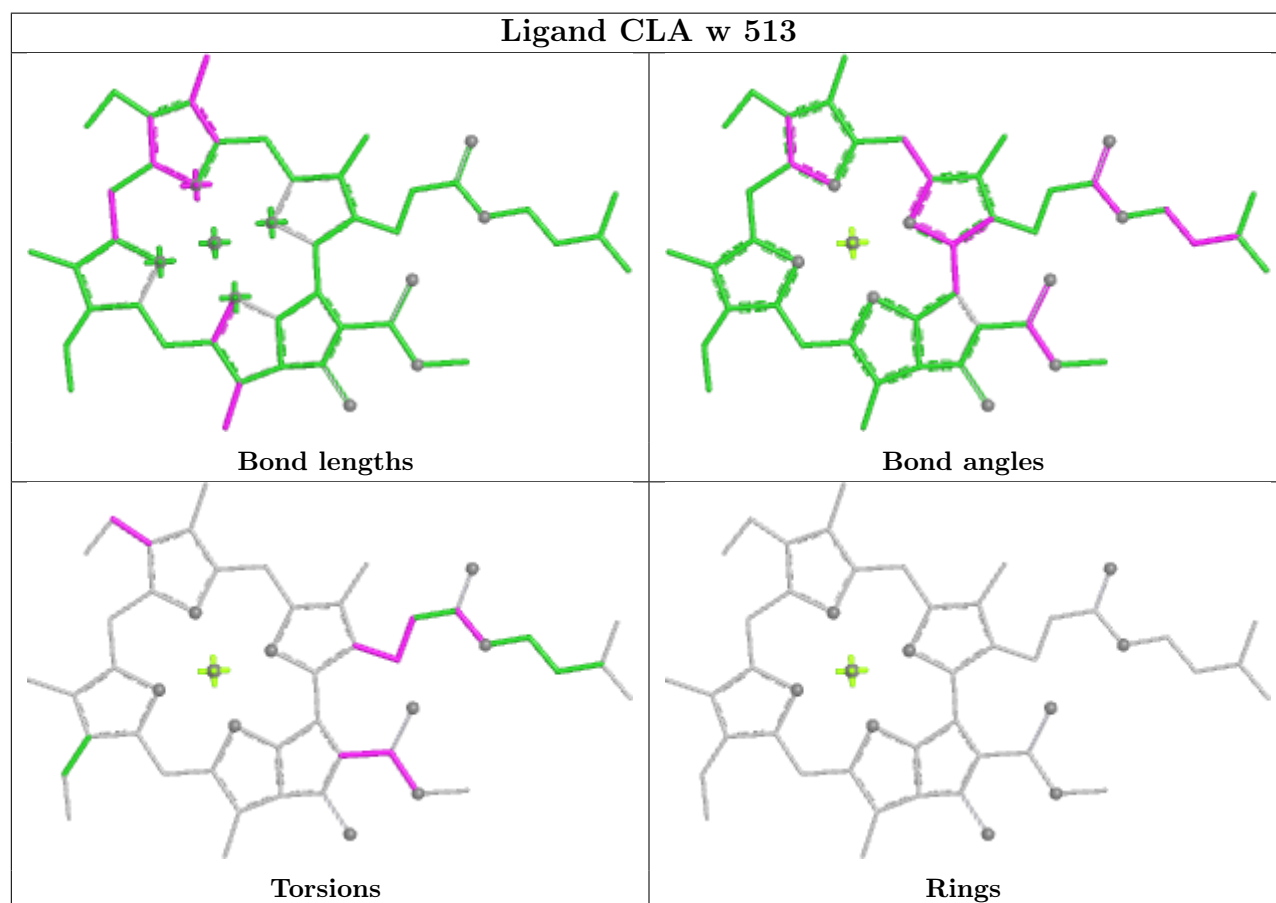
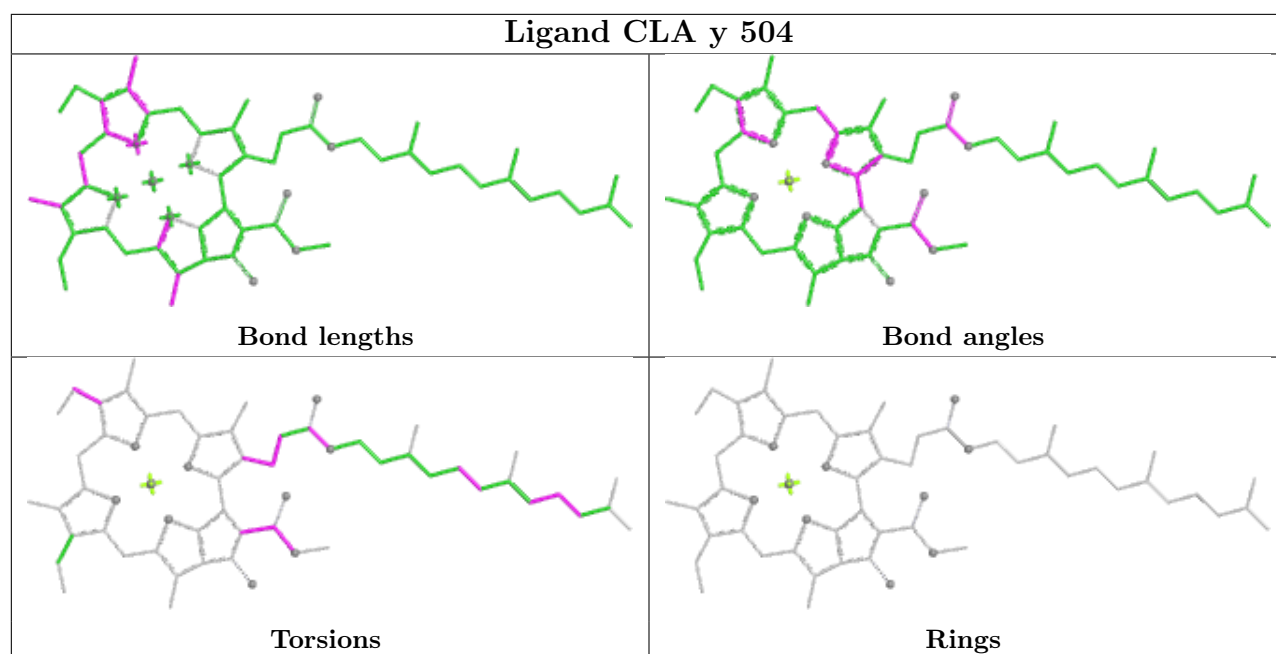
Ligand CLA t 515

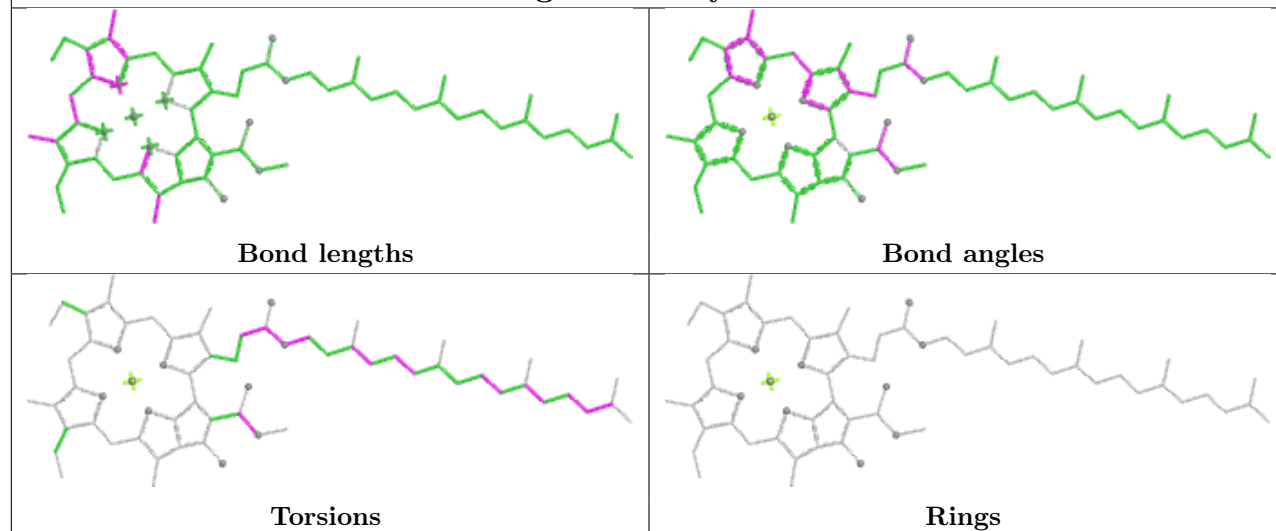
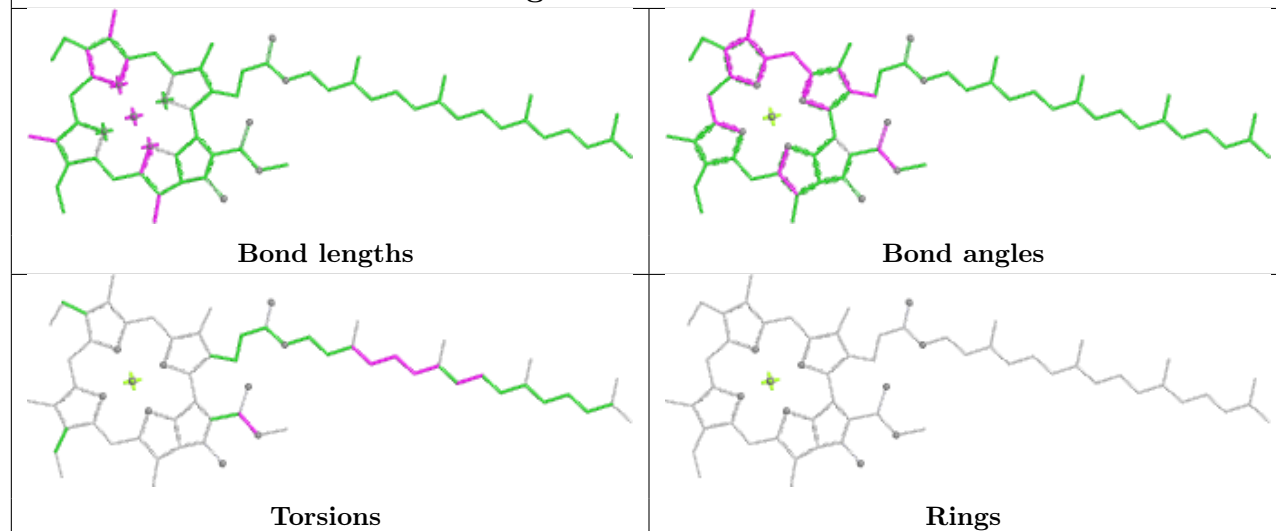


Ligand CLA o 508

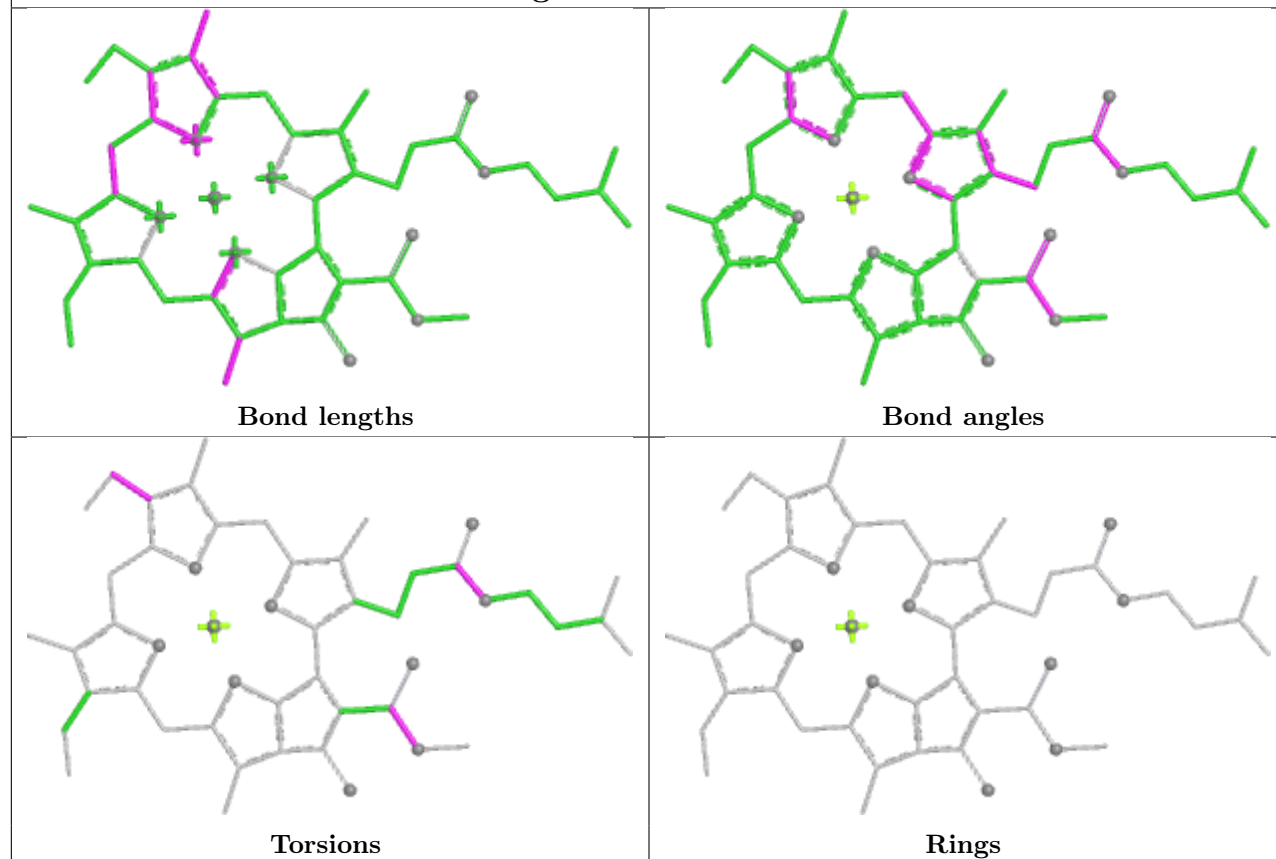




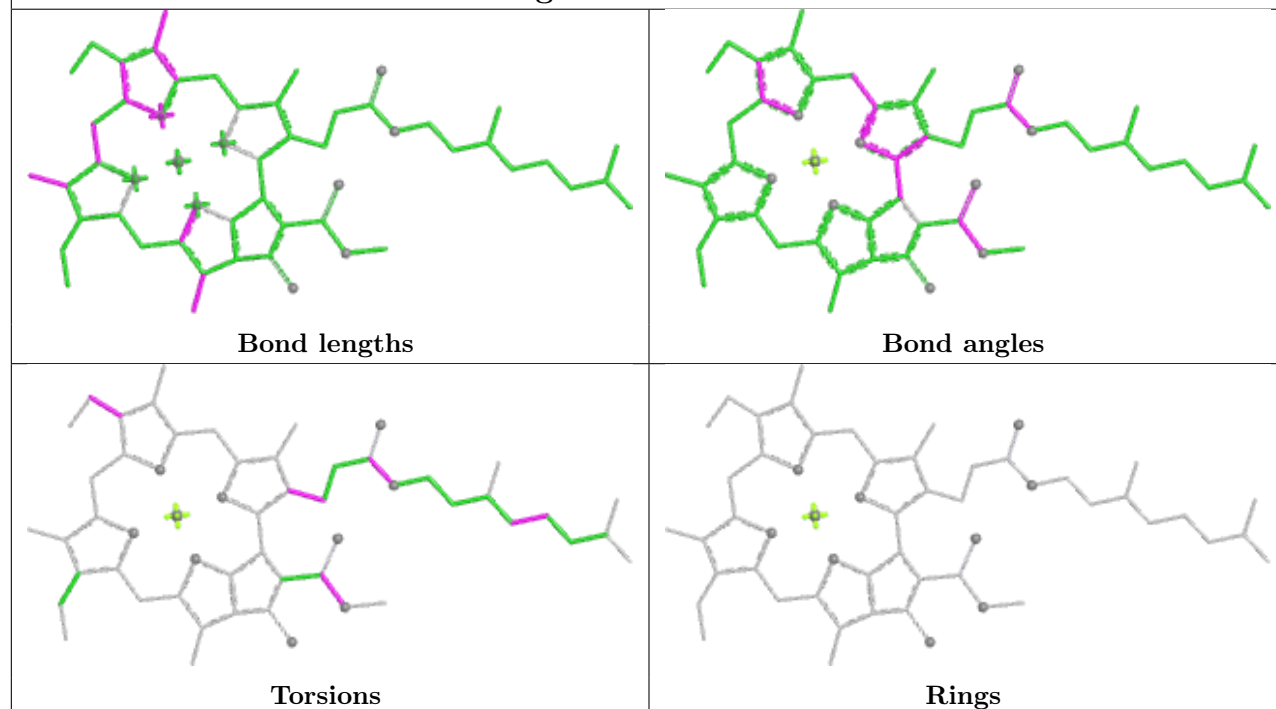


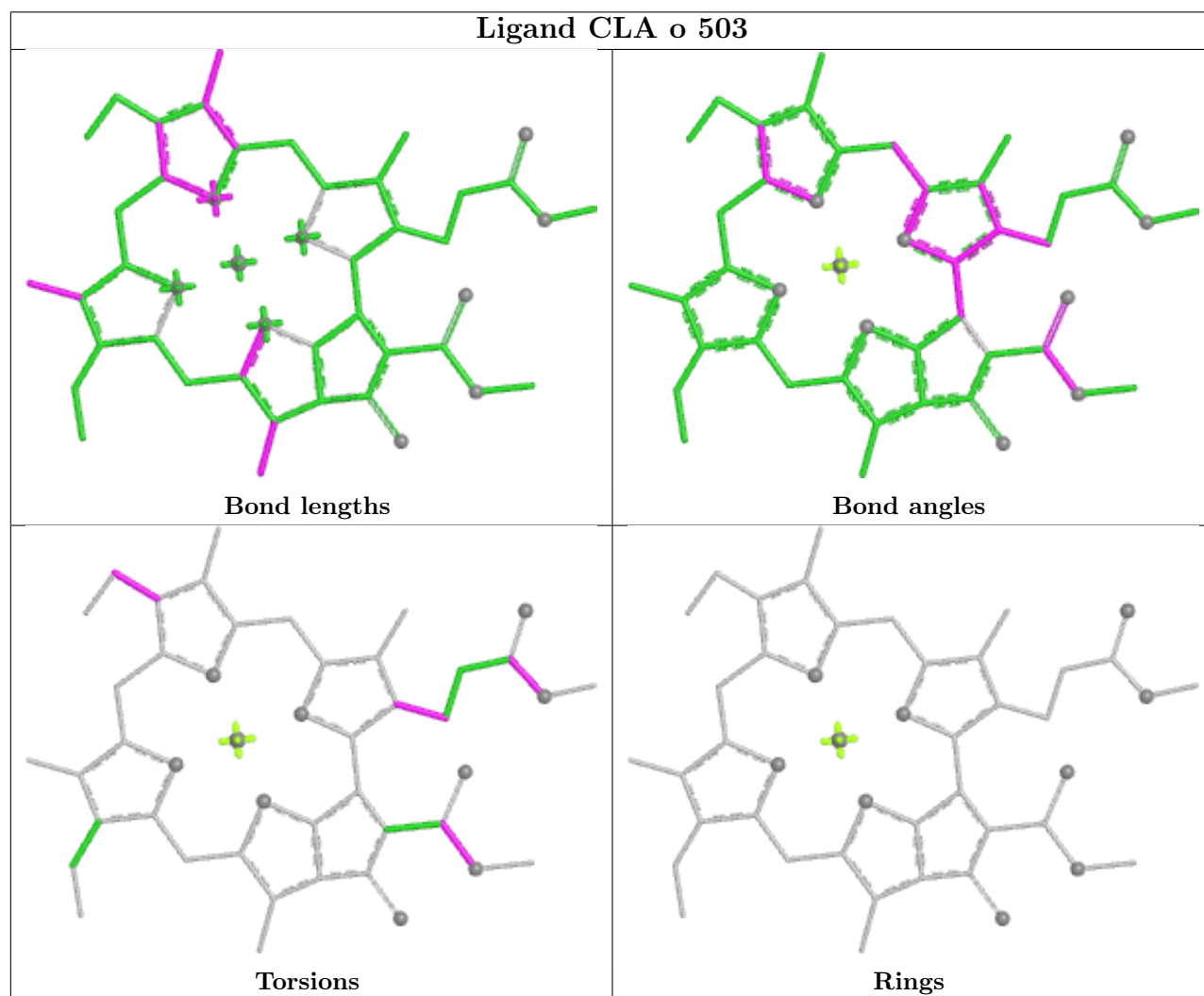
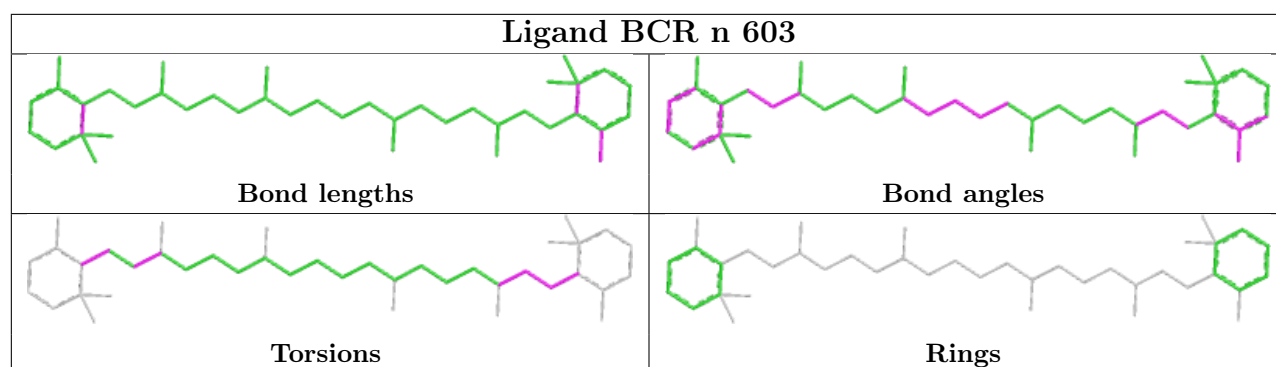
Ligand CLA y 511**Ligand CLA b 1226**

Ligand CLA w 501

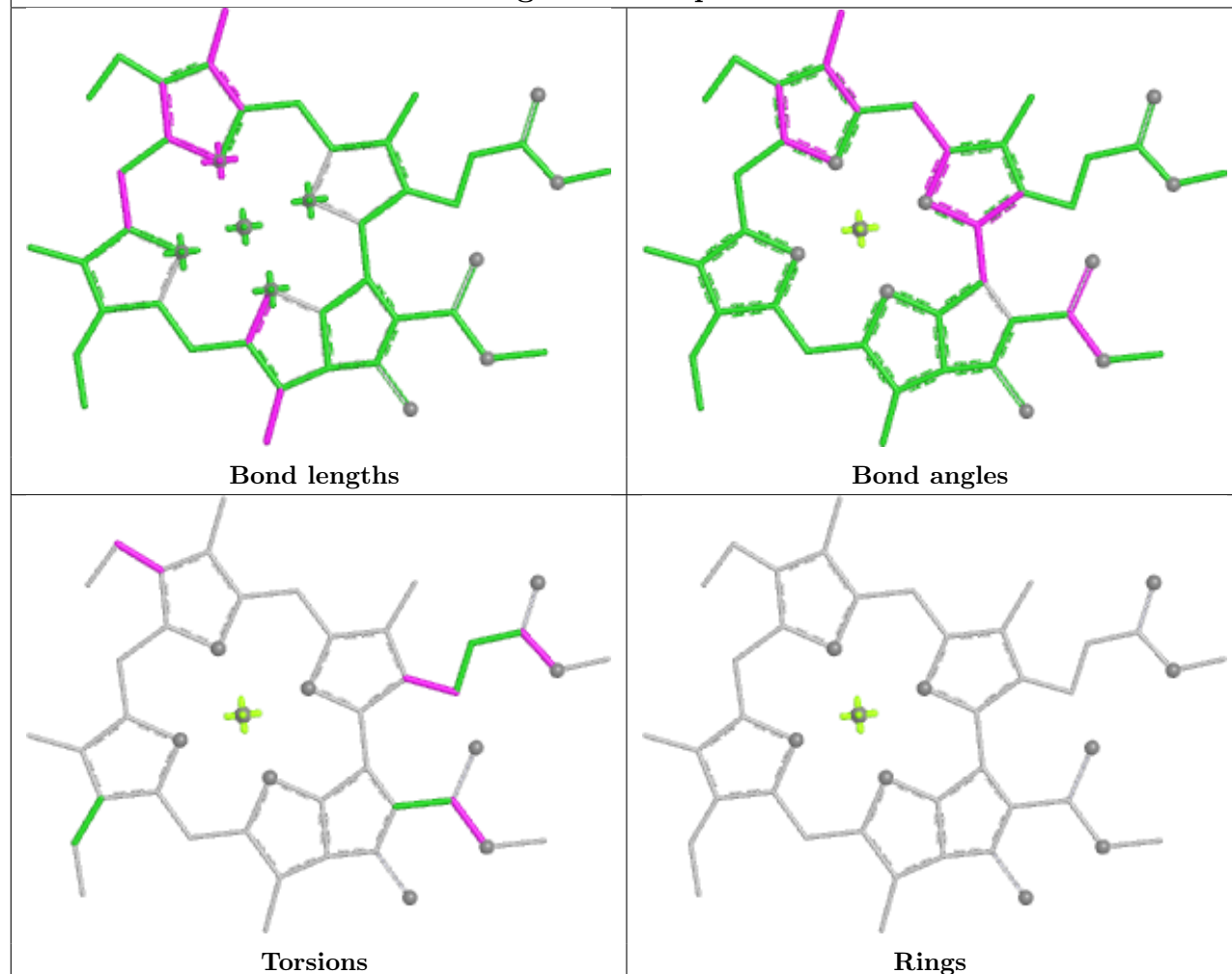


Ligand CLA v 508

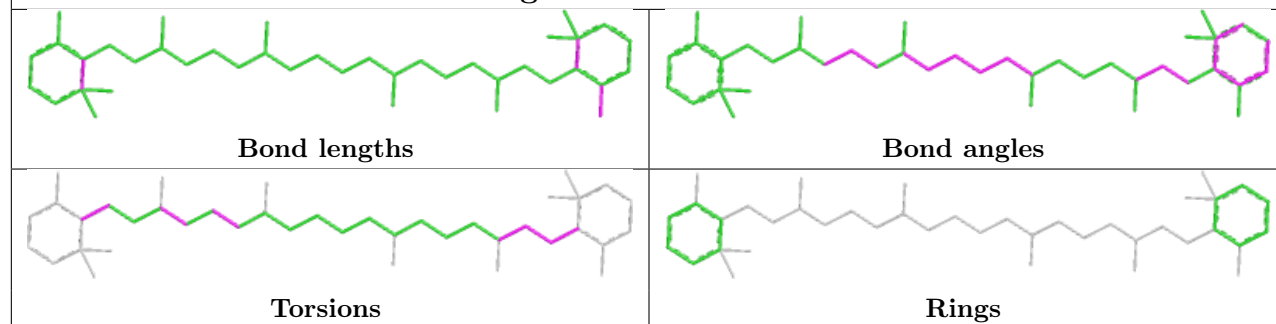


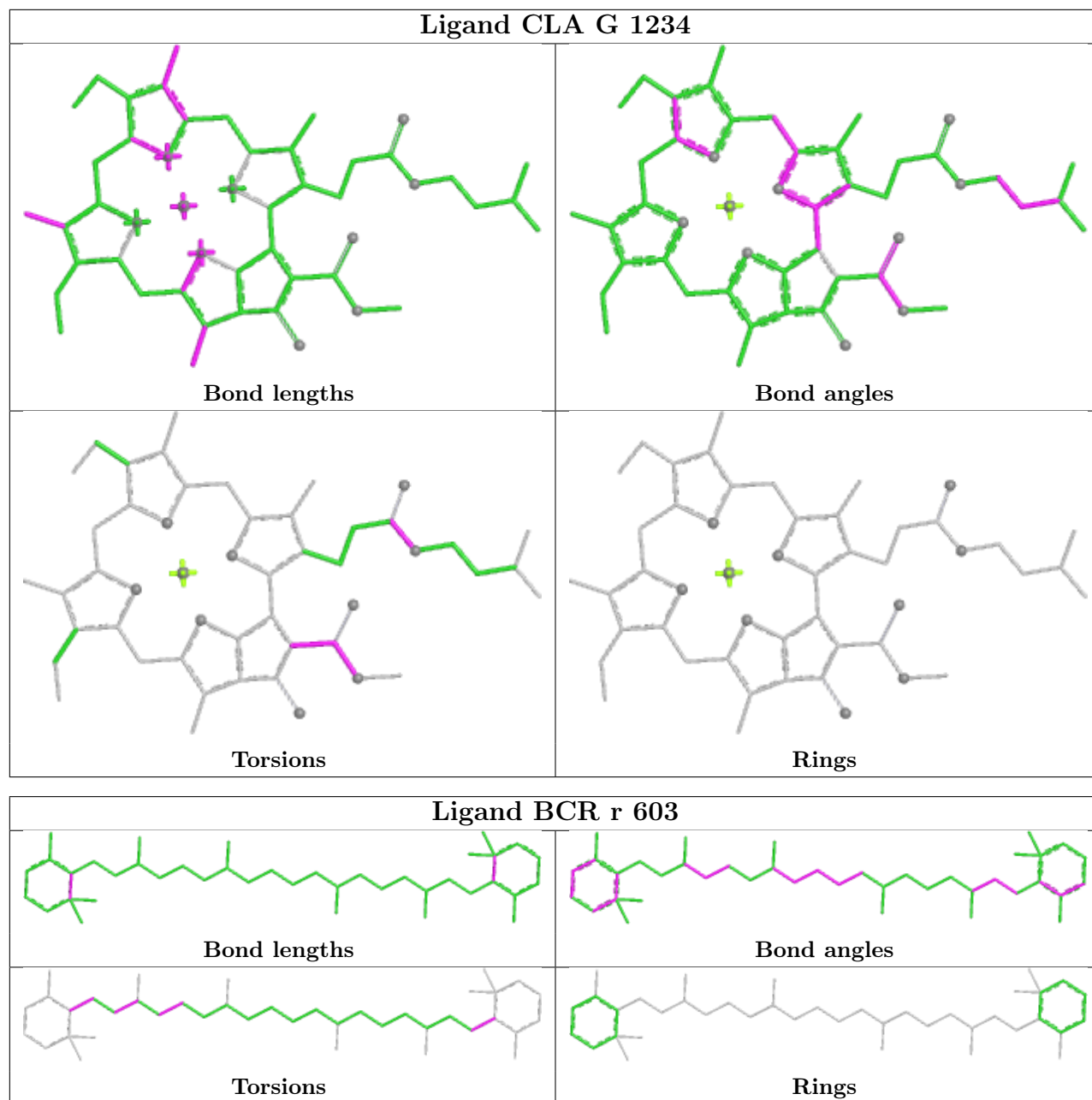


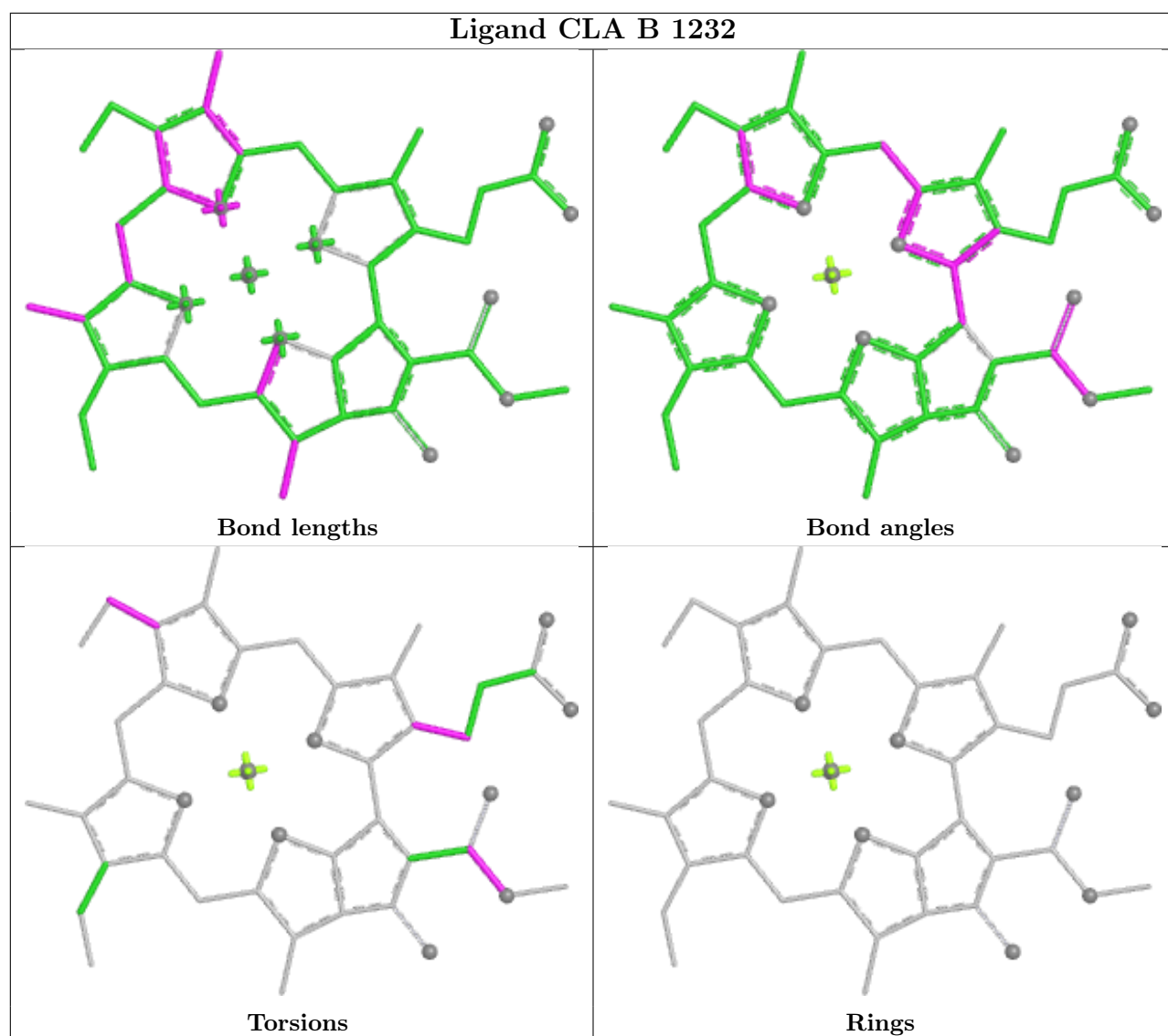
Ligand CLA q 516



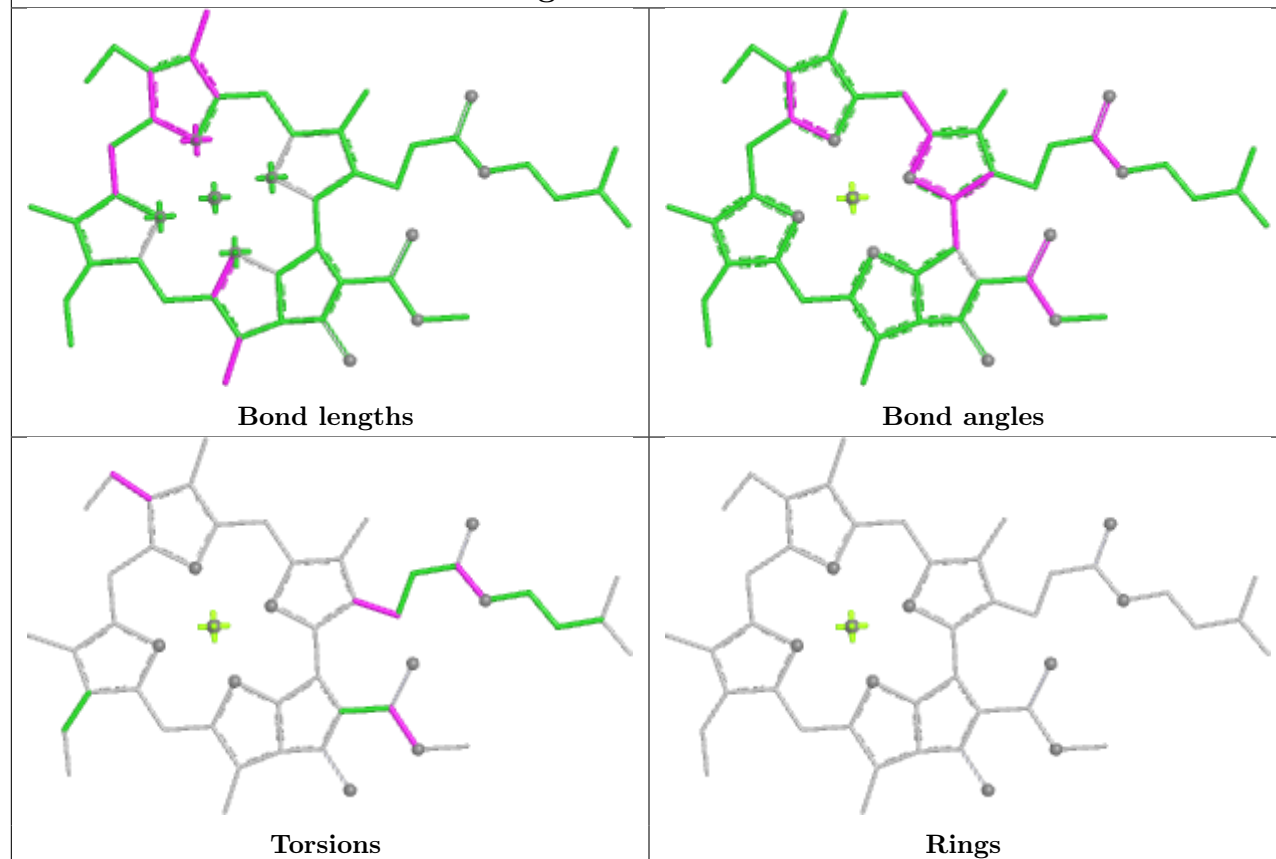
Ligand BCR G 4017



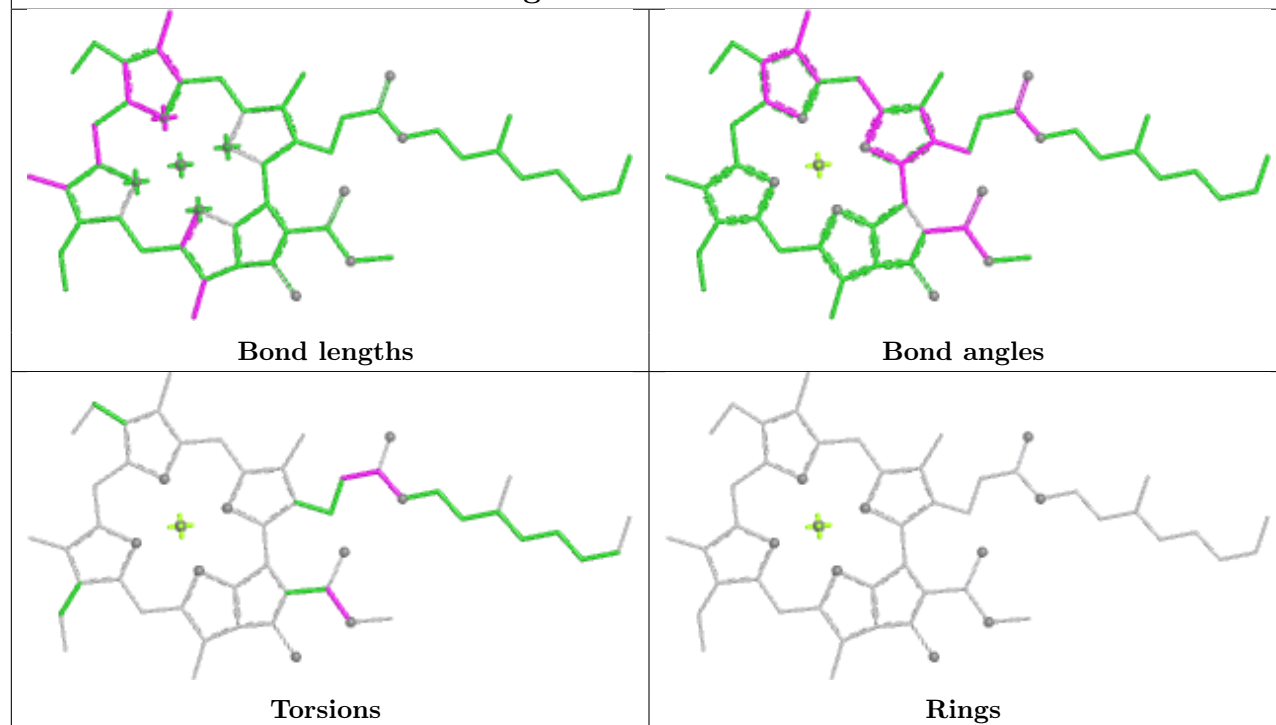


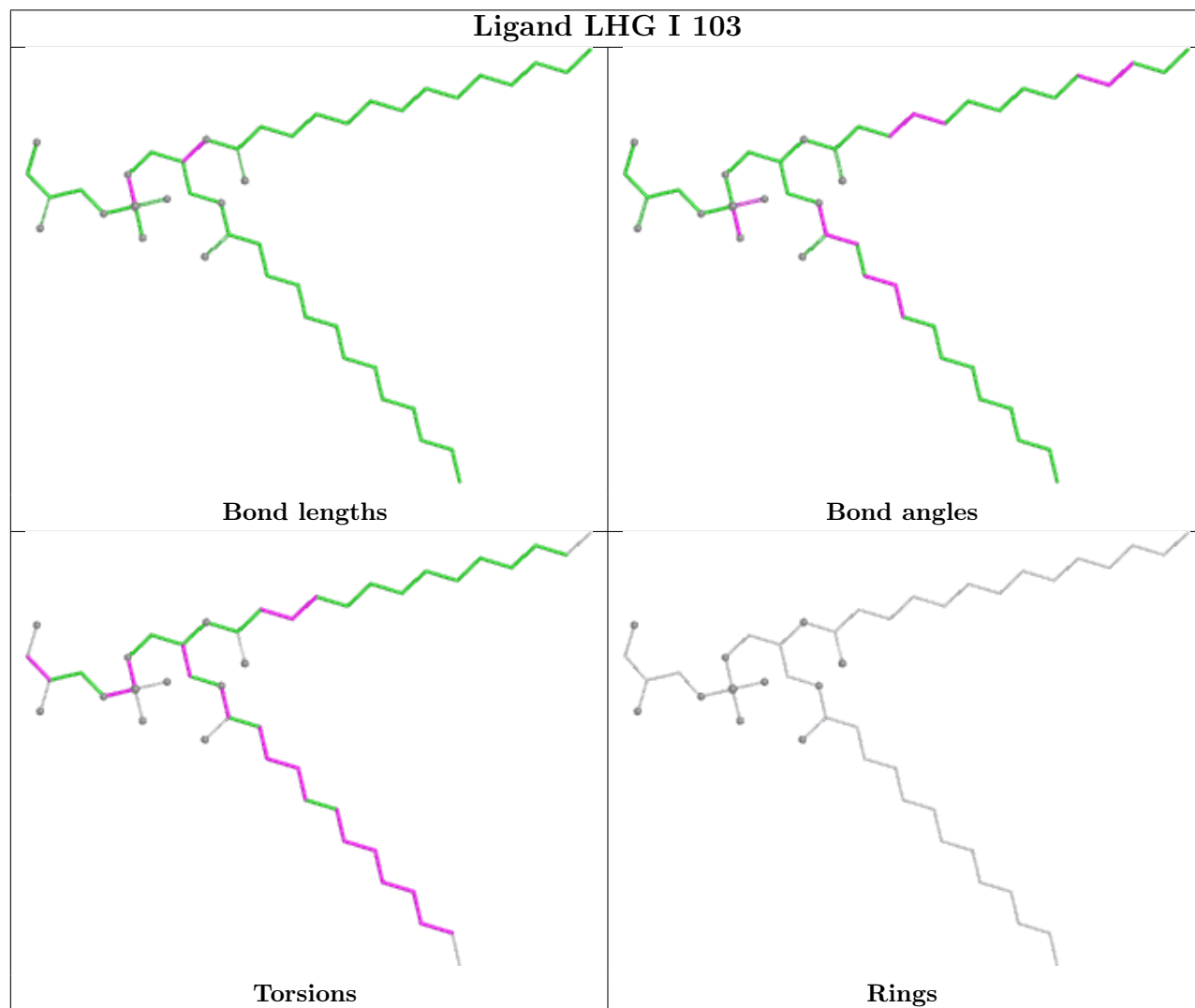
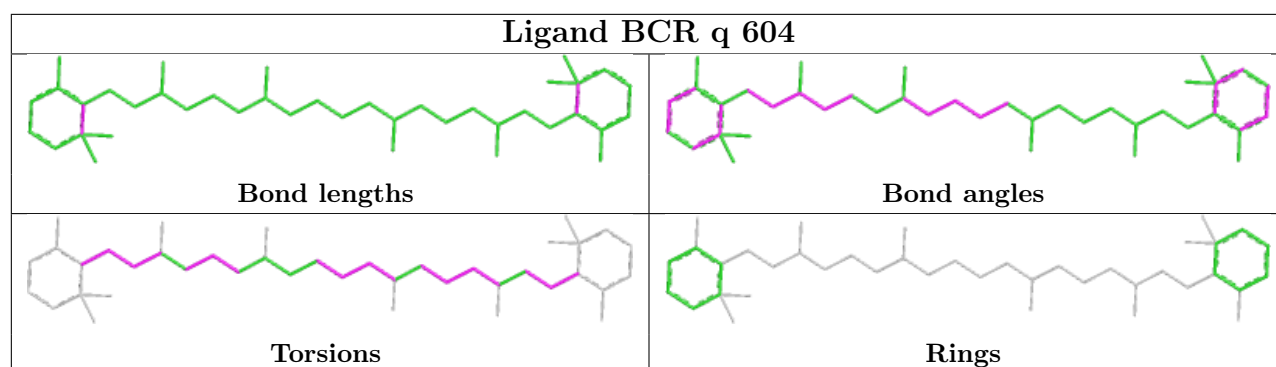


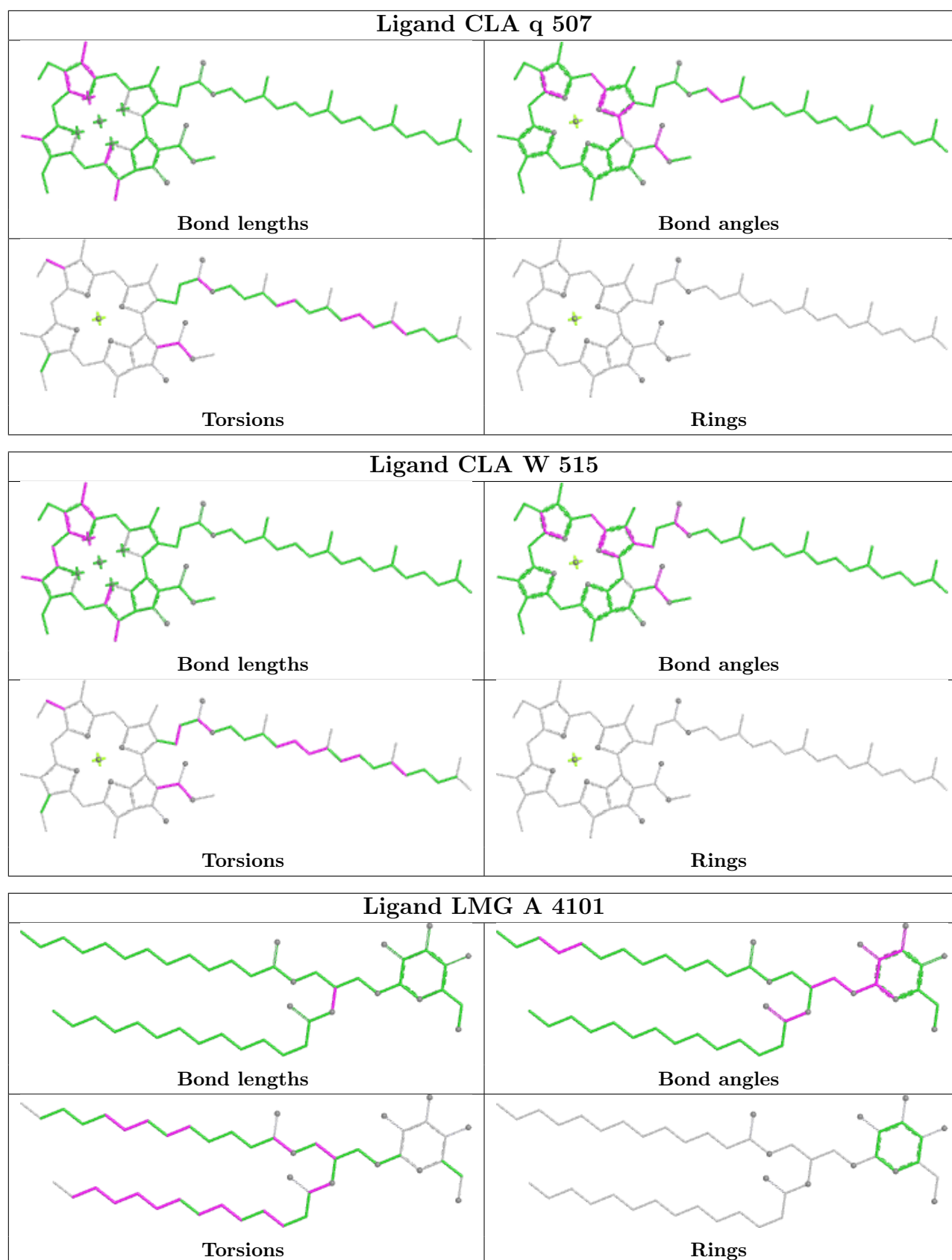
Ligand CLA r 513

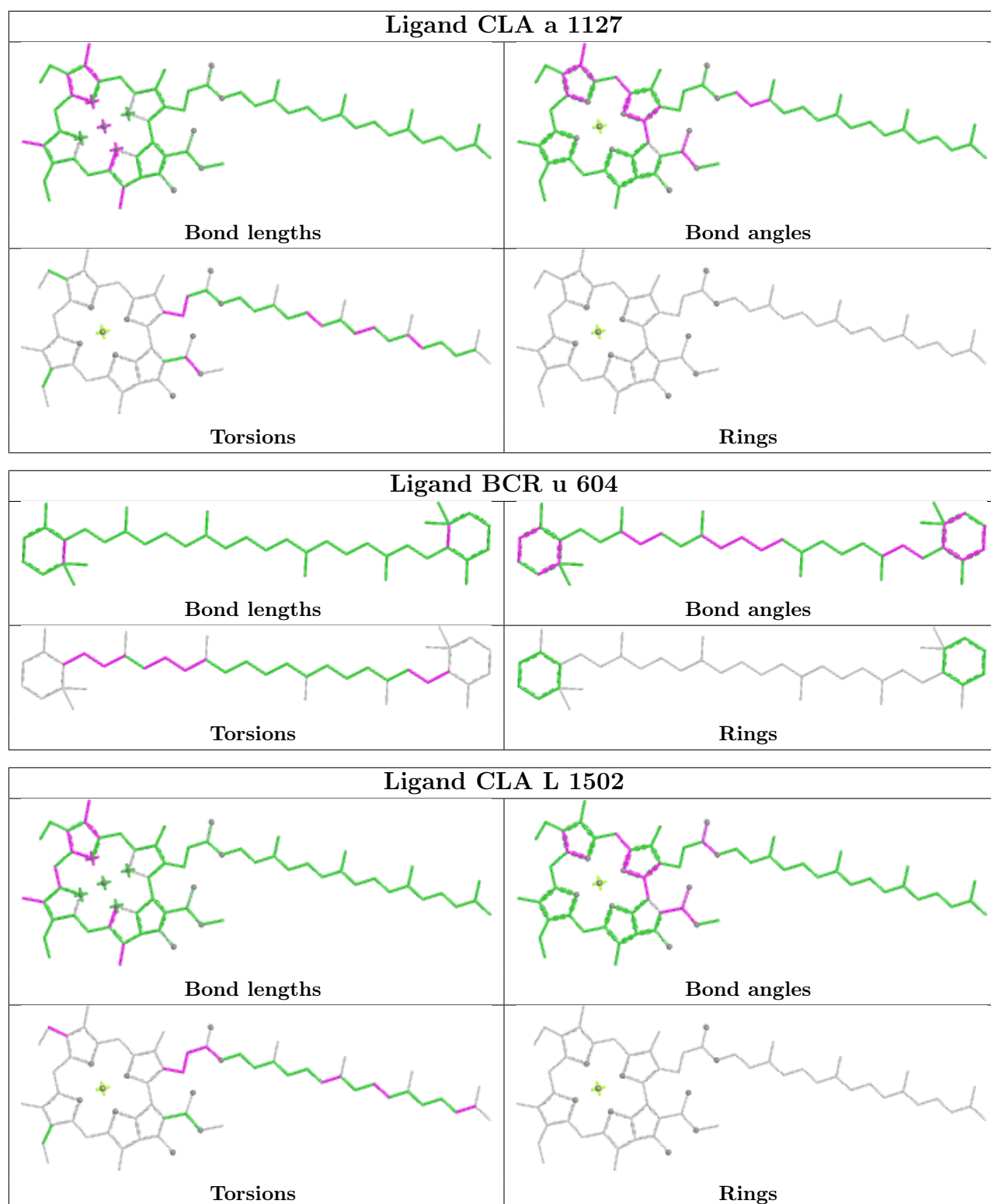


Ligand CLA B 1220

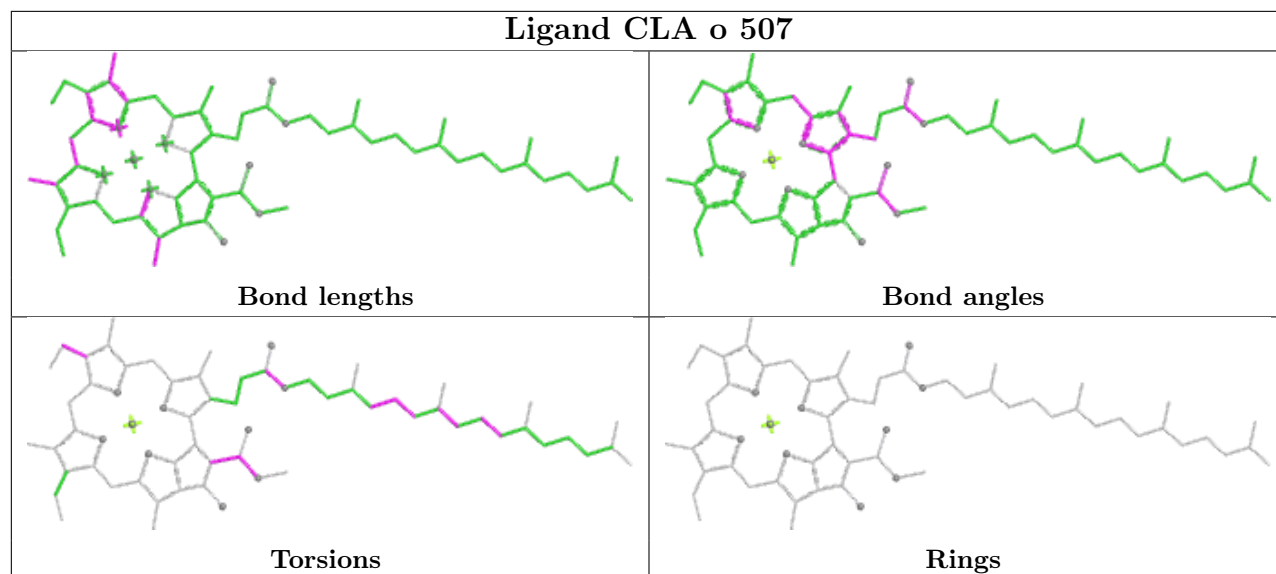




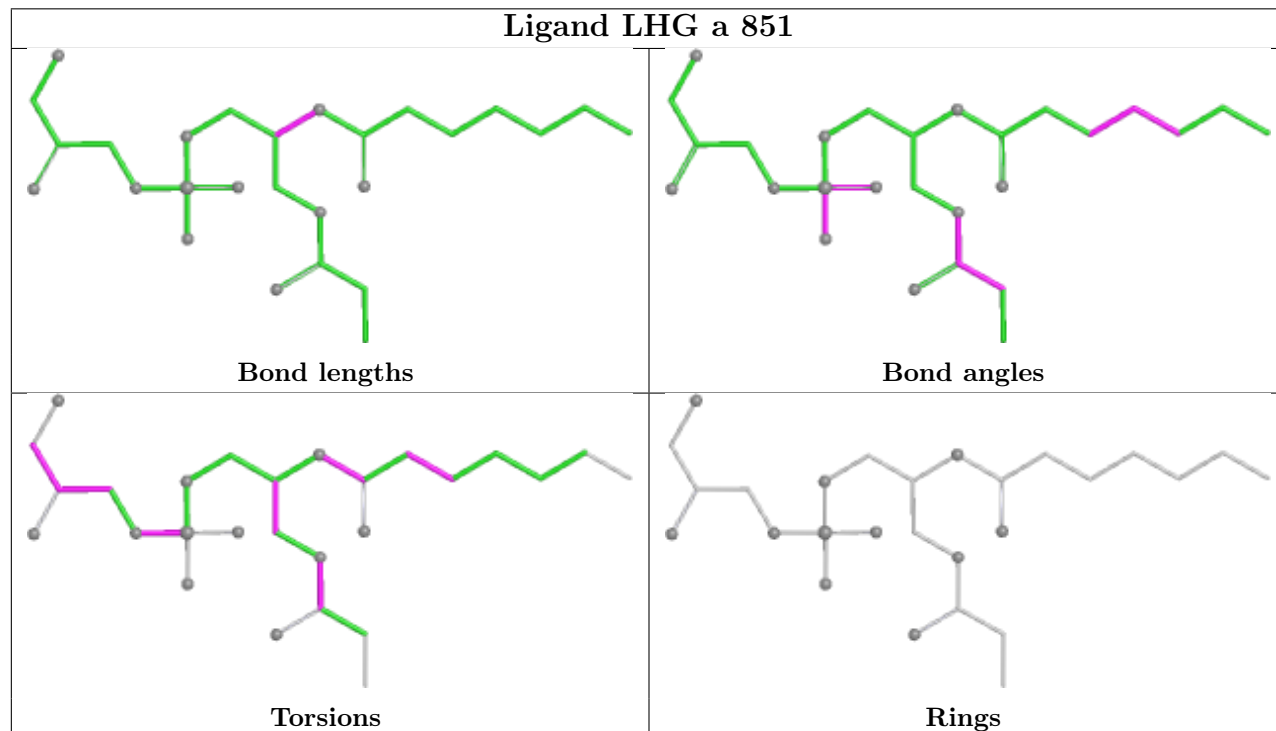




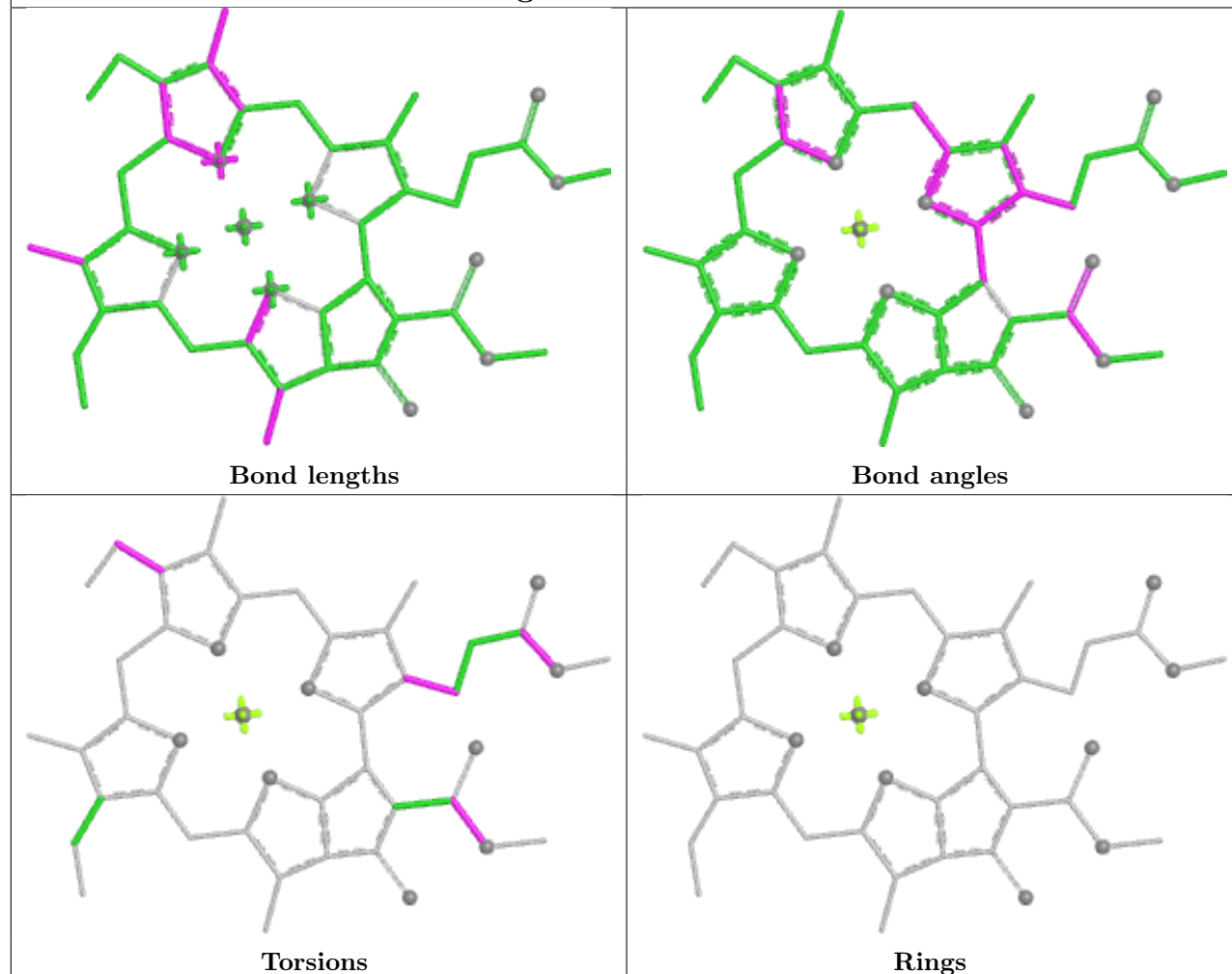
Ligand CLA o 507



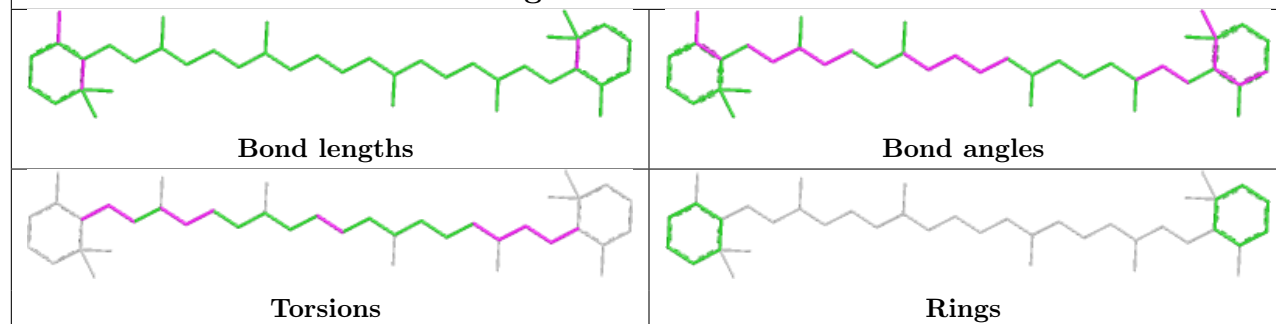
Ligand LHG a 851

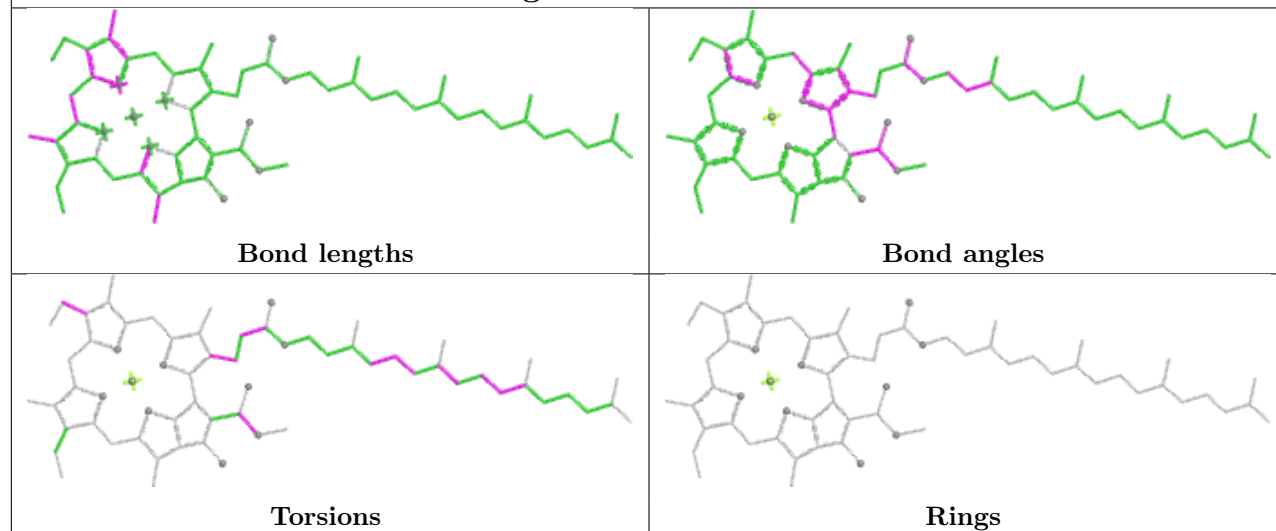
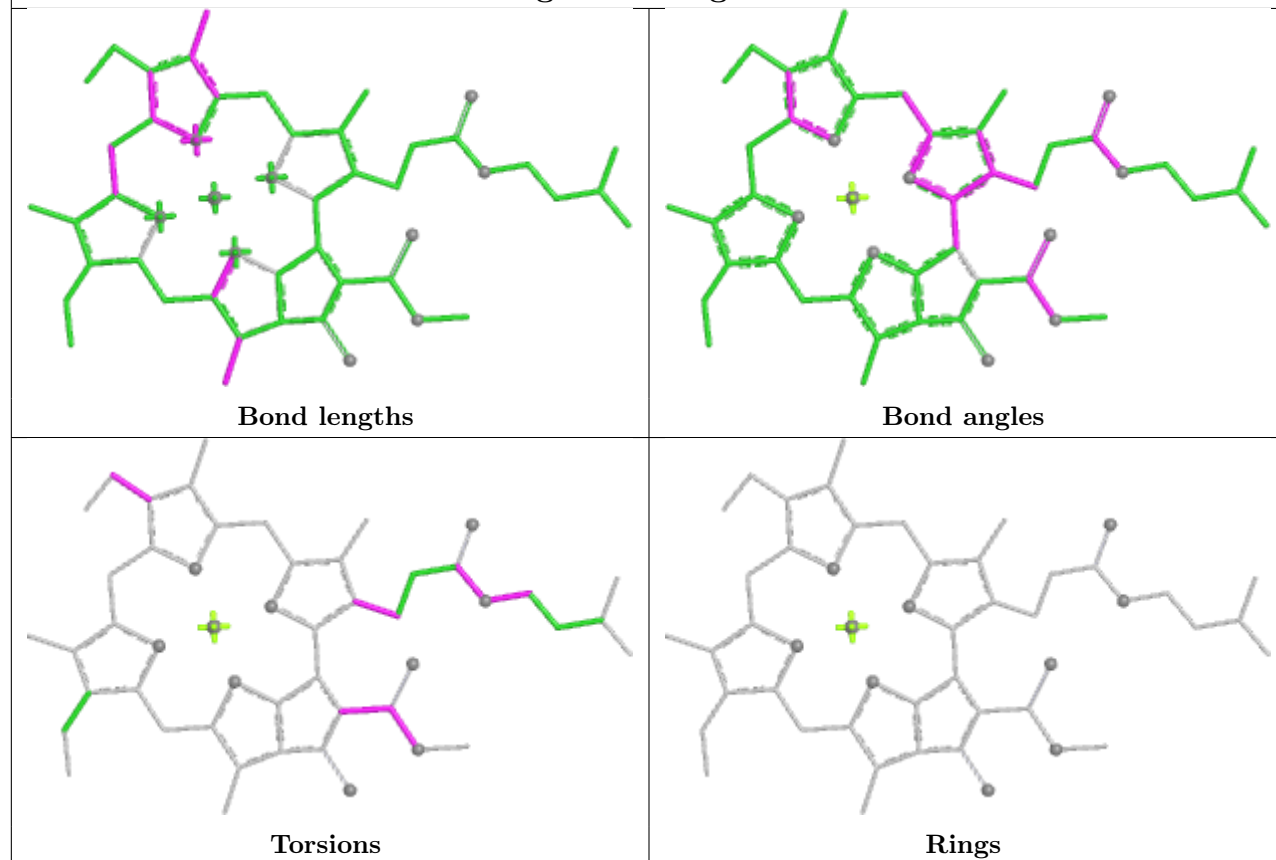


Ligand CLA u 503

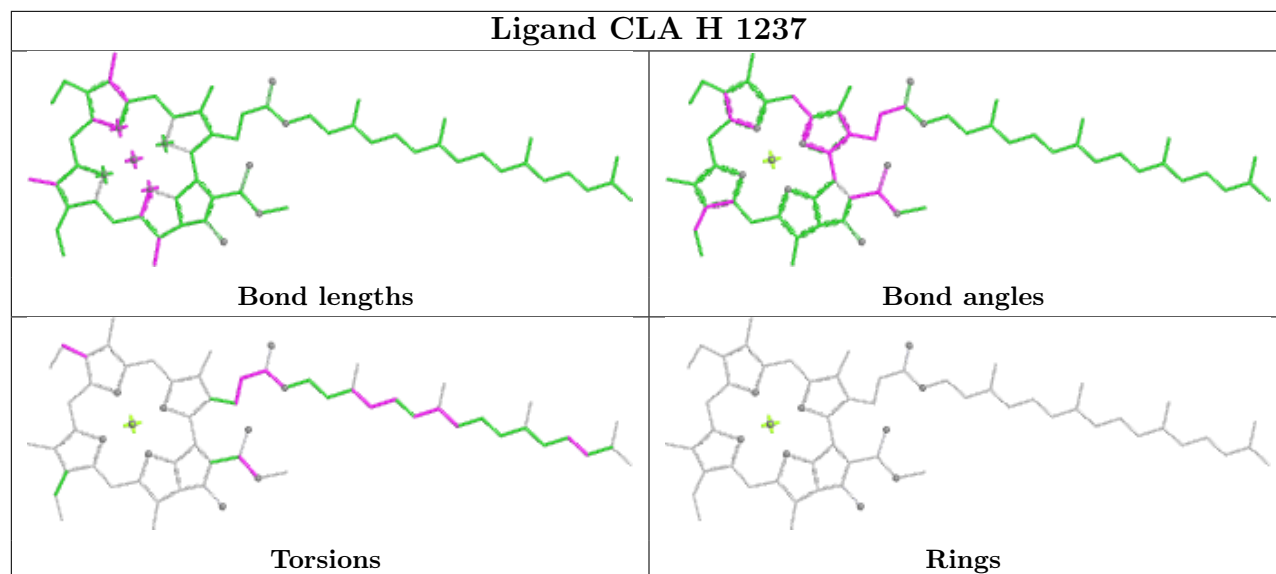


Ligand BCR S 4015

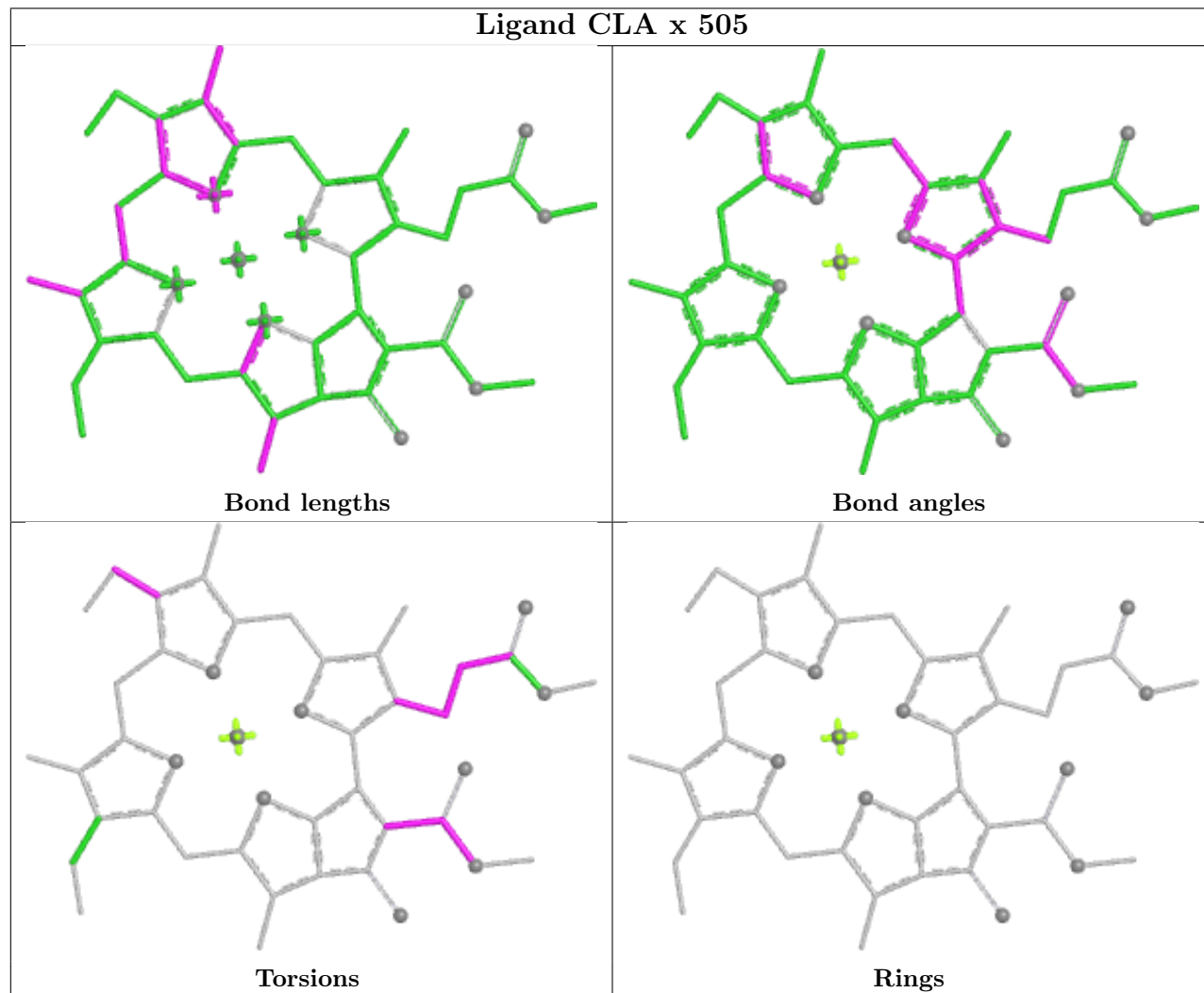


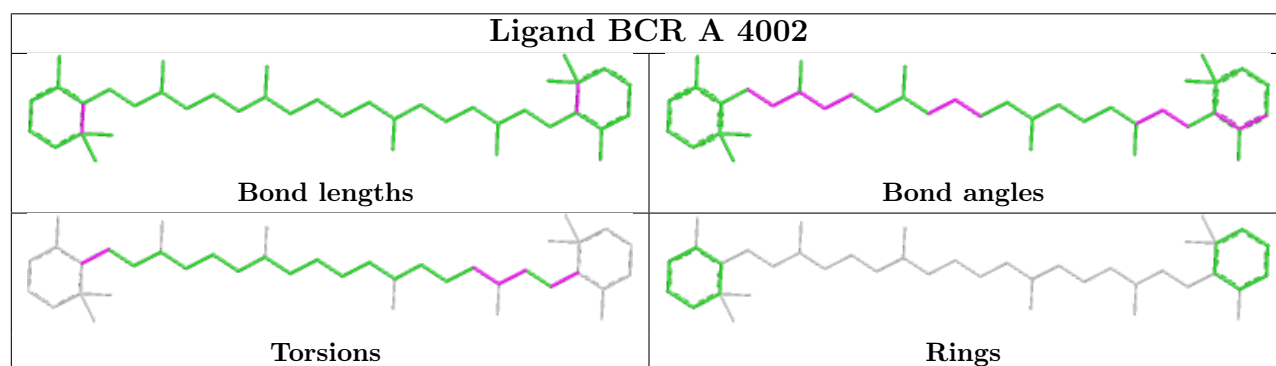
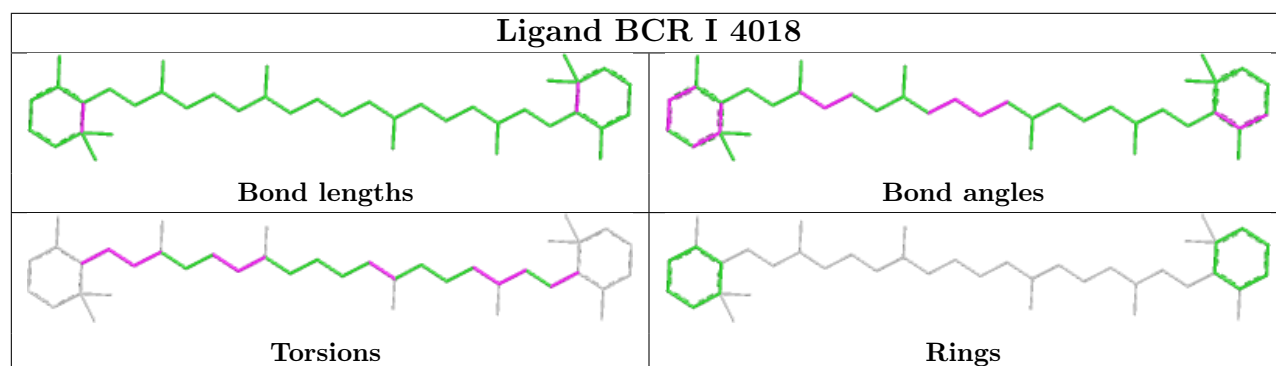
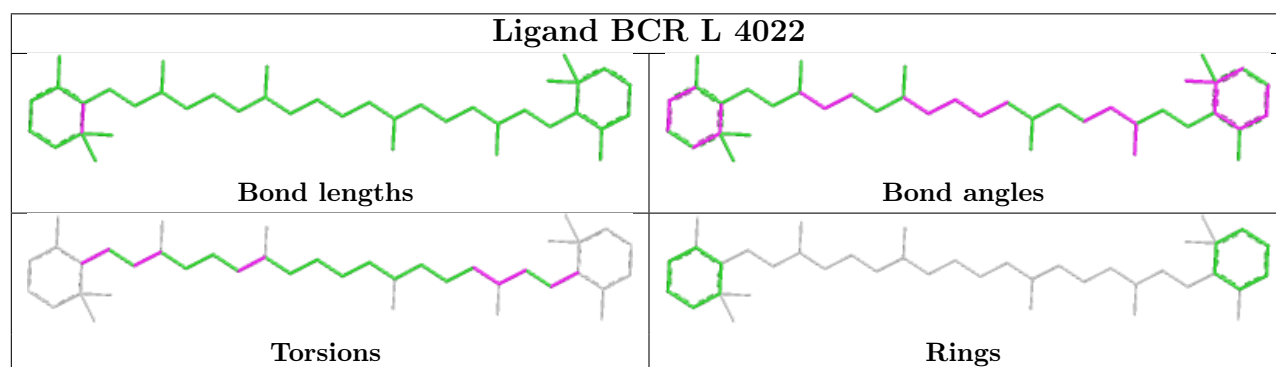
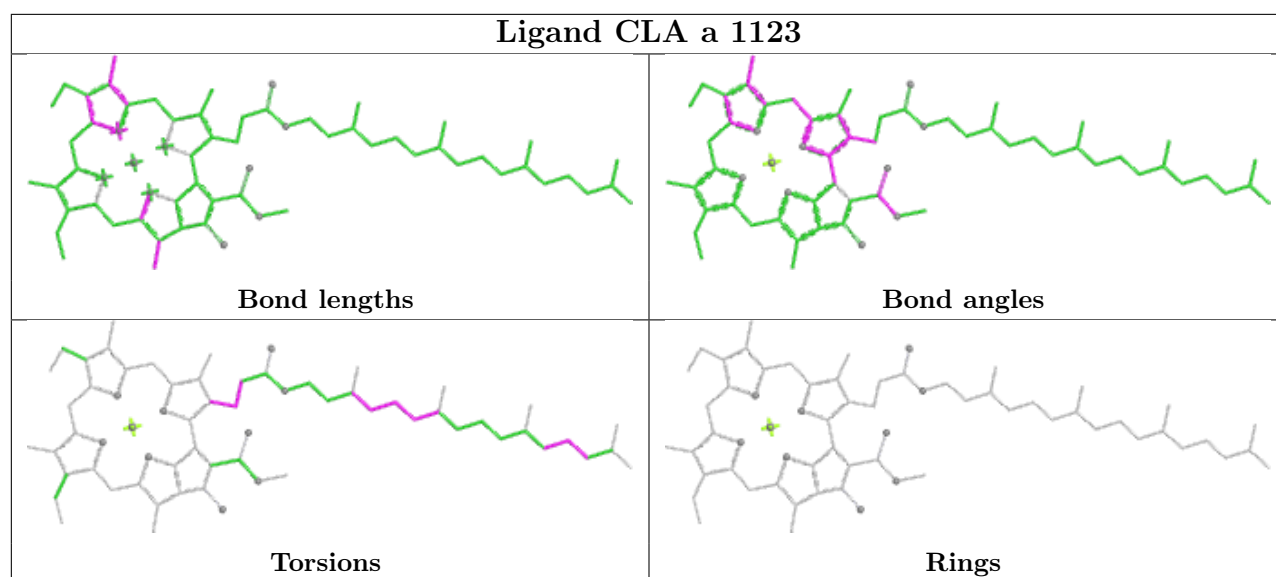
Ligand CLA A 1126**Ligand CLA g 501**

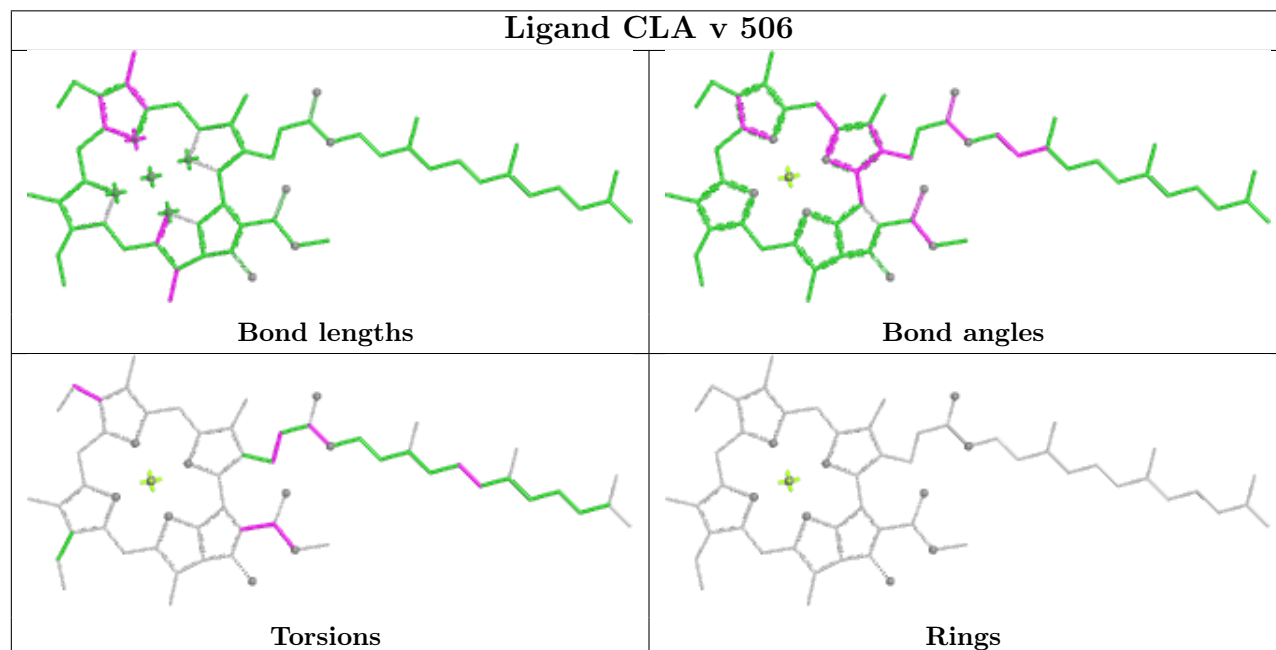
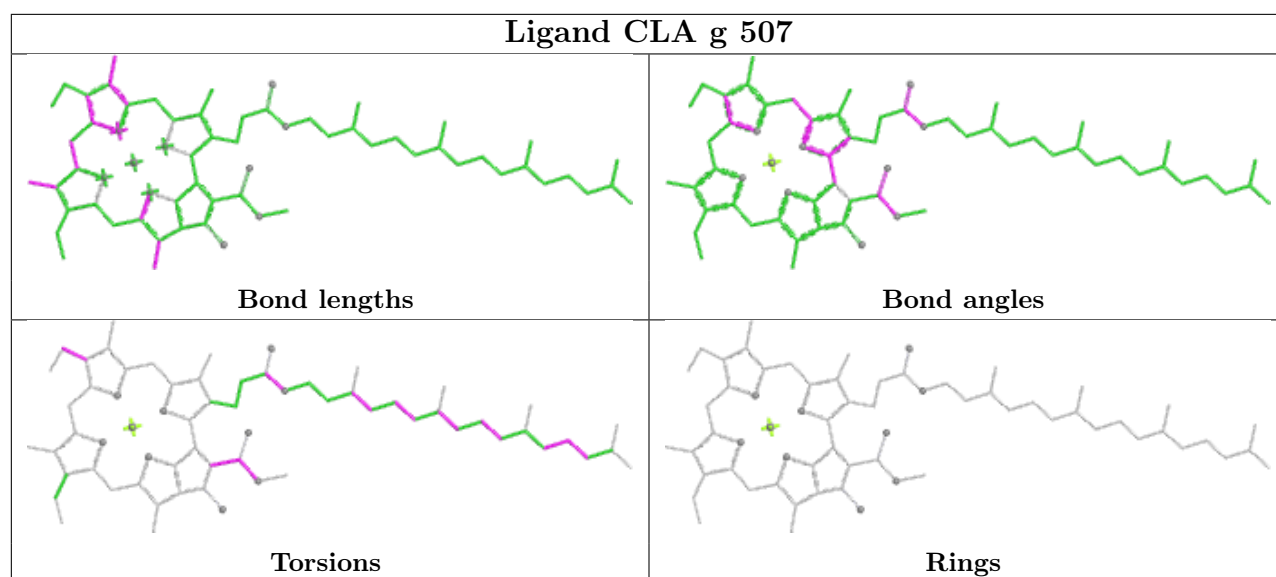
Ligand CLA H 1237



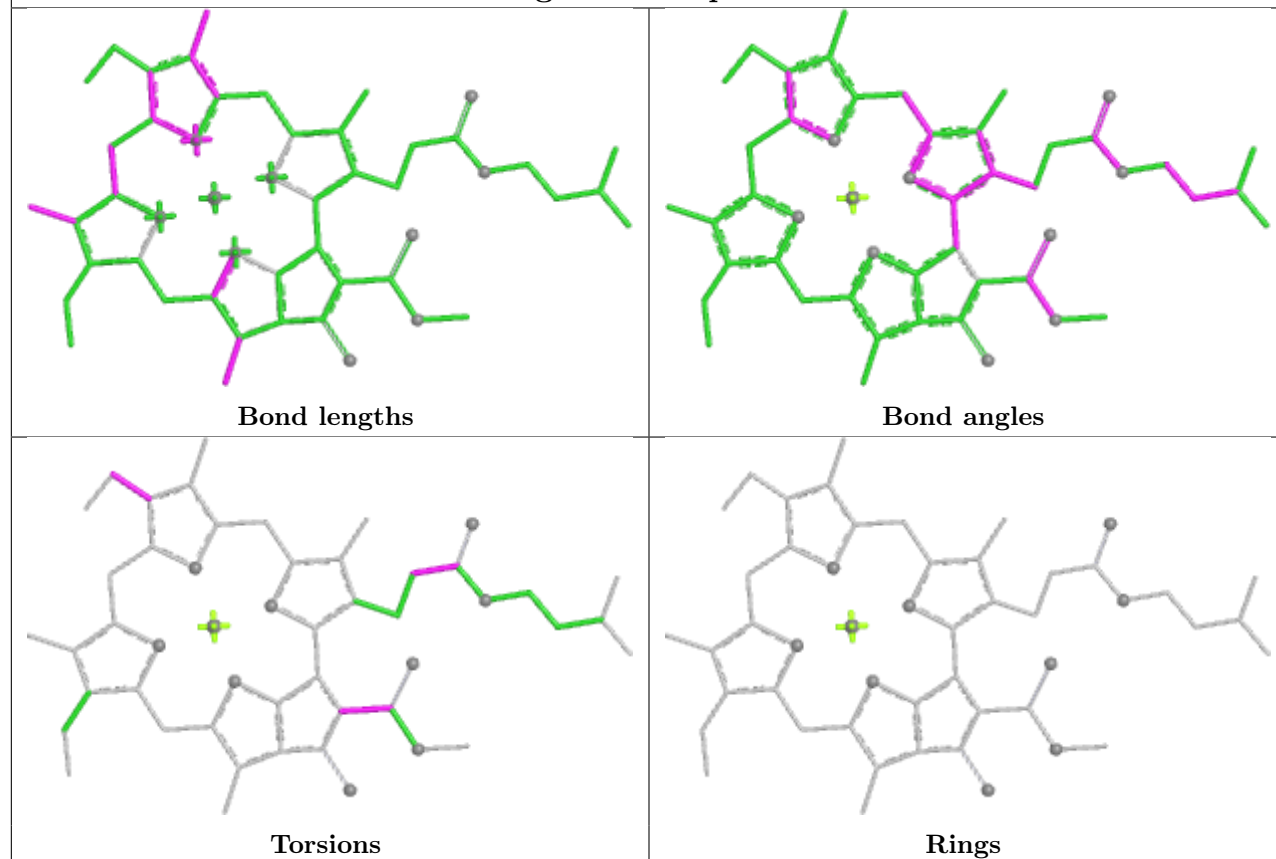
Ligand CLA x 505



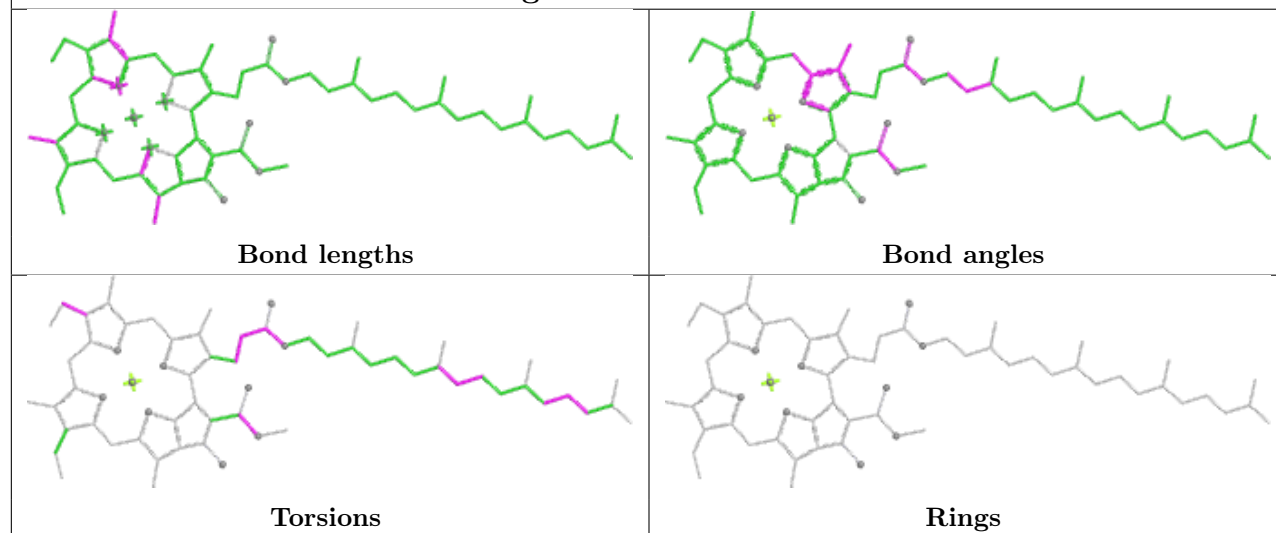


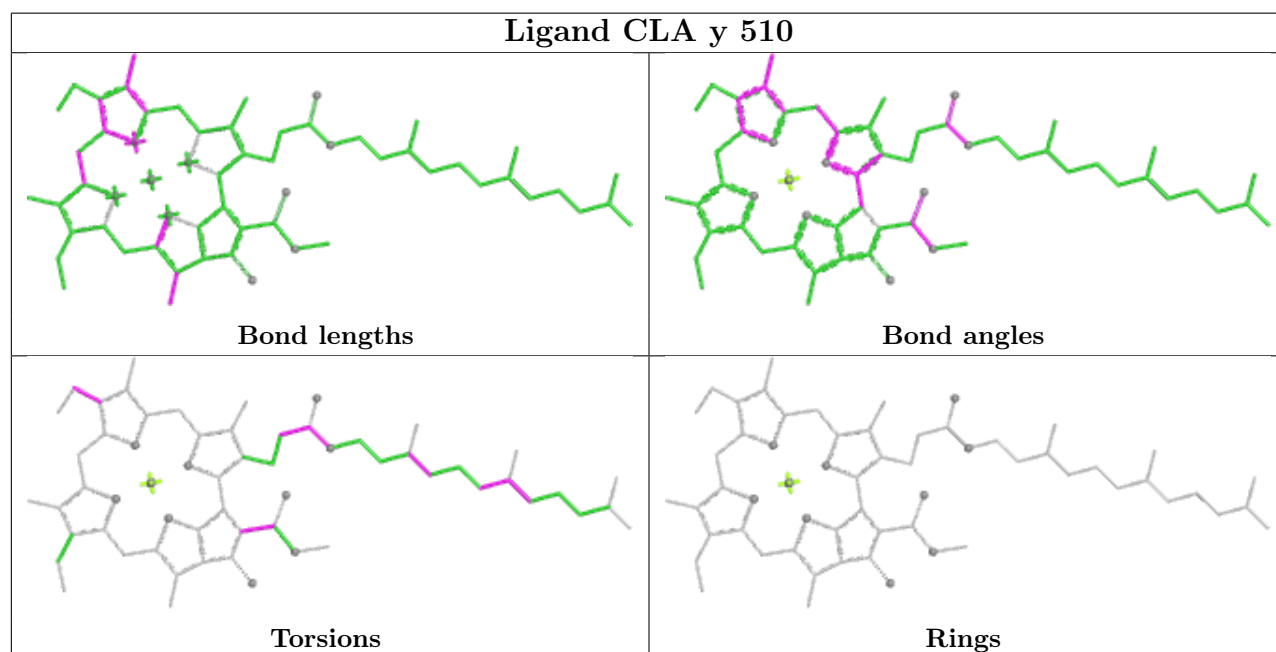
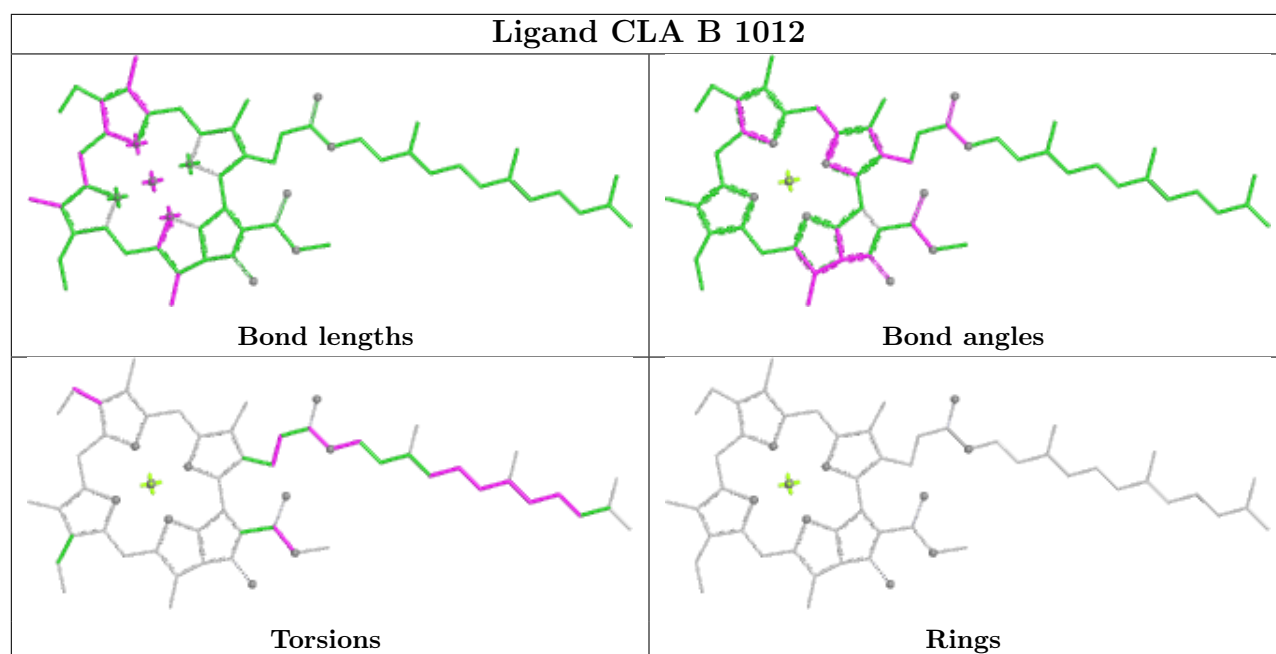


Ligand CLA p 514

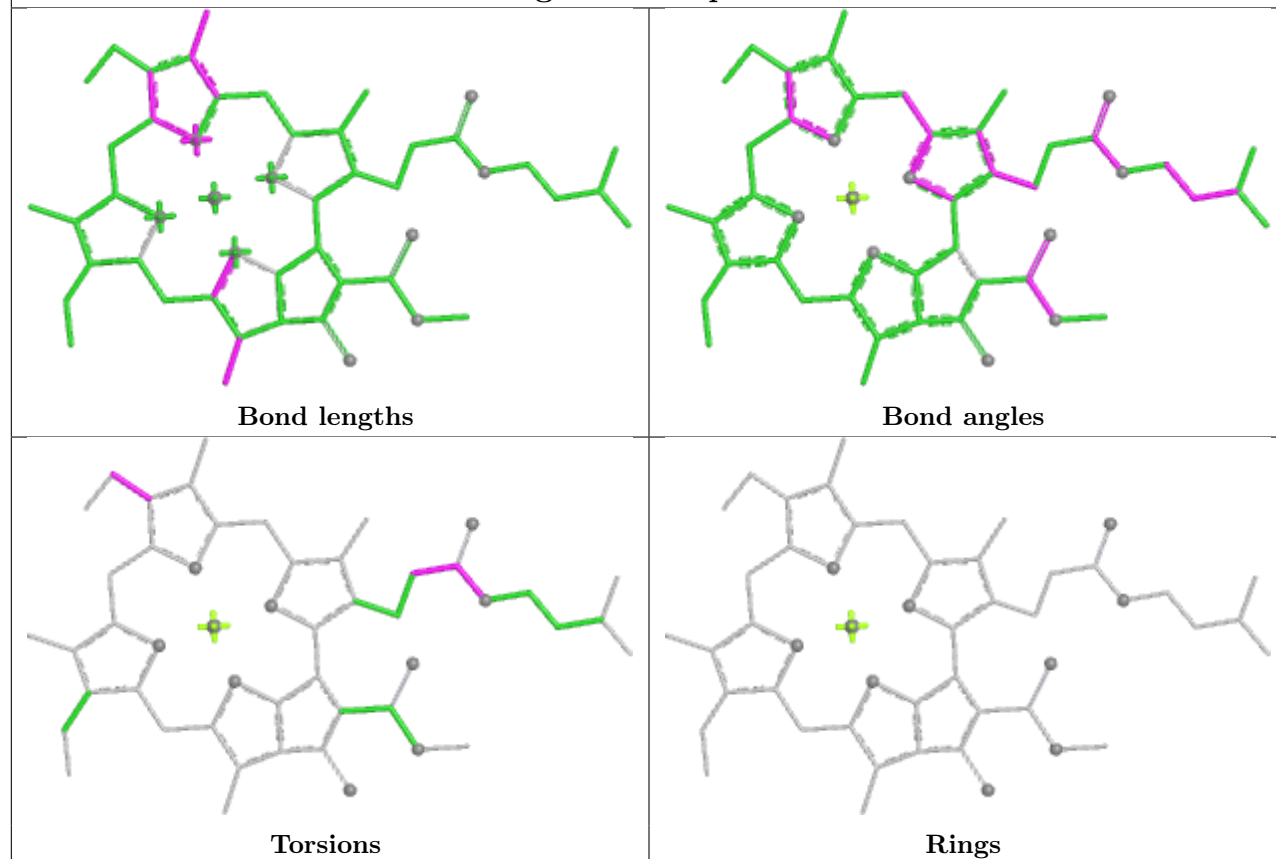


Ligand CLA G 1021

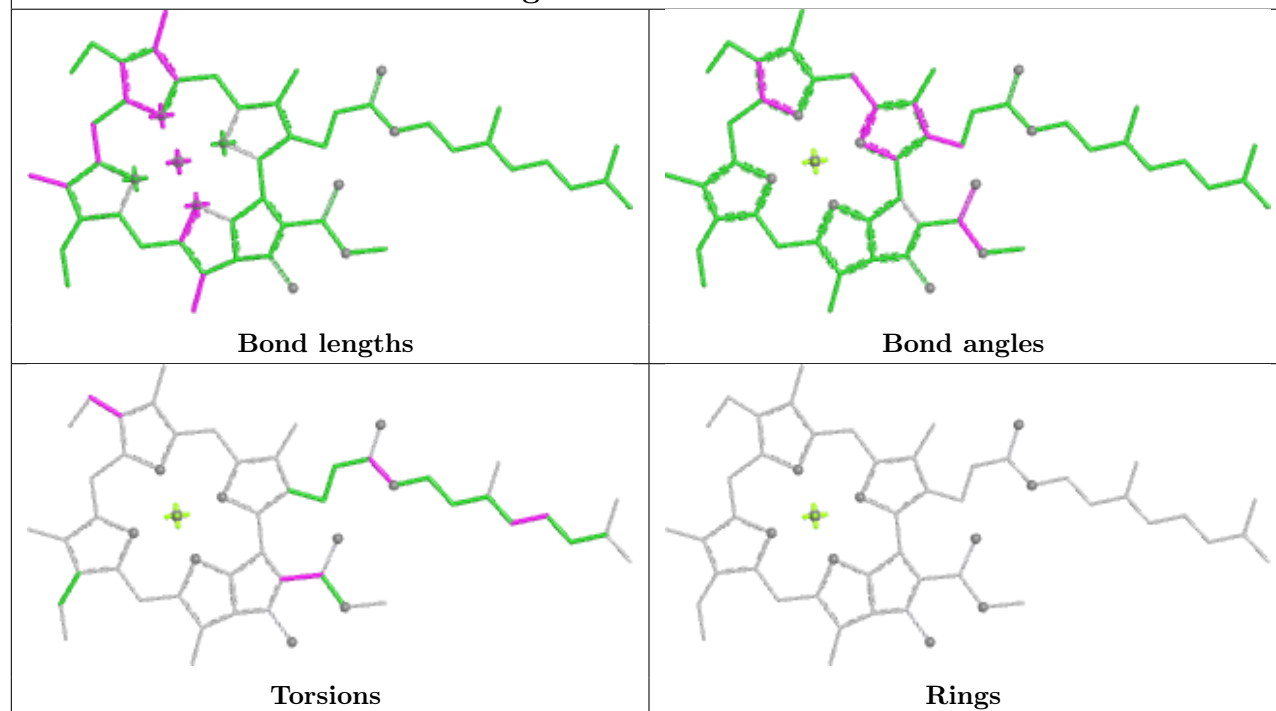


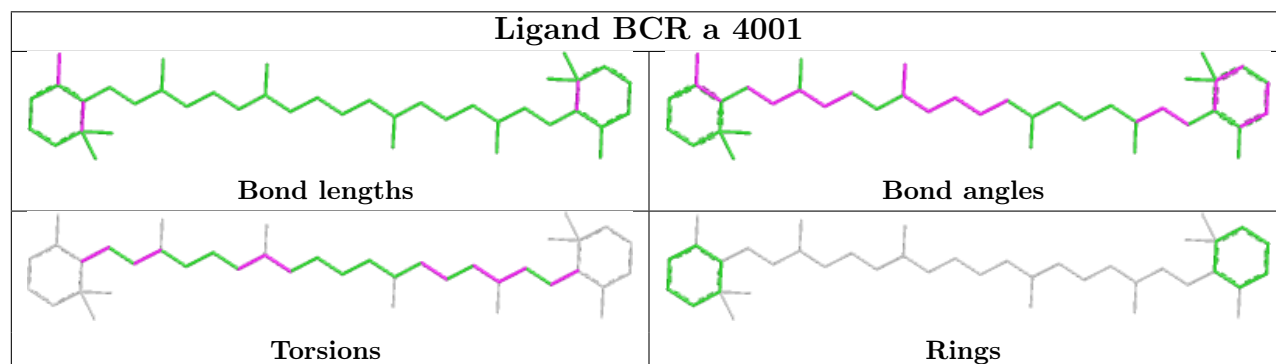
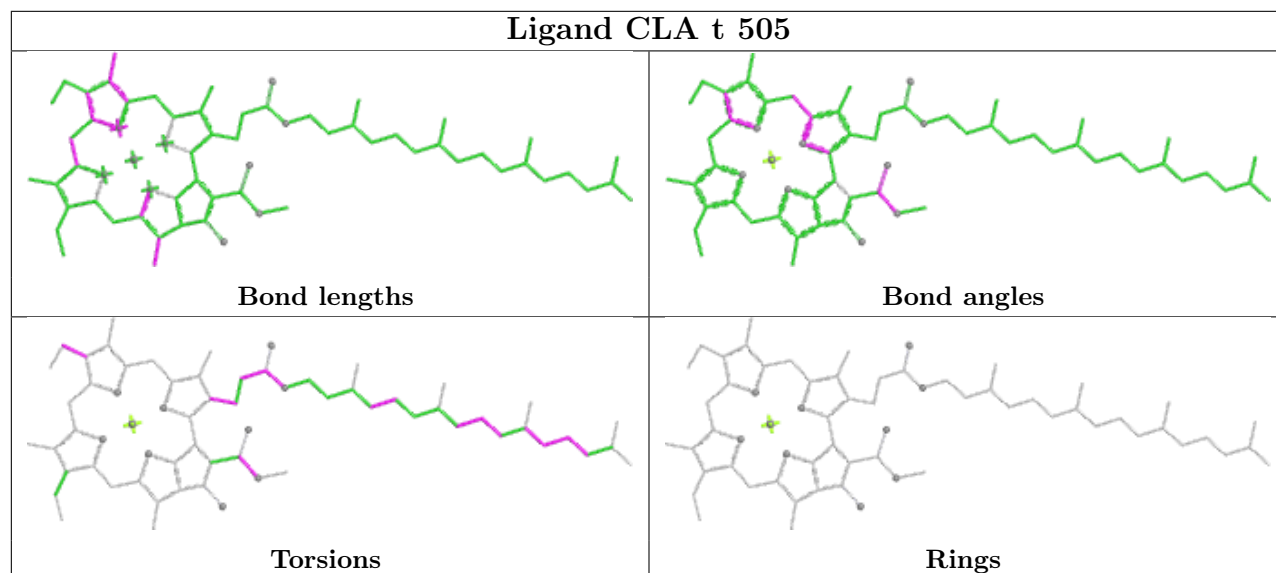
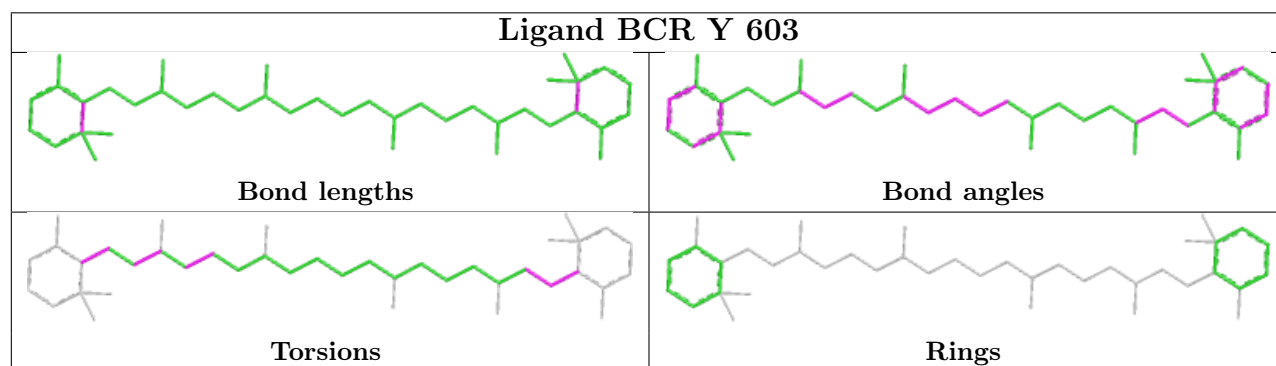
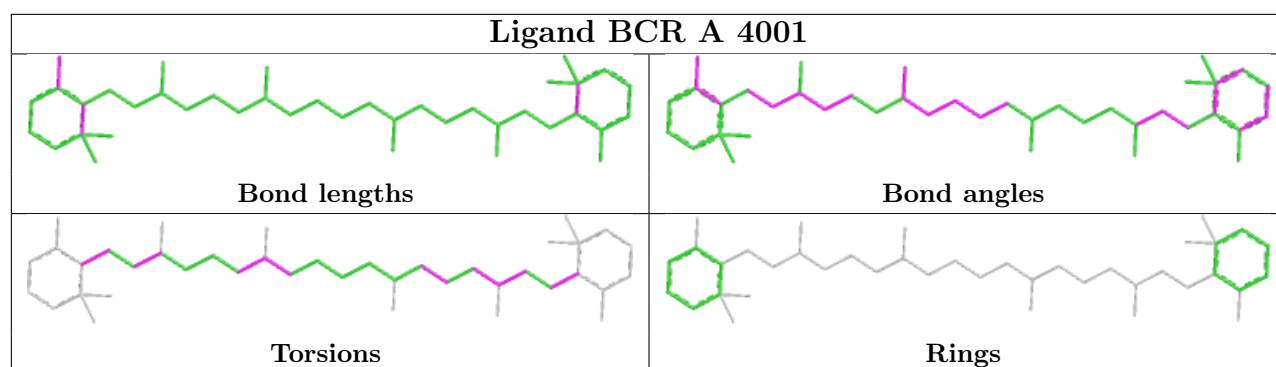


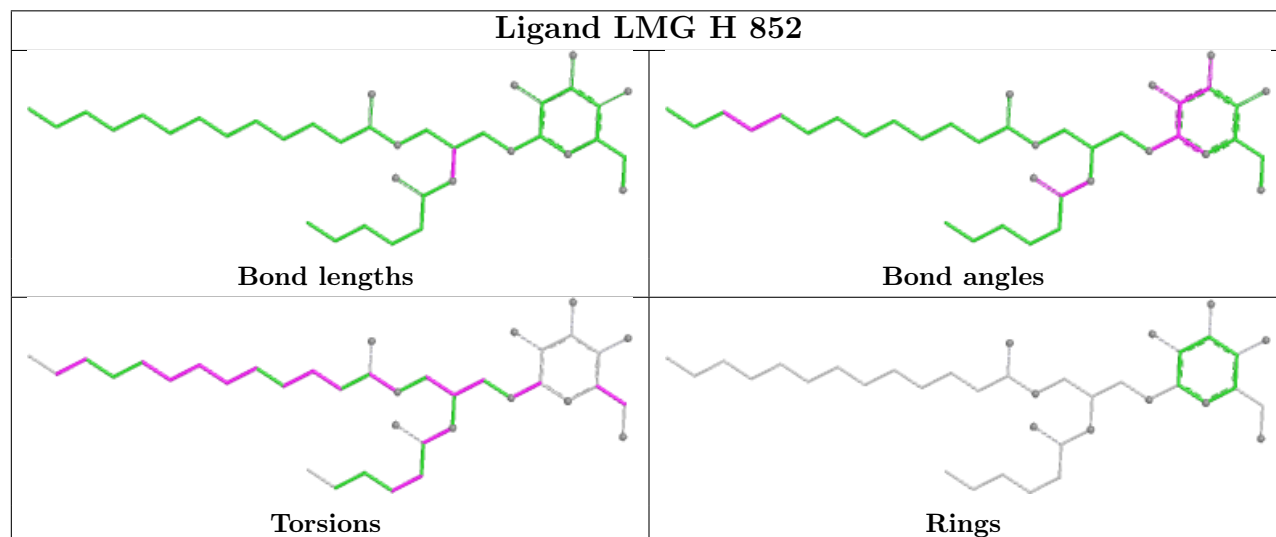
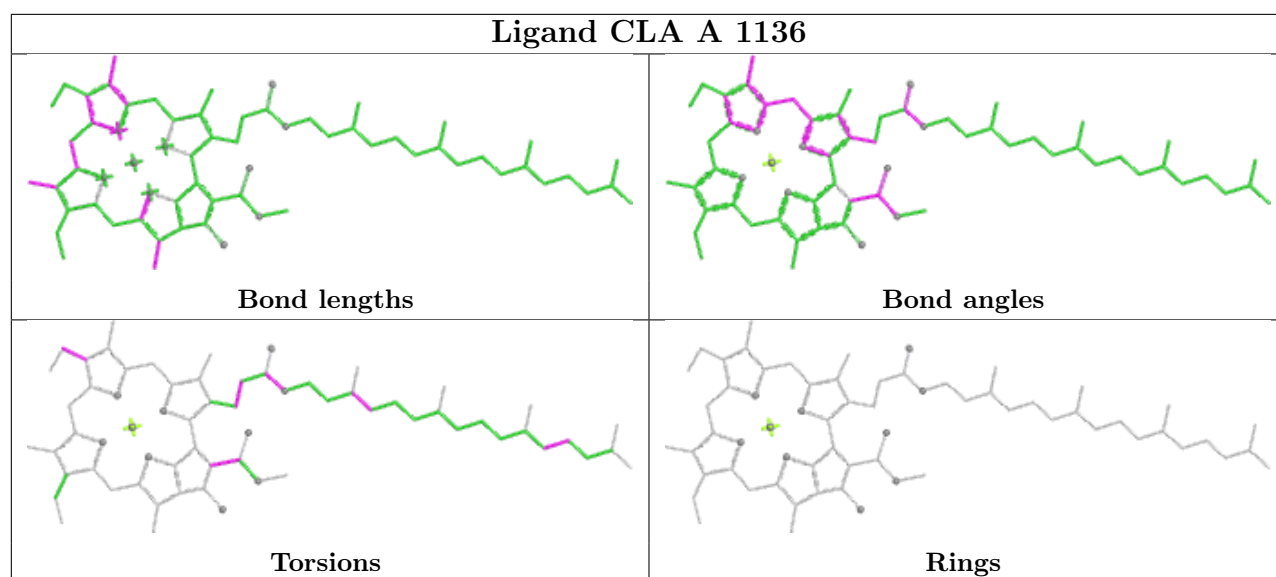
Ligand CLA p 502



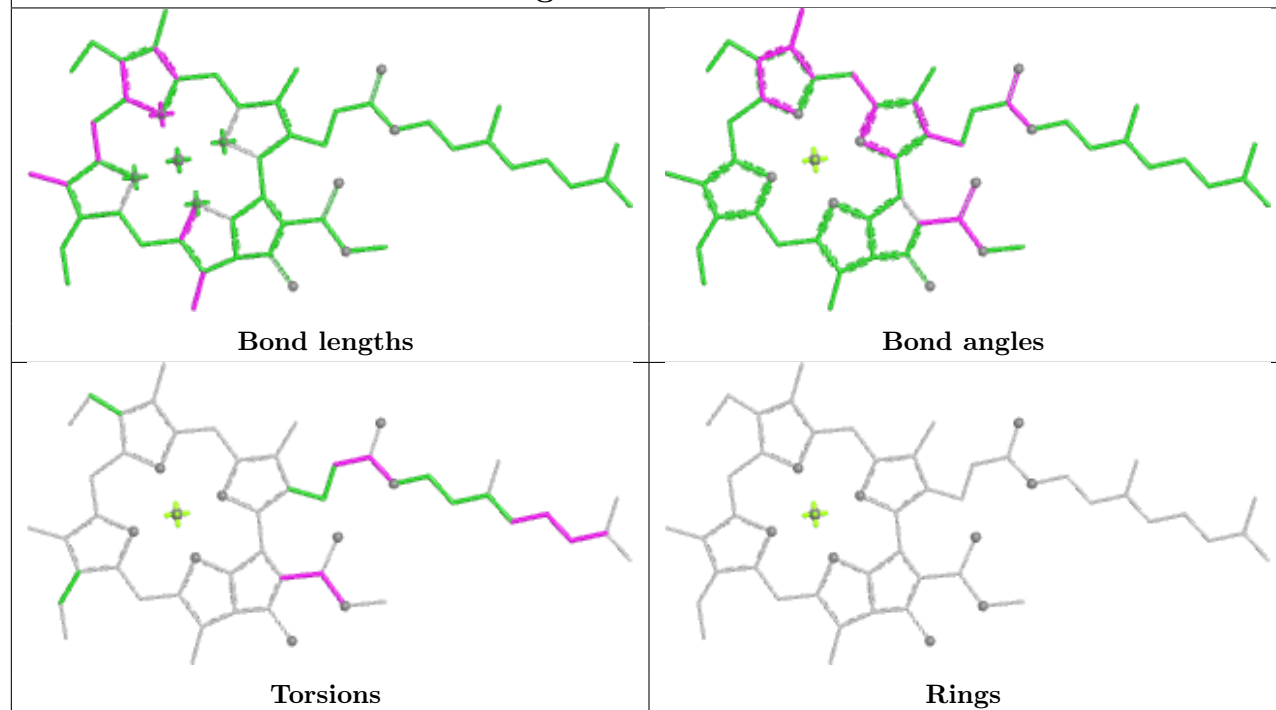
Ligand CLA H 1118



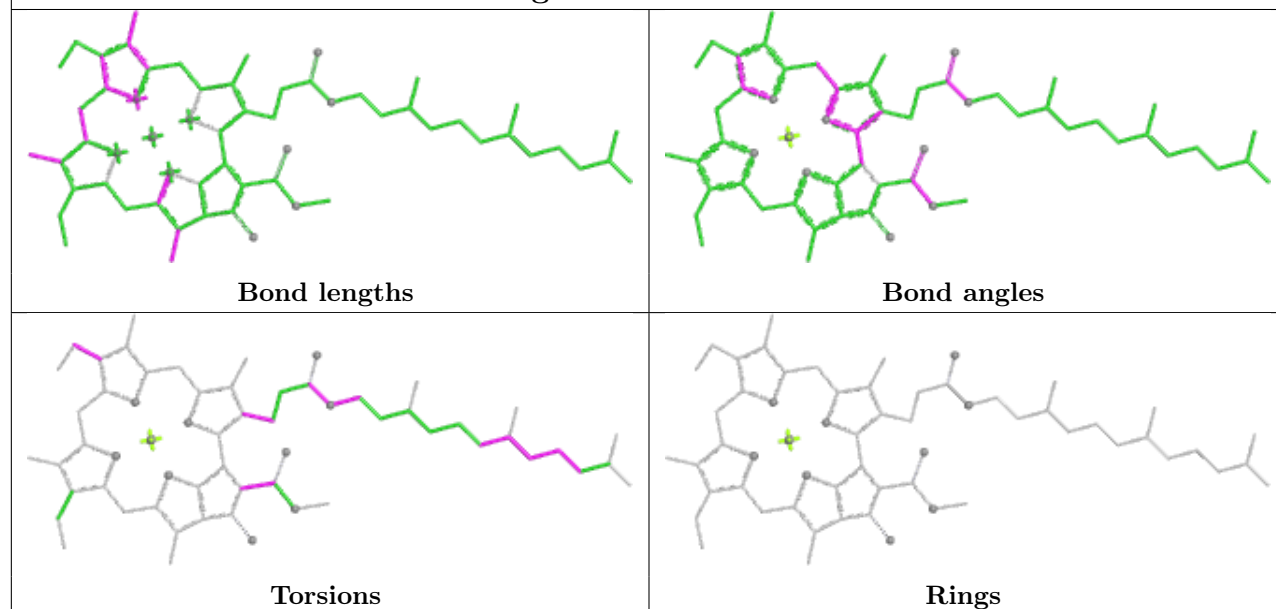


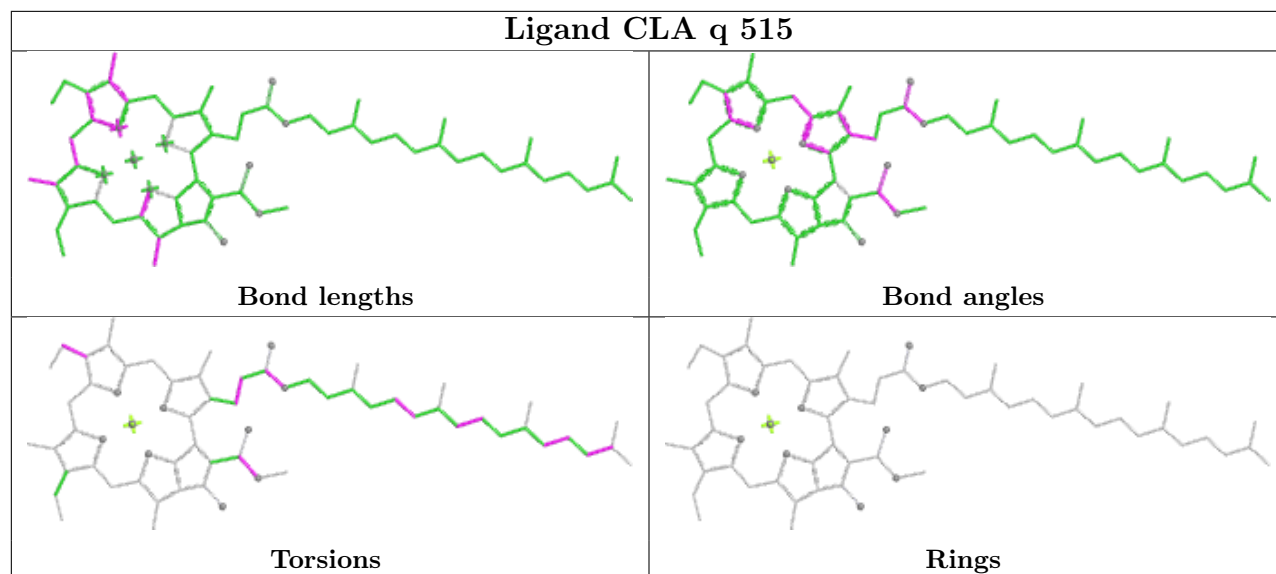
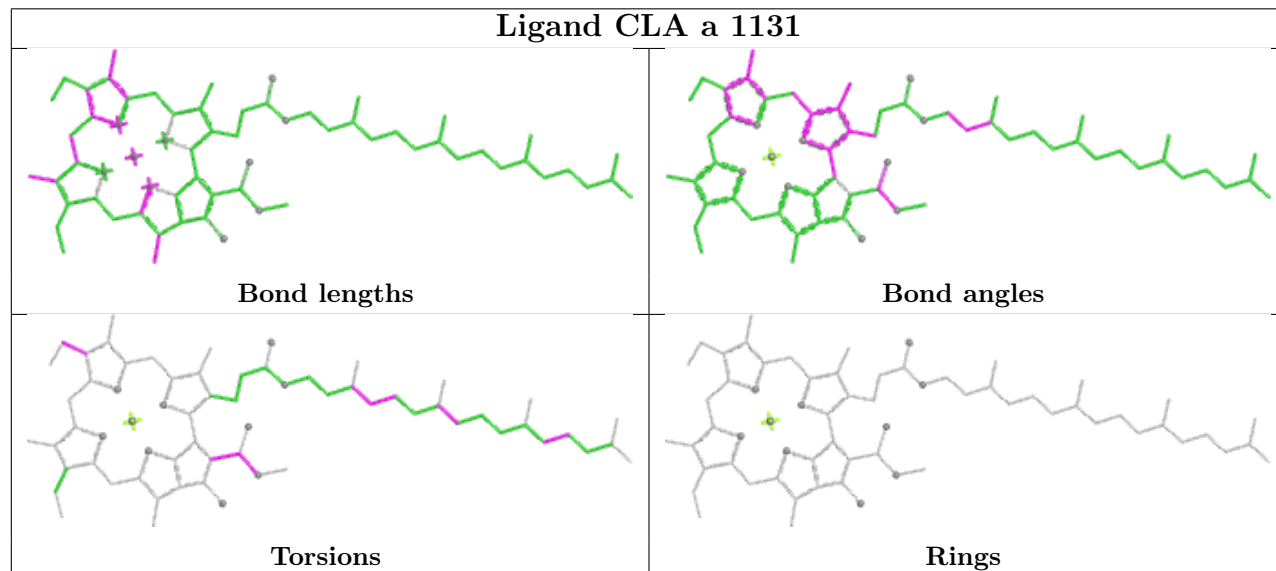


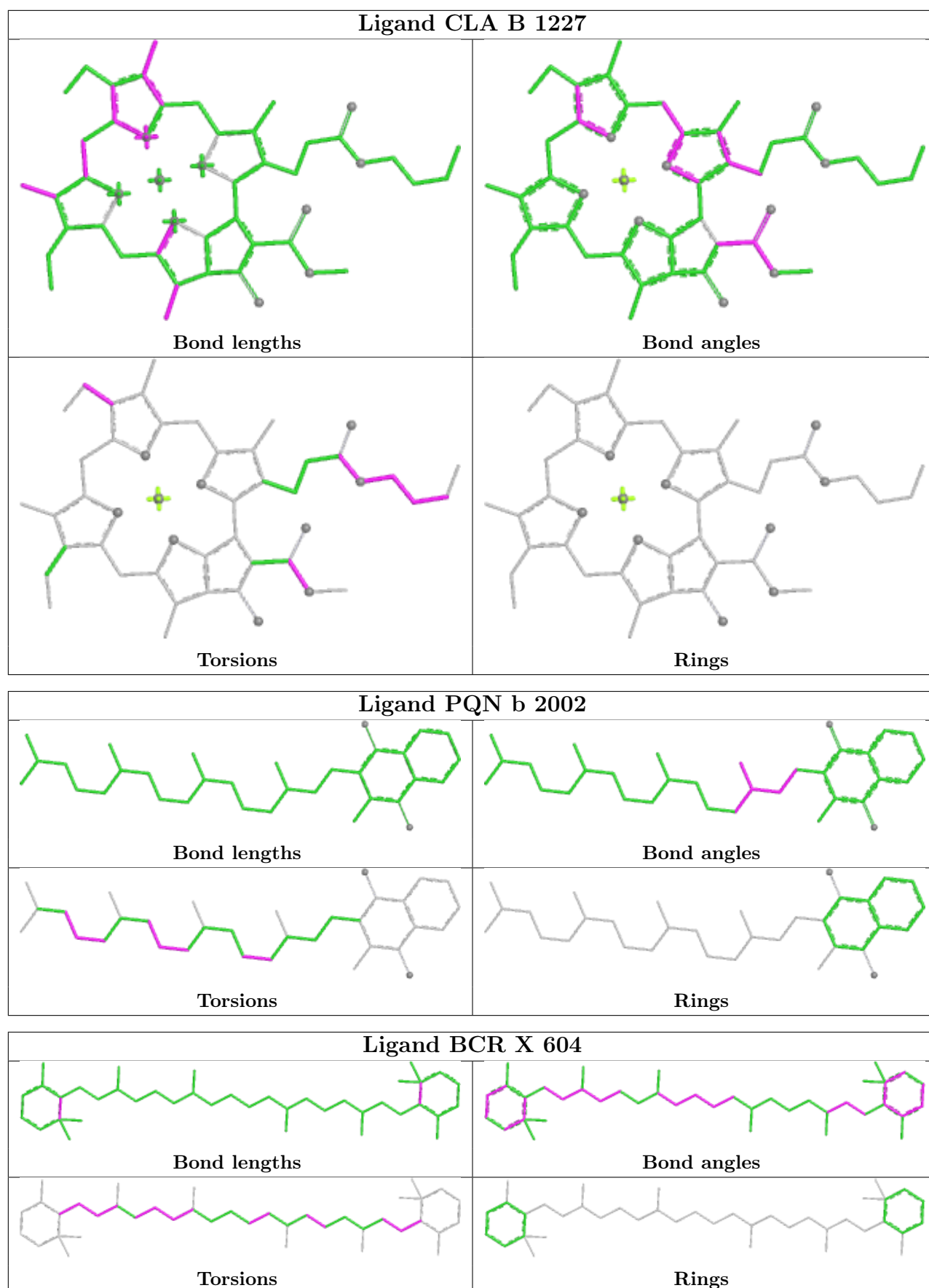
Ligand CLA o 517

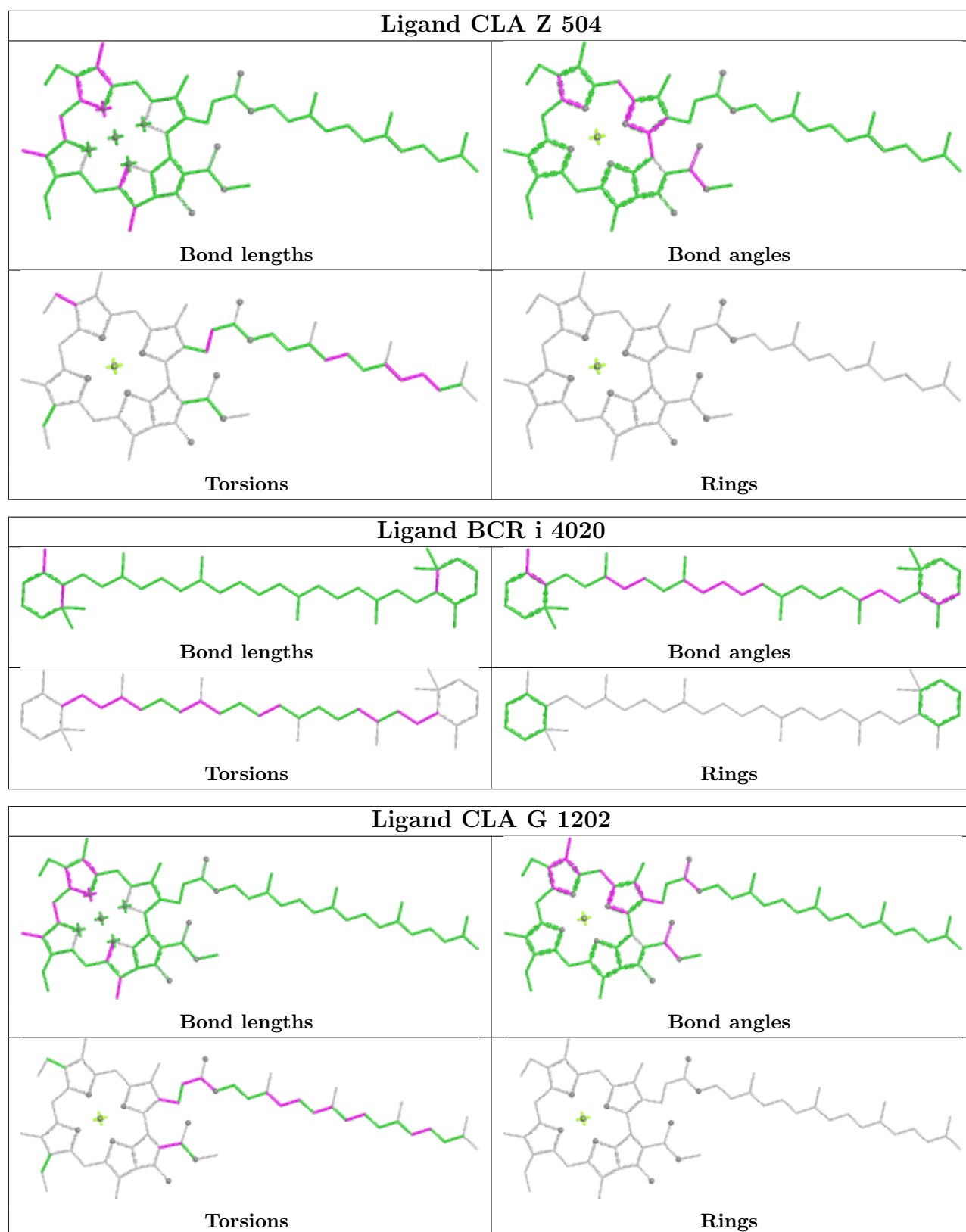


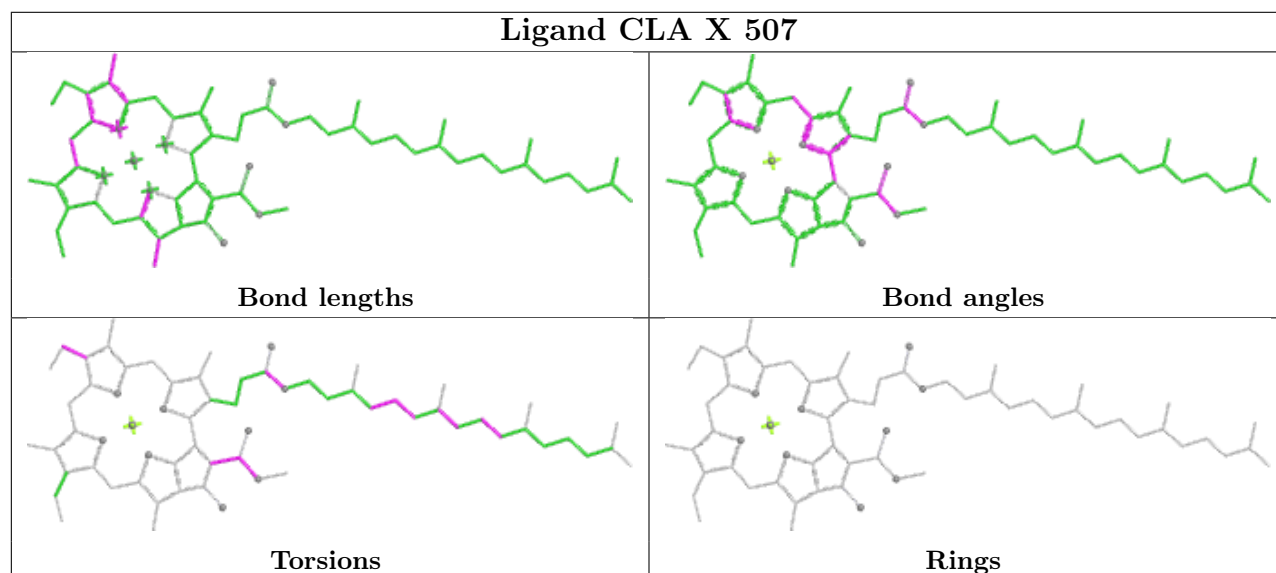
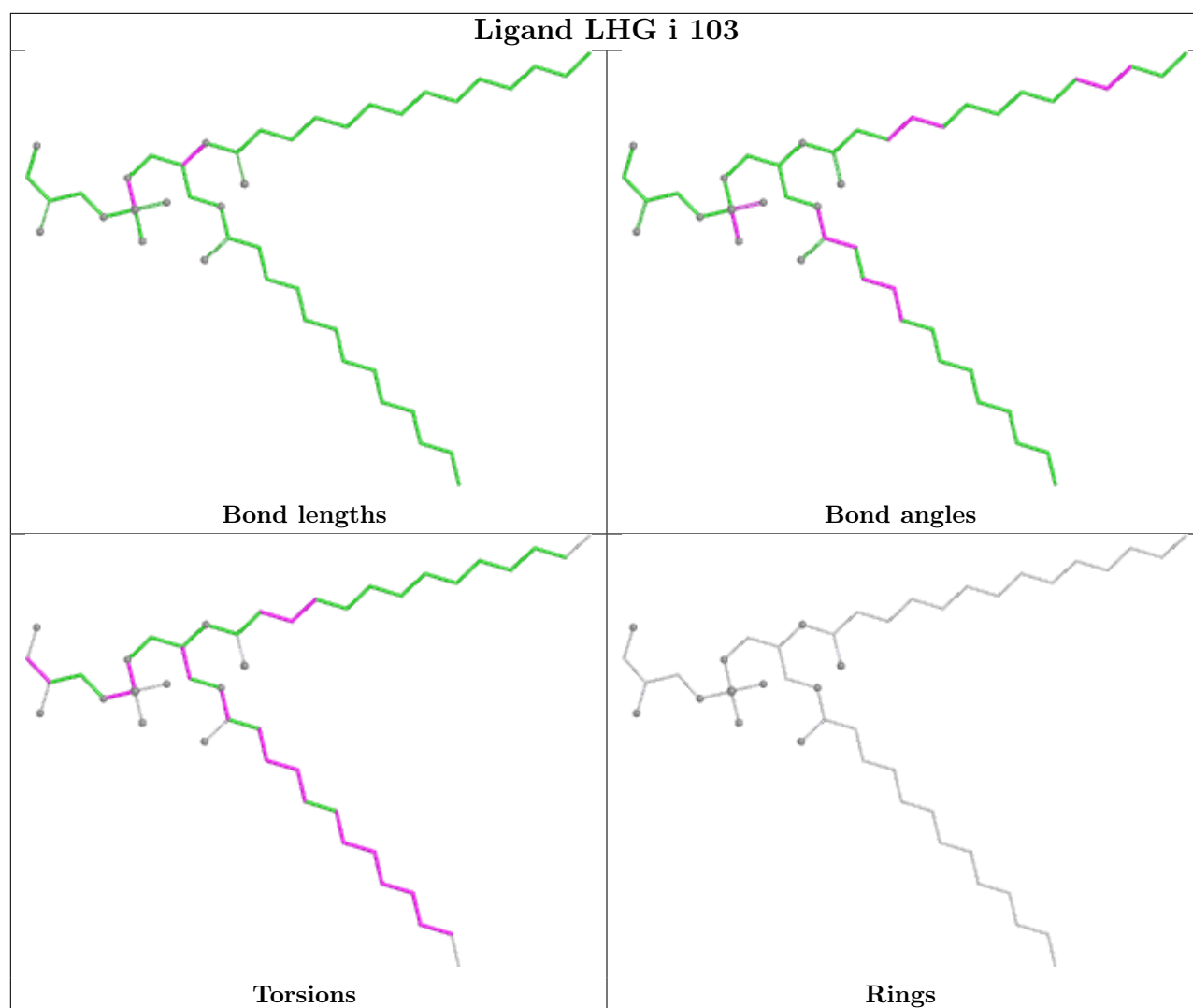
Ligand CLA Y 504

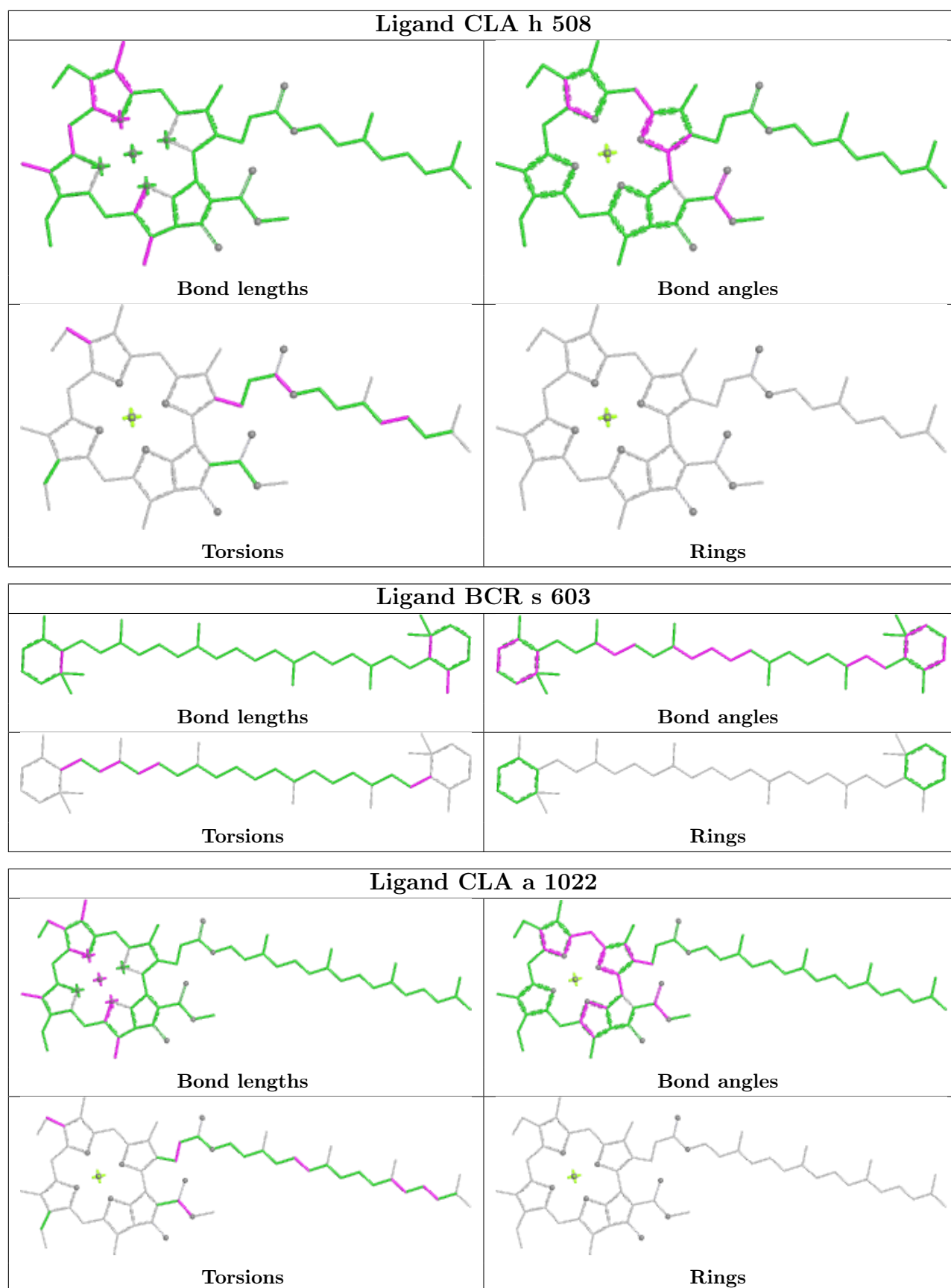


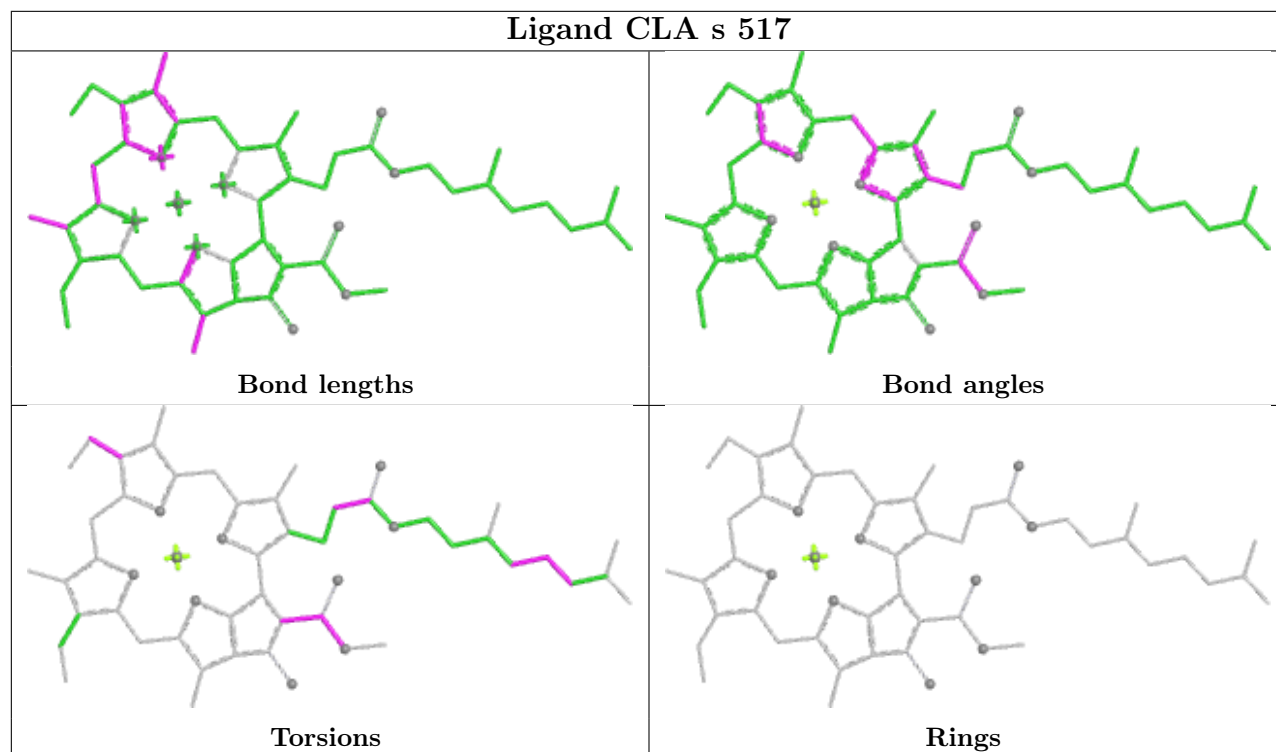
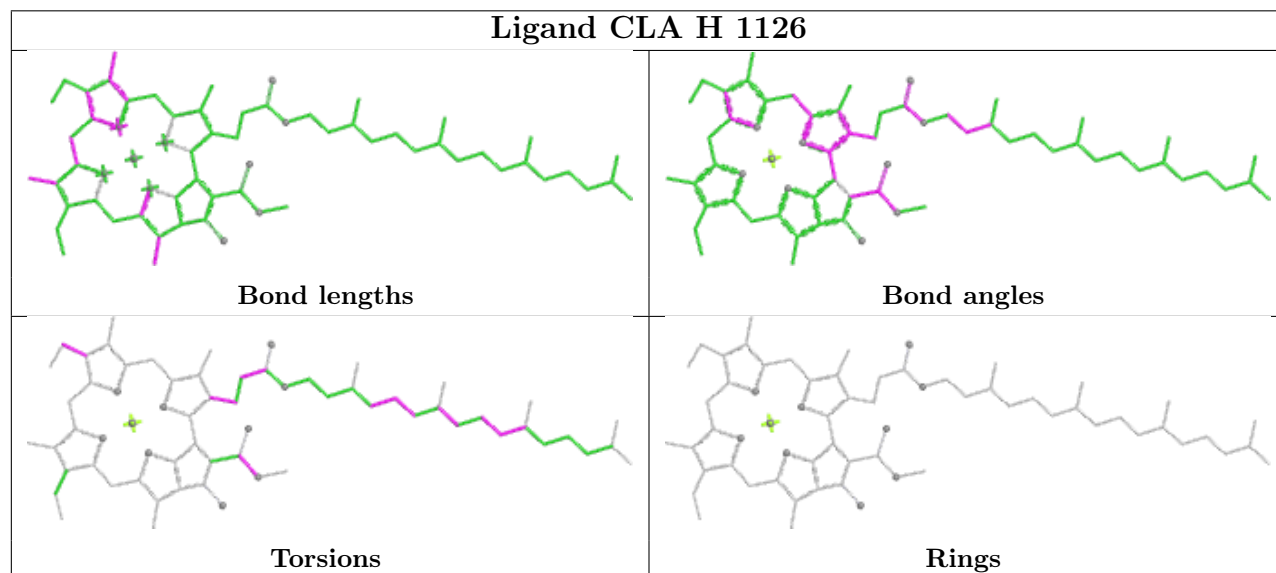
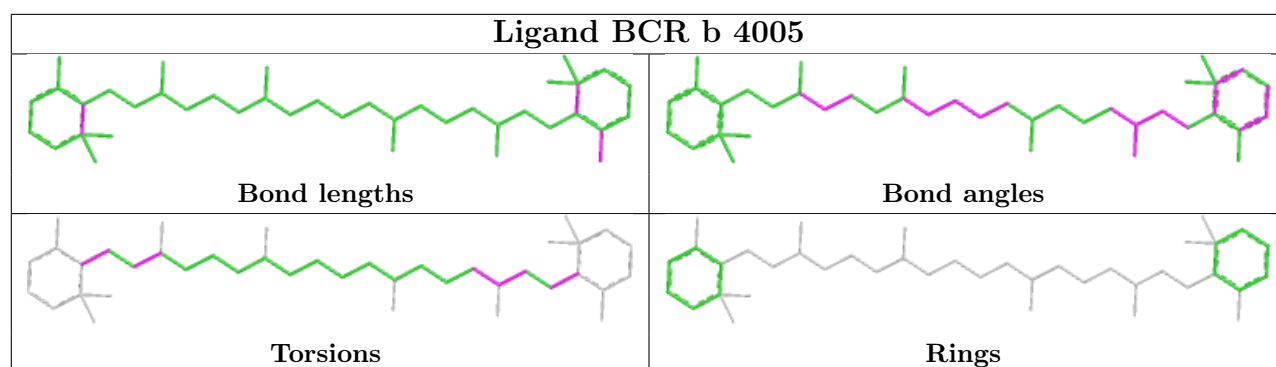
Ligand CLA q 515**Ligand CLA a 1131**

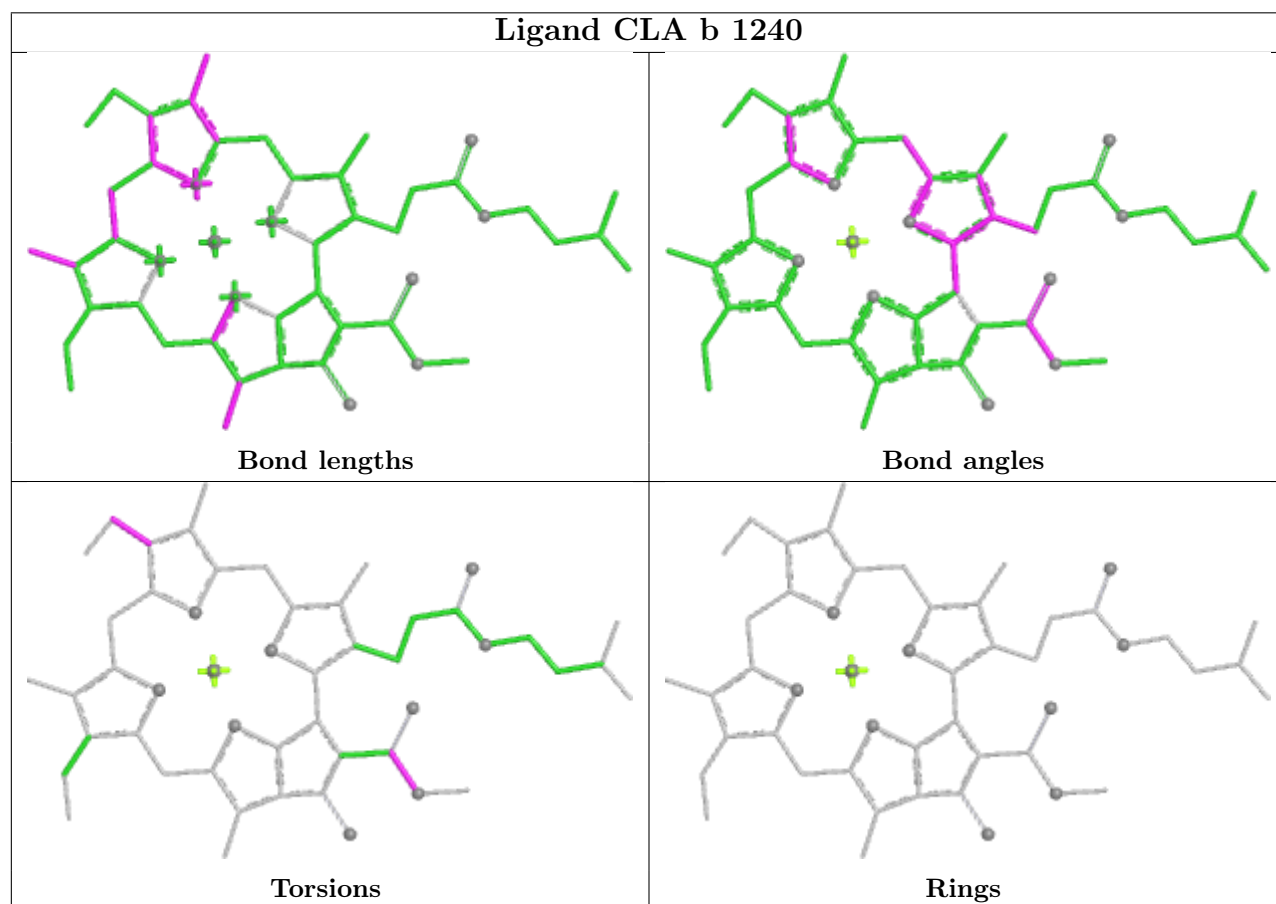
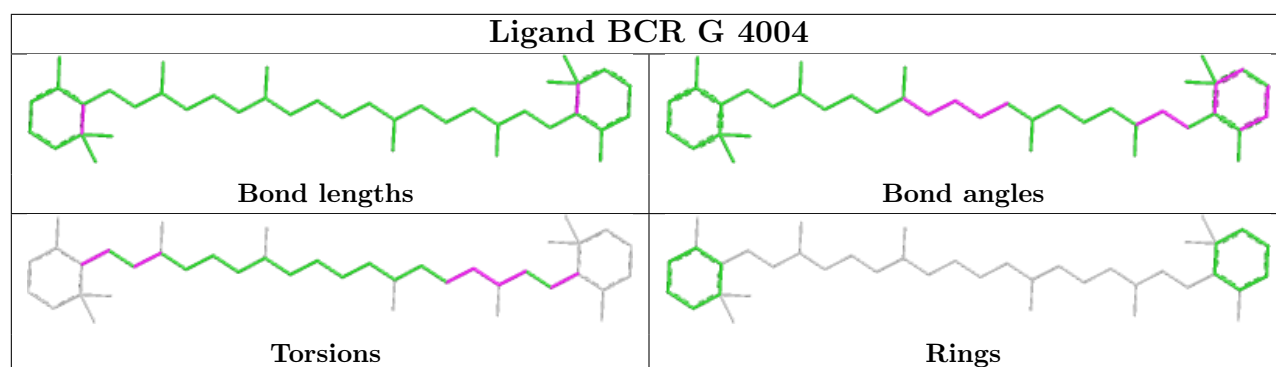




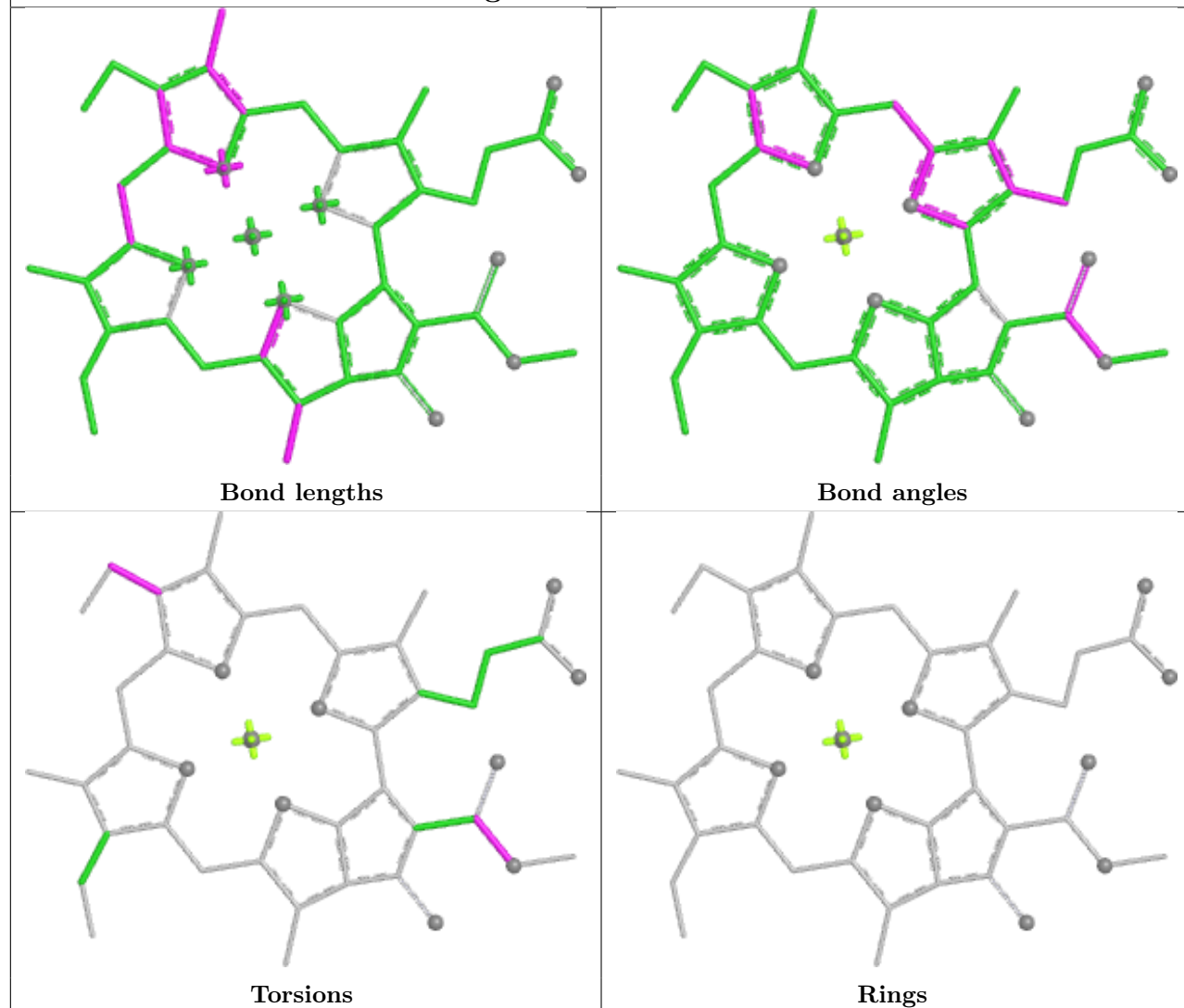




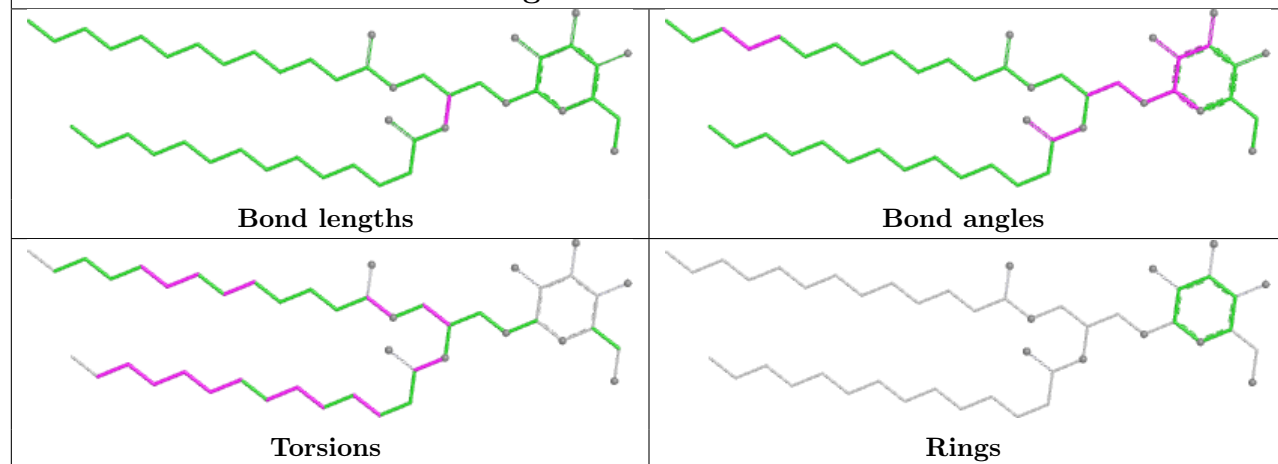


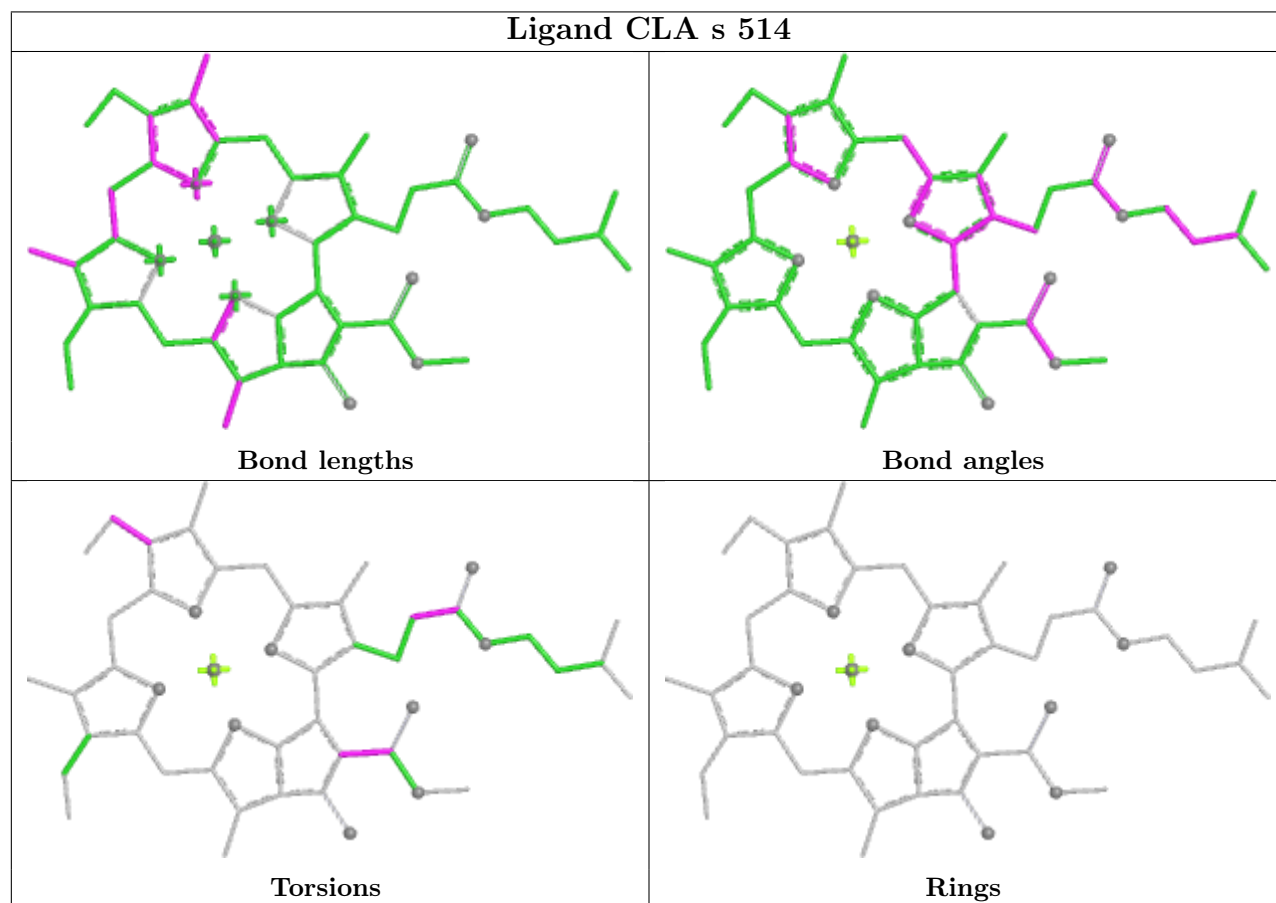
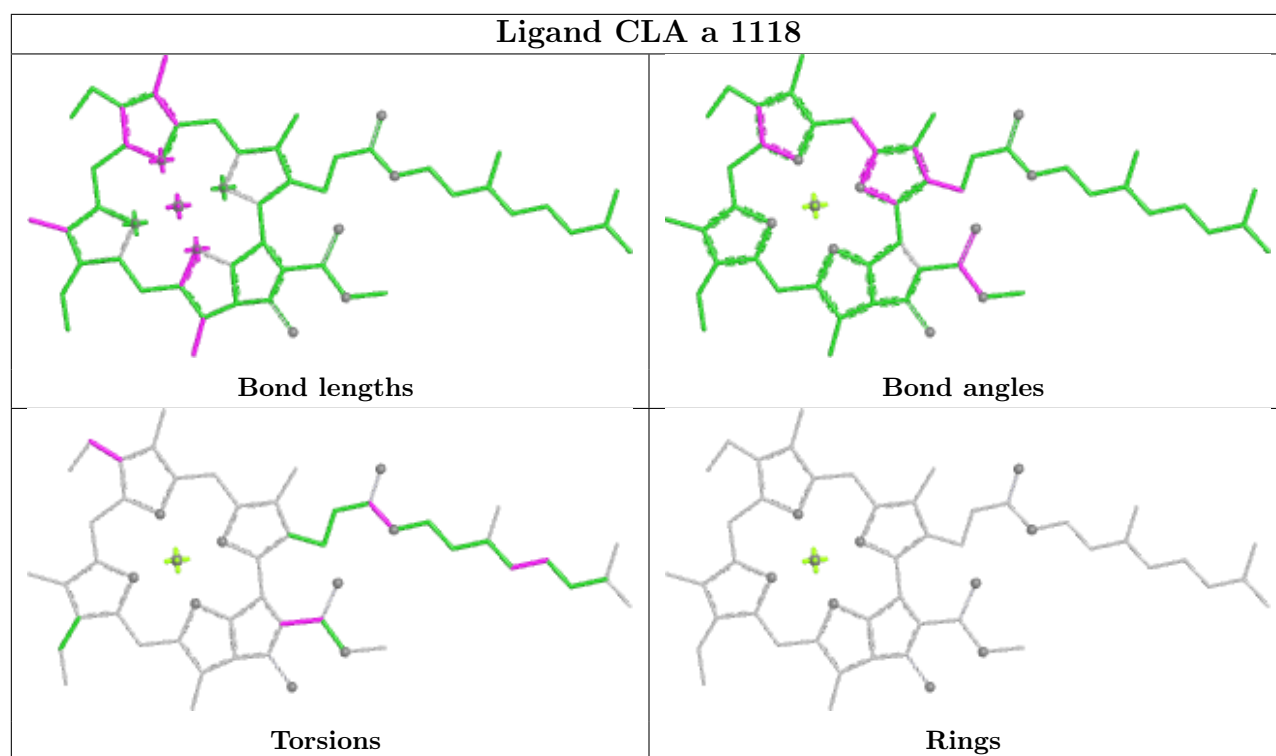


Ligand CLA B 1208

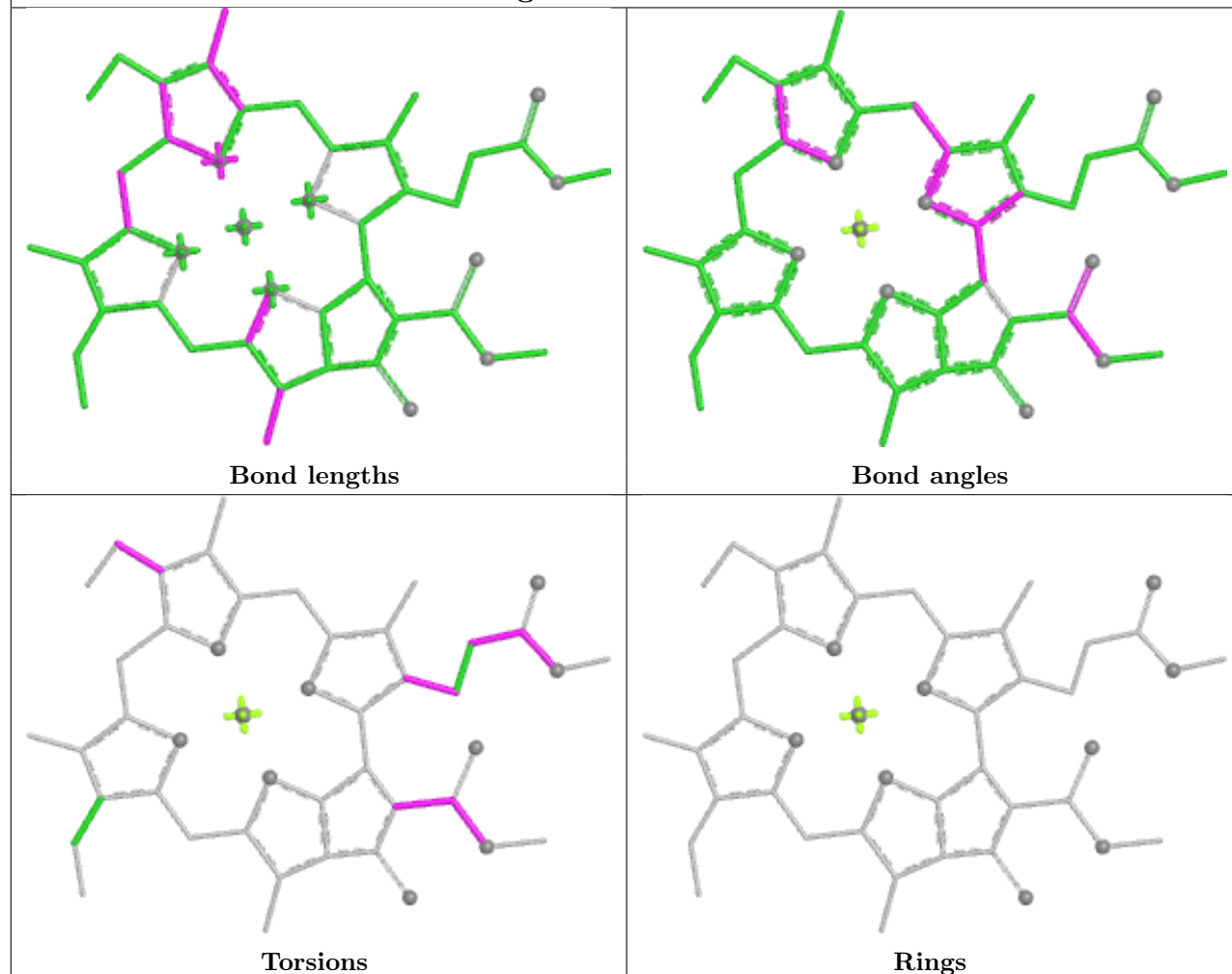


Ligand LMG a 4101

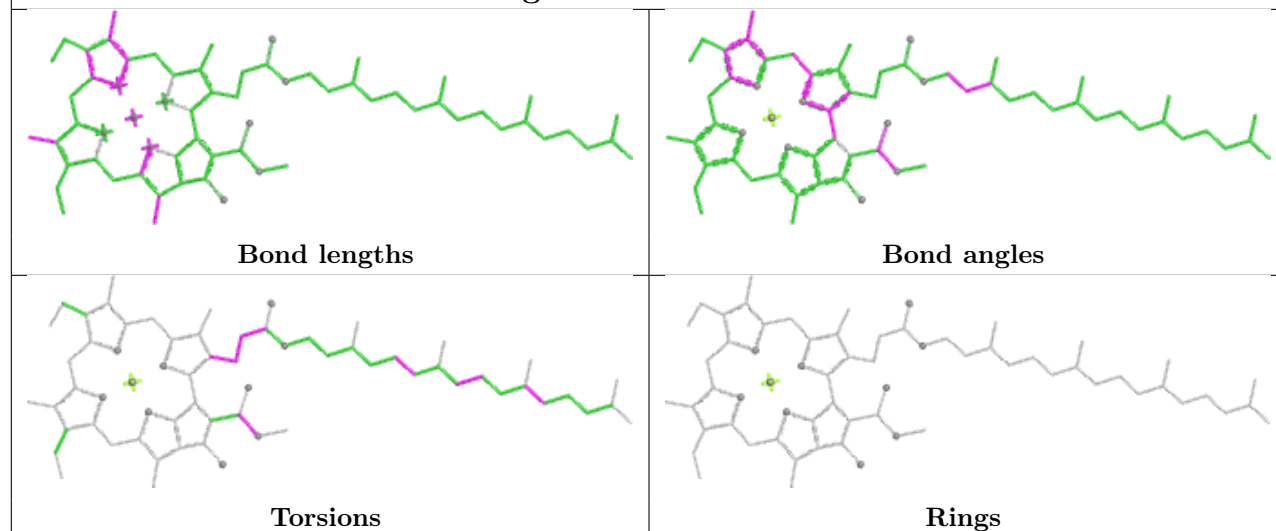


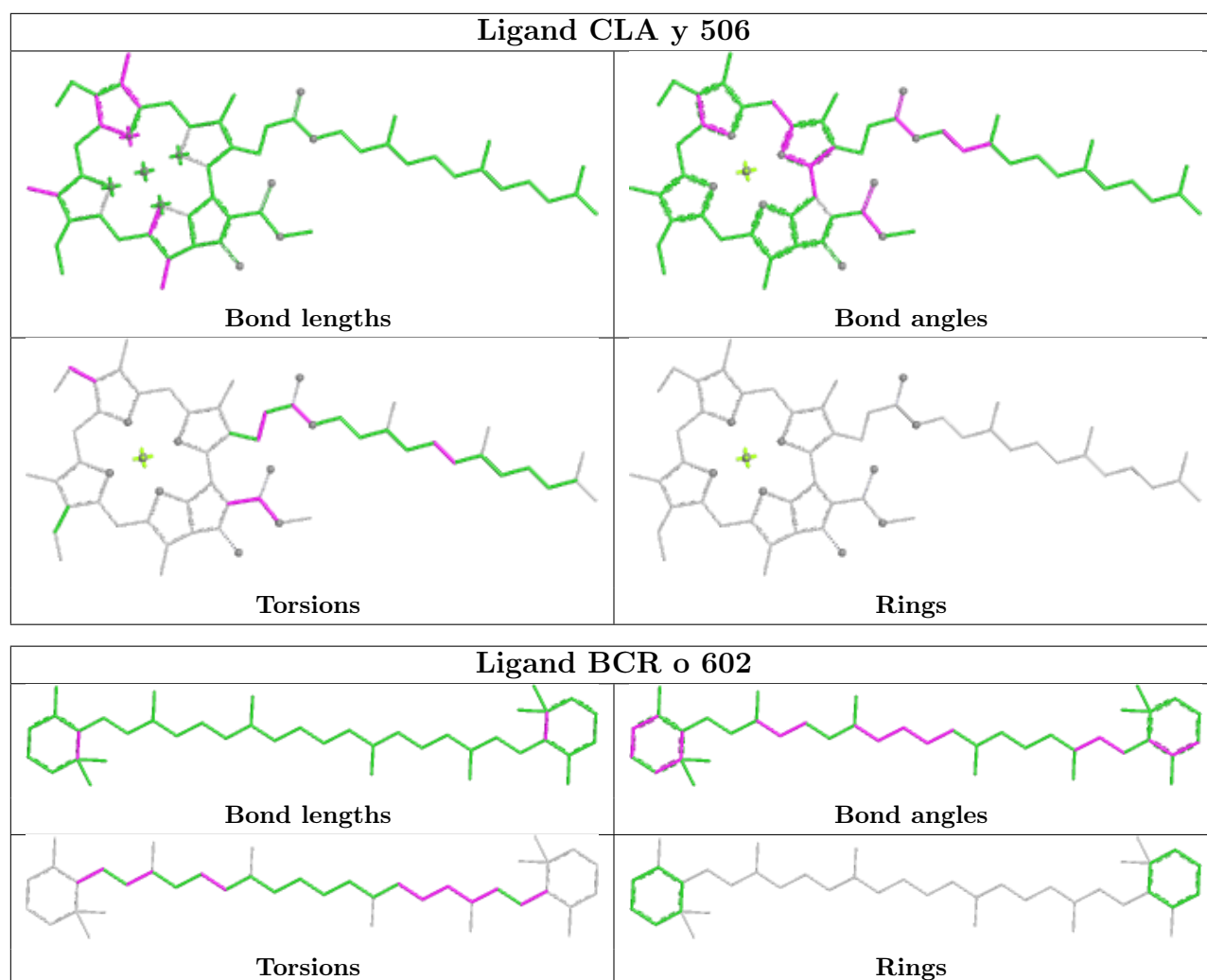


Ligand CLA v 503

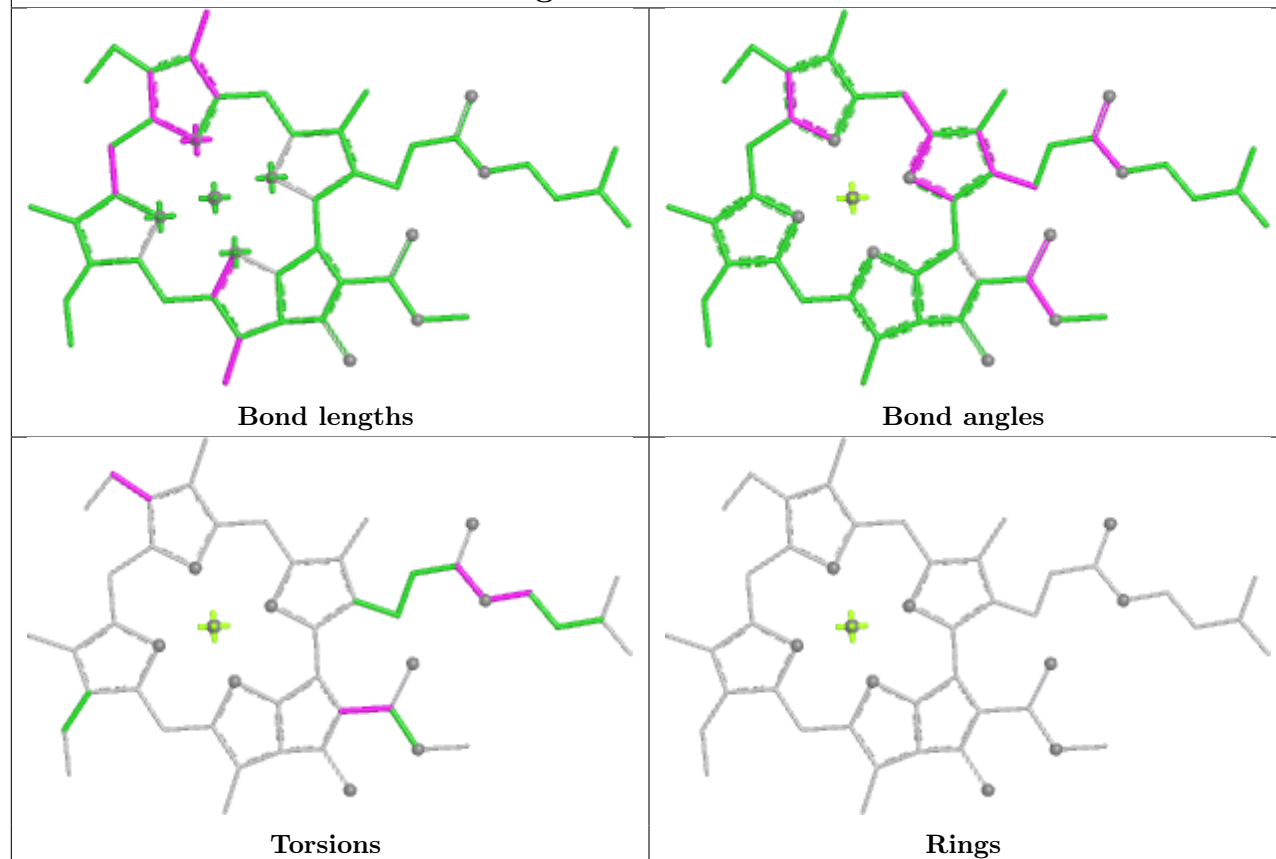


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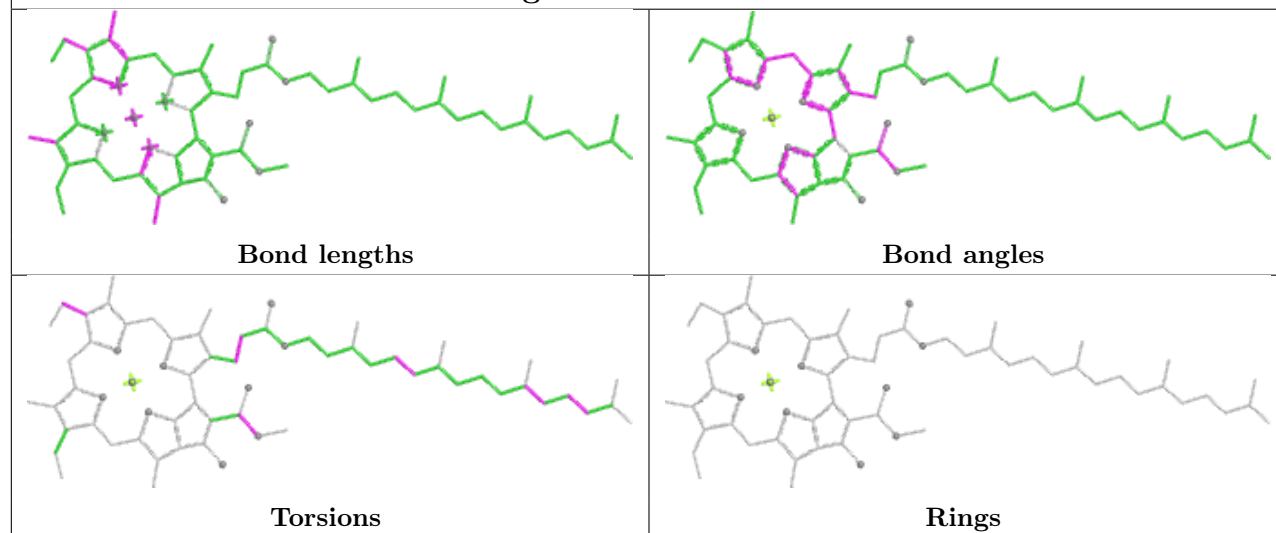




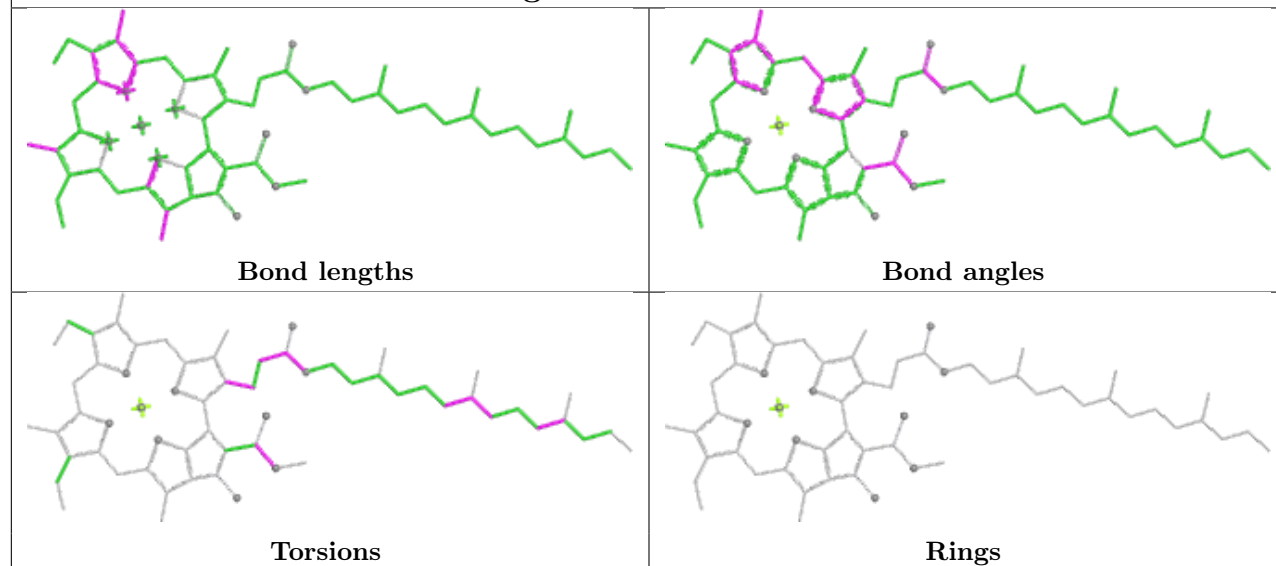
Ligand CLA x 501



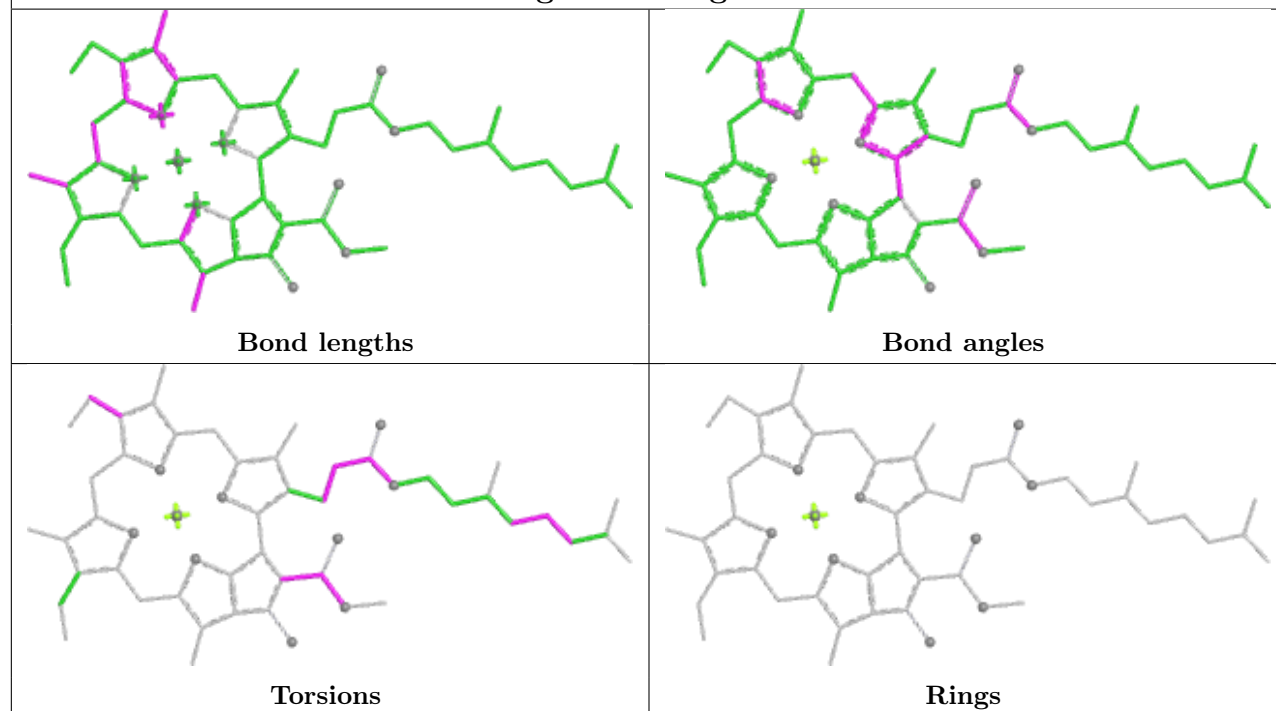
Ligand CLA A 1022

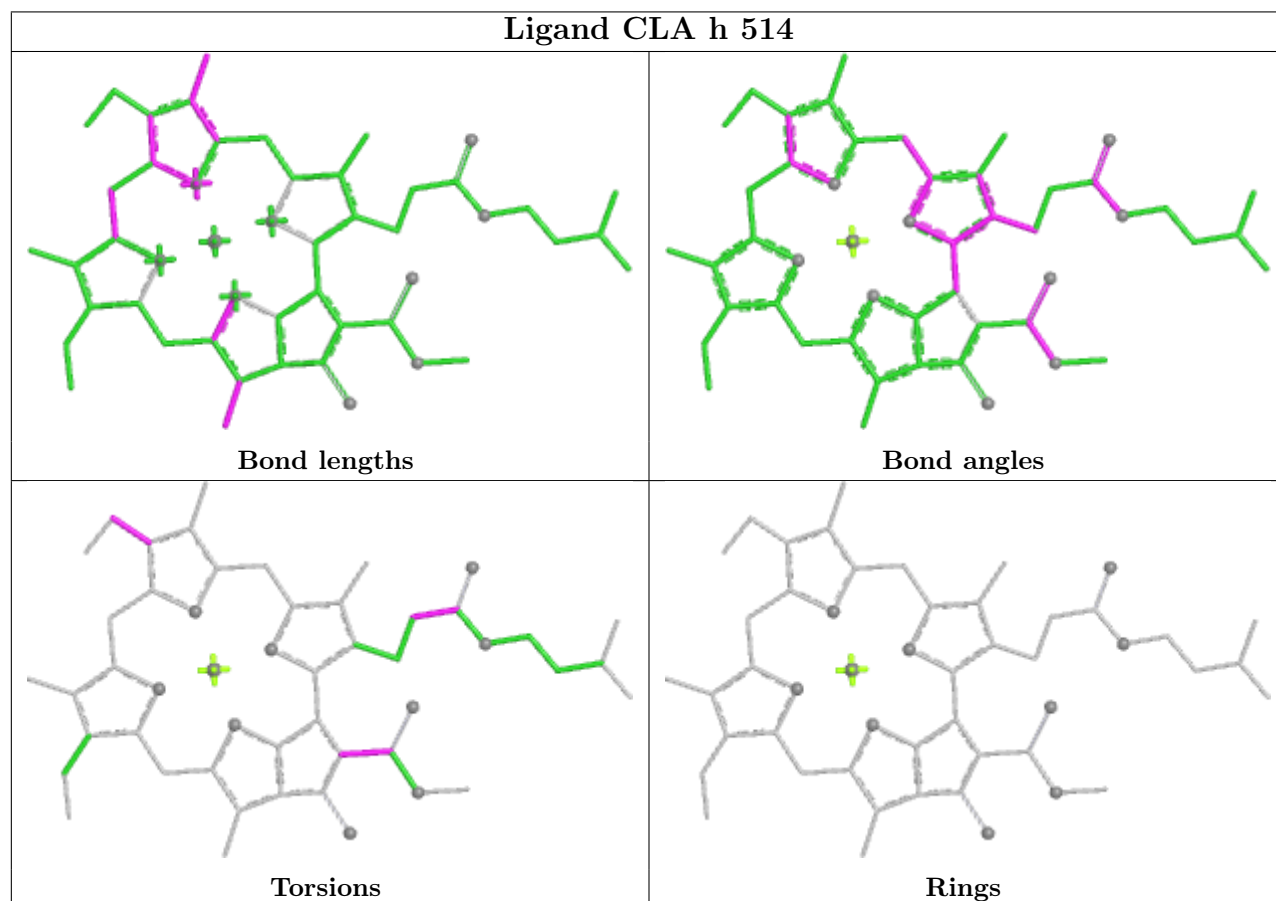
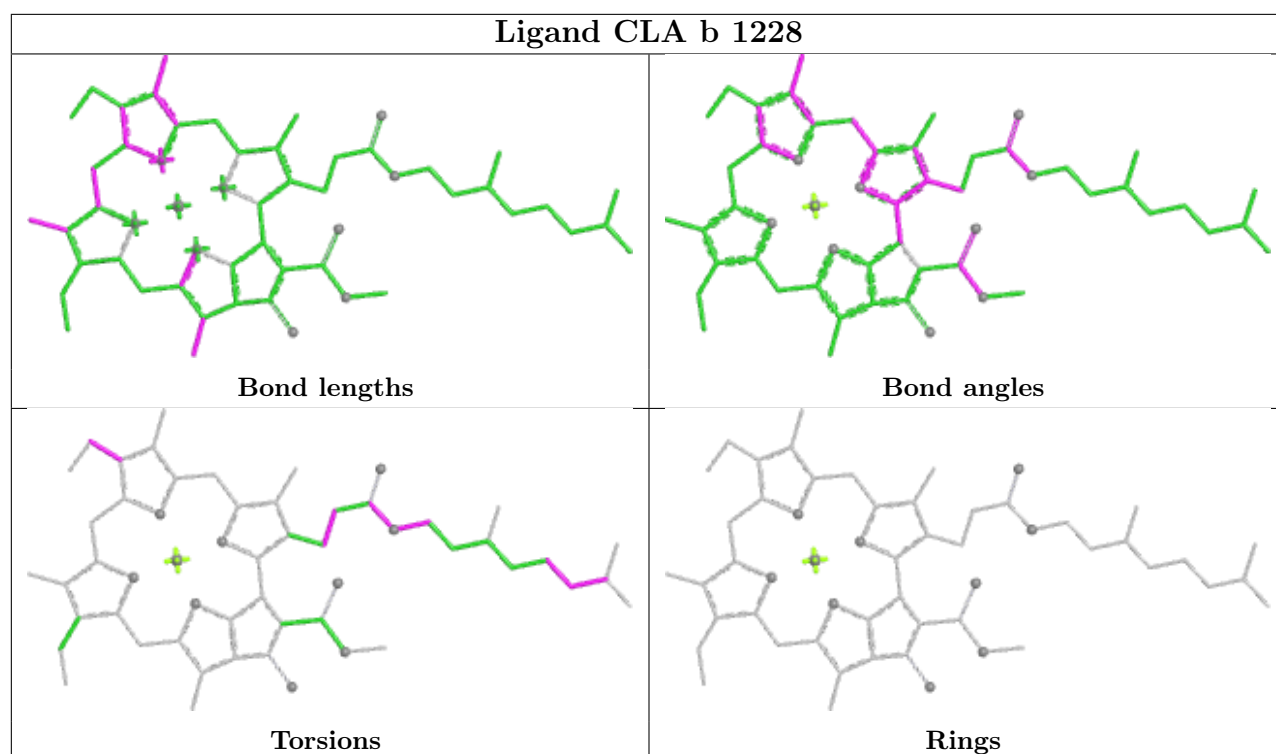


Ligand CLA B 1235

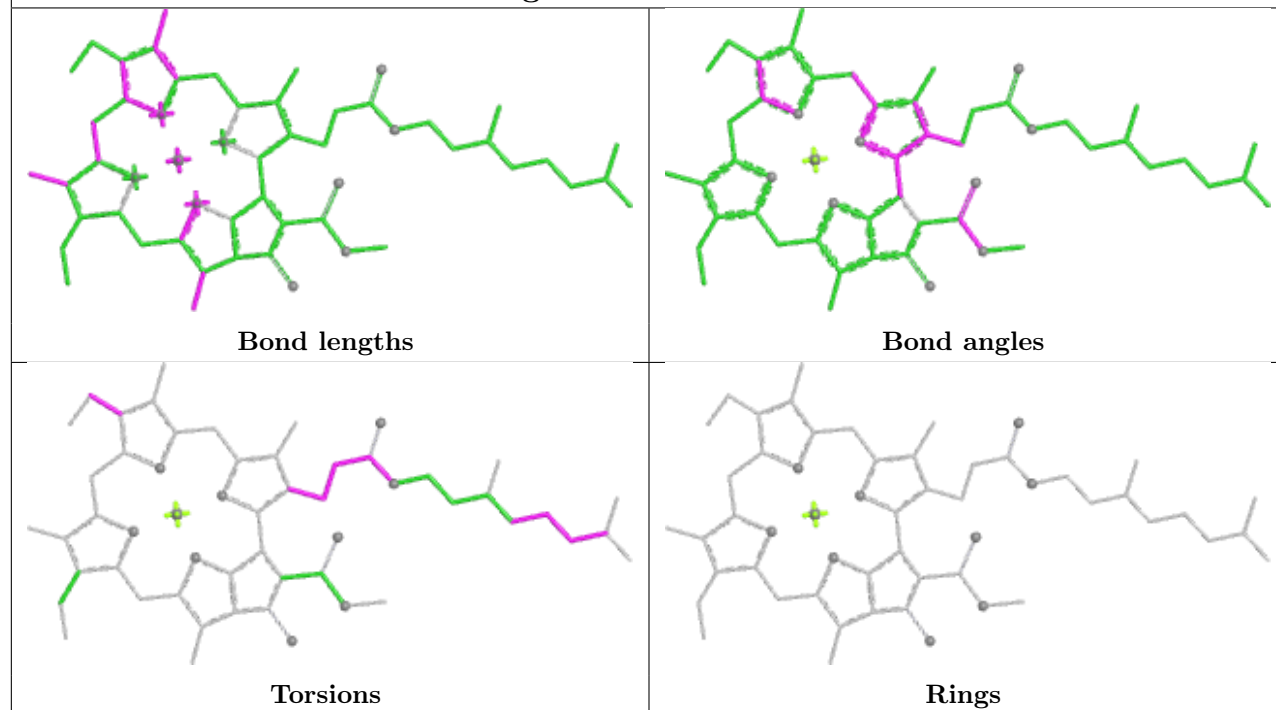


Ligand CLA g 517

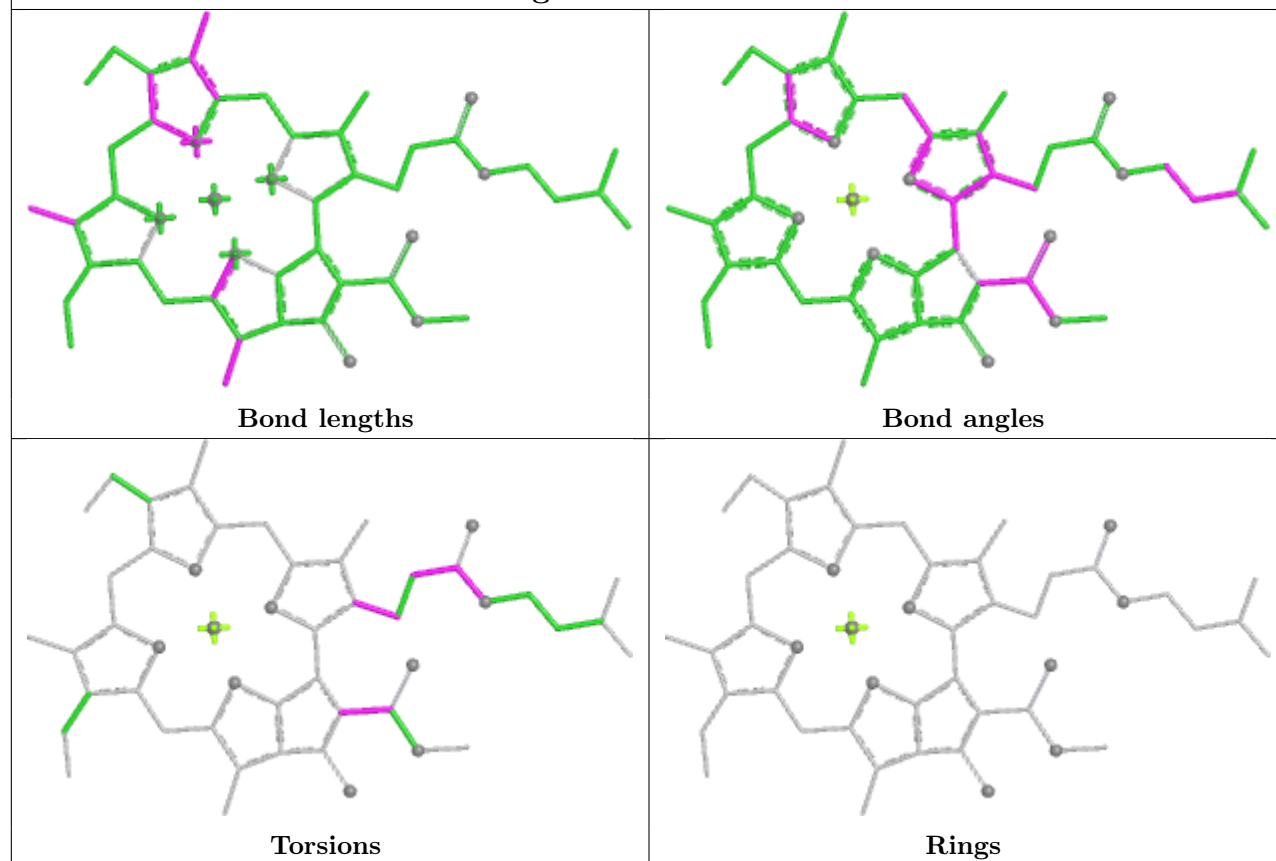




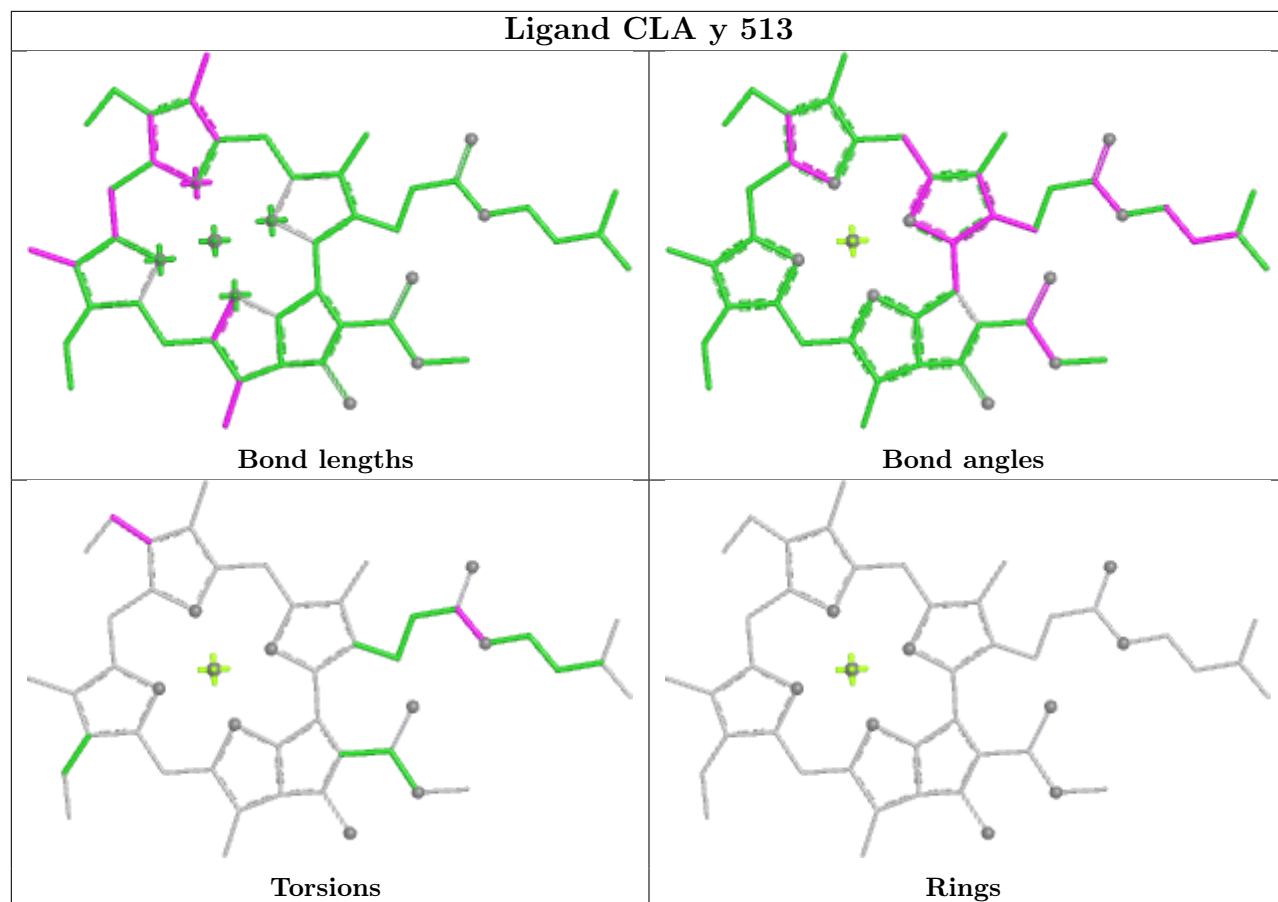
Ligand CLA H 1111



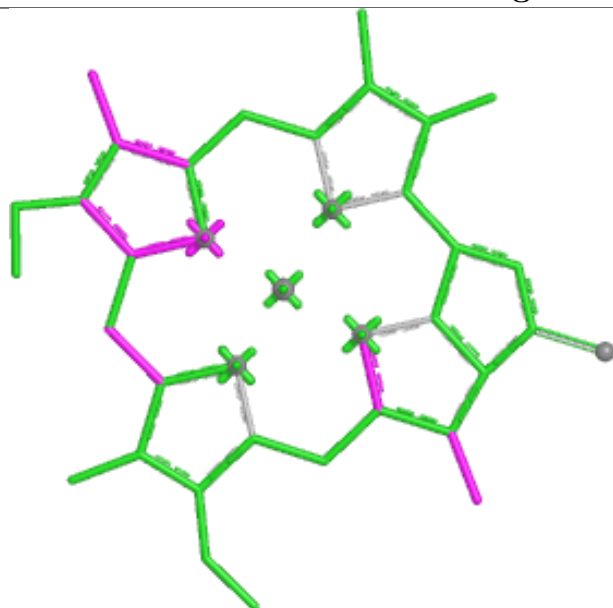
Ligand CLA w 502



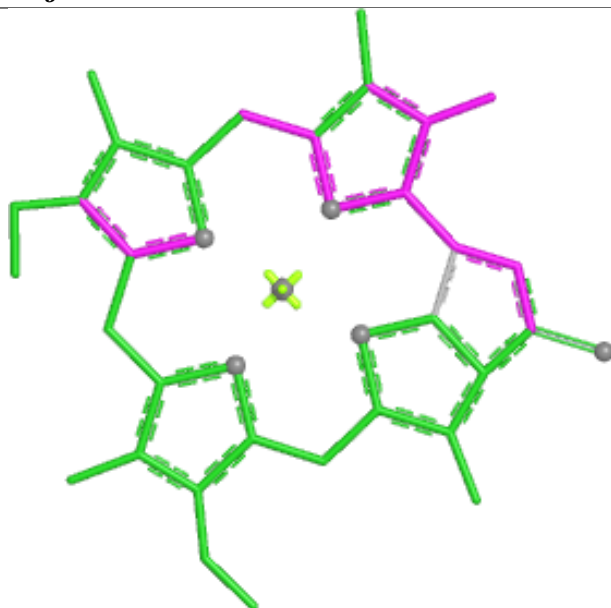
Ligand CLA y 513



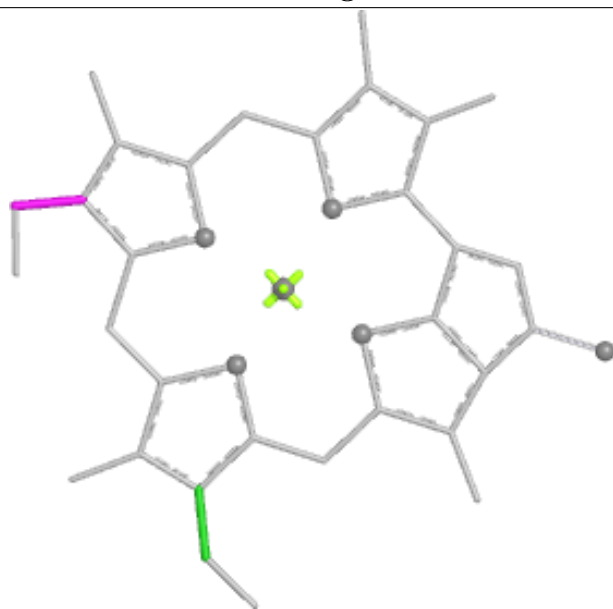
Ligand CLA j 1303



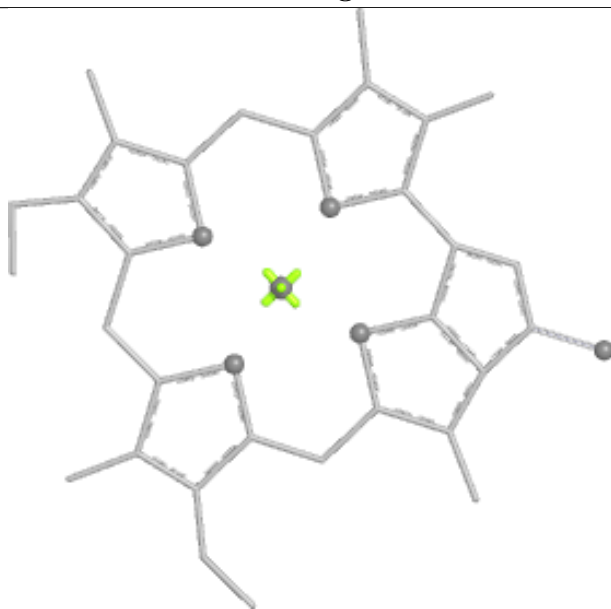
Bond lengths



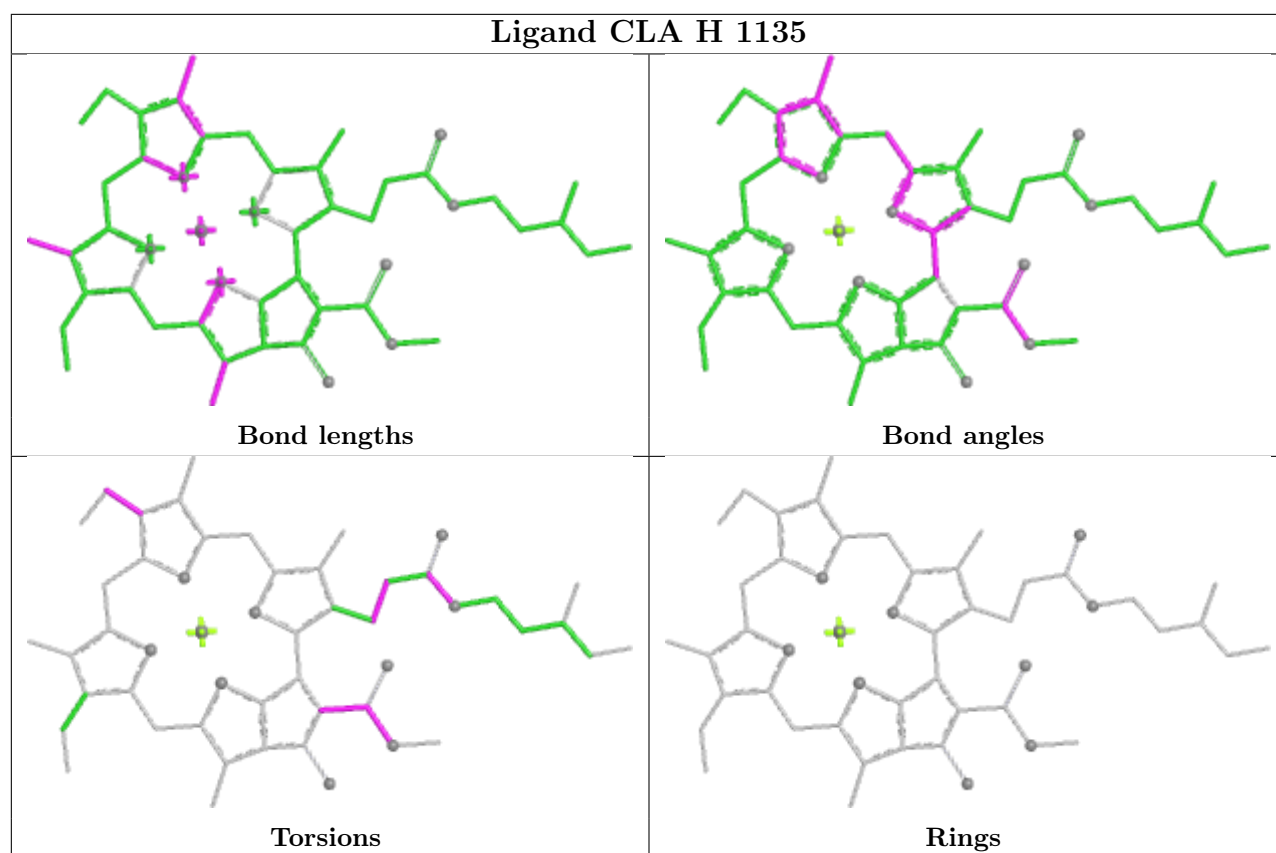
Bond angles



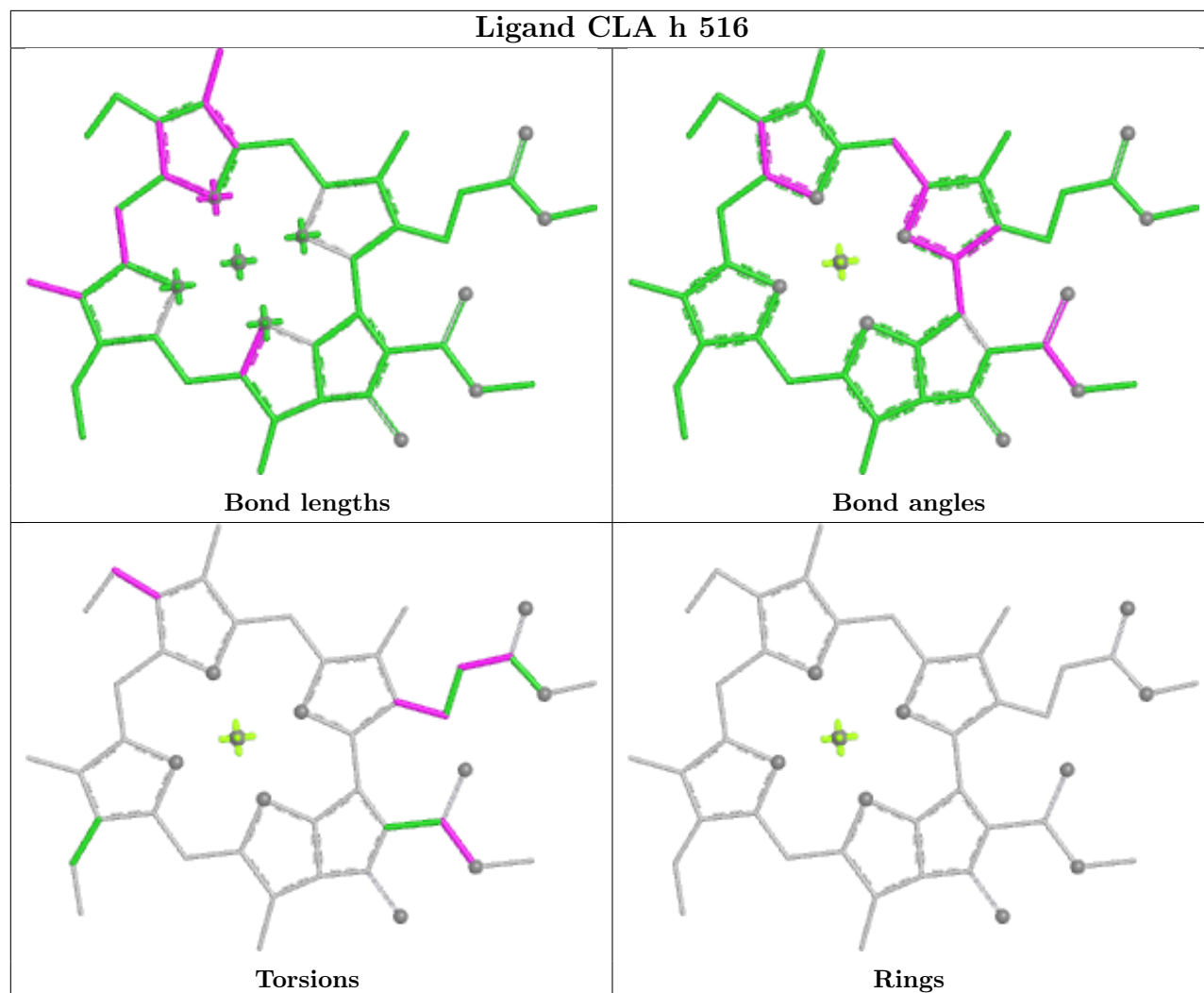
Torsions

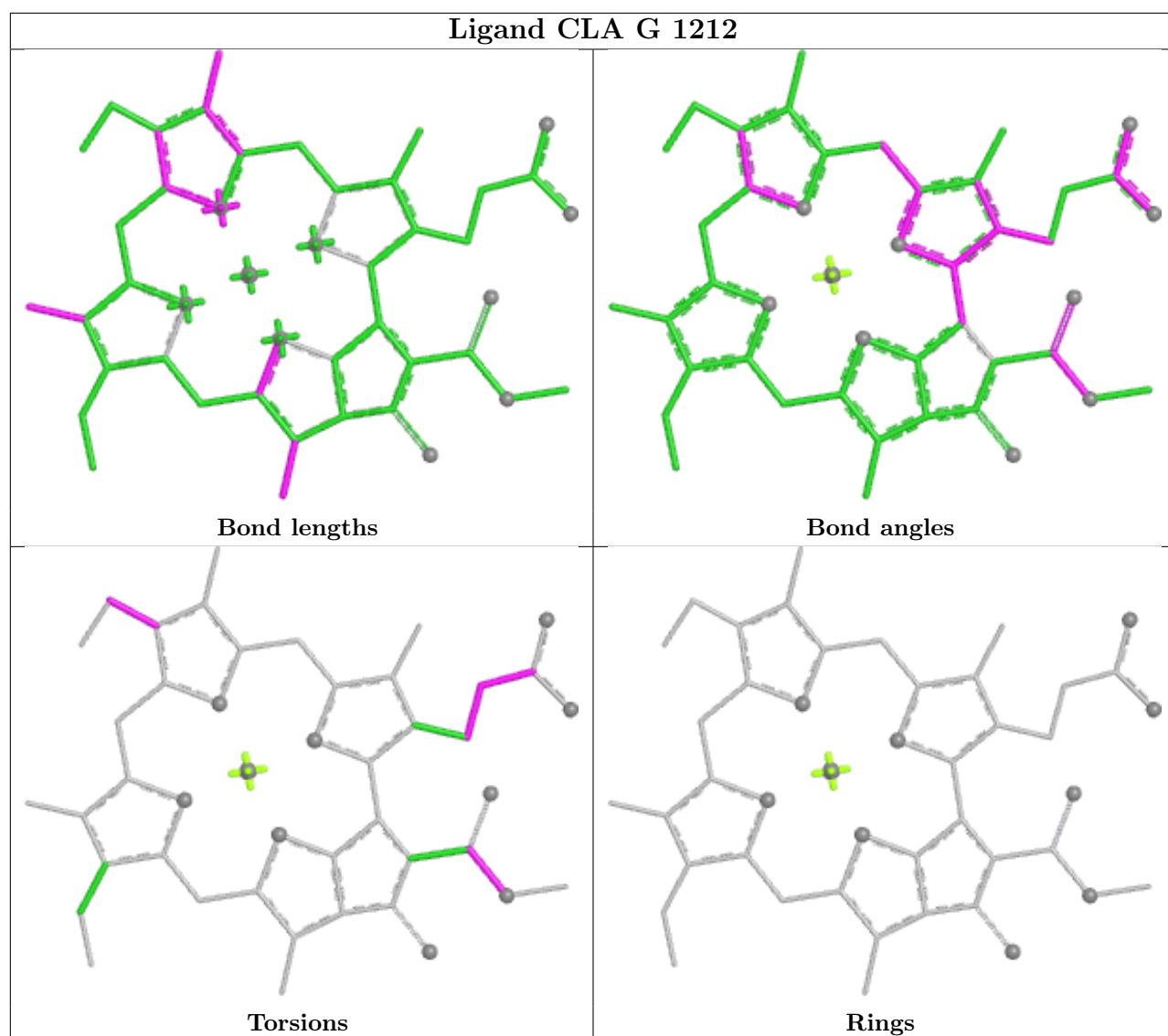


Rings

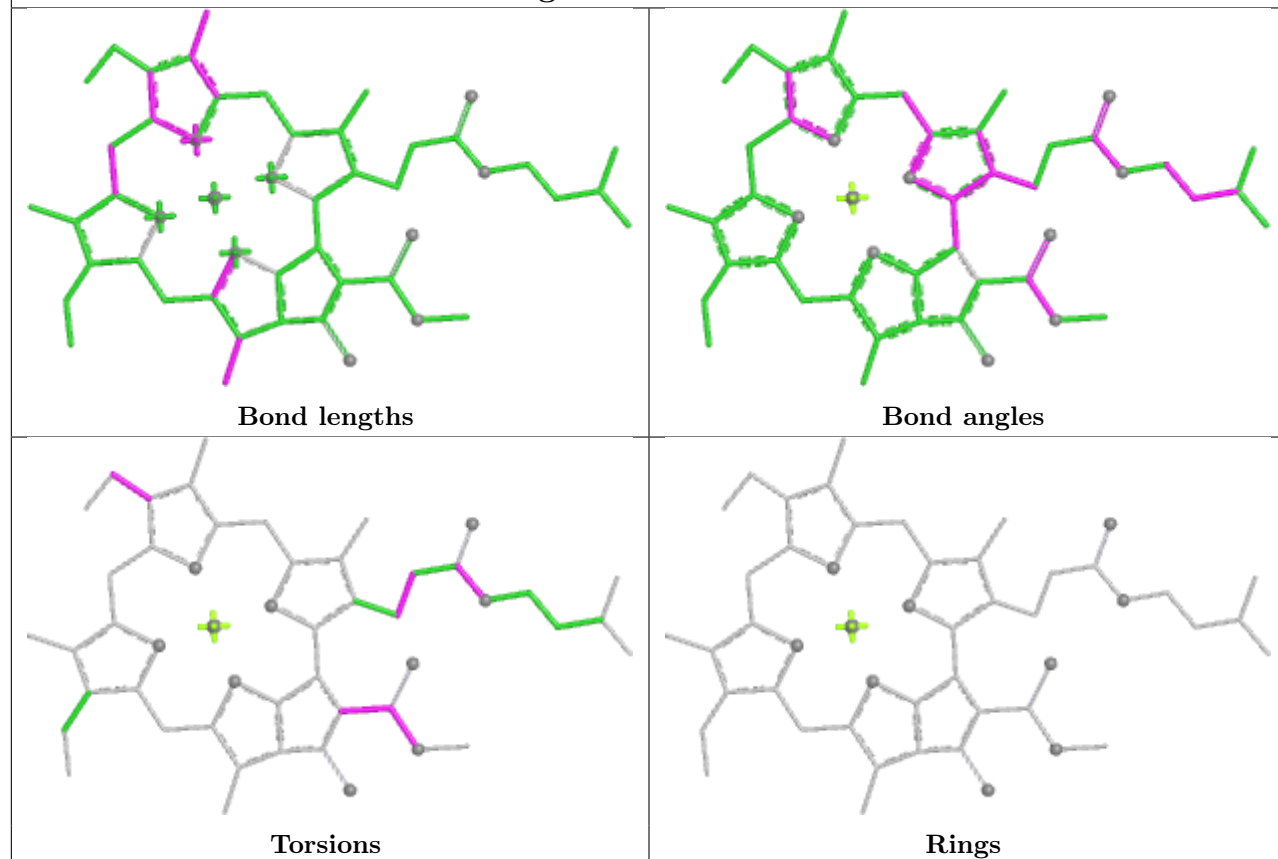


Ligand CLA h 516

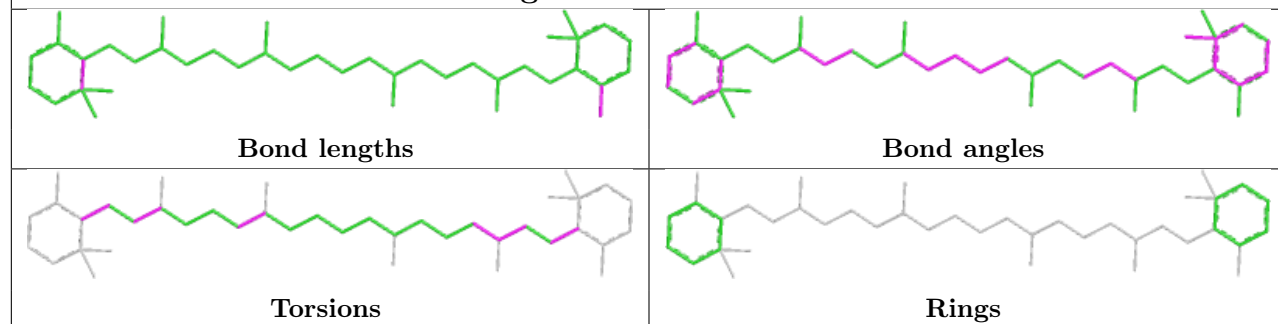


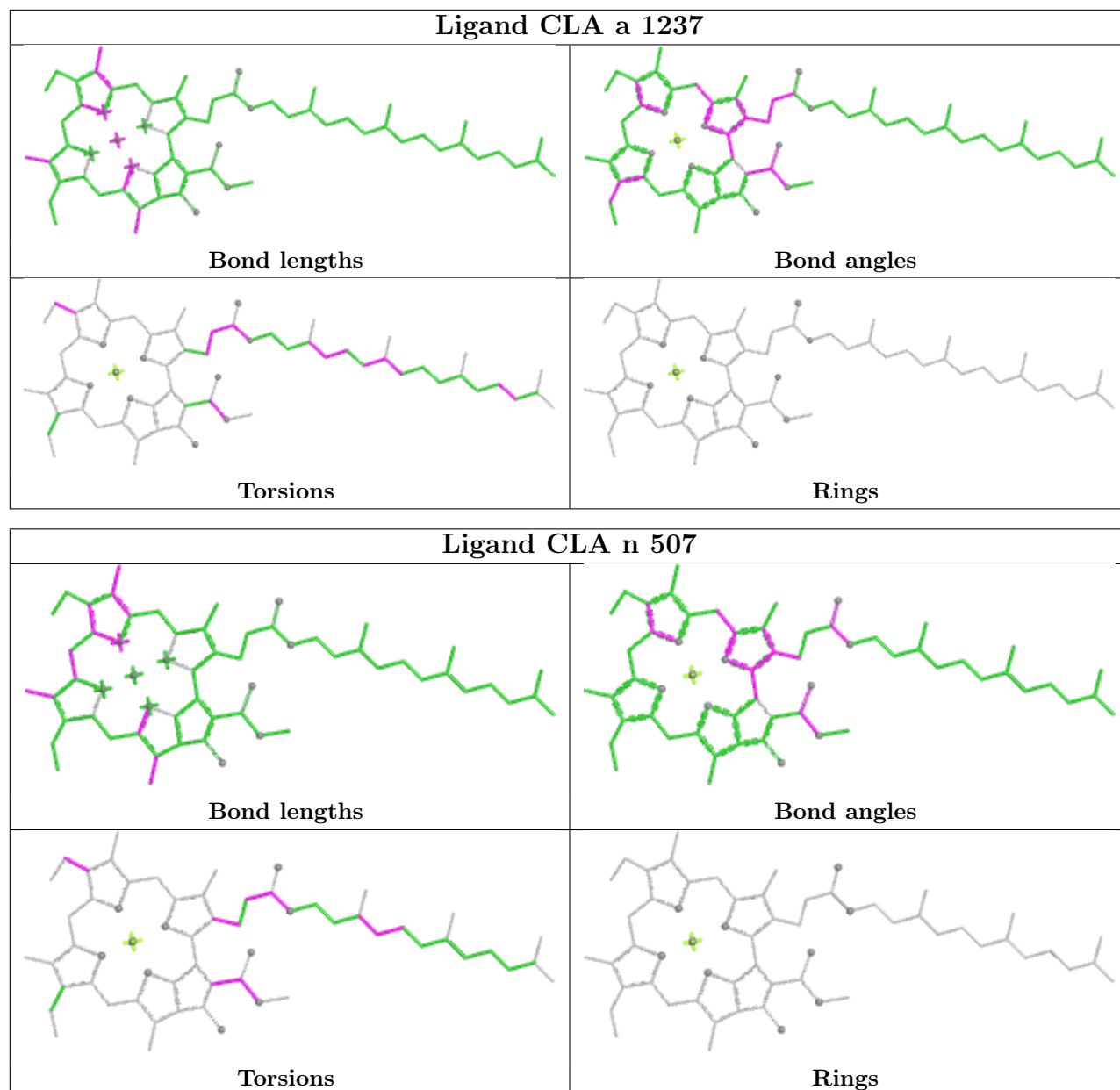


Ligand CLA t 501

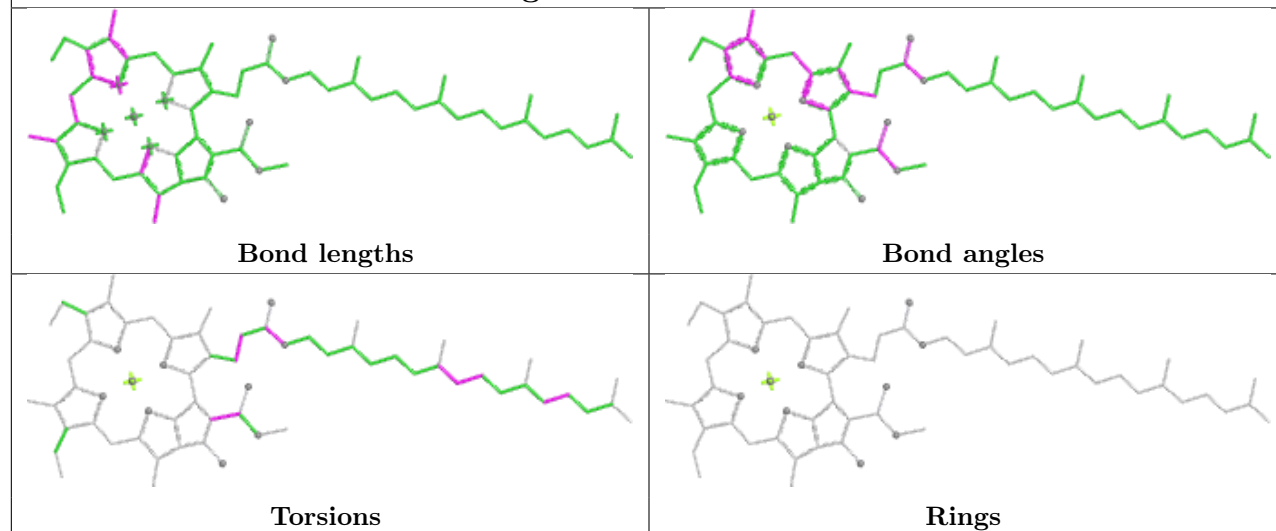


Ligand BCR U 4022

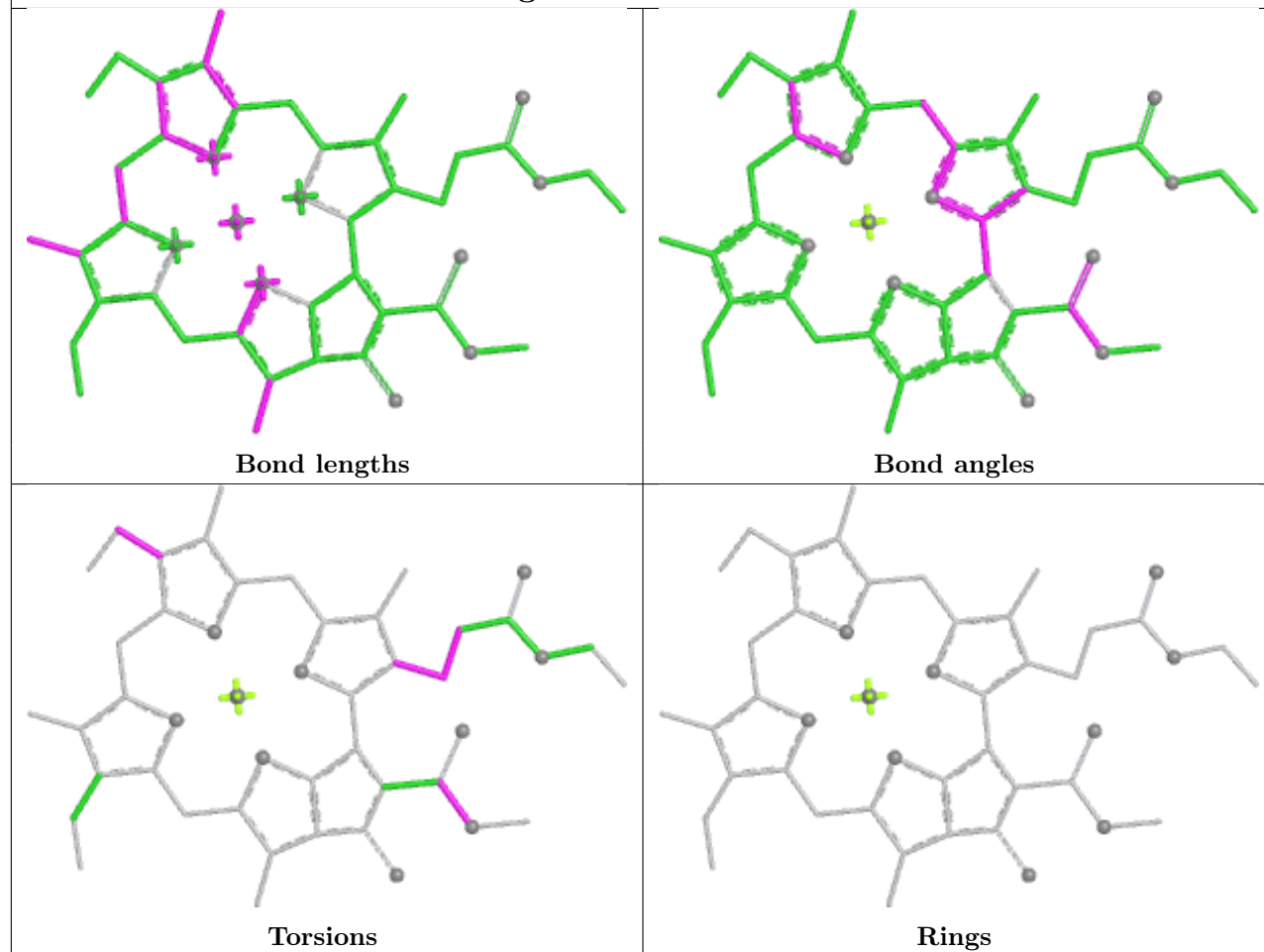


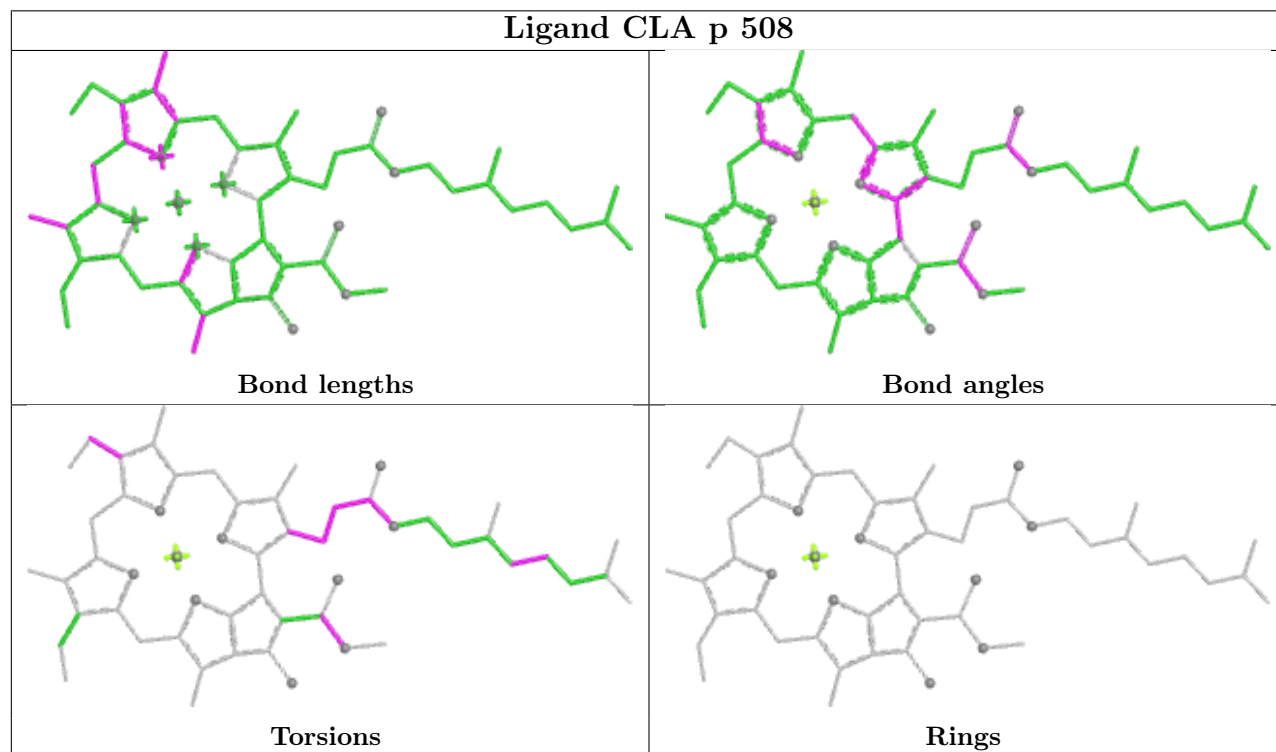
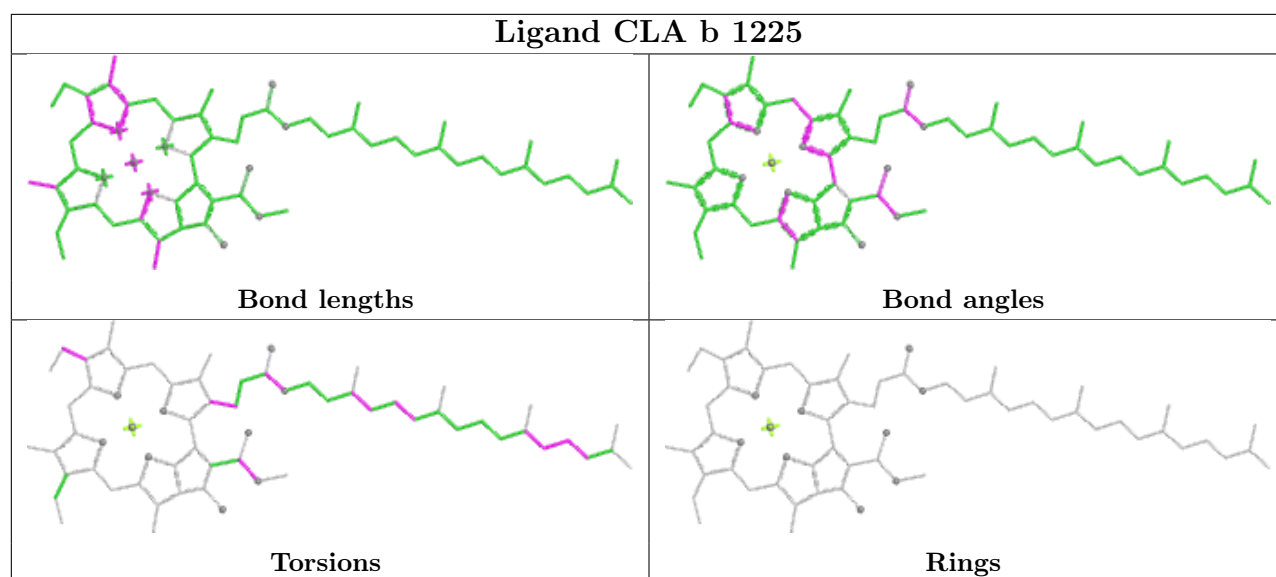


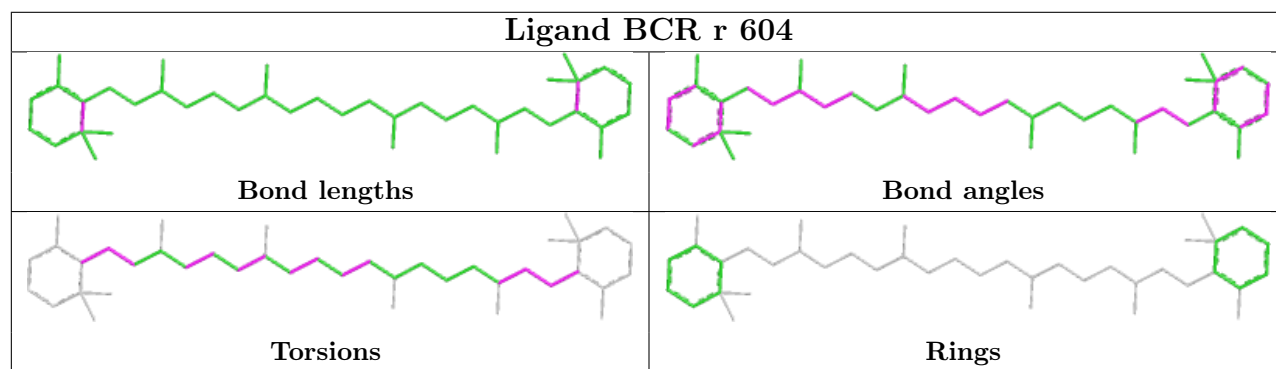
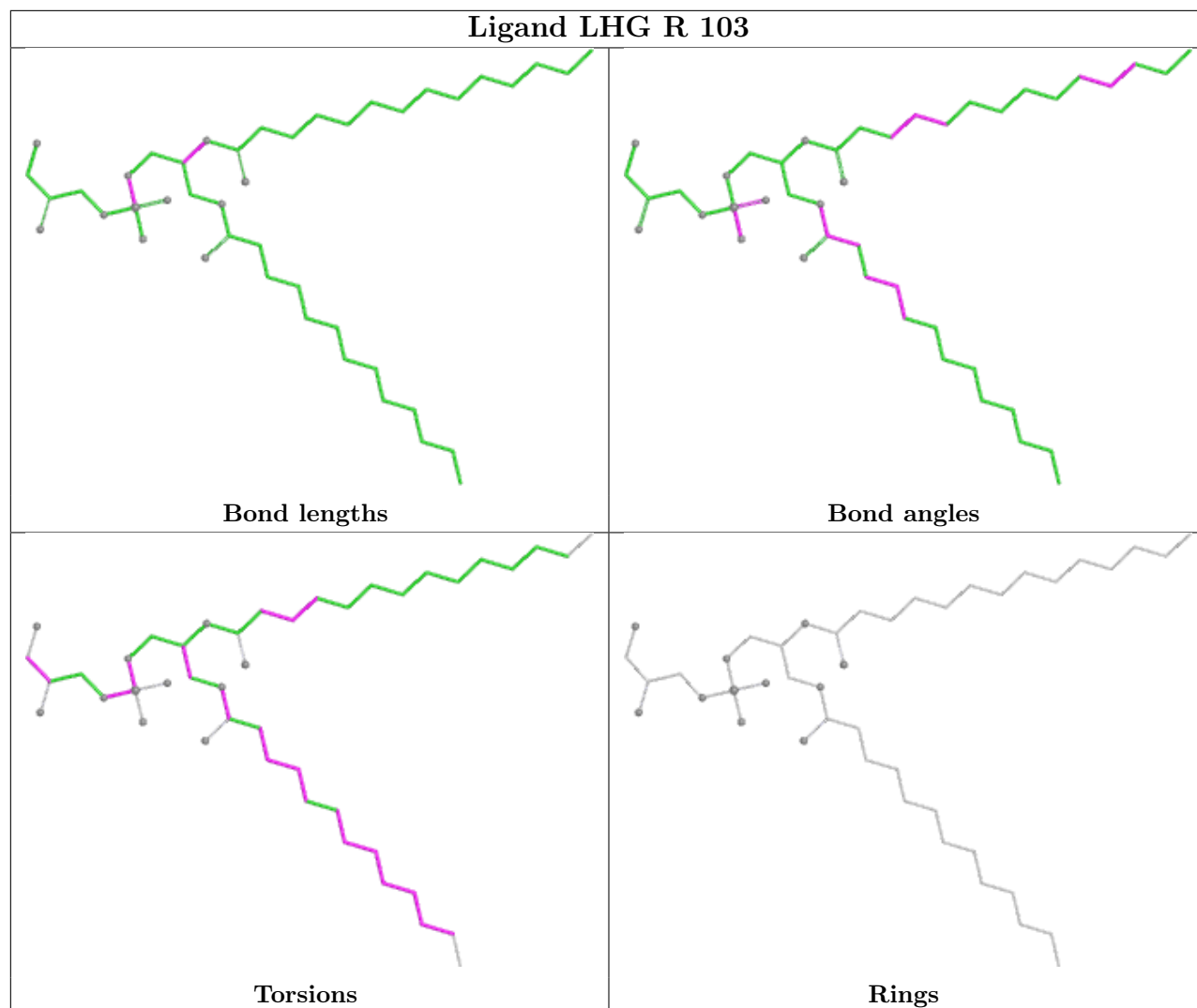
Ligand CLA G 1211



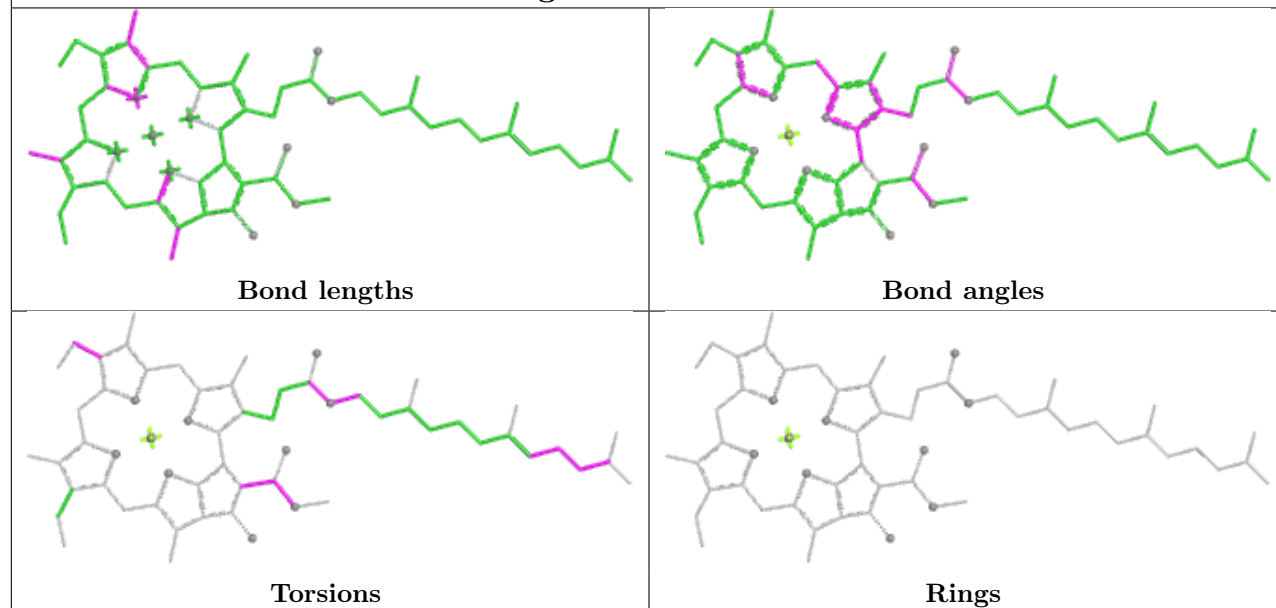
Ligand CLA B 1216



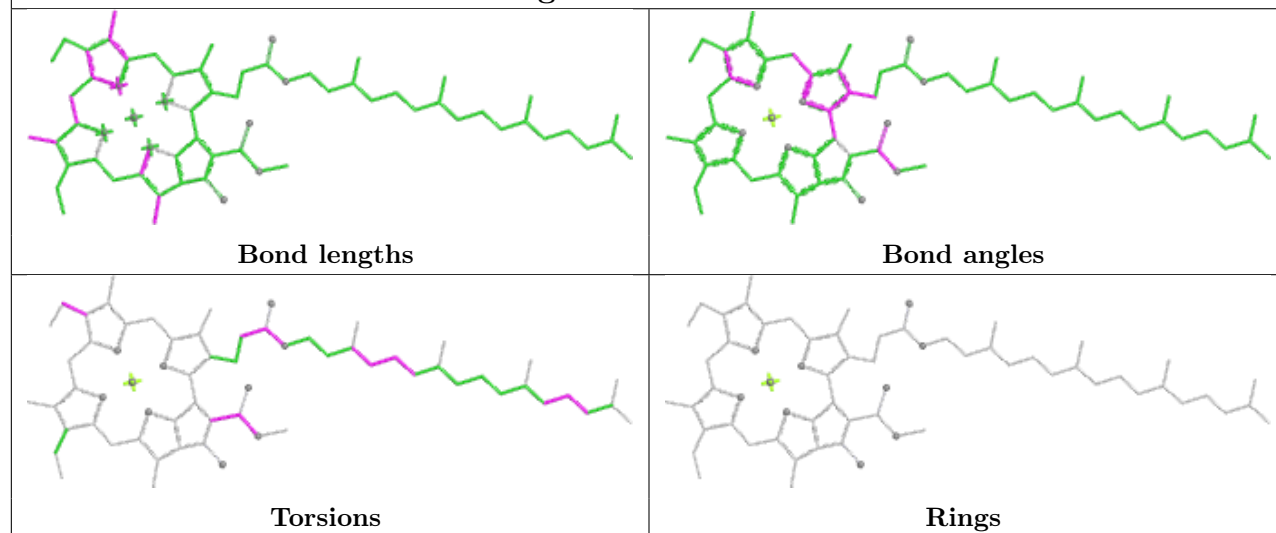


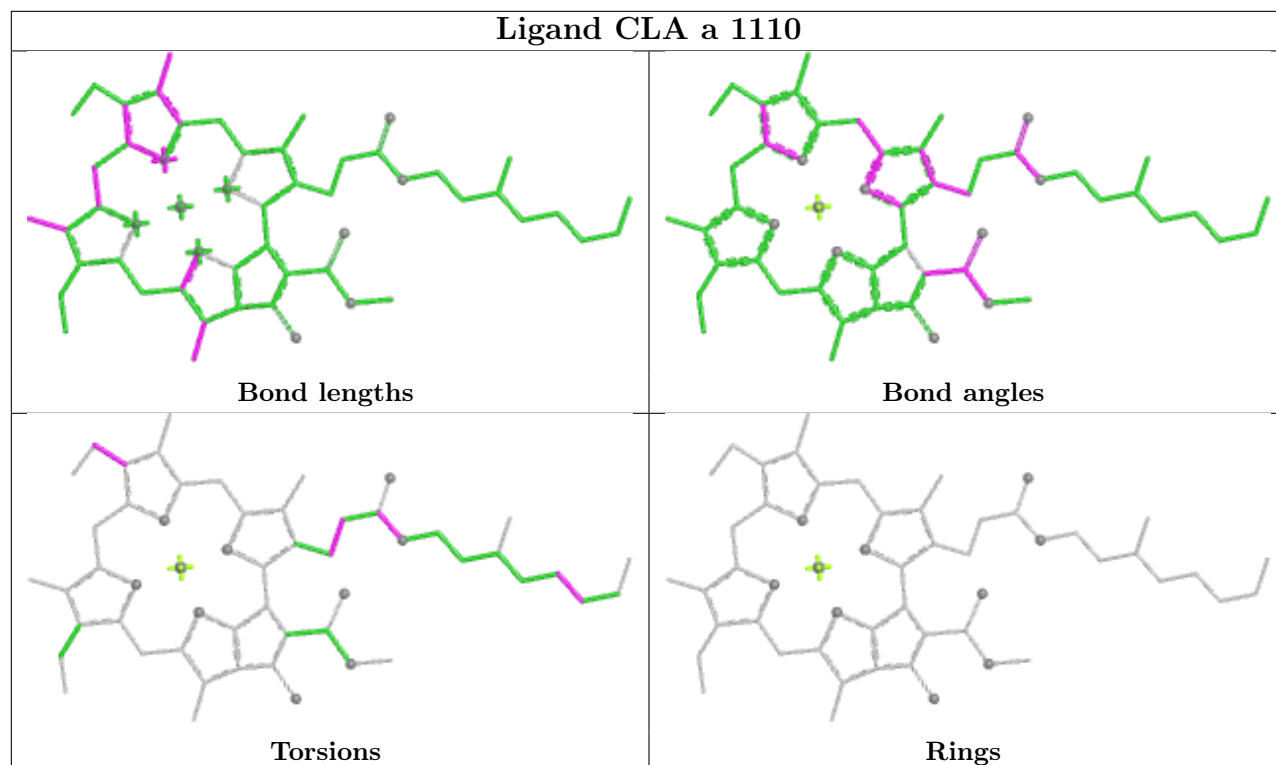
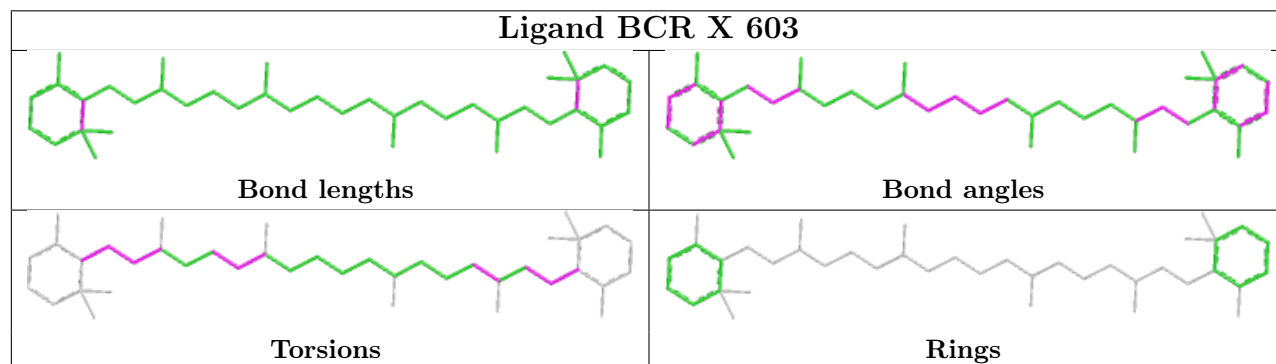
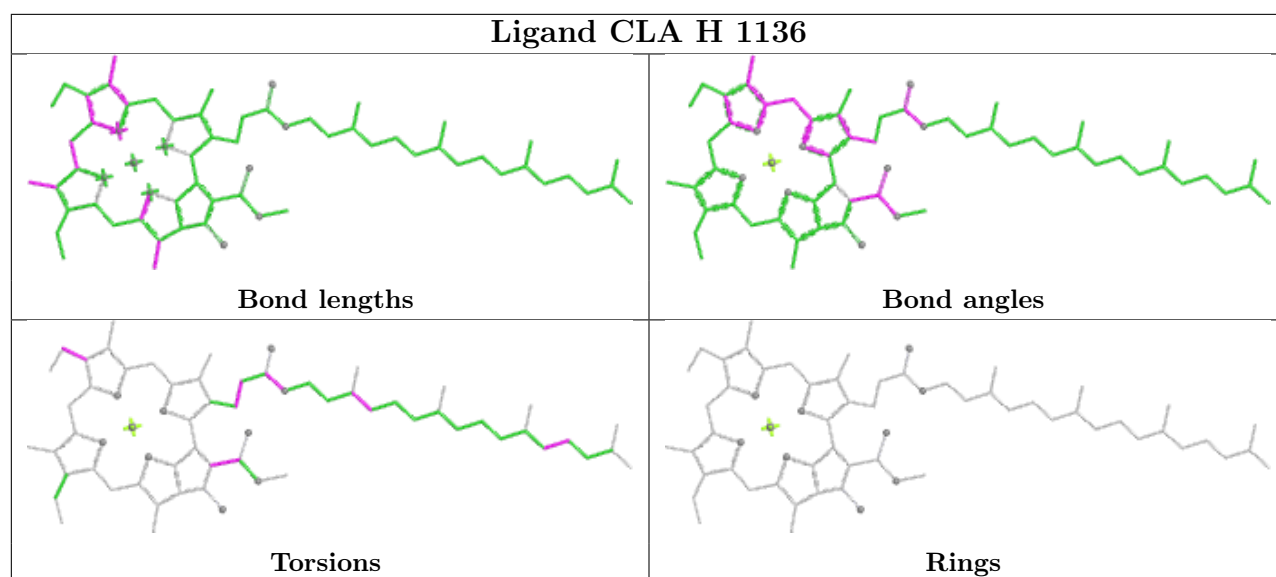


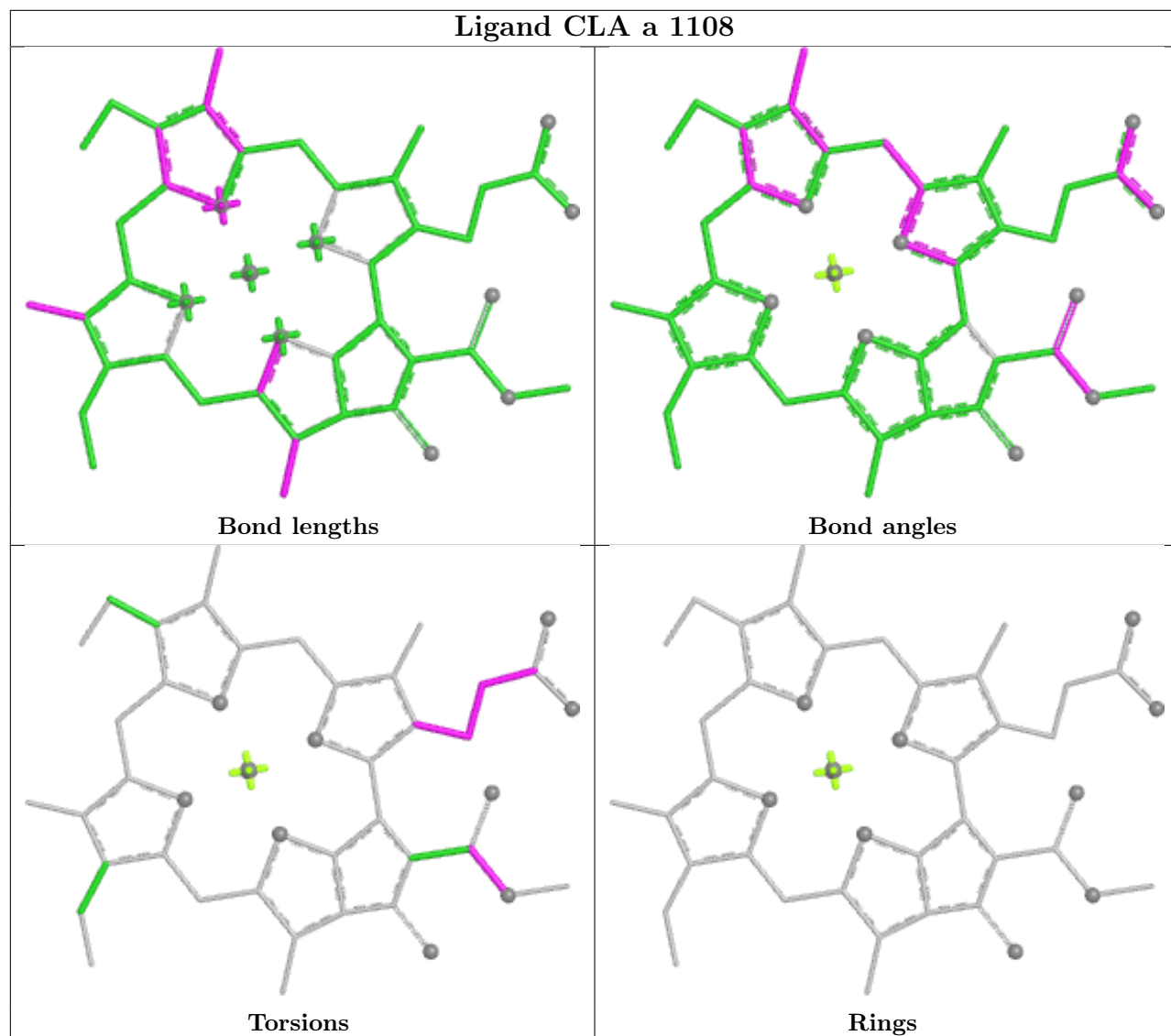
Ligand CLA s 506

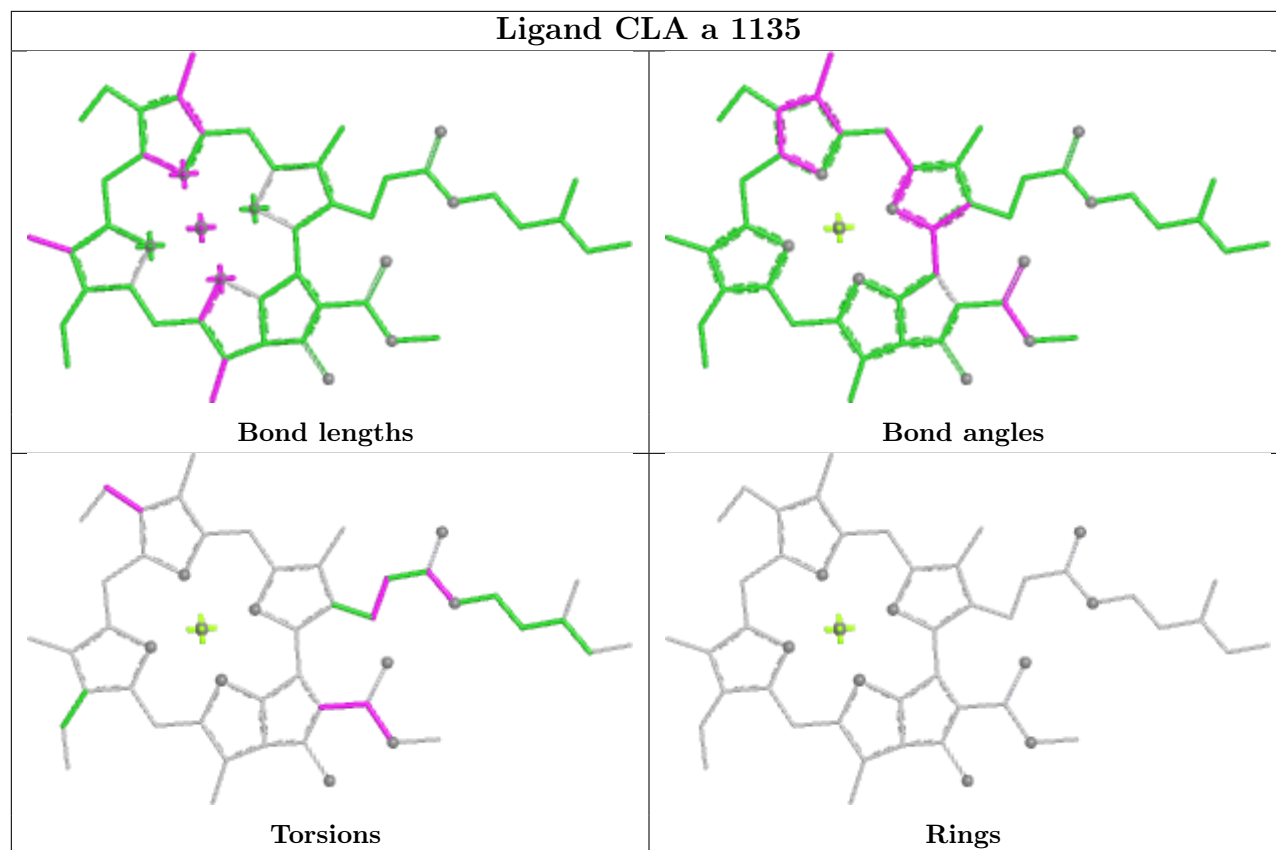


Ligand CLA r 507

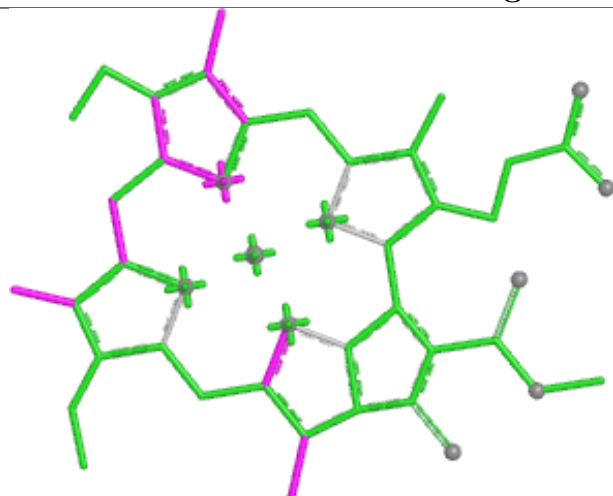




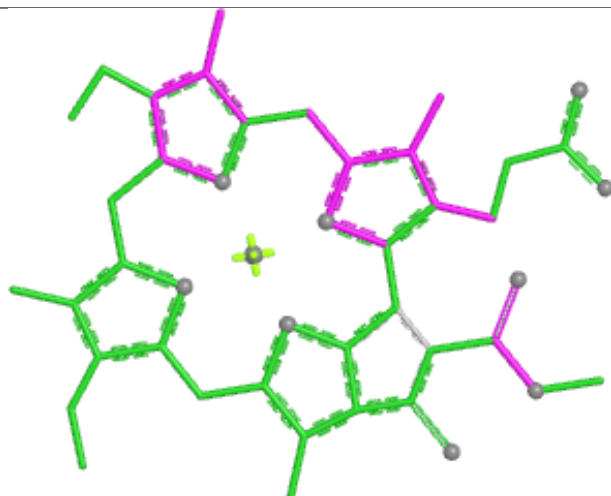




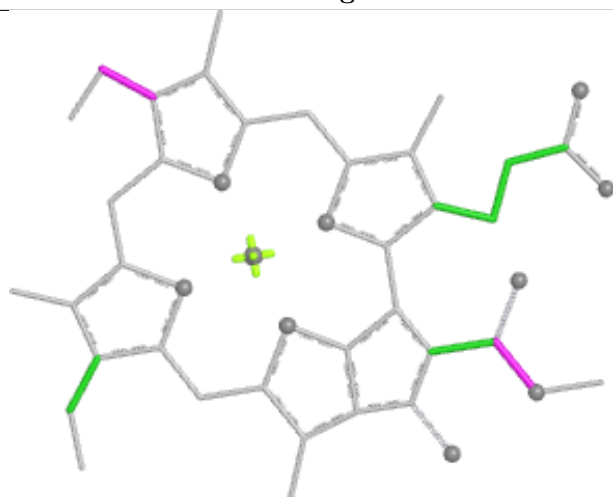
Ligand CLA G 1231



Bond lengths



Bond angles

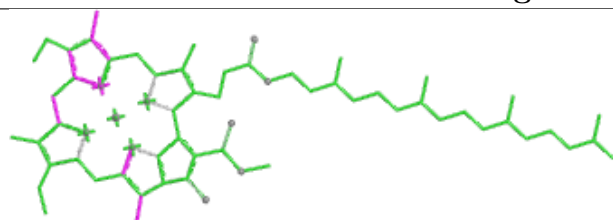


Torsions

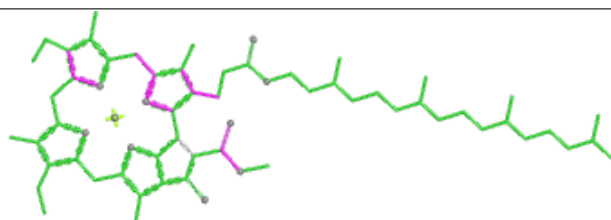


Rings

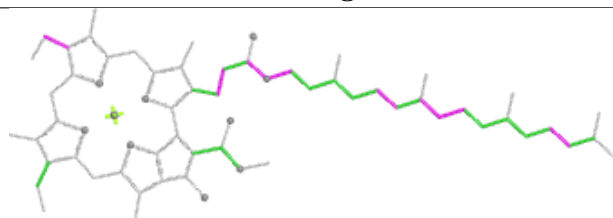
Ligand CLA X 515



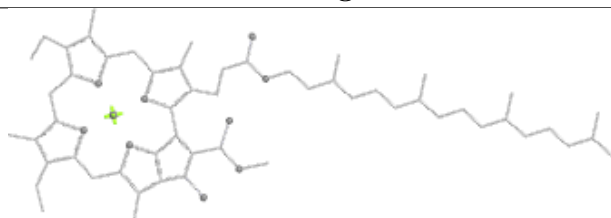
Bond lengths



Bond angles

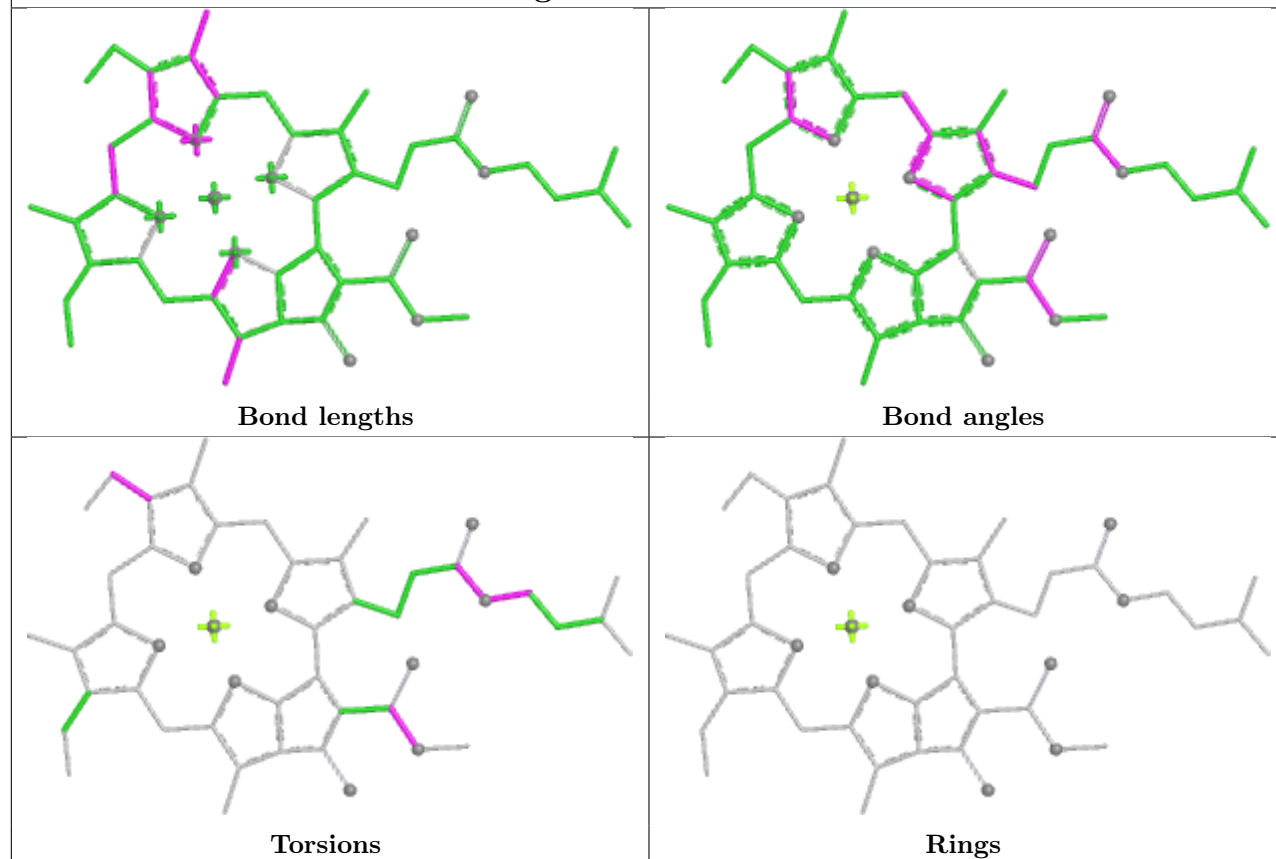


Torsions

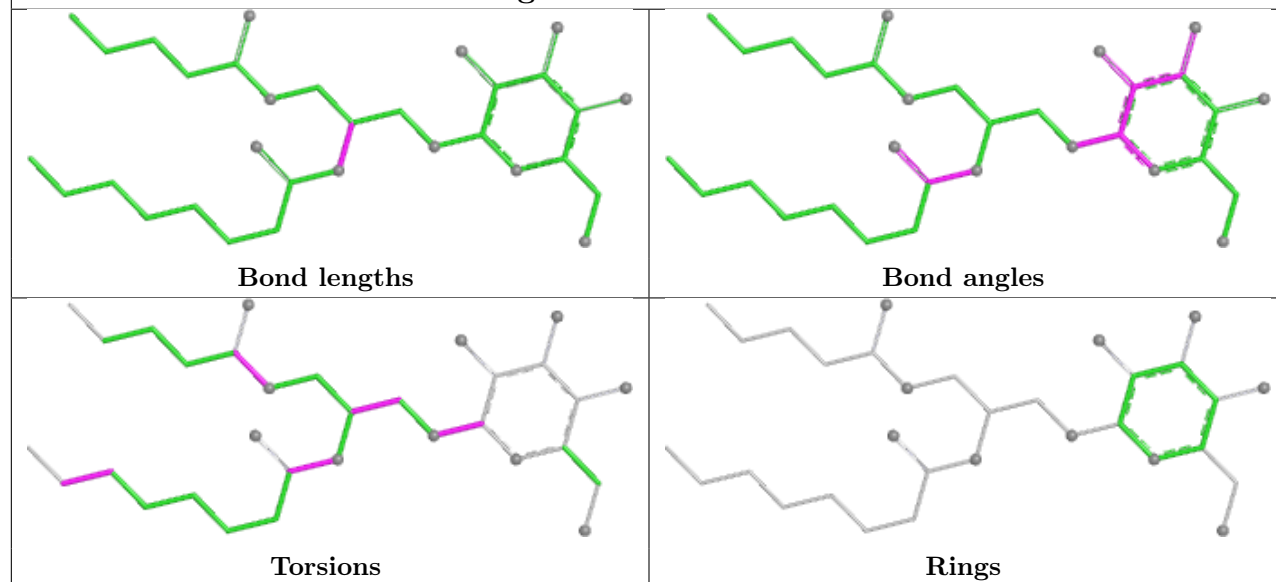


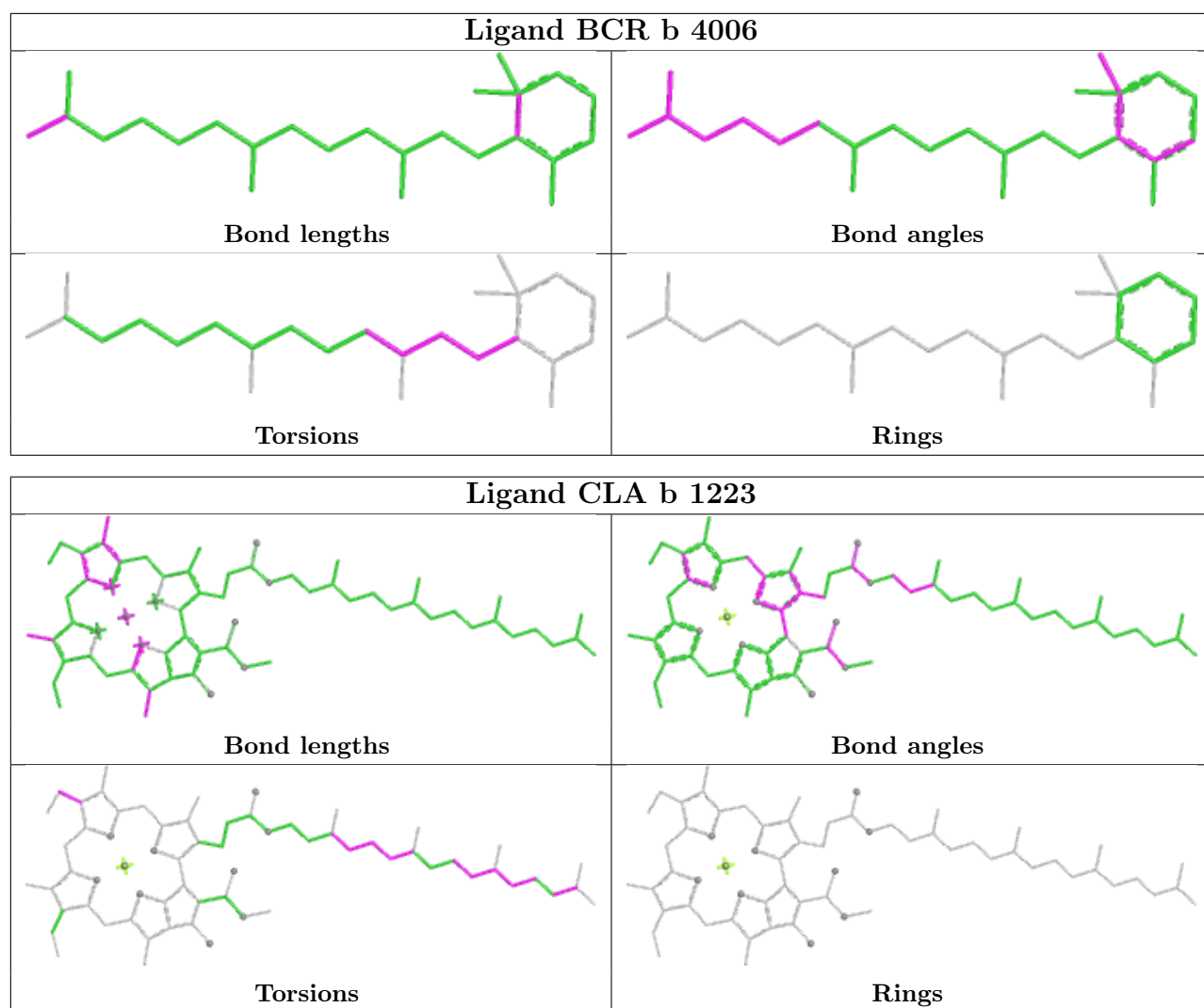
Rings

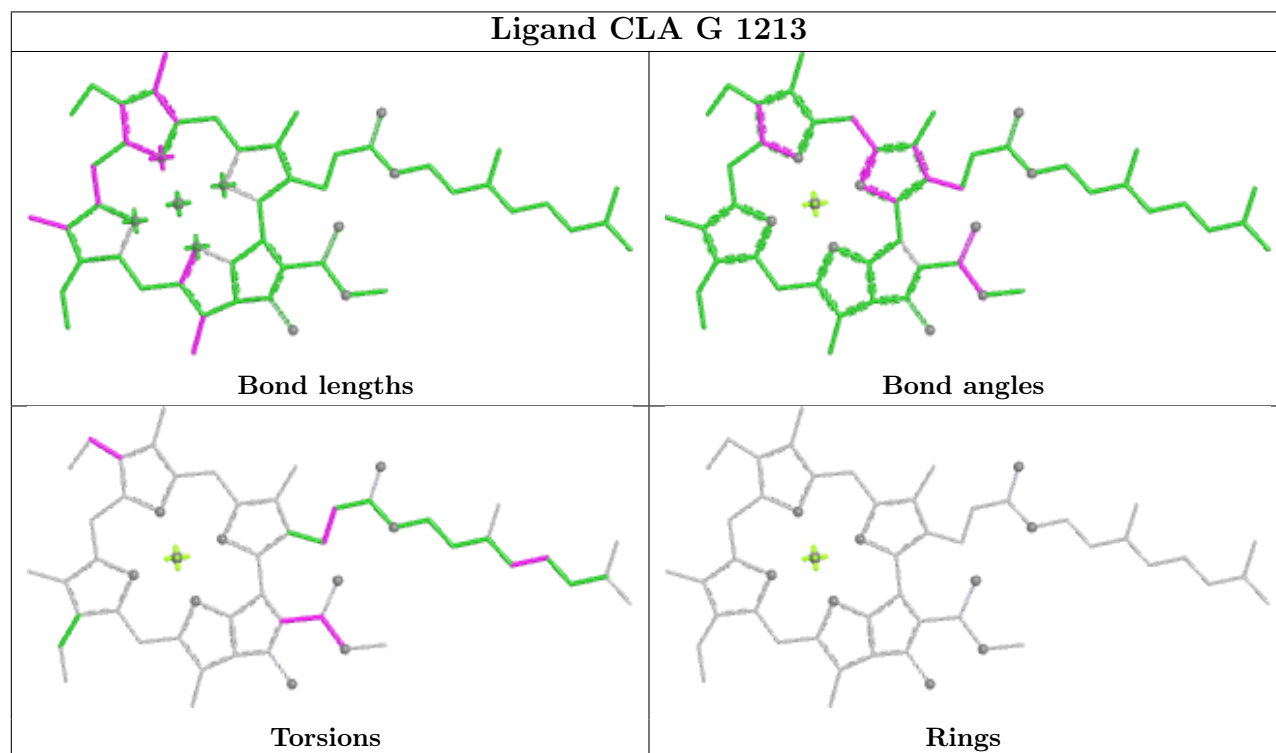
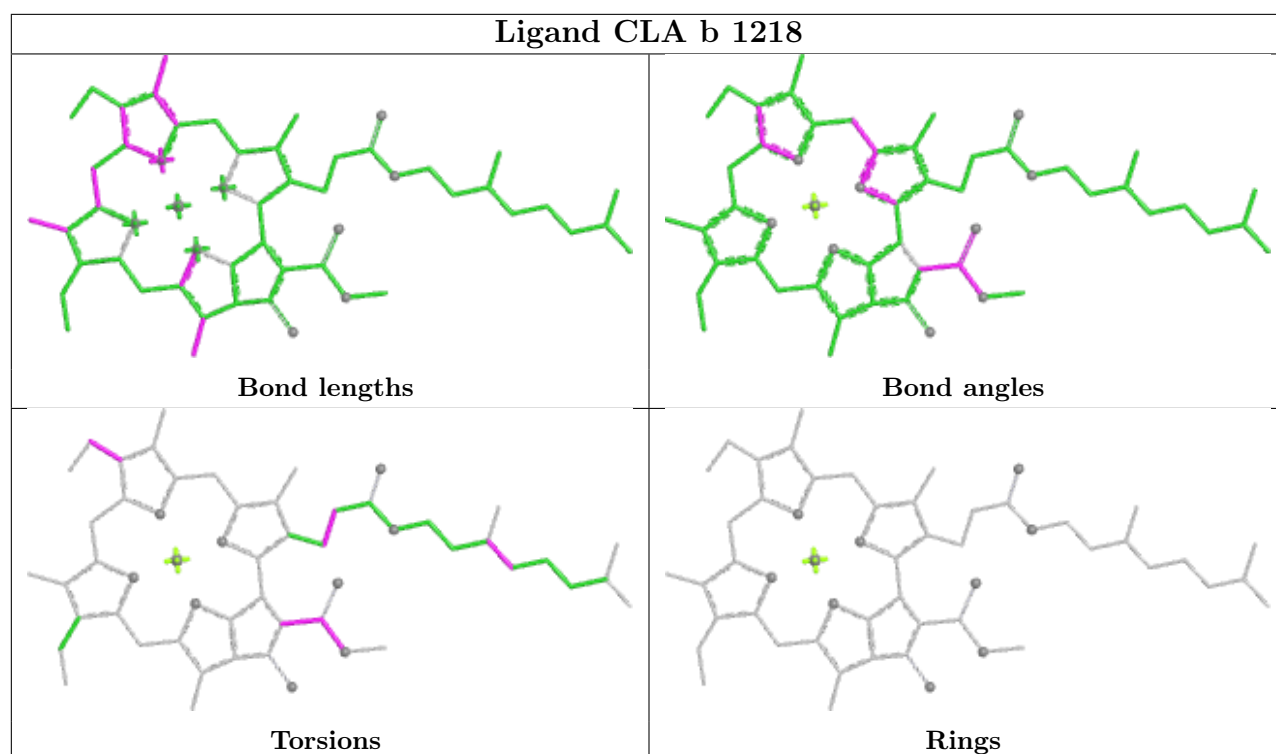
Ligand CLA Z 501

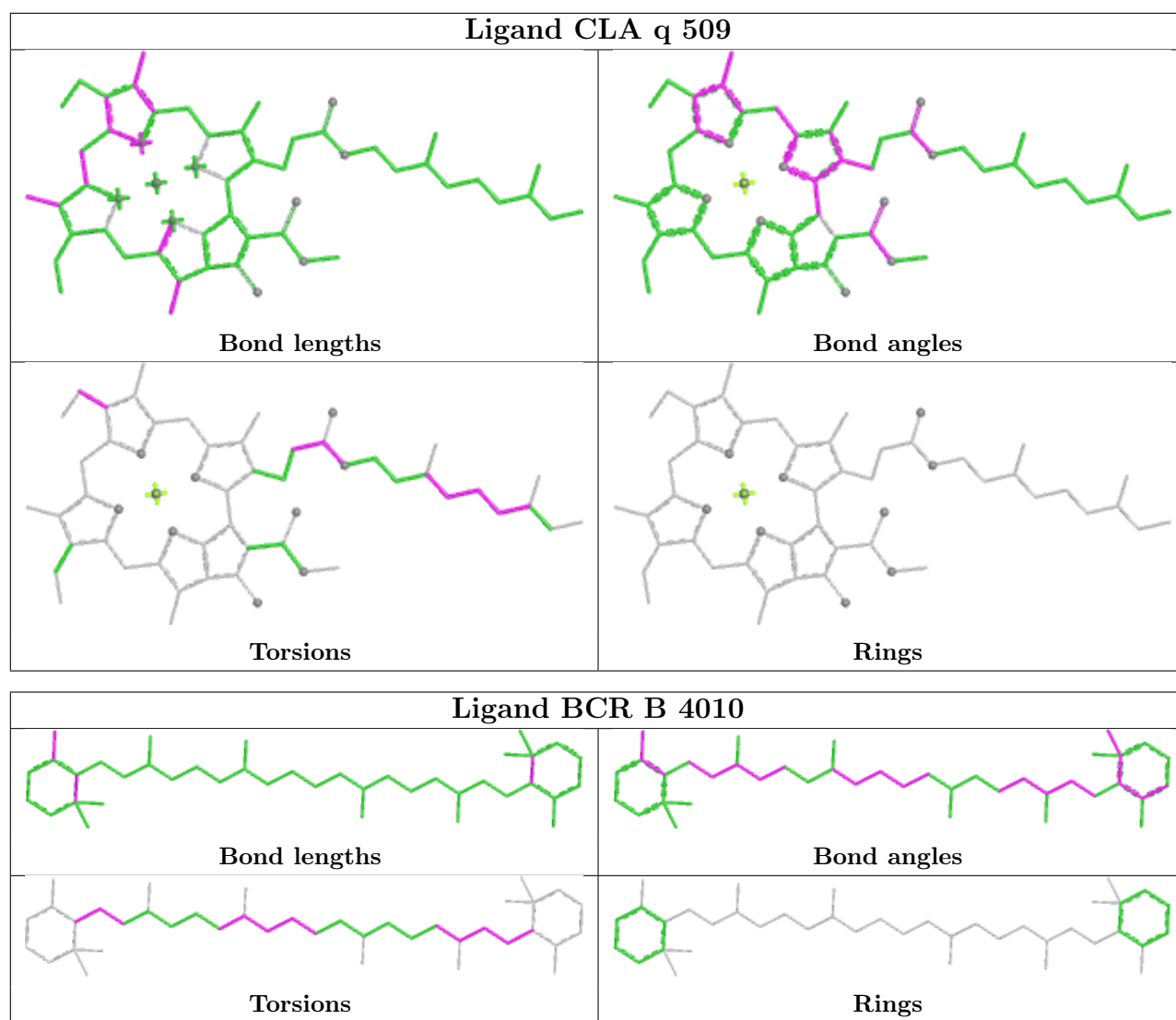


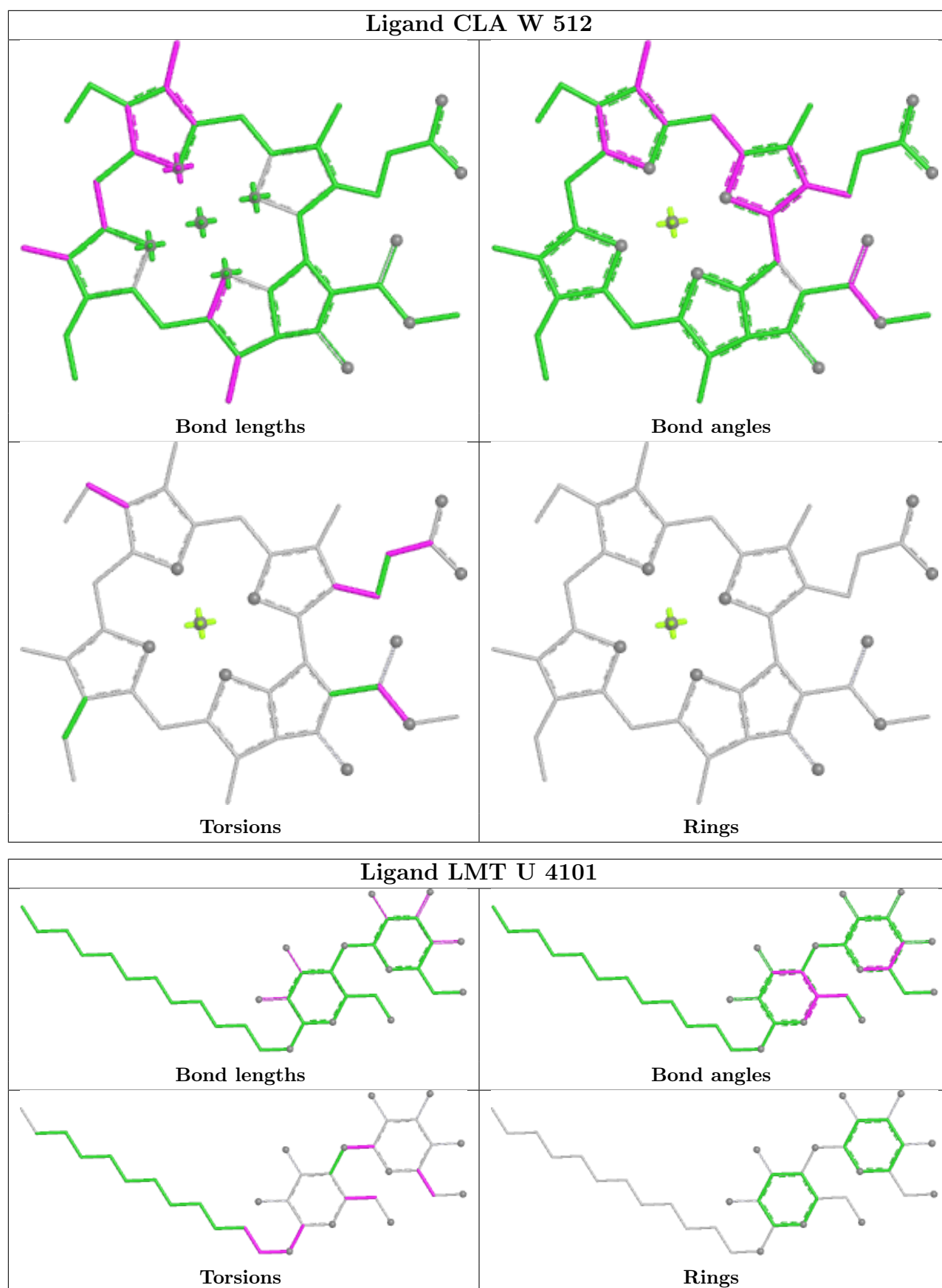
Ligand LMG H 4201



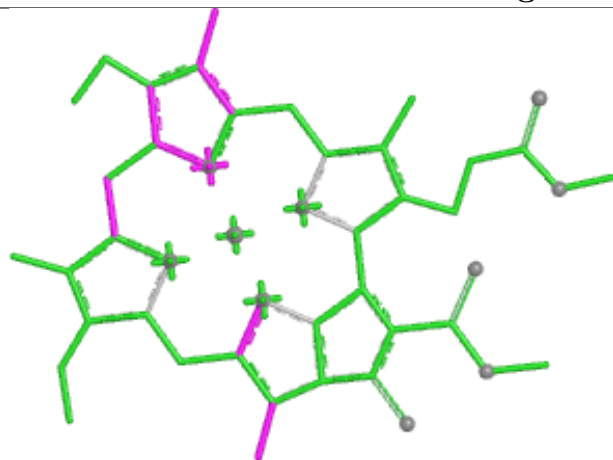




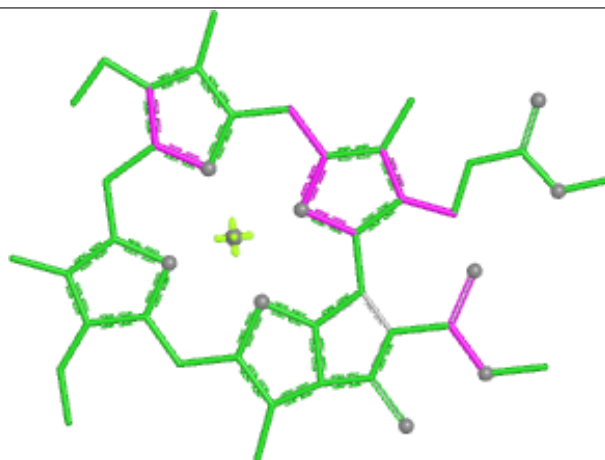




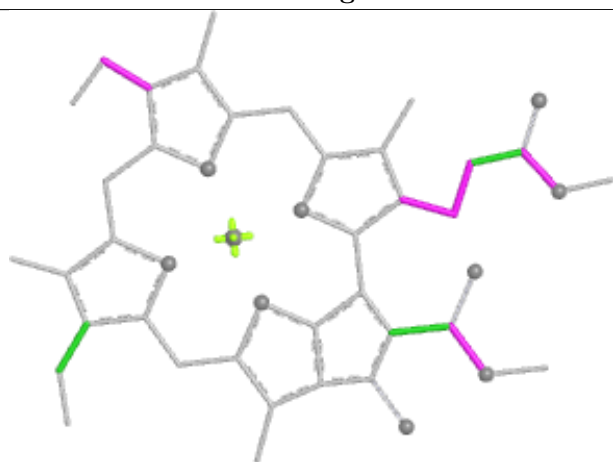
Ligand CLA v 501



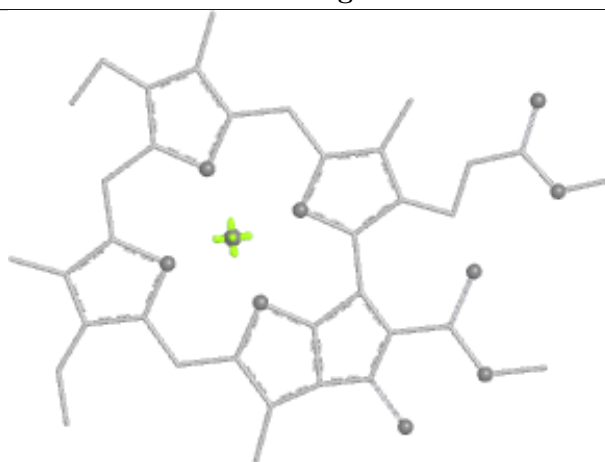
Bond lengths



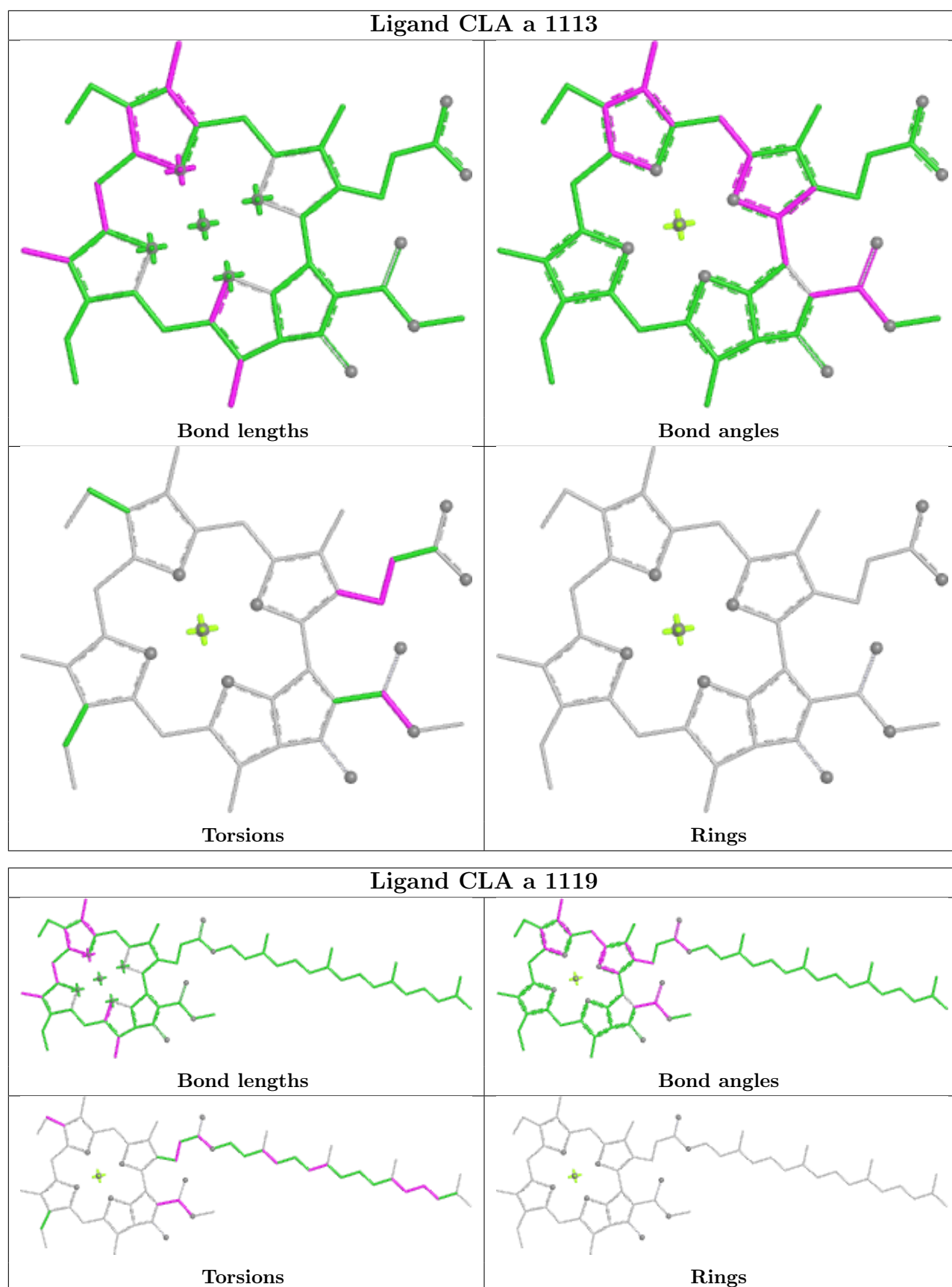
Bond angles

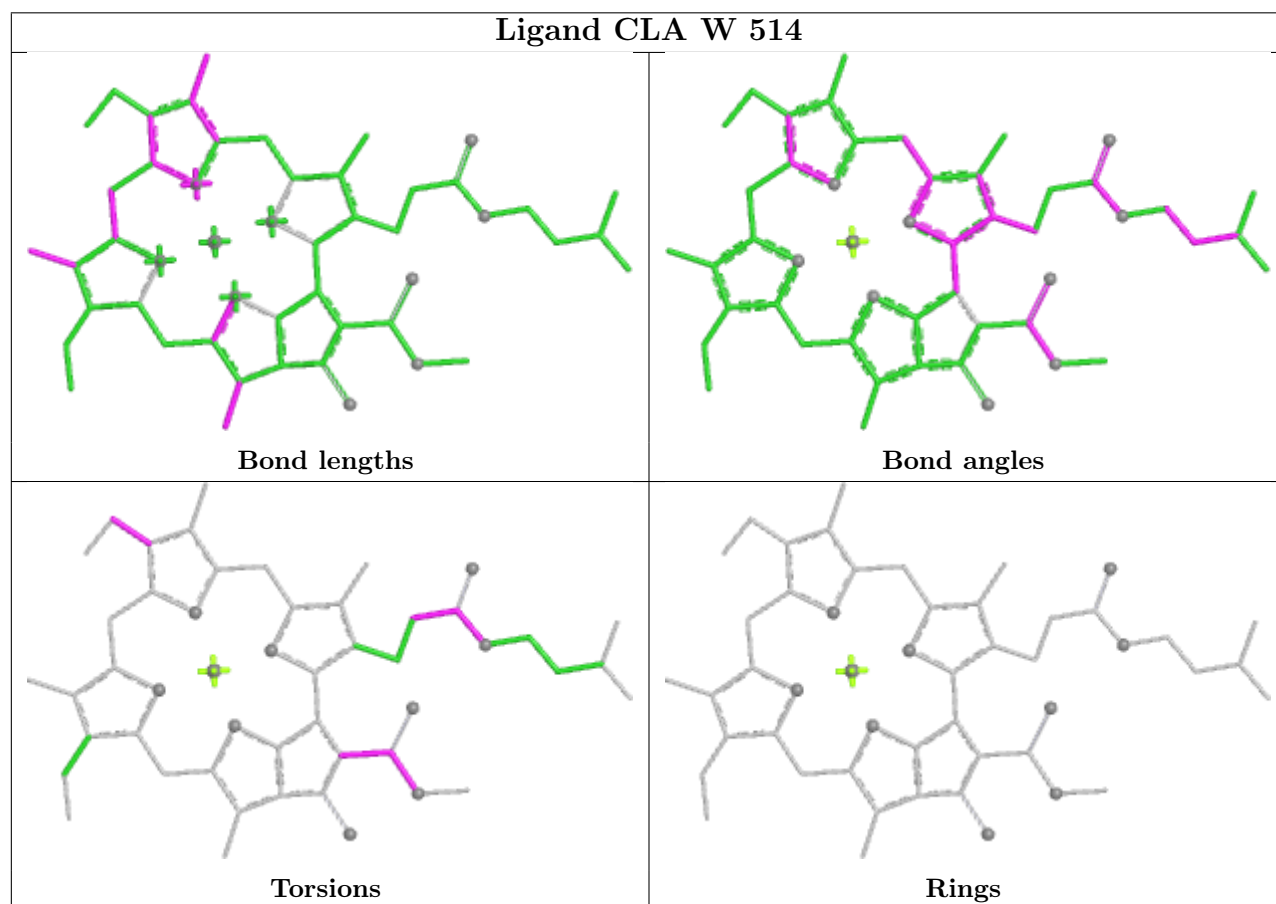
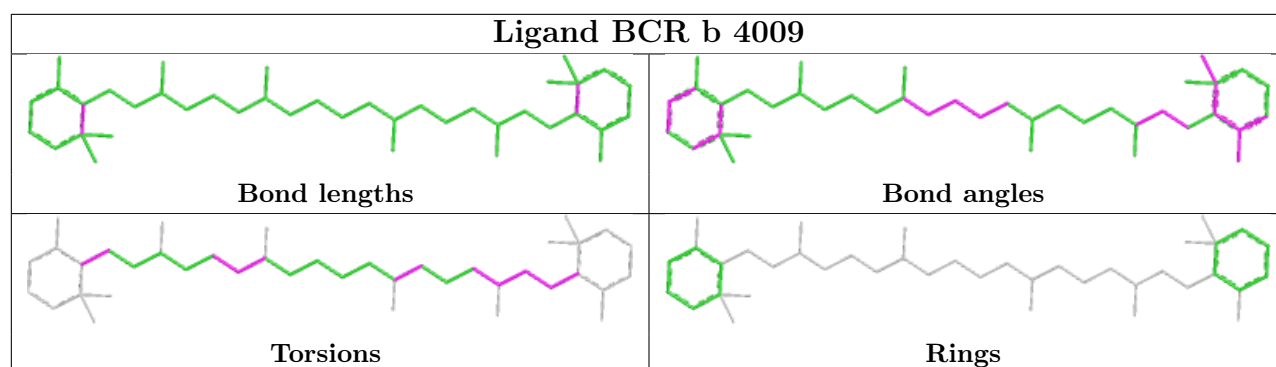


Torsions

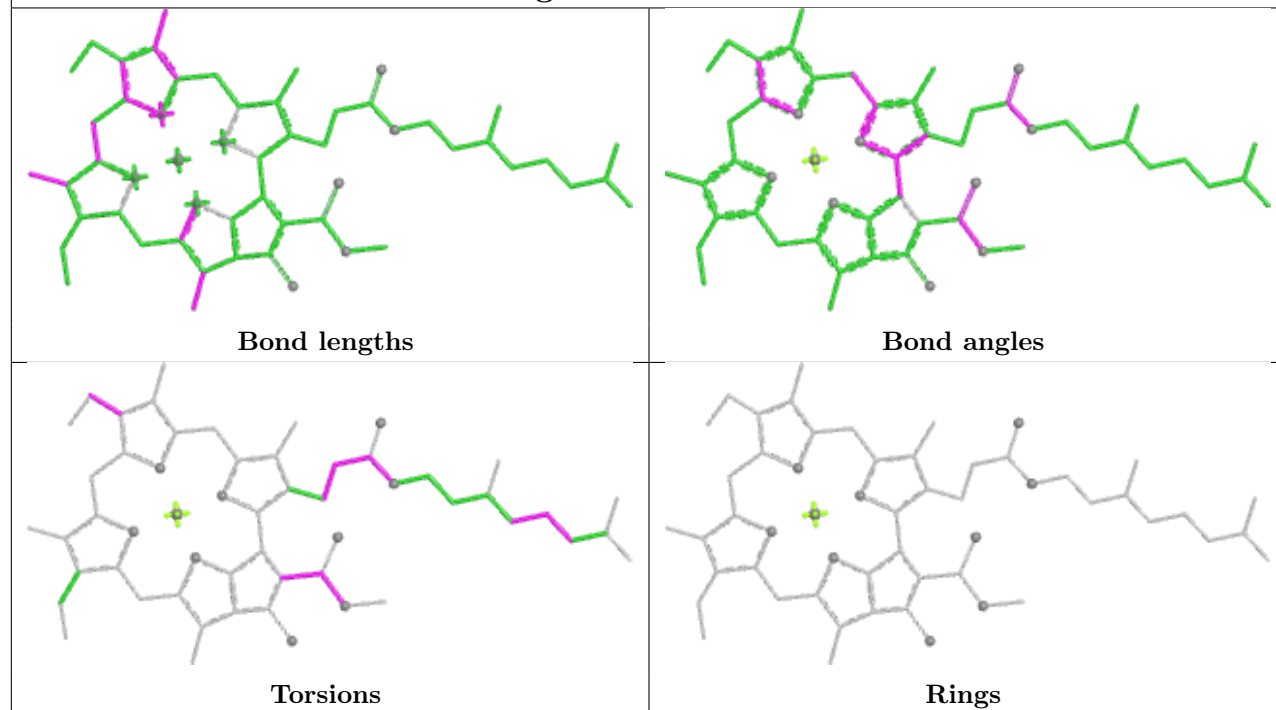


Rings

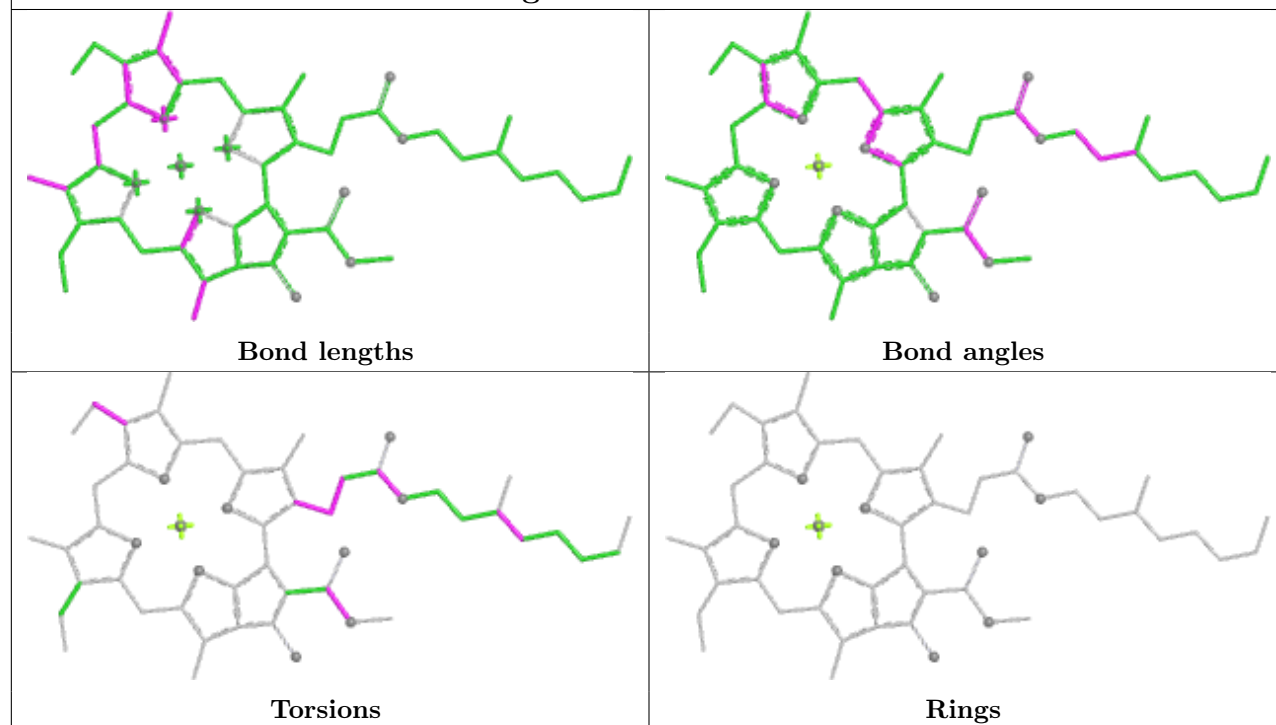




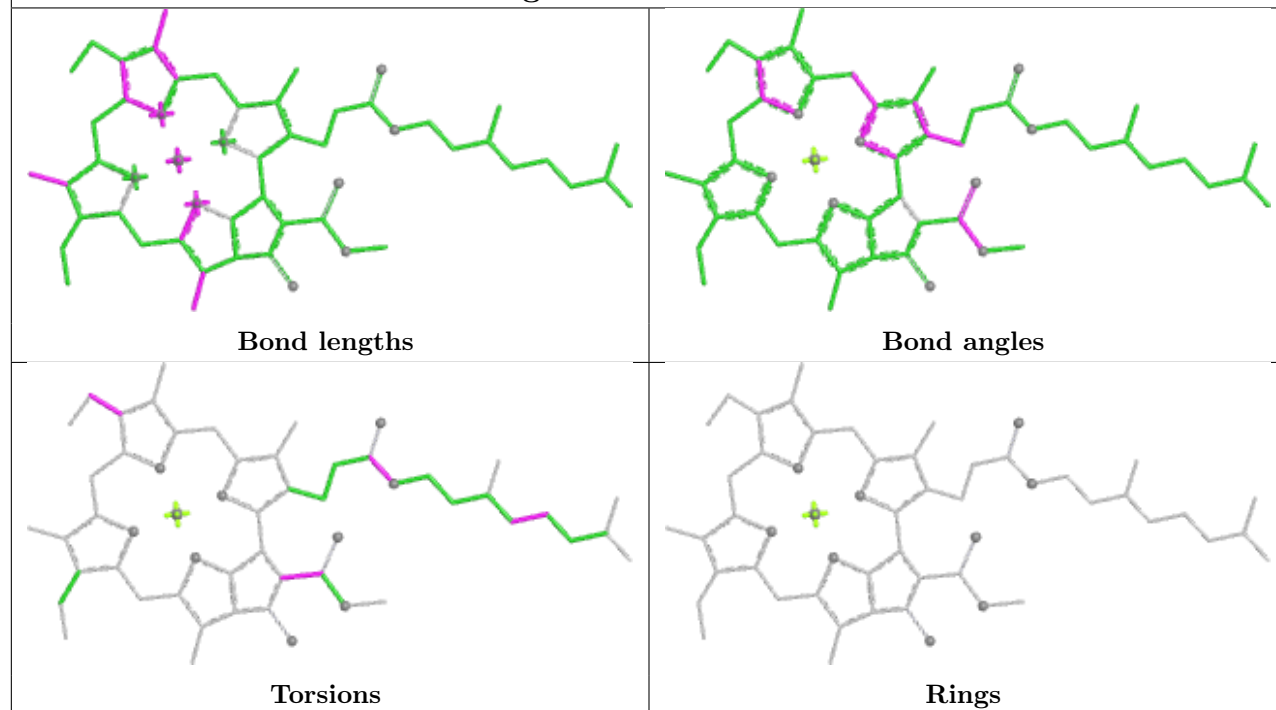
Ligand CLA x 517



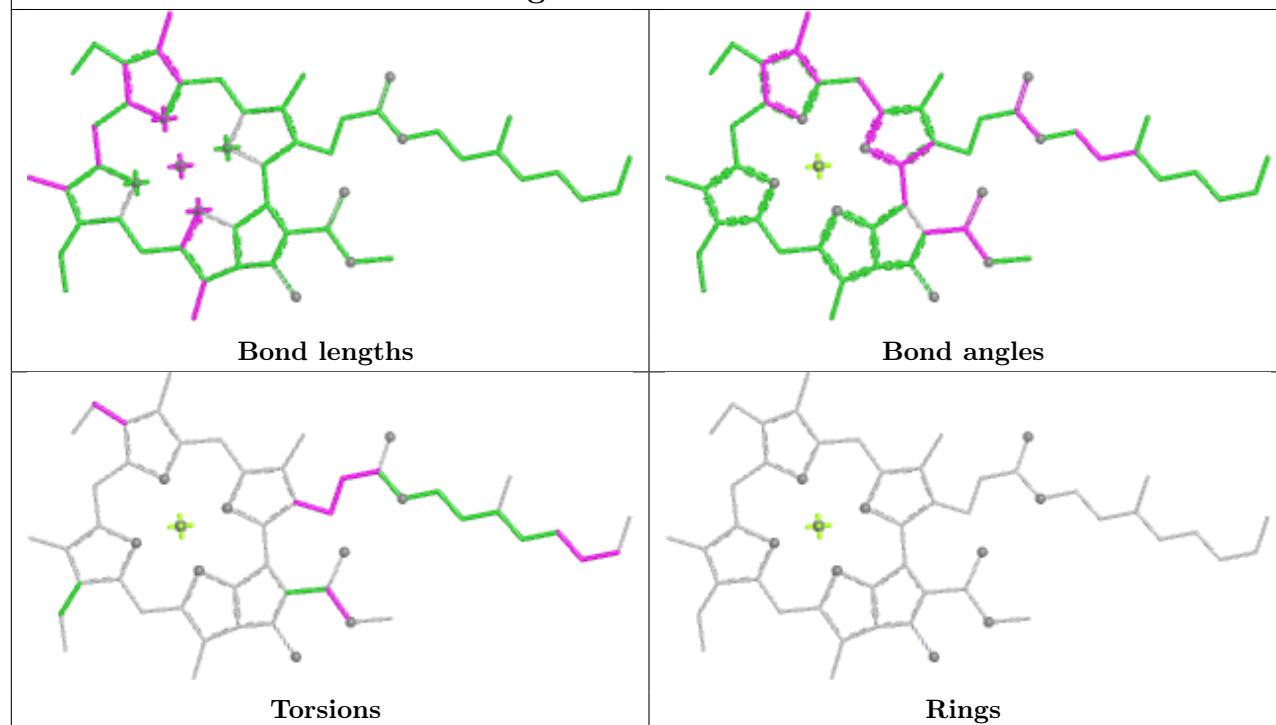
Ligand CLA H 1133



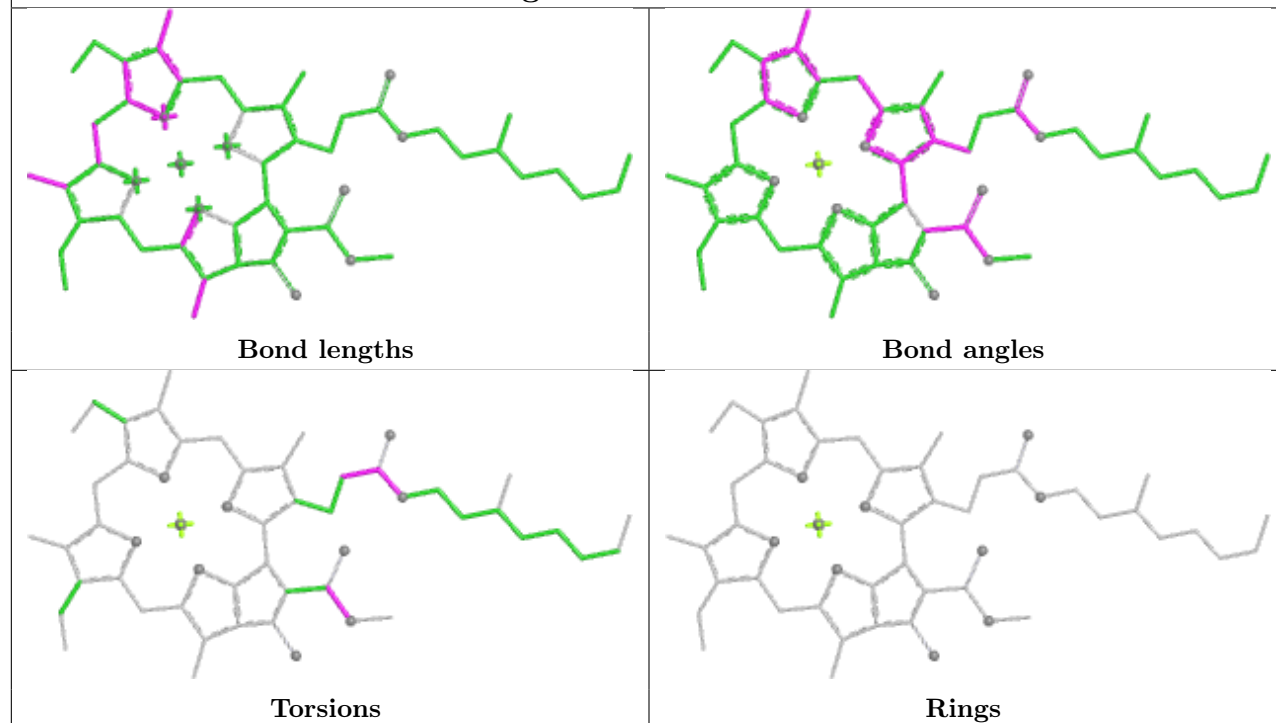
Ligand CLA A 1118



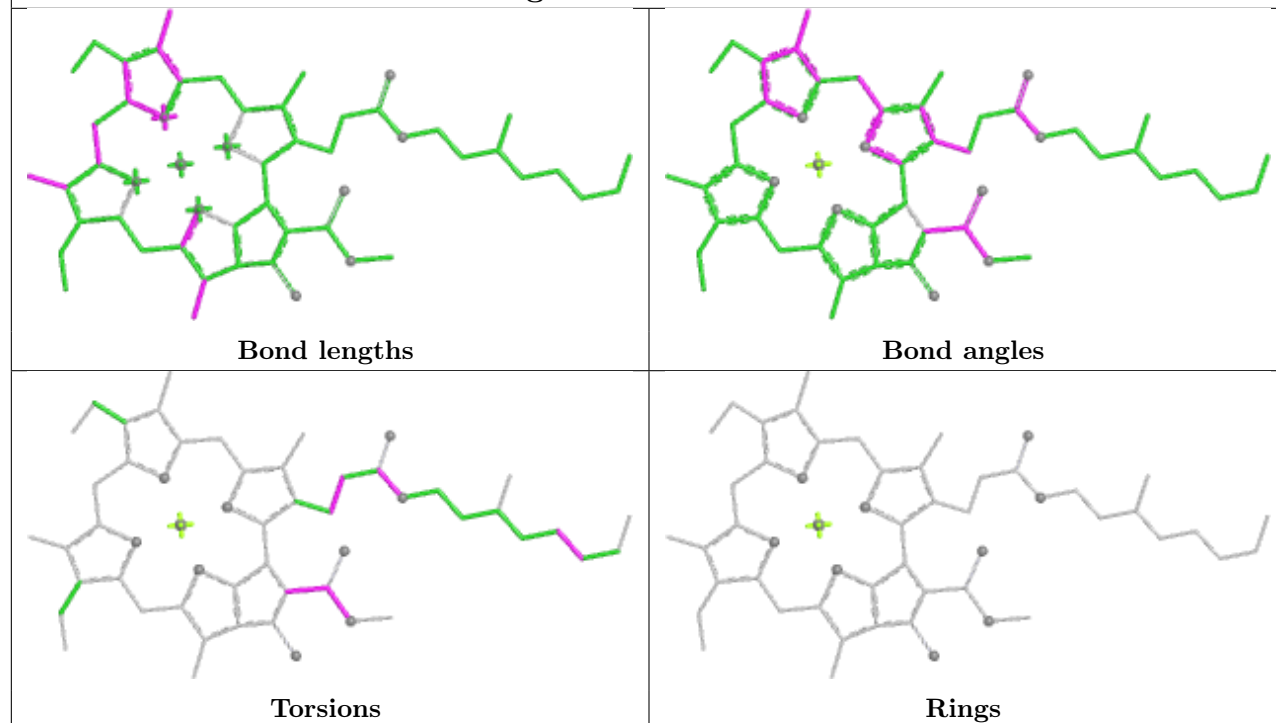
Ligand CLA a 1116



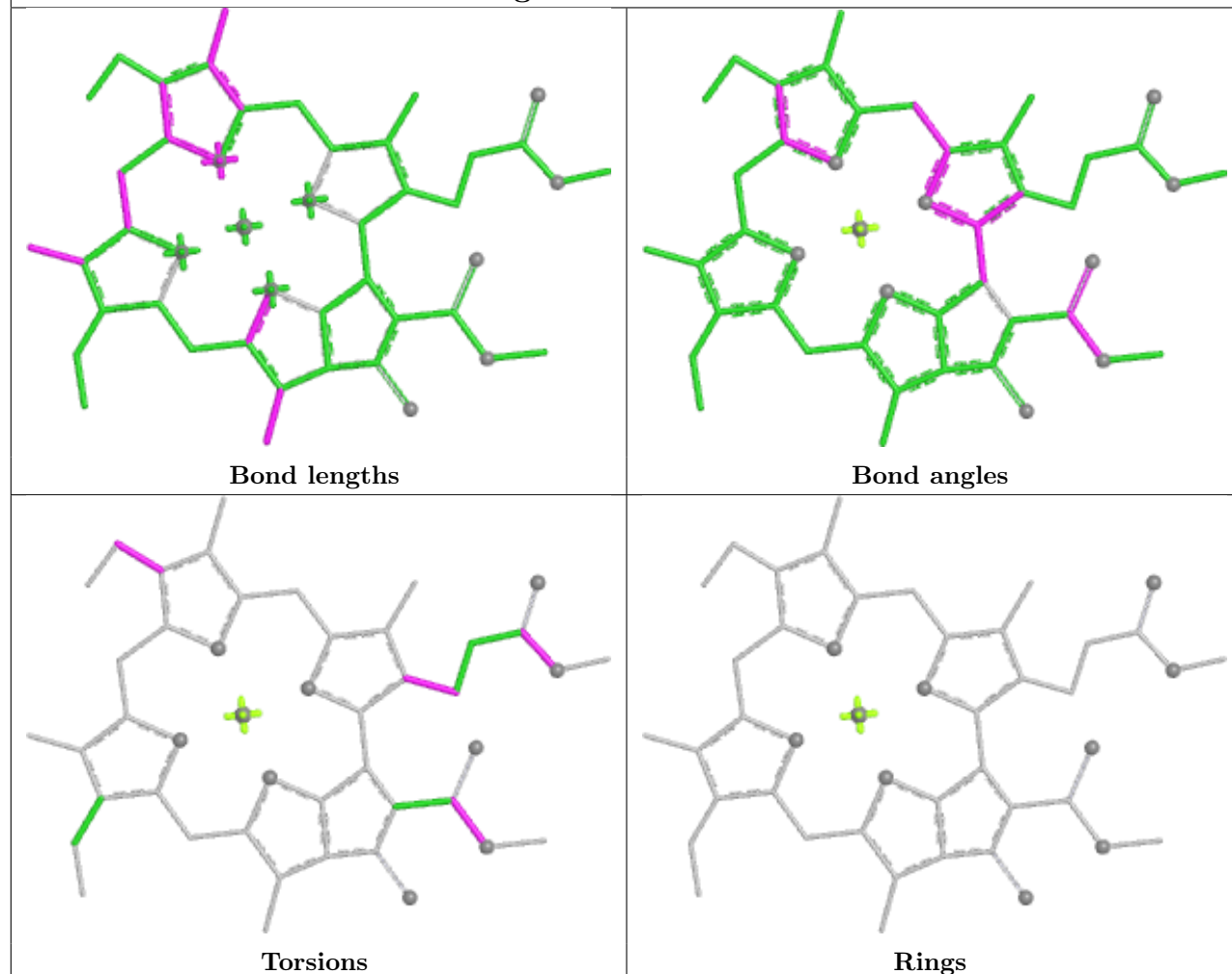
Ligand CLA G 1220



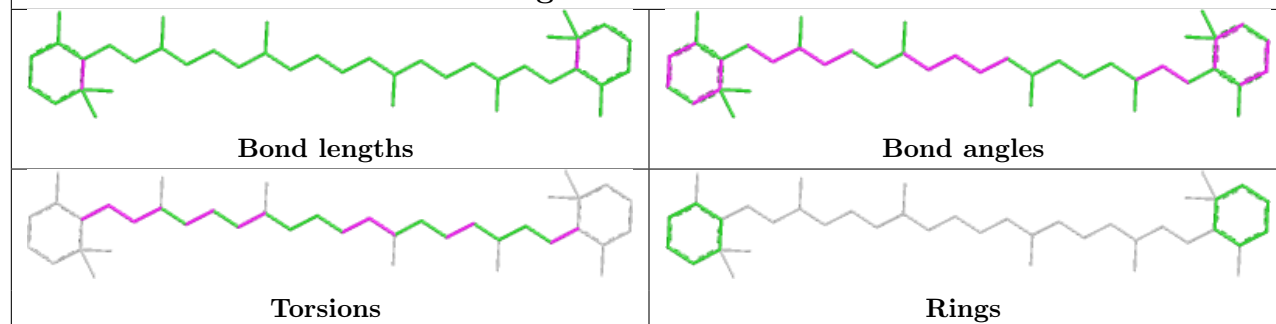
Ligand CLA b 1201



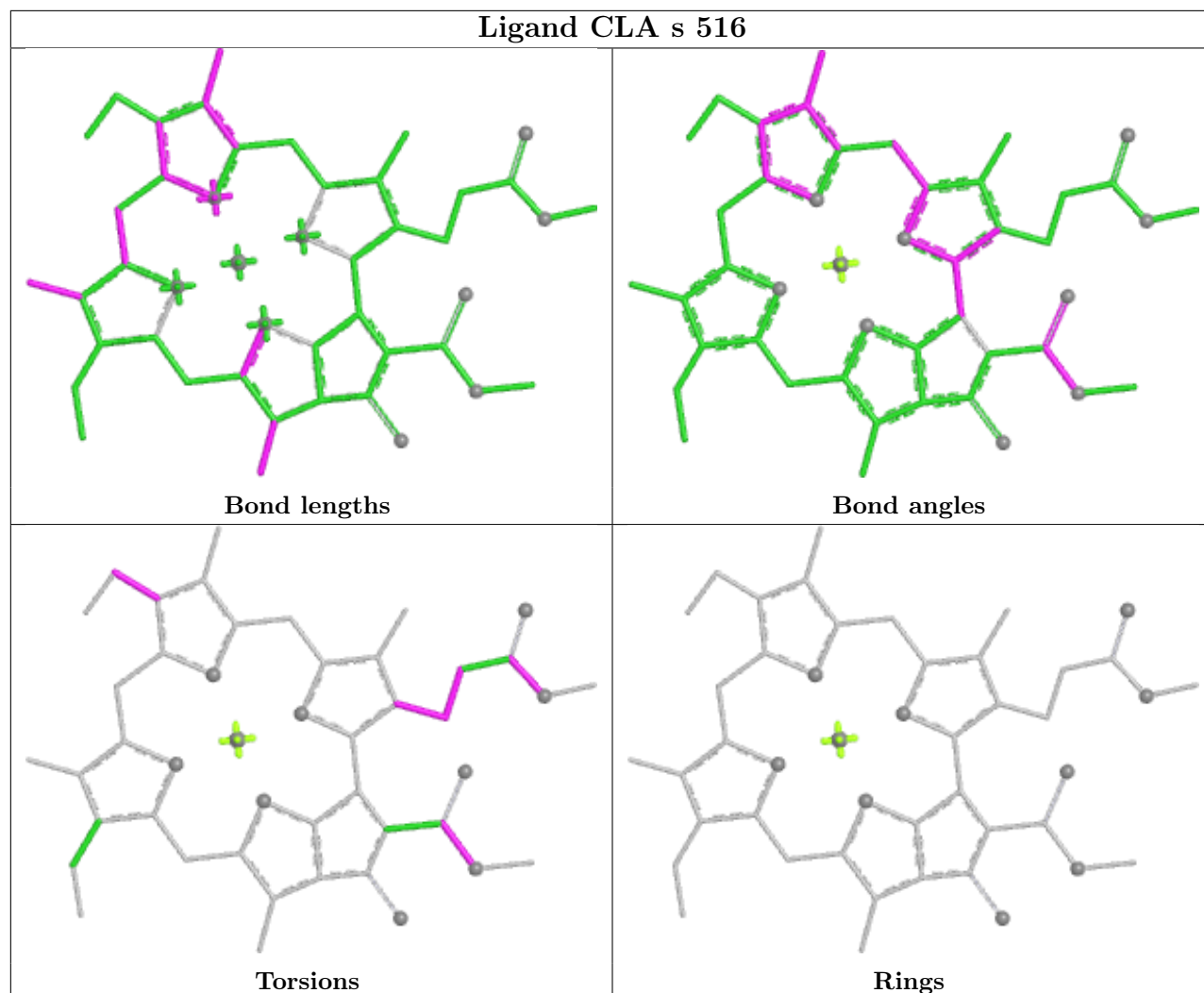
Ligand CLA w 516

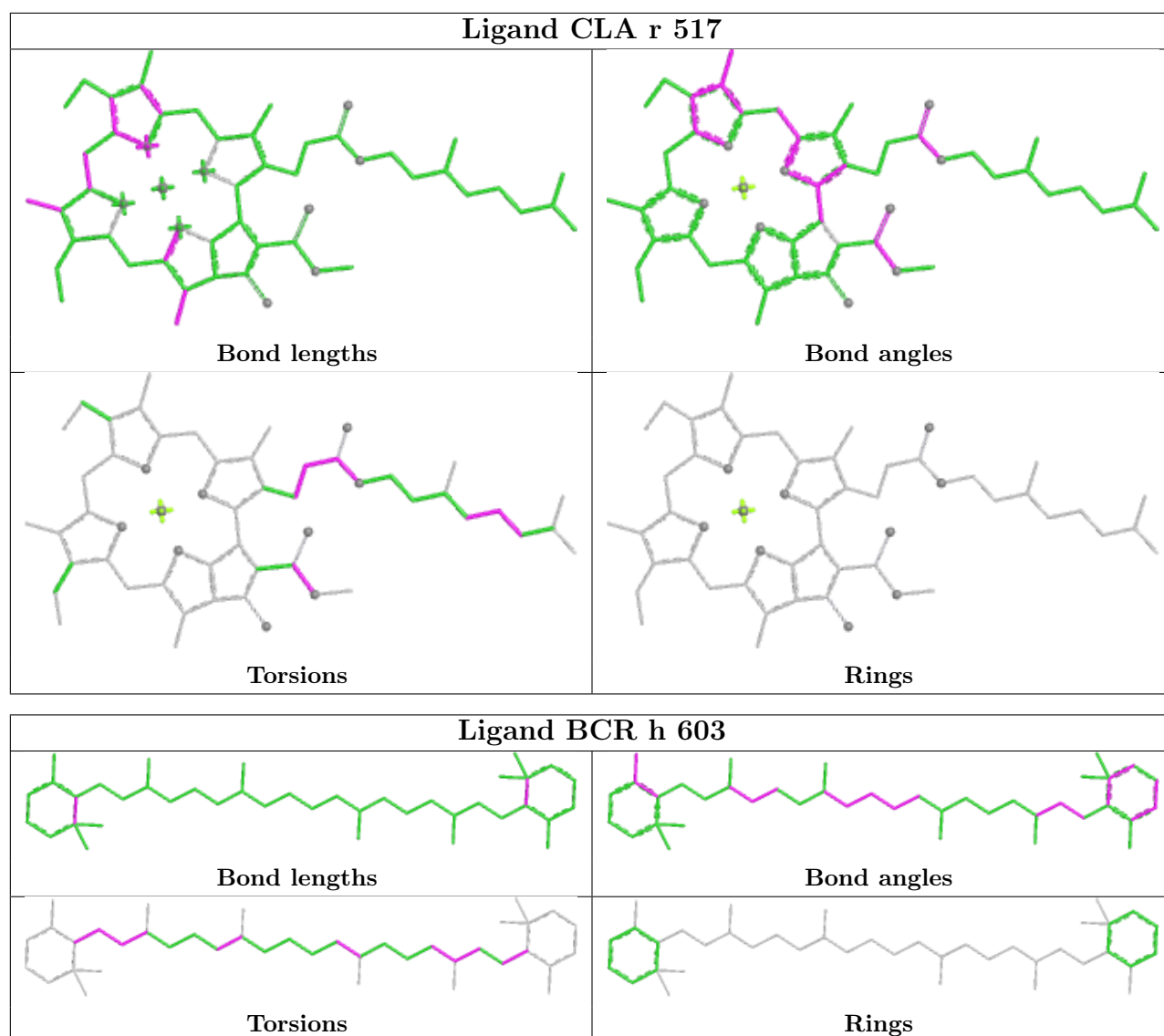


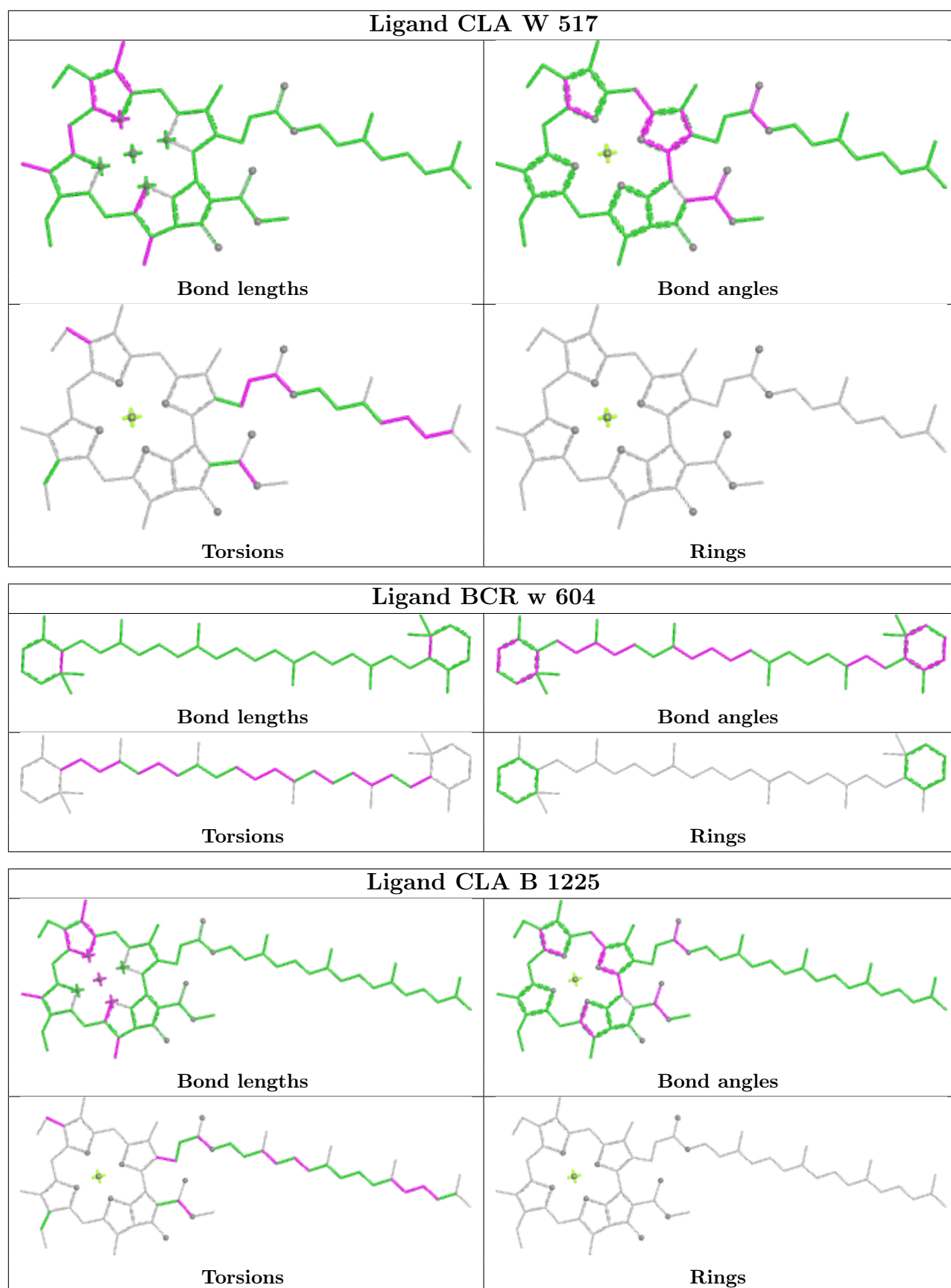
Ligand BCR t 601

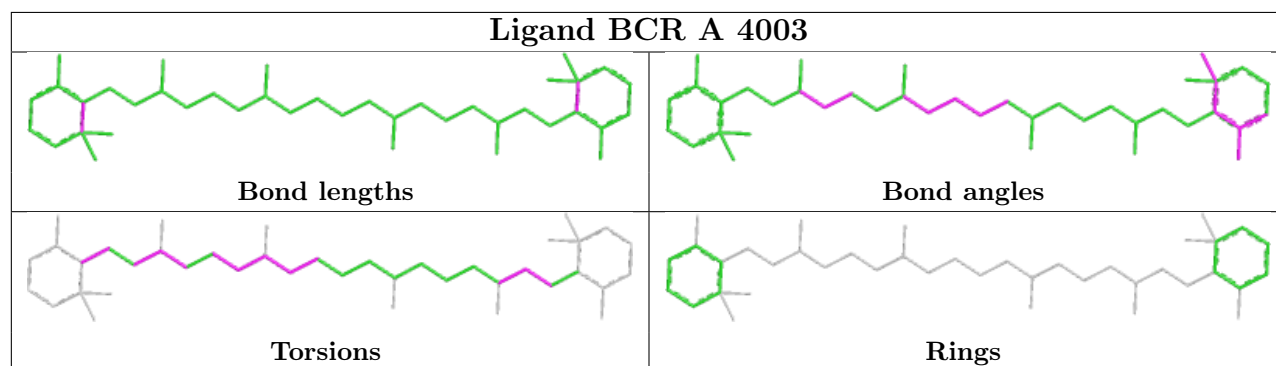
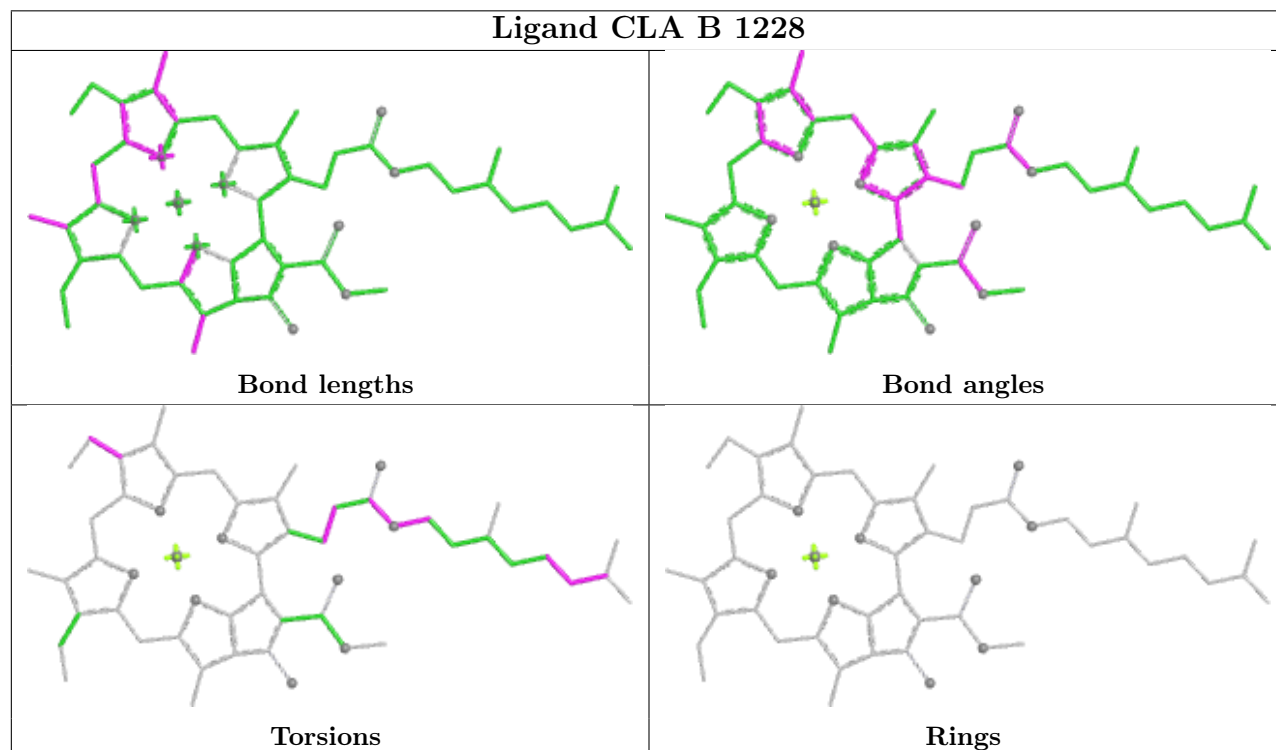
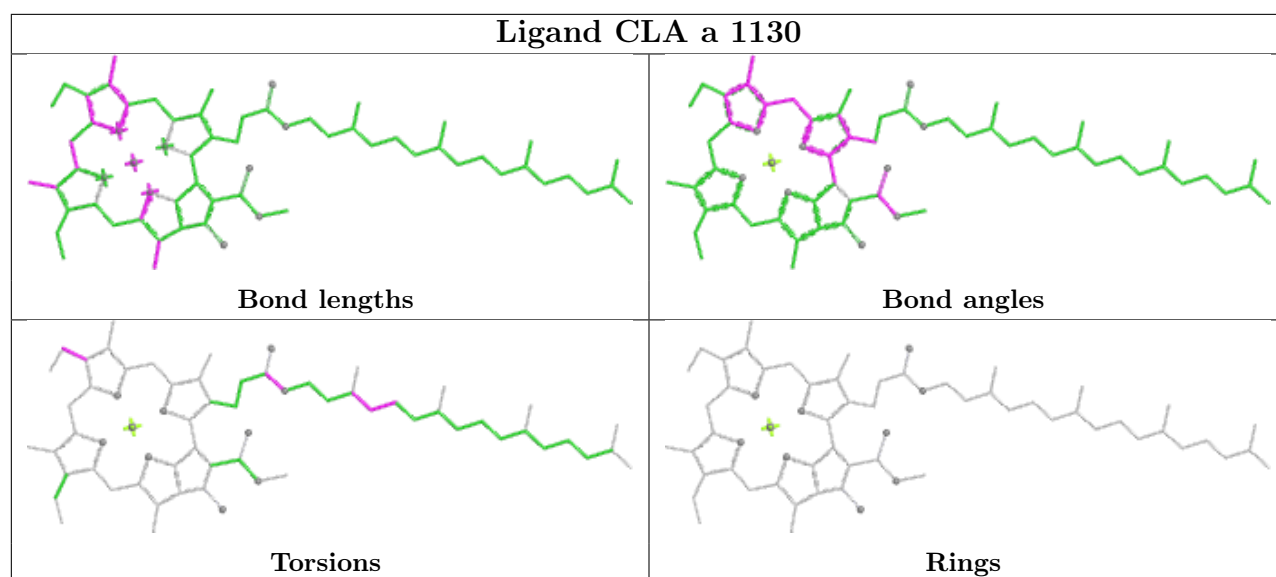


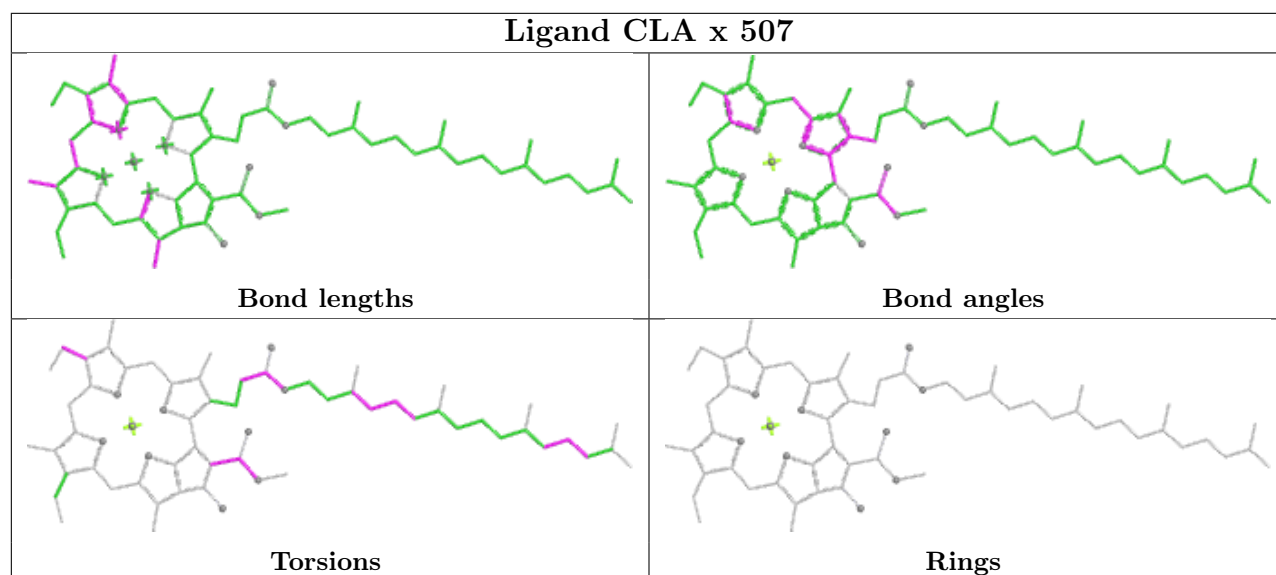
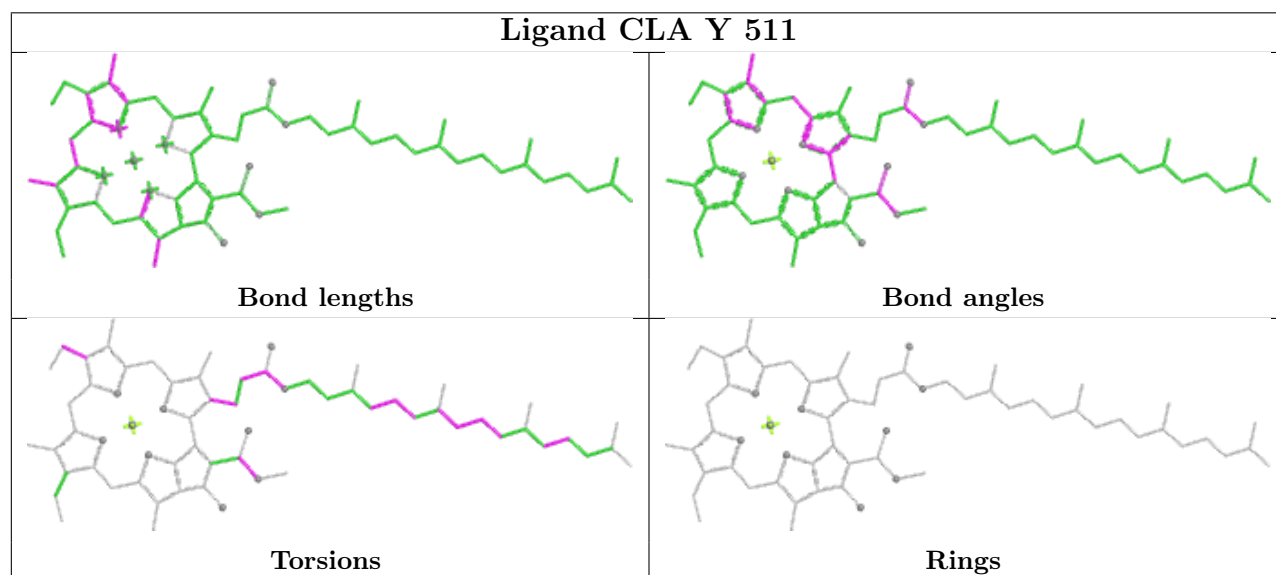
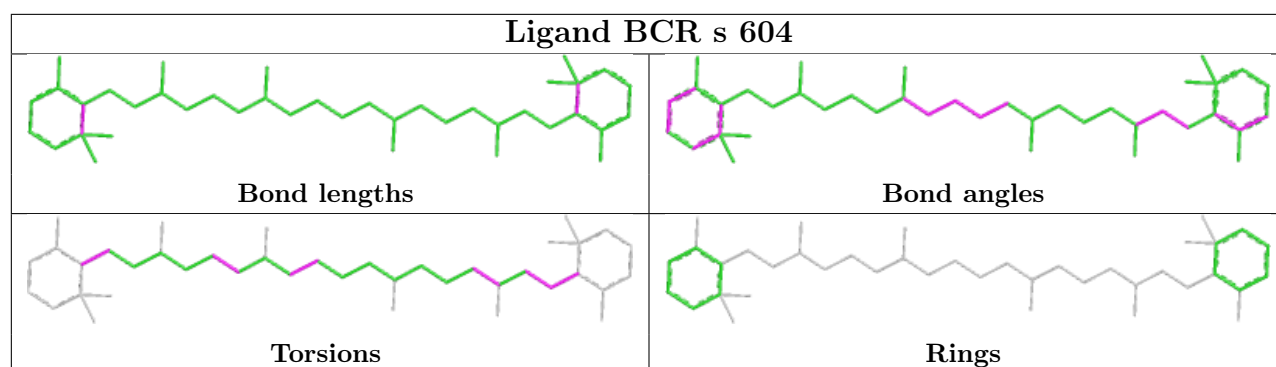
Ligand CLA s 516

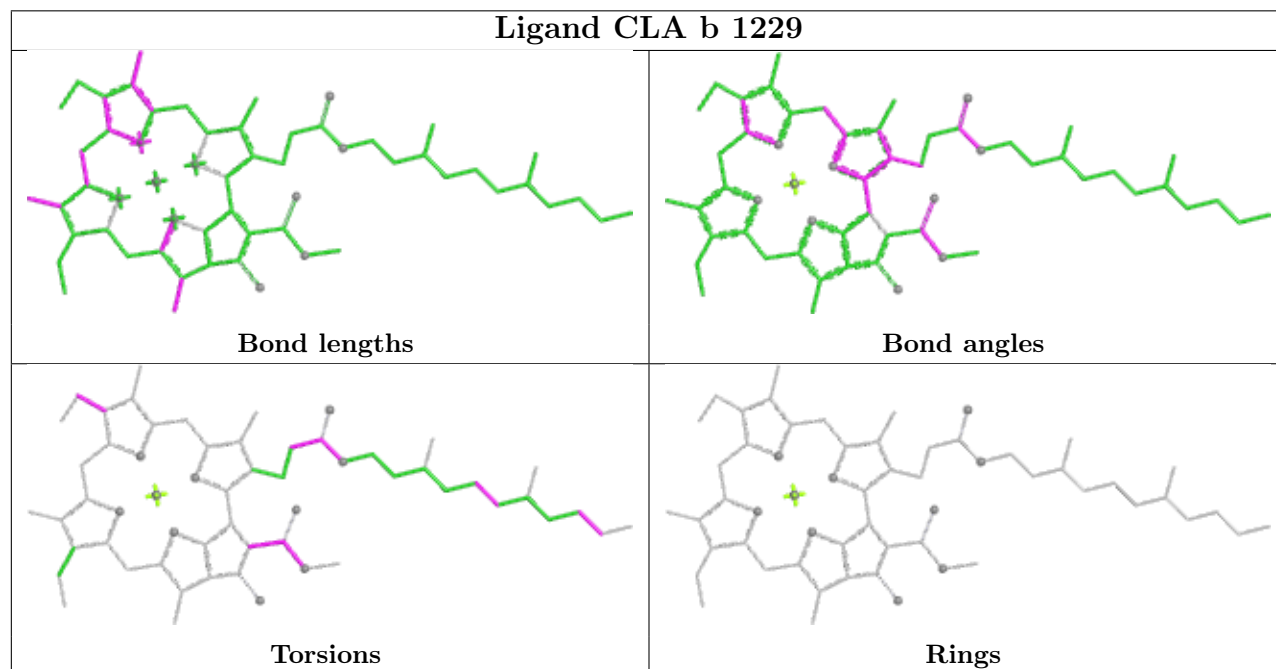
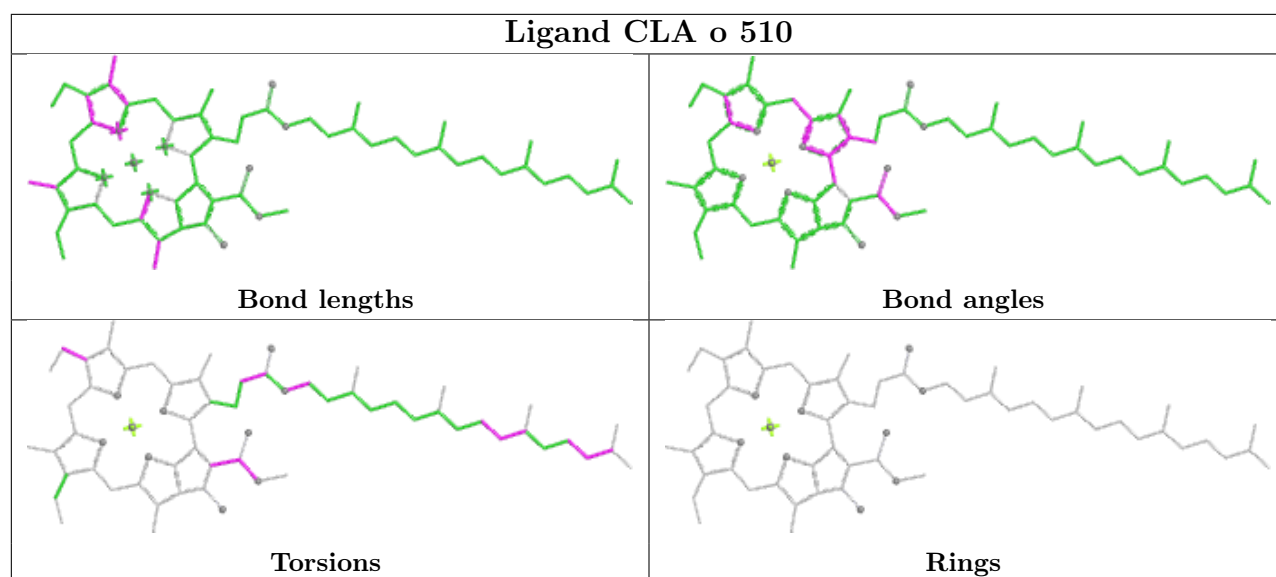


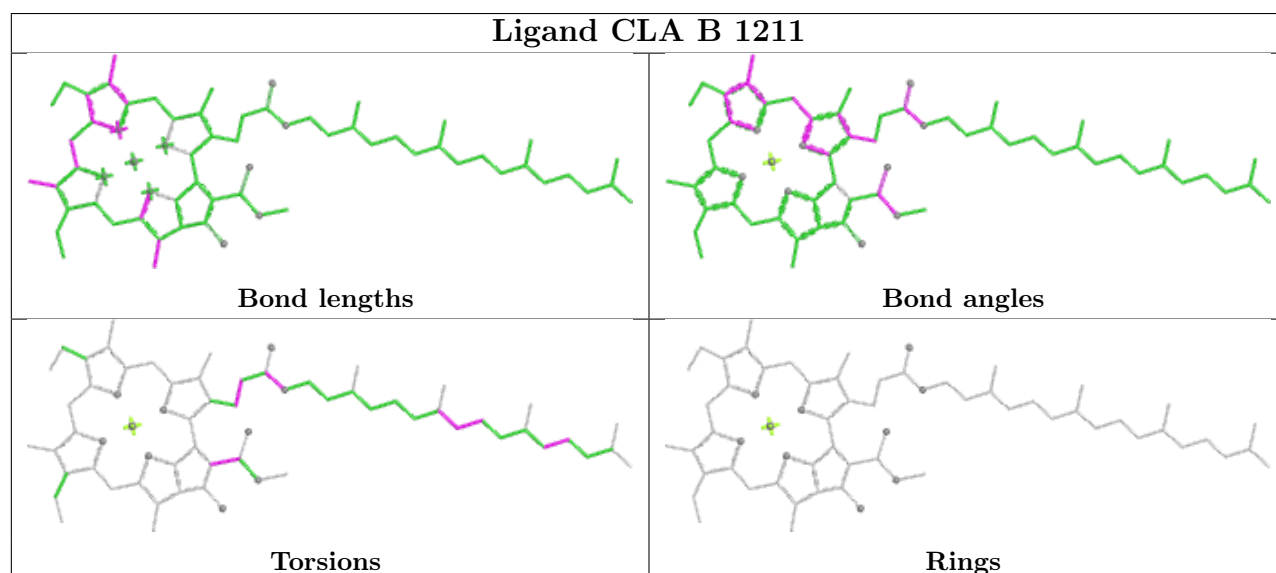
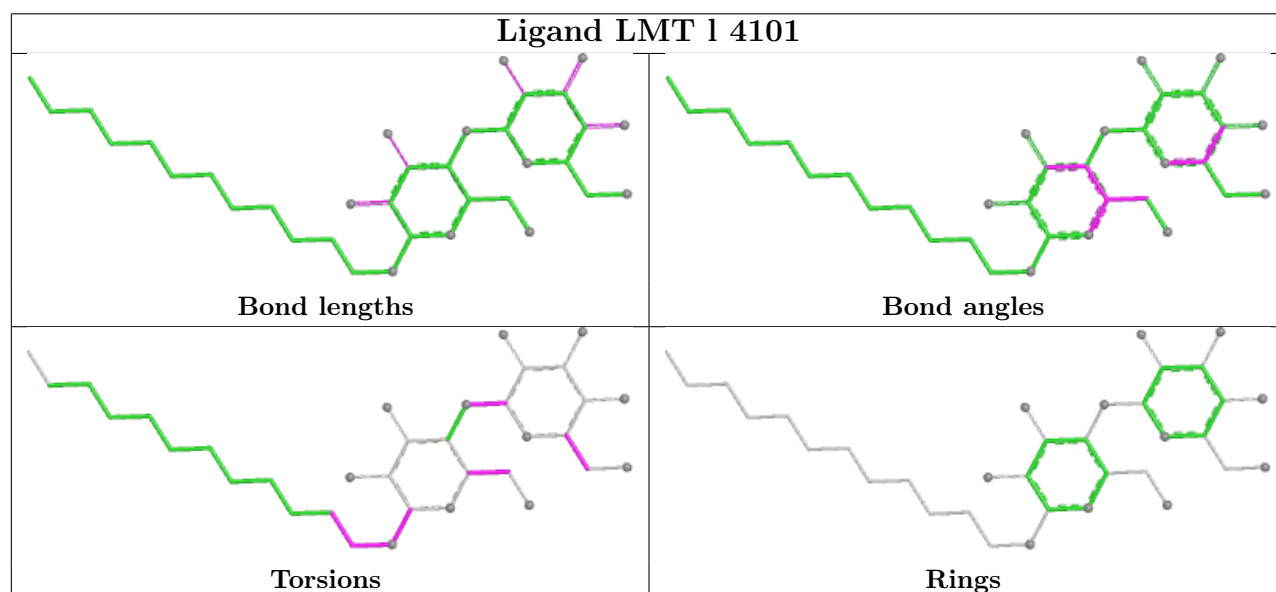
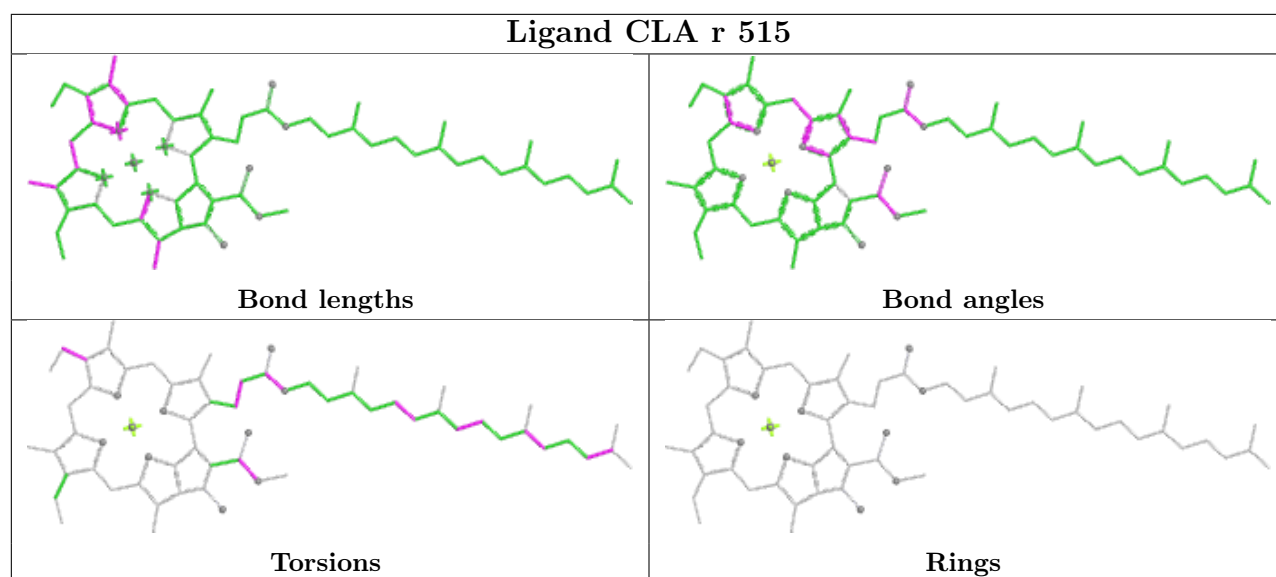




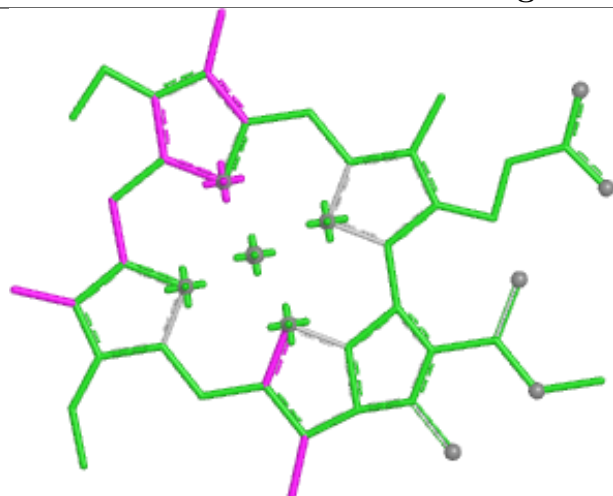




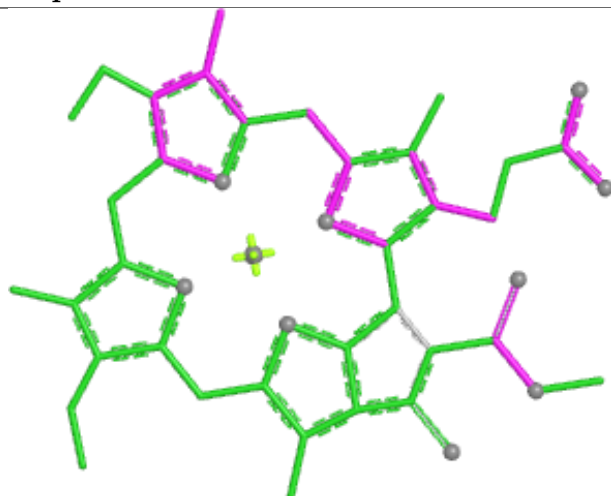




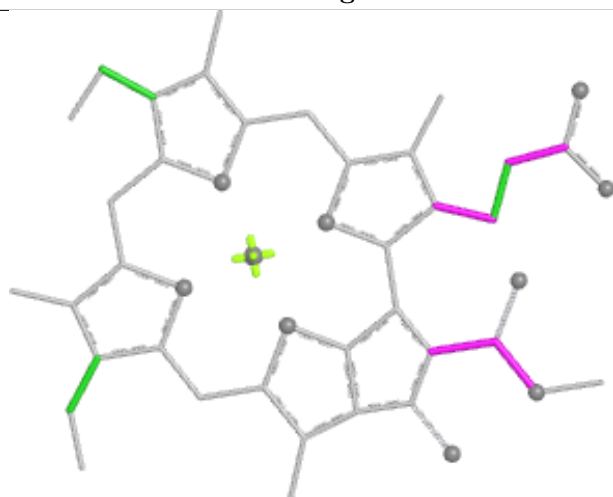
Ligand CLA p 512



Bond lengths



Bond angles

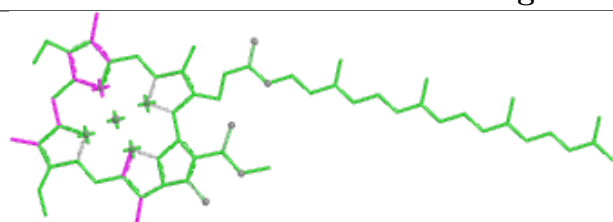


Torsions

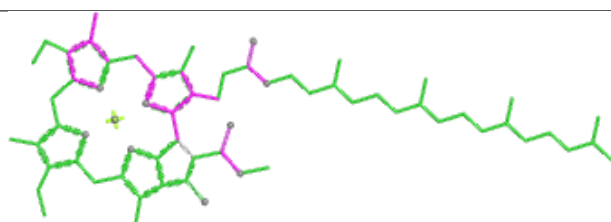


Rings

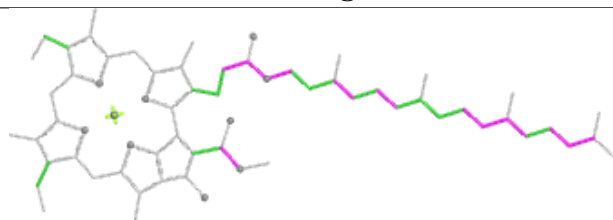
Ligand CLA h 511



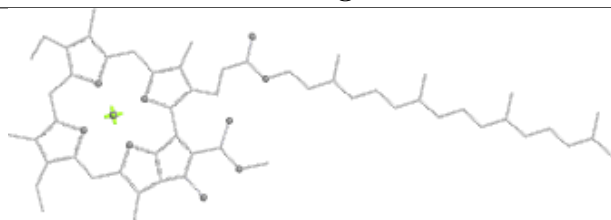
Bond lengths



Bond angles

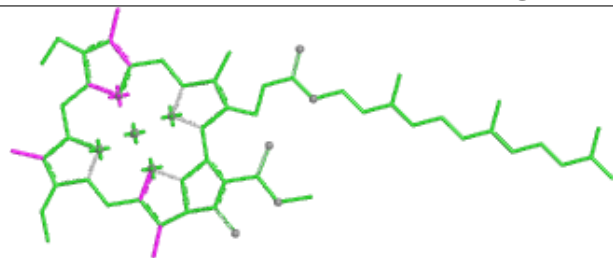


Torsions

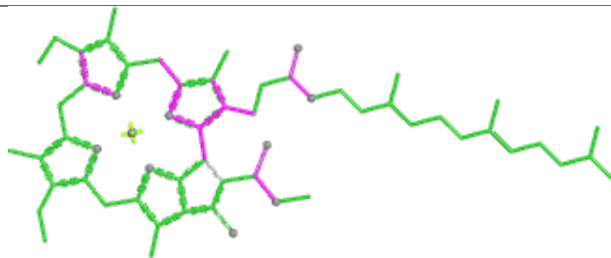


Rings

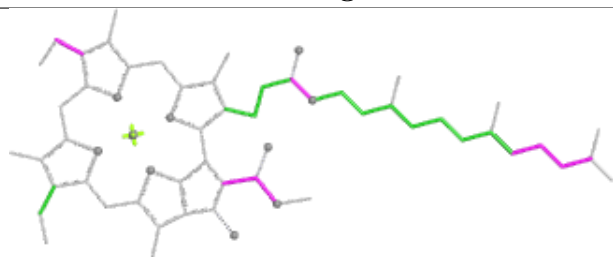
Ligand CLA Y 506



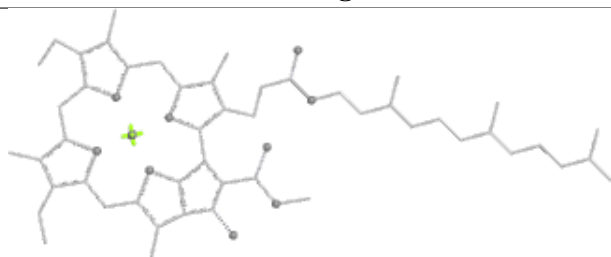
Bond lengths



Bond angles

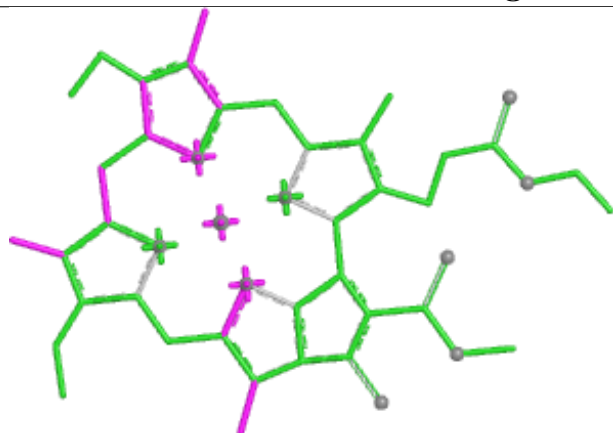


Torsions

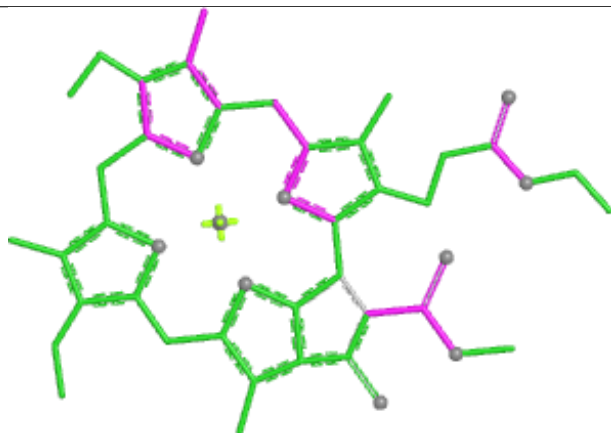


Rings

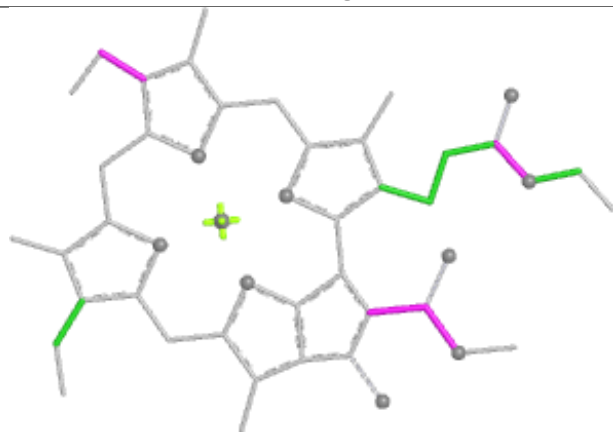
Ligand CLA H 1137



Bond lengths



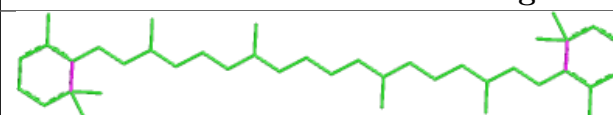
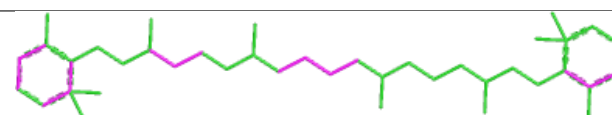
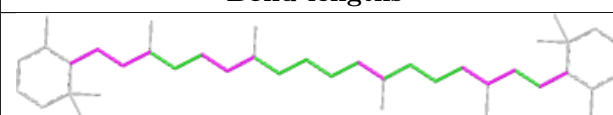
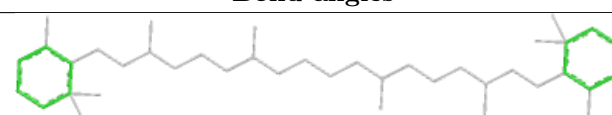
Bond angles

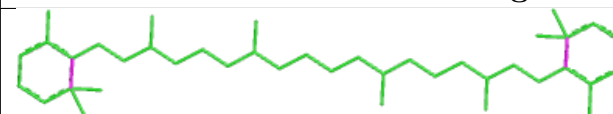
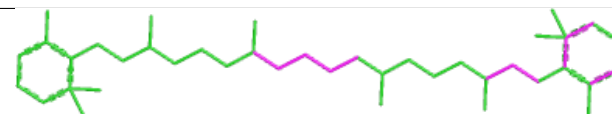
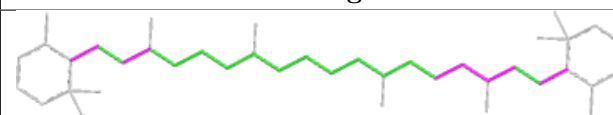
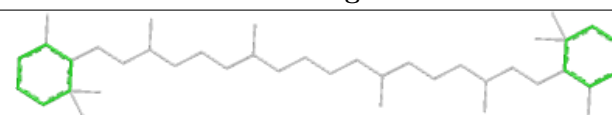


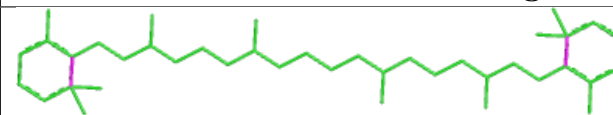
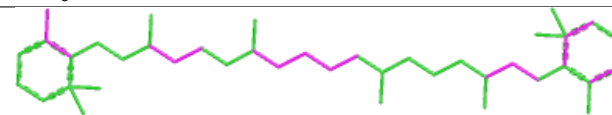
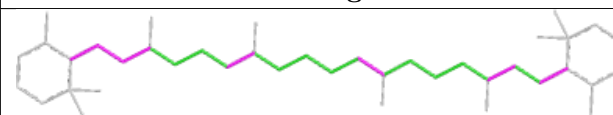
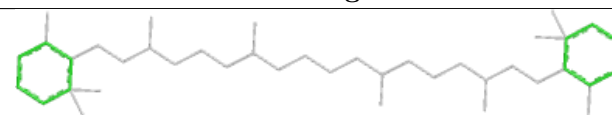
Torsions



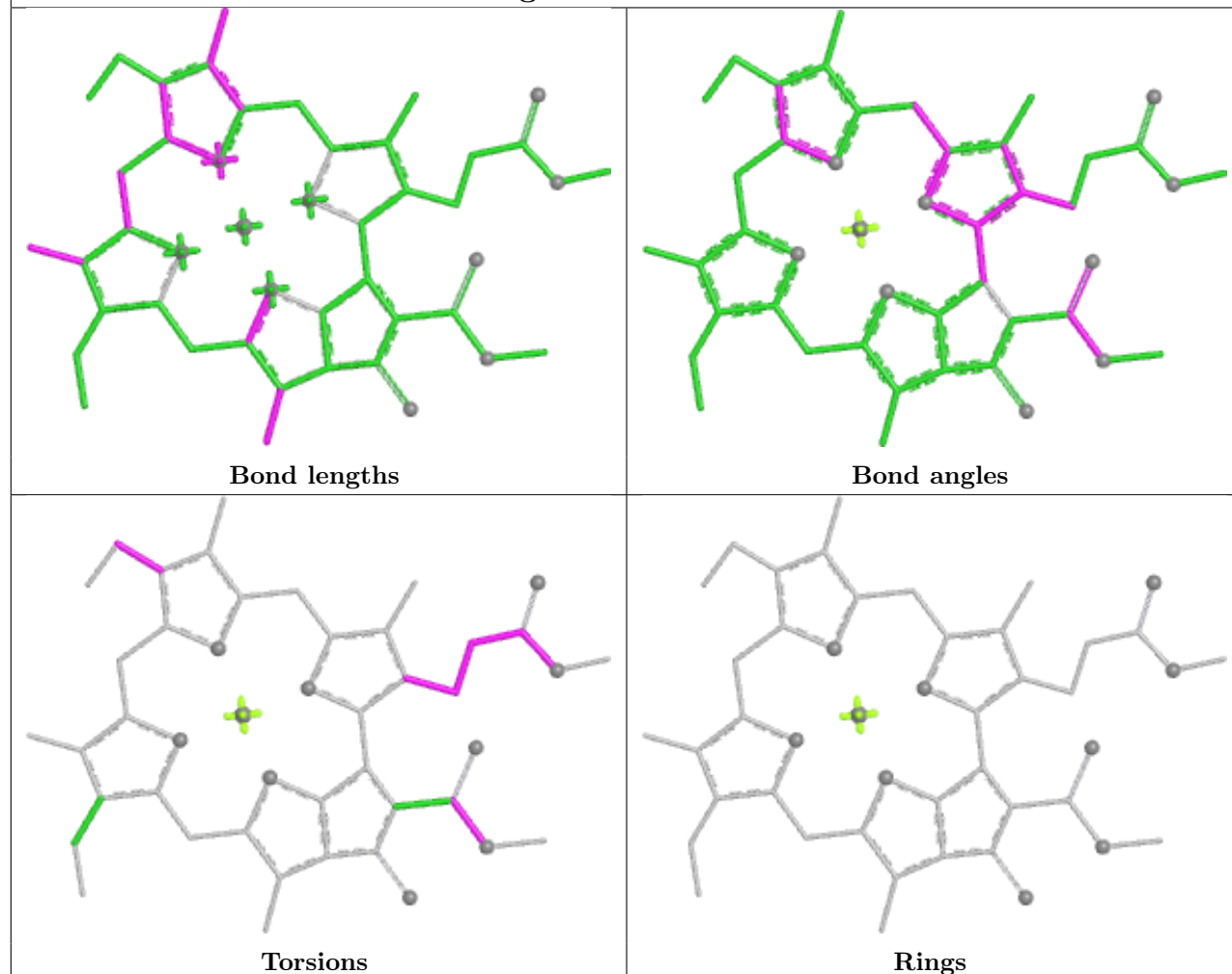
Rings

Ligand BCR i 4018	
	
Bond lengths	Bond angles
	
Torsions	Rings

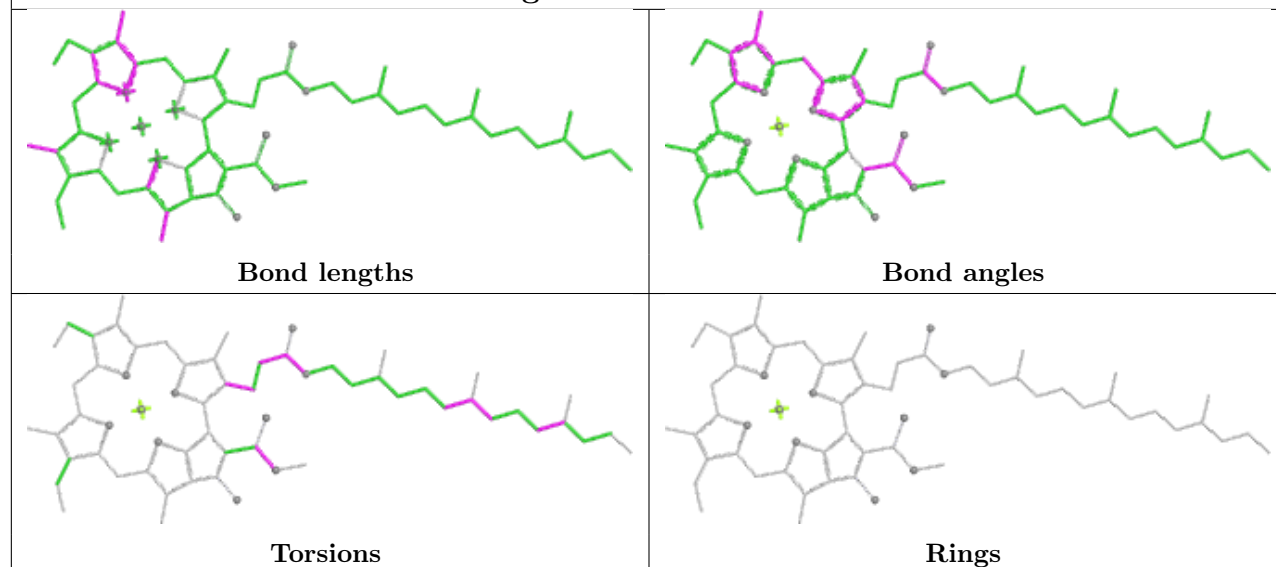
Ligand BCR B 4004	
	
Bond lengths	Bond angles
	
Torsions	Rings

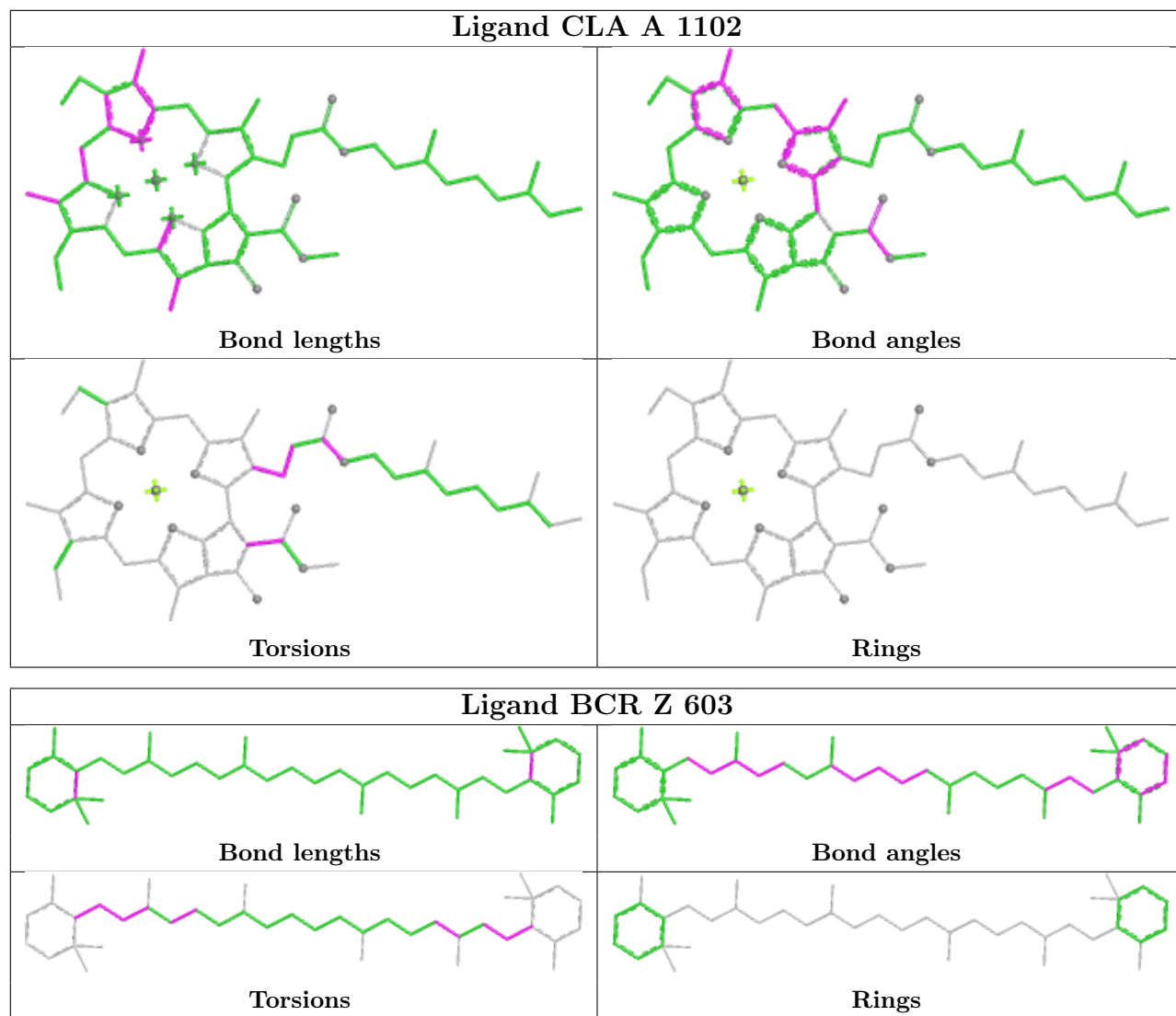
Ligand BCR y 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA r 503

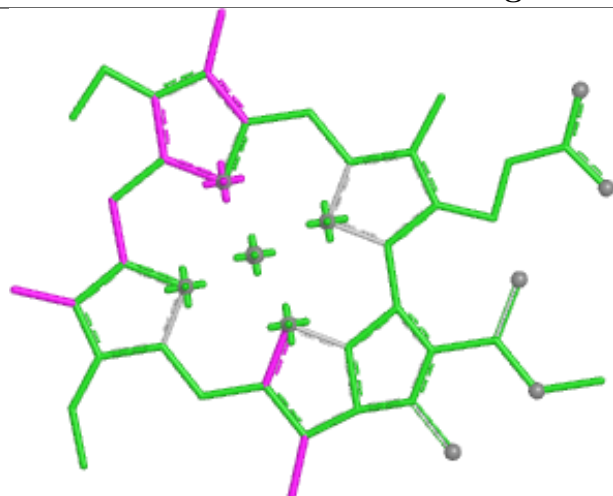


Ligand CLA G 1235

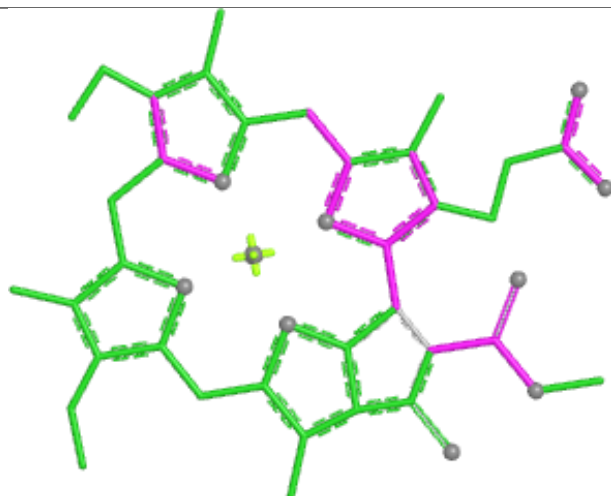




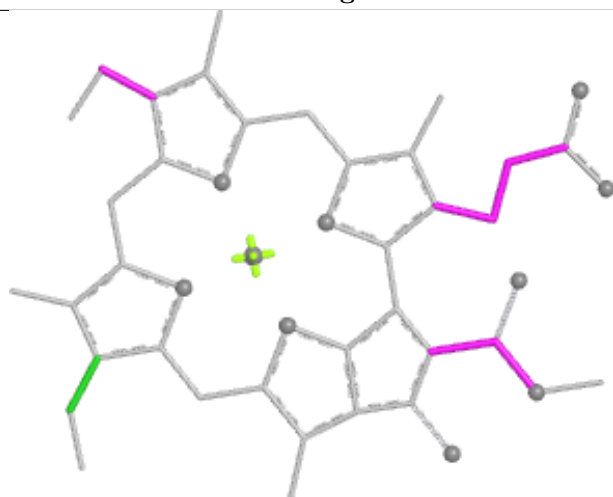
Ligand CLA A 1134



Bond lengths



Bond angles

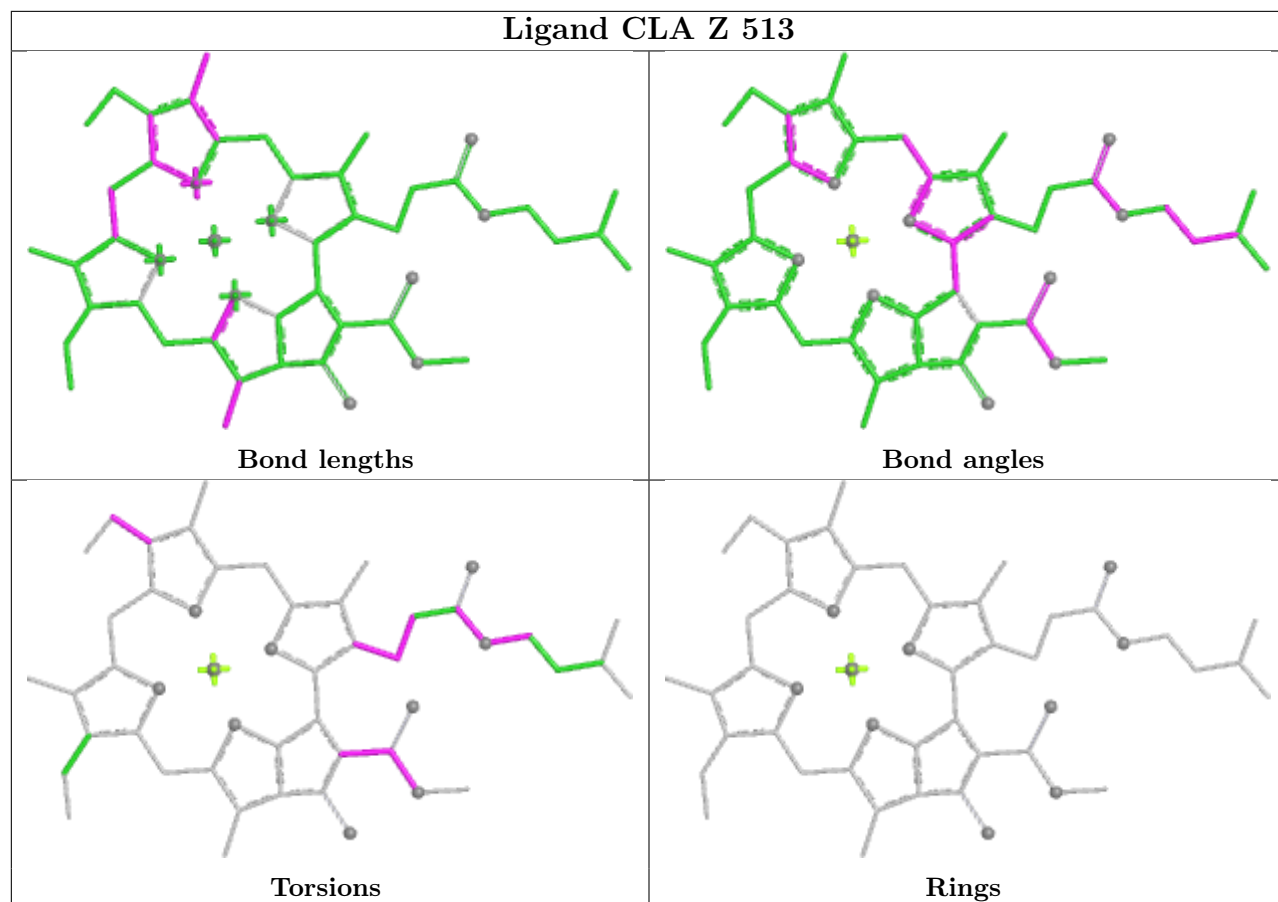


Torsions

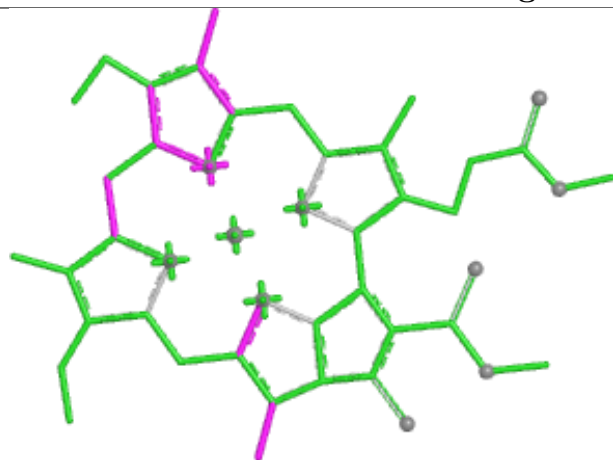


Rings

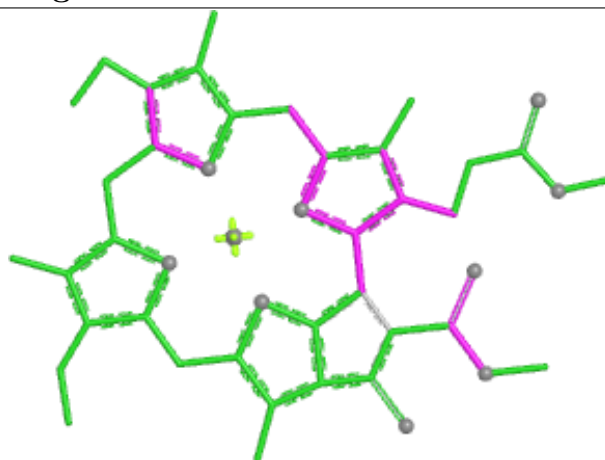
Ligand CLA Z 513



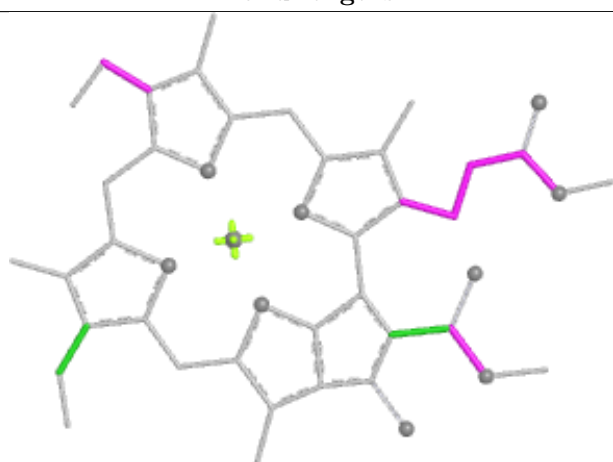
Ligand CLA g 503



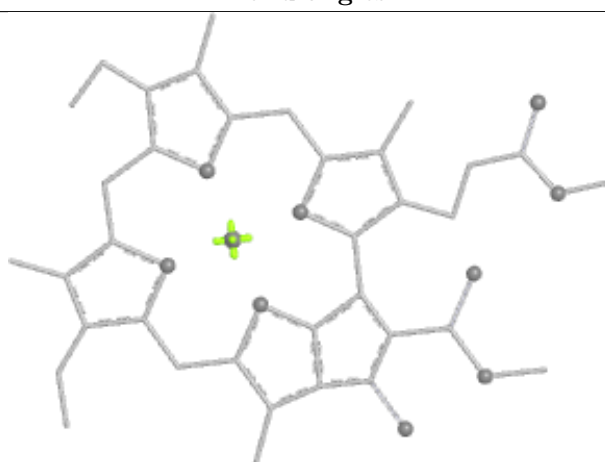
Bond lengths



Bond angles

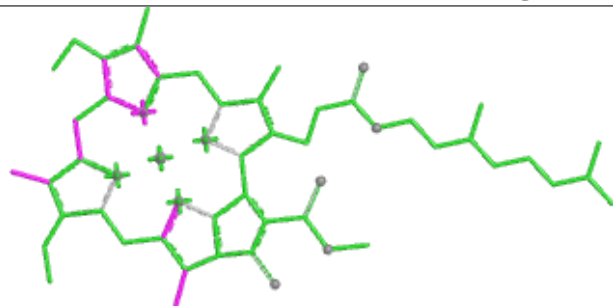


Torsions

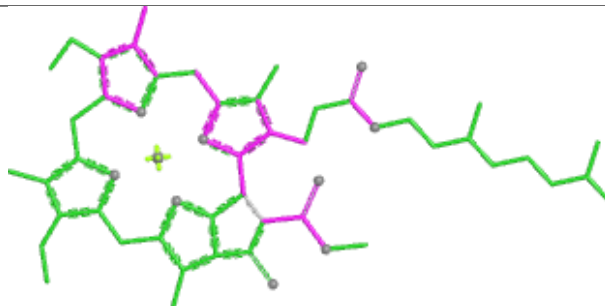


Rings

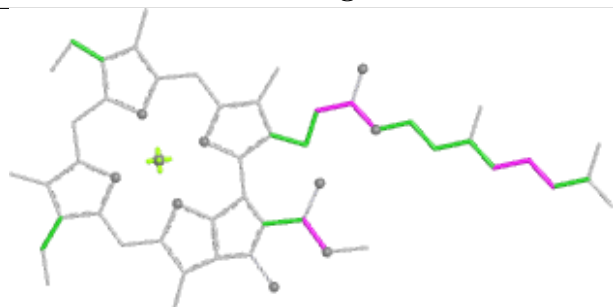
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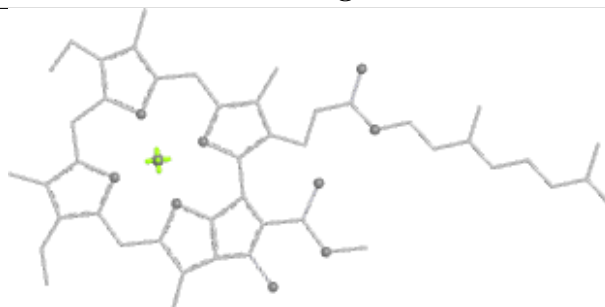
Bond lengths



Bond angles

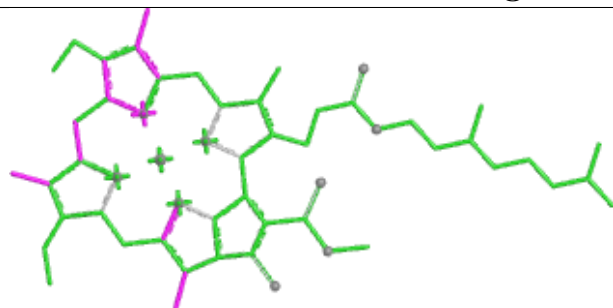


Torsions

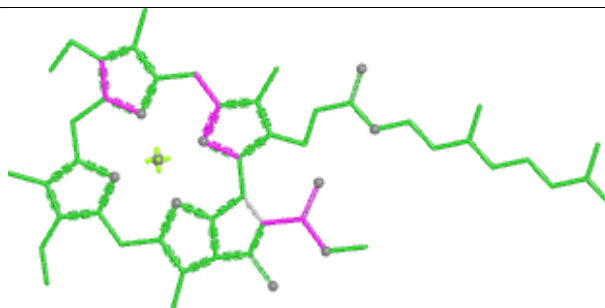


Rings

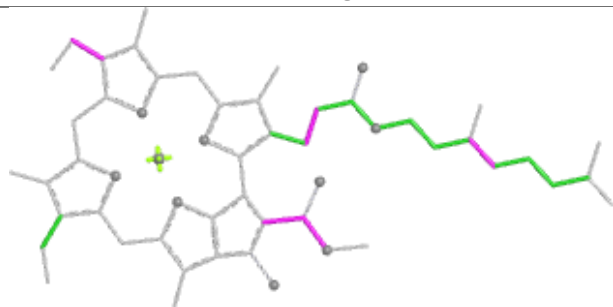
Ligand CLA G 1218



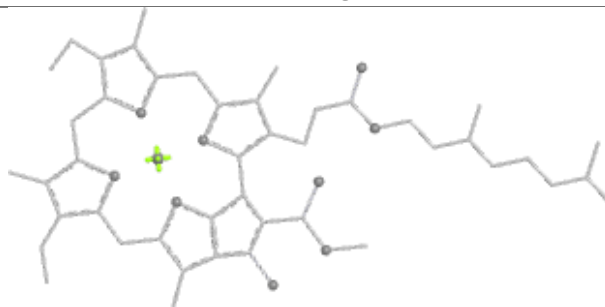
Bond lengths



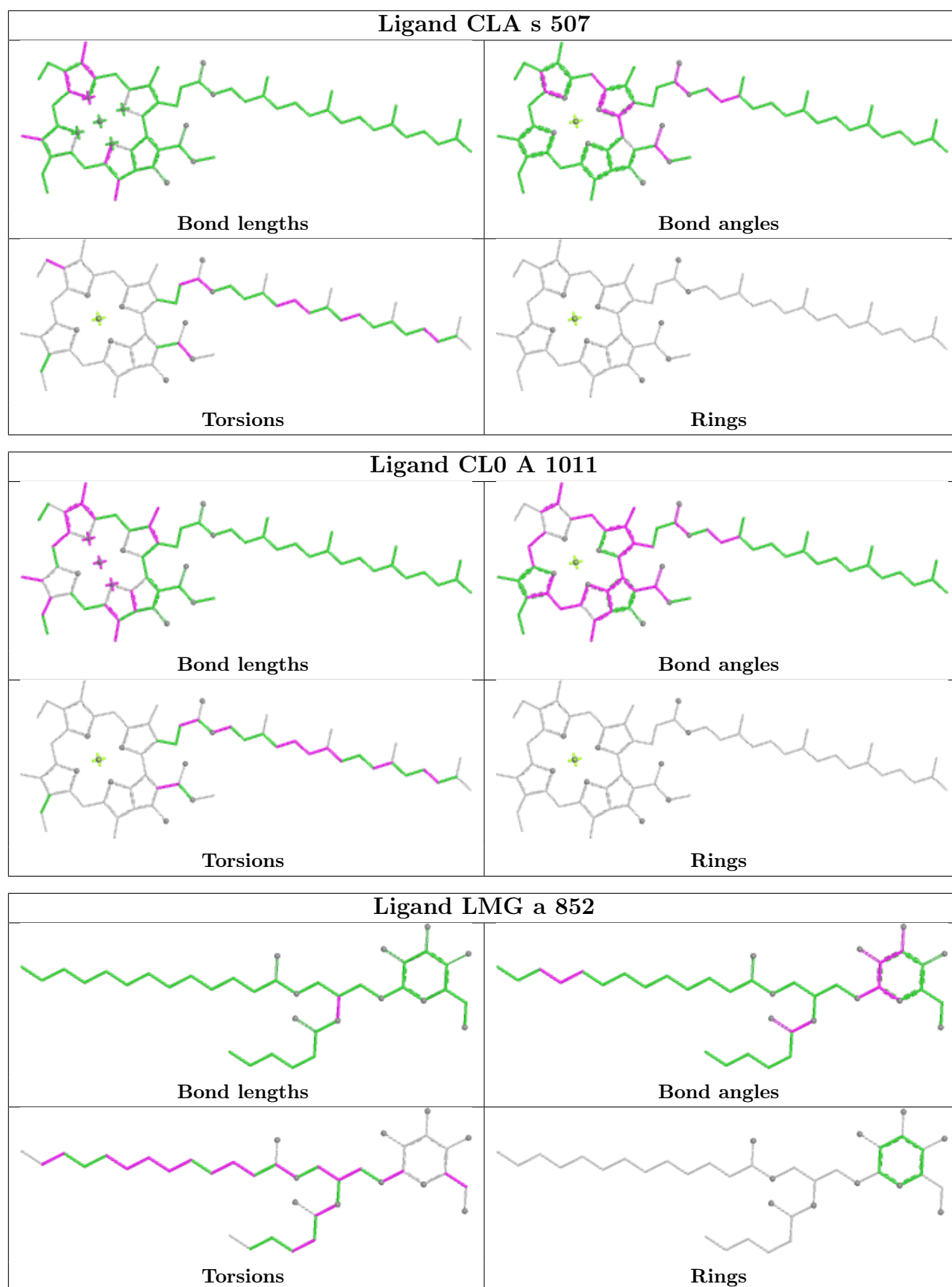
Bond angles



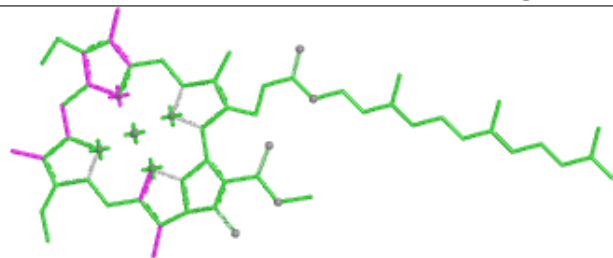
Torsions



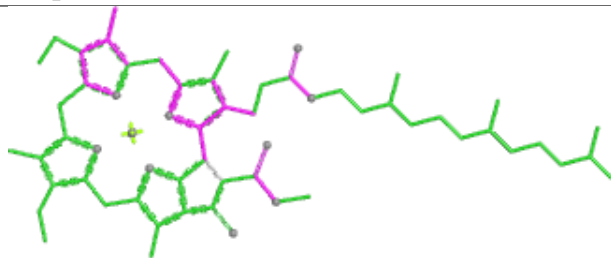
Rings



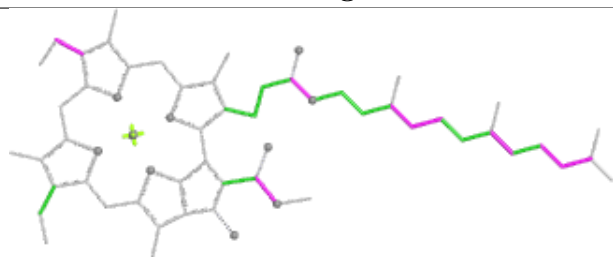
Ligand CLA p 509



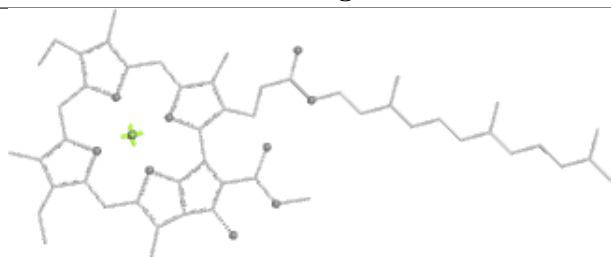
Bond lengths



Bond angles

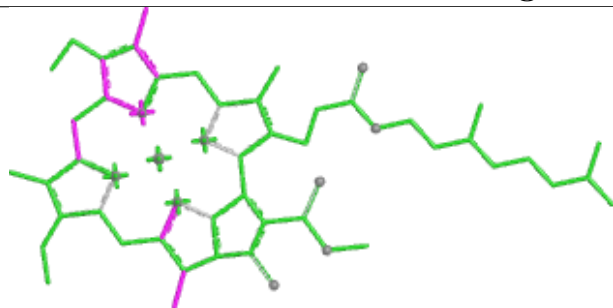


Torsions

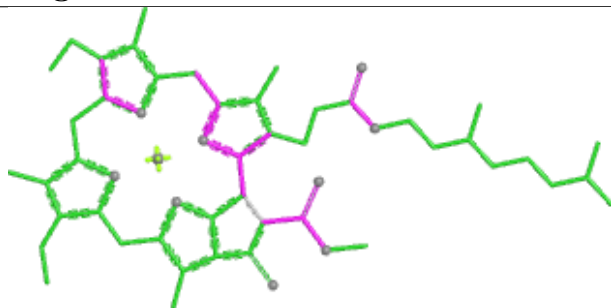


Rings

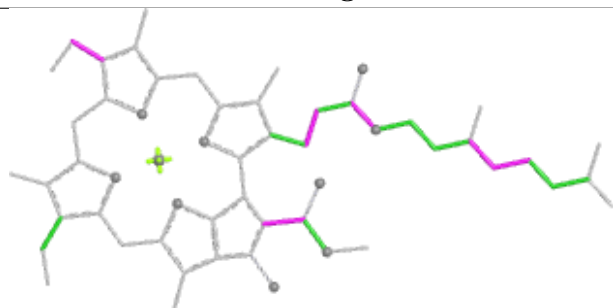
Ligand CLA g 510



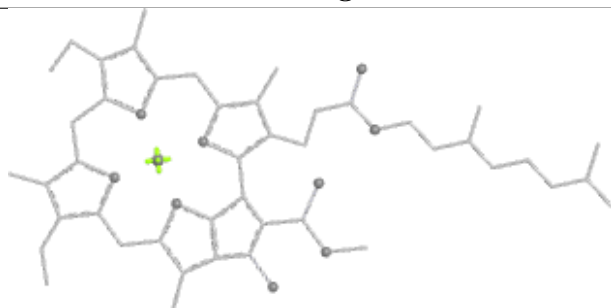
Bond lengths



Bond angles

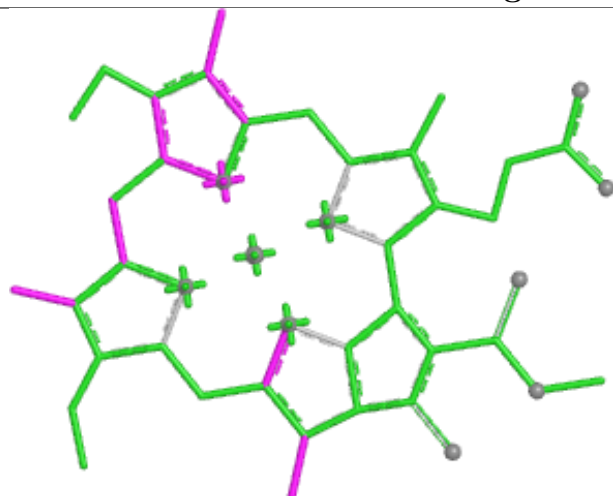


Torsions

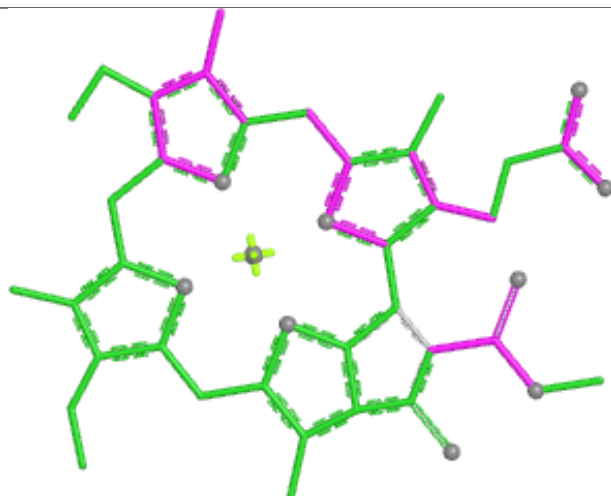


Rings

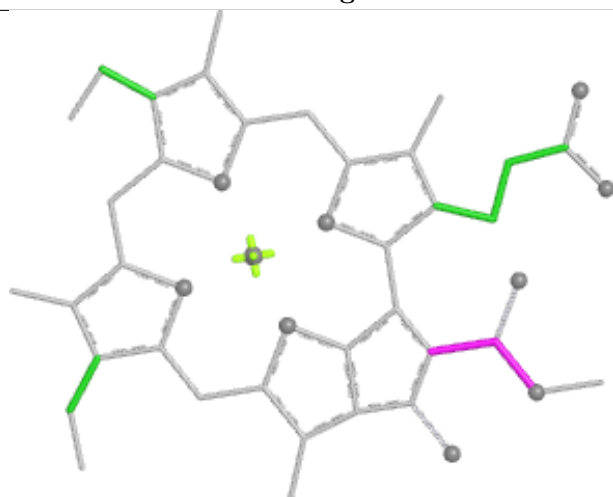
Ligand CLA G 1230



Bond lengths



Bond angles

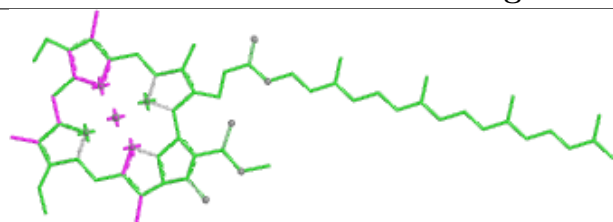


Torsions

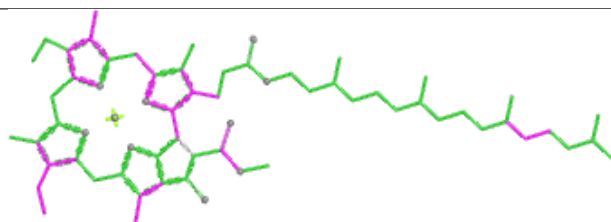


Rings

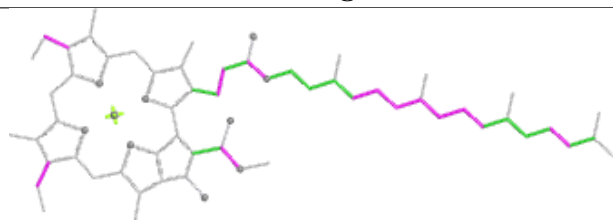
Ligand CLA G 1023



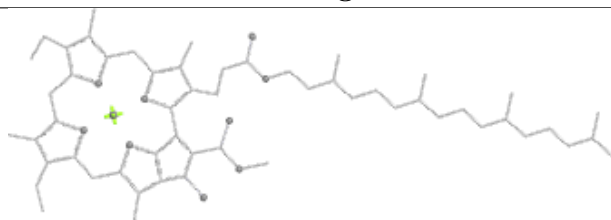
Bond lengths



Bond angles

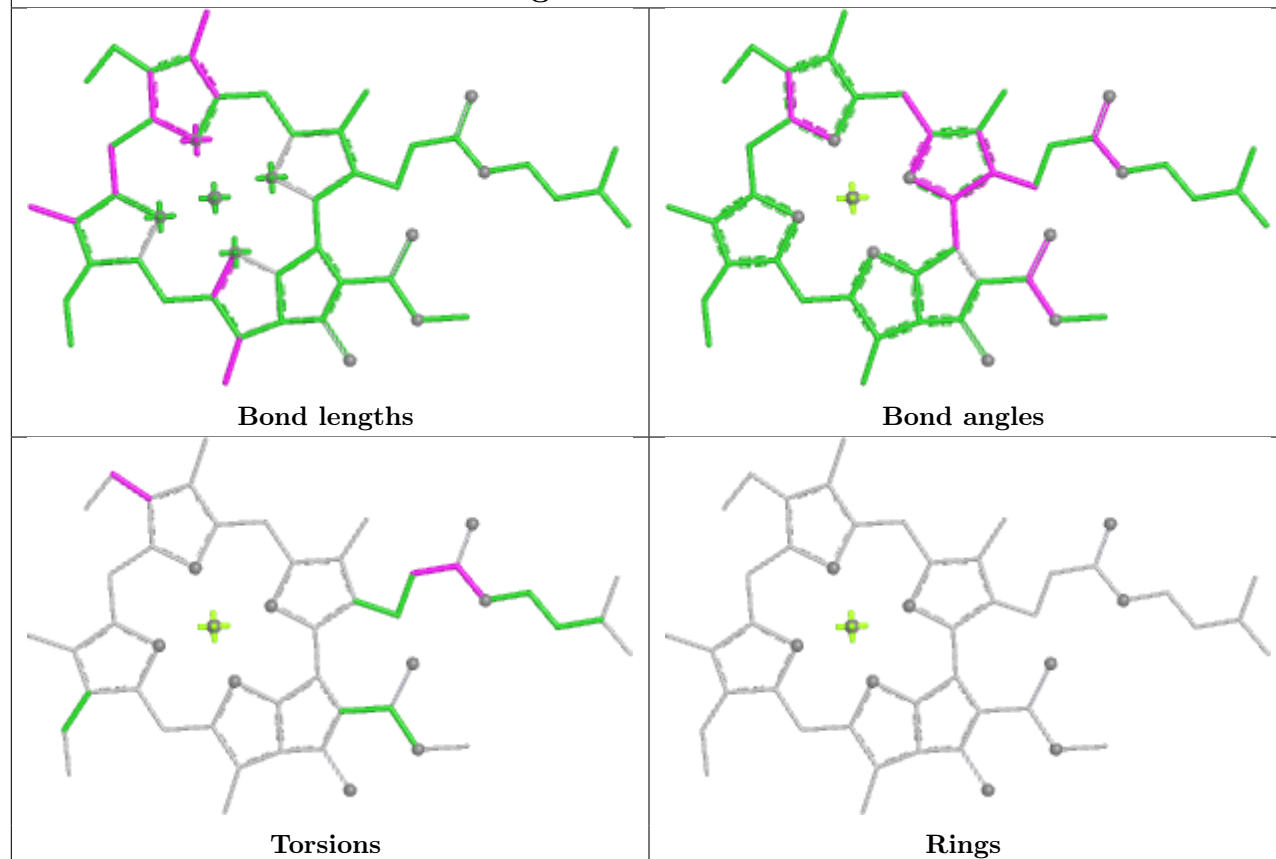


Torsions

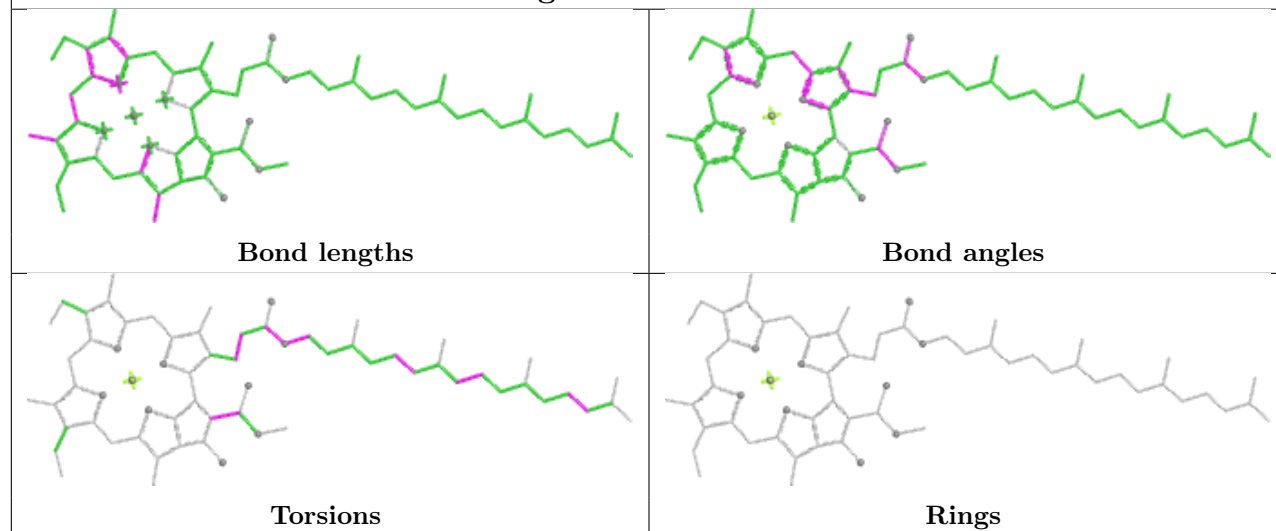


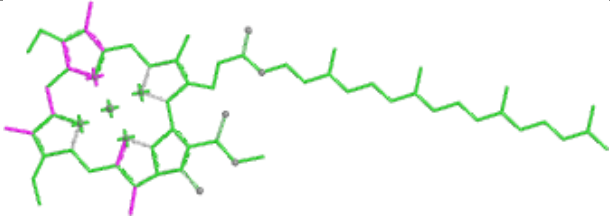
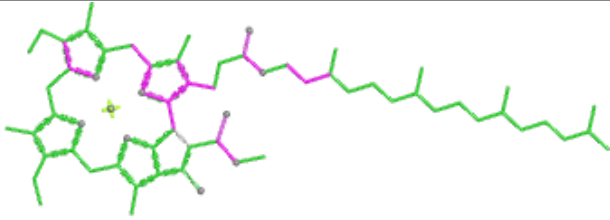
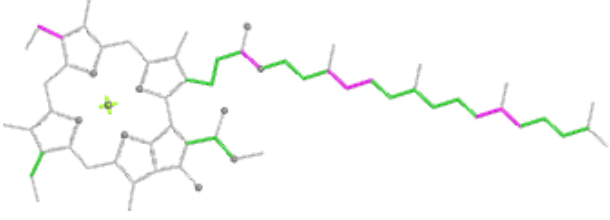
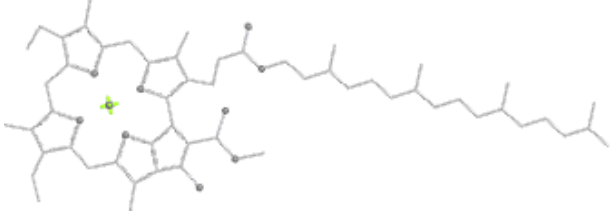
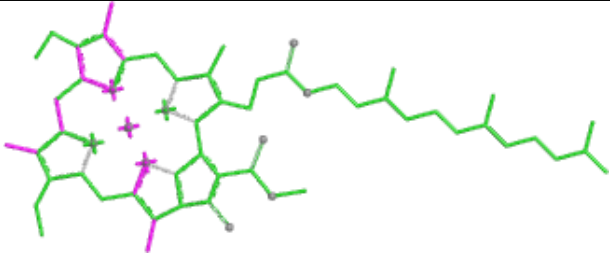
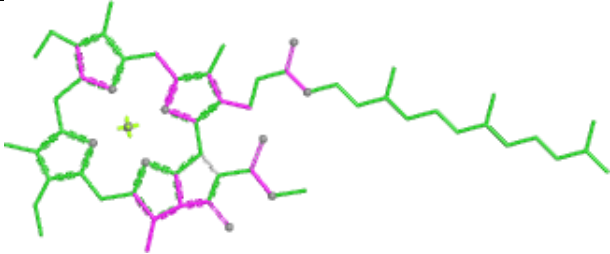
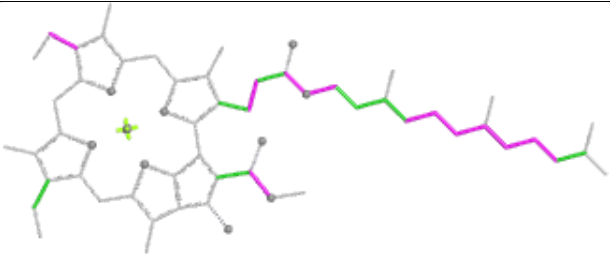
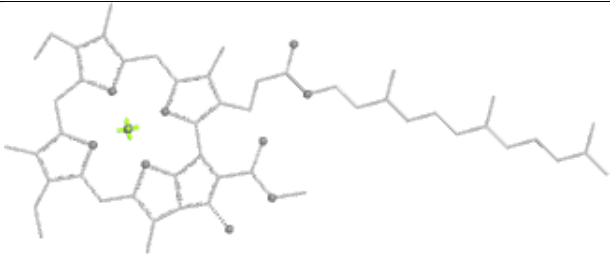
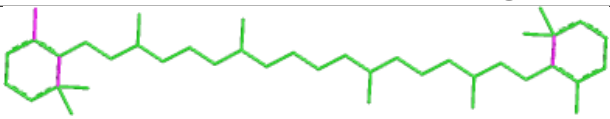
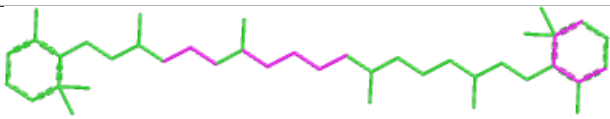
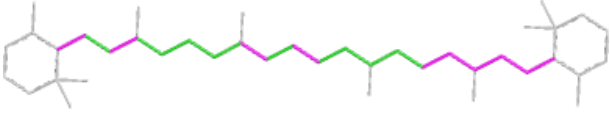
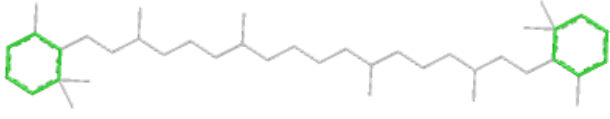
Rings

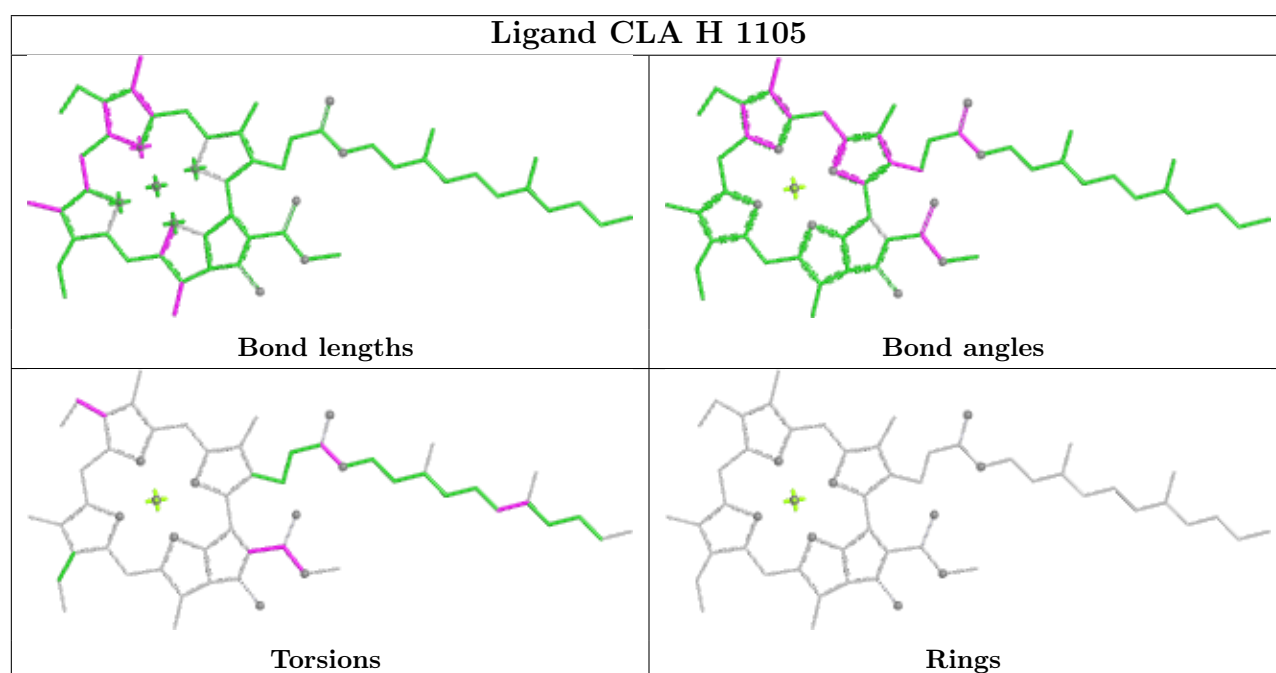
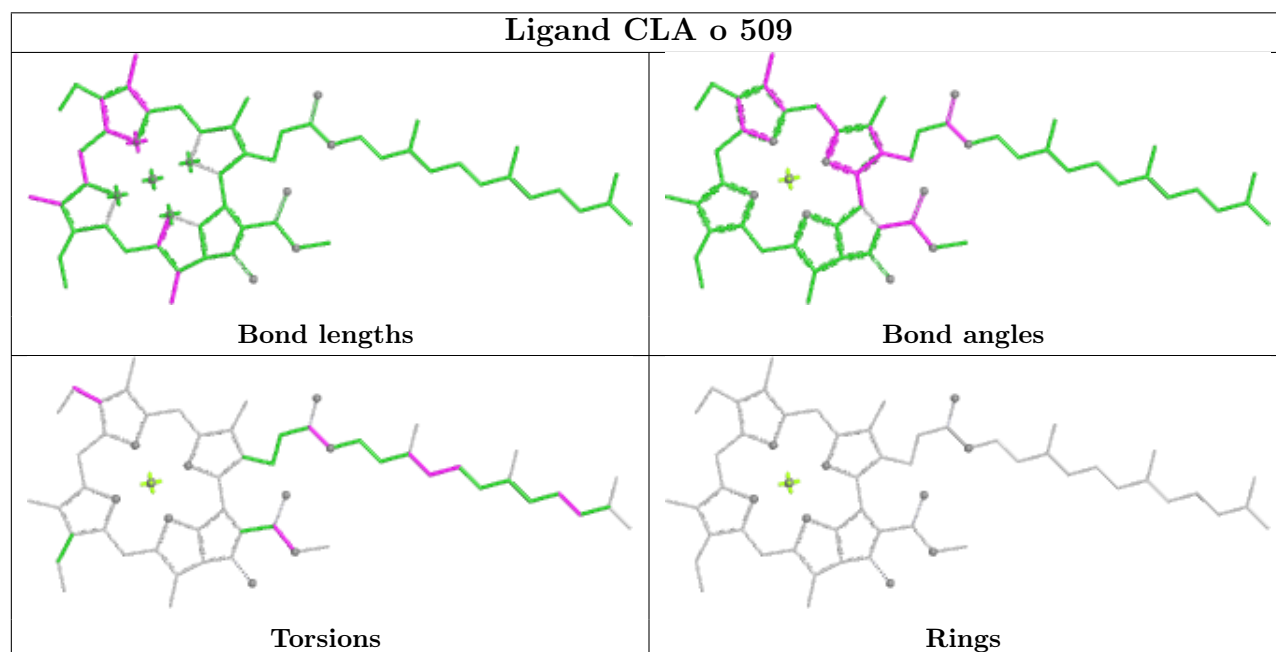
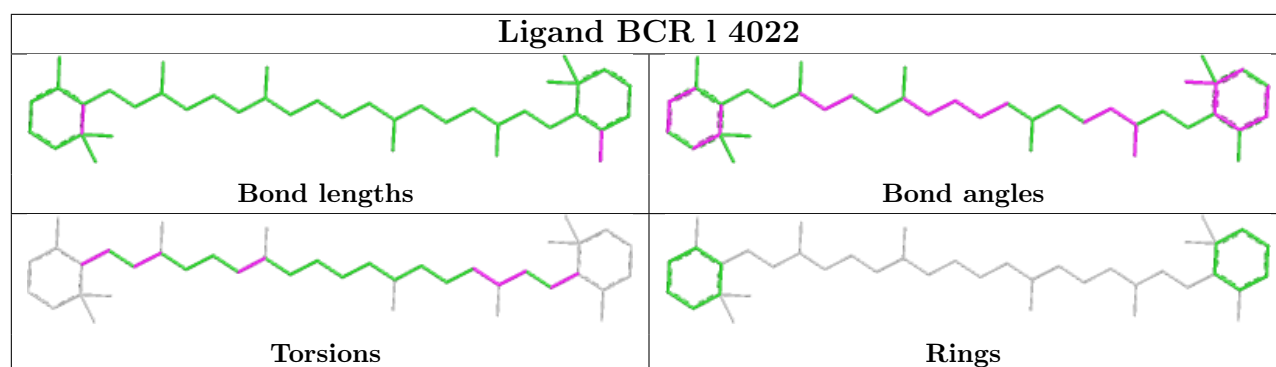
Ligand CLA Y 513

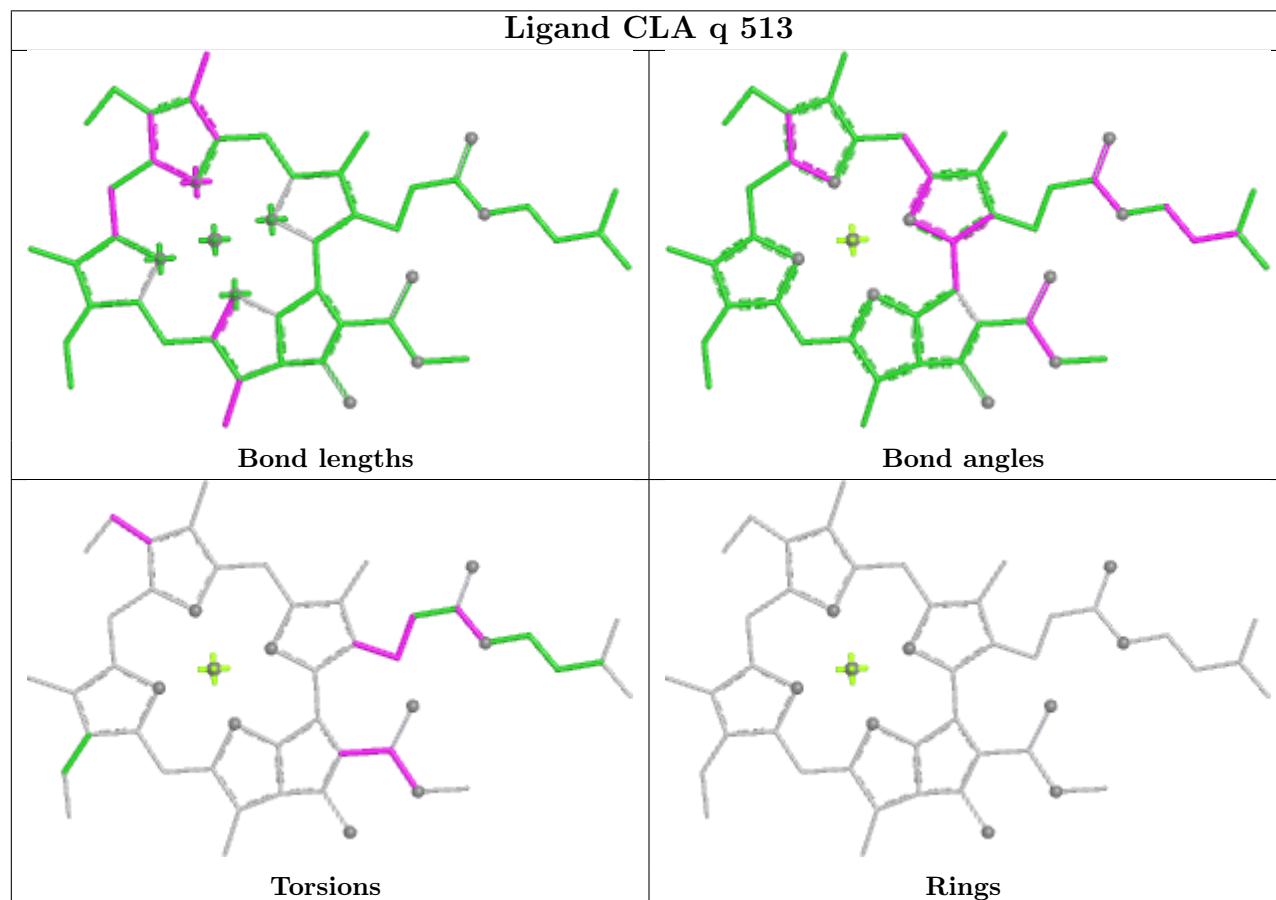
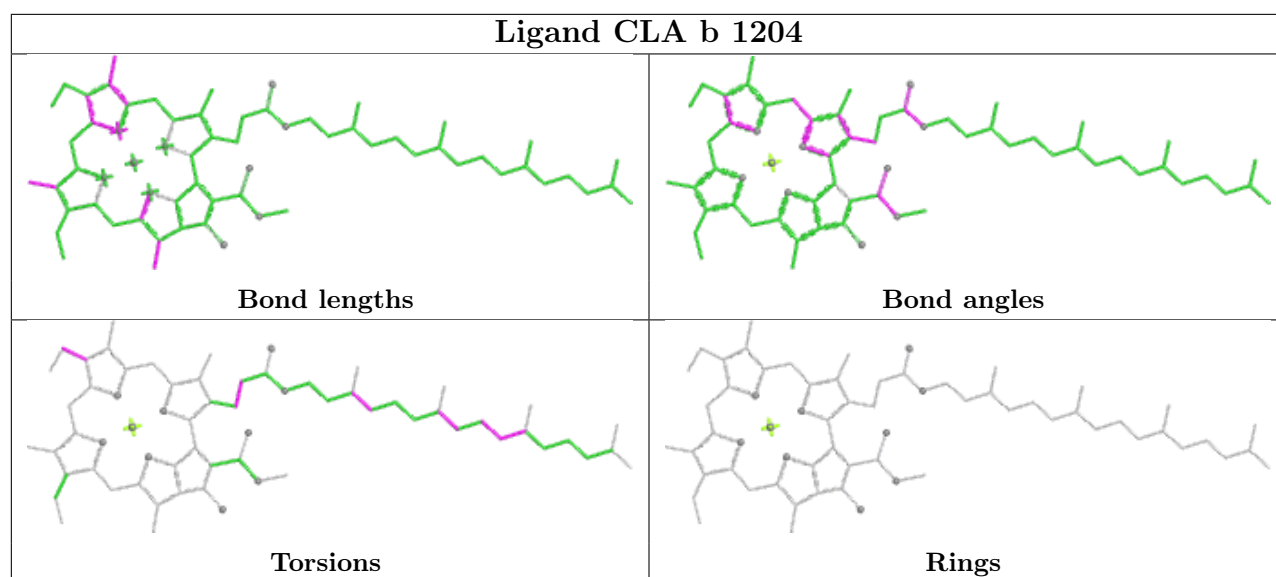


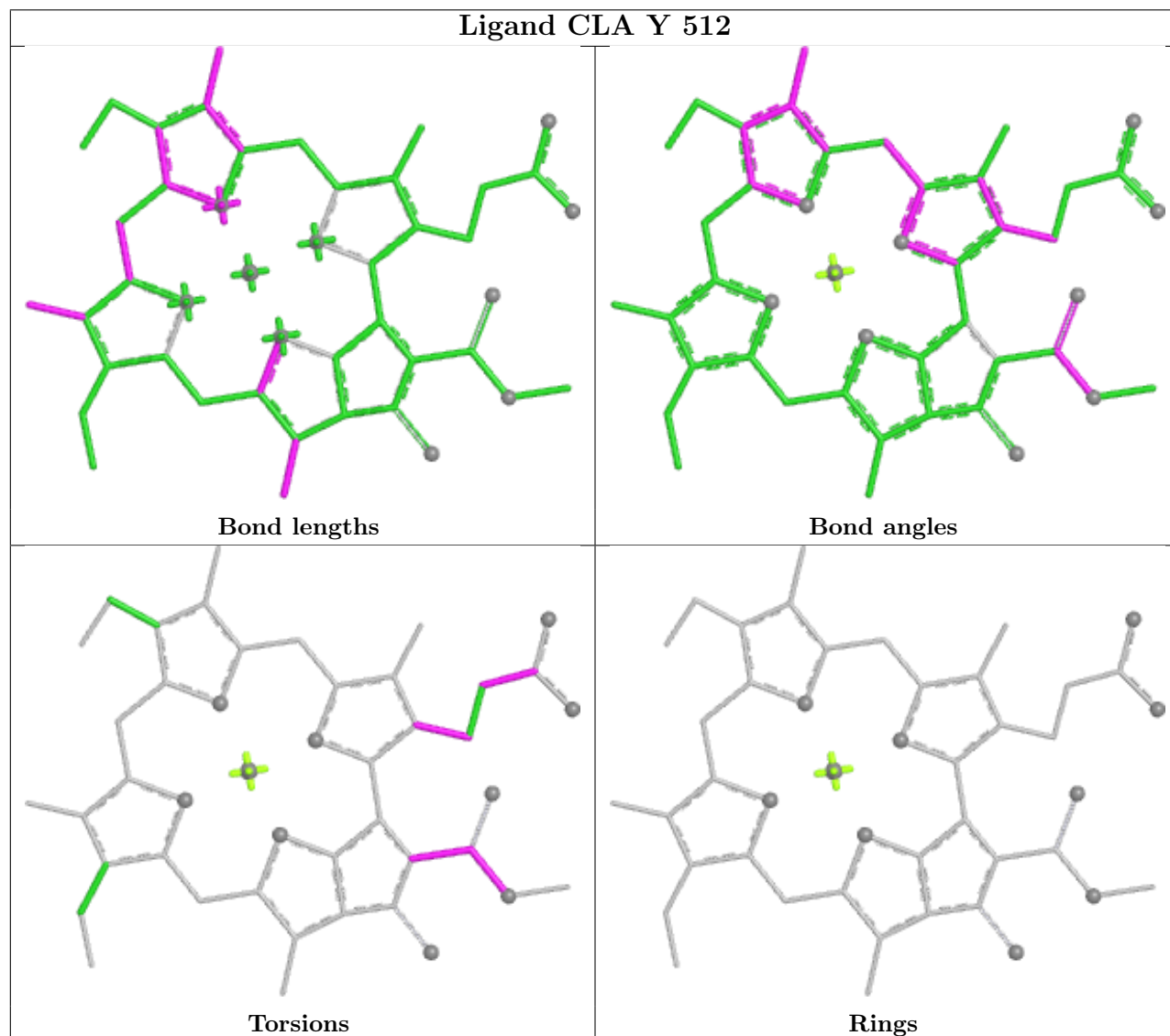
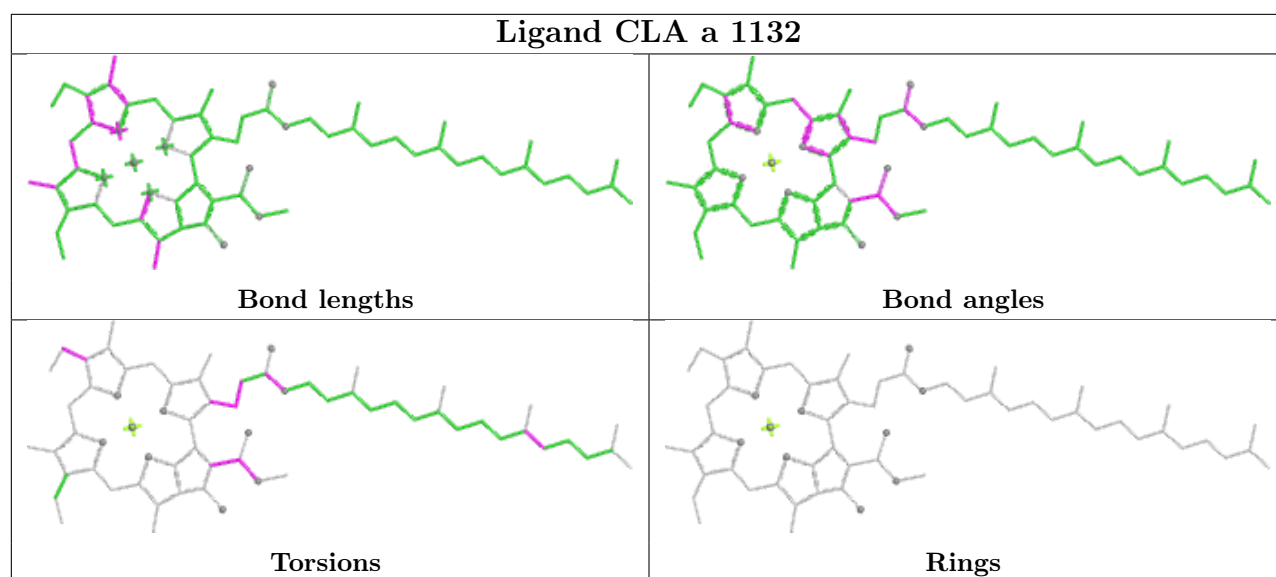
Ligand CLA s 515

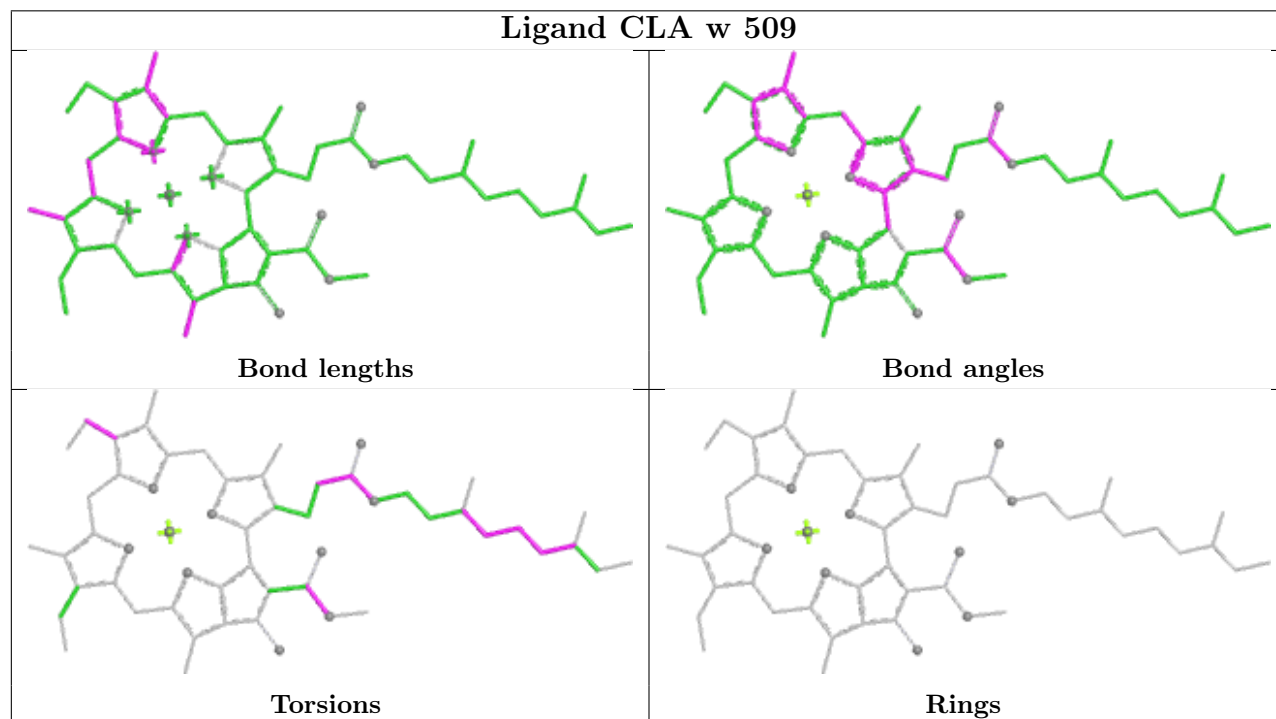
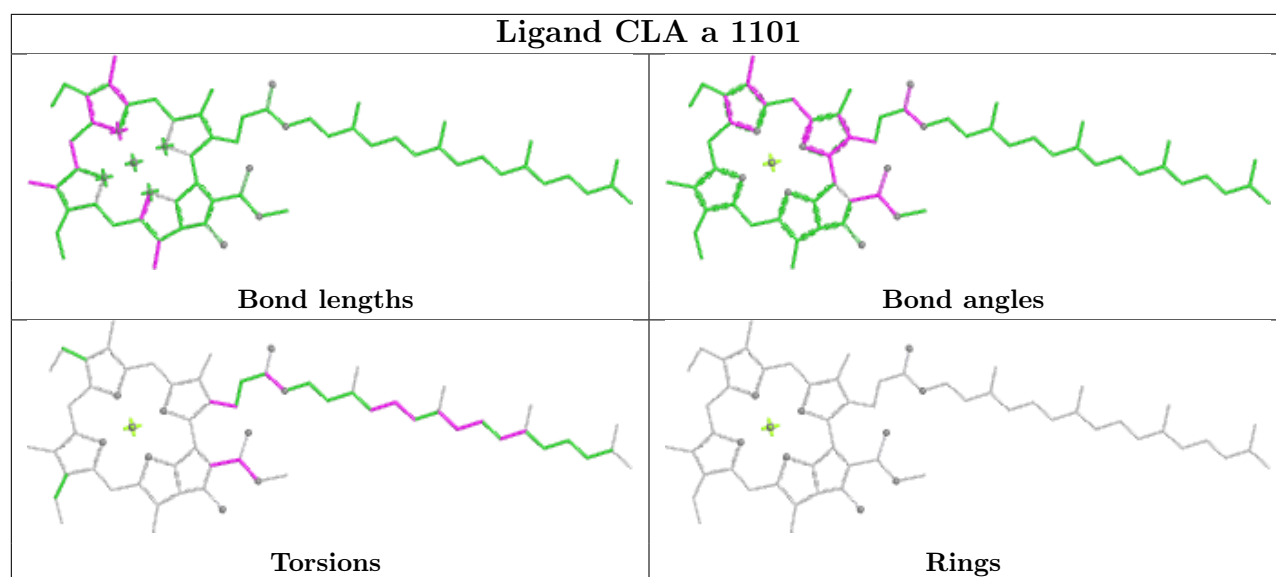


Ligand CLA a 1138	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA G 1012	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 4014	
 Bond lengths	 Bond angles
 Torsions	 Rings

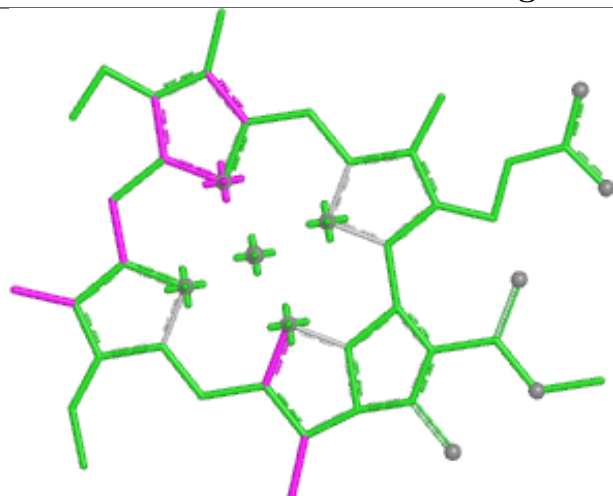




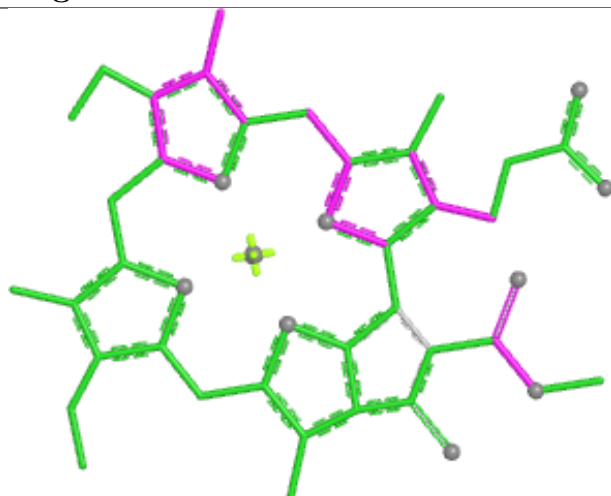




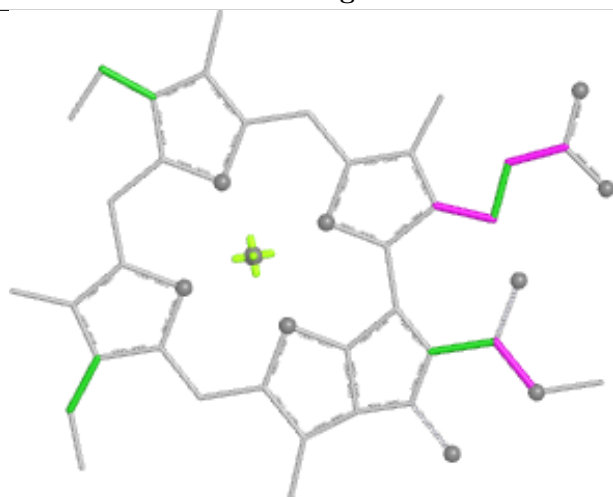
Ligand CLA g 512



Bond lengths



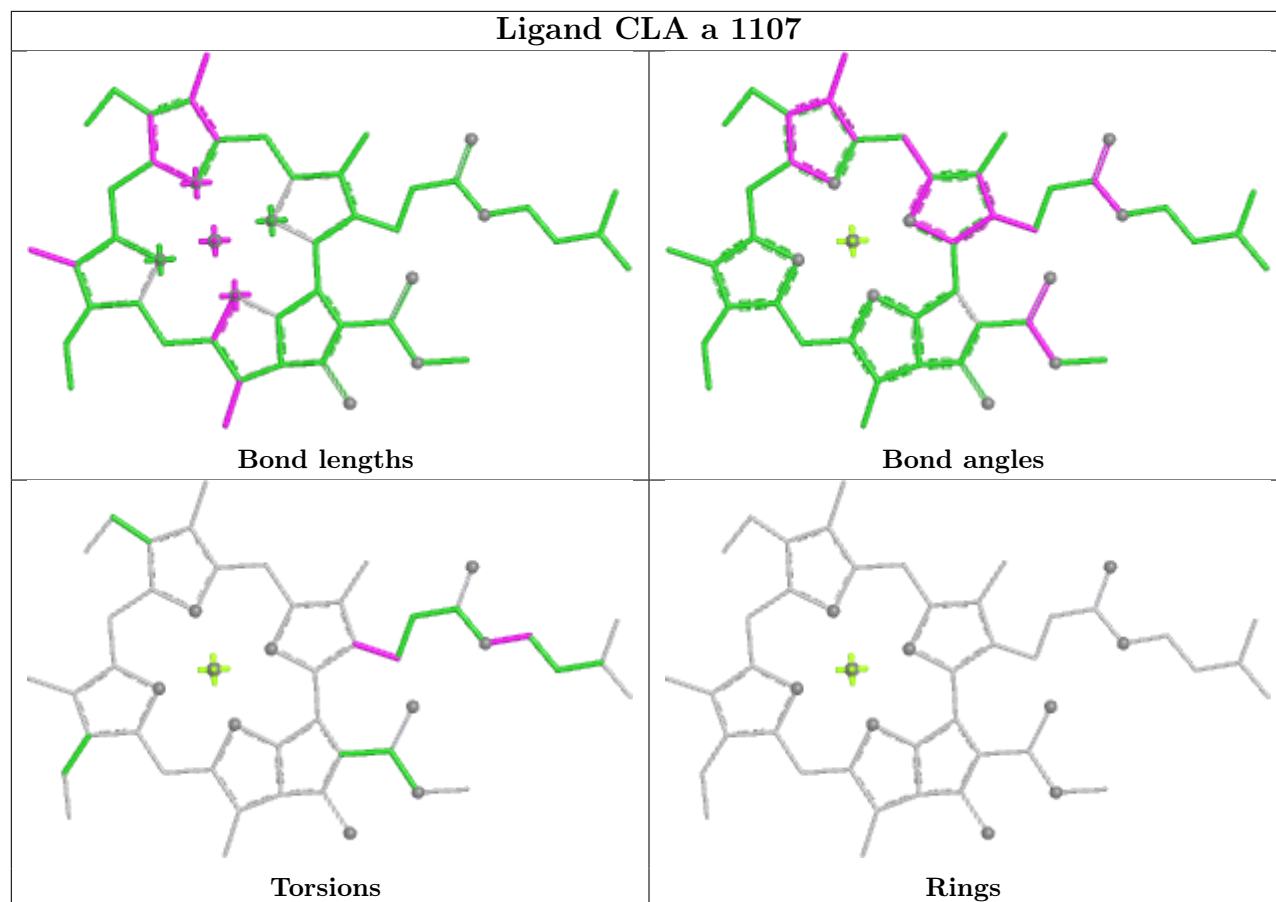
Bond angles



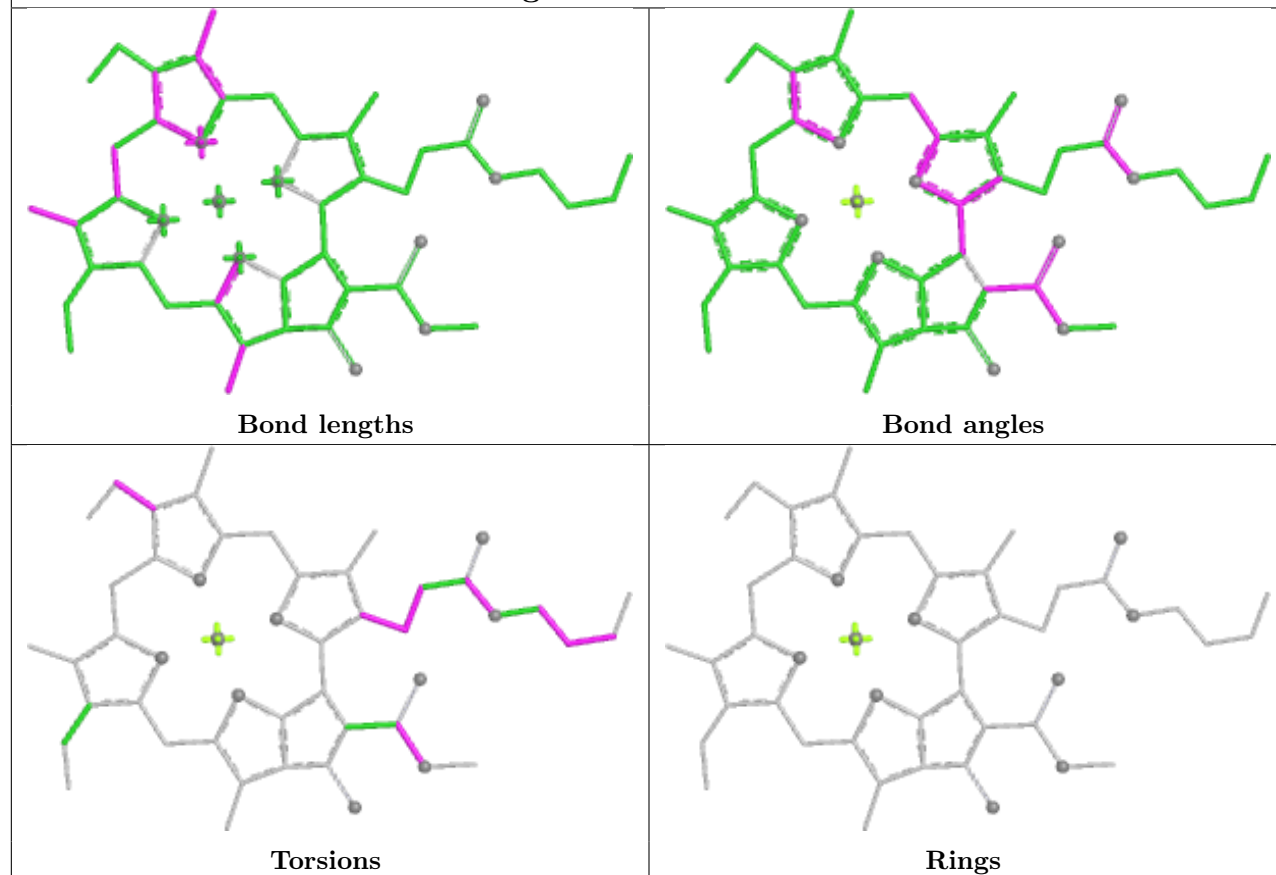
Torsions



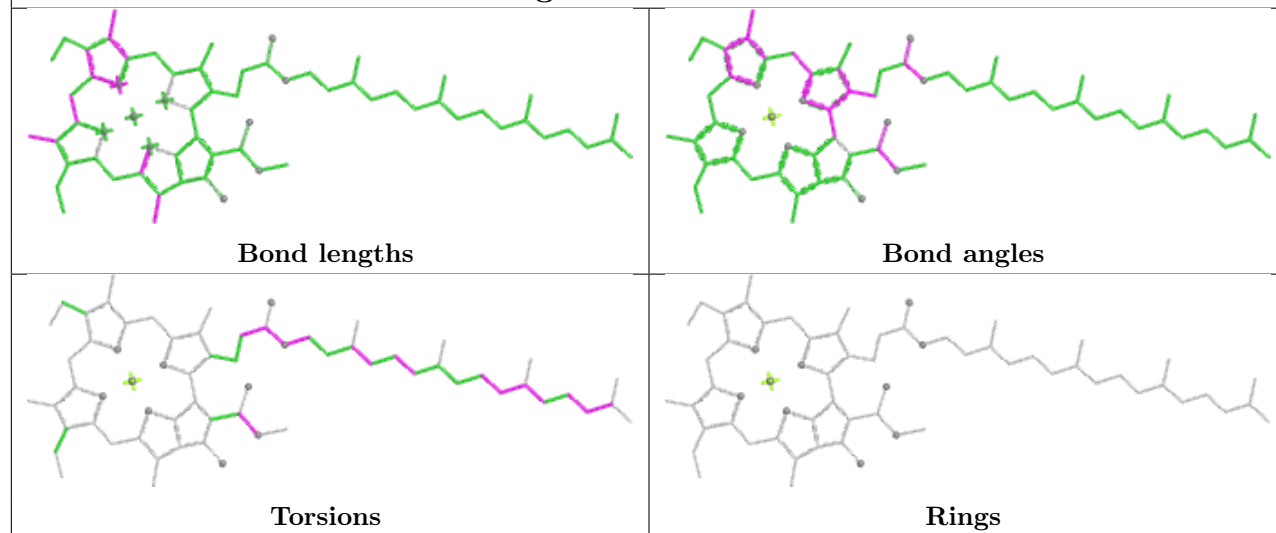
Rings



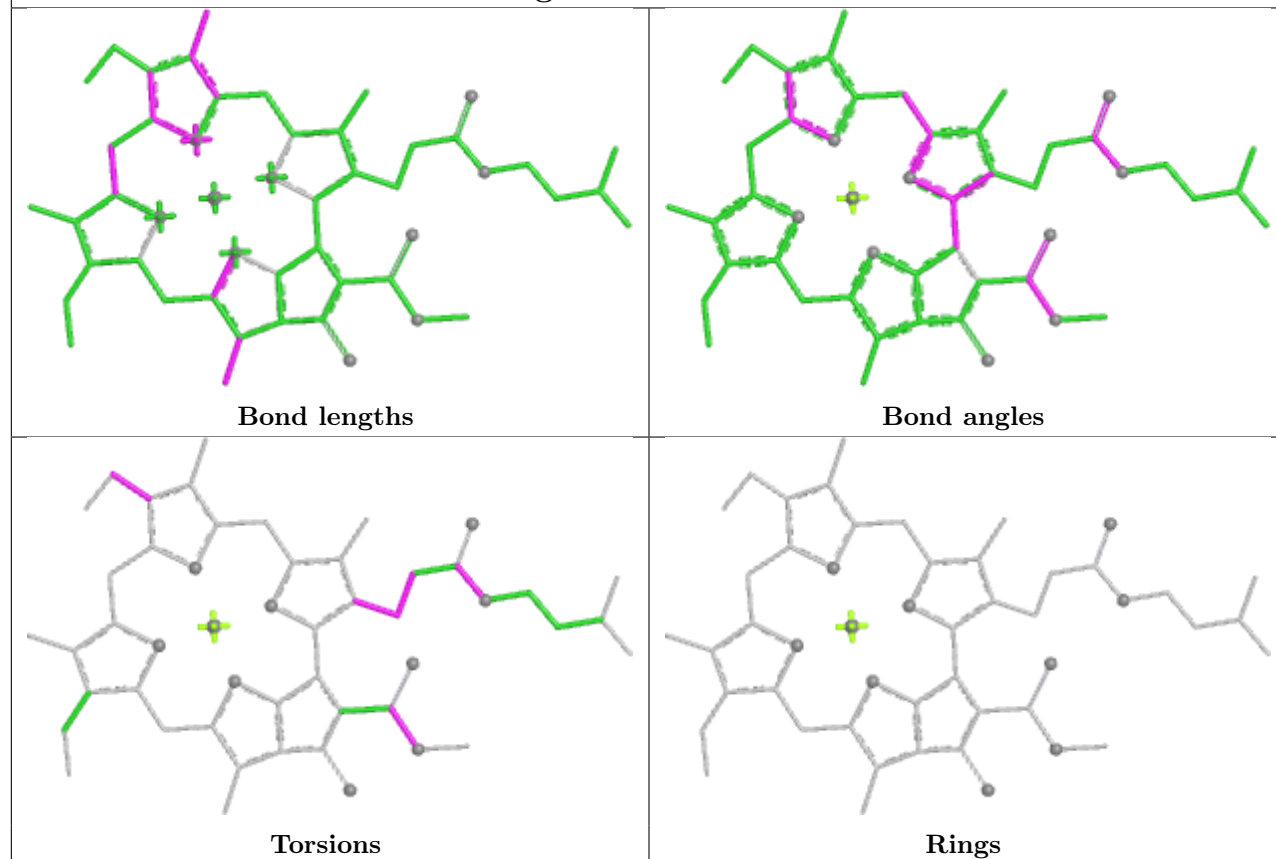
Ligand CLA H 1120



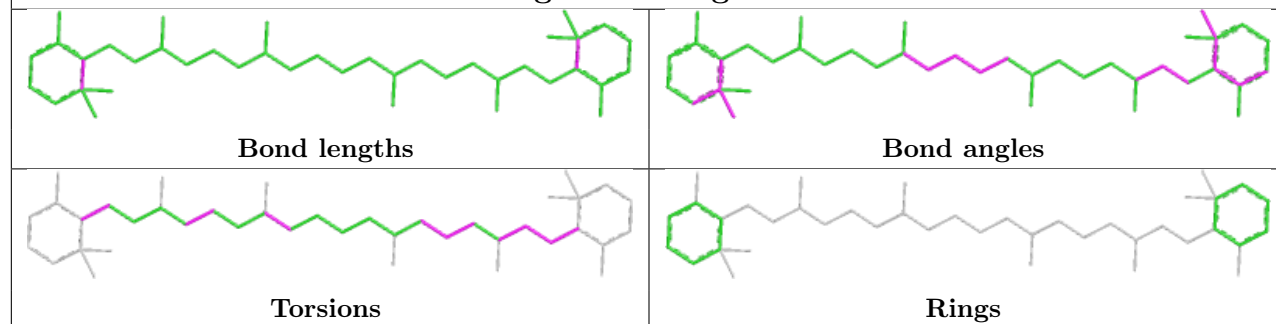
Ligand CLA v 511

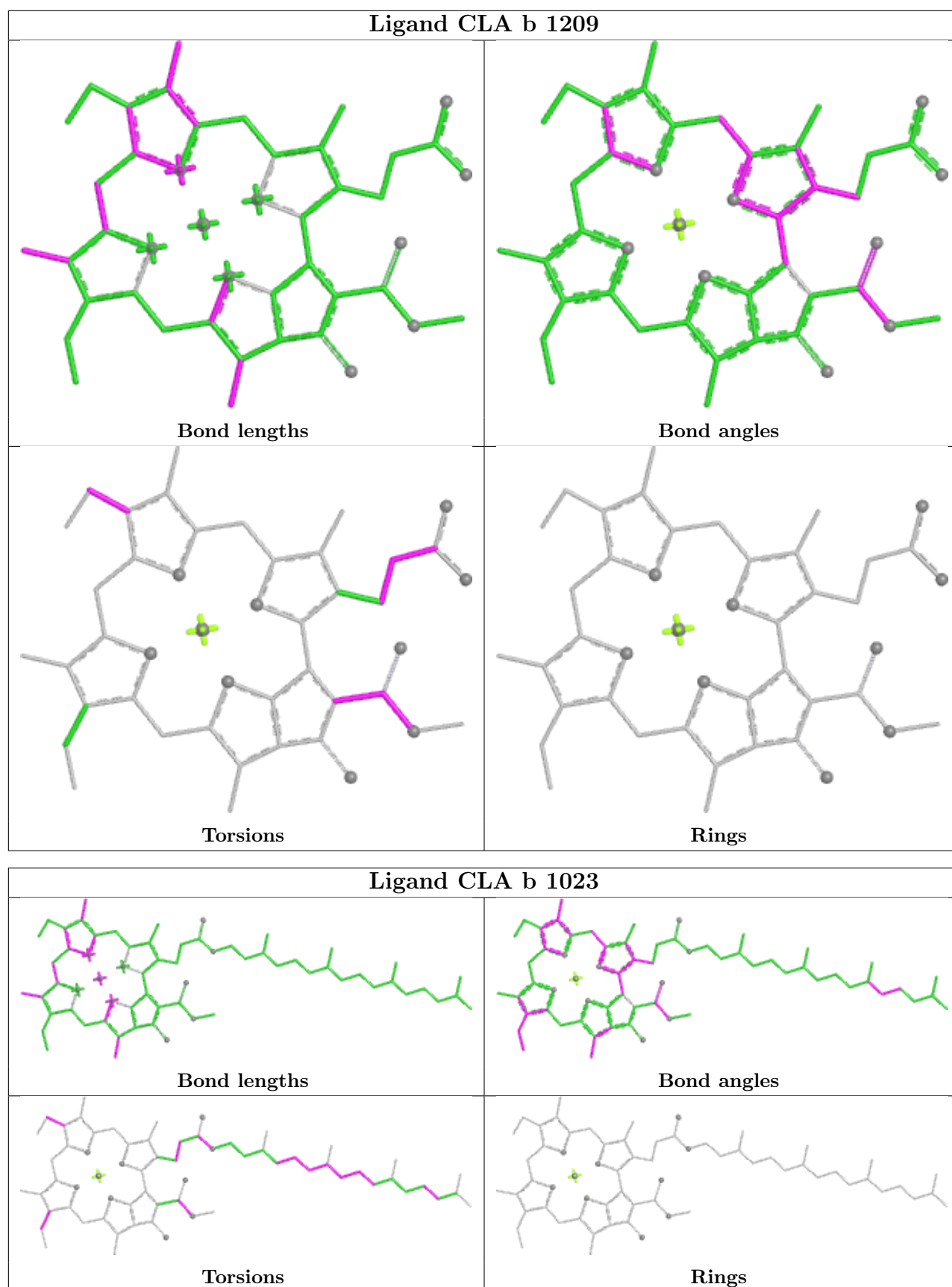


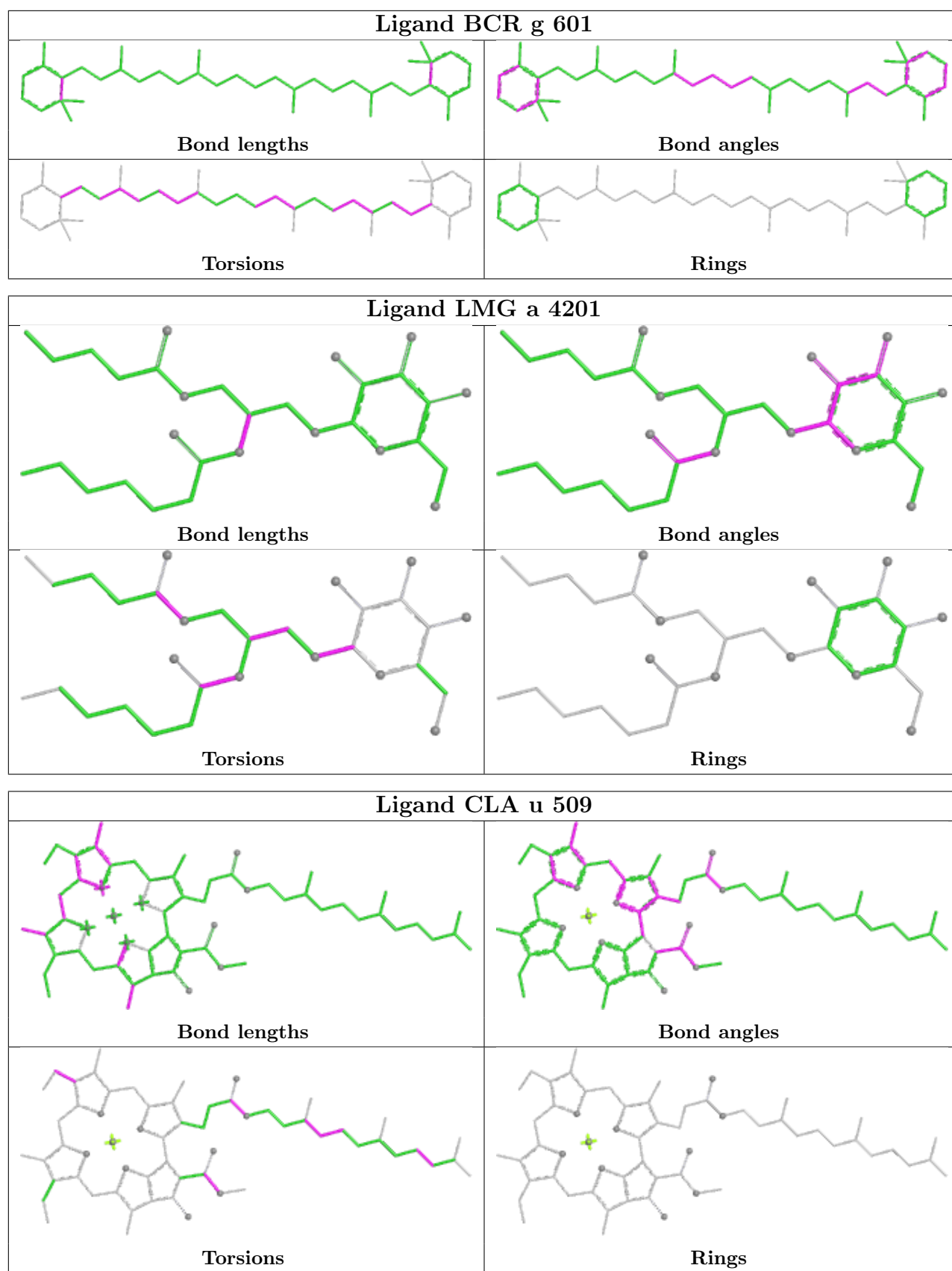
Ligand CLA u 513

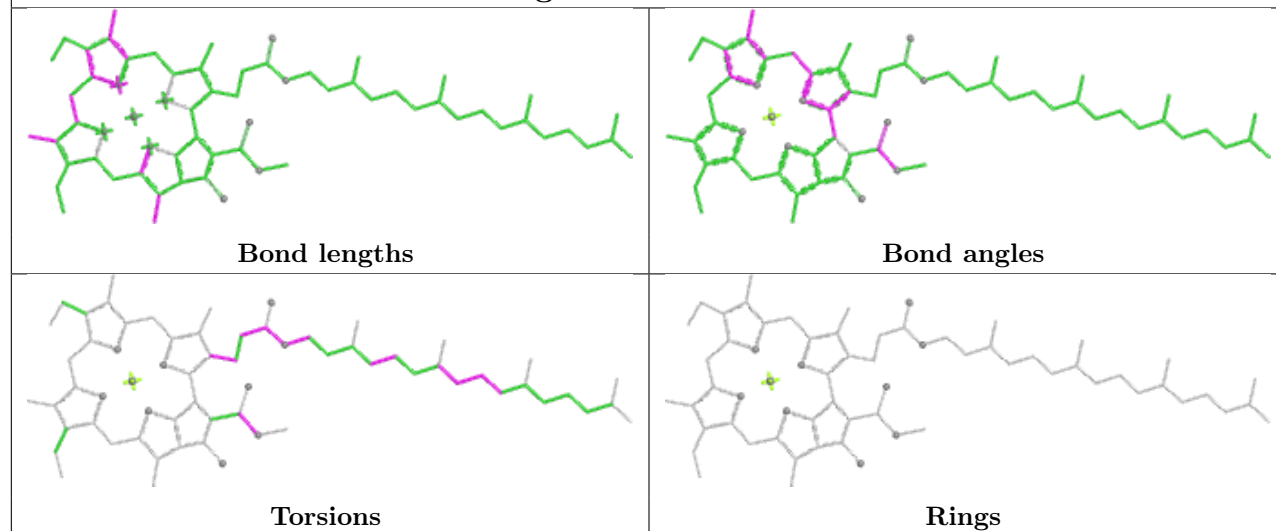
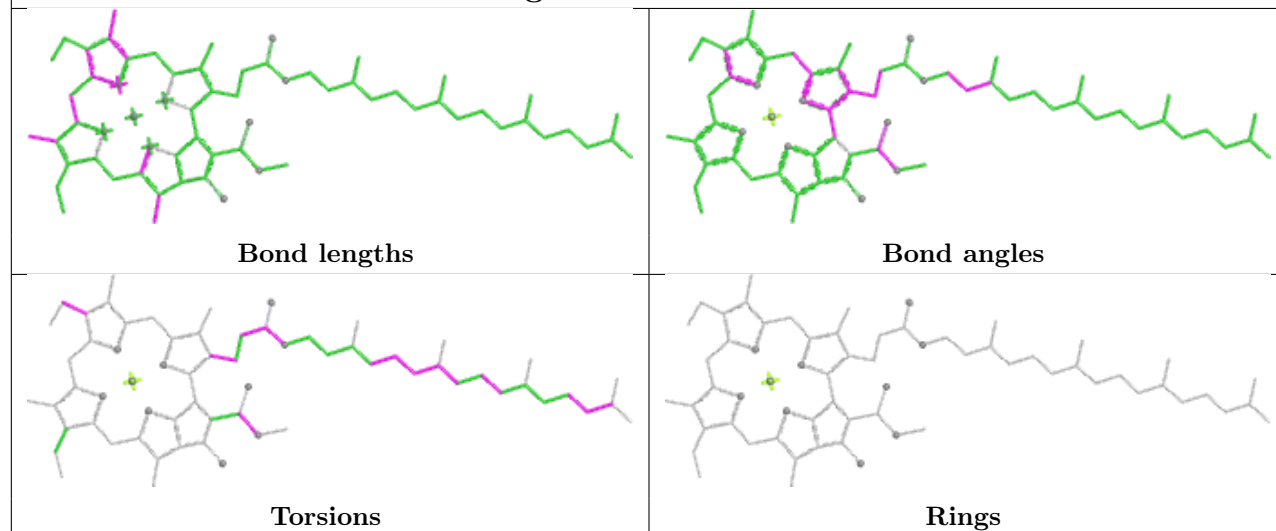


Ligand BCR g 602

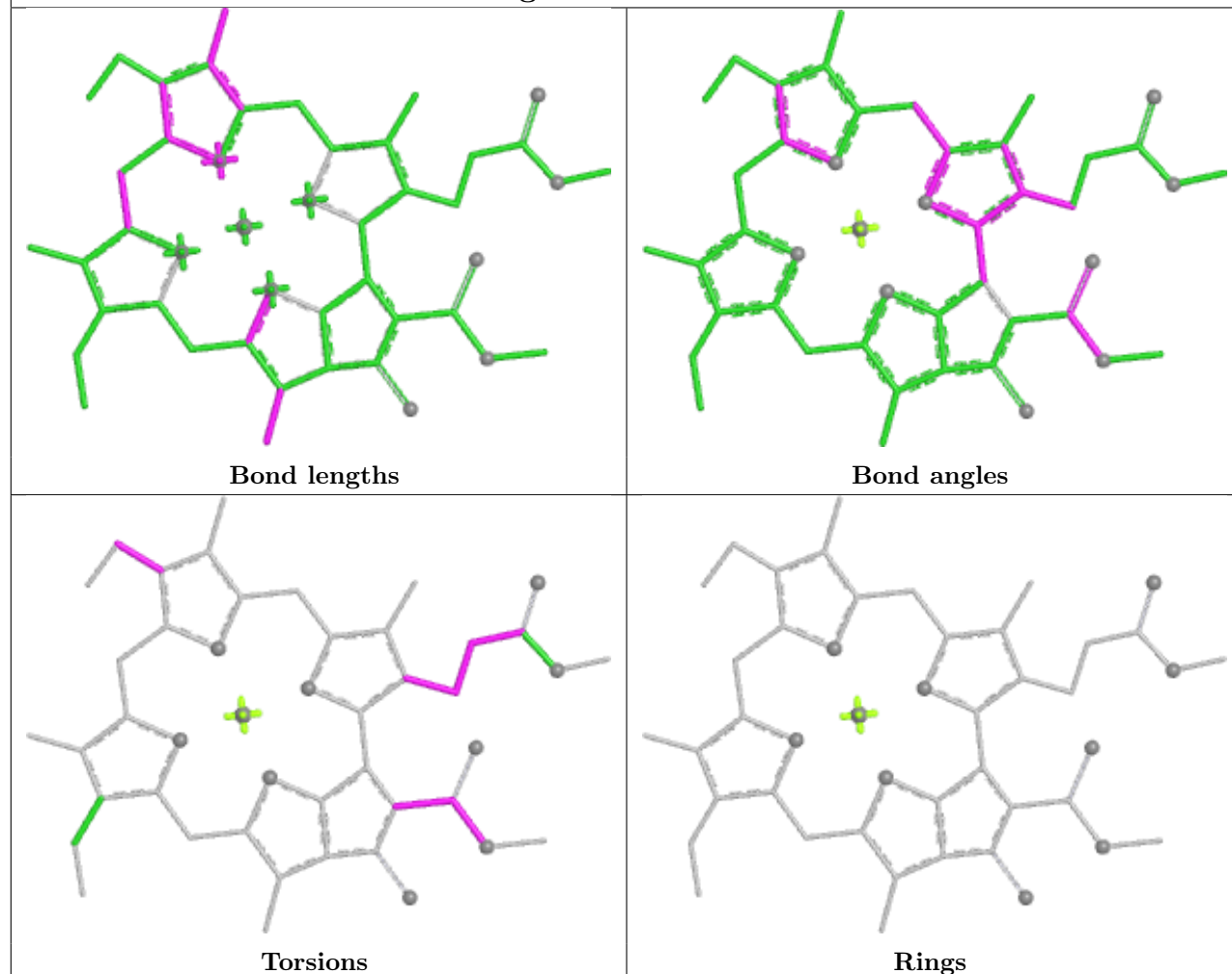




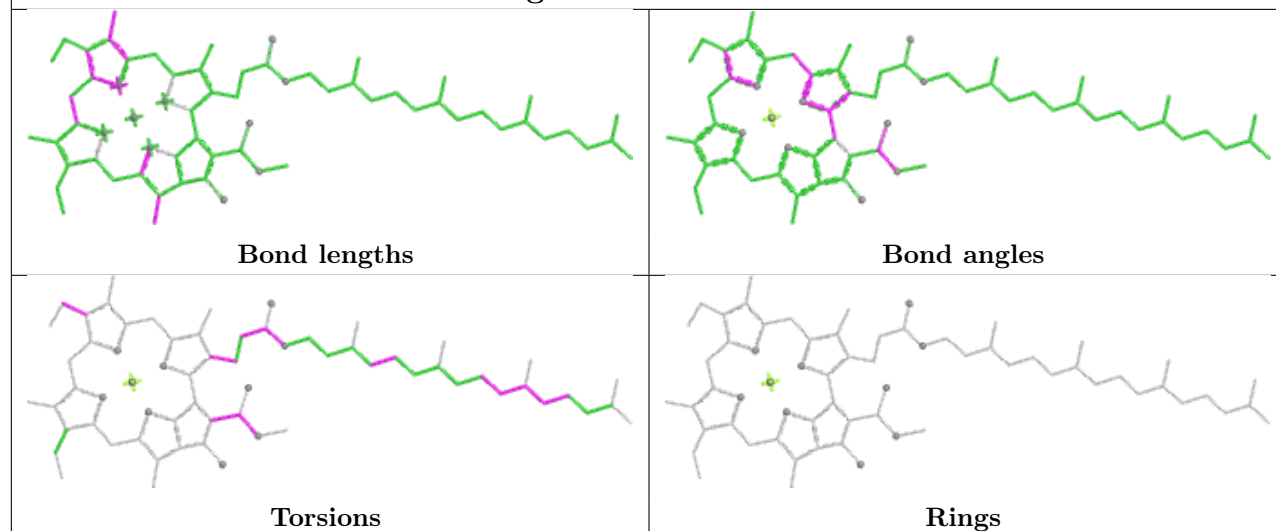


Ligand CLA n 511**Ligand CLA L 1501**

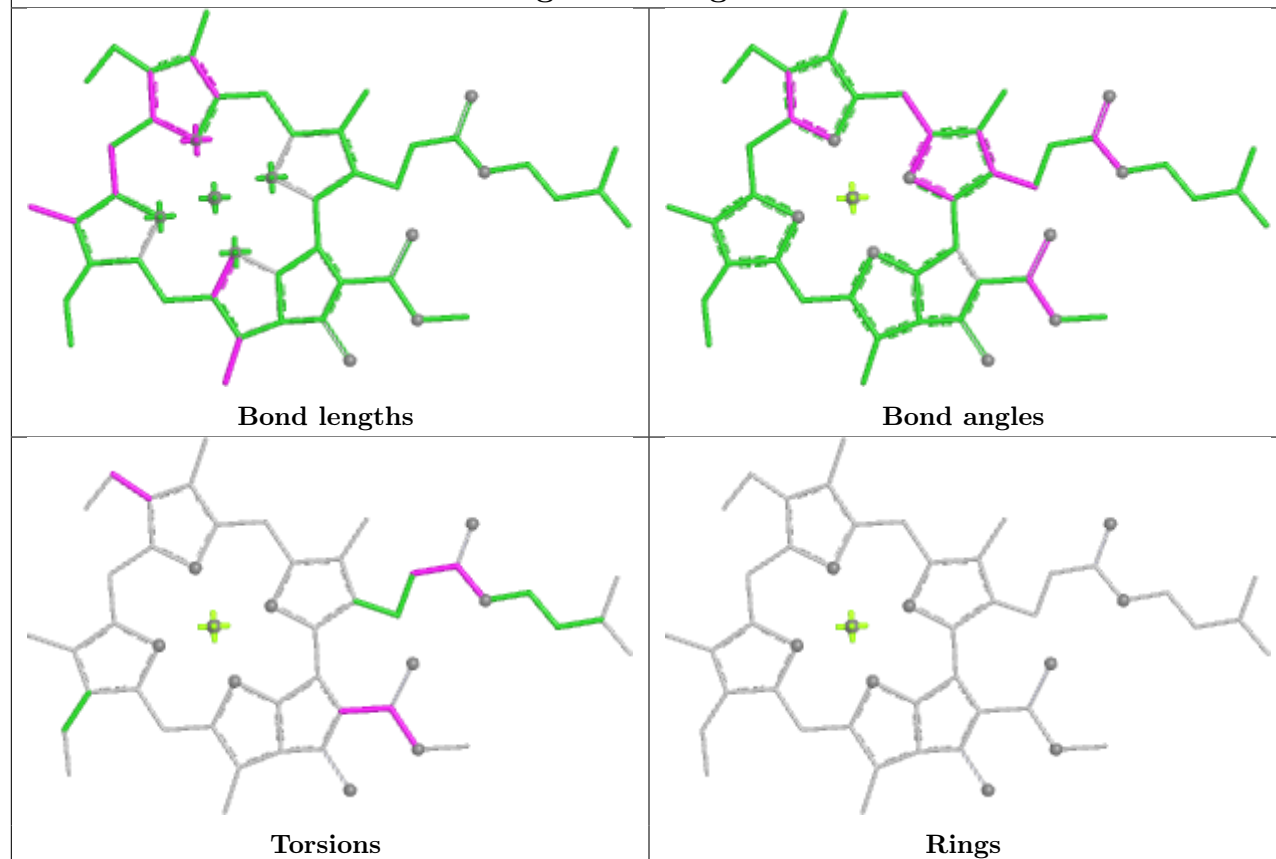
Ligand CLA r 505



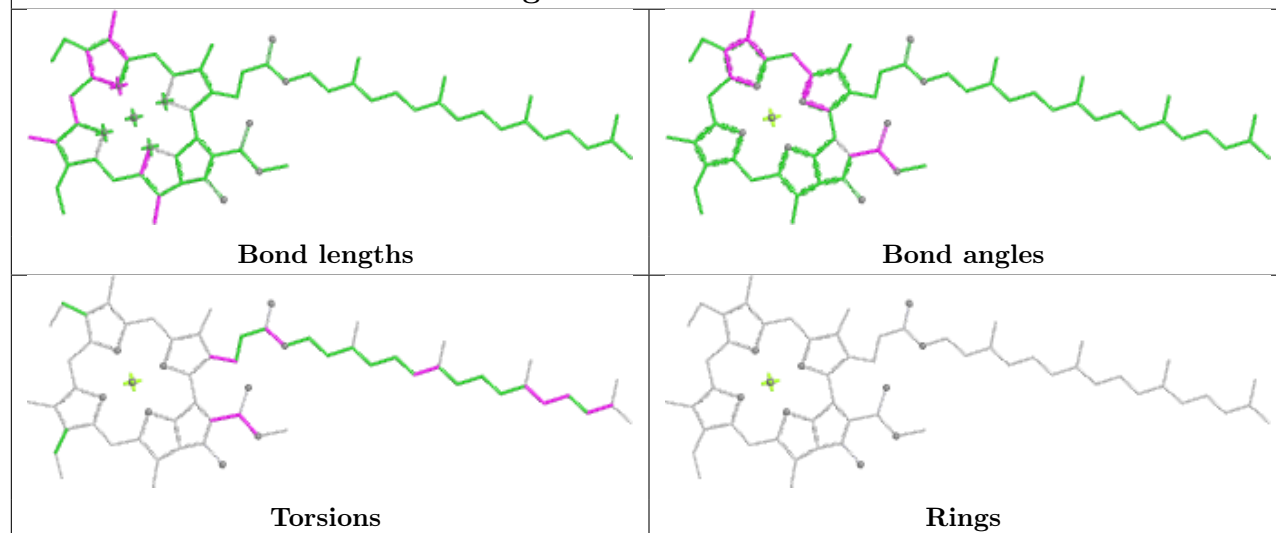
Ligand CLA W 505

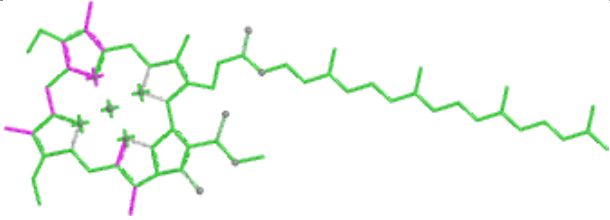
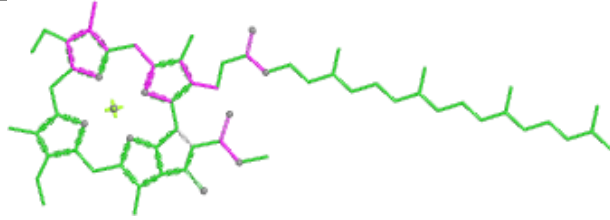
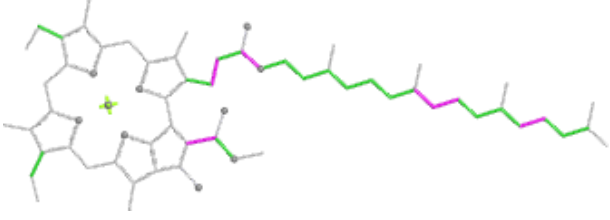
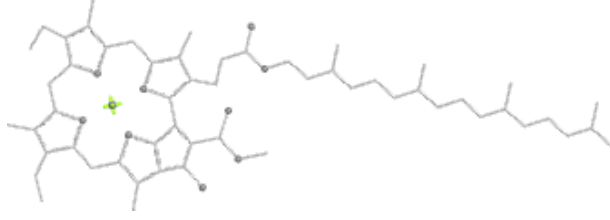
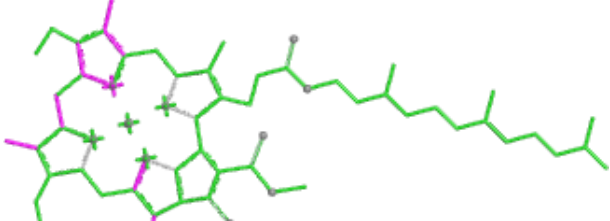
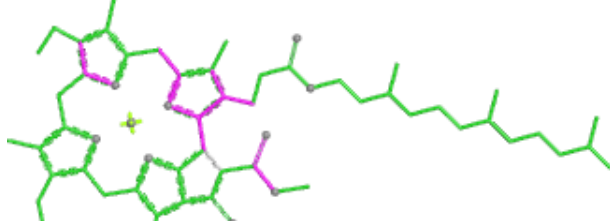
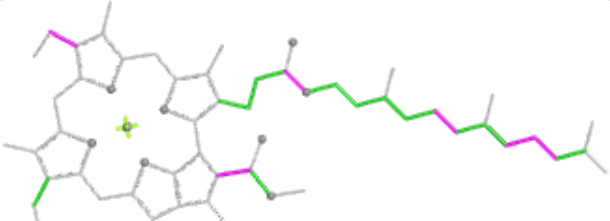
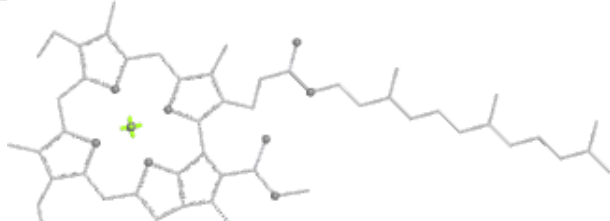
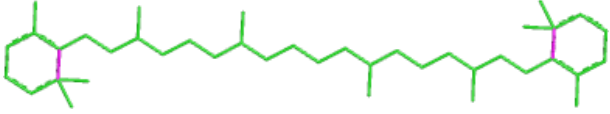
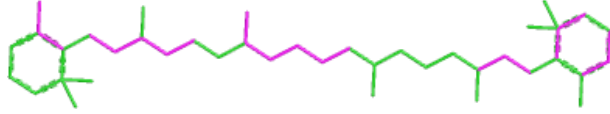
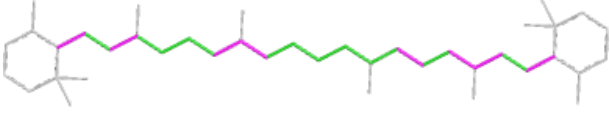
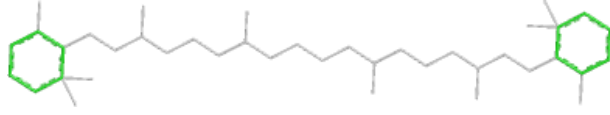


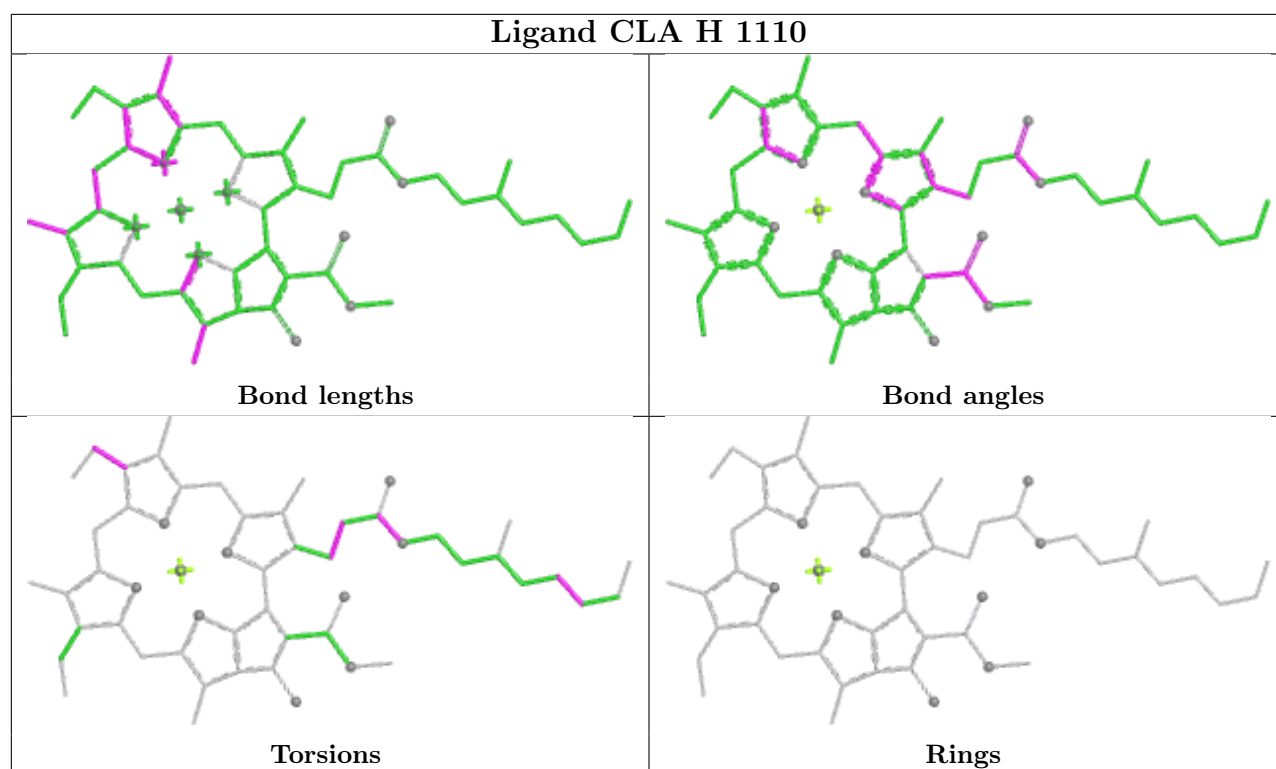
Ligand CLA g 513



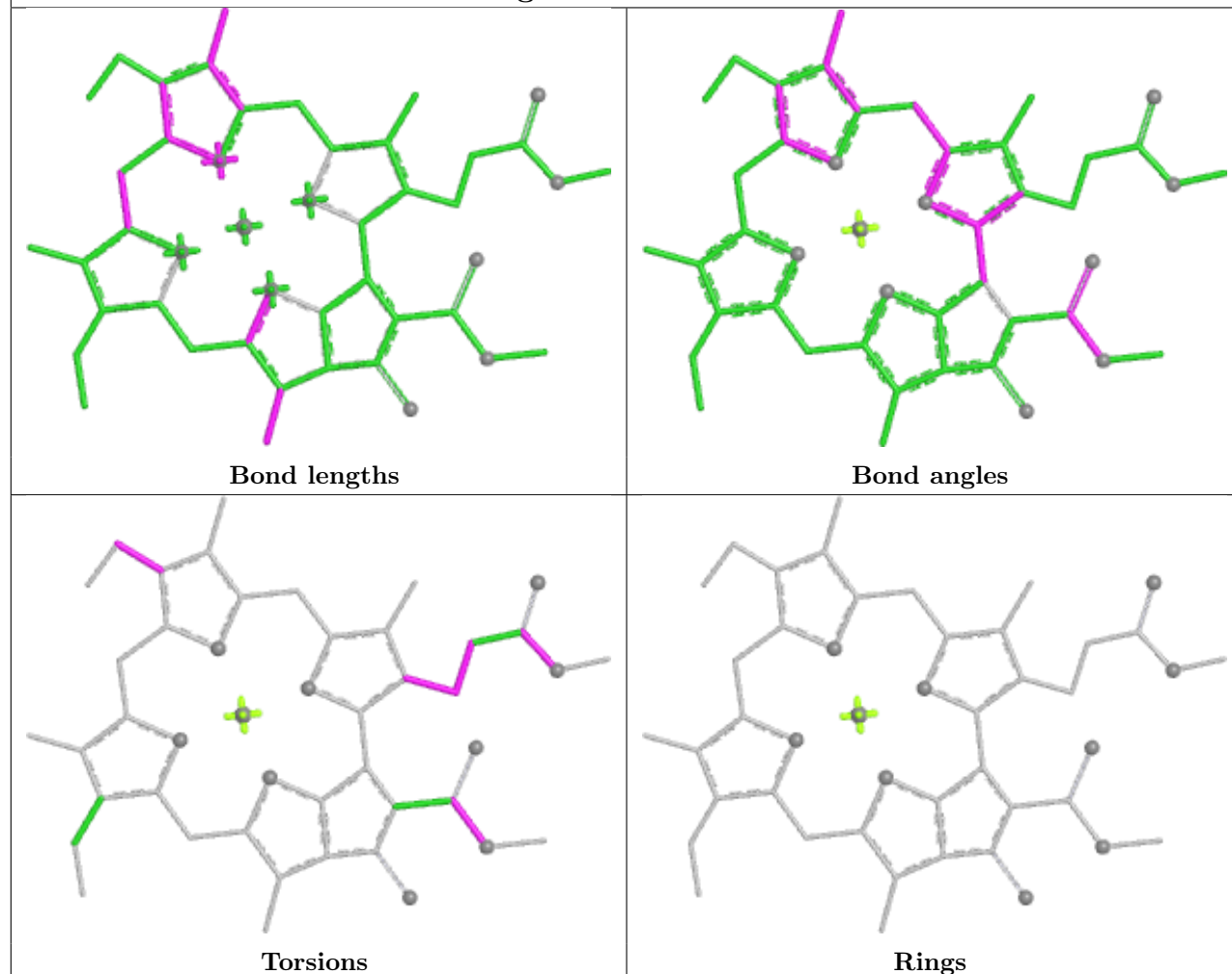
Ligand CLA A 1117



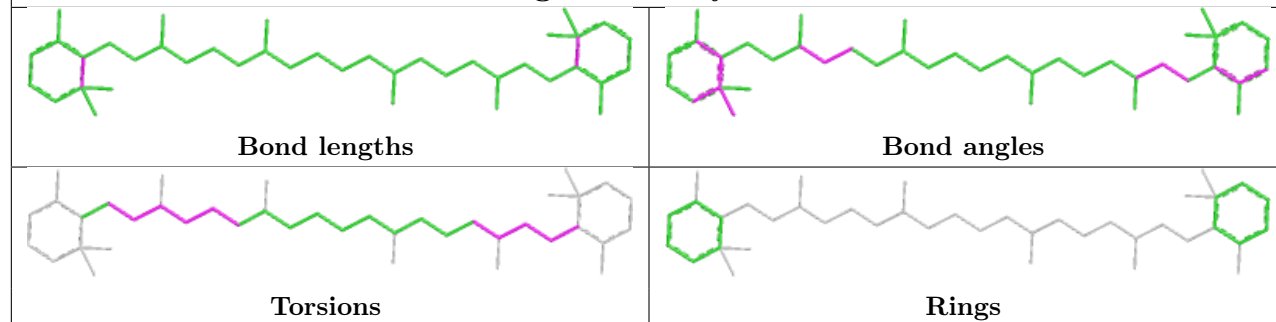
Ligand CLA b 1211	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA w 506	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 4001	
 Bond lengths	 Bond angles
 Torsions	 Rings



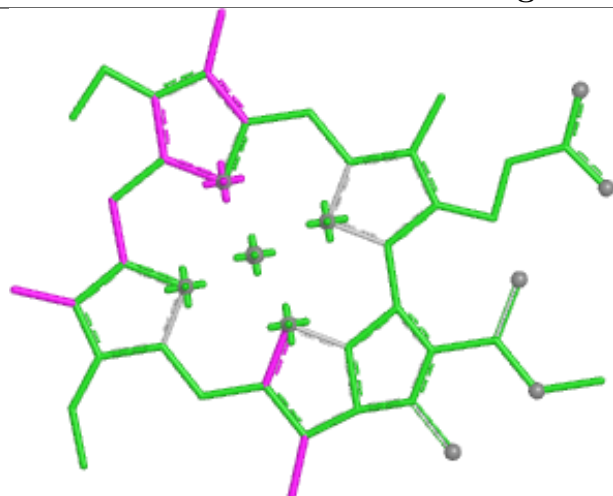
Ligand CLA x 516



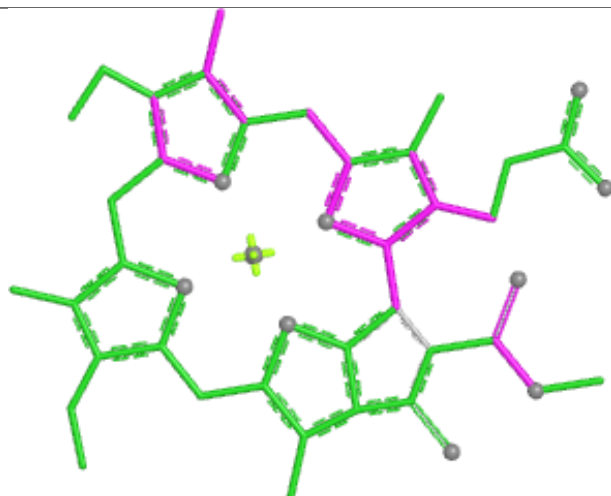
Ligand BCR y 604



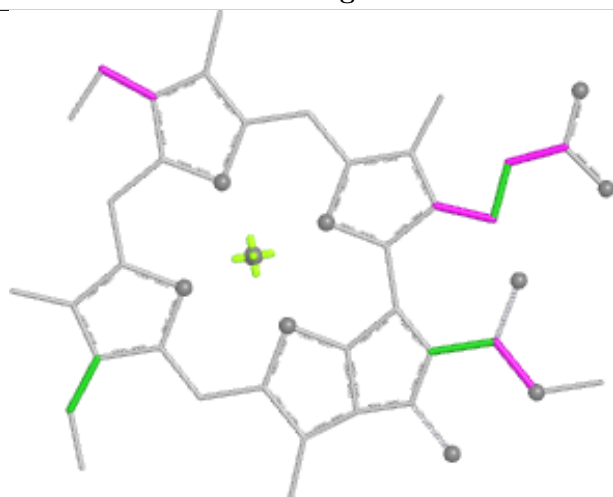
Ligand CLA n 512



Bond lengths



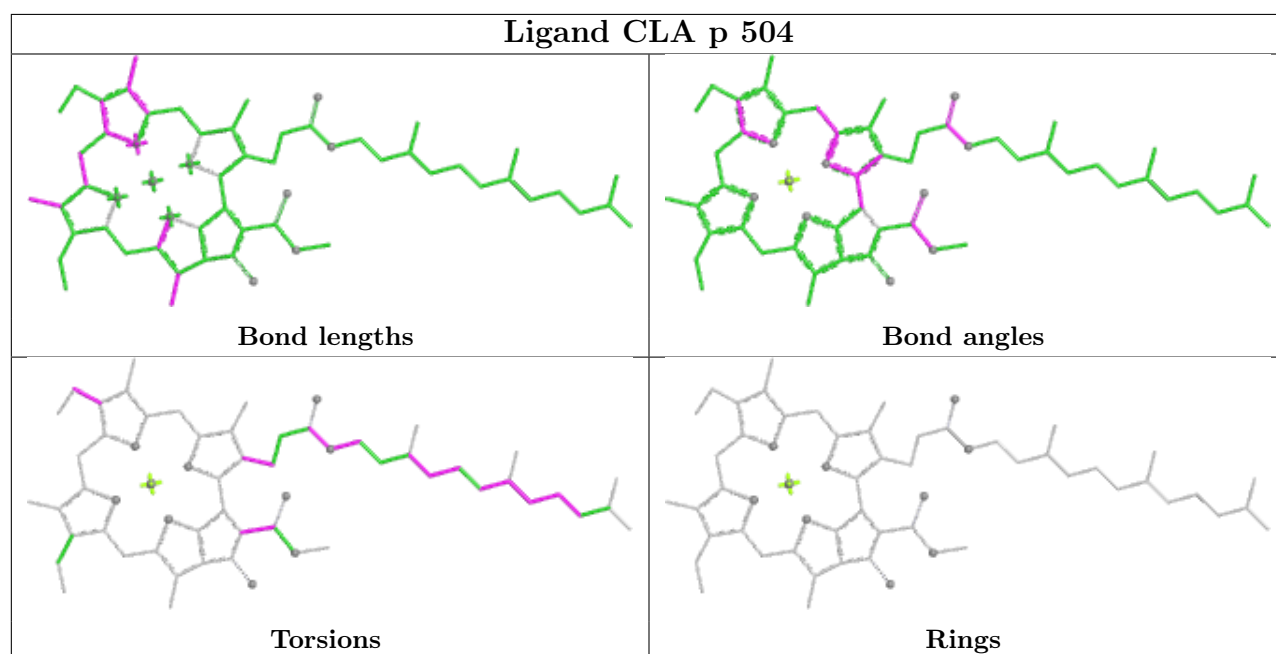
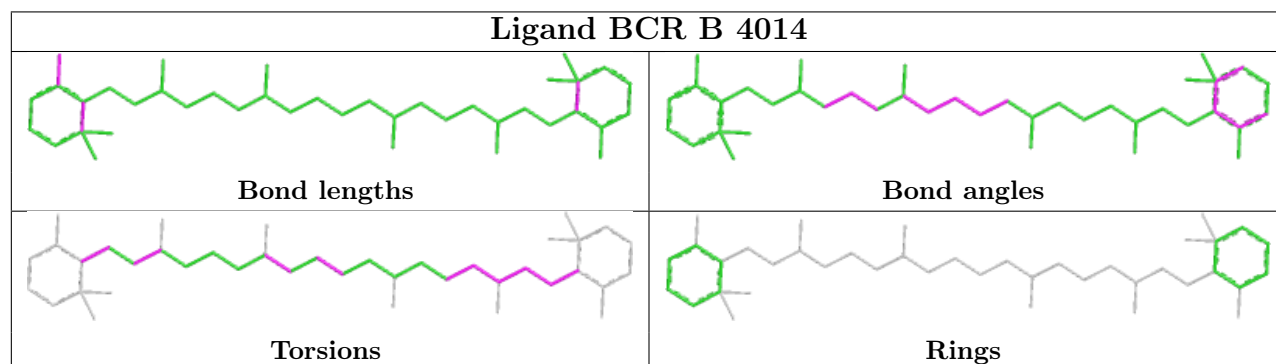
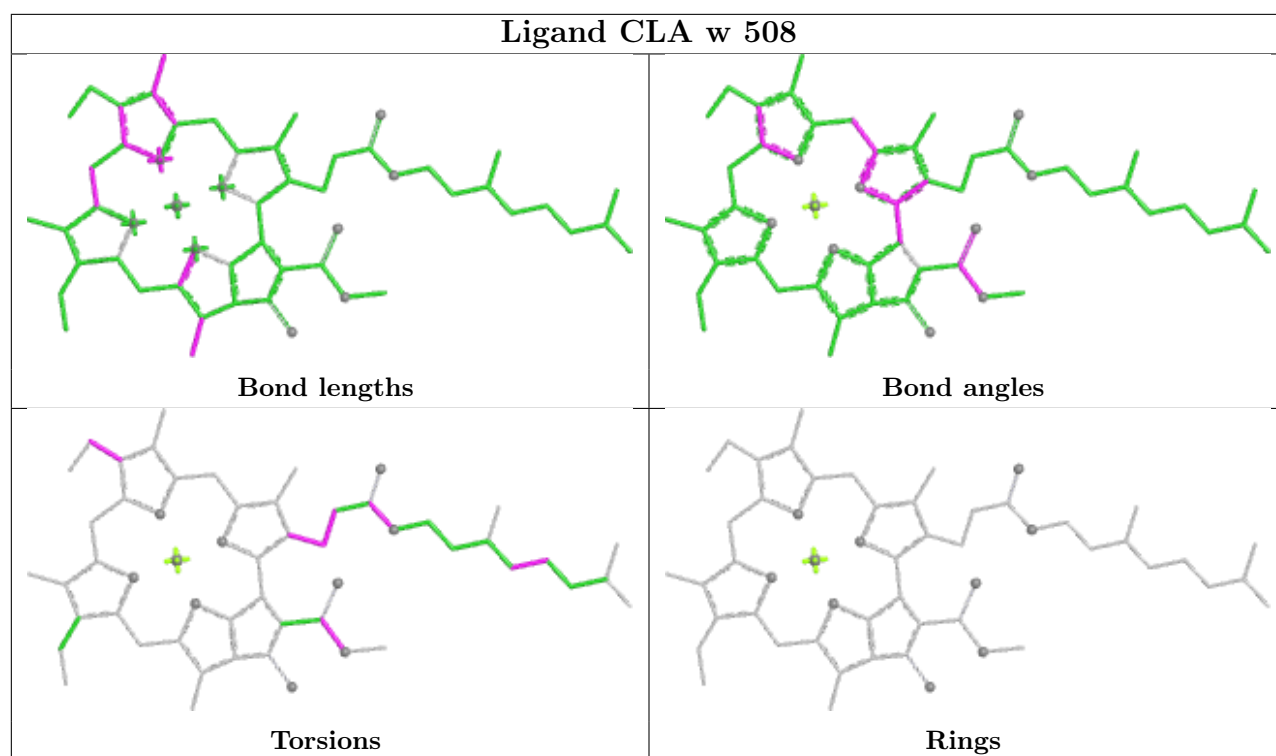
Bond angles



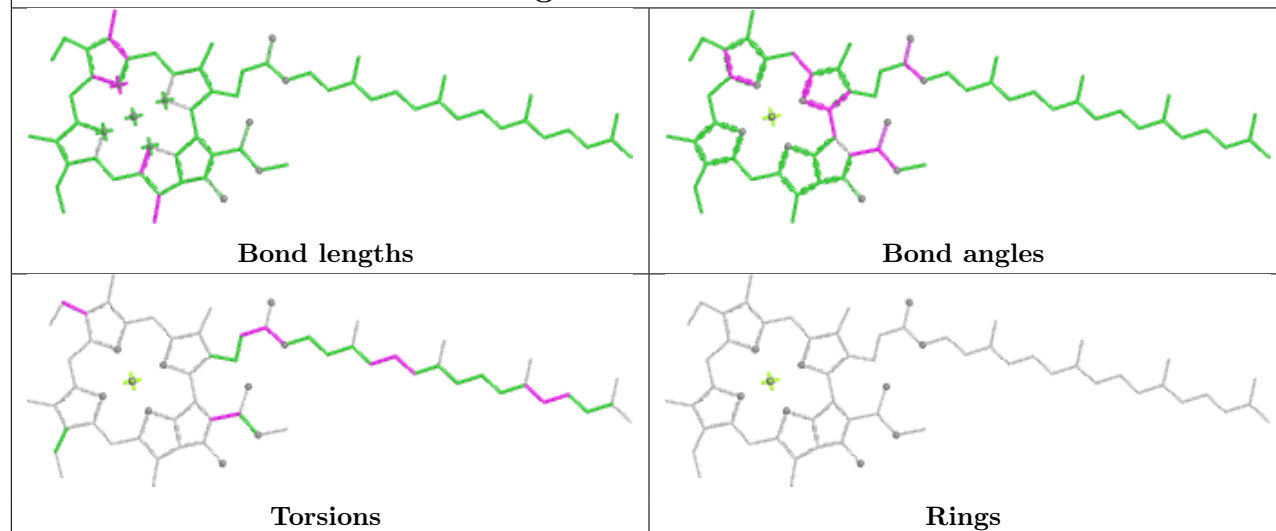
Torsions



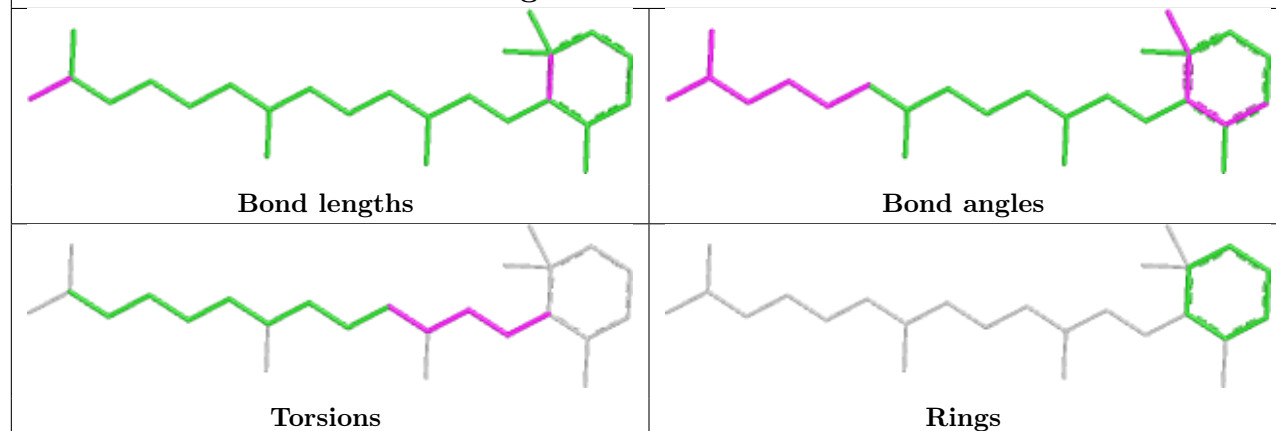
Rings



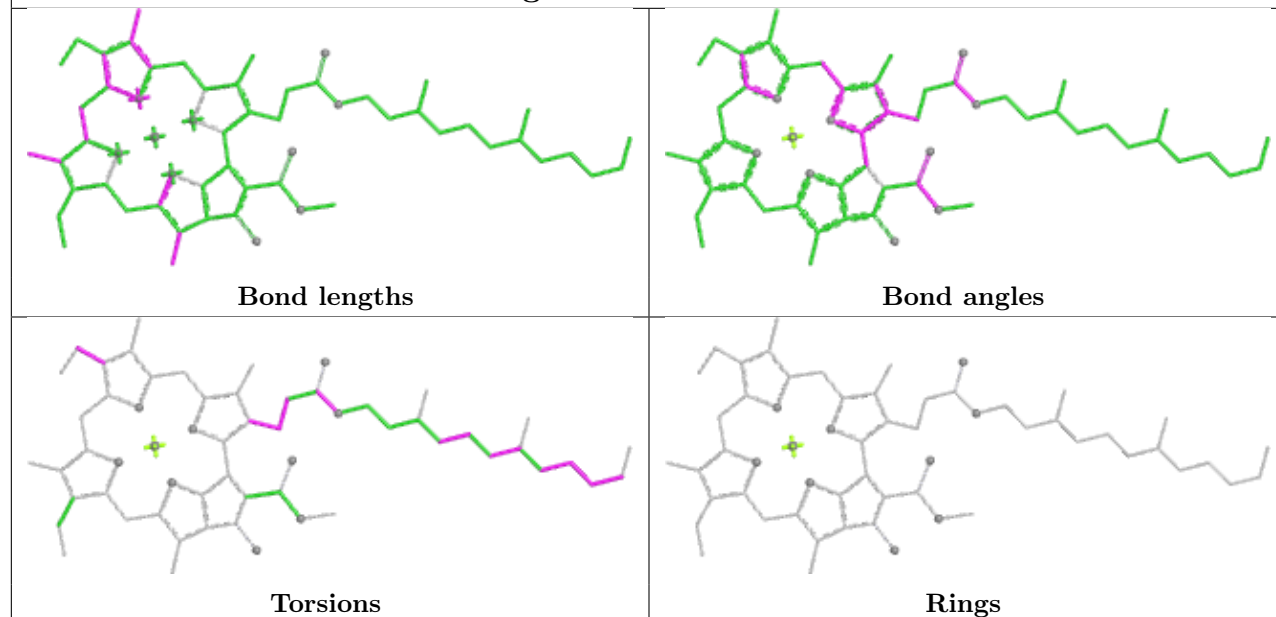
Ligand CLA n 510



Ligand BCR G 4006



Ligand CLA A 1122



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.

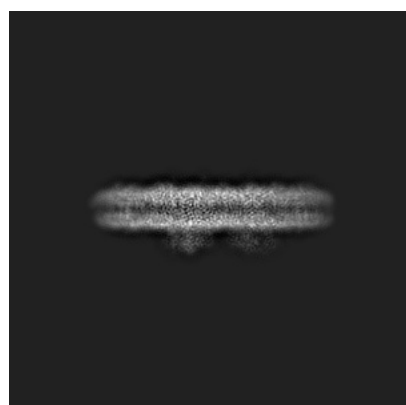
6 Map visualisation [i](#)

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.

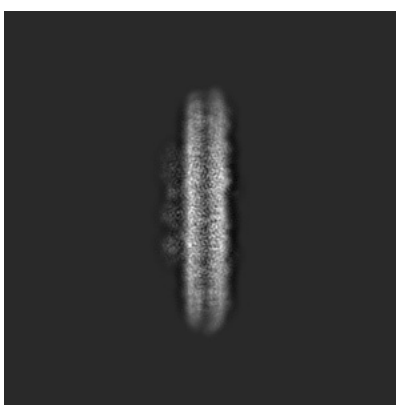
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

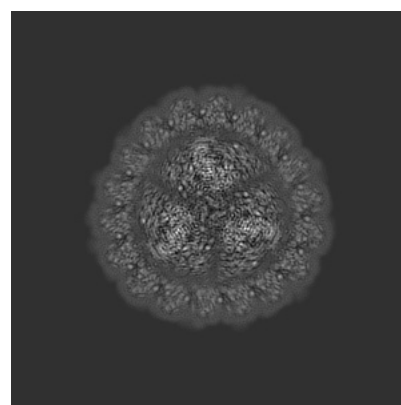
6.1.1 Primary map



X



Y

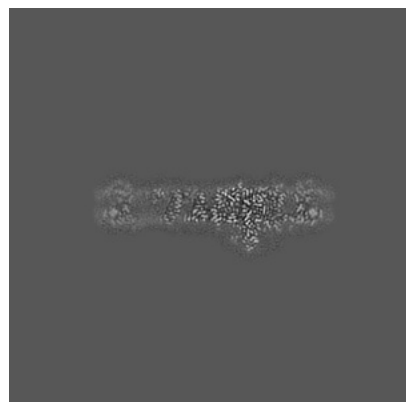


Z

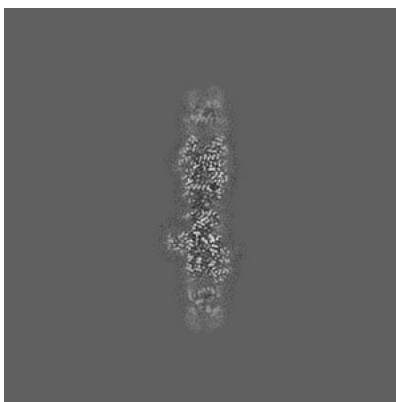
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

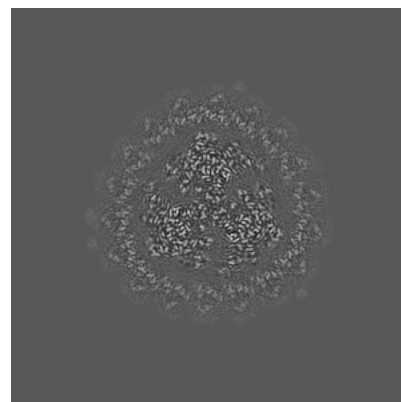
6.2.1 Primary map



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](#)

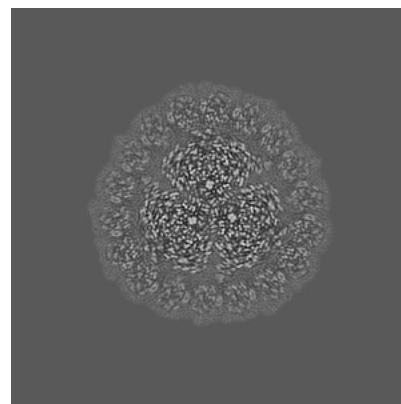
6.3.1 Primary map



X Index: 239



Y Index: 227

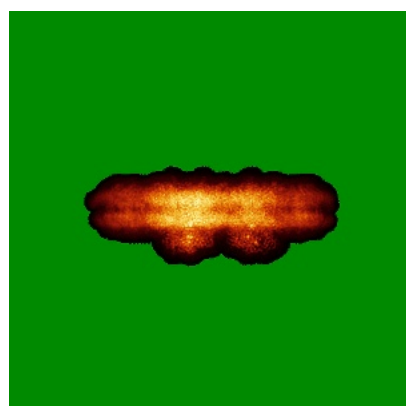


Z Index: 238

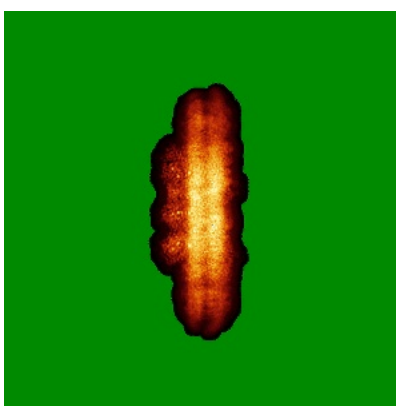
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

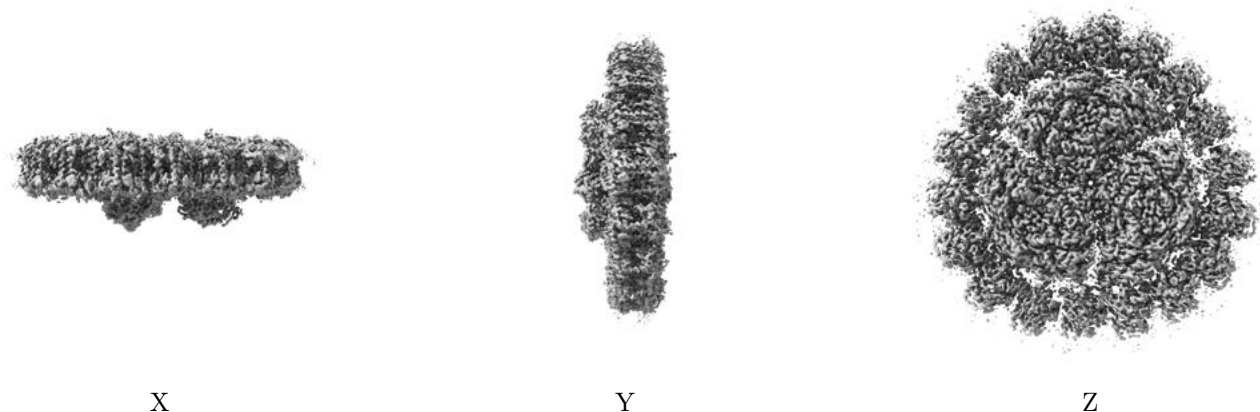


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

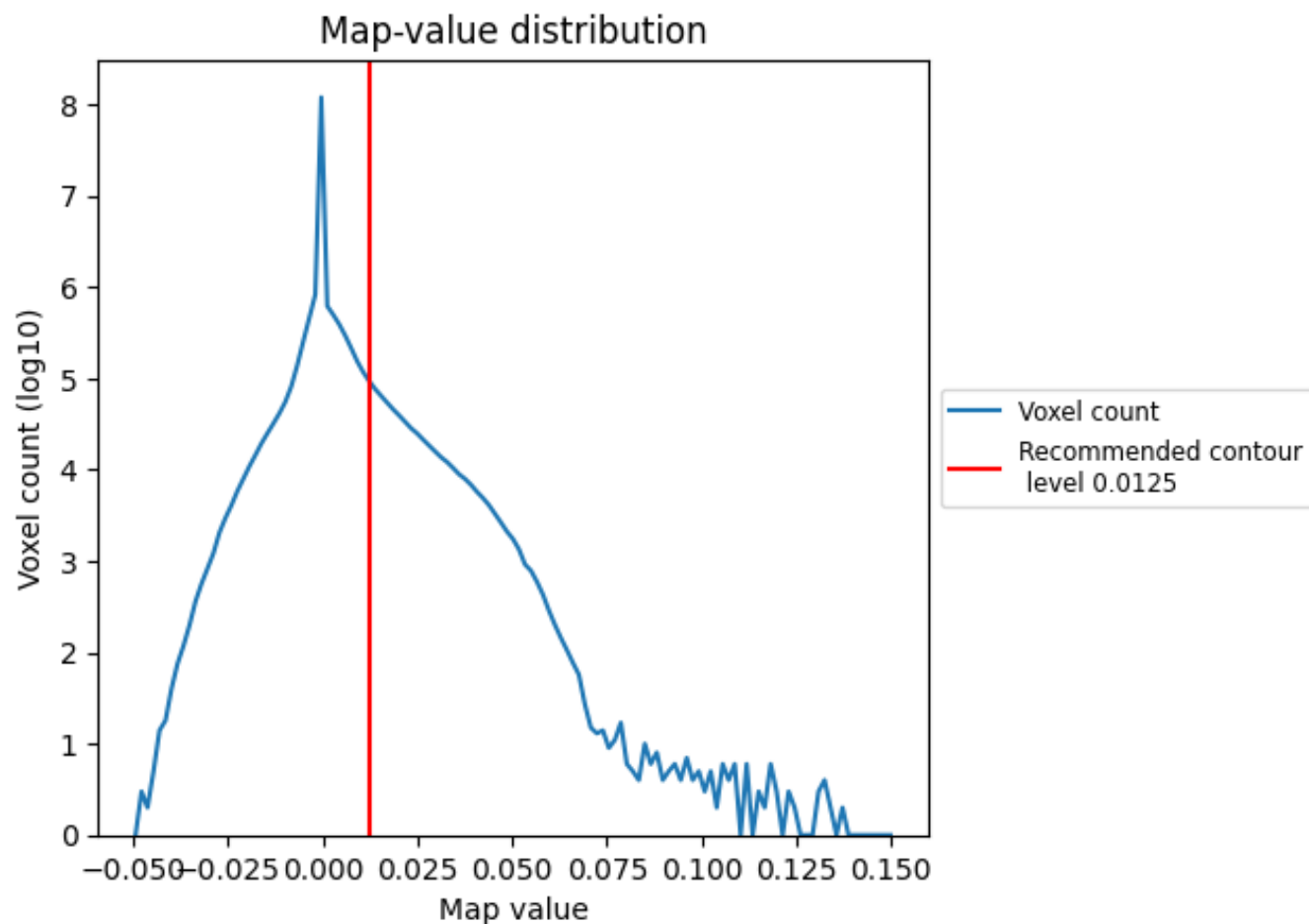
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

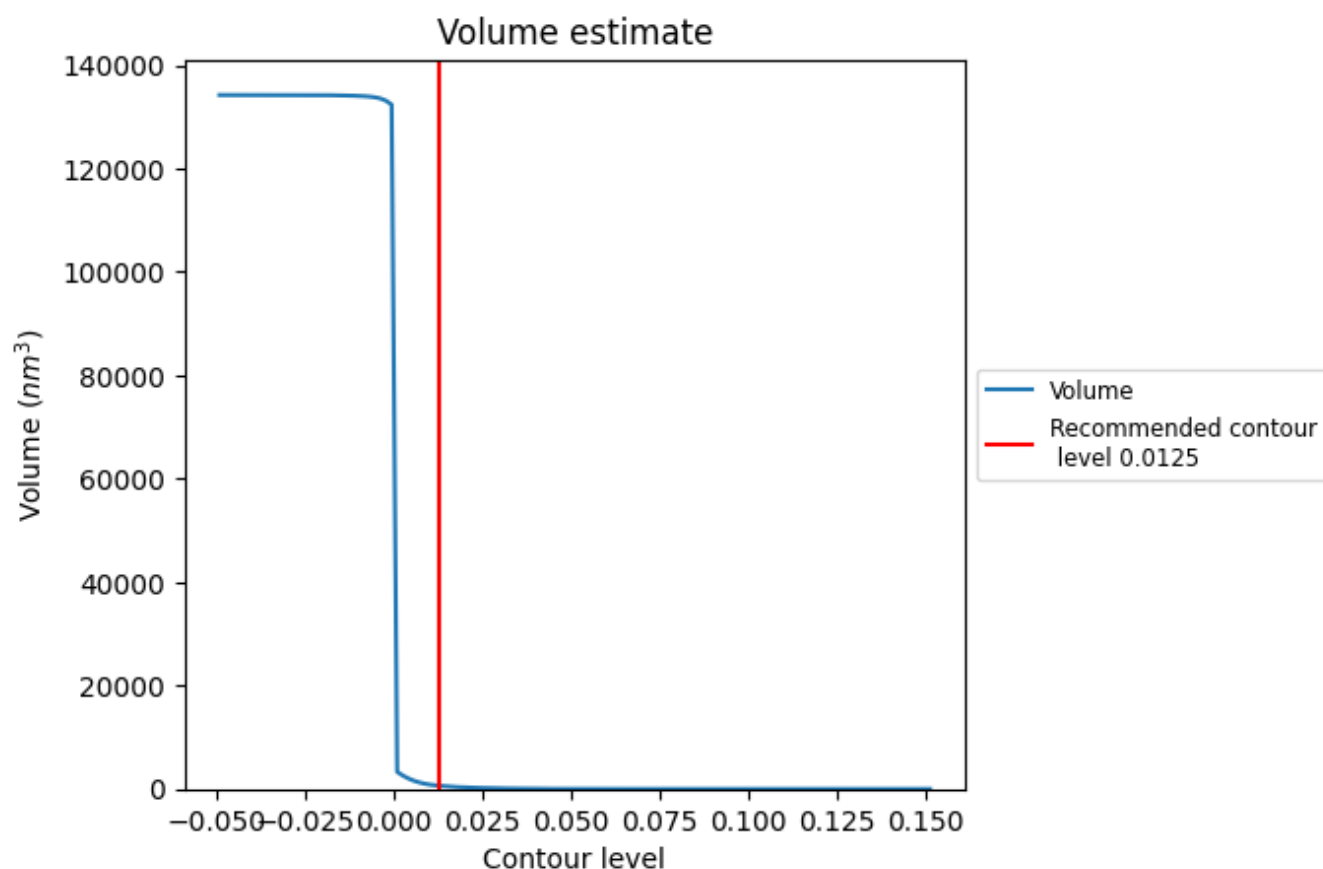
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

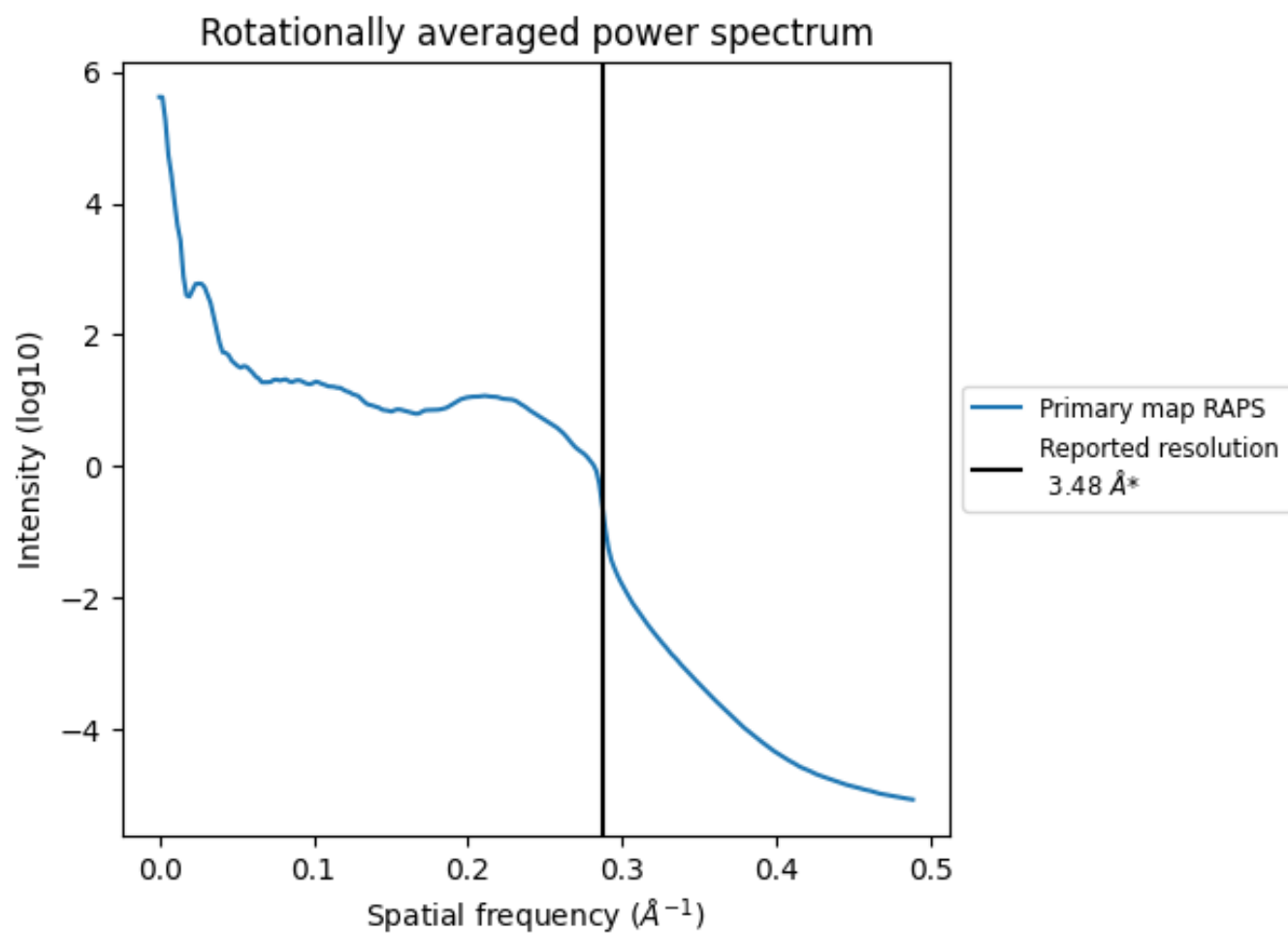
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 642 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 ⓘ

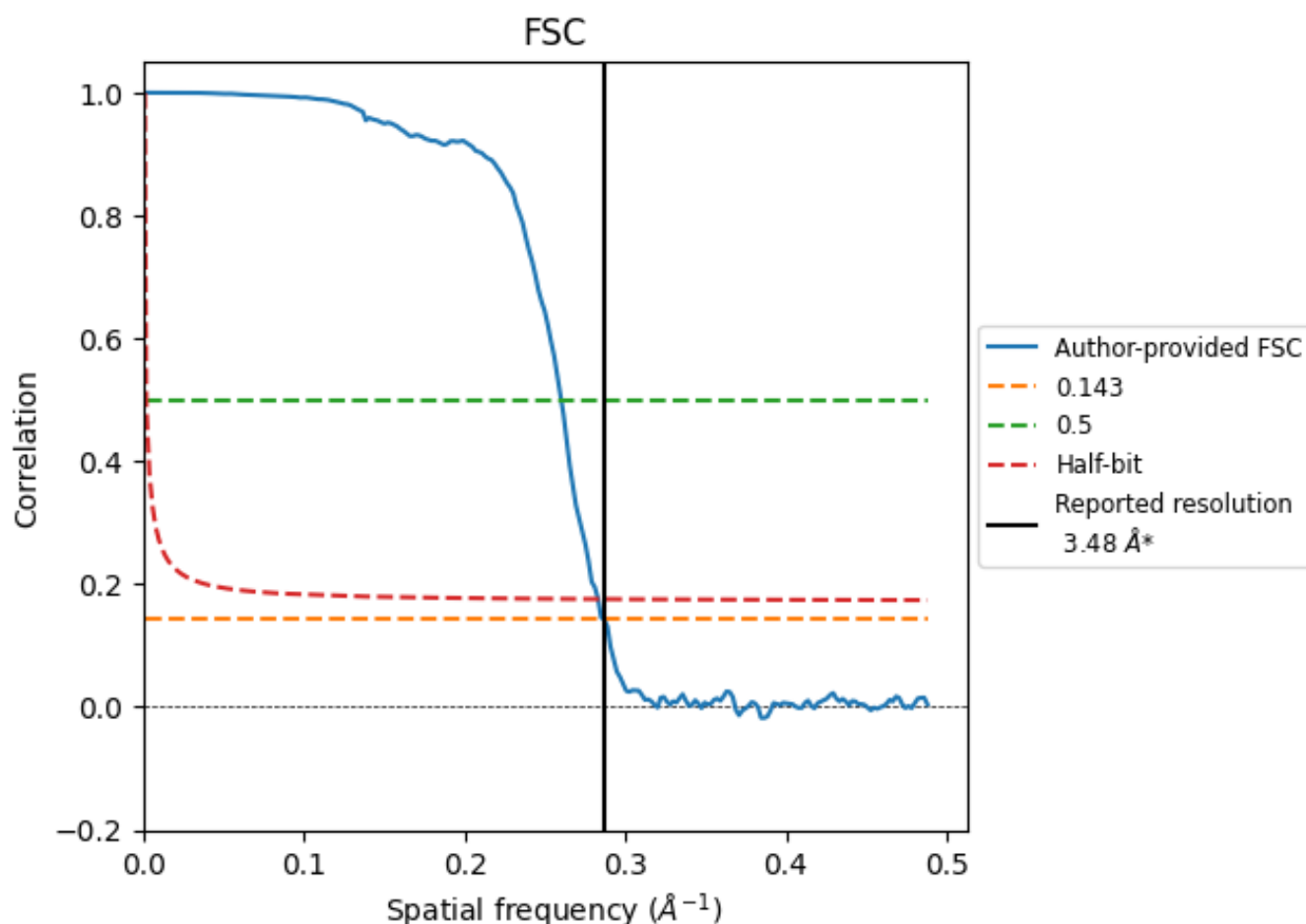


*Reported resolution corresponds to spatial frequency of 0.287 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.287 Å⁻¹

8.2 Resolution estimates [i](#)

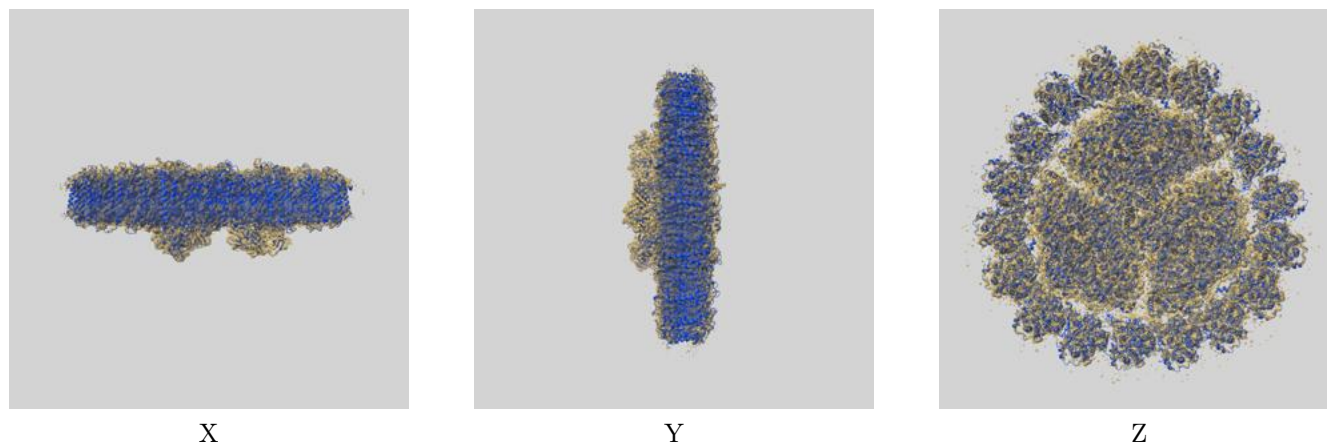
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.48	-	-
Author-provided FSC curve	3.49	3.84	3.53
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

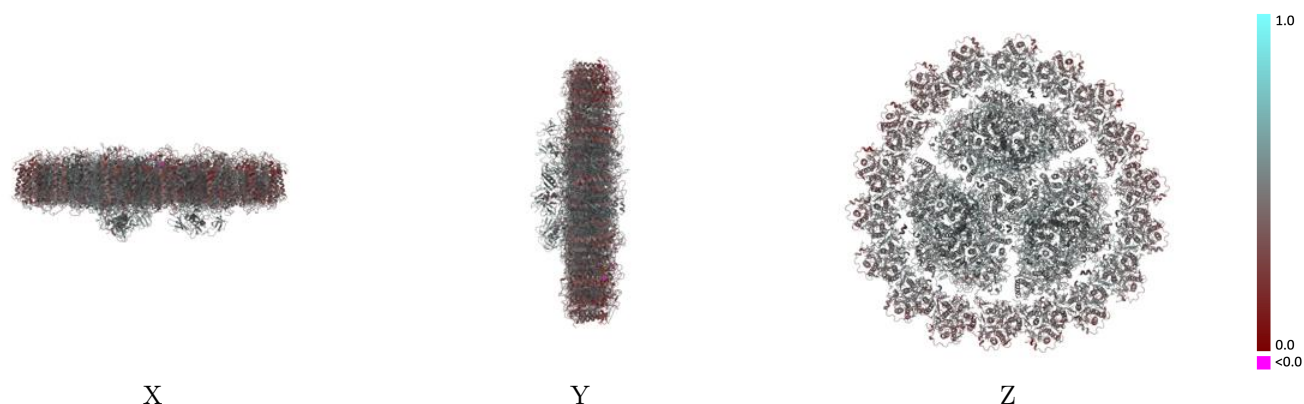
This section contains information regarding the fit between EMDB map EMD-0524 and PDB model 6NWA. Per-residue inclusion information can be found in section [3](#) on page [65](#).

9.1 Map-model overlay [i](#)



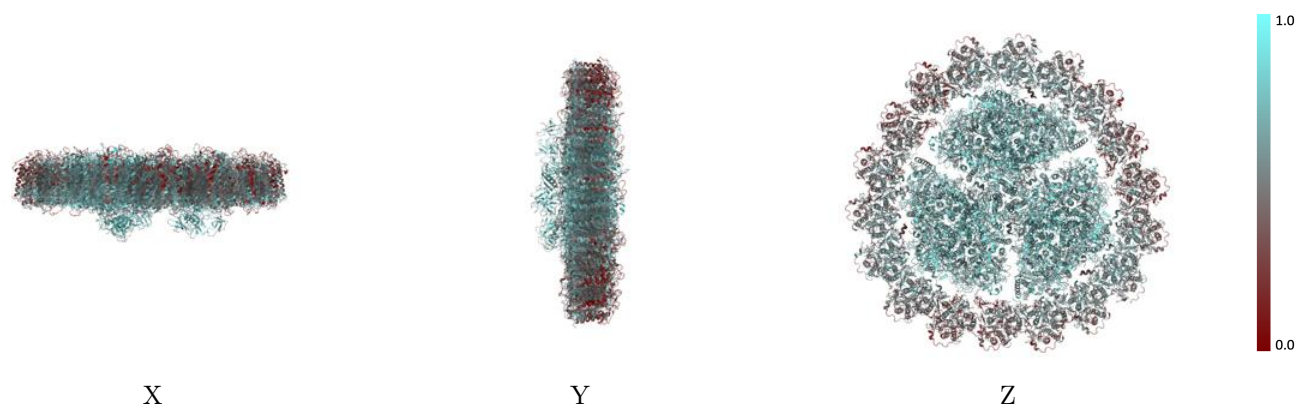
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



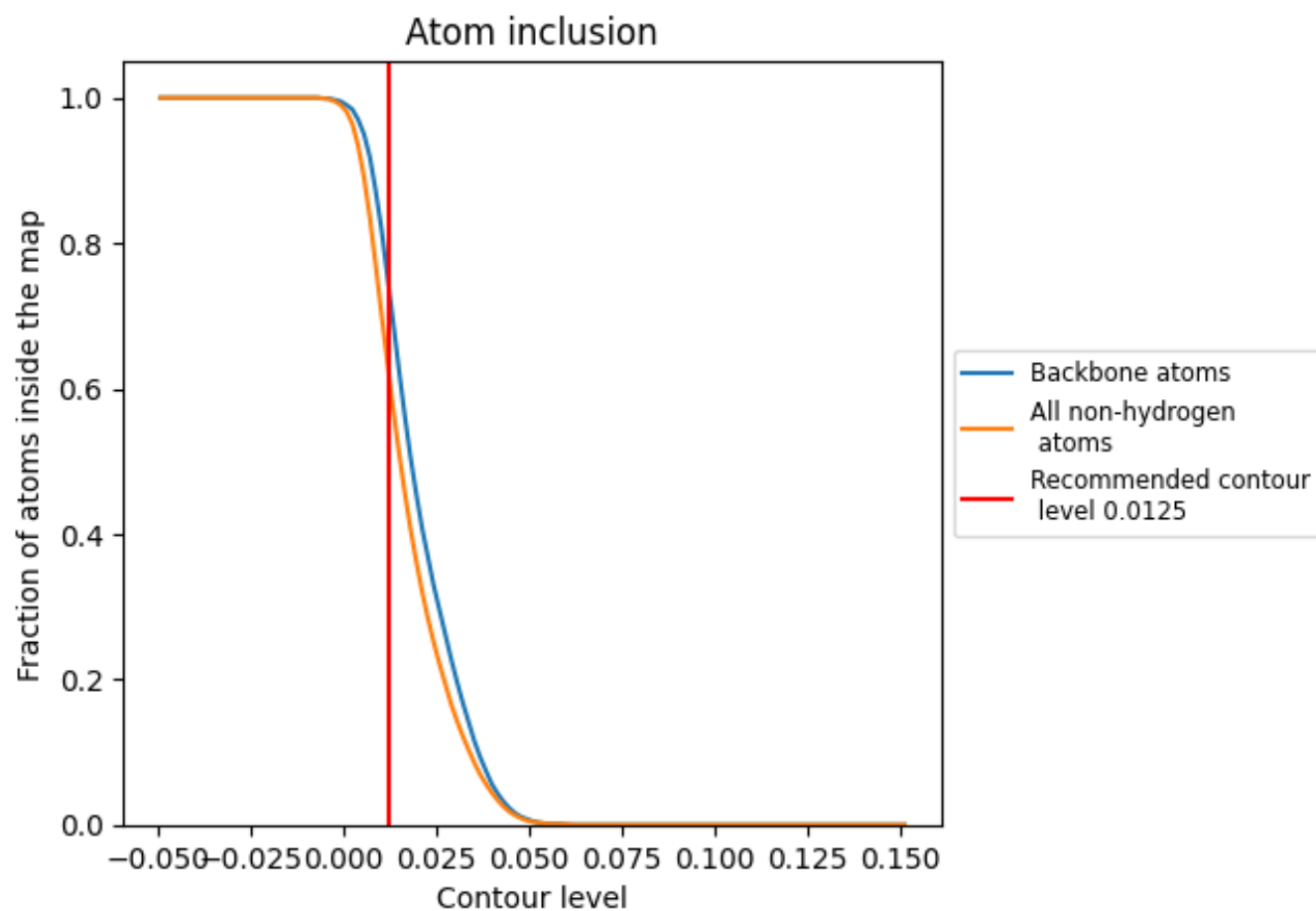
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.6100	 0.4590
A	 0.7410	 0.5070
B	 0.7360	 0.5030
C	 0.7990	 0.5080
D	 0.7050	 0.5070
E	 0.7060	 0.4990
F	 0.6980	 0.4740
G	 0.7370	 0.5030
H	 0.7440	 0.5120
I	 0.7630	 0.5330
J	 0.6770	 0.4880
K	 0.6250	 0.4280
L	 0.7250	 0.5040
M	 0.6150	 0.4870
N	 0.7970	 0.5060
O	 0.6980	 0.5080
P	 0.6930	 0.5020
Q	 0.6950	 0.4790
R	 0.7720	 0.5320
S	 0.6750	 0.4990
T	 0.6040	 0.4130
U	 0.7280	 0.5080
V	 0.6400	 0.4670
W	 0.4010	 0.3750
X	 0.5100	 0.4280
Y	 0.5550	 0.4440
Z	 0.5090	 0.4170
a	 0.7470	 0.5120
b	 0.7400	 0.4980
c	 0.8120	 0.5120
d	 0.7130	 0.5070
e	 0.7120	 0.4910
f	 0.7000	 0.4690
g	 0.4620	 0.3980
h	 0.3900	 0.3840



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Chain	Atom inclusion	Q-score
i	 0.7530	 0.5260
j	 0.6810	 0.4840
k	 0.6050	 0.4380
l	 0.7260	 0.5090
m	 0.6510	 0.4870
n	 0.4000	 0.3750
o	 0.5070	 0.4270
p	 0.5640	 0.4490
q	 0.5150	 0.4220
r	 0.4660	 0.4010
s	 0.5640	 0.4540
t	 0.4100	 0.3800
u	 0.5090	 0.4350
v	 0.3930	 0.3890
w	 0.5150	 0.4210
x	 0.4690	 0.4060
y	 0.3850	 0.3830