



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 06:36 PM EST

PDB ID : 7UMH
EMDB ID : EMD-26601
Title : Energetic robustness to large scale structural dynamics in a photosynthetic supercomplex
Authors : Harris, D.; Toporik, H.; Schlau-Cohen, G.S.; Mazor, Y.
Deposited on : 2022-04-07
Resolution : 2.60 Å(reported)
Based on initial model : 6NWA

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

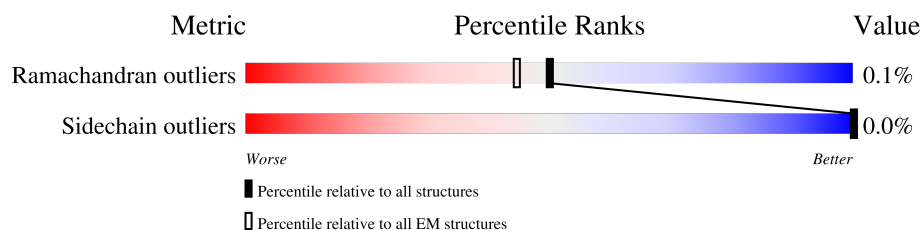
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	98% .
1	H	751	98% .
1	a	751	98% .
2	B	731	100% .
2	G	731	100% .
2	b	731	100% .
3	C	81	99% .
3	N	81	99% .
3	c	81	99% .

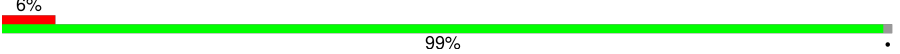
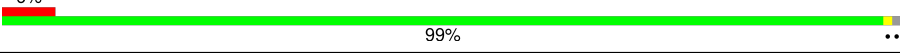
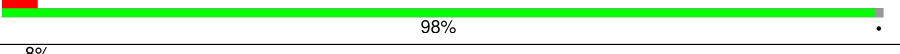
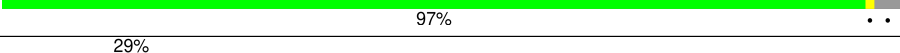
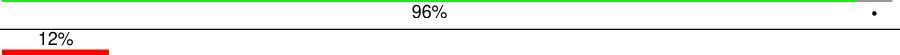
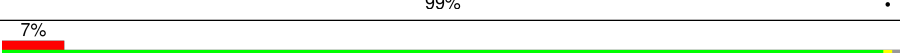
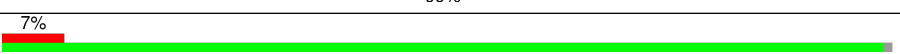

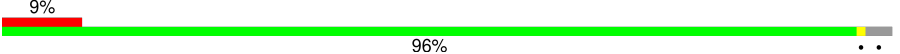
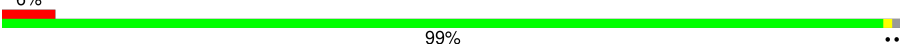
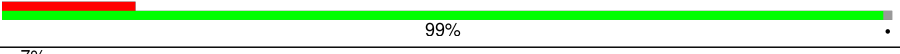
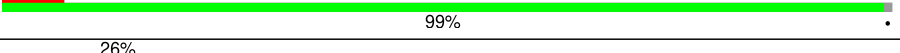
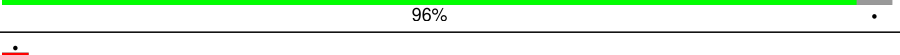
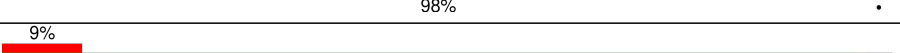
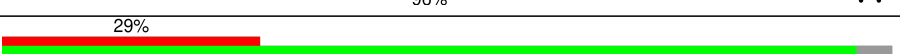

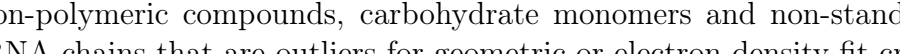
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	141	
4	P	141	
4	d	141	
5	E	74	
5	O	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	K	86	
9	T	86	
9	k	86	
10	L	157	
10	U	157	
10	l	157	
11	M	31	
11	V	31	
11	m	31	
12	W	342	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
12	X	342	 6% 99%
12	Y	342	 6% 99%
12	Z	342	 1% 98%
12	g	342	 8% 97%
12	h	342	 29% 96%
12	n	342	 12% 99%
12	o	342	 7% 99%
12	p	342	 7% 99%
12	q	342	 5% 98%
12	r	342	 9% 96%
12	s	342	 6% 99%
12	t	342	 15% 99%
12	u	342	 7% 99%
12	v	342	 26% 96%
12	w	342	 1% 98%
12	x	342	 9% 96%
12	y	342	 29% 96%

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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	A	1104	X	-	-	-
16	CLA	A	1105	X	-	-	-
16	CLA	A	1106	X	-	-	-
16	CLA	A	1109	X	-	-	-
16	CLA	A	1110	X	-	-	-
16	CLA	A	1111	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	1119	X	-	-	-
16	CLA	A	1121	X	-	-	-
16	CLA	A	1122	X	-	-	-
16	CLA	A	1124	X	-	-	-
16	CLA	A	1126	X	-	-	-
16	CLA	A	1127	X	-	-	-
16	CLA	A	1128	X	-	-	-
16	CLA	A	1130	X	-	-	-
16	CLA	A	1132	X	-	-	-
16	CLA	A	1133	X	-	-	-
16	CLA	A	1135	X	-	-	-
16	CLA	A	1136	X	-	-	-
16	CLA	A	1137	X	-	-	-
16	CLA	A	1138	X	-	-	-
16	CLA	A	1139	X	-	-	-
16	CLA	A	1140	X	-	-	-
16	CLA	A	1237	X	-	-	-
16	CLA	A	1801	X	-	-	-
16	CLA	B	1012	X	-	-	-
16	CLA	B	1021	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	1208	X	-	-	-
16	CLA	B	1209	X	-	-	-
16	CLA	B	1211	X	-	-	-
16	CLA	B	1212	X	-	-	-
16	CLA	B	1213	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	B	1214	X	-	-	-
16	CLA	B	1215	X	-	-	-
16	CLA	B	1220	X	-	-	-
16	CLA	B	1223	X	-	-	-
16	CLA	B	1224	X	-	-	-
16	CLA	B	1227	X	-	-	-
16	CLA	B	1229	X	-	-	-
16	CLA	B	1230	X	-	-	-
16	CLA	B	1231	X	-	-	-
16	CLA	B	1232	X	-	-	-
16	CLA	B	1234	X	-	-	-
16	CLA	B	1235	X	-	-	-
16	CLA	B	1236	X	-	-	-
16	CLA	B	1238	X	-	-	-
16	CLA	B	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	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	1208	X	-	-	-
16	CLA	G	1209	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	1220	X	-	-	-
16	CLA	G	1221	X	-	-	-
16	CLA	G	1223	X	-	-	-
16	CLA	G	1224	X	-	-	-
16	CLA	G	1225	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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	G	1234	X	-	-	-
16	CLA	G	1235	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	1109	X	-	-	-
16	CLA	H	1110	X	-	-	-
16	CLA	H	1111	X	-	-	-
16	CLA	H	1113	X	-	-	-
16	CLA	H	1114	X	-	-	-
16	CLA	H	1116	X	-	-	-
16	CLA	H	1117	X	-	-	-
16	CLA	H	1119	X	-	-	-
16	CLA	H	1121	X	-	-	-
16	CLA	H	1124	X	-	-	-
16	CLA	H	1126	X	-	-	-
16	CLA	H	1127	X	-	-	-
16	CLA	H	1128	X	-	-	-
16	CLA	H	1131	X	-	-	-
16	CLA	H	1132	X	-	-	-
16	CLA	H	1136	X	-	-	-
16	CLA	H	1137	X	-	-	-
16	CLA	H	1138	X	-	-	-
16	CLA	H	1139	X	-	-	-
16	CLA	H	1140	X	-	-	-
16	CLA	H	1237	X	-	-	-
16	CLA	H	1801	X	-	-	-
16	CLA	J	1302	X	-	-	-
16	CLA	K	4002	X	-	-	-
16	CLA	K	4003	X	-	-	-
16	CLA	K	4004	X	-	-	-
16	CLA	L	1503	X	-	-	-
16	CLA	Q	1301	X	-	-	-
16	CLA	Q	1302	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	S	1302	X	-	-	-
16	CLA	T	4002	X	-	-	-
16	CLA	T	4003	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	508	X	-	-	-
16	CLA	W	509	X	-	-	-
16	CLA	W	511	X	-	-	-
16	CLA	W	512	X	-	-	-
16	CLA	W	514	X	-	-	-
16	CLA	W	515	X	-	-	-
16	CLA	W	517	X	-	-	-
16	CLA	X	502	X	-	-	-
16	CLA	X	505	X	-	-	-
16	CLA	X	506	X	-	-	-
16	CLA	X	508	X	-	-	-
16	CLA	X	509	X	-	-	-
16	CLA	X	511	X	-	-	-
16	CLA	X	514	X	-	-	-
16	CLA	X	515	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	508	X	-	-	-
16	CLA	Y	509	X	-	-	-
16	CLA	Y	511	X	-	-	-
16	CLA	Y	512	X	-	-	-
16	CLA	Y	514	X	-	-	-
16	CLA	Y	515	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	507	X	-	-	-
16	CLA	Z	508	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	Z	509	X	-	-	-
16	CLA	Z	511	X	-	-	-
16	CLA	Z	512	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	1109	X	-	-	-
16	CLA	a	1110	X	-	-	-
16	CLA	a	1111	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	1119	X	-	-	-
16	CLA	a	1121	X	-	-	-
16	CLA	a	1124	X	-	-	-
16	CLA	a	1126	X	-	-	-
16	CLA	a	1127	X	-	-	-
16	CLA	a	1128	X	-	-	-
16	CLA	a	1132	X	-	-	-
16	CLA	a	1135	X	-	-	-
16	CLA	a	1136	X	-	-	-
16	CLA	a	1137	X	-	-	-
16	CLA	a	1138	X	-	-	-
16	CLA	a	1139	X	-	-	-
16	CLA	a	1237	X	-	-	-
16	CLA	a	1801	X	-	-	-
16	CLA	b	1012	X	-	-	-
16	CLA	b	1021	X	-	-	-
16	CLA	b	1201	X	-	-	-
16	CLA	b	1202	X	-	-	-
16	CLA	b	1203	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	b	1204	X	-	-	-
16	CLA	b	1205	X	-	-	-
16	CLA	b	1206	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	1216	X	-	-	-
16	CLA	b	1221	X	-	-	-
16	CLA	b	1223	X	-	-	-
16	CLA	b	1224	X	-	-	-
16	CLA	b	1226	X	-	-	-
16	CLA	b	1227	X	-	-	-
16	CLA	b	1228	X	-	-	-
16	CLA	b	1229	X	-	-	-
16	CLA	b	1231	X	-	-	-
16	CLA	b	1232	X	-	-	-
16	CLA	b	1234	X	-	-	-
16	CLA	b	1235	X	-	-	-
16	CLA	b	1238	X	-	-	-
16	CLA	b	1240	X	-	-	-
16	CLA	f	1301	X	-	-	-
16	CLA	f	1302	X	-	-	-
16	CLA	g	502	X	-	-	-
16	CLA	g	504	X	-	-	-
16	CLA	g	505	X	-	-	-
16	CLA	g	507	X	-	-	-
16	CLA	g	508	X	-	-	-
16	CLA	g	509	X	-	-	-
16	CLA	g	511	X	-	-	-
16	CLA	g	512	X	-	-	-
16	CLA	g	514	X	-	-	-
16	CLA	g	515	X	-	-	-
16	CLA	g	516	X	-	-	-
16	CLA	h	502	X	-	-	-
16	CLA	h	503	X	-	-	-
16	CLA	h	506	X	-	-	-
16	CLA	h	507	X	-	-	-
16	CLA	h	508	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	h	509	X	-	-	-
16	CLA	h	511	X	-	-	-
16	CLA	h	513	X	-	-	-
16	CLA	h	515	X	-	-	-
16	CLA	h	516	X	-	-	-
16	CLA	h	517	X	-	-	-
16	CLA	k	4002	X	-	-	-
16	CLA	k	4003	X	-	-	-
16	CLA	k	4004	X	-	-	-
16	CLA	l	1503	X	-	-	-
16	CLA	n	501	X	-	-	-
16	CLA	n	502	X	-	-	-
16	CLA	n	503	X	-	-	-
16	CLA	n	505	X	-	-	-
16	CLA	n	507	X	-	-	-
16	CLA	n	508	X	-	-	-
16	CLA	n	509	X	-	-	-
16	CLA	n	512	X	-	-	-
16	CLA	n	514	X	-	-	-
16	CLA	n	515	X	-	-	-
16	CLA	n	517	X	-	-	-
16	CLA	o	502	X	-	-	-
16	CLA	o	505	X	-	-	-
16	CLA	o	506	X	-	-	-
16	CLA	o	508	X	-	-	-
16	CLA	o	509	X	-	-	-
16	CLA	o	511	X	-	-	-
16	CLA	o	512	X	-	-	-
16	CLA	o	514	X	-	-	-
16	CLA	o	515	X	-	-	-
16	CLA	p	501	X	-	-	-
16	CLA	p	502	X	-	-	-
16	CLA	p	503	X	-	-	-
16	CLA	p	508	X	-	-	-
16	CLA	p	509	X	-	-	-
16	CLA	p	511	X	-	-	-
16	CLA	p	512	X	-	-	-
16	CLA	p	514	X	-	-	-
16	CLA	p	515	X	-	-	-
16	CLA	p	516	X	-	-	-
16	CLA	q	501	X	-	-	-
16	CLA	q	502	X	-	-	-

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 140516 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
			5787	3791	984	985	27		
1	H	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		
1	a	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	730	Total	C	N	O	S	0	0
			5775	3801	968	991	15		
2	G	730	Total	C	N	O	S	0	0
			5775	3801	968	991	15		
2	b	730	Total	C	N	O	S	0	0
			5775	3801	968	991	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	N	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		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		
4	d	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	68	Total	C	N	O		0	0
			537	337	95	105			
5	O	68	Total	C	N	O		0	0
			537	337	95	105			
5	e	68	Total	C	N	O		0	0
			537	337	95	105			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		
6	Q	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		
6	f	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		

- 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	R	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		

- 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
			311	210	46	52	3		
8	S	39	Total	C	N	O	S	0	0
			311	210	46	52	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	39	Total	C	N	O	S	0	0
			311	210	46	52	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	77	Total	C	N	O	S	0	0
			538	353	89	92	4		
9	T	77	Total	C	N	O	S	0	0
			538	353	89	92	4		
9	k	77	Total	C	N	O	S	0	0
			538	353	89	92	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		
10	U	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		
10	l	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		

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

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

- Molecule 12 is a protein called Iron stress-induced chlorophyll-binding protein.

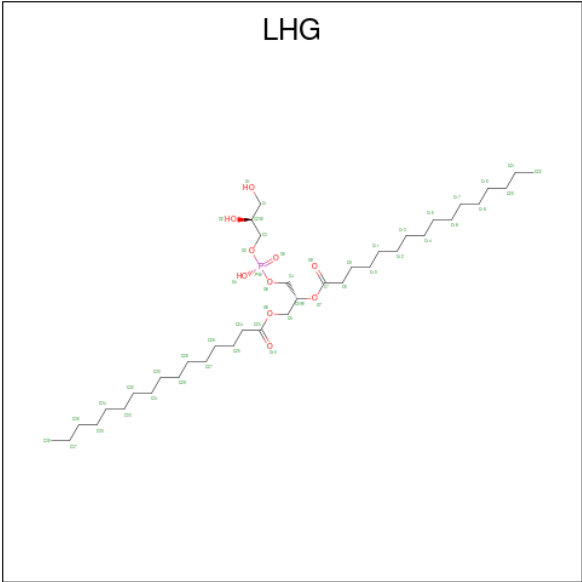
Mol	Chain	Residues	Atoms					AltConf	Trace
12	W	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	X	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	Y	340	Total	C	N	O	S	0	0
			2622	1744	428	445	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	g	333	Total	C	N	O	S	0	0
			2573	1714	420	434	5		
12	h	330	Total	C	N	O	S	0	0
			2538	1692	412	429	5		
12	n	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	o	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	p	340	Total	C	N	O	S	0	0
			2622	1744	428	445	5		
12	q	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	r	332	Total	C	N	O	S	0	0
			2566	1709	419	433	5		
12	s	339	Total	C	N	O	S	0	0
			2617	1741	427	444	5		
12	t	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	u	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	v	330	Total	C	N	O	S	0	0
			2538	1692	412	429	5		
12	w	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	x	332	Total	C	N	O	S	0	0
			2566	1709	419	433	5		
12	y	330	Total	C	N	O	S	0	0
			2532	1689	409	429	5		

- Molecule 13 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



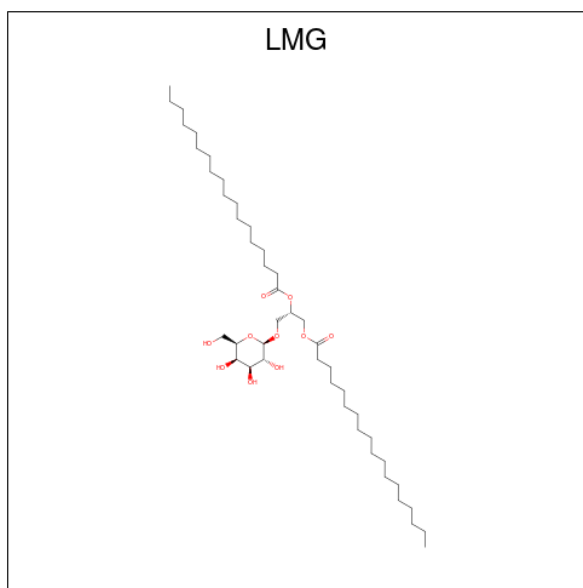
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			43	32	10	1	
13	A	1	Total	C	O	P	0
			26	15	10	1	
13	B	1	Total	C	O	P	0
			38	27	10	1	
13	G	1	Total	C	O	P	0
			38	27	10	1	
13	H	1	Total	C	O	P	0
			43	32	10	1	
13	H	1	Total	C	O	P	0
			26	15	10	1	
13	I	1	Total	C	O	P	0
			40	29	10	1	
13	R	1	Total	C	O	P	0
			40	29	10	1	
13	X	1	Total	C	O	P	0
			27	16	10	1	
13	Y	1	Total	C	O	P	0
			32	21	10	1	
13	a	1	Total	C	O	P	0
			43	32	10	1	
13	a	1	Total	C	O	P	0
			26	15	10	1	
13	b	1	Total	C	O	P	0
			38	27	10	1	
13	g	1	Total	C	O	P	0
			31	20	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
13	i	1	Total	C	O	P	0
			40	29	10	1	
13	o	1	Total	C	O	P	0
			27	16	10	1	
13	p	1	Total	C	O	P	0
			32	21	10	1	
13	r	1	Total	C	O	P	0
			31	20	10	1	
13	s	1	Total	C	O	P	0
			32	21	10	1	
13	u	1	Total	C	O	P	0
			27	16	10	1	
13	x	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 14 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



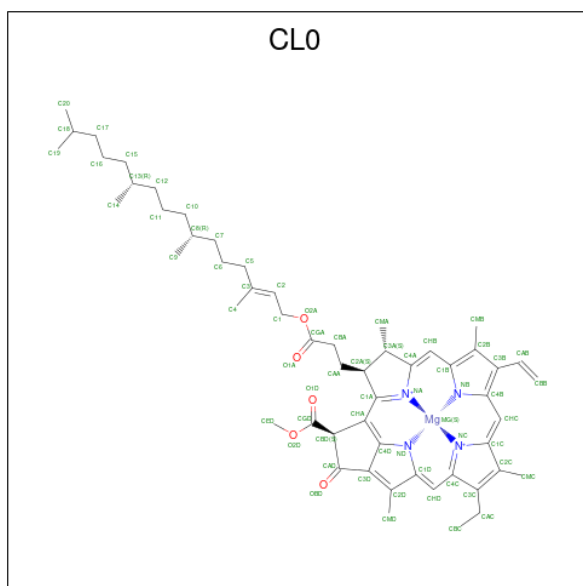
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	O		0
			38	28	10		
14	A	1	Total	C	O		0
			46	36	10		
14	A	1	Total	C	O		0
			32	22	10		
14	B	1	Total	C	O		0
			43	33	10		

Continued on next page...

Continued from previous page...

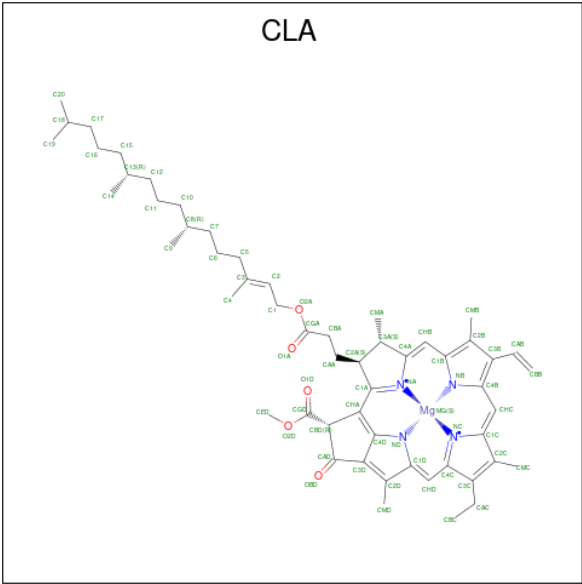
Mol	Chain	Residues	Atoms			AltConf
14	F	1	Total	C	O	0
			27	17	10	
14	G	1	Total	C	O	0
			43	33	10	
14	H	1	Total	C	O	0
			38	28	10	
14	H	1	Total	C	O	0
			46	36	10	
14	H	1	Total	C	O	0
			32	22	10	
14	Q	1	Total	C	O	0
			27	17	10	
14	a	1	Total	C	O	0
			38	28	10	
14	a	1	Total	C	O	0
			46	36	10	
14	a	1	Total	C	O	0
			32	22	10	
14	b	1	Total	C	O	0
			43	33	10	
14	f	1	Total	C	O	0
			27	17	10	

- Molecule 15 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 16 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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	

Continued on next page...

Continued from previous page...

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
			46	36	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
			60	50	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	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	A	1	Total 60	C 50	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 60	C 50	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 46	C 36	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 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

Continued on next page...

Continued from previous page...

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 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 53	C 43	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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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 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 50	C 40	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 46	C 36	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 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	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 54	C 44	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 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 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 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 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 46	C 36	Mg 1	N 4	O 5	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	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	K	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
16	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	L	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 46	C 36	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 37	C 31	Mg 1	N 4	O 1	0
16	T	1	Total 45	C 35	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 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 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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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 60	C 50	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 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 46	C 36	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
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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 65	C 55	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 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 65	C 55	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
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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
			60	50	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
			46	36	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			60	50	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
			54	44	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
			51	41	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
			47	37	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
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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 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 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
16	f	1	Total 46	C 36	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 46	C 36	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 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 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 46	C 36	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	h	1	Total 46	C 36	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 46	C 36	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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 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 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 46	C 36	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 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	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	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	l	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	l	1	Total 60	C 50	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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
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 65	C 55	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 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 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 46	C 36	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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
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 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 46	C 36	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 65	C 55	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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
16	p	1	Total 65	C 55	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 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 65	C 55	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 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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	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 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 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
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 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 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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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 65	C 55	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 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 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 46	C 36	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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 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 46	C 36	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	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 65	C 55	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 65	C 55	Mg 1	N 4	O 5	0
16	v	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
16	v	1	Total 65	C 55	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 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 65	C 55	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	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 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 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 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 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

Continued on next page...

Continued from previous page...

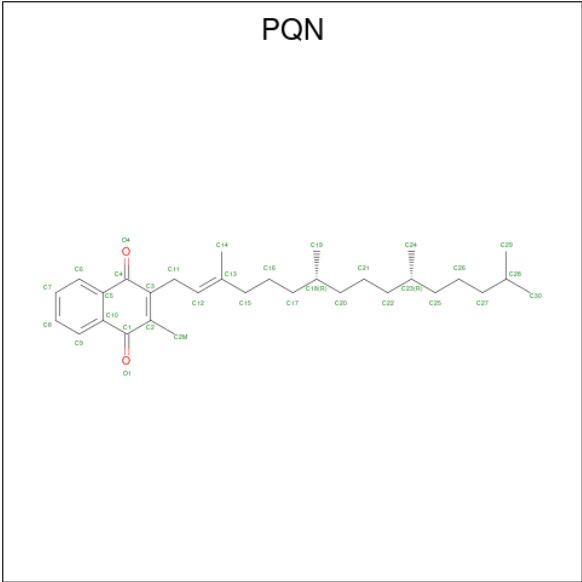
Mol	Chain	Residues	Atoms					AltConf
16	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	w	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	w	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	x	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	x	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	x	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total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

Continued on next page...

Continued from previous page...

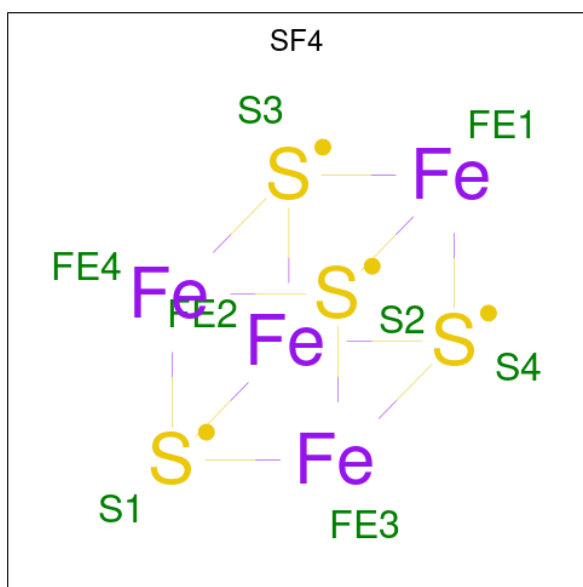
Mol	Chain	Residues	Atoms					AltConf
16	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0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

- Molecule 17 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



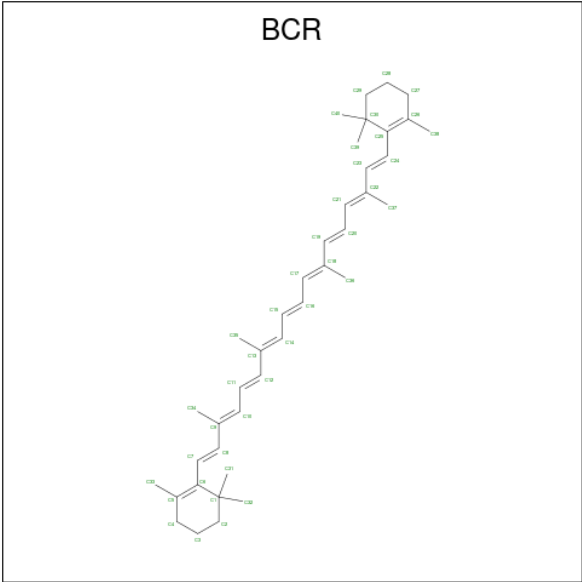
Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	C	O	0
			33	31	2	
17	B	1	Total	C	O	0
			33	31	2	
17	G	1	Total	C	O	0
			33	31	2	
17	H	1	Total	C	O	0
			33	31	2	
17	a	1	Total	C	O	0
			33	31	2	
17	b	1	Total	C	O	0
			33	31	2	

- Molecule 18 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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	H	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	
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	

- Molecule 19 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



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	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			30	30	
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	F	1	Total	C	0
			40	40	
19	G	1	Total	C	0
			40	40	
19	G	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
19	G	1	Total C 30 30	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	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	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	K	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	Q	1	Total C 40 40	0
19	R	1	Total C 40 40	0
19	S	1	Total C 40 40	0
19	S	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
19	S	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	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
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
19	Z	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
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 30 30	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	f	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	h	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	h	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
19	k	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	n	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
19	r	1	Total C 40 40	0
19	r	1	Total C 40 40	0
19	r	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

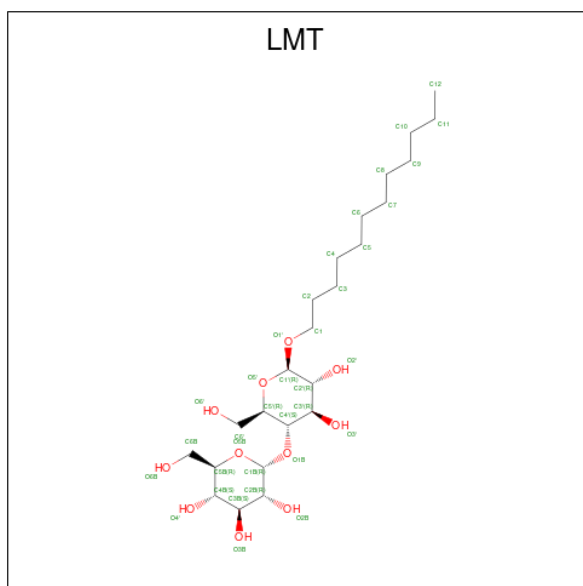
Mol	Chain	Residues	Atoms	AltConf
19	r	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	v	1	Total C 40 40	0
19	v	1	Total C 40 40	0
19	v	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
19	x	1	Total C 40 40	0
19	x	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
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

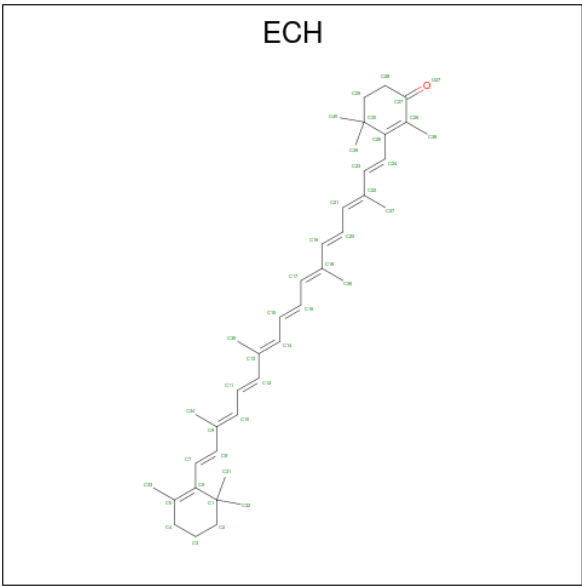
- Molecule 20 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 21 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: $C_{40}H_{54}O$) (labeled

as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	B	1	Total	C	O	0
			41	40	1	
21	G	1	Total	C	O	0
			41	40	1	
21	I	1	Total	C	O	0
			41	40	1	
21	M	1	Total	C	O	0
			41	40	1	
21	R	1	Total	C	O	0
			41	40	1	
21	V	1	Total	C	O	0
			41	40	1	
21	b	1	Total	C	O	0
			41	40	1	
21	i	1	Total	C	O	0
			41	40	1	
21	m	1	Total	C	O	0
			41	40	1	

- Molecule 22 is CALCIUM ION (three-letter code: CA) (formula: Ca).

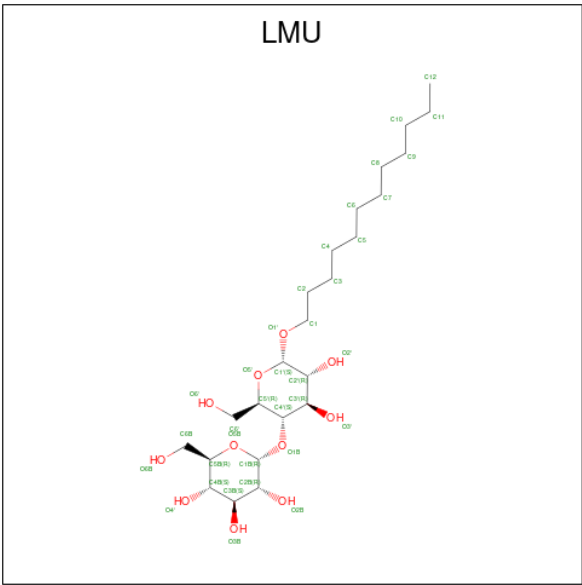
Mol	Chain	Residues	Atoms		AltConf
22	L	1	Total	Ca	0
			1	1	
22	U	1	Total	Ca	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
22	l	1	1	1	0

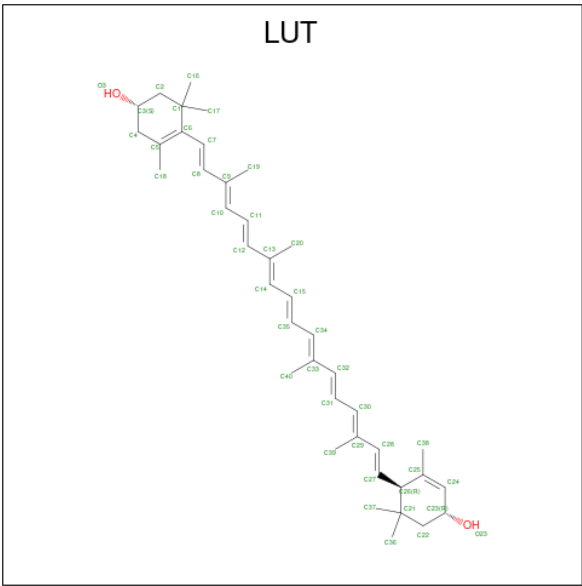
- Molecule 23 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	Y	1	35	24	11	0
23	Z	1	35	24	11	0
23	g	1	35	24	11	0
23	p	1	35	24	11	0
23	q	1	35	24	11	0
23	r	1	35	24	11	0
23	s	1	35	24	11	0
23	w	1	35	24	11	0
23	x	1	35	24	11	0

- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3

,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
24	Z	1	Total	C	O	0
			42	40	2	
24	q	1	Total	C	O	0
			42	40	2	
24	w	1	Total	C	O	0
			42	40	2	

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		AltConf
25	A	56	Total	O	0
			56	56	
25	B	52	Total	O	0
			52	52	
25	C	7	Total	O	0
			7	7	
25	D	3	Total	O	0
			3	3	
25	E	4	Total	O	0
			4	4	
25	F	3	Total	O	0
			3	3	
25	G	55	Total	O	0
			55	55	
25	H	52	Total	O	0
			52	52	

Continued on next page...

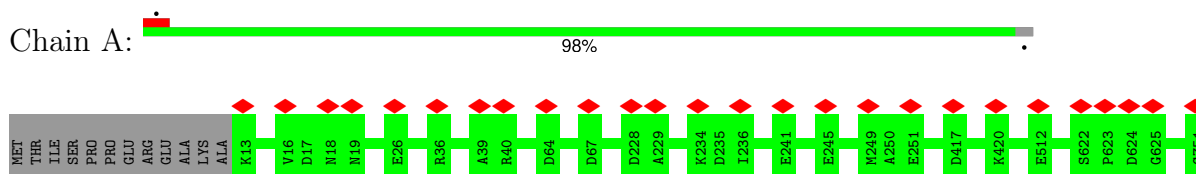
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
25	I	1	Total 1	O 1	0
25	J	1	Total 1	O 1	0
25	L	5	Total 5	O 5	0
25	N	13	Total 13	O 13	0
25	O	11	Total 11	O 11	0
25	P	6	Total 6	O 6	0
25	Q	4	Total 4	O 4	0
25	R	1	Total 1	O 1	0
25	S	3	Total 3	O 3	0
25	U	3	Total 3	O 3	0
25	a	57	Total 57	O 57	0
25	b	74	Total 74	O 74	0
25	c	17	Total 17	O 17	0
25	d	7	Total 7	O 7	0
25	e	10	Total 10	O 10	0
25	f	7	Total 7	O 7	0
25	i	1	Total 1	O 1	0
25	j	1	Total 1	O 1	0
25	k	1	Total 1	O 1	0
25	l	6	Total 6	O 6	0

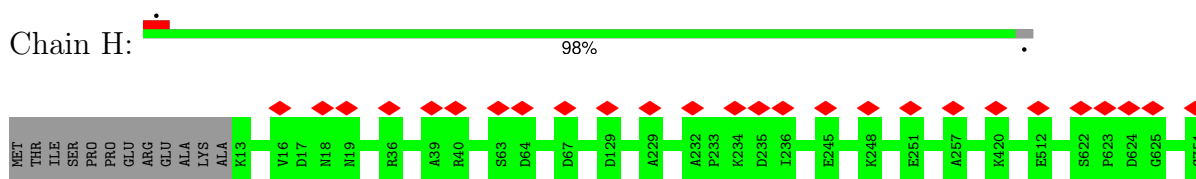
3 Residue-property plots

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

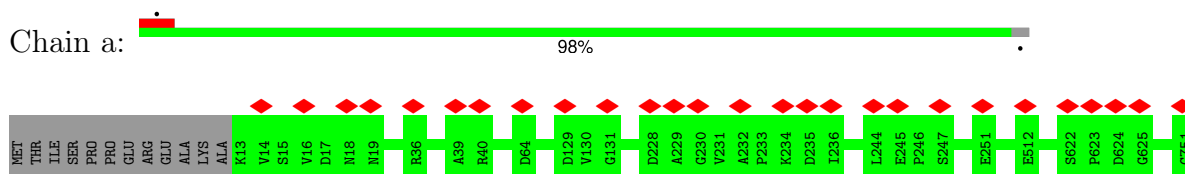
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



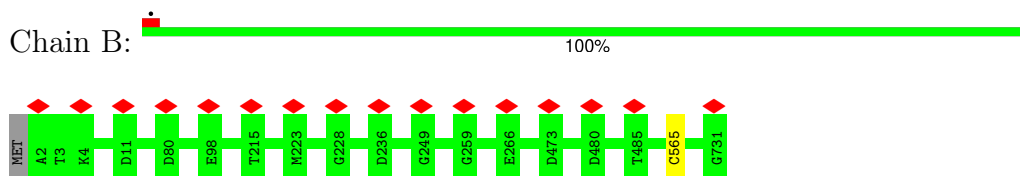
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



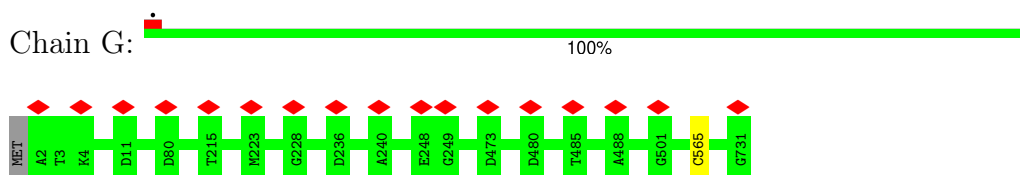
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



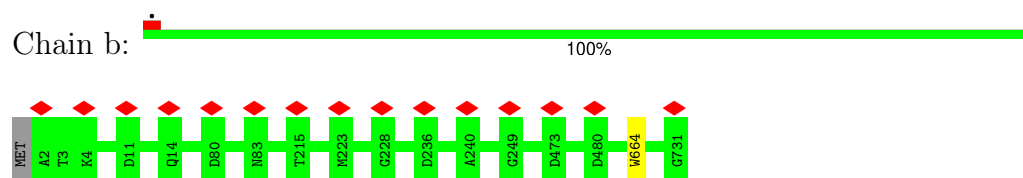
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



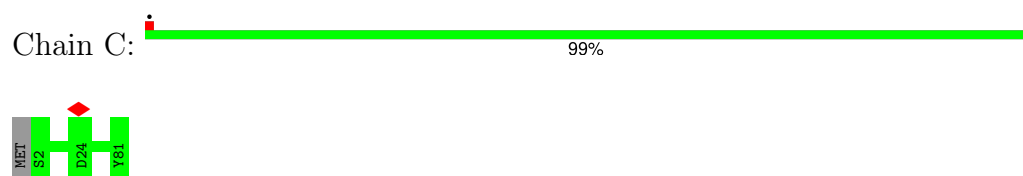
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



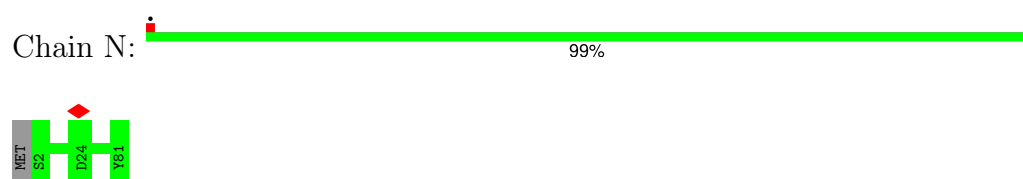
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



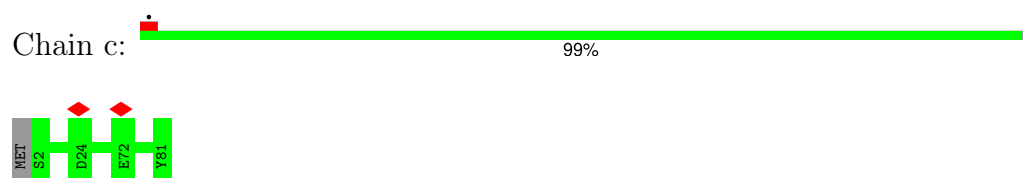
- Molecule 3: Photosystem I iron-sulfur center



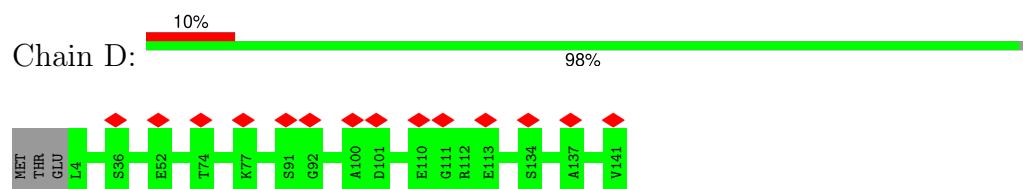
- Molecule 3: Photosystem I iron-sulfur center



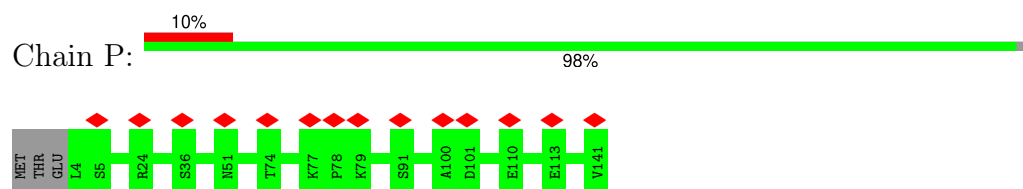
- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II

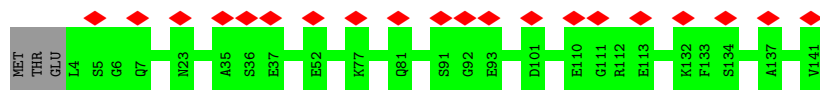


- Molecule 4: Photosystem I reaction center subunit II

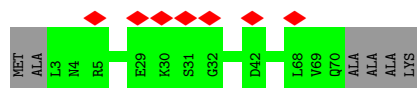


- Molecule 4: Photosystem I reaction center subunit II

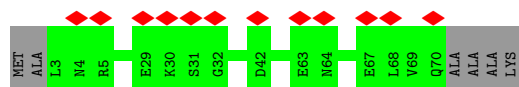
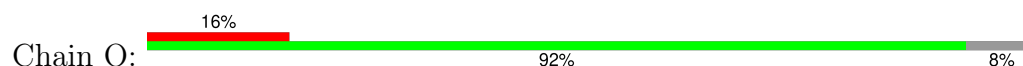




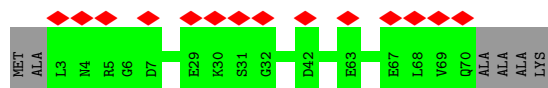
- Molecule 5: Photosystem I reaction center subunit IV



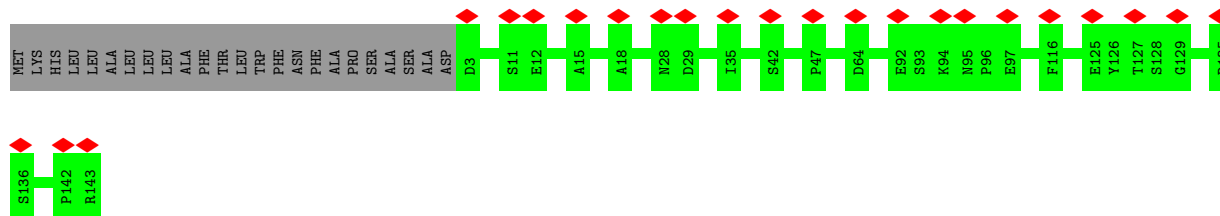
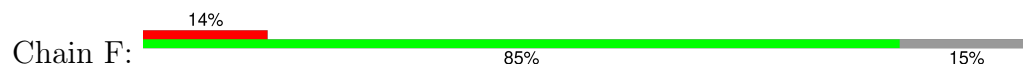
- Molecule 5: Photosystem I reaction center subunit IV



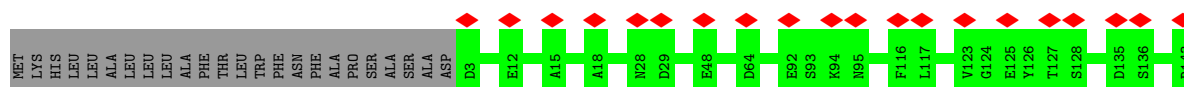
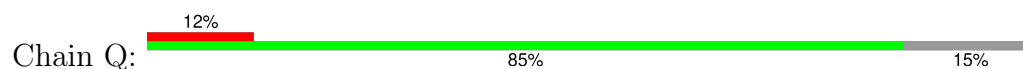
- Molecule 5: Photosystem I reaction center subunit IV



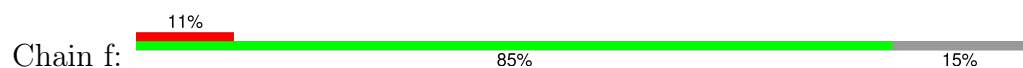
- Molecule 6: Photosystem I reaction center subunit III

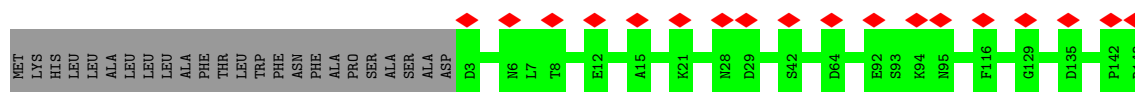


- Molecule 6: Photosystem I reaction center subunit III

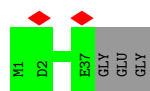
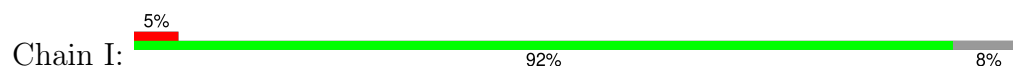


- Molecule 6: Photosystem I reaction center subunit III

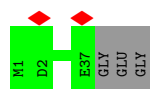
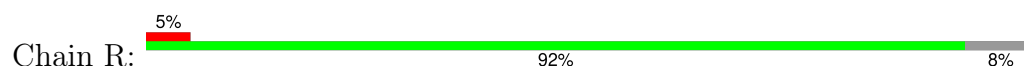




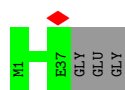
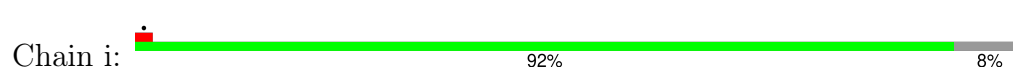
- Molecule 7: Photosystem I reaction center subunit VIII



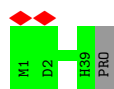
- Molecule 7: Photosystem I reaction center subunit VIII



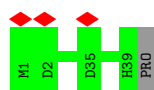
- Molecule 7: Photosystem I reaction center subunit VIII



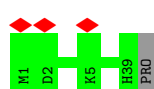
- Molecule 8: Photosystem I reaction center subunit IX



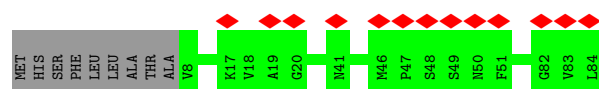
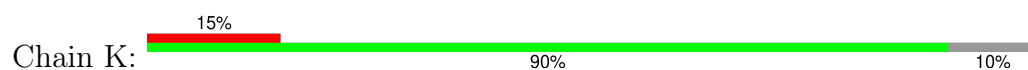
- Molecule 8: Photosystem I reaction center subunit IX



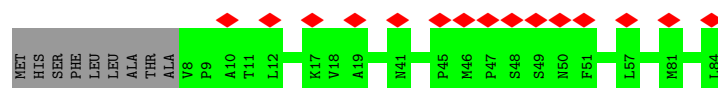
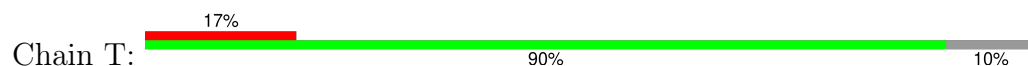
- Molecule 8: Photosystem I reaction center subunit IX



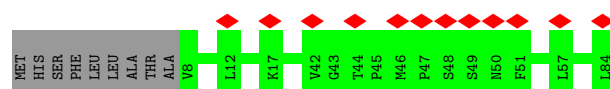
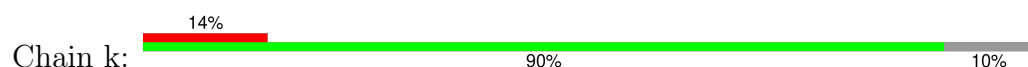
- Molecule 9: Photosystem I reaction center subunit Psak 1



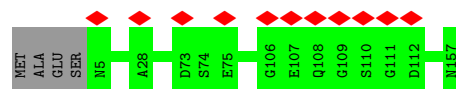
- Molecule 9: Photosystem I reaction center subunit PsaK 1



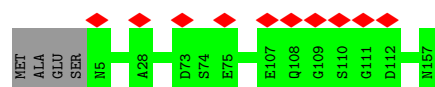
- Molecule 9: Photosystem I reaction center subunit PsaK 1



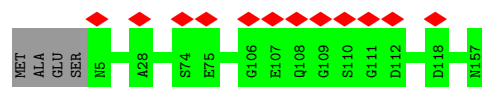
- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII

Chain V:  6% 100%



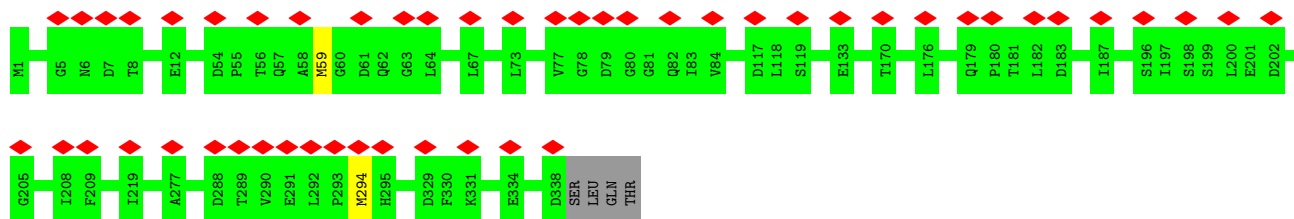
- Molecule 11: Photosystem I reaction center subunit XII

Chain m:  6% 100%



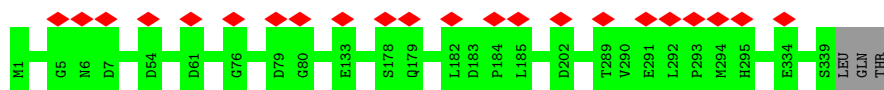
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain W:  15% 98%



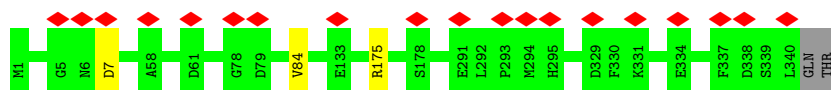
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain X:  6% 99%



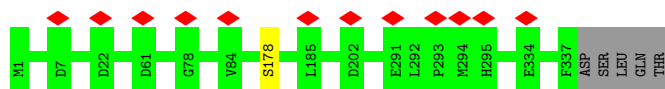
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain Y:  6% 99%

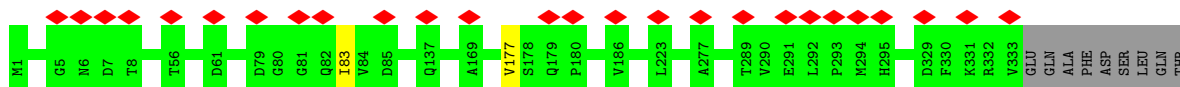


- Molecule 12: Iron stress-induced chlorophyll-binding protein

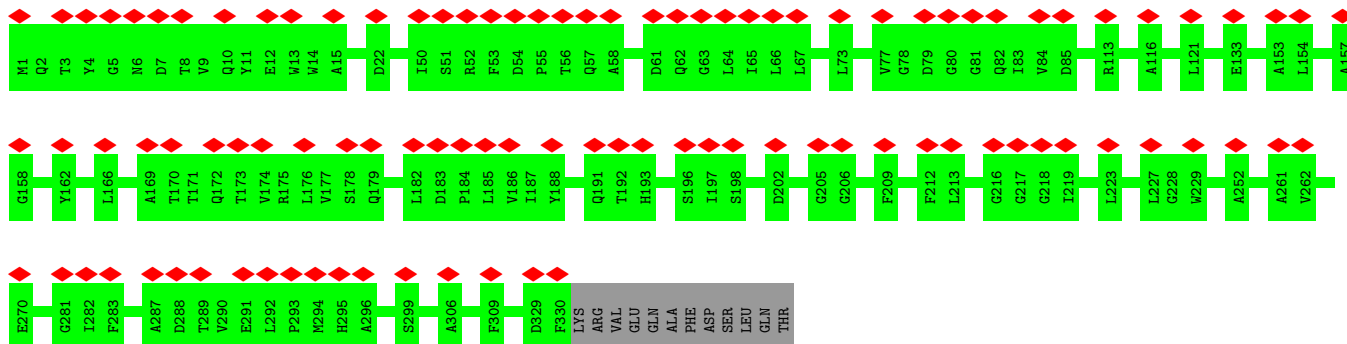
Chain Z:  6% 98%



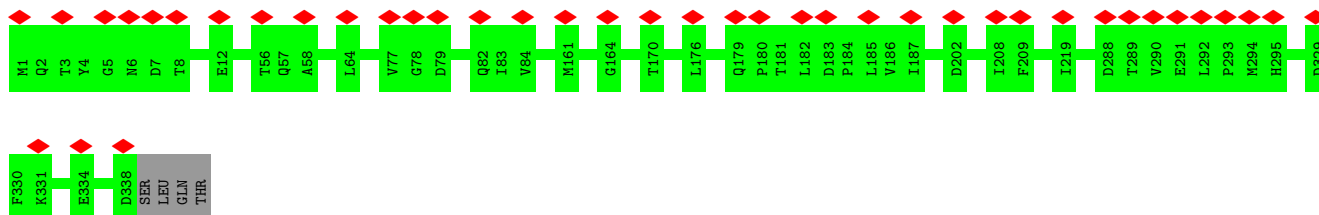
- Molecule 12: Iron stress-induced chlorophyll-binding protein



- Molecule 12: Iron stress-induced chlorophyll-binding protein



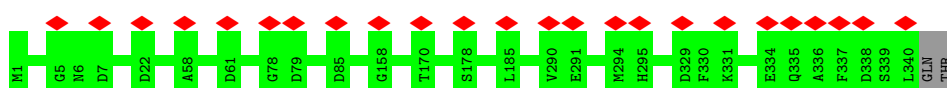
- Molecule 12: Iron stress-induced chlorophyll-binding protein



- Molecule 12: Iron stress-induced chlorophyll-binding protein

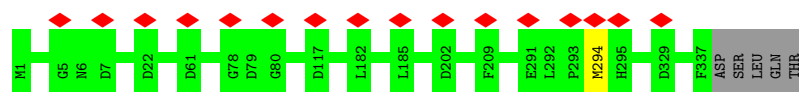


- Molecule 12: Iron stress-induced chlorophyll-binding protein



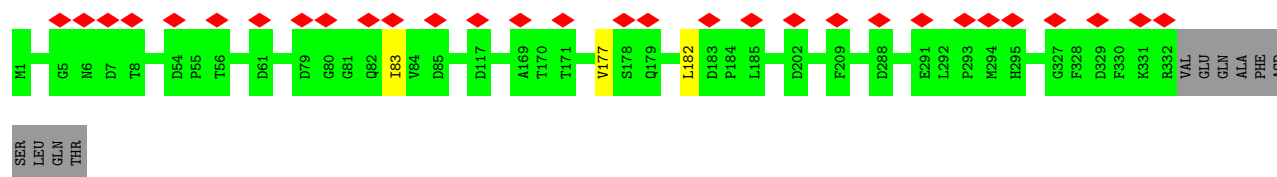
- Molecule 12: Iron stress-induced chlorophyll-binding protein





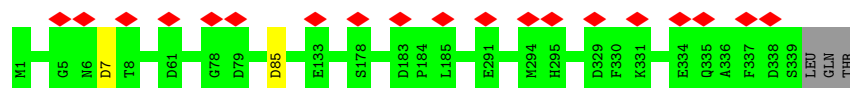
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain r: 96%



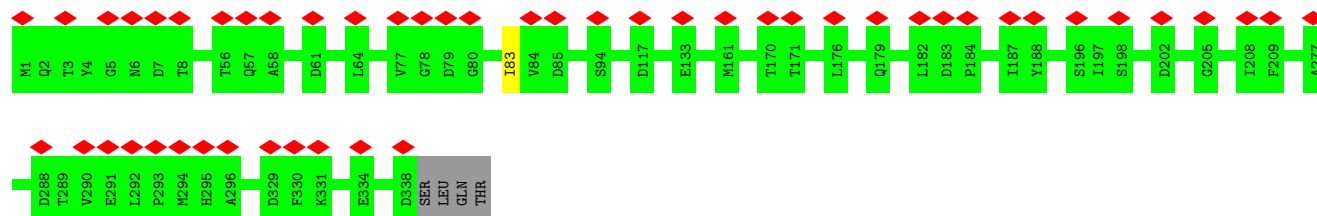
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain s: 99%



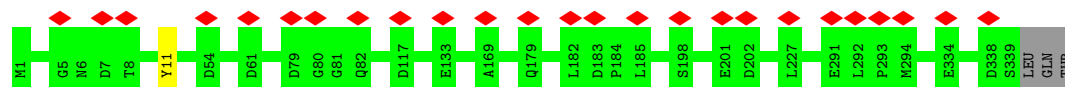
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain t: 99%



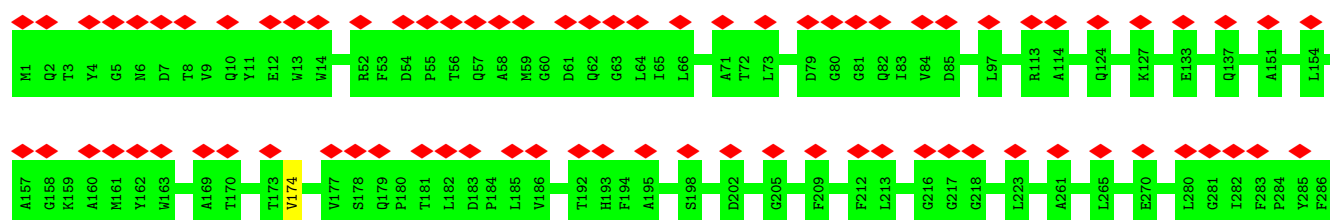
- Molecule 12: Iron stress-induced chlorophyll-binding protein

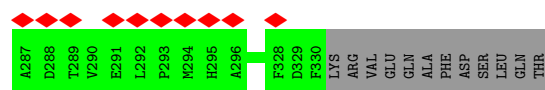
Chain u: 99%



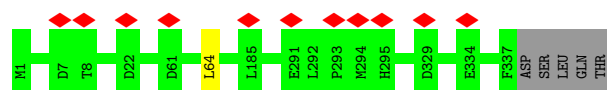
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain v: 96%

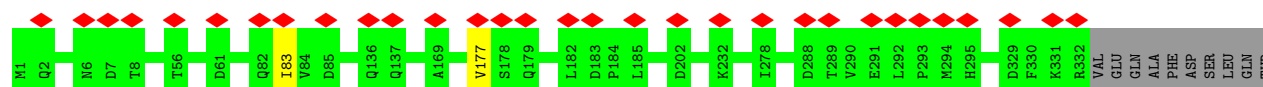




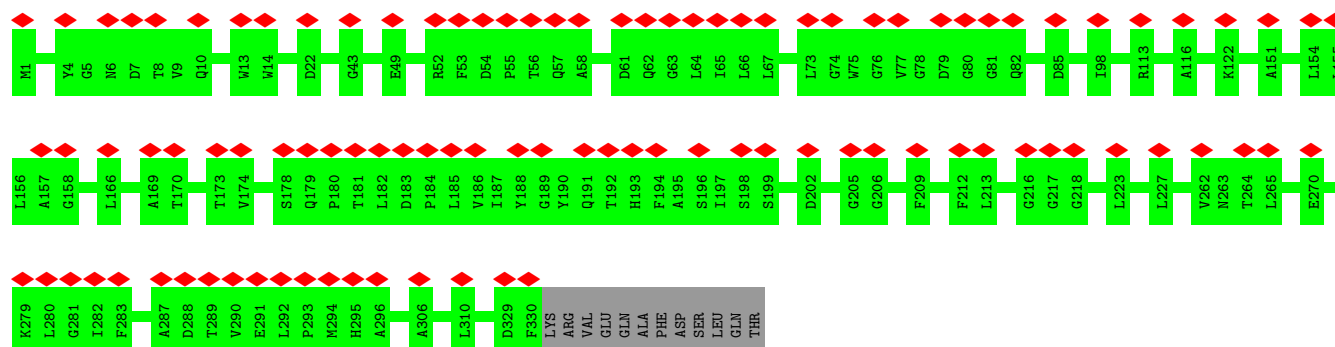
- Molecule 12: Iron stress-induced chlorophyll-binding protein



- Molecule 12: Iron stress-induced chlorophyll-binding protein



- Molecule 12: Iron stress-induced chlorophyll-binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	143739	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)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	70.466	Depositor
Minimum map value	-42.667	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	2.305	Depositor
Recommended contour level	9.2	Depositor
Map size (\AA)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.31	0/5985	0.50	0/8158
1	H	0.31	0/5985	0.51	0/8158
1	a	0.31	0/5985	0.51	0/8158
2	B	0.31	0/5986	0.51	1/8185 (0.0%)
2	G	0.31	1/5986 (0.0%)	0.51	0/8185
2	b	0.31	0/5986	0.51	0/8185
3	C	0.30	0/610	0.58	0/826
3	N	0.31	0/610	0.58	0/826
3	c	0.31	0/610	0.61	0/826
4	D	0.28	0/1102	0.55	0/1485
4	P	0.28	0/1102	0.53	0/1485
4	d	0.29	0/1102	0.53	0/1485
5	E	0.29	0/546	0.54	0/738
5	O	0.28	0/546	0.51	0/738
5	e	0.29	0/546	0.55	0/738
6	F	0.28	0/1130	0.54	0/1535
6	Q	0.28	0/1130	0.54	0/1535
6	f	0.29	0/1130	0.54	0/1535
7	I	0.32	0/304	0.57	0/416
7	R	0.34	0/304	0.59	0/416
7	i	0.31	0/304	0.56	0/416
8	J	0.30	0/319	0.53	0/431
8	S	0.30	0/319	0.54	0/431
8	j	0.32	0/319	0.52	0/431
9	K	0.27	0/549	0.47	0/745
9	T	0.27	0/549	0.51	0/745
9	k	0.27	0/549	0.48	0/745
10	L	0.29	0/1180	0.52	0/1603
10	U	0.30	0/1180	0.53	0/1603
10	l	0.30	0/1180	0.53	0/1603
11	M	0.26	0/241	0.50	0/326
11	V	0.27	0/241	0.58	0/326

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	m	0.29	0/241	0.53	0/326
12	W	0.28	0/2691	0.52	0/3678
12	X	0.28	0/2712	0.51	0/3703
12	Y	0.30	0/2712	0.52	0/3704
12	Z	0.29	0/2693	0.50	0/3678
12	g	0.28	0/2662	0.51	0/3636
12	h	0.28	0/2627	0.51	0/3592
12	n	0.27	0/2691	0.48	0/3678
12	o	0.28	0/2712	0.52	0/3703
12	p	0.29	0/2712	0.51	0/3704
12	q	0.28	0/2693	0.49	0/3678
12	r	0.29	0/2655	0.53	1/3626 (0.0%)
12	s	0.29	0/2707	0.52	0/3697
12	t	0.27	0/2691	0.50	0/3678
12	u	0.28	0/2712	0.50	0/3703
12	v	0.27	0/2627	0.50	0/3592
12	w	0.28	0/2693	0.51	1/3678 (0.0%)
12	x	0.28	0/2655	0.52	0/3626
12	y	0.27	0/2621	0.51	0/3585
All	All	0.29	1/102122 (0.0%)	0.51	3/139283 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1
12	Y	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	565	CYS	CB-SG	-5.05	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	565	CYS	CA-CB-SG	6.14	125.06	114.00
12	r	182	LEU	CA-CB-CG	5.39	127.69	115.30
12	w	64	LEU	CA-CB-CG	5.13	127.09	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	Y	84	VAL	Peptide
2	b	664	TRP	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [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%)	712 (97%)	25 (3%)	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	728/731 (100%)	713 (98%)	15 (2%)	0	100	100
2	G	728/731 (100%)	712 (98%)	16 (2%)	0	100	100
2	b	728/731 (100%)	711 (98%)	17 (2%)	0	100	100
3	C	78/81 (96%)	78 (100%)	0	0	100	100
3	N	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	c	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	136/141 (96%)	126 (93%)	10 (7%)	0	100	100
4	P	136/141 (96%)	126 (93%)	10 (7%)	0	100	100
4	d	136/141 (96%)	130 (96%)	6 (4%)	0	100	100
5	E	66/74 (89%)	65 (98%)	1 (2%)	0	100	100
5	O	66/74 (89%)	64 (97%)	2 (3%)	0	100	100
5	e	66/74 (89%)	64 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	139/165 (84%)	135 (97%)	4 (3%)	0	100	100
6	Q	139/165 (84%)	134 (96%)	5 (4%)	0	100	100
6	f	139/165 (84%)	134 (96%)	5 (4%)	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%)	37 (100%)	0	0	100	100
8	S	37/40 (92%)	37 (100%)	0	0	100	100
8	j	37/40 (92%)	37 (100%)	0	0	100	100
9	K	75/86 (87%)	74 (99%)	1 (1%)	0	100	100
9	T	75/86 (87%)	74 (99%)	1 (1%)	0	100	100
9	k	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
10	L	151/157 (96%)	150 (99%)	1 (1%)	0	100	100
10	U	151/157 (96%)	148 (98%)	3 (2%)	0	100	100
10	l	151/157 (96%)	147 (97%)	4 (3%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	V	29/31 (94%)	29 (100%)	0	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
12	W	336/342 (98%)	317 (94%)	18 (5%)	1 (0%)	37	59
12	X	337/342 (98%)	318 (94%)	19 (6%)	0	100	100
12	Y	338/342 (99%)	320 (95%)	17 (5%)	1 (0%)	37	59
12	Z	335/342 (98%)	326 (97%)	8 (2%)	1 (0%)	37	59
12	g	331/342 (97%)	304 (92%)	25 (8%)	2 (1%)	22	43
12	h	328/342 (96%)	308 (94%)	20 (6%)	0	100	100
12	n	336/342 (98%)	322 (96%)	14 (4%)	0	100	100
12	o	337/342 (98%)	318 (94%)	17 (5%)	2 (1%)	22	43
12	p	338/342 (99%)	317 (94%)	21 (6%)	0	100	100
12	q	335/342 (98%)	326 (97%)	9 (3%)	0	100	100
12	r	330/342 (96%)	316 (96%)	12 (4%)	2 (1%)	22	43
12	s	337/342 (98%)	321 (95%)	14 (4%)	2 (1%)	22	43
12	t	336/342 (98%)	319 (95%)	16 (5%)	1 (0%)	37	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	u	337/342 (98%)	322 (96%)	14 (4%)	1 (0%)	37	59
12	v	328/342 (96%)	312 (95%)	15 (5%)	1 (0%)	37	59
12	w	335/342 (98%)	322 (96%)	13 (4%)	0	100	100
12	x	330/342 (96%)	311 (94%)	17 (5%)	2 (1%)	22	43
12	y	328/342 (96%)	307 (94%)	21 (6%)	0	100	100
All	All	12645/13047 (97%)	12150 (96%)	479 (4%)	16 (0%)	50	71

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	W	59	MET
12	v	174	VAL
12	s	85	ASP
12	o	11	TYR
12	s	7	ASP

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%)	593 (100%)	0	100	100
1	H	593/603 (98%)	593 (100%)	0	100	100
1	a	593/603 (98%)	593 (100%)	0	100	100
2	B	582/583 (100%)	582 (100%)	0	100	100
2	G	582/583 (100%)	582 (100%)	0	100	100
2	b	582/583 (100%)	582 (100%)	0	100	100
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	113/116 (97%)	113 (100%)	0	100	100
4	P	113/116 (97%)	113 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	113/116 (97%)	113 (100%)	0	100	100
5	E	58/60 (97%)	58 (100%)	0	100	100
5	O	58/60 (97%)	58 (100%)	0	100	100
5	e	58/60 (97%)	58 (100%)	0	100	100
6	F	118/137 (86%)	118 (100%)	0	100	100
6	Q	118/137 (86%)	118 (100%)	0	100	100
6	f	118/137 (86%)	118 (100%)	0	100	100
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	34/35 (97%)	34 (100%)	0	100	100
8	S	34/35 (97%)	34 (100%)	0	100	100
8	j	34/35 (97%)	34 (100%)	0	100	100
9	K	55/62 (89%)	55 (100%)	0	100	100
9	T	55/62 (89%)	55 (100%)	0	100	100
9	k	55/62 (89%)	55 (100%)	0	100	100
10	L	115/118 (98%)	115 (100%)	0	100	100
10	U	115/118 (98%)	115 (100%)	0	100	100
10	l	115/118 (98%)	115 (100%)	0	100	100
11	M	25/25 (100%)	25 (100%)	0	100	100
11	V	25/25 (100%)	25 (100%)	0	100	100
11	m	25/25 (100%)	25 (100%)	0	100	100
12	W	252/260 (97%)	251 (100%)	1 (0%)	89	96
12	X	256/260 (98%)	256 (100%)	0	100	100
12	Y	255/260 (98%)	254 (100%)	1 (0%)	89	96
12	Z	253/260 (97%)	253 (100%)	0	100	100
12	g	251/260 (96%)	251 (100%)	0	100	100
12	h	246/260 (95%)	246 (100%)	0	100	100
12	n	252/260 (97%)	252 (100%)	0	100	100
12	o	256/260 (98%)	256 (100%)	0	100	100
12	p	255/260 (98%)	255 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	q	253/260 (97%)	252 (100%)	1 (0%)	89	96
12	r	250/260 (96%)	250 (100%)	0	100	100
12	s	255/260 (98%)	255 (100%)	0	100	100
12	t	252/260 (97%)	252 (100%)	0	100	100
12	u	256/260 (98%)	256 (100%)	0	100	100
12	v	246/260 (95%)	246 (100%)	0	100	100
12	w	253/260 (97%)	253 (100%)	0	100	100
12	x	250/260 (96%)	250 (100%)	0	100	100
12	y	245/260 (94%)	245 (100%)	0	100	100
All	All	9912/10200 (97%)	9909 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	W	294	MET
12	Y	175	ARG
12	q	294	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
12	s	136	GLN
12	x	62	GLN
12	t	191	GLN
12	v	137	GLN
9	T	26	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 798 ligands modelled in this entry, 3 are monoatomic - leaving 795 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	501	-	48,58,73	1.36	3 (6%)	56,95,113	1.16	5 (8%)
19	BCR	a	4008	-	41,41,41	0.91	1 (2%)	56,56,56	1.35	6 (10%)
13	LHG	o	605	-	26,26,48	0.85	0	29,32,54	1.27	2 (6%)
19	BCR	B	4009	-	30,30,41	0.84	0	39,39,56	1.32	5 (12%)
16	CLA	H	1113	-	43,53,73	1.44	3 (6%)	50,89,113	1.18	3 (6%)
16	CLA	u	511	-	63,73,73	1.15	3 (4%)	74,113,113	1.11	3 (4%)
16	CLA	G	1203	-	63,73,73	1.15	3 (4%)	74,113,113	1.10	4 (5%)
19	BCR	G	4010	-	41,41,41	0.94	0	56,56,56	1.39	9 (16%)
21	ECH	R	4020	-	42,42,42	0.99	3 (7%)	55,58,58	1.93	14 (25%)
16	CLA	s	502	-	48,58,73	1.35	4 (8%)	56,95,113	1.03	2 (3%)
19	BCR	A	4011	-	41,41,41	0.88	0	56,56,56	1.29	4 (7%)
16	CLA	q	507	-	63,73,73	1.19	3 (4%)	74,113,113	1.06	3 (4%)
20	LMT	H	4202	-	36,36,36	1.16	5 (13%)	47,47,47	0.91	0
16	CLA	G	1213	-	53,63,73	1.30	3 (5%)	62,101,113	1.05	3 (4%)
16	CLA	X	509	-	58,68,73	1.20	3 (5%)	68,107,113	0.94	4 (5%)
16	CLA	W	514	-	48,58,73	1.34	3 (6%)	56,95,113	1.05	4 (7%)
16	CLA	p	516	-	44,54,73	1.37	3 (6%)	51,90,113	1.00	2 (3%)
16	CLA	a	1137	-	45,55,73	1.35	3 (6%)	52,91,113	1.03	4 (7%)
19	BCR	s	603	-	41,41,41	0.86	0	56,56,56	1.18	6 (10%)
19	BCR	Z	604	-	41,41,41	0.87	0	56,56,56	1.24	6 (10%)
16	CLA	q	504	-	63,73,73	1.18	3 (4%)	74,113,113	1.07	3 (4%)
13	LHG	Y	605	-	31,31,48	0.78	1 (3%)	34,37,54	1.29	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	p	504	-	63,73,73	1.17	3 (4%)	74,113,113	0.95	2 (2%)
21	ECH	V	4021	-	42,42,42	0.84	1 (2%)	55,58,58	1.55	7 (12%)
16	CLA	b	1215	-	58,68,73	1.19	3 (5%)	68,107,113	1.14	3 (4%)
16	CLA	a	1114	-	44,54,73	1.41	3 (6%)	51,90,113	1.24	3 (5%)
16	CLA	b	1202	-	63,73,73	1.17	3 (4%)	74,113,113	0.92	2 (2%)
16	CLA	o	508	12	53,63,73	1.30	3 (5%)	62,101,113	0.90	2 (3%)
16	CLA	v	503	-	44,54,73	1.40	3 (6%)	51,90,113	1.15	3 (5%)
16	CLA	b	1021	-	63,73,73	1.15	3 (4%)	74,113,113	1.05	4 (5%)
16	CLA	g	505	-	63,73,73	1.18	3 (4%)	74,113,113	1.17	5 (6%)
16	CLA	h	505	-	63,73,73	1.21	3 (4%)	74,113,113	1.13	4 (5%)
16	CLA	A	1110	-	52,62,73	1.27	3 (5%)	60,99,113	0.94	2 (3%)
16	CLA	a	1124	25	58,68,73	1.23	3 (5%)	68,107,113	0.99	2 (2%)
16	CLA	a	1106	1	63,73,73	1.15	3 (4%)	74,113,113	1.10	3 (4%)
16	CLA	b	1216	25	45,55,73	1.43	3 (6%)	52,91,113	1.42	5 (9%)
16	CLA	k	4004	-	53,63,73	1.30	3 (5%)	62,101,113	0.94	4 (6%)
16	CLA	H	1013	-	63,73,73	1.14	4 (6%)	74,113,113	1.21	9 (12%)
13	LHG	A	849	-	42,42,48	0.69	1 (2%)	45,48,54	1.23	5 (11%)
16	CLA	o	504	-	58,68,73	1.23	3 (5%)	68,107,113	1.00	3 (4%)
21	ECH	b	4006	-	42,42,42	0.85	2 (4%)	55,58,58	1.52	8 (14%)
16	CLA	H	1138	-	63,73,73	1.16	3 (4%)	74,113,113	0.96	3 (4%)
16	CLA	a	1123	-	63,73,73	1.16	3 (4%)	74,113,113	1.02	4 (5%)
16	CLA	y	508	-	53,63,73	1.31	3 (5%)	62,101,113	1.16	4 (6%)
16	CLA	b	1213	-	53,63,73	1.28	4 (7%)	62,101,113	1.08	5 (8%)
16	CLA	n	513	-	44,54,73	1.41	3 (6%)	51,90,113	0.95	3 (5%)
16	CLA	W	509	-	58,68,73	1.21	3 (5%)	68,107,113	1.03	3 (4%)
16	CLA	n	514	-	48,58,73	1.35	4 (8%)	56,95,113	1.03	4 (7%)
16	CLA	U	1502	-	58,68,73	1.17	3 (5%)	68,107,113	1.08	3 (4%)
16	CLA	Y	505	-	63,73,73	1.17	3 (4%)	74,113,113	1.01	5 (6%)
16	CLA	b	1221	25	63,73,73	1.19	3 (4%)	74,113,113	1.07	3 (4%)
16	CLA	w	514	-	48,58,73	1.34	3 (6%)	56,95,113	1.02	4 (7%)
16	CLA	r	504	-	63,73,73	1.18	3 (4%)	74,113,113	0.93	2 (2%)
19	BCR	G	4017	-	41,41,41	0.87	0	56,56,56	1.18	6 (10%)
13	LHG	I	103	-	39,39,48	0.68	2 (5%)	42,45,54	1.23	4 (9%)
16	CLA	a	1112	-	43,53,73	1.40	3 (6%)	50,89,113	0.95	2 (4%)
16	CLA	h	516	-	44,54,73	1.43	3 (6%)	51,90,113	1.06	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	Y	504	-	63,73,73	1.18	3 (4%)	74,113,113	0.95	2 (2%)
16	CLA	B	1218	-	53,63,73	1.29	3 (5%)	62,101,113	1.09	4 (6%)
19	BCR	t	601	-	41,41,41	0.83	0	56,56,56	1.18	6 (10%)
23	LMU	q	605	-	36,36,36	0.83	0	47,47,47	1.13	4 (8%)
16	CLA	A	1104	-	63,73,73	1.18	3 (4%)	74,113,113	0.92	4 (5%)
14	LMG	B	848	-	43,43,55	0.87	1 (2%)	51,51,63	1.28	6 (11%)
16	CLA	A	1113	-	43,53,73	1.43	3 (6%)	50,89,113	1.05	2 (4%)
16	CLA	x	504	-	63,73,73	1.19	3 (4%)	74,113,113	0.97	4 (5%)
19	BCR	X	603	-	41,41,41	0.85	0	56,56,56	1.15	4 (7%)
19	BCR	U	4022	-	41,41,41	0.88	0	56,56,56	1.32	6 (10%)
16	CLA	G	1235	-	60,70,73	1.16	3 (5%)	70,109,113	1.18	7 (10%)
16	CLA	W	505	-	63,73,73	1.19	3 (4%)	74,113,113	1.12	5 (6%)
13	LHG	a	849	-	42,42,48	0.71	1 (2%)	45,48,54	1.22	4 (8%)
16	CLA	G	1226	-	58,68,73	1.20	4 (6%)	68,107,113	1.07	4 (5%)
16	CLA	Z	512	12	63,73,73	1.18	4 (6%)	74,113,113	1.10	3 (4%)
19	BCR	y	601	-	41,41,41	0.83	0	56,56,56	1.24	6 (10%)
16	CLA	L	1502	-	58,68,73	1.16	3 (5%)	68,107,113	1.08	3 (4%)
16	CLA	H	1126	-	63,73,73	1.17	3 (4%)	74,113,113	1.12	4 (5%)
16	CLA	y	514	-	48,58,73	1.40	4 (8%)	56,95,113	1.05	5 (8%)
19	BCR	G	4005	-	41,41,41	0.85	0	56,56,56	1.14	4 (7%)
16	CLA	G	1210	-	63,73,73	1.17	3 (4%)	74,113,113	1.04	4 (5%)
15	CL0	H	1011	-	63,73,73	1.21	4 (6%)	74,113,113	1.05	6 (8%)
16	CLA	o	502	-	48,58,73	1.33	4 (8%)	56,95,113	0.98	3 (5%)
16	CLA	w	510	-	58,68,73	1.23	3 (5%)	68,107,113	0.95	1 (1%)
16	CLA	g	501	-	48,58,73	1.33	3 (6%)	56,95,113	1.00	3 (5%)
16	CLA	h	501	-	44,54,73	1.44	3 (6%)	51,90,113	1.15	4 (7%)
16	CLA	U	1503	-	63,73,73	1.16	3 (4%)	74,113,113	0.88	3 (4%)
16	CLA	W	510	-	63,73,73	1.20	3 (4%)	74,113,113	0.98	4 (5%)
16	CLA	G	1217	-	43,53,73	1.42	3 (6%)	50,89,113	0.98	2 (4%)
19	BCR	H	4011	-	41,41,41	0.88	0	56,56,56	1.26	6 (10%)
19	BCR	n	603	-	41,41,41	0.83	0	56,56,56	1.20	5 (8%)
19	BCR	w	603	-	41,41,41	0.85	0	56,56,56	1.17	6 (10%)
16	CLA	G	1023	-	63,73,73	1.19	5 (7%)	74,113,113	1.09	6 (8%)
18	SF4	A	3001	-	0,12,12	-	-	-	-	-
16	CLA	s	511	-	63,73,73	1.14	3 (4%)	74,113,113	1.04	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	CLA	b	1201	-	52,62,73	1.30	3 (5%)	60,99,113	1.13	3 (5%)
16	CLA	B	1209	-	43,53,73	1.43	3 (6%)	50,89,113	1.04	2 (4%)
16	CLA	G	1215	-	58,68,73	1.17	3 (5%)	68,107,113	1.09	2 (2%)
16	CLA	w	511	-	63,73,73	1.16	3 (4%)	74,113,113	1.03	4 (5%)
19	BCR	j	4012	-	41,41,41	0.88	0	56,56,56	1.29	7 (12%)
16	CLA	A	1129	-	44,54,73	1.35	3 (6%)	51,90,113	1.08	3 (5%)
16	CLA	k	4002	-	43,53,73	1.45	3 (6%)	50,89,113	1.06	3 (6%)
16	CLA	q	512	12	63,73,73	1.18	4 (6%)	74,113,113	1.01	2 (2%)
16	CLA	G	1216	25	45,55,73	1.38	3 (6%)	52,91,113	1.29	3 (5%)
19	BCR	w	602	-	41,41,41	0.86	0	56,56,56	1.26	7 (12%)
16	CLA	u	515	-	63,73,73	1.14	3 (4%)	74,113,113	1.04	4 (5%)
17	PQN	A	2001	-	34,34,34	0.37	0	43,45,45	1.08	2 (4%)
16	CLA	Y	512	12	63,73,73	1.19	4 (6%)	74,113,113	1.19	7 (9%)
16	CLA	x	515	-	63,73,73	1.17	3 (4%)	74,113,113	1.12	5 (6%)
16	CLA	X	503	-	44,54,73	1.38	3 (6%)	51,90,113	0.98	1 (1%)
16	CLA	G	1230	-	43,53,73	1.40	3 (6%)	50,89,113	0.96	1 (2%)
21	ECH	I	4020	-	42,42,42	0.88	1 (2%)	55,58,58	1.90	14 (25%)
16	CLA	W	502	-	48,58,73	1.37	4 (8%)	56,95,113	1.10	4 (7%)
16	CLA	a	1022	-	63,73,73	1.17	3 (4%)	74,113,113	1.04	7 (9%)
16	CLA	u	502	-	48,58,73	1.35	4 (8%)	56,95,113	1.04	2 (3%)
16	CLA	Y	506	-	58,68,73	1.24	3 (5%)	68,107,113	1.07	4 (5%)
13	LHG	u	605	-	26,26,48	0.83	0	29,32,54	1.27	2 (6%)
16	CLA	b	1219	-	43,53,73	1.46	3 (6%)	50,89,113	1.08	3 (6%)
16	CLA	s	505	-	63,73,73	1.20	3 (4%)	74,113,113	1.09	5 (6%)
16	CLA	B	1229	-	56,66,73	1.26	3 (5%)	65,104,113	1.02	4 (6%)
13	LHG	x	605	-	30,30,48	0.78	1 (3%)	33,36,54	1.28	3 (9%)
16	CLA	A	1128	-	63,73,73	1.15	4 (6%)	74,113,113	1.12	5 (6%)
19	BCR	Y	602	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)
16	CLA	Z	514	-	48,58,73	1.34	3 (6%)	56,95,113	1.10	4 (7%)
14	LMG	a	4101	-	46,46,55	0.90	2 (4%)	54,54,63	1.22	4 (7%)
20	LMT	A	4202	-	36,36,36	1.16	5 (13%)	47,47,47	0.92	0
19	BCR	k	4001	-	41,41,41	0.86	0	56,56,56	1.30	6 (10%)
16	CLA	F	1302	6	44,54,73	1.44	3 (6%)	51,90,113	0.99	2 (3%)
16	CLA	b	1225	-	63,73,73	1.16	4 (6%)	74,113,113	0.98	4 (5%)
16	CLA	H	1115	-	52,62,73	1.27	3 (5%)	60,99,113	1.17	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	1219	-	43,53,73	1.44	3 (6%)	50,89,113	1.07	2 (4%)
19	BCR	i	4018	-	41,41,41	0.87	0	56,56,56	1.23	8 (14%)
16	CLA	s	509	-	58,68,73	1.21	3 (5%)	68,107,113	1.00	4 (5%)
16	CLA	b	1208	-	43,53,73	1.40	3 (6%)	50,89,113	1.10	4 (8%)
19	BCR	p	601	-	41,41,41	0.87	0	56,56,56	1.32	8 (14%)
16	CLA	b	1222	25	48,58,73	1.36	3 (6%)	56,95,113	1.06	3 (5%)
16	CLA	a	1102	16	54,64,73	1.25	3 (5%)	63,102,113	0.95	2 (3%)
16	CLA	b	1238	25	63,73,73	1.13	3 (4%)	74,113,113	1.00	5 (6%)
16	CLA	W	512	12	58,68,73	1.23	4 (6%)	68,107,113	1.07	4 (5%)
16	CLA	X	507	12	63,73,73	1.20	3 (4%)	74,113,113	0.88	3 (4%)
16	CLA	b	1212	-	43,53,73	1.44	3 (6%)	50,89,113	1.22	3 (6%)
16	CLA	G	1209	-	43,53,73	1.44	3 (6%)	50,89,113	1.09	2 (4%)
19	BCR	l	4022	-	41,41,41	0.89	1 (2%)	56,56,56	1.41	8 (14%)
16	CLA	W	508	12	53,63,73	1.28	3 (5%)	62,101,113	0.89	2 (3%)
19	BCR	o	604	-	41,41,41	0.88	0	56,56,56	1.31	10 (17%)
13	LHG	R	103	-	39,39,48	0.68	2 (5%)	42,45,54	1.24	4 (9%)
16	CLA	B	1203	-	63,73,73	1.16	3 (4%)	74,113,113	1.08	4 (5%)
16	CLA	o	514	-	48,58,73	1.40	4 (8%)	56,95,113	1.34	4 (7%)
16	CLA	B	1235	-	60,70,73	1.17	3 (5%)	70,109,113	1.22	8 (11%)
16	CLA	p	514	-	48,58,73	1.34	3 (6%)	56,95,113	1.02	3 (5%)
19	BCR	T	4005	-	41,41,41	0.85	0	56,56,56	1.26	7 (12%)
16	CLA	G	1221	25	63,73,73	1.18	3 (4%)	74,113,113	1.07	3 (4%)
13	LHG	b	4018	16	37,37,48	0.71	0	40,43,54	1.31	5 (12%)
19	BCR	j	4013	-	41,41,41	0.86	0	56,56,56	1.26	7 (12%)
16	CLA	a	1107	1	48,58,73	1.35	3 (6%)	56,95,113	1.08	2 (3%)
19	BCR	h	601	-	41,41,41	0.84	0	56,56,56	1.28	7 (12%)
16	CLA	A	1115	-	52,62,73	1.28	4 (7%)	60,99,113	1.20	3 (5%)
16	CLA	H	1139	25	58,68,73	1.23	3 (5%)	68,107,113	0.94	3 (4%)
16	CLA	Z	510	-	58,68,73	1.24	3 (5%)	68,107,113	0.99	2 (2%)
17	PQN	a	2001	-	34,34,34	0.39	0	43,45,45	1.06	2 (4%)
16	CLA	G	1201	-	52,62,73	1.31	3 (5%)	60,99,113	1.02	2 (3%)
16	CLA	G	1218	-	53,63,73	1.30	3 (5%)	62,101,113	1.03	3 (4%)
16	CLA	H	1123	-	63,73,73	1.18	3 (4%)	74,113,113	0.97	4 (5%)
16	CLA	n	511	-	63,73,73	1.19	3 (4%)	74,113,113	1.00	4 (5%)
16	CLA	A	1111	-	53,63,73	1.28	4 (7%)	62,101,113	1.21	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	a	1013	-	63,73,73	1.14	4 (6%)	74,113,113	1.16	4 (5%)
14	LMG	G	848	-	43,43,55	0.86	0	51,51,63	1.27	7 (13%)
16	CLA	a	1138	-	63,73,73	1.17	3 (4%)	74,113,113	0.93	3 (4%)
14	LMG	H	4201	-	32,32,55	0.98	1 (3%)	40,40,63	1.17	3 (7%)
16	CLA	u	509	-	58,68,73	1.20	3 (5%)	68,107,113	1.02	4 (5%)
16	CLA	X	512	12	63,73,73	1.13	3 (4%)	74,113,113	1.00	5 (6%)
16	CLA	B	1221	25	63,73,73	1.17	3 (4%)	74,113,113	0.96	1 (1%)
16	CLA	Y	517	12	53,63,73	1.29	3 (5%)	62,101,113	0.95	1 (1%)
16	CLA	W	517	12	53,63,73	1.29	3 (5%)	62,101,113	0.92	2 (3%)
19	BCR	u	602	-	41,41,41	0.88	0	56,56,56	1.36	6 (10%)
16	CLA	x	513	-	44,54,73	1.42	3 (6%)	51,90,113	0.98	1 (1%)
16	CLA	A	1103	-	63,73,73	1.17	3 (4%)	74,113,113	0.96	1 (1%)
13	LHG	X	605	-	26,26,48	0.82	0	29,32,54	1.27	2 (6%)
16	CLA	p	502	-	48,58,73	1.33	3 (6%)	56,95,113	0.99	3 (5%)
16	CLA	A	1106	1	63,73,73	1.15	3 (4%)	74,113,113	1.13	4 (5%)
16	CLA	b	1203	-	63,73,73	1.15	3 (4%)	74,113,113	1.05	5 (6%)
16	CLA	v	506	-	58,68,73	1.24	3 (5%)	68,107,113	1.10	5 (7%)
16	CLA	x	514	-	48,58,73	1.33	3 (6%)	56,95,113	1.05	4 (7%)
16	CLA	A	1133	-	52,62,73	1.26	4 (7%)	60,99,113	1.10	4 (6%)
16	CLA	a	1125	-	63,73,73	1.18	4 (6%)	74,113,113	1.04	3 (4%)
16	CLA	a	1131	-	63,73,73	1.15	3 (4%)	74,113,113	1.04	2 (2%)
16	CLA	Y	509	-	58,68,73	1.20	3 (5%)	68,107,113	1.04	3 (4%)
16	CLA	G	1227	-	47,57,73	1.30	4 (8%)	53,93,113	1.12	4 (7%)
16	CLA	Z	515	-	63,73,73	1.18	3 (4%)	74,113,113	1.11	3 (4%)
16	CLA	o	505	-	63,73,73	1.17	3 (4%)	74,113,113	1.02	3 (4%)
16	CLA	r	516	-	44,54,73	1.40	3 (6%)	51,90,113	1.09	3 (5%)
16	CLA	p	505	-	63,73,73	1.19	3 (4%)	74,113,113	1.04	4 (5%)
16	CLA	A	1132	-	63,73,73	1.12	3 (4%)	74,113,113	1.08	3 (4%)
16	CLA	G	1207	-	63,73,73	1.18	3 (4%)	74,113,113	1.15	5 (6%)
19	BCR	R	4018	-	41,41,41	0.85	0	56,56,56	1.20	7 (12%)
16	CLA	G	1231	25	43,53,73	1.44	3 (6%)	50,89,113	1.09	3 (6%)
16	CLA	A	1123	25	63,73,73	1.18	3 (4%)	74,113,113	1.10	4 (5%)
16	CLA	A	1136	-	63,73,73	1.14	3 (4%)	74,113,113	0.92	2 (2%)
16	CLA	A	1801	13	44,54,73	1.36	3 (6%)	51,90,113	1.23	4 (7%)
16	CLA	A	1105	-	56,66,73	1.24	3 (5%)	65,104,113	0.96	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	CLA	a	1122	-	57,67,73	1.25	3 (5%)	66,105,113	1.02	2 (3%)
16	CLA	p	510	-	63,73,73	1.19	3 (4%)	74,113,113	0.99	2 (2%)
16	CLA	v	511	-	63,73,73	1.18	3 (4%)	74,113,113	1.06	4 (5%)
16	CLA	g	513	-	44,54,73	1.41	3 (6%)	51,90,113	0.89	3 (5%)
23	LMU	r	606	-	36,36,36	0.87	0	47,47,47	1.10	2 (4%)
16	CLA	t	502	-	48,58,73	1.36	4 (8%)	56,95,113	1.01	3 (5%)
16	CLA	t	504	-	58,68,73	1.25	3 (5%)	68,107,113	0.97	3 (4%)
19	BCR	b	4004	-	41,41,41	0.84	0	56,56,56	1.26	6 (10%)
19	BCR	p	604	-	41,41,41	0.87	0	56,56,56	1.23	6 (10%)
16	CLA	T	4003	9	43,53,73	1.44	3 (6%)	50,89,113	0.99	2 (4%)
19	BCR	H	4002	-	41,41,41	0.85	0	56,56,56	1.19	5 (8%)
19	BCR	p	603	-	41,41,41	0.86	0	56,56,56	1.21	5 (8%)
19	BCR	b	4009	-	30,30,41	0.85	0	39,39,56	1.35	6 (15%)
19	BCR	h	603	-	41,41,41	0.83	0	56,56,56	1.19	4 (7%)
16	CLA	b	1220	-	52,62,73	1.34	4 (7%)	60,99,113	1.03	4 (6%)
16	CLA	w	505	-	63,73,73	1.16	3 (4%)	74,113,113	1.04	5 (6%)
16	CLA	k	4003	9	43,53,73	1.45	3 (6%)	50,89,113	1.05	2 (4%)
16	CLA	a	1126	-	63,73,73	1.16	3 (4%)	74,113,113	1.11	3 (4%)
16	CLA	o	510	-	58,68,73	1.24	3 (5%)	68,107,113	0.92	3 (4%)
19	BCR	b	4005	-	41,41,41	0.85	0	56,56,56	1.15	5 (8%)
23	LMU	s	606	-	36,36,36	0.83	0	47,47,47	1.27	4 (8%)
19	BCR	G	4009	-	30,30,41	0.84	0	39,39,56	1.32	5 (12%)
16	CLA	t	514	-	48,58,73	1.36	3 (6%)	56,95,113	1.06	4 (7%)
15	CL0	a	1011	-	63,73,73	1.21	4 (6%)	74,113,113	0.99	5 (6%)
16	CLA	h	510	-	63,73,73	1.19	3 (4%)	74,113,113	0.95	4 (5%)
16	CLA	o	515	-	63,73,73	1.13	3 (4%)	74,113,113	1.04	4 (5%)
16	CLA	b	1227	-	47,57,73	1.31	4 (8%)	53,93,113	1.09	4 (7%)
19	BCR	t	604	-	41,41,41	0.83	0	56,56,56	1.23	4 (7%)
16	CLA	H	1101	-	63,73,73	1.16	3 (4%)	74,113,113	1.00	2 (2%)
16	CLA	n	509	-	58,68,73	1.21	3 (5%)	68,107,113	0.94	4 (5%)
16	CLA	g	510	-	63,73,73	1.19	3 (4%)	74,113,113	1.08	4 (5%)
16	CLA	v	510	-	63,73,73	1.21	3 (4%)	74,113,113	0.98	5 (6%)
19	BCR	Z	603	-	41,41,41	0.85	0	56,56,56	1.17	4 (7%)
16	CLA	G	1222	25	48,58,73	1.36	4 (8%)	56,95,113	1.06	5 (8%)
16	CLA	A	1117	-	63,73,73	1.14	3 (4%)	74,113,113	1.17	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	T	4002	-	43,53,73	1.45	3 (6%)	50,89,113	0.95	2 (4%)
16	CLA	q	502	-	48,58,73	1.31	4 (8%)	56,95,113	0.96	1 (1%)
18	SF4	C	102	-	0,12,12	-	-	-	-	-
16	CLA	Y	501	-	48,58,73	1.35	3 (6%)	56,95,113	1.12	4 (7%)
16	CLA	F	1301	25	43,53,73	1.41	3 (6%)	50,89,113	1.13	3 (6%)
16	CLA	G	1208	-	43,53,73	1.39	3 (6%)	50,89,113	1.14	4 (8%)
16	CLA	g	516	-	44,54,73	1.40	3 (6%)	51,90,113	1.16	2 (3%)
16	CLA	v	516	-	44,54,73	1.42	3 (6%)	51,90,113	0.90	2 (3%)
21	ECH	i	4020	-	42,42,42	0.84	1 (2%)	55,58,58	1.84	10 (18%)
16	CLA	B	1210	-	63,73,73	1.17	3 (4%)	74,113,113	1.08	4 (5%)
16	CLA	Z	503	-	44,54,73	1.43	4 (9%)	51,90,113	1.00	2 (3%)
20	LMT	L	4101	-	36,36,36	1.17	6 (16%)	47,47,47	1.15	3 (6%)
16	CLA	y	505	-	63,73,73	1.21	3 (4%)	74,113,113	1.21	4 (5%)
16	CLA	a	1134	1	43,53,73	1.41	3 (6%)	50,89,113	1.12	3 (6%)
23	LMU	Z	605	-	36,36,36	0.87	0	47,47,47	1.20	4 (8%)
23	LMU	w	605	-	36,36,36	0.84	0	47,47,47	1.10	4 (8%)
16	CLA	T	4004	-	53,63,73	1.31	3 (5%)	62,101,113	1.10	3 (4%)
14	LMG	F	4017	-	27,27,55	1.10	2 (7%)	35,35,63	1.16	3 (8%)
16	CLA	H	1119	25	63,73,73	1.13	3 (4%)	74,113,113	0.94	2 (2%)
19	BCR	x	604	-	41,41,41	0.88	0	56,56,56	1.29	6 (10%)
16	CLA	B	1217	-	43,53,73	1.44	3 (6%)	50,89,113	1.00	1 (2%)
16	CLA	Z	506	-	58,68,73	1.23	3 (5%)	68,107,113	0.98	2 (2%)
16	CLA	H	1130	-	58,68,73	1.17	3 (5%)	68,107,113	0.95	5 (7%)
16	CLA	h	502	-	48,58,73	1.37	3 (6%)	56,95,113	0.96	4 (7%)
16	CLA	B	1204	-	63,73,73	1.16	3 (4%)	74,113,113	0.88	1 (1%)
16	CLA	B	1023	-	63,73,73	1.20	4 (6%)	74,113,113	1.09	4 (5%)
13	LHG	A	851	16	25,25,48	0.87	1 (4%)	28,31,54	1.27	2 (7%)
16	CLA	t	510	-	63,73,73	1.18	3 (4%)	74,113,113	0.96	4 (5%)
16	CLA	q	510	-	58,68,73	1.21	3 (5%)	68,107,113	0.92	3 (4%)
16	CLA	g	502	-	48,58,73	1.31	3 (6%)	56,95,113	0.93	0
19	BCR	B	4014	-	41,41,41	0.88	0	56,56,56	1.25	7 (12%)
13	LHG	r	605	-	30,30,48	0.81	2 (6%)	33,36,54	1.28	3 (9%)
16	CLA	G	1206	2	63,73,73	1.16	3 (4%)	74,113,113	0.91	2 (2%)
16	CLA	Z	511	-	63,73,73	1.15	4 (6%)	74,113,113	1.11	4 (5%)
16	CLA	p	506	-	58,68,73	1.24	3 (5%)	68,107,113	1.08	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	g	507	-	63,73,73	1.21	3 (4%)	74,113,113	0.92	4 (5%)
19	BCR	v	601	-	41,41,41	0.83	0	56,56,56	1.30	7 (12%)
16	CLA	t	513	-	44,54,73	1.42	3 (6%)	51,90,113	1.04	4 (7%)
19	BCR	y	604	-	41,41,41	0.87	0	56,56,56	1.29	7 (12%)
16	CLA	B	1227	-	47,57,73	1.32	4 (8%)	53,93,113	1.12	4 (7%)
16	CLA	h	503	-	44,54,73	1.44	3 (6%)	51,90,113	1.17	3 (5%)
16	CLA	n	505	-	63,73,73	1.20	4 (6%)	74,113,113	1.19	4 (5%)
16	CLA	n	507	-	63,73,73	1.21	3 (4%)	74,113,113	0.93	3 (4%)
16	CLA	w	513	-	48,58,73	1.36	3 (6%)	56,95,113	1.07	3 (5%)
16	CLA	w	501	-	48,58,73	1.34	3 (6%)	56,95,113	0.99	3 (5%)
16	CLA	Z	507	-	63,73,73	1.20	3 (4%)	74,113,113	1.01	3 (4%)
16	CLA	B	1207	-	63,73,73	1.19	4 (6%)	74,113,113	1.16	6 (8%)
16	CLA	g	506	-	58,68,73	1.23	3 (5%)	68,107,113	0.98	5 (7%)
16	CLA	p	511	-	63,73,73	1.14	3 (4%)	74,113,113	1.07	5 (6%)
16	CLA	A	1119	25	63,73,73	1.12	3 (4%)	74,113,113	1.00	4 (5%)
16	CLA	t	506	-	58,68,73	1.24	3 (5%)	68,107,113	1.04	4 (5%)
16	CLA	H	1132	-	63,73,73	1.13	3 (4%)	74,113,113	1.04	3 (4%)
13	LHG	i	103	-	39,39,48	0.69	2 (5%)	42,45,54	1.24	5 (11%)
16	CLA	L	1501	10	58,68,73	1.19	3 (5%)	68,107,113	0.97	4 (5%)
16	CLA	Z	504	-	63,73,73	1.17	4 (6%)	74,113,113	1.03	5 (6%)
16	CLA	q	506	-	58,68,73	1.25	3 (5%)	68,107,113	0.97	2 (2%)
16	CLA	o	513	-	44,54,73	1.39	3 (6%)	51,90,113	0.90	0
16	CLA	B	1213	-	53,63,73	1.27	4 (7%)	62,101,113	1.00	3 (4%)
16	CLA	B	1223	-	63,73,73	1.17	3 (4%)	74,113,113	1.01	2 (2%)
16	CLA	A	1118	-	53,63,73	1.28	3 (5%)	62,101,113	0.95	2 (3%)
16	CLA	g	511	-	63,73,73	1.16	3 (4%)	74,113,113	0.96	2 (2%)
16	CLA	u	517	12	53,63,73	1.30	3 (5%)	62,101,113	0.99	3 (4%)
19	BCR	Y	604	-	41,41,41	0.86	0	56,56,56	1.16	6 (10%)
21	ECH	m	4021	-	42,42,42	0.84	0	55,58,58	1.55	9 (16%)
16	CLA	r	515	-	63,73,73	1.18	3 (4%)	74,113,113	1.09	4 (5%)
16	CLA	U	1501	10	58,68,73	1.20	3 (5%)	68,107,113	1.00	3 (4%)
16	CLA	n	506	-	58,68,73	1.23	3 (5%)	68,107,113	1.05	4 (5%)
16	CLA	h	511	-	63,73,73	1.20	4 (6%)	74,113,113	1.00	7 (9%)
16	CLA	r	509	-	63,73,73	1.15	3 (4%)	74,113,113	0.95	3 (4%)
19	BCR	A	4003	-	41,41,41	0.85	0	56,56,56	1.29	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	t	516	-	44,54,73	1.41	3 (6%)	51,90,113	1.05	2 (3%)
16	CLA	y	501	-	44,54,73	1.40	3 (6%)	51,90,113	1.19	3 (5%)
20	LMT	U	4101	-	36,36,36	1.16	6 (16%)	47,47,47	1.09	1 (2%)
17	PQN	b	2002	-	34,34,34	0.36	0	43,45,45	1.06	2 (4%)
16	CLA	A	1120	-	47,57,73	1.31	3 (6%)	53,93,113	1.13	5 (9%)
16	CLA	A	1122	-	57,67,73	1.25	3 (5%)	66,105,113	0.97	4 (6%)
16	CLA	A	1127	-	63,73,73	1.17	4 (6%)	74,113,113	1.06	3 (4%)
16	CLA	x	510	-	63,73,73	1.19	3 (4%)	74,113,113	1.01	3 (4%)
16	CLA	g	508	12	53,63,73	1.29	3 (5%)	62,101,113	0.91	2 (3%)
16	CLA	v	508	-	53,63,73	1.32	4 (7%)	62,101,113	1.24	5 (8%)
16	CLA	A	1102	16	54,64,73	1.26	3 (5%)	63,102,113	0.87	1 (1%)
13	LHG	H	849	-	42,42,48	0.68	0	45,48,54	1.21	4 (8%)
16	CLA	u	516	-	44,54,73	1.38	3 (6%)	51,90,113	1.08	3 (5%)
16	CLA	t	507	-	63,73,73	1.22	3 (4%)	74,113,113	0.88	2 (2%)
16	CLA	K	4004	-	53,63,73	1.31	3 (5%)	62,101,113	1.08	4 (6%)
16	CLA	H	1112	-	43,53,73	1.41	3 (6%)	50,89,113	0.97	2 (4%)
16	CLA	h	504	-	58,68,73	1.26	3 (5%)	68,107,113	1.14	5 (7%)
14	LMG	a	4201	-	32,32,55	0.98	1 (3%)	40,40,63	1.17	3 (7%)
19	BCR	U	4019	-	41,41,41	0.86	0	56,56,56	1.49	8 (14%)
19	BCR	o	601	-	41,41,41	0.88	1 (2%)	56,56,56	1.37	8 (14%)
16	CLA	q	515	-	63,73,73	1.18	3 (4%)	74,113,113	1.13	4 (5%)
16	CLA	A	1124	25	58,68,73	1.22	3 (5%)	68,107,113	1.03	3 (4%)
16	CLA	A	1237	25	63,73,73	1.20	4 (6%)	74,113,113	1.10	5 (6%)
16	CLA	n	503	-	44,54,73	1.41	3 (6%)	51,90,113	1.17	4 (7%)
16	CLA	w	515	-	63,73,73	1.17	3 (4%)	74,113,113	1.10	3 (4%)
19	BCR	G	4004	-	41,41,41	0.83	0	56,56,56	1.25	6 (10%)
16	CLA	Y	508	12	53,63,73	1.27	3 (5%)	62,101,113	0.94	3 (4%)
16	CLA	t	503	-	44,54,73	1.42	3 (6%)	51,90,113	1.20	4 (7%)
19	BCR	q	602	-	41,41,41	0.85	0	56,56,56	1.24	6 (10%)
16	CLA	w	503	-	44,54,73	1.43	4 (9%)	51,90,113	1.06	3 (5%)
16	CLA	x	507	-	63,73,73	1.21	3 (4%)	74,113,113	0.97	3 (4%)
16	CLA	A	1130	-	58,68,73	1.20	3 (5%)	68,107,113	0.91	3 (4%)
19	BCR	h	604	-	41,41,41	0.86	0	56,56,56	1.25	6 (10%)
16	CLA	q	517	12	53,63,73	1.29	3 (5%)	62,101,113	1.04	4 (6%)
19	BCR	n	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	g	509	-	63,73,73	1.16	4 (6%)	74,113,113	0.99	2 (2%)
16	CLA	G	1012	25	53,63,73	1.24	3 (5%)	62,101,113	1.22	8 (12%)
16	CLA	b	1228	-	53,63,73	1.28	3 (5%)	62,101,113	1.01	3 (4%)
16	CLA	w	509	-	63,73,73	1.15	3 (4%)	74,113,113	0.94	3 (4%)
16	CLA	B	1212	-	43,53,73	1.43	3 (6%)	50,89,113	1.17	4 (8%)
21	ECH	M	4021	-	42,42,42	0.86	0	55,58,58	1.53	9 (16%)
13	LHG	H	851	16	25,25,48	0.88	1 (4%)	28,31,54	1.27	2 (7%)
19	BCR	r	604	-	41,41,41	0.89	0	56,56,56	1.27	6 (10%)
16	CLA	u	501	-	44,54,73	1.40	3 (6%)	51,90,113	0.93	3 (5%)
19	BCR	L	4019	-	41,41,41	0.90	0	56,56,56	1.41	6 (10%)
16	CLA	y	513	-	44,54,73	1.42	3 (6%)	51,90,113	0.94	2 (3%)
19	BCR	x	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)
16	CLA	A	1112	-	43,53,73	1.40	3 (6%)	50,89,113	1.04	3 (6%)
19	BCR	I	4018	-	41,41,41	0.86	0	56,56,56	1.27	8 (14%)
16	CLA	r	517	12	53,63,73	1.29	3 (5%)	62,101,113	0.95	2 (3%)
16	CLA	a	1109	16	63,73,73	1.17	3 (4%)	74,113,113	1.11	4 (5%)
16	CLA	l	1501	10	58,68,73	1.20	3 (5%)	68,107,113	0.98	3 (4%)
16	CLA	H	1106	1	63,73,73	1.15	3 (4%)	74,113,113	1.09	3 (4%)
16	CLA	A	1114	-	44,54,73	1.39	3 (6%)	51,90,113	1.21	4 (7%)
16	CLA	H	1104	-	63,73,73	1.18	4 (6%)	74,113,113	0.99	4 (5%)
16	CLA	X	515	-	63,73,73	1.15	3 (4%)	74,113,113	1.05	4 (5%)
16	CLA	u	512	12	63,73,73	1.15	4 (6%)	74,113,113	1.03	2 (2%)
16	CLA	x	506	-	58,68,73	1.24	4 (6%)	68,107,113	1.06	4 (5%)
16	CLA	y	503	-	44,54,73	1.45	4 (9%)	51,90,113	1.14	4 (7%)
16	CLA	u	508	12	53,63,73	1.30	3 (5%)	62,101,113	0.93	2 (3%)
13	LHG	g	605	-	30,30,48	0.80	2 (6%)	33,36,54	1.26	3 (9%)
21	ECH	B	4006	-	42,42,42	0.74	0	55,58,58	1.53	11 (20%)
16	CLA	W	501	-	48,58,73	1.34	3 (6%)	56,95,113	1.11	3 (5%)
16	CLA	r	507	-	63,73,73	1.21	3 (4%)	74,113,113	0.92	3 (4%)
19	BCR	k	4005	-	41,41,41	0.85	0	56,56,56	1.26	5 (8%)
19	BCR	T	4001	-	41,41,41	0.86	1 (2%)	56,56,56	1.26	7 (12%)
16	CLA	a	1116	-	52,62,73	1.24	3 (5%)	60,99,113	0.95	3 (5%)
16	CLA	B	1226	-	58,68,73	1.21	4 (6%)	68,107,113	1.02	3 (4%)
16	CLA	x	511	-	63,73,73	1.17	4 (6%)	74,113,113	0.90	2 (2%)
16	CLA	H	1108	-	43,53,73	1.40	3 (6%)	50,89,113	1.19	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	CLA	a	1135	-	49,59,73	1.34	4 (8%)	56,96,113	1.06	3 (5%)
16	CLA	r	508	12	53,63,73	1.30	3 (5%)	62,101,113	0.93	2 (3%)
16	CLA	s	507	12	63,73,73	1.20	3 (4%)	74,113,113	0.90	3 (4%)
19	BCR	G	4014	-	41,41,41	0.90	1 (2%)	56,56,56	1.29	8 (14%)
14	LMG	H	4101	-	46,46,55	0.91	1 (2%)	54,54,63	1.23	4 (7%)
14	LMG	b	848	-	43,43,55	0.86	1 (2%)	51,51,63	1.28	6 (11%)
16	CLA	A	1126	-	63,73,73	1.15	3 (4%)	74,113,113	1.15	2 (2%)
16	CLA	H	1107	1	48,58,73	1.35	3 (6%)	56,95,113	1.02	4 (7%)
15	CL0	A	1011	-	63,73,73	1.22	4 (6%)	74,113,113	1.02	5 (6%)
16	CLA	B	1224	-	58,68,73	1.24	4 (6%)	68,107,113	1.10	3 (4%)
16	CLA	B	1231	25	43,53,73	1.43	3 (6%)	50,89,113	1.14	3 (6%)
16	CLA	p	513	-	44,54,73	1.40	3 (6%)	51,90,113	0.91	2 (3%)
16	CLA	G	1219	-	43,53,73	1.44	3 (6%)	50,89,113	1.03	3 (6%)
16	CLA	W	516	-	44,54,73	1.41	3 (6%)	51,90,113	1.04	2 (3%)
16	CLA	b	1226	-	58,68,73	1.21	4 (6%)	68,107,113	1.03	3 (4%)
19	BCR	u	601	-	41,41,41	0.91	1 (2%)	56,56,56	1.38	9 (16%)
19	BCR	t	603	-	41,41,41	0.84	0	56,56,56	1.18	4 (7%)
19	BCR	S	4015	-	41,41,41	0.87	0	56,56,56	1.20	8 (14%)
16	CLA	B	1208	-	43,53,73	1.40	3 (6%)	50,89,113	1.11	4 (8%)
16	CLA	t	517	12	53,63,73	1.28	3 (5%)	62,101,113	0.90	1 (1%)
16	CLA	u	514	-	48,58,73	1.36	3 (6%)	56,95,113	1.16	4 (7%)
19	BCR	r	603	-	41,41,41	0.83	0	56,56,56	1.20	6 (10%)
16	CLA	t	501	-	48,58,73	1.35	3 (6%)	56,95,113	1.12	3 (5%)
14	LMG	f	4017	-	27,27,55	1.09	2 (7%)	35,35,63	1.16	3 (8%)
16	CLA	A	1135	-	49,59,73	1.31	4 (8%)	56,96,113	1.13	4 (7%)
16	CLA	q	508	12	53,63,73	1.28	3 (5%)	62,101,113	1.11	4 (6%)
19	BCR	B	4017	-	41,41,41	0.88	0	56,56,56	1.22	6 (10%)
16	CLA	G	1202	-	63,73,73	1.15	3 (4%)	74,113,113	0.91	3 (4%)
16	CLA	A	1121	-	49,59,73	1.34	3 (6%)	56,96,113	1.04	2 (3%)
16	CLA	W	513	-	44,54,73	1.43	3 (6%)	51,90,113	1.00	2 (3%)
19	BCR	A	4002	-	41,41,41	0.84	0	56,56,56	1.15	3 (5%)
16	CLA	o	506	-	58,68,73	1.24	4 (6%)	68,107,113	1.05	4 (5%)
19	BCR	B	4010	-	41,41,41	0.91	0	56,56,56	1.35	8 (14%)
16	CLA	H	1124	-	58,68,73	1.21	3 (5%)	68,107,113	0.89	1 (1%)
16	CLA	H	1237	25	63,73,73	1.18	4 (6%)	74,113,113	1.09	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	w	506	-	58,68,73	1.24	4 (6%)	68,107,113	1.06	3 (4%)
16	CLA	Q	1301	25	43,53,73	1.42	3 (6%)	50,89,113	1.12	4 (8%)
19	BCR	J	4012	-	41,41,41	0.87	0	56,56,56	1.31	8 (14%)
16	CLA	W	503	-	44,54,73	1.39	3 (6%)	51,90,113	1.15	4 (7%)
19	BCR	X	602	-	41,41,41	0.88	0	56,56,56	1.36	7 (12%)
19	BCR	b	4014	-	41,41,41	0.91	0	56,56,56	1.45	8 (14%)
16	CLA	a	1115	-	52,62,73	1.28	3 (5%)	60,99,113	1.10	2 (3%)
19	BCR	A	4007	-	41,41,41	0.91	1 (2%)	56,56,56	1.40	9 (16%)
16	CLA	H	1140	-	63,73,73	1.16	4 (6%)	74,113,113	1.03	2 (2%)
16	CLA	x	509	-	63,73,73	1.14	3 (4%)	74,113,113	0.97	4 (5%)
16	CLA	o	511	-	63,73,73	1.15	3 (4%)	74,113,113	1.04	5 (6%)
16	CLA	s	513	-	44,54,73	1.41	3 (6%)	51,90,113	1.08	3 (5%)
16	CLA	W	507	-	63,73,73	1.22	3 (4%)	74,113,113	0.89	2 (2%)
14	LMG	a	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.24	4 (8%)
24	LUT	w	601	-	42,43,43	0.74	0	51,60,60	1.46	7 (13%)
16	CLA	v	512	12	63,73,73	1.20	3 (4%)	74,113,113	1.04	6 (8%)
16	CLA	W	515	-	63,73,73	1.18	3 (4%)	74,113,113	1.01	4 (5%)
16	CLA	a	1103	-	63,73,73	1.17	3 (4%)	74,113,113	0.97	2 (2%)
16	CLA	r	512	12	63,73,73	1.19	4 (6%)	74,113,113	1.19	4 (5%)
16	CLA	X	508	12	53,63,73	1.30	3 (5%)	62,101,113	0.87	2 (3%)
19	BCR	A	4008	-	41,41,41	0.89	0	56,56,56	1.35	8 (14%)
16	CLA	l	1502	-	58,68,73	1.15	3 (5%)	68,107,113	1.10	3 (4%)
16	CLA	q	514	-	48,58,73	1.34	3 (6%)	56,95,113	1.14	4 (7%)
16	CLA	p	503	-	44,54,73	1.36	4 (9%)	51,90,113	1.08	5 (9%)
20	LMT	a	4202	-	36,36,36	1.17	5 (13%)	47,47,47	0.93	0
16	CLA	X	504	-	58,68,73	1.24	3 (5%)	68,107,113	1.14	3 (4%)
16	CLA	s	512	12	63,73,73	1.20	4 (6%)	74,113,113	1.15	6 (8%)
16	CLA	B	1234	-	48,58,73	1.31	4 (8%)	56,95,113	1.19	5 (8%)
23	LMU	p	606	-	36,36,36	0.83	0	47,47,47	1.33	5 (10%)
16	CLA	H	1131	-	63,73,73	1.16	3 (4%)	74,113,113	1.02	3 (4%)
19	BCR	Y	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)
16	CLA	r	514	-	48,58,73	1.34	3 (6%)	56,95,113	1.05	4 (7%)
16	CLA	s	516	-	44,54,73	1.38	3 (6%)	51,90,113	1.02	2 (3%)
16	CLA	B	1012	25	53,63,73	1.25	3 (5%)	62,101,113	1.16	6 (9%)
16	CLA	G	1234	-	48,58,73	1.29	4 (8%)	56,95,113	1.23	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	b	1210	-	63,73,73	1.19	3 (4%)	74,113,113	1.04	5 (6%)
16	CLA	b	1229	-	56,66,73	1.26	3 (5%)	65,104,113	0.98	4 (6%)
16	CLA	Y	510	-	63,73,73	1.19	3 (4%)	74,113,113	0.97	3 (4%)
16	CLA	p	509	-	58,68,73	1.20	3 (5%)	68,107,113	0.97	3 (4%)
16	CLA	A	1107	1	48,58,73	1.35	3 (6%)	56,95,113	1.06	3 (5%)
16	CLA	a	1101	-	63,73,73	1.16	3 (4%)	74,113,113	1.05	4 (5%)
16	CLA	o	517	12	53,63,73	1.28	3 (5%)	62,101,113	0.92	2 (3%)
16	CLA	t	511	-	63,73,73	1.17	3 (4%)	74,113,113	1.02	4 (5%)
19	BCR	g	604	-	41,41,41	0.88	0	56,56,56	1.28	6 (10%)
16	CLA	A	1013	-	63,73,73	1.12	4 (6%)	74,113,113	1.21	8 (10%)
16	CLA	v	509	-	63,73,73	1.17	4 (6%)	74,113,113	0.98	5 (6%)
16	CLA	b	1217	-	43,53,73	1.42	3 (6%)	50,89,113	1.16	4 (8%)
16	CLA	r	505	-	63,73,73	1.18	3 (4%)	74,113,113	1.15	4 (5%)
19	BCR	y	603	-	41,41,41	0.83	0	56,56,56	1.17	5 (8%)
16	CLA	o	509	-	58,68,73	1.20	3 (5%)	68,107,113	0.91	4 (5%)
23	LMU	g	606	-	36,36,36	0.86	0	47,47,47	1.32	5 (10%)
16	CLA	B	1236	-	48,58,73	1.32	4 (8%)	56,95,113	1.05	3 (5%)
16	CLA	Y	515	-	63,73,73	1.14	3 (4%)	74,113,113	1.02	4 (5%)
16	CLA	H	1022	25	63,73,73	1.14	3 (4%)	74,113,113	1.06	6 (8%)
16	CLA	B	1201	-	52,62,73	1.30	3 (5%)	60,99,113	1.01	2 (3%)
16	CLA	A	1131	-	63,73,73	1.16	3 (4%)	74,113,113	1.05	3 (4%)
16	CLA	H	1133	-	52,62,73	1.28	4 (7%)	60,99,113	1.15	3 (5%)
19	BCR	q	603	-	41,41,41	0.84	0	56,56,56	1.16	5 (8%)
23	LMU	Y	606	-	36,36,36	0.84	0	47,47,47	1.36	6 (12%)
16	CLA	H	1135	-	49,59,73	1.33	4 (8%)	56,96,113	1.15	3 (5%)
16	CLA	J	1303	-	35,45,73	1.56	4 (11%)	42,78,113	0.98	2 (4%)
16	CLA	Z	516	-	44,54,73	1.38	3 (6%)	51,90,113	0.98	2 (3%)
16	CLA	A	1101	-	63,73,73	1.17	3 (4%)	74,113,113	0.99	6 (8%)
23	LMU	x	606	-	36,36,36	0.88	0	47,47,47	1.26	6 (12%)
16	CLA	w	507	-	63,73,73	1.20	3 (4%)	74,113,113	0.85	2 (2%)
16	CLA	b	1207	-	63,73,73	1.19	3 (4%)	74,113,113	1.15	4 (5%)
16	CLA	Z	509	-	63,73,73	1.15	3 (4%)	74,113,113	0.96	2 (2%)
16	CLA	s	506	-	58,68,73	1.25	4 (6%)	68,107,113	1.06	6 (8%)
16	CLA	B	1239	-	63,73,73	1.17	3 (4%)	74,113,113	1.09	4 (5%)
16	CLA	y	506	-	58,68,73	1.23	3 (5%)	68,107,113	1.11	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	a	1104	-	63,73,73	1.17	4 (6%)	74,113,113	1.00	3 (4%)
16	CLA	a	1113	-	43,53,73	1.44	4 (9%)	50,89,113	1.14	2 (4%)
16	CLA	K	4003	9	43,53,73	1.46	3 (6%)	50,89,113	1.03	2 (4%)
14	LMG	H	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.23	4 (8%)
16	CLA	G	1225	-	63,73,73	1.16	4 (6%)	74,113,113	1.06	3 (4%)
16	CLA	H	1127	-	63,73,73	1.18	4 (6%)	74,113,113	1.11	4 (5%)
13	LHG	a	851	16	25,25,48	0.88	2 (8%)	28,31,54	1.26	2 (7%)
16	CLA	a	1132	-	63,73,73	1.11	3 (4%)	74,113,113	1.15	3 (4%)
19	BCR	B	4004	-	41,41,41	0.83	0	56,56,56	1.26	5 (8%)
16	CLA	G	1224	-	58,68,73	1.24	4 (6%)	68,107,113	1.11	3 (4%)
16	CLA	B	1214	-	53,63,73	1.26	3 (5%)	62,101,113	1.18	3 (4%)
16	CLA	a	1801	13	44,54,73	1.39	3 (6%)	51,90,113	1.22	3 (5%)
16	CLA	H	1111	-	53,63,73	1.28	3 (5%)	62,101,113	1.03	2 (3%)
16	CLA	a	1136	-	63,73,73	1.14	3 (4%)	74,113,113	0.95	2 (2%)
16	CLA	y	511	-	63,73,73	1.19	3 (4%)	74,113,113	1.11	4 (5%)
16	CLA	a	1108	-	43,53,73	1.42	3 (6%)	50,89,113	1.20	3 (6%)
16	CLA	p	517	12	53,63,73	1.29	3 (5%)	62,101,113	0.93	2 (3%)
24	LUT	Z	601	-	42,43,43	0.81	1 (2%)	51,60,60	1.48	6 (11%)
19	BCR	u	604	-	41,41,41	0.89	0	56,56,56	1.35	10 (17%)
16	CLA	t	509	-	58,68,73	1.22	3 (5%)	68,107,113	1.08	4 (5%)
13	LHG	s	605	-	31,31,48	0.79	1 (3%)	34,37,54	1.28	4 (11%)
16	CLA	w	512	12	63,73,73	1.17	4 (6%)	74,113,113	1.10	5 (6%)
16	CLA	A	1109	16	63,73,73	1.18	3 (4%)	74,113,113	1.07	4 (5%)
16	CLA	x	503	-	44,54,73	1.40	3 (6%)	51,90,113	1.04	2 (3%)
16	CLA	y	507	-	63,73,73	1.21	3 (4%)	74,113,113	0.87	2 (2%)
16	CLA	u	513	-	44,54,73	1.40	3 (6%)	51,90,113	0.93	2 (3%)
16	CLA	v	517	-	53,63,73	1.33	3 (5%)	62,101,113	1.00	4 (6%)
16	CLA	X	505	-	63,73,73	1.17	3 (4%)	74,113,113	1.10	5 (6%)
16	CLA	h	506	-	58,68,73	1.26	4 (6%)	68,107,113	1.22	6 (8%)
16	CLA	s	508	12	53,63,73	1.28	3 (5%)	62,101,113	0.95	4 (6%)
16	CLA	y	504	-	58,68,73	1.25	4 (6%)	68,107,113	1.02	5 (7%)
16	CLA	b	1231	25	43,53,73	1.44	3 (6%)	50,89,113	1.17	3 (6%)
16	CLA	A	1134	1	43,53,73	1.42	3 (6%)	50,89,113	0.99	1 (2%)
19	BCR	Z	602	-	41,41,41	0.87	0	56,56,56	1.36	8 (14%)
16	CLA	b	1224	-	58,68,73	1.23	4 (6%)	68,107,113	1.24	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	b	1234	-	48,58,73	1.33	3 (6%)	56,95,113	1.19	7 (12%)
18	SF4	H	3001	-	0,12,12	-	-	-	-	-
16	CLA	B	1220	-	51,61,73	1.36	3 (5%)	59,98,113	1.05	5 (8%)
16	CLA	f	1301	25	43,53,73	1.42	3 (6%)	50,89,113	1.04	4 (8%)
16	CLA	Y	516	-	44,54,73	1.38	3 (6%)	51,90,113	1.05	2 (3%)
16	CLA	H	1129	-	44,54,73	1.34	3 (6%)	51,90,113	1.03	3 (5%)
16	CLA	b	1235	-	60,70,73	1.21	4 (6%)	70,109,113	1.13	7 (10%)
19	BCR	r	602	-	41,41,41	0.86	0	56,56,56	1.24	4 (7%)
19	BCR	W	601	-	41,41,41	0.86	0	56,56,56	1.27	8 (14%)
16	CLA	Z	508	12	53,63,73	1.28	3 (5%)	62,101,113	1.10	4 (6%)
16	CLA	h	507	-	63,73,73	1.18	3 (4%)	74,113,113	1.08	4 (5%)
16	CLA	b	1230	-	43,53,73	1.41	3 (6%)	50,89,113	1.10	3 (6%)
16	CLA	a	1140	-	63,73,73	1.15	3 (4%)	74,113,113	1.00	2 (2%)
16	CLA	K	4002	-	43,53,73	1.44	3 (6%)	50,89,113	0.96	2 (4%)
16	CLA	y	512	12	63,73,73	1.20	3 (4%)	74,113,113	0.91	3 (4%)
16	CLA	S	1303	-	35,45,73	1.56	4 (11%)	42,78,113	0.98	2 (4%)
16	CLA	s	517	12	53,63,73	1.32	3 (5%)	62,101,113	0.98	2 (3%)
16	CLA	b	1232	25	43,53,73	1.45	3 (6%)	50,89,113	1.33	3 (6%)
16	CLA	v	513	-	44,54,73	1.44	3 (6%)	51,90,113	0.95	2 (3%)
16	CLA	q	511	-	63,73,73	1.16	3 (4%)	74,113,113	1.09	4 (5%)
16	CLA	o	503	-	44,54,73	1.39	3 (6%)	51,90,113	0.97	2 (3%)
16	CLA	v	501	-	44,54,73	1.43	3 (6%)	51,90,113	1.07	4 (7%)
16	CLA	H	1128	-	63,73,73	1.17	4 (6%)	74,113,113	1.05	5 (6%)
16	CLA	r	513	-	44,54,73	1.42	3 (6%)	51,90,113	0.99	3 (5%)
16	CLA	t	512	12	63,73,73	1.19	4 (6%)	74,113,113	1.11	4 (5%)
14	LMG	Q	4017	-	27,27,55	1.07	1 (3%)	35,35,63	1.18	3 (8%)
16	CLA	G	1223	-	63,73,73	1.17	3 (4%)	74,113,113	1.07	4 (5%)
16	CLA	j	1302	8	43,53,73	1.47	3 (6%)	50,89,113	1.00	3 (6%)
16	CLA	y	510	-	63,73,73	1.19	3 (4%)	74,113,113	0.91	3 (4%)
19	BCR	H	4007	-	41,41,41	0.91	1 (2%)	56,56,56	1.30	7 (12%)
16	CLA	r	503	-	44,54,73	1.39	3 (6%)	51,90,113	1.01	2 (3%)
16	CLA	B	1211	-	63,73,73	1.18	4 (6%)	74,113,113	0.97	3 (4%)
19	BCR	x	602	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)
16	CLA	X	506	-	58,68,73	1.23	4 (6%)	68,107,113	1.26	4 (5%)
16	CLA	X	514	-	48,58,73	1.38	4 (8%)	56,95,113	1.29	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	CLA	j	1303	-	35,45,73	1.56	4 (11%)	42,78,113	1.02	2 (4%)
16	CLA	n	512	12	63,73,73	1.18	4 (6%)	74,113,113	1.06	4 (5%)
16	CLA	t	508	12	53,63,73	1.28	3 (5%)	62,101,113	0.94	2 (3%)
19	BCR	J	4013	-	41,41,41	0.86	0	56,56,56	1.23	8 (14%)
19	BCR	K	4001	-	41,41,41	0.86	0	56,56,56	1.31	7 (12%)
19	BCR	W	603	-	41,41,41	0.85	0	56,56,56	1.21	3 (5%)
14	LMG	A	4101	-	46,46,55	0.93	2 (4%)	54,54,63	1.23	4 (7%)
16	CLA	n	516	-	44,54,73	1.41	3 (6%)	51,90,113	0.85	1 (1%)
16	CLA	G	1205	-	63,73,73	1.16	4 (6%)	74,113,113	1.09	4 (5%)
16	CLA	H	1122	-	57,67,73	1.23	3 (5%)	66,105,113	0.96	3 (4%)
16	CLA	g	503	-	44,54,73	1.41	3 (6%)	51,90,113	0.99	2 (3%)
16	CLA	X	511	-	63,73,73	1.14	3 (4%)	74,113,113	1.11	6 (8%)
16	CLA	q	505	-	63,73,73	1.16	4 (6%)	74,113,113	1.17	8 (10%)
16	CLA	p	507	12	63,73,73	1.20	3 (4%)	74,113,113	0.94	3 (4%)
19	BCR	o	603	-	41,41,41	0.87	0	56,56,56	1.31	8 (14%)
16	CLA	a	1111	-	53,63,73	1.28	3 (5%)	62,101,113	1.03	2 (3%)
16	CLA	b	1223	-	63,73,73	1.18	3 (4%)	74,113,113	1.06	1 (1%)
16	CLA	u	503	-	44,54,73	1.39	3 (6%)	51,90,113	0.94	2 (3%)
16	CLA	g	515	-	63,73,73	1.19	3 (4%)	74,113,113	1.12	4 (5%)
16	CLA	a	1110	-	52,62,73	1.25	3 (5%)	60,99,113	0.97	2 (3%)
18	SF4	N	101	-	0,12,12	-	-	-	-	-
16	CLA	x	516	-	44,54,73	1.39	3 (6%)	51,90,113	1.14	3 (5%)
16	CLA	A	1138	-	63,73,73	1.16	3 (4%)	74,113,113	0.90	3 (4%)
19	BCR	b	4017	-	41,41,41	0.87	0	56,56,56	1.16	4 (7%)
16	CLA	g	517	12	53,63,73	1.32	3 (5%)	62,101,113	0.89	1 (1%)
16	CLA	v	514	-	48,58,73	1.38	3 (6%)	56,95,113	0.97	2 (3%)
19	BCR	g	601	-	41,41,41	0.88	0	56,56,56	1.44	9 (16%)
16	CLA	G	1214	-	53,63,73	1.24	4 (7%)	62,101,113	1.09	3 (4%)
16	CLA	a	1133	-	52,62,73	1.30	3 (5%)	60,99,113	0.92	2 (3%)
19	BCR	b	4010	-	41,41,41	0.91	0	56,56,56	1.33	7 (12%)
16	CLA	X	510	-	58,68,73	1.23	3 (5%)	68,107,113	0.91	2 (2%)
16	CLA	b	1205	-	63,73,73	1.16	3 (4%)	74,113,113	1.05	4 (5%)
16	CLA	H	1125	-	63,73,73	1.18	3 (4%)	74,113,113	0.96	2 (2%)
16	CLA	a	1237	25	63,73,73	1.19	4 (6%)	74,113,113	1.12	5 (6%)
19	BCR	q	604	-	41,41,41	0.87	0	56,56,56	1.26	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	G	1212	-	43,53,73	1.45	3 (6%)	50,89,113	1.23	4 (8%)
16	CLA	H	1120	-	47,57,73	1.31	3 (6%)	53,93,113	1.19	5 (9%)
13	LHG	p	605	-	31,31,48	0.77	1 (3%)	34,37,54	1.29	4 (11%)
16	CLA	b	1218	-	53,63,73	1.29	3 (5%)	62,101,113	1.00	5 (8%)
16	CLA	Z	505	-	63,73,73	1.19	3 (4%)	74,113,113	0.93	3 (4%)
16	CLA	h	517	-	53,63,73	1.31	3 (5%)	62,101,113	0.96	4 (6%)
16	CLA	H	1110	-	52,62,73	1.27	3 (5%)	60,99,113	0.97	3 (5%)
16	CLA	r	510	-	63,73,73	1.18	3 (4%)	74,113,113	0.96	2 (2%)
20	LMT	l	4101	-	36,36,36	1.16	6 (16%)	47,47,47	1.09	1 (2%)
16	CLA	o	512	12	63,73,73	1.17	4 (6%)	74,113,113	1.18	5 (6%)
19	BCR	X	601	-	41,41,41	0.87	1 (2%)	56,56,56	1.33	6 (10%)
16	CLA	W	504	-	58,68,73	1.26	3 (5%)	68,107,113	0.97	3 (4%)
16	CLA	x	501	-	48,58,73	1.36	3 (6%)	56,95,113	1.22	4 (7%)
13	LHG	B	4018	16	37,37,48	0.72	1 (2%)	40,43,54	1.32	5 (12%)
17	PQN	G	2002	-	34,34,34	0.38	0	43,45,45	1.04	2 (4%)
16	CLA	G	1236	-	48,58,73	1.32	3 (6%)	56,95,113	1.05	2 (3%)
16	CLA	X	517	12	53,63,73	1.28	3 (5%)	62,101,113	0.95	4 (6%)
19	BCR	r	601	-	41,41,41	0.86	1 (2%)	56,56,56	1.29	7 (12%)
16	CLA	G	1220	-	52,62,73	1.31	3 (5%)	60,99,113	1.04	3 (5%)
18	SF4	c	101	-	0,12,12	-	-	-	-	-
16	CLA	s	515	-	63,73,73	1.14	3 (4%)	74,113,113	0.98	4 (5%)
16	CLA	q	513	-	48,58,73	1.36	3 (6%)	56,95,113	1.01	3 (5%)
19	BCR	l	4019	-	41,41,41	0.88	0	56,56,56	1.44	8 (14%)
21	ECH	G	4006	-	42,42,42	0.79	0	55,58,58	1.50	8 (14%)
16	CLA	q	501	-	48,58,73	1.35	3 (6%)	56,95,113	0.99	3 (5%)
16	CLA	s	504	-	63,73,73	1.18	3 (4%)	74,113,113	0.90	2 (2%)
19	BCR	g	603	-	41,41,41	0.84	0	56,56,56	1.21	6 (10%)
19	BCR	v	603	-	41,41,41	0.85	0	56,56,56	1.27	8 (14%)
16	CLA	n	508	12	53,63,73	1.29	3 (5%)	62,101,113	0.92	1 (1%)
19	BCR	W	604	-	41,41,41	0.86	0	56,56,56	1.37	9 (16%)
16	CLA	b	1012	25	53,63,73	1.23	3 (5%)	62,101,113	1.24	8 (12%)
14	LMG	A	4201	-	32,32,55	1.00	1 (3%)	40,40,63	1.18	3 (7%)
16	CLA	H	1103	-	63,73,73	1.16	3 (4%)	74,113,113	0.99	3 (4%)
16	CLA	b	1211	-	63,73,73	1.18	3 (4%)	74,113,113	0.94	3 (4%)
19	BCR	Q	4016	-	41,41,41	0.86	0	56,56,56	1.28	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	CLA	t	505	-	63,73,73	1.19	3 (4%)	74,113,113	1.18	5 (6%)
18	SF4	a	3001	-	0,12,12	-	-	-		
16	CLA	Y	502	-	48,58,73	1.34	3 (6%)	56,95,113	0.97	3 (5%)
16	CLA	a	1129	-	44,54,73	1.33	3 (6%)	51,90,113	1.07	3 (5%)
19	BCR	f	4016	-	41,41,41	0.87	0	56,56,56	1.29	5 (8%)
16	CLA	X	502	-	48,58,73	1.32	4 (8%)	56,95,113	0.94	2 (3%)
19	BCR	s	604	-	41,41,41	0.87	0	56,56,56	1.22	5 (8%)
19	BCR	L	4022	-	41,41,41	0.86	0	56,56,56	1.30	6 (10%)
19	BCR	o	602	-	41,41,41	0.88	0	56,56,56	1.37	7 (12%)
16	CLA	n	517	12	53,63,73	1.27	3 (5%)	62,101,113	0.90	1 (1%)
16	CLA	B	1216	25	45,55,73	1.40	4 (8%)	52,91,113	1.09	3 (5%)
16	CLA	q	516	-	44,54,73	1.38	3 (6%)	51,90,113	0.89	1 (1%)
16	CLA	p	512	12	63,73,73	1.21	4 (6%)	74,113,113	1.16	5 (6%)
16	CLA	r	501	-	48,58,73	1.34	3 (6%)	56,95,113	1.15	4 (7%)
16	CLA	Y	514	-	48,58,73	1.35	3 (6%)	56,95,113	1.07	4 (7%)
16	CLA	l	1503	-	63,73,73	1.16	3 (4%)	74,113,113	0.91	3 (4%)
18	SF4	C	101	-	0,12,12	-	-	-		
16	CLA	B	1240	13	44,54,73	1.43	3 (6%)	51,90,113	1.17	3 (5%)
16	CLA	G	1229	-	56,66,73	1.26	3 (5%)	65,104,113	1.03	4 (6%)
16	CLA	G	1232	25	43,53,73	1.44	3 (6%)	50,89,113	1.25	5 (10%)
16	CLA	x	517	12	53,63,73	1.30	3 (5%)	62,101,113	0.90	2 (3%)
16	CLA	h	508	-	53,63,73	1.30	3 (5%)	62,101,113	1.05	4 (6%)
16	CLA	B	1230	-	43,53,73	1.40	3 (6%)	50,89,113	1.05	2 (4%)
16	CLA	g	512	12	63,73,73	1.20	4 (6%)	74,113,113	1.14	4 (5%)
16	CLA	J	1302	8	43,53,73	1.47	3 (6%)	50,89,113	1.09	3 (6%)
16	CLA	s	503	-	44,54,73	1.40	4 (9%)	51,90,113	1.17	4 (7%)
16	CLA	B	1222	25	48,58,73	1.36	3 (6%)	56,95,113	1.02	3 (5%)
19	BCR	H	4008	-	41,41,41	0.90	1 (2%)	56,56,56	1.36	4 (7%)
16	CLA	Q	1302	6	44,54,73	1.42	3 (6%)	51,90,113	0.98	2 (3%)
16	CLA	X	513	-	44,54,73	1.38	3 (6%)	51,90,113	1.02	2 (3%)
18	SF4	c	102	-	0,12,12	-	-	-		
16	CLA	h	512	12	63,73,73	1.21	4 (6%)	74,113,113	0.95	4 (5%)
16	CLA	n	502	-	48,58,73	1.35	4 (8%)	56,95,113	1.06	2 (3%)
19	BCR	j	4015	-	41,41,41	0.88	0	56,56,56	1.22	7 (12%)
16	CLA	a	1121	-	49,59,73	1.35	3 (6%)	56,96,113	1.07	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	a	1128	-	63,73,73	1.14	4 (6%)	74,113,113	1.07	5 (6%)
16	CLA	b	1023	-	63,73,73	1.18	4 (6%)	74,113,113	1.09	3 (4%)
14	LMG	A	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.23	4 (8%)
16	CLA	w	502	-	48,58,73	1.32	4 (8%)	56,95,113	1.10	3 (5%)
16	CLA	q	503	-	44,54,73	1.42	4 (9%)	51,90,113	1.20	4 (7%)
16	CLA	s	510	-	63,73,73	1.18	3 (4%)	74,113,113	0.92	3 (4%)
16	CLA	H	1137	-	45,55,73	1.35	3 (6%)	52,91,113	1.01	4 (7%)
16	CLA	G	1228	-	53,63,73	1.27	3 (5%)	62,101,113	1.02	3 (4%)
16	CLA	y	517	-	53,63,73	1.33	3 (5%)	62,101,113	1.23	5 (8%)
16	CLA	A	1140	-	63,73,73	1.16	4 (6%)	74,113,113	1.07	3 (4%)
16	CLA	g	514	-	48,58,73	1.34	4 (8%)	56,95,113	1.02	4 (7%)
19	BCR	a	4007	-	41,41,41	0.89	1 (2%)	56,56,56	1.30	5 (8%)
19	BCR	a	4011	-	41,41,41	0.89	0	56,56,56	1.26	5 (8%)
16	CLA	a	1117	-	63,73,73	1.12	3 (4%)	74,113,113	1.17	6 (8%)
16	CLA	b	1240	13	44,54,73	1.42	3 (6%)	51,90,113	1.11	2 (3%)
16	CLA	W	506	-	58,68,73	1.22	3 (5%)	68,107,113	1.05	4 (5%)
16	CLA	B	1215	-	58,68,73	1.16	3 (5%)	68,107,113	1.12	3 (4%)
16	CLA	a	1105	-	56,66,73	1.25	3 (5%)	65,104,113	0.98	4 (6%)
19	BCR	S	4013	-	41,41,41	0.87	0	56,56,56	1.32	7 (12%)
19	BCR	a	4003	-	41,41,41	0.87	0	56,56,56	1.22	4 (7%)
16	CLA	B	1225	-	63,73,73	1.15	4 (6%)	74,113,113	1.05	4 (5%)
16	CLA	f	1302	6	44,54,73	1.43	3 (6%)	51,90,113	1.00	2 (3%)
19	BCR	w	604	-	41,41,41	0.87	0	56,56,56	1.27	6 (10%)
16	CLA	a	1120	-	47,57,73	1.32	3 (6%)	53,93,113	1.23	5 (9%)
16	CLA	h	514	-	48,58,73	1.37	3 (6%)	56,95,113	1.01	4 (7%)
16	CLA	W	511	-	63,73,73	1.18	3 (4%)	74,113,113	1.07	6 (8%)
16	CLA	v	502	-	48,58,73	1.34	3 (6%)	56,95,113	0.96	3 (5%)
19	BCR	Y	603	-	41,41,41	0.85	0	56,56,56	1.16	4 (7%)
16	CLA	H	1116	-	52,62,73	1.23	4 (7%)	60,99,113	1.06	4 (6%)
16	CLA	y	502	-	48,58,73	1.36	3 (6%)	56,95,113	0.97	3 (5%)
16	CLA	B	1206	2	63,73,73	1.15	3 (4%)	74,113,113	0.92	4 (5%)
19	BCR	x	603	-	41,41,41	0.85	0	56,56,56	1.26	6 (10%)
16	CLA	b	1204	-	63,73,73	1.17	3 (4%)	74,113,113	0.92	2 (2%)
16	CLA	q	509	-	63,73,73	1.13	3 (4%)	74,113,113	0.96	4 (5%)
16	CLA	B	1238	25	63,73,73	1.14	3 (4%)	74,113,113	0.98	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	H	1102	16	54,64,73	1.24	3 (5%)	63,102,113	0.91	2 (3%)
16	CLA	H	1136	-	63,73,73	1.14	3 (4%)	74,113,113	0.94	2 (2%)
16	CLA	A	1137	-	45,55,73	1.36	3 (6%)	52,91,113	0.98	4 (7%)
16	CLA	H	1801	13	44,54,73	1.36	3 (6%)	51,90,113	1.14	4 (7%)
16	CLA	u	510	-	58,68,73	1.24	3 (5%)	68,107,113	0.89	3 (4%)
16	CLA	h	509	-	63,73,73	1.19	4 (6%)	74,113,113	1.01	4 (5%)
16	CLA	G	1211	-	63,73,73	1.20	3 (4%)	74,113,113	0.97	2 (2%)
16	CLA	A	1022	25	63,73,73	1.17	3 (4%)	74,113,113	1.00	6 (8%)
16	CLA	p	508	12	53,63,73	1.29	3 (5%)	62,101,113	0.97	4 (6%)
16	CLA	A	1125	-	63,73,73	1.18	3 (4%)	74,113,113	0.96	3 (4%)
16	CLA	n	515	-	63,73,73	1.17	3 (4%)	74,113,113	1.02	3 (4%)
16	CLA	G	1021	-	63,73,73	1.16	3 (4%)	74,113,113	1.11	4 (5%)
16	CLA	a	1130	-	58,68,73	1.18	3 (5%)	68,107,113	0.96	4 (5%)
13	LHG	G	4018	16	37,37,48	0.73	1 (2%)	40,43,54	1.32	5 (12%)
16	CLA	v	515	-	63,73,73	1.21	3 (4%)	74,113,113	1.09	5 (6%)
16	CLA	w	508	12	53,63,73	1.28	3 (5%)	62,101,113	1.00	4 (6%)
19	BCR	X	604	-	41,41,41	0.88	0	56,56,56	1.31	5 (8%)
19	BCR	v	604	-	41,41,41	0.86	0	56,56,56	1.28	8 (14%)
16	CLA	A	1139	25	58,68,73	1.22	3 (5%)	68,107,113	1.03	3 (4%)
16	CLA	b	1206	2	63,73,73	1.14	3 (4%)	74,113,113	0.95	3 (4%)
16	CLA	y	515	-	63,73,73	1.20	3 (4%)	74,113,113	1.06	6 (8%)
16	CLA	B	1205	-	63,73,73	1.18	3 (4%)	74,113,113	1.03	3 (4%)
16	CLA	Z	517	12	53,63,73	1.31	3 (5%)	62,101,113	0.97	2 (3%)
16	CLA	u	507	12	63,73,73	1.20	3 (4%)	74,113,113	0.93	3 (4%)
16	CLA	G	1204	-	63,73,73	1.17	3 (4%)	74,113,113	0.94	2 (2%)
16	CLA	w	504	-	63,73,73	1.17	3 (4%)	74,113,113	0.96	4 (5%)
16	CLA	H	1134	1	43,53,73	1.41	3 (6%)	50,89,113	0.98	1 (2%)
16	CLA	x	512	12	63,73,73	1.19	4 (6%)	74,113,113	1.09	4 (5%)
16	CLA	a	1118	-	53,63,73	1.28	3 (5%)	62,101,113	0.89	1 (1%)
16	CLA	v	505	-	63,73,73	1.23	3 (4%)	74,113,113	1.21	4 (5%)
18	SF4	N	102	-	0,12,12	-	-	-	-	-
19	BCR	H	4003	-	41,41,41	0.86	0	56,56,56	1.22	4 (7%)
16	CLA	s	501	-	48,58,73	1.36	3 (6%)	56,95,113	1.15	4 (7%)
16	CLA	b	1209	-	43,53,73	1.43	3 (6%)	50,89,113	1.06	2 (4%)
16	CLA	t	515	-	63,73,73	1.19	3 (4%)	74,113,113	1.09	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	CLA	o	501	-	44,54,73	1.38	3 (6%)	51,90,113	1.04	3 (5%)
19	BCR	B	4005	-	41,41,41	0.85	0	56,56,56	1.17	4 (7%)
19	BCR	u	603	-	41,41,41	0.88	0	56,56,56	1.35	8 (14%)
16	CLA	n	504	-	58,68,73	1.25	3 (5%)	68,107,113	1.05	3 (4%)
19	BCR	p	602	-	41,41,41	0.87	0	56,56,56	1.31	7 (12%)
16	CLA	H	1109	16	63,73,73	1.18	3 (4%)	74,113,113	1.06	4 (5%)
17	PQN	H	2001	-	34,34,34	0.38	0	43,45,45	1.06	2 (4%)
16	CLA	h	515	-	63,73,73	1.20	3 (4%)	74,113,113	1.13	6 (8%)
16	CLA	H	1117	-	63,73,73	1.12	3 (4%)	74,113,113	1.16	6 (8%)
16	CLA	Z	502	-	48,58,73	1.32	4 (8%)	56,95,113	1.03	3 (5%)
16	CLA	a	1139	25	53,63,73	1.28	3 (5%)	62,101,113	0.96	4 (6%)
16	CLA	A	1116	-	52,62,73	1.22	3 (5%)	60,99,113	1.14	6 (10%)
16	CLA	p	515	-	63,73,73	1.14	3 (4%)	74,113,113	1.02	4 (5%)
19	BCR	s	602	-	41,41,41	0.87	0	56,56,56	1.32	8 (14%)
16	CLA	G	1238	25	63,73,73	1.14	3 (4%)	74,113,113	0.96	3 (4%)
16	CLA	B	1202	-	63,73,73	1.19	3 (4%)	74,113,113	0.92	2 (2%)
19	BCR	n	604	-	41,41,41	0.86	0	56,56,56	1.33	7 (12%)
17	PQN	B	2002	-	34,34,34	0.36	0	43,45,45	1.04	2 (4%)
16	CLA	w	516	-	44,54,73	1.38	3 (6%)	51,90,113	0.96	3 (5%)
19	BCR	S	4012	-	41,41,41	0.88	0	56,56,56	1.28	7 (12%)
16	CLA	X	501	-	44,54,73	1.38	3 (6%)	51,90,113	1.01	3 (5%)
24	LUT	q	601	-	42,43,43	0.77	0	51,60,60	1.51	9 (17%)
16	CLA	G	1240	13	44,54,73	1.43	3 (6%)	51,90,113	1.25	4 (7%)
16	CLA	u	506	-	58,68,73	1.29	4 (6%)	68,107,113	1.63	9 (13%)
19	BCR	K	4005	-	41,41,41	0.86	0	56,56,56	1.28	6 (10%)
16	CLA	Y	513	-	44,54,73	1.41	3 (6%)	51,90,113	0.96	3 (5%)
16	CLA	o	516	-	44,54,73	1.39	3 (6%)	51,90,113	0.95	1 (1%)
16	CLA	w	517	12	53,63,73	1.29	4 (7%)	62,101,113	0.99	1 (1%)
16	CLA	Z	501	-	48,58,73	1.34	3 (6%)	56,95,113	1.00	4 (7%)
16	CLA	Y	503	-	44,54,73	1.36	3 (6%)	51,90,113	1.09	3 (5%)
16	CLA	Y	511	-	63,73,73	1.15	3 (4%)	74,113,113	1.05	5 (6%)
16	CLA	G	1239	-	63,73,73	1.17	3 (4%)	74,113,113	1.12	5 (6%)
16	CLA	Z	513	-	48,58,73	1.34	3 (6%)	56,95,113	0.99	3 (5%)
16	CLA	H	1121	-	49,59,73	1.35	3 (6%)	56,96,113	1.09	2 (3%)
16	CLA	r	506	-	58,68,73	1.22	3 (5%)	68,107,113	1.03	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	CLA	y	509	-	63,73,73	1.18	3 (4%)	74,113,113	0.87	3 (4%)
16	CLA	o	507	12	63,73,73	1.22	3 (4%)	74,113,113	0.97	2 (2%)
16	CLA	s	514	-	48,58,73	1.34	3 (6%)	56,95,113	1.23	4 (7%)
16	CLA	a	1127	-	63,73,73	1.18	4 (6%)	74,113,113	1.06	3 (4%)
16	CLA	b	1236	-	48,58,73	1.32	3 (6%)	56,95,113	1.13	4 (7%)
19	BCR	s	601	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)
16	CLA	L	1503	25	63,73,73	1.16	3 (4%)	74,113,113	0.90	3 (4%)
19	BCR	a	4002	-	41,41,41	0.85	0	56,56,56	1.18	5 (8%)
16	CLA	S	1302	8	43,53,73	1.45	3 (6%)	50,89,113	1.00	3 (6%)
16	CLA	X	516	-	44,54,73	1.38	3 (6%)	51,90,113	1.00	2 (3%)
16	CLA	r	511	-	63,73,73	1.17	3 (4%)	74,113,113	0.90	2 (2%)
16	CLA	n	510	-	63,73,73	1.20	3 (4%)	74,113,113	1.03	3 (4%)
16	CLA	u	504	-	58,68,73	1.24	3 (5%)	68,107,113	0.95	3 (4%)
16	CLA	v	507	12	63,73,73	1.22	3 (4%)	74,113,113	1.01	4 (5%)
16	CLA	A	1108	-	43,53,73	1.42	3 (6%)	50,89,113	0.97	1 (2%)
16	CLA	B	1228	-	53,63,73	1.29	3 (5%)	62,101,113	1.02	3 (4%)
16	CLA	p	501	-	48,58,73	1.35	3 (6%)	56,95,113	1.12	4 (7%)
19	BCR	J	4015	-	41,41,41	0.87	0	56,56,56	1.26	9 (16%)
16	CLA	b	1214	-	53,63,73	1.25	3 (5%)	62,101,113	1.01	3 (4%)
16	CLA	g	504	-	63,73,73	1.19	3 (4%)	74,113,113	0.96	4 (5%)
16	CLA	v	504	-	58,68,73	1.24	3 (5%)	68,107,113	0.98	4 (5%)
16	CLA	x	502	-	48,58,73	1.34	4 (8%)	56,95,113	0.99	2 (3%)
16	CLA	H	1118	-	53,63,73	1.29	3 (5%)	62,101,113	1.00	5 (8%)
16	CLA	b	1239	-	63,73,73	1.16	3 (4%)	74,113,113	1.02	6 (8%)
16	CLA	x	508	12	53,63,73	1.31	3 (5%)	62,101,113	0.91	2 (3%)
16	CLA	H	1105	-	56,66,73	1.23	3 (5%)	65,104,113	1.03	4 (6%)
16	CLA	B	1232	-	43,53,73	1.41	3 (6%)	50,89,113	1.27	4 (8%)
16	CLA	Y	507	12	63,73,73	1.20	3 (4%)	74,113,113	0.93	3 (4%)
16	CLA	h	513	-	44,54,73	1.43	3 (6%)	51,90,113	0.92	2 (3%)
19	BCR	F	4016	-	41,41,41	0.86	0	56,56,56	1.31	8 (14%)
16	CLA	B	1021	-	63,73,73	1.16	3 (4%)	74,113,113	1.08	4 (5%)
16	CLA	r	502	-	48,58,73	1.32	3 (6%)	56,95,113	0.96	1 (1%)
16	CLA	u	505	-	63,73,73	1.17	3 (4%)	74,113,113	1.04	4 (5%)
16	CLA	a	1119	-	63,73,73	1.13	3 (4%)	74,113,113	0.95	4 (5%)
16	CLA	H	1114	-	44,54,73	1.40	3 (6%)	51,90,113	1.21	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	x	505	-	63,73,73	1.17	3 (4%)	74,113,113	1.22	5 (6%)
16	CLA	y	516	-	44,54,73	1.44	3 (6%)	51,90,113	1.10	4 (7%)
19	BCR	g	602	-	41,41,41	0.86	0	56,56,56	1.28	7 (12%)

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	501	-	1/1/12/20	8/19/97/115	-
19	BCR	a	4008	-	-	10/29/63/63	0/2/2/2
13	LHG	o	605	-	-	12/31/31/53	-
19	BCR	B	4009	-	-	7/24/41/63	0/1/1/2
16	CLA	H	1113	-	1/1/11/20	0/13/91/115	-
16	CLA	u	511	-	1/1/15/20	7/37/115/115	-
16	CLA	G	1203	-	1/1/15/20	14/37/115/115	-
19	BCR	G	4010	-	-	17/29/63/63	0/2/2/2
21	ECH	R	4020	-	-	11/29/66/66	0/2/2/2
16	CLA	s	502	-	1/1/12/20	5/19/97/115	-
19	BCR	A	4011	-	-	17/29/63/63	0/2/2/2
16	CLA	q	507	-	1/1/15/20	11/37/115/115	-
20	LMT	H	4202	-	-	8/21/61/61	0/2/2/2
16	CLA	G	1213	-	1/1/13/20	7/25/103/115	-
16	CLA	X	509	-	1/1/14/20	12/31/109/115	-
16	CLA	W	514	-	1/1/12/20	7/19/97/115	-
16	CLA	p	516	-	1/1/11/20	7/15/93/115	-
16	CLA	a	1137	-	1/1/11/20	4/16/94/115	-
19	BCR	s	603	-	-	7/29/63/63	0/2/2/2
19	BCR	Z	604	-	-	19/29/63/63	0/2/2/2
16	CLA	q	504	-	1/1/15/20	13/37/115/115	-
13	LHG	Y	605	-	-	16/36/36/53	-
16	CLA	p	504	-	-	15/37/115/115	-
21	ECH	V	4021	-	-	14/29/66/66	0/2/2/2
16	CLA	b	1215	-	-	5/31/109/115	-
16	CLA	a	1114	-	1/1/11/20	8/15/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	b	1202	-	1/1/15/20	16/37/115/115	-
16	CLA	o	508	12	1/1/13/20	12/25/103/115	-
16	CLA	v	503	-	1/1/11/20	6/15/93/115	-
16	CLA	b	1021	-	1/1/15/20	16/37/115/115	-
16	CLA	g	505	-	1/1/15/20	9/37/115/115	-
16	CLA	h	505	-	-	5/37/115/115	-
16	CLA	A	1110	-	1/1/12/20	8/24/102/115	-
16	CLA	a	1124	25	1/1/14/20	7/31/109/115	-
16	CLA	a	1106	1	1/1/15/20	16/37/115/115	-
16	CLA	b	1216	25	1/1/11/20	0/16/94/115	-
16	CLA	k	4004	-	1/1/13/20	6/25/103/115	-
16	CLA	H	1013	-	1/1/15/20	13/37/115/115	-
13	LHG	A	849	-	-	19/47/47/53	-
16	CLA	o	504	-	-	9/31/109/115	-
21	ECH	b	4006	-	-	9/29/66/66	0/2/2/2
16	CLA	H	1138	-	1/1/15/20	9/37/115/115	-
16	CLA	a	1123	-	-	13/37/115/115	-
16	CLA	y	508	-	1/1/13/20	9/25/103/115	-
16	CLA	b	1213	-	1/1/13/20	5/25/103/115	-
16	CLA	n	513	-	-	8/15/93/115	-
16	CLA	W	509	-	1/1/14/20	4/31/109/115	-
16	CLA	n	514	-	1/1/12/20	6/19/97/115	-
16	CLA	U	1502	-	-	8/31/109/115	-
16	CLA	Y	505	-	1/1/15/20	13/37/115/115	-
16	CLA	b	1221	25	1/1/15/20	19/37/115/115	-
16	CLA	w	514	-	1/1/12/20	7/19/97/115	-
16	CLA	r	504	-	1/1/15/20	16/37/115/115	-
19	BCR	G	4017	-	-	13/29/63/63	0/2/2/2
13	LHG	I	103	-	-	20/44/44/53	-
16	CLA	h	516	-	1/1/11/20	6/15/93/115	-
16	CLA	a	1112	-	-	5/13/91/115	-
16	CLA	Y	504	-	1/1/15/20	15/37/115/115	-
16	CLA	B	1218	-	-	7/25/103/115	-
19	BCR	t	601	-	-	14/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LMU	q	605	-	-	5/21/61/61	0/2/2/2
16	CLA	A	1104	-	1/1/15/20	18/37/115/115	-
14	LMG	B	848	-	-	18/38/58/70	0/1/1/1
16	CLA	A	1113	-	1/1/11/20	6/13/91/115	-
16	CLA	x	504	-	1/1/15/20	20/37/115/115	-
19	BCR	X	603	-	-	12/29/63/63	0/2/2/2
19	BCR	U	4022	-	-	16/29/63/63	0/2/2/2
16	CLA	G	1235	-	1/1/14/20	9/34/112/115	-
16	CLA	W	505	-	1/1/15/20	18/37/115/115	-
13	LHG	a	849	-	-	17/47/47/53	-
16	CLA	Z	512	12	1/1/15/20	13/37/115/115	-
16	CLA	G	1226	-	-	17/31/109/115	-
19	BCR	y	601	-	-	15/29/63/63	0/2/2/2
16	CLA	L	1502	-	-	8/31/109/115	-
16	CLA	H	1126	-	1/1/15/20	11/37/115/115	-
16	CLA	y	514	-	-	6/19/97/115	-
19	BCR	G	4005	-	-	11/29/63/63	0/2/2/2
16	CLA	G	1210	-	-	15/37/115/115	-
15	CL0	H	1011	-	2/2/20/25	6/37/135/135	-
16	CLA	o	502	-	1/1/12/20	7/19/97/115	-
16	CLA	w	510	-	-	9/31/109/115	-
16	CLA	g	501	-	-	6/19/97/115	-
16	CLA	h	501	-	-	7/15/93/115	-
16	CLA	U	1503	-	1/1/15/20	9/37/115/115	-
16	CLA	W	510	-	-	14/37/115/115	-
16	CLA	G	1217	-	-	7/13/91/115	-
19	BCR	H	4011	-	-	16/29/63/63	0/2/2/2
19	BCR	n	603	-	-	12/29/63/63	0/2/2/2
19	BCR	w	603	-	-	13/29/63/63	0/2/2/2
16	CLA	G	1023	-	-	8/37/115/115	-
18	SF4	A	3001	-	-	-	0/6/5/5
16	CLA	s	511	-	1/1/15/20	13/37/115/115	-
16	CLA	b	1201	-	1/1/12/20	4/24/102/115	-
16	CLA	B	1209	-	1/1/11/20	5/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	G	1215	-	1/1/14/20	6/31/109/115	-
16	CLA	w	511	-	1/1/15/20	8/37/115/115	-
19	BCR	j	4012	-	-	10/29/63/63	0/2/2/2
16	CLA	A	1129	-	-	5/15/93/115	-
16	CLA	k	4002	-	1/1/11/20	5/13/91/115	-
16	CLA	q	512	12	1/1/15/20	14/37/115/115	-
16	CLA	G	1216	25	1/1/11/20	3/16/94/115	-
19	BCR	w	602	-	-	11/29/63/63	0/2/2/2
16	CLA	u	515	-	-	16/37/115/115	-
17	PQN	A	2001	-	-	3/23/43/43	0/2/2/2
16	CLA	Y	512	12	1/1/15/20	8/37/115/115	-
16	CLA	x	515	-	1/1/15/20	9/37/115/115	-
16	CLA	X	503	-	-	10/15/93/115	-
16	CLA	G	1230	-	1/1/11/20	6/13/91/115	-
21	ECH	I	4020	-	-	11/29/66/66	0/2/2/2
16	CLA	W	502	-	1/1/12/20	9/19/97/115	-
16	CLA	a	1022	-	1/1/15/20	8/37/115/115	-
16	CLA	u	502	-	1/1/12/20	6/19/97/115	-
16	CLA	Y	506	-	-	12/31/109/115	-
13	LHG	u	605	-	-	12/31/31/53	-
16	CLA	s	505	-	1/1/15/20	11/37/115/115	-
16	CLA	b	1219	-	-	5/13/91/115	-
16	CLA	B	1229	-	1/1/13/20	8/29/107/115	-
13	LHG	x	605	-	-	20/35/35/53	-
16	CLA	A	1128	-	1/1/15/20	19/37/115/115	-
19	BCR	Y	602	-	-	10/29/63/63	0/2/2/2
16	CLA	Z	514	-	1/1/12/20	8/19/97/115	-
14	LMG	a	4101	-	-	21/41/61/70	0/1/1/1
20	LMT	A	4202	-	-	7/21/61/61	0/2/2/2
19	BCR	k	4001	-	-	12/29/63/63	0/2/2/2
16	CLA	F	1302	6	1/1/11/20	7/15/93/115	-
16	CLA	b	1225	-	-	12/37/115/115	-
16	CLA	H	1115	-	-	9/24/102/115	-
16	CLA	B	1219	-	-	4/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	i	4018	-	-	13/29/63/63	0/2/2/2
16	CLA	s	509	-	1/1/14/20	14/31/109/115	-
16	CLA	b	1208	-	1/1/11/20	6/13/91/115	-
19	BCR	p	601	-	-	9/29/63/63	0/2/2/2
16	CLA	b	1222	25	-	7/19/97/115	-
16	CLA	a	1102	16	1/1/13/20	6/27/105/115	-
16	CLA	b	1238	25	1/1/15/20	16/37/115/115	-
16	CLA	W	512	12	1/1/14/20	16/31/109/115	-
16	CLA	X	507	12	-	8/37/115/115	-
16	CLA	b	1212	-	1/1/11/20	3/13/91/115	-
16	CLA	G	1209	-	1/1/11/20	3/13/91/115	-
19	BCR	l	4022	-	-	18/29/63/63	0/2/2/2
16	CLA	W	508	12	1/1/13/20	7/25/103/115	-
19	BCR	o	604	-	-	18/29/63/63	0/2/2/2
16	CLA	B	1203	-	1/1/15/20	14/37/115/115	-
16	CLA	o	514	-	1/1/12/20	7/19/97/115	-
13	LHG	R	103	-	-	23/44/44/53	-
16	CLA	B	1235	-	1/1/14/20	10/34/112/115	-
16	CLA	p	514	-	1/1/12/20	7/19/97/115	-
19	BCR	T	4005	-	-	9/29/63/63	0/2/2/2
16	CLA	G	1221	25	1/1/15/20	18/37/115/115	-
13	LHG	b	4018	16	-	16/42/42/53	-
19	BCR	j	4013	-	-	11/29/63/63	0/2/2/2
16	CLA	a	1107	1	-	6/19/97/115	-
19	BCR	h	601	-	-	14/29/63/63	0/2/2/2
16	CLA	A	1115	-	1/1/12/20	8/24/102/115	-
16	CLA	H	1139	25	1/1/14/20	11/31/109/115	-
16	CLA	Z	510	-	-	10/31/109/115	-
17	PQN	a	2001	-	-	5/23/43/43	0/2/2/2
16	CLA	G	1201	-	1/1/12/20	4/24/102/115	-
16	CLA	G	1218	-	-	12/25/103/115	-
16	CLA	H	1123	-	-	10/37/115/115	-
16	CLA	n	511	-	-	6/37/115/115	-
16	CLA	A	1111	-	1/1/13/20	6/25/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	a	1013	-	1/1/15/20	12/37/115/115	-
14	LMG	G	848	-	-	18/38/58/70	0/1/1/1
16	CLA	a	1138	-	1/1/15/20	13/37/115/115	-
14	LMG	H	4201	-	-	10/27/47/70	0/1/1/1
16	CLA	u	509	-	1/1/14/20	6/31/109/115	-
16	CLA	X	512	12	-	10/37/115/115	-
16	CLA	B	1221	25	-	13/37/115/115	-
16	CLA	Y	517	12	-	9/25/103/115	-
16	CLA	W	517	12	1/1/13/20	9/25/103/115	-
19	BCR	u	602	-	-	13/29/63/63	0/2/2/2
16	CLA	x	513	-	-	8/15/93/115	-
16	CLA	A	1103	-	1/1/15/20	9/37/115/115	-
16	CLA	p	502	-	1/1/12/20	3/19/97/115	-
13	LHG	X	605	-	-	12/31/31/53	-
16	CLA	A	1106	1	1/1/15/20	14/37/115/115	-
16	CLA	b	1203	-	1/1/15/20	14/37/115/115	-
16	CLA	v	506	-	1/1/14/20	5/31/109/115	-
16	CLA	x	514	-	1/1/12/20	6/19/97/115	-
16	CLA	A	1133	-	1/1/12/20	9/24/102/115	-
16	CLA	a	1125	-	-	9/37/115/115	-
16	CLA	a	1131	-	-	12/37/115/115	-
16	CLA	Y	509	-	1/1/14/20	15/31/109/115	-
16	CLA	o	505	-	1/1/15/20	14/37/115/115	-
16	CLA	Z	515	-	1/1/15/20	10/37/115/115	-
16	CLA	r	516	-	1/1/11/20	3/15/93/115	-
16	CLA	G	1227	-	-	8/18/96/115	-
16	CLA	p	505	-	-	12/37/115/115	-
16	CLA	A	1132	-	1/1/15/20	15/37/115/115	-
16	CLA	G	1207	-	-	12/37/115/115	-
19	BCR	R	4018	-	-	13/29/63/63	0/2/2/2
16	CLA	G	1231	25	1/1/11/20	3/13/91/115	-
16	CLA	A	1801	13	1/1/11/20	8/15/93/115	-
16	CLA	A	1136	-	1/1/15/20	5/37/115/115	-
16	CLA	A	1123	25	-	8/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	1105	-	1/1/13/20	9/29/107/115	-
16	CLA	v	511	-	1/1/15/20	9/37/115/115	-
16	CLA	a	1122	-	-	8/30/108/115	-
16	CLA	p	510	-	-	10/37/115/115	-
16	CLA	g	513	-	-	9/15/93/115	-
23	LMU	r	606	-	-	6/21/61/61	0/2/2/2
16	CLA	t	502	-	1/1/12/20	9/19/97/115	-
16	CLA	t	504	-	1/1/14/20	5/31/109/115	-
19	BCR	b	4004	-	-	11/29/63/63	0/2/2/2
19	BCR	p	604	-	-	15/29/63/63	0/2/2/2
16	CLA	T	4003	9	1/1/11/20	9/13/91/115	-
19	BCR	H	4002	-	-	11/29/63/63	0/2/2/2
19	BCR	p	603	-	-	7/29/63/63	0/2/2/2
19	BCR	b	4009	-	-	7/24/41/63	0/1/1/2
19	BCR	h	603	-	-	11/29/63/63	0/2/2/2
16	CLA	b	1220	-	-	11/24/102/115	-
16	CLA	w	505	-	-	8/37/115/115	-
16	CLA	k	4003	9	1/1/11/20	5/13/91/115	-
16	CLA	a	1126	-	1/1/15/20	11/37/115/115	-
16	CLA	o	510	-	-	5/31/109/115	-
19	BCR	b	4005	-	-	12/29/63/63	0/2/2/2
23	LMU	s	606	-	-	6/21/61/61	0/2/2/2
19	BCR	G	4009	-	-	7/24/41/63	0/1/1/2
16	CLA	t	514	-	1/1/12/20	7/19/97/115	-
15	CL0	a	1011	-	2/2/20/25	7/37/135/135	-
16	CLA	o	515	-	1/1/15/20	15/37/115/115	-
16	CLA	h	510	-	-	7/37/115/115	-
16	CLA	b	1227	-	1/1/11/20	5/18/96/115	-
19	BCR	t	604	-	-	14/29/63/63	0/2/2/2
16	CLA	H	1101	-	1/1/15/20	16/37/115/115	-
16	CLA	n	509	-	1/1/14/20	8/31/109/115	-
16	CLA	g	510	-	-	10/37/115/115	-
16	CLA	v	510	-	-	6/37/115/115	-
19	BCR	Z	603	-	-	8/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	G	1222	25	-	6/19/97/115	-
16	CLA	A	1117	-	1/1/15/20	6/37/115/115	-
16	CLA	T	4002	-	1/1/11/20	5/13/91/115	-
16	CLA	q	502	-	1/1/12/20	6/19/97/115	-
18	SF4	C	102	-	-	-	0/6/5/5
16	CLA	Y	501	-	1/1/12/20	6/19/97/115	-
16	CLA	F	1301	25	1/1/11/20	2/13/91/115	-
16	CLA	G	1208	-	1/1/11/20	6/13/91/115	-
16	CLA	g	516	-	1/1/11/20	4/15/93/115	-
16	CLA	v	516	-	1/1/11/20	4/15/93/115	-
21	ECH	i	4020	-	-	12/29/66/66	0/2/2/2
16	CLA	Z	503	-	1/1/11/20	8/15/93/115	-
16	CLA	B	1210	-	-	13/37/115/115	-
20	LMT	L	4101	-	-	9/21/61/61	0/2/2/2
16	CLA	y	505	-	1/1/15/20	8/37/115/115	-
16	CLA	a	1134	1	-	4/13/91/115	-
23	LMU	Z	605	-	-	5/21/61/61	0/2/2/2
23	LMU	w	605	-	-	5/21/61/61	0/2/2/2
16	CLA	T	4004	-	-	3/25/103/115	-
14	LMG	F	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	H	1119	25	1/1/15/20	11/37/115/115	-
19	BCR	x	604	-	-	12/29/63/63	0/2/2/2
16	CLA	B	1217	-	-	5/13/91/115	-
16	CLA	Z	506	-	-	7/31/109/115	-
16	CLA	H	1130	-	-	9/31/109/115	-
16	CLA	h	502	-	1/1/12/20	5/19/97/115	-
16	CLA	B	1204	-	1/1/15/20	7/37/115/115	-
16	CLA	B	1023	-	-	8/37/115/115	-
13	LHG	A	851	16	-	7/30/30/53	-
16	CLA	t	510	-	-	9/37/115/115	-
16	CLA	q	510	-	-	8/31/109/115	-
16	CLA	g	502	-	1/1/12/20	4/19/97/115	-
19	BCR	B	4014	-	-	16/29/63/63	0/2/2/2
13	LHG	r	605	-	-	17/35/35/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	G	1206	2	1/1/15/20	11/37/115/115	-
16	CLA	Z	511	-	1/1/15/20	3/37/115/115	-
16	CLA	p	506	-	-	13/31/109/115	-
16	CLA	g	507	-	1/1/15/20	7/37/115/115	-
19	BCR	v	601	-	-	11/29/63/63	0/2/2/2
16	CLA	t	513	-	-	6/15/93/115	-
19	BCR	y	604	-	-	11/29/63/63	0/2/2/2
16	CLA	B	1227	-	1/1/11/20	10/18/96/115	-
16	CLA	h	503	-	1/1/11/20	5/15/93/115	-
16	CLA	n	505	-	1/1/15/20	20/37/115/115	-
16	CLA	n	507	-	1/1/15/20	9/37/115/115	-
16	CLA	w	513	-	-	7/19/97/115	-
16	CLA	w	501	-	1/1/12/20	10/19/97/115	-
16	CLA	Z	507	-	1/1/15/20	14/37/115/115	-
16	CLA	B	1207	-	-	16/37/115/115	-
16	CLA	g	506	-	-	9/31/109/115	-
16	CLA	p	511	-	1/1/15/20	14/37/115/115	-
16	CLA	A	1119	25	1/1/15/20	5/37/115/115	-
16	CLA	t	506	-	1/1/14/20	11/31/109/115	-
16	CLA	H	1132	-	1/1/15/20	15/37/115/115	-
16	CLA	q	506	-	1/1/14/20	10/31/109/115	-
13	LHG	i	103	-	-	22/44/44/53	-
16	CLA	Z	504	-	1/1/15/20	12/37/115/115	-
16	CLA	L	1501	10	-	12/31/109/115	-
16	CLA	o	513	-	-	4/15/93/115	-
16	CLA	B	1213	-	1/1/13/20	7/25/103/115	-
16	CLA	B	1223	-	1/1/15/20	9/37/115/115	-
16	CLA	A	1118	-	-	9/25/103/115	-
16	CLA	g	511	-	1/1/15/20	8/37/115/115	-
16	CLA	u	517	12	-	6/25/103/115	-
19	BCR	Y	604	-	-	14/29/63/63	0/2/2/2
21	ECH	m	4021	-	-	14/29/66/66	0/2/2/2
16	CLA	r	515	-	1/1/15/20	11/37/115/115	-
16	CLA	U	1501	10	-	12/31/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	n	506	-	-	7/31/109/115	-
16	CLA	h	511	-	1/1/15/20	13/37/115/115	-
16	CLA	r	509	-	-	9/37/115/115	-
19	BCR	A	4003	-	-	9/29/63/63	0/2/2/2
16	CLA	t	516	-	1/1/11/20	7/15/93/115	-
16	CLA	y	501	-	1/1/11/20	6/15/93/115	-
20	LMT	U	4101	-	-	8/21/61/61	0/2/2/2
17	PQN	b	2002	-	-	8/23/43/43	0/2/2/2
16	CLA	A	1122	-	1/1/13/20	7/30/108/115	-
16	CLA	A	1120	-	-	6/18/96/115	-
16	CLA	A	1127	-	1/1/15/20	4/37/115/115	-
16	CLA	x	510	-	-	11/37/115/115	-
16	CLA	g	508	12	1/1/13/20	5/25/103/115	-
16	CLA	v	508	-	1/1/13/20	11/25/103/115	-
16	CLA	A	1102	16	1/1/13/20	6/27/105/115	-
13	LHG	H	849	-	-	17/47/47/53	-
16	CLA	u	516	-	1/1/11/20	7/15/93/115	-
16	CLA	t	507	-	1/1/15/20	9/37/115/115	-
16	CLA	K	4004	-	1/1/13/20	4/25/103/115	-
16	CLA	H	1112	-	-	2/13/91/115	-
16	CLA	h	504	-	-	14/31/109/115	-
14	LMG	a	4201	-	-	11/27/47/70	0/1/1/1
19	BCR	U	4019	-	-	10/29/63/63	0/2/2/2
19	BCR	o	601	-	-	8/29/63/63	0/2/2/2
16	CLA	q	515	-	1/1/15/20	10/37/115/115	-
16	CLA	A	1124	25	1/1/14/20	6/31/109/115	-
16	CLA	A	1237	25	1/1/15/20	10/37/115/115	-
16	CLA	n	503	-	1/1/11/20	7/15/93/115	-
16	CLA	w	515	-	1/1/15/20	12/37/115/115	-
19	BCR	G	4004	-	-	11/29/63/63	0/2/2/2
16	CLA	Y	508	12	1/1/13/20	11/25/103/115	-
16	CLA	t	503	-	1/1/11/20	5/15/93/115	-
19	BCR	q	602	-	-	12/29/63/63	0/2/2/2
16	CLA	w	503	-	1/1/11/20	8/15/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	x	507	-	1/1/15/20	8/37/115/115	-
16	CLA	A	1130	-	1/1/14/20	9/31/109/115	-
19	BCR	h	604	-	-	13/29/63/63	0/2/2/2
16	CLA	q	517	12	-	9/25/103/115	-
19	BCR	n	601	-	-	12/29/63/63	0/2/2/2
16	CLA	g	509	-	1/1/15/20	8/37/115/115	-
16	CLA	G	1012	25	1/1/13/20	7/25/103/115	-
16	CLA	b	1228	-	1/1/13/20	11/25/103/115	-
16	CLA	w	509	-	1/1/15/20	11/37/115/115	-
16	CLA	B	1212	-	1/1/11/20	5/13/91/115	-
21	ECH	M	4021	-	-	15/29/66/66	0/2/2/2
13	LHG	H	851	16	-	7/30/30/53	-
19	BCR	r	604	-	-	15/29/63/63	0/2/2/2
16	CLA	u	501	-	-	5/15/93/115	-
19	BCR	L	4019	-	-	13/29/63/63	0/2/2/2
16	CLA	y	513	-	1/1/11/20	5/15/93/115	-
19	BCR	x	601	-	-	11/29/63/63	0/2/2/2
16	CLA	A	1112	-	-	4/13/91/115	-
19	BCR	I	4018	-	-	11/29/63/63	0/2/2/2
16	CLA	r	517	12	-	10/25/103/115	-
16	CLA	a	1109	16	1/1/15/20	7/37/115/115	-
16	CLA	l	1501	10	-	14/31/109/115	-
16	CLA	H	1106	1	1/1/15/20	15/37/115/115	-
16	CLA	A	1114	-	1/1/11/20	7/15/93/115	-
16	CLA	H	1104	-	1/1/15/20	15/37/115/115	-
16	CLA	X	515	-	1/1/15/20	15/37/115/115	-
16	CLA	y	503	-	1/1/11/20	4/15/93/115	-
16	CLA	u	512	12	-	11/37/115/115	-
16	CLA	x	506	-	-	12/31/109/115	-
16	CLA	u	508	12	1/1/13/20	10/25/103/115	-
13	LHG	g	605	-	-	16/35/35/53	-
21	ECH	B	4006	-	-	10/29/66/66	0/2/2/2
16	CLA	W	501	-	1/1/12/20	8/19/97/115	-
16	CLA	r	507	-	1/1/15/20	11/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	k	4005	-	-	7/29/63/63	0/2/2/2
19	BCR	T	4001	-	-	12/29/63/63	0/2/2/2
16	CLA	a	1116	-	1/1/12/20	8/24/102/115	-
16	CLA	B	1226	-	-	14/31/109/115	-
16	CLA	x	511	-	-	6/37/115/115	-
16	CLA	H	1108	-	-	4/13/91/115	-
16	CLA	a	1135	-	1/1/12/20	2/21/99/115	-
16	CLA	r	508	12	1/1/13/20	7/25/103/115	-
16	CLA	s	507	12	-	9/37/115/115	-
19	BCR	G	4014	-	-	16/29/63/63	0/2/2/2
14	LMG	H	4101	-	-	23/41/61/70	0/1/1/1
16	CLA	A	1126	-	1/1/15/20	11/37/115/115	-
14	LMG	b	848	-	-	19/38/58/70	0/1/1/1
16	CLA	H	1107	1	-	4/19/97/115	-
15	CL0	A	1011	-	2/2/20/25	8/37/135/135	-
16	CLA	B	1224	-	1/1/14/20	10/31/109/115	-
16	CLA	B	1231	25	1/1/11/20	7/13/91/115	-
16	CLA	p	513	-	-	6/15/93/115	-
16	CLA	G	1219	-	-	6/13/91/115	-
16	CLA	W	516	-	-	5/15/93/115	-
16	CLA	b	1226	-	1/1/14/20	16/31/109/115	-
19	BCR	u	601	-	-	8/29/63/63	0/2/2/2
19	BCR	t	603	-	-	11/29/63/63	0/2/2/2
19	BCR	S	4015	-	-	10/29/63/63	0/2/2/2
16	CLA	B	1208	-	1/1/11/20	4/13/91/115	-
16	CLA	t	517	12	1/1/13/20	6/25/103/115	-
16	CLA	u	514	-	1/1/12/20	4/19/97/115	-
19	BCR	r	603	-	-	11/29/63/63	0/2/2/2
16	CLA	t	501	-	1/1/12/20	7/19/97/115	-
16	CLA	A	1135	-	1/1/12/20	2/21/99/115	-
14	LMG	f	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	q	508	12	1/1/13/20	8/25/103/115	-
19	BCR	B	4017	-	-	11/29/63/63	0/2/2/2
16	CLA	G	1202	-	1/1/15/20	16/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	1121	-	1/1/12/20	6/21/99/115	-
16	CLA	W	513	-	-	8/15/93/115	-
19	BCR	A	4002	-	-	12/29/63/63	0/2/2/2
16	CLA	o	506	-	1/1/14/20	15/31/109/115	-
19	BCR	B	4010	-	-	16/29/63/63	0/2/2/2
16	CLA	H	1124	-	1/1/14/20	5/31/109/115	-
16	CLA	H	1237	25	1/1/15/20	10/37/115/115	-
16	CLA	w	506	-	-	5/31/109/115	-
16	CLA	Q	1301	25	1/1/11/20	0/13/91/115	-
19	BCR	J	4012	-	-	12/29/63/63	0/2/2/2
16	CLA	W	503	-	1/1/11/20	8/15/93/115	-
19	BCR	X	602	-	-	17/29/63/63	0/2/2/2
19	BCR	b	4014	-	-	15/29/63/63	0/2/2/2
16	CLA	a	1115	-	1/1/12/20	8/24/102/115	-
19	BCR	A	4007	-	-	7/29/63/63	0/2/2/2
16	CLA	H	1140	-	1/1/15/20	13/37/115/115	-
16	CLA	x	509	-	1/1/15/20	12/37/115/115	-
16	CLA	o	511	-	1/1/15/20	9/37/115/115	-
16	CLA	s	513	-	-	7/15/93/115	-
16	CLA	W	507	-	-	10/37/115/115	-
14	LMG	a	852	-	-	10/33/53/70	0/1/1/1
24	LUT	w	601	-	-	7/29/67/67	0/2/2/2
16	CLA	v	512	12	-	11/37/115/115	-
16	CLA	W	515	-	1/1/15/20	15/37/115/115	-
16	CLA	a	1103	-	1/1/15/20	12/37/115/115	-
16	CLA	r	512	12	1/1/15/20	9/37/115/115	-
16	CLA	X	508	12	1/1/13/20	13/25/103/115	-
19	BCR	A	4008	-	-	12/29/63/63	0/2/2/2
16	CLA	l	1502	-	-	8/31/109/115	-
16	CLA	q	514	-	1/1/12/20	9/19/97/115	-
16	CLA	p	503	-	1/1/11/20	5/15/93/115	-
20	LMT	a	4202	-	-	8/21/61/61	0/2/2/2
16	CLA	X	504	-	-	15/31/109/115	-
16	CLA	s	512	12	1/1/15/20	7/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	1234	-	1/1/12/20	5/19/97/115	-
23	LMU	p	606	-	-	9/21/61/61	0/2/2/2
16	CLA	H	1131	-	1/1/15/20	9/37/115/115	-
19	BCR	Y	601	-	-	12/29/63/63	0/2/2/2
16	CLA	r	514	-	1/1/12/20	9/19/97/115	-
16	CLA	s	516	-	-	9/15/93/115	-
16	CLA	B	1012	25	1/1/13/20	11/25/103/115	-
16	CLA	G	1234	-	1/1/12/20	3/19/97/115	-
16	CLA	b	1210	-	1/1/15/20	12/37/115/115	-
16	CLA	b	1229	-	1/1/13/20	8/29/107/115	-
16	CLA	Y	510	-	-	10/37/115/115	-
16	CLA	p	509	-	1/1/14/20	19/31/109/115	-
16	CLA	A	1107	1	-	4/19/97/115	-
16	CLA	a	1101	-	1/1/15/20	18/37/115/115	-
16	CLA	t	511	-	1/1/15/20	8/37/115/115	-
16	CLA	o	517	12	-	9/25/103/115	-
19	BCR	g	604	-	-	16/29/63/63	0/2/2/2
16	CLA	A	1013	-	1/1/15/20	13/37/115/115	-
16	CLA	v	509	-	-	14/37/115/115	-
16	CLA	b	1217	-	-	1/13/91/115	-
16	CLA	r	505	-	-	11/37/115/115	-
19	BCR	y	603	-	-	11/29/63/63	0/2/2/2
16	CLA	o	509	-	1/1/14/20	9/31/109/115	-
23	LMU	g	606	-	-	5/21/61/61	0/2/2/2
16	CLA	B	1236	-	1/1/12/20	9/19/97/115	-
16	CLA	Y	515	-	1/1/15/20	8/37/115/115	-
16	CLA	H	1022	25	1/1/15/20	10/37/115/115	-
16	CLA	B	1201	-	1/1/12/20	4/24/102/115	-
16	CLA	A	1131	-	-	12/37/115/115	-
16	CLA	H	1133	-	-	8/24/102/115	-
19	BCR	q	603	-	-	6/29/63/63	0/2/2/2
23	LMU	Y	606	-	-	6/21/61/61	0/2/2/2
16	CLA	H	1135	-	-	3/21/99/115	-
16	CLA	J	1303	-	-	0/2/76/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	Z	516	-	1/1/11/20	9/15/93/115	-
16	CLA	A	1101	-	1/1/15/20	14/37/115/115	-
23	LMU	x	606	-	-	14/21/61/61	0/2/2/2
16	CLA	w	507	-	1/1/15/20	9/37/115/115	-
16	CLA	b	1207	-	-	12/37/115/115	-
16	CLA	Z	509	-	1/1/15/20	15/37/115/115	-
16	CLA	s	506	-	-	9/31/109/115	-
16	CLA	y	506	-	1/1/14/20	9/31/109/115	-
16	CLA	B	1239	-	-	13/37/115/115	-
16	CLA	a	1104	-	1/1/15/20	16/37/115/115	-
16	CLA	a	1113	-	1/1/11/20	2/13/91/115	-
16	CLA	K	4003	9	1/1/11/20	8/13/91/115	-
14	LMG	H	852	-	-	6/33/53/70	0/1/1/1
16	CLA	G	1225	-	1/1/15/20	10/37/115/115	-
16	CLA	H	1127	-	1/1/15/20	6/37/115/115	-
13	LHG	a	851	16	-	9/30/30/53	-
16	CLA	a	1132	-	1/1/15/20	14/37/115/115	-
19	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
16	CLA	G	1224	-	1/1/14/20	12/31/109/115	-
16	CLA	B	1214	-	1/1/13/20	8/25/103/115	-
16	CLA	a	1801	13	1/1/11/20	6/15/93/115	-
16	CLA	H	1111	-	1/1/13/20	8/25/103/115	-
16	CLA	a	1136	-	1/1/15/20	9/37/115/115	-
16	CLA	y	511	-	1/1/15/20	11/37/115/115	-
16	CLA	a	1108	-	-	6/13/91/115	-
16	CLA	p	517	12	-	8/25/103/115	-
24	LUT	Z	601	-	-	7/29/67/67	0/2/2/2
19	BCR	u	604	-	-	17/29/63/63	0/2/2/2
16	CLA	t	509	-	1/1/14/20	5/31/109/115	-
16	CLA	w	512	12	1/1/15/20	11/37/115/115	-
13	LHG	s	605	-	-	12/36/36/53	-
16	CLA	A	1109	16	1/1/15/20	7/37/115/115	-
16	CLA	x	503	-	-	7/15/93/115	-
16	CLA	y	507	-	-	11/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	u	513	-	-	6/15/93/115	-
16	CLA	v	517	-	1/1/13/20	14/25/103/115	-
16	CLA	X	505	-	1/1/15/20	10/37/115/115	-
16	CLA	h	506	-	1/1/14/20	9/31/109/115	-
16	CLA	s	508	12	1/1/13/20	8/25/103/115	-
16	CLA	y	504	-	-	12/31/109/115	-
16	CLA	b	1231	25	1/1/11/20	6/13/91/115	-
16	CLA	A	1134	1	-	4/13/91/115	-
19	BCR	Z	602	-	-	11/29/63/63	0/2/2/2
16	CLA	b	1224	-	1/1/14/20	8/31/109/115	-
16	CLA	b	1234	-	1/1/12/20	3/19/97/115	-
18	SF4	H	3001	-	-	-	0/6/5/5
16	CLA	B	1220	-	1/1/12/20	11/23/101/115	-
16	CLA	f	1301	25	1/1/11/20	2/13/91/115	-
16	CLA	Y	516	-	-	9/15/93/115	-
16	CLA	H	1129	-	-	4/15/93/115	-
16	CLA	b	1235	-	1/1/14/20	12/34/112/115	-
19	BCR	r	602	-	-	16/29/63/63	0/2/2/2
19	BCR	W	601	-	-	16/29/63/63	0/2/2/2
16	CLA	Z	508	12	1/1/13/20	7/25/103/115	-
16	CLA	h	507	-	1/1/15/20	13/37/115/115	-
16	CLA	b	1230	-	-	5/13/91/115	-
16	CLA	a	1140	-	-	11/37/115/115	-
16	CLA	K	4002	-	1/1/11/20	2/13/91/115	-
16	CLA	y	512	12	-	12/37/115/115	-
16	CLA	S	1303	-	-	0/2/76/115	-
16	CLA	s	517	12	-	8/25/103/115	-
16	CLA	b	1232	25	1/1/11/20	6/13/91/115	-
16	CLA	v	513	-	1/1/11/20	2/15/93/115	-
16	CLA	q	511	-	-	4/37/115/115	-
16	CLA	o	503	-	-	3/15/93/115	-
16	CLA	v	501	-	-	6/15/93/115	-
16	CLA	H	1128	-	1/1/15/20	16/37/115/115	-
16	CLA	r	513	-	-	11/15/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	t	512	12	1/1/15/20	9/37/115/115	-
14	LMG	Q	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	G	1223	-	1/1/15/20	4/37/115/115	-
16	CLA	j	1302	8	-	6/13/91/115	-
16	CLA	y	510	-	-	6/37/115/115	-
19	BCR	H	4007	-	-	8/29/63/63	0/2/2/2
16	CLA	r	503	-	-	8/15/93/115	-
16	CLA	B	1211	-	1/1/15/20	15/37/115/115	-
19	BCR	x	602	-	-	17/29/63/63	0/2/2/2
16	CLA	X	506	-	1/1/14/20	12/31/109/115	-
16	CLA	X	514	-	1/1/12/20	2/19/97/115	-
16	CLA	j	1303	-	-	0/2/76/115	-
16	CLA	n	512	12	1/1/15/20	18/37/115/115	-
16	CLA	t	508	12	1/1/13/20	7/25/103/115	-
19	BCR	J	4013	-	-	9/29/63/63	0/2/2/2
19	BCR	K	4001	-	-	11/29/63/63	0/2/2/2
19	BCR	W	603	-	-	13/29/63/63	0/2/2/2
14	LMG	A	4101	-	-	24/41/61/70	0/1/1/1
16	CLA	n	516	-	-	6/15/93/115	-
16	CLA	G	1205	-	1/1/15/20	8/37/115/115	-
16	CLA	H	1122	-	-	7/30/108/115	-
16	CLA	g	503	-	-	8/15/93/115	-
16	CLA	X	511	-	1/1/15/20	10/37/115/115	-
16	CLA	q	505	-	1/1/15/20	12/37/115/115	-
16	CLA	p	507	12	-	7/37/115/115	-
19	BCR	o	603	-	-	9/29/63/63	0/2/2/2
16	CLA	a	1111	-	1/1/13/20	8/25/103/115	-
16	CLA	b	1223	-	1/1/15/20	9/37/115/115	-
16	CLA	u	503	-	-	7/15/93/115	-
16	CLA	g	515	-	1/1/15/20	8/37/115/115	-
16	CLA	a	1110	-	1/1/12/20	7/24/102/115	-
18	SF4	N	101	-	-	-	0/6/5/5
16	CLA	x	516	-	1/1/11/20	4/15/93/115	-
16	CLA	A	1138	-	1/1/15/20	10/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	b	4017	-	-	12/29/63/63	0/2/2/2
16	CLA	v	514	-	1/1/12/20	6/19/97/115	-
16	CLA	g	517	12	-	9/25/103/115	-
19	BCR	g	601	-	-	17/29/63/63	0/2/2/2
16	CLA	G	1214	-	1/1/13/20	11/25/103/115	-
16	CLA	a	1133	-	-	6/24/102/115	-
19	BCR	b	4010	-	-	15/29/63/63	0/2/2/2
16	CLA	b	1205	-	1/1/15/20	10/37/115/115	-
16	CLA	X	510	-	-	8/31/109/115	-
16	CLA	H	1125	-	-	10/37/115/115	-
16	CLA	a	1237	25	1/1/15/20	12/37/115/115	-
19	BCR	q	604	-	-	15/29/63/63	0/2/2/2
16	CLA	G	1212	-	1/1/11/20	7/13/91/115	-
16	CLA	H	1120	-	-	7/18/96/115	-
13	LHG	p	605	-	-	13/36/36/53	-
16	CLA	h	517	-	1/1/13/20	9/25/103/115	-
16	CLA	Z	505	-	1/1/15/20	12/37/115/115	-
16	CLA	b	1218	-	-	7/25/103/115	-
16	CLA	H	1110	-	1/1/12/20	7/24/102/115	-
16	CLA	r	510	-	-	11/37/115/115	-
20	LMT	l	4101	-	-	7/21/61/61	0/2/2/2
16	CLA	o	512	12	1/1/15/20	7/37/115/115	-
19	BCR	X	601	-	-	10/29/63/63	0/2/2/2
16	CLA	W	504	-	1/1/14/20	4/31/109/115	-
16	CLA	x	501	-	-	6/19/97/115	-
13	LHG	B	4018	16	-	17/42/42/53	-
17	PQN	G	2002	-	-	10/23/43/43	0/2/2/2
16	CLA	G	1236	-	-	5/19/97/115	-
16	CLA	X	517	12	-	5/25/103/115	-
19	BCR	r	601	-	-	15/29/63/63	0/2/2/2
16	CLA	G	1220	-	1/1/12/20	13/24/102/115	-
18	SF4	c	101	-	-	-	0/6/5/5
16	CLA	s	515	-	1/1/15/20	11/37/115/115	-
16	CLA	q	513	-	-	7/19/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	l	4019	-	-	12/29/63/63	0/2/2/2
21	ECH	G	4006	-	-	10/29/66/66	0/2/2/2
16	CLA	q	501	-	1/1/12/20	7/19/97/115	-
16	CLA	s	504	-	1/1/15/20	14/37/115/115	-
19	BCR	g	603	-	-	15/29/63/63	0/2/2/2
19	BCR	v	603	-	-	12/29/63/63	0/2/2/2
16	CLA	n	508	12	1/1/13/20	7/25/103/115	-
19	BCR	W	604	-	-	10/29/63/63	0/2/2/2
16	CLA	b	1012	25	1/1/13/20	10/25/103/115	-
14	LMG	A	4201	-	-	13/27/47/70	0/1/1/1
16	CLA	H	1103	-	1/1/15/20	12/37/115/115	-
16	CLA	b	1211	-	1/1/15/20	12/37/115/115	-
19	BCR	Q	4016	-	-	11/29/63/63	0/2/2/2
16	CLA	t	505	-	-	10/37/115/115	-
18	SF4	a	3001	-	-	-	0/6/5/5
16	CLA	Y	502	-	1/1/12/20	4/19/97/115	-
16	CLA	a	1129	-	-	2/15/93/115	-
19	BCR	f	4016	-	-	11/29/63/63	0/2/2/2
16	CLA	X	502	-	1/1/12/20	5/19/97/115	-
19	BCR	s	604	-	-	16/29/63/63	0/2/2/2
19	BCR	L	4022	-	-	14/29/63/63	0/2/2/2
19	BCR	o	602	-	-	14/29/63/63	0/2/2/2
16	CLA	n	517	12	1/1/13/20	9/25/103/115	-
16	CLA	B	1216	25	-	4/16/94/115	-
16	CLA	q	516	-	1/1/11/20	9/15/93/115	-
16	CLA	p	512	12	1/1/15/20	9/37/115/115	-
16	CLA	r	501	-	1/1/12/20	4/19/97/115	-
16	CLA	Y	514	-	1/1/12/20	6/19/97/115	-
16	CLA	l	1503	-	1/1/15/20	12/37/115/115	-
18	SF4	C	101	-	-	-	0/6/5/5
16	CLA	B	1240	13	1/1/11/20	5/15/93/115	-
16	CLA	G	1229	-	1/1/13/20	9/29/107/115	-
16	CLA	G	1232	25	1/1/11/20	5/13/91/115	-
16	CLA	x	517	12	-	7/25/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	h	508	-	1/1/13/20	10/25/103/115	-
16	CLA	B	1230	-	1/1/11/20	6/13/91/115	-
16	CLA	g	512	12	1/1/15/20	8/37/115/115	-
16	CLA	J	1302	8	1/1/11/20	4/13/91/115	-
16	CLA	s	503	-	1/1/11/20	8/15/93/115	-
16	CLA	B	1222	25	-	6/19/97/115	-
19	BCR	H	4008	-	-	13/29/63/63	0/2/2/2
16	CLA	Q	1302	6	1/1/11/20	4/15/93/115	-
16	CLA	X	513	-	-	7/15/93/115	-
18	SF4	c	102	-	-	-	0/6/5/5
16	CLA	n	502	-	1/1/12/20	5/19/97/115	-
16	CLA	h	512	12	-	16/37/115/115	-
19	BCR	j	4015	-	-	14/29/63/63	0/2/2/2
16	CLA	a	1121	-	1/1/12/20	5/21/99/115	-
16	CLA	a	1128	-	1/1/15/20	17/37/115/115	-
16	CLA	b	1023	-	-	10/37/115/115	-
16	CLA	w	502	-	1/1/12/20	6/19/97/115	-
14	LMG	A	852	-	-	10/33/53/70	0/1/1/1
16	CLA	q	503	-	1/1/11/20	8/15/93/115	-
16	CLA	s	510	-	-	8/37/115/115	-
16	CLA	H	1137	-	1/1/11/20	4/16/94/115	-
16	CLA	G	1228	-	1/1/13/20	13/25/103/115	-
16	CLA	y	517	-	1/1/13/20	13/25/103/115	-
16	CLA	A	1140	-	1/1/15/20	11/37/115/115	-
16	CLA	g	514	-	1/1/12/20	6/19/97/115	-
19	BCR	a	4007	-	-	7/29/63/63	0/2/2/2
19	BCR	a	4011	-	-	16/29/63/63	0/2/2/2
16	CLA	a	1117	-	1/1/15/20	9/37/115/115	-
16	CLA	b	1240	13	1/1/11/20	4/15/93/115	-
16	CLA	W	506	-	-	9/31/109/115	-
16	CLA	B	1215	-	1/1/14/20	6/31/109/115	-
16	CLA	a	1105	-	1/1/13/20	7/29/107/115	-
19	BCR	S	4013	-	-	10/29/63/63	0/2/2/2
19	BCR	a	4003	-	-	12/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	f	1302	6	1/1/11/20	7/15/93/115	-
16	CLA	B	1225	-	-	11/37/115/115	-
19	BCR	w	604	-	-	17/29/63/63	0/2/2/2
16	CLA	a	1120	-	-	7/18/96/115	-
16	CLA	h	514	-	-	6/19/97/115	-
16	CLA	W	511	-	1/1/15/20	8/37/115/115	-
16	CLA	v	502	-	1/1/12/20	5/19/97/115	-
19	BCR	Y	603	-	-	8/29/63/63	0/2/2/2
16	CLA	H	1116	-	1/1/12/20	8/24/102/115	-
16	CLA	y	502	-	1/1/12/20	4/19/97/115	-
16	CLA	B	1206	2	1/1/15/20	17/37/115/115	-
19	BCR	x	603	-	-	14/29/63/63	0/2/2/2
16	CLA	b	1204	-	1/1/15/20	11/37/115/115	-
16	CLA	q	509	-	1/1/15/20	11/37/115/115	-
16	CLA	B	1238	25	1/1/15/20	7/37/115/115	-
16	CLA	H	1102	16	1/1/13/20	5/27/105/115	-
16	CLA	H	1136	-	1/1/15/20	8/37/115/115	-
16	CLA	A	1137	-	1/1/11/20	5/16/94/115	-
16	CLA	H	1801	13	1/1/11/20	4/15/93/115	-
16	CLA	u	510	-	-	8/31/109/115	-
16	CLA	h	509	-	1/1/15/20	16/37/115/115	-
16	CLA	G	1211	-	-	20/37/115/115	-
16	CLA	A	1022	25	1/1/15/20	10/37/115/115	-
16	CLA	p	508	12	1/1/13/20	8/25/103/115	-
16	CLA	A	1125	-	-	10/37/115/115	-
16	CLA	n	515	-	1/1/15/20	14/37/115/115	-
16	CLA	G	1021	-	1/1/15/20	13/37/115/115	-
16	CLA	a	1130	-	-	9/31/109/115	-
16	CLA	v	515	-	1/1/15/20	16/37/115/115	-
16	CLA	w	508	12	1/1/13/20	6/25/103/115	-
13	LHG	G	4018	16	-	12/42/42/53	-
19	BCR	X	604	-	-	19/29/63/63	0/2/2/2
19	BCR	v	604	-	-	12/29/63/63	0/2/2/2
16	CLA	A	1139	25	1/1/14/20	14/31/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	b	1206	2	1/1/15/20	15/37/115/115	-
16	CLA	y	515	-	1/1/15/20	15/37/115/115	-
16	CLA	B	1205	-	1/1/15/20	8/37/115/115	-
16	CLA	Z	517	12	1/1/13/20	4/25/103/115	-
16	CLA	u	507	12	1/1/15/20	10/37/115/115	-
16	CLA	G	1204	-	1/1/15/20	7/37/115/115	-
16	CLA	w	504	-	1/1/15/20	11/37/115/115	-
16	CLA	H	1134	1	-	2/13/91/115	-
16	CLA	x	512	12	-	7/37/115/115	-
16	CLA	a	1118	-	-	9/25/103/115	-
16	CLA	v	505	-	-	11/37/115/115	-
18	SF4	N	102	-	-	-	0/6/5/5
19	BCR	H	4003	-	-	10/29/63/63	0/2/2/2
16	CLA	s	501	-	1/1/12/20	7/19/97/115	-
16	CLA	b	1209	-	1/1/11/20	3/13/91/115	-
16	CLA	t	515	-	1/1/15/20	13/37/115/115	-
16	CLA	o	501	-	-	7/15/93/115	-
19	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
19	BCR	u	603	-	-	9/29/63/63	0/2/2/2
16	CLA	n	504	-	-	4/31/109/115	-
19	BCR	p	602	-	-	11/29/63/63	0/2/2/2
16	CLA	H	1109	16	1/1/15/20	9/37/115/115	-
17	PQN	H	2001	-	-	3/23/43/43	0/2/2/2
16	CLA	h	515	-	1/1/15/20	17/37/115/115	-
16	CLA	H	1117	-	1/1/15/20	8/37/115/115	-
16	CLA	Z	502	-	1/1/12/20	5/19/97/115	-
16	CLA	a	1139	25	1/1/13/20	4/25/103/115	-
16	CLA	A	1116	-	1/1/12/20	10/24/102/115	-
16	CLA	p	515	-	1/1/15/20	13/37/115/115	-
19	BCR	s	602	-	-	11/29/63/63	0/2/2/2
16	CLA	G	1238	25	1/1/15/20	9/37/115/115	-
16	CLA	B	1202	-	1/1/15/20	16/37/115/115	-
19	BCR	n	604	-	-	13/29/63/63	0/2/2/2
17	PQN	B	2002	-	-	9/23/43/43	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	w	516	-	1/1/11/20	8/15/93/115	-
19	BCR	S	4012	-	-	10/29/63/63	0/2/2/2
16	CLA	X	501	-	-	7/15/93/115	-
24	LUT	q	601	-	-	7/29/67/67	0/2/2/2
16	CLA	G	1240	13	1/1/11/20	4/15/93/115	-
16	CLA	u	506	-	1/1/14/20	11/31/109/115	-
19	BCR	K	4005	-	-	9/29/63/63	0/2/2/2
16	CLA	Y	513	-	-	8/15/93/115	-
16	CLA	o	516	-	-	9/15/93/115	-
16	CLA	w	517	12	1/1/13/20	6/25/103/115	-
16	CLA	Z	501	-	1/1/12/20	7/19/97/115	-
16	CLA	Y	503	-	1/1/11/20	5/15/93/115	-
16	CLA	Y	511	-	1/1/15/20	13/37/115/115	-
16	CLA	G	1239	-	1/1/15/20	14/37/115/115	-
16	CLA	Z	513	-	-	7/19/97/115	-
16	CLA	H	1121	-	1/1/12/20	7/21/99/115	-
16	CLA	r	506	-	-	10/31/109/115	-
16	CLA	y	509	-	1/1/15/20	19/37/115/115	-
16	CLA	o	507	12	-	11/37/115/115	-
16	CLA	s	514	-	1/1/12/20	6/19/97/115	-
16	CLA	a	1127	-	1/1/15/20	3/37/115/115	-
16	CLA	b	1236	-	-	7/19/97/115	-
19	BCR	s	601	-	-	12/29/63/63	0/2/2/2
16	CLA	L	1503	25	1/1/15/20	11/37/115/115	-
19	BCR	a	4002	-	-	12/29/63/63	0/2/2/2
16	CLA	S	1302	8	1/1/11/20	5/13/91/115	-
16	CLA	X	516	-	-	6/15/93/115	-
16	CLA	r	511	-	1/1/15/20	6/37/115/115	-
16	CLA	n	510	-	-	14/37/115/115	-
16	CLA	u	504	-	-	17/31/109/115	-
16	CLA	v	507	12	-	8/37/115/115	-
16	CLA	A	1108	-	-	2/13/91/115	-
16	CLA	B	1228	-	-	13/25/103/115	-
16	CLA	p	501	-	1/1/12/20	5/19/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	J	4015	-	-	7/29/63/63	0/2/2/2
16	CLA	b	1214	-	1/1/13/20	5/25/103/115	-
16	CLA	g	504	-	1/1/15/20	20/37/115/115	-
16	CLA	v	504	-	1/1/14/20	13/31/109/115	-
16	CLA	x	502	-	1/1/12/20	4/19/97/115	-
16	CLA	H	1118	-	-	11/25/103/115	-
16	CLA	x	508	12	1/1/13/20	10/25/103/115	-
16	CLA	b	1239	-	-	13/37/115/115	-
16	CLA	H	1105	-	1/1/13/20	8/29/107/115	-
16	CLA	B	1232	-	1/1/11/20	6/13/91/115	-
16	CLA	h	513	-	1/1/11/20	6/15/93/115	-
16	CLA	Y	507	12	-	8/37/115/115	-
19	BCR	F	4016	-	-	9/29/63/63	0/2/2/2
16	CLA	B	1021	-	1/1/15/20	12/37/115/115	-
16	CLA	r	502	-	1/1/12/20	5/19/97/115	-
16	CLA	u	505	-	1/1/15/20	12/37/115/115	-
16	CLA	a	1119	-	1/1/15/20	7/37/115/115	-
16	CLA	H	1114	-	1/1/11/20	7/15/93/115	-
16	CLA	x	505	-	1/1/15/20	8/37/115/115	-
16	CLA	y	516	-	1/1/11/20	6/15/93/115	-
19	BCR	g	602	-	-	14/29/63/63	0/2/2/2

The worst 5 of 1993 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	u	506	CLA	CHB-C4A	6.36	1.39	1.33
16	o	514	CLA	CHB-C4A	6.33	1.38	1.33
16	v	507	CLA	CHB-C4A	6.29	1.38	1.33
15	A	1011	CL0	CHB-C4A	6.25	1.38	1.33
16	b	1216	CLA	CHB-C4A	6.24	1.38	1.33

The worst 5 of 3103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	u	506	CLA	C4A-NA-C1A	8.41	110.52	106.68
21	i	4020	ECH	C8-C9-C10	6.94	129.93	119.01
16	x	505	CLA	C4A-NA-C1A	6.63	109.70	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	v	505	CLA	C4A-NA-C1A	6.60	109.69	106.68
16	b	1216	CLA	C4A-NA-C1A	6.57	109.68	106.68

5 of 405 chirality outliers are listed below:

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

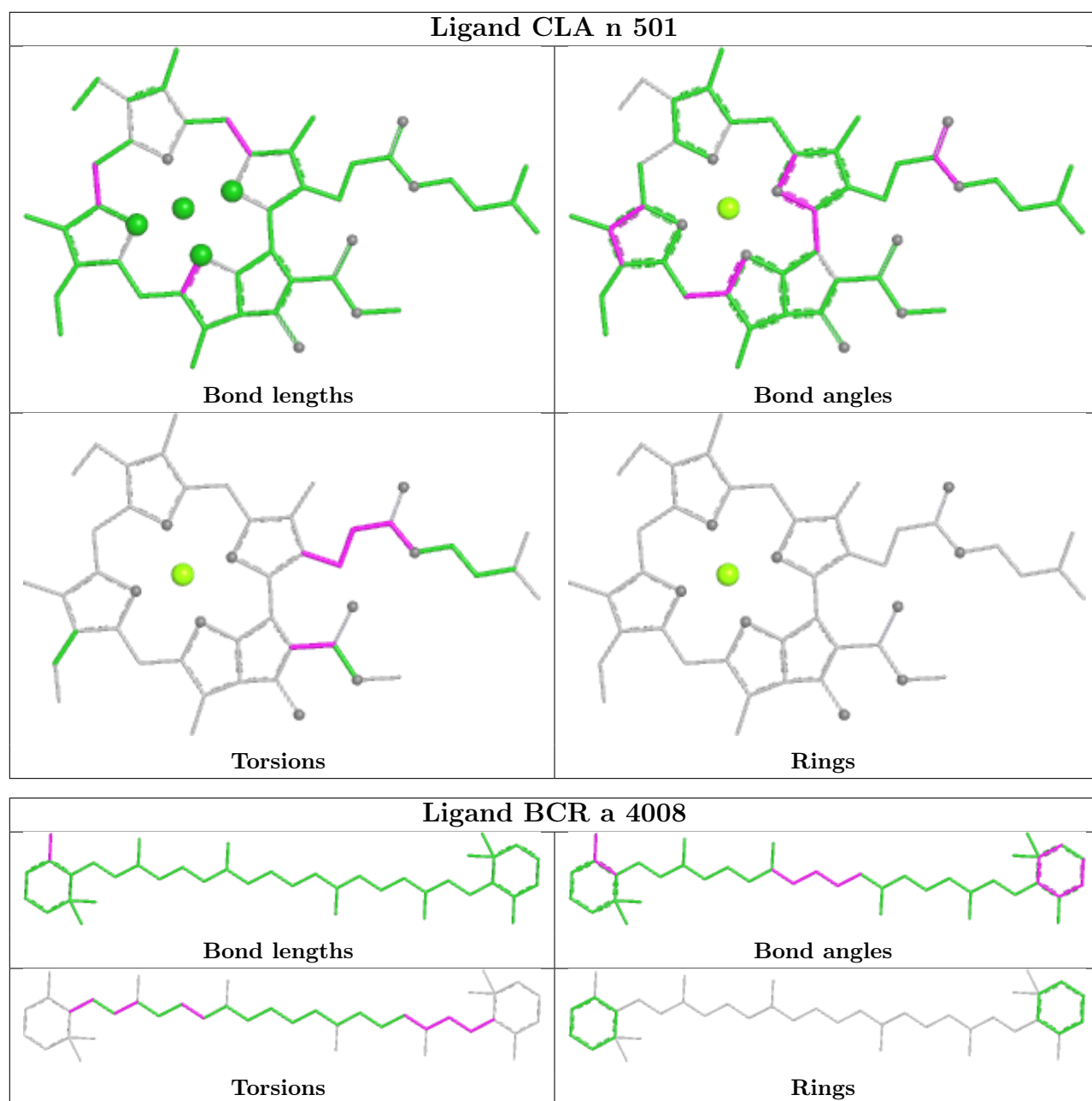
5 of 7417 torsion outliers are listed below:

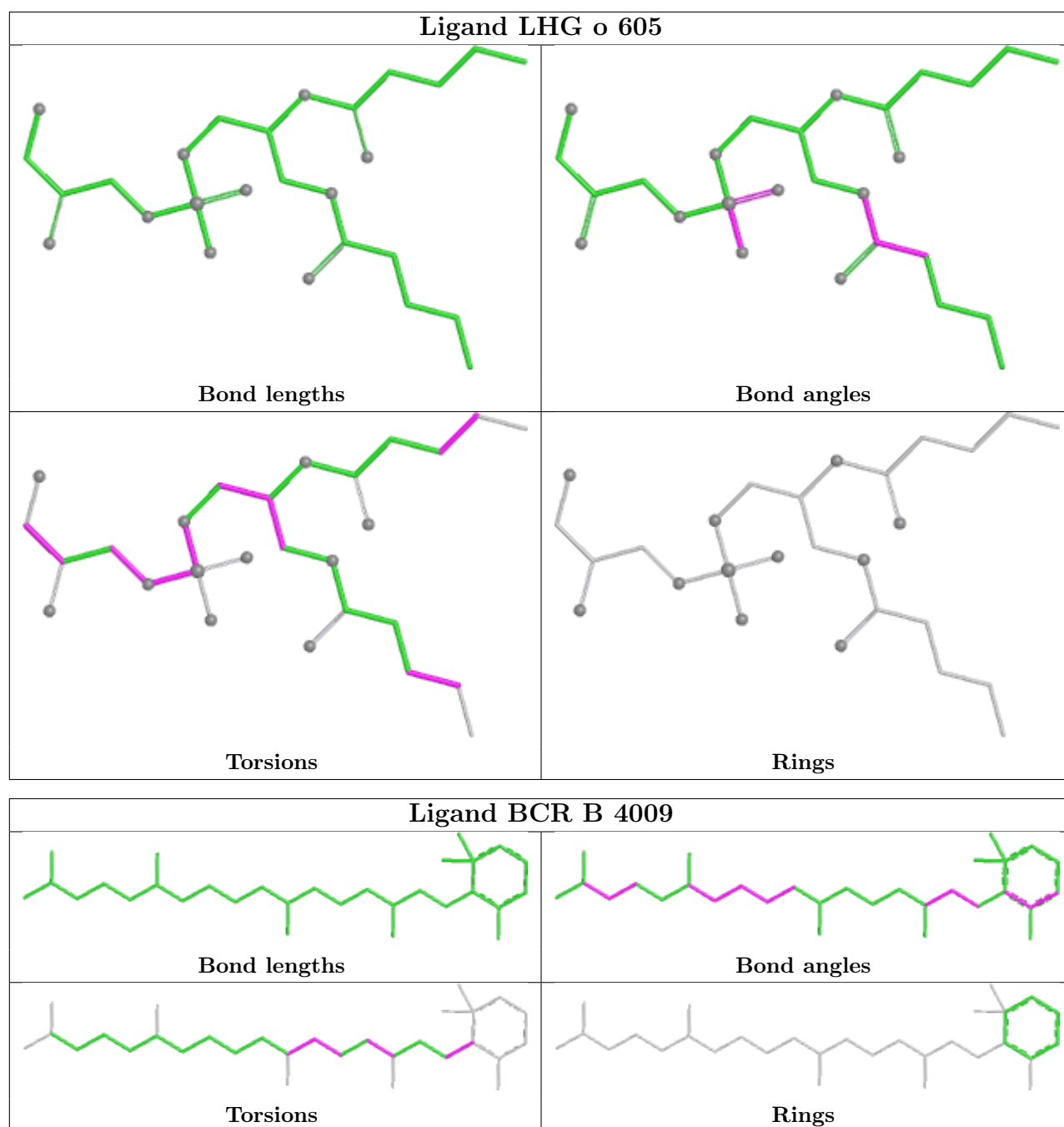
Mol	Chain	Res	Type	Atoms
13	A	849	LHG	O1-C1-C2-O2
13	A	849	LHG	O1-C1-C2-C3
13	A	849	LHG	C3-O3-P-O5
13	A	851	LHG	C3-O3-P-O5
13	B	4018	LHG	O1-C1-C2-O2

There are no ring outliers.

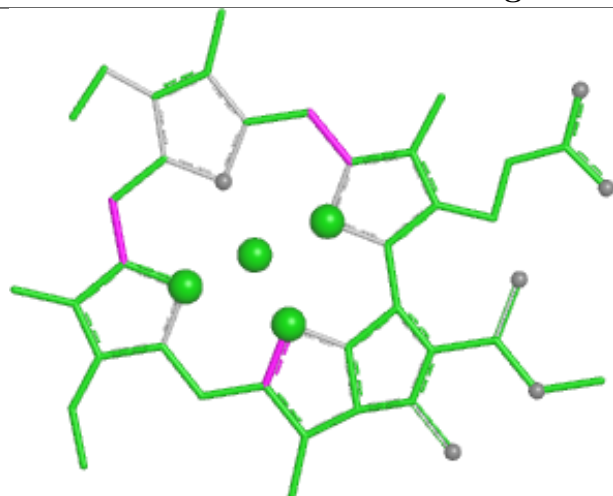
No monomer is involved in short contacts.

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

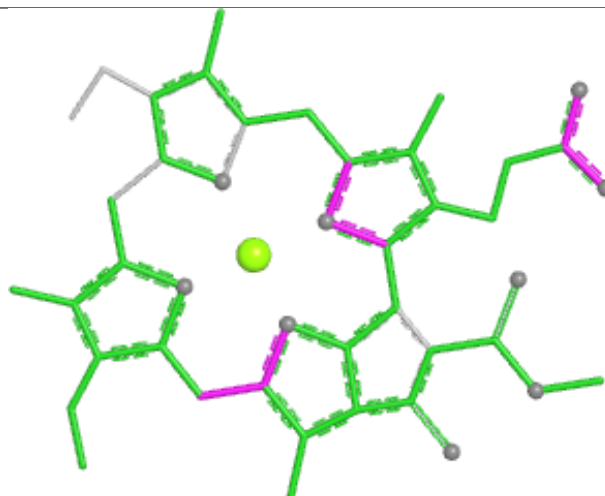




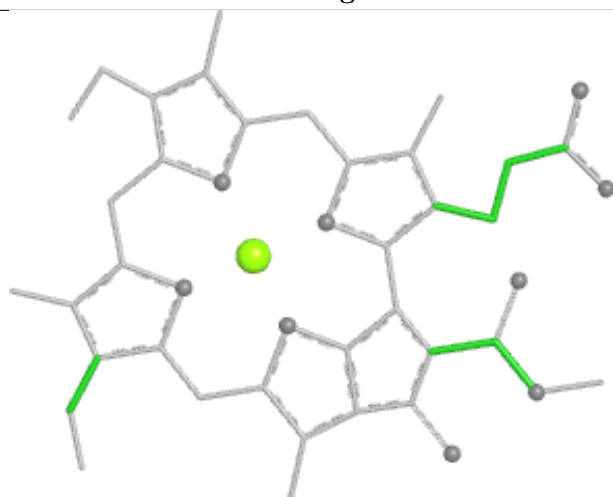
Ligand CLA H 1113



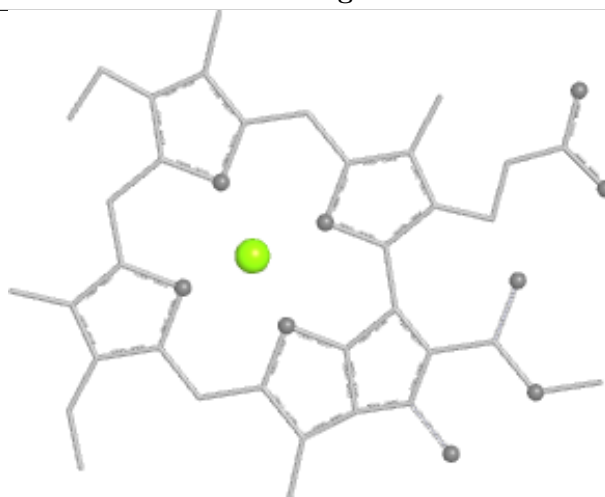
Bond lengths



Bond angles

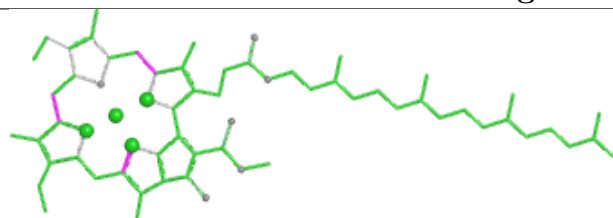


Torsions

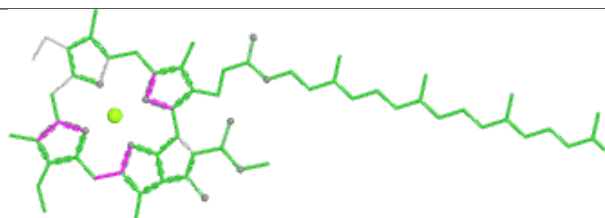


Rings

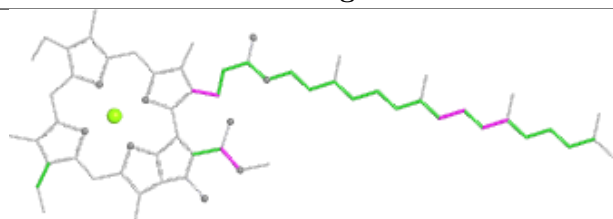
Ligand CLA u 511



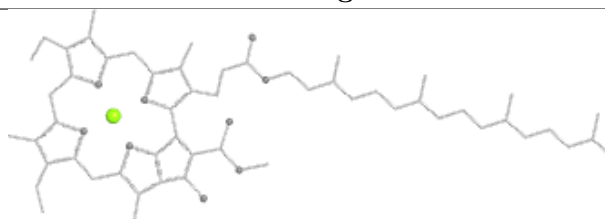
Bond lengths



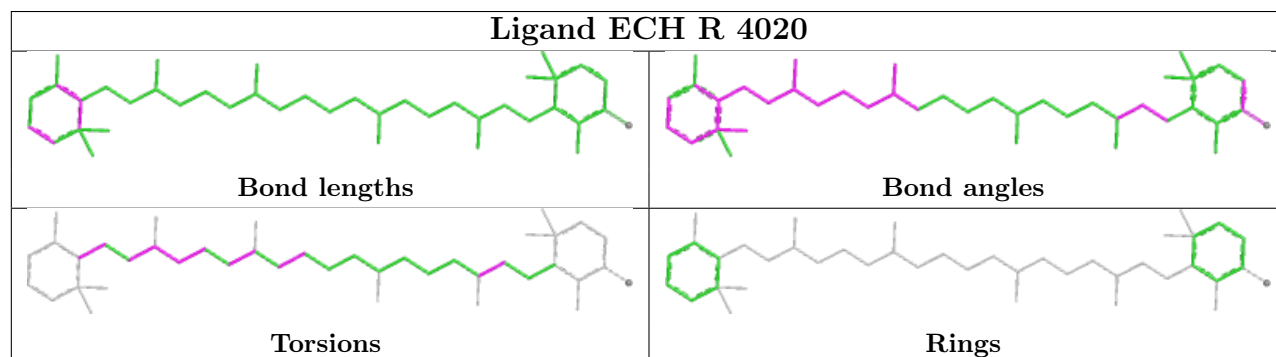
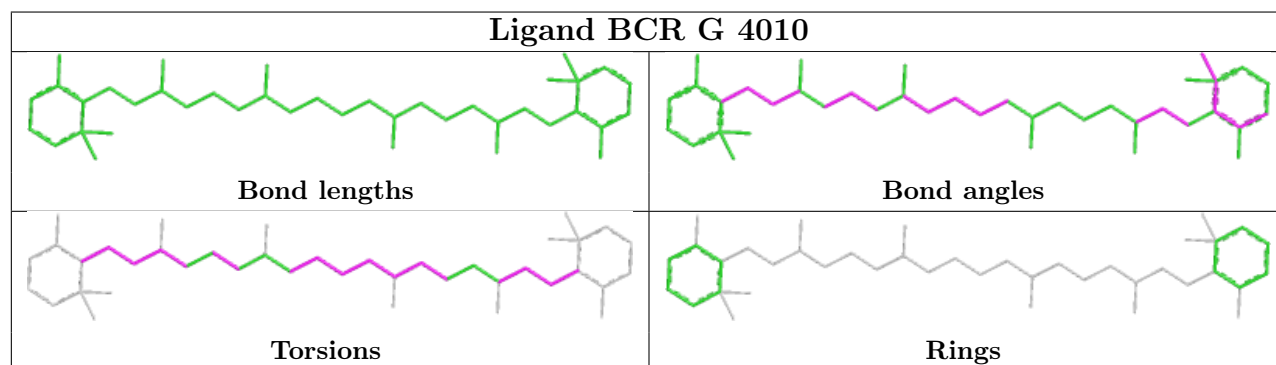
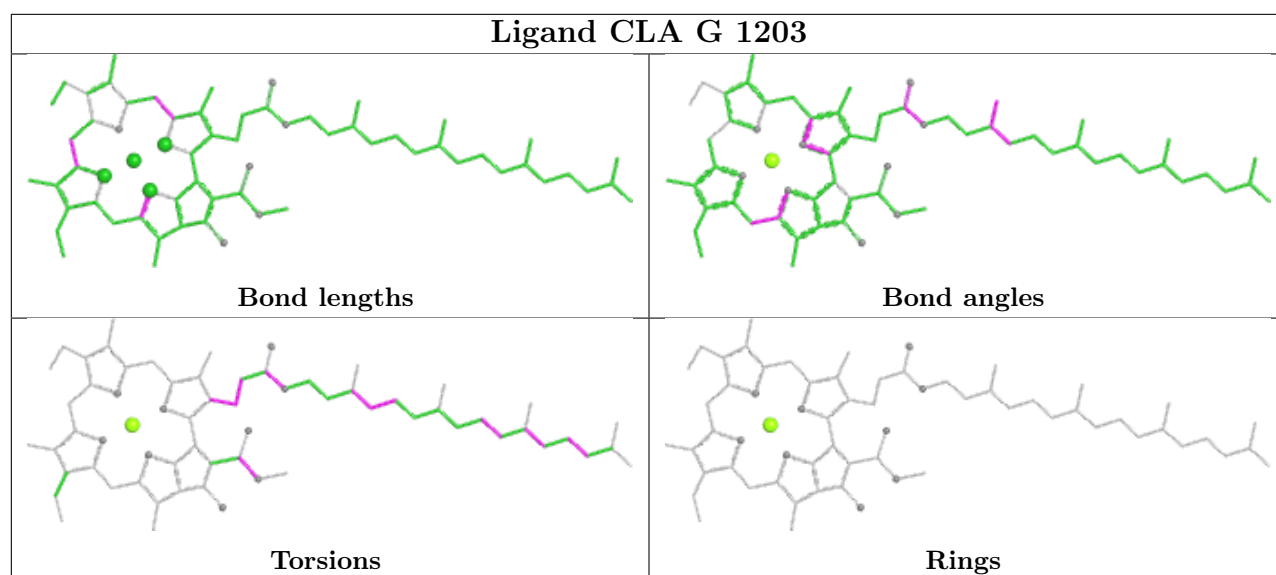
Bond angles

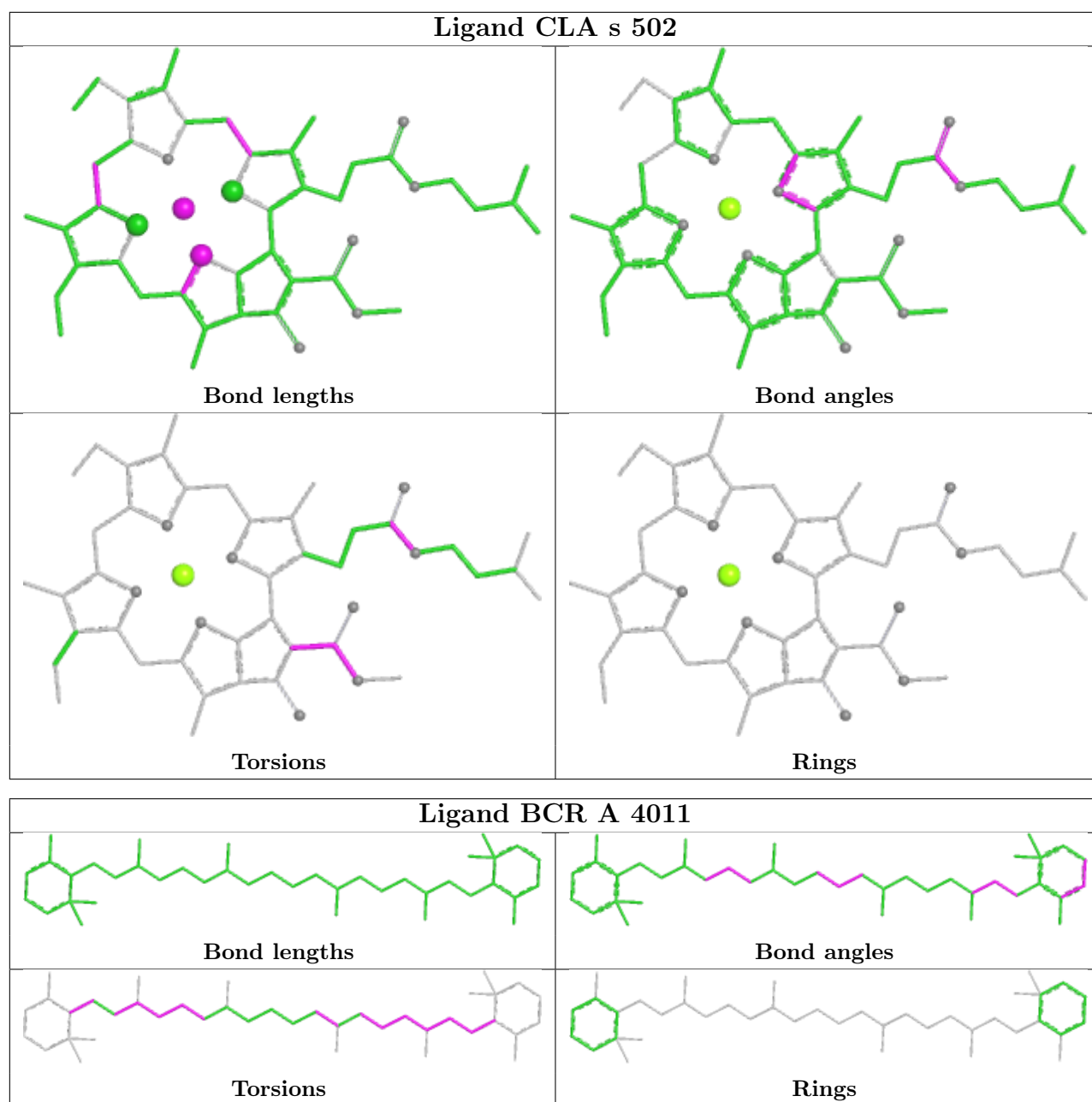


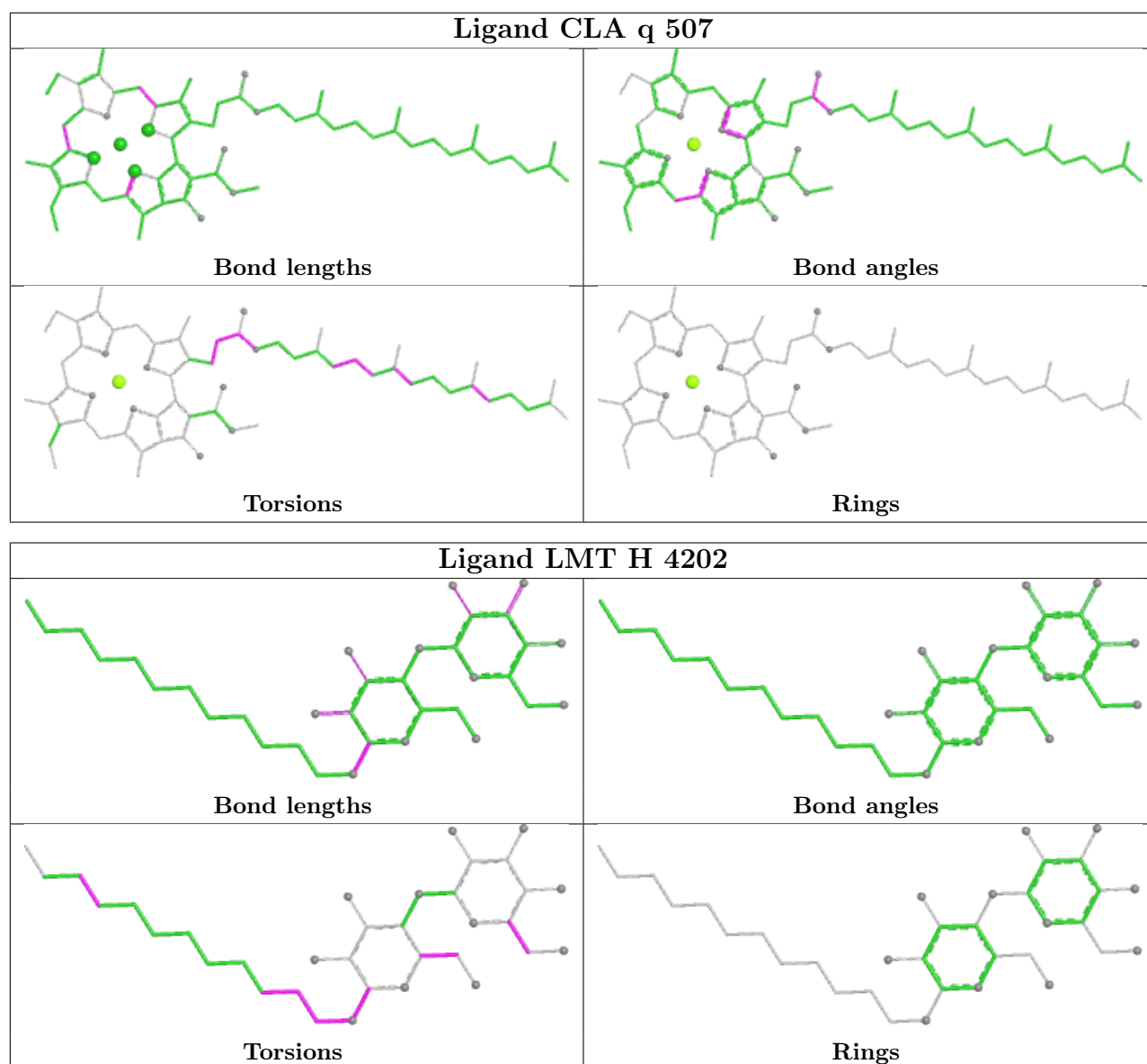
Torsions



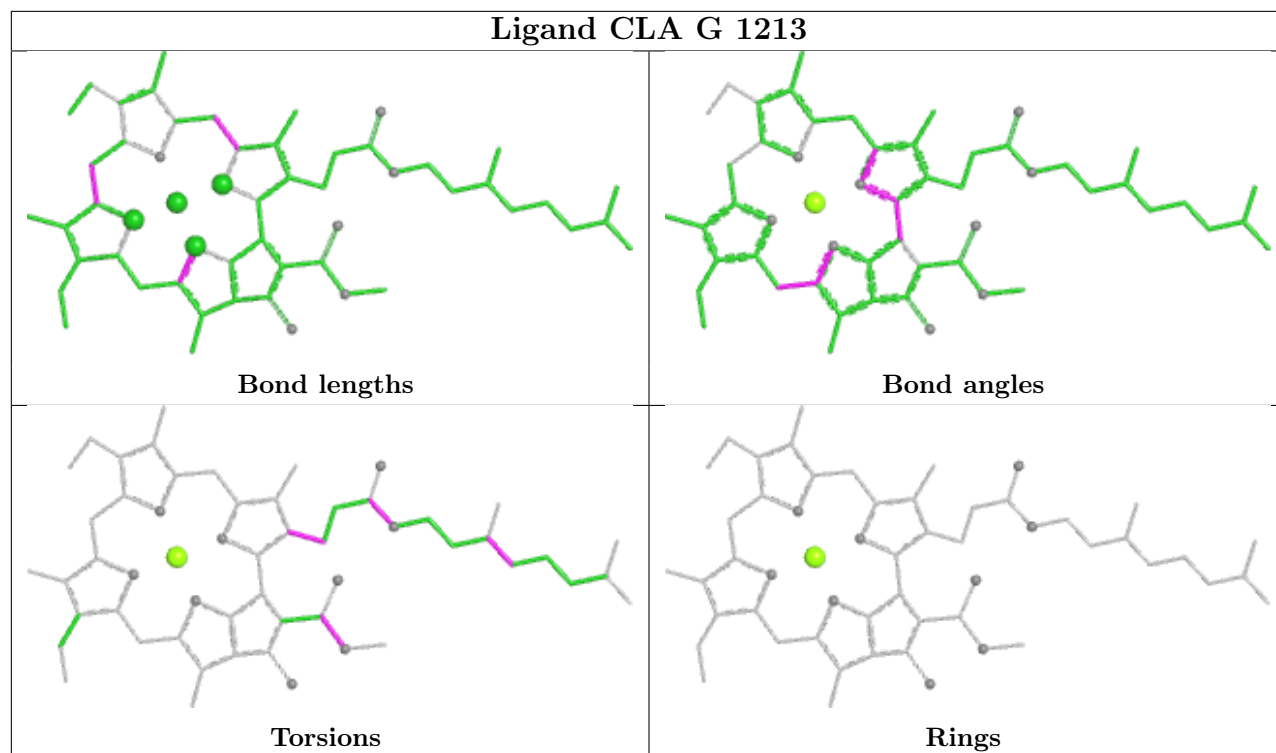
Rings



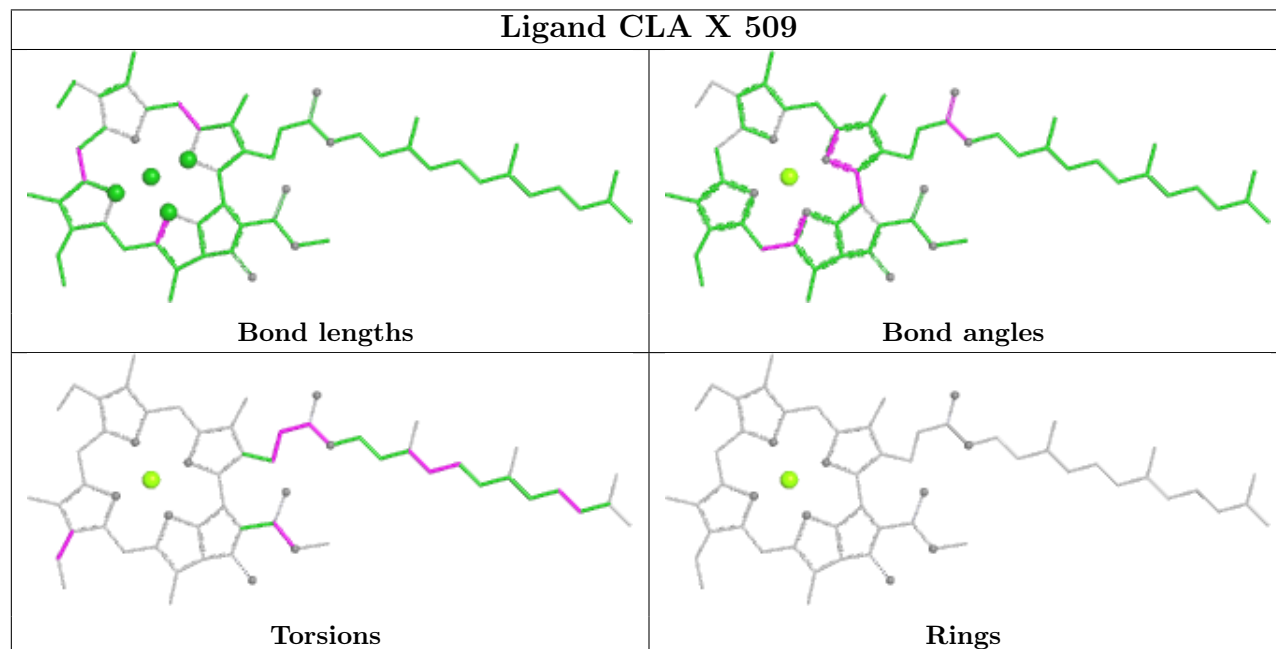


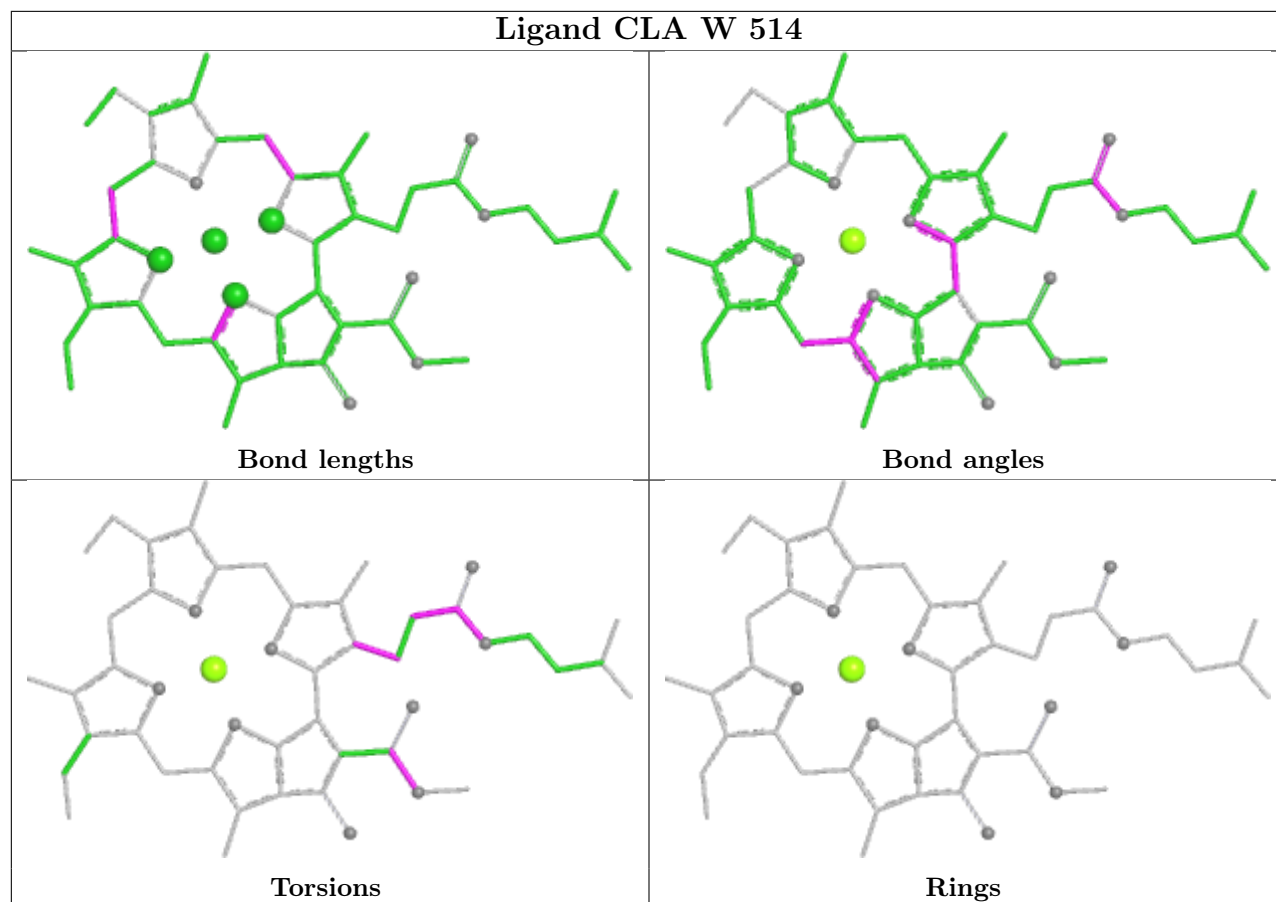


Ligand CLA G 1213

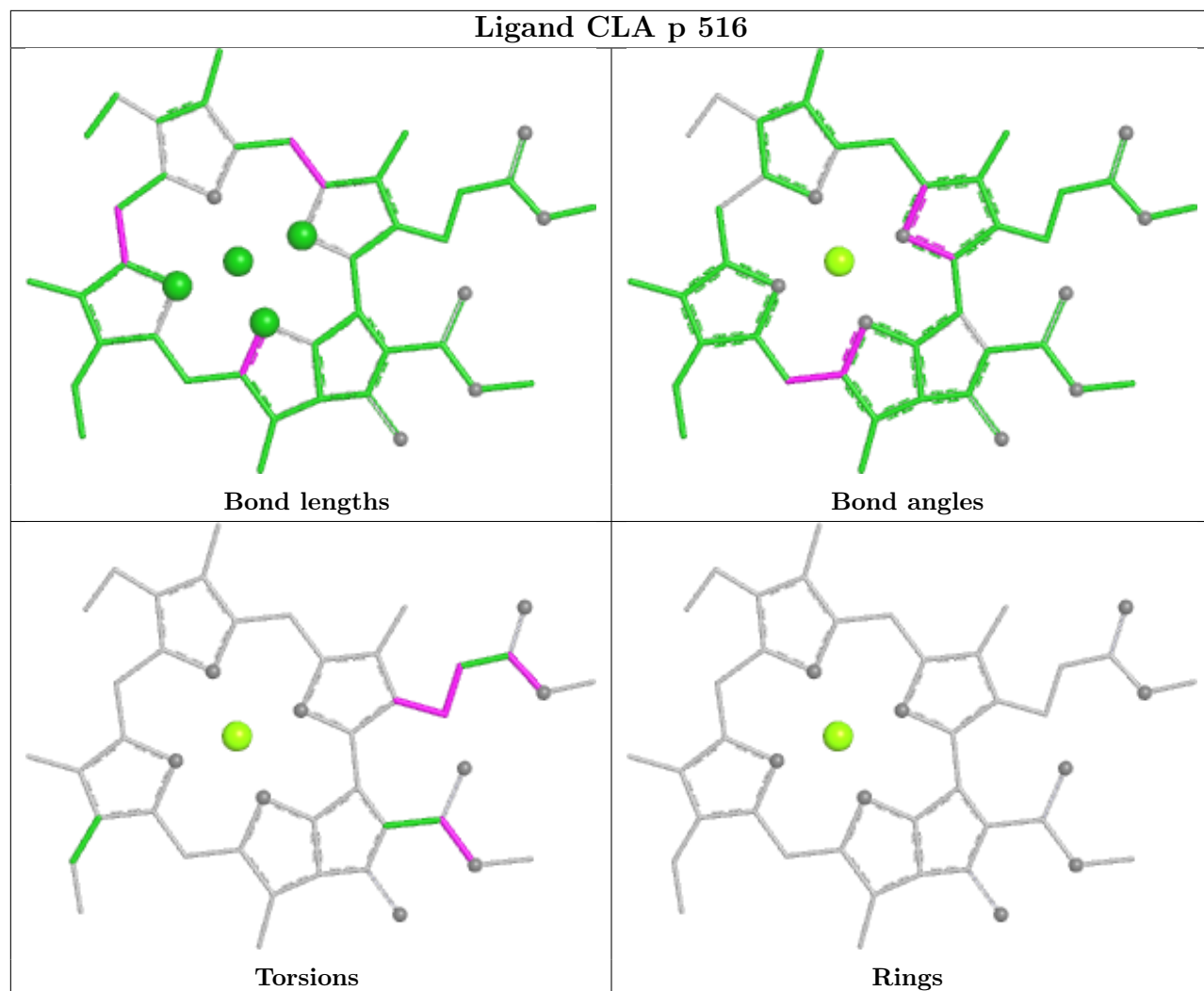


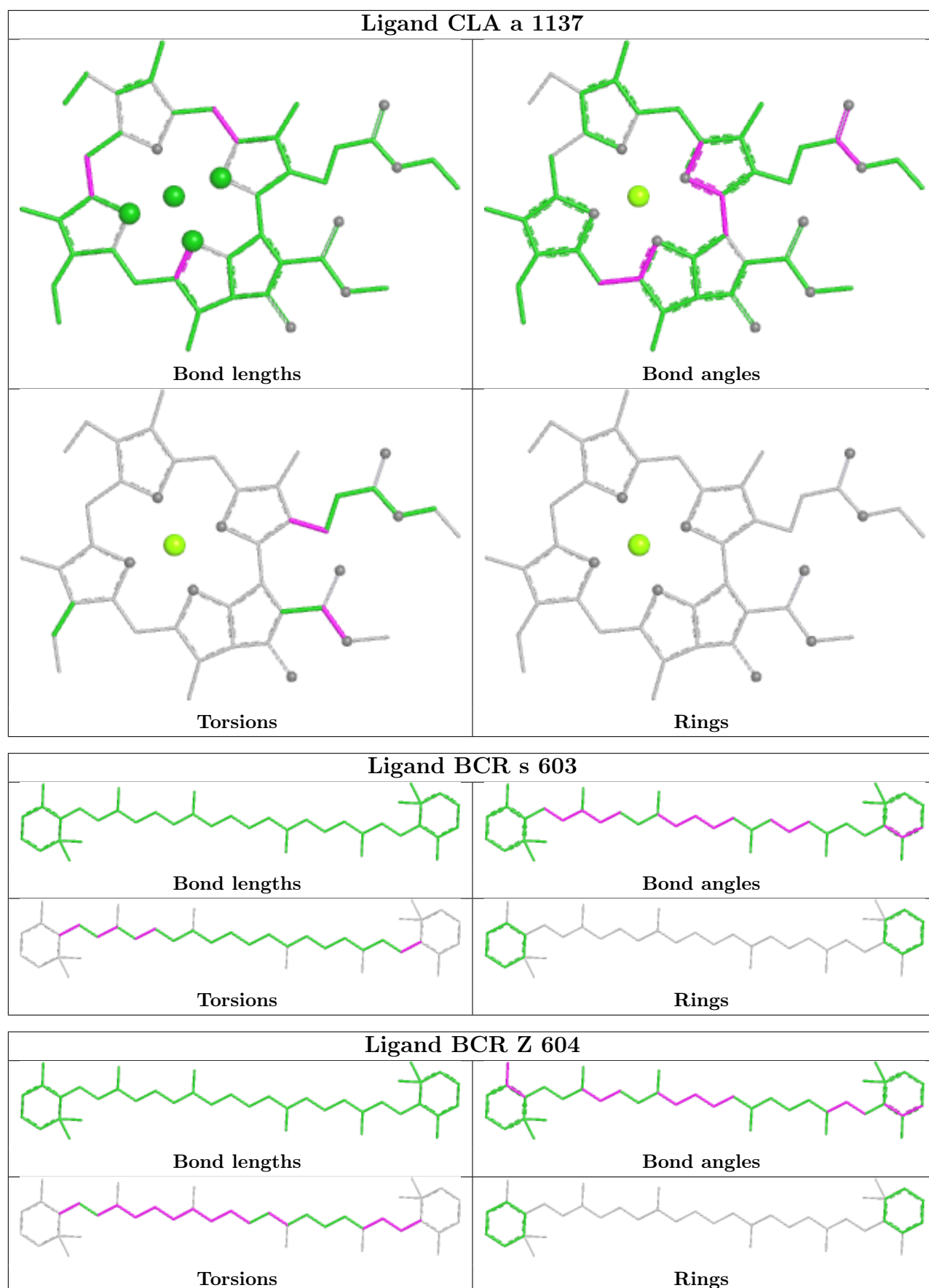
Ligand CLA X 509

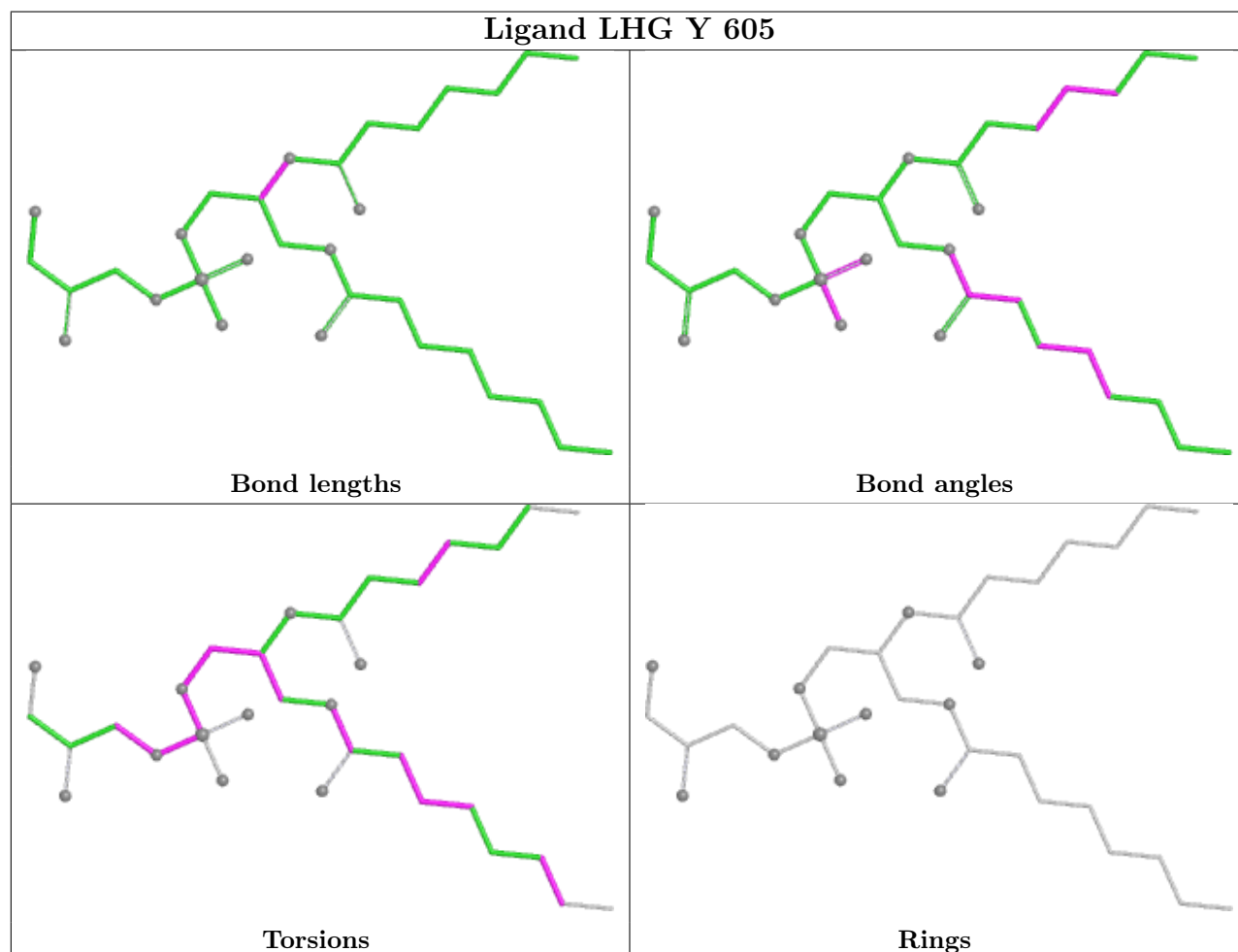
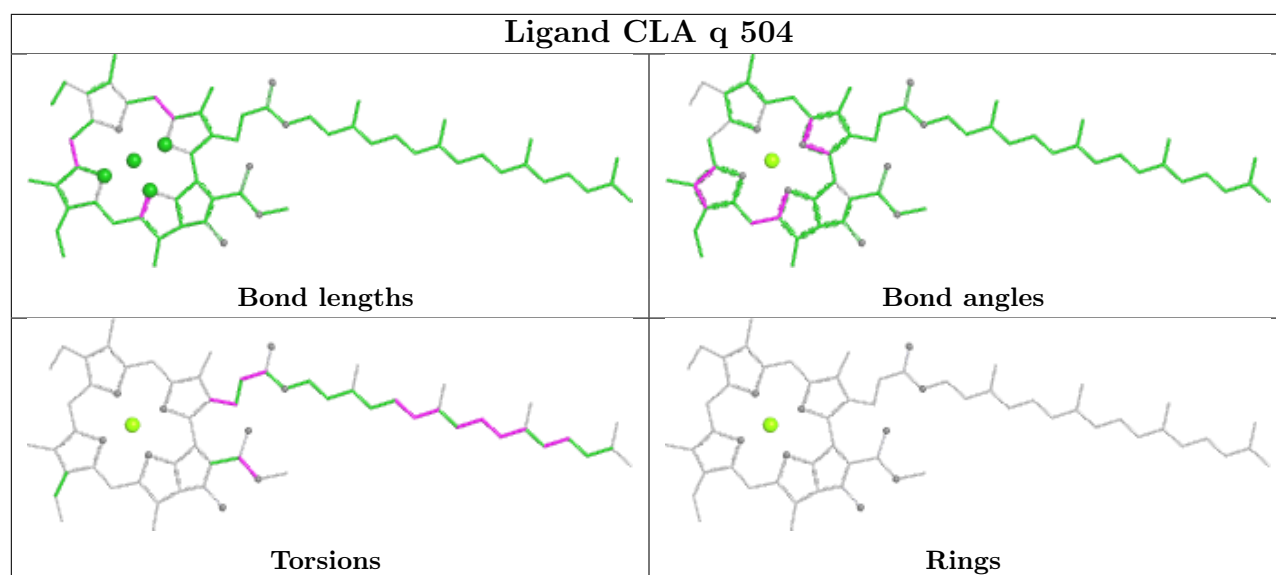


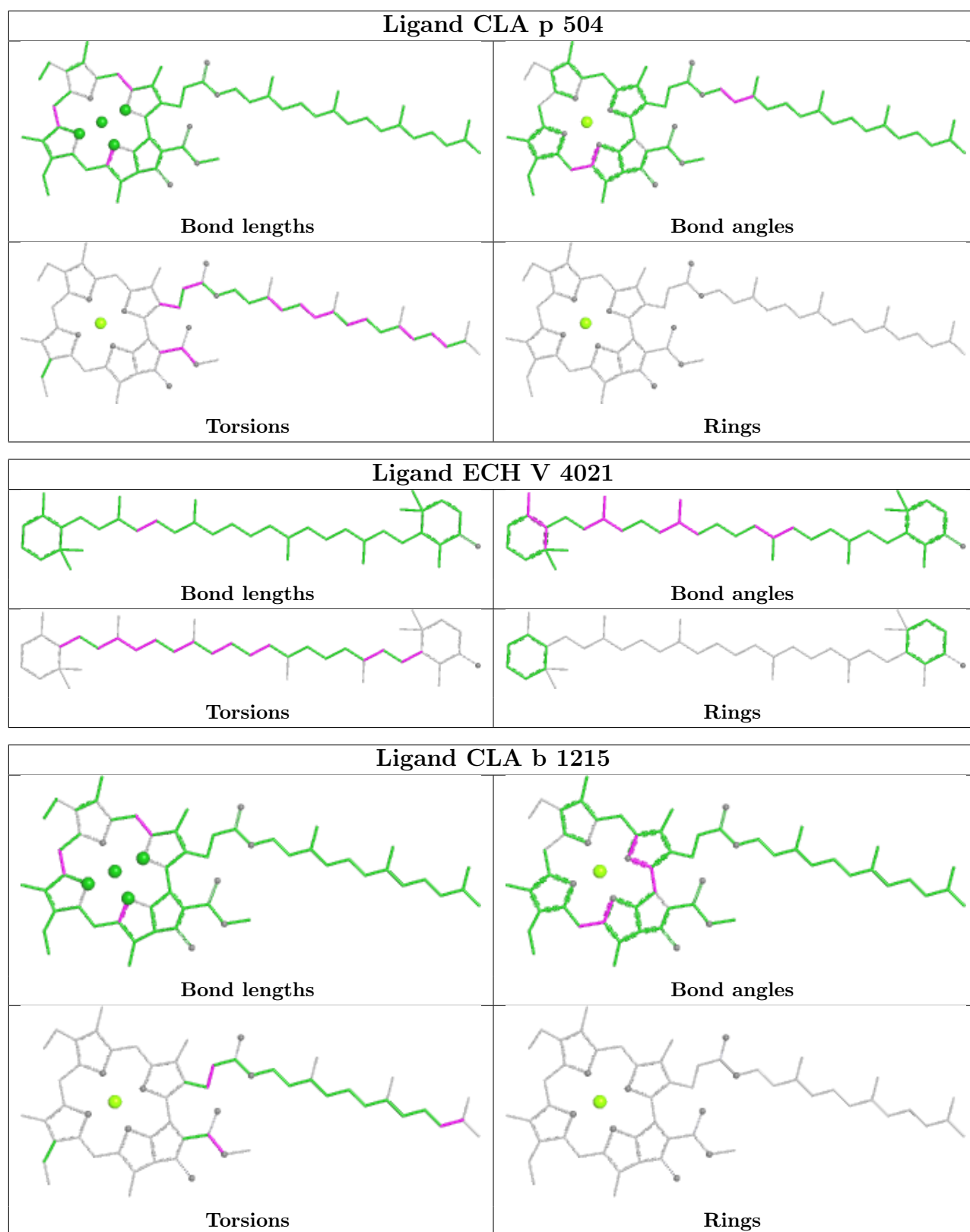


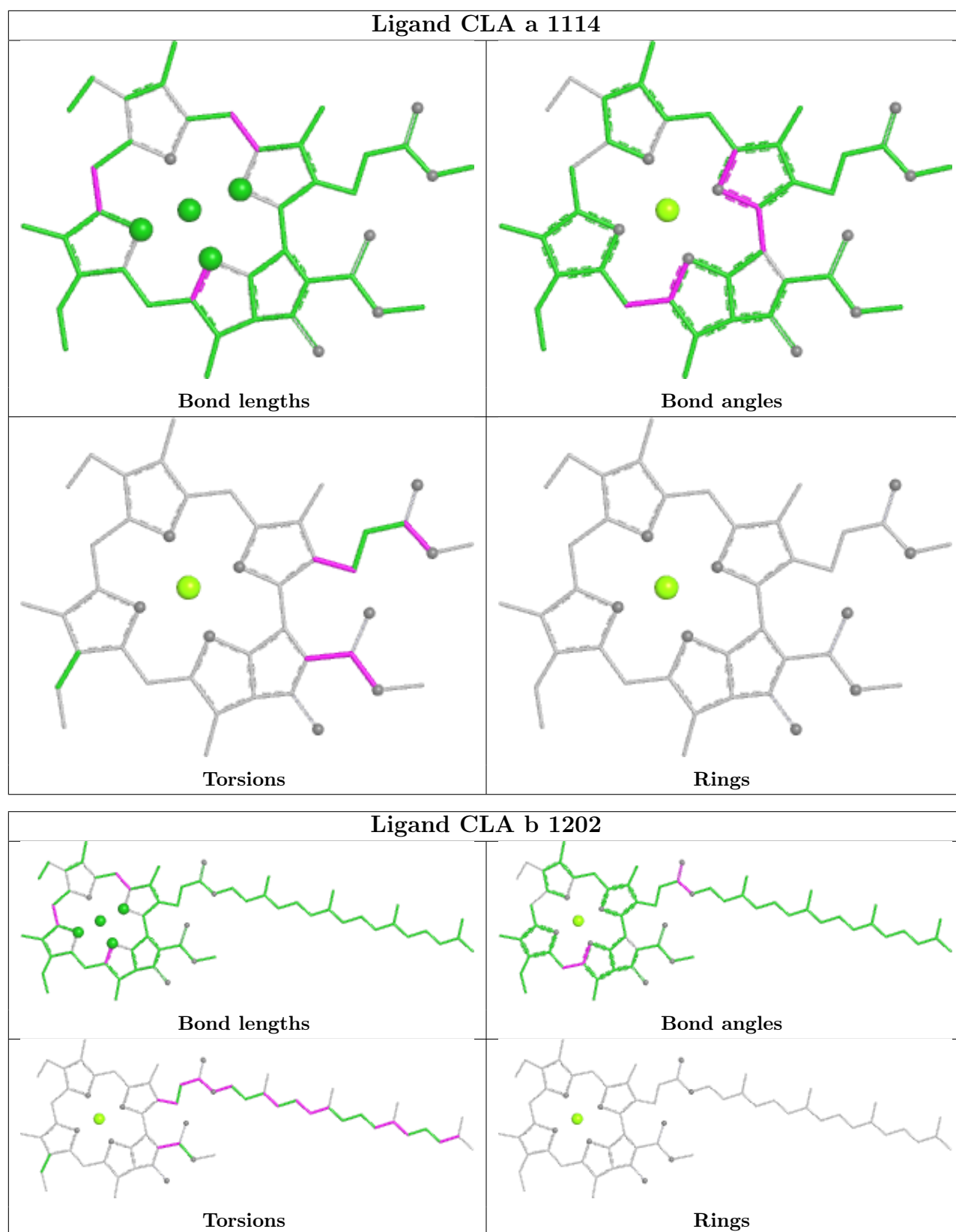
Ligand CLA p 516

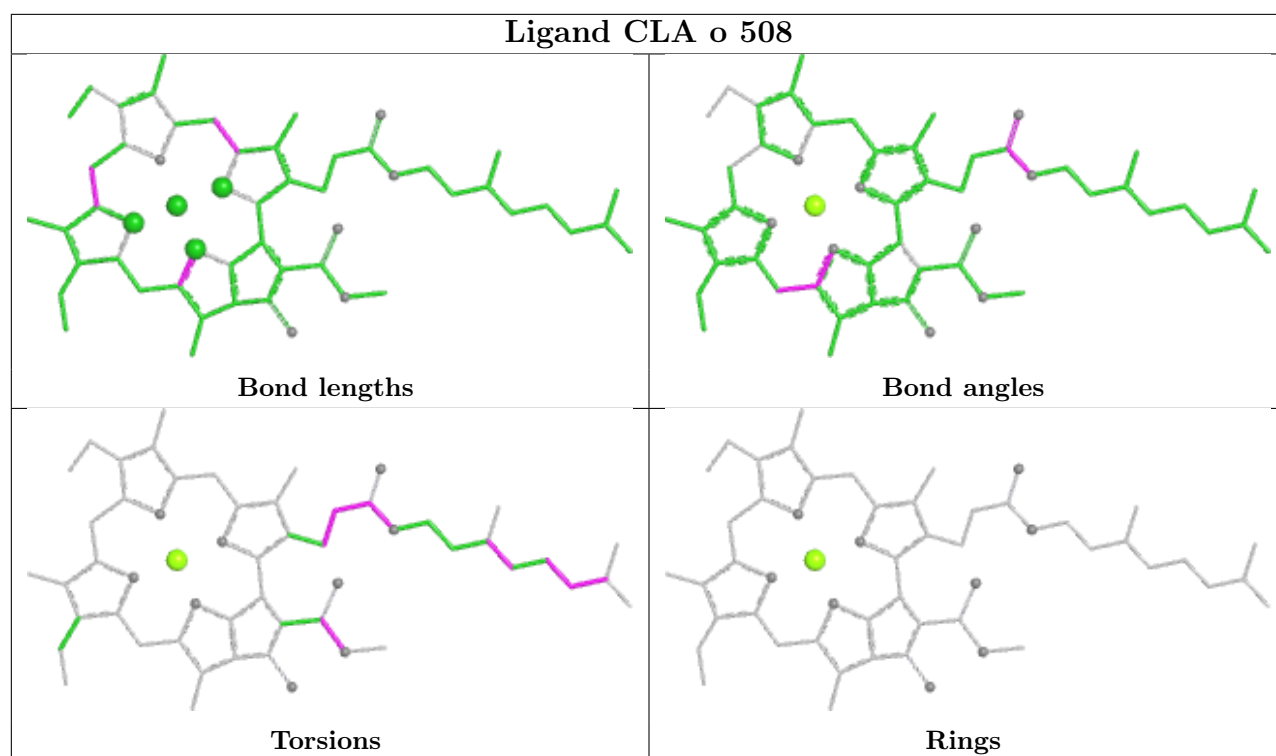




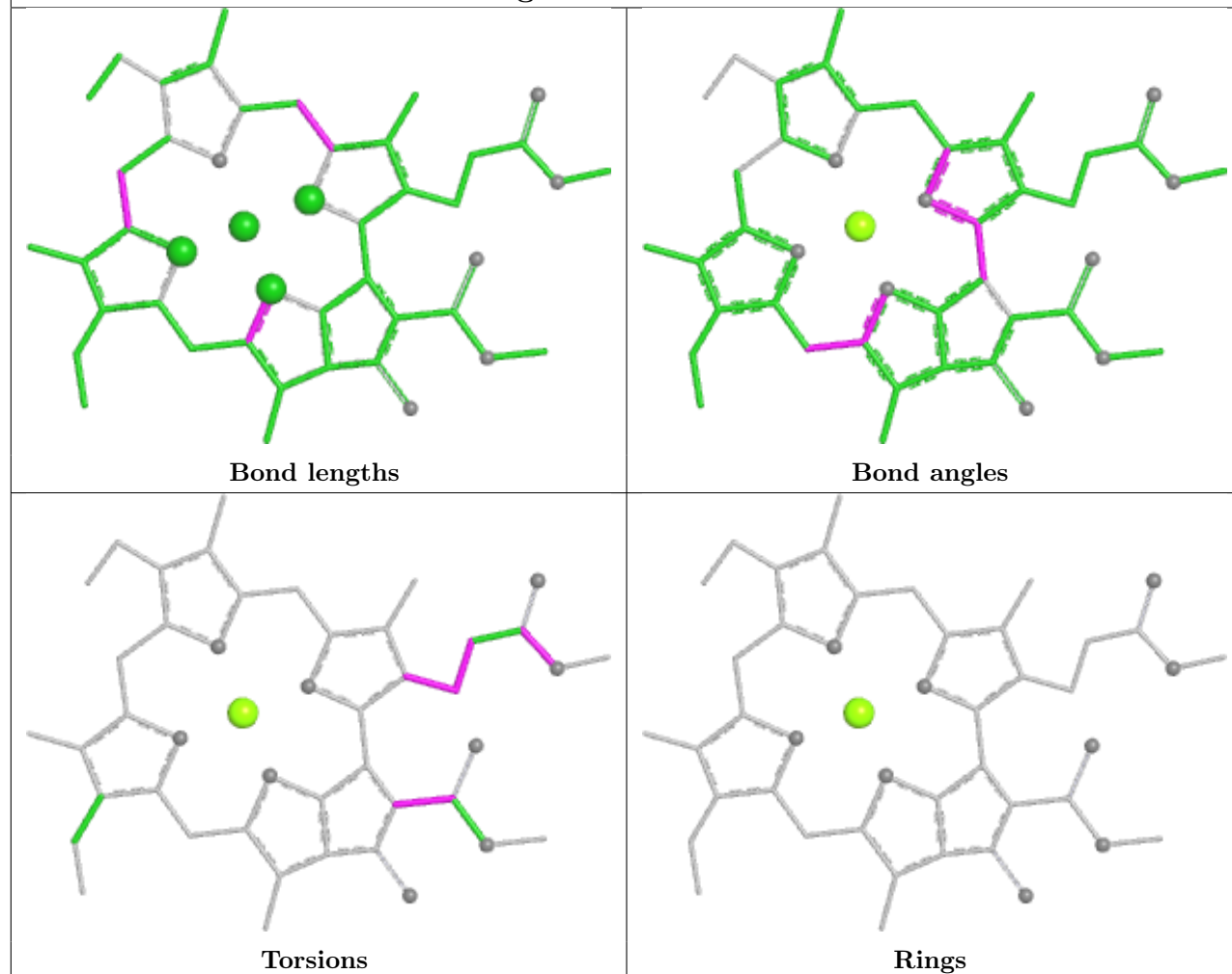




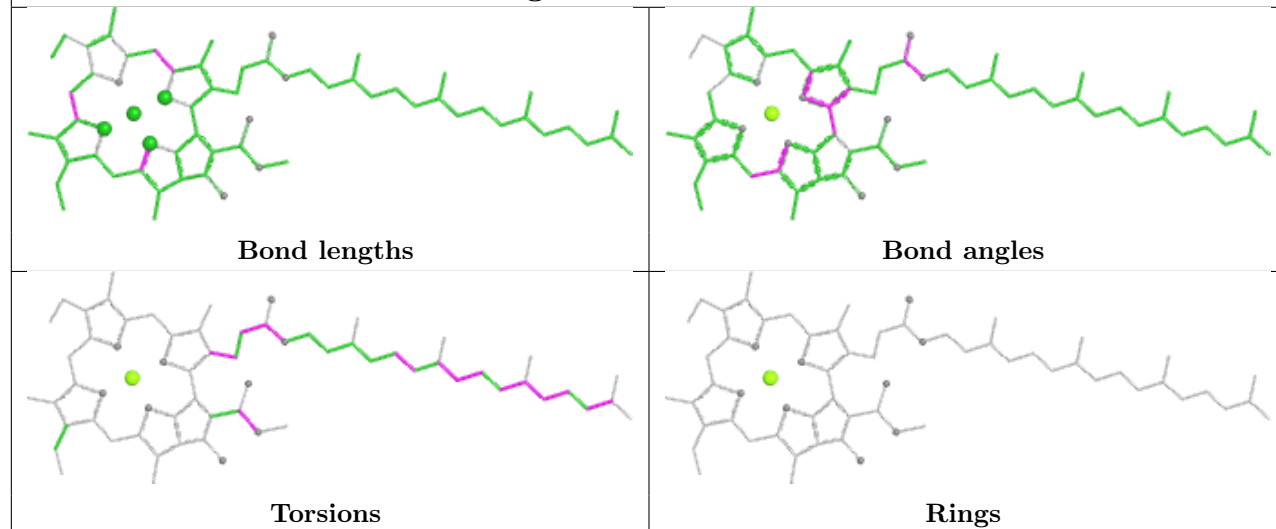


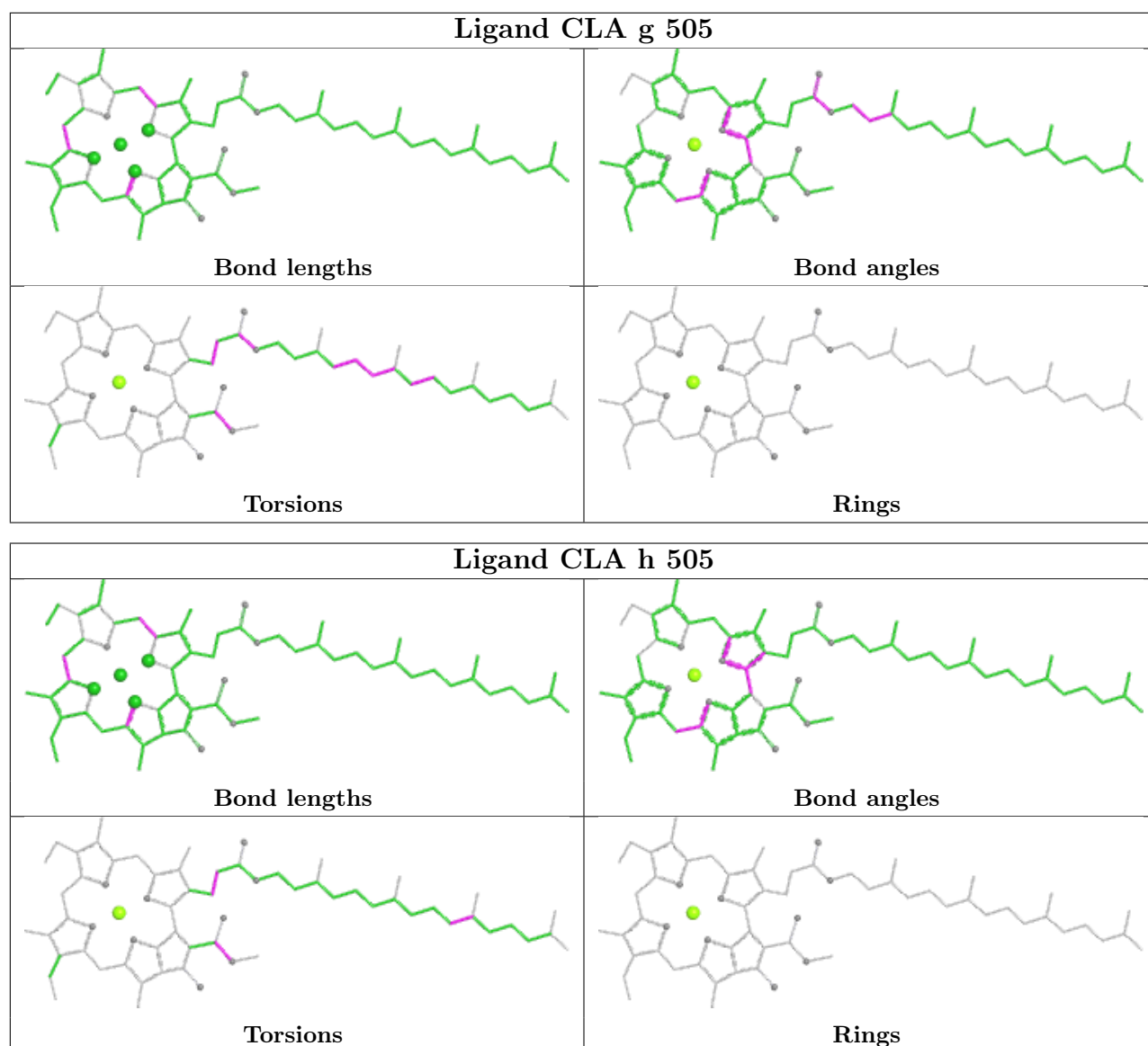


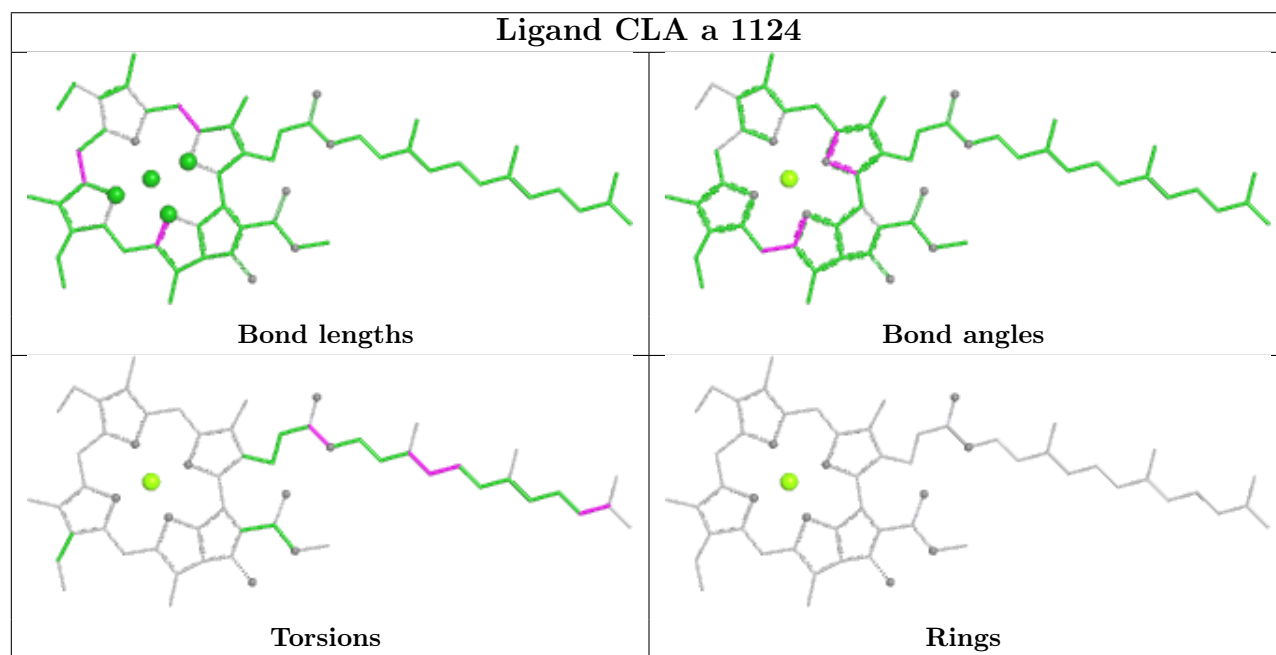
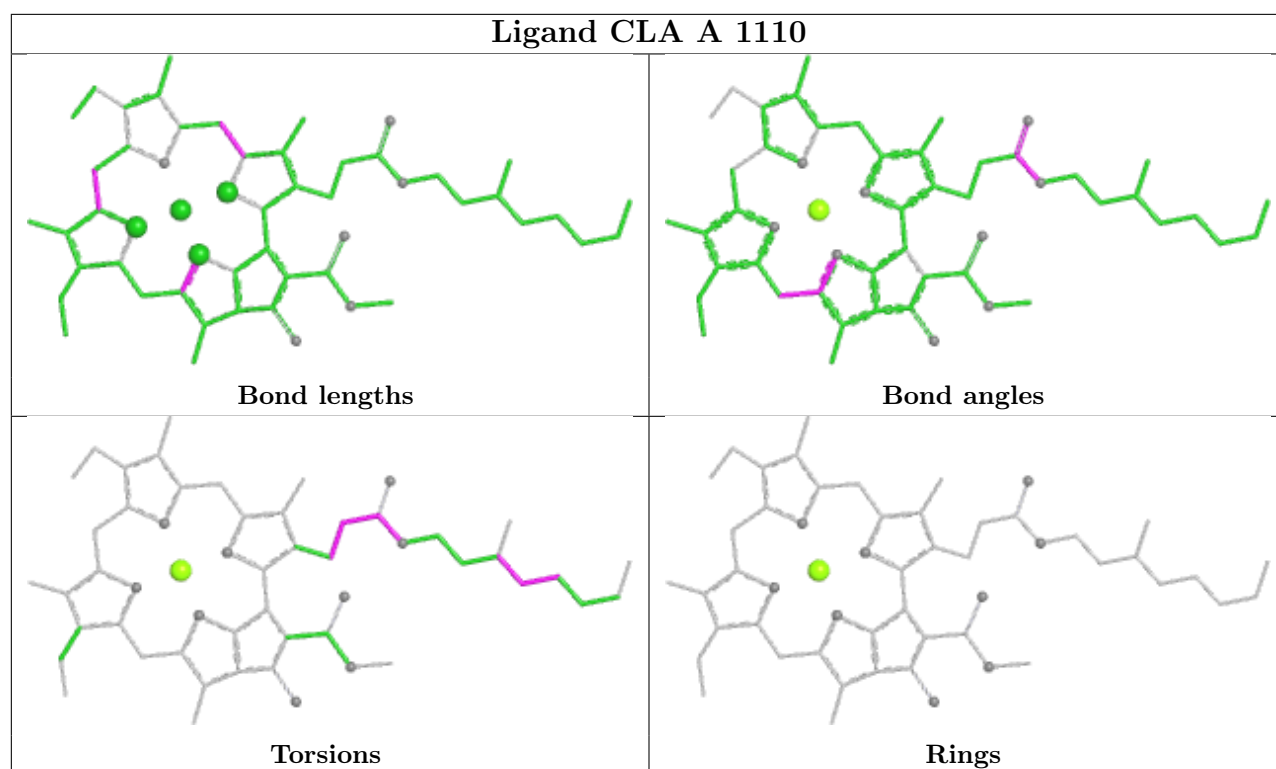
Ligand CLA v 503

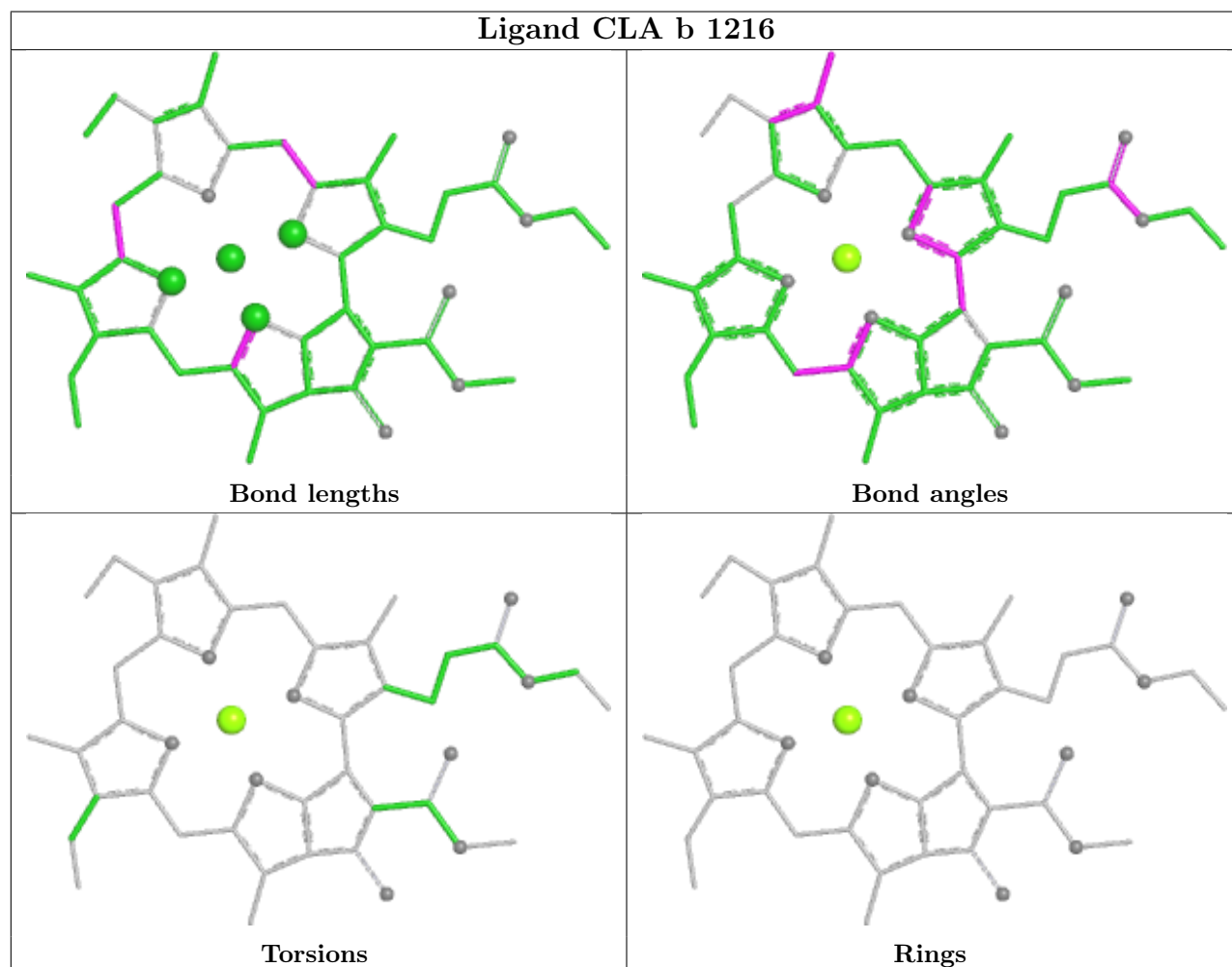
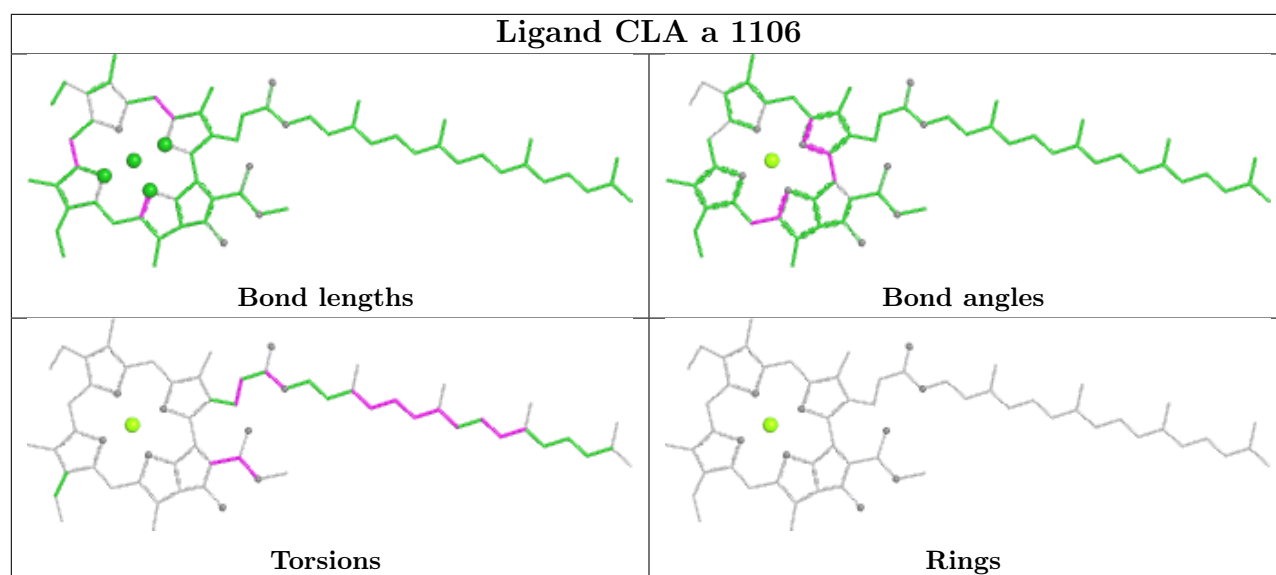


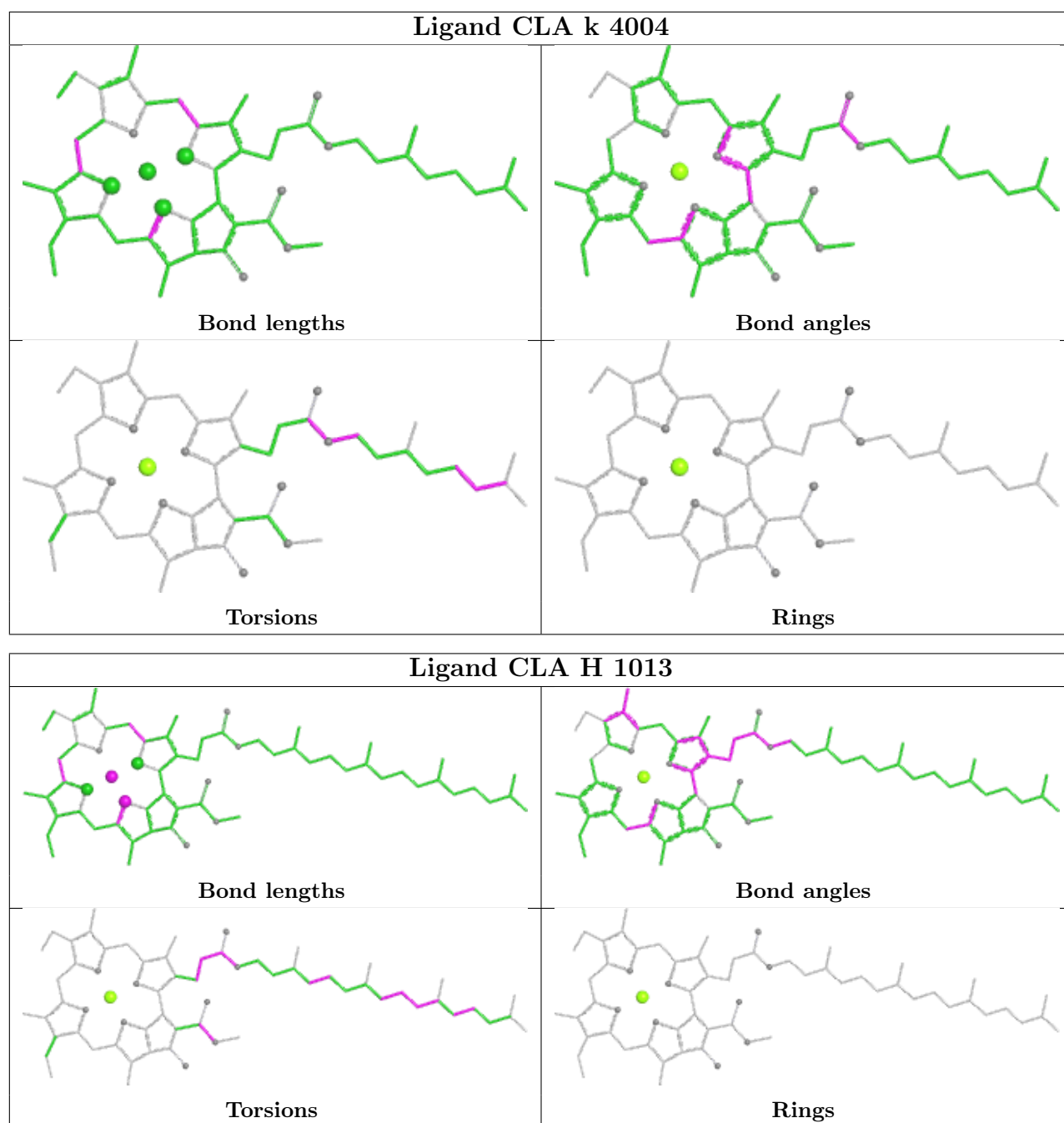
Ligand CLA b 1021

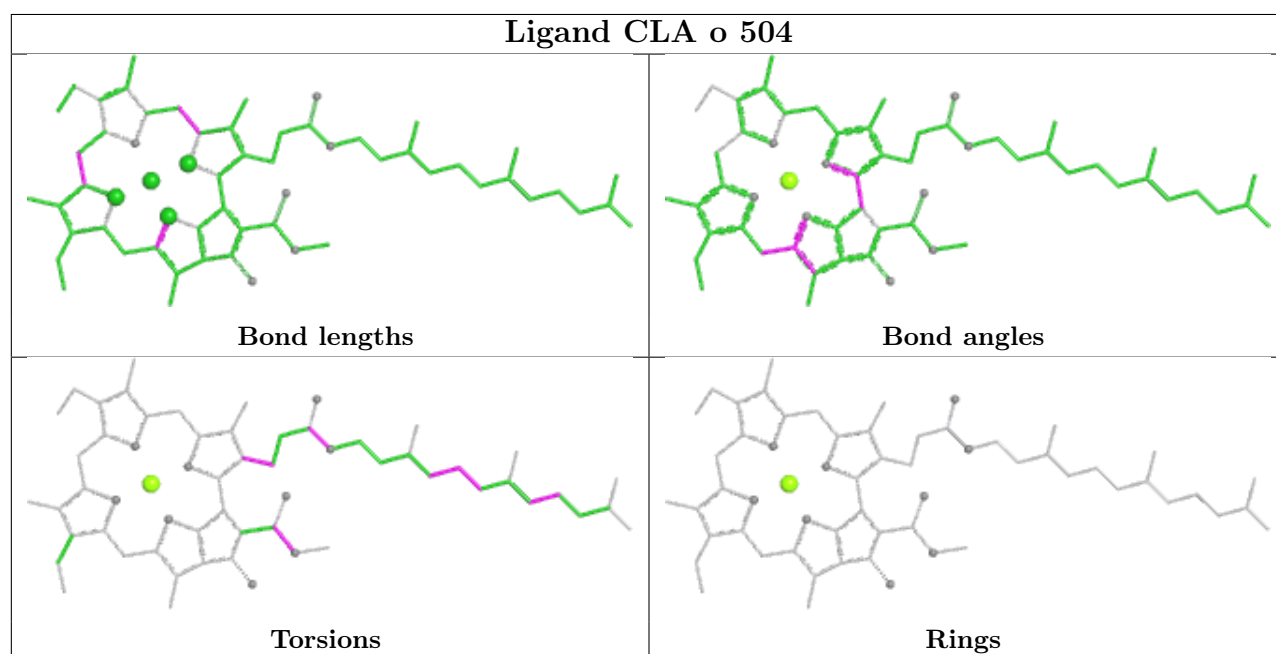
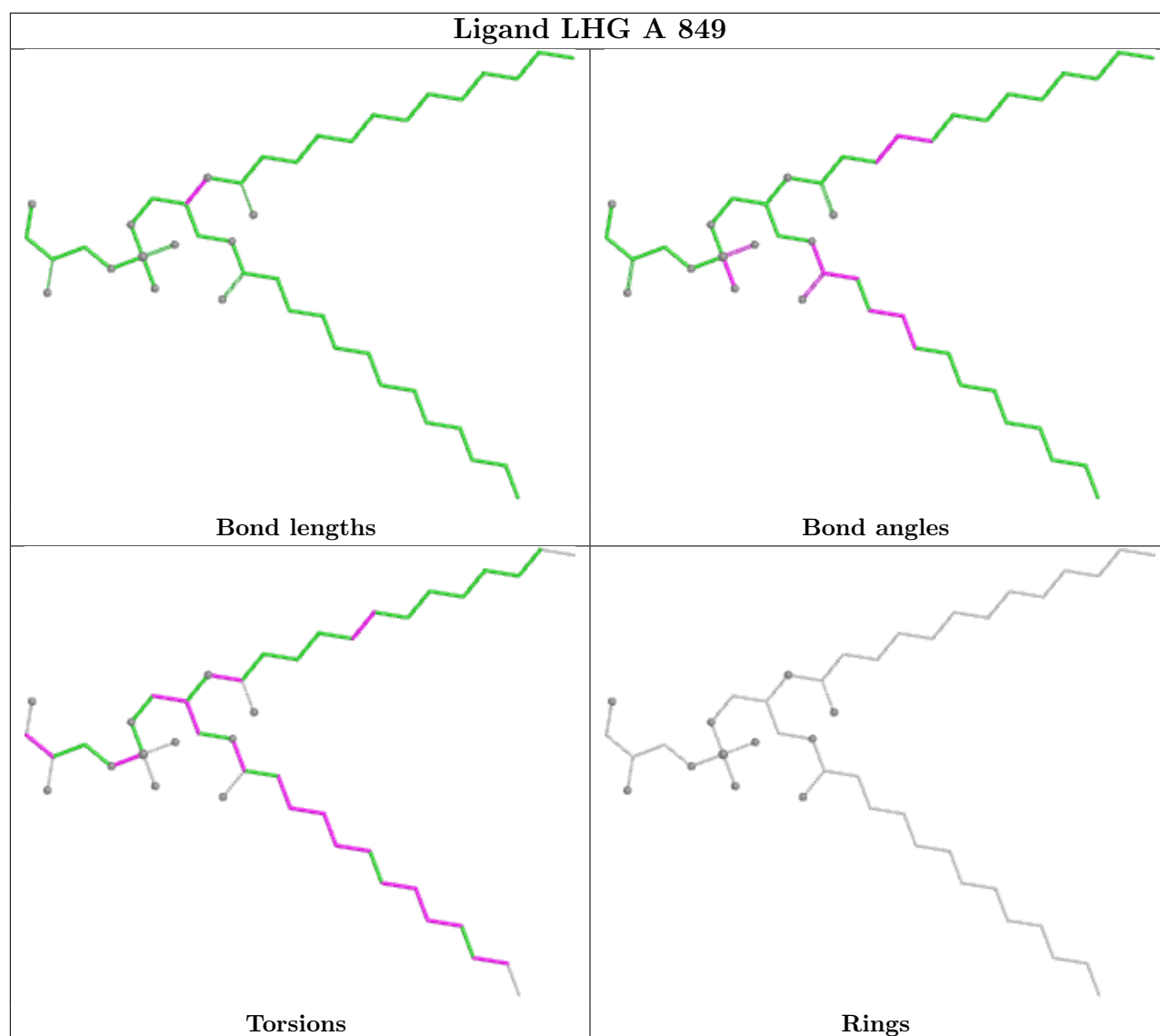


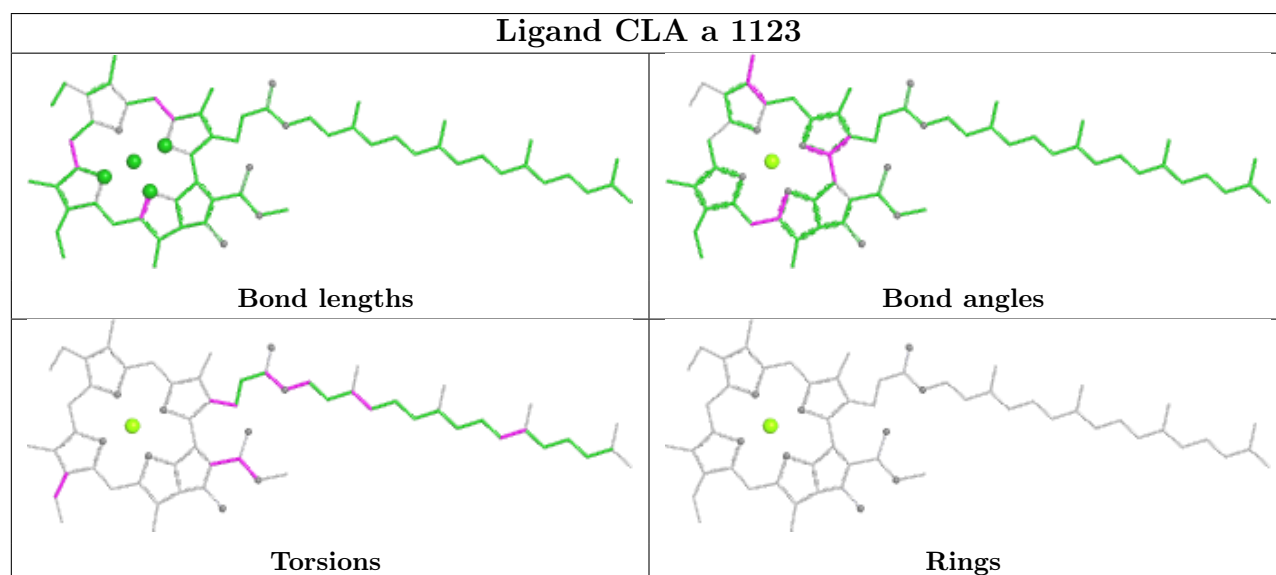
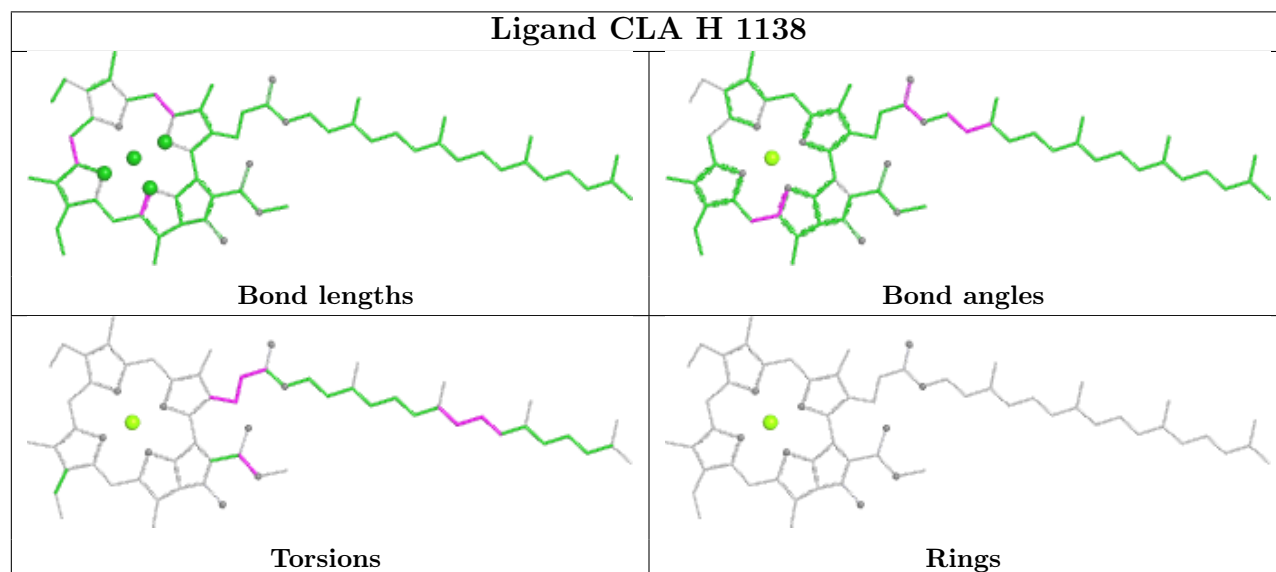
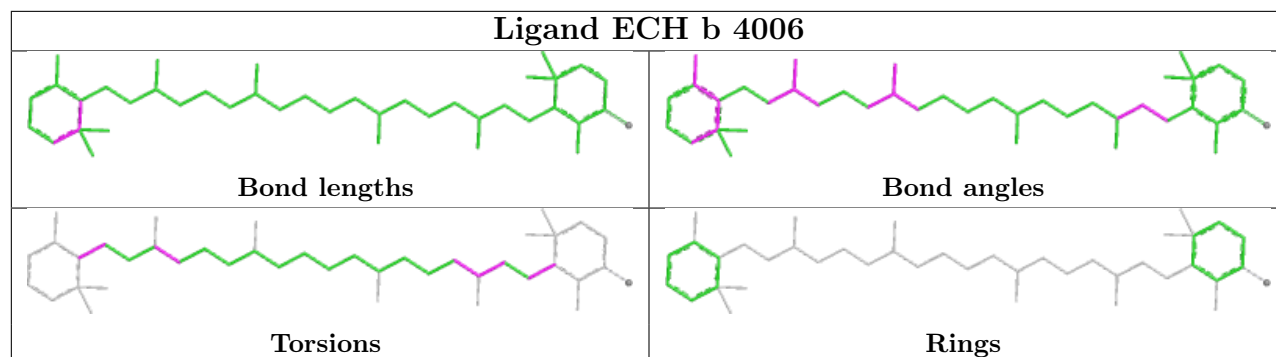




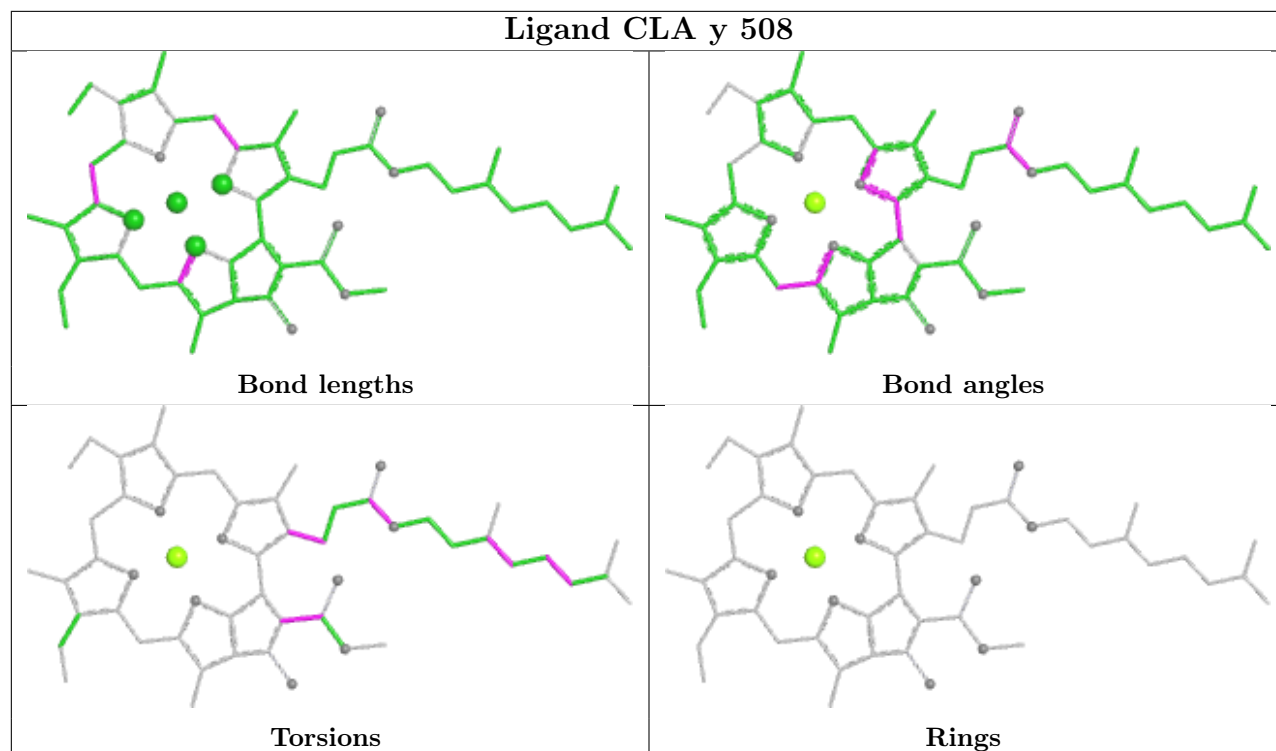




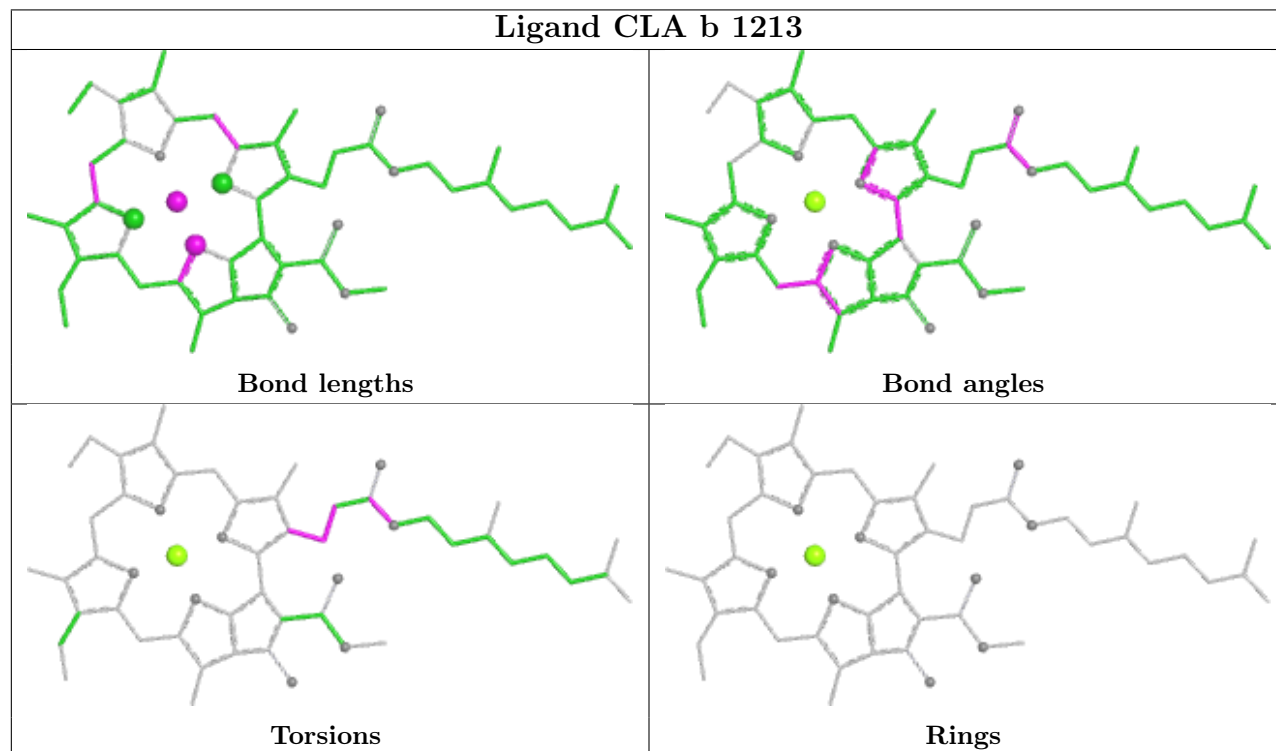




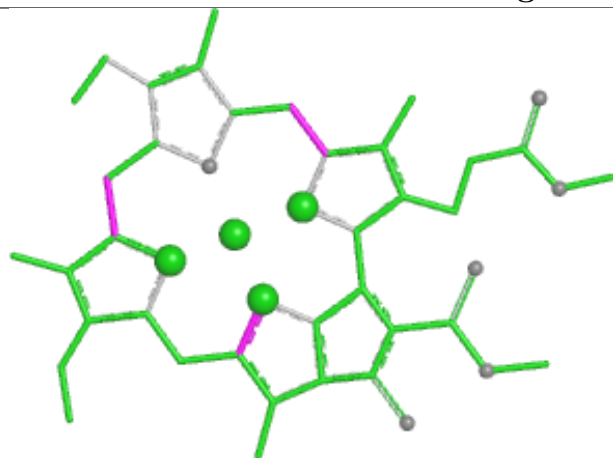
Ligand CLA y 508



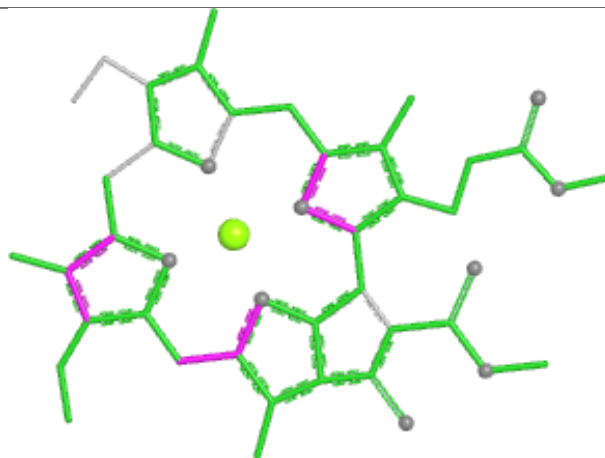
Ligand CLA b 1213



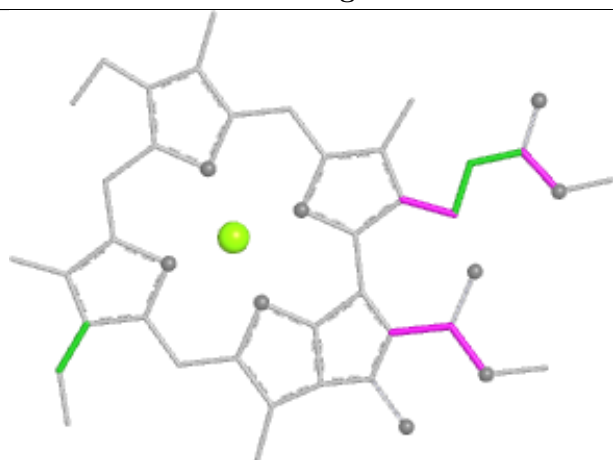
Ligand CLA n 513



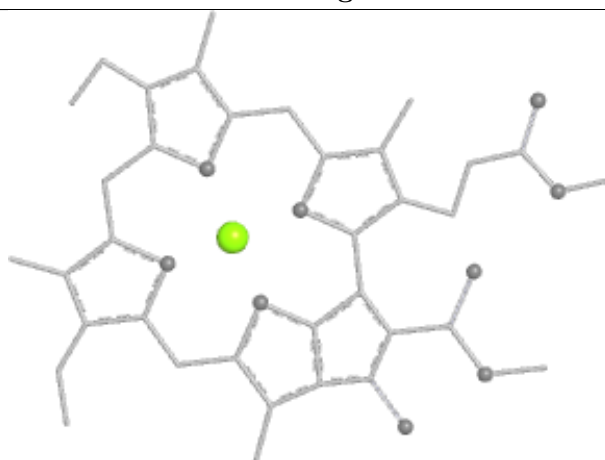
Bond lengths



Bond angles

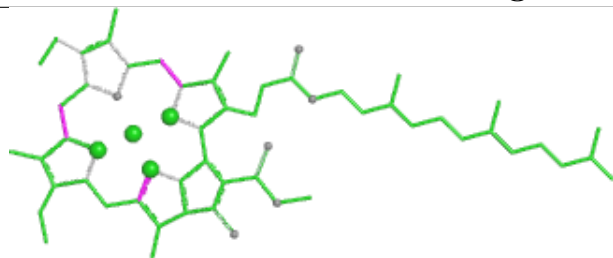


Torsions

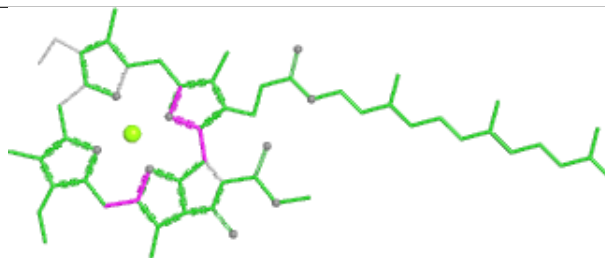


Rings

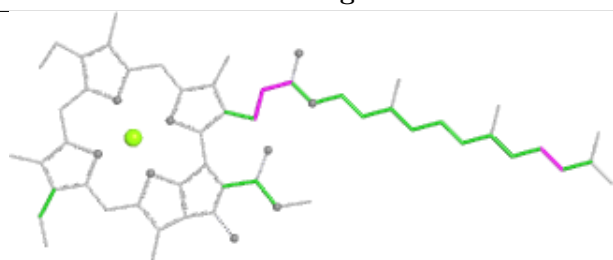
Ligand CLA W 509



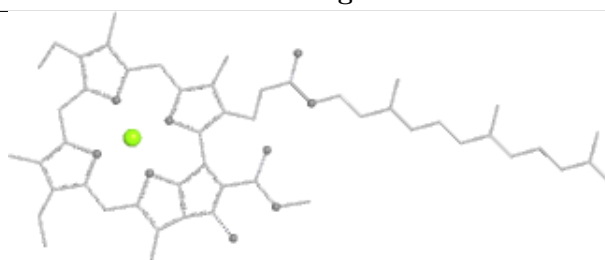
Bond lengths



Bond angles

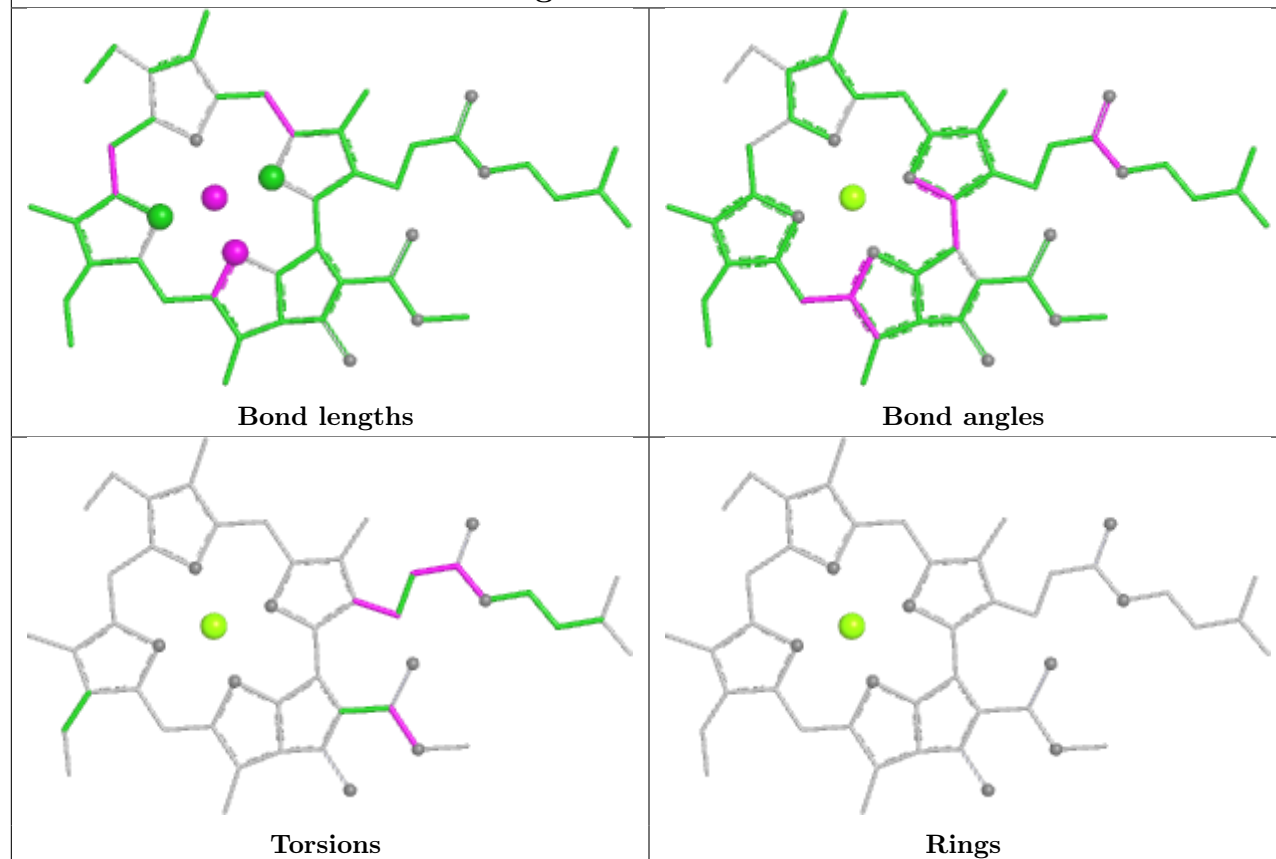


Torsions

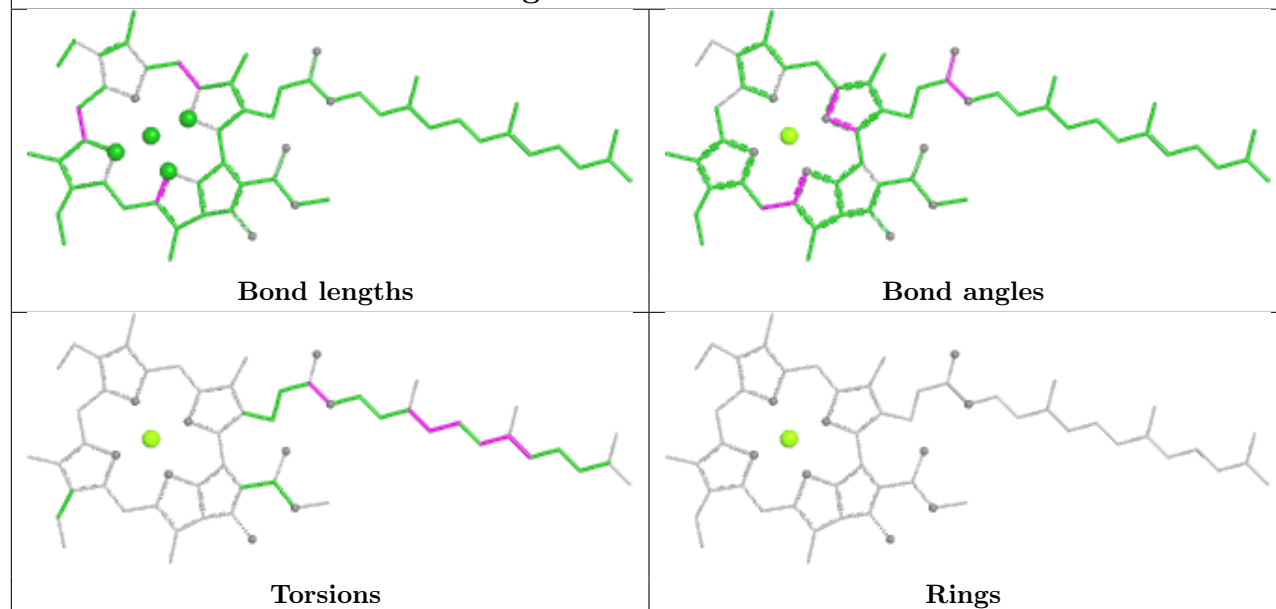


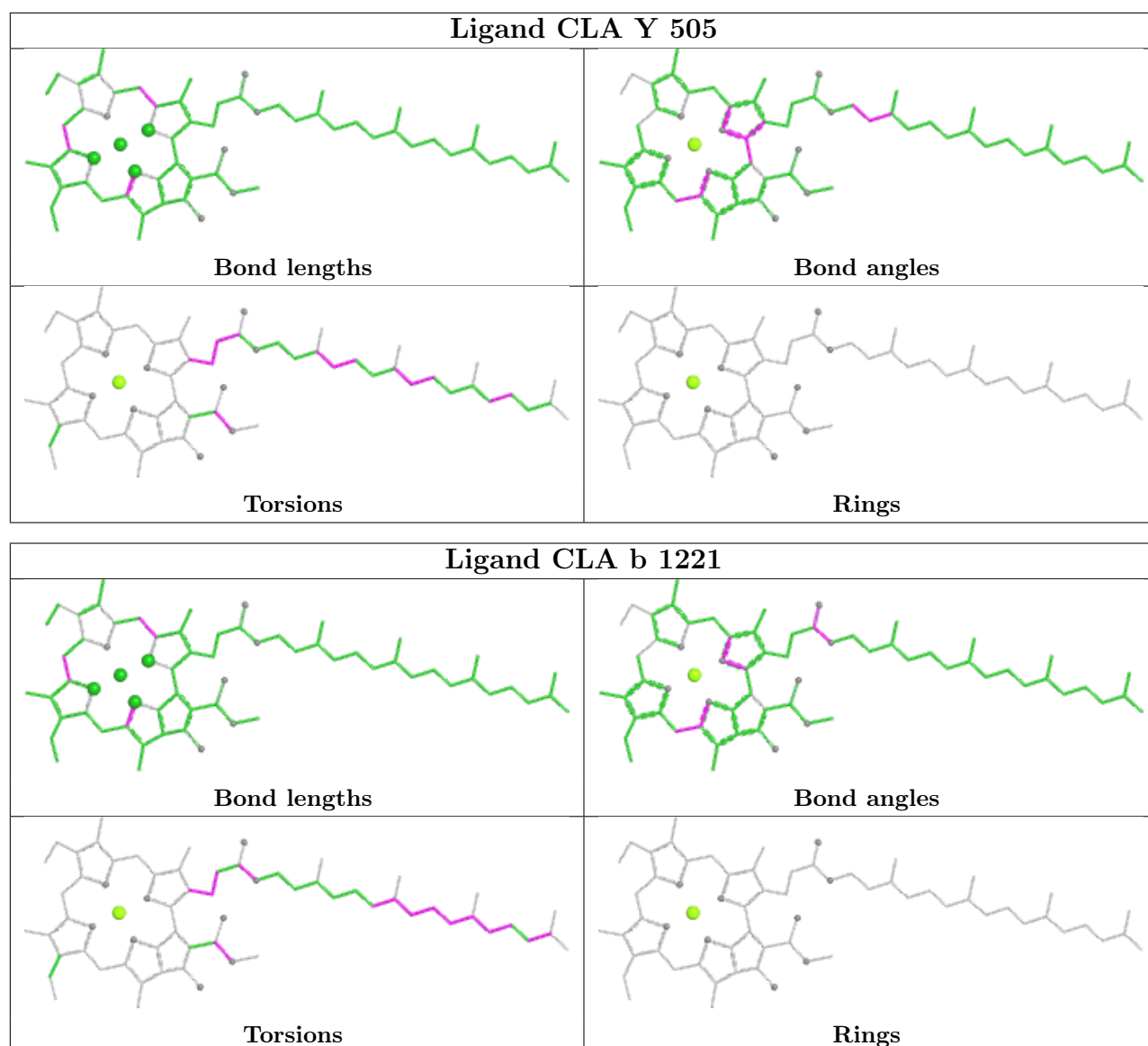
Rings

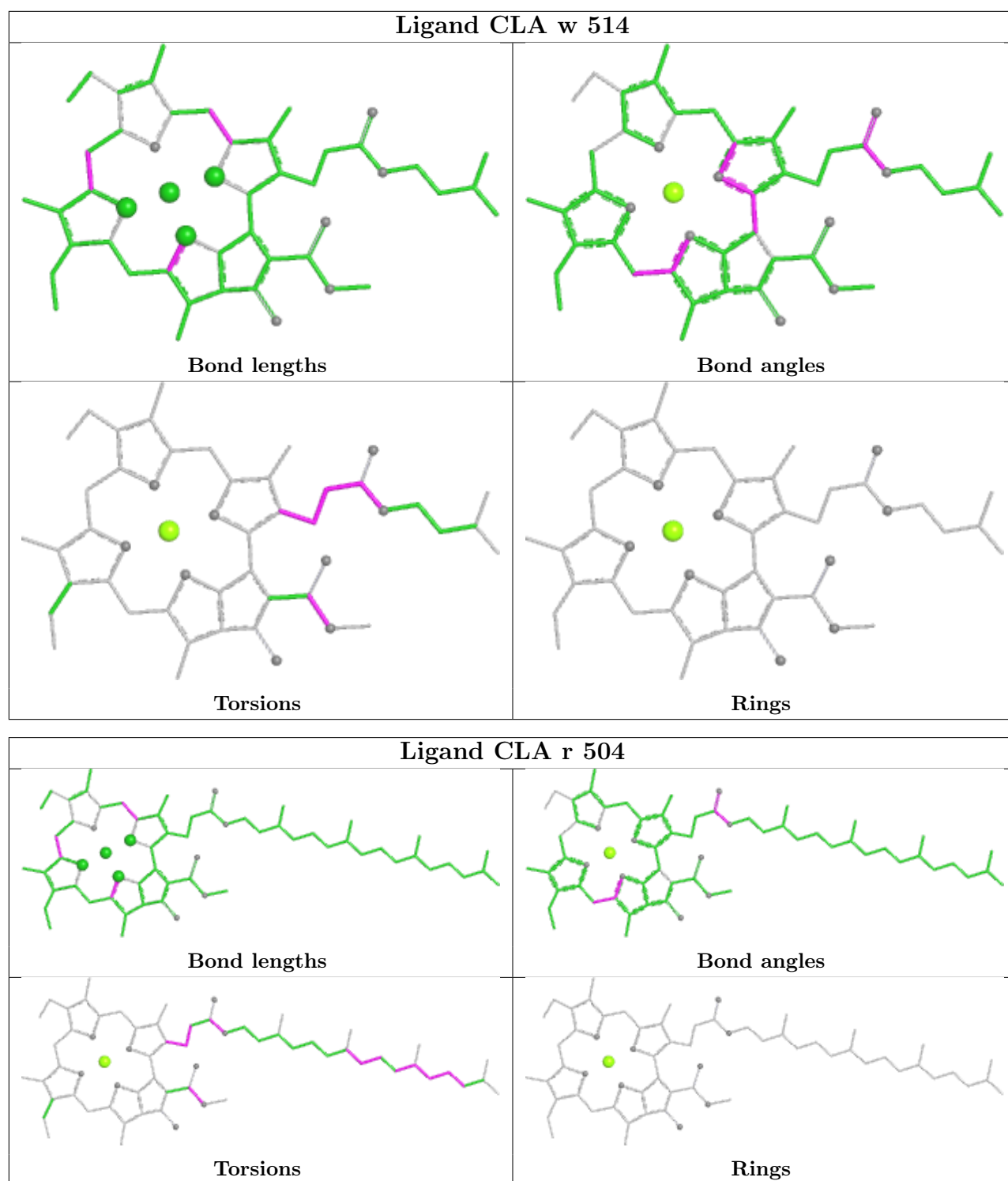
Ligand CLA n 514

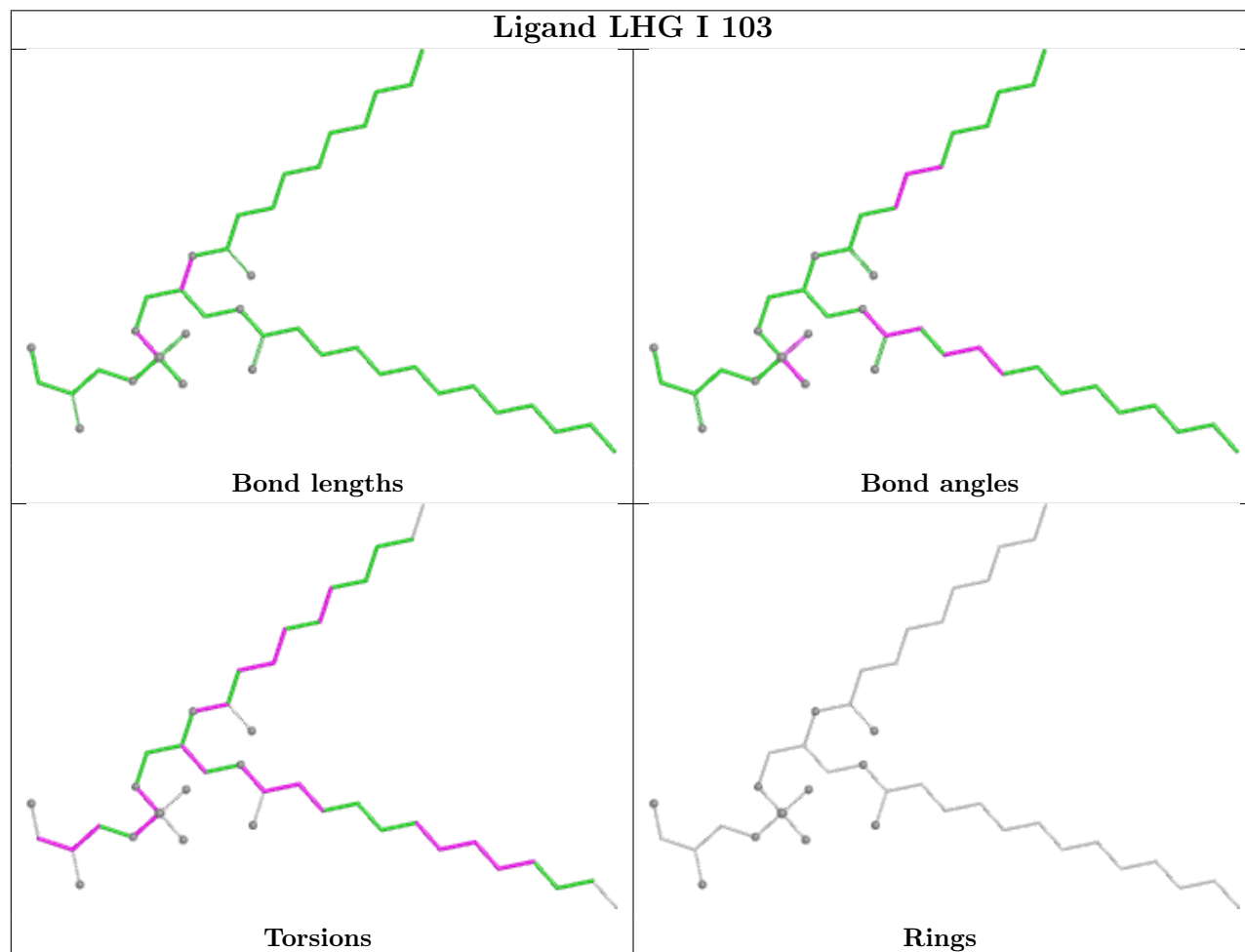
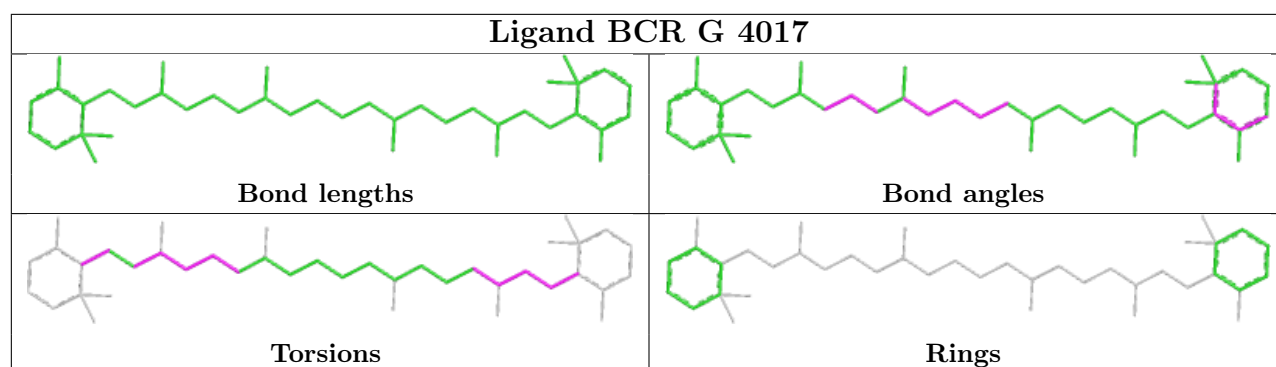


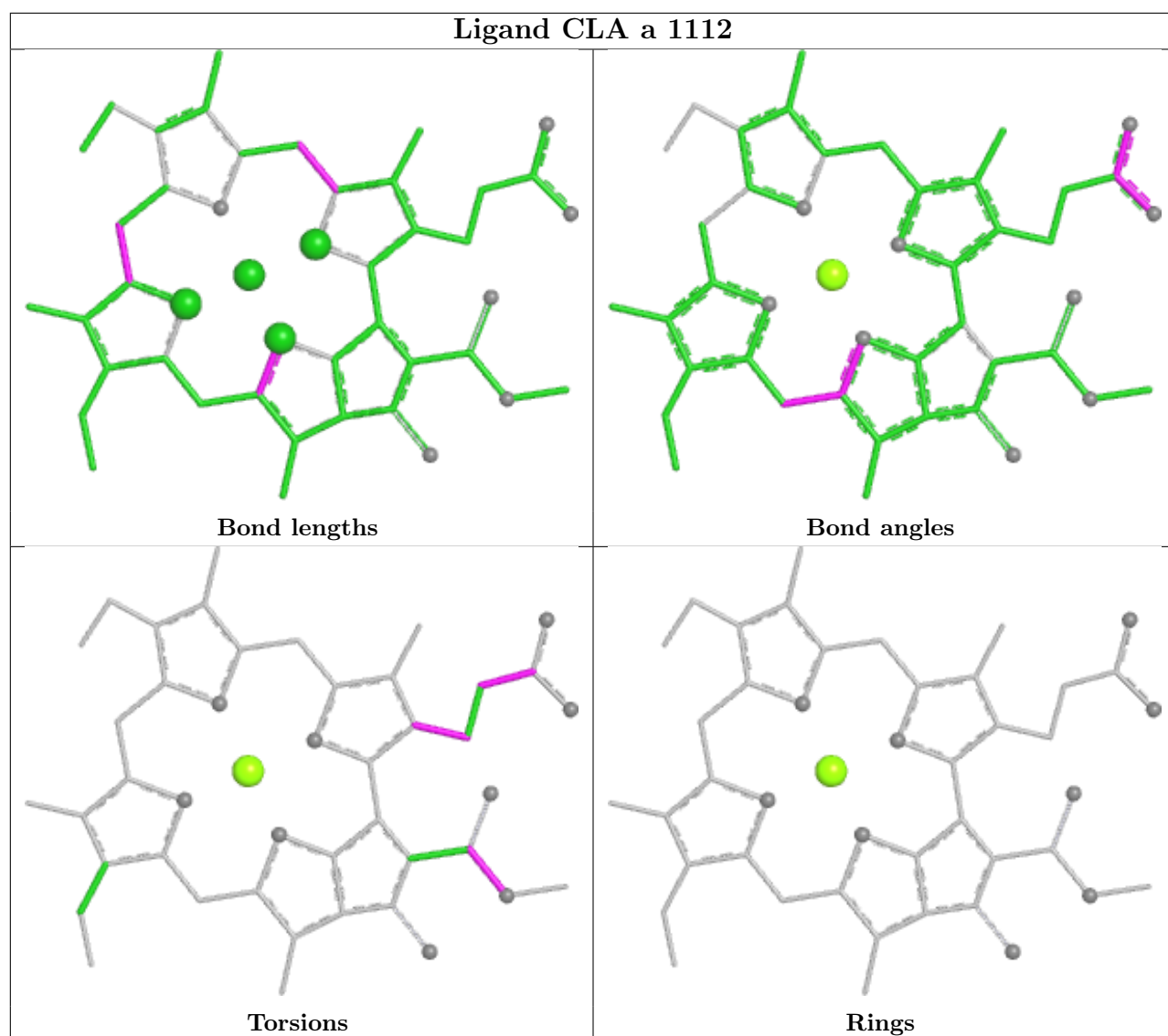
Ligand CLA U 1502



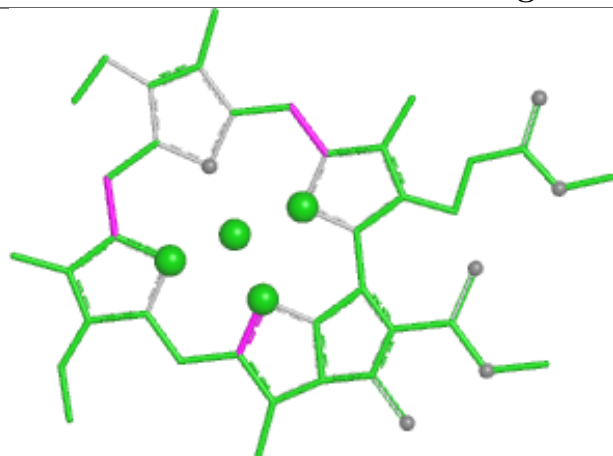




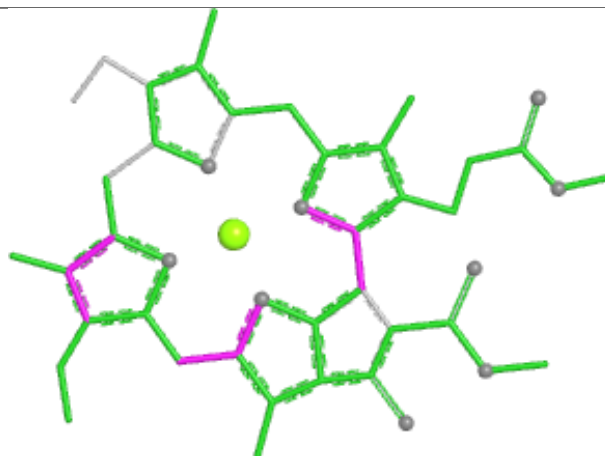




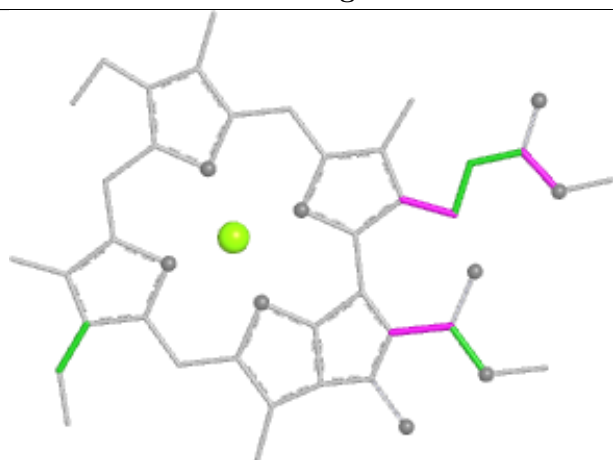
Ligand CLA h 516



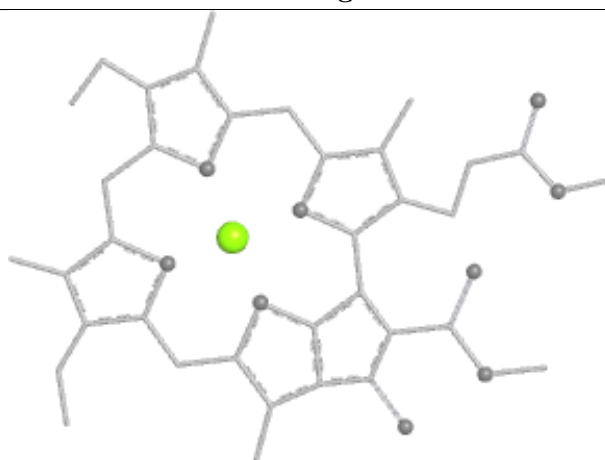
Bond lengths



Bond angles

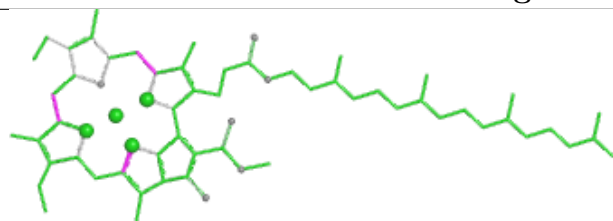


Torsions

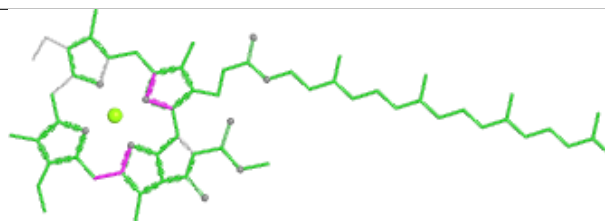


Rings

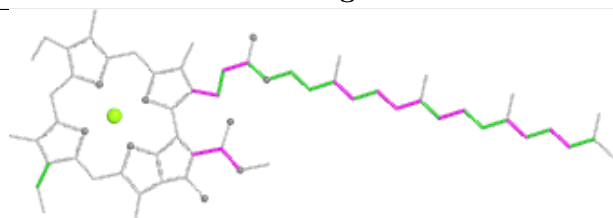
Ligand CLA Y 504



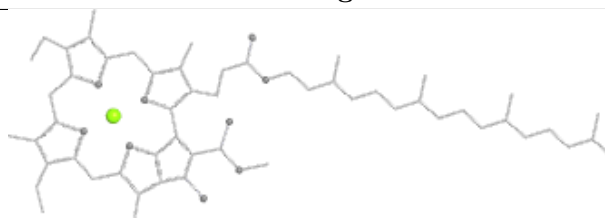
Bond lengths



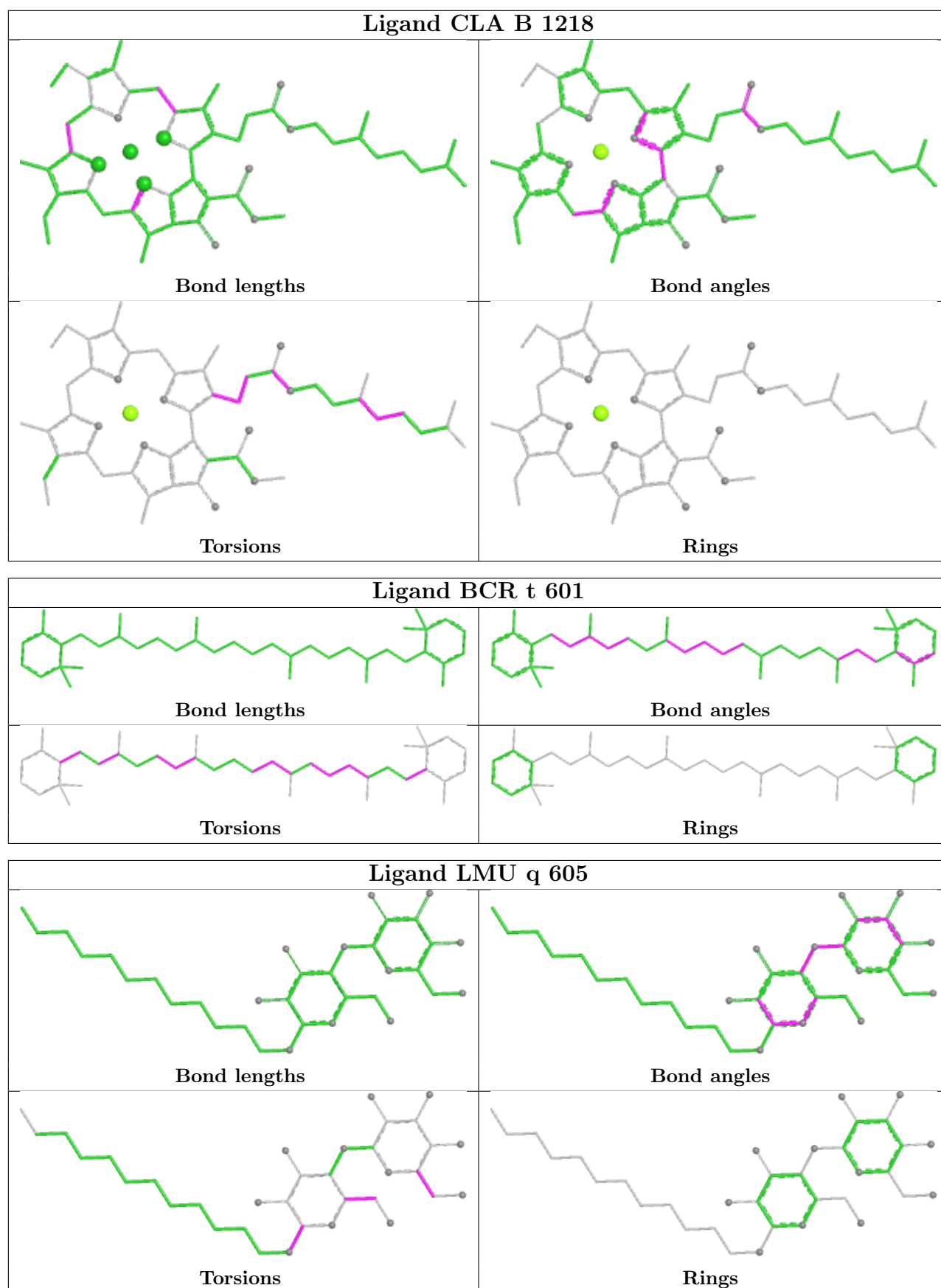
Bond angles

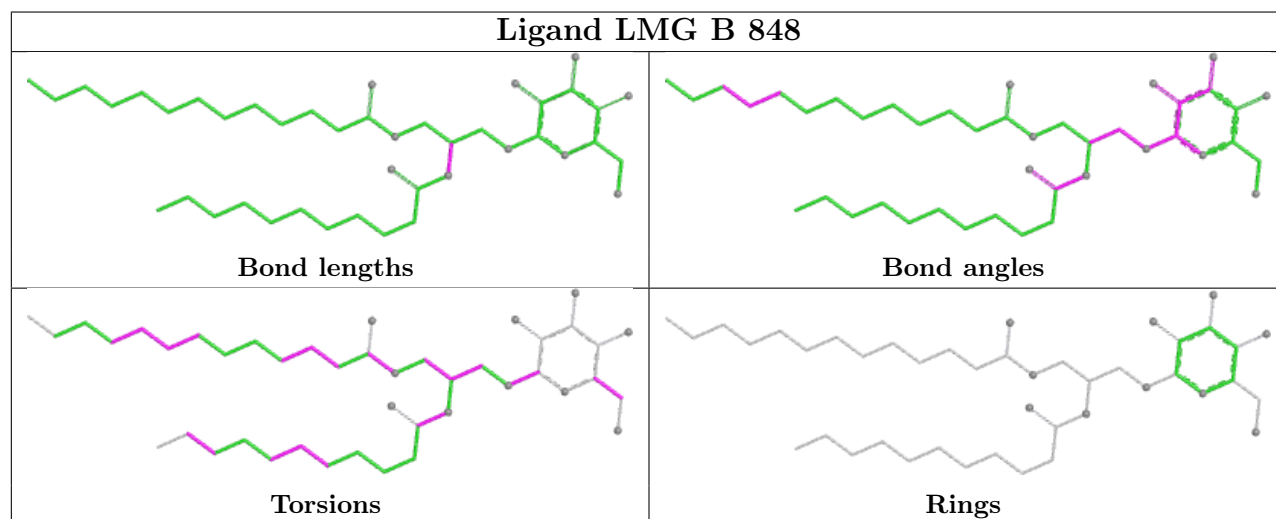
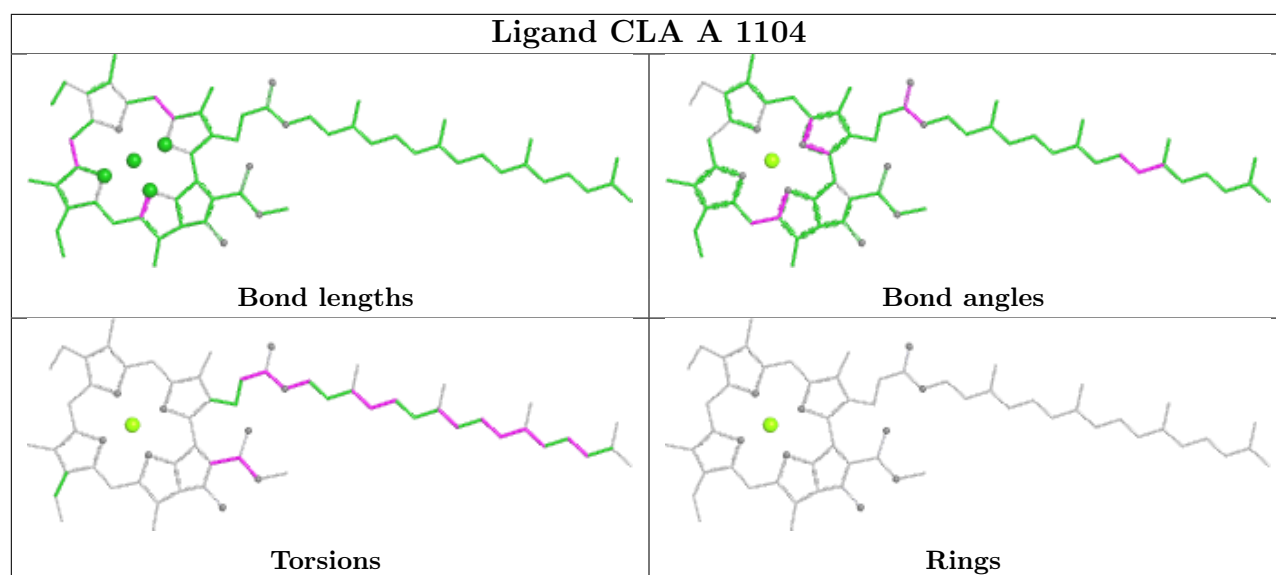


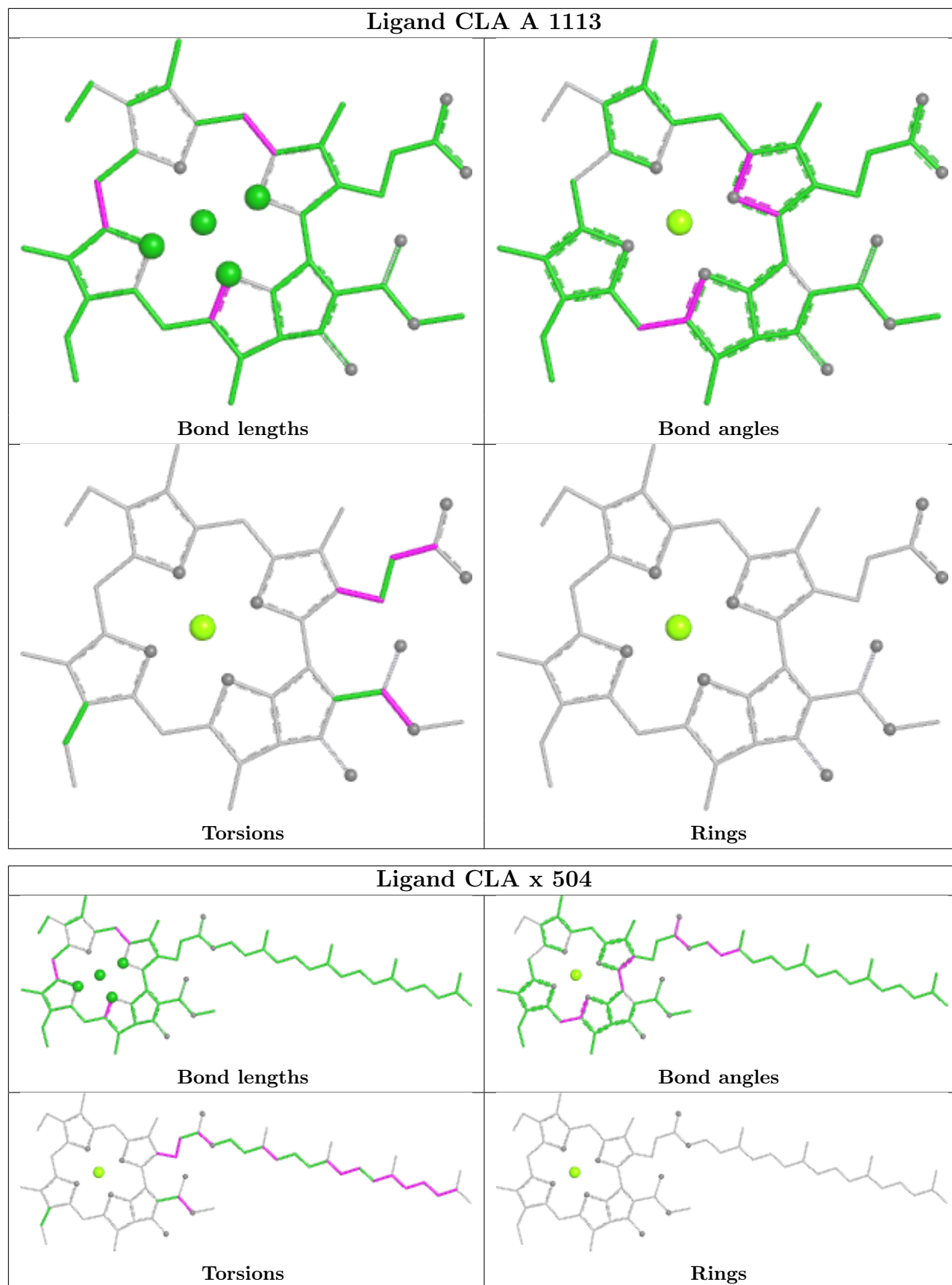
Torsions

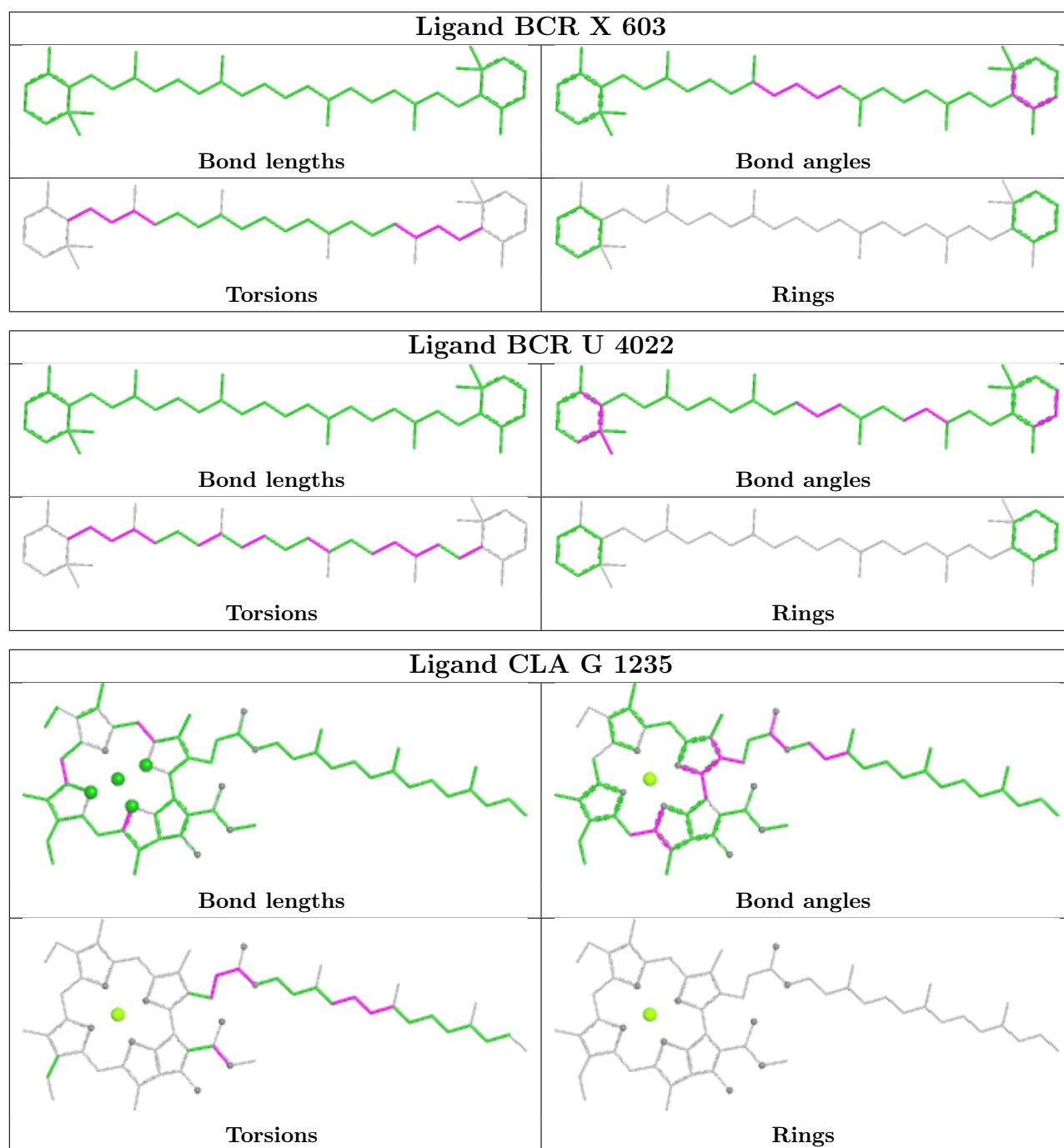


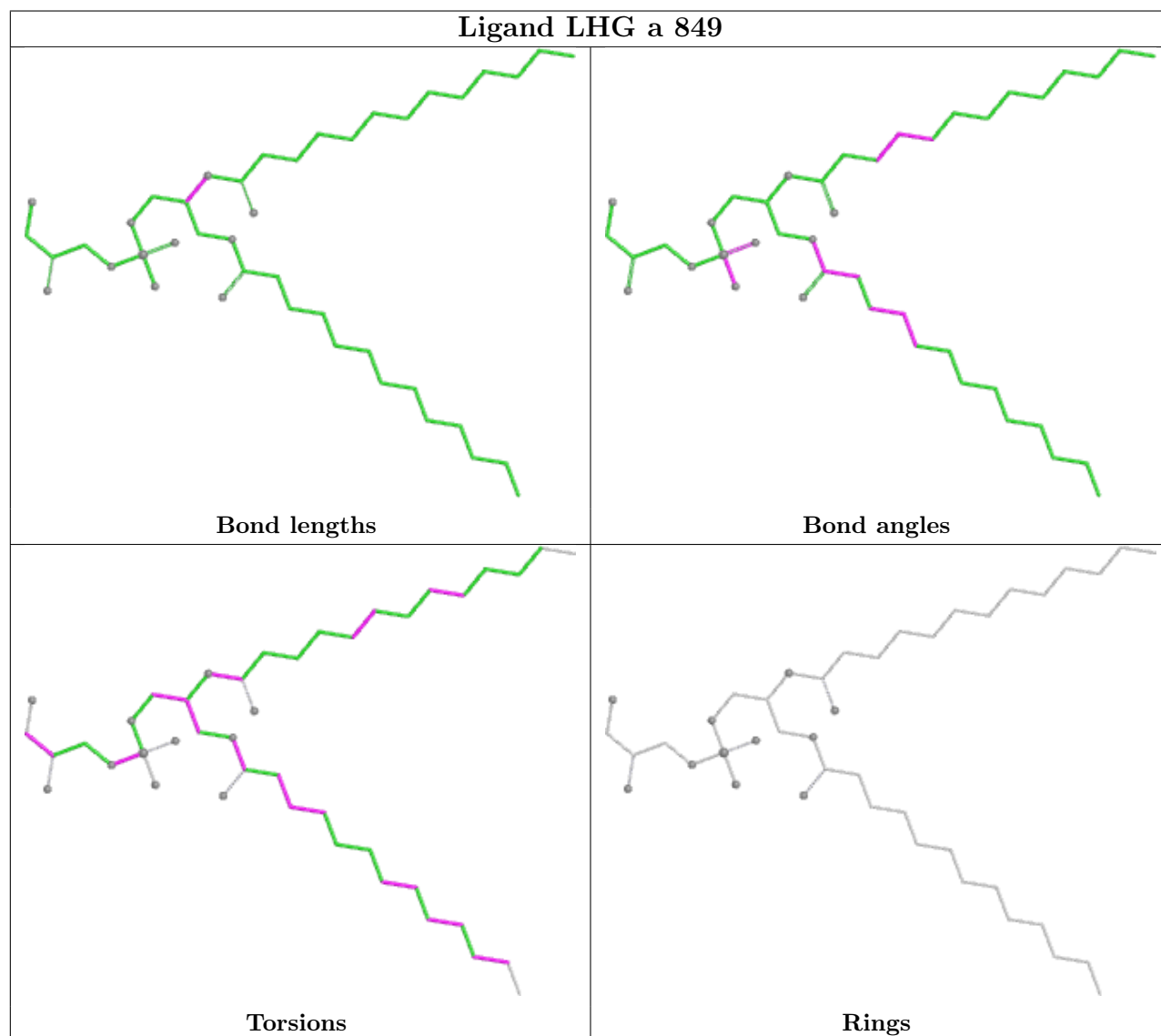
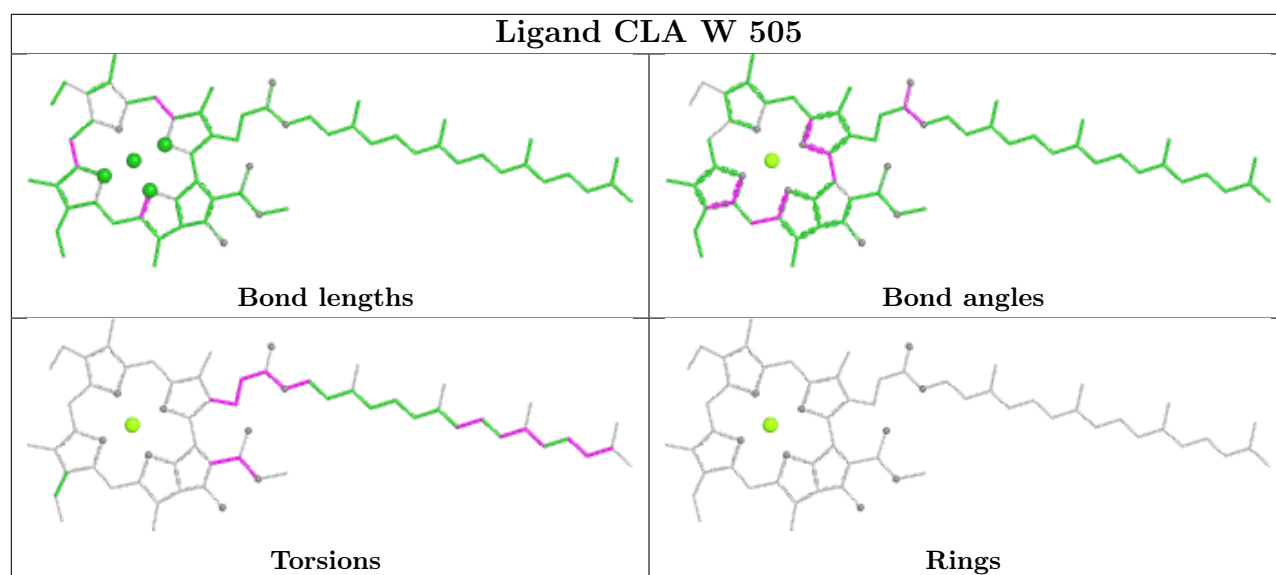
Rings

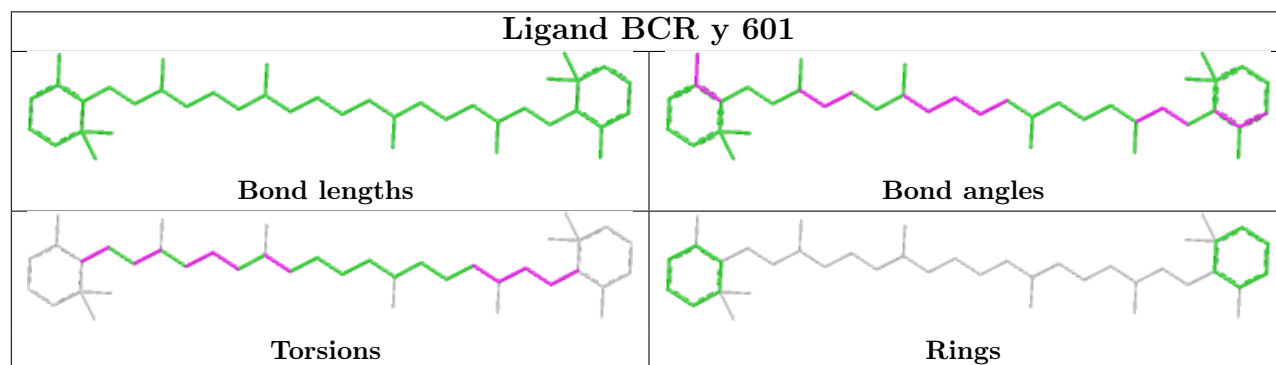
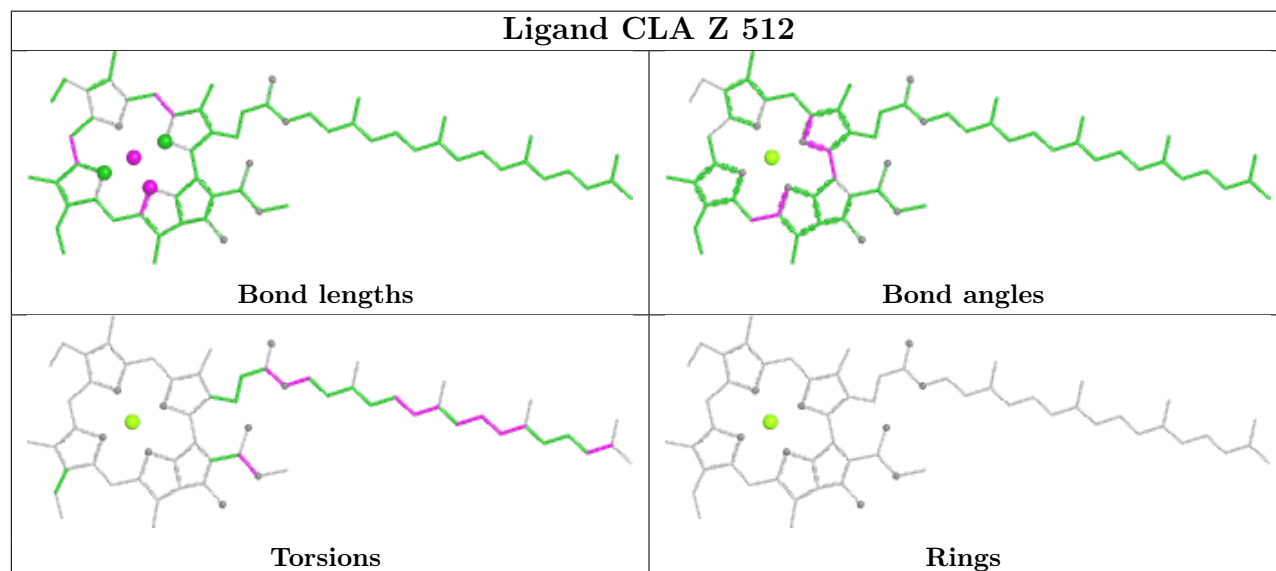
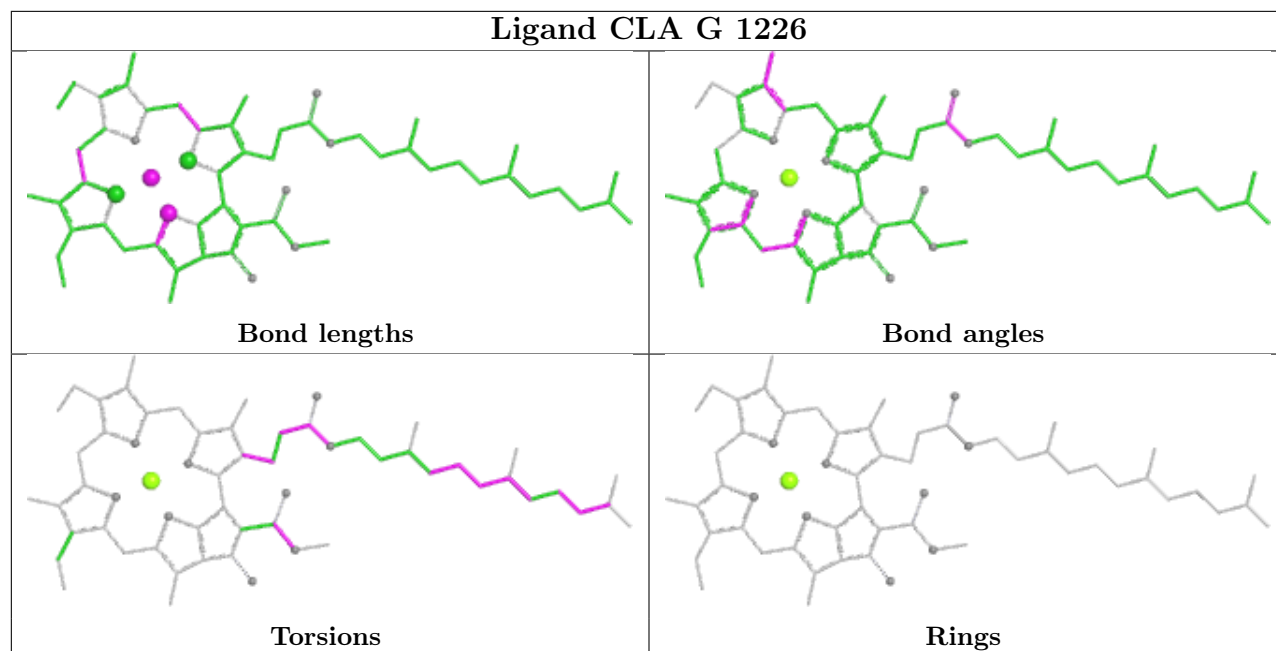


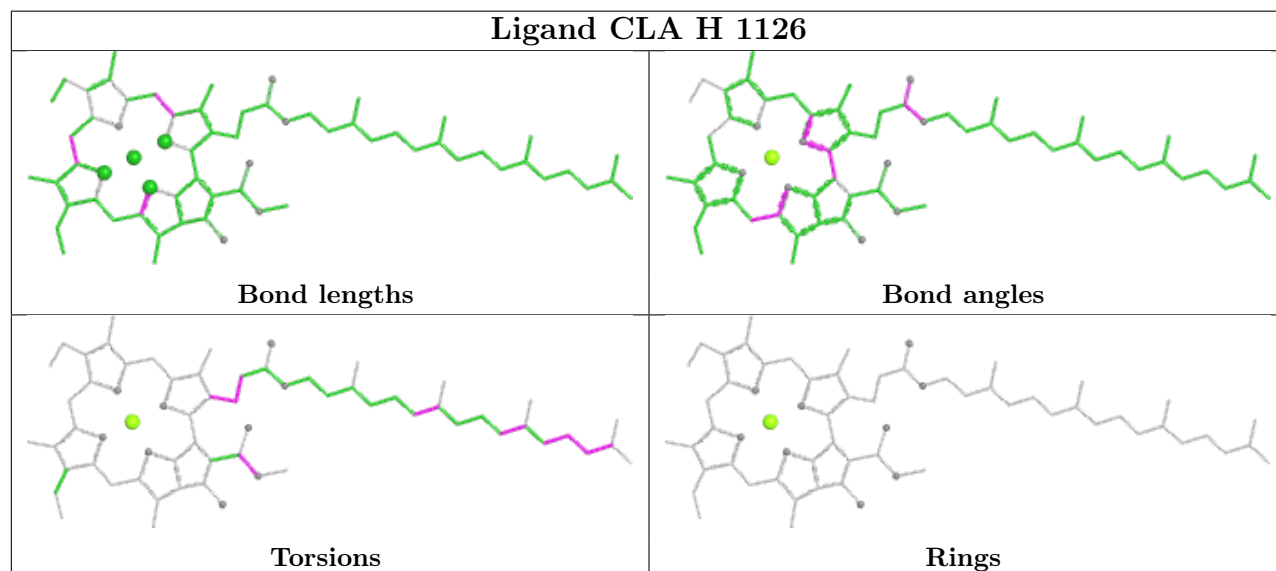
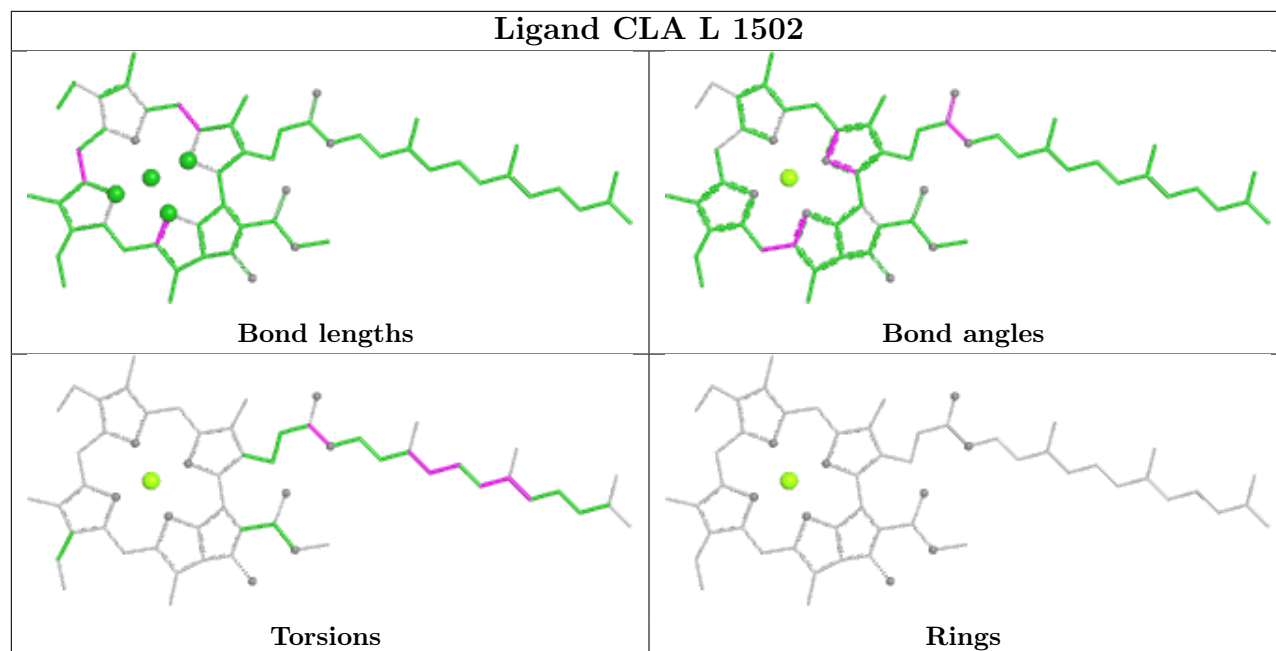


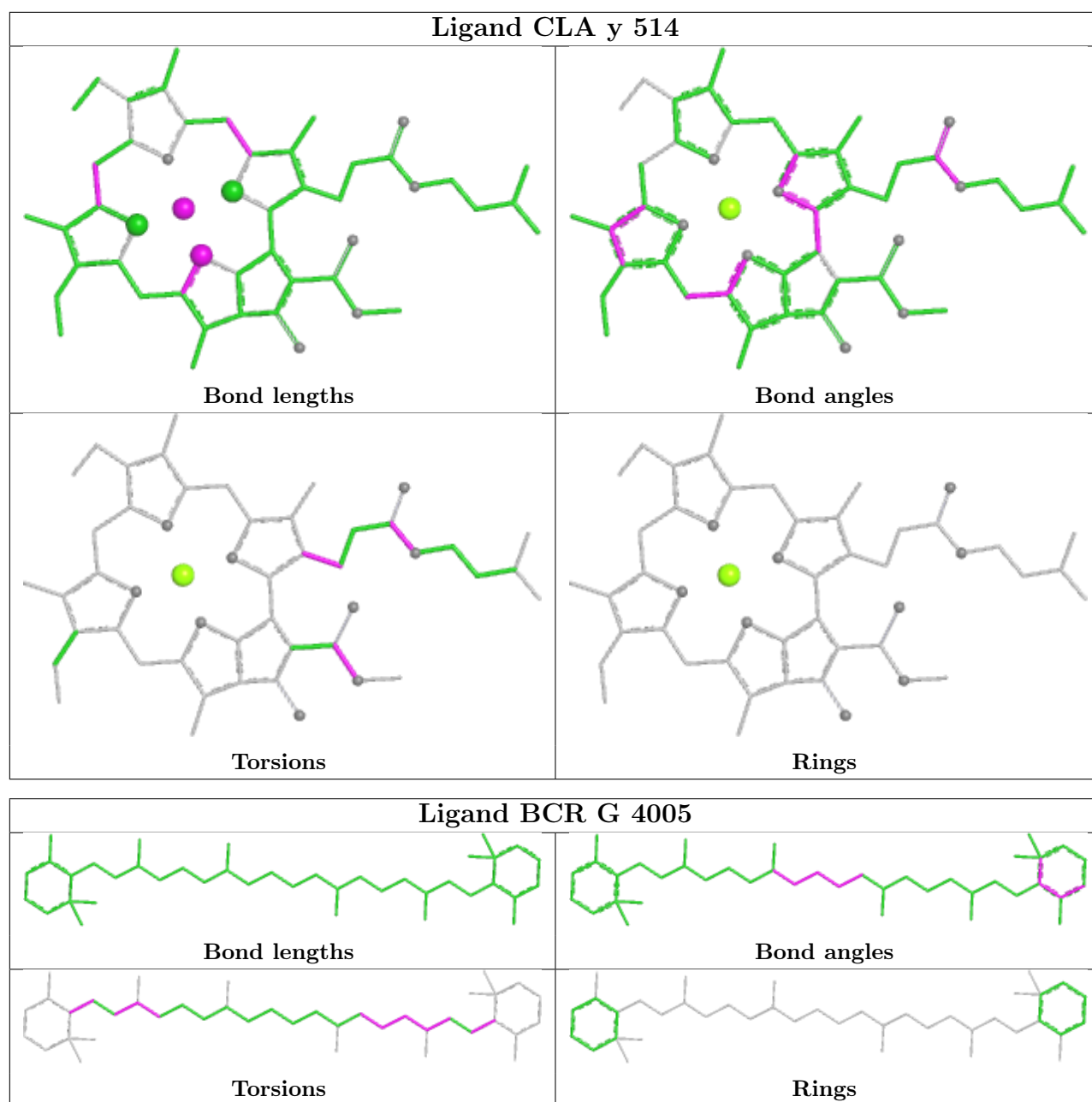


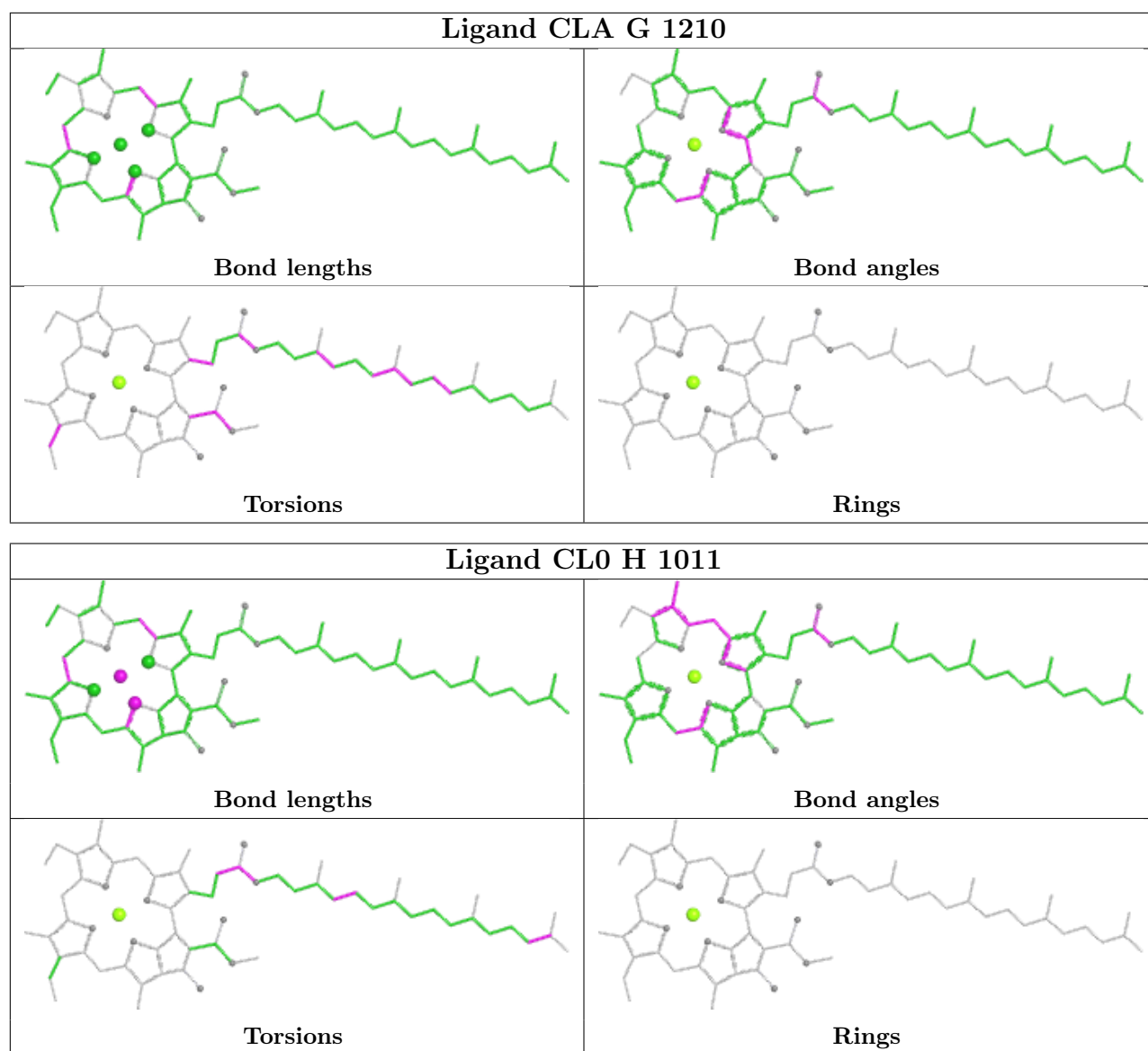




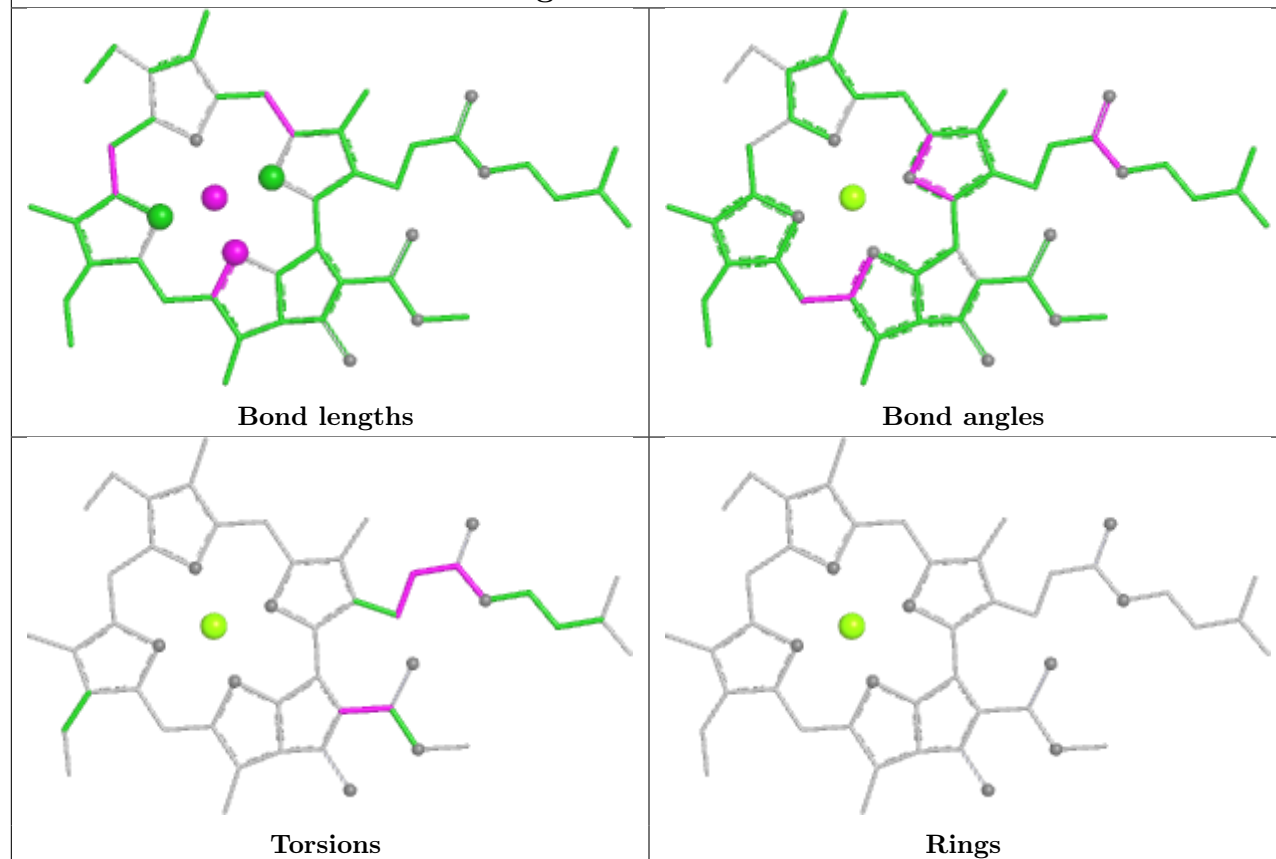




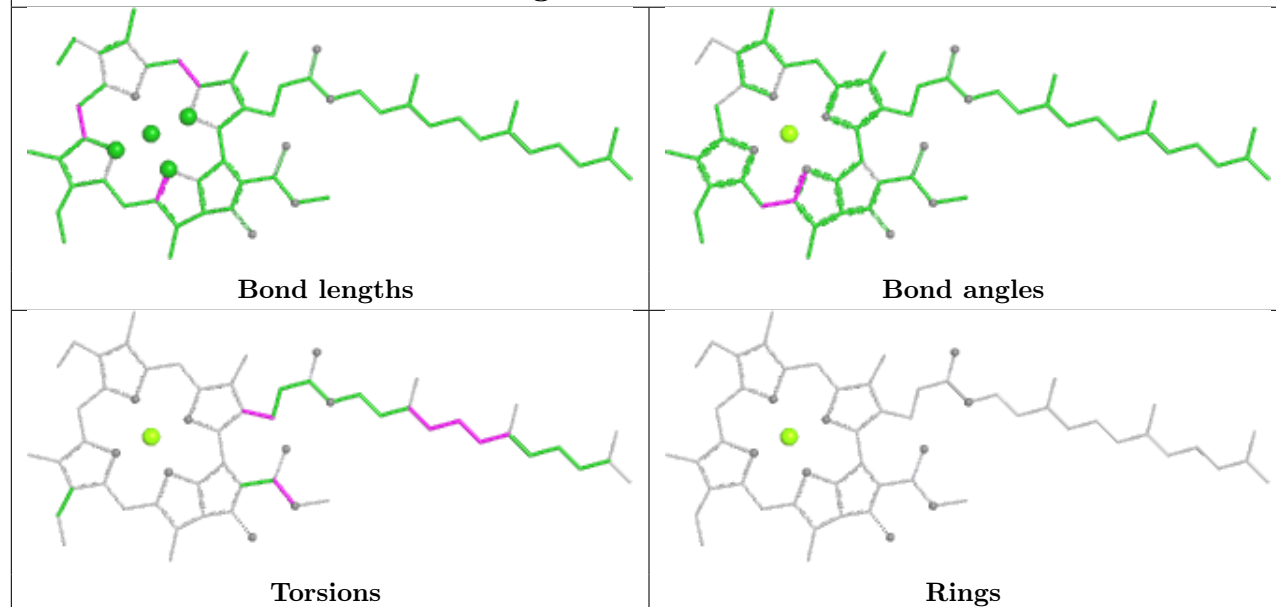


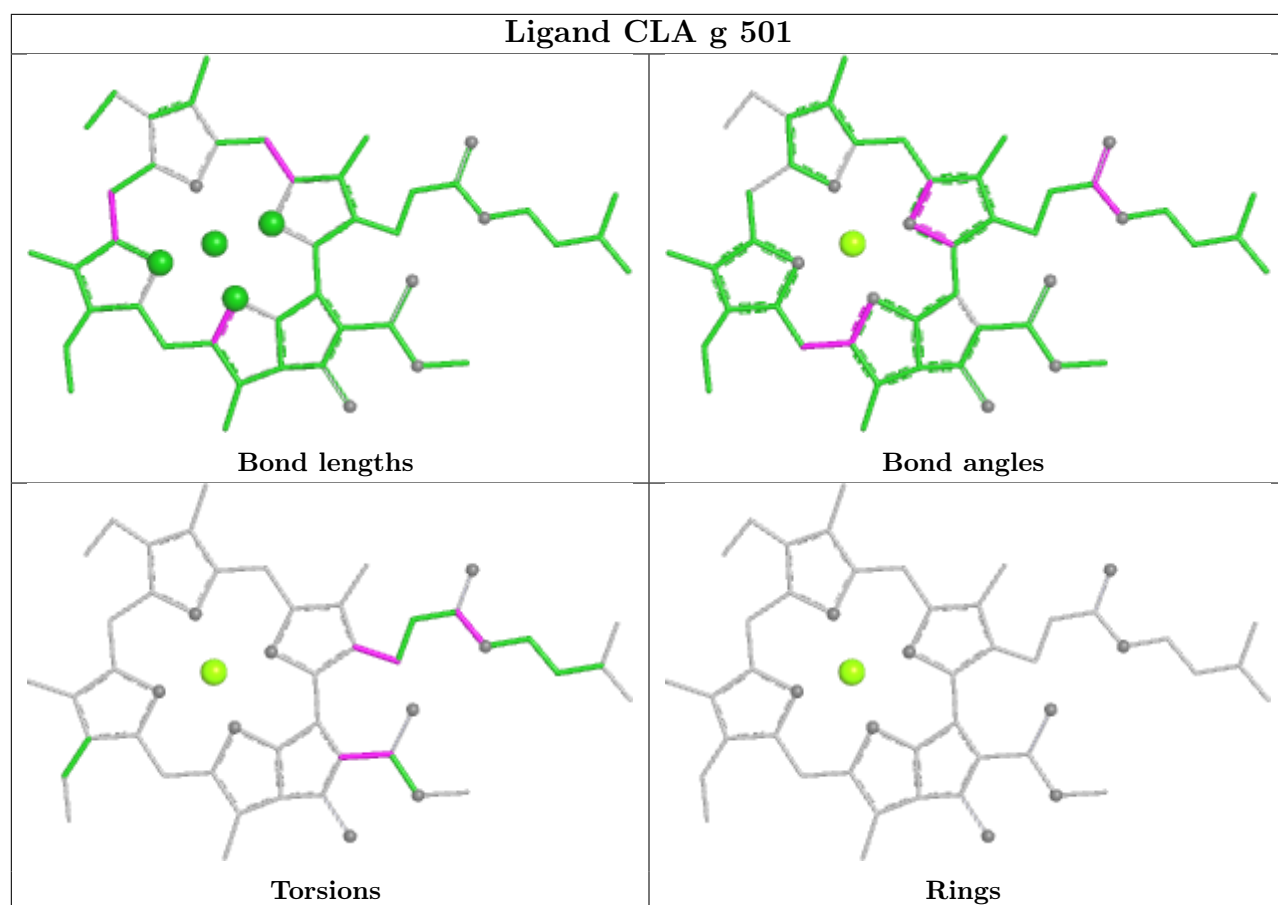


Ligand CLA o 502

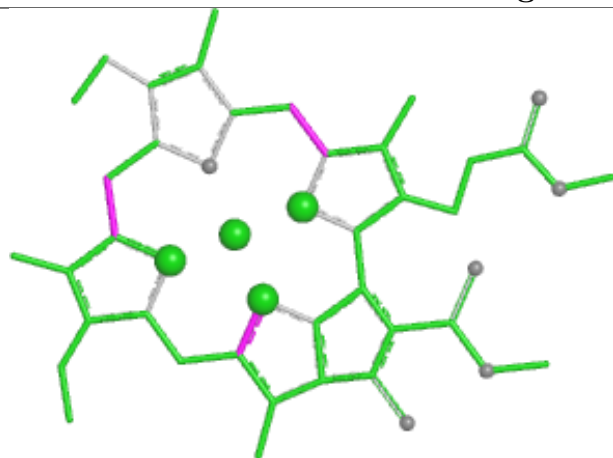


Ligand CLA w 510

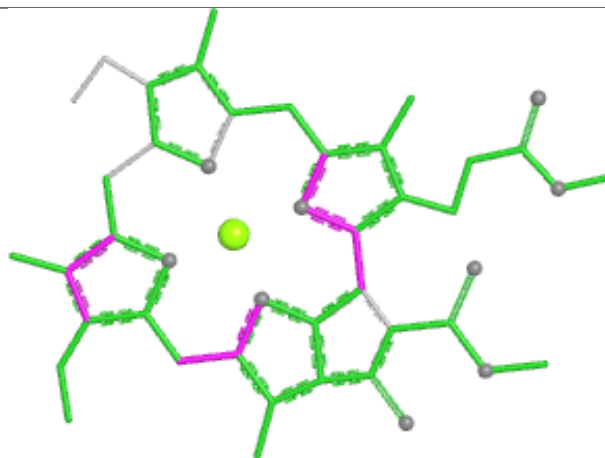




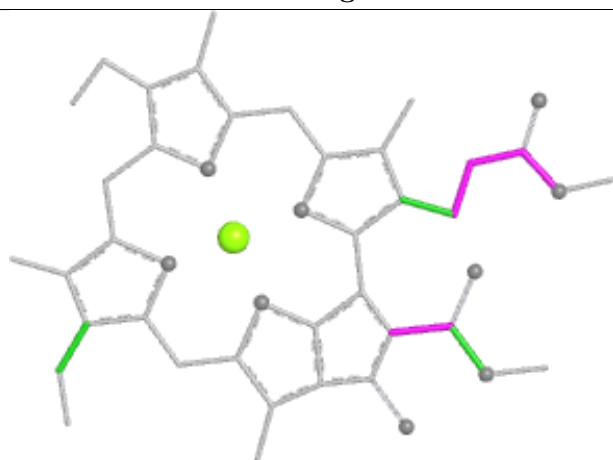
Ligand CLA h 501



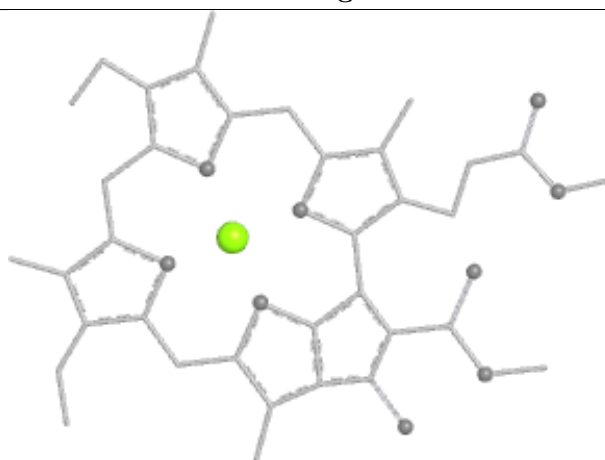
Bond lengths



Bond angles

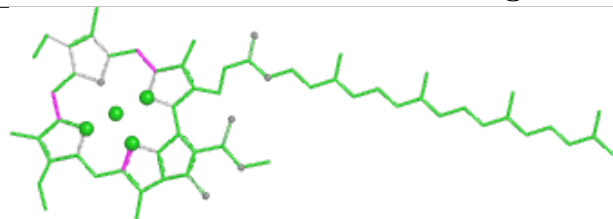


Torsions

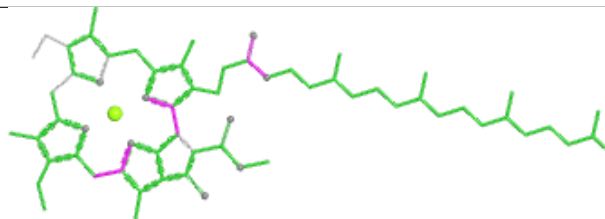


Rings

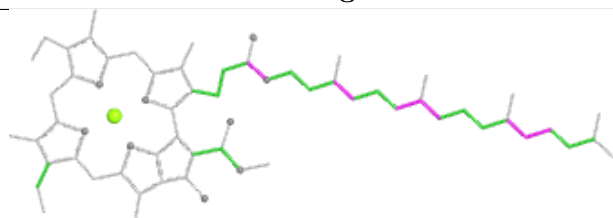
Ligand CLA U 1503



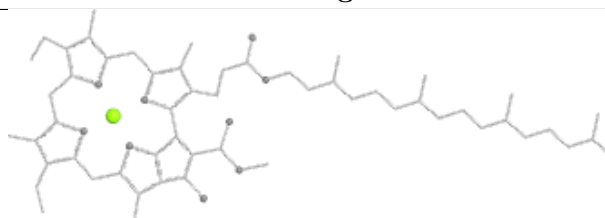
Bond lengths



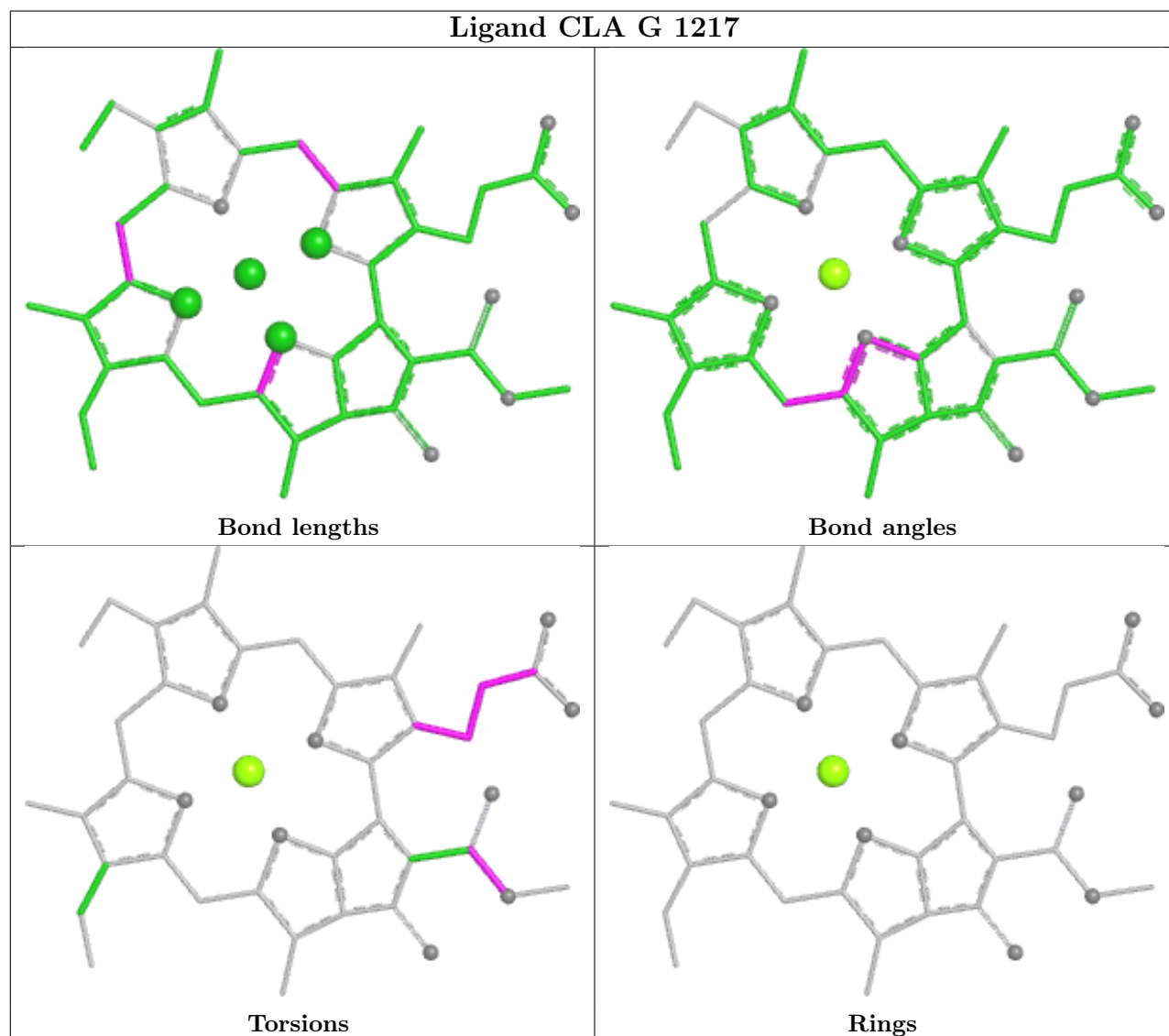
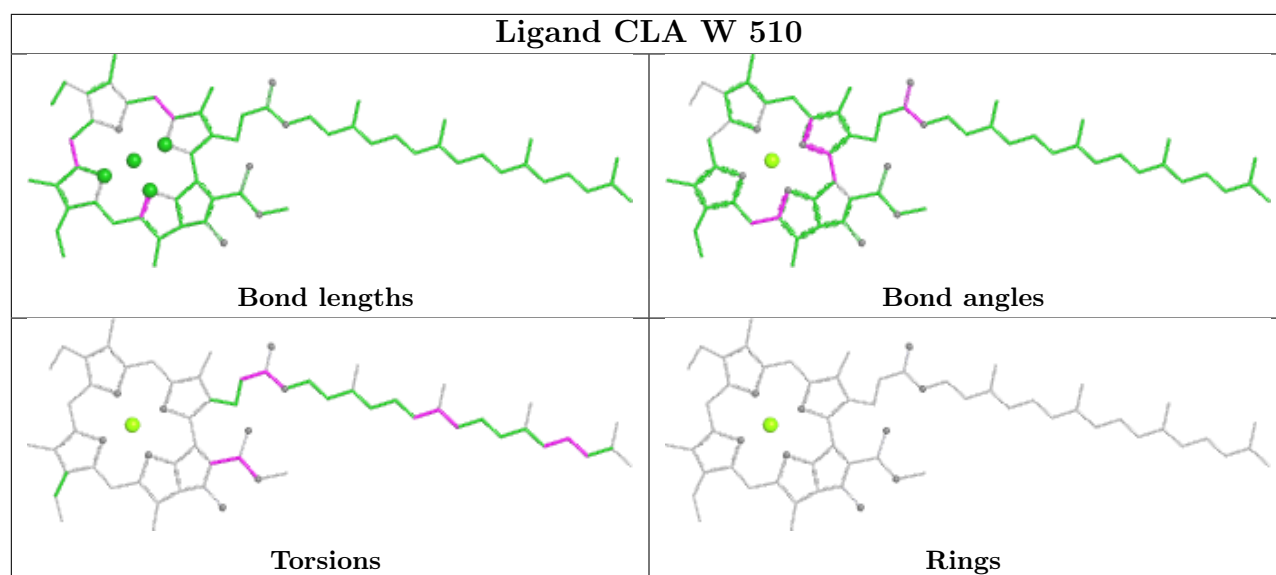
Bond angles

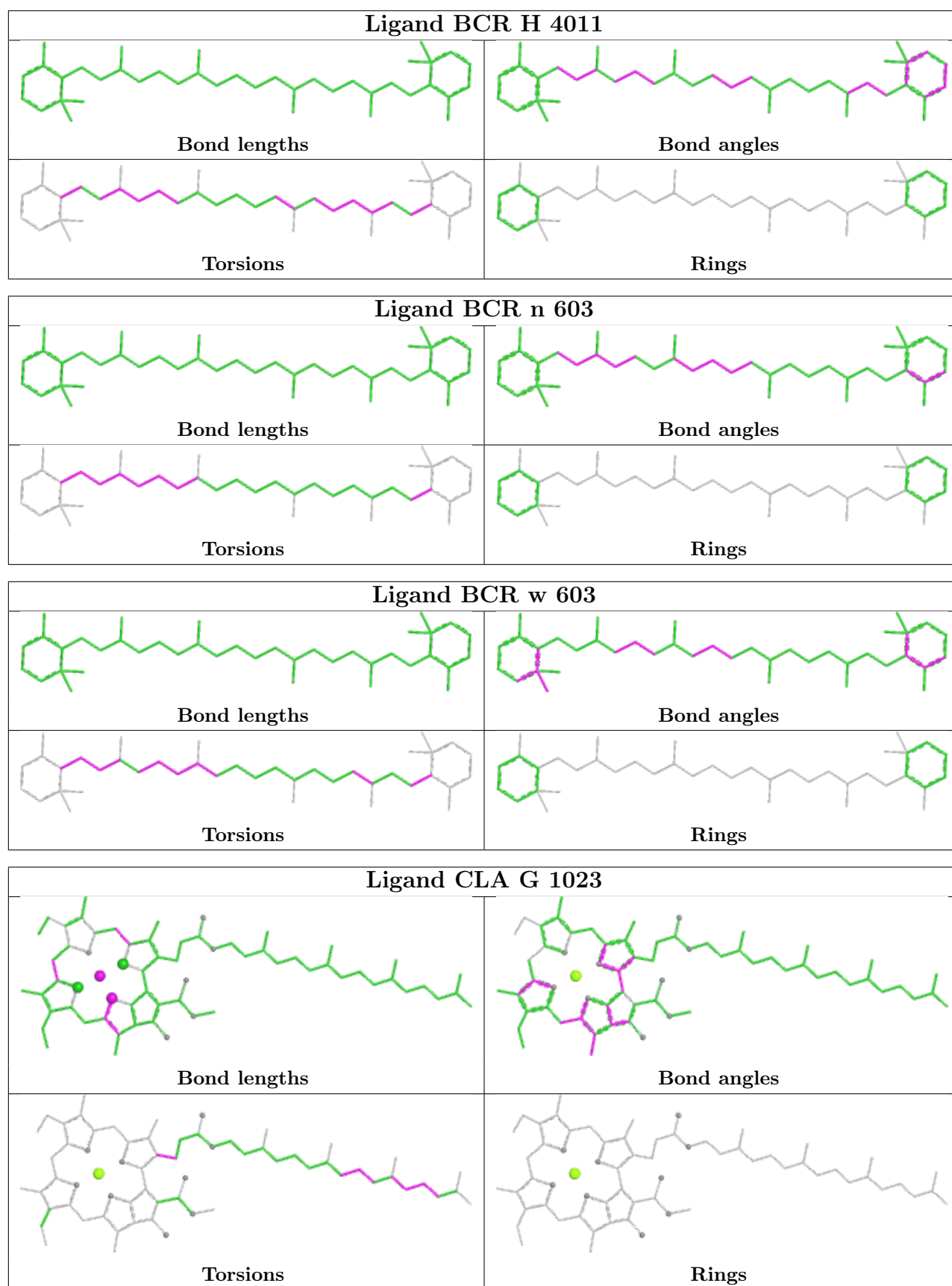


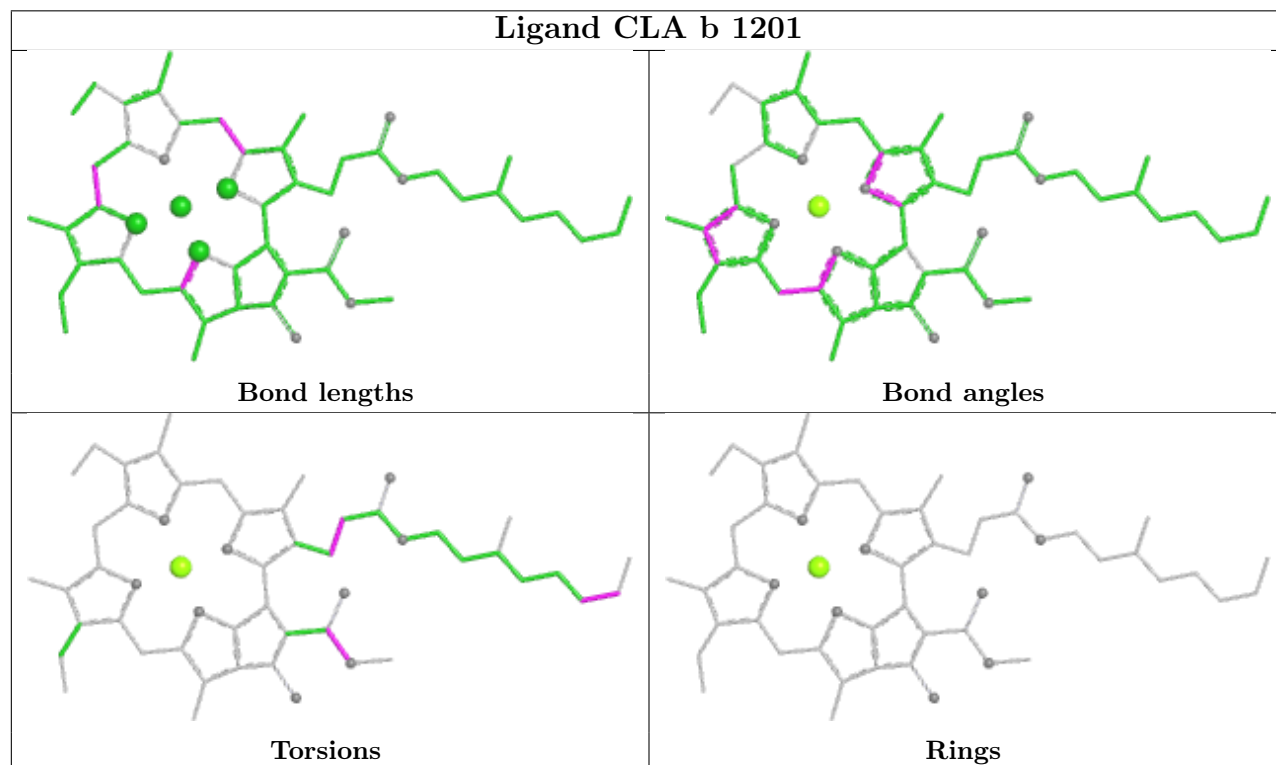
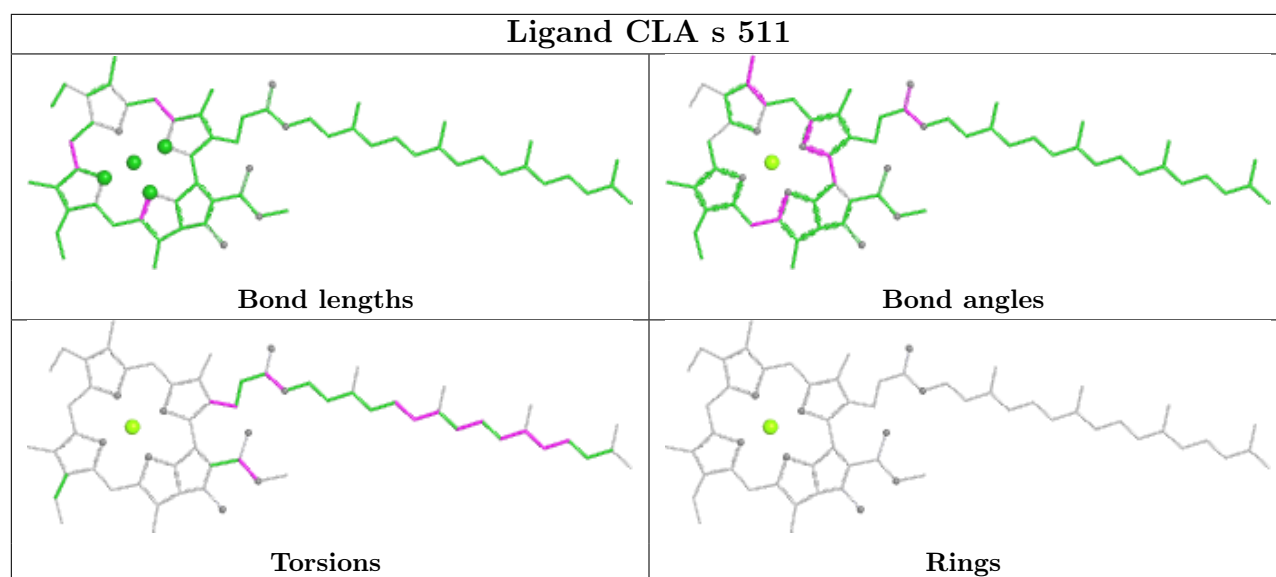
Torsions



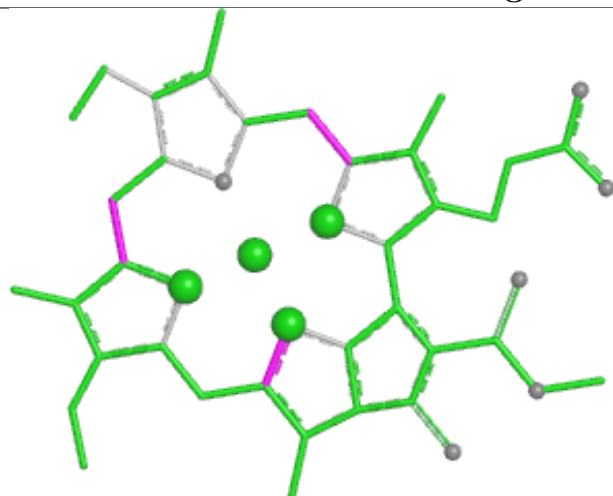
Rings



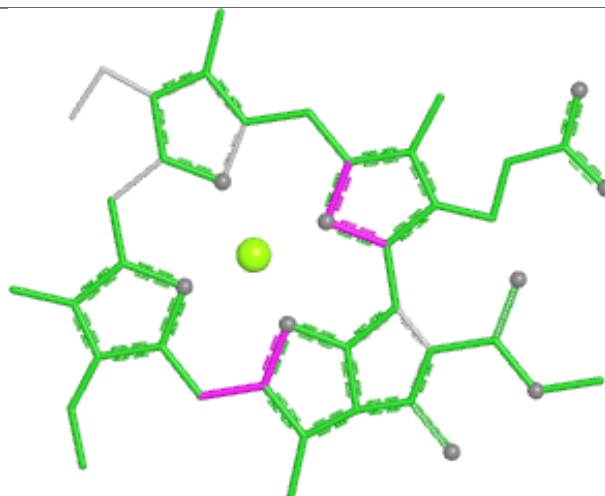




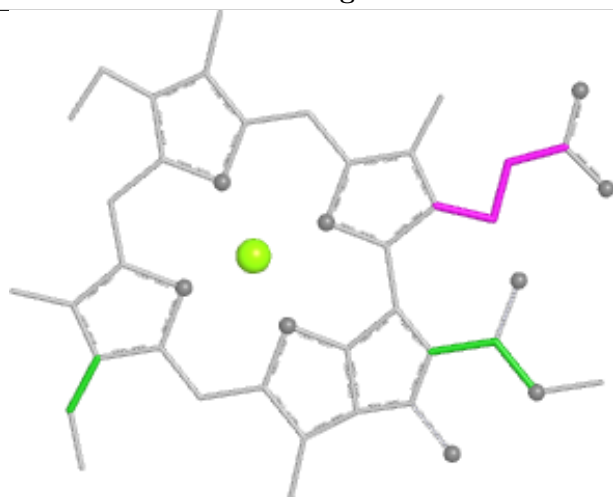
Ligand CLA B 1209



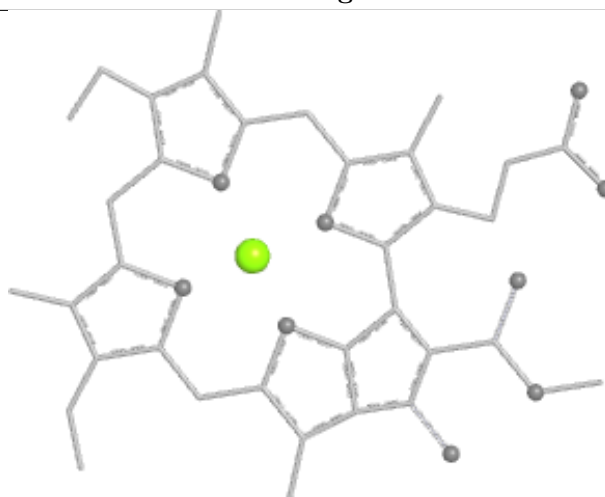
Bond lengths



Bond angles

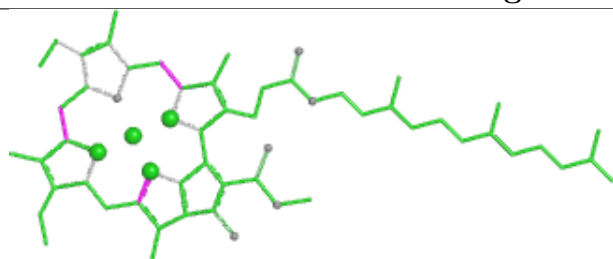


Torsions

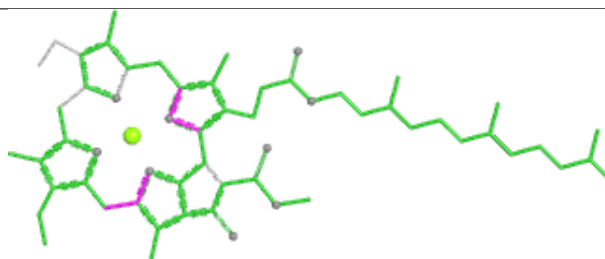


Rings

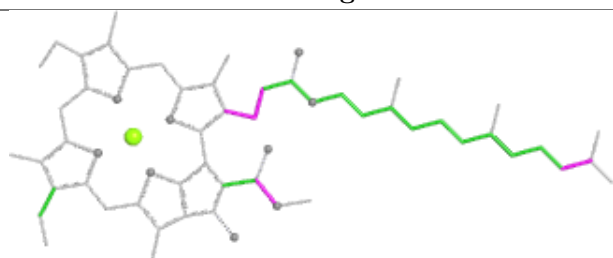
Ligand CLA G 1215



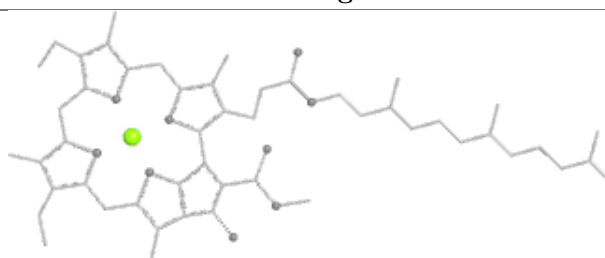
Bond lengths



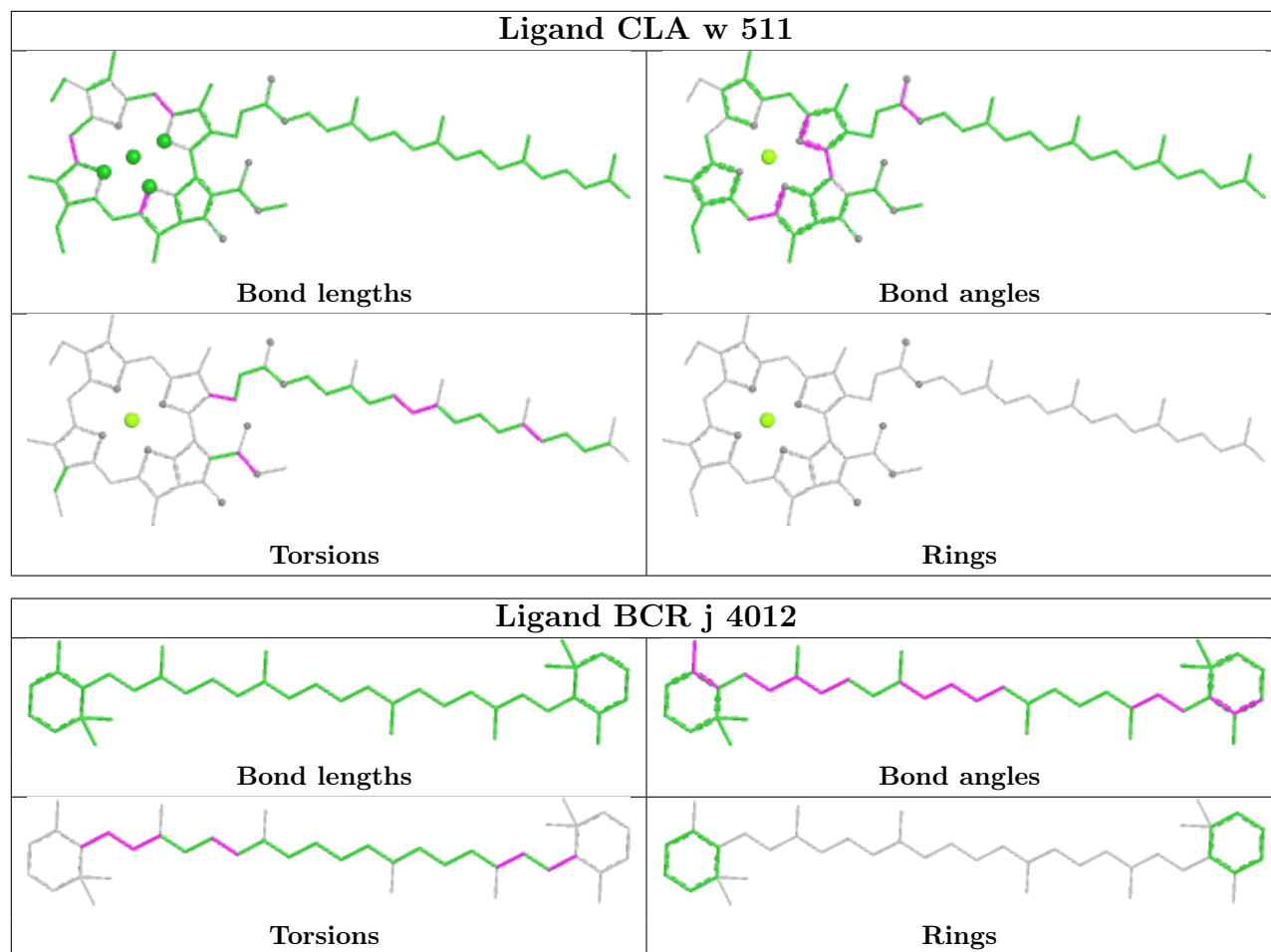
Bond angles



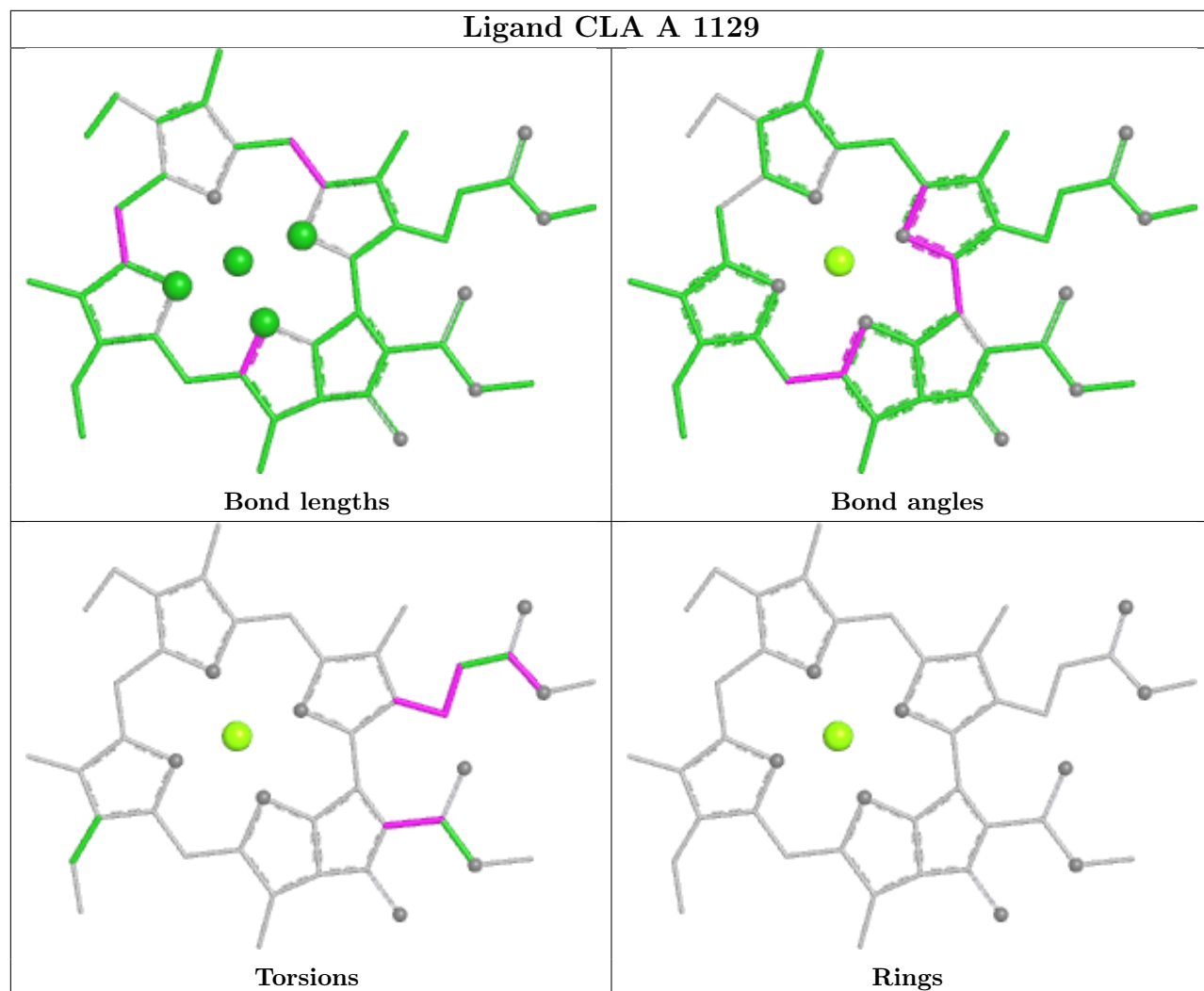
Torsions

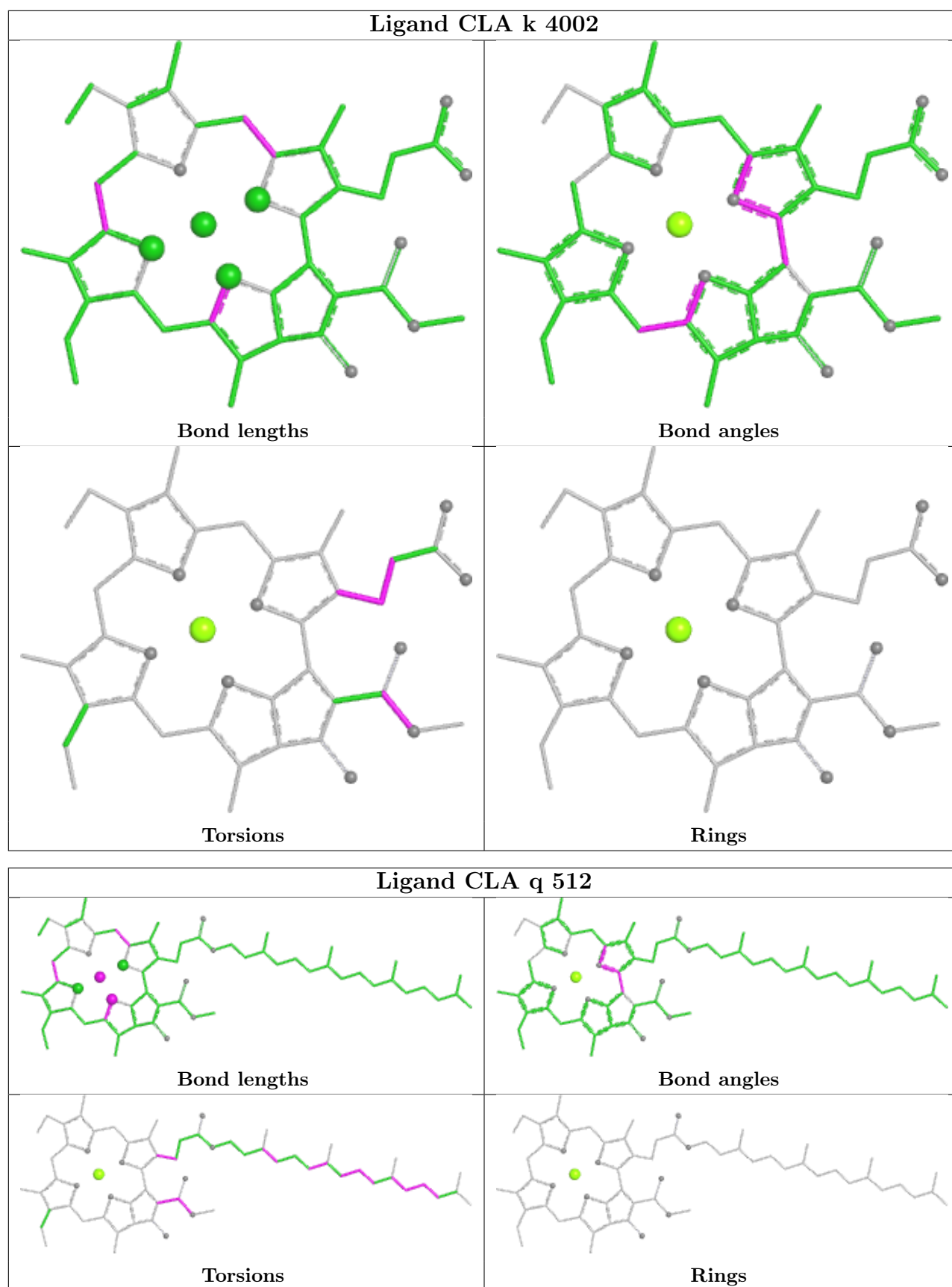


Rings

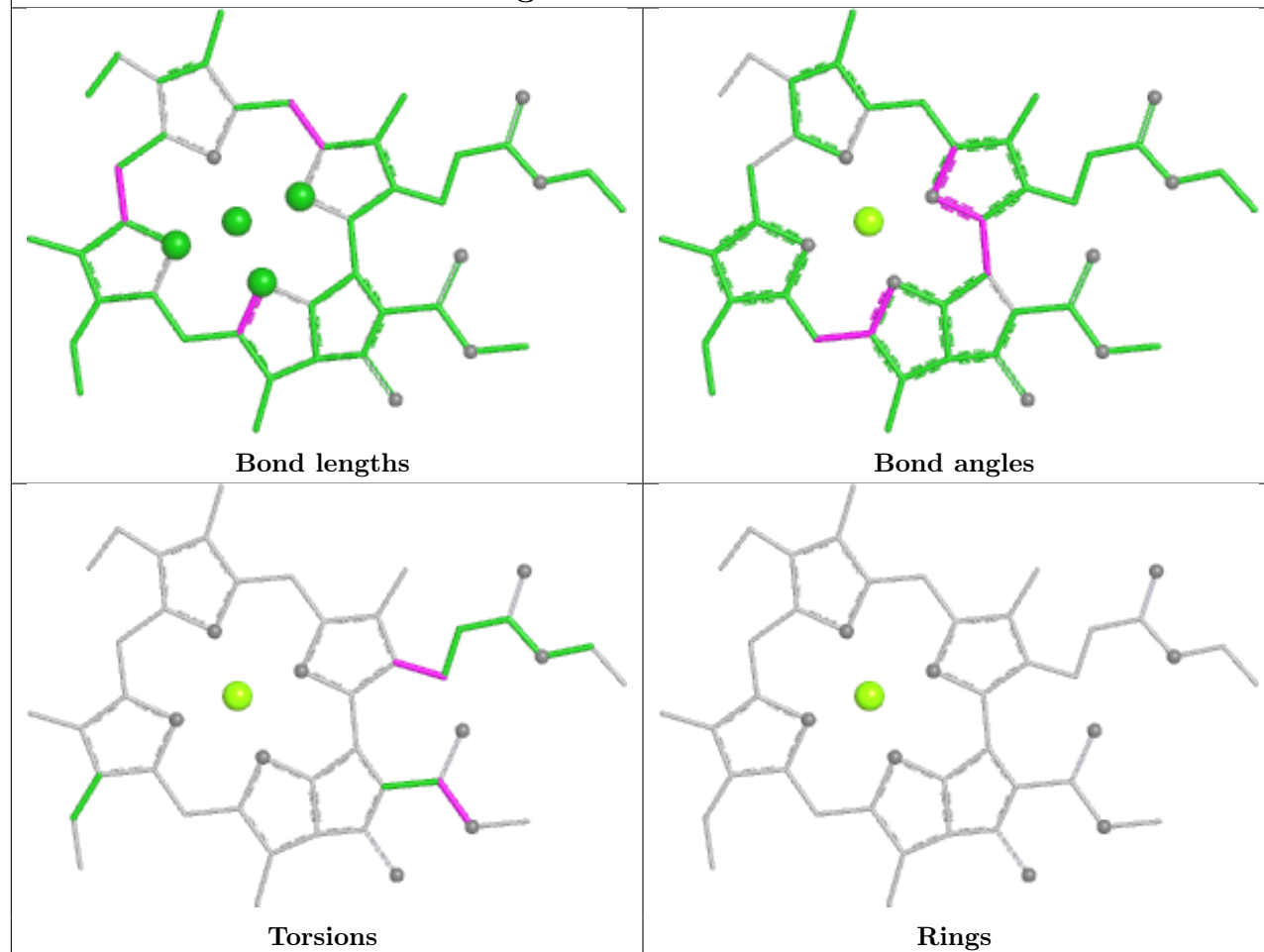


Ligand CLA A 1129

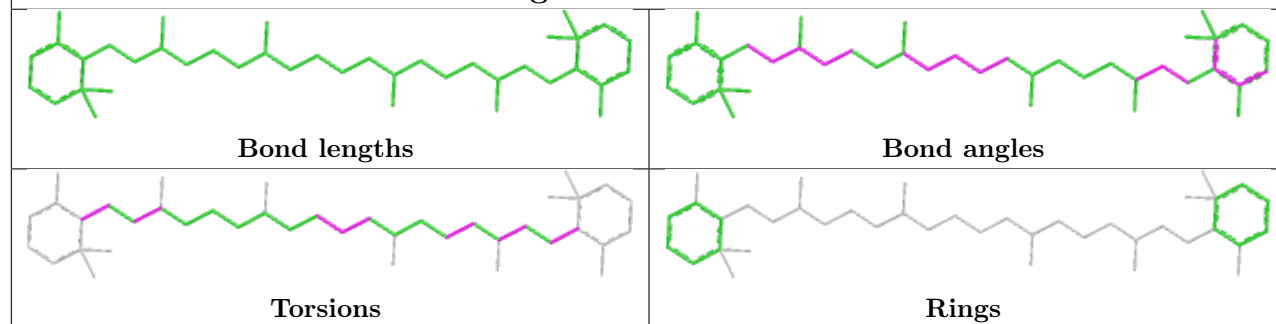


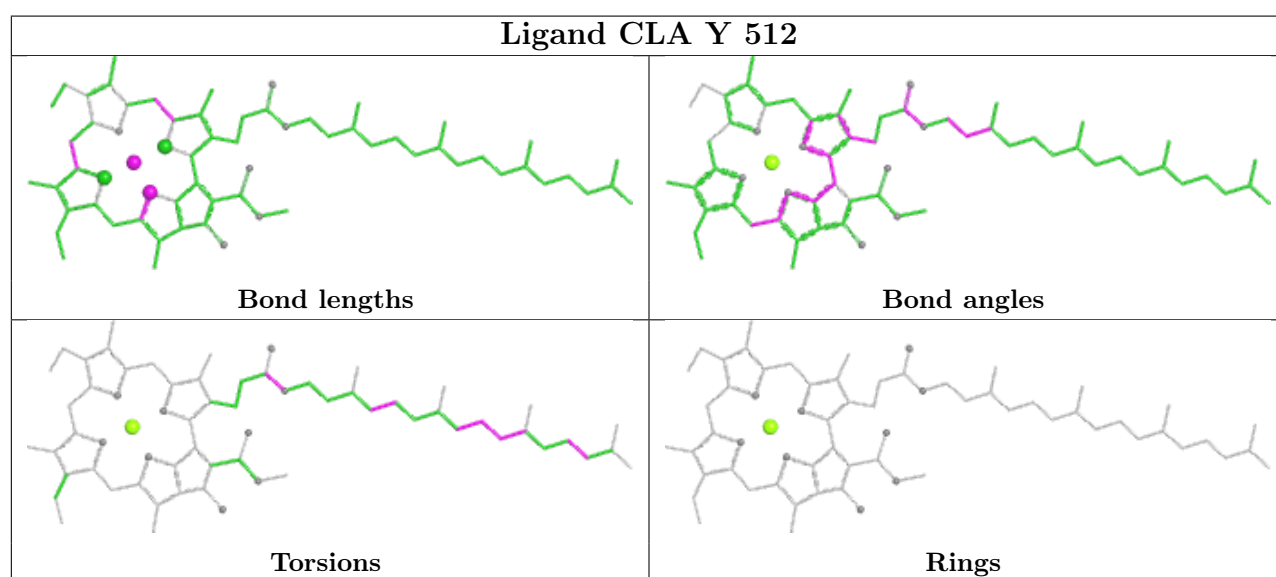
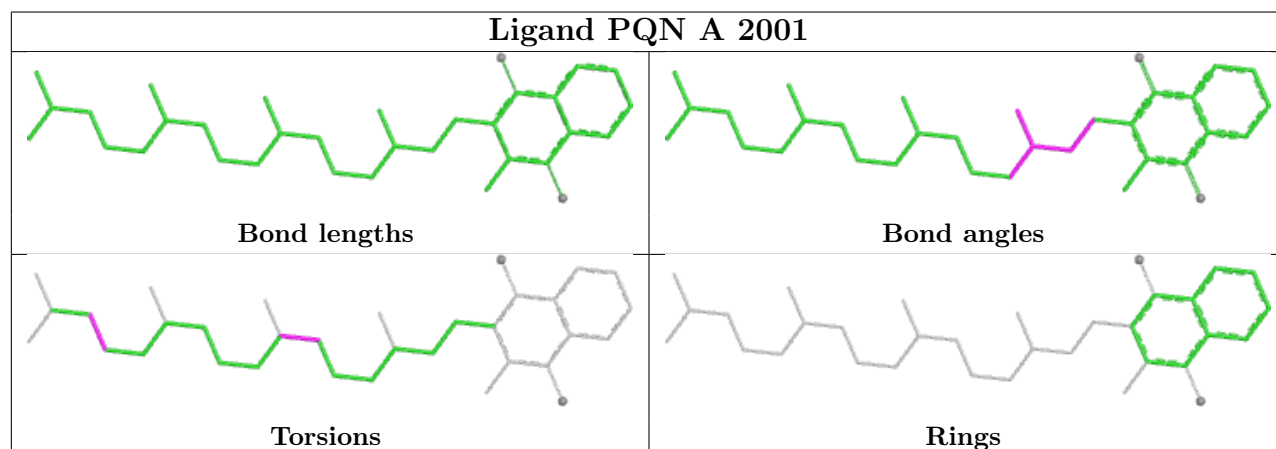
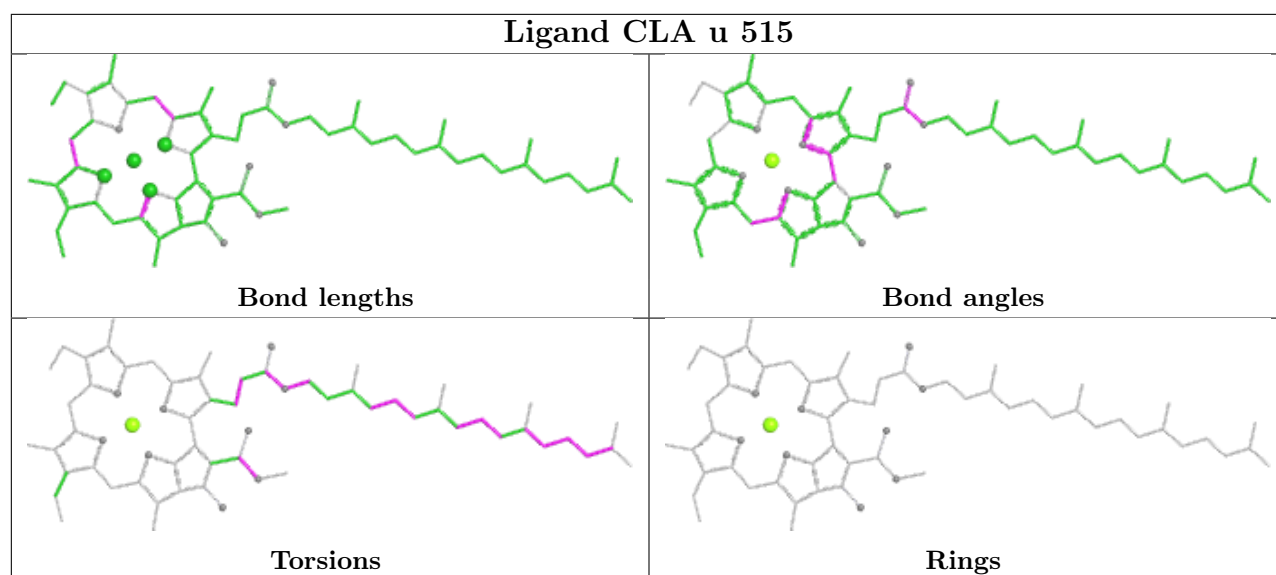


Ligand CLA G 1216

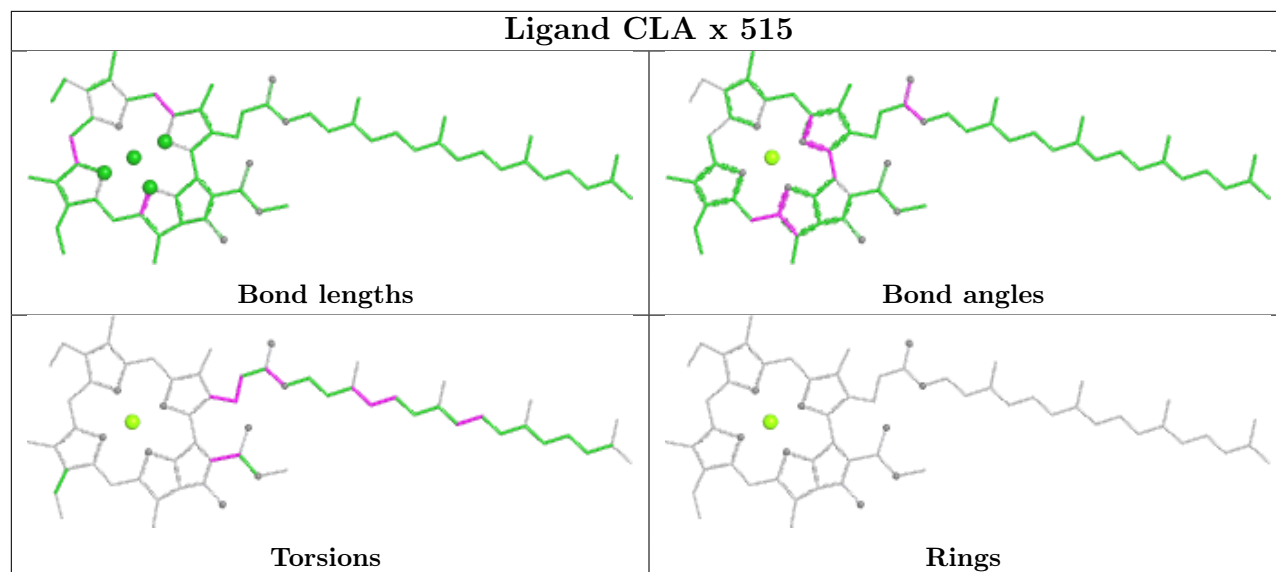


Ligand BCR w 602

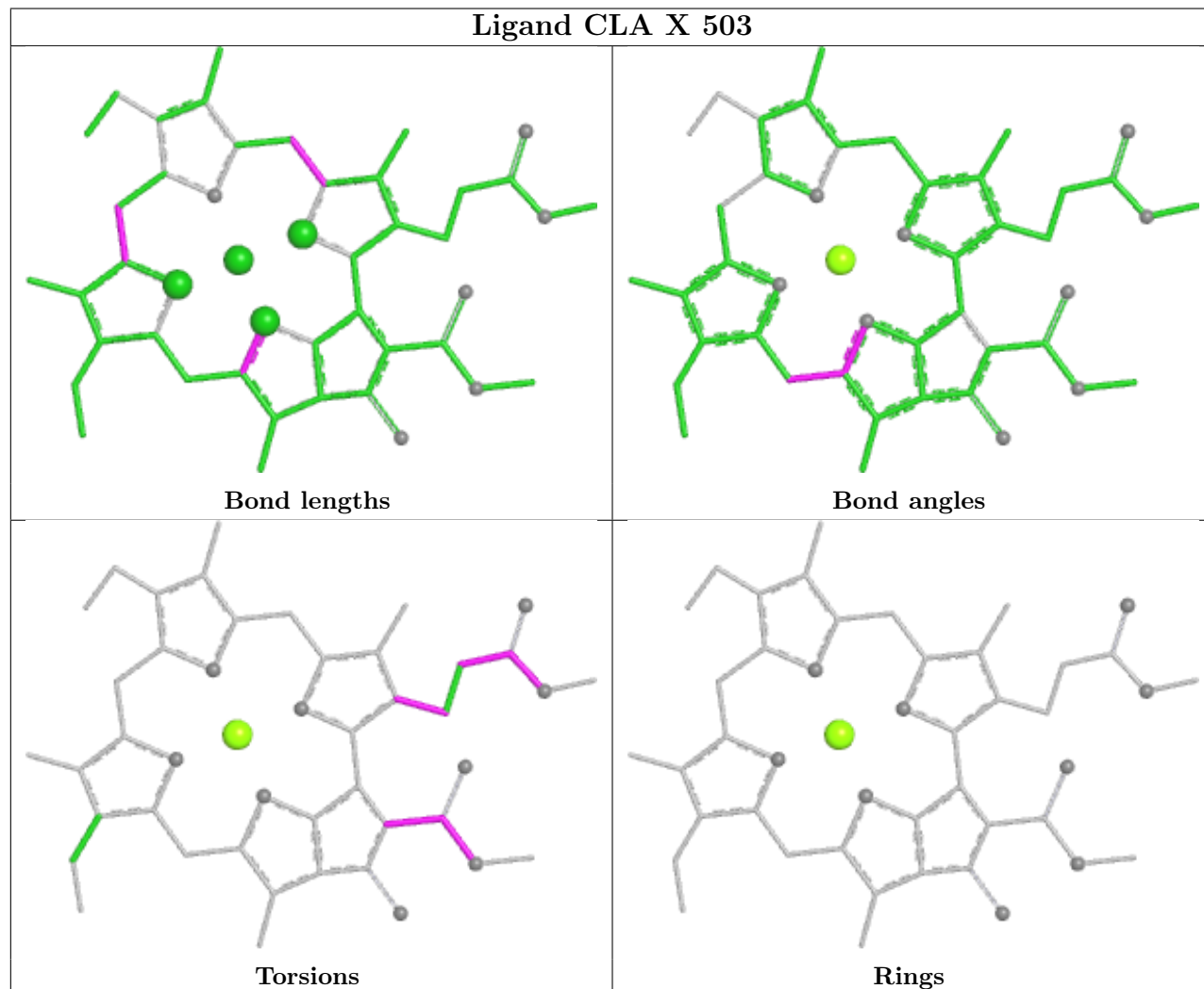




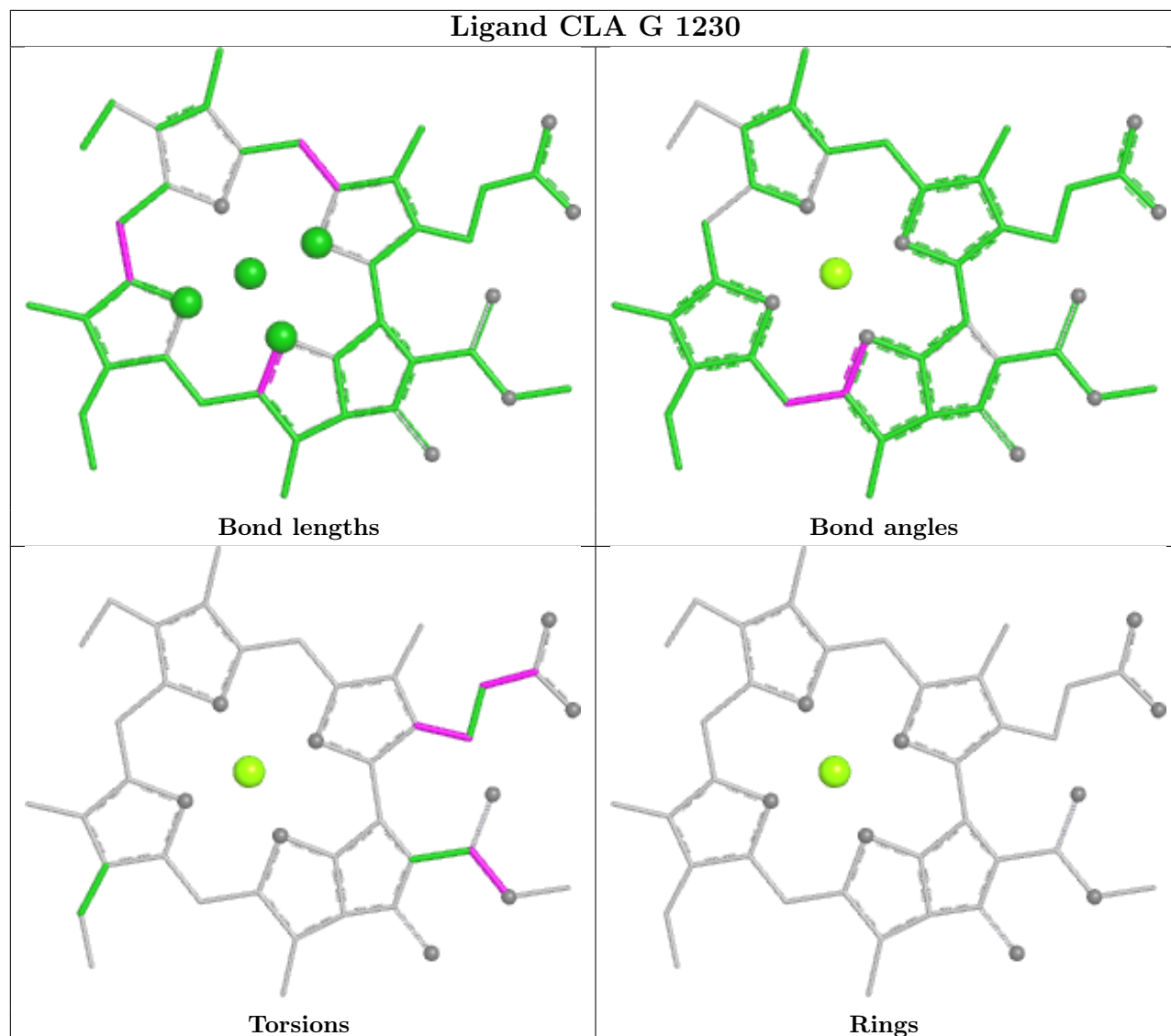
Ligand CLA x 515



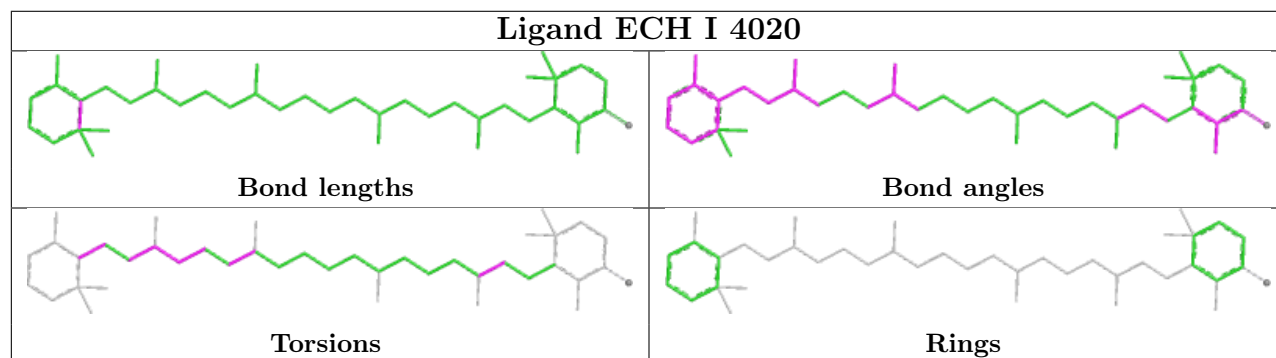
Ligand CLA X 503

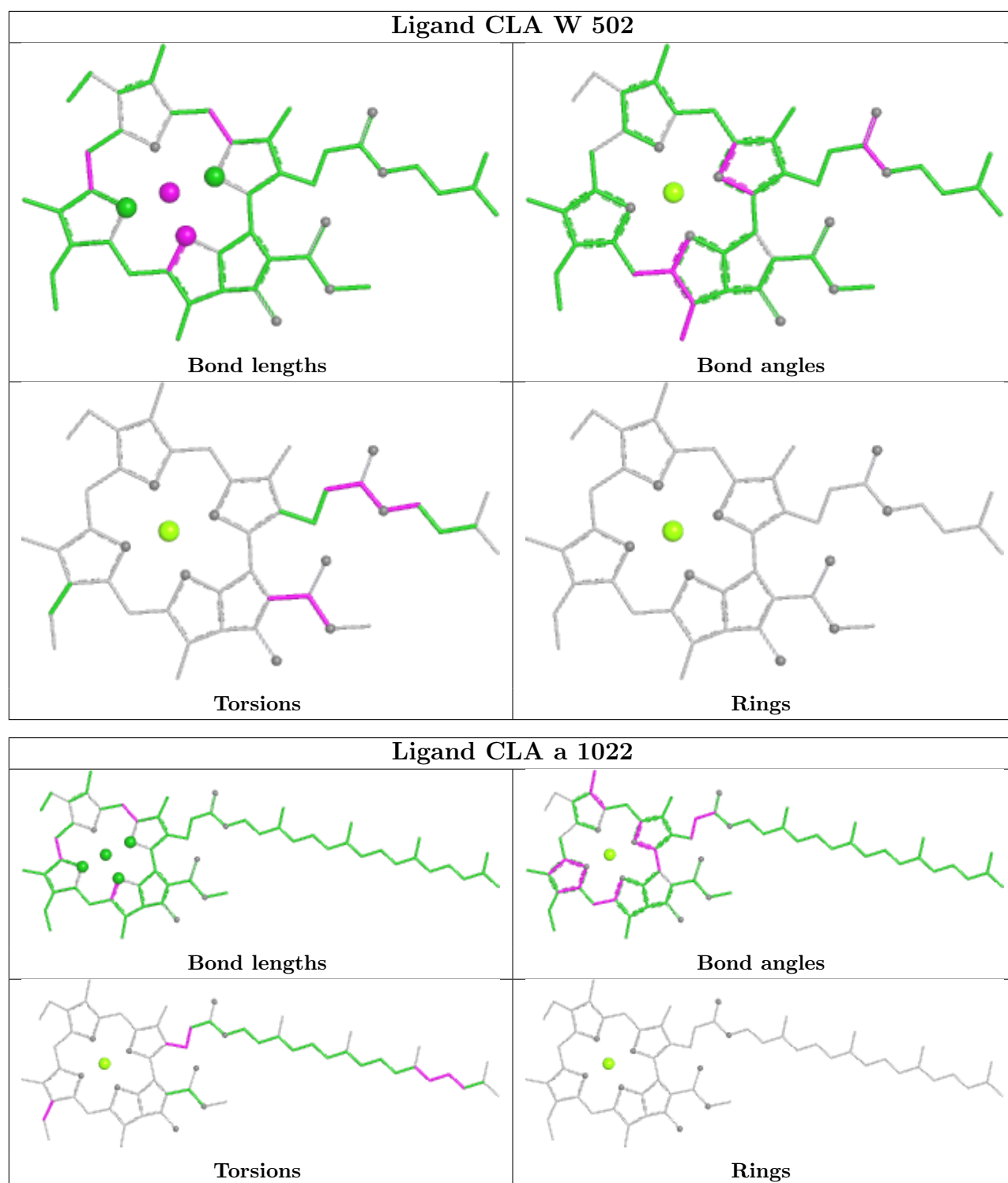


Ligand CLA G 1230

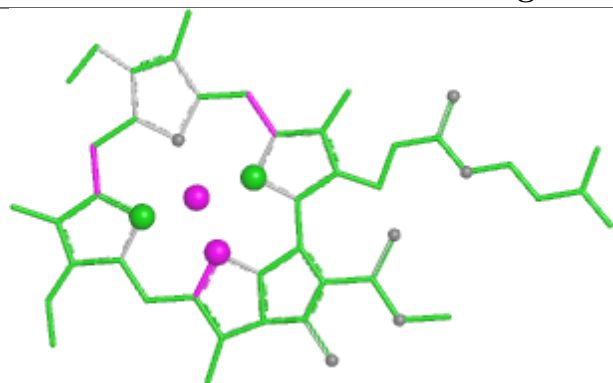


Ligand ECH I 4020

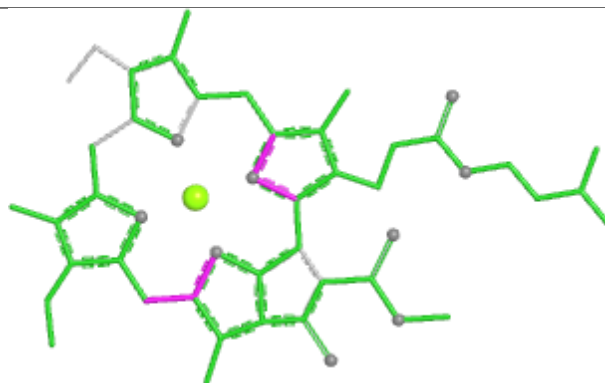




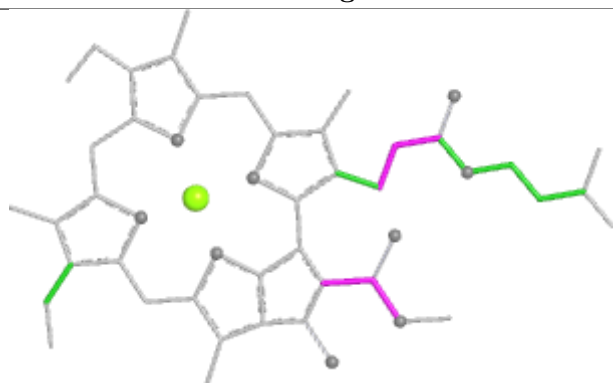
Ligand CLA u 502



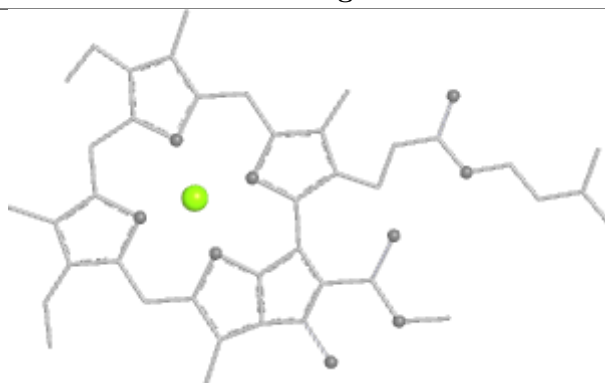
Bond lengths



Bond angles

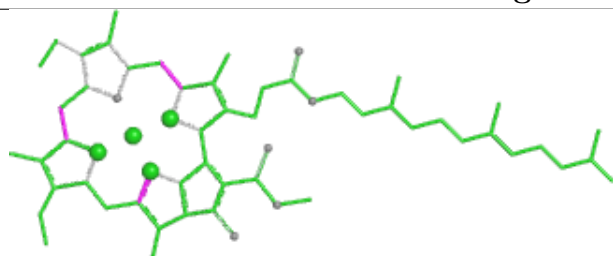


Torsions

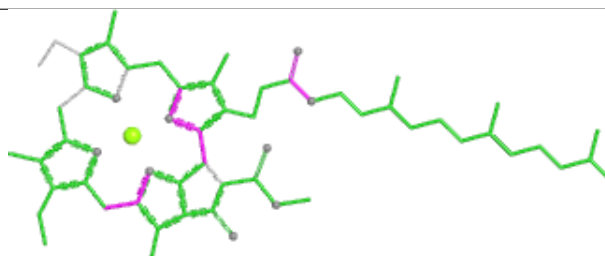


Rings

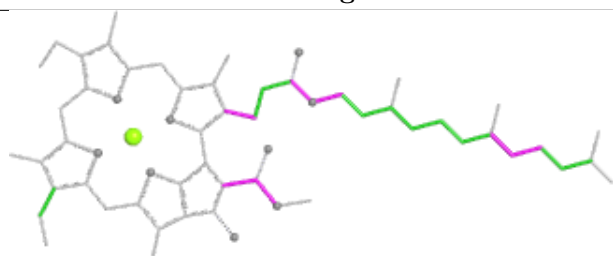
Ligand CLA Y 506



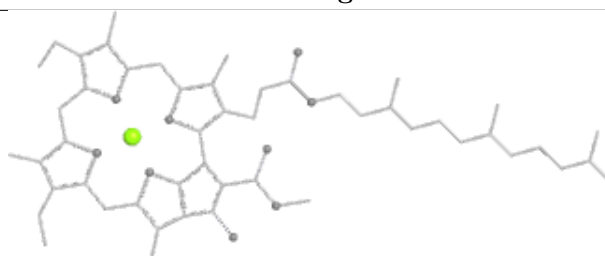
Bond lengths



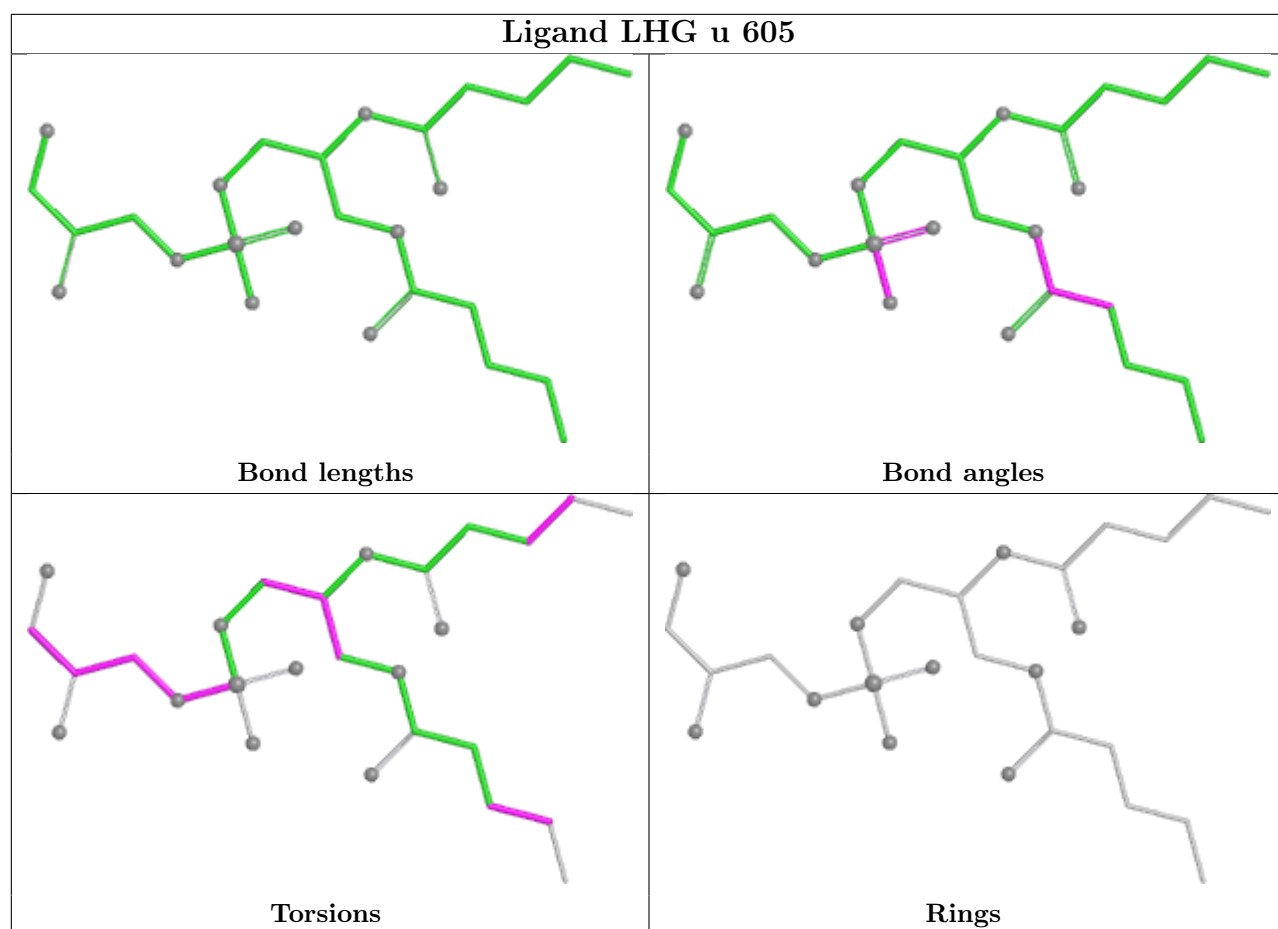
Bond angles

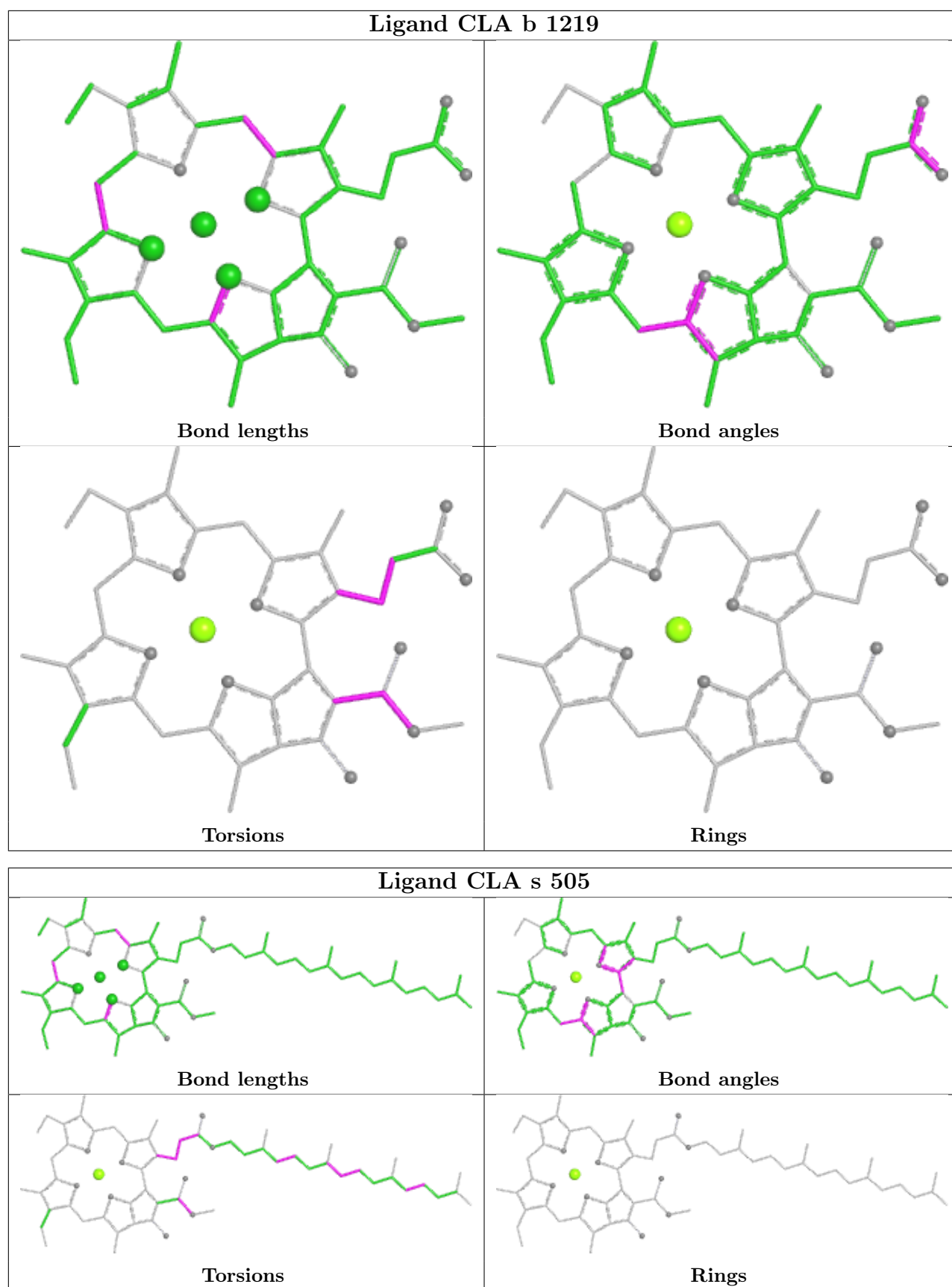


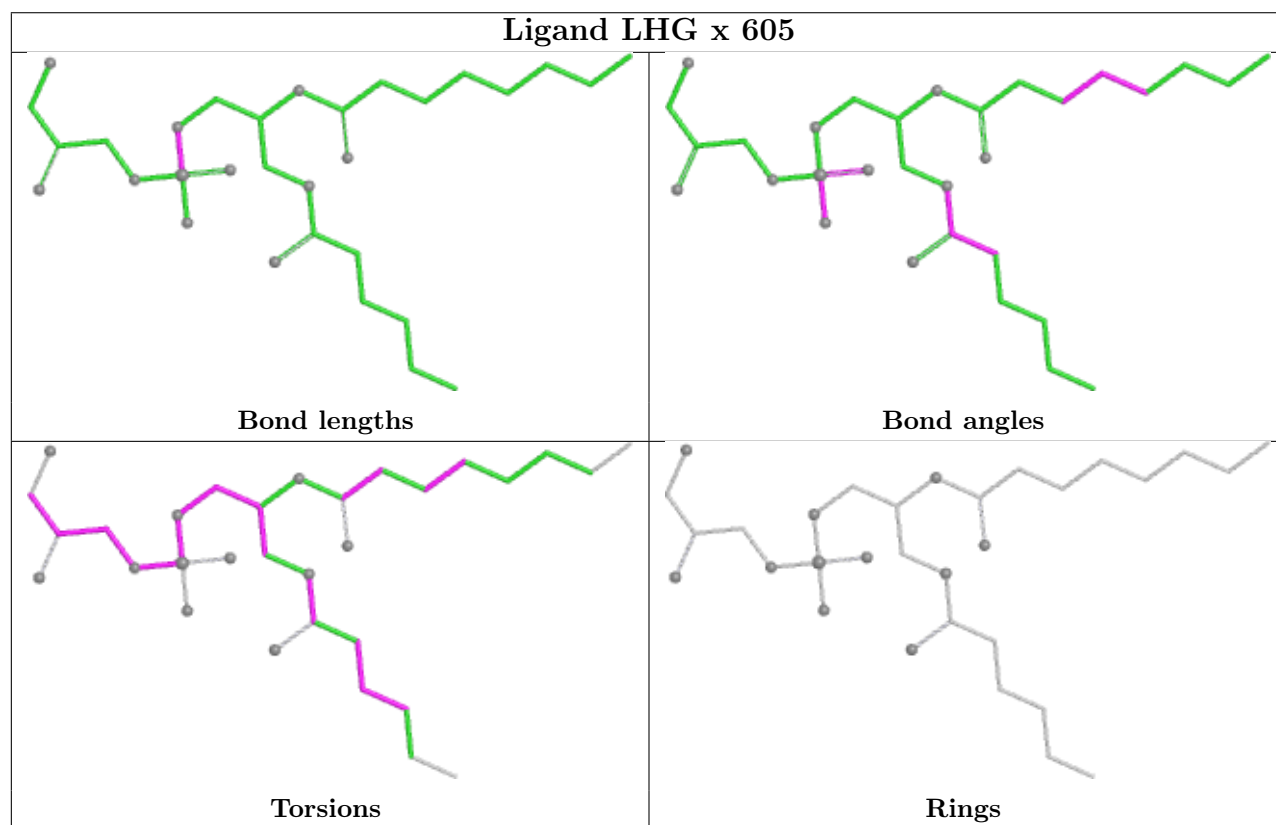
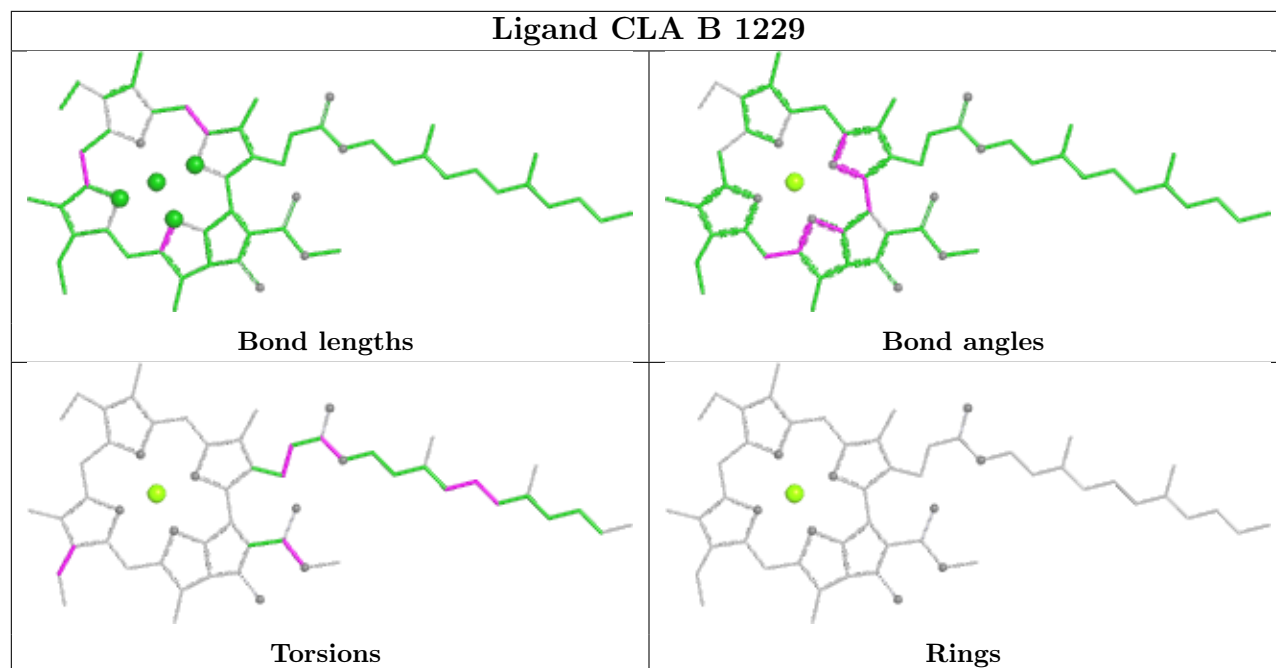
Torsions

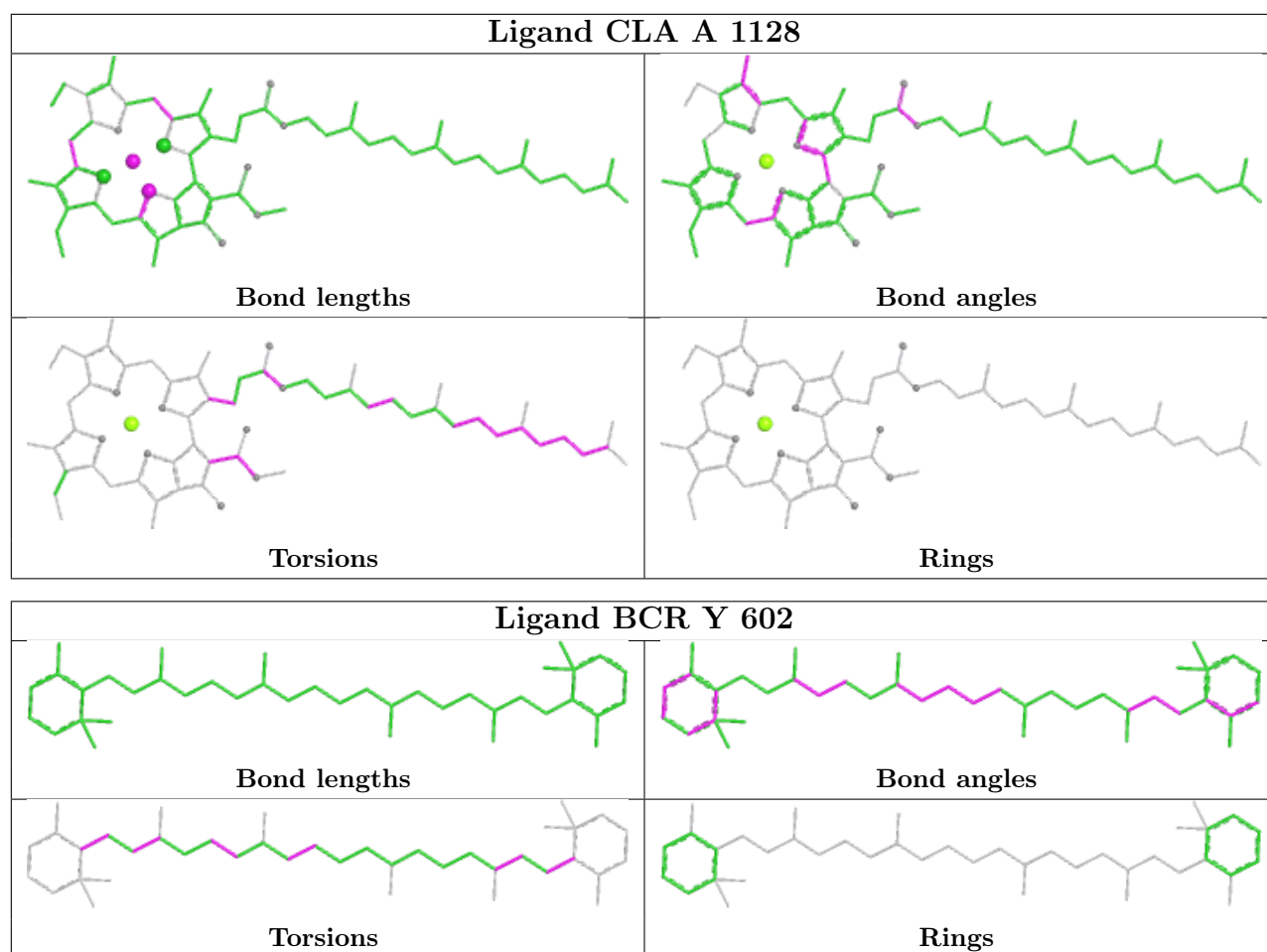


Rings

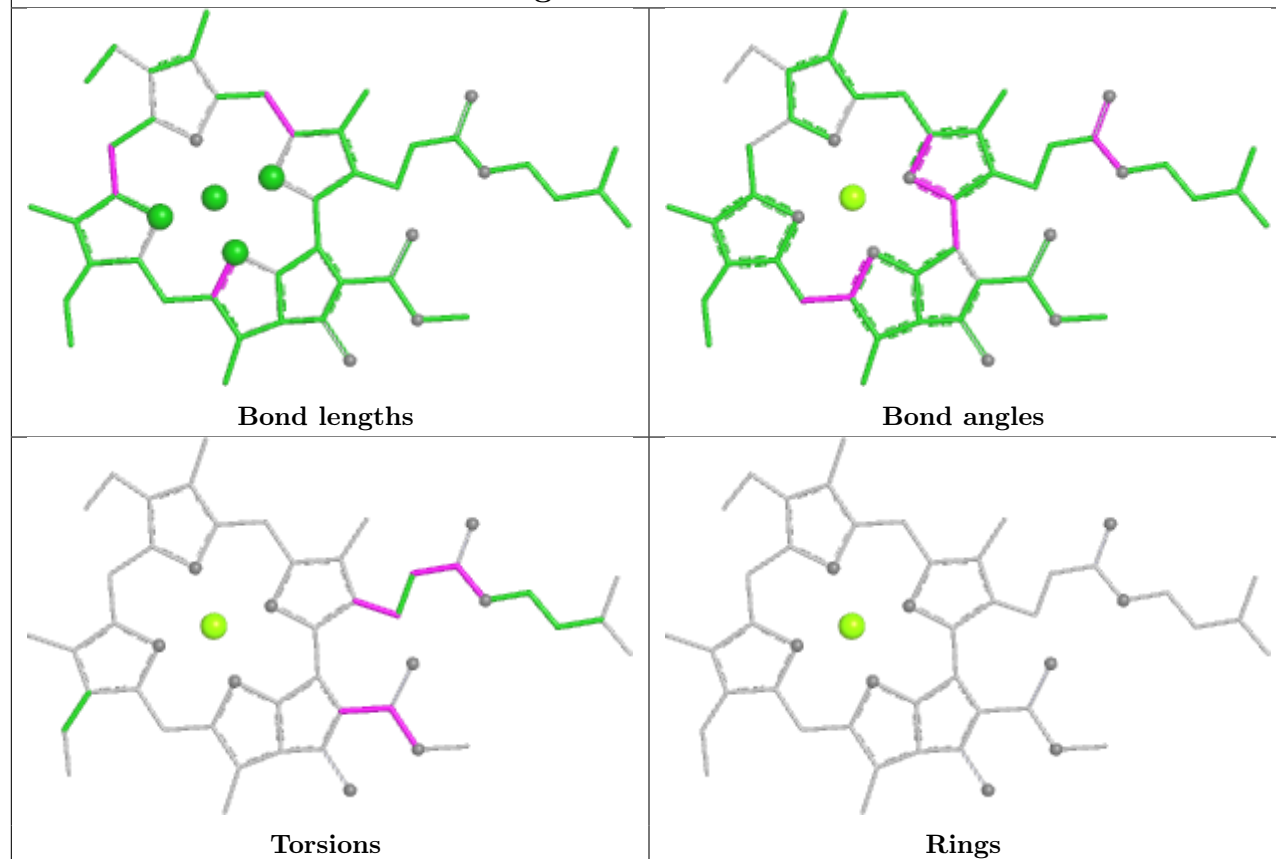




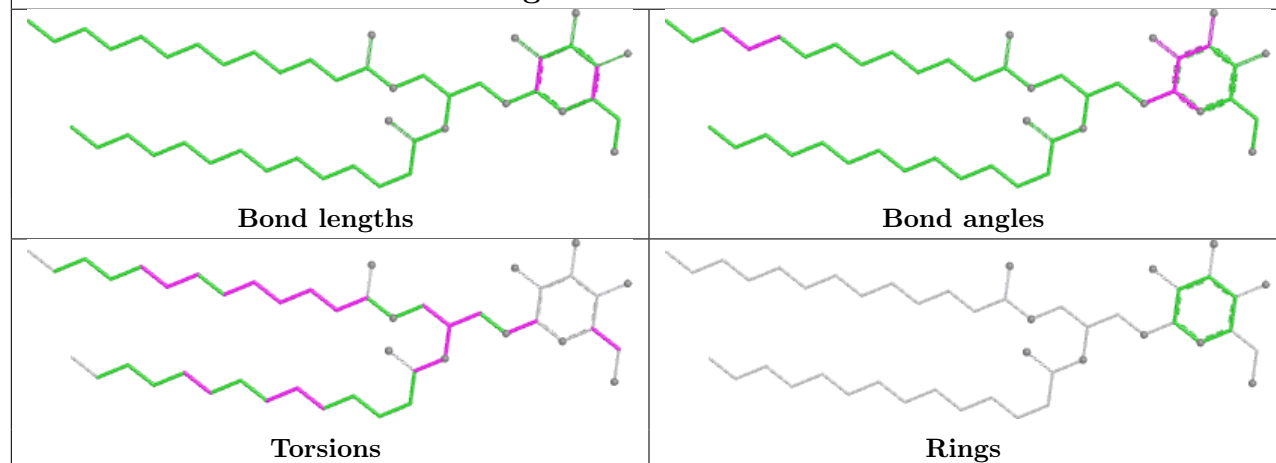


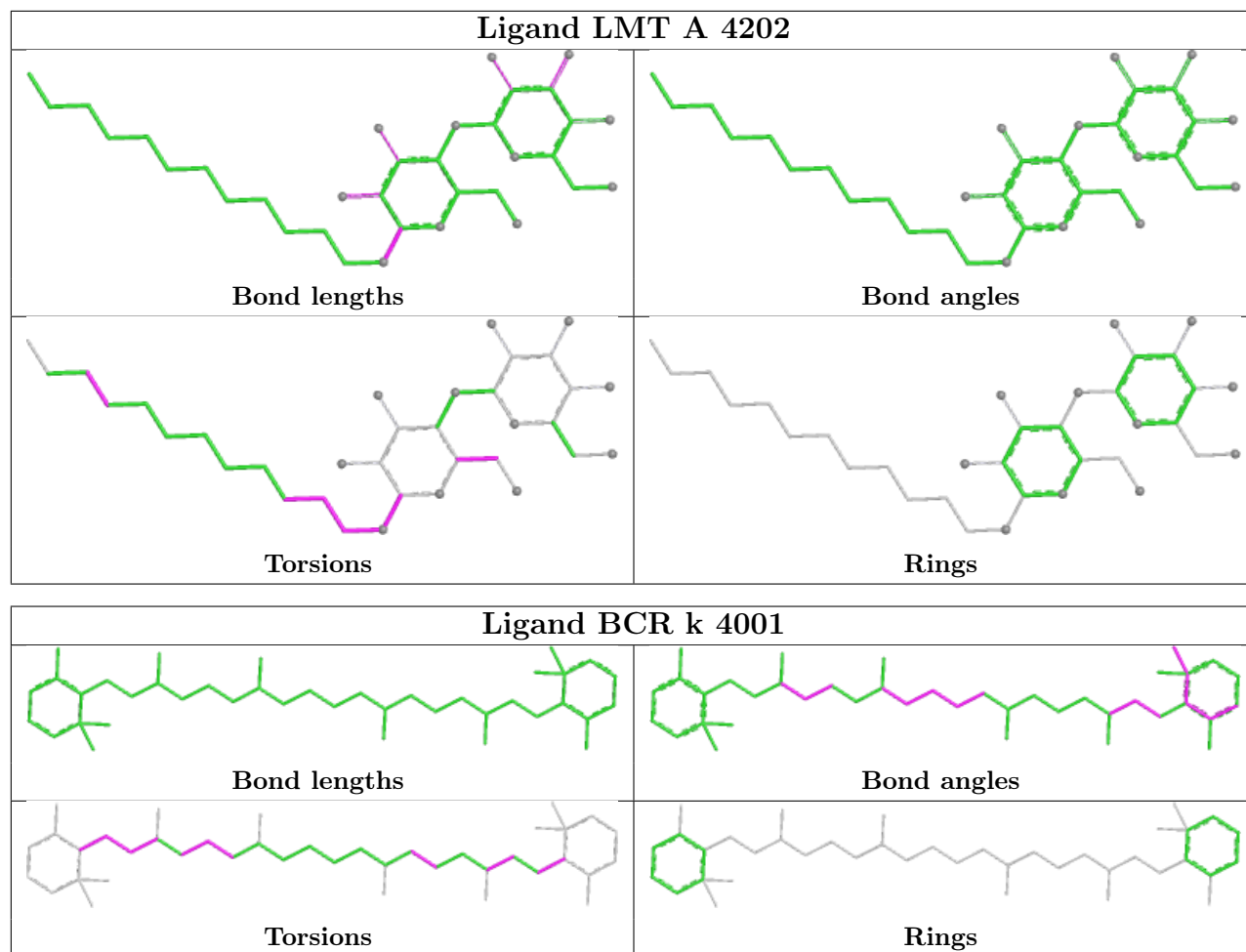


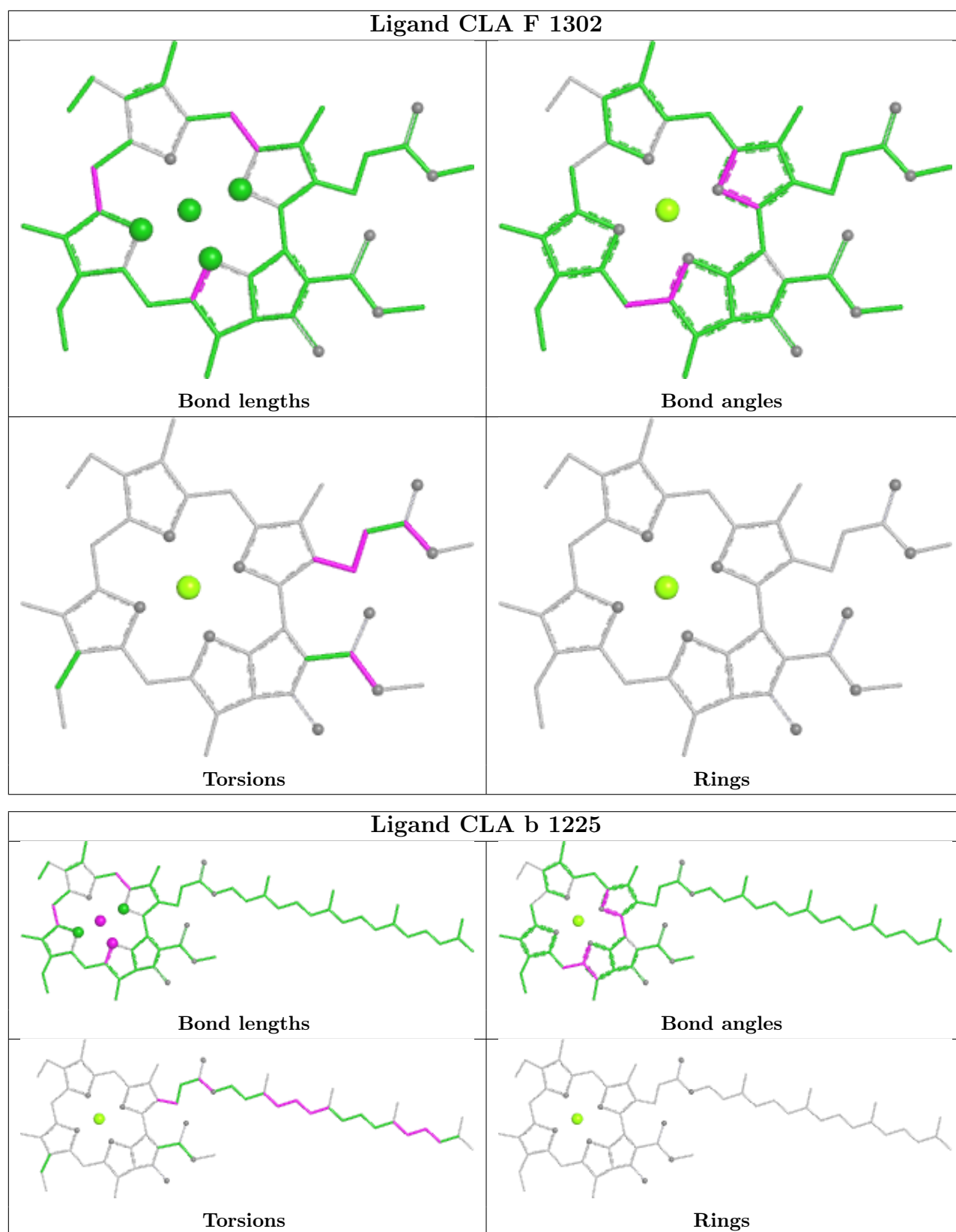
Ligand CLA Z 514

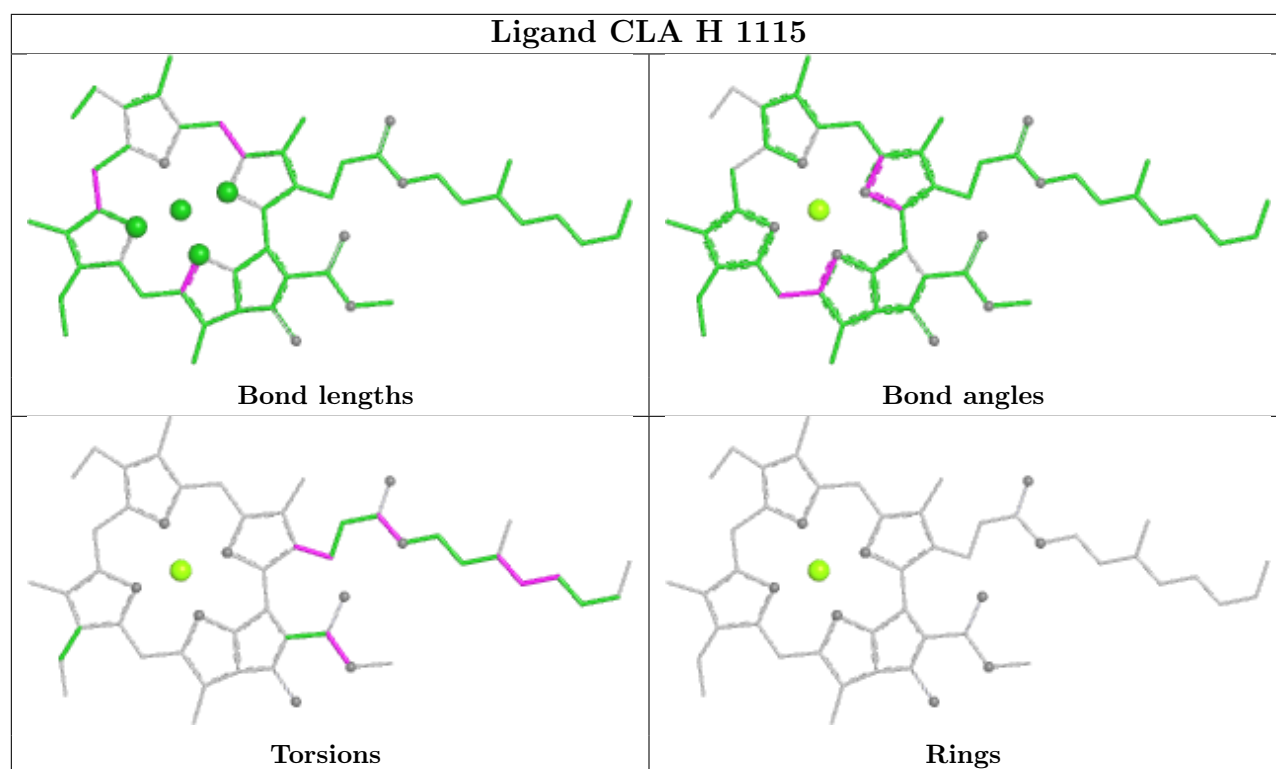


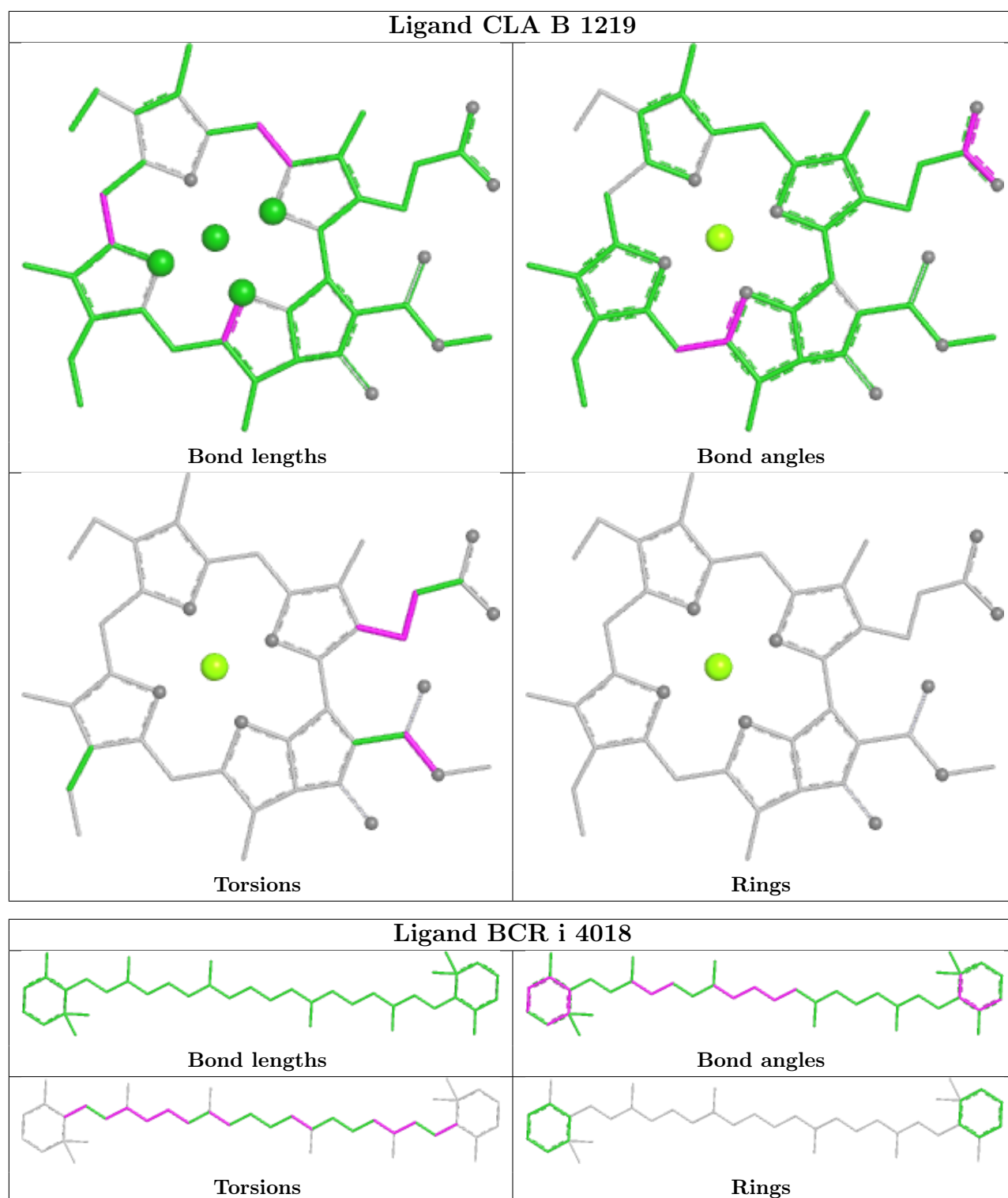
Ligand LMG a 4101



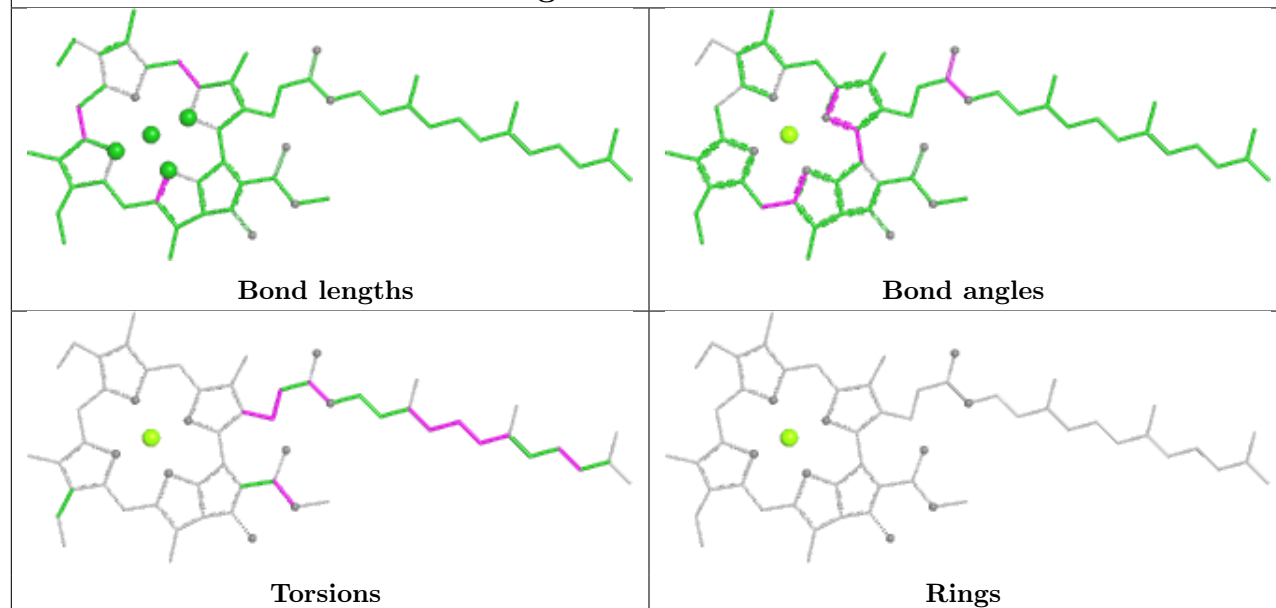




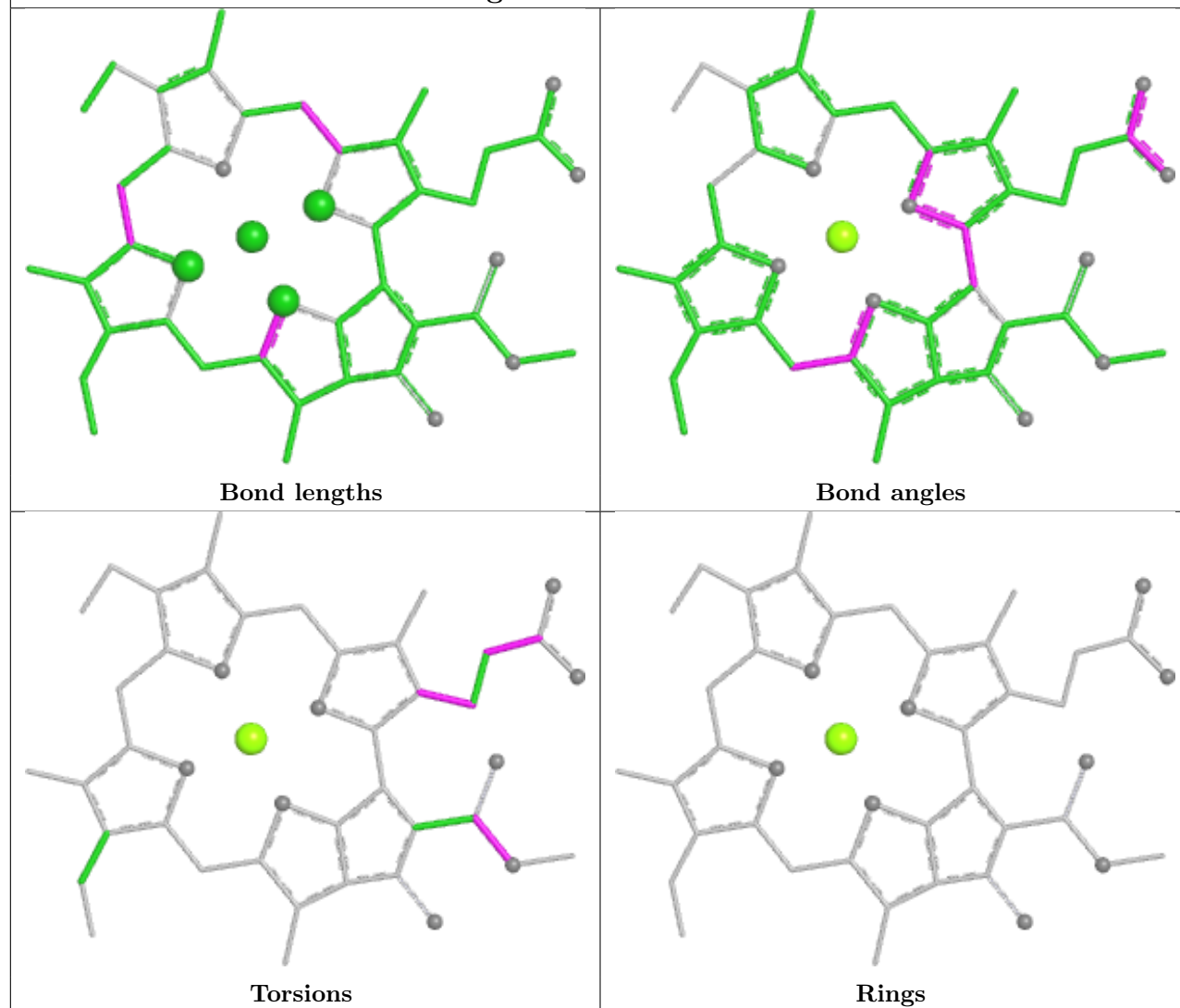


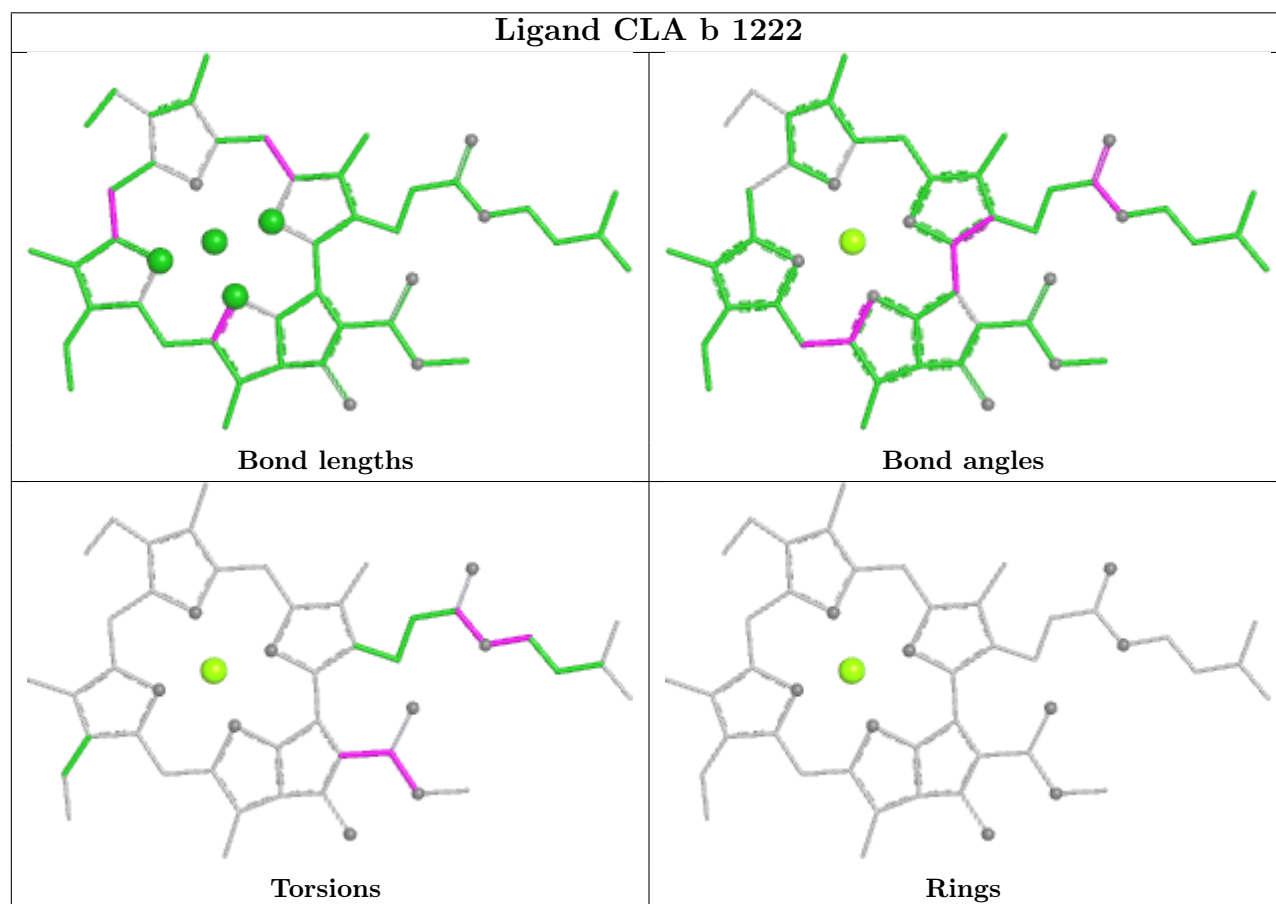
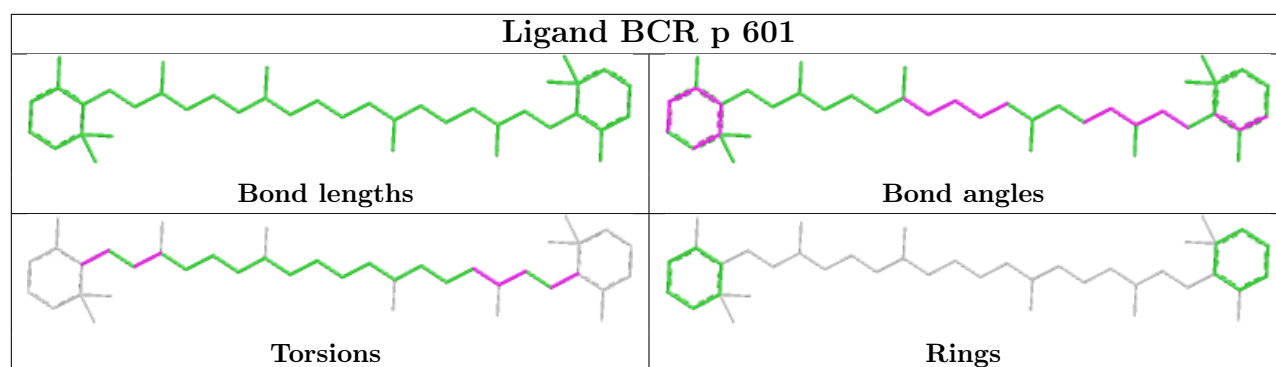


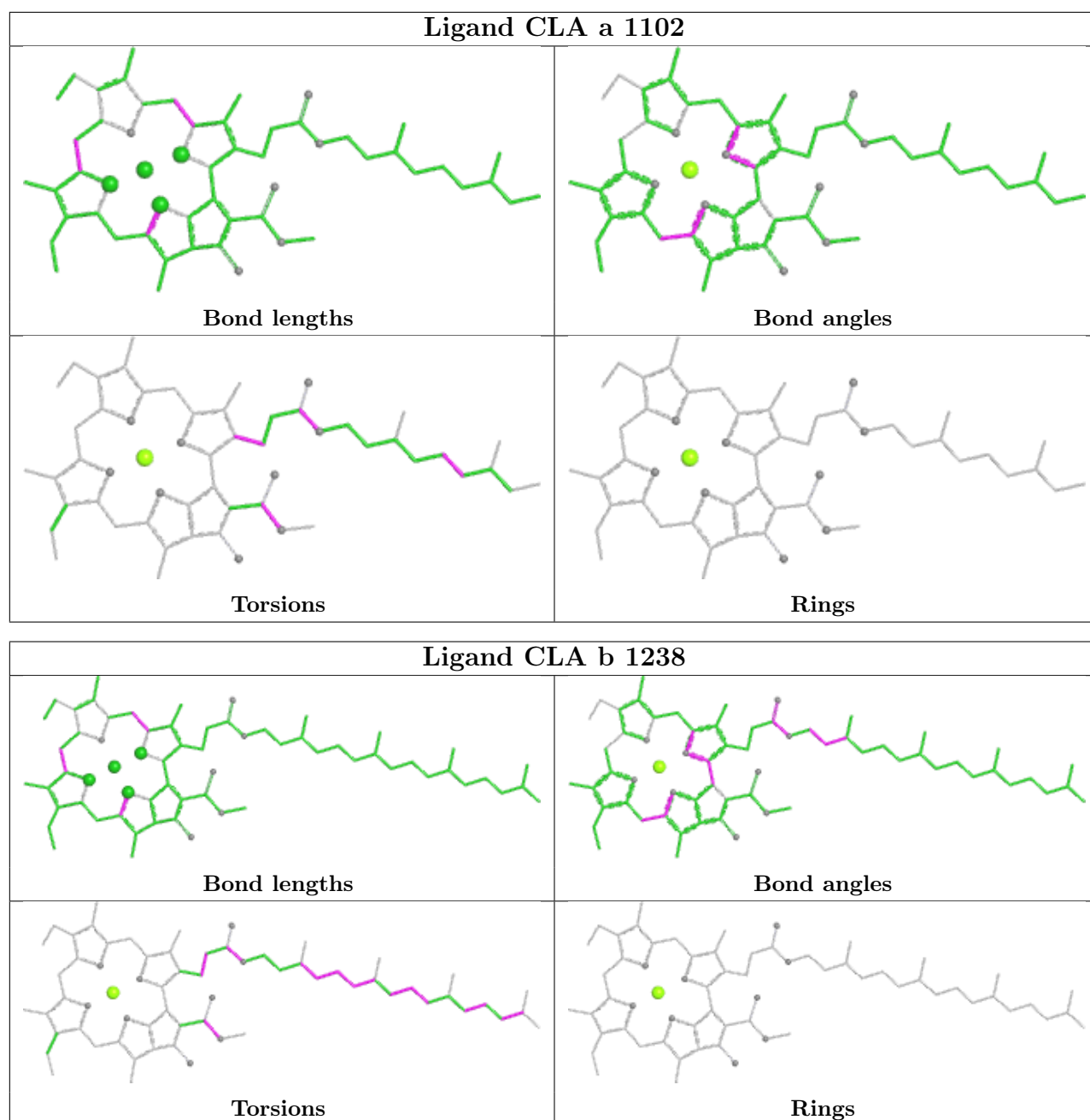
Ligand CLA s 509

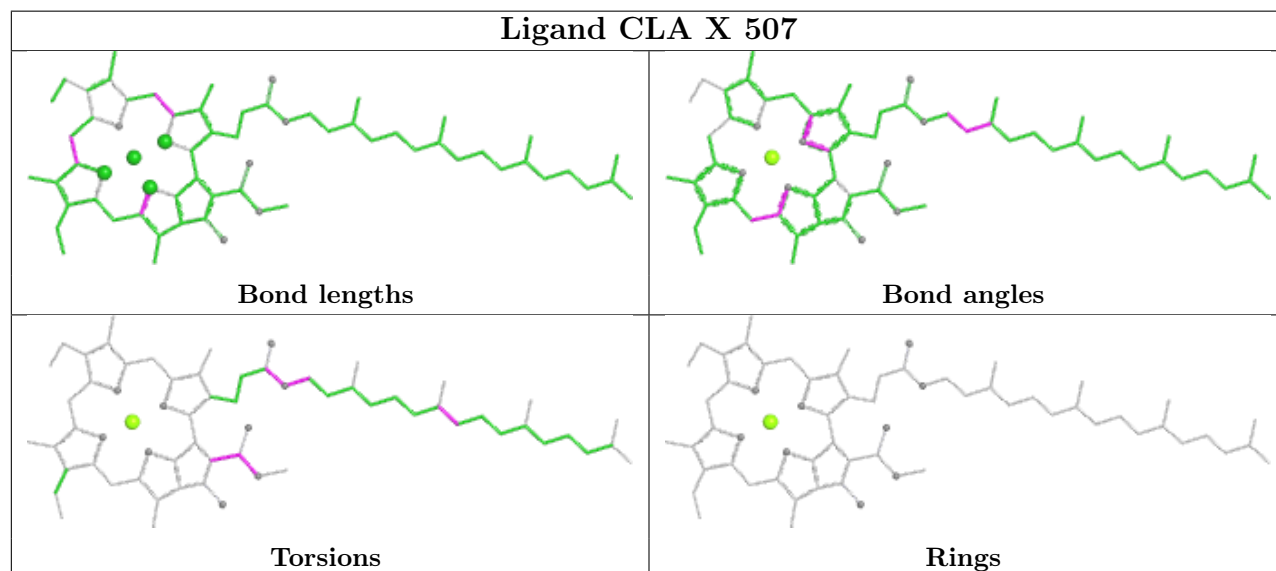
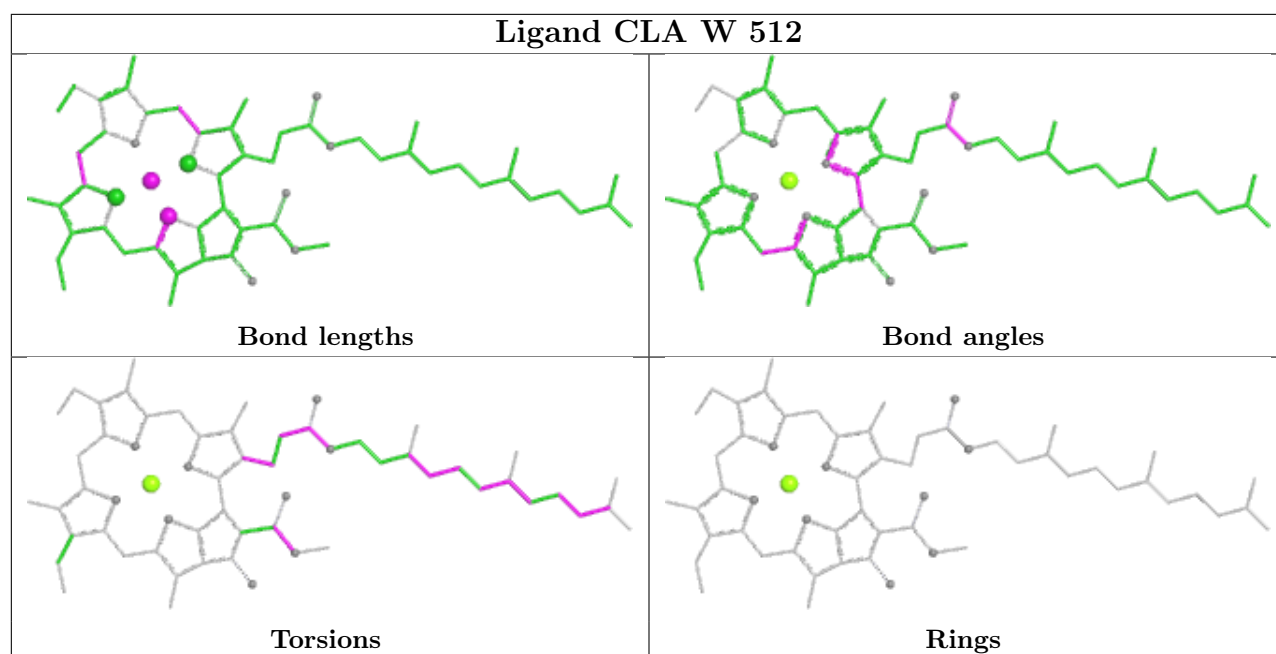


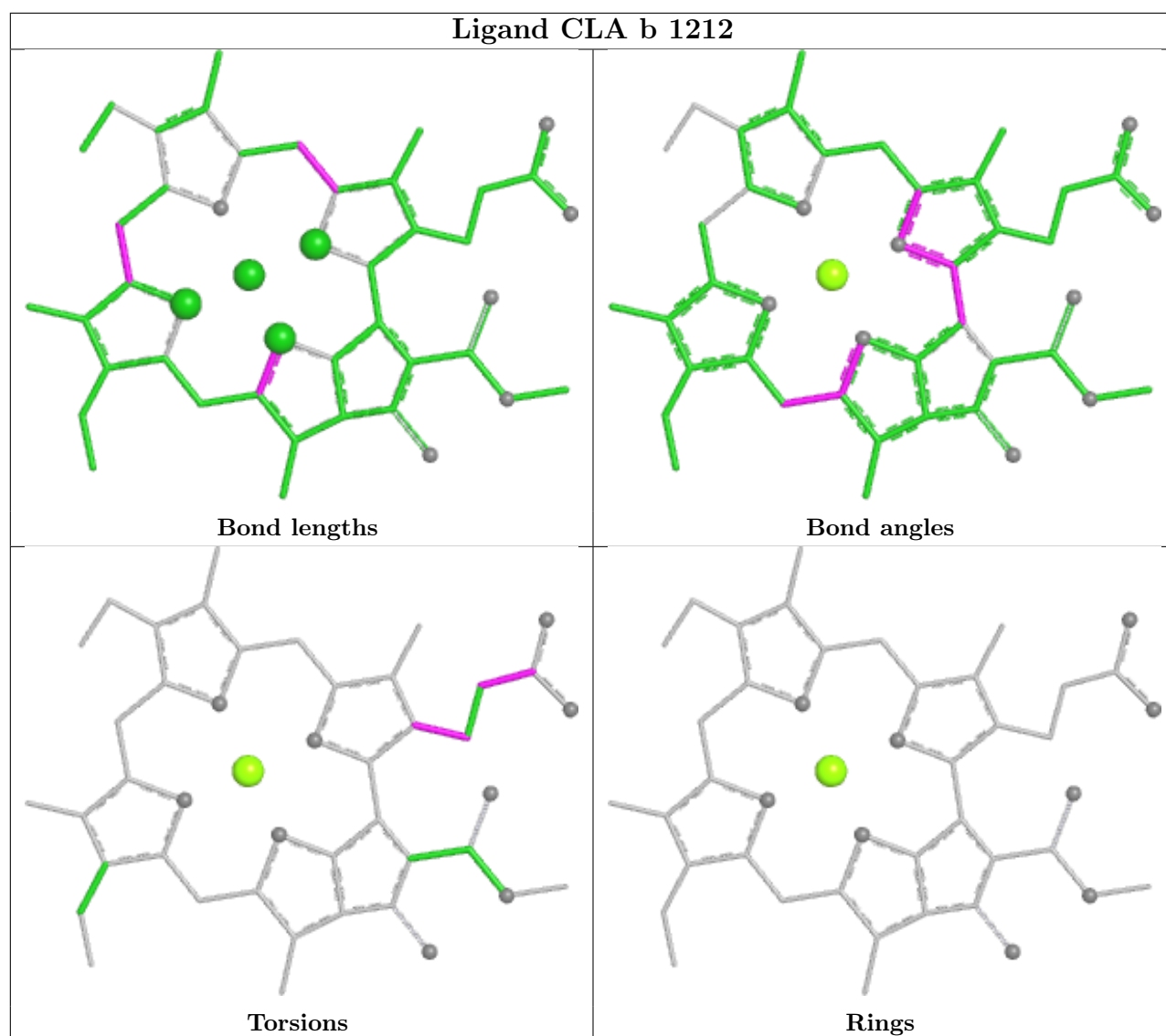
Ligand CLA b 1208



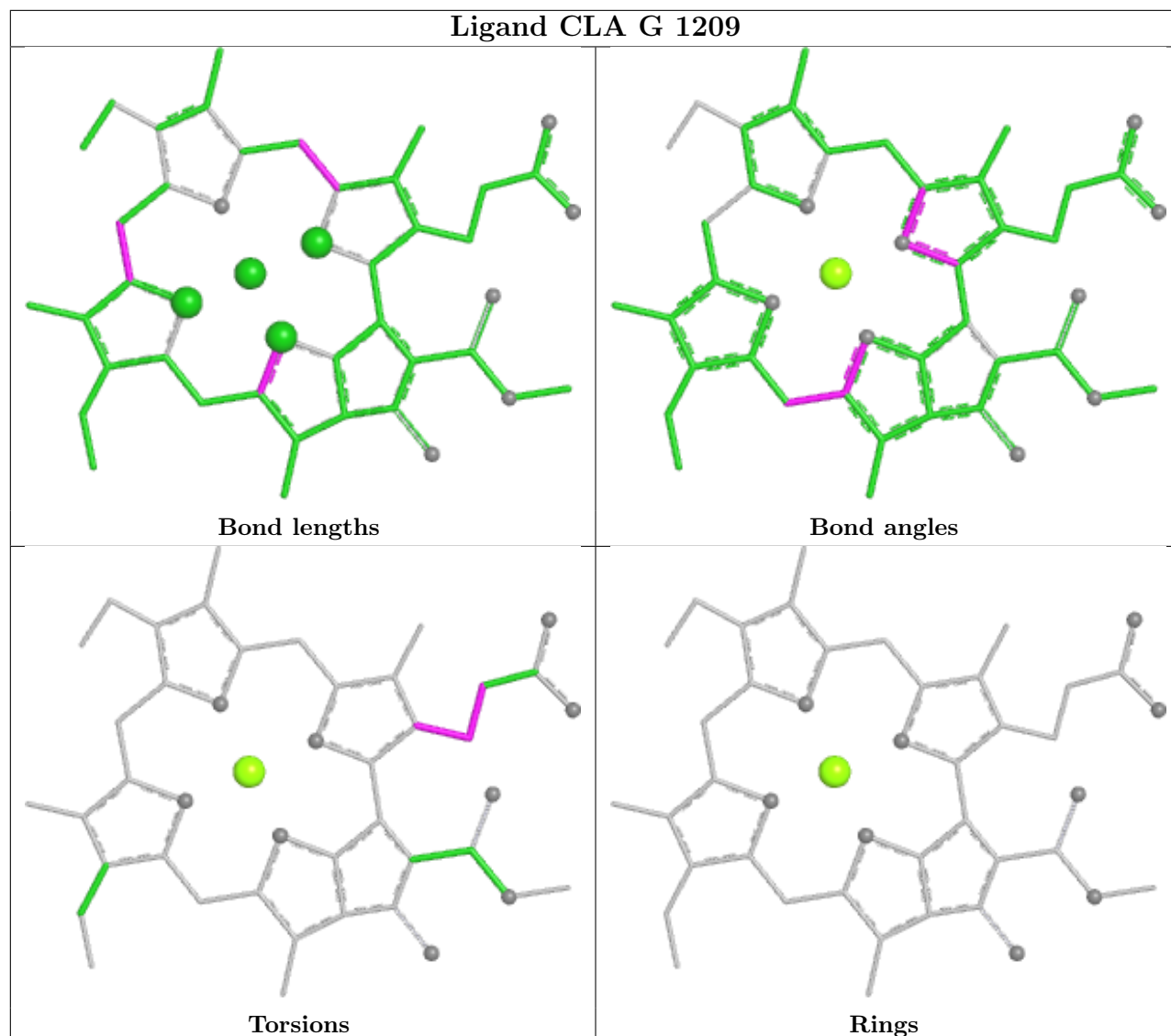




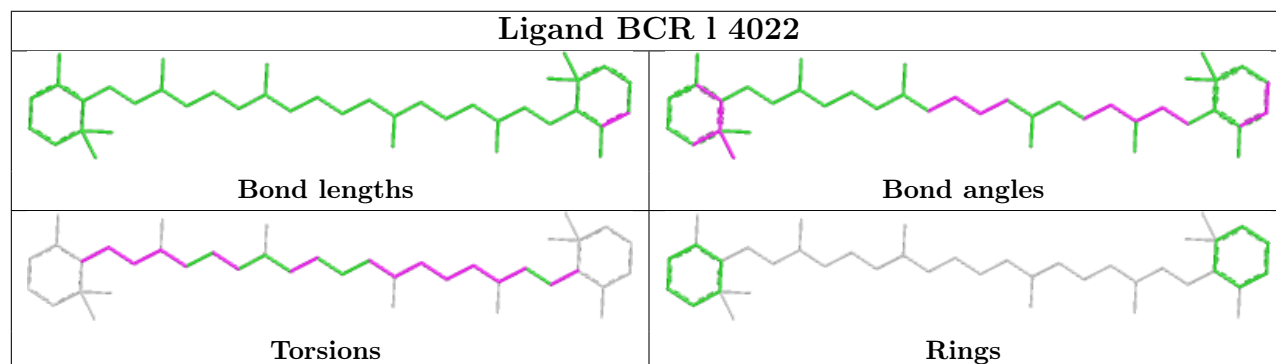


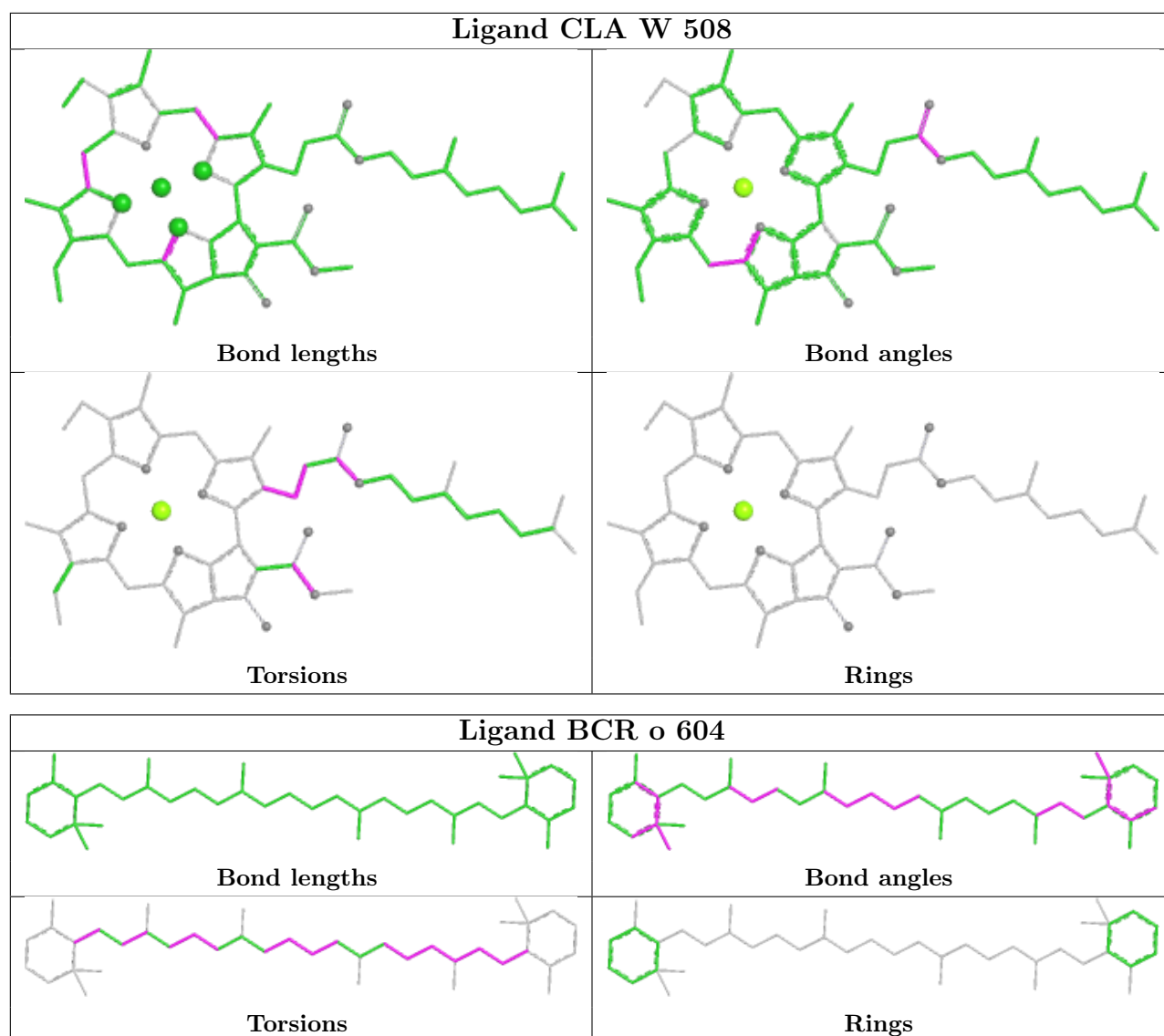


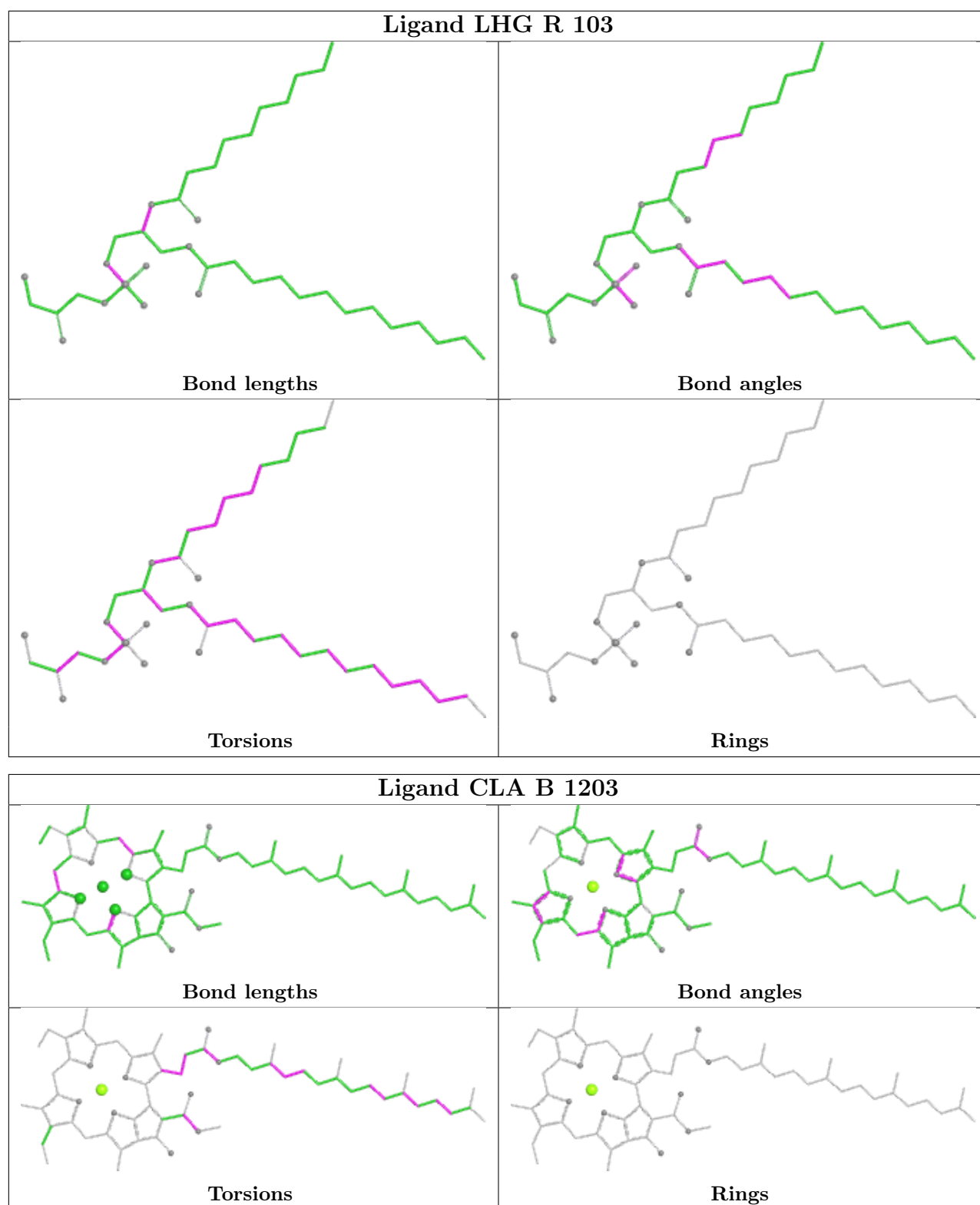
Ligand CLA G 1209



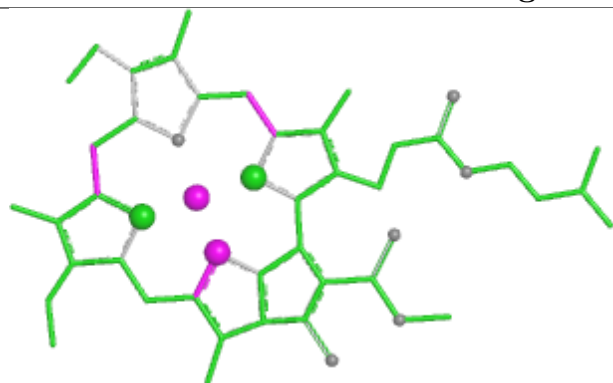
Ligand BCR 1 4022



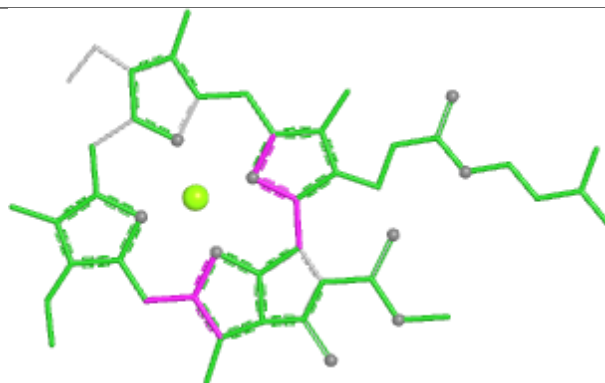




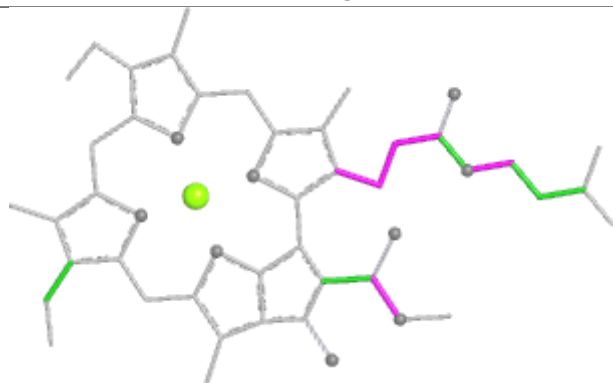
Ligand CLA o 514



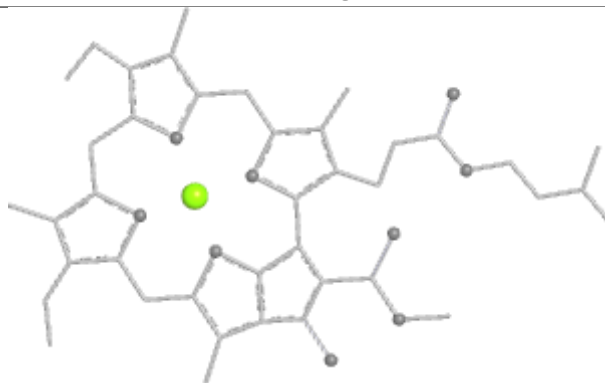
Bond lengths



Bond angles

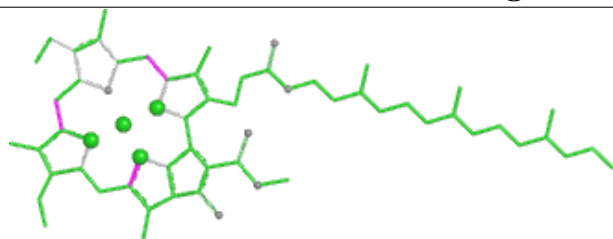


Torsions

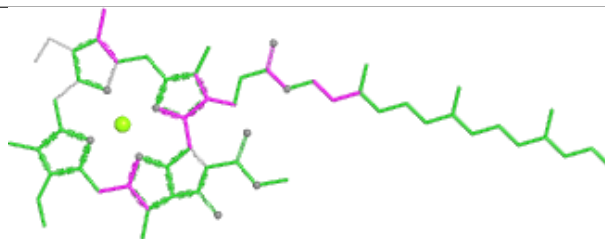


Rings

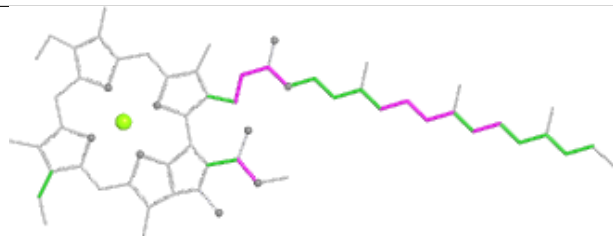
Ligand CLA B 1235



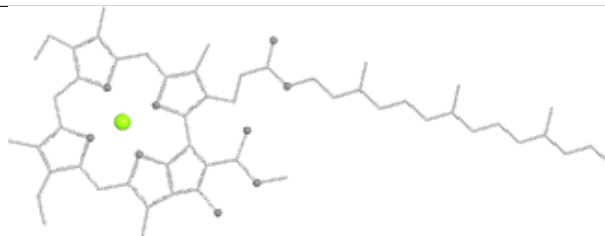
Bond lengths



Bond angles

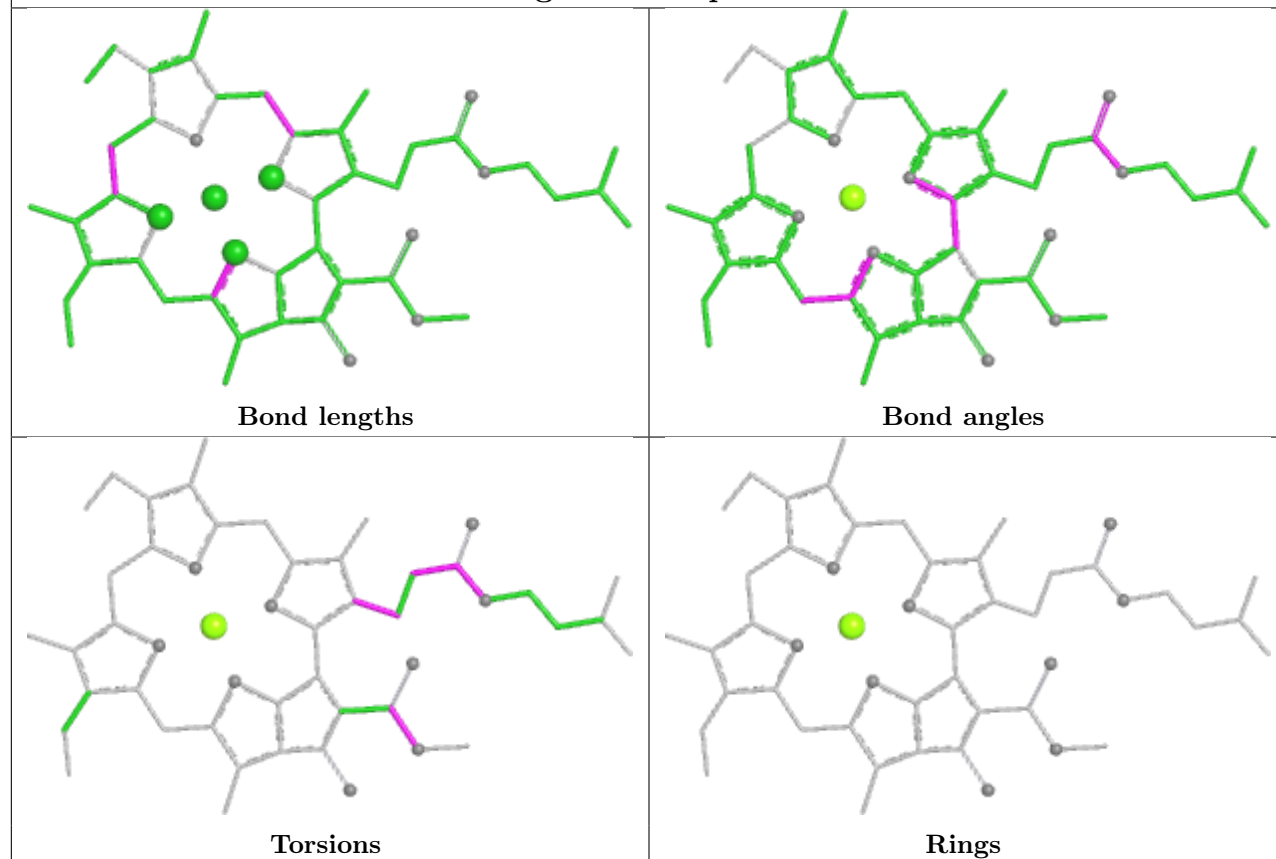


Torsions

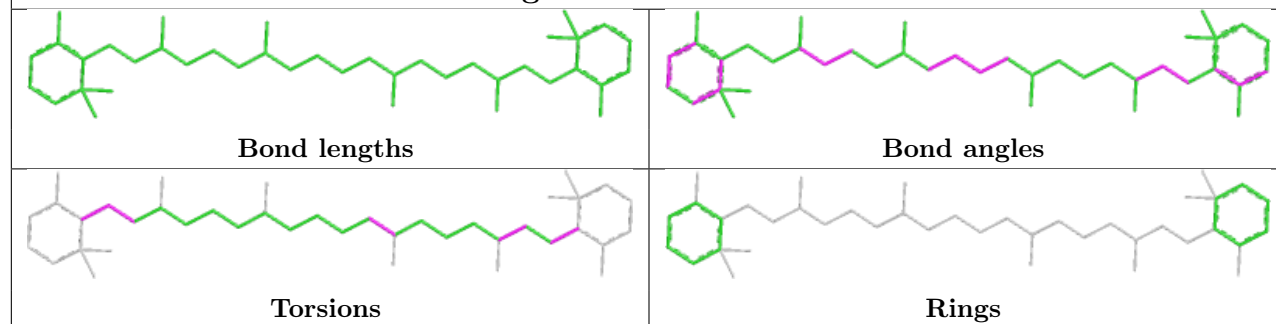


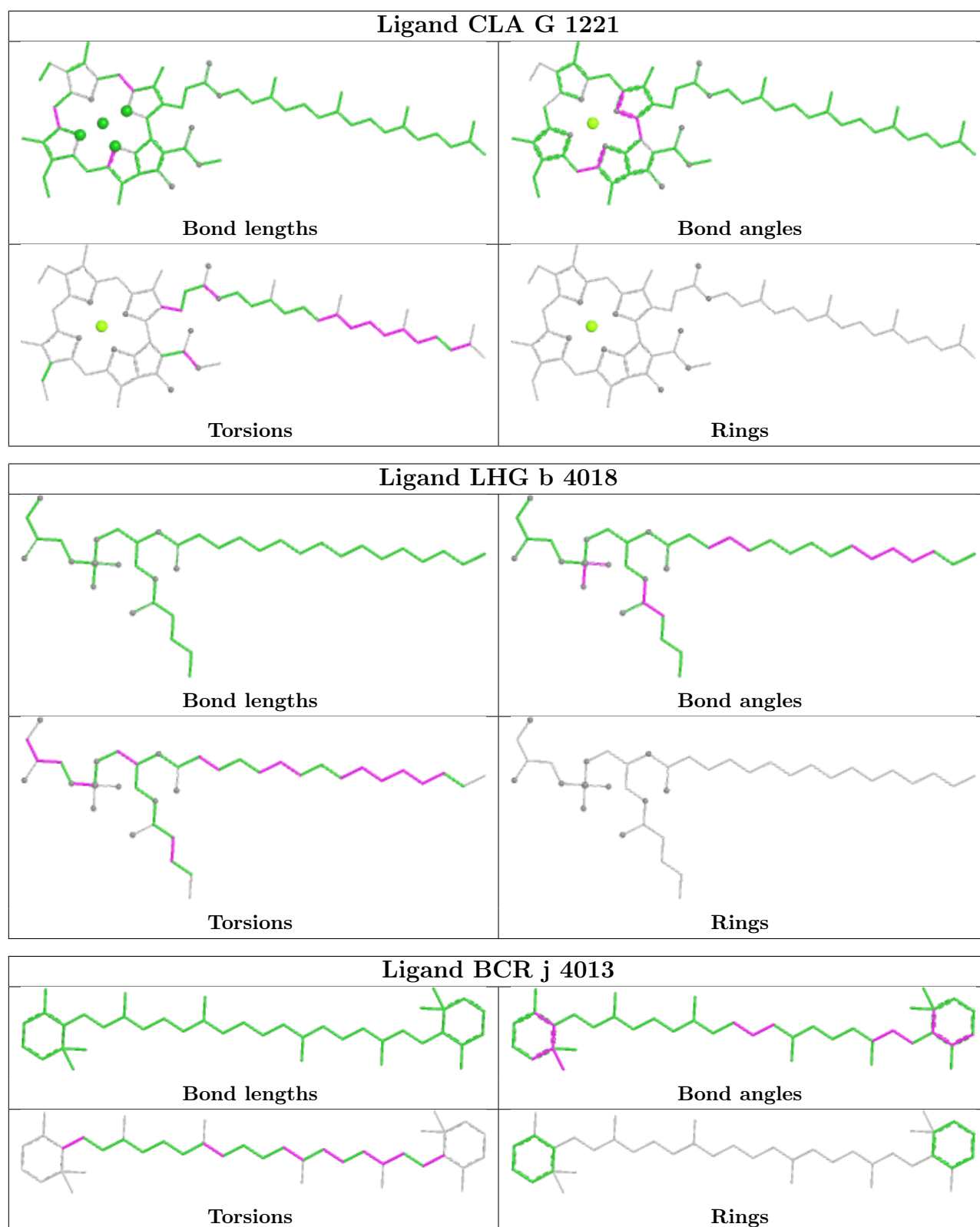
Rings

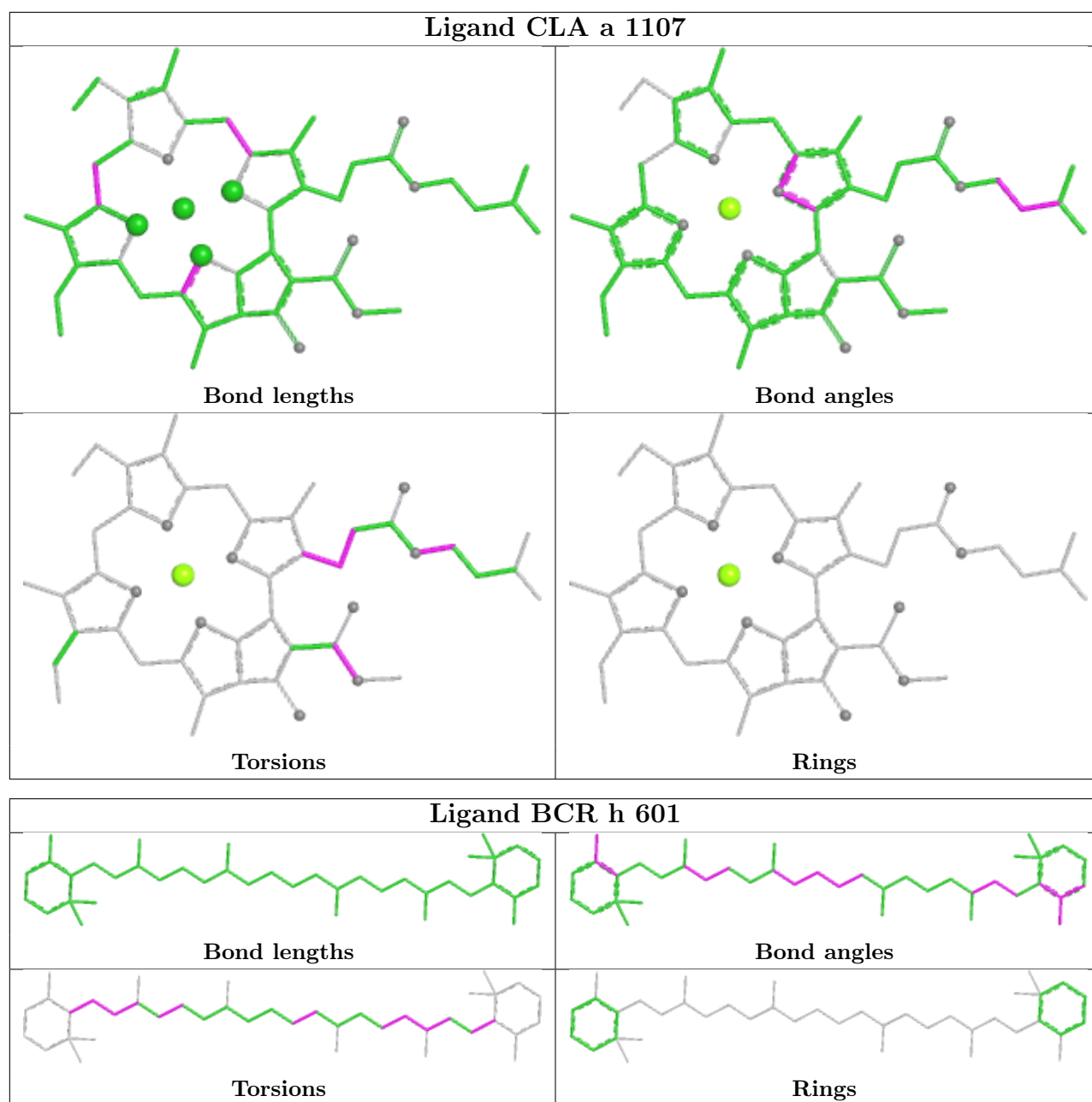
Ligand CLA p 514

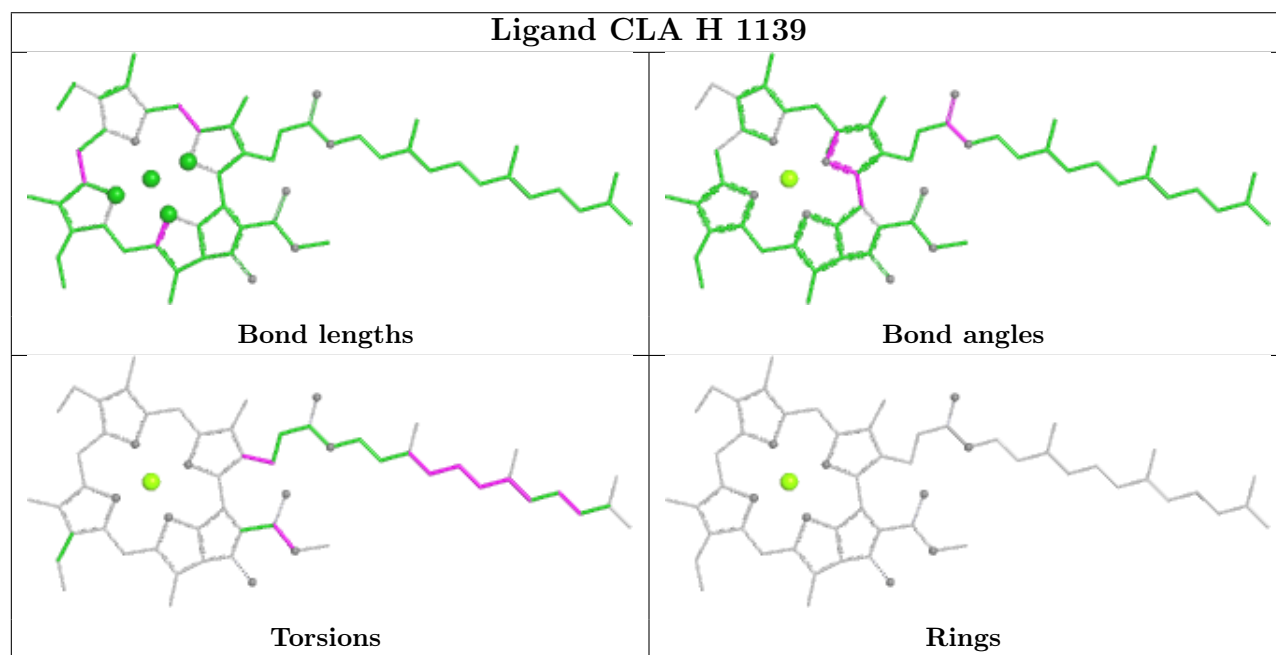
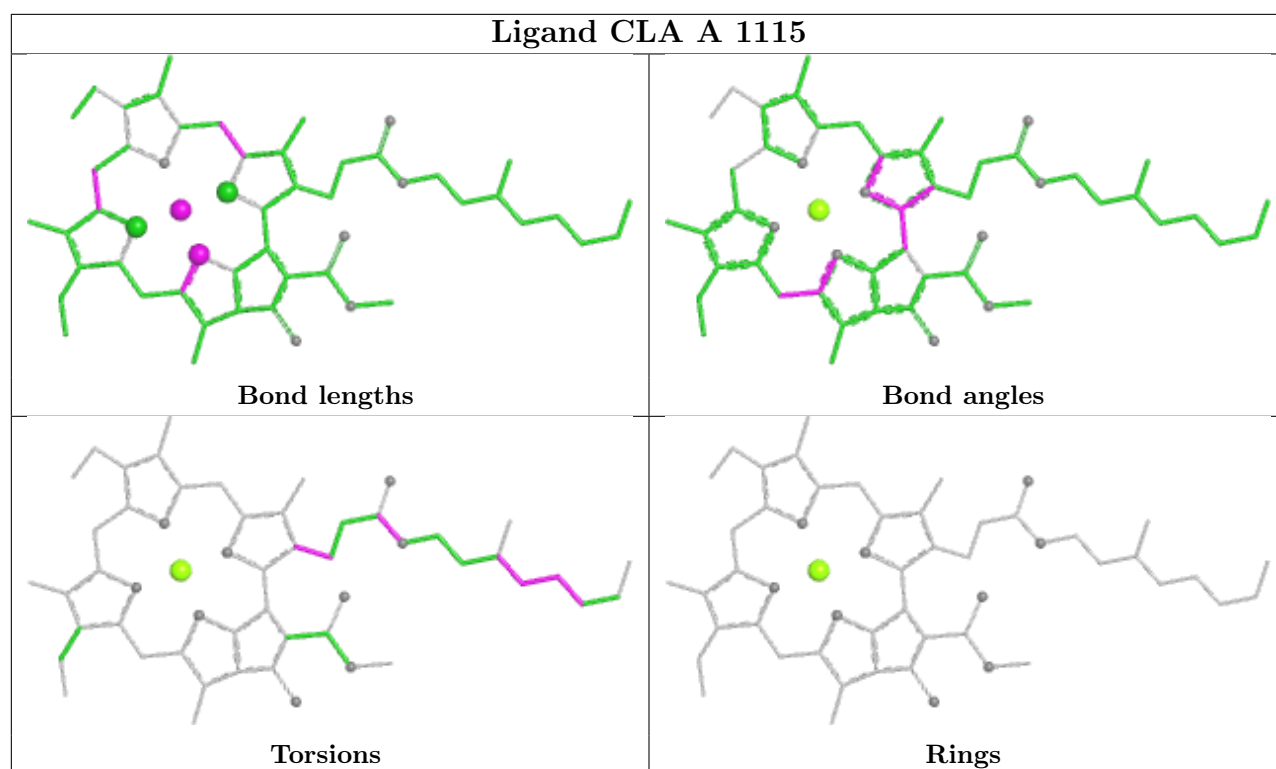


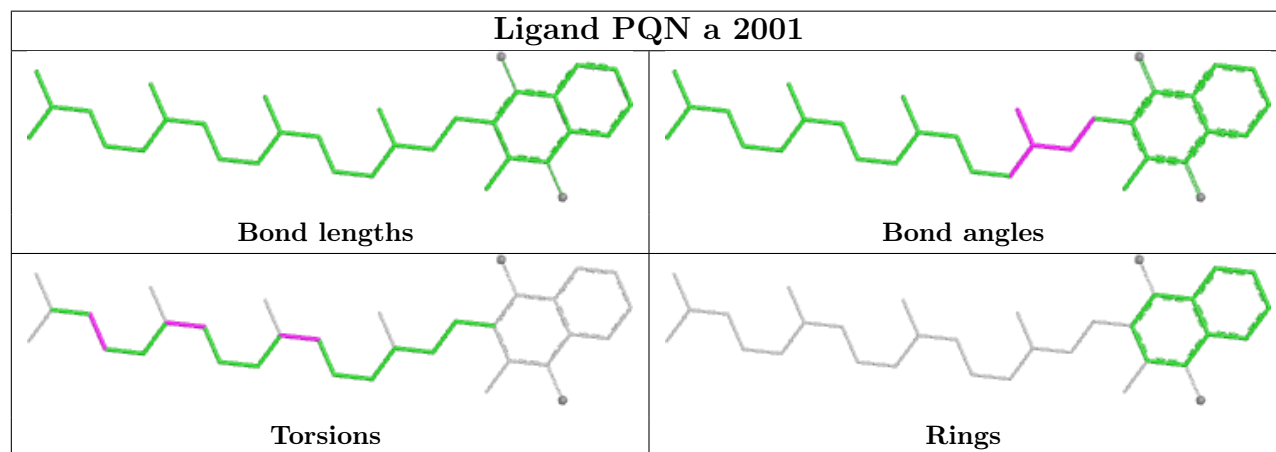
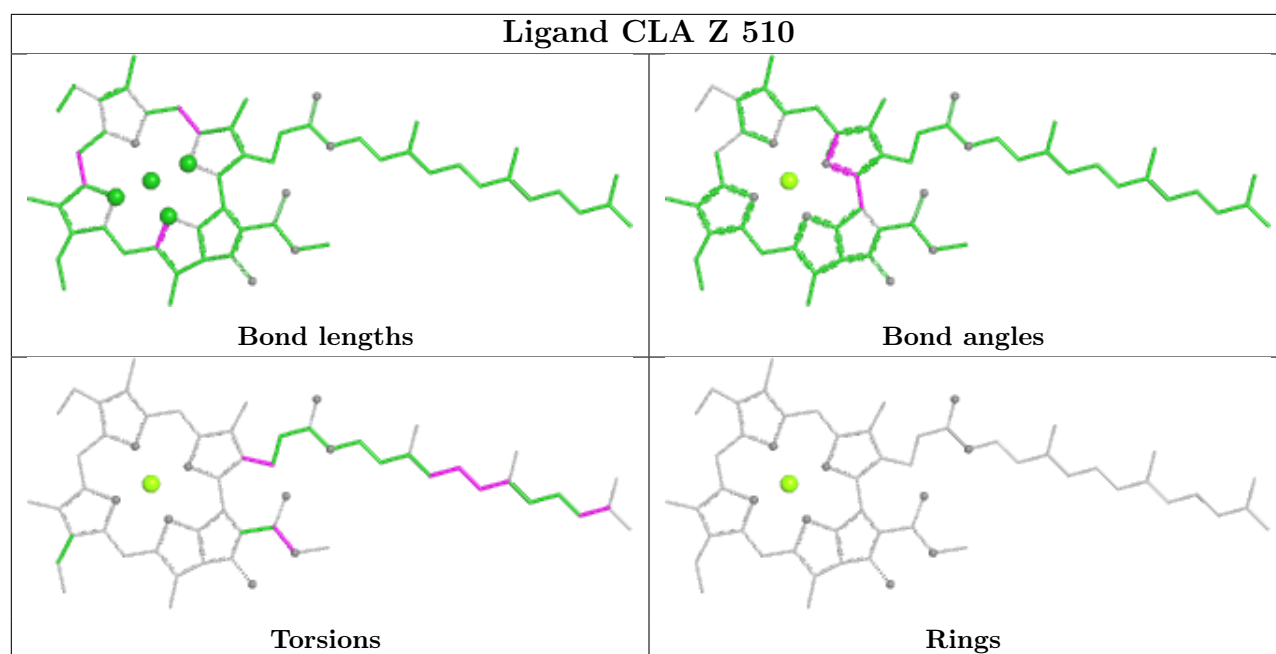
Ligand BCR T 4005

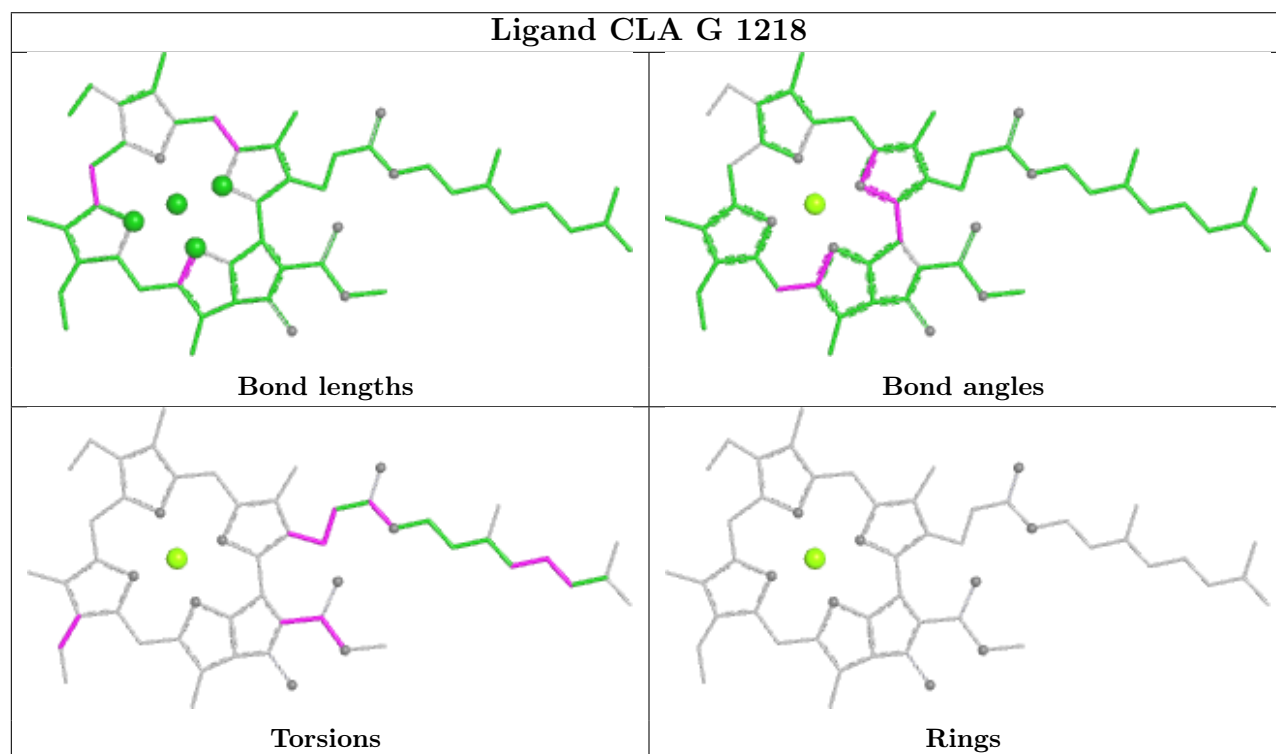
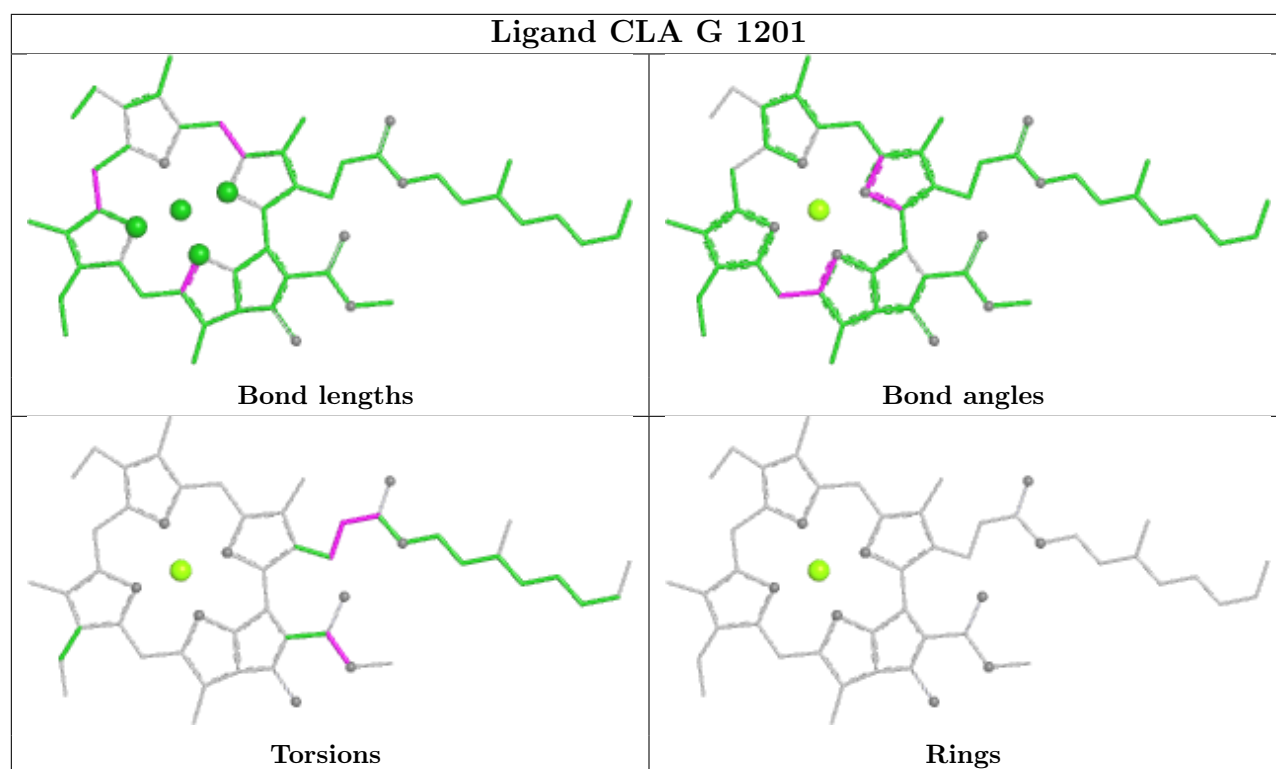


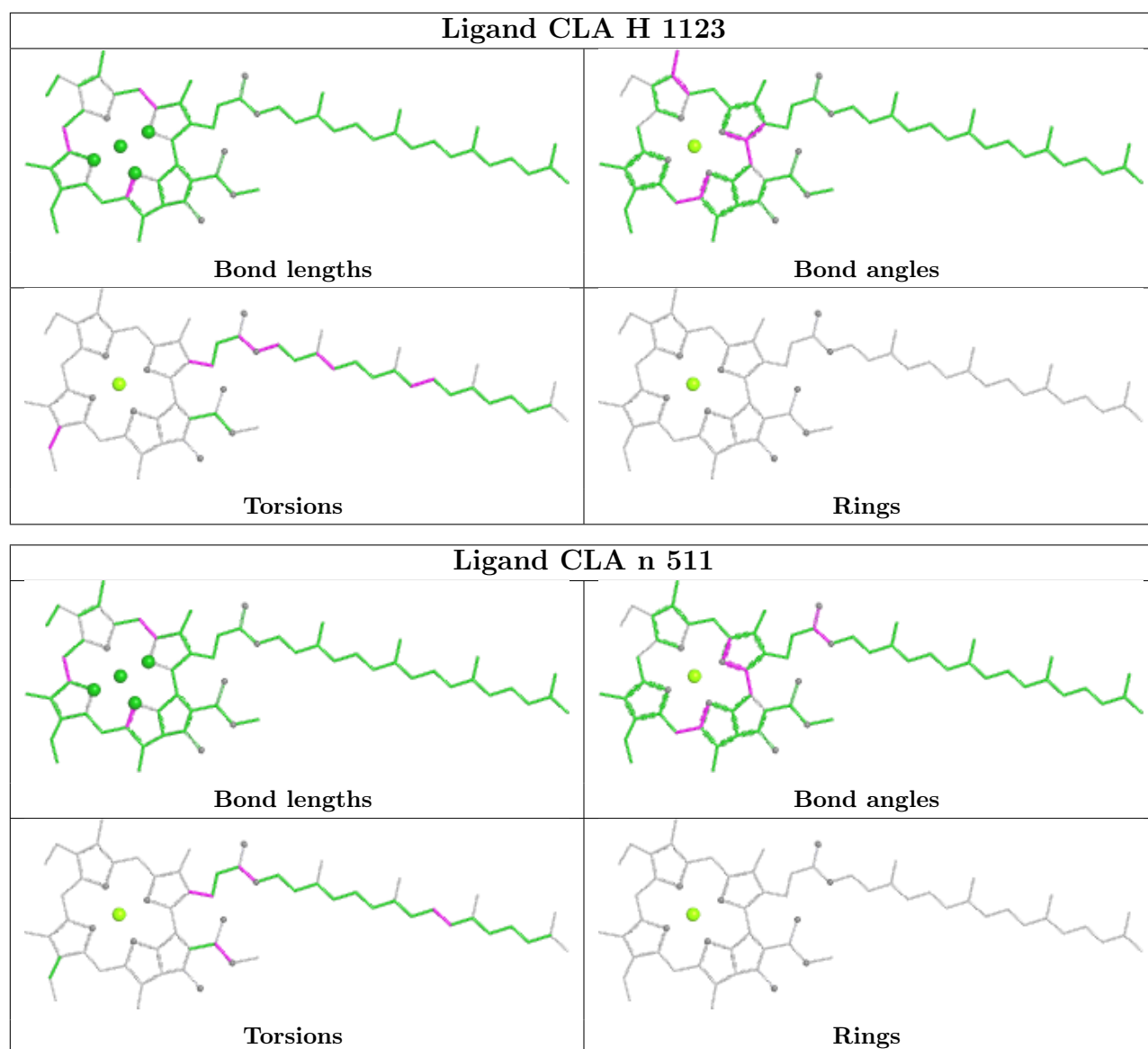


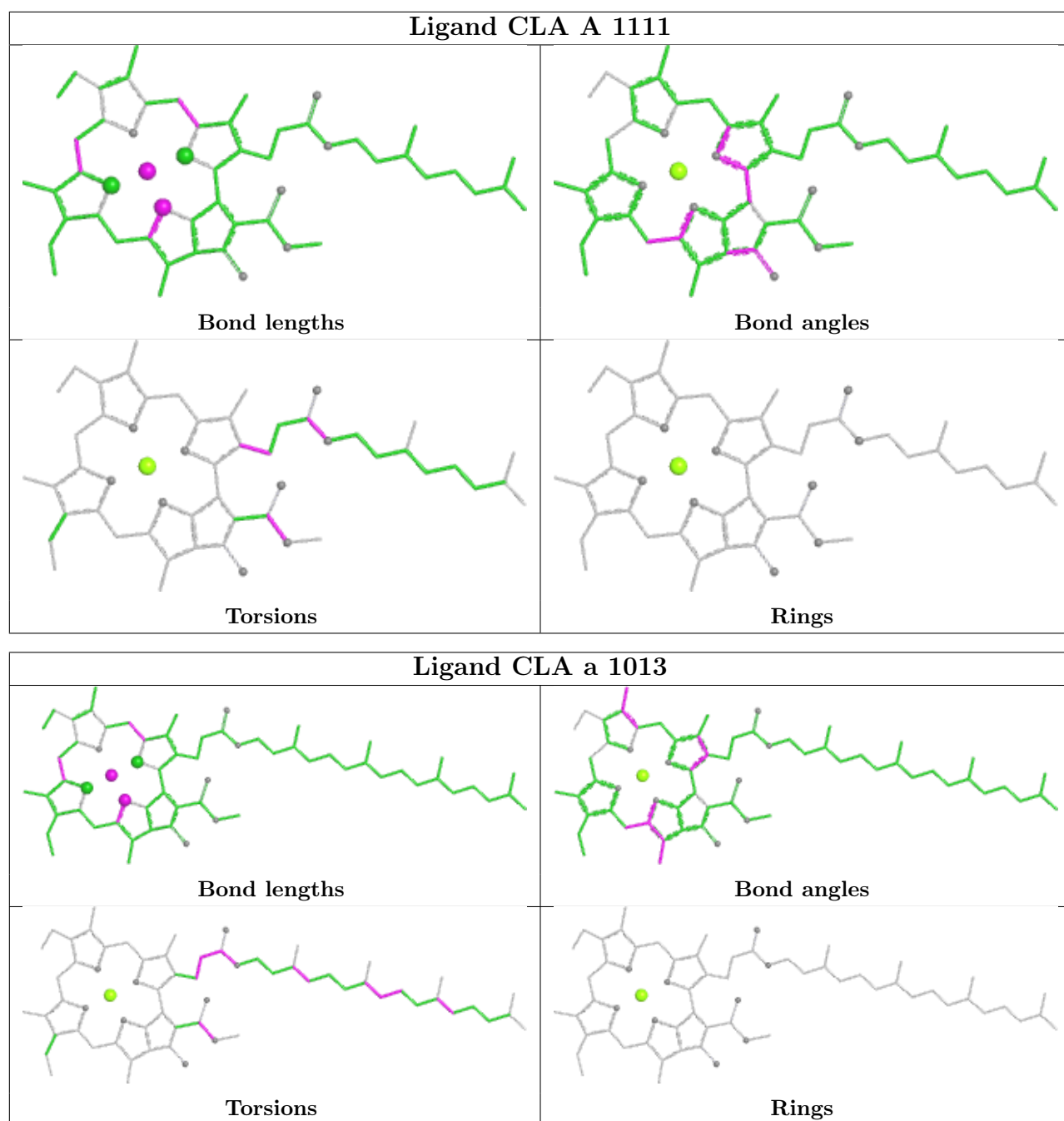


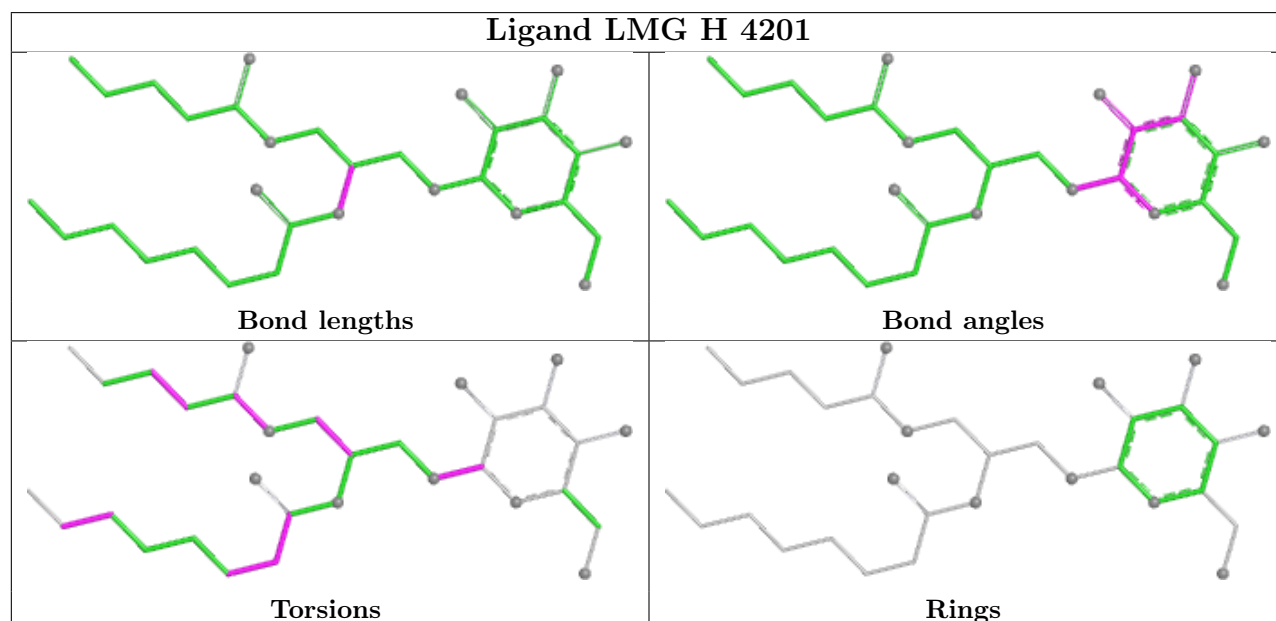
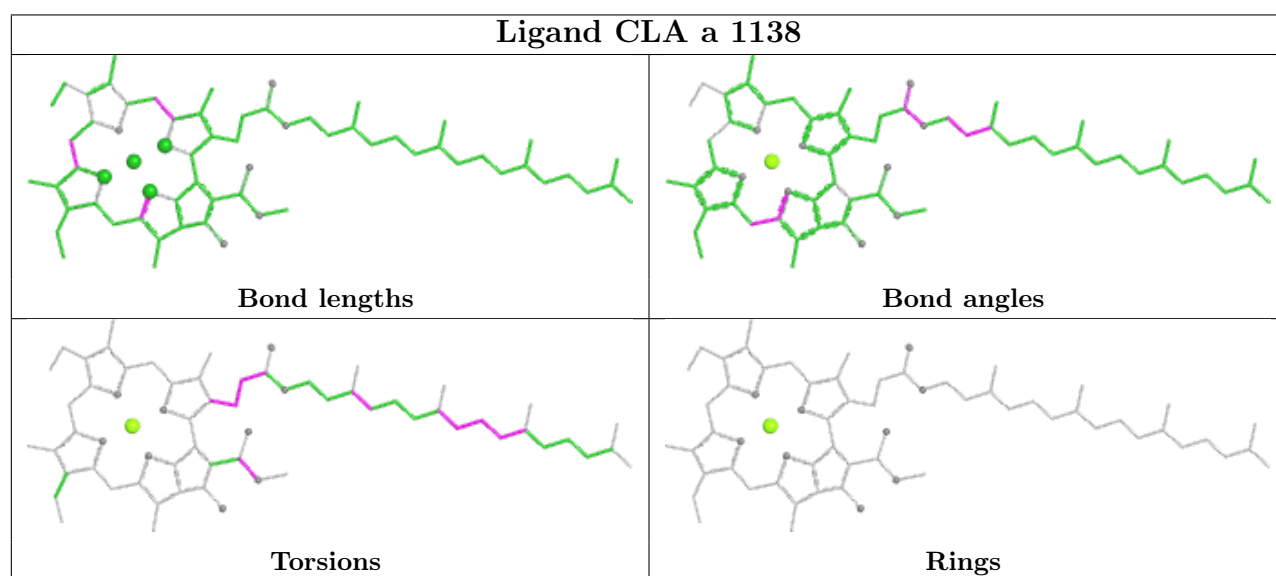
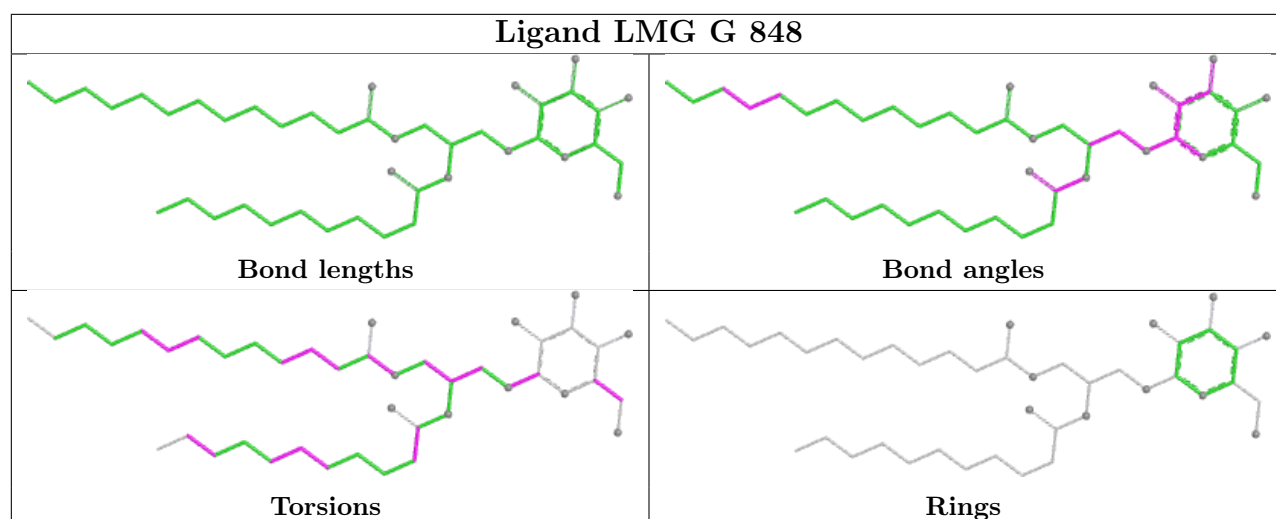


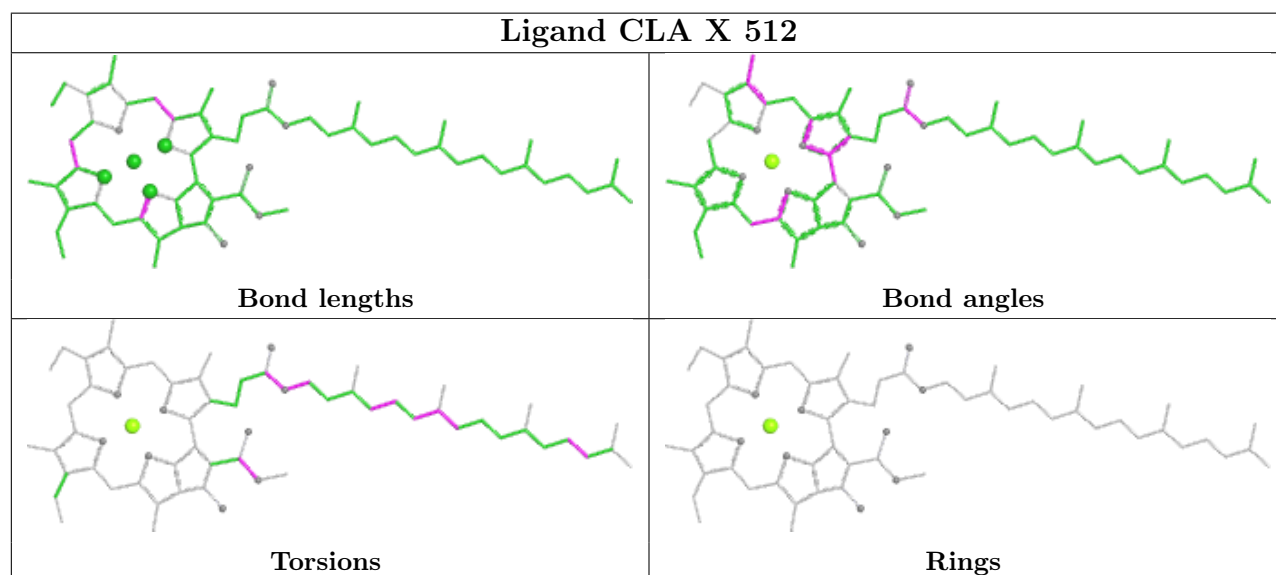
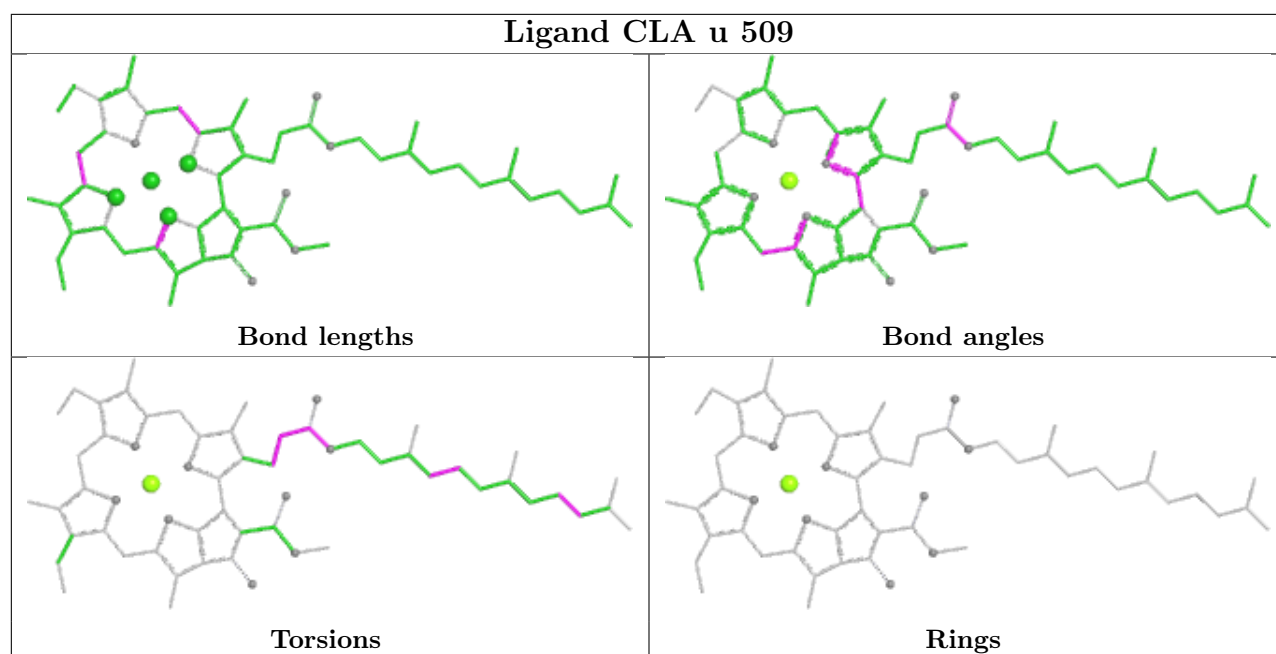


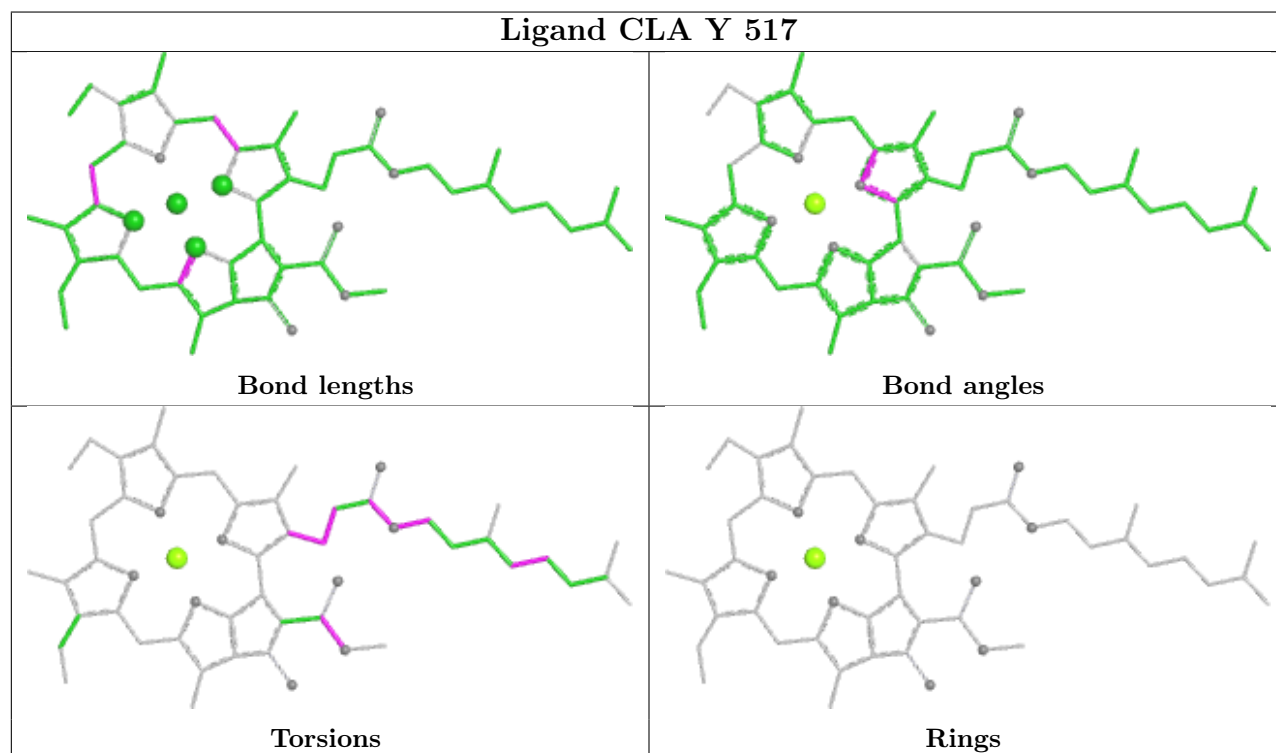
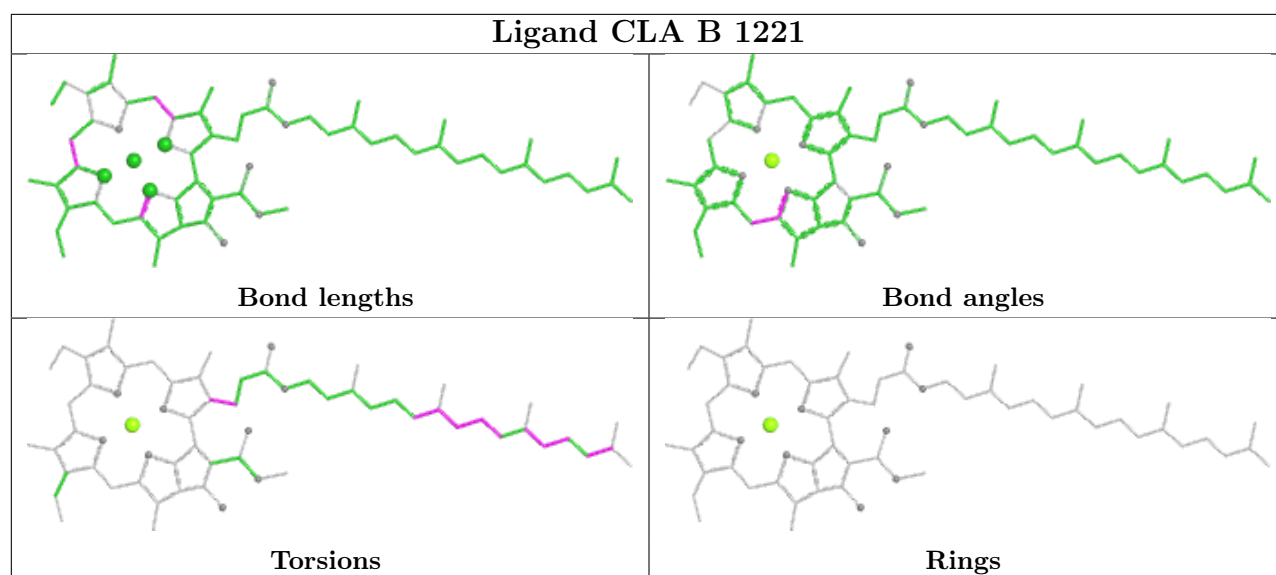


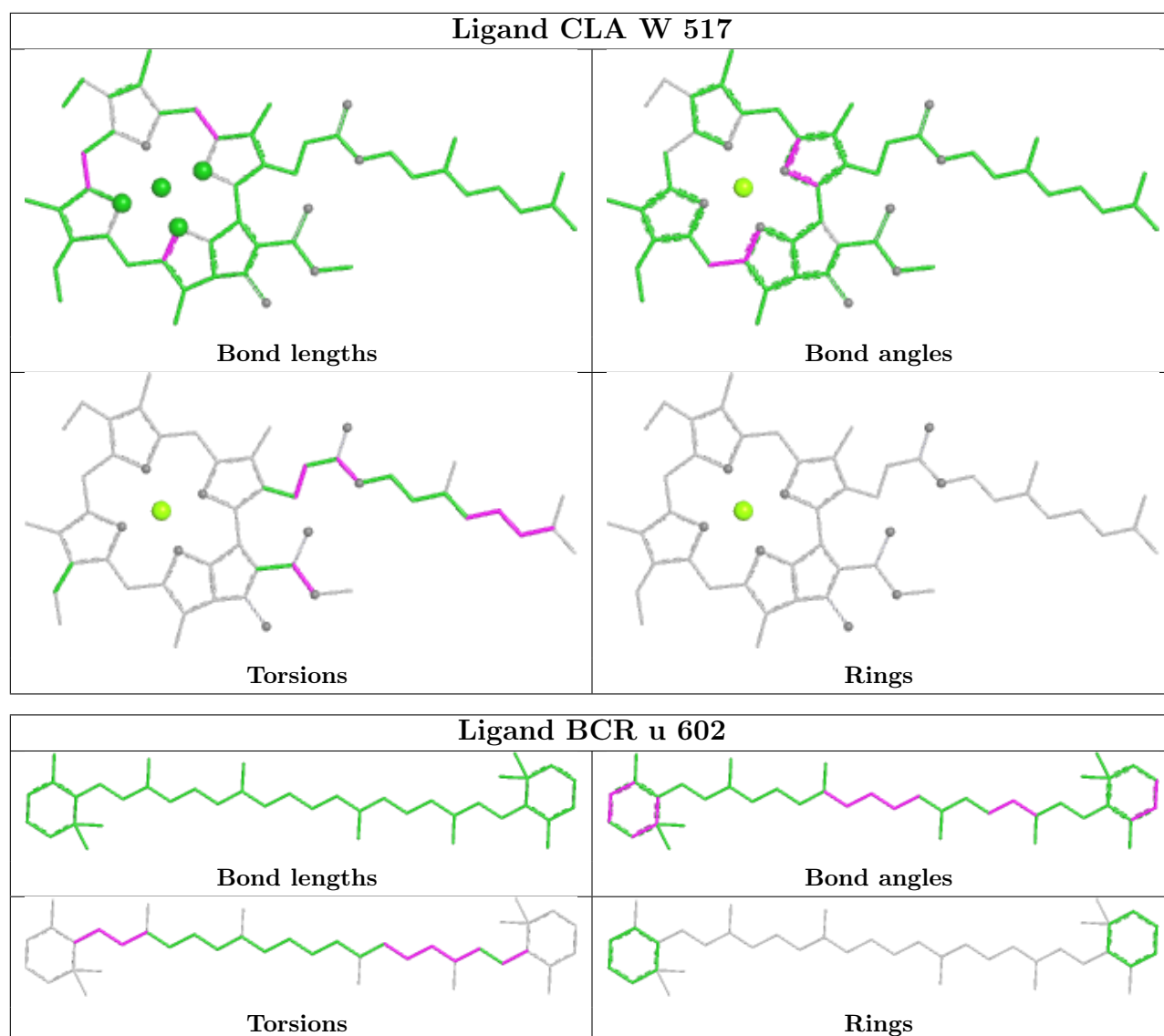


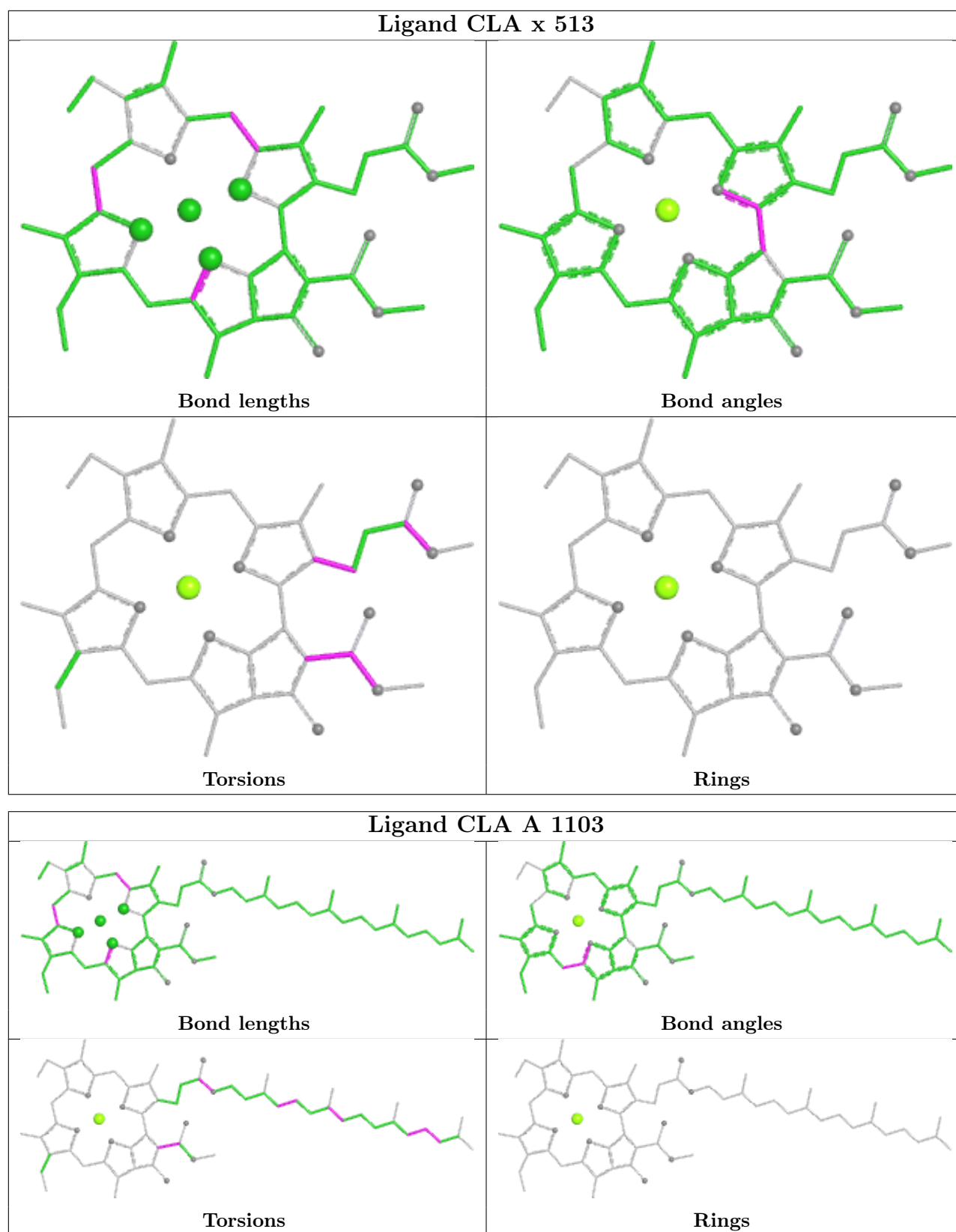


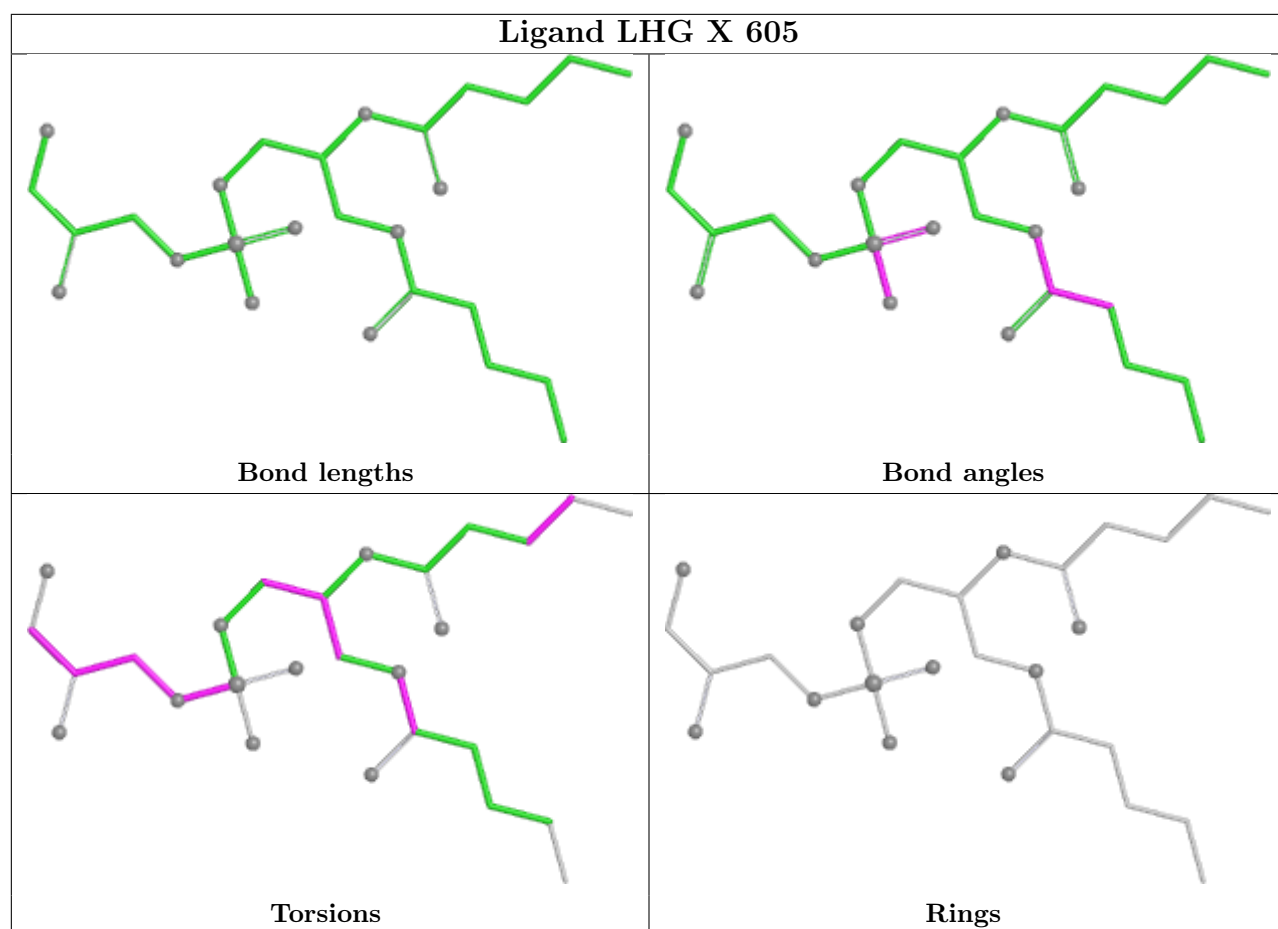




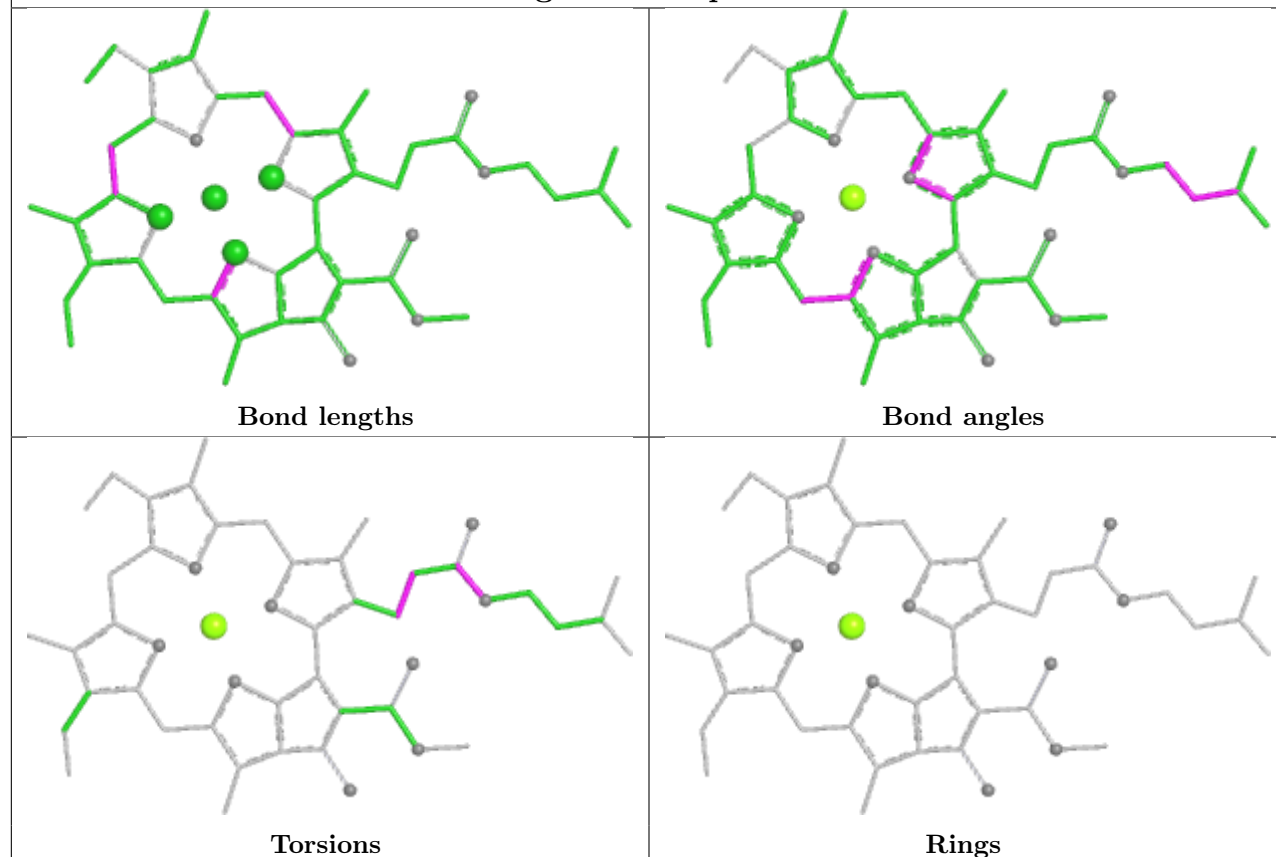




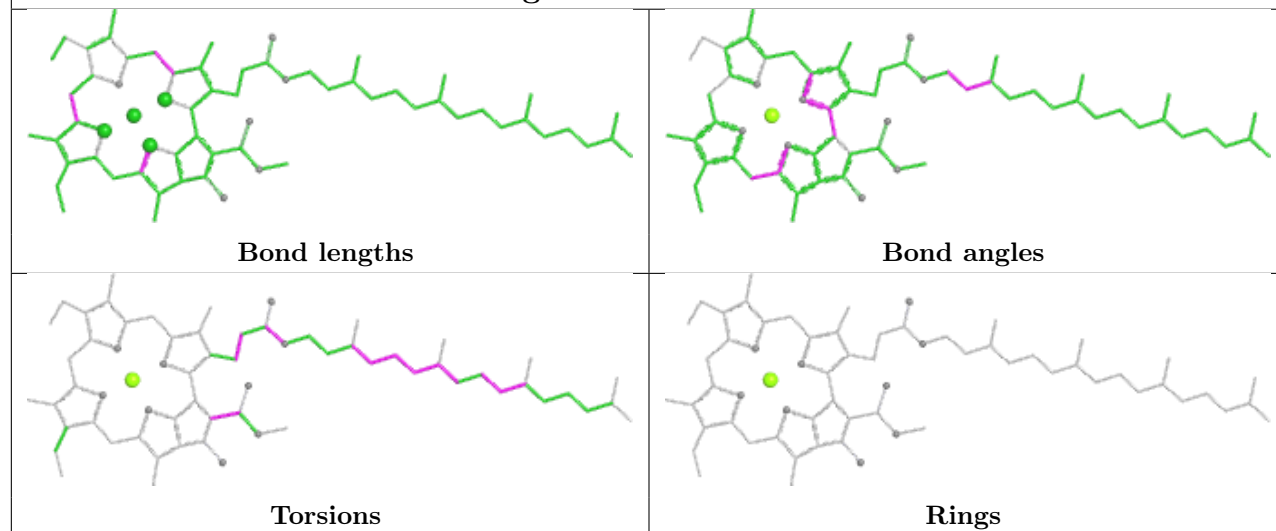


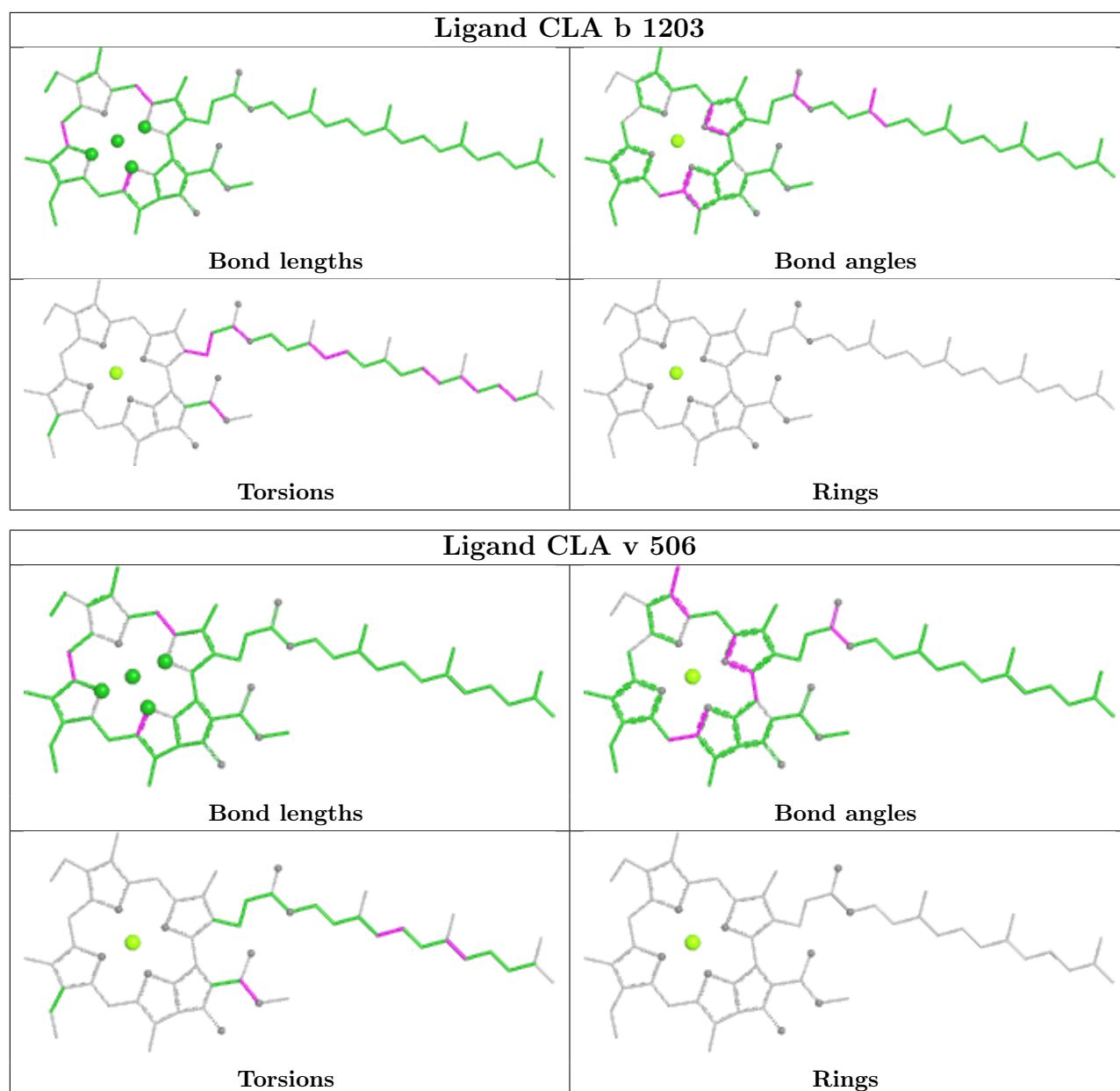


Ligand CLA p 502

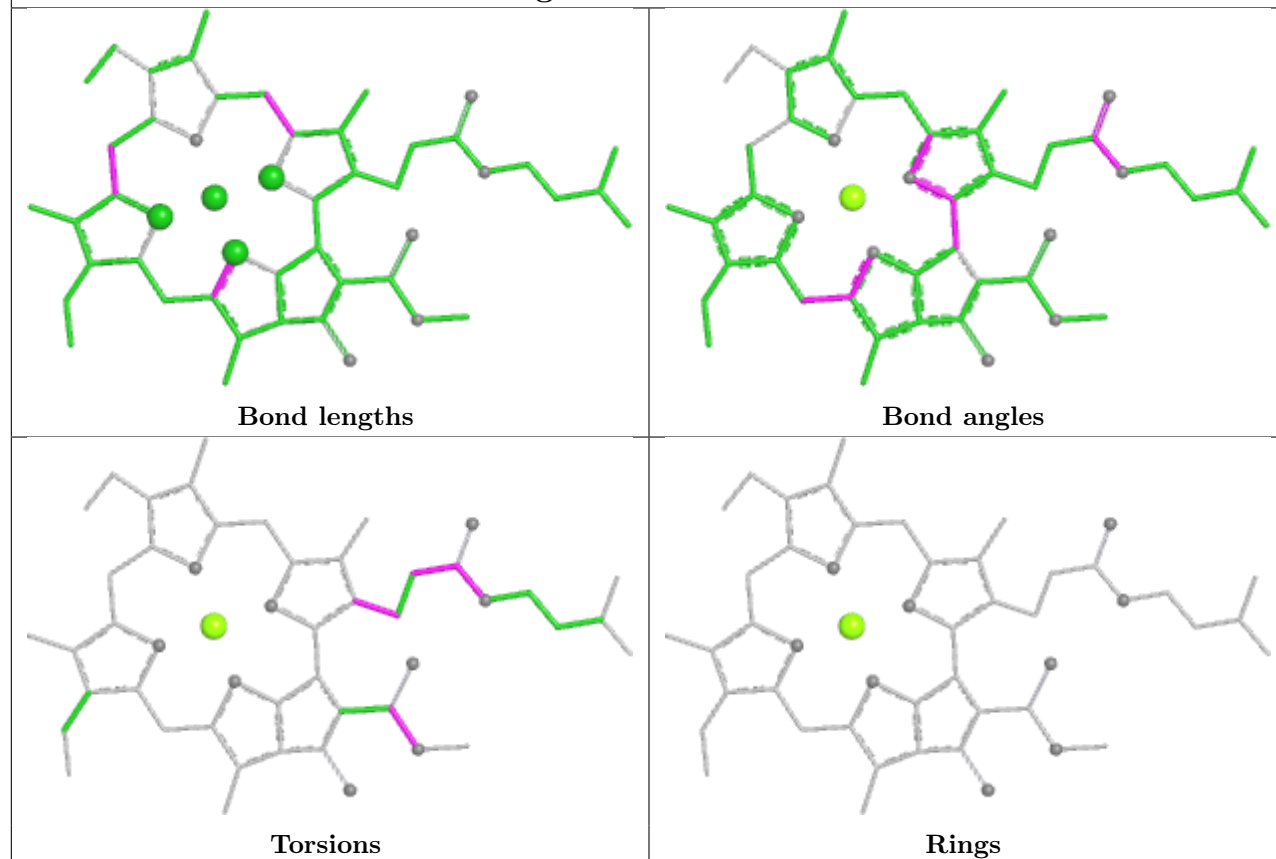


Ligand CLA A 1106

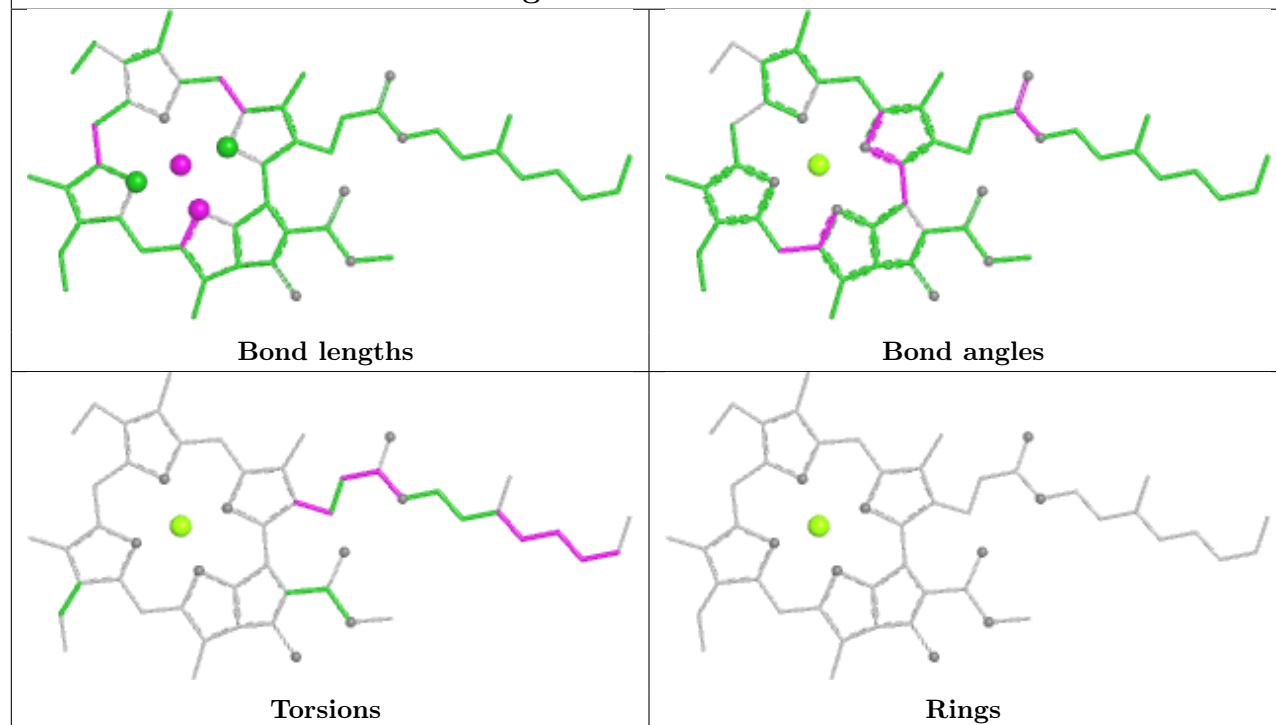


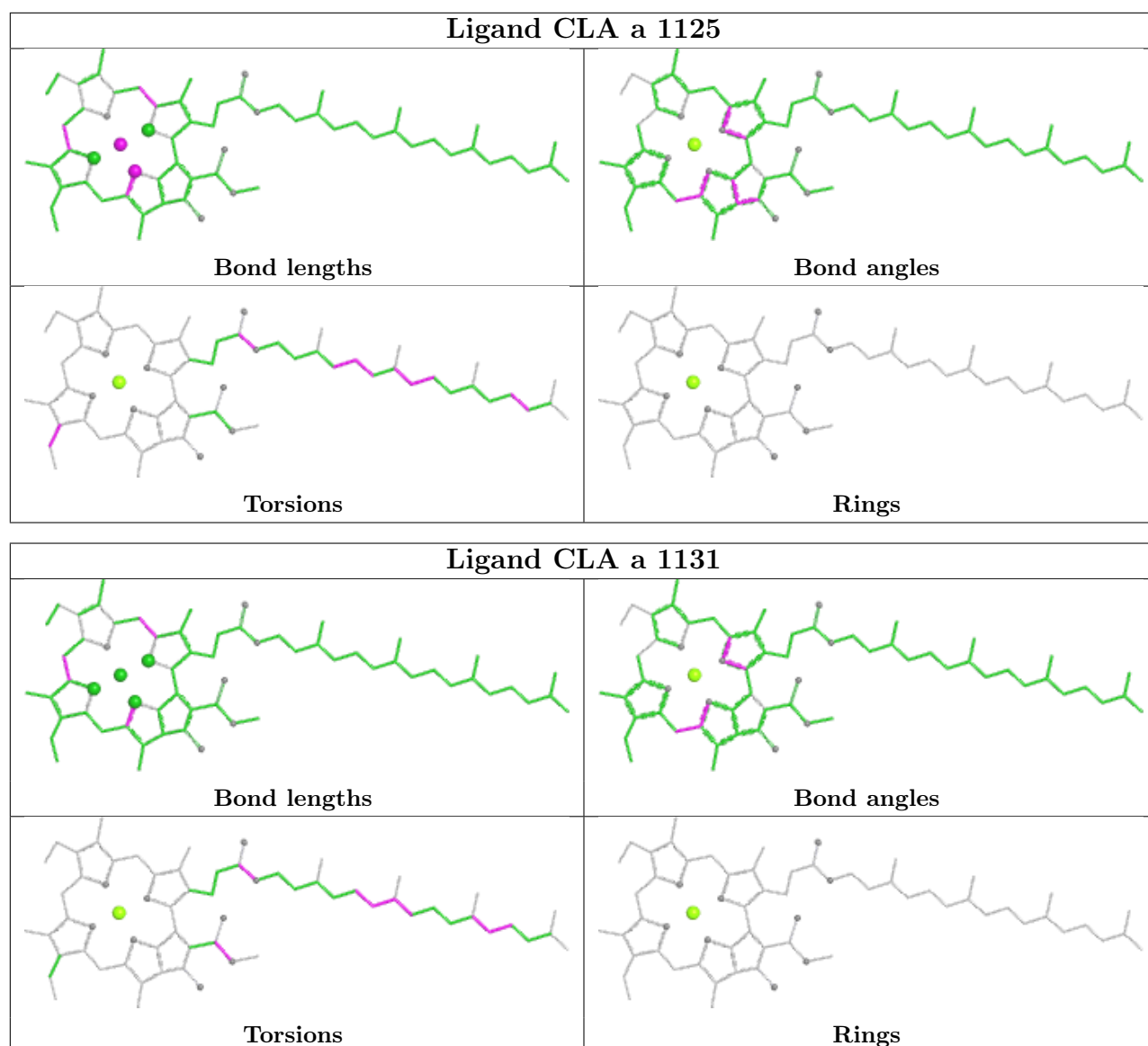


Ligand CLA x 514

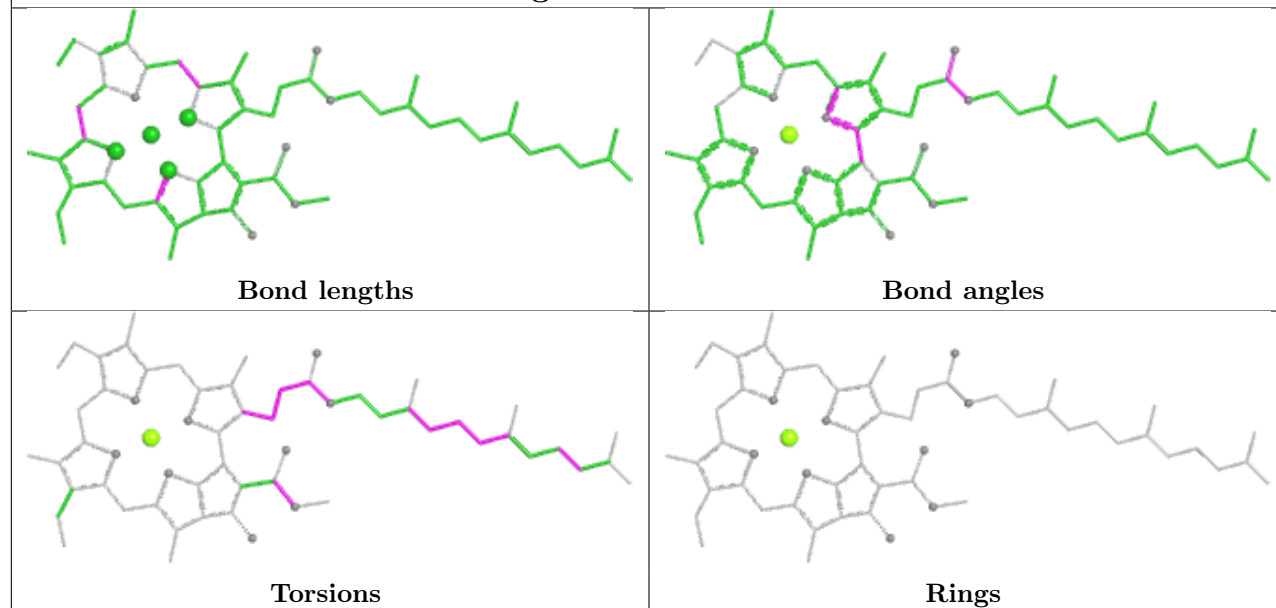


Ligand CLA A 1133

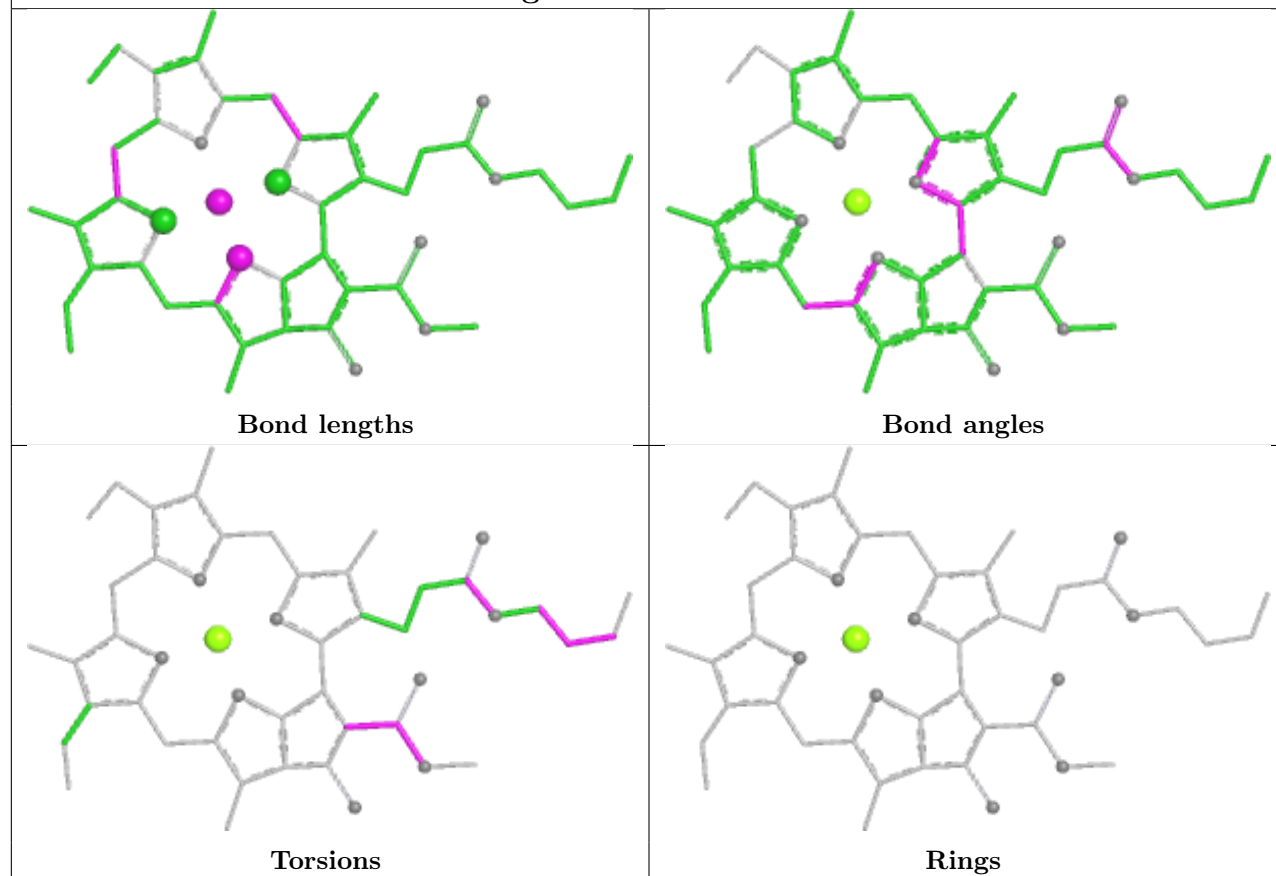


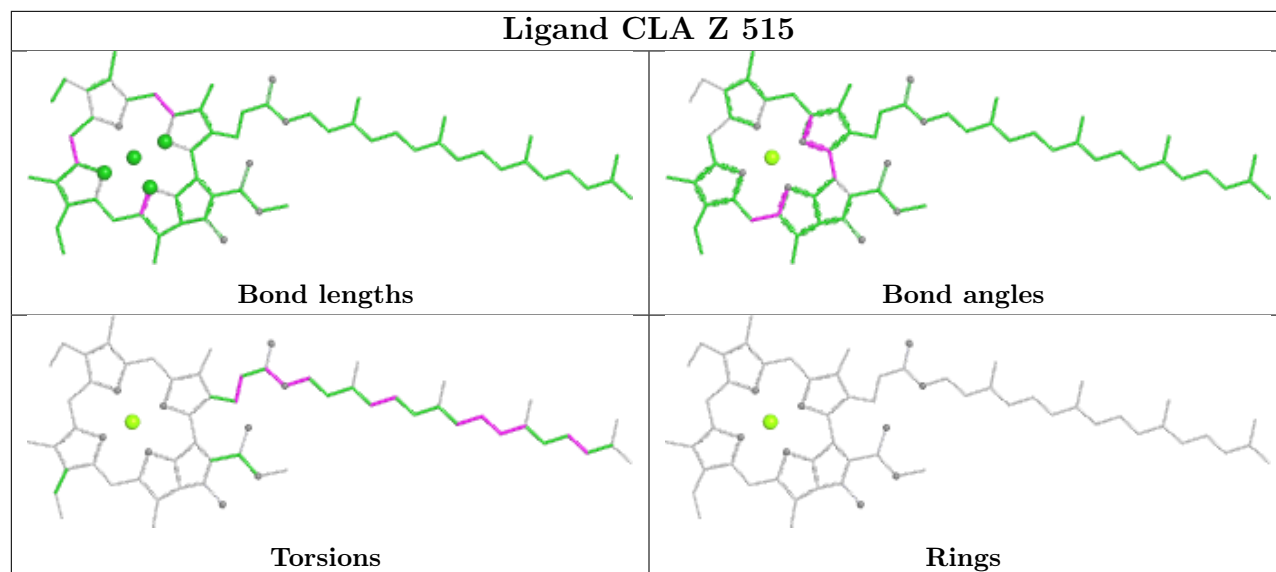
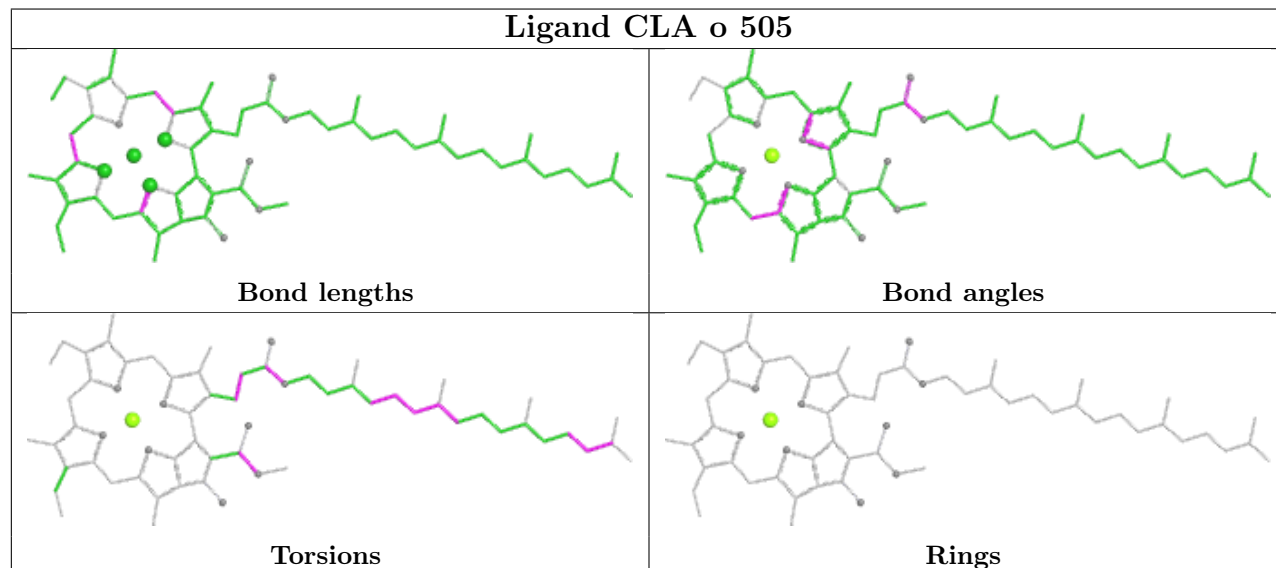


Ligand CLA Y 509

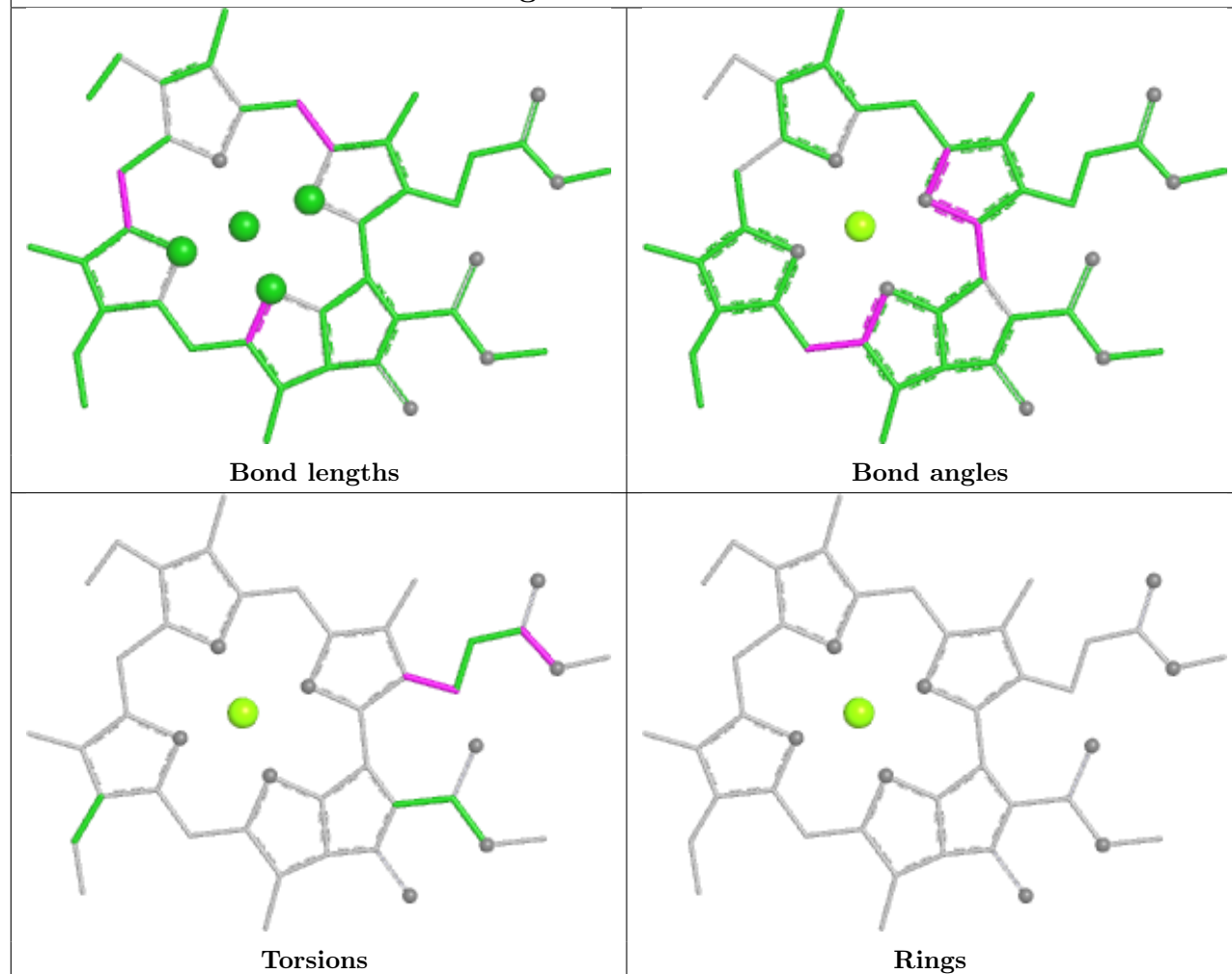


Ligand CLA G 1227

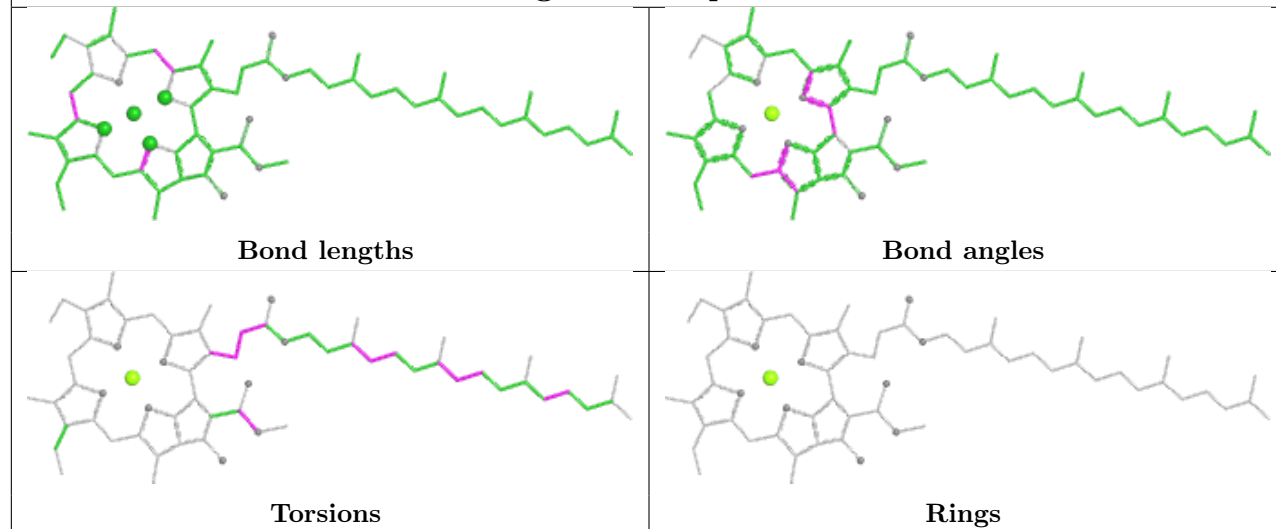


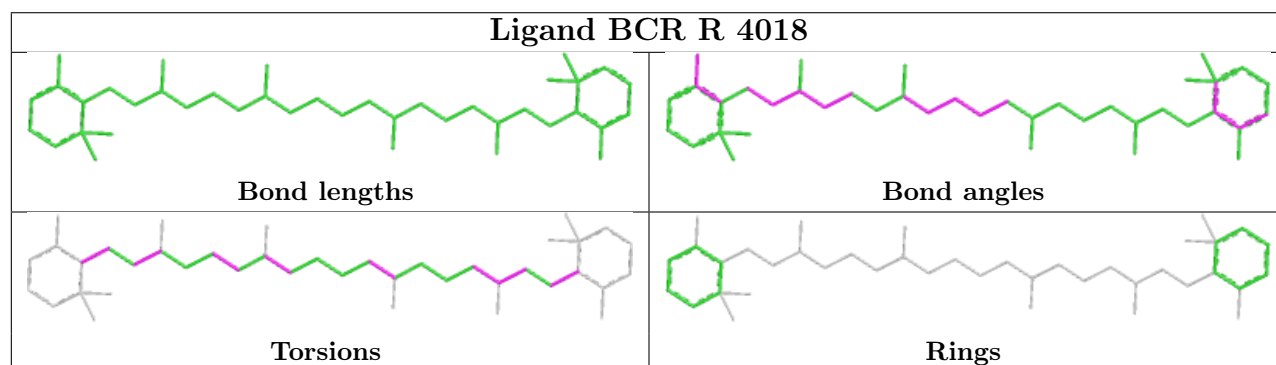
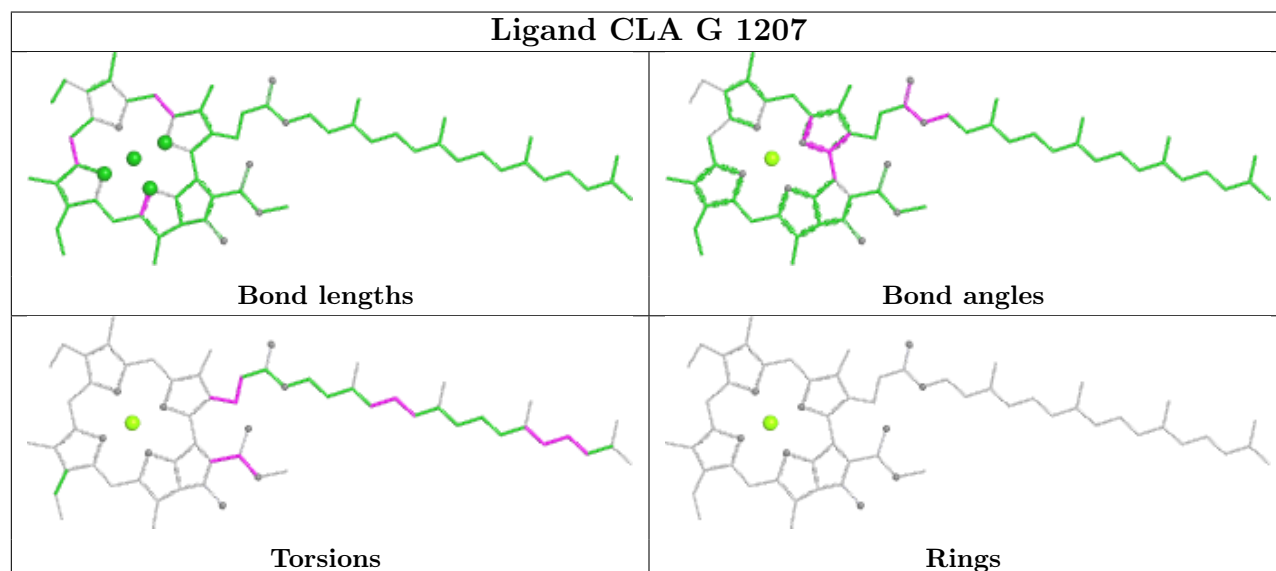
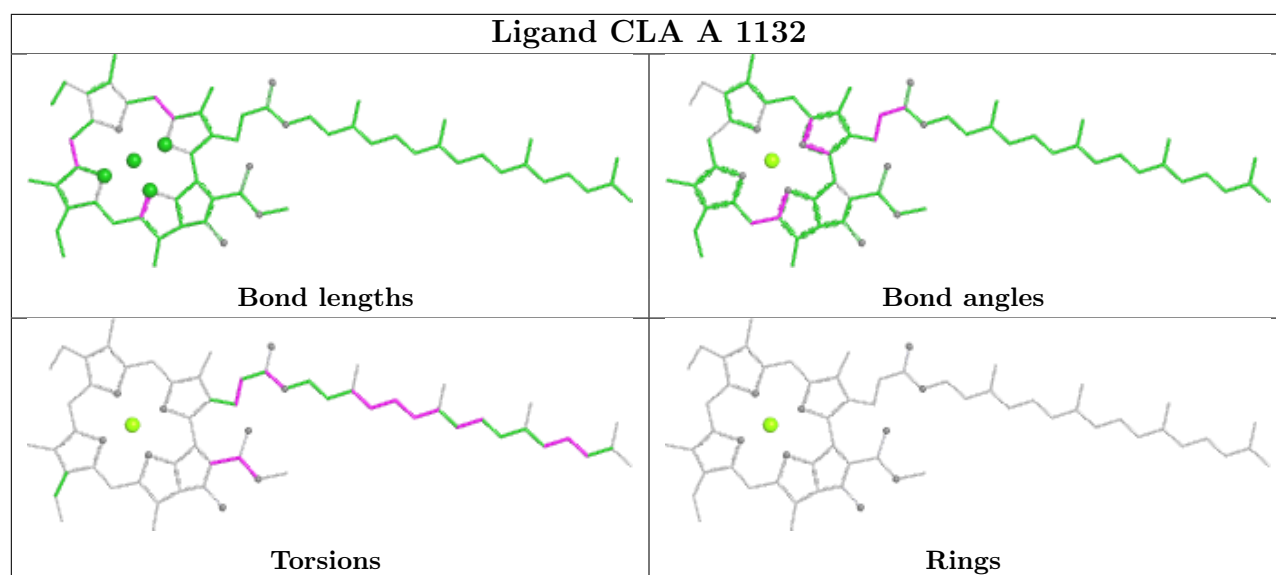
Ligand CLA Z 515**Ligand CLA o 505**

Ligand CLA r 516

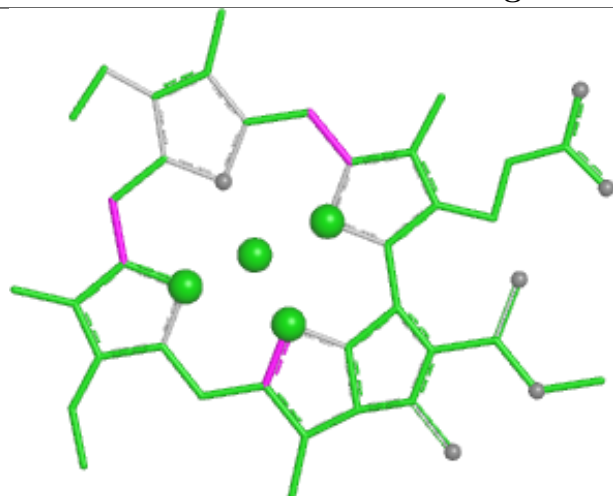


Ligand CLA p 505

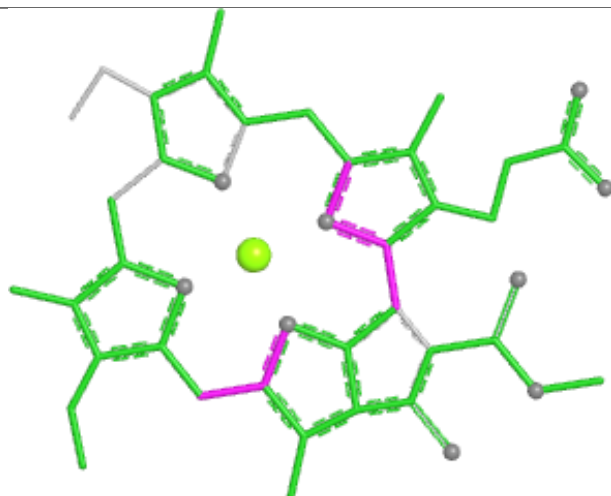




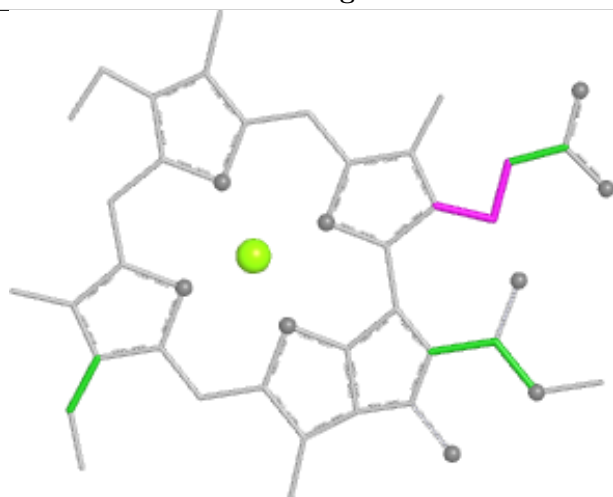
Ligand CLA G 1231



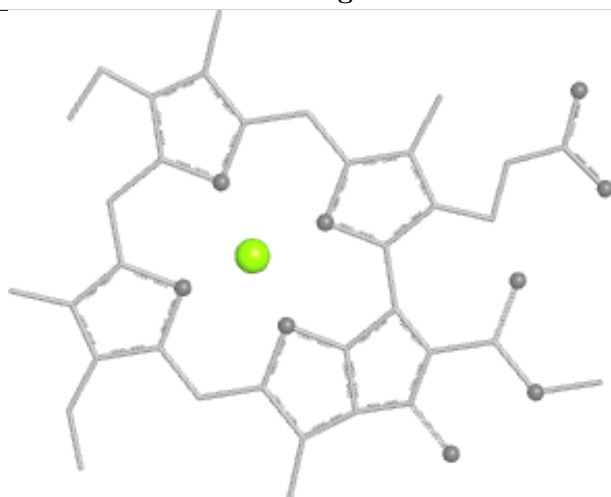
Bond lengths



Bond angles

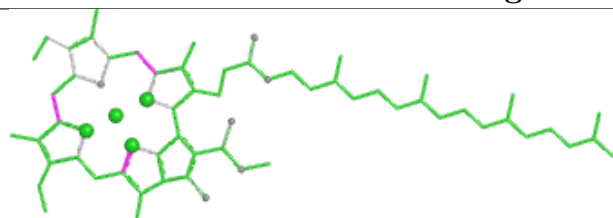


Torsions

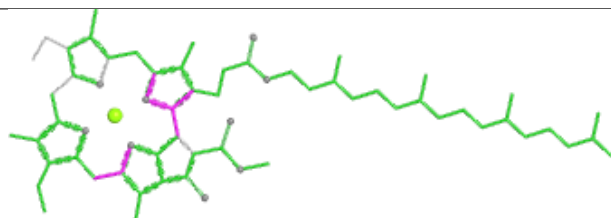


Rings

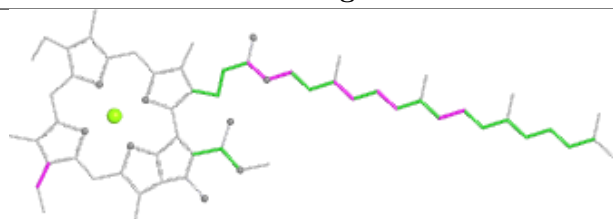
Ligand CLA A 1123



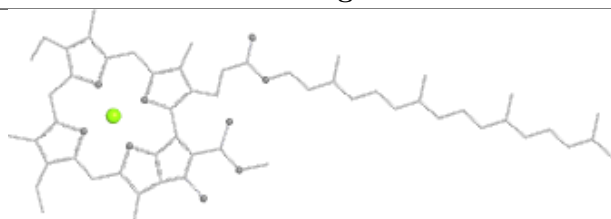
Bond lengths



Bond angles

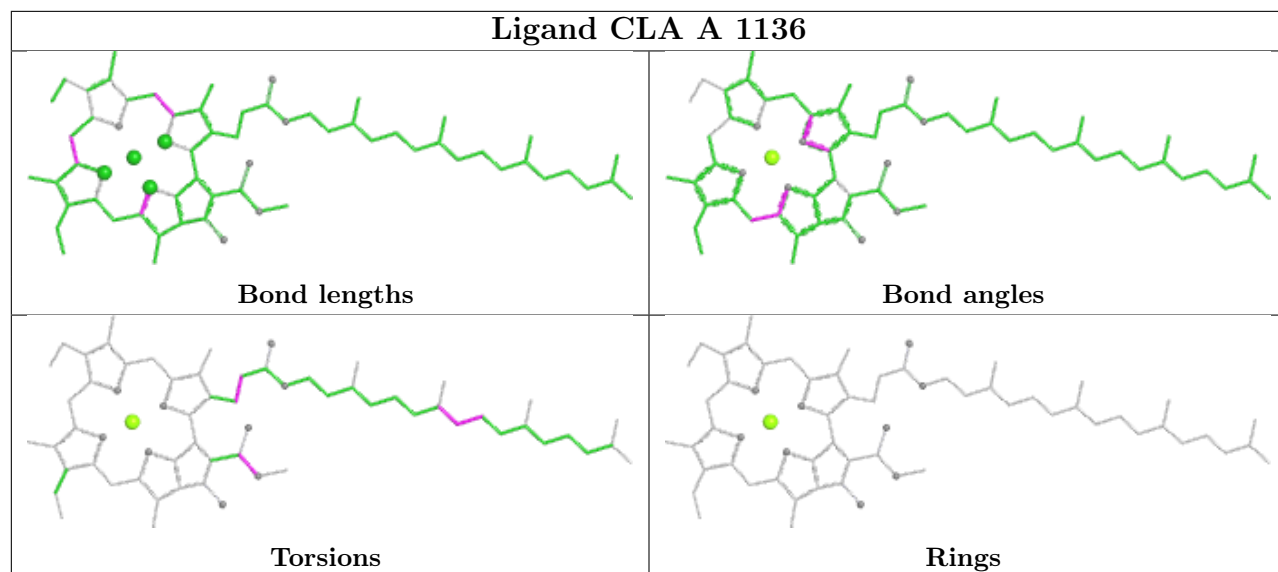


Torsions

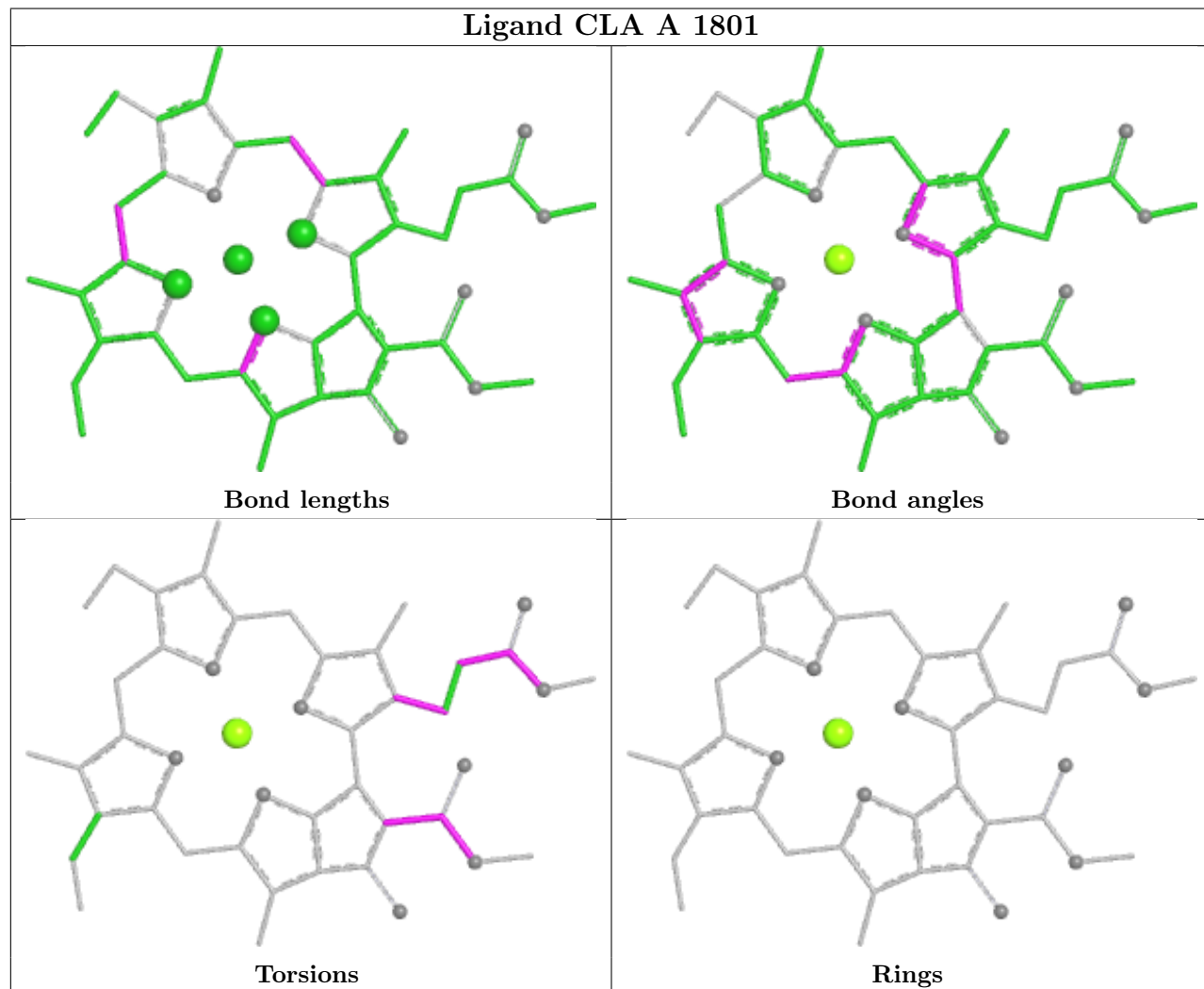


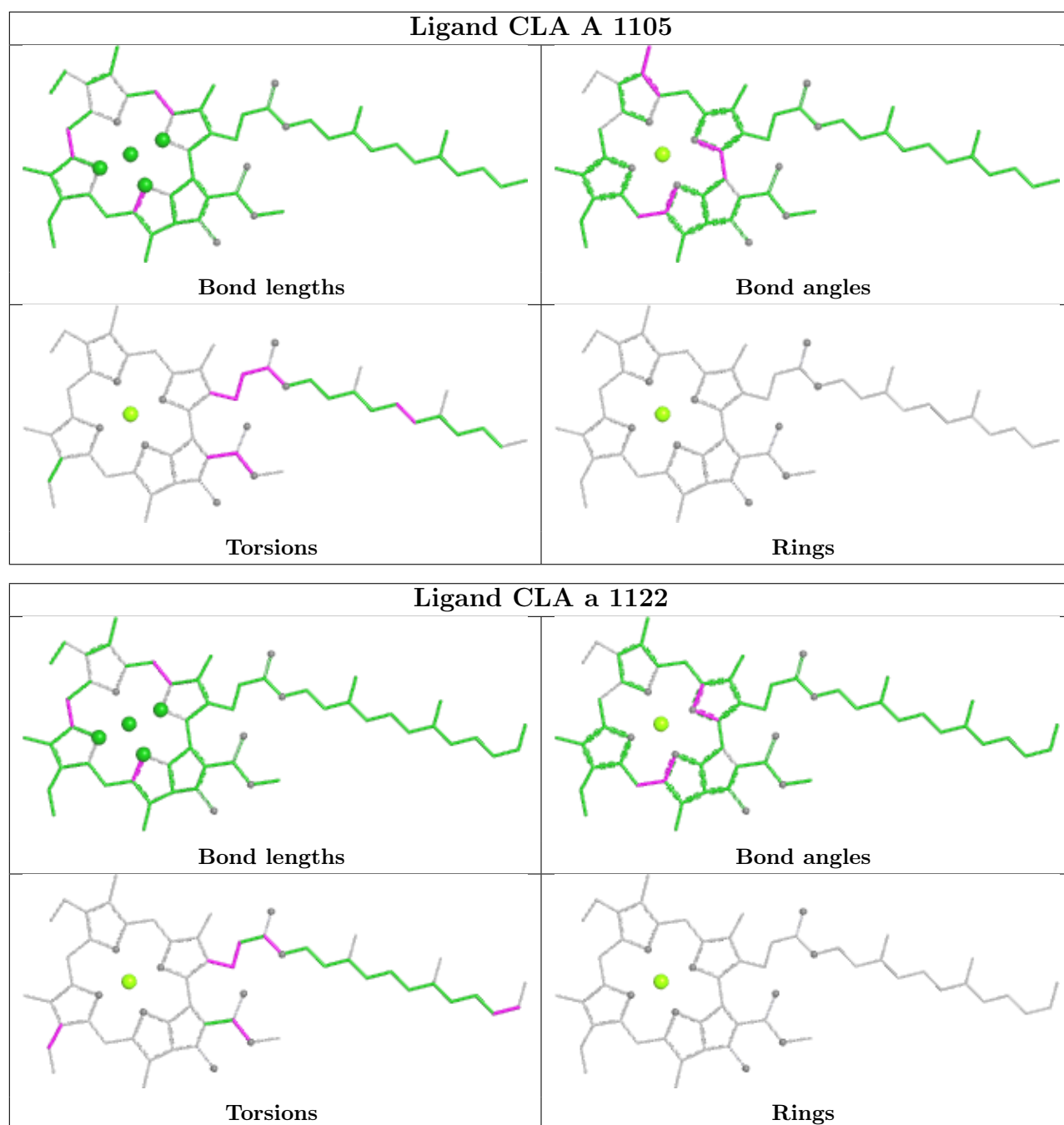
Rings

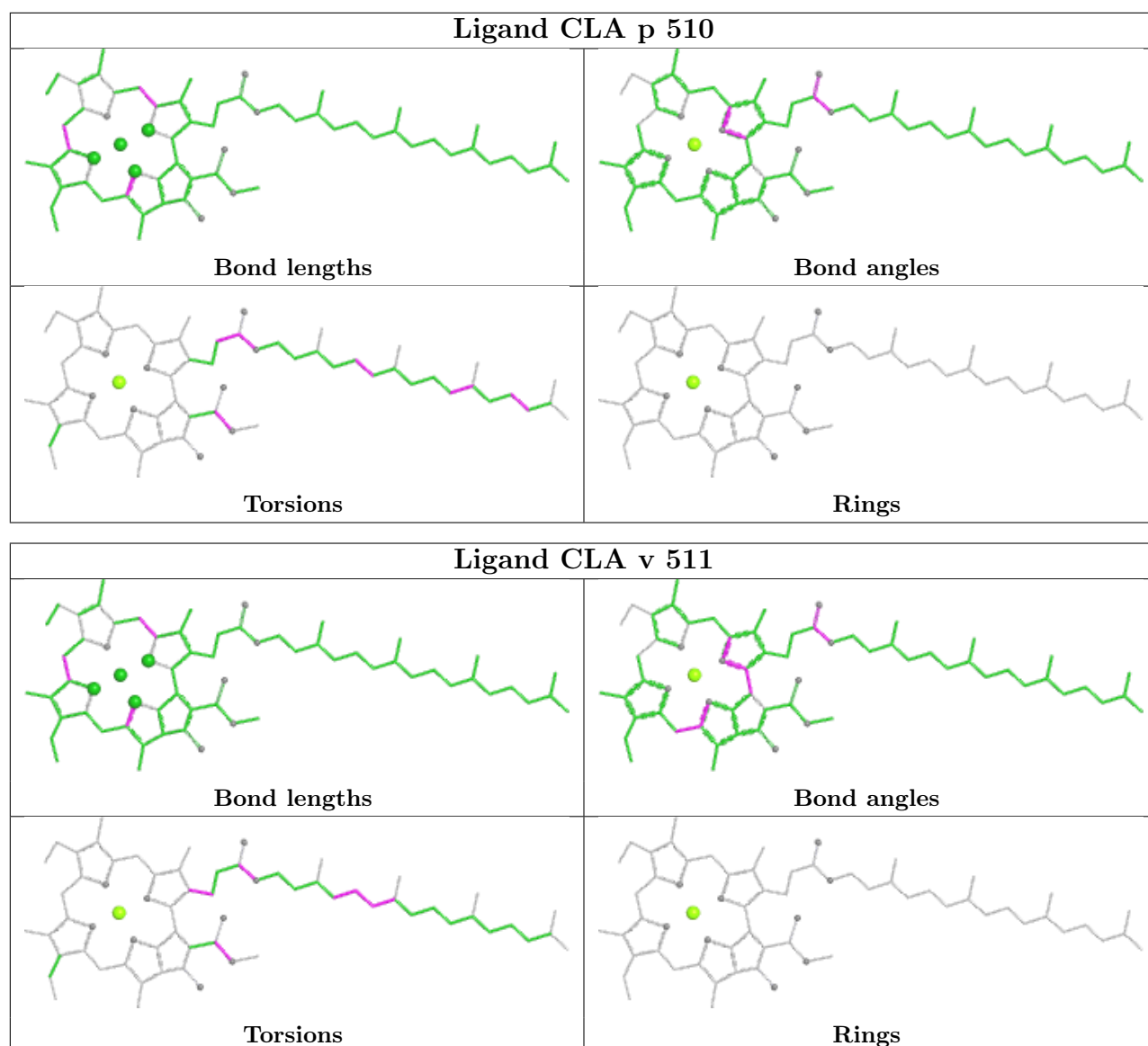
Ligand CLA A 1136



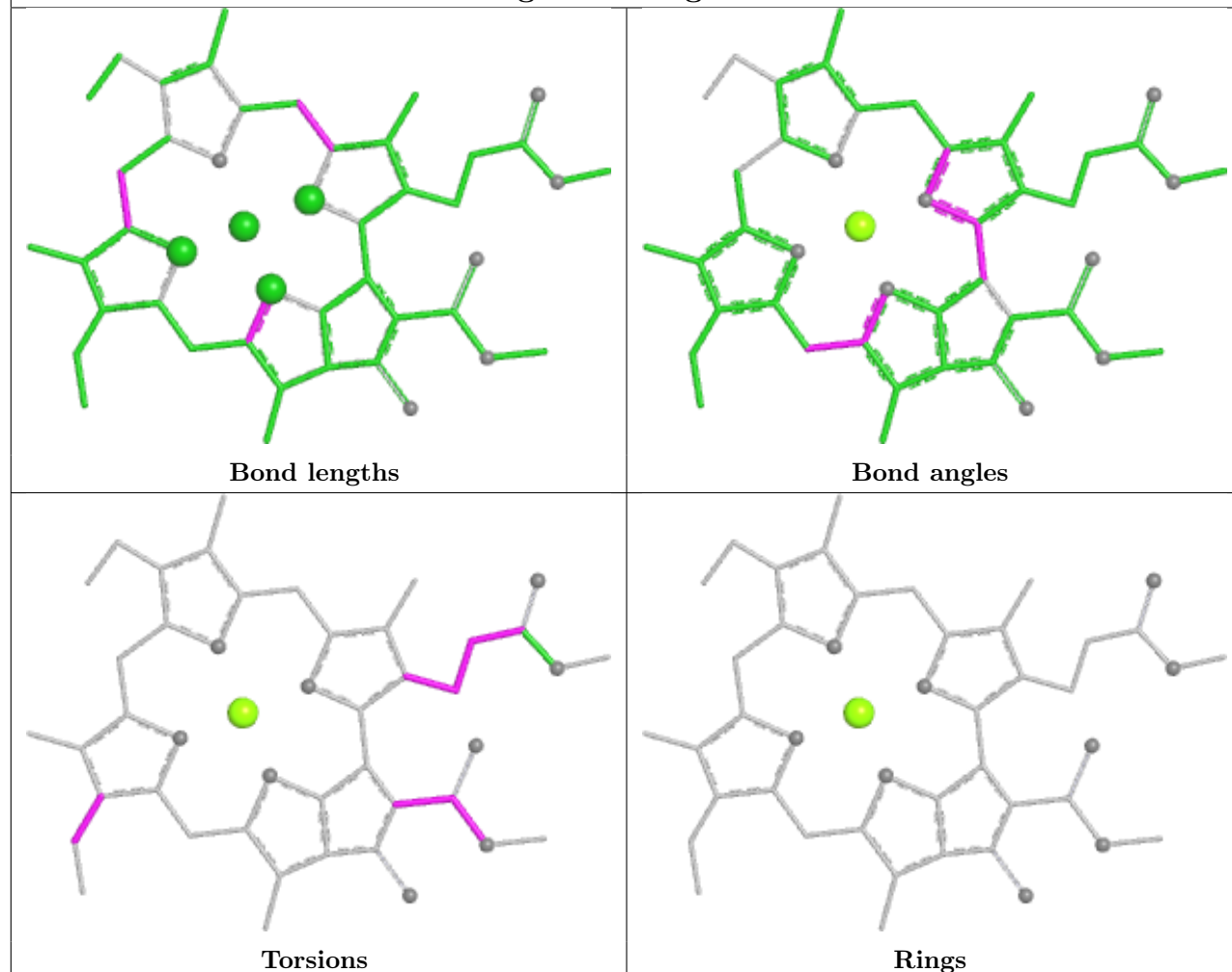
Ligand CLA A 1801



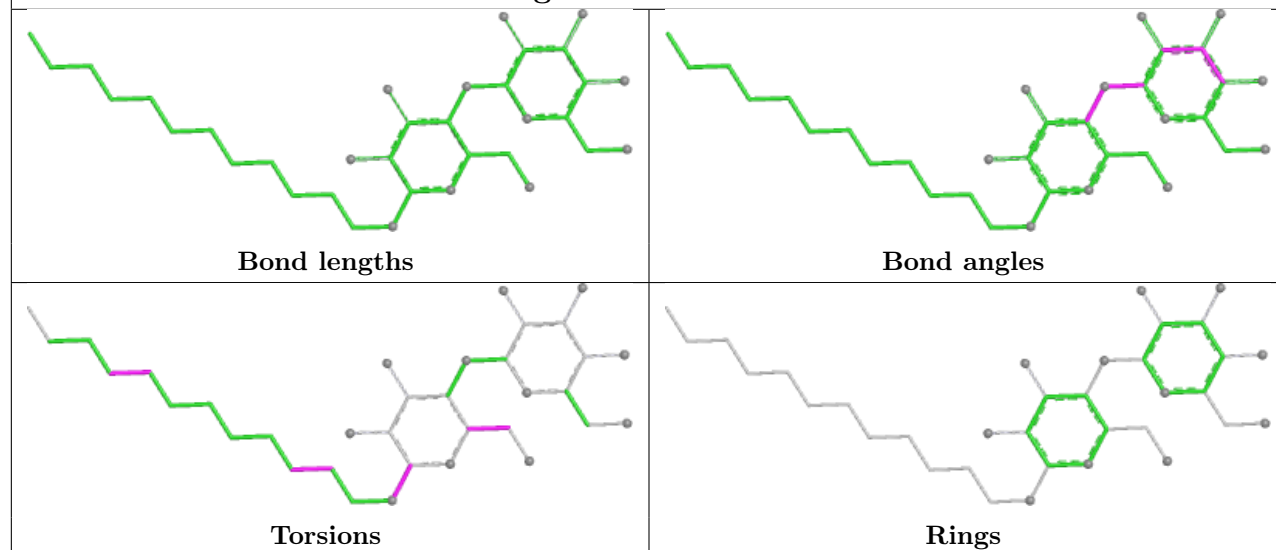




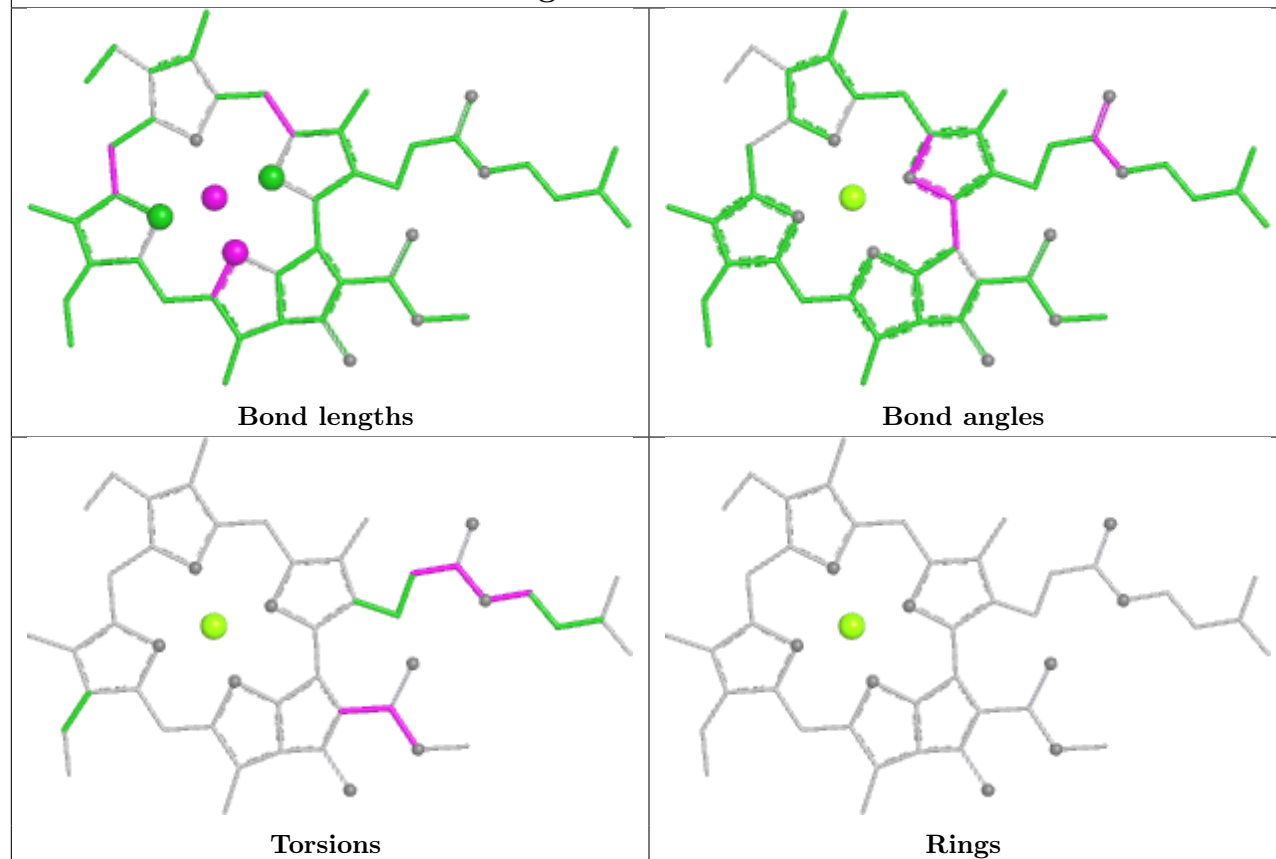
Ligand CLA g 513



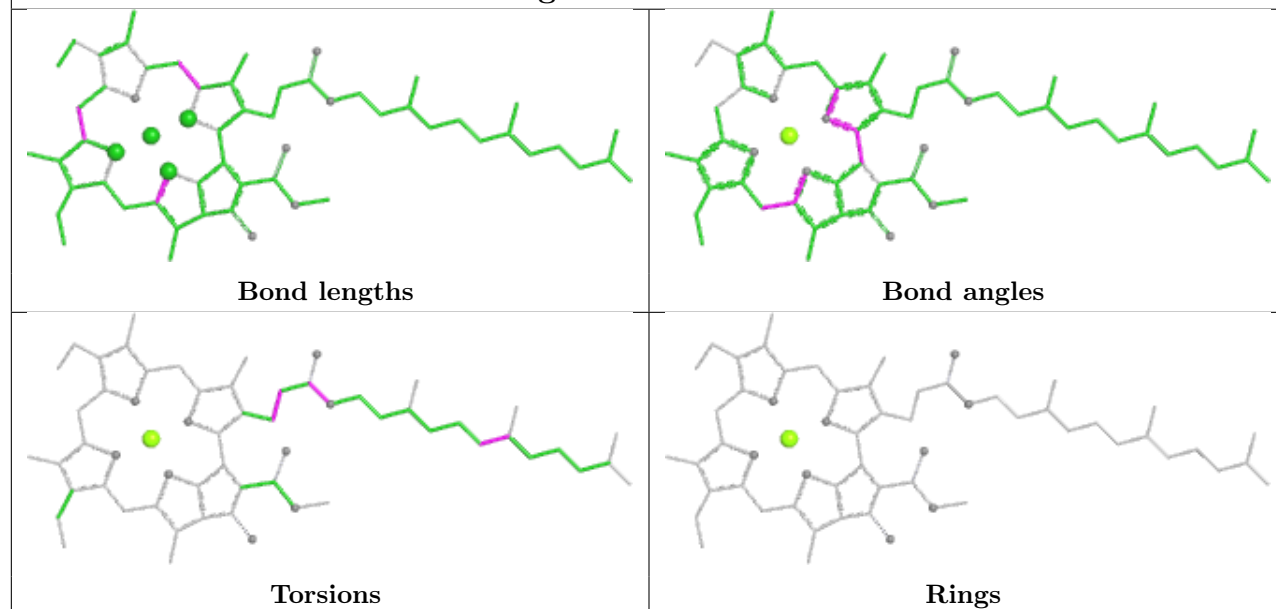
Ligand LMU r 606

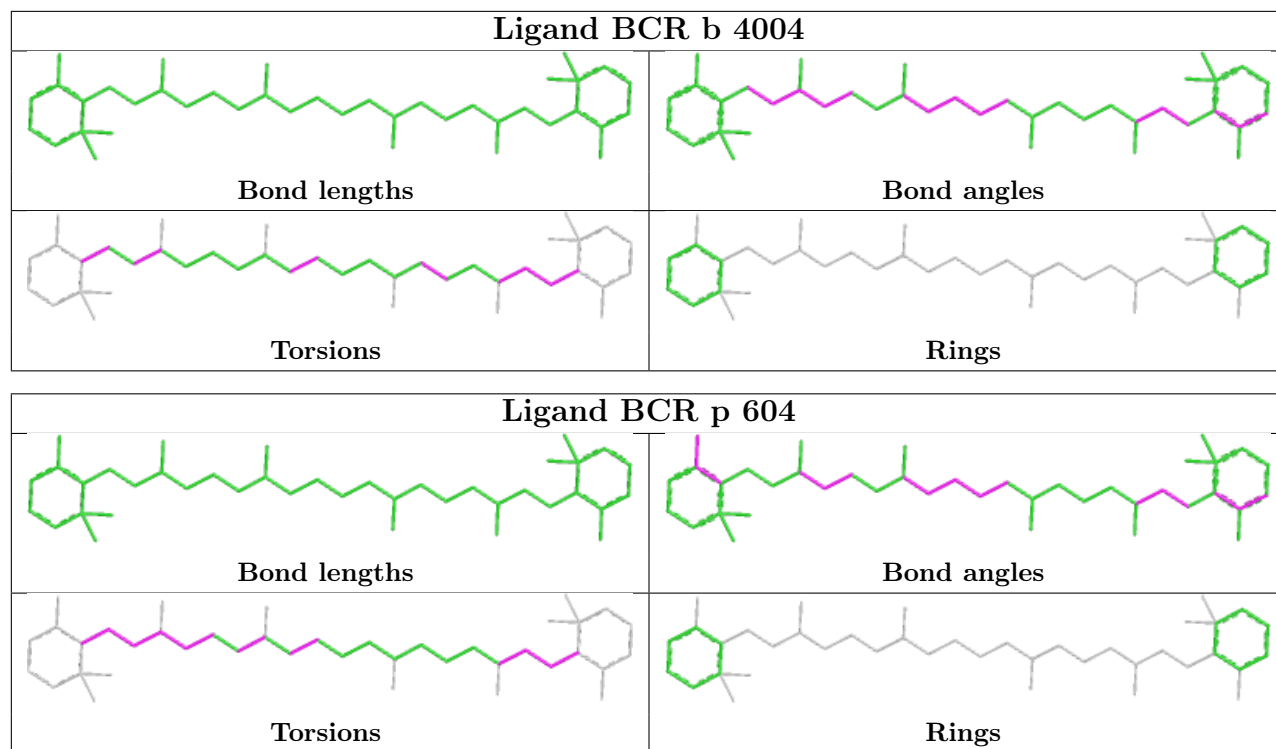


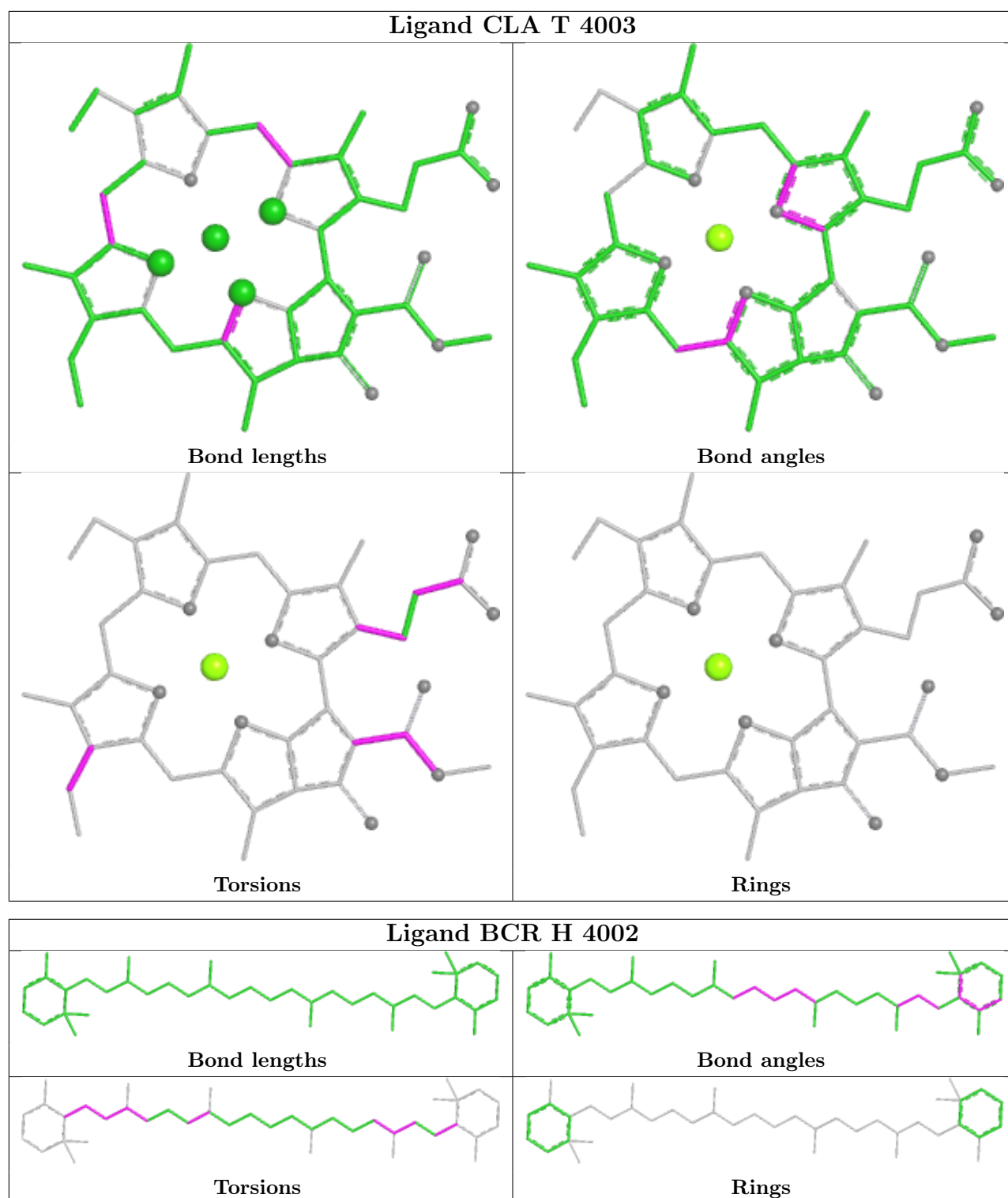
Ligand CLA t 502

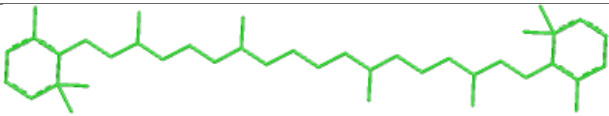
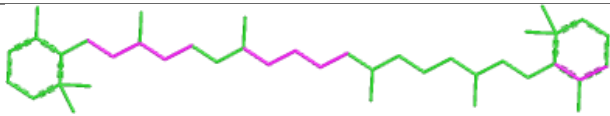
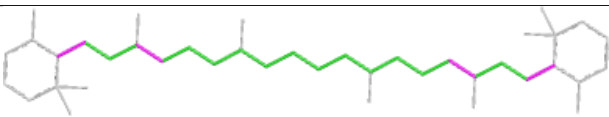
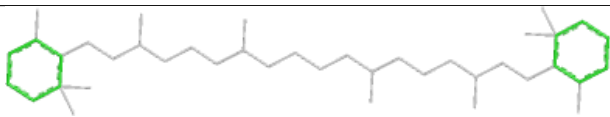


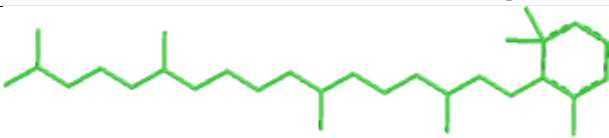
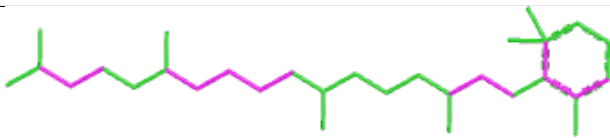
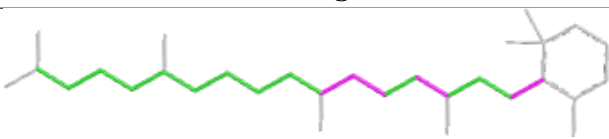
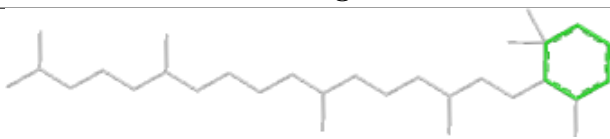
Ligand CLA t 504

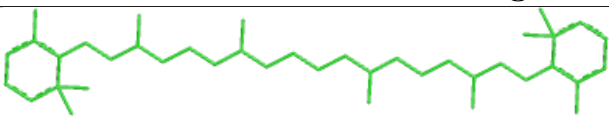
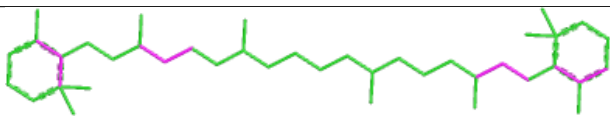

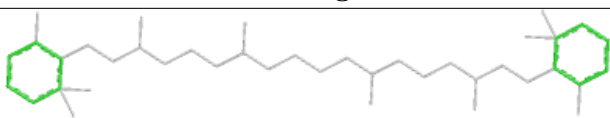


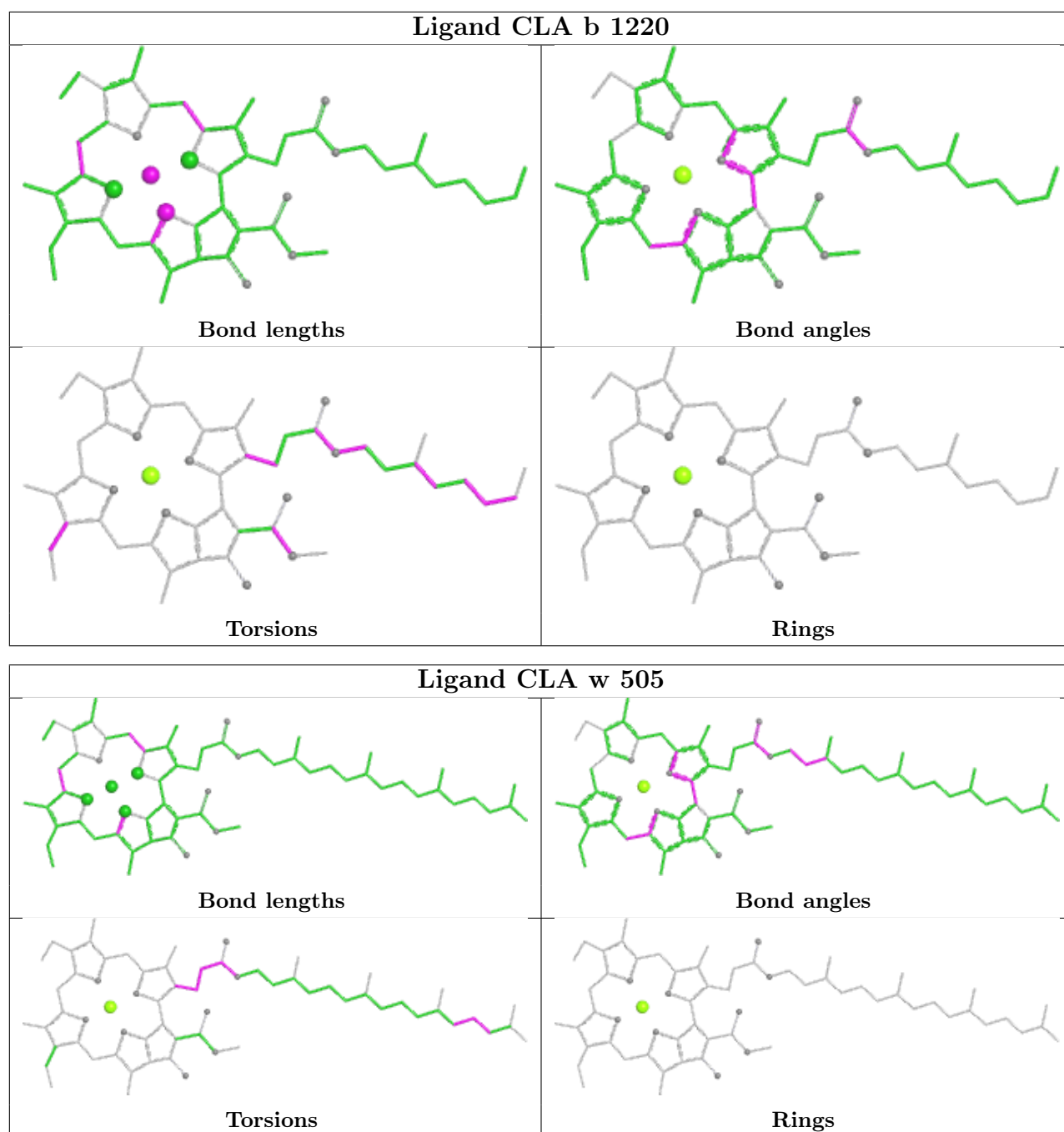


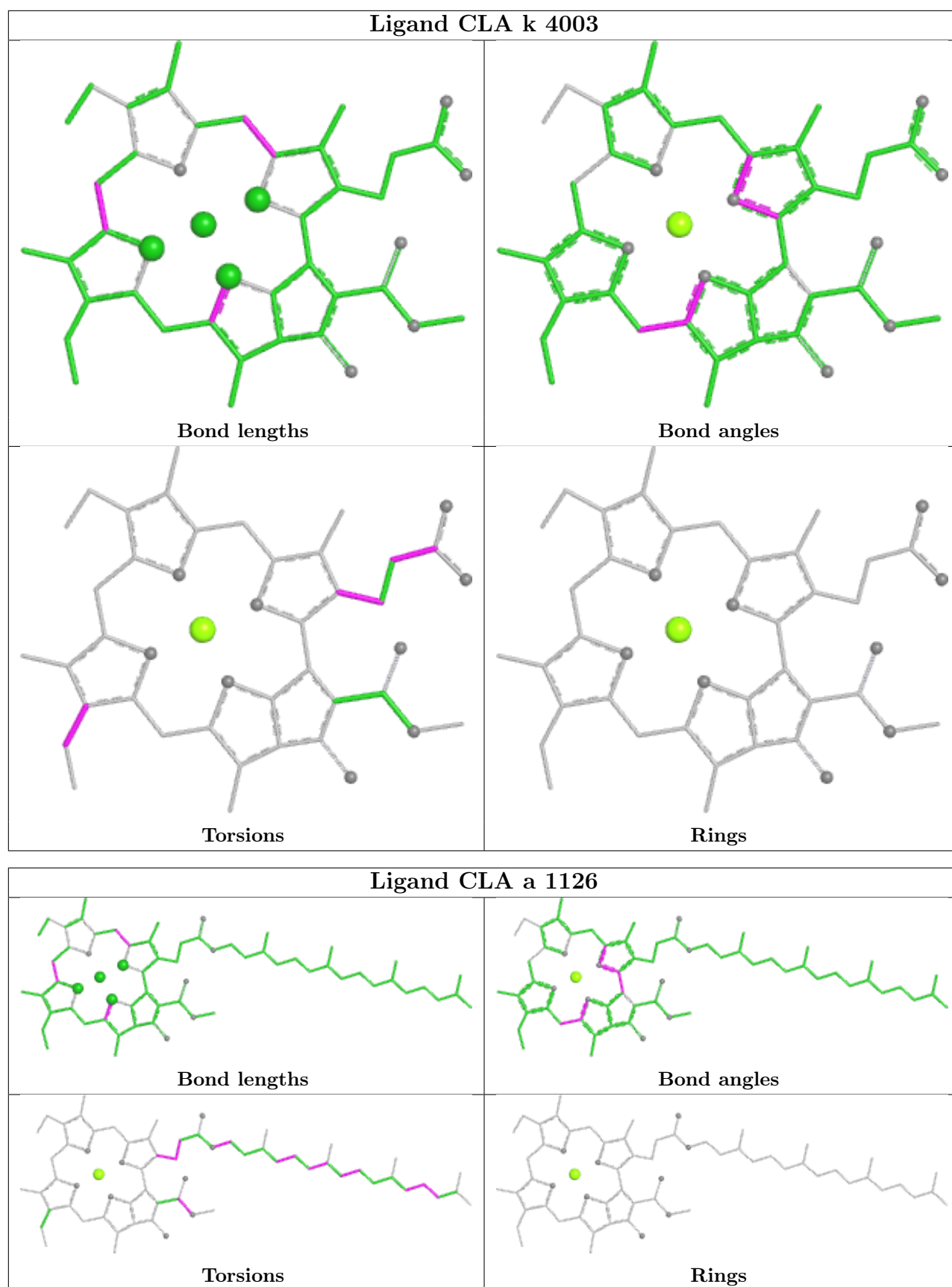


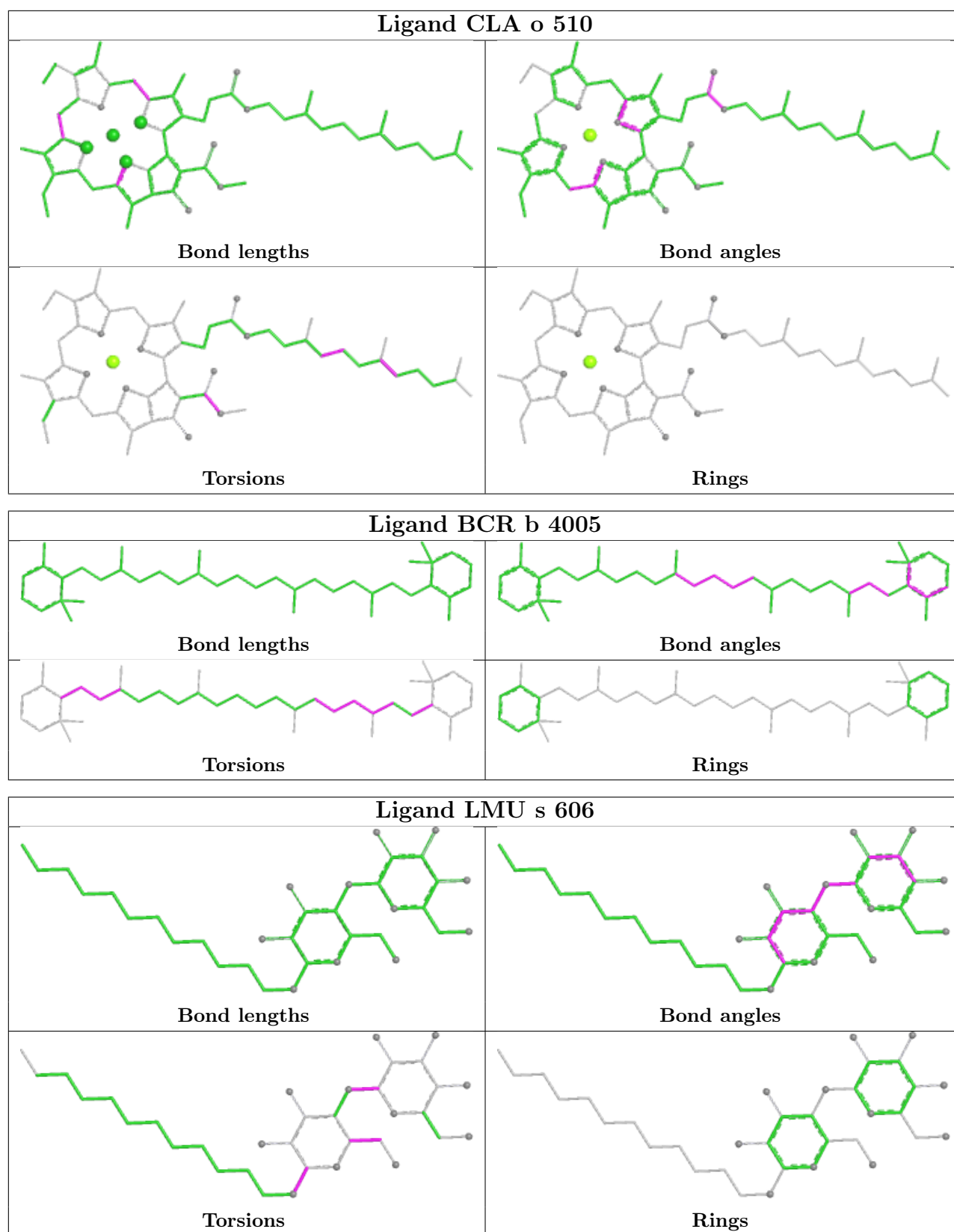
Ligand BCR p 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

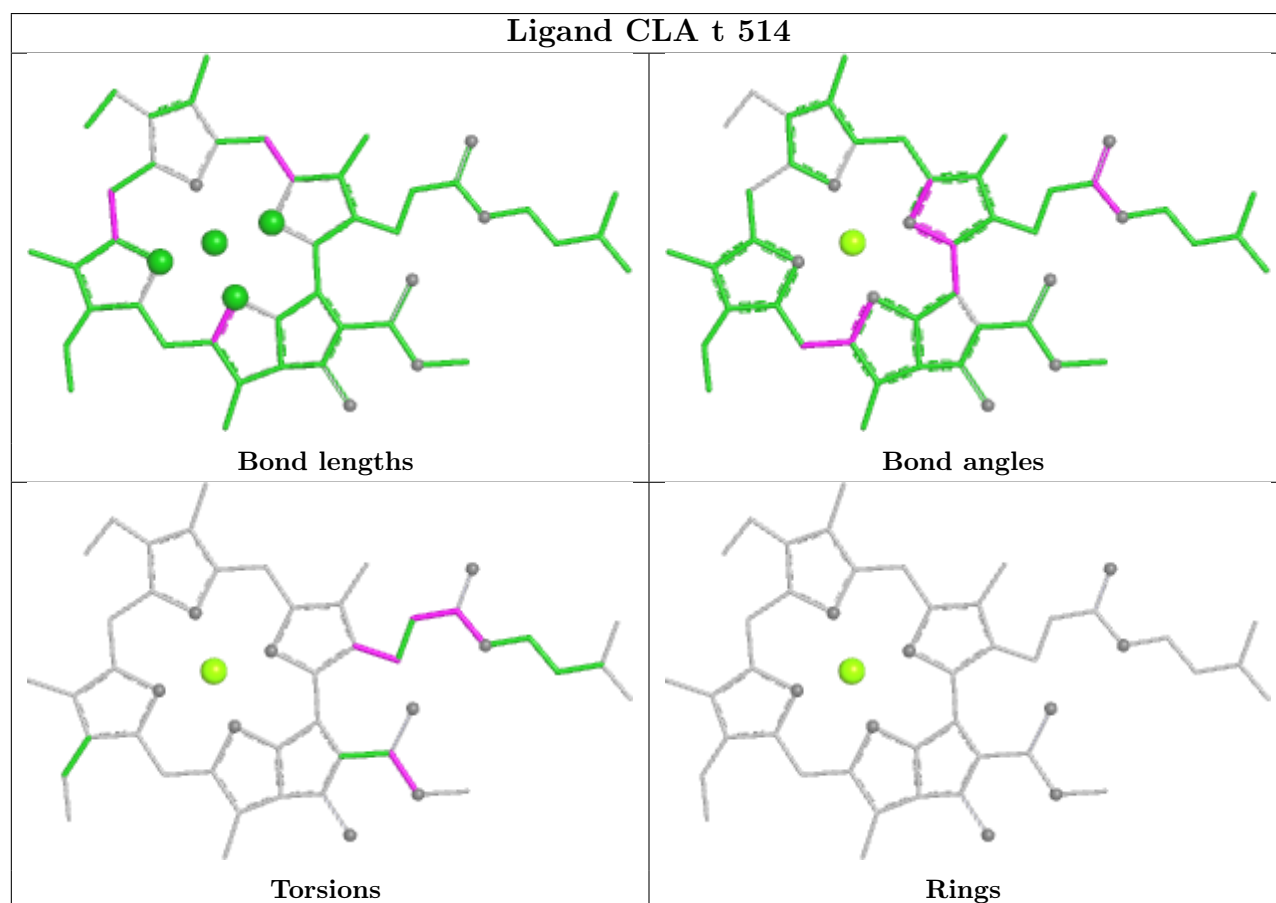
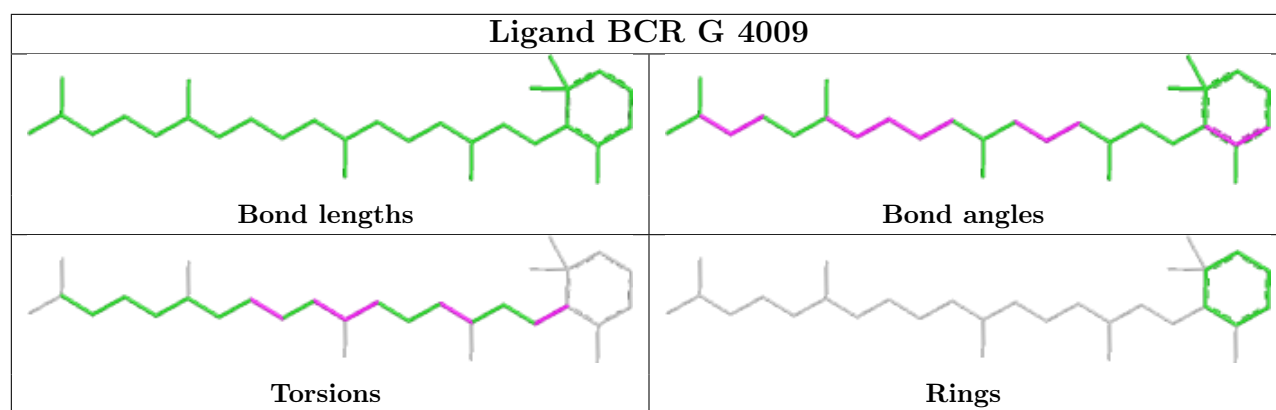
Ligand BCR b 4009	
	
Bond lengths	Bond angles
	
Torsions	Rings

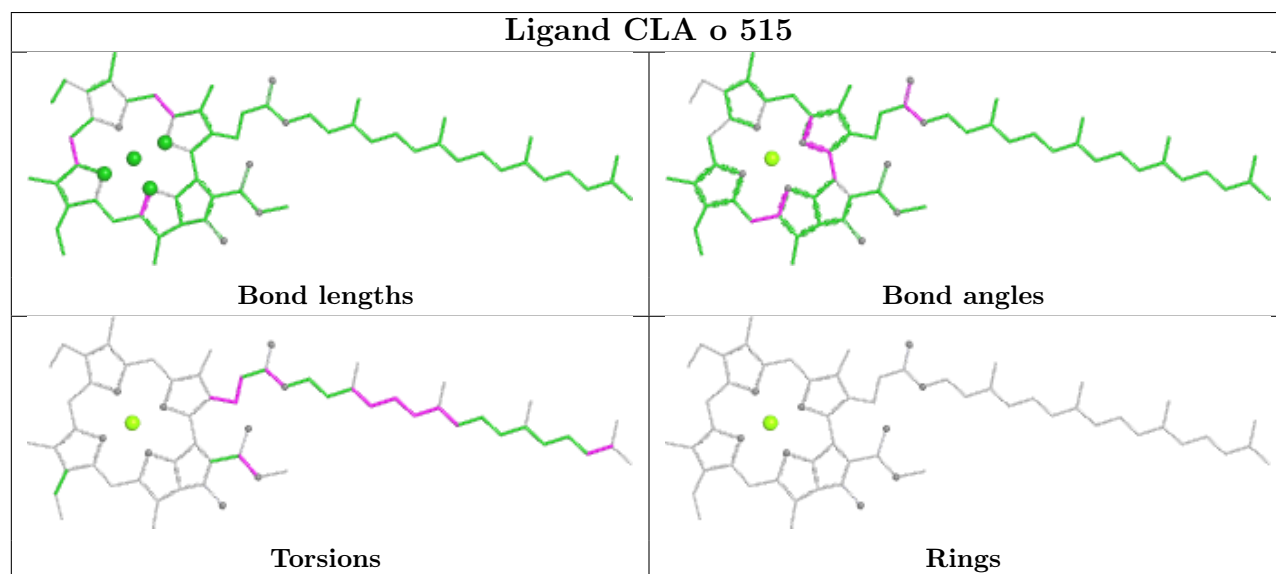
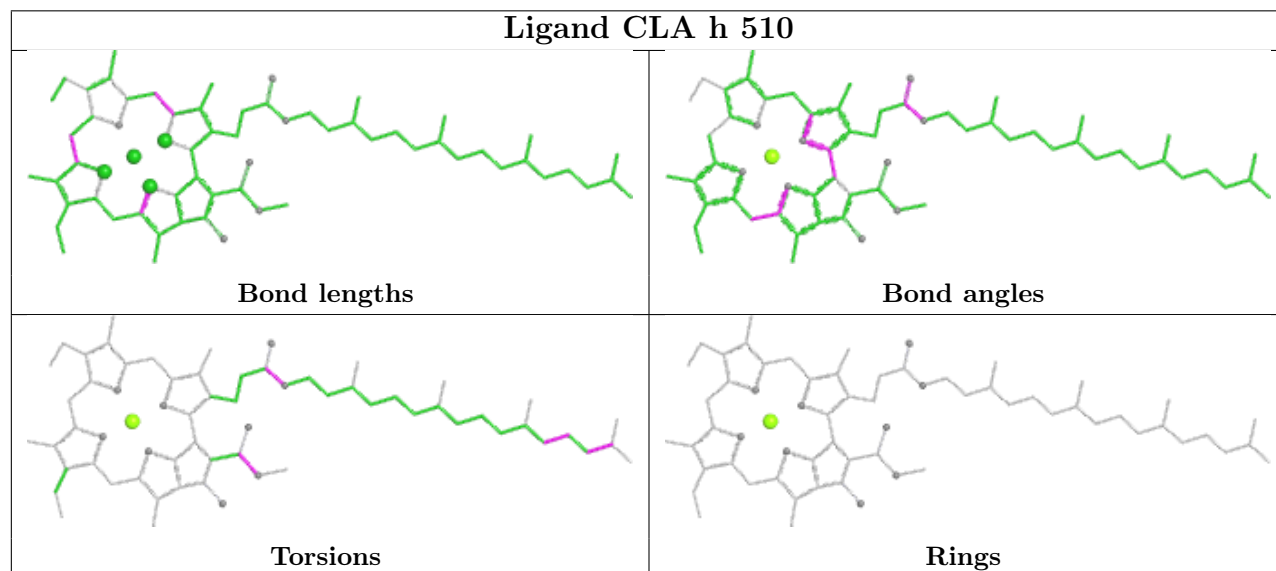
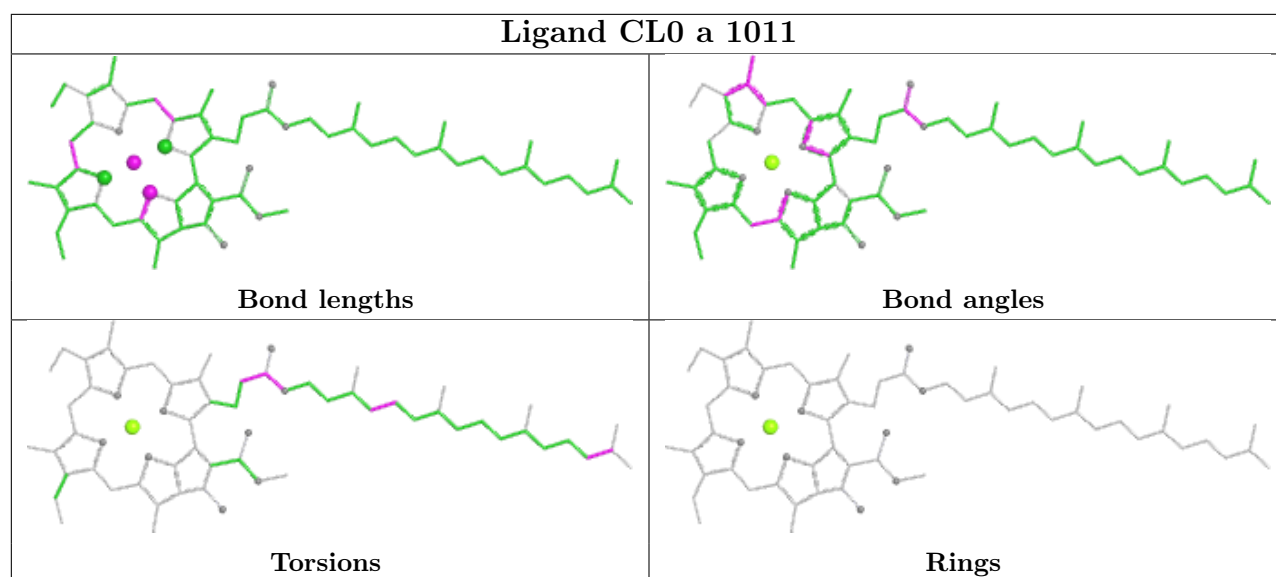
Ligand BCR h 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

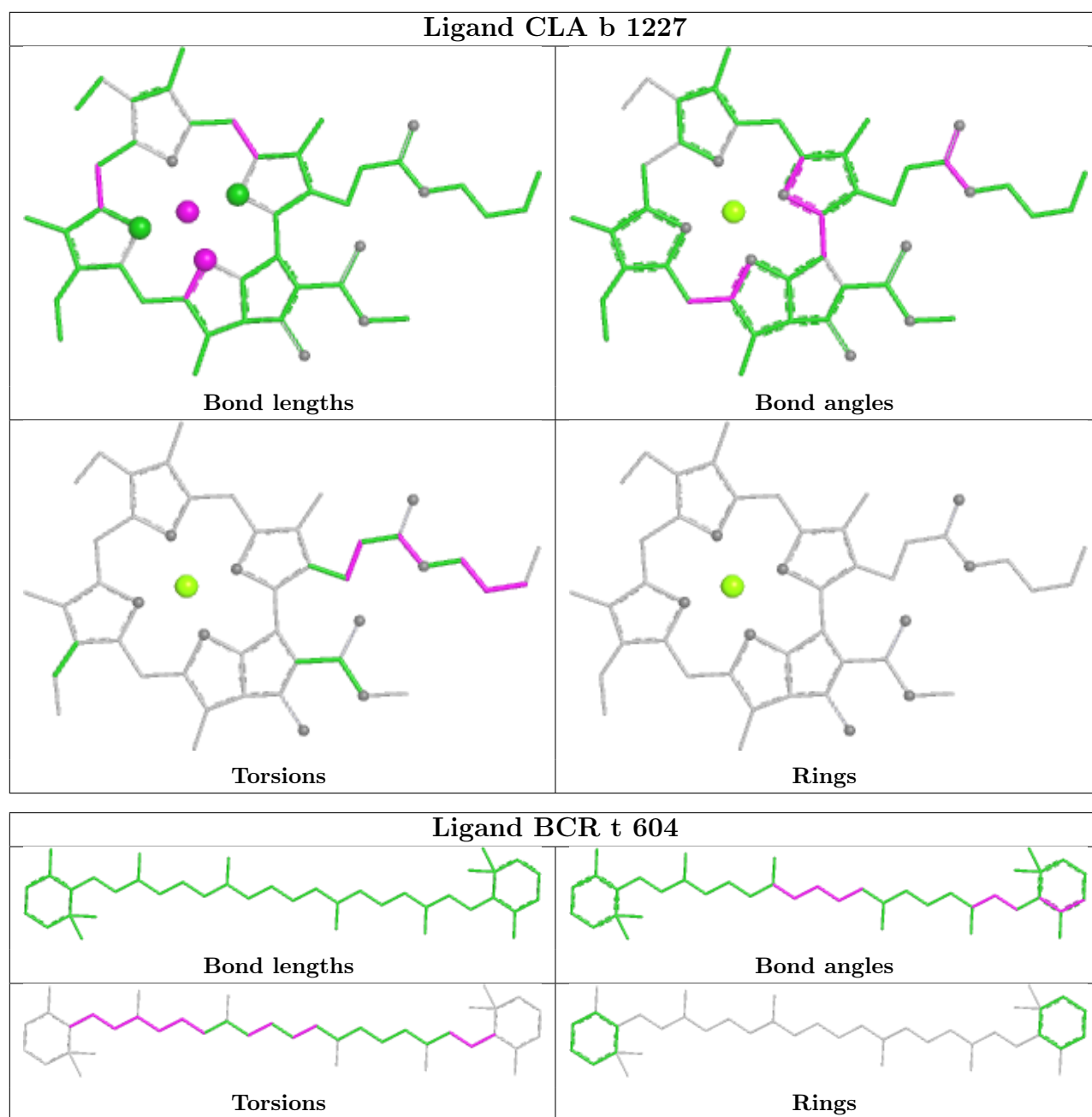


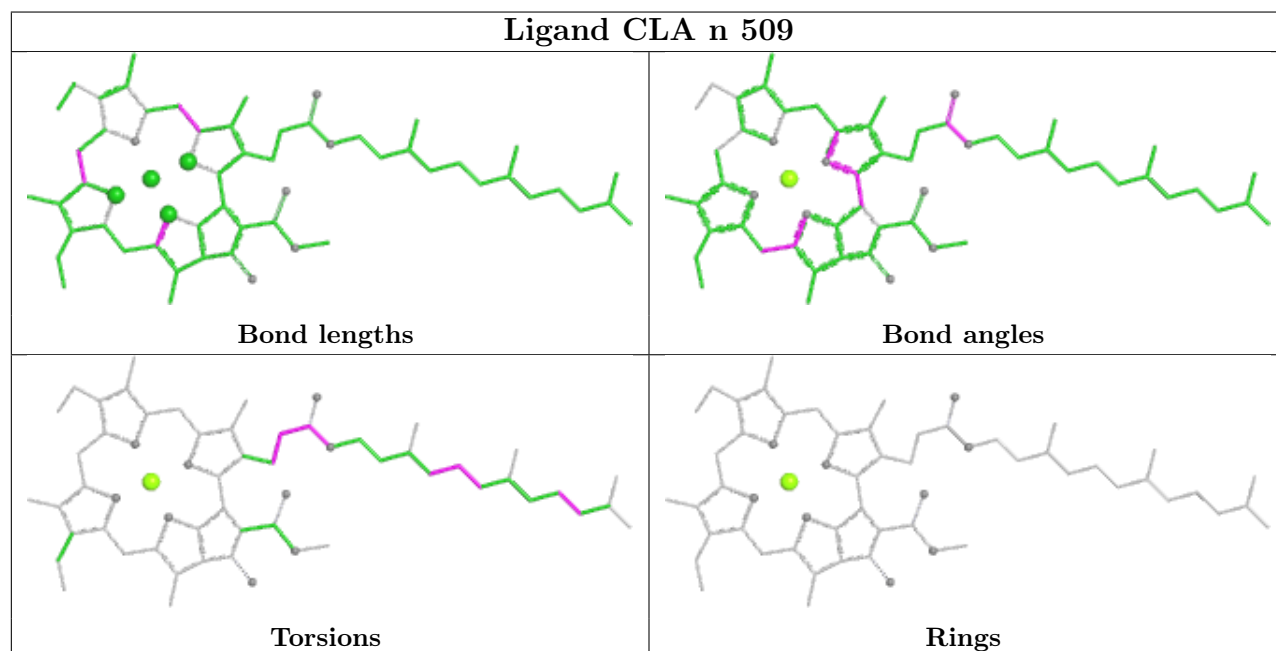
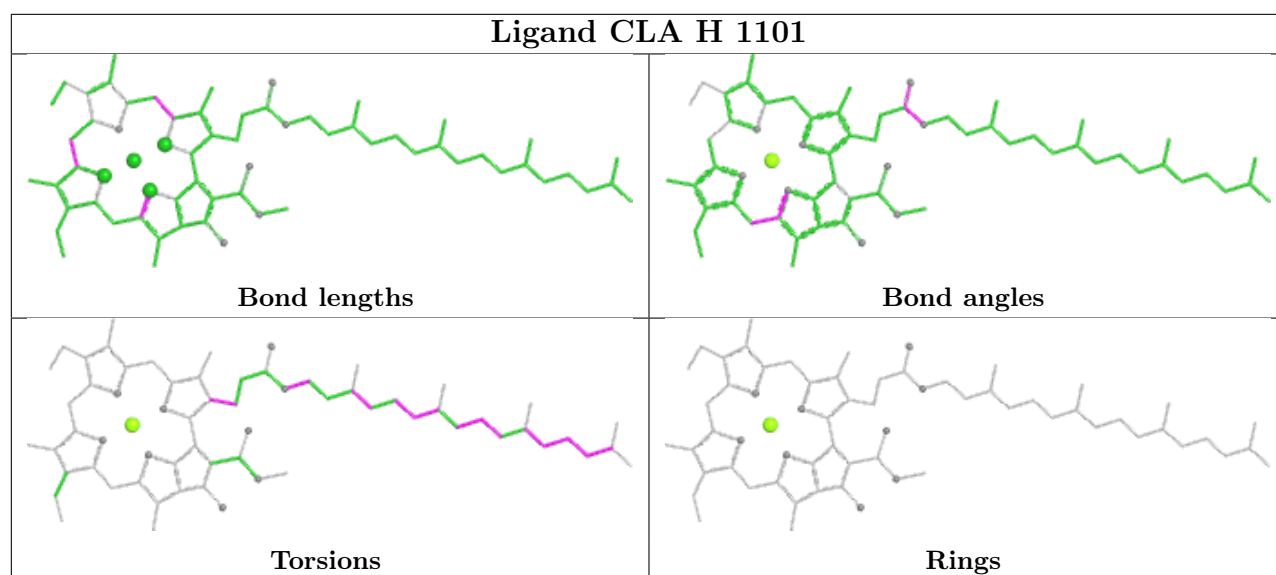


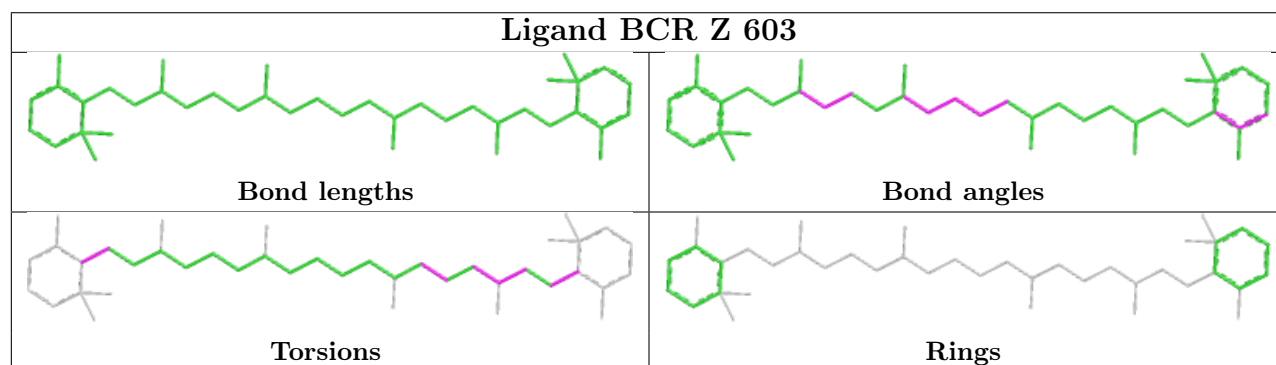
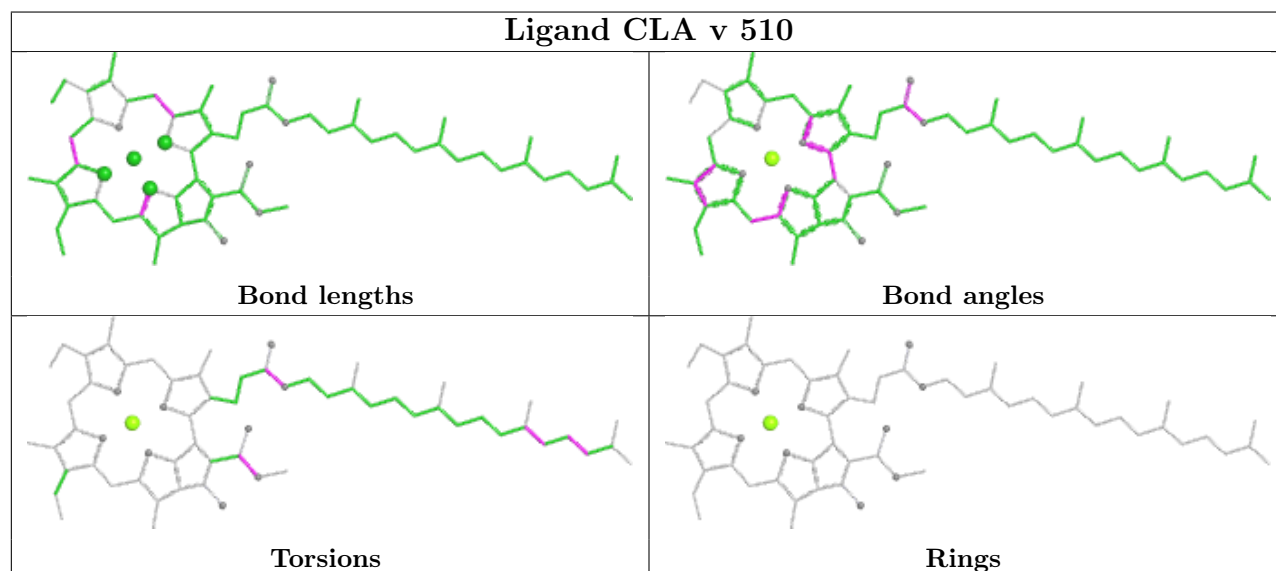
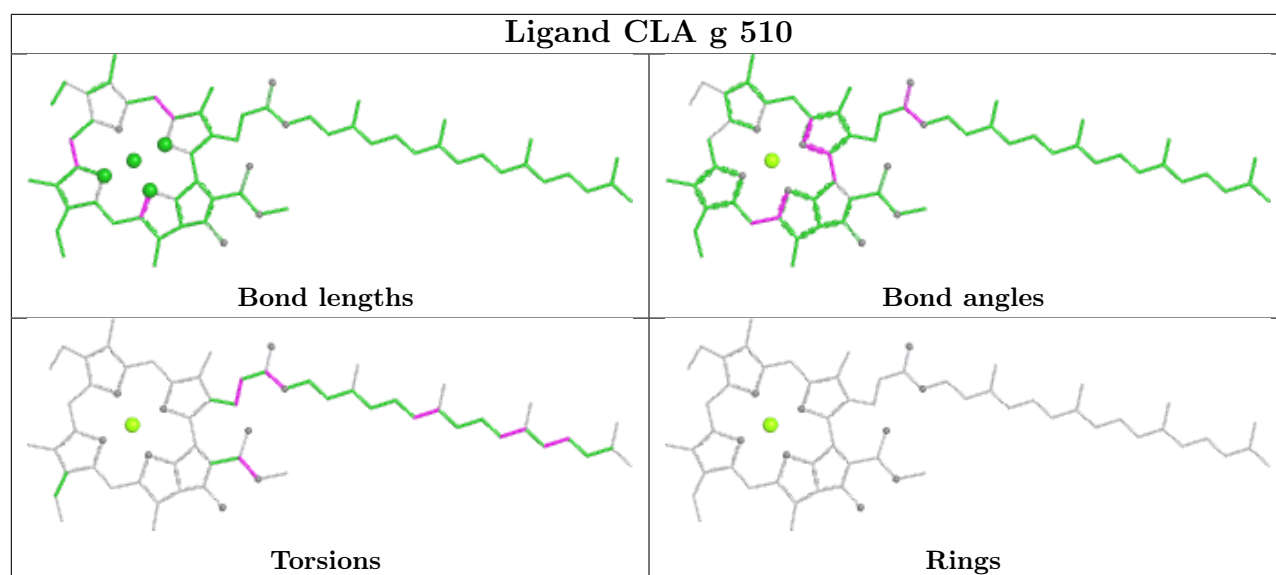




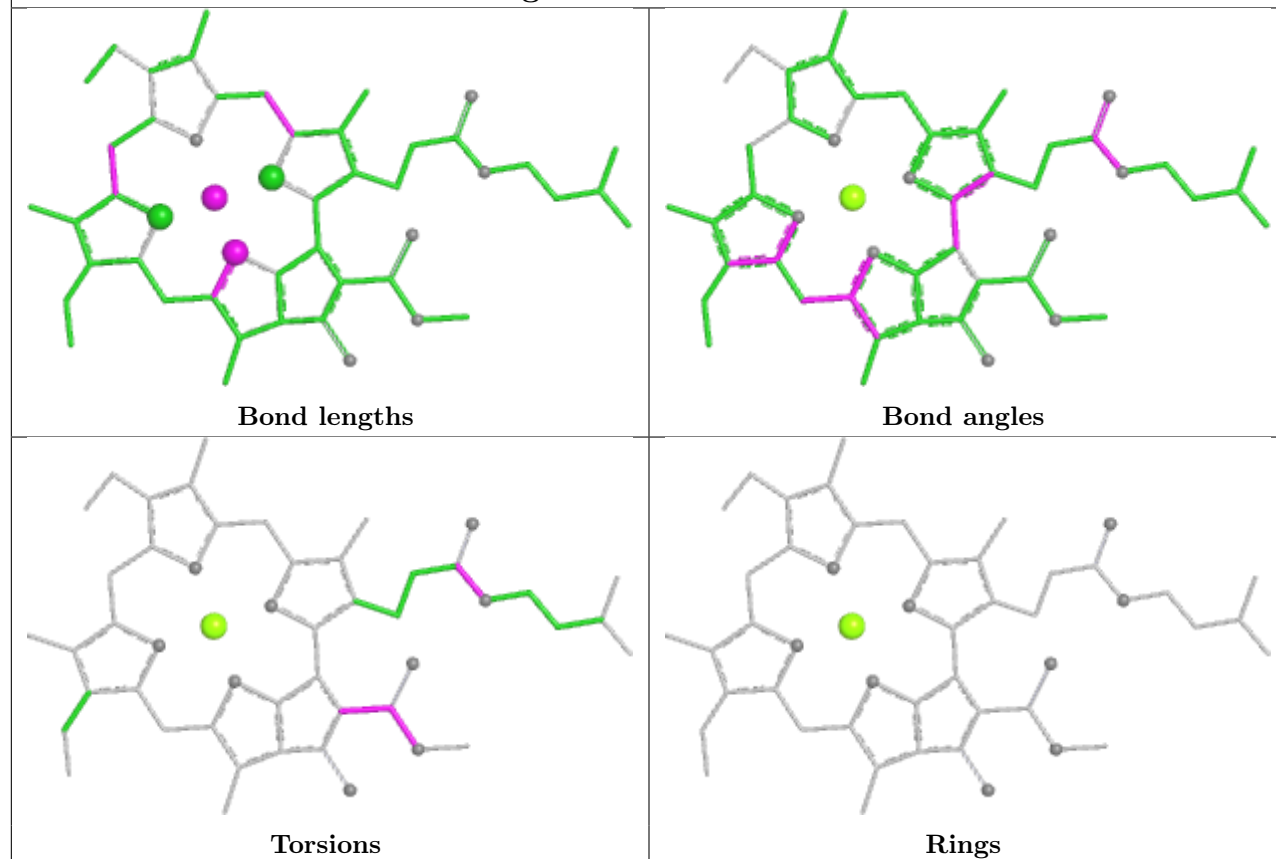




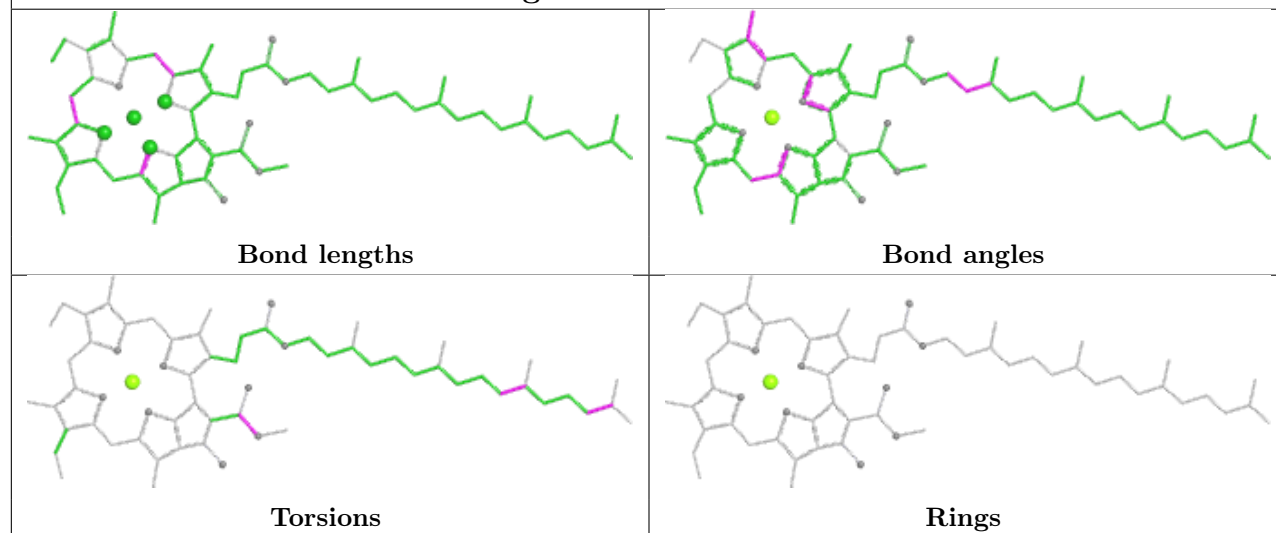


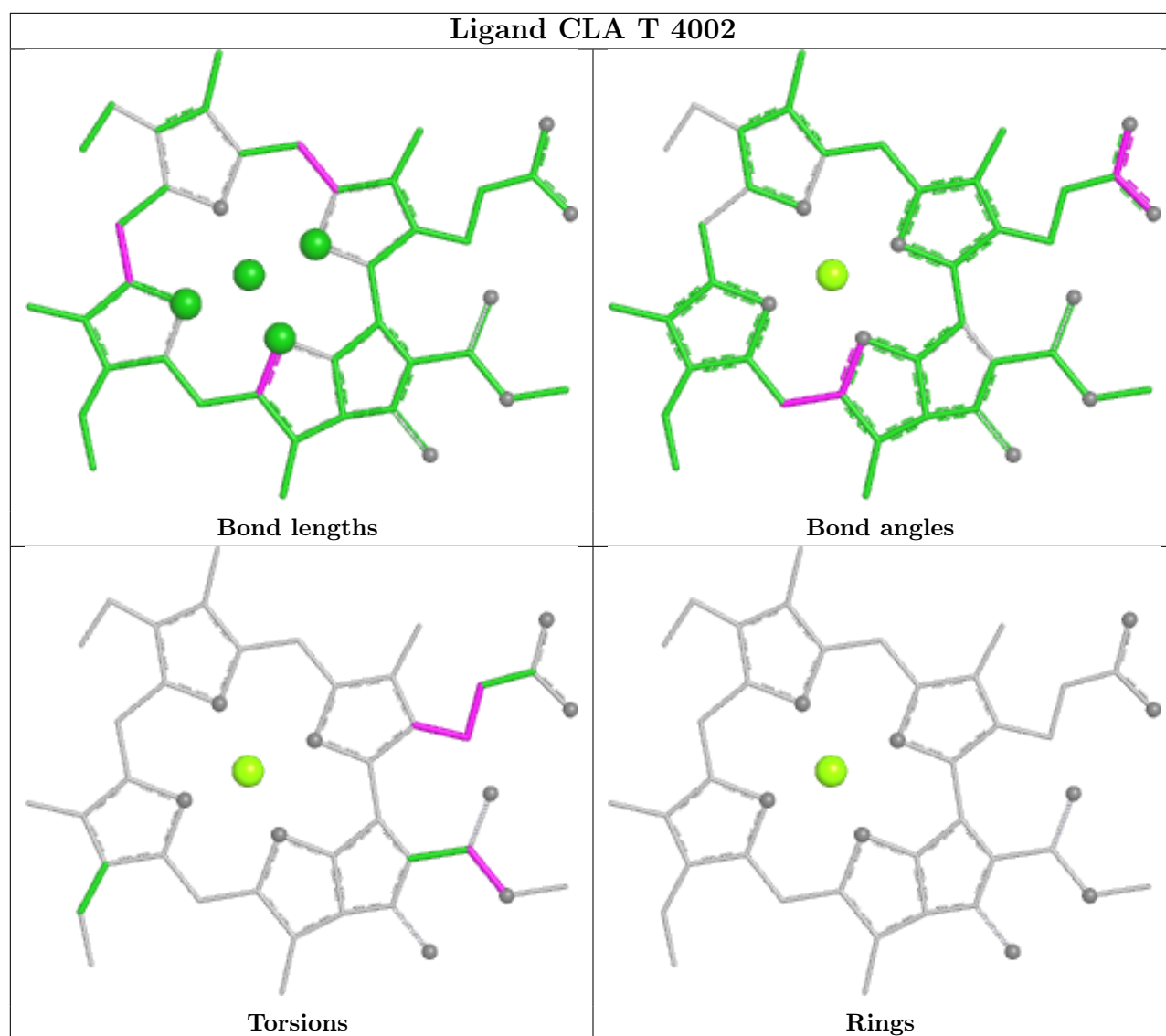


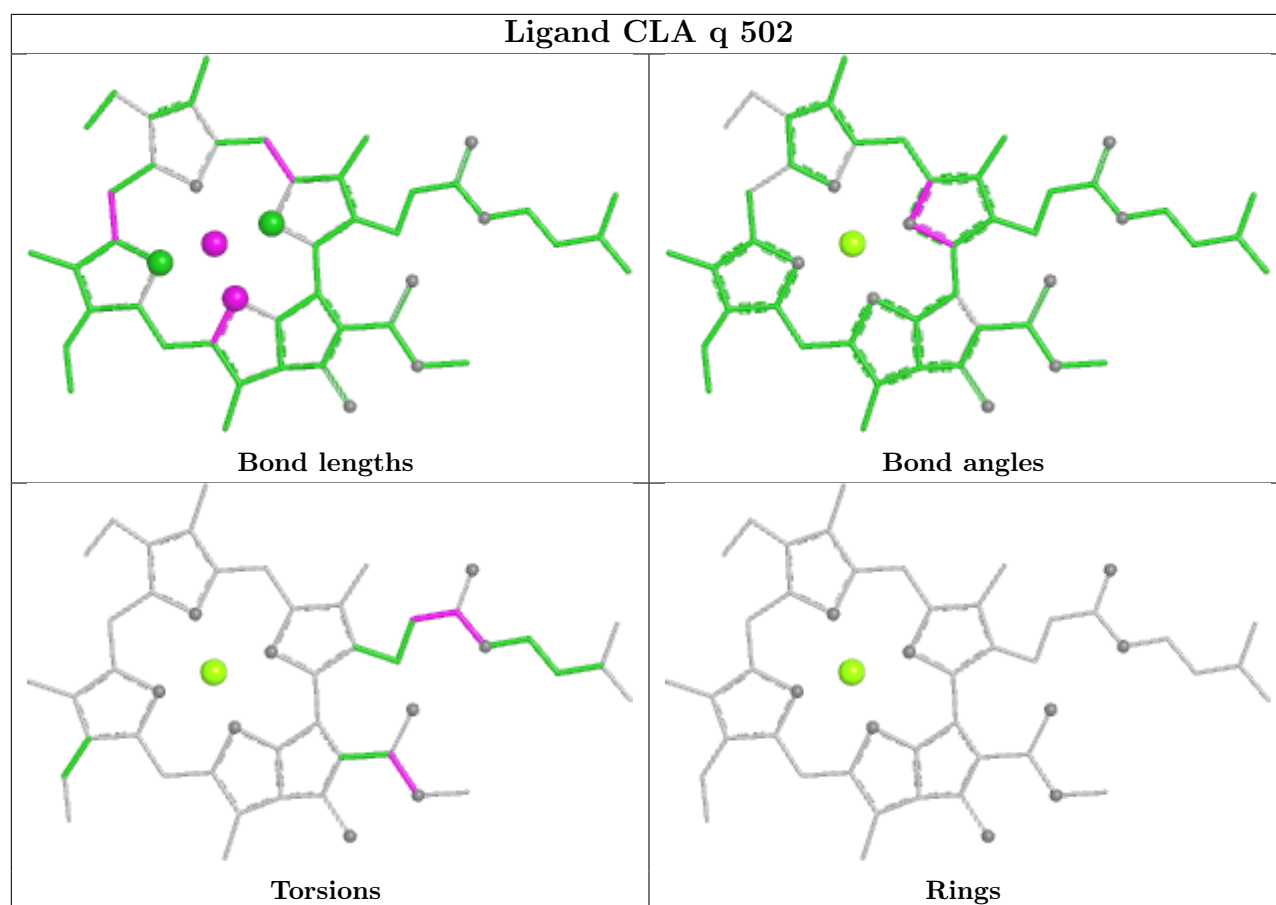
Ligand CLA G 1222

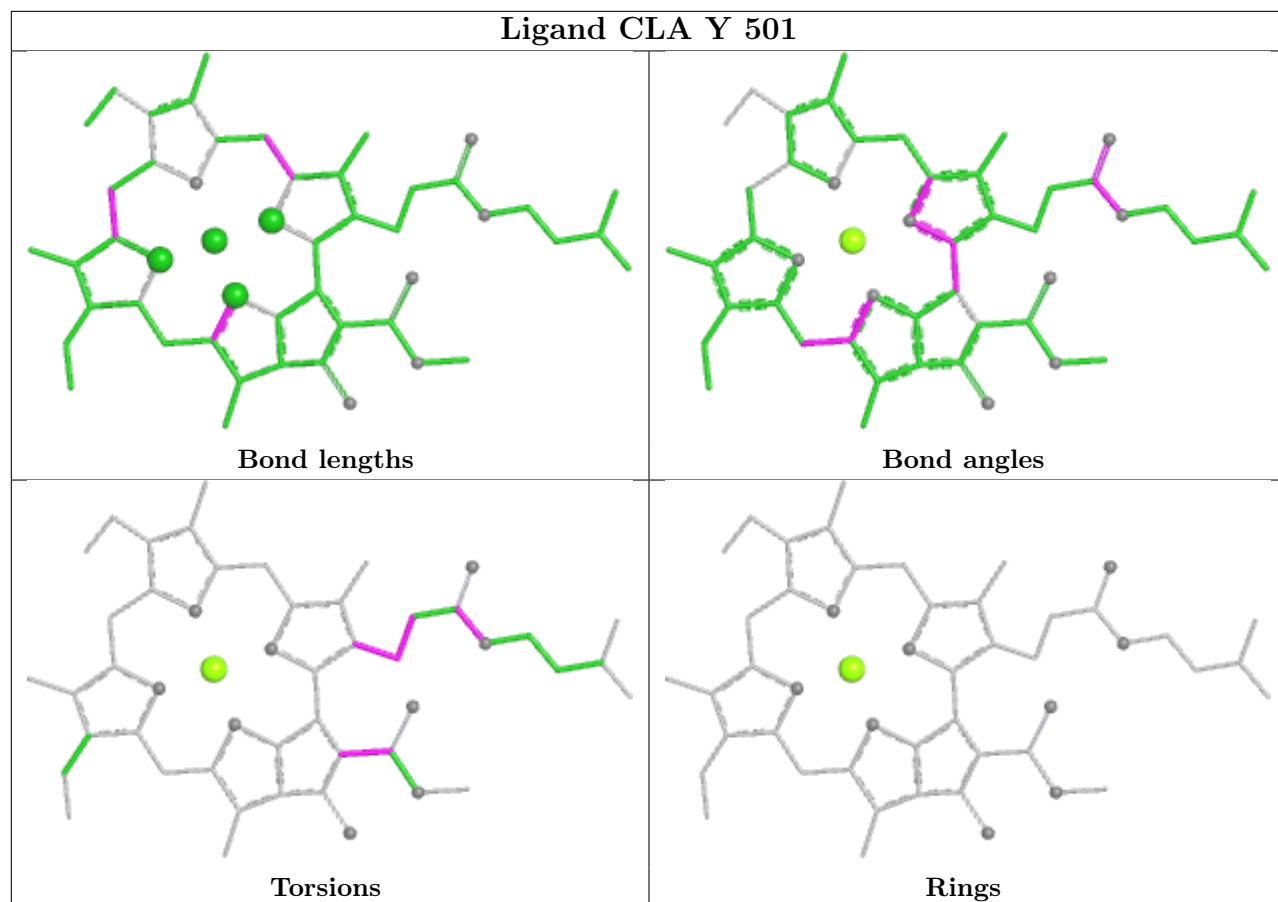


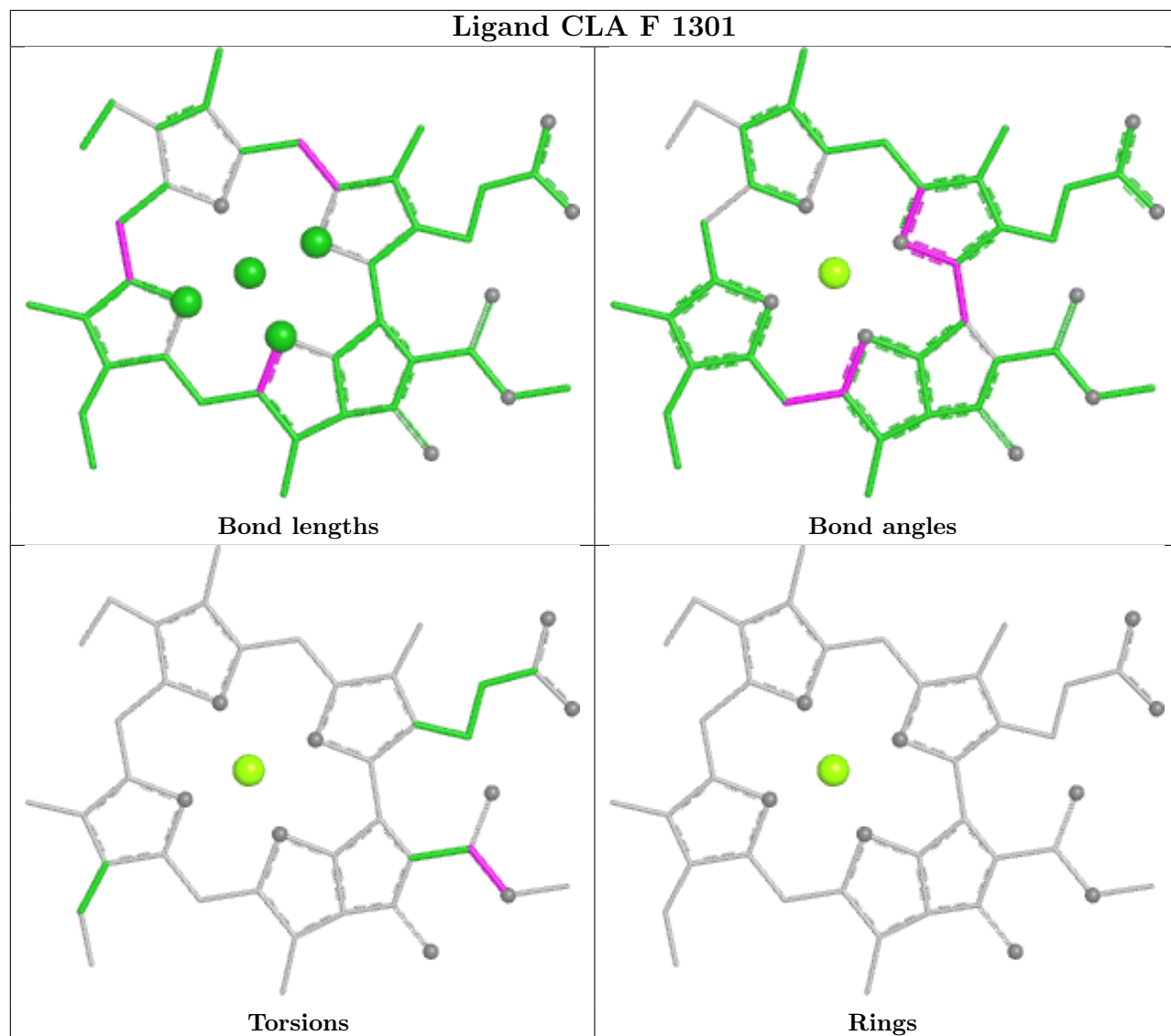
Ligand CLA A 1117



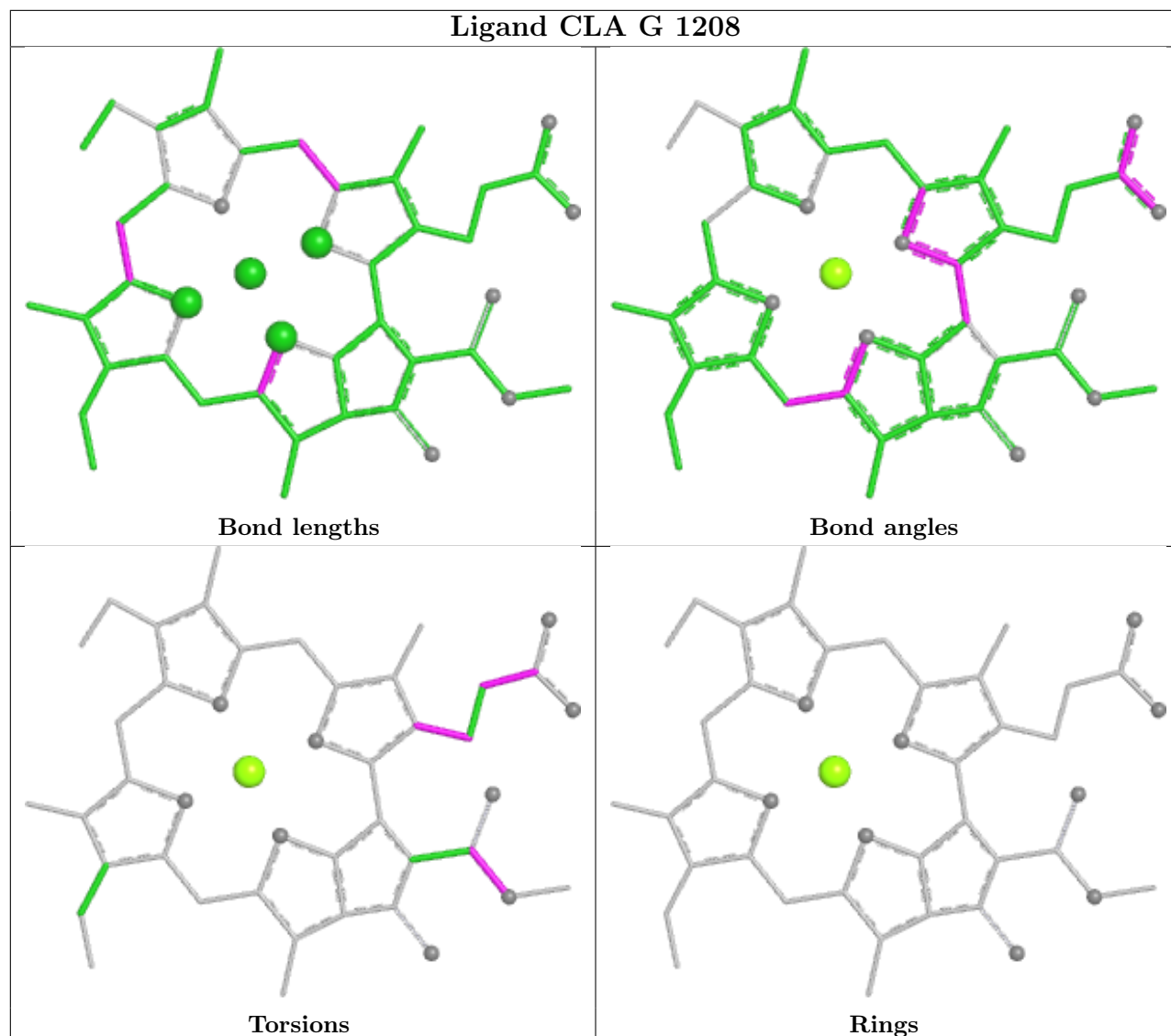




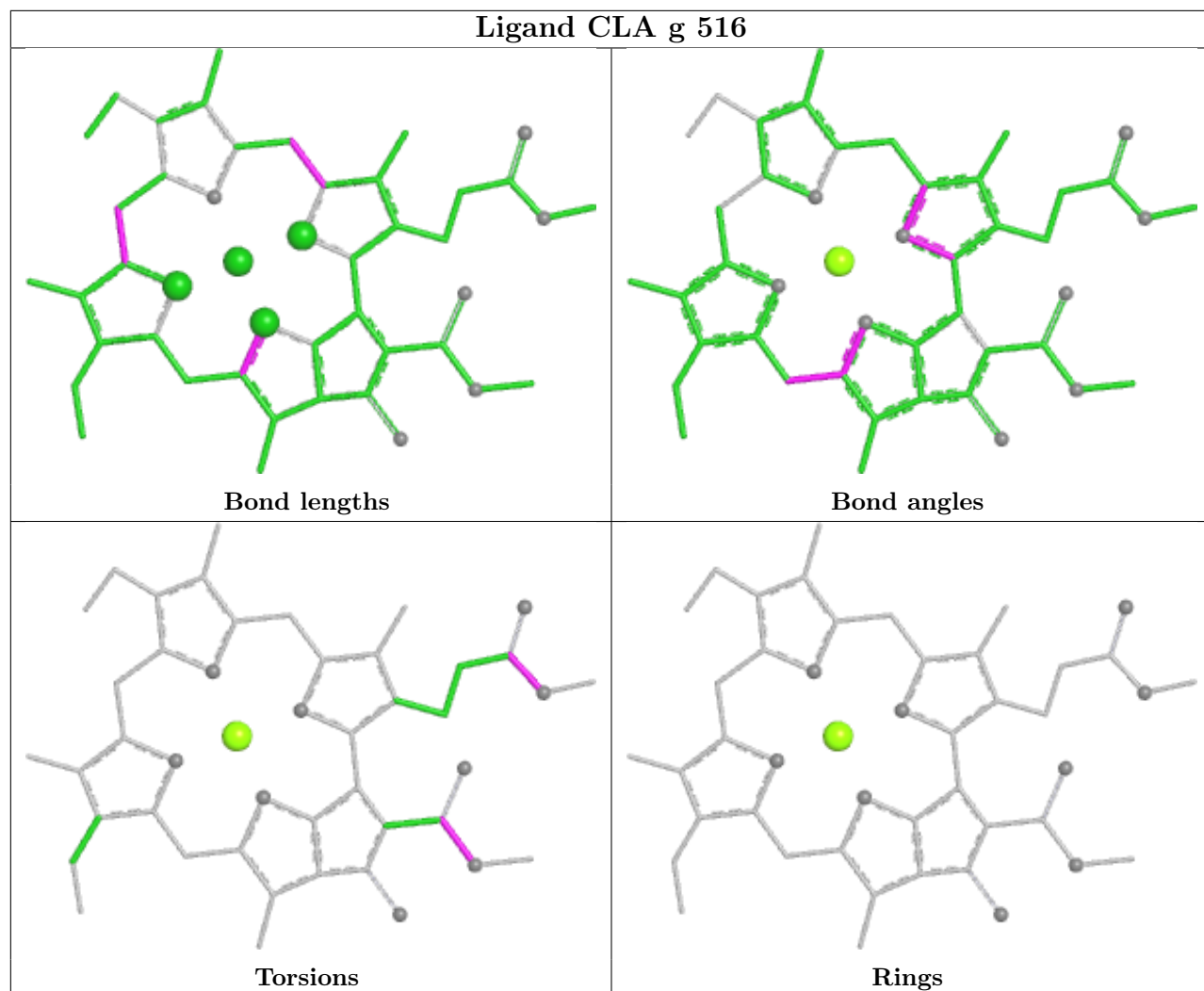




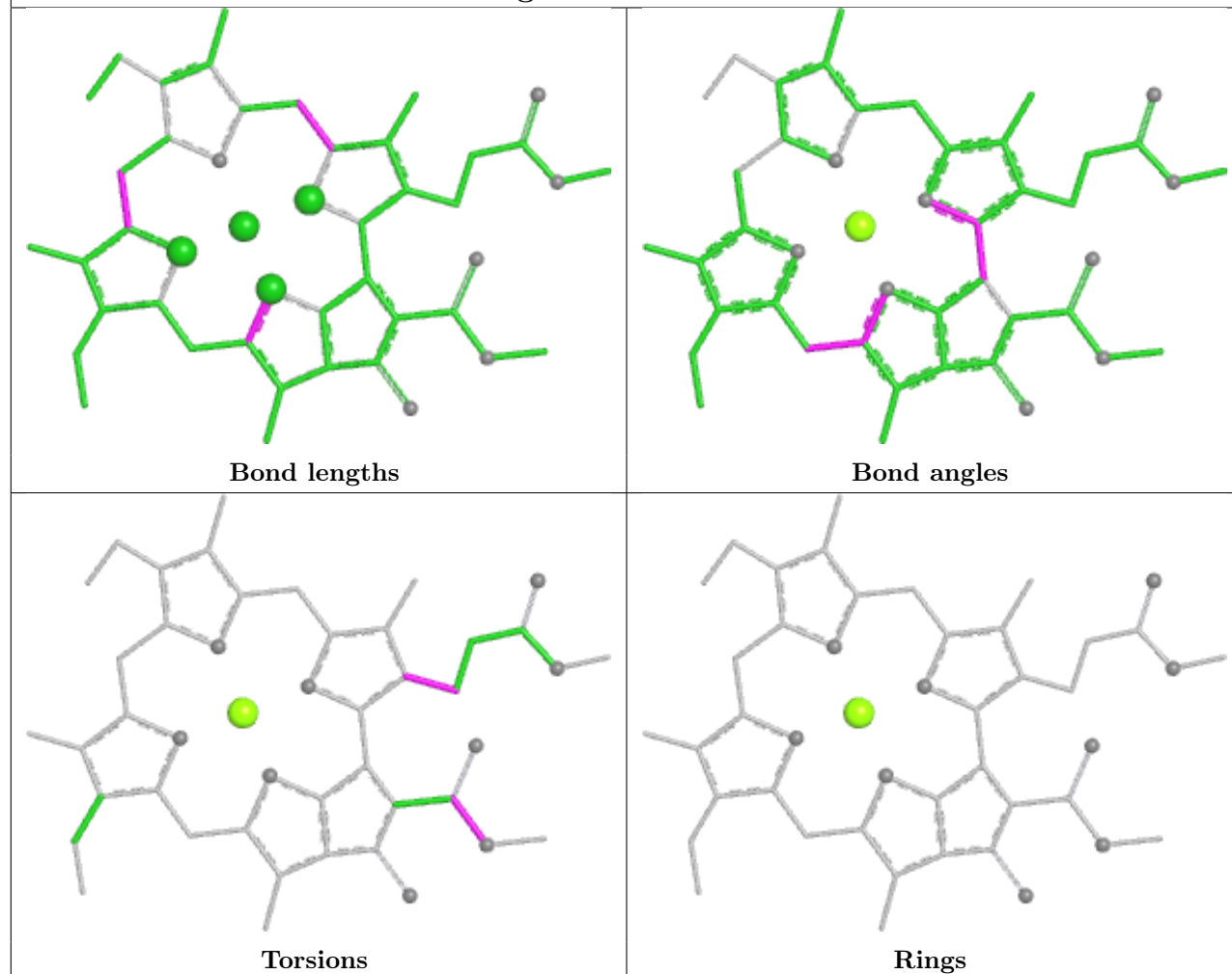
Ligand CLA G 1208



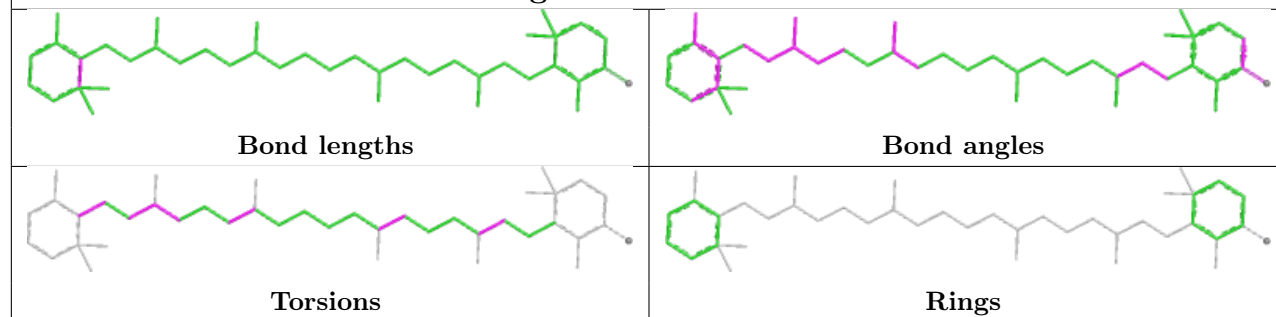
Ligand CLA g 516

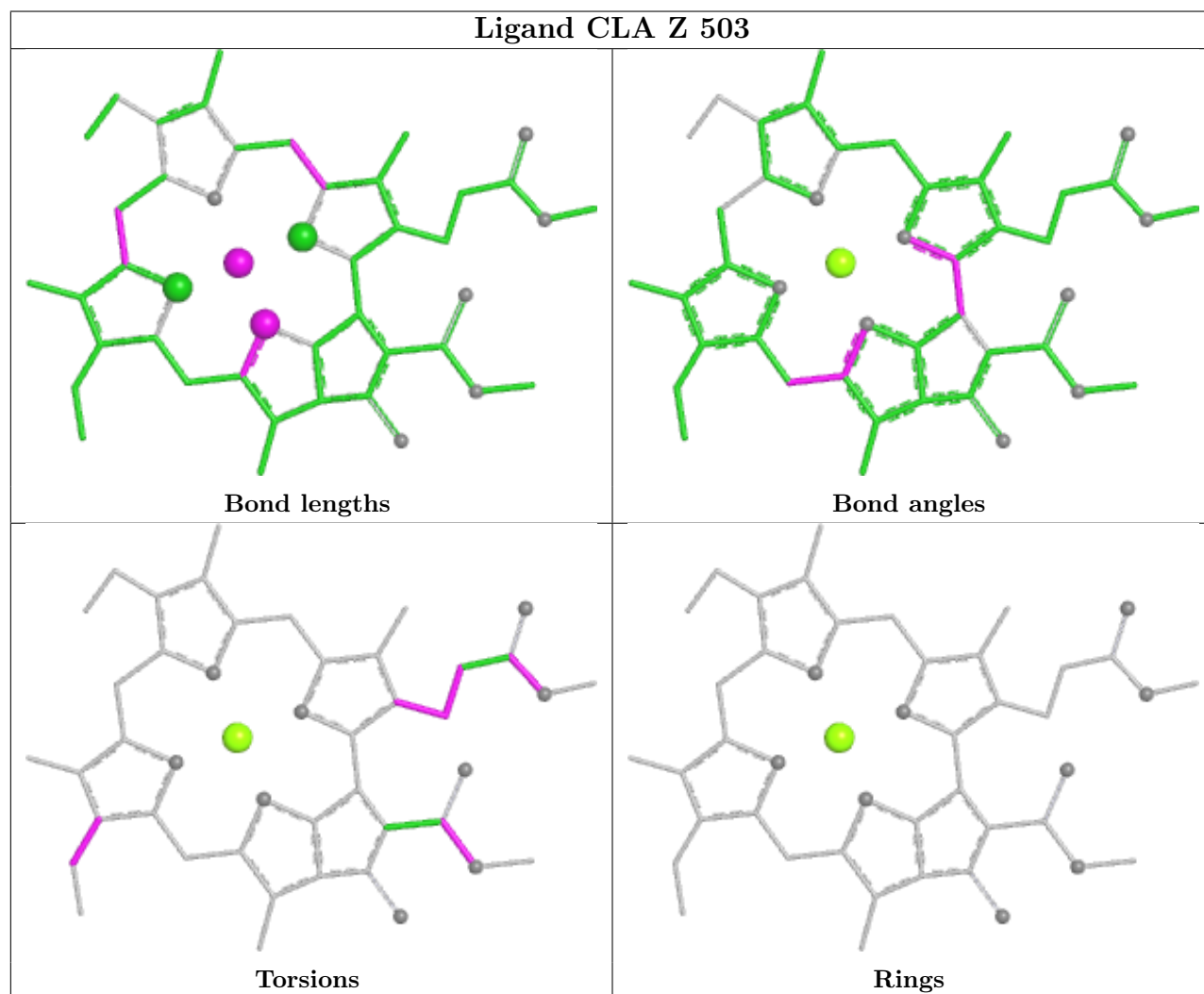
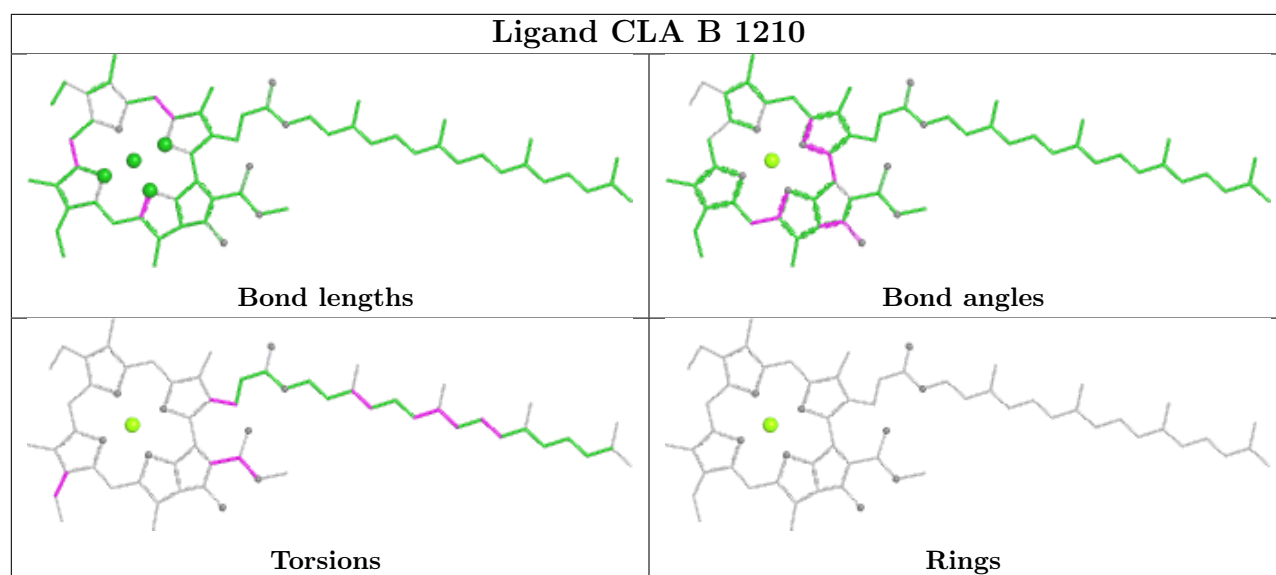


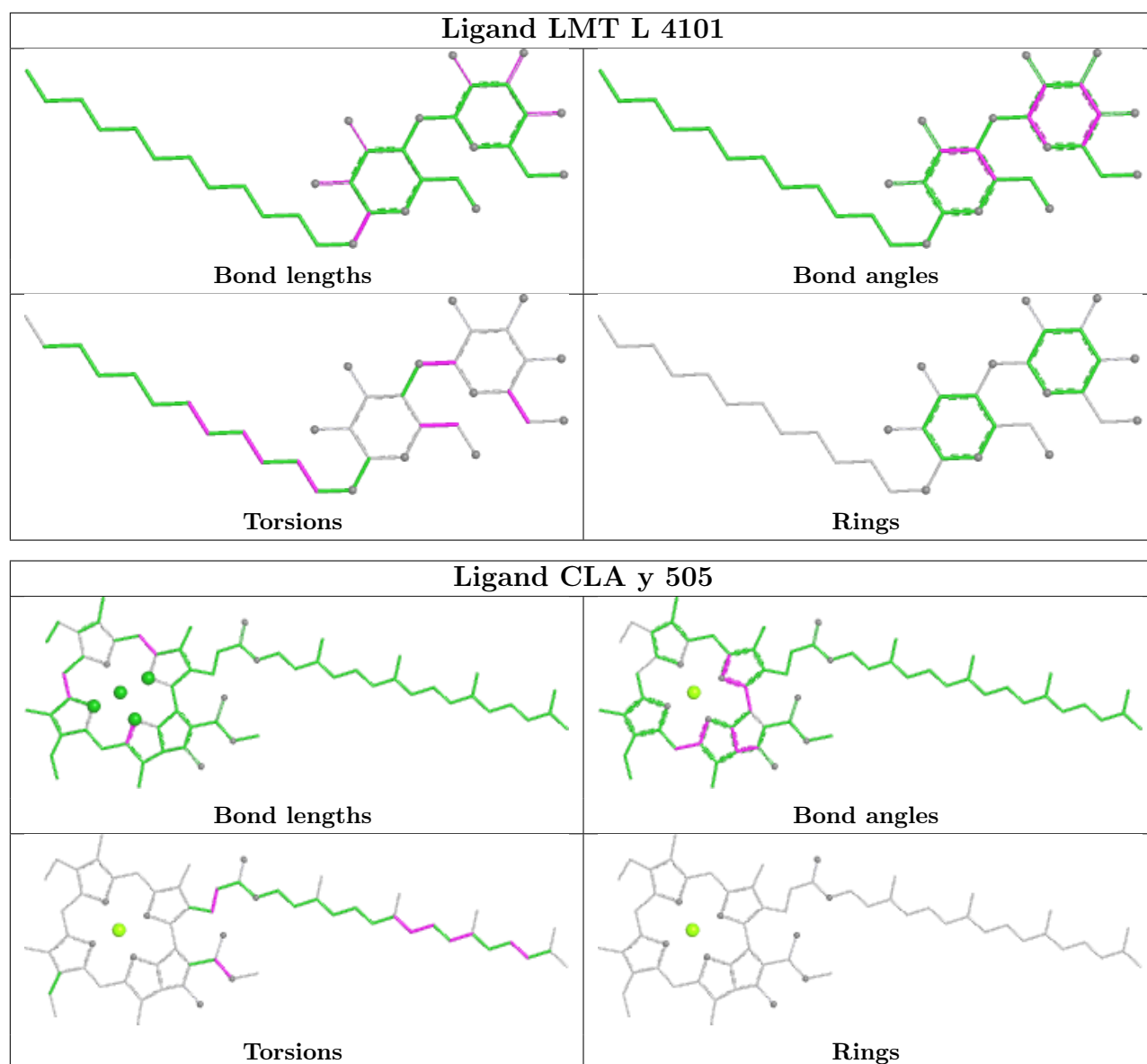
Ligand CLA v 516

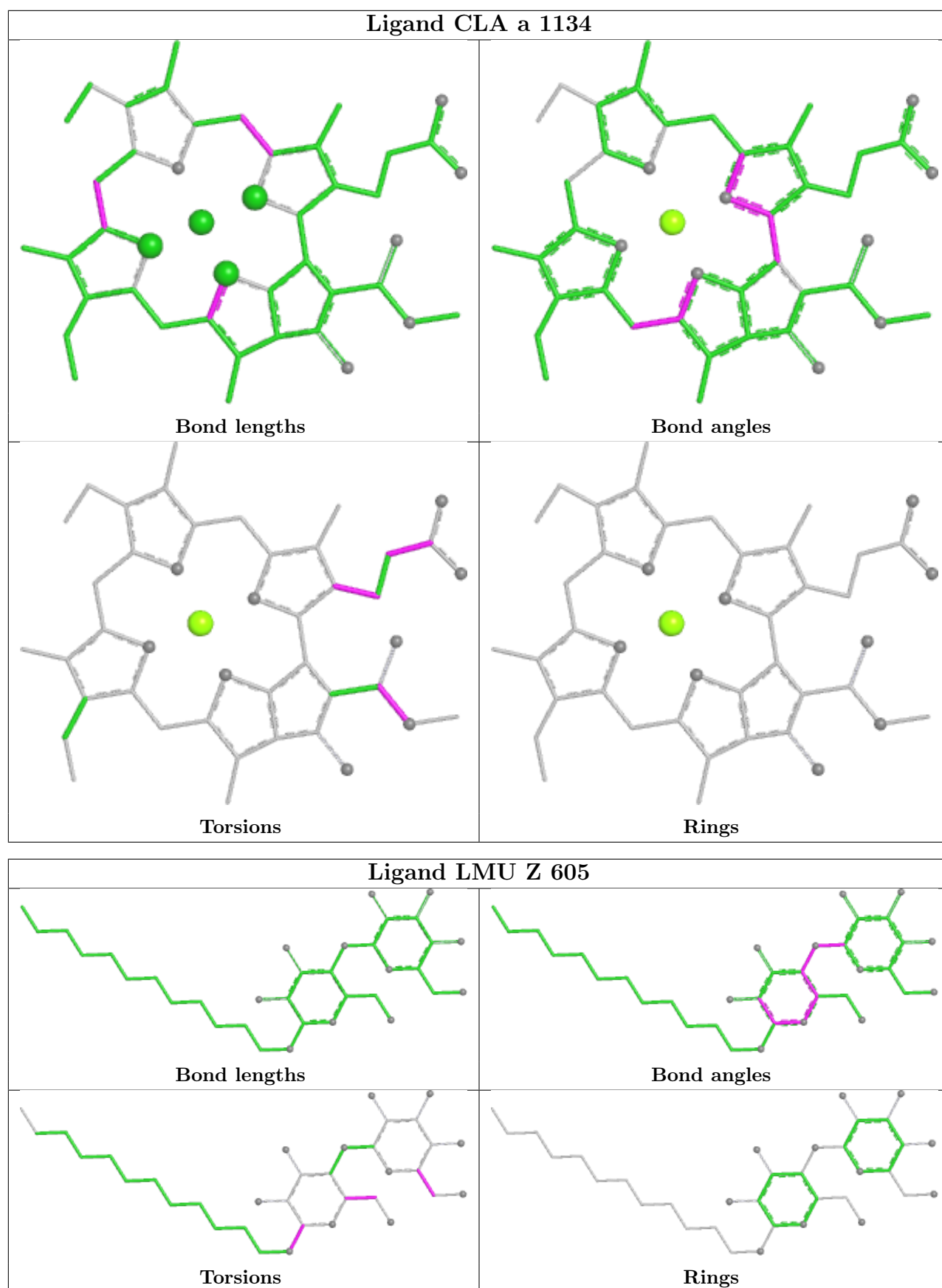


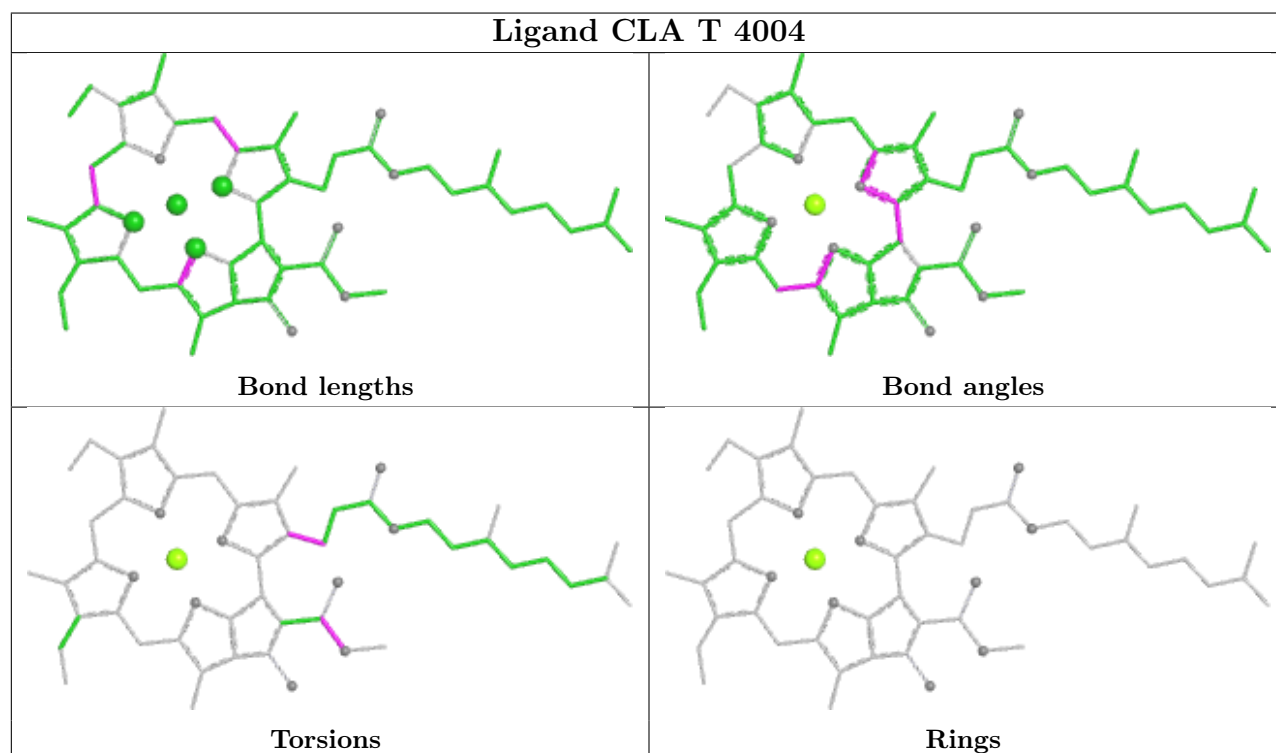
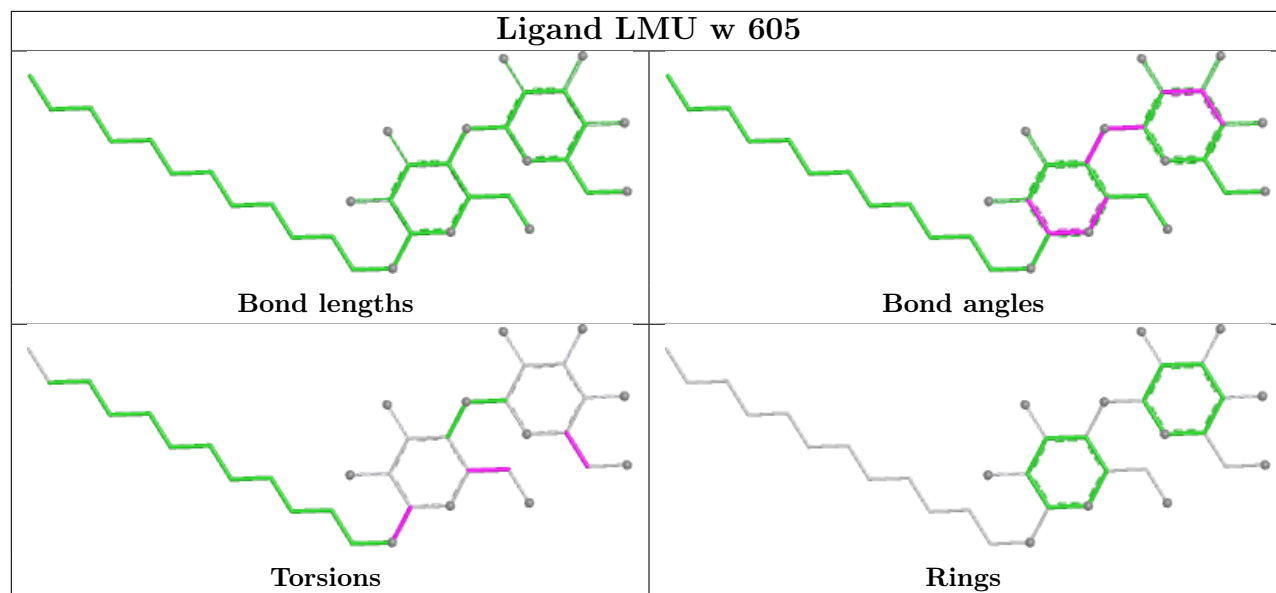
Ligand ECH i 4020

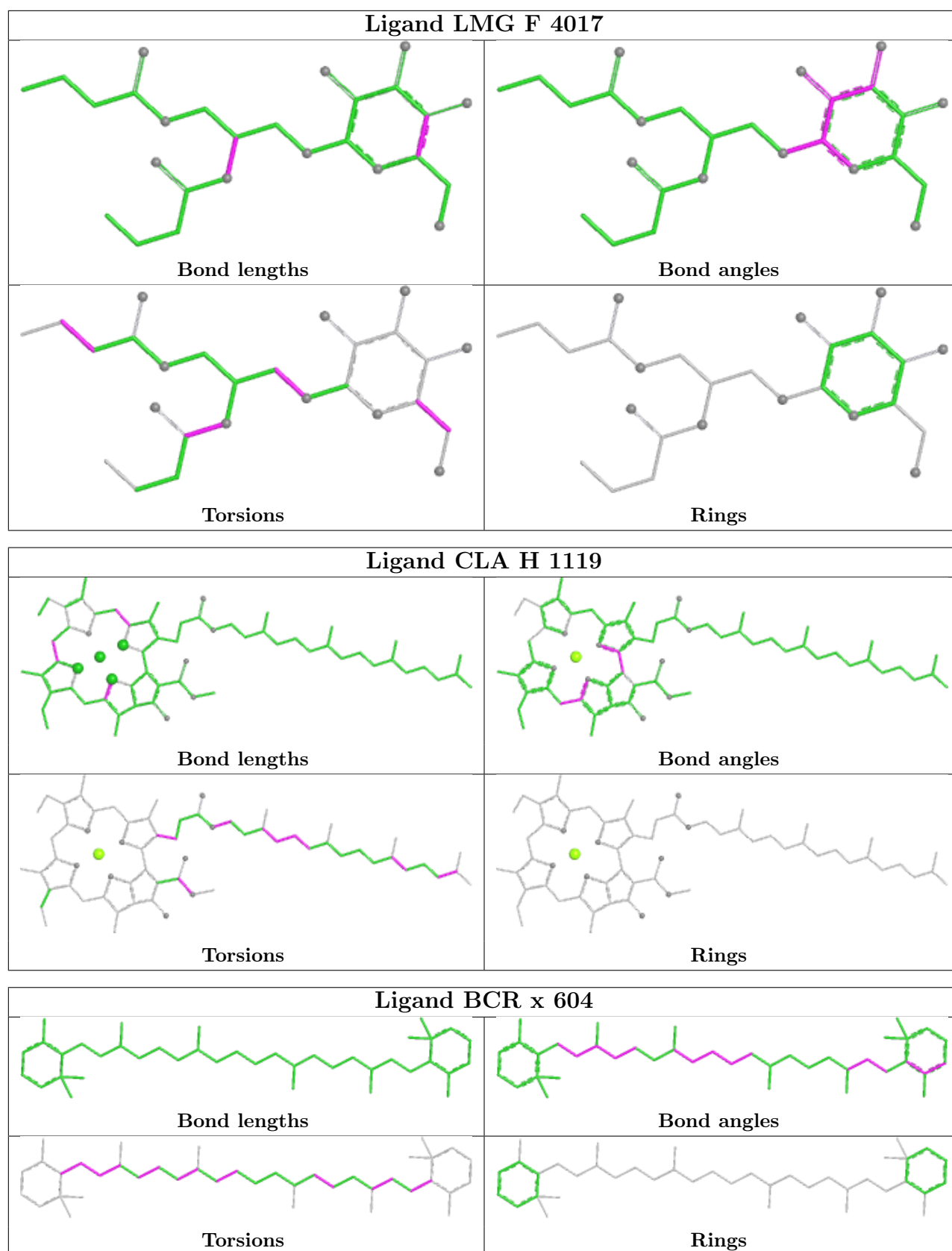




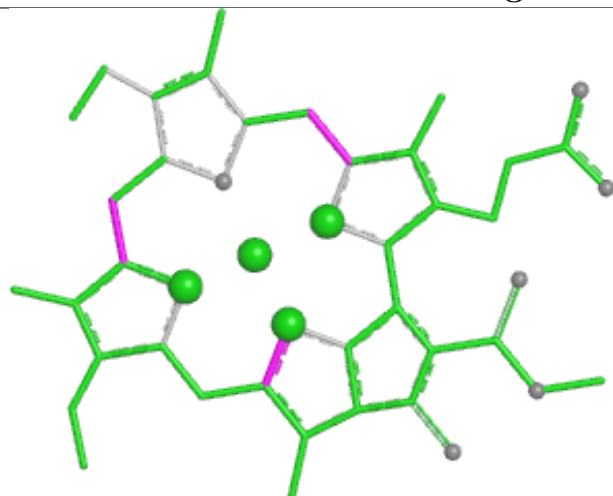




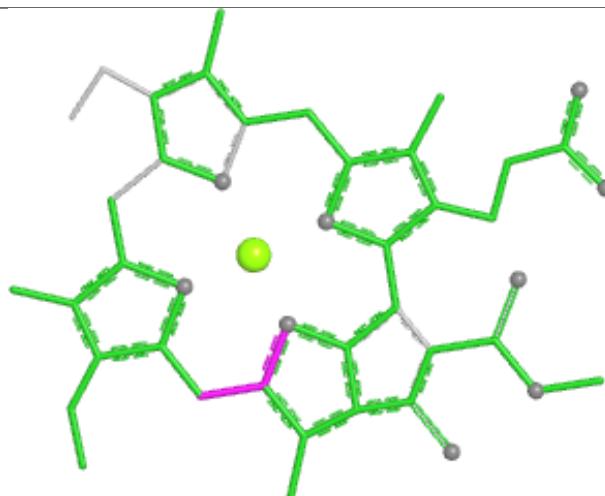




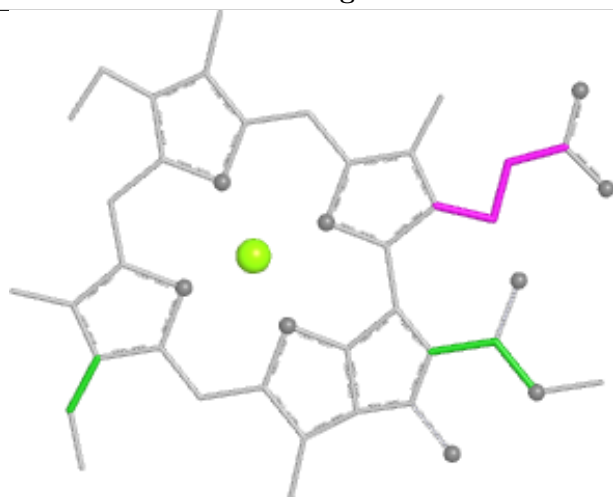
Ligand CLA B 1217



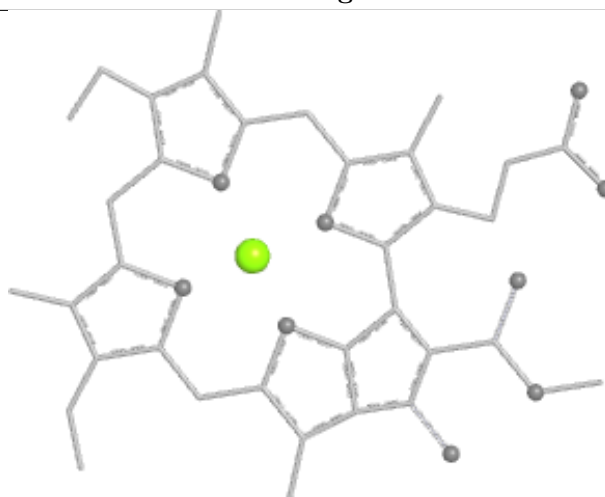
Bond lengths



Bond angles

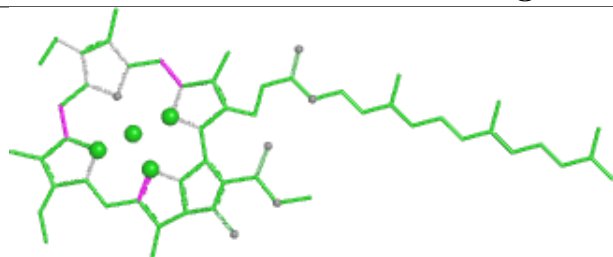


Torsions

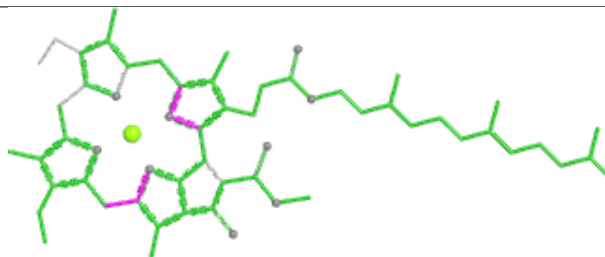


Rings

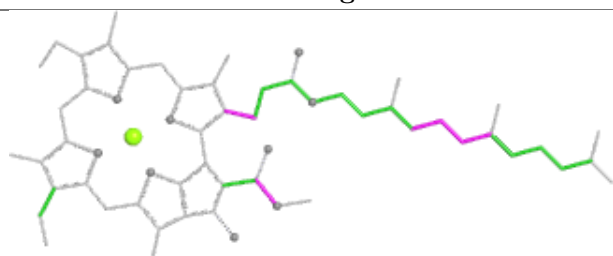
Ligand CLA Z 506



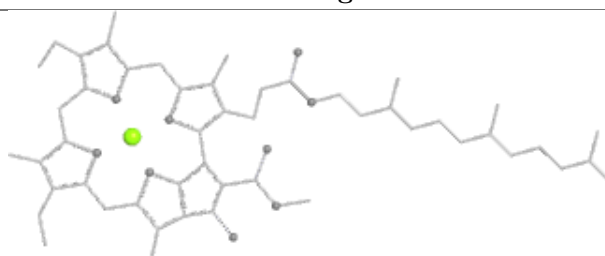
Bond lengths



Bond angles

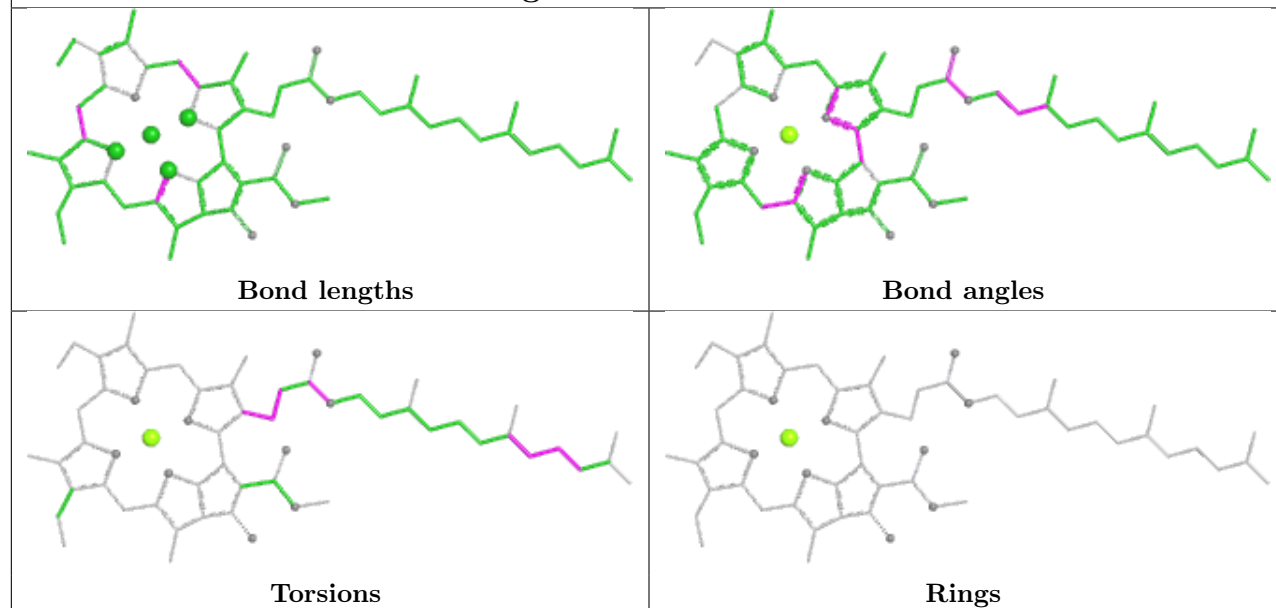


Torsions

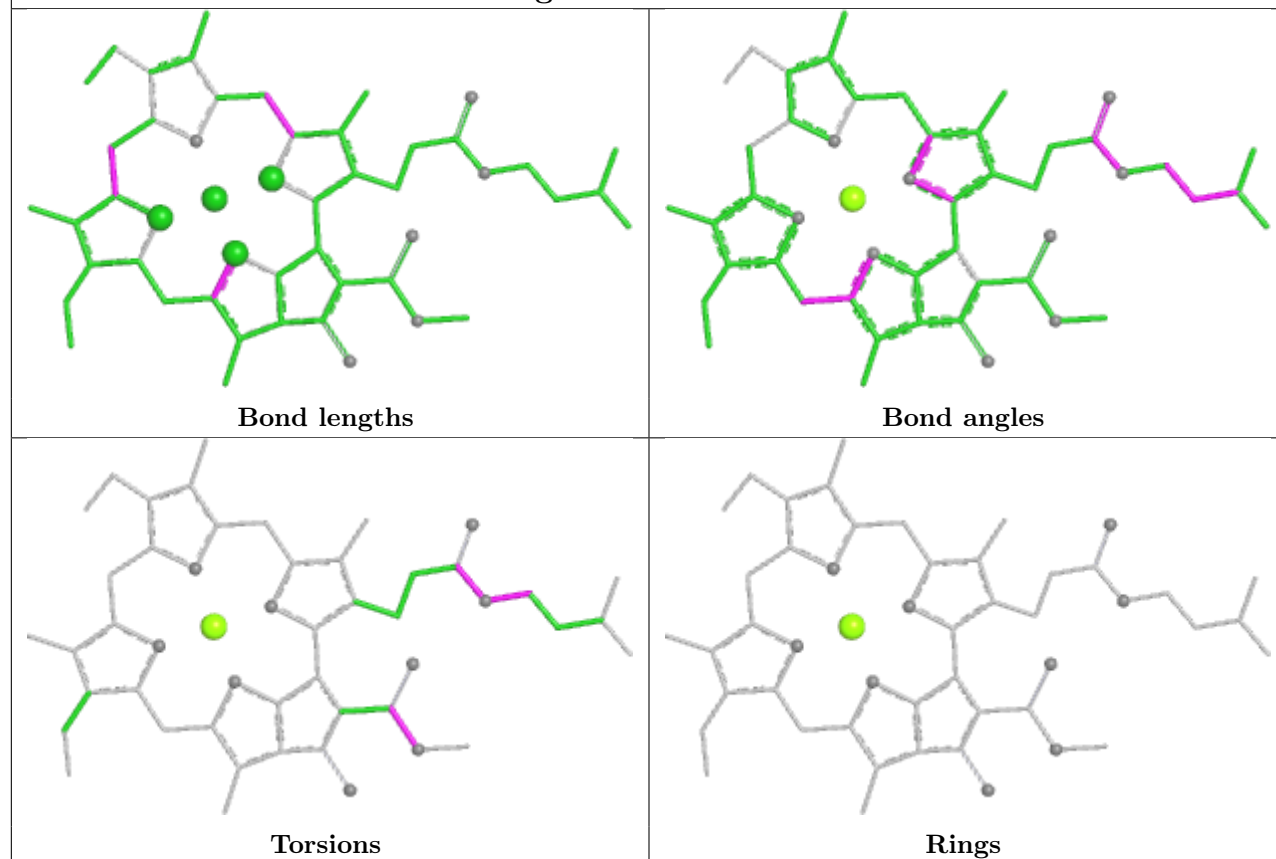


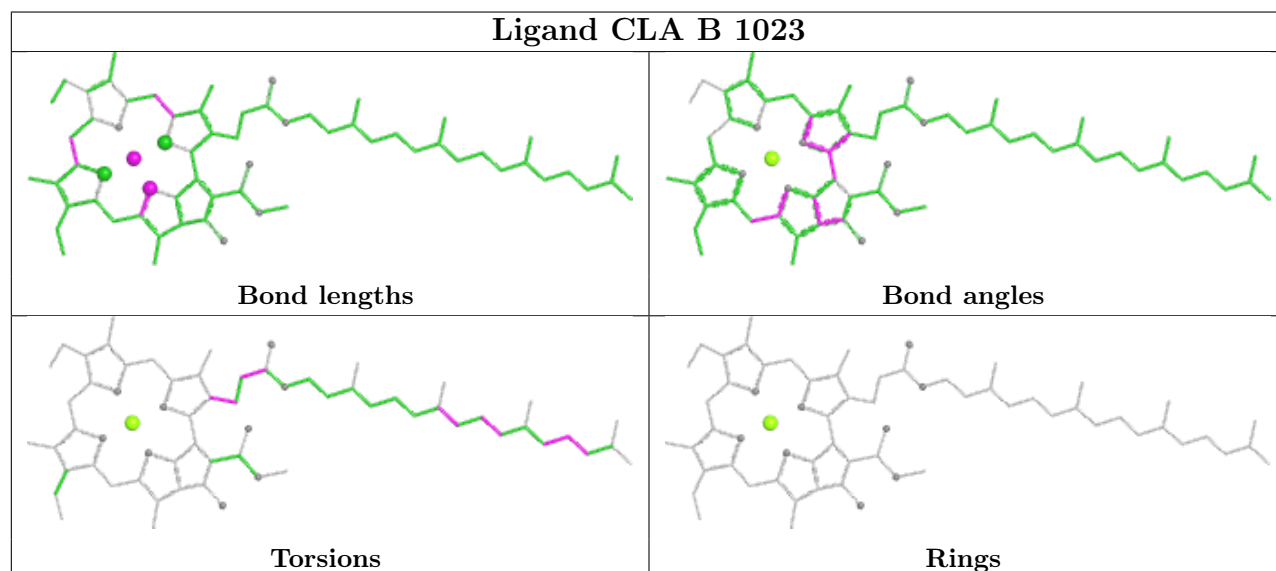
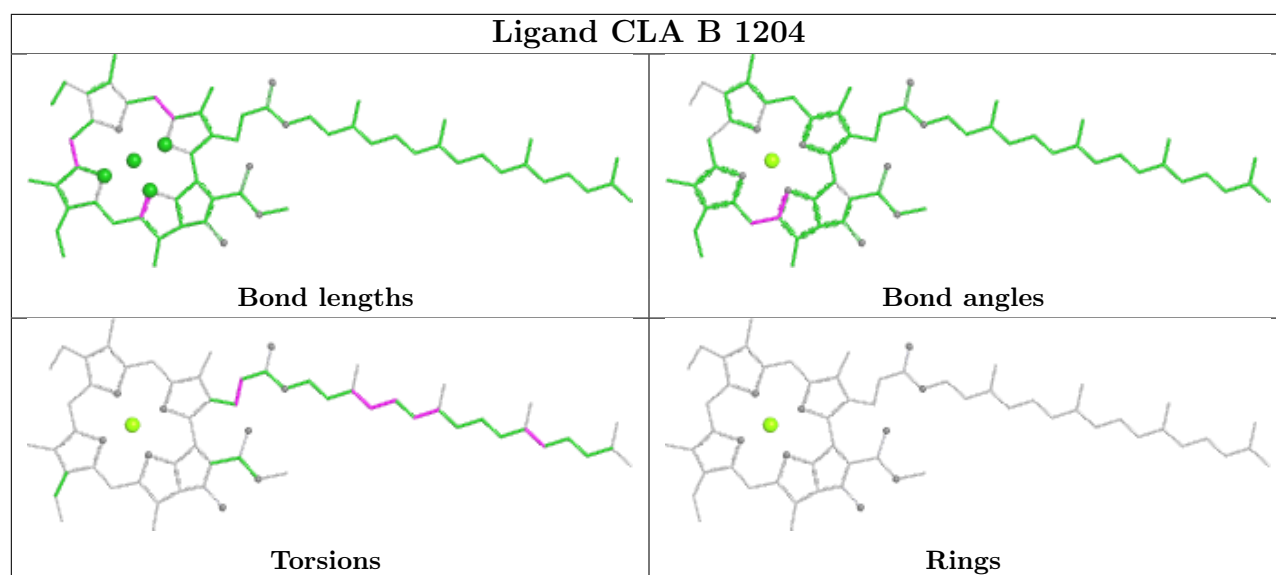
Rings

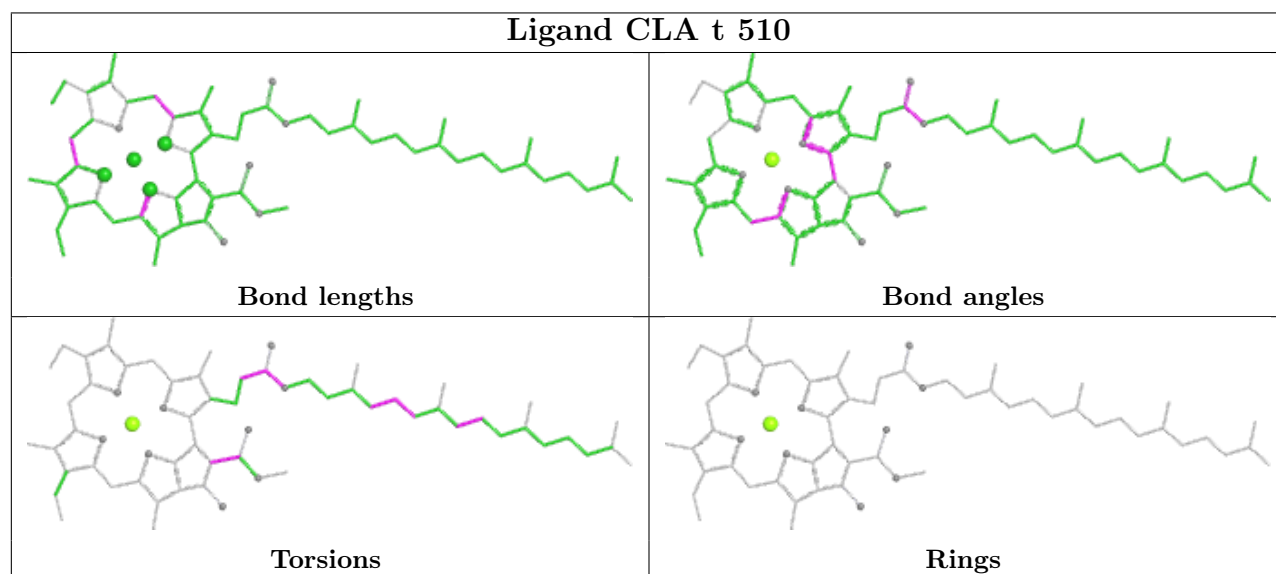
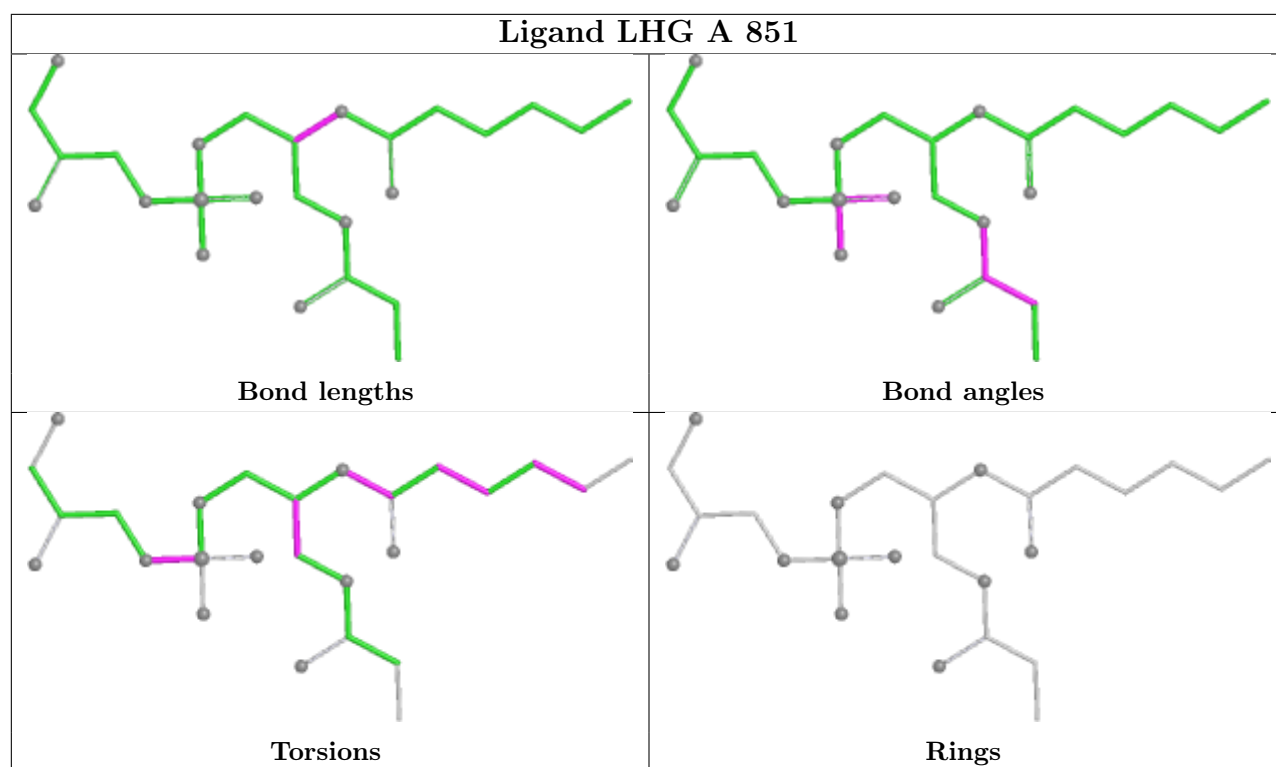
Ligand CLA H 1130



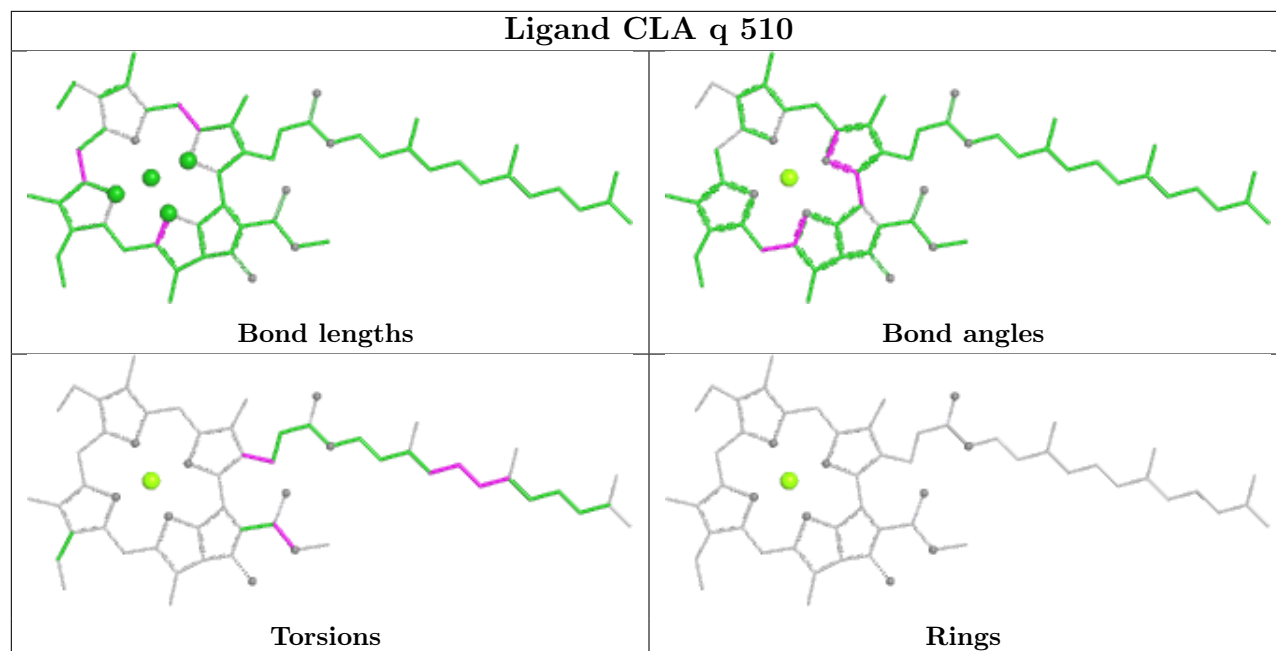
Ligand CLA h 502



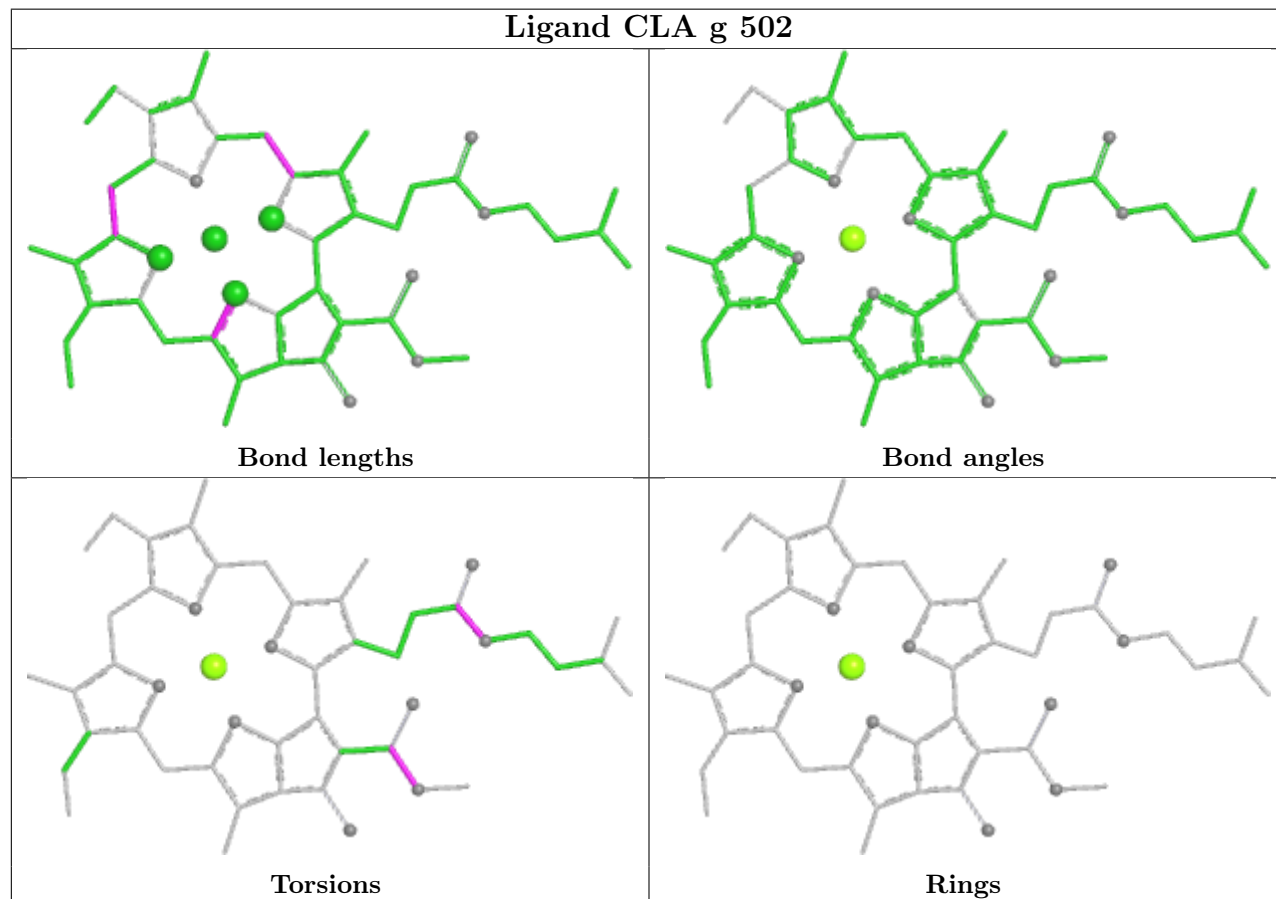


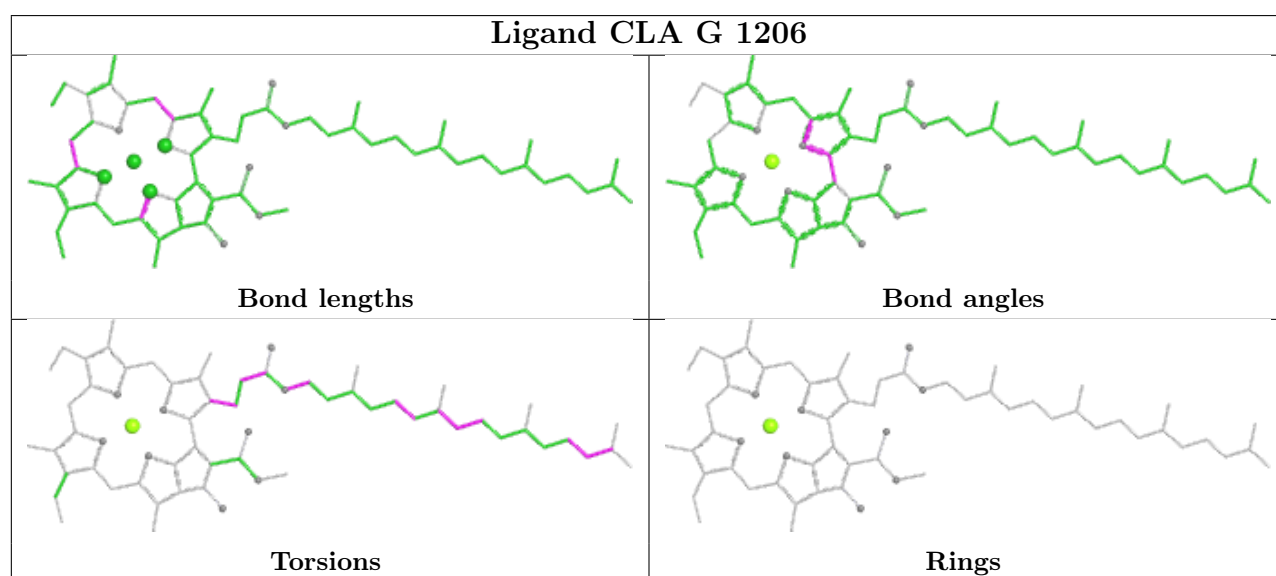
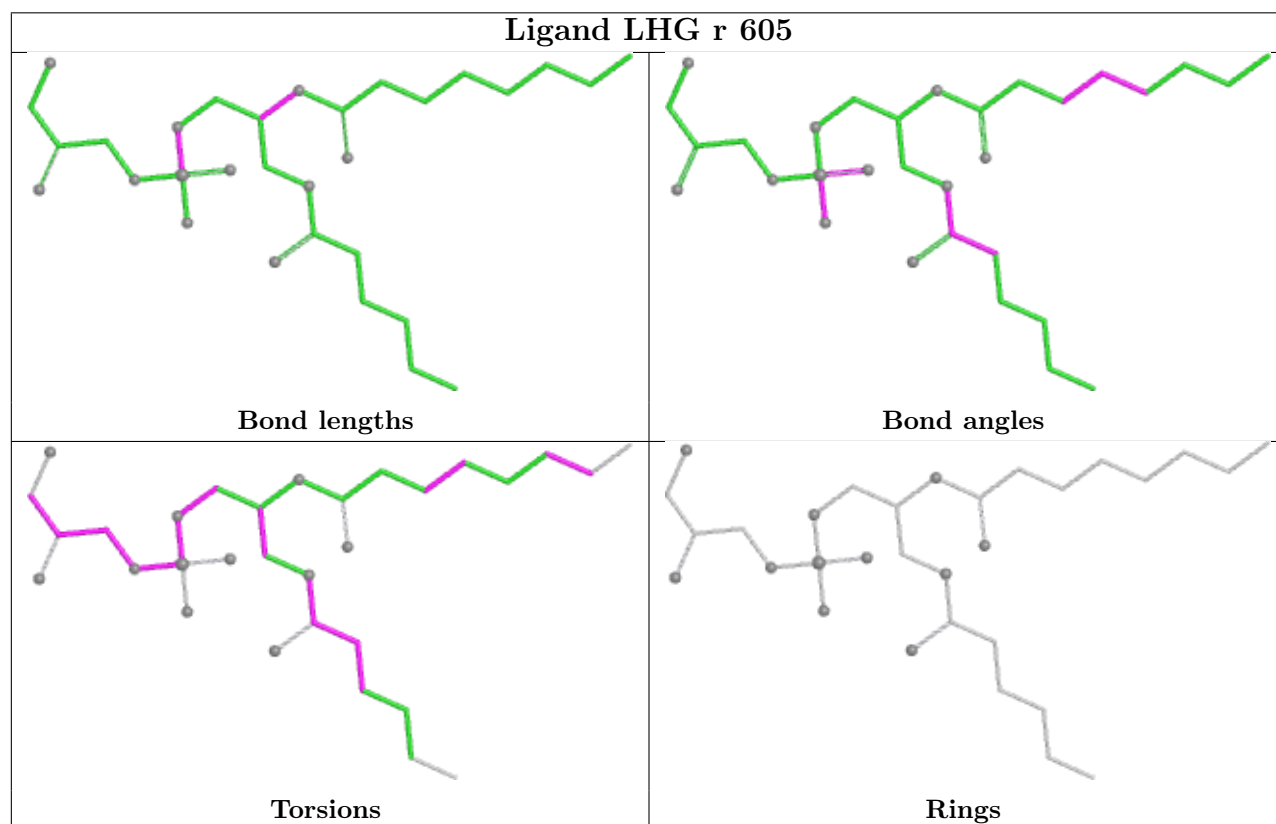
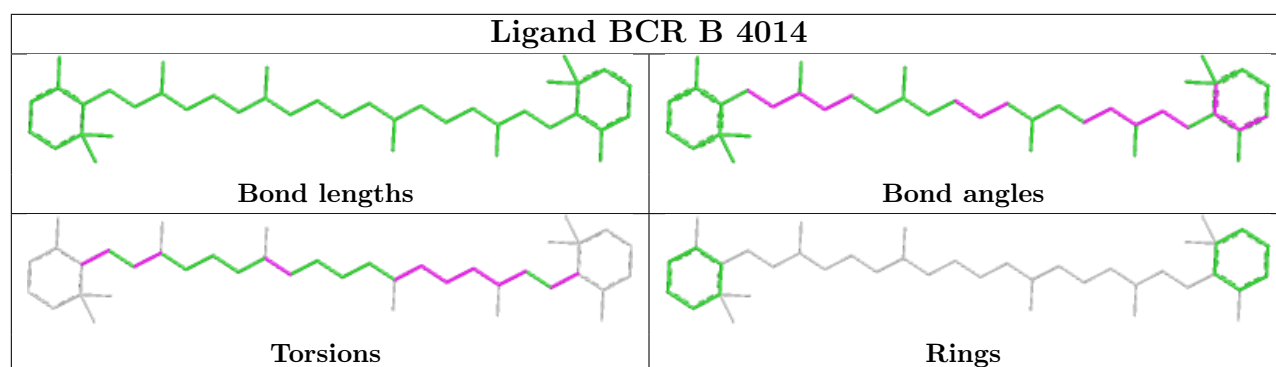


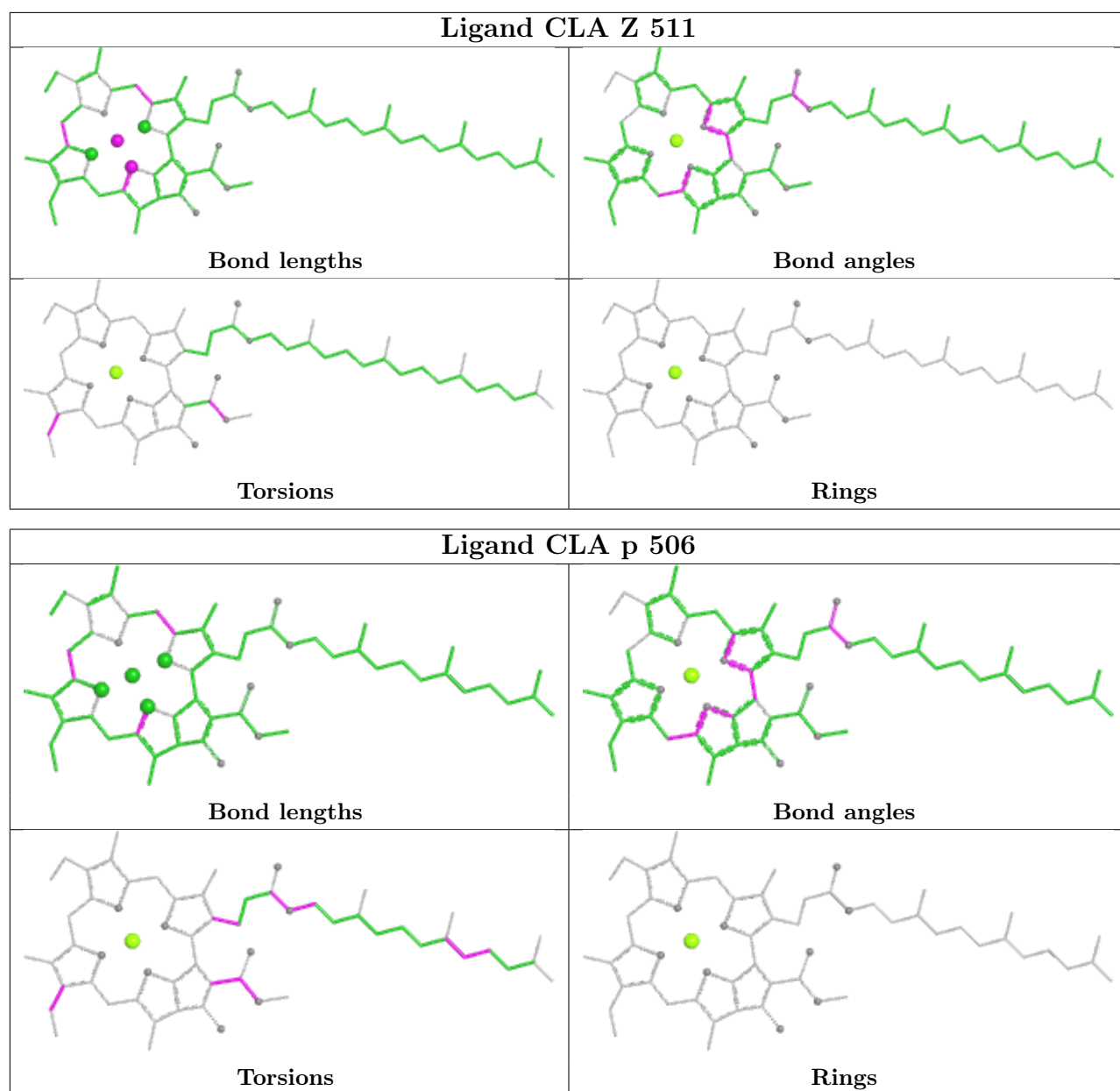
Ligand CLA q 510

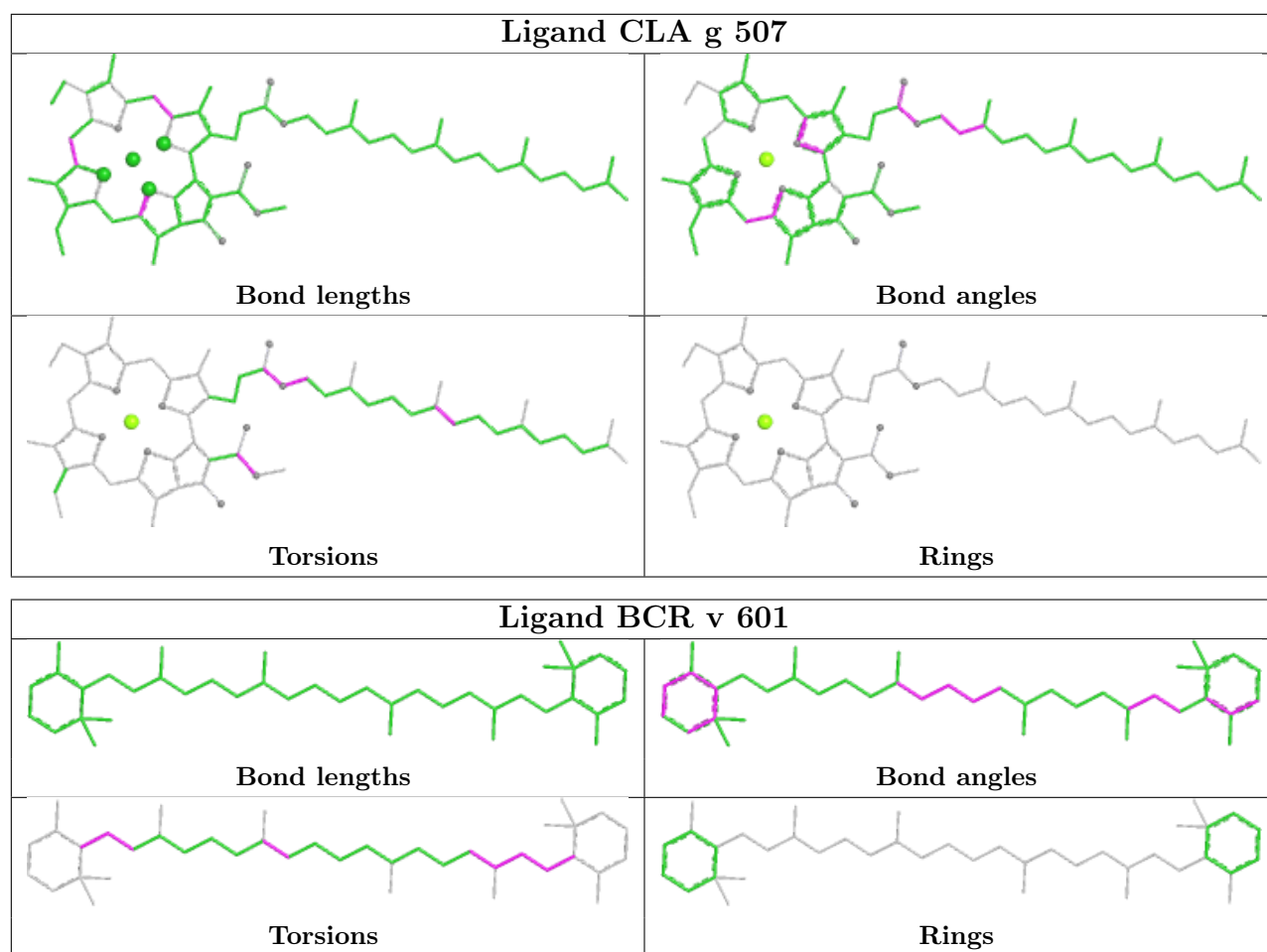


Ligand CLA g 502

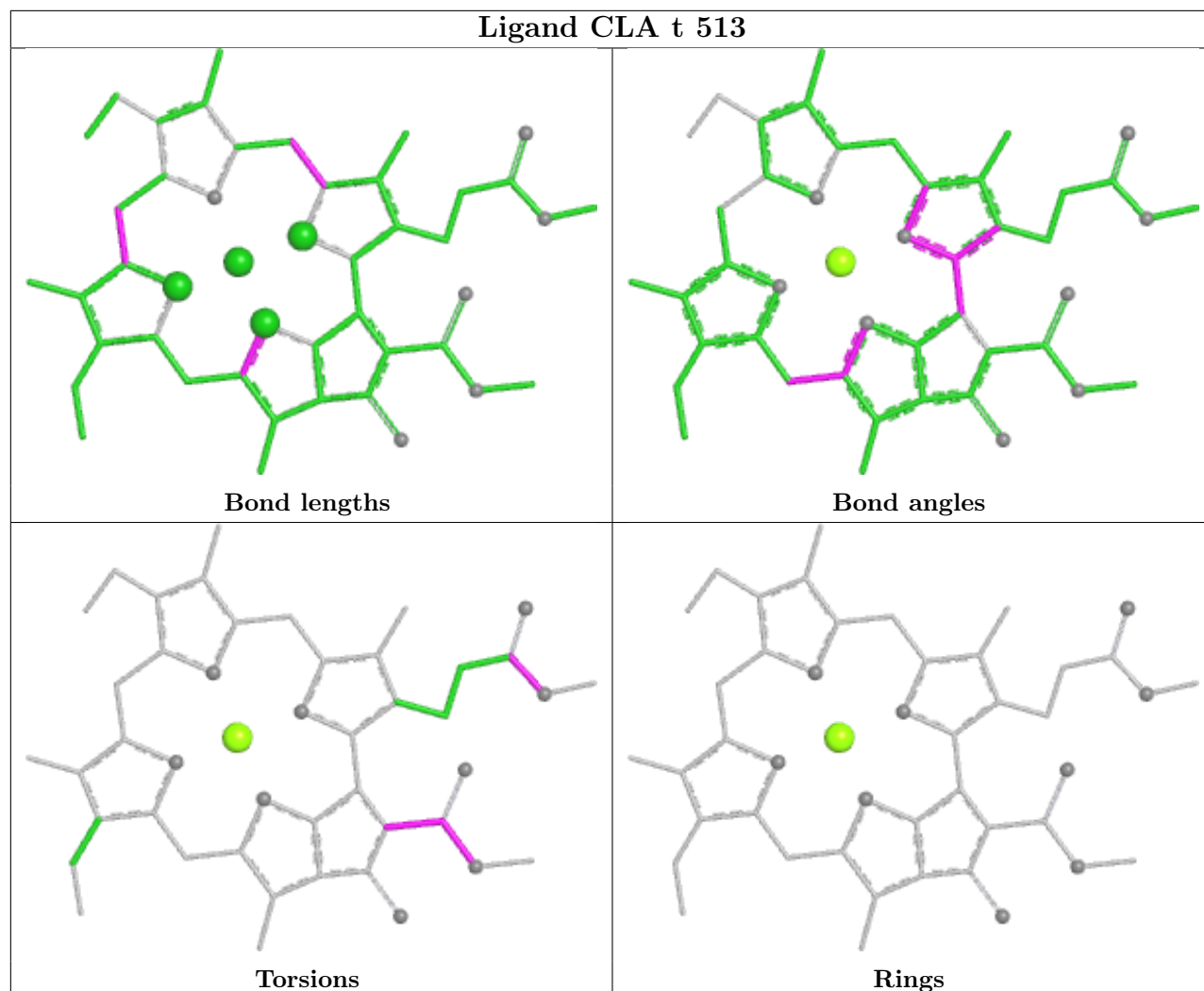




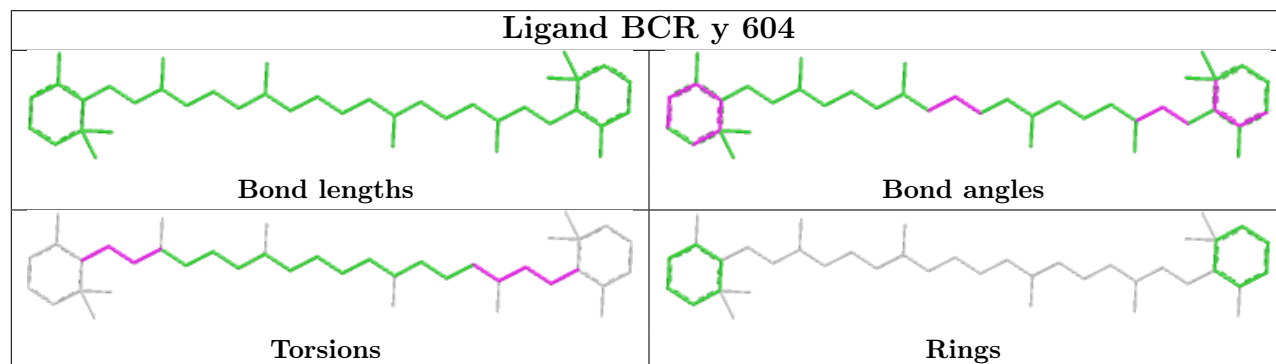


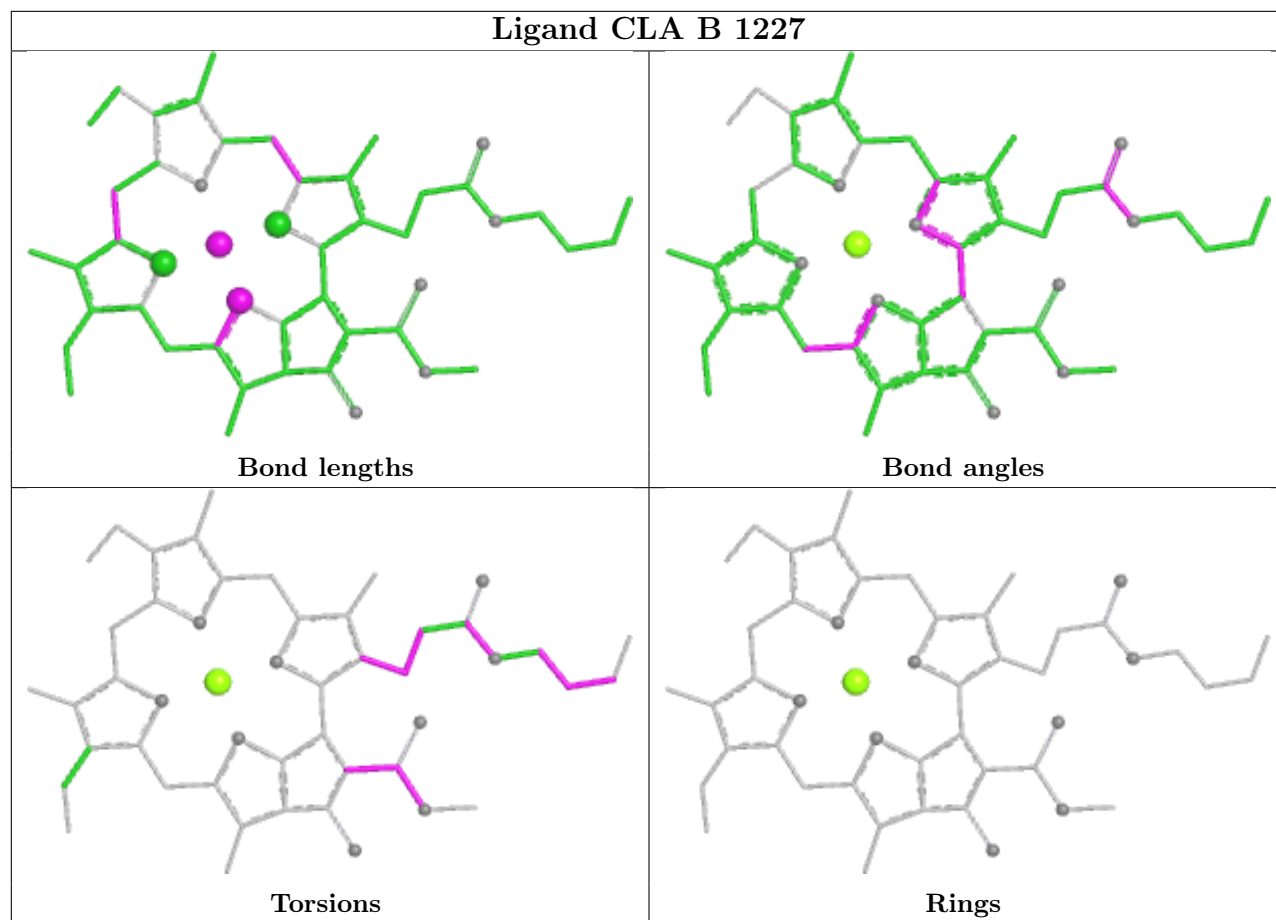


Ligand CLA t 513

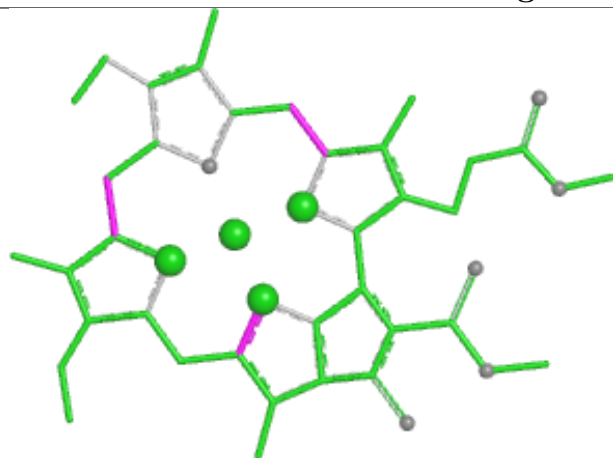


Ligand BCR y 604

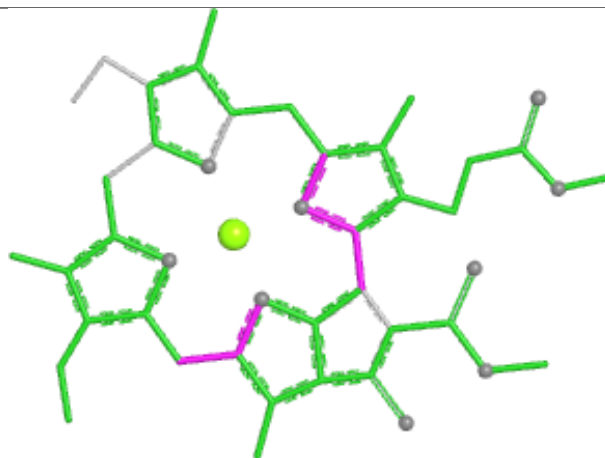




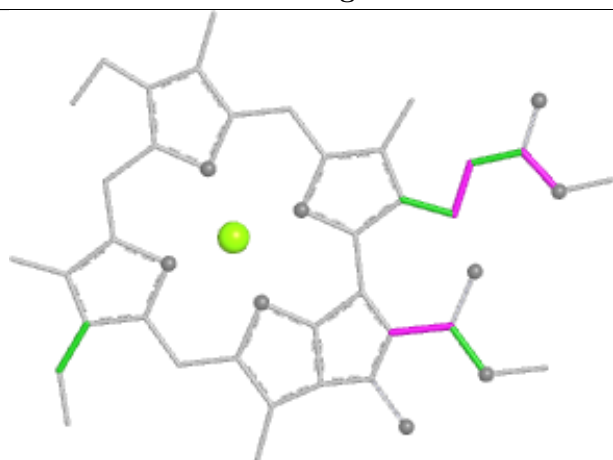
Ligand CLA h 503



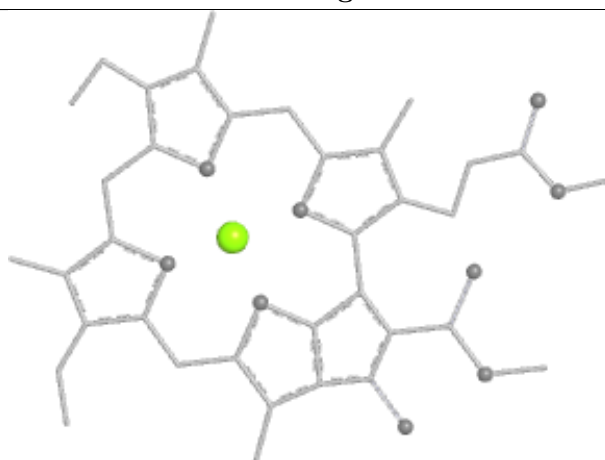
Bond lengths



Bond angles

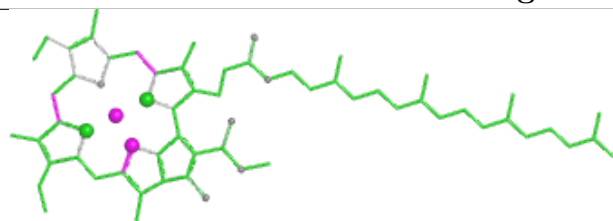


Torsions

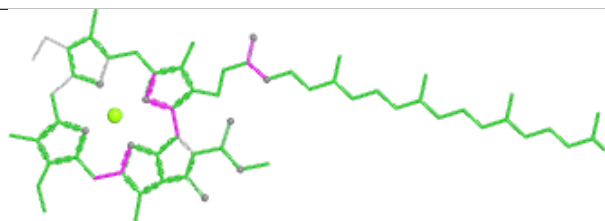


Rings

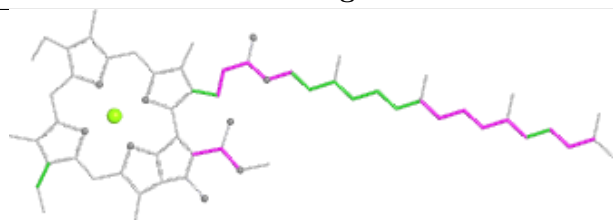
Ligand CLA n 505



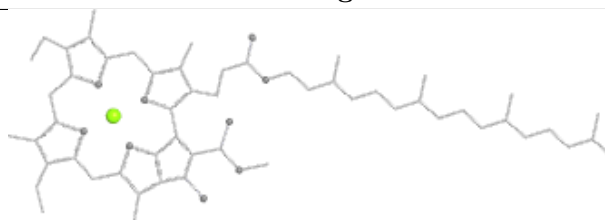
Bond lengths



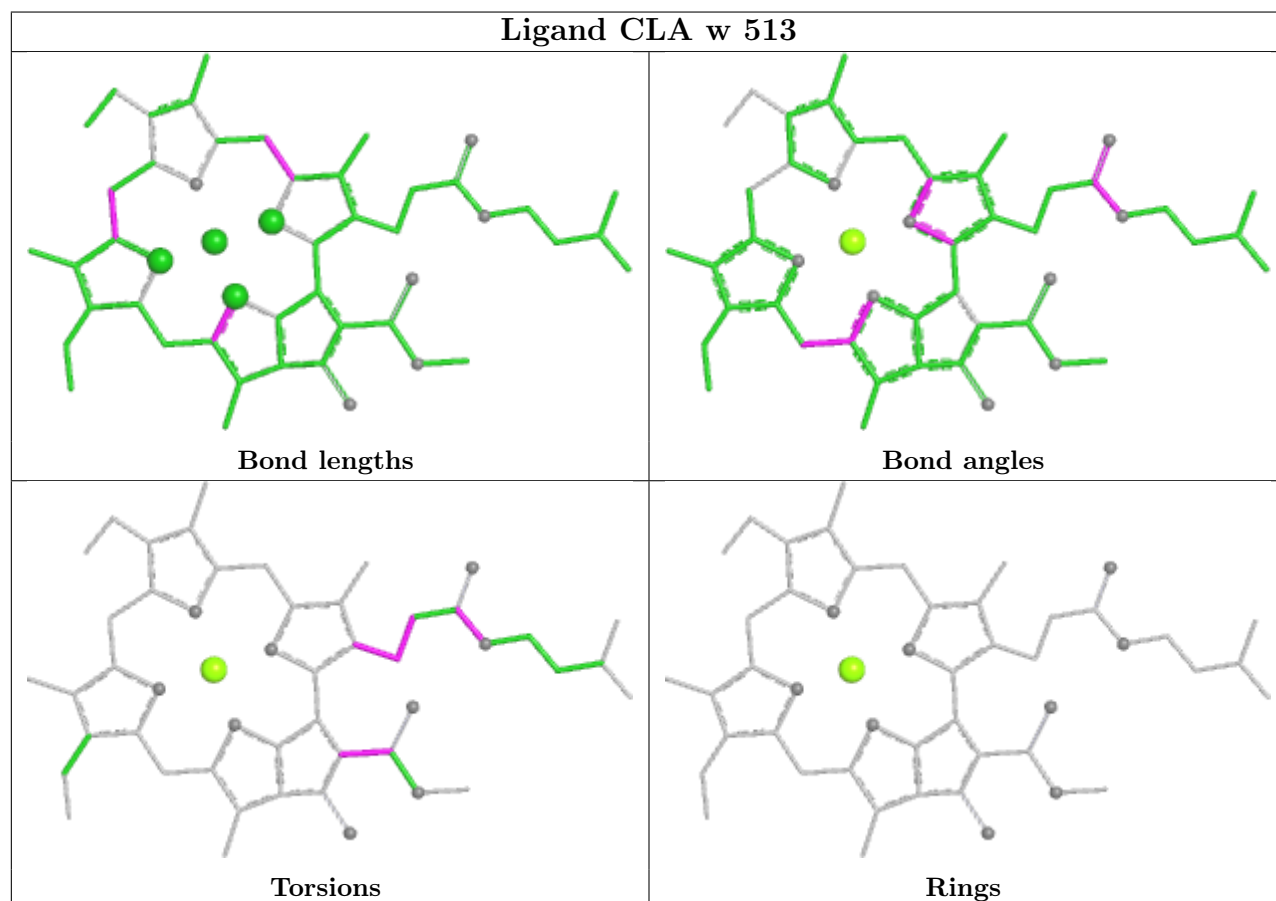
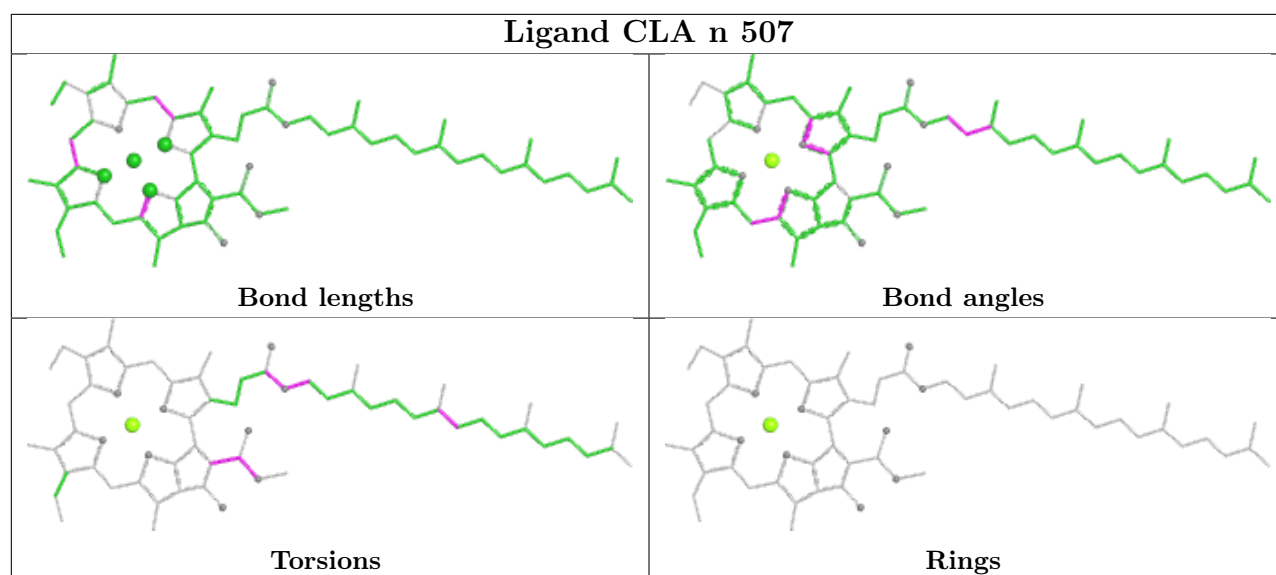
Bond angles

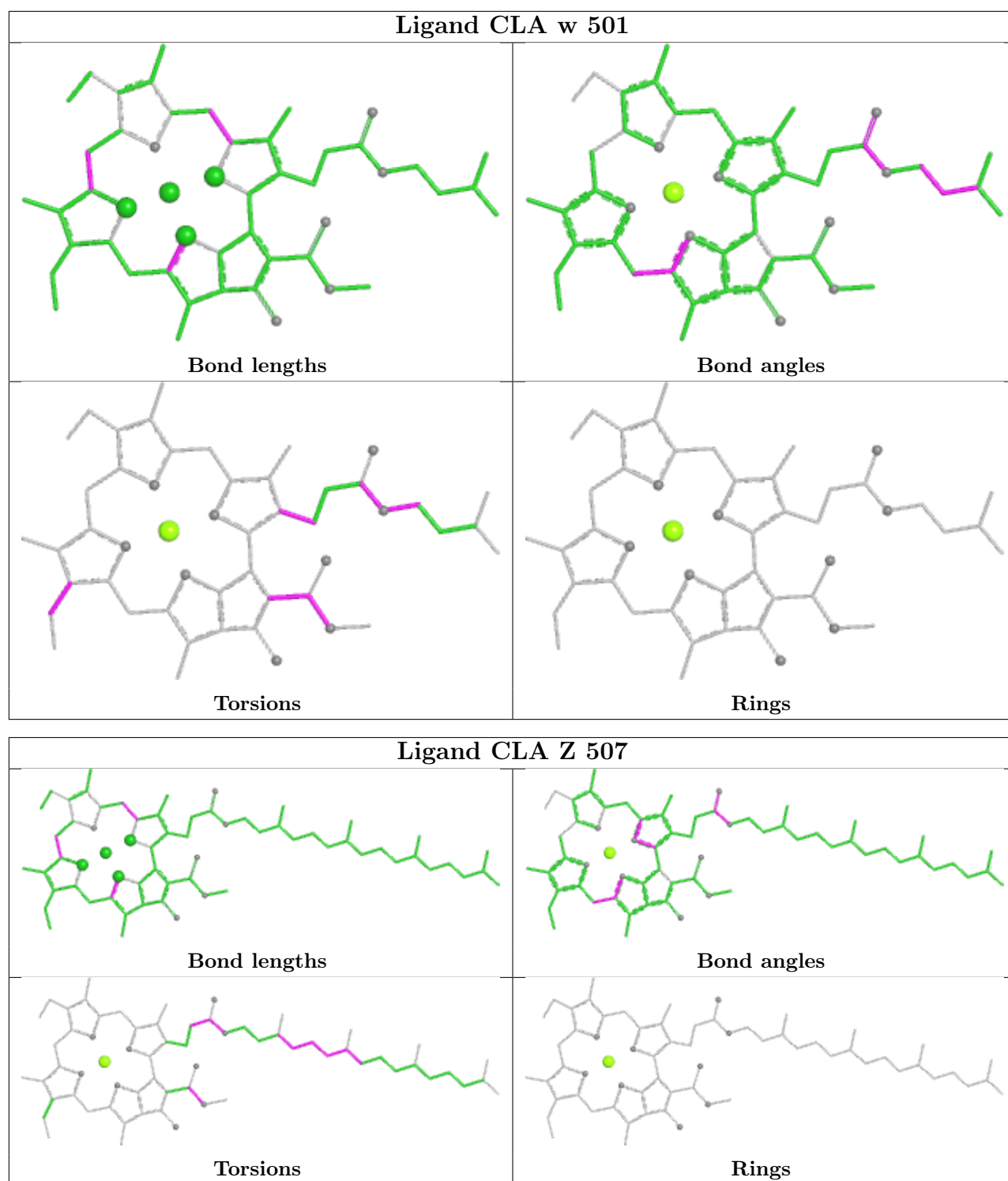


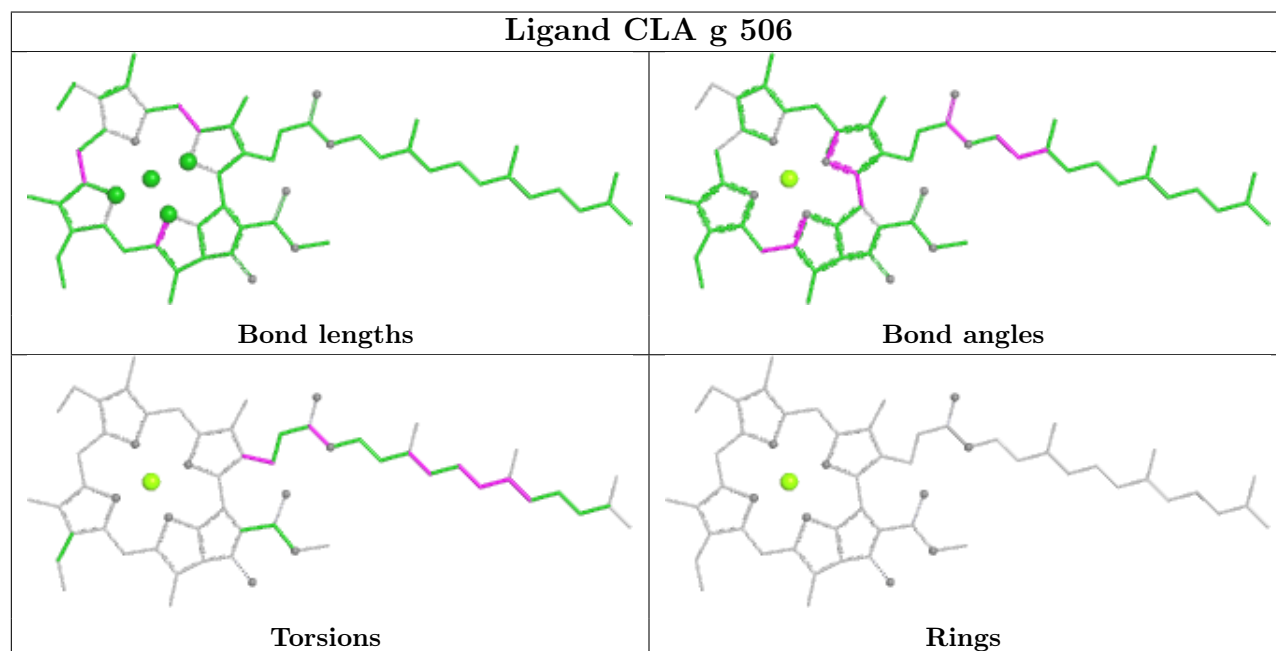
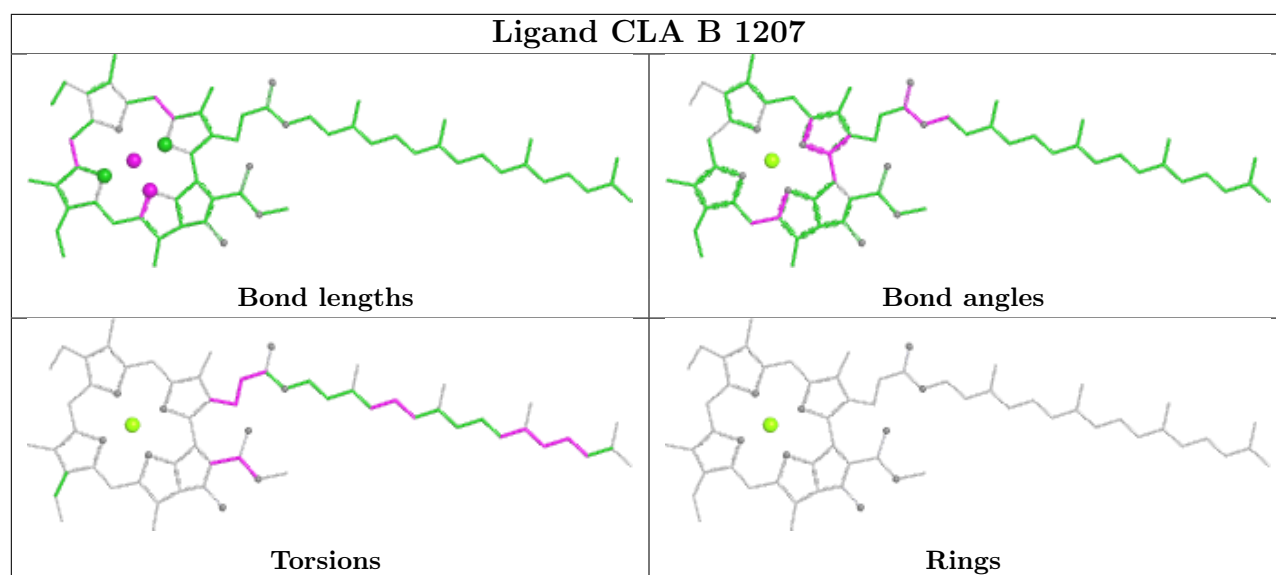
Torsions

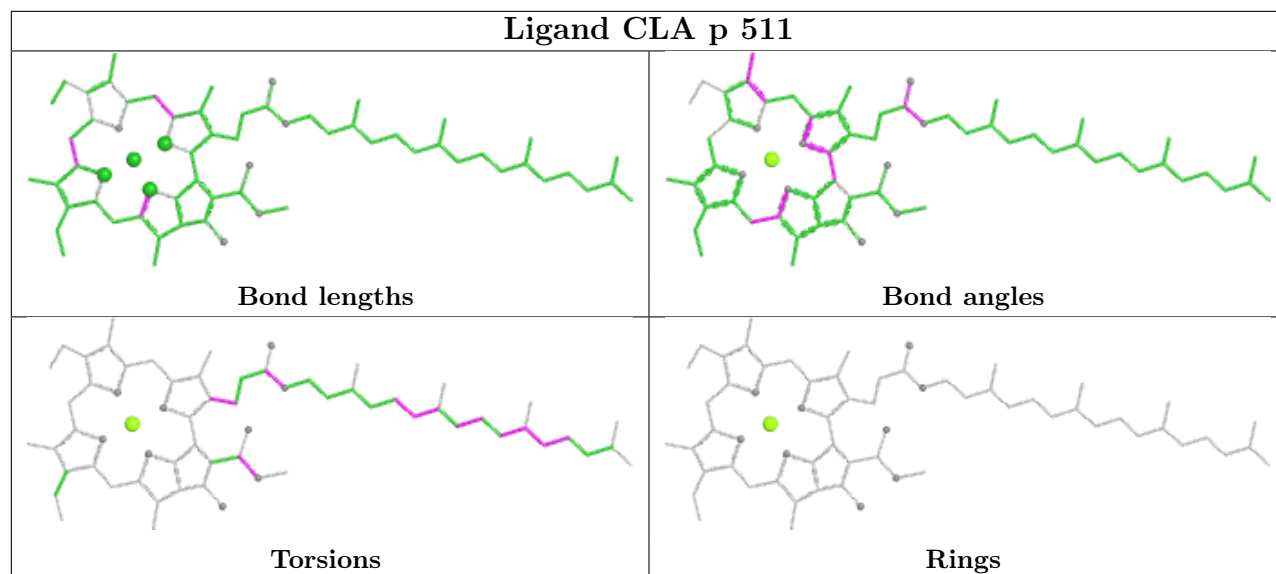
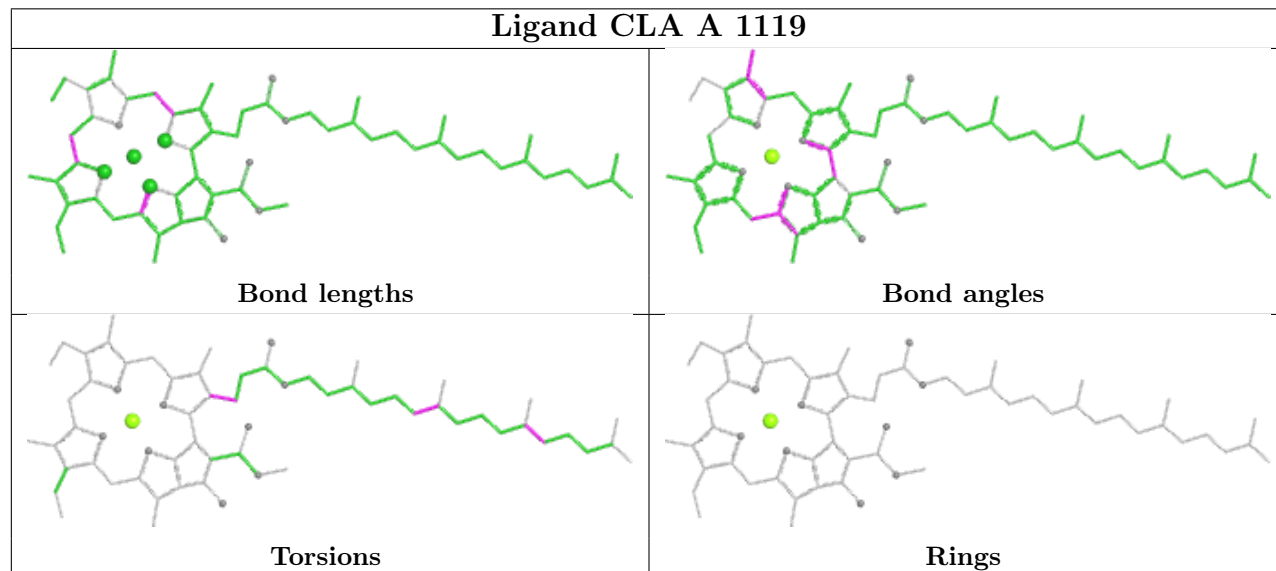


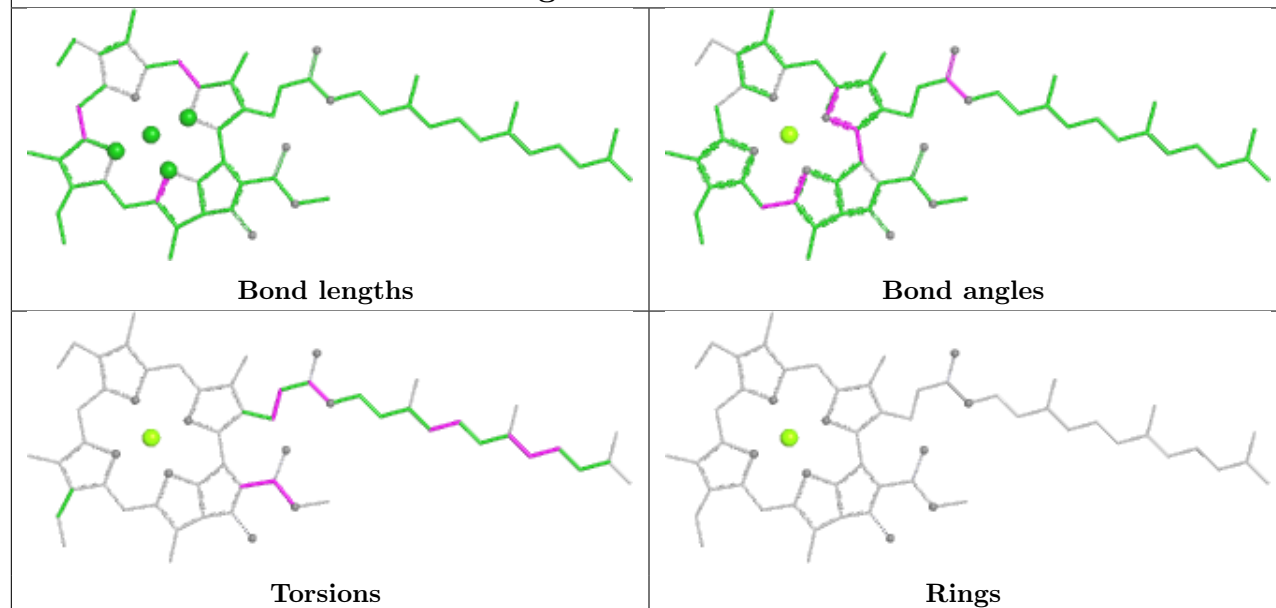
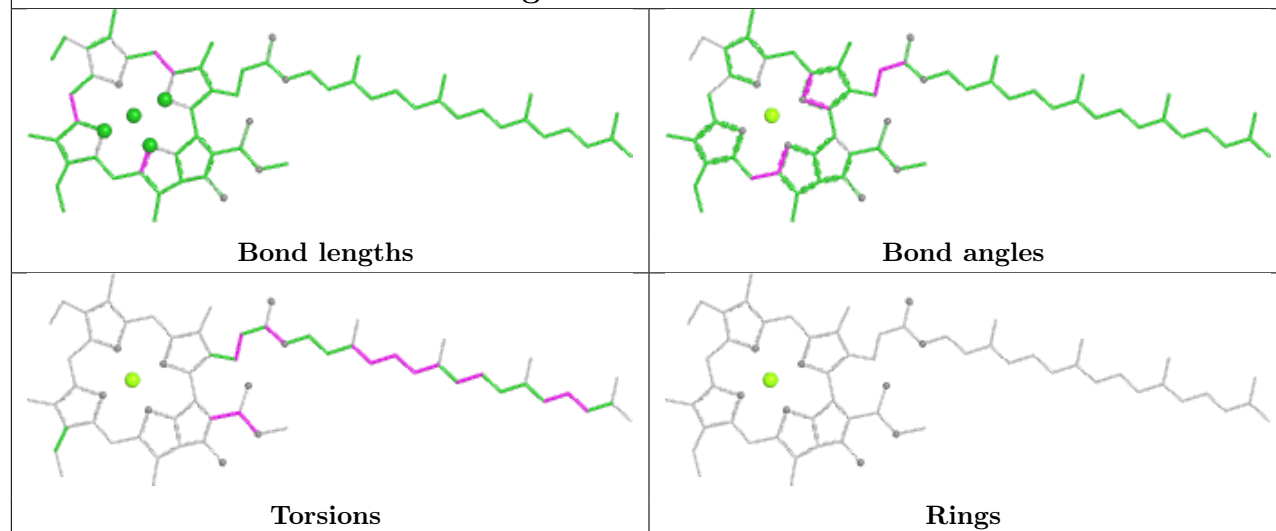
Rings



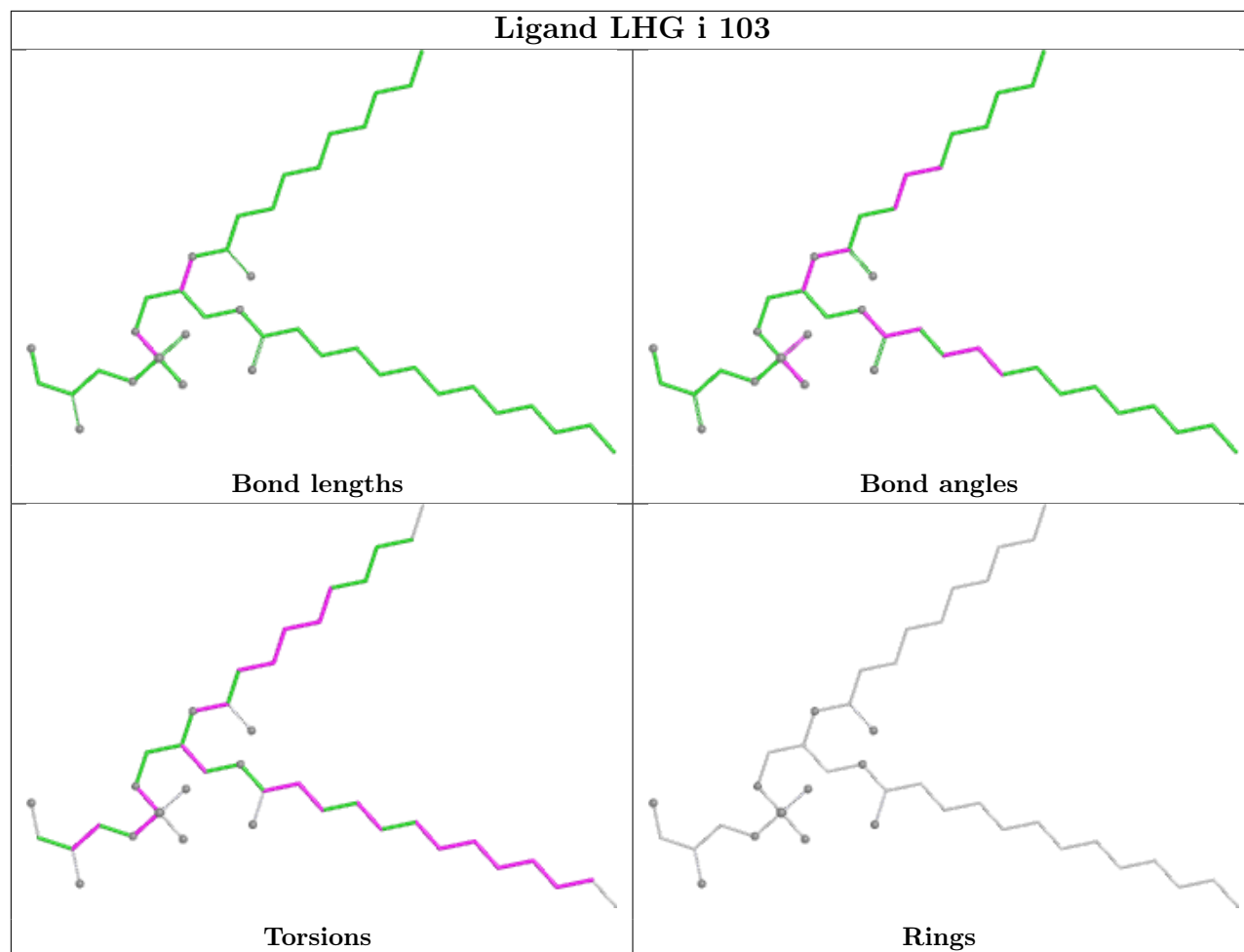




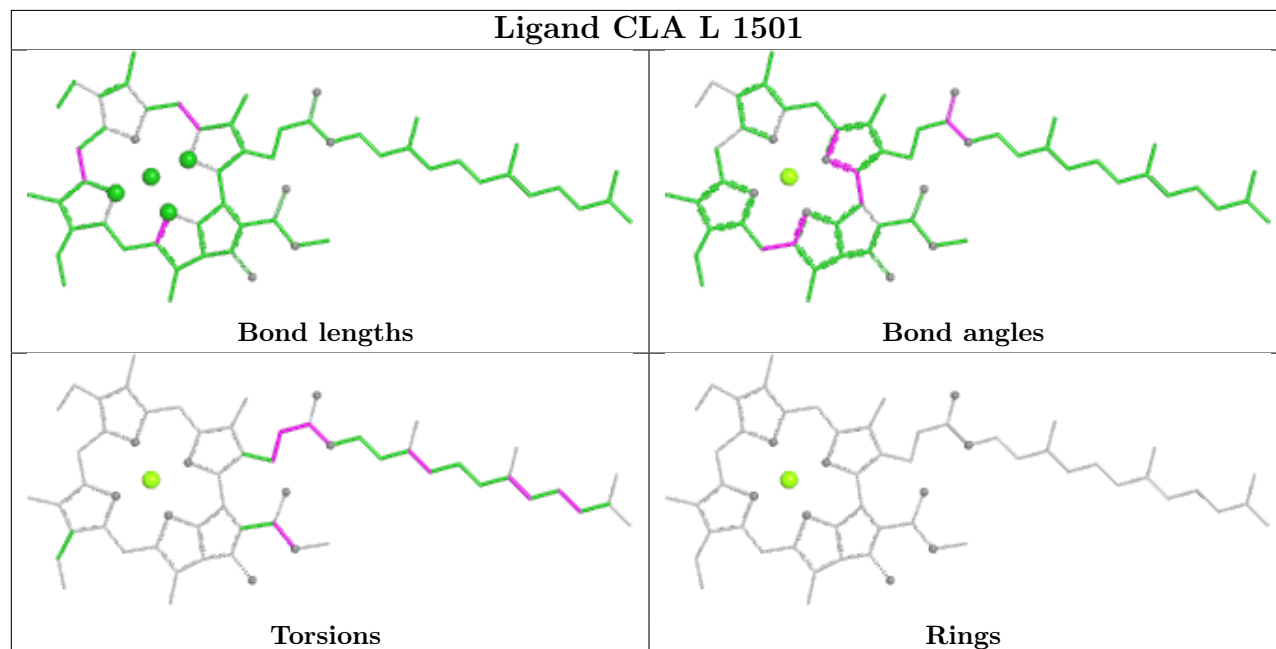
Ligand CLA p 511**Ligand CLA A 1119**

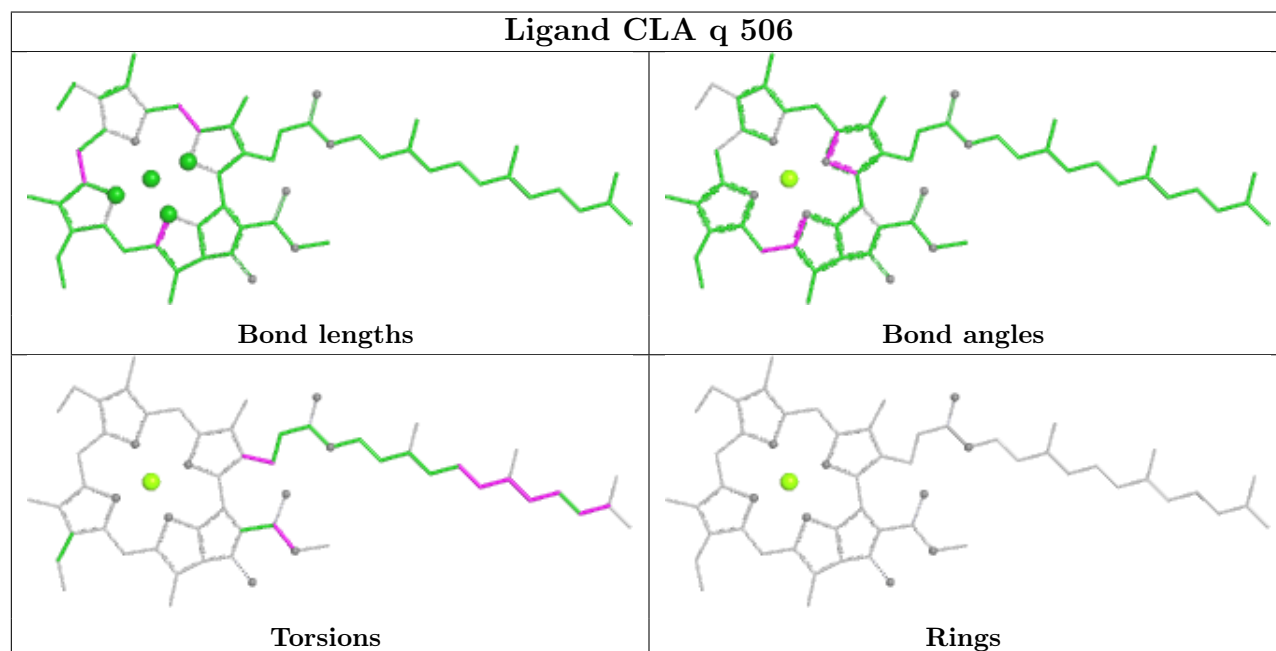
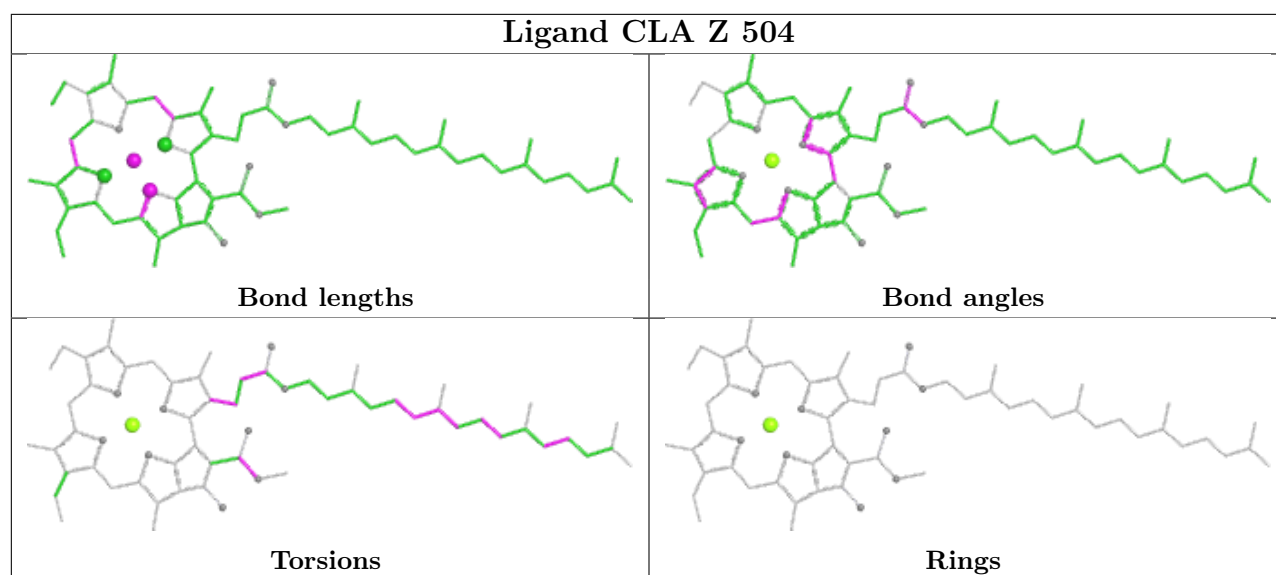
Ligand CLA t 506**Ligand CLA H 1132**

Ligand LHG i 103

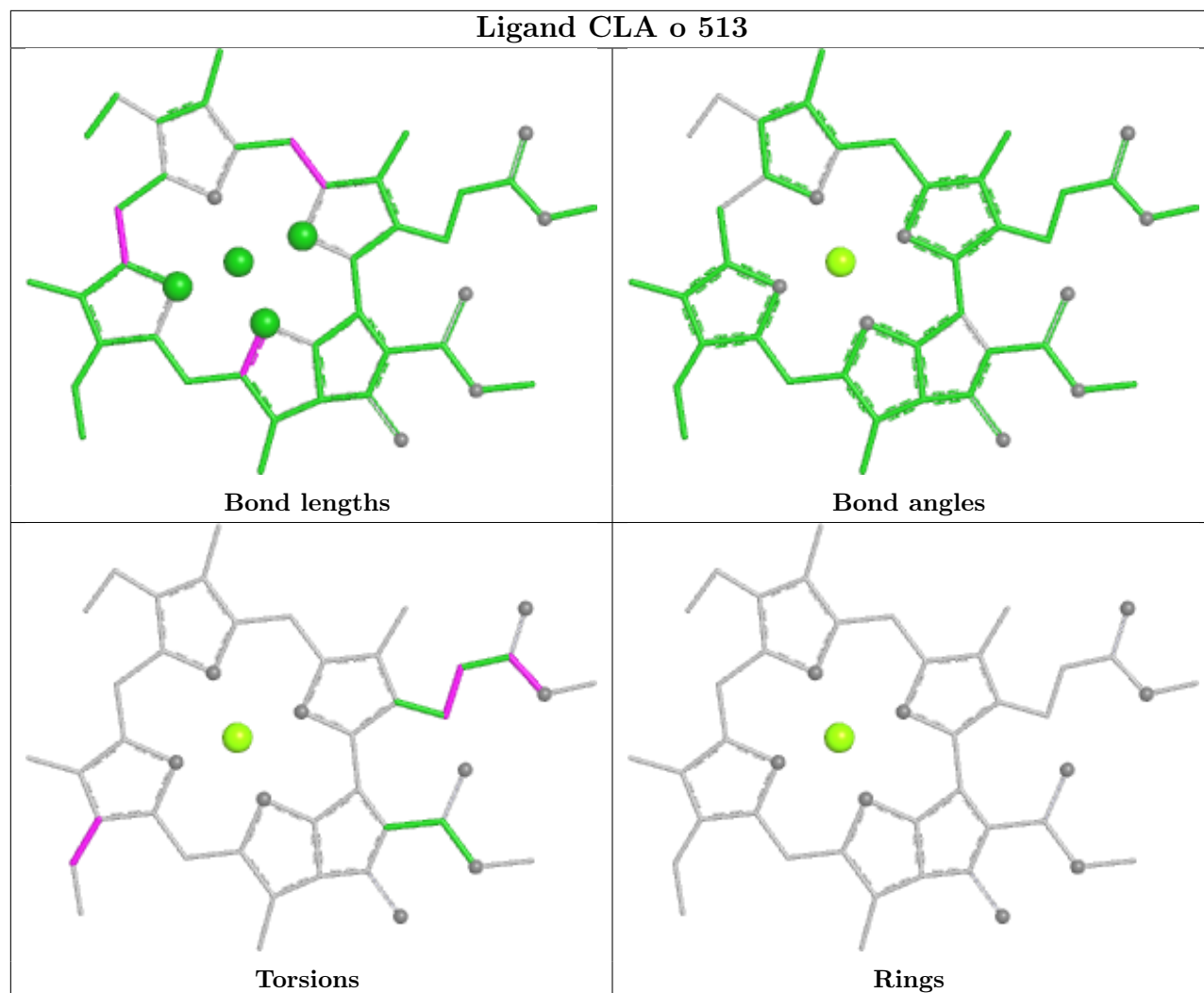


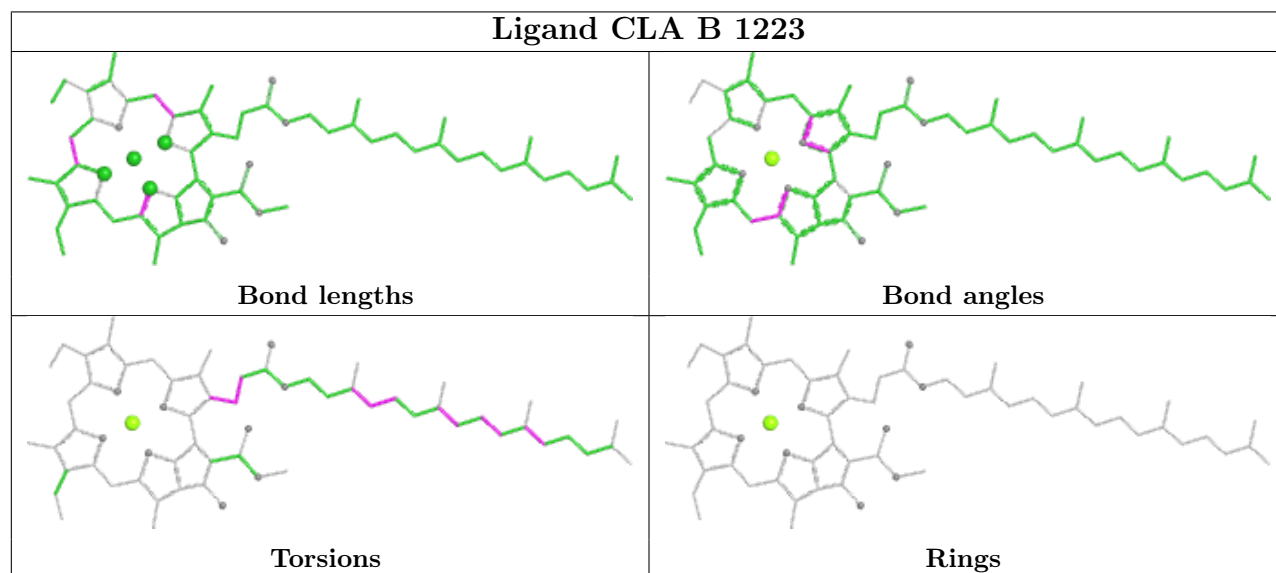
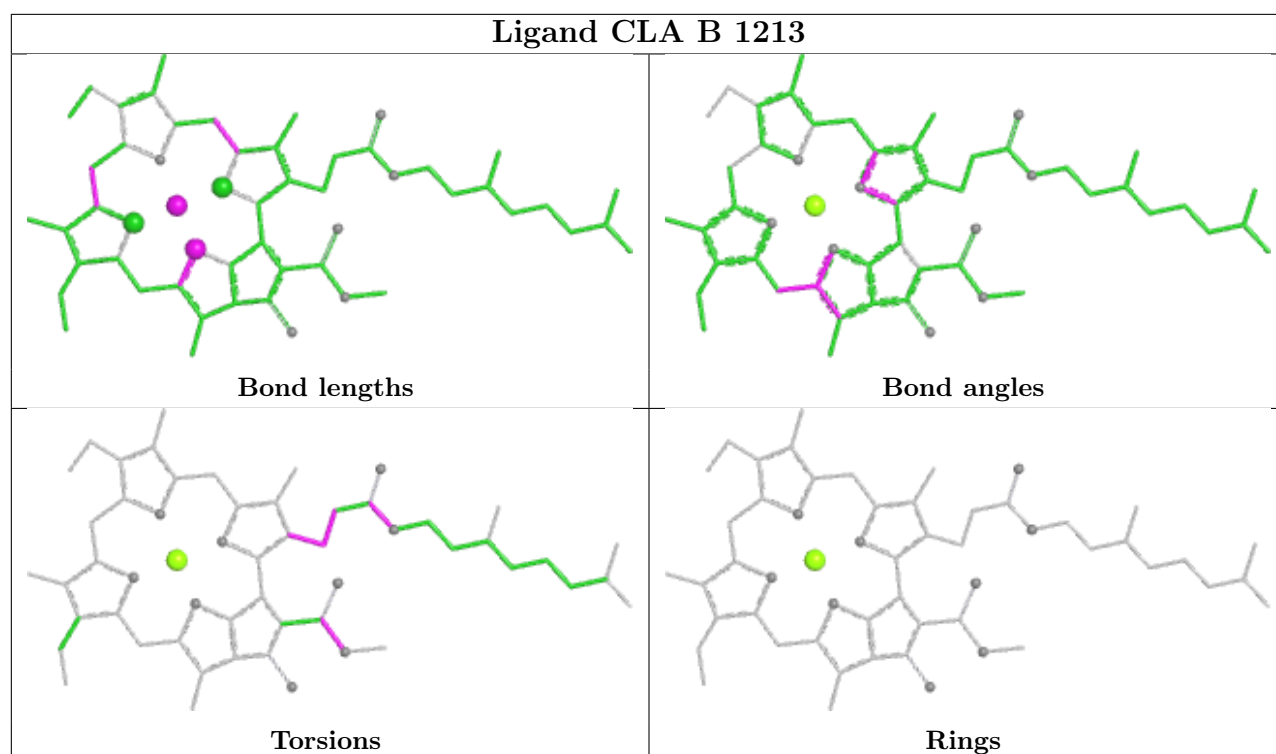
Ligand CLA L 1501



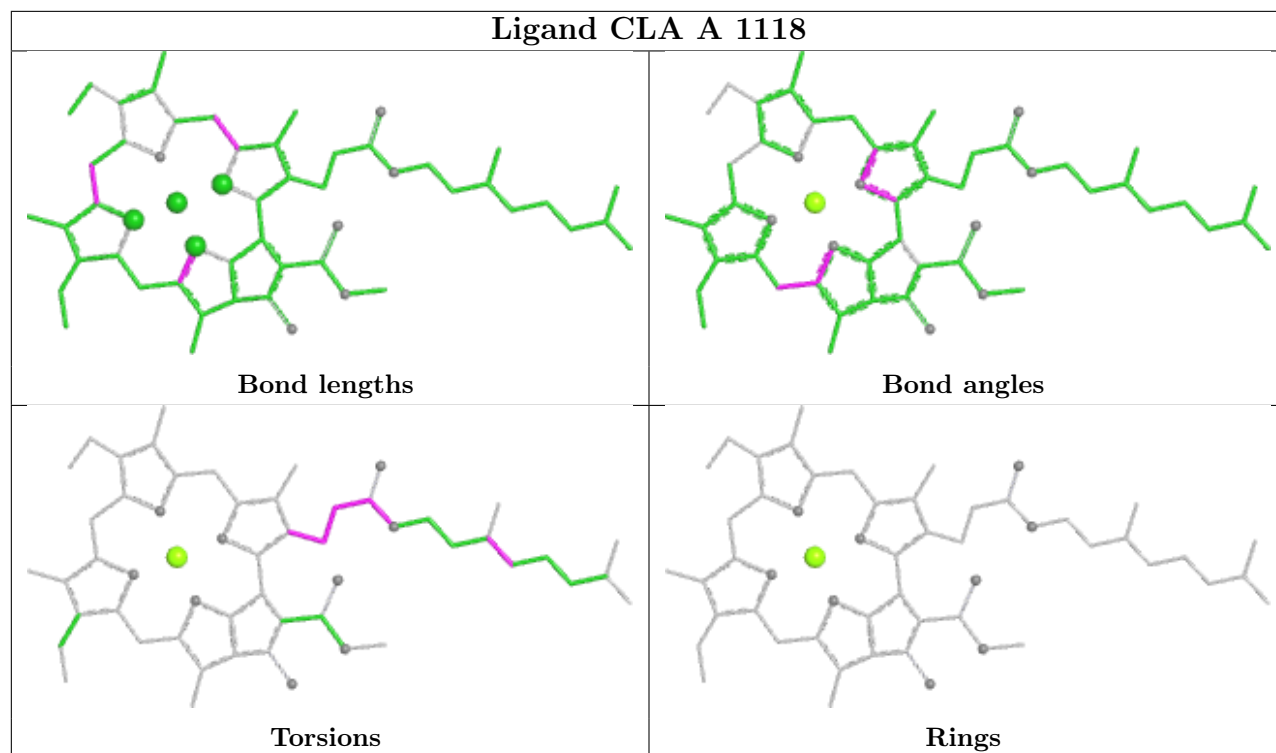


Ligand CLA o 513

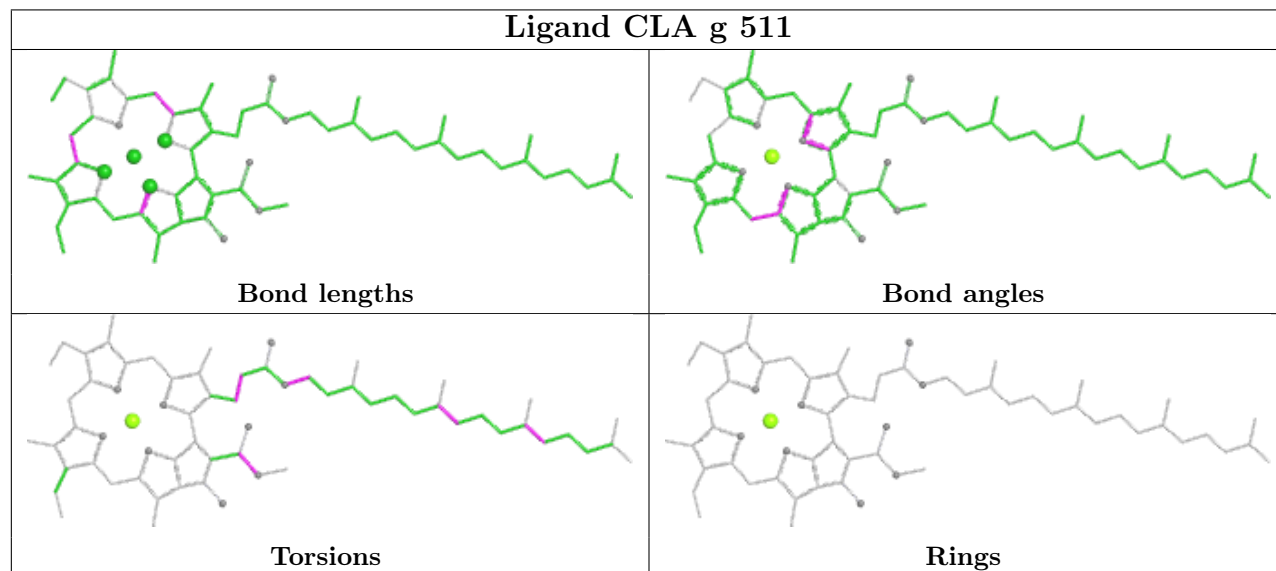


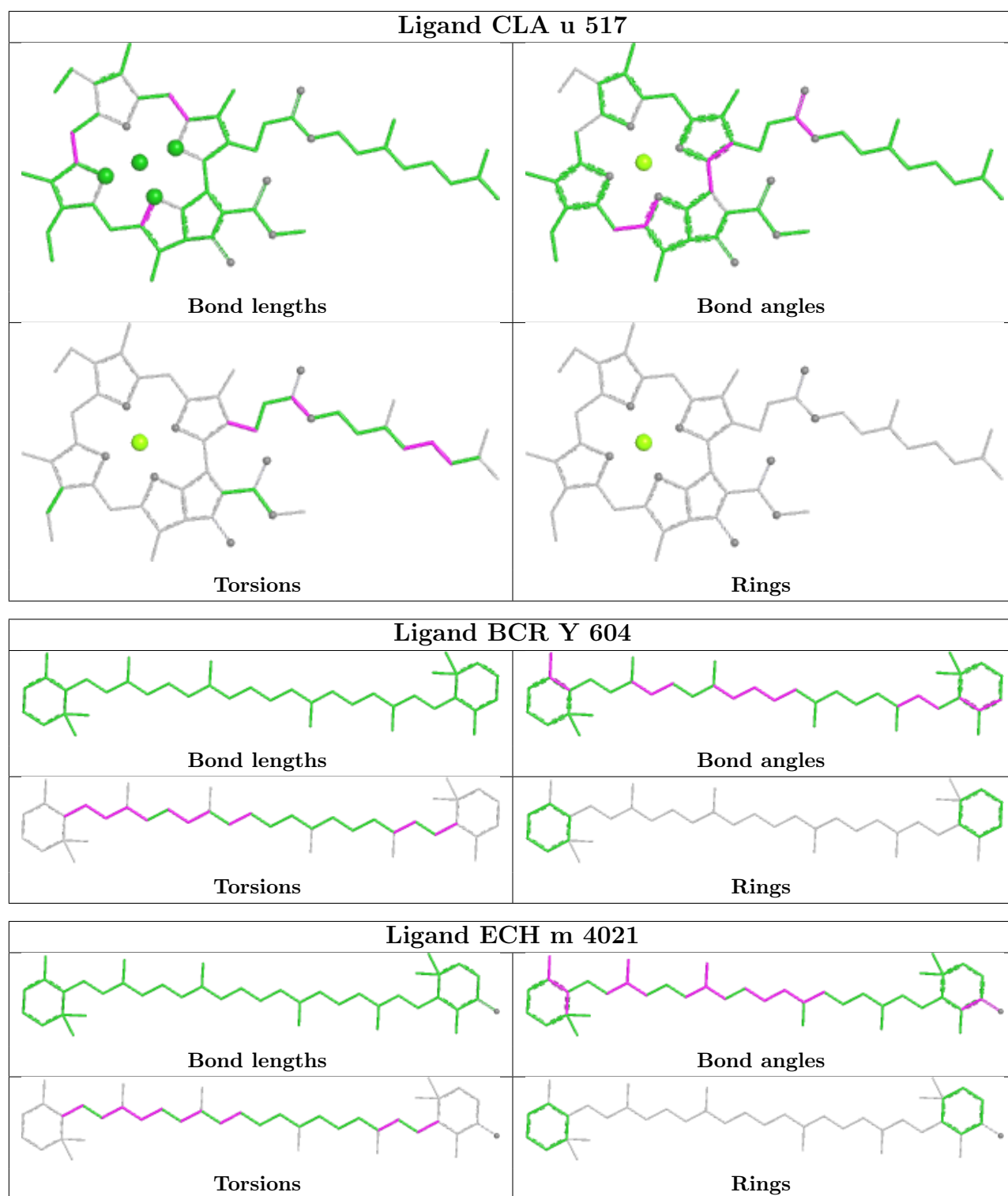


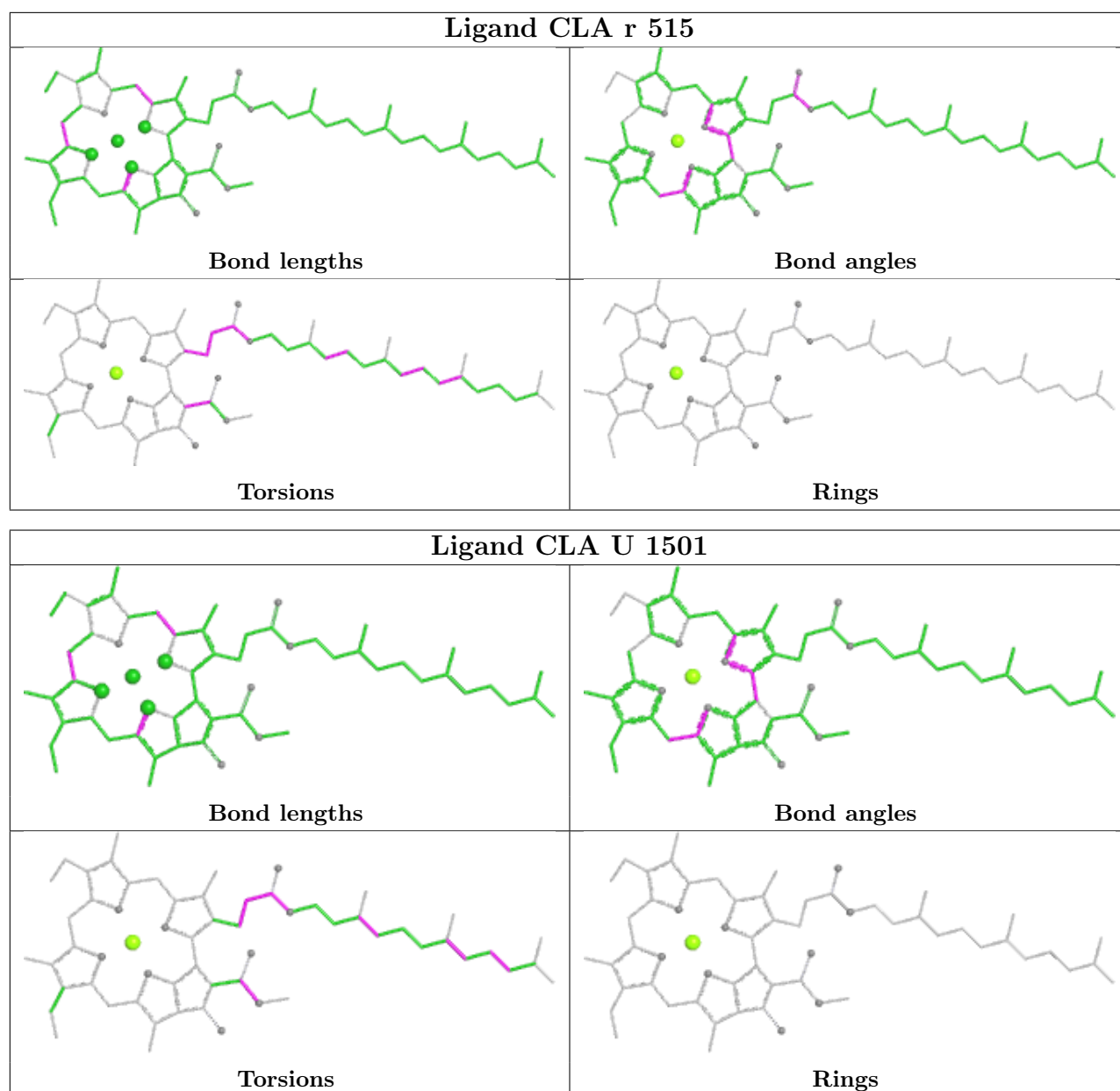
Ligand CLA A 1118

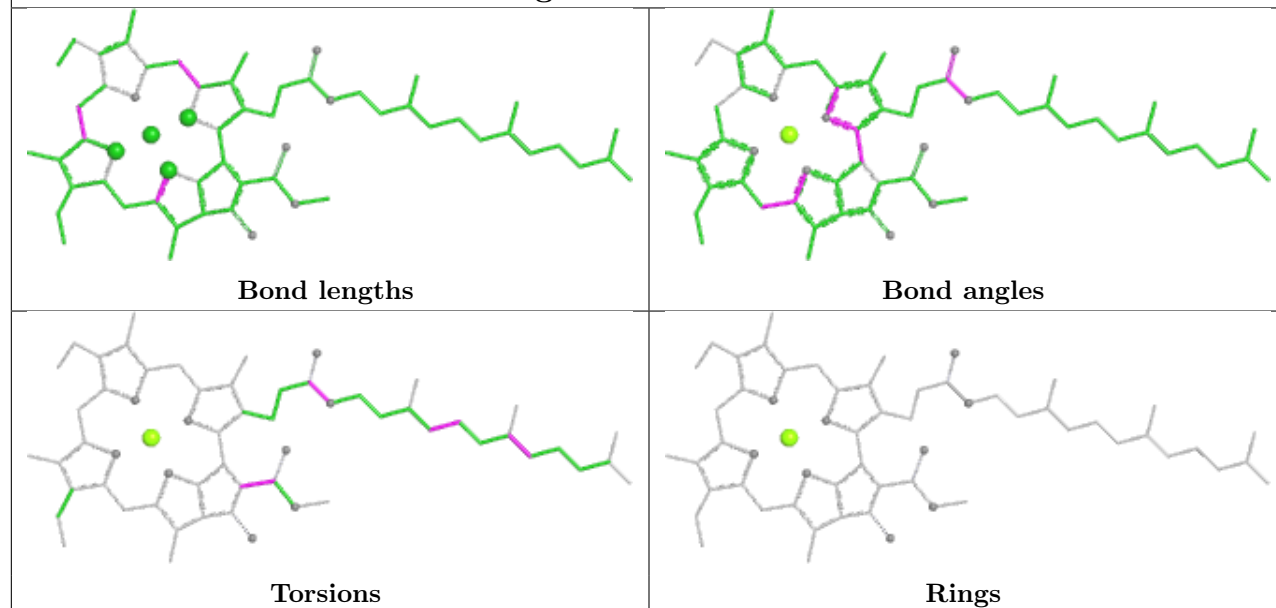
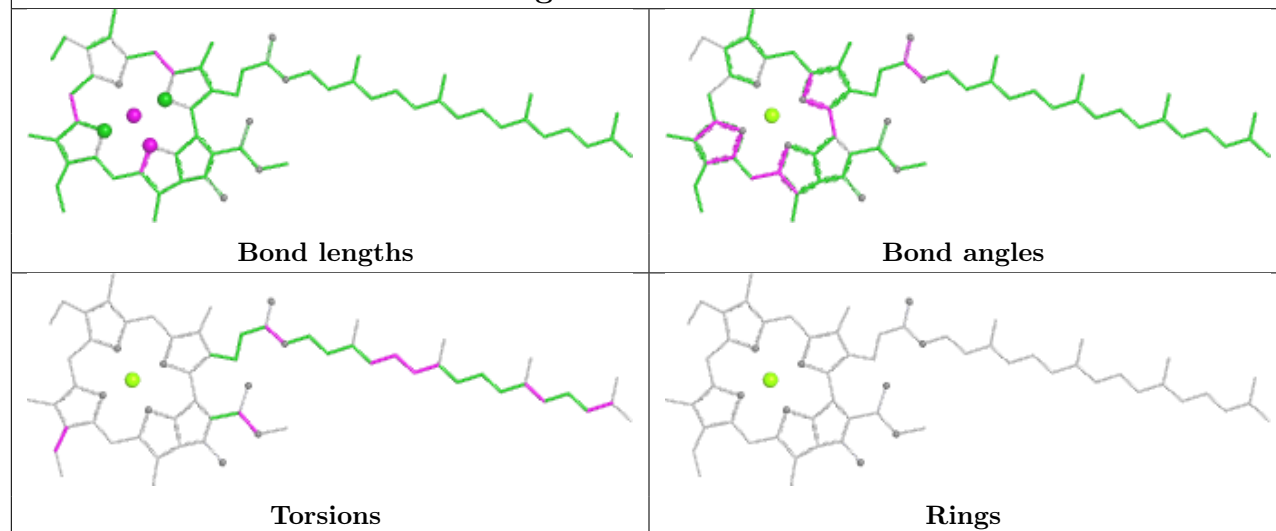


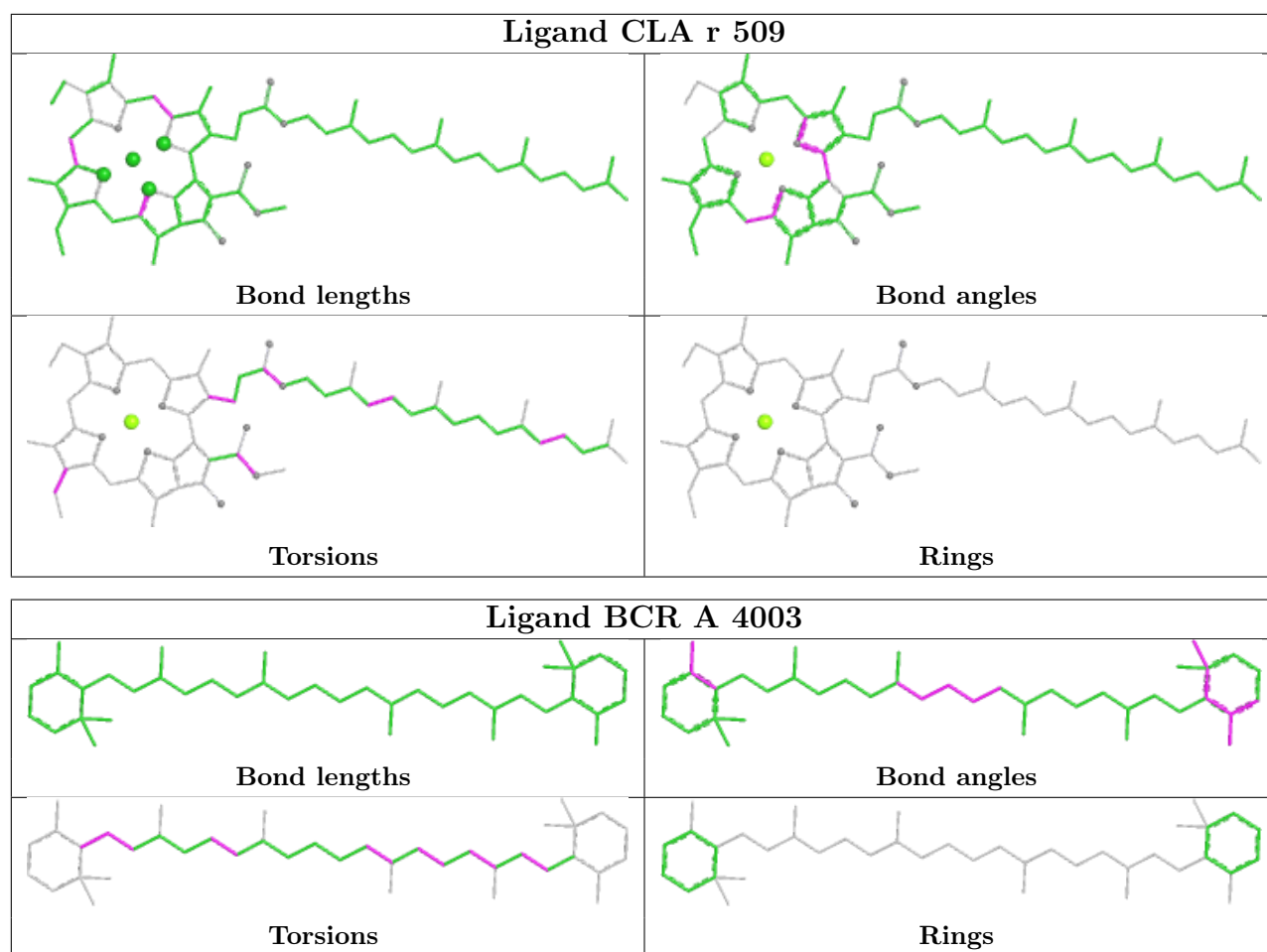
Ligand CLA g 511



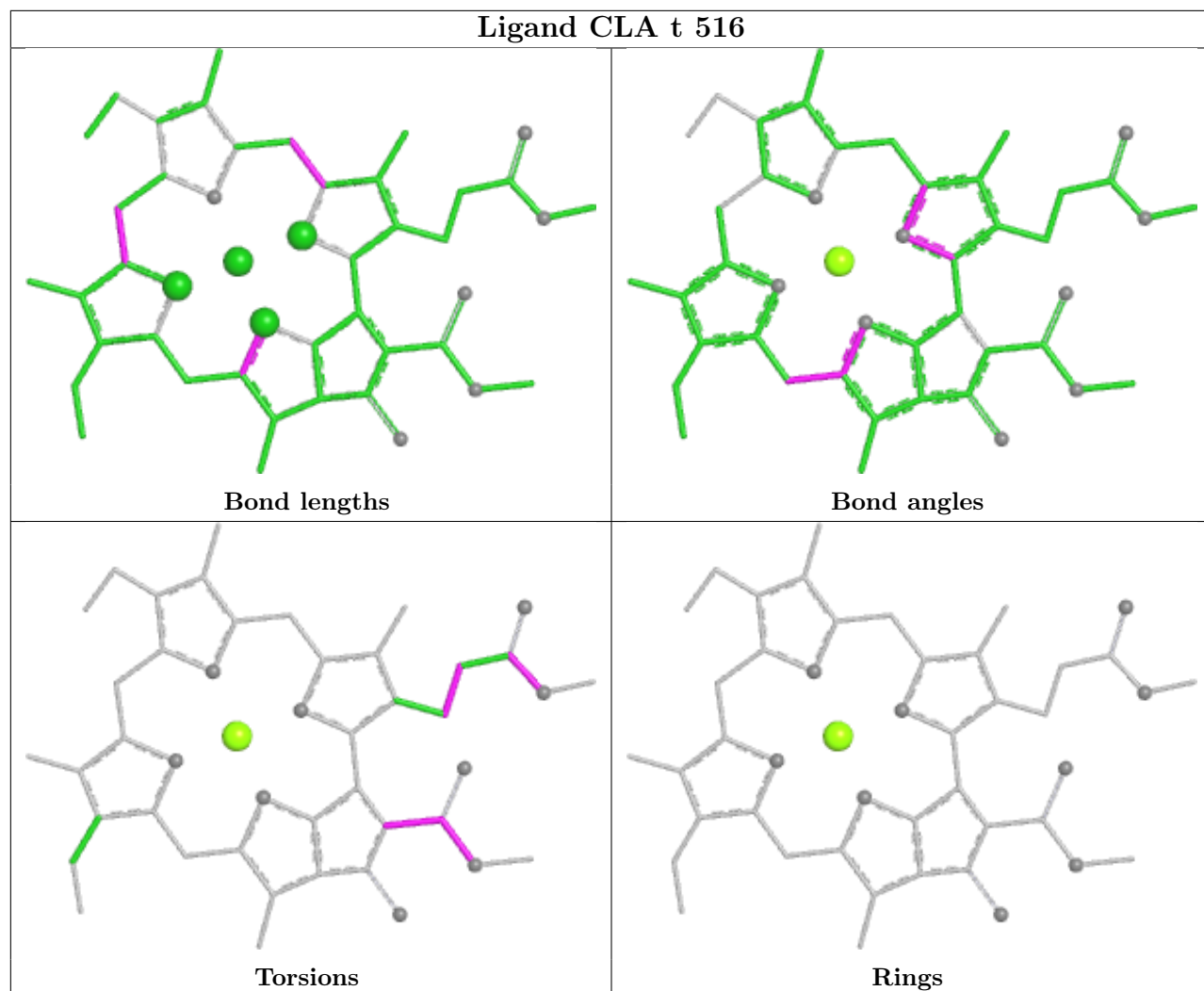




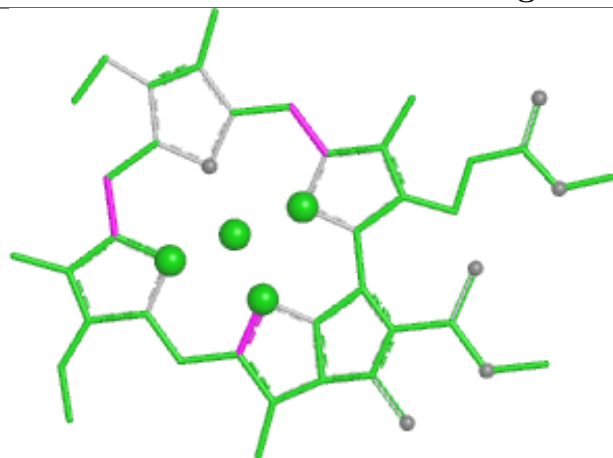
Ligand CLA n 506**Ligand CLA h 511**



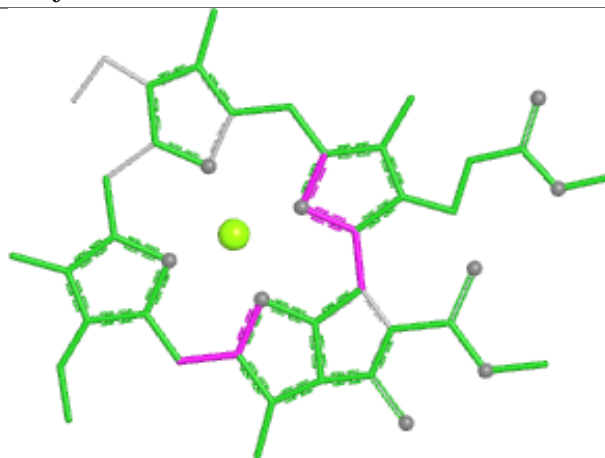
Ligand CLA t 516



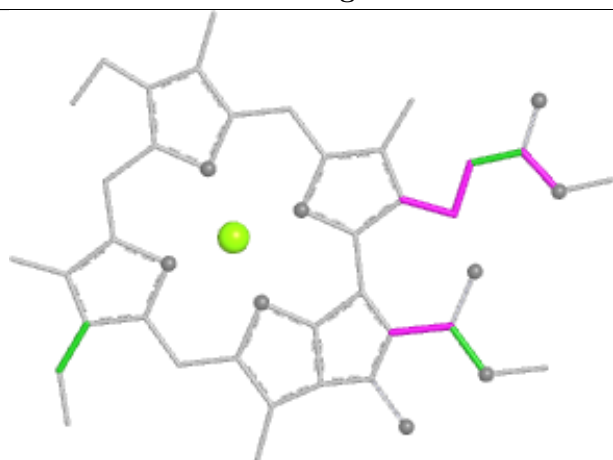
Ligand CLA y 501



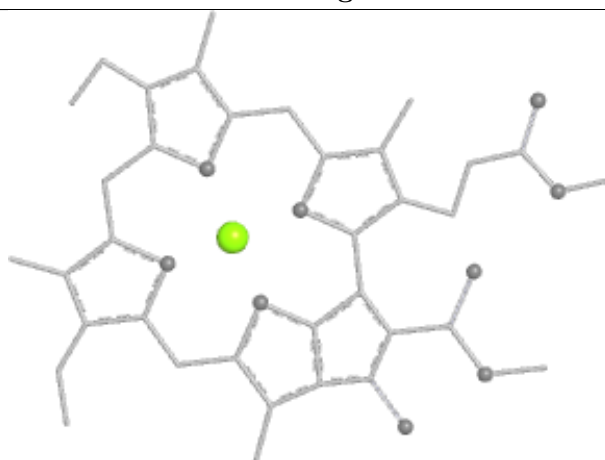
Bond lengths



Bond angles

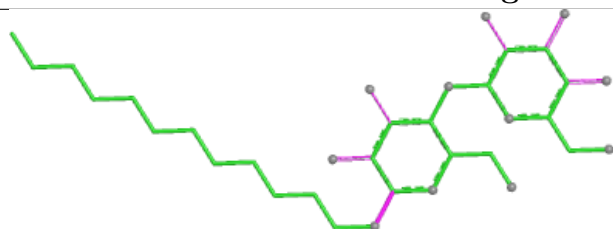


Torsions

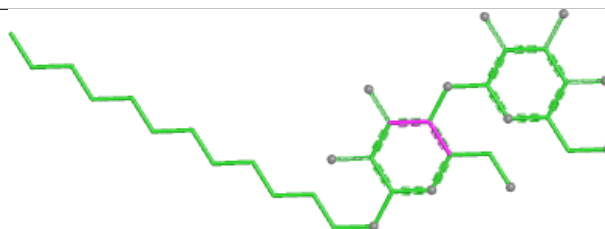


Rings

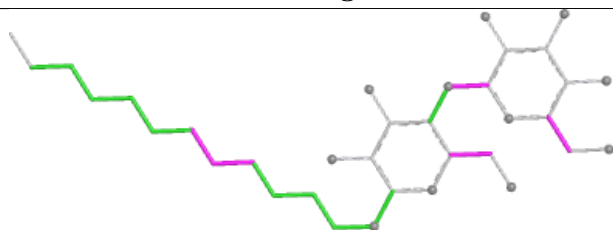
Ligand LMT U 4101



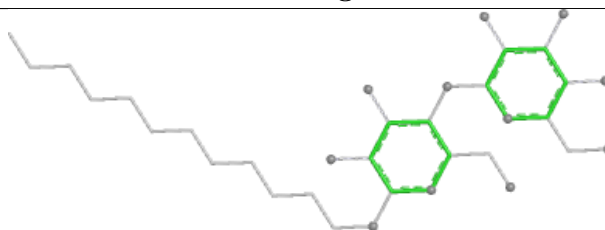
Bond lengths



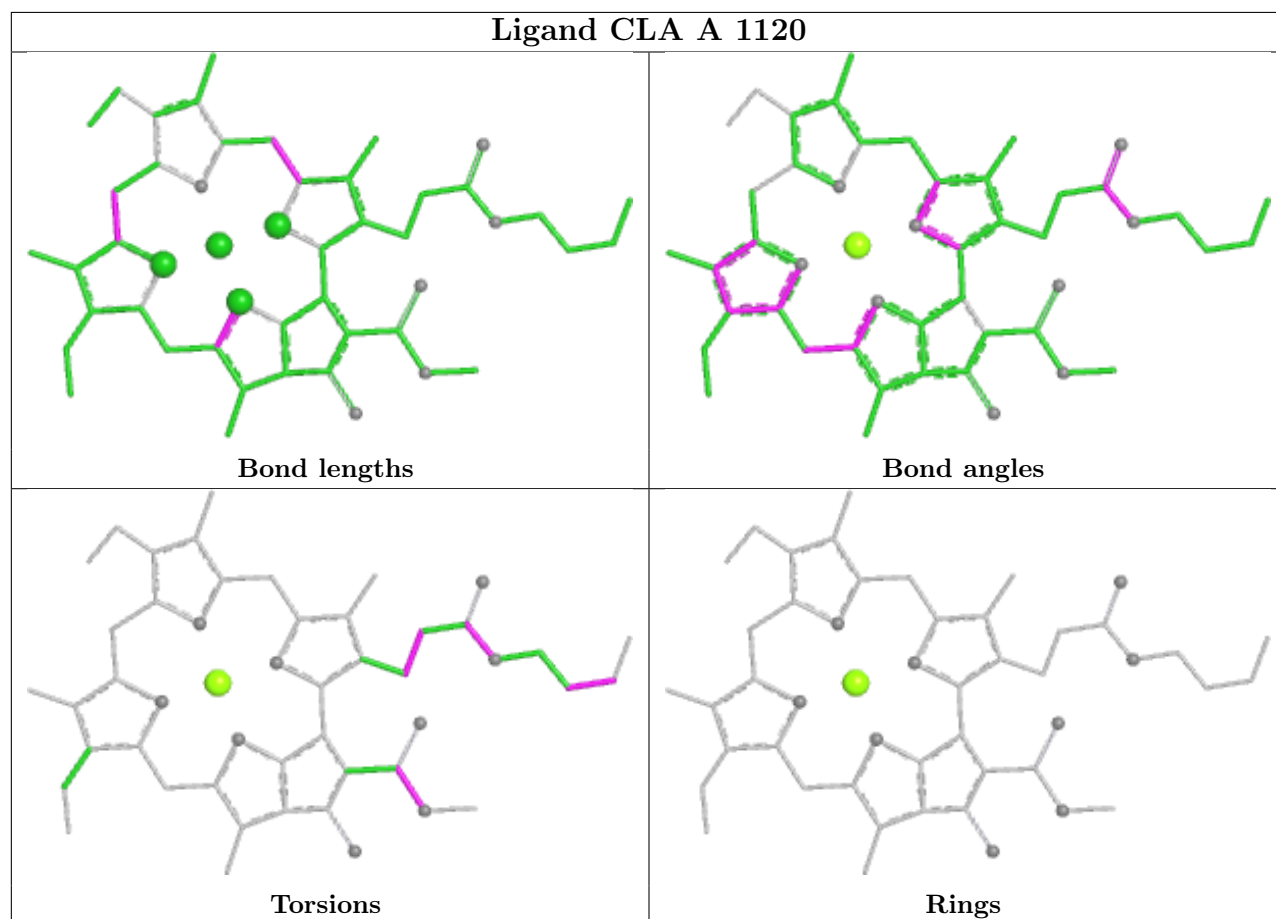
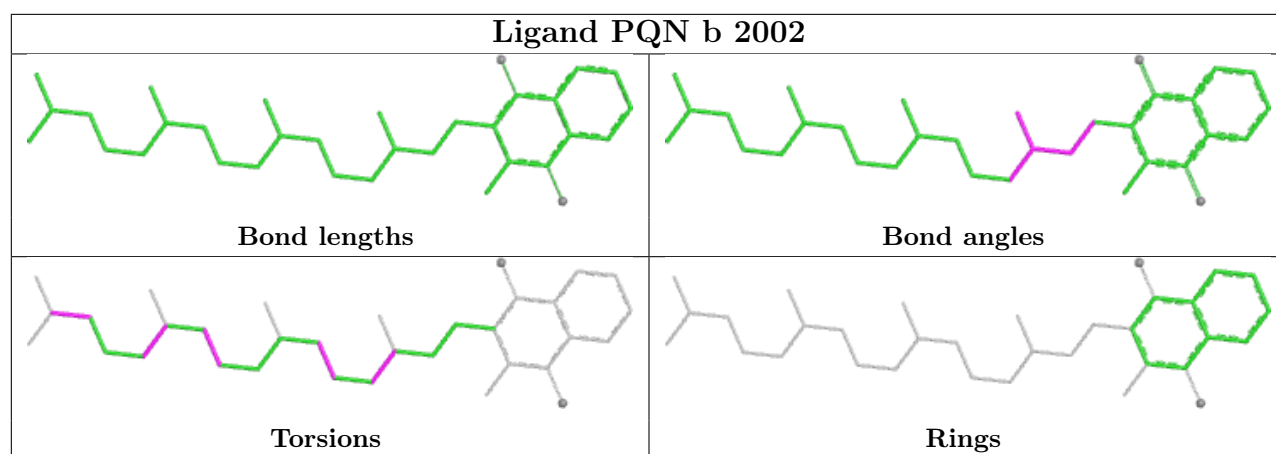
Bond angles



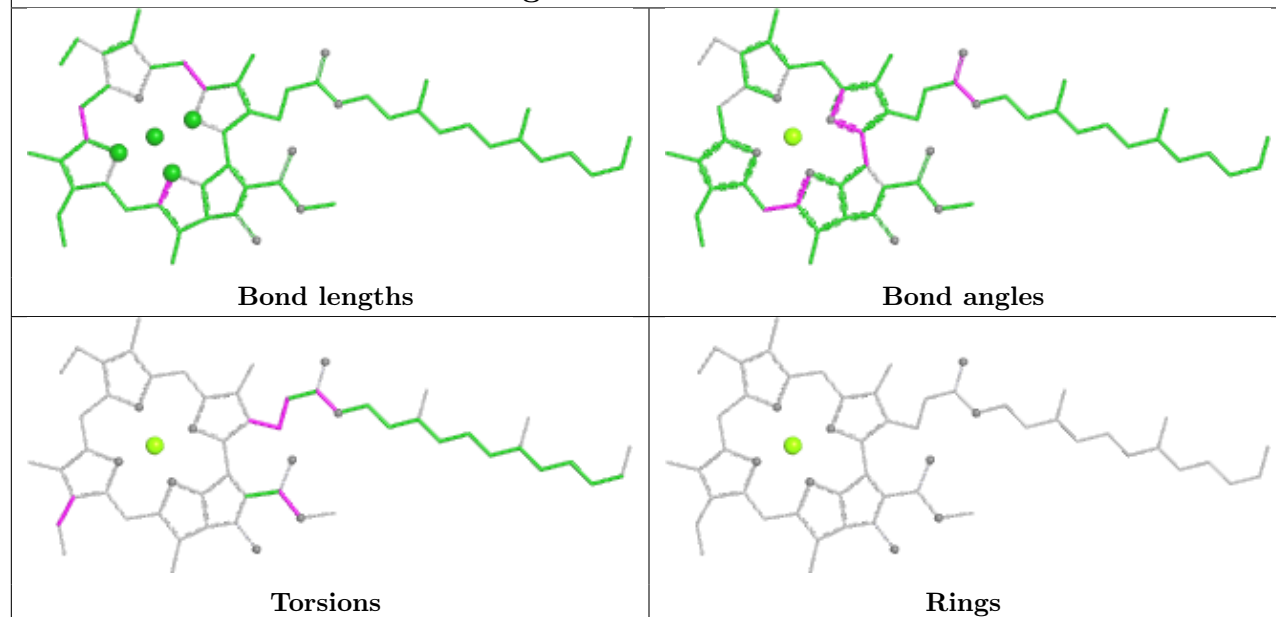
Torsions



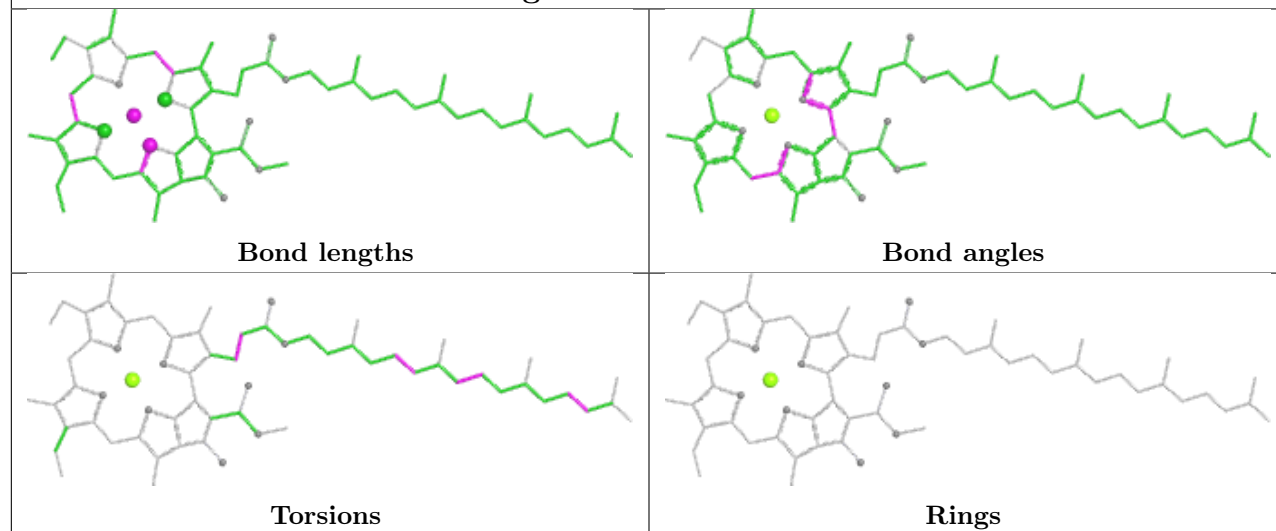
Rings

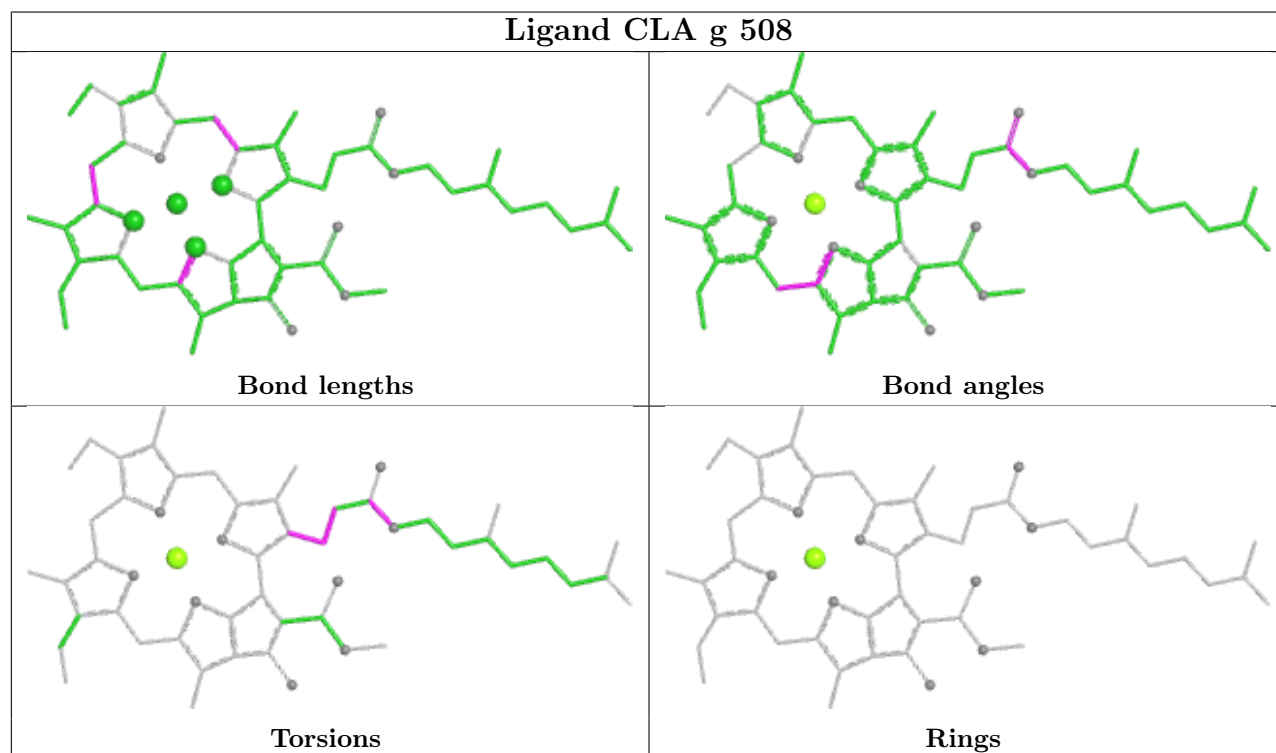
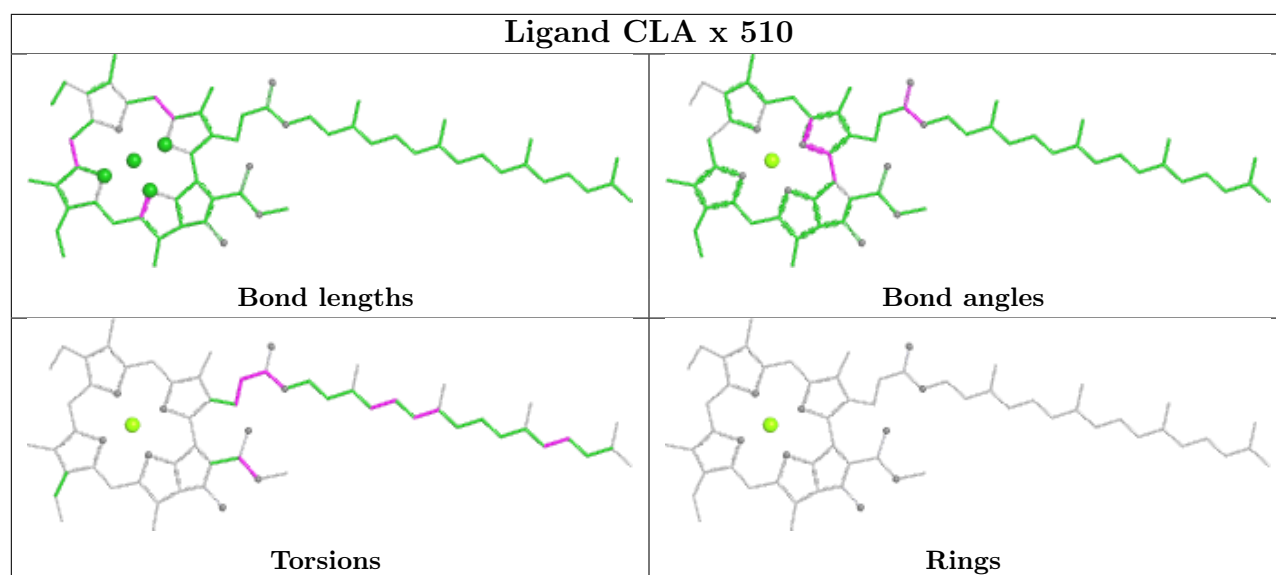


Ligand CLA A 1122

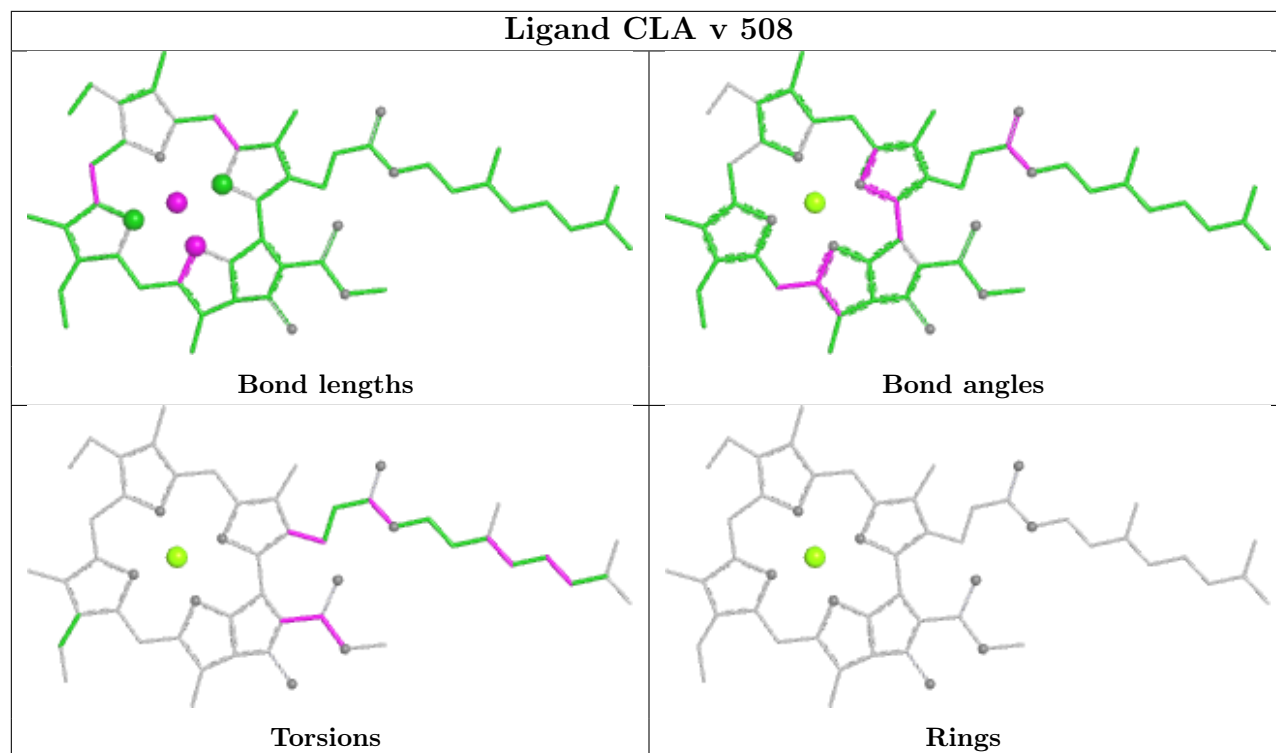


Ligand CLA A 1127

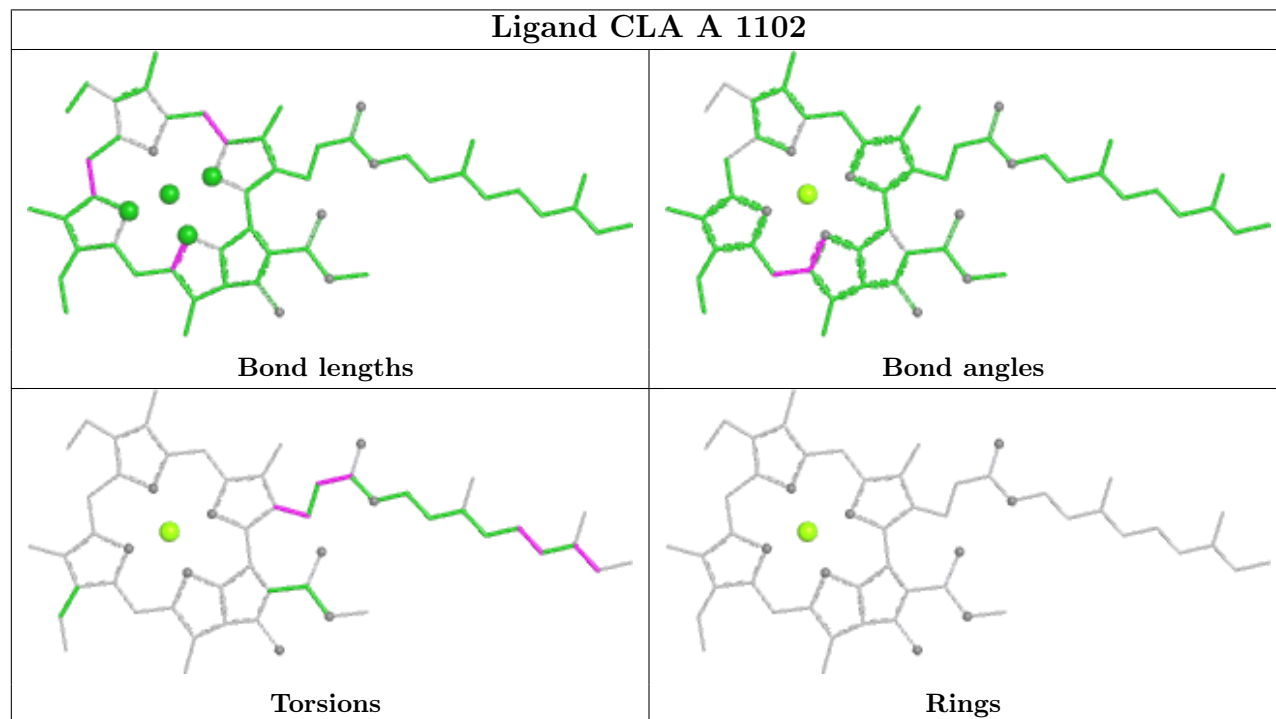


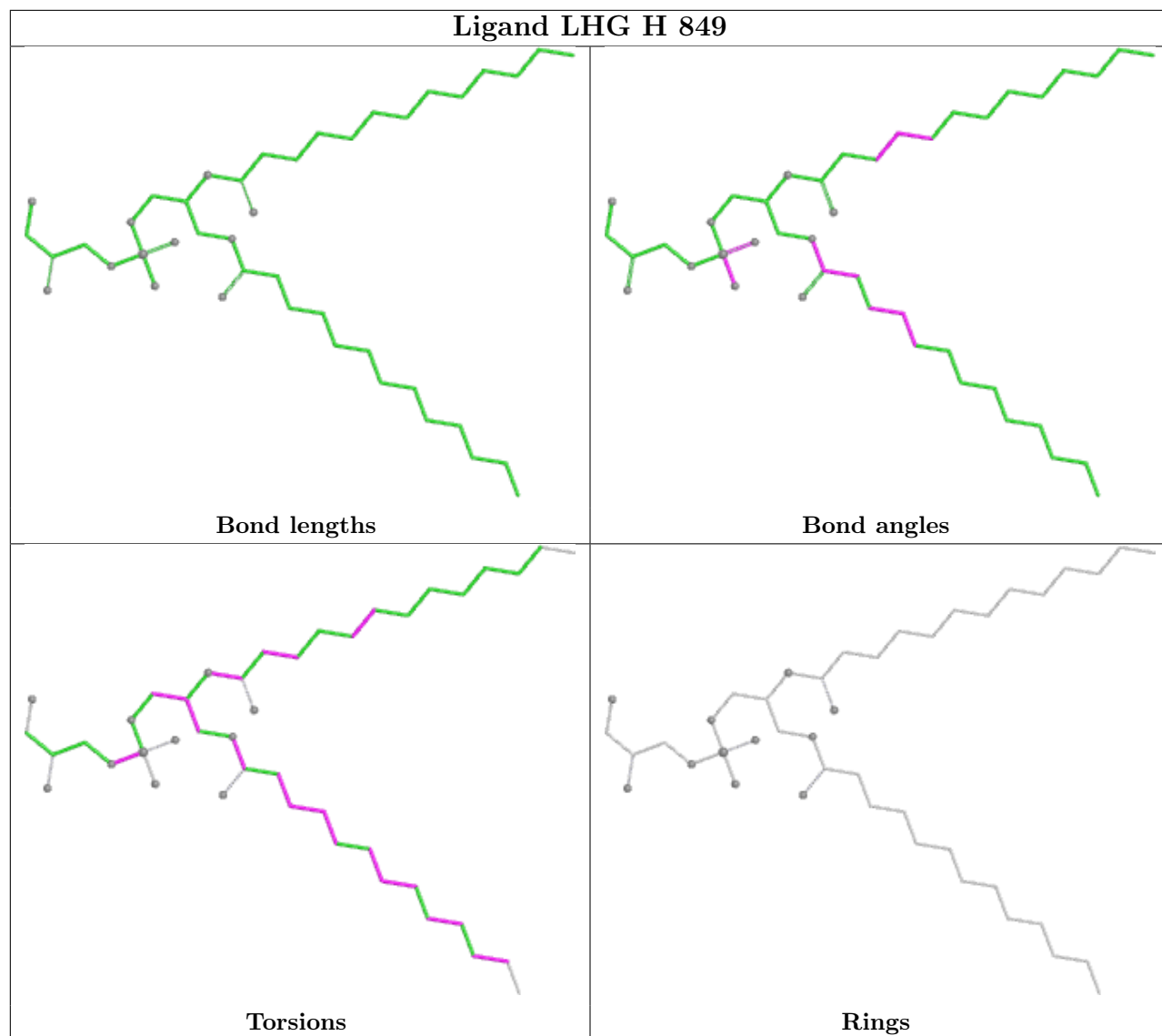


Ligand CLA v 508

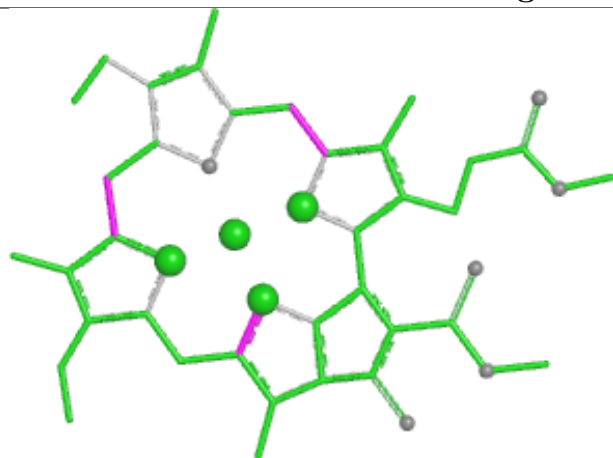


Ligand CLA A 1102

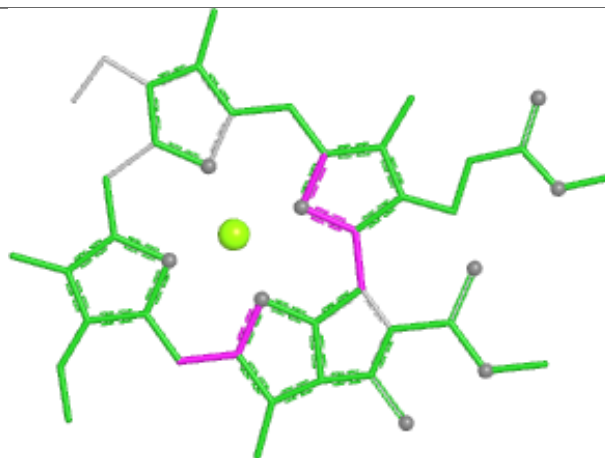




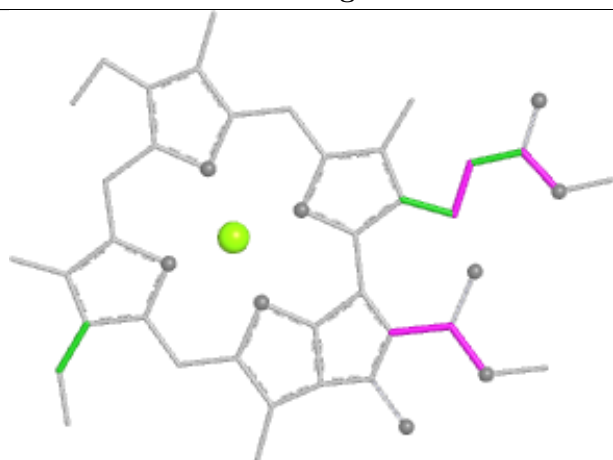
Ligand CLA u 516



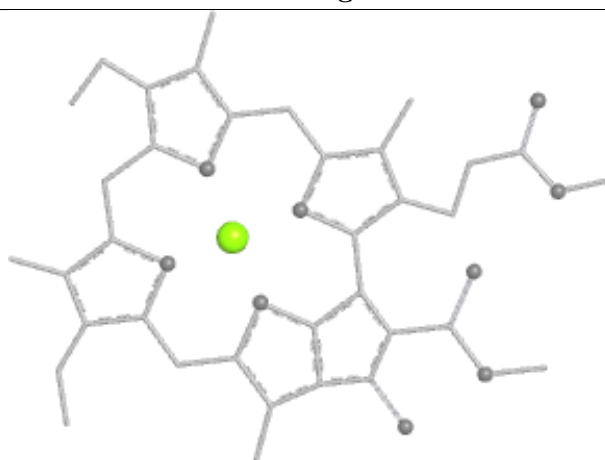
Bond lengths



Bond angles

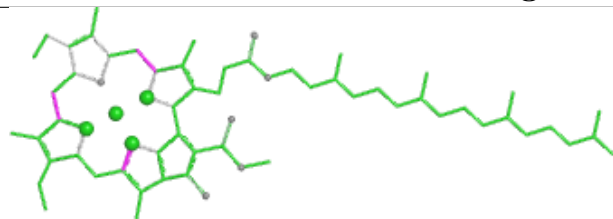


Torsions

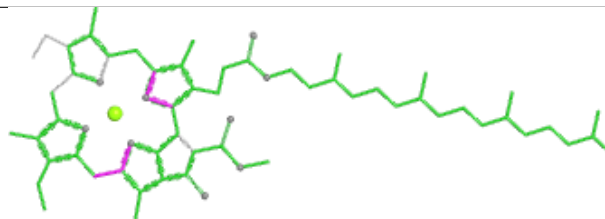


Rings

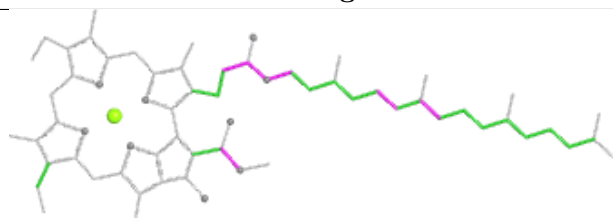
Ligand CLA t 507



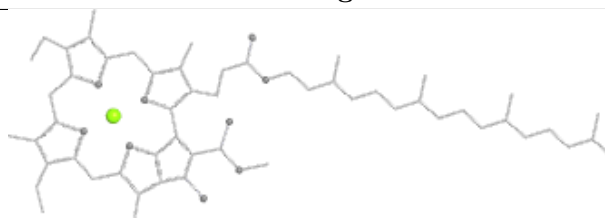
Bond lengths



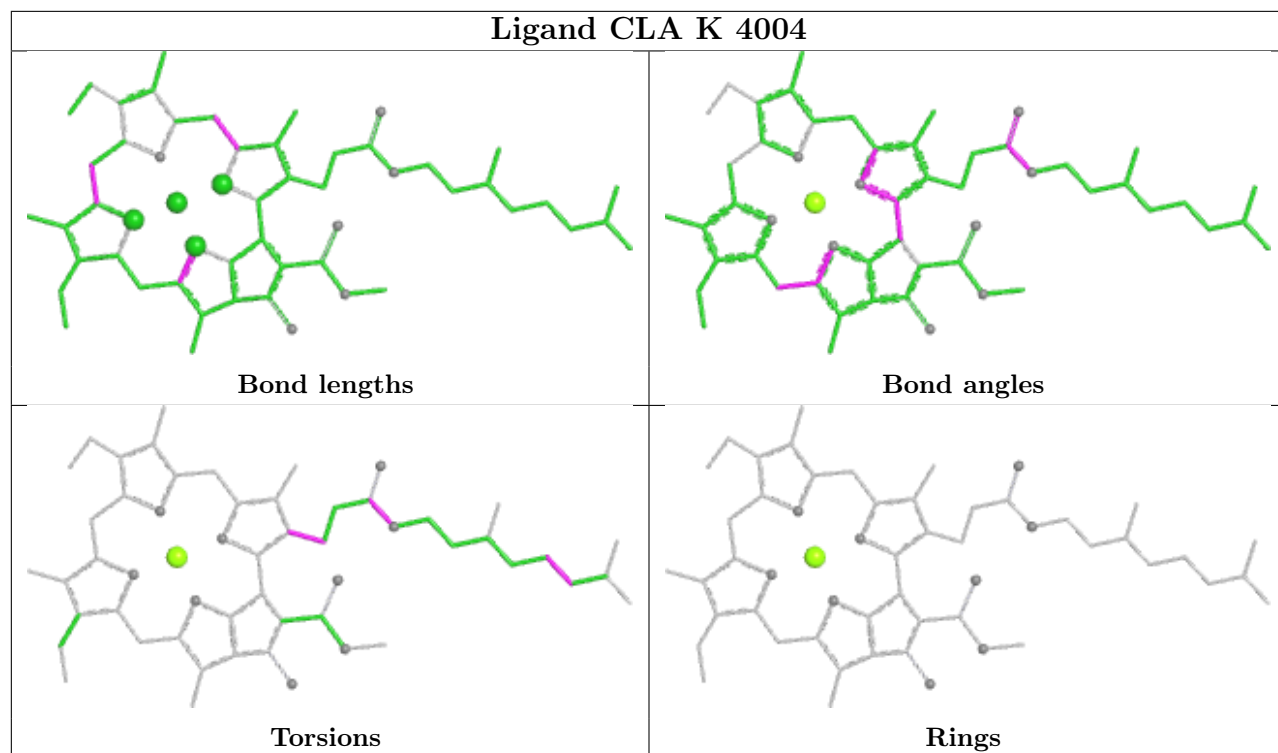
Bond angles



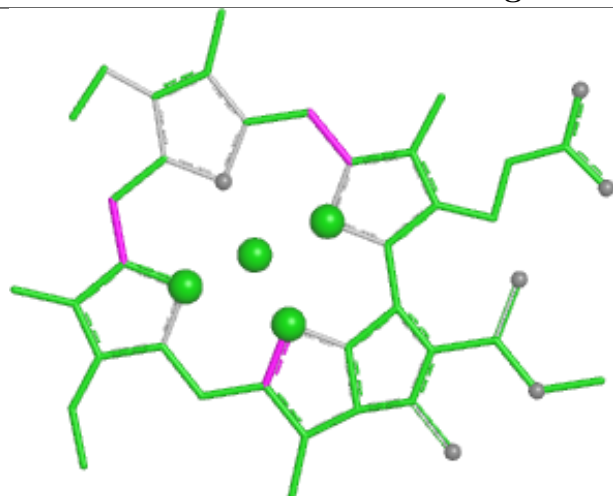
Torsions



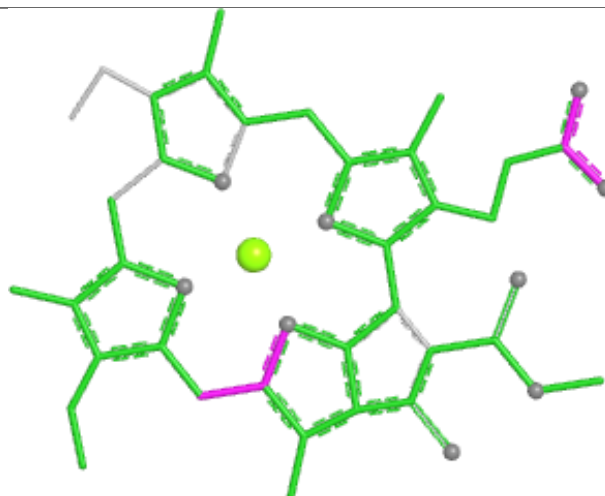
Rings



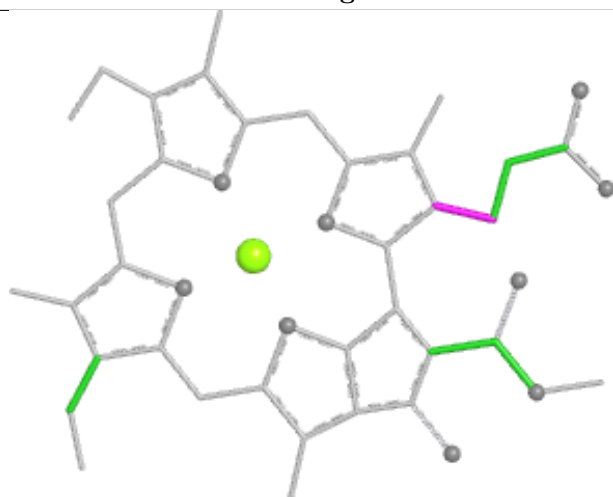
Ligand CLA H 1112



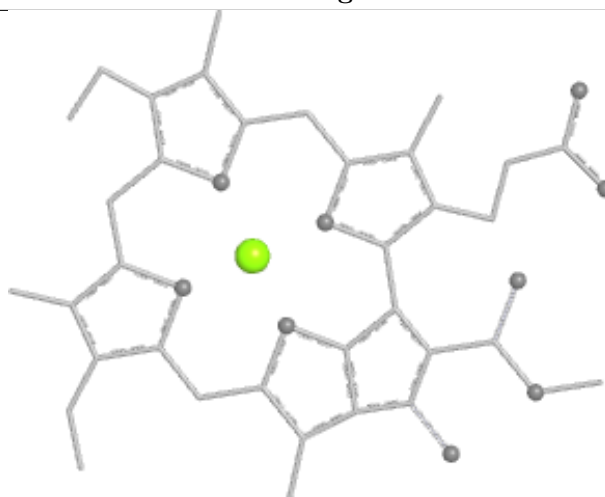
Bond lengths



Bond angles

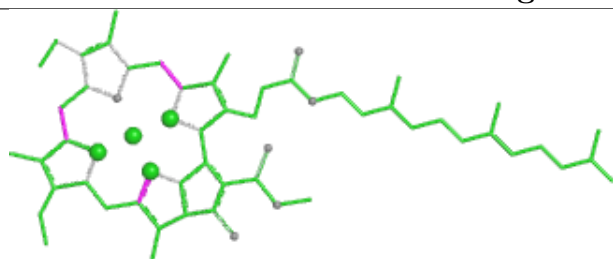


Torsions

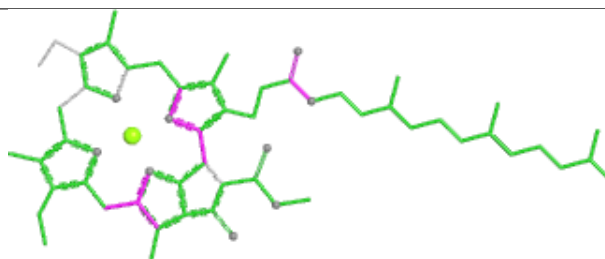


Rings

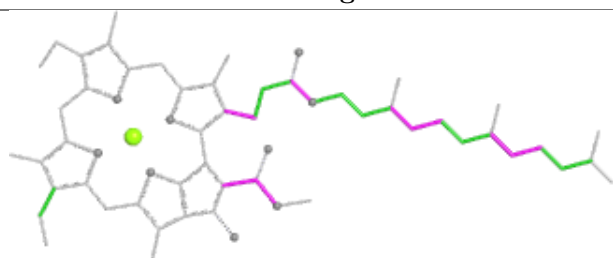
Ligand CLA h 504



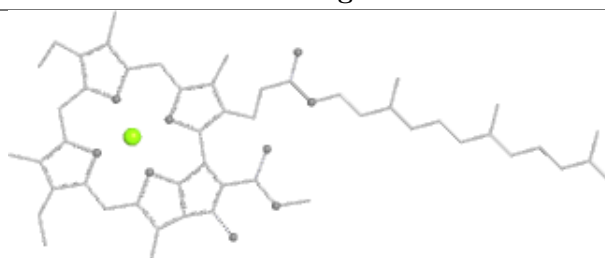
Bond lengths



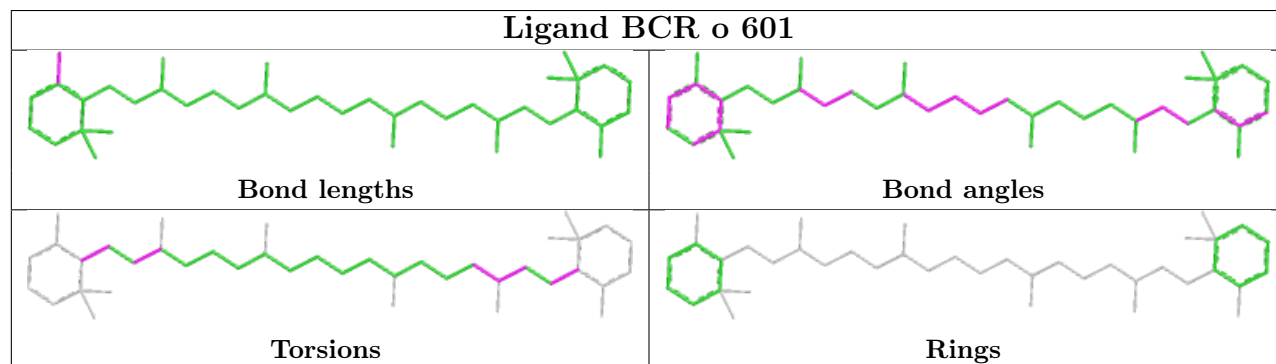
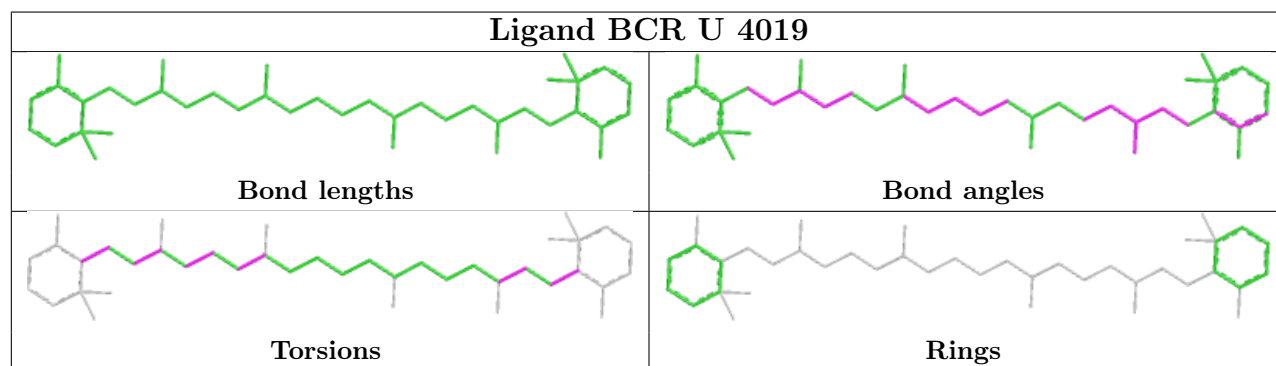
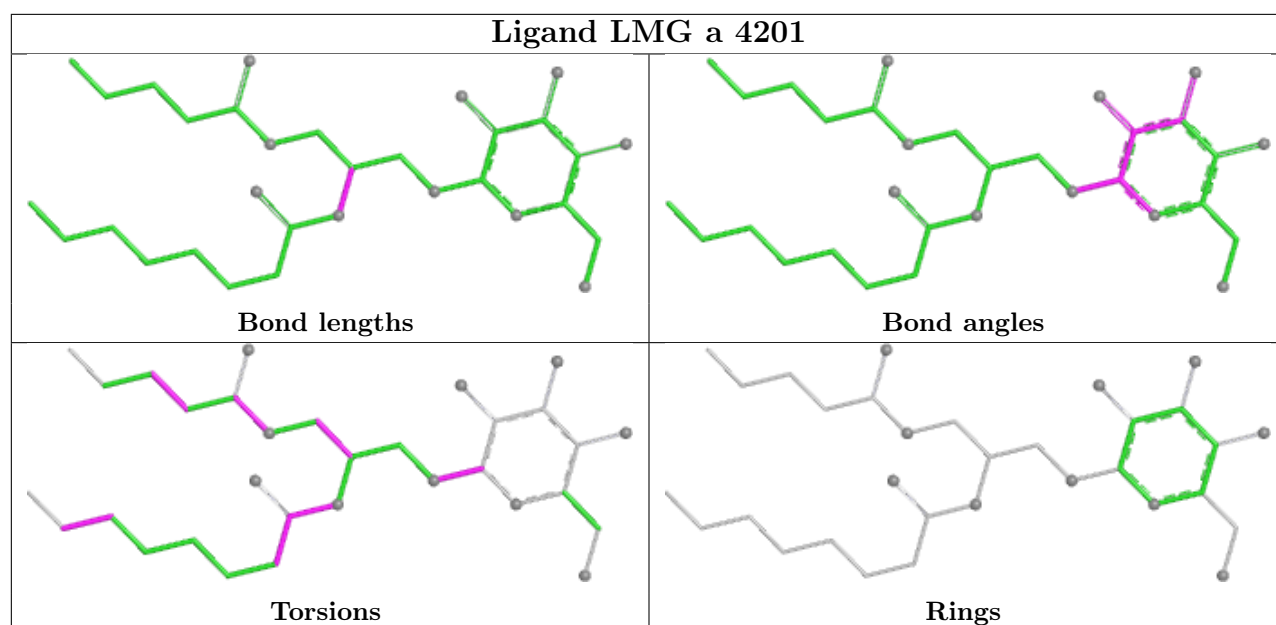
Bond angles

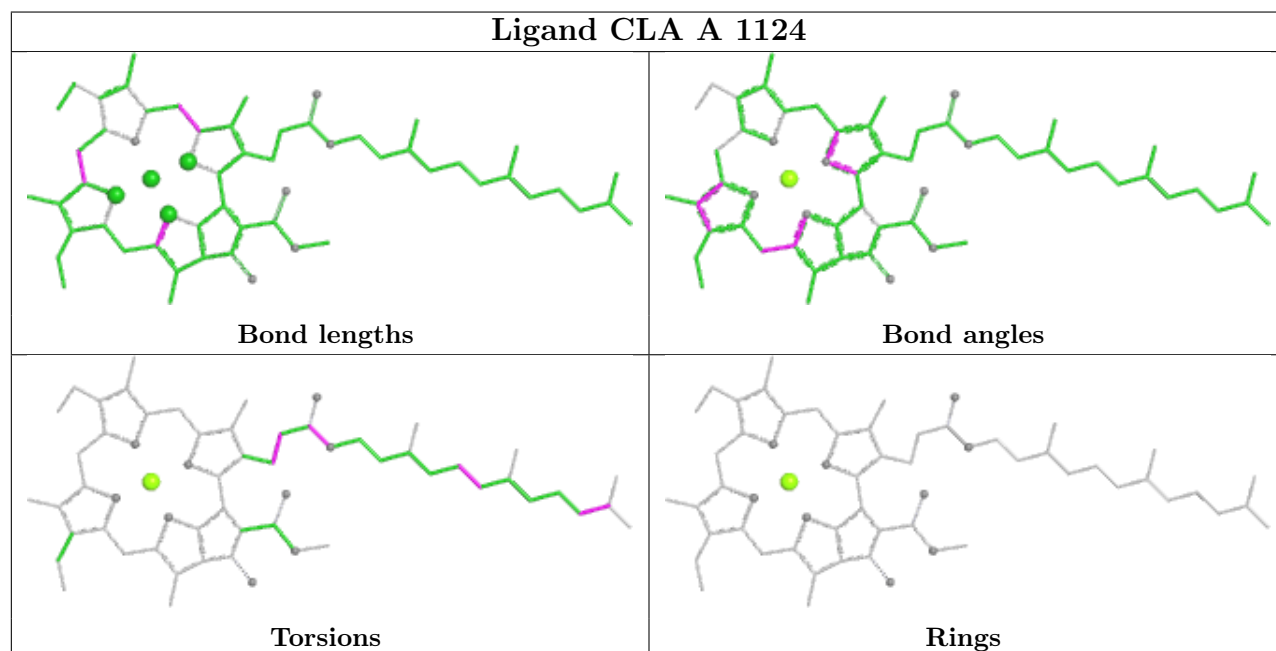
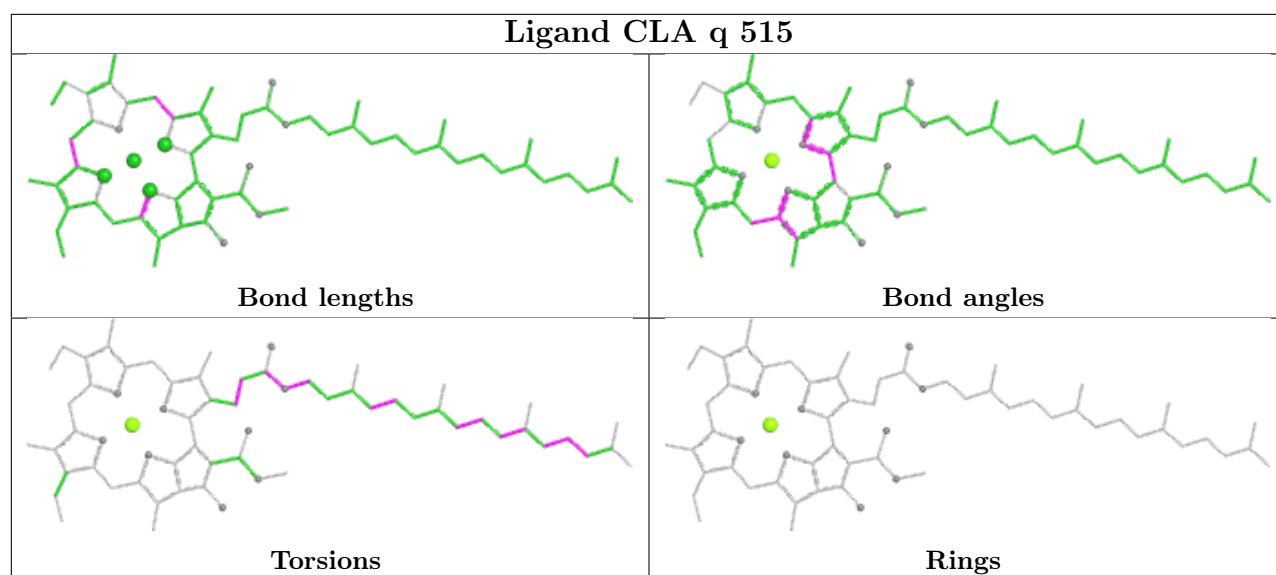


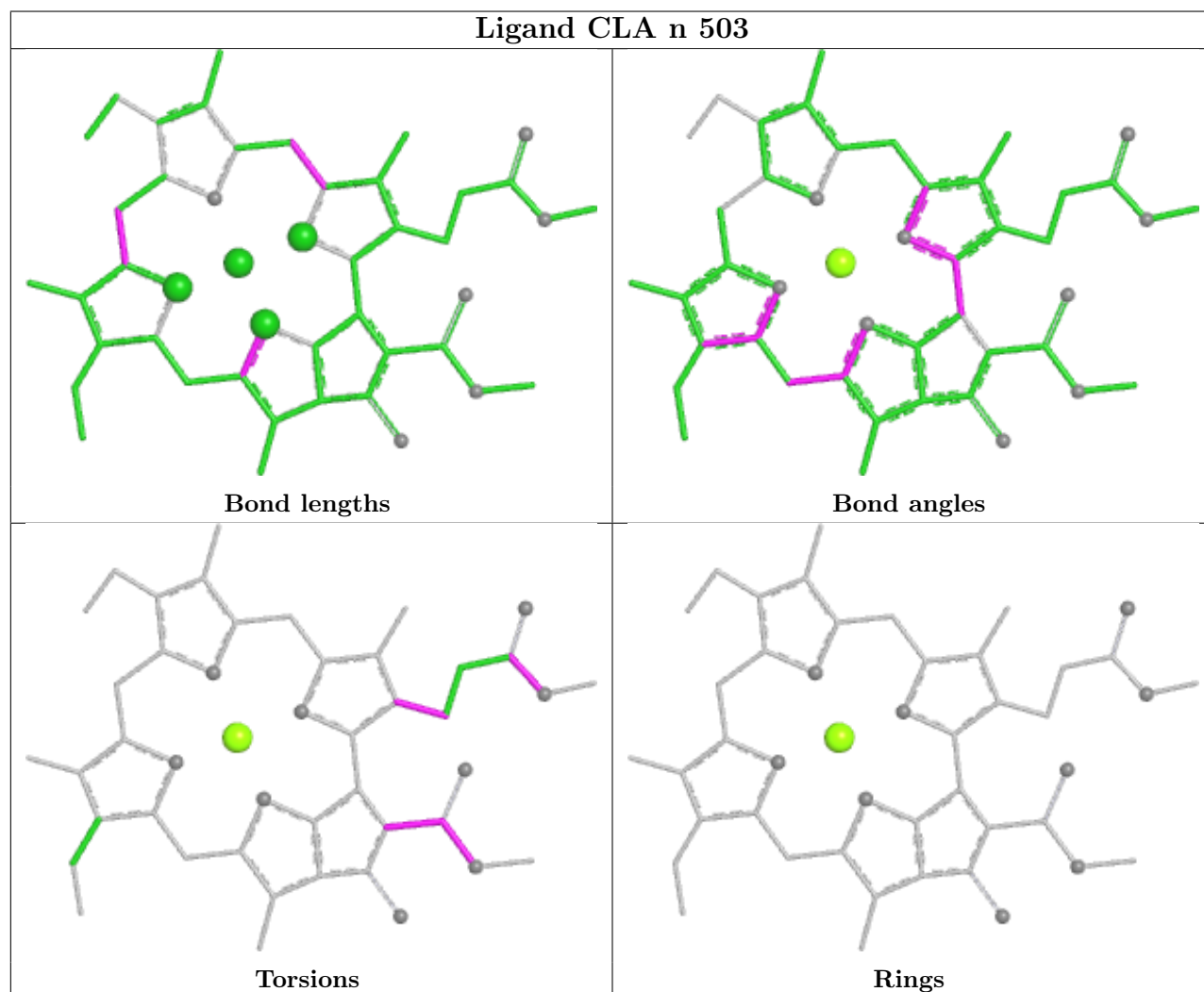
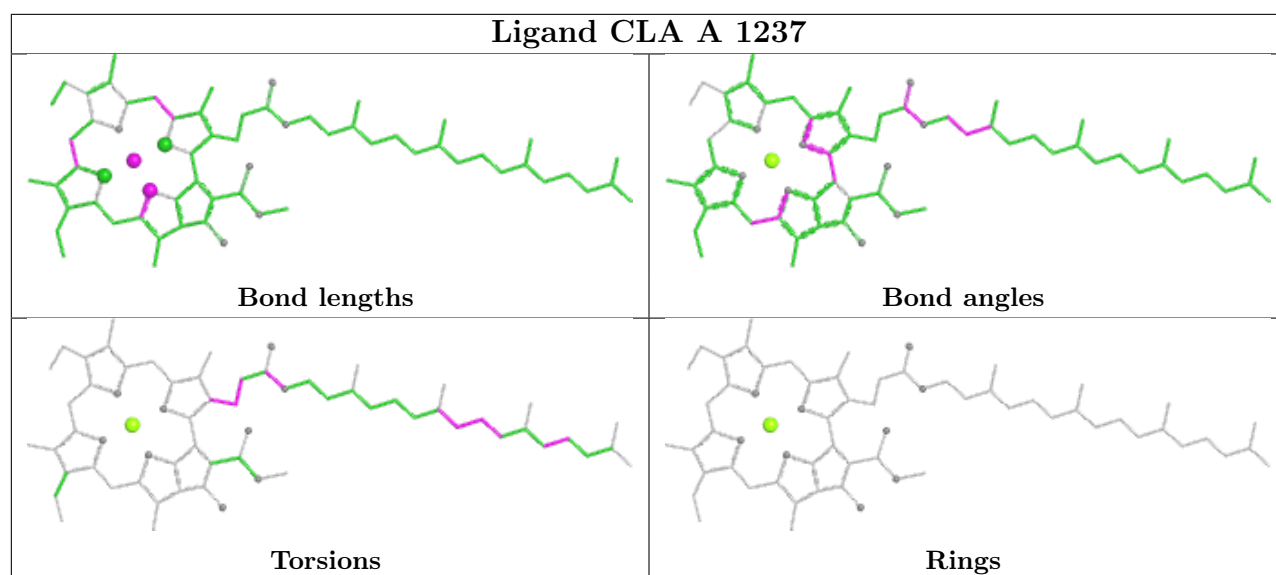
Torsions

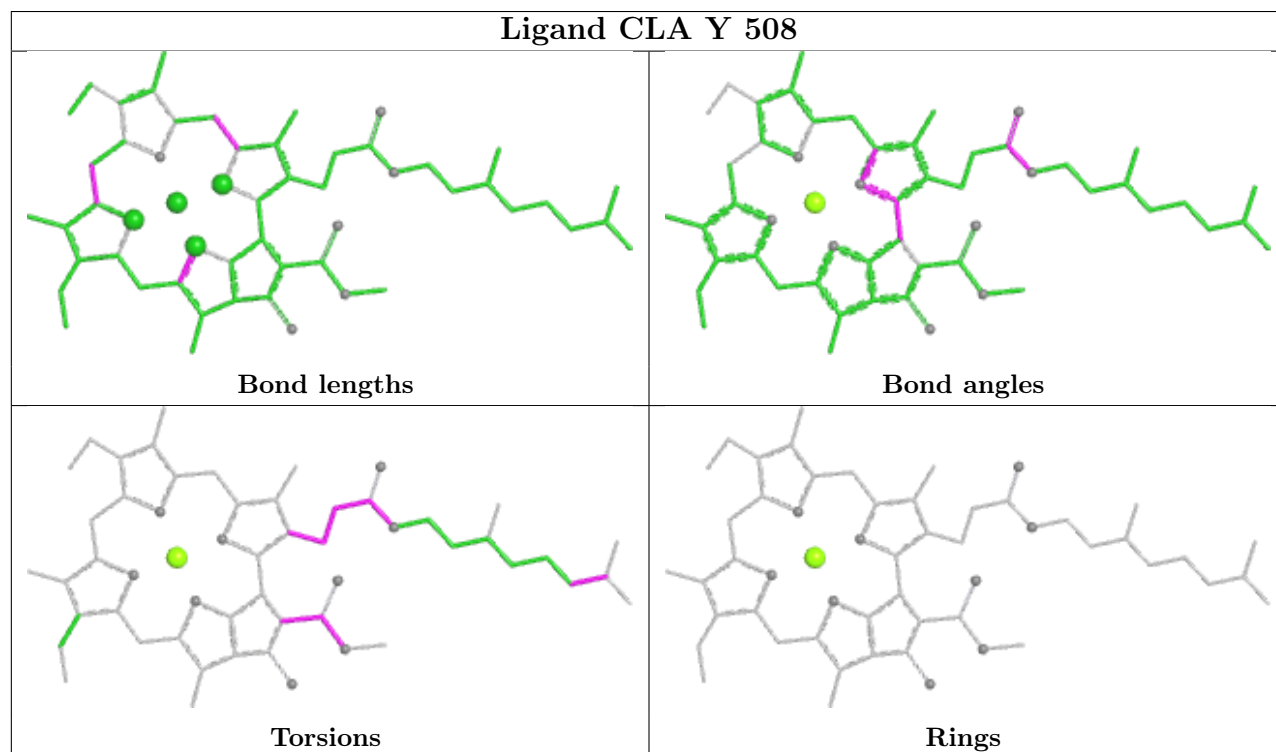
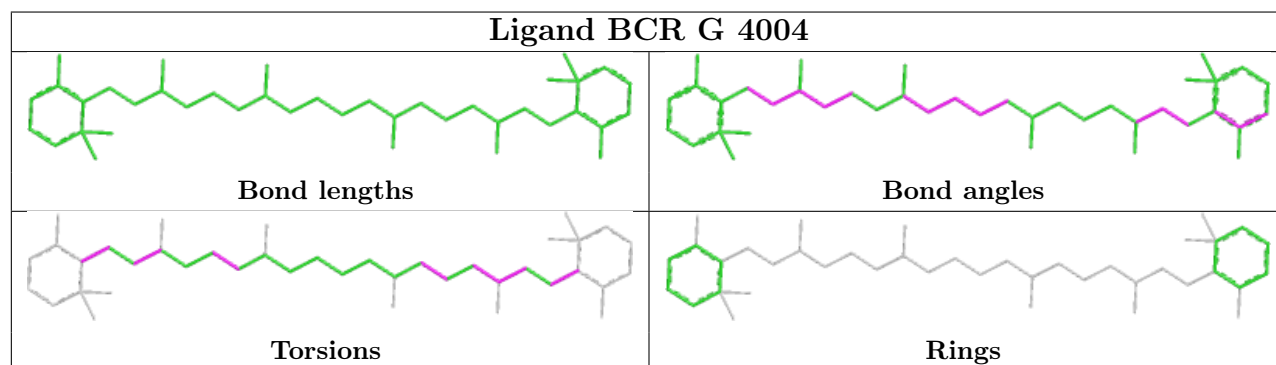
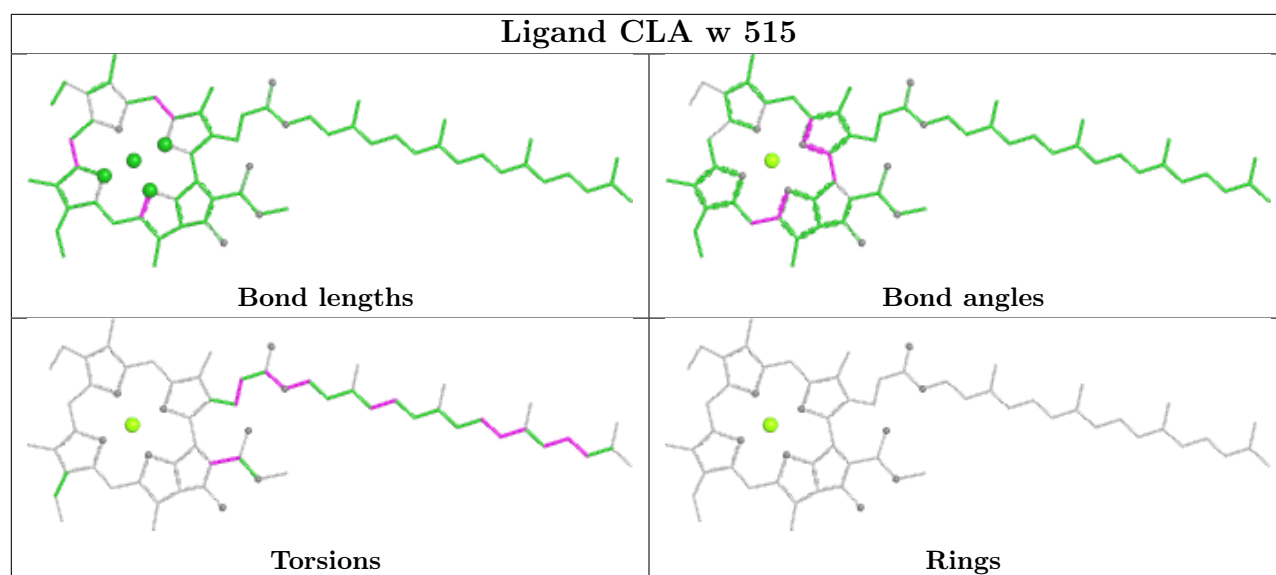


Rings

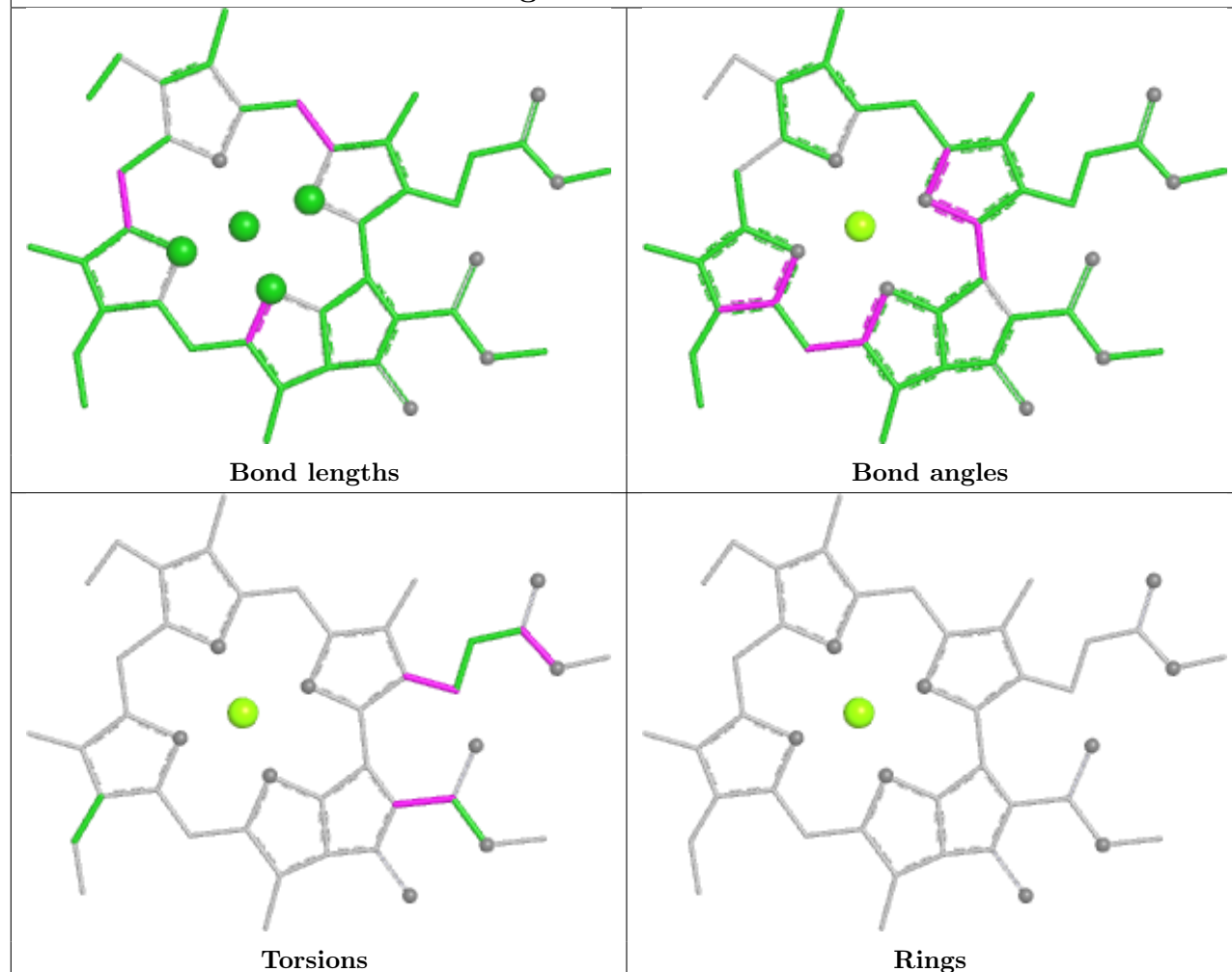




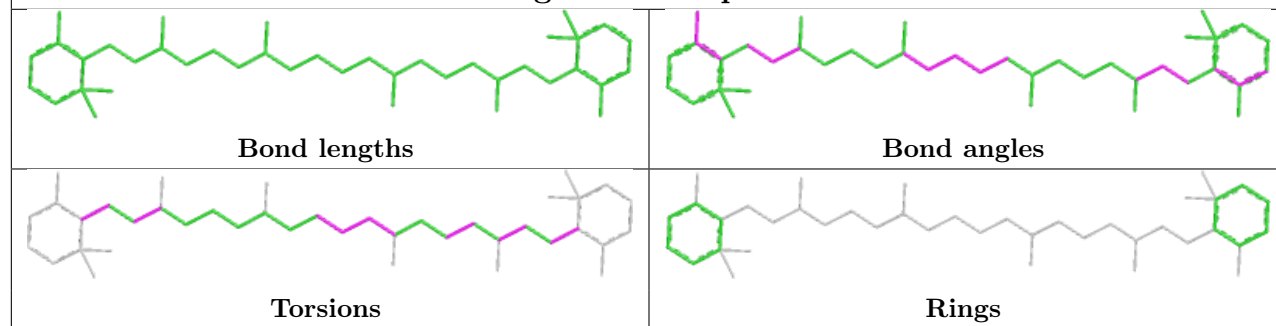


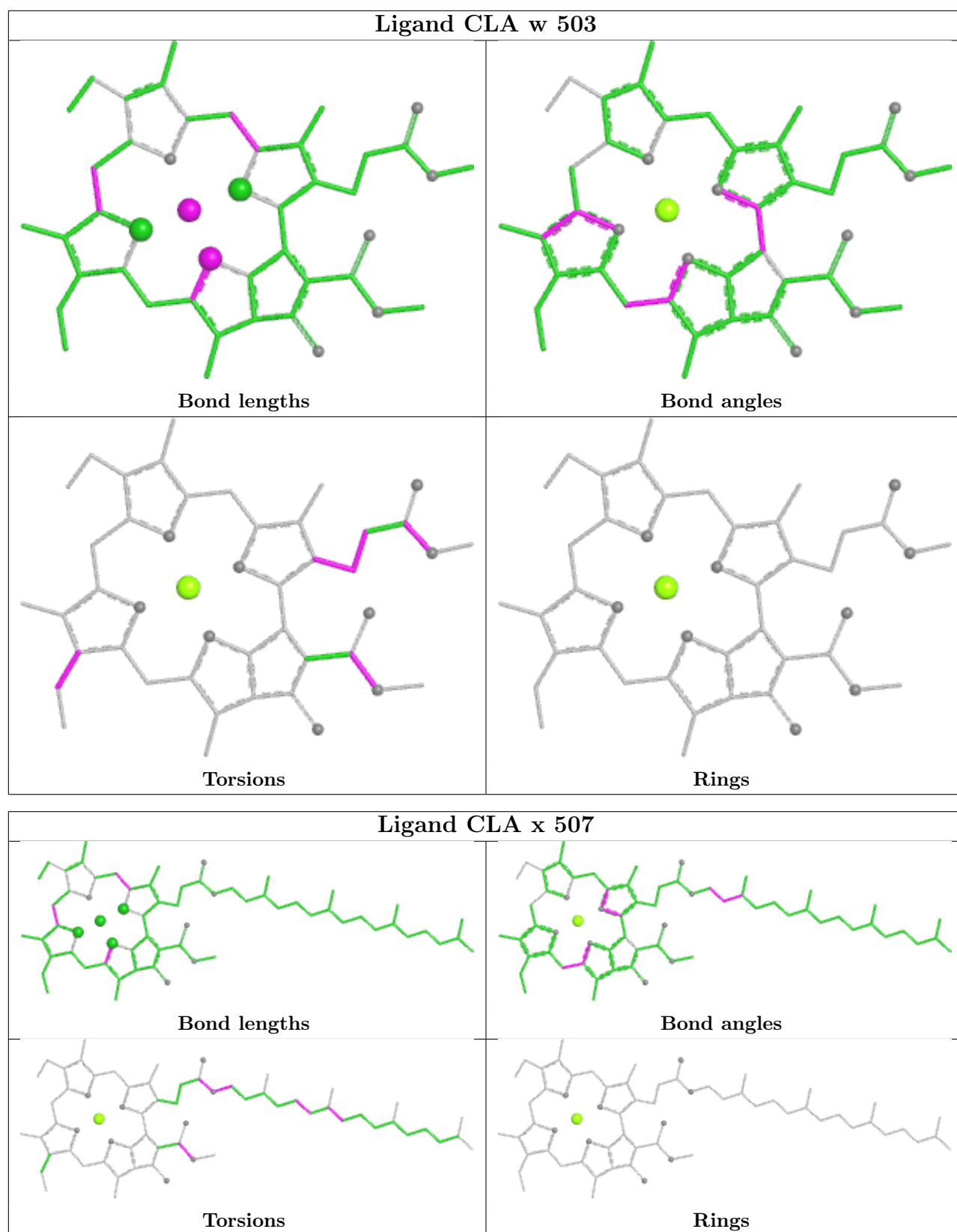


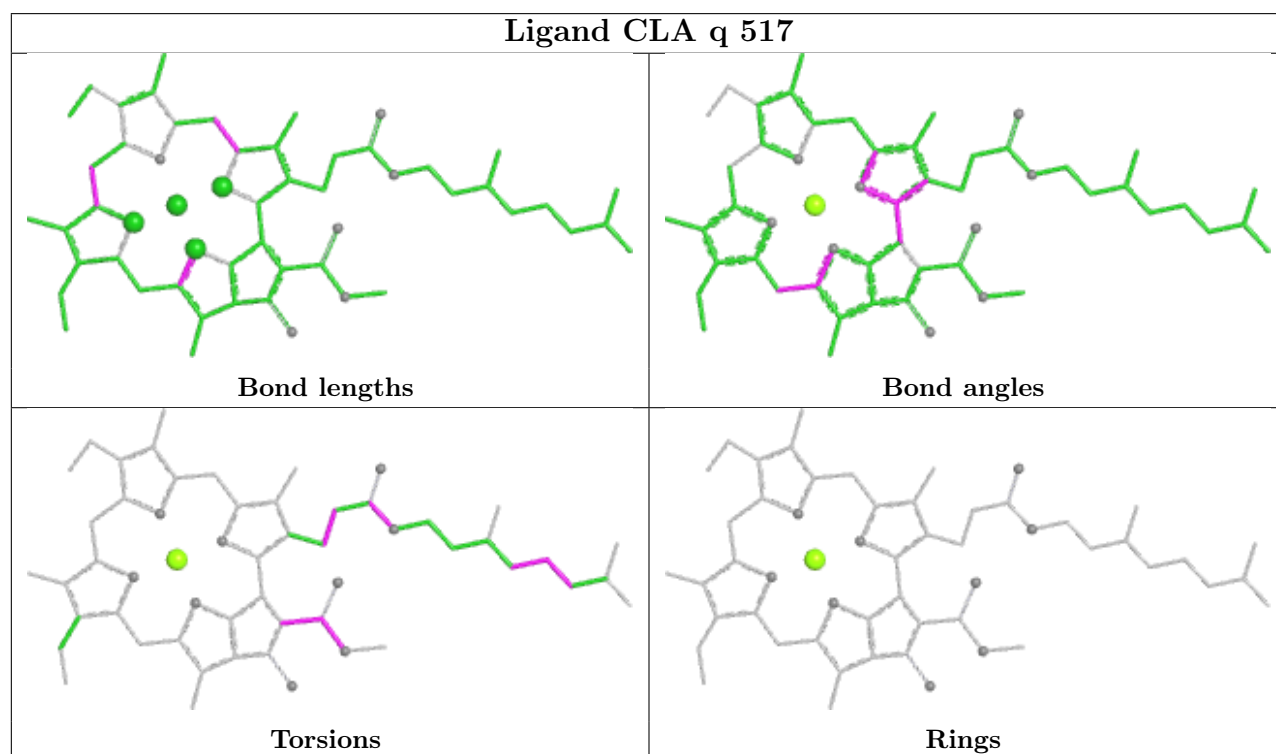
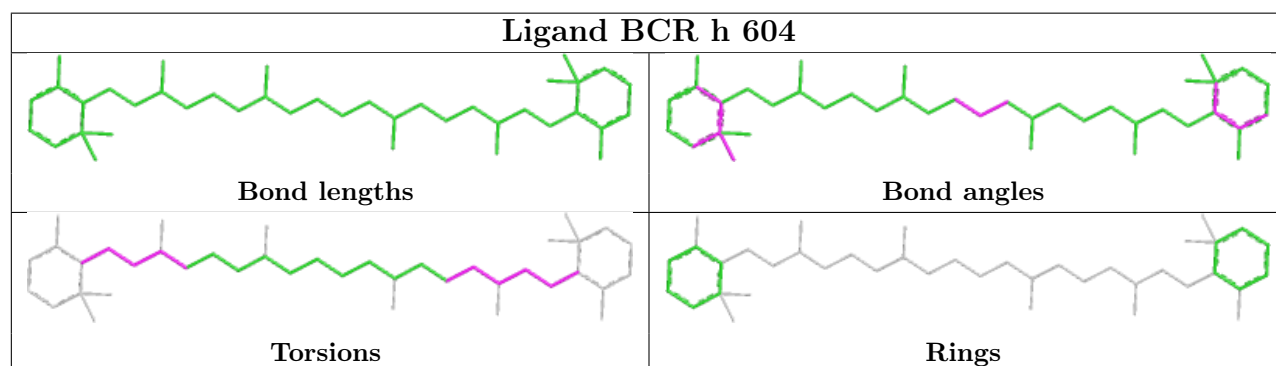
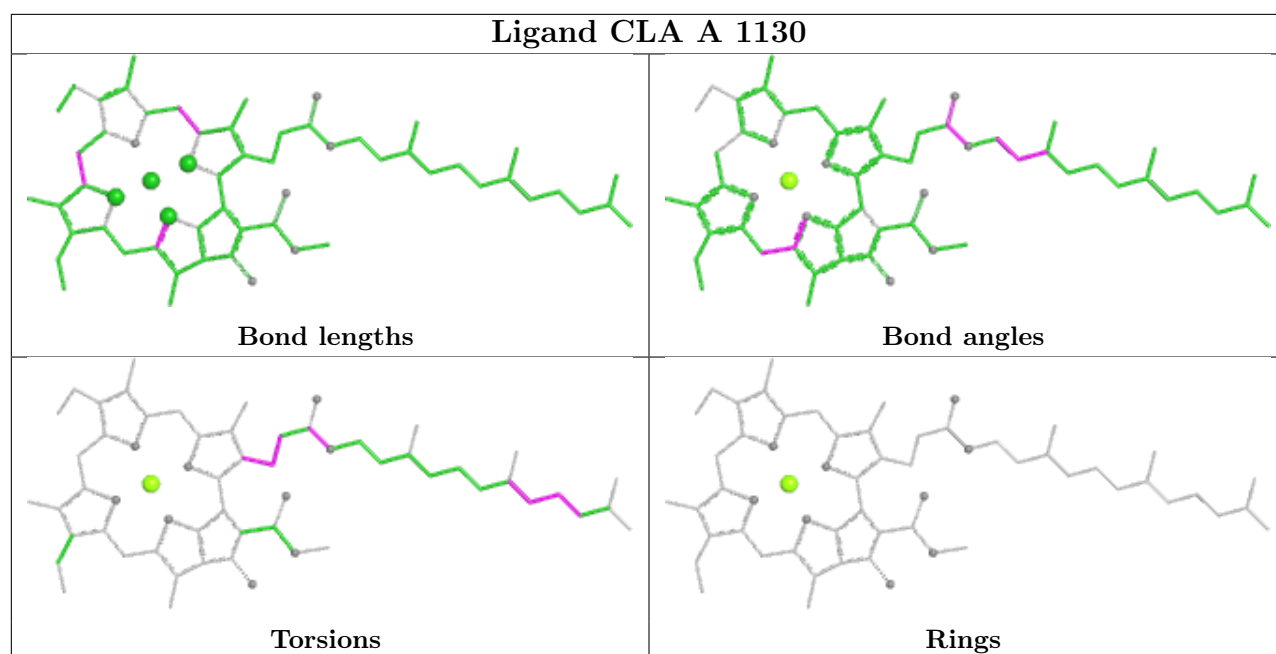
Ligand CLA t 503

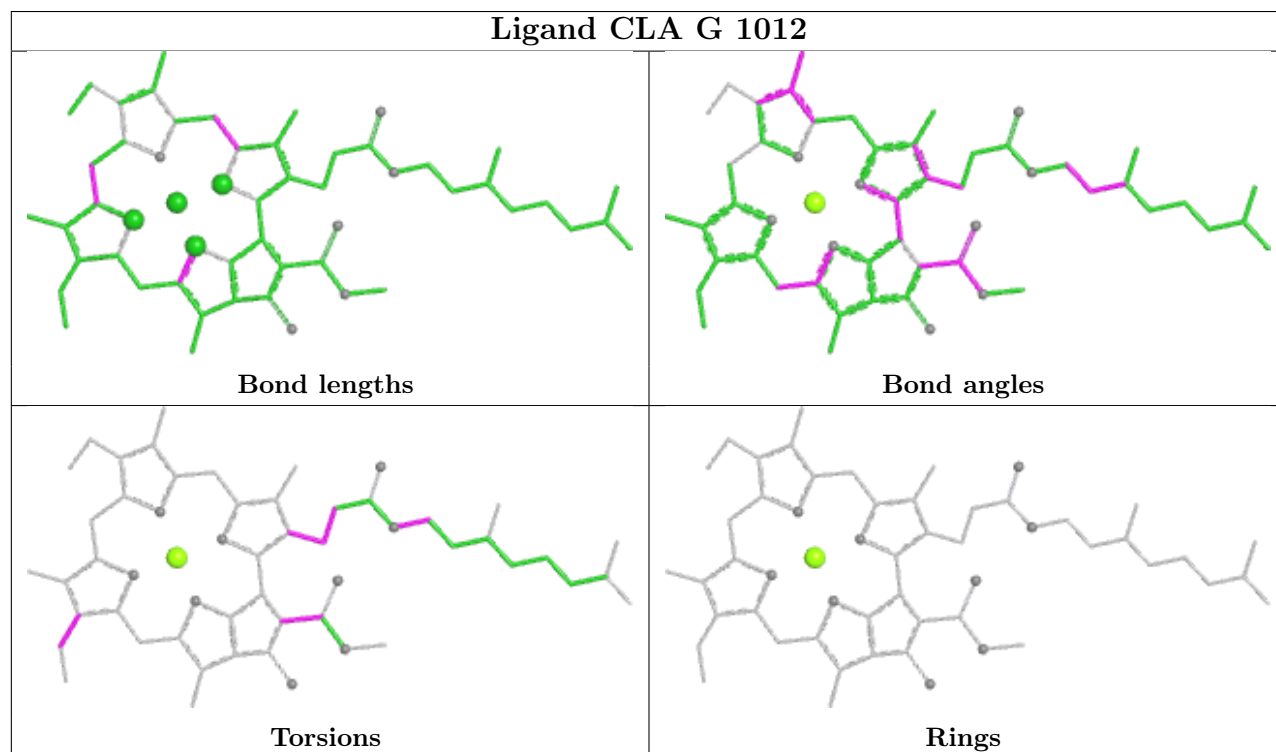
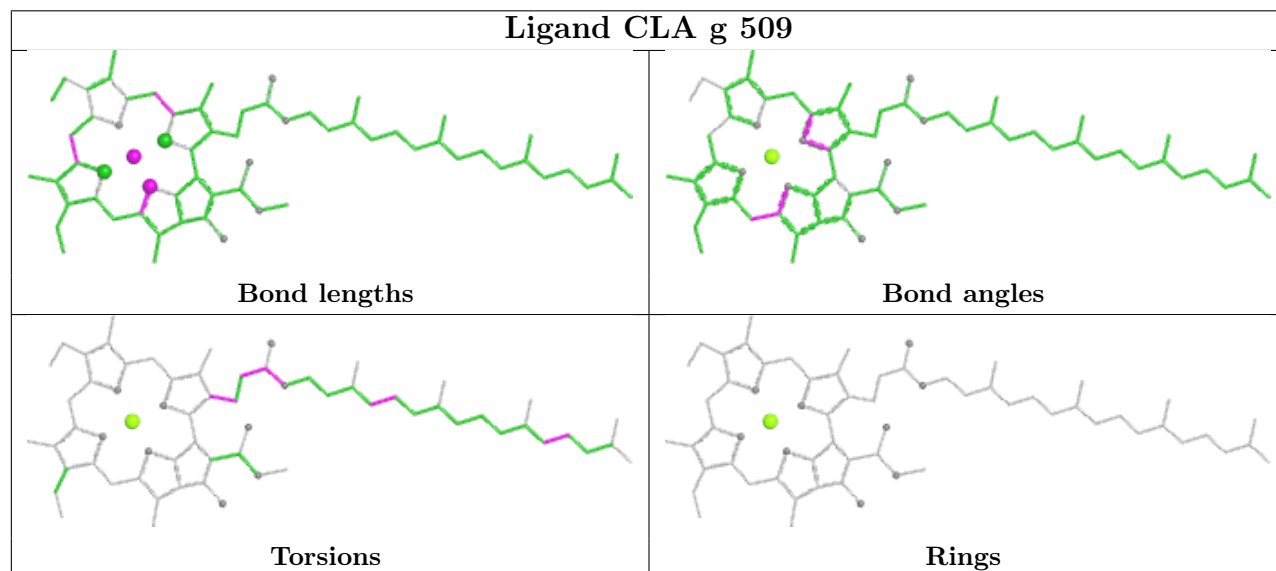
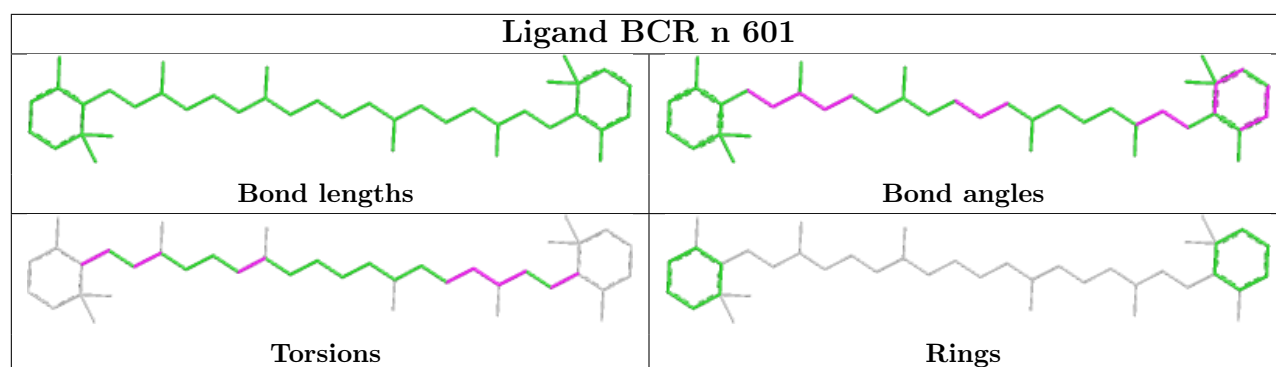


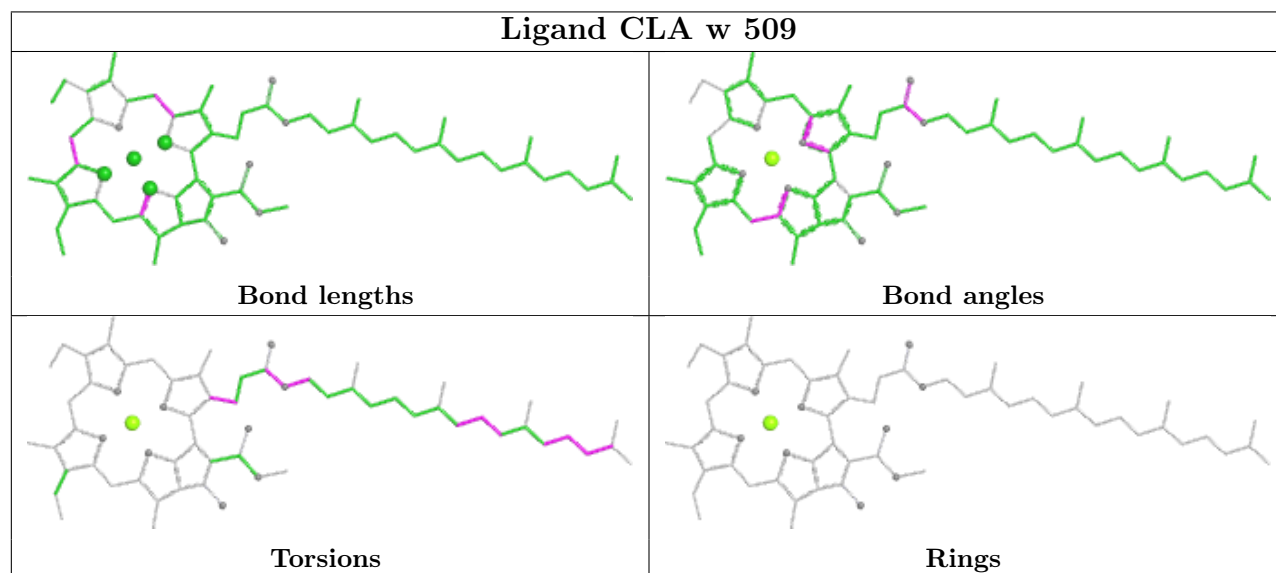
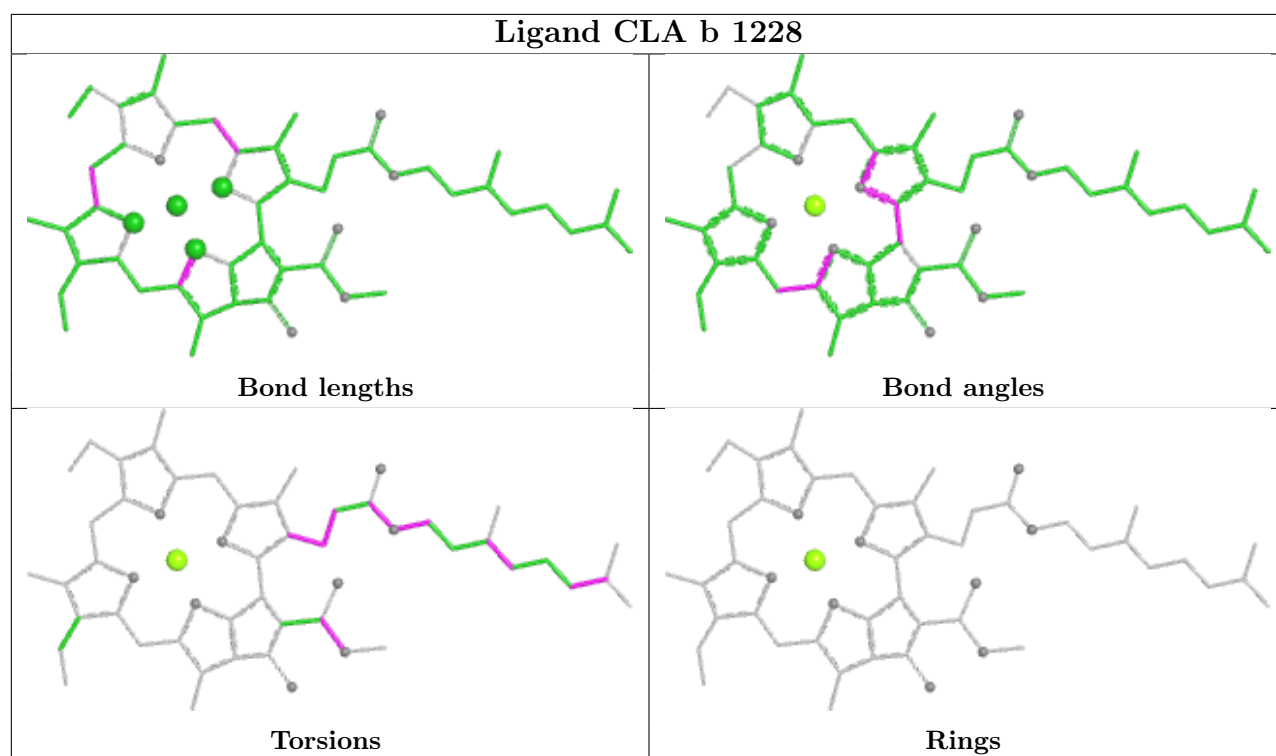
Ligand BCR q 602



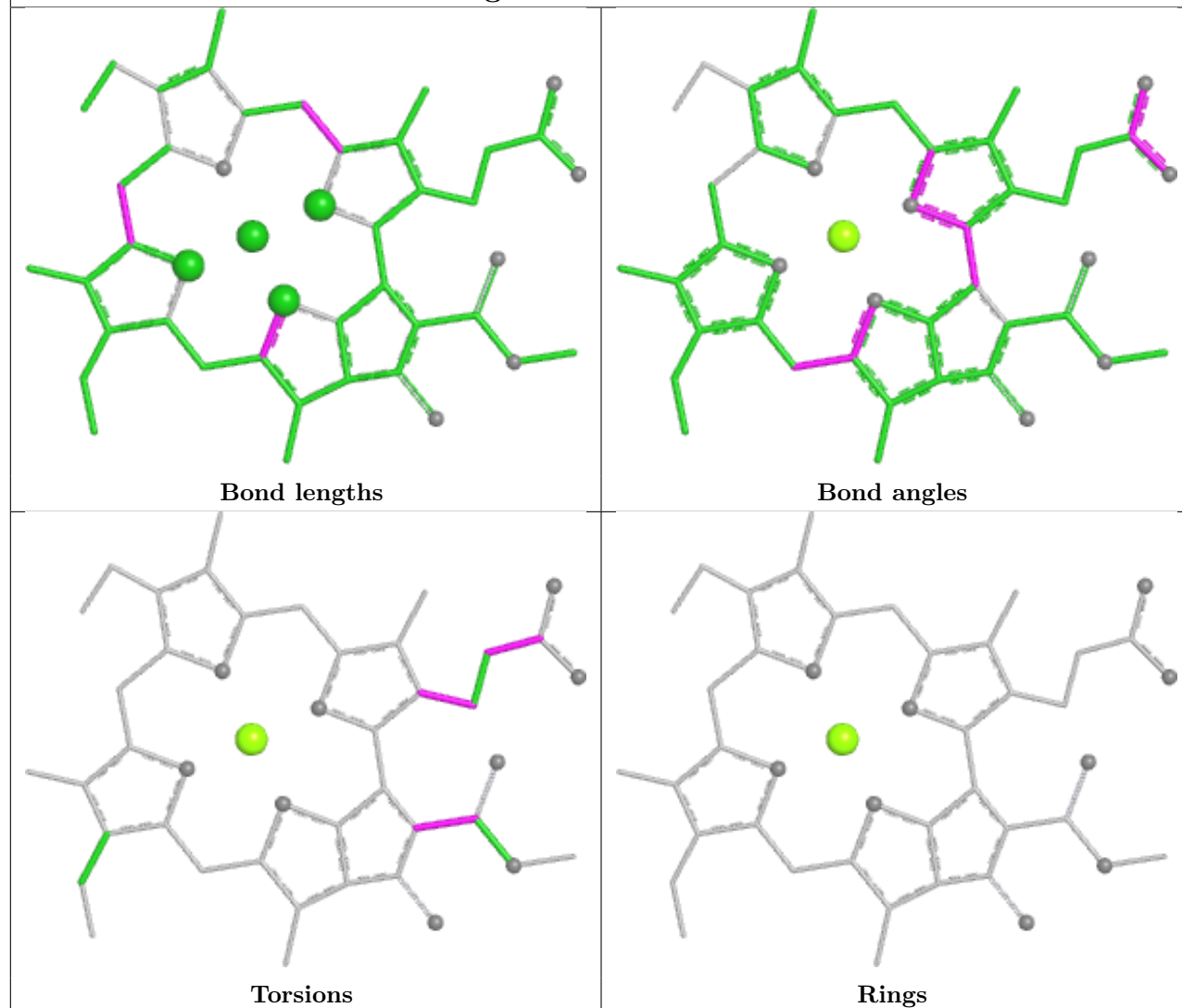




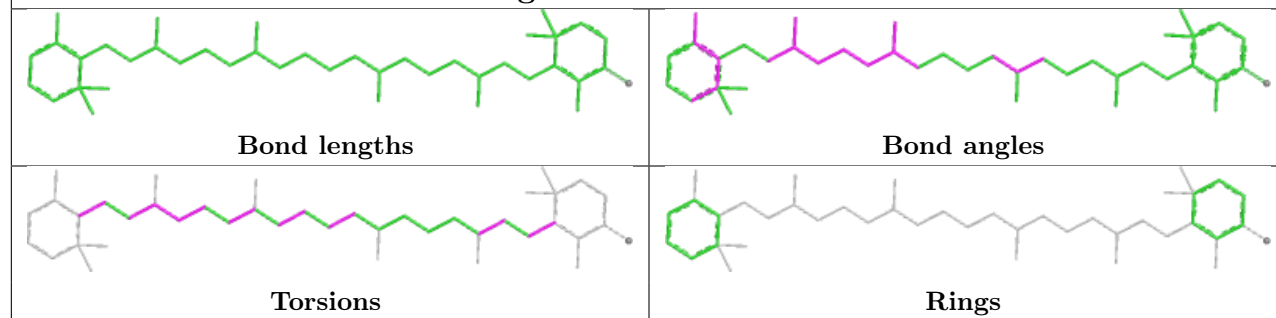


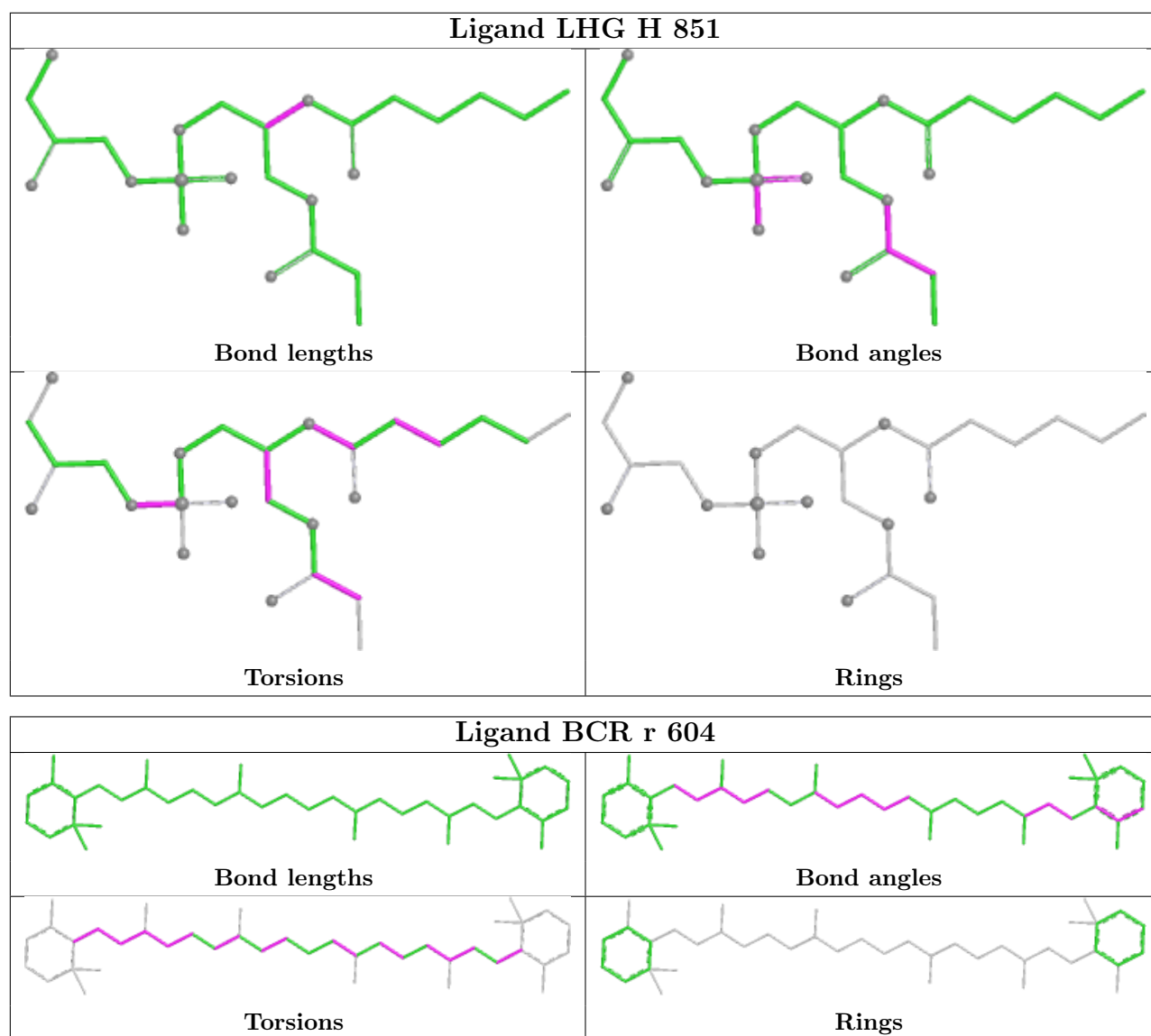


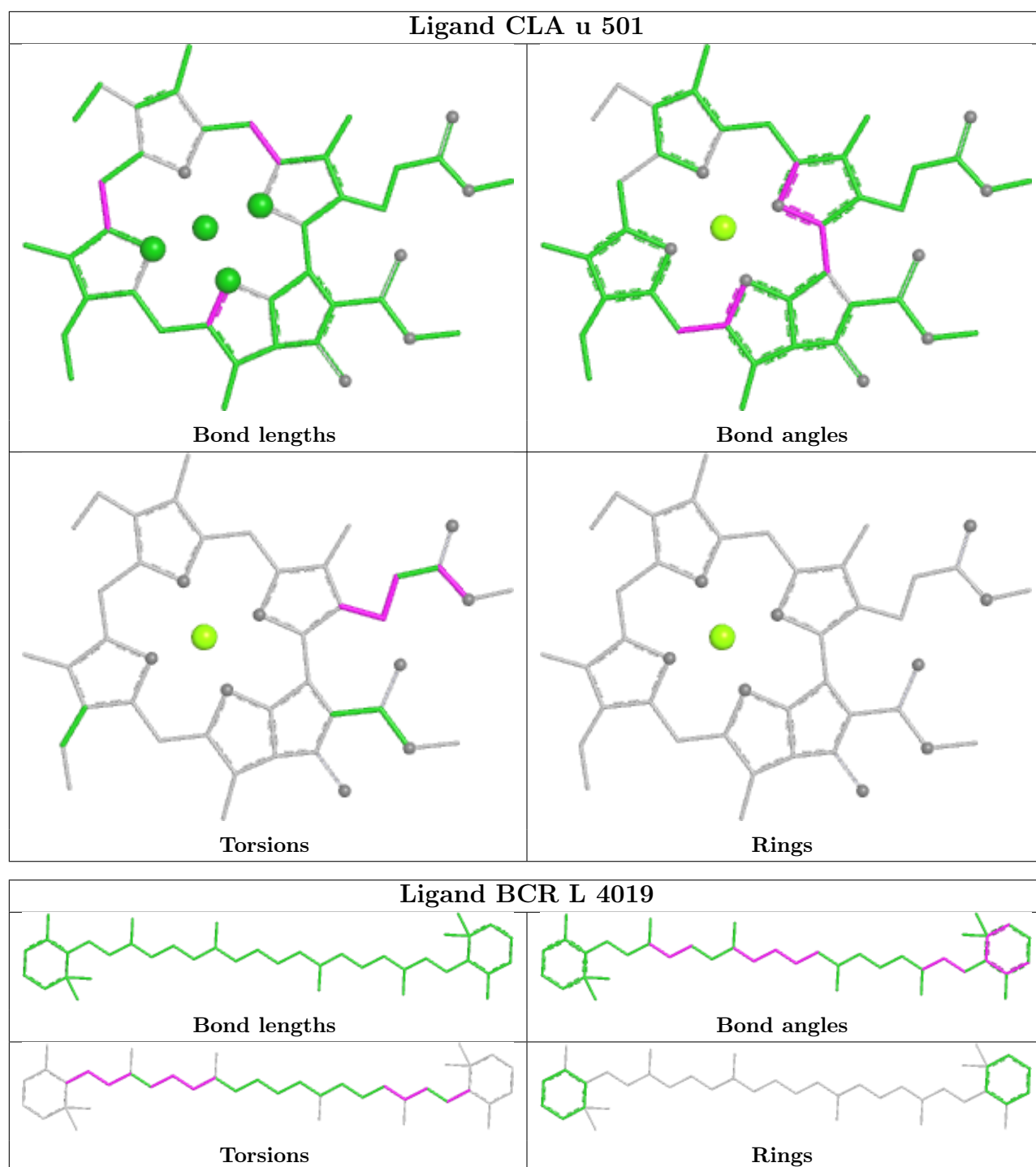
Ligand CLA B 1212



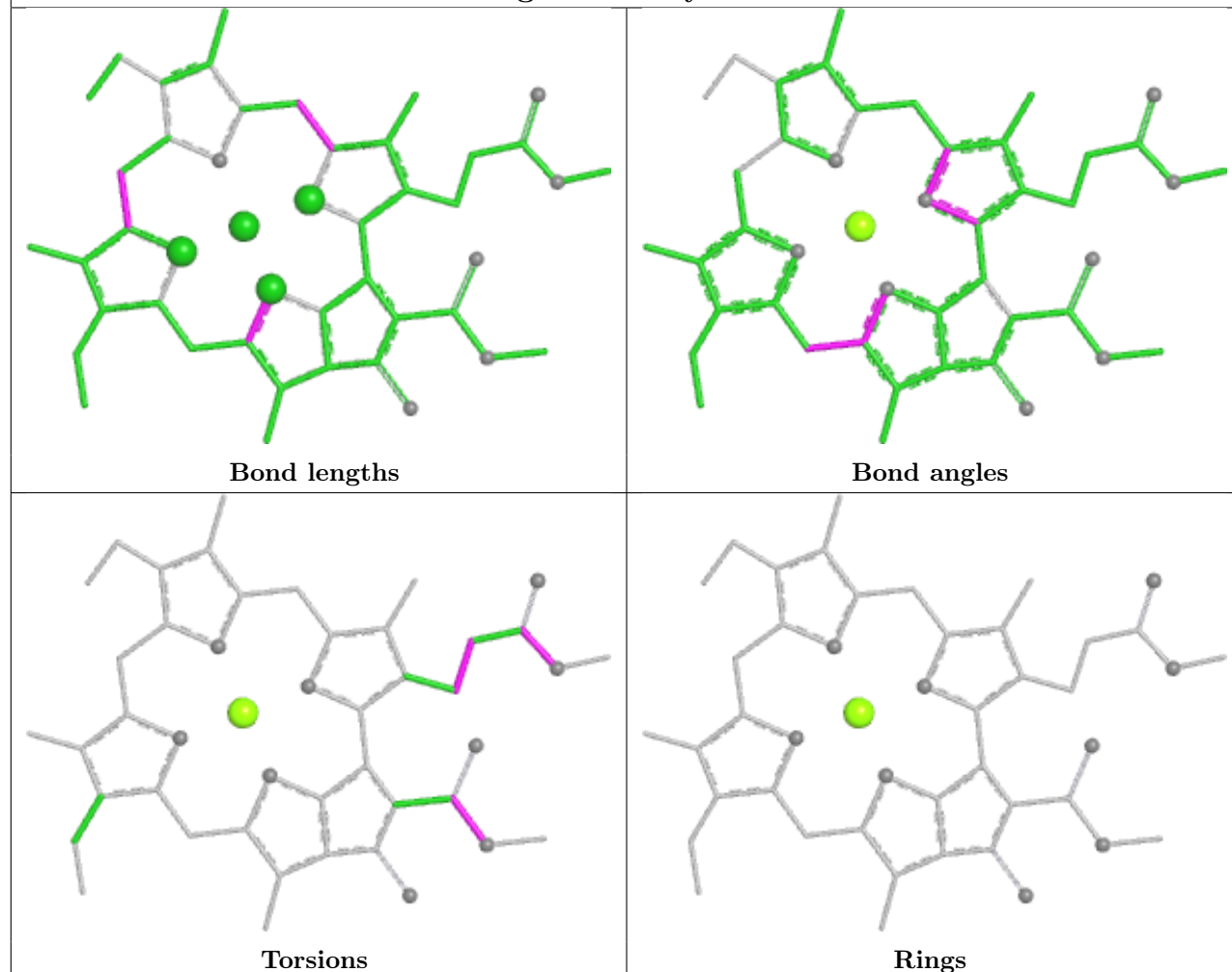
Ligand ECH M 4021



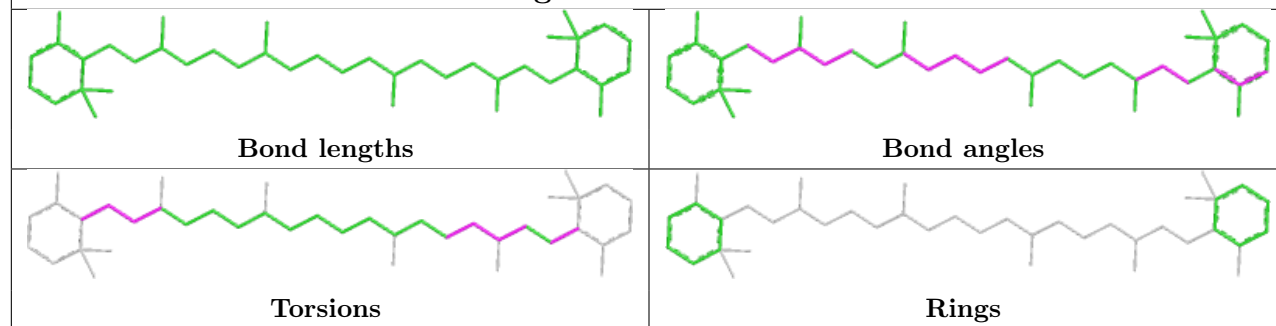




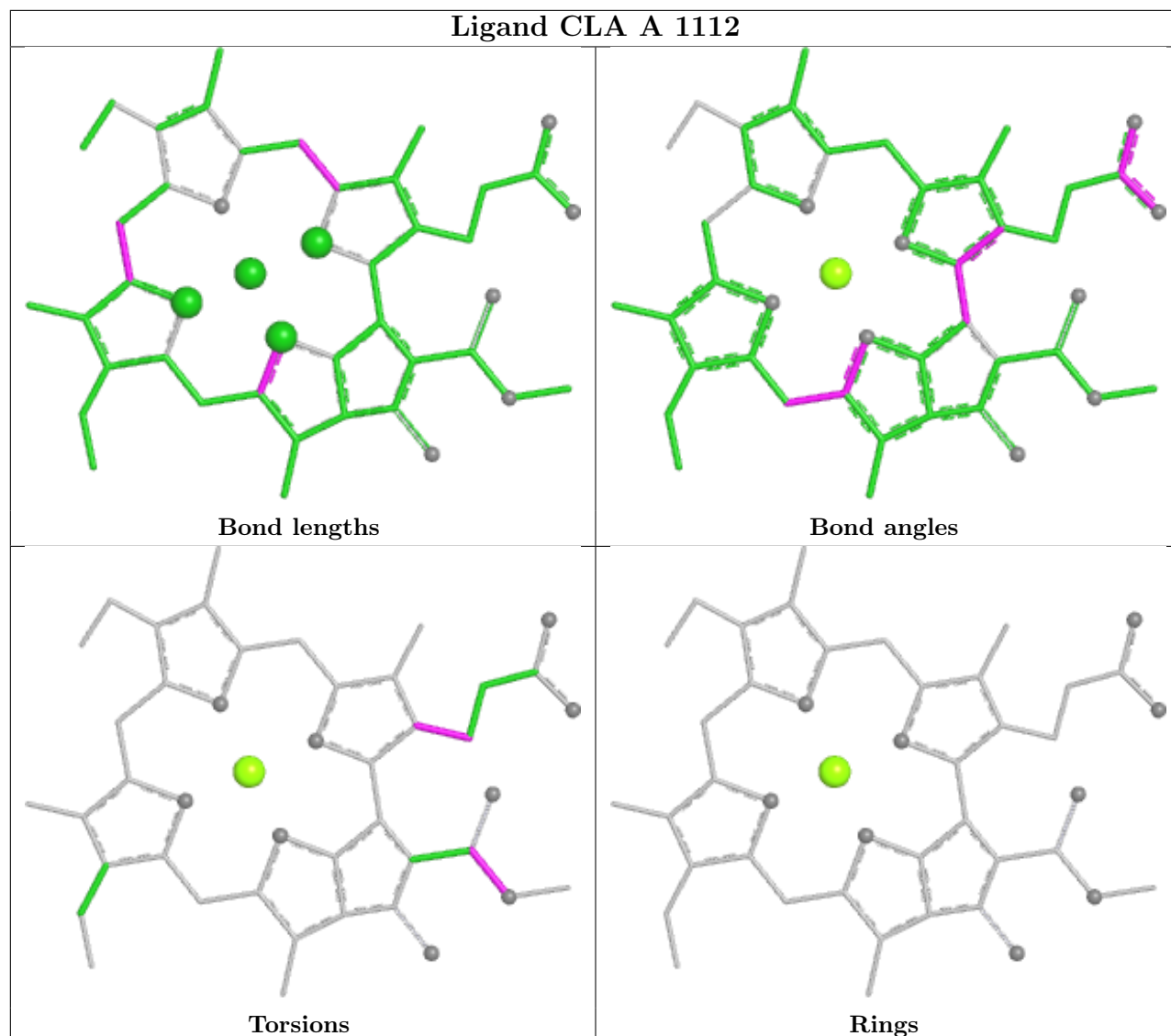
Ligand CLA y 513



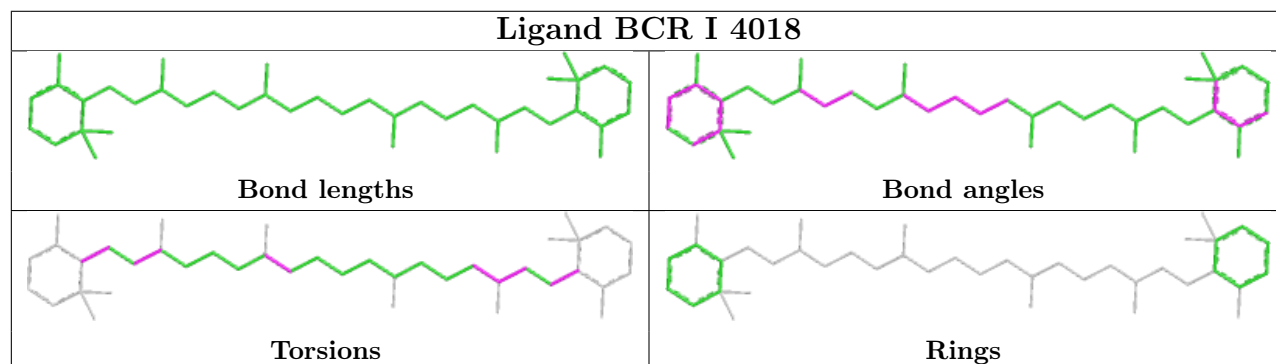
Ligand BCR x 601



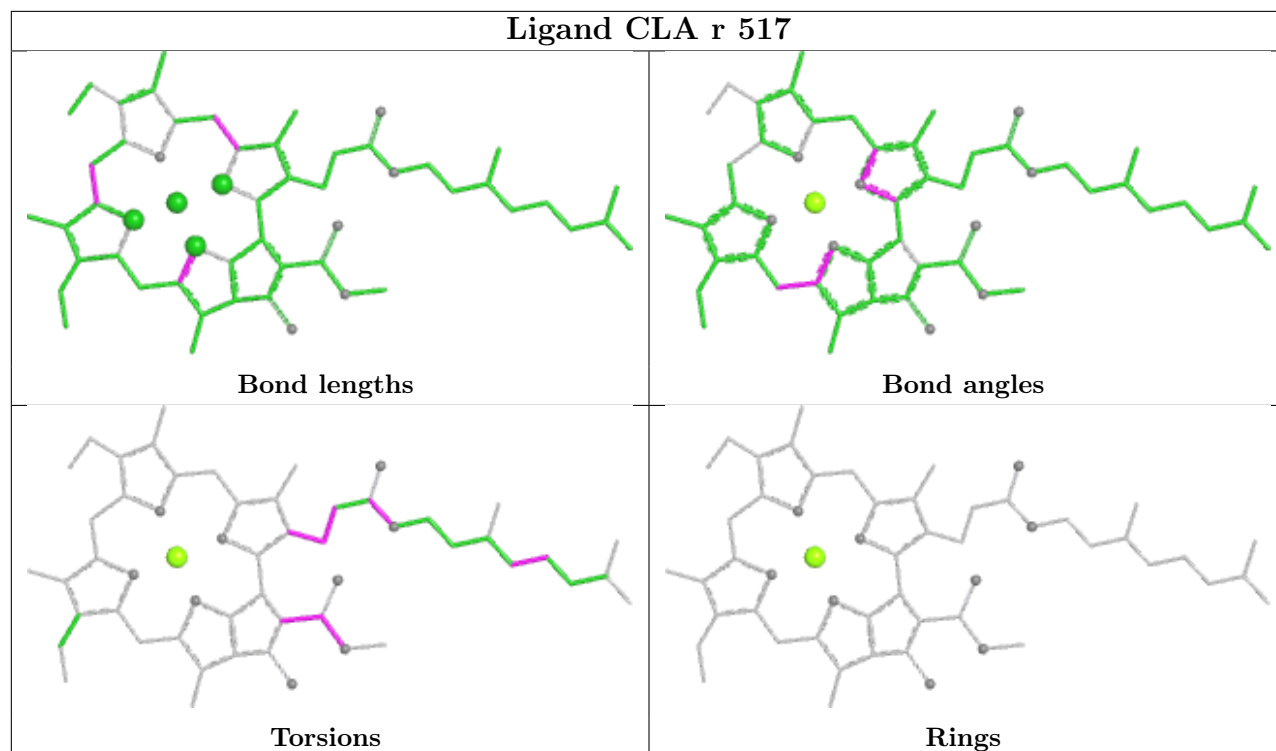
Ligand CLA A 1112



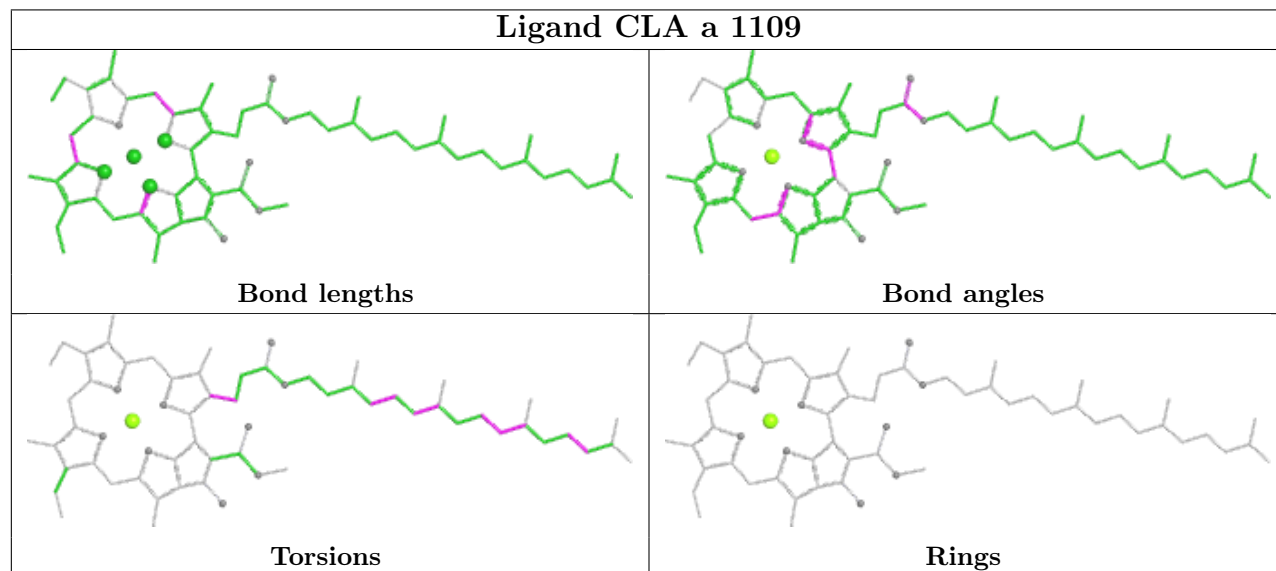
Ligand BCR I 4018

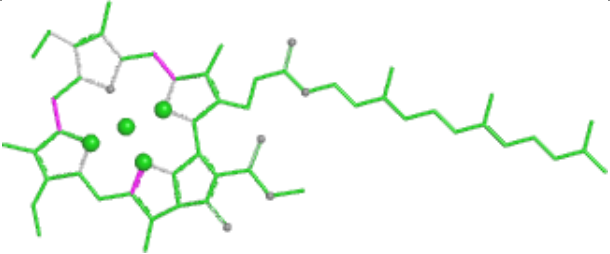
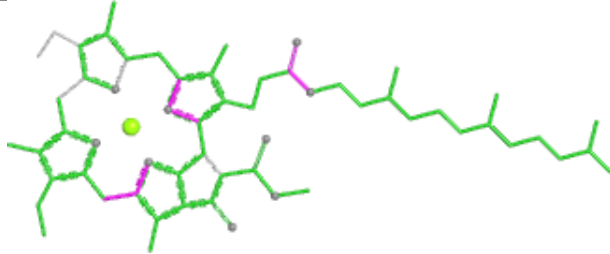
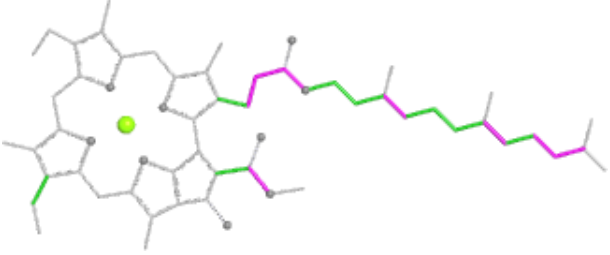
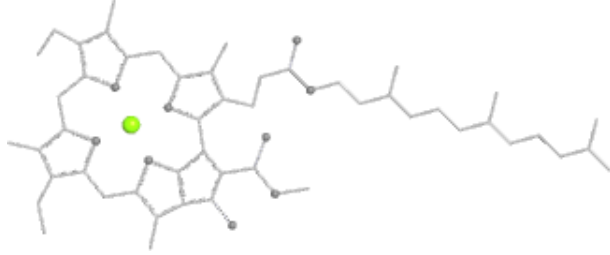
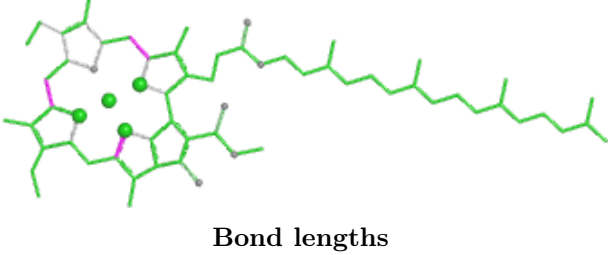
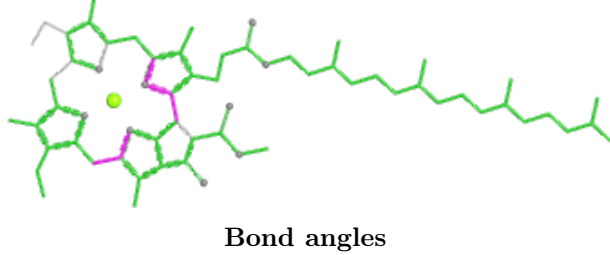
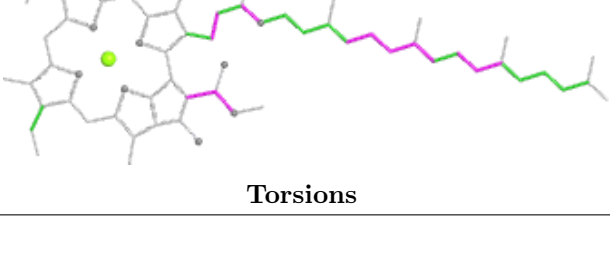
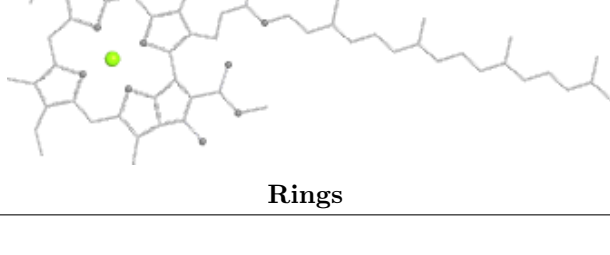


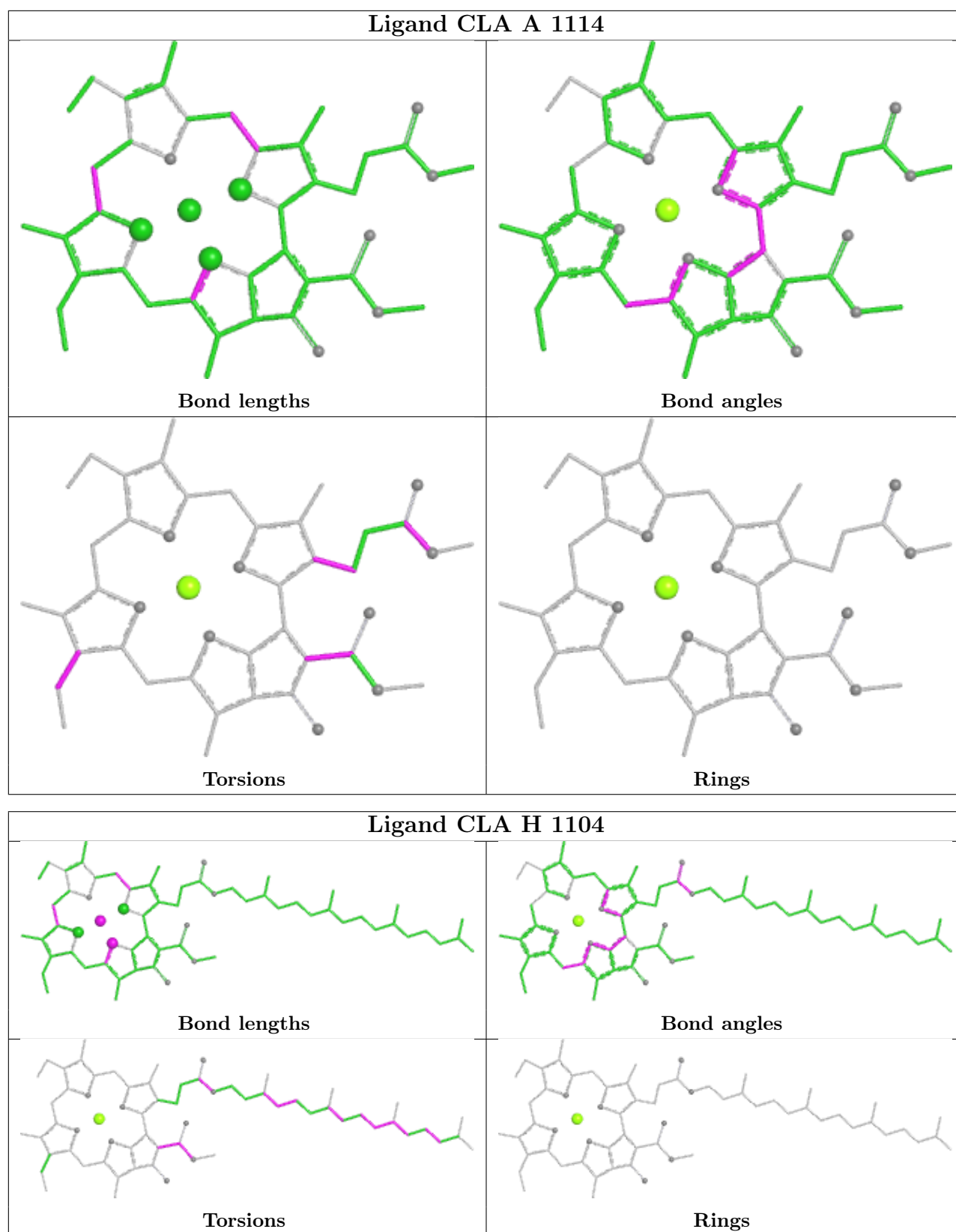
Ligand CLA r 517

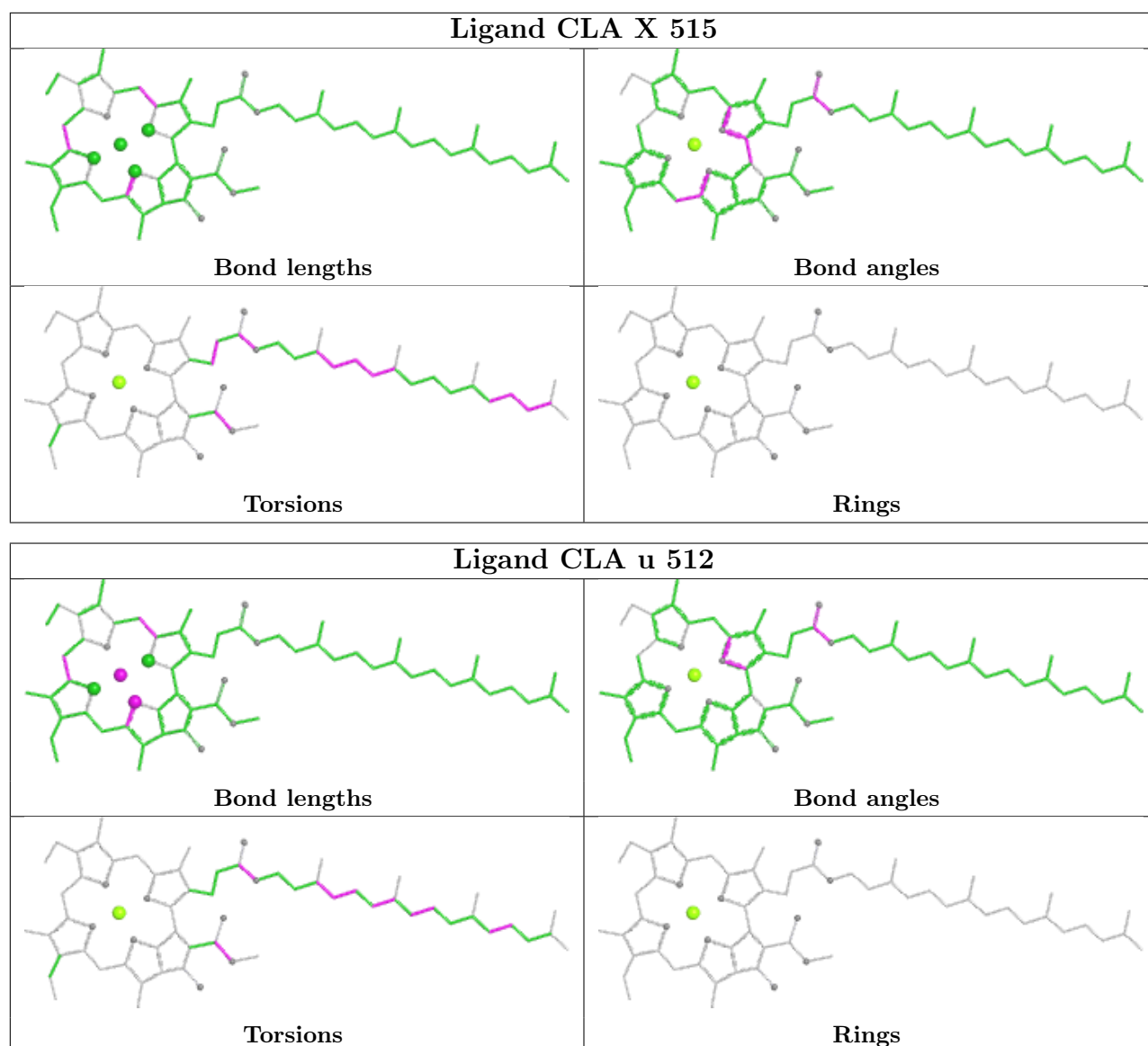


Ligand CLA a 1109

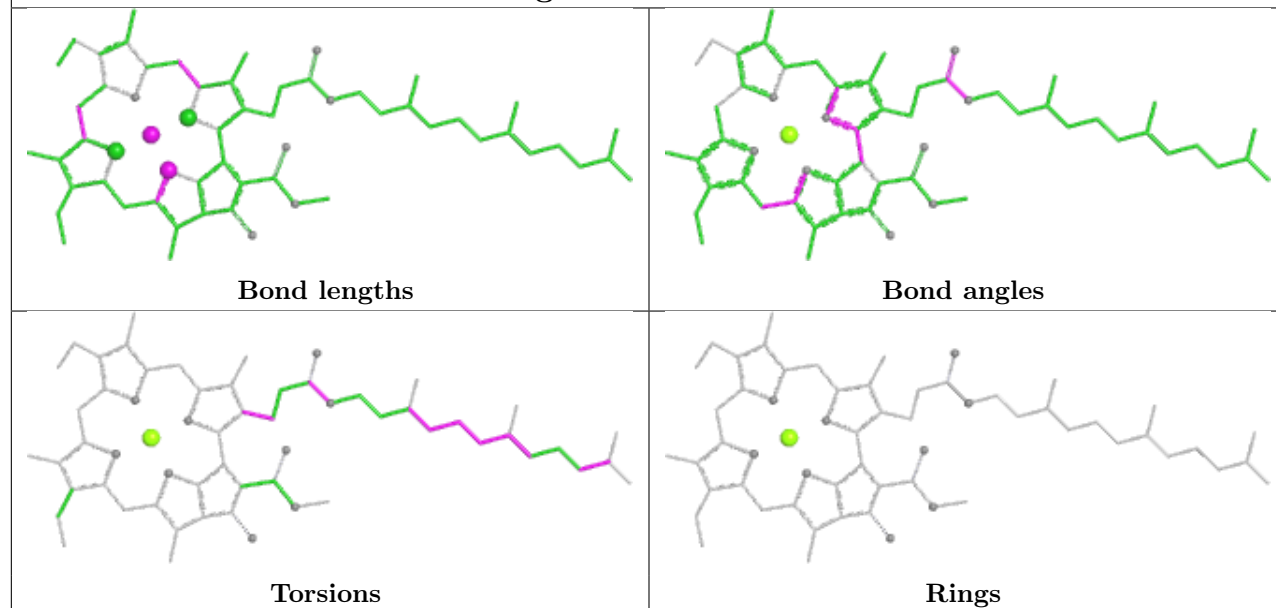


Ligand CLA I 1501	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA H 1106	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

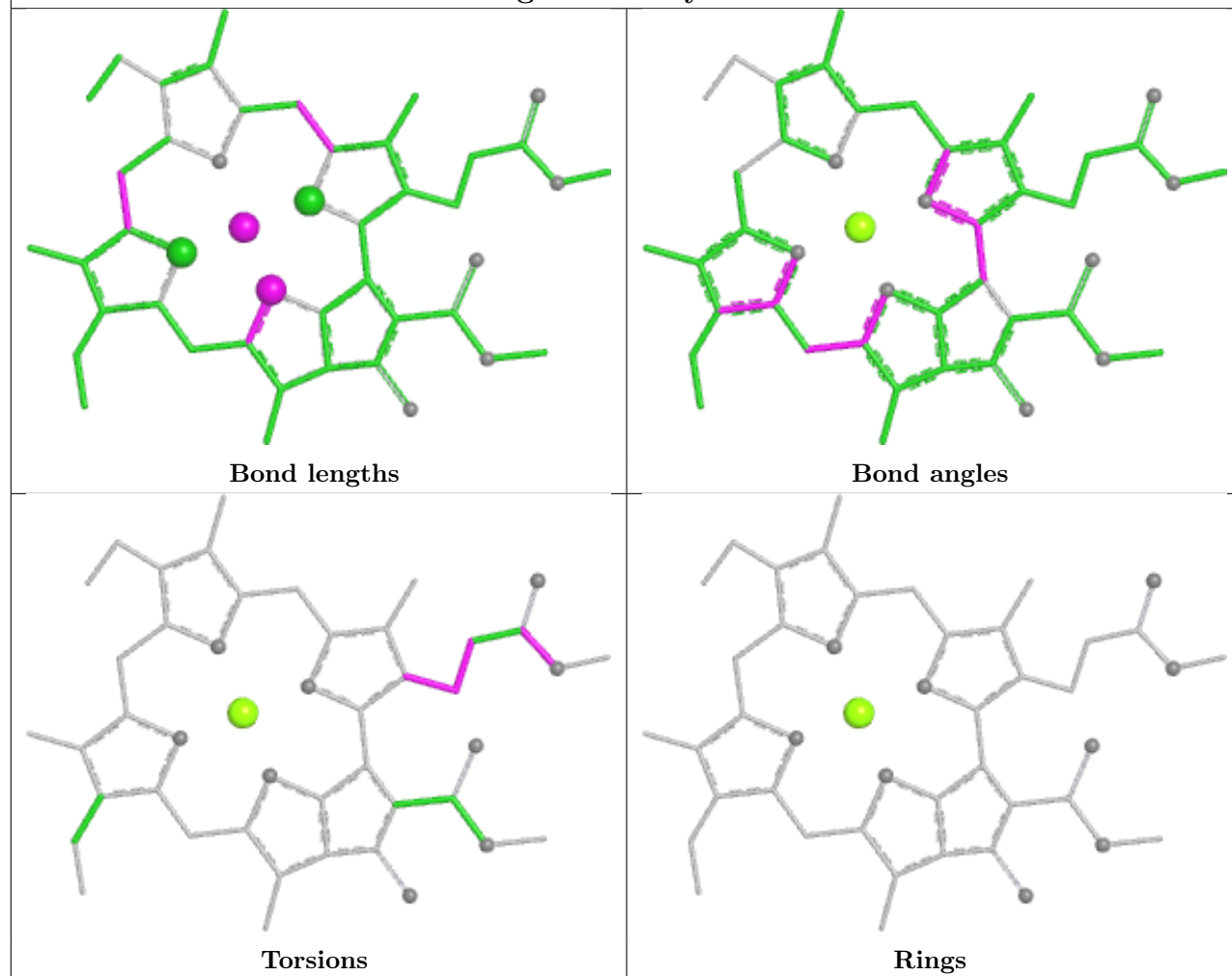




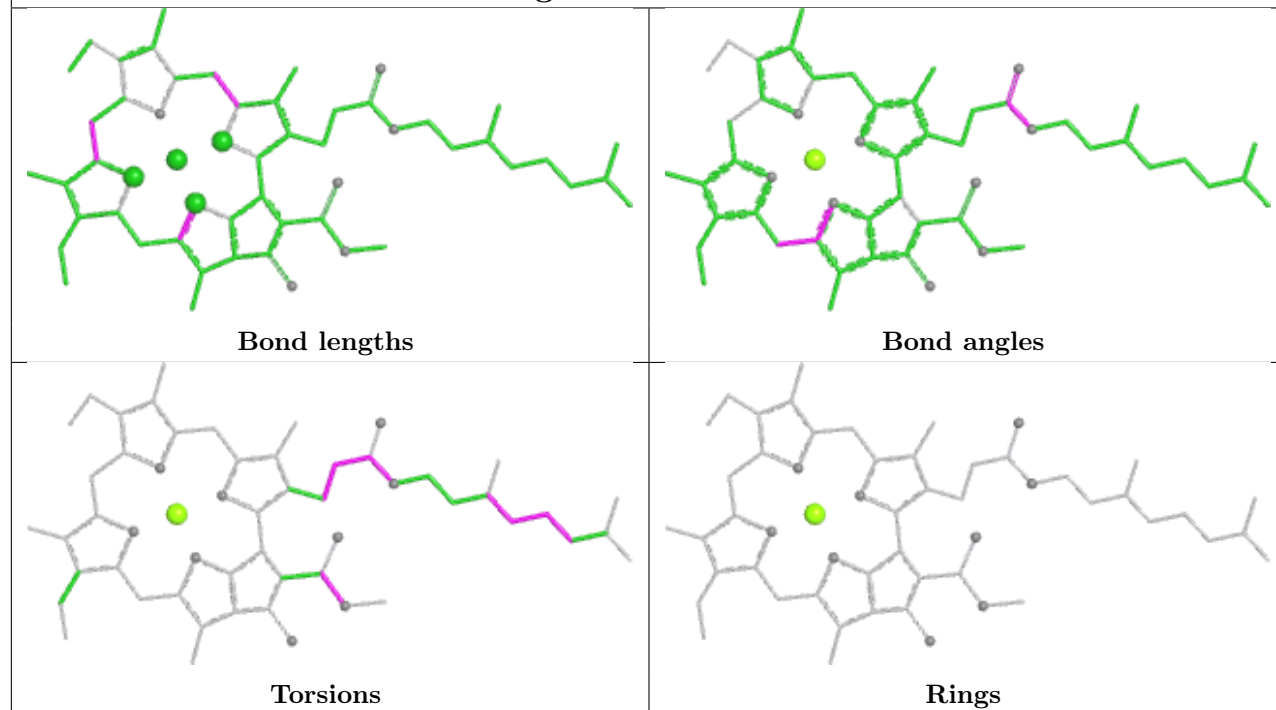
Ligand CLA x 506



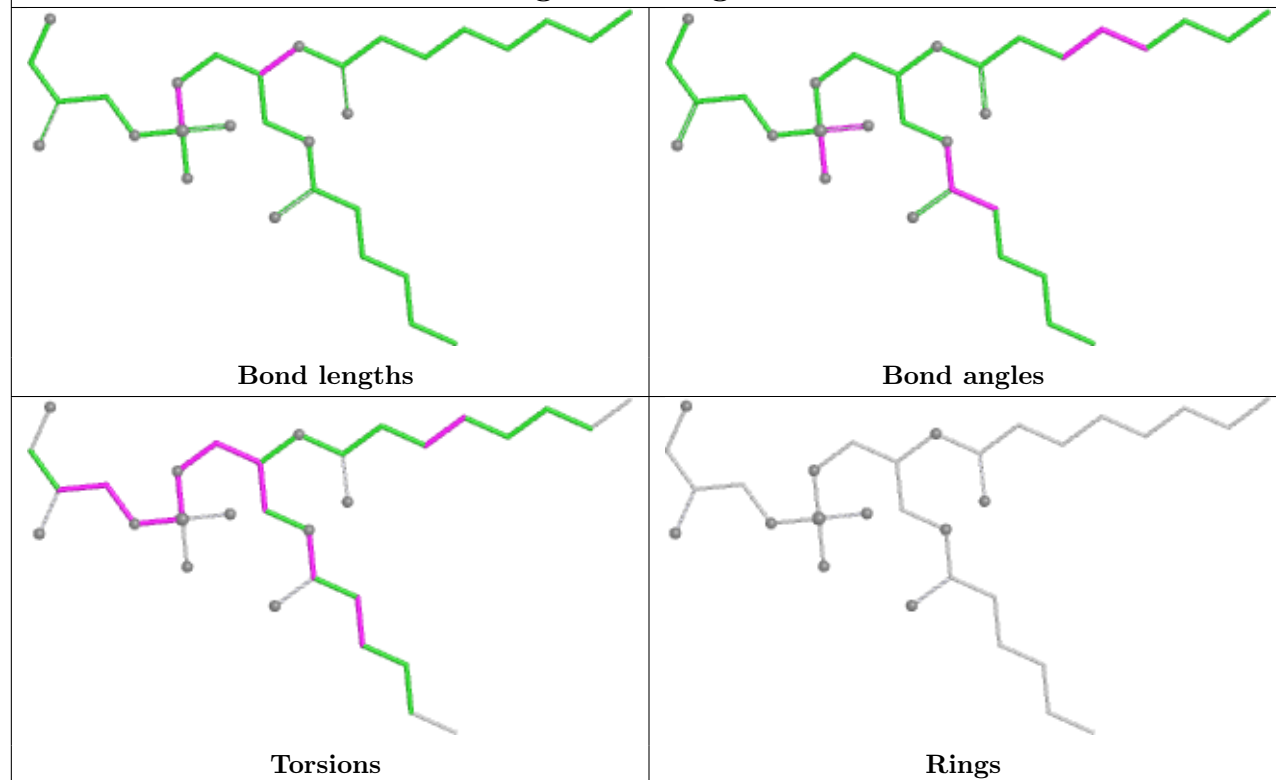
Ligand CLA y 503

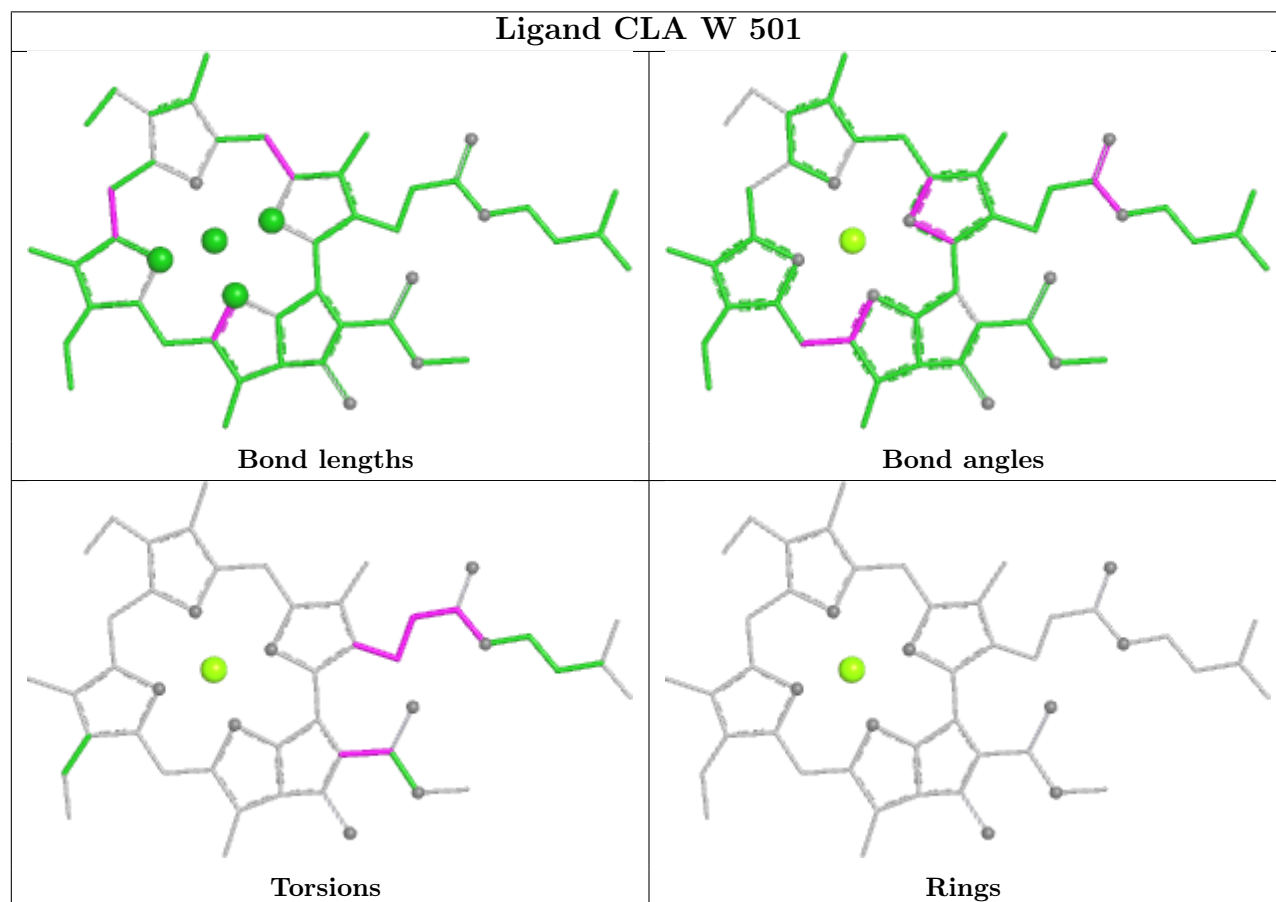
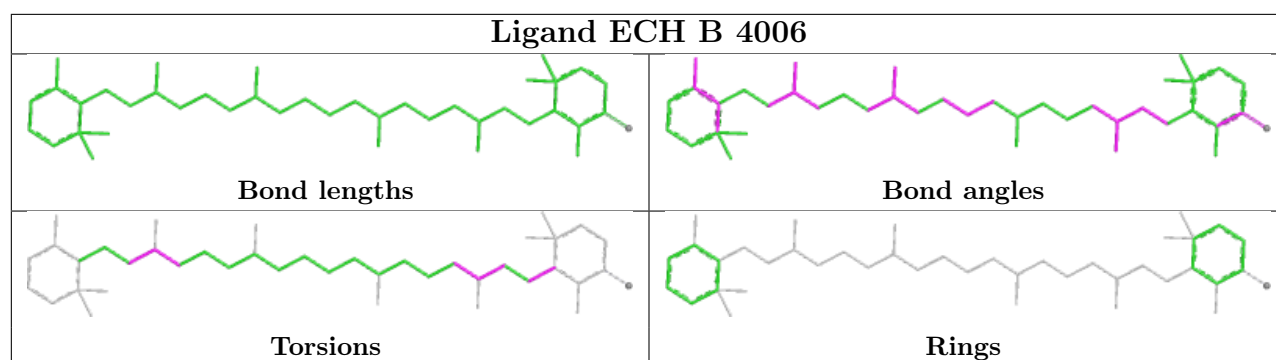


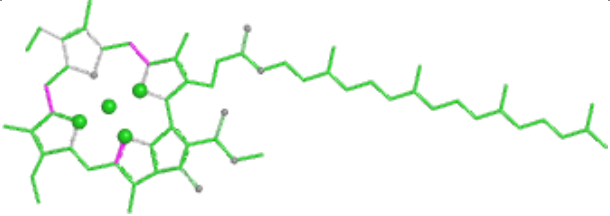
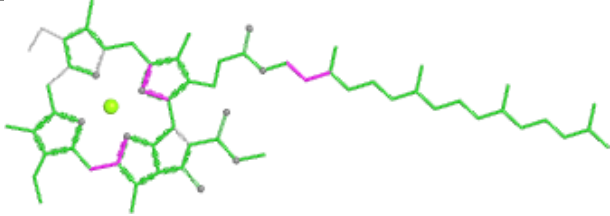
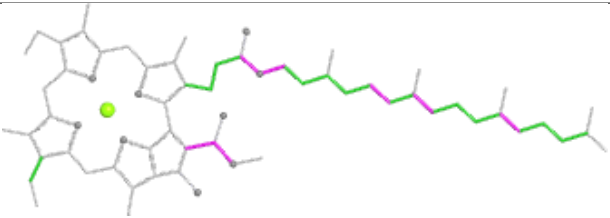
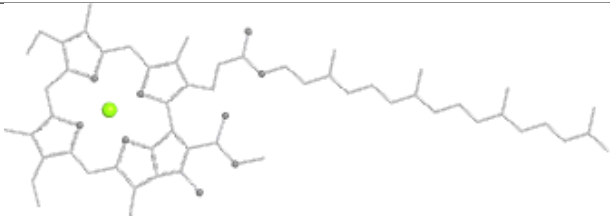
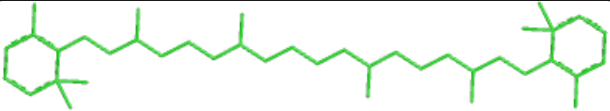
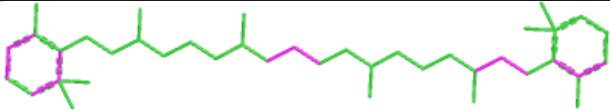
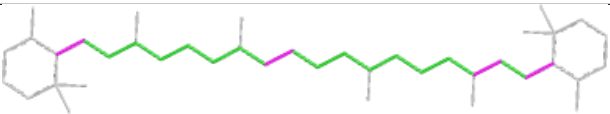
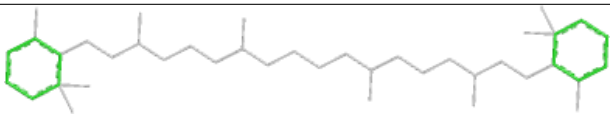
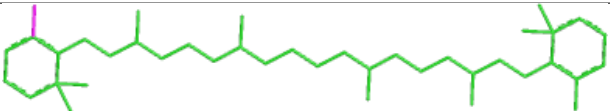
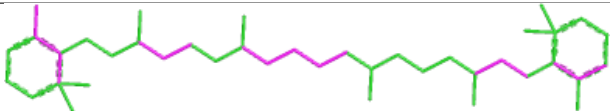
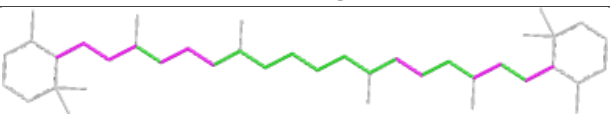
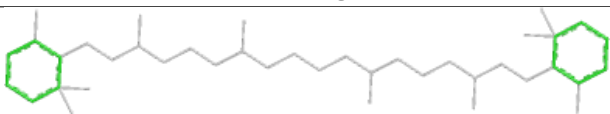
Ligand CLA u 508

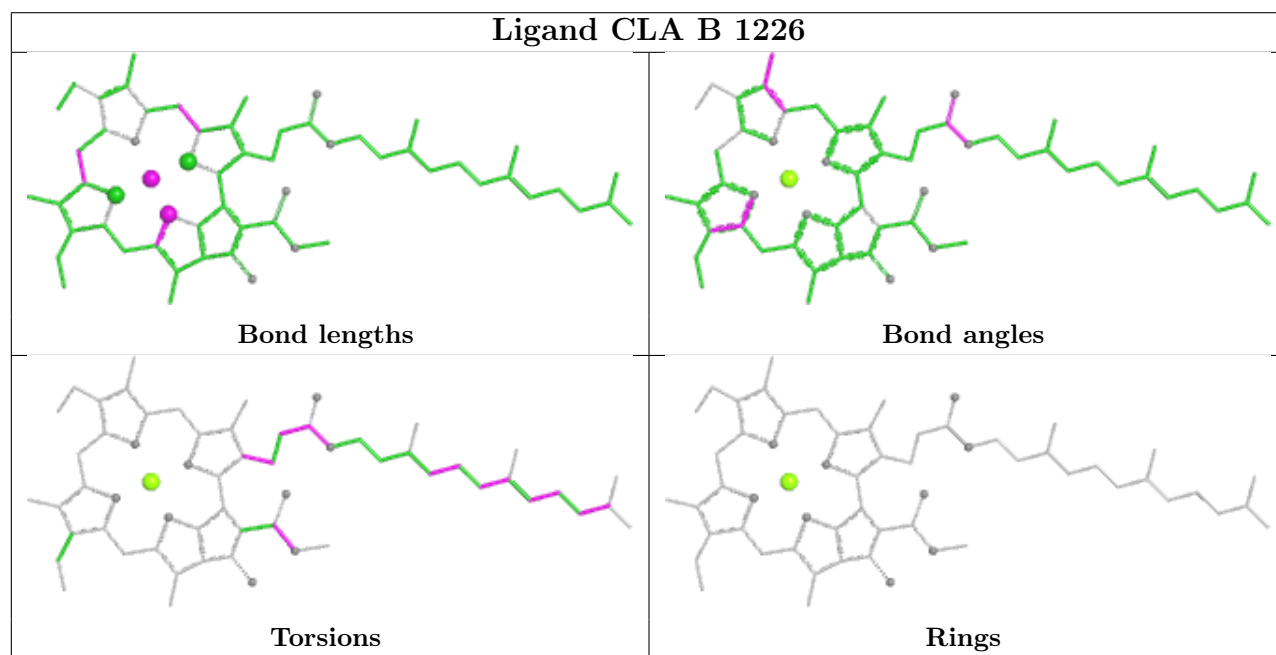
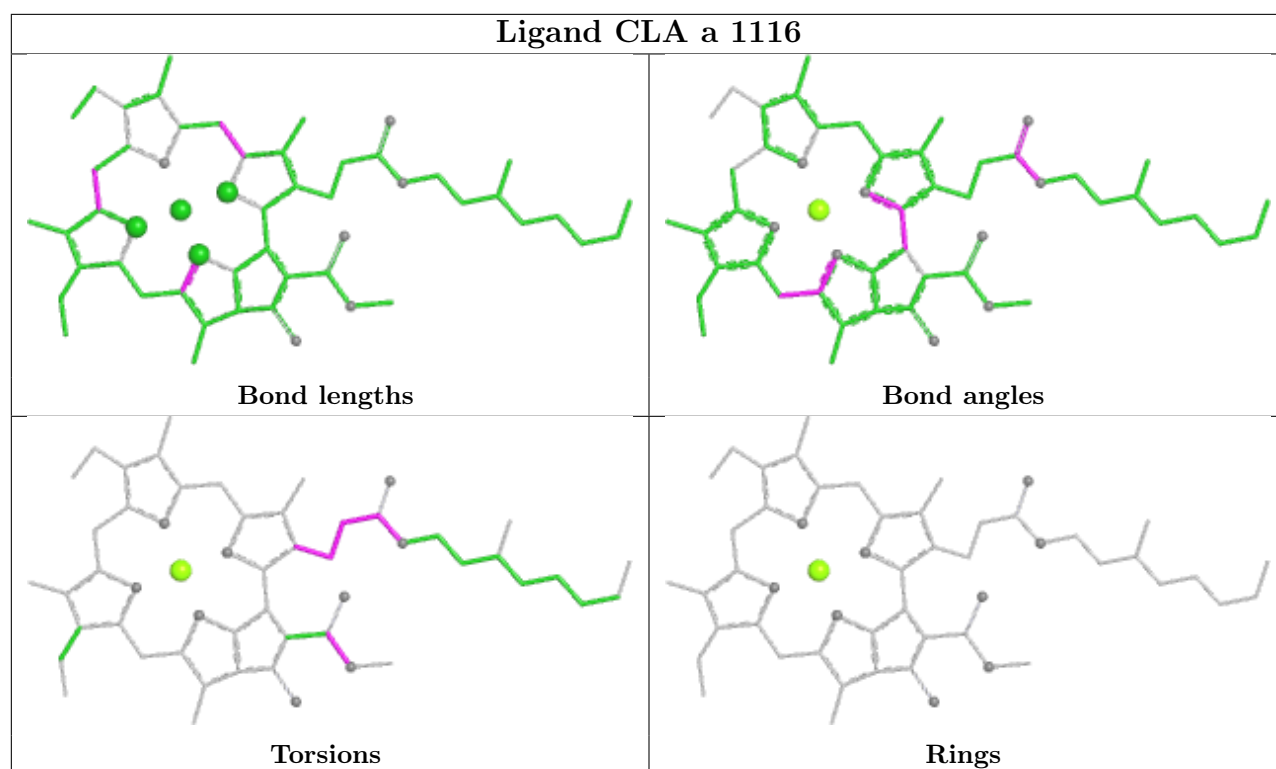


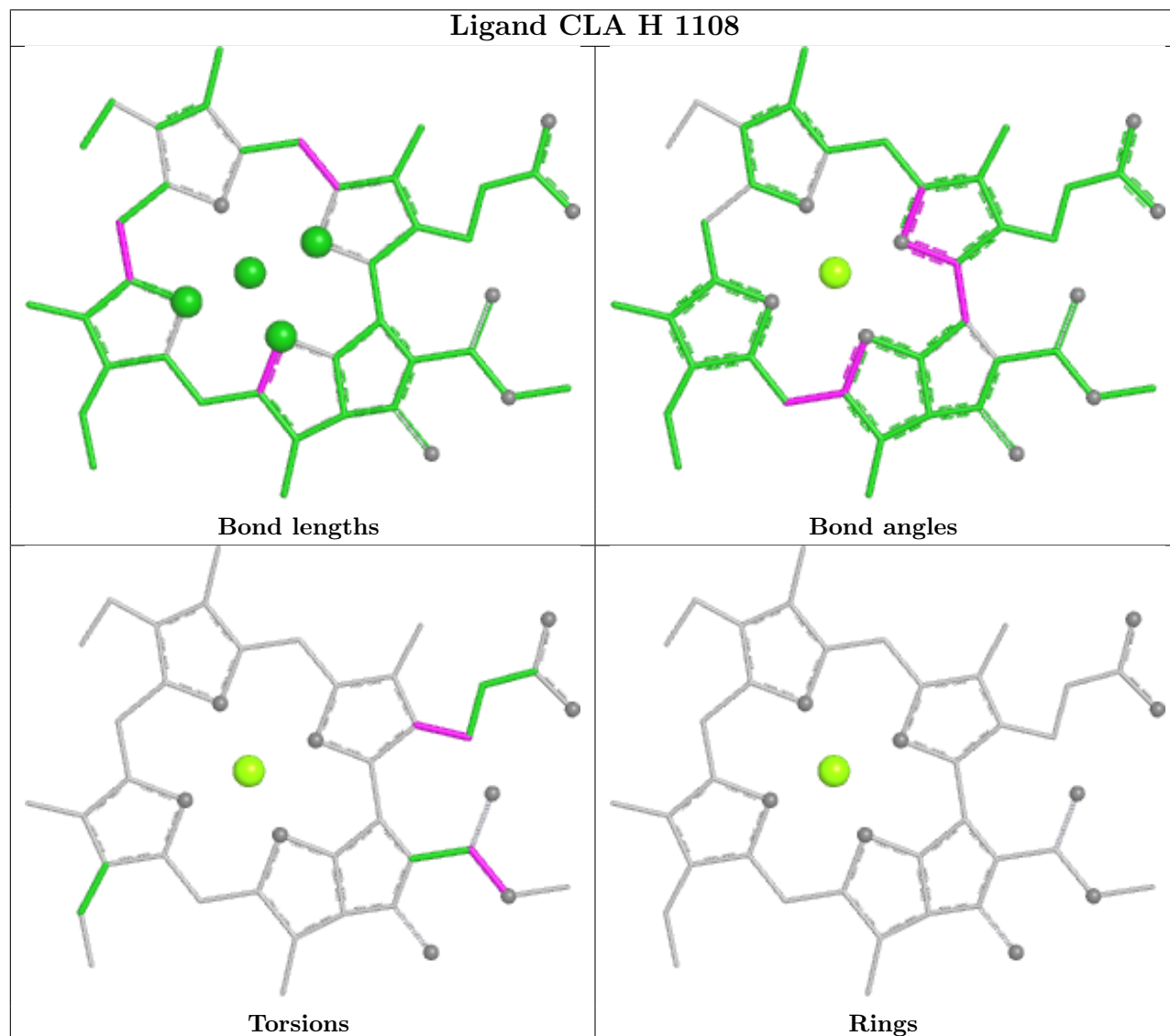
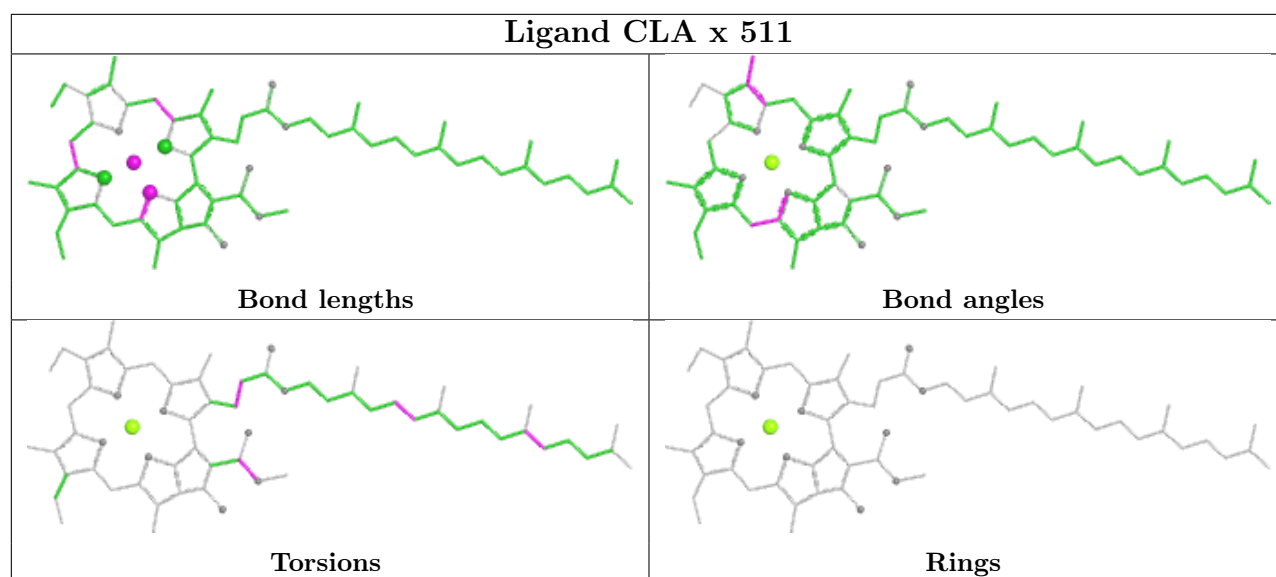
Ligand LHG g 605

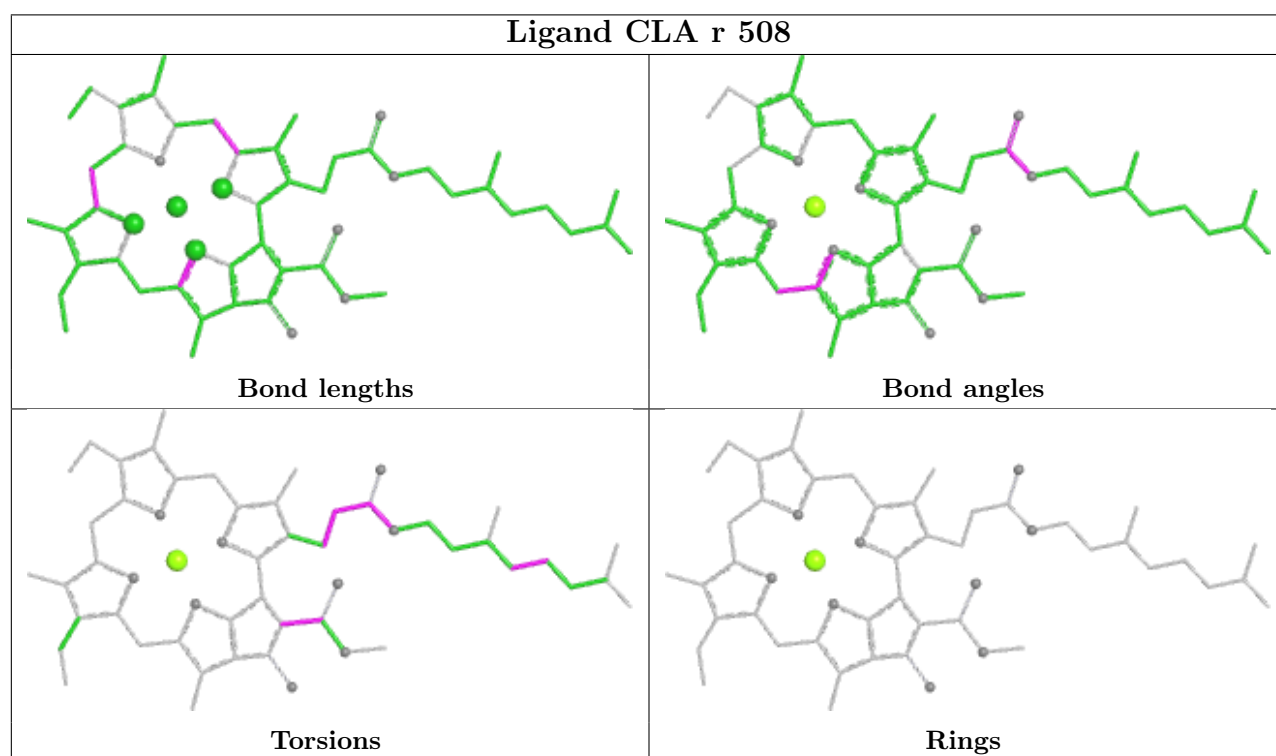
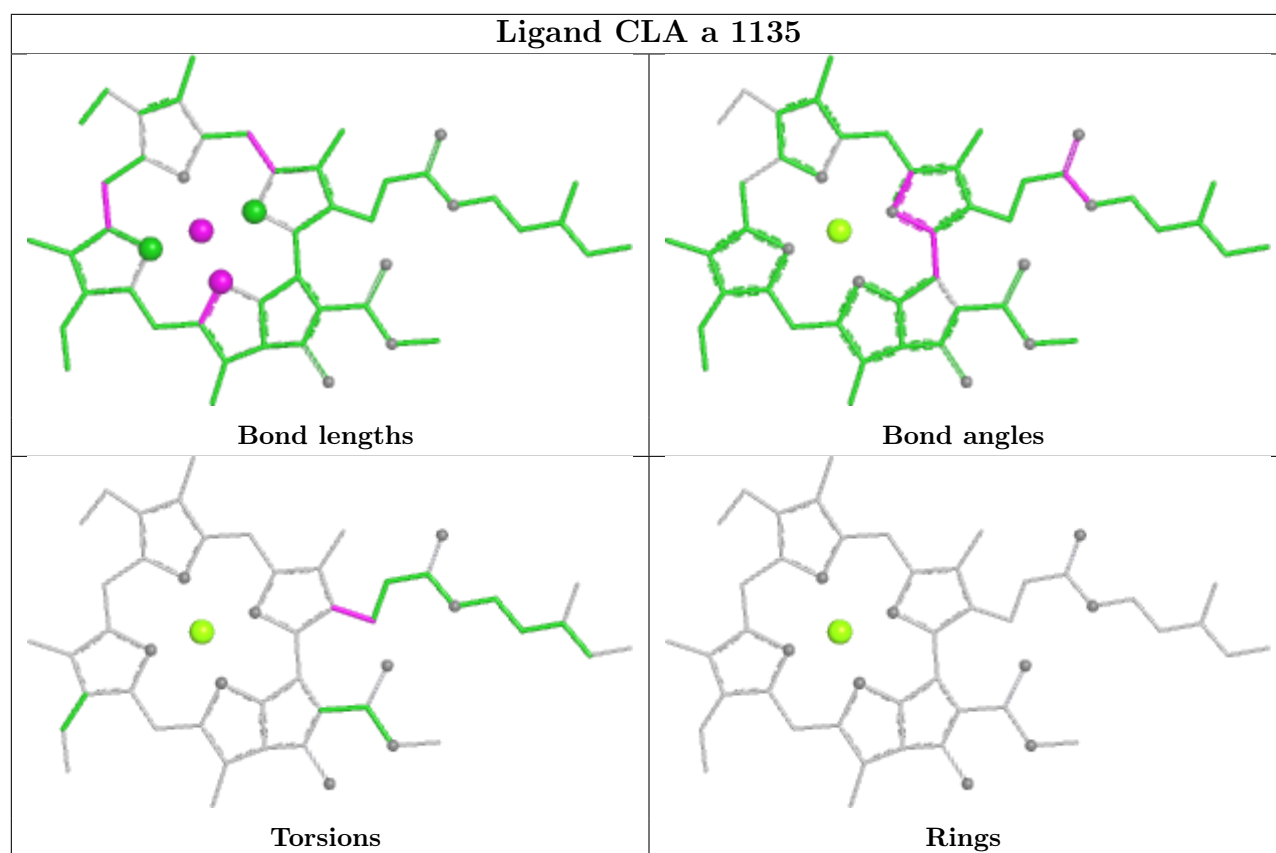


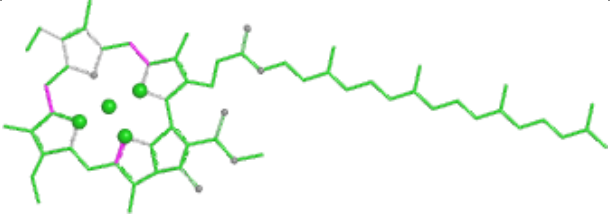
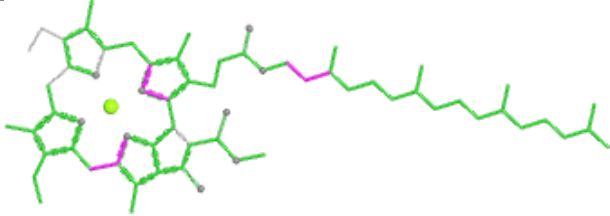
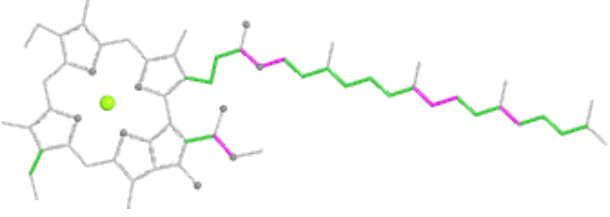
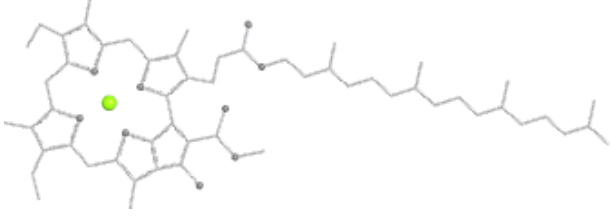
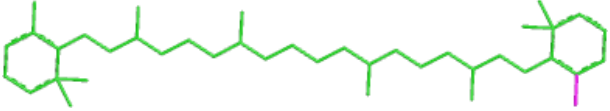
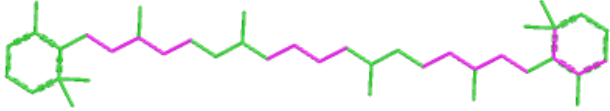

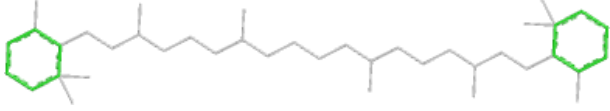
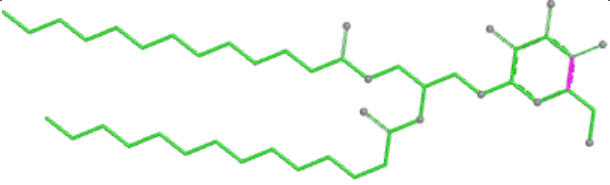
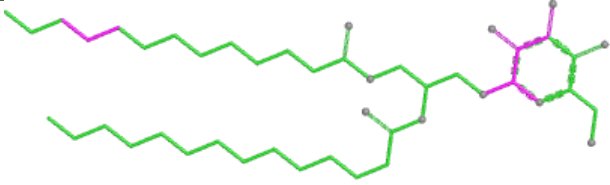
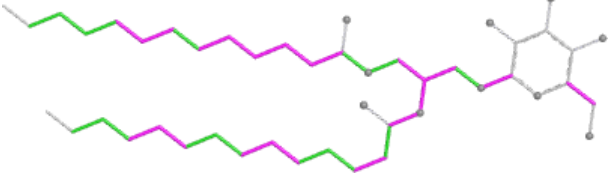
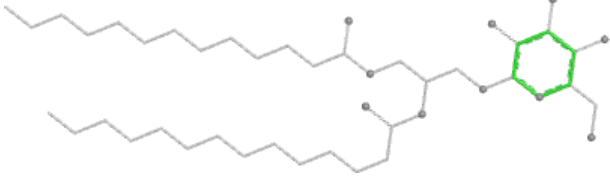


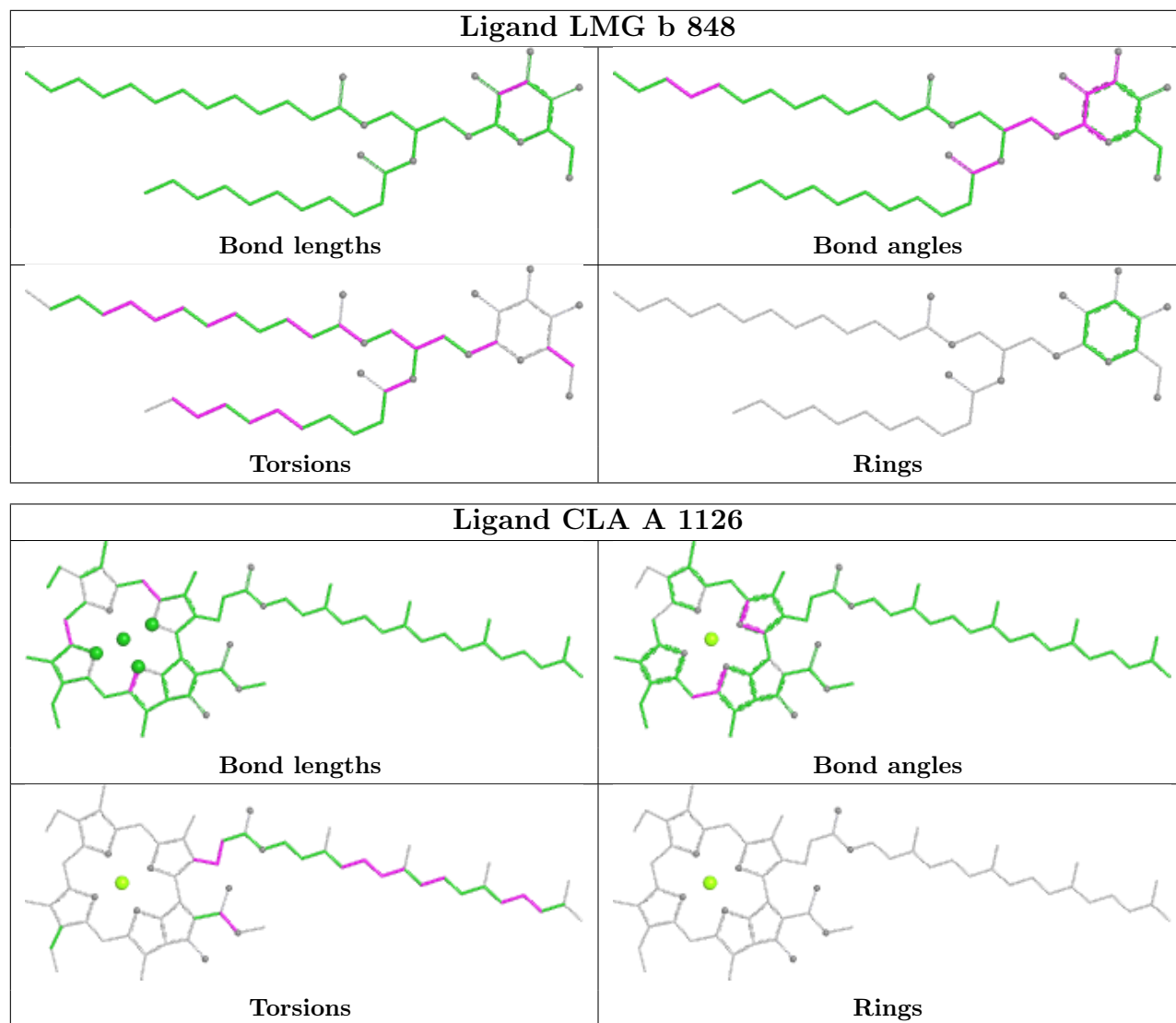
Ligand CLA r 507	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR k 4005	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR T 4001	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



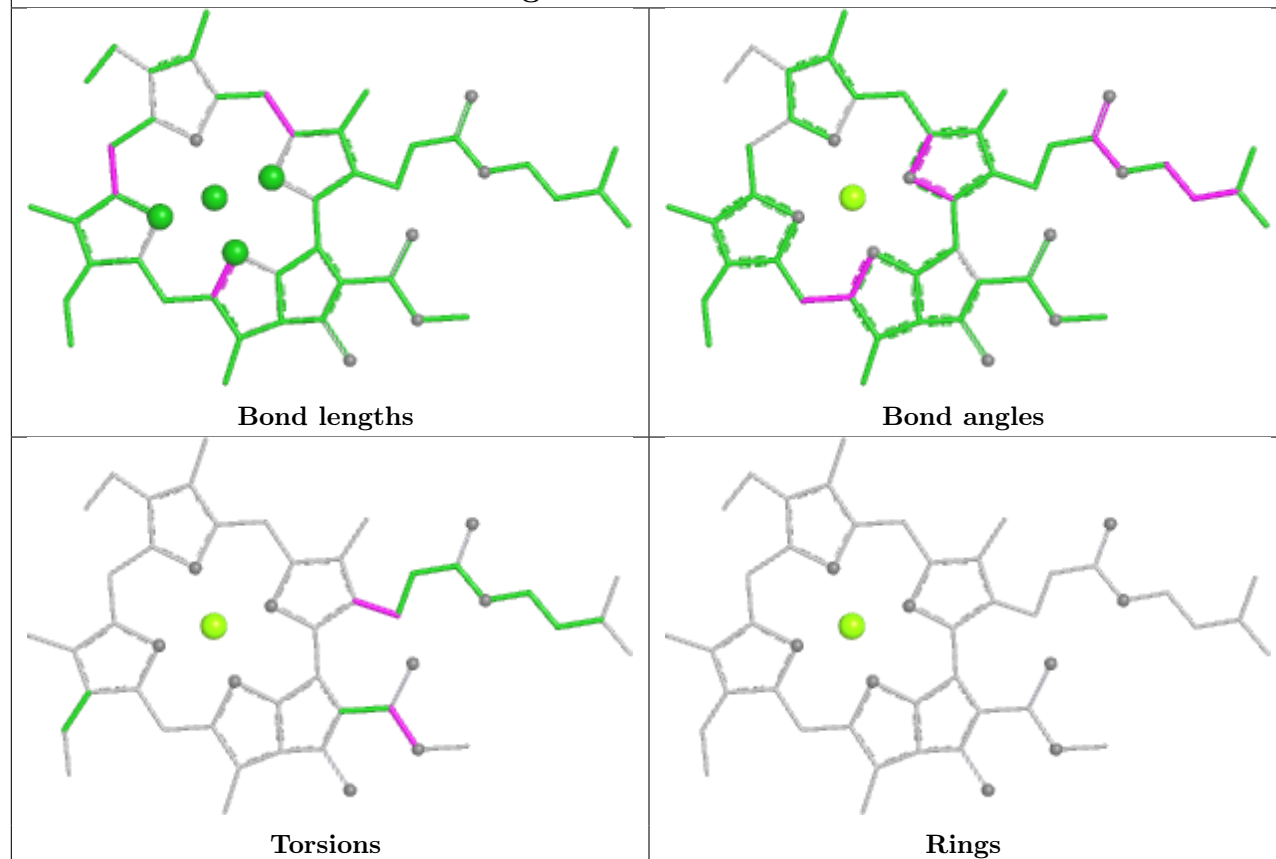




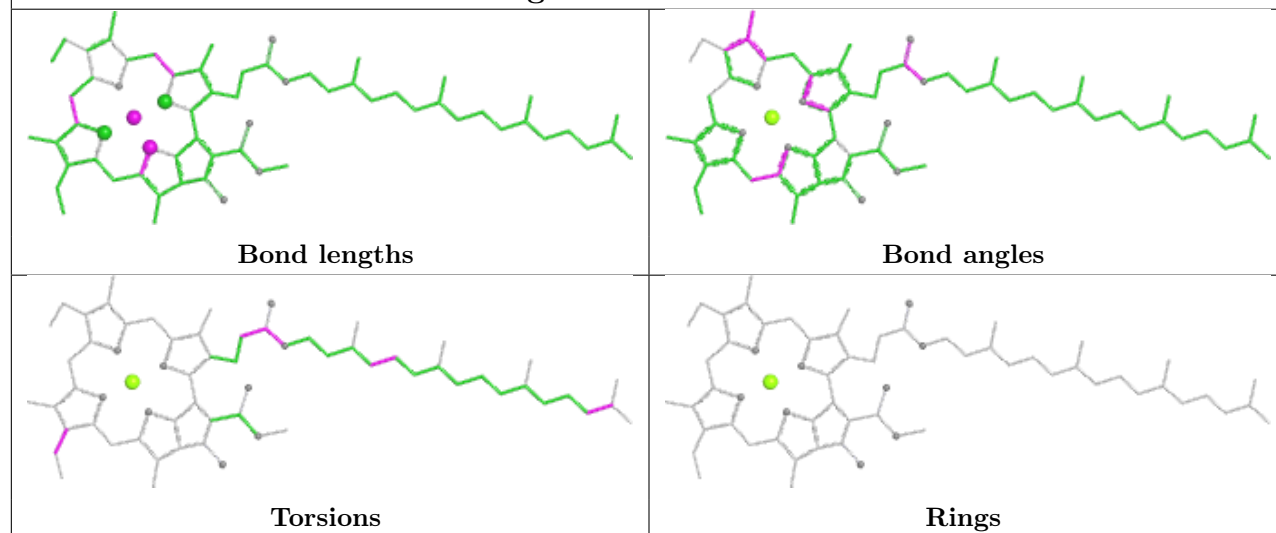
Ligand CLA s 507	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR G 4014	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG H 4101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



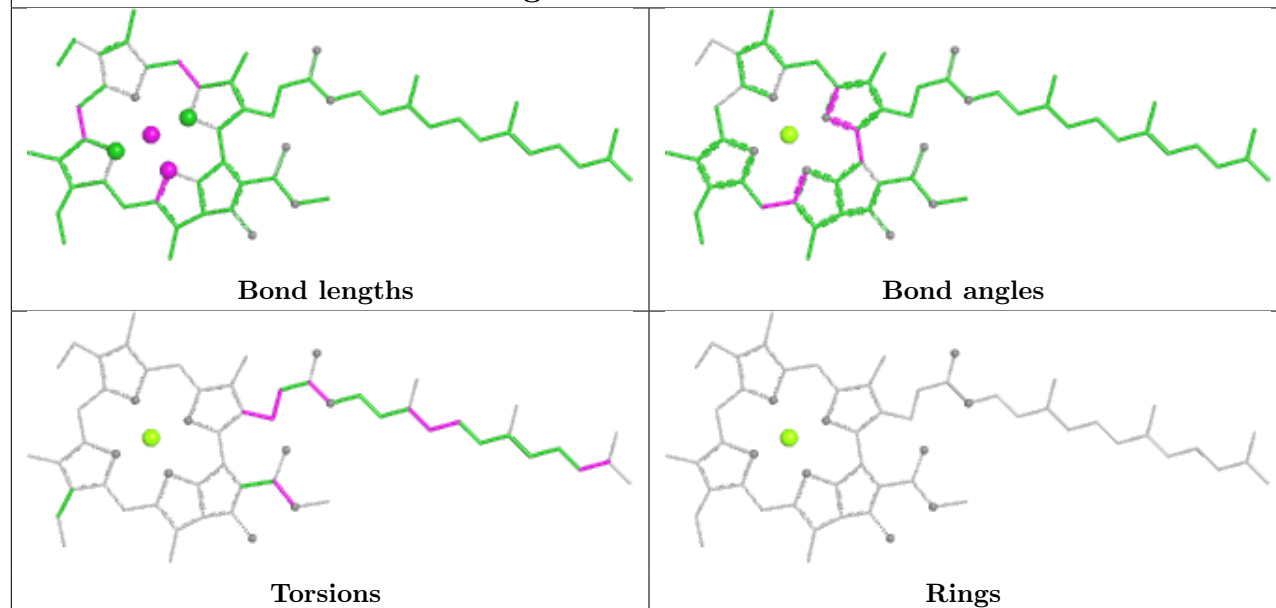
Ligand CLA H 1107



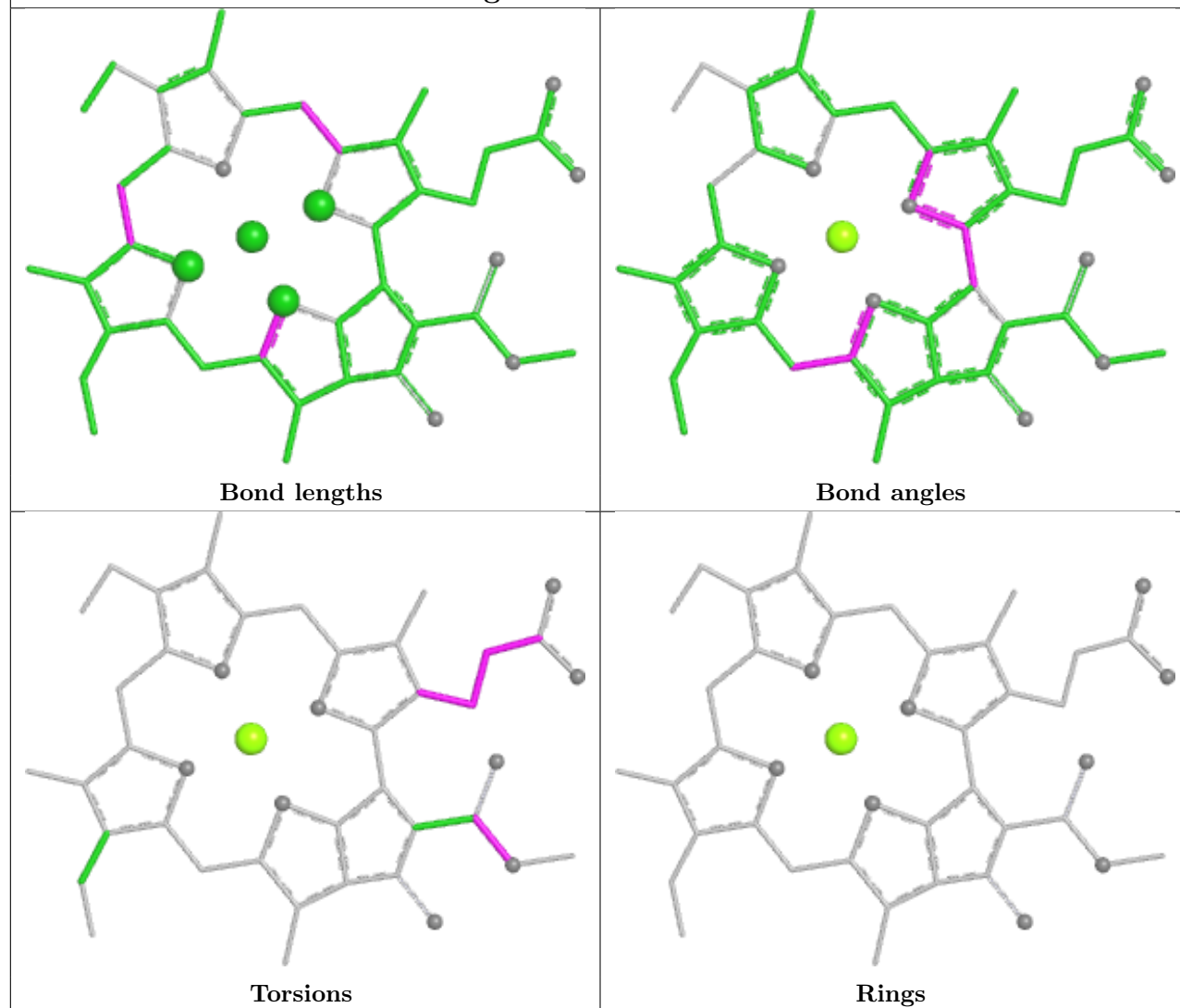
Ligand CL0 A 1011



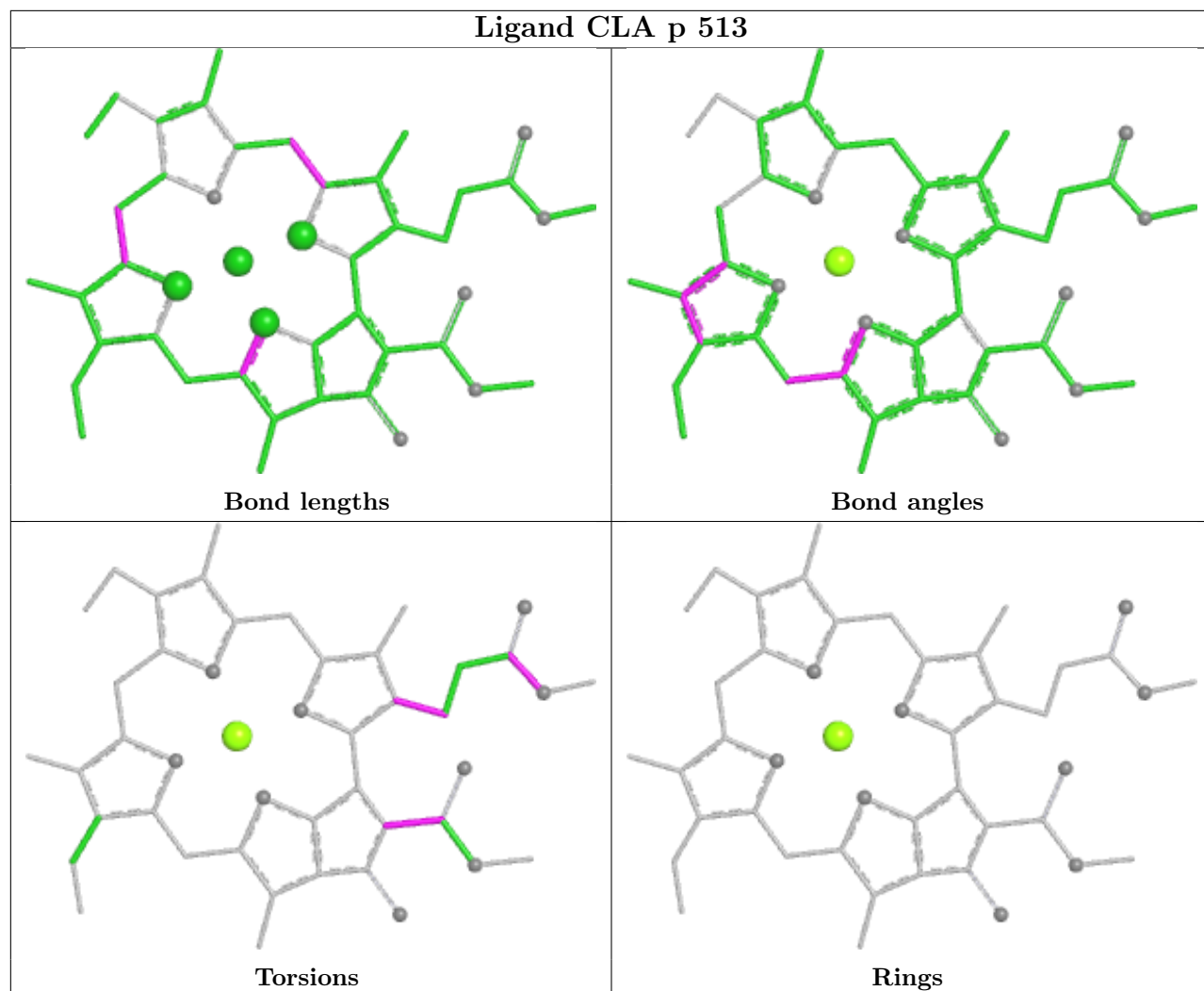
Ligand CLA B 1224



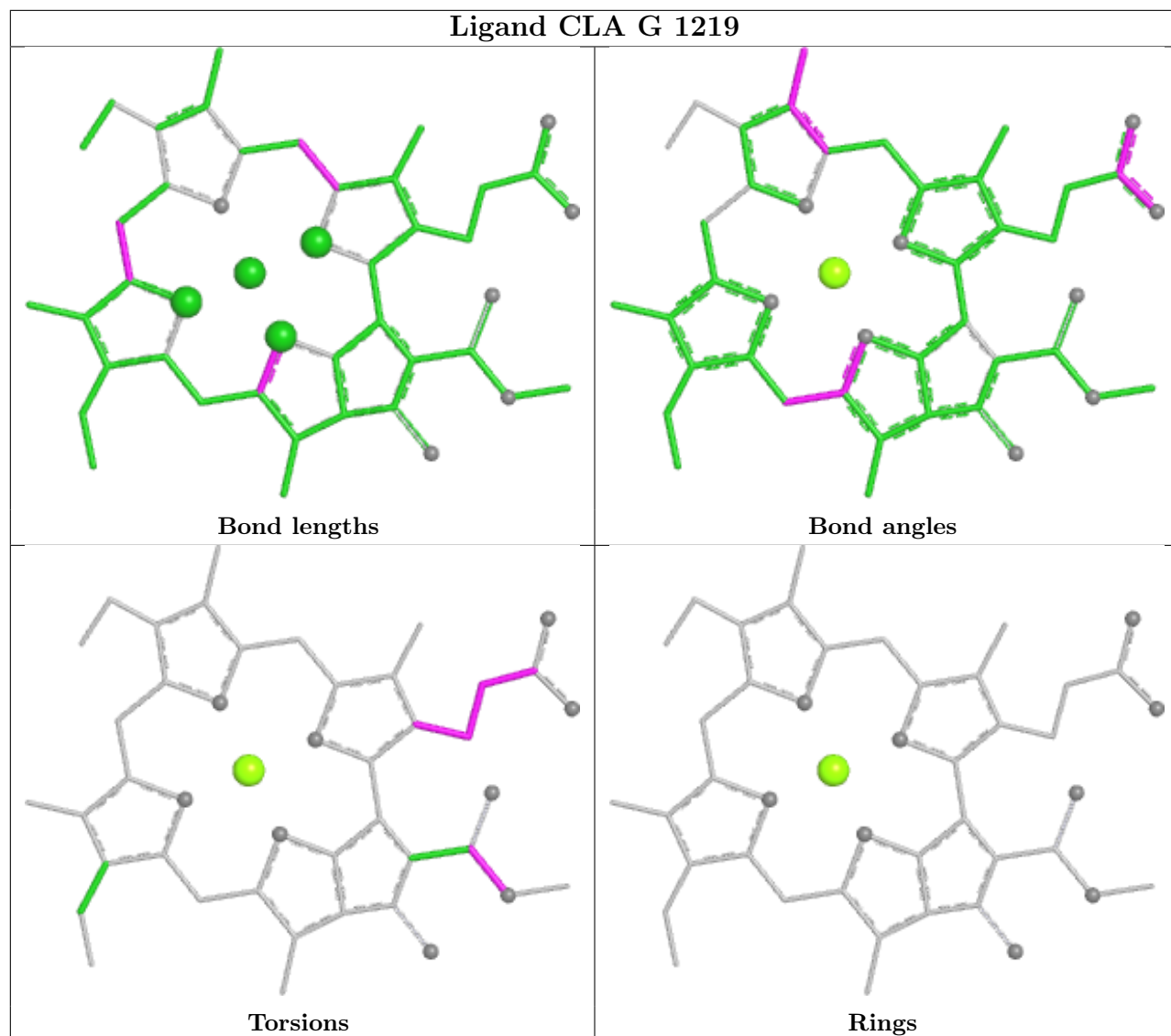
Ligand CLA B 1231

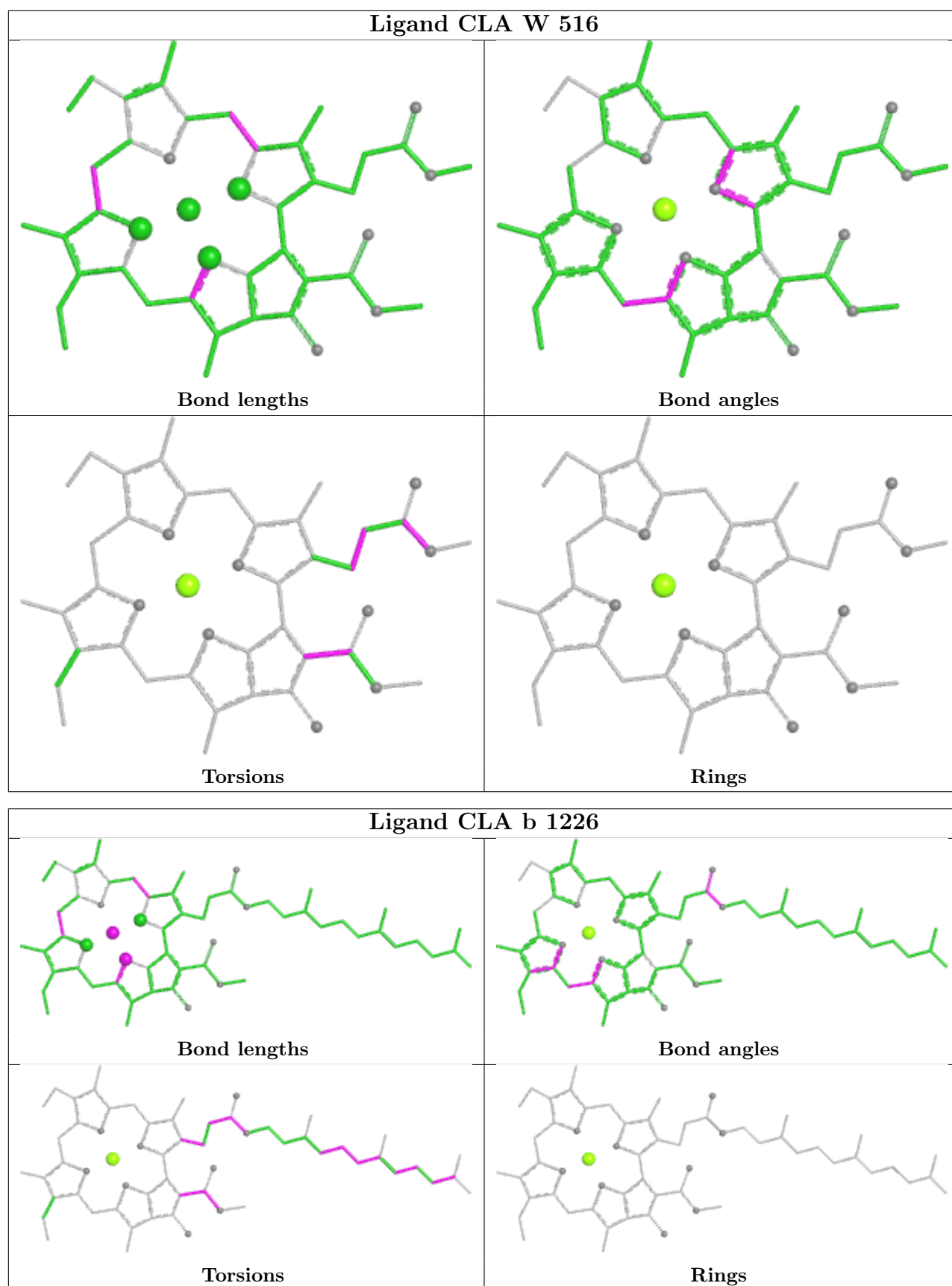


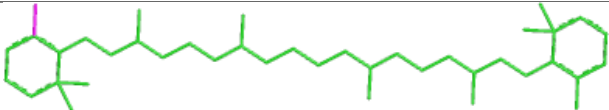
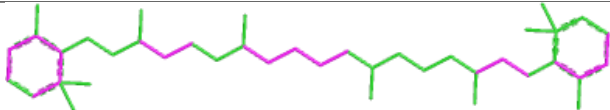
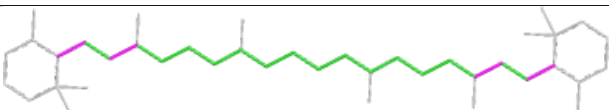
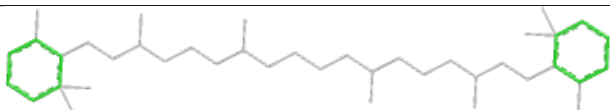
Ligand CLA p 513


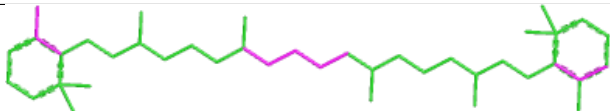
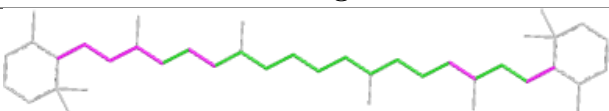
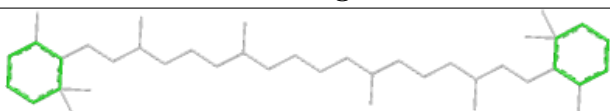


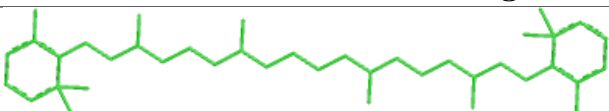
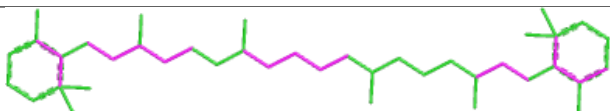
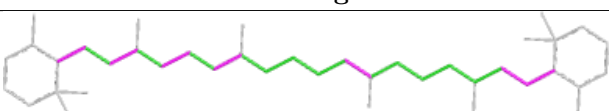
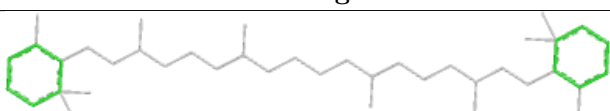
Ligand CLA G 1219

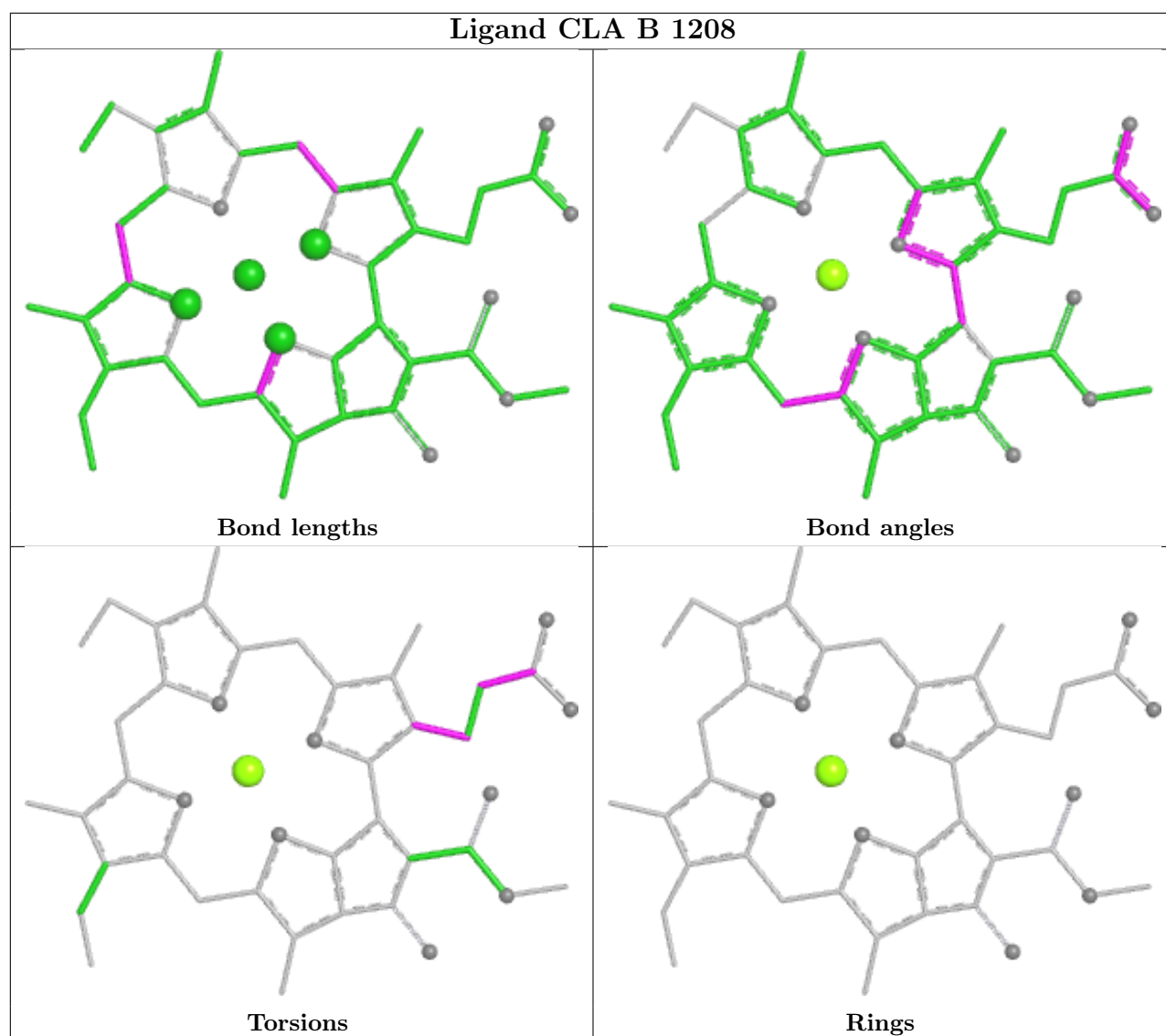




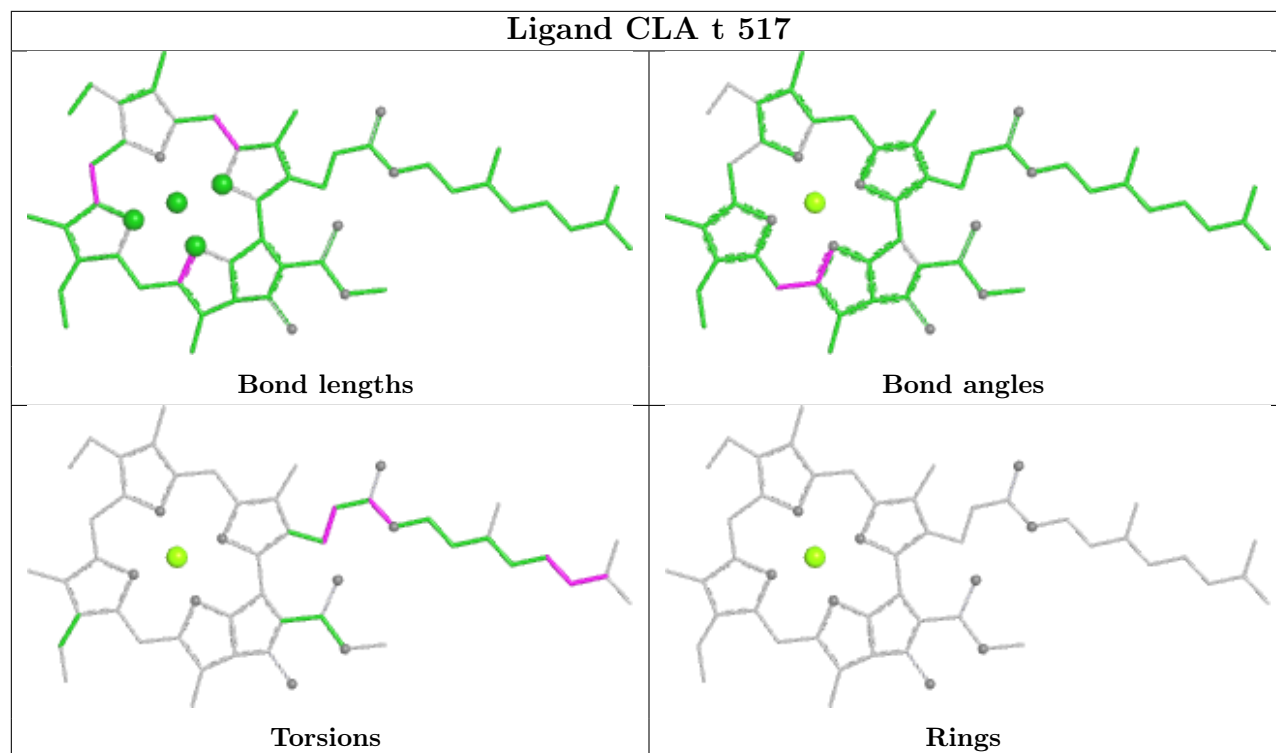
Ligand BCR u 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR t 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

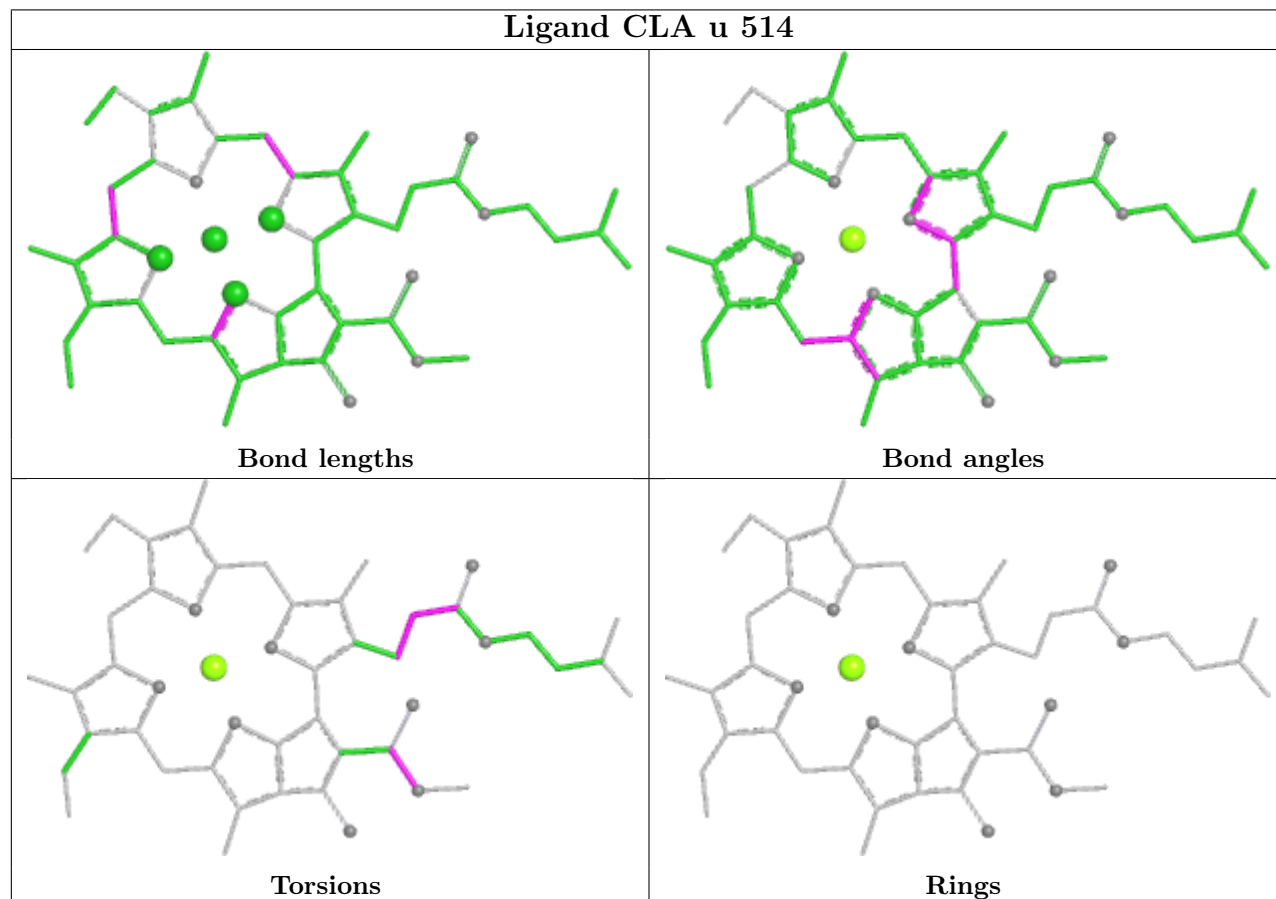
Ligand BCR S 4015	
	
Bond lengths	Bond angles
	
Torsions	Rings

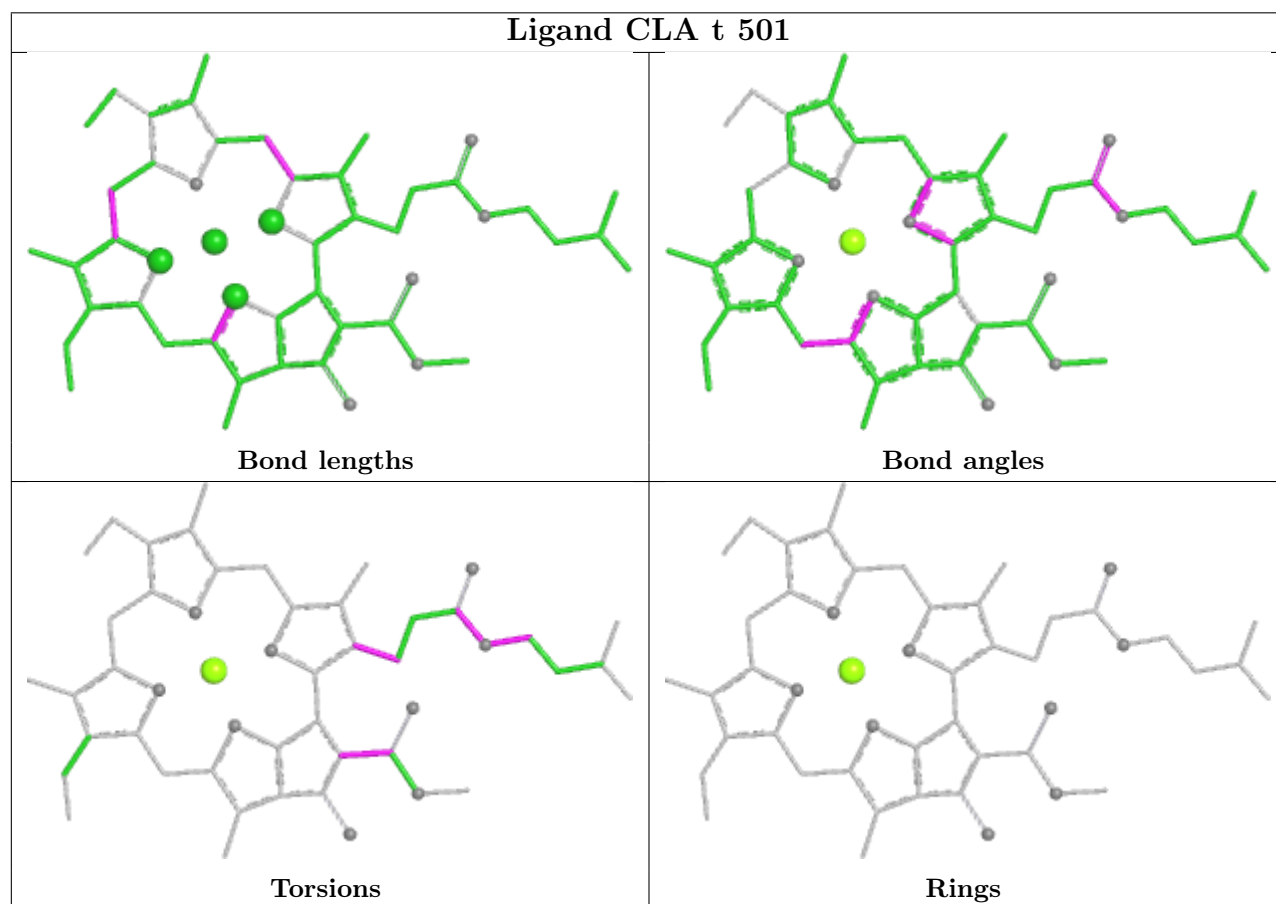
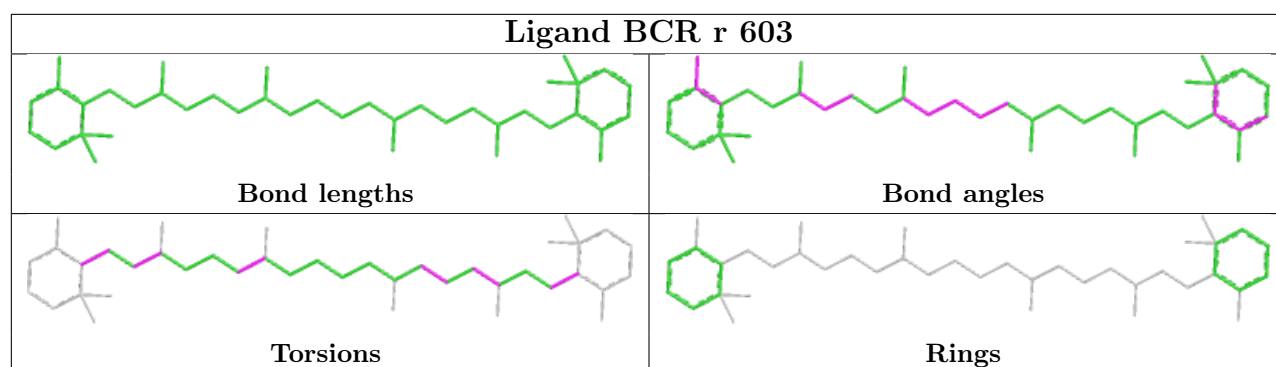


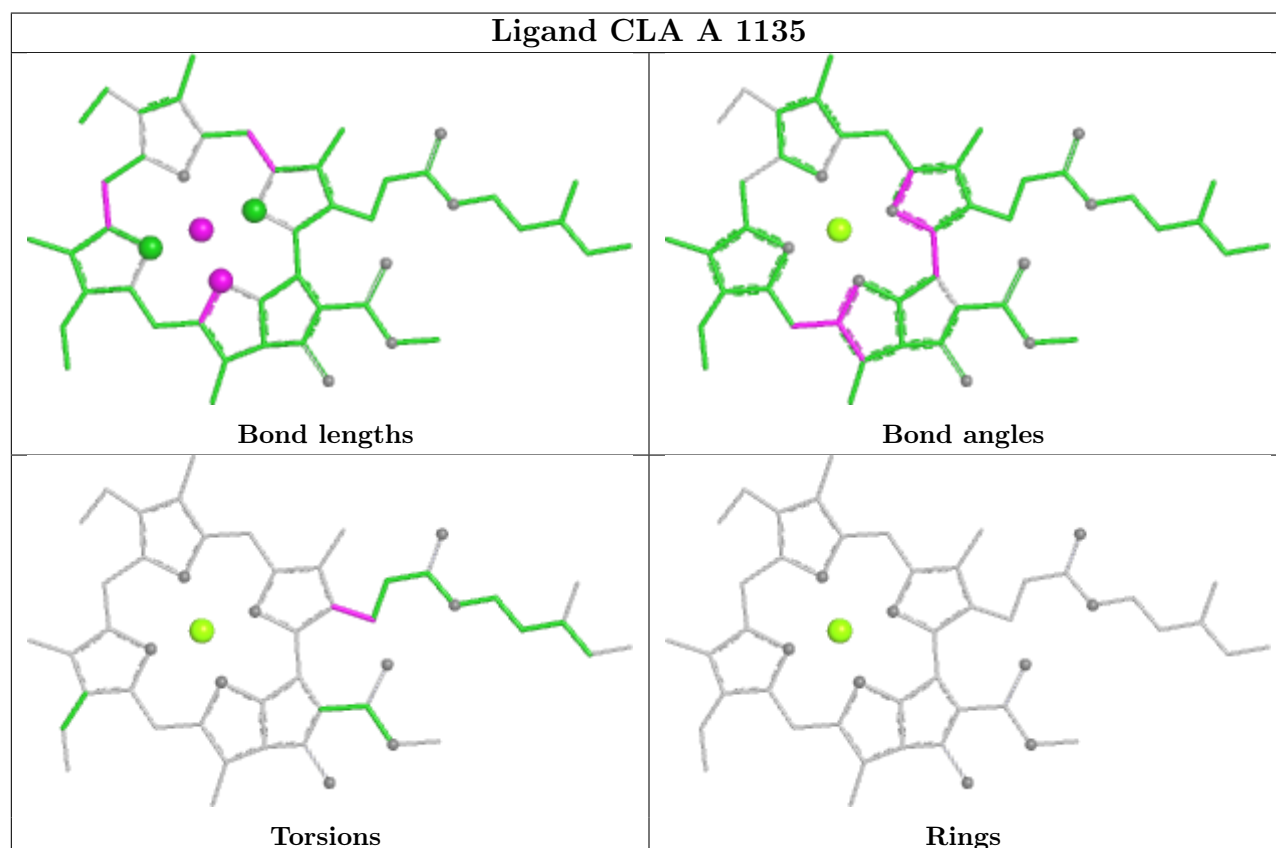
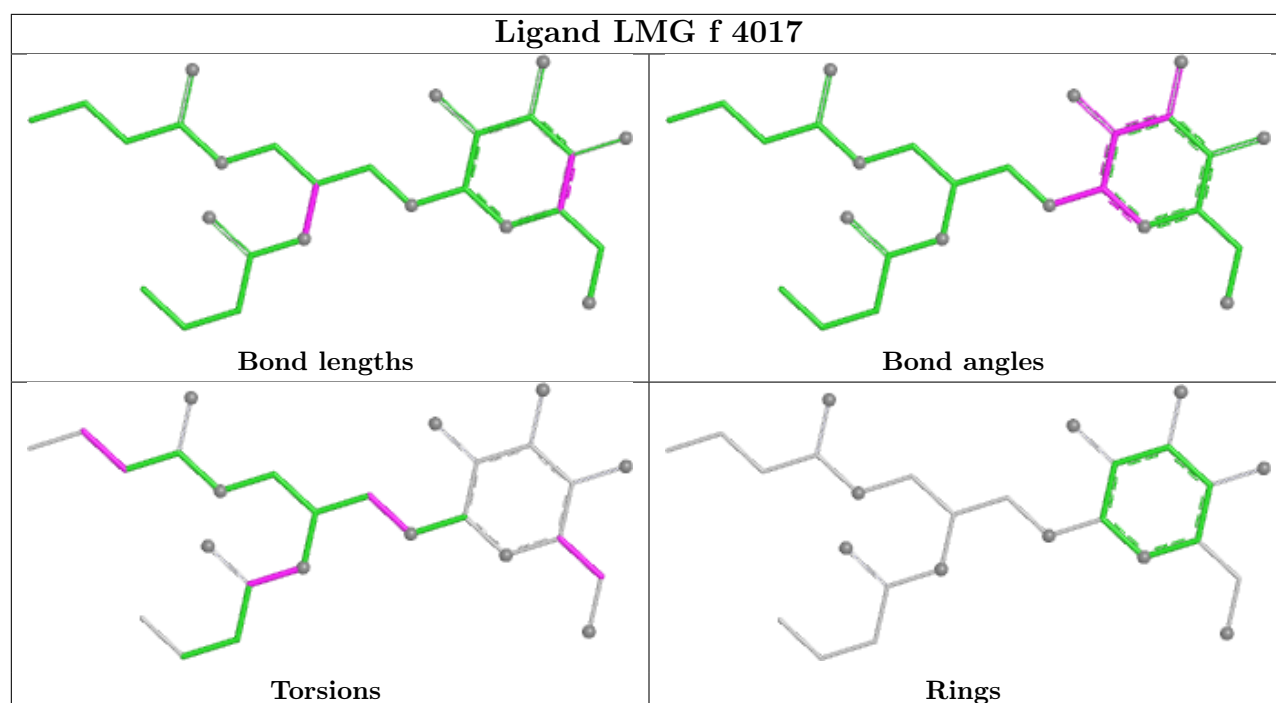
Ligand CLA t 517

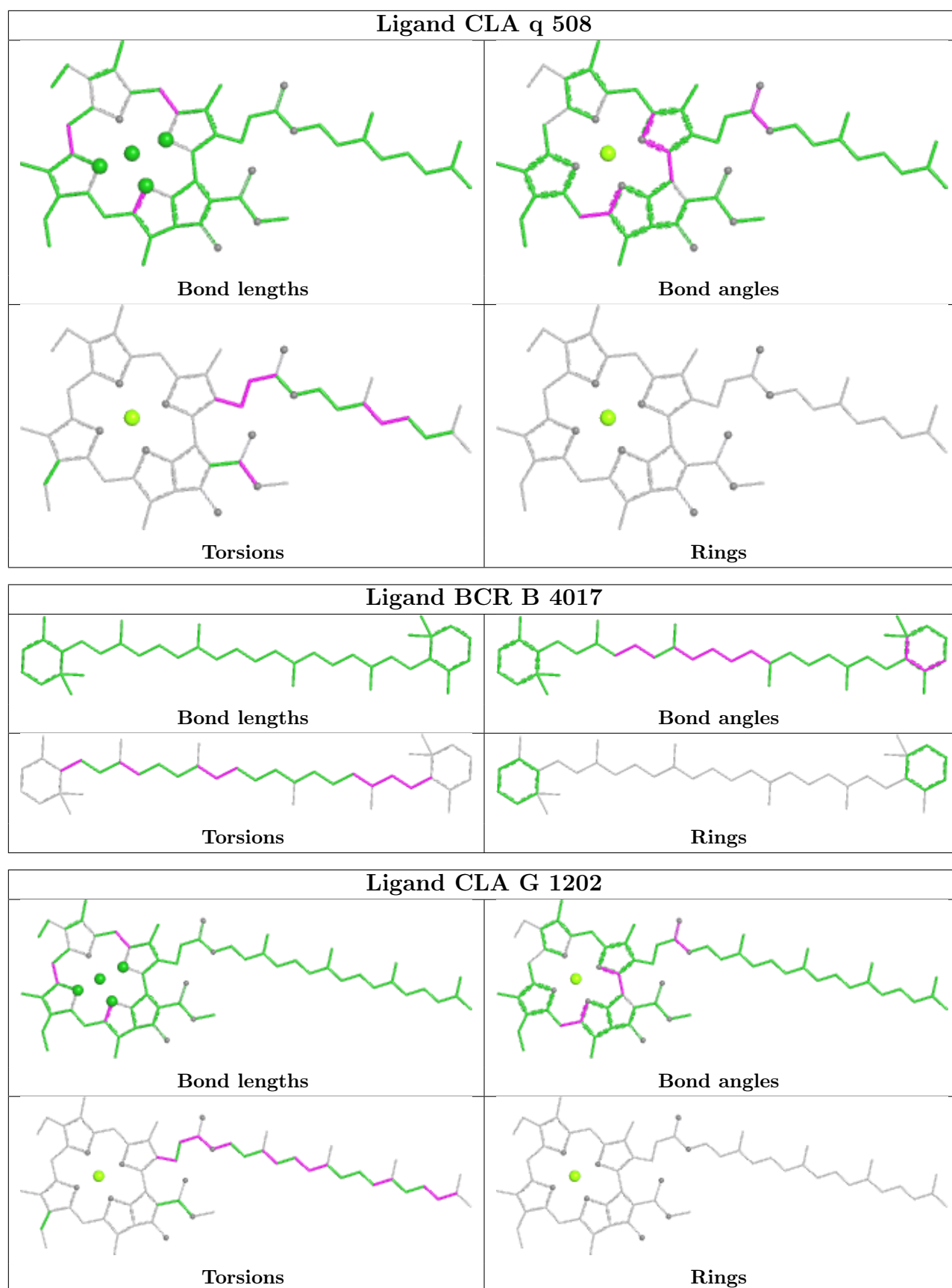


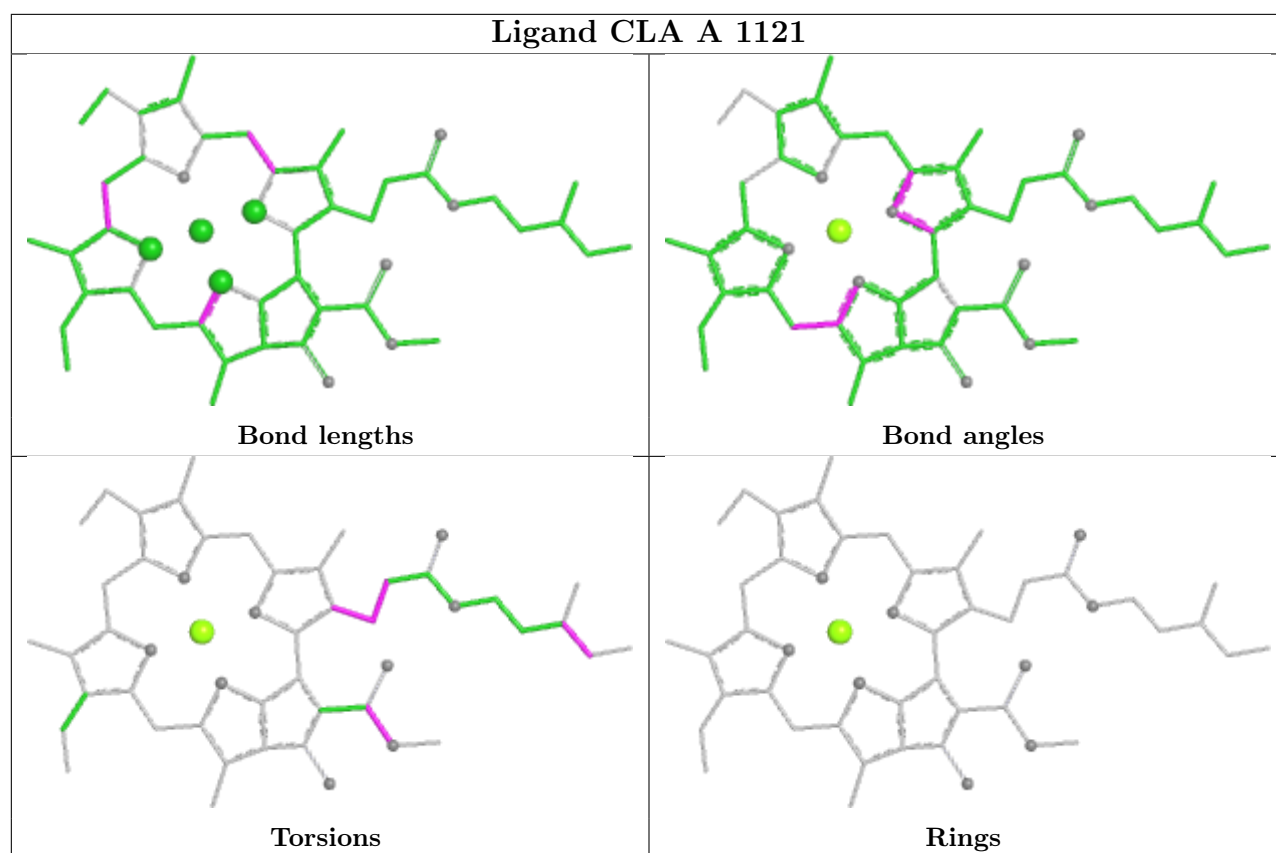
Ligand CLA u 514

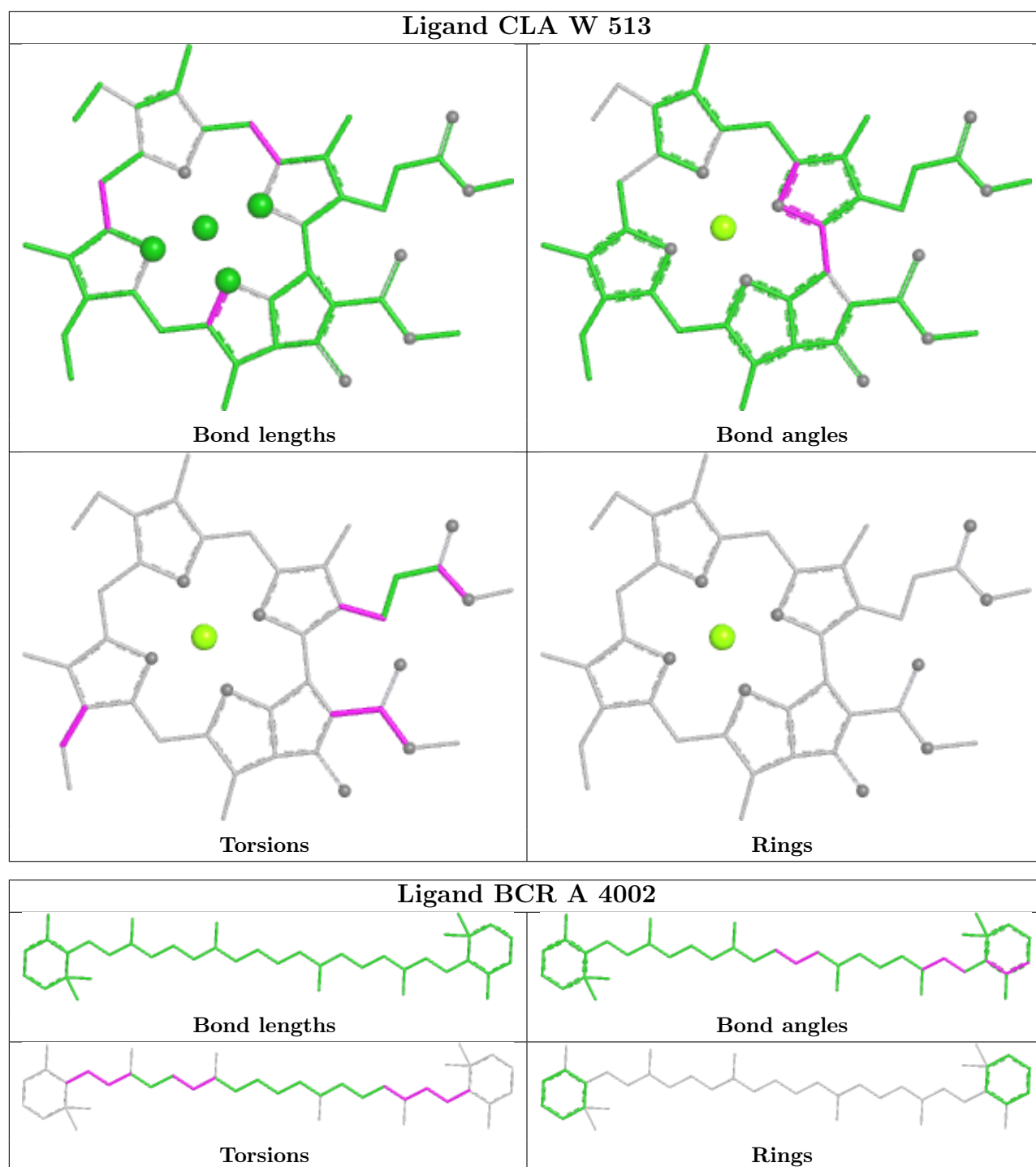


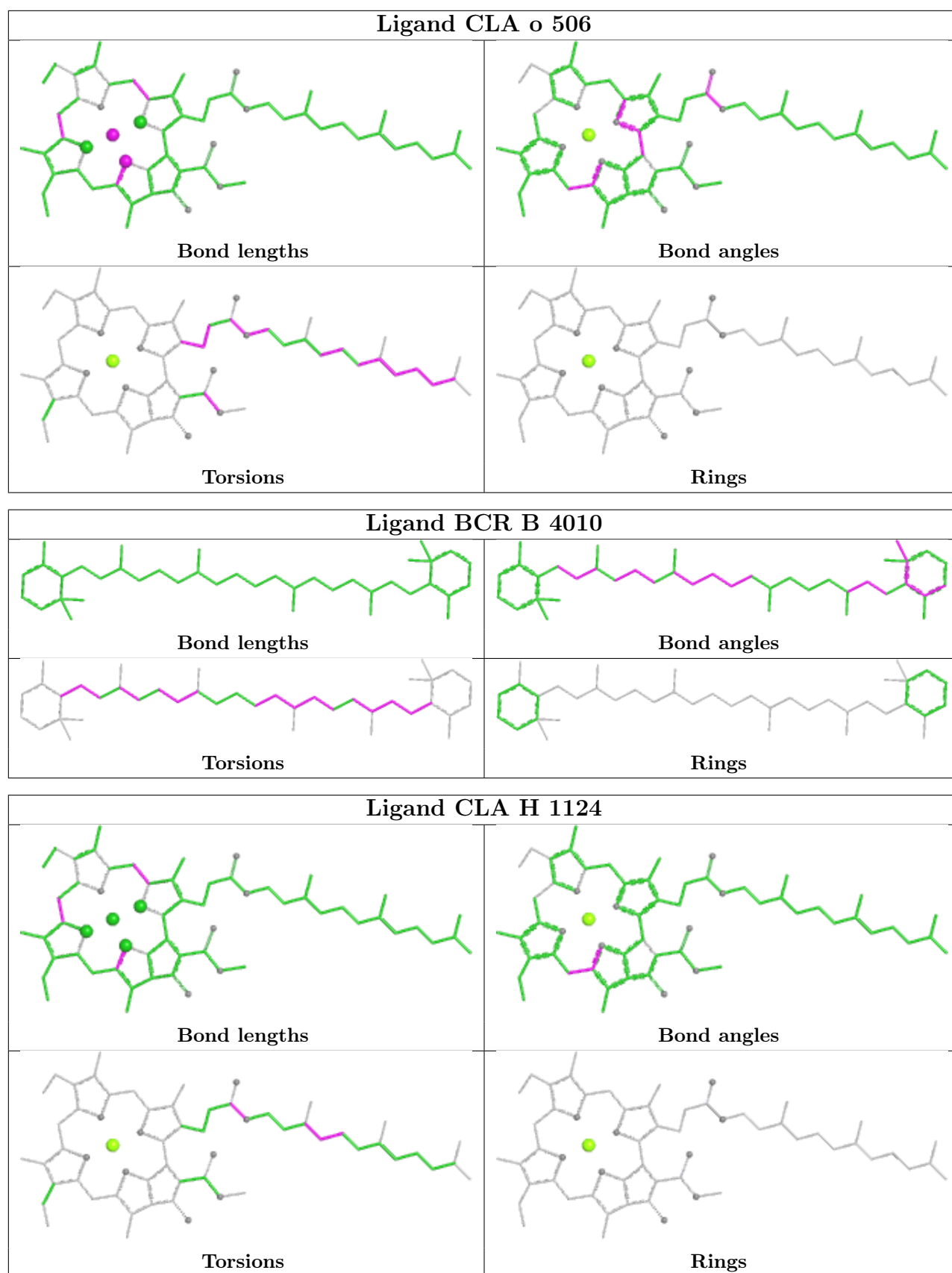


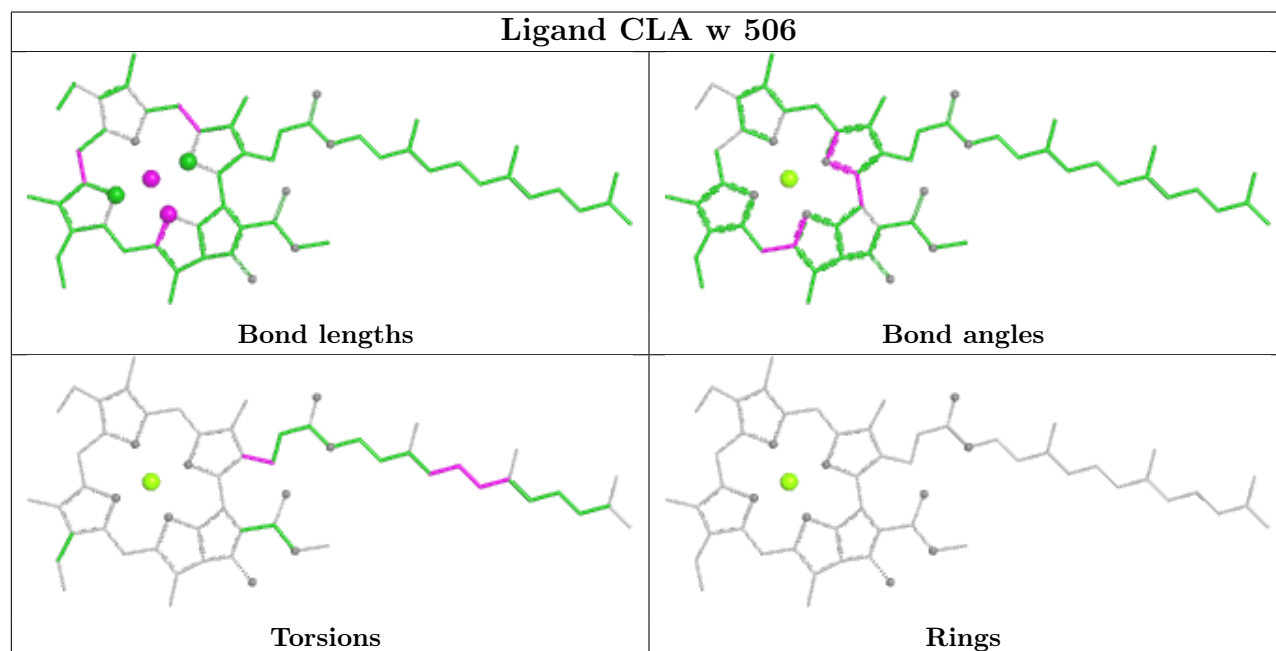
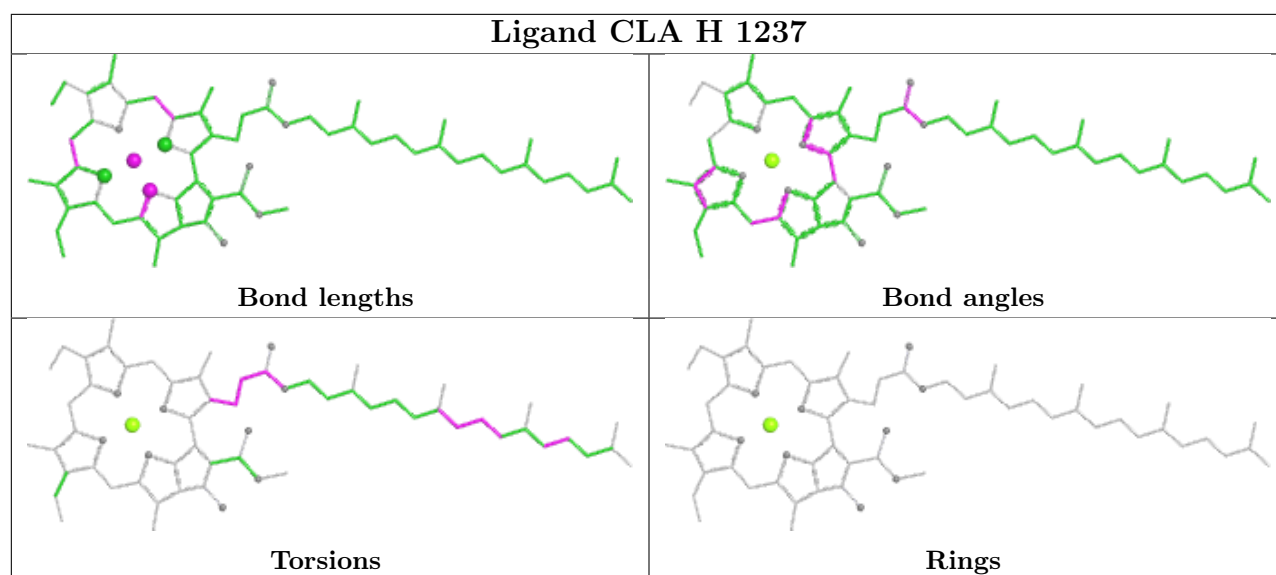


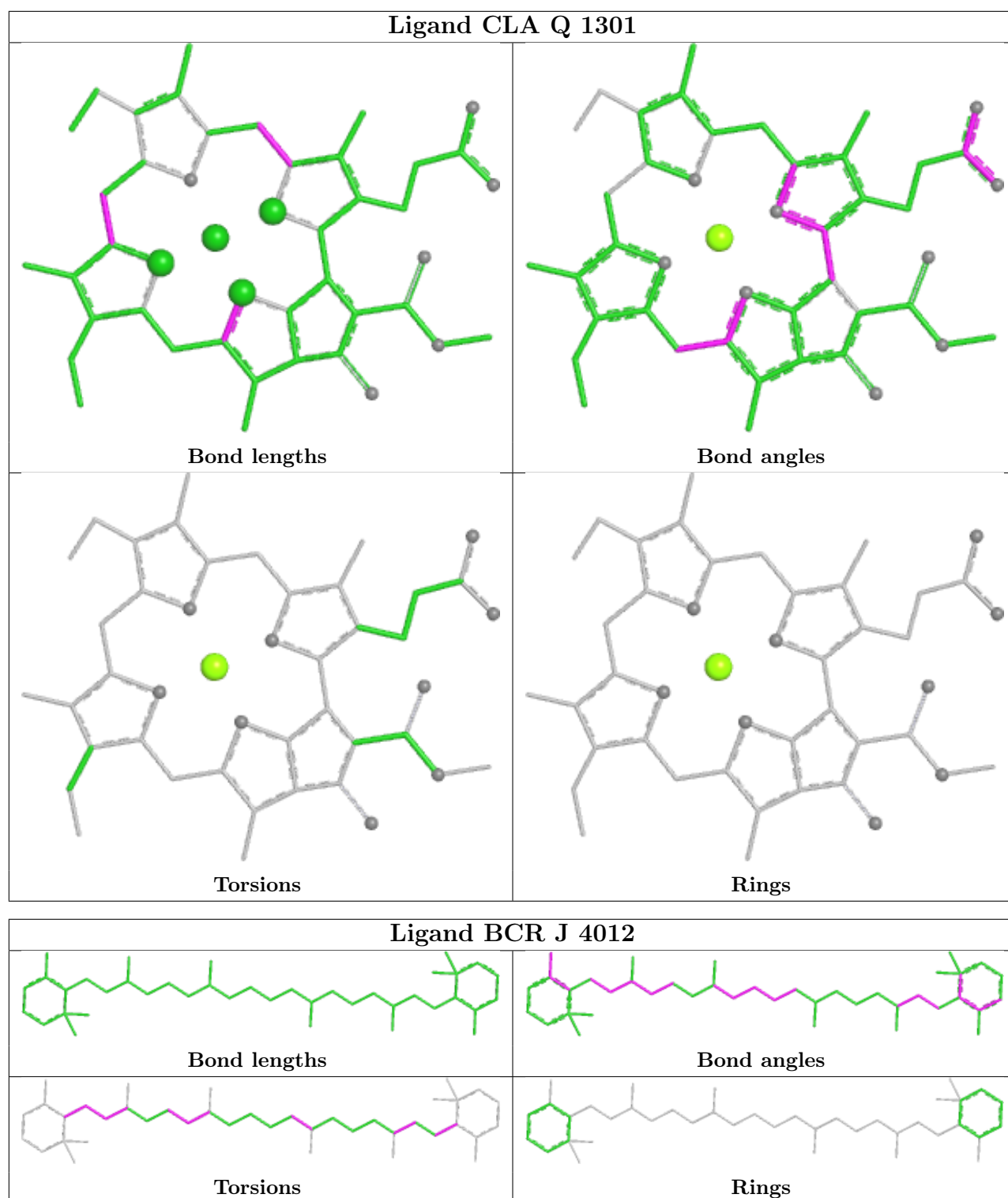


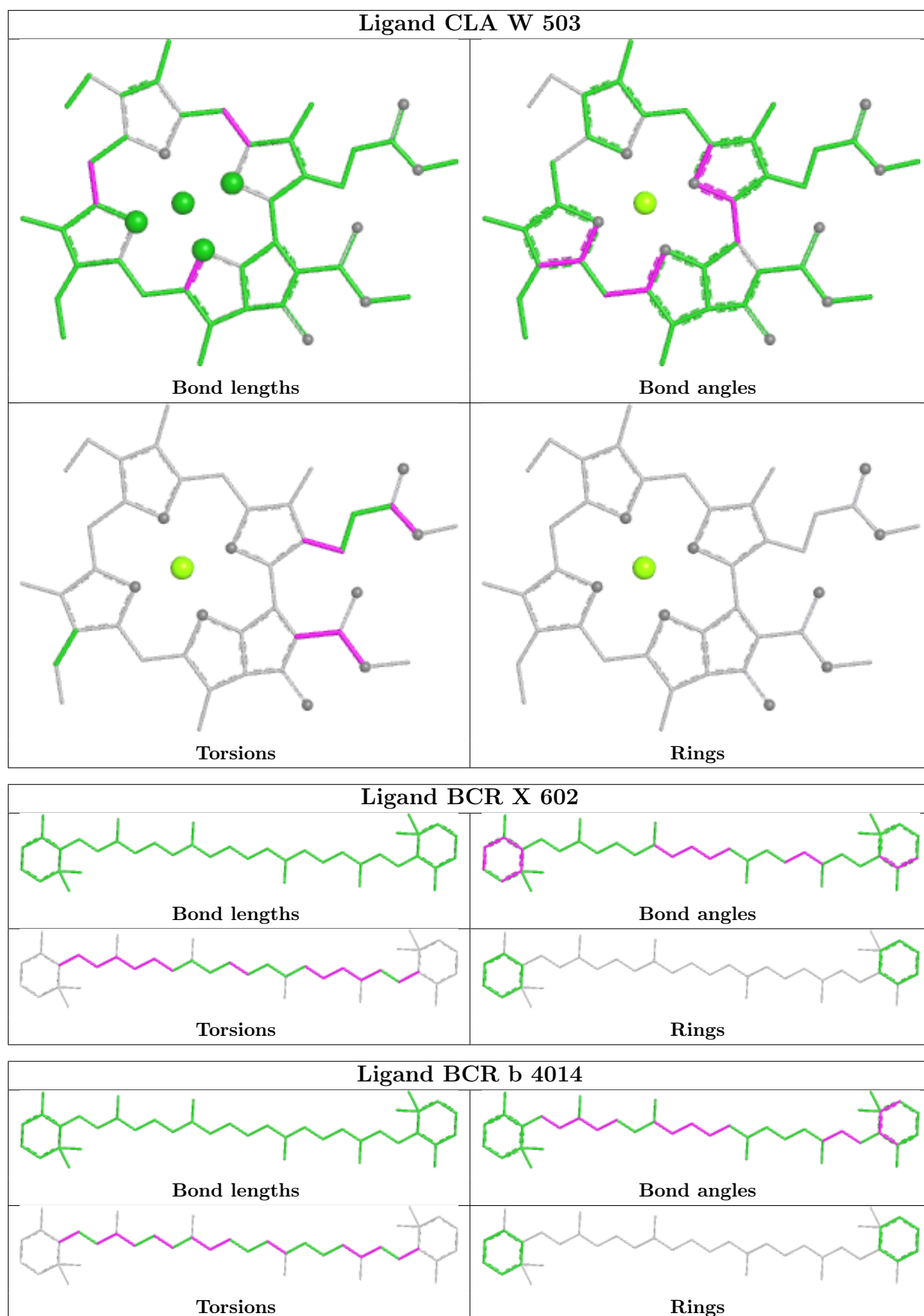


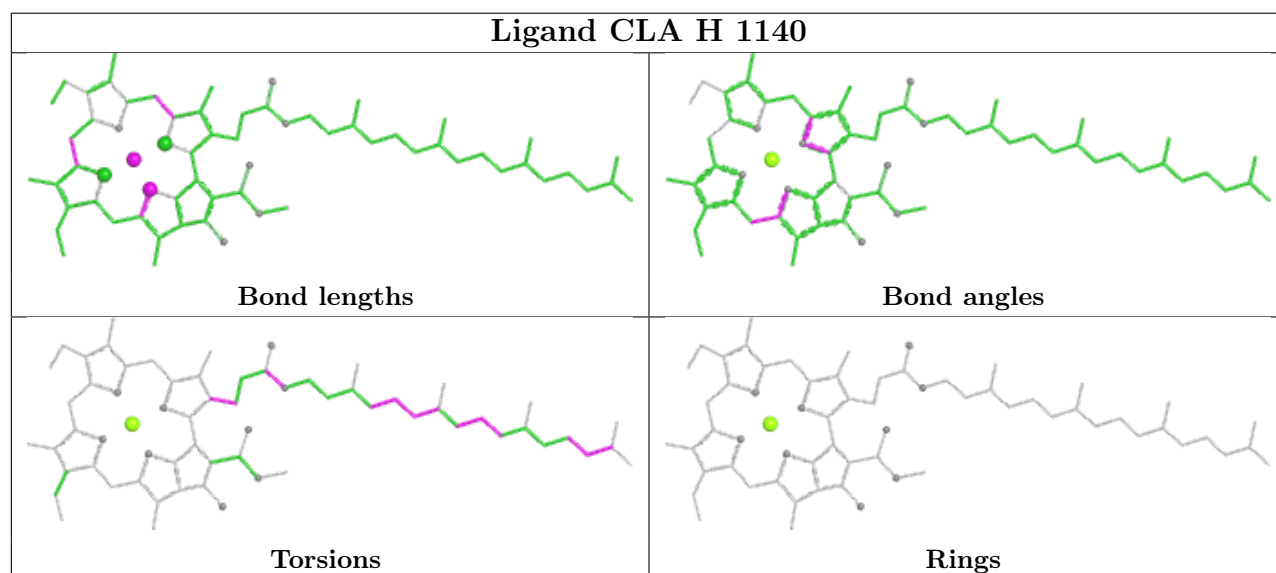
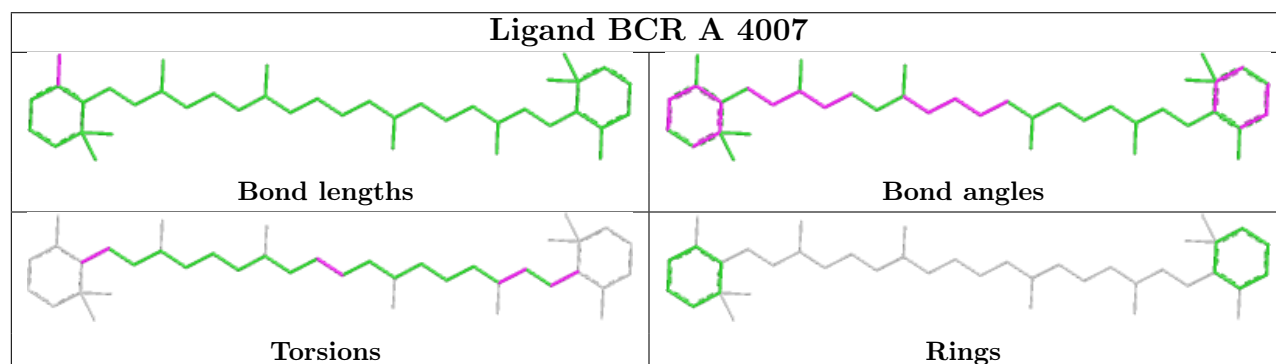
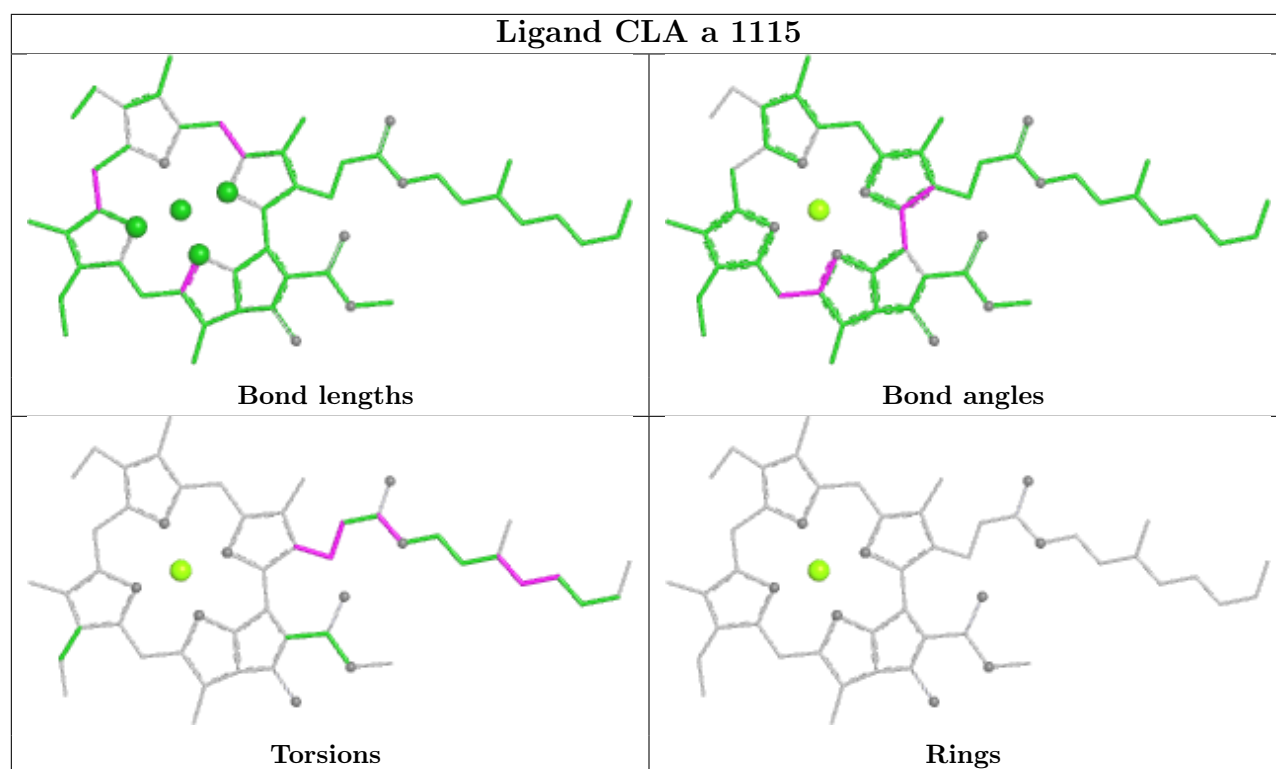


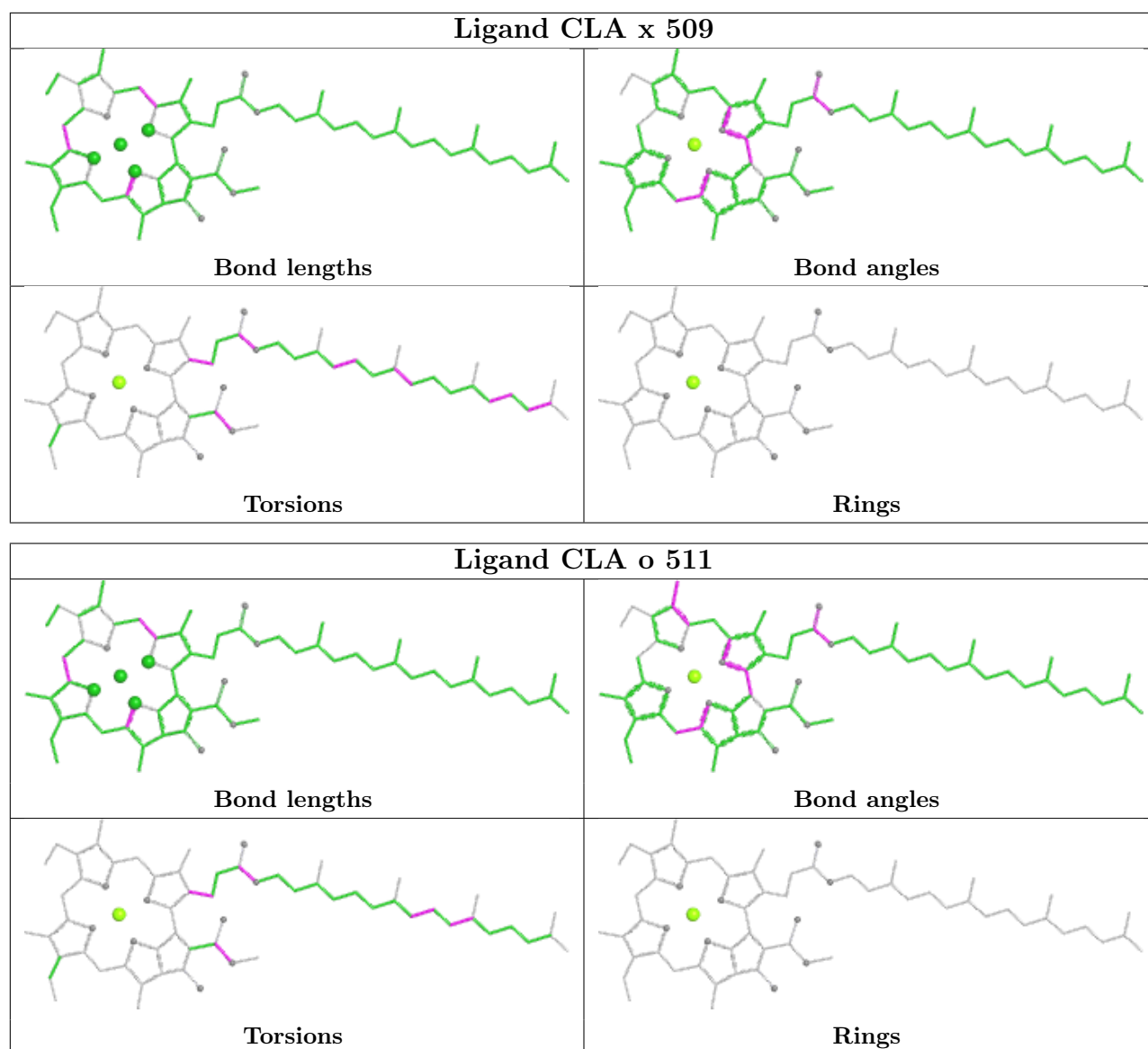




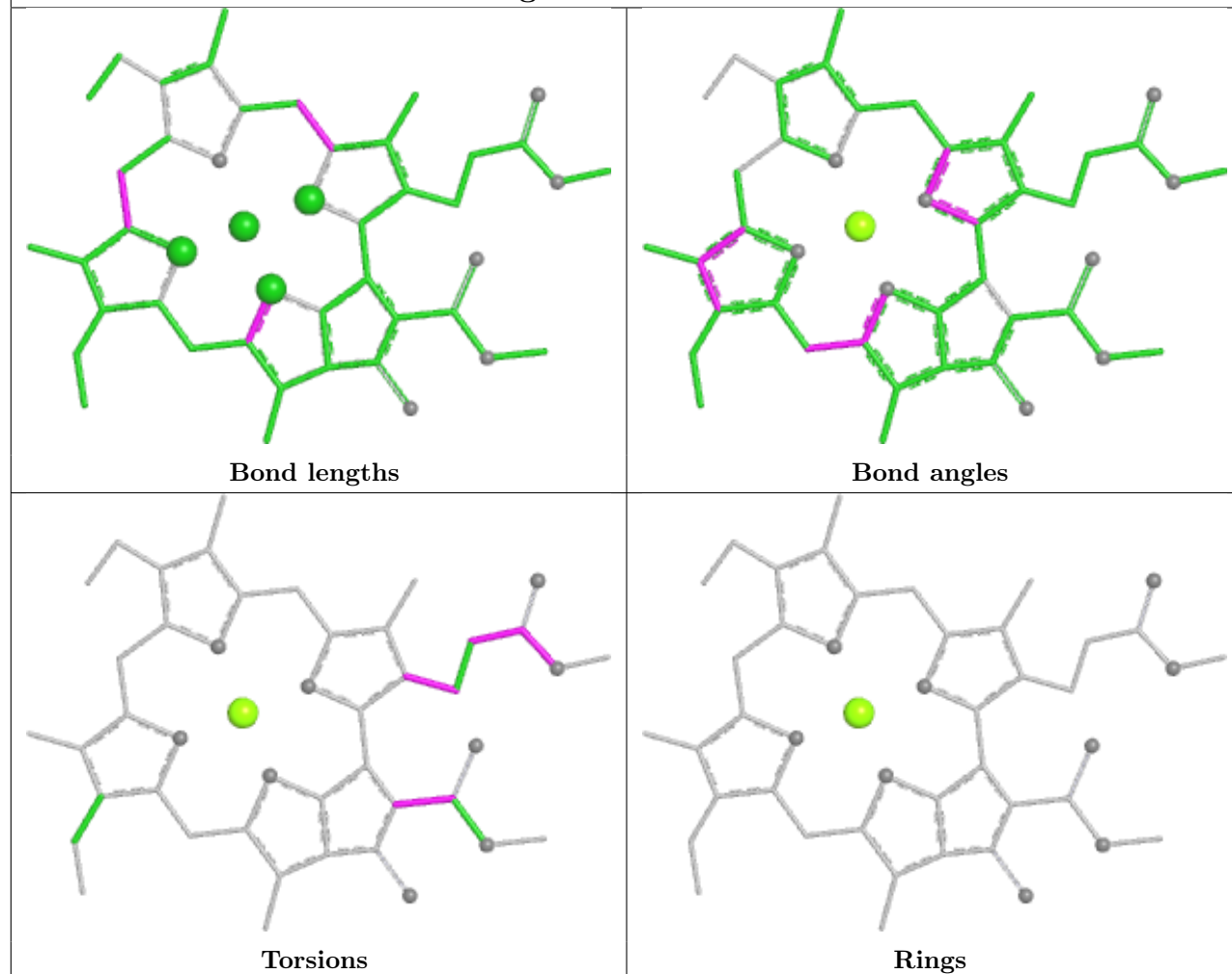




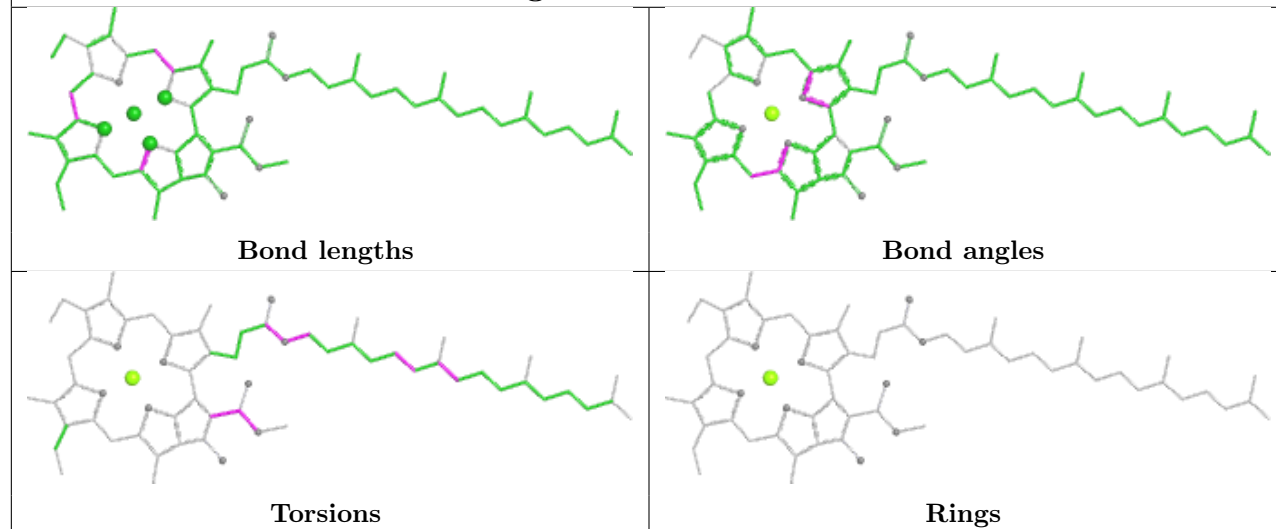


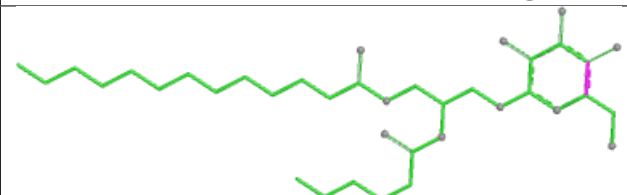
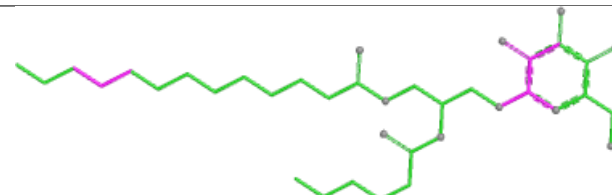
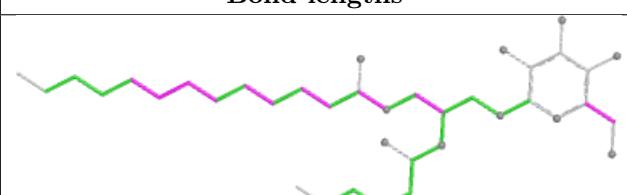
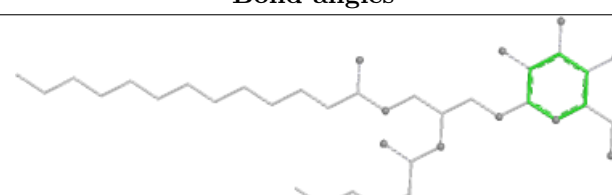


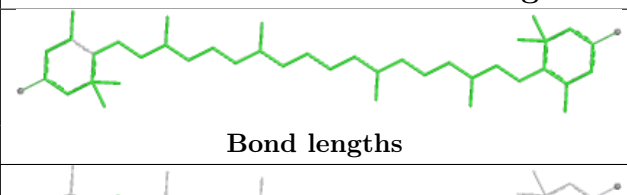
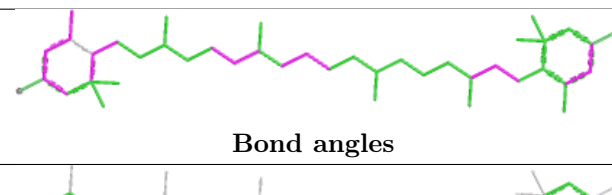
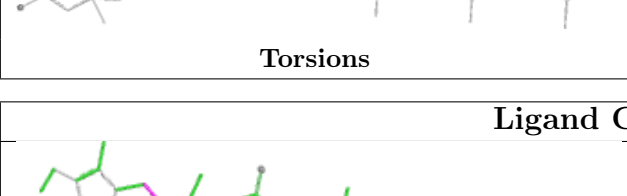

Ligand CLA s 513

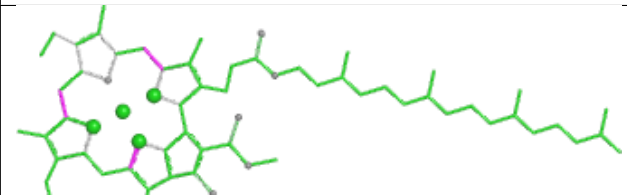
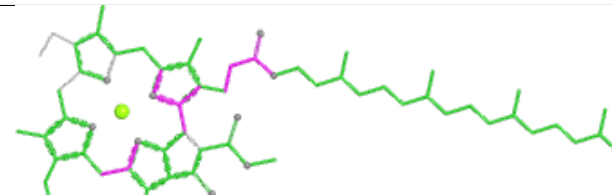
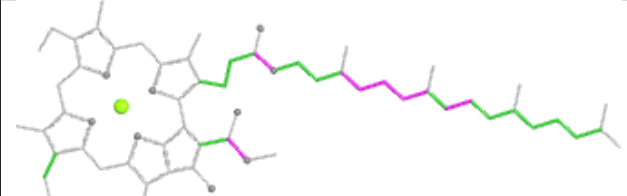
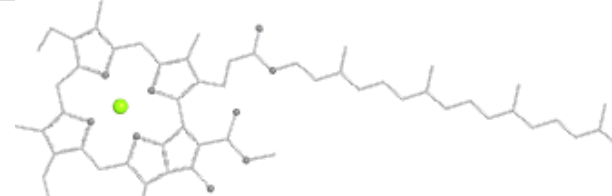


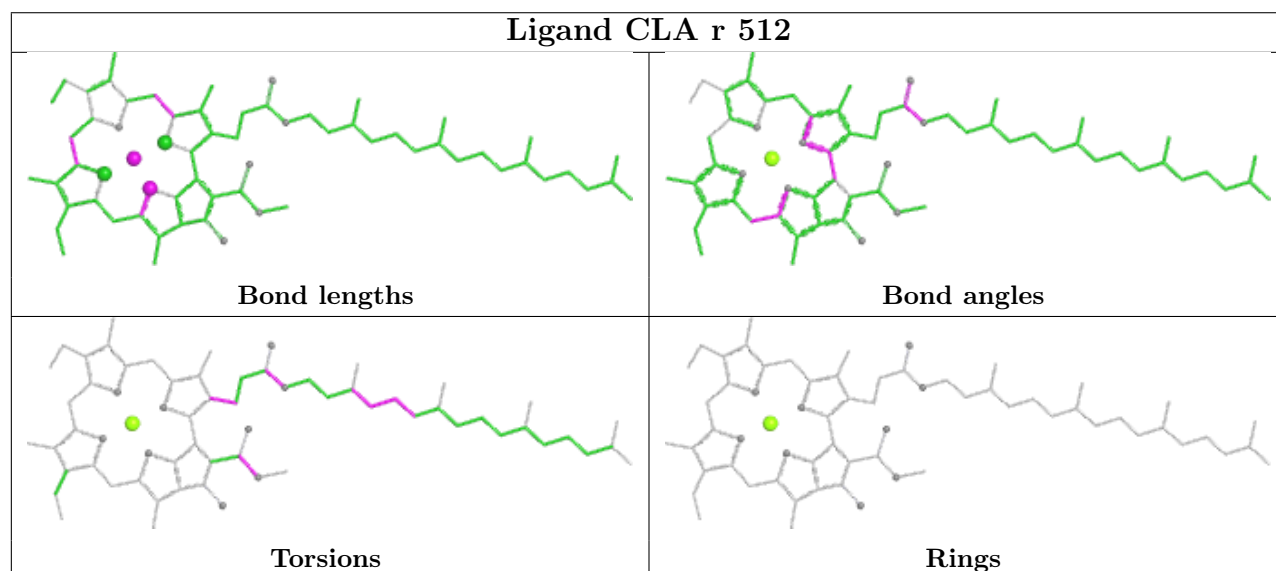
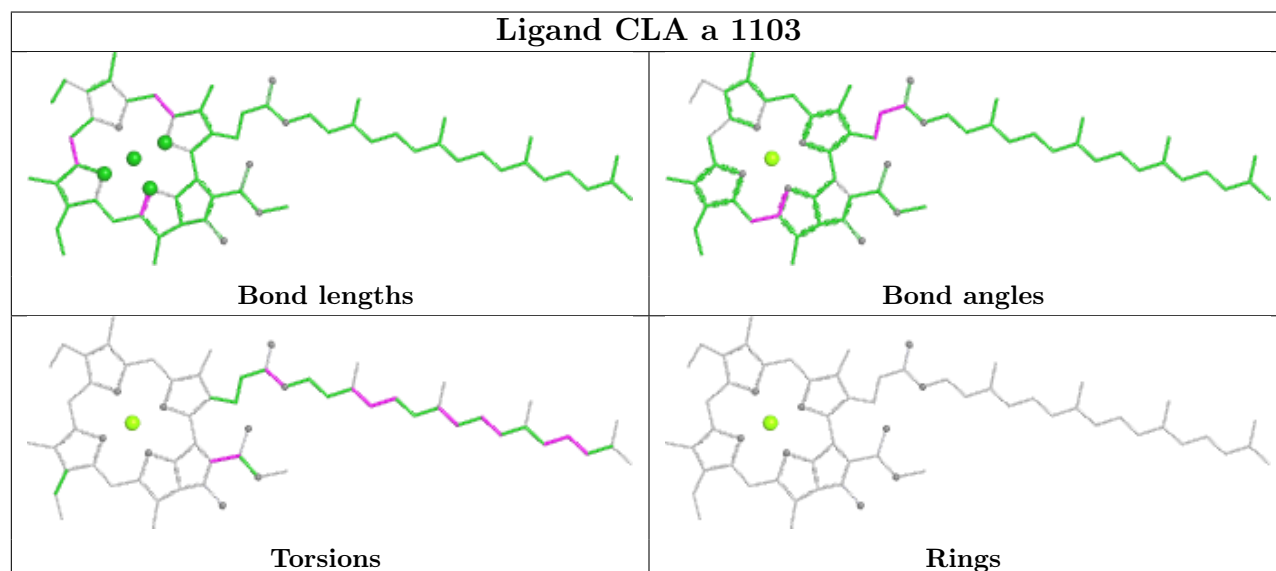
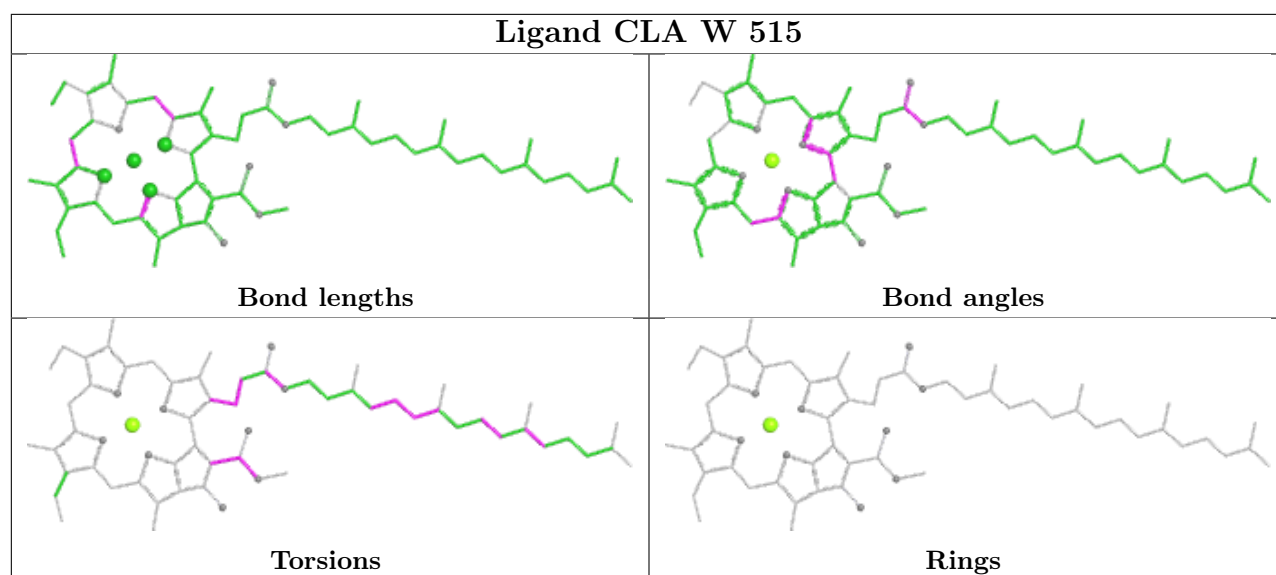
Ligand CLA W 507

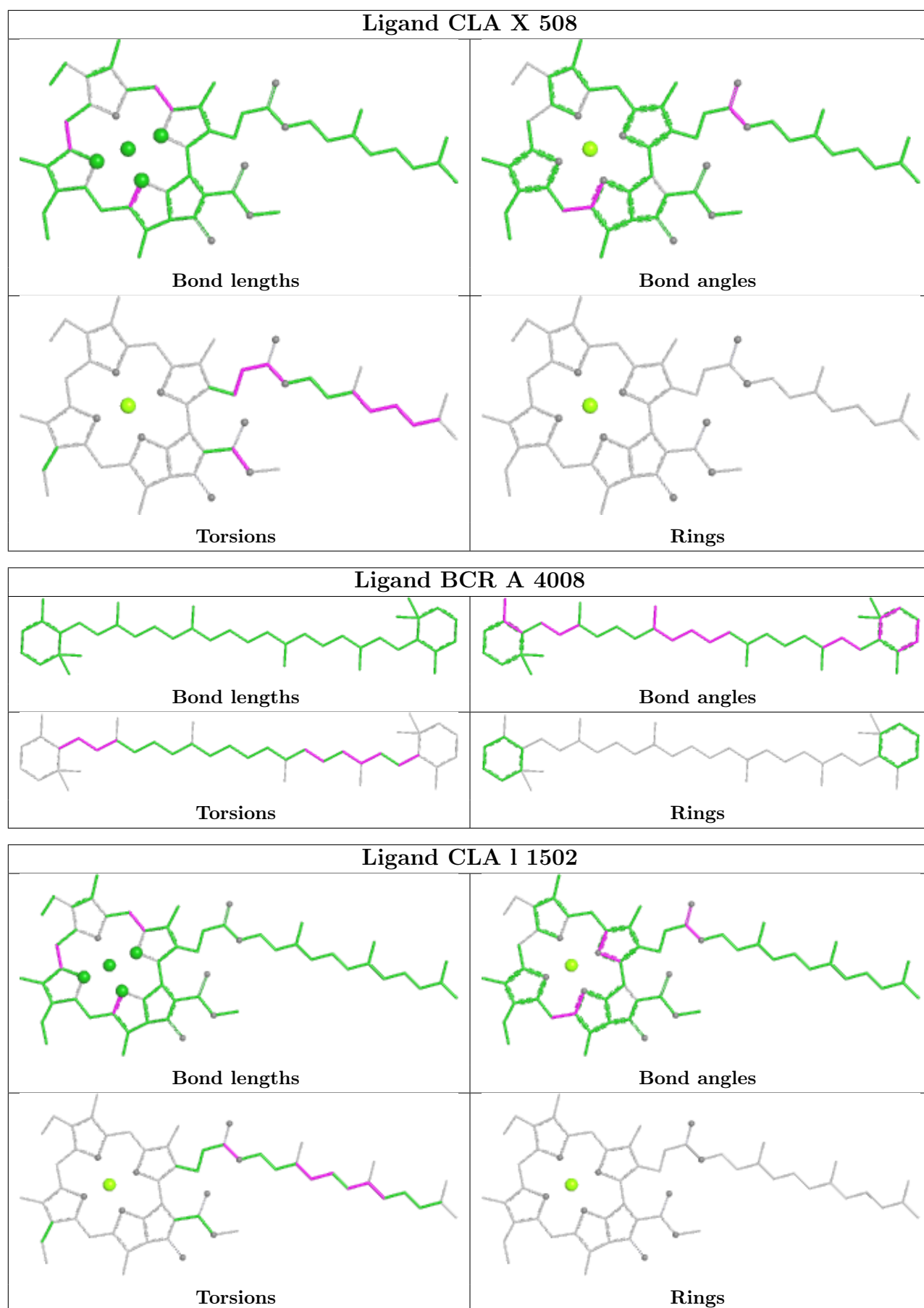


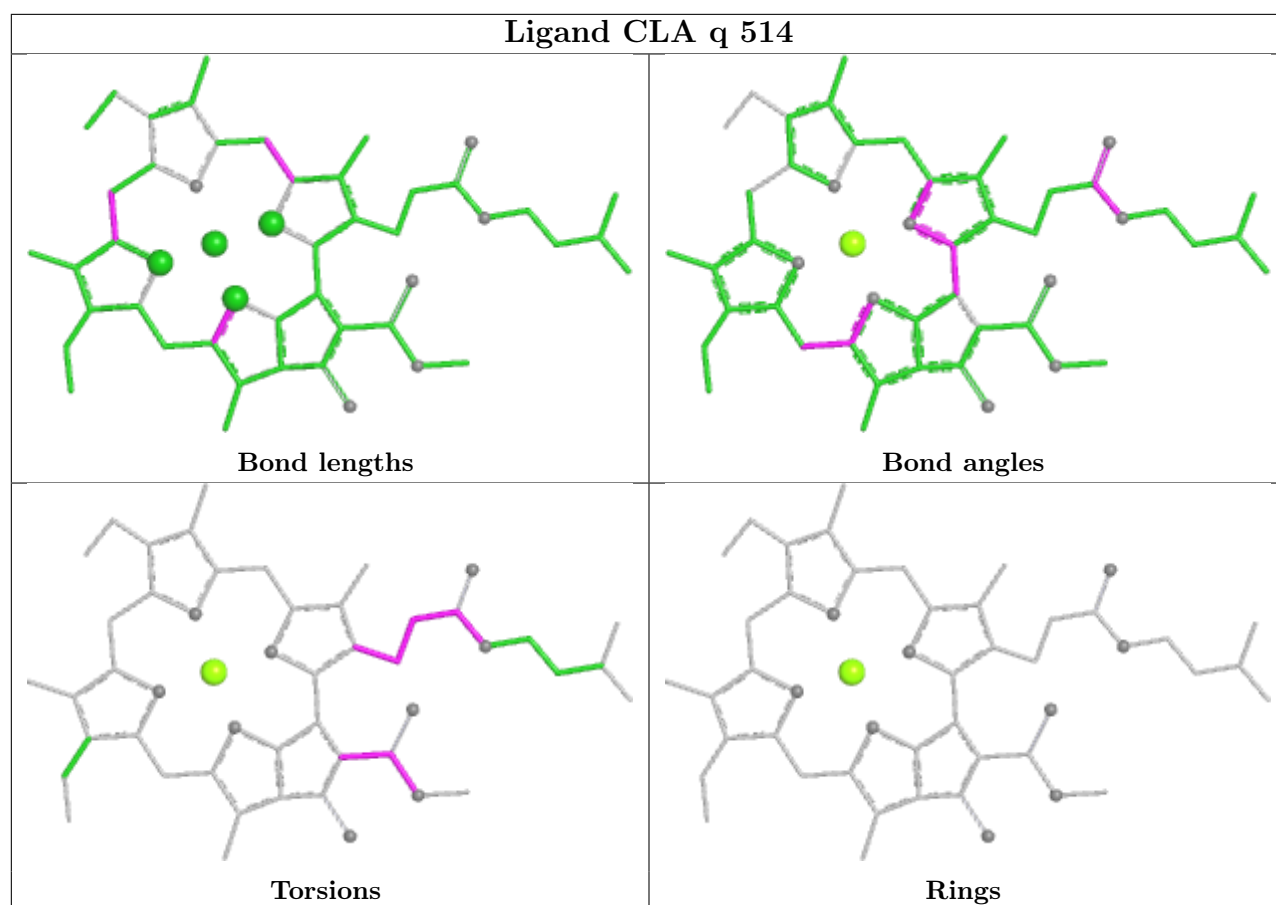
Ligand LMG a 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT w 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

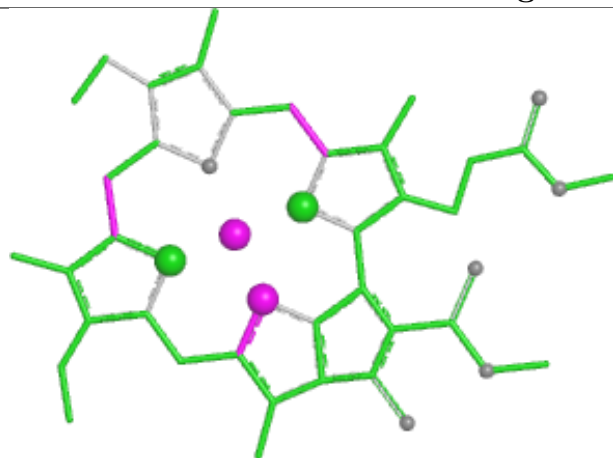
Ligand CLA v 512	
	
Bond lengths	Bond angles
	
Torsions	Rings



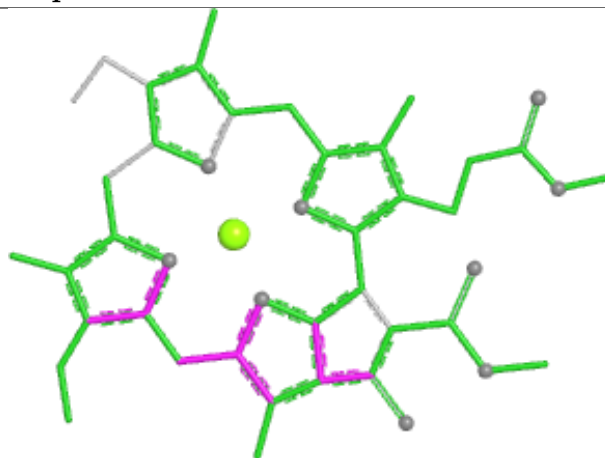




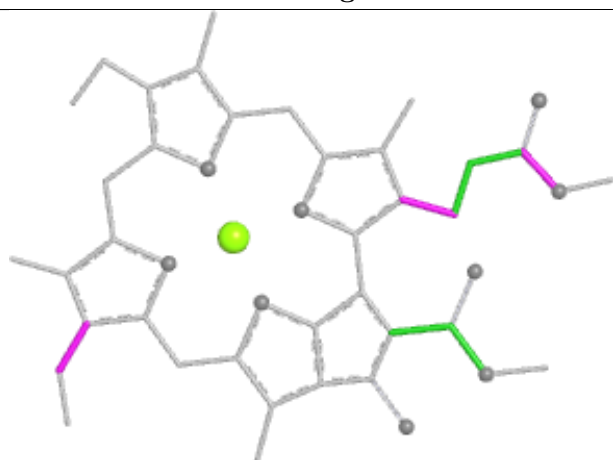
Ligand CLA p 503



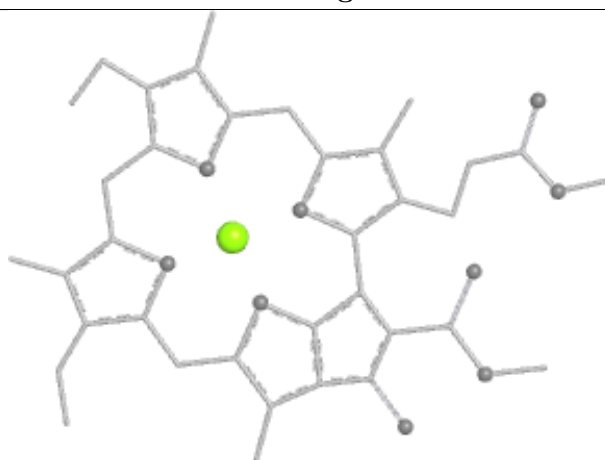
Bond lengths



Bond angles

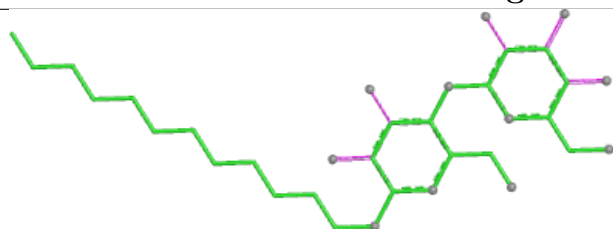


Torsions

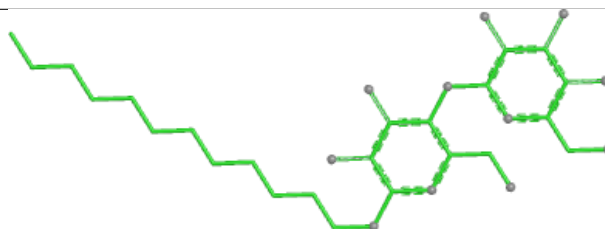


Rings

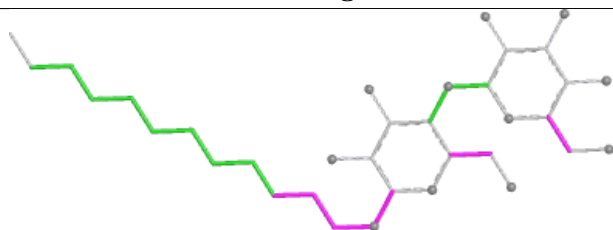
Ligand LMT a 4202



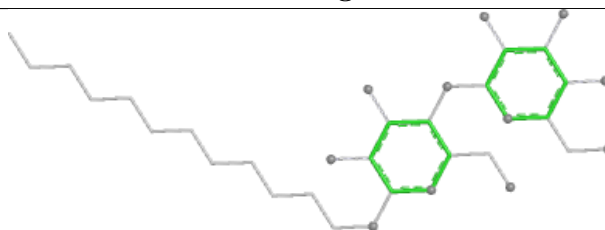
Bond lengths



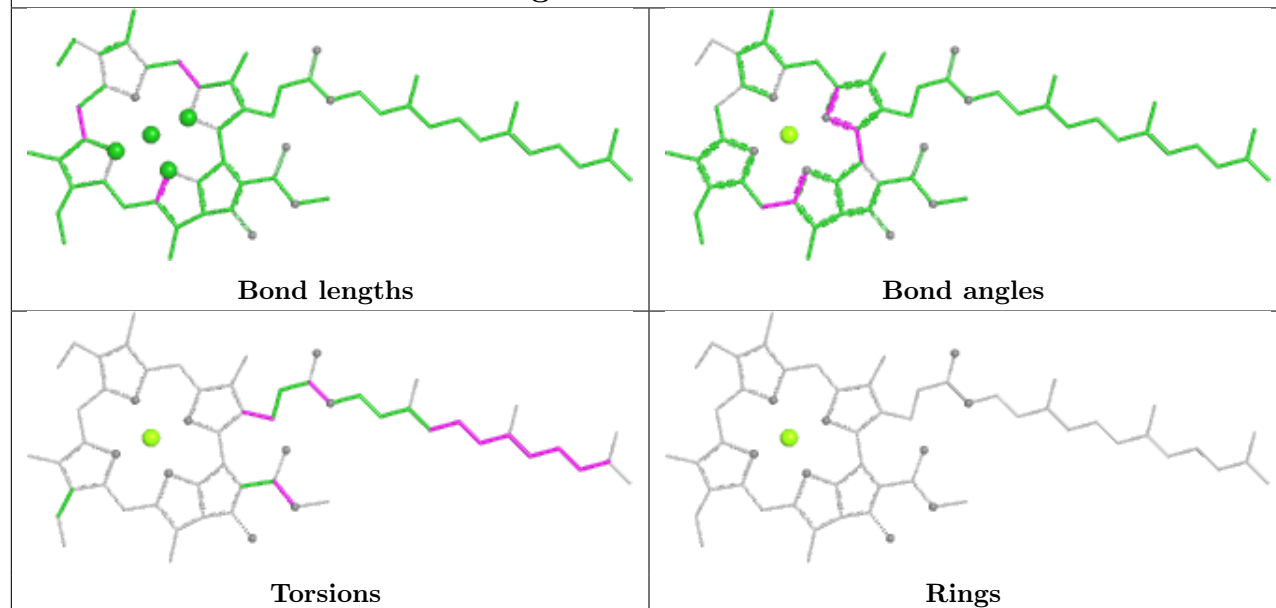
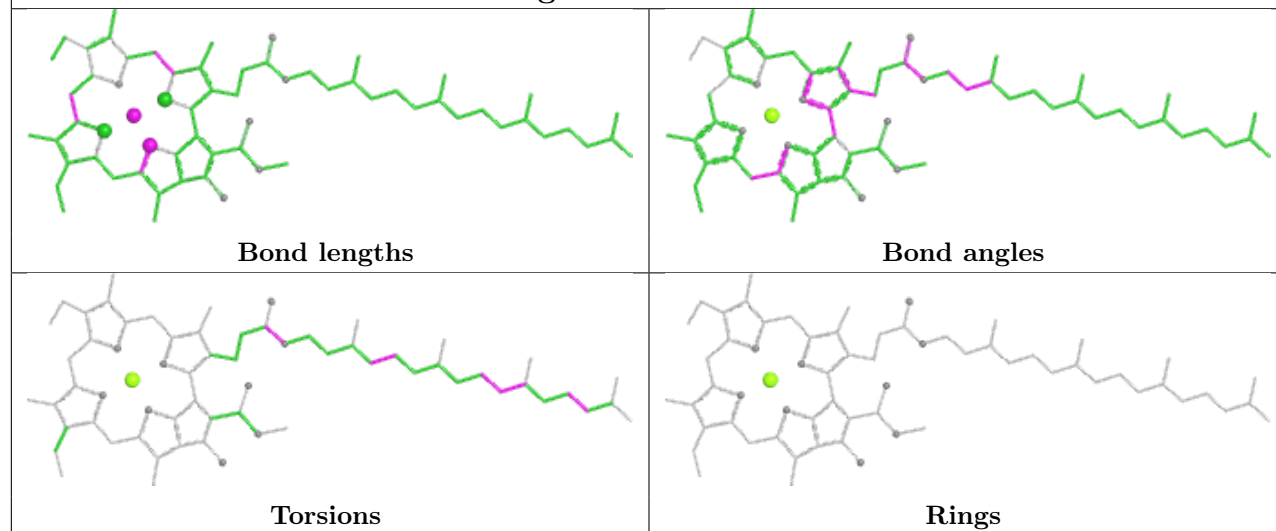
Bond angles



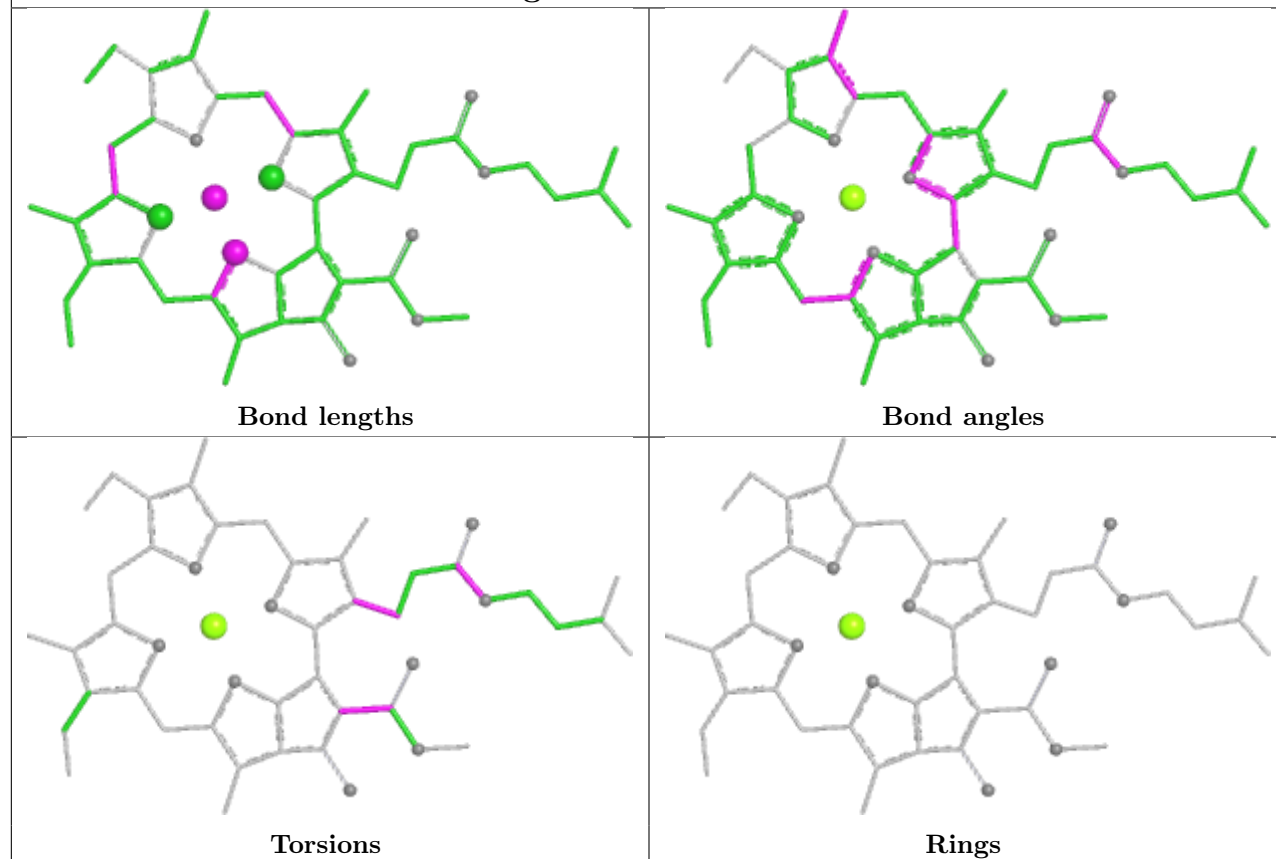
Torsions



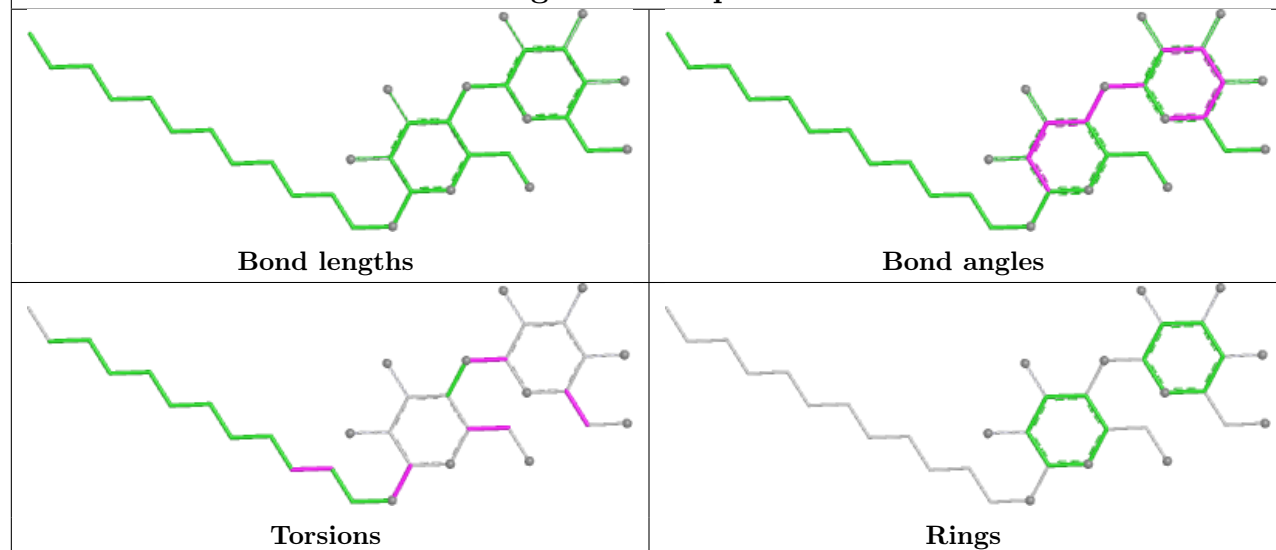
Rings

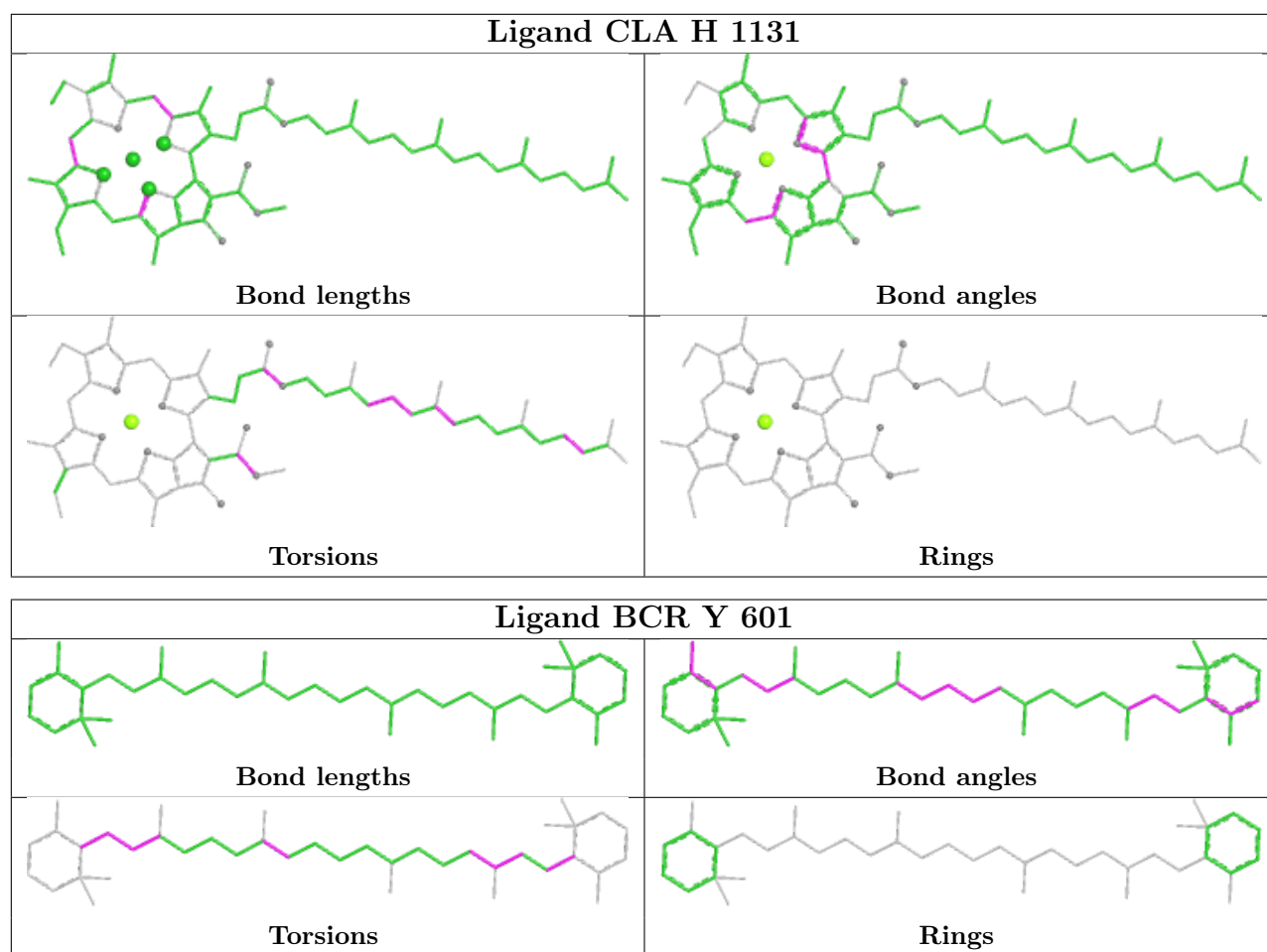
Ligand CLA X 504**Ligand CLA s 512**

Ligand CLA B 1234

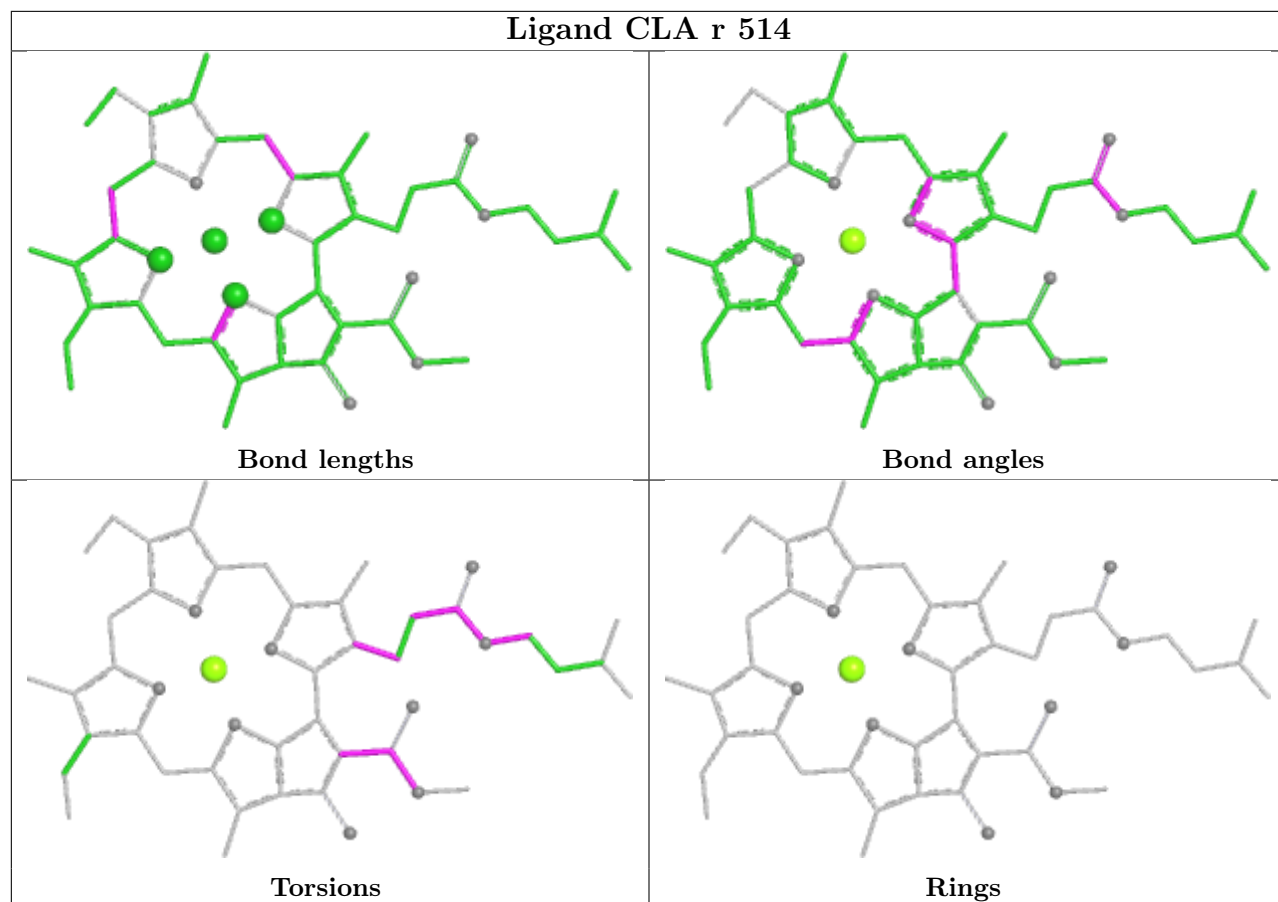


Ligand LMU p 606

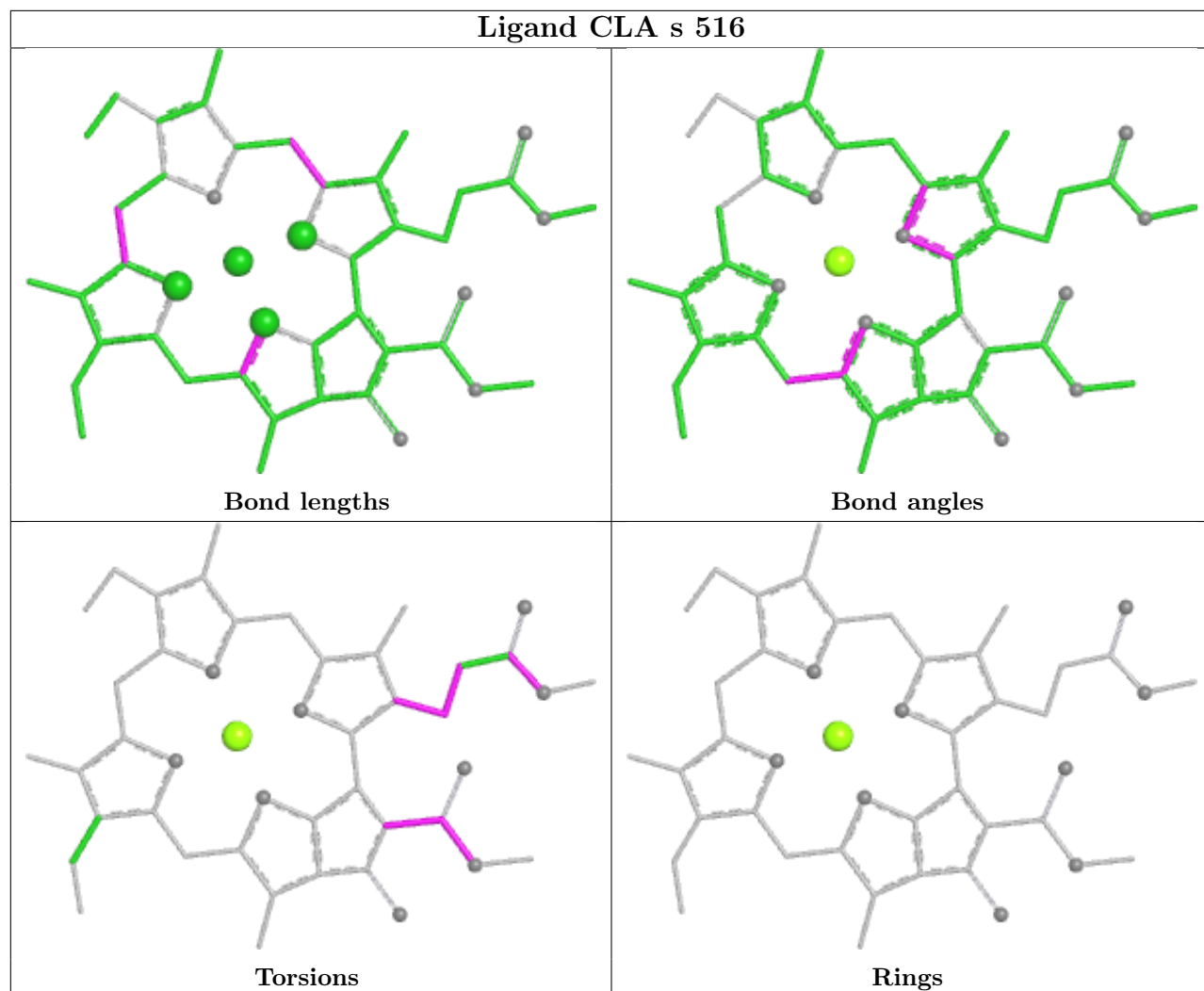




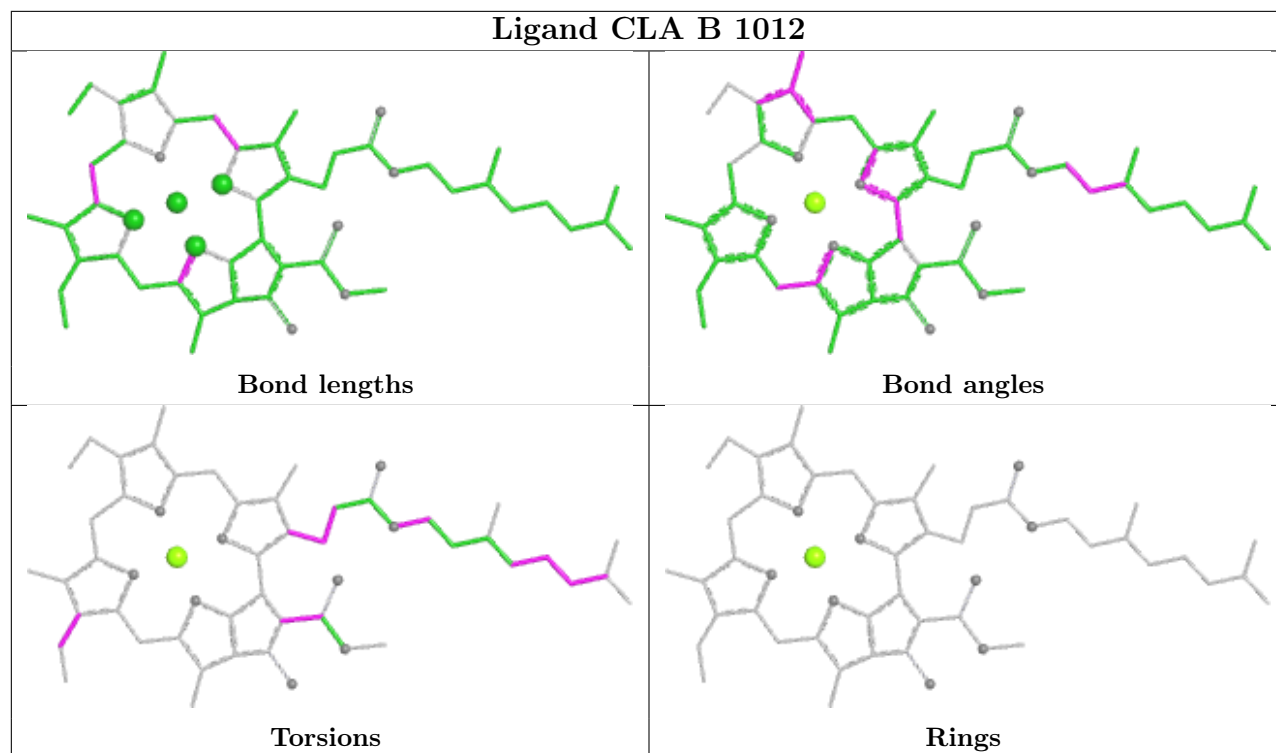
Ligand CLA r 514



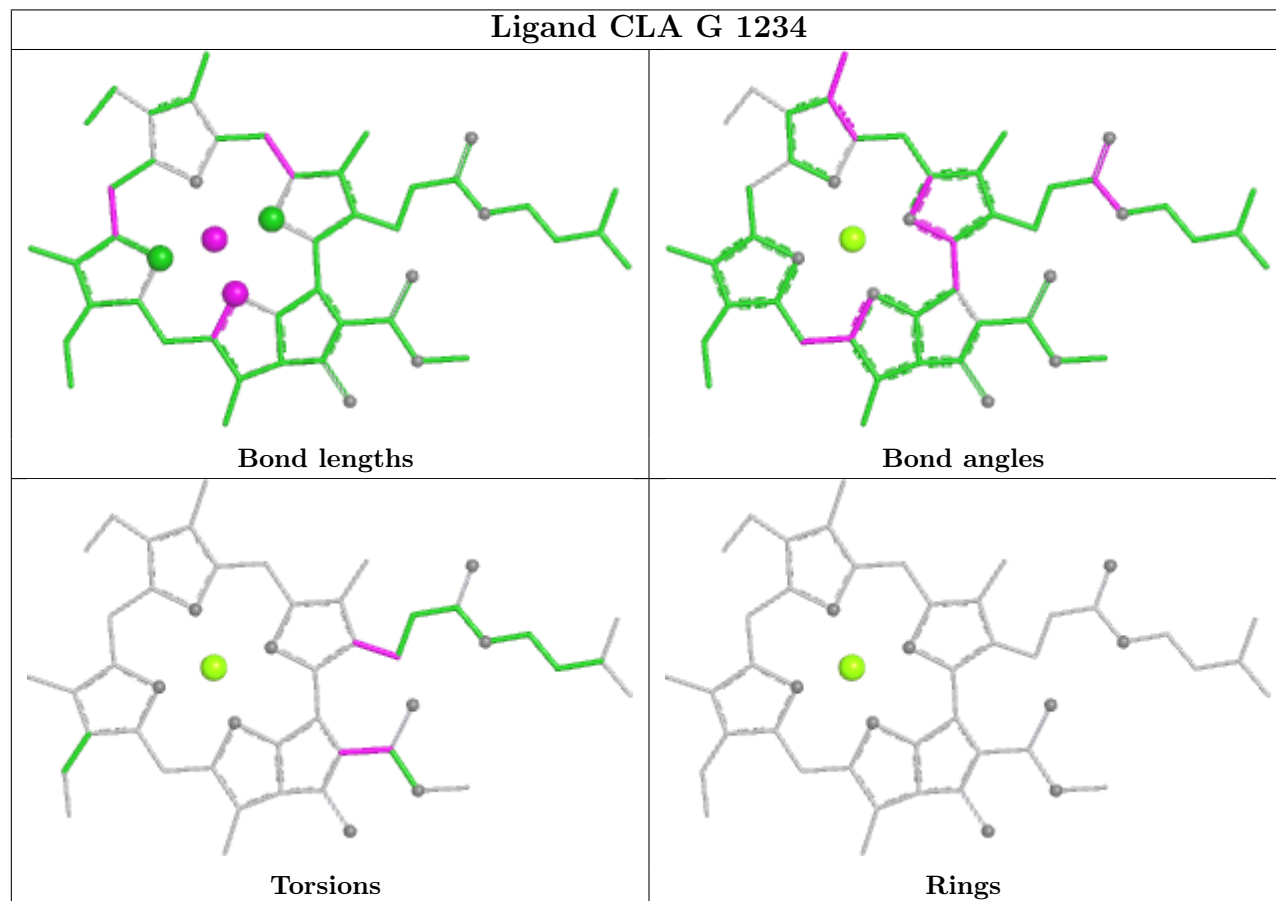
Ligand CLA s 516

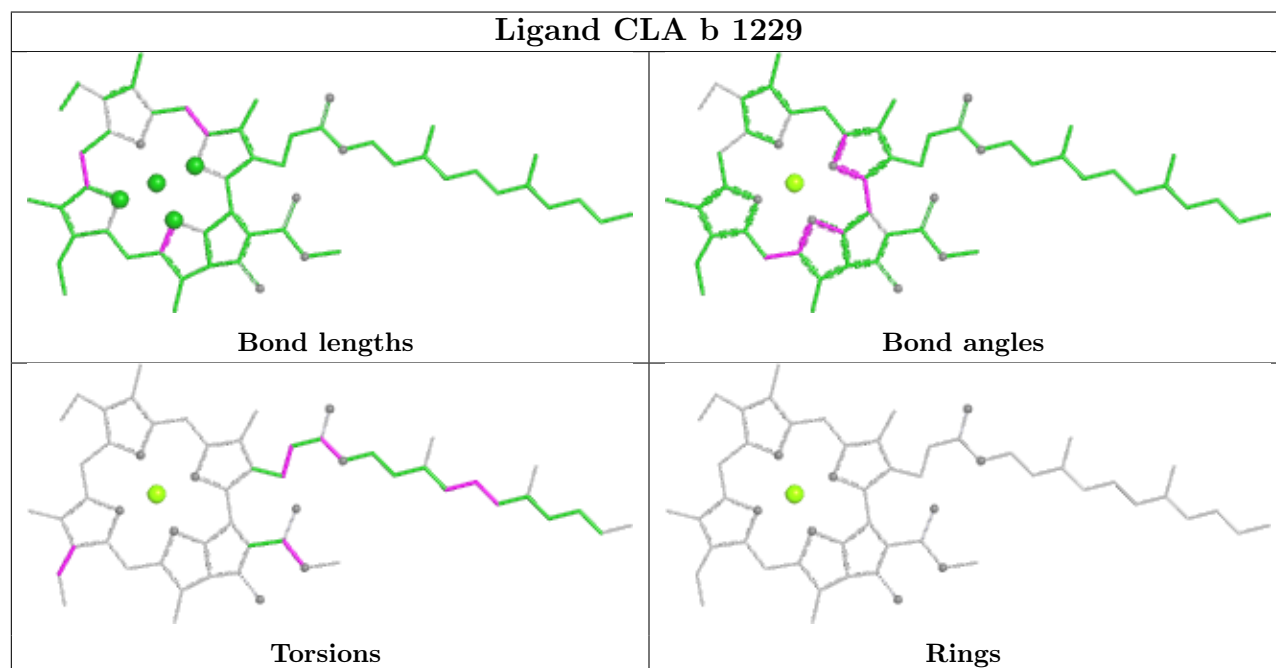
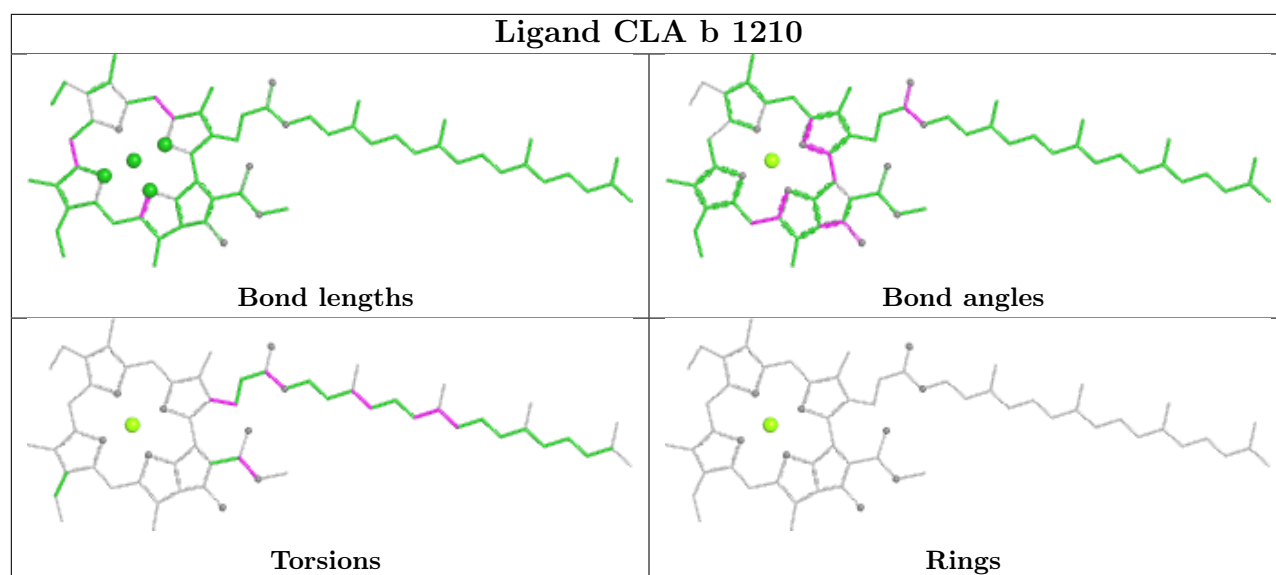


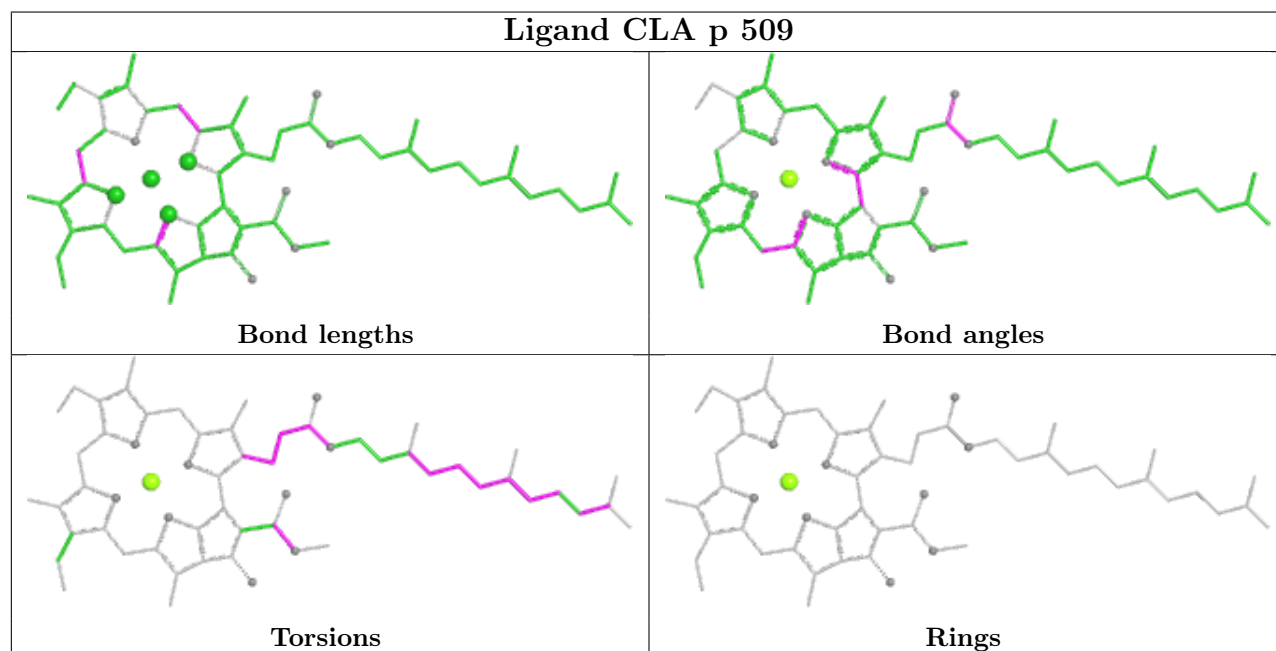
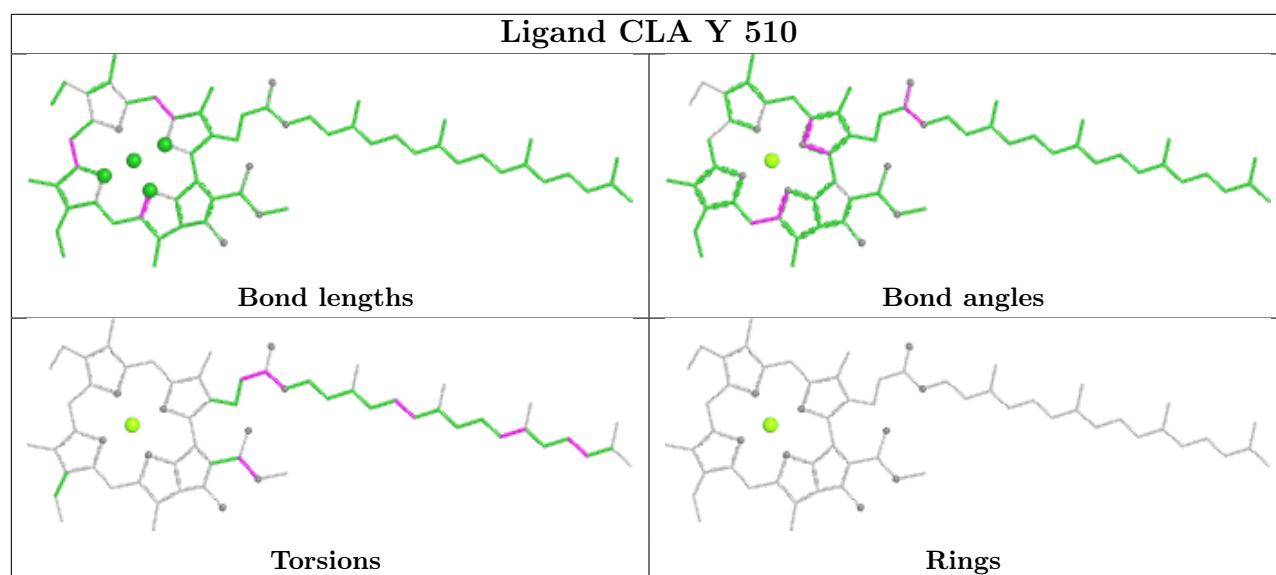
Ligand CLA B 1012



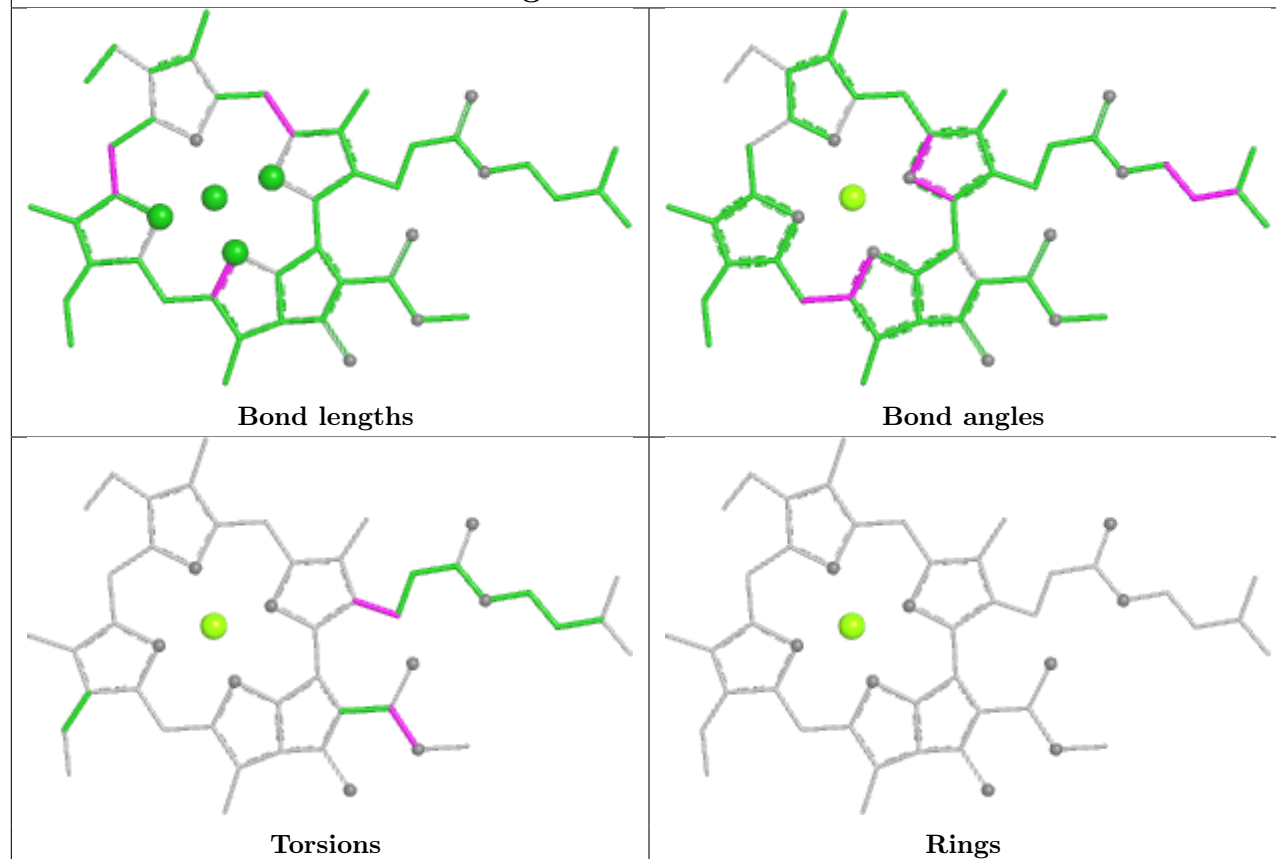
Ligand CLA G 1234



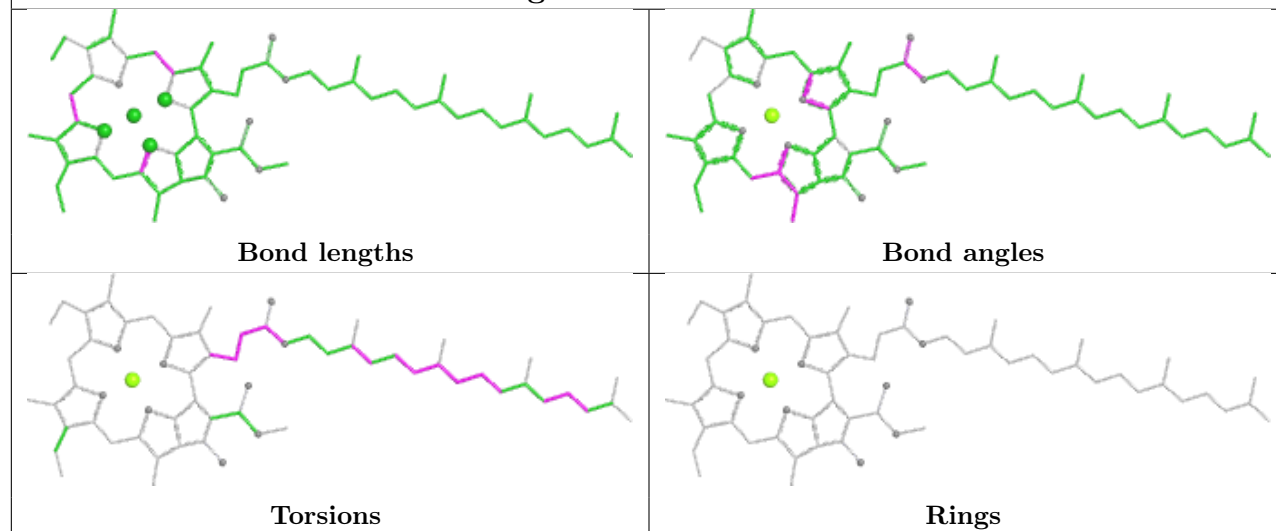


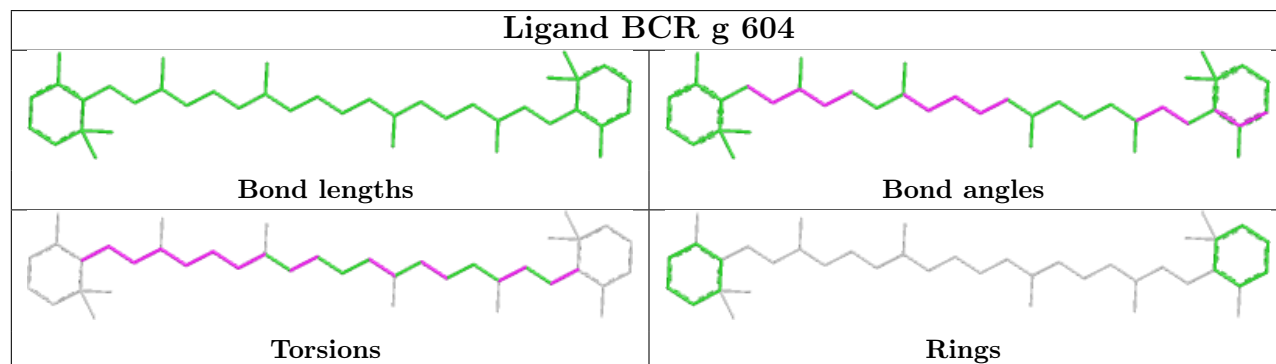
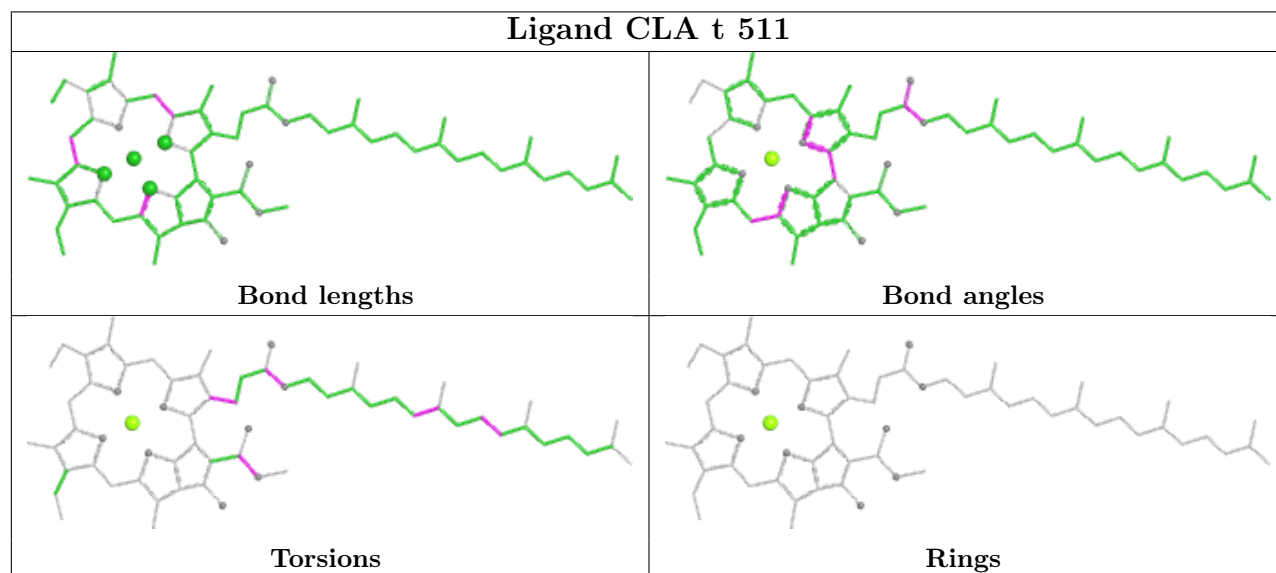
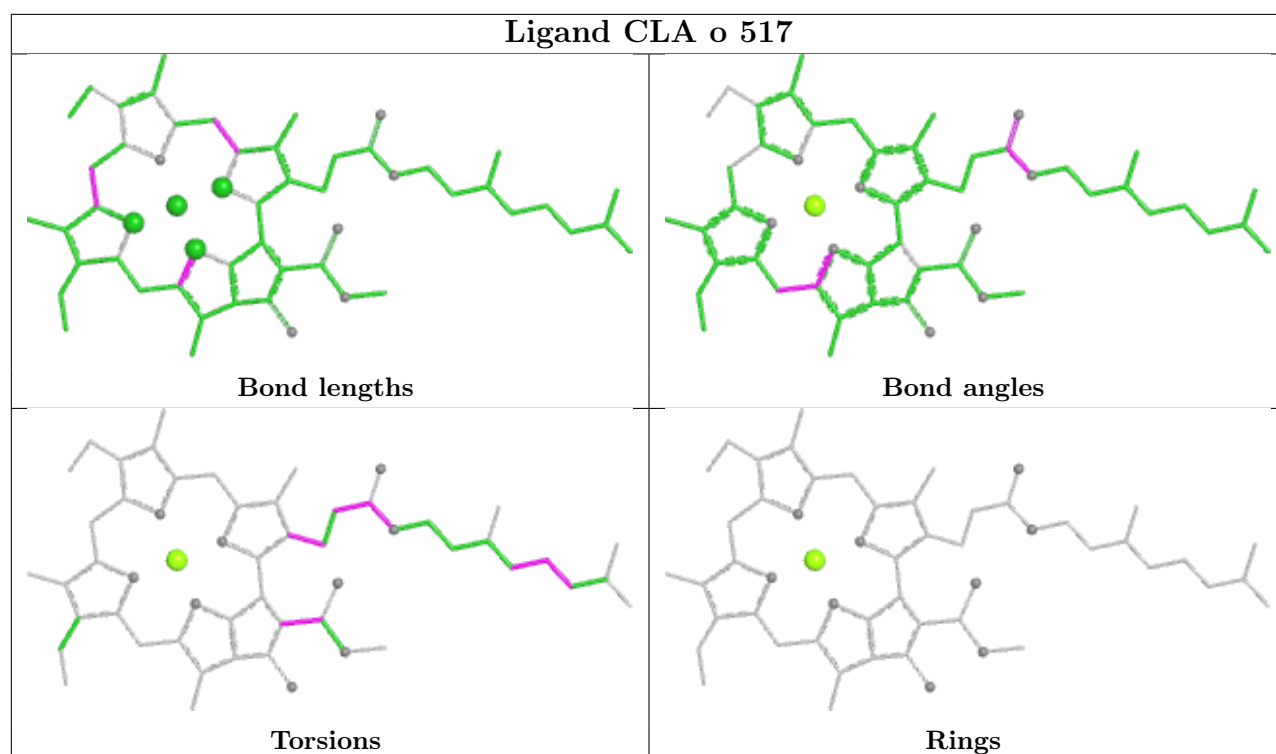


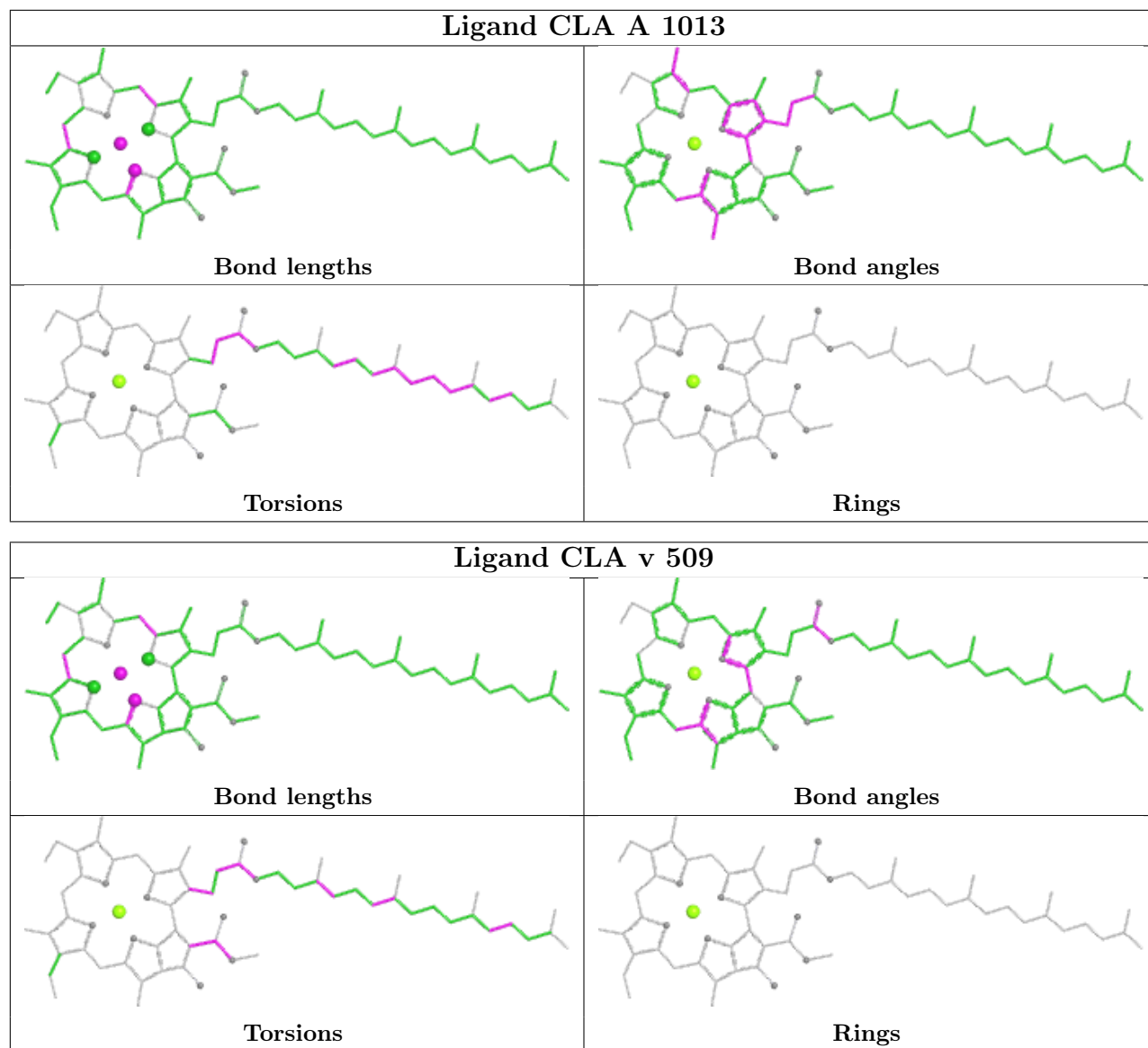
Ligand CLA A 1107

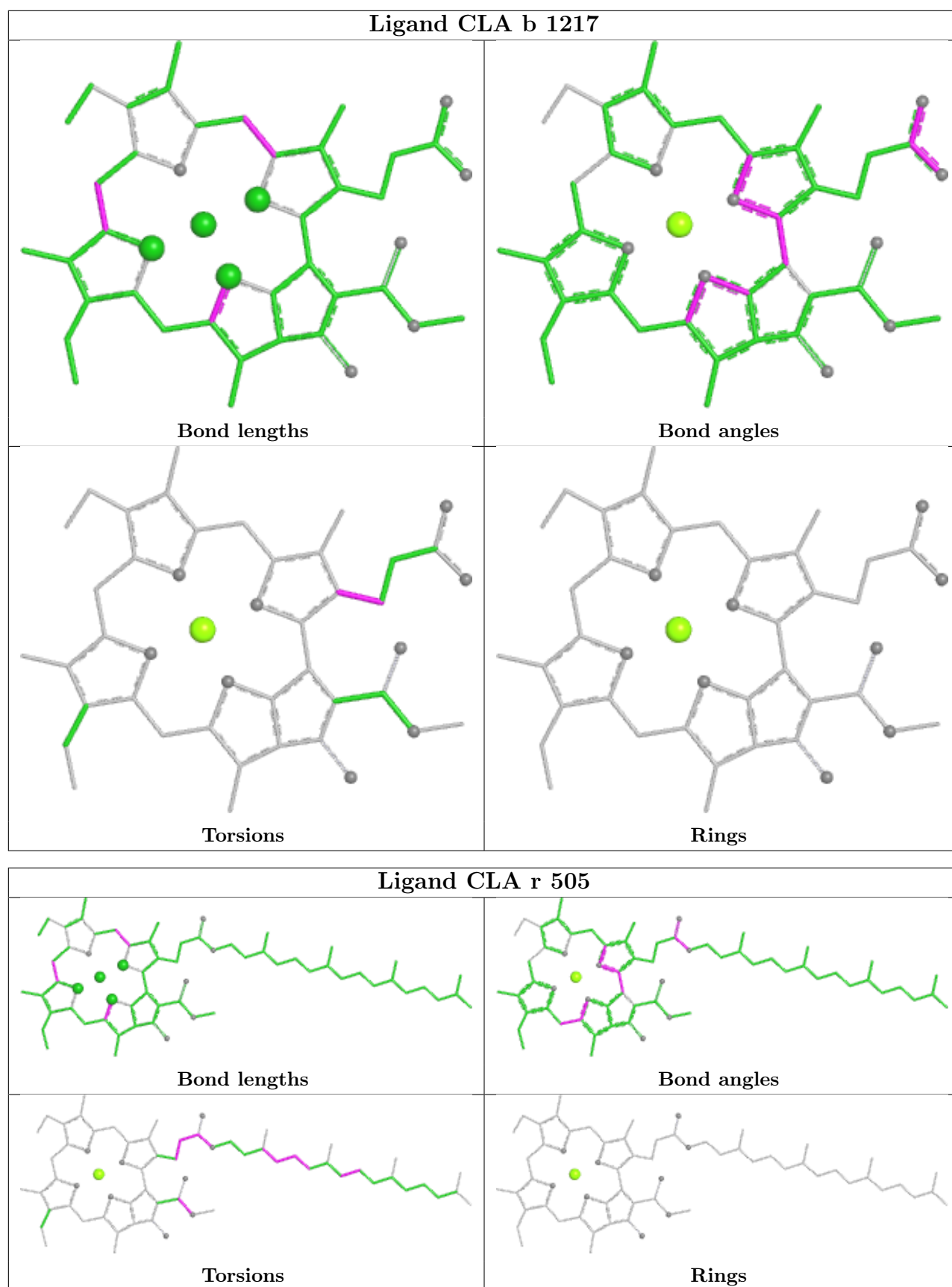


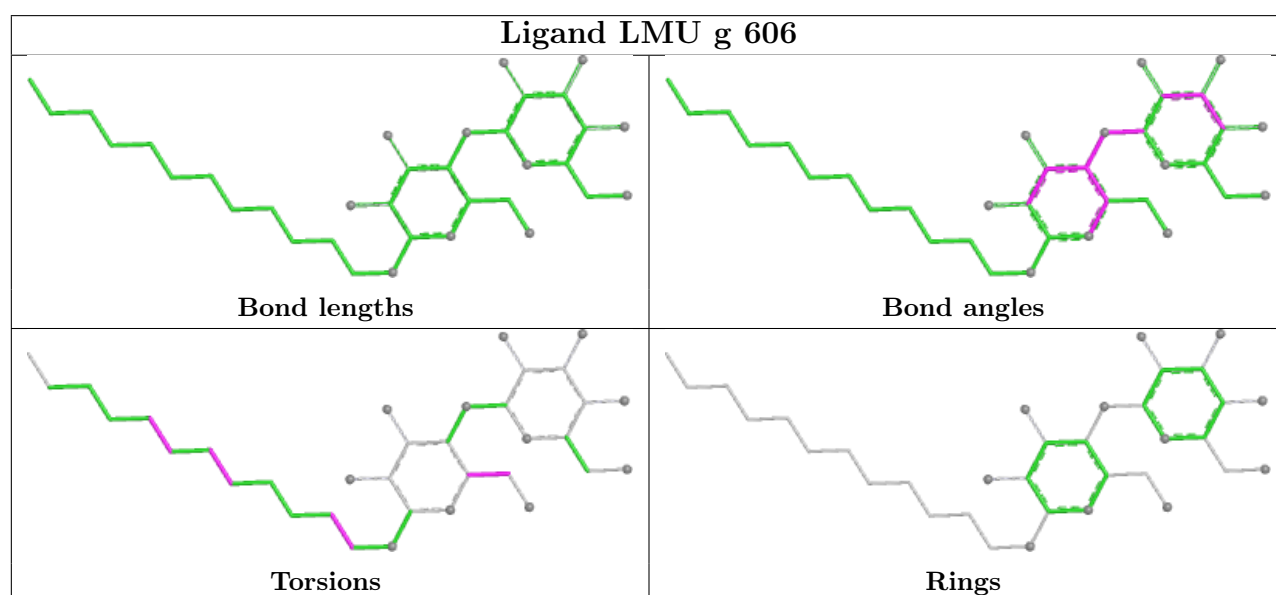
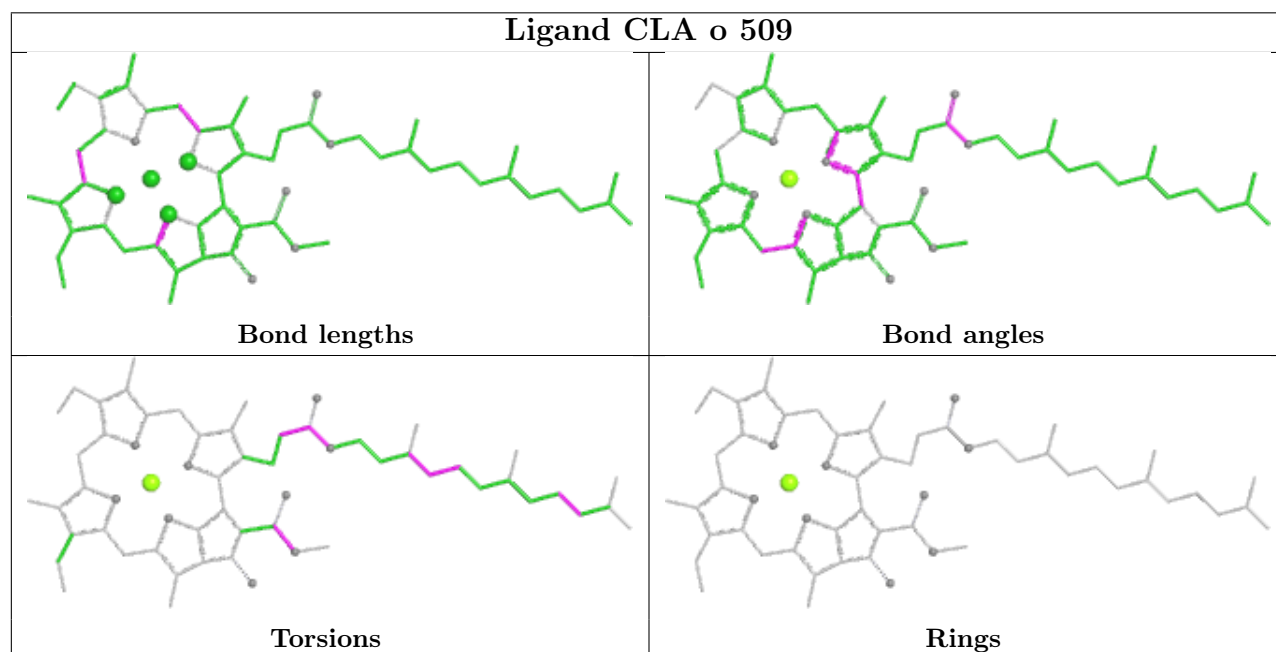
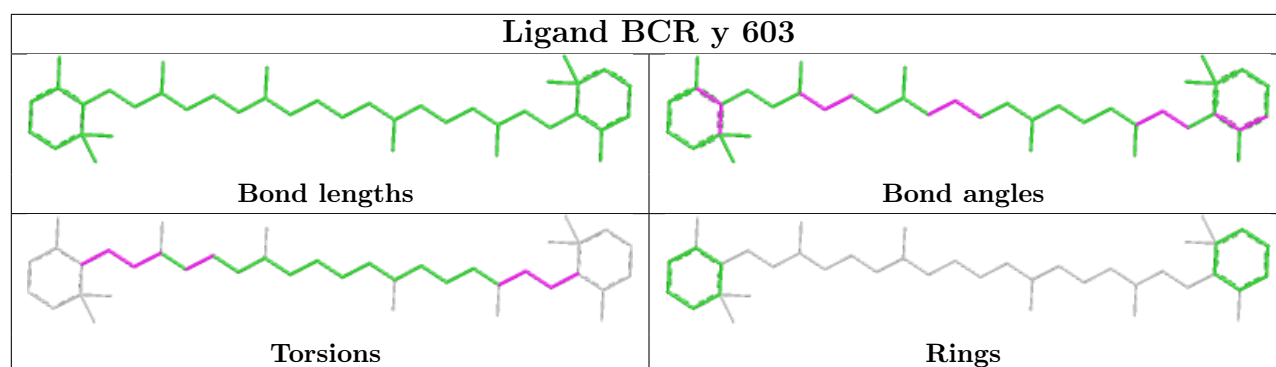
Ligand CLA a 1101



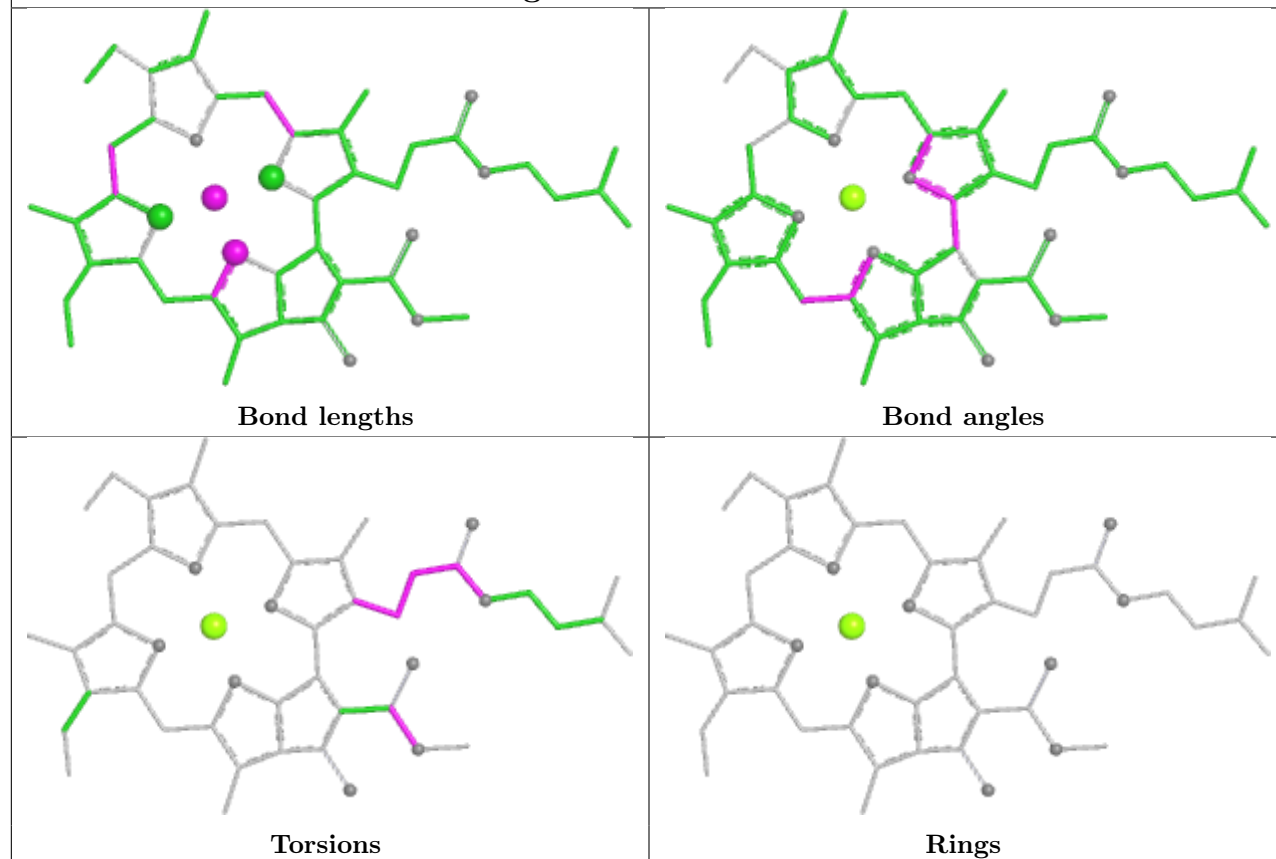




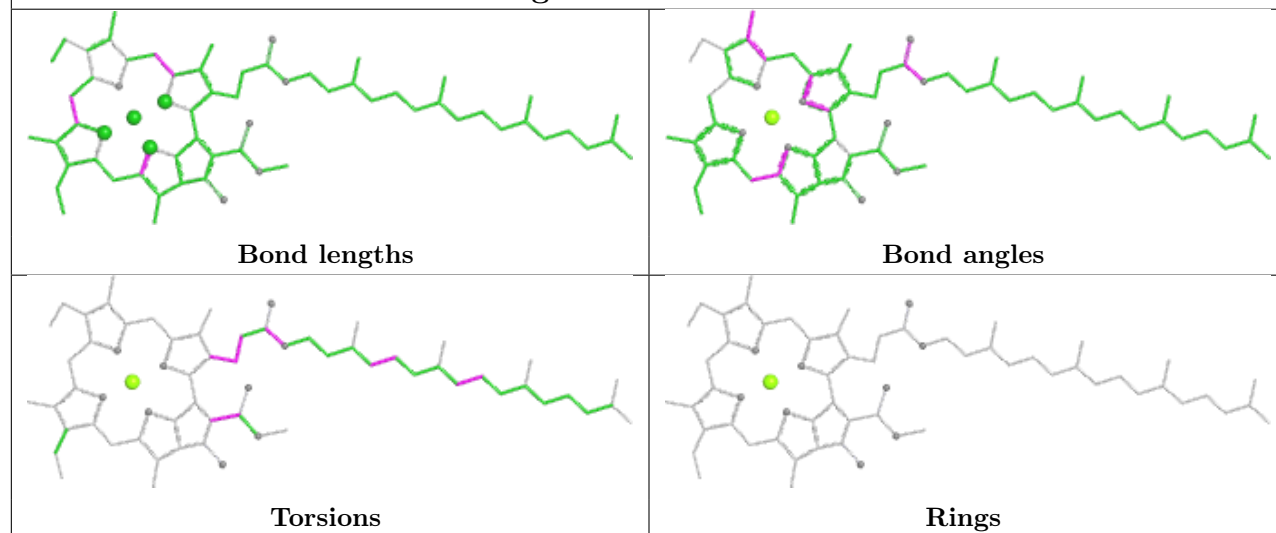


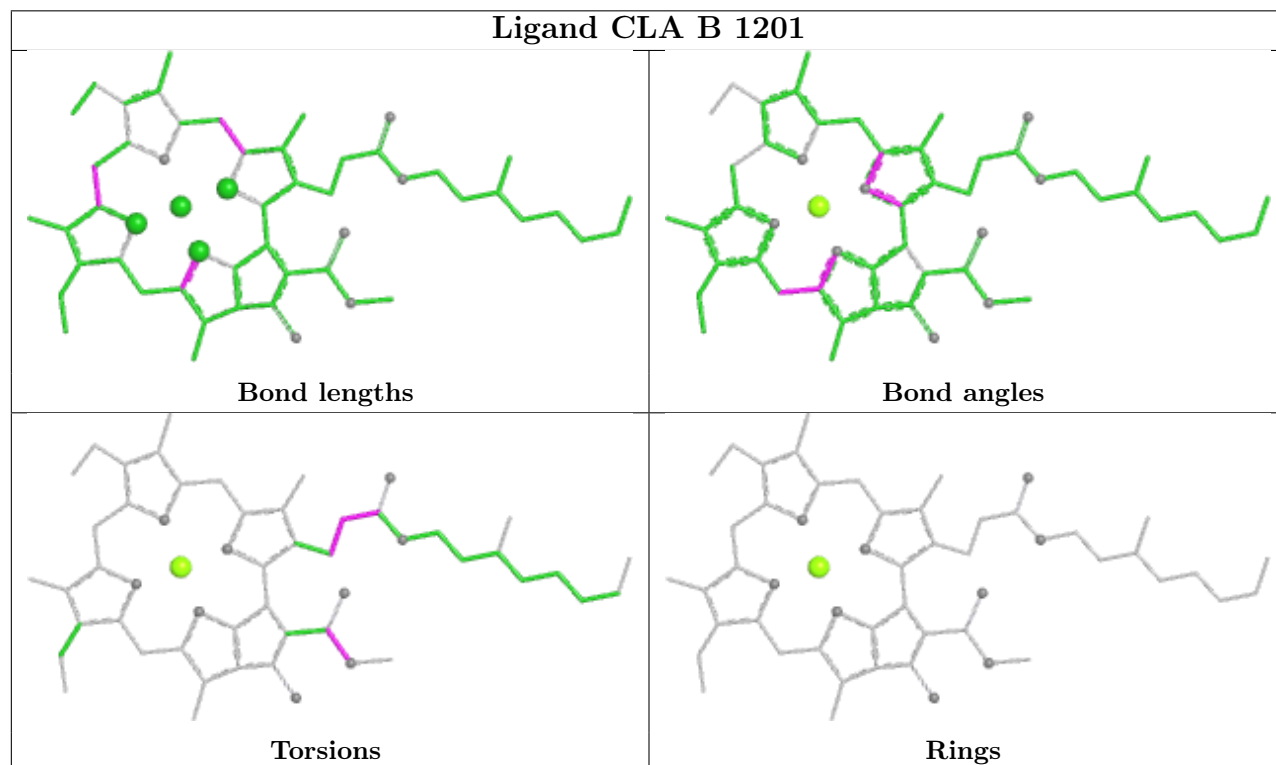
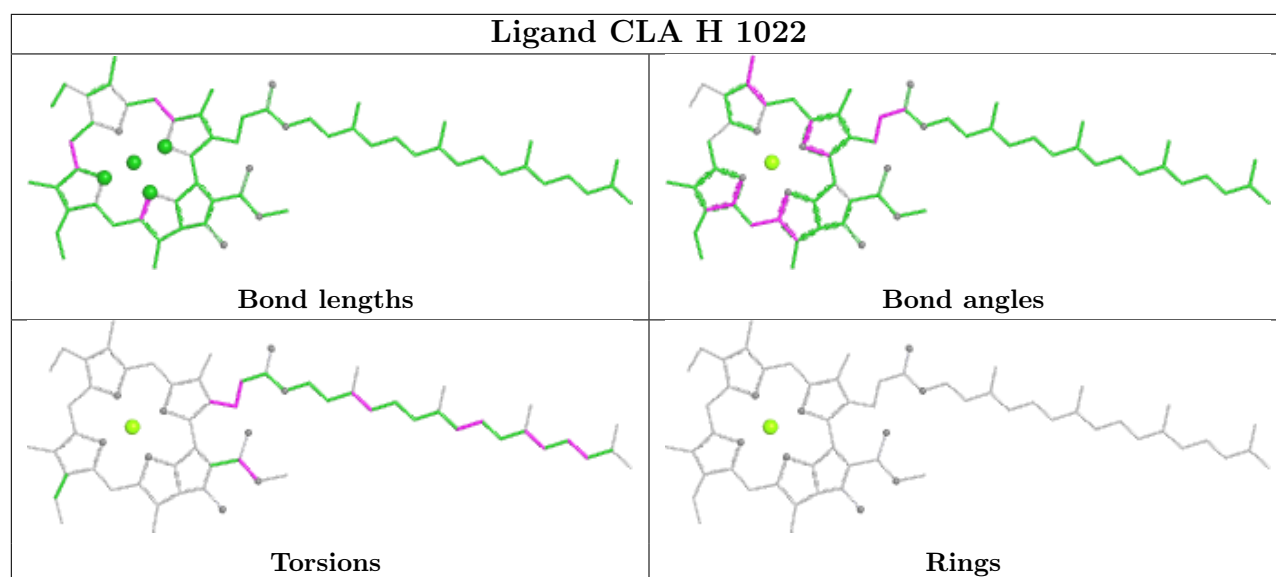


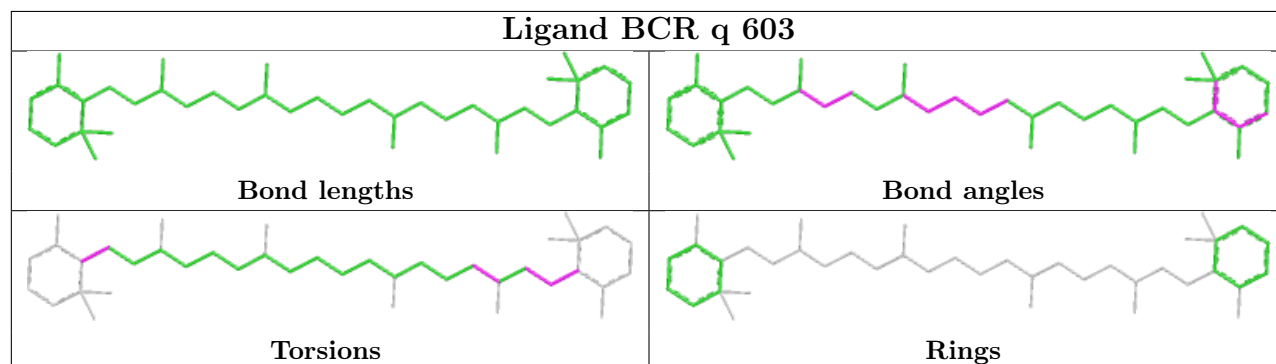
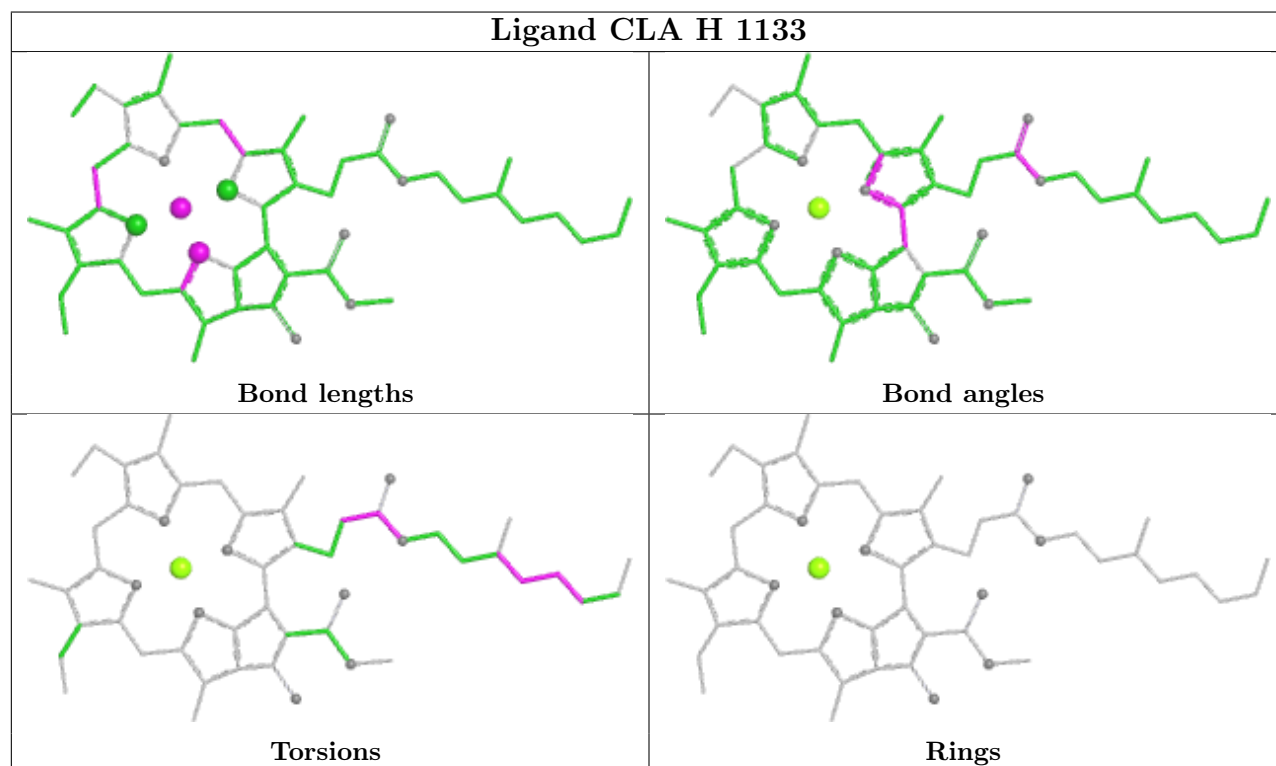
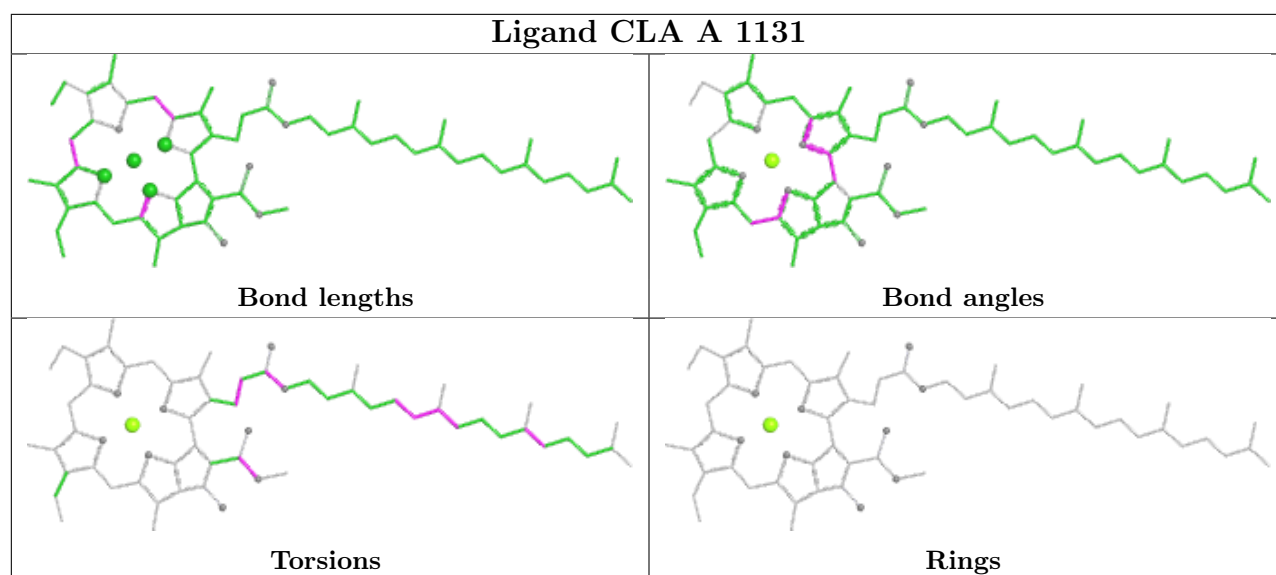
Ligand CLA B 1236

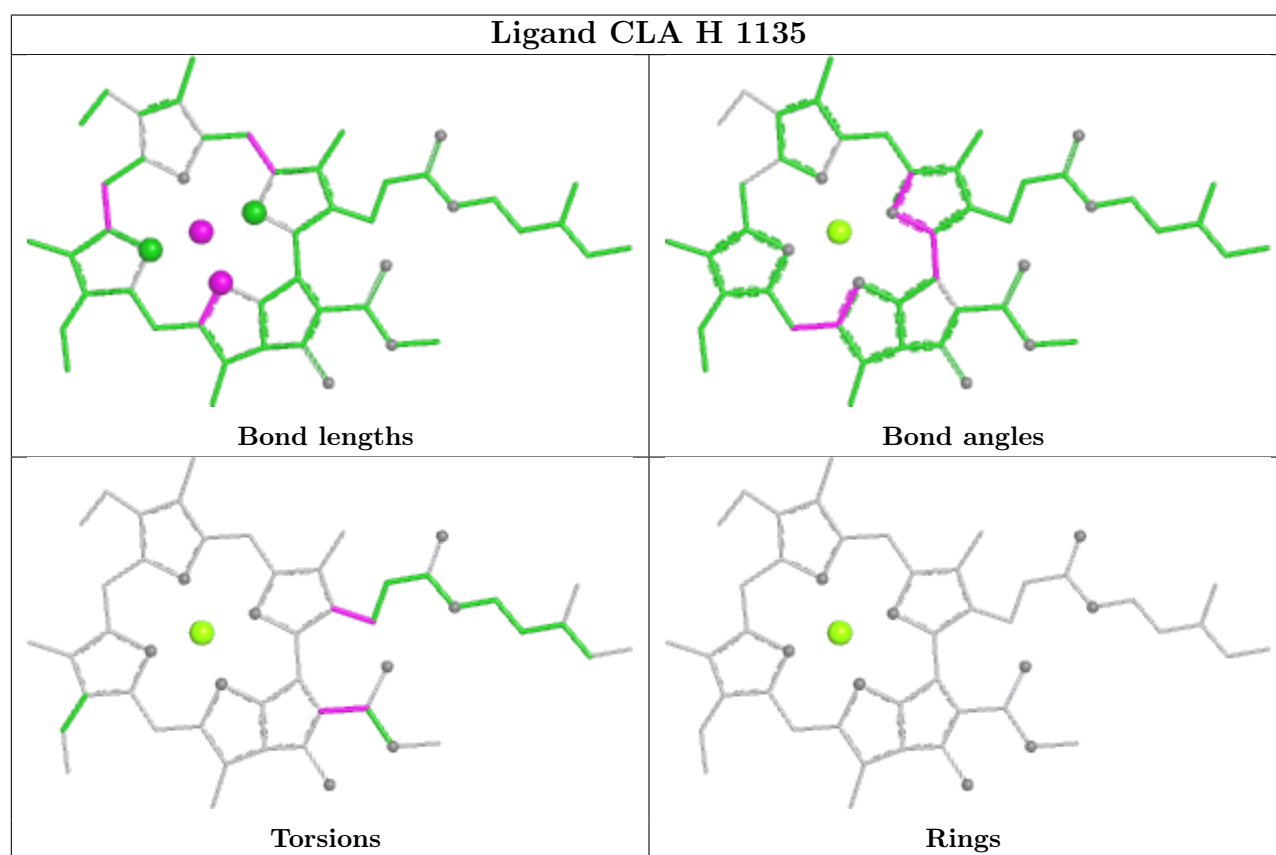
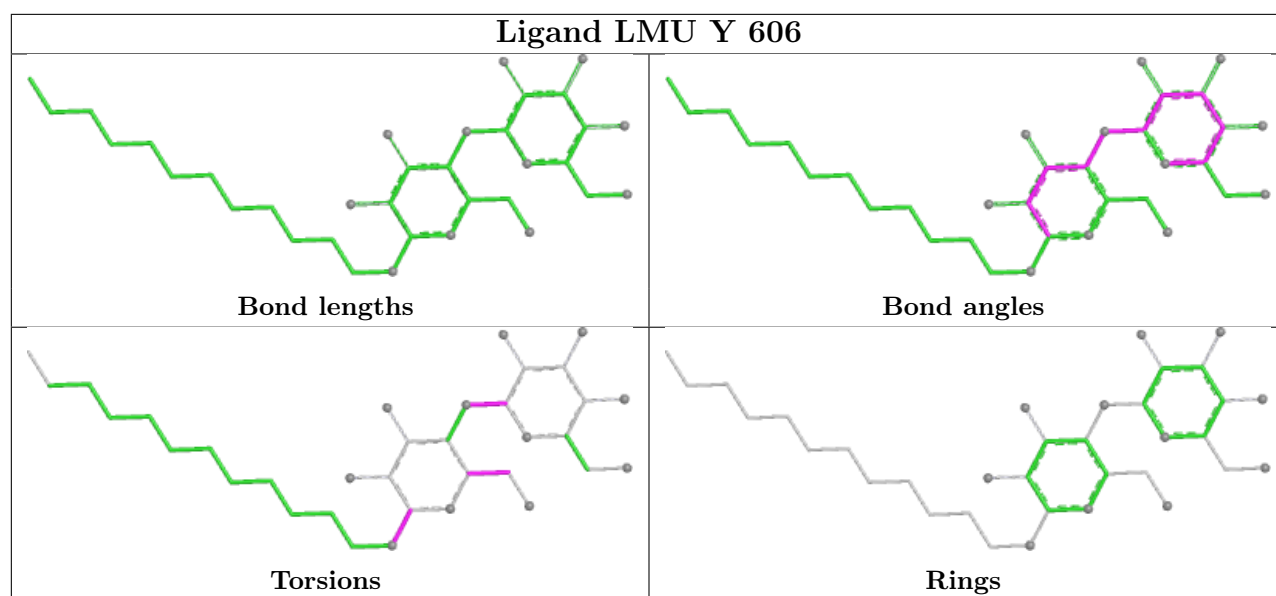


Ligand CLA Y 515

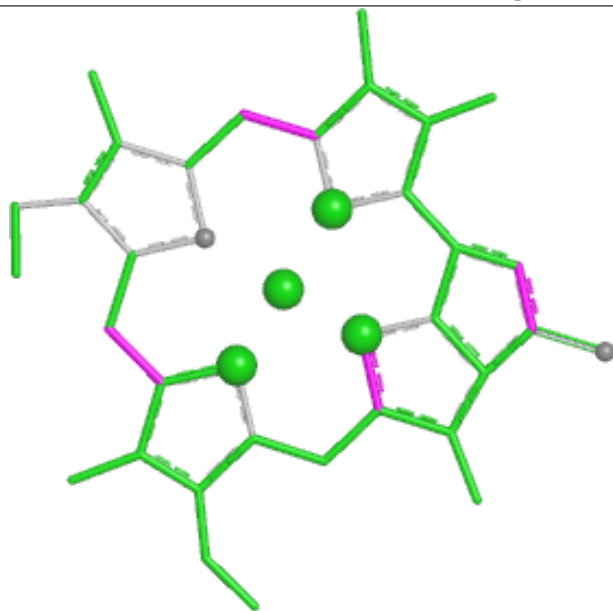




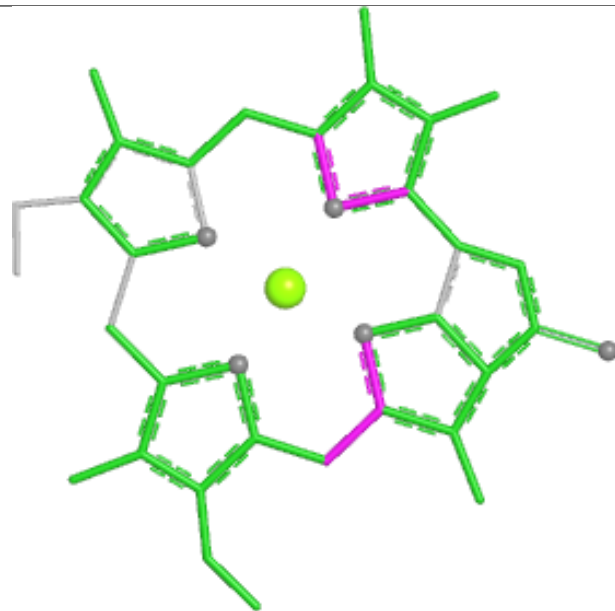




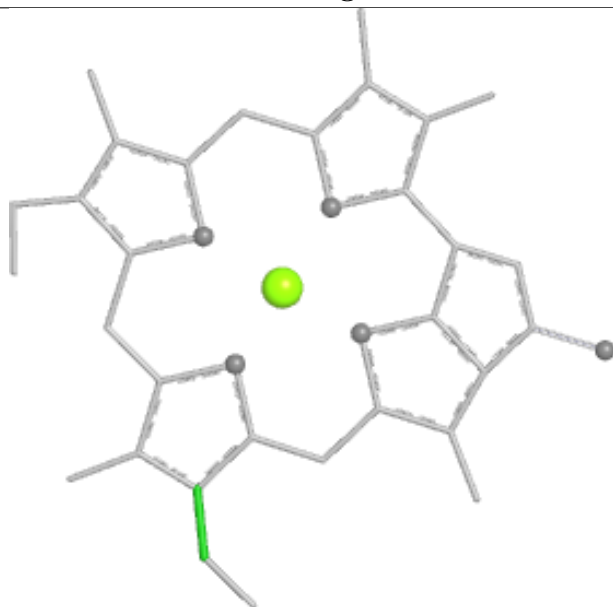
Ligand CLA J 1303



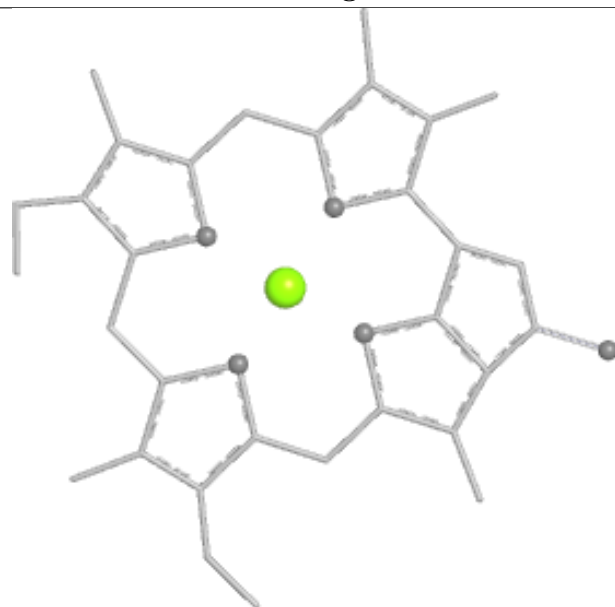
Bond lengths



Bond angles

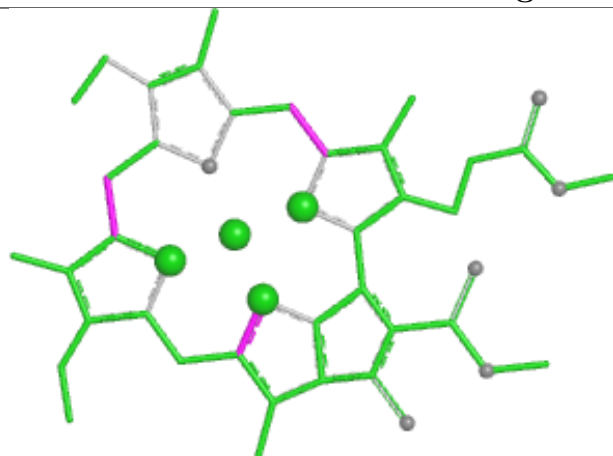


Torsions

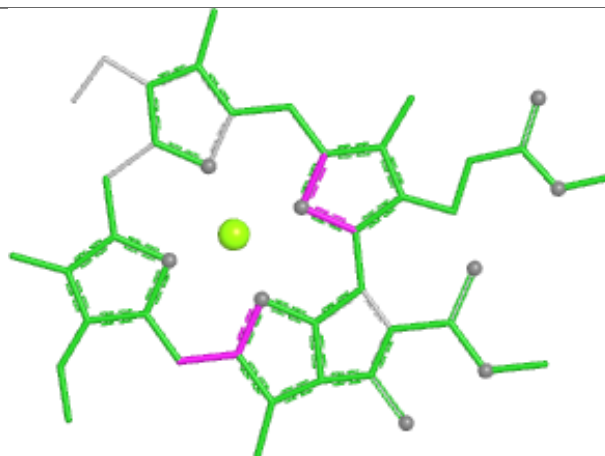


Rings

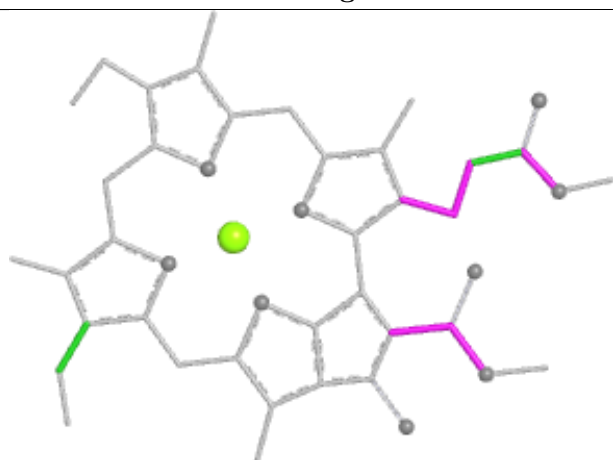
Ligand CLA Z 516



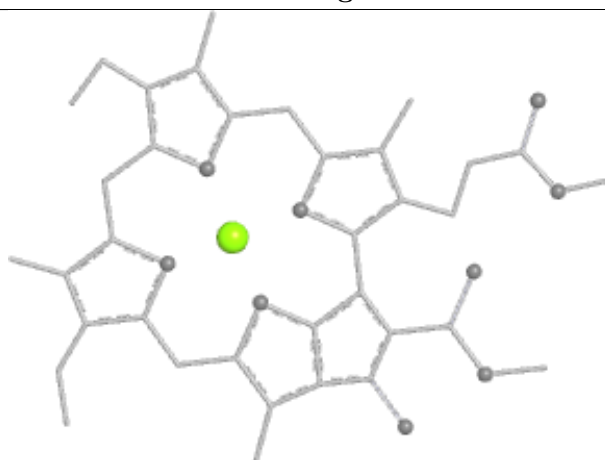
Bond lengths



Bond angles

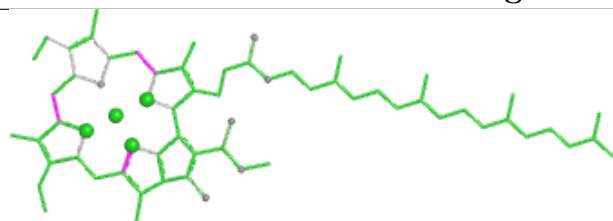


Torsions

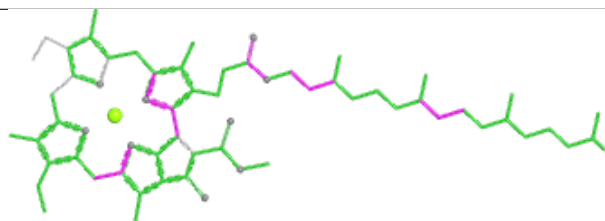


Rings

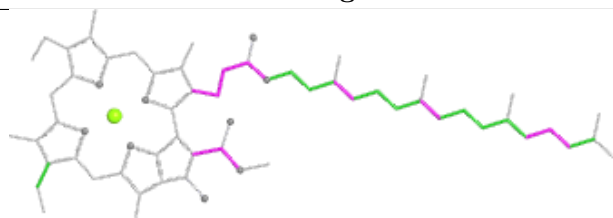
Ligand CLA A 1101



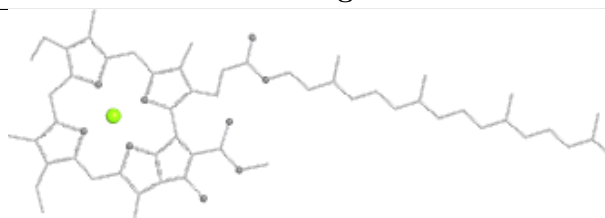
Bond lengths



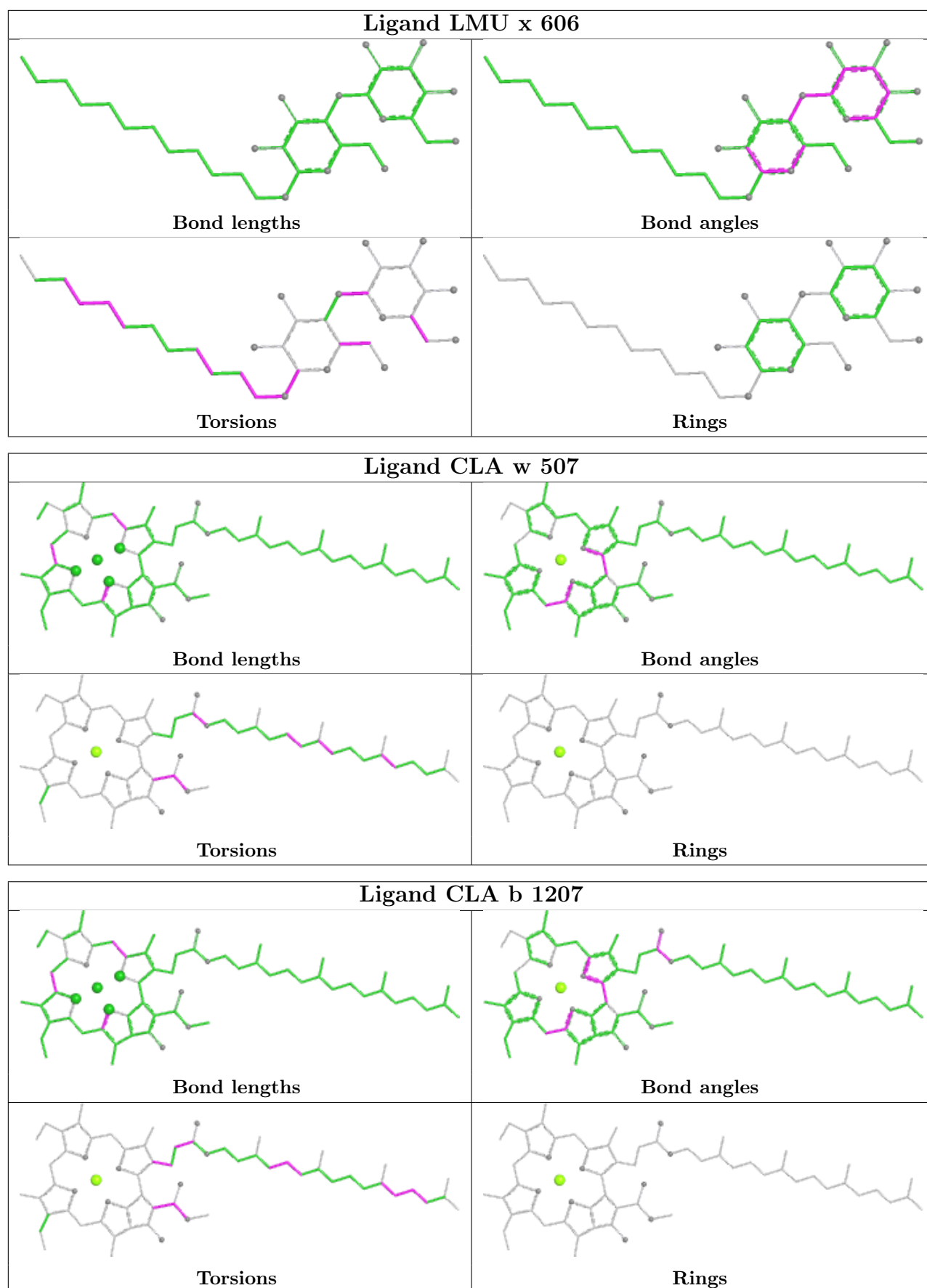
Bond angles

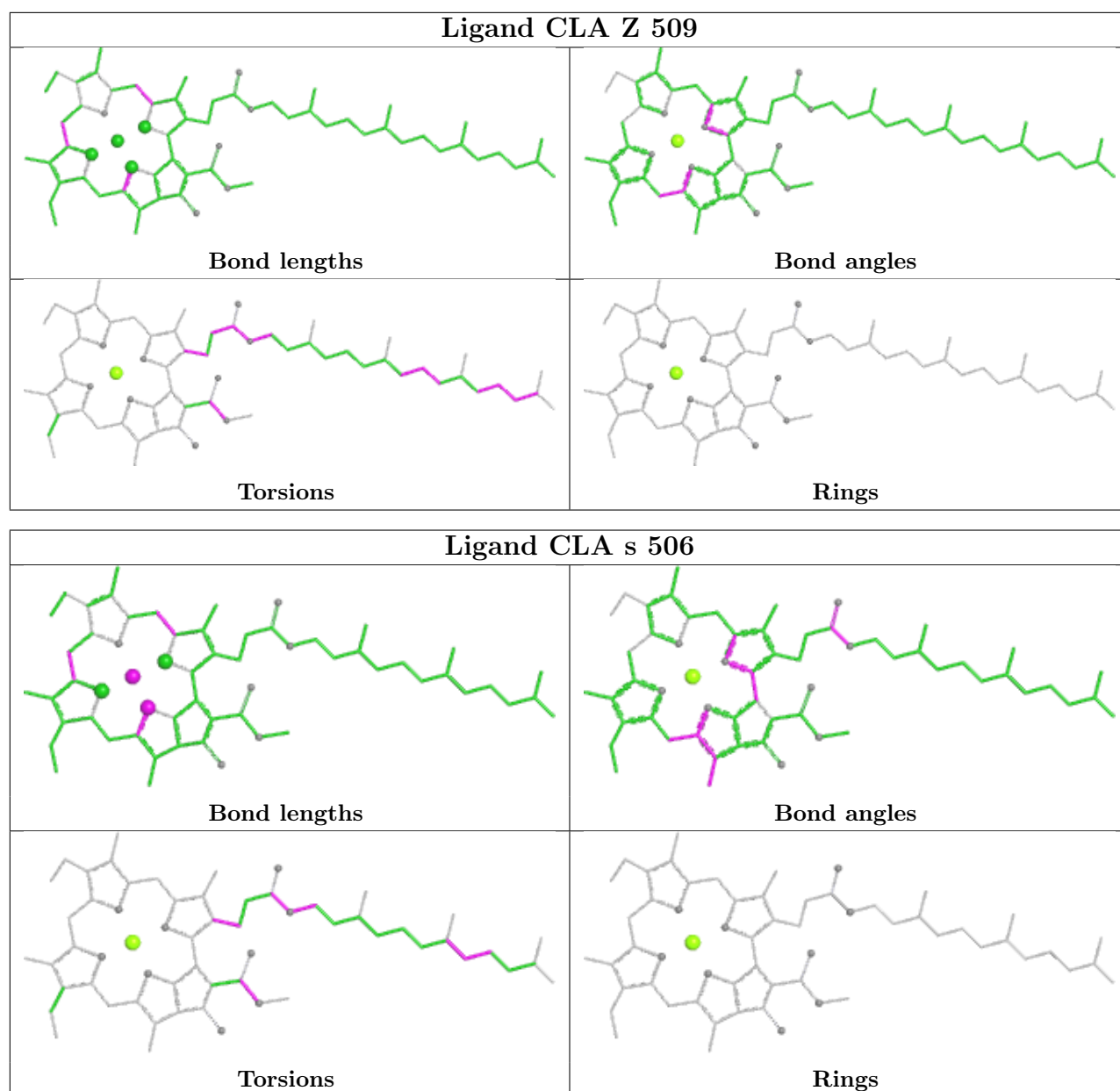


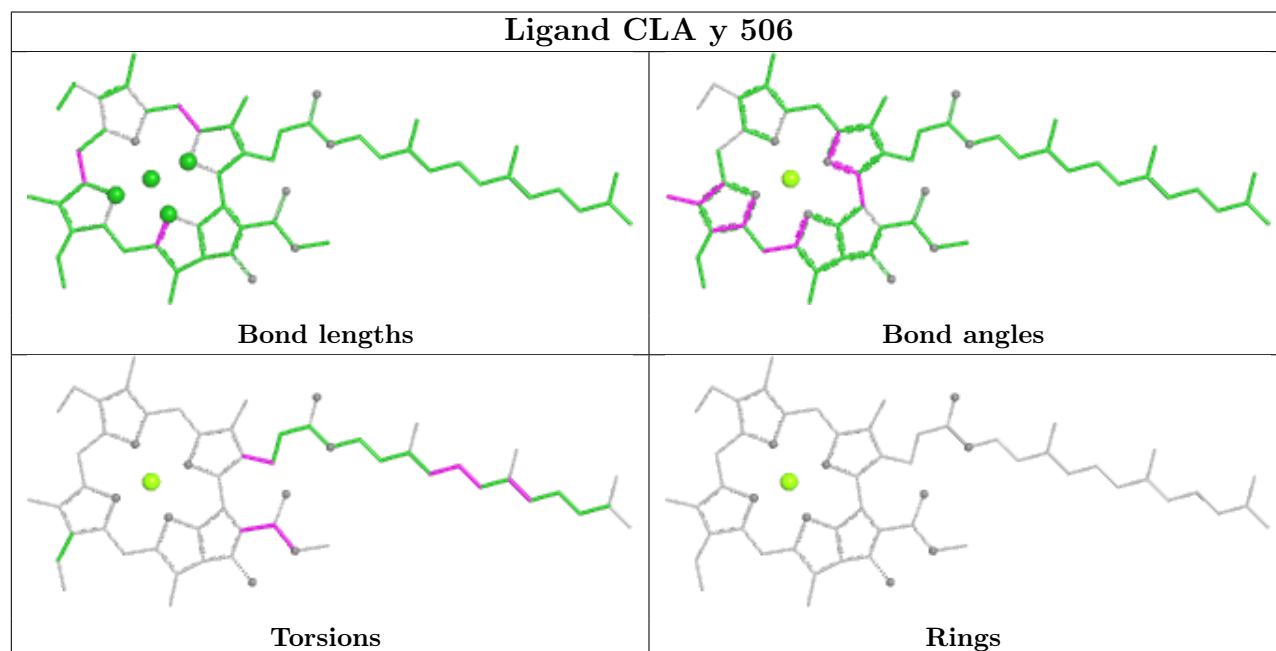
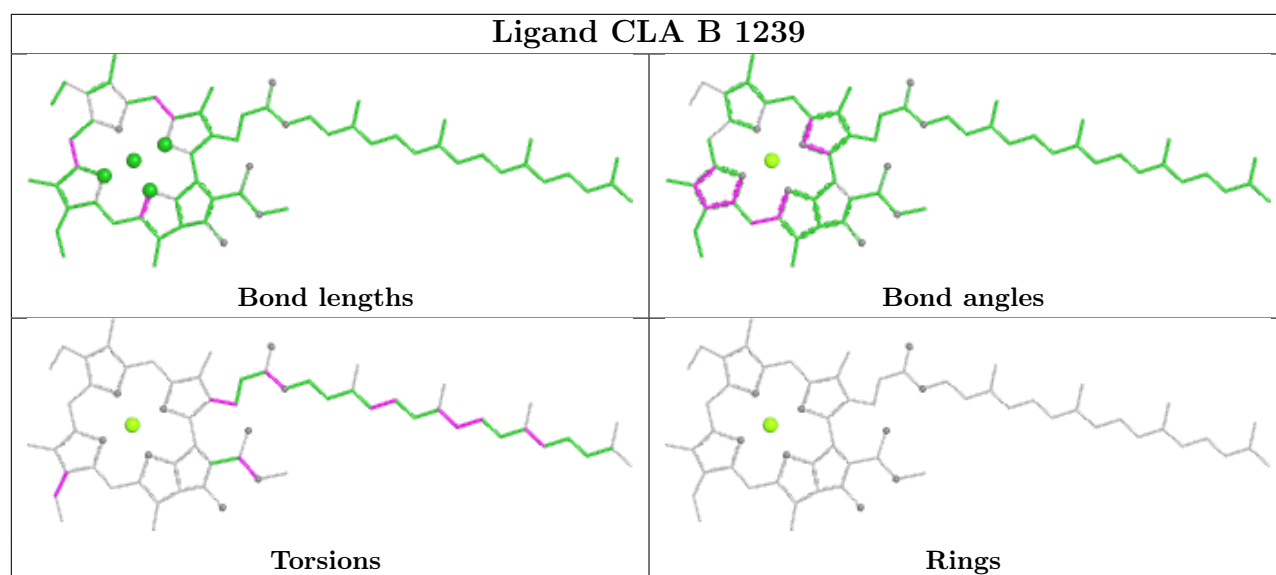
Torsions

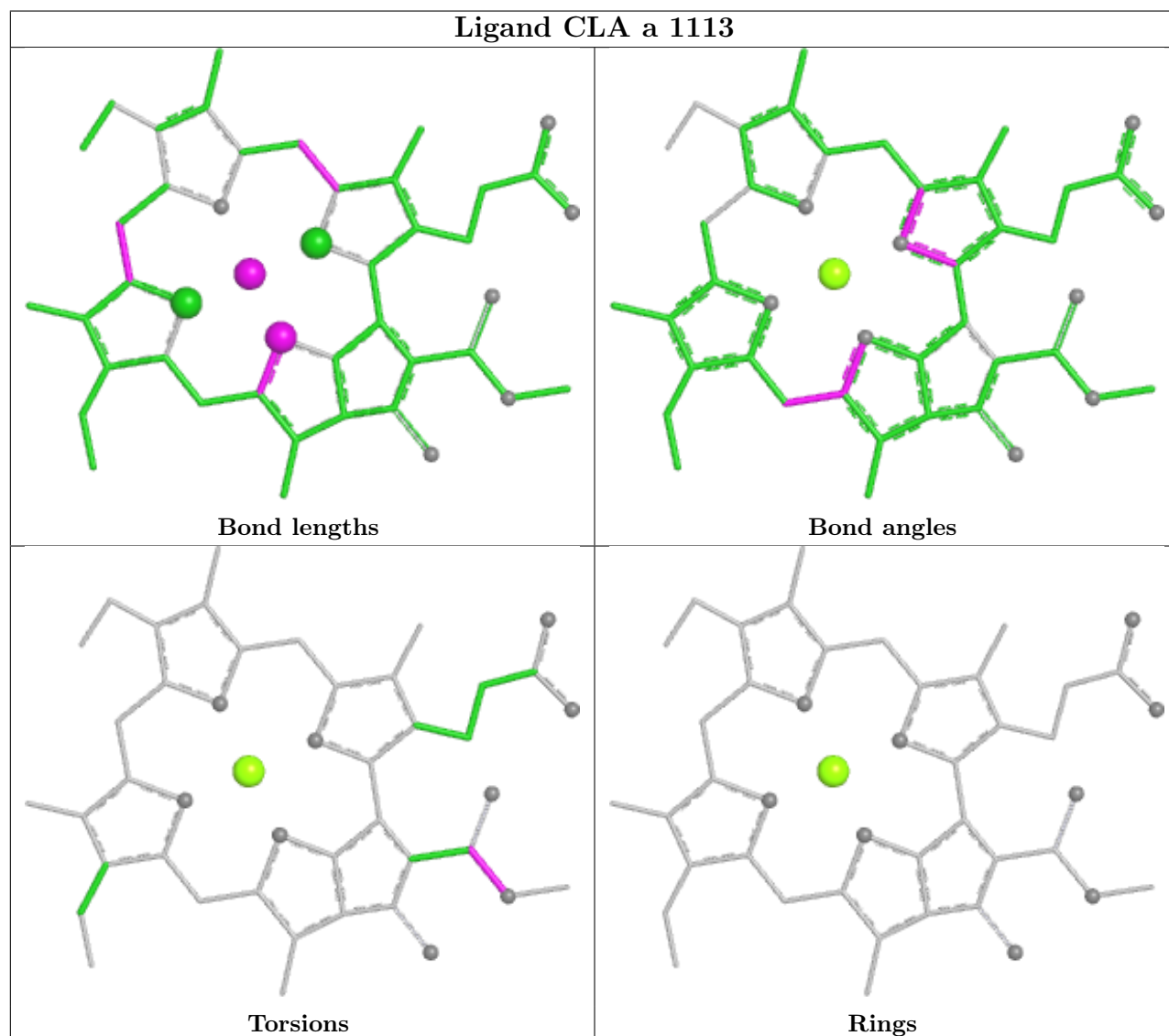
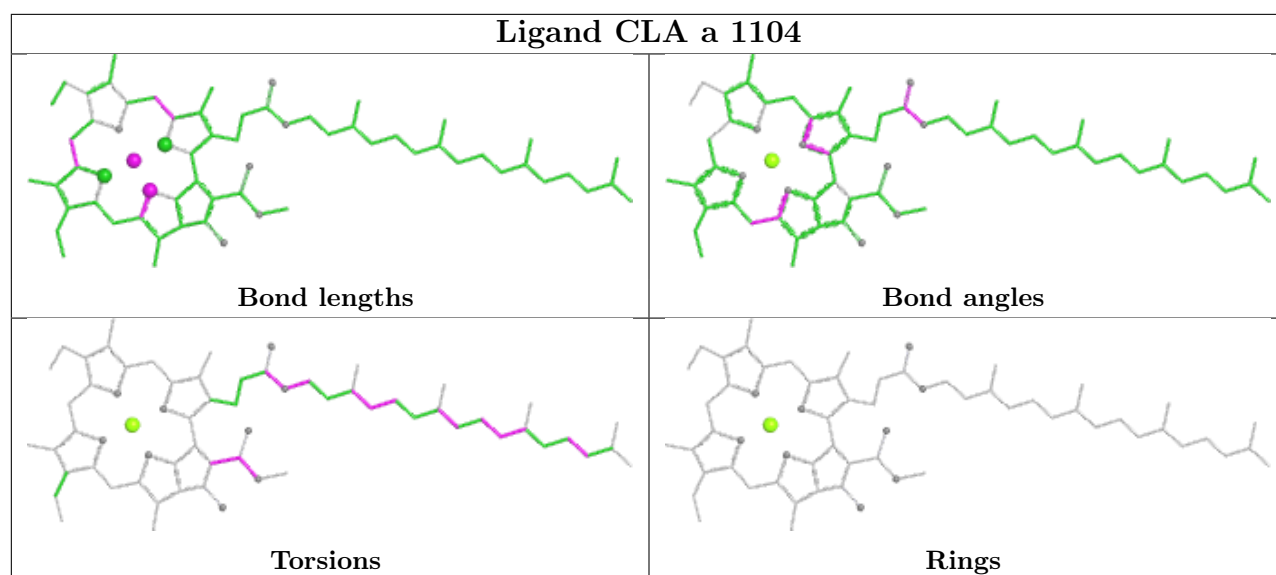


Rings

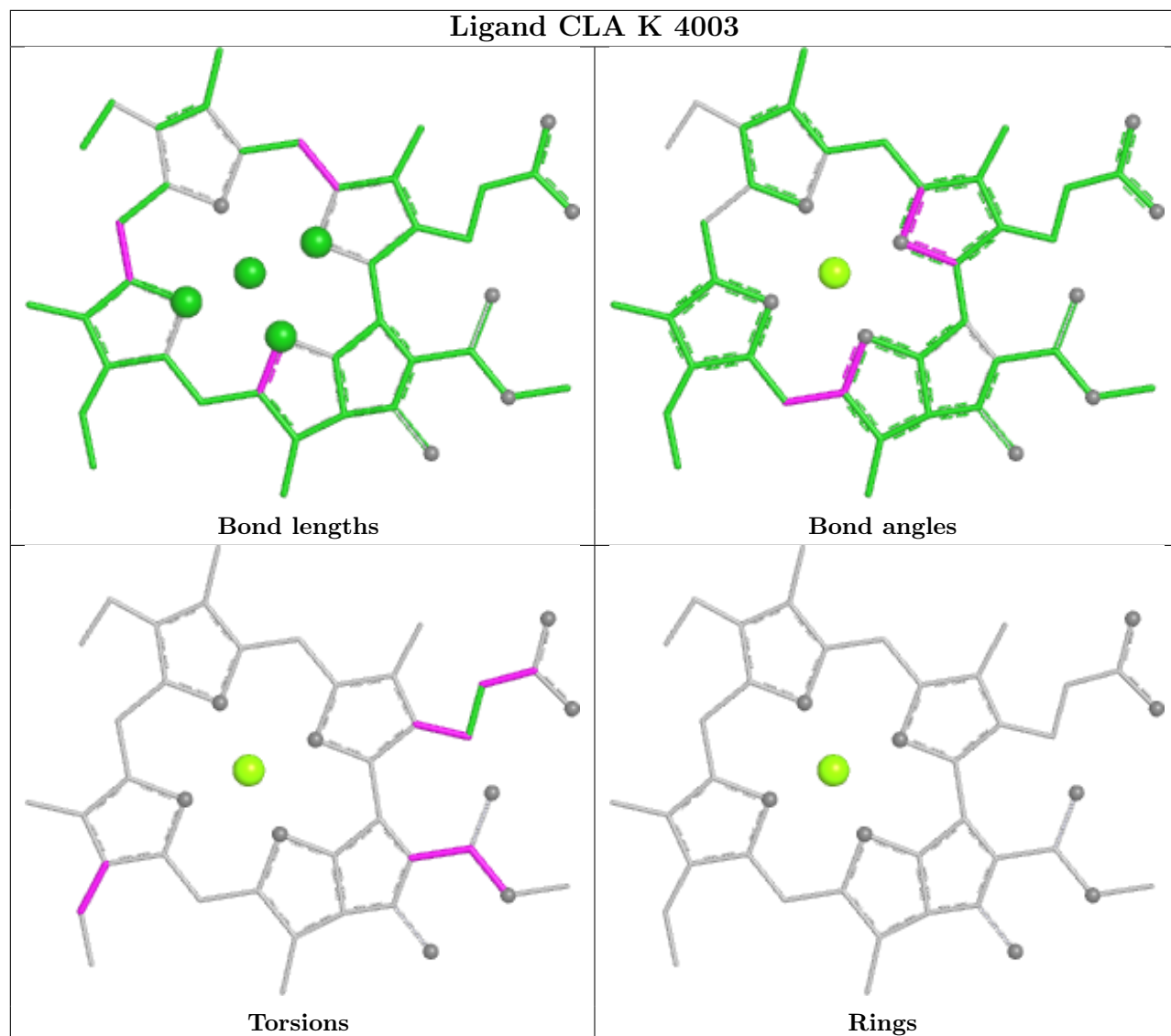




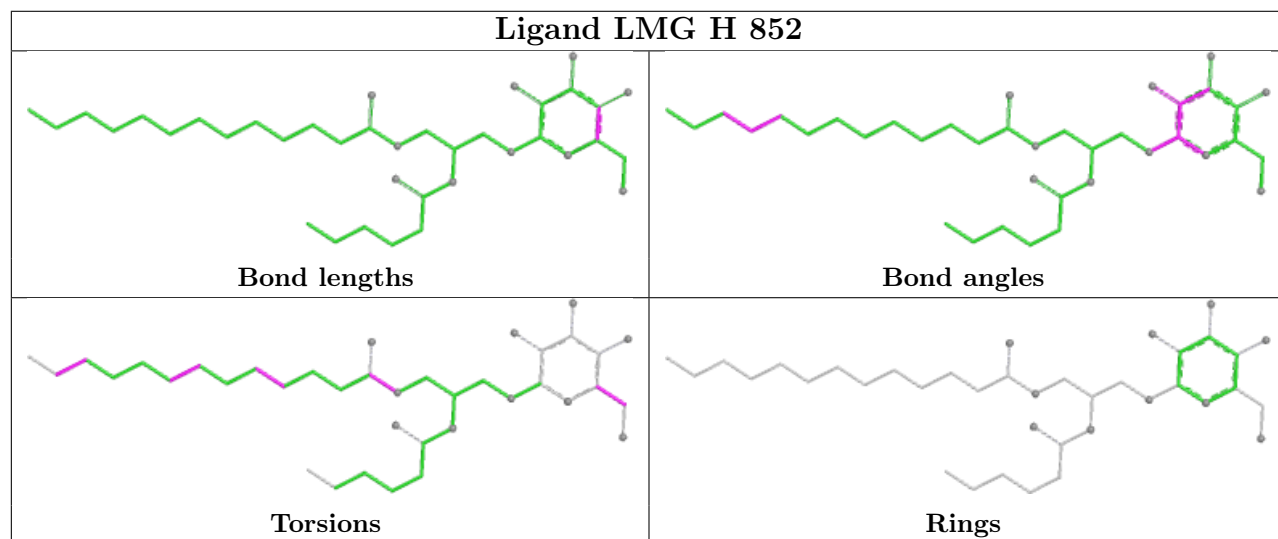


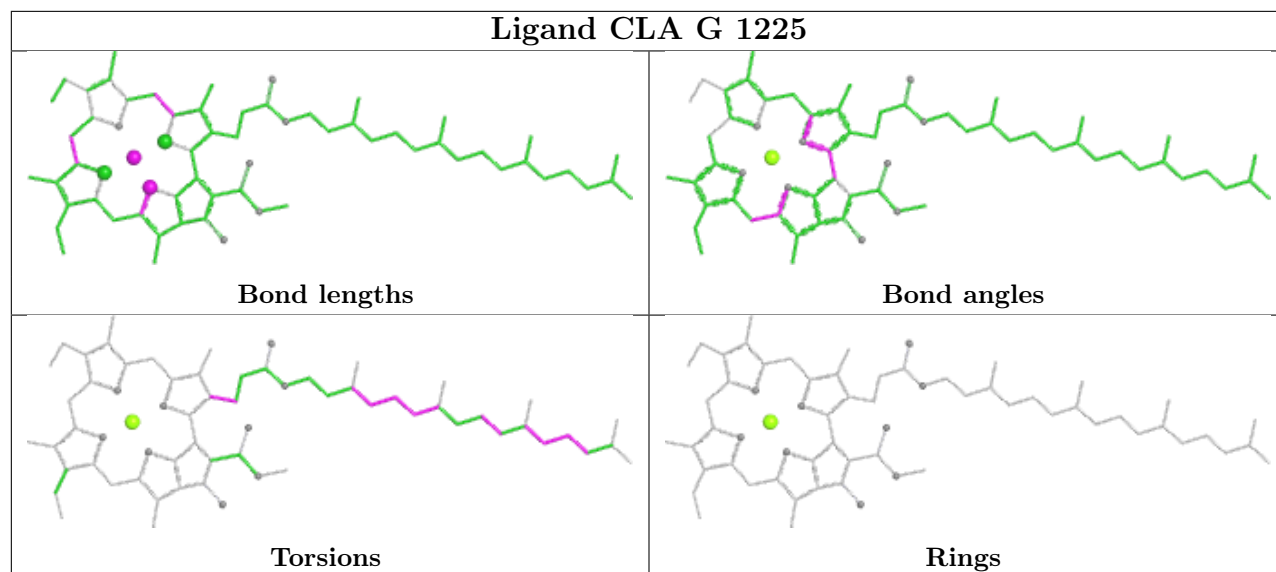
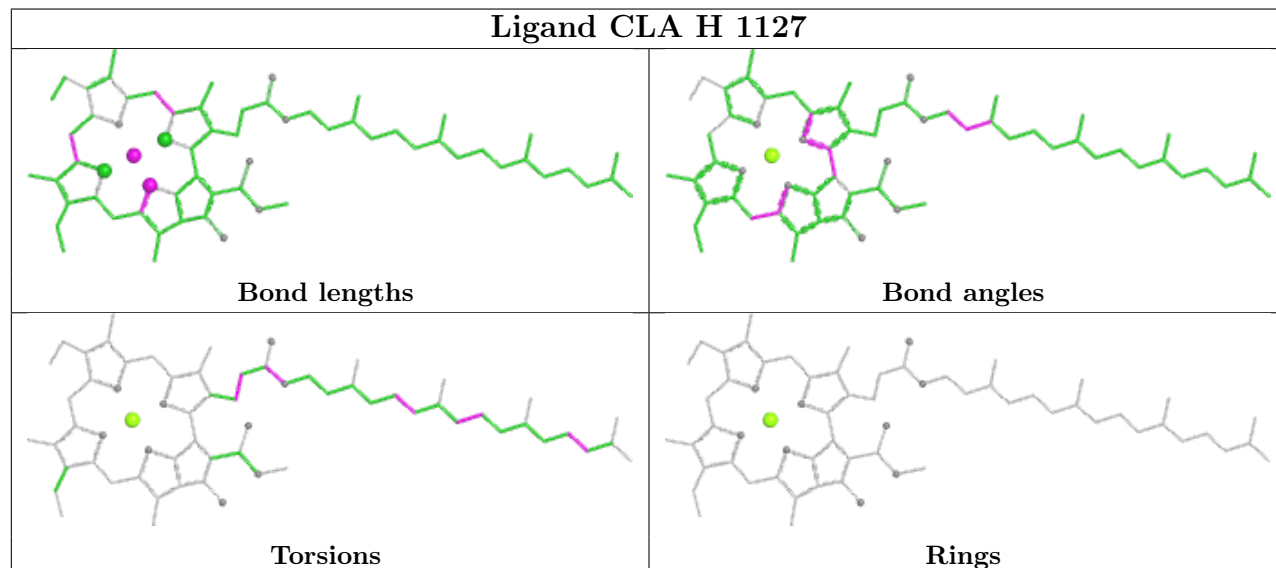


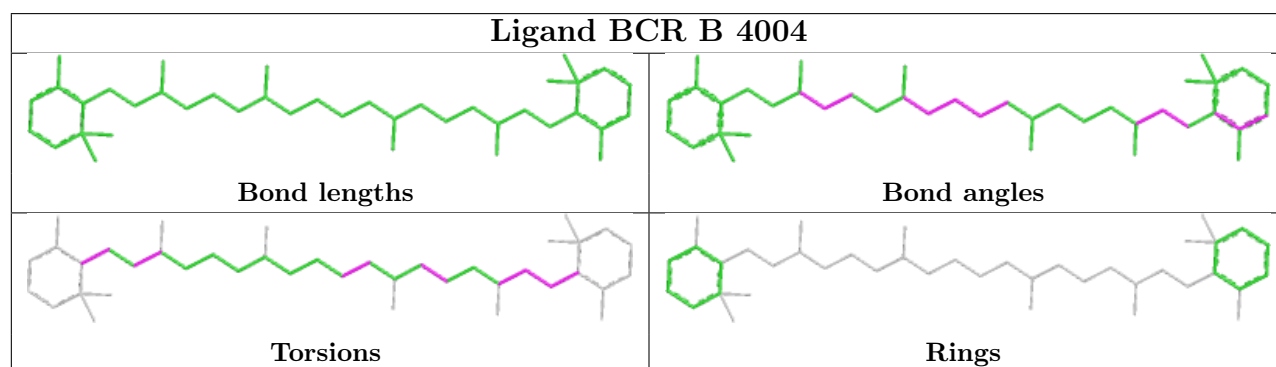
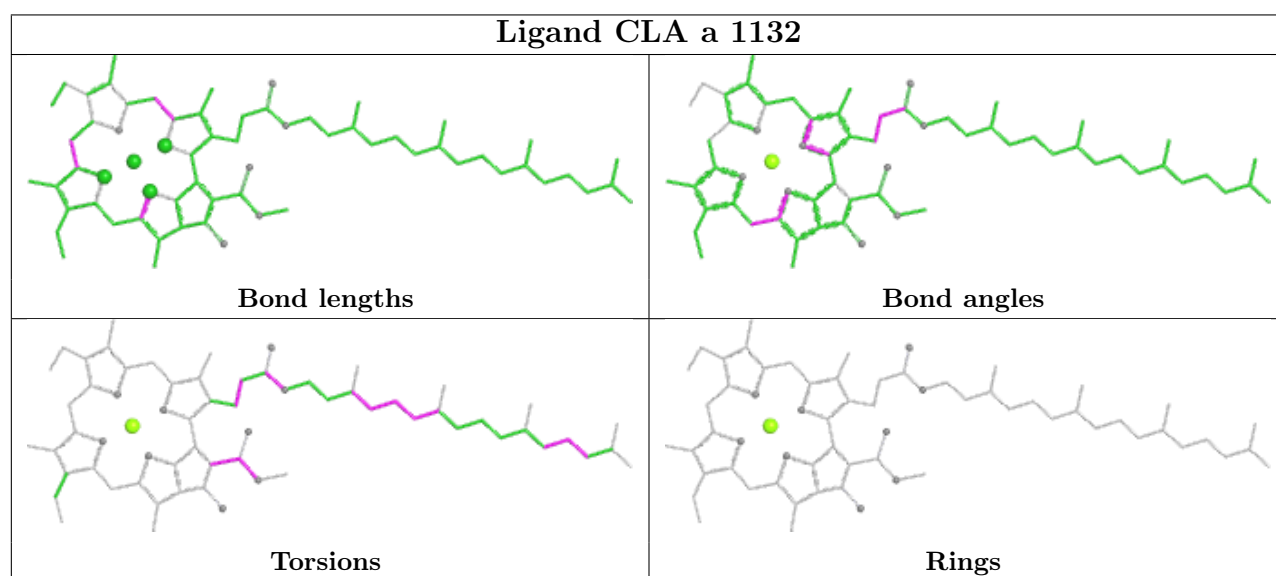
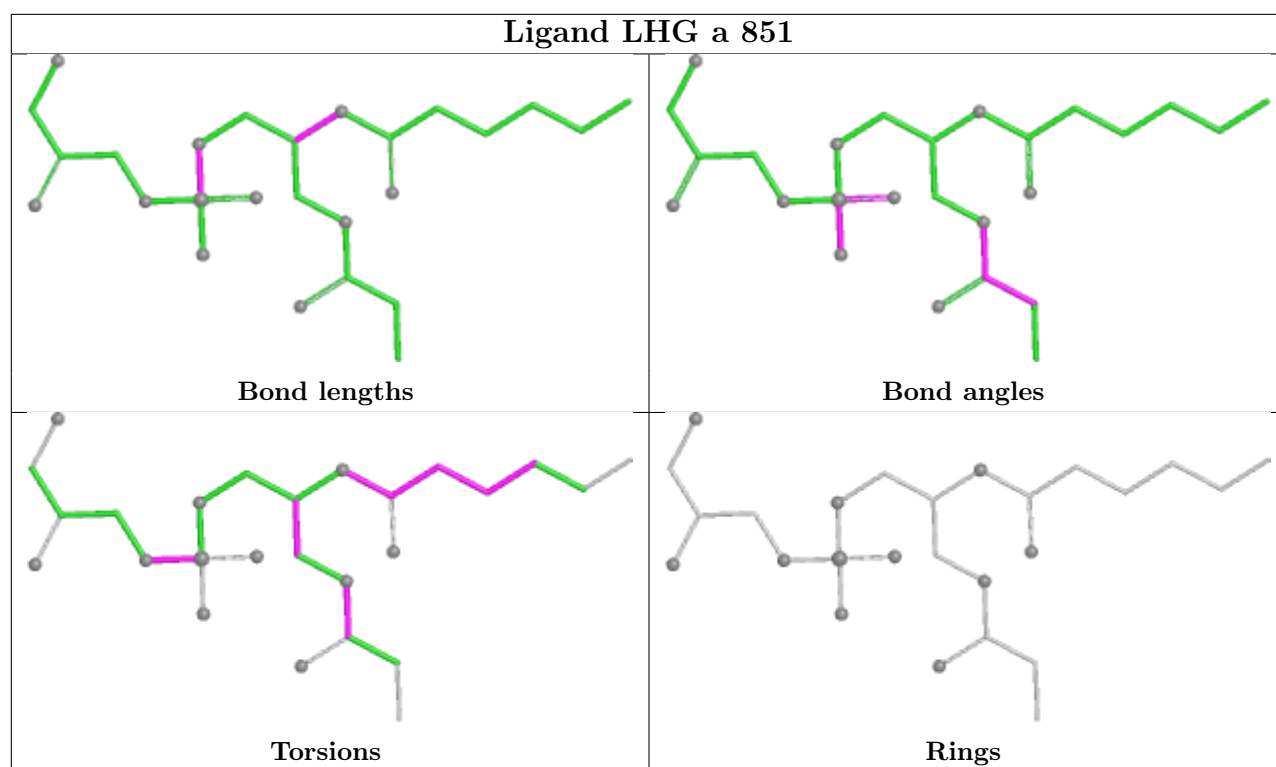
Ligand CLA K 4003



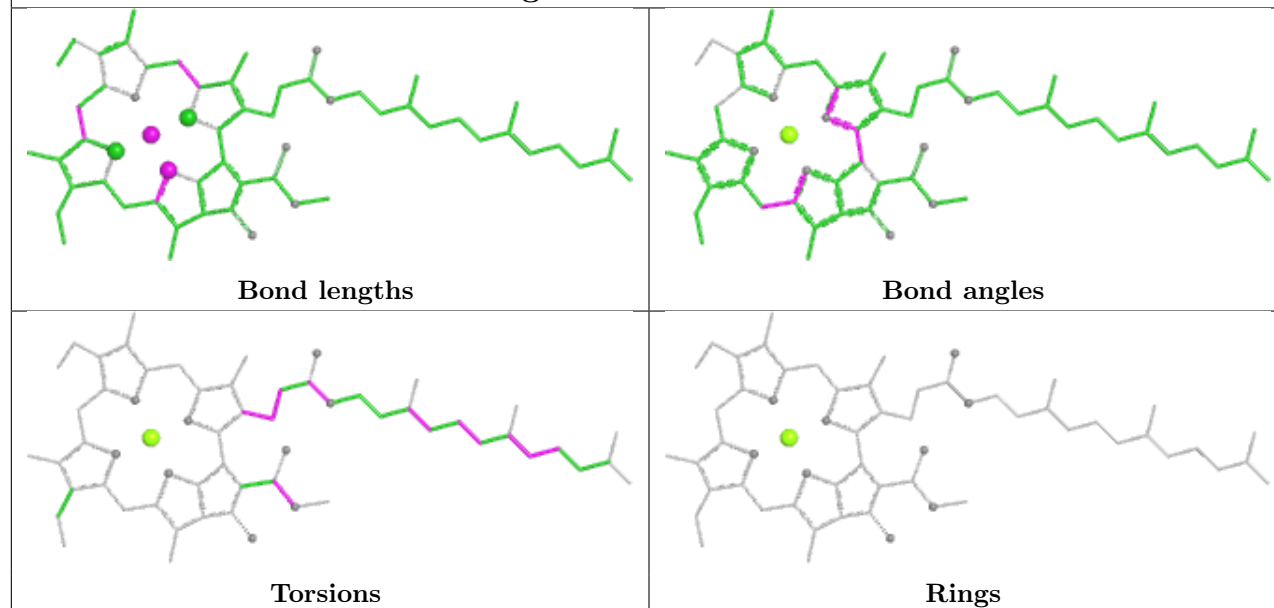
Ligand LMG H 852



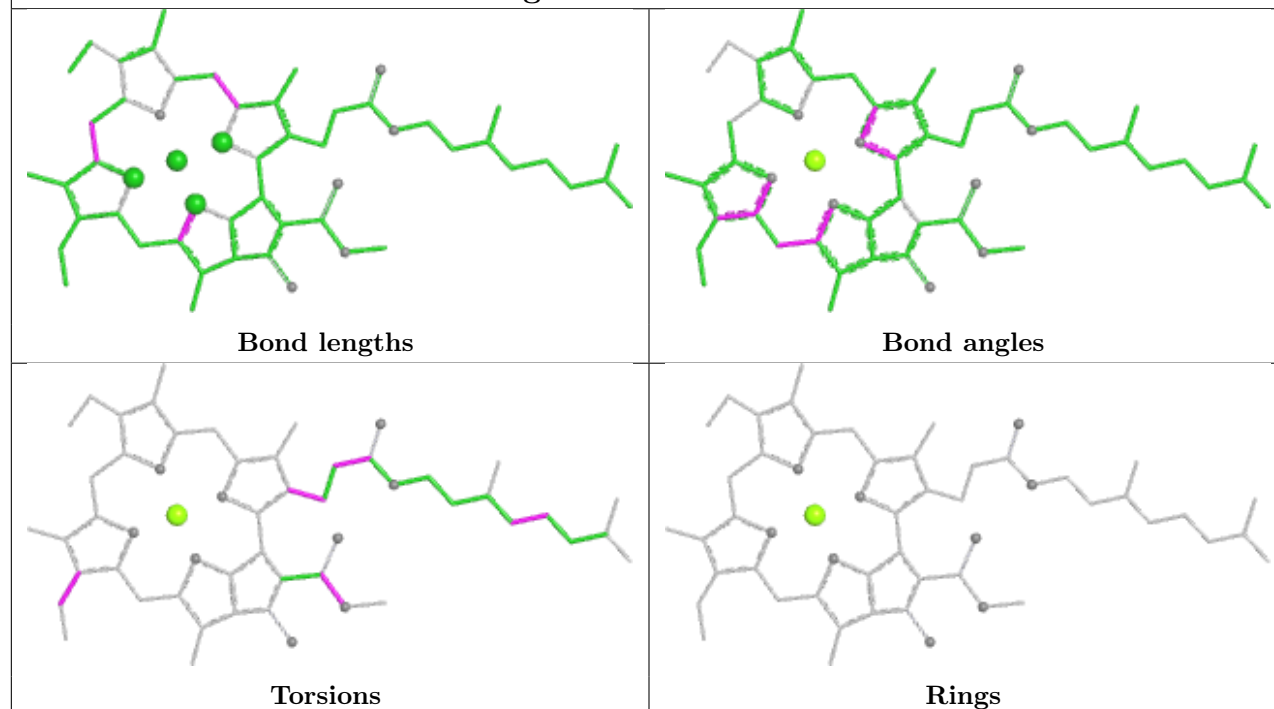
Ligand CLA G 1225**Ligand CLA H 1127**

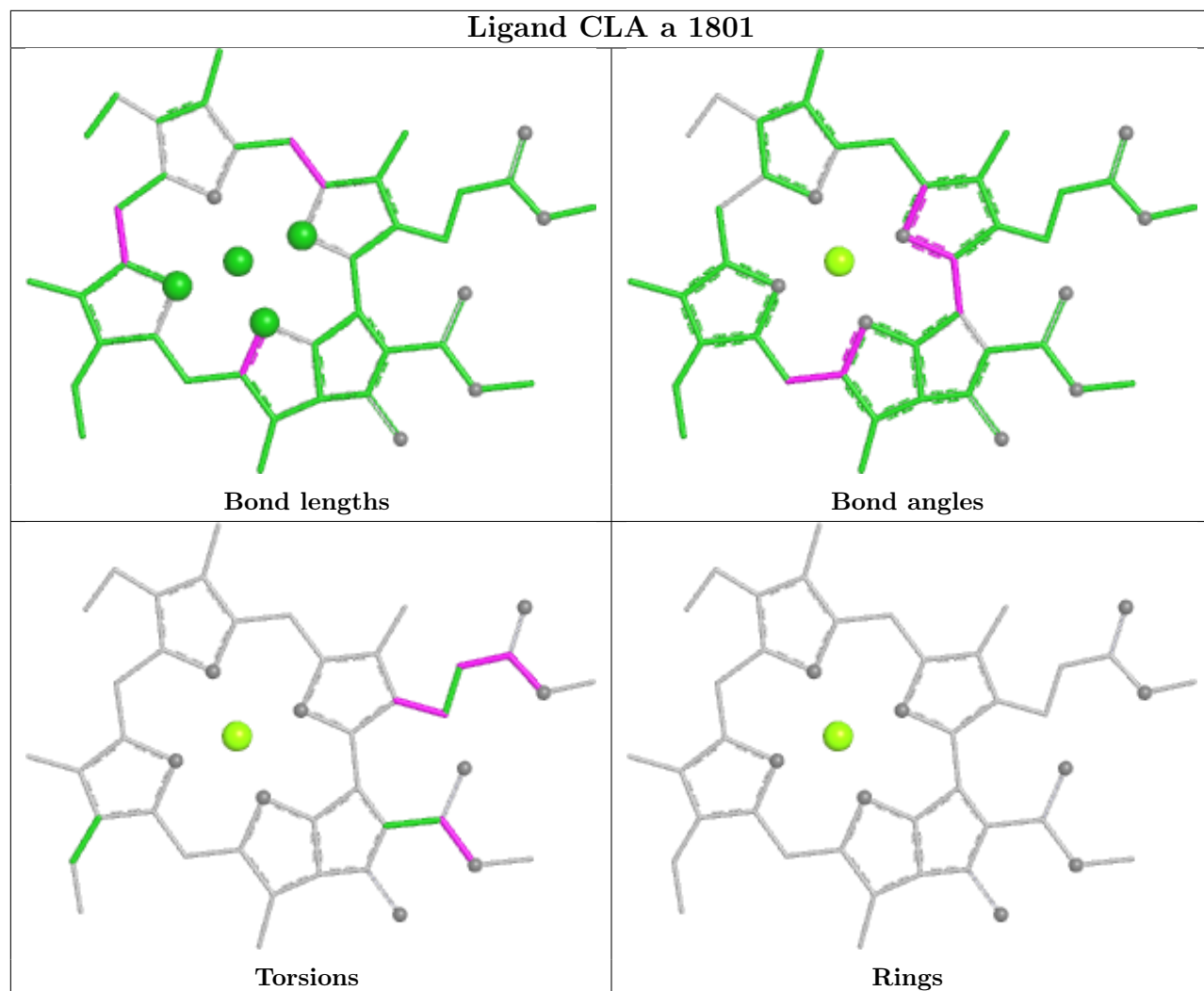


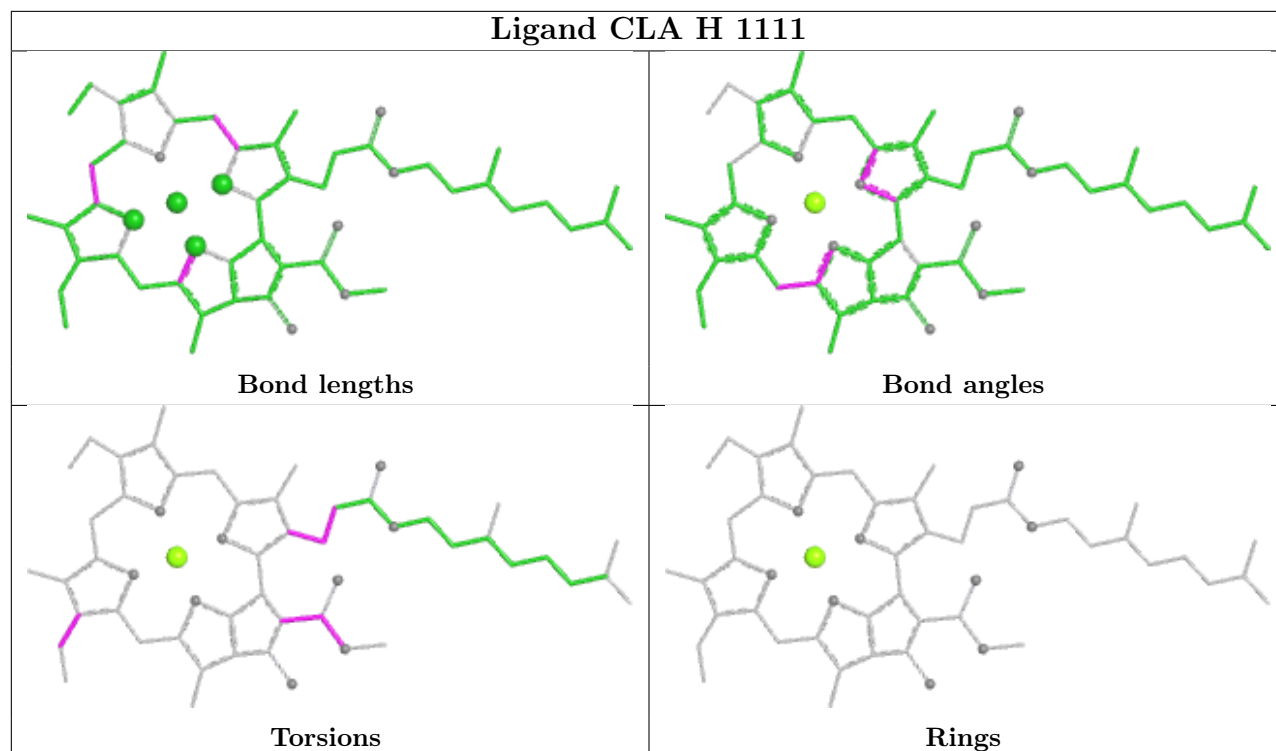
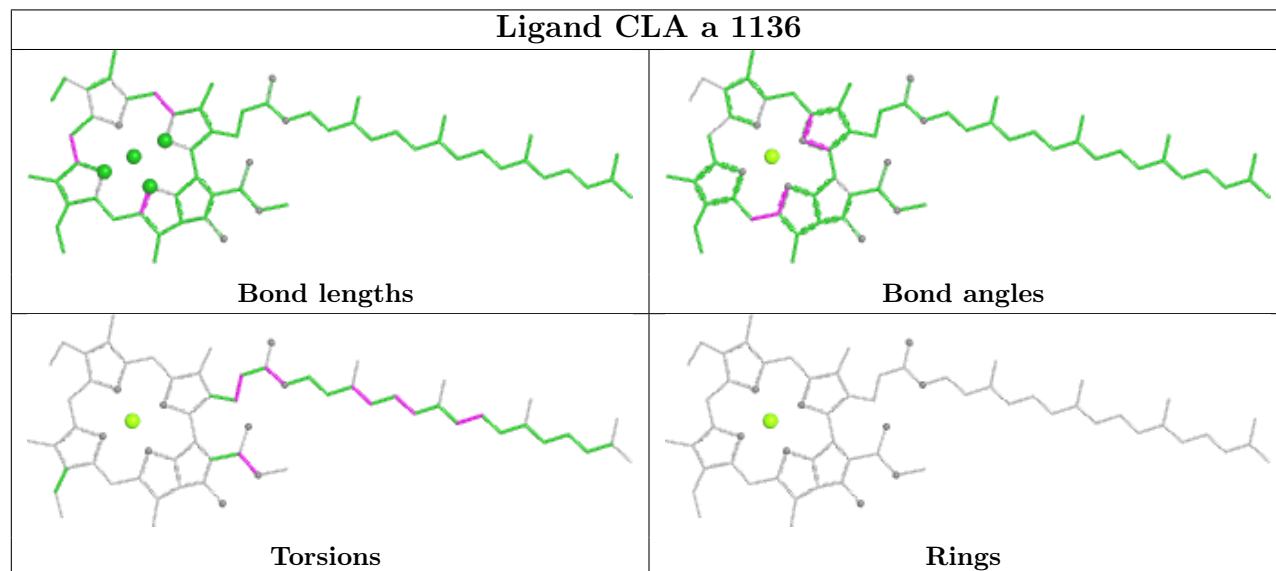
Ligand CLA G 1224

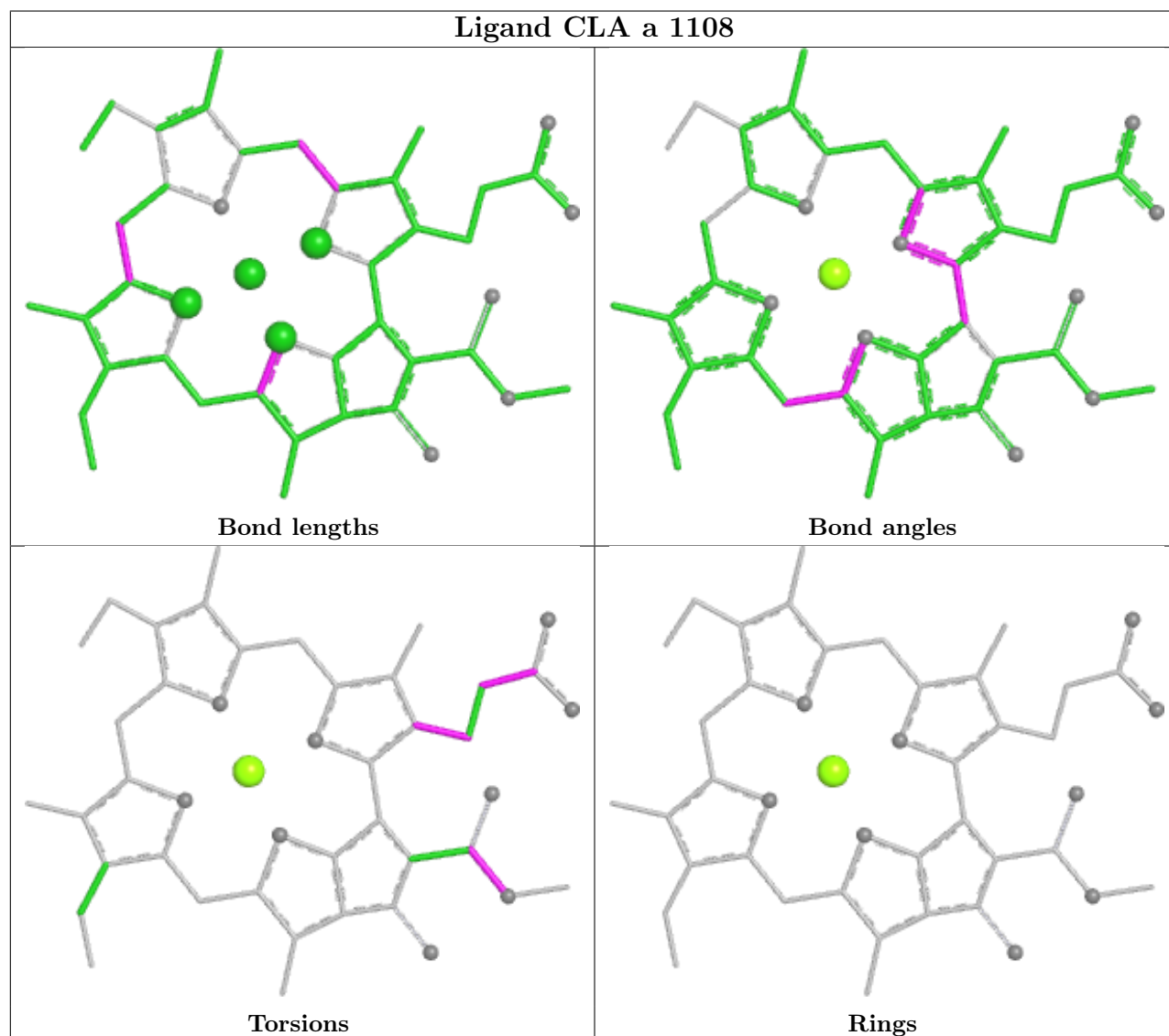
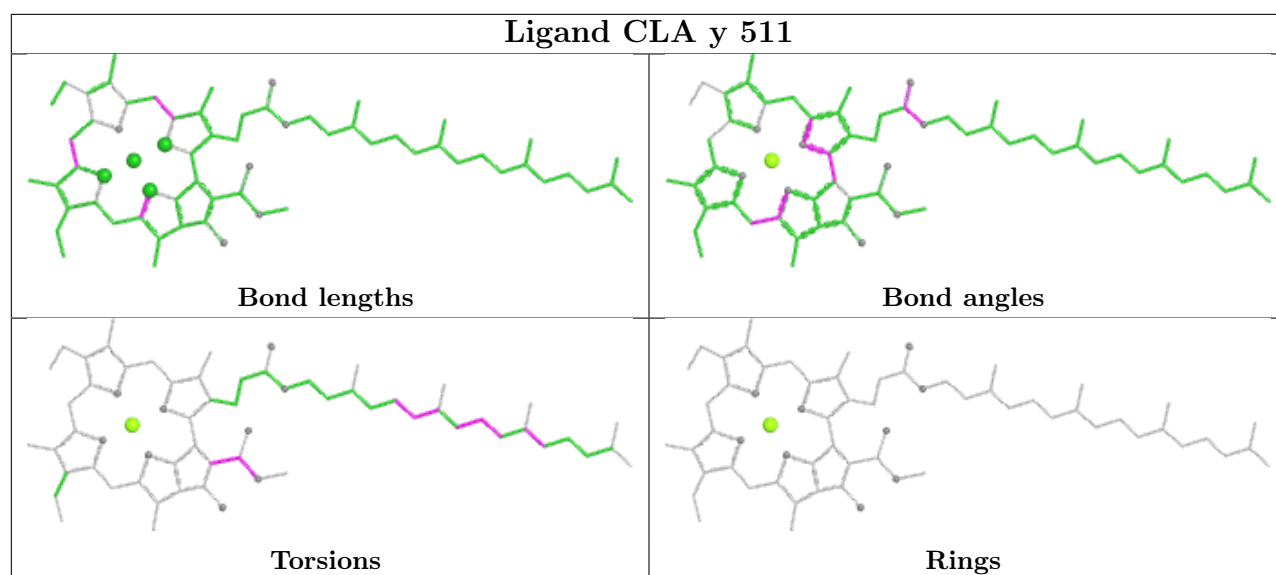


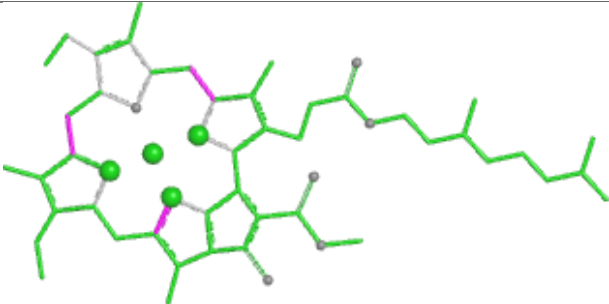
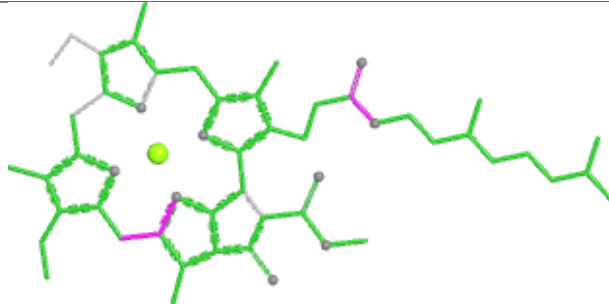
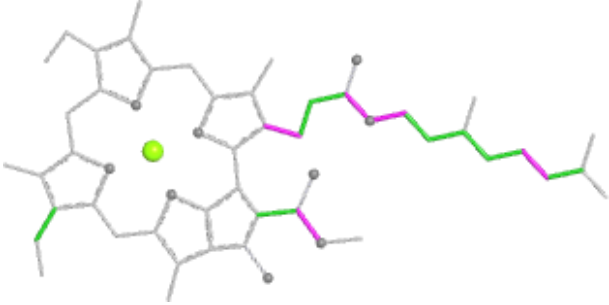
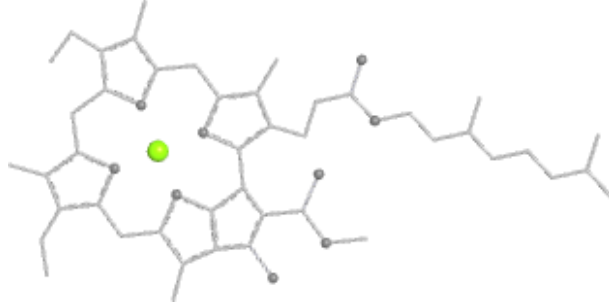
Ligand CLA B 1214

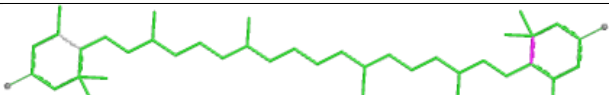
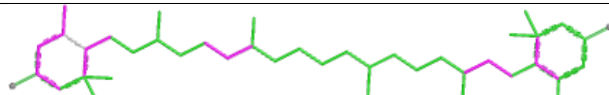
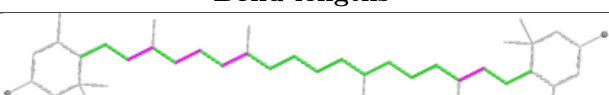
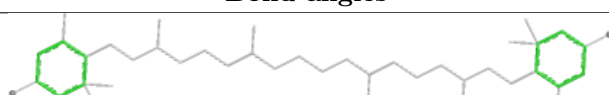


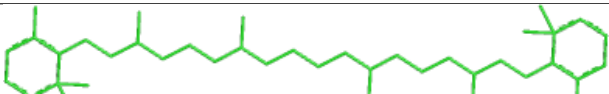
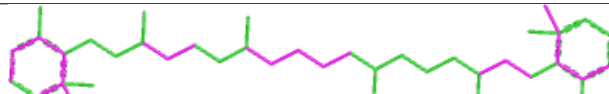

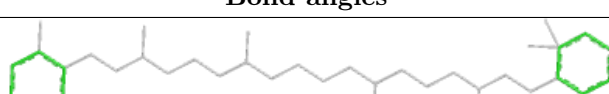


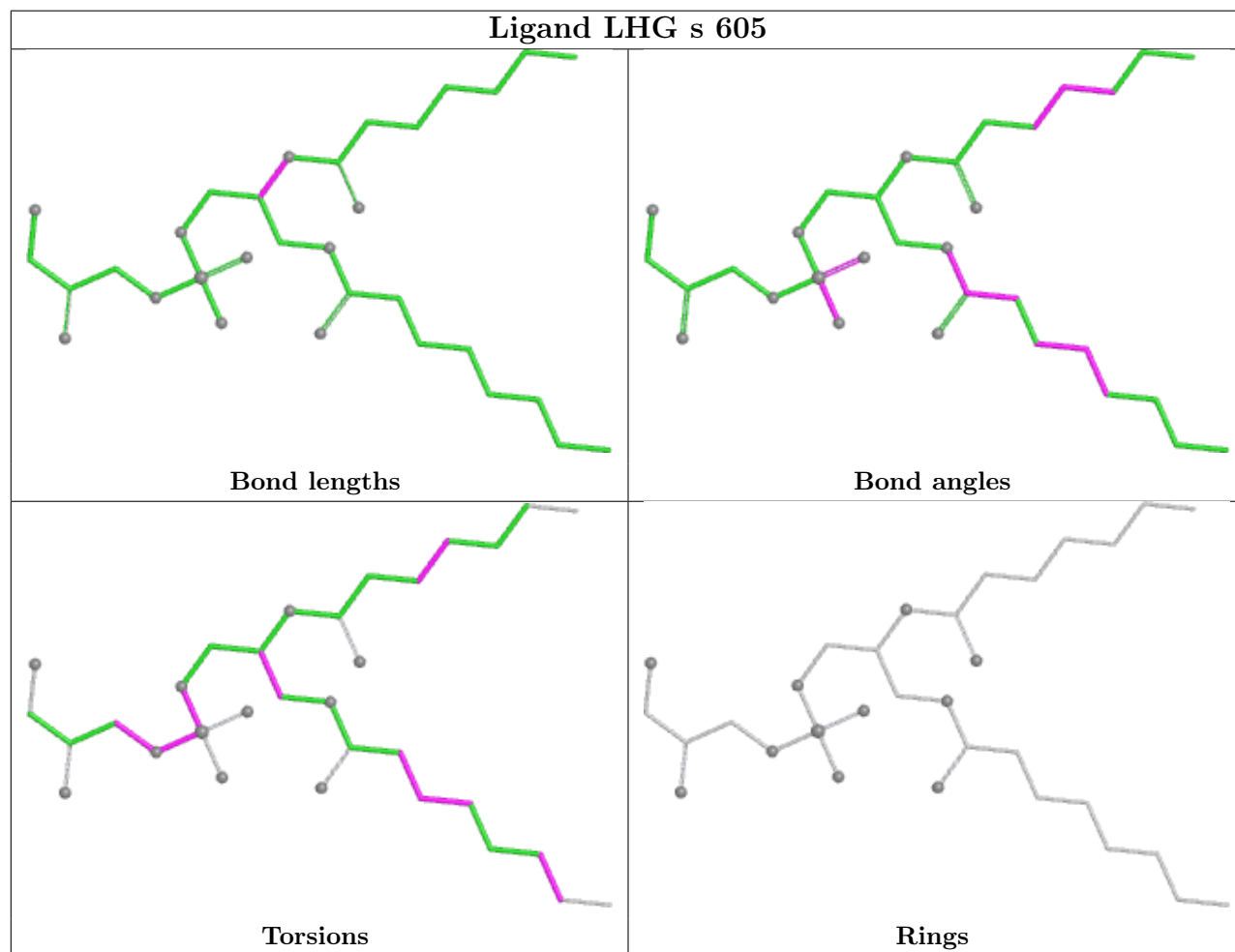
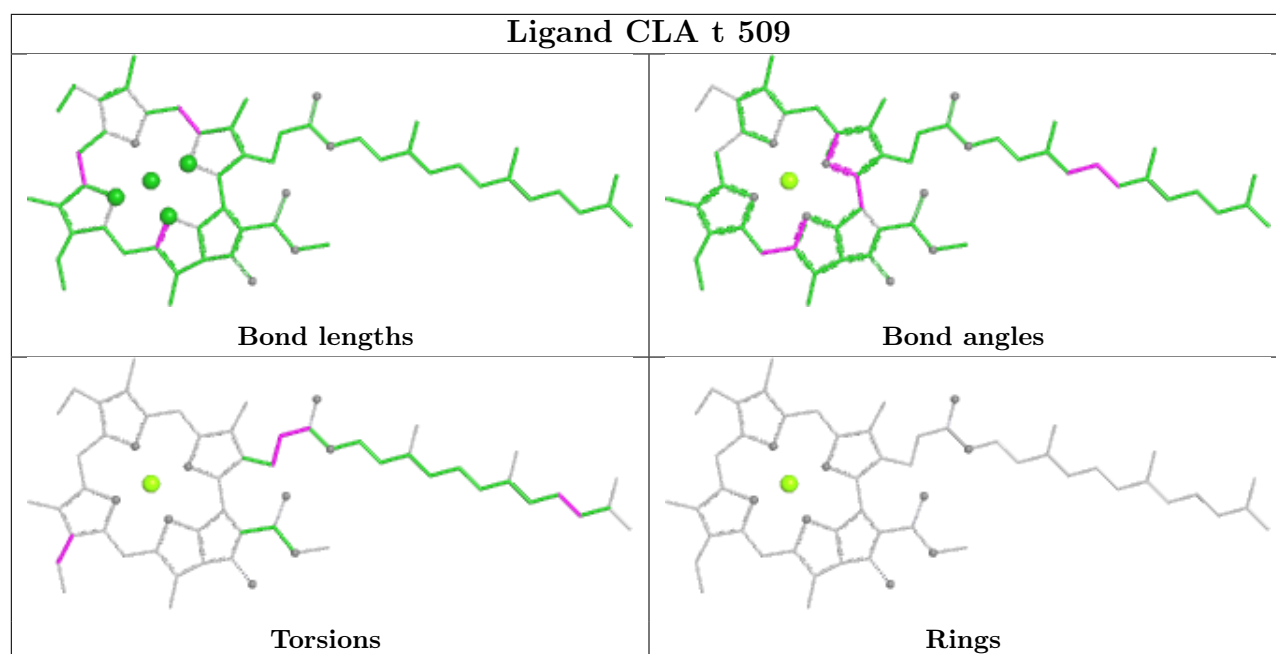
Ligand CLA H 1111**Ligand CLA a 1136**

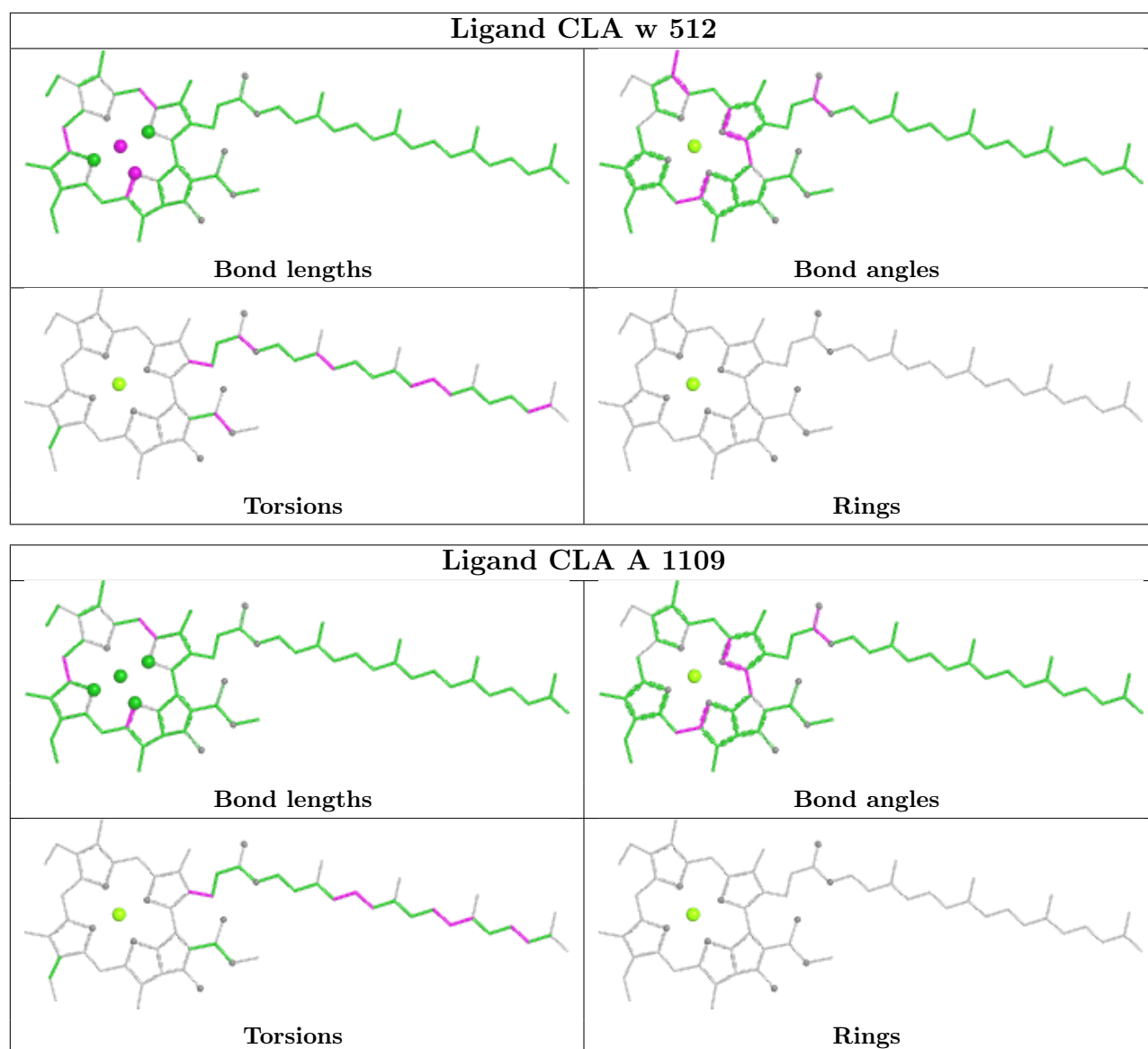


Ligand CLA p 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

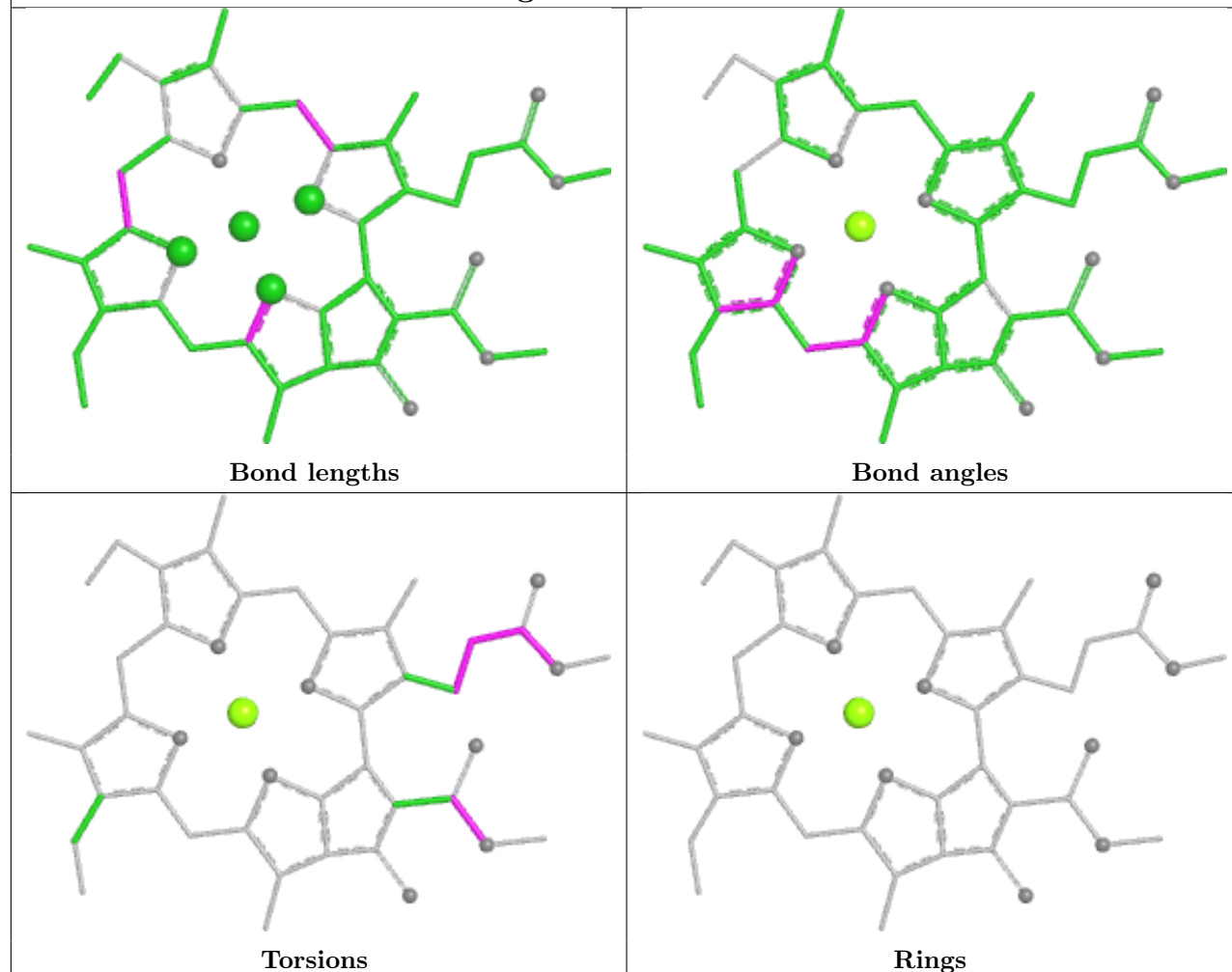
Ligand LUT Z 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR u 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

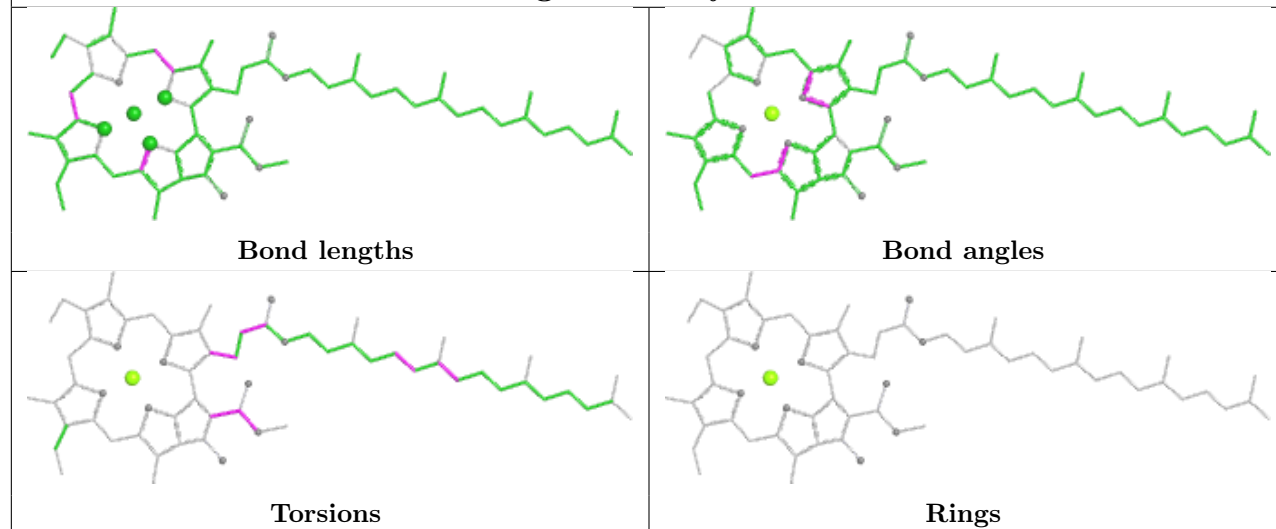




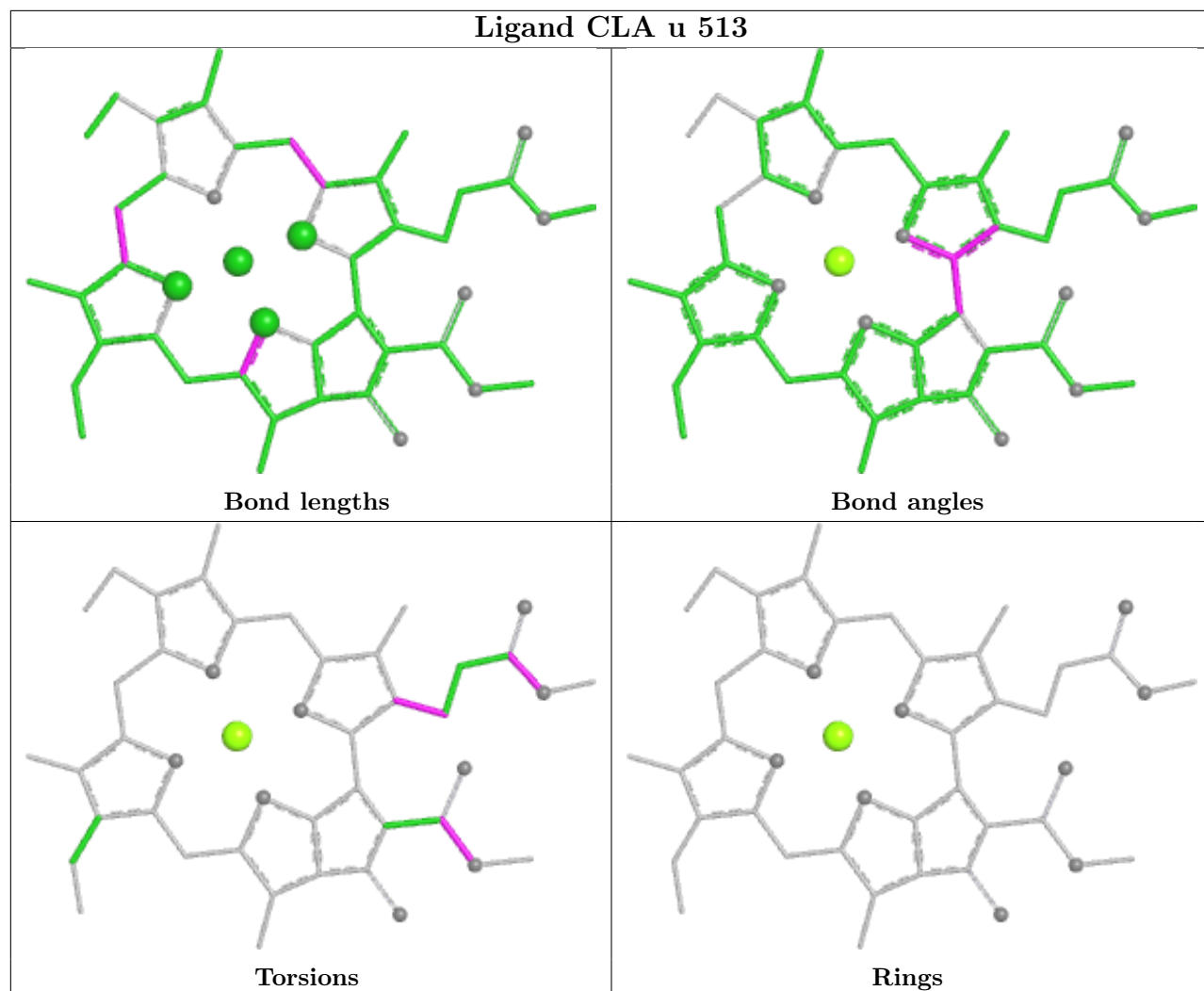
Ligand CLA x 503



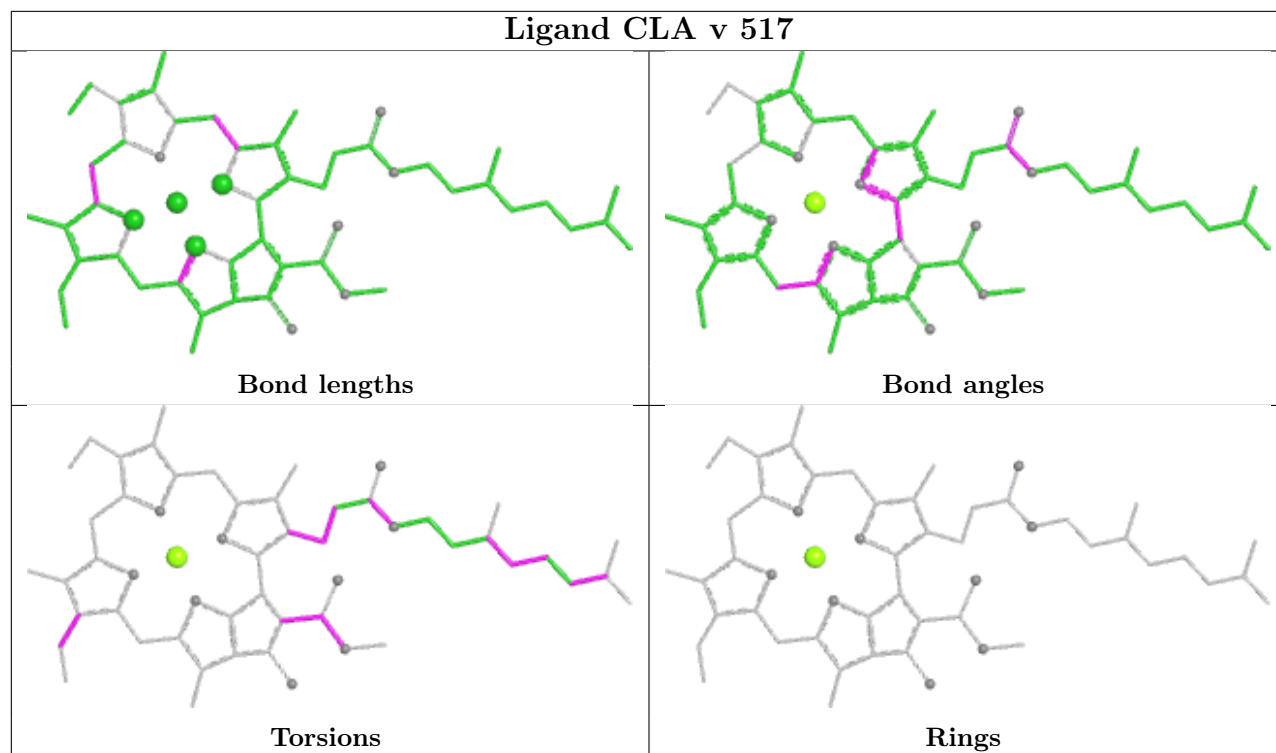
Ligand CLA y 507



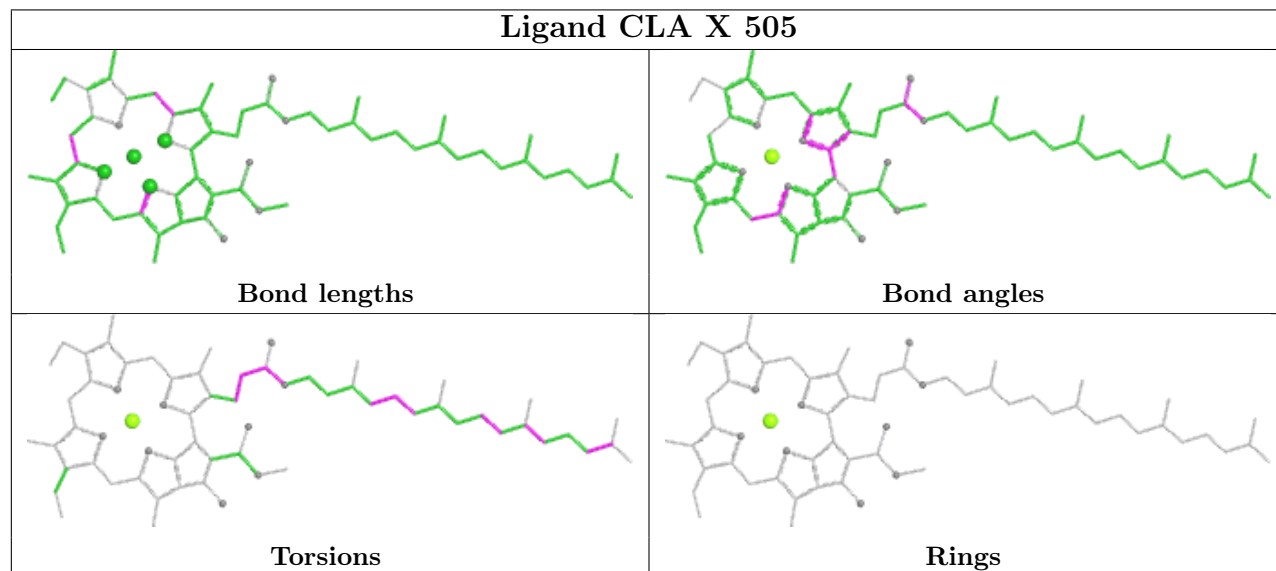
Ligand CLA u 513



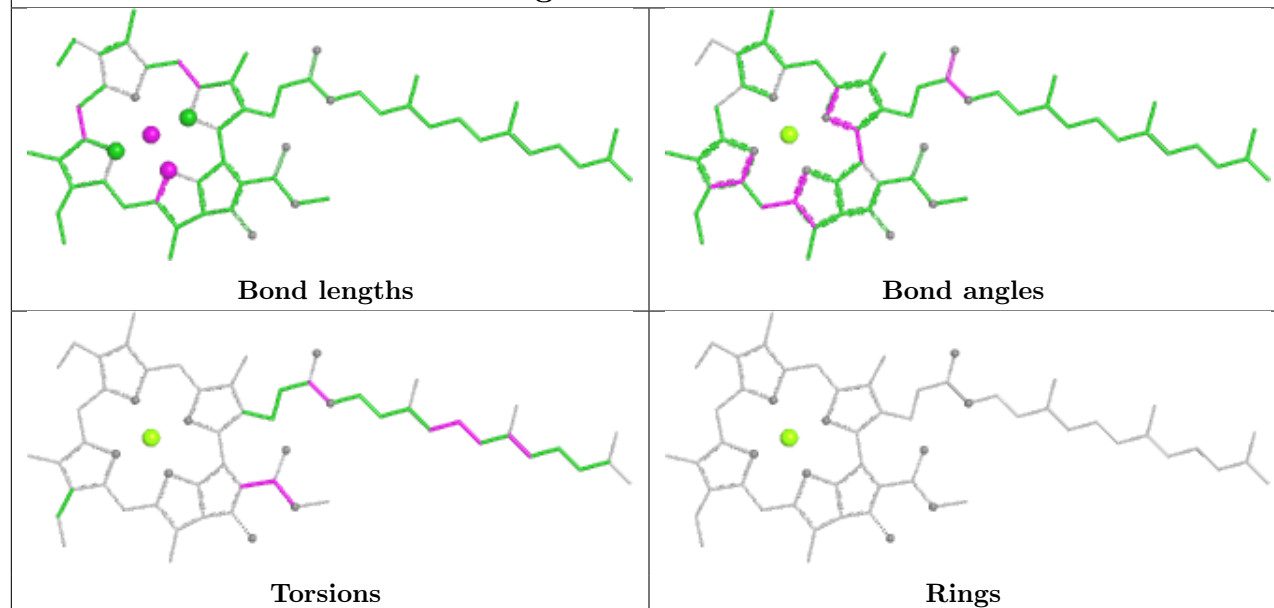
Ligand CLA v 517



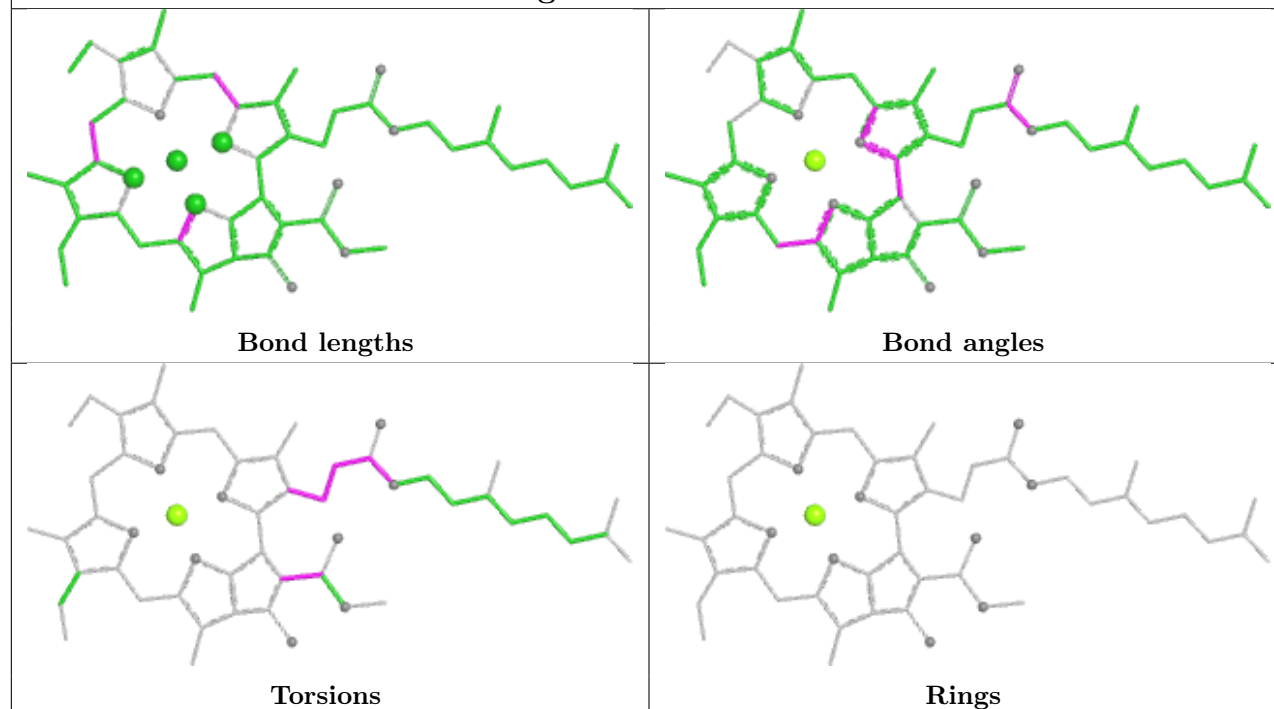
Ligand CLA X 505

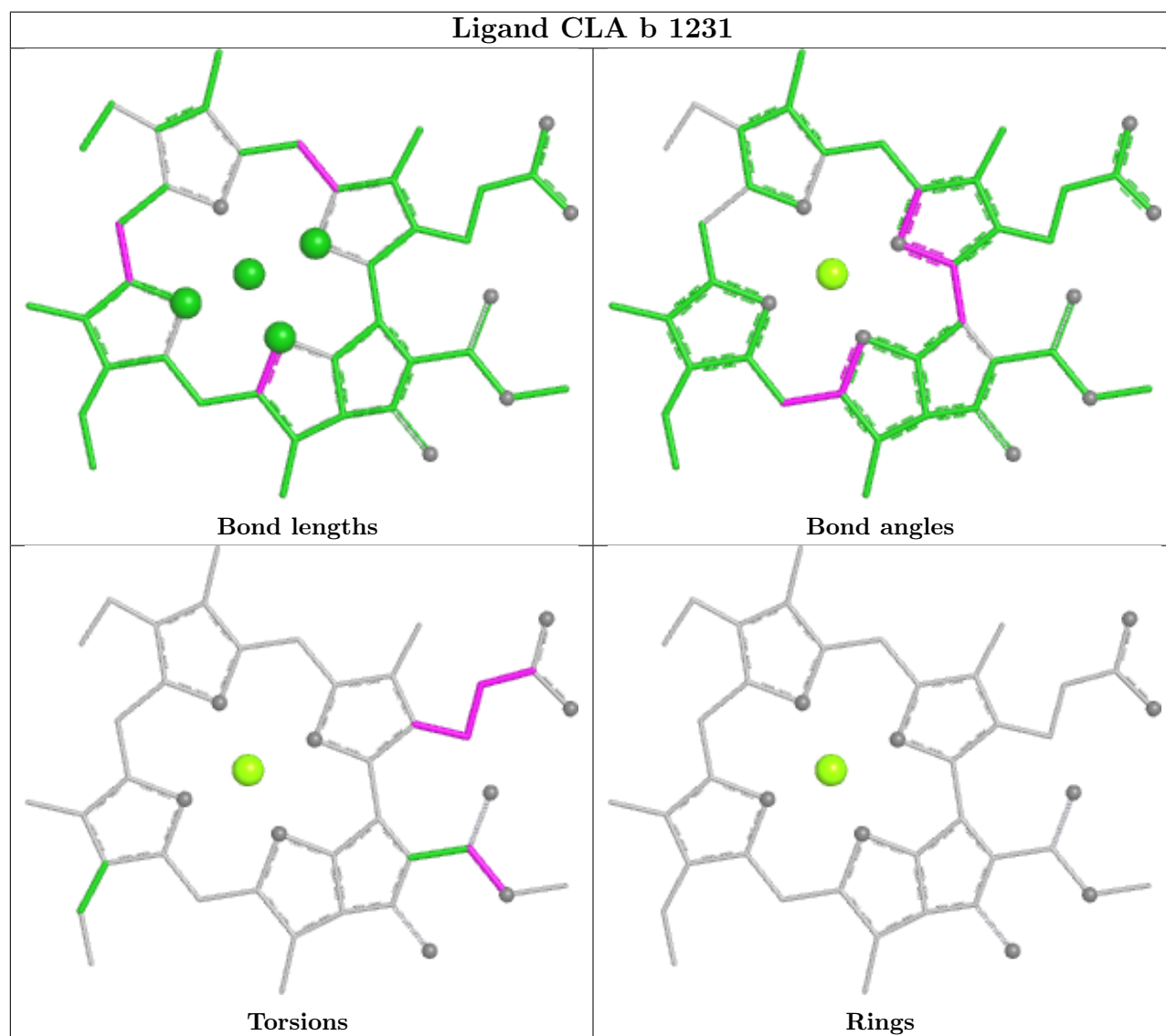
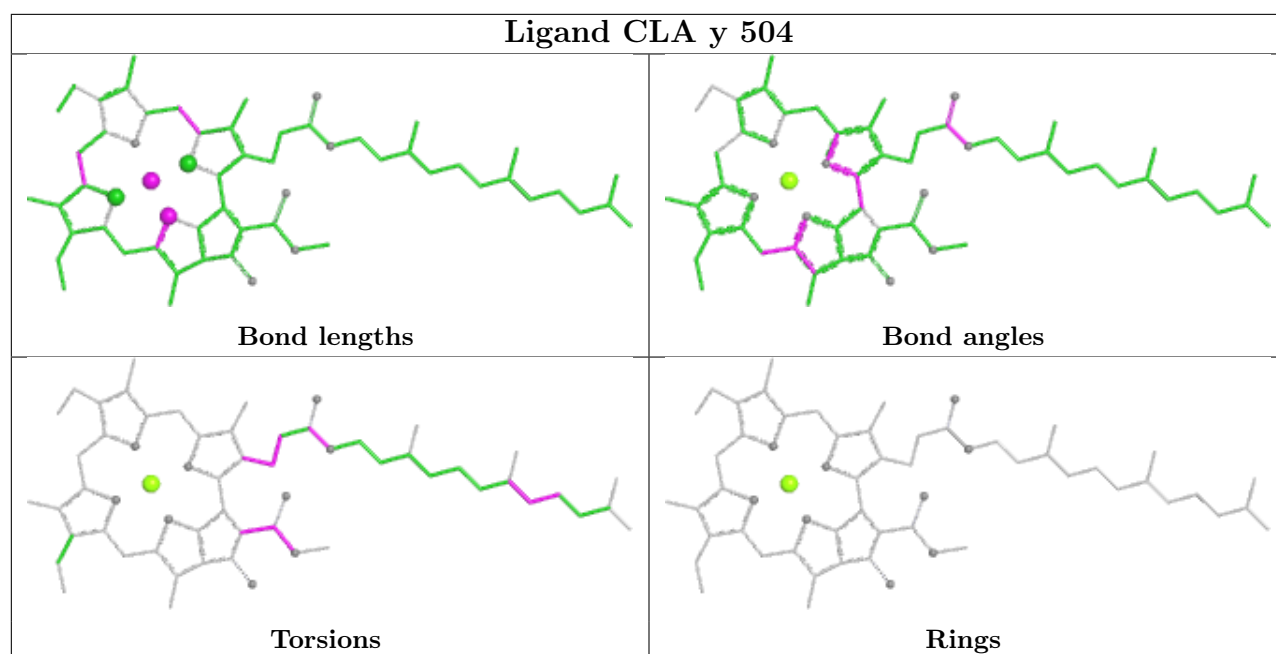


Ligand CLA h 506

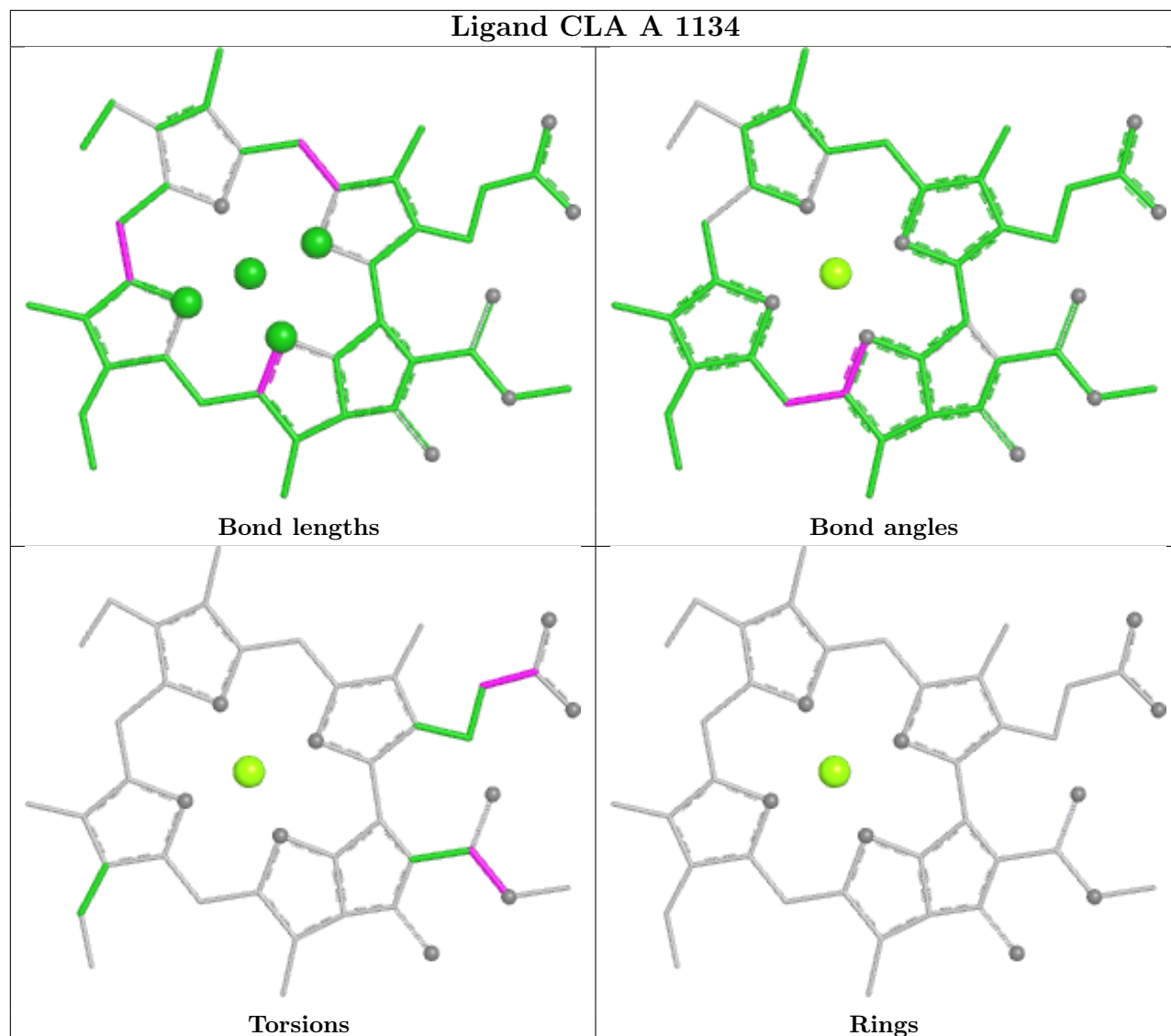


Ligand CLA s 508

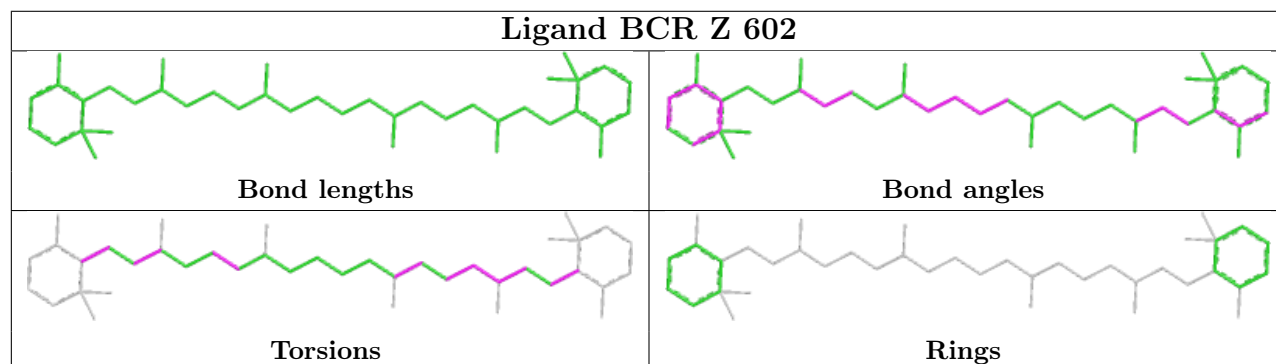


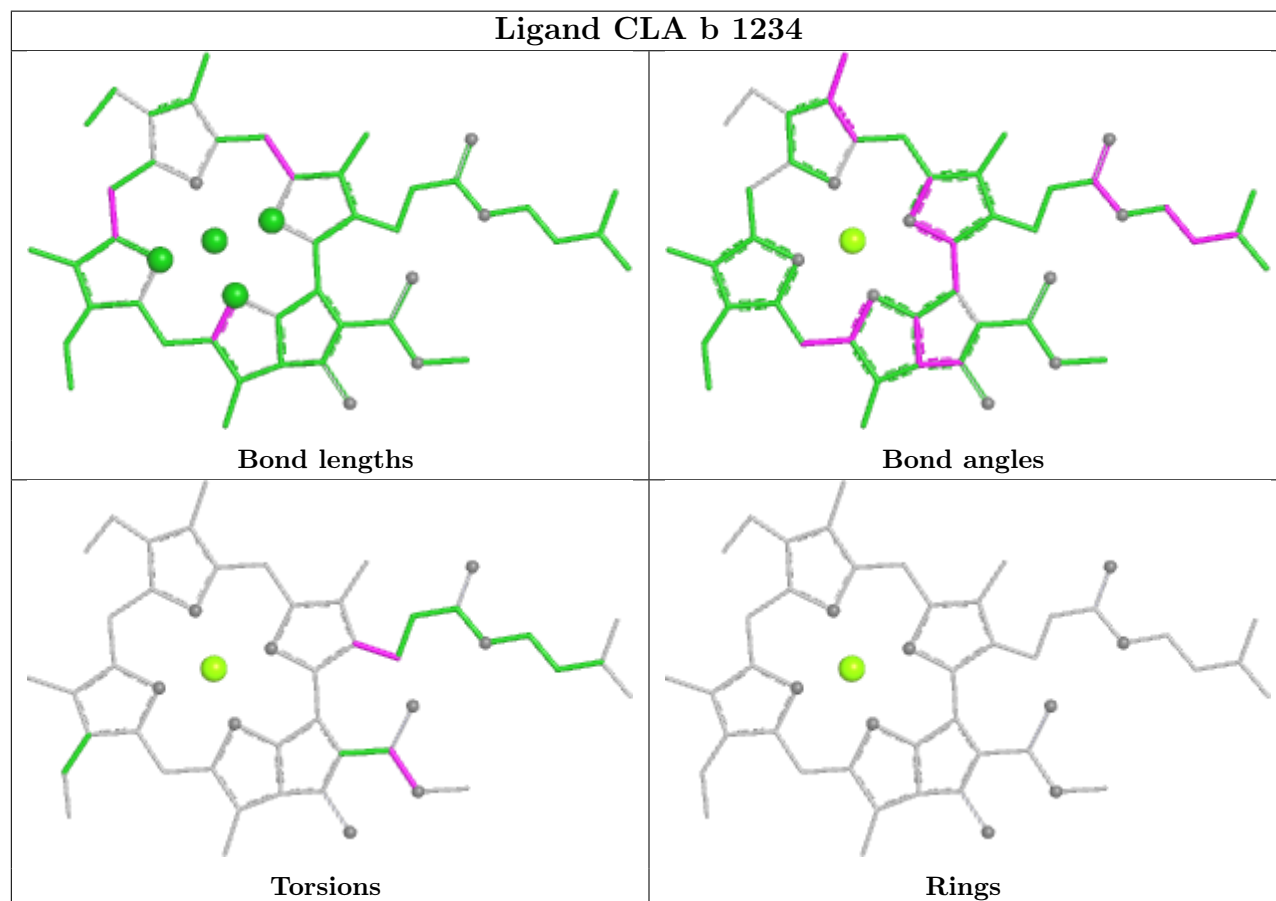
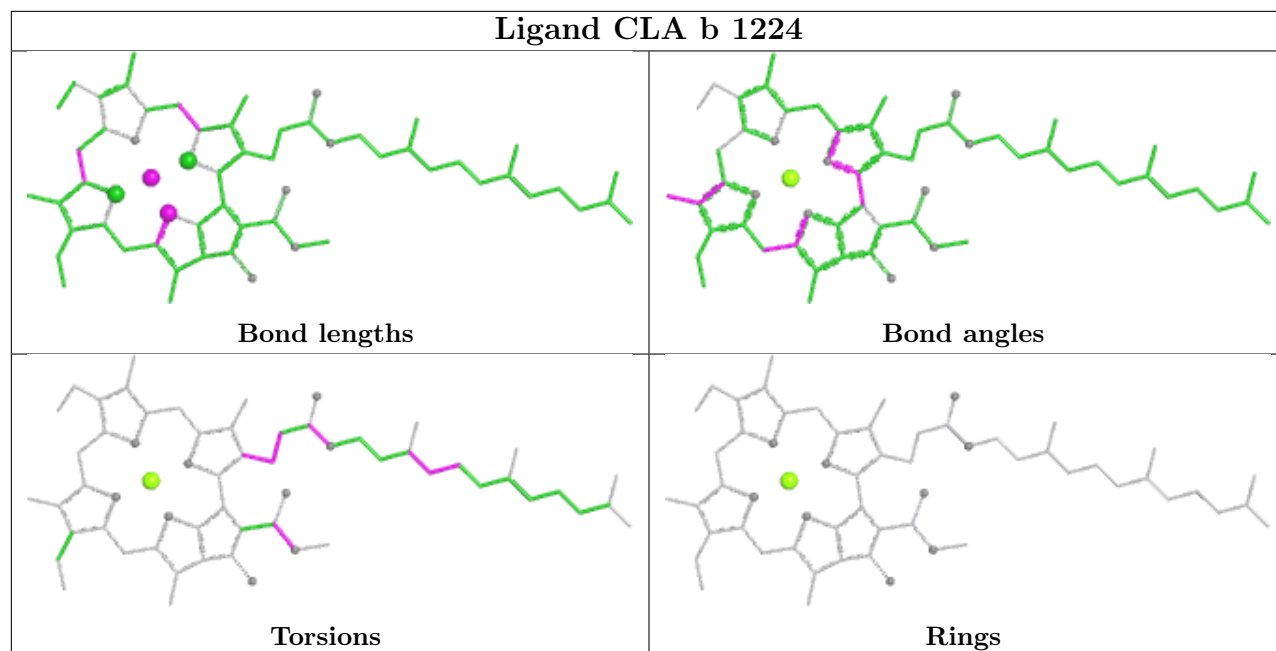


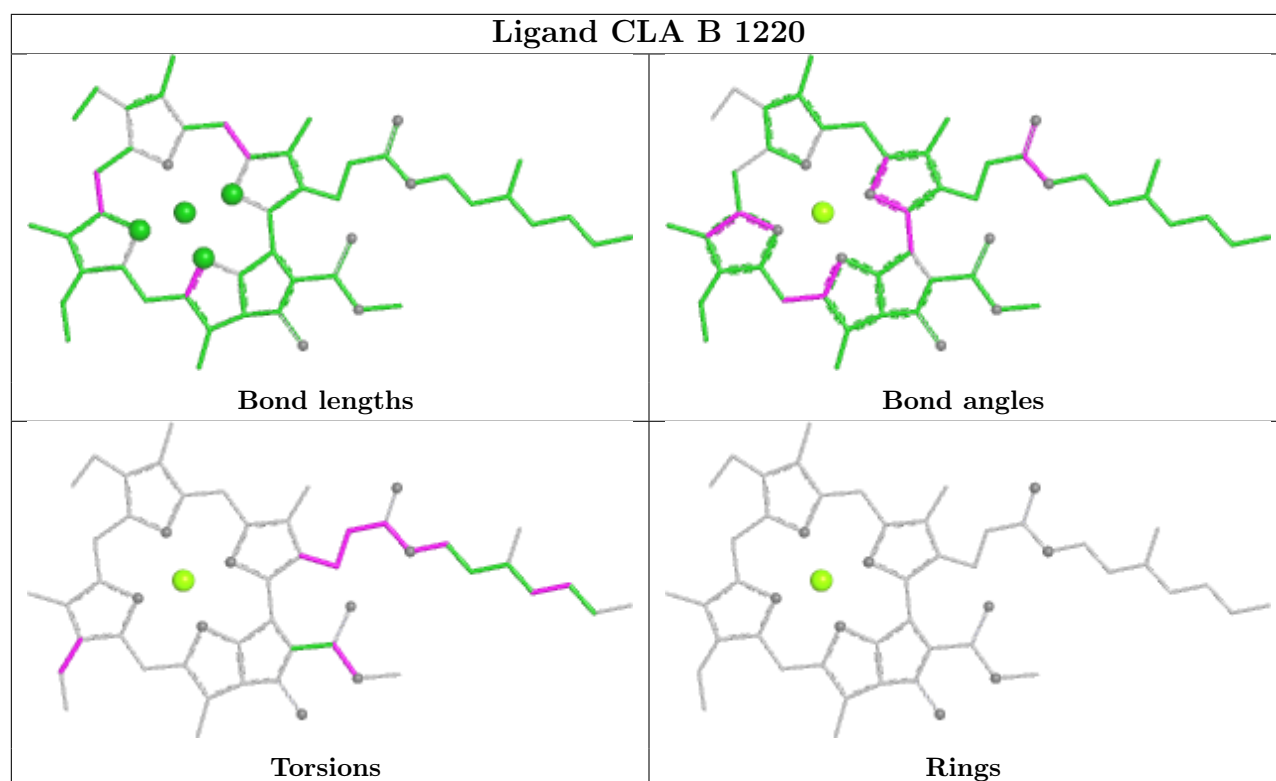
Ligand CLA A 1134

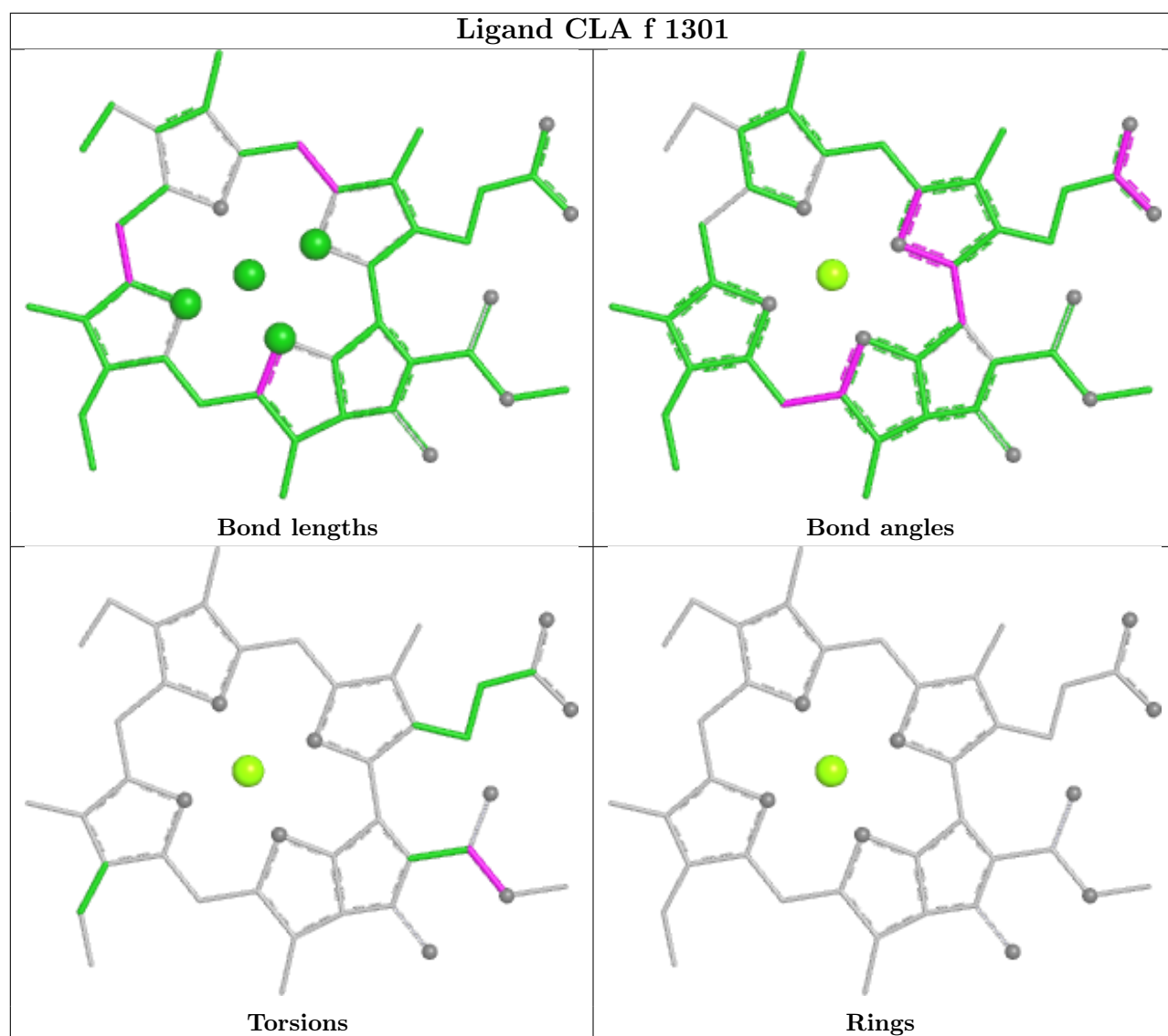


Ligand BCR Z 602

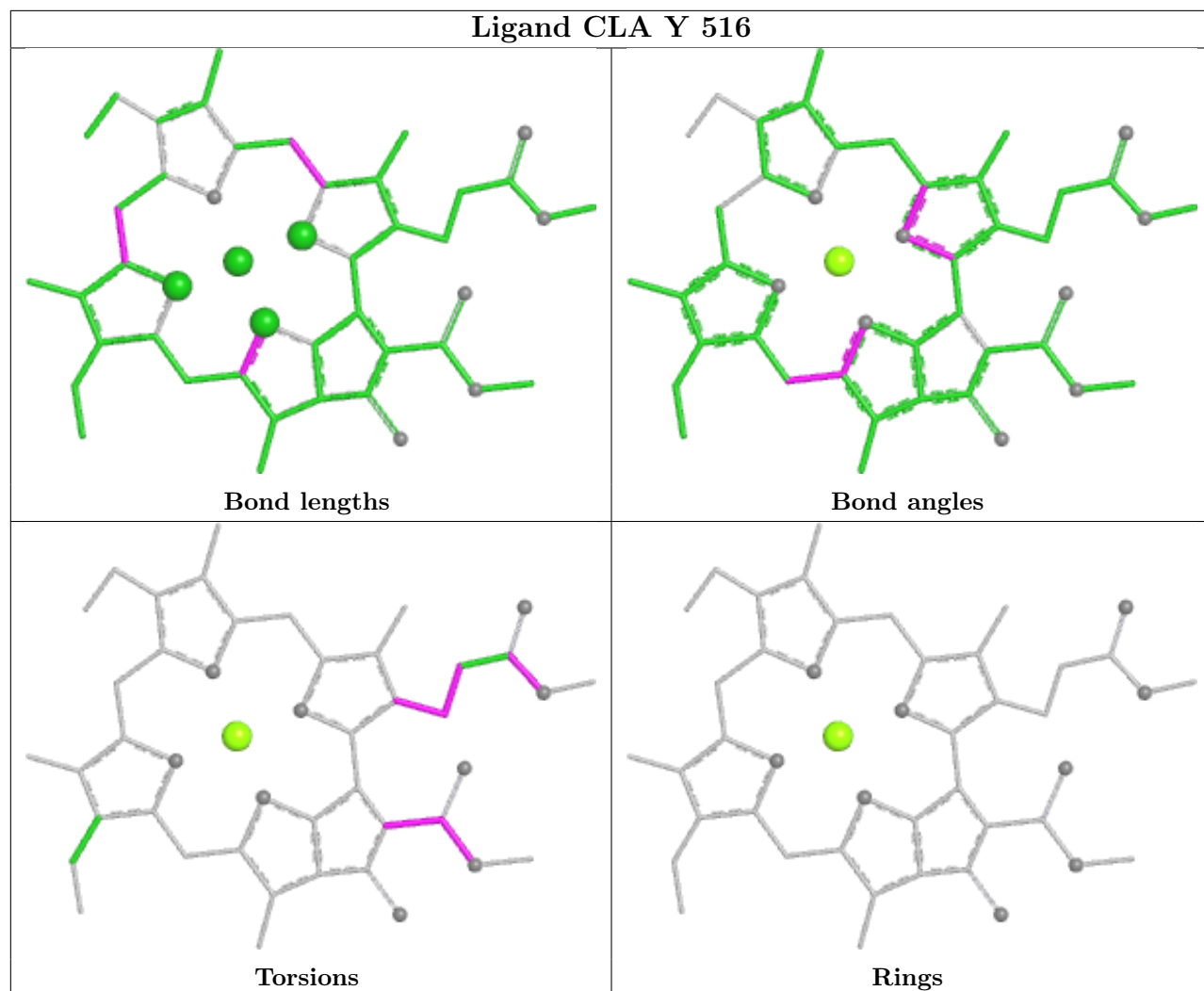




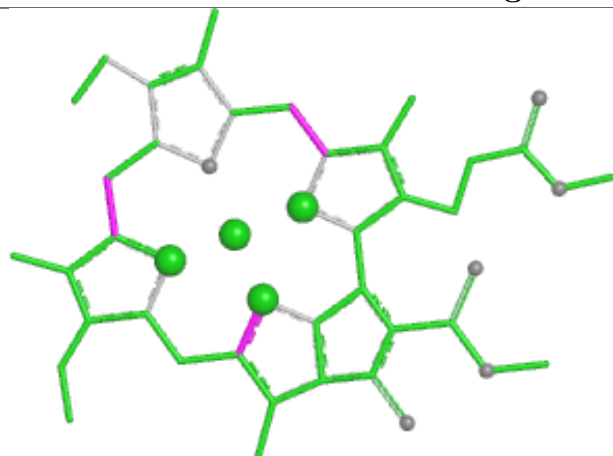




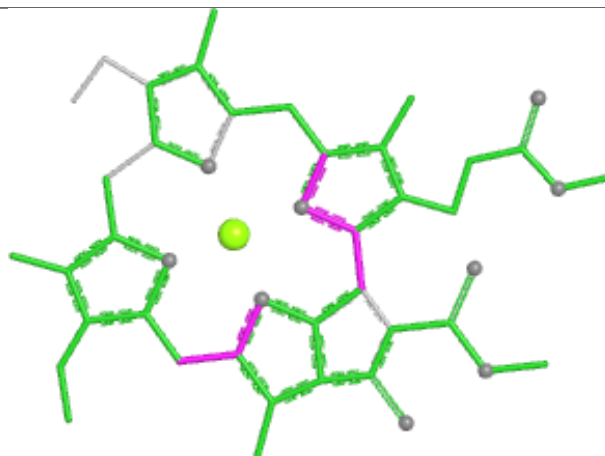
Ligand CLA Y 516



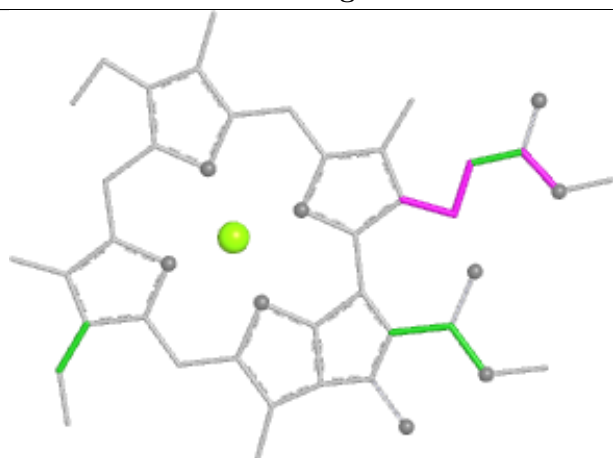
Ligand CLA H 1129



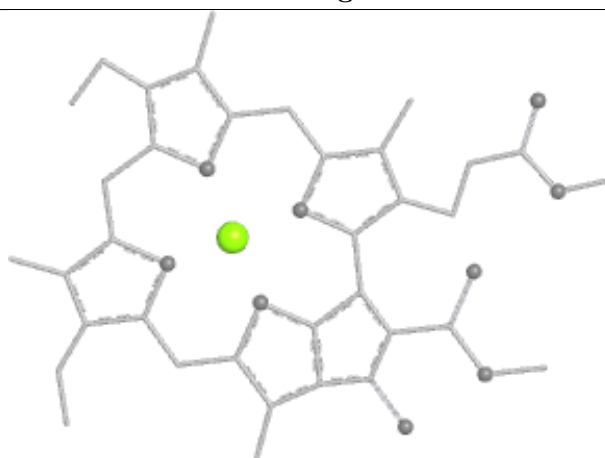
Bond lengths



Bond angles

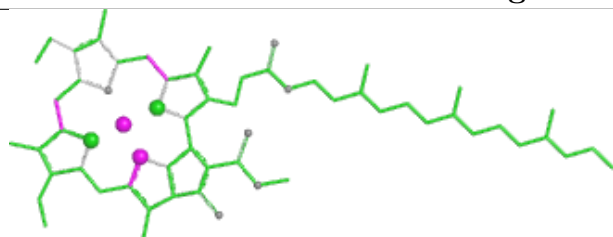


Torsions

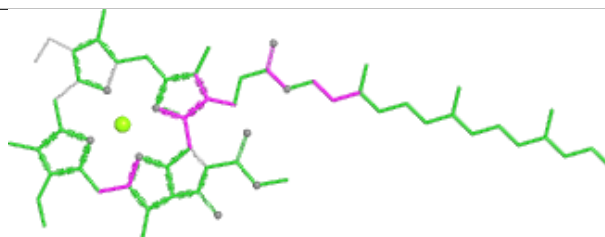


Rings

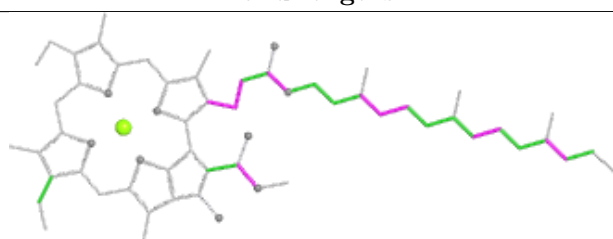
Ligand CLA b 1235



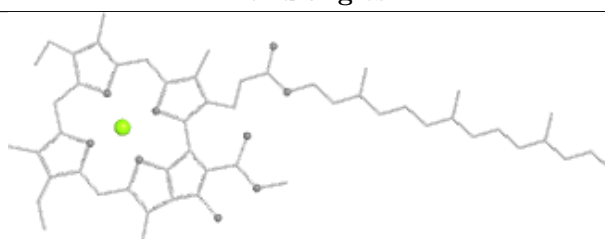
Bond lengths



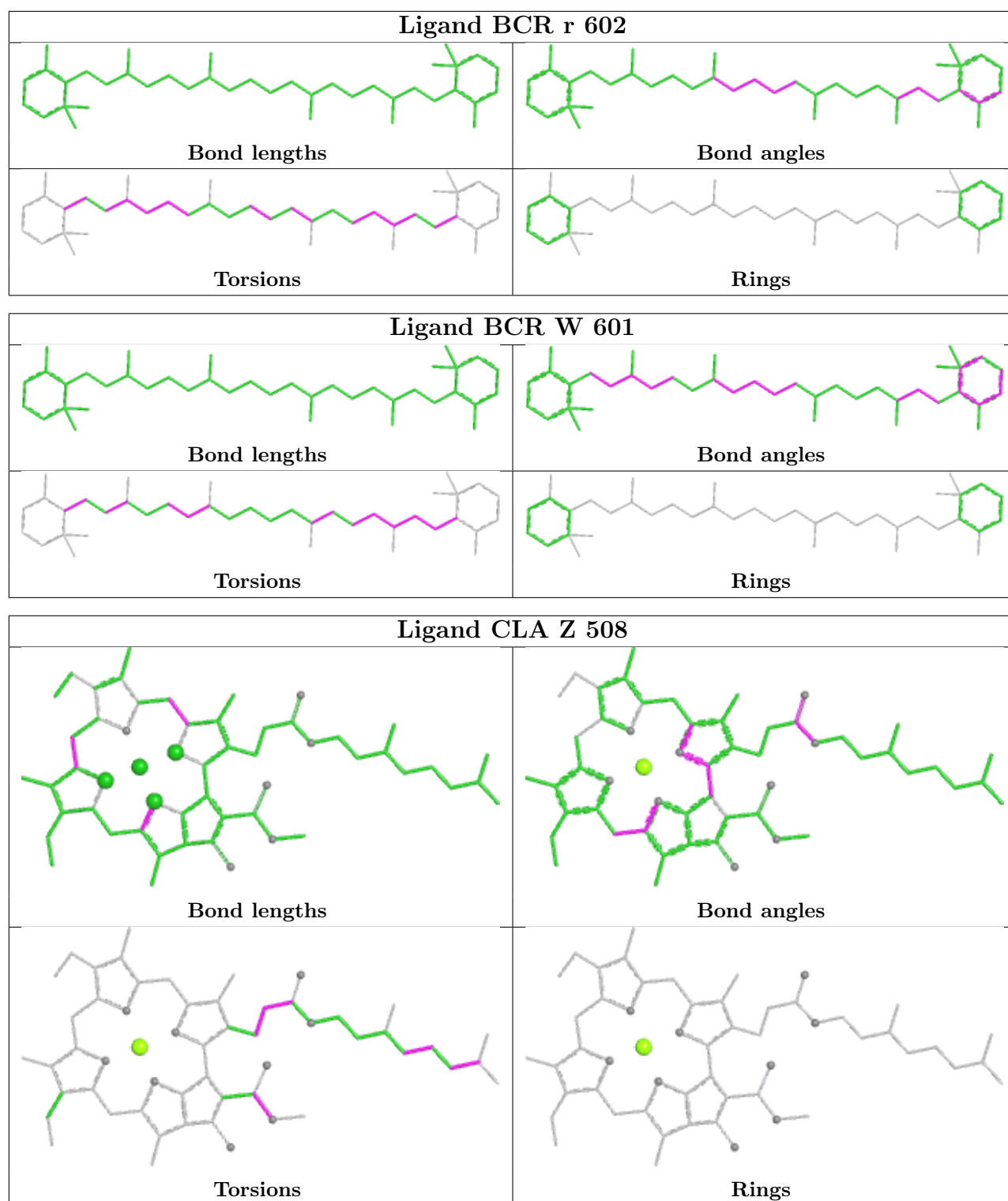
Bond angles

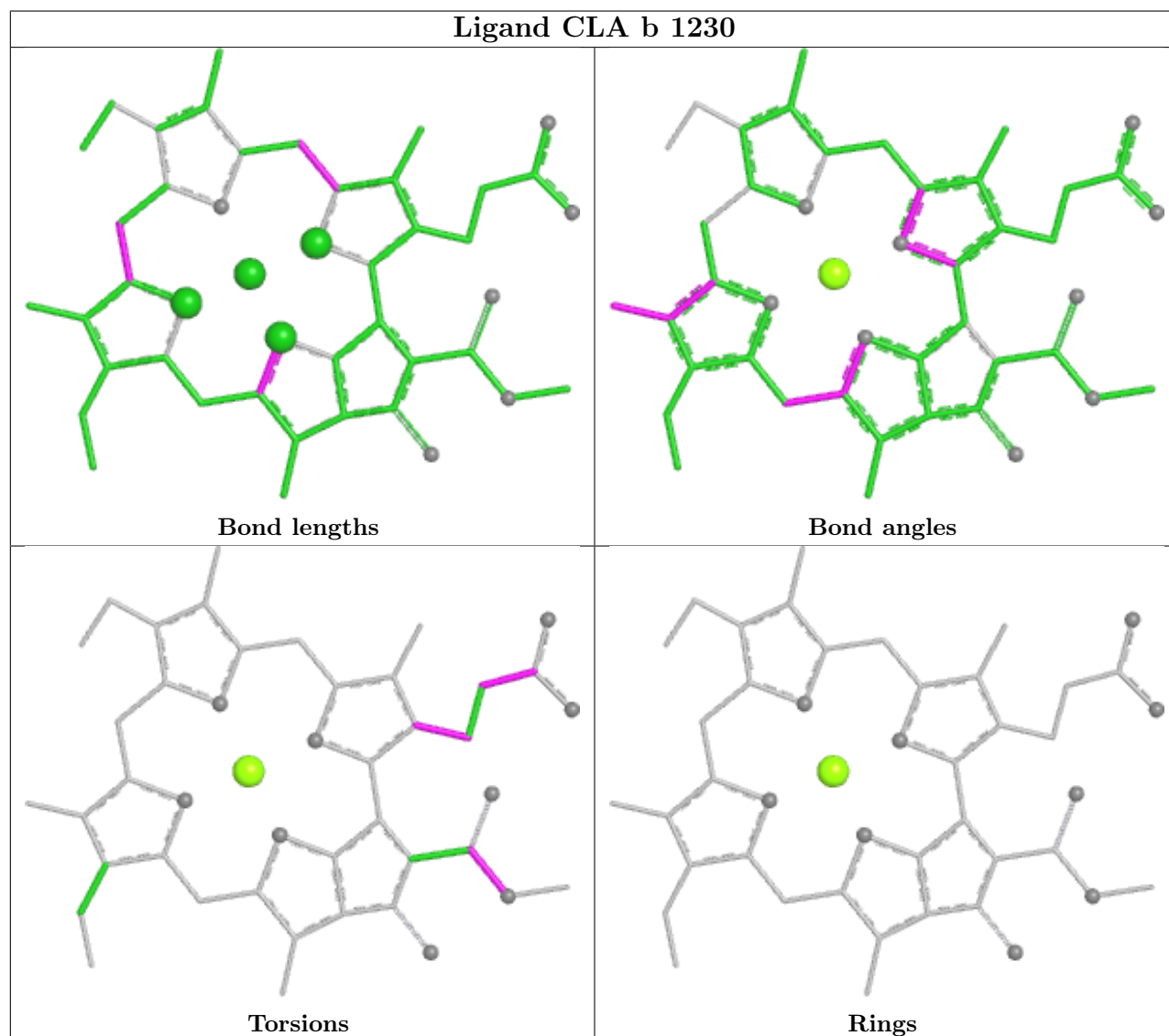
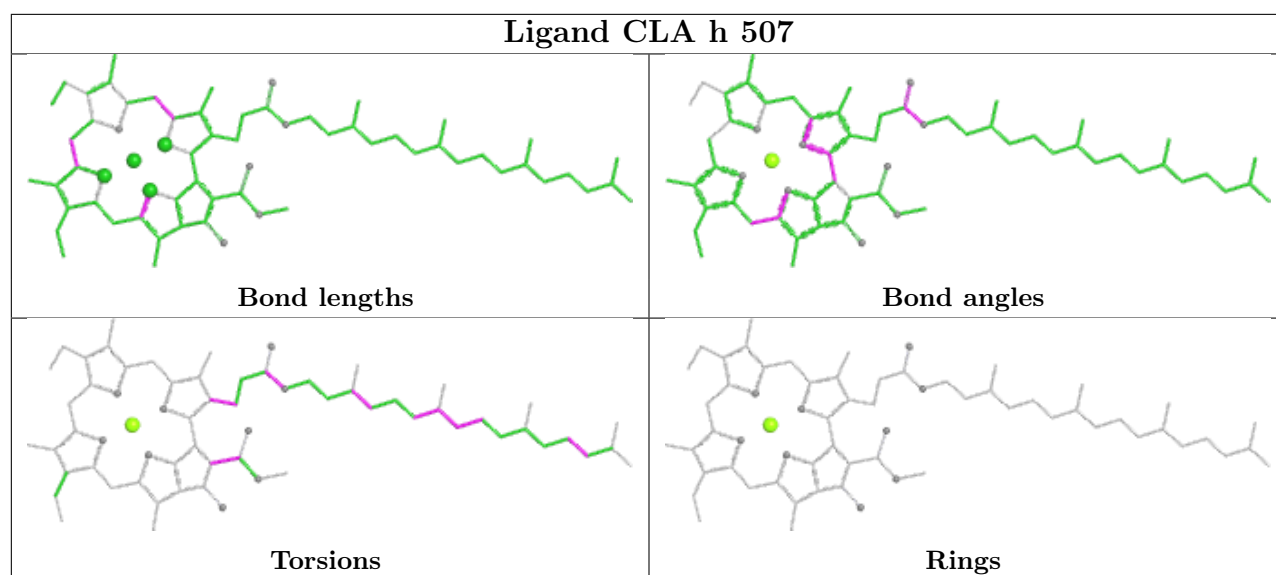


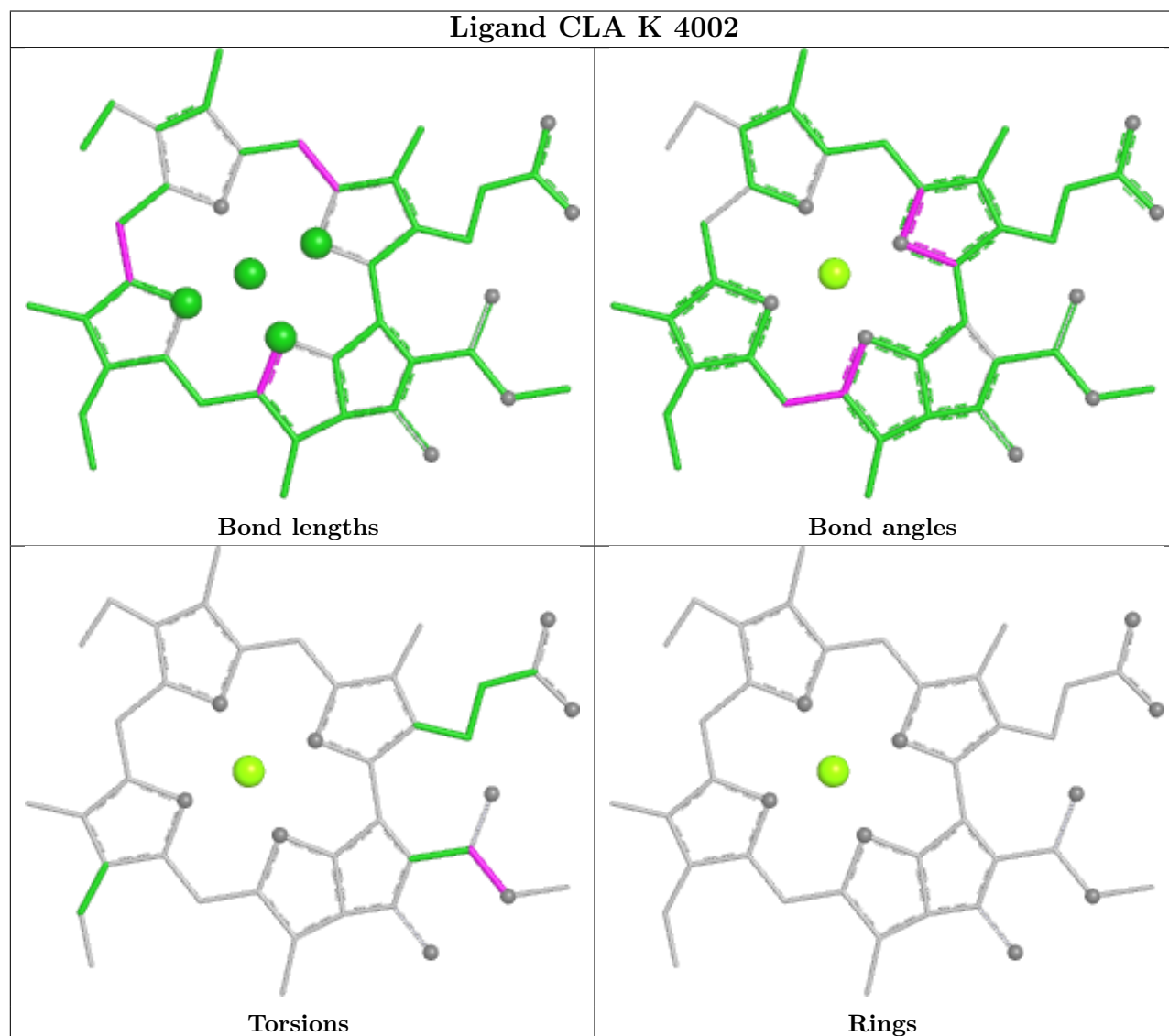
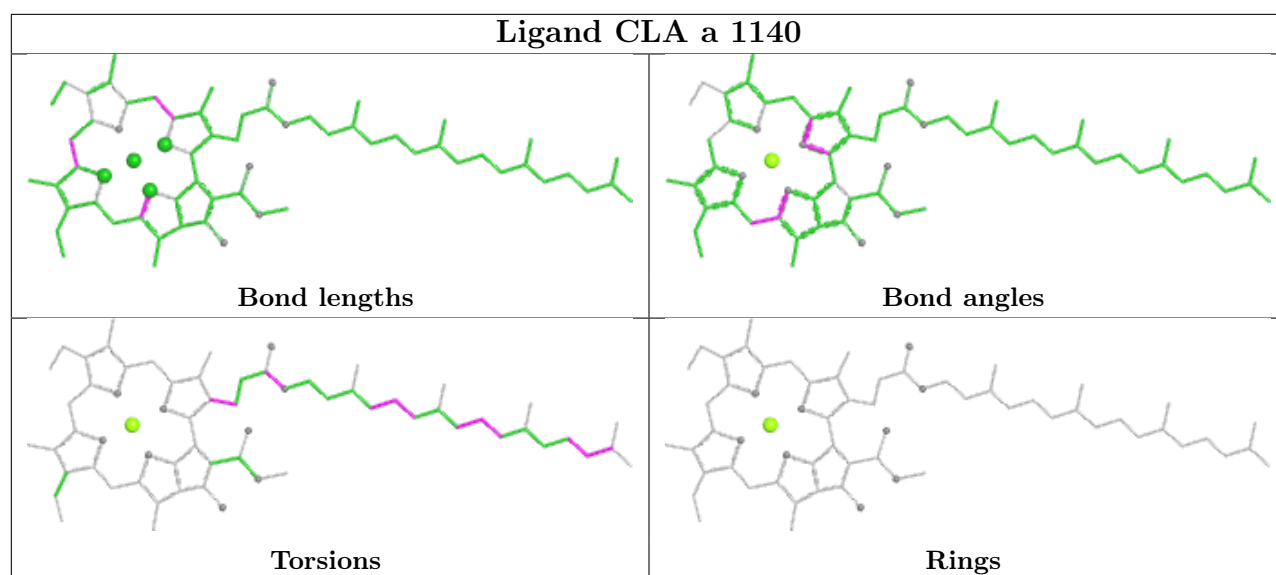
Torsions

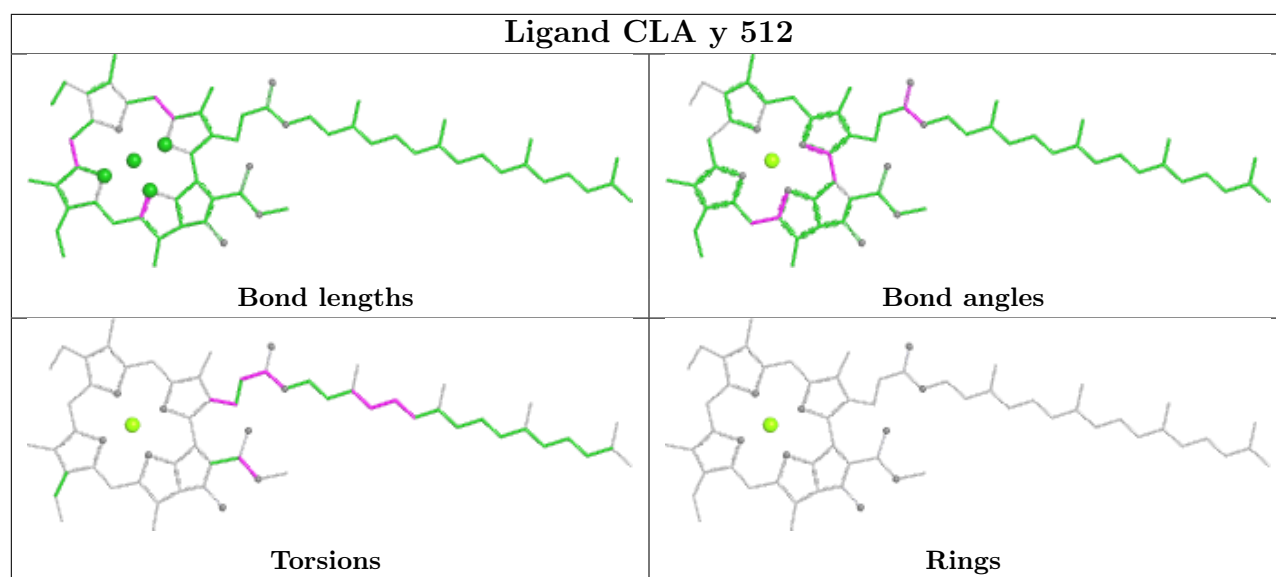


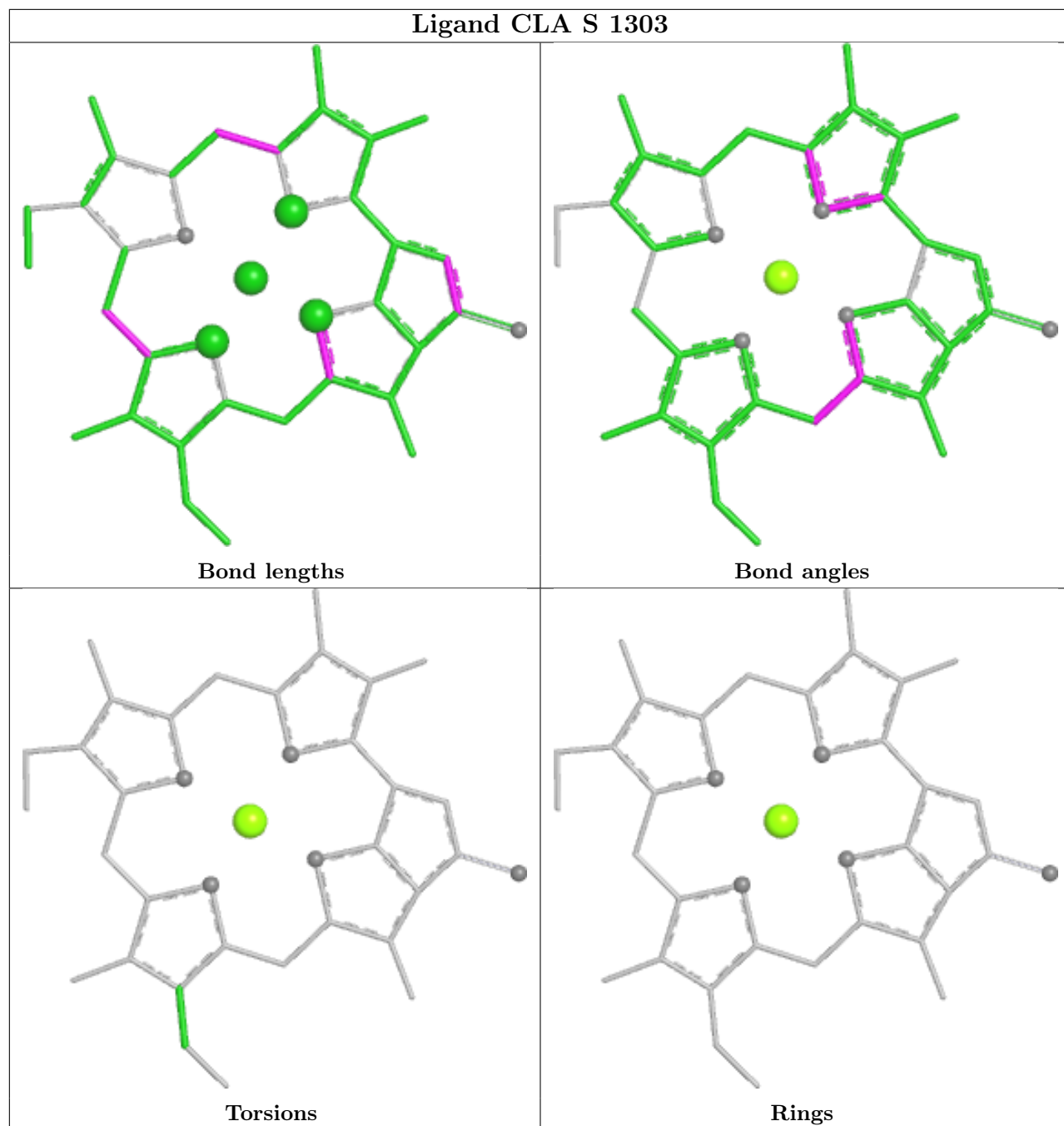
Rings

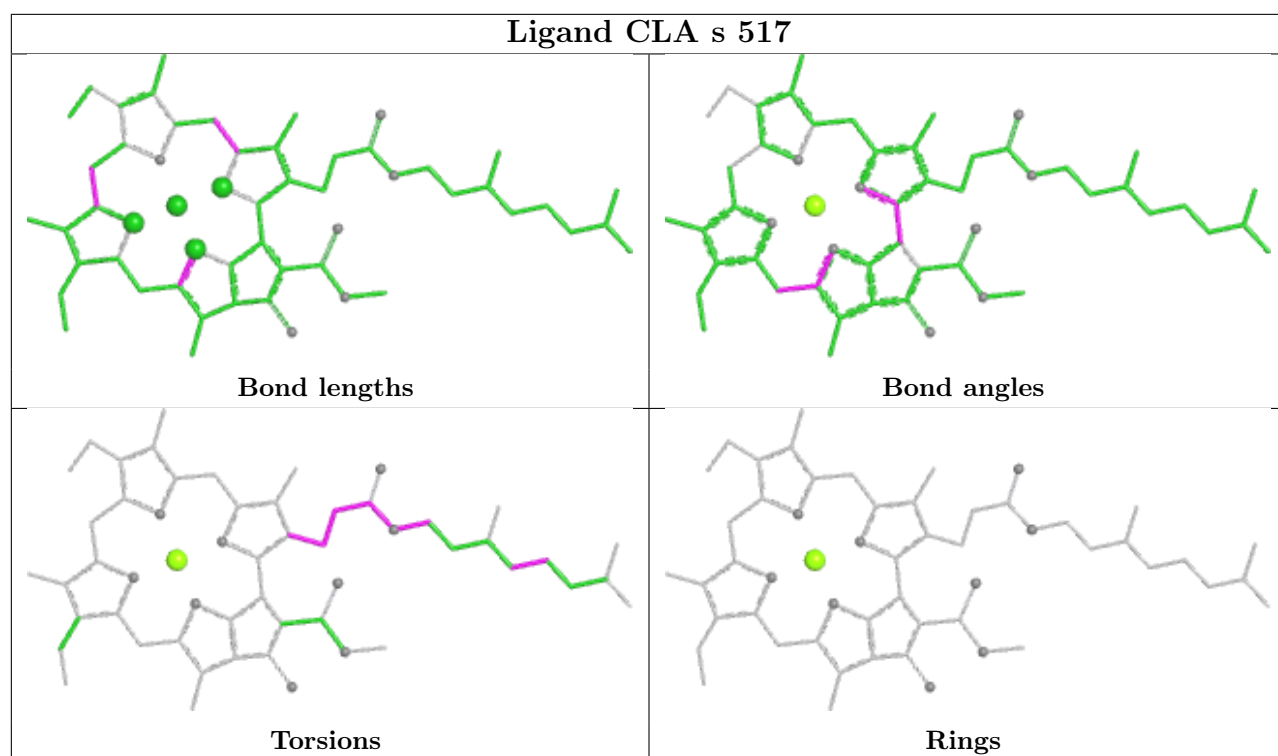


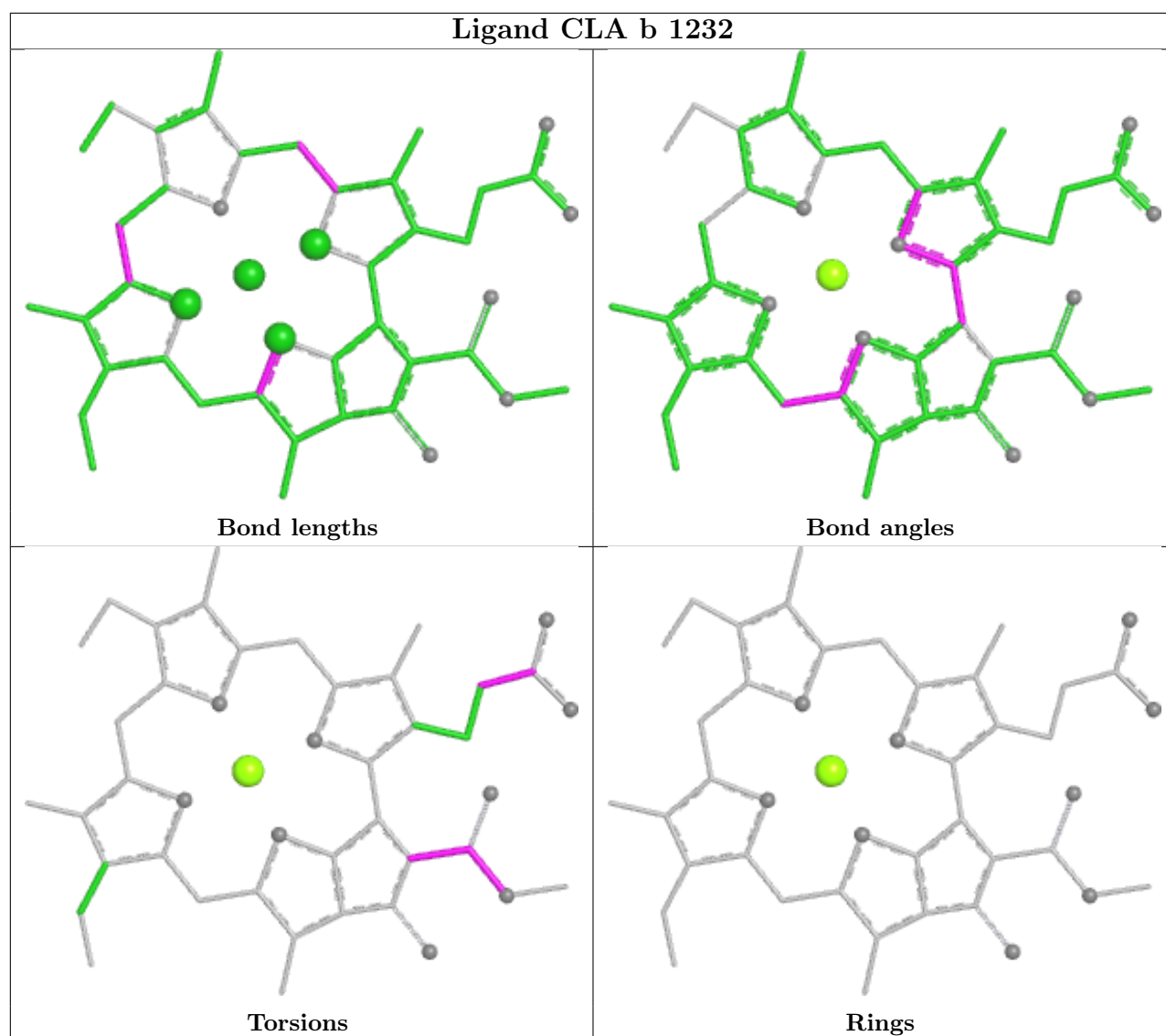




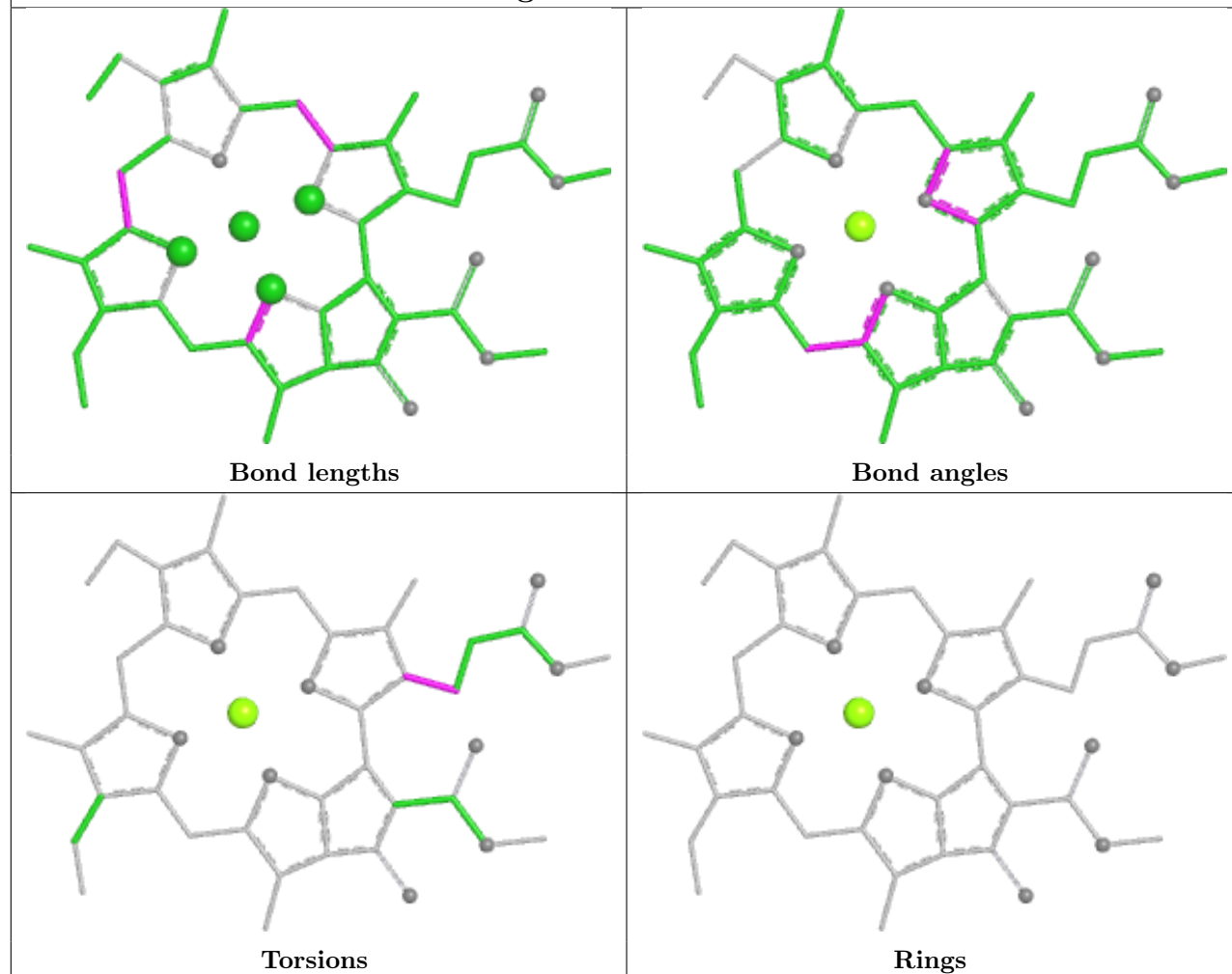




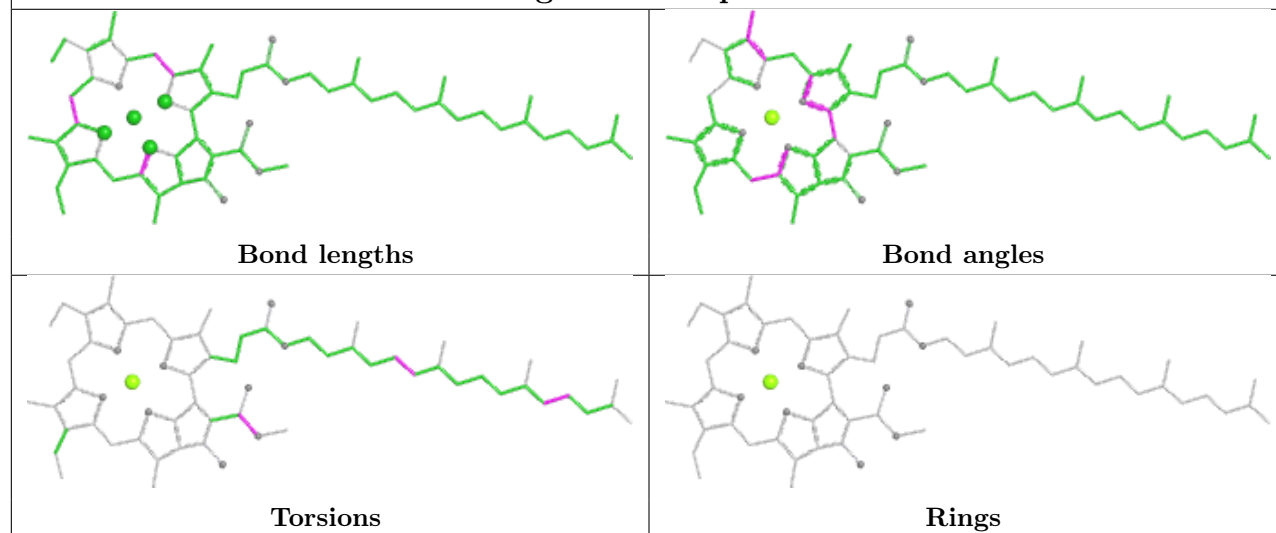




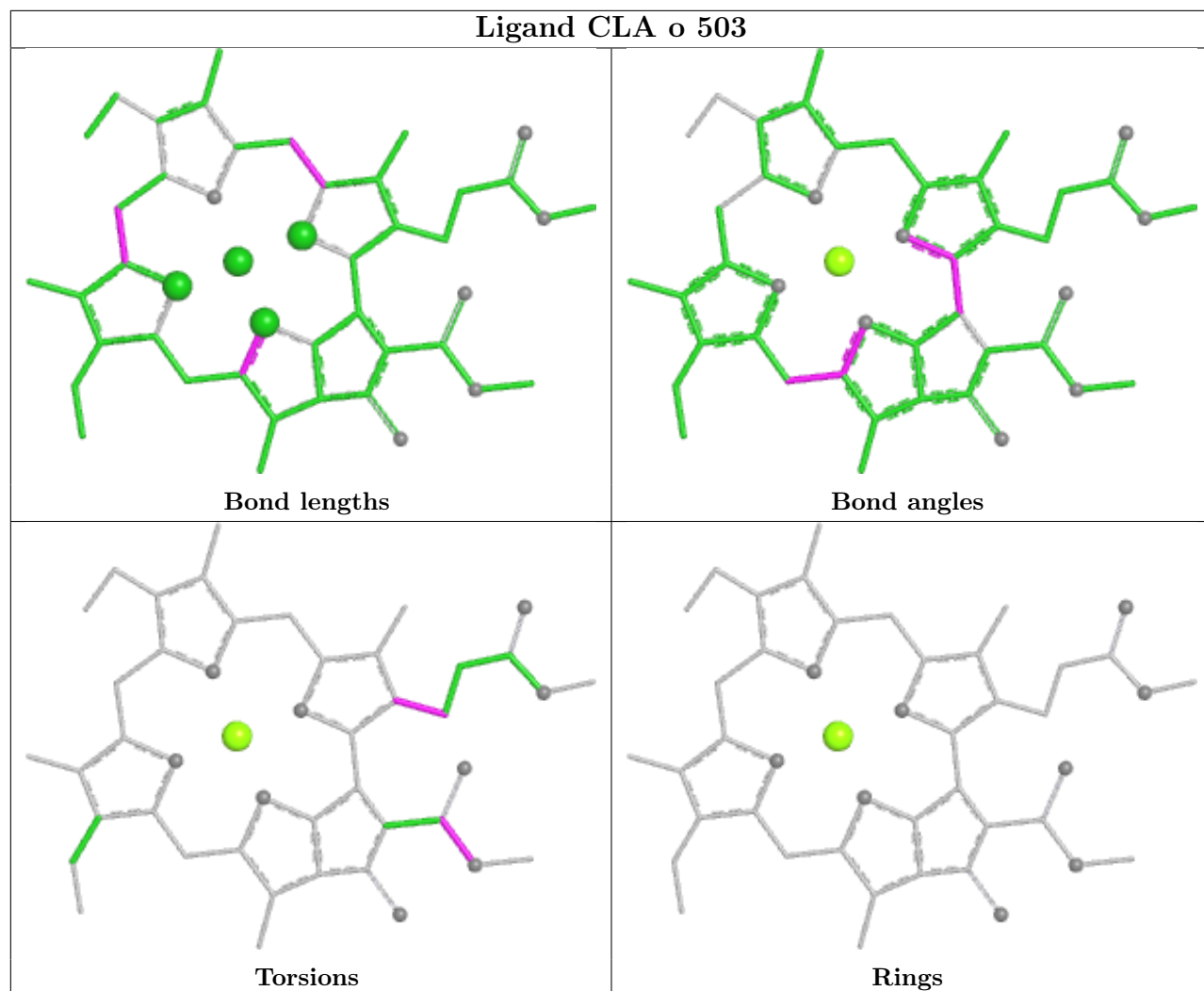
Ligand CLA v 513



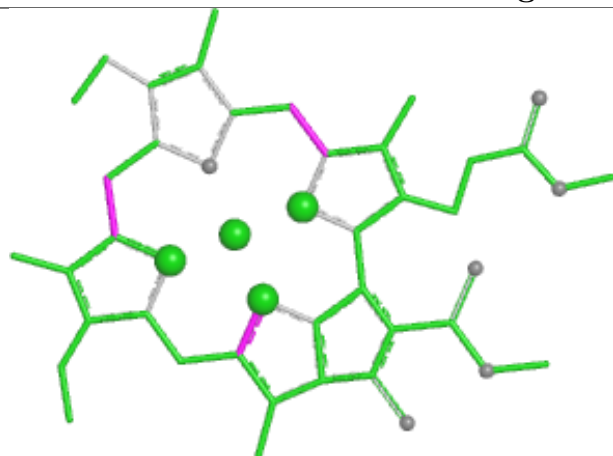
Ligand CLA q 511



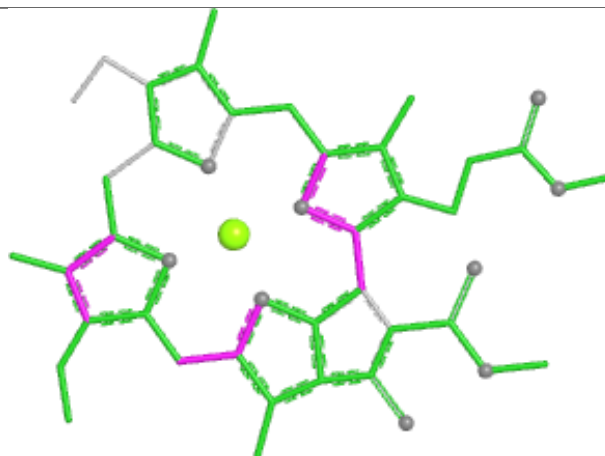
Ligand CLA o 503



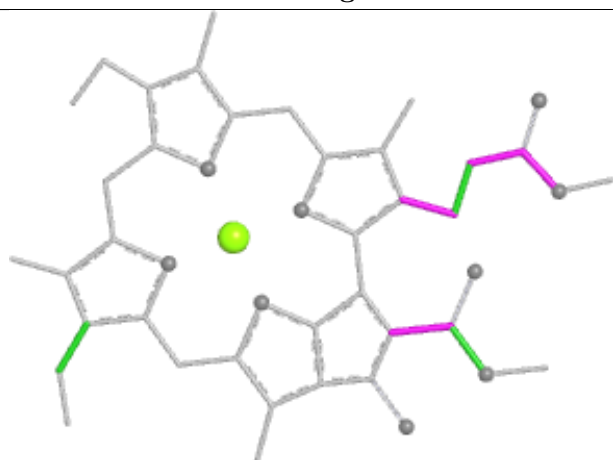
Ligand CLA v 501



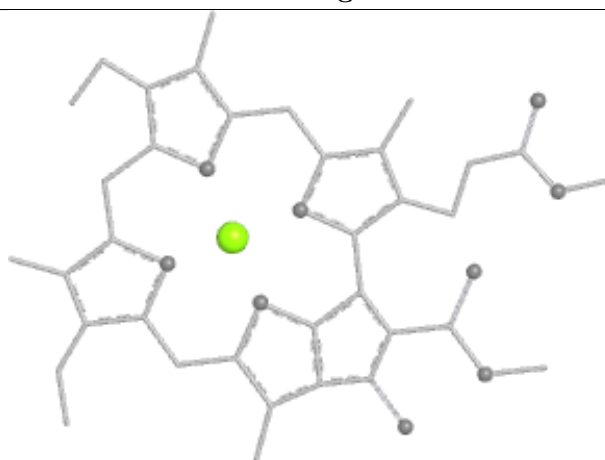
Bond lengths



Bond angles

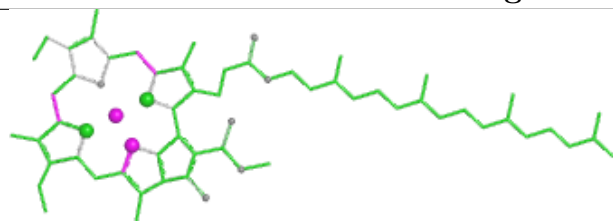


Torsions

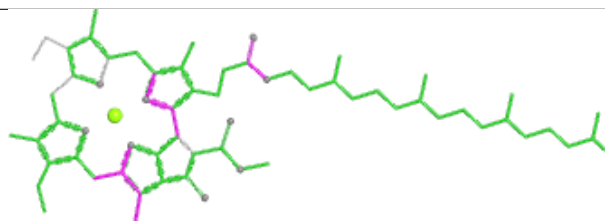


Rings

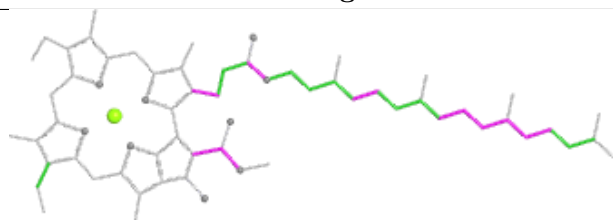
Ligand CLA H 1128



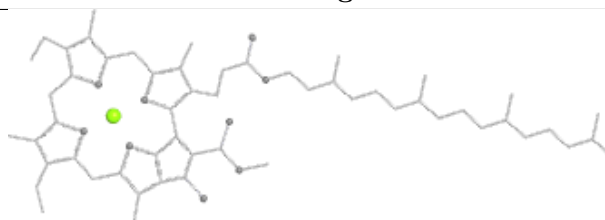
Bond lengths



Bond angles

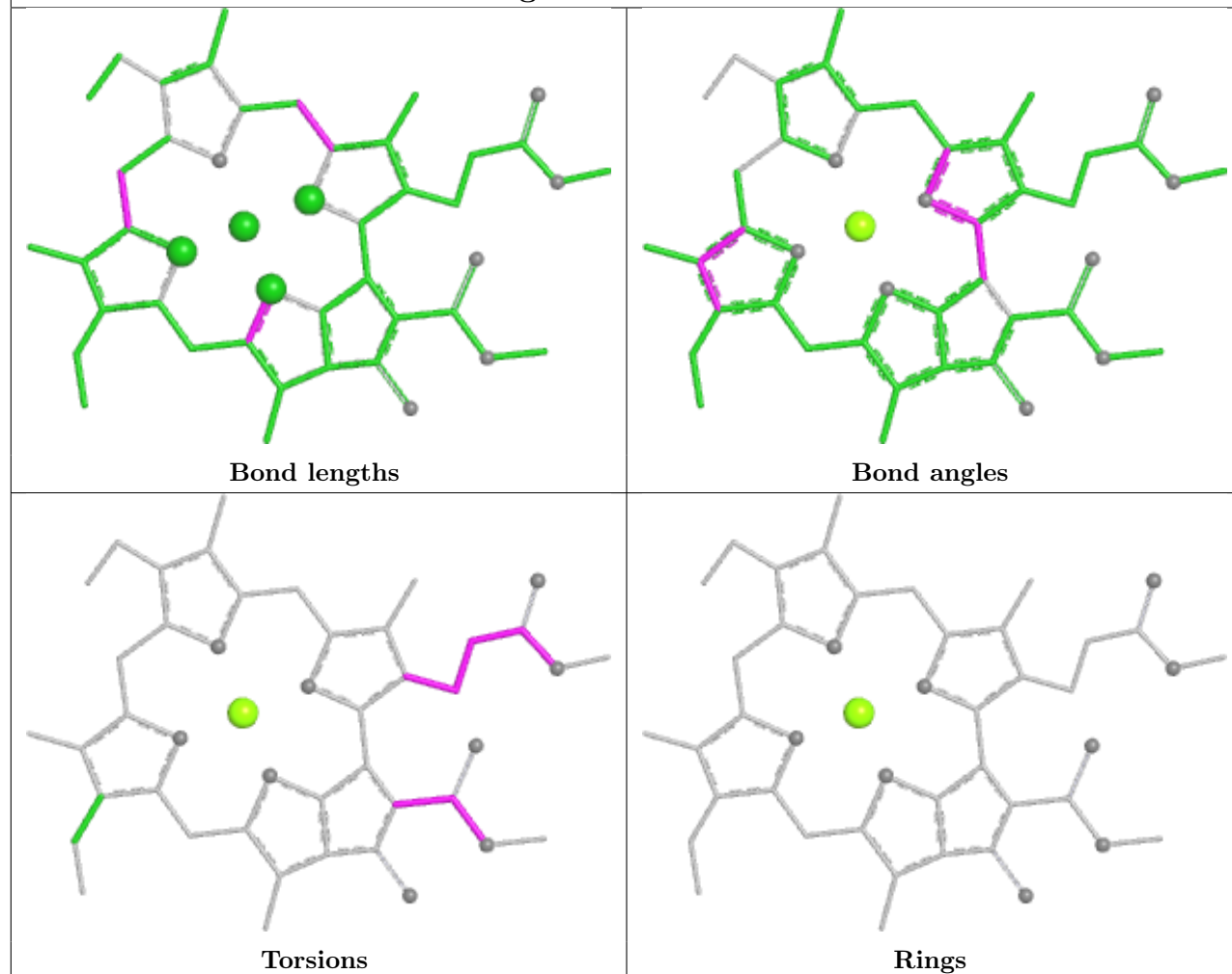


Torsions

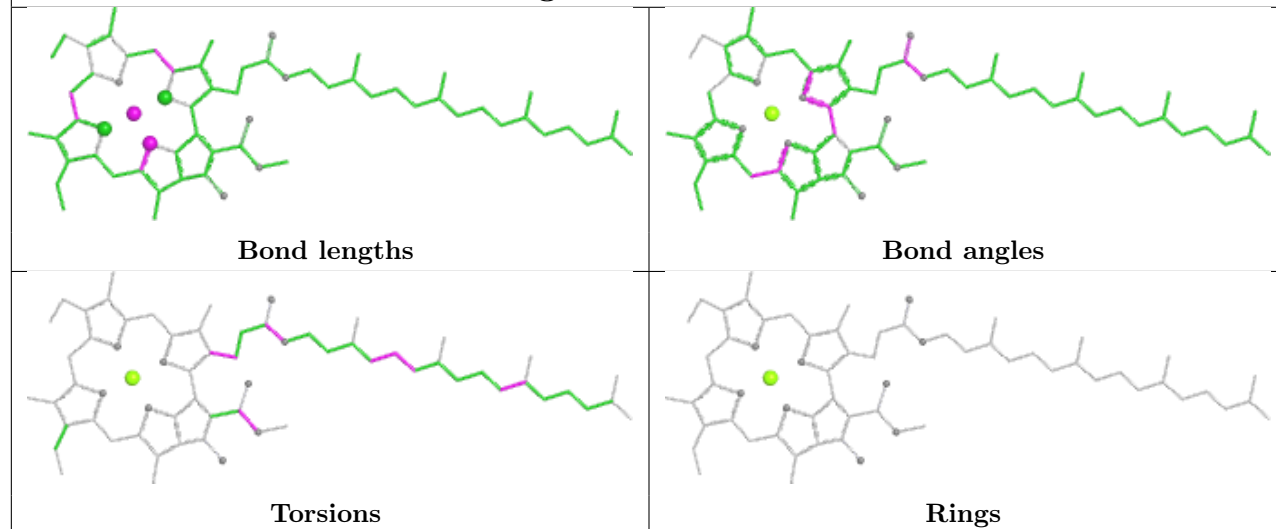


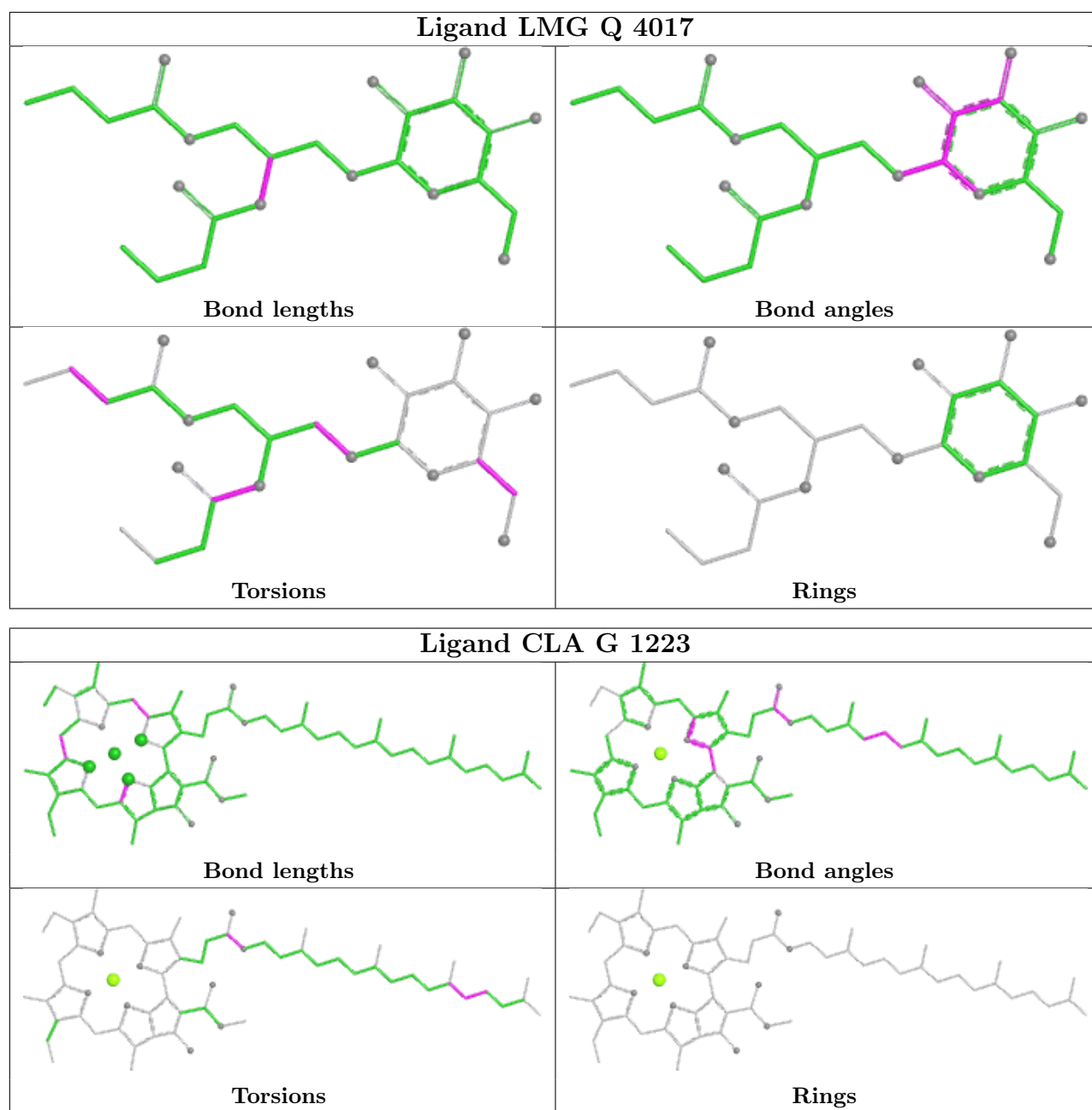
Rings

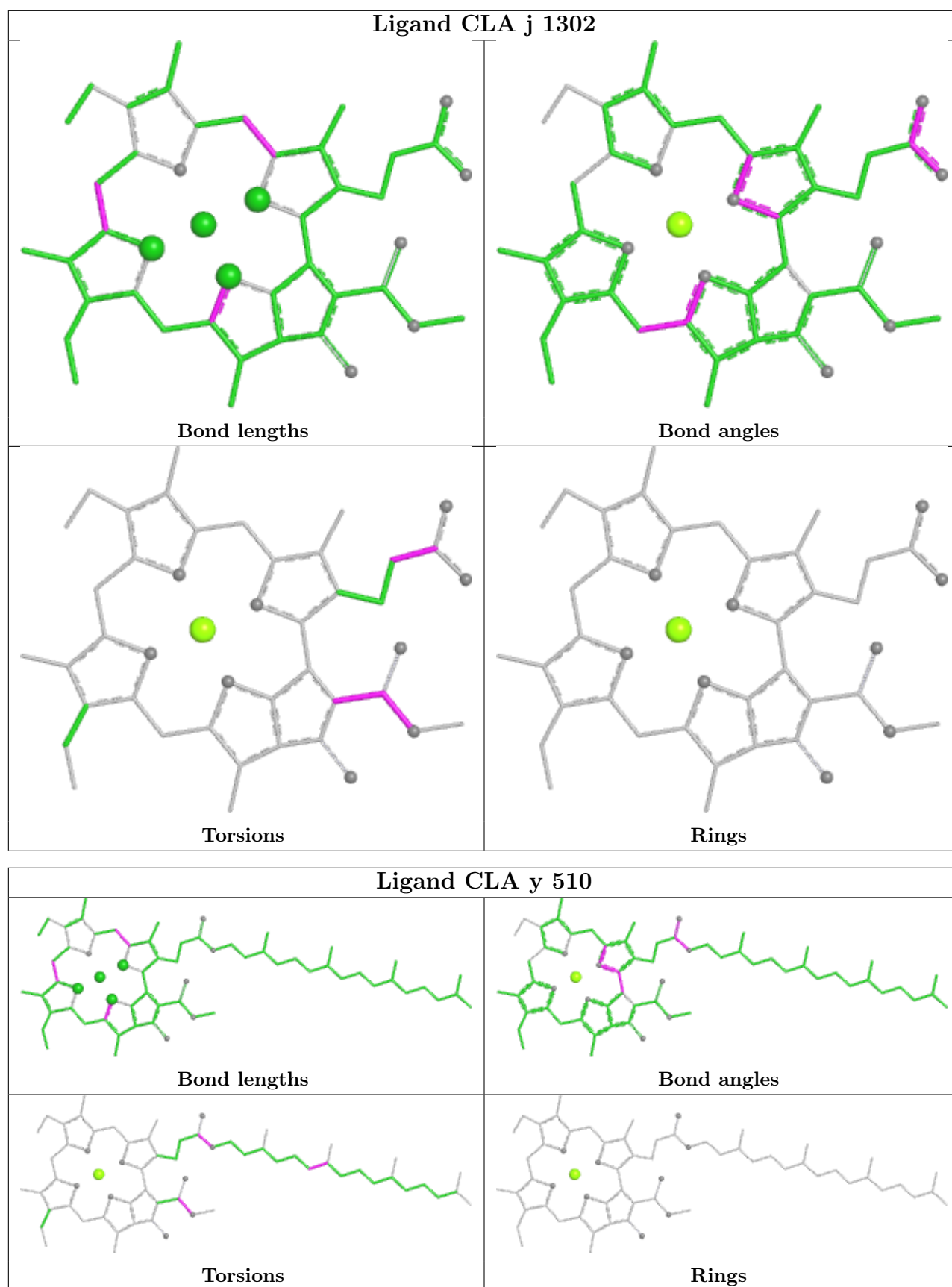
Ligand CLA r 513

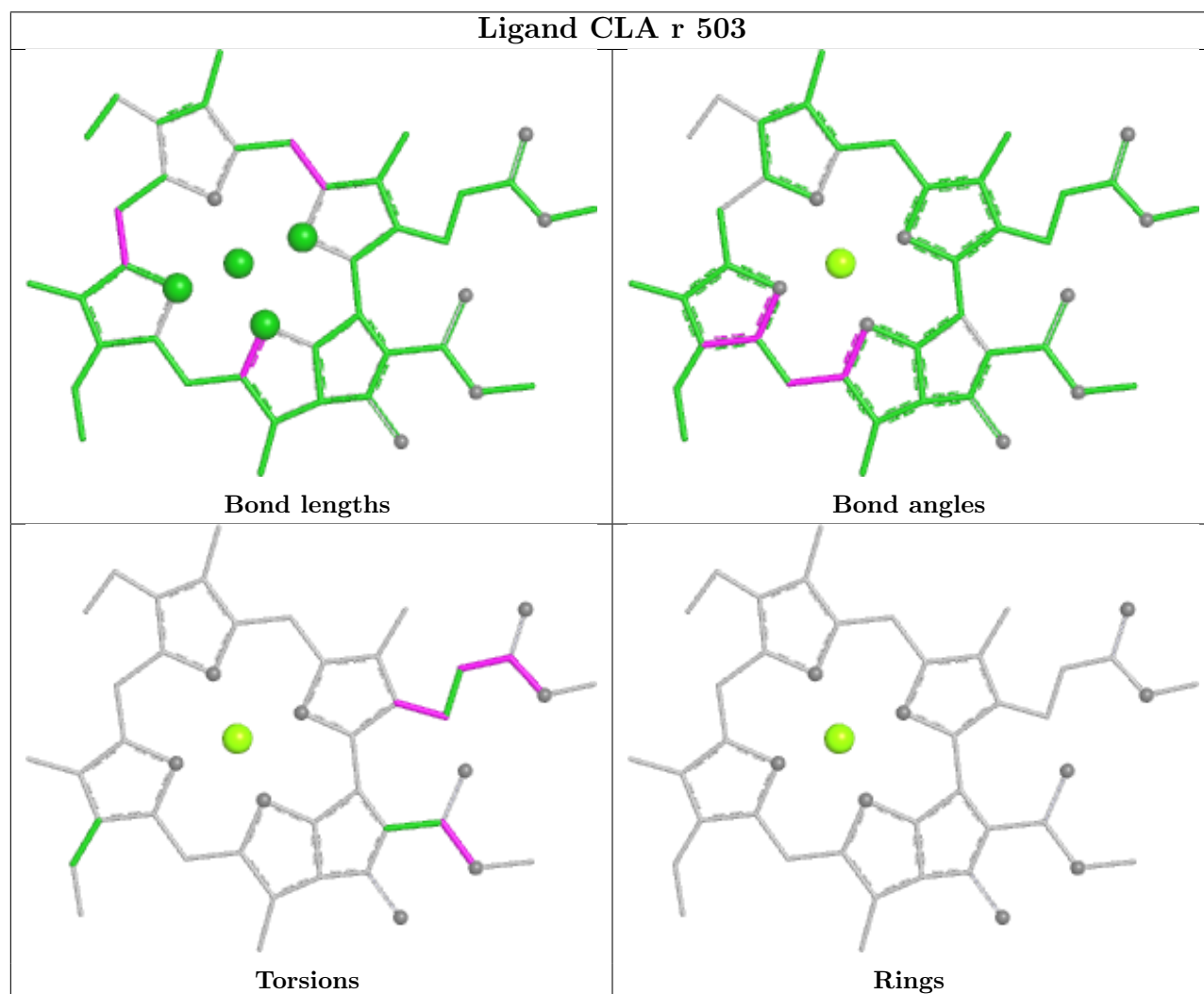
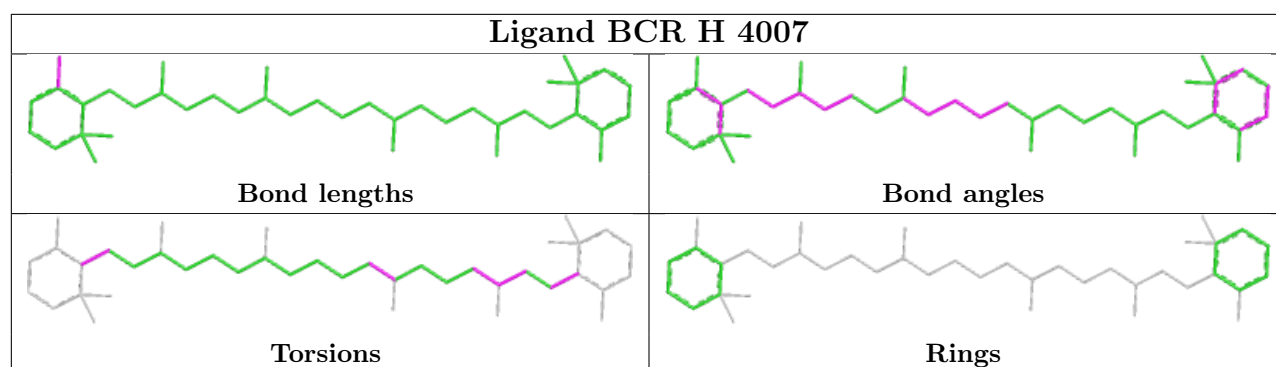


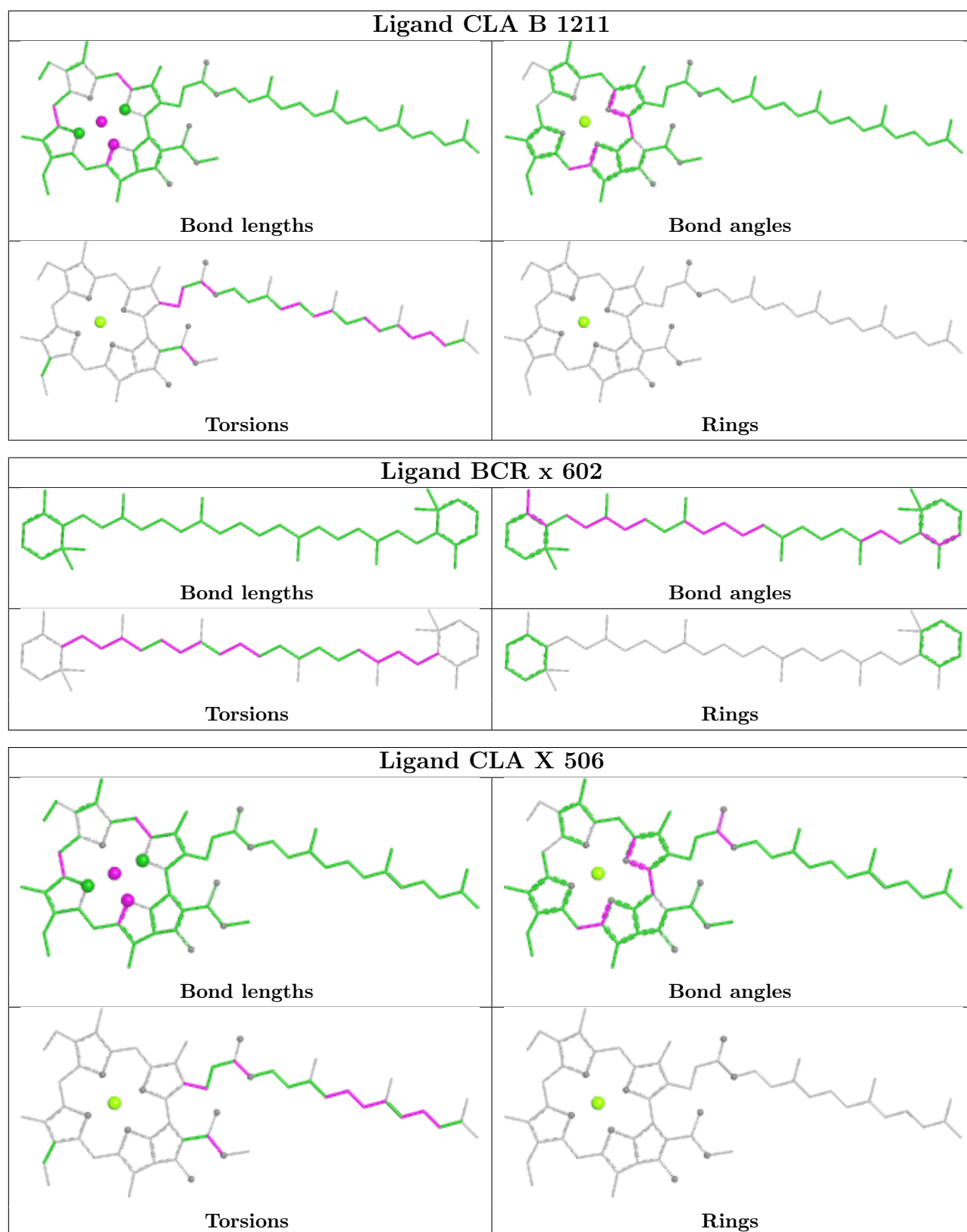
Ligand CLA t 512

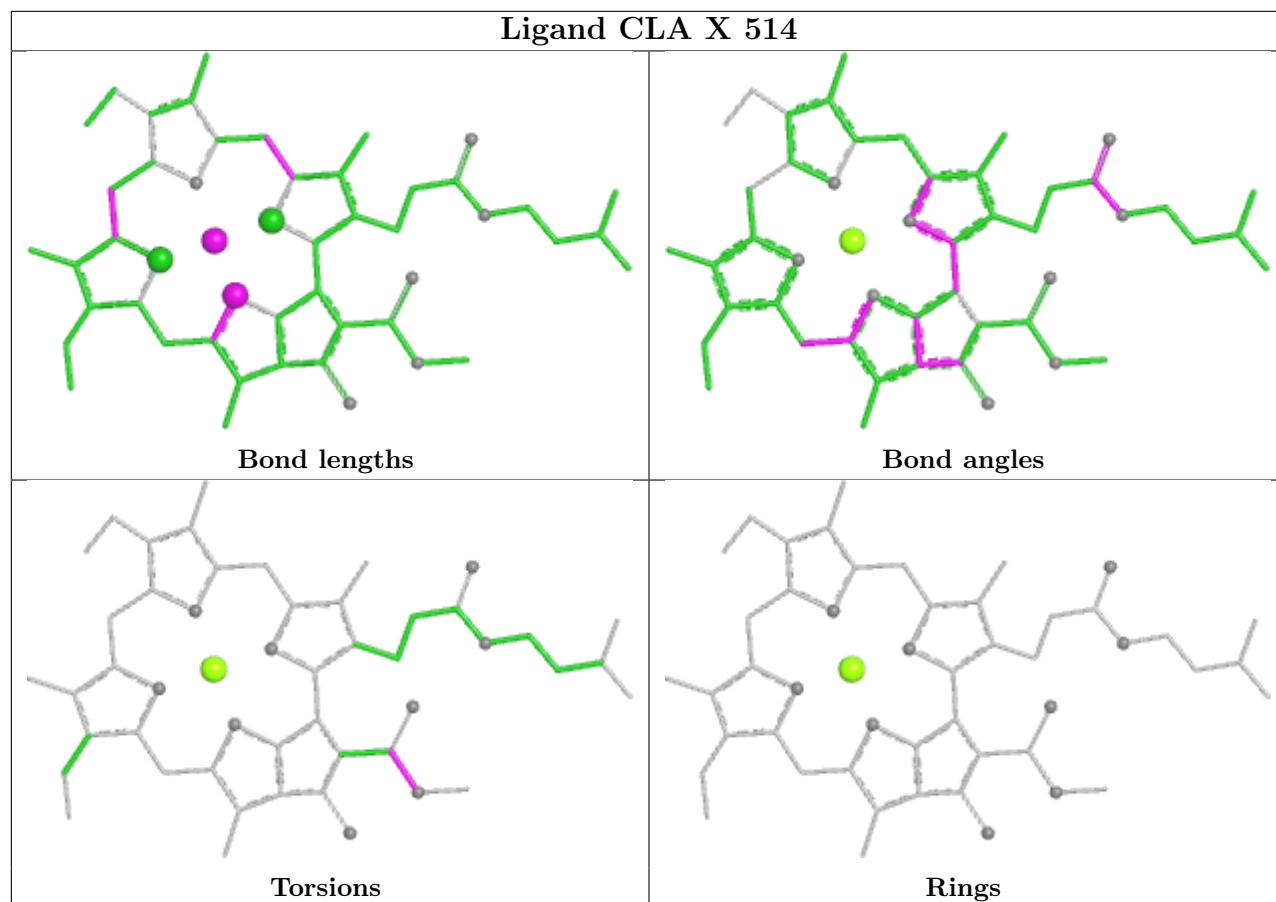




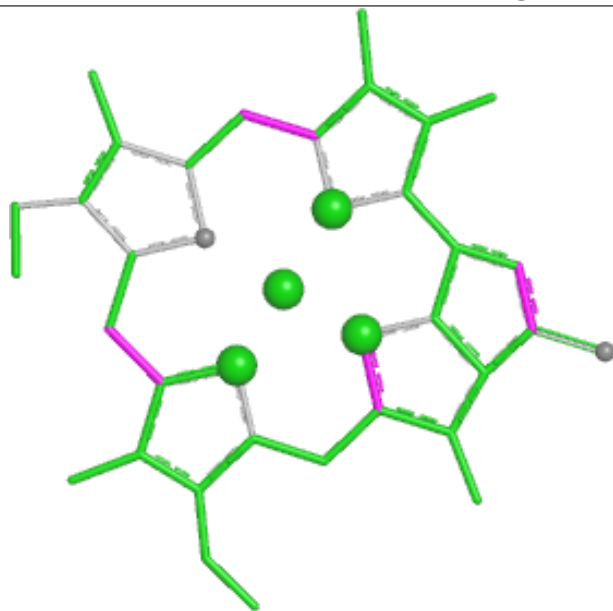




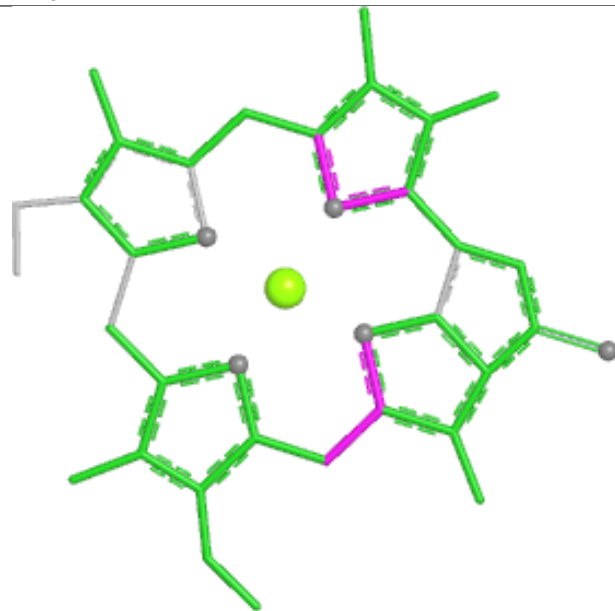




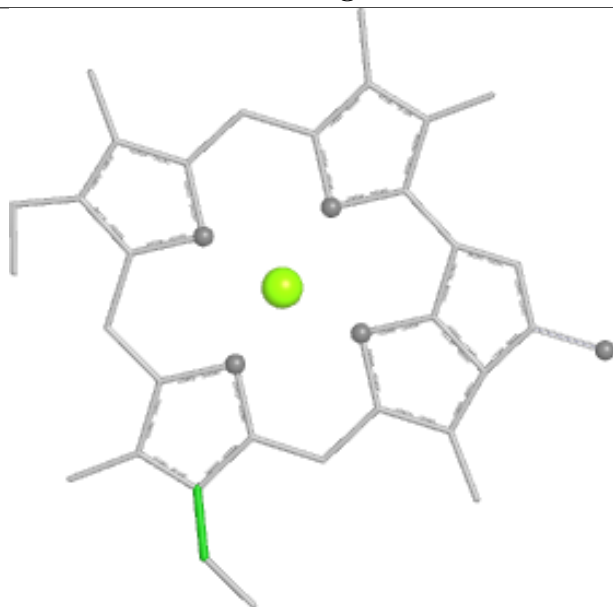
Ligand CLA j 1303



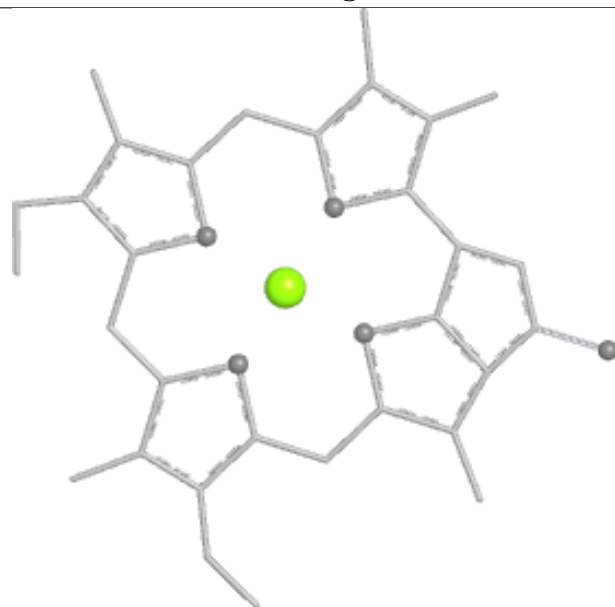
Bond lengths



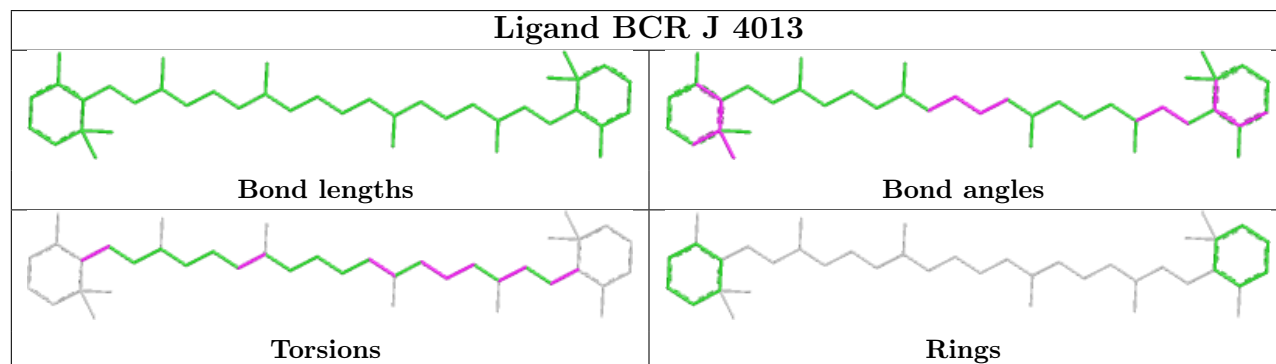
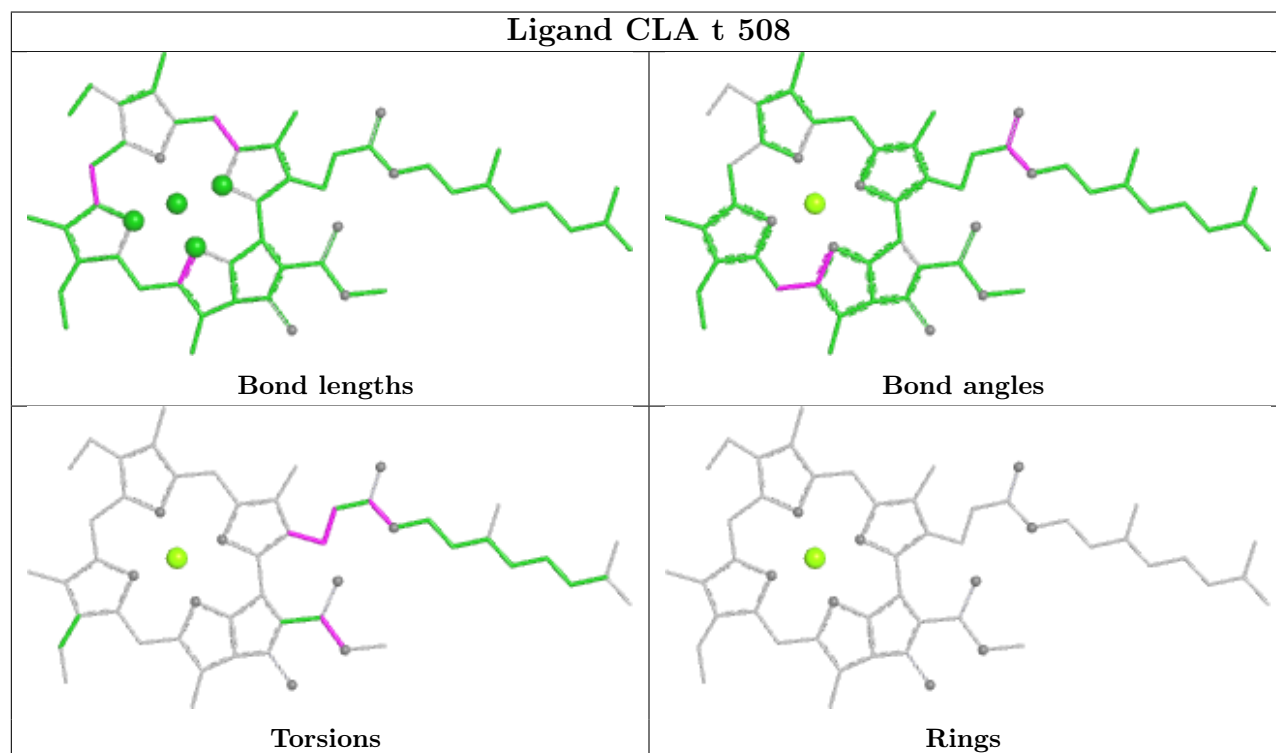
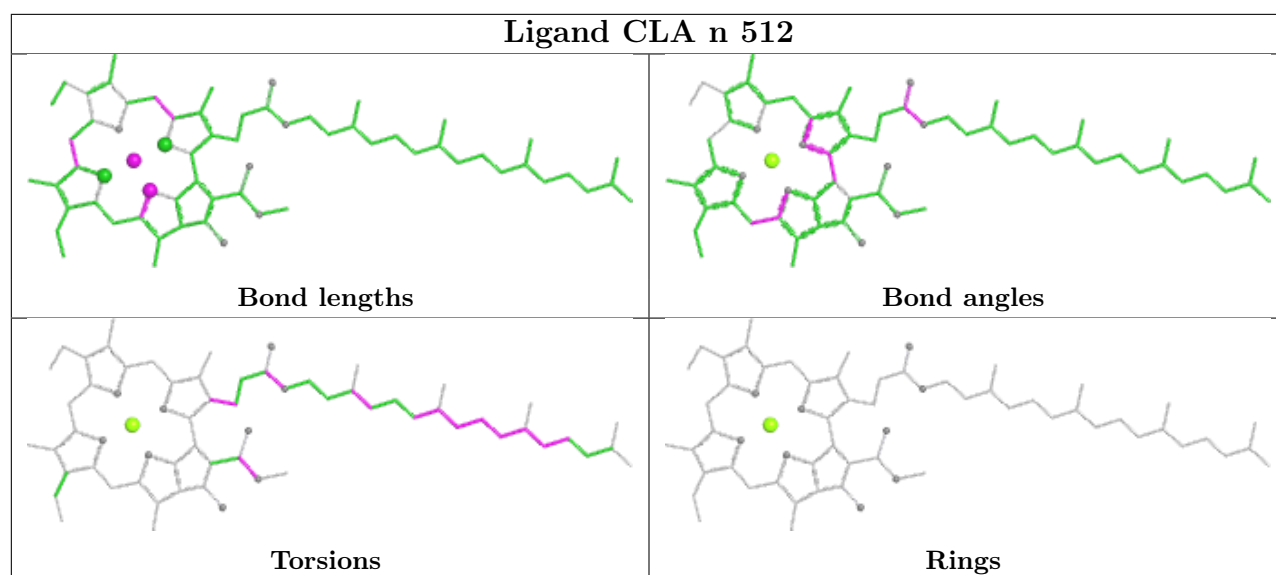
Bond angles

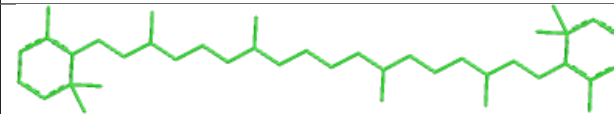
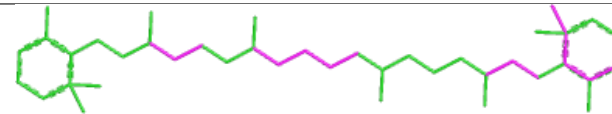
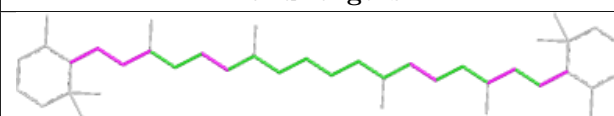
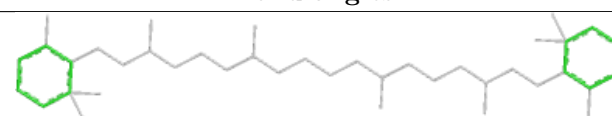


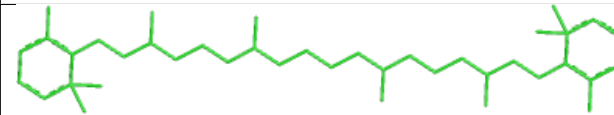
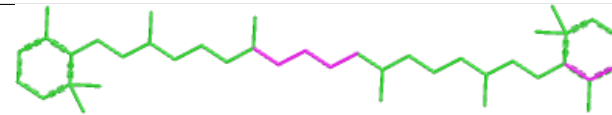
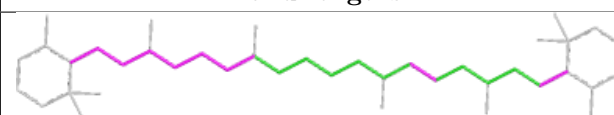
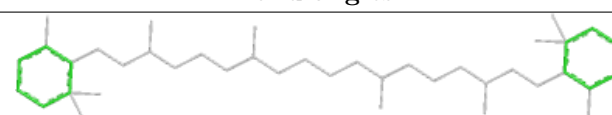
Torsions

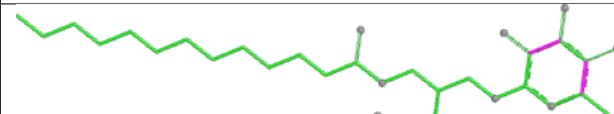
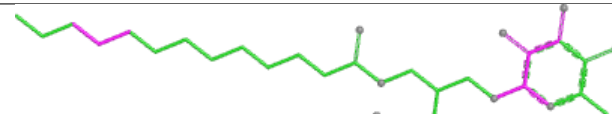
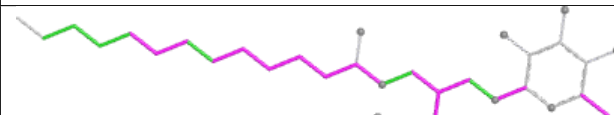
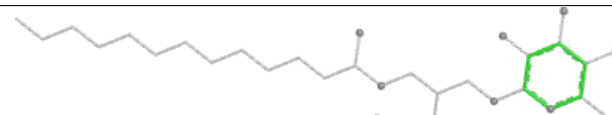


Rings

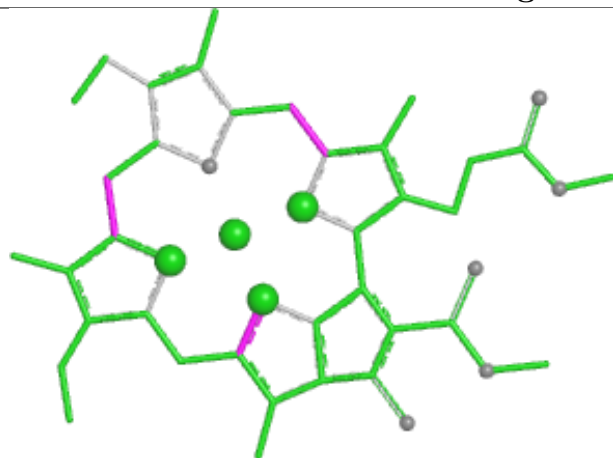


Ligand BCR K 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

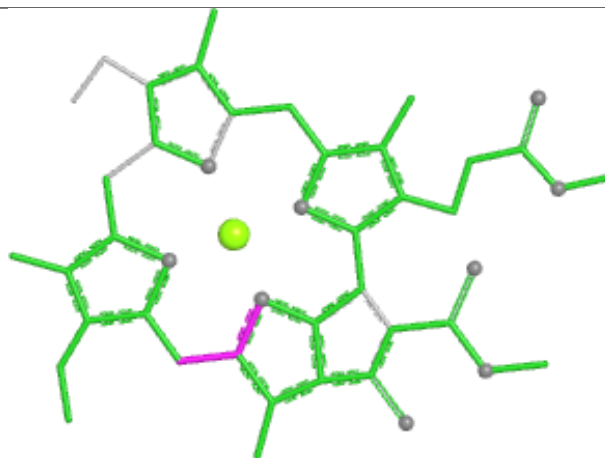
Ligand BCR W 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG A 4101	
	
Bond lengths	Bond angles
	
Torsions	Rings

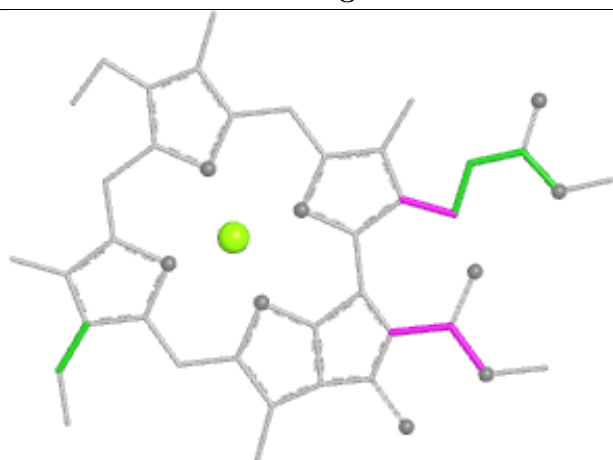
Ligand CLA n 516



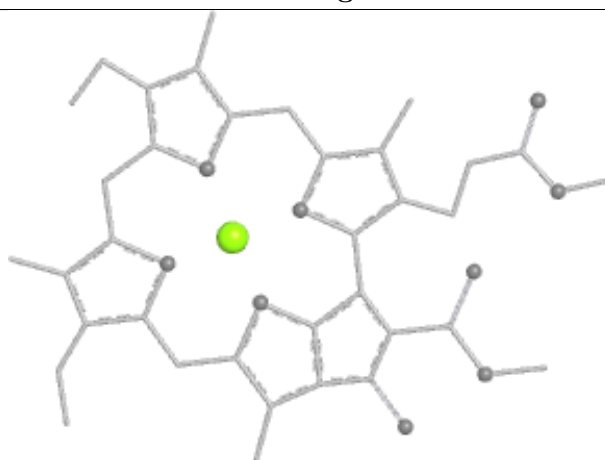
Bond lengths



Bond angles

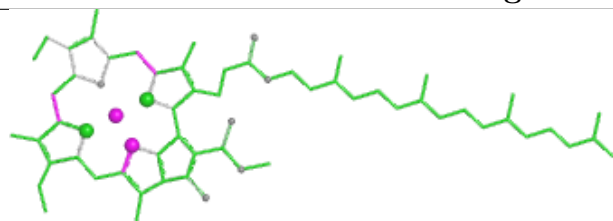


Torsions

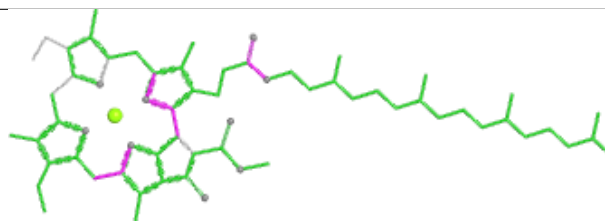


Rings

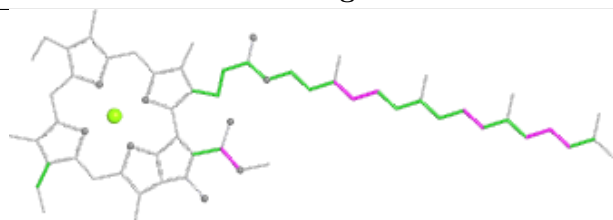
Ligand CLA G 1205



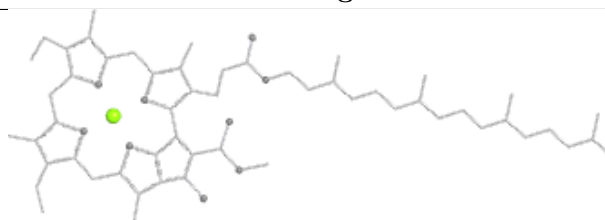
Bond lengths



Bond angles

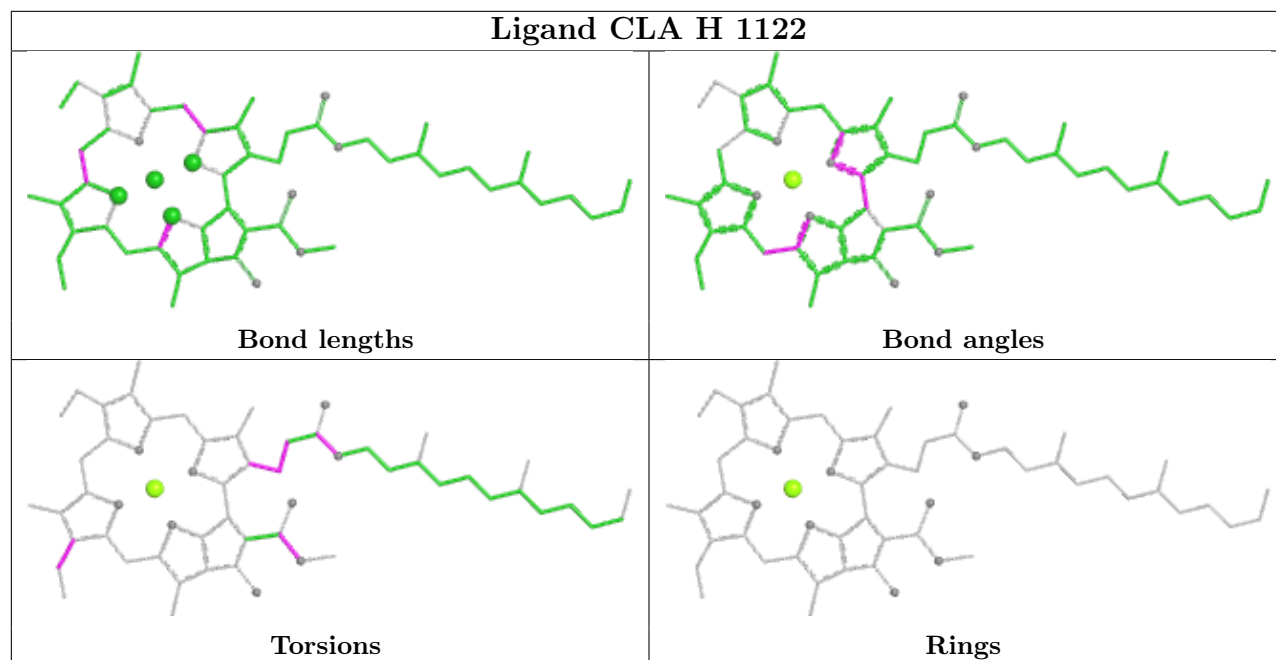


Torsions

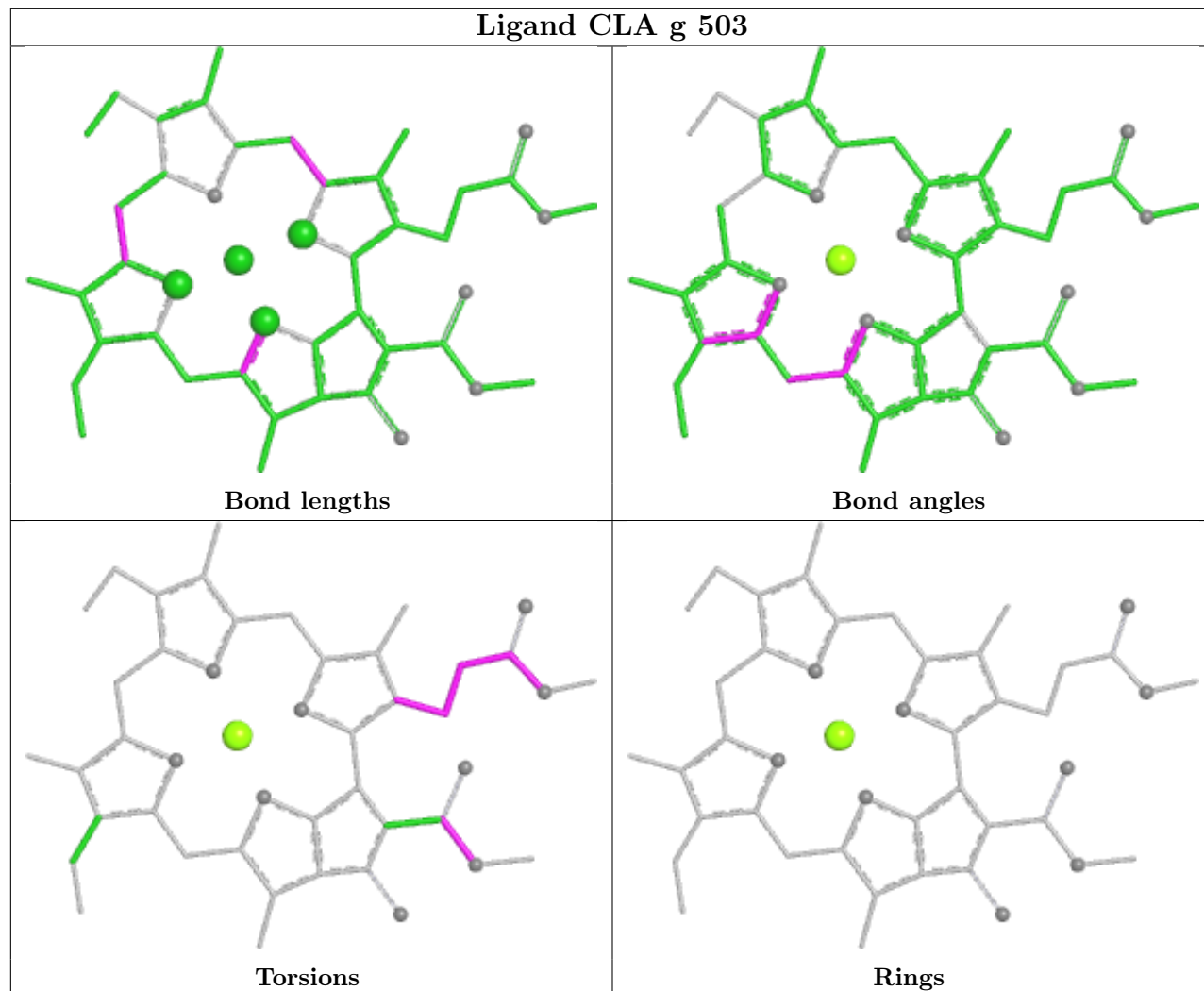


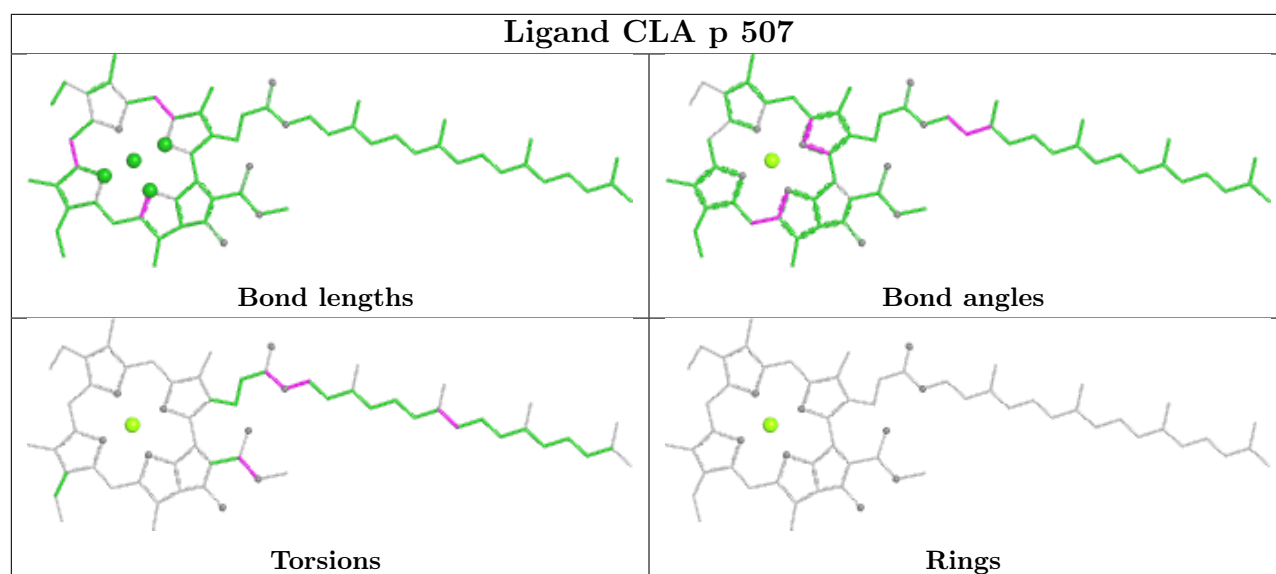
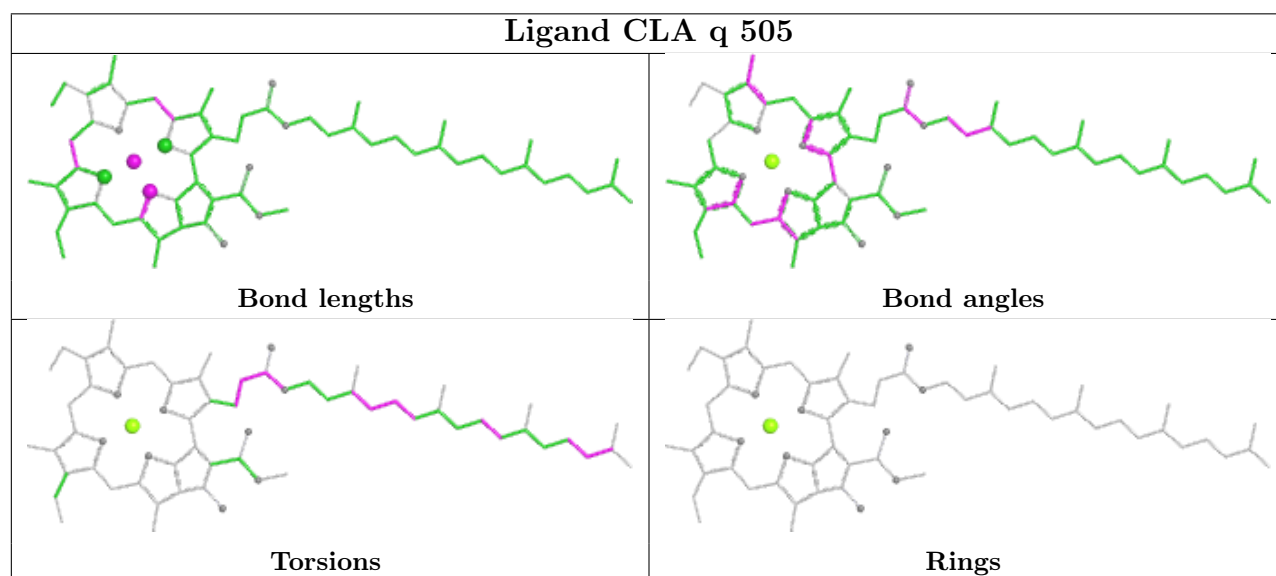
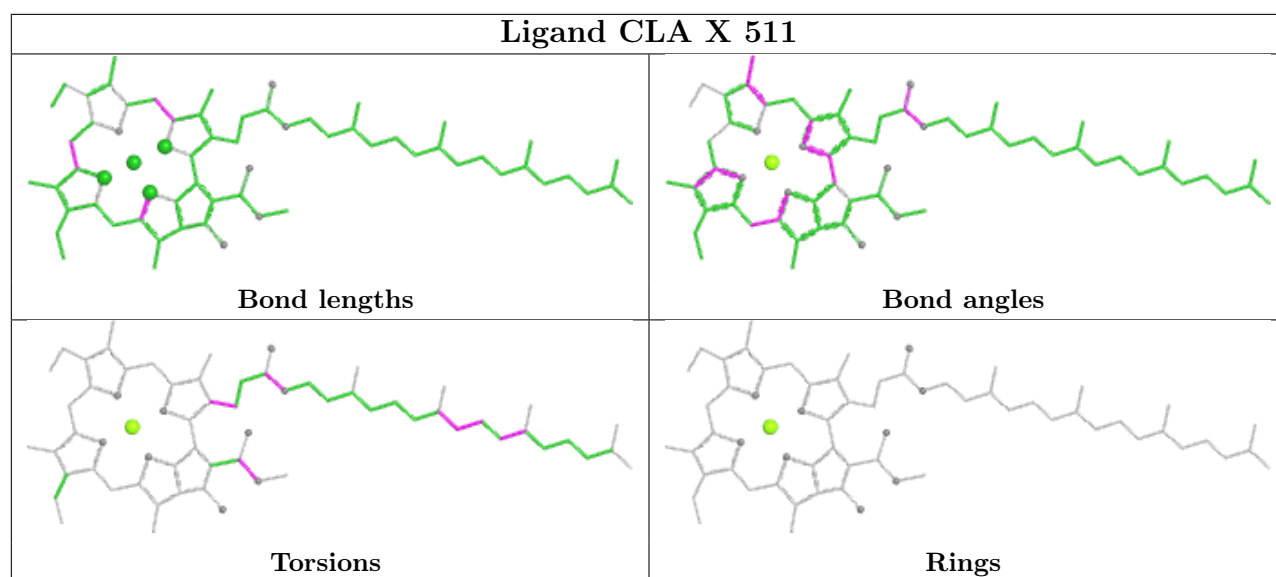
Rings

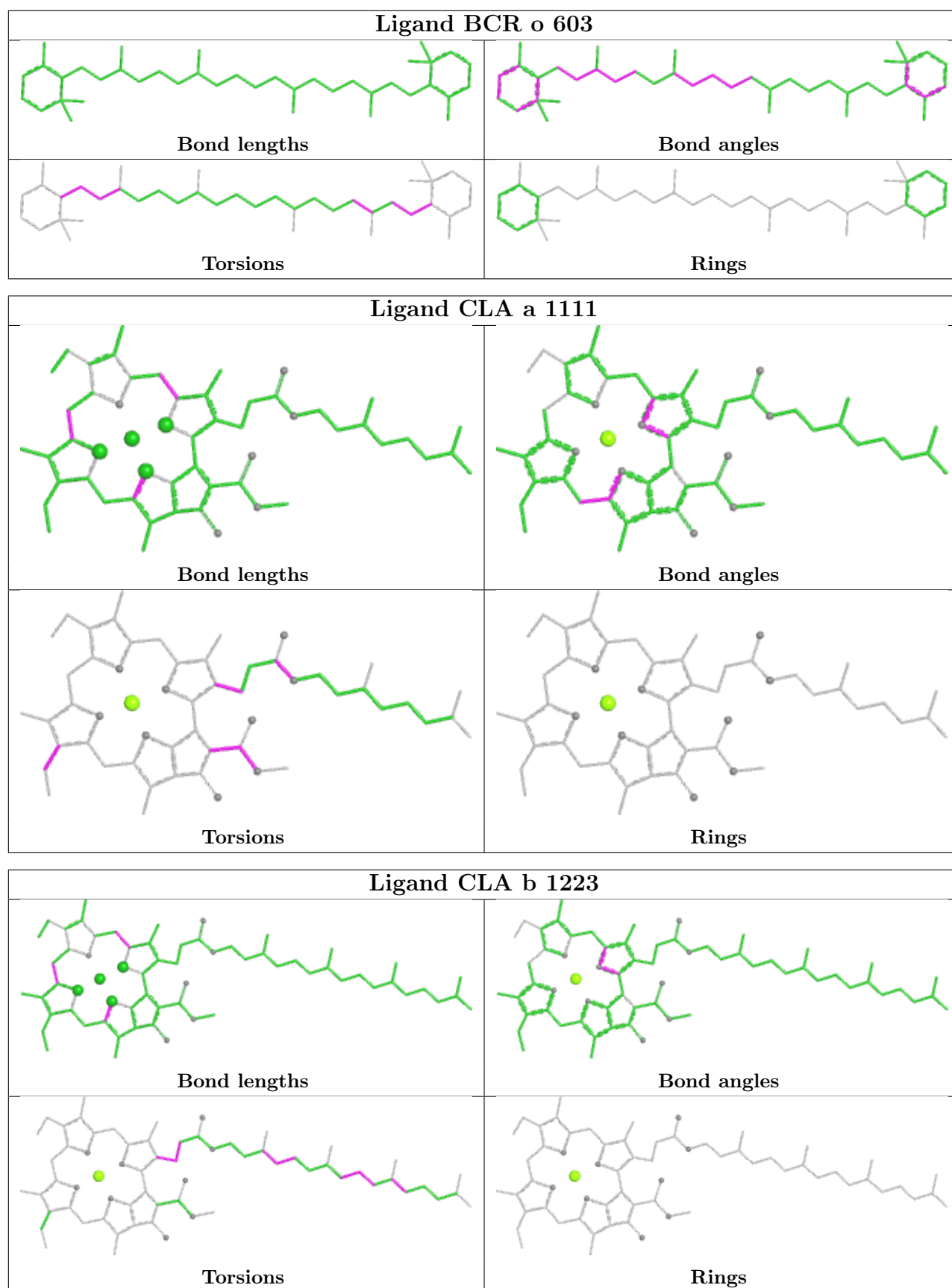
Ligand CLA H 1122



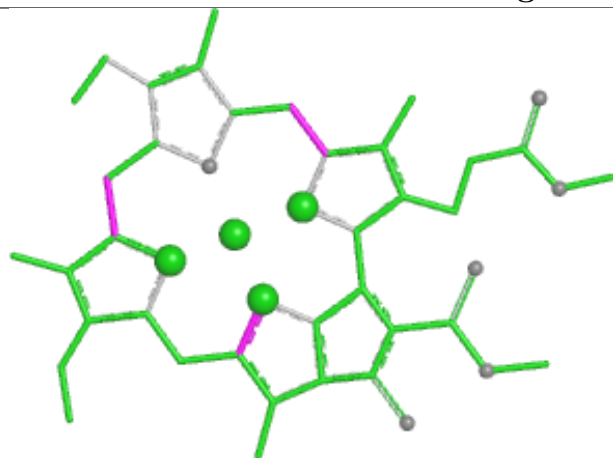
Ligand CLA g 503



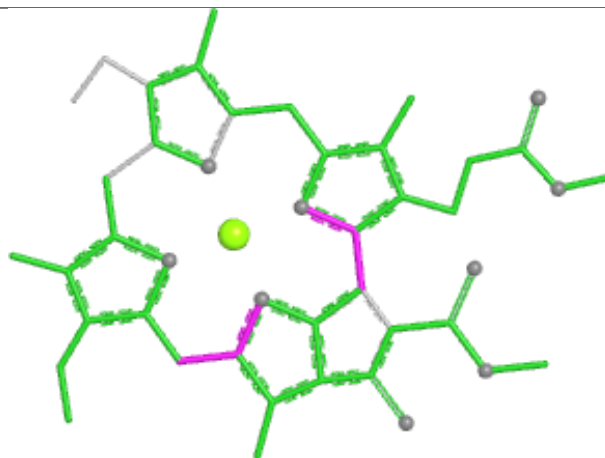




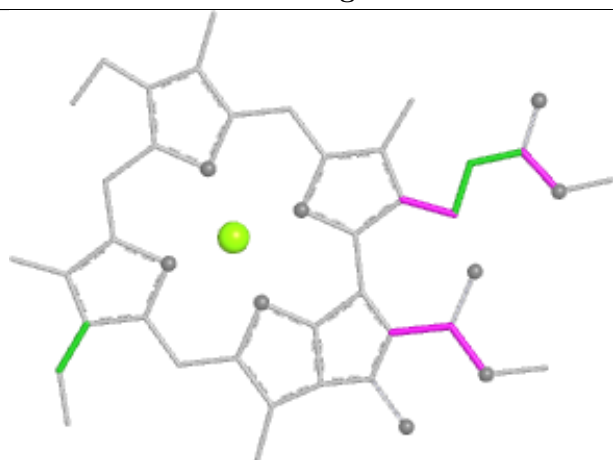
Ligand CLA u 503



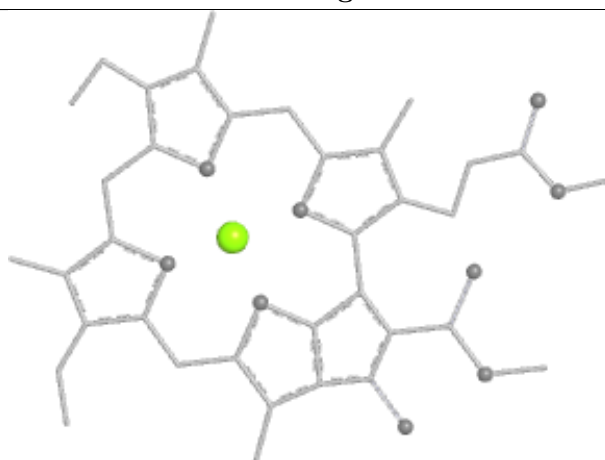
Bond lengths



Bond angles

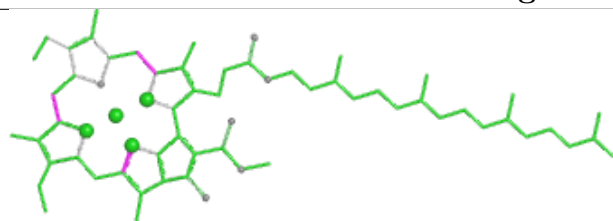


Torsions

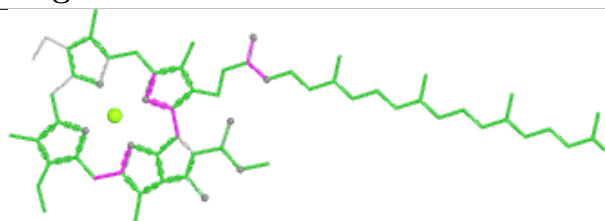


Rings

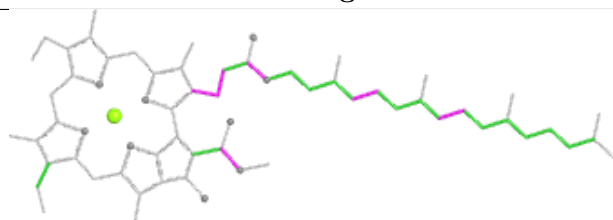
Ligand CLA g 515



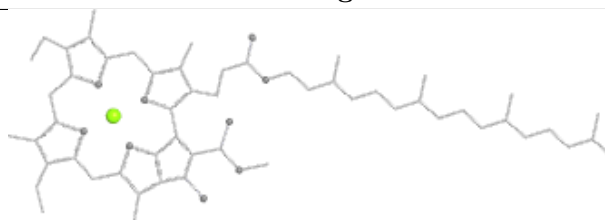
Bond lengths



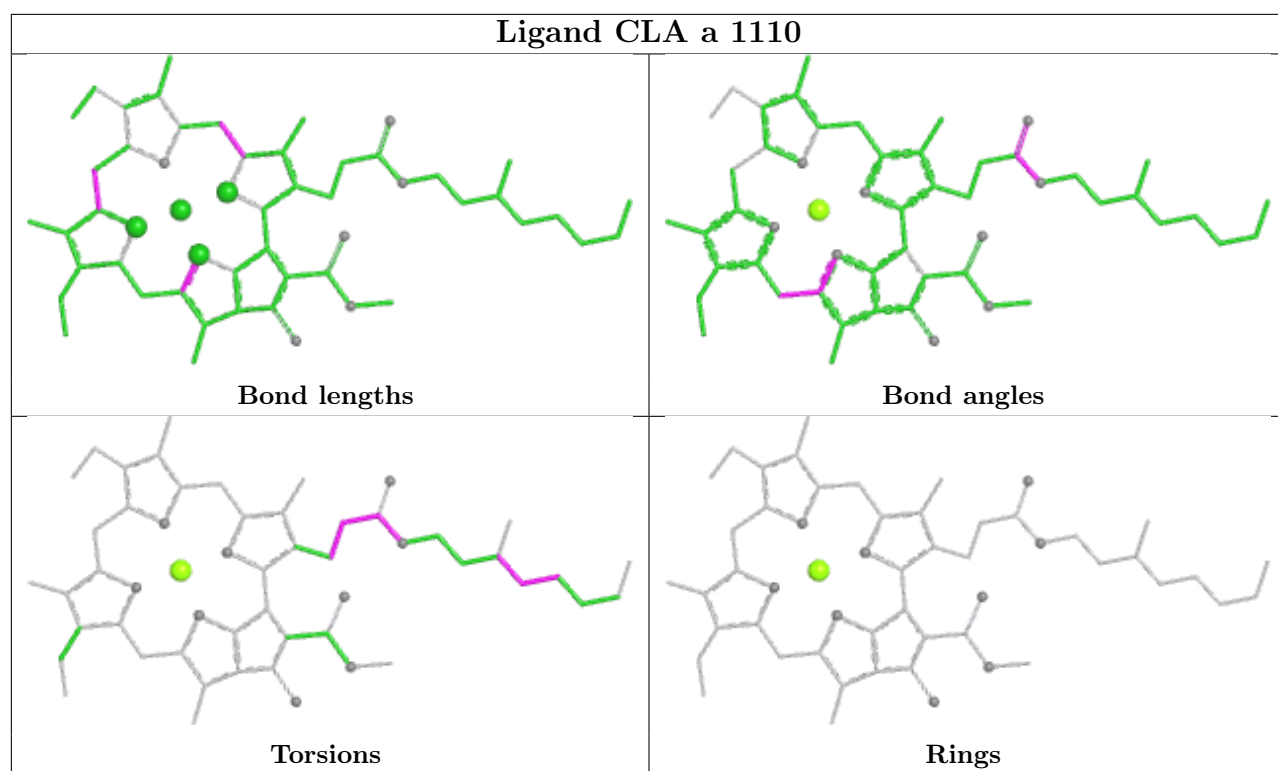
Bond angles

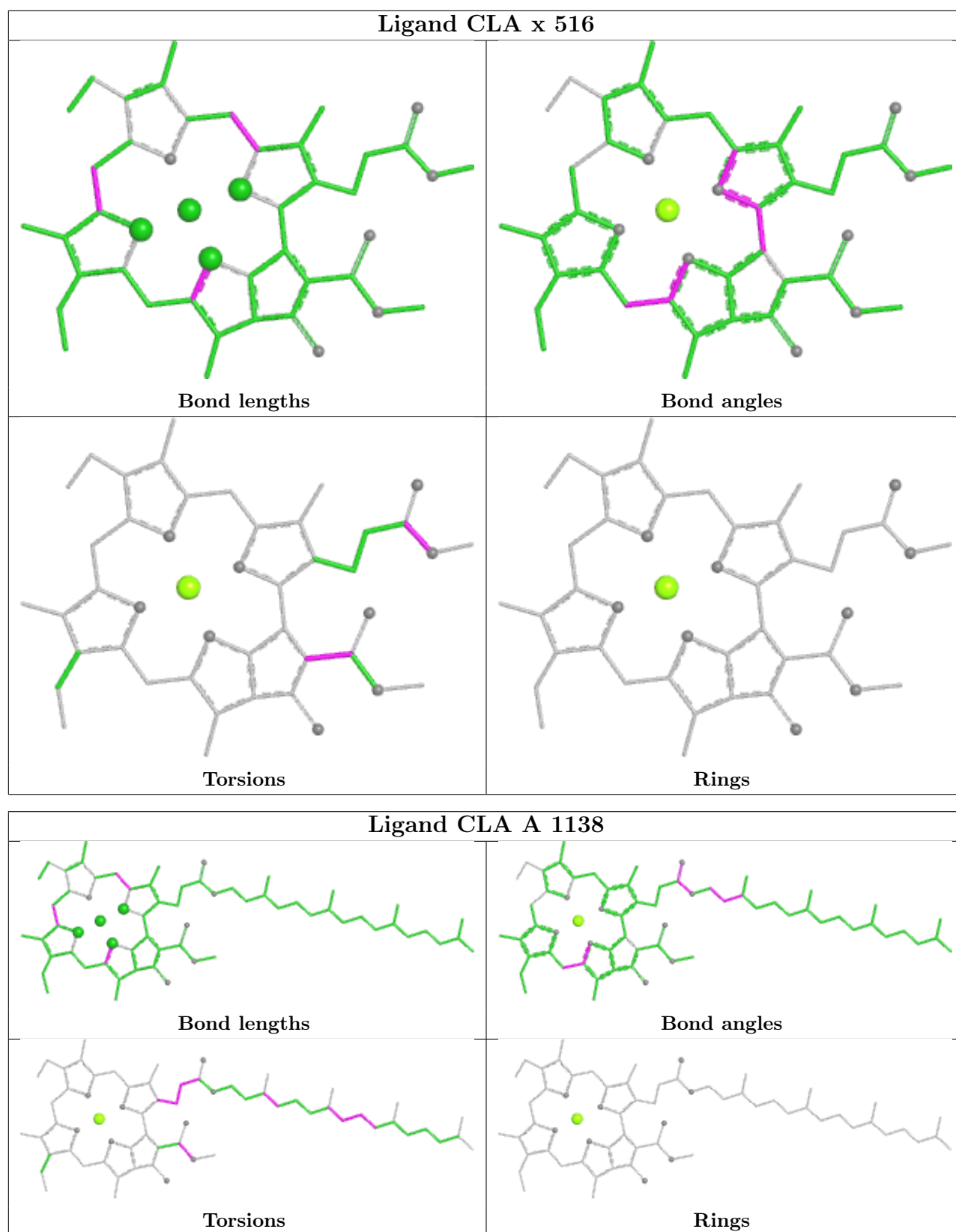


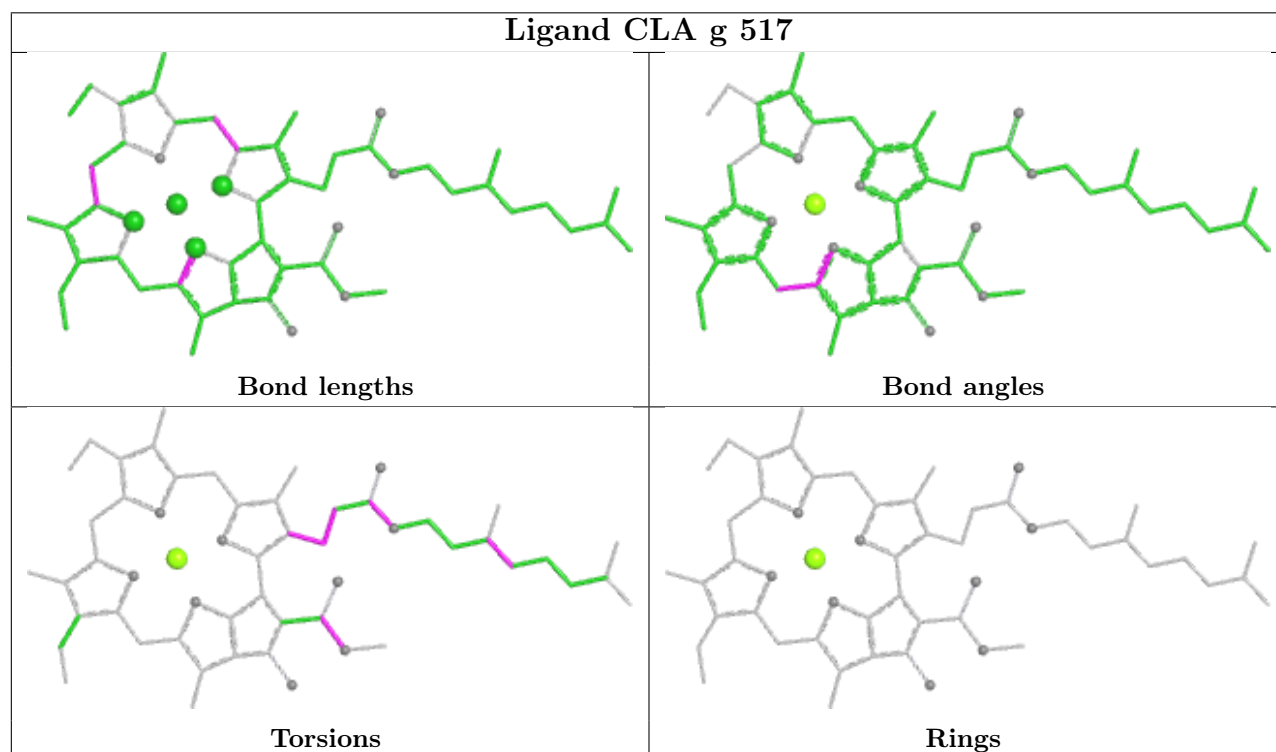
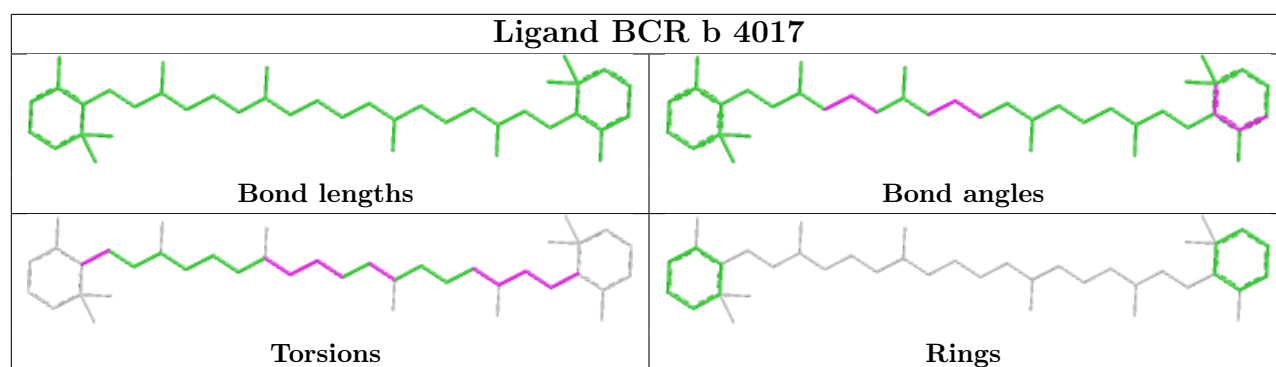
Torsions

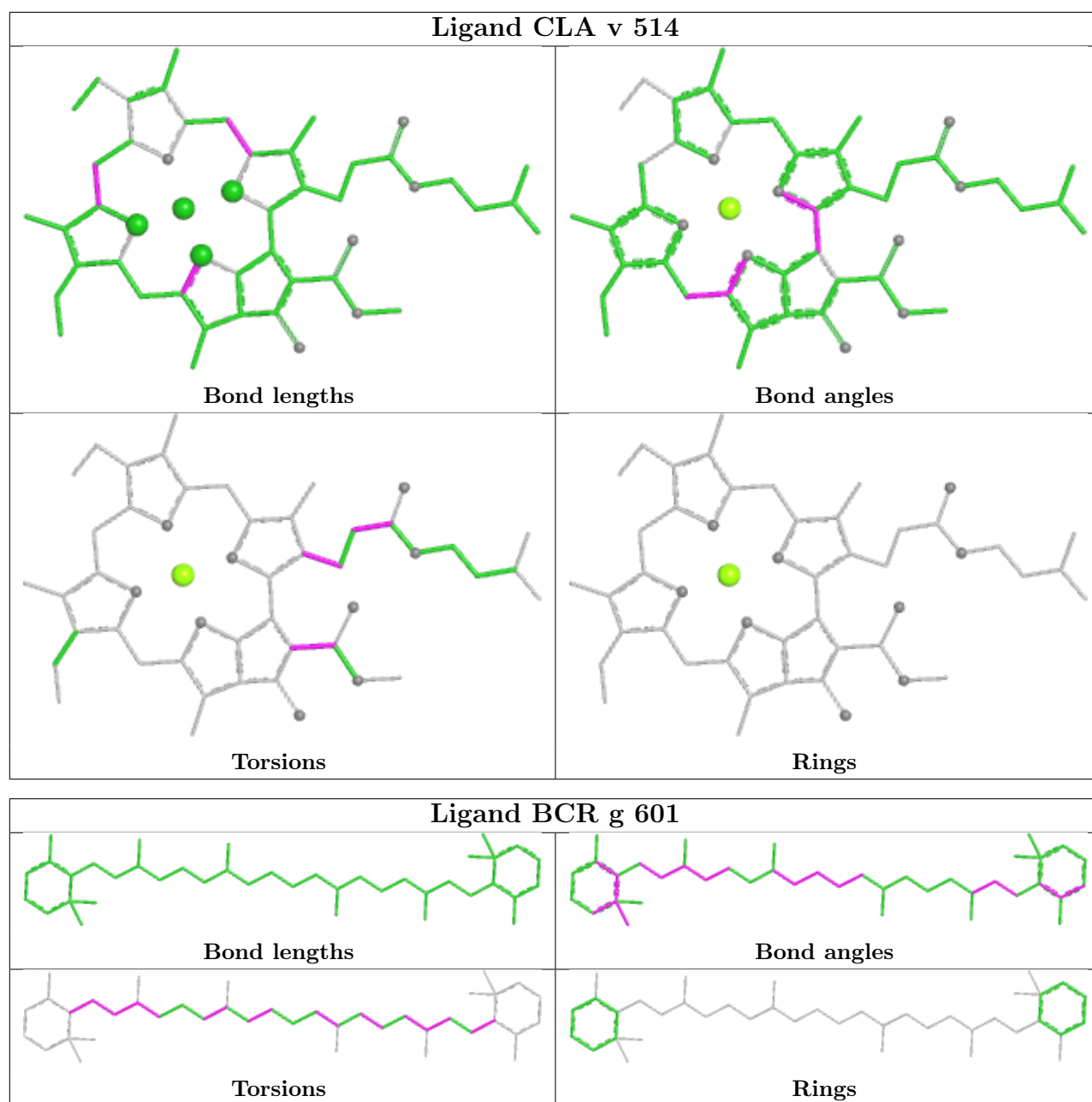


Rings

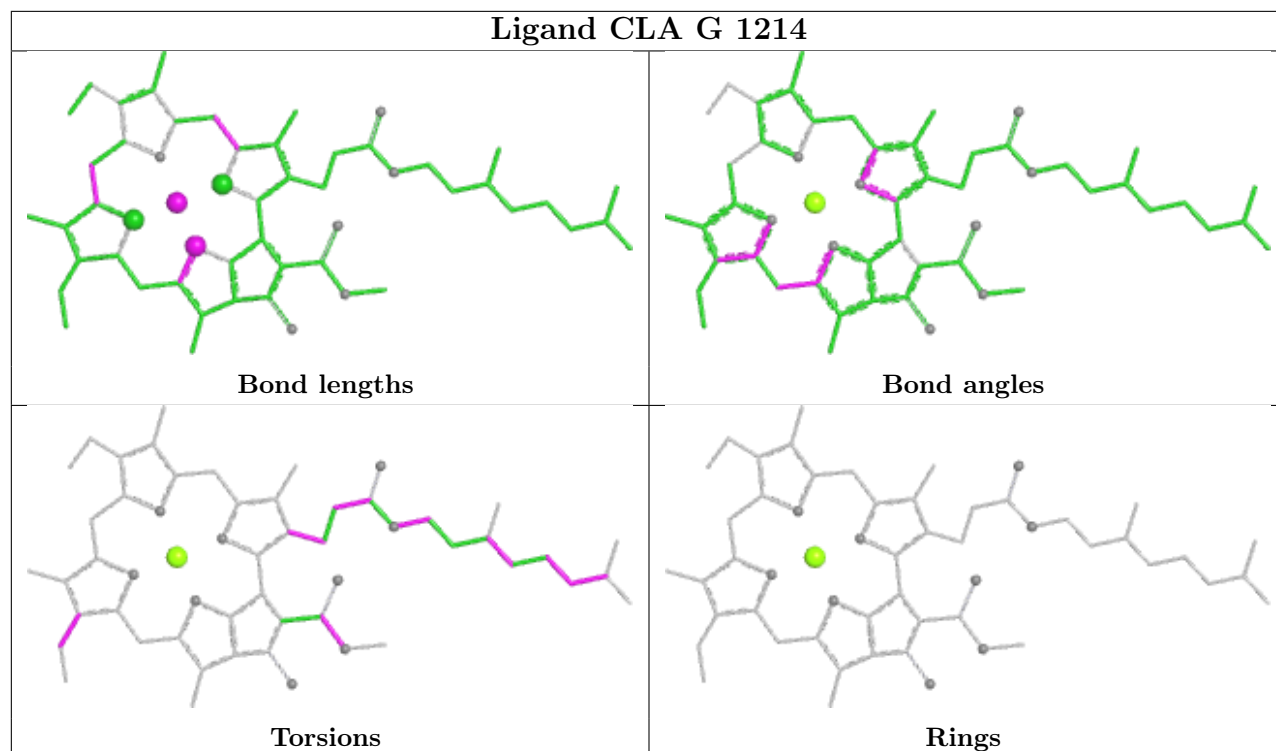




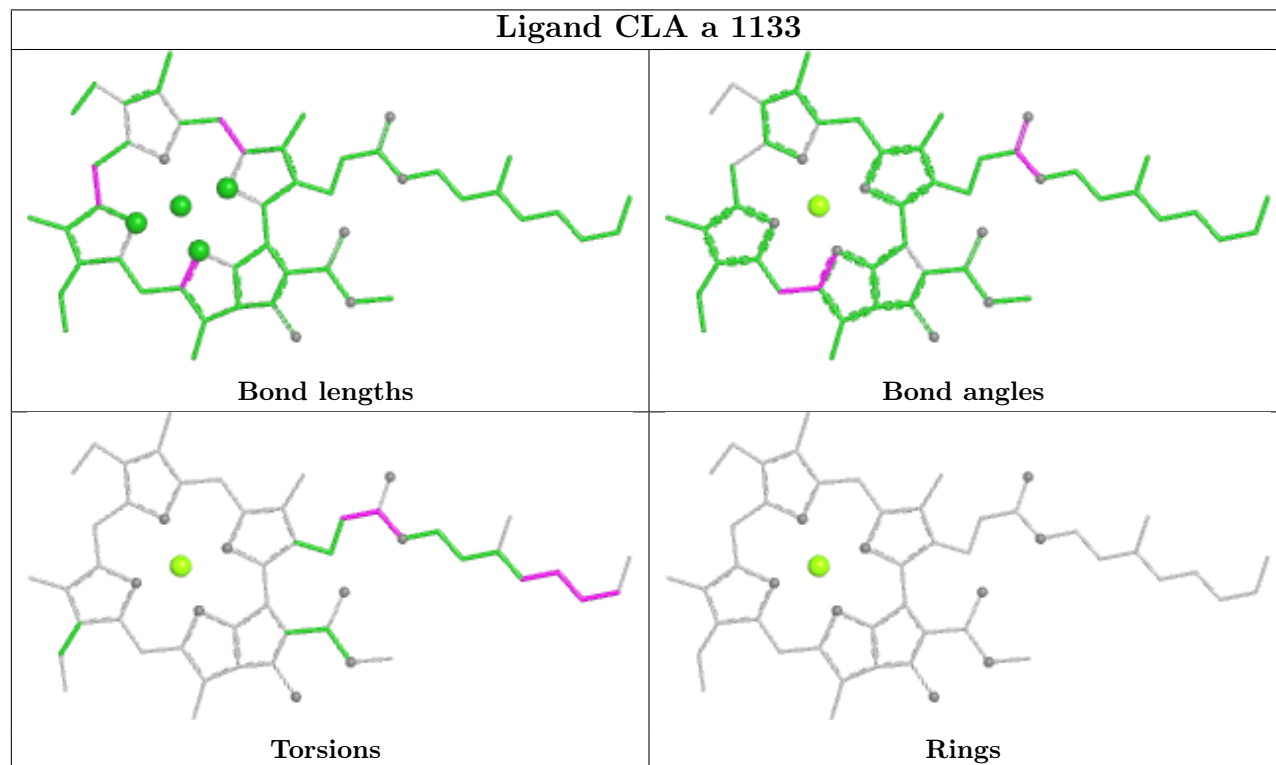


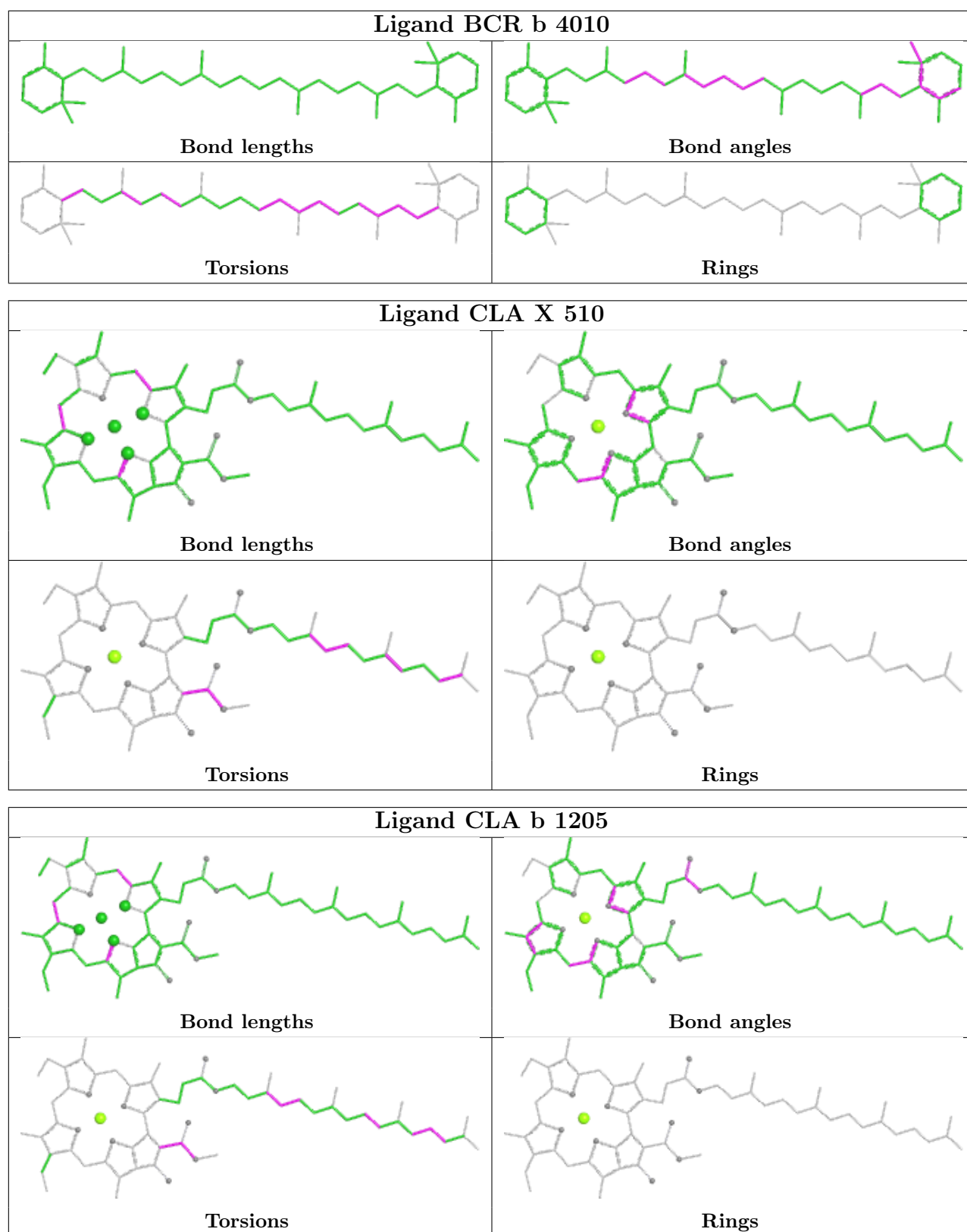


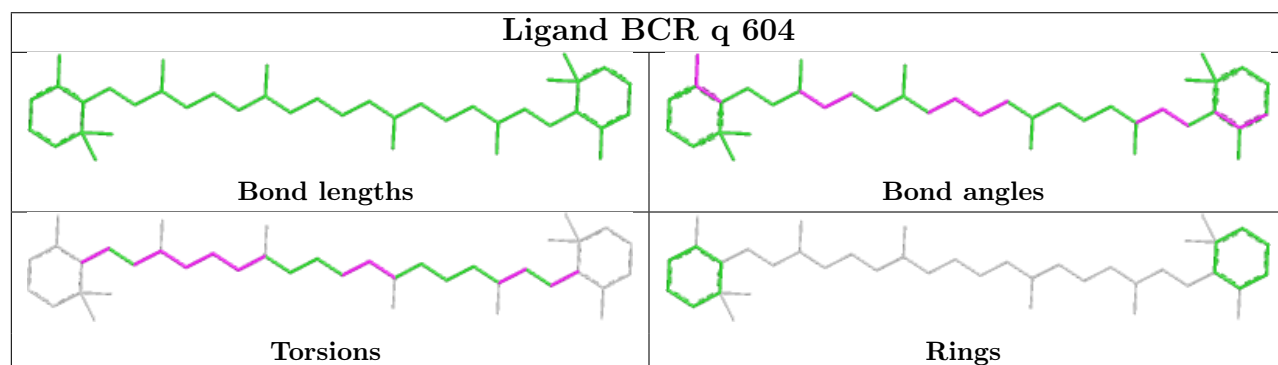
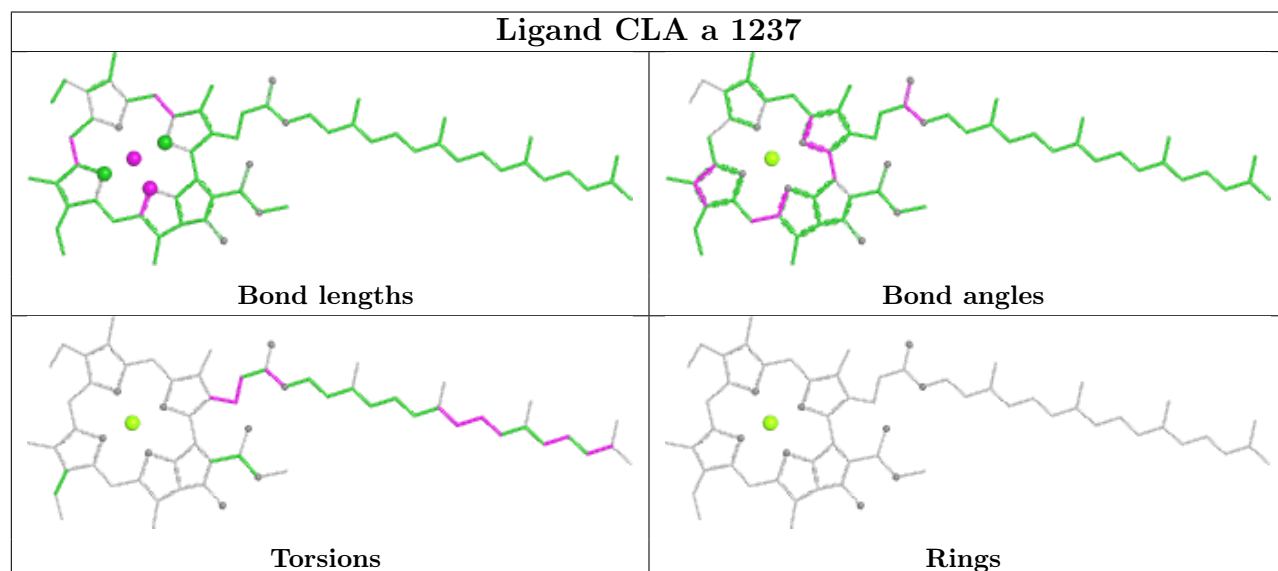
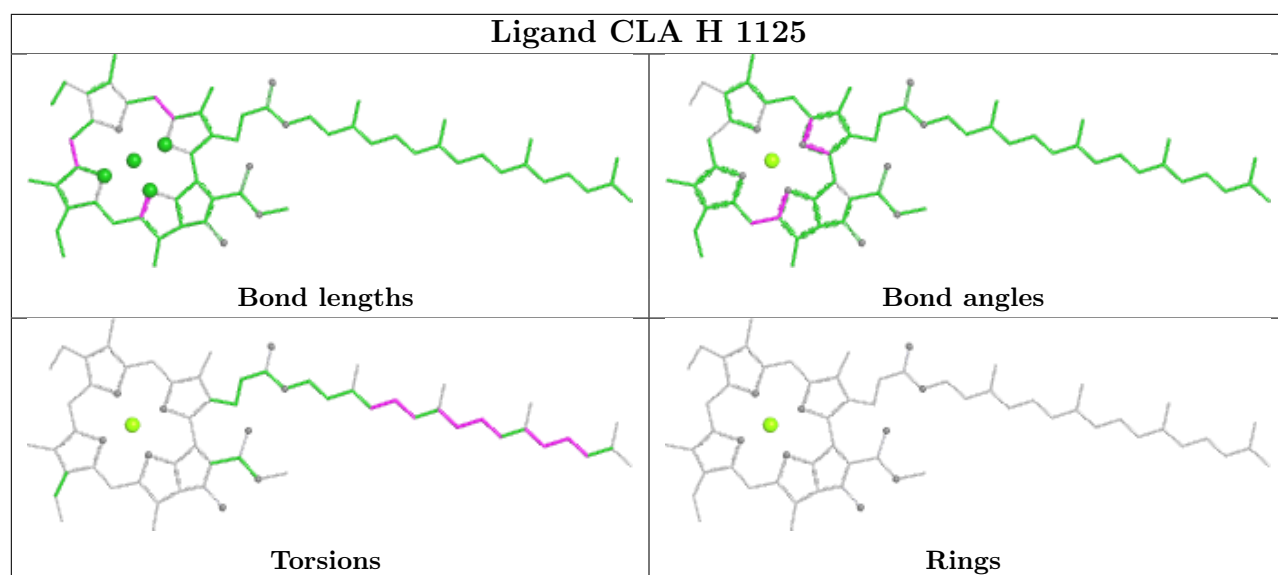
Ligand CLA G 1214



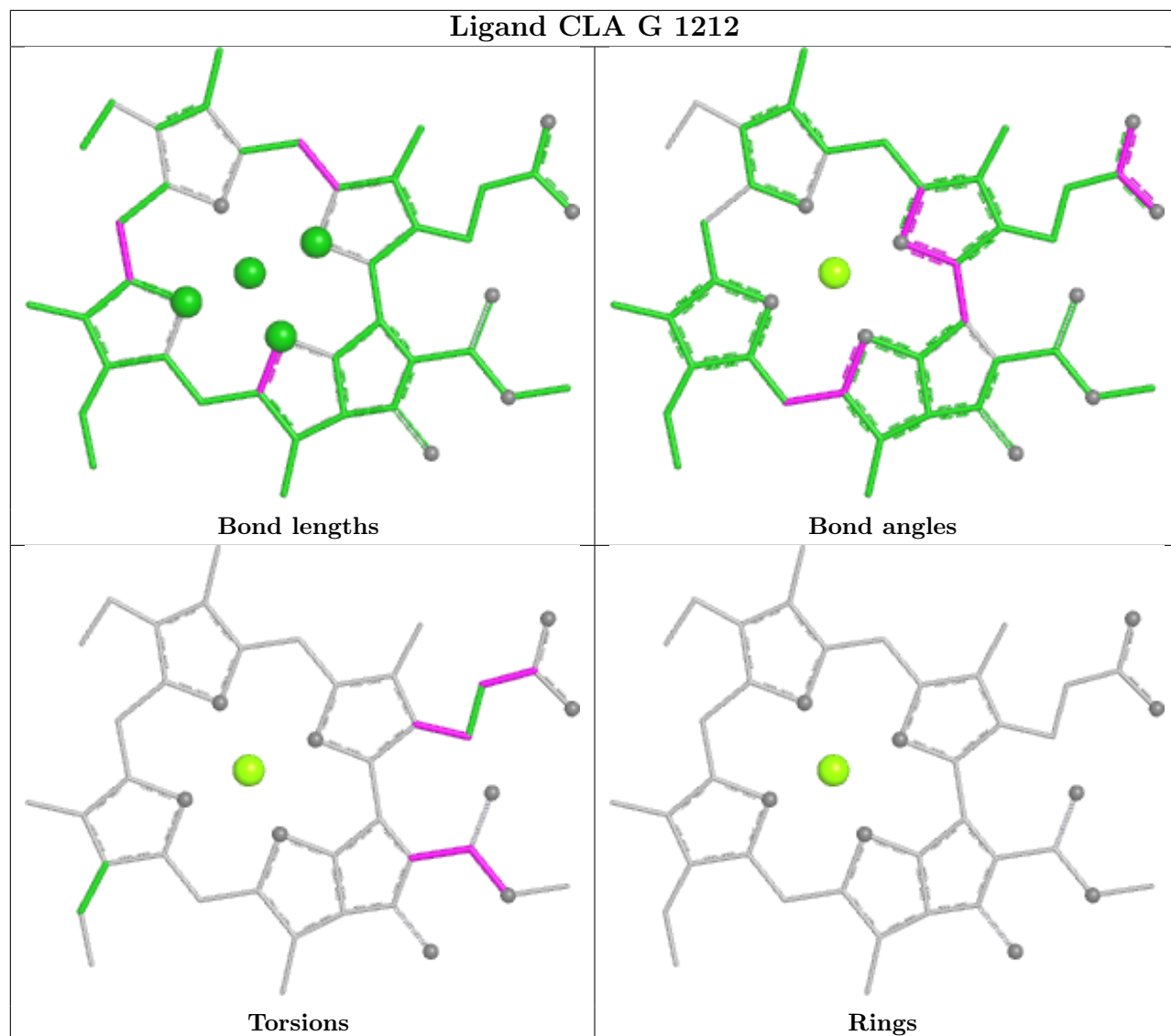
Ligand CLA a 1133

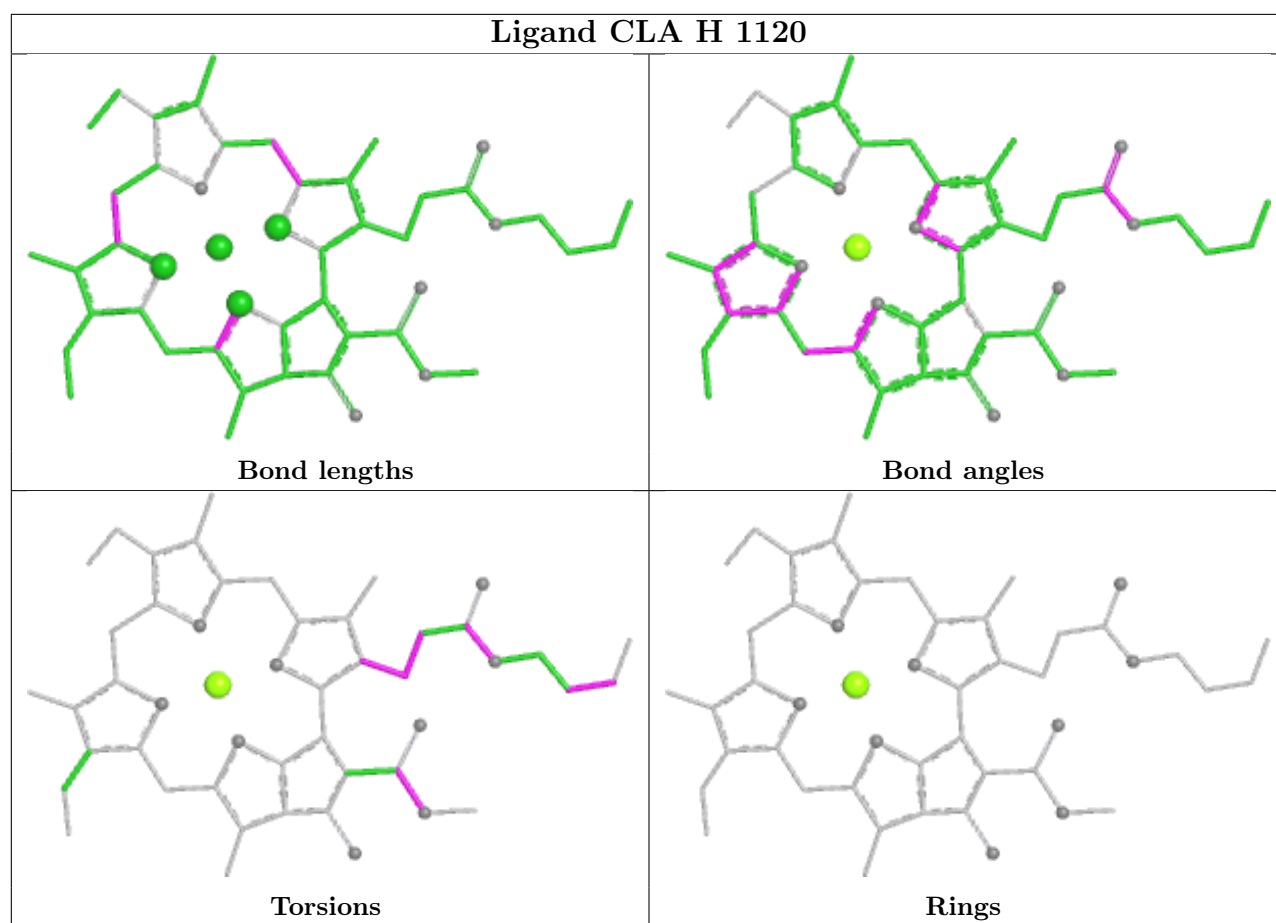


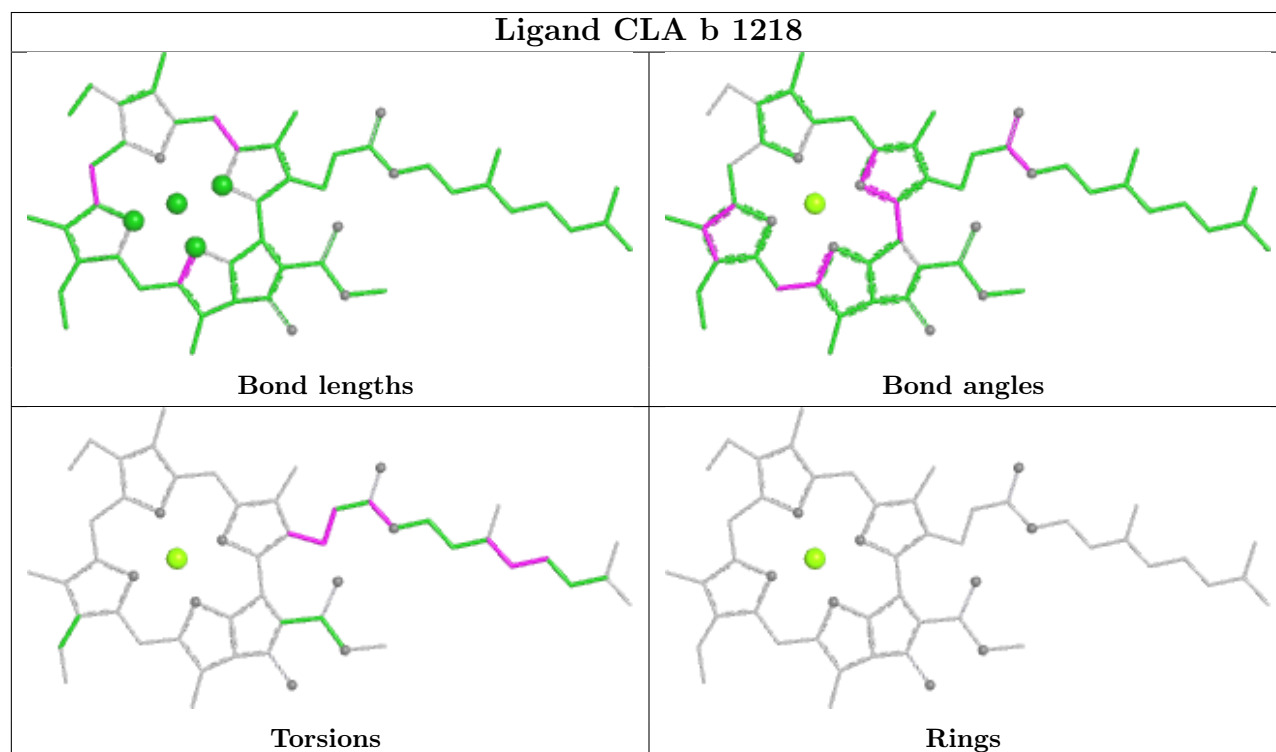
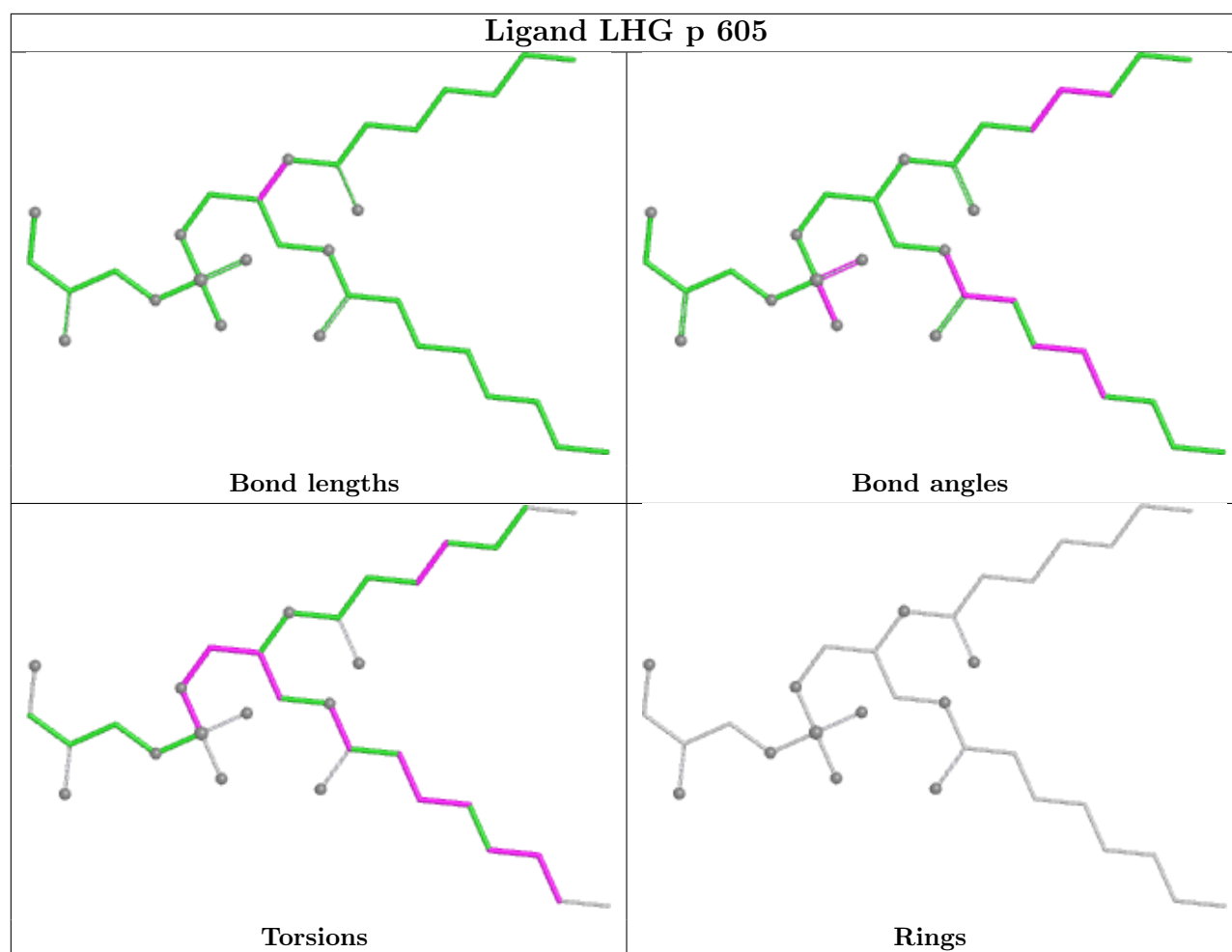


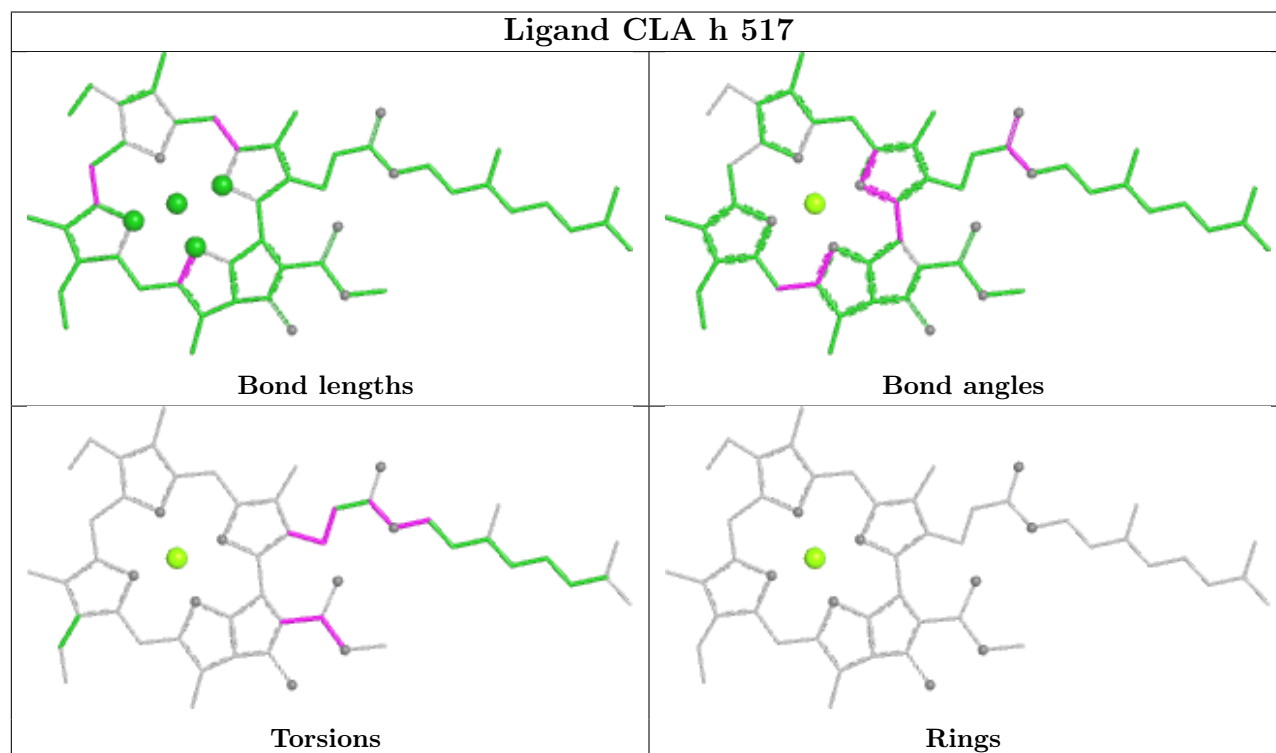
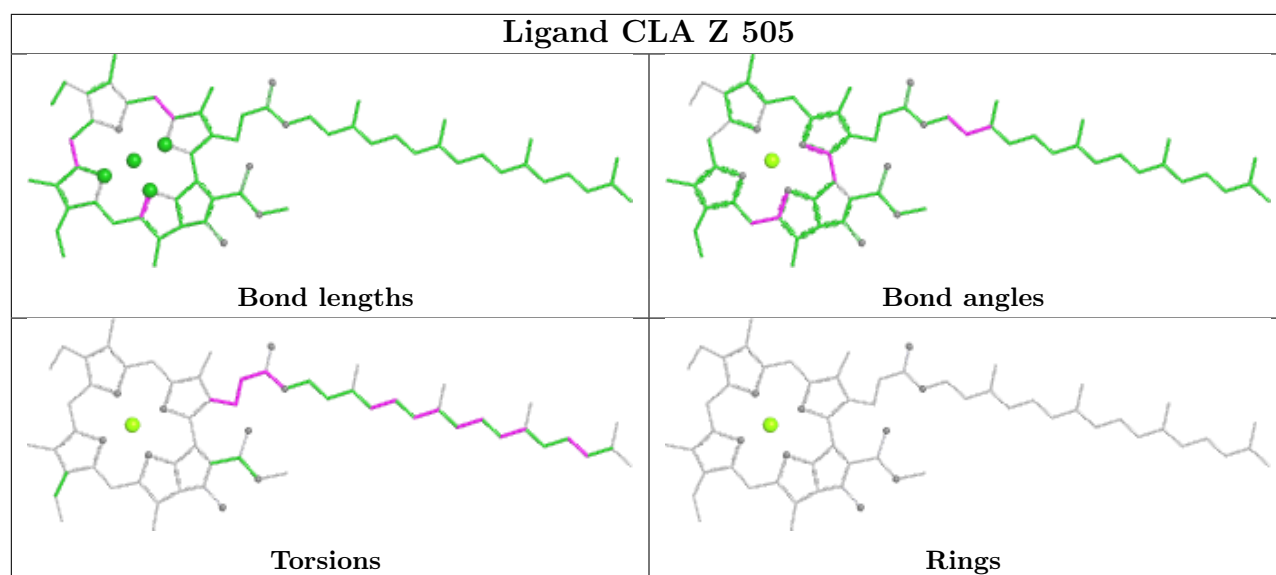


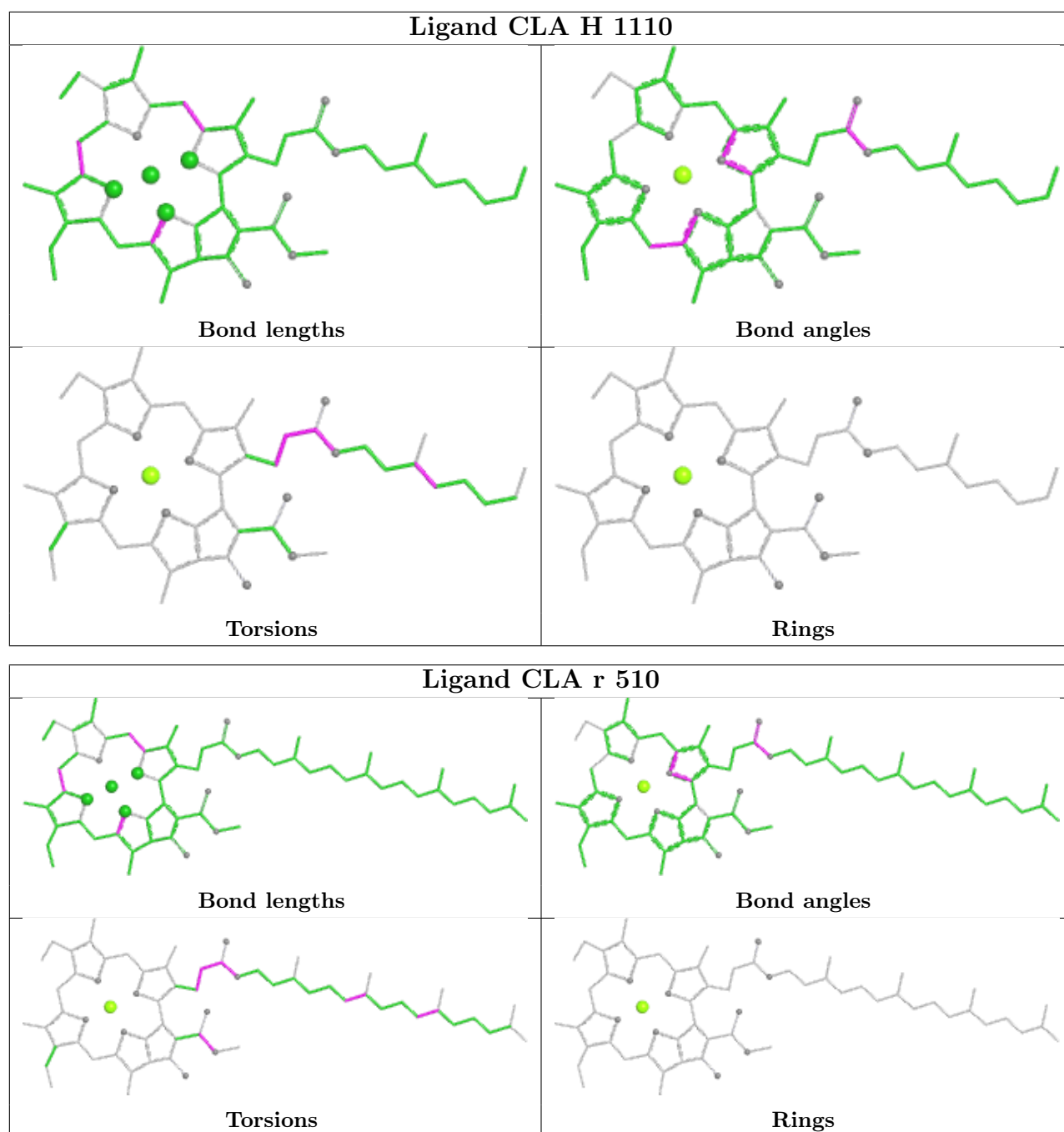
Ligand CLA G 1212

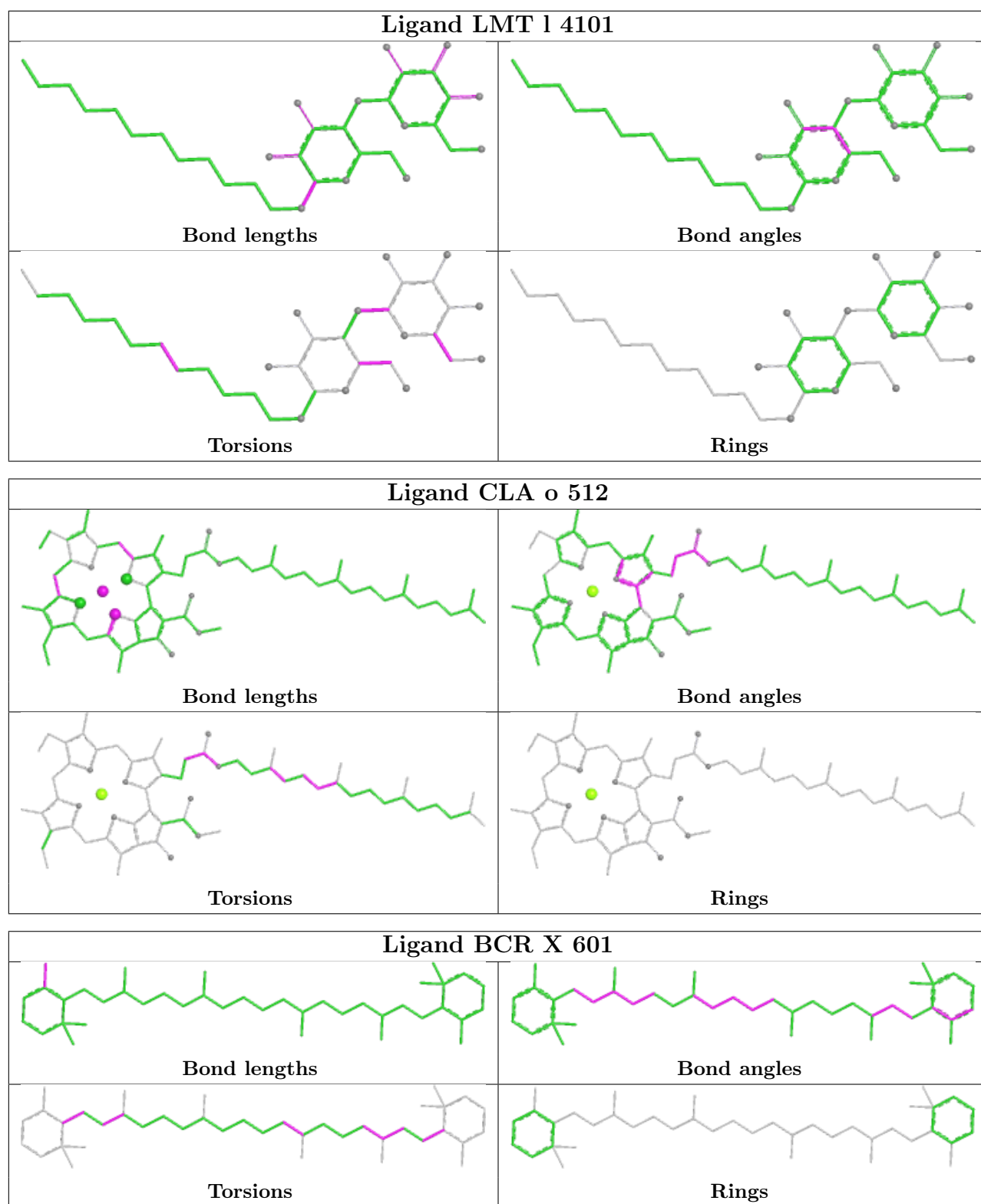


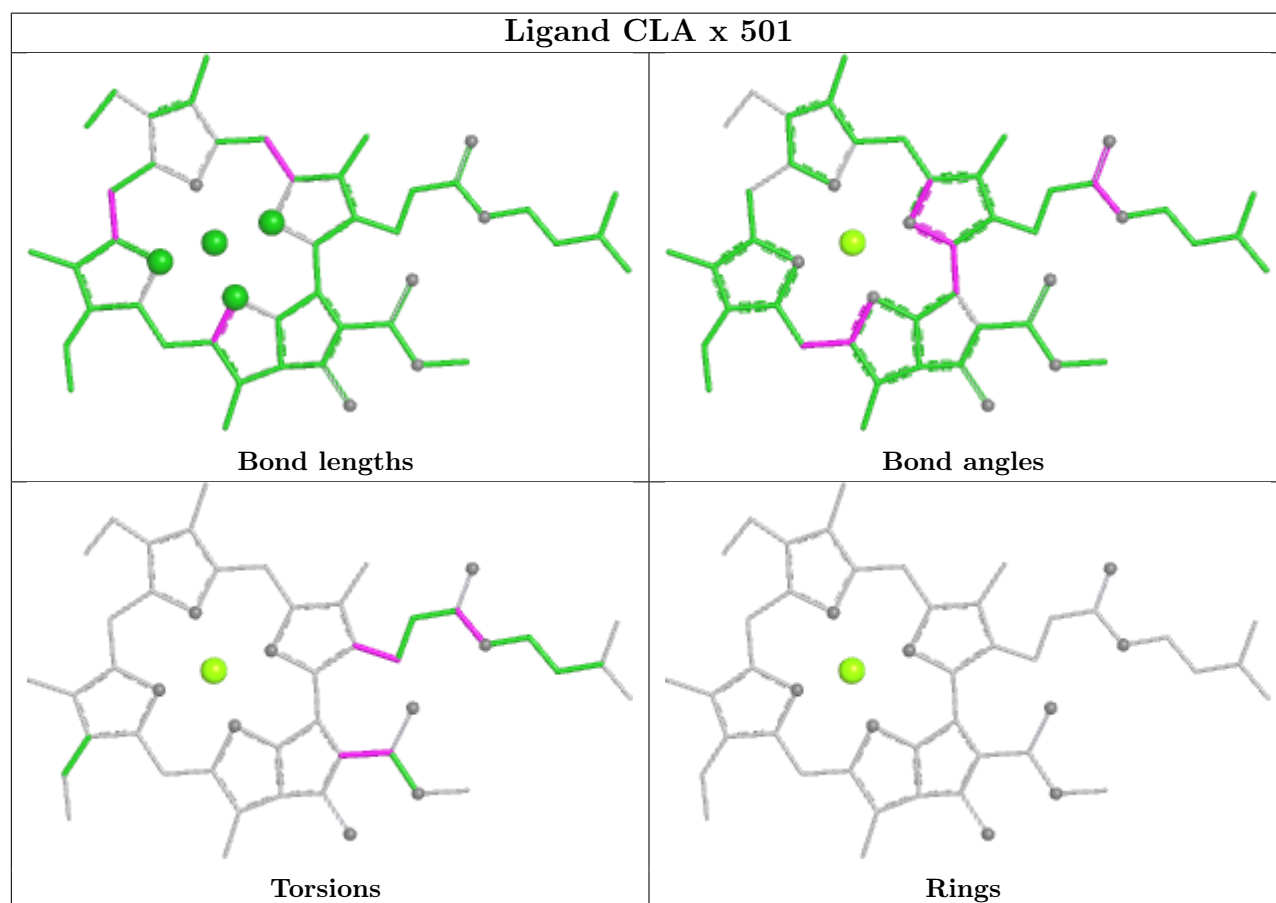
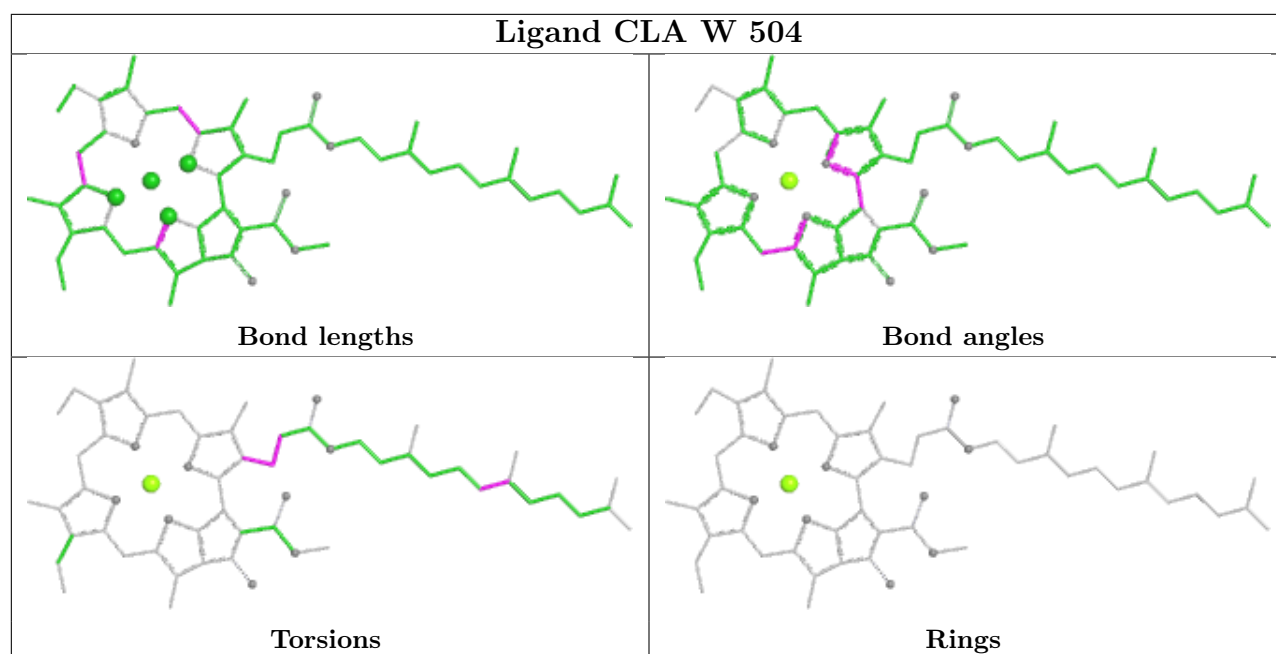


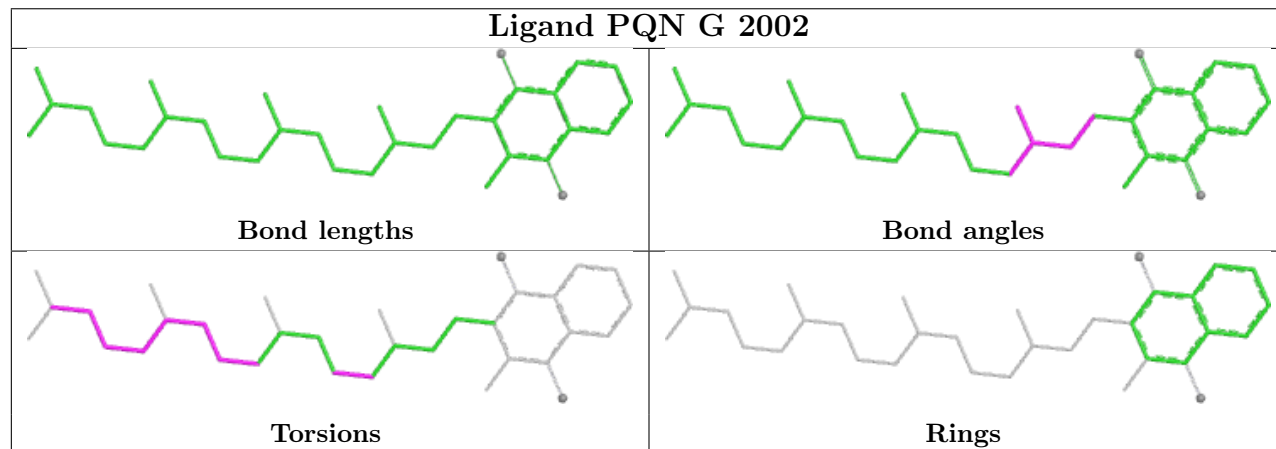
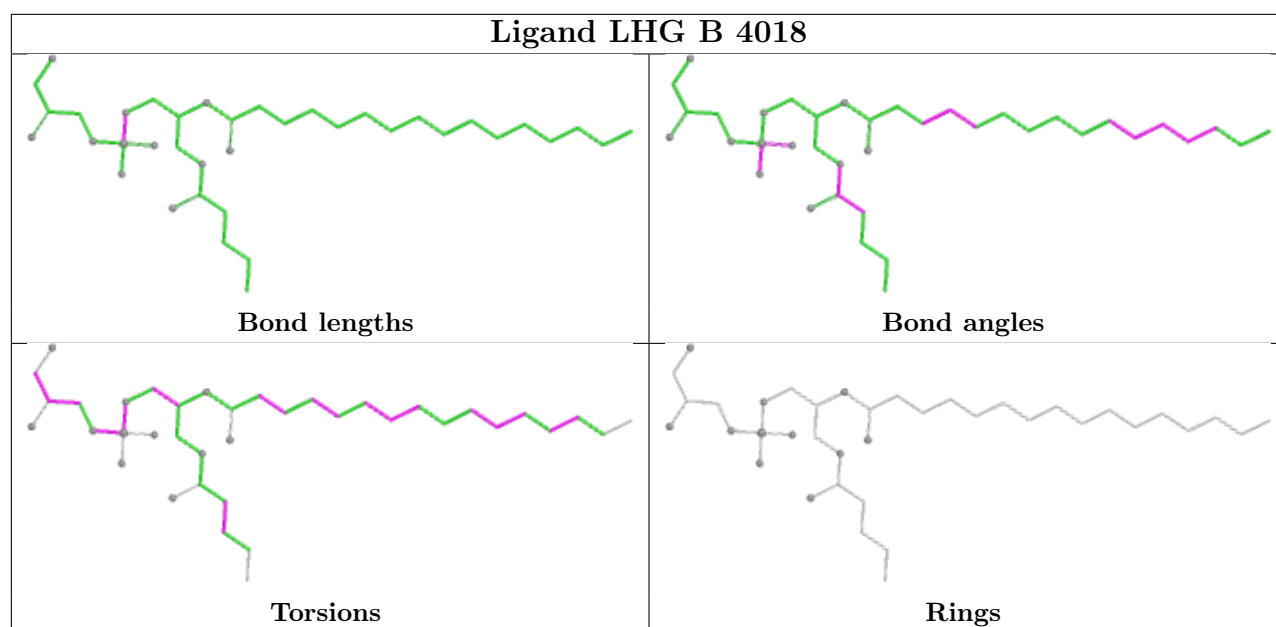




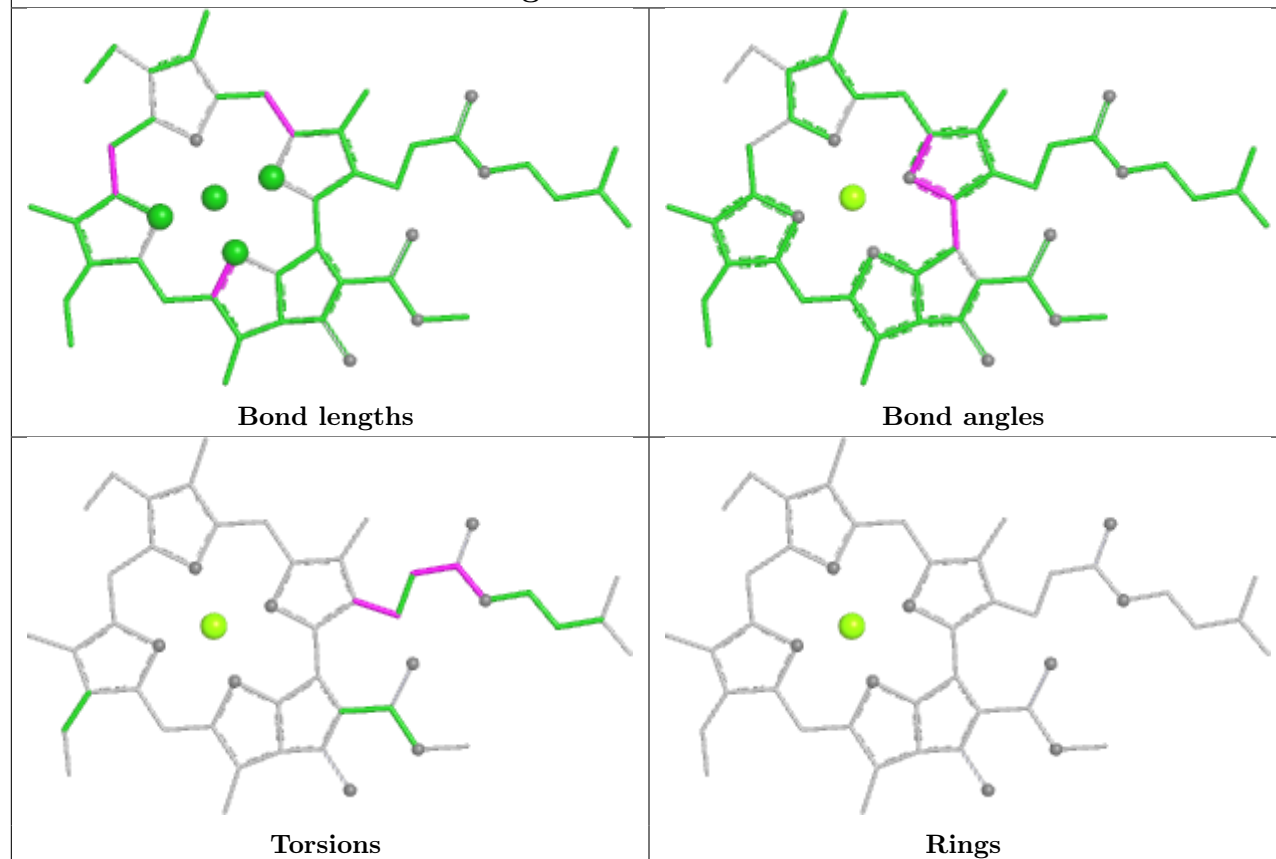




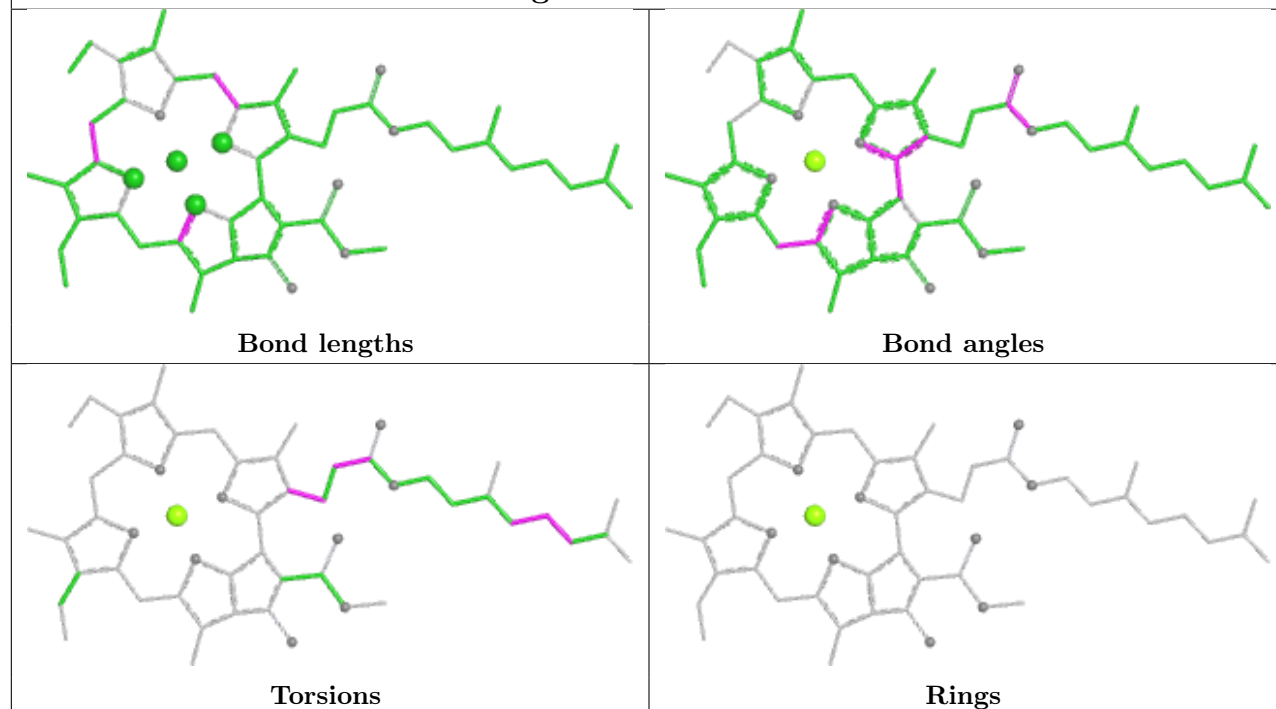


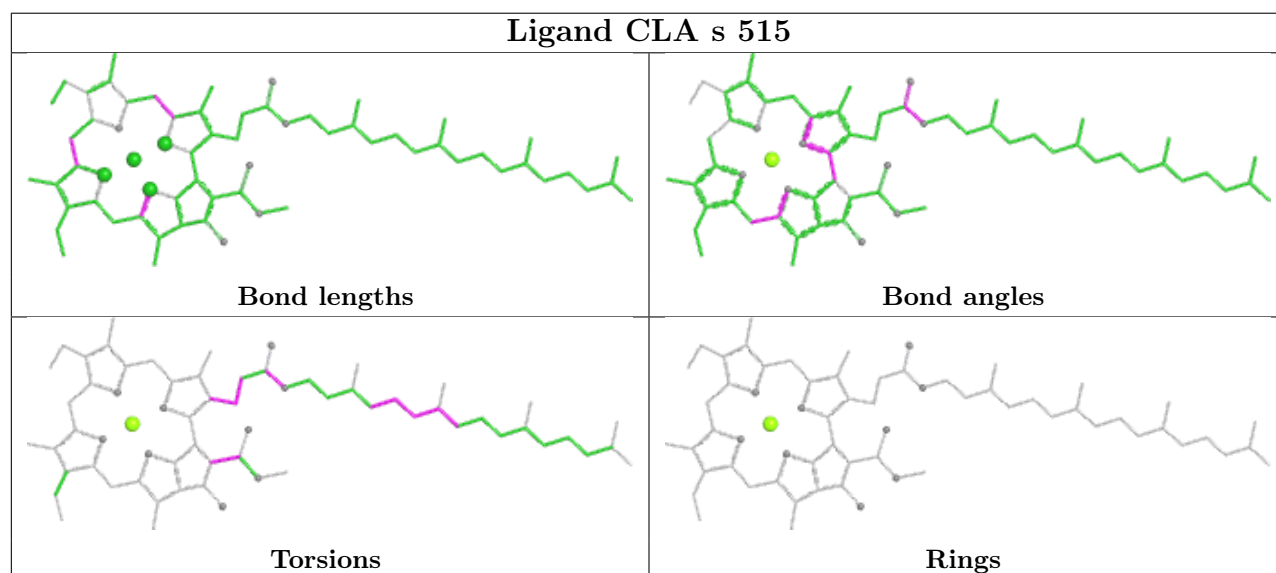
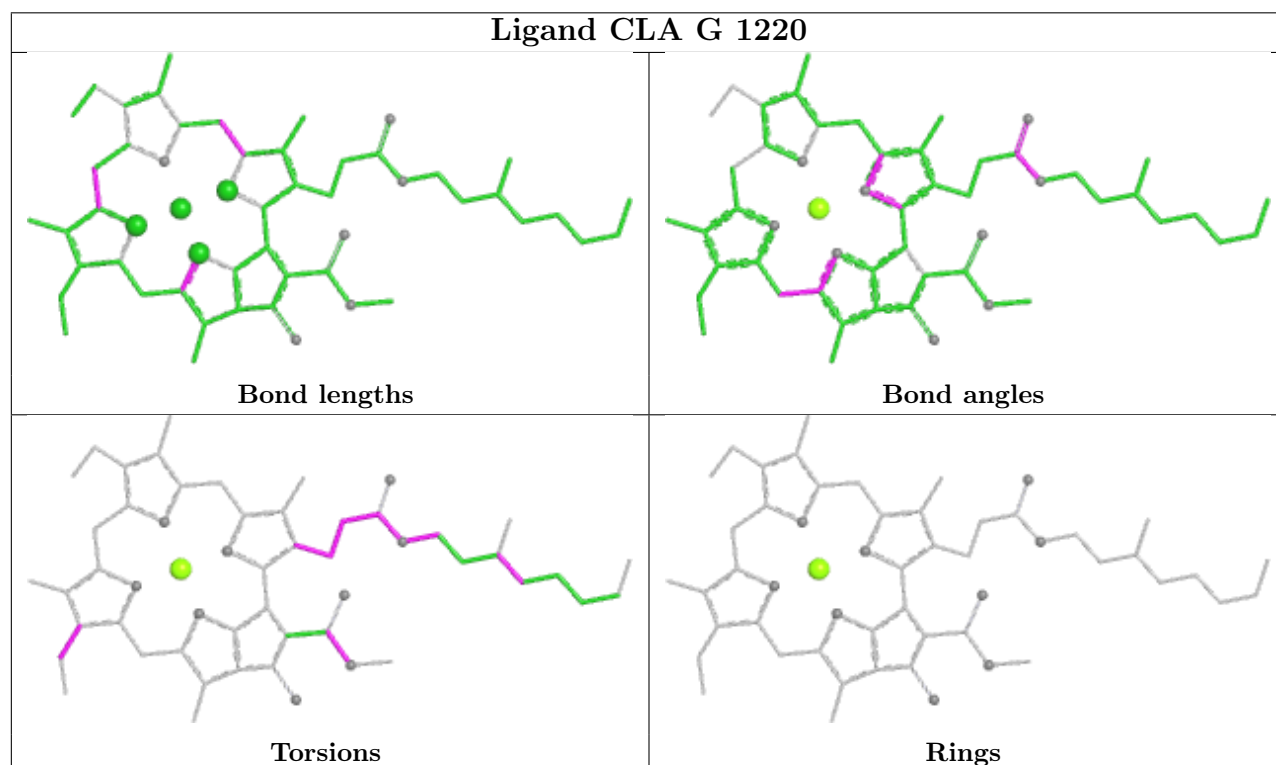
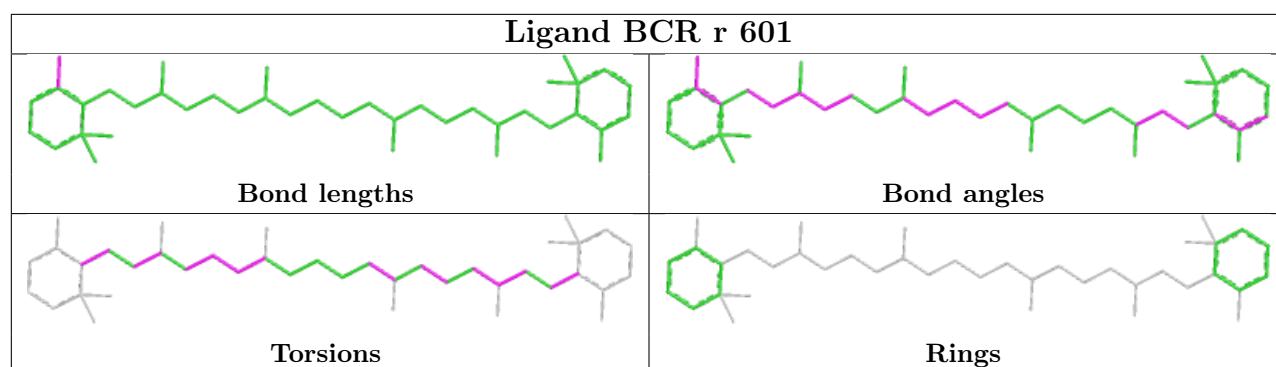


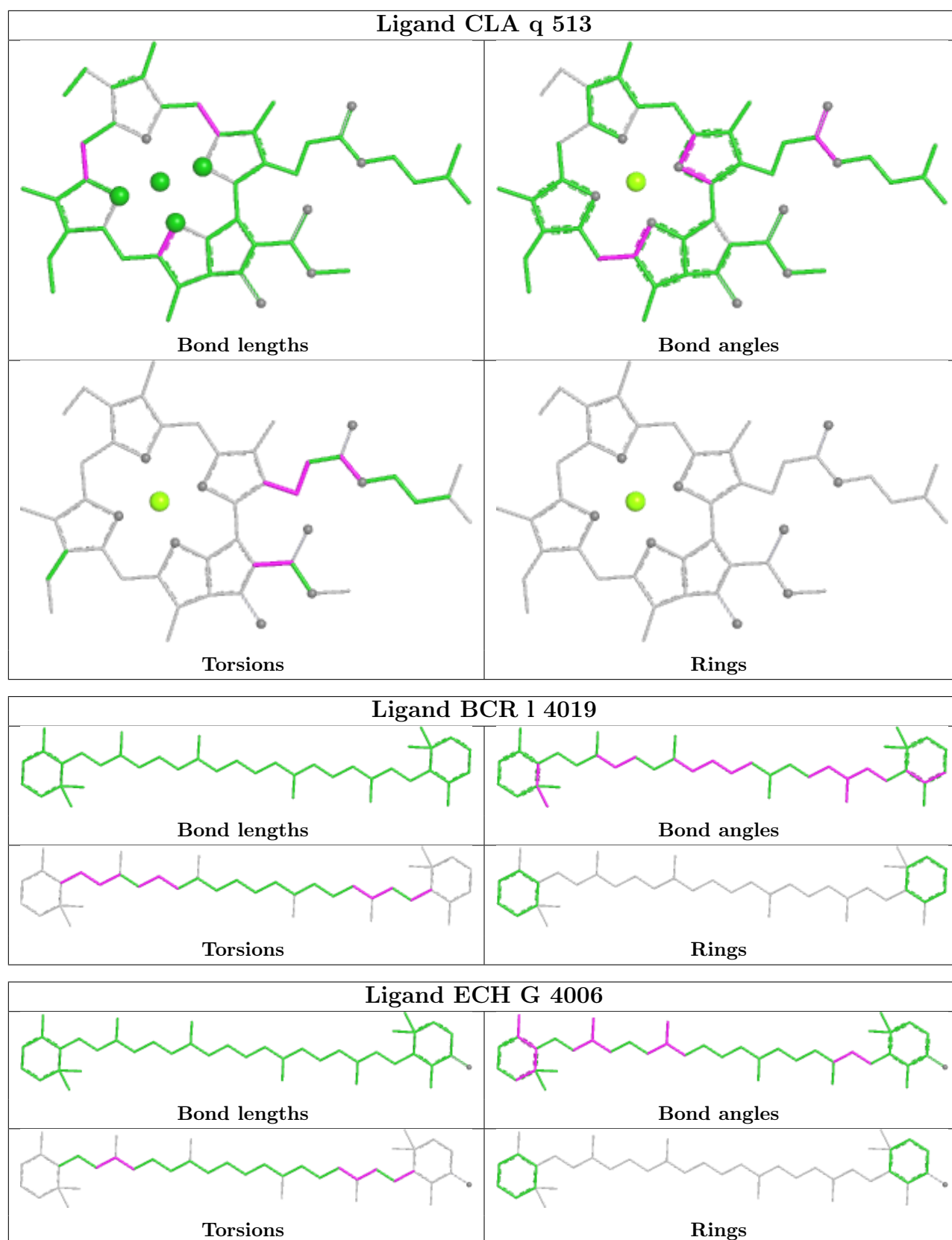
Ligand CLA G 1236



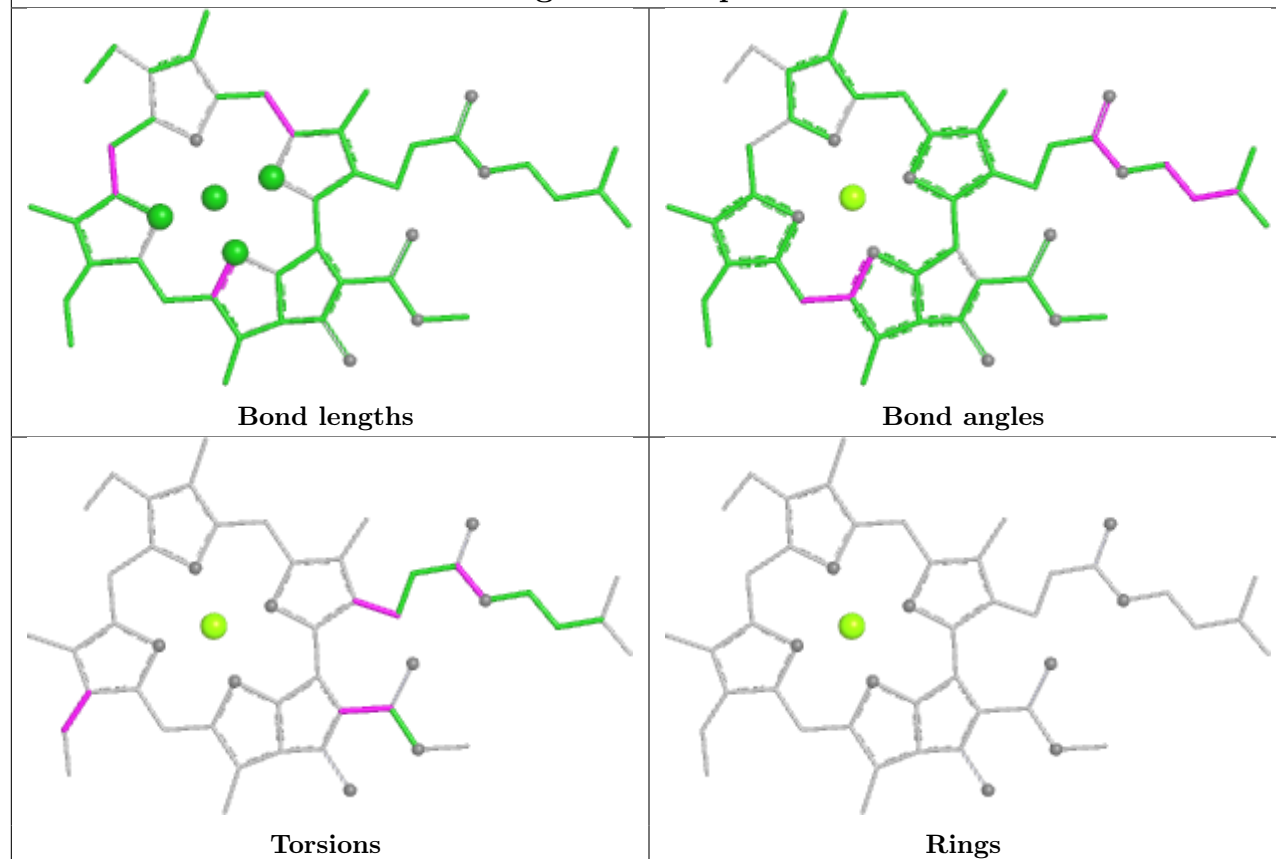
Ligand CLA X 517



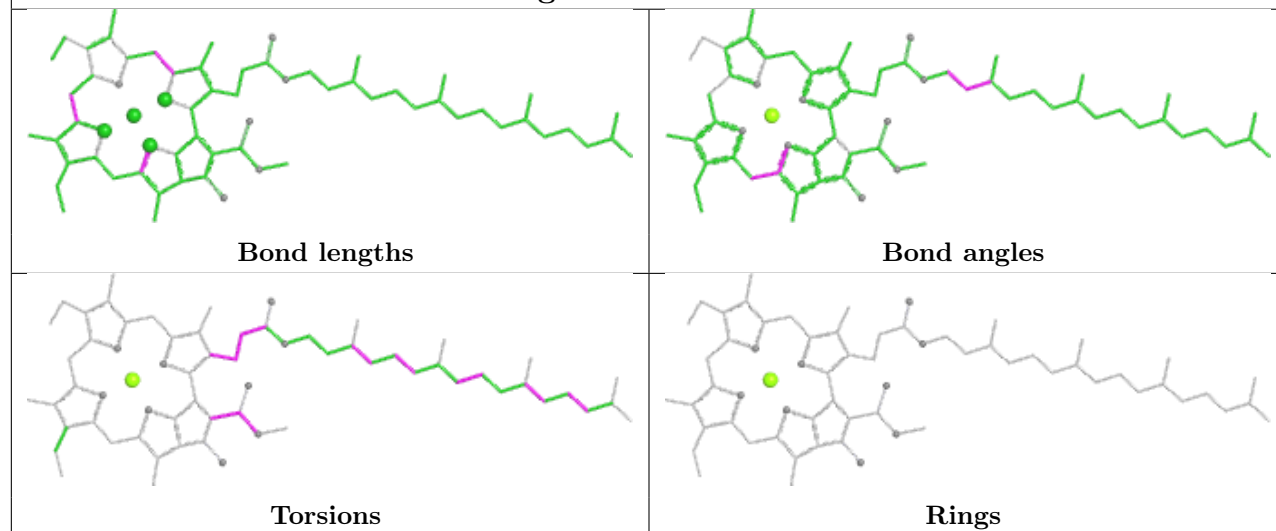


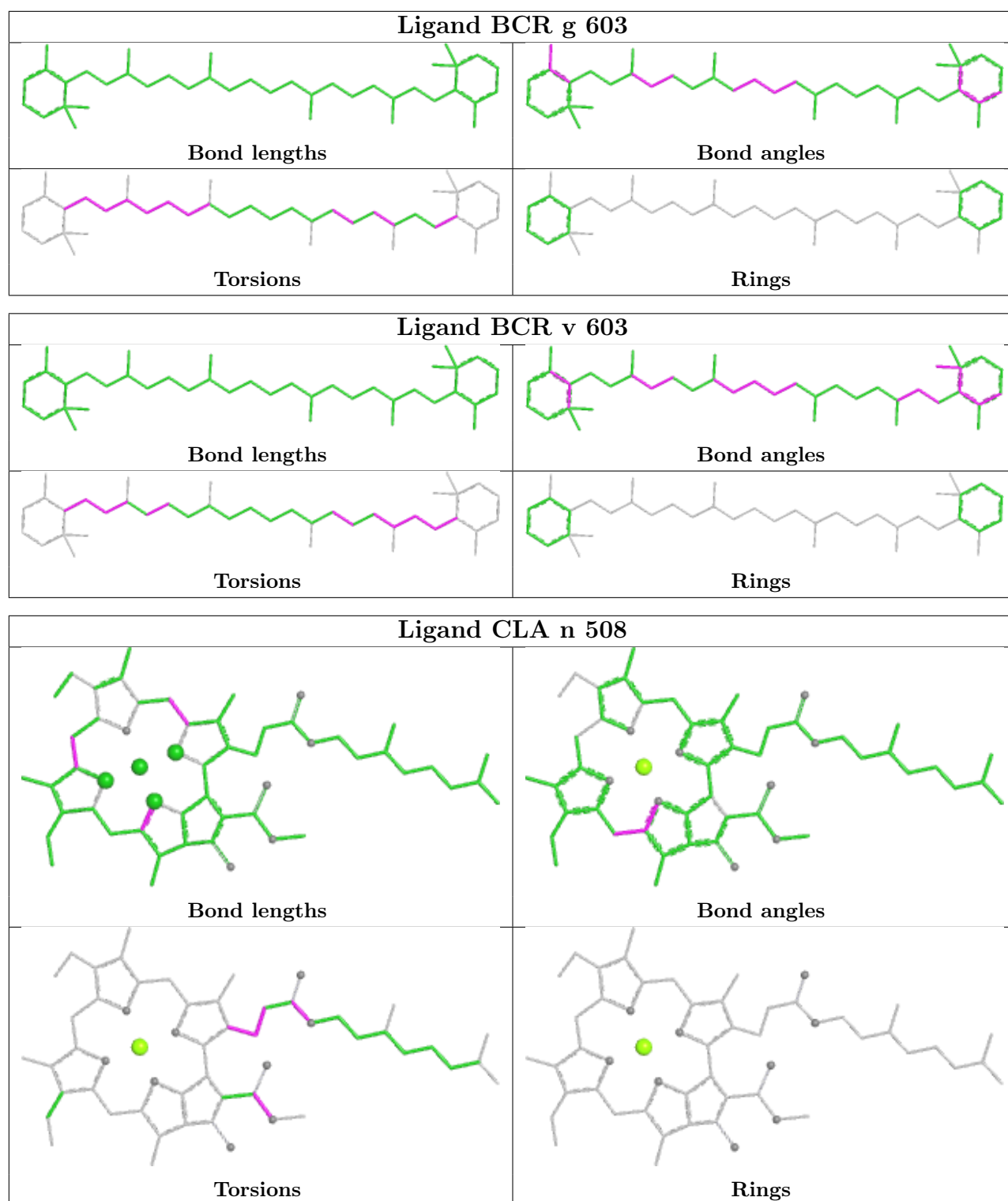


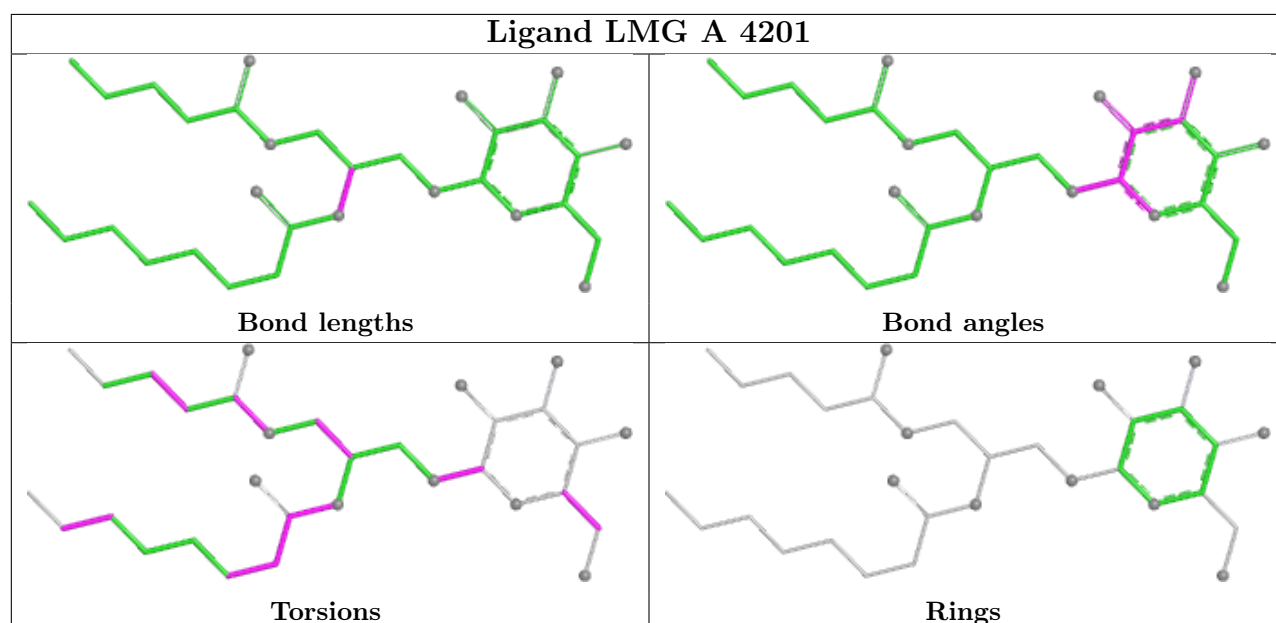
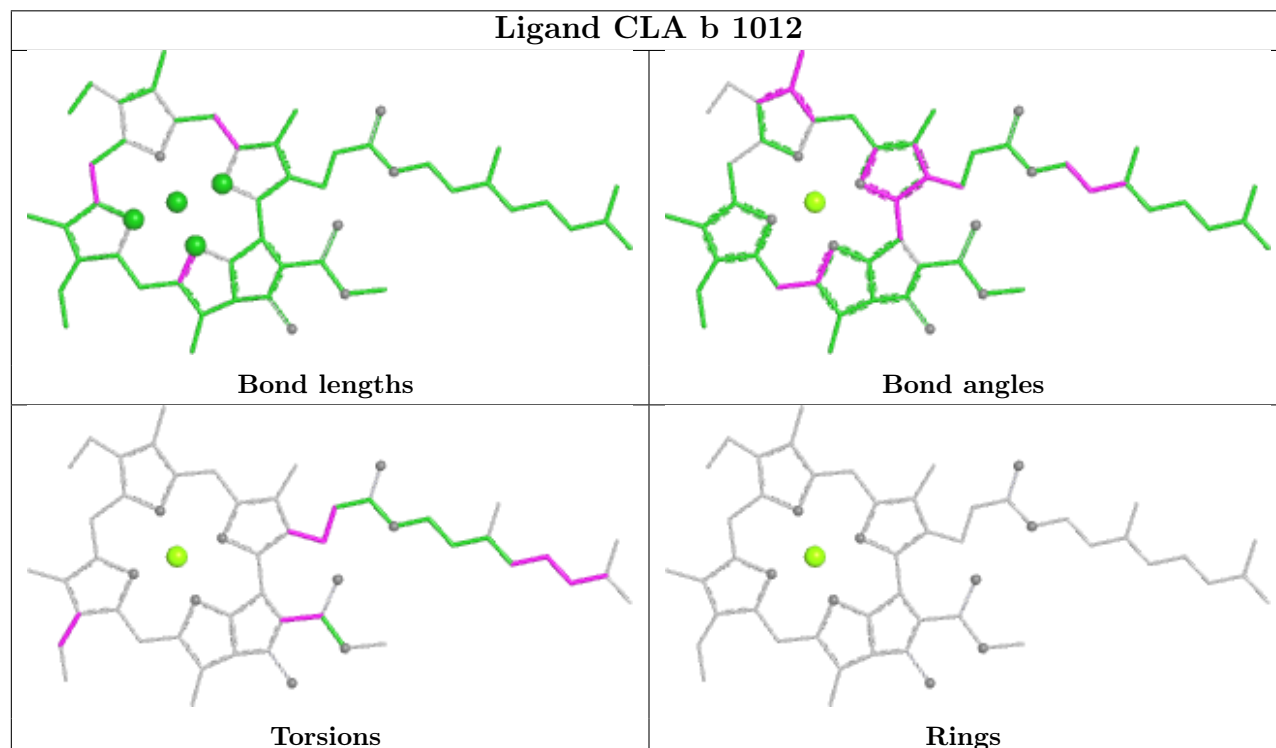
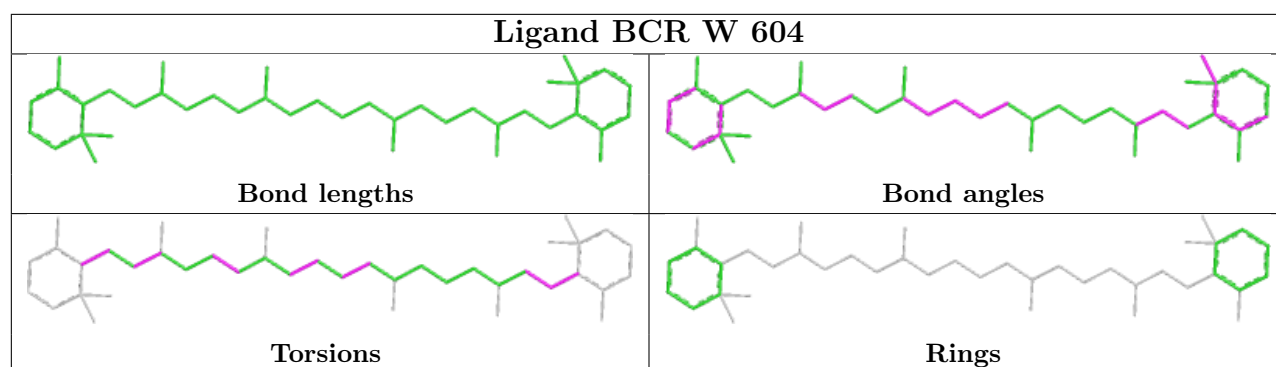
Ligand CLA q 501

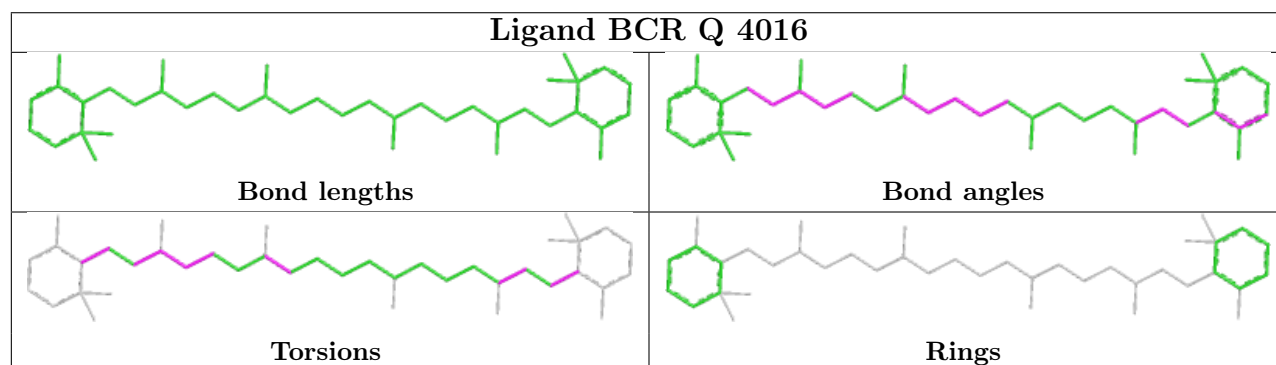
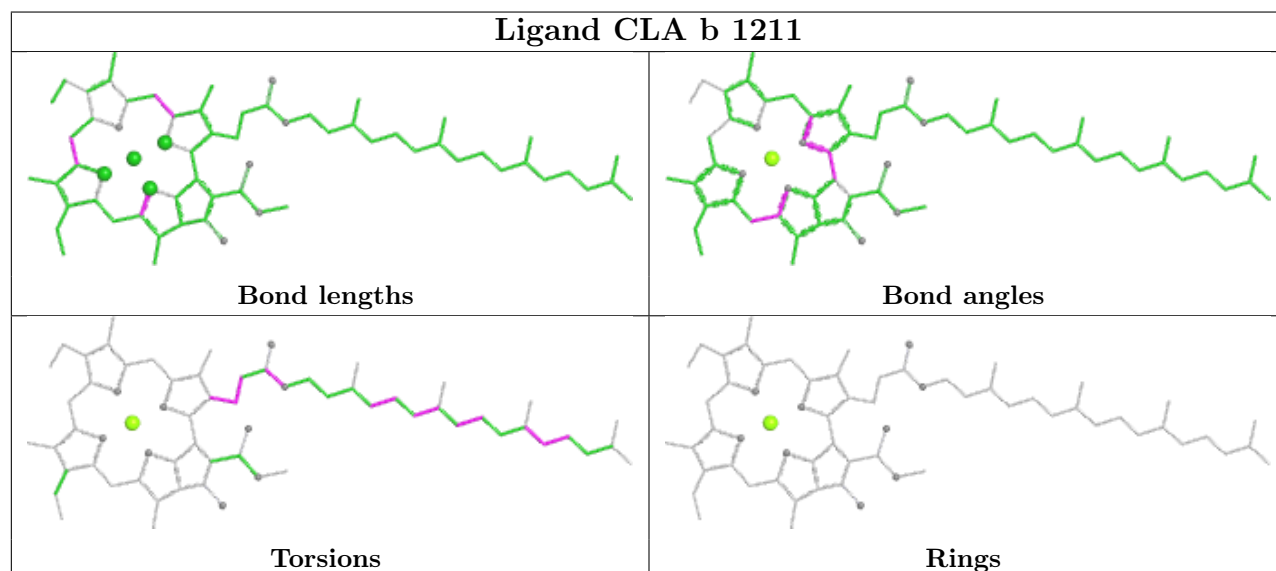
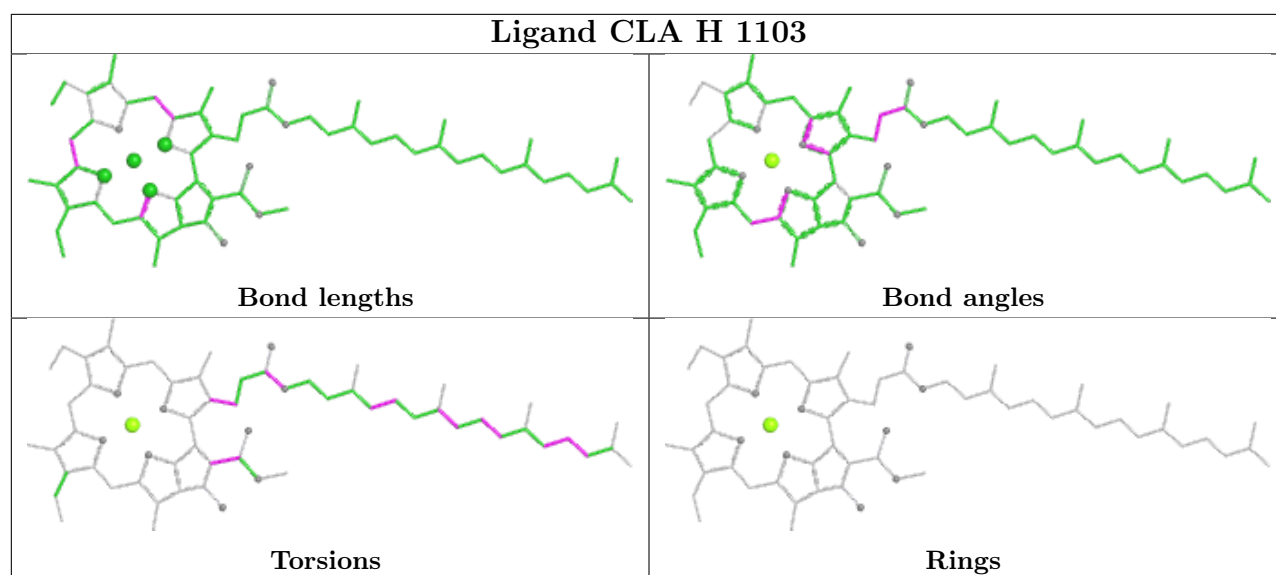


Ligand CLA s 504

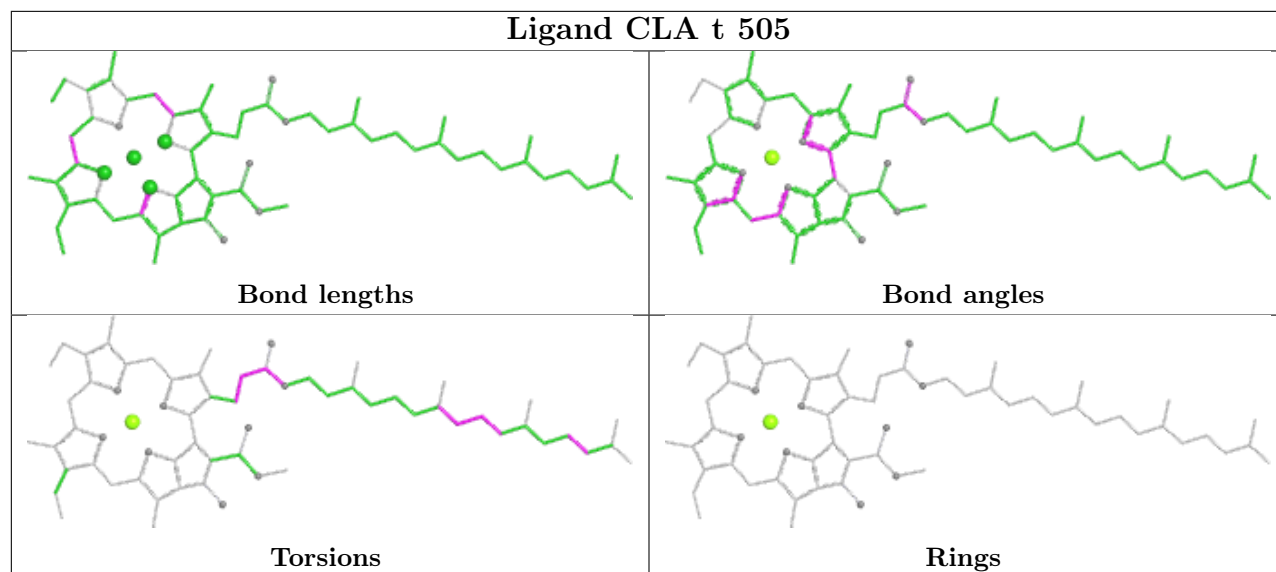




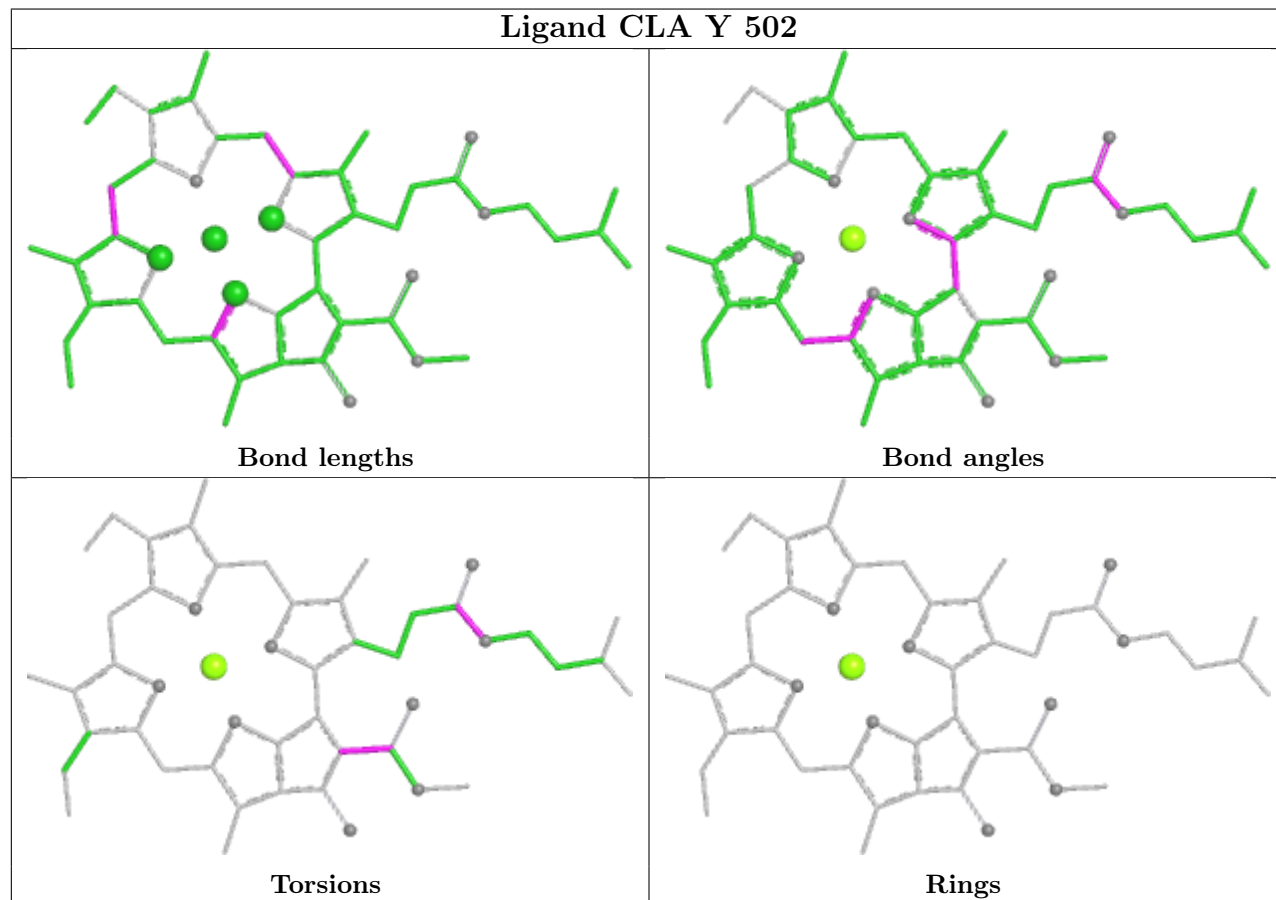


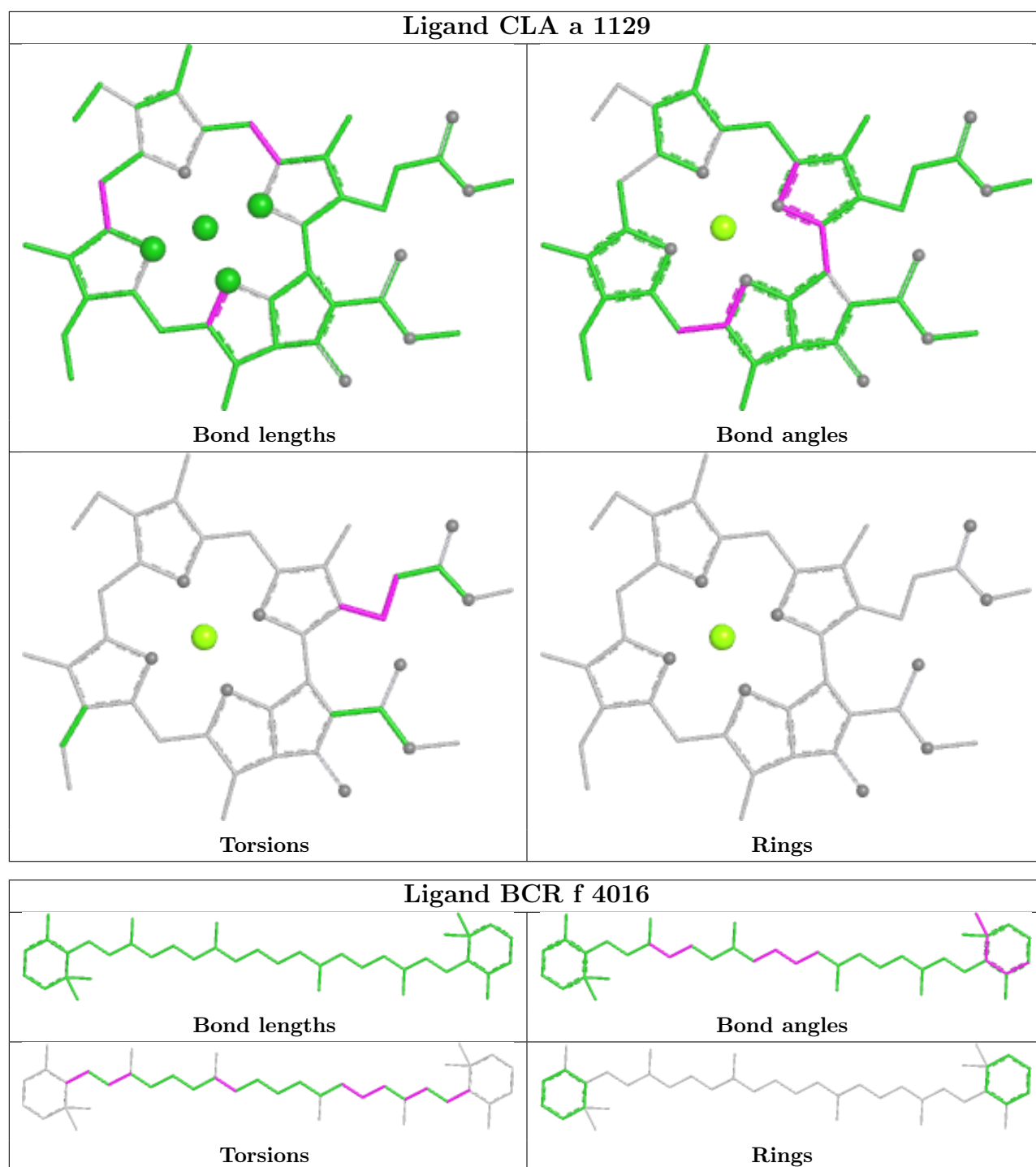


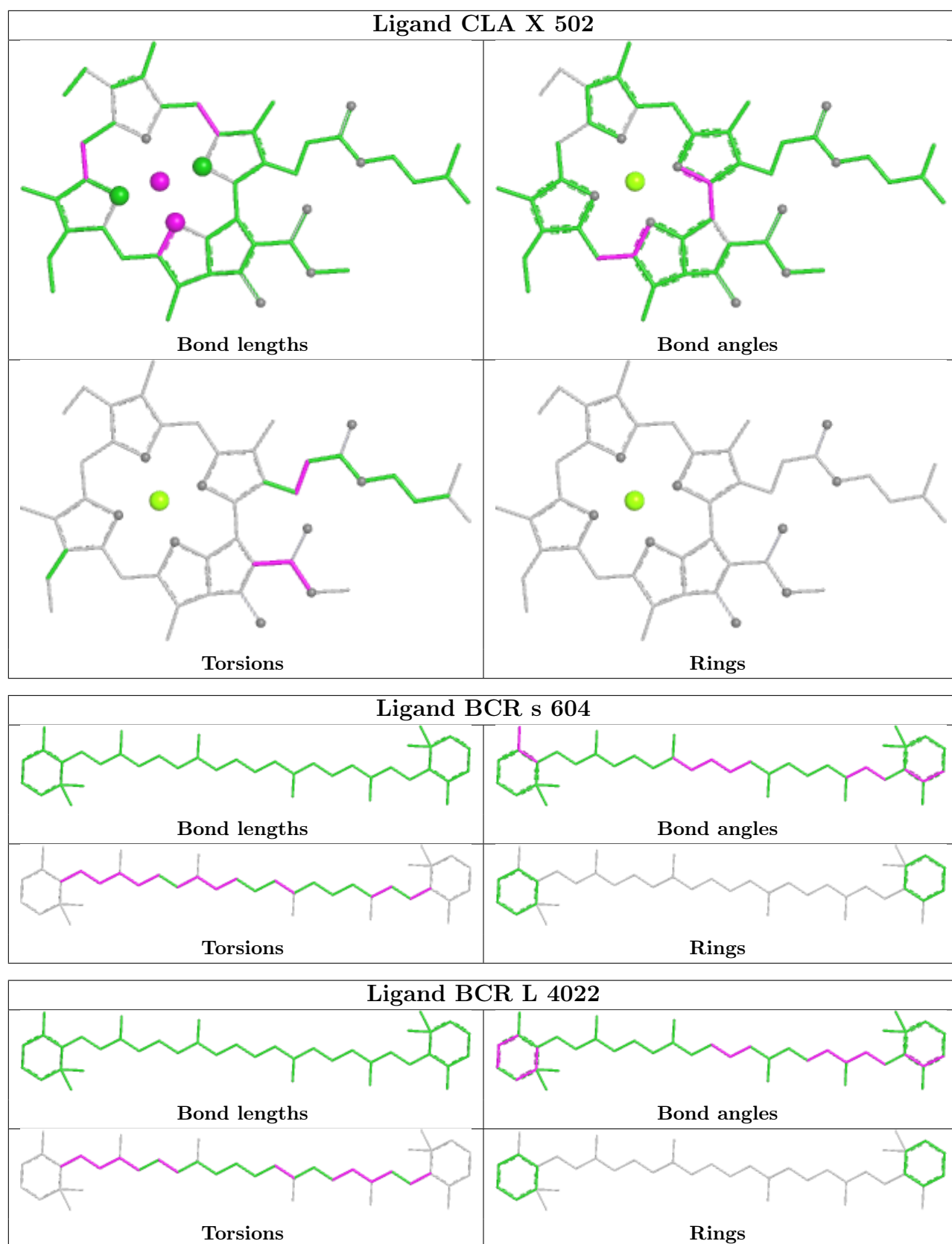
Ligand CLA t 505

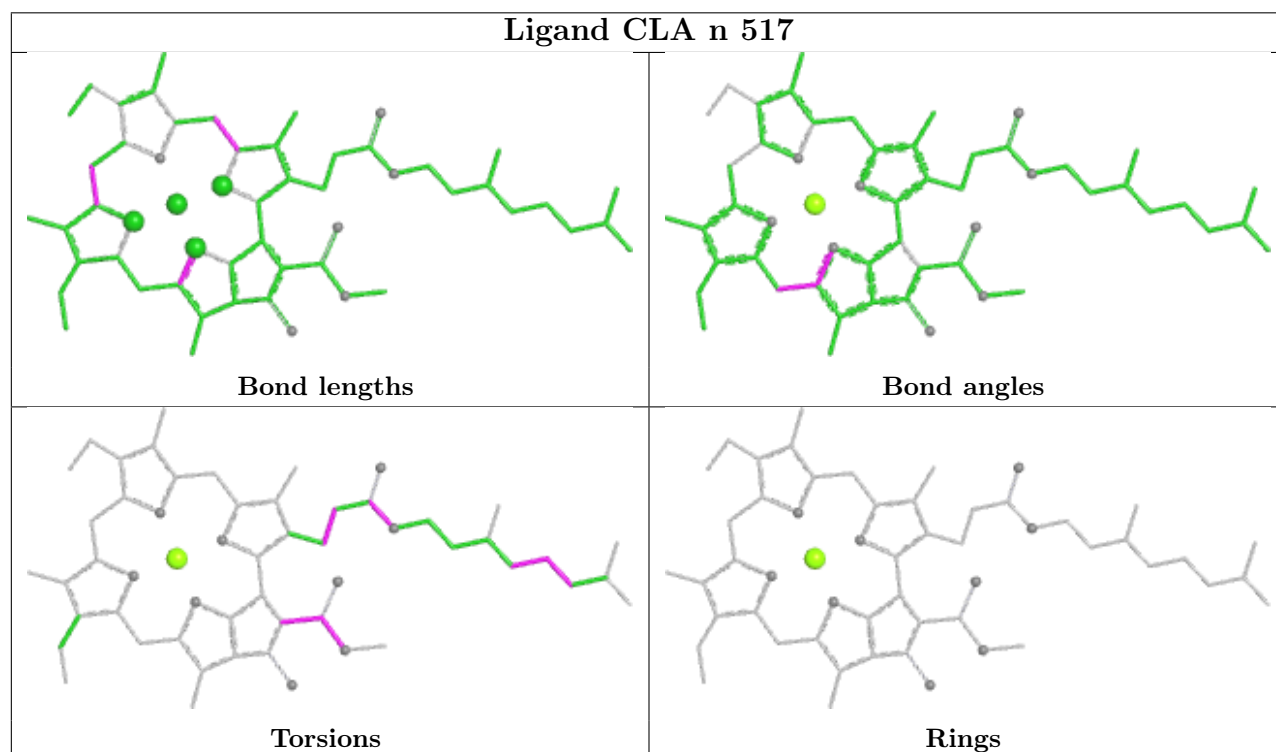
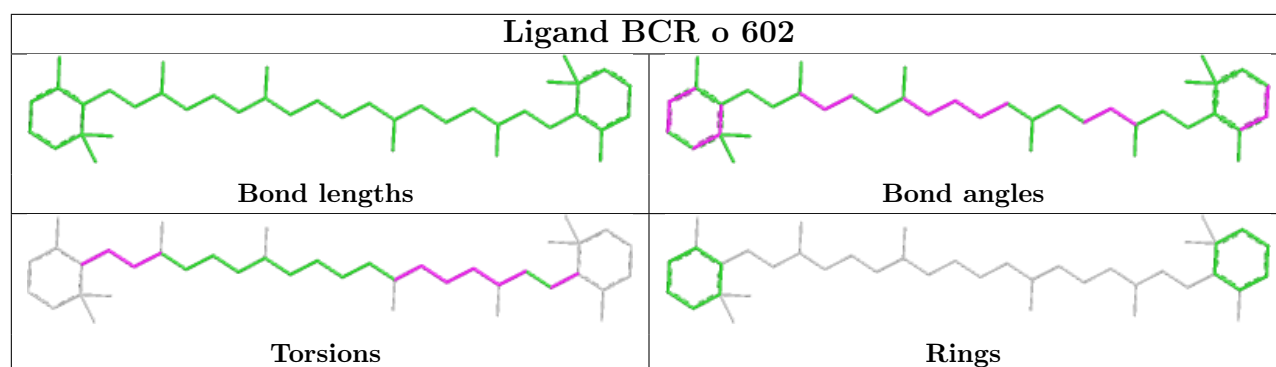


Ligand CLA Y 502

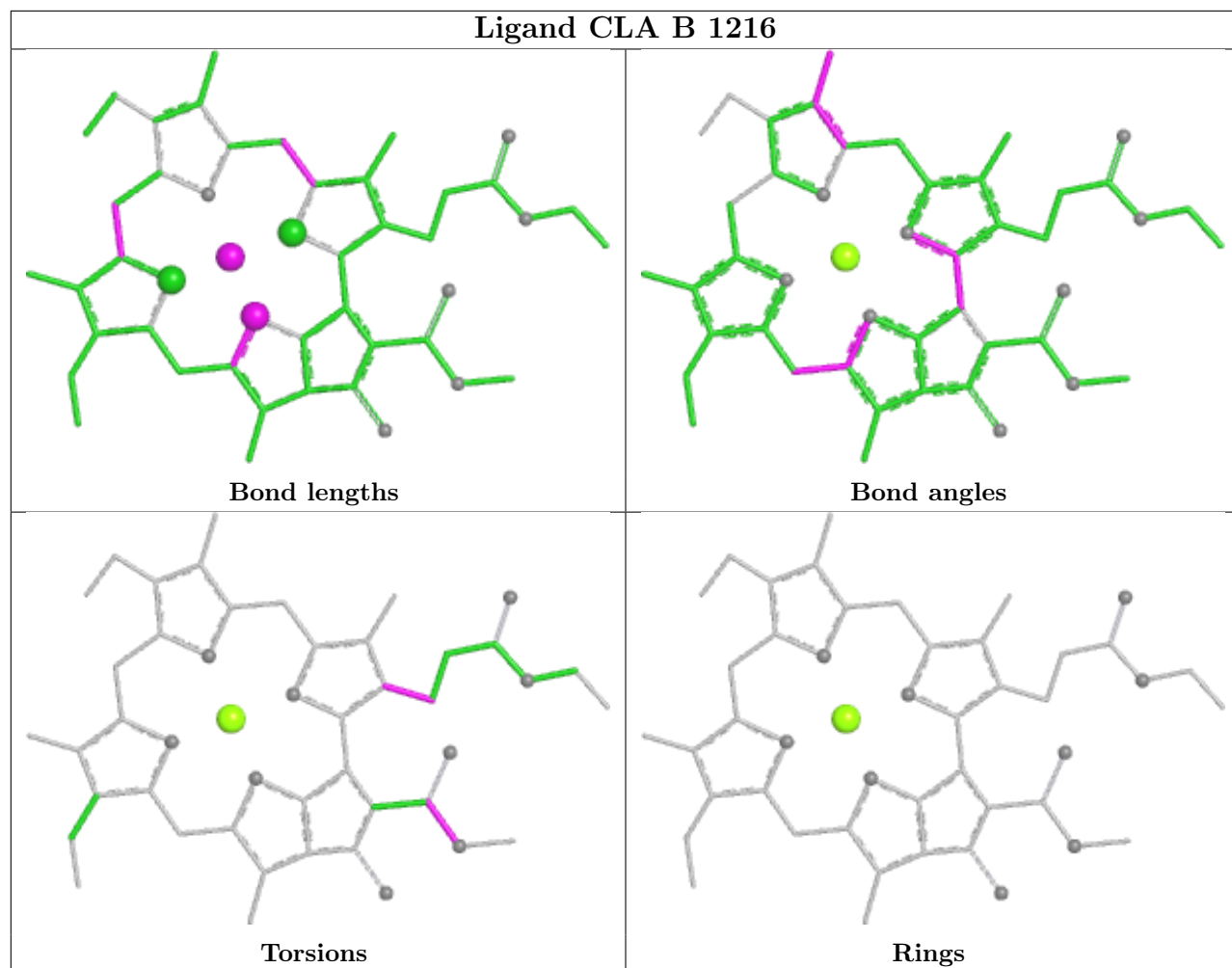




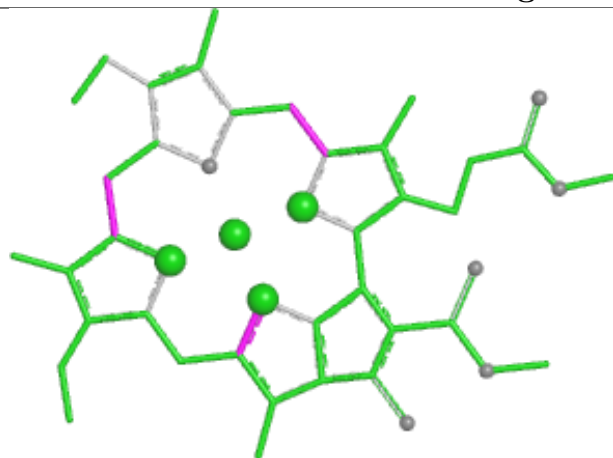




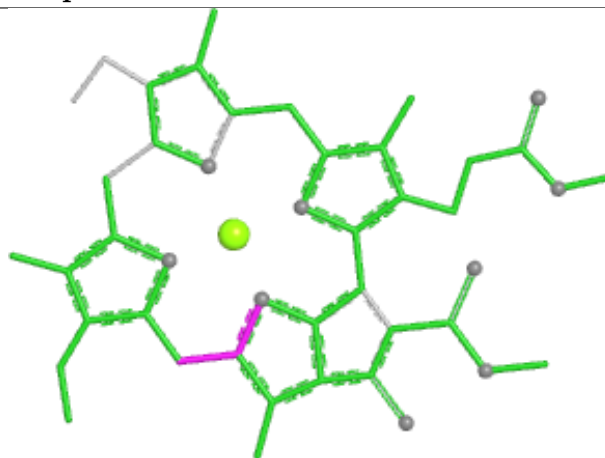
Ligand CLA B 1216



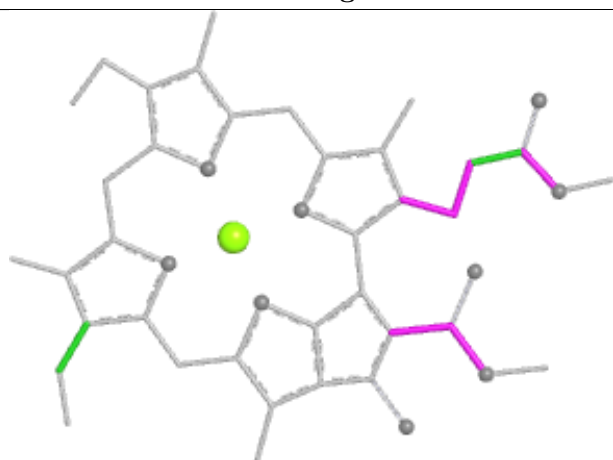
Ligand CLA q 516



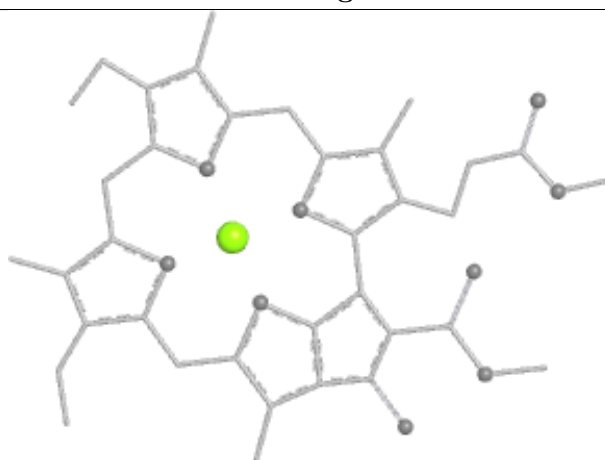
Bond lengths



Bond angles

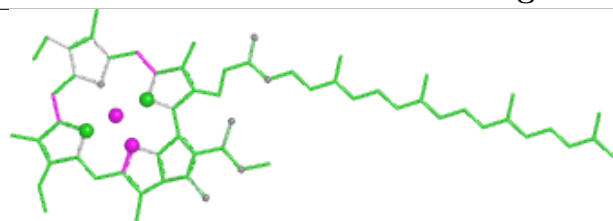


Torsions

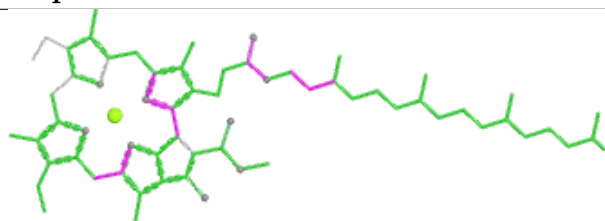


Rings

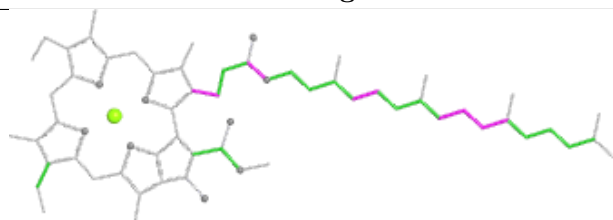
Ligand CLA p 512



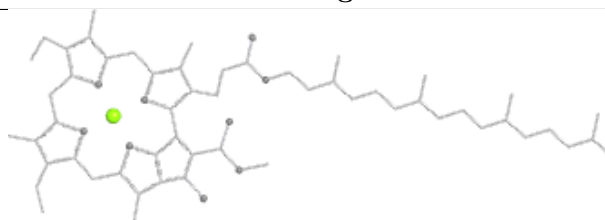
Bond lengths



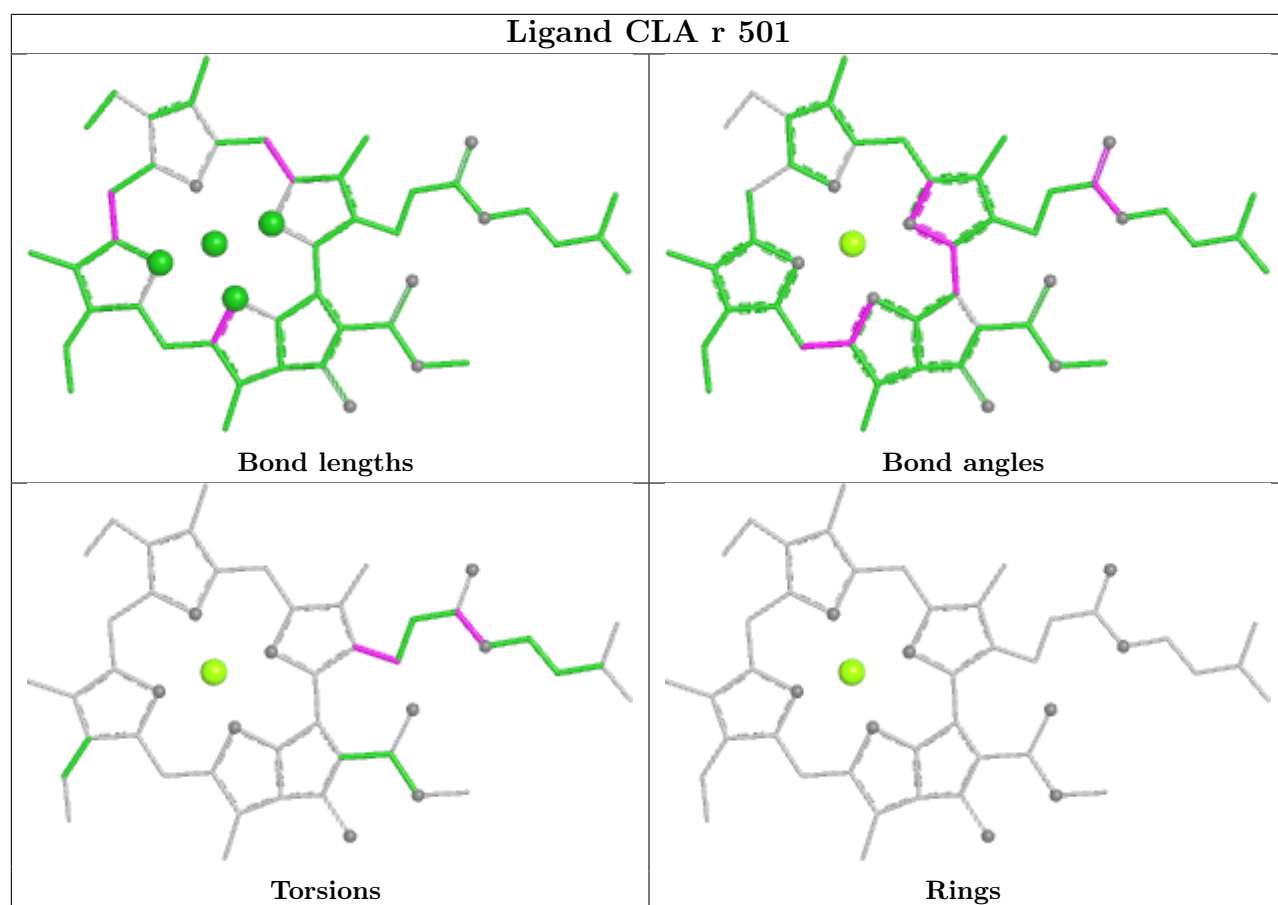
Bond angles



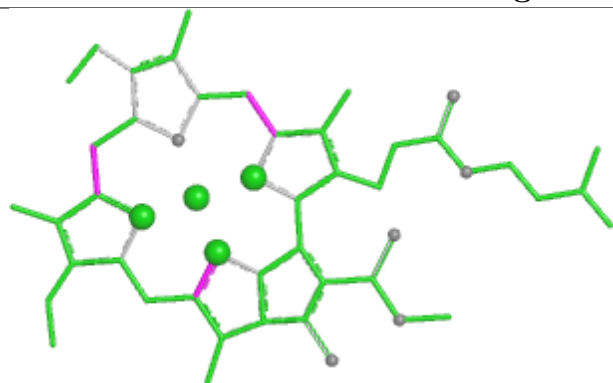
Torsions



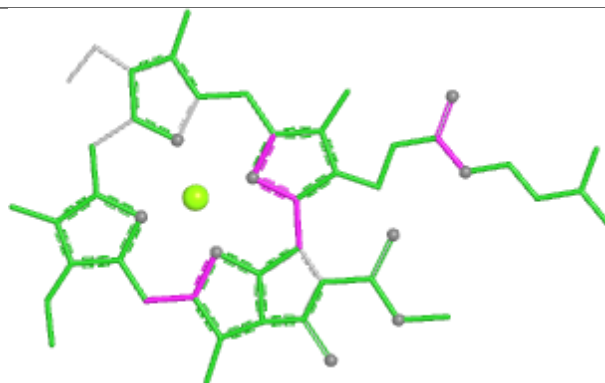
Rings



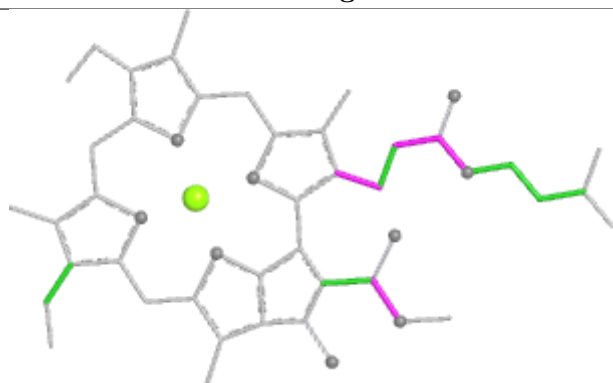
Ligand CLA Y 514



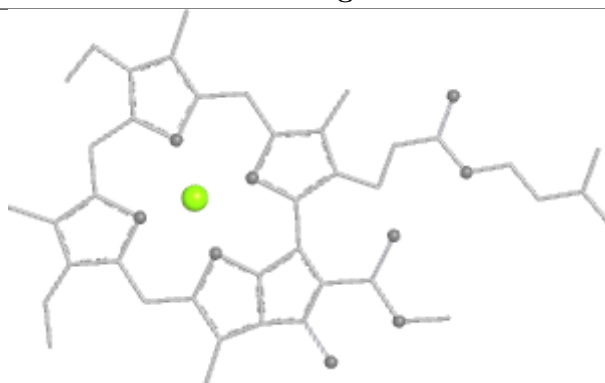
Bond lengths



Bond angles

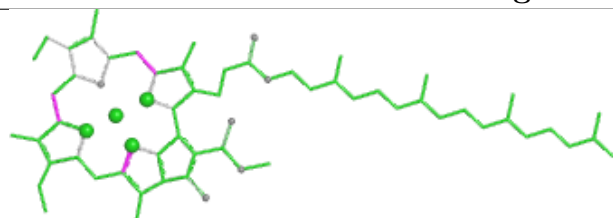


Torsions

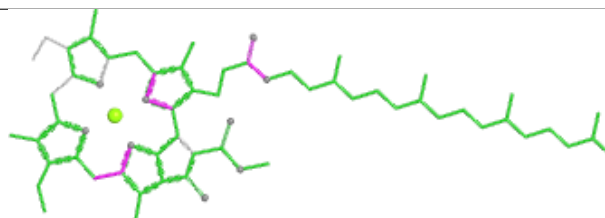


Rings

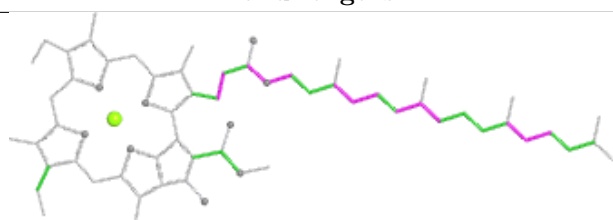
Ligand CLA I 1503



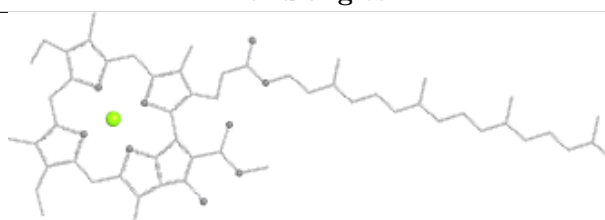
Bond lengths



Bond angles

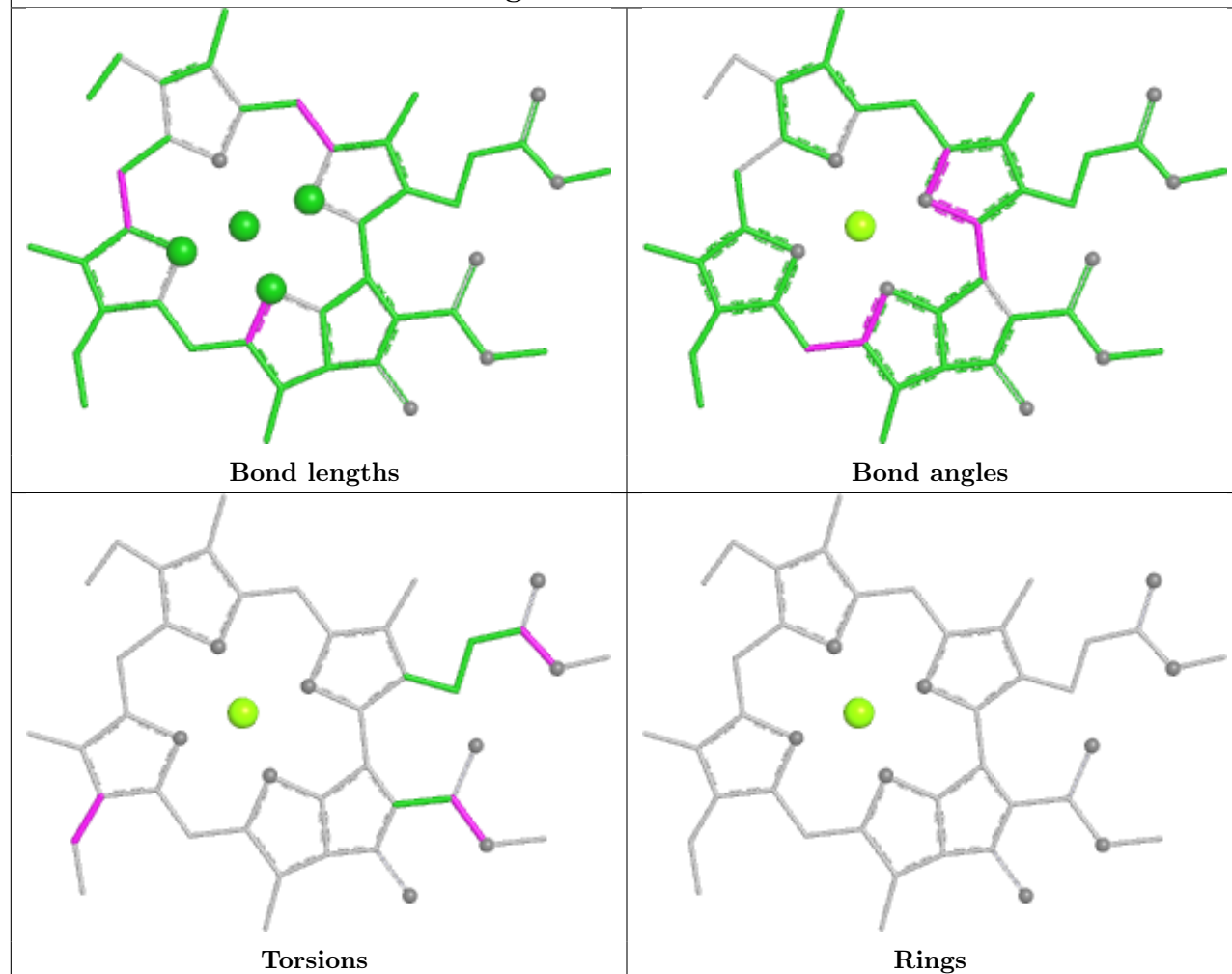


Torsions

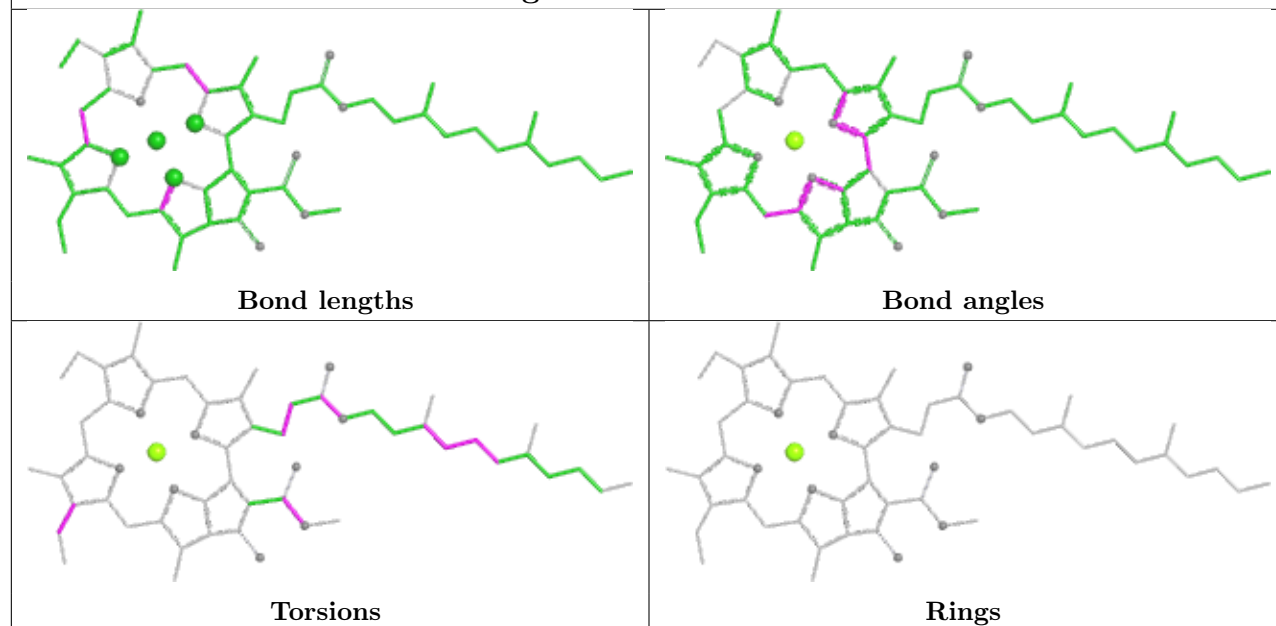


Rings

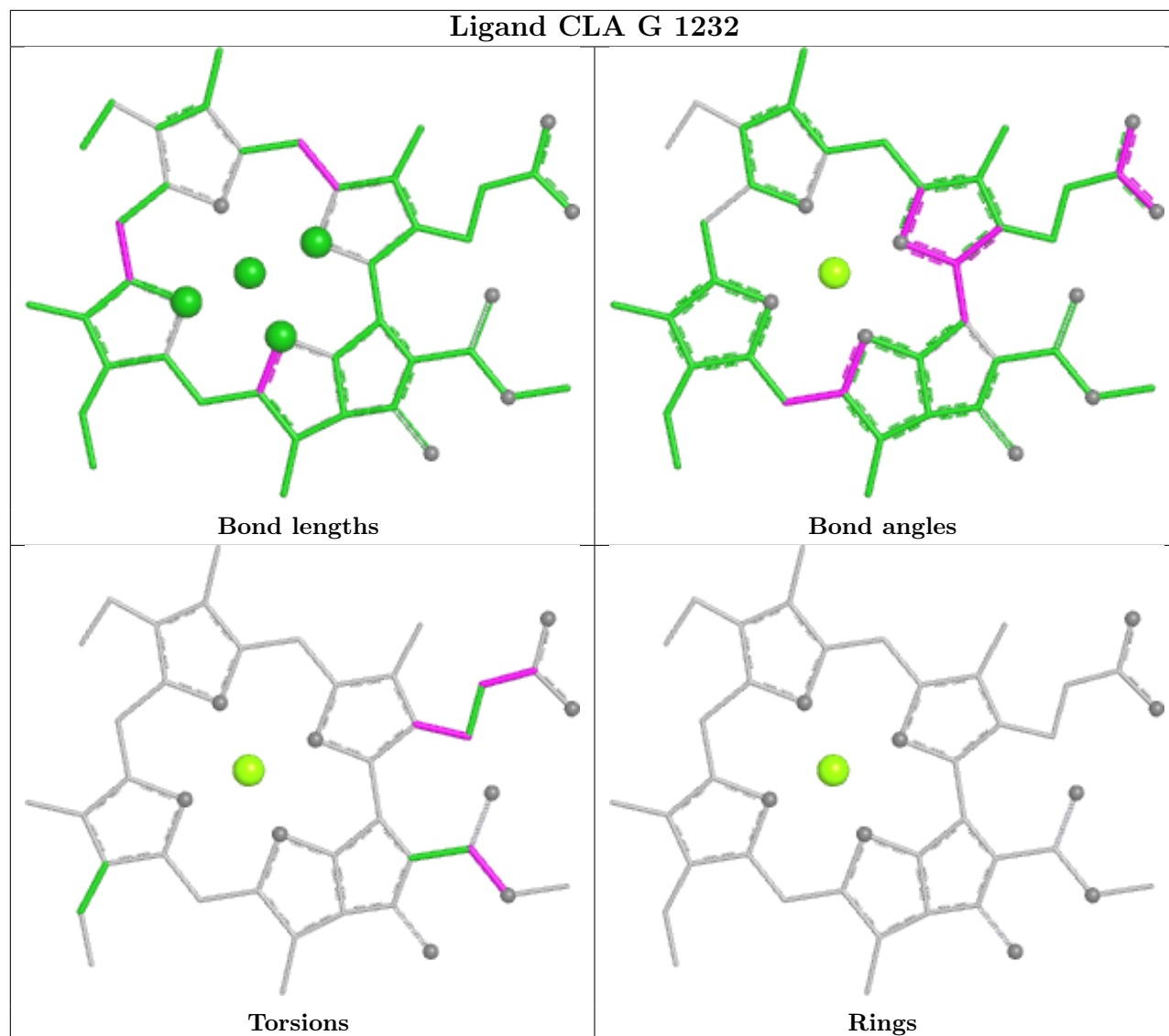
Ligand CLA B 1240



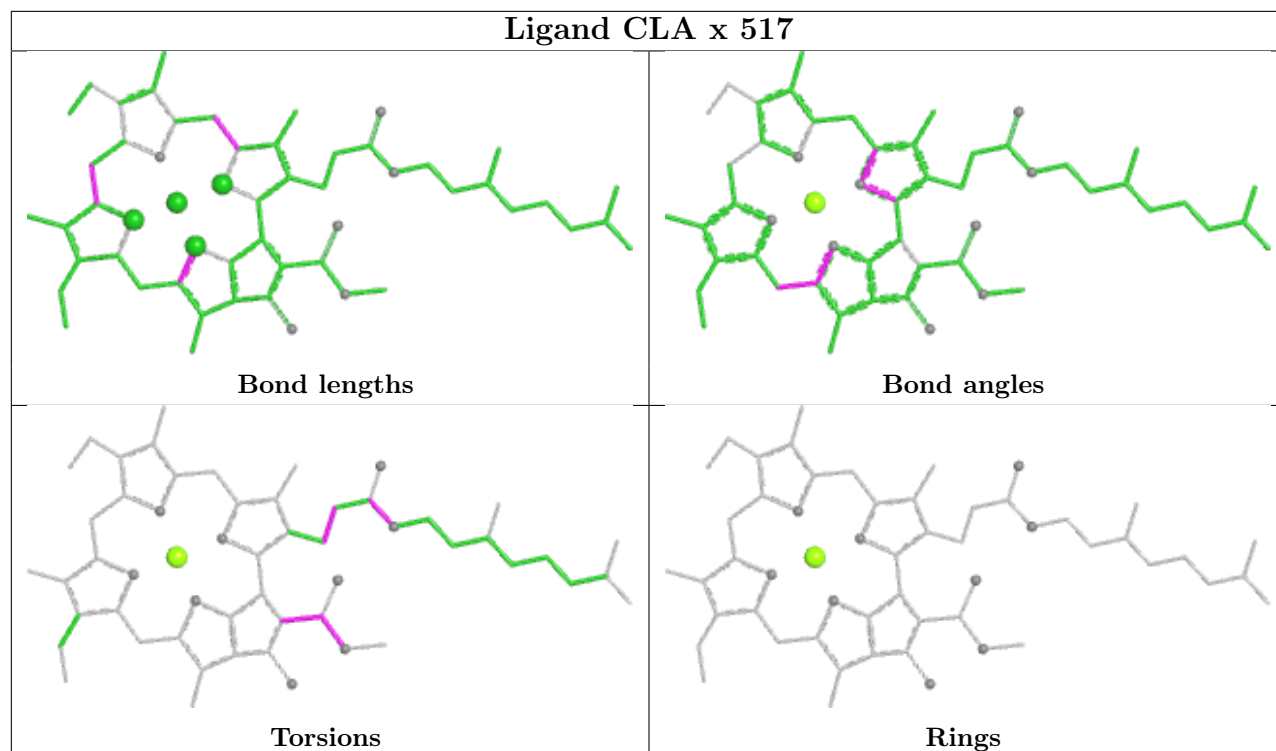
Ligand CLA G 1229



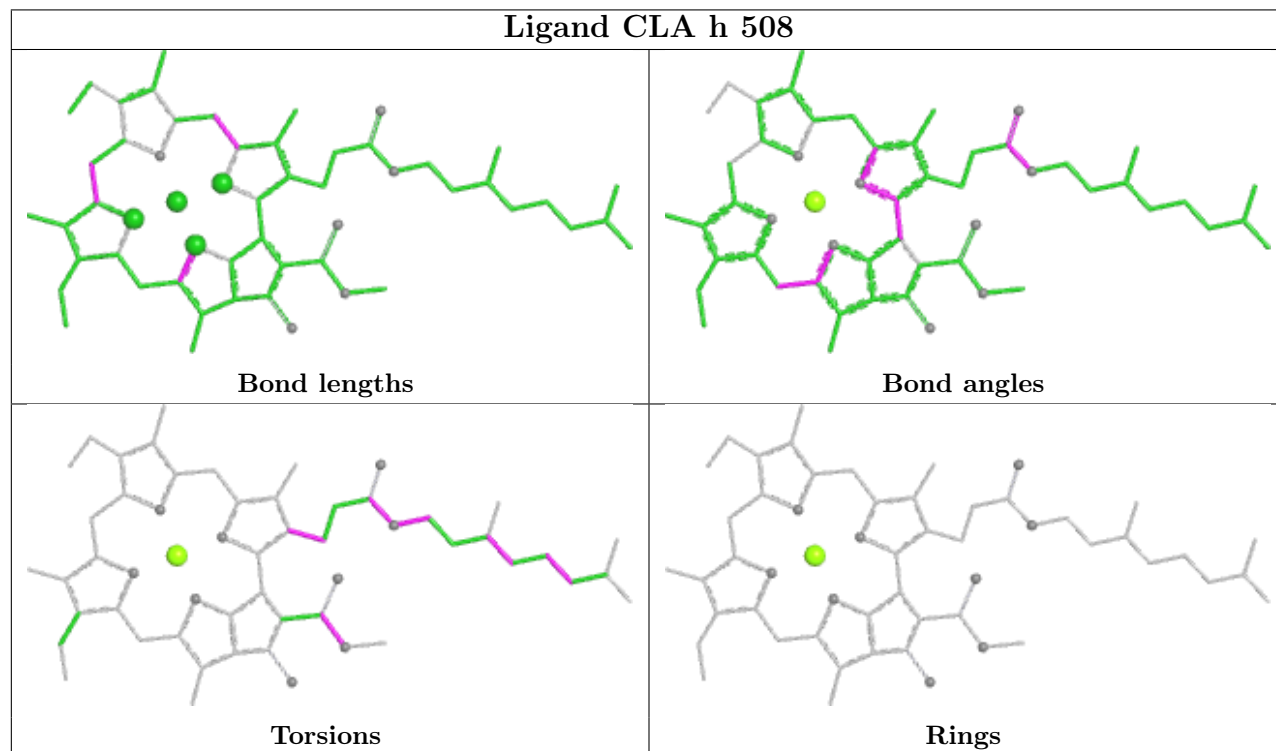
Ligand CLA G 1232



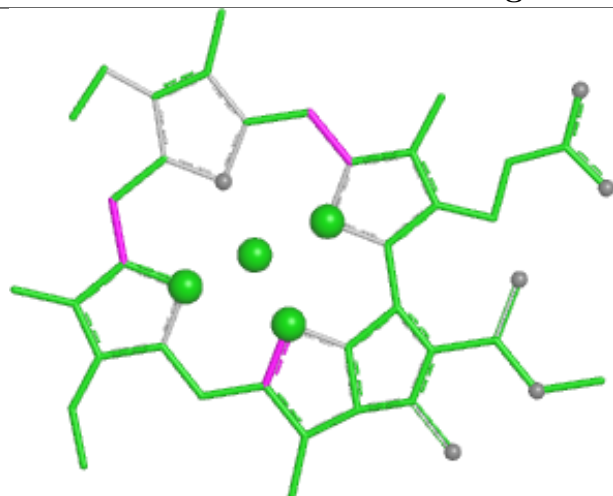
Ligand CLA x 517



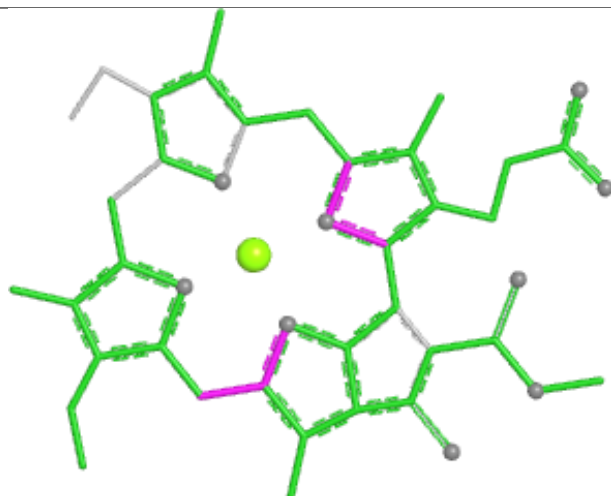
Ligand CLA h 508



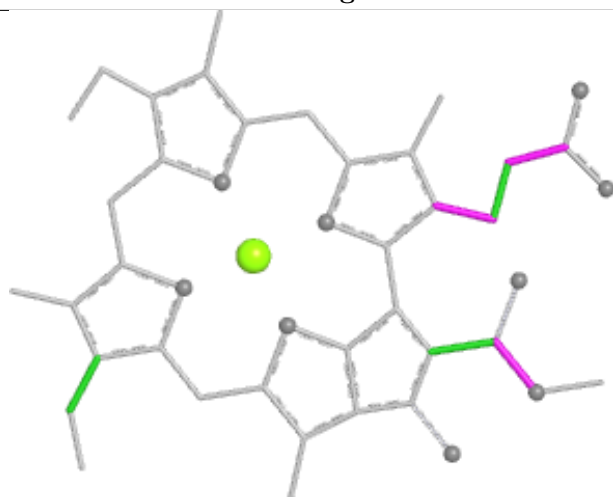
Ligand CLA B 1230



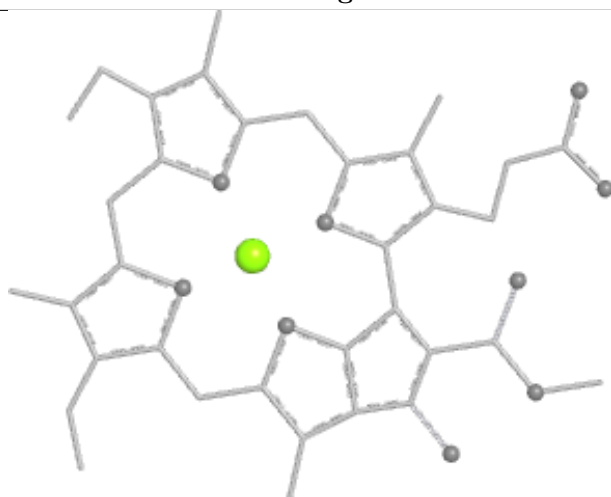
Bond lengths



Bond angles

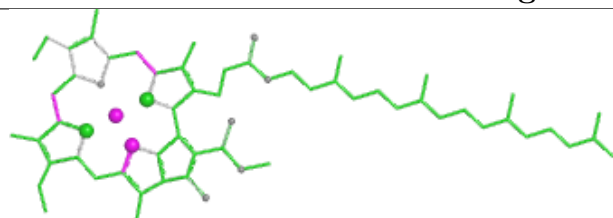


Torsions

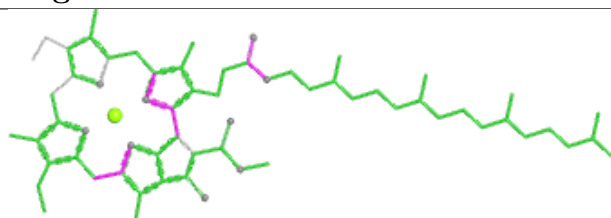


Rings

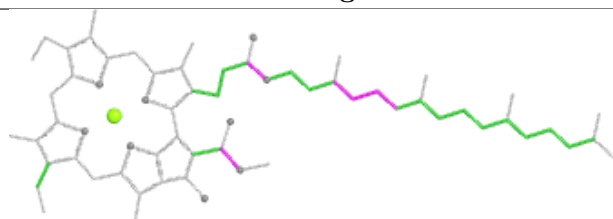
Ligand CLA g 512



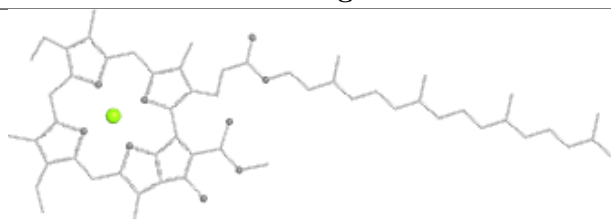
Bond lengths



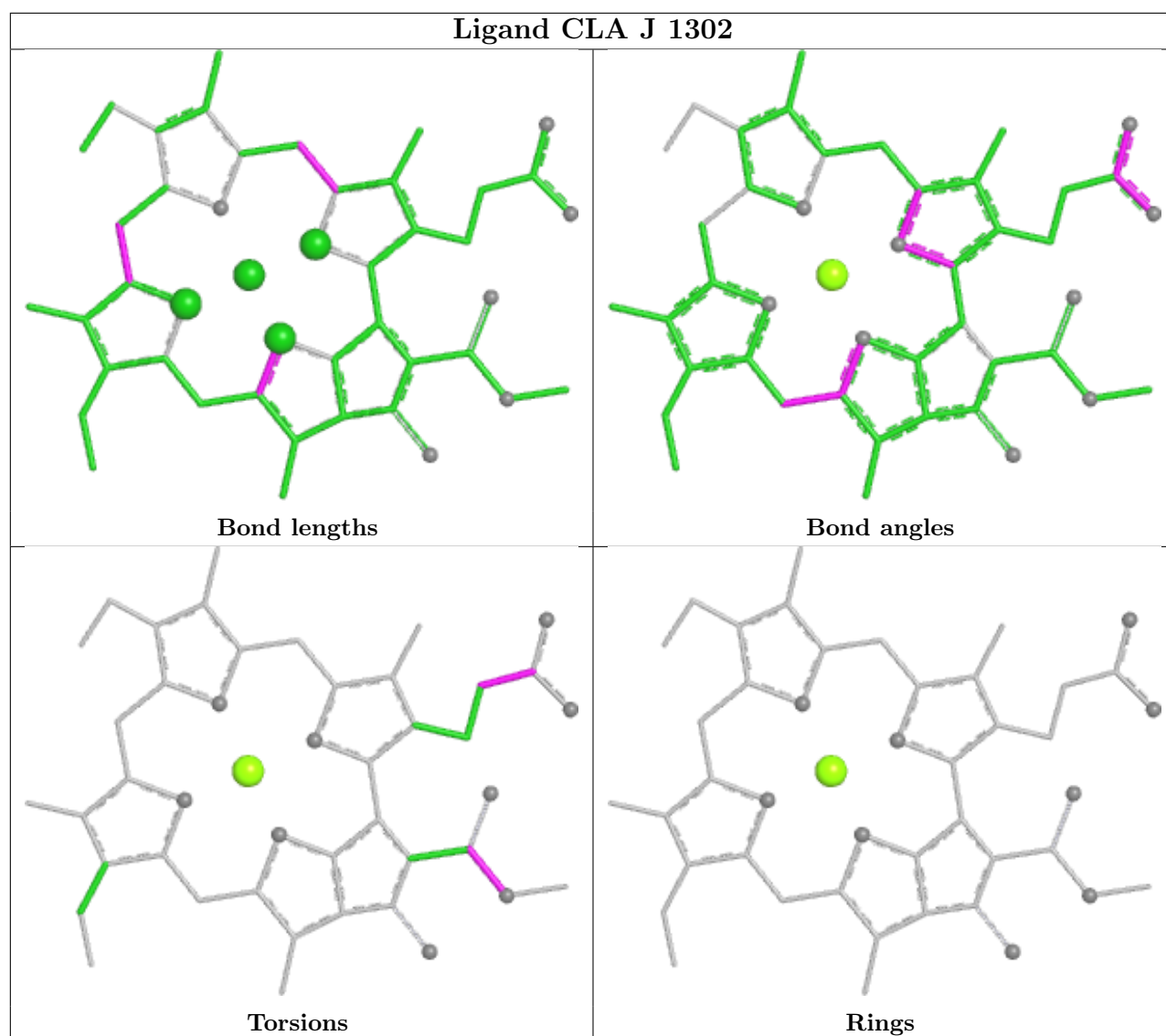
Bond angles



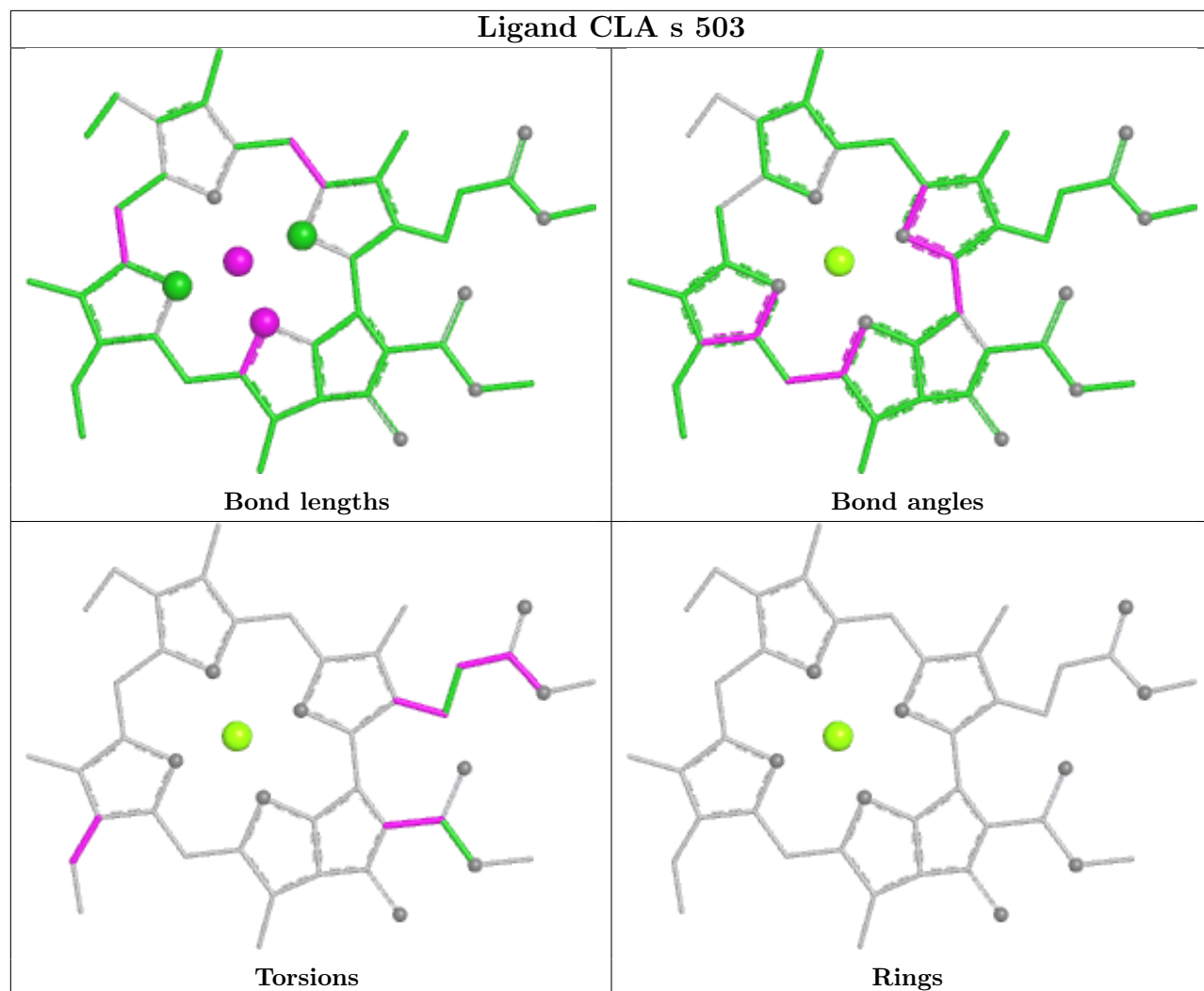
Torsions

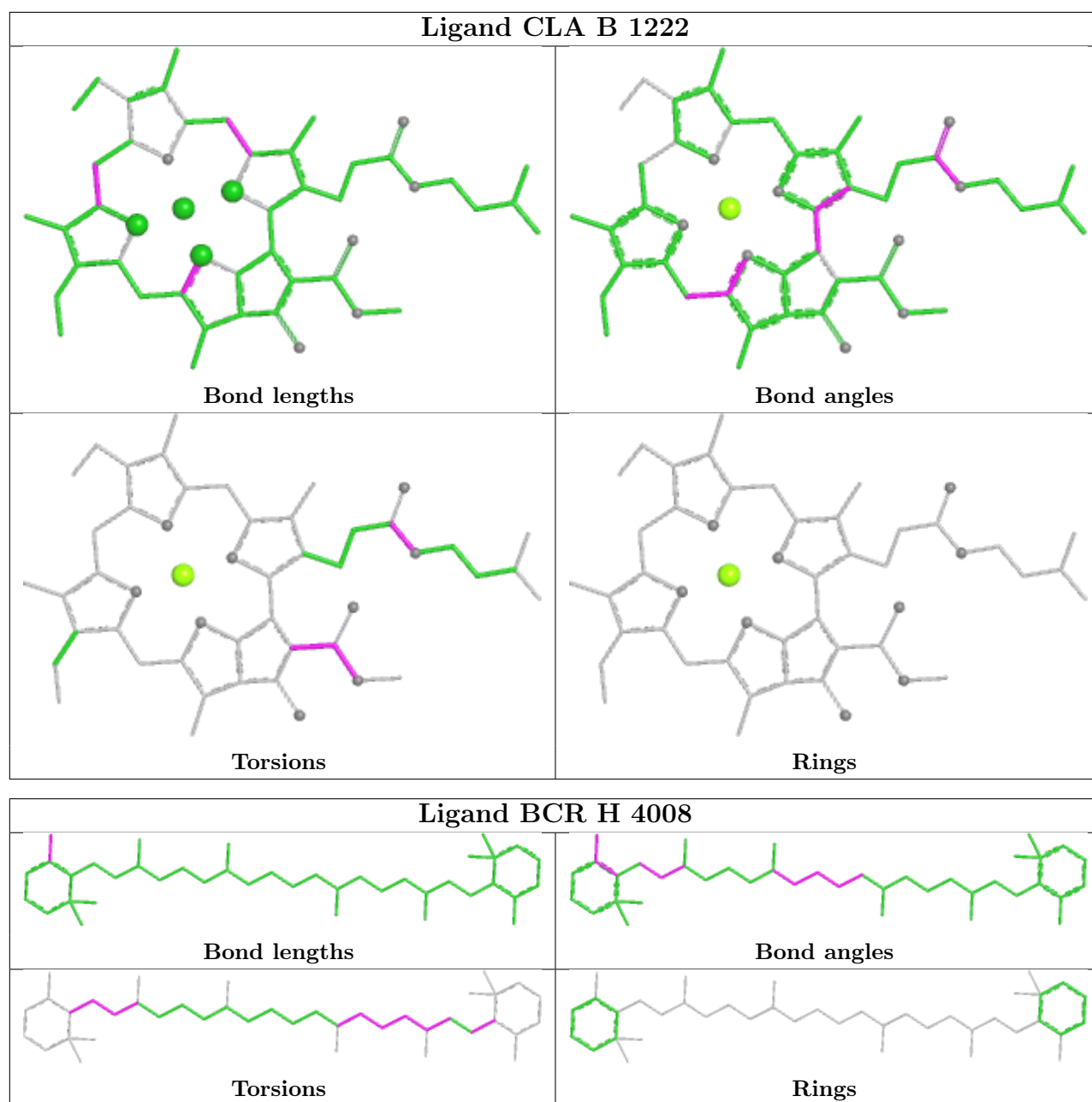


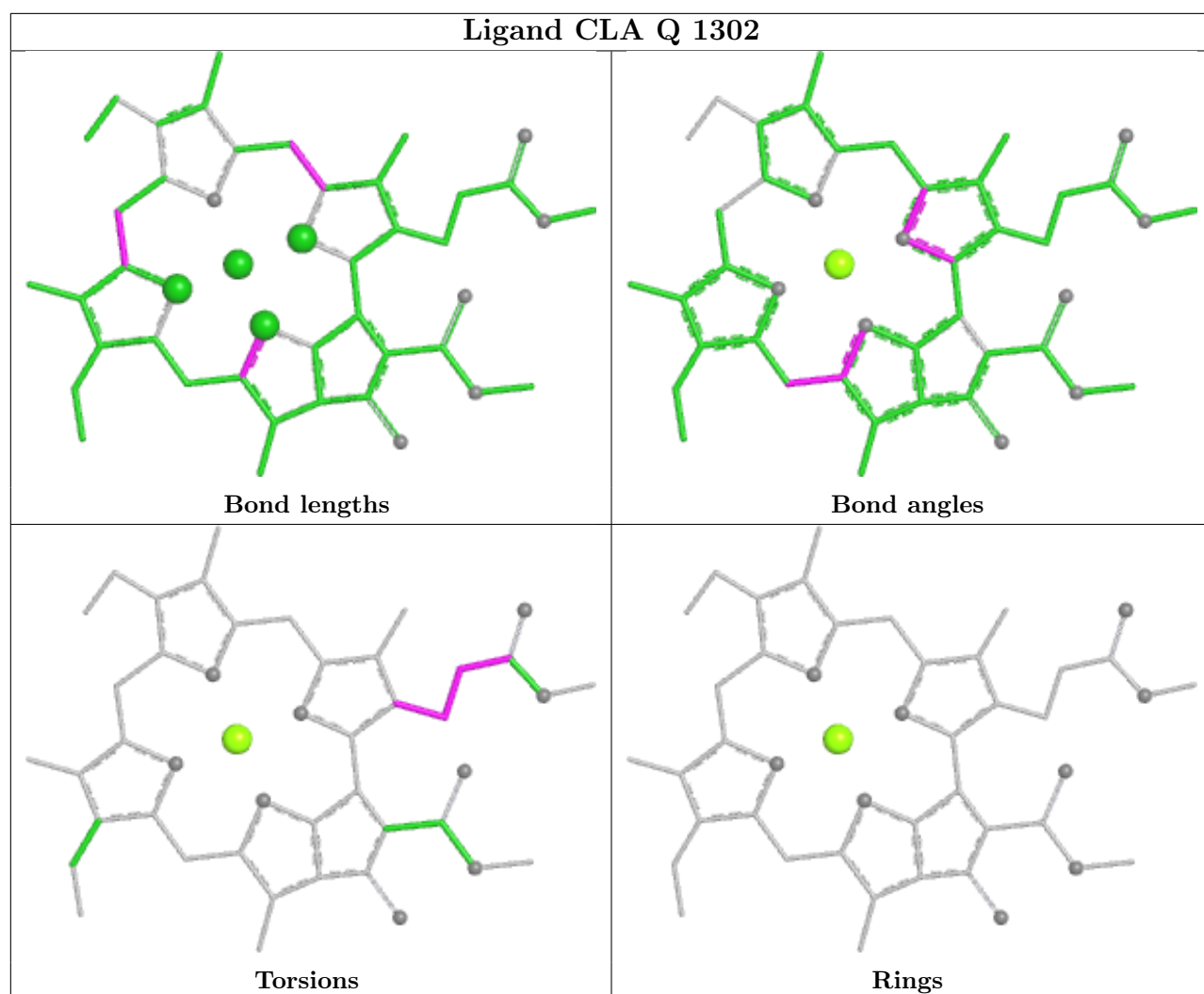
Rings



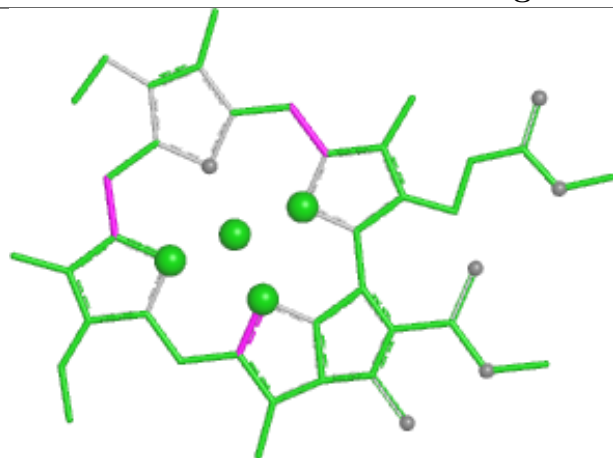
Ligand CLA s 503



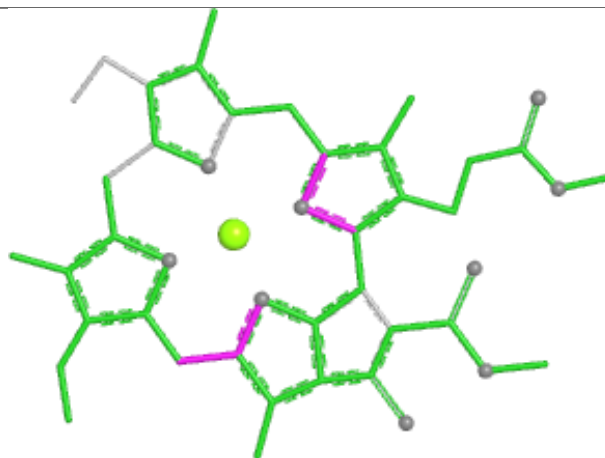




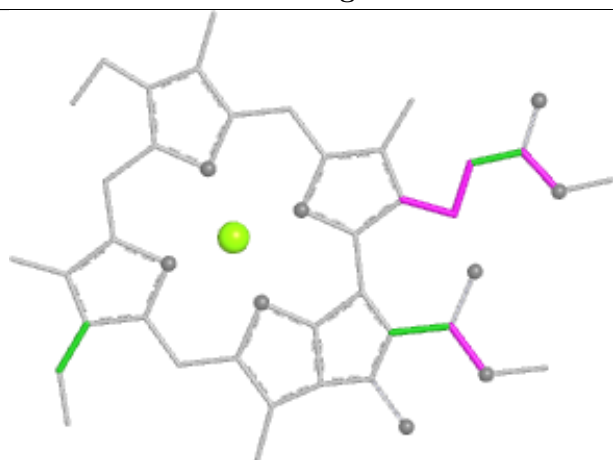
Ligand CLA X 513



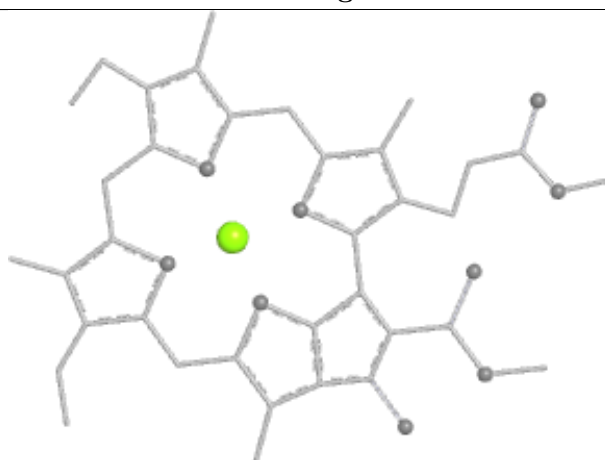
Bond lengths



Bond angles

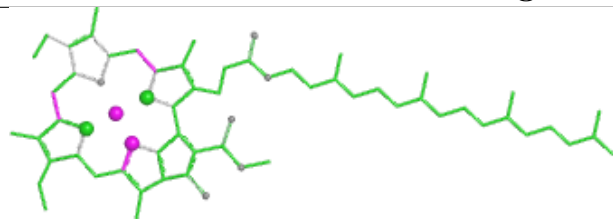


Torsions

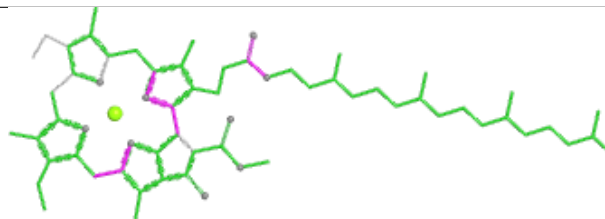


Rings

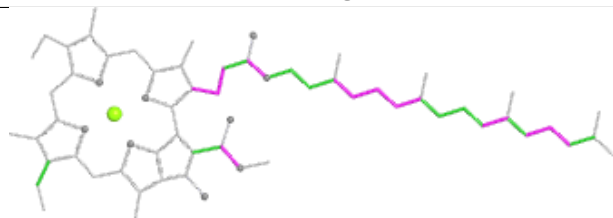
Ligand CLA h 512



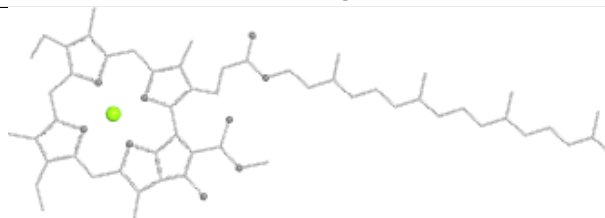
Bond lengths



Bond angles

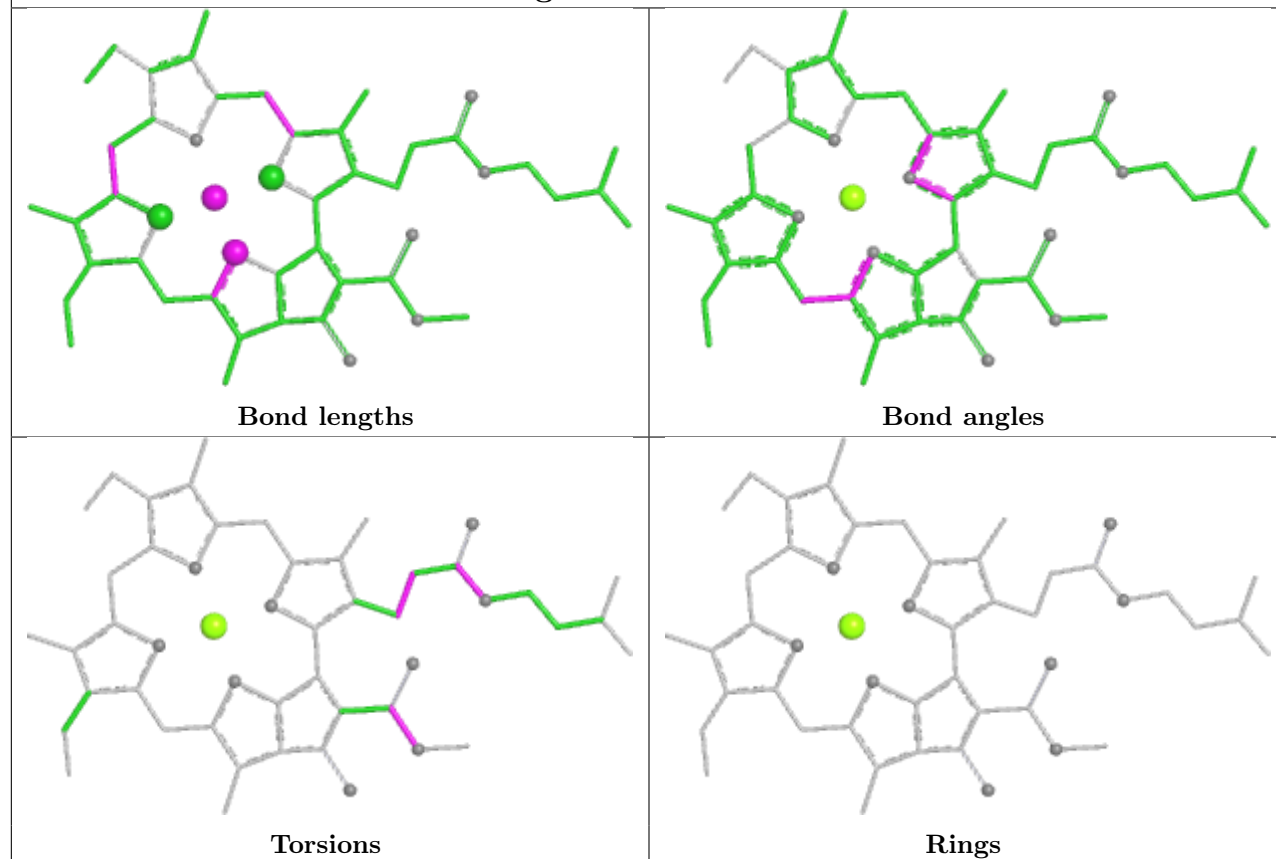


Torsions

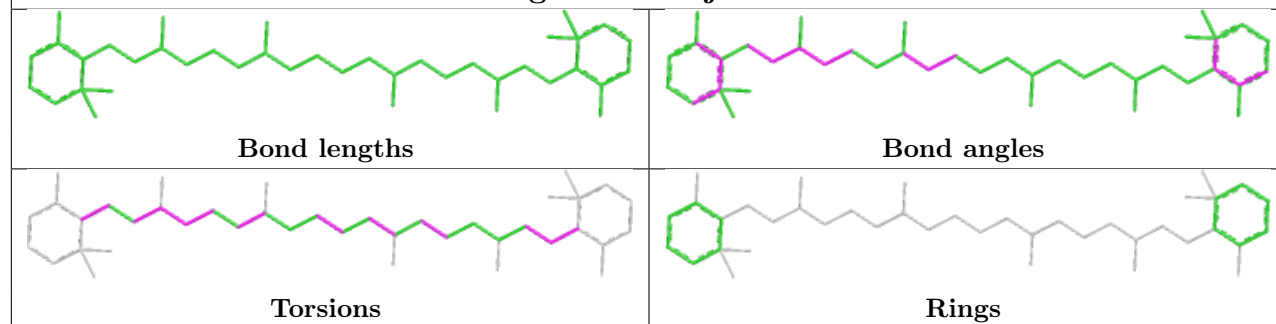


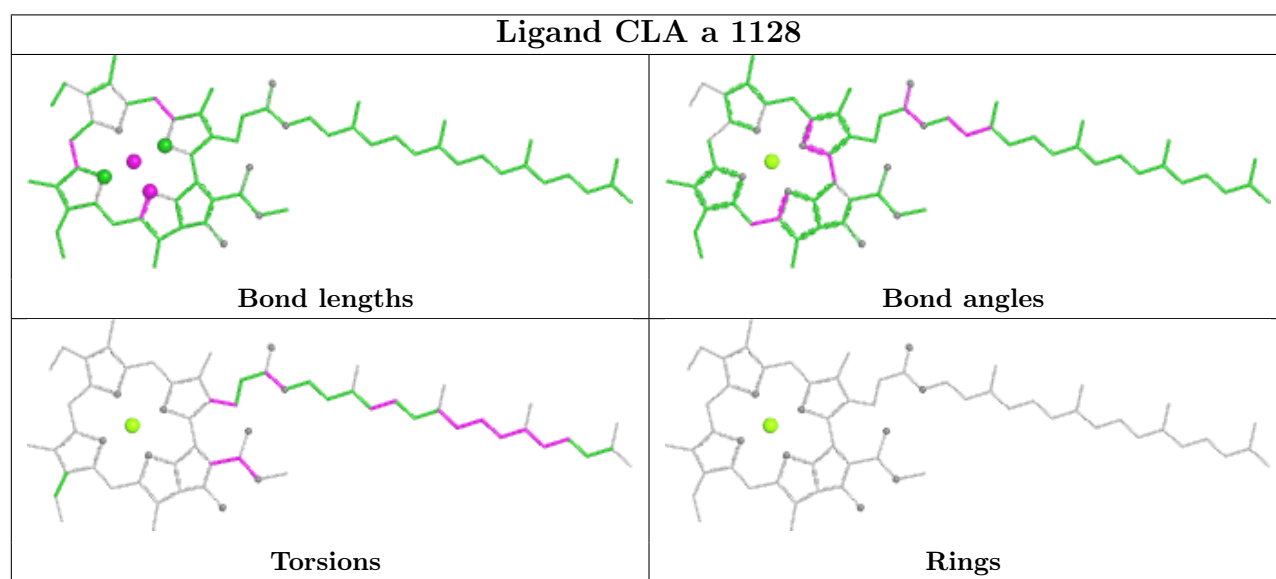
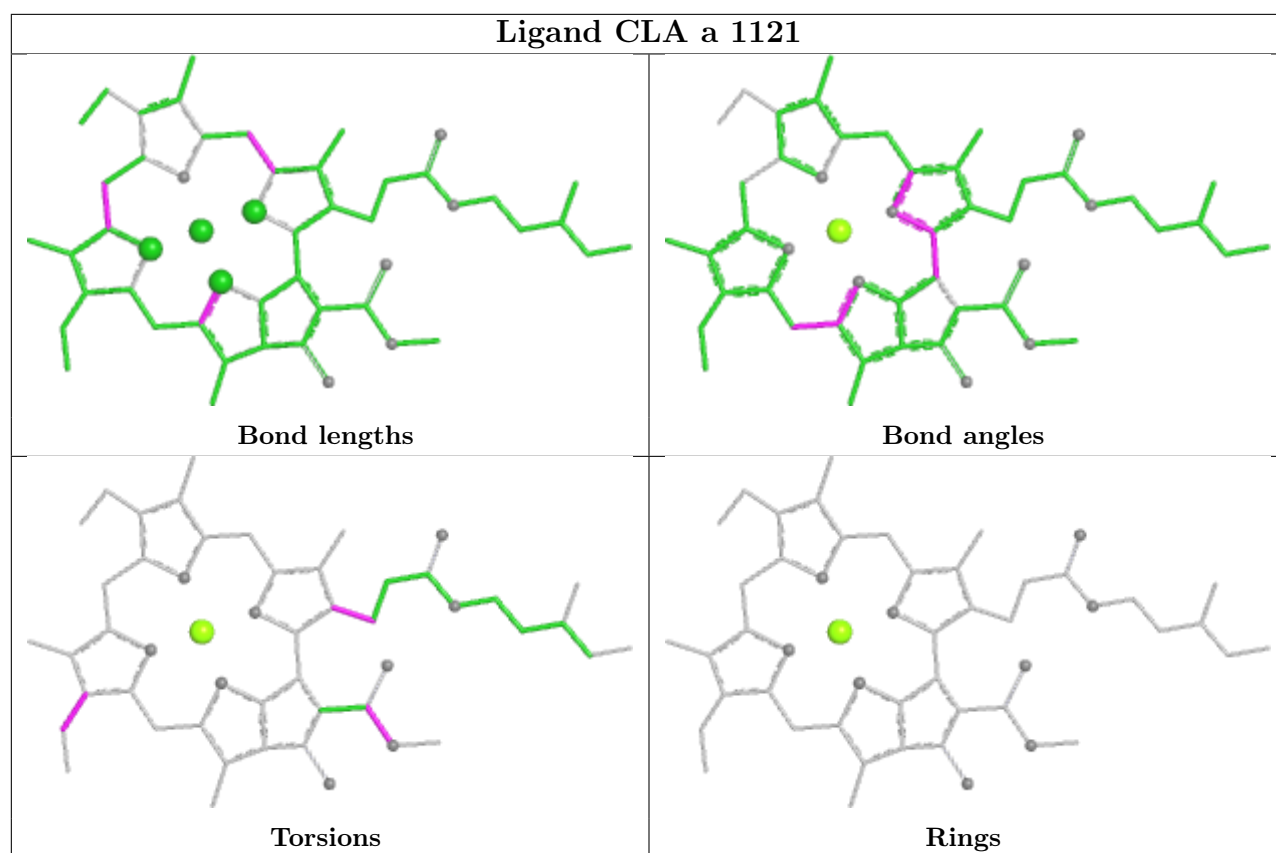
Rings

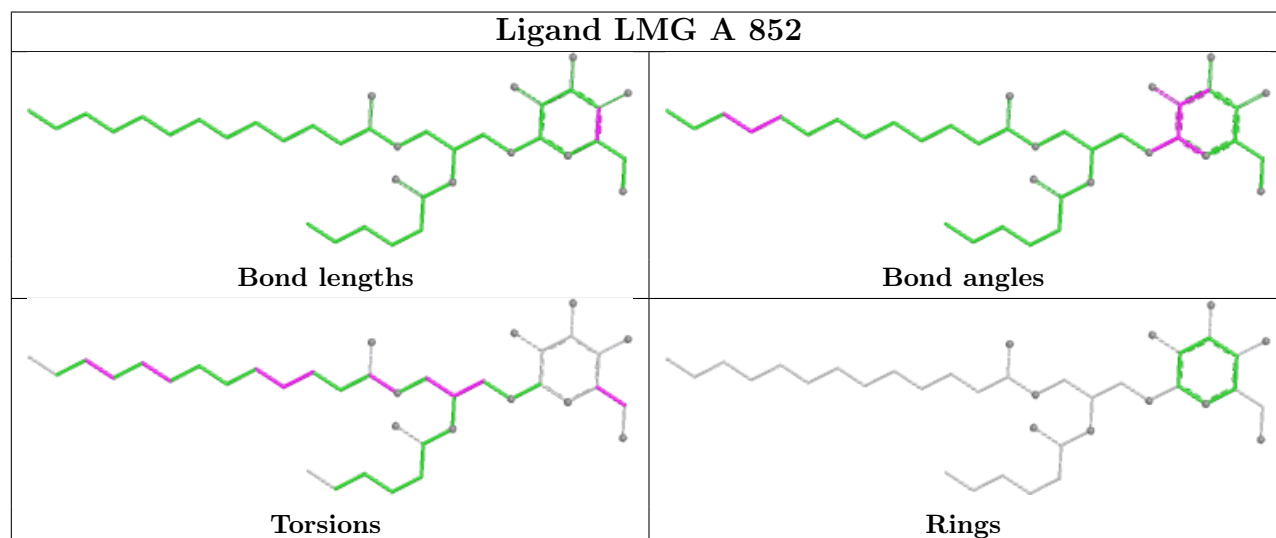
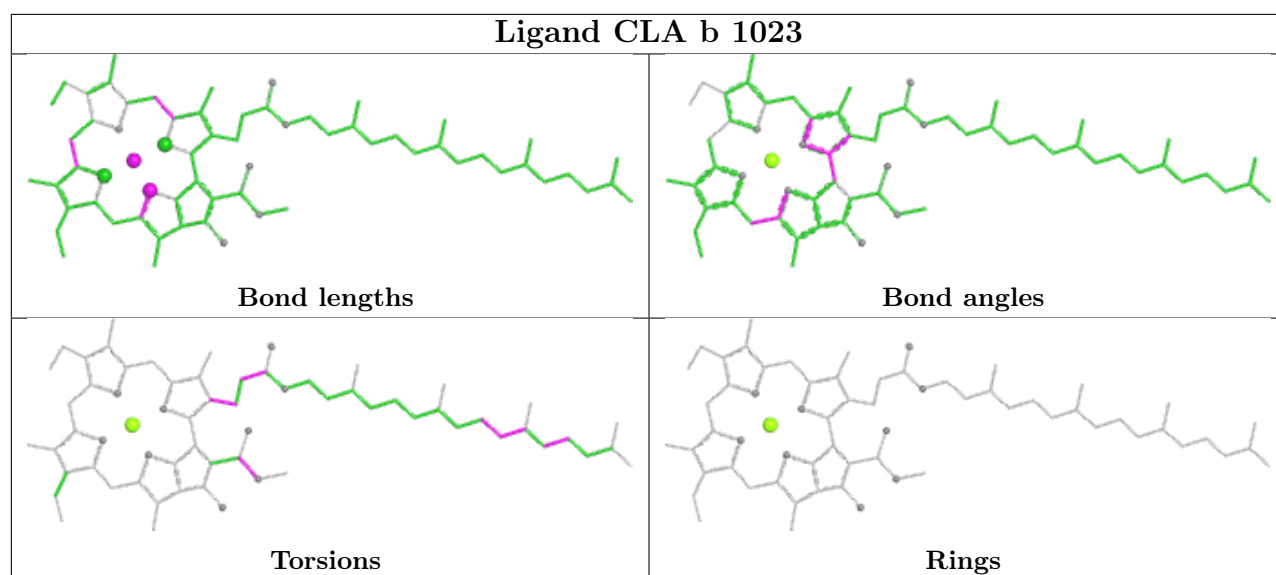
Ligand CLA n 502

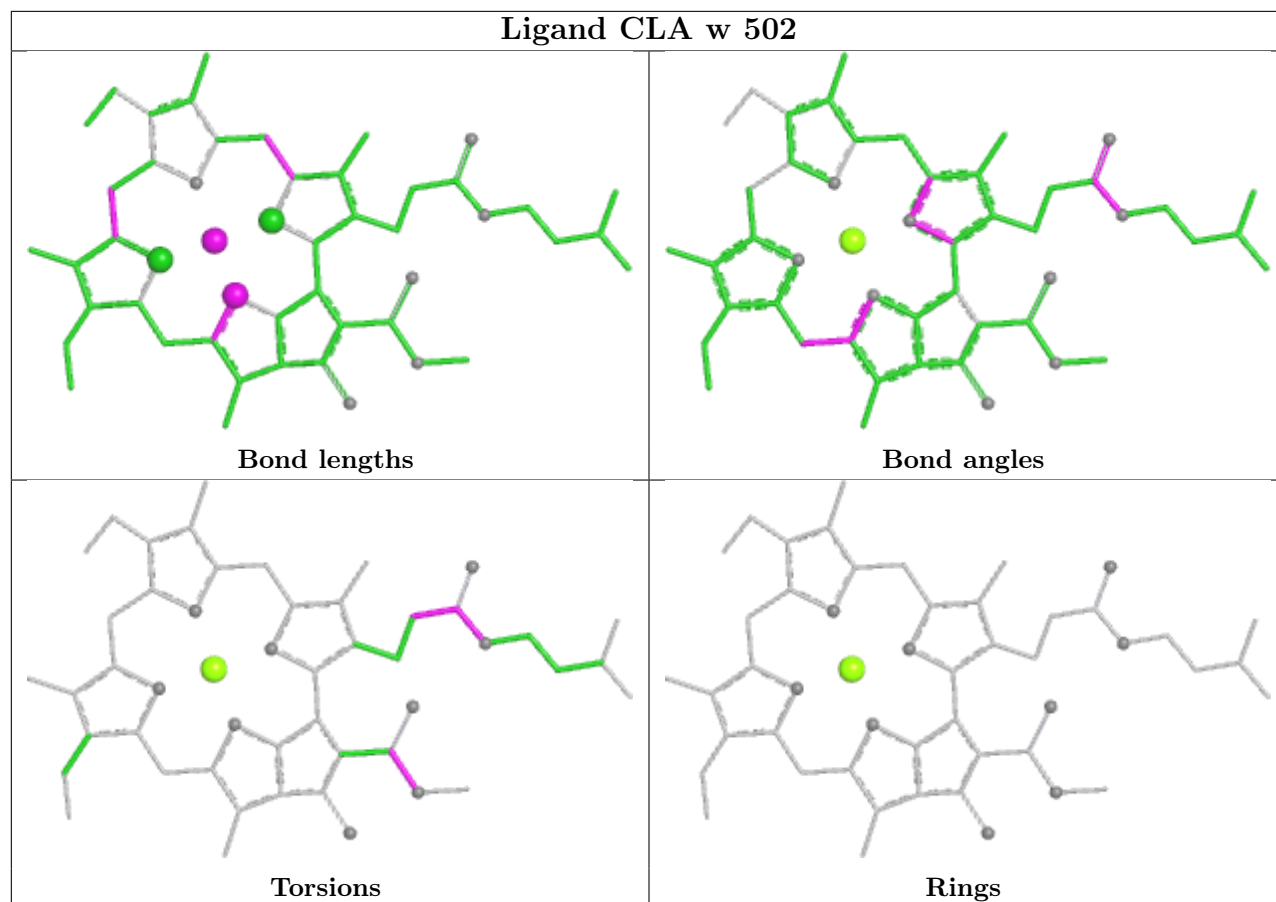


Ligand BCR j 4015

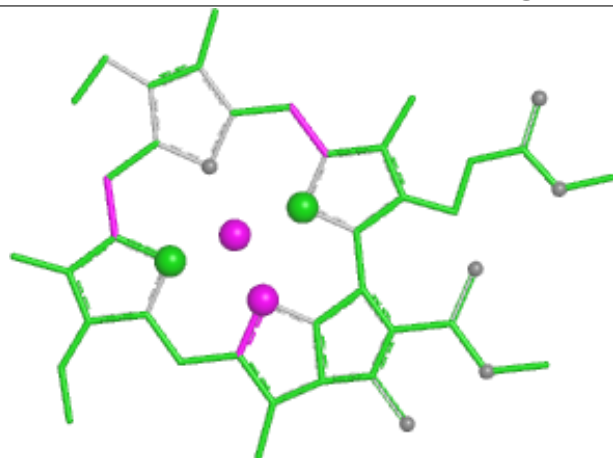




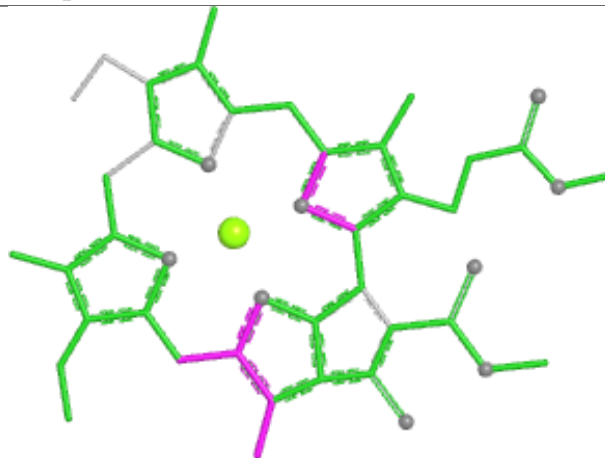




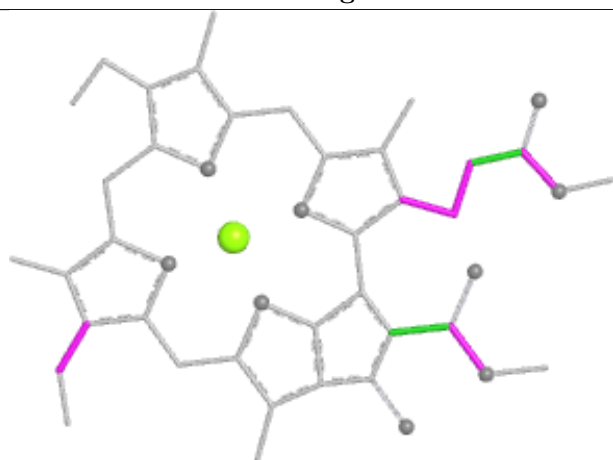
Ligand CLA q 503



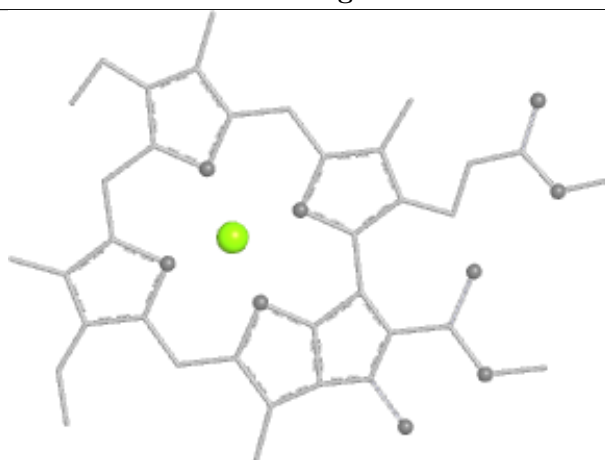
Bond lengths



Bond angles

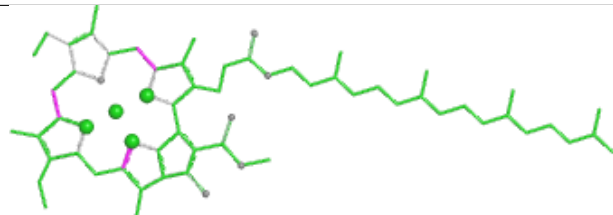


Torsions

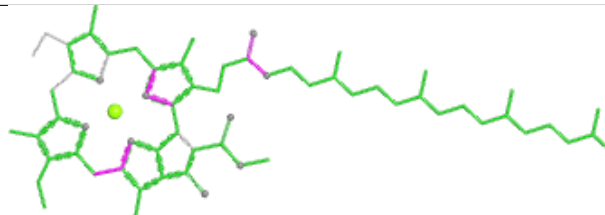


Rings

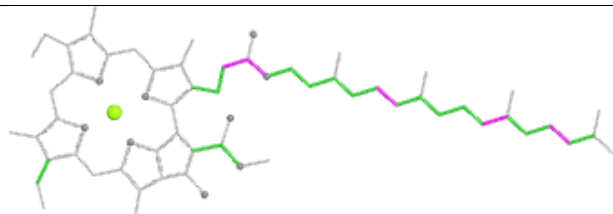
Ligand CLA s 510



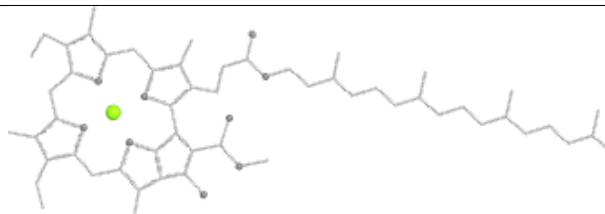
Bond lengths



Bond angles

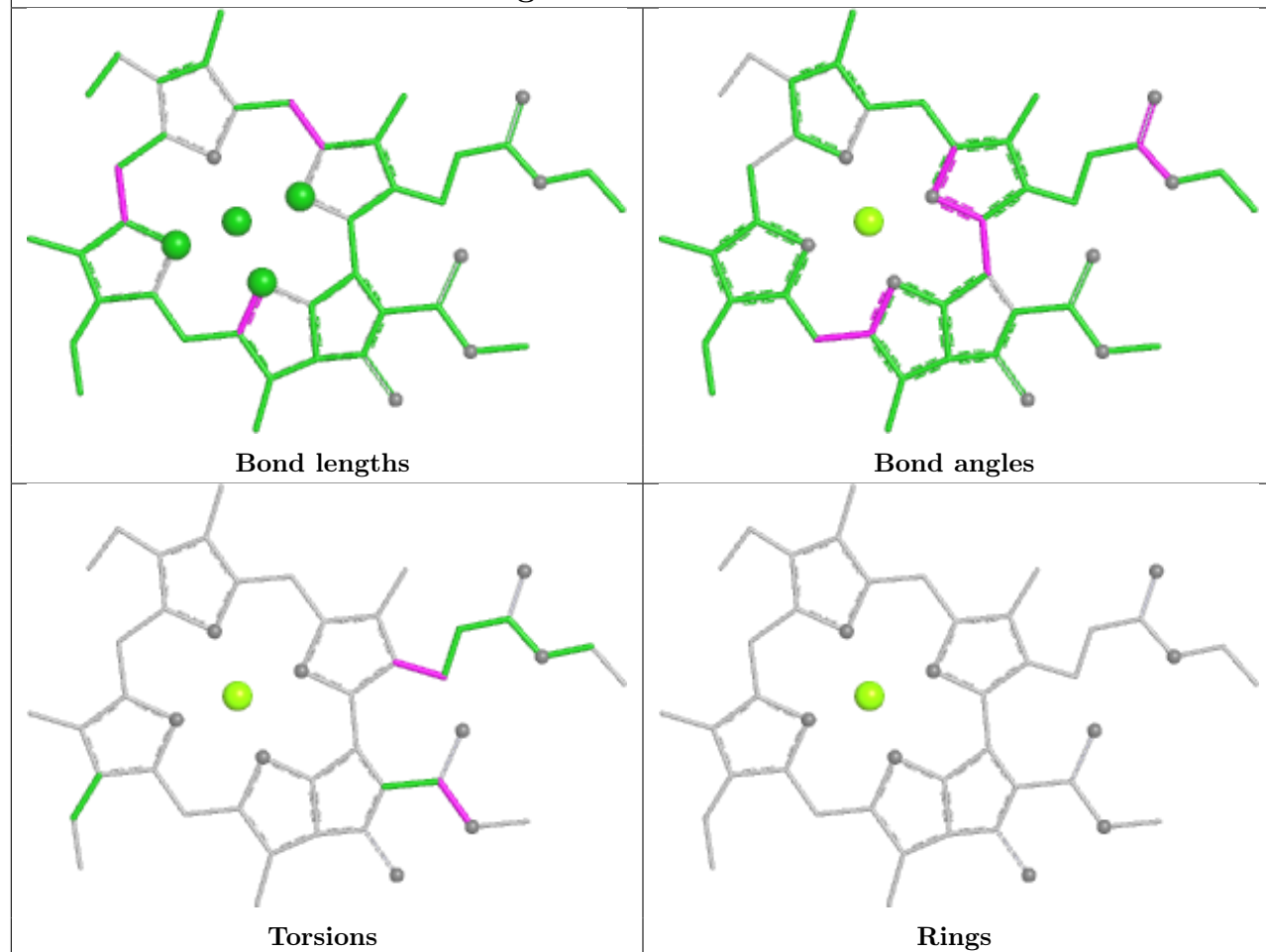


Torsions

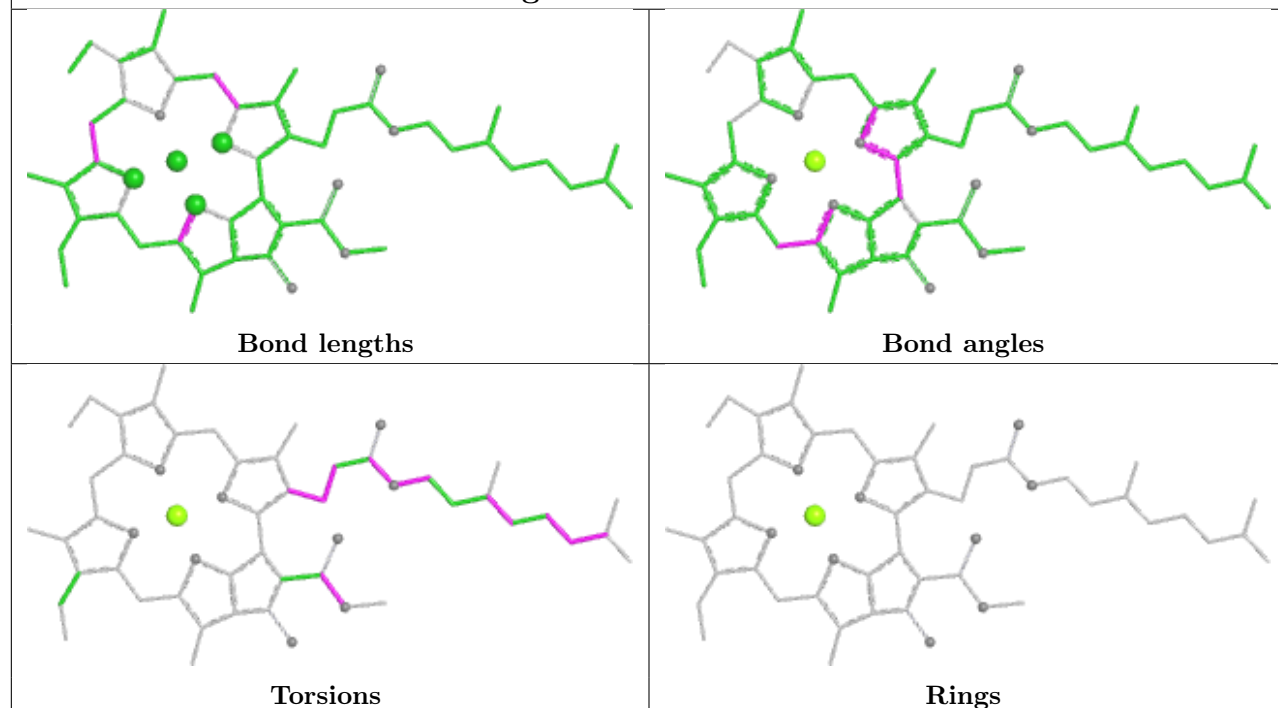


Rings

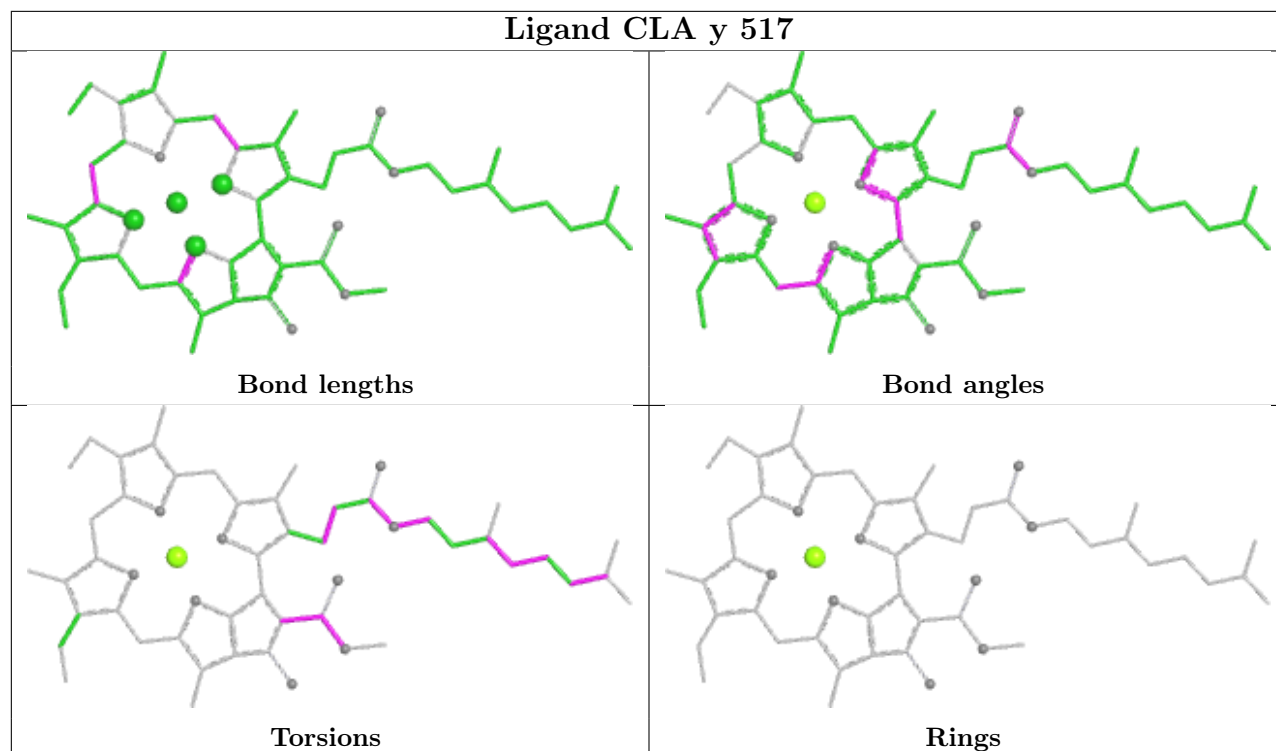
Ligand CLA H 1137



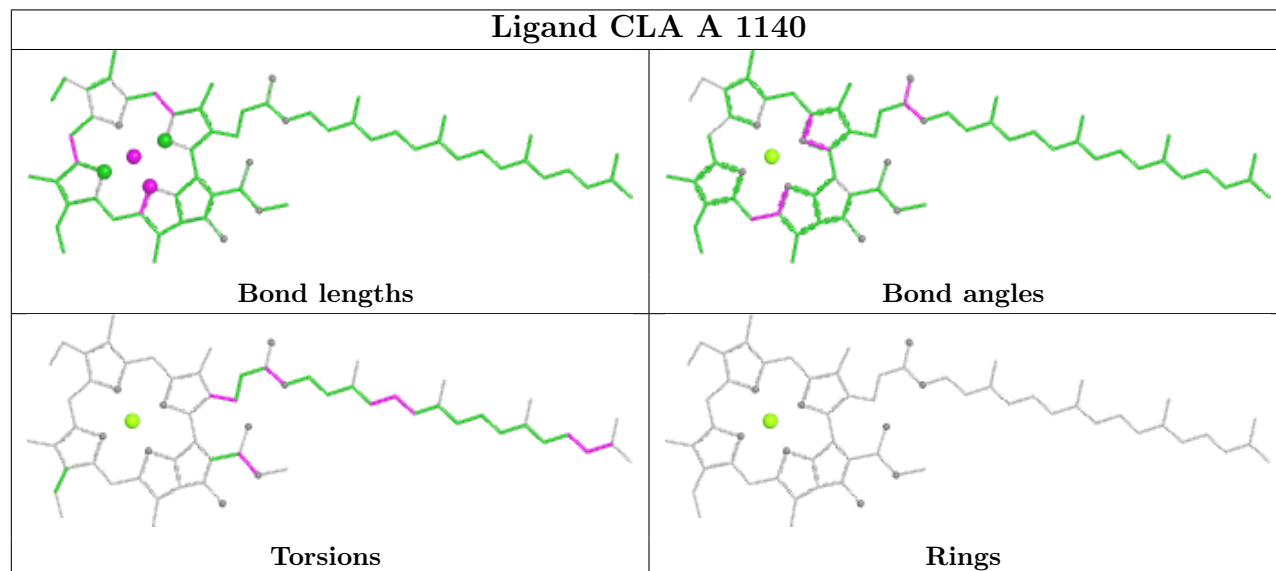
Ligand CLA G 1228

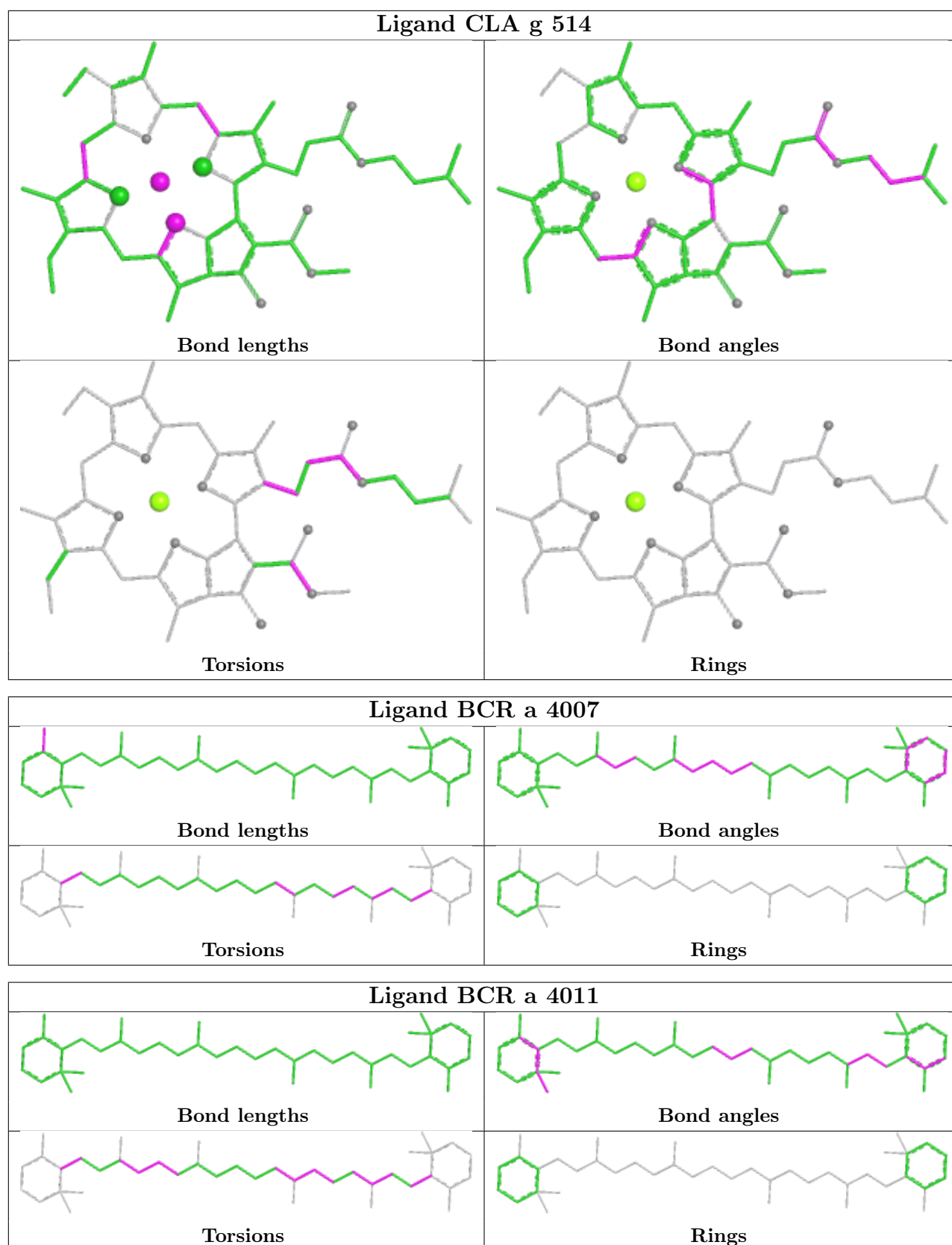


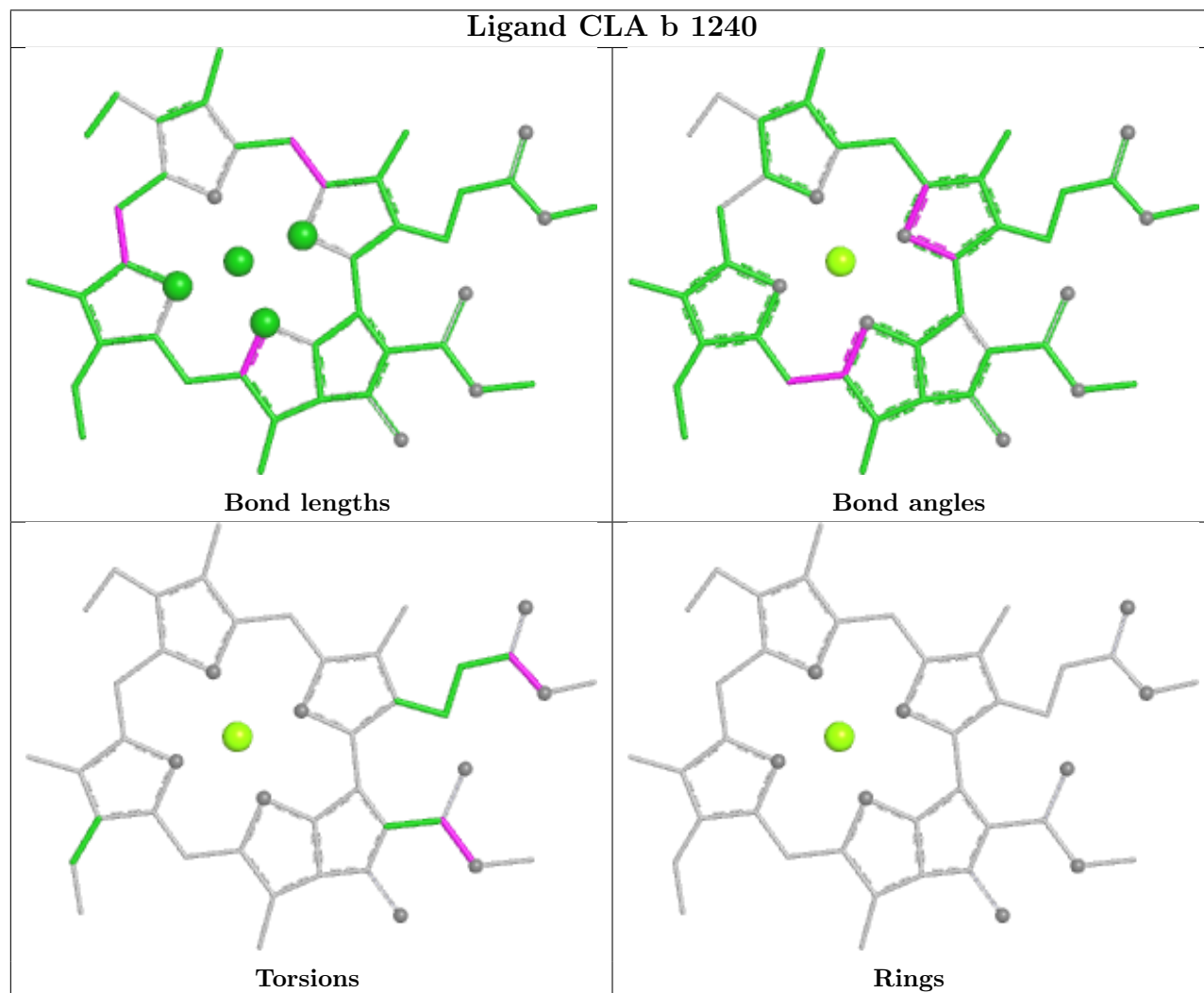
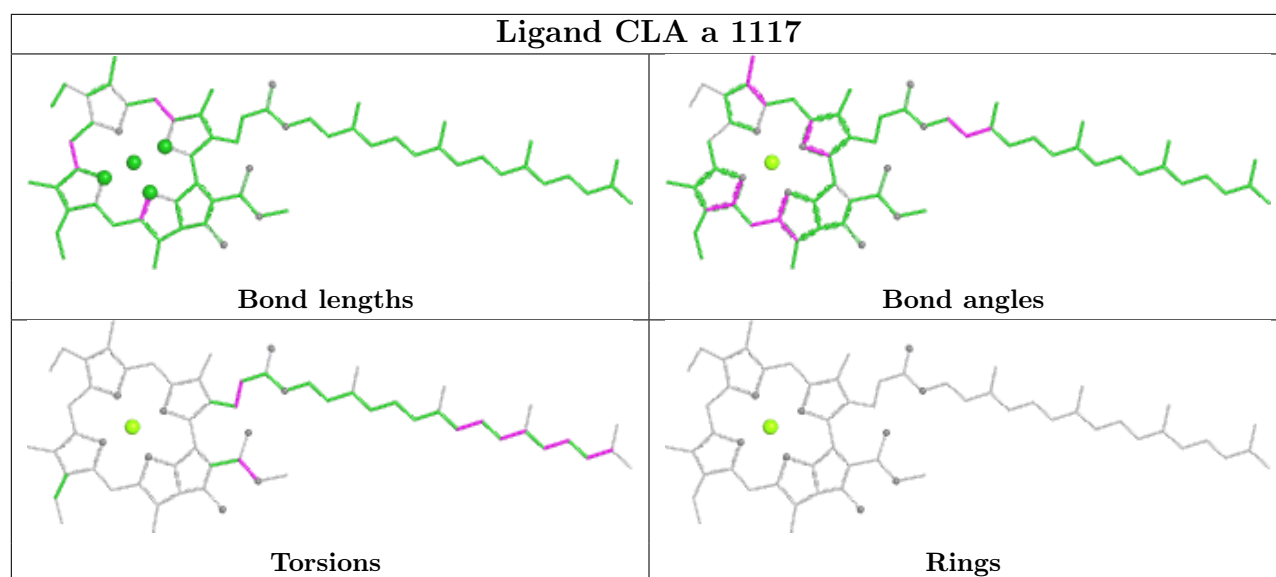
Ligand CLA y 517

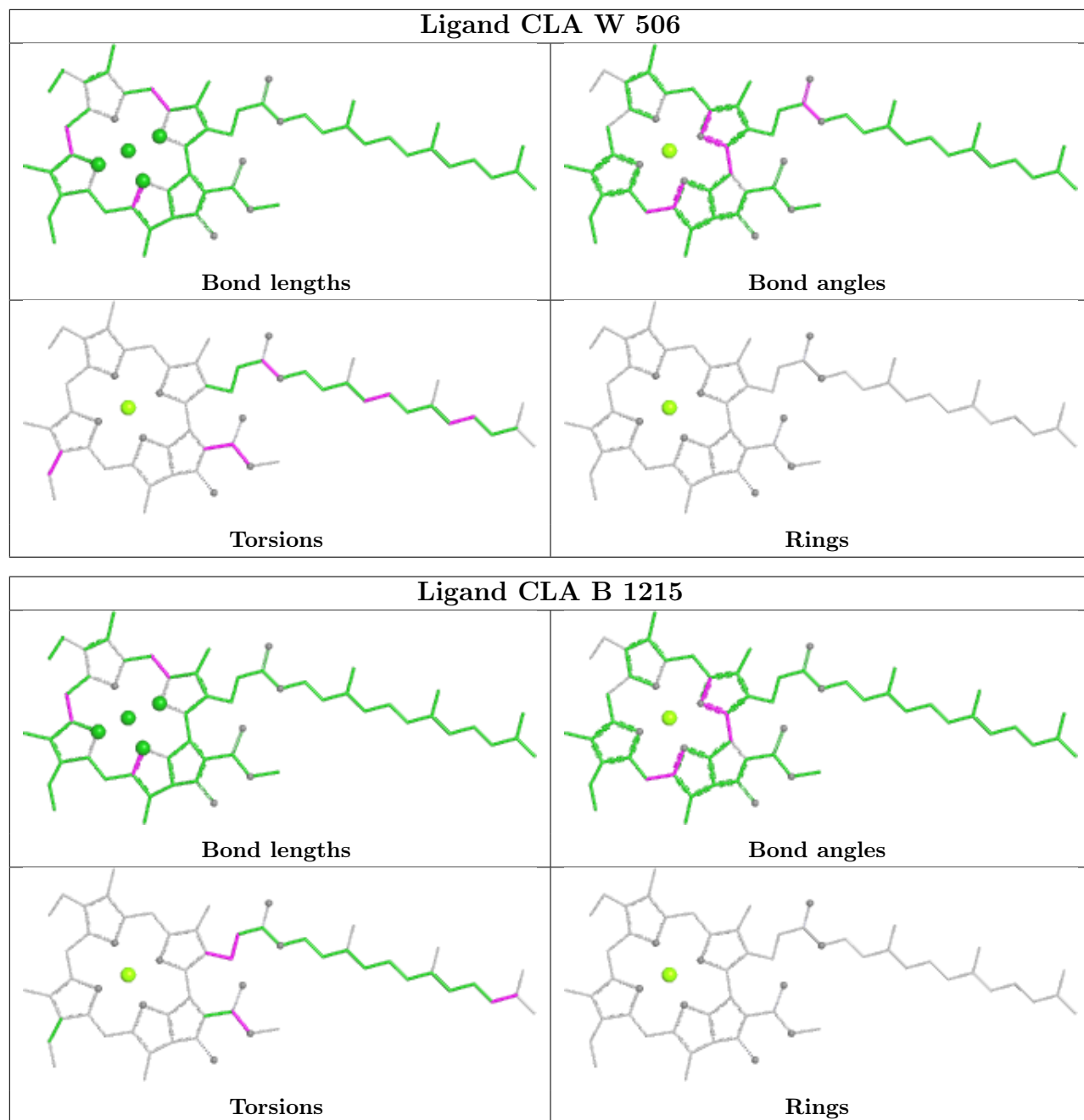


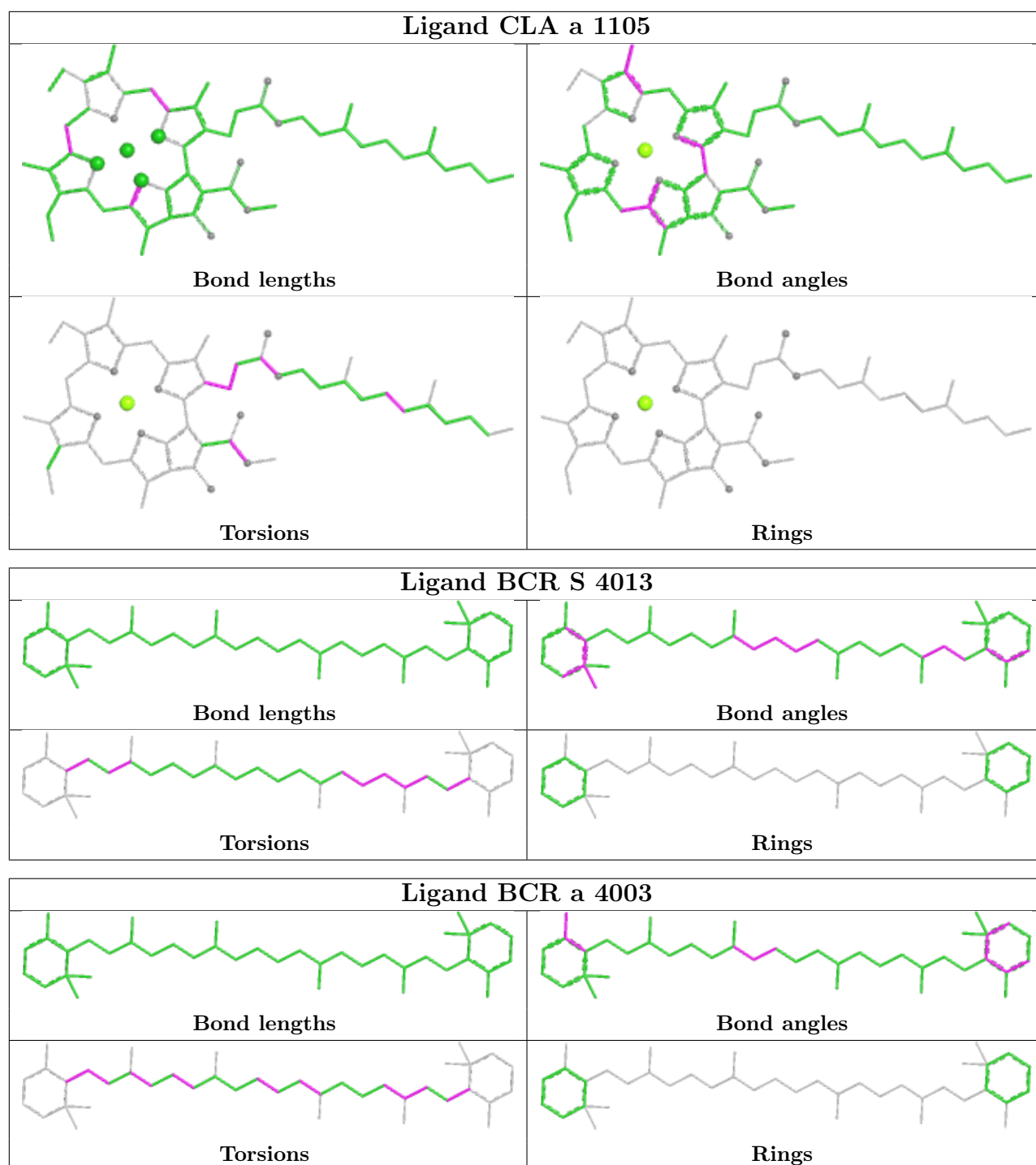
Ligand CLA A 1140



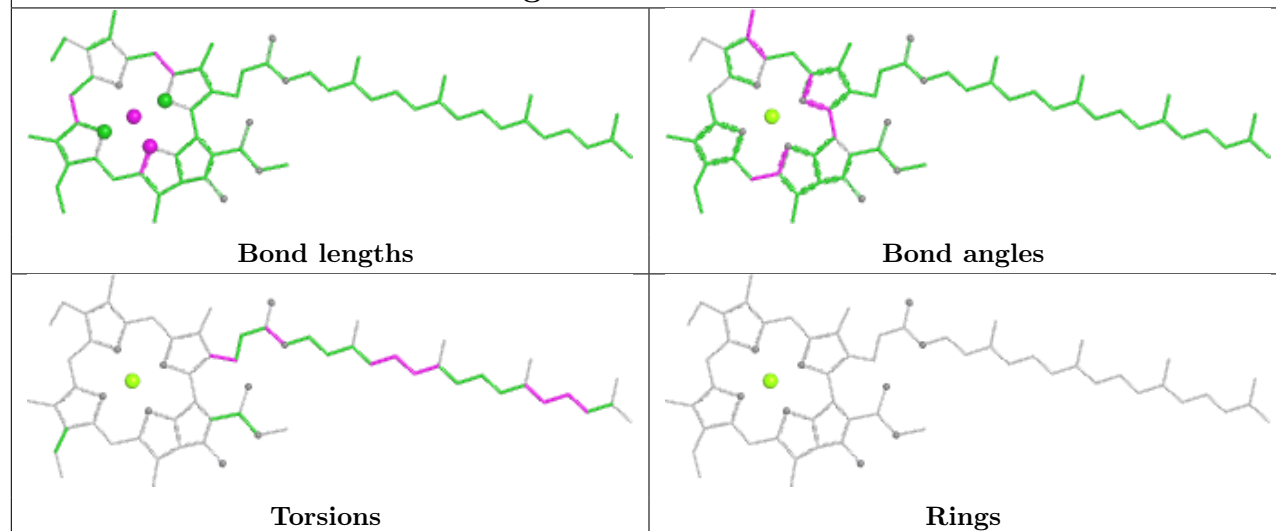




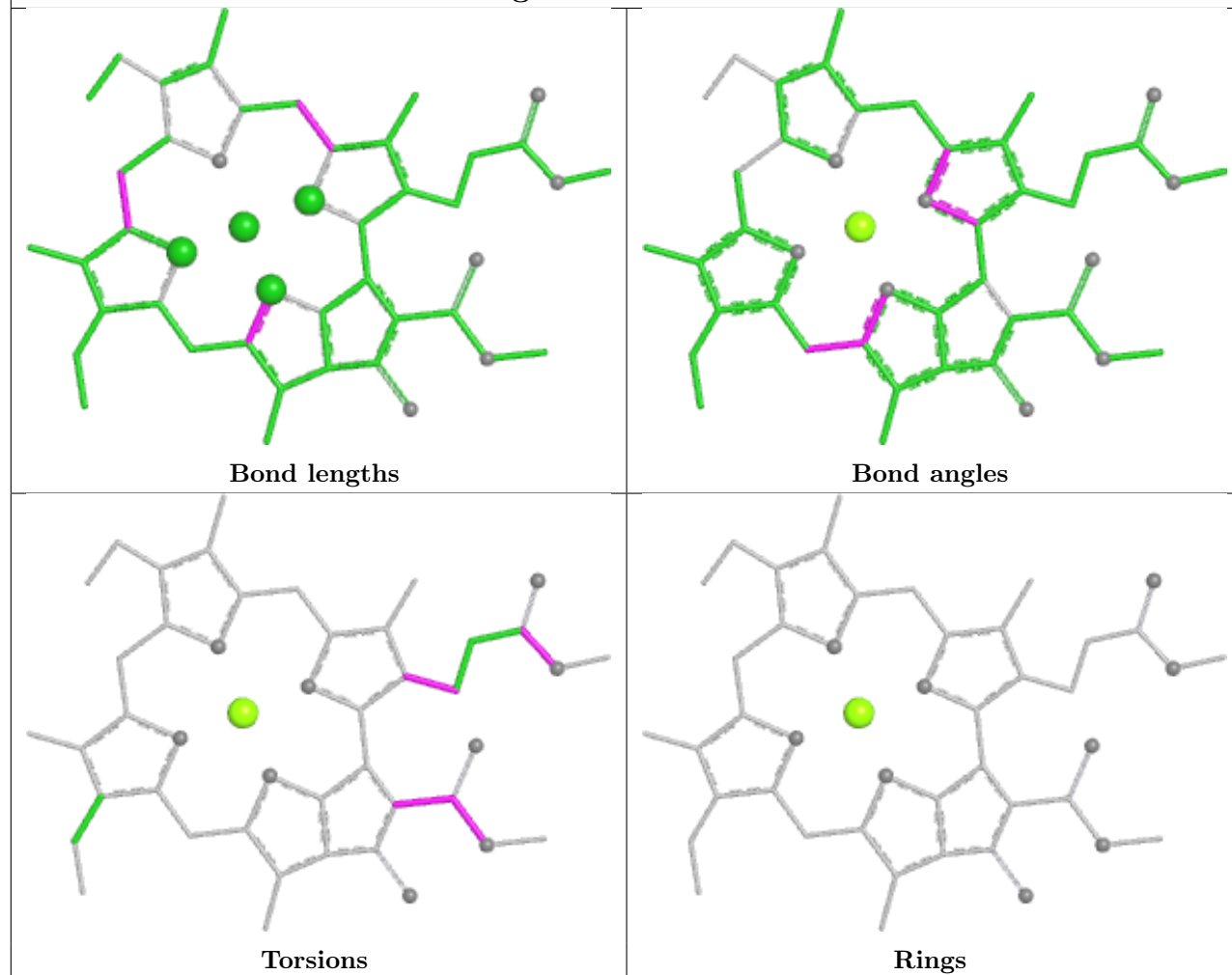


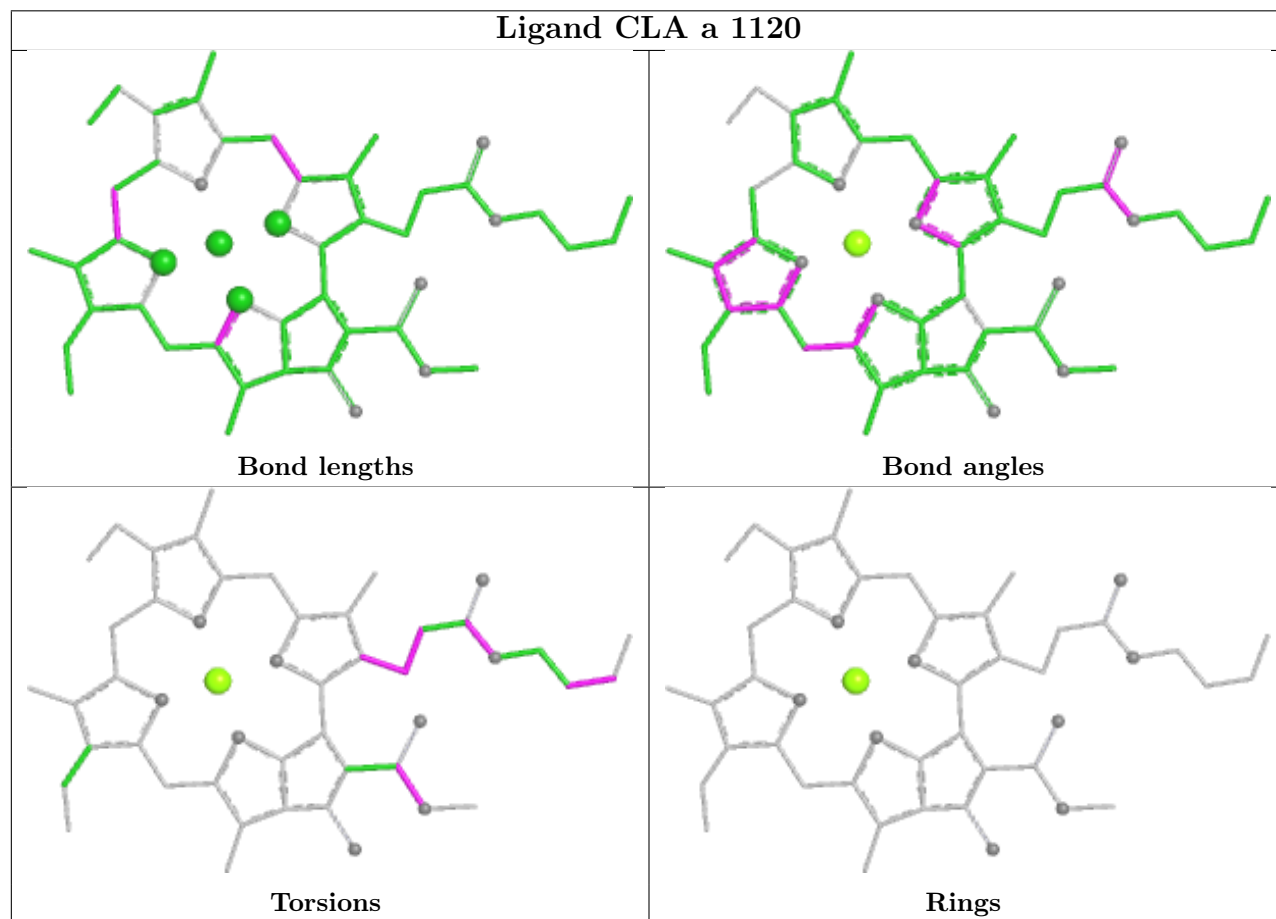
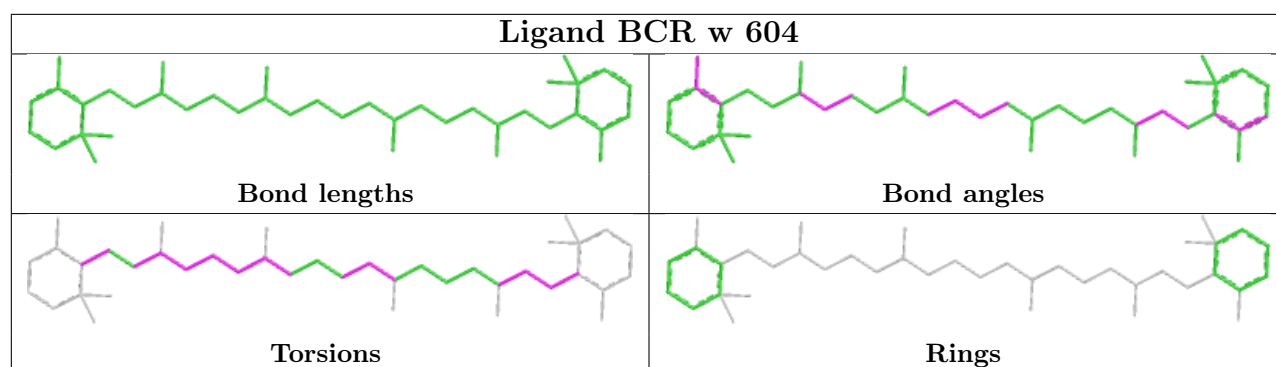


Ligand CLA B 1225

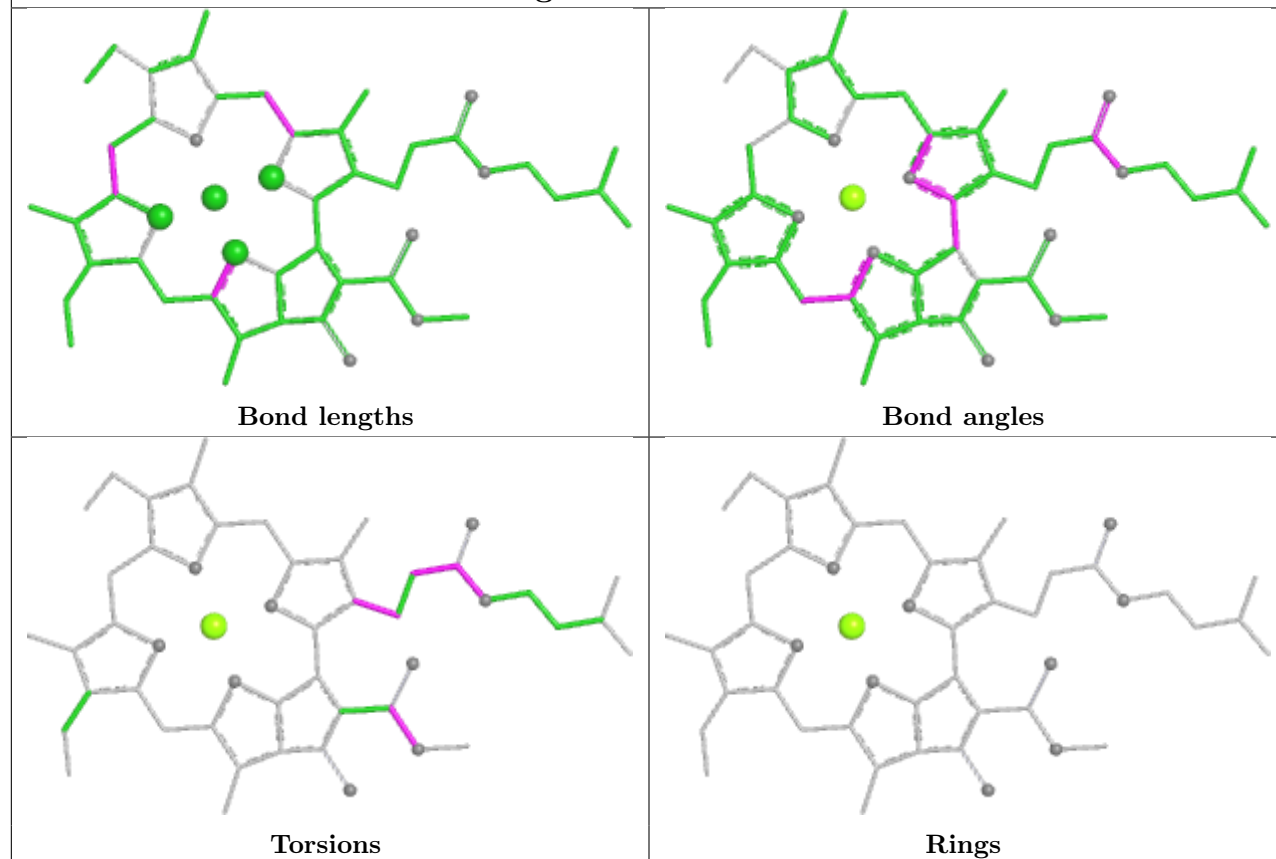


Ligand CLA f 1302

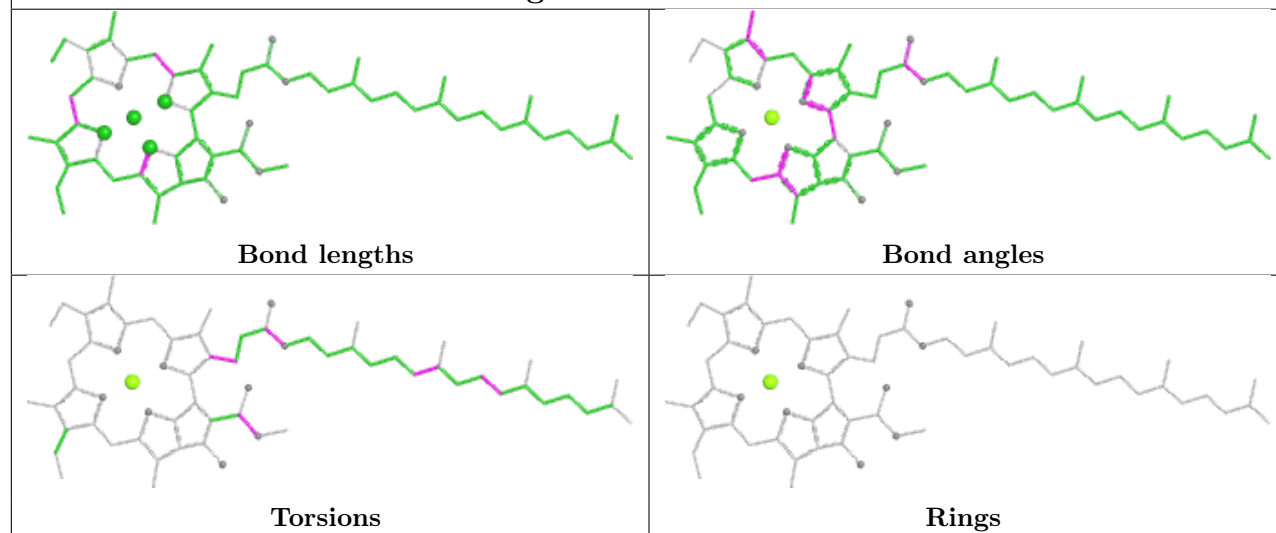


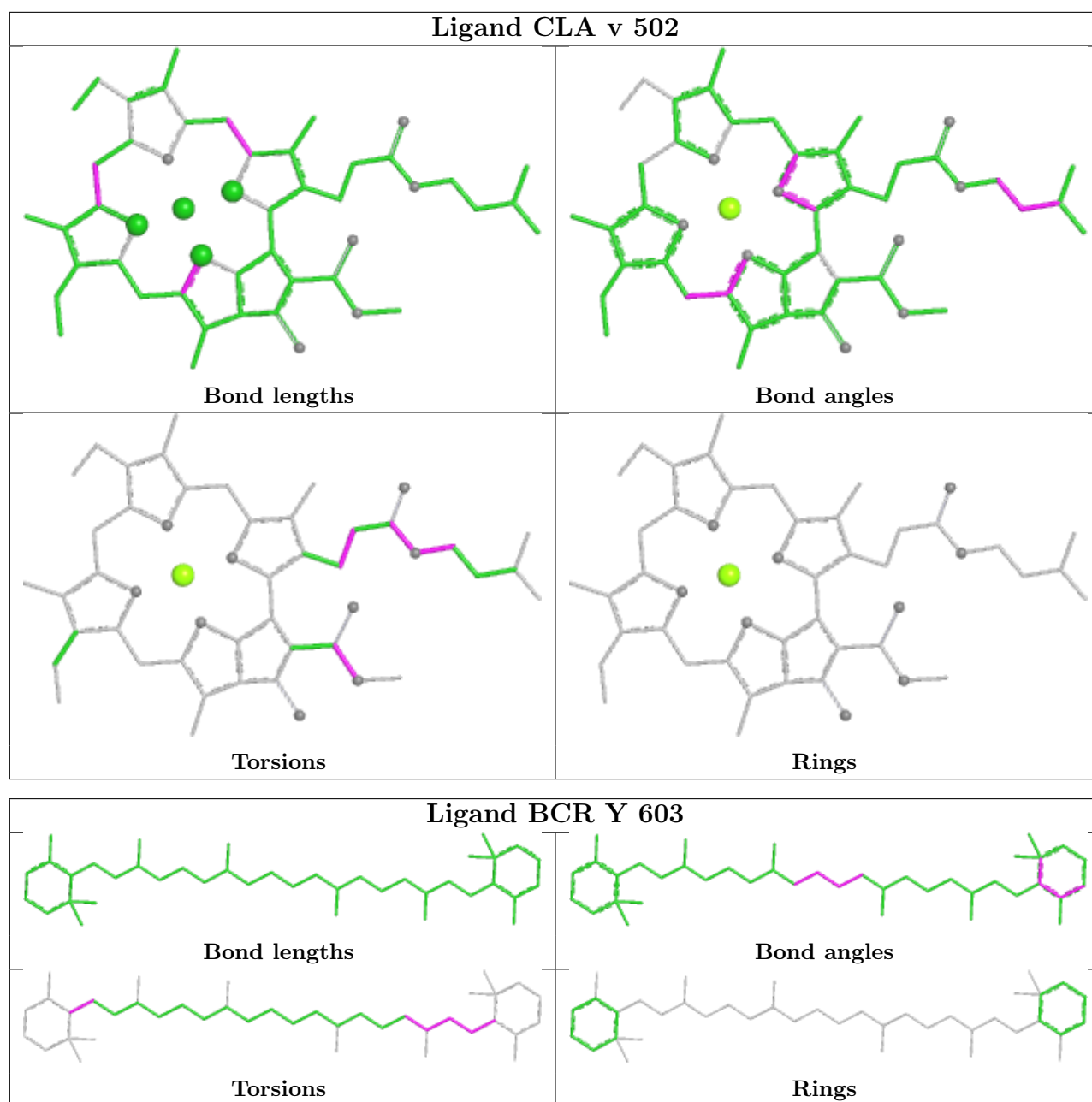


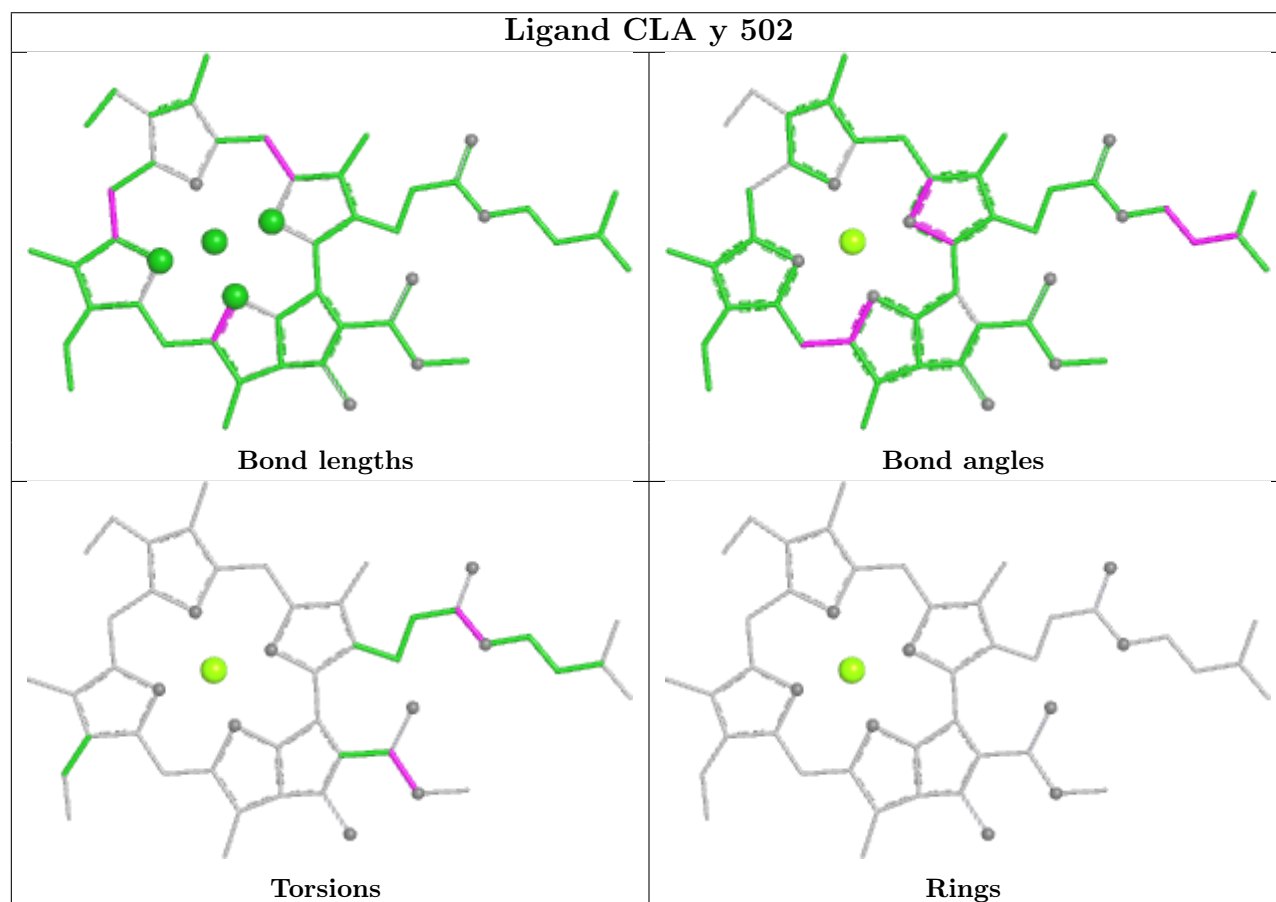
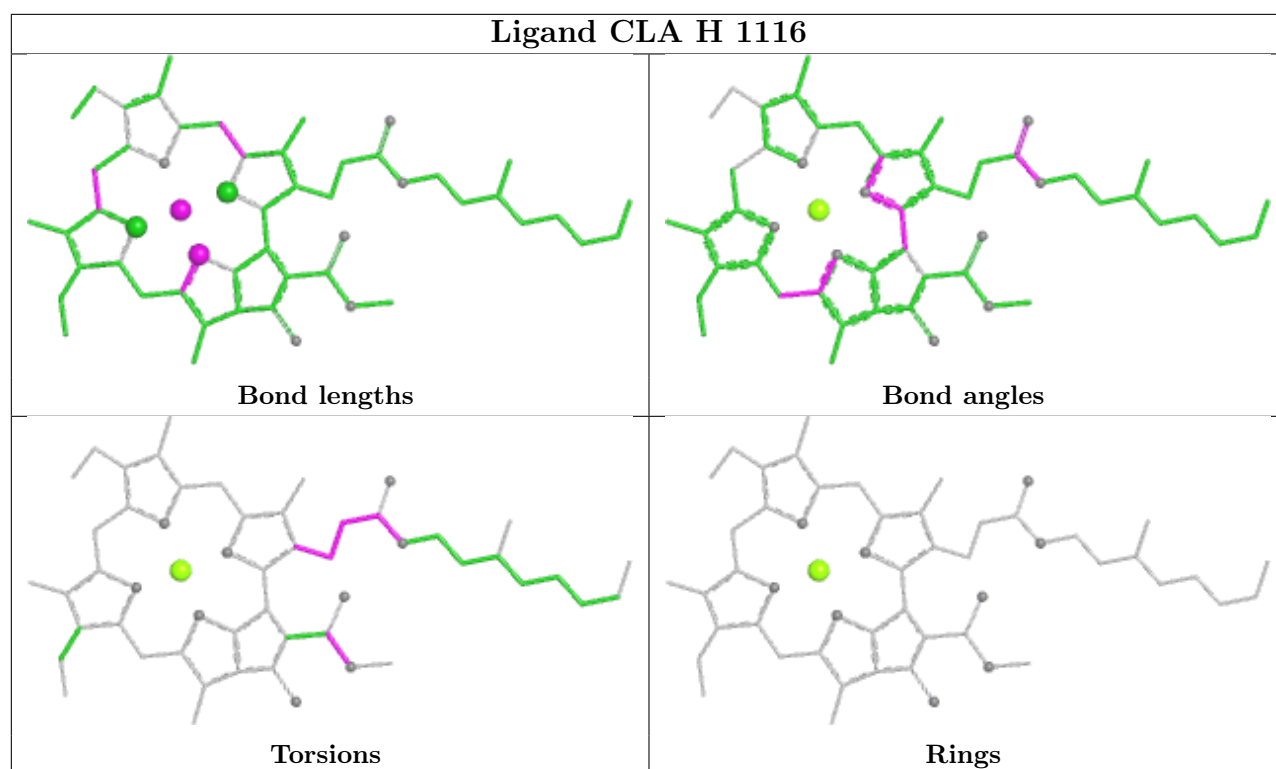
Ligand CLA h 514

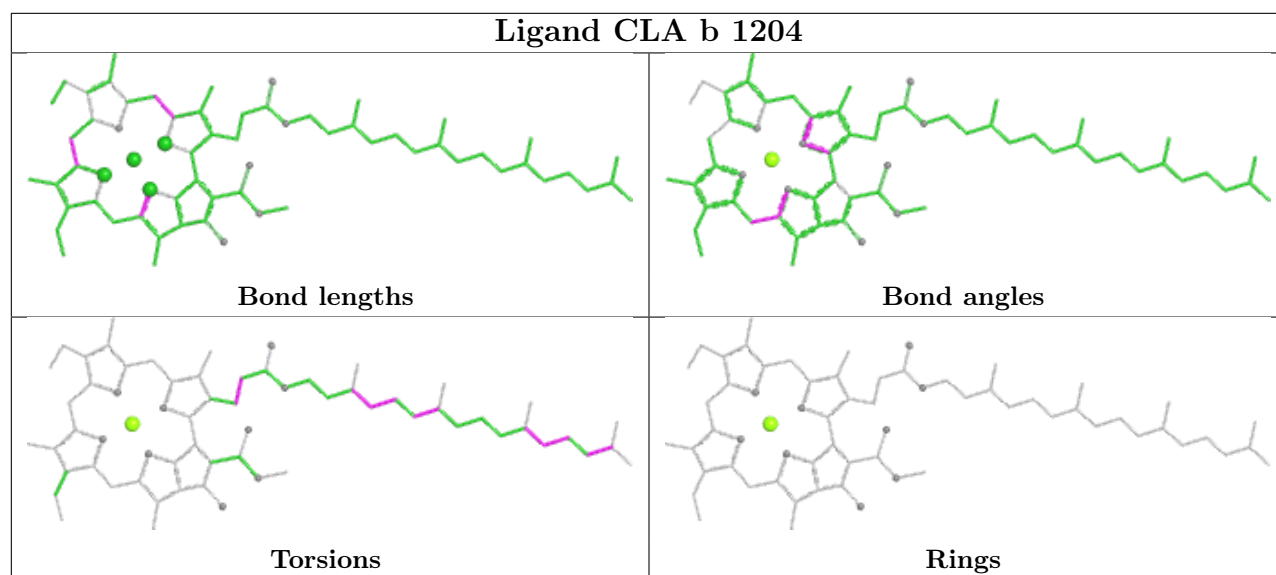
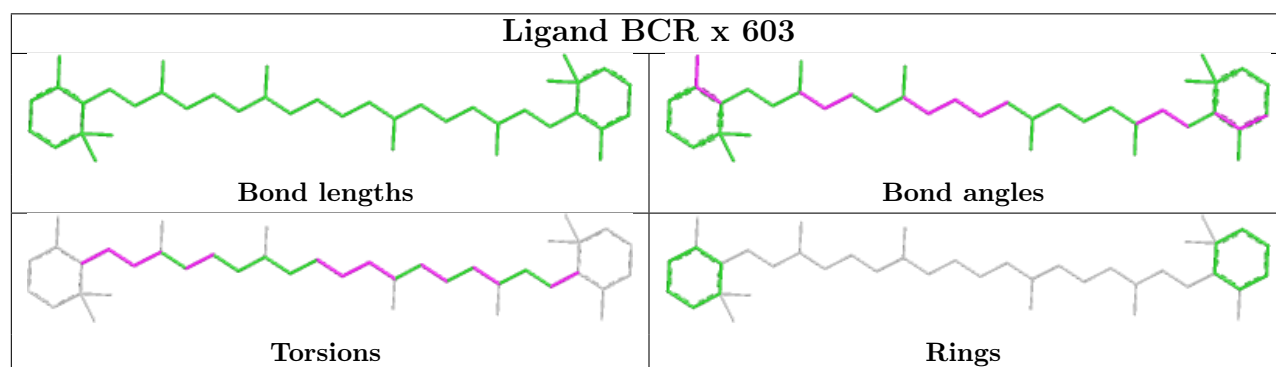
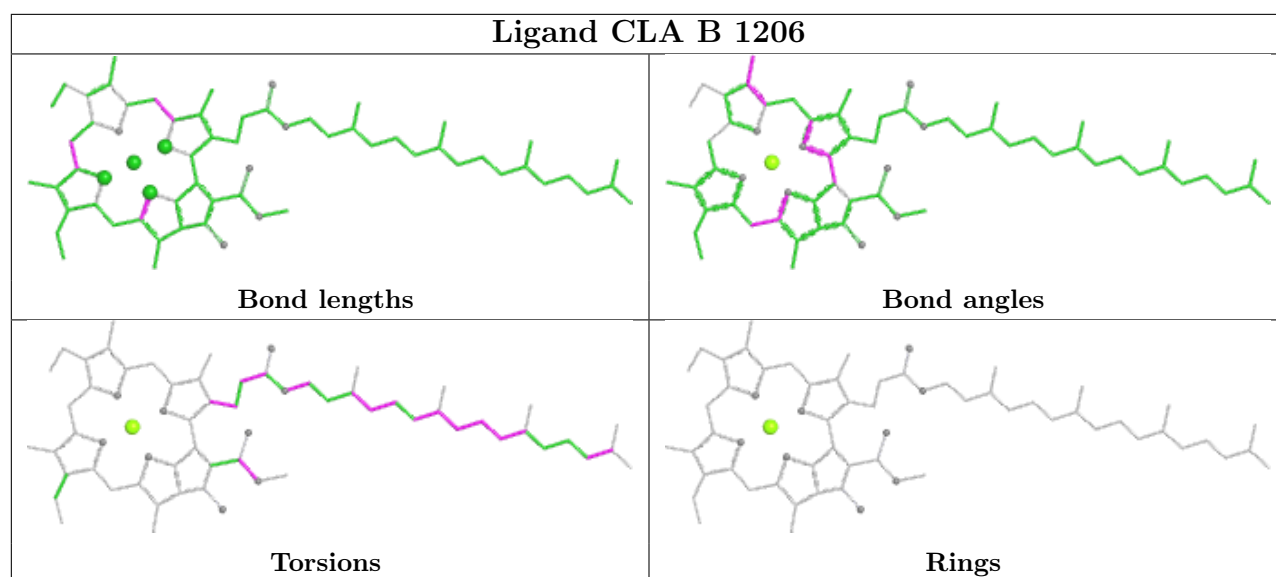


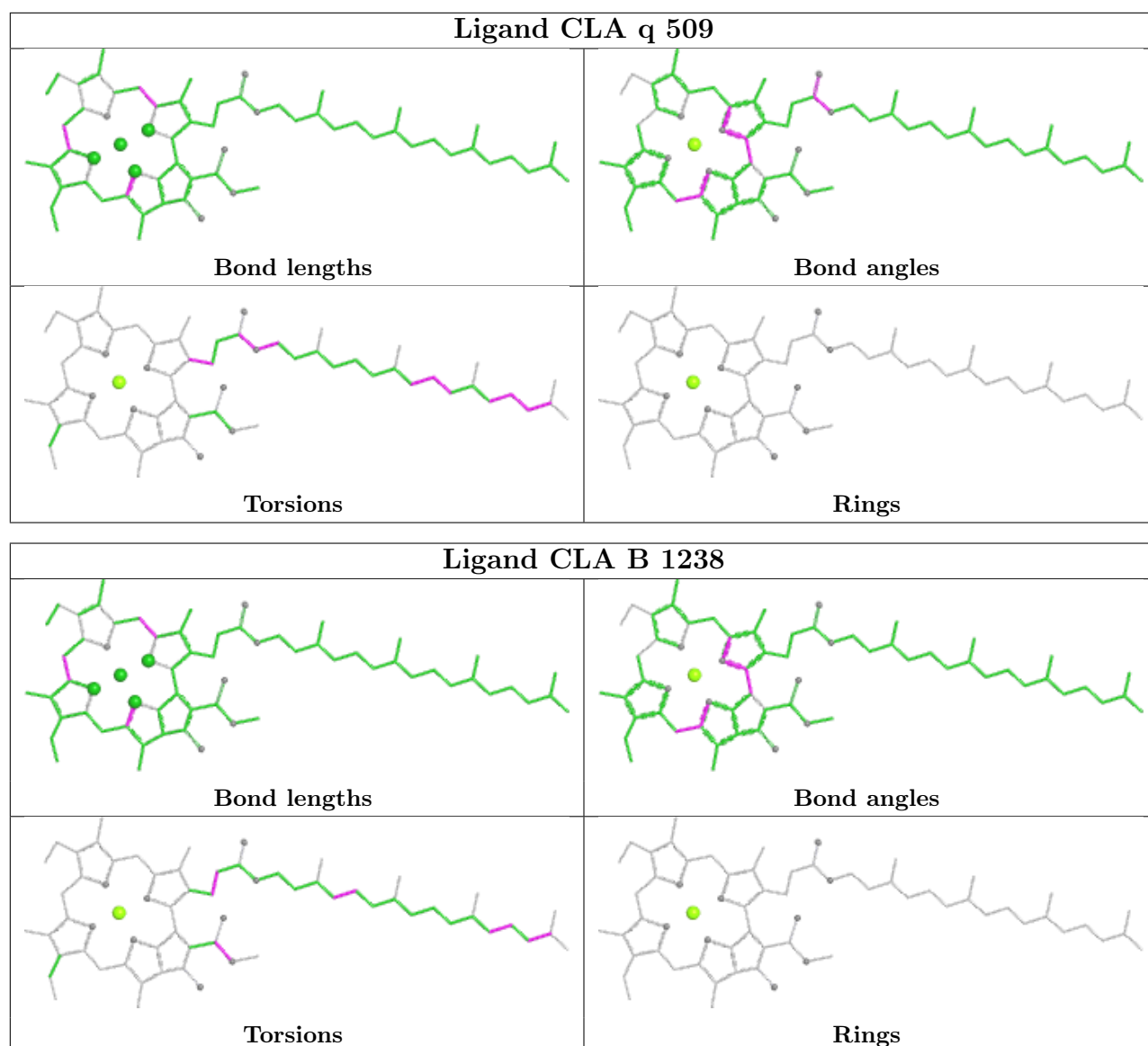
Ligand CLA W 511

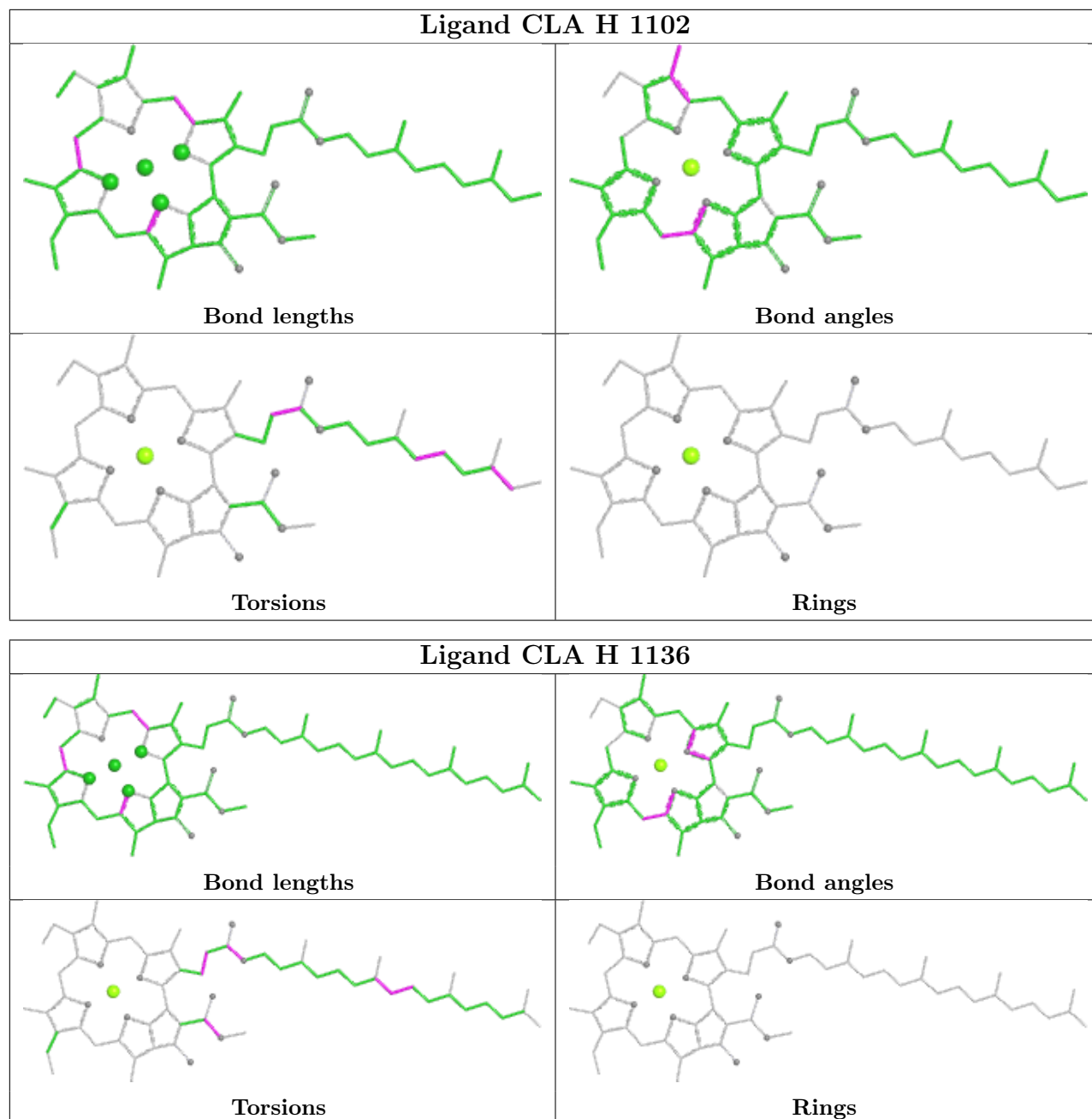




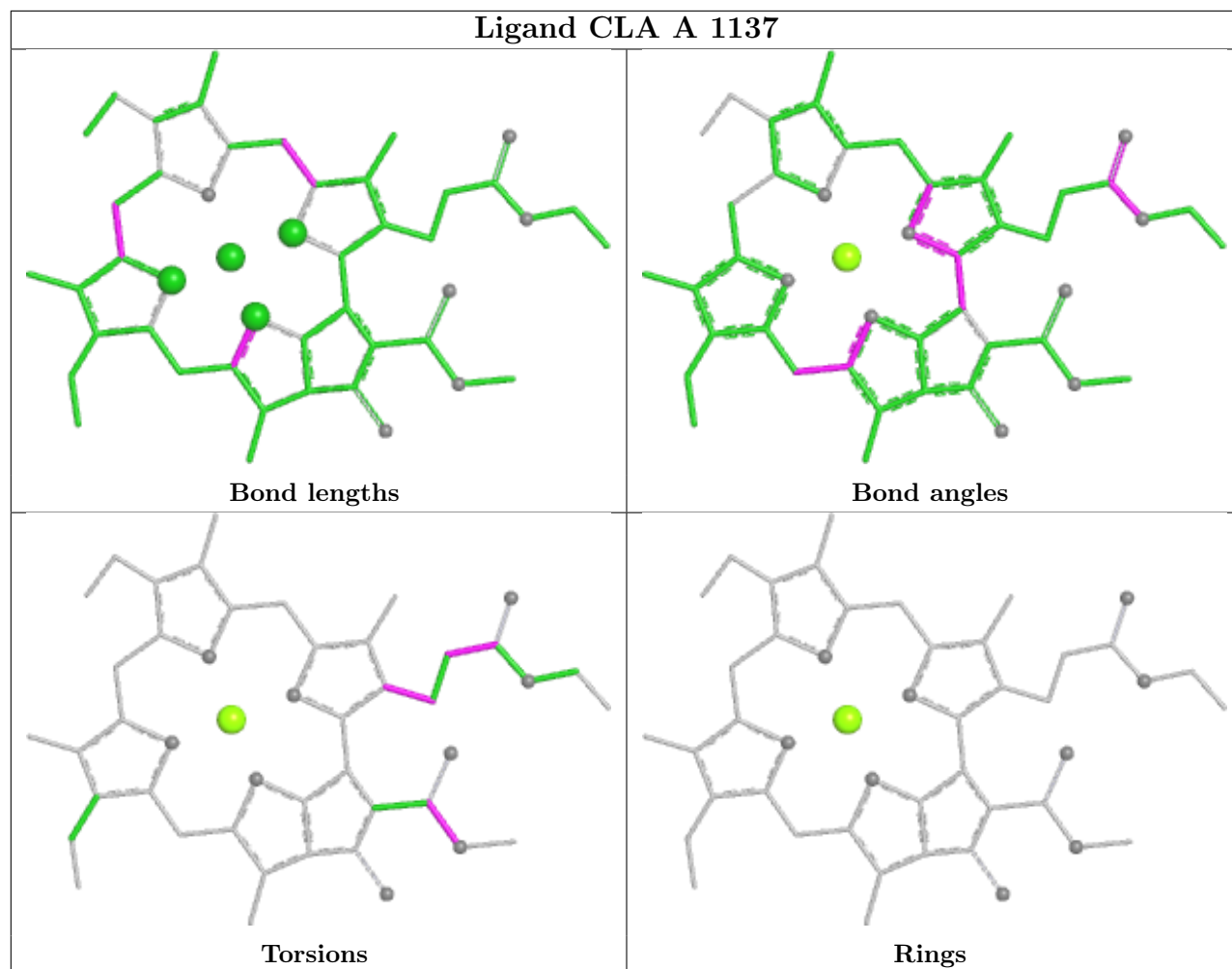


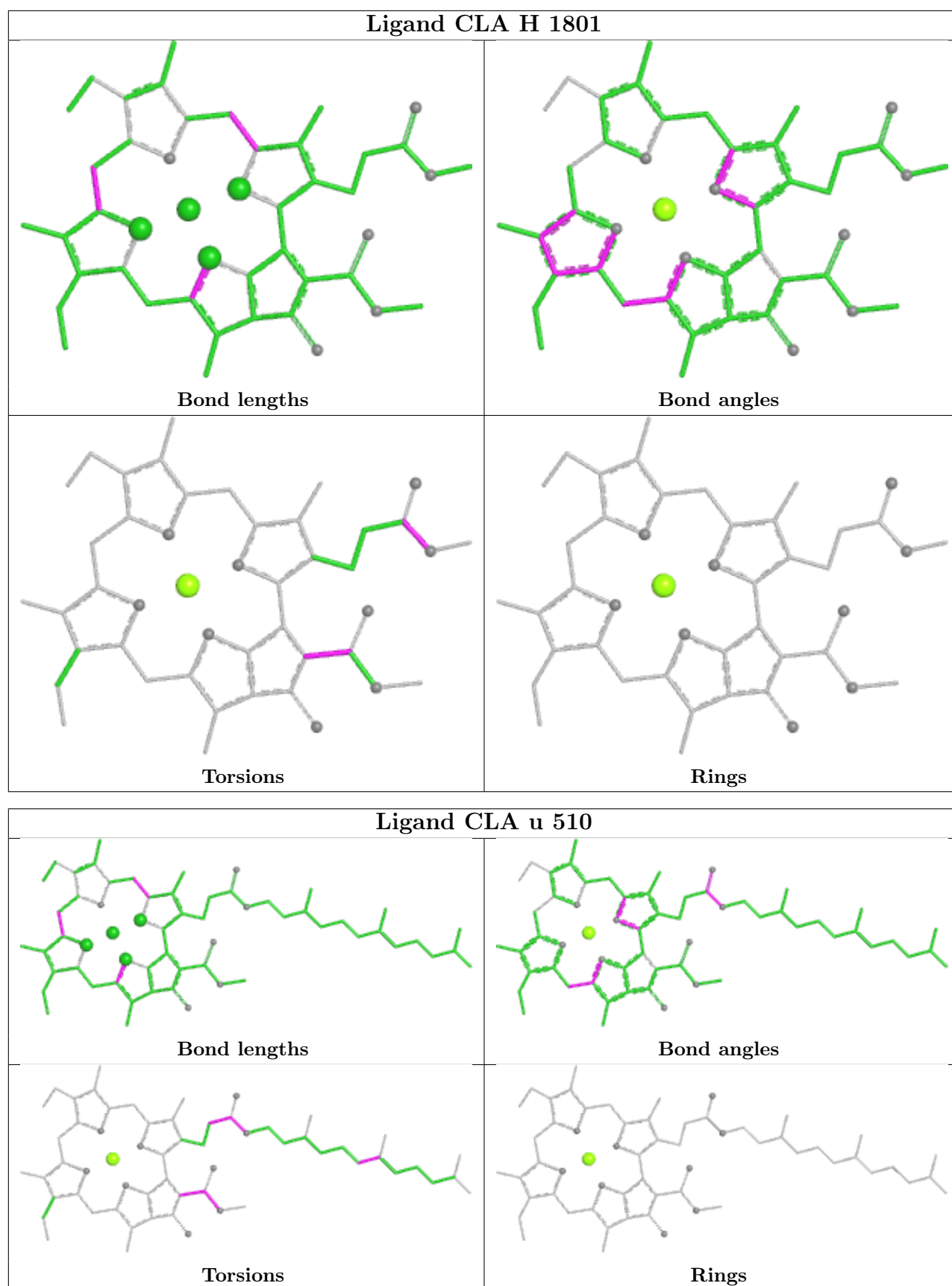


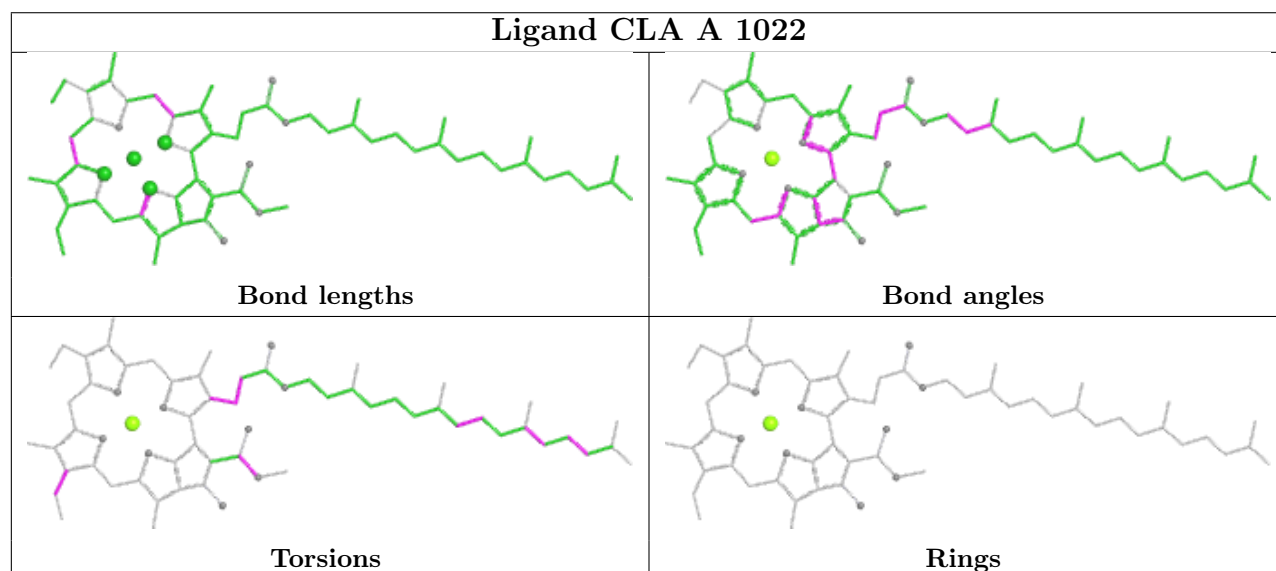
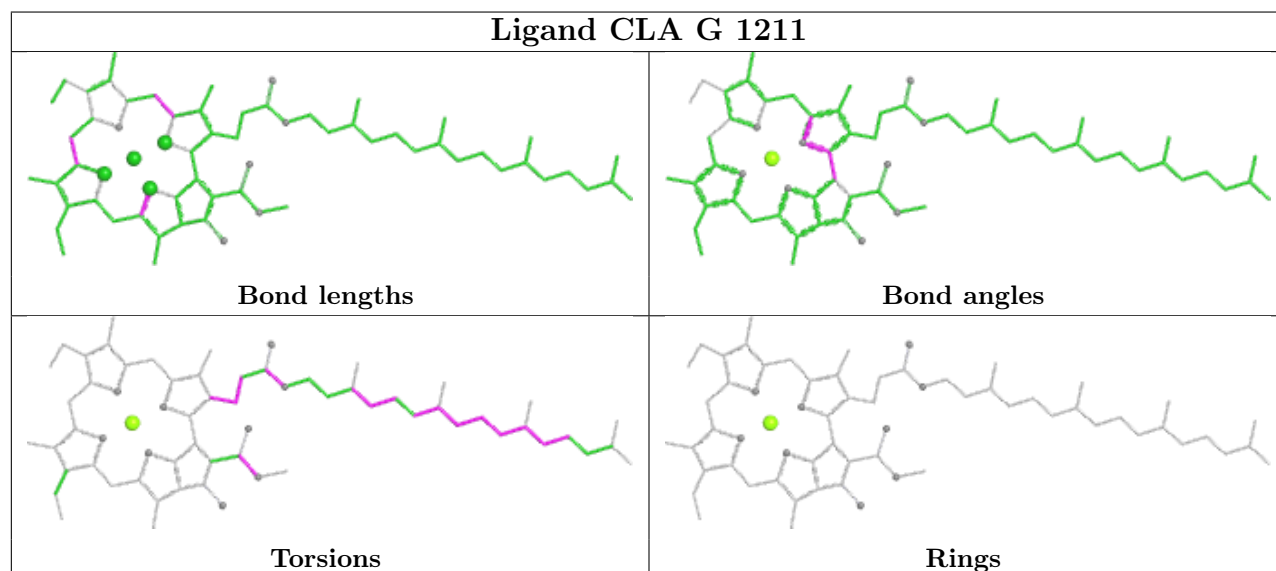
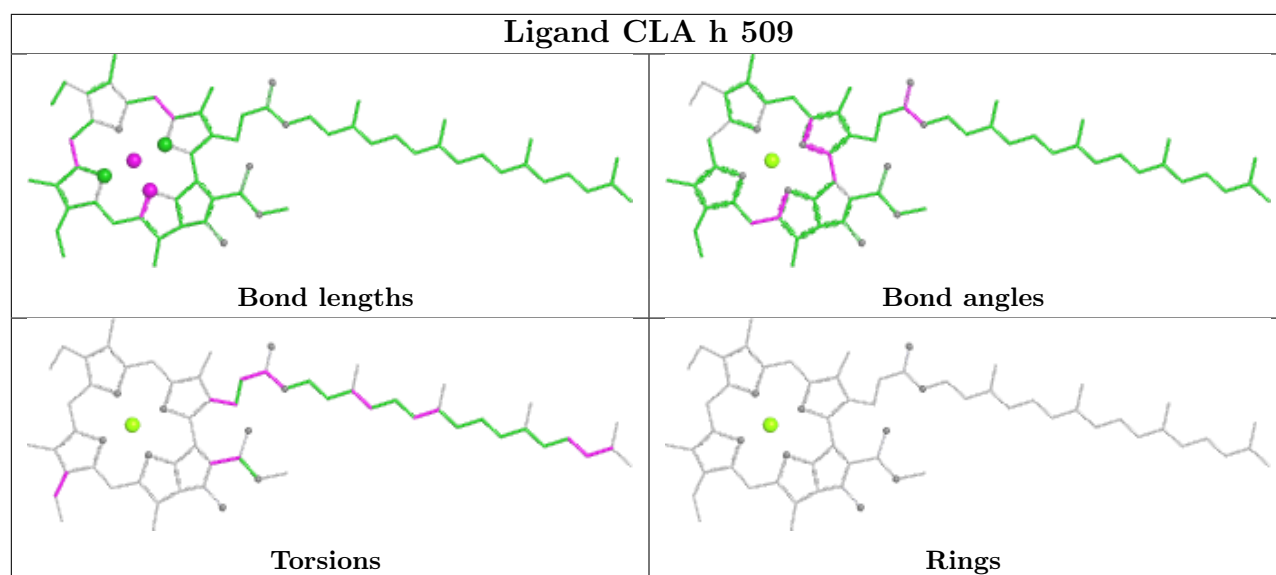




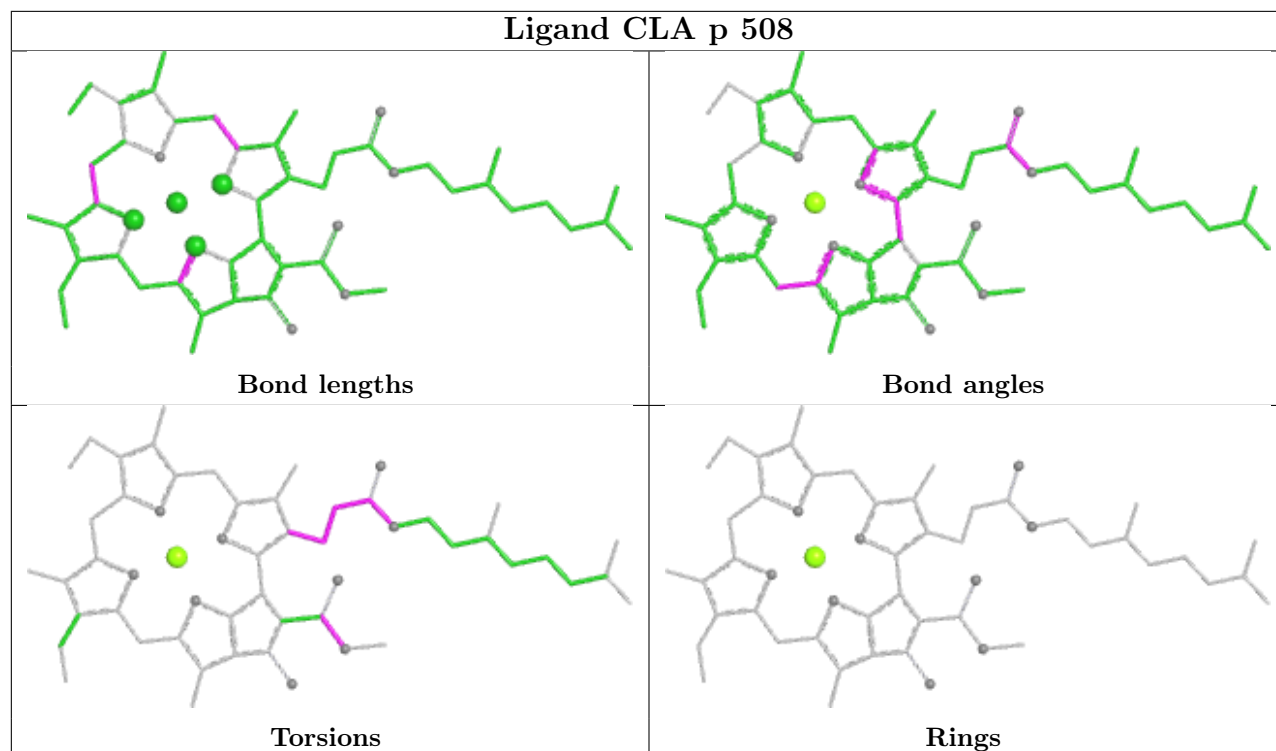
Ligand CLA A 1137



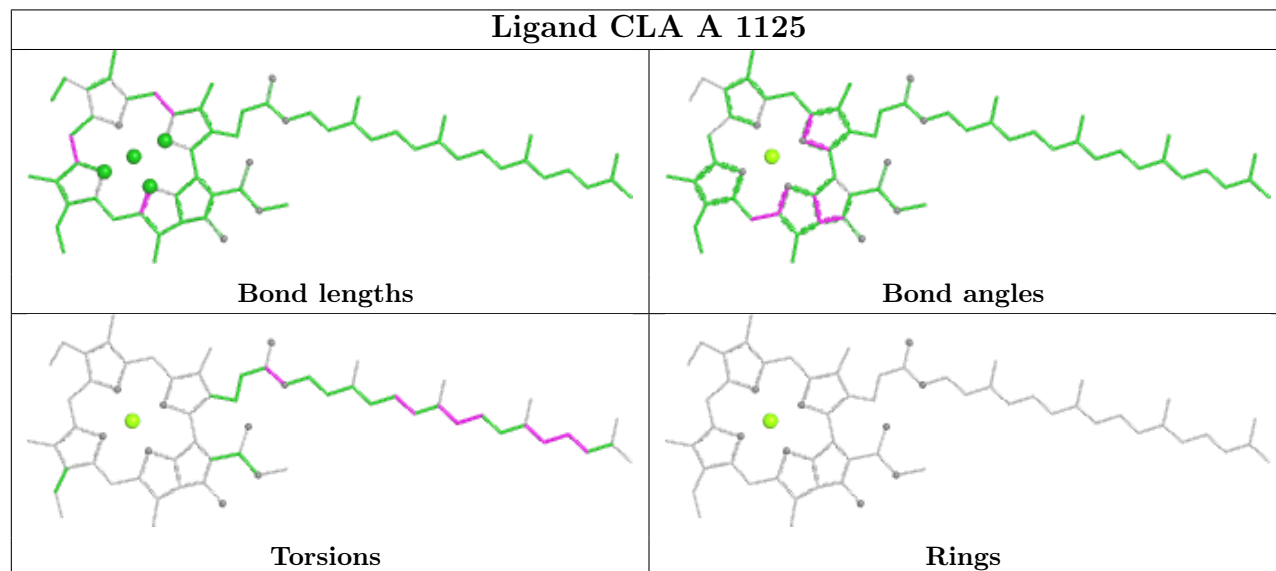


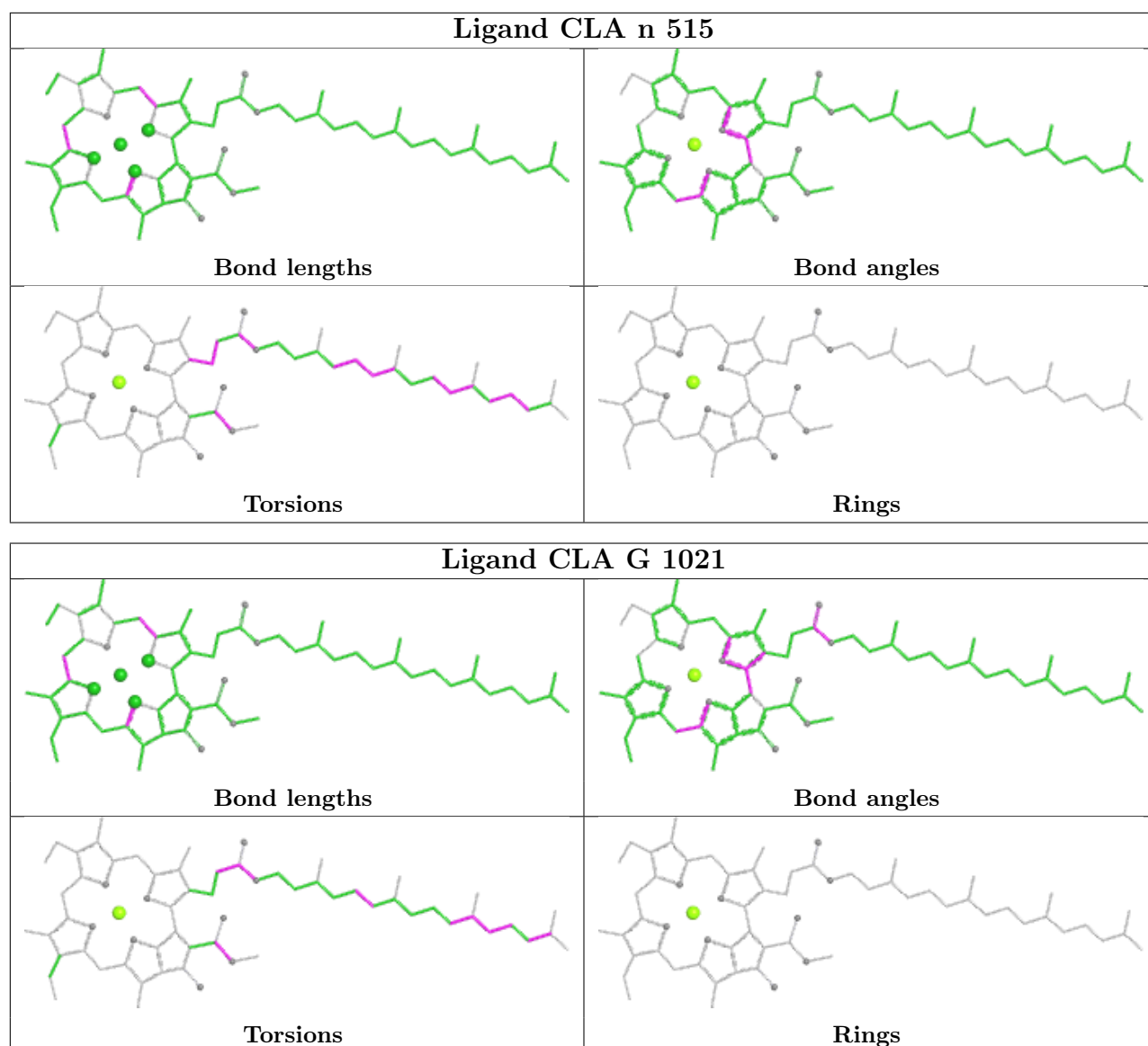


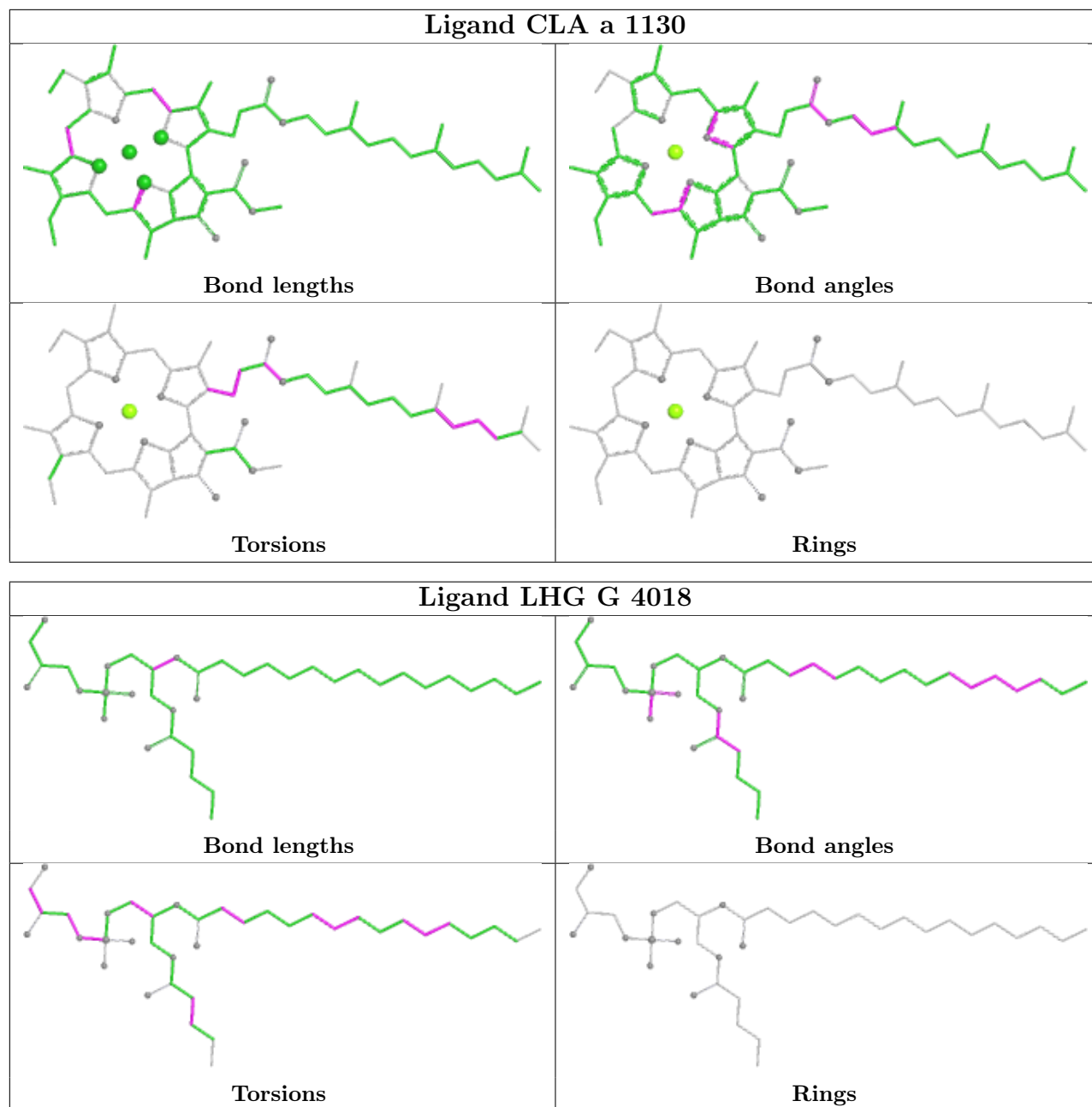
Ligand CLA p 508

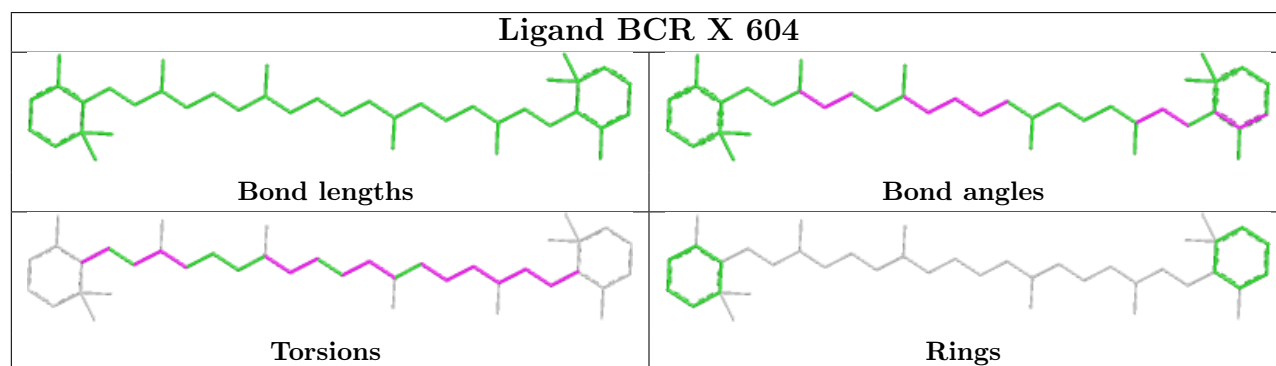
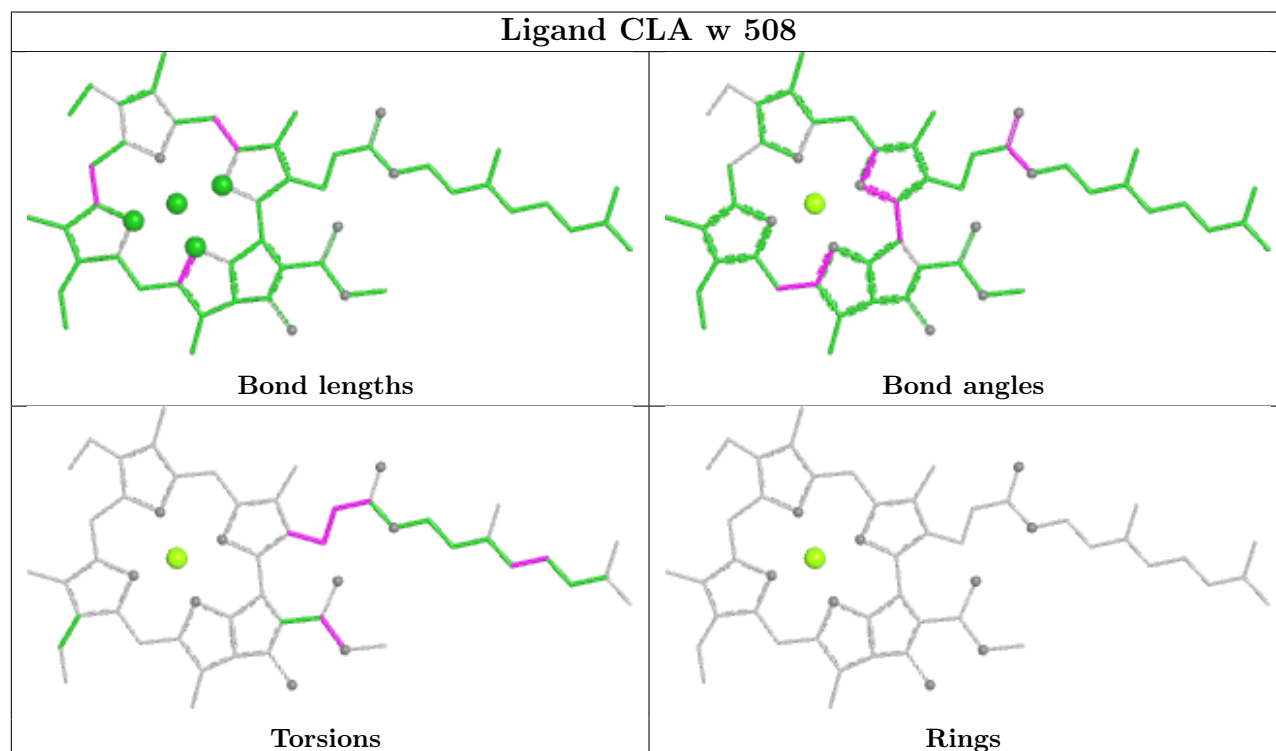
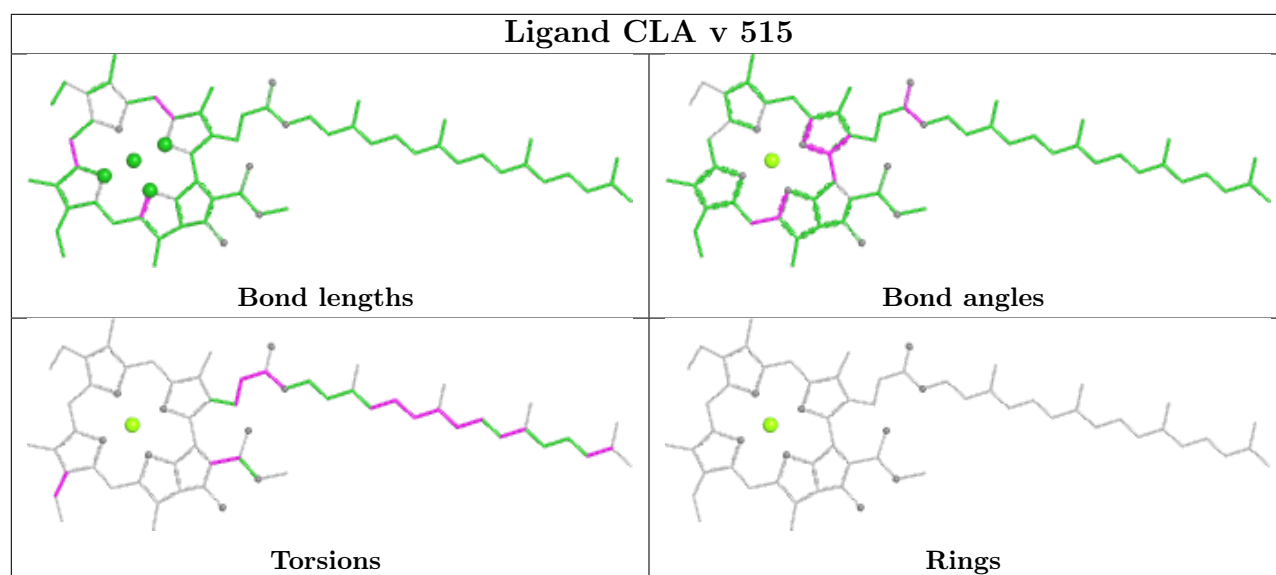


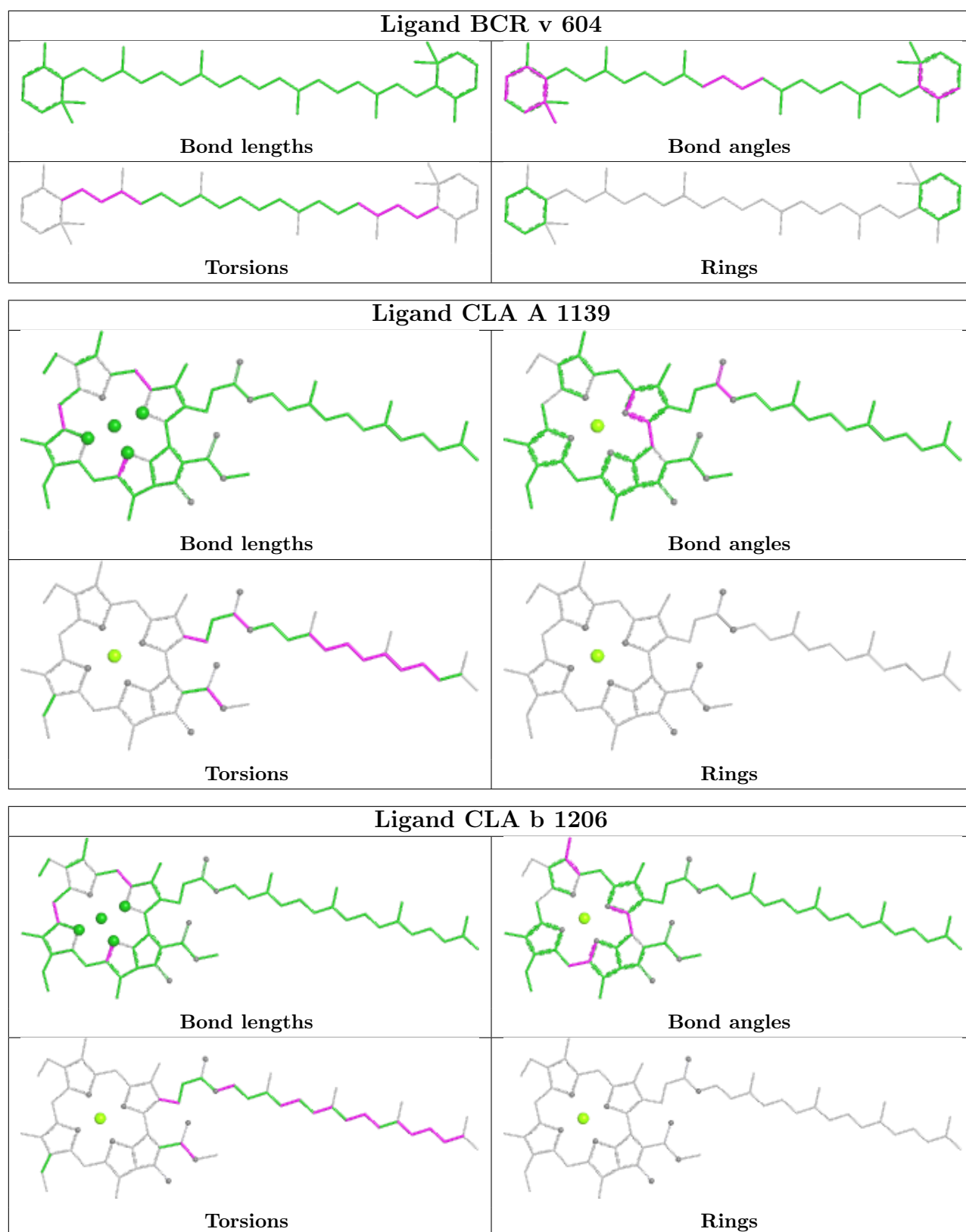
Ligand CLA A 1125

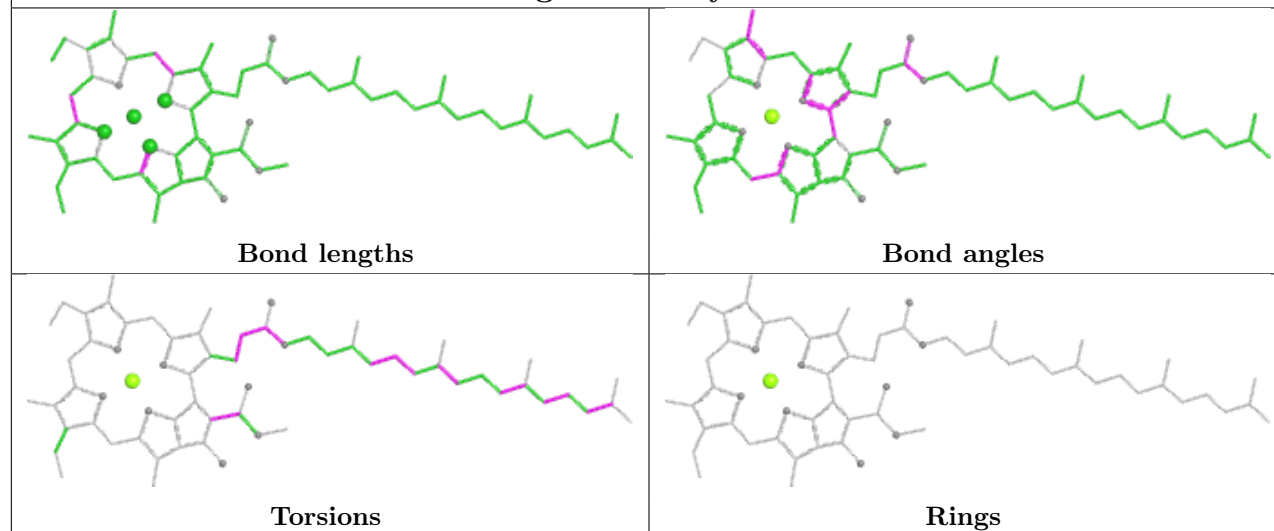
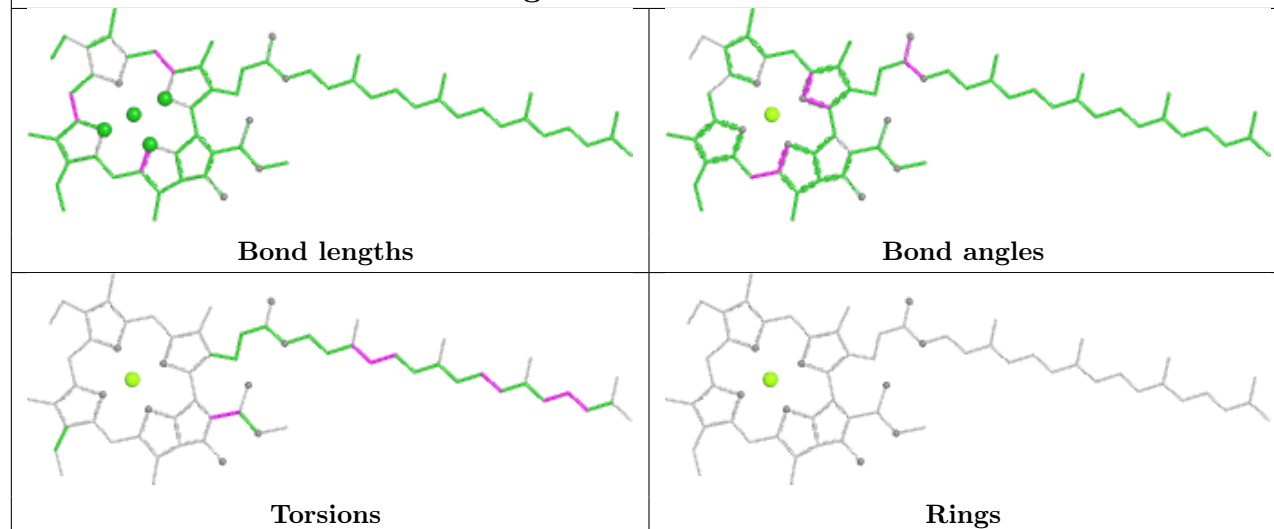




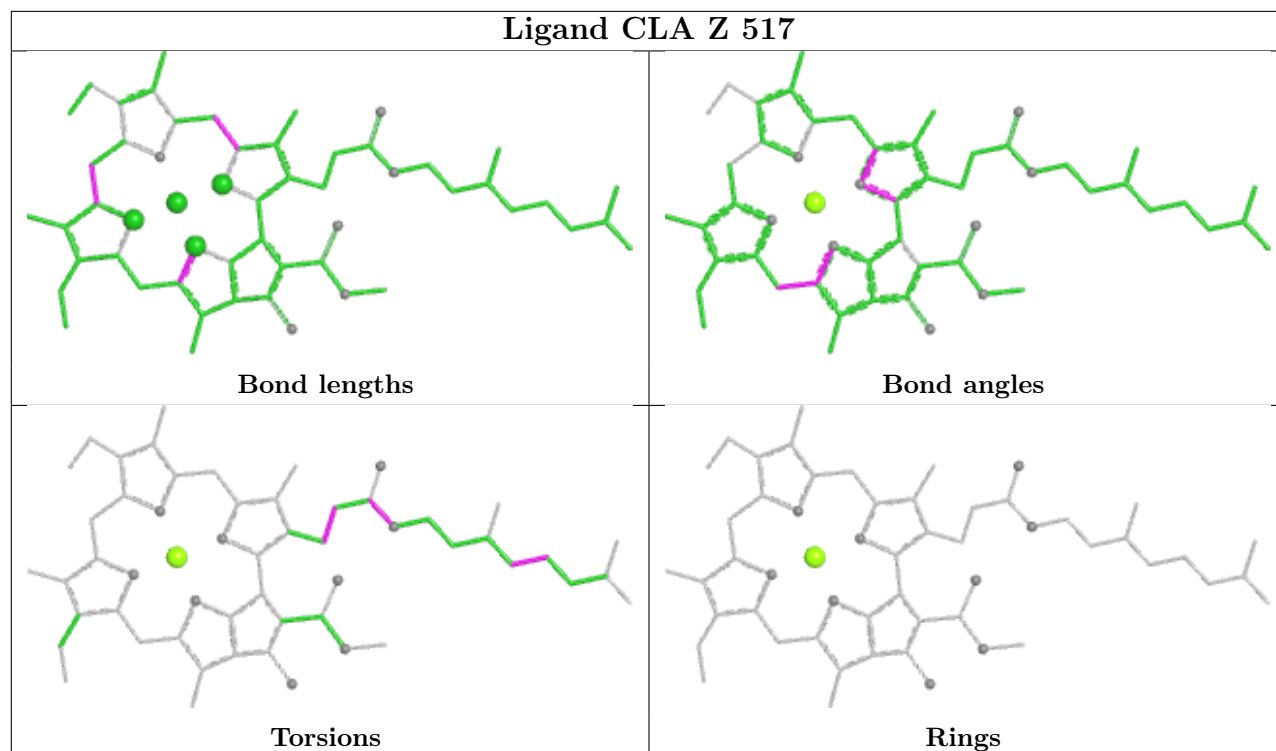




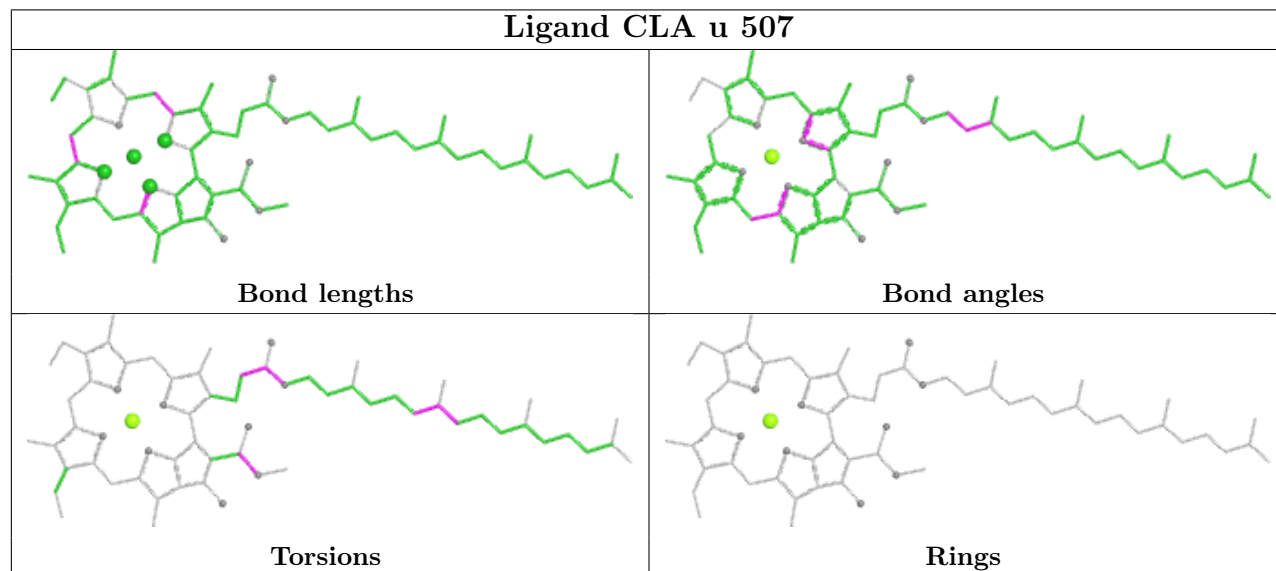


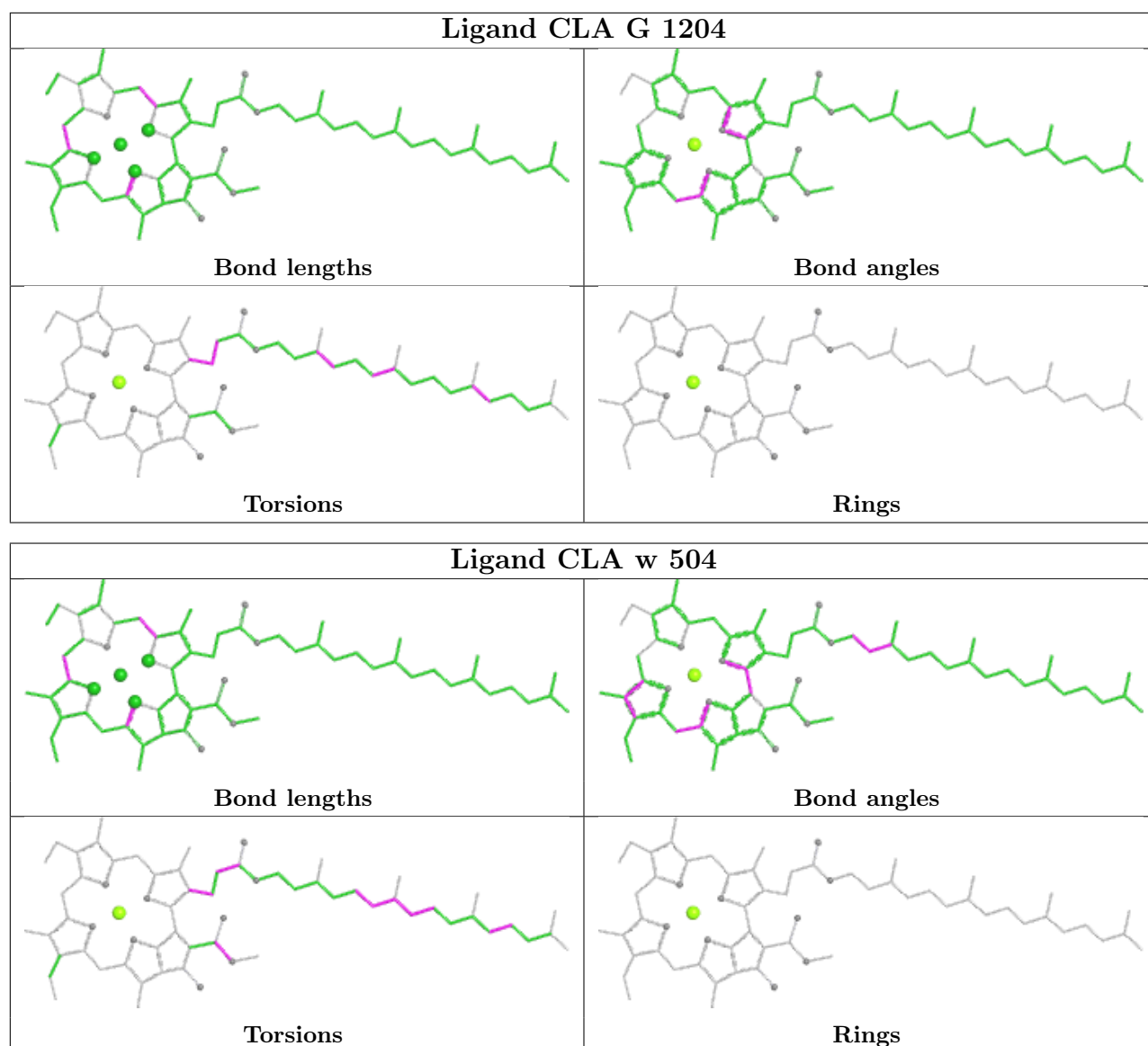
Ligand CLA y 515**Ligand CLA B 1205**

Ligand CLA Z 517

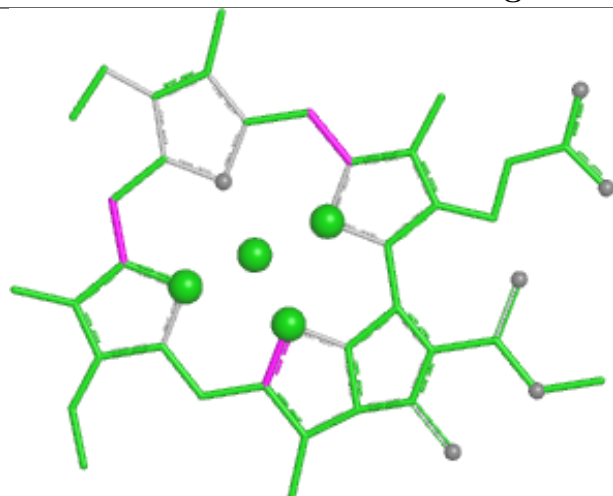


Ligand CLA u 507

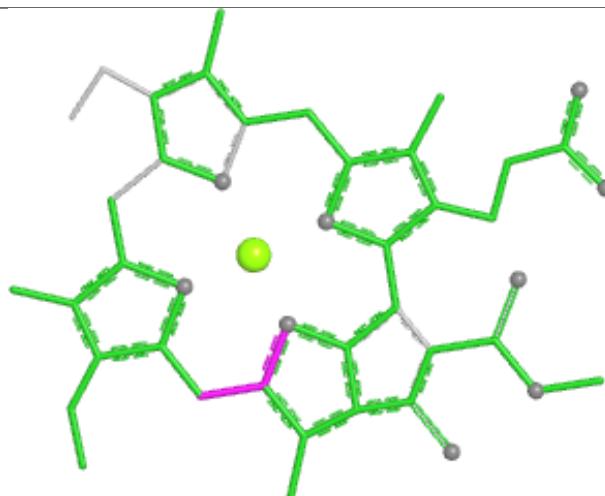




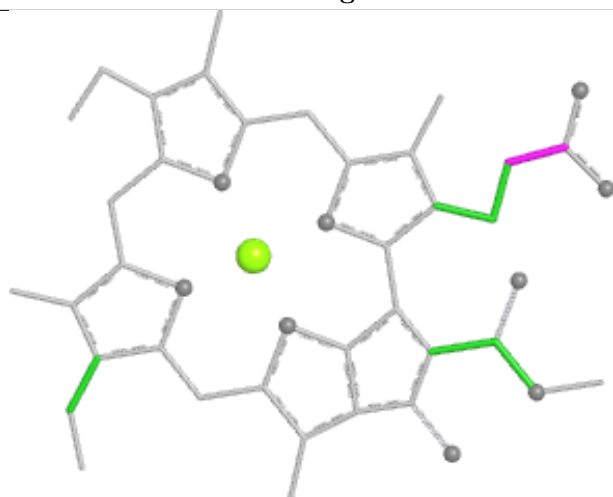
Ligand CLA H 1134



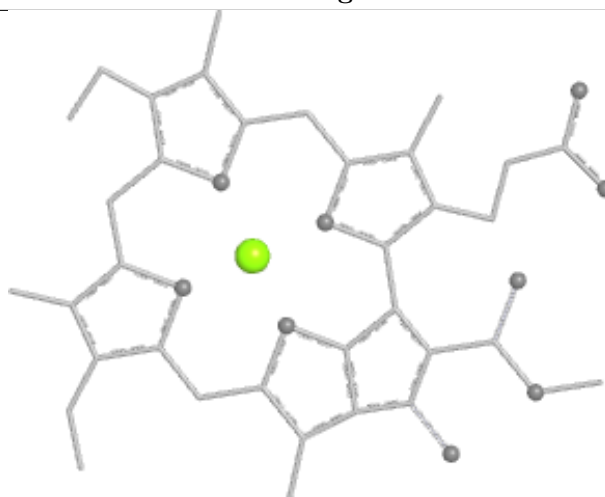
Bond lengths



Bond angles

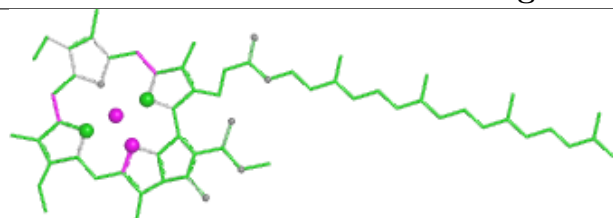


Torsions

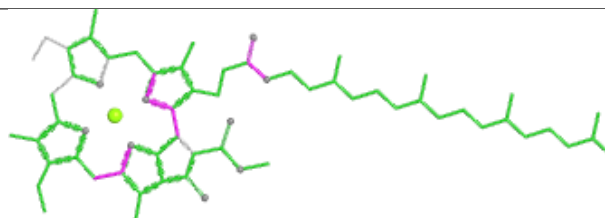


Rings

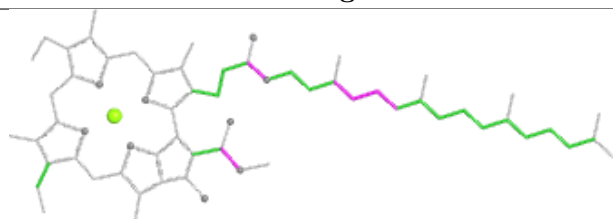
Ligand CLA x 512



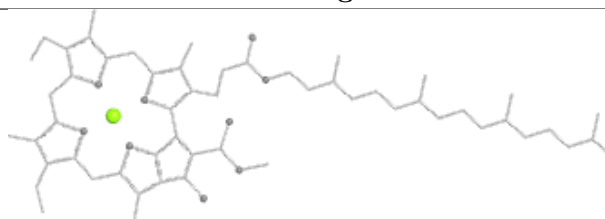
Bond lengths



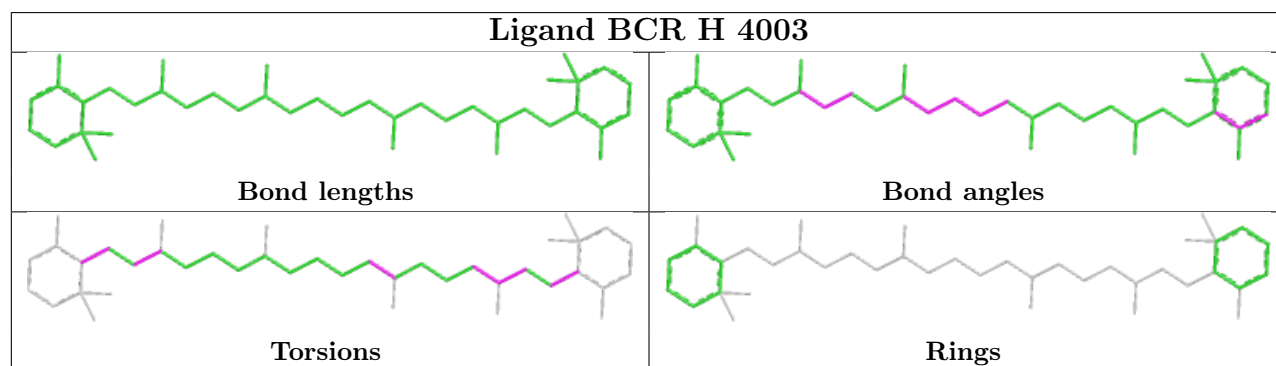
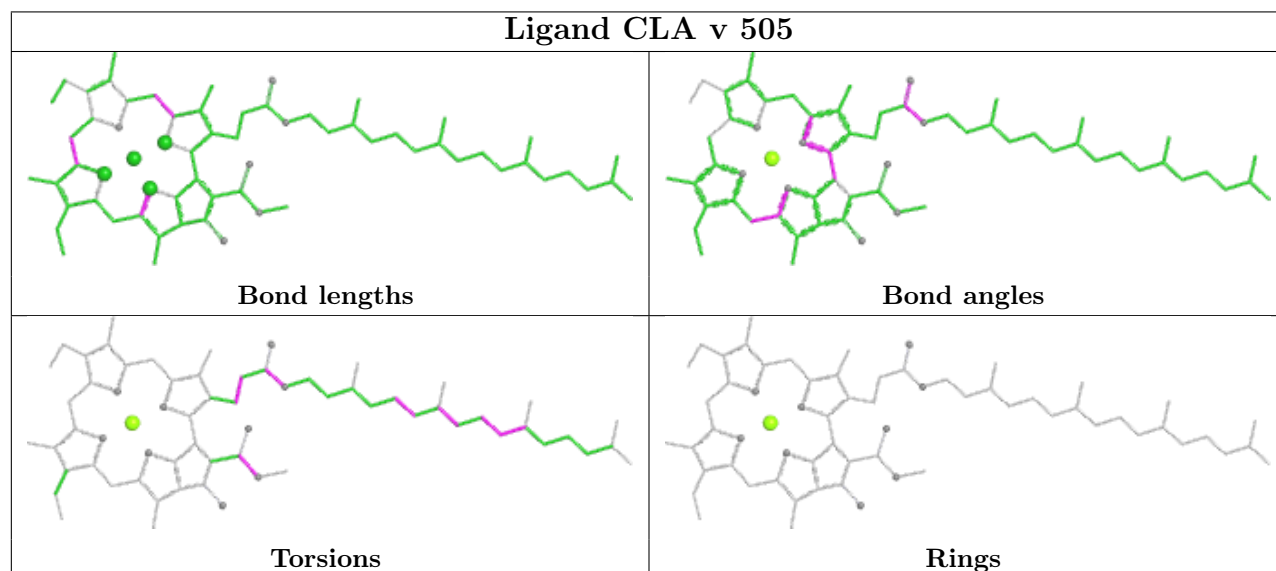
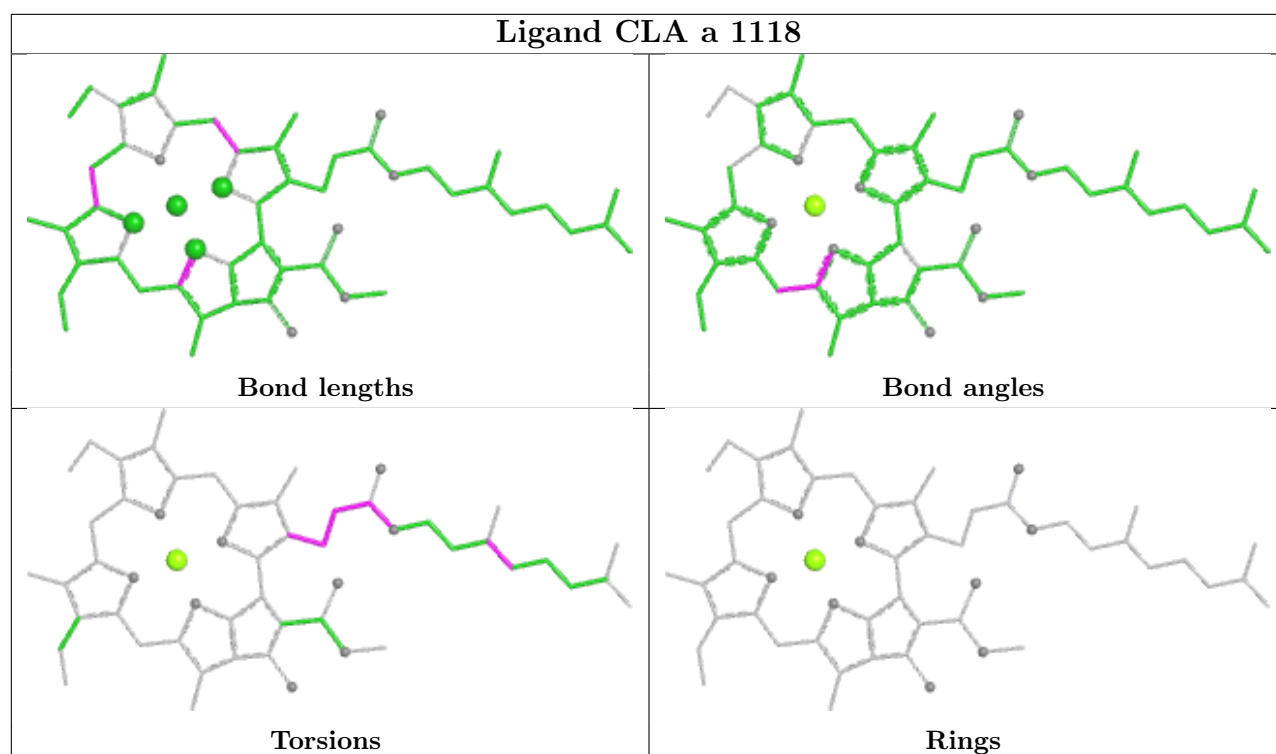
Bond angles

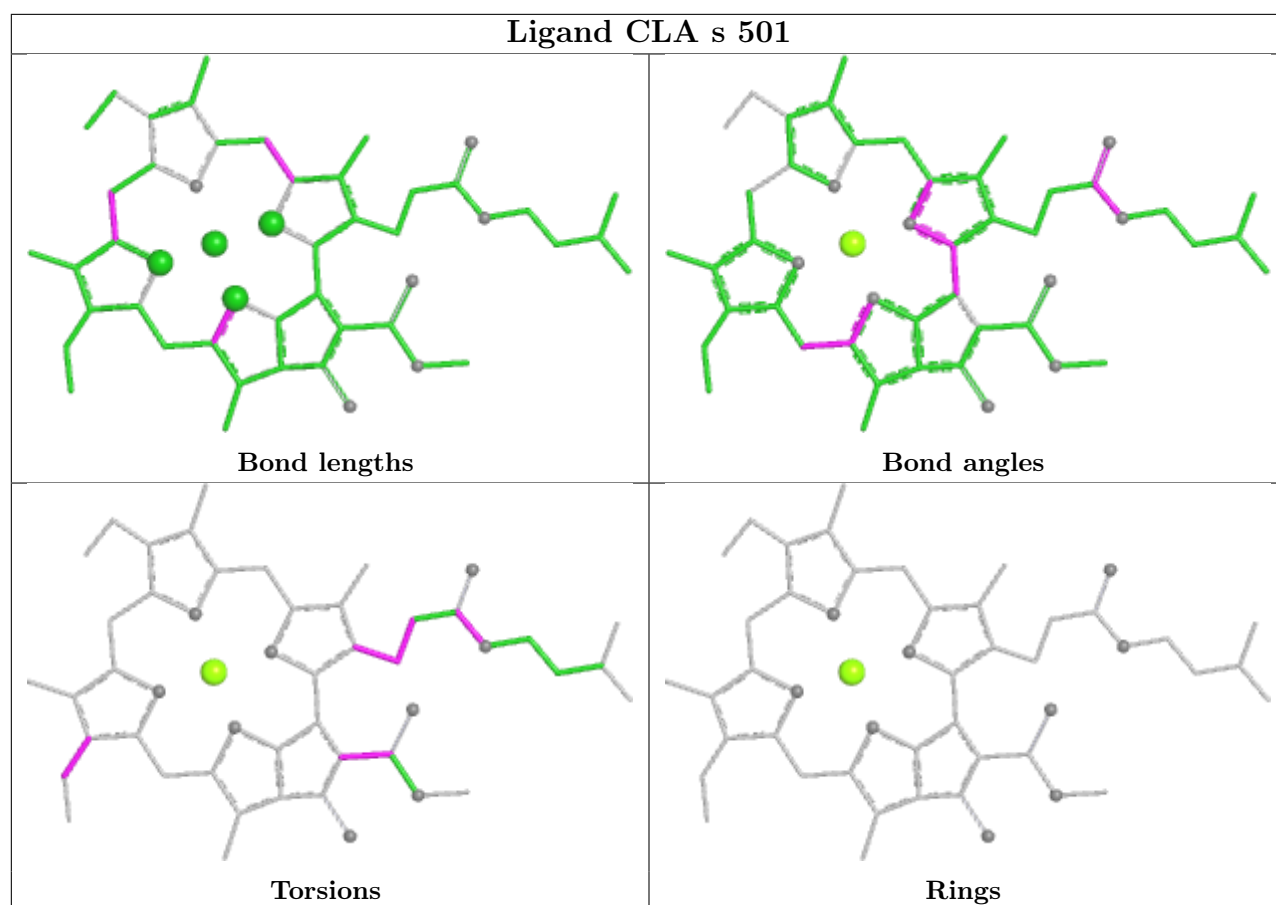


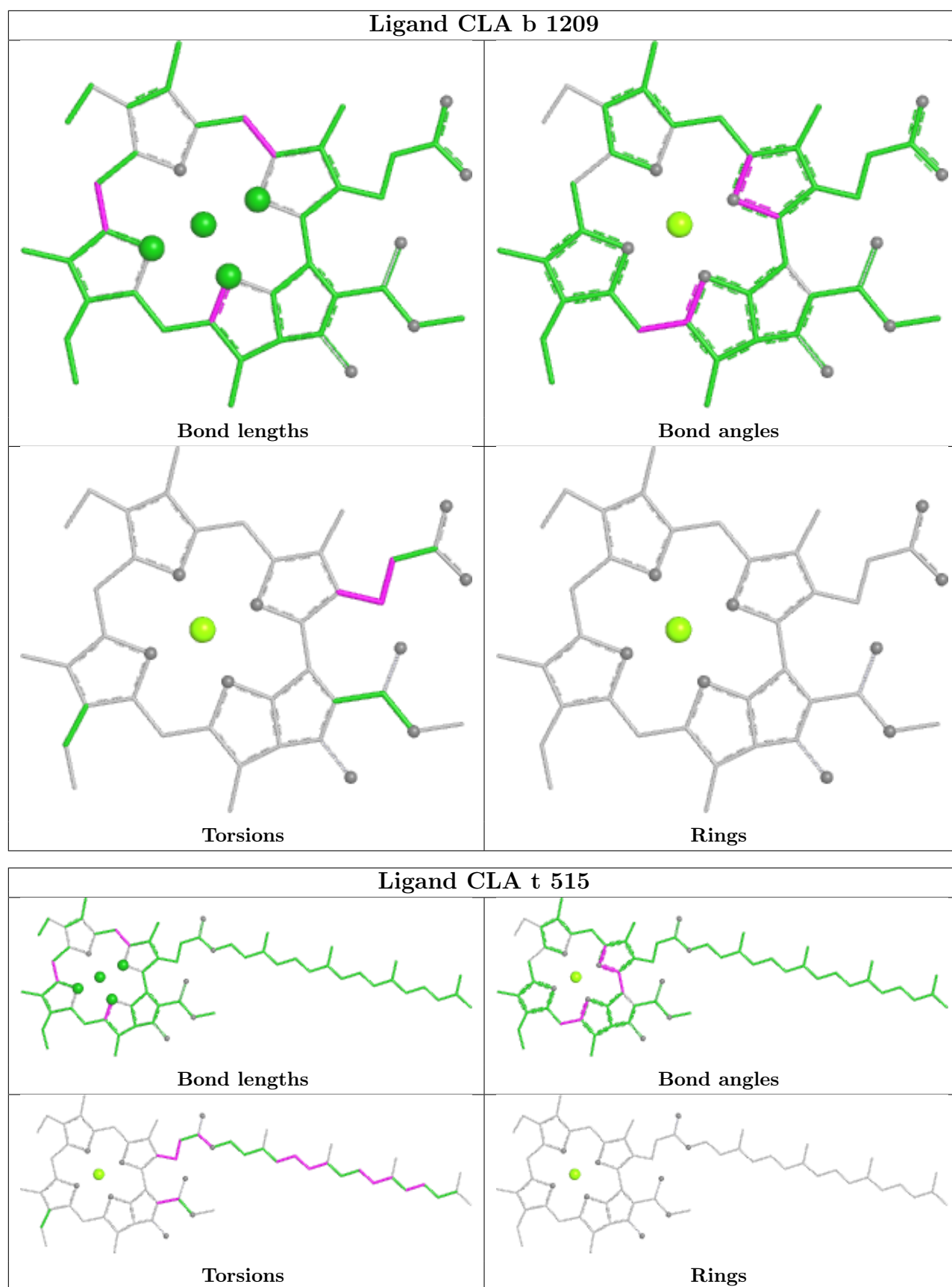
Torsions

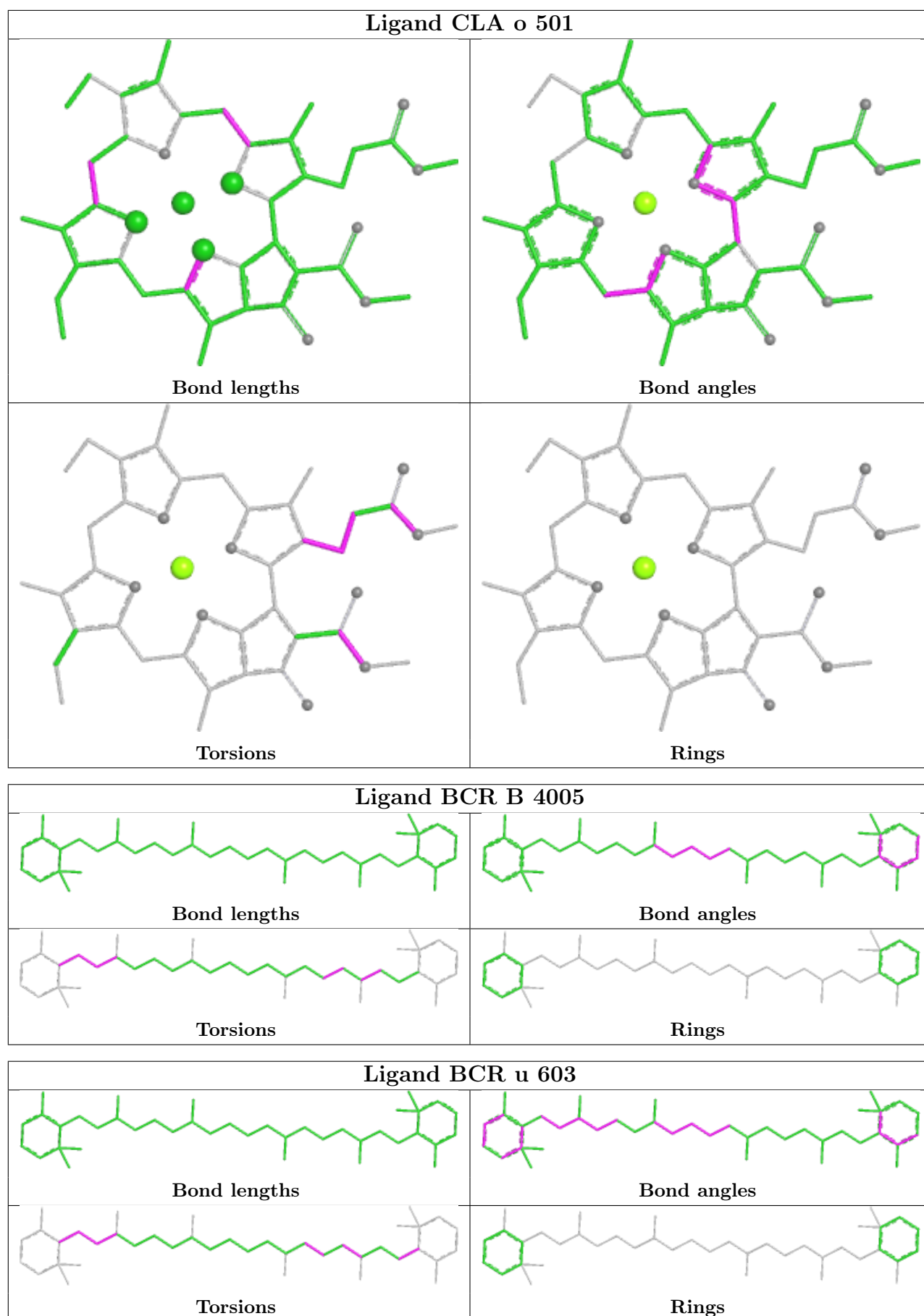


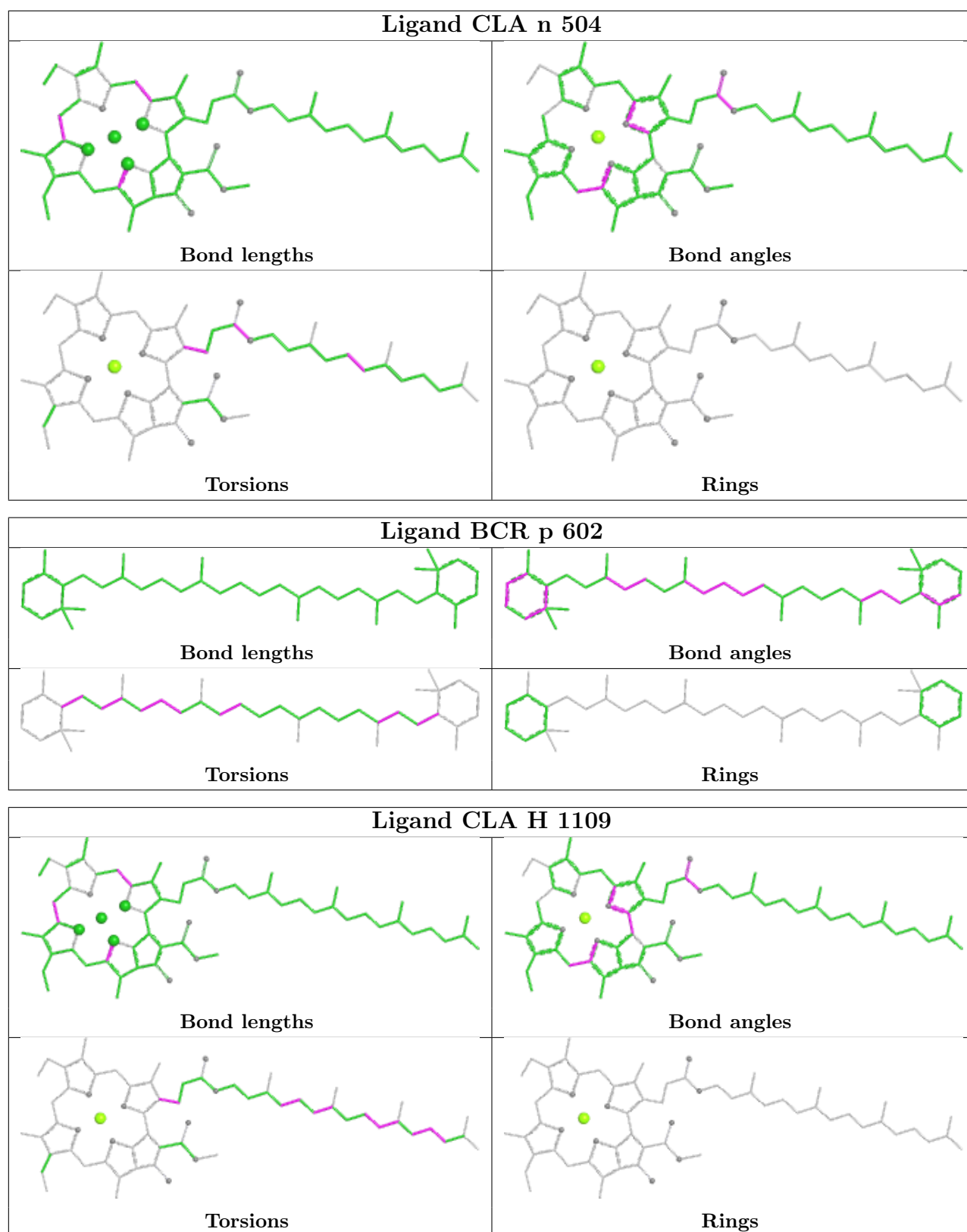
Rings

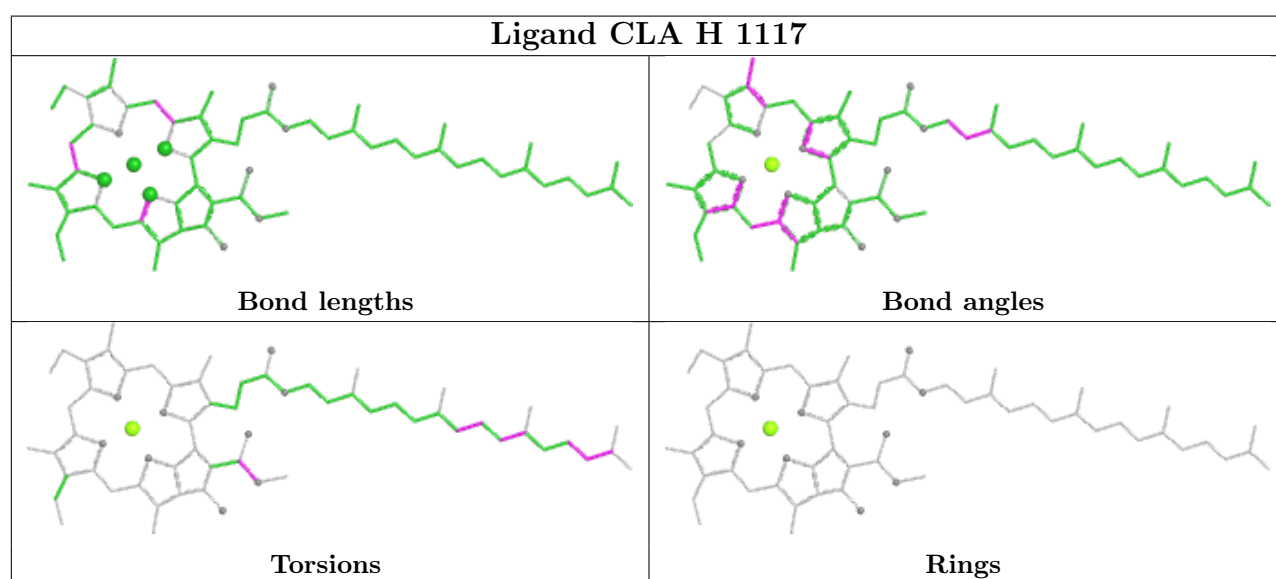
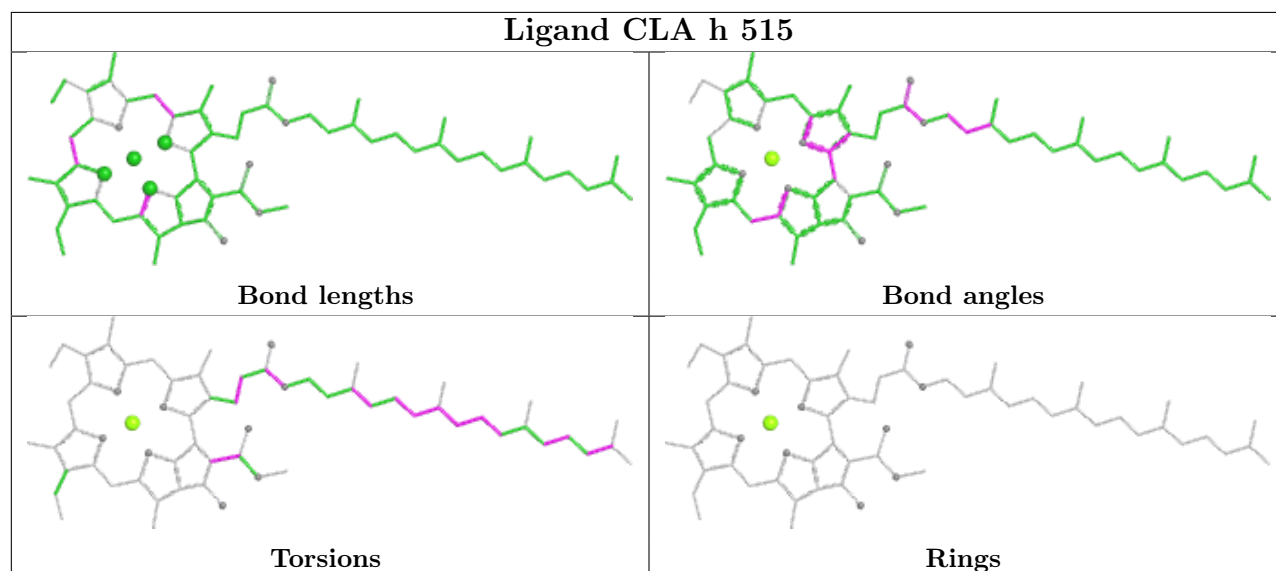
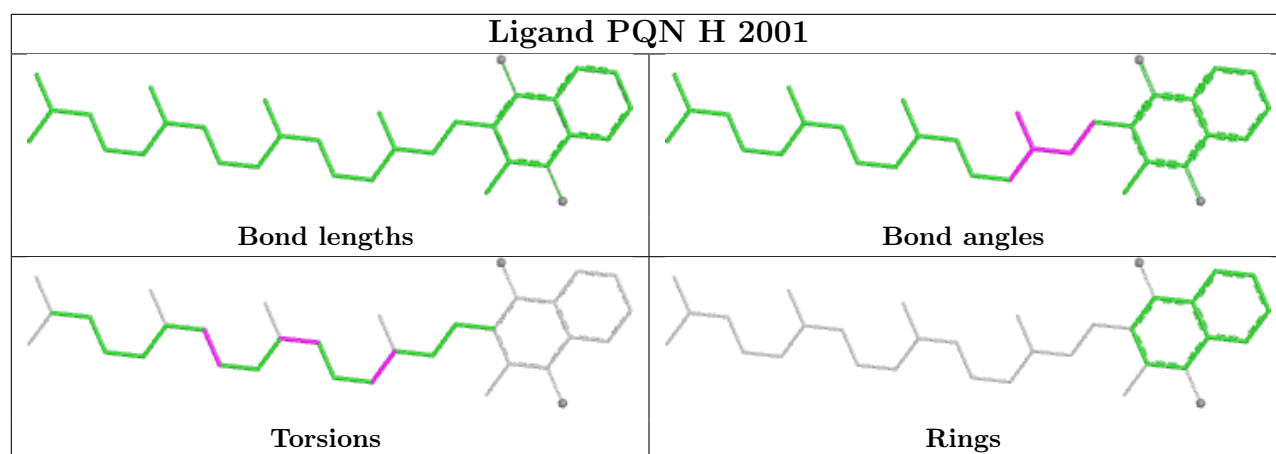




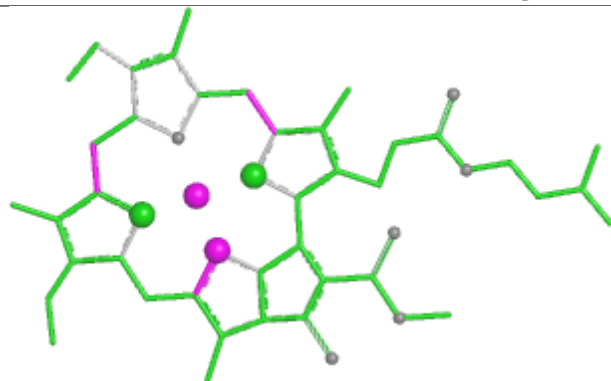




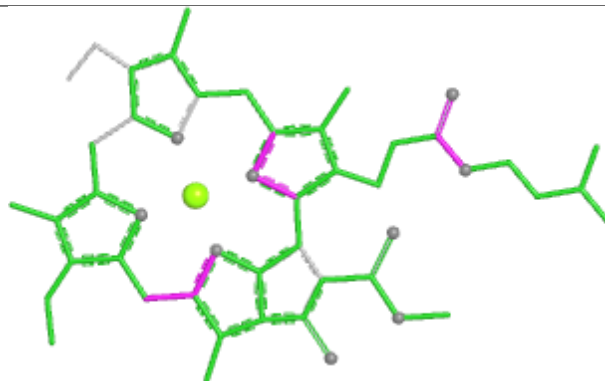




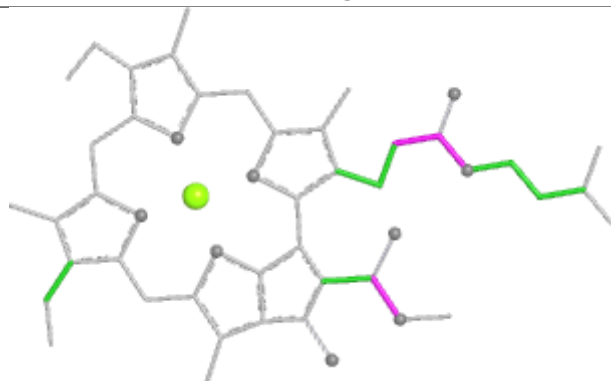
Ligand CLA Z 502



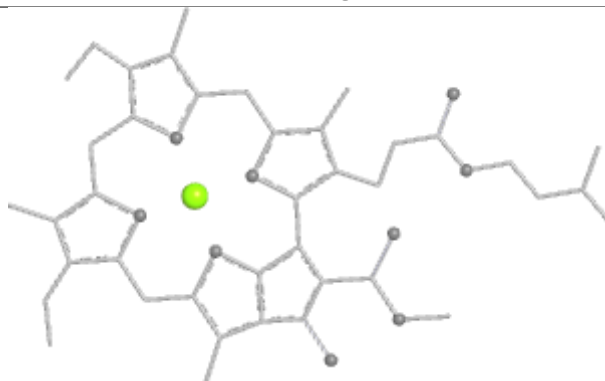
Bond lengths



Bond angles

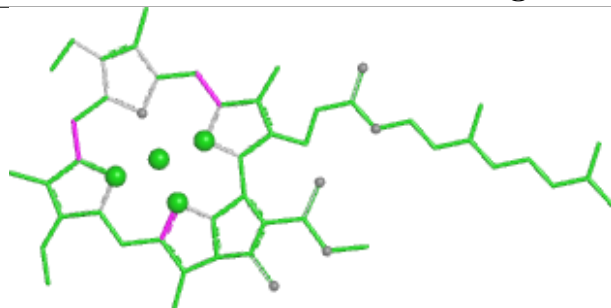


Torsions

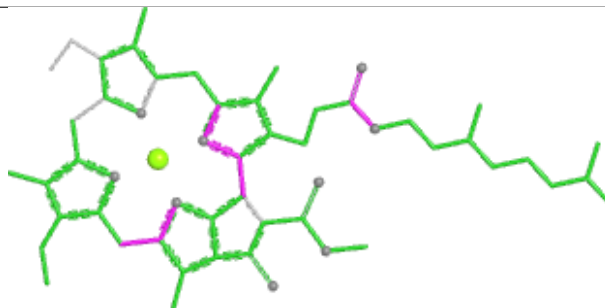


Rings

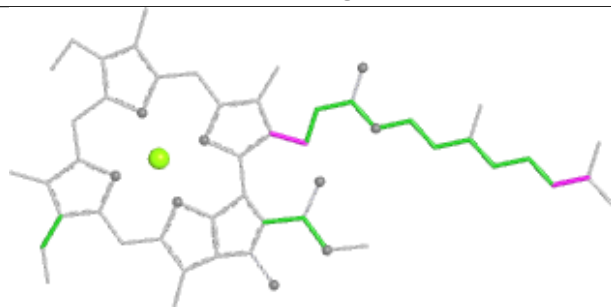
Ligand CLA a 1139



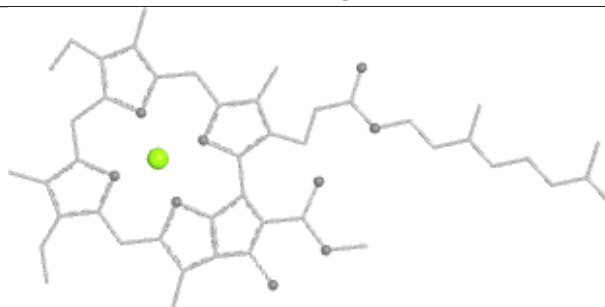
Bond lengths



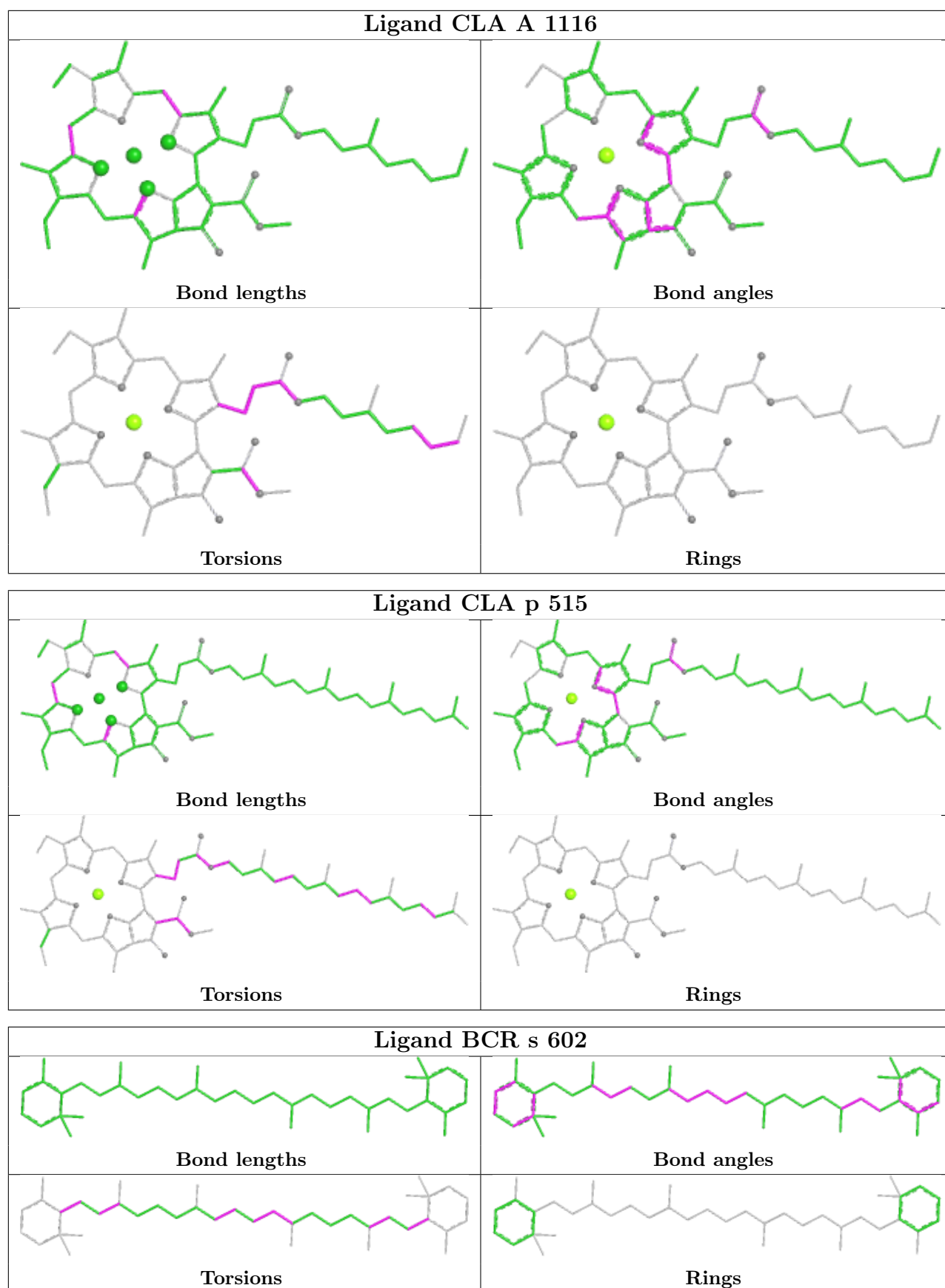
Bond angles

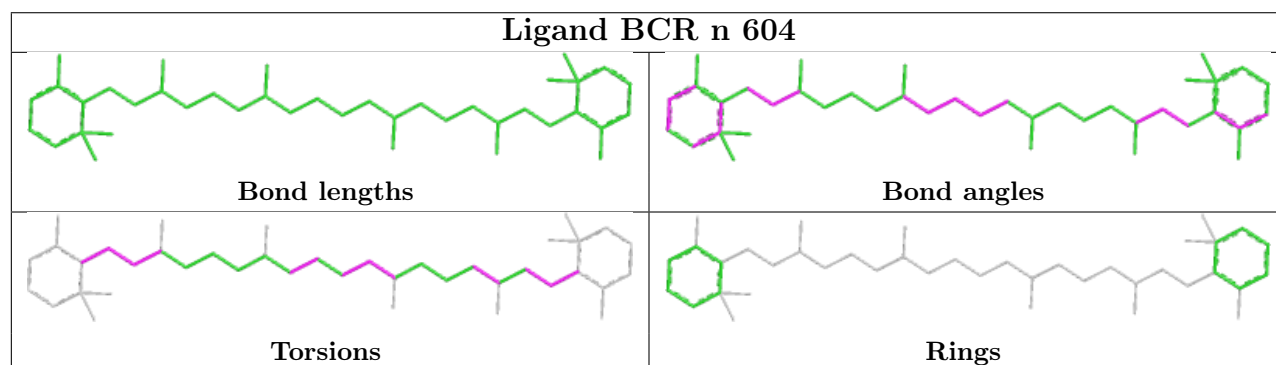
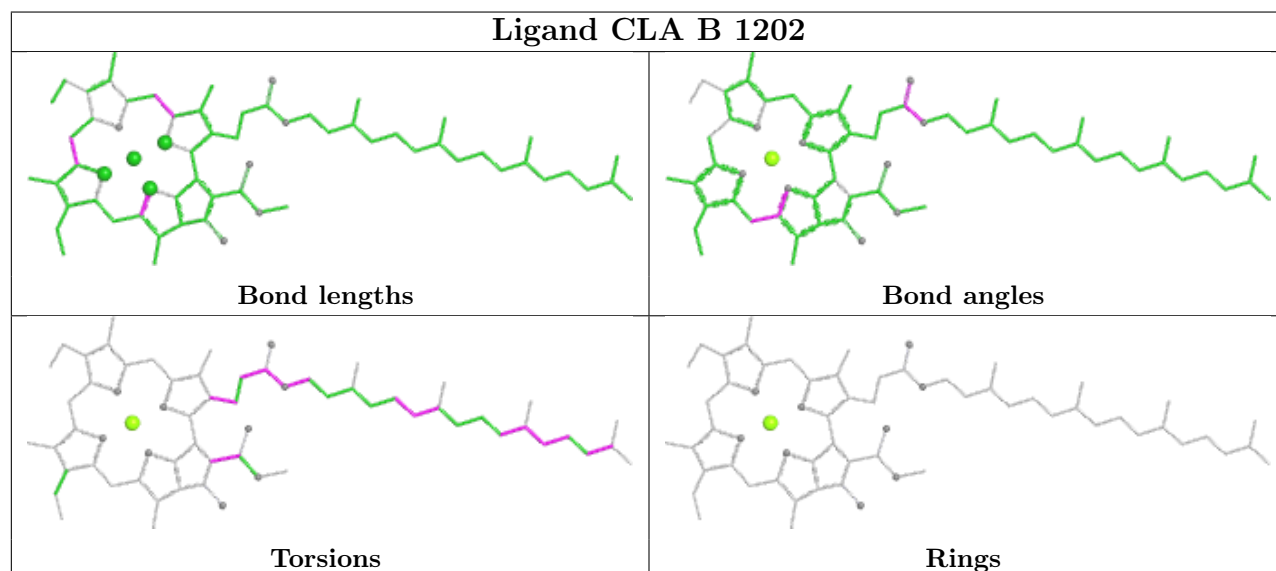
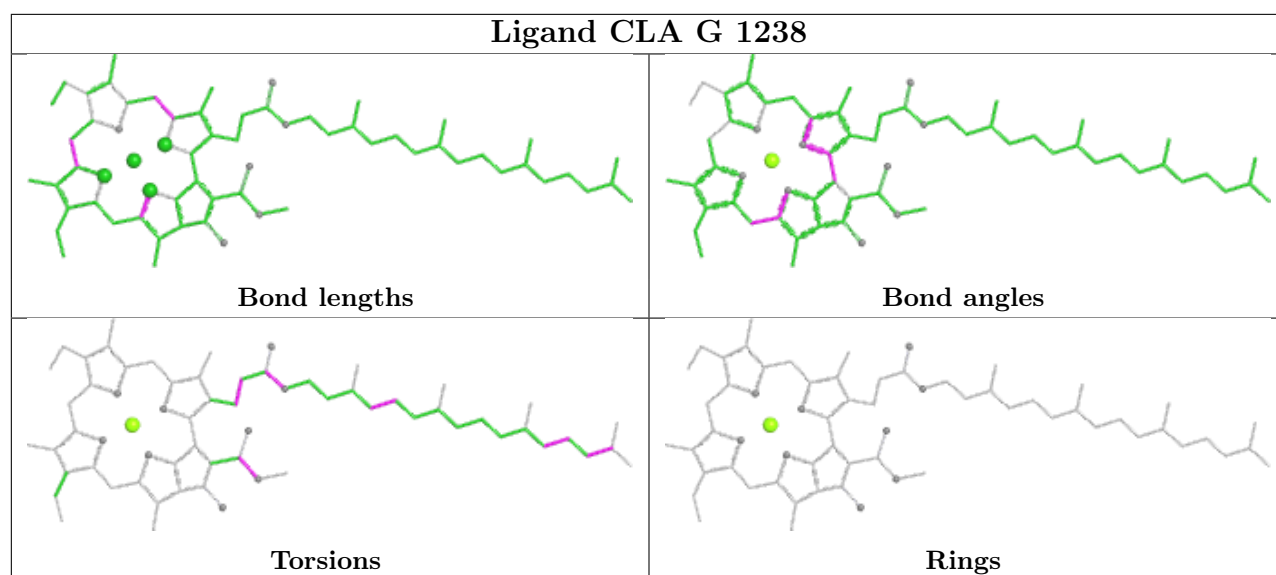


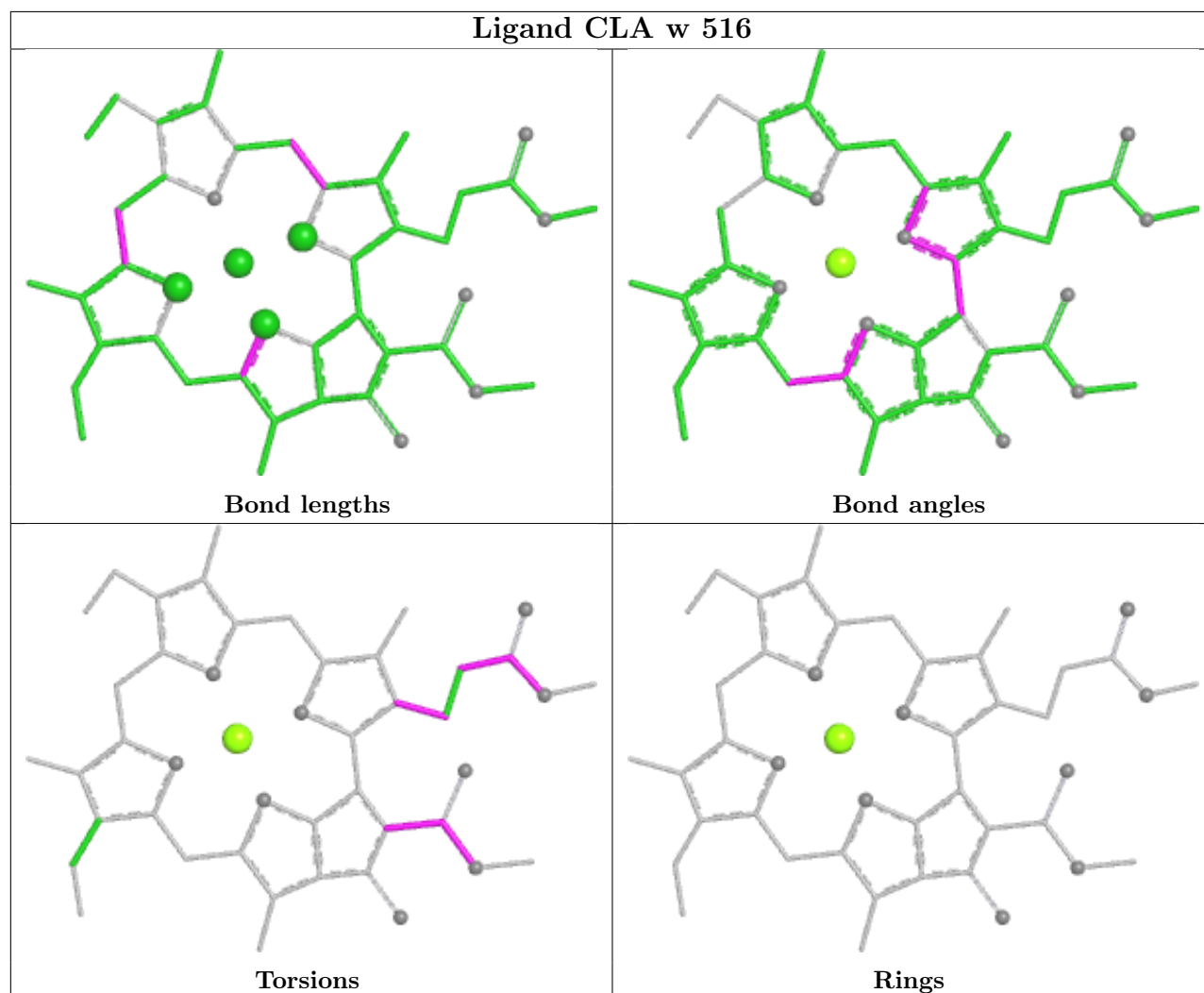
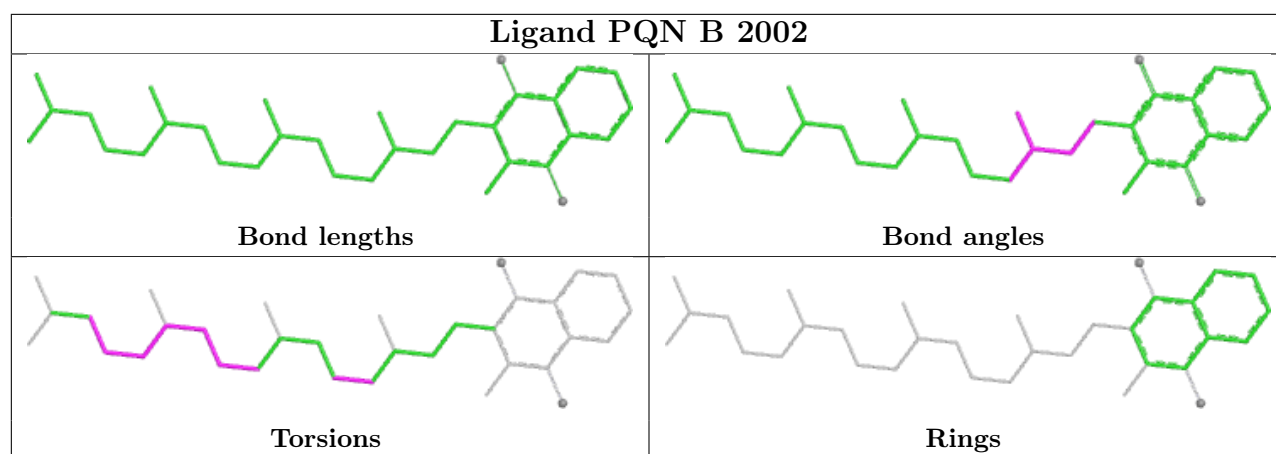
Torsions

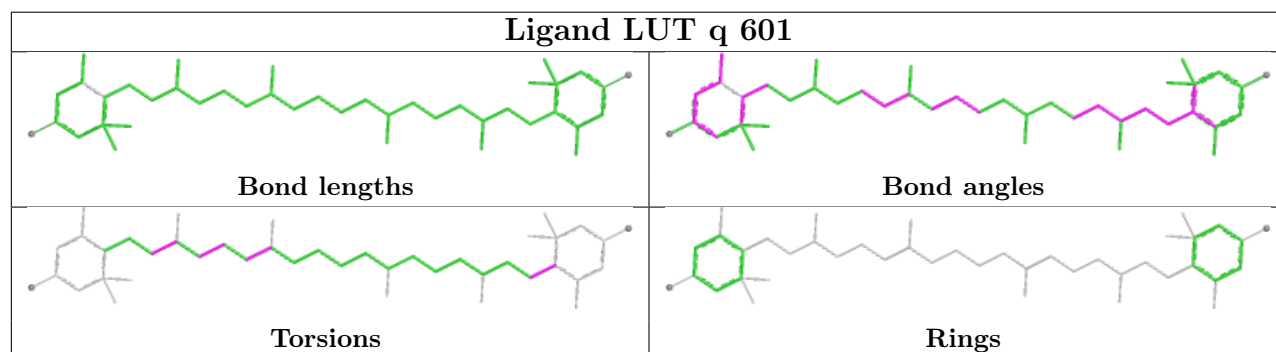
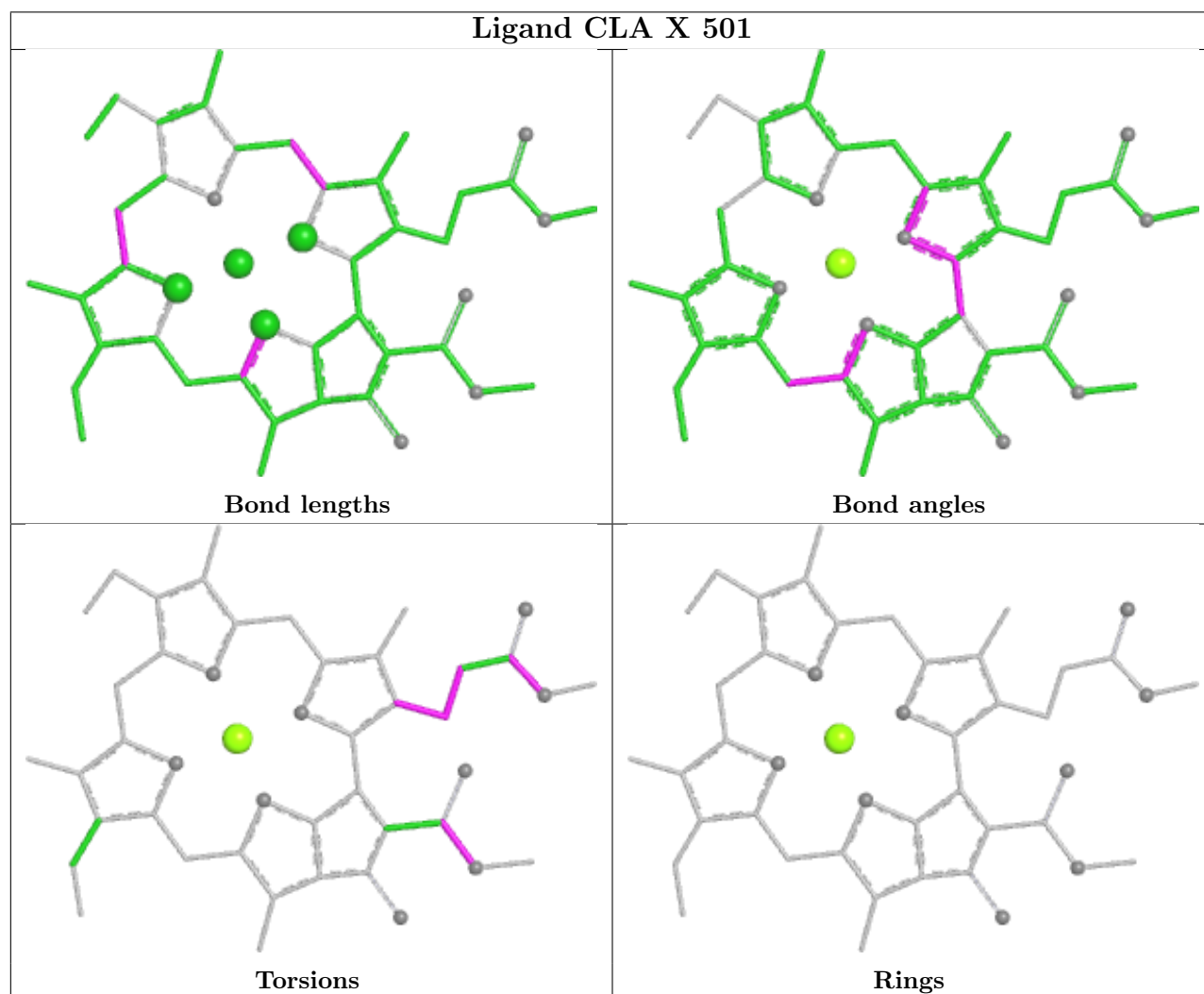
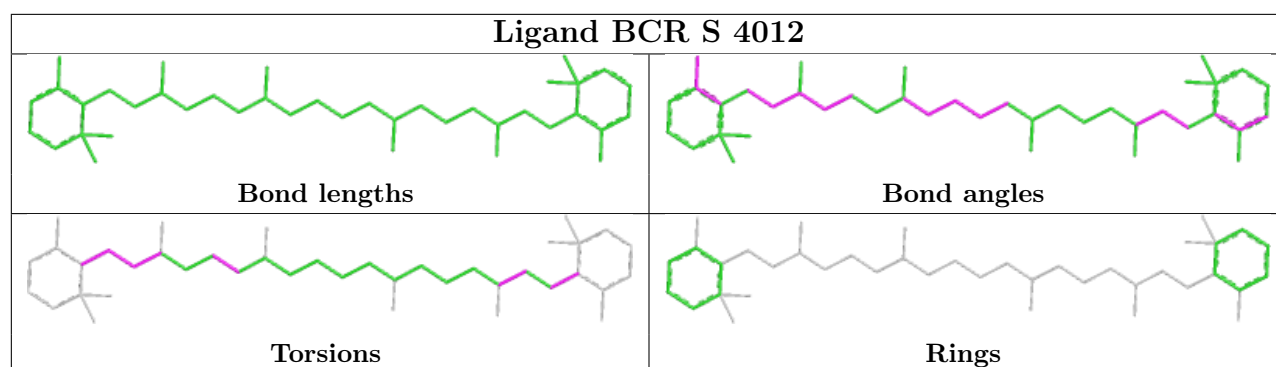


Rings

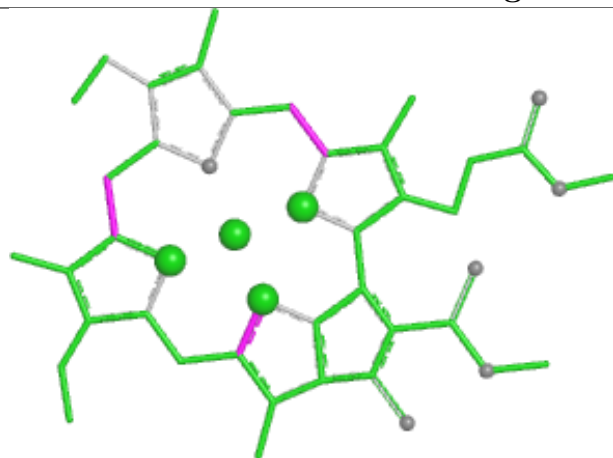




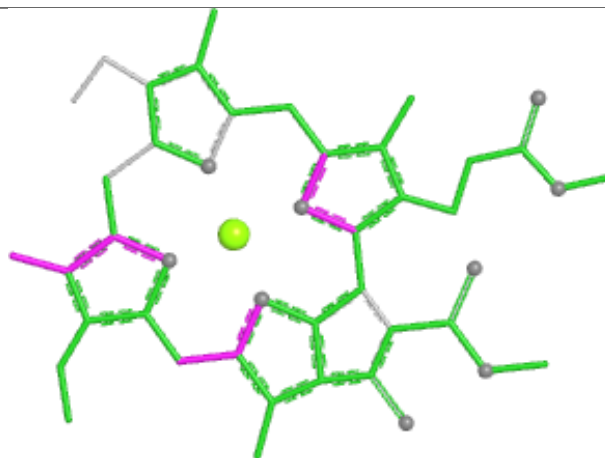




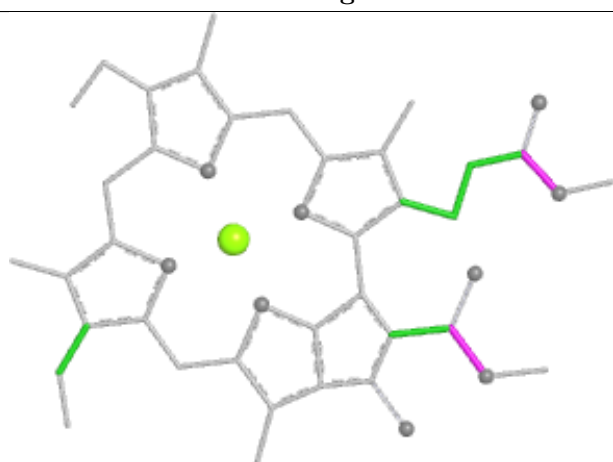
Ligand CLA G 1240



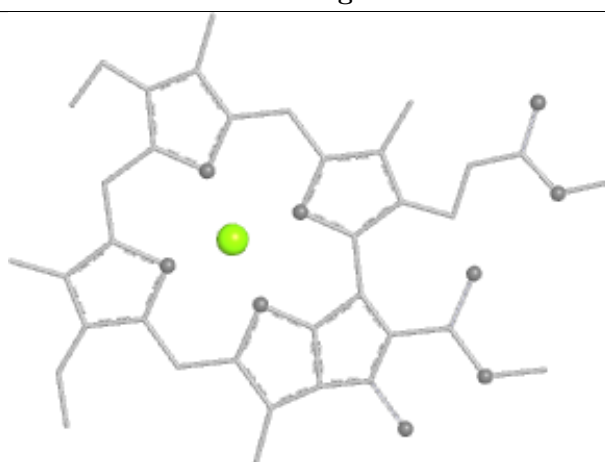
Bond lengths



Bond angles

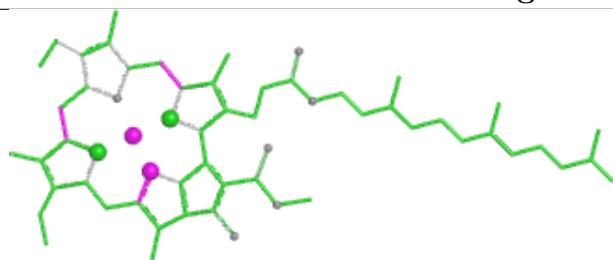


Torsions

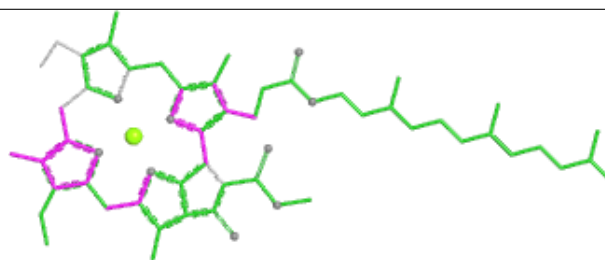


Rings

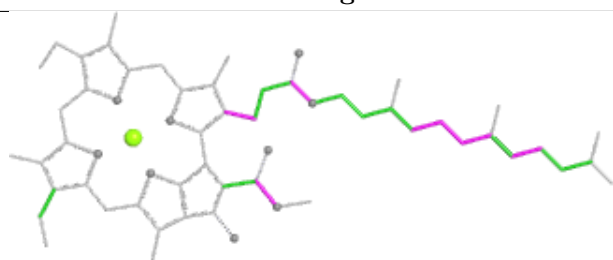
Ligand CLA u 506



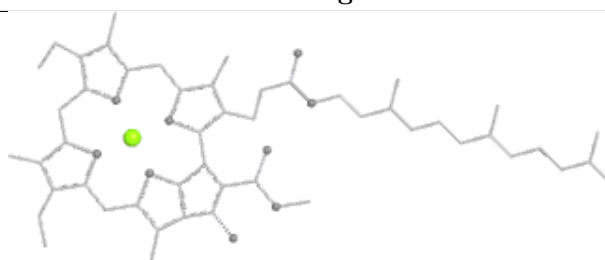
Bond lengths



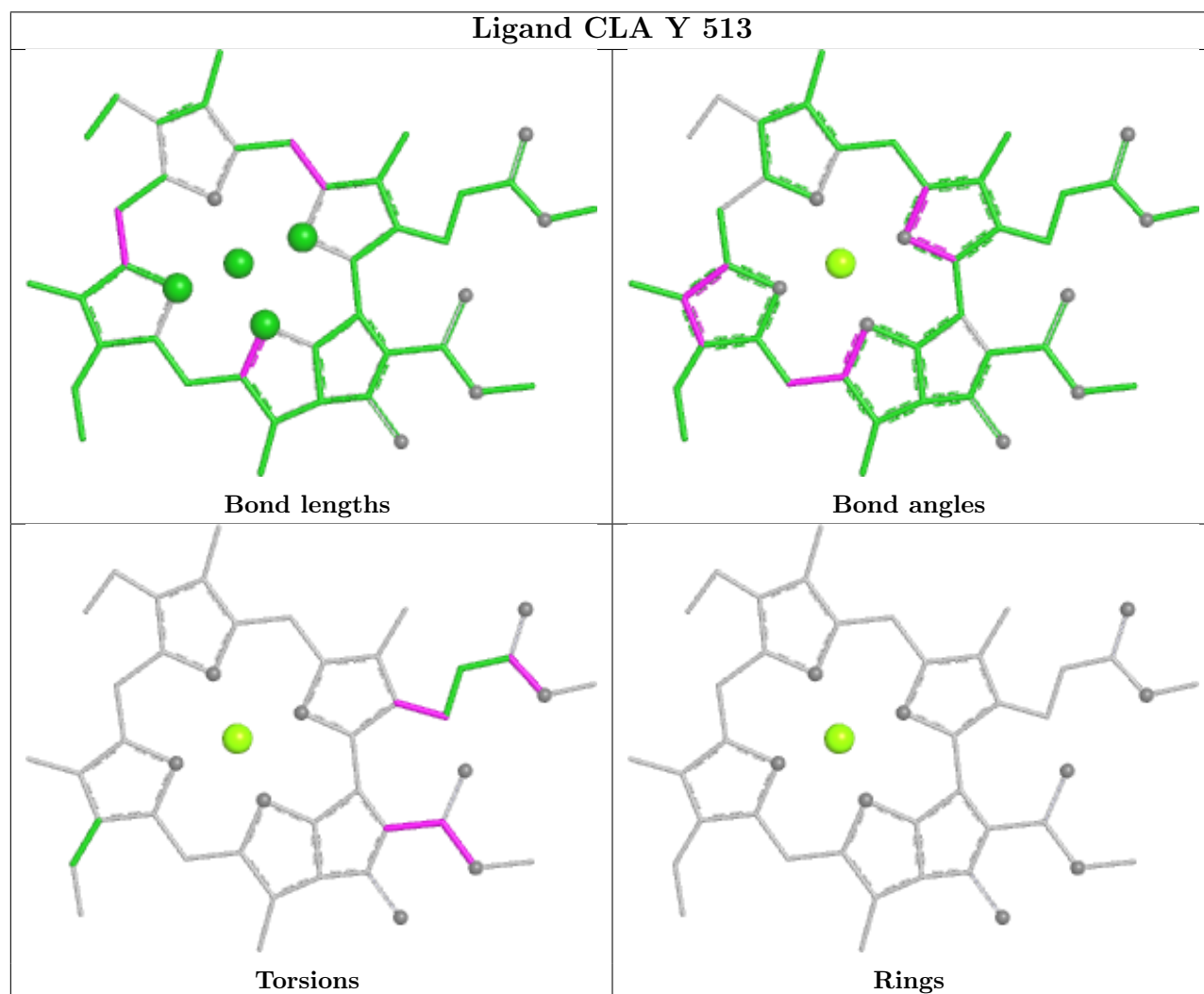
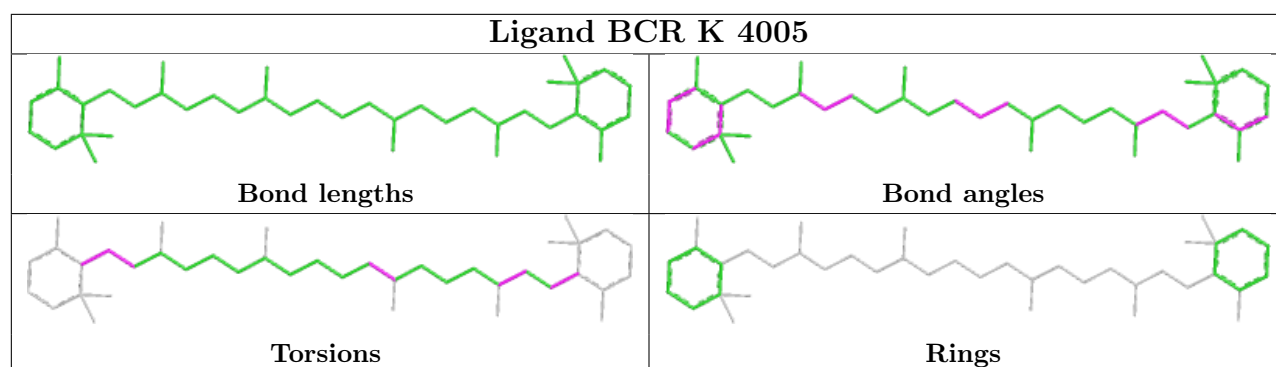
Bond angles



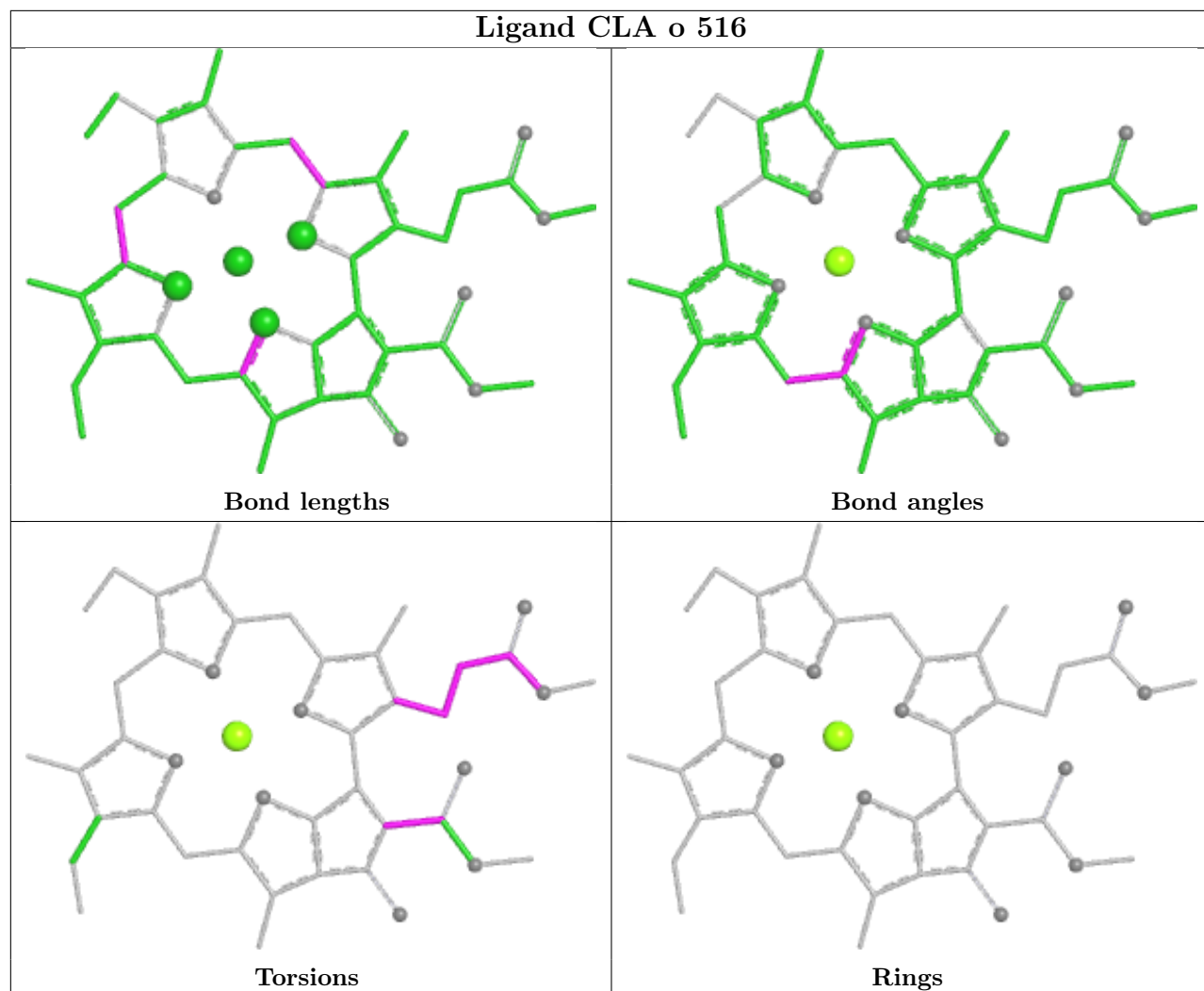
Torsions

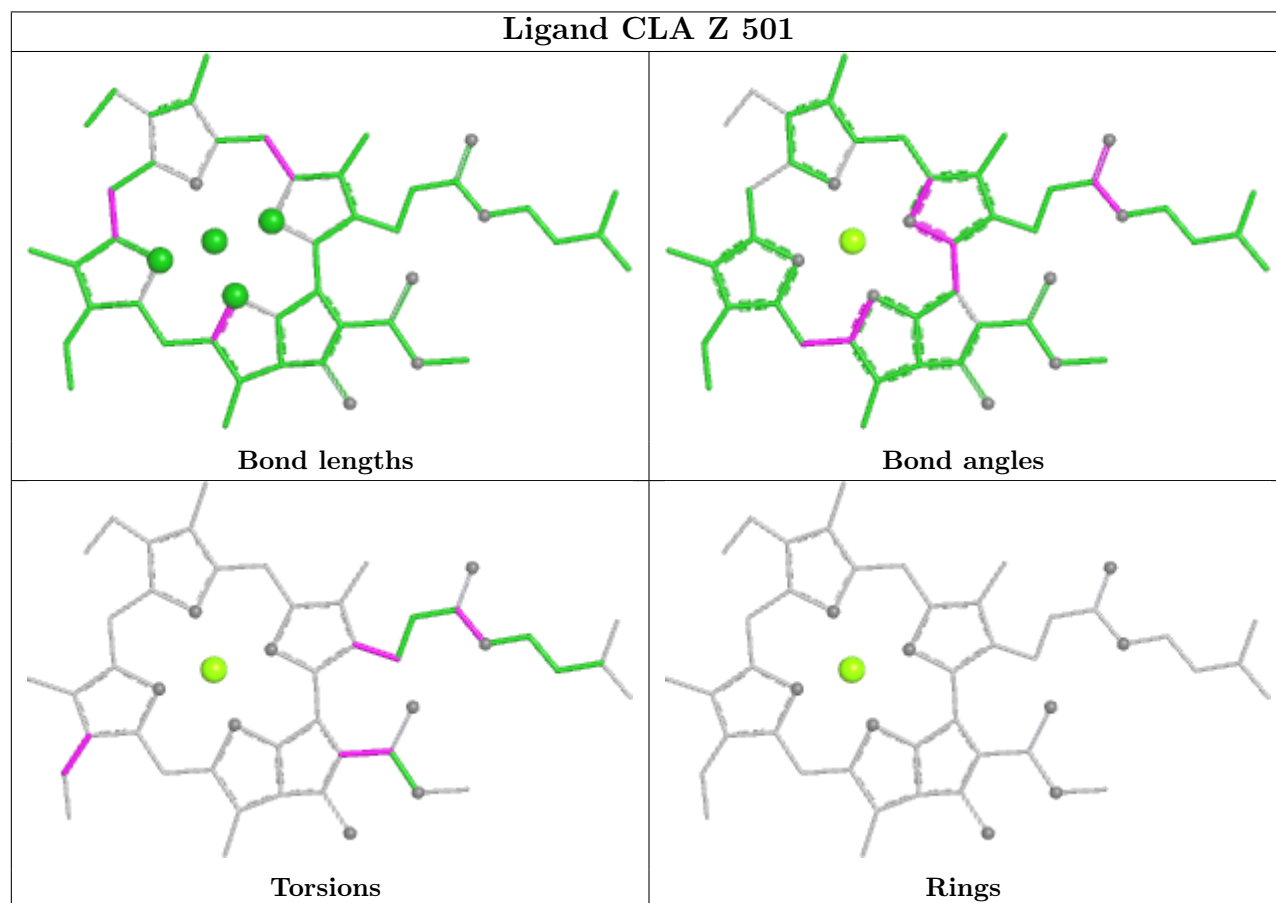
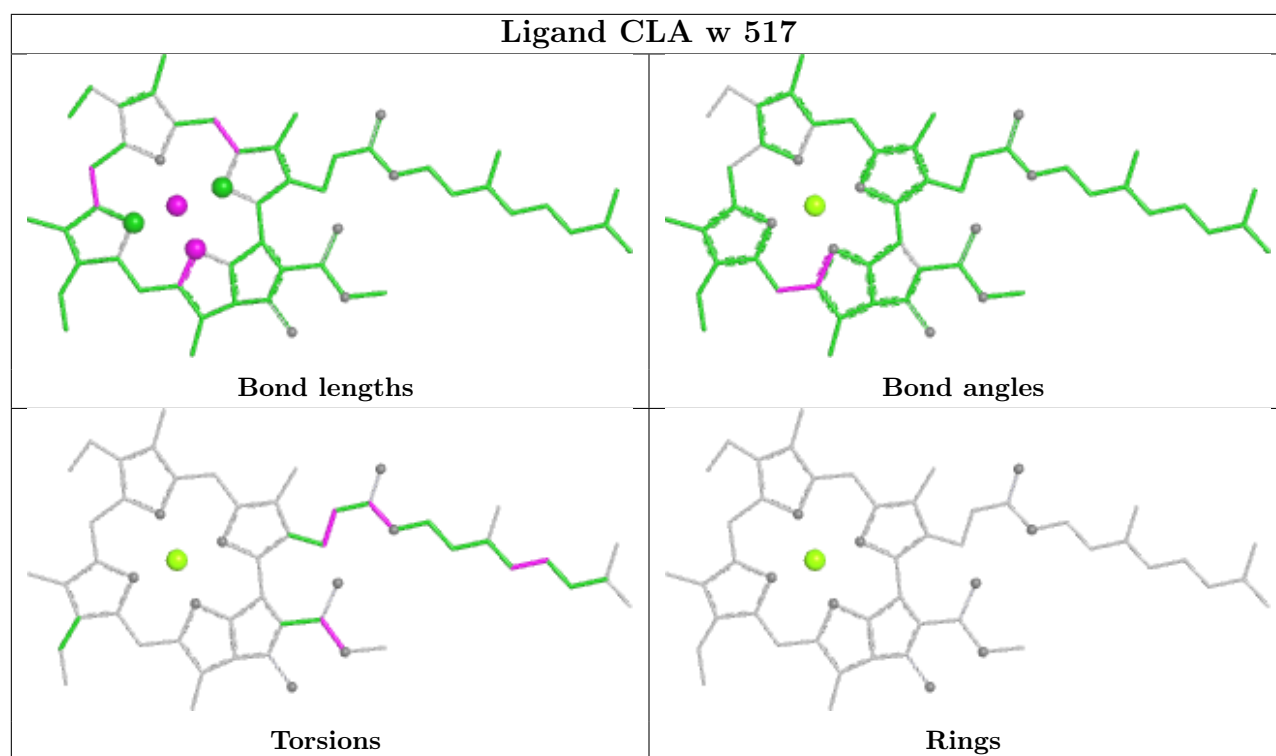


Rings

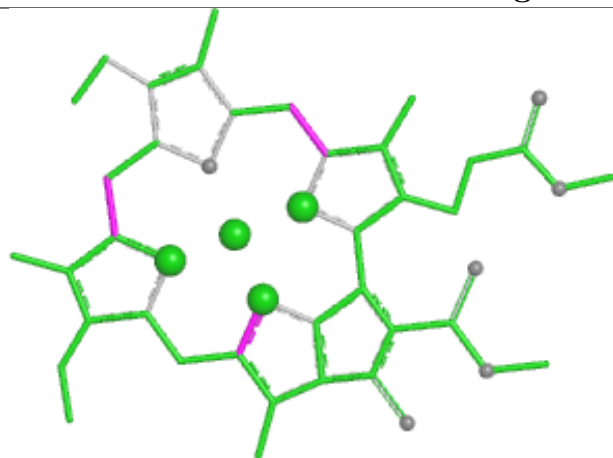


Ligand CLA o 516

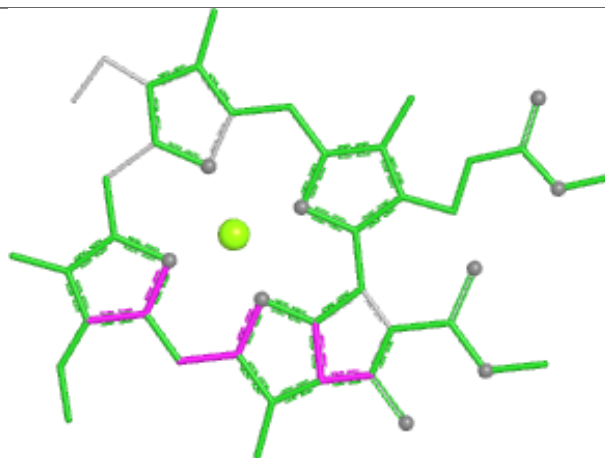




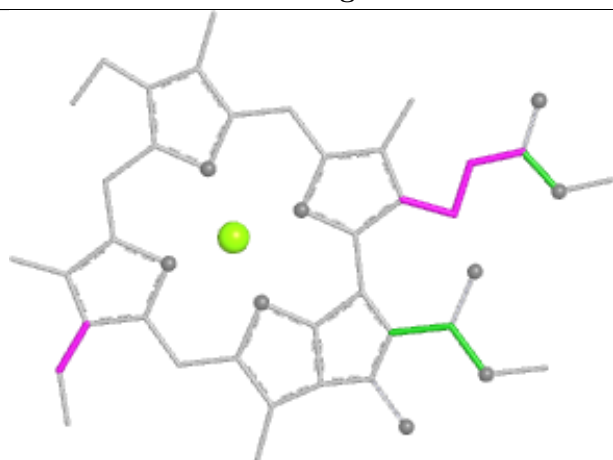
Ligand CLA Y 503



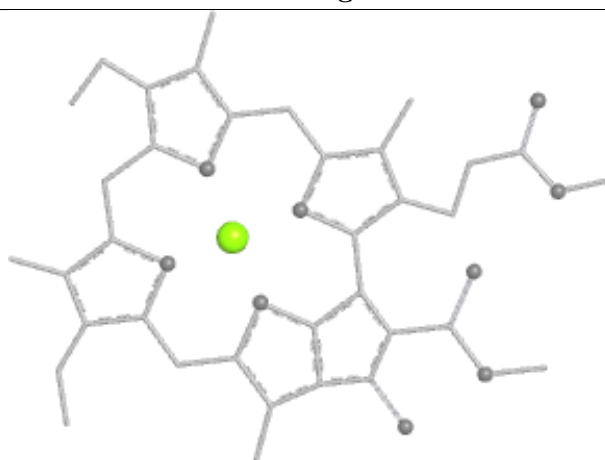
Bond lengths



Bond angles

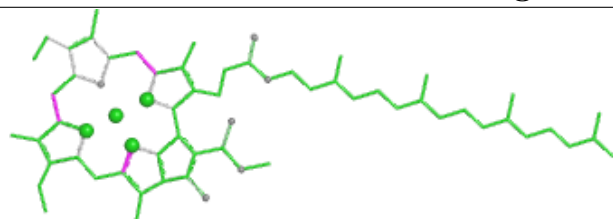


Torsions

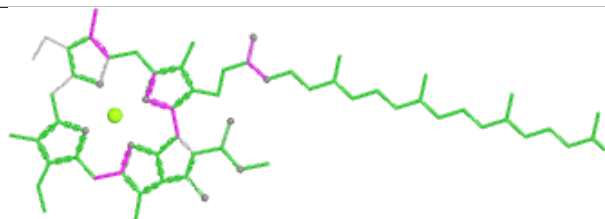


Rings

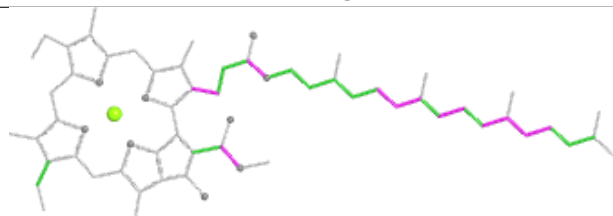
Ligand CLA Y 511



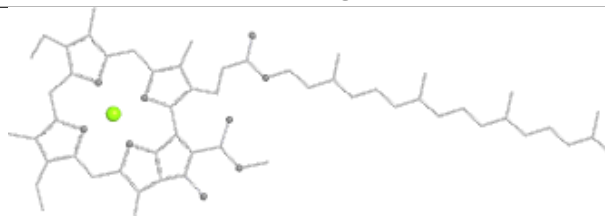
Bond lengths



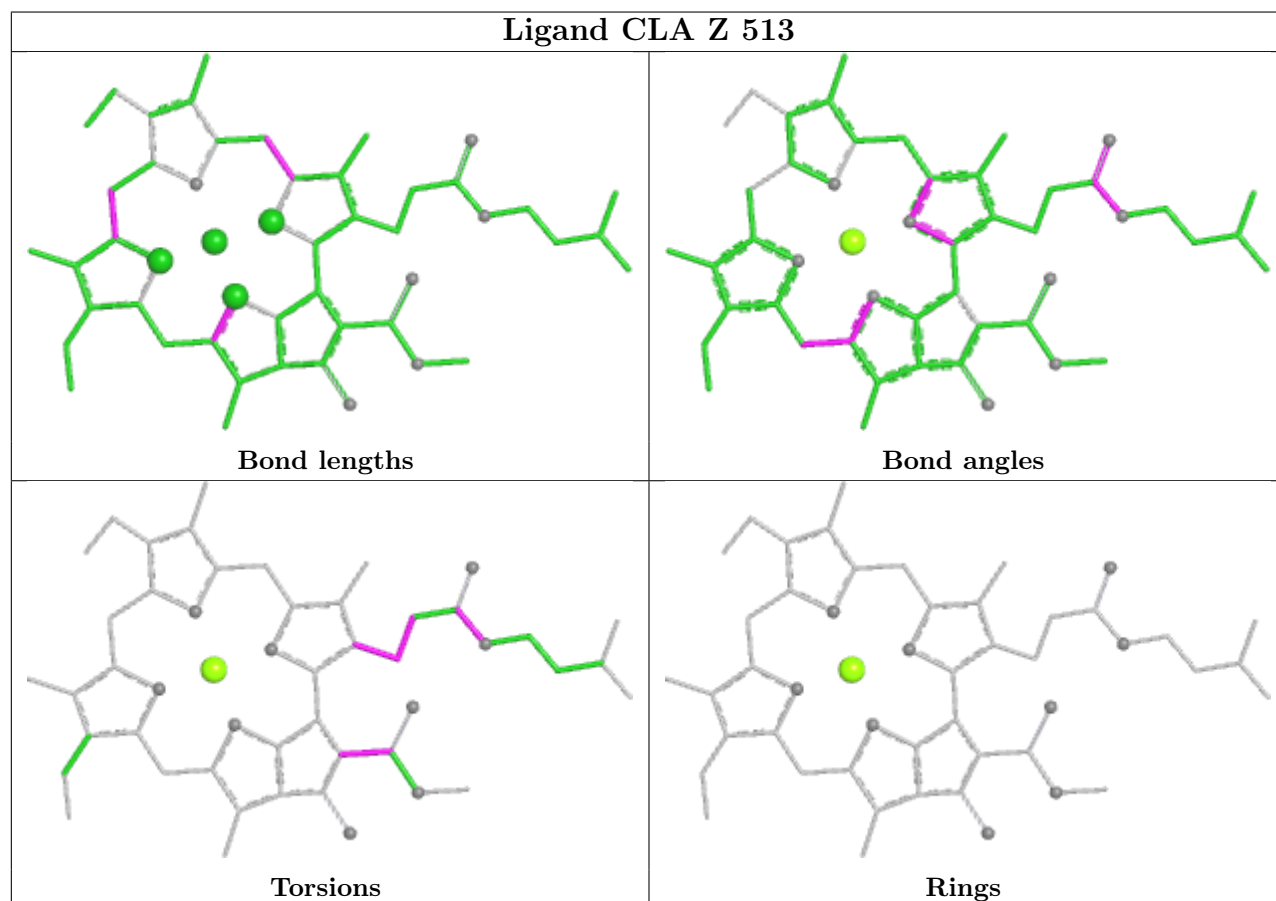
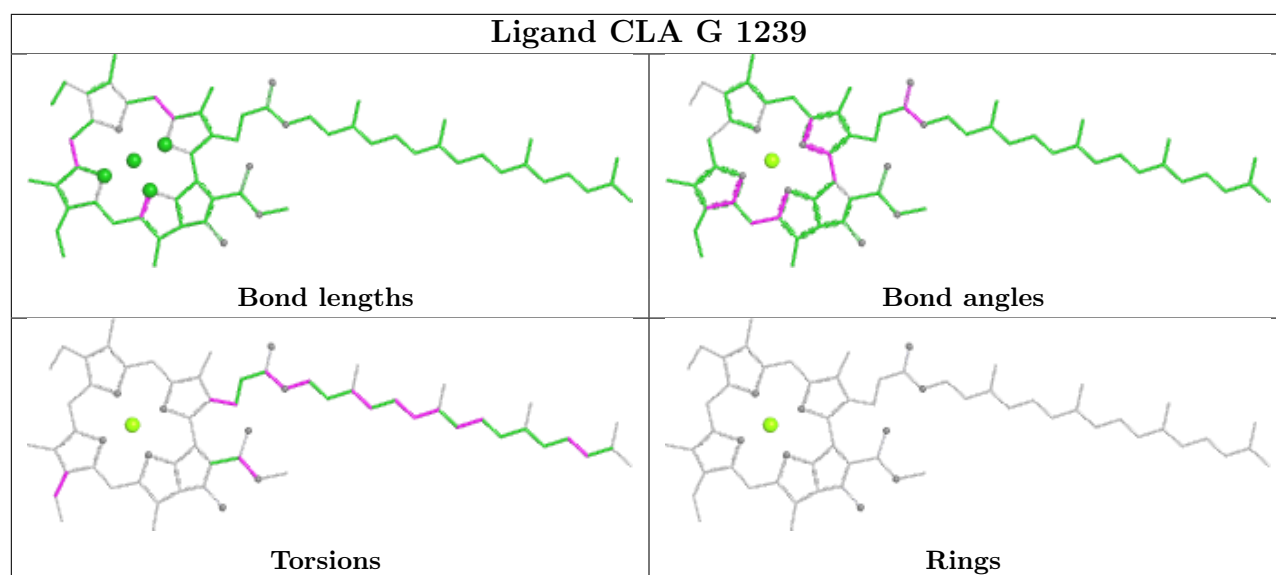
Bond angles



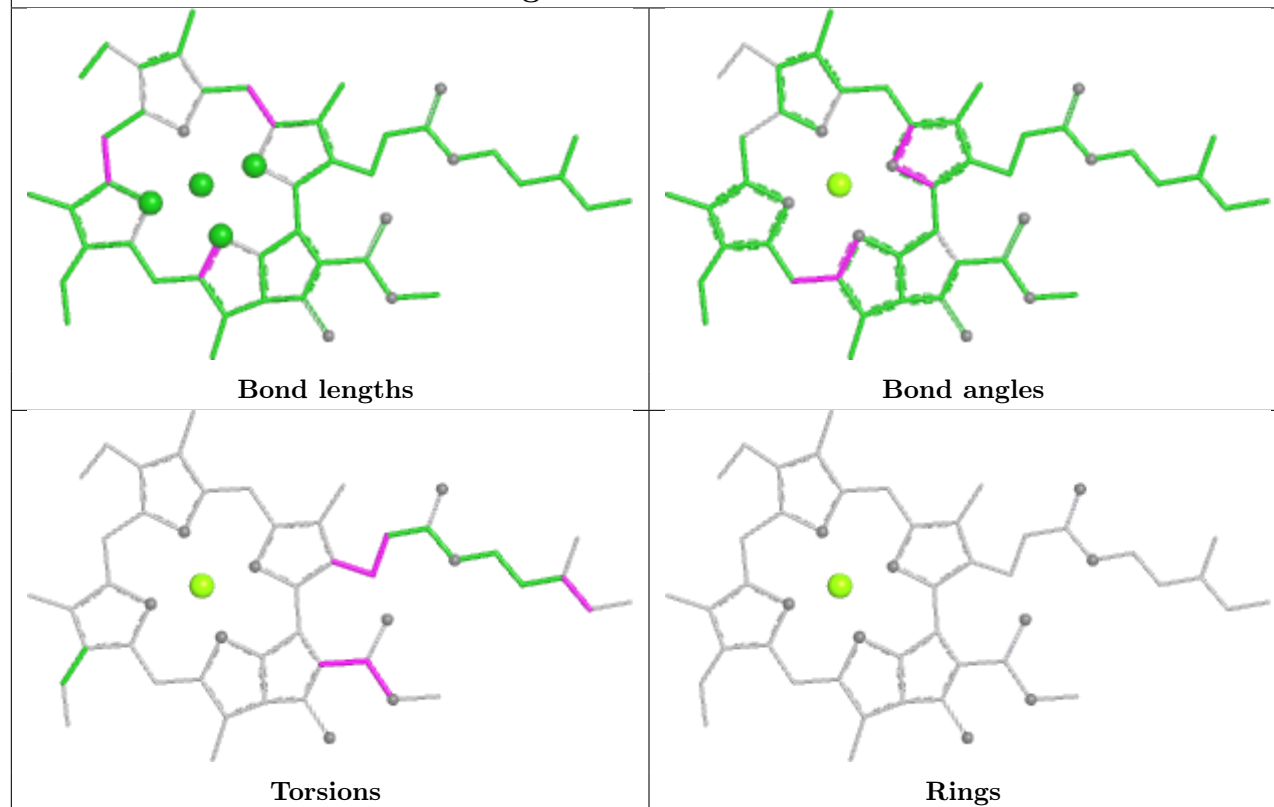
Torsions



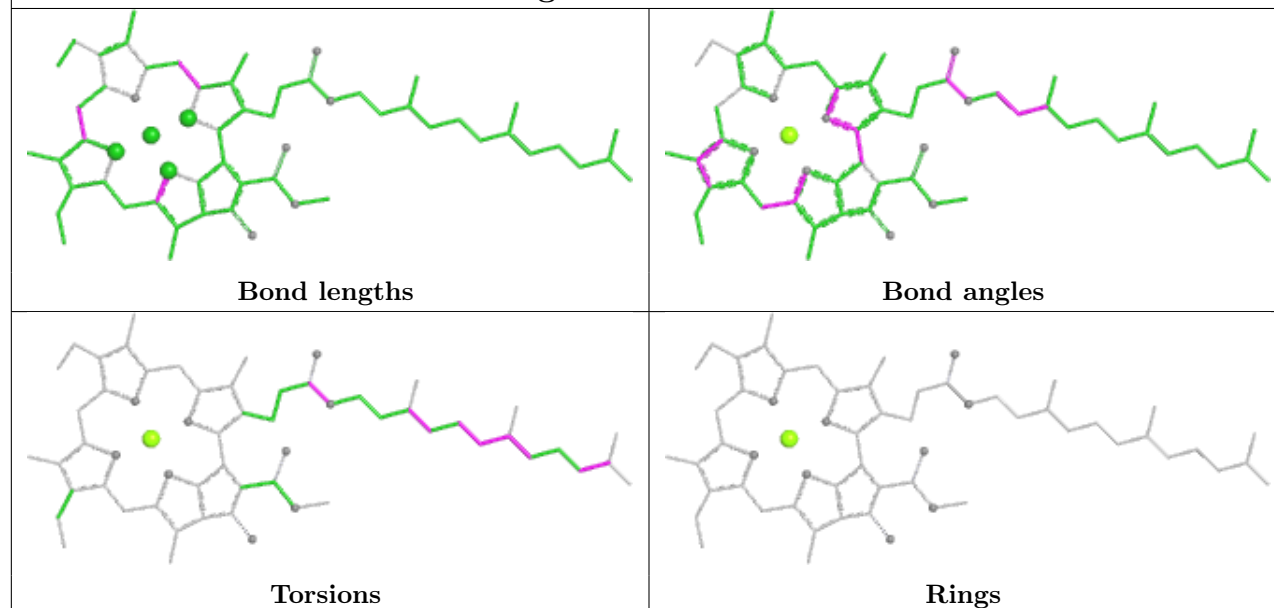
Rings

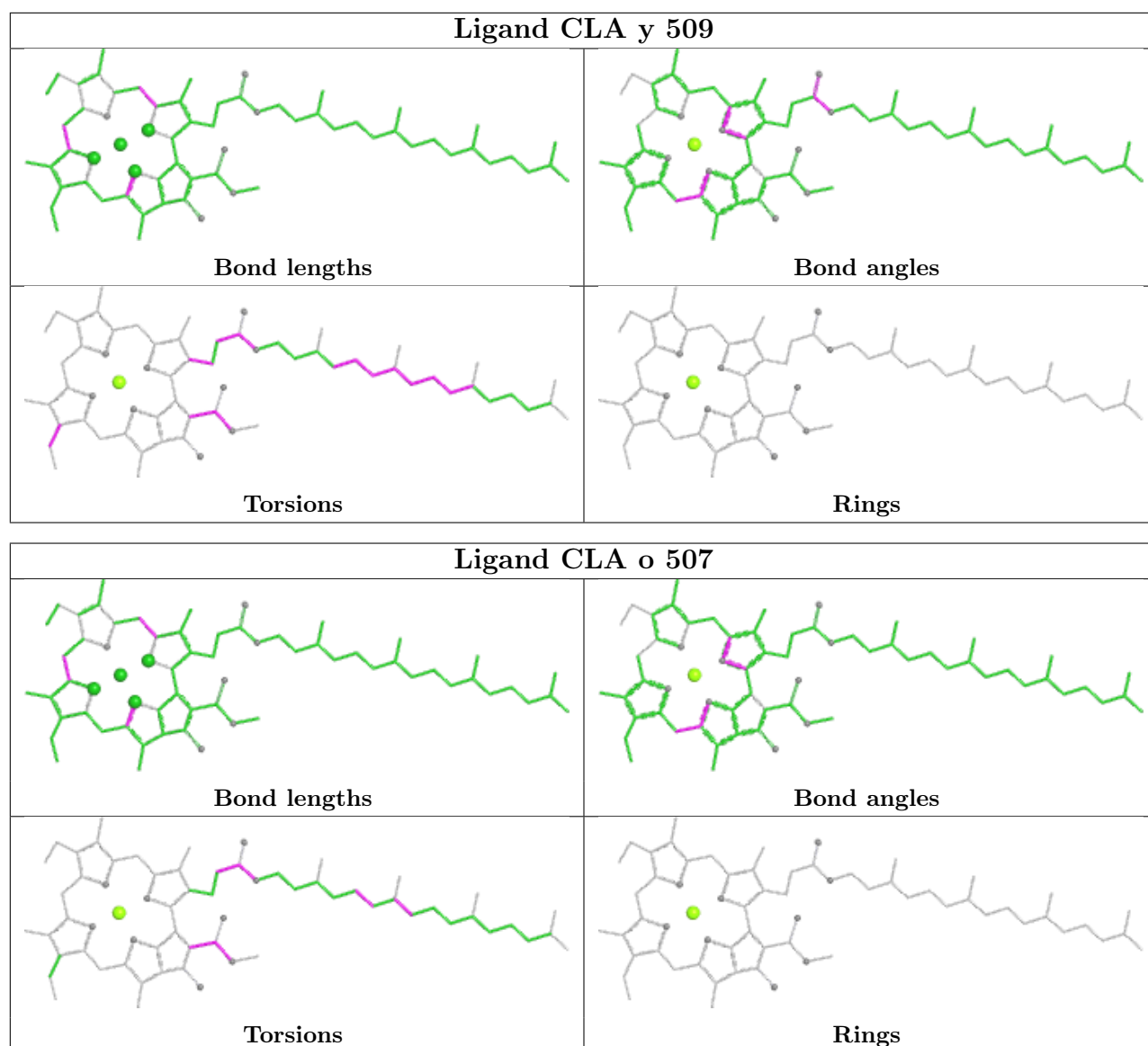


Ligand CLA H 1121

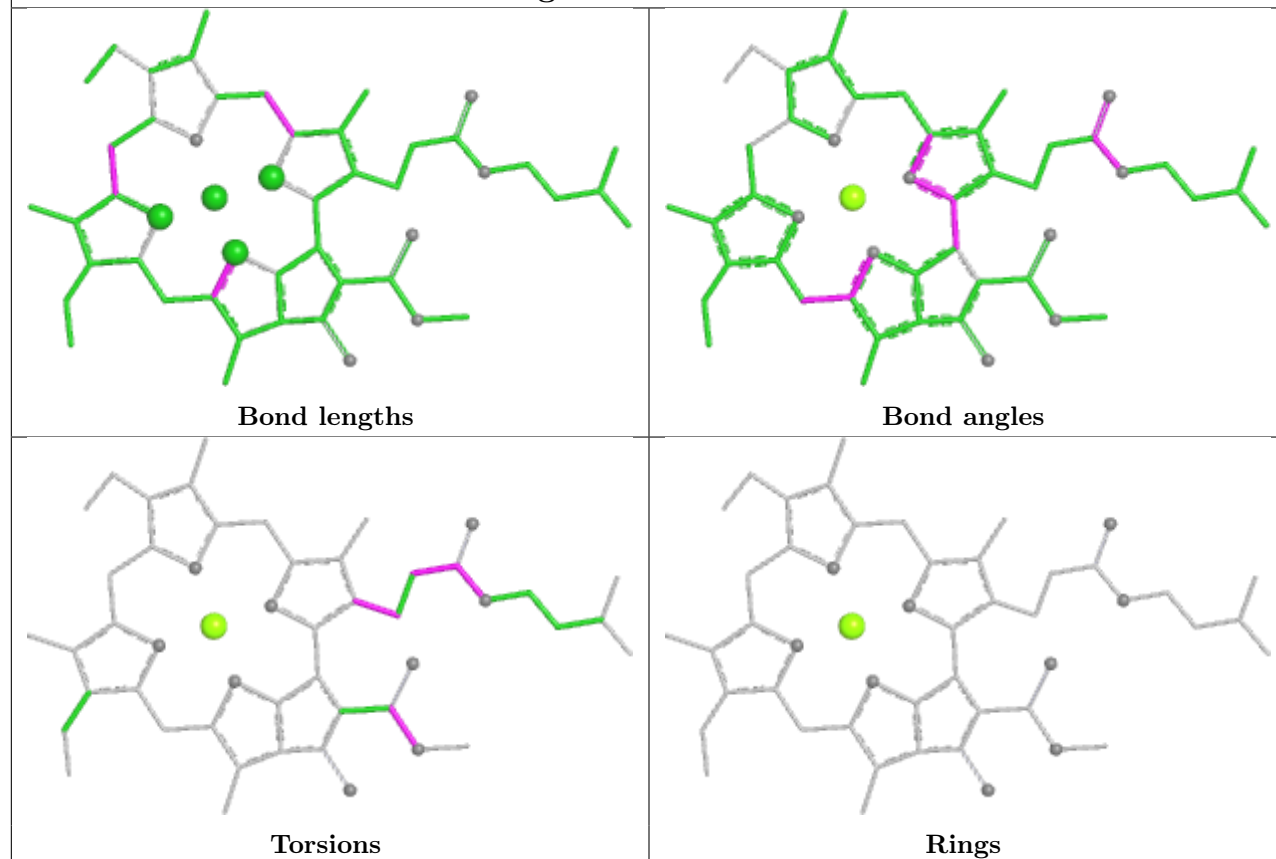


Ligand CLA r 506

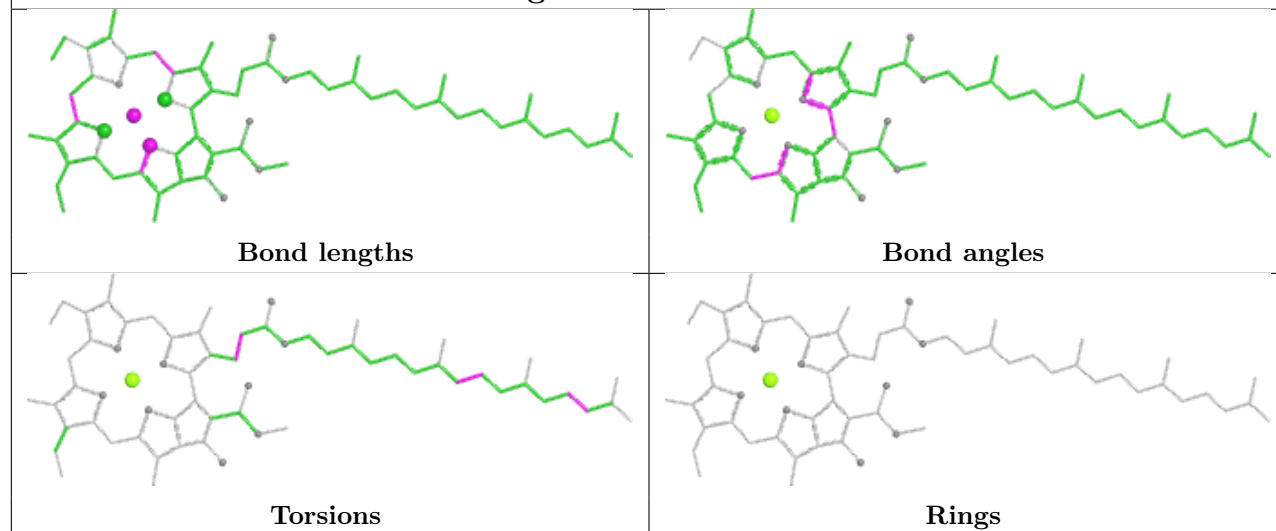


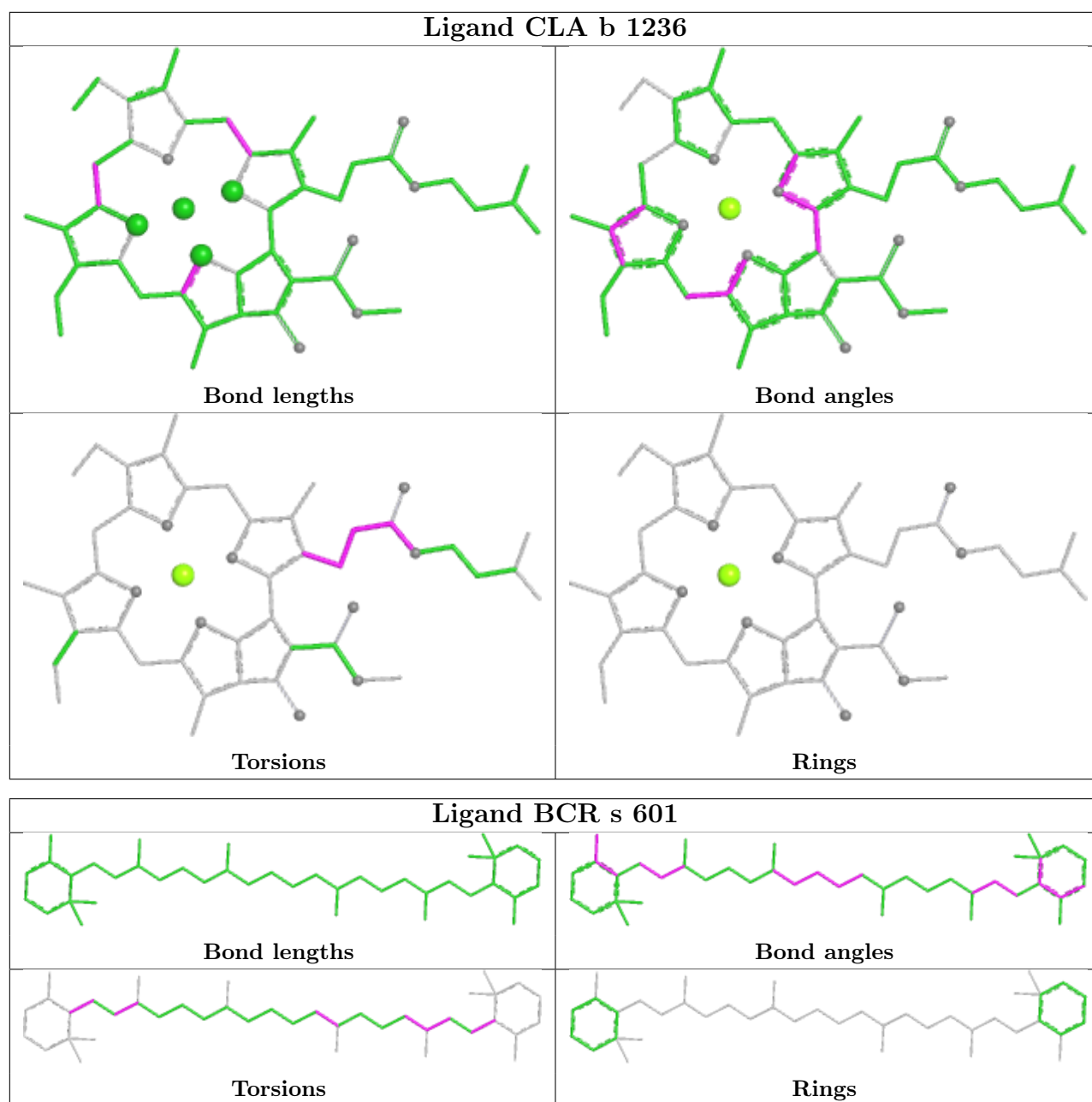


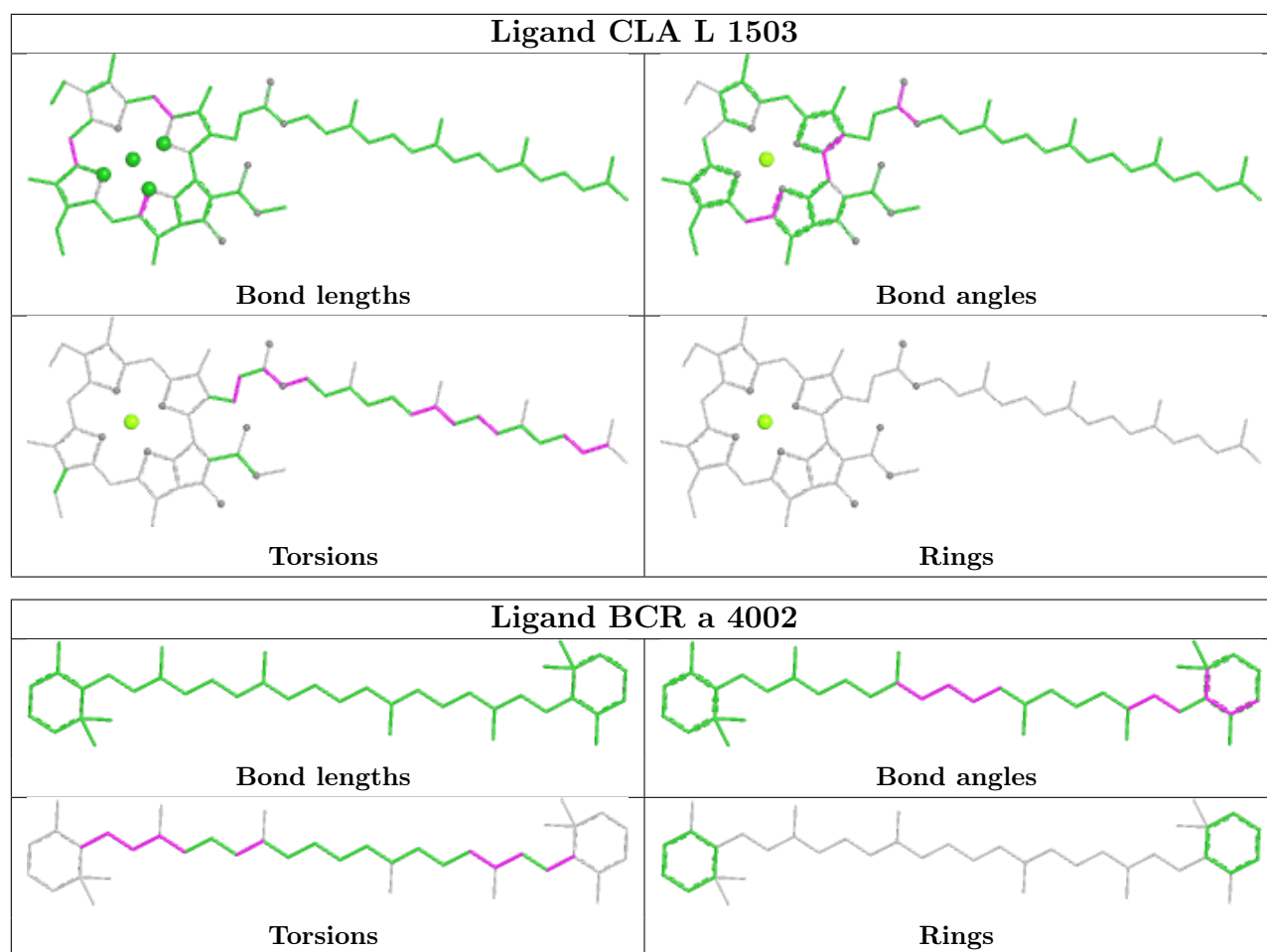
Ligand CLA s 514

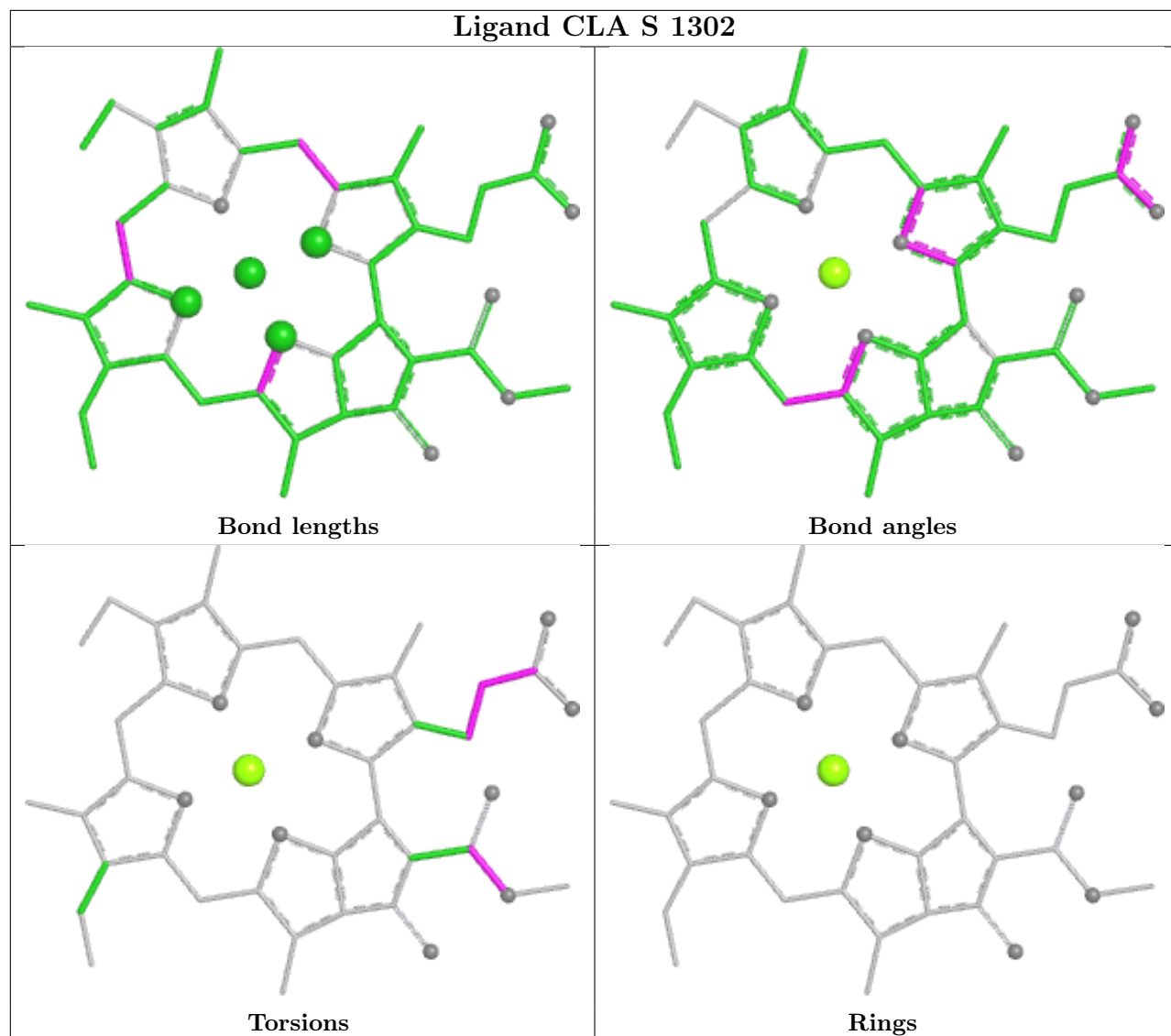


Ligand CLA a 1127

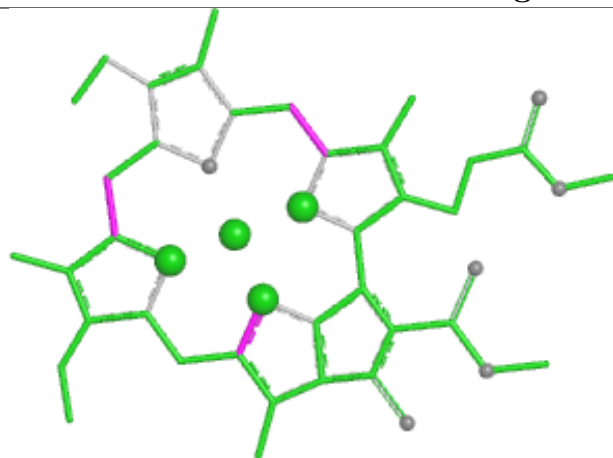




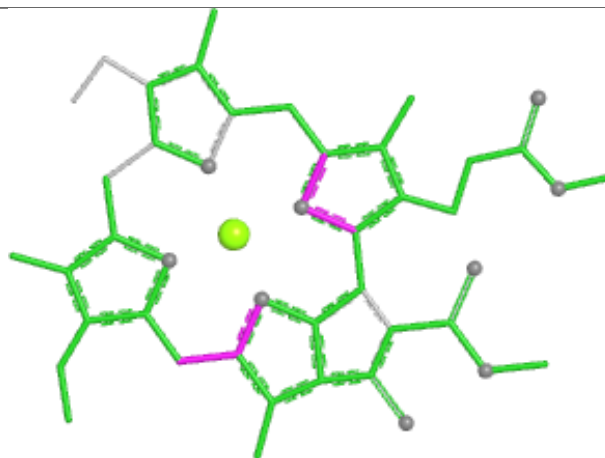




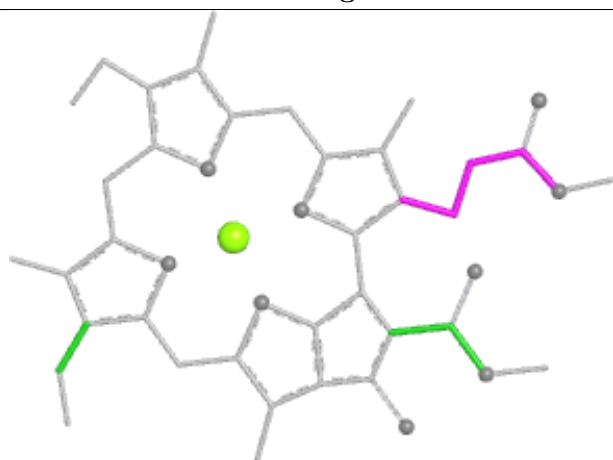
Ligand CLA X 516



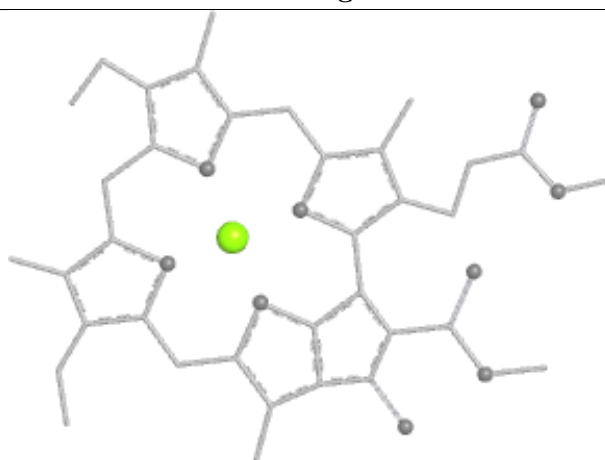
Bond lengths



Bond angles

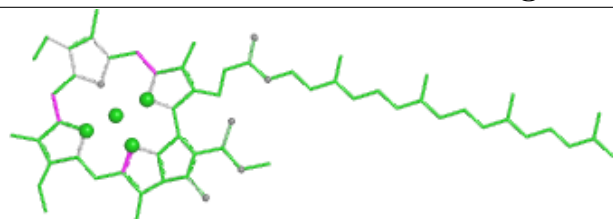


Torsions

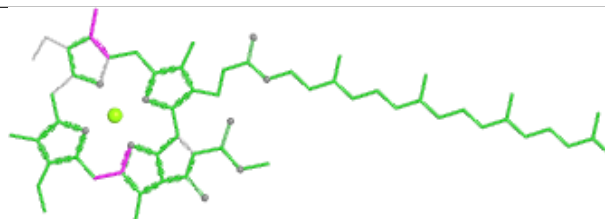


Rings

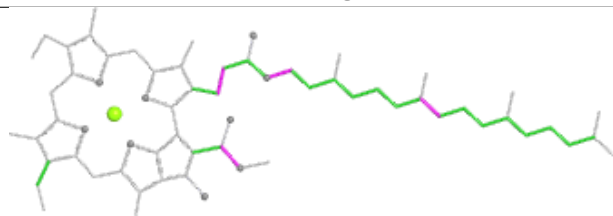
Ligand CLA r 511



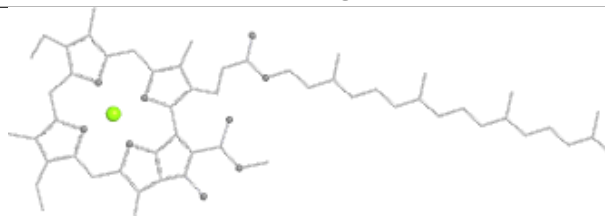
Bond lengths



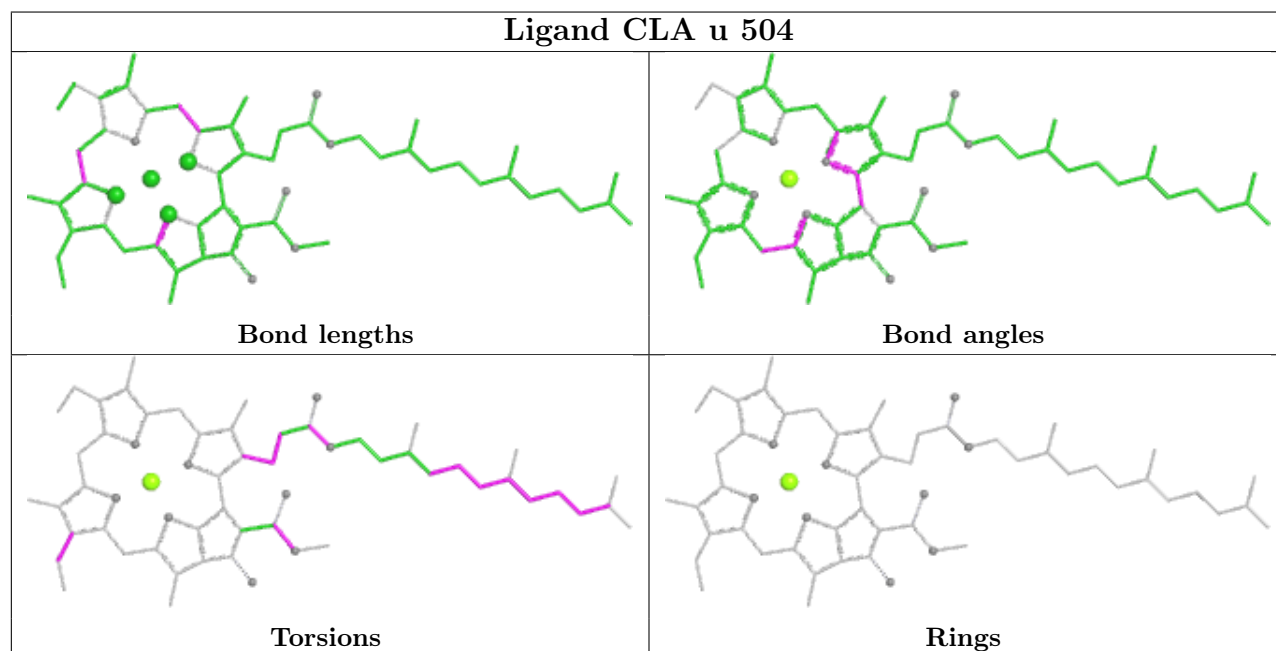
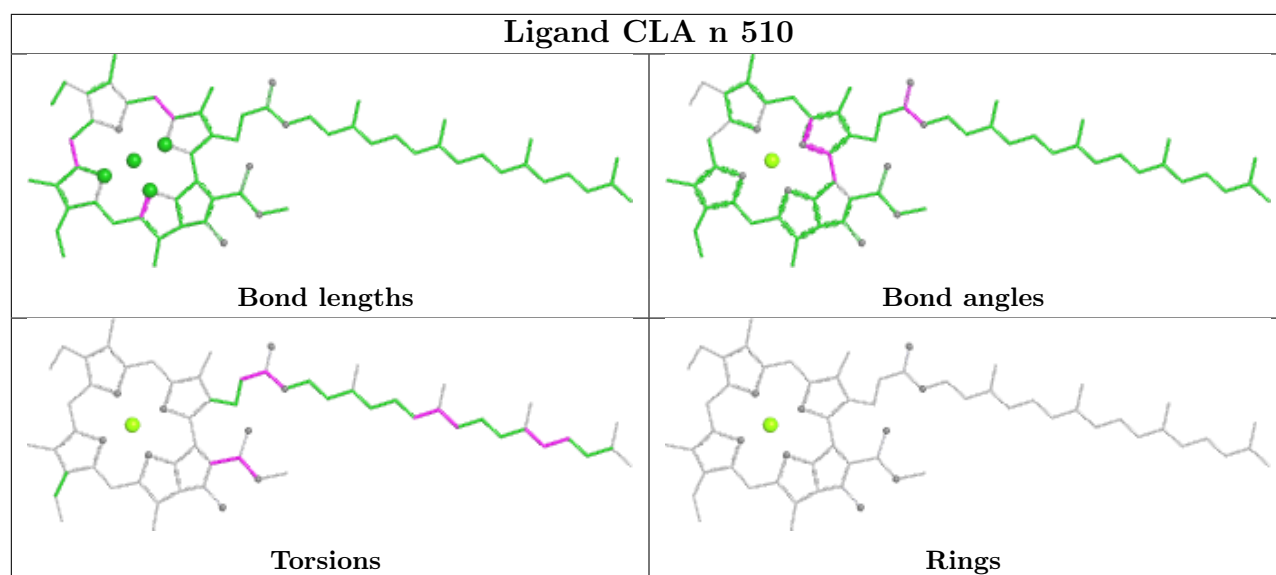
Bond angles

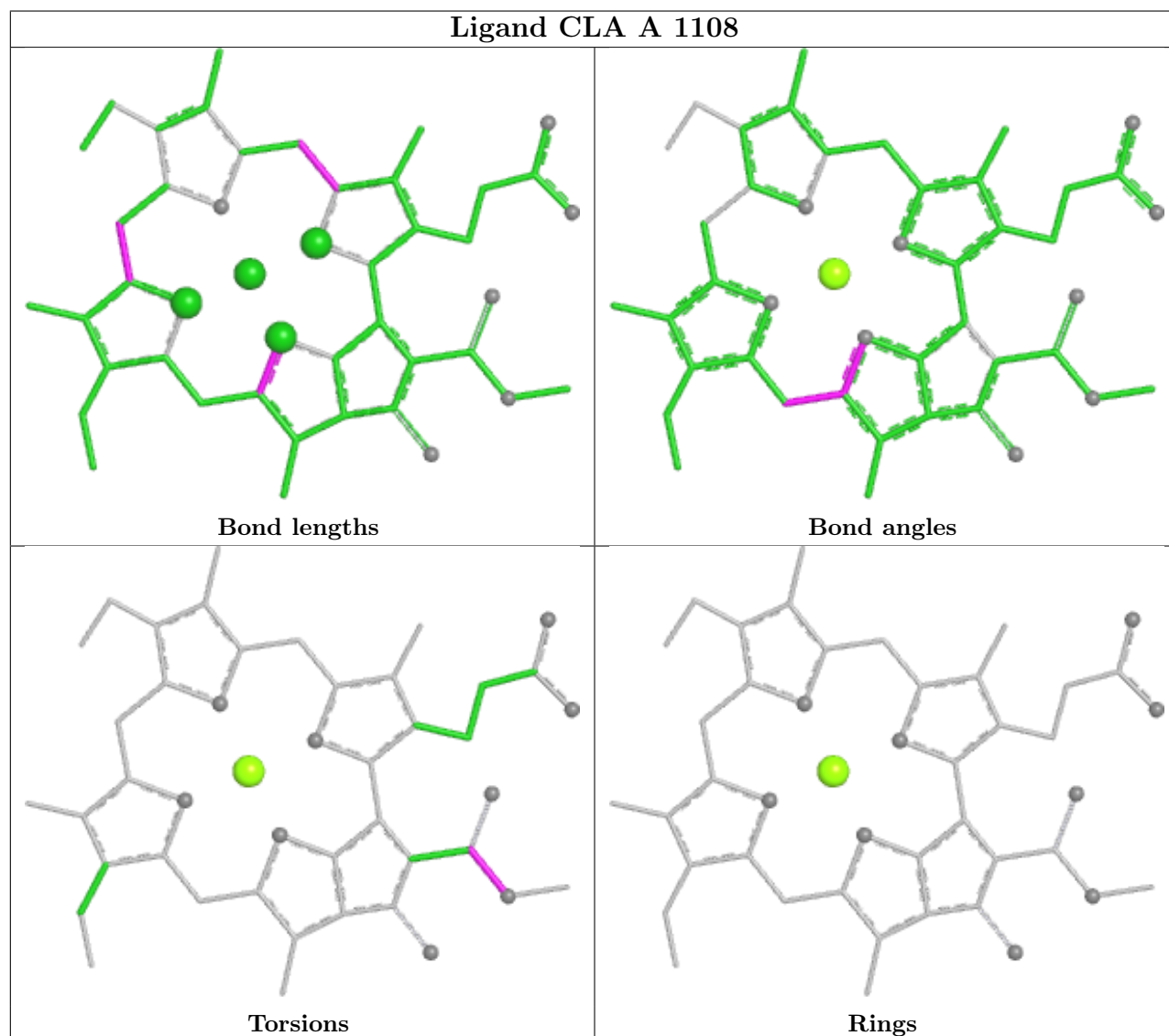
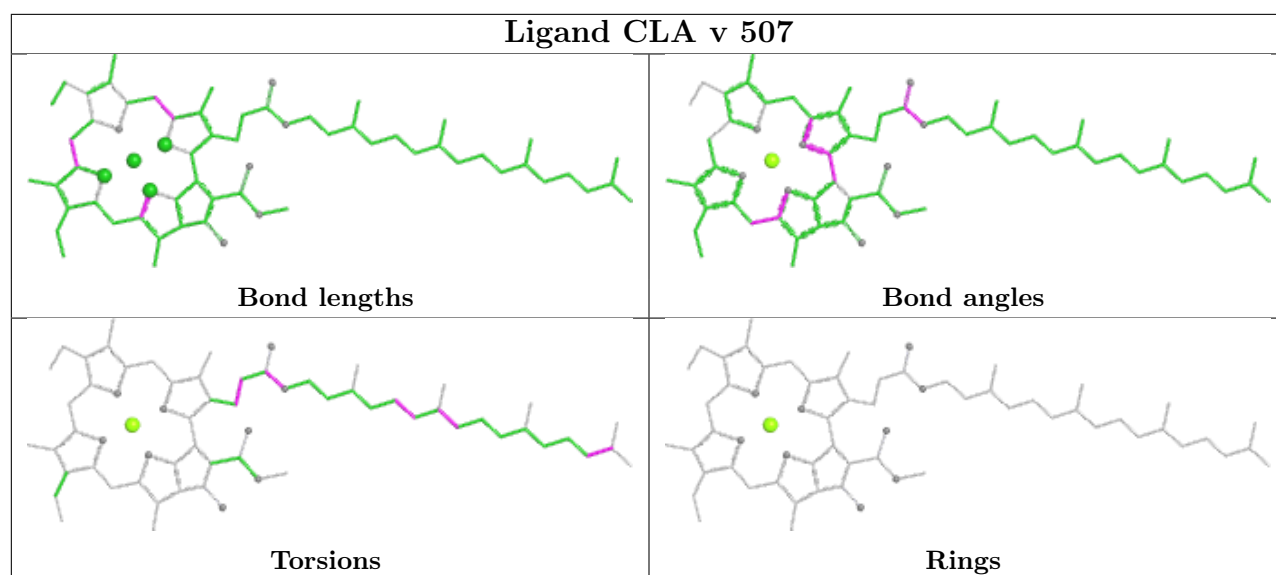


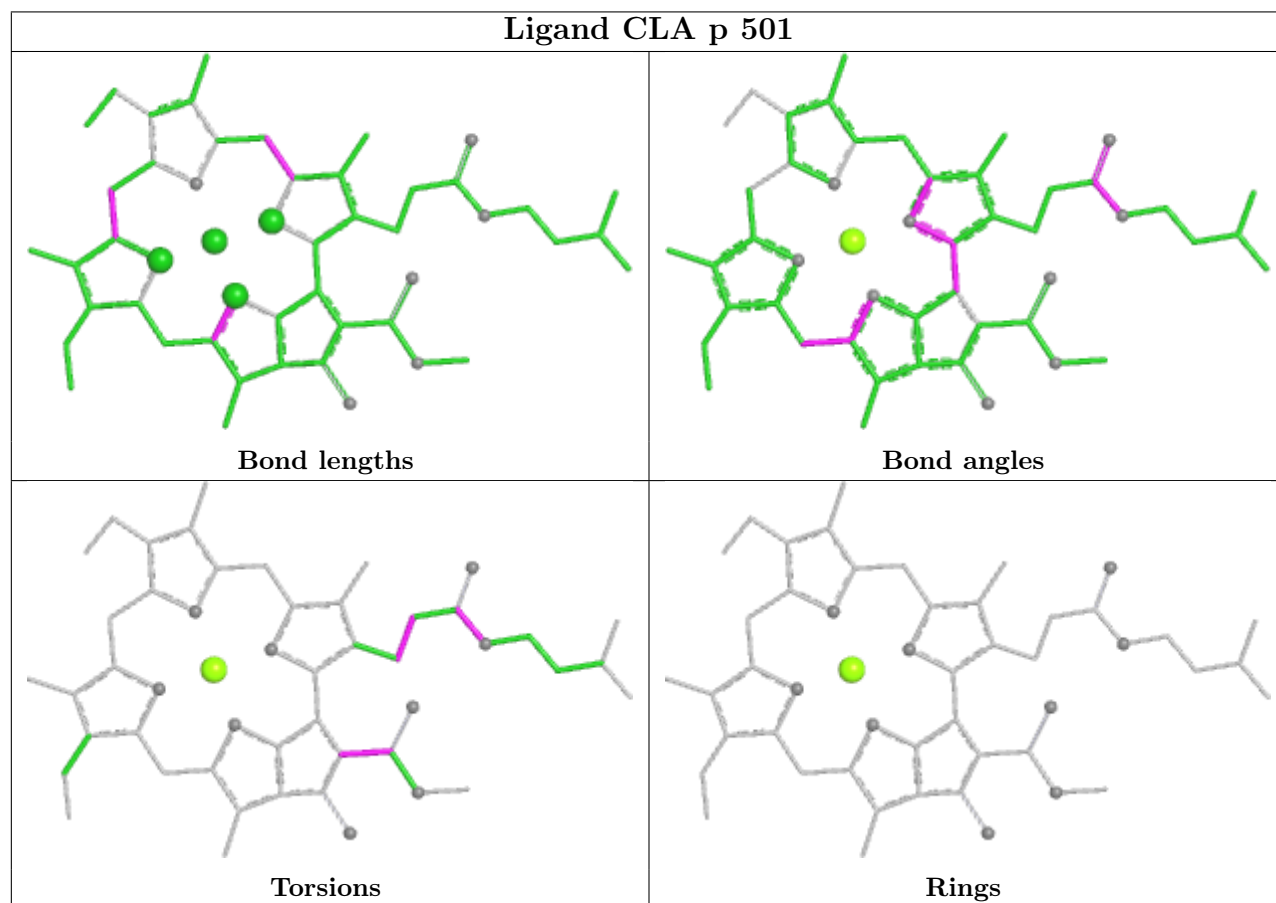
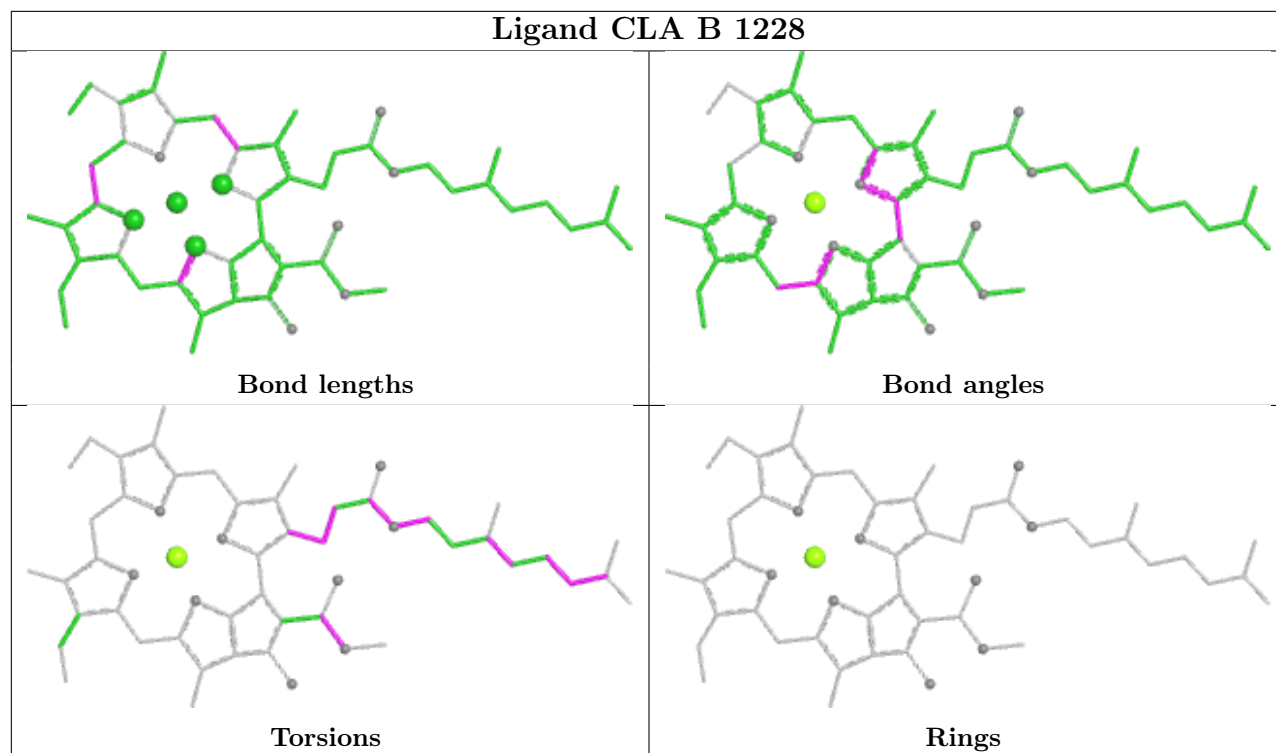
Torsions

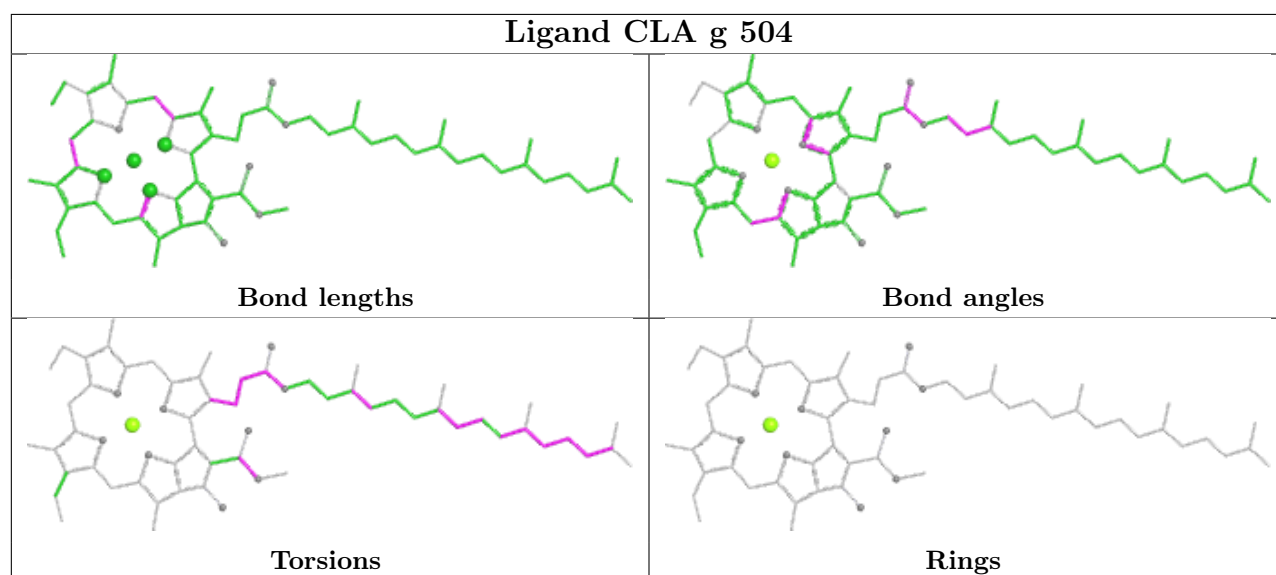
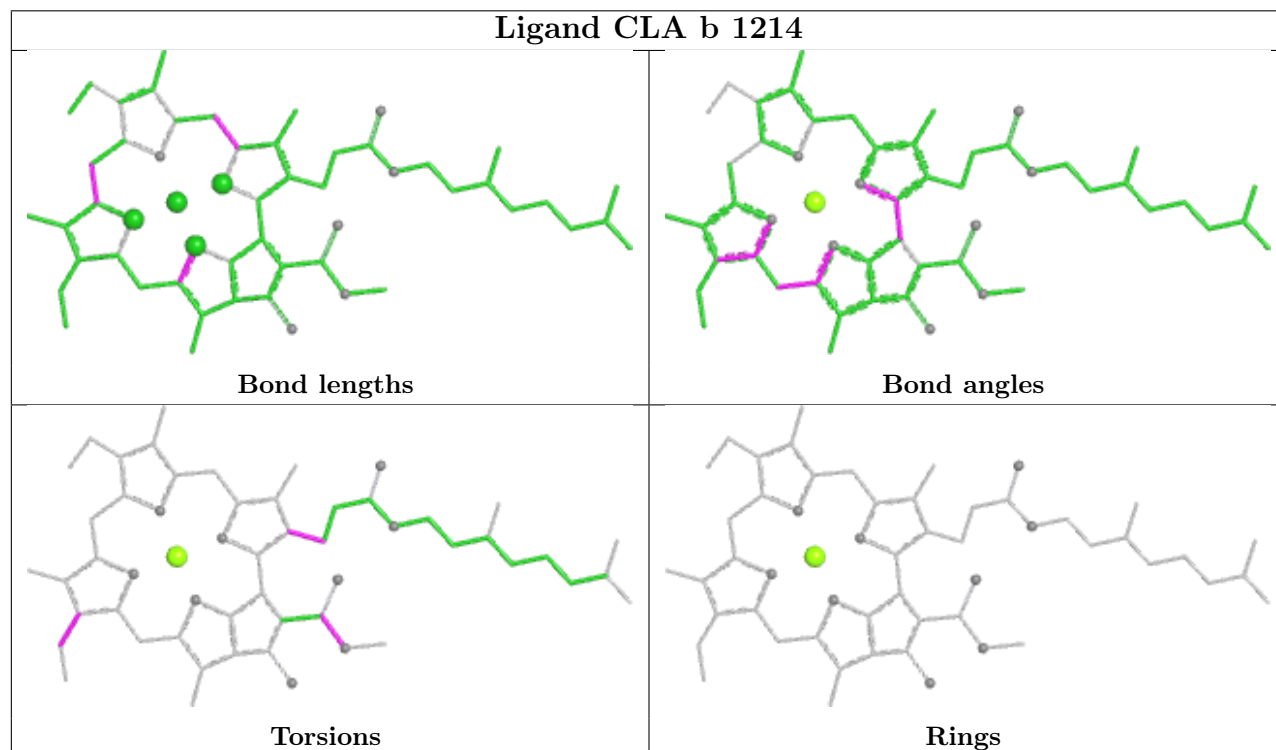
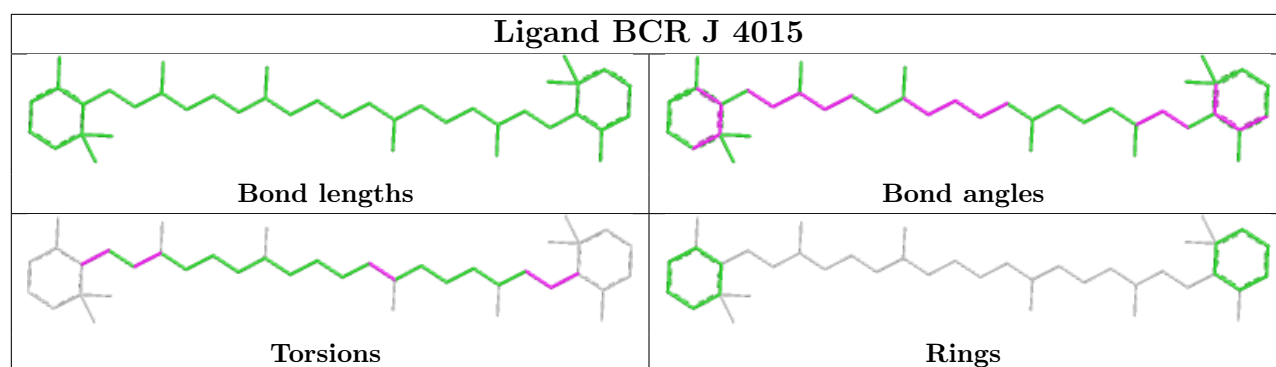


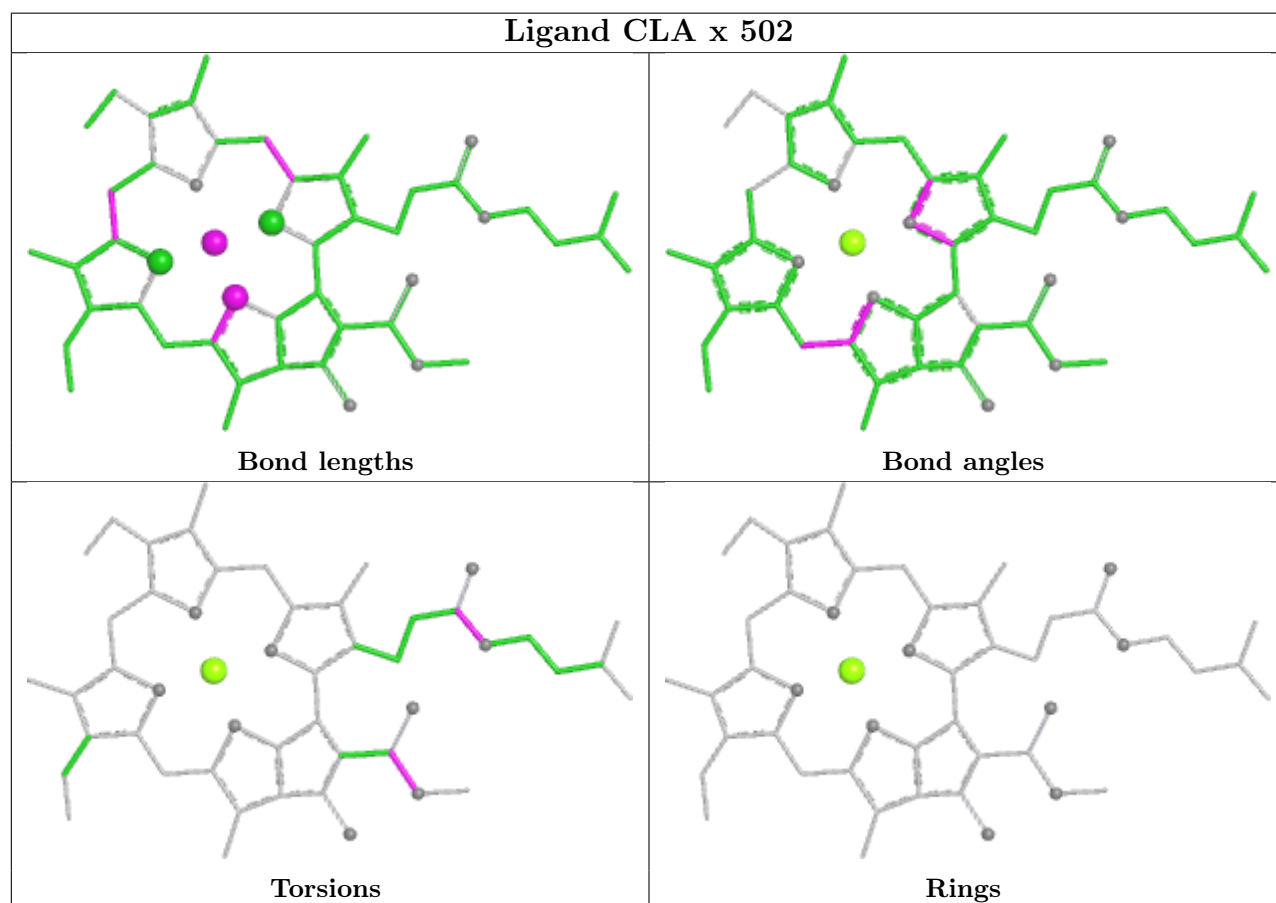
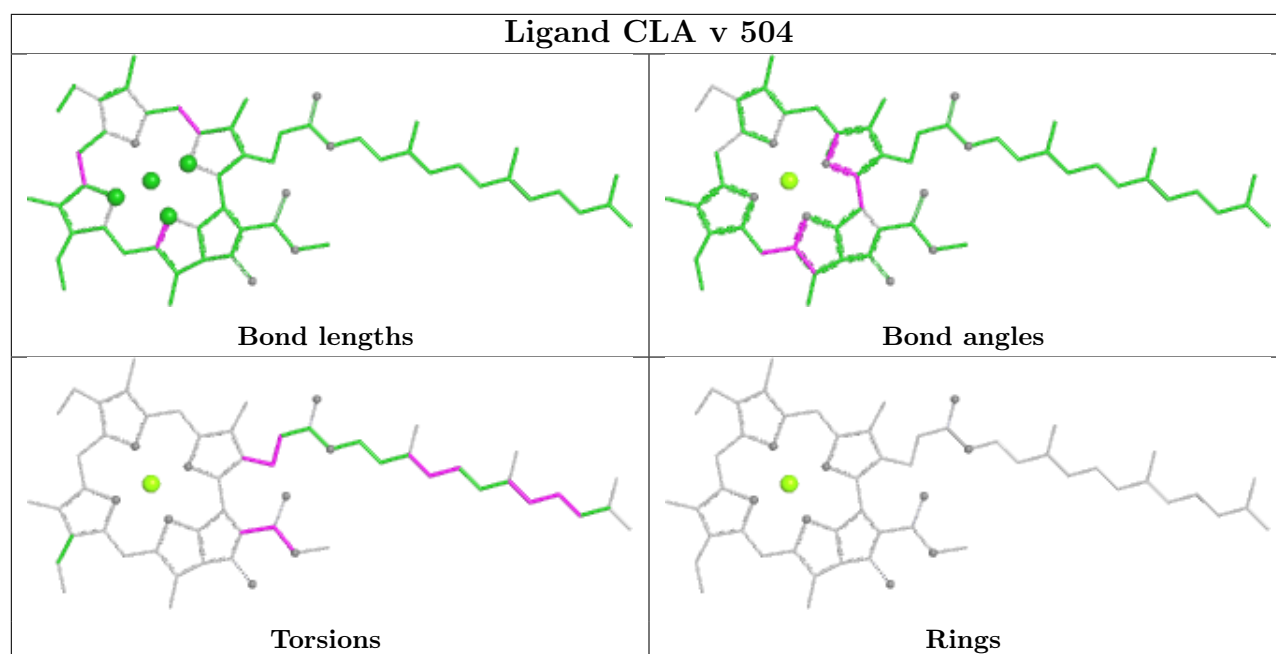
Rings

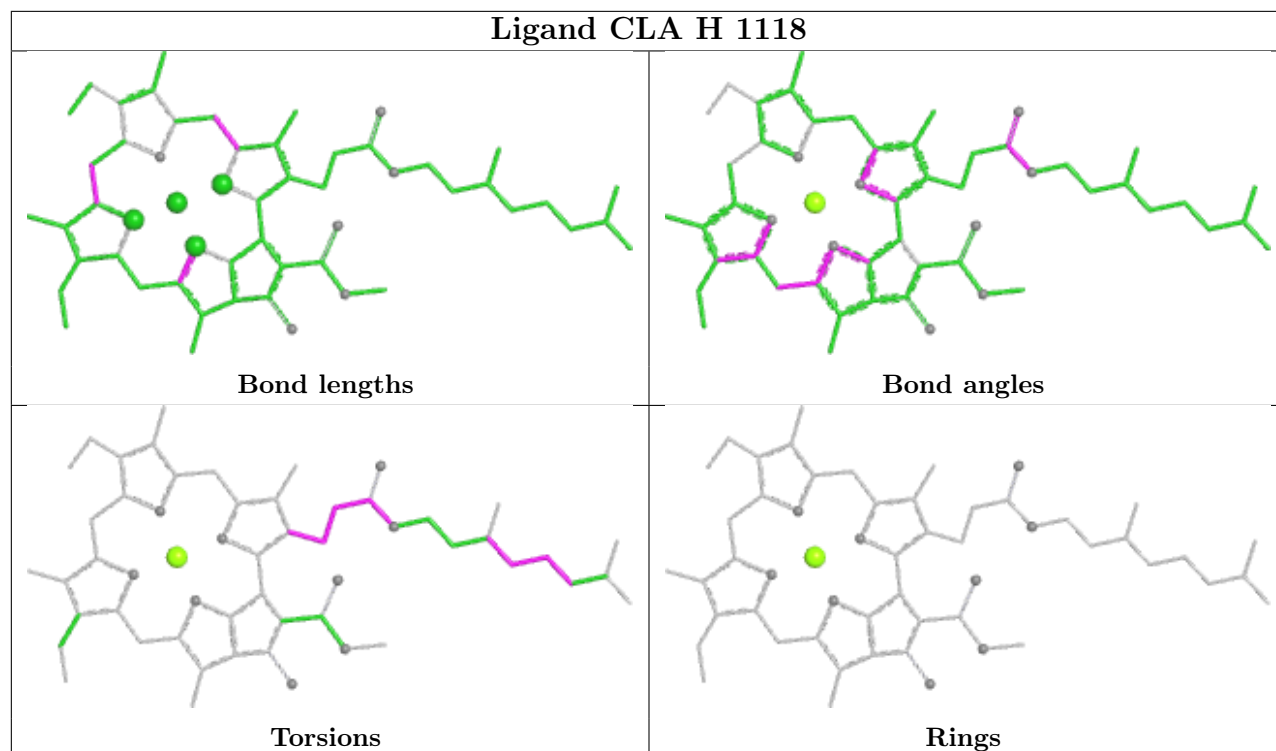
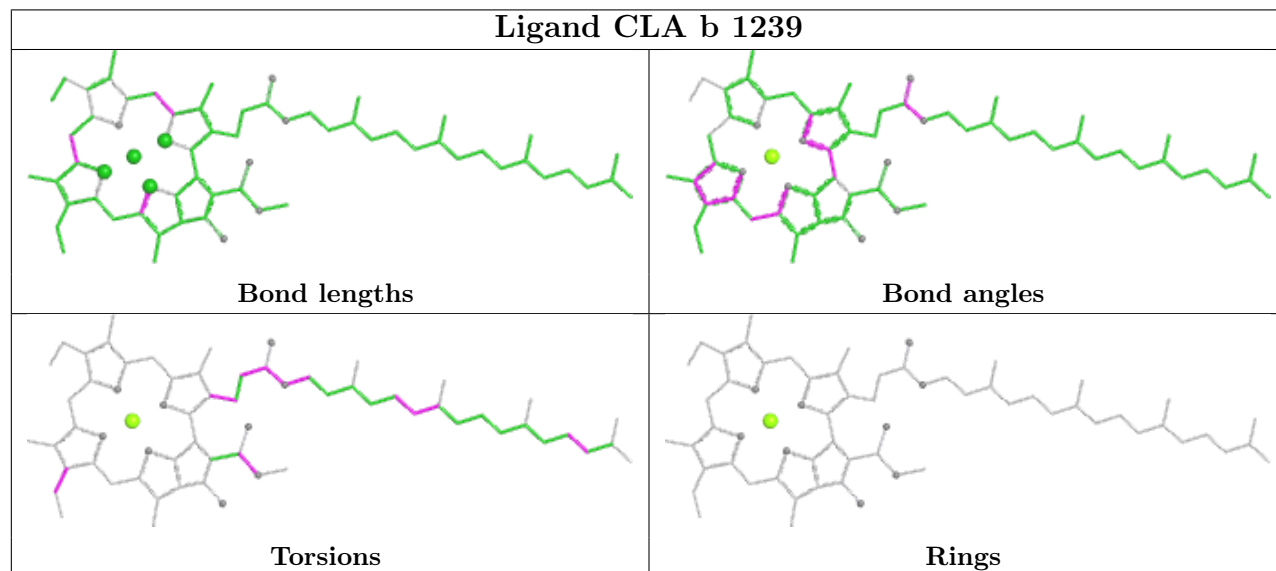




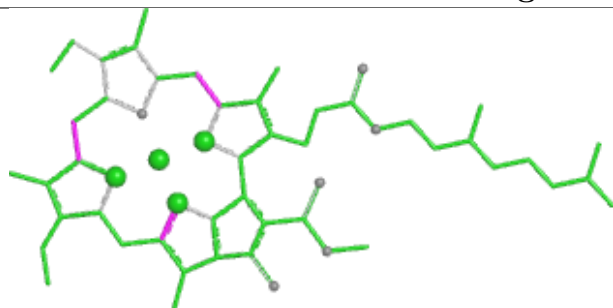




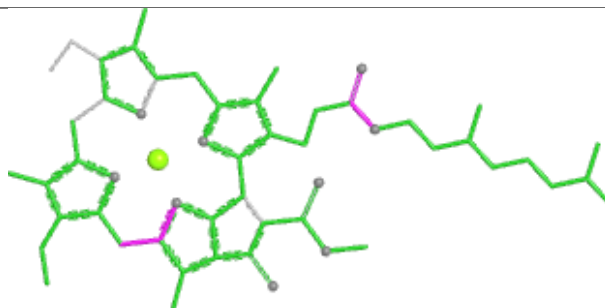


Ligand CLA H 1118**Ligand CLA b 1239**

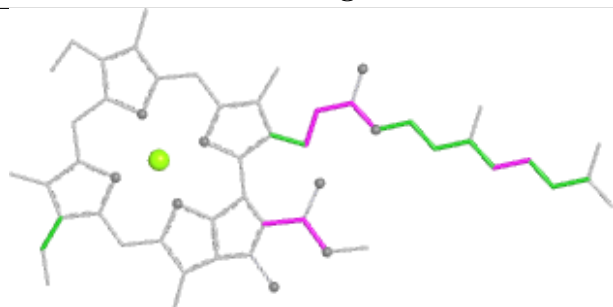
Ligand CLA x 508



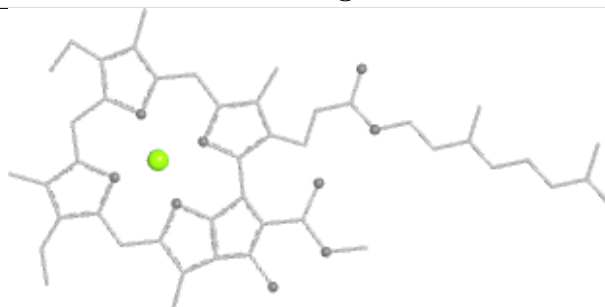
Bond lengths



Bond angles

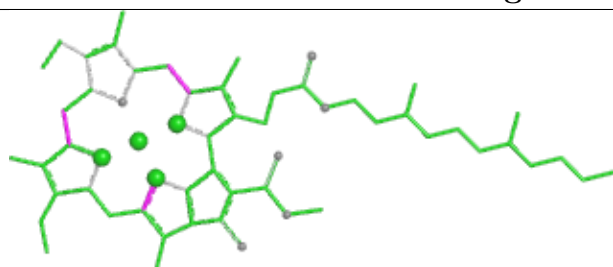


Torsions

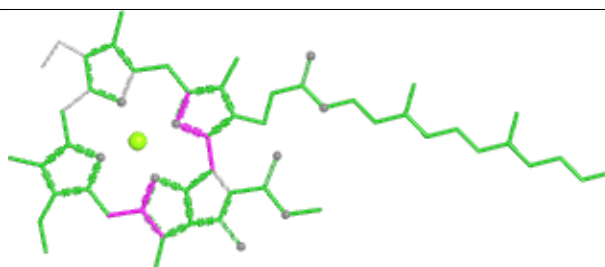


Rings

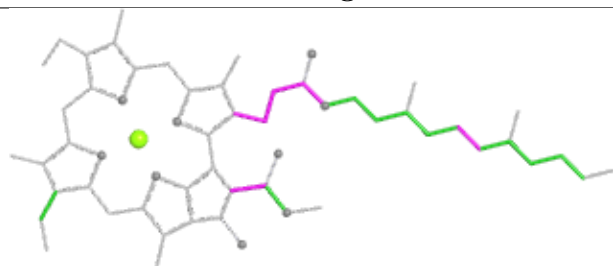
Ligand CLA H 1105



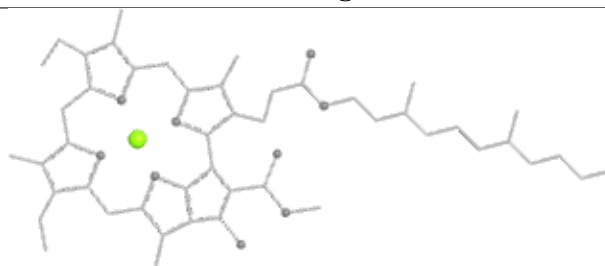
Bond lengths



Bond angles

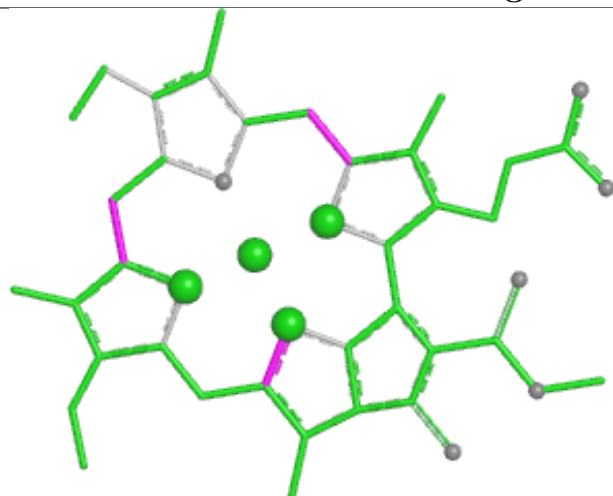


Torsions

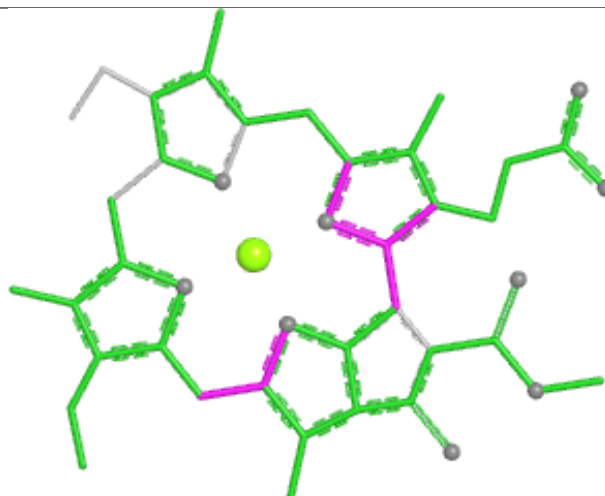


Rings

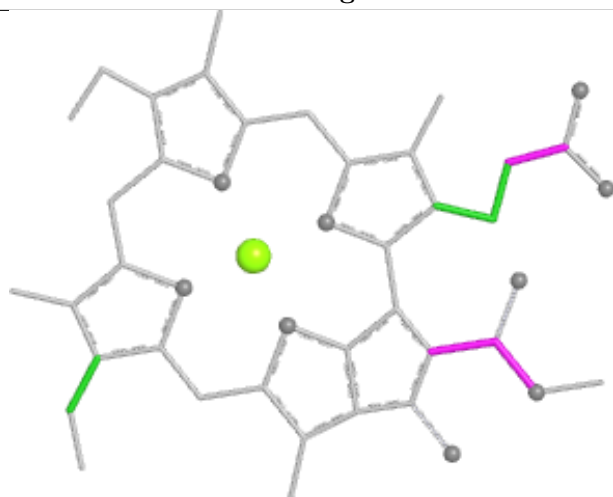
Ligand CLA B 1232



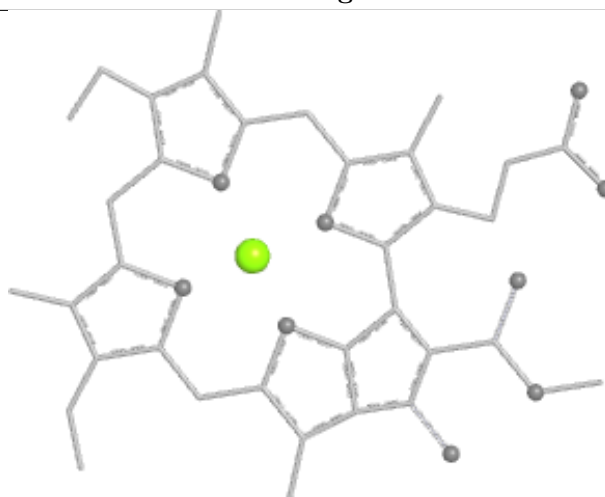
Bond lengths



Bond angles

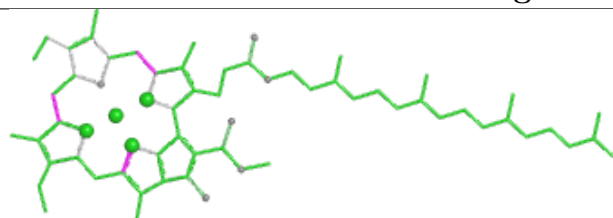


Torsions

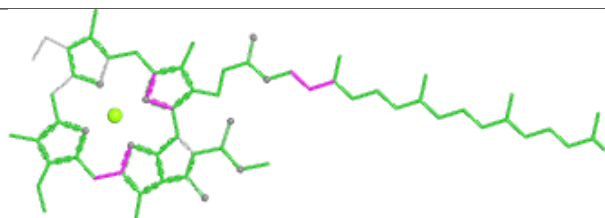


Rings

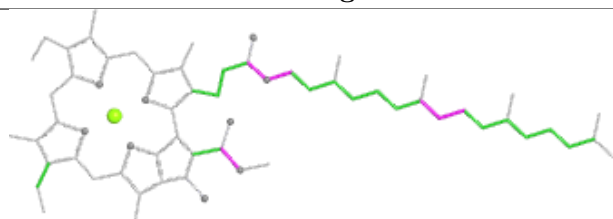
Ligand CLA Y 507



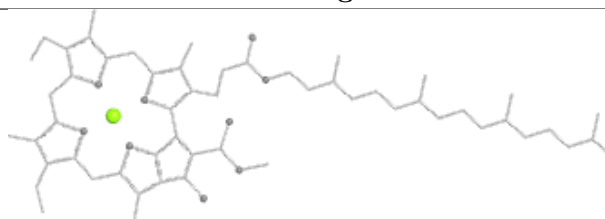
Bond lengths



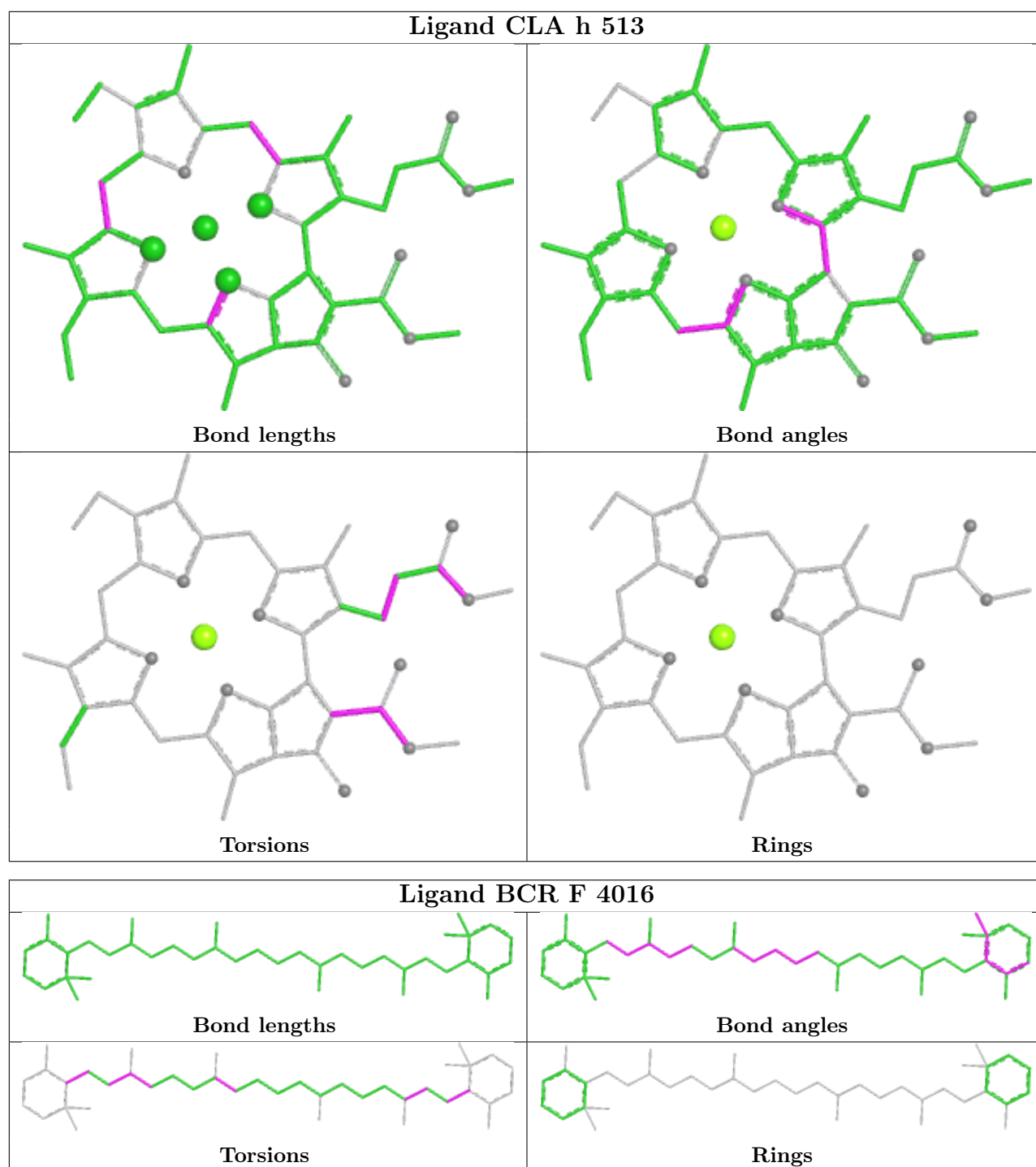
Bond angles

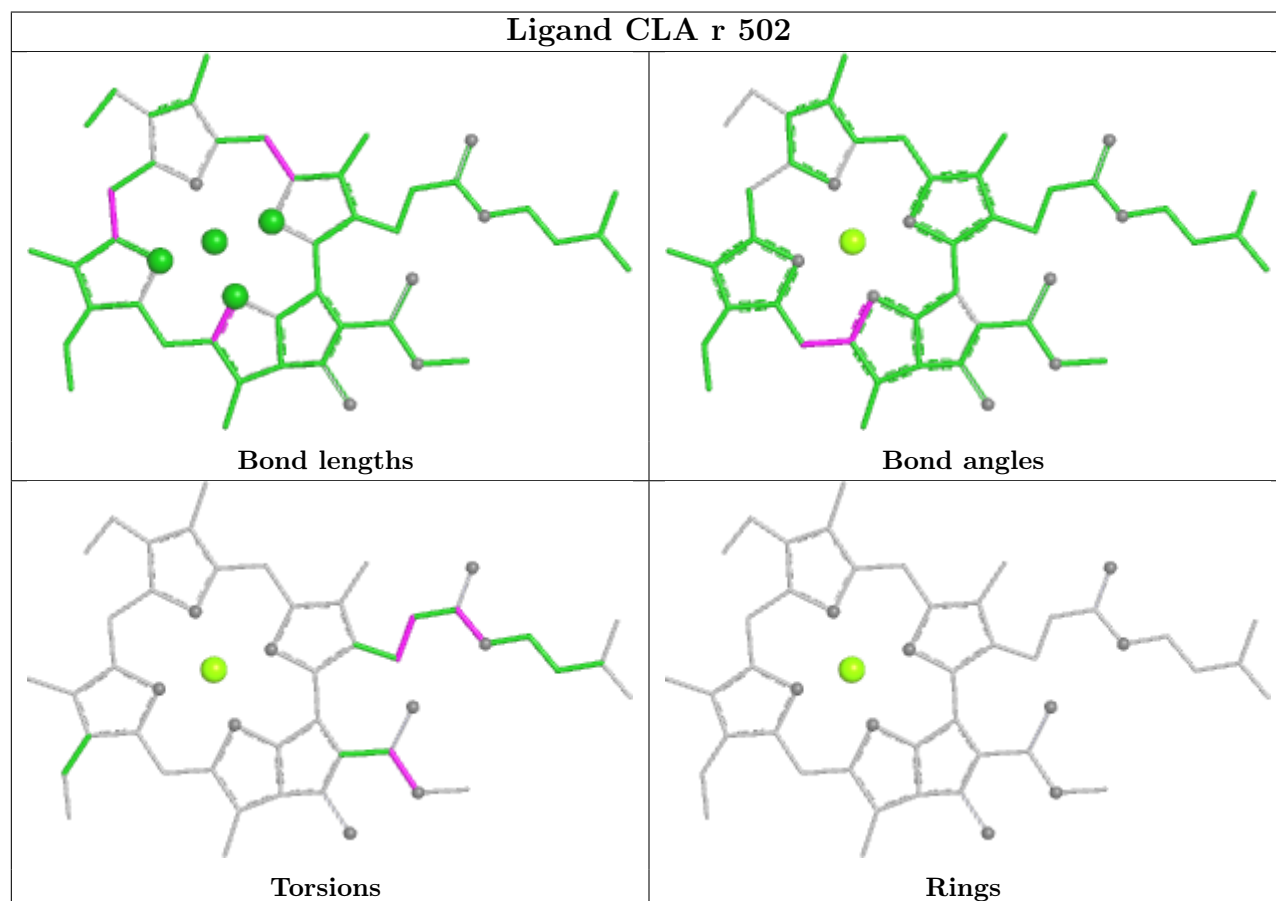
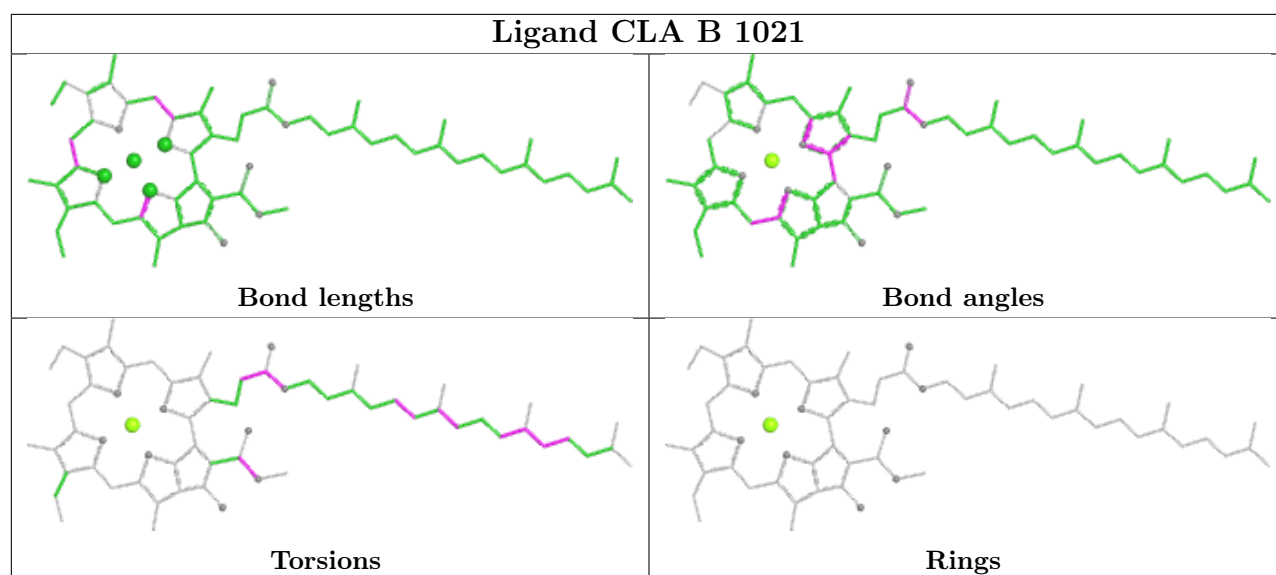


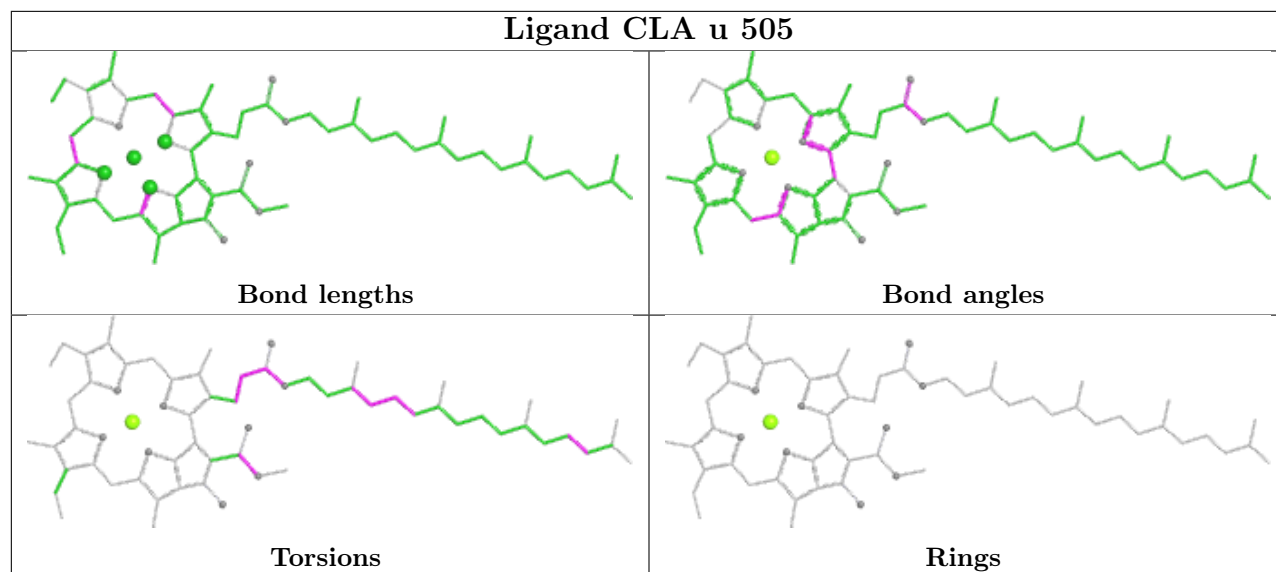
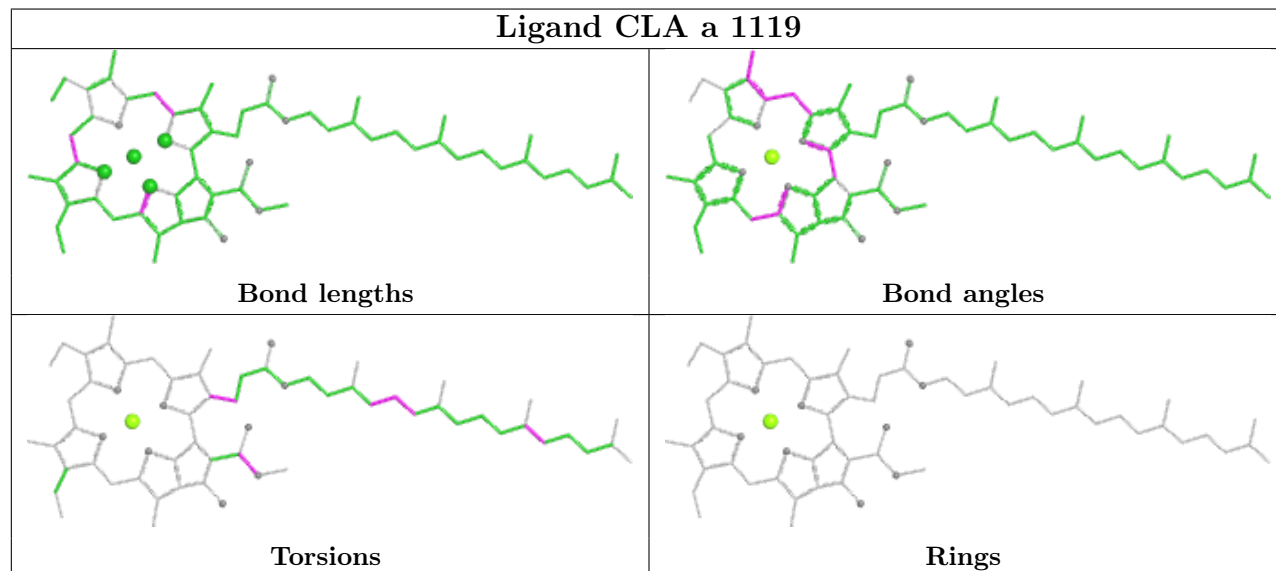
Torsions



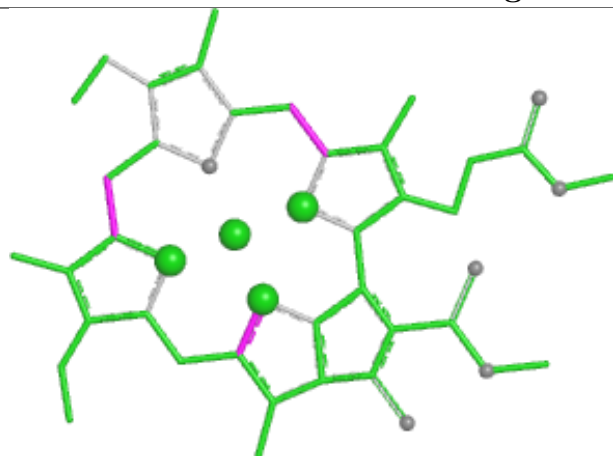
Rings



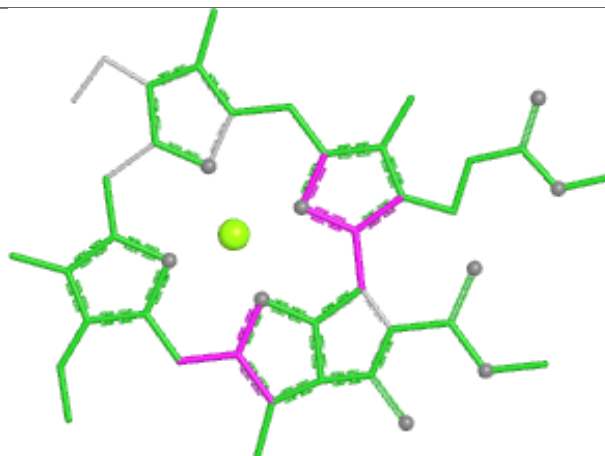


Ligand CLA u 505**Ligand CLA a 1119**

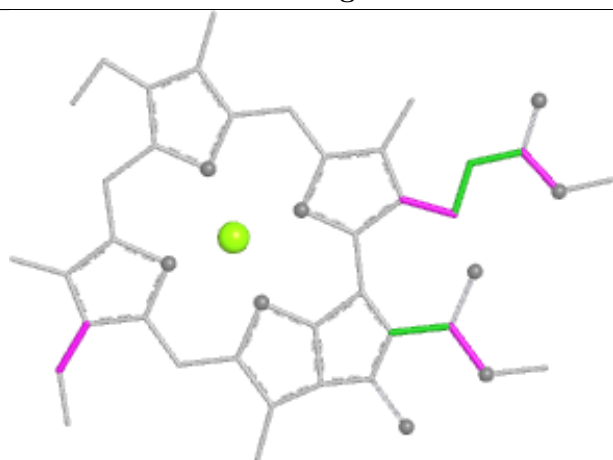
Ligand CLA H 1114



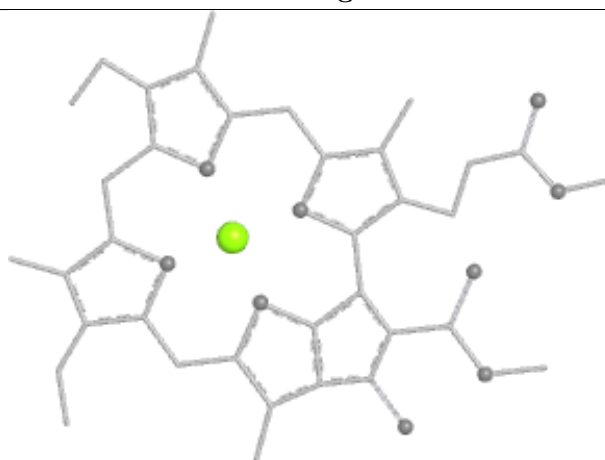
Bond lengths



Bond angles

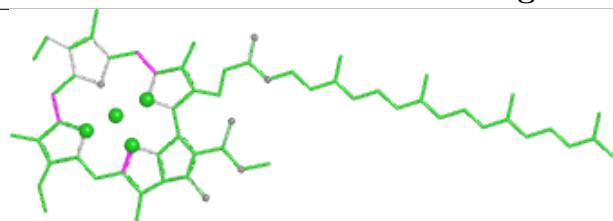


Torsions

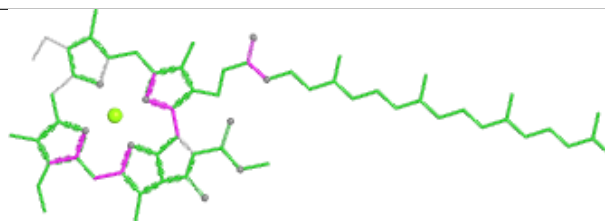


Rings

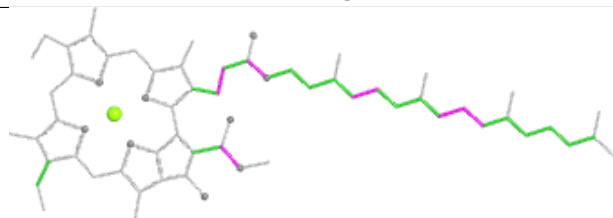
Ligand CLA x 505



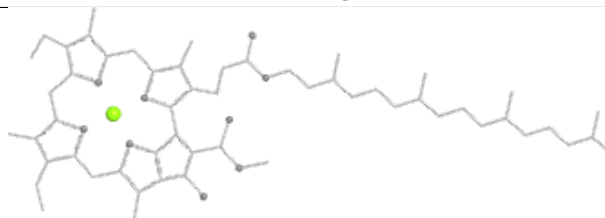
Bond lengths



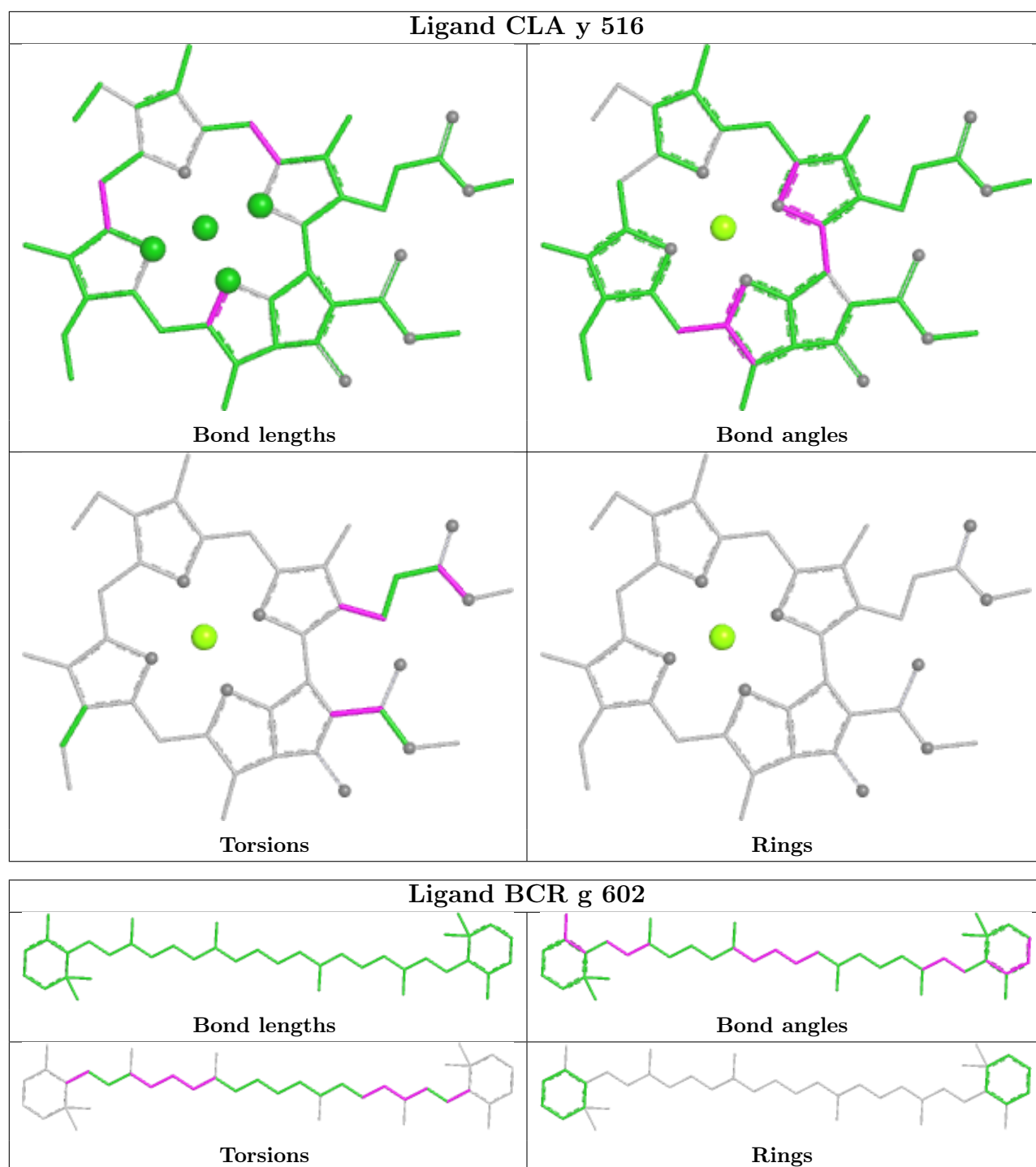
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

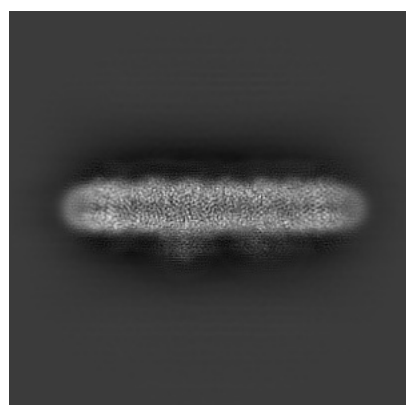
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26601. These allow visual inspection of the internal detail of the map and identification of artifacts.

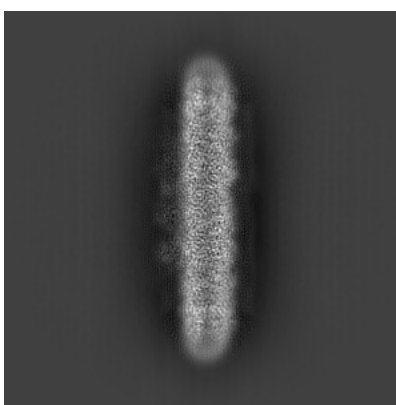
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

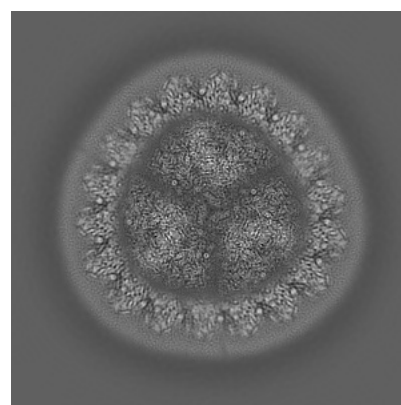
6.1.1 Primary map



X



Y

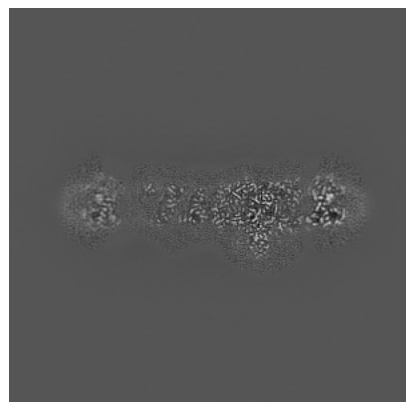


Z

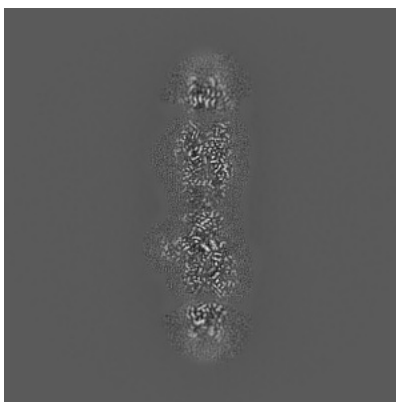
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

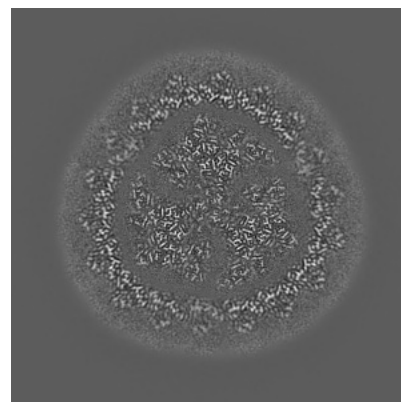
6.2.1 Primary map



X Index: 200



Y Index: 200

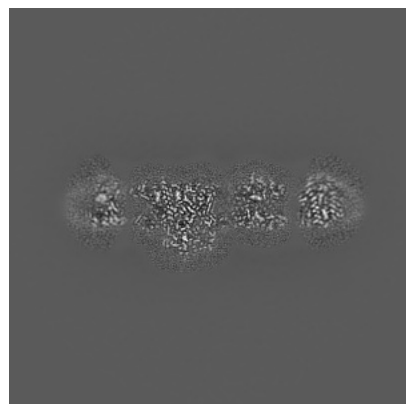


Z Index: 200

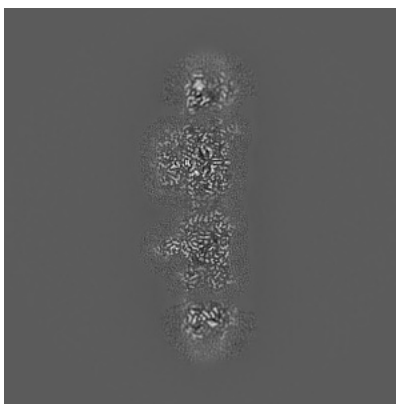
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

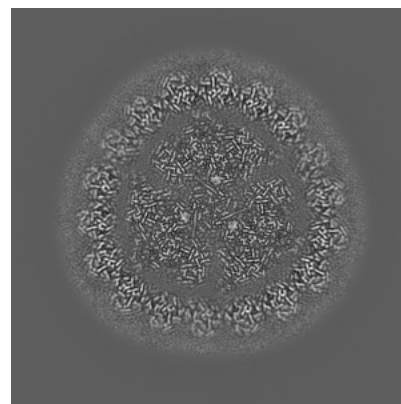
6.3.1 Primary map



X Index: 160



Y Index: 177

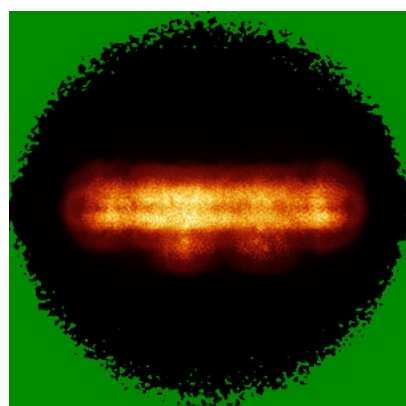


Z Index: 193

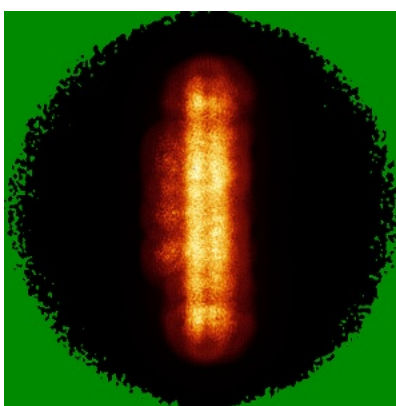
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

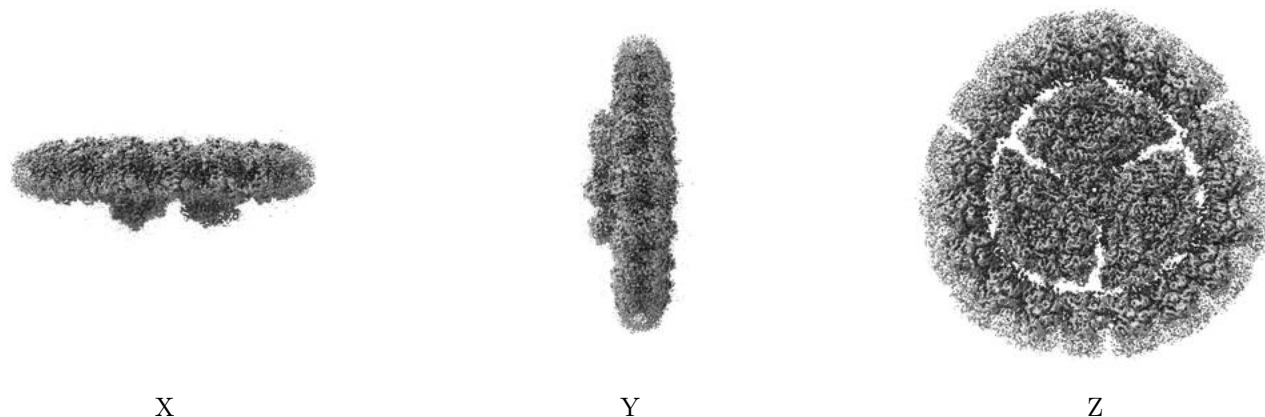


Z

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

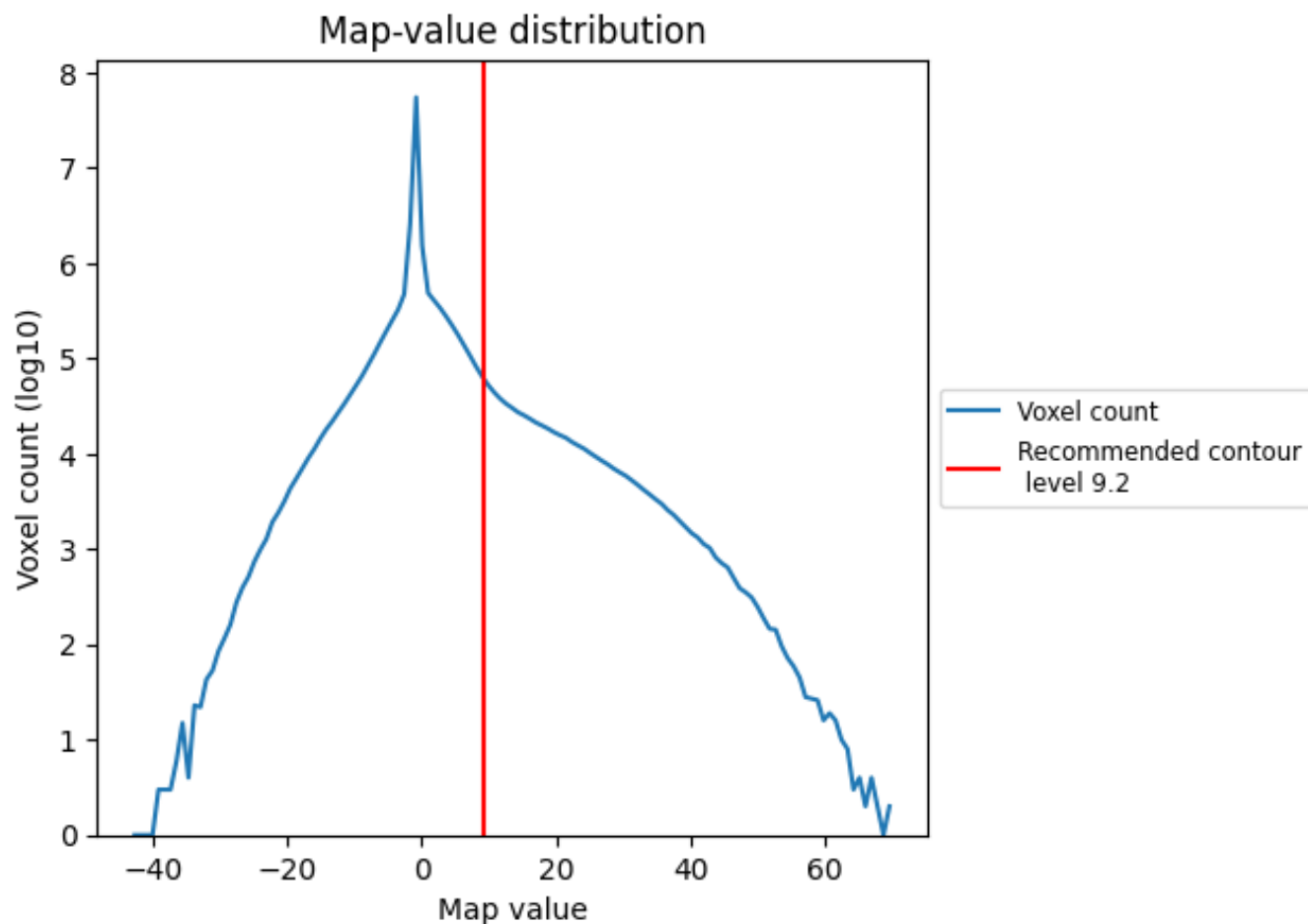
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

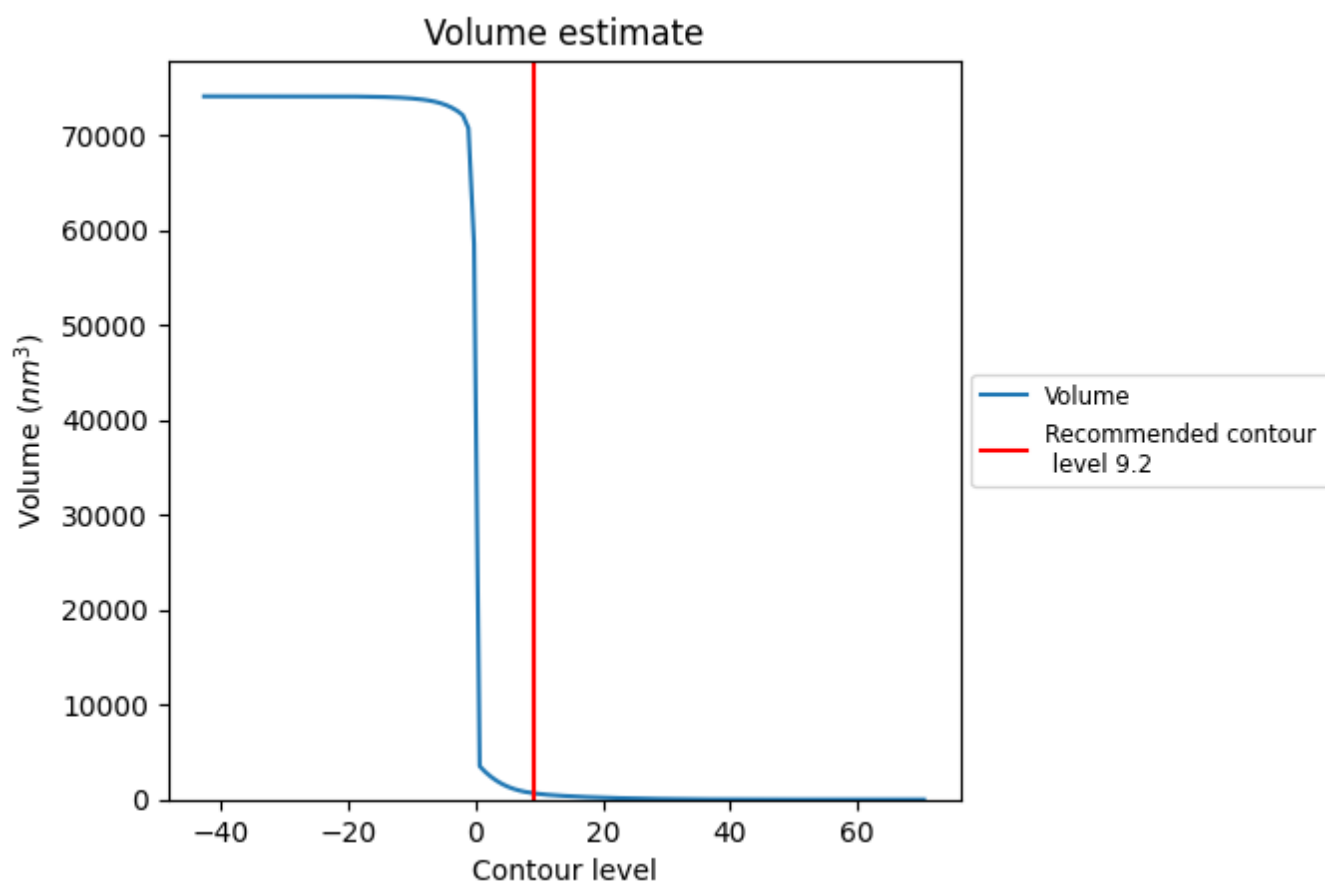
This section contains the results of statistical analysis of the map.

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.

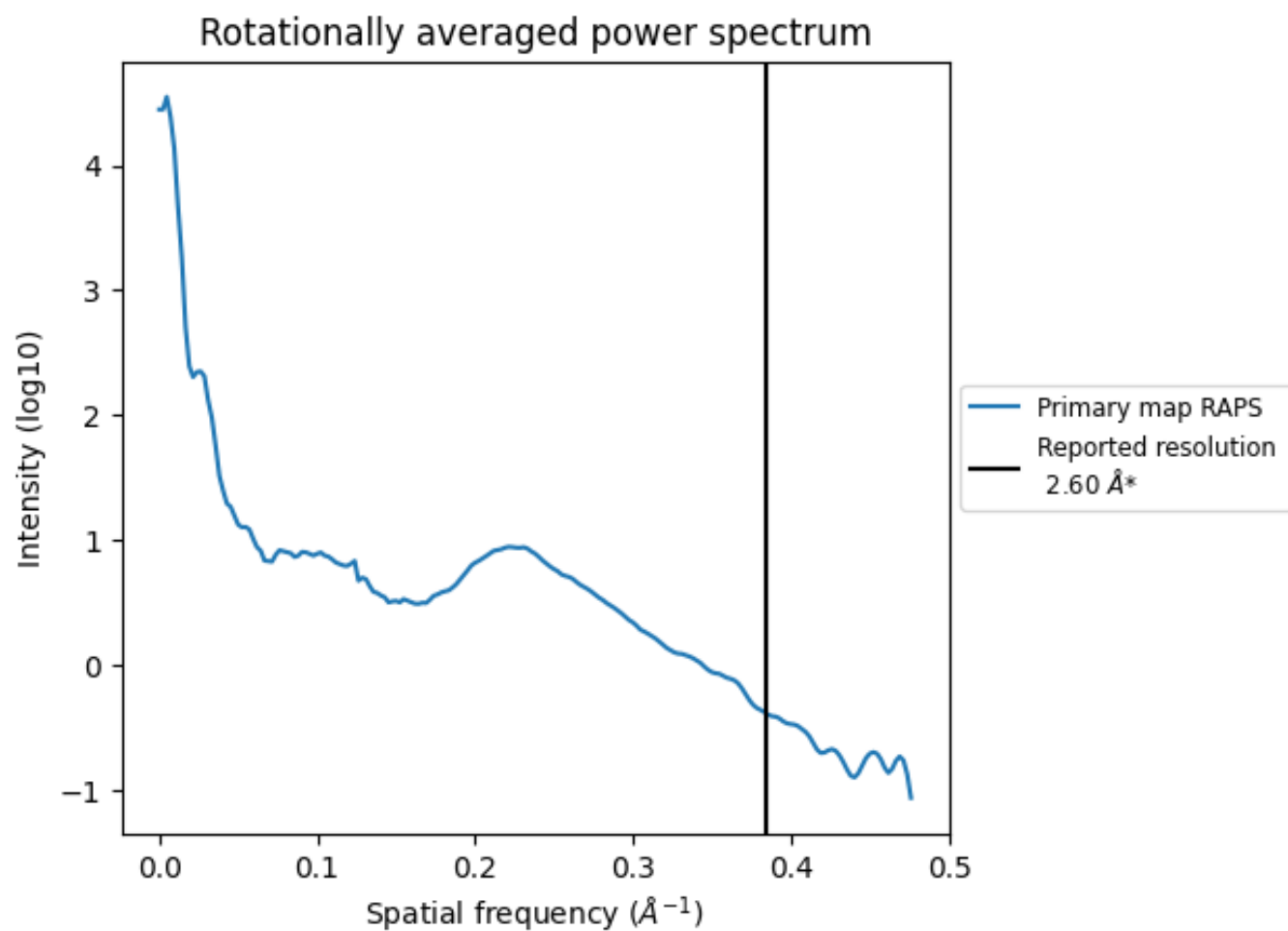
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 657 nm³; this corresponds to an approximate mass of 594 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 0.385 Å⁻¹

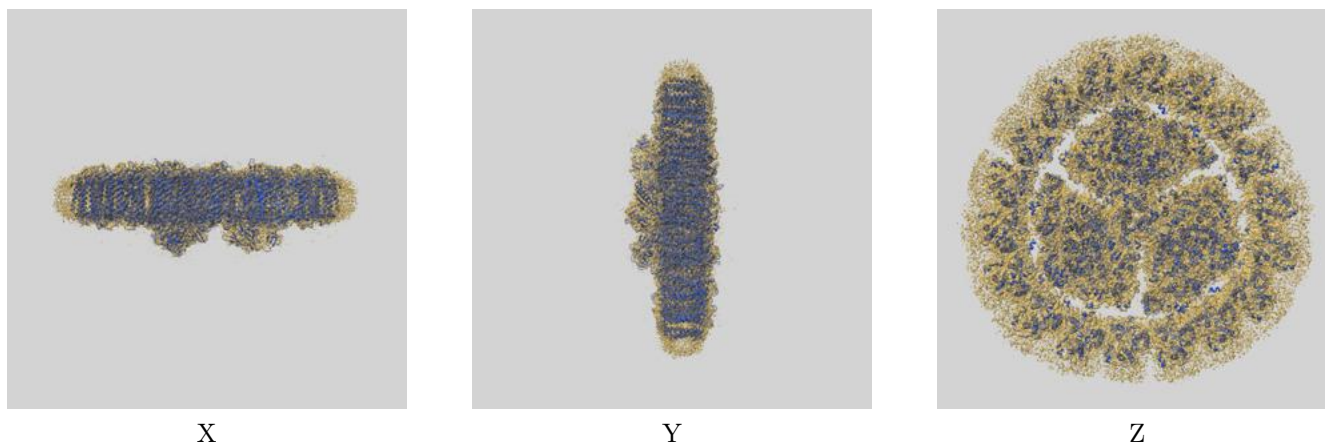
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

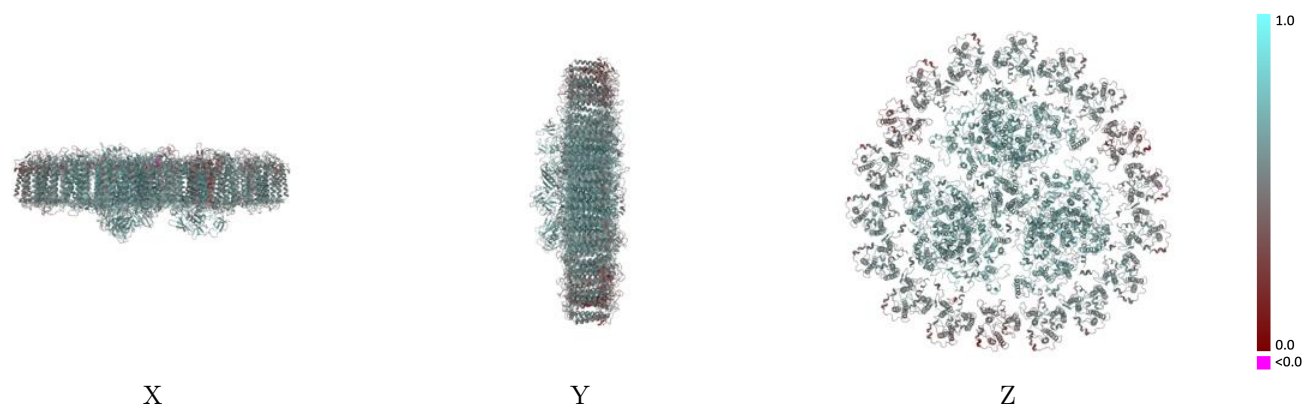
This section contains information regarding the fit between EMDB map EMD-26601 and PDB model 7UMH. Per-residue inclusion information can be found in section [3](#) on page [64](#).

9.1 Map-model overlay [i](#)



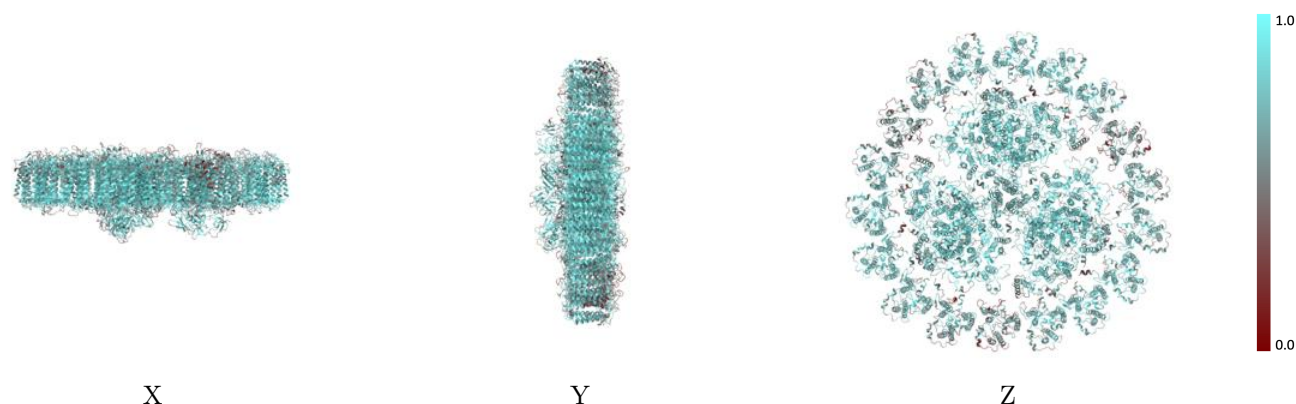
The images above show the 3D surface view of the map at the recommended contour level 9.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



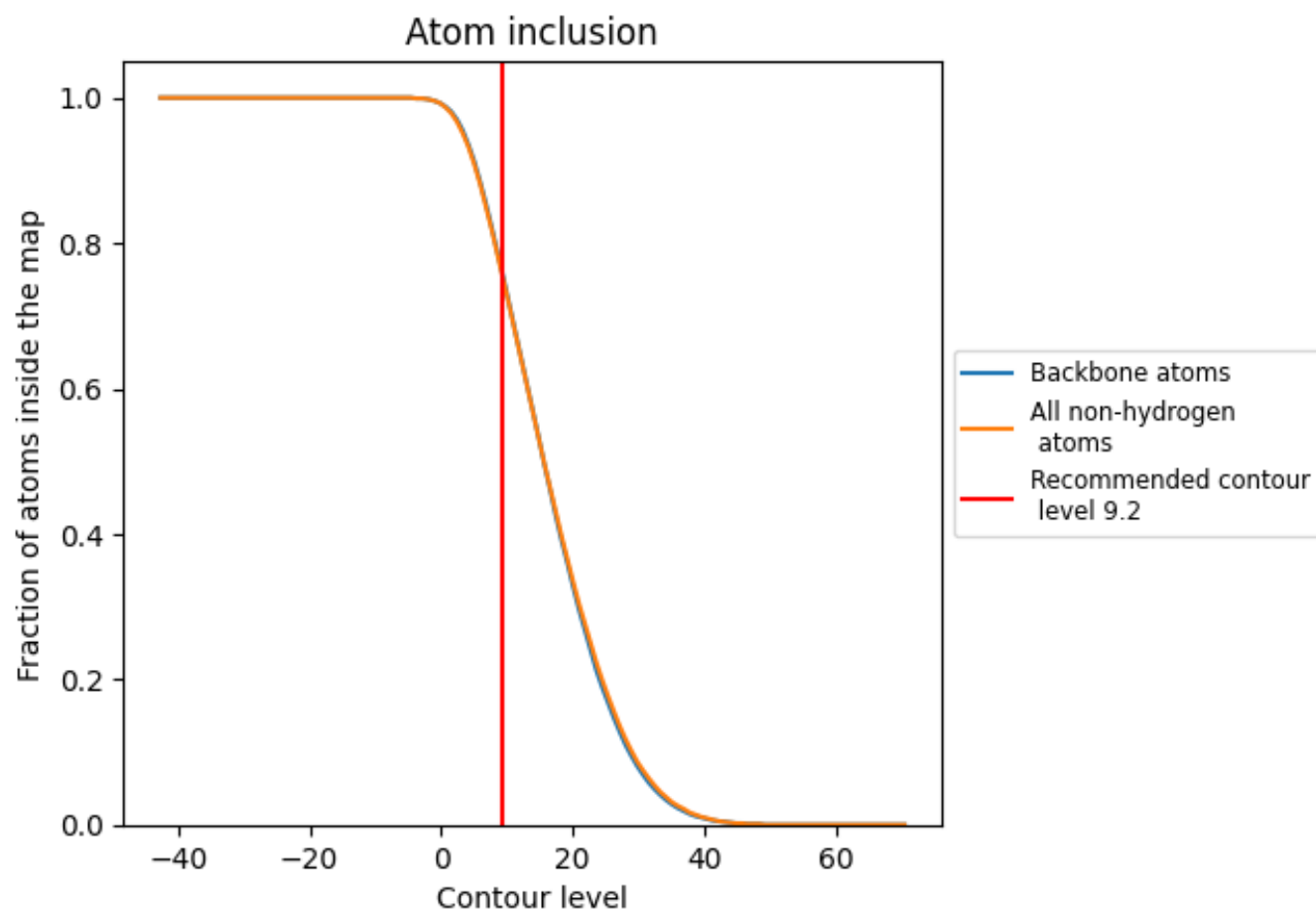
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (9.2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (9.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7600	 0.5830
A	 0.8500	 0.6590
B	 0.8530	 0.6580
C	 0.8720	 0.6440
D	 0.7320	 0.6010
E	 0.7110	 0.5910
F	 0.6610	 0.6030
G	 0.8570	 0.6580
H	 0.8550	 0.6590
I	 0.7320	 0.6300
J	 0.7310	 0.6300
K	 0.5930	 0.5910
L	 0.7710	 0.6360
M	 0.7140	 0.6350
N	 0.8740	 0.6450
O	 0.6800	 0.5860
P	 0.7240	 0.6040
Q	 0.6700	 0.6070
R	 0.7320	 0.6350
S	 0.7270	 0.6340
T	 0.6090	 0.5850
U	 0.7720	 0.6400
V	 0.6770	 0.6170
W	 0.6650	 0.5000
X	 0.7490	 0.5360
Y	 0.7840	 0.5560
Z	 0.7720	 0.5460
a	 0.8490	 0.6620
b	 0.8570	 0.6610
c	 0.8700	 0.6500
d	 0.7210	 0.6020
e	 0.6720	 0.5800
f	 0.6720	 0.6070
g	 0.7050	 0.5260
h	 0.5270	 0.4200



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.7370	 0.6290
j	 0.7590	 0.6360
k	 0.6030	 0.5890
l	 0.7650	 0.6350
m	 0.7140	 0.6350
n	 0.6720	 0.5010
o	 0.7400	 0.5370
p	 0.7770	 0.5570
q	 0.7590	 0.5430
r	 0.6990	 0.5170
s	 0.7750	 0.5550
t	 0.6620	 0.4980
u	 0.7400	 0.5300
v	 0.5460	 0.4350
w	 0.7620	 0.5450
x	 0.6830	 0.5150
y	 0.5320	 0.4260