



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 02:59 AM JST

PDB ID : 6KIG
EMDB ID : EMD-9995
Title : Structure of cyanobacterial photosystem I-IsiA supercomplex
Authors : Cao, P.; Cao, D.F.; Si, L.; Su, X.D.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on : 2019-07-18
Resolution : 2.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

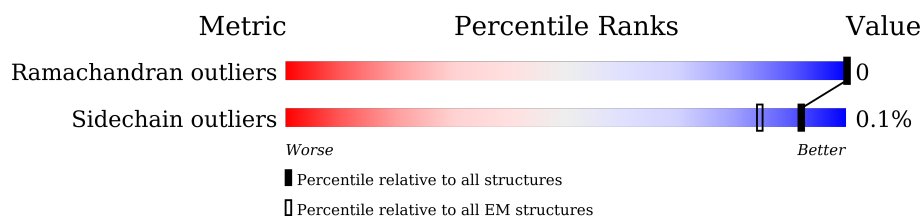
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

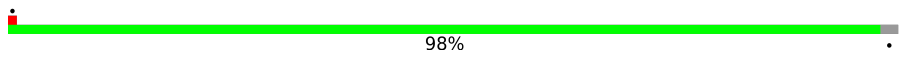
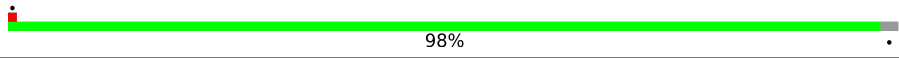
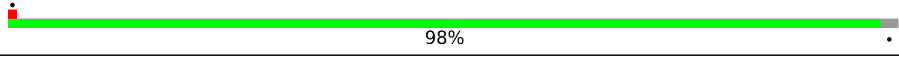
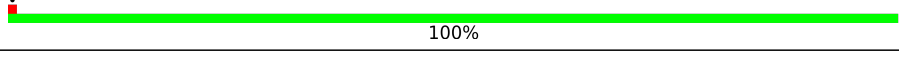
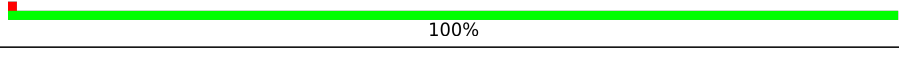
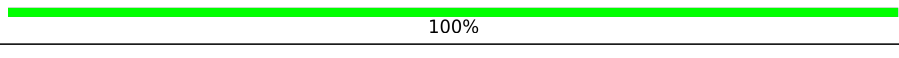
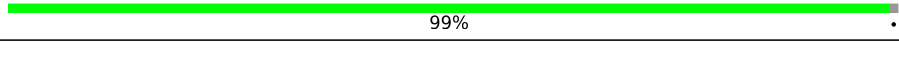
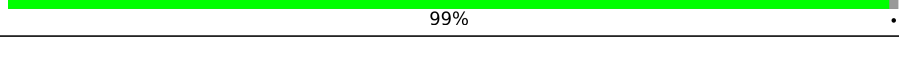
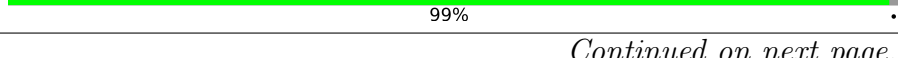
The reported resolution of this entry is 2.90 Å.

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.



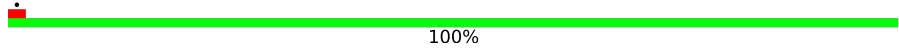
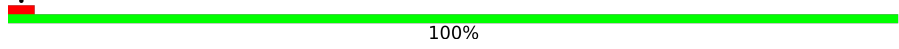
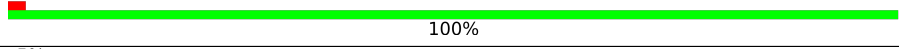
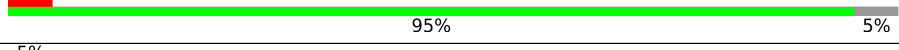
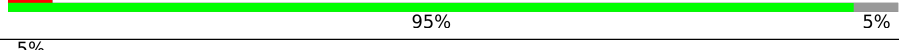
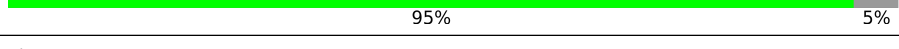
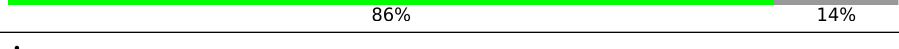
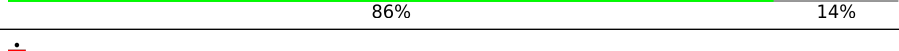
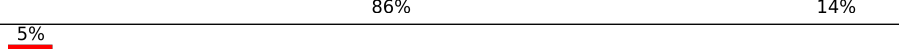
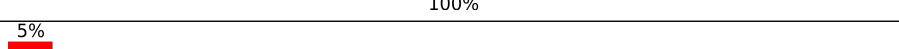
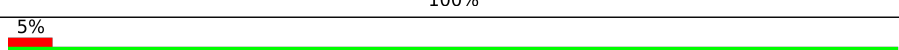
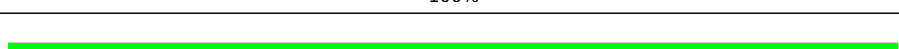
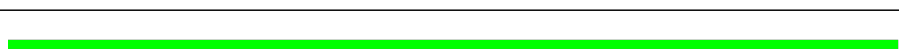
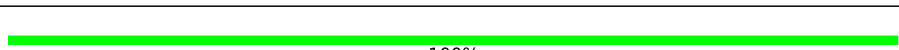
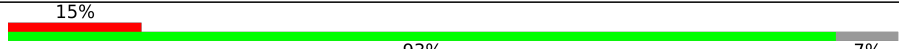
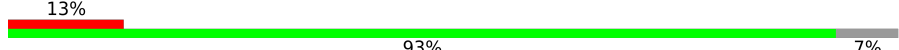
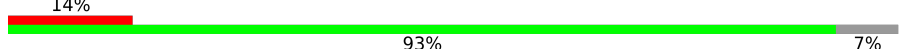
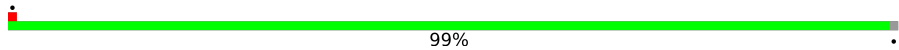
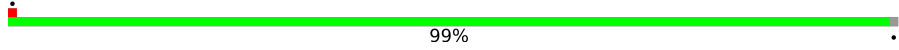
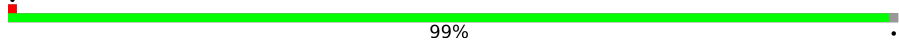
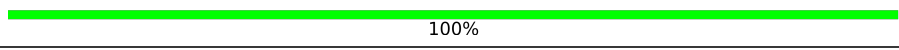
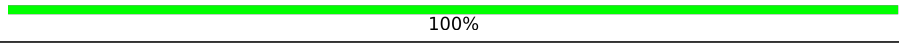
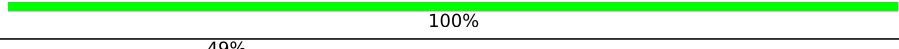
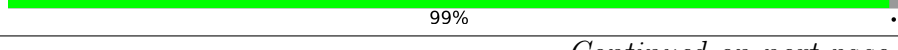

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	763	 98%
1	G	763	 98%
1	e	763	 98%
2	B	734	 100%
2	H	734	 100%
2	f	734	 100%
3	C	81	 99%
3	N	81	 99%
3	g	81	 99%

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Mol	Chain	Length	Quality of chain
4	D	141	
4	O	141	
4	h	141	
5	E	75	
5	Q	75	
5	i	75	
6	F	159	
6	R	159	
6	j	159	
7	I	38	
7	S	38	
7	k	38	
8	J	41	
8	T	41	
8	l	41	
9	K	84	
9	U	84	
9	m	84	
10	L	166	
10	V	166	
10	n	166	
11	M	29	
11	W	29	
11	o	29	
12	1	342	

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Mol	Chain	Length	Quality of chain
12	2	342	40% 99% .
12	3	342	59% 99% .
12	4	342	94% 99% .
12	5	342	98% 99% .
12	6	342	91% 99% .
12	Y	342	49% 99% .
12	Z	342	38% 99% .
12	a	342	60% 99% .
12	b	342	95% 99% .
12	c	342	98% 99% .
12	d	342	90% 99% .
12	q	342	51% 99% .
12	r	342	41% 99% .
12	s	342	59% 99% .
12	t	342	93% 99% .
12	u	342	99% 99% .
12	v	342	90% 99% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	1	501	X	-	-	-
13	CLA	1	502	X	-	-	-
13	CLA	1	503	X	-	-	-
13	CLA	1	504	X	-	-	-
13	CLA	1	505	X	-	-	-
13	CLA	1	506	X	-	-	-
13	CLA	1	507	X	-	-	-
13	CLA	1	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	1	509	X	-	-	-
13	CLA	1	510	X	-	-	-
13	CLA	1	511	X	-	-	-
13	CLA	1	512	X	-	-	-
13	CLA	1	513	X	-	-	-
13	CLA	1	516	X	-	-	-
13	CLA	1	517	X	-	-	-
13	CLA	1	518	X	-	-	-
13	CLA	1	519	X	-	-	-
13	CLA	2	501	X	-	-	-
13	CLA	2	502	X	-	-	-
13	CLA	2	503	X	-	-	-
13	CLA	2	504	X	-	-	-
13	CLA	2	505	X	-	-	-
13	CLA	2	506	X	-	-	-
13	CLA	2	507	X	-	-	-
13	CLA	2	508	X	-	-	-
13	CLA	2	509	X	-	-	-
13	CLA	2	510	X	-	-	-
13	CLA	2	511	X	-	-	-
13	CLA	2	512	X	-	-	-
13	CLA	2	513	X	-	-	-
13	CLA	2	516	X	-	-	-
13	CLA	2	517	X	-	-	-
13	CLA	2	518	X	-	-	-
13	CLA	2	519	X	-	-	-
13	CLA	3	501	X	-	-	-
13	CLA	3	502	X	-	-	-
13	CLA	3	503	X	-	-	-
13	CLA	3	504	X	-	-	-
13	CLA	3	505	X	-	-	-
13	CLA	3	506	X	-	-	-
13	CLA	3	507	X	-	-	-
13	CLA	3	508	X	-	-	-
13	CLA	3	509	X	-	-	-
13	CLA	3	510	X	-	-	-
13	CLA	3	511	X	-	-	-
13	CLA	3	512	X	-	-	-
13	CLA	3	513	X	-	-	-
13	CLA	3	516	X	-	-	-
13	CLA	3	517	X	-	-	-
13	CLA	3	518	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	3	519	X	-	-	-
13	CLA	4	501	X	-	-	-
13	CLA	4	502	X	-	-	-
13	CLA	4	503	X	-	-	-
13	CLA	4	504	X	-	-	-
13	CLA	4	505	X	-	-	-
13	CLA	4	506	X	-	-	-
13	CLA	4	507	X	-	-	-
13	CLA	4	508	X	-	-	-
13	CLA	4	509	X	-	-	-
13	CLA	4	510	X	-	-	-
13	CLA	4	511	X	-	-	-
13	CLA	4	512	X	-	-	-
13	CLA	4	513	X	-	-	-
13	CLA	4	516	X	-	-	-
13	CLA	4	517	X	-	-	-
13	CLA	4	518	X	-	-	-
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13	CLA	6	502	X	-	-	-
13	CLA	6	503	X	-	-	-
13	CLA	6	504	X	-	-	-
13	CLA	6	505	X	-	-	-
13	CLA	6	506	X	-	-	-
13	CLA	6	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	6	508	X	-	-	-
13	CLA	6	509	X	-	-	-
13	CLA	6	510	X	-	-	-
13	CLA	6	511	X	-	-	-
13	CLA	6	512	X	-	-	-
13	CLA	6	513	X	-	-	-
13	CLA	6	516	X	-	-	-
13	CLA	6	517	X	-	-	-
13	CLA	6	518	X	-	-	-
13	CLA	6	519	X	-	-	-
13	CLA	A	1011	X	-	-	-
13	CLA	A	1013	X	-	-	-
13	CLA	A	1022	X	-	-	-
13	CLA	A	1101	X	-	-	-
13	CLA	A	1102	X	-	-	-
13	CLA	A	1103	X	-	-	-
13	CLA	A	1104	X	-	-	-
13	CLA	A	1105	X	-	-	-
13	CLA	A	1106	X	-	-	-
13	CLA	A	1107	X	-	-	-
13	CLA	A	1108	X	-	-	-
13	CLA	A	1109	X	-	-	-
13	CLA	A	1110	X	-	-	-
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13	CLA	A	1114	X	-	-	-
13	CLA	A	1115	X	-	-	-
13	CLA	A	1116	X	-	-	-
13	CLA	A	1117	X	-	-	-
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13	CLA	A	1119	X	-	-	-
13	CLA	A	1120	X	-	-	-
13	CLA	A	1121	X	-	-	-
13	CLA	A	1122	X	-	-	-
13	CLA	A	1123	X	-	-	-
13	CLA	A	1124	X	-	-	-
13	CLA	A	1125	X	-	-	-
13	CLA	A	1126	X	-	-	-
13	CLA	A	1127	X	-	-	-
13	CLA	A	1128	X	-	-	-
13	CLA	A	1129	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	1130	X	-	-	-
13	CLA	A	1131	X	-	-	-
13	CLA	A	1132	X	-	-	-
13	CLA	A	1133	X	-	-	-
13	CLA	A	1134	X	-	-	-
13	CLA	A	1135	X	-	-	-
13	CLA	A	1136	X	-	-	-
13	CLA	A	1137	X	-	-	-
13	CLA	A	1138	X	-	-	-
13	CLA	A	1139	X	-	-	-
13	CLA	A	1140	X	-	-	-
13	CLA	A	1237	X	-	-	-
13	CLA	A	1801	X	-	-	-
13	CLA	B	1012	X	-	-	-
13	CLA	B	1021	X	-	-	-
13	CLA	B	1023	X	-	-	-
13	CLA	B	1201	X	-	-	-
13	CLA	B	1202	X	-	-	-
13	CLA	B	1203	X	-	-	-
13	CLA	B	1204	X	-	-	-
13	CLA	B	1205	X	-	-	-
13	CLA	B	1206	X	-	-	-
13	CLA	B	1207	X	-	-	-
13	CLA	B	1208	X	-	-	-
13	CLA	B	1209	X	-	-	-
13	CLA	B	1210	X	-	-	-
13	CLA	B	1211	X	-	-	-
13	CLA	B	1212	X	-	-	-
13	CLA	B	1213	X	-	-	-
13	CLA	B	1214	X	-	-	-
13	CLA	B	1215	X	-	-	-
13	CLA	B	1216	X	-	-	-
13	CLA	B	1217	X	-	-	-
13	CLA	B	1218	X	-	-	-
13	CLA	B	1219	X	-	-	-
13	CLA	B	1220	X	-	-	-
13	CLA	B	1221	X	-	-	-
13	CLA	B	1222	X	-	-	-
13	CLA	B	1223	X	-	-	-
13	CLA	B	1224	X	-	-	-
13	CLA	B	1225	X	-	-	-
13	CLA	B	1226	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	1227	X	-	-	-
13	CLA	B	1228	X	-	-	-
13	CLA	B	1229	X	-	-	-
13	CLA	B	1230	X	-	-	-
13	CLA	B	1231	X	-	-	-
13	CLA	B	1232	X	-	-	-
13	CLA	B	1234	X	-	-	-
13	CLA	B	1235	X	-	-	-
13	CLA	B	1238	X	-	-	-
13	CLA	B	1239	X	-	-	-
13	CLA	F	1301	X	-	-	-
13	CLA	F	1302	X	-	-	-
13	CLA	G	1011	X	-	-	-
13	CLA	G	1013	X	-	-	-
13	CLA	G	1022	X	-	-	-
13	CLA	G	1101	X	-	-	-
13	CLA	G	1102	X	-	-	-
13	CLA	G	1103	X	-	-	-
13	CLA	G	1104	X	-	-	-
13	CLA	G	1105	X	-	-	-
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13	CLA	G	1117	X	-	-	-
13	CLA	G	1118	X	-	-	-
13	CLA	G	1119	X	-	-	-
13	CLA	G	1120	X	-	-	-
13	CLA	G	1121	X	-	-	-
13	CLA	G	1122	X	-	-	-
13	CLA	G	1123	X	-	-	-
13	CLA	G	1124	X	-	-	-
13	CLA	G	1125	X	-	-	-
13	CLA	G	1126	X	-	-	-
13	CLA	G	1127	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	G	1128	X	-	-	-
13	CLA	G	1129	X	-	-	-
13	CLA	G	1130	X	-	-	-
13	CLA	G	1131	X	-	-	-
13	CLA	G	1132	X	-	-	-
13	CLA	G	1133	X	-	-	-
13	CLA	G	1134	X	-	-	-
13	CLA	G	1135	X	-	-	-
13	CLA	G	1136	X	-	-	-
13	CLA	G	1137	X	-	-	-
13	CLA	G	1138	X	-	-	-
13	CLA	G	1139	X	-	-	-
13	CLA	G	1140	X	-	-	-
13	CLA	G	1237	X	-	-	-
13	CLA	G	1801	X	-	-	-
13	CLA	H	1012	X	-	-	-
13	CLA	H	1021	X	-	-	-
13	CLA	H	1023	X	-	-	-
13	CLA	H	1201	X	-	-	-
13	CLA	H	1202	X	-	-	-
13	CLA	H	1203	X	-	-	-
13	CLA	H	1204	X	-	-	-
13	CLA	H	1205	X	-	-	-
13	CLA	H	1206	X	-	-	-
13	CLA	H	1207	X	-	-	-
13	CLA	H	1208	X	-	-	-
13	CLA	H	1209	X	-	-	-
13	CLA	H	1210	X	-	-	-
13	CLA	H	1211	X	-	-	-
13	CLA	H	1212	X	-	-	-
13	CLA	H	1213	X	-	-	-
13	CLA	H	1214	X	-	-	-
13	CLA	H	1215	X	-	-	-
13	CLA	H	1216	X	-	-	-
13	CLA	H	1217	X	-	-	-
13	CLA	H	1218	X	-	-	-
13	CLA	H	1219	X	-	-	-
13	CLA	H	1220	X	-	-	-
13	CLA	H	1221	X	-	-	-
13	CLA	H	1222	X	-	-	-
13	CLA	H	1223	X	-	-	-
13	CLA	H	1224	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	H	1225	X	-	-	-
13	CLA	H	1226	X	-	-	-
13	CLA	H	1227	X	-	-	-
13	CLA	H	1228	X	-	-	-
13	CLA	H	1229	X	-	-	-
13	CLA	H	1230	X	-	-	-
13	CLA	H	1231	X	-	-	-
13	CLA	H	1232	X	-	-	-
13	CLA	H	1234	X	-	-	-
13	CLA	H	1235	X	-	-	-
13	CLA	H	1238	X	-	-	-
13	CLA	H	1239	X	-	-	-
13	CLA	J	1302	X	-	-	-
13	CLA	J	1303	X	-	-	-
13	CLA	K	1103	X	-	-	-
13	CLA	K	1105	X	-	-	-
13	CLA	K	1401	X	-	-	-
13	CLA	L	1501	X	-	-	-
13	CLA	L	1502	X	-	-	-
13	CLA	L	1503	X	-	-	-
13	CLA	R	1301	X	-	-	-
13	CLA	R	1302	X	-	-	-
13	CLA	T	1302	X	-	-	-
13	CLA	T	1303	X	-	-	-
13	CLA	U	1103	X	-	-	-
13	CLA	U	1105	X	-	-	-
13	CLA	U	1401	X	-	-	-
13	CLA	V	1501	X	-	-	-
13	CLA	V	1502	X	-	-	-
13	CLA	V	1503	X	-	-	-
13	CLA	Y	501	X	-	-	-
13	CLA	Y	502	X	-	-	-
13	CLA	Y	503	X	-	-	-
13	CLA	Y	504	X	-	-	-
13	CLA	Y	505	X	-	-	-
13	CLA	Y	506	X	-	-	-
13	CLA	Y	507	X	-	-	-
13	CLA	Y	508	X	-	-	-
13	CLA	Y	509	X	-	-	-
13	CLA	Y	510	X	-	-	-
13	CLA	Y	511	X	-	-	-
13	CLA	Y	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	Y	513	X	-	-	-
13	CLA	Y	516	X	-	-	-
13	CLA	Y	517	X	-	-	-
13	CLA	Y	518	X	-	-	-
13	CLA	Y	519	X	-	-	-
13	CLA	Z	501	X	-	-	-
13	CLA	Z	502	X	-	-	-
13	CLA	Z	503	X	-	-	-
13	CLA	Z	504	X	-	-	-
13	CLA	Z	505	X	-	-	-
13	CLA	Z	506	X	-	-	-
13	CLA	Z	507	X	-	-	-
13	CLA	Z	508	X	-	-	-
13	CLA	Z	509	X	-	-	-
13	CLA	Z	510	X	-	-	-
13	CLA	Z	511	X	-	-	-
13	CLA	Z	512	X	-	-	-
13	CLA	Z	513	X	-	-	-
13	CLA	Z	516	X	-	-	-
13	CLA	Z	517	X	-	-	-
13	CLA	Z	518	X	-	-	-
13	CLA	Z	519	X	-	-	-
13	CLA	a	501	X	-	-	-
13	CLA	a	502	X	-	-	-
13	CLA	a	503	X	-	-	-
13	CLA	a	504	X	-	-	-
13	CLA	a	505	X	-	-	-
13	CLA	a	506	X	-	-	-
13	CLA	a	507	X	-	-	-
13	CLA	a	508	X	-	-	-
13	CLA	a	509	X	-	-	-
13	CLA	a	510	X	-	-	-
13	CLA	a	511	X	-	-	-
13	CLA	a	512	X	-	-	-
13	CLA	a	513	X	-	-	-
13	CLA	a	516	X	-	-	-
13	CLA	a	517	X	-	-	-
13	CLA	a	518	X	-	-	-
13	CLA	a	519	X	-	-	-
13	CLA	b	501	X	-	-	-
13	CLA	b	502	X	-	-	-
13	CLA	b	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	b	504	X	-	-	-
13	CLA	b	505	X	-	-	-
13	CLA	b	506	X	-	-	-
13	CLA	b	507	X	-	-	-
13	CLA	b	508	X	-	-	-
13	CLA	b	509	X	-	-	-
13	CLA	b	510	X	-	-	-
13	CLA	b	511	X	-	-	-
13	CLA	b	512	X	-	-	-
13	CLA	b	513	X	-	-	-
13	CLA	b	516	X	-	-	-
13	CLA	b	517	X	-	-	-
13	CLA	b	518	X	-	-	-
13	CLA	b	519	X	-	-	-
13	CLA	c	501	X	-	-	-
13	CLA	c	502	X	-	-	-
13	CLA	c	503	X	-	-	-
13	CLA	c	504	X	-	-	-
13	CLA	c	505	X	-	-	-
13	CLA	c	506	X	-	-	-
13	CLA	c	507	X	-	-	-
13	CLA	c	508	X	-	-	-
13	CLA	c	509	X	-	-	-
13	CLA	c	510	X	-	-	-
13	CLA	c	511	X	-	-	-
13	CLA	c	512	X	-	-	-
13	CLA	c	513	X	-	-	-
13	CLA	c	516	X	-	-	-
13	CLA	c	517	X	-	-	-
13	CLA	c	518	X	-	-	-
13	CLA	c	519	X	-	-	-
13	CLA	d	501	X	-	-	-
13	CLA	d	502	X	-	-	-
13	CLA	d	503	X	-	-	-
13	CLA	d	504	X	-	-	-
13	CLA	d	505	X	-	-	-
13	CLA	d	506	X	-	-	-
13	CLA	d	507	X	-	-	-
13	CLA	d	508	X	-	-	-
13	CLA	d	509	X	-	-	-
13	CLA	d	510	X	-	-	-
13	CLA	d	511	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	d	512	X	-	-	-
13	CLA	d	513	X	-	-	-
13	CLA	d	516	X	-	-	-
13	CLA	d	517	X	-	-	-
13	CLA	d	518	X	-	-	-
13	CLA	d	519	X	-	-	-
13	CLA	e	1011	X	-	-	-
13	CLA	e	1013	X	-	-	-
13	CLA	e	1022	X	-	-	-
13	CLA	e	1101	X	-	-	-
13	CLA	e	1102	X	-	-	-
13	CLA	e	1103	X	-	-	-
13	CLA	e	1104	X	-	-	-
13	CLA	e	1105	X	-	-	-
13	CLA	e	1106	X	-	-	-
13	CLA	e	1107	X	-	-	-
13	CLA	e	1108	X	-	-	-
13	CLA	e	1109	X	-	-	-
13	CLA	e	1110	X	-	-	-
13	CLA	e	1111	X	-	-	-
13	CLA	e	1112	X	-	-	-
13	CLA	e	1113	X	-	-	-
13	CLA	e	1114	X	-	-	-
13	CLA	e	1115	X	-	-	-
13	CLA	e	1116	X	-	-	-
13	CLA	e	1117	X	-	-	-
13	CLA	e	1118	X	-	-	-
13	CLA	e	1119	X	-	-	-
13	CLA	e	1120	X	-	-	-
13	CLA	e	1121	X	-	-	-
13	CLA	e	1122	X	-	-	-
13	CLA	e	1123	X	-	-	-
13	CLA	e	1124	X	-	-	-
13	CLA	e	1125	X	-	-	-
13	CLA	e	1126	X	-	-	-
13	CLA	e	1127	X	-	-	-
13	CLA	e	1128	X	-	-	-
13	CLA	e	1129	X	-	-	-
13	CLA	e	1130	X	-	-	-
13	CLA	e	1131	X	-	-	-
13	CLA	e	1132	X	-	-	-
13	CLA	e	1133	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	e	1134	X	-	-	-
13	CLA	e	1135	X	-	-	-
13	CLA	e	1136	X	-	-	-
13	CLA	e	1137	X	-	-	-
13	CLA	e	1138	X	-	-	-
13	CLA	e	1139	X	-	-	-
13	CLA	e	1140	X	-	-	-
13	CLA	e	1237	X	-	-	-
13	CLA	e	1801	X	-	-	-
13	CLA	f	1012	X	-	-	-
13	CLA	f	1021	X	-	-	-
13	CLA	f	1023	X	-	-	-
13	CLA	f	1201	X	-	-	-
13	CLA	f	1202	X	-	-	-
13	CLA	f	1203	X	-	-	-
13	CLA	f	1204	X	-	-	-
13	CLA	f	1205	X	-	-	-
13	CLA	f	1206	X	-	-	-
13	CLA	f	1207	X	-	-	-
13	CLA	f	1208	X	-	-	-
13	CLA	f	1209	X	-	-	-
13	CLA	f	1210	X	-	-	-
13	CLA	f	1211	X	-	-	-
13	CLA	f	1212	X	-	-	-
13	CLA	f	1213	X	-	-	-
13	CLA	f	1214	X	-	-	-
13	CLA	f	1215	X	-	-	-
13	CLA	f	1216	X	-	-	-
13	CLA	f	1217	X	-	-	-
13	CLA	f	1218	X	-	-	-
13	CLA	f	1219	X	-	-	-
13	CLA	f	1220	X	-	-	-
13	CLA	f	1221	X	-	-	-
13	CLA	f	1222	X	-	-	-
13	CLA	f	1223	X	-	-	-
13	CLA	f	1224	X	-	-	-
13	CLA	f	1225	X	-	-	-
13	CLA	f	1226	X	-	-	-
13	CLA	f	1227	X	-	-	-
13	CLA	f	1228	X	-	-	-
13	CLA	f	1229	X	-	-	-
13	CLA	f	1230	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	f	1231	X	-	-	-
13	CLA	f	1232	X	-	-	-
13	CLA	f	1234	X	-	-	-
13	CLA	f	1235	X	-	-	-
13	CLA	f	1238	X	-	-	-
13	CLA	f	1239	X	-	-	-
13	CLA	j	1301	X	-	-	-
13	CLA	j	1302	X	-	-	-
13	CLA	l	1302	X	-	-	-
13	CLA	l	1303	X	-	-	-
13	CLA	m	1103	X	-	-	-
13	CLA	m	1105	X	-	-	-
13	CLA	m	1401	X	-	-	-
13	CLA	n	1501	X	-	-	-
13	CLA	n	1502	X	-	-	-
13	CLA	n	1503	X	-	-	-
13	CLA	q	501	X	-	-	-
13	CLA	q	502	X	-	-	-
13	CLA	q	503	X	-	-	-
13	CLA	q	504	X	-	-	-
13	CLA	q	505	X	-	-	-
13	CLA	q	506	X	-	-	-
13	CLA	q	507	X	-	-	-
13	CLA	q	508	X	-	-	-
13	CLA	q	509	X	-	-	-
13	CLA	q	510	X	-	-	-
13	CLA	q	511	X	-	-	-
13	CLA	q	512	X	-	-	-
13	CLA	q	513	X	-	-	-
13	CLA	q	516	X	-	-	-
13	CLA	q	517	X	-	-	-
13	CLA	q	518	X	-	-	-
13	CLA	q	519	X	-	-	-
13	CLA	r	501	X	-	-	-
13	CLA	r	502	X	-	-	-
13	CLA	r	503	X	-	-	-
13	CLA	r	504	X	-	-	-
13	CLA	r	505	X	-	-	-
13	CLA	r	506	X	-	-	-
13	CLA	r	507	X	-	-	-
13	CLA	r	508	X	-	-	-
13	CLA	r	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	r	510	X	-	-	-
13	CLA	r	511	X	-	-	-
13	CLA	r	512	X	-	-	-
13	CLA	r	513	X	-	-	-
13	CLA	r	516	X	-	-	-
13	CLA	r	517	X	-	-	-
13	CLA	r	518	X	-	-	-
13	CLA	r	519	X	-	-	-
13	CLA	s	501	X	-	-	-
13	CLA	s	502	X	-	-	-
13	CLA	s	503	X	-	-	-
13	CLA	s	504	X	-	-	-
13	CLA	s	505	X	-	-	-
13	CLA	s	506	X	-	-	-
13	CLA	s	507	X	-	-	-
13	CLA	s	508	X	-	-	-
13	CLA	s	509	X	-	-	-
13	CLA	s	510	X	-	-	-
13	CLA	s	511	X	-	-	-
13	CLA	s	512	X	-	-	-
13	CLA	s	513	X	-	-	-
13	CLA	s	516	X	-	-	-
13	CLA	s	517	X	-	-	-
13	CLA	s	518	X	-	-	-
13	CLA	s	519	X	-	-	-
13	CLA	t	501	X	-	-	-
13	CLA	t	502	X	-	-	-
13	CLA	t	503	X	-	-	-
13	CLA	t	504	X	-	-	-
13	CLA	t	505	X	-	-	-
13	CLA	t	506	X	-	-	-
13	CLA	t	507	X	-	-	-
13	CLA	t	508	X	-	-	-
13	CLA	t	509	X	-	-	-
13	CLA	t	510	X	-	-	-
13	CLA	t	511	X	-	-	-
13	CLA	t	512	X	-	-	-
13	CLA	t	513	X	-	-	-
13	CLA	t	516	X	-	-	-
13	CLA	t	517	X	-	-	-
13	CLA	t	518	X	-	-	-
13	CLA	t	519	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	u	501	X	-	-	-
13	CLA	u	502	X	-	-	-
13	CLA	u	503	X	-	-	-
13	CLA	u	504	X	-	-	-
13	CLA	u	505	X	-	-	-
13	CLA	u	506	X	-	-	-
13	CLA	u	507	X	-	-	-
13	CLA	u	508	X	-	-	-
13	CLA	u	509	X	-	-	-
13	CLA	u	510	X	-	-	-
13	CLA	u	511	X	-	-	-
13	CLA	u	512	X	-	-	-
13	CLA	u	513	X	-	-	-
13	CLA	u	516	X	-	-	-
13	CLA	u	517	X	-	-	-
13	CLA	u	518	X	-	-	-
13	CLA	u	519	X	-	-	-
13	CLA	v	501	X	-	-	-
13	CLA	v	502	X	-	-	-
13	CLA	v	503	X	-	-	-
13	CLA	v	504	X	-	-	-
13	CLA	v	505	X	-	-	-
13	CLA	v	506	X	-	-	-
13	CLA	v	507	X	-	-	-
13	CLA	v	508	X	-	-	-
13	CLA	v	509	X	-	-	-
13	CLA	v	510	X	-	-	-
13	CLA	v	511	X	-	-	-
13	CLA	v	512	X	-	-	-
13	CLA	v	513	X	-	-	-
13	CLA	v	516	X	-	-	-
13	CLA	v	517	X	-	-	-
13	CLA	v	518	X	-	-	-
13	CLA	v	519	X	-	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 143022 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	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		
1	G	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		
1	e	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5789	3811	970	994	14		
2	H	733	Total	C	N	O	S	0	0
			5789	3811	970	994	14		
2	f	733	Total	C	N	O	S	0	0
			5789	3811	970	994	14		

- 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
			598	368	103	116	11		
3	N	80	Total	C	N	O	S	0	0
			598	368	103	116	11		
3	g	80	Total	C	N	O	S	0	0
			598	368	103	116	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	141	Total	C	N	O	S	0	0
			1098	702	187	208	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	141	Total	C	N	O	S	0	0
			1098	702	187	208	1		
4	h	141	Total	C	N	O	S	0	0
			1098	702	187	208	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	71	Total	C	N	O		0	0
			543	343	95	105			
5	Q	71	Total	C	N	O		0	0
			543	343	95	105			
5	i	71	Total	C	N	O		0	0
			543	343	95	105			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	136	Total	C	N	O	S	0	0
			1036	670	174	190	2		
6	R	136	Total	C	N	O	S	0	0
			1036	670	174	190	2		
6	j	136	Total	C	N	O	S	0	0
			1036	670	174	190	2		

- Molecule 7 is a protein called Photosystem I PsaI protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			282	191	38	51	2		
7	S	38	Total	C	N	O	S	0	0
			282	191	38	51	2		
7	k	38	Total	C	N	O	S	0	0
			282	191	38	51	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			335	228	52	54	1		
8	T	41	Total	C	N	O	S	0	0
			335	228	52	54	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	l	41	Total	C	N	O	S	0	0
			335	228	52	54	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	78	Total	C	N	O	S	0	0
			549	364	91	93	1		
9	U	78	Total	C	N	O	S	0	0
			549	364	91	93	1		
9	m	78	Total	C	N	O	S	0	0
			549	364	91	93	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	164	Total	C	N	O	S	0	0
			1210	782	201	225	2		
10	V	164	Total	C	N	O	S	0	0
			1210	782	201	225	2		
10	n	164	Total	C	N	O	S	0	0
			1210	782	201	225	2		

- Molecule 11 is a protein called Psam.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	29	Total	C	N	O	S	0	0
			228	151	36	40	1		
11	W	29	Total	C	N	O	S	0	0
			228	151	36	40	1		
11	o	29	Total	C	N	O	S	0	0
			228	151	36	40	1		

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

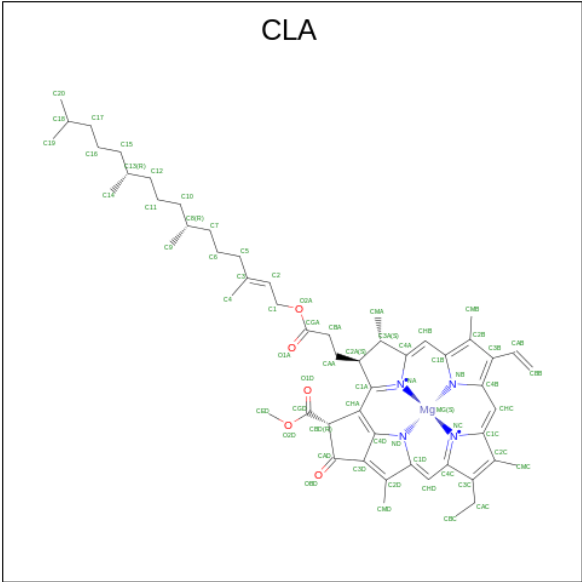
Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	2	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	3	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	4	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	5	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	6	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	Y	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	Z	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	a	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	b	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	c	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	d	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	q	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	r	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	s	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	t	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	u	339	Total 2605	C 1722	N 428	O 448	S 7	0	0
12	v	339	Total 2605	C 1722	N 428	O 448	S 7	0	0

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	J	1	Total 58	C 48	Mg 1	N 4	O 5	0
13	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	1	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	1	1	Total 64	C 54	Mg 1	N 4	O 5	0
13	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	2	1	Total 53	C 43	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	3	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	6	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	G	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	H	1	Total 57	C 47	Mg 1	N 4	O 5	0
13	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	H	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	T	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	U	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	V	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	Y	1	Total 64	C 54	Mg 1	N 4	O 5	0
13	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	Y	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 53	C 43	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 61	C 51	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	d	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	d	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	d	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	e	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 53	C 43	Mg 1	N 4	O 5	0
13	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	e	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	e	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	e	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	f	1	Total 57	C 47	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	l	1	Total 58	C 48	Mg 1	N 4	O 5	0
13	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	m	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	m	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	m	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	q	1	Total 64	C 54	Mg 1	N 4	O 5	0
13	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	q	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	q	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	q	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	r	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	r	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	r	1	Total 53	C 43	Mg 1	N 4	O 5	0
13	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	s	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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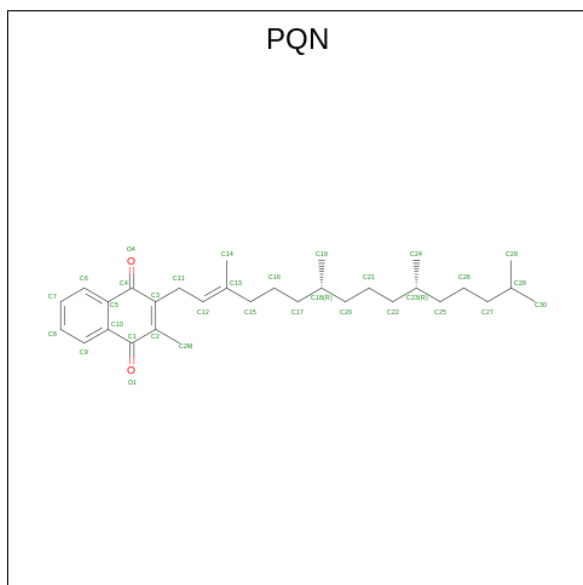
Mol	Chain	Residues	Atoms					AltConf
13	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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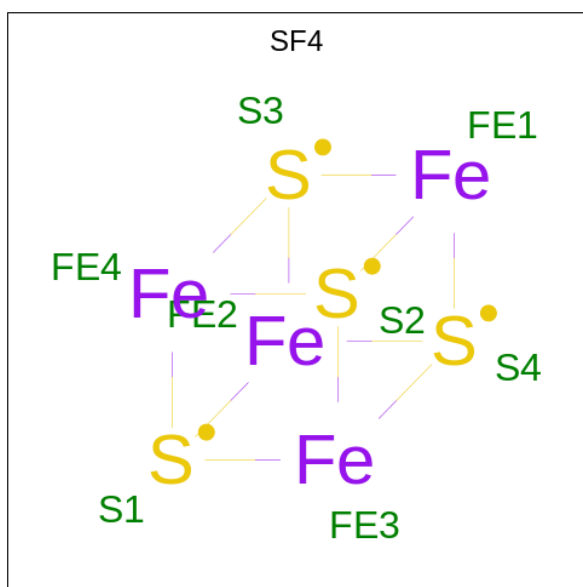
Mol	Chain	Residues	Atoms					AltConf
13	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	v	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



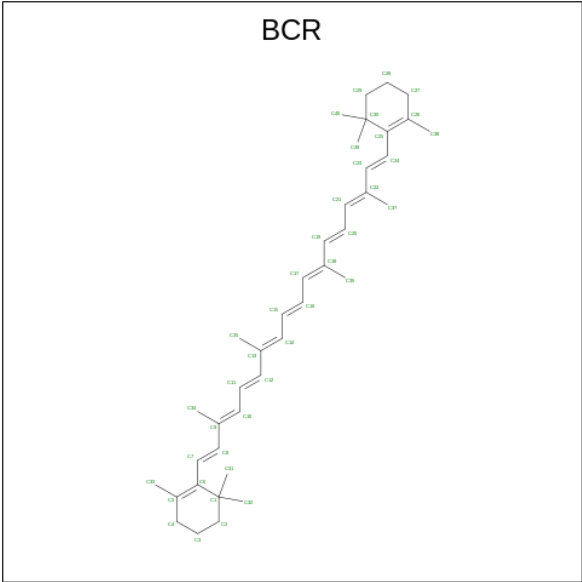
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			33	31	2	
14	B	1	Total	C	O	0
			33	31	2	
14	G	1	Total	C	O	0
			33	31	2	
14	H	1	Total	C	O	0
			33	31	2	
14	e	1	Total	C	O	0
			33	31	2	
14	f	1	Total	C	O	0
			33	31	2	

- Molecule 15 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	Fe	S	0
			8	4	4	
15	C	1	Total	Fe	S	
			8	4	4	
15	C	1	Total	Fe	S	
			8	4	4	
15	G	1	Total	Fe	S	
			8	4	4	
15	N	1	Total	Fe	S	
			8	4	4	
15	N	1	Total	Fe	S	0
			8	4	4	
15	e	1	Total	Fe	S	
			8	4	4	
15	g	1	Total	Fe	S	
			8	4	4	
15	g	1	Total	Fe	S	
			8	4	4	

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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Mol	Chain	Residues	Atoms	AltConf
16	I	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	K	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	M	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	3	1	Total C 40 40	0
16	3	1	Total C 40 40	0
16	3	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	3	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	4	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	5	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	G	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	H	1	Total C 40 40	0
16	R	1	Total C 40 40	0
16	S	1	Total C 40 40	0
16	T	1	Total C 40 40	0
16	T	1	Total C 40 40	0
16	T	1	Total C 40 40	0
16	U	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	V	1	Total C 40 40	0
16	W	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Y	1	Total C 40 40	0
16	Z	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	Z	1	Total C 40 40	0
16	Z	1	Total C 40 40	0
16	Z	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	c	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	d	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	e	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	k	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	m	1	Total C 40 40	0
16	n	1	Total C 40 40	0
16	n	1	Total C 40 40	0
16	n	1	Total C 40 40	0
16	n	1	Total C 40 40	0

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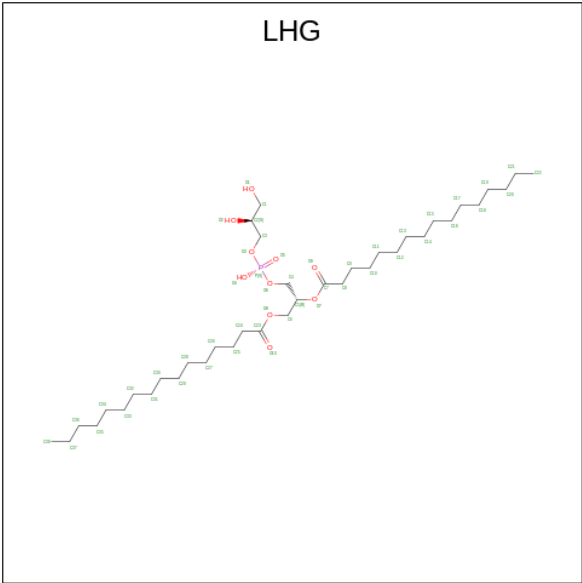
Mol	Chain	Residues	Atoms	AltConf
16	o	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	q	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	r	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	s	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	t	1	Total C 40 40	0
16	u	1	Total C 40 40	0
16	u	1	Total C 40 40	0
16	u	1	Total C 40 40	0
16	u	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
16	v	1	Total	C	0
			40	40	
16	v	1	Total	C	0
			40	40	
16	v	1	Total	C	0
			40	40	
16	v	1	Total	C	0
			40	40	

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			39	28	10	1	
17	A	1	Total	C	O	P	0
			36	25	10	1	
17	A	1	Total	C	O	P	0
			45	34	10	1	
17	A	1	Total	C	O	P	0
			45	34	10	1	
17	A	1	Total	C	O	P	0
			47	36	10	1	
17	A	1	Total	C	O	P	0
			35	24	10	1	
17	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total 49	C 38	O 10	P 1	0
17	A	1	Total 41	C 30	O 10	P 1	0
17	B	1	Total 39	C 28	O 10	P 1	0
17	B	1	Total 44	C 33	O 10	P 1	0
17	I	1	Total 44	C 33	O 10	P 1	0
17	L	1	Total 38	C 27	O 10	P 1	0
17	L	1	Total 41	C 30	O 10	P 1	0
17	L	1	Total 49	C 38	O 10	P 1	0
17	G	1	Total 39	C 28	O 10	P 1	0
17	G	1	Total 36	C 25	O 10	P 1	0
17	G	1	Total 45	C 34	O 10	P 1	0
17	G	1	Total 45	C 34	O 10	P 1	0
17	G	1	Total 47	C 36	O 10	P 1	0
17	G	1	Total 35	C 24	O 10	P 1	0
17	G	1	Total 49	C 38	O 10	P 1	0
17	G	1	Total 49	C 38	O 10	P 1	0
17	G	1	Total 41	C 30	O 10	P 1	0
17	H	1	Total 39	C 28	O 10	P 1	0
17	H	1	Total 44	C 33	O 10	P 1	0
17	S	1	Total 44	C 33	O 10	P 1	0
17	V	1	Total 38	C 27	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
17	V	1	Total	C	O	P	0
			41	30	10	1	
17	V	1	Total	C	O	P	0
			49	38	10	1	
17	e	1	Total	C	O	P	0
			39	28	10	1	
17	e	1	Total	C	O	P	0
			36	25	10	1	
17	e	1	Total	C	O	P	0
			45	34	10	1	
17	e	1	Total	C	O	P	0
			45	34	10	1	
17	e	1	Total	C	O	P	0
			47	36	10	1	
17	e	1	Total	C	O	P	0
			35	24	10	1	
17	e	1	Total	C	O	P	0
			49	38	10	1	
17	e	1	Total	C	O	P	0
			49	38	10	1	
17	e	1	Total	C	O	P	0
			41	30	10	1	
17	f	1	Total	C	O	P	0
			39	28	10	1	
17	f	1	Total	C	O	P	0
			44	33	10	1	
17	k	1	Total	C	O	P	0
			44	33	10	1	
17	n	1	Total	C	O	P	0
			38	27	10	1	
17	n	1	Total	C	O	P	0
			41	30	10	1	
17	n	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 18 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).

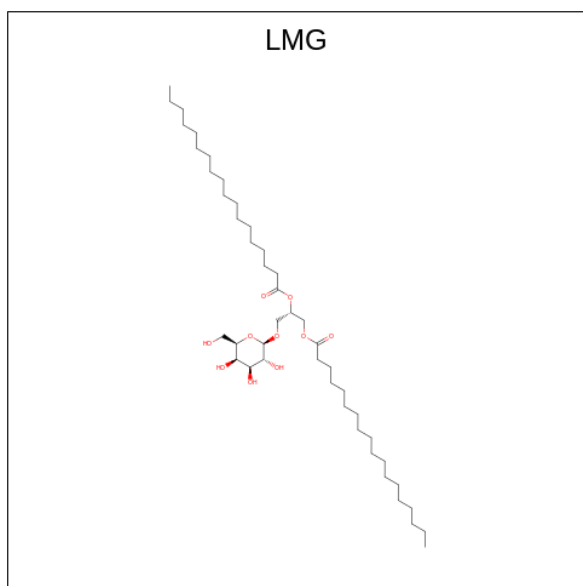


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Mol	Chain	Residues	Atoms			AltConf
18	f	1	Total	C	O	0
			35	24	11	
18	l	1	Total	C	O	0
			22	16	6	
18	q	1	Total	C	O	0
			19	13	6	
18	r	1	Total	C	O	0
			23	17	6	

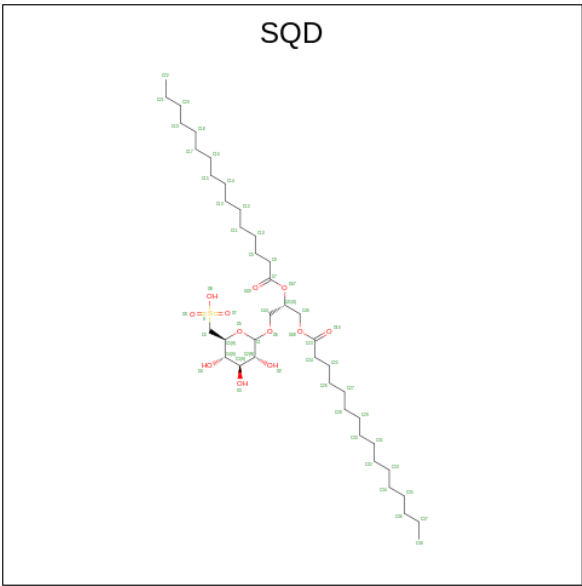
- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
19	B	1	Total	C	O	0
			54	44	10	
19	J	1	Total	C	O	0
			35	25	10	
19	H	1	Total	C	O	0
			54	44	10	
19	T	1	Total	C	O	0
			35	25	10	
19	f	1	Total	C	O	0
			54	44	10	
19	l	1	Total	C	O	0
			35	25	10	

- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				AltConf
20	B	1	Total	C	O	S	0
			45	32	12	1	
20	L	1	Total	C	O	S	0
			51	38	12	1	
20	1	1	Total	C	O	S	0
			48	35	12	1	
20	2	1	Total	C	O	S	0
			43	30	12	1	
20	3	1	Total	C	O	S	0
			43	30	12	1	
20	4	1	Total	C	O	S	0
			26	13	12	1	
20	5	1	Total	C	O	S	0
			29	16	12	1	
20	6	1	Total	C	O	S	0
			26	13	12	1	
20	H	1	Total	C	O	S	0
			45	32	12	1	
20	V	1	Total	C	O	S	0
			51	38	12	1	
20	Y	1	Total	C	O	S	0
			48	35	12	1	
20	Z	1	Total	C	O	S	0
			43	30	12	1	
20	a	1	Total	C	O	S	0
			43	30	12	1	

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Mol	Chain	Residues	Atoms				AltConf
20	b	1	Total	C	O	S	0
			26	13	12	1	
20	c	1	Total	C	O	S	0
			29	16	12	1	
20	d	1	Total	C	O	S	0
			26	13	12	1	
20	f	1	Total	C	O	S	0
			45	32	12	1	
20	n	1	Total	C	O	S	0
			51	38	12	1	
20	q	1	Total	C	O	S	0
			48	35	12	1	
20	r	1	Total	C	O	S	0
			43	30	12	1	
20	s	1	Total	C	O	S	0
			43	30	12	1	
20	t	1	Total	C	O	S	0
			26	13	12	1	
20	u	1	Total	C	O	S	0
			29	16	12	1	
20	v	1	Total	C	O	S	0
			26	13	12	1	

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	A	9	Total	O	0
			9	9	
21	B	7	Total	O	0
			7	7	
21	F	1	Total	O	0
			1	1	
21	L	1	Total	O	0
			1	1	
21	G	9	Total	O	0
			9	9	
21	H	7	Total	O	0
			7	7	
21	R	1	Total	O	0
			1	1	
21	V	1	Total	O	0
			1	1	

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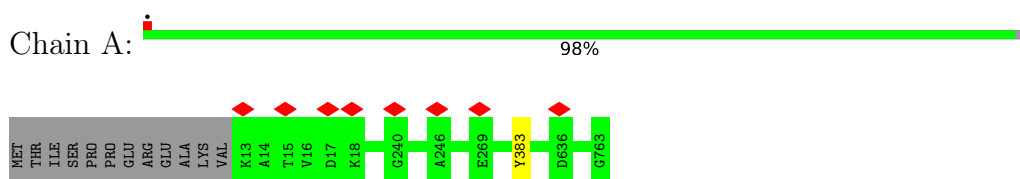
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Mol	Chain	Residues	Atoms		AltConf
21	e	9	Total 9	O 9	0
21	f	7	Total 7	O 7	0
21	j	1	Total 1	O 1	0
21	n	1	Total 1	O 1	0

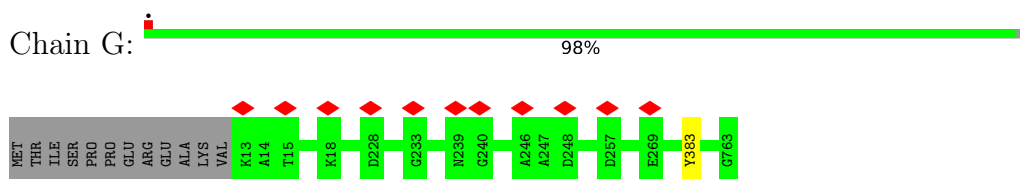
3 Residue-property plots [i](#)

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

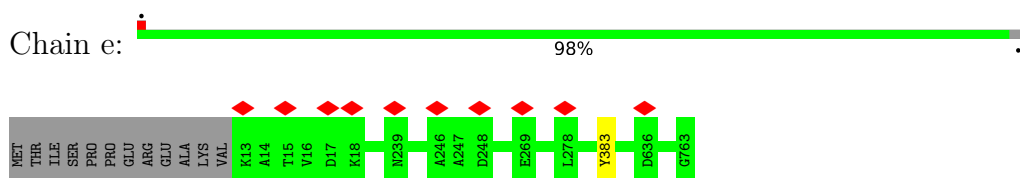
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



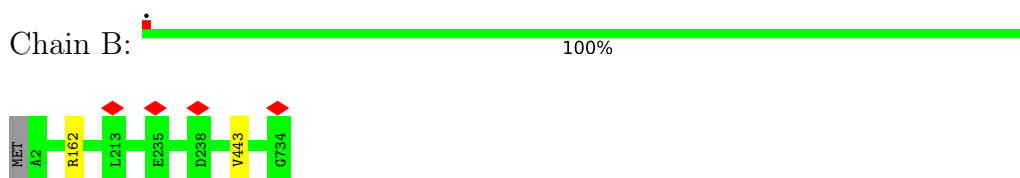
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



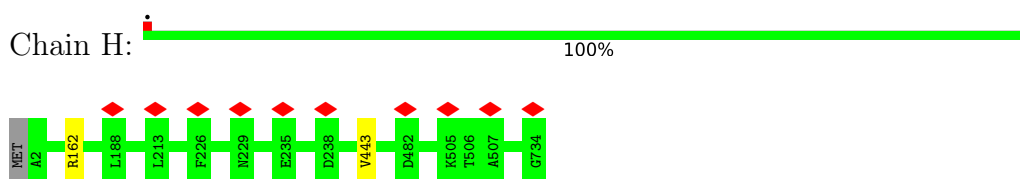
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

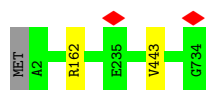


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain f:  100%



- Molecule 3: Photosystem I iron-sulfur center

Chain C:  99%



- Molecule 3: Photosystem I iron-sulfur center

Chain N:  99%



- Molecule 3: Photosystem I iron-sulfur center

Chain g:  99%



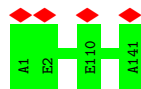
- Molecule 4: Photosystem I reaction center subunit II

Chain D:  100%



- Molecule 4: Photosystem I reaction center subunit II

Chain O:  100%



- Molecule 4: Photosystem I reaction center subunit II

Chain h:  100%



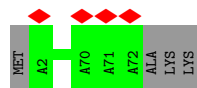
- Molecule 5: Photosystem I reaction center subunit IV



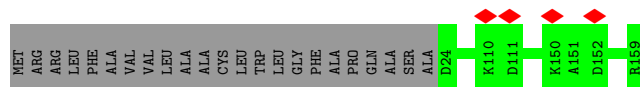
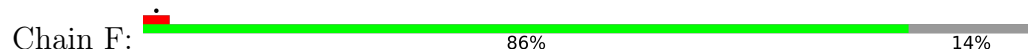
- Molecule 5: Photosystem I reaction center subunit IV



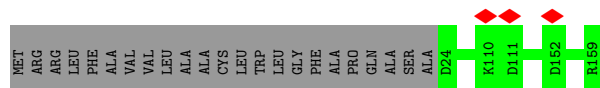
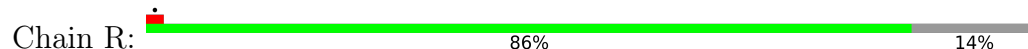
- Molecule 5: Photosystem I reaction center subunit IV



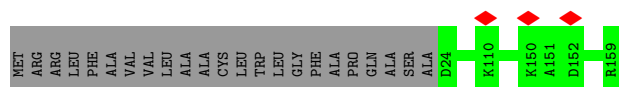
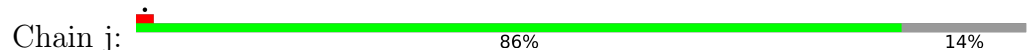
- Molecule 6: Photosystem I reaction center subunit III



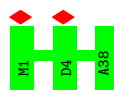
- Molecule 6: Photosystem I reaction center subunit III



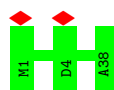
- Molecule 6: Photosystem I reaction center subunit III



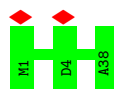
- Molecule 7: Photosystem I PsaI protein



- Molecule 7: Photosystem I PsaI protein



- Molecule 7: Photosystem I PsaI protein



- Molecule 8: Photosystem I reaction center subunit IX



There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem I reaction center subunit IX



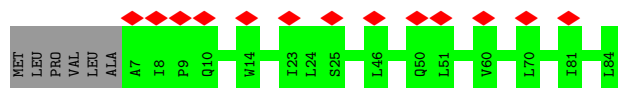
There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem I reaction center subunit IX



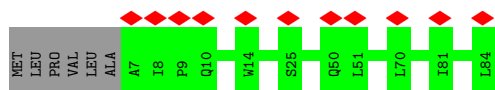
There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem I reaction center subunit PsaK

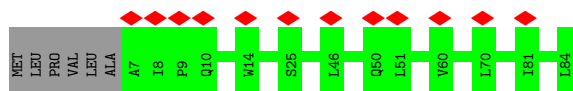


- Molecule 9: Photosystem I reaction center subunit PsaK

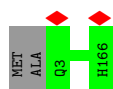




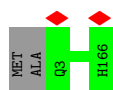
- Molecule 9: Photosystem I reaction center subunit PsaK



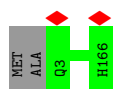
- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 11: PsaM



There are no outlier residues recorded for this chain.

- Molecule 11: PsaM



There are no outlier residues recorded for this chain.

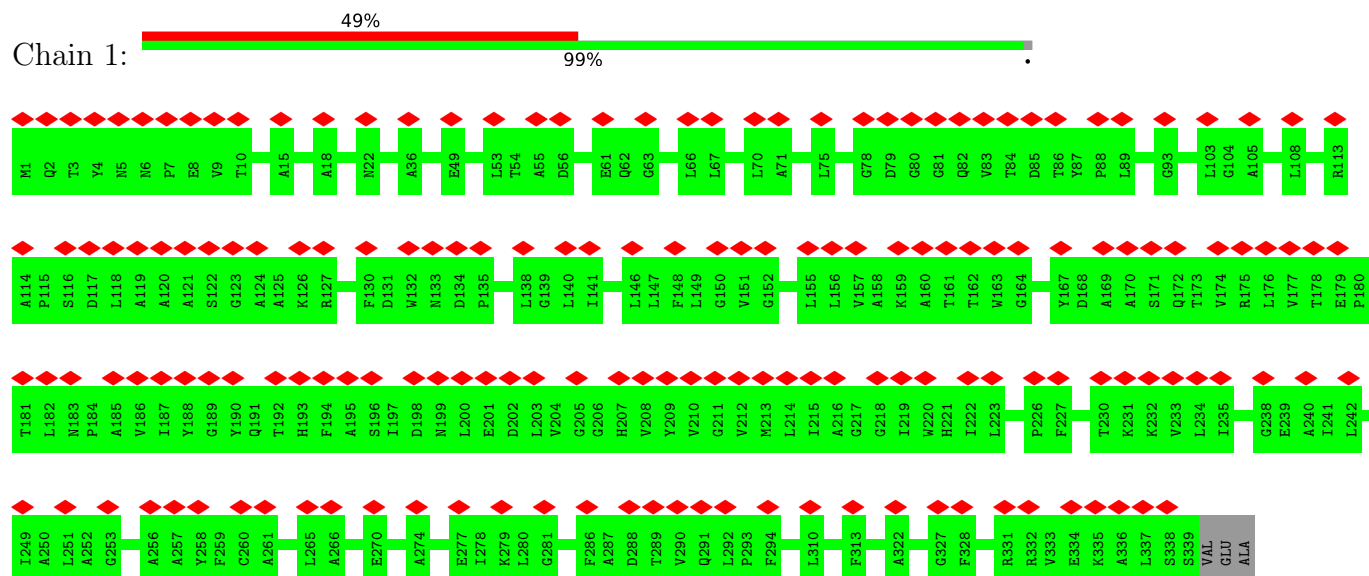
- Molecule 11: PsaM



There are no outlier residues recorded for this chain.

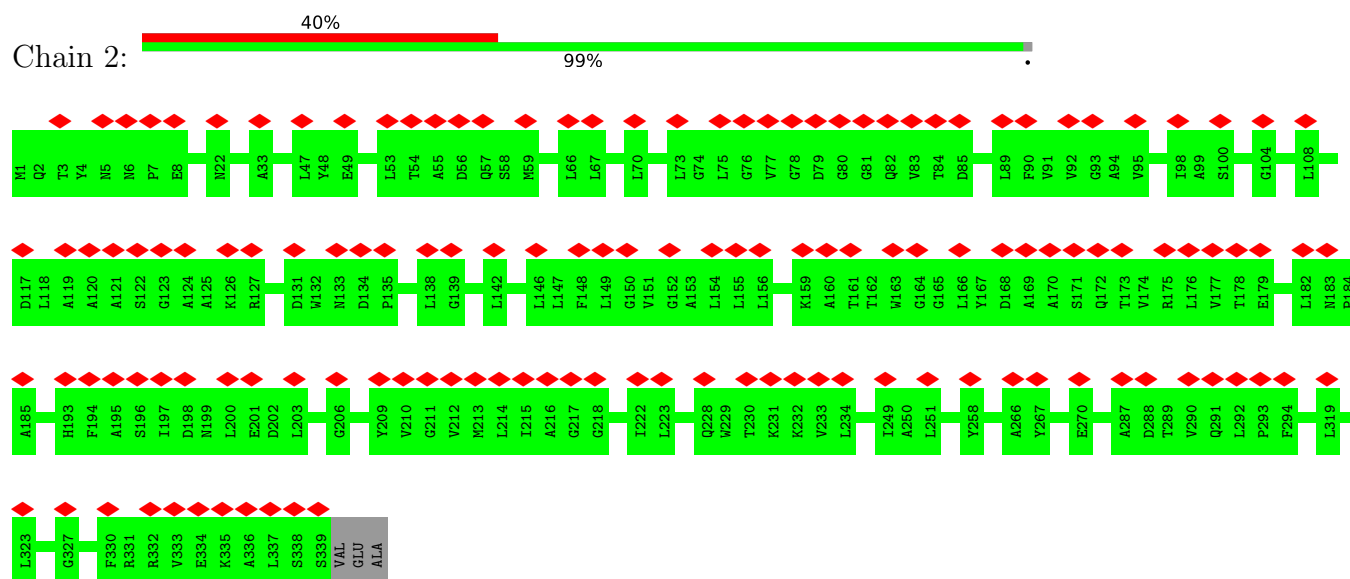
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain 1:



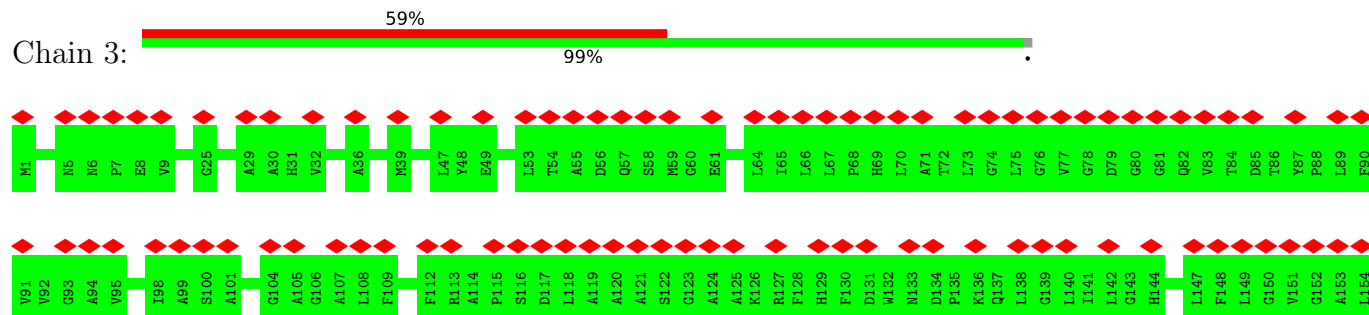
• Molecule 12: Iron stress-induced chlorophyll-binding protein

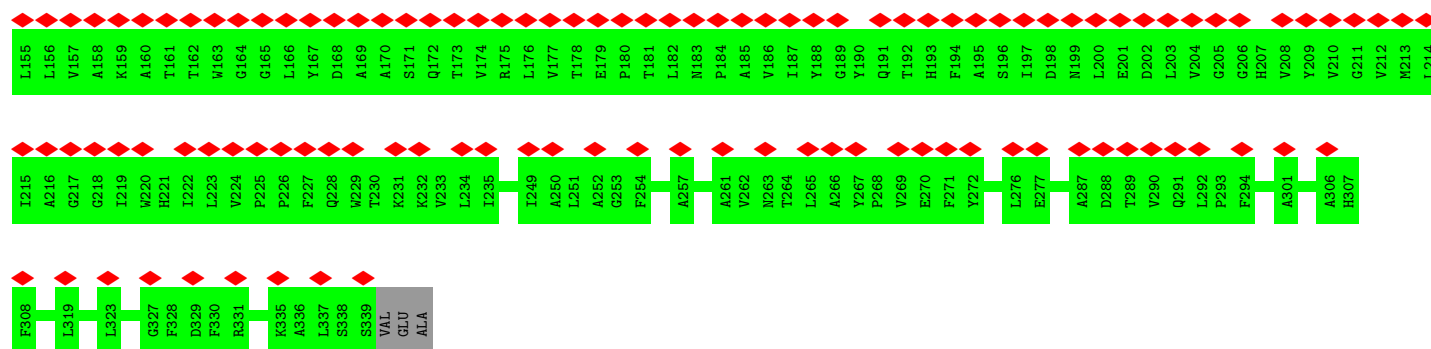
Chain 2:



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

Chain 3:

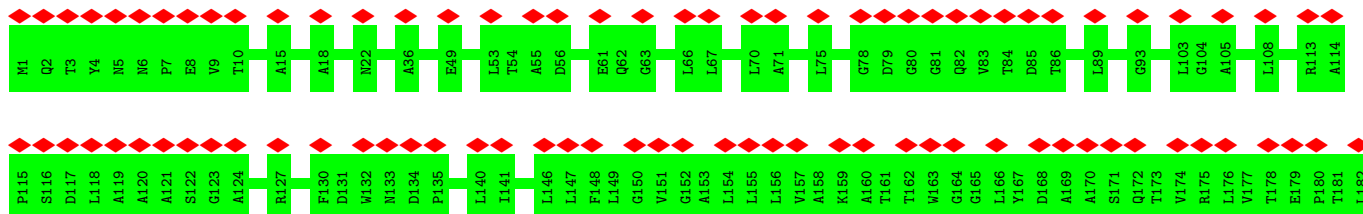


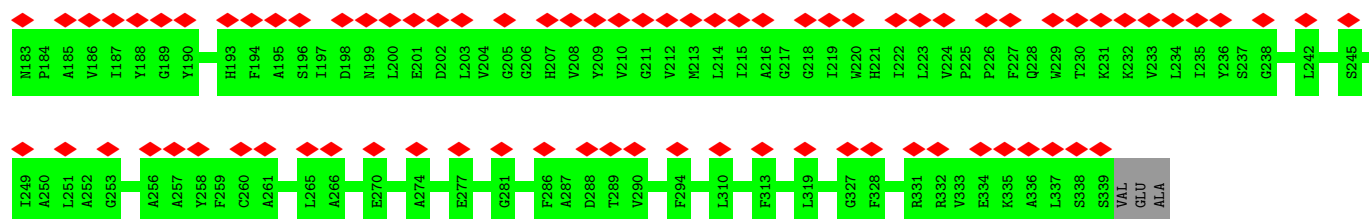


- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain 4: 94% 99%







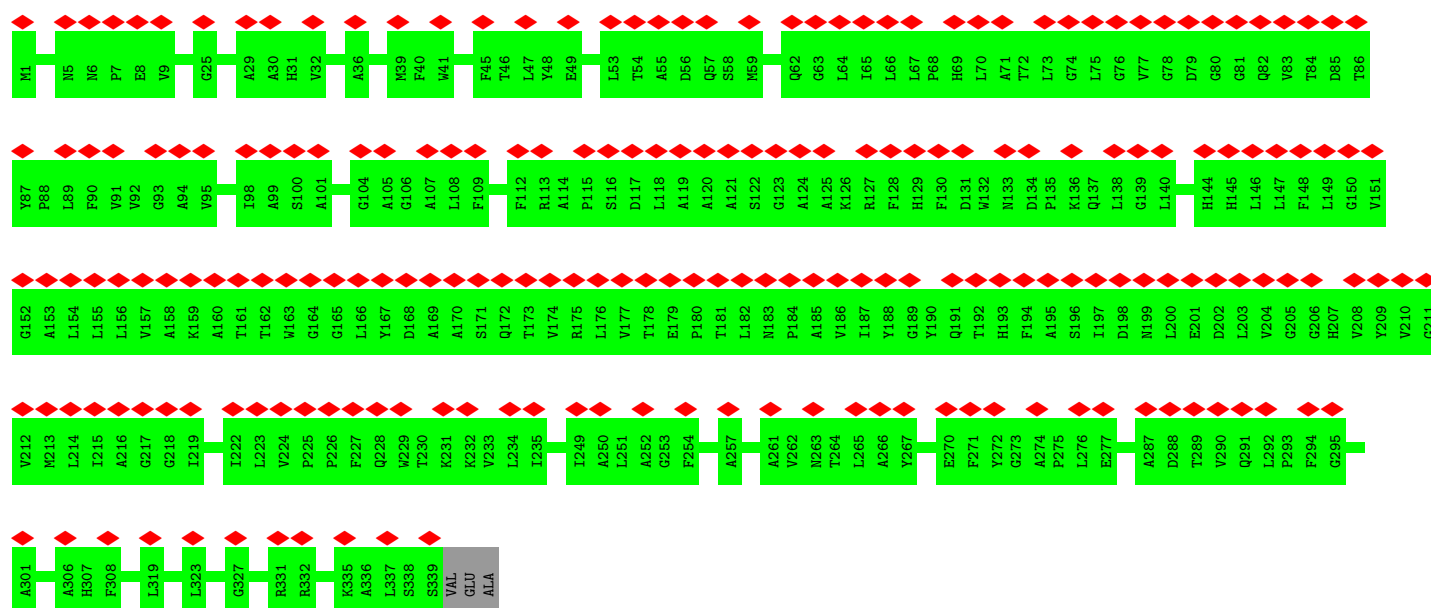
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain Z: 38% 99%



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

Chain a: 60% 99%



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

Chain b: 

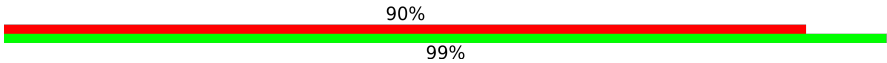


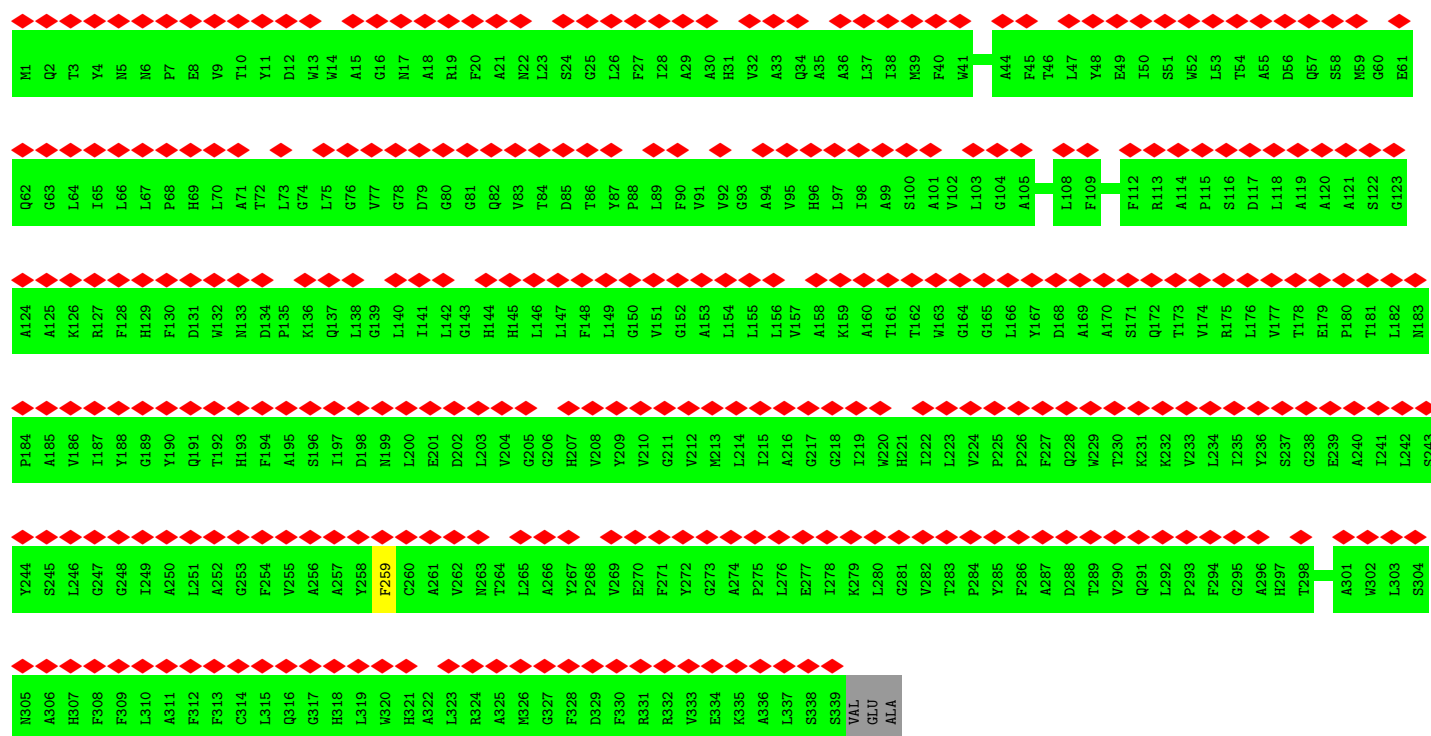
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain c: 



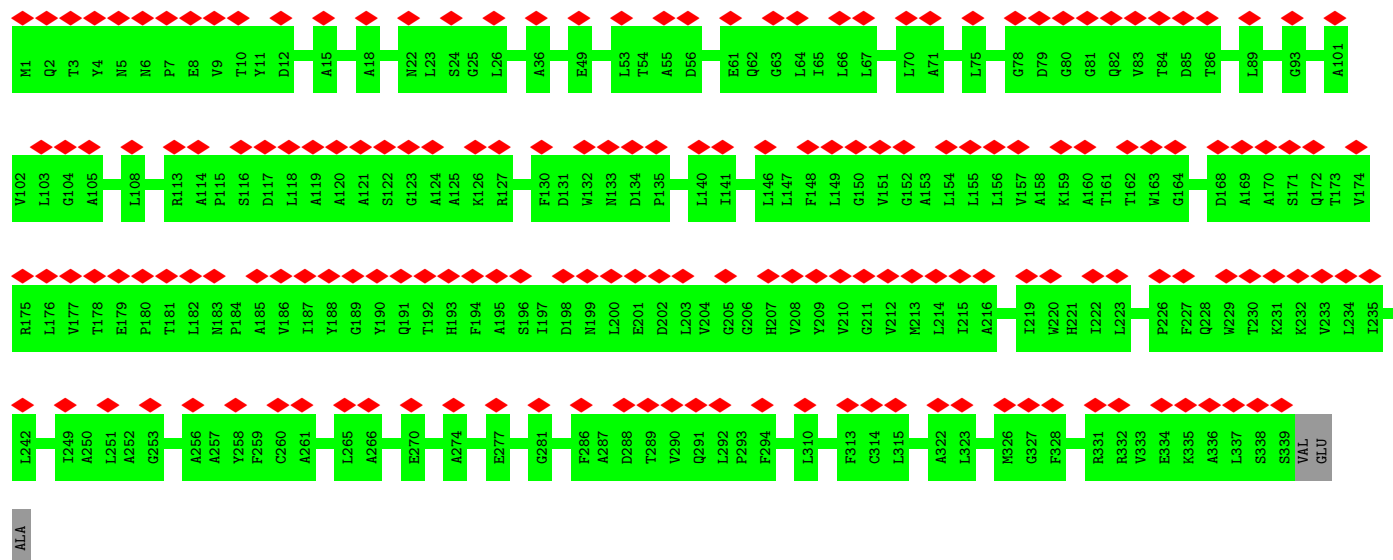
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain d: 

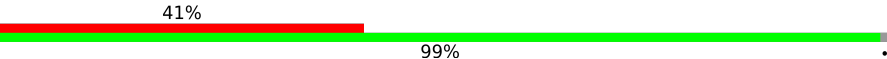


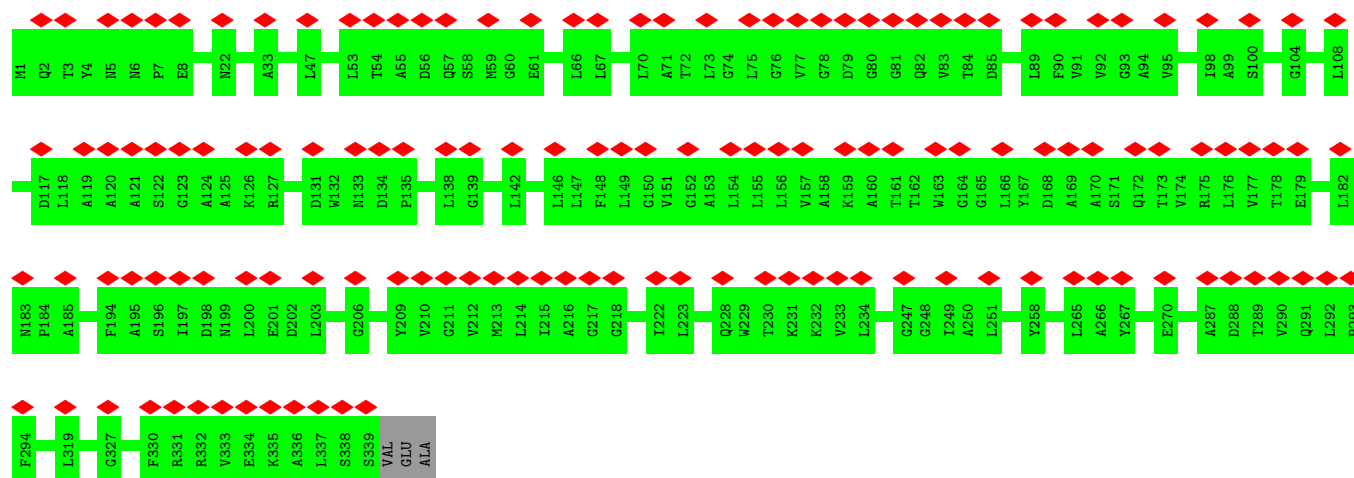
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain q: 



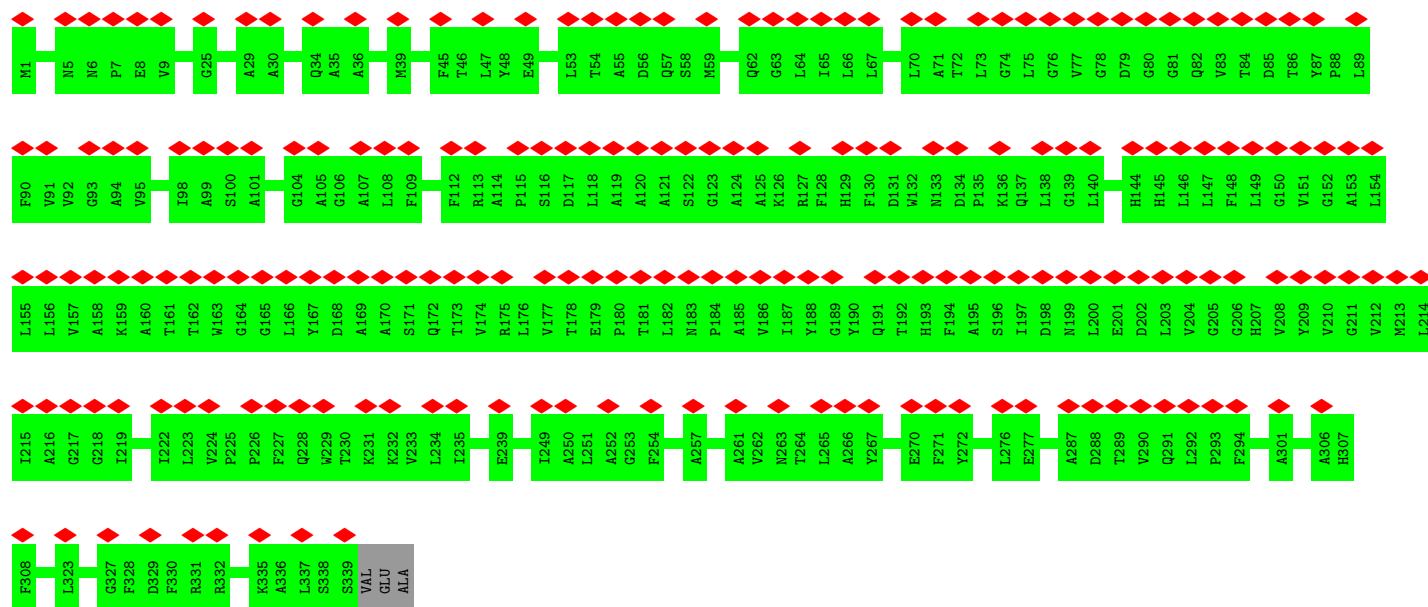
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain r: 



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

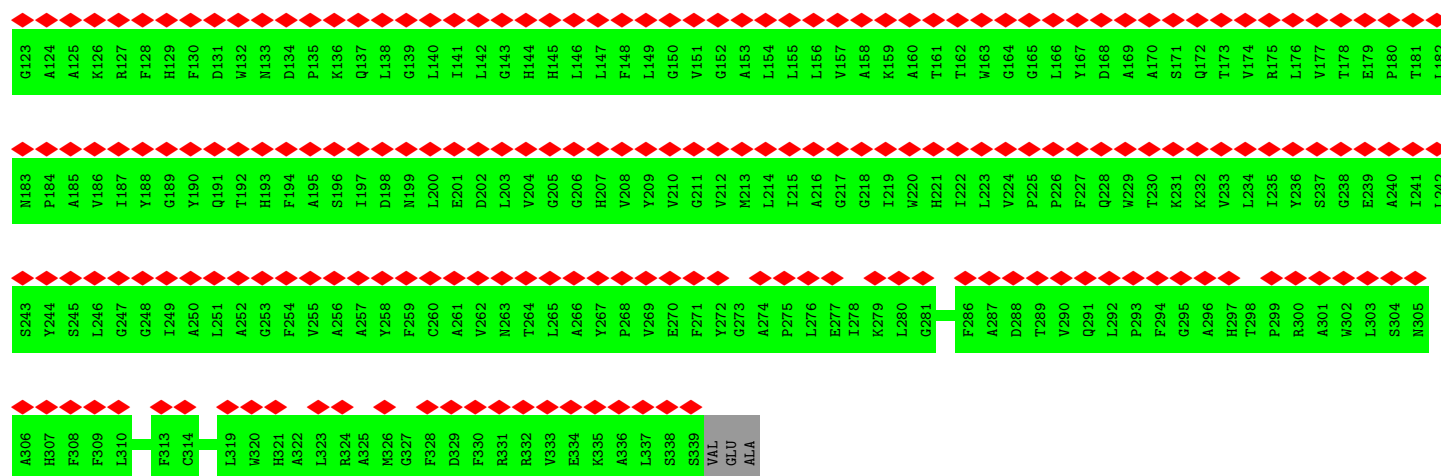
Chain s: 59% 99%



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

Chain t: 93% 99%





• 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, C3	Depositor
Number of particles used	63332	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.170	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: LMU, LHG, CLA, BCR, LMG, SF4, PQN, SQD

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	0.42	0/6064	0.53	0/8274
1	G	0.42	0/6064	0.53	0/8274
1	e	0.42	0/6064	0.53	0/8274
2	B	0.42	0/5999	0.53	0/8199
2	H	0.42	0/5999	0.53	0/8199
2	f	0.42	0/5999	0.53	0/8199
3	C	0.42	0/608	0.56	0/823
3	N	0.42	0/608	0.56	0/823
3	g	0.43	0/608	0.56	0/823
4	D	0.37	0/1124	0.54	0/1516
4	O	0.37	0/1124	0.54	0/1516
4	h	0.37	0/1124	0.54	0/1516
5	E	0.38	0/553	0.46	0/750
5	Q	0.38	0/553	0.46	0/750
5	i	0.38	0/553	0.46	0/750
6	F	0.36	0/1062	0.50	0/1442
6	R	0.36	0/1062	0.50	0/1442
6	j	0.36	0/1062	0.50	0/1442
7	I	0.38	0/289	0.62	0/393
7	S	0.38	0/289	0.62	0/393
7	k	0.38	0/289	0.62	0/393
8	J	0.41	0/346	0.57	0/469
8	T	0.41	0/346	0.57	0/469
8	l	0.41	0/346	0.57	0/469
9	K	0.31	0/560	0.56	0/765
9	U	0.31	0/560	0.56	0/765
9	m	0.31	0/560	0.56	0/765
10	L	0.36	0/1242	0.51	0/1696
10	V	0.36	0/1242	0.51	0/1696
10	n	0.36	0/1242	0.51	0/1696
11	M	0.37	0/231	0.54	0/314
11	W	0.37	0/231	0.54	0/314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	o	0.37	0/231	0.54	0/314
12	1	0.28	0/2689	0.47	0/3678
12	2	0.28	0/2689	0.48	0/3678
12	3	0.27	0/2689	0.46	0/3678
12	4	0.27	0/2689	0.47	0/3678
12	5	0.27	0/2689	0.46	0/3678
12	6	0.27	0/2689	0.45	0/3678
12	Y	0.29	0/2689	0.47	0/3678
12	Z	0.29	0/2689	0.48	0/3678
12	a	0.27	0/2689	0.46	0/3678
12	b	0.27	0/2689	0.47	0/3678
12	c	0.27	0/2689	0.46	0/3678
12	d	0.27	0/2689	0.45	0/3678
12	q	0.29	0/2689	0.47	0/3678
12	r	0.29	0/2689	0.48	0/3678
12	s	0.27	0/2689	0.46	0/3678
12	t	0.27	0/2689	0.47	0/3678
12	u	0.27	0/2689	0.46	0/3678
12	v	0.27	0/2689	0.45	0/3678
All	All	0.35	0/102636	0.50	0/140127

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	749/763 (98%)	723 (96%)	26 (4%)	0	100	100
1	G	749/763 (98%)	723 (96%)	26 (4%)	0	100	100
1	e	749/763 (98%)	723 (96%)	26 (4%)	0	100	100
2	B	731/734 (100%)	711 (97%)	20 (3%)	0	100	100
2	H	731/734 (100%)	711 (97%)	20 (3%)	0	100	100
2	f	731/734 (100%)	711 (97%)	20 (3%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	N	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	g	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
4	O	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
4	h	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
5	E	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
5	Q	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
5	i	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
6	F	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
6	R	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
6	j	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
7	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	S	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	k	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
8	T	39/41 (95%)	39 (100%)	0	0	100	100
8	l	39/41 (95%)	39 (100%)	0	0	100	100
9	K	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
9	U	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
9	m	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
10	L	162/166 (98%)	157 (97%)	5 (3%)	0	100	100
10	V	162/166 (98%)	157 (97%)	5 (3%)	0	100	100
10	n	162/166 (98%)	157 (97%)	5 (3%)	0	100	100
11	M	27/29 (93%)	27 (100%)	0	0	100	100
11	W	27/29 (93%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	o	27/29 (93%)	27 (100%)	0	0	100	100
12	1	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	2	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	3	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	4	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
12	5	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	6	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	Y	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	Z	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	a	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	b	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
12	c	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	d	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	q	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	r	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	s	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	t	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
12	u	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	v	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
All	All	12786/13089 (98%)	12420 (97%)	366 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	600/611 (98%)	599 (100%)	1 (0%)	92	98
1	G	600/611 (98%)	599 (100%)	1 (0%)	92	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	600/611 (98%)	599 (100%)	1 (0%)	92	98
2	B	583/584 (100%)	581 (100%)	2 (0%)	91	97
2	H	583/584 (100%)	581 (100%)	2 (0%)	91	97
2	f	583/584 (100%)	581 (100%)	2 (0%)	91	97
3	C	67/68 (98%)	67 (100%)	0	100	100
3	N	67/68 (98%)	67 (100%)	0	100	100
3	g	67/68 (98%)	67 (100%)	0	100	100
4	D	114/114 (100%)	114 (100%)	0	100	100
4	O	114/114 (100%)	114 (100%)	0	100	100
4	h	114/114 (100%)	114 (100%)	0	100	100
5	E	56/59 (95%)	56 (100%)	0	100	100
5	Q	56/59 (95%)	56 (100%)	0	100	100
5	i	56/59 (95%)	56 (100%)	0	100	100
6	F	105/121 (87%)	105 (100%)	0	100	100
6	R	105/121 (87%)	105 (100%)	0	100	100
6	j	105/121 (87%)	105 (100%)	0	100	100
7	I	30/30 (100%)	30 (100%)	0	100	100
7	S	30/30 (100%)	30 (100%)	0	100	100
7	k	30/30 (100%)	30 (100%)	0	100	100
8	J	35/35 (100%)	35 (100%)	0	100	100
8	T	35/35 (100%)	35 (100%)	0	100	100
8	l	35/35 (100%)	35 (100%)	0	100	100
9	K	56/61 (92%)	56 (100%)	0	100	100
9	U	56/61 (92%)	56 (100%)	0	100	100
9	m	56/61 (92%)	56 (100%)	0	100	100
10	L	127/128 (99%)	127 (100%)	0	100	100
10	V	127/128 (99%)	127 (100%)	0	100	100
10	n	127/128 (99%)	127 (100%)	0	100	100
11	M	24/24 (100%)	24 (100%)	0	100	100
11	W	24/24 (100%)	24 (100%)	0	100	100
11	o	24/24 (100%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	1	257/259 (99%)	257 (100%)	0	100	100
12	2	257/259 (99%)	257 (100%)	0	100	100
12	3	257/259 (99%)	257 (100%)	0	100	100
12	4	257/259 (99%)	257 (100%)	0	100	100
12	5	257/259 (99%)	257 (100%)	0	100	100
12	6	257/259 (99%)	256 (100%)	1 (0%)	89	97
12	Y	257/259 (99%)	257 (100%)	0	100	100
12	Z	257/259 (99%)	257 (100%)	0	100	100
12	a	257/259 (99%)	257 (100%)	0	100	100
12	b	257/259 (99%)	257 (100%)	0	100	100
12	c	257/259 (99%)	257 (100%)	0	100	100
12	d	257/259 (99%)	256 (100%)	1 (0%)	89	97
12	q	257/259 (99%)	257 (100%)	0	100	100
12	r	257/259 (99%)	257 (100%)	0	100	100
12	s	257/259 (99%)	257 (100%)	0	100	100
12	t	257/259 (99%)	257 (100%)	0	100	100
12	u	257/259 (99%)	257 (100%)	0	100	100
12	v	257/259 (99%)	256 (100%)	1 (0%)	89	97
All	All	10017/10167 (98%)	10005 (100%)	12 (0%)	92	98

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	d	259	PHE
1	e	383	TYR
12	v	259	PHE
2	f	162	ARG
12	6	259	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	e	179	HIS
2	f	603	GLN
1	e	192	ASN

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Mol	Chain	Res	Type
2	f	34	HIS
10	n	3	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

846 ligands are modelled in this entry.

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	BCR	2	524	-	41,41,41	0.73	0	56,56,56	1.67	12 (21%)
13	CLA	6	516	12	45,53,73	1.79	6 (13%)	52,89,113	1.60	8 (15%)
13	CLA	q	519	12	50,58,73	1.66	10 (20%)	58,95,113	1.50	8 (13%)
14	PQN	f	2002	-	34,34,34	2.87	11 (32%)	42,45,45	2.18	4 (9%)
13	CLA	4	503	12	55,63,73	1.63	6 (10%)	64,101,113	1.54	11 (17%)
13	CLA	u	508	12	45,53,73	1.78	7 (15%)	52,89,113	1.73	6 (11%)
13	CLA	6	508	12	45,53,73	1.77	7 (15%)	52,89,113	1.67	7 (13%)
17	LHG	H	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.21	5 (10%)
18	LMU	1	902	-	19,19,36	1.22	1 (5%)	24,24,47	1.10	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	t	519	12	55,63,73	1.59	9 (16%)	64,101,113	1.50	6 (9%)
13	CLA	G	1022	21	65,73,73	1.48	9 (13%)	76,113,113	1.48	9 (11%)
13	CLA	Y	507	-	60,68,73	1.52	6 (10%)	70,107,113	1.53	9 (12%)
13	CLA	Z	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.48	7 (9%)
16	BCR	d	521	-	41,41,41	0.66	0	56,56,56	1.91	12 (21%)
16	BCR	H	4005	-	41,41,41	0.70	0	56,56,56	1.78	11 (19%)
13	CLA	H	1220	2	55,63,73	1.55	9 (16%)	64,101,113	1.67	11 (17%)
13	CLA	T	1303	8	65,73,73	1.44	7 (10%)	76,113,113	1.51	11 (14%)
17	LHG	e	5003	13	40,40,48	0.74	1 (2%)	43,46,54	1.33	6 (13%)
13	CLA	v	519	12	46,54,73	1.76	6 (13%)	53,90,113	1.59	6 (11%)
16	BCR	L	4219	-	41,41,41	0.78	0	56,56,56	1.80	12 (21%)
13	CLA	f	1236	2	55,63,73	1.63	7 (12%)	64,101,113	1.43	8 (12%)
13	CLA	r	508	12	55,63,73	1.63	8 (14%)	64,101,113	1.59	9 (14%)
13	CLA	U	1401	-	55,63,73	1.59	7 (12%)	64,101,113	1.55	9 (14%)
16	BCR	A	4003	-	41,41,41	0.78	0	56,56,56	1.73	11 (19%)
20	SQD	6	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.91	10 (29%)
13	CLA	6	509	12	45,53,73	1.77	6 (13%)	52,89,113	1.63	6 (11%)
13	CLA	Z	517	-	45,53,73	1.77	7 (15%)	52,89,113	1.62	6 (11%)
13	CLA	A	1101	1	65,73,73	1.49	8 (12%)	76,113,113	1.45	9 (11%)
13	CLA	H	1201	2	60,68,73	1.48	7 (11%)	70,107,113	1.66	8 (11%)
16	BCR	2	522	-	41,41,41	0.71	0	56,56,56	1.75	18 (32%)
16	BCR	M	4021	-	41,41,41	0.71	0	56,56,56	1.82	14 (25%)
13	CLA	f	1228	2	55,63,73	1.53	7 (12%)	64,101,113	1.67	8 (12%)
13	CLA	Z	513	12	65,73,73	1.50	8 (12%)	76,113,113	1.38	7 (9%)
13	CLA	B	1217	2	57,65,73	1.52	7 (12%)	66,103,113	1.54	8 (12%)
13	CLA	u	518	12	55,63,73	1.60	6 (10%)	64,101,113	1.45	7 (10%)
13	CLA	4	504	-	45,53,73	1.77	6 (13%)	52,89,113	1.63	7 (13%)
13	CLA	G	1101	1	65,73,73	1.49	8 (12%)	76,113,113	1.45	9 (11%)
13	CLA	c	503	12	55,63,73	1.64	6 (10%)	64,101,113	1.53	8 (12%)
16	BCR	f	4017	-	41,41,41	0.80	0	56,56,56	1.57	11 (19%)
19	LMG	H	5002	-	54,54,55	0.79	2 (3%)	62,62,63	1.43	10 (16%)
13	CLA	A	1107	1	65,73,73	1.47	10 (15%)	76,113,113	1.43	9 (11%)
13	CLA	r	510	12	65,73,73	1.46	7 (10%)	76,113,113	1.43	6 (7%)
16	BCR	Z	522	-	41,41,41	0.71	0	56,56,56	1.75	18 (32%)
13	CLA	A	1011	1	65,73,73	1.45	6 (9%)	76,113,113	1.63	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	LHG	A	5004	-	35,35,48	0.74	1 (2%)	38,41,54	1.25	4 (10%)
13	CLA	m	1401	-	55,63,73	1.59	8 (14%)	64,101,113	1.56	9 (14%)
13	CLA	5	502	12	50,58,73	1.71	8 (16%)	58,95,113	1.54	7 (12%)
13	CLA	B	1219	2	65,73,73	1.48	7 (10%)	76,113,113	1.33	9 (11%)
13	CLA	r	504	-	50,58,73	1.68	7 (14%)	58,95,113	1.58	8 (13%)
13	CLA	Y	510	12	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
13	CLA	f	1202	2	65,73,73	1.44	7 (10%)	76,113,113	1.65	10 (13%)
13	CLA	G	1801	17	45,53,73	1.72	7 (15%)	52,89,113	1.83	8 (15%)
13	CLA	s	501	12	65,73,73	1.45	7 (10%)	76,113,113	1.52	7 (9%)
13	CLA	5	512	12	45,53,73	1.76	7 (15%)	52,89,113	1.58	7 (13%)
13	CLA	H	1214	2	65,73,73	1.49	9 (13%)	76,113,113	1.51	7 (9%)
13	CLA	A	1116	1	60,68,73	1.51	7 (11%)	70,107,113	1.50	7 (10%)
16	BCR	V	4020	-	41,41,41	0.83	0	56,56,56	1.95	16 (28%)
13	CLA	2	501	12	65,73,73	1.48	7 (10%)	76,113,113	1.47	7 (9%)
13	CLA	A	1130	1	65,73,73	1.47	7 (10%)	76,113,113	1.52	10 (13%)
13	CLA	5	508	12	45,53,73	1.78	7 (15%)	52,89,113	1.73	6 (11%)
20	SQD	a	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.59	12 (23%)
16	BCR	I	4018	-	41,41,41	0.77	0	56,56,56	1.84	15 (26%)
19	LMG	J	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.25	7 (16%)
13	CLA	H	1224	2	60,68,73	1.47	7 (11%)	70,107,113	1.58	8 (11%)
13	CLA	Y	511	12	55,63,73	1.61	6 (10%)	64,101,113	1.58	8 (12%)
13	CLA	A	1110	1	51,59,73	1.66	7 (13%)	59,96,113	1.60	7 (11%)
13	CLA	u	519	12	46,54,73	1.75	9 (19%)	53,90,113	1.55	6 (11%)
16	BCR	H	4009	-	41,41,41	0.81	0	56,56,56	1.91	21 (37%)
13	CLA	6	504	-	45,53,73	1.78	5 (11%)	52,89,113	1.68	8 (15%)
13	CLA	A	1131	1	65,73,73	1.45	9 (13%)	76,113,113	1.43	9 (11%)
13	CLA	c	504	-	45,53,73	1.77	5 (11%)	52,89,113	1.63	7 (13%)
13	CLA	r	507	-	65,73,73	1.44	7 (10%)	76,113,113	1.48	7 (9%)
13	CLA	B	1215	2	65,73,73	1.44	8 (12%)	76,113,113	1.57	8 (10%)
13	CLA	H	1232	21	50,58,73	1.62	7 (14%)	58,95,113	1.82	6 (10%)
13	CLA	A	1109	1	65,73,73	1.41	7 (10%)	76,113,113	1.52	7 (9%)
16	BCR	l	4013	-	41,41,41	0.76	0	56,56,56	1.96	15 (26%)
13	CLA	2	517	-	45,53,73	1.77	7 (15%)	52,89,113	1.63	6 (11%)
18	LMU	G	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.00	2 (7%)
13	CLA	G	1110	1	51,59,73	1.65	7 (13%)	59,96,113	1.60	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	1133	1	65,73,73	1.39	8 (12%)	76,113,113	1.49	6 (7%)
13	CLA	A	1125	1	65,73,73	1.43	8 (12%)	76,113,113	1.55	9 (11%)
13	CLA	d	501	12	60,68,73	1.53	6 (10%)	70,107,113	1.51	7 (10%)
13	CLA	u	502	12	50,58,73	1.71	8 (16%)	58,95,113	1.55	7 (12%)
13	CLA	2	518	12	65,73,73	1.46	6 (9%)	76,113,113	1.48	7 (9%)
13	CLA	G	1109	1	65,73,73	1.41	7 (10%)	76,113,113	1.52	7 (9%)
13	CLA	f	1234	2	65,73,73	1.42	8 (12%)	76,113,113	1.69	13 (17%)
16	BCR	G	4001	-	41,41,41	0.76	0	56,56,56	1.72	11 (19%)
13	CLA	q	508	12	55,63,73	1.60	7 (12%)	64,101,113	1.70	9 (14%)
13	CLA	H	1215	2	65,73,73	1.44	8 (12%)	76,113,113	1.57	8 (10%)
13	CLA	G	1133	1	65,73,73	1.39	7 (10%)	76,113,113	1.49	6 (7%)
16	BCR	U	4104	-	41,41,41	0.74	0	56,56,56	1.86	15 (26%)
13	CLA	B	1211	2	56,64,73	1.53	7 (12%)	65,102,113	1.78	6 (9%)
13	CLA	c	507	-	45,53,73	1.74	6 (13%)	52,89,113	1.69	8 (15%)
13	CLA	A	1124	21	56,64,73	1.58	6 (10%)	65,102,113	1.63	12 (18%)
13	CLA	s	507	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	8 (10%)
16	BCR	b	524	-	41,41,41	0.67	0	56,56,56	1.85	15 (26%)
13	CLA	B	1231	21	65,73,73	1.37	7 (10%)	76,113,113	1.56	8 (10%)
13	CLA	d	517	-	45,53,73	1.78	7 (15%)	52,89,113	1.58	6 (11%)
16	BCR	4	522	-	41,41,41	0.74	0	56,56,56	1.85	18 (32%)
13	CLA	2	507	-	65,73,73	1.44	6 (9%)	76,113,113	1.48	7 (9%)
13	CLA	d	513	12	45,53,73	1.84	6 (13%)	52,89,113	1.54	6 (11%)
13	CLA	b	508	12	45,53,73	1.82	8 (17%)	52,89,113	1.75	10 (19%)
13	CLA	A	1117	1	65,73,73	1.43	10 (15%)	76,113,113	1.69	12 (15%)
13	CLA	2	506	12	55,63,73	1.61	7 (12%)	64,101,113	1.55	6 (9%)
13	CLA	u	506	12	45,53,73	1.78	6 (13%)	52,89,113	1.66	7 (13%)
13	CLA	v	506	12	45,53,73	1.79	7 (15%)	52,89,113	1.65	6 (11%)
16	BCR	Y	523	-	41,41,41	0.71	0	56,56,56	1.64	16 (28%)
16	BCR	Y	524	-	41,41,41	0.73	0	56,56,56	1.82	15 (26%)
16	BCR	n	4020	-	41,41,41	0.82	0	56,56,56	1.95	15 (26%)
13	CLA	e	1130	1	65,73,73	1.47	7 (10%)	76,113,113	1.52	10 (13%)
17	LHG	e	5005	-	44,44,48	0.67	1 (2%)	47,50,54	1.27	6 (12%)
13	CLA	A	1118	1	60,68,73	1.49	8 (13%)	70,107,113	1.49	8 (11%)
17	LHG	V	5218	-	37,37,48	0.75	2 (5%)	40,43,54	1.23	4 (10%)
13	CLA	e	1110	1	51,59,73	1.66	7 (13%)	59,96,113	1.61	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	Y	508	12	55,63,73	1.60	7 (12%)	64,101,113	1.71	10 (15%)
13	CLA	Z	518	12	65,73,73	1.46	6 (9%)	76,113,113	1.48	7 (9%)
13	CLA	b	516	12	45,53,73	1.77	6 (13%)	52,89,113	1.58	7 (13%)
13	CLA	t	512	12	45,53,73	1.79	6 (13%)	52,89,113	1.62	6 (11%)
13	CLA	d	507	-	45,53,73	1.77	6 (13%)	52,89,113	1.66	8 (15%)
13	CLA	q	507	-	60,68,73	1.53	6 (10%)	70,107,113	1.54	9 (12%)
13	CLA	B	1201	2	60,68,73	1.48	7 (11%)	70,107,113	1.65	8 (11%)
13	CLA	s	517	-	45,53,73	1.77	7 (15%)	52,89,113	1.58	6 (11%)
13	CLA	f	1239	2	65,73,73	1.49	7 (10%)	76,113,113	1.62	14 (18%)
16	BCR	5	521	-	41,41,41	0.68	0	56,56,56	1.94	16 (28%)
13	CLA	H	1212	2	55,63,73	1.54	8 (14%)	64,101,113	1.64	8 (12%)
13	CLA	c	502	12	50,58,73	1.71	8 (16%)	58,95,113	1.54	7 (12%)
16	BCR	s	521	-	41,41,41	0.66	0	56,56,56	1.76	10 (17%)
16	BCR	r	524	-	41,41,41	0.73	0	56,56,56	1.67	12 (21%)
13	CLA	A	1138	1	65,73,73	1.44	7 (10%)	76,113,113	1.46	8 (10%)
13	CLA	f	1218	2	60,68,73	1.47	7 (11%)	70,107,113	1.53	6 (8%)
13	CLA	3	501	12	65,73,73	1.44	7 (10%)	76,113,113	1.53	7 (9%)
13	CLA	5	509	12	65,73,73	1.46	7 (10%)	76,113,113	1.48	8 (10%)
16	BCR	6	523	-	41,41,41	0.70	0	56,56,56	1.73	14 (25%)
20	SQD	2	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.61	10 (19%)
13	CLA	t	507	-	45,53,73	1.77	6 (13%)	52,89,113	1.69	8 (15%)
13	CLA	2	510	12	65,73,73	1.46	6 (9%)	76,113,113	1.44	6 (7%)
17	LHG	e	5007	-	46,46,48	0.66	1 (2%)	49,52,54	1.24	5 (10%)
13	CLA	f	1211	2	56,64,73	1.53	7 (12%)	65,102,113	1.77	6 (9%)
13	CLA	G	1138	1	65,73,73	1.44	7 (10%)	76,113,113	1.45	8 (10%)
13	CLA	r	503	12	65,73,73	1.48	7 (10%)	76,113,113	1.45	7 (9%)
16	BCR	f	4010	-	41,41,41	0.94	3 (7%)	56,56,56	2.28	23 (41%)
16	BCR	t	524	-	41,41,41	0.68	0	56,56,56	1.84	15 (26%)
13	CLA	b	502	12	50,58,73	1.69	6 (12%)	58,95,113	1.59	7 (12%)
17	LHG	A	5006	-	44,44,48	0.62	0	47,50,54	1.26	5 (10%)
13	CLA	3	517	-	45,53,73	1.78	7 (15%)	52,89,113	1.58	6 (11%)
13	CLA	r	516	12	45,53,73	1.77	6 (13%)	52,89,113	1.66	7 (13%)
16	BCR	G	4002	-	41,41,41	0.81	1 (2%)	56,56,56	1.85	14 (25%)
16	BCR	a	521	-	41,41,41	0.68	0	56,56,56	1.75	10 (17%)
16	BCR	A	4008	-	41,41,41	0.84	1 (2%)	56,56,56	2.03	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	K	1401	-	55,63,73	1.59	8 (14%)	64,101,113	1.55	9 (14%)
13	CLA	4	513	12	45,53,73	1.80	7 (15%)	52,89,113	1.62	6 (11%)
13	CLA	Y	502	12	60,68,73	1.55	7 (11%)	70,107,113	1.47	7 (10%)
13	CLA	e	1801	17	45,53,73	1.72	7 (15%)	52,89,113	1.83	8 (15%)
13	CLA	d	509	12	45,53,73	1.77	6 (13%)	52,89,113	1.62	6 (11%)
13	CLA	G	1125	1	65,73,73	1.43	7 (10%)	76,113,113	1.55	9 (11%)
13	CLA	5	519	12	46,54,73	1.76	9 (19%)	53,90,113	1.55	6 (11%)
13	CLA	v	510	12	45,53,73	1.80	6 (13%)	52,89,113	1.58	7 (13%)
20	SQD	Z	822	-	42,43,54	1.07	5 (11%)	51,54,65	1.61	10 (19%)
13	CLA	H	1217	2	57,65,73	1.52	7 (12%)	66,103,113	1.54	9 (13%)
13	CLA	e	1112	1	50,58,73	1.63	9 (18%)	58,95,113	1.72	8 (13%)
13	CLA	3	507	-	65,73,73	1.46	6 (9%)	76,113,113	1.44	8 (10%)
14	PQN	B	2002	-	34,34,34	2.88	11 (32%)	42,45,45	2.18	4 (9%)
13	CLA	1	507	-	60,68,73	1.52	6 (10%)	70,107,113	1.53	9 (12%)
13	CLA	a	501	12	65,73,73	1.44	7 (10%)	76,113,113	1.53	7 (9%)
16	BCR	4	524	-	41,41,41	0.67	0	56,56,56	1.84	15 (26%)
13	CLA	1	501	12	65,73,73	1.49	7 (10%)	76,113,113	1.44	8 (10%)
13	CLA	G	1122	1	60,68,73	1.50	9 (15%)	70,107,113	1.53	8 (11%)
13	CLA	B	1239	2	65,73,73	1.49	7 (10%)	76,113,113	1.63	14 (18%)
13	CLA	s	510	12	65,73,73	1.47	6 (9%)	76,113,113	1.46	9 (11%)
16	BCR	e	4002	-	41,41,41	0.81	0	56,56,56	1.85	14 (25%)
13	CLA	G	1108	1	54,62,73	1.61	7 (12%)	62,99,113	1.48	6 (9%)
13	CLA	4	508	12	45,53,73	1.82	8 (17%)	52,89,113	1.75	10 (19%)
18	LMU	A	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.07	2 (4%)
13	CLA	K	1103	9	50,58,73	1.64	9 (18%)	58,95,113	1.68	12 (20%)
13	CLA	H	1231	21	65,73,73	1.37	7 (10%)	76,113,113	1.56	8 (10%)
13	CLA	a	517	-	45,53,73	1.77	7 (15%)	52,89,113	1.58	6 (11%)
13	CLA	5	506	12	45,53,73	1.78	6 (13%)	52,89,113	1.66	7 (13%)
13	CLA	s	506	12	50,58,73	1.69	7 (14%)	58,95,113	1.67	6 (10%)
13	CLA	b	505	12	65,73,73	1.47	6 (9%)	76,113,113	1.37	6 (7%)
13	CLA	J	1303	8	65,73,73	1.44	7 (10%)	76,113,113	1.51	12 (15%)
13	CLA	4	516	12	45,53,73	1.78	6 (13%)	52,89,113	1.58	7 (13%)
13	CLA	n	1502	10	65,73,73	1.43	7 (10%)	76,113,113	1.48	8 (10%)
18	LMU	G	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.07	2 (4%)
13	CLA	f	1232	21	50,58,73	1.62	7 (14%)	58,95,113	1.82	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	f	4006	-	41,41,41	0.72	0	56,56,56	1.98	20 (35%)
13	CLA	3	502	12	50,58,73	1.69	7 (14%)	58,95,113	1.62	8 (13%)
13	CLA	d	511	12	45,53,73	1.79	6 (13%)	52,89,113	1.66	6 (11%)
16	BCR	s	524	-	41,41,41	0.73	0	56,56,56	1.82	17 (30%)
13	CLA	4	505	12	65,73,73	1.47	6 (9%)	76,113,113	1.37	7 (9%)
13	CLA	e	1103	1	65,73,73	1.43	7 (10%)	76,113,113	1.64	8 (10%)
16	BCR	1	521	-	41,41,41	0.66	0	56,56,56	1.81	11 (19%)
16	BCR	3	524	-	41,41,41	0.74	0	56,56,56	1.81	17 (30%)
15	SF4	g	3002	3	0,12,12	-	-	-	-	-
13	CLA	Y	519	12	50,58,73	1.65	10 (20%)	58,95,113	1.50	8 (13%)
13	CLA	s	508	12	55,63,73	1.63	7 (12%)	64,101,113	1.59	8 (12%)
13	CLA	1	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.50	7 (9%)
13	CLA	a	507	-	65,73,73	1.46	6 (9%)	76,113,113	1.44	8 (10%)
13	CLA	G	1237	21	65,73,73	1.48	9 (13%)	76,113,113	1.50	11 (14%)
13	CLA	d	506	12	45,53,73	1.79	6 (13%)	52,89,113	1.65	6 (11%)
13	CLA	q	506	12	45,53,73	1.77	7 (15%)	52,89,113	1.69	6 (11%)
16	BCR	B	4010	-	41,41,41	0.94	3 (7%)	56,56,56	2.28	23 (41%)
13	CLA	Z	510	12	65,73,73	1.46	7 (10%)	76,113,113	1.44	6 (7%)
13	CLA	Y	518	12	60,68,73	1.52	9 (15%)	70,107,113	1.52	8 (11%)
13	CLA	A	1111	1	65,73,73	1.46	7 (10%)	76,113,113	1.49	7 (9%)
13	CLA	H	1240	17	65,73,73	1.47	6 (9%)	76,113,113	1.44	9 (11%)
13	CLA	b	512	12	45,53,73	1.78	6 (13%)	52,89,113	1.62	6 (11%)
13	CLA	s	516	12	45,53,73	1.78	6 (13%)	52,89,113	1.85	12 (23%)
13	CLA	4	502	12	50,58,73	1.69	6 (12%)	58,95,113	1.60	7 (12%)
20	SQD	4	822	-	25,26,54	1.31	4 (16%)	34,37,65	1.84	9 (26%)
20	SQD	v	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.91	10 (29%)
13	CLA	G	1106	1	65,73,73	1.41	9 (13%)	76,113,113	1.55	9 (11%)
13	CLA	2	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.48	7 (9%)
13	CLA	G	1121	1	55,63,73	1.58	8 (14%)	64,101,113	1.59	11 (17%)
13	CLA	2	516	12	45,53,73	1.77	6 (13%)	52,89,113	1.64	7 (13%)
13	CLA	3	516	12	45,53,73	1.77	6 (13%)	52,89,113	1.85	12 (23%)
13	CLA	q	509	12	65,73,73	1.46	7 (10%)	76,113,113	1.50	7 (9%)
13	CLA	r	505	12	65,73,73	1.44	6 (9%)	76,113,113	1.40	8 (10%)
13	CLA	a	511	12	50,58,73	1.70	6 (12%)	58,95,113	1.61	6 (10%)
14	PQN	e	2001	-	34,34,34	2.88	11 (32%)	42,45,45	2.11	7 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	G	4008	-	41,41,41	0.84	1 (2%)	56,56,56	2.03	16 (28%)
13	CLA	t	516	12	45,53,73	1.78	6 (13%)	52,89,113	1.59	7 (13%)
17	LHG	G	5008	-	34,34,48	0.76	1 (2%)	37,40,54	1.28	4 (10%)
13	CLA	s	511	12	50,58,73	1.71	6 (12%)	58,95,113	1.62	6 (10%)
13	CLA	u	511	12	55,63,73	1.62	6 (10%)	64,101,113	1.53	7 (10%)
13	CLA	2	511	12	55,63,73	1.62	6 (10%)	64,101,113	1.57	7 (10%)
16	BCR	l	4012	-	41,41,41	0.70	0	56,56,56	1.66	13 (23%)
13	CLA	t	505	12	65,73,73	1.46	6 (9%)	76,113,113	1.36	6 (7%)
13	CLA	e	1138	1	65,73,73	1.44	7 (10%)	76,113,113	1.46	8 (10%)
13	CLA	e	1139	21	65,73,73	1.46	7 (10%)	76,113,113	1.34	9 (11%)
16	BCR	Z	524	-	41,41,41	0.74	0	56,56,56	1.67	12 (21%)
13	CLA	A	1115	1	60,68,73	1.47	7 (11%)	70,107,113	1.59	8 (11%)
13	CLA	e	1136	1	60,68,73	1.53	8 (13%)	70,107,113	1.56	11 (15%)
13	CLA	Y	506	12	45,53,73	1.77	6 (13%)	52,89,113	1.68	6 (11%)
13	CLA	3	519	12	55,63,73	1.61	9 (16%)	64,101,113	1.50	7 (10%)
13	CLA	B	1232	21	50,58,73	1.62	7 (14%)	58,95,113	1.82	6 (10%)
13	CLA	b	519	12	55,63,73	1.58	9 (16%)	64,101,113	1.49	6 (9%)
13	CLA	2	513	12	65,73,73	1.50	8 (12%)	76,113,113	1.38	6 (7%)
13	CLA	Z	508	12	55,63,73	1.63	8 (14%)	64,101,113	1.58	9 (14%)
13	CLA	e	1237	21	65,73,73	1.49	9 (13%)	76,113,113	1.50	11 (14%)
13	CLA	s	502	12	50,58,73	1.68	7 (14%)	58,95,113	1.62	8 (13%)
19	LMG	l	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.24	7 (16%)
16	BCR	n	4022	-	41,41,41	0.75	0	56,56,56	1.90	15 (26%)
13	CLA	j	1301	21	65,73,73	1.46	7 (10%)	76,113,113	1.38	8 (10%)
13	CLA	B	1223	2	65,73,73	1.41	7 (10%)	76,113,113	1.56	6 (7%)
13	CLA	e	1022	21	65,73,73	1.48	9 (13%)	76,113,113	1.48	9 (11%)
13	CLA	G	1116	1	60,68,73	1.51	8 (13%)	70,107,113	1.50	7 (10%)
13	CLA	Z	516	12	45,53,73	1.77	7 (15%)	52,89,113	1.64	7 (13%)
15	SF4	G	3001	2,1	0,12,12	-	-	-	-	-
16	BCR	L	4020	-	41,41,41	0.83	0	56,56,56	1.95	16 (28%)
13	CLA	e	1121	1	55,63,73	1.59	7 (12%)	64,101,113	1.58	11 (17%)
13	CLA	G	1130	1	65,73,73	1.47	7 (10%)	76,113,113	1.52	10 (13%)
16	BCR	b	523	-	41,41,41	0.70	0	56,56,56	1.65	12 (21%)
16	BCR	e	4008	-	41,41,41	0.84	1 (2%)	56,56,56	2.02	17 (30%)
17	LHG	L	5221	-	48,48,48	0.65	2 (4%)	51,54,54	1.30	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	e	1111	1	65,73,73	1.46	7 (10%)	76,113,113	1.48	7 (9%)
13	CLA	f	1238	21	65,73,73	1.41	7 (10%)	76,113,113	1.57	10 (13%)
13	CLA	Z	511	12	55,63,73	1.62	6 (10%)	64,101,113	1.57	7 (10%)
16	BCR	a	524	-	41,41,41	0.74	0	56,56,56	1.81	17 (30%)
13	CLA	e	1117	1	65,73,73	1.43	10 (15%)	76,113,113	1.69	12 (15%)
13	CLA	e	1120	1	53,61,73	1.56	7 (13%)	61,98,113	1.68	7 (11%)
13	CLA	A	1123	21	65,73,73	1.40	7 (10%)	76,113,113	1.51	8 (10%)
13	CLA	B	1238	21	65,73,73	1.41	7 (10%)	76,113,113	1.57	10 (13%)
13	CLA	v	505	12	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
16	BCR	B	4014	-	41,41,41	0.74	0	56,56,56	1.85	13 (23%)
13	CLA	e	1135	1	52,60,73	1.54	8 (15%)	60,97,113	1.71	10 (16%)
13	CLA	2	504	-	50,58,73	1.68	7 (14%)	58,95,113	1.59	8 (13%)
13	CLA	b	506	12	45,53,73	1.79	6 (13%)	52,89,113	1.63	6 (11%)
20	SQD	H	1852	-	44,45,54	1.02	4 (9%)	53,56,65	1.84	14 (26%)
13	CLA	q	503	12	64,72,73	1.50	6 (9%)	74,111,113	1.46	8 (10%)
13	CLA	r	513	12	65,73,73	1.50	8 (12%)	76,113,113	1.38	6 (7%)
13	CLA	t	501	12	60,68,73	1.55	5 (8%)	70,107,113	1.44	6 (8%)
17	LHG	A	5007	-	46,46,48	0.67	1 (2%)	49,52,54	1.24	5 (10%)
13	CLA	e	1115	1	60,68,73	1.46	7 (11%)	70,107,113	1.59	8 (11%)
17	LHG	n	5218	-	37,37,48	0.75	2 (5%)	40,43,54	1.23	4 (10%)
13	CLA	H	1210	2	65,73,73	1.42	8 (12%)	76,113,113	1.53	12 (15%)
13	CLA	t	511	12	45,53,73	1.80	6 (13%)	52,89,113	1.70	7 (13%)
16	BCR	m	4104	-	41,41,41	0.74	0	56,56,56	1.86	15 (26%)
13	CLA	B	1225	2	65,73,73	1.42	9 (13%)	76,113,113	1.45	7 (9%)
13	CLA	L	1501	10	65,73,73	1.47	7 (10%)	76,113,113	1.52	9 (11%)
13	CLA	q	511	12	55,63,73	1.60	6 (10%)	64,101,113	1.57	8 (12%)
16	BCR	J	4012	-	41,41,41	0.70	0	56,56,56	1.66	13 (23%)
13	CLA	d	510	12	45,53,73	1.80	5 (11%)	52,89,113	1.57	7 (13%)
13	CLA	r	519	12	55,63,73	1.61	8 (14%)	64,101,113	1.46	9 (14%)
16	BCR	t	522	-	41,41,41	0.73	0	56,56,56	1.85	18 (32%)
13	CLA	5	505	12	61,69,73	1.51	6 (9%)	71,108,113	1.39	6 (8%)
13	CLA	H	1211	2	56,64,73	1.53	7 (12%)	65,102,113	1.79	6 (9%)
13	CLA	s	505	12	65,73,73	1.46	6 (9%)	76,113,113	1.37	6 (7%)
13	CLA	e	1124	21	56,64,73	1.58	6 (10%)	65,102,113	1.62	12 (18%)
13	CLA	t	518	12	55,63,73	1.62	7 (12%)	64,101,113	1.49	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	A	4011	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
13	CLA	r	517	-	45,53,73	1.77	7 (15%)	52,89,113	1.64	6 (11%)
13	CLA	G	1113	1	45,53,73	1.68	7 (15%)	52,89,113	1.76	6 (11%)
13	CLA	3	505	12	65,73,73	1.46	6 (9%)	76,113,113	1.36	6 (7%)
13	CLA	G	1120	1	53,61,73	1.56	7 (13%)	61,98,113	1.68	7 (11%)
13	CLA	Z	502	12	60,68,73	1.56	8 (13%)	70,107,113	1.44	7 (10%)
16	BCR	t	523	-	41,41,41	0.69	0	56,56,56	1.65	13 (23%)
13	CLA	Z	504	-	50,58,73	1.68	6 (12%)	58,95,113	1.58	8 (13%)
16	BCR	W	4021	-	41,41,41	0.71	0	56,56,56	1.82	14 (25%)
16	BCR	r	521	-	41,41,41	0.66	0	56,56,56	1.86	11 (19%)
16	BCR	r	523	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
13	CLA	a	502	12	50,58,73	1.68	7 (14%)	58,95,113	1.62	8 (13%)
13	CLA	s	518	12	55,63,73	1.61	7 (12%)	64,101,113	1.48	7 (10%)
13	CLA	e	1101	1	65,73,73	1.49	8 (12%)	76,113,113	1.45	9 (11%)
13	CLA	6	502	12	50,58,73	1.68	6 (12%)	58,95,113	1.60	7 (12%)
16	BCR	k	4018	-	41,41,41	0.77	0	56,56,56	1.84	15 (26%)
17	LHG	A	5009	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
14	PQN	H	2002	-	34,34,34	2.87	11 (32%)	42,45,45	2.17	4 (9%)
13	CLA	t	506	12	45,53,73	1.80	6 (13%)	52,89,113	1.65	7 (13%)
16	BCR	H	4004	-	41,41,41	0.72	0	56,56,56	1.85	13 (23%)
13	CLA	a	508	12	55,63,73	1.65	7 (12%)	64,101,113	1.60	8 (12%)
17	LHG	G	5009	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
13	CLA	v	501	12	60,68,73	1.53	7 (11%)	70,107,113	1.51	7 (10%)
16	BCR	n	4219	-	41,41,41	0.78	0	56,56,56	1.81	12 (21%)
13	CLA	f	1214	2	65,73,73	1.49	9 (13%)	76,113,113	1.51	7 (9%)
20	SQD	u	822	-	28,29,54	1.26	5 (17%)	37,40,65	1.92	13 (35%)
13	CLA	Y	513	12	55,63,73	1.62	7 (12%)	64,101,113	1.49	6 (9%)
13	CLA	t	503	12	55,63,73	1.63	6 (10%)	64,101,113	1.54	12 (18%)
13	CLA	A	1140	1	65,73,73	1.49	8 (12%)	76,113,113	1.47	12 (15%)
13	CLA	6	503	12	52,60,73	1.67	6 (11%)	60,97,113	1.58	9 (15%)
16	BCR	c	523	-	41,41,41	0.74	0	56,56,56	1.78	16 (28%)
15	SF4	C	3003	3	0,12,12	-	-	-	-	-
13	CLA	B	1213	2	65,73,73	1.40	7 (10%)	76,113,113	1.54	10 (13%)
13	CLA	H	1205	2	65,73,73	1.46	9 (13%)	76,113,113	1.54	9 (11%)
13	CLA	V	1501	10	65,73,73	1.46	7 (10%)	76,113,113	1.52	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	V	4019	-	41,41,41	0.74	0	56,56,56	1.92	14 (25%)
17	LHG	G	5004	-	35,35,48	0.74	1 (2%)	38,41,54	1.25	4 (10%)
13	CLA	q	513	12	55,63,73	1.61	7 (12%)	64,101,113	1.50	6 (9%)
16	BCR	4	523	-	41,41,41	0.69	0	56,56,56	1.65	12 (21%)
13	CLA	1	519	12	50,58,73	1.66	10 (20%)	58,95,113	1.50	8 (13%)
13	CLA	d	502	12	50,58,73	1.68	6 (12%)	58,95,113	1.60	7 (12%)
16	BCR	T	4013	-	41,41,41	0.76	0	56,56,56	1.96	15 (26%)
13	CLA	5	504	-	45,53,73	1.77	5 (11%)	52,89,113	1.64	7 (13%)
13	CLA	s	504	-	45,53,73	1.75	6 (13%)	52,89,113	1.69	6 (11%)
13	CLA	B	1214	2	65,73,73	1.49	9 (13%)	76,113,113	1.50	7 (9%)
17	LHG	e	5009	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
13	CLA	B	1203	2	65,73,73	1.44	9 (13%)	76,113,113	1.46	7 (9%)
16	BCR	d	524	-	41,41,41	0.75	0	56,56,56	1.87	13 (23%)
13	CLA	A	1104	1	65,73,73	1.40	7 (10%)	76,113,113	1.53	10 (13%)
16	BCR	V	4022	-	41,41,41	0.76	0	56,56,56	1.90	14 (25%)
20	SQD	f	1852	-	44,45,54	1.01	4 (9%)	53,56,65	1.84	14 (26%)
13	CLA	6	505	12	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
13	CLA	U	1103	9	50,58,73	1.64	9 (18%)	58,95,113	1.69	11 (18%)
13	CLA	Y	512	12	52,60,73	1.65	6 (11%)	60,97,113	1.53	6 (10%)
13	CLA	v	507	-	45,53,73	1.77	6 (13%)	52,89,113	1.66	8 (15%)
13	CLA	2	519	12	55,63,73	1.61	9 (16%)	64,101,113	1.46	9 (14%)
13	CLA	d	508	12	45,53,73	1.77	7 (15%)	52,89,113	1.67	7 (13%)
16	BCR	o	4021	-	41,41,41	0.71	0	56,56,56	1.81	14 (25%)
13	CLA	l	1302	8	58,66,73	1.52	8 (13%)	67,104,113	1.53	8 (11%)
13	CLA	U	1105	9	45,53,73	1.79	8 (17%)	52,89,113	1.85	11 (21%)
13	CLA	e	1114	21	50,58,73	1.68	8 (16%)	58,95,113	1.64	7 (12%)
17	LHG	A	5001	-	48,48,48	0.78	1 (2%)	51,54,54	1.26	6 (11%)
13	CLA	d	516	12	45,53,73	1.79	6 (13%)	52,89,113	1.61	8 (15%)
13	CLA	Z	505	12	65,73,73	1.44	6 (9%)	76,113,113	1.41	8 (10%)
13	CLA	q	504	-	45,53,73	1.79	7 (15%)	52,89,113	1.61	8 (15%)
13	CLA	B	1240	17	65,73,73	1.47	6 (9%)	76,113,113	1.44	9 (11%)
13	CLA	c	501	12	65,73,73	1.46	7 (10%)	76,113,113	1.48	7 (9%)
16	BCR	2	523	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
13	CLA	G	1119	21	65,73,73	1.46	9 (13%)	76,113,113	1.51	9 (11%)
13	CLA	G	1137	1	65,73,73	1.44	7 (10%)	76,113,113	1.51	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	c	512	12	45,53,73	1.75	6 (13%)	52,89,113	1.59	7 (13%)
13	CLA	G	1123	21	65,73,73	1.40	7 (10%)	76,113,113	1.50	8 (10%)
13	CLA	v	517	-	45,53,73	1.79	6 (13%)	52,89,113	1.59	6 (11%)
13	CLA	e	1113	1	45,53,73	1.67	7 (15%)	52,89,113	1.77	6 (11%)
13	CLA	f	1205	2	65,73,73	1.45	9 (13%)	76,113,113	1.53	9 (11%)
16	BCR	t	521	-	41,41,41	0.65	0	56,56,56	1.78	11 (19%)
13	CLA	R	1302	6	45,53,73	1.76	7 (15%)	52,89,113	1.59	6 (11%)
13	CLA	c	517	-	45,53,73	1.81	6 (13%)	52,89,113	1.55	6 (11%)
13	CLA	L	1502	10	65,73,73	1.43	7 (10%)	76,113,113	1.49	8 (10%)
13	CLA	f	1219	2	65,73,73	1.47	7 (10%)	76,113,113	1.33	9 (11%)
13	CLA	B	1012	21	65,73,73	1.46	9 (13%)	76,113,113	1.54	8 (10%)
17	LHG	G	5005	-	44,44,48	0.67	1 (2%)	47,50,54	1.27	6 (12%)
16	BCR	c	521	-	41,41,41	0.69	0	56,56,56	1.94	16 (28%)
13	CLA	m	1105	9	45,53,73	1.79	9 (20%)	52,89,113	1.85	11 (21%)
13	CLA	t	517	-	45,53,73	1.77	7 (15%)	52,89,113	1.66	8 (15%)
13	CLA	v	504	-	45,53,73	1.76	5 (11%)	52,89,113	1.68	8 (15%)
16	BCR	G	4011	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
16	BCR	F	4016	-	41,41,41	0.74	0	56,56,56	1.78	13 (23%)
16	BCR	B	4004	-	41,41,41	0.72	0	56,56,56	1.85	13 (23%)
13	CLA	t	513	12	45,53,73	1.80	7 (15%)	52,89,113	1.62	6 (11%)
16	BCR	H	4010	-	41,41,41	0.94	3 (7%)	56,56,56	2.28	23 (41%)
13	CLA	f	1230	2	60,68,73	1.53	9 (15%)	70,107,113	1.53	10 (14%)
13	CLA	a	519	12	55,63,73	1.61	7 (12%)	64,101,113	1.50	7 (10%)
16	BCR	Z	523	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
16	BCR	H	4014	-	41,41,41	0.74	0	56,56,56	1.84	13 (23%)
13	CLA	a	516	12	45,53,73	1.77	6 (13%)	52,89,113	1.85	12 (23%)
13	CLA	e	1133	1	65,73,73	1.39	7 (10%)	76,113,113	1.48	6 (7%)
17	LHG	e	5002	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	5 (12%)
13	CLA	r	512	12	53,61,73	1.61	7 (13%)	61,98,113	1.47	5 (8%)
13	CLA	A	1105	1	55,63,73	1.52	7 (12%)	64,101,113	1.69	9 (14%)
13	CLA	u	503	12	55,63,73	1.63	6 (10%)	64,101,113	1.53	8 (12%)
13	CLA	A	1137	1	65,73,73	1.44	7 (10%)	76,113,113	1.50	8 (10%)
13	CLA	5	510	12	45,53,73	1.76	6 (13%)	52,89,113	1.60	7 (13%)
13	CLA	f	1206	2	65,73,73	1.44	10 (15%)	76,113,113	1.58	7 (9%)
13	CLA	a	513	12	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	J	1302	8	58,66,73	1.52	8 (13%)	67,104,113	1.51	8 (11%)
13	CLA	r	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.48	7 (9%)
16	BCR	r	522	-	41,41,41	0.70	0	56,56,56	1.75	17 (30%)
13	CLA	b	513	12	45,53,73	1.80	7 (15%)	52,89,113	1.62	6 (11%)
13	CLA	r	502	12	60,68,73	1.57	8 (13%)	70,107,113	1.44	8 (11%)
13	CLA	e	1134	1	56,64,73	1.57	8 (14%)	65,102,113	1.54	8 (12%)
13	CLA	r	518	12	65,73,73	1.46	7 (10%)	76,113,113	1.48	7 (9%)
13	CLA	B	1205	2	65,73,73	1.46	9 (13%)	76,113,113	1.53	9 (11%)
13	CLA	B	1236	2	55,63,73	1.63	7 (12%)	64,101,113	1.43	8 (12%)
16	BCR	f	4014	-	41,41,41	0.74	0	56,56,56	1.84	13 (23%)
13	CLA	H	1012	21	65,73,73	1.46	9 (13%)	76,113,113	1.54	8 (10%)
13	CLA	f	1021	2	65,73,73	1.42	8 (12%)	76,113,113	1.44	9 (11%)
13	CLA	A	1022	21	65,73,73	1.47	10 (15%)	76,113,113	1.49	9 (11%)
13	CLA	t	504	-	45,53,73	1.77	6 (13%)	52,89,113	1.63	7 (13%)
16	BCR	5	524	-	41,41,41	0.68	0	56,56,56	1.67	14 (25%)
16	BCR	e	4001	-	41,41,41	0.76	0	56,56,56	1.72	11 (19%)
16	BCR	1	522	-	41,41,41	0.73	0	56,56,56	1.91	19 (33%)
13	CLA	B	1210	2	65,73,73	1.42	8 (12%)	76,113,113	1.53	12 (15%)
13	CLA	q	512	12	52,60,73	1.64	6 (11%)	60,97,113	1.53	6 (10%)
13	CLA	e	1128	1	65,73,73	1.54	10 (15%)	76,113,113	1.61	7 (9%)
13	CLA	u	513	12	45,53,73	1.82	8 (17%)	52,89,113	1.56	7 (13%)
13	CLA	Z	519	12	55,63,73	1.61	9 (16%)	64,101,113	1.46	9 (14%)
13	CLA	a	506	12	50,58,73	1.70	7 (14%)	58,95,113	1.67	6 (10%)
13	CLA	6	519	12	46,54,73	1.76	6 (13%)	53,90,113	1.59	6 (11%)
17	LHG	G	5006	-	44,44,48	0.62	0	47,50,54	1.25	5 (10%)
13	CLA	q	510	12	65,73,73	1.47	5 (7%)	76,113,113	1.41	7 (9%)
13	CLA	H	1223	2	65,73,73	1.40	7 (10%)	76,113,113	1.55	6 (7%)
16	BCR	B	4005	-	41,41,41	0.70	0	56,56,56	1.78	11 (19%)
17	LHG	n	5220	-	40,40,48	0.65	0	43,46,54	1.23	4 (9%)
13	CLA	d	505	12	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
17	LHG	B	1842	13	38,38,48	0.66	0	41,44,54	1.23	4 (9%)
17	LHG	G	5002	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	5 (12%)
16	BCR	6	521	-	41,41,41	0.66	0	56,56,56	1.91	12 (21%)
17	LHG	I	5001	-	43,43,48	0.64	0	46,49,54	1.22	4 (8%)
13	CLA	s	512	12	45,53,73	1.74	7 (15%)	52,89,113	1.62	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	LMU	Y	902	-	19,19,36	1.22	1 (5%)	24,24,47	1.10	3 (12%)
17	LHG	A	5003	13	40,40,48	0.74	1 (2%)	43,46,54	1.34	6 (13%)
13	CLA	l	1303	8	65,73,73	1.43	7 (10%)	76,113,113	1.51	12 (15%)
13	CLA	5	516	12	45,53,73	1.78	6 (13%)	52,89,113	1.59	6 (11%)
13	CLA	b	504	-	45,53,73	1.76	6 (13%)	52,89,113	1.63	7 (13%)
13	CLA	1	508	12	55,63,73	1.60	7 (12%)	64,101,113	1.70	9 (14%)
13	CLA	f	1227	2	65,73,73	1.47	9 (13%)	76,113,113	1.47	9 (11%)
13	CLA	v	513	12	45,53,73	1.82	6 (13%)	52,89,113	1.54	6 (11%)
16	BCR	v	524	-	41,41,41	0.76	0	56,56,56	1.87	13 (23%)
13	CLA	A	1113	1	45,53,73	1.67	7 (15%)	52,89,113	1.77	6 (11%)
16	BCR	q	524	-	41,41,41	0.73	0	56,56,56	1.82	15 (26%)
13	CLA	d	518	12	55,63,73	1.61	6 (10%)	64,101,113	1.50	7 (10%)
13	CLA	A	1132	1	65,73,73	1.43	10 (15%)	76,113,113	1.48	10 (13%)
13	CLA	f	1222	21	60,68,73	1.50	7 (11%)	70,107,113	1.54	10 (14%)
18	LMU	f	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.11	3 (6%)
15	SF4	g	3003	3	0,12,12	-	-	-	-	-
13	CLA	u	512	12	45,53,73	1.77	7 (15%)	52,89,113	1.59	7 (13%)
13	CLA	u	504	-	45,53,73	1.78	6 (13%)	52,89,113	1.64	7 (13%)
13	CLA	v	508	12	45,53,73	1.77	7 (15%)	52,89,113	1.68	7 (13%)
13	CLA	u	510	12	45,53,73	1.77	6 (13%)	52,89,113	1.60	7 (13%)
13	CLA	G	1132	1	65,73,73	1.42	9 (13%)	76,113,113	1.47	10 (13%)
13	CLA	Y	505	12	65,73,73	1.45	6 (9%)	76,113,113	1.39	7 (9%)
13	CLA	Z	503	12	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
16	BCR	5	522	-	41,41,41	0.74	0	56,56,56	1.93	20 (35%)
16	BCR	d	523	-	41,41,41	0.70	0	56,56,56	1.73	14 (25%)
13	CLA	q	516	12	45,53,73	1.79	6 (13%)	52,89,113	1.79	10 (19%)
13	CLA	Z	506	12	55,63,73	1.61	7 (12%)	64,101,113	1.55	6 (9%)
20	SQD	r	822	-	42,43,54	1.07	5 (11%)	51,54,65	1.61	10 (19%)
13	CLA	Y	503	12	64,72,73	1.49	6 (9%)	74,111,113	1.45	8 (10%)
13	CLA	5	518	12	55,63,73	1.60	6 (10%)	64,101,113	1.45	7 (10%)
15	SF4	e	3001	2,1	0,12,12	-	-	-	-	-
13	CLA	G	1105	1	55,63,73	1.51	7 (12%)	64,101,113	1.70	9 (14%)
13	CLA	H	1219	2	65,73,73	1.48	7 (10%)	76,113,113	1.33	9 (11%)
13	CLA	f	1225	2	65,73,73	1.41	9 (13%)	76,113,113	1.45	7 (9%)
13	CLA	v	511	12	45,53,73	1.78	6 (13%)	52,89,113	1.67	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	c	516	12	45,53,73	1.79	6 (13%)	52,89,113	1.60	6 (11%)
18	LMU	A	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.00	1 (3%)
13	CLA	B	1206	2	65,73,73	1.44	10 (15%)	76,113,113	1.58	7 (9%)
13	CLA	s	503	12	65,73,73	1.50	6 (9%)	76,113,113	1.41	9 (11%)
13	CLA	e	1131	1	65,73,73	1.44	9 (13%)	76,113,113	1.43	9 (11%)
14	PQN	G	2001	-	34,34,34	2.87	11 (32%)	42,45,45	2.12	7 (16%)
13	CLA	H	1203	2	65,73,73	1.44	8 (12%)	76,113,113	1.46	7 (9%)
16	BCR	V	4219	-	41,41,41	0.77	0	56,56,56	1.80	12 (21%)
13	CLA	A	1136	1	60,68,73	1.52	8 (13%)	70,107,113	1.56	11 (15%)
13	CLA	e	1122	1	60,68,73	1.49	9 (15%)	70,107,113	1.53	8 (11%)
13	CLA	3	510	12	65,73,73	1.46	6 (9%)	76,113,113	1.46	9 (11%)
13	CLA	f	1201	2	60,68,73	1.48	7 (11%)	70,107,113	1.66	8 (11%)
13	CLA	G	1104	1	65,73,73	1.40	7 (10%)	76,113,113	1.53	10 (13%)
16	BCR	S	4018	-	41,41,41	0.77	0	56,56,56	1.84	15 (26%)
13	CLA	v	502	12	50,58,73	1.68	6 (12%)	58,95,113	1.60	6 (10%)
13	CLA	q	502	12	60,68,73	1.54	7 (11%)	70,107,113	1.47	7 (10%)
13	CLA	q	518	12	60,68,73	1.52	9 (15%)	70,107,113	1.53	8 (11%)
15	SF4	N	3003	3	0,12,12	-	-	-	-	-
13	CLA	1	512	12	52,60,73	1.64	6 (11%)	60,97,113	1.53	6 (10%)
13	CLA	G	1136	1	60,68,73	1.52	8 (13%)	70,107,113	1.55	11 (15%)
13	CLA	B	1209	2	52,60,73	1.66	8 (15%)	60,97,113	1.67	8 (13%)
13	CLA	v	509	12	45,53,73	1.77	6 (13%)	52,89,113	1.63	6 (11%)
16	BCR	1	524	-	41,41,41	0.73	0	56,56,56	1.82	15 (26%)
13	CLA	a	512	12	45,53,73	1.75	7 (15%)	52,89,113	1.62	5 (9%)
16	BCR	T	4015	-	41,41,41	0.78	0	56,56,56	1.82	14 (25%)
13	CLA	3	512	12	45,53,73	1.74	7 (15%)	52,89,113	1.61	5 (9%)
13	CLA	B	1229	2	65,73,73	1.43	7 (10%)	76,113,113	1.57	10 (13%)
13	CLA	a	510	12	65,73,73	1.47	6 (9%)	76,113,113	1.47	9 (11%)
13	CLA	f	1012	21	65,73,73	1.46	9 (13%)	76,113,113	1.54	8 (10%)
13	CLA	f	1208	2	65,73,73	1.42	7 (10%)	76,113,113	1.42	8 (10%)
13	CLA	6	512	12	45,53,73	1.77	6 (13%)	52,89,113	1.58	5 (9%)
16	BCR	b	522	-	41,41,41	0.74	0	56,56,56	1.85	18 (32%)
16	BCR	G	4003	-	41,41,41	0.78	0	56,56,56	1.73	11 (19%)
13	CLA	b	518	12	55,63,73	1.62	7 (12%)	64,101,113	1.49	7 (10%)
13	CLA	c	508	12	45,53,73	1.77	7 (15%)	52,89,113	1.73	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	v	523	-	41,41,41	0.70	0	56,56,56	1.73	14 (25%)
13	CLA	f	1207	2	65,73,73	1.46	9 (13%)	76,113,113	1.38	6 (7%)
16	BCR	Y	522	-	41,41,41	0.73	0	56,56,56	1.91	20 (35%)
13	CLA	3	503	12	65,73,73	1.50	6 (9%)	76,113,113	1.41	9 (11%)
13	CLA	T	1302	8	58,66,73	1.53	8 (13%)	67,104,113	1.51	8 (11%)
13	CLA	e	1140	1	65,73,73	1.49	7 (10%)	76,113,113	1.47	12 (15%)
13	CLA	B	1227	2	65,73,73	1.46	9 (13%)	76,113,113	1.47	9 (11%)
13	CLA	1	516	12	45,53,73	1.79	6 (13%)	52,89,113	1.79	10 (19%)
13	CLA	f	1221	21	65,73,73	1.49	8 (12%)	76,113,113	1.65	12 (15%)
20	SQD	5	822	-	28,29,54	1.25	5 (17%)	37,40,65	1.92	13 (35%)
20	SQD	s	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.59	12 (23%)
16	BCR	J	4013	-	41,41,41	0.76	0	56,56,56	1.96	15 (26%)
13	CLA	H	1213	2	65,73,73	1.40	7 (10%)	76,113,113	1.54	10 (13%)
13	CLA	B	1222	21	60,68,73	1.50	7 (11%)	70,107,113	1.54	10 (14%)
20	SQD	t	822	-	25,26,54	1.31	4 (16%)	34,37,65	1.84	9 (26%)
14	PQN	A	2001	-	34,34,34	2.88	11 (32%)	42,45,45	2.11	7 (16%)
13	CLA	f	1215	2	65,73,73	1.44	8 (12%)	76,113,113	1.57	7 (9%)
16	BCR	B	4017	-	41,41,41	0.80	0	56,56,56	1.57	11 (19%)
17	LHG	e	5008	-	34,34,48	0.77	1 (2%)	37,40,54	1.28	4 (10%)
13	CLA	e	1119	21	65,73,73	1.45	9 (13%)	76,113,113	1.52	9 (11%)
13	CLA	B	1235	2	65,73,73	1.43	7 (10%)	76,113,113	1.54	10 (13%)
13	CLA	6	511	12	45,53,73	1.78	6 (13%)	52,89,113	1.66	6 (11%)
13	CLA	G	1107	1	65,73,73	1.47	10 (15%)	76,113,113	1.43	9 (11%)
13	CLA	A	1126	1	65,73,73	1.39	7 (10%)	76,113,113	1.60	8 (10%)
13	CLA	H	1209	2	52,60,73	1.66	8 (15%)	60,97,113	1.67	8 (13%)
13	CLA	A	1127	1	65,73,73	1.41	7 (10%)	76,113,113	1.50	9 (11%)
13	CLA	q	501	12	65,73,73	1.50	7 (10%)	76,113,113	1.43	8 (10%)
13	CLA	a	518	12	55,63,73	1.61	7 (12%)	64,101,113	1.47	7 (10%)
16	BCR	c	522	-	41,41,41	0.74	0	56,56,56	1.93	20 (35%)
20	SQD	q	822	-	47,48,54	0.99	5 (10%)	56,59,65	1.74	13 (23%)
16	BCR	u	524	-	41,41,41	0.68	0	56,56,56	1.67	14 (25%)
13	CLA	B	1021	2	65,73,73	1.42	8 (12%)	76,113,113	1.44	9 (11%)
16	BCR	B	4009	-	41,41,41	0.81	0	56,56,56	1.91	21 (37%)
13	CLA	1	502	12	60,68,73	1.55	7 (11%)	70,107,113	1.47	7 (10%)
13	CLA	G	1127	1	65,73,73	1.41	7 (10%)	76,113,113	1.50	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	c	518	12	55,63,73	1.60	6 (10%)	64,101,113	1.45	7 (10%)
13	CLA	4	519	12	55,63,73	1.58	9 (16%)	64,101,113	1.49	6 (9%)
13	CLA	e	1102	1	65,73,73	1.42	7 (10%)	76,113,113	1.49	7 (9%)
13	CLA	e	1106	1	65,73,73	1.41	9 (13%)	76,113,113	1.54	9 (11%)
15	SF4	N	3002	3	0,12,12	-	-	-		
13	CLA	A	1128	1	65,73,73	1.53	10 (15%)	76,113,113	1.61	7 (9%)
13	CLA	B	1208	2	65,73,73	1.43	7 (10%)	76,113,113	1.42	8 (10%)
13	CLA	A	1102	1	65,73,73	1.42	6 (9%)	76,113,113	1.49	7 (9%)
13	CLA	j	1302	6	45,53,73	1.76	7 (15%)	52,89,113	1.58	6 (11%)
13	CLA	n	1501	10	65,73,73	1.46	8 (12%)	76,113,113	1.52	9 (11%)
13	CLA	r	501	12	65,73,73	1.49	7 (10%)	76,113,113	1.47	7 (9%)
13	CLA	t	509	12	65,73,73	1.48	6 (9%)	76,113,113	1.50	8 (10%)
16	BCR	a	523	-	41,41,41	0.69	0	56,56,56	1.76	15 (26%)
17	LHG	G	5001	-	48,48,48	0.78	1 (2%)	51,54,54	1.26	6 (11%)
13	CLA	b	501	12	60,68,73	1.54	5 (8%)	70,107,113	1.46	6 (8%)
13	CLA	2	502	12	60,68,73	1.56	8 (13%)	70,107,113	1.45	7 (10%)
16	BCR	n	4019	-	41,41,41	0.73	0	56,56,56	1.92	14 (25%)
13	CLA	A	1134	1	56,64,73	1.57	8 (14%)	65,102,113	1.55	8 (12%)
18	LMU	l	5105	-	22,22,36	1.14	1 (4%)	27,27,47	0.81	0
16	BCR	e	4011	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
13	CLA	u	516	12	45,53,73	1.78	6 (13%)	52,89,113	1.59	6 (11%)
17	LHG	f	1842	13	38,38,48	0.65	0	41,44,54	1.23	4 (9%)
17	LHG	G	5003	13	40,40,48	0.74	0	43,46,54	1.34	6 (13%)
13	CLA	H	1238	21	65,73,73	1.41	7 (10%)	76,113,113	1.57	10 (13%)
13	CLA	3	506	12	50,58,73	1.70	7 (14%)	58,95,113	1.67	6 (10%)
17	LHG	f	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.22	5 (10%)
13	CLA	r	511	12	55,63,73	1.62	6 (10%)	64,101,113	1.56	7 (10%)
13	CLA	f	1223	2	65,73,73	1.42	7 (10%)	76,113,113	1.56	6 (7%)
20	SQD	L	5216	-	50,51,54	0.97	5 (10%)	59,62,65	1.63	11 (18%)
13	CLA	b	503	12	55,63,73	1.64	6 (10%)	64,101,113	1.55	11 (17%)
13	CLA	2	512	12	53,61,73	1.61	7 (13%)	61,98,113	1.48	5 (8%)
13	CLA	A	1135	1	52,60,73	1.53	8 (15%)	60,97,113	1.72	10 (16%)
13	CLA	G	1013	-	65,73,73	1.43	8 (12%)	76,113,113	1.75	9 (11%)
13	CLA	5	507	-	45,53,73	1.75	6 (13%)	52,89,113	1.68	8 (15%)
13	CLA	2	508	12	55,63,73	1.62	8 (14%)	64,101,113	1.59	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	LHG	G	5007	-	46,46,48	0.67	1 (2%)	49,52,54	1.24	5 (10%)
13	CLA	F	1301	21	65,73,73	1.46	7 (10%)	76,113,113	1.39	8 (10%)
13	CLA	4	506	12	45,53,73	1.80	6 (13%)	52,89,113	1.64	6 (11%)
13	CLA	B	1220	2	55,63,73	1.54	9 (16%)	64,101,113	1.67	11 (17%)
13	CLA	B	1207	2	65,73,73	1.46	9 (13%)	76,113,113	1.38	6 (7%)
13	CLA	2	505	12	65,73,73	1.44	6 (9%)	76,113,113	1.41	8 (10%)
20	SQD	3	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.59	12 (23%)
13	CLA	B	1221	21	65,73,73	1.48	8 (12%)	76,113,113	1.66	12 (15%)
13	CLA	F	1302	6	45,53,73	1.76	7 (15%)	52,89,113	1.59	6 (11%)
13	CLA	e	1011	1	65,73,73	1.45	6 (9%)	76,113,113	1.63	12 (15%)
13	CLA	f	1204	2	65,73,73	1.38	8 (12%)	76,113,113	1.43	9 (11%)
13	CLA	q	505	12	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
16	BCR	H	4006	-	41,41,41	0.73	0	56,56,56	1.98	19 (33%)
16	BCR	Y	521	-	41,41,41	0.65	0	56,56,56	1.80	11 (19%)
18	LMU	B	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.11	3 (6%)
20	SQD	1	822	-	47,48,54	0.99	5 (10%)	56,59,65	1.74	13 (23%)
16	BCR	A	4007	-	41,41,41	0.74	0	56,56,56	2.11	18 (32%)
15	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
16	BCR	5	523	-	41,41,41	0.75	0	56,56,56	1.78	16 (28%)
13	CLA	c	519	12	46,54,73	1.76	9 (19%)	53,90,113	1.56	6 (11%)
16	BCR	G	4007	-	41,41,41	0.75	0	56,56,56	2.10	18 (32%)
13	CLA	f	1216	21	60,68,73	1.57	10 (16%)	70,107,113	1.44	6 (8%)
13	CLA	G	1118	1	60,68,73	1.49	8 (13%)	70,107,113	1.49	8 (11%)
16	BCR	e	4007	-	41,41,41	0.74	0	56,56,56	2.11	18 (32%)
13	CLA	H	1239	2	65,73,73	1.48	7 (10%)	76,113,113	1.63	14 (18%)
16	BCR	s	522	-	41,41,41	0.68	0	56,56,56	1.91	15 (26%)
13	CLA	H	1206	2	65,73,73	1.44	10 (15%)	76,113,113	1.58	7 (9%)
16	BCR	f	4005	-	41,41,41	0.70	0	56,56,56	1.78	11 (19%)
13	CLA	A	1801	17	45,53,73	1.72	7 (15%)	52,89,113	1.83	8 (15%)
13	CLA	H	1230	2	60,68,73	1.53	9 (15%)	70,107,113	1.52	10 (14%)
13	CLA	Y	501	12	65,73,73	1.49	7 (10%)	76,113,113	1.43	8 (10%)
13	CLA	H	1236	2	55,63,73	1.63	7 (12%)	64,101,113	1.42	8 (12%)
13	CLA	u	505	12	61,69,73	1.51	6 (9%)	71,108,113	1.40	6 (8%)
13	CLA	A	1121	1	55,63,73	1.58	7 (12%)	64,101,113	1.58	11 (17%)
17	LHG	A	5008	-	34,34,48	0.76	1 (2%)	37,40,54	1.28	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	b	517	-	45,53,73	1.78	6 (13%)	52,89,113	1.66	8 (15%)
13	CLA	G	1128	1	65,73,73	1.53	10 (15%)	76,113,113	1.61	6 (7%)
16	BCR	q	523	-	41,41,41	0.71	0	56,56,56	1.64	16 (28%)
13	CLA	a	503	12	65,73,73	1.50	6 (9%)	76,113,113	1.41	9 (11%)
13	CLA	5	501	12	65,73,73	1.46	6 (9%)	76,113,113	1.47	7 (9%)
13	CLA	f	1023	-	65,73,73	1.41	8 (12%)	76,113,113	1.84	14 (18%)
16	BCR	u	522	-	41,41,41	0.74	0	56,56,56	1.93	20 (35%)
13	CLA	e	1108	1	54,62,73	1.61	7 (12%)	62,99,113	1.49	6 (9%)
20	SQD	b	822	-	25,26,54	1.31	4 (16%)	34,37,65	1.85	9 (26%)
18	LMU	H	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.10	3 (6%)
13	CLA	Y	517	-	45,53,73	1.78	7 (15%)	52,89,113	1.58	6 (11%)
13	CLA	B	1226	2	65,73,73	1.56	10 (15%)	76,113,113	1.82	14 (18%)
13	CLA	5	511	12	55,63,73	1.61	6 (10%)	64,101,113	1.52	7 (10%)
13	CLA	c	506	12	45,53,73	1.77	5 (11%)	52,89,113	1.66	7 (13%)
13	CLA	G	1114	21	50,58,73	1.67	8 (16%)	58,95,113	1.64	7 (12%)
13	CLA	Y	504	-	45,53,73	1.80	8 (17%)	52,89,113	1.61	8 (15%)
13	CLA	e	1118	1	60,68,73	1.50	7 (11%)	70,107,113	1.49	8 (11%)
13	CLA	u	509	12	65,73,73	1.45	7 (10%)	76,113,113	1.49	8 (10%)
13	CLA	5	517	-	45,53,73	1.80	7 (15%)	52,89,113	1.55	6 (11%)
16	BCR	b	521	-	41,41,41	0.64	0	56,56,56	1.78	11 (19%)
13	CLA	1	505	12	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
18	LMU	e	1848	-	36,36,36	1.14	2 (5%)	47,47,47	1.07	2 (4%)
13	CLA	b	507	-	45,53,73	1.75	6 (13%)	52,89,113	1.68	8 (15%)
17	LHG	L	5218	-	37,37,48	0.75	2 (5%)	40,43,54	1.23	4 (10%)
17	LHG	L	5220	-	40,40,48	0.65	0	43,46,54	1.23	4 (9%)
18	LMU	e	1849	-	23,23,36	1.16	1 (4%)	28,28,47	1.00	2 (7%)
13	CLA	G	1124	21	56,64,73	1.58	6 (10%)	65,102,113	1.64	12 (18%)
13	CLA	Z	512	12	53,61,73	1.61	6 (11%)	61,98,113	1.48	5 (8%)
13	CLA	H	1227	2	65,73,73	1.46	9 (13%)	76,113,113	1.46	9 (11%)
17	LHG	n	5221	-	48,48,48	0.65	2 (4%)	51,54,54	1.30	6 (11%)
16	BCR	s	523	-	41,41,41	0.69	0	56,56,56	1.76	15 (26%)
13	CLA	B	1202	2	65,73,73	1.44	7 (10%)	76,113,113	1.65	9 (11%)
16	BCR	4	521	-	41,41,41	0.64	0	56,56,56	1.78	11 (19%)
13	CLA	f	1209	2	52,60,73	1.66	8 (15%)	60,97,113	1.67	8 (13%)
13	CLA	6	513	12	45,53,73	1.83	5 (11%)	52,89,113	1.54	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	1234	2	65,73,73	1.43	8 (12%)	76,113,113	1.69	13 (17%)
17	LHG	e	5006	-	44,44,48	0.62	0	47,50,54	1.26	5 (10%)
13	CLA	H	1235	2	65,73,73	1.43	8 (12%)	76,113,113	1.54	10 (13%)
13	CLA	a	505	12	65,73,73	1.45	6 (9%)	76,113,113	1.36	6 (7%)
13	CLA	v	516	12	45,53,73	1.78	5 (11%)	52,89,113	1.60	8 (15%)
13	CLA	5	503	12	55,63,73	1.63	6 (10%)	64,101,113	1.53	8 (12%)
13	CLA	A	1114	21	50,58,73	1.68	8 (16%)	58,95,113	1.64	7 (12%)
13	CLA	1	518	12	60,68,73	1.53	10 (16%)	70,107,113	1.53	8 (11%)
13	CLA	f	1203	2	65,73,73	1.44	8 (12%)	76,113,113	1.46	7 (9%)
13	CLA	G	1011	1	65,73,73	1.46	6 (9%)	76,113,113	1.63	12 (15%)
13	CLA	G	1134	1	56,64,73	1.57	7 (12%)	65,102,113	1.55	8 (12%)
13	CLA	e	1109	1	65,73,73	1.42	7 (10%)	76,113,113	1.52	7 (9%)
13	CLA	B	1218	2	60,68,73	1.47	7 (11%)	70,107,113	1.52	7 (10%)
13	CLA	G	1126	1	65,73,73	1.38	6 (9%)	76,113,113	1.60	8 (10%)
16	BCR	1	523	-	41,41,41	0.71	0	56,56,56	1.63	16 (28%)
13	CLA	B	1216	21	60,68,73	1.56	10 (16%)	70,107,113	1.43	7 (10%)
13	CLA	b	510	12	50,58,73	1.69	6 (12%)	58,95,113	1.62	7 (12%)
16	BCR	6	522	-	41,41,41	0.70	0	56,56,56	1.84	14 (25%)
13	CLA	1	503	12	64,72,73	1.50	6 (9%)	74,111,113	1.46	7 (9%)
17	LHG	V	5220	-	40,40,48	0.64	0	43,46,54	1.23	4 (9%)
20	SQD	d	822	-	25,26,54	1.30	4 (16%)	34,37,65	1.91	10 (29%)
13	CLA	6	518	12	55,63,73	1.61	6 (10%)	64,101,113	1.49	7 (10%)
13	CLA	Y	516	12	45,53,73	1.79	6 (13%)	52,89,113	1.78	10 (19%)
17	LHG	V	5221	-	48,48,48	0.65	2 (4%)	51,54,54	1.30	6 (11%)
16	BCR	3	523	-	41,41,41	0.69	0	56,56,56	1.76	15 (26%)
17	LHG	e	5004	-	35,35,48	0.74	1 (2%)	38,41,54	1.25	4 (10%)
13	CLA	A	1103	1	65,73,73	1.43	7 (10%)	76,113,113	1.64	8 (10%)
16	BCR	B	4006	-	41,41,41	0.72	0	56,56,56	1.99	19 (33%)
16	BCR	J	4015	-	41,41,41	0.78	0	56,56,56	1.82	14 (25%)
13	CLA	4	507	-	45,53,73	1.76	6 (13%)	52,89,113	1.68	8 (15%)
16	BCR	q	521	-	41,41,41	0.65	0	56,56,56	1.80	11 (19%)
13	CLA	2	503	12	65,73,73	1.47	6 (9%)	76,113,113	1.45	7 (9%)
13	CLA	A	1122	1	60,68,73	1.50	9 (15%)	70,107,113	1.53	8 (11%)
13	CLA	e	1137	1	65,73,73	1.45	7 (10%)	76,113,113	1.50	8 (10%)
13	CLA	A	1108	1	54,62,73	1.61	7 (12%)	62,99,113	1.48	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	3	518	12	55,63,73	1.61	7 (12%)	64,101,113	1.48	7 (10%)
17	LHG	B	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.21	5 (10%)
13	CLA	4	512	12	45,53,73	1.79	6 (13%)	52,89,113	1.62	6 (11%)
13	CLA	d	512	12	45,53,73	1.77	6 (13%)	52,89,113	1.59	5 (9%)
13	CLA	G	1117	1	65,73,73	1.43	10 (15%)	76,113,113	1.69	12 (15%)
13	CLA	d	504	-	45,53,73	1.77	5 (11%)	52,89,113	1.68	7 (13%)
13	CLA	f	1226	2	65,73,73	1.56	10 (15%)	76,113,113	1.82	14 (18%)
13	CLA	f	1220	2	55,63,73	1.54	9 (16%)	64,101,113	1.67	11 (17%)
13	CLA	3	511	12	50,58,73	1.70	6 (12%)	58,95,113	1.62	6 (10%)
13	CLA	4	510	12	50,58,73	1.68	6 (12%)	58,95,113	1.62	7 (12%)
13	CLA	Y	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.51	7 (9%)
13	CLA	e	1126	1	65,73,73	1.39	7 (10%)	76,113,113	1.60	8 (10%)
13	CLA	v	512	12	45,53,73	1.77	6 (13%)	52,89,113	1.58	5 (9%)
20	SQD	B	1852	-	44,45,54	1.02	4 (9%)	53,56,65	1.84	14 (26%)
13	CLA	B	1230	2	60,68,73	1.54	9 (15%)	70,107,113	1.53	10 (14%)
16	BCR	K	4104	-	41,41,41	0.74	0	56,56,56	1.86	15 (26%)
16	BCR	j	4016	-	41,41,41	0.74	0	56,56,56	1.79	13 (23%)
13	CLA	B	1204	2	65,73,73	1.38	8 (12%)	76,113,113	1.43	9 (11%)
13	CLA	5	513	12	45,53,73	1.81	8 (17%)	52,89,113	1.57	6 (11%)
13	CLA	G	1140	1	65,73,73	1.49	8 (12%)	76,113,113	1.48	12 (15%)
13	CLA	e	1105	1	55,63,73	1.52	7 (12%)	64,101,113	1.69	9 (14%)
16	BCR	f	4009	-	41,41,41	0.81	0	56,56,56	1.91	21 (37%)
13	CLA	l	517	-	45,53,73	1.78	7 (15%)	52,89,113	1.58	6 (11%)
13	CLA	H	1023	-	65,73,73	1.40	8 (12%)	76,113,113	1.85	15 (19%)
16	BCR	u	521	-	41,41,41	0.68	0	56,56,56	1.94	16 (28%)
13	CLA	G	1135	1	52,60,73	1.53	8 (15%)	60,97,113	1.71	10 (16%)
16	BCR	R	4016	-	41,41,41	0.75	0	56,56,56	1.78	13 (23%)
16	BCR	u	523	-	41,41,41	0.74	0	56,56,56	1.78	16 (28%)
16	BCR	v	521	-	41,41,41	0.66	0	56,56,56	1.91	12 (21%)
13	CLA	t	510	12	50,58,73	1.68	6 (12%)	58,95,113	1.62	7 (12%)
13	CLA	H	1221	21	65,73,73	1.48	8 (12%)	76,113,113	1.66	12 (15%)
13	CLA	H	1222	21	60,68,73	1.49	7 (11%)	70,107,113	1.54	10 (14%)
13	CLA	b	511	12	45,53,73	1.80	6 (13%)	52,89,113	1.69	7 (13%)
17	LHG	e	5001	-	48,48,48	0.78	1 (2%)	51,54,54	1.26	6 (11%)
13	CLA	l	506	12	45,53,73	1.77	6 (13%)	52,89,113	1.68	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	H	4017	-	41,41,41	0.79	0	56,56,56	1.58	11 (19%)
13	CLA	a	504	-	45,53,73	1.75	6 (13%)	52,89,113	1.69	6 (11%)
19	LMG	f	5002	-	54,54,55	0.80	3 (5%)	62,62,63	1.43	10 (16%)
13	CLA	d	519	12	46,54,73	1.76	6 (13%)	53,90,113	1.59	6 (11%)
13	CLA	q	517	-	45,53,73	1.78	7 (15%)	52,89,113	1.57	6 (11%)
16	BCR	q	522	-	41,41,41	0.74	0	56,56,56	1.90	19 (33%)
13	CLA	1	504	-	45,53,73	1.79	8 (17%)	52,89,113	1.61	8 (15%)
13	CLA	m	1103	9	50,58,73	1.66	9 (18%)	58,95,113	1.68	12 (20%)
13	CLA	H	1021	2	65,73,73	1.42	8 (12%)	76,113,113	1.43	9 (11%)
13	CLA	f	1213	2	65,73,73	1.40	7 (10%)	76,113,113	1.54	10 (13%)
13	CLA	A	1112	1	50,58,73	1.63	9 (18%)	58,95,113	1.72	9 (15%)
13	CLA	4	501	12	60,68,73	1.54	5 (8%)	70,107,113	1.45	6 (8%)
13	CLA	u	501	12	65,73,73	1.47	6 (9%)	76,113,113	1.47	7 (9%)
13	CLA	3	504	-	45,53,73	1.75	6 (13%)	52,89,113	1.69	6 (11%)
16	BCR	L	4022	-	41,41,41	0.76	0	56,56,56	1.90	14 (25%)
18	LMU	Z	901	-	23,23,36	1.10	1 (4%)	28,28,47	0.94	0
16	BCR	2	521	-	41,41,41	0.66	0	56,56,56	1.87	11 (19%)
13	CLA	c	509	12	65,73,73	1.46	7 (10%)	76,113,113	1.49	8 (10%)
16	BCR	3	521	-	41,41,41	0.67	0	56,56,56	1.76	10 (17%)
13	CLA	G	1112	1	50,58,73	1.63	9 (18%)	58,95,113	1.72	9 (15%)
16	BCR	c	524	-	41,41,41	0.69	0	56,56,56	1.67	15 (26%)
16	BCR	A	4002	-	41,41,41	0.81	1 (2%)	56,56,56	1.85	15 (26%)
18	LMU	T	5105	-	22,22,36	1.14	1 (4%)	27,27,47	0.81	0
13	CLA	n	1503	21	60,68,73	1.49	7 (11%)	70,107,113	1.55	7 (10%)
13	CLA	4	517	-	45,53,73	1.79	6 (13%)	52,89,113	1.66	8 (15%)
13	CLA	G	1103	1	65,73,73	1.43	7 (10%)	76,113,113	1.64	8 (10%)
13	CLA	H	1216	21	60,68,73	1.56	10 (16%)	70,107,113	1.43	6 (8%)
13	CLA	u	517	-	45,53,73	1.80	7 (15%)	52,89,113	1.56	6 (11%)
16	BCR	f	4004	-	41,41,41	0.72	0	56,56,56	1.85	13 (23%)
13	CLA	c	510	12	45,53,73	1.76	6 (13%)	52,89,113	1.60	7 (13%)
13	CLA	L	1503	21	60,68,73	1.49	7 (11%)	70,107,113	1.55	7 (10%)
16	BCR	L	4019	-	41,41,41	0.73	0	56,56,56	1.92	14 (25%)
13	CLA	b	509	12	65,73,73	1.47	6 (9%)	76,113,113	1.50	9 (11%)
13	CLA	V	1503	21	60,68,73	1.49	7 (11%)	70,107,113	1.56	7 (10%)
13	CLA	G	1131	1	65,73,73	1.45	9 (13%)	76,113,113	1.43	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	LHG	H	1842	13	38,38,48	0.66	0	41,44,54	1.23	4 (9%)
13	CLA	t	502	12	50,58,73	1.68	7 (14%)	58,95,113	1.59	7 (12%)
16	BCR	d	522	-	41,41,41	0.70	0	56,56,56	1.84	14 (25%)
17	LHG	k	5001	-	43,43,48	0.64	0	46,49,54	1.22	4 (8%)
20	SQD	Y	822	-	47,48,54	0.99	5 (10%)	56,59,65	1.74	13 (23%)
13	CLA	4	509	12	65,73,73	1.47	6 (9%)	76,113,113	1.51	8 (10%)
13	CLA	f	1224	2	60,68,73	1.47	7 (11%)	70,107,113	1.59	8 (11%)
13	CLA	c	511	12	55,63,73	1.61	6 (10%)	64,101,113	1.53	7 (10%)
18	LMU	r	901	-	23,23,36	1.10	1 (4%)	28,28,47	0.94	0
13	CLA	6	501	12	60,68,73	1.53	6 (10%)	70,107,113	1.51	7 (10%)
16	BCR	Z	521	-	41,41,41	0.66	0	56,56,56	1.86	11 (19%)
13	CLA	f	1240	17	65,73,73	1.47	6 (9%)	76,113,113	1.44	9 (11%)
13	CLA	6	510	12	45,53,73	1.80	6 (13%)	52,89,113	1.57	7 (13%)
13	CLA	H	1207	2	65,73,73	1.47	9 (13%)	76,113,113	1.39	6 (7%)
15	SF4	C	3002	3	0,12,12	-	-	-	-	-
16	BCR	T	4012	-	41,41,41	0.70	0	56,56,56	1.66	13 (23%)
13	CLA	e	1132	1	65,73,73	1.43	10 (15%)	76,113,113	1.47	10 (13%)
16	BCR	e	4003	-	41,41,41	0.78	0	56,56,56	1.73	11 (19%)
13	CLA	r	506	12	55,63,73	1.61	6 (10%)	64,101,113	1.55	6 (9%)
13	CLA	l	513	12	55,63,73	1.61	7 (12%)	64,101,113	1.49	6 (9%)
13	CLA	c	513	12	45,53,73	1.81	8 (17%)	52,89,113	1.57	6 (11%)
20	SQD	n	5216	-	50,51,54	0.97	5 (10%)	59,62,65	1.63	11 (18%)
13	CLA	6	517	-	45,53,73	1.78	7 (15%)	52,89,113	1.59	6 (11%)
19	LMG	T	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.25	7 (16%)
20	SQD	c	822	-	28,29,54	1.25	5 (17%)	37,40,65	1.92	13 (35%)
16	BCR	l	4015	-	41,41,41	0.79	0	56,56,56	1.82	14 (25%)
13	CLA	Z	507	-	65,73,73	1.44	6 (9%)	76,113,113	1.48	7 (9%)
13	CLA	s	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.51	8 (10%)
13	CLA	B	1228	2	55,63,73	1.52	7 (12%)	64,101,113	1.68	8 (12%)
19	LMG	B	5002	-	54,54,55	0.79	2 (3%)	62,62,63	1.43	10 (16%)
13	CLA	l	510	12	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
13	CLA	e	1125	1	65,73,73	1.42	8 (12%)	76,113,113	1.56	9 (11%)
13	CLA	G	1102	1	65,73,73	1.42	6 (9%)	76,113,113	1.49	7 (9%)
13	CLA	R	1301	21	65,73,73	1.47	7 (10%)	76,113,113	1.39	8 (10%)
13	CLA	e	1013	-	65,73,73	1.42	8 (12%)	76,113,113	1.75	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	A	4001	-	41,41,41	0.76	0	56,56,56	1.72	11 (19%)
13	CLA	t	508	12	45,53,73	1.82	8 (17%)	52,89,113	1.75	10 (19%)
13	CLA	H	1225	2	65,73,73	1.41	9 (13%)	76,113,113	1.44	7 (9%)
13	CLA	e	1107	1	65,73,73	1.46	10 (15%)	76,113,113	1.43	10 (13%)
13	CLA	G	1111	1	65,73,73	1.47	7 (10%)	76,113,113	1.49	7 (9%)
13	CLA	6	507	-	45,53,73	1.77	6 (13%)	52,89,113	1.66	8 (15%)
18	LMU	J	5105	-	22,22,36	1.14	1 (4%)	27,27,47	0.81	0
13	CLA	1	511	12	55,63,73	1.60	6 (10%)	64,101,113	1.58	8 (12%)
13	CLA	e	1104	1	65,73,73	1.40	7 (10%)	76,113,113	1.52	10 (13%)
13	CLA	f	1229	2	65,73,73	1.44	7 (10%)	76,113,113	1.57	10 (13%)
13	CLA	6	506	12	45,53,73	1.79	5 (11%)	52,89,113	1.66	6 (11%)
13	CLA	3	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.51	8 (10%)
13	CLA	s	519	12	55,63,73	1.60	8 (14%)	64,101,113	1.49	7 (10%)
13	CLA	d	503	12	52,60,73	1.66	6 (11%)	60,97,113	1.57	9 (15%)
13	CLA	v	503	12	52,60,73	1.67	6 (11%)	60,97,113	1.58	9 (15%)
13	CLA	s	513	12	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
13	CLA	3	508	12	55,63,73	1.65	7 (12%)	64,101,113	1.60	8 (12%)
13	CLA	H	1226	2	65,73,73	1.56	10 (15%)	76,113,113	1.82	13 (17%)
20	SQD	V	5216	-	50,51,54	0.97	5 (10%)	59,62,65	1.64	10 (16%)
13	CLA	f	1235	2	65,73,73	1.42	8 (12%)	76,113,113	1.54	10 (13%)
13	CLA	G	1115	1	60,68,73	1.47	7 (11%)	70,107,113	1.59	8 (11%)
13	CLA	4	518	12	55,63,73	1.61	6 (10%)	64,101,113	1.48	7 (10%)
13	CLA	A	1129	1	51,59,73	1.61	10 (19%)	59,96,113	1.61	8 (13%)
13	CLA	B	1212	2	55,63,73	1.53	7 (12%)	64,101,113	1.64	8 (12%)
13	CLA	4	511	12	45,53,73	1.79	6 (13%)	52,89,113	1.70	7 (13%)
13	CLA	A	1120	1	53,61,73	1.56	7 (13%)	61,98,113	1.67	7 (11%)
13	CLA	B	1023	-	65,73,73	1.41	8 (12%)	76,113,113	1.85	14 (18%)
13	CLA	H	1208	2	65,73,73	1.42	7 (10%)	76,113,113	1.43	8 (10%)
13	CLA	H	1228	2	55,63,73	1.52	7 (12%)	64,101,113	1.68	9 (14%)
13	CLA	f	1210	2	65,73,73	1.43	8 (12%)	76,113,113	1.53	12 (15%)
13	CLA	H	1229	2	65,73,73	1.43	7 (10%)	76,113,113	1.57	10 (13%)
13	CLA	c	505	12	61,69,73	1.51	6 (9%)	71,108,113	1.40	6 (8%)
13	CLA	f	1212	2	55,63,73	1.53	7 (12%)	64,101,113	1.65	8 (12%)
13	CLA	G	1129	1	51,59,73	1.61	10 (19%)	59,96,113	1.61	8 (13%)
13	CLA	u	507	-	45,53,73	1.75	6 (13%)	52,89,113	1.68	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	1224	2	60,68,73	1.47	7 (11%)	70,107,113	1.59	8 (11%)
18	LMU	q	902	-	19,19,36	1.22	1 (5%)	24,24,47	1.10	3 (12%)
13	CLA	H	1202	2	65,73,73	1.44	7 (10%)	76,113,113	1.65	9 (11%)
17	LHG	A	5002	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	5 (12%)
17	LHG	A	5005	-	44,44,48	0.67	1 (2%)	47,50,54	1.27	6 (12%)
18	LMU	2	901	-	23,23,36	1.10	1 (4%)	28,28,47	0.94	0
16	BCR	a	522	-	41,41,41	0.67	0	56,56,56	1.91	16 (28%)
13	CLA	A	1119	21	65,73,73	1.46	9 (13%)	76,113,113	1.52	9 (11%)
13	CLA	H	1204	2	65,73,73	1.38	8 (12%)	76,113,113	1.43	9 (11%)
13	CLA	e	1123	21	65,73,73	1.40	7 (10%)	76,113,113	1.51	8 (10%)
13	CLA	A	1139	21	65,73,73	1.45	7 (10%)	76,113,113	1.33	9 (11%)
13	CLA	3	513	12	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
13	CLA	H	1234	2	65,73,73	1.43	8 (12%)	76,113,113	1.68	13 (17%)
13	CLA	a	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.50	8 (10%)
16	BCR	6	524	-	41,41,41	0.75	0	56,56,56	1.86	13 (23%)
13	CLA	G	1139	21	65,73,73	1.45	7 (10%)	76,113,113	1.33	9 (11%)
13	CLA	A	1237	21	65,73,73	1.49	9 (13%)	76,113,113	1.50	11 (14%)
13	CLA	Z	501	12	65,73,73	1.48	7 (10%)	76,113,113	1.47	7 (9%)
13	CLA	f	1217	2	57,65,73	1.51	7 (12%)	66,103,113	1.54	8 (12%)
13	CLA	f	1231	21	65,73,73	1.38	7 (10%)	76,113,113	1.57	8 (10%)
13	CLA	e	1127	1	65,73,73	1.42	7 (10%)	76,113,113	1.50	9 (11%)
13	CLA	H	1218	2	60,68,73	1.47	7 (11%)	70,107,113	1.52	6 (8%)
13	CLA	V	1502	10	65,73,73	1.43	7 (10%)	76,113,113	1.49	8 (10%)
16	BCR	v	522	-	41,41,41	0.69	0	56,56,56	1.84	15 (26%)
16	BCR	3	522	-	41,41,41	0.67	0	56,56,56	1.91	16 (28%)
13	CLA	K	1105	9	45,53,73	1.79	8 (17%)	52,89,113	1.86	11 (21%)
17	LHG	S	5001	-	43,43,48	0.64	0	46,49,54	1.22	4 (8%)
13	CLA	v	518	12	55,63,73	1.61	6 (10%)	64,101,113	1.49	7 (10%)
13	CLA	A	1106	1	65,73,73	1.41	9 (13%)	76,113,113	1.54	9 (11%)
13	CLA	e	1129	1	51,59,73	1.60	10 (19%)	59,96,113	1.61	8 (13%)
13	CLA	A	1013	-	65,73,73	1.42	8 (12%)	76,113,113	1.75	9 (11%)
13	CLA	e	1116	1	60,68,73	1.51	8 (13%)	70,107,113	1.49	7 (10%)

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	BCR	2	524	-	-	2/29/63/63	0/2/2/2
13	CLA	6	516	12	1/1/11/20	8/13/91/115	-
13	CLA	q	519	12	1/1/12/20	6/19/97/115	-
14	PQN	f	2002	-	-	9/23/43/43	0/2/2/2
13	CLA	4	503	12	1/1/13/20	1/25/103/115	-
13	CLA	u	508	12	1/1/11/20	4/13/91/115	-
13	CLA	6	508	12	1/1/11/20	3/13/91/115	-
17	LHG	H	1855	-	-	28/48/48/53	-
18	LMU	1	902	-	-	6/10/30/61	0/1/1/2
13	CLA	t	519	12	1/1/13/20	12/25/103/115	-
13	CLA	G	1022	21	1/1/15/20	8/37/115/115	-
13	CLA	Y	507	-	1/1/14/20	15/31/109/115	-
13	CLA	Z	509	12	1/1/15/20	6/37/115/115	-
16	BCR	d	521	-	-	5/29/63/63	0/2/2/2
16	BCR	H	4005	-	-	6/29/63/63	0/2/2/2
13	CLA	H	1220	2	1/1/13/20	9/25/103/115	-
13	CLA	T	1303	8	1/1/15/20	18/37/115/115	-
17	LHG	e	5003	13	-	17/45/45/53	-
13	CLA	v	519	12	1/1/11/20	6/15/93/115	-
16	BCR	L	4219	-	-	2/29/63/63	0/2/2/2
13	CLA	f	1236	2	-	3/25/103/115	-
13	CLA	r	508	12	1/1/13/20	6/25/103/115	-
13	CLA	U	1401	-	1/1/13/20	8/25/103/115	-
16	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
20	SQD	6	822	-	-	9/19/39/69	0/1/1/1
13	CLA	6	509	12	1/1/11/20	5/13/91/115	-
13	CLA	Z	517	-	1/1/11/20	4/13/91/115	-
13	CLA	A	1101	1	1/1/15/20	13/37/115/115	-
13	CLA	H	1201	2	1/1/14/20	11/31/109/115	-
16	BCR	2	522	-	-	6/29/63/63	0/2/2/2
16	BCR	M	4021	-	-	7/29/63/63	0/2/2/2
13	CLA	f	1228	2	1/1/13/20	8/25/103/115	-
13	CLA	Z	513	12	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1217	2	1/1/13/20	12/28/106/115	-
13	CLA	u	518	12	1/1/13/20	11/25/103/115	-
13	CLA	4	504	-	1/1/11/20	5/13/91/115	-
13	CLA	G	1101	1	1/1/15/20	13/37/115/115	-
13	CLA	c	503	12	1/1/13/20	10/25/103/115	-
16	BCR	f	4017	-	-	2/29/63/63	0/2/2/2
19	LMG	H	5002	-	-	24/49/69/70	0/1/1/1
13	CLA	A	1107	1	1/1/15/20	14/37/115/115	-
13	CLA	r	510	12	1/1/15/20	9/37/115/115	-
16	BCR	Z	522	-	-	6/29/63/63	0/2/2/2
13	CLA	A	1011	1	1/1/15/20	10/37/115/115	-
17	LHG	A	5004	-	-	21/40/40/53	-
13	CLA	m	1401	-	1/1/13/20	8/25/103/115	-
13	CLA	5	502	12	1/1/12/20	5/19/97/115	-
13	CLA	B	1219	2	1/1/15/20	17/37/115/115	-
13	CLA	r	504	-	1/1/12/20	5/19/97/115	-
13	CLA	Y	510	12	1/1/15/20	11/37/115/115	-
13	CLA	f	1202	2	1/1/15/20	13/37/115/115	-
13	CLA	G	1801	17	1/1/11/20	5/13/91/115	-
13	CLA	s	501	12	1/1/15/20	6/37/115/115	-
13	CLA	5	512	12	1/1/11/20	5/13/91/115	-
13	CLA	H	1214	2	1/1/15/20	13/37/115/115	-
13	CLA	A	1116	1	1/1/14/20	15/31/109/115	-
16	BCR	V	4020	-	-	4/29/63/63	0/2/2/2
13	CLA	2	501	12	1/1/15/20	12/37/115/115	-
13	CLA	A	1130	1	1/1/15/20	7/37/115/115	-
13	CLA	5	508	12	1/1/11/20	4/13/91/115	-
20	SQD	a	822	-	-	21/38/58/69	0/1/1/1
16	BCR	I	4018	-	-	1/29/63/63	0/2/2/2
19	LMG	J	5104	-	-	17/30/50/70	0/1/1/1
13	CLA	H	1224	2	1/1/14/20	13/31/109/115	-
13	CLA	Y	511	12	1/1/13/20	4/25/103/115	-
13	CLA	A	1110	1	1/1/12/20	9/21/99/115	-
13	CLA	u	519	12	1/1/11/20	8/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	H	4009	-	-	1/29/63/63	0/2/2/2
13	CLA	6	504	-	1/1/11/20	6/13/91/115	-
13	CLA	A	1131	1	1/1/15/20	6/37/115/115	-
13	CLA	c	504	-	1/1/11/20	3/13/91/115	-
13	CLA	r	507	-	1/1/15/20	14/37/115/115	-
13	CLA	B	1215	2	1/1/15/20	19/37/115/115	-
13	CLA	H	1232	21	1/1/12/20	6/19/97/115	-
13	CLA	A	1109	1	1/1/15/20	9/37/115/115	-
16	BCR	l	4013	-	-	4/29/63/63	0/2/2/2
13	CLA	2	517	-	1/1/11/20	4/13/91/115	-
18	LMU	G	1849	-	-	6/14/34/61	0/1/1/2
13	CLA	G	1110	1	1/1/12/20	9/21/99/115	-
13	CLA	A	1133	1	1/1/15/20	15/37/115/115	-
13	CLA	A	1125	1	1/1/15/20	14/37/115/115	-
13	CLA	d	501	12	1/1/14/20	16/31/109/115	-
13	CLA	u	502	12	1/1/12/20	5/19/97/115	-
13	CLA	2	518	12	1/1/15/20	16/37/115/115	-
13	CLA	G	1109	1	1/1/15/20	9/37/115/115	-
13	CLA	f	1234	2	1/1/15/20	13/37/115/115	-
16	BCR	G	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	q	508	12	1/1/13/20	9/25/103/115	-
13	CLA	H	1215	2	1/1/15/20	19/37/115/115	-
13	CLA	G	1133	1	1/1/15/20	15/37/115/115	-
16	BCR	U	4104	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1211	2	1/1/13/20	4/27/105/115	-
13	CLA	c	507	-	1/1/11/20	5/13/91/115	-
13	CLA	A	1124	21	1/1/13/20	11/27/105/115	-
13	CLA	s	507	-	1/1/15/20	13/37/115/115	-
16	BCR	b	524	-	-	4/29/63/63	0/2/2/2
13	CLA	B	1231	21	1/1/15/20	8/37/115/115	-
13	CLA	d	517	-	1/1/11/20	9/13/91/115	-
16	BCR	4	522	-	-	4/29/63/63	0/2/2/2
13	CLA	2	507	-	1/1/15/20	14/37/115/115	-
13	CLA	d	513	12	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	508	12	1/1/11/20	4/13/91/115	-
13	CLA	A	1117	1	1/1/15/20	12/37/115/115	-
13	CLA	2	506	12	1/1/13/20	8/25/103/115	-
13	CLA	u	506	12	1/1/11/20	5/13/91/115	-
13	CLA	v	506	12	1/1/11/20	5/13/91/115	-
16	BCR	Y	523	-	-	6/29/63/63	0/2/2/2
16	BCR	Y	524	-	-	2/29/63/63	0/2/2/2
16	BCR	n	4020	-	-	4/29/63/63	0/2/2/2
13	CLA	e	1130	1	1/1/15/20	7/37/115/115	-
17	LHG	e	5005	-	-	29/49/49/53	-
13	CLA	A	1118	1	1/1/14/20	12/31/109/115	-
17	LHG	V	5218	-	-	23/42/42/53	-
13	CLA	e	1110	1	1/1/12/20	9/21/99/115	-
13	CLA	Y	508	12	1/1/13/20	9/25/103/115	-
13	CLA	Z	518	12	1/1/15/20	16/37/115/115	-
13	CLA	b	516	12	1/1/11/20	7/13/91/115	-
13	CLA	t	512	12	1/1/11/20	3/13/91/115	-
13	CLA	d	507	-	1/1/11/20	4/13/91/115	-
13	CLA	q	507	-	1/1/14/20	15/31/109/115	-
13	CLA	B	1201	2	1/1/14/20	11/31/109/115	-
13	CLA	s	517	-	1/1/11/20	7/13/91/115	-
13	CLA	f	1239	2	1/1/15/20	15/37/115/115	-
16	BCR	5	521	-	-	7/29/63/63	0/2/2/2
13	CLA	H	1212	2	1/1/13/20	11/25/103/115	-
13	CLA	c	502	12	1/1/12/20	5/19/97/115	-
16	BCR	s	521	-	-	7/29/63/63	0/2/2/2
16	BCR	r	524	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1138	1	1/1/15/20	12/37/115/115	-
13	CLA	f	1218	2	1/1/14/20	7/31/109/115	-
13	CLA	3	501	12	1/1/15/20	6/37/115/115	-
13	CLA	5	509	12	1/1/15/20	12/37/115/115	-
16	BCR	6	523	-	-	4/29/63/63	0/2/2/2
20	SQD	2	822	-	-	13/38/58/69	0/1/1/1
13	CLA	t	507	-	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	2	510	12	1/1/15/20	9/37/115/115	-
17	LHG	e	5007	-	-	24/51/51/53	-
13	CLA	f	1211	2	1/1/13/20	4/27/105/115	-
13	CLA	G	1138	1	1/1/15/20	12/37/115/115	-
13	CLA	r	503	12	1/1/15/20	9/37/115/115	-
16	BCR	f	4010	-	-	5/29/63/63	0/2/2/2
16	BCR	t	524	-	-	4/29/63/63	0/2/2/2
13	CLA	b	502	12	1/1/12/20	5/19/97/115	-
17	LHG	A	5006	-	-	24/49/49/53	-
13	CLA	3	517	-	1/1/11/20	7/13/91/115	-
13	CLA	r	516	12	1/1/11/20	8/13/91/115	-
16	BCR	G	4002	-	-	0/29/63/63	0/2/2/2
16	BCR	a	521	-	-	7/29/63/63	0/2/2/2
16	BCR	A	4008	-	-	7/29/63/63	0/2/2/2
13	CLA	K	1401	-	1/1/13/20	8/25/103/115	-
13	CLA	4	513	12	1/1/11/20	7/13/91/115	-
13	CLA	Y	502	12	1/1/14/20	14/31/109/115	-
13	CLA	e	1801	17	1/1/11/20	5/13/91/115	-
13	CLA	d	509	12	1/1/11/20	6/13/91/115	-
13	CLA	G	1125	1	1/1/15/20	14/37/115/115	-
13	CLA	5	519	12	1/1/11/20	8/15/93/115	-
13	CLA	v	510	12	1/1/11/20	7/13/91/115	-
20	SQD	Z	822	-	-	13/38/58/69	0/1/1/1
13	CLA	H	1217	2	1/1/13/20	12/28/106/115	-
13	CLA	e	1112	1	1/1/12/20	3/19/97/115	-
13	CLA	3	507	-	1/1/15/20	13/37/115/115	-
14	PQN	B	2002	-	-	9/23/43/43	0/2/2/2
13	CLA	1	507	-	1/1/14/20	15/31/109/115	-
13	CLA	a	501	12	1/1/15/20	6/37/115/115	-
16	BCR	4	524	-	-	4/29/63/63	0/2/2/2
13	CLA	1	501	12	1/1/15/20	18/37/115/115	-
13	CLA	G	1122	1	1/1/14/20	14/31/109/115	-
13	CLA	B	1239	2	1/1/15/20	15/37/115/115	-
13	CLA	s	510	12	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	e	4002	-	-	0/29/63/63	0/2/2/2
13	CLA	G	1108	1	1/1/12/20	16/24/102/115	-
13	CLA	4	508	12	1/1/11/20	4/13/91/115	-
18	LMU	A	1848	-	-	7/21/61/61	0/2/2/2
13	CLA	K	1103	9	1/1/12/20	7/19/97/115	-
13	CLA	H	1231	21	1/1/15/20	8/37/115/115	-
13	CLA	a	517	-	1/1/11/20	7/13/91/115	-
13	CLA	5	506	12	1/1/11/20	5/13/91/115	-
13	CLA	s	506	12	1/1/12/20	5/19/97/115	-
13	CLA	b	505	12	1/1/15/20	11/37/115/115	-
13	CLA	J	1303	8	1/1/15/20	18/37/115/115	-
13	CLA	4	516	12	1/1/11/20	7/13/91/115	-
13	CLA	n	1502	10	1/1/15/20	8/37/115/115	-
18	LMU	G	1848	-	-	7/21/61/61	0/2/2/2
13	CLA	f	1232	21	1/1/12/20	6/19/97/115	-
16	BCR	f	4006	-	-	4/29/63/63	0/2/2/2
13	CLA	3	502	12	1/1/12/20	4/19/97/115	-
13	CLA	d	511	12	1/1/11/20	4/13/91/115	-
16	BCR	s	524	-	-	5/29/63/63	0/2/2/2
13	CLA	4	505	12	1/1/15/20	11/37/115/115	-
13	CLA	e	1103	1	1/1/15/20	20/37/115/115	-
16	BCR	1	521	-	-	7/29/63/63	0/2/2/2
16	BCR	3	524	-	-	5/29/63/63	0/2/2/2
15	SF4	g	3002	3	-	-	0/6/5/5
13	CLA	Y	519	12	1/1/12/20	6/19/97/115	-
13	CLA	s	508	12	1/1/13/20	7/25/103/115	-
13	CLA	1	509	12	1/1/15/20	6/37/115/115	-
13	CLA	a	507	-	1/1/15/20	13/37/115/115	-
13	CLA	G	1237	21	1/1/15/20	18/37/115/115	-
13	CLA	d	506	12	1/1/11/20	5/13/91/115	-
13	CLA	q	506	12	1/1/11/20	6/13/91/115	-
16	BCR	B	4010	-	-	5/29/63/63	0/2/2/2
13	CLA	Z	510	12	1/1/15/20	9/37/115/115	-
13	CLA	Y	518	12	1/1/14/20	15/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1111	1	1/1/15/20	14/37/115/115	-
13	CLA	s	516	12	1/1/11/20	9/13/91/115	-
13	CLA	b	512	12	1/1/11/20	3/13/91/115	-
13	CLA	H	1240	17	-	13/37/115/115	-
13	CLA	4	502	12	1/1/12/20	5/19/97/115	-
20	SQD	4	822	-	-	8/19/39/69	0/1/1/1
20	SQD	v	822	-	-	9/19/39/69	0/1/1/1
13	CLA	G	1106	1	1/1/15/20	21/37/115/115	-
13	CLA	2	509	12	1/1/15/20	6/37/115/115	-
13	CLA	G	1121	1	1/1/13/20	6/25/103/115	-
13	CLA	2	516	12	1/1/11/20	8/13/91/115	-
13	CLA	3	516	12	1/1/11/20	9/13/91/115	-
13	CLA	q	509	12	1/1/15/20	6/37/115/115	-
13	CLA	r	505	12	1/1/15/20	14/37/115/115	-
13	CLA	a	511	12	1/1/12/20	5/19/97/115	-
14	PQN	e	2001	-	-	14/23/43/43	0/2/2/2
16	BCR	G	4008	-	-	7/29/63/63	0/2/2/2
13	CLA	t	516	12	1/1/11/20	7/13/91/115	-
17	LHG	G	5008	-	-	19/39/39/53	-
13	CLA	s	511	12	1/1/12/20	5/19/97/115	-
13	CLA	u	511	12	1/1/13/20	5/25/103/115	-
13	CLA	2	511	12	1/1/13/20	4/25/103/115	-
16	BCR	l	4012	-	-	9/29/63/63	0/2/2/2
13	CLA	t	505	12	1/1/15/20	11/37/115/115	-
13	CLA	e	1138	1	1/1/15/20	12/37/115/115	-
13	CLA	e	1139	21	1/1/15/20	12/37/115/115	-
16	BCR	Z	524	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1115	1	1/1/14/20	10/31/109/115	-
13	CLA	e	1136	1	1/1/14/20	5/31/109/115	-
13	CLA	Y	506	12	1/1/11/20	6/13/91/115	-
13	CLA	3	519	12	1/1/13/20	8/25/103/115	-
13	CLA	B	1232	21	1/1/12/20	6/19/97/115	-
13	CLA	b	519	12	1/1/13/20	12/25/103/115	-
13	CLA	2	513	12	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	Z	508	12	1/1/13/20	6/25/103/115	-
13	CLA	e	1237	21	1/1/15/20	19/37/115/115	-
13	CLA	s	502	12	1/1/12/20	4/19/97/115	-
19	LMG	l	5104	-	-	17/30/50/70	0/1/1/1
16	BCR	n	4022	-	-	2/29/63/63	0/2/2/2
13	CLA	j	1301	21	1/1/15/20	11/37/115/115	-
13	CLA	B	1223	2	1/1/15/20	14/37/115/115	-
13	CLA	e	1022	21	1/1/15/20	8/37/115/115	-
13	CLA	G	1116	1	1/1/14/20	15/31/109/115	-
13	CLA	Z	516	12	1/1/11/20	8/13/91/115	-
16	BCR	L	4020	-	-	4/29/63/63	0/2/2/2
15	SF4	G	3001	2,1	-	-	0/6/5/5
13	CLA	e	1121	1	1/1/13/20	6/25/103/115	-
13	CLA	G	1130	1	1/1/15/20	7/37/115/115	-
16	BCR	b	523	-	-	5/29/63/63	0/2/2/2
16	BCR	e	4008	-	-	7/29/63/63	0/2/2/2
17	LHG	L	5221	-	-	30/53/53/53	-
13	CLA	e	1111	1	1/1/15/20	14/37/115/115	-
13	CLA	f	1238	21	1/1/15/20	4/37/115/115	-
13	CLA	Z	511	12	1/1/13/20	4/25/103/115	-
16	BCR	a	524	-	-	5/29/63/63	0/2/2/2
13	CLA	e	1117	1	1/1/15/20	12/37/115/115	-
13	CLA	e	1120	1	1/1/12/20	4/23/101/115	-
13	CLA	A	1123	21	1/1/15/20	11/37/115/115	-
13	CLA	B	1238	21	1/1/15/20	4/37/115/115	-
13	CLA	v	505	12	1/1/15/20	15/37/115/115	-
16	BCR	B	4014	-	-	9/29/63/63	0/2/2/2
13	CLA	e	1135	1	1/1/12/20	10/22/100/115	-
13	CLA	2	504	-	1/1/12/20	5/19/97/115	-
13	CLA	b	506	12	1/1/11/20	2/13/91/115	-
20	SQD	H	1852	-	-	19/40/60/69	0/1/1/1
13	CLA	q	503	12	1/1/14/20	9/36/114/115	-
13	CLA	r	513	12	1/1/15/20	15/37/115/115	-
13	CLA	t	501	12	1/1/14/20	12/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LHG	A	5007	-	-	24/51/51/53	-
13	CLA	e	1115	1	1/1/14/20	10/31/109/115	-
17	LHG	n	5218	-	-	23/42/42/53	-
13	CLA	H	1210	2	1/1/15/20	19/37/115/115	-
13	CLA	t	511	12	1/1/11/20	3/13/91/115	-
16	BCR	m	4104	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1225	2	1/1/15/20	8/37/115/115	-
13	CLA	L	1501	10	1/1/15/20	18/37/115/115	-
13	CLA	q	511	12	1/1/13/20	4/25/103/115	-
16	BCR	J	4012	-	-	9/29/63/63	0/2/2/2
13	CLA	d	510	12	1/1/11/20	7/13/91/115	-
13	CLA	r	519	12	1/1/13/20	9/25/103/115	-
16	BCR	t	522	-	-	4/29/63/63	0/2/2/2
13	CLA	5	505	12	1/1/14/20	16/33/111/115	-
13	CLA	H	1211	2	1/1/13/20	4/27/105/115	-
13	CLA	s	505	12	1/1/15/20	18/37/115/115	-
13	CLA	e	1124	21	1/1/13/20	11/27/105/115	-
13	CLA	t	518	12	1/1/13/20	8/25/103/115	-
16	BCR	A	4011	-	-	12/29/63/63	0/2/2/2
13	CLA	r	517	-	1/1/11/20	4/13/91/115	-
13	CLA	G	1113	1	1/1/11/20	5/13/91/115	-
13	CLA	3	505	12	1/1/15/20	17/37/115/115	-
13	CLA	G	1120	1	1/1/12/20	4/23/101/115	-
13	CLA	Z	502	12	1/1/14/20	11/31/109/115	-
16	BCR	t	523	-	-	5/29/63/63	0/2/2/2
13	CLA	Z	504	-	1/1/12/20	5/19/97/115	-
16	BCR	W	4021	-	-	7/29/63/63	0/2/2/2
16	BCR	r	521	-	-	4/29/63/63	0/2/2/2
16	BCR	r	523	-	-	6/29/63/63	0/2/2/2
13	CLA	a	502	12	1/1/12/20	4/19/97/115	-
13	CLA	s	518	12	1/1/13/20	10/25/103/115	-
13	CLA	e	1101	1	1/1/15/20	13/37/115/115	-
13	CLA	6	502	12	1/1/12/20	5/19/97/115	-
16	BCR	k	4018	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LHG	A	5009	-	-	28/53/53/53	-
14	PQN	H	2002	-	-	9/23/43/43	0/2/2/2
13	CLA	t	506	12	1/1/11/20	2/13/91/115	-
16	BCR	H	4004	-	-	8/29/63/63	0/2/2/2
13	CLA	a	508	12	1/1/13/20	7/25/103/115	-
17	LHG	G	5009	-	-	28/53/53/53	-
13	CLA	v	501	12	1/1/14/20	16/31/109/115	-
16	BCR	n	4219	-	-	2/29/63/63	0/2/2/2
13	CLA	f	1214	2	1/1/15/20	13/37/115/115	-
20	SQD	u	822	-	-	7/24/44/69	0/1/1/1
13	CLA	Y	513	12	1/1/13/20	2/25/103/115	-
13	CLA	t	503	12	1/1/13/20	1/25/103/115	-
13	CLA	A	1140	1	1/1/15/20	11/37/115/115	-
13	CLA	6	503	12	1/1/12/20	8/22/100/115	-
16	BCR	c	523	-	-	4/29/63/63	0/2/2/2
15	SF4	C	3003	3	-	-	0/6/5/5
13	CLA	B	1213	2	1/1/15/20	14/37/115/115	-
13	CLA	H	1205	2	1/1/15/20	10/37/115/115	-
13	CLA	V	1501	10	1/1/15/20	18/37/115/115	-
16	BCR	V	4019	-	-	6/29/63/63	0/2/2/2
17	LHG	G	5004	-	-	21/40/40/53	-
13	CLA	q	513	12	1/1/13/20	2/25/103/115	-
16	BCR	4	523	-	-	5/29/63/63	0/2/2/2
13	CLA	1	519	12	1/1/12/20	6/19/97/115	-
13	CLA	d	502	12	1/1/12/20	5/19/97/115	-
16	BCR	T	4013	-	-	4/29/63/63	0/2/2/2
13	CLA	5	504	-	1/1/11/20	3/13/91/115	-
13	CLA	s	504	-	1/1/11/20	6/13/91/115	-
13	CLA	B	1214	2	1/1/15/20	13/37/115/115	-
17	LHG	e	5009	-	-	28/53/53/53	-
13	CLA	B	1203	2	1/1/15/20	16/37/115/115	-
16	BCR	d	524	-	-	5/29/63/63	0/2/2/2
13	CLA	A	1104	1	1/1/15/20	12/37/115/115	-
16	BCR	V	4022	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	SQD	f	1852	-	-	19/40/60/69	0/1/1/1
13	CLA	6	505	12	1/1/15/20	15/37/115/115	-
13	CLA	U	1103	9	1/1/12/20	7/19/97/115	-
13	CLA	Y	512	12	1/1/12/20	9/22/100/115	-
13	CLA	v	507	-	1/1/11/20	4/13/91/115	-
13	CLA	2	519	12	1/1/13/20	9/25/103/115	-
13	CLA	d	508	12	1/1/11/20	3/13/91/115	-
16	BCR	o	4021	-	-	7/29/63/63	0/2/2/2
13	CLA	l	1302	8	1/1/13/20	13/29/107/115	-
13	CLA	U	1105	9	1/1/11/20	9/13/91/115	-
13	CLA	e	1114	21	1/1/12/20	2/19/97/115	-
17	LHG	A	5001	-	-	25/53/53/53	-
13	CLA	d	516	12	1/1/11/20	8/13/91/115	-
13	CLA	Z	505	12	1/1/15/20	14/37/115/115	-
13	CLA	q	504	-	1/1/11/20	5/13/91/115	-
13	CLA	B	1240	17	-	13/37/115/115	-
13	CLA	c	501	12	1/1/15/20	19/37/115/115	-
16	BCR	2	523	-	-	6/29/63/63	0/2/2/2
13	CLA	G	1119	21	1/1/15/20	15/37/115/115	-
13	CLA	G	1137	1	1/1/15/20	19/37/115/115	-
13	CLA	c	512	12	1/1/11/20	5/13/91/115	-
13	CLA	G	1123	21	1/1/15/20	11/37/115/115	-
13	CLA	v	517	-	1/1/11/20	9/13/91/115	-
13	CLA	e	1113	1	1/1/11/20	5/13/91/115	-
13	CLA	f	1205	2	1/1/15/20	10/37/115/115	-
16	BCR	t	521	-	-	10/29/63/63	0/2/2/2
13	CLA	R	1302	6	1/1/11/20	8/13/91/115	-
13	CLA	c	517	-	1/1/11/20	9/13/91/115	-
13	CLA	L	1502	10	1/1/15/20	8/37/115/115	-
13	CLA	f	1219	2	1/1/15/20	17/37/115/115	-
13	CLA	B	1012	21	1/1/15/20	16/37/115/115	-
17	LHG	G	5005	-	-	29/49/49/53	-
16	BCR	c	521	-	-	7/29/63/63	0/2/2/2
13	CLA	m	1105	9	1/1/11/20	9/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	t	517	-	1/1/11/20	5/13/91/115	-
13	CLA	v	504	-	1/1/11/20	6/13/91/115	-
16	BCR	G	4011	-	-	12/29/63/63	0/2/2/2
16	BCR	F	4016	-	-	2/29/63/63	0/2/2/2
16	BCR	B	4004	-	-	8/29/63/63	0/2/2/2
13	CLA	t	513	12	1/1/11/20	7/13/91/115	-
16	BCR	H	4010	-	-	5/29/63/63	0/2/2/2
13	CLA	f	1230	2	1/1/14/20	10/31/109/115	-
13	CLA	a	519	12	1/1/13/20	8/25/103/115	-
16	BCR	Z	523	-	-	6/29/63/63	0/2/2/2
16	BCR	H	4014	-	-	9/29/63/63	0/2/2/2
13	CLA	a	516	12	1/1/11/20	9/13/91/115	-
13	CLA	e	1133	1	1/1/15/20	15/37/115/115	-
17	LHG	e	5002	-	-	26/43/43/53	-
13	CLA	r	512	12	1/1/12/20	5/23/101/115	-
13	CLA	A	1105	1	1/1/13/20	6/25/103/115	-
13	CLA	u	503	12	1/1/13/20	10/25/103/115	-
13	CLA	A	1137	1	1/1/15/20	19/37/115/115	-
13	CLA	5	510	12	1/1/11/20	7/13/91/115	-
13	CLA	f	1206	2	1/1/15/20	15/37/115/115	-
13	CLA	a	513	12	1/1/15/20	13/37/115/115	-
13	CLA	J	1302	8	1/1/13/20	13/29/107/115	-
13	CLA	r	509	12	1/1/15/20	6/37/115/115	-
16	BCR	r	522	-	-	6/29/63/63	0/2/2/2
13	CLA	b	513	12	1/1/11/20	7/13/91/115	-
13	CLA	r	502	12	1/1/14/20	11/31/109/115	-
13	CLA	e	1134	1	1/1/13/20	11/27/105/115	-
13	CLA	r	518	12	1/1/15/20	16/37/115/115	-
13	CLA	B	1205	2	1/1/15/20	10/37/115/115	-
13	CLA	B	1236	2	-	3/25/103/115	-
16	BCR	f	4014	-	-	9/29/63/63	0/2/2/2
13	CLA	H	1012	21	1/1/15/20	16/37/115/115	-
13	CLA	f	1021	2	1/1/15/20	11/37/115/115	-
13	CLA	A	1022	21	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	t	504	-	1/1/11/20	5/13/91/115	-
16	BCR	5	524	-	-	2/29/63/63	0/2/2/2
16	BCR	e	4001	-	-	8/29/63/63	0/2/2/2
16	BCR	1	522	-	-	6/29/63/63	0/2/2/2
13	CLA	B	1210	2	1/1/15/20	19/37/115/115	-
13	CLA	q	512	12	1/1/12/20	10/22/100/115	-
13	CLA	e	1128	1	1/1/15/20	12/37/115/115	-
13	CLA	u	513	12	1/1/11/20	4/13/91/115	-
13	CLA	Z	519	12	1/1/13/20	9/25/103/115	-
13	CLA	a	506	12	1/1/12/20	5/19/97/115	-
13	CLA	6	519	12	1/1/11/20	6/15/93/115	-
17	LHG	G	5006	-	-	24/49/49/53	-
13	CLA	q	510	12	1/1/15/20	11/37/115/115	-
13	CLA	H	1223	2	1/1/15/20	14/37/115/115	-
16	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
17	LHG	n	5220	-	-	24/45/45/53	-
13	CLA	d	505	12	1/1/15/20	15/37/115/115	-
17	LHG	B	1842	13	-	22/43/43/53	-
17	LHG	G	5002	-	-	26/43/43/53	-
16	BCR	6	521	-	-	5/29/63/63	0/2/2/2
17	LHG	I	5001	-	-	22/48/48/53	-
13	CLA	s	512	12	1/1/11/20	3/13/91/115	-
18	LMU	Y	902	-	-	6/10/30/61	0/1/1/2
17	LHG	A	5003	13	-	17/45/45/53	-
13	CLA	l	1303	8	1/1/15/20	18/37/115/115	-
13	CLA	5	516	12	1/1/11/20	2/13/91/115	-
13	CLA	b	504	-	1/1/11/20	5/13/91/115	-
13	CLA	1	508	12	1/1/13/20	9/25/103/115	-
13	CLA	f	1227	2	1/1/15/20	12/37/115/115	-
13	CLA	v	513	12	1/1/11/20	3/13/91/115	-
16	BCR	v	524	-	-	5/29/63/63	0/2/2/2
13	CLA	A	1113	1	1/1/11/20	5/13/91/115	-
16	BCR	q	524	-	-	2/29/63/63	0/2/2/2
13	CLA	d	518	12	1/1/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1132	1	1/1/15/20	15/37/115/115	-
13	CLA	f	1222	21	1/1/14/20	7/31/109/115	-
18	LMU	f	1843	-	-	12/21/61/61	0/2/2/2
15	SF4	g	3003	3	-	-	0/6/5/5
13	CLA	u	512	12	1/1/11/20	5/13/91/115	-
13	CLA	u	504	-	1/1/11/20	3/13/91/115	-
13	CLA	v	508	12	1/1/11/20	3/13/91/115	-
13	CLA	u	510	12	1/1/11/20	7/13/91/115	-
13	CLA	G	1132	1	1/1/15/20	15/37/115/115	-
13	CLA	Y	505	12	1/1/15/20	11/37/115/115	-
13	CLA	Z	503	12	1/1/15/20	9/37/115/115	-
16	BCR	5	522	-	-	5/29/63/63	0/2/2/2
16	BCR	d	523	-	-	4/29/63/63	0/2/2/2
13	CLA	q	516	12	1/1/11/20	13/13/91/115	-
13	CLA	Z	506	12	1/1/13/20	8/25/103/115	-
20	SQD	r	822	-	-	13/38/58/69	0/1/1/1
13	CLA	Y	503	12	1/1/14/20	9/36/114/115	-
13	CLA	5	518	12	1/1/13/20	11/25/103/115	-
15	SF4	e	3001	2,1	-	-	0/6/5/5
13	CLA	G	1105	1	1/1/13/20	6/25/103/115	-
13	CLA	H	1219	2	1/1/15/20	17/37/115/115	-
13	CLA	f	1225	2	1/1/15/20	7/37/115/115	-
13	CLA	v	511	12	1/1/11/20	4/13/91/115	-
13	CLA	c	516	12	1/1/11/20	2/13/91/115	-
18	LMU	A	1849	-	-	6/14/34/61	0/1/1/2
13	CLA	B	1206	2	1/1/15/20	15/37/115/115	-
13	CLA	s	503	12	1/1/15/20	7/37/115/115	-
13	CLA	e	1131	1	1/1/15/20	6/37/115/115	-
14	PQN	G	2001	-	-	14/23/43/43	0/2/2/2
13	CLA	H	1203	2	1/1/15/20	16/37/115/115	-
16	BCR	V	4219	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1136	1	1/1/14/20	5/31/109/115	-
13	CLA	e	1122	1	1/1/14/20	14/31/109/115	-
13	CLA	3	510	12	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	f	1201	2	1/1/14/20	11/31/109/115	-
13	CLA	G	1104	1	1/1/15/20	12/37/115/115	-
16	BCR	S	4018	-	-	1/29/63/63	0/2/2/2
13	CLA	v	502	12	1/1/12/20	5/19/97/115	-
13	CLA	q	502	12	1/1/14/20	14/31/109/115	-
13	CLA	q	518	12	1/1/14/20	15/31/109/115	-
15	SF4	N	3003	3	-	-	0/6/5/5
13	CLA	1	512	12	1/1/12/20	10/22/100/115	-
13	CLA	G	1136	1	1/1/14/20	5/31/109/115	-
13	CLA	B	1209	2	1/1/12/20	8/22/100/115	-
13	CLA	v	509	12	1/1/11/20	6/13/91/115	-
16	BCR	1	524	-	-	2/29/63/63	0/2/2/2
13	CLA	a	512	12	1/1/11/20	3/13/91/115	-
16	BCR	T	4015	-	-	5/29/63/63	0/2/2/2
13	CLA	3	512	12	1/1/11/20	3/13/91/115	-
13	CLA	B	1229	2	1/1/15/20	13/37/115/115	-
13	CLA	a	510	12	1/1/15/20	17/37/115/115	-
13	CLA	f	1012	21	1/1/15/20	16/37/115/115	-
13	CLA	f	1208	2	1/1/15/20	15/37/115/115	-
13	CLA	6	512	12	1/1/11/20	6/13/91/115	-
16	BCR	b	522	-	-	4/29/63/63	0/2/2/2
16	BCR	G	4003	-	-	0/29/63/63	0/2/2/2
13	CLA	b	518	12	1/1/13/20	8/25/103/115	-
13	CLA	c	508	12	1/1/11/20	4/13/91/115	-
16	BCR	v	523	-	-	4/29/63/63	0/2/2/2
13	CLA	f	1207	2	1/1/15/20	14/37/115/115	-
16	BCR	Y	522	-	-	6/29/63/63	0/2/2/2
13	CLA	3	503	12	1/1/15/20	7/37/115/115	-
13	CLA	T	1302	8	1/1/13/20	13/29/107/115	-
13	CLA	e	1140	1	1/1/15/20	11/37/115/115	-
13	CLA	B	1227	2	1/1/15/20	12/37/115/115	-
13	CLA	1	516	12	1/1/11/20	13/13/91/115	-
13	CLA	f	1221	21	1/1/15/20	14/37/115/115	-
20	SQD	5	822	-	-	7/24/44/69	0/1/1/1
20	SQD	s	822	-	-	21/38/58/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	J	4013	-	-	4/29/63/63	0/2/2/2
13	CLA	H	1213	2	1/1/15/20	14/37/115/115	-
13	CLA	B	1222	21	1/1/14/20	7/31/109/115	-
20	SQD	t	822	-	-	8/19/39/69	0/1/1/1
14	PQN	A	2001	-	-	14/23/43/43	0/2/2/2
13	CLA	f	1215	2	1/1/15/20	19/37/115/115	-
16	BCR	B	4017	-	-	2/29/63/63	0/2/2/2
17	LHG	e	5008	-	-	19/39/39/53	-
13	CLA	e	1119	21	1/1/15/20	15/37/115/115	-
13	CLA	B	1235	2	1/1/15/20	6/37/115/115	-
13	CLA	6	511	12	1/1/11/20	4/13/91/115	-
13	CLA	G	1107	1	1/1/15/20	14/37/115/115	-
13	CLA	A	1126	1	1/1/15/20	18/37/115/115	-
13	CLA	H	1209	2	1/1/12/20	8/22/100/115	-
13	CLA	A	1127	1	1/1/15/20	12/37/115/115	-
13	CLA	q	501	12	1/1/15/20	18/37/115/115	-
13	CLA	a	518	12	1/1/13/20	10/25/103/115	-
16	BCR	c	522	-	-	5/29/63/63	0/2/2/2
20	SQD	q	822	-	-	20/43/63/69	0/1/1/1
16	BCR	u	524	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1021	2	1/1/15/20	10/37/115/115	-
16	BCR	B	4009	-	-	1/29/63/63	0/2/2/2
13	CLA	l	502	12	1/1/14/20	14/31/109/115	-
13	CLA	G	1127	1	1/1/15/20	12/37/115/115	-
13	CLA	c	518	12	1/1/13/20	11/25/103/115	-
13	CLA	4	519	12	1/1/13/20	12/25/103/115	-
13	CLA	e	1102	1	1/1/15/20	11/37/115/115	-
13	CLA	e	1106	1	1/1/15/20	21/37/115/115	-
15	SF4	N	3002	3	-	-	0/6/5/5
13	CLA	A	1128	1	1/1/15/20	12/37/115/115	-
13	CLA	B	1208	2	1/1/15/20	15/37/115/115	-
13	CLA	A	1102	1	1/1/15/20	11/37/115/115	-
13	CLA	j	1302	6	1/1/11/20	8/13/91/115	-
13	CLA	n	1501	10	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	r	501	12	1/1/15/20	12/37/115/115	-
13	CLA	t	509	12	1/1/15/20	7/37/115/115	-
16	BCR	a	523	-	-	4/29/63/63	0/2/2/2
17	LHG	G	5001	-	-	25/53/53/53	-
13	CLA	b	501	12	1/1/14/20	12/31/109/115	-
13	CLA	2	502	12	1/1/14/20	11/31/109/115	-
16	BCR	n	4019	-	-	6/29/63/63	0/2/2/2
13	CLA	A	1134	1	1/1/13/20	11/27/105/115	-
18	LMU	l	5105	-	-	8/13/33/61	0/1/1/2
16	BCR	e	4011	-	-	13/29/63/63	0/2/2/2
13	CLA	u	516	12	1/1/11/20	2/13/91/115	-
17	LHG	f	1842	13	-	22/43/43/53	-
17	LHG	G	5003	13	-	16/45/45/53	-
13	CLA	H	1238	21	1/1/15/20	4/37/115/115	-
13	CLA	3	506	12	1/1/12/20	5/19/97/115	-
17	LHG	f	1855	-	-	28/48/48/53	-
13	CLA	r	511	12	1/1/13/20	4/25/103/115	-
13	CLA	f	1223	2	1/1/15/20	14/37/115/115	-
20	SQD	L	5216	-	-	17/46/66/69	0/1/1/1
13	CLA	b	503	12	1/1/13/20	1/25/103/115	-
13	CLA	2	512	12	1/1/12/20	5/23/101/115	-
13	CLA	A	1135	1	1/1/12/20	10/22/100/115	-
13	CLA	G	1013	-	1/1/15/20	11/37/115/115	-
13	CLA	5	507	-	1/1/11/20	5/13/91/115	-
13	CLA	2	508	12	1/1/13/20	6/25/103/115	-
17	LHG	G	5007	-	-	24/51/51/53	-
13	CLA	F	1301	21	1/1/15/20	11/37/115/115	-
13	CLA	4	506	12	1/1/11/20	2/13/91/115	-
13	CLA	B	1220	2	1/1/13/20	9/25/103/115	-
13	CLA	B	1207	2	1/1/15/20	14/37/115/115	-
13	CLA	2	505	12	1/1/15/20	14/37/115/115	-
20	SQD	3	822	-	-	21/38/58/69	0/1/1/1
13	CLA	B	1221	21	1/1/15/20	14/37/115/115	-
13	CLA	F	1302	6	1/1/11/20	8/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	e	1011	1	1/1/15/20	10/37/115/115	-
13	CLA	f	1204	2	1/1/15/20	12/37/115/115	-
13	CLA	q	505	12	1/1/15/20	11/37/115/115	-
16	BCR	H	4006	-	-	4/29/63/63	0/2/2/2
16	BCR	Y	521	-	-	6/29/63/63	0/2/2/2
18	LMU	B	1843	-	-	12/21/61/61	0/2/2/2
20	SQD	1	822	-	-	20/43/63/69	0/1/1/1
16	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
15	SF4	A	3001	2,1	-	-	0/6/5/5
16	BCR	5	523	-	-	4/29/63/63	0/2/2/2
13	CLA	c	519	12	1/1/11/20	8/15/93/115	-
16	BCR	G	4007	-	-	0/29/63/63	0/2/2/2
13	CLA	f	1216	21	1/1/14/20	5/31/109/115	-
13	CLA	G	1118	1	1/1/14/20	12/31/109/115	-
16	BCR	e	4007	-	-	0/29/63/63	0/2/2/2
13	CLA	H	1239	2	1/1/15/20	15/37/115/115	-
16	BCR	s	522	-	-	5/29/63/63	0/2/2/2
13	CLA	H	1206	2	1/1/15/20	15/37/115/115	-
16	BCR	f	4005	-	-	6/29/63/63	0/2/2/2
13	CLA	A	1801	17	1/1/11/20	5/13/91/115	-
13	CLA	H	1230	2	1/1/14/20	10/31/109/115	-
13	CLA	Y	501	12	1/1/15/20	18/37/115/115	-
13	CLA	H	1236	2	-	3/25/103/115	-
13	CLA	u	505	12	1/1/14/20	16/33/111/115	-
13	CLA	A	1121	1	1/1/13/20	6/25/103/115	-
17	LHG	A	5008	-	-	19/39/39/53	-
13	CLA	b	517	-	1/1/11/20	5/13/91/115	-
13	CLA	G	1128	1	1/1/15/20	12/37/115/115	-
16	BCR	q	523	-	-	6/29/63/63	0/2/2/2
13	CLA	a	503	12	1/1/15/20	7/37/115/115	-
13	CLA	5	501	12	1/1/15/20	19/37/115/115	-
13	CLA	f	1023	-	1/1/15/20	10/37/115/115	-
16	BCR	u	522	-	-	5/29/63/63	0/2/2/2
13	CLA	e	1108	1	1/1/12/20	16/24/102/115	-
20	SQD	b	822	-	-	8/19/39/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LMU	H	1843	-	-	12/21/61/61	0/2/2/2
13	CLA	Y	517	-	1/1/11/20	4/13/91/115	-
13	CLA	B	1226	2	1/1/15/20	12/37/115/115	-
13	CLA	5	511	12	1/1/13/20	5/25/103/115	-
13	CLA	c	506	12	1/1/11/20	5/13/91/115	-
13	CLA	G	1114	21	1/1/12/20	2/19/97/115	-
13	CLA	Y	504	-	1/1/11/20	5/13/91/115	-
13	CLA	e	1118	1	1/1/14/20	12/31/109/115	-
13	CLA	u	509	12	1/1/15/20	12/37/115/115	-
13	CLA	5	517	-	1/1/11/20	9/13/91/115	-
16	BCR	b	521	-	-	10/29/63/63	0/2/2/2
13	CLA	l	505	12	1/1/15/20	11/37/115/115	-
18	LMU	e	1848	-	-	7/21/61/61	0/2/2/2
13	CLA	b	507	-	1/1/11/20	6/13/91/115	-
17	LHG	L	5218	-	-	23/42/42/53	-
17	LHG	L	5220	-	-	24/45/45/53	-
18	LMU	e	1849	-	-	6/14/34/61	0/1/1/2
13	CLA	G	1124	21	1/1/13/20	11/27/105/115	-
13	CLA	Z	512	12	1/1/12/20	5/23/101/115	-
13	CLA	H	1227	2	1/1/15/20	12/37/115/115	-
17	LHG	n	5221	-	-	30/53/53/53	-
16	BCR	s	523	-	-	4/29/63/63	0/2/2/2
13	CLA	B	1202	2	1/1/15/20	13/37/115/115	-
16	BCR	4	521	-	-	10/29/63/63	0/2/2/2
13	CLA	f	1209	2	1/1/12/20	8/22/100/115	-
13	CLA	6	513	12	1/1/11/20	3/13/91/115	-
13	CLA	B	1234	2	1/1/15/20	13/37/115/115	-
17	LHG	e	5006	-	-	24/49/49/53	-
13	CLA	H	1235	2	1/1/15/20	6/37/115/115	-
13	CLA	a	505	12	1/1/15/20	17/37/115/115	-
13	CLA	v	516	12	1/1/11/20	8/13/91/115	-
13	CLA	5	503	12	1/1/13/20	10/25/103/115	-
13	CLA	A	1114	21	1/1/12/20	2/19/97/115	-
13	CLA	l	518	12	1/1/14/20	15/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	f	1203	2	1/1/15/20	16/37/115/115	-
13	CLA	G	1011	1	1/1/15/20	10/37/115/115	-
13	CLA	G	1134	1	1/1/13/20	11/27/105/115	-
13	CLA	e	1109	1	1/1/15/20	9/37/115/115	-
13	CLA	B	1218	2	1/1/14/20	7/31/109/115	-
13	CLA	G	1126	1	1/1/15/20	18/37/115/115	-
16	BCR	1	523	-	-	6/29/63/63	0/2/2/2
13	CLA	B	1216	21	1/1/14/20	5/31/109/115	-
13	CLA	b	510	12	1/1/12/20	5/19/97/115	-
16	BCR	6	522	-	-	5/29/63/63	0/2/2/2
13	CLA	1	503	12	1/1/14/20	9/36/114/115	-
17	LHG	V	5220	-	-	24/45/45/53	-
20	SQD	d	822	-	-	9/19/39/69	0/1/1/1
13	CLA	6	518	12	1/1/13/20	10/25/103/115	-
13	CLA	Y	516	12	1/1/11/20	13/13/91/115	-
17	LHG	V	5221	-	-	30/53/53/53	-
16	BCR	3	523	-	-	4/29/63/63	0/2/2/2
17	LHG	e	5004	-	-	21/40/40/53	-
13	CLA	A	1103	1	1/1/15/20	20/37/115/115	-
16	BCR	B	4006	-	-	4/29/63/63	0/2/2/2
16	BCR	J	4015	-	-	5/29/63/63	0/2/2/2
13	CLA	4	507	-	1/1/11/20	6/13/91/115	-
16	BCR	q	521	-	-	7/29/63/63	0/2/2/2
13	CLA	2	503	12	1/1/15/20	9/37/115/115	-
13	CLA	A	1122	1	1/1/14/20	14/31/109/115	-
13	CLA	e	1137	1	1/1/15/20	19/37/115/115	-
13	CLA	A	1108	1	1/1/12/20	16/24/102/115	-
13	CLA	3	518	12	1/1/13/20	10/25/103/115	-
17	LHG	B	1855	-	-	28/48/48/53	-
13	CLA	4	512	12	1/1/11/20	3/13/91/115	-
13	CLA	d	512	12	1/1/11/20	6/13/91/115	-
13	CLA	G	1117	1	1/1/15/20	12/37/115/115	-
13	CLA	d	504	-	1/1/11/20	6/13/91/115	-
13	CLA	f	1226	2	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	f	1220	2	1/1/13/20	9/25/103/115	-
13	CLA	3	511	12	1/1/12/20	5/19/97/115	-
13	CLA	4	510	12	1/1/12/20	5/19/97/115	-
13	CLA	Y	509	12	1/1/15/20	6/37/115/115	-
13	CLA	e	1126	1	1/1/15/20	18/37/115/115	-
13	CLA	v	512	12	1/1/11/20	6/13/91/115	-
20	SQD	B	1852	-	-	19/40/60/69	0/1/1/1
13	CLA	B	1230	2	1/1/14/20	10/31/109/115	-
16	BCR	K	4104	-	-	2/29/63/63	0/2/2/2
16	BCR	j	4016	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1204	2	1/1/15/20	12/37/115/115	-
13	CLA	5	513	12	1/1/11/20	4/13/91/115	-
13	CLA	G	1140	1	1/1/15/20	11/37/115/115	-
13	CLA	e	1105	1	1/1/13/20	6/25/103/115	-
16	BCR	f	4009	-	-	1/29/63/63	0/2/2/2
13	CLA	l	517	-	1/1/11/20	4/13/91/115	-
13	CLA	H	1023	-	1/1/15/20	10/37/115/115	-
16	BCR	u	521	-	-	7/29/63/63	0/2/2/2
13	CLA	G	1135	1	1/1/12/20	10/22/100/115	-
16	BCR	R	4016	-	-	2/29/63/63	0/2/2/2
16	BCR	u	523	-	-	4/29/63/63	0/2/2/2
16	BCR	v	521	-	-	5/29/63/63	0/2/2/2
13	CLA	t	510	12	1/1/12/20	5/19/97/115	-
13	CLA	H	1221	21	1/1/15/20	14/37/115/115	-
13	CLA	H	1222	21	1/1/14/20	7/31/109/115	-
13	CLA	b	511	12	1/1/11/20	3/13/91/115	-
17	LHG	e	5001	-	-	25/53/53/53	-
13	CLA	l	506	12	1/1/11/20	6/13/91/115	-
16	BCR	H	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	a	504	-	1/1/11/20	6/13/91/115	-
19	LMG	f	5002	-	-	24/49/69/70	0/1/1/1
13	CLA	d	519	12	1/1/11/20	6/15/93/115	-
13	CLA	q	517	-	1/1/11/20	4/13/91/115	-
16	BCR	q	522	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	1	504	-	1/1/11/20	5/13/91/115	-
13	CLA	m	1103	9	1/1/12/20	7/19/97/115	-
13	CLA	H	1021	2	1/1/15/20	11/37/115/115	-
13	CLA	f	1213	2	1/1/15/20	14/37/115/115	-
13	CLA	A	1112	1	1/1/12/20	3/19/97/115	-
13	CLA	4	501	12	1/1/14/20	12/31/109/115	-
13	CLA	u	501	12	1/1/15/20	19/37/115/115	-
13	CLA	3	504	-	1/1/11/20	6/13/91/115	-
16	BCR	L	4022	-	-	2/29/63/63	0/2/2/2
18	LMU	Z	901	-	-	8/14/34/61	0/1/1/2
16	BCR	2	521	-	-	4/29/63/63	0/2/2/2
13	CLA	c	509	12	1/1/15/20	12/37/115/115	-
16	BCR	3	521	-	-	7/29/63/63	0/2/2/2
13	CLA	G	1112	1	1/1/12/20	3/19/97/115	-
16	BCR	c	524	-	-	2/29/63/63	0/2/2/2
16	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
18	LMU	T	5105	-	-	8/13/33/61	0/1/1/2
13	CLA	n	1503	21	1/1/14/20	10/31/109/115	-
13	CLA	4	517	-	1/1/11/20	5/13/91/115	-
13	CLA	G	1103	1	1/1/15/20	20/37/115/115	-
13	CLA	H	1216	21	1/1/14/20	5/31/109/115	-
13	CLA	u	517	-	1/1/11/20	9/13/91/115	-
16	BCR	f	4004	-	-	8/29/63/63	0/2/2/2
13	CLA	c	510	12	1/1/11/20	7/13/91/115	-
13	CLA	L	1503	21	1/1/14/20	10/31/109/115	-
16	BCR	L	4019	-	-	6/29/63/63	0/2/2/2
13	CLA	b	509	12	1/1/15/20	7/37/115/115	-
13	CLA	V	1503	21	1/1/14/20	10/31/109/115	-
13	CLA	G	1131	1	1/1/15/20	6/37/115/115	-
17	LHG	H	1842	13	-	22/43/43/53	-
13	CLA	t	502	12	1/1/12/20	5/19/97/115	-
16	BCR	d	522	-	-	5/29/63/63	0/2/2/2
17	LHG	k	5001	-	-	22/48/48/53	-
20	SQD	Y	822	-	-	20/43/63/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	4	509	12	1/1/15/20	7/37/115/115	-
13	CLA	f	1224	2	1/1/14/20	13/31/109/115	-
13	CLA	c	511	12	1/1/13/20	5/25/103/115	-
18	LMU	r	901	-	-	8/14/34/61	0/1/1/2
13	CLA	6	501	12	1/1/14/20	16/31/109/115	-
16	BCR	Z	521	-	-	4/29/63/63	0/2/2/2
13	CLA	f	1240	17	-	13/37/115/115	-
13	CLA	6	510	12	1/1/11/20	7/13/91/115	-
13	CLA	H	1207	2	1/1/15/20	14/37/115/115	-
16	BCR	T	4012	-	-	9/29/63/63	0/2/2/2
15	SF4	C	3002	3	-	-	0/6/5/5
13	CLA	e	1132	1	1/1/15/20	15/37/115/115	-
16	BCR	e	4003	-	-	0/29/63/63	0/2/2/2
13	CLA	r	506	12	1/1/13/20	8/25/103/115	-
13	CLA	l	513	12	1/1/13/20	2/25/103/115	-
13	CLA	c	513	12	1/1/11/20	4/13/91/115	-
20	SQD	n	5216	-	-	17/46/66/69	0/1/1/1
13	CLA	6	517	-	1/1/11/20	9/13/91/115	-
19	LMG	T	5104	-	-	17/30/50/70	0/1/1/1
20	SQD	c	822	-	-	7/24/44/69	0/1/1/1
16	BCR	l	4015	-	-	5/29/63/63	0/2/2/2
13	CLA	Z	507	-	1/1/15/20	14/37/115/115	-
13	CLA	s	509	12	1/1/15/20	4/37/115/115	-
13	CLA	B	1228	2	1/1/13/20	8/25/103/115	-
19	LMG	B	5002	-	-	24/49/69/70	0/1/1/1
13	CLA	l	510	12	1/1/15/20	11/37/115/115	-
13	CLA	e	1125	1	1/1/15/20	14/37/115/115	-
13	CLA	G	1102	1	1/1/15/20	11/37/115/115	-
13	CLA	R	1301	21	1/1/15/20	11/37/115/115	-
13	CLA	e	1013	-	1/1/15/20	11/37/115/115	-
16	BCR	A	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	t	508	12	1/1/11/20	4/13/91/115	-
13	CLA	H	1225	2	1/1/15/20	7/37/115/115	-
13	CLA	e	1107	1	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	G	1111	1	1/1/15/20	14/37/115/115	-
13	CLA	6	507	-	1/1/11/20	4/13/91/115	-
18	LMU	J	5105	-	-	8/13/33/61	0/1/1/2
13	CLA	1	511	12	1/1/13/20	4/25/103/115	-
13	CLA	e	1104	1	1/1/15/20	12/37/115/115	-
13	CLA	f	1229	2	1/1/15/20	13/37/115/115	-
13	CLA	6	506	12	1/1/11/20	5/13/91/115	-
13	CLA	3	509	12	1/1/15/20	4/37/115/115	-
13	CLA	s	519	12	1/1/13/20	8/25/103/115	-
13	CLA	d	503	12	1/1/12/20	8/22/100/115	-
13	CLA	v	503	12	1/1/12/20	8/22/100/115	-
13	CLA	s	513	12	1/1/15/20	13/37/115/115	-
13	CLA	3	508	12	1/1/13/20	7/25/103/115	-
13	CLA	H	1226	2	1/1/15/20	12/37/115/115	-
20	SQD	V	5216	-	-	17/46/66/69	0/1/1/1
13	CLA	f	1235	2	1/1/15/20	6/37/115/115	-
13	CLA	G	1115	1	1/1/14/20	10/31/109/115	-
13	CLA	4	518	12	1/1/13/20	8/25/103/115	-
13	CLA	A	1129	1	1/1/12/20	5/21/99/115	-
13	CLA	B	1212	2	1/1/13/20	11/25/103/115	-
13	CLA	4	511	12	1/1/11/20	3/13/91/115	-
13	CLA	A	1120	1	1/1/12/20	4/23/101/115	-
13	CLA	B	1023	-	1/1/15/20	10/37/115/115	-
13	CLA	H	1208	2	1/1/15/20	15/37/115/115	-
13	CLA	H	1228	2	1/1/13/20	8/25/103/115	-
13	CLA	f	1210	2	1/1/15/20	19/37/115/115	-
13	CLA	H	1229	2	1/1/15/20	13/37/115/115	-
13	CLA	c	505	12	1/1/14/20	16/33/111/115	-
13	CLA	f	1212	2	1/1/13/20	11/25/103/115	-
13	CLA	G	1129	1	1/1/12/20	5/21/99/115	-
13	CLA	u	507	-	1/1/11/20	5/13/91/115	-
13	CLA	B	1224	2	1/1/14/20	13/31/109/115	-
18	LMU	q	902	-	-	6/10/30/61	0/1/1/2
13	CLA	H	1202	2	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LHG	A	5002	-	-	26/43/43/53	-
17	LHG	A	5005	-	-	29/49/49/53	-
18	LMU	2	901	-	-	8/14/34/61	0/1/1/2
16	BCR	a	522	-	-	5/29/63/63	0/2/2/2
13	CLA	A	1119	21	1/1/15/20	15/37/115/115	-
13	CLA	H	1204	2	1/1/15/20	12/37/115/115	-
13	CLA	e	1123	21	1/1/15/20	11/37/115/115	-
13	CLA	A	1139	21	1/1/15/20	12/37/115/115	-
13	CLA	3	513	12	1/1/15/20	13/37/115/115	-
13	CLA	H	1234	2	1/1/15/20	13/37/115/115	-
13	CLA	a	509	12	1/1/15/20	4/37/115/115	-
16	BCR	6	524	-	-	5/29/63/63	0/2/2/2
13	CLA	G	1139	21	1/1/15/20	12/37/115/115	-
13	CLA	A	1237	21	1/1/15/20	19/37/115/115	-
13	CLA	Z	501	12	1/1/15/20	12/37/115/115	-
13	CLA	f	1217	2	1/1/13/20	12/28/106/115	-
13	CLA	f	1231	21	1/1/15/20	8/37/115/115	-
13	CLA	e	1127	1	1/1/15/20	12/37/115/115	-
13	CLA	H	1218	2	1/1/14/20	7/31/109/115	-
13	CLA	V	1502	10	1/1/15/20	8/37/115/115	-
16	BCR	v	522	-	-	5/29/63/63	0/2/2/2
16	BCR	3	522	-	-	5/29/63/63	0/2/2/2
13	CLA	K	1105	9	1/1/11/20	9/13/91/115	-
17	LHG	S	5001	-	-	22/48/48/53	-
13	CLA	v	518	12	1/1/13/20	10/25/103/115	-
13	CLA	A	1106	1	1/1/15/20	21/37/115/115	-
13	CLA	e	1129	1	1/1/12/20	5/21/99/115	-
13	CLA	A	1013	-	1/1/15/20	11/37/115/115	-
13	CLA	e	1116	1	1/1/14/20	15/31/109/115	-

The worst 5 of 4509 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	2002	PQN	C12-C13	8.71	1.53	1.33
14	f	2002	PQN	C12-C13	8.70	1.53	1.33
14	H	2002	PQN	C12-C13	8.70	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	2001	PQN	C12-C13	8.66	1.53	1.33
14	e	2001	PQN	C12-C13	8.66	1.53	1.33

The worst 5 of 7438 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	f	2002	PQN	C11-C12-C13	-9.00	111.81	126.79
14	B	2002	PQN	C11-C12-C13	-9.00	111.81	126.79
13	H	1211	CLA	C4A-NA-C1A	8.99	110.75	106.71
14	H	2002	PQN	C11-C12-C13	-8.98	111.85	126.79
13	B	1211	CLA	C4A-NA-C1A	8.88	110.70	106.71

5 of 588 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	1011	CLA	ND
13	A	1013	CLA	ND
13	A	1102	CLA	ND
13	A	1103	CLA	ND
13	A	1104	CLA	ND

5 of 8073 torsion outliers are listed below:

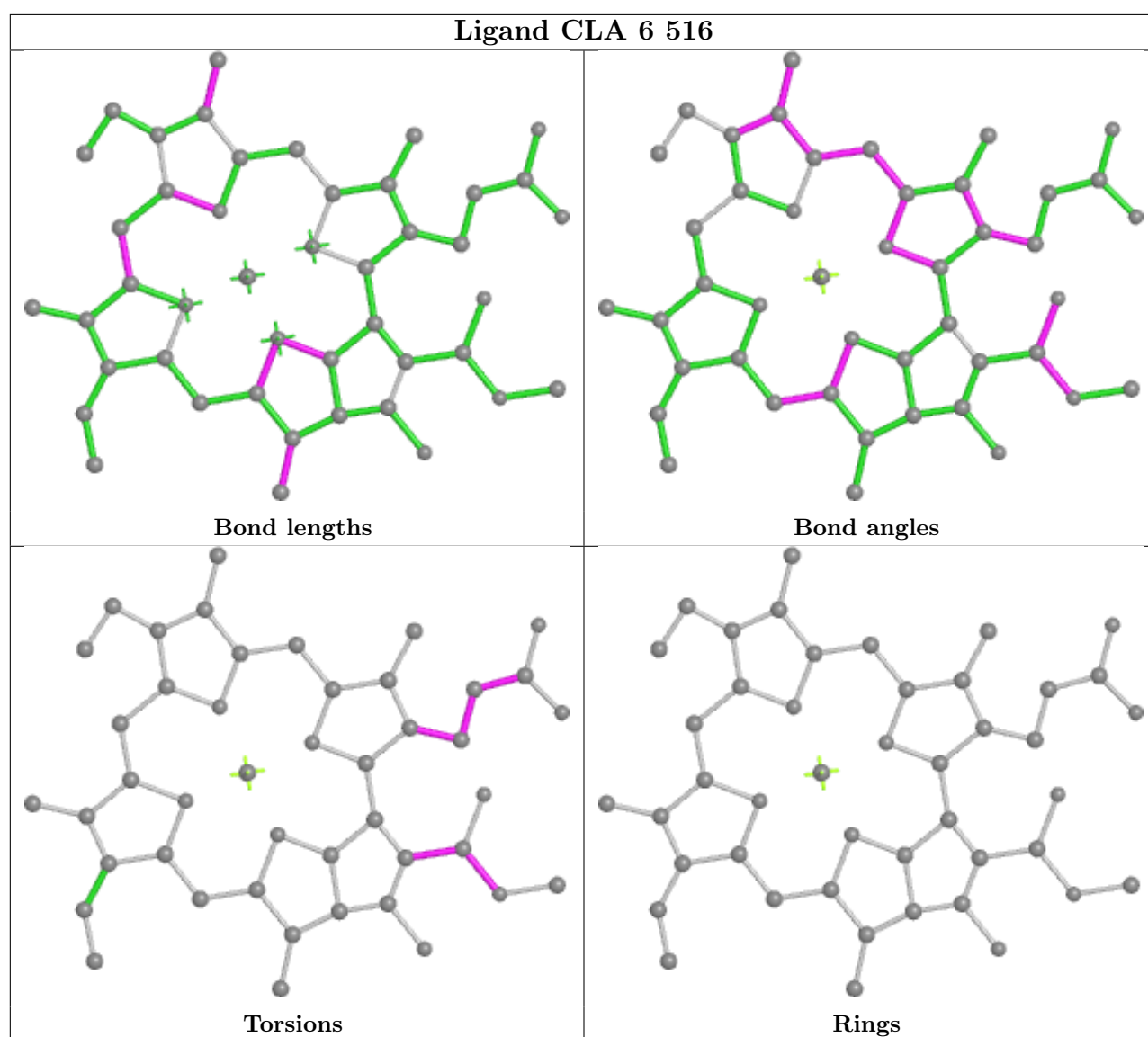
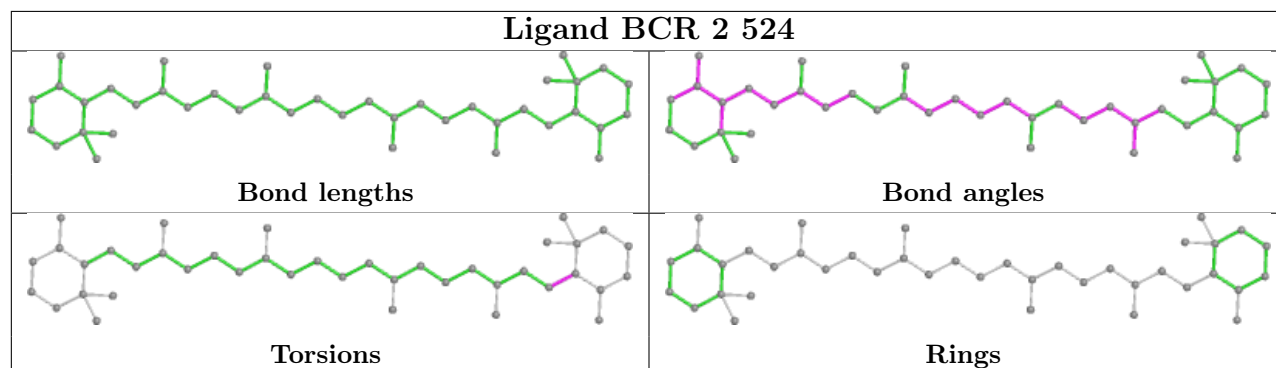
Mol	Chain	Res	Type	Atoms
13	A	1011	CLA	CHA-CBD-CGD-O1D
13	A	1102	CLA	C3A-C2A-CAA-CBA
13	A	1103	CLA	C1A-C2A-CAA-CBA
13	A	1103	CLA	CHA-CBD-CGD-O1D
13	A	1103	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

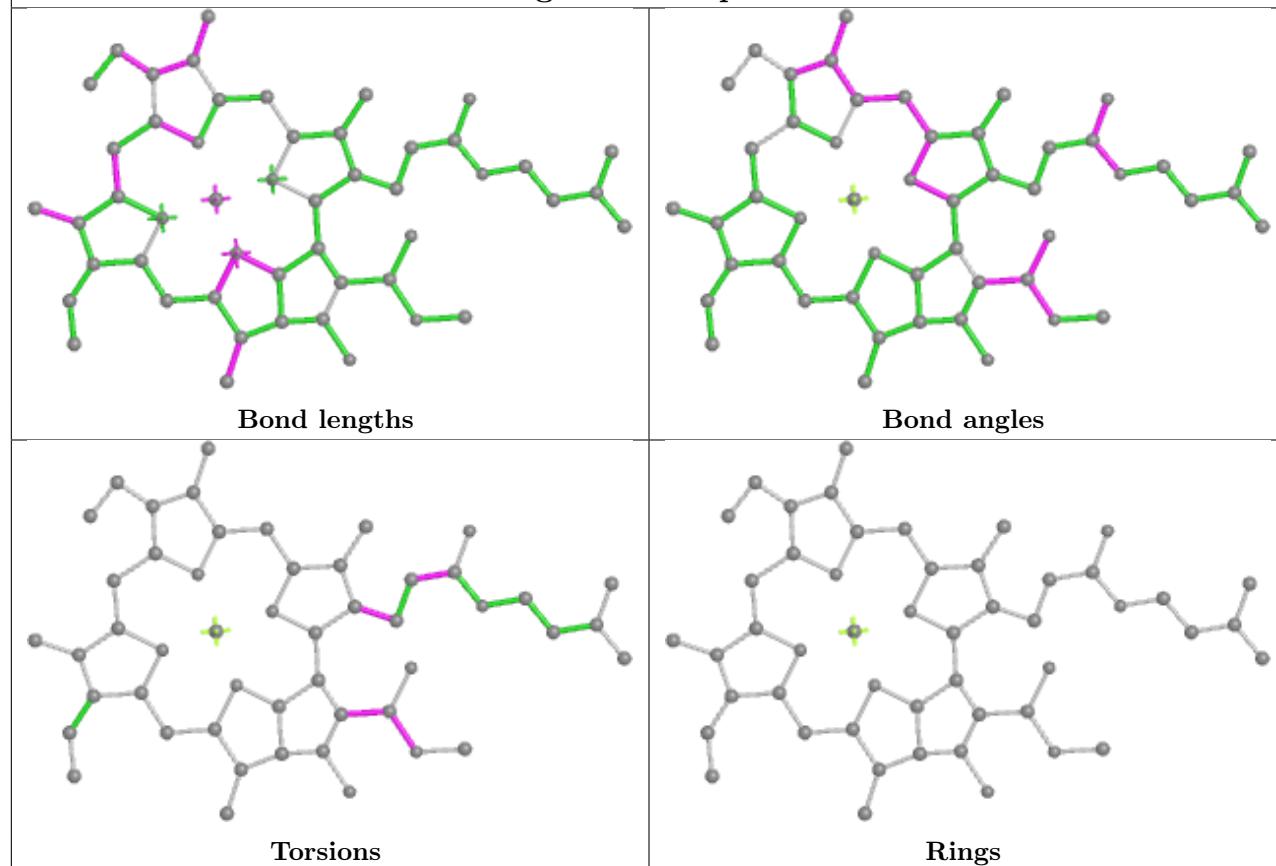
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

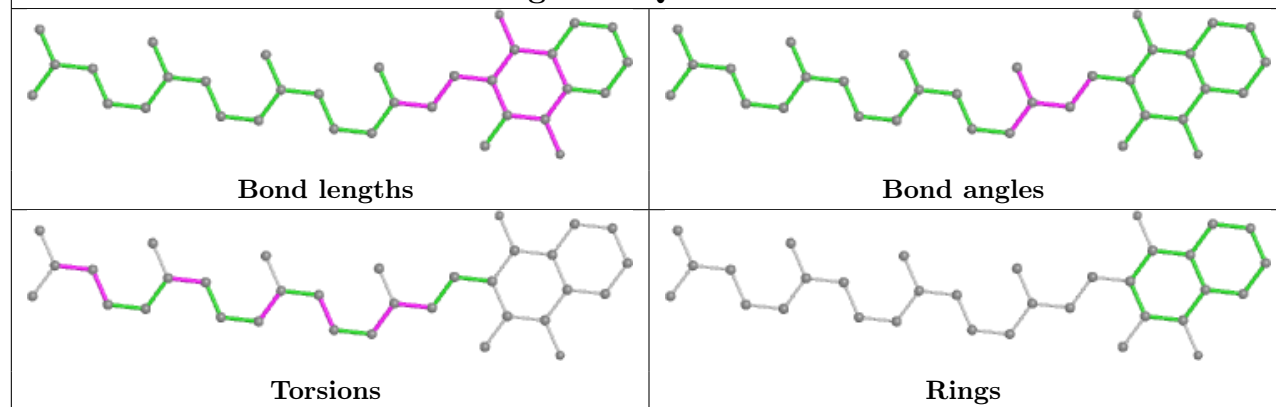
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

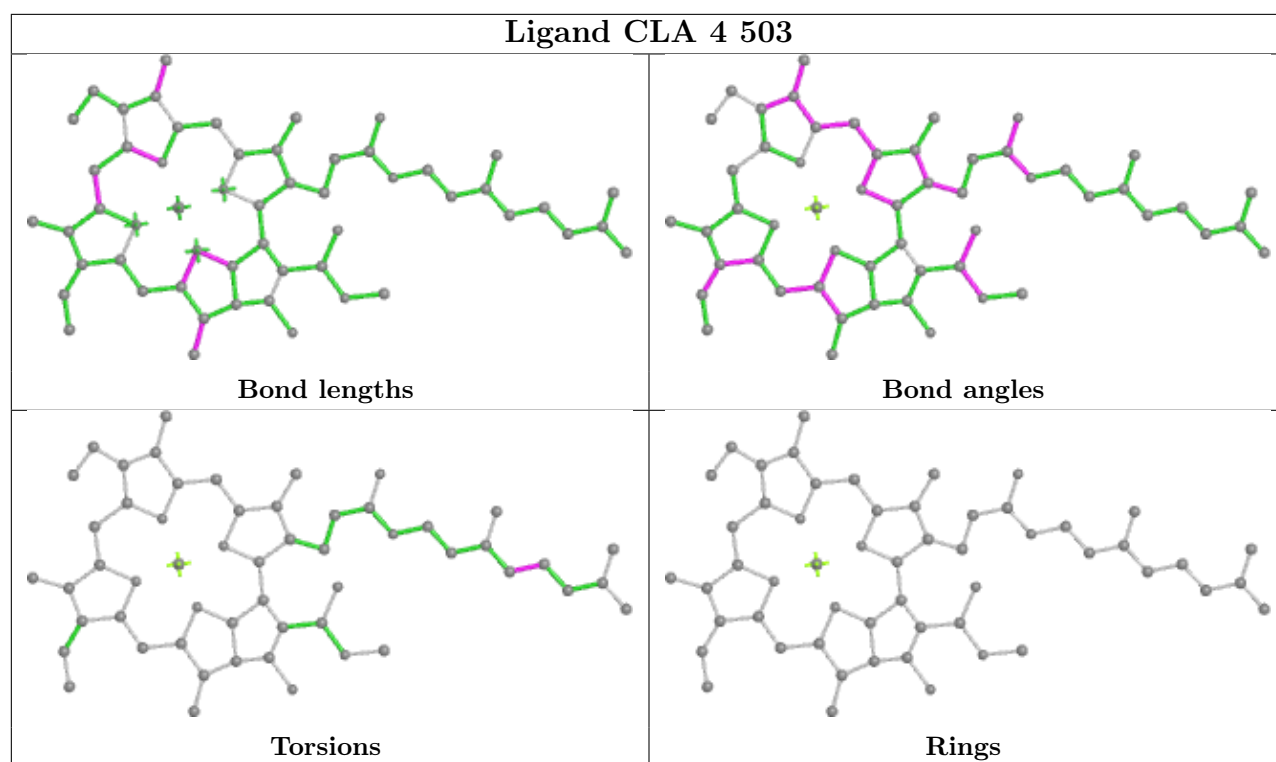


Ligand CLA q 519

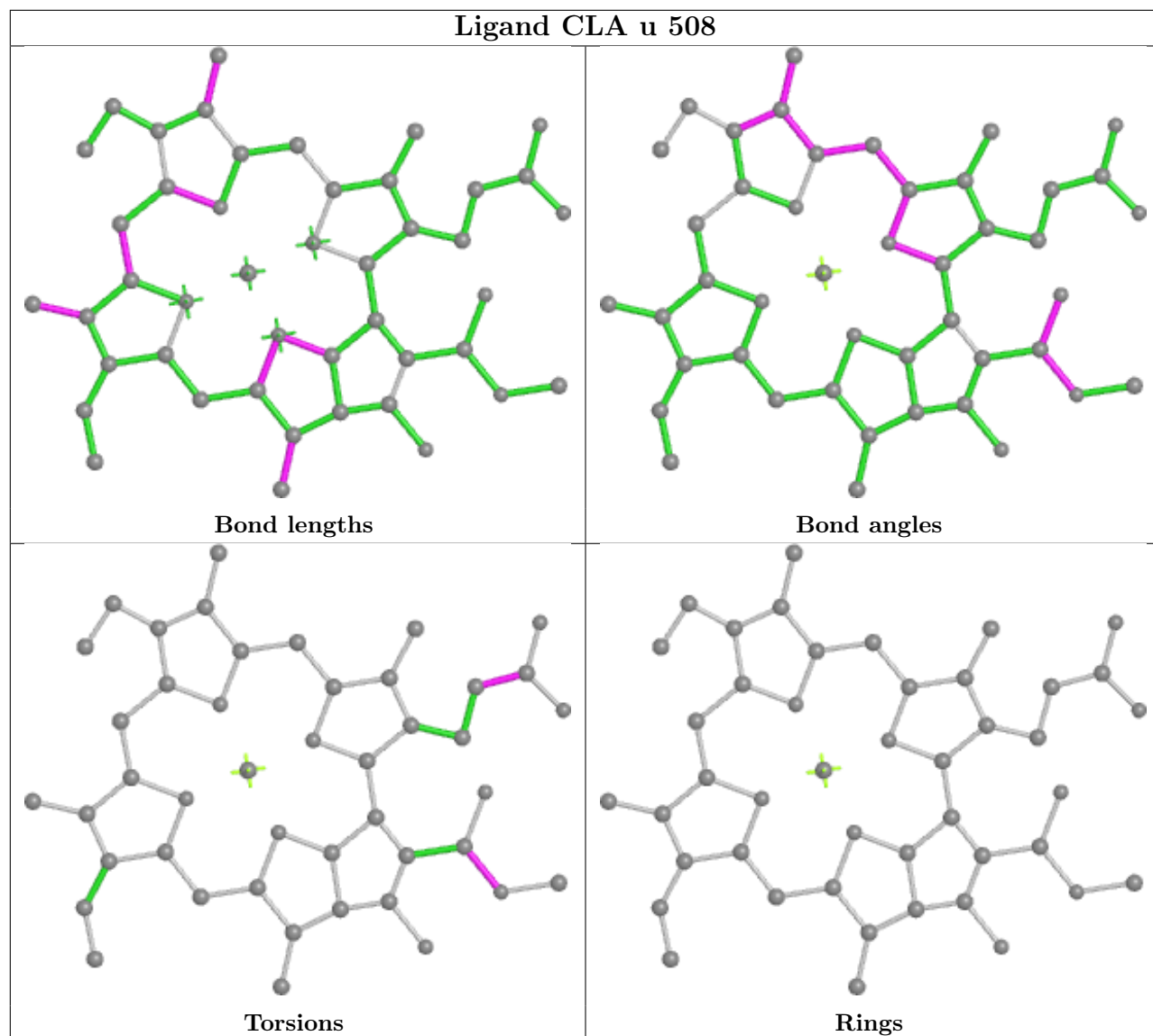


Ligand PQN f 2002

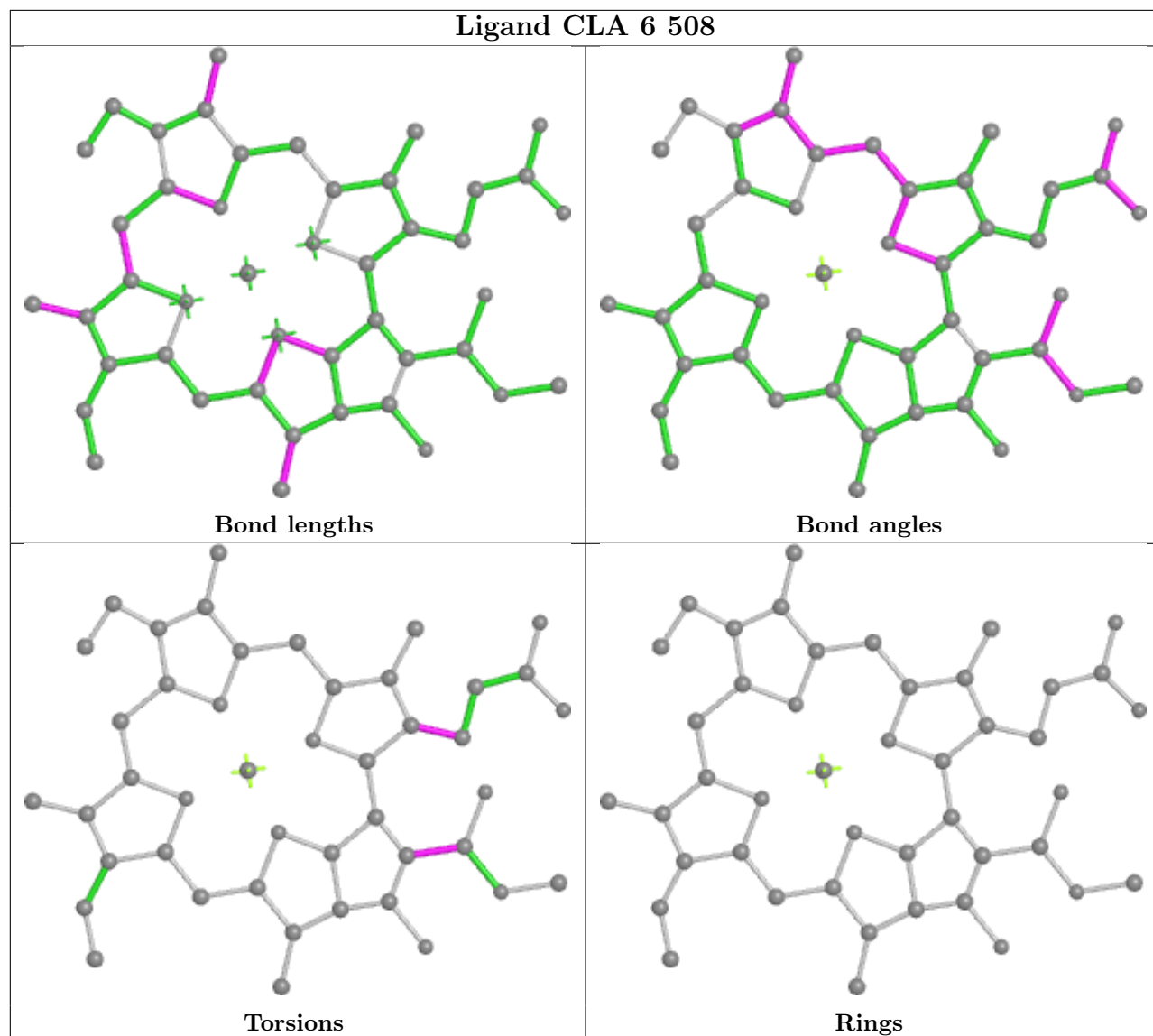


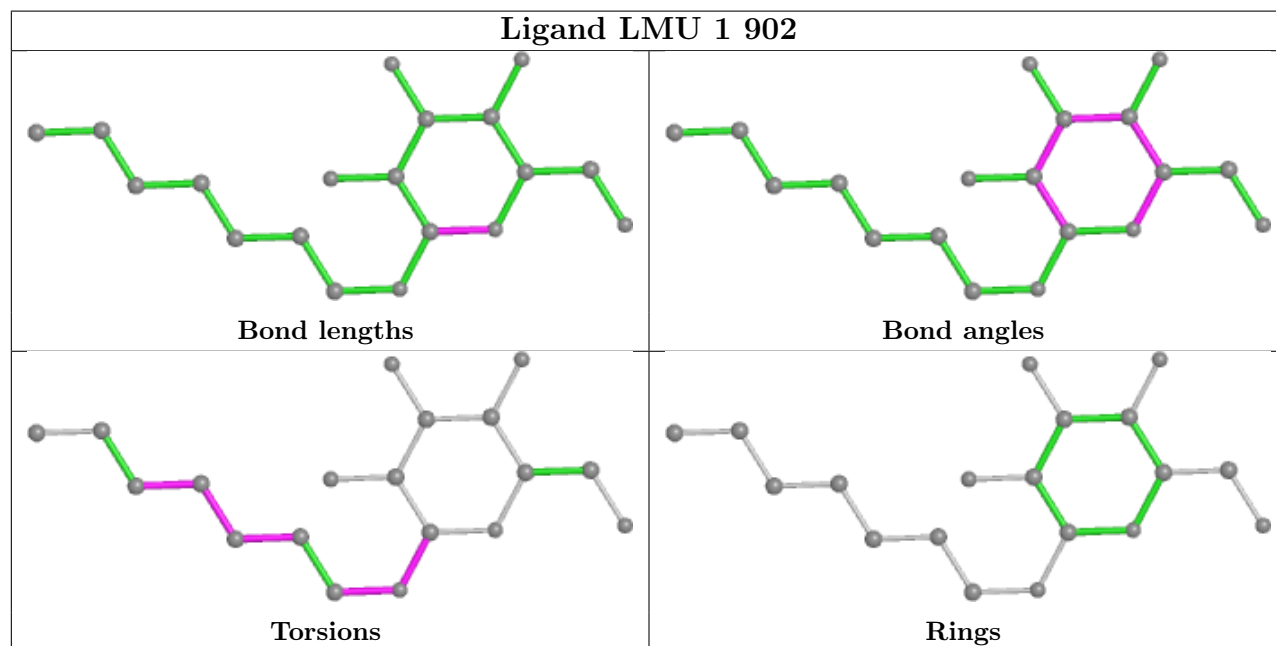
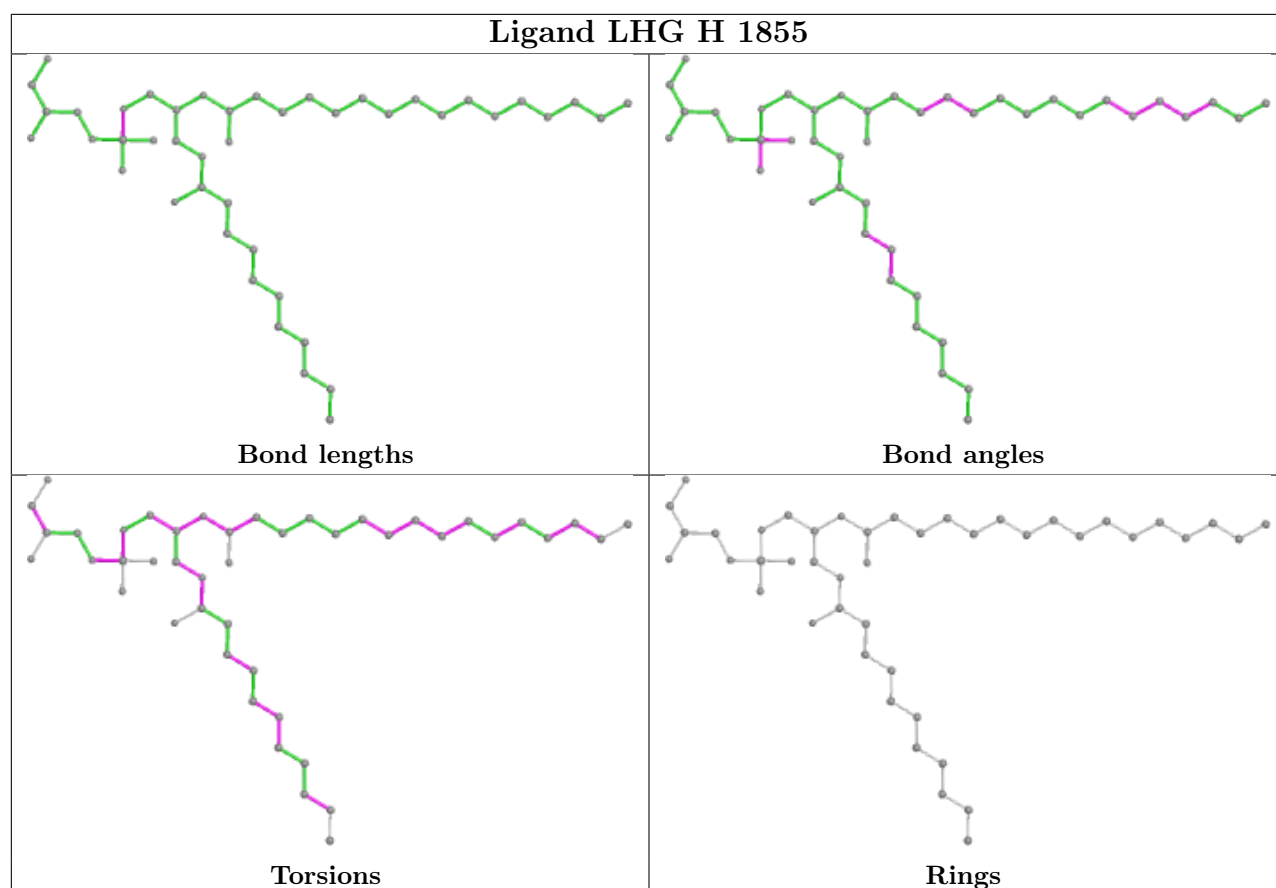


Ligand CLA u 508

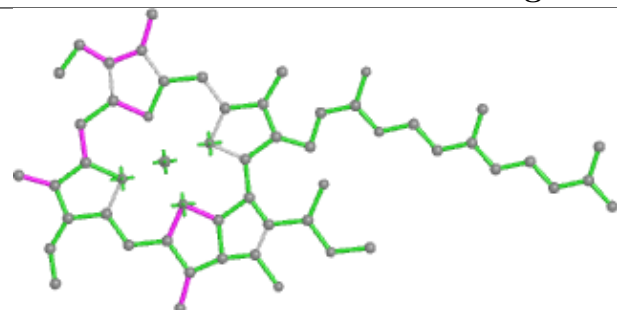


Ligand CLA 6 508

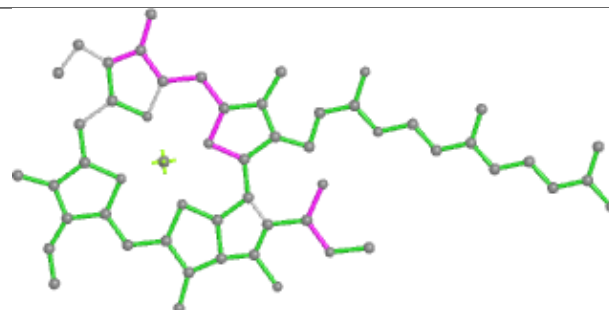




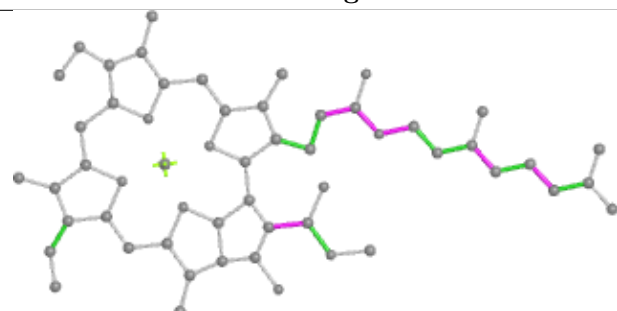
Ligand CLA t 519



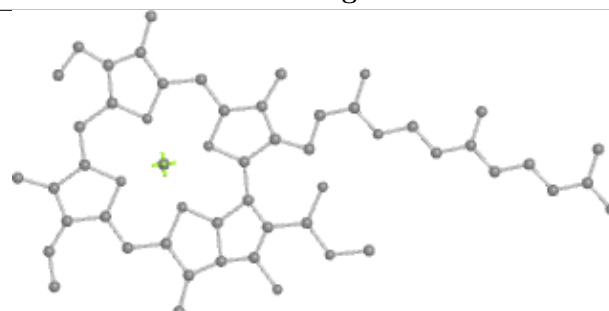
Bond lengths



Bond angles

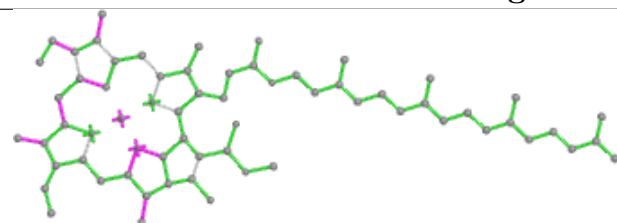


Torsions

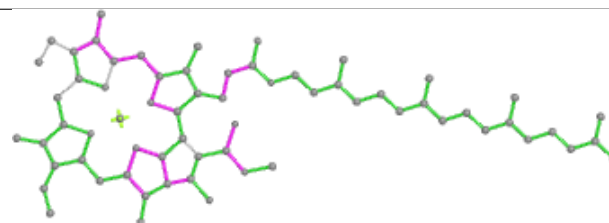


Rings

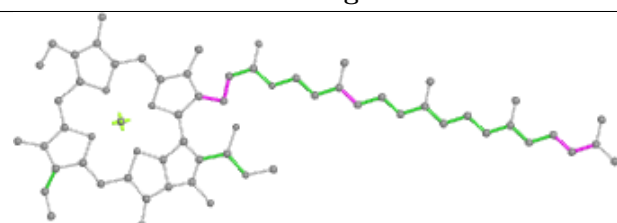
Ligand CLA G 1022



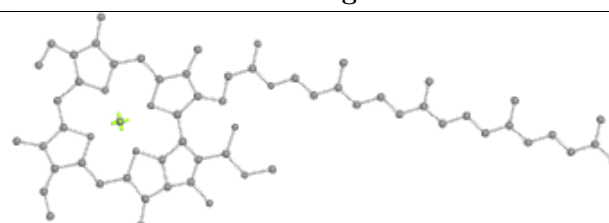
Bond lengths



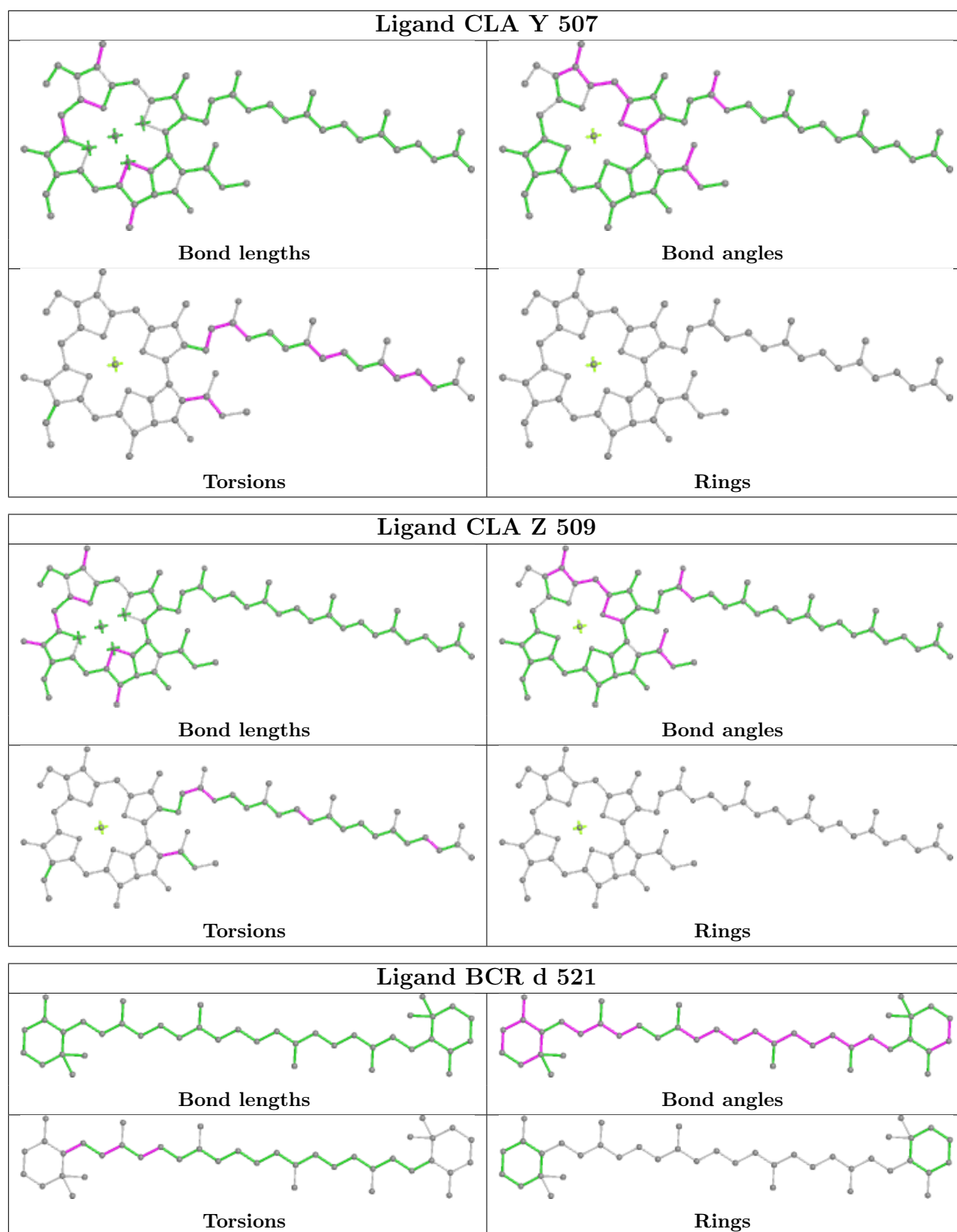
Bond angles

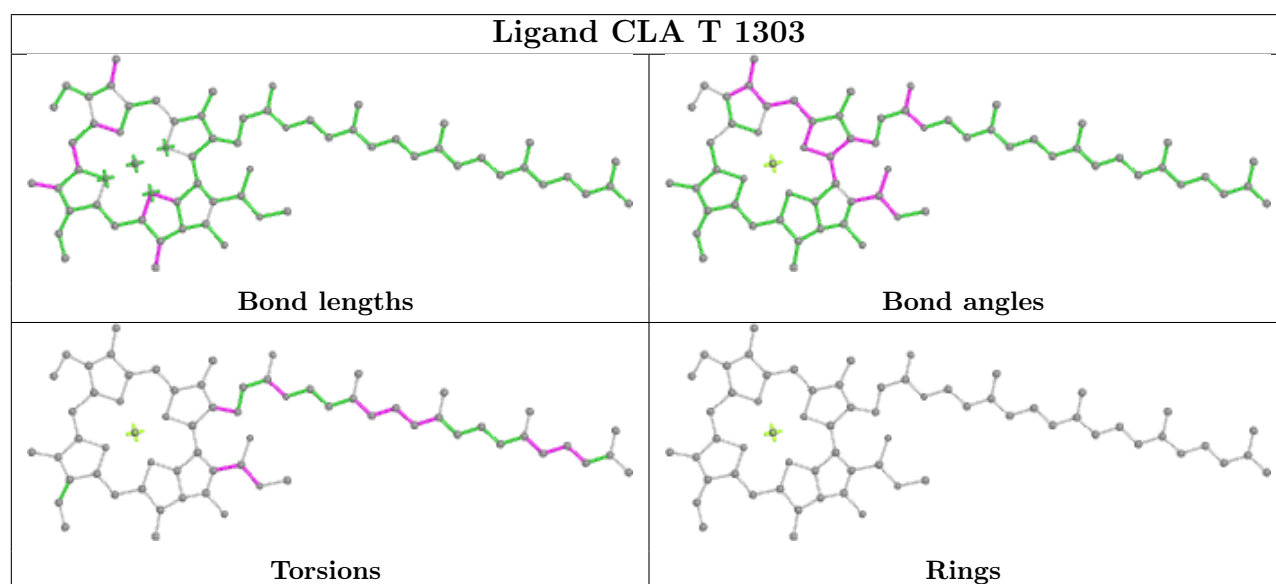
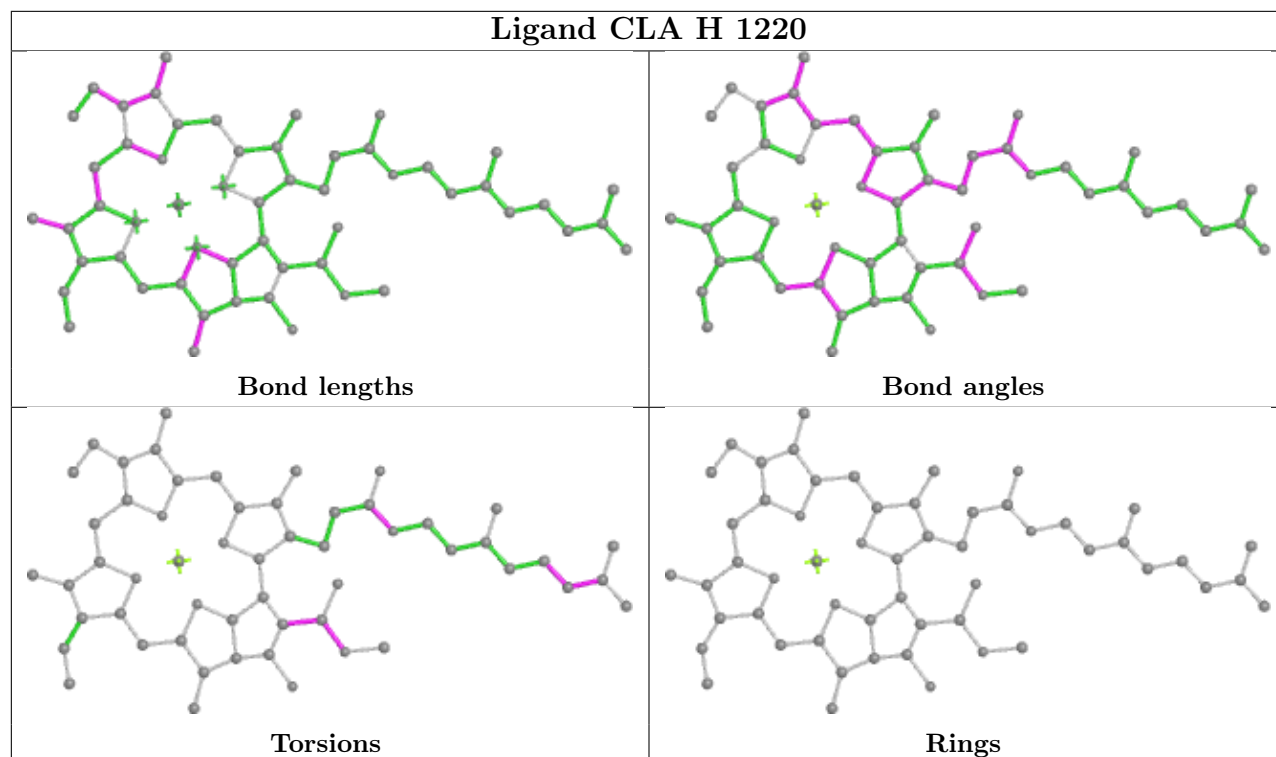
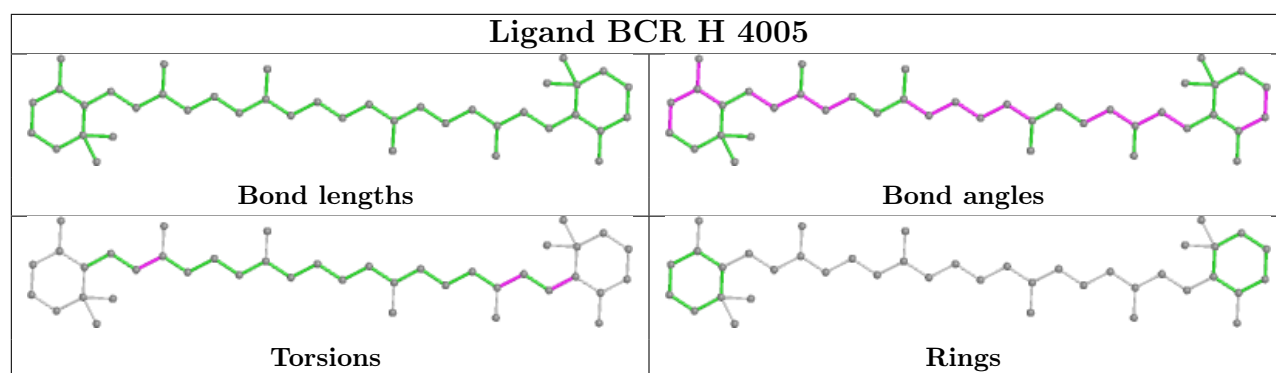


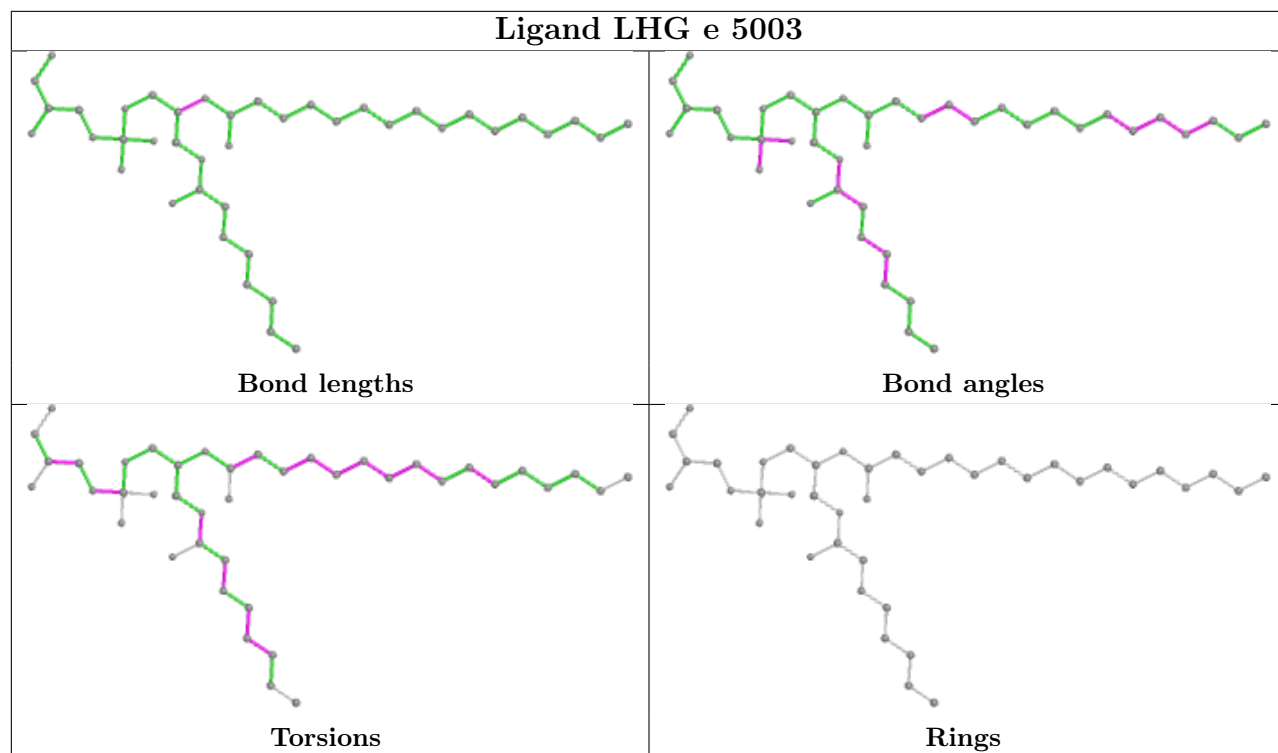
Torsions



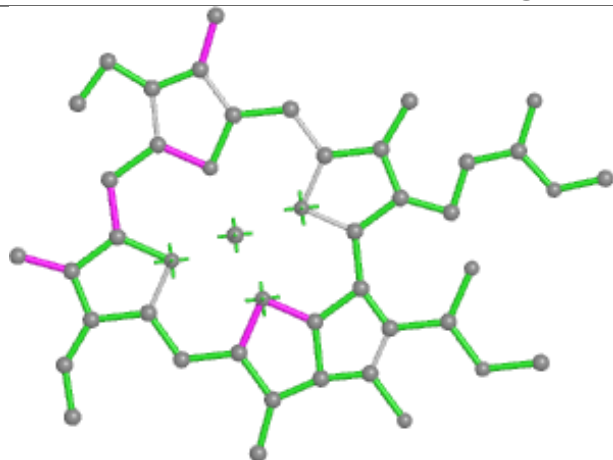
Rings



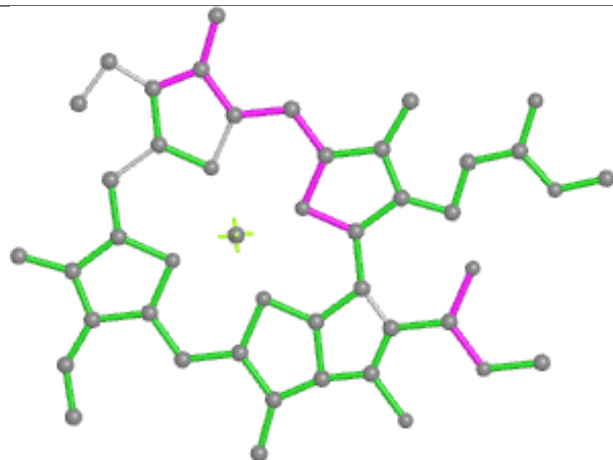




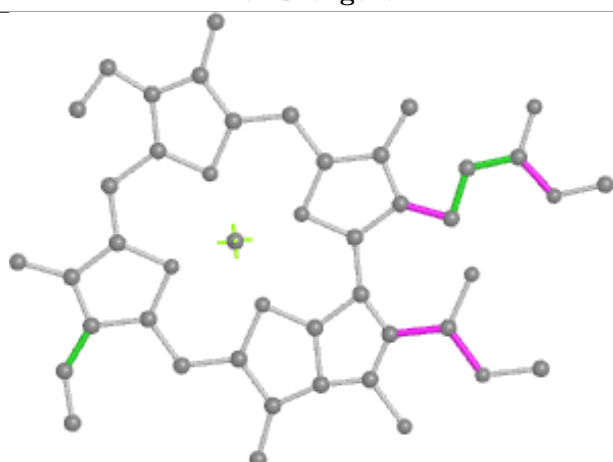
Ligand CLA v 519



Bond lengths



Bond angles

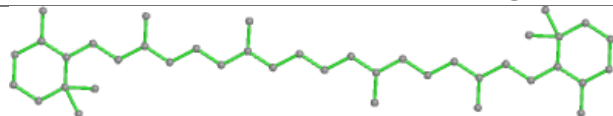


Torsions

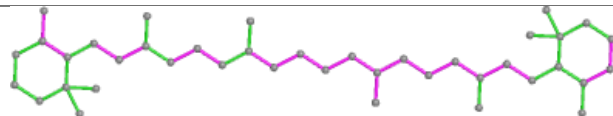


Rings

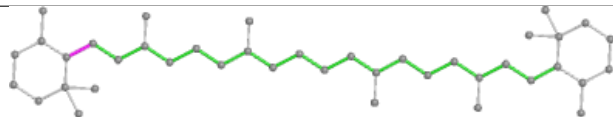
Ligand BCR L 4219



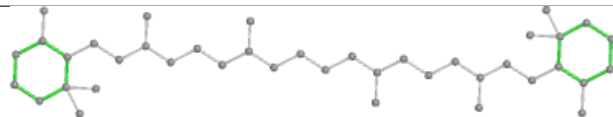
Bond lengths



Bond angles

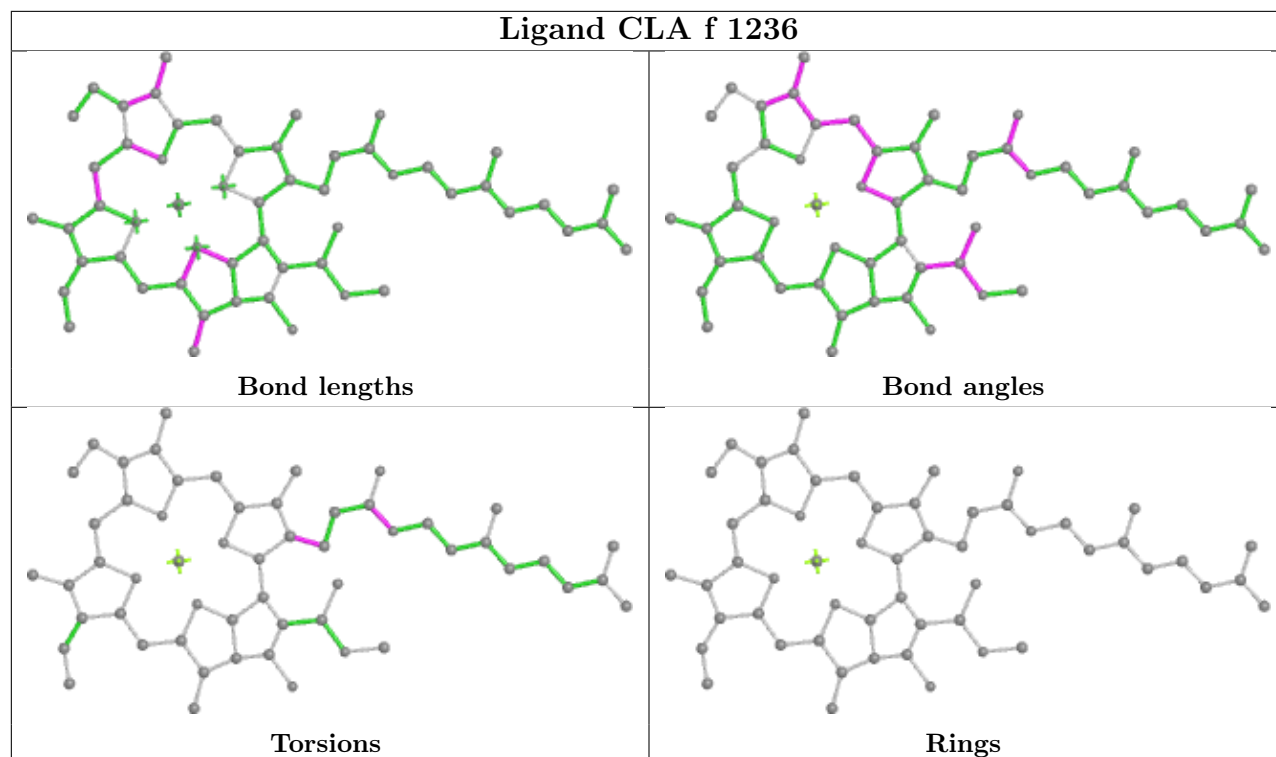


Torsions

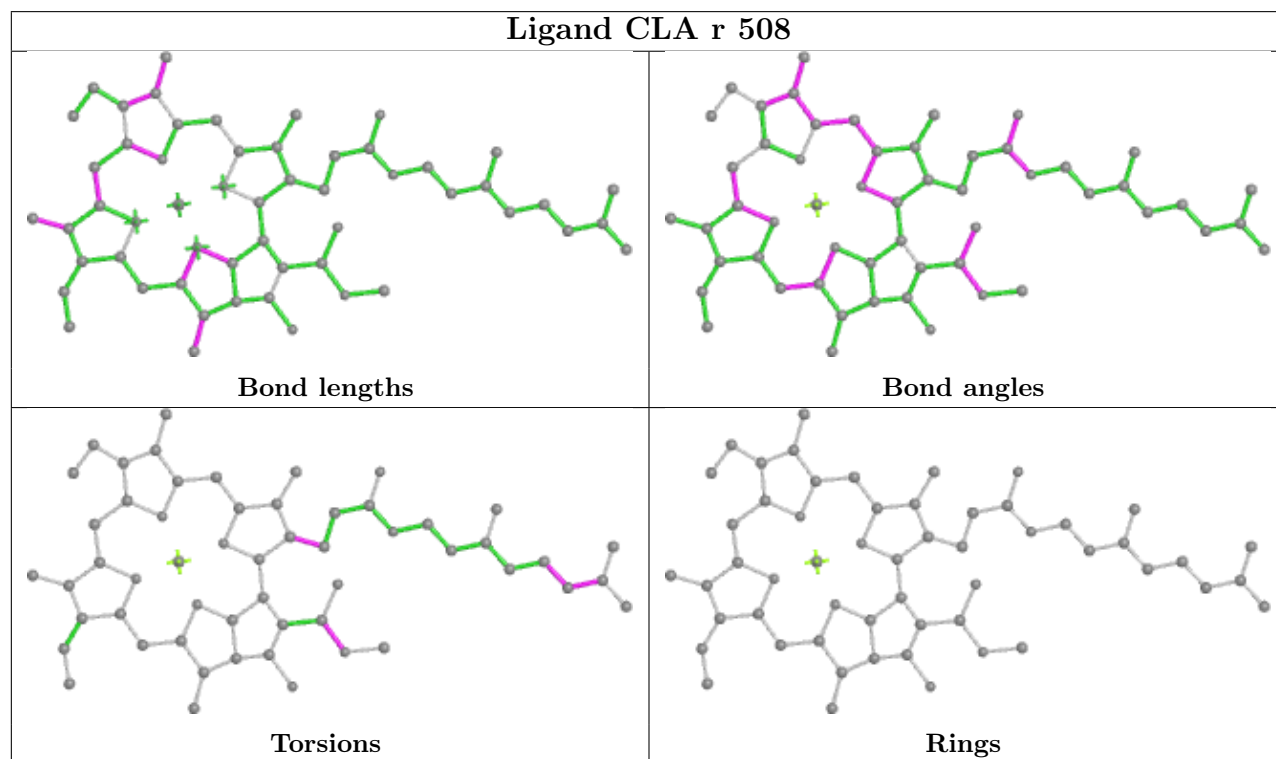


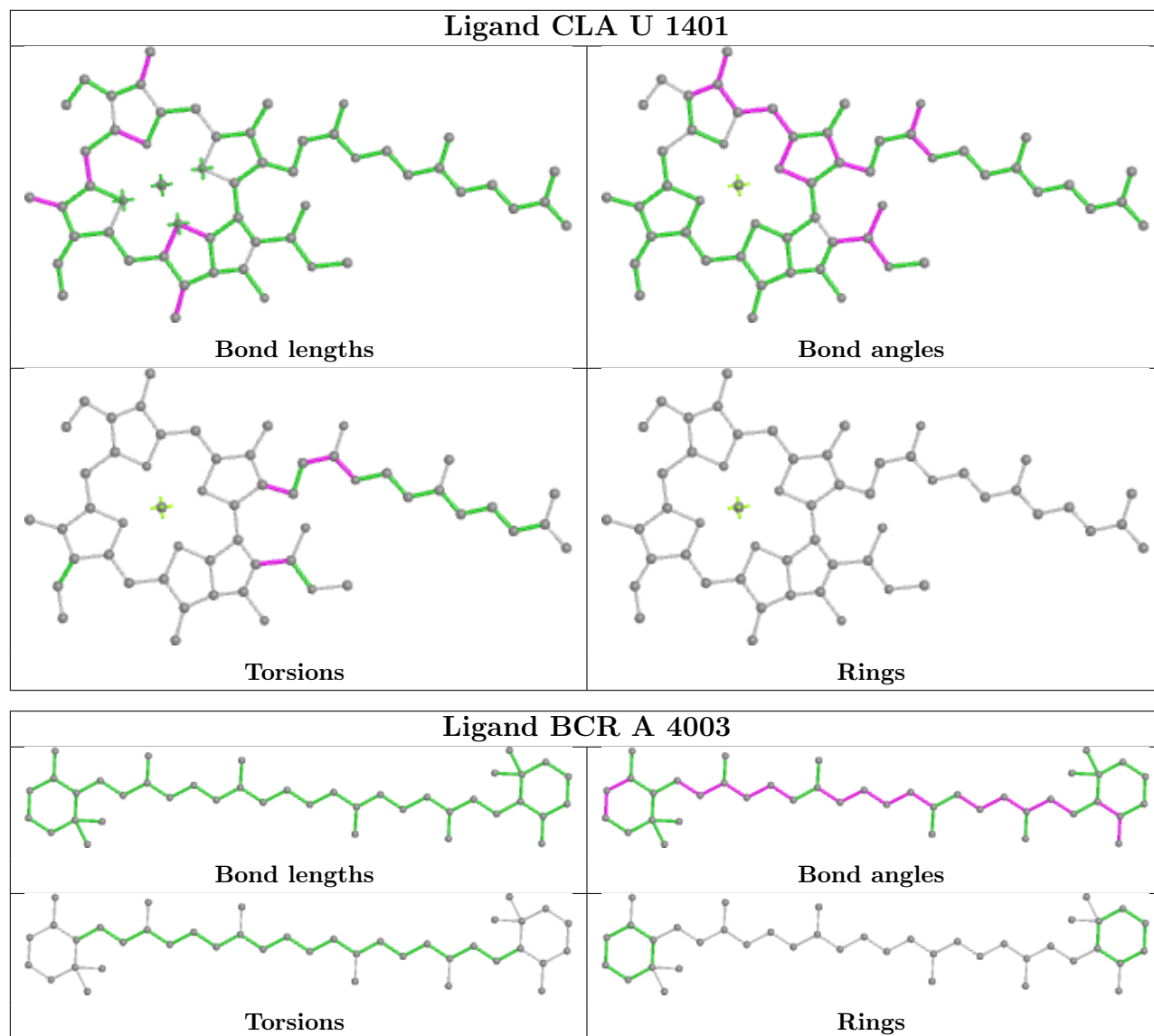
Rings

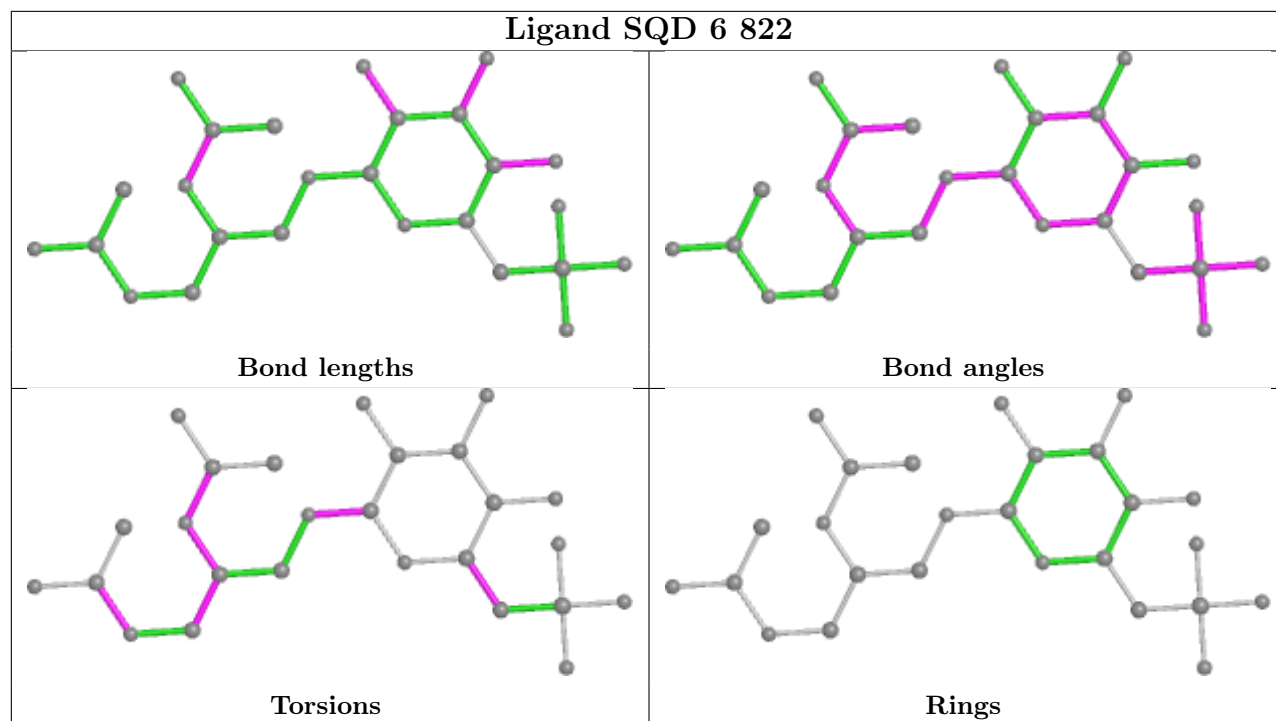
Ligand CLA f 1236



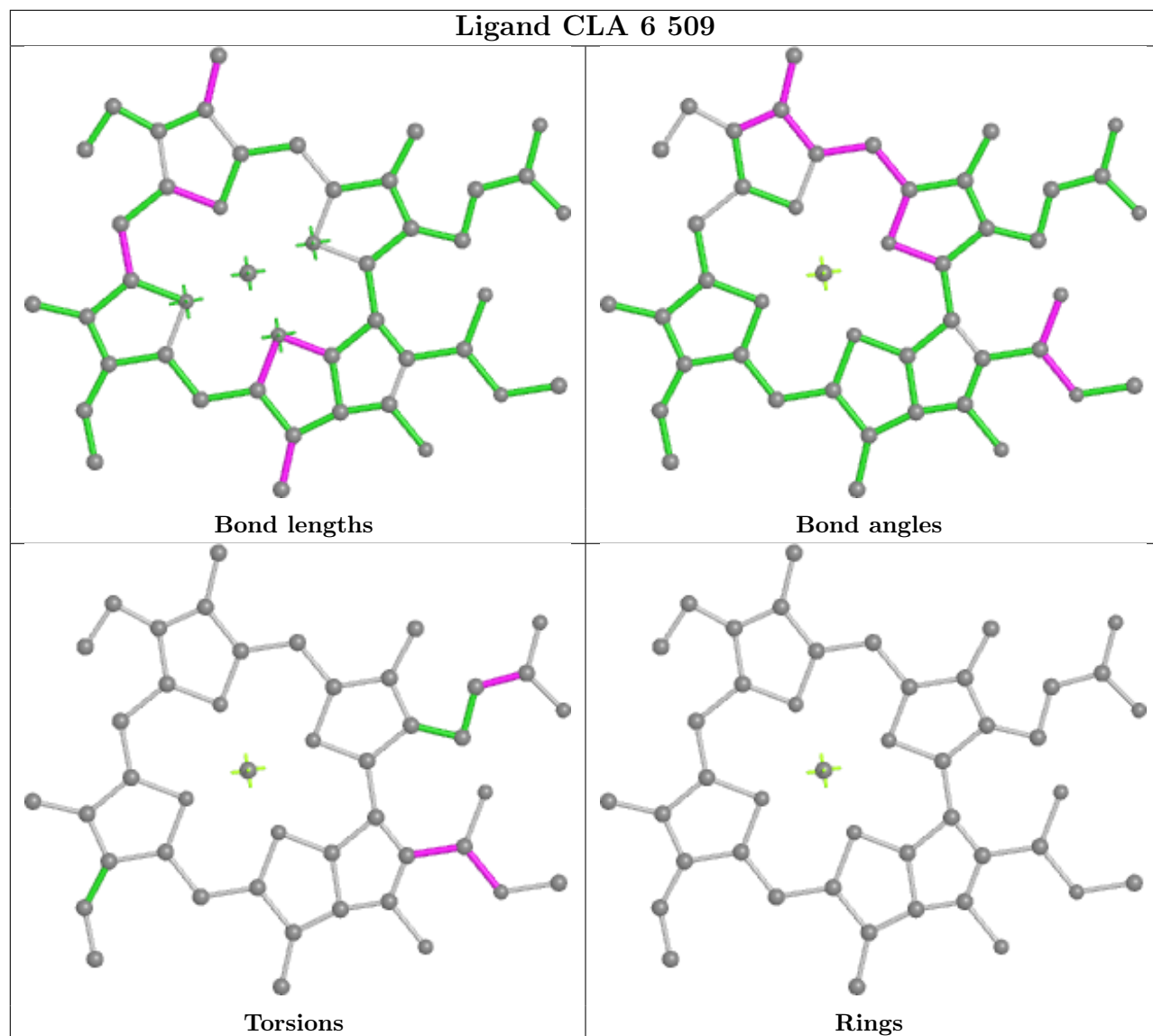
Ligand CLA r 508



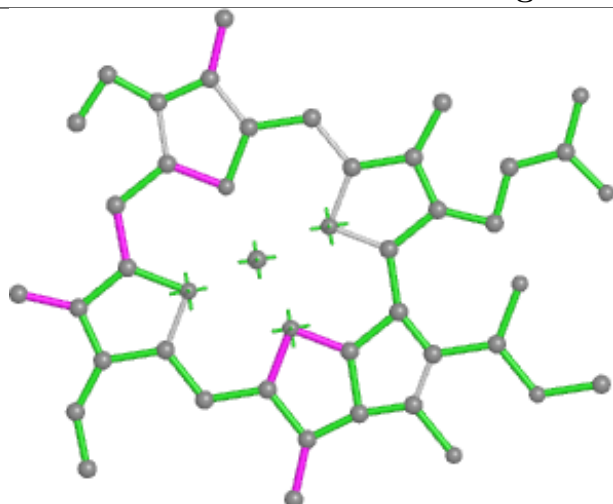




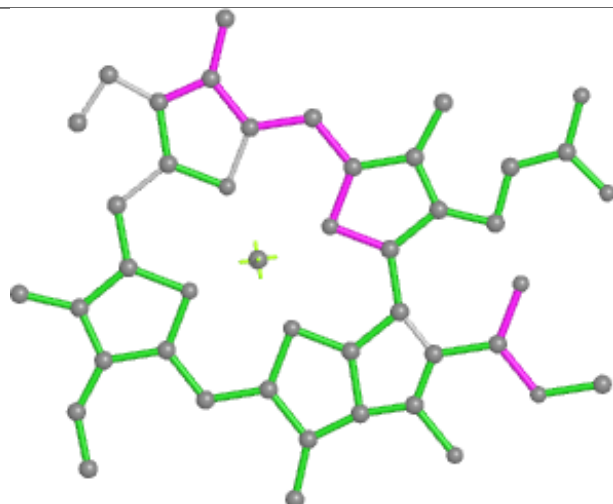
Ligand CLA 6 509



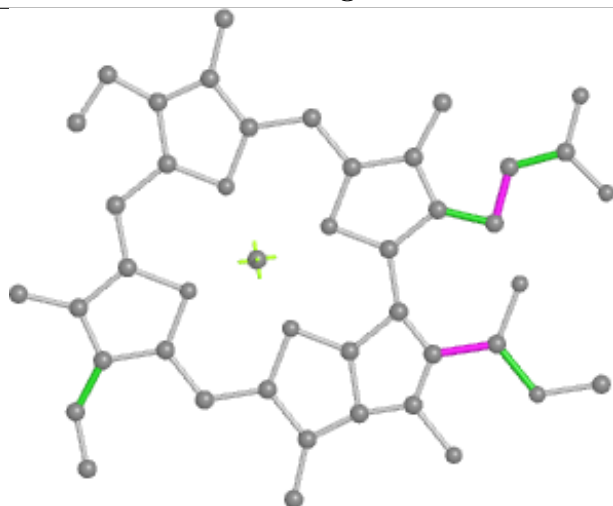
Ligand CLA Z 517



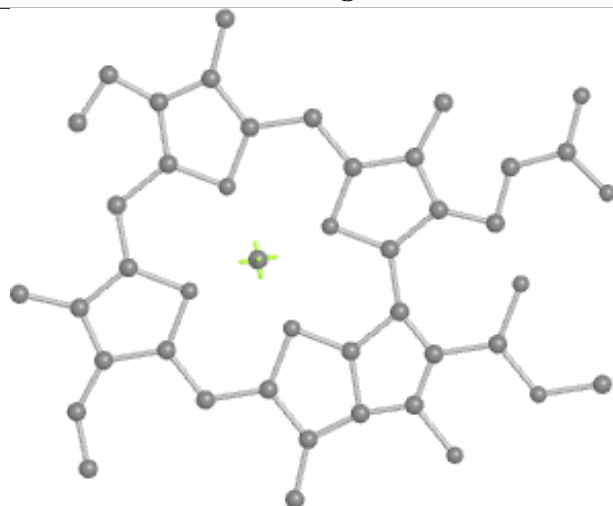
Bond lengths



Bond angles

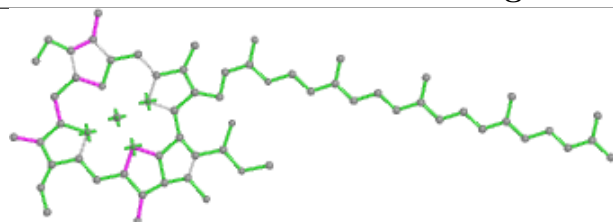


Torsions

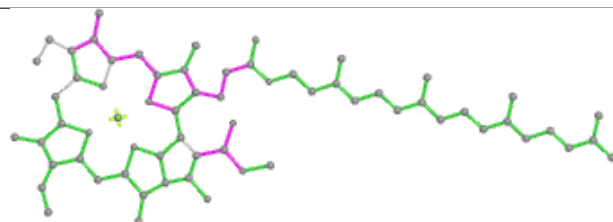


Rings

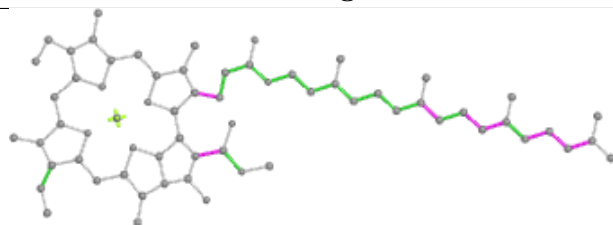
Ligand CLA A 1101



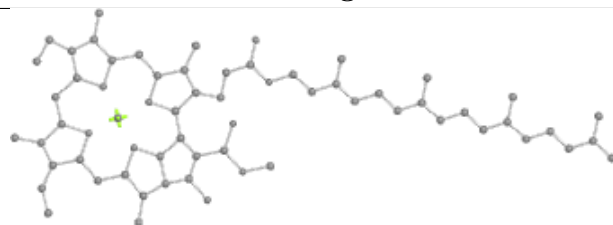
Bond lengths



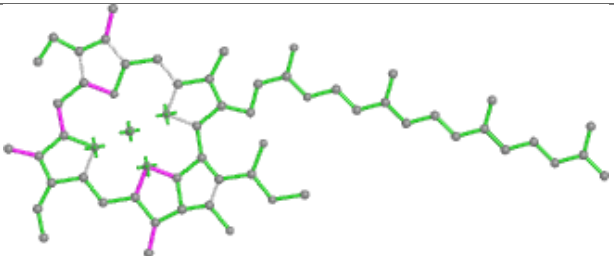
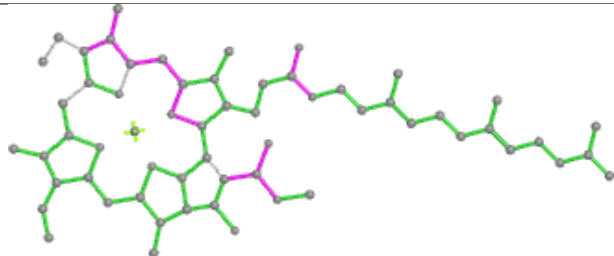
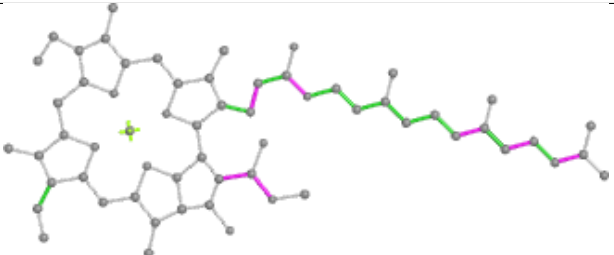
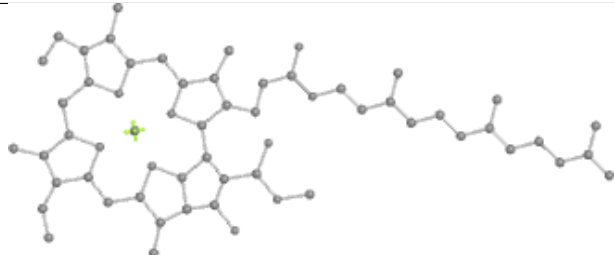
Bond angles

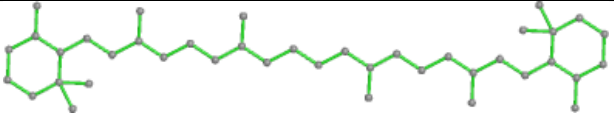
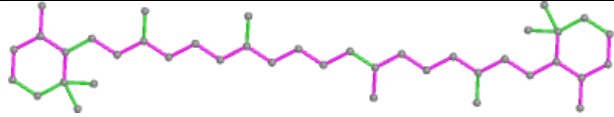
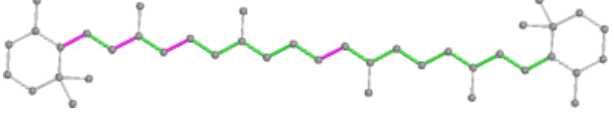
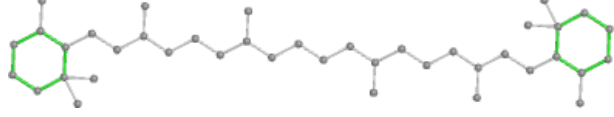


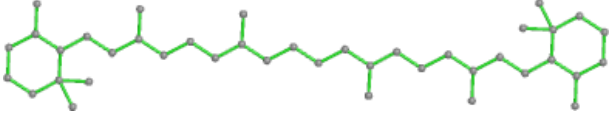
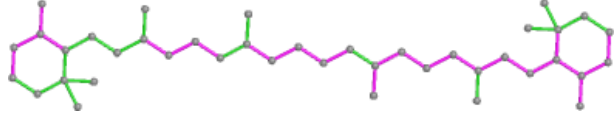
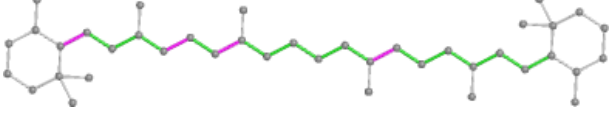
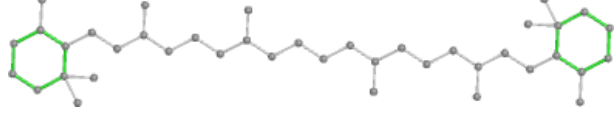
Torsions



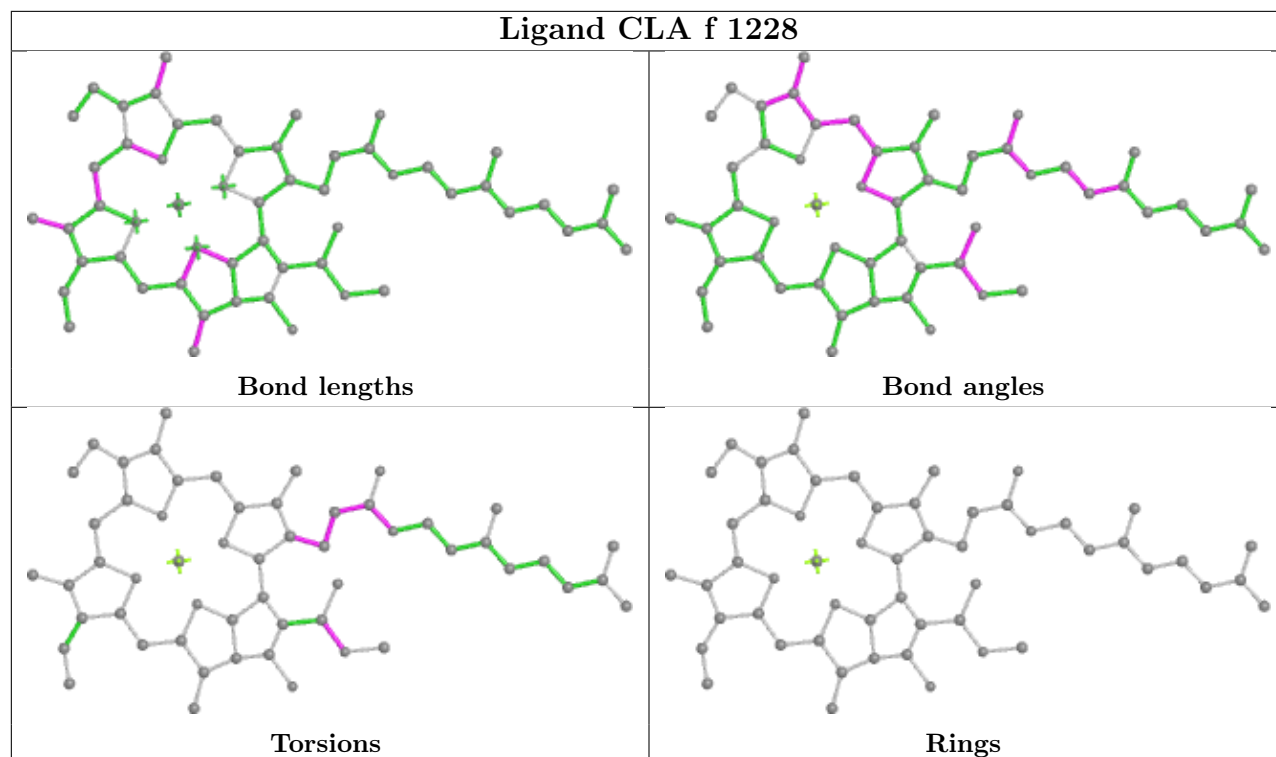
Rings

Ligand CLA H 1201	
	
Bond lengths	Bond angles
	
Torsions	Rings

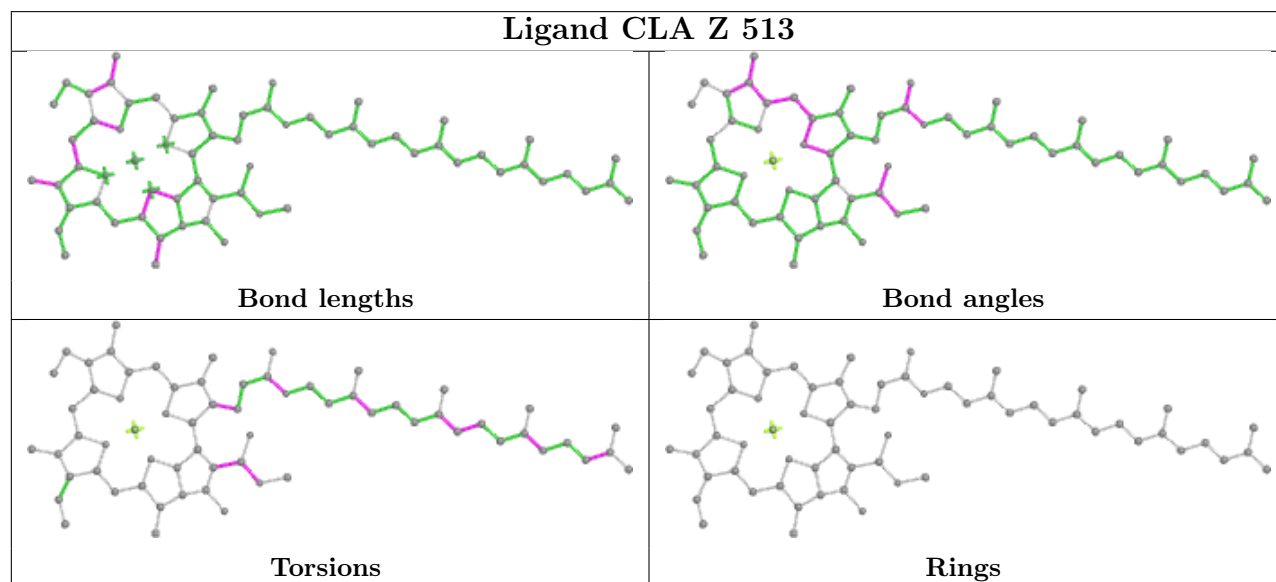
Ligand BCR 2 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR M 4021	
	
Bond lengths	Bond angles
	
Torsions	Rings

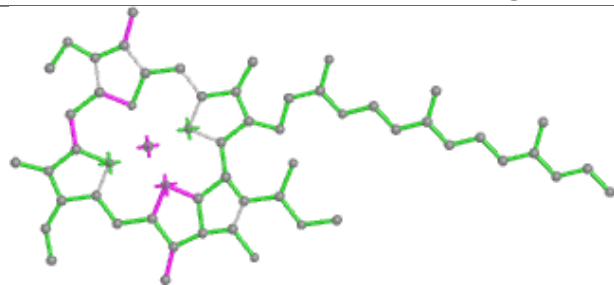
Ligand CLA f 1228



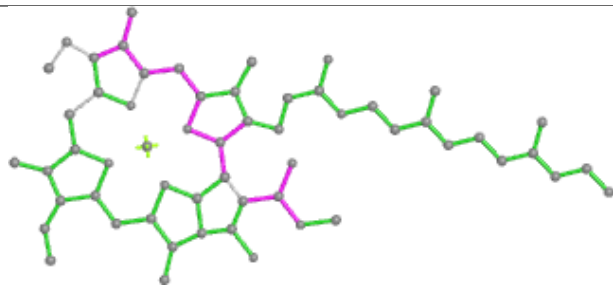
Ligand CLA Z 513



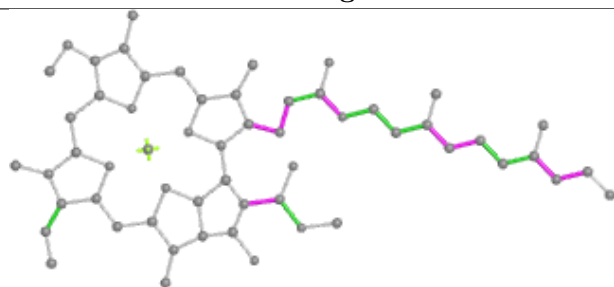
Ligand CLA B 1217



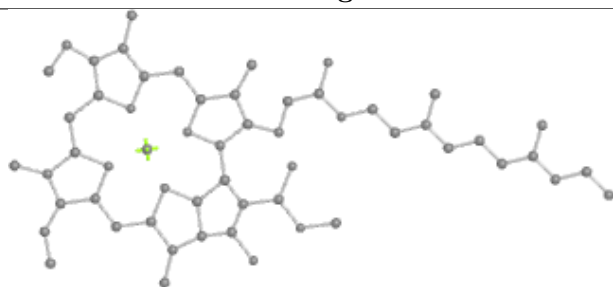
Bond lengths



Bond angles

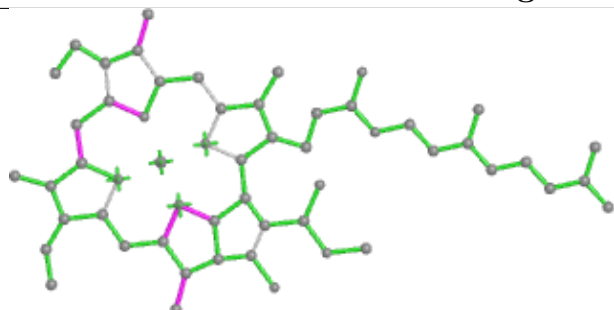


Torsions

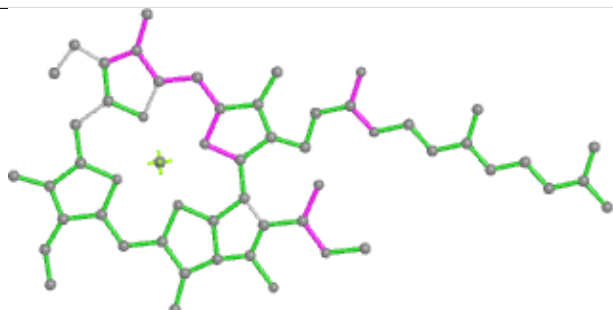


Rings

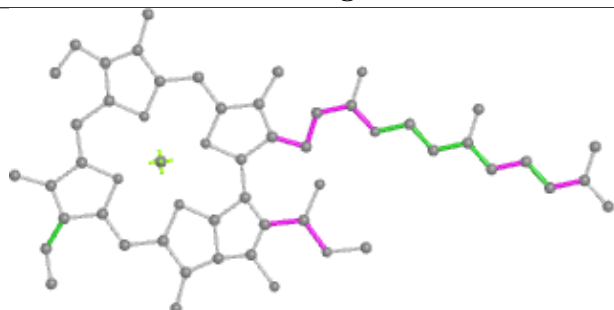
Ligand CLA u 518



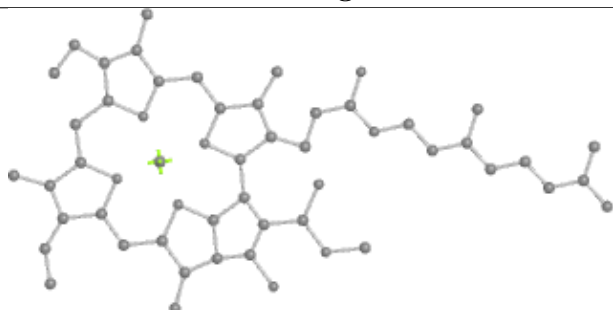
Bond lengths



Bond angles

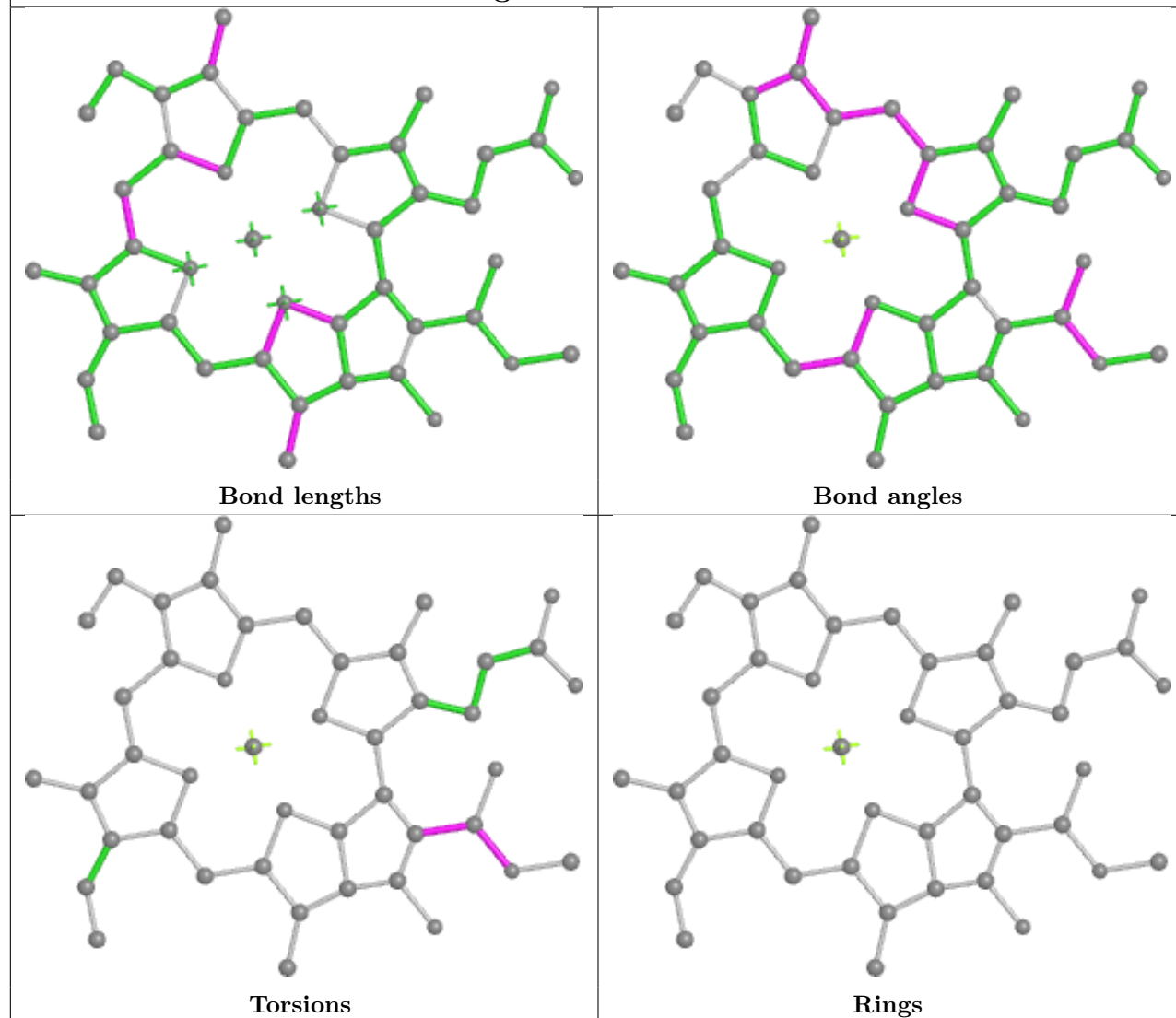


Torsions

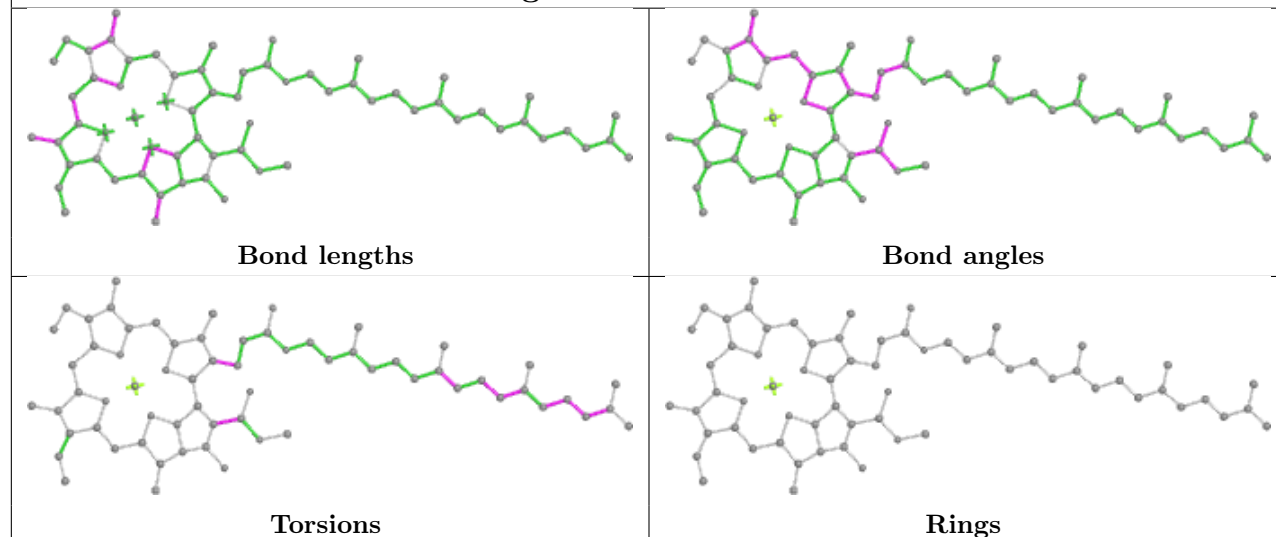


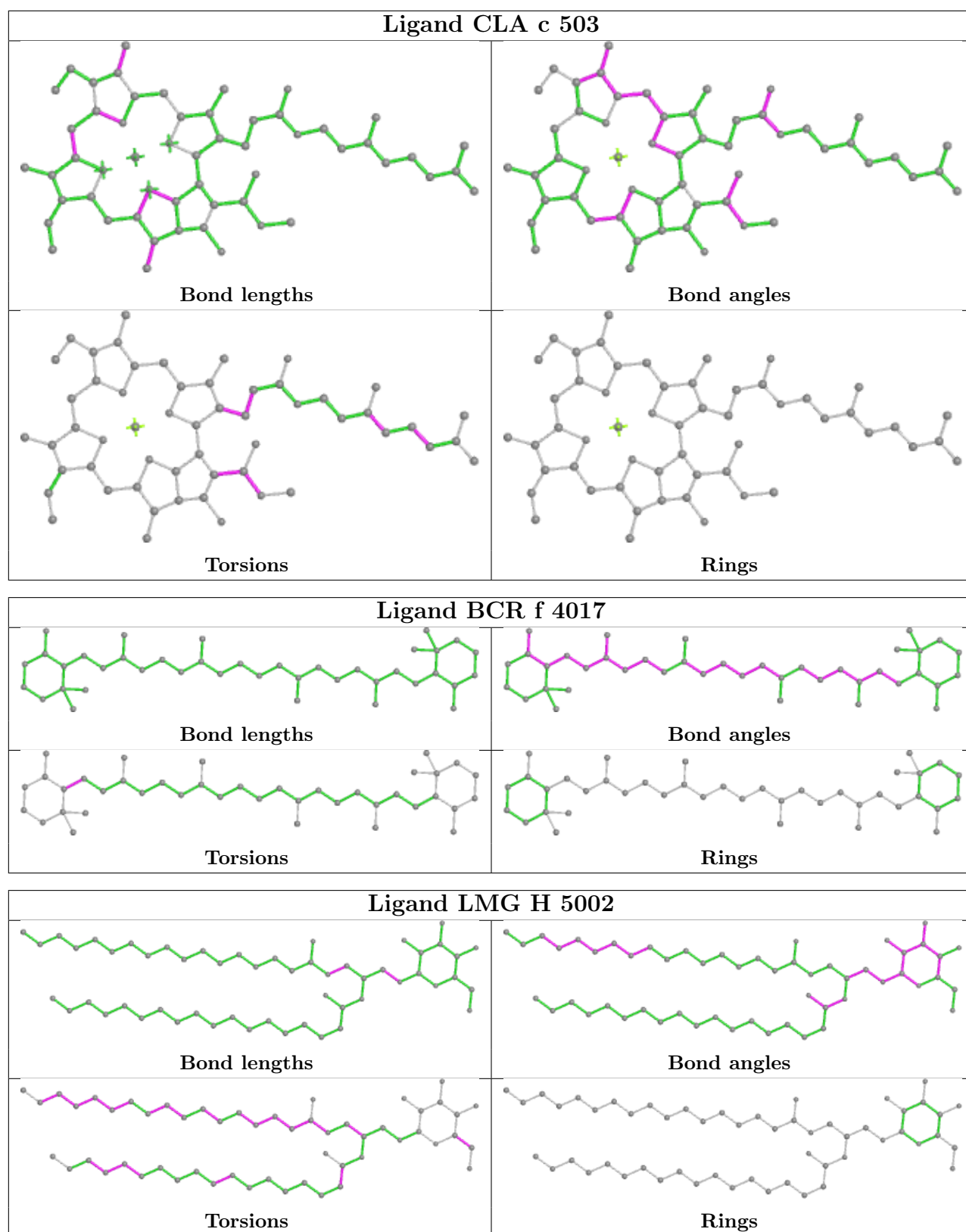
Rings

Ligand CLA 4 504

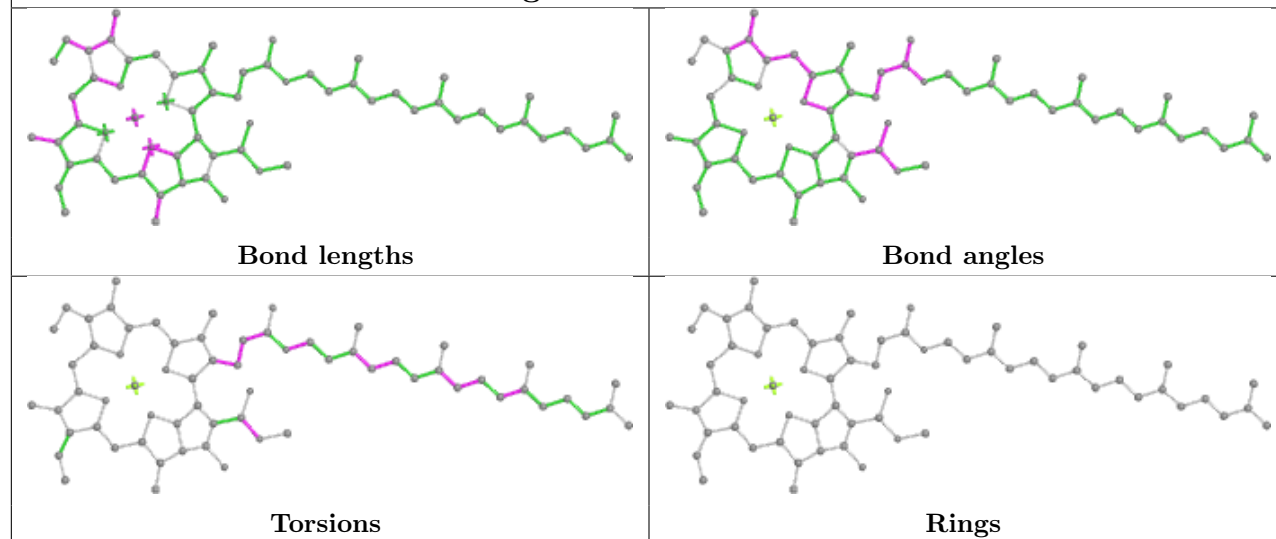


Ligand CLA G 1101

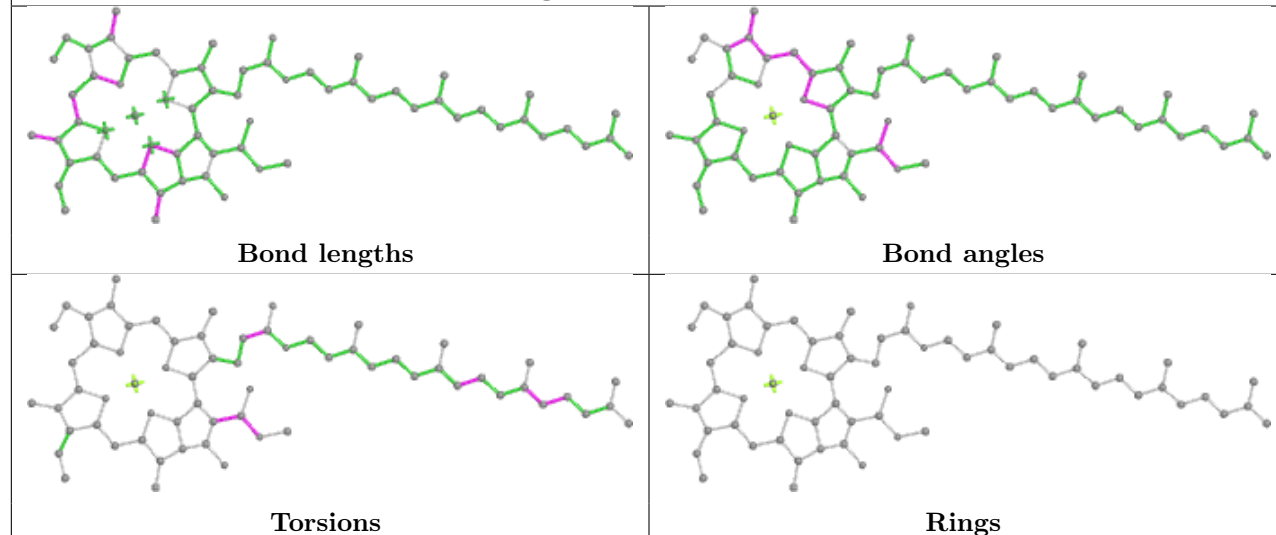




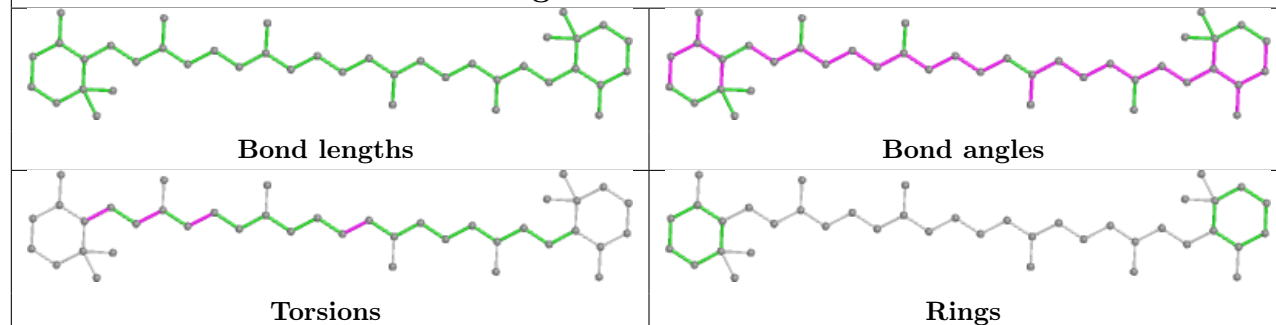
Ligand CLA A 1107

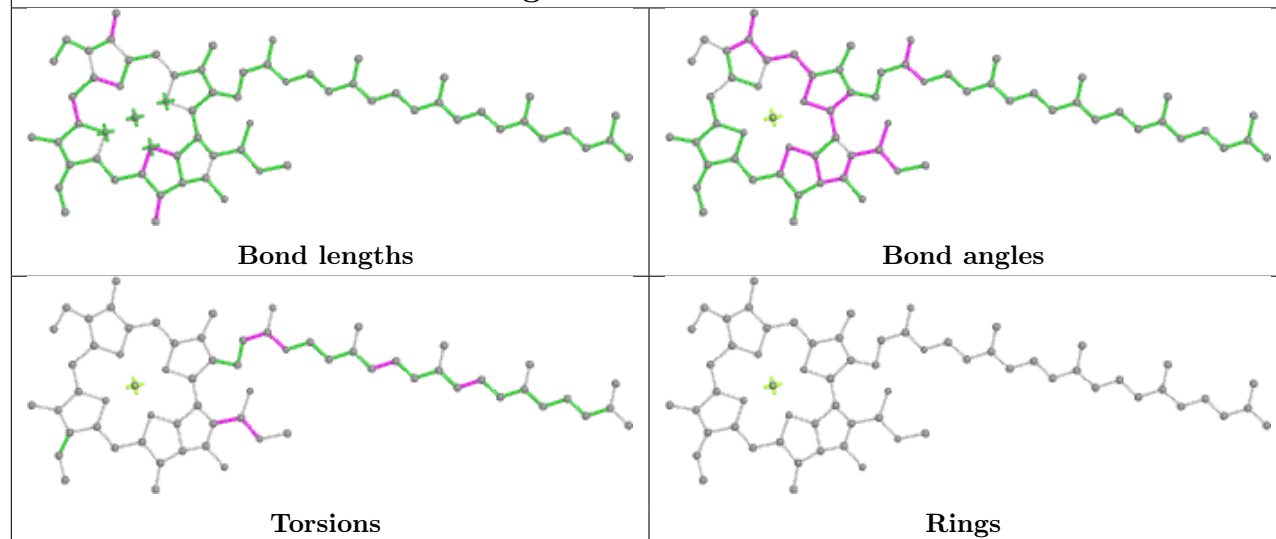
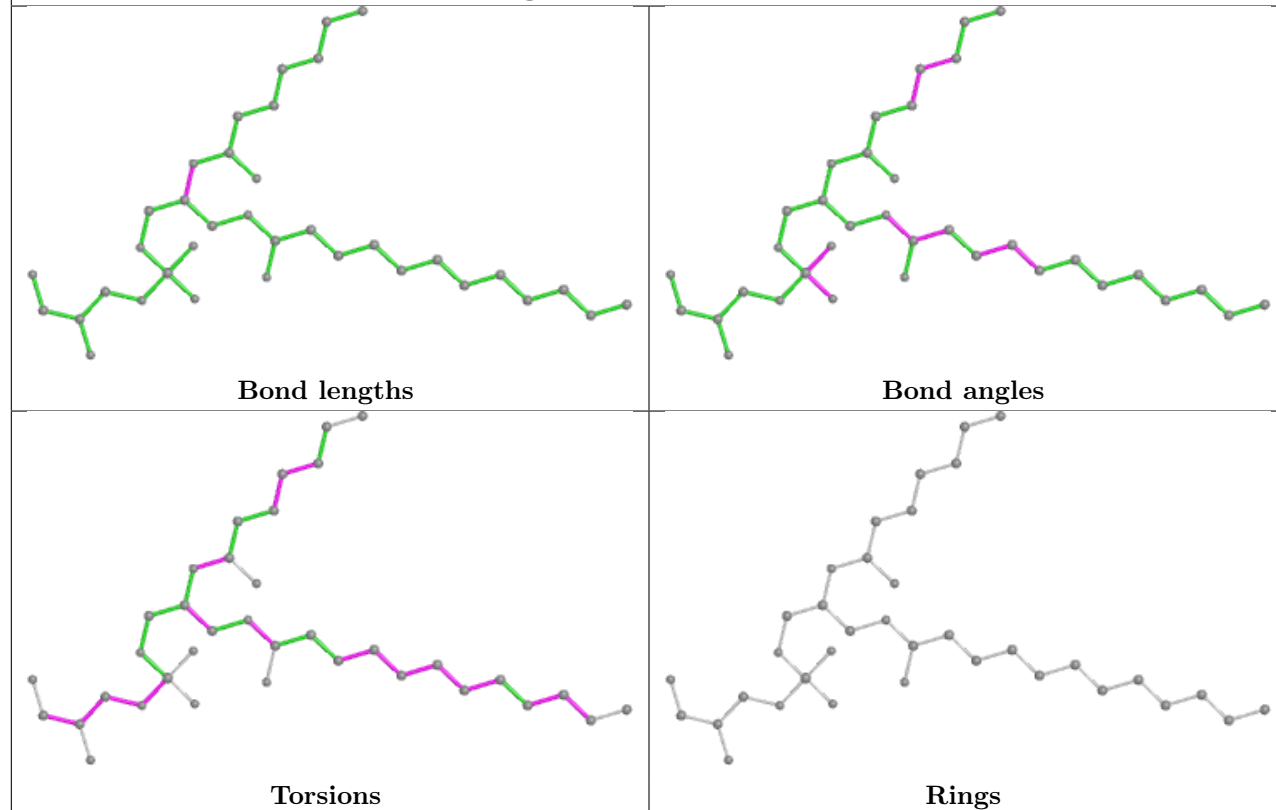


Ligand CLA r 510

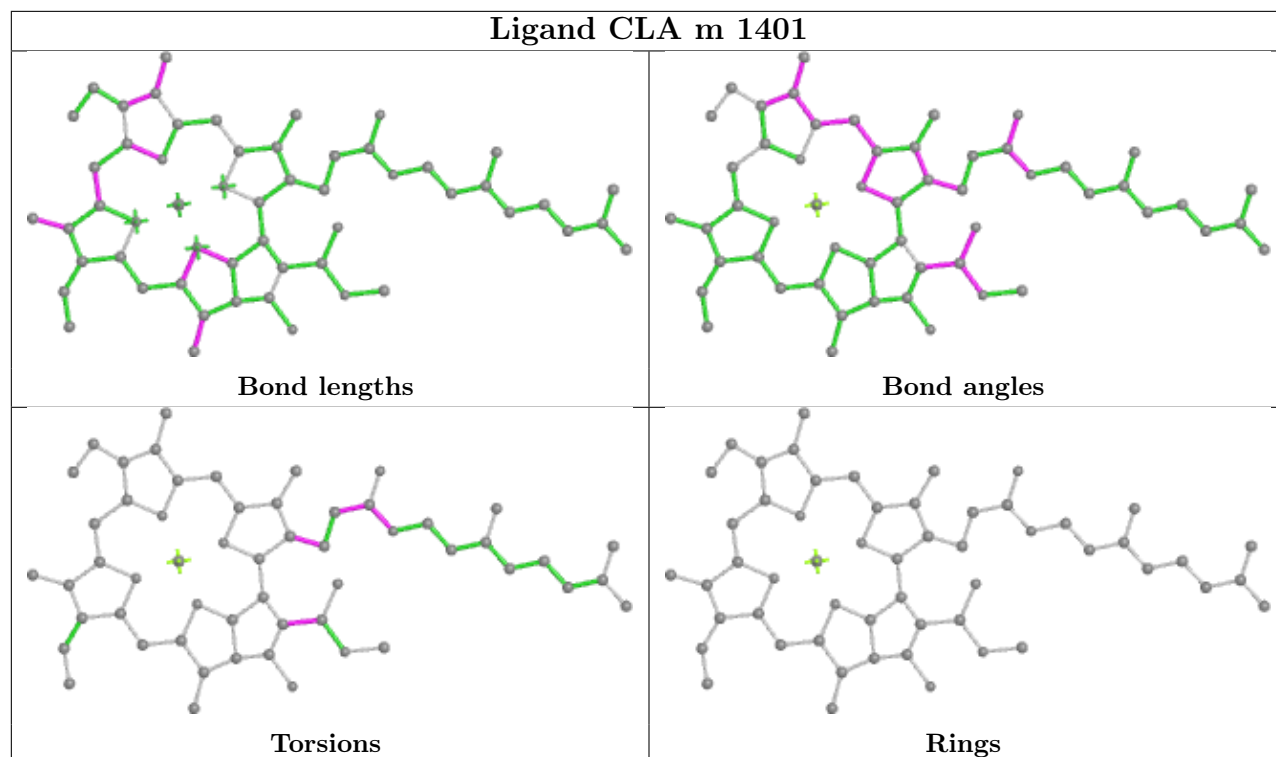


Ligand BCR Z 522

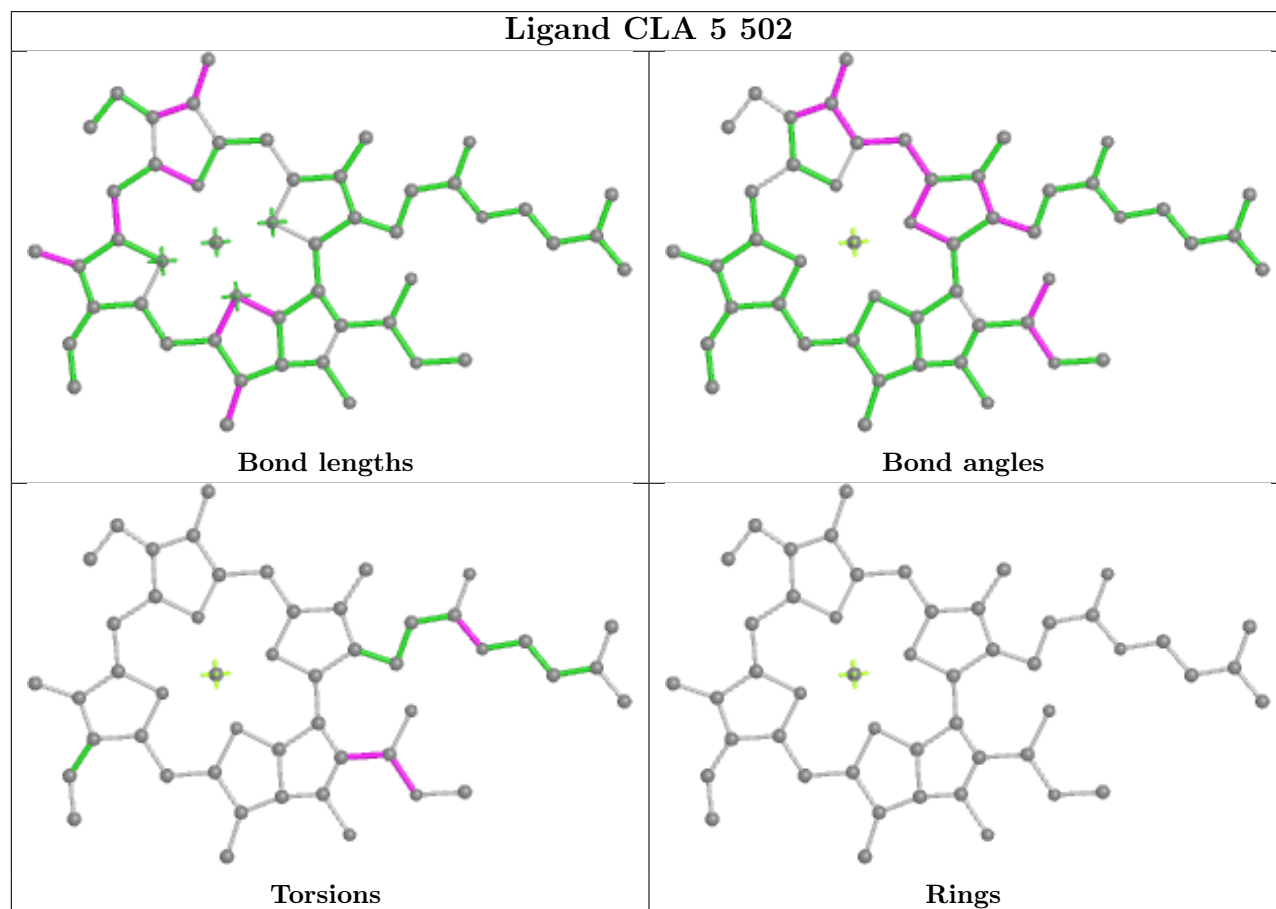


Ligand CLA A 1011**Ligand LHG A 5004**

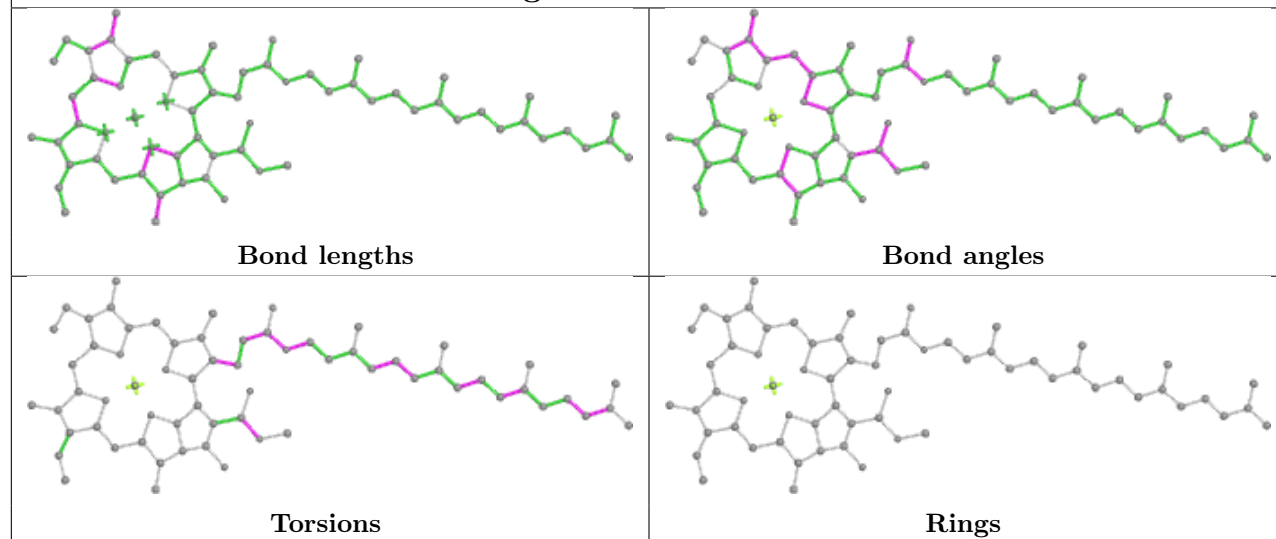
Ligand CLA m 1401



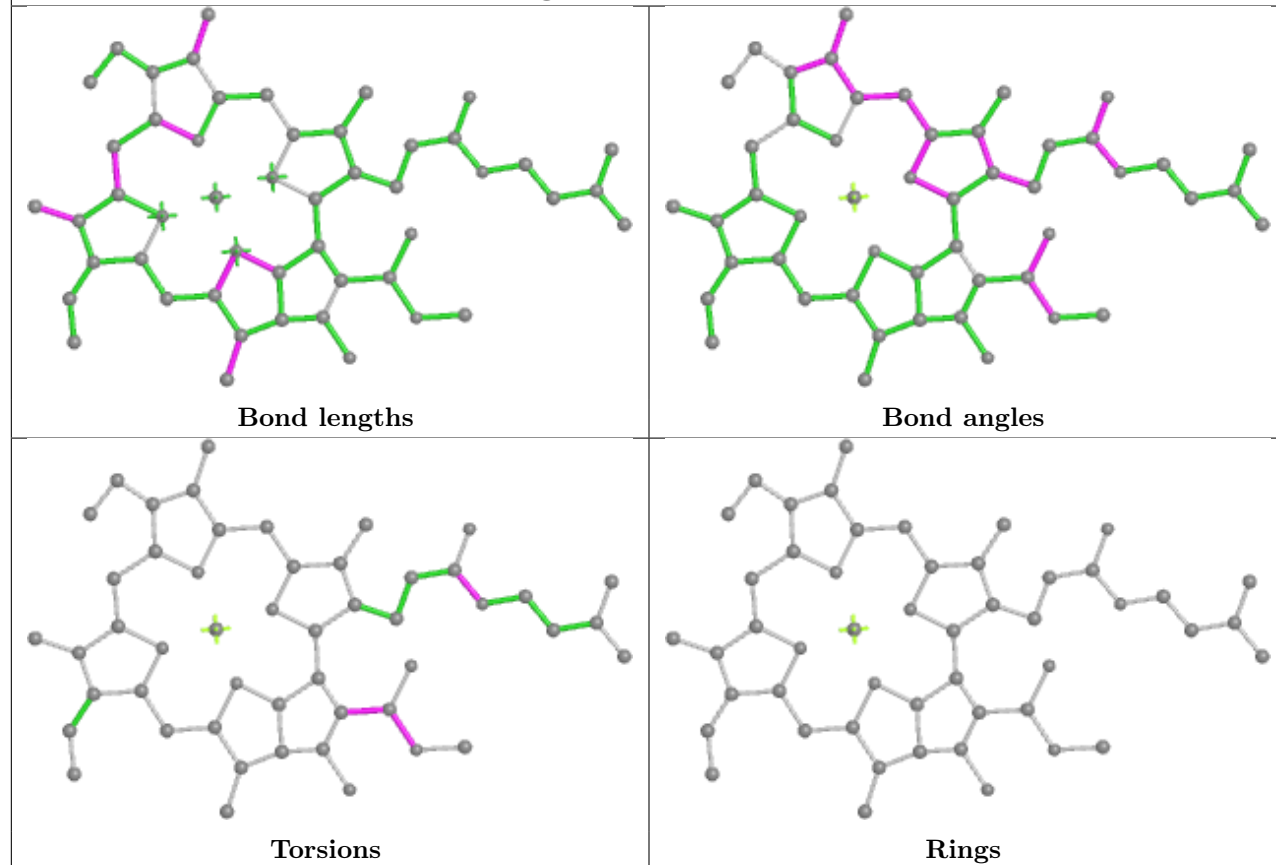
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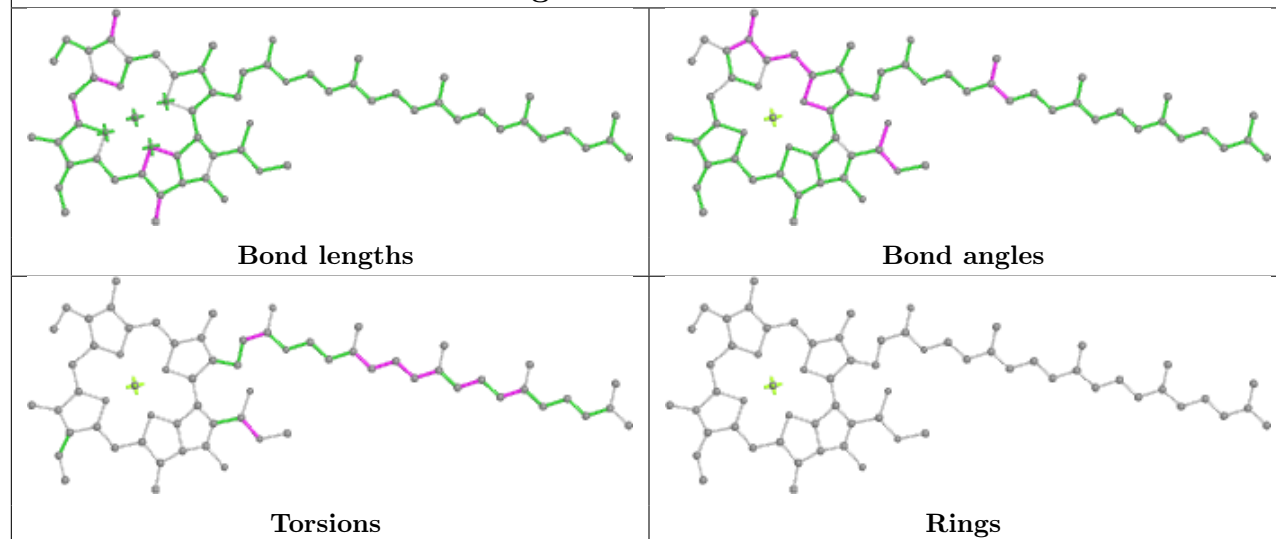
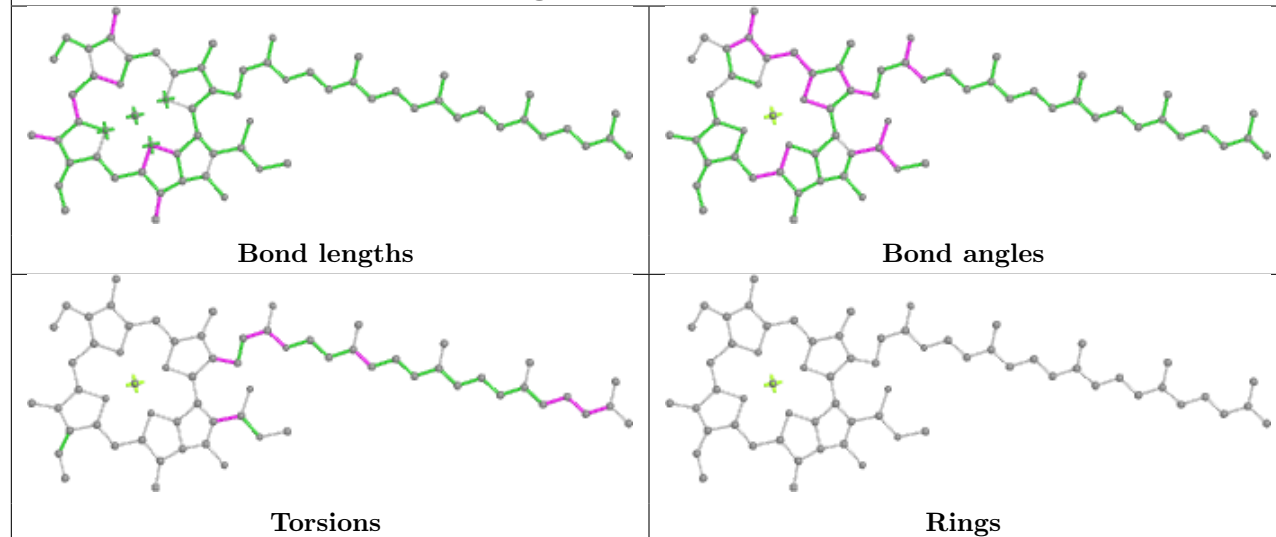


Ligand CLA B 1219

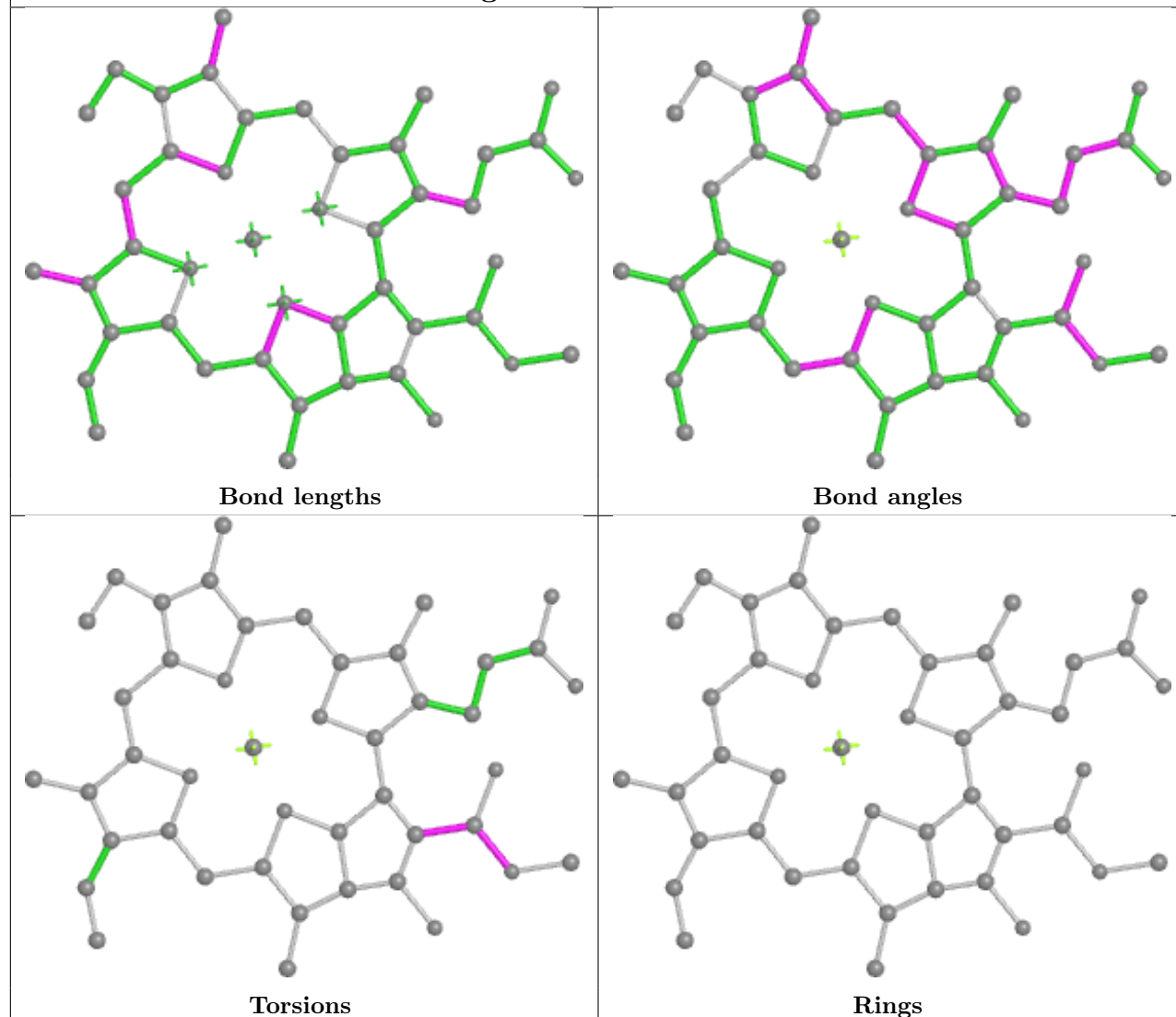


Ligand CLA r 504

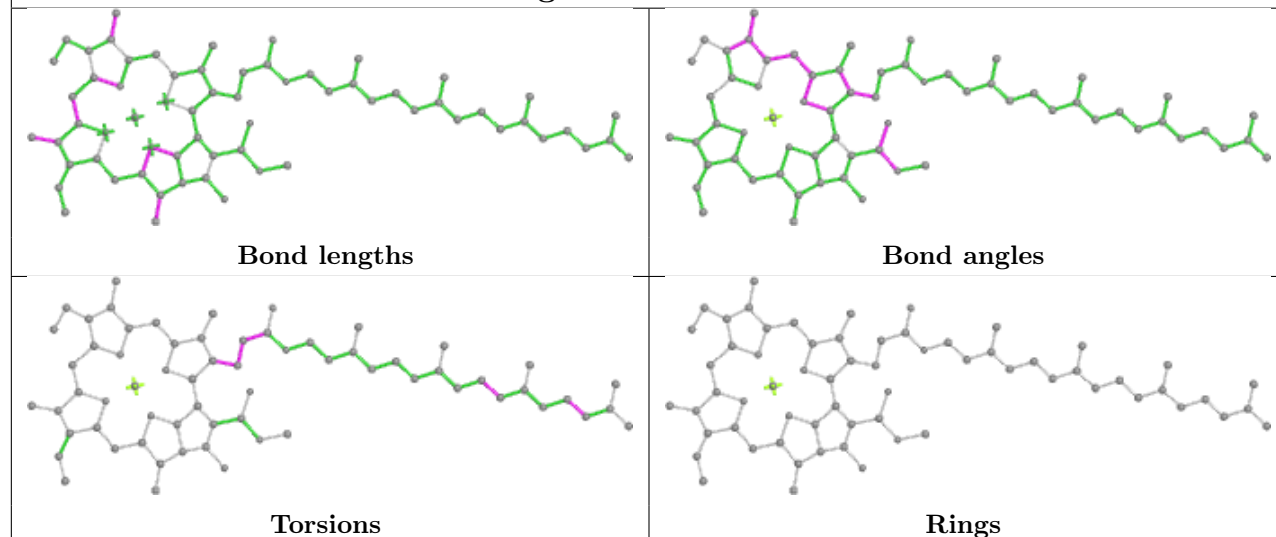


Ligand CLA Y 510**Ligand CLA f 1202**

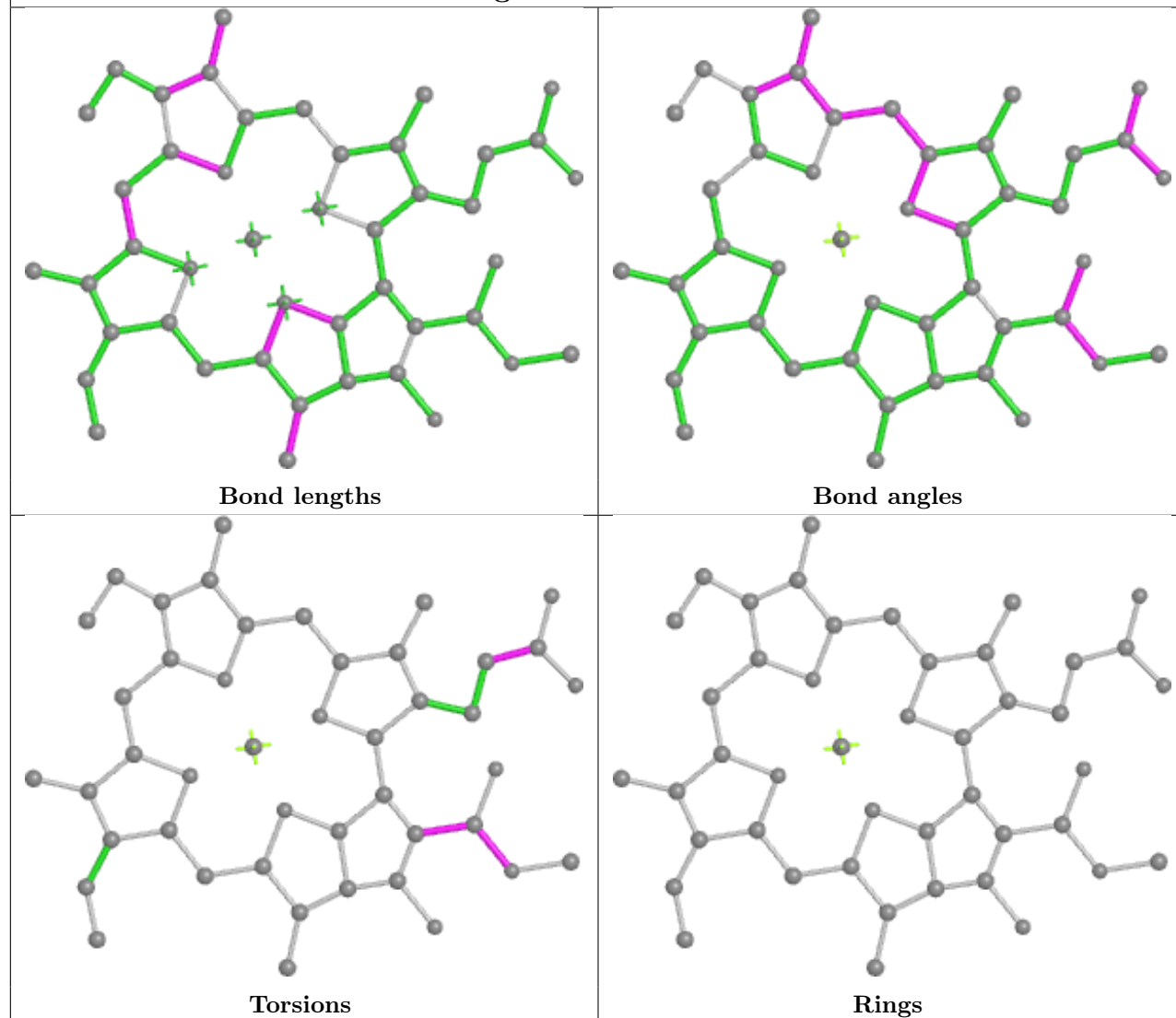
Ligand CLA G 1801



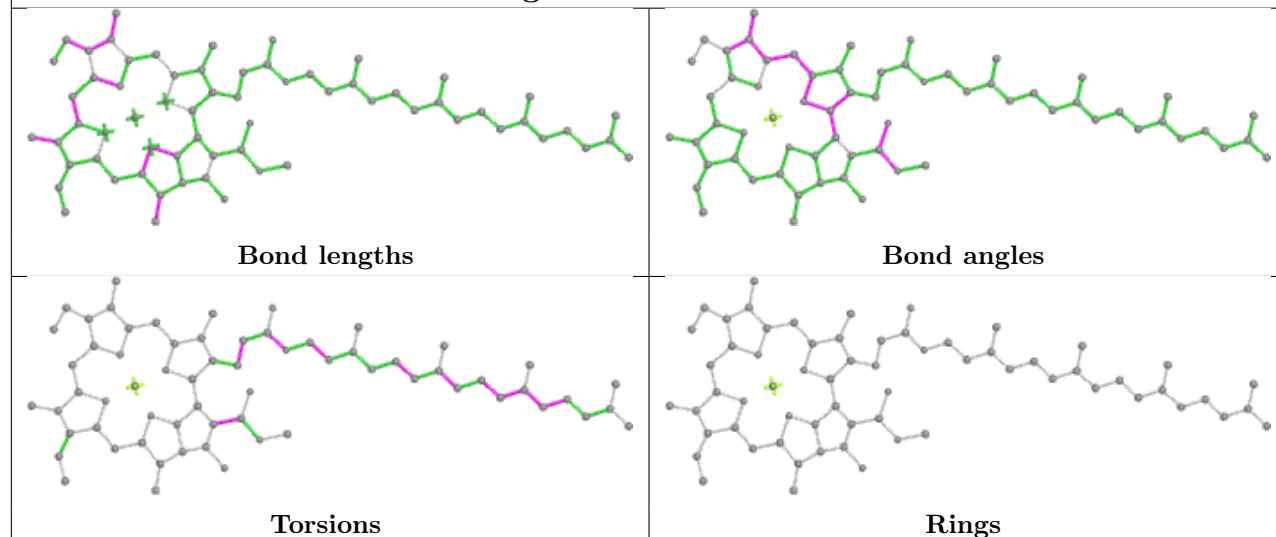
Ligand CLA s 501

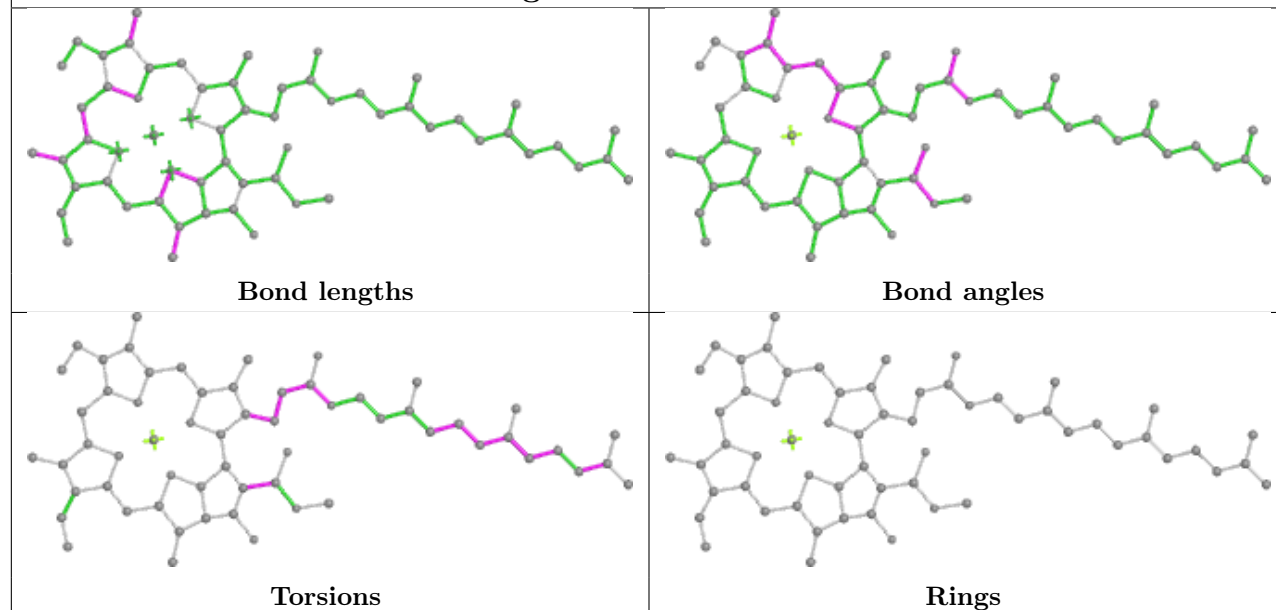
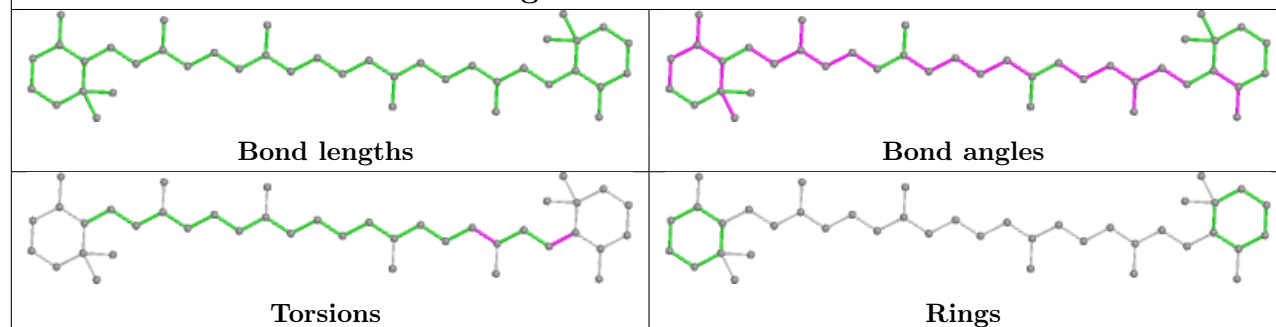
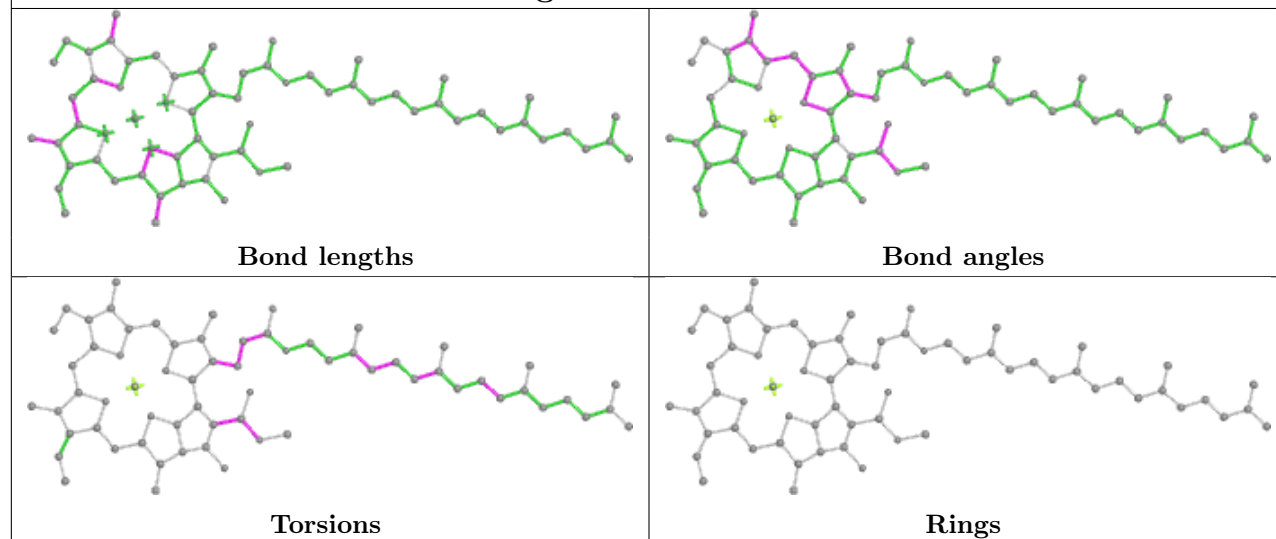


Ligand CLA 5 512

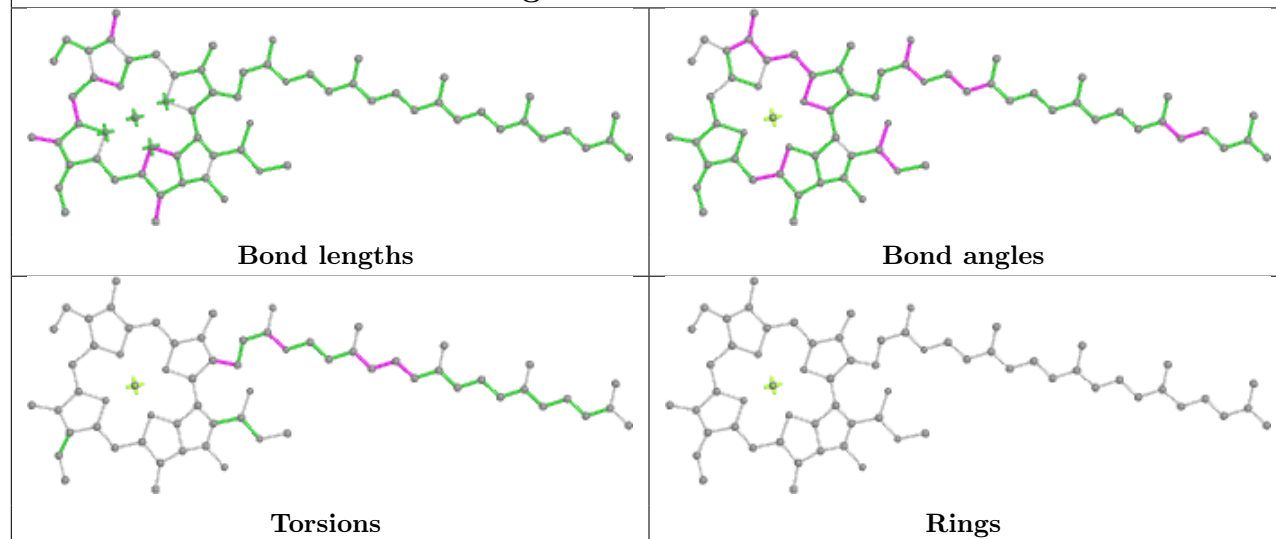


Ligand CLA H 1214

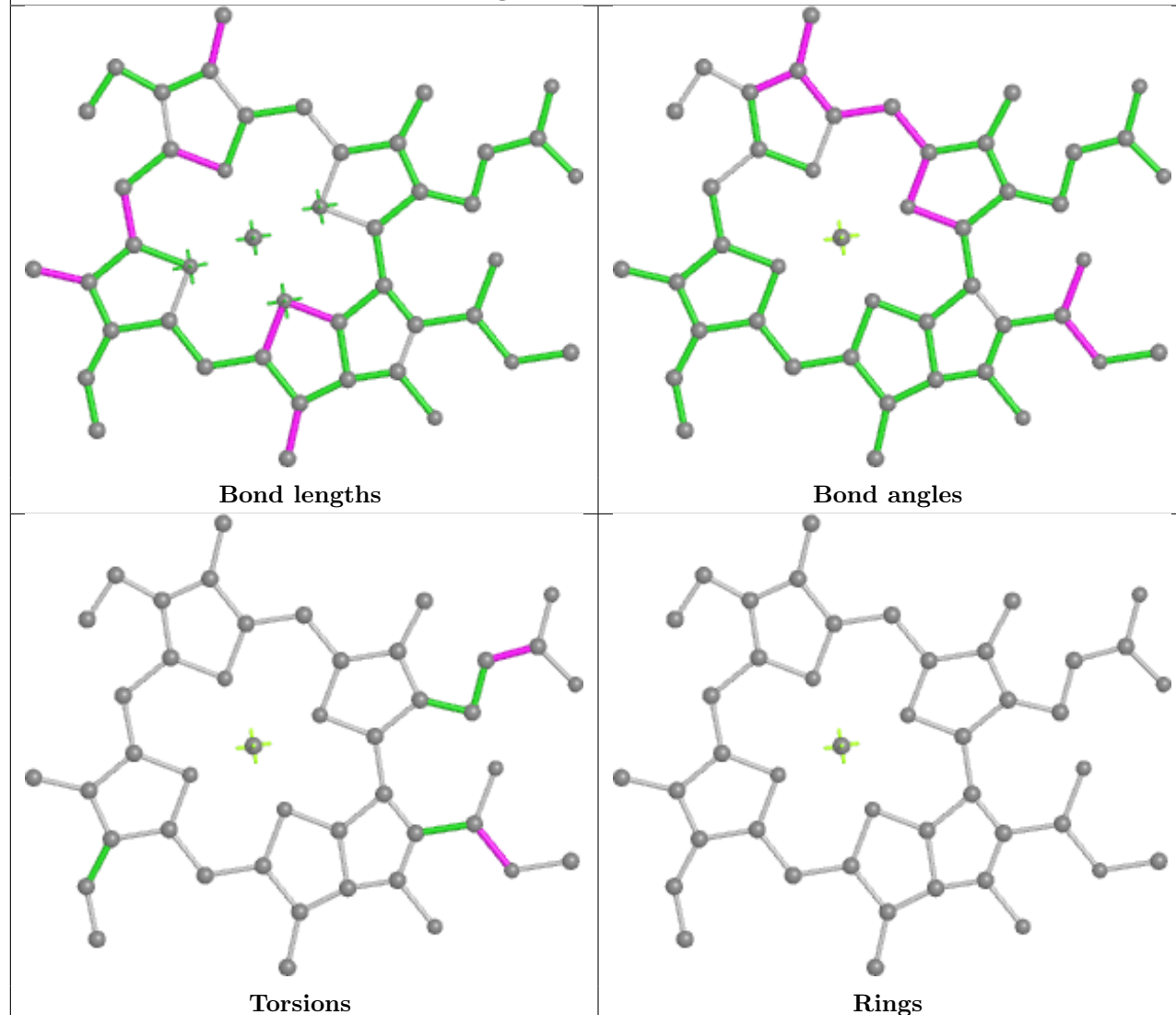


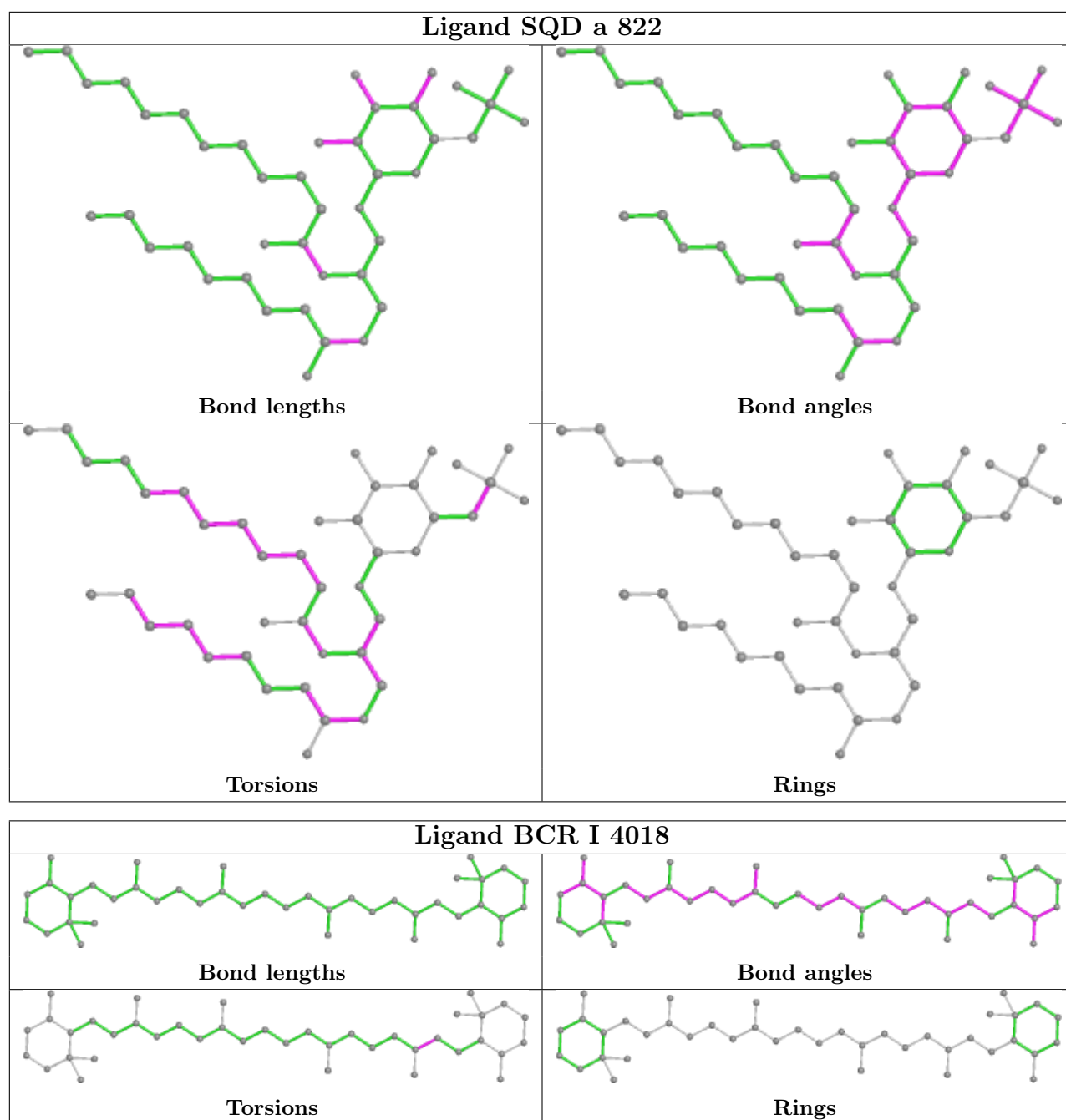
Ligand CLA A 1116**Ligand BCR V 4020****Ligand CLA 2 501**

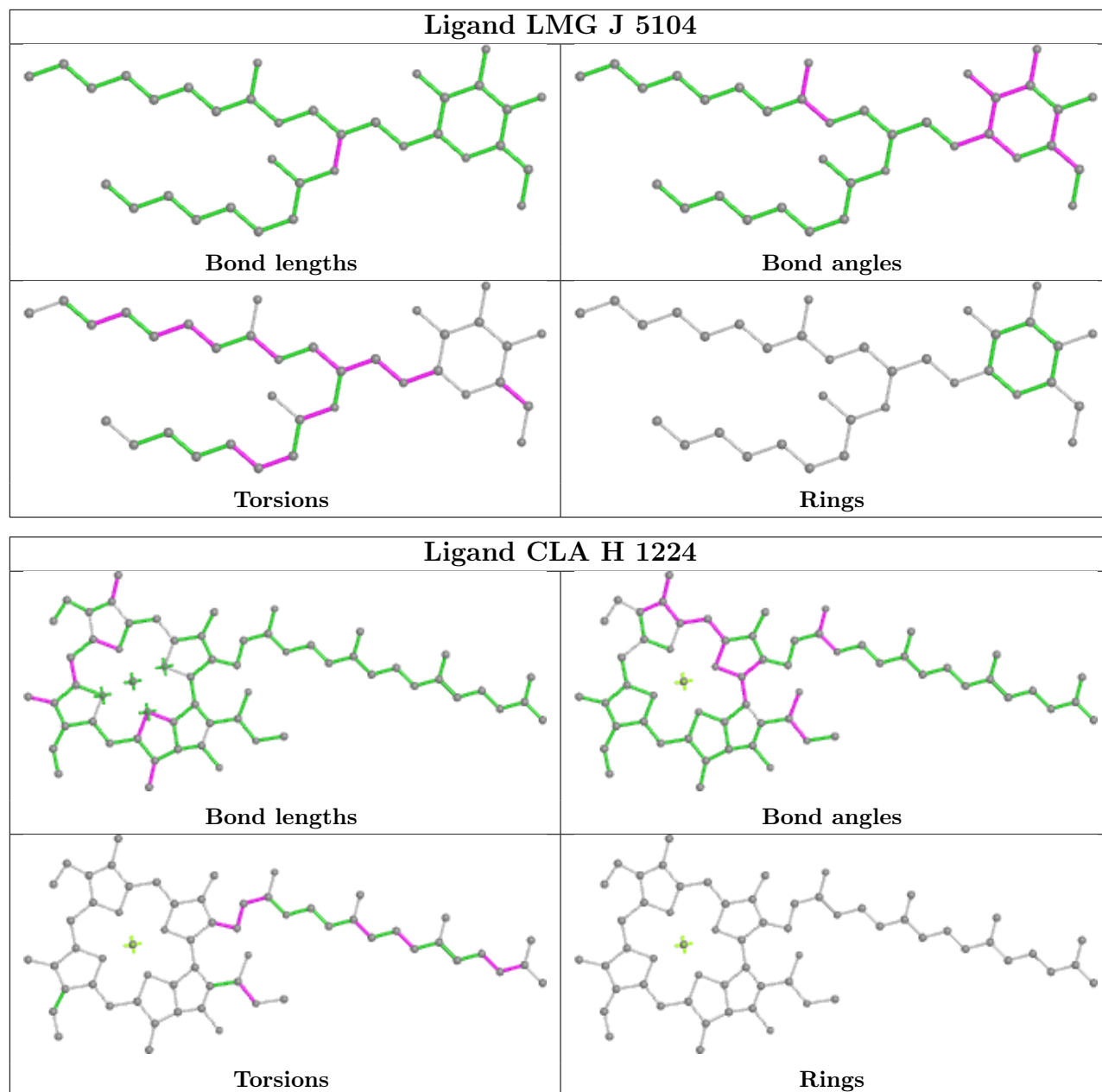
Ligand CLA A 1130



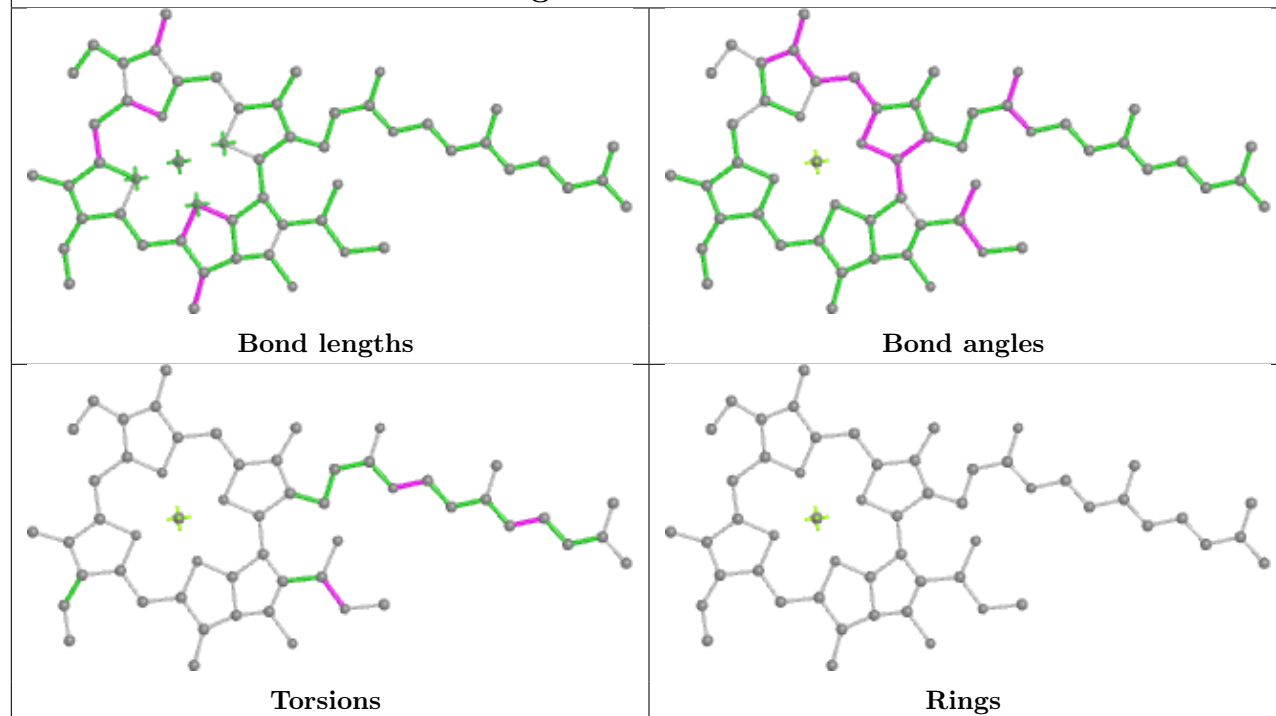
Ligand CLA 5 508



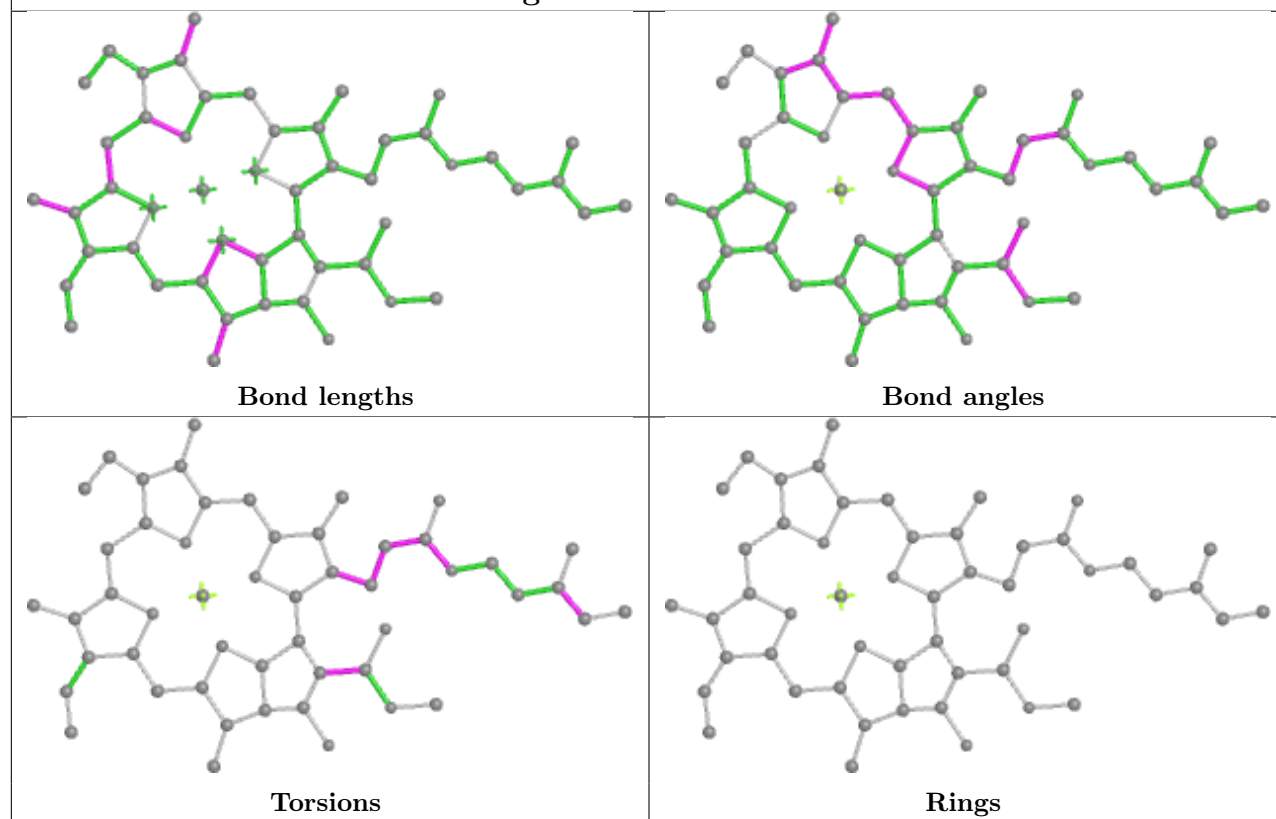




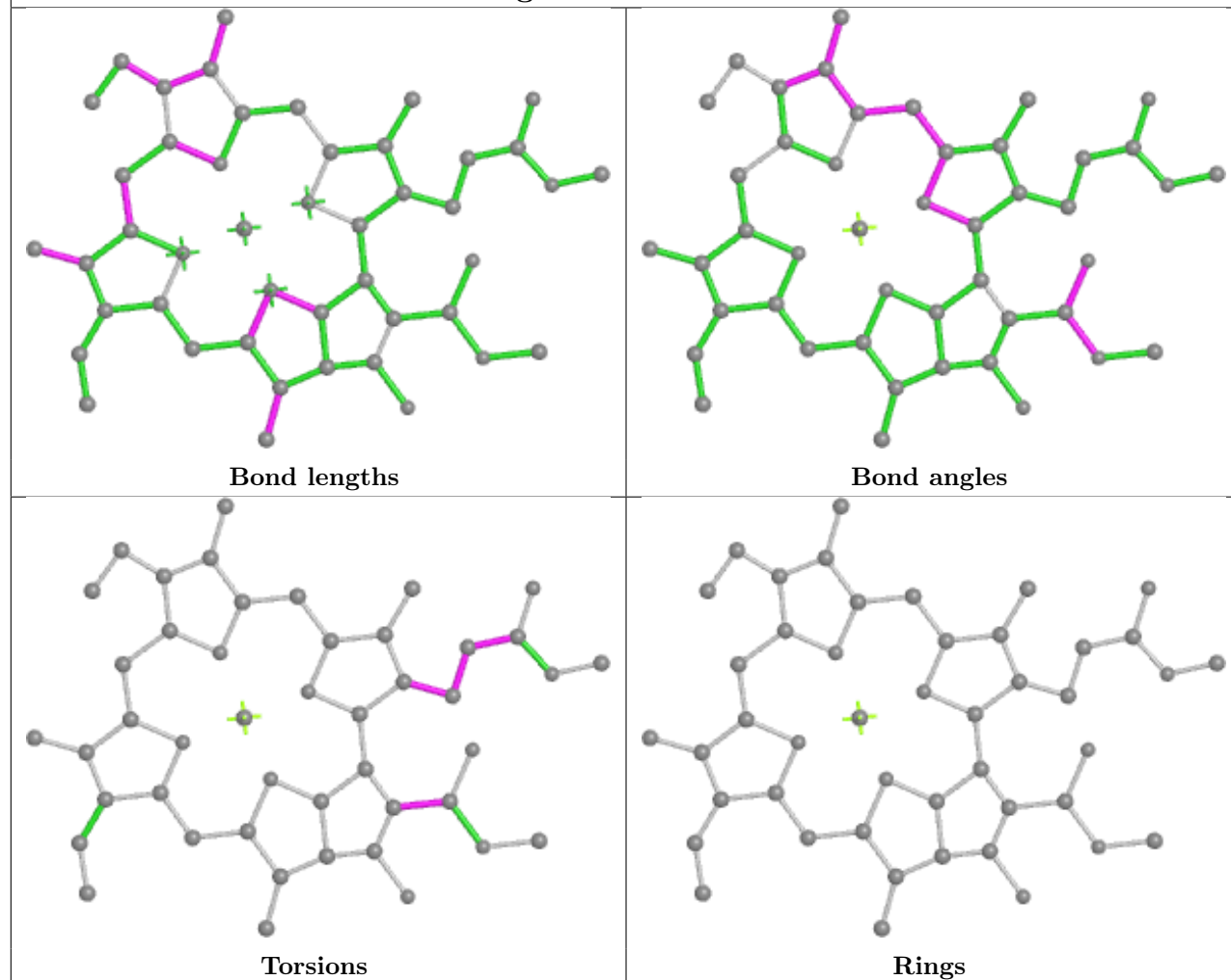
Ligand CLA Y 511



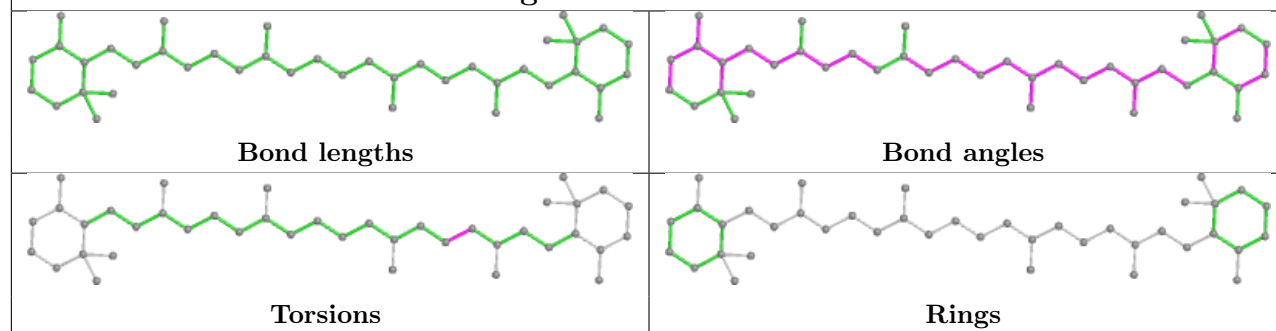
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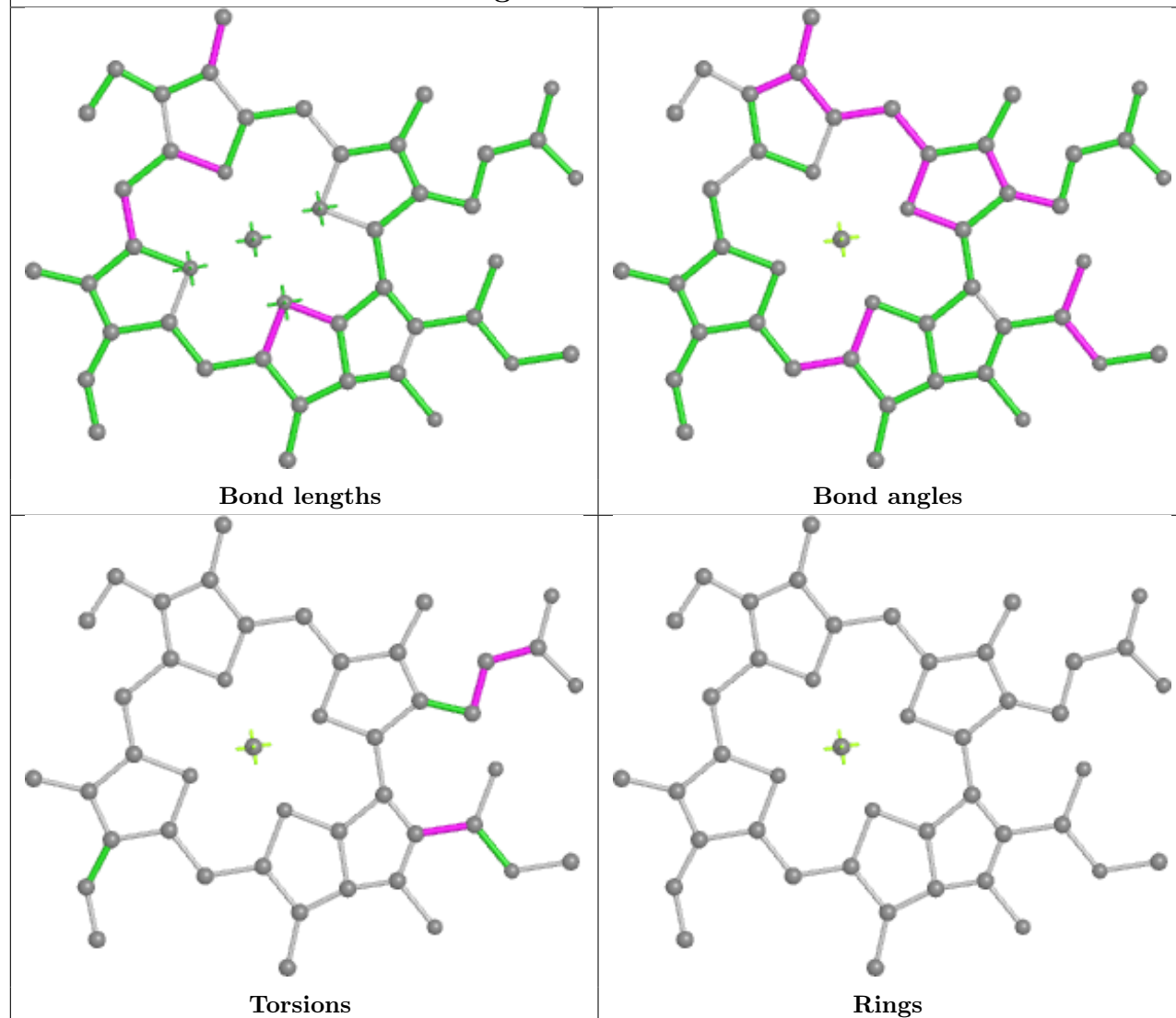
Ligand CLA u 519



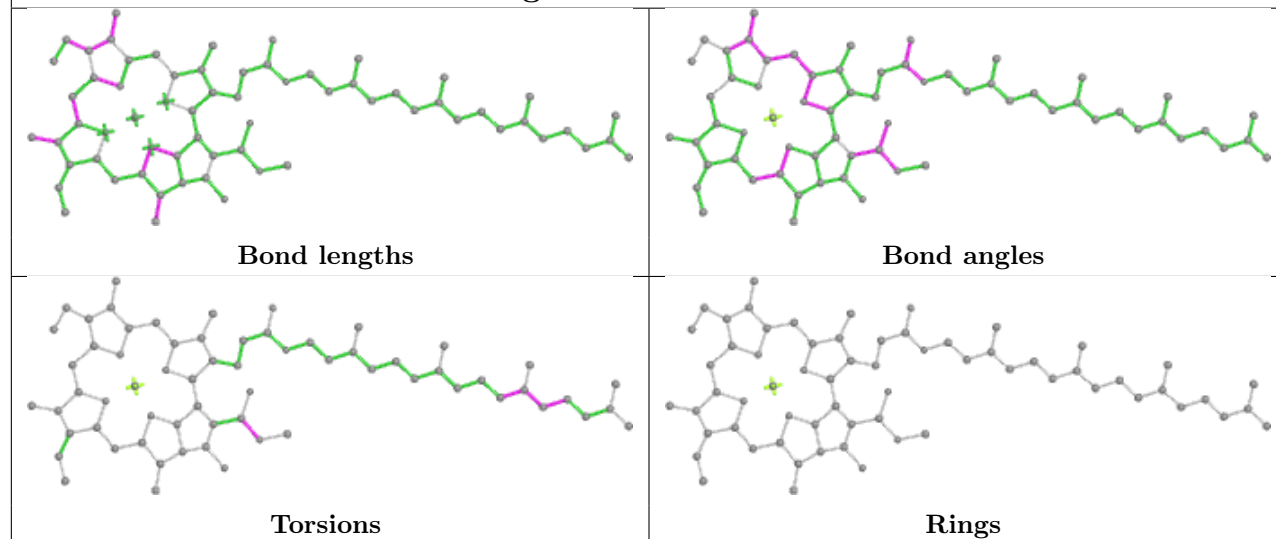
Ligand BCR H 4009



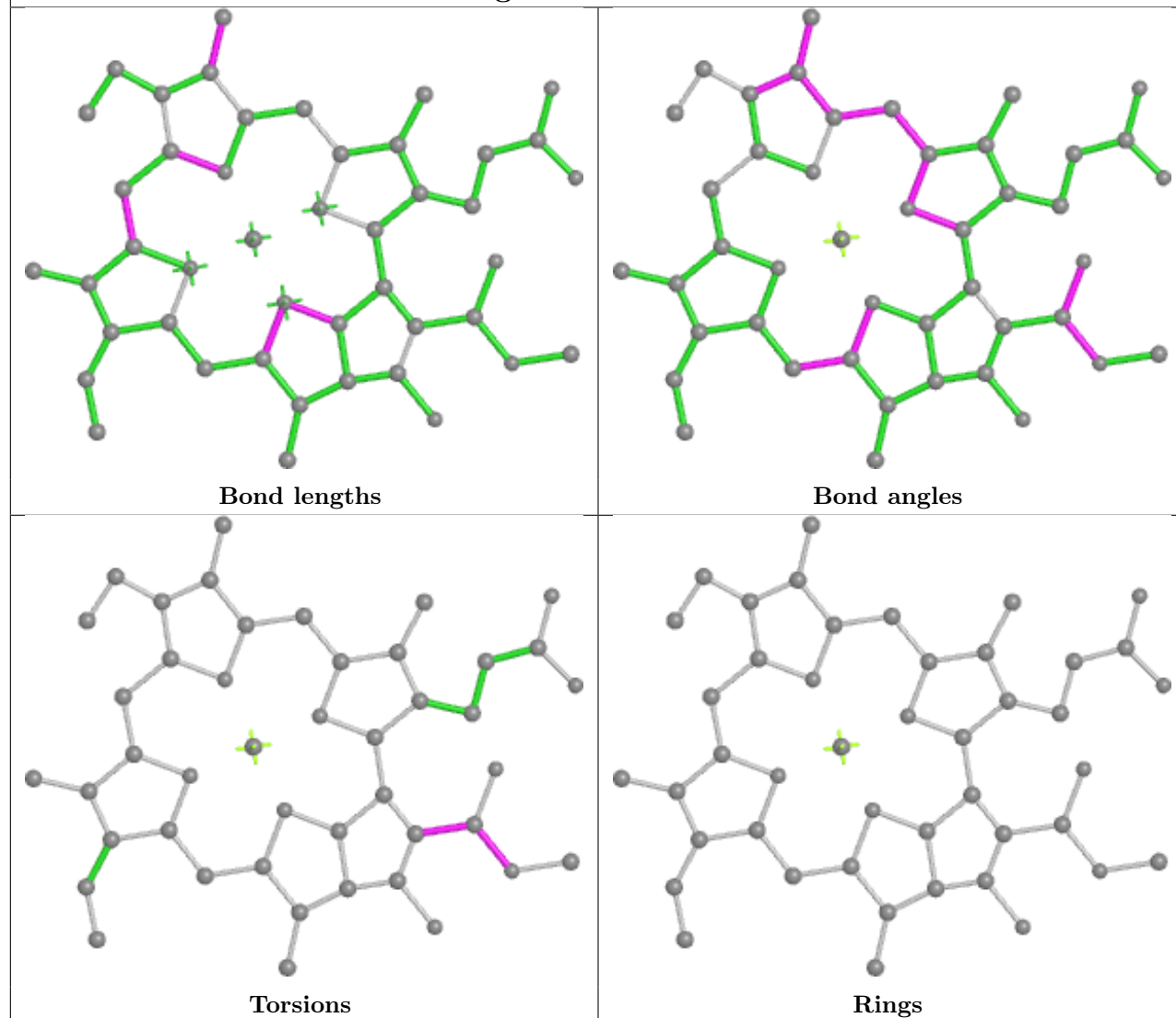
Ligand CLA 6 504



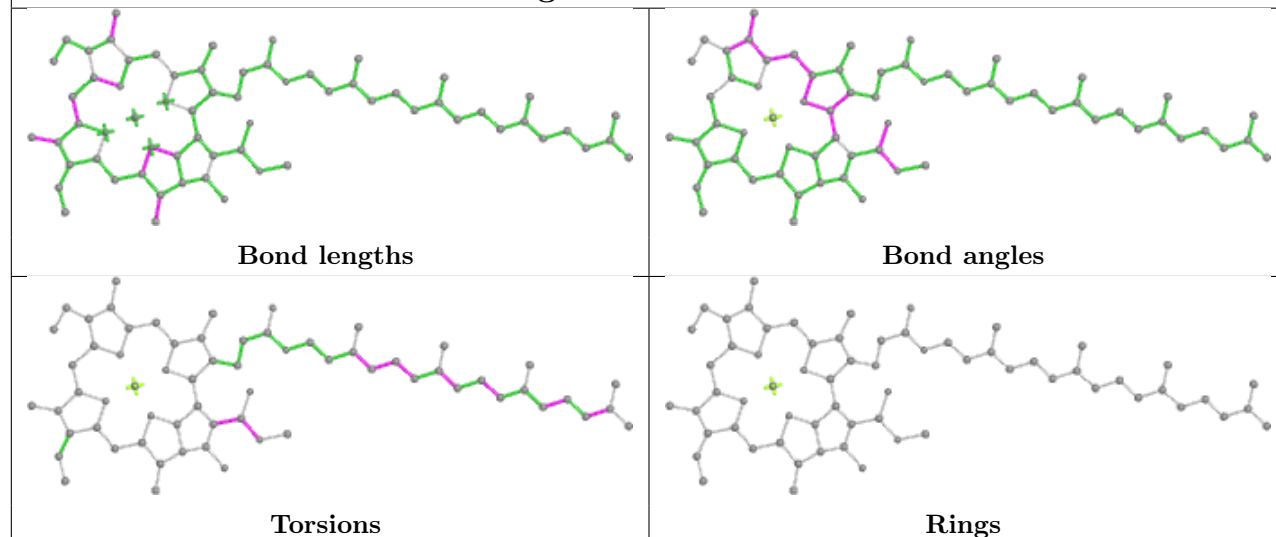
Ligand CLA A 1131



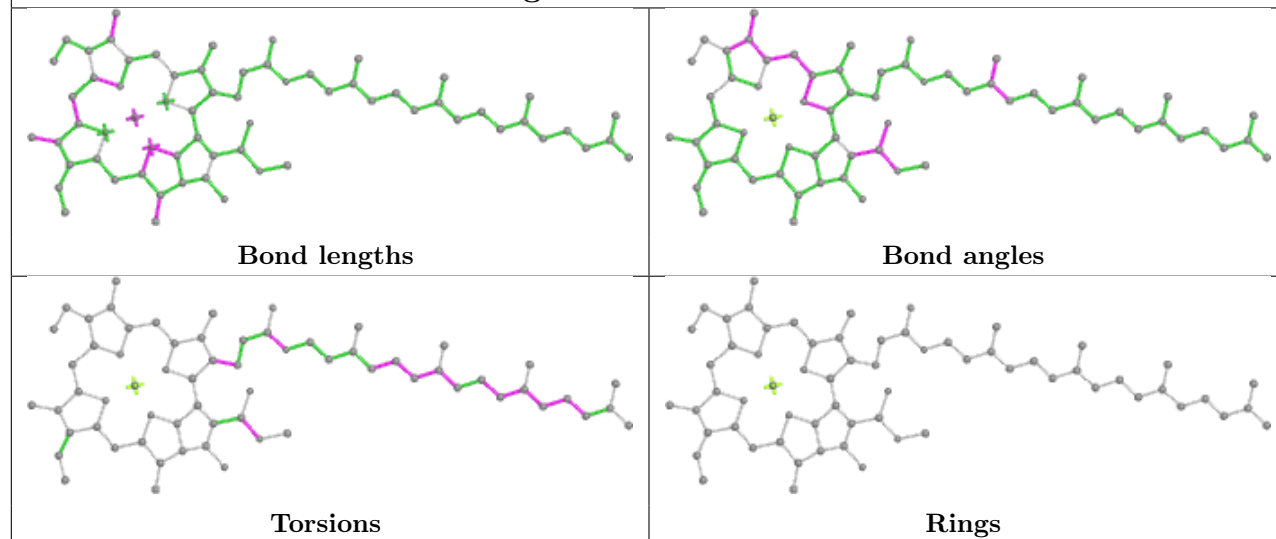
Ligand CLA c 504



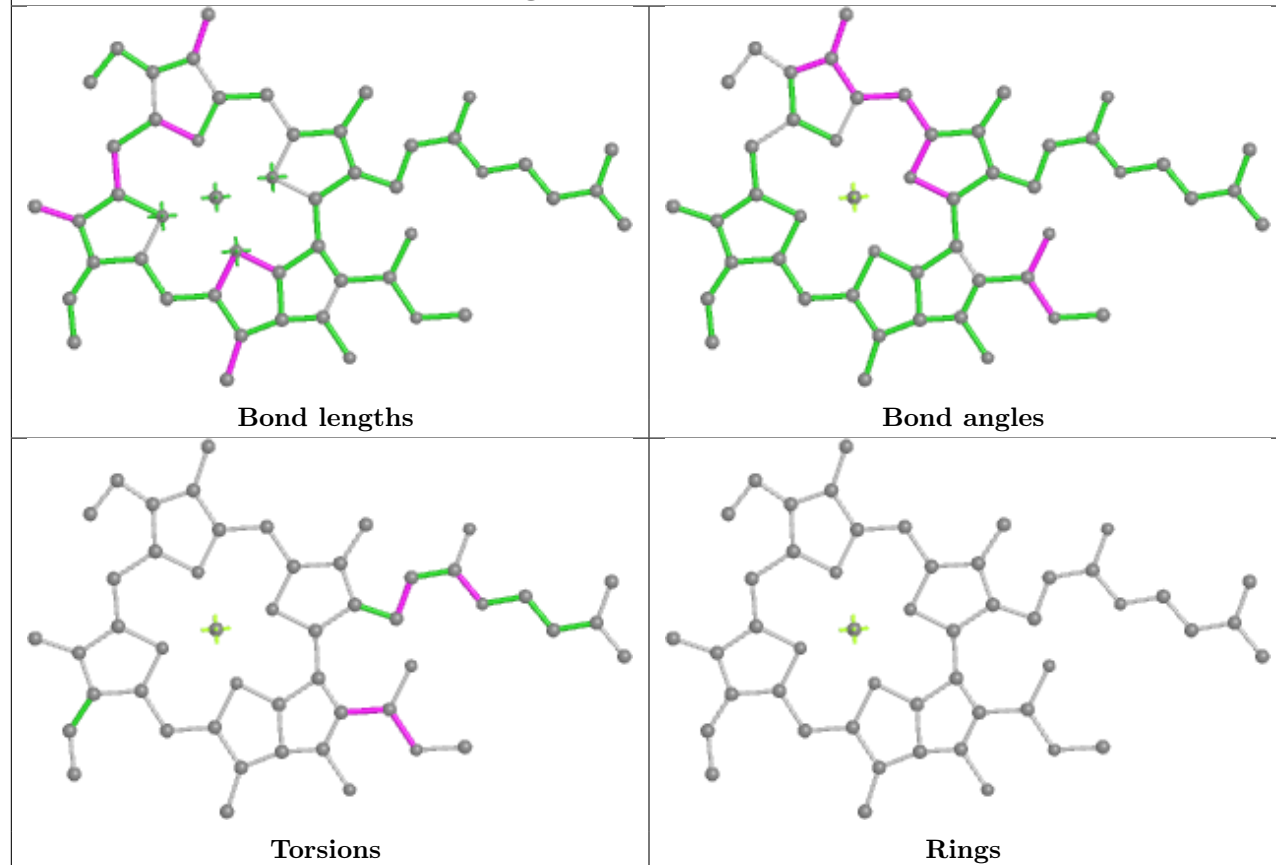
Ligand CLA r 507

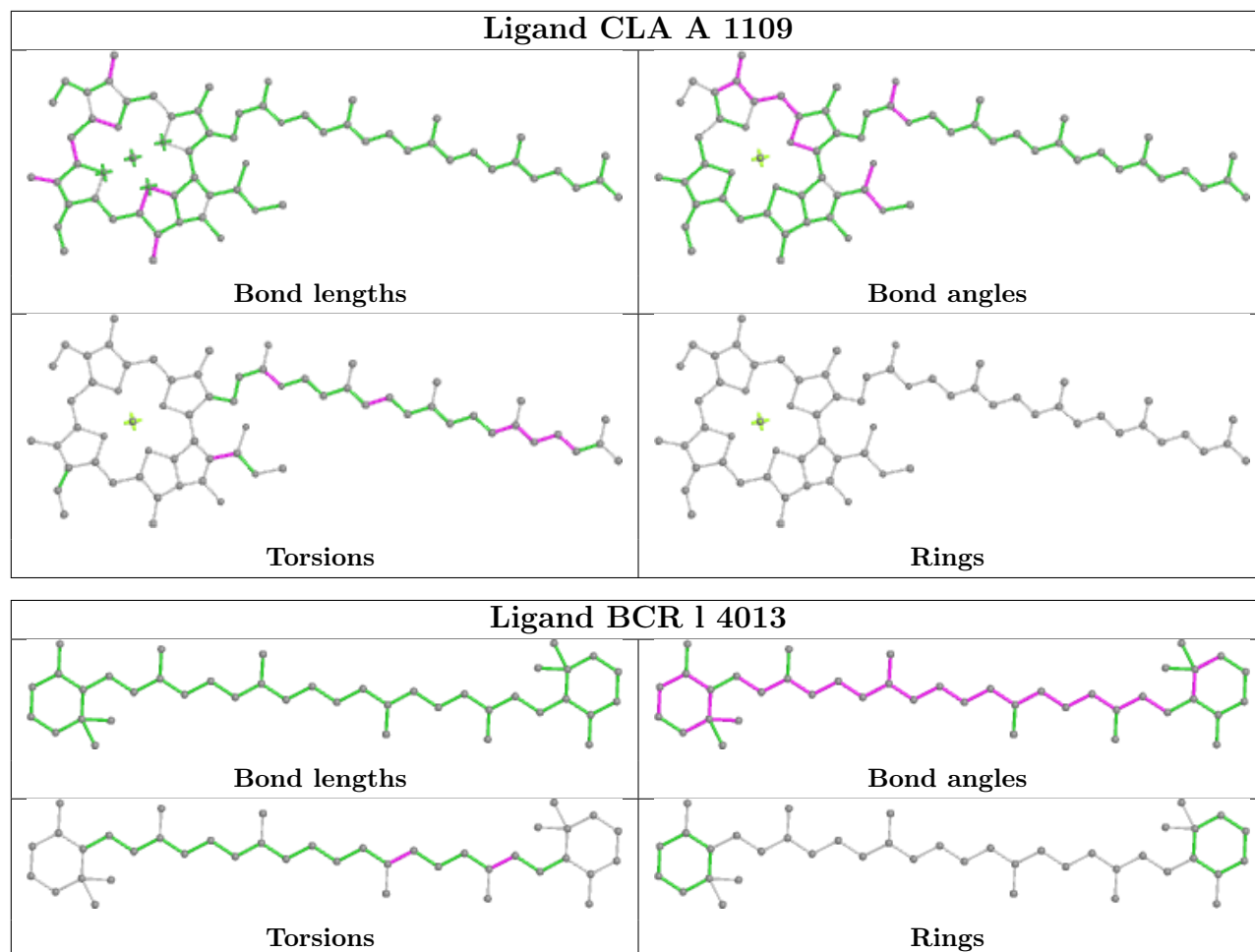


Ligand CLA B 1215

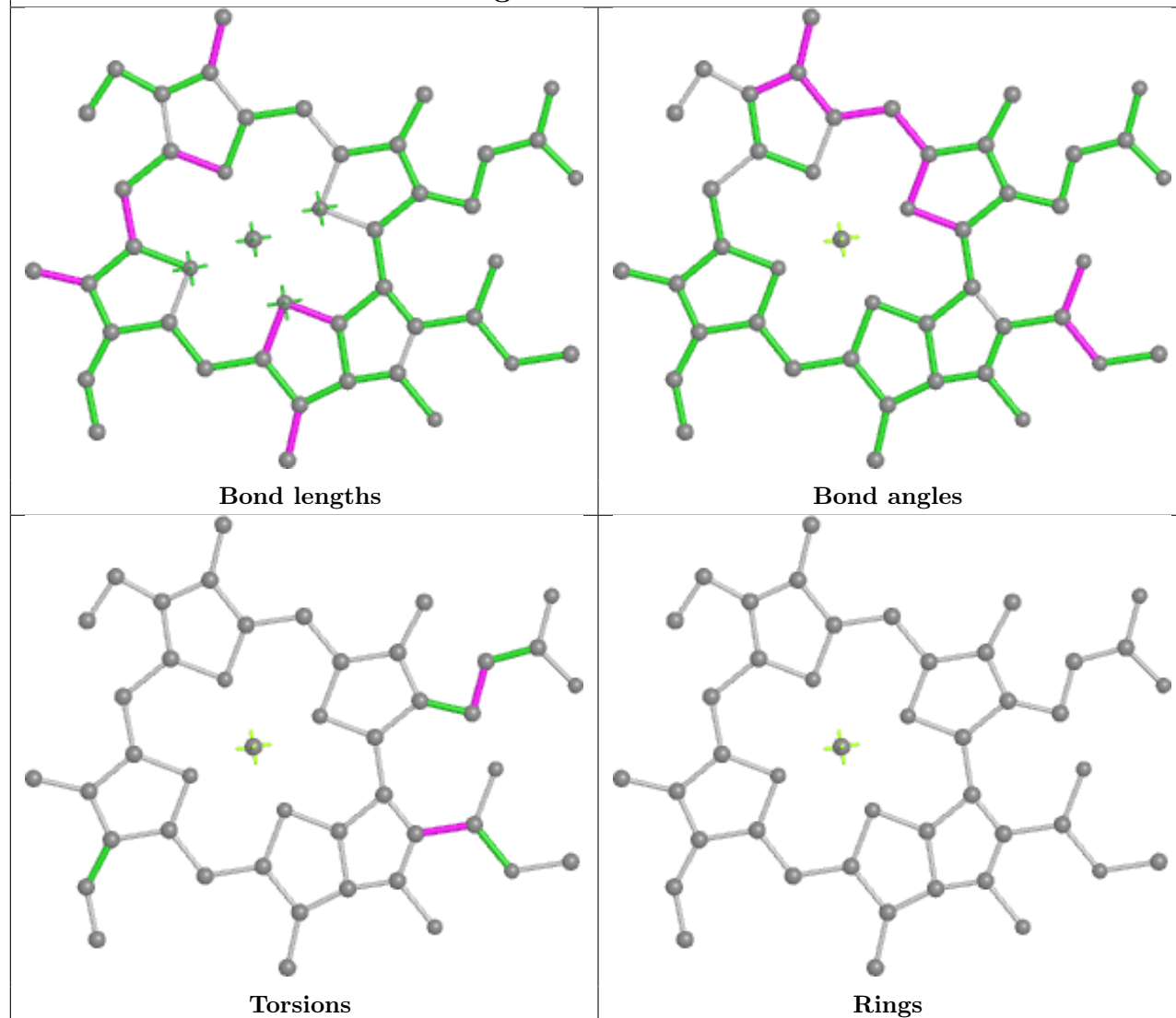


Ligand CLA H 1232

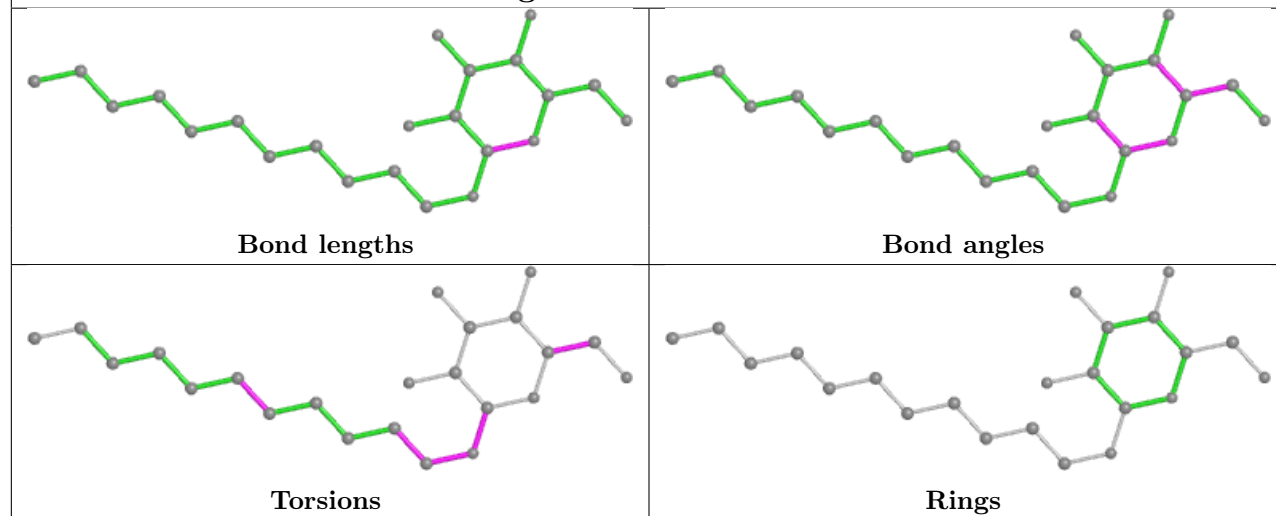


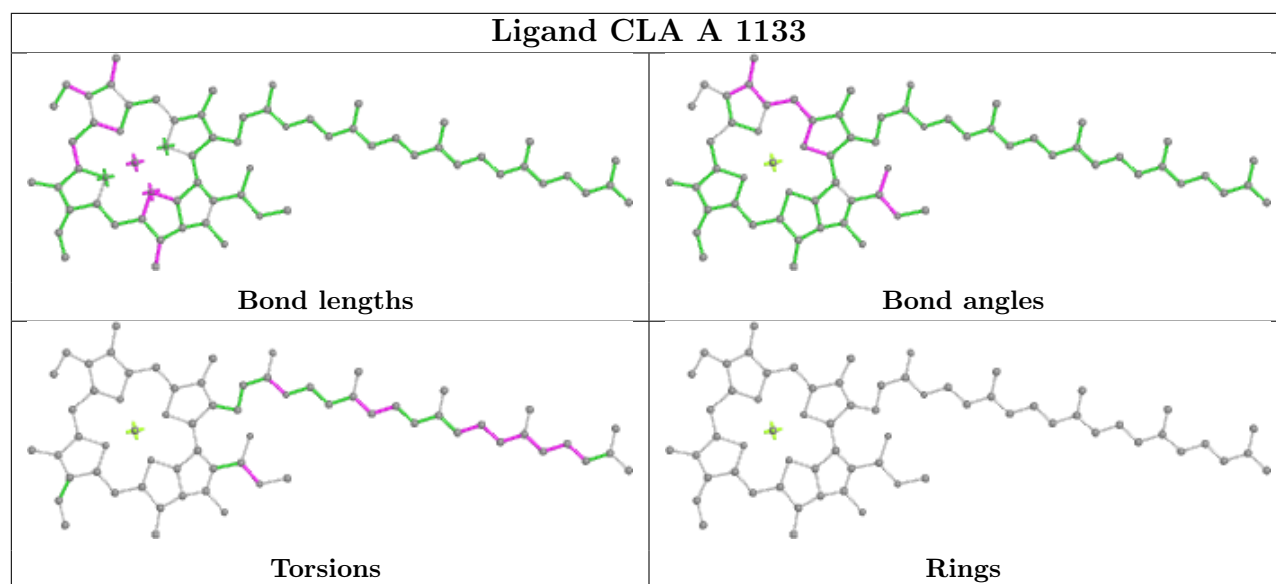
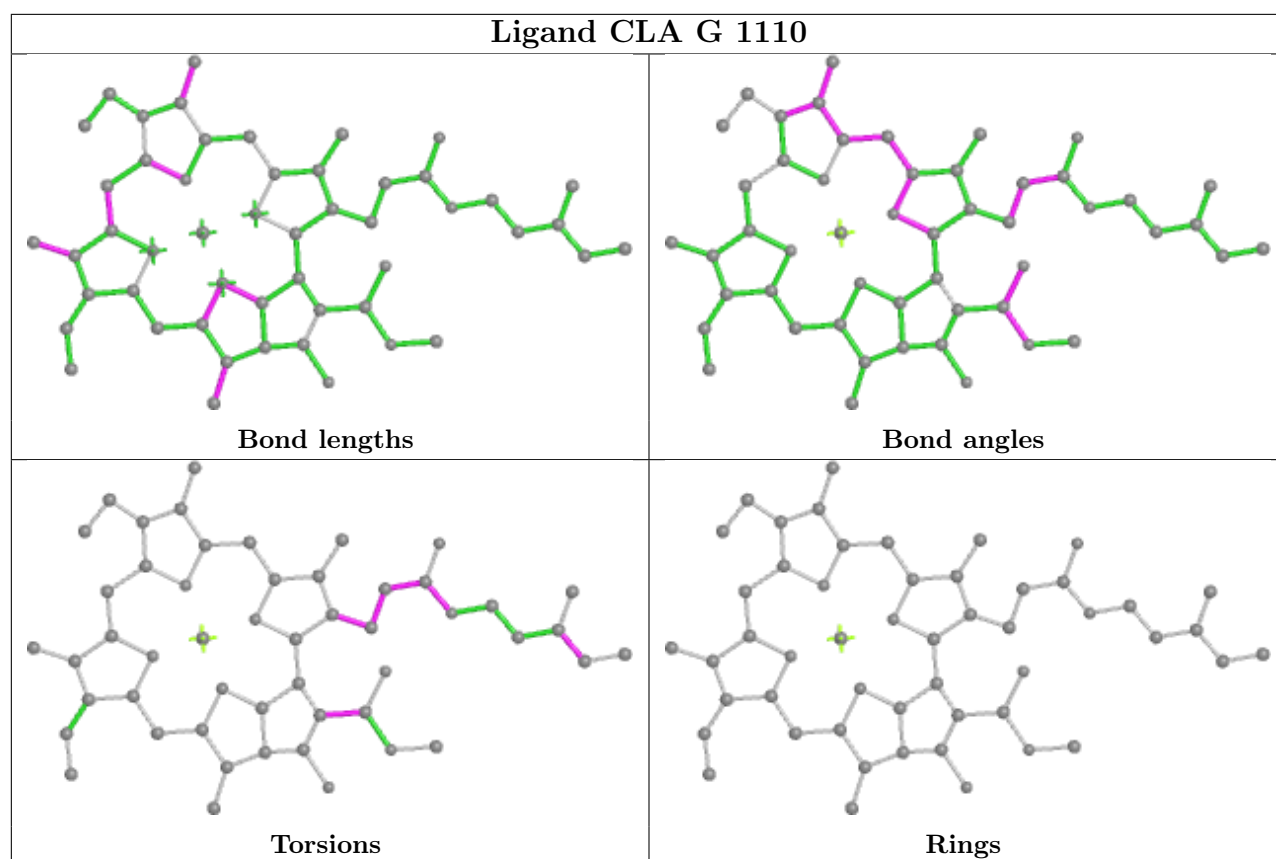


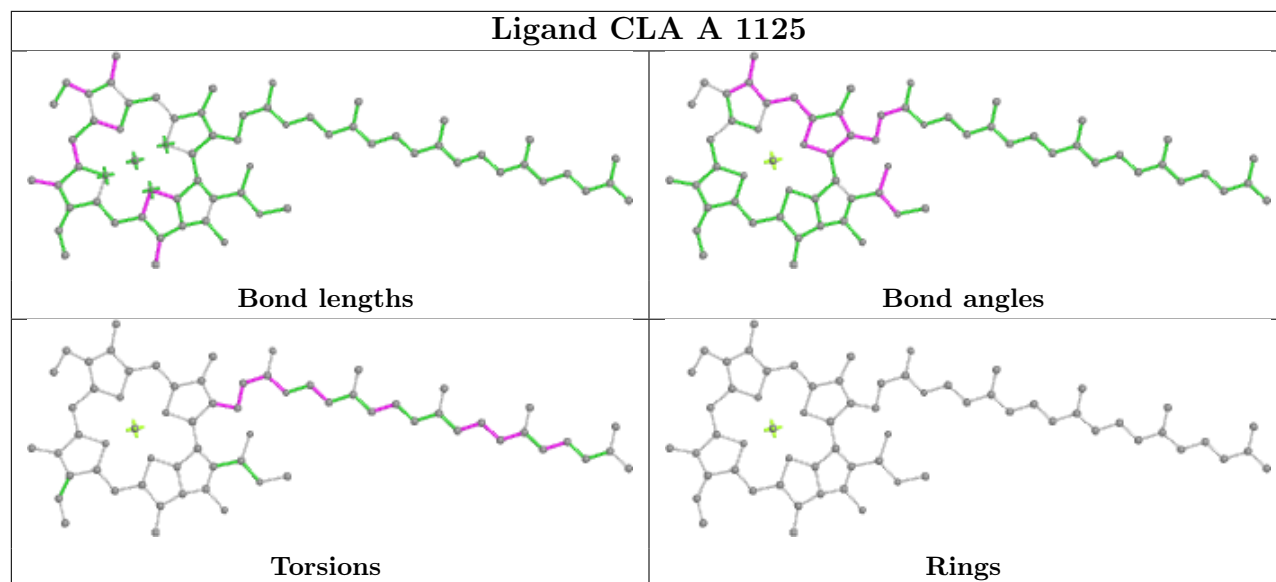
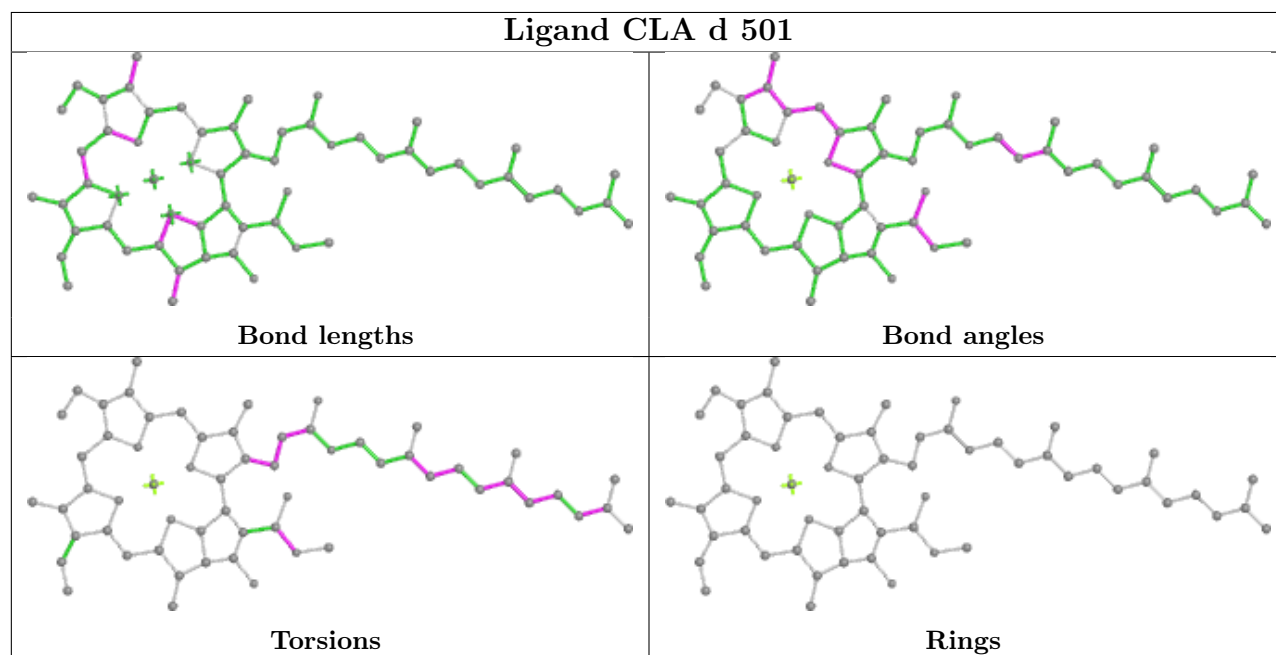
Ligand CLA 2 517



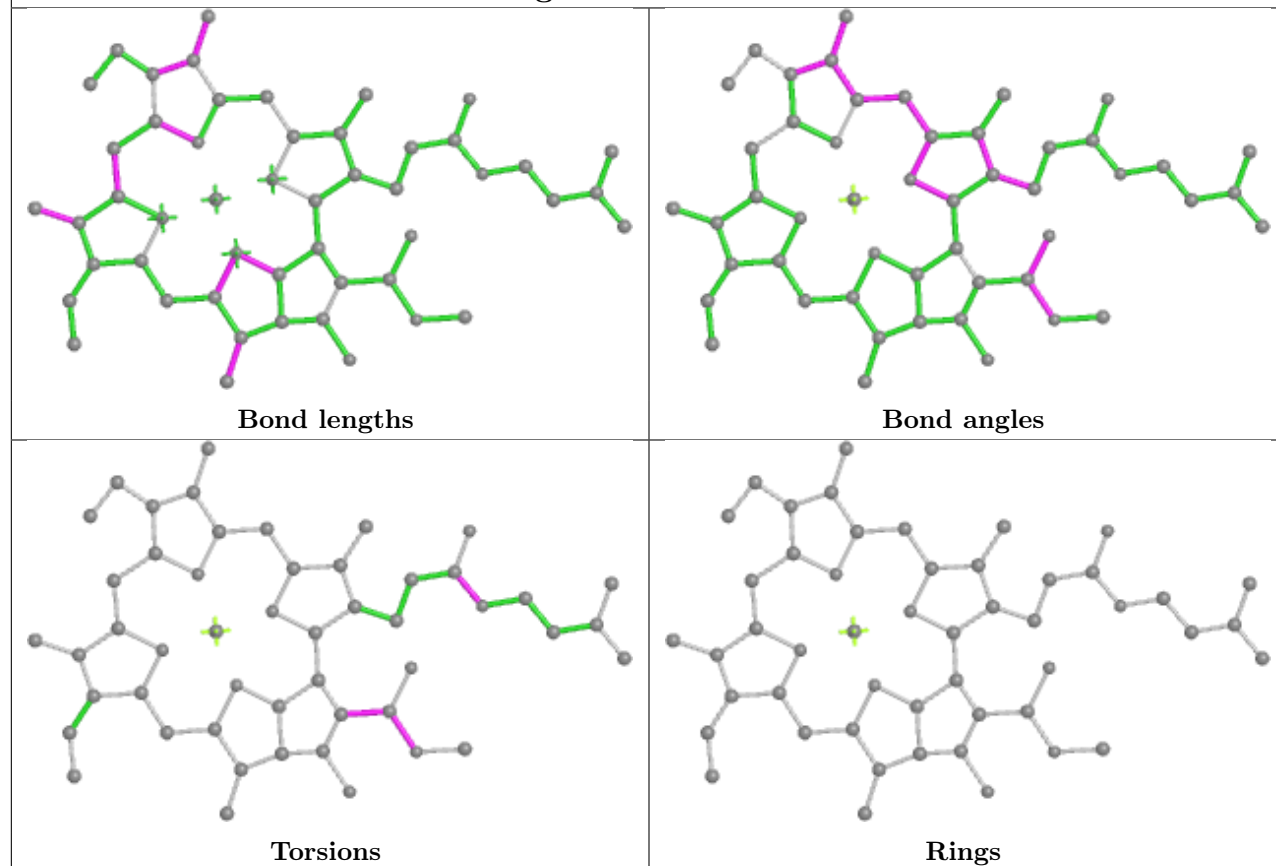
Ligand LMU G 1849



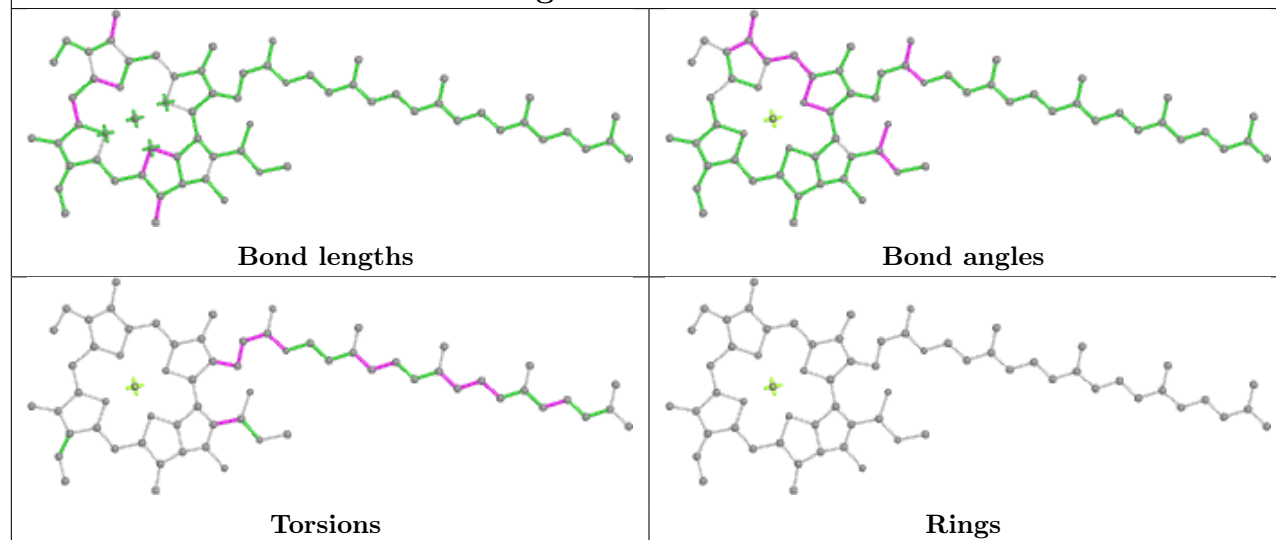


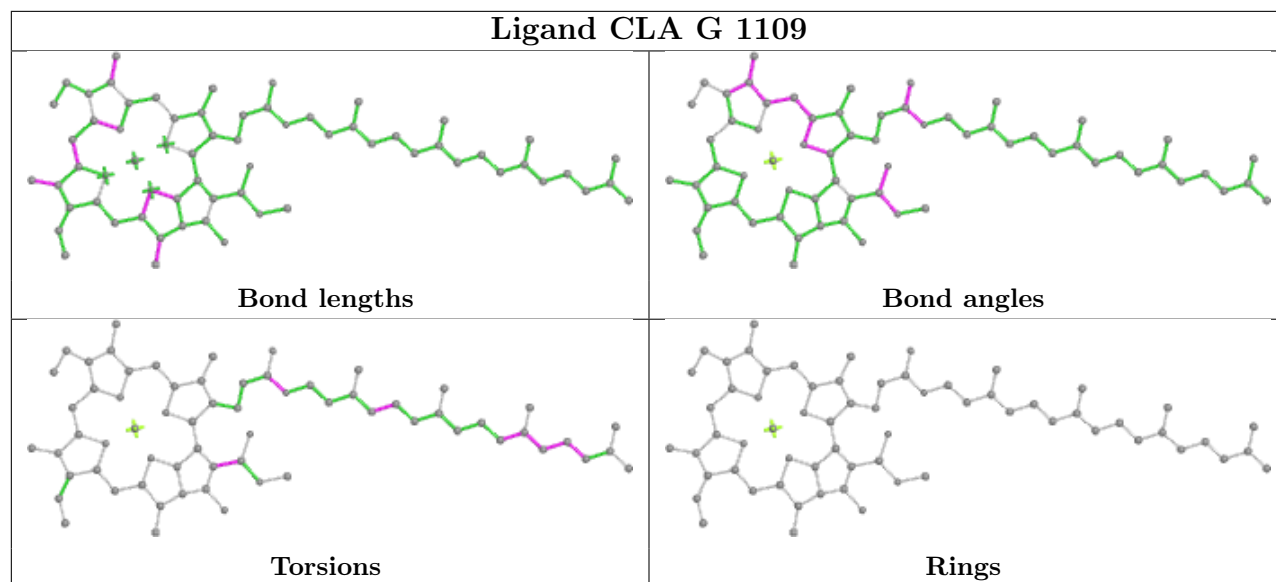
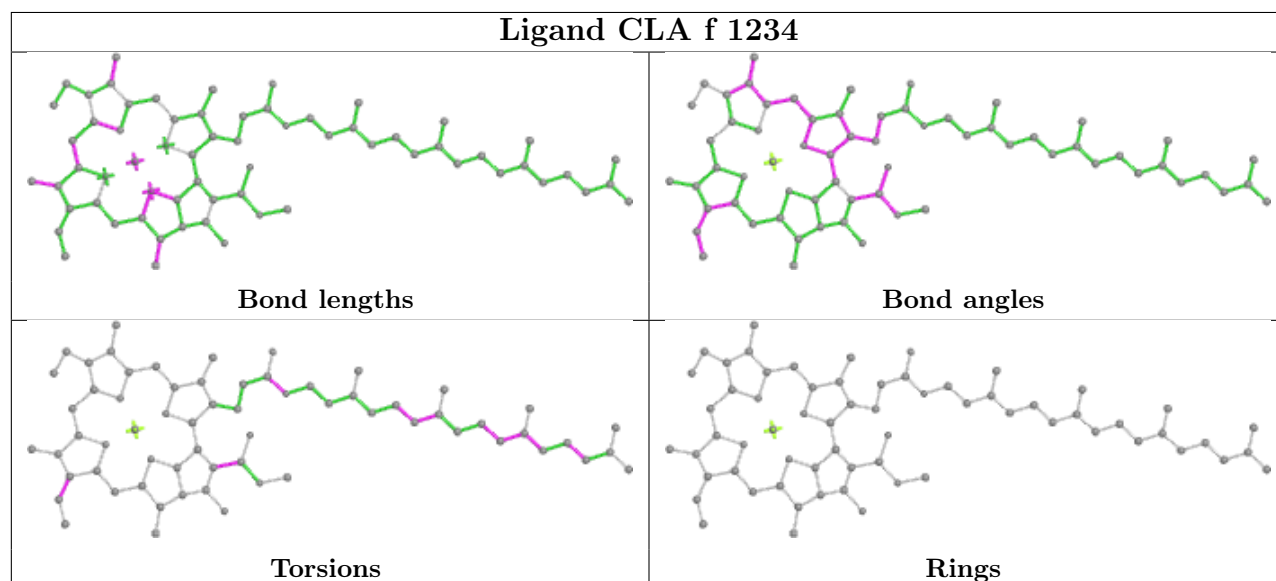
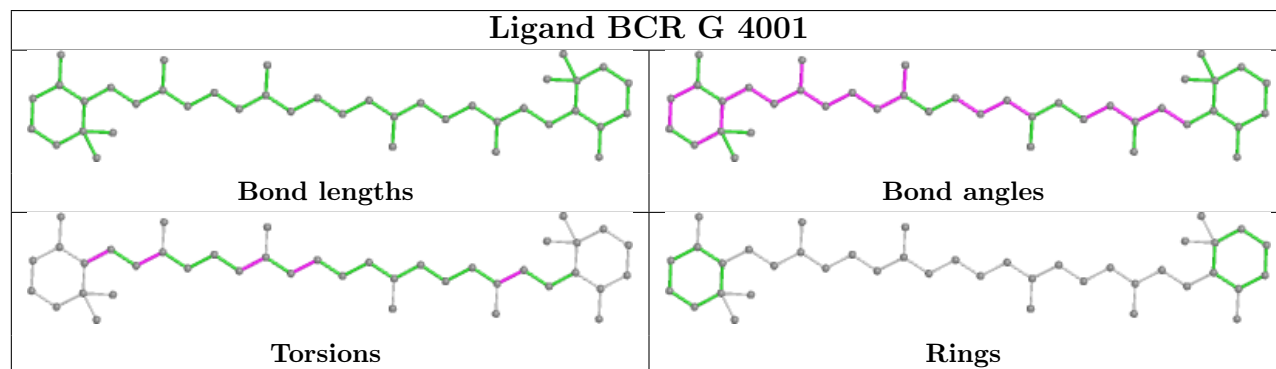
Ligand CLA A 1125**Ligand CLA d 501**

Ligand CLA u 502

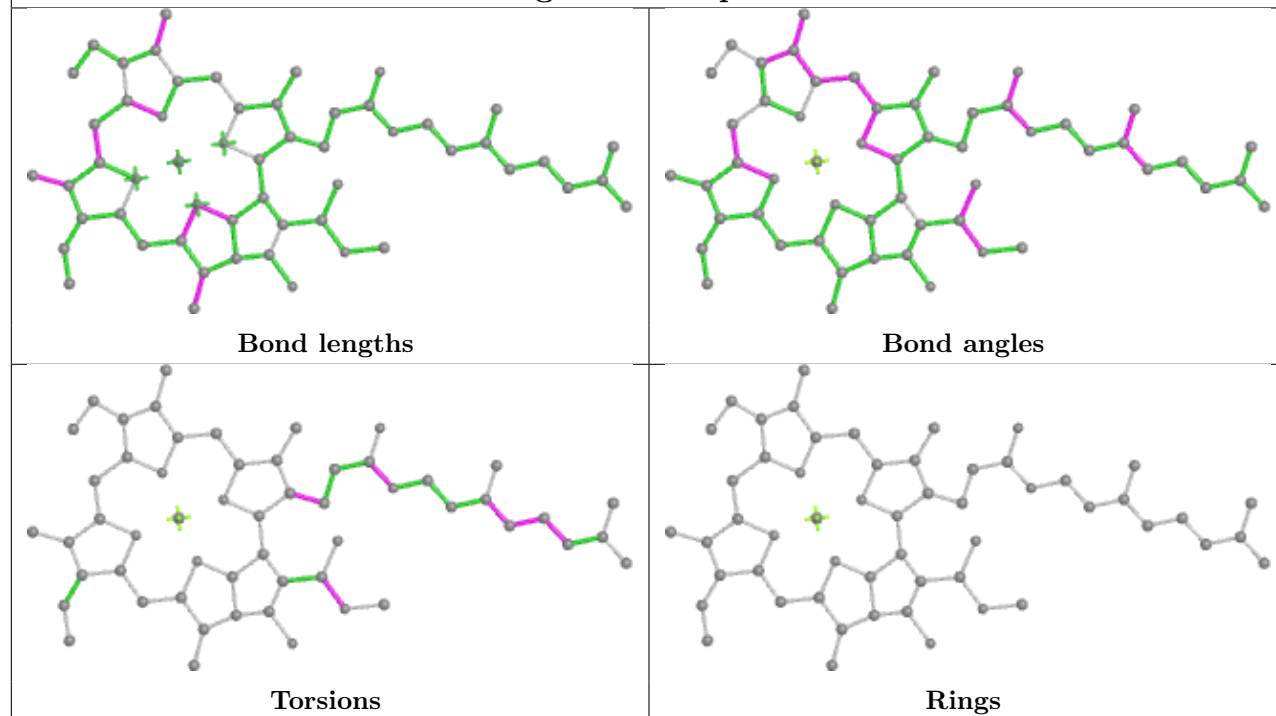


Ligand CLA 2 518

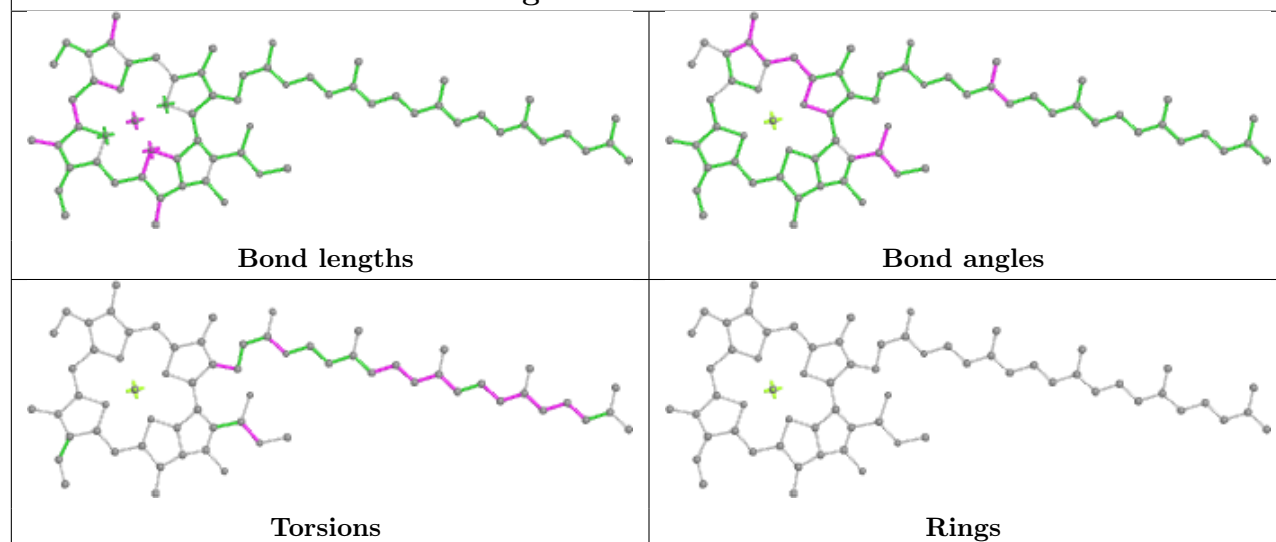


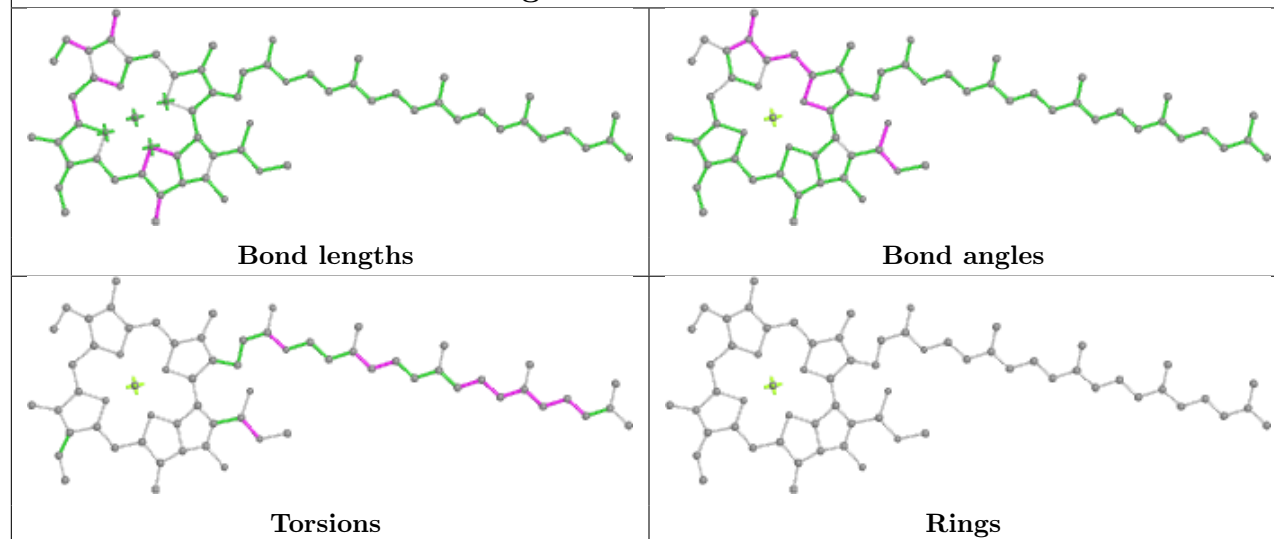
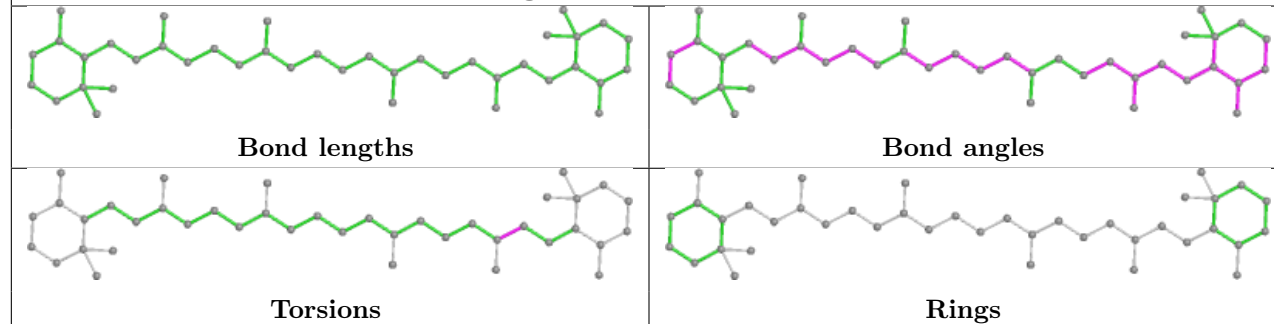
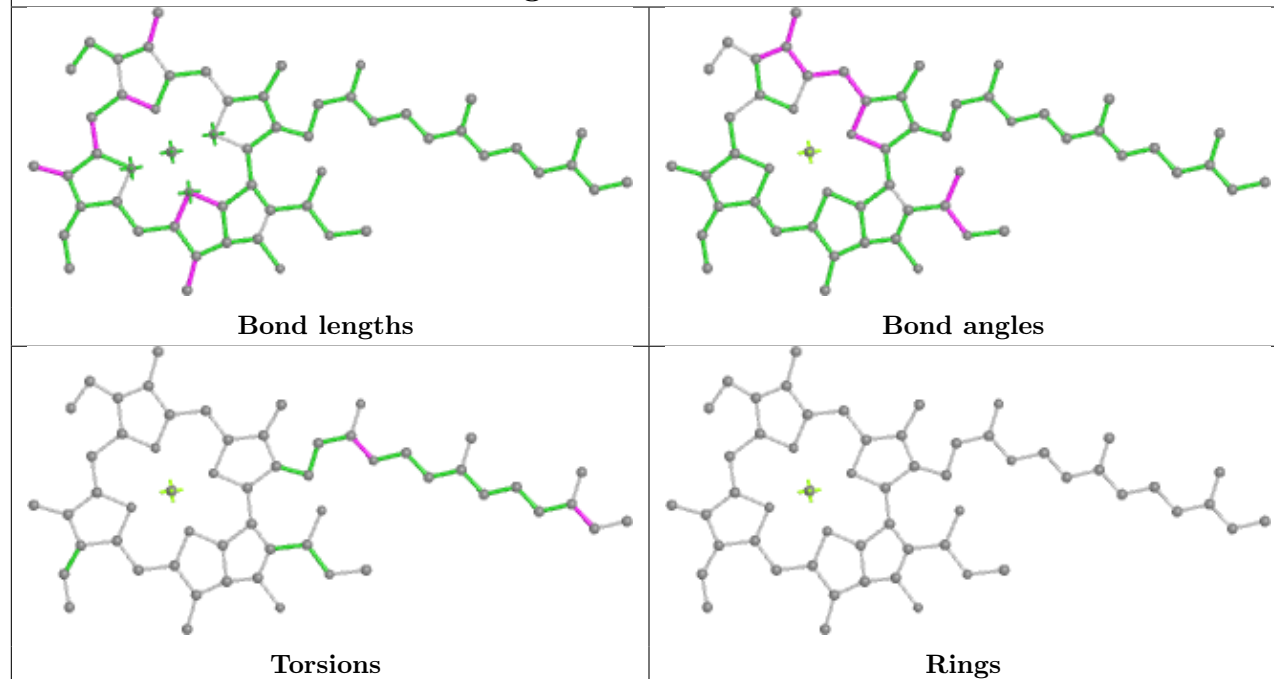
Ligand CLA G 1109**Ligand CLA f 1234****Ligand BCR G 4001**

Ligand CLA q 508

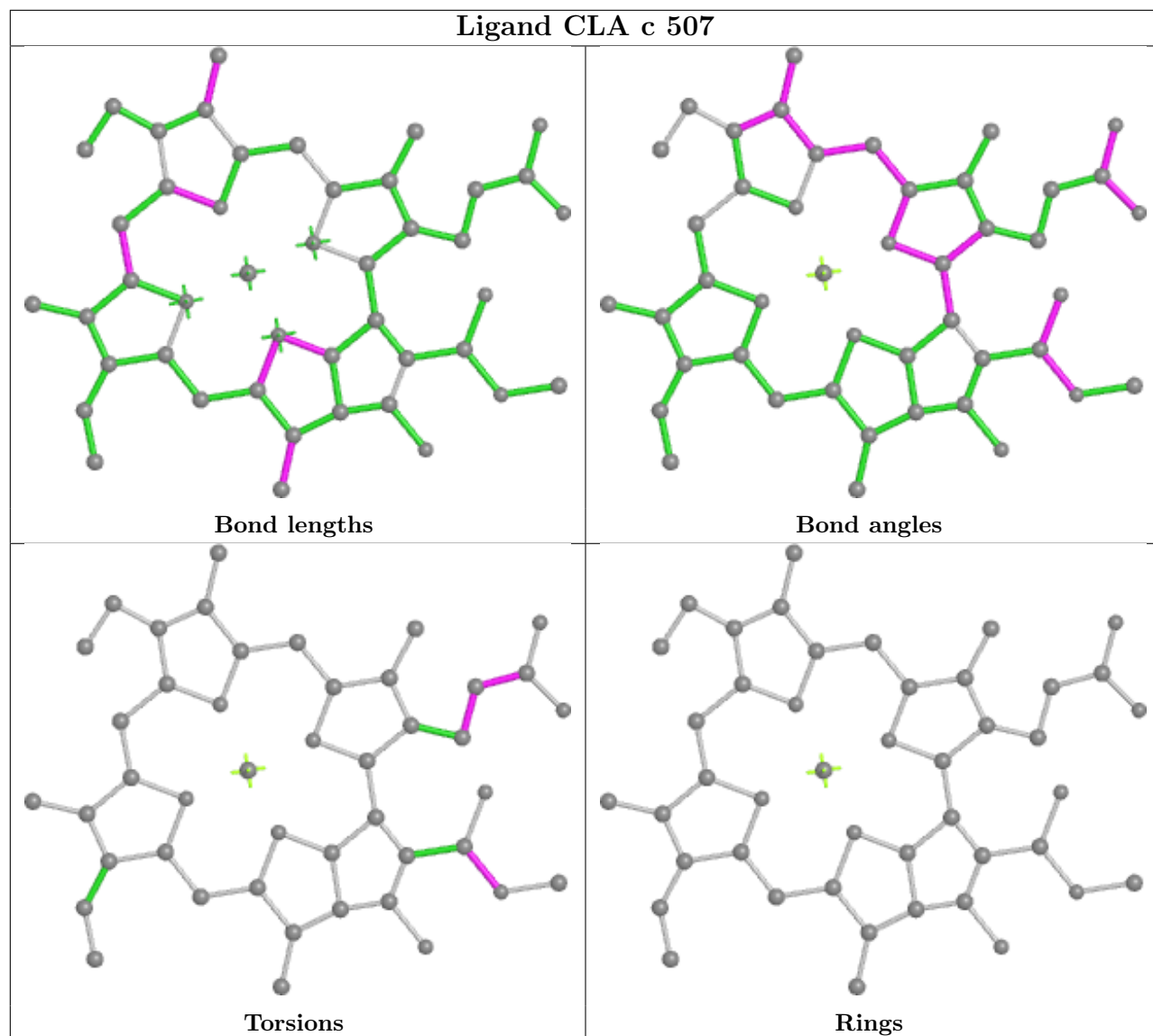


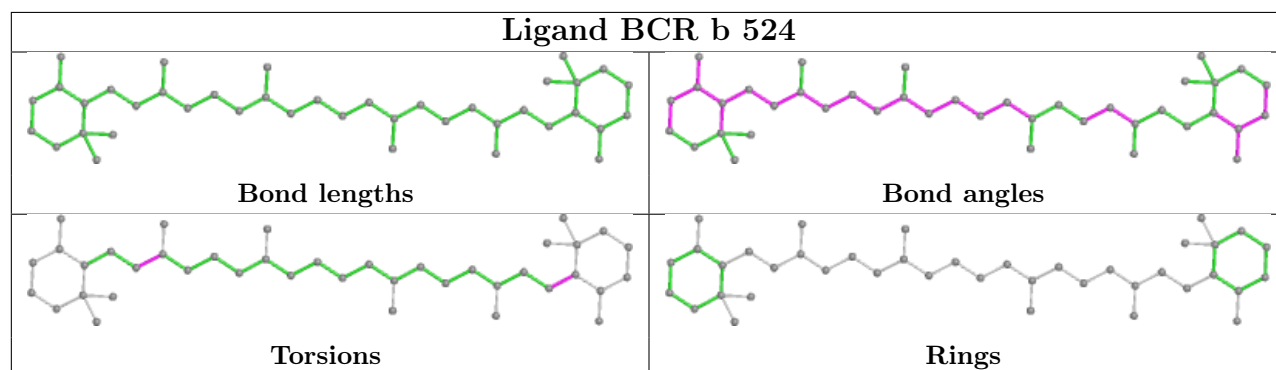
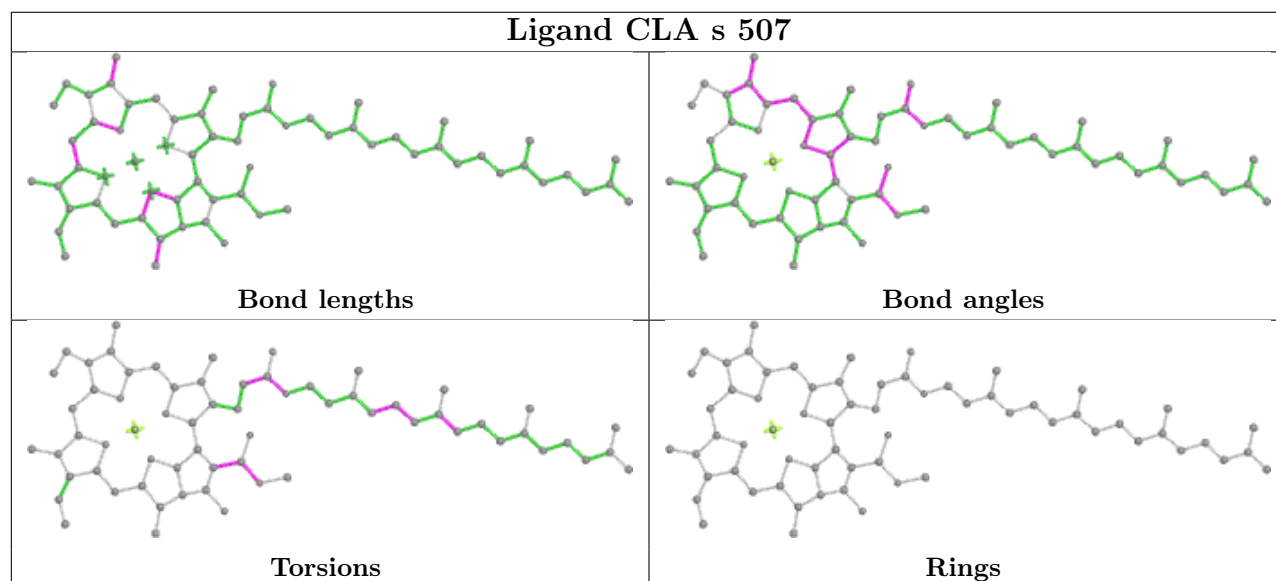
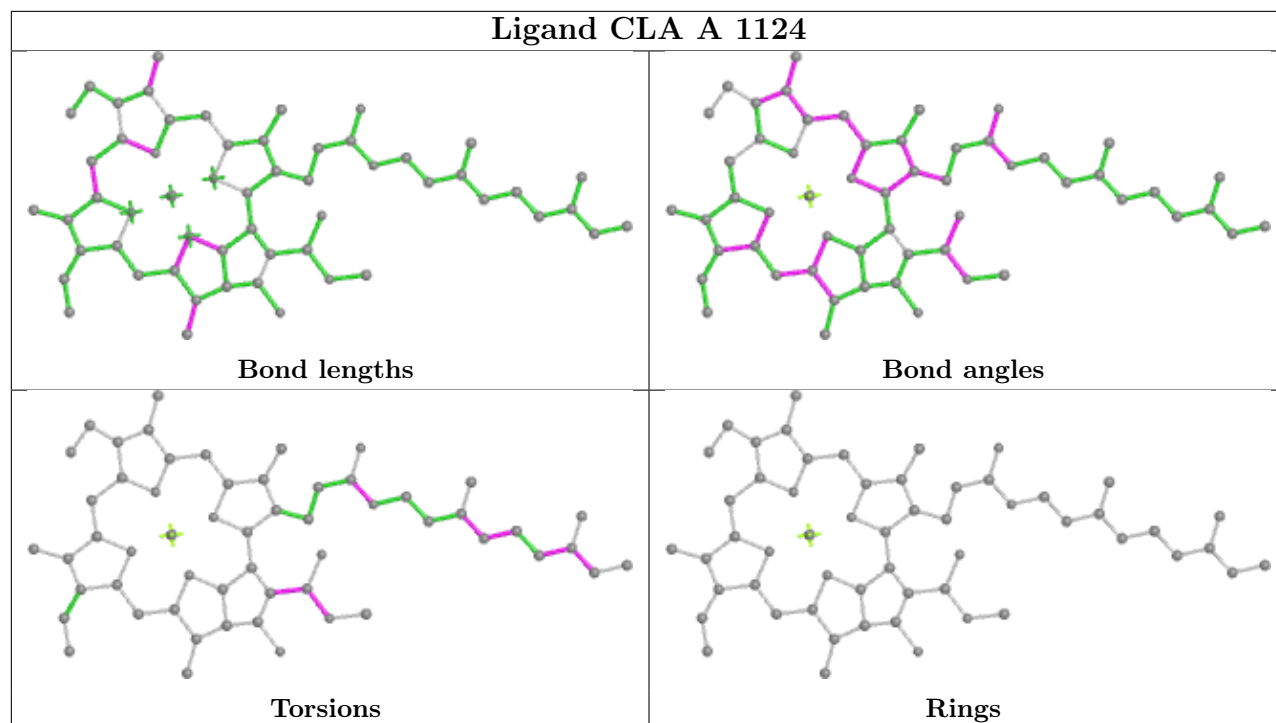
Ligand CLA H 1215



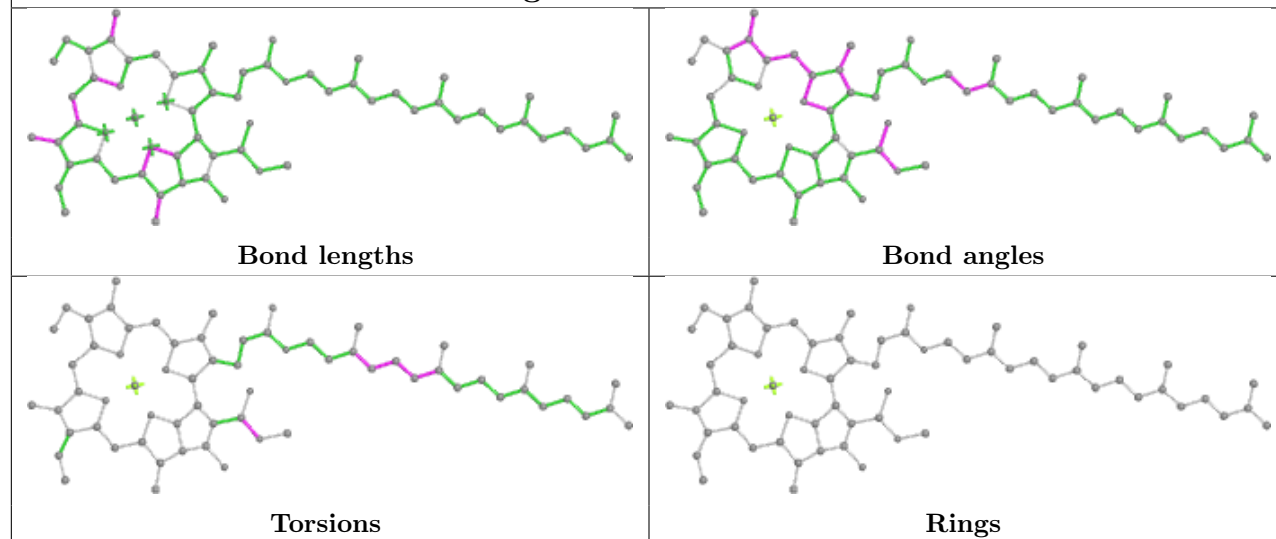
Ligand CLA G 1133**Ligand BCR U 4104****Ligand CLA B 1211**

Ligand CLA c 507

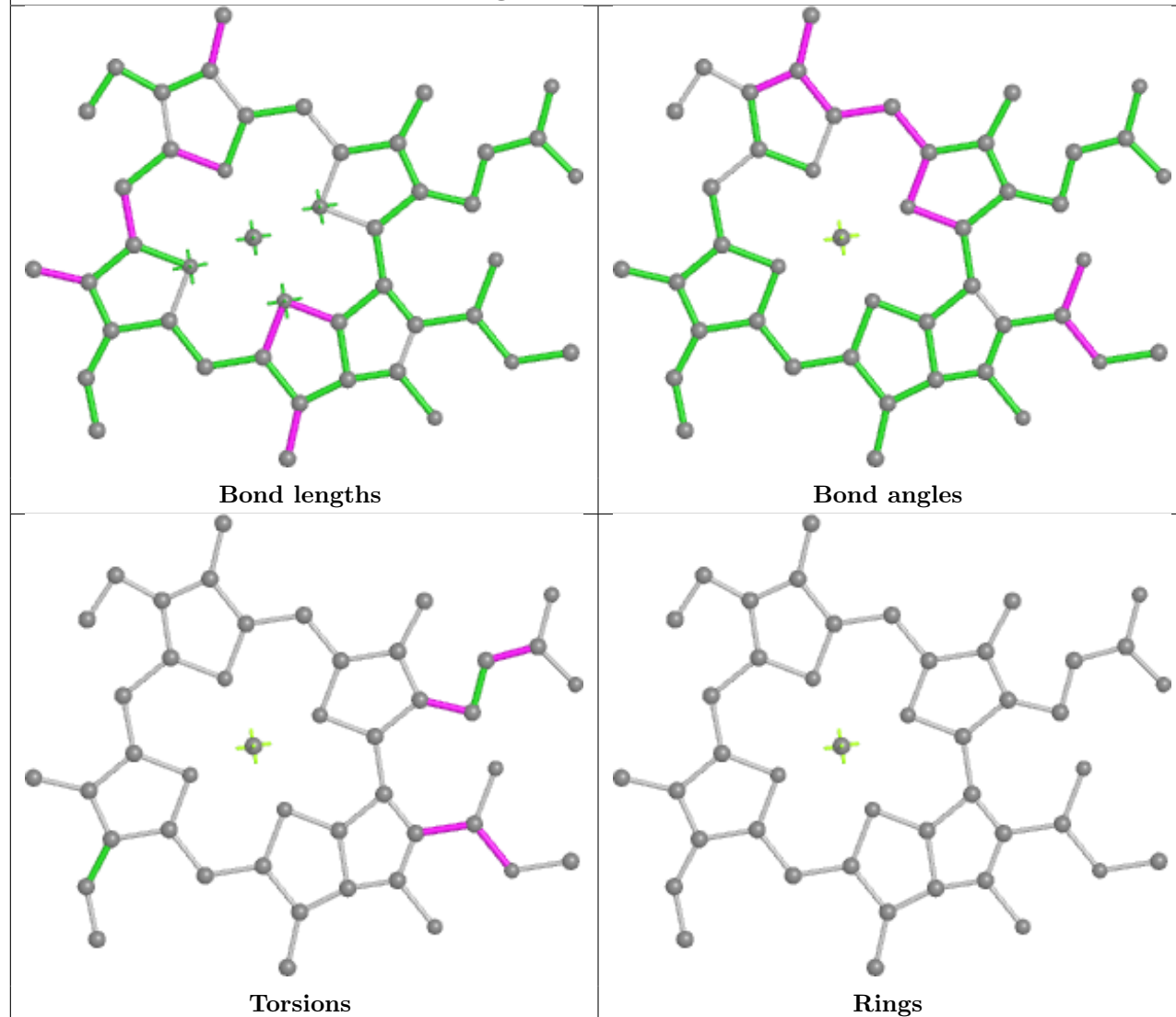


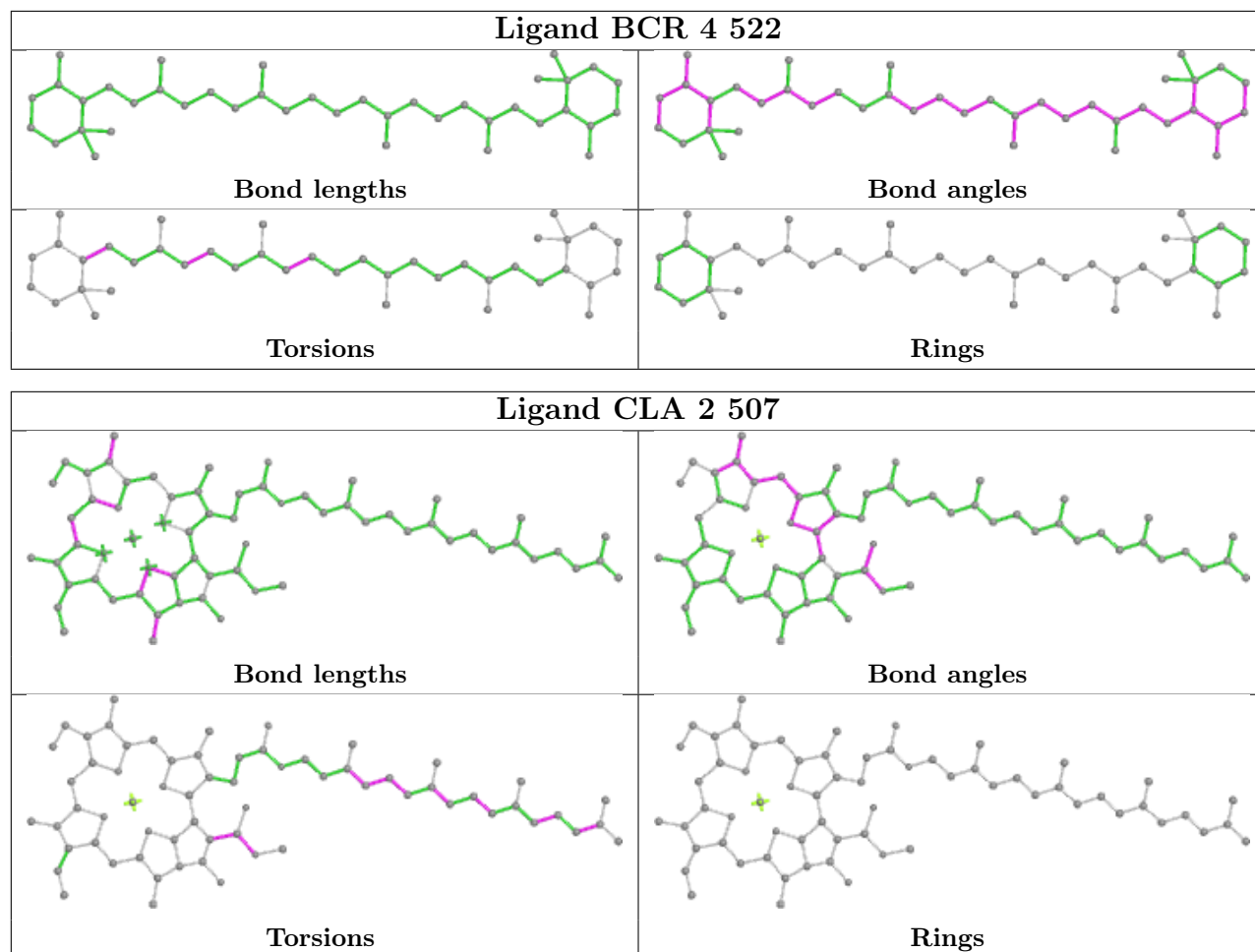


Ligand CLA B 1231

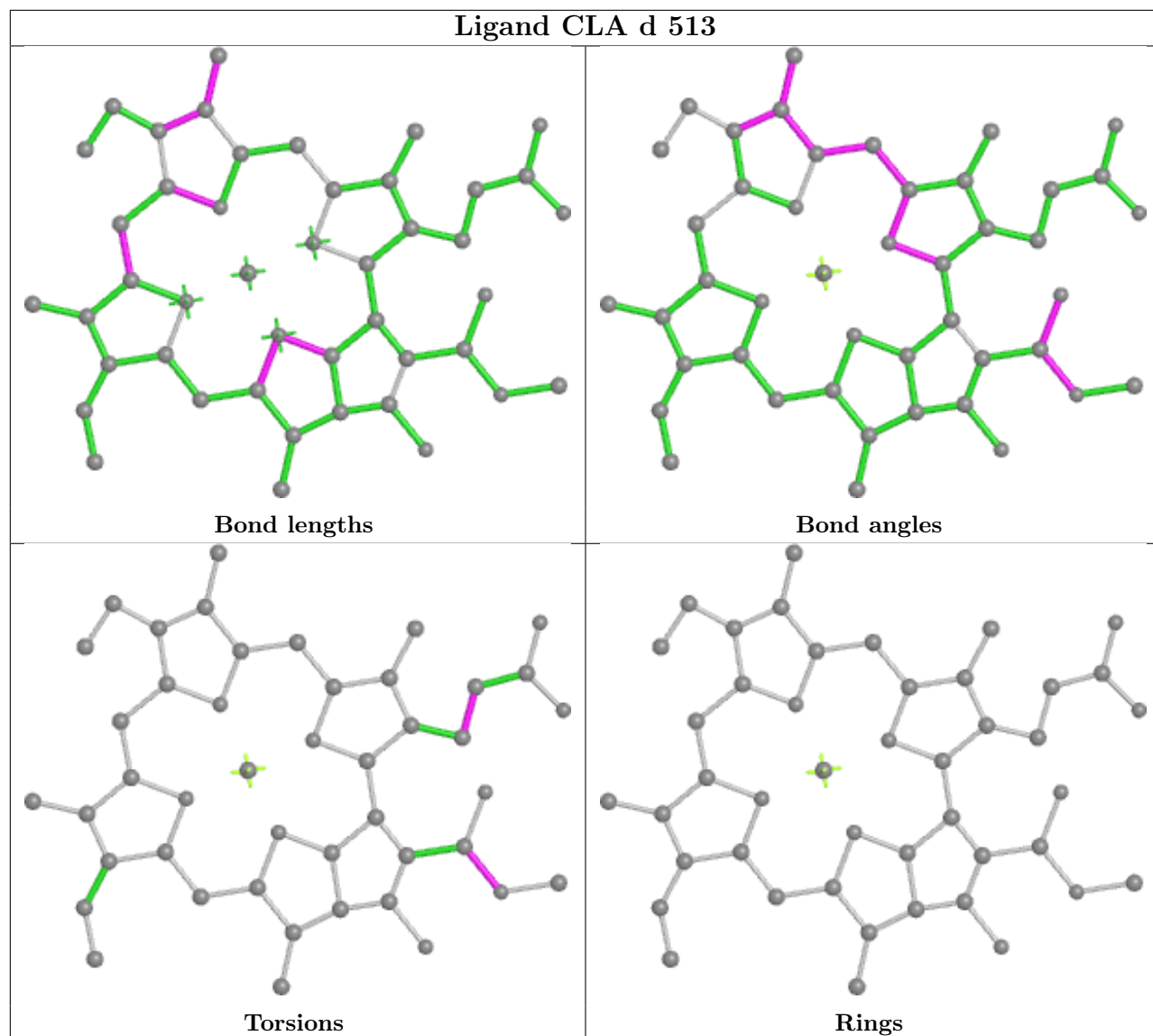


Ligand CLA d 517

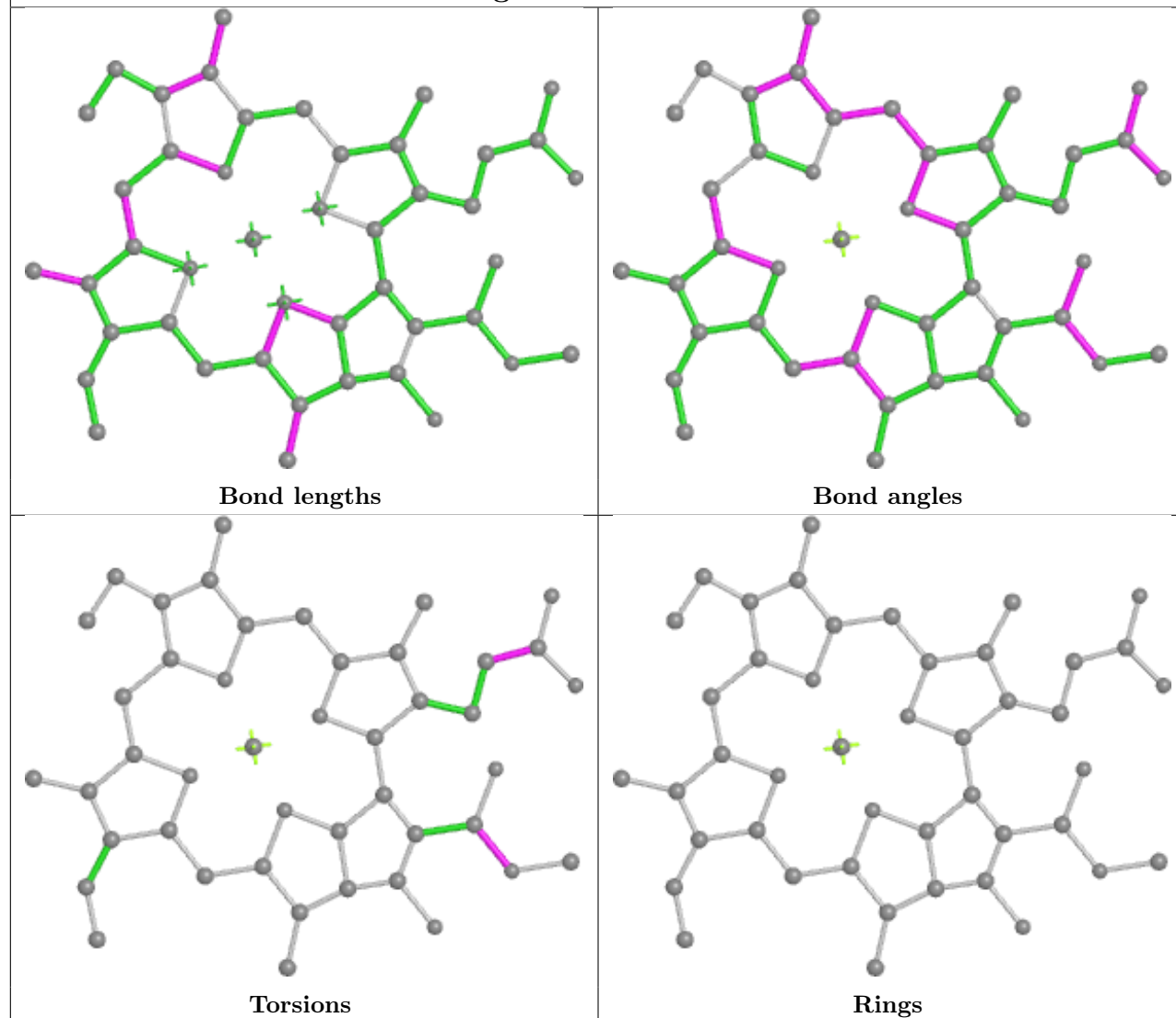




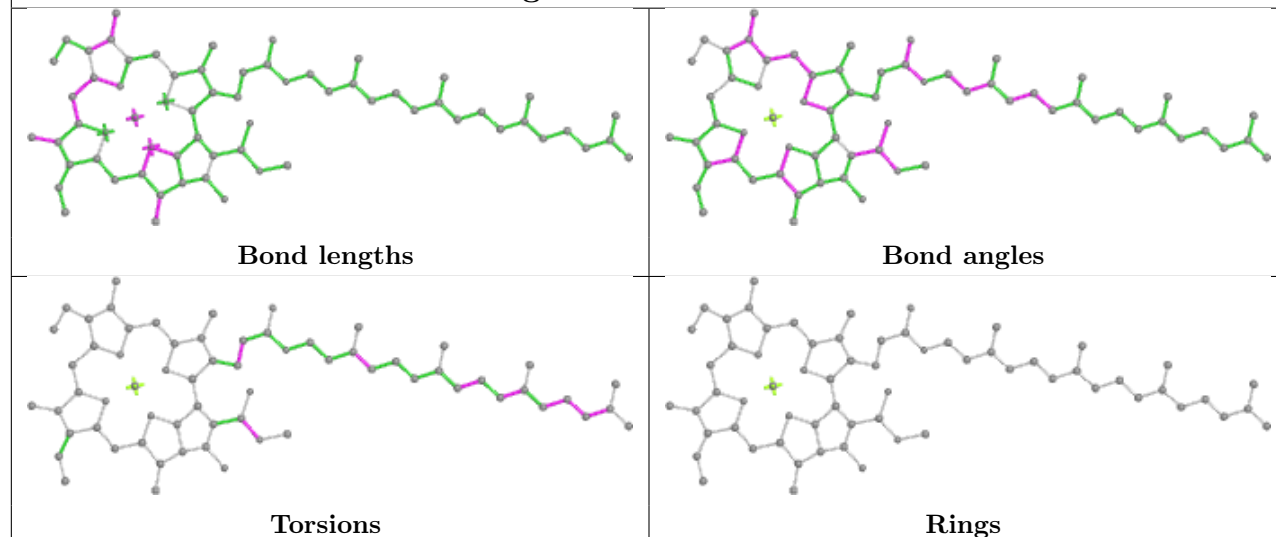
Ligand CLA d 513

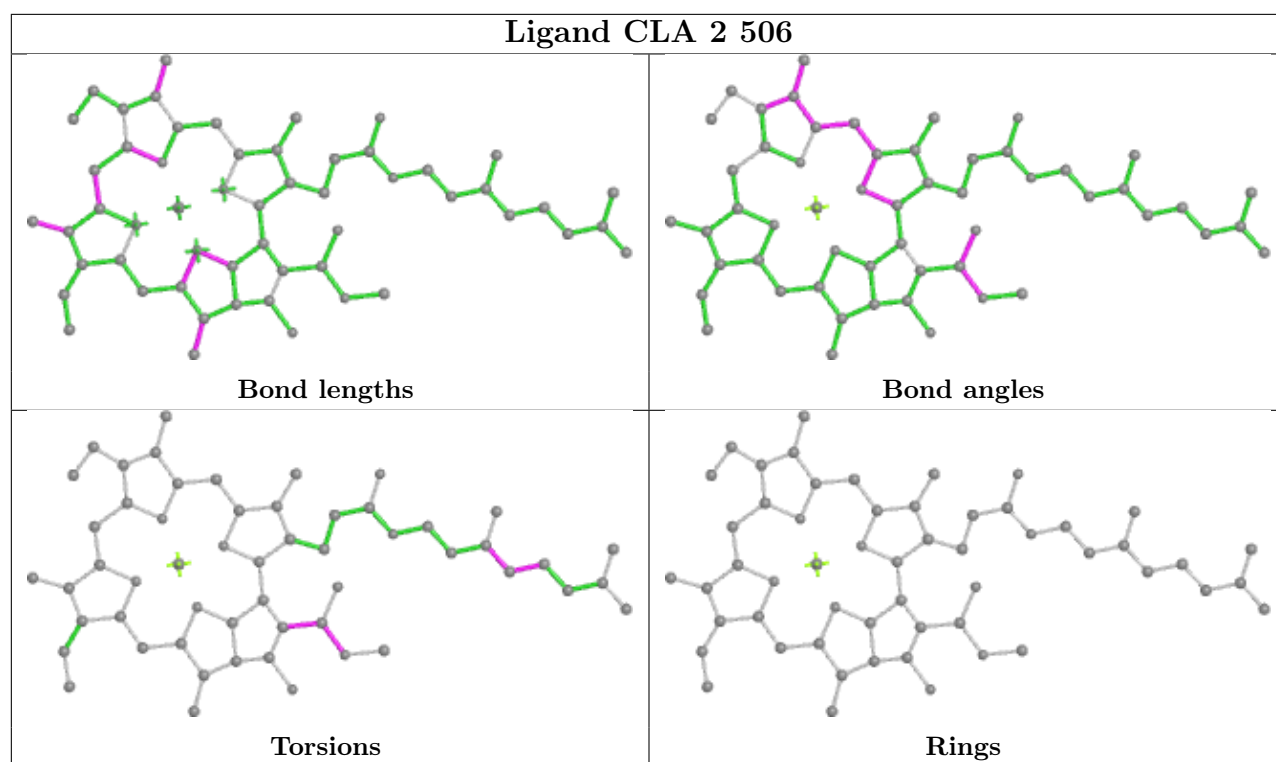


Ligand CLA b 508

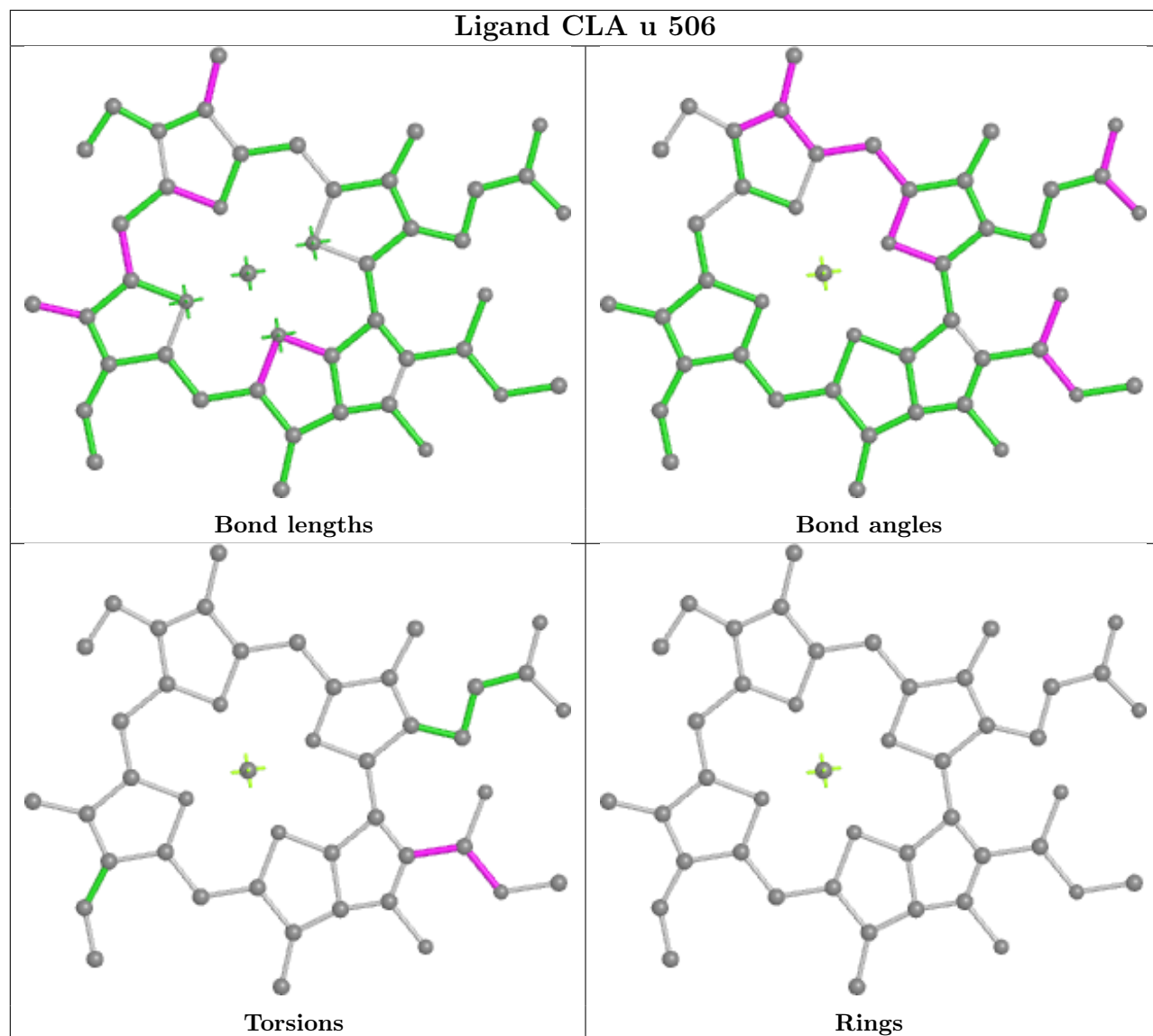


Ligand CLA A 1117

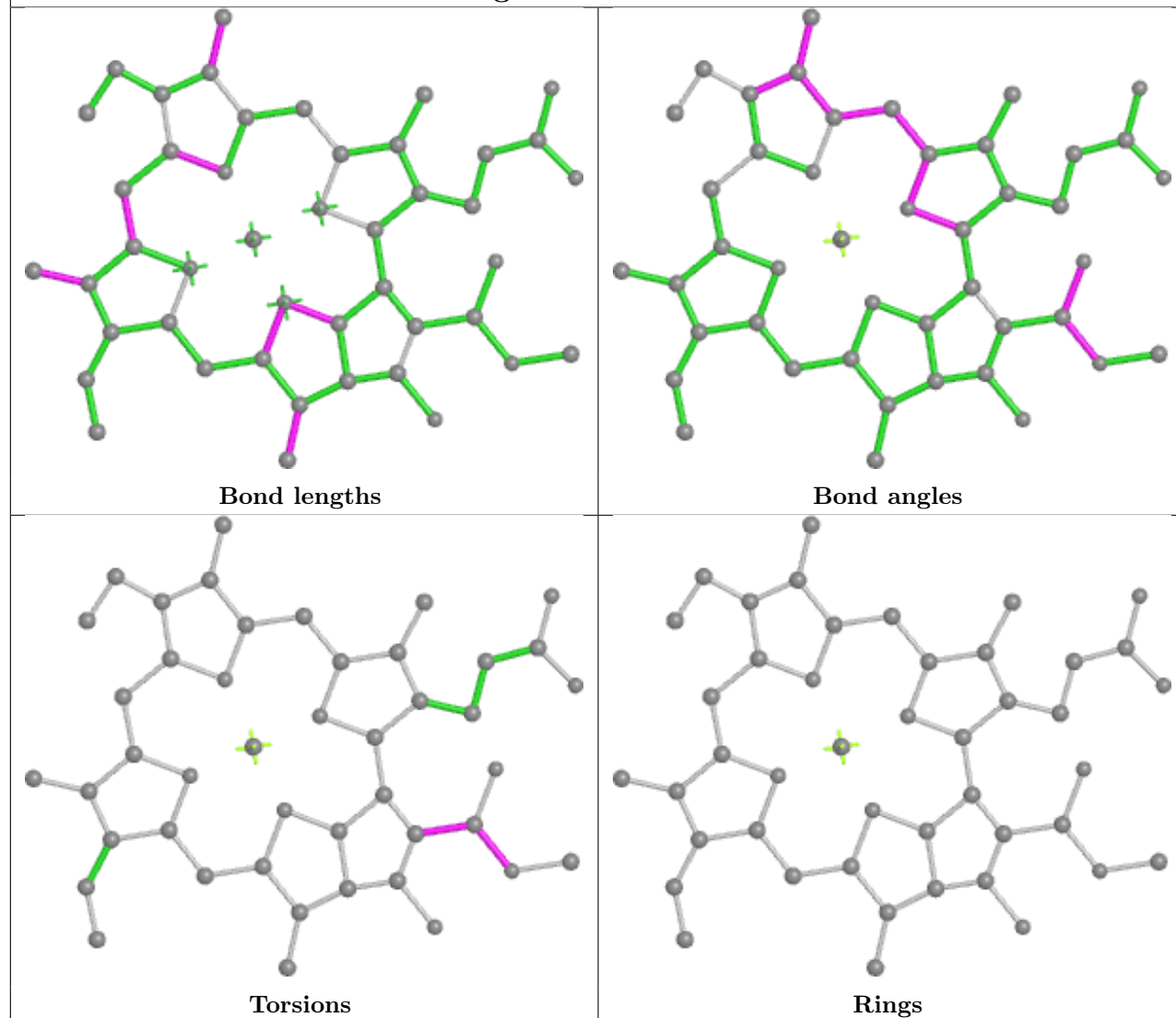




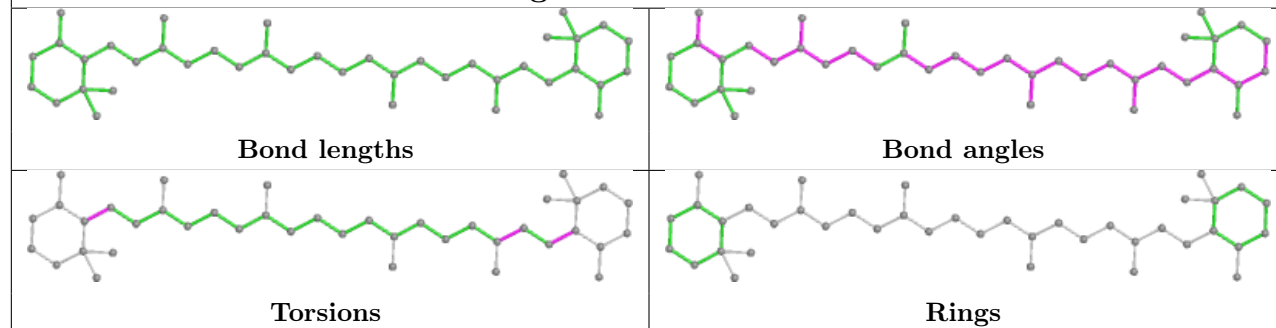
Ligand CLA u 506

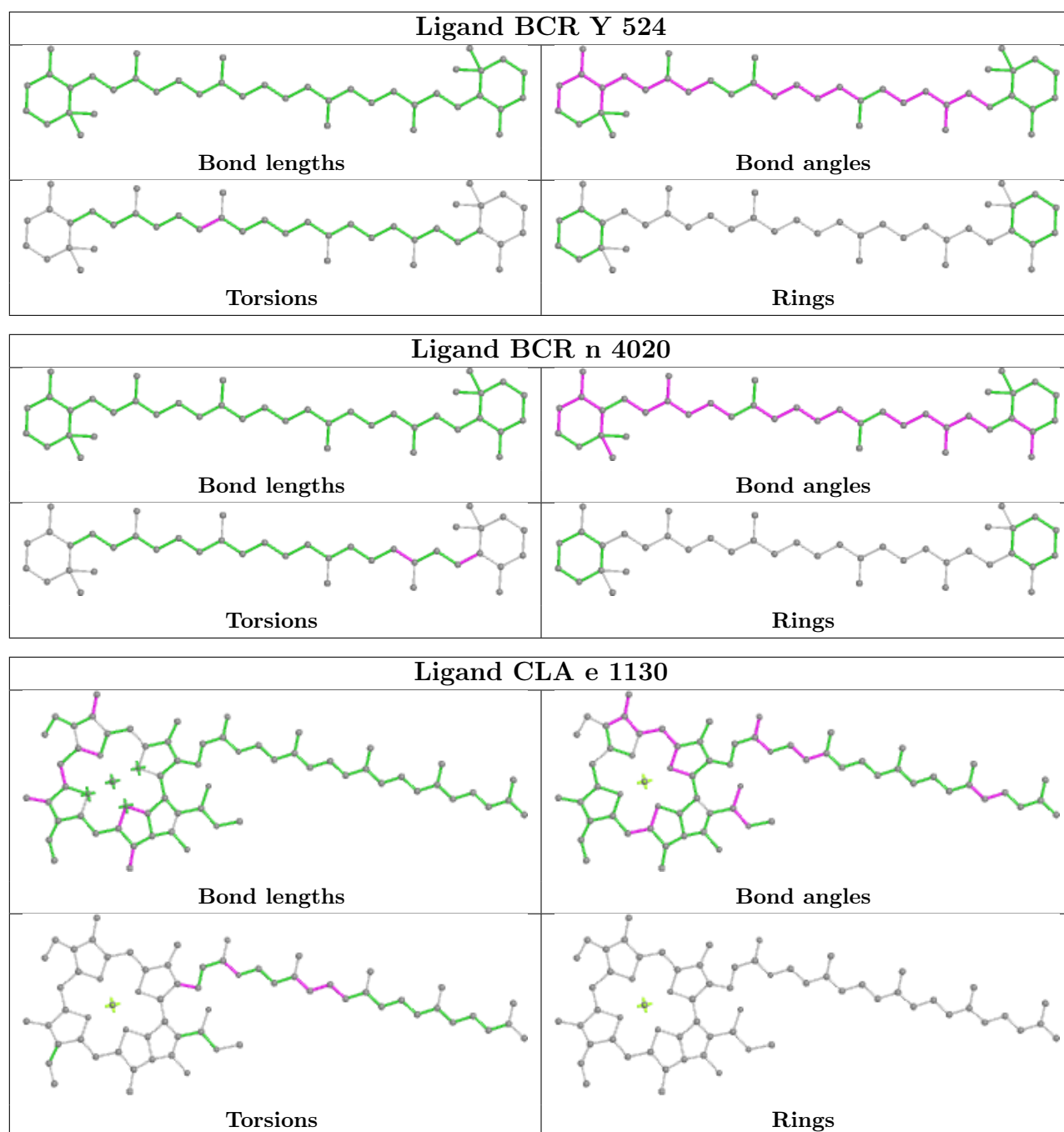


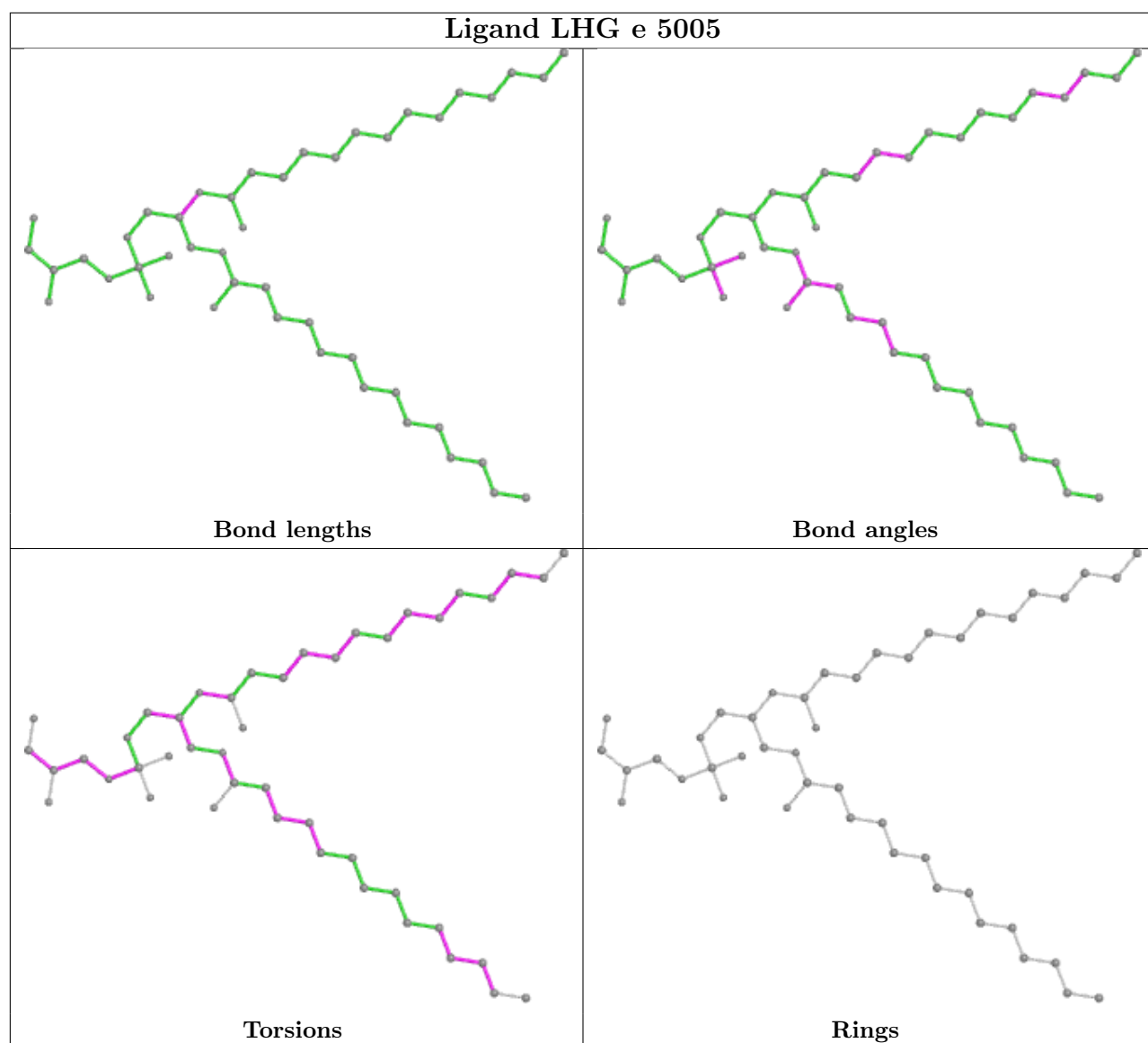
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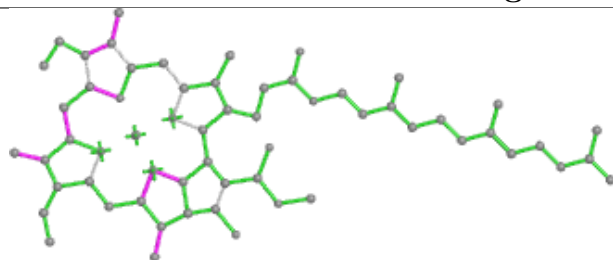
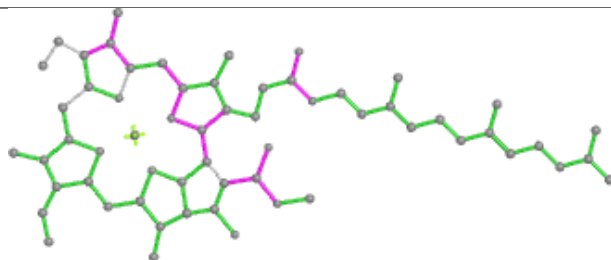
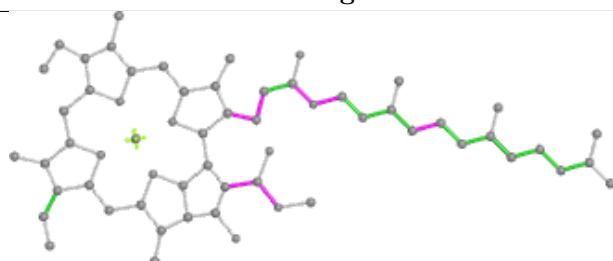
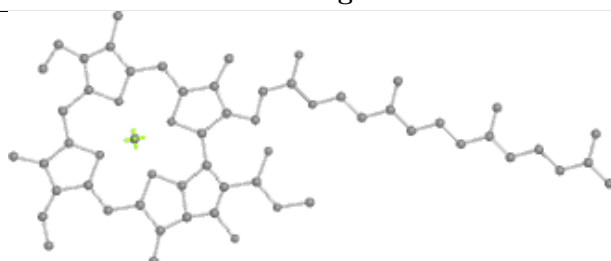
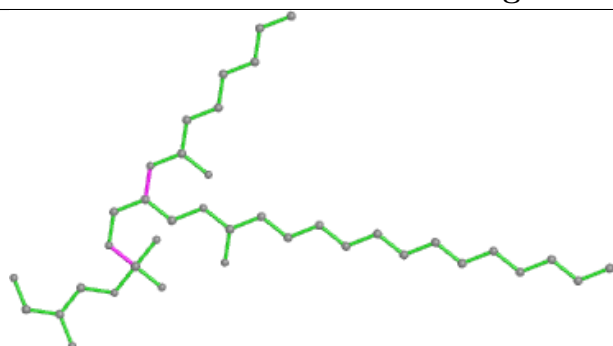
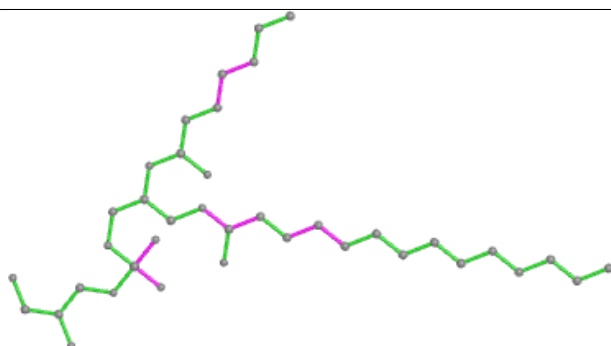
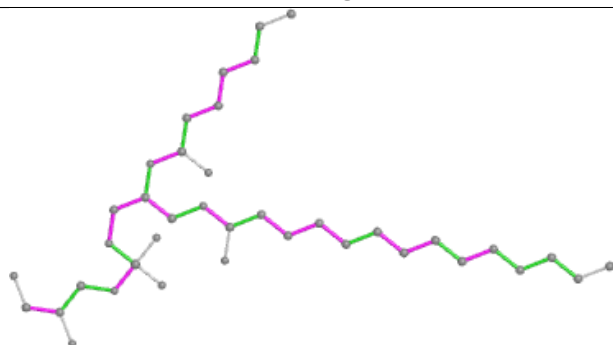
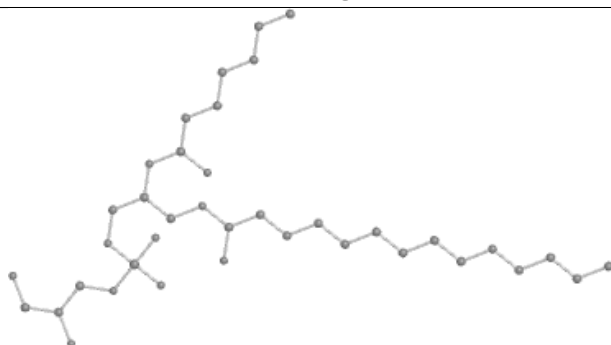


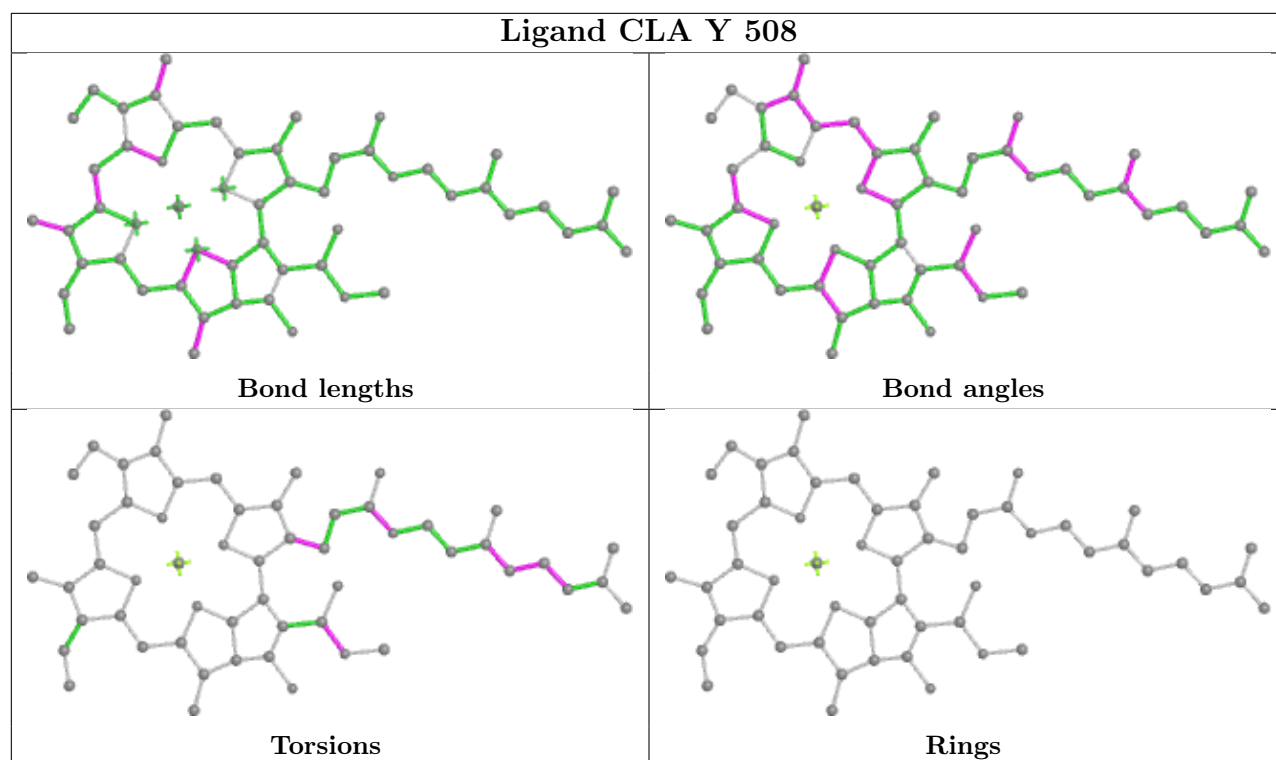
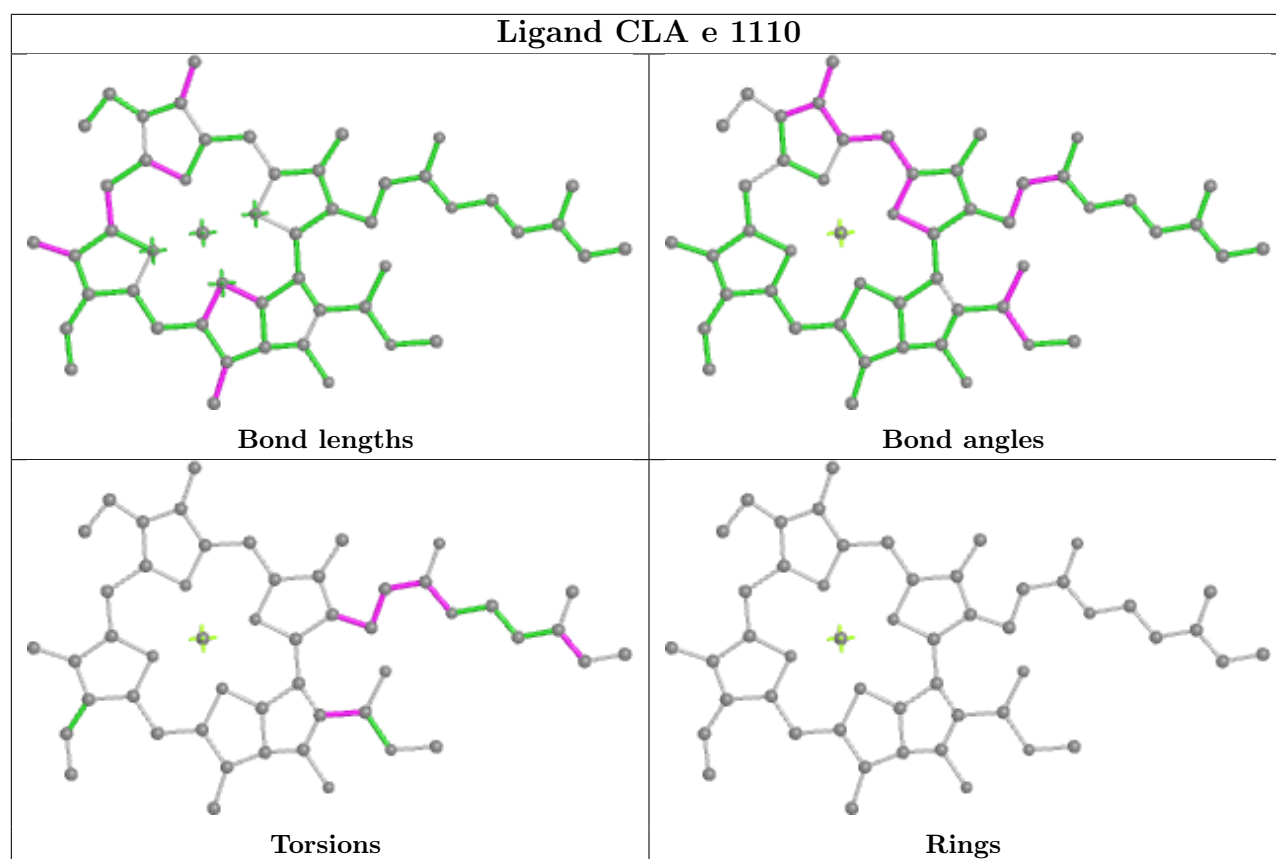
Ligand BCR Y 523



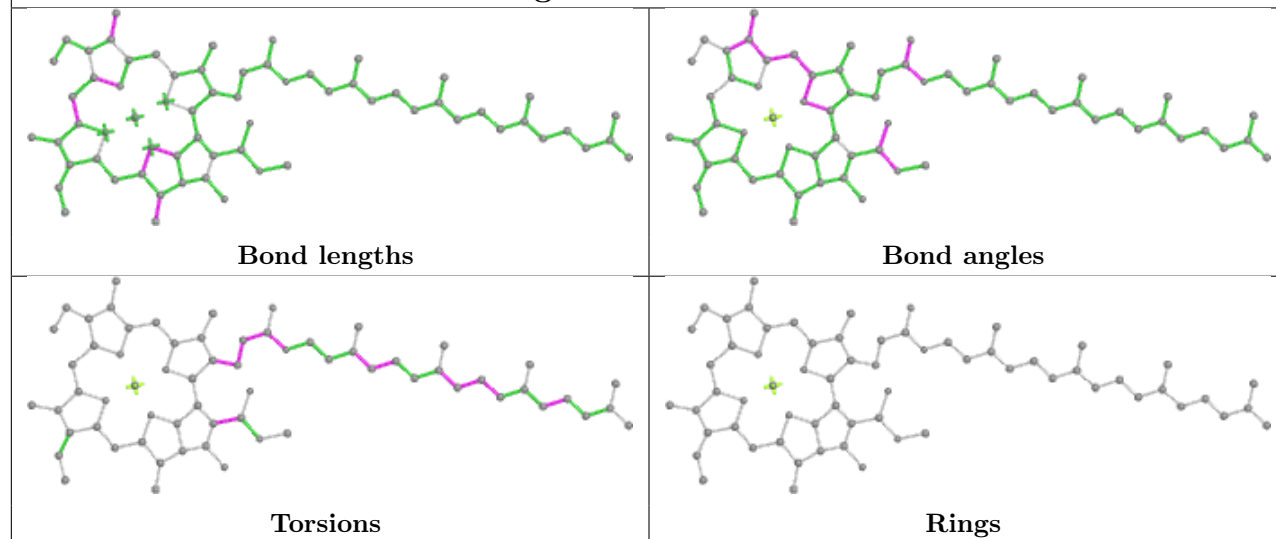




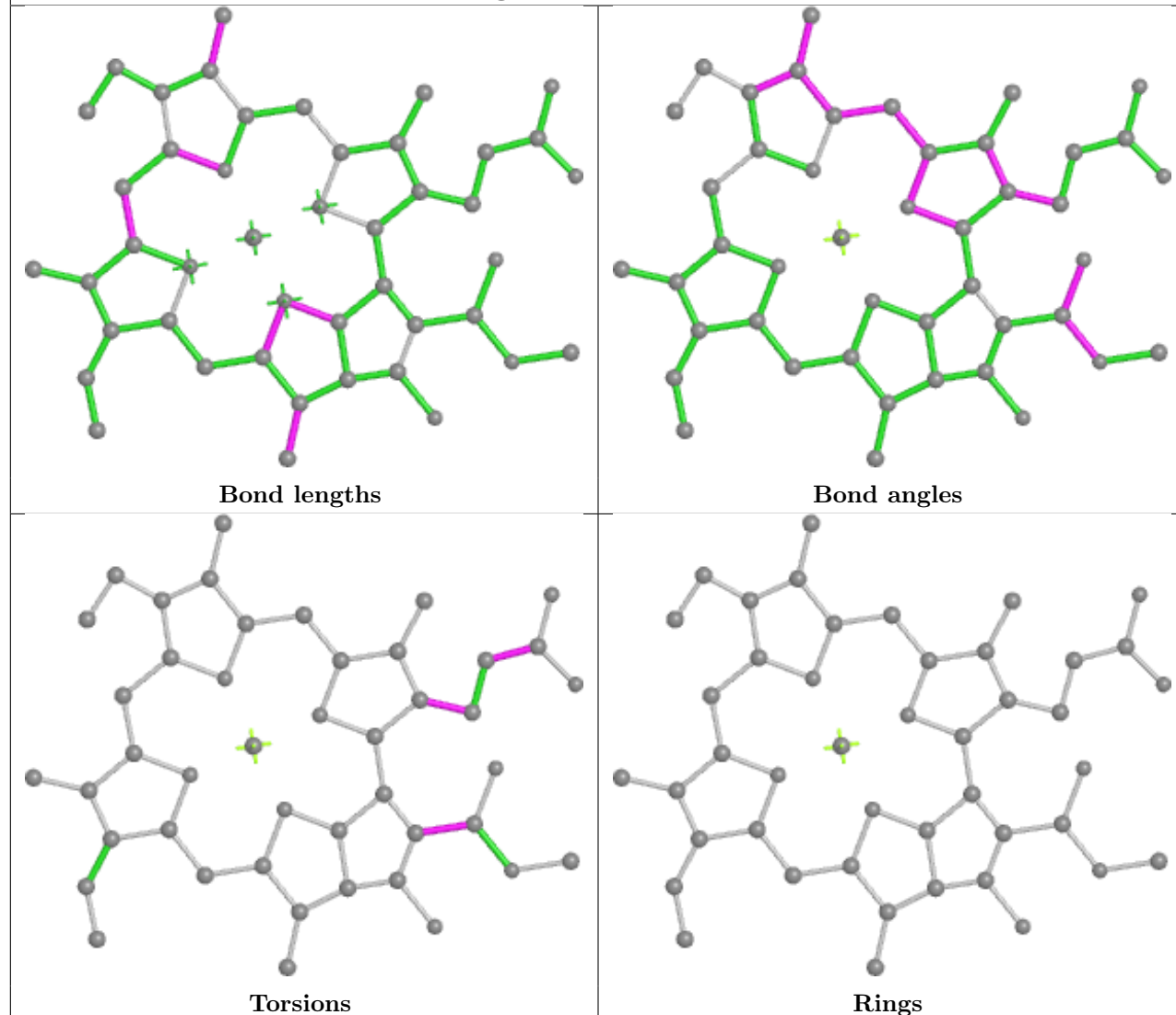
Ligand CLA A 1118**Bond lengths****Bond angles****Torsions****Rings****Ligand LHG V 5218****Bond lengths****Bond angles****Torsions****Rings**



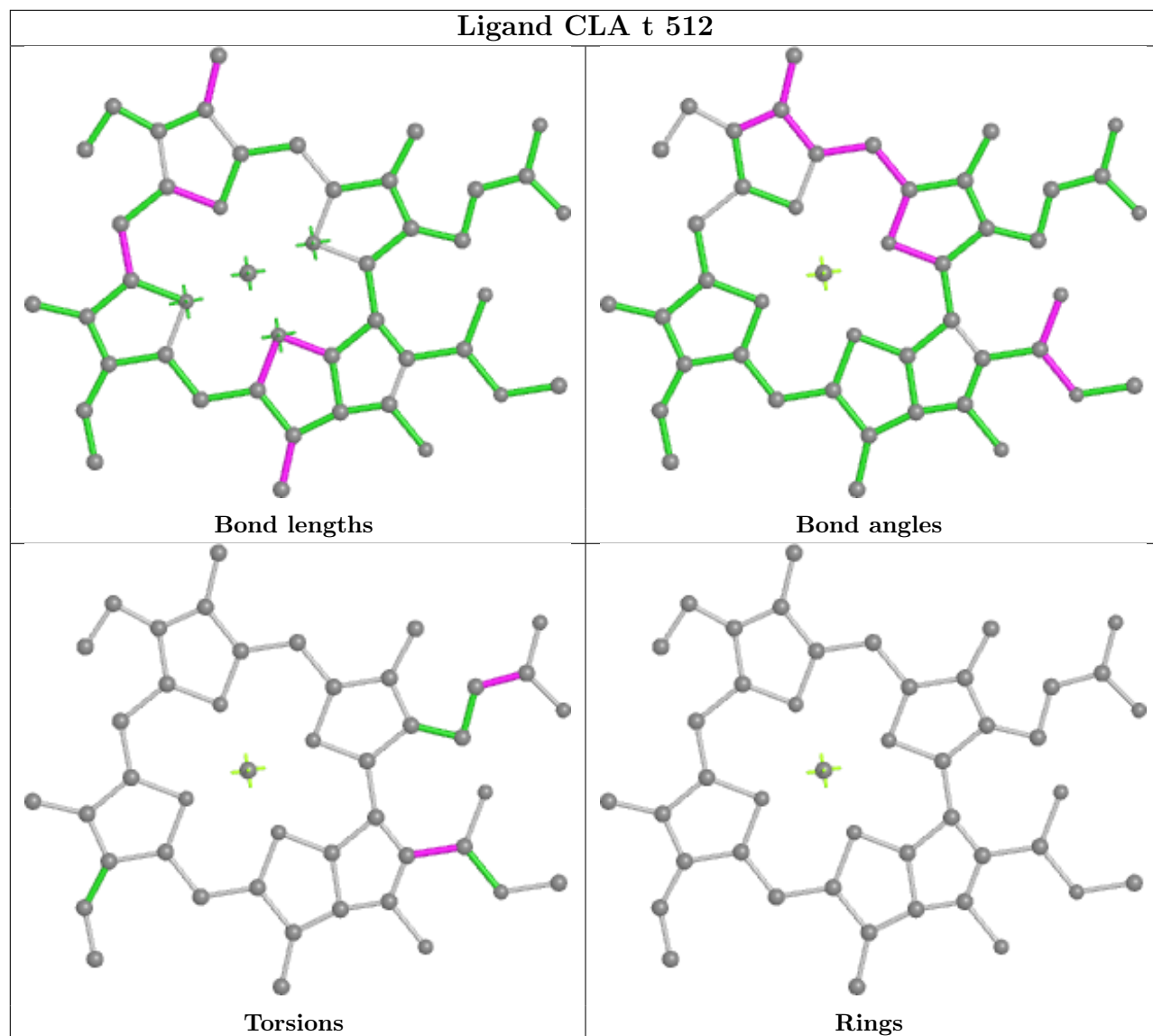
Ligand CLA Z 518



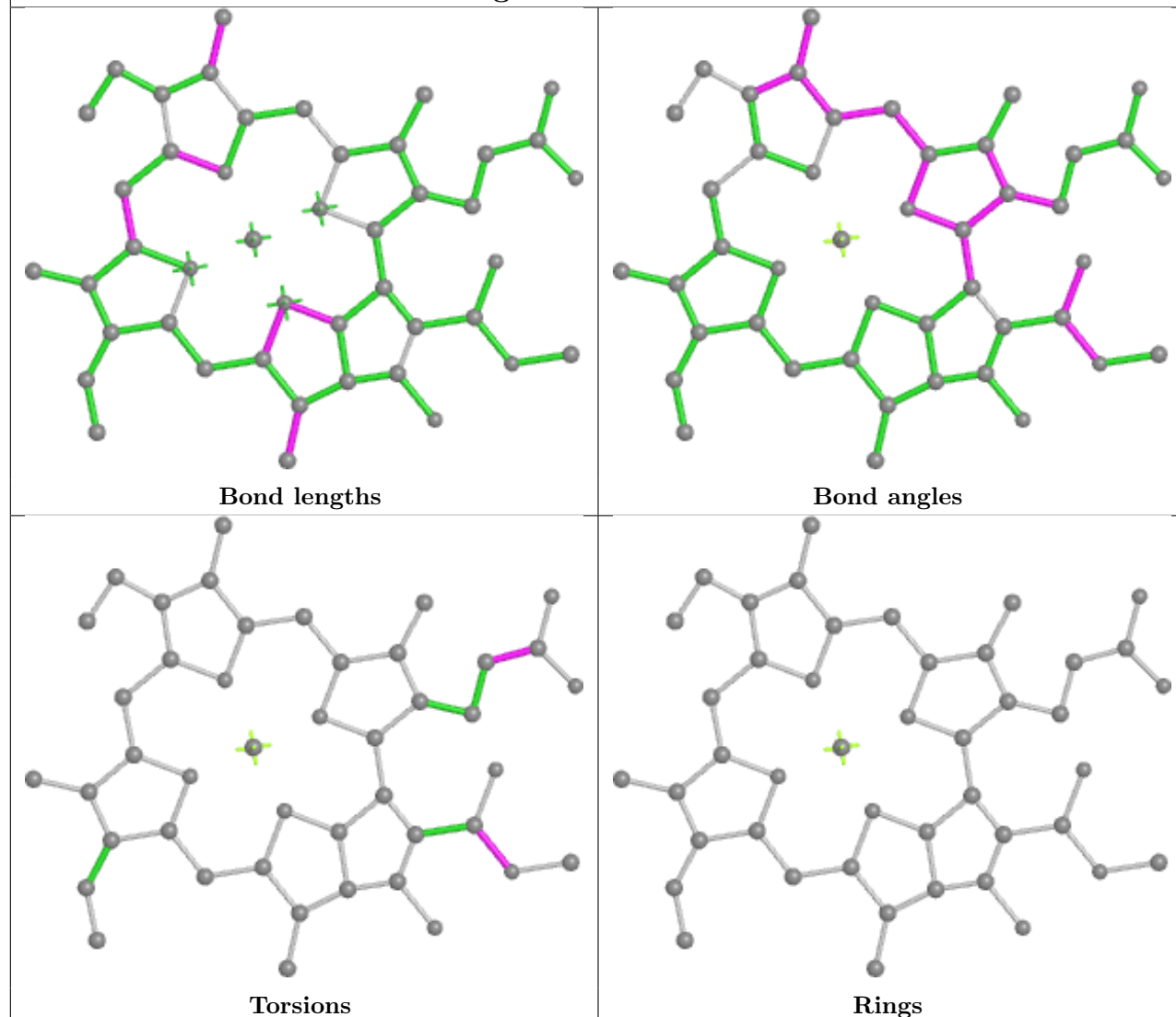
Ligand CLA b 516



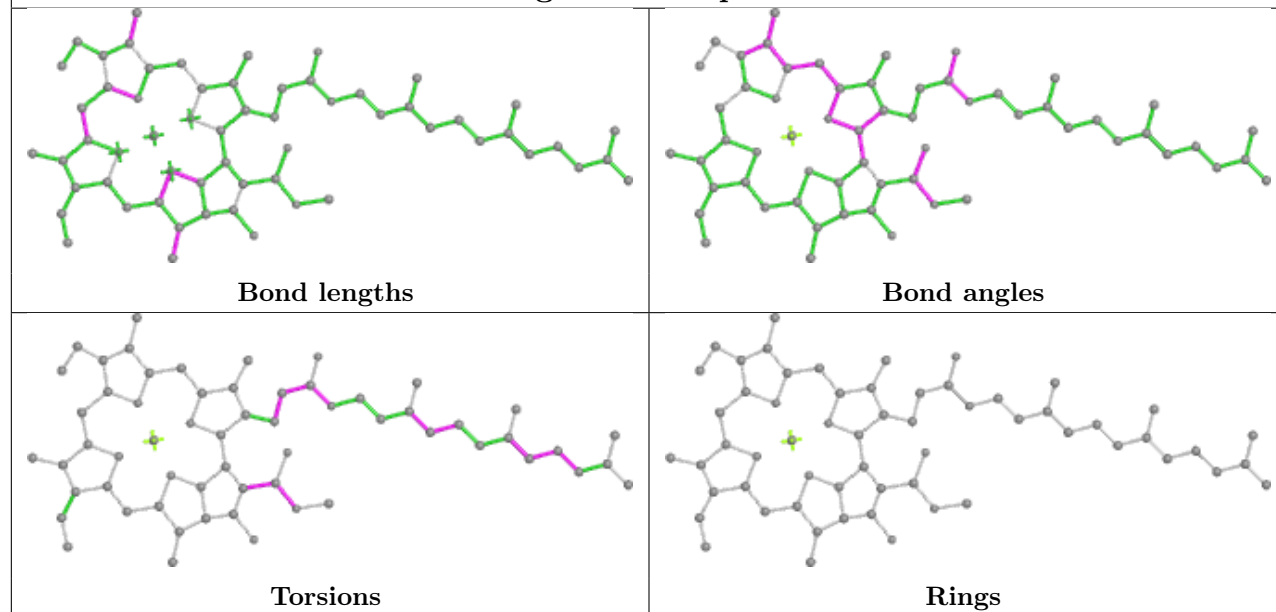
Ligand CLA t 512



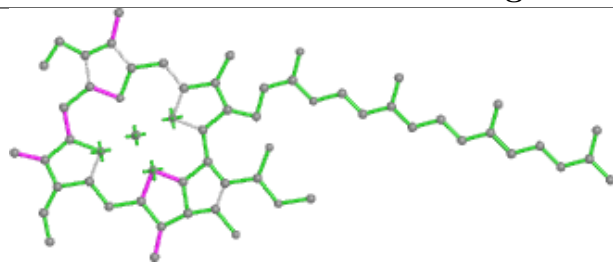
Ligand CLA d 507



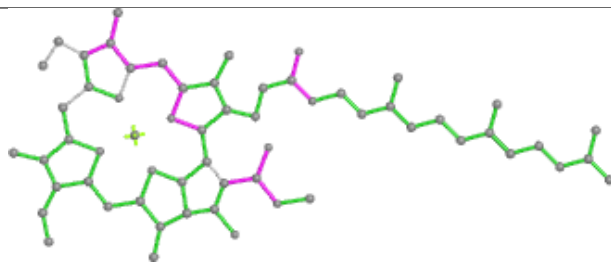
Ligand CLA q 507



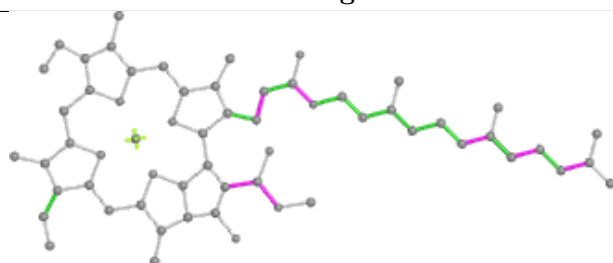
Ligand CLA B 1201



Bond lengths



Bond angles

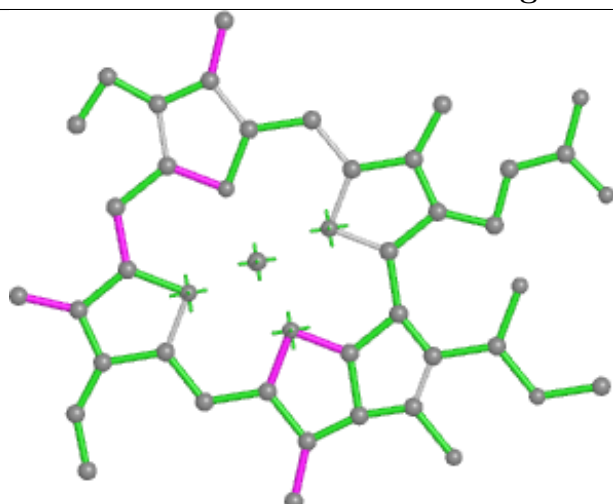


Torsions

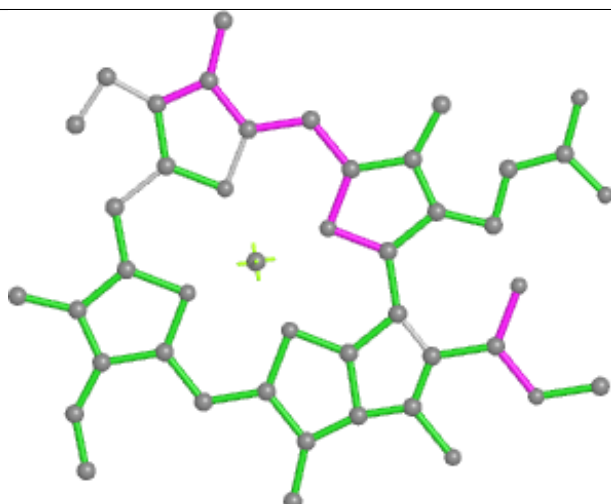


Rings

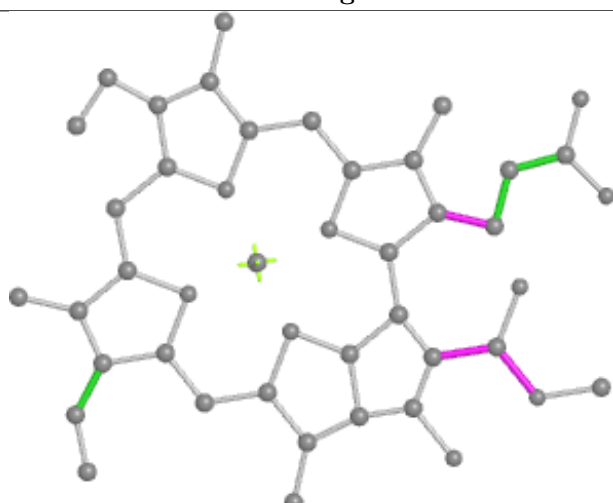
Ligand CLA s 517



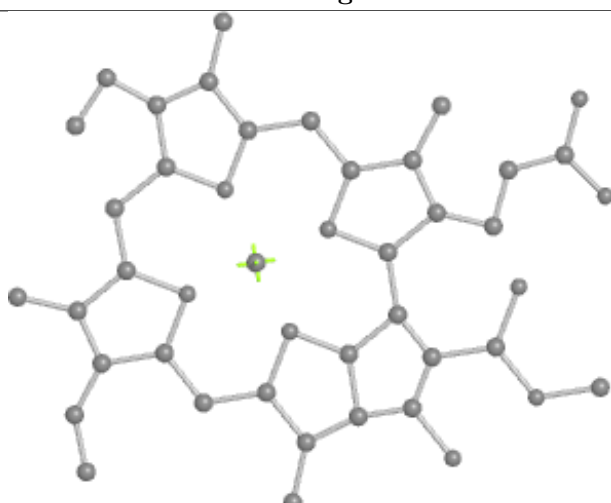
Bond lengths



Bond angles

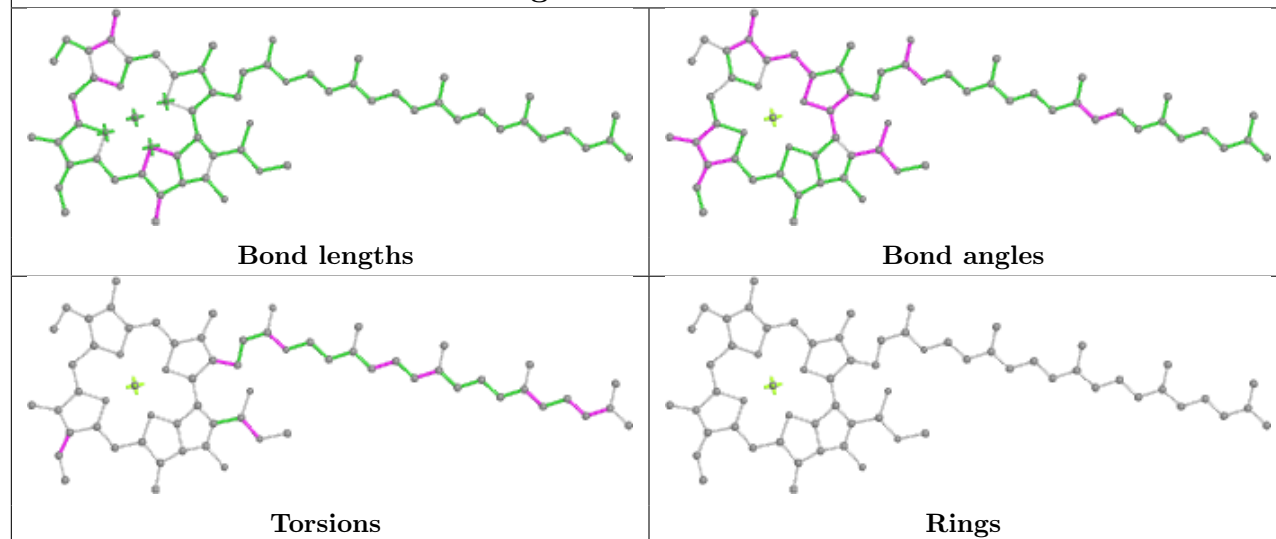


Torsions

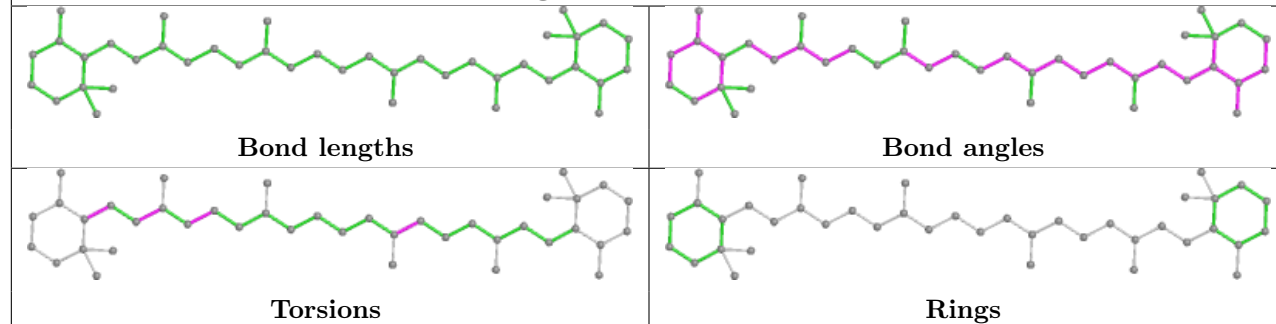


Rings

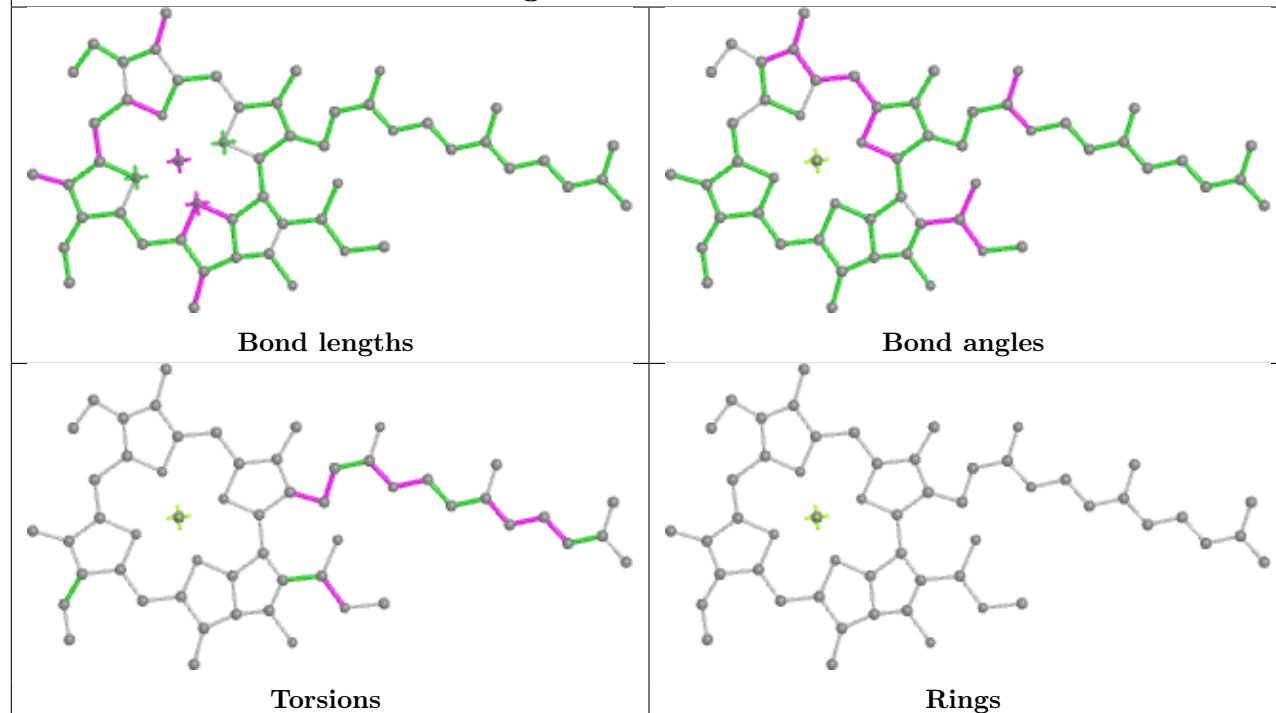
Ligand CLA f 1239

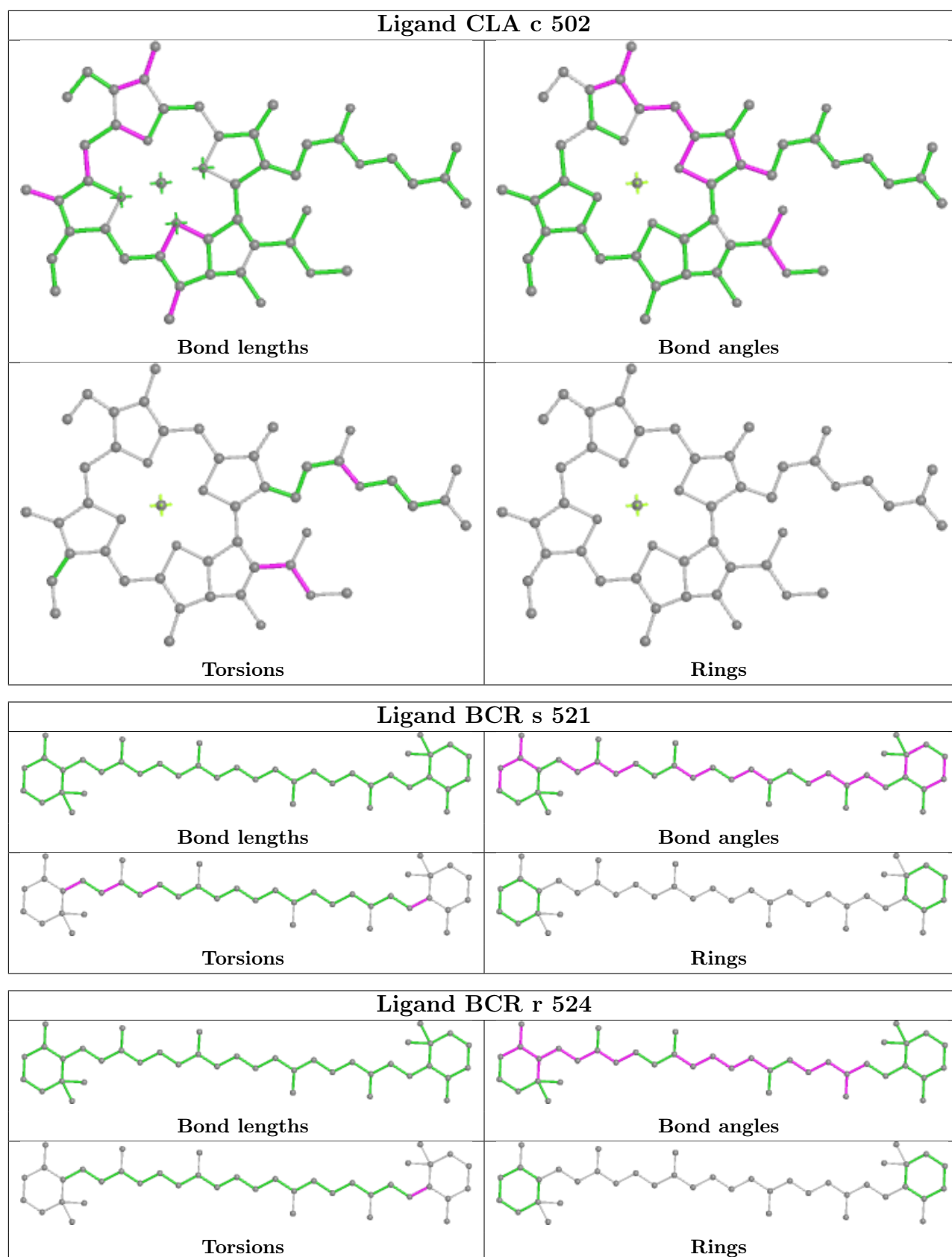


Ligand BCR 5 521

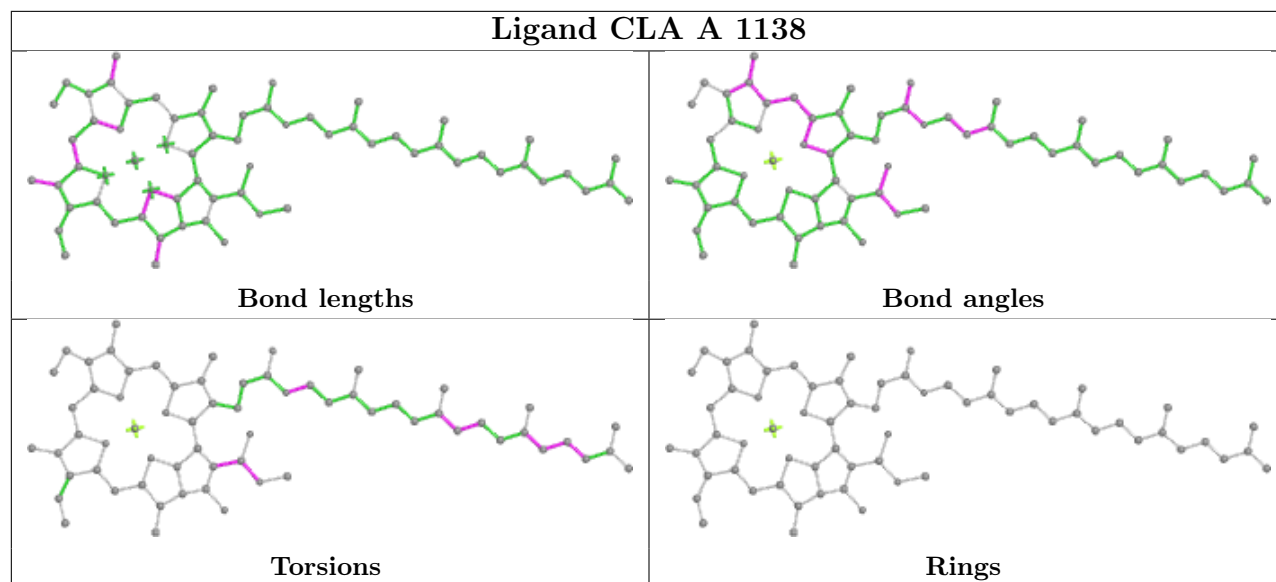


Ligand CLA H 1212

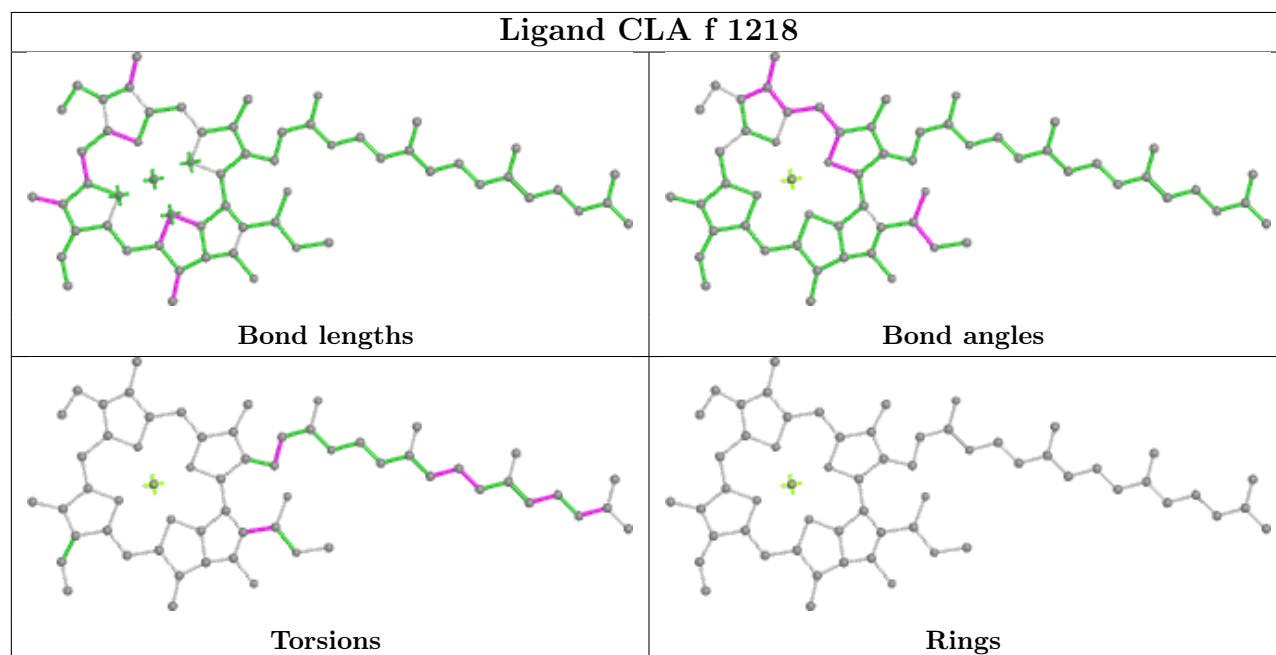


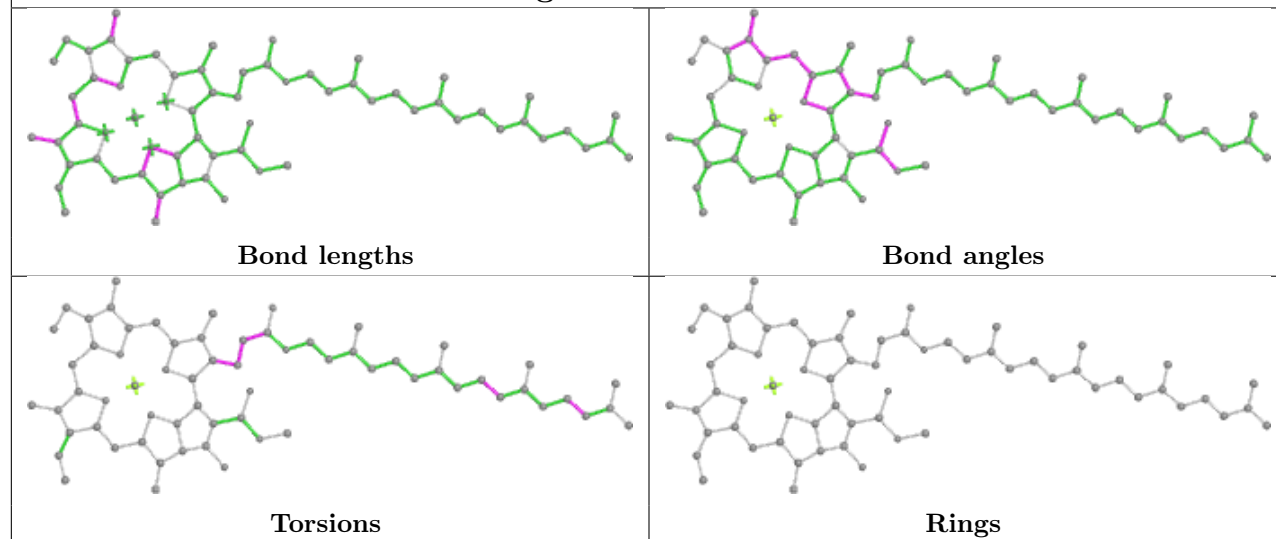
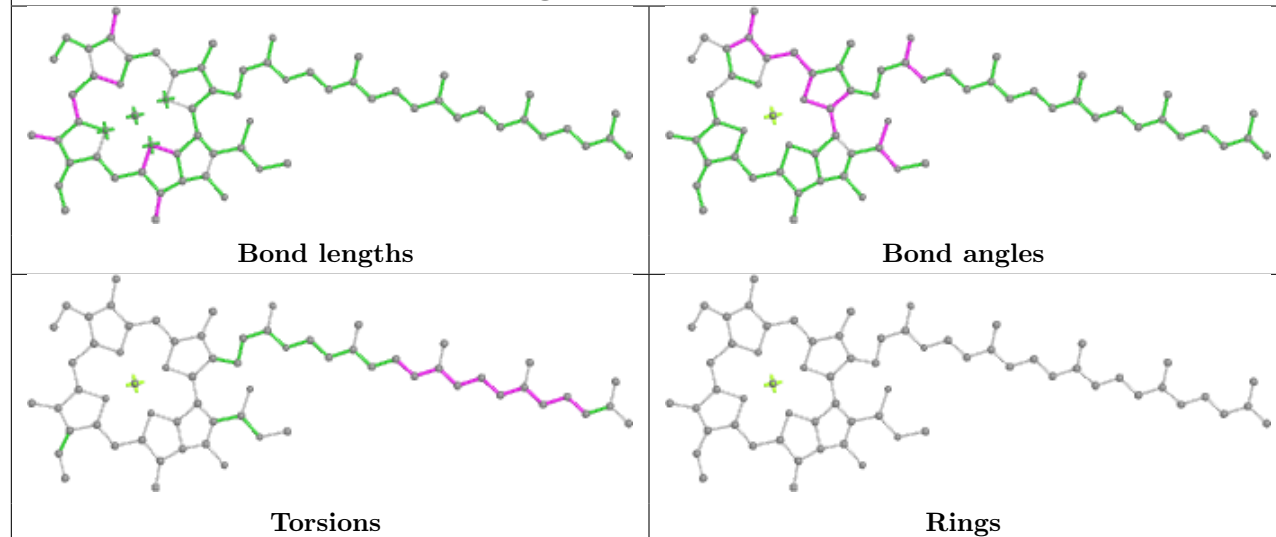
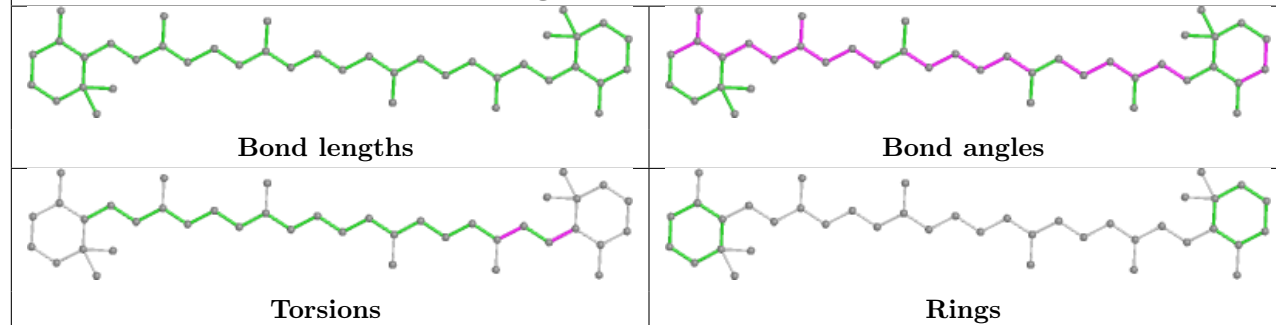


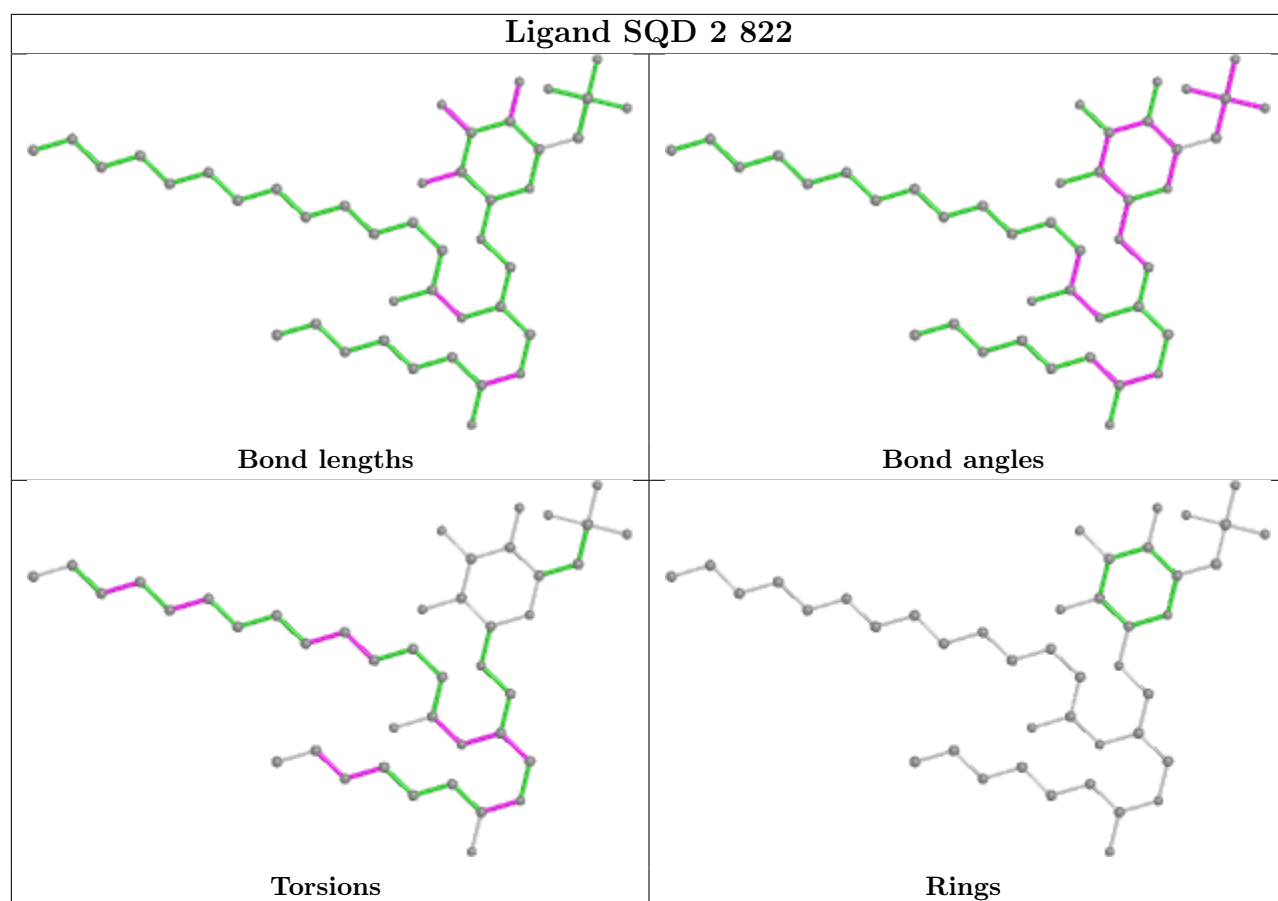
Ligand CLA A 1138



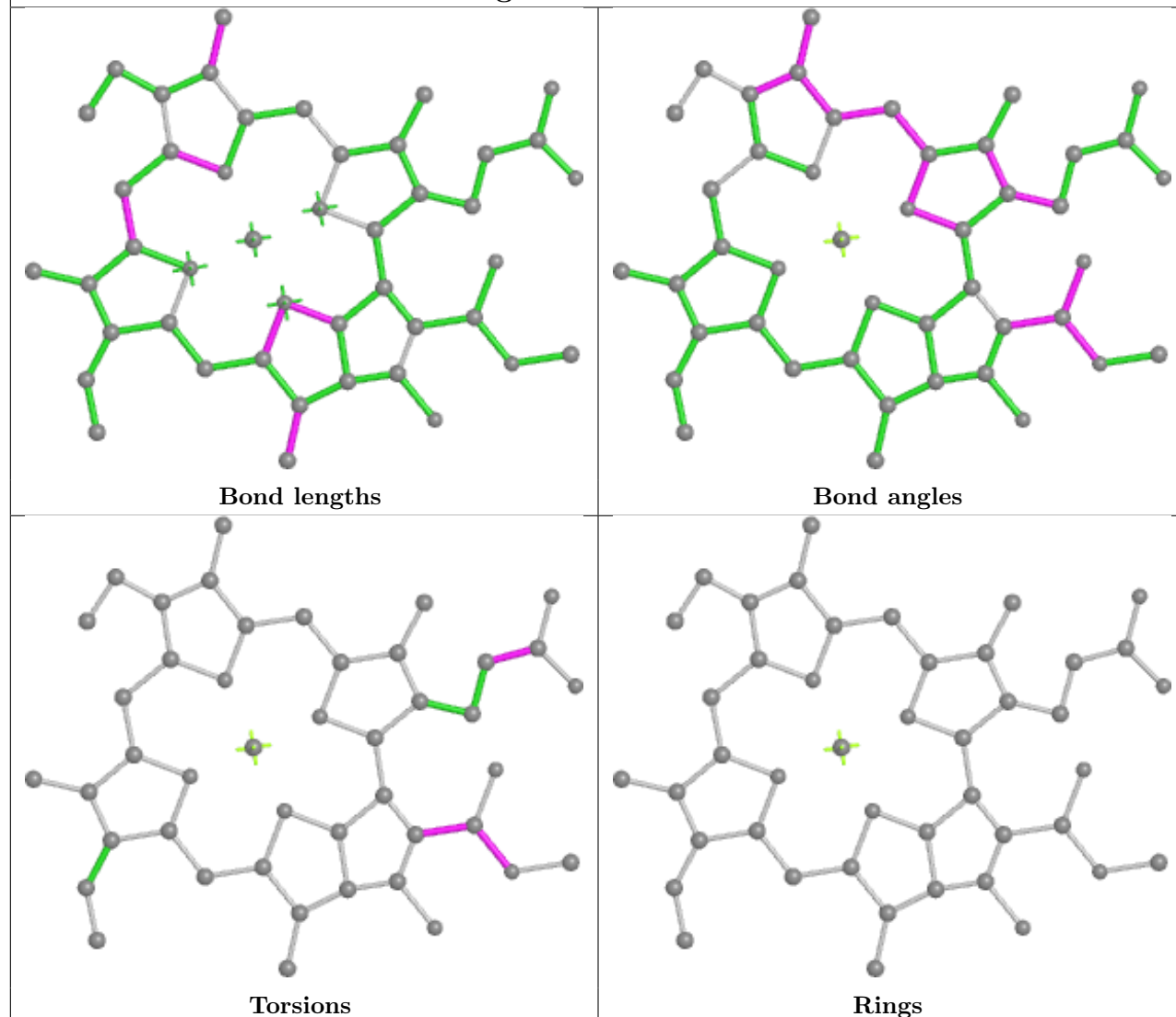
Ligand CLA f 1218



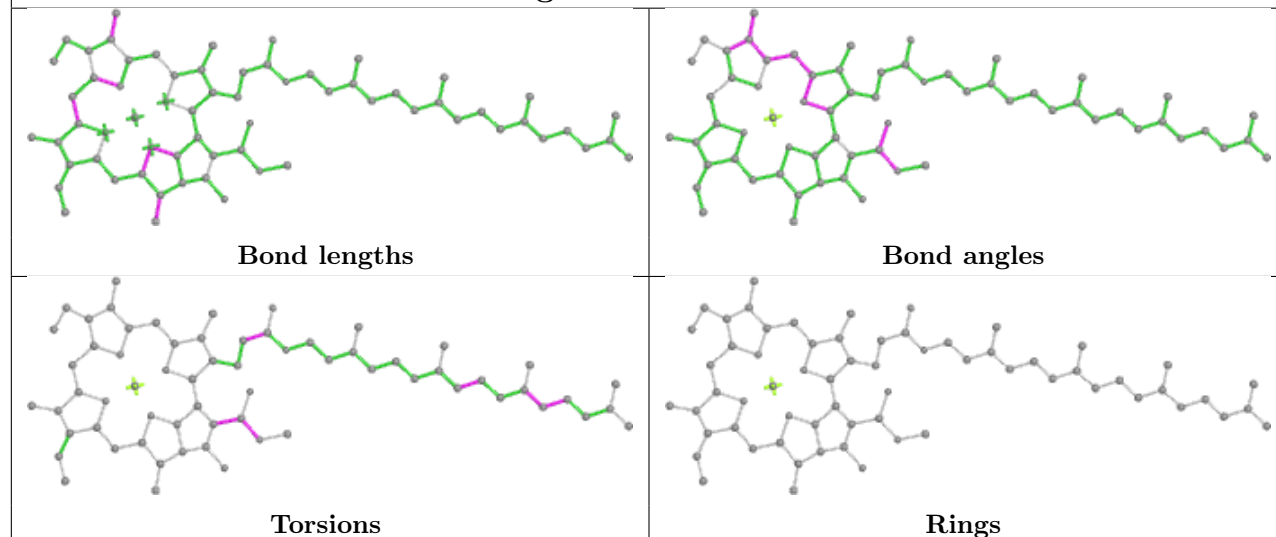
Ligand CLA 3 501**Ligand CLA 5 509****Ligand BCR 6 523**

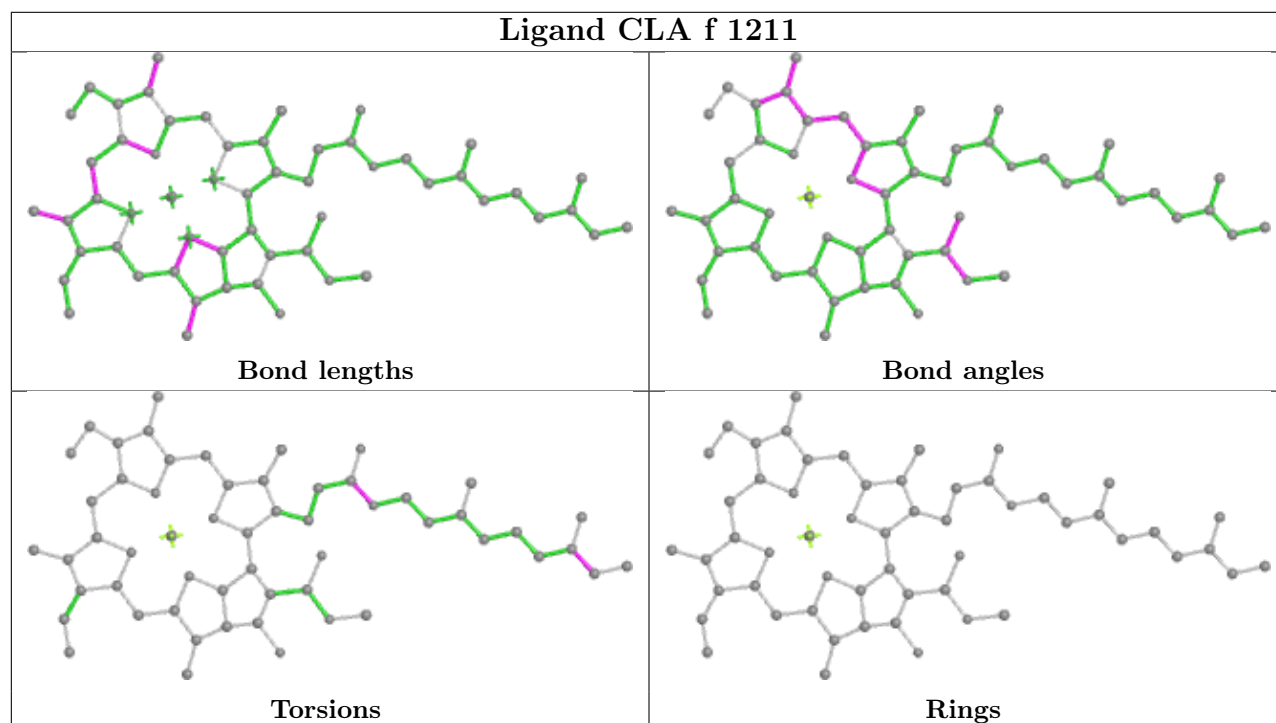
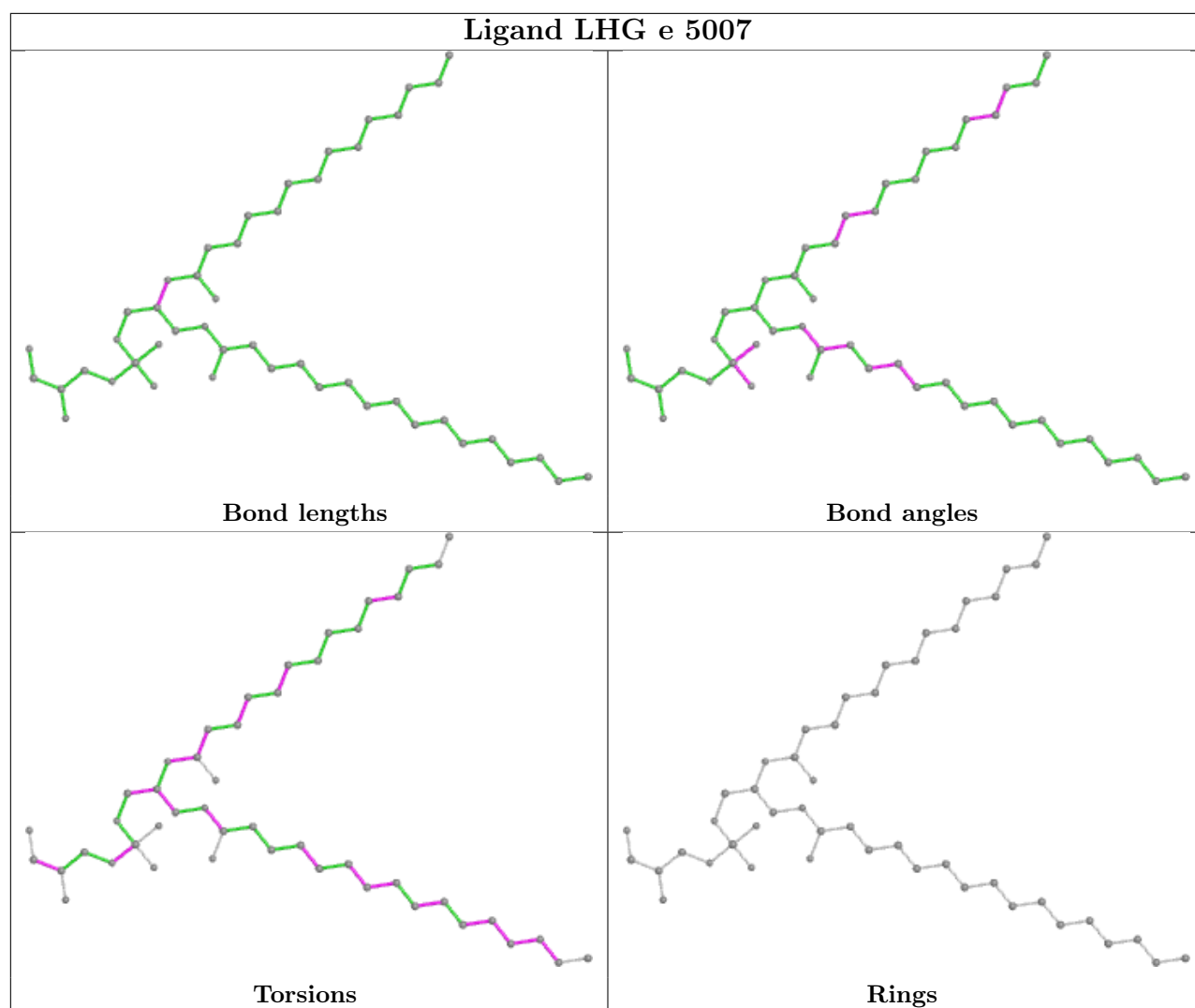


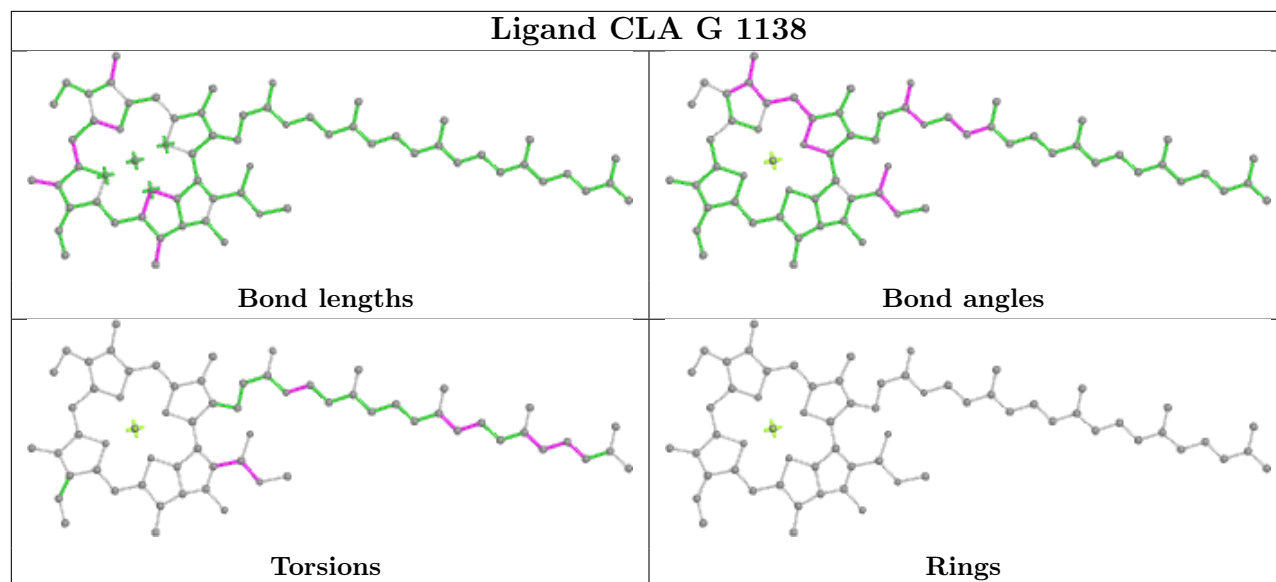
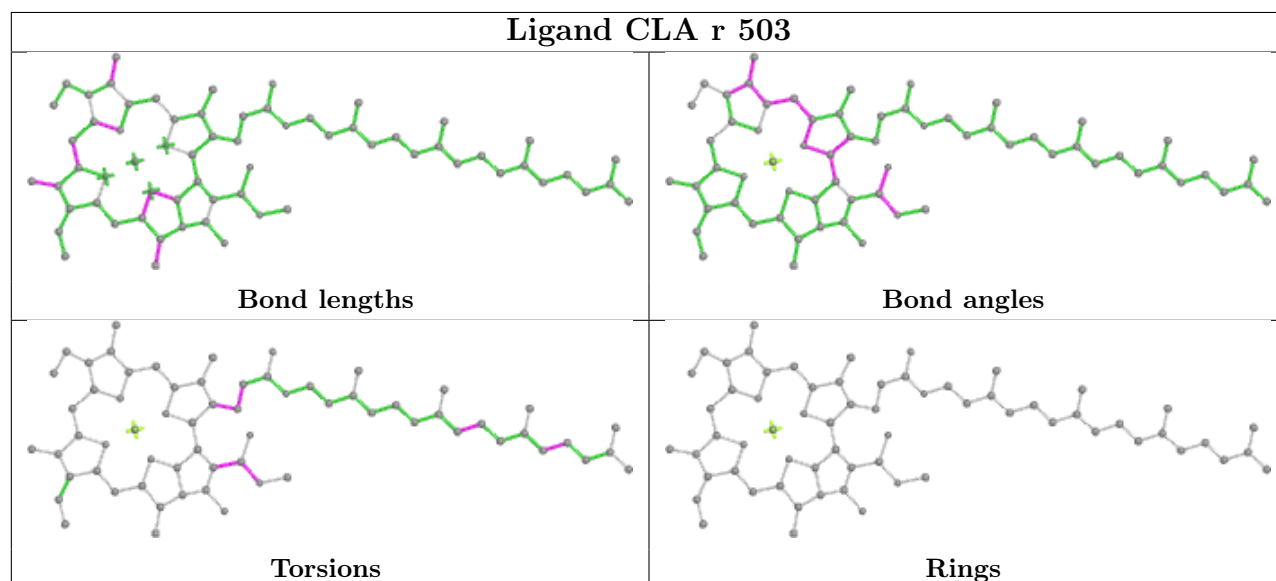
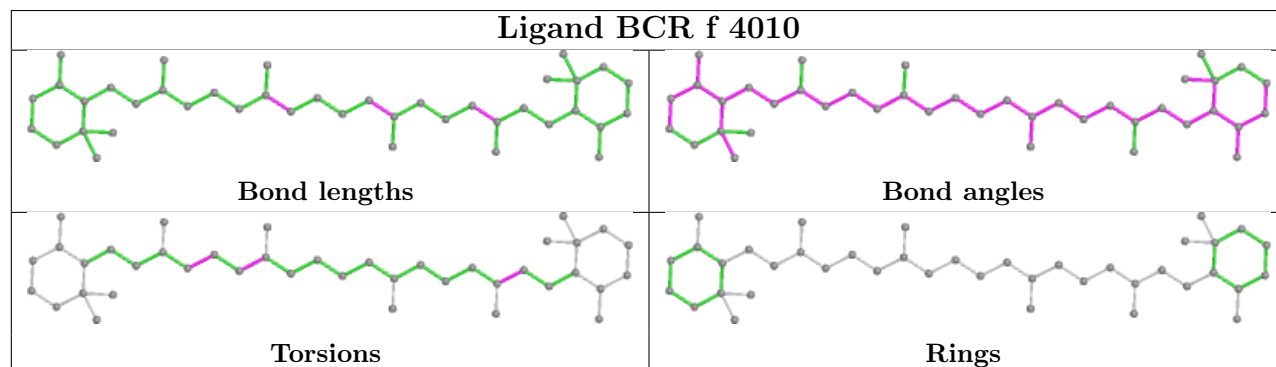
Ligand CLA t 507

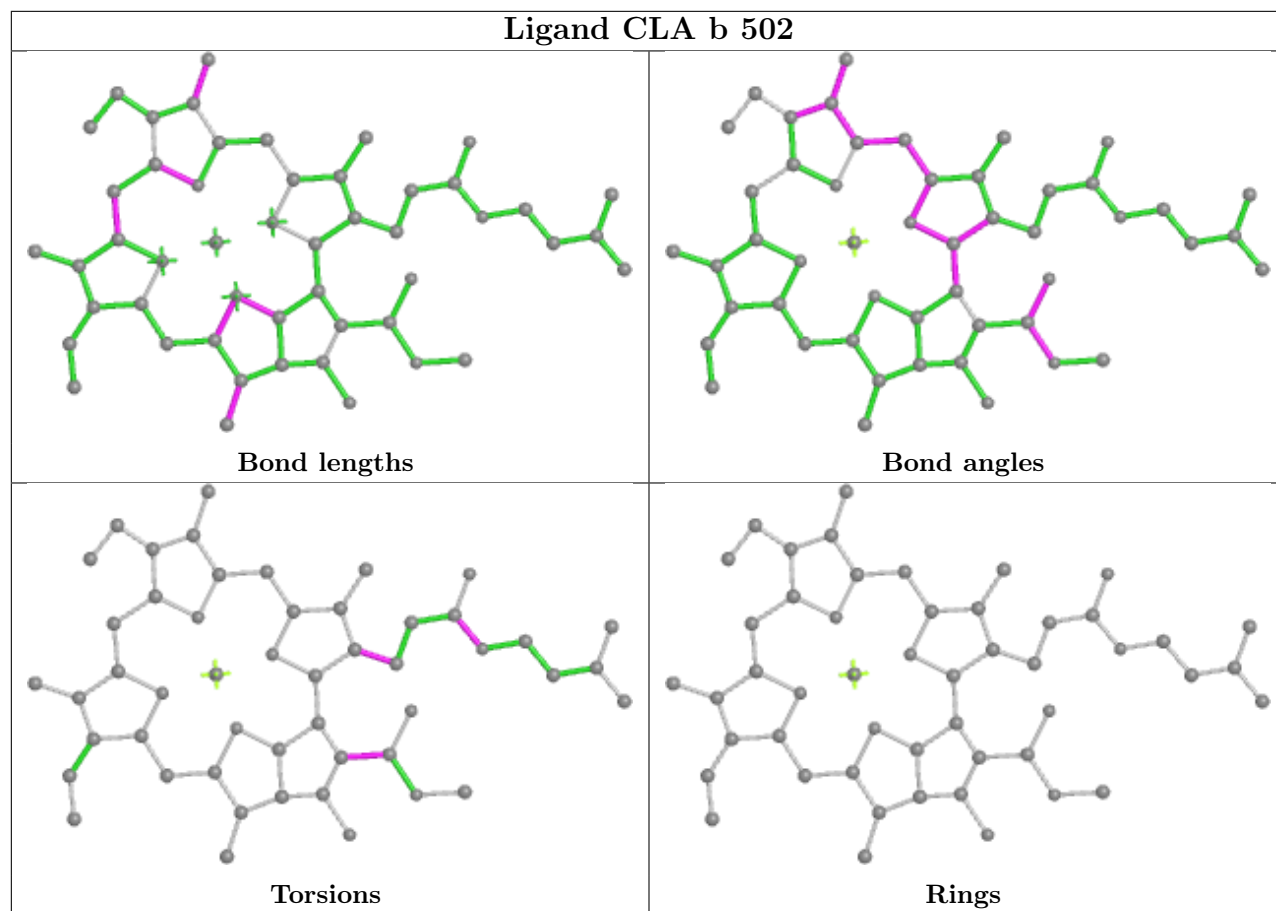
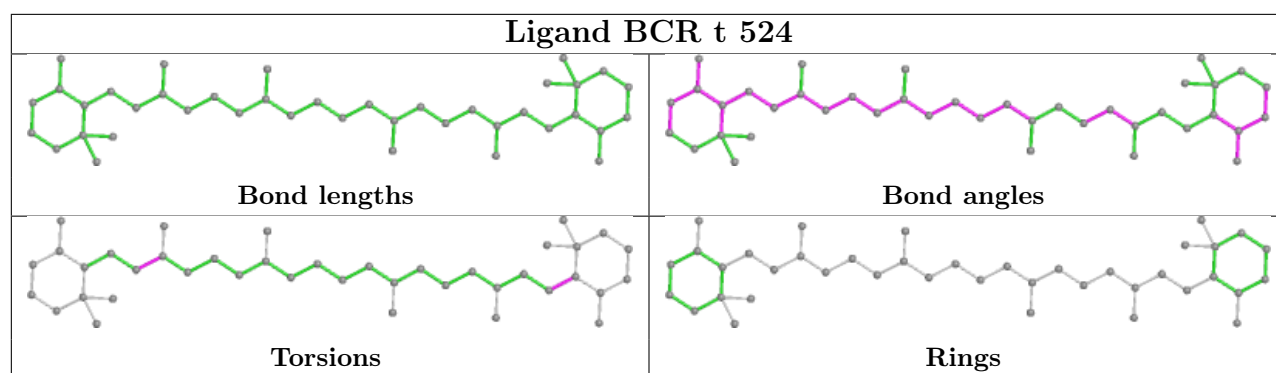


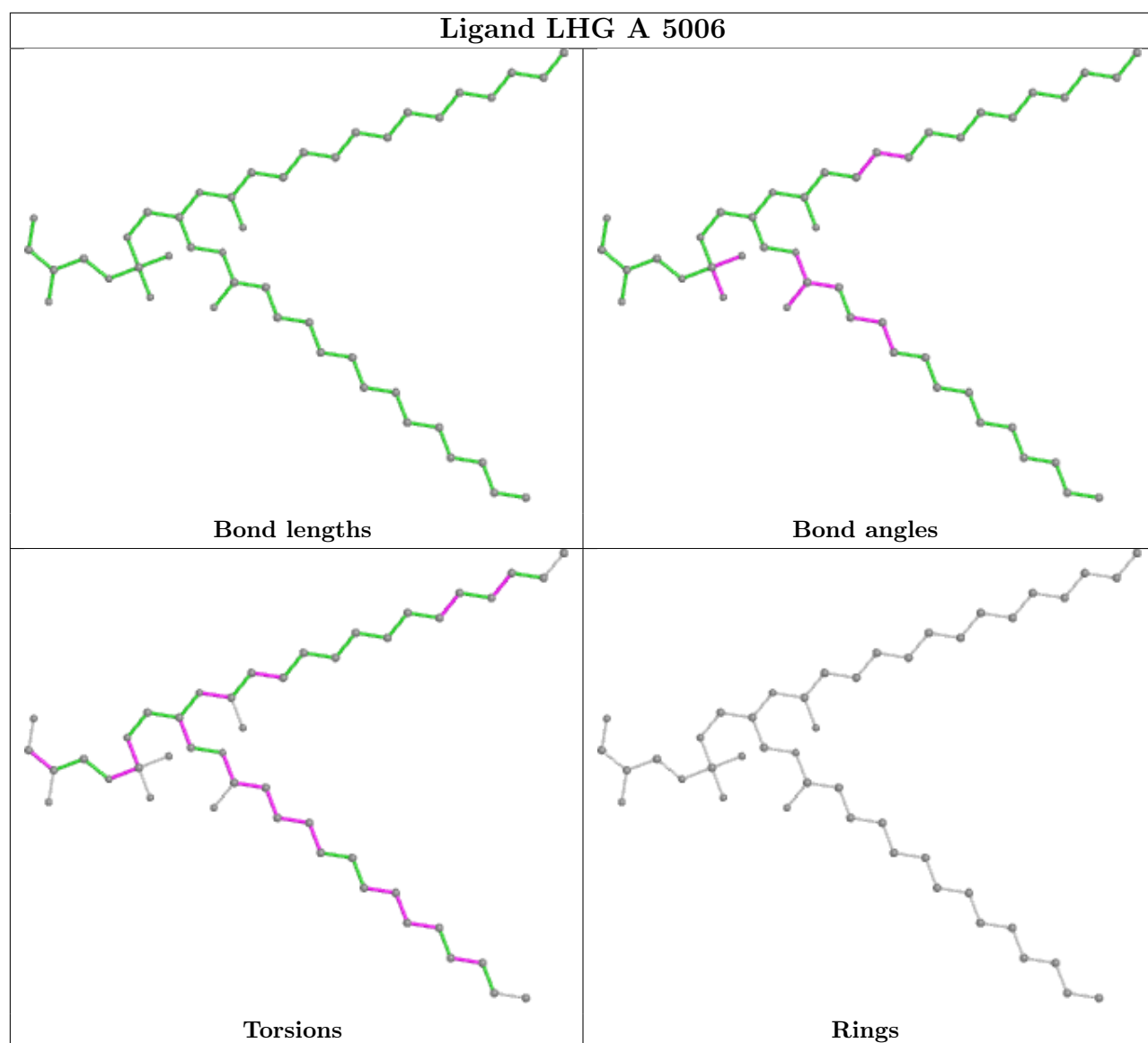
Ligand CLA 2 510



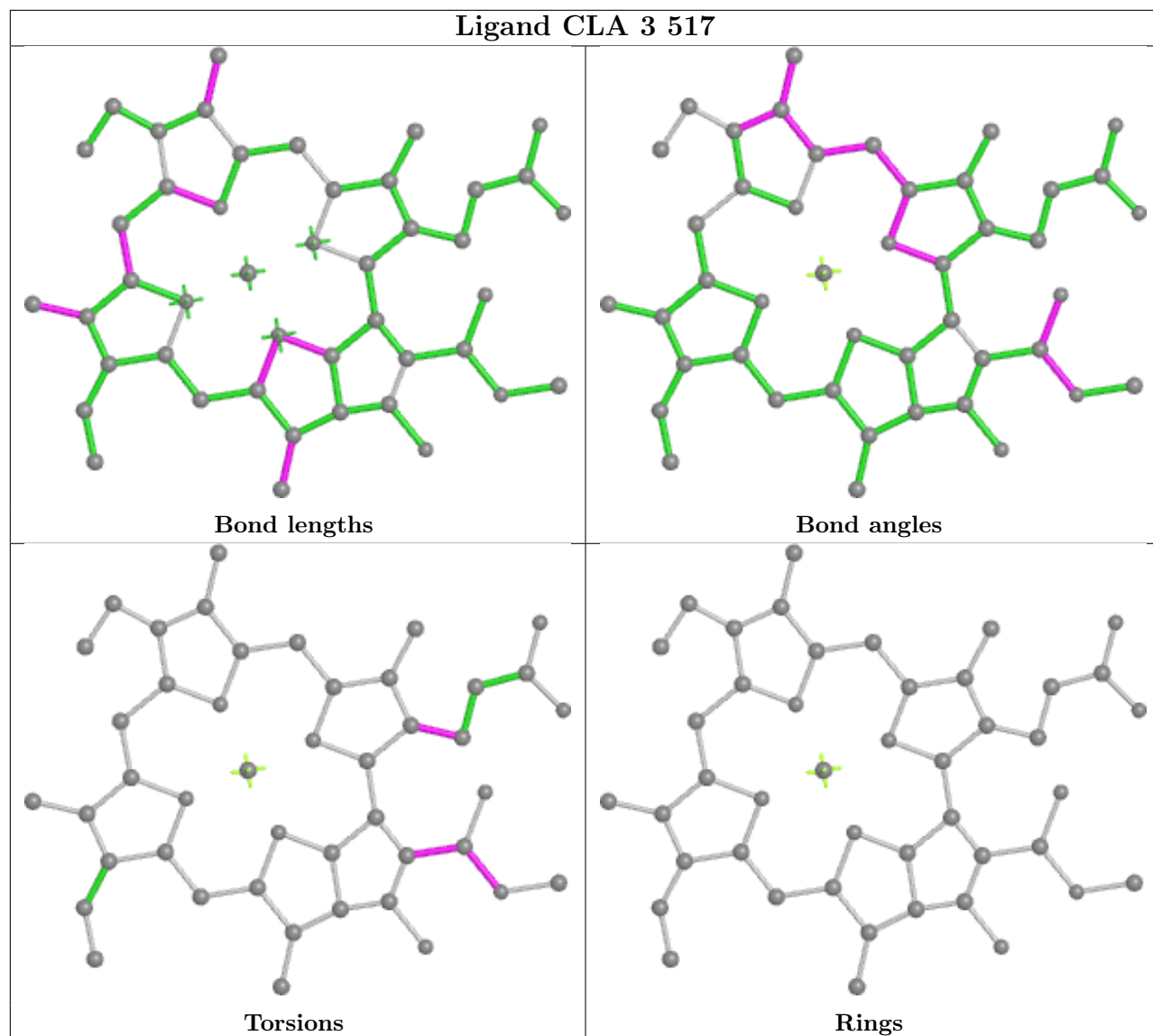


Ligand CLA G 1138**Ligand CLA r 503****Ligand BCR f 4010**

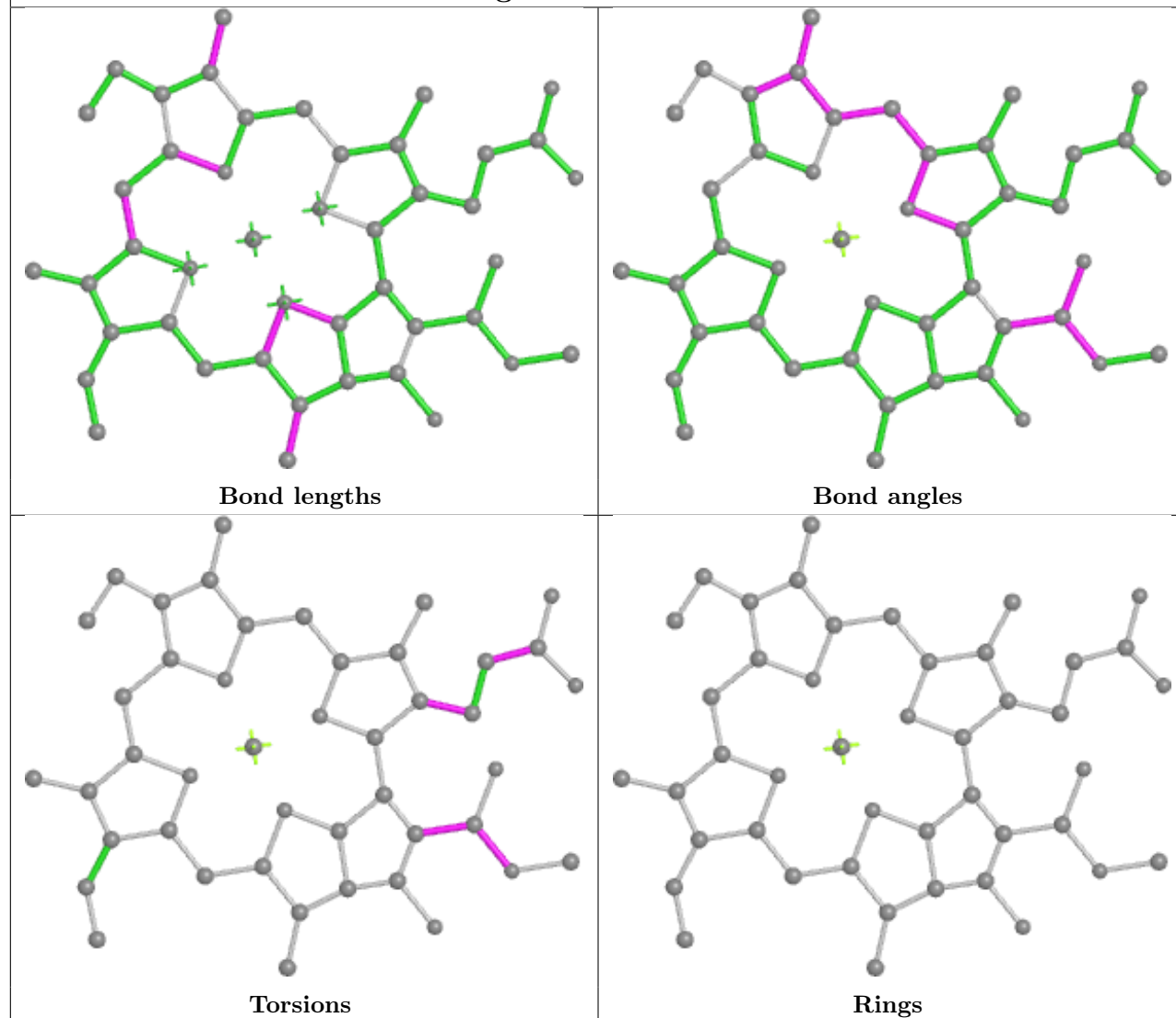




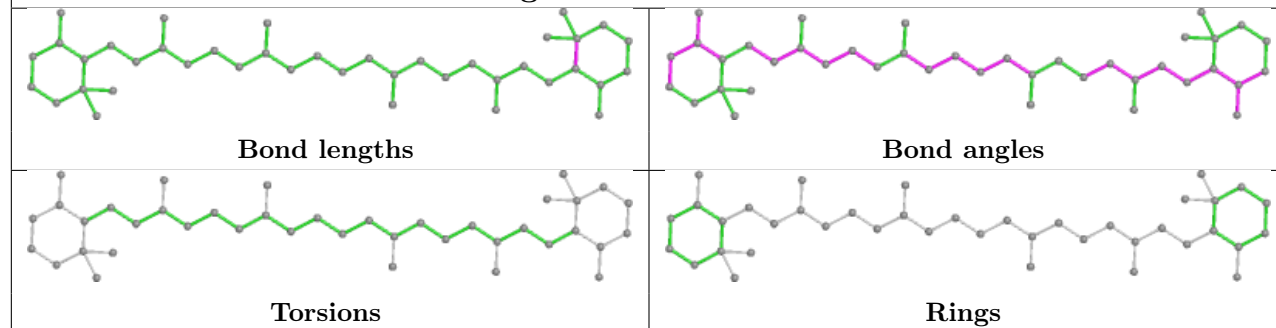
Ligand CLA 3 517

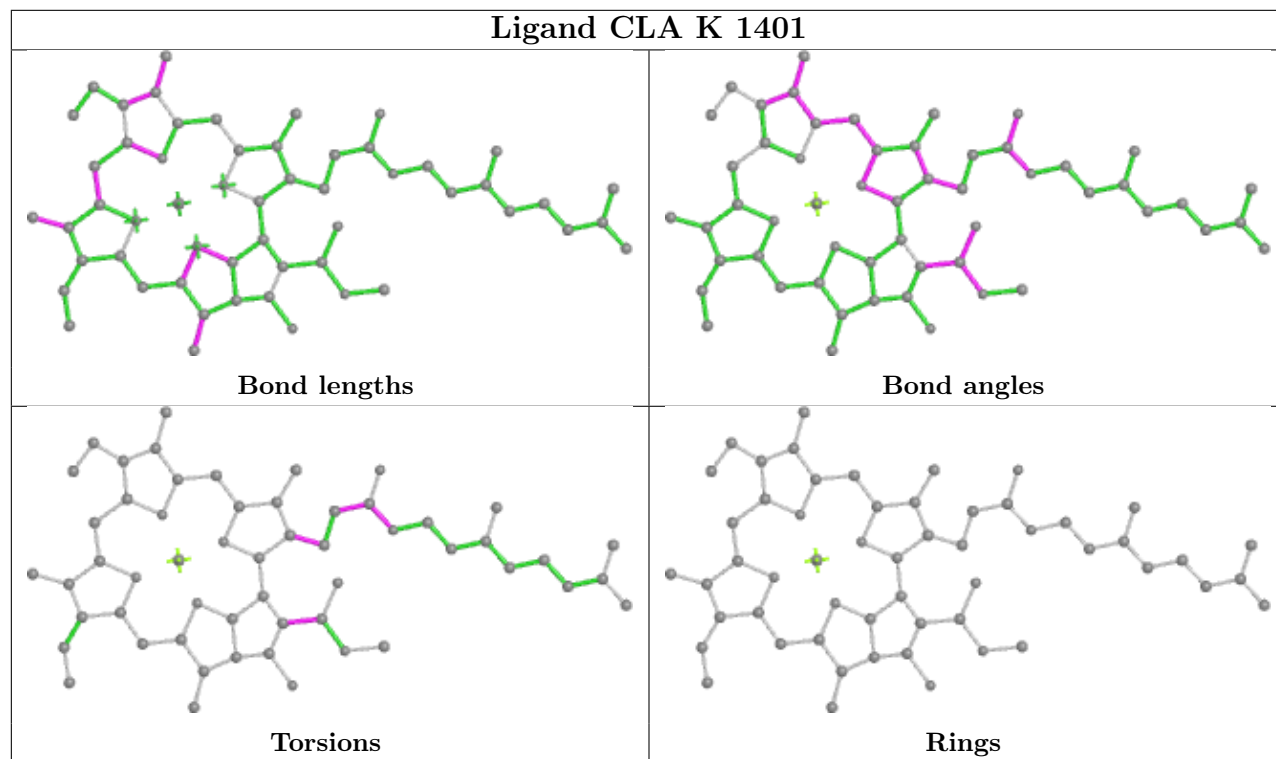
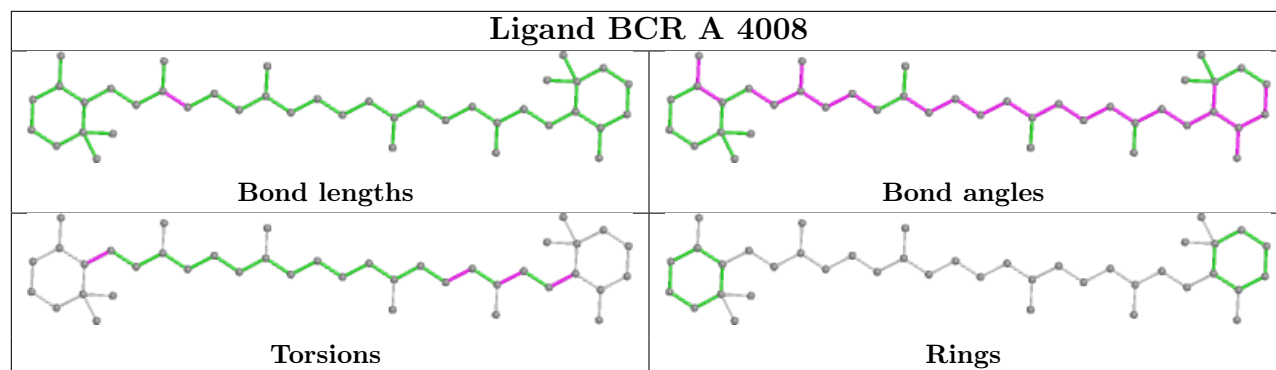
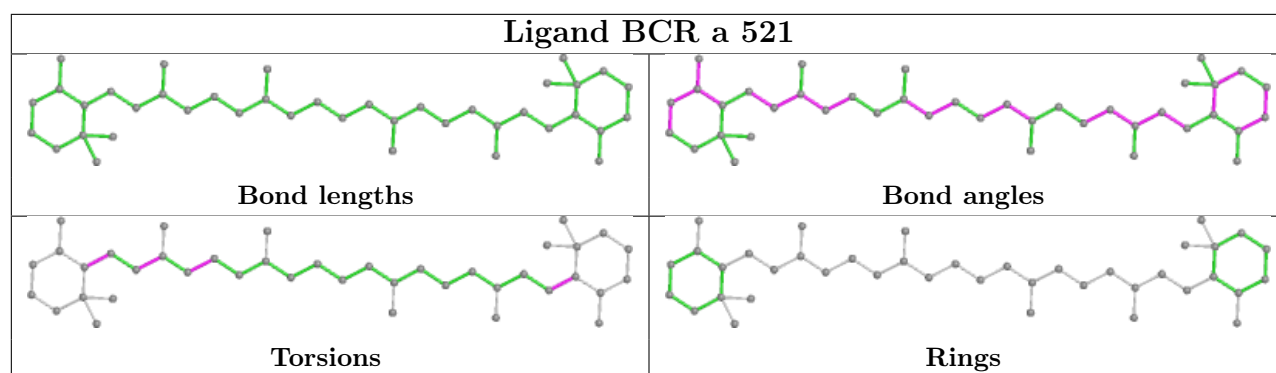


Ligand CLA r 516

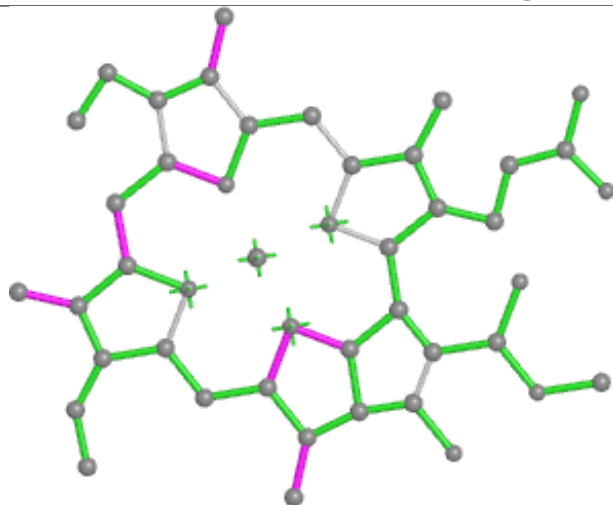


Ligand BCR G 4002

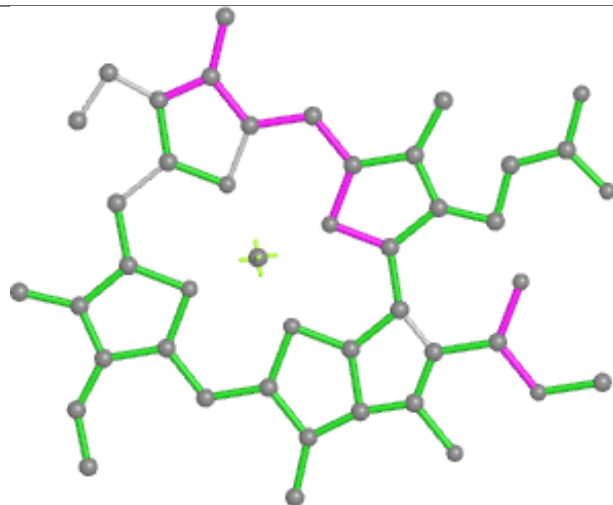




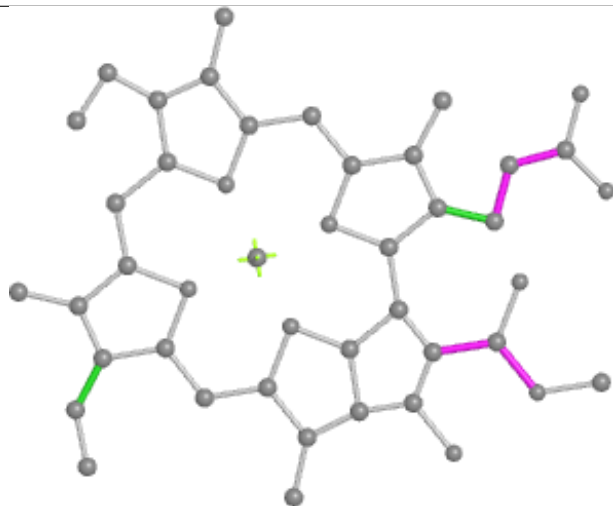
Ligand CLA 4 513



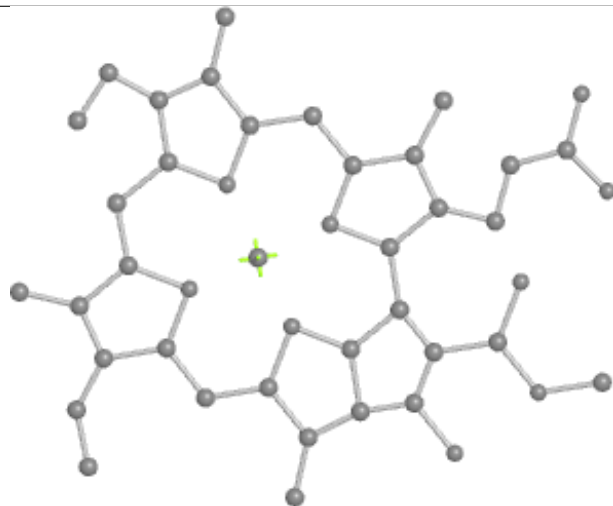
Bond lengths



Bond angles

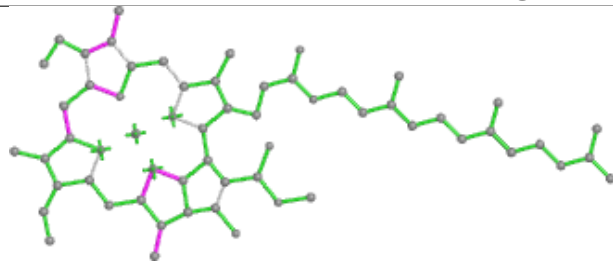


Torsions

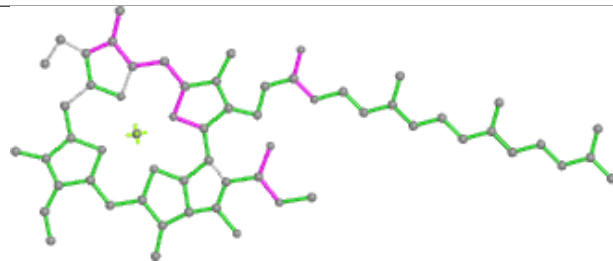


Rings

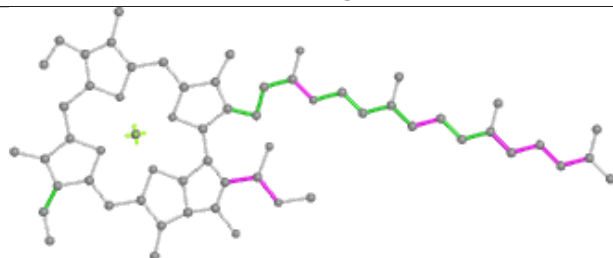
Ligand CLA Y 502



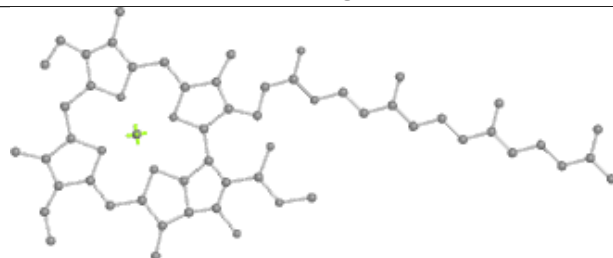
Bond lengths



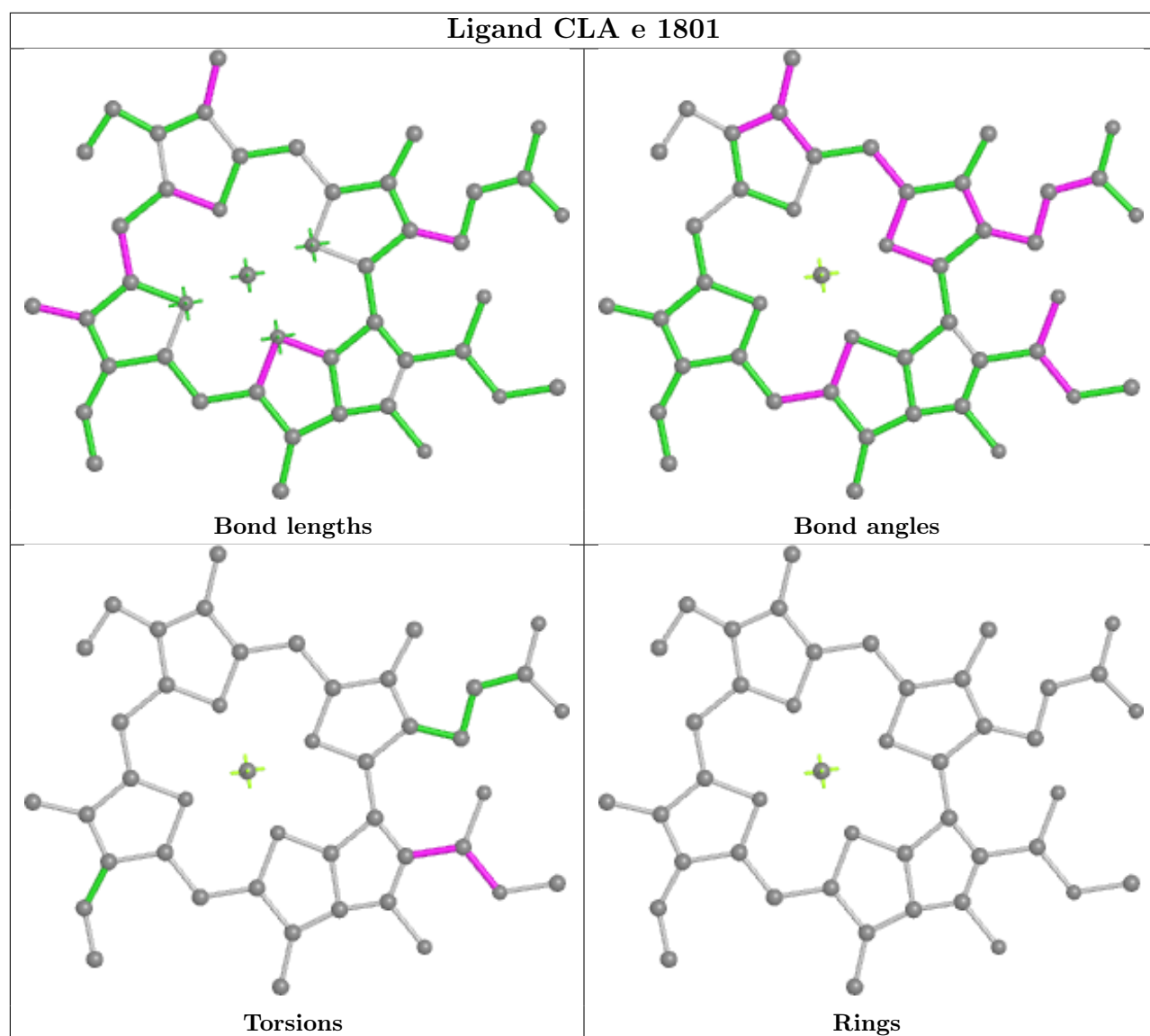
Bond angles



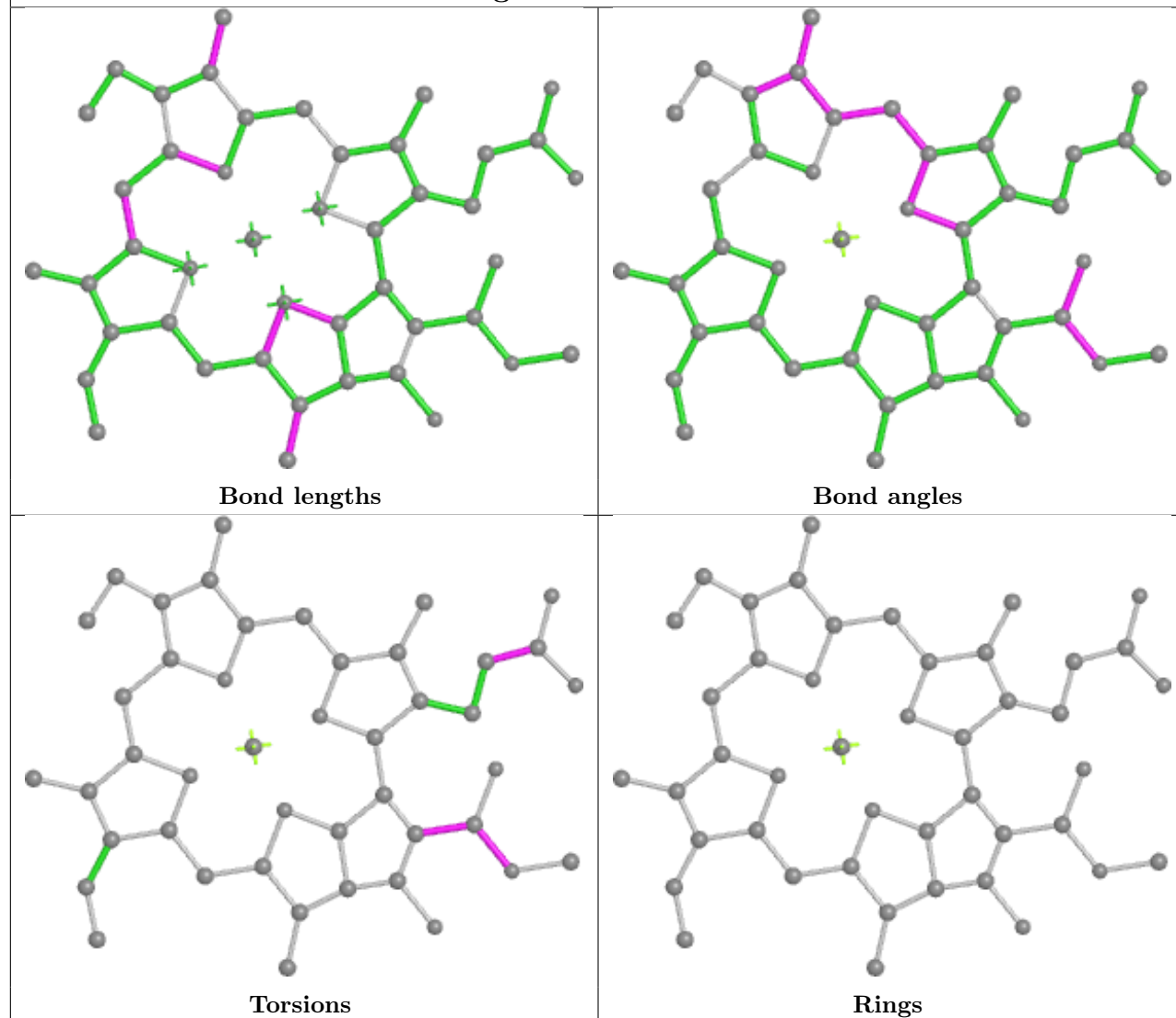
Torsions



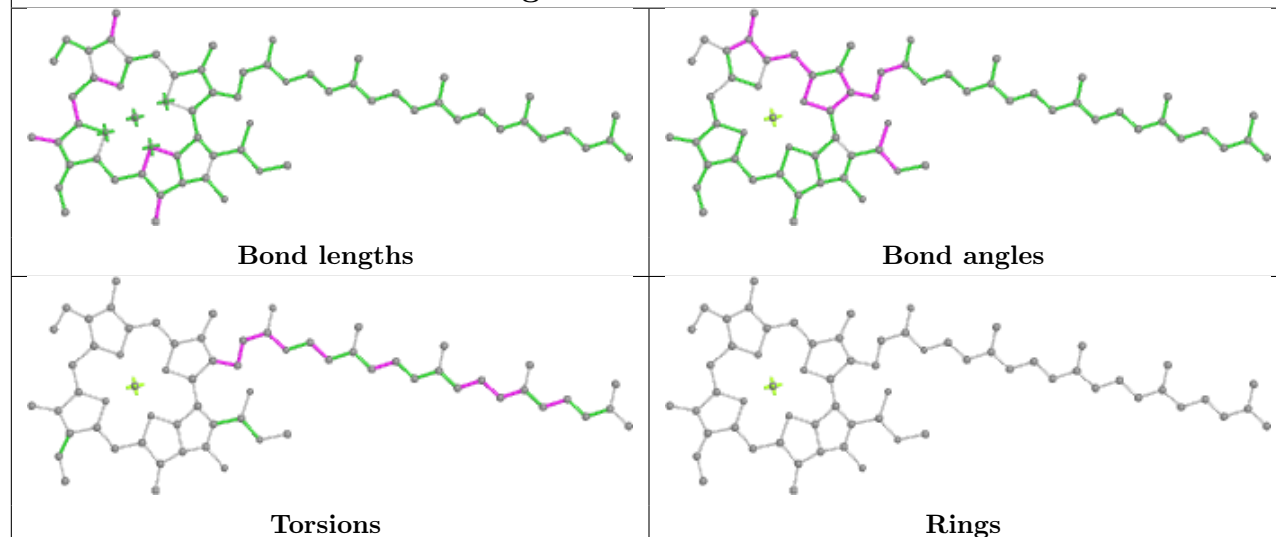
Rings



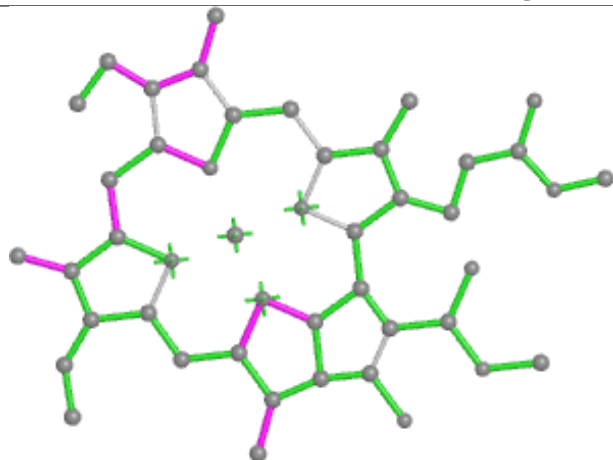
Ligand CLA d 509



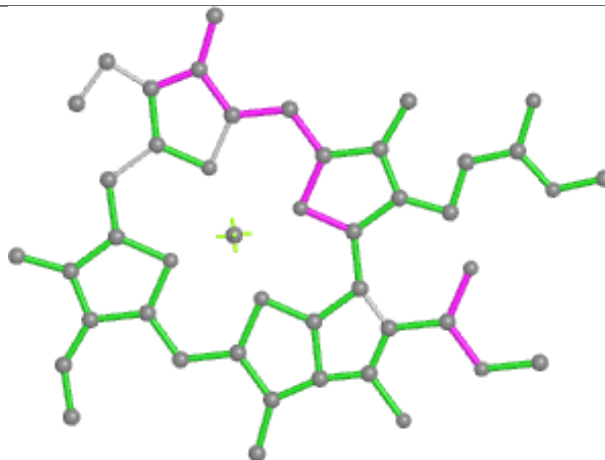
Ligand CLA G 1125



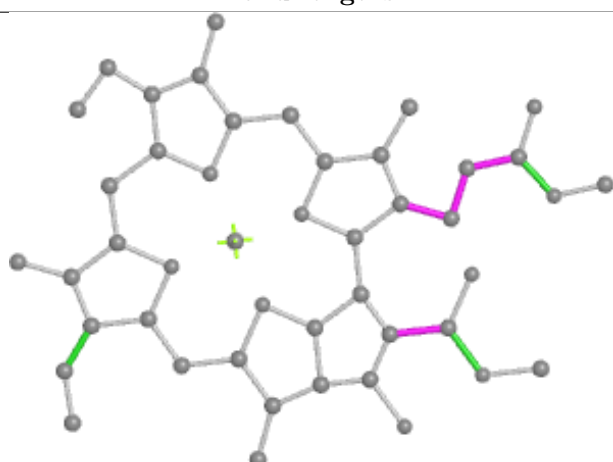
Ligand CLA 5 519



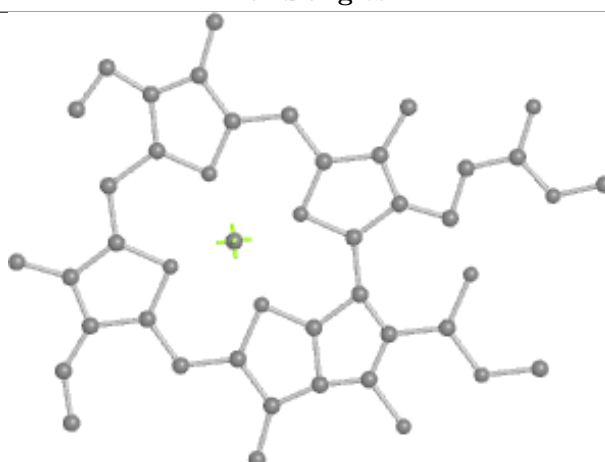
Bond lengths



Bond angles

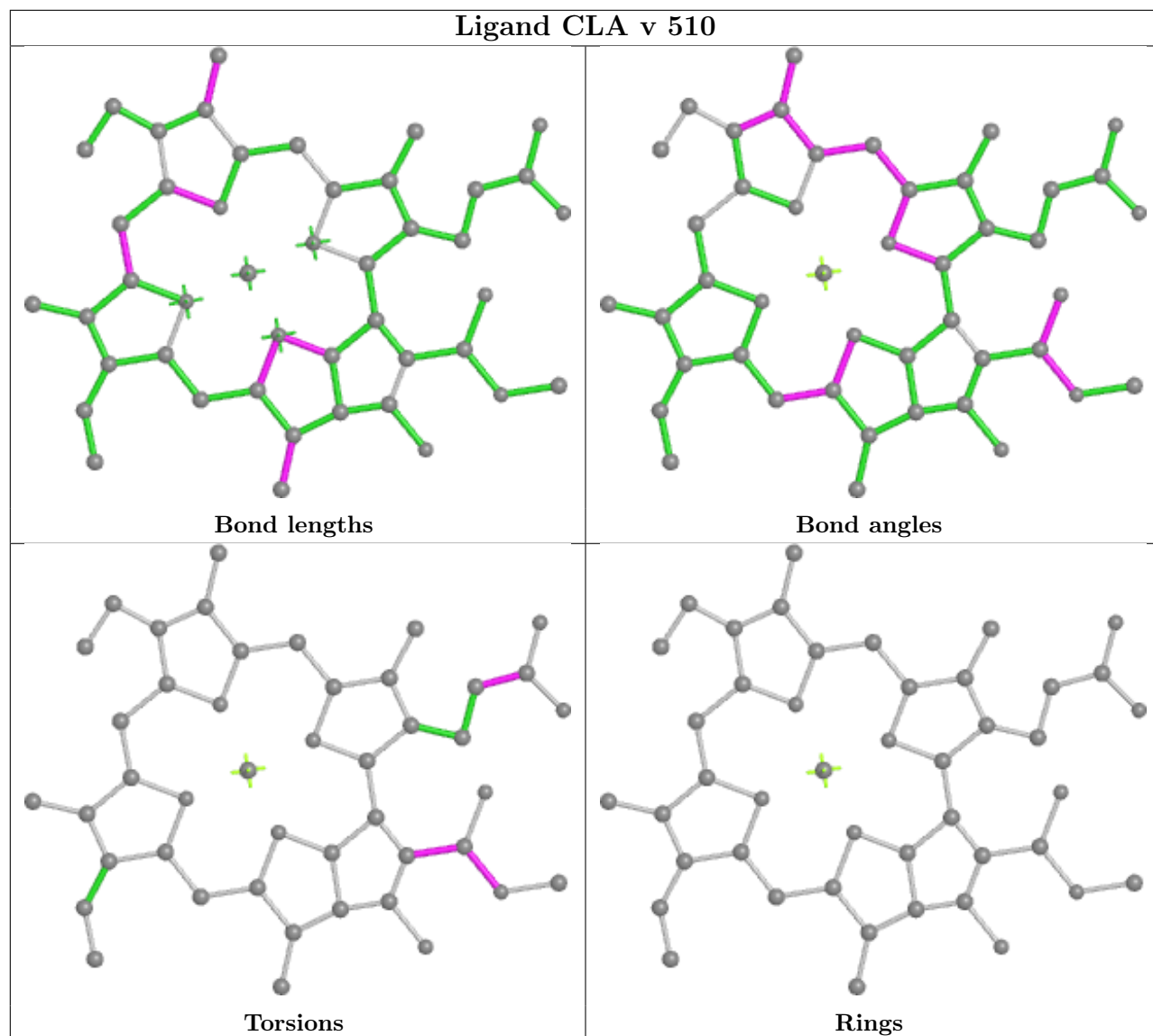


Torsions

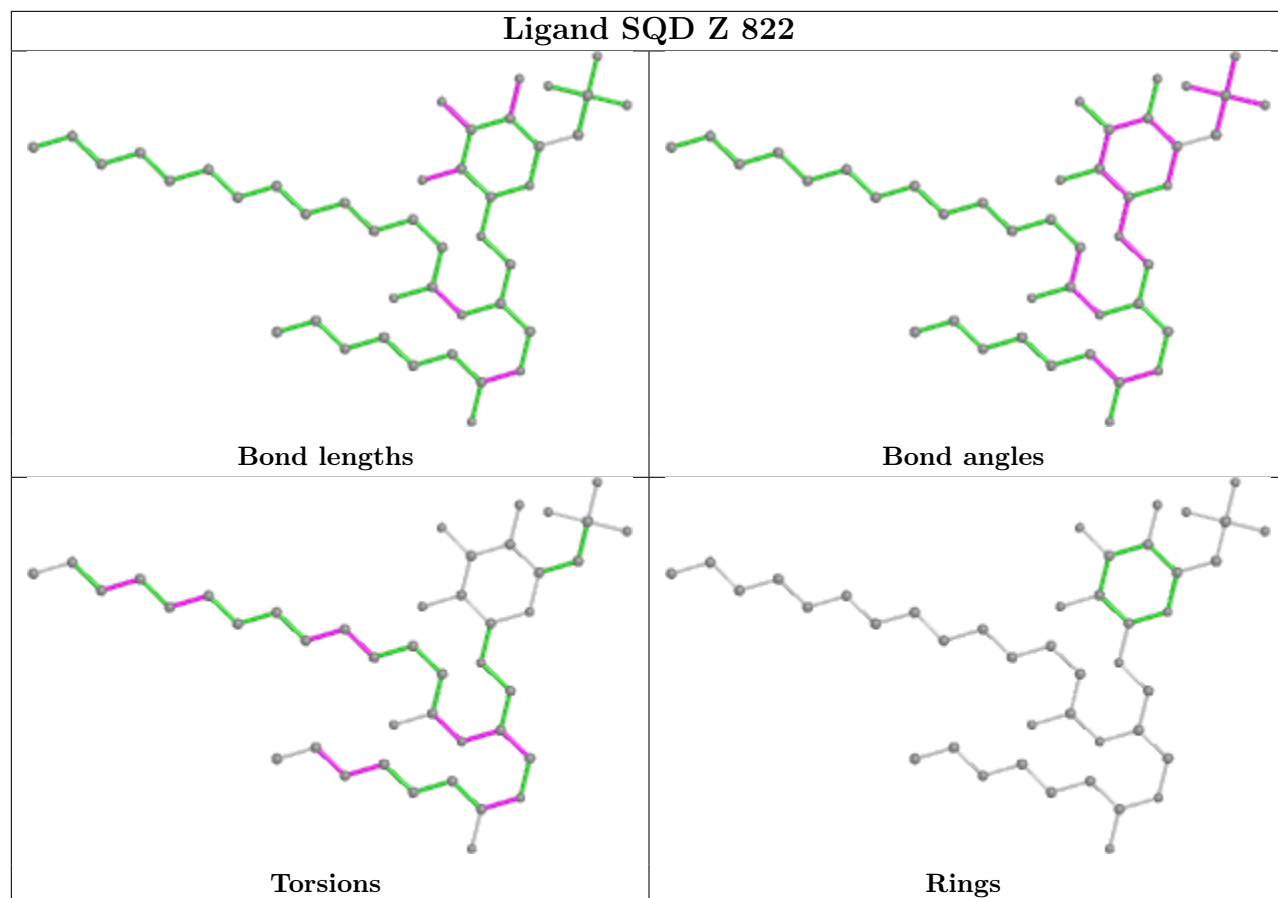


Rings

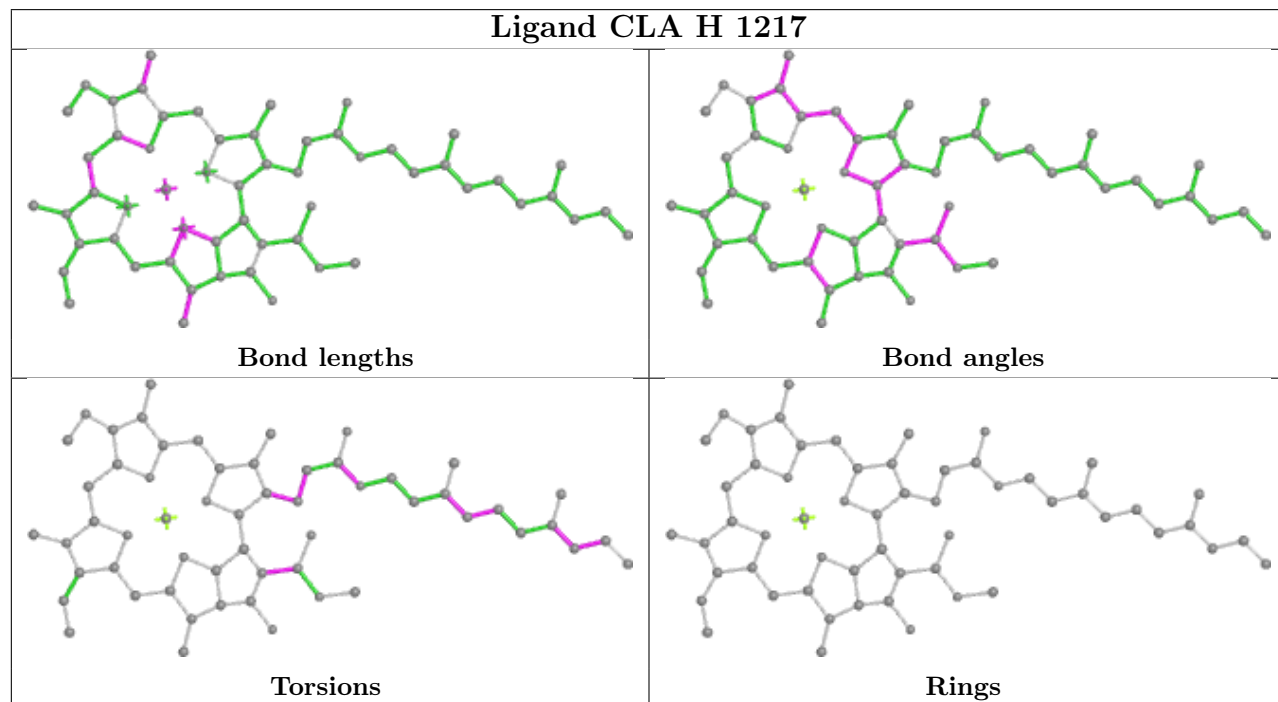
Ligand CLA v 510

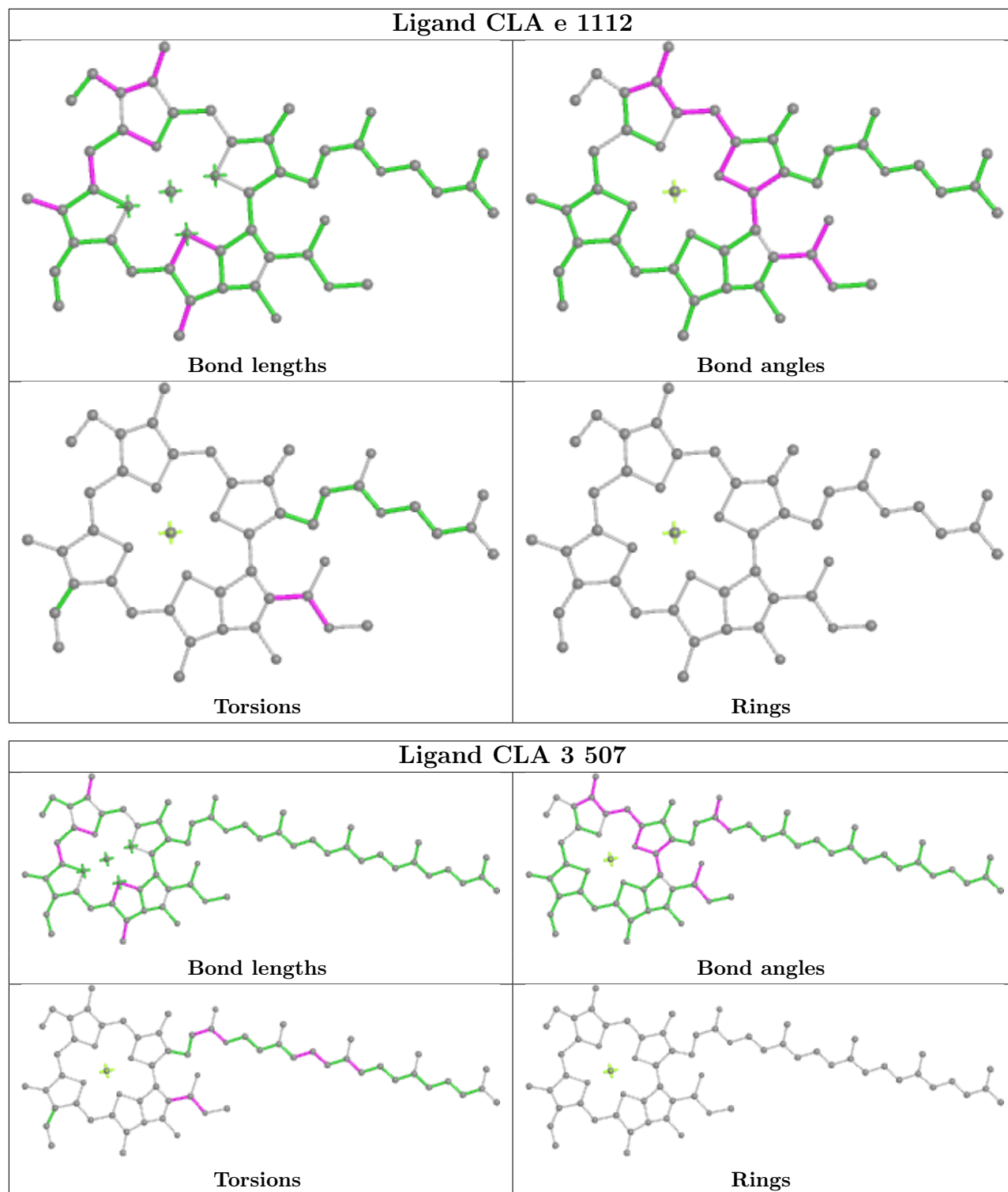


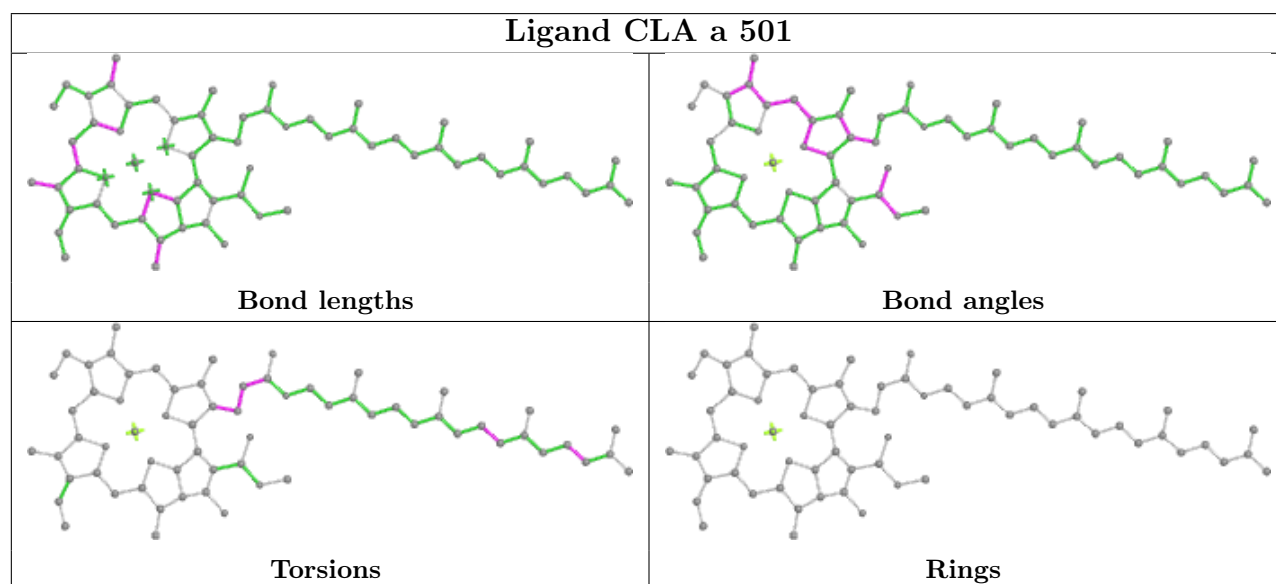
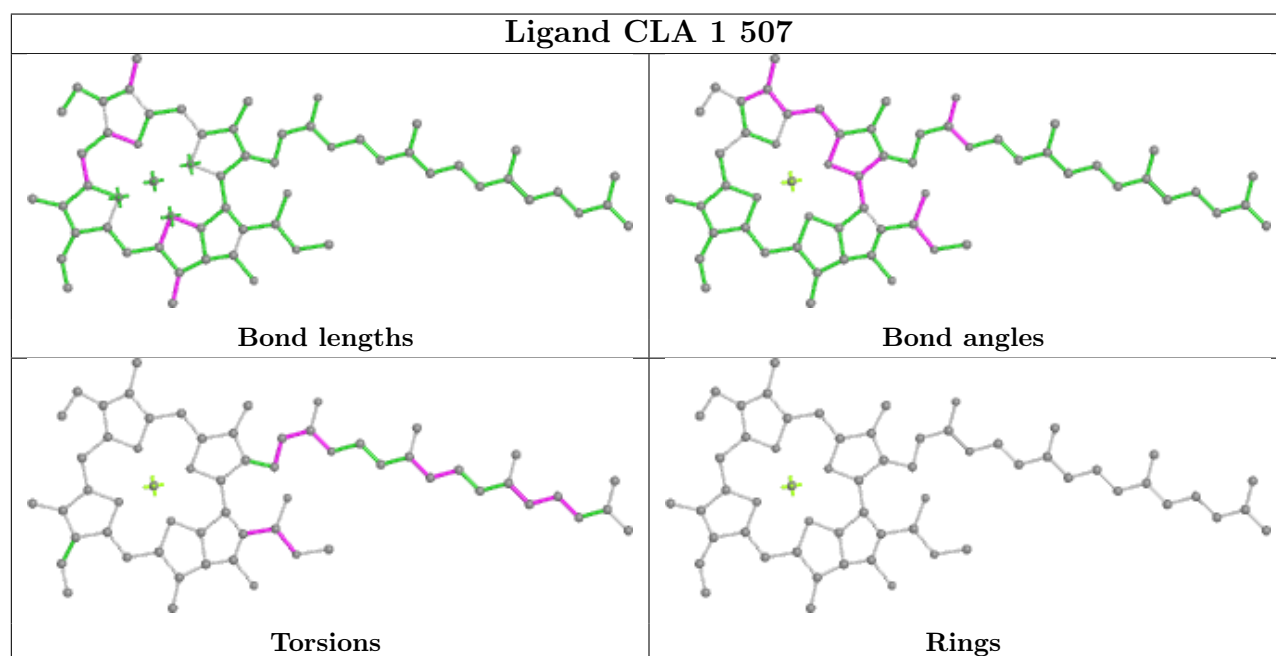
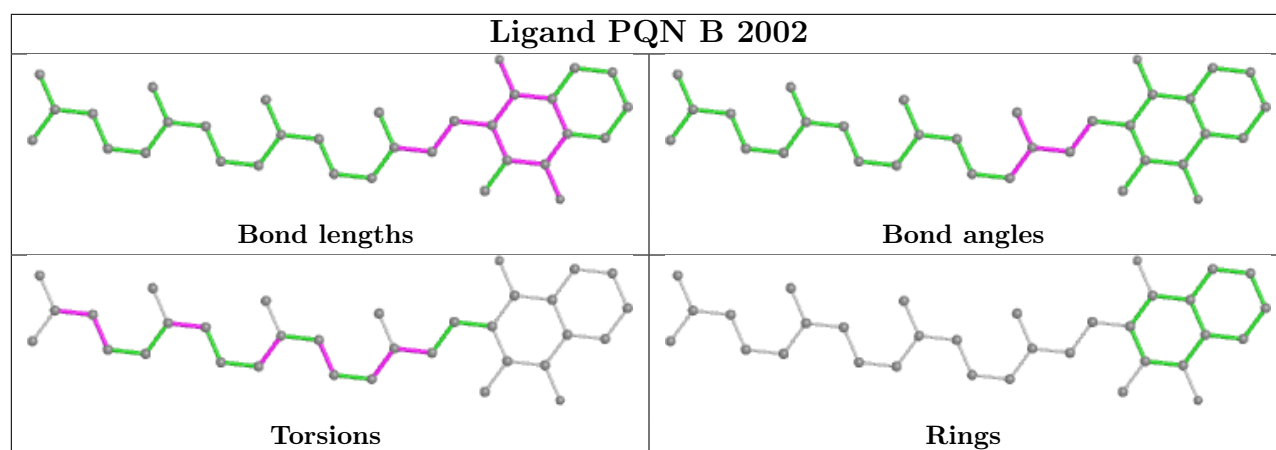
Ligand SQD Z 822

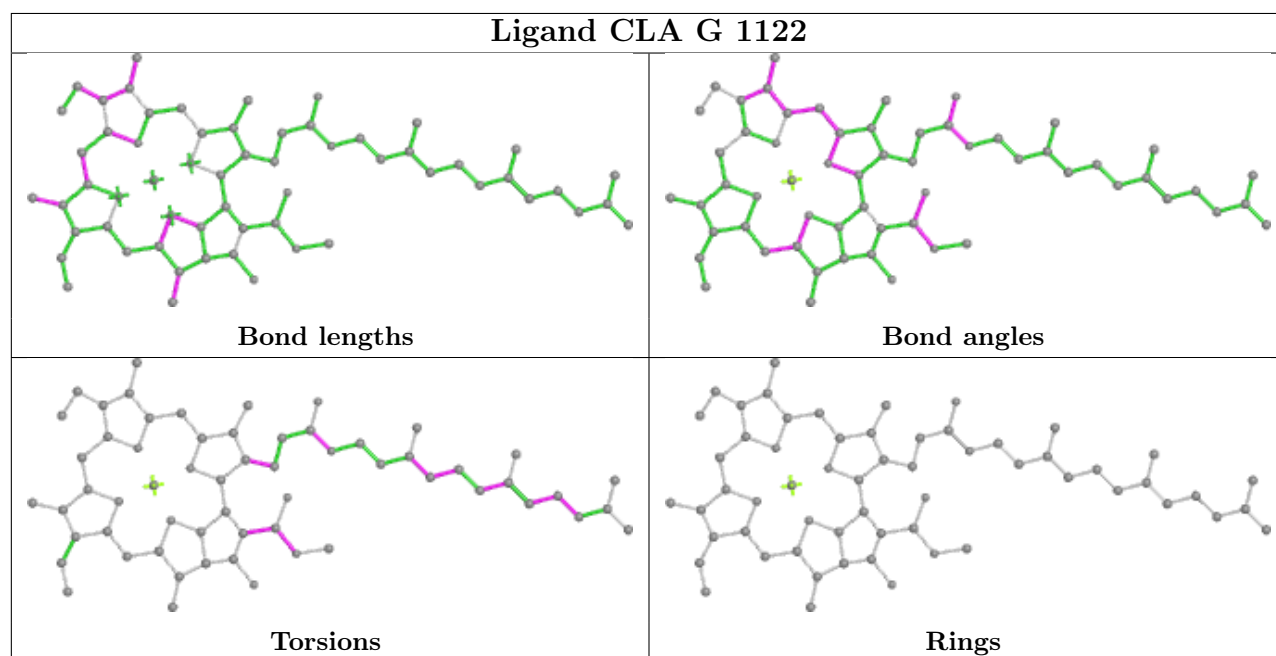
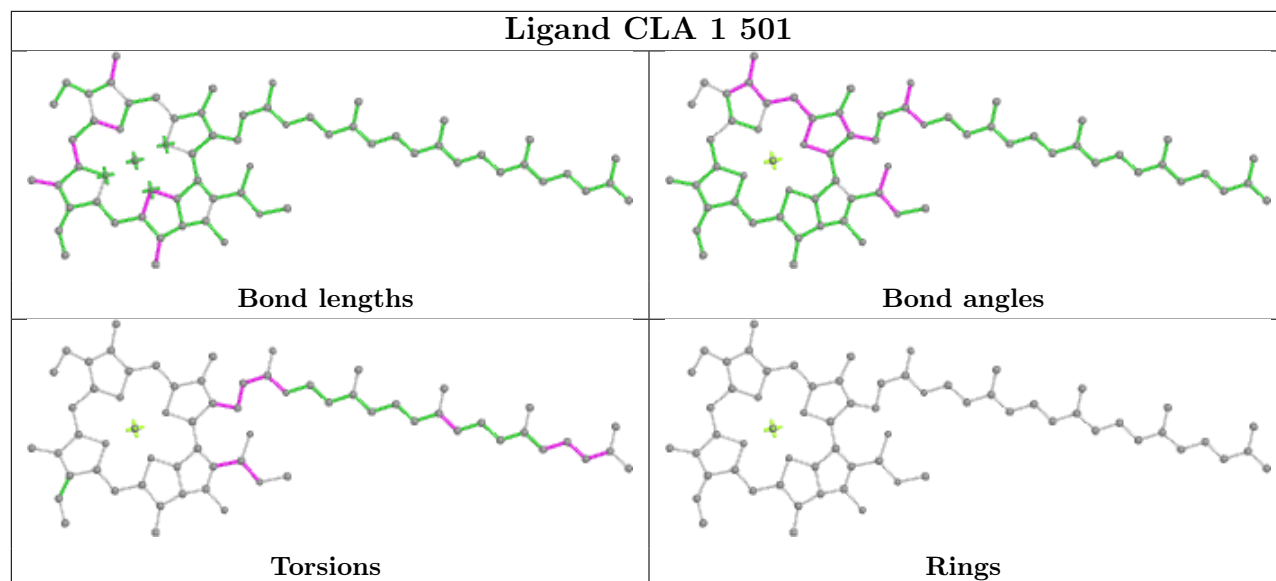
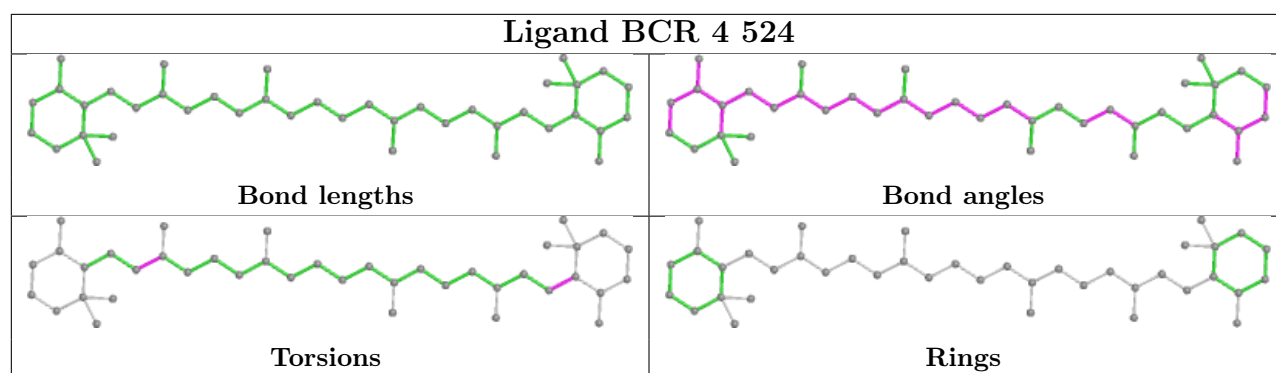


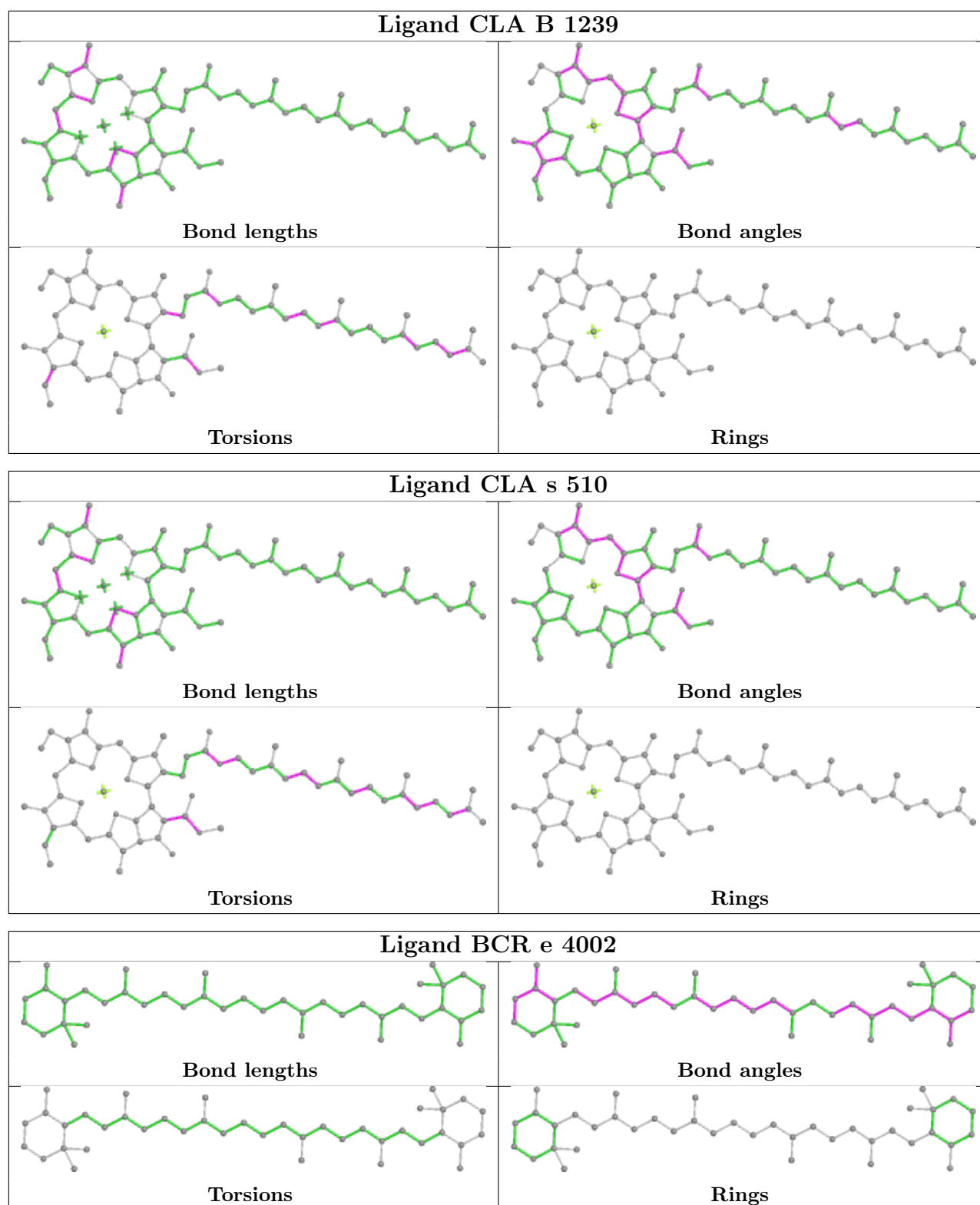
Ligand CLA H 1217

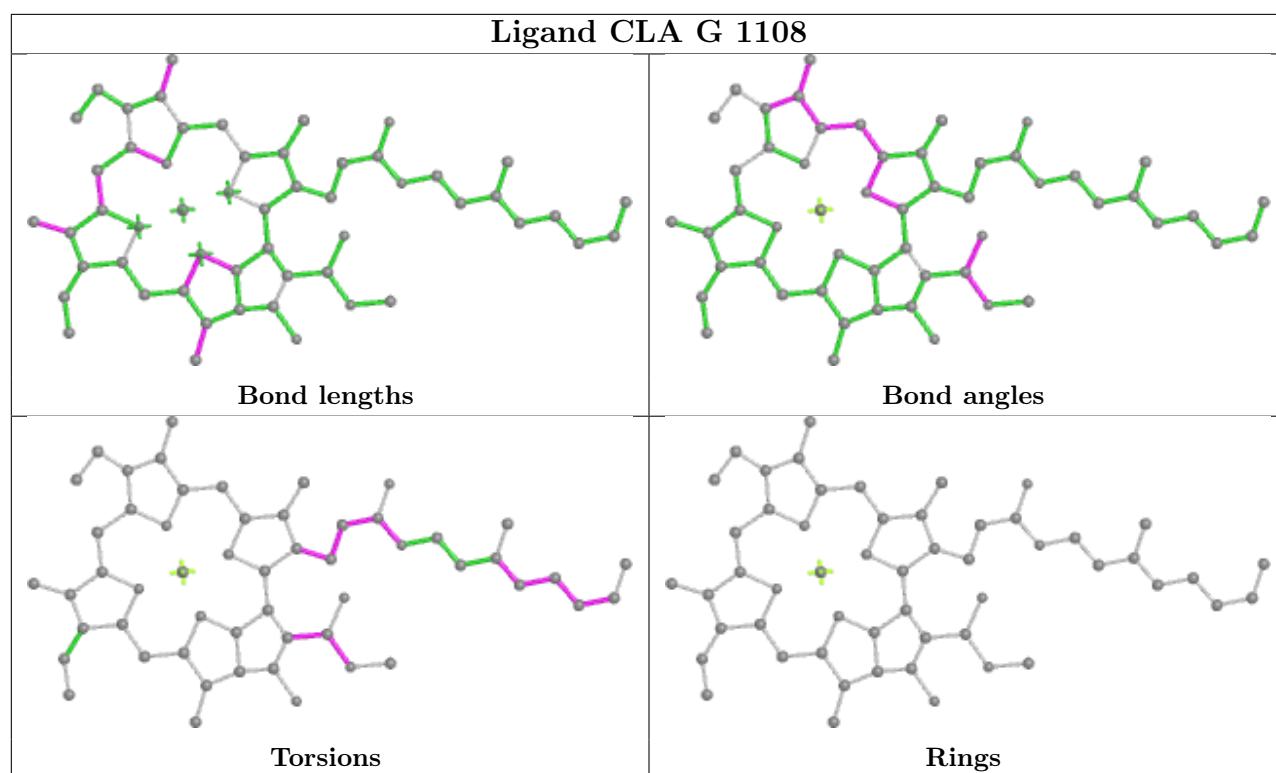




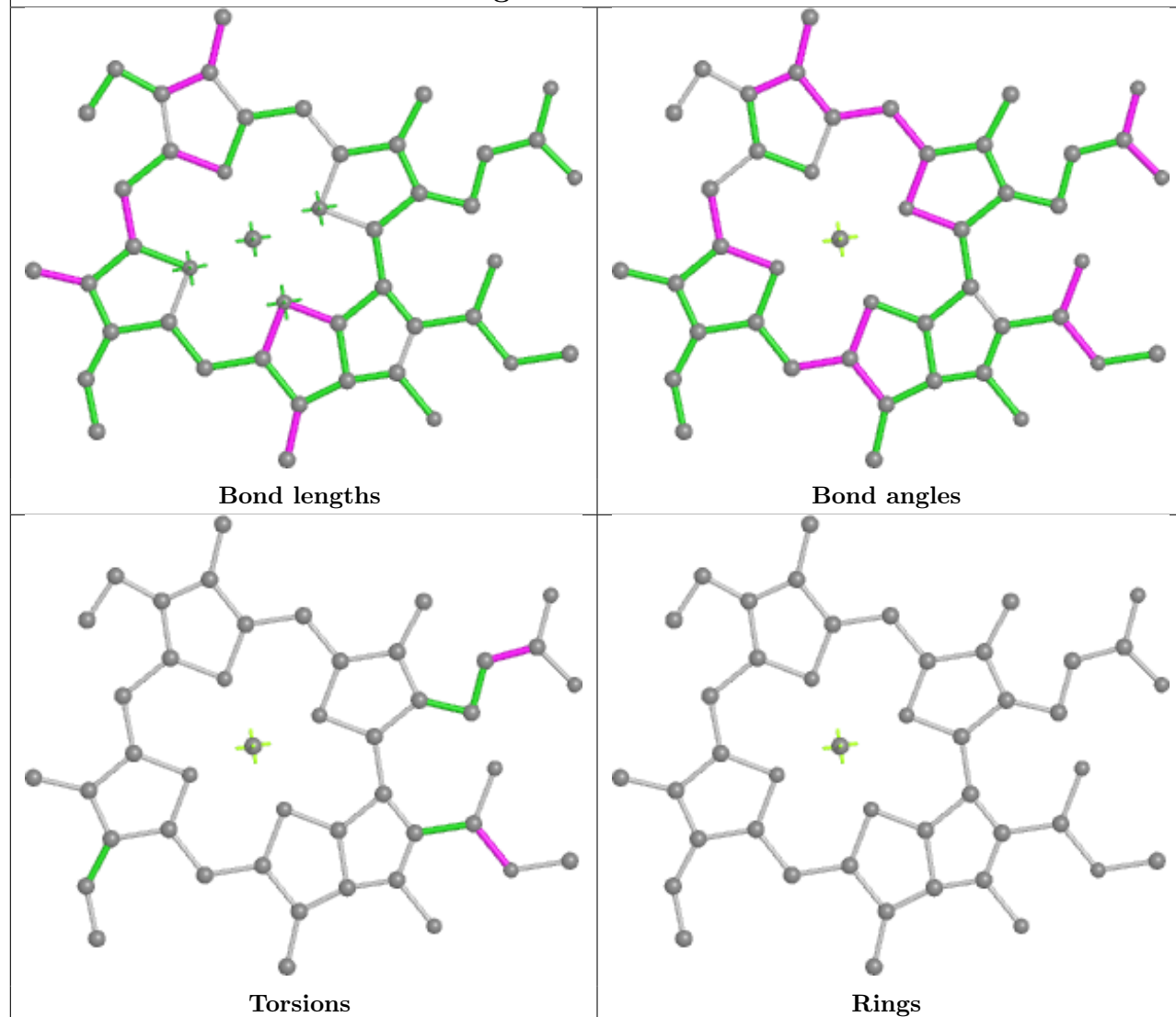




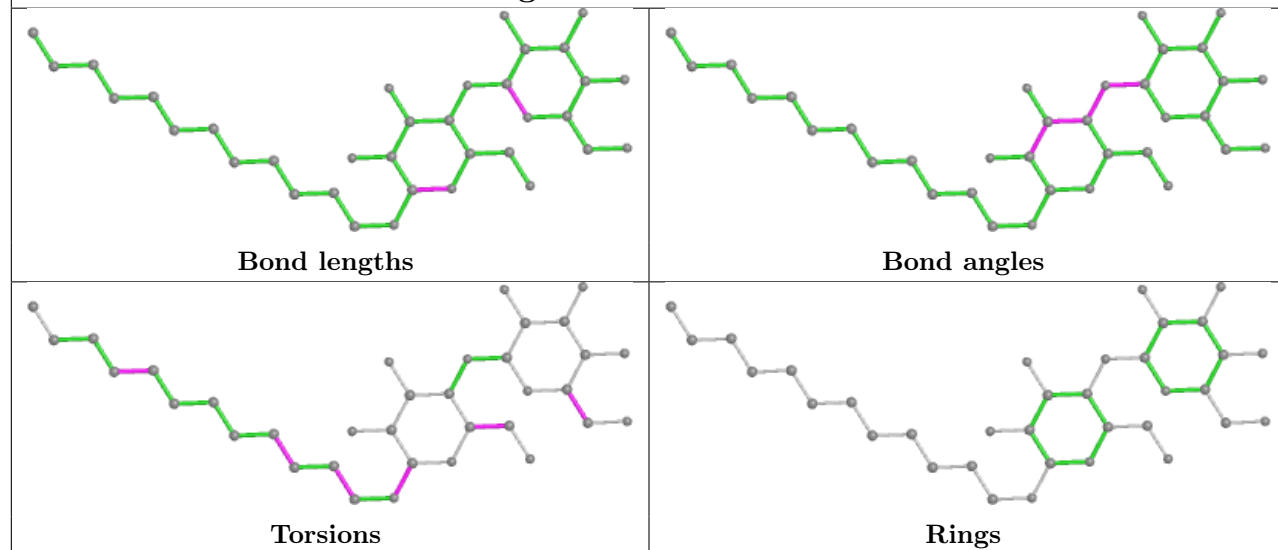




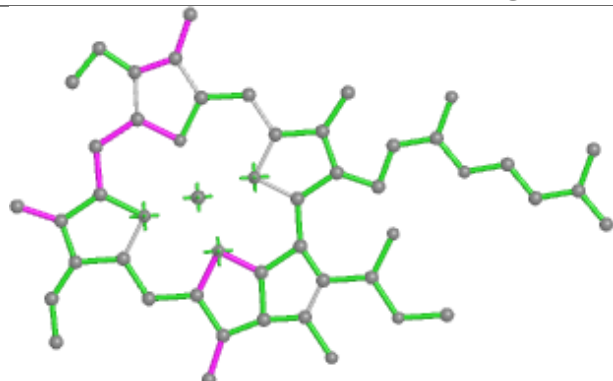
Ligand CLA 4 508



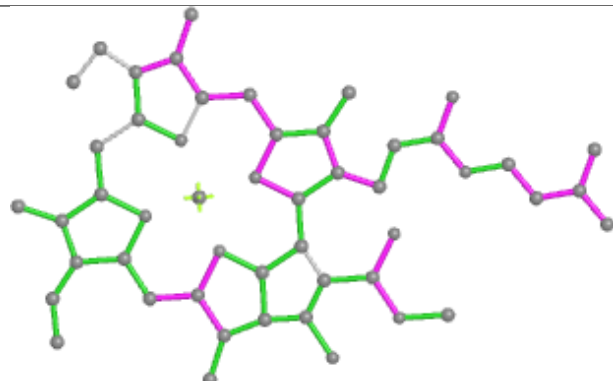
Ligand LMU A 1848



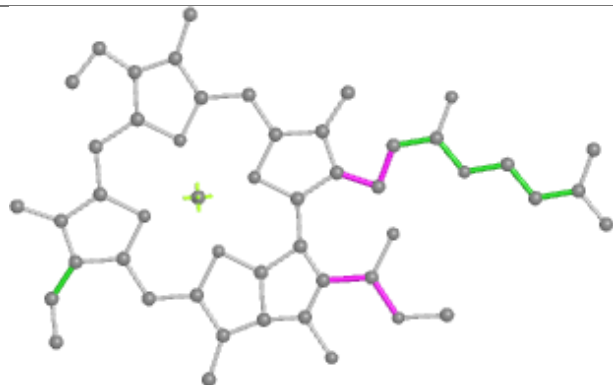
Ligand CLA K 1103



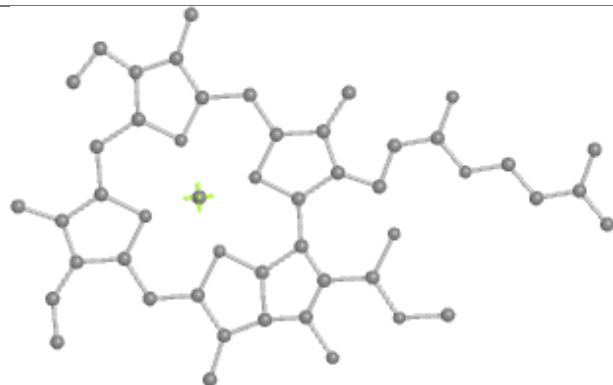
Bond lengths



Bond angles

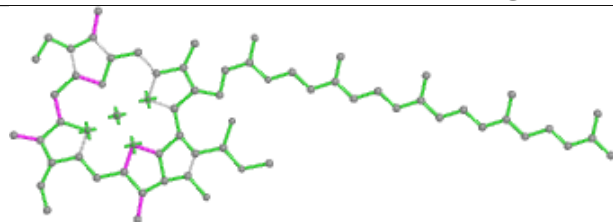


Torsions

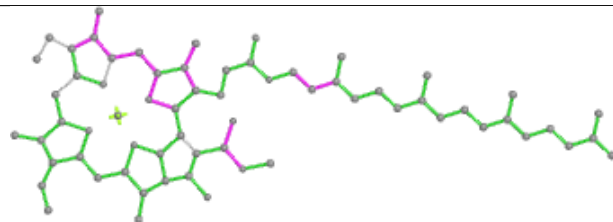


Rings

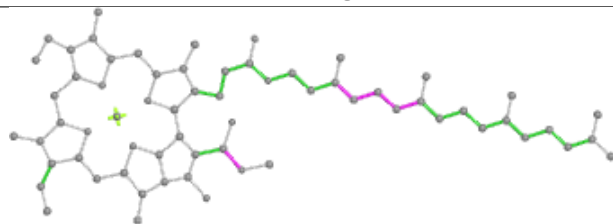
Ligand CLA H 1231



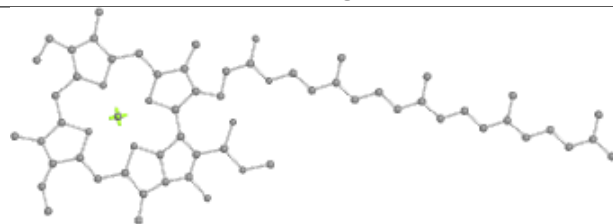
Bond lengths



Bond angles

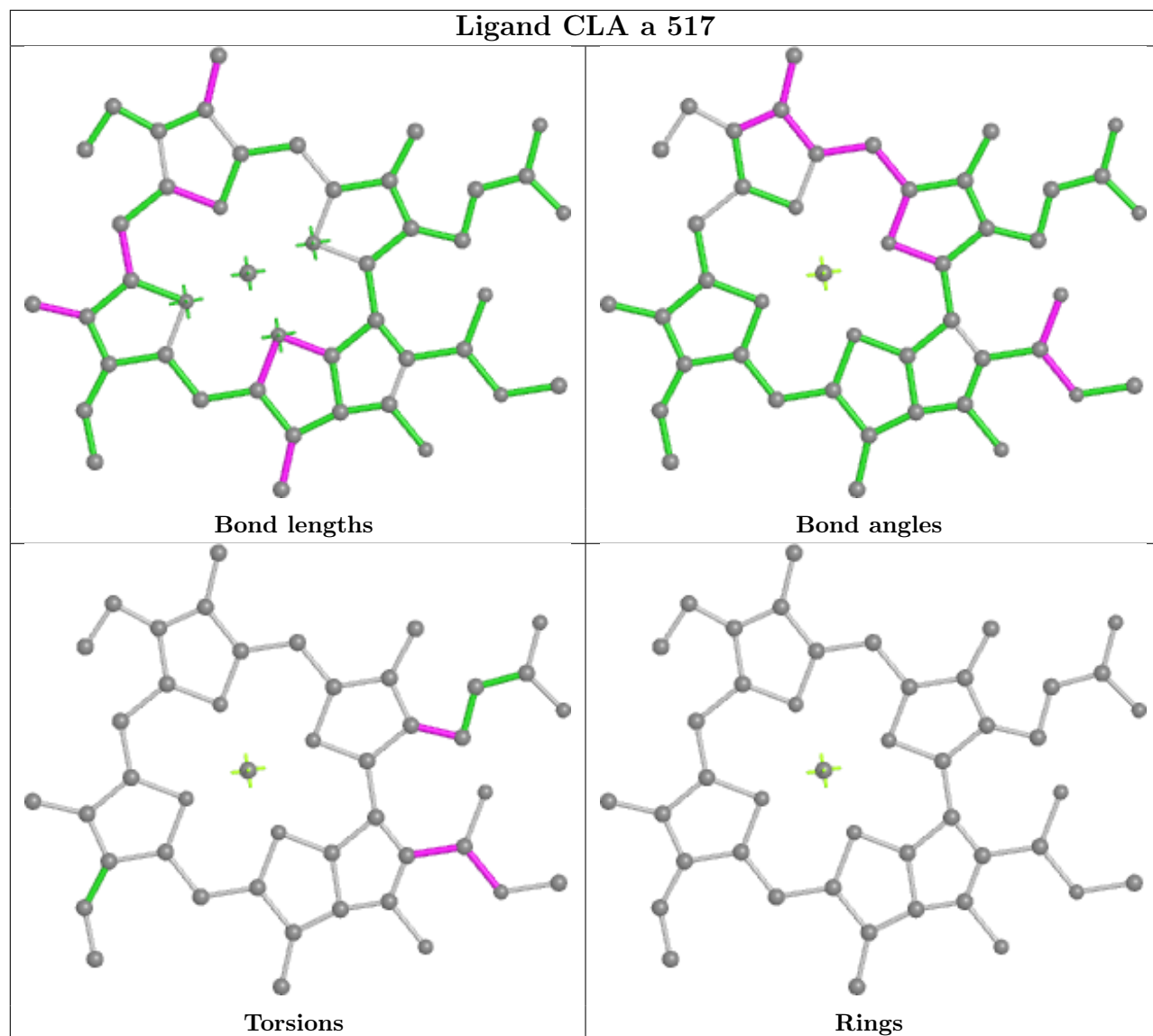


Torsions

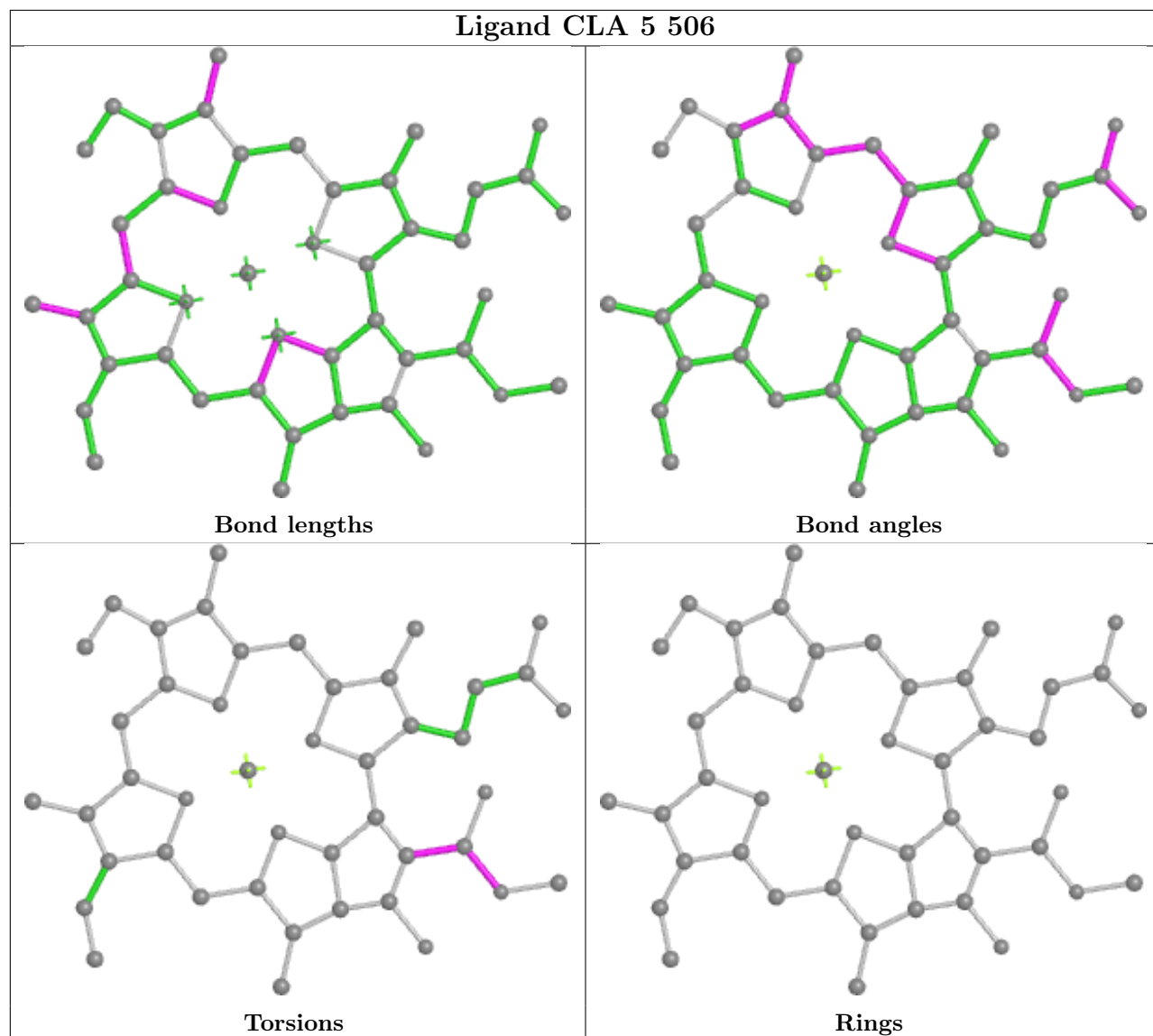


Rings

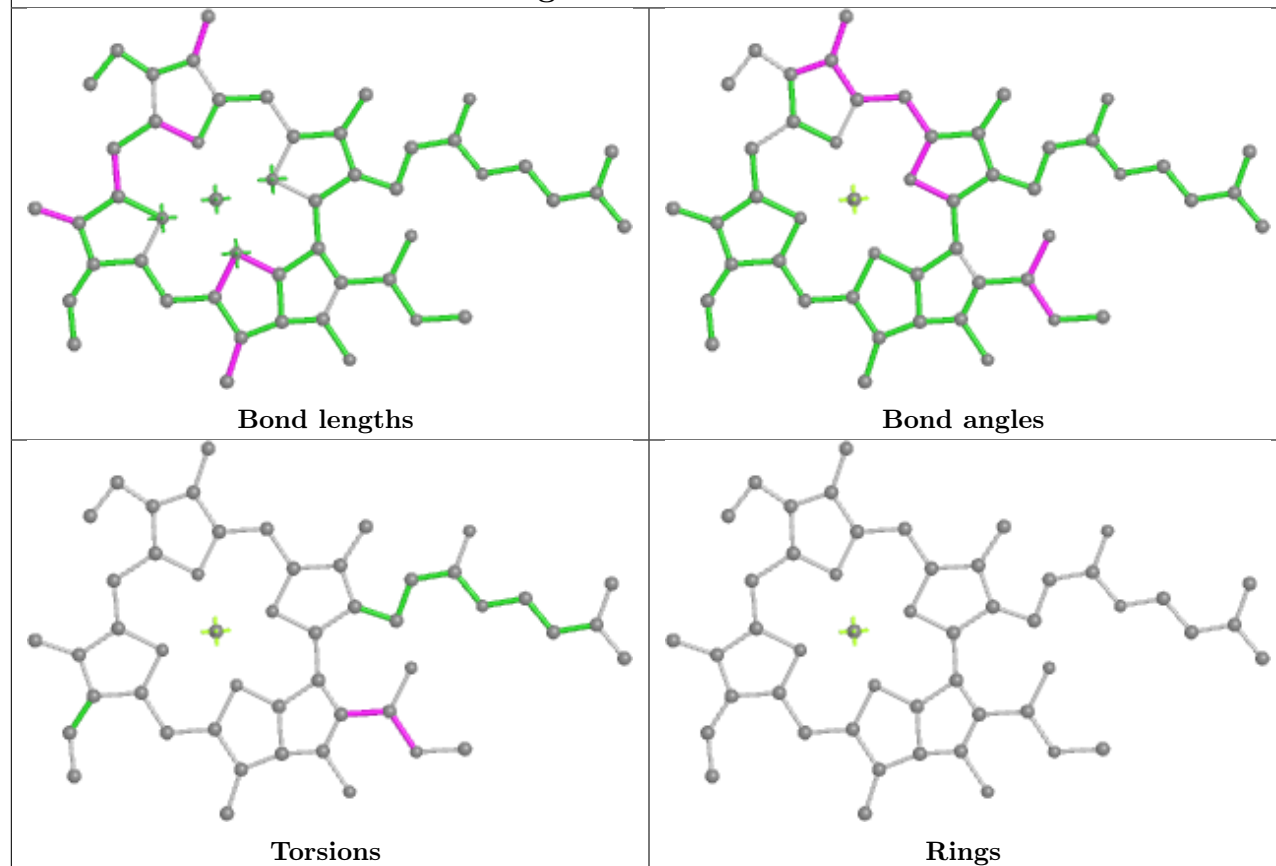
Ligand CLA a 517



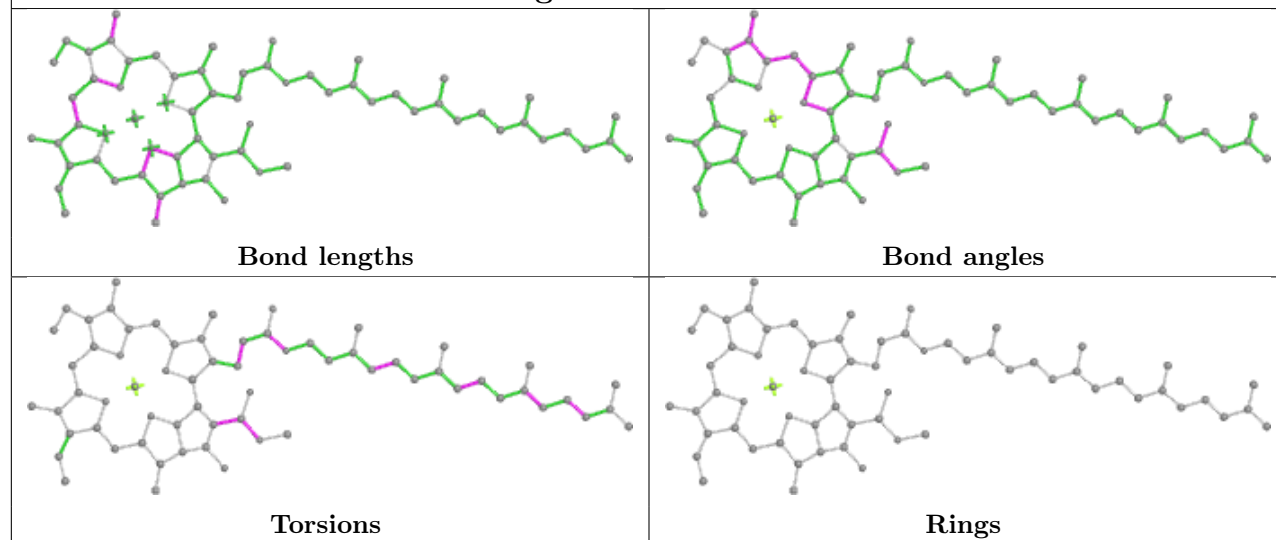
Ligand CLA 5 506

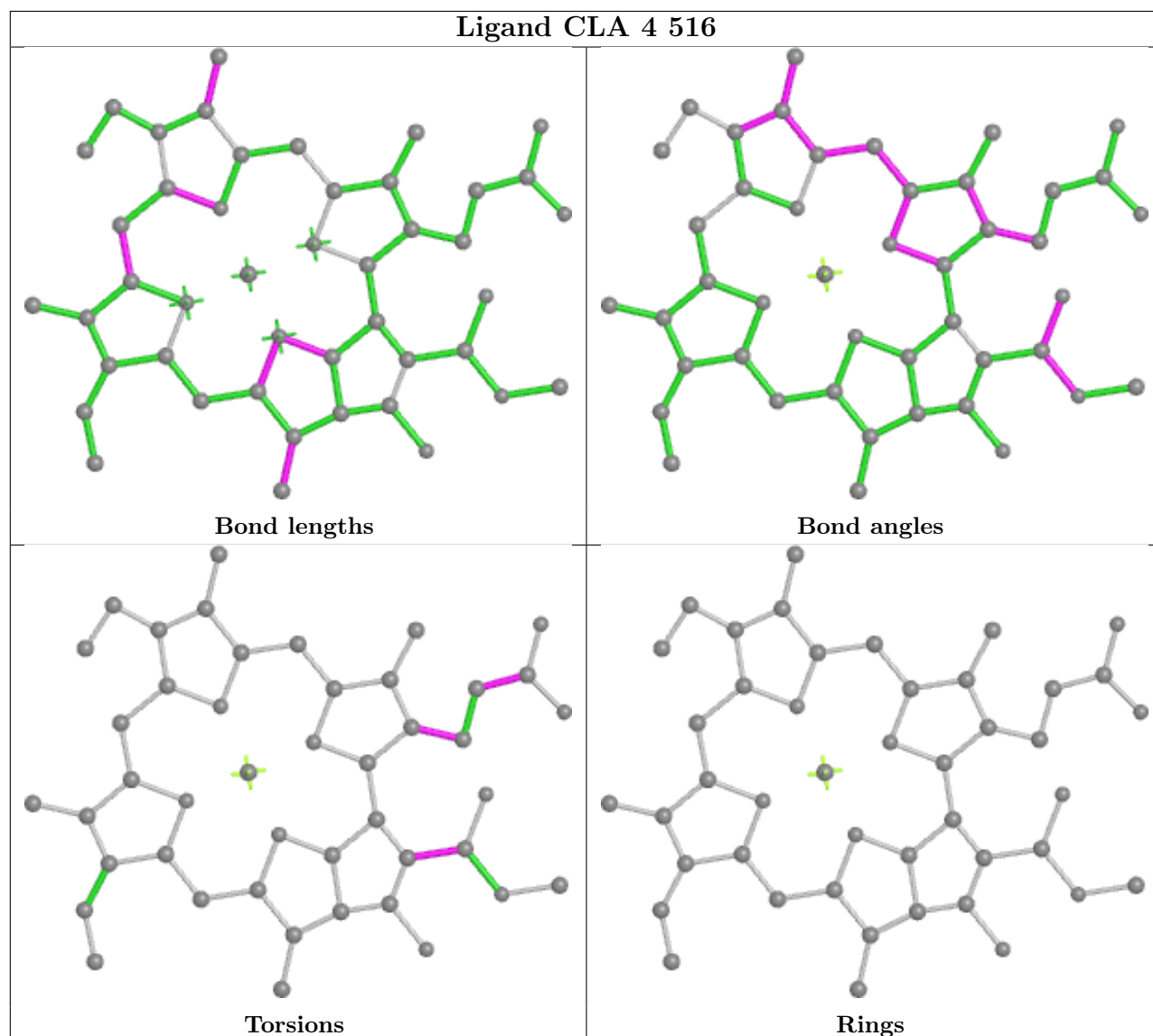
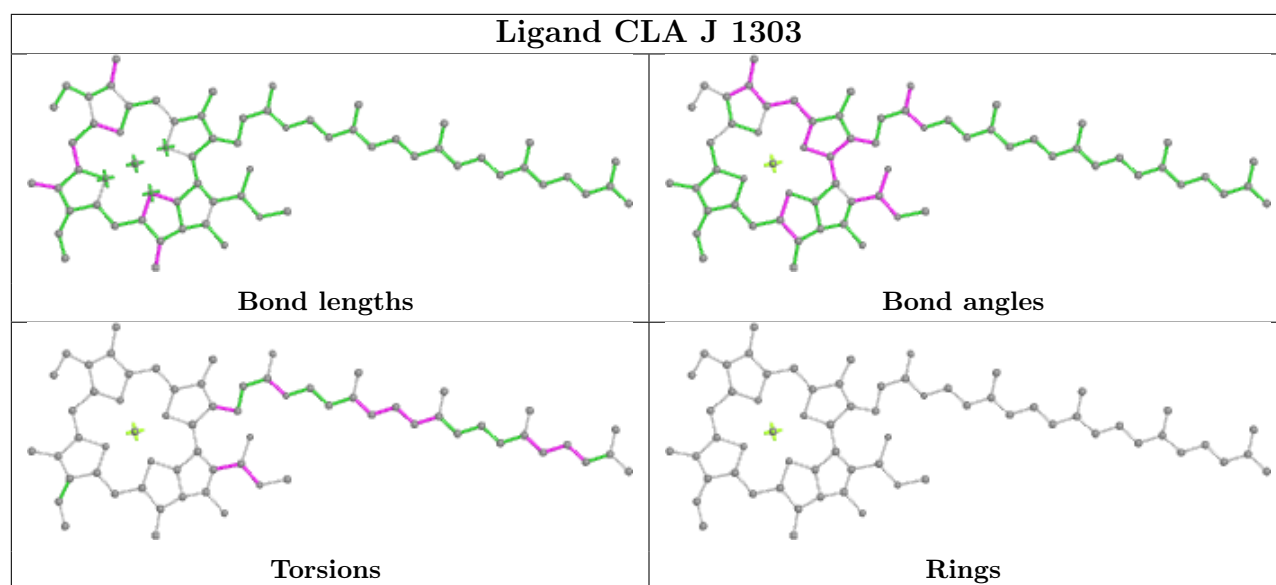


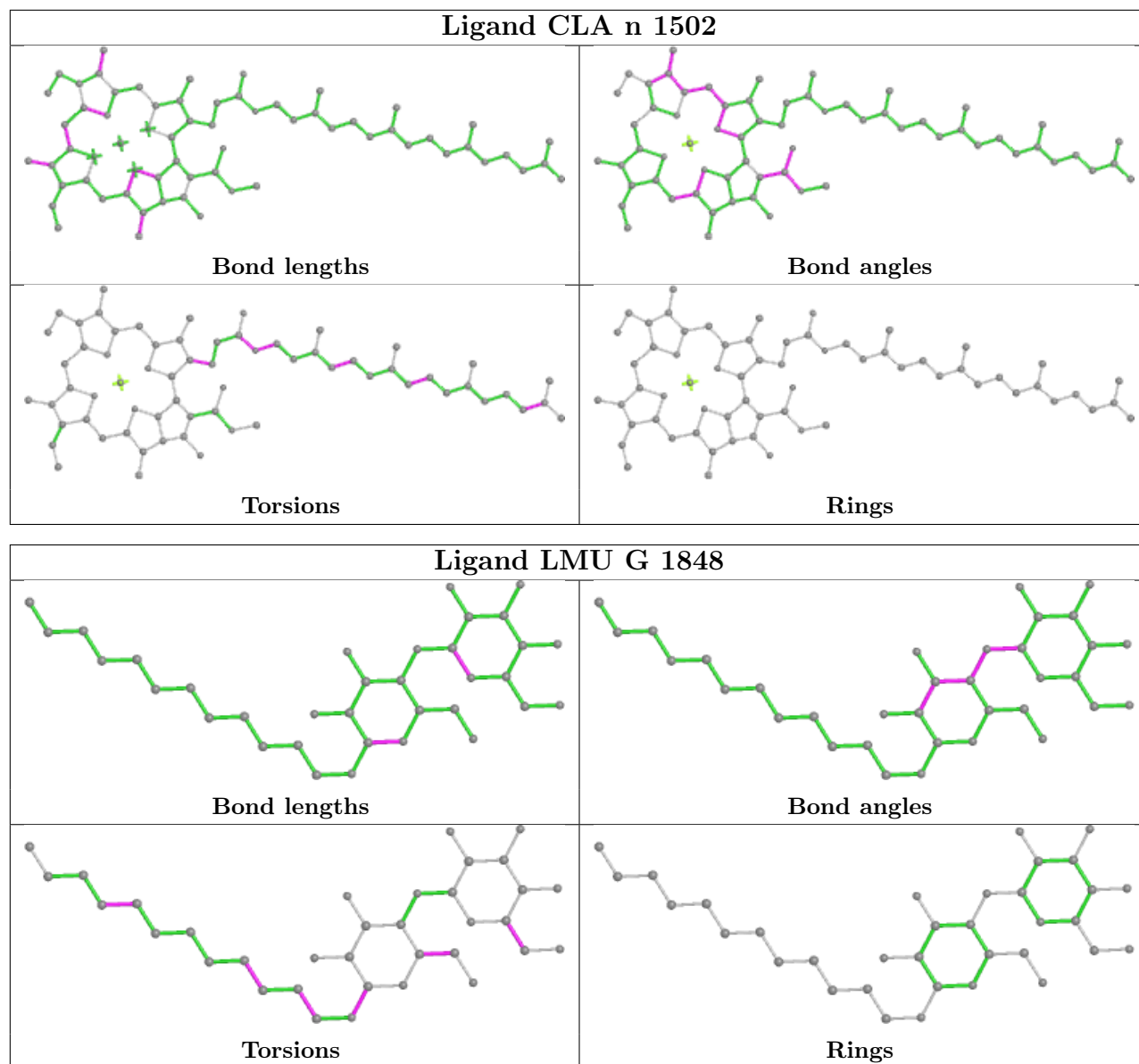
Ligand CLA s 506

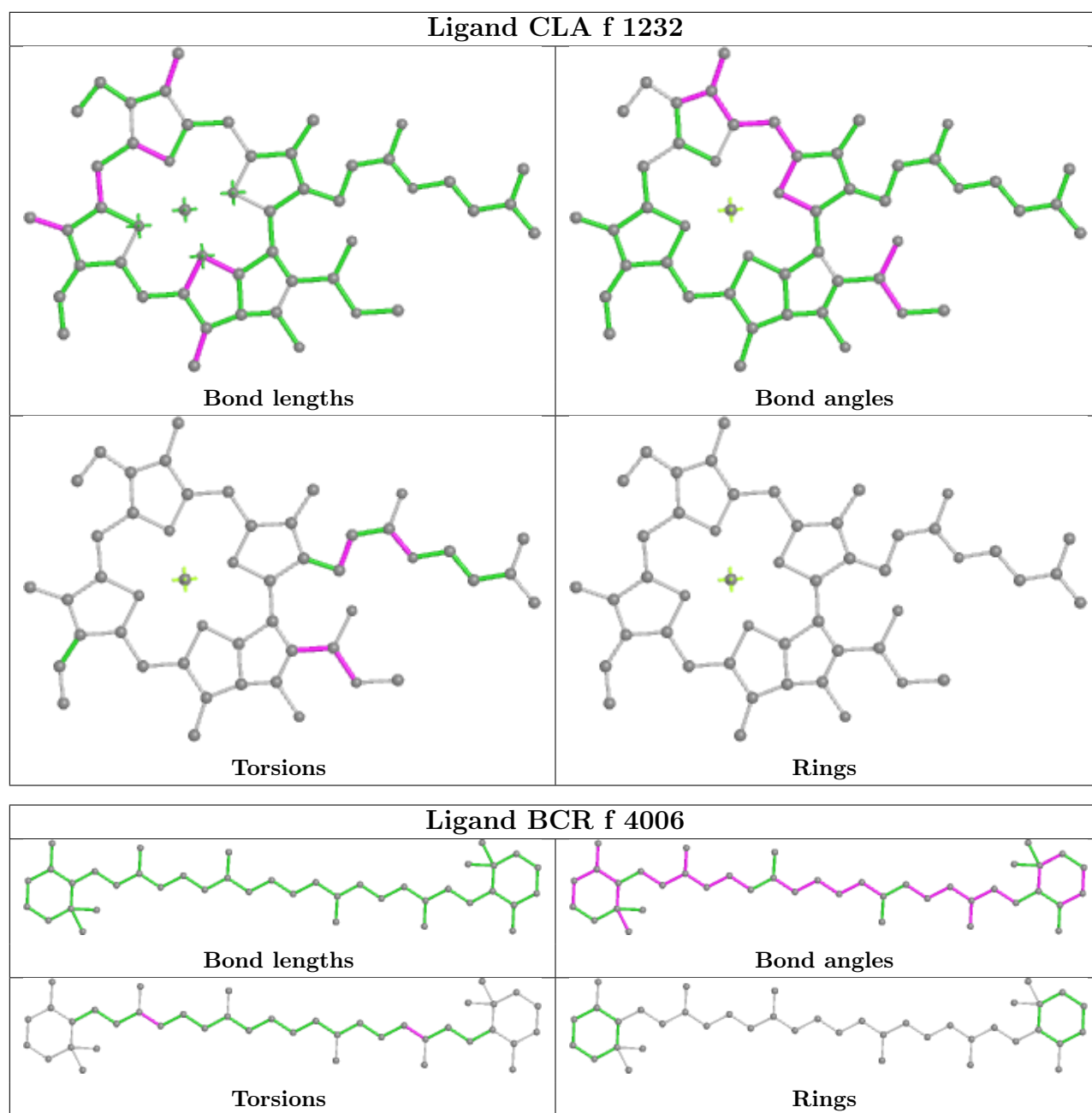


Ligand CLA b 505

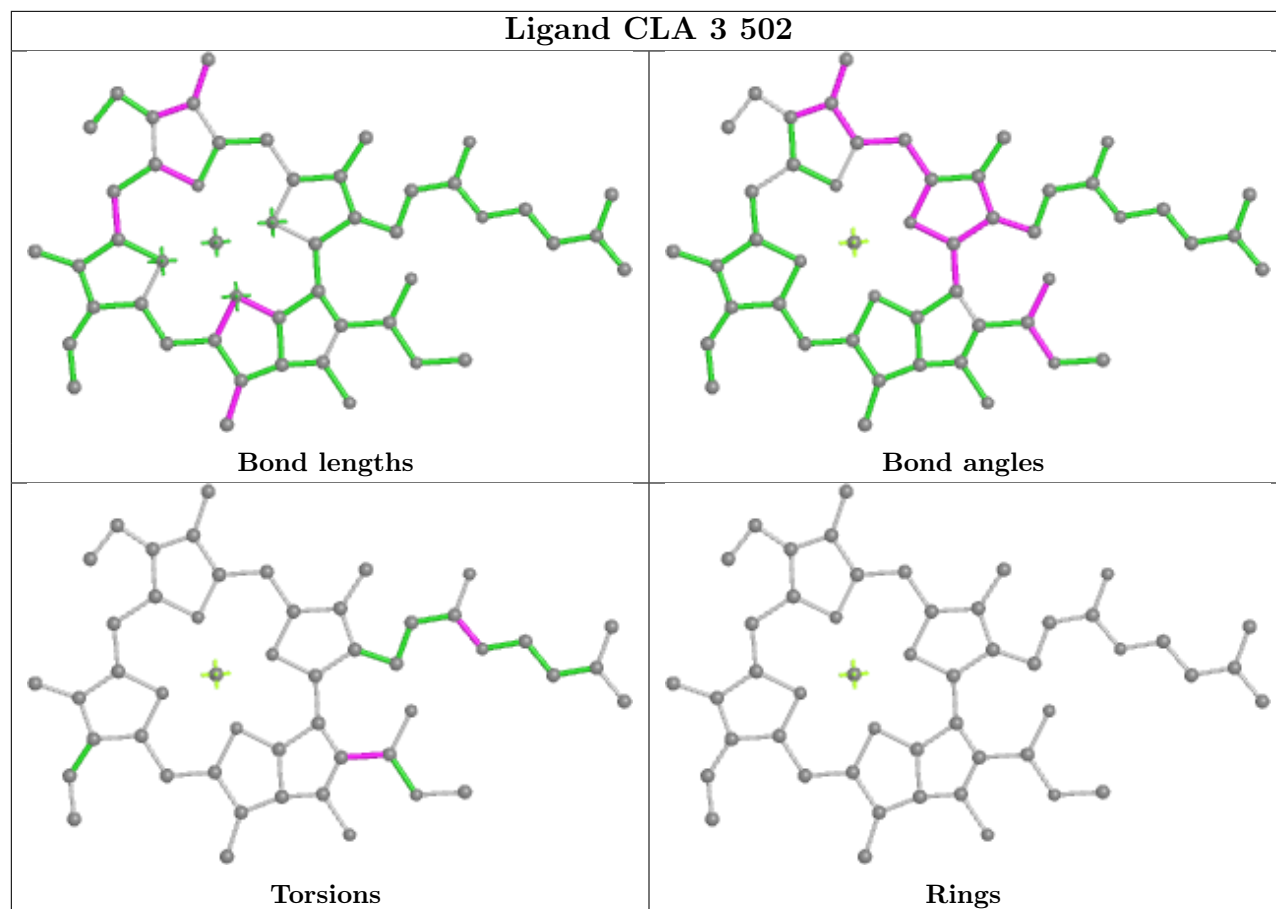




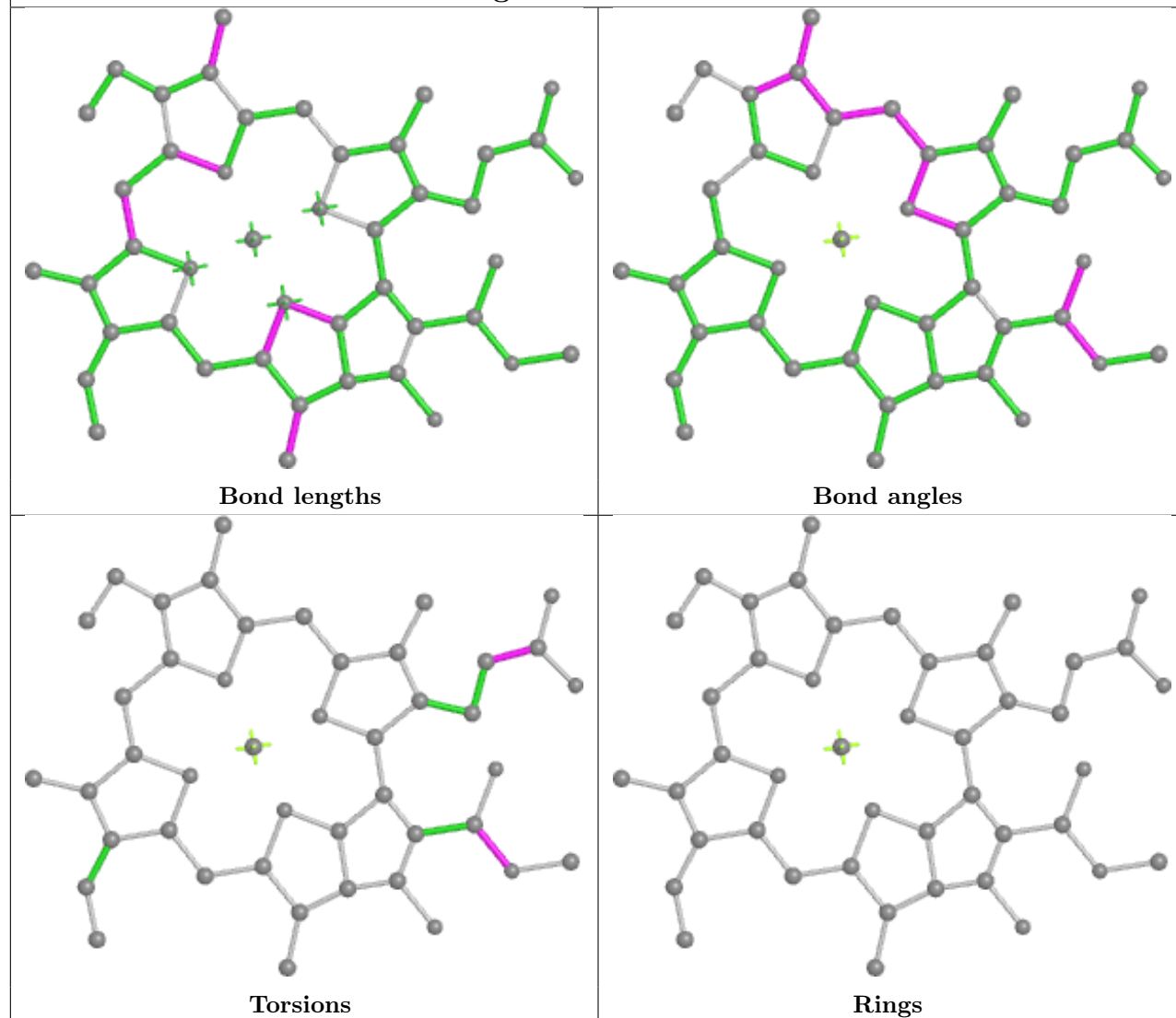




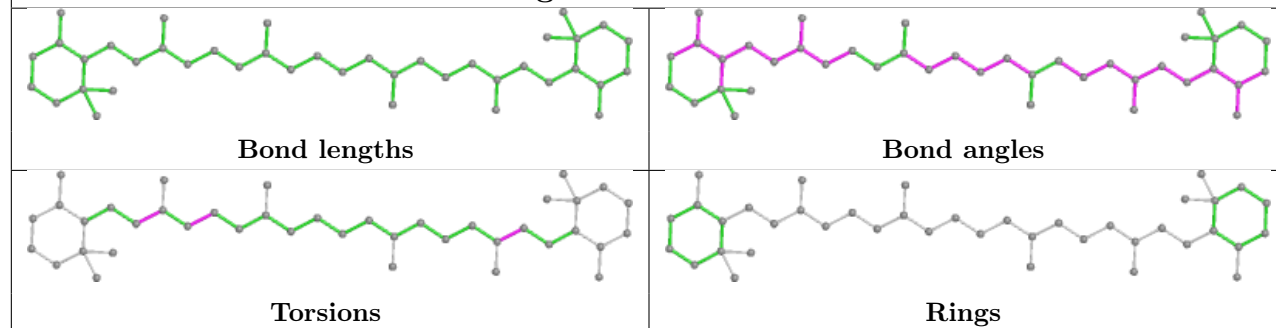
Ligand CLA 3 502

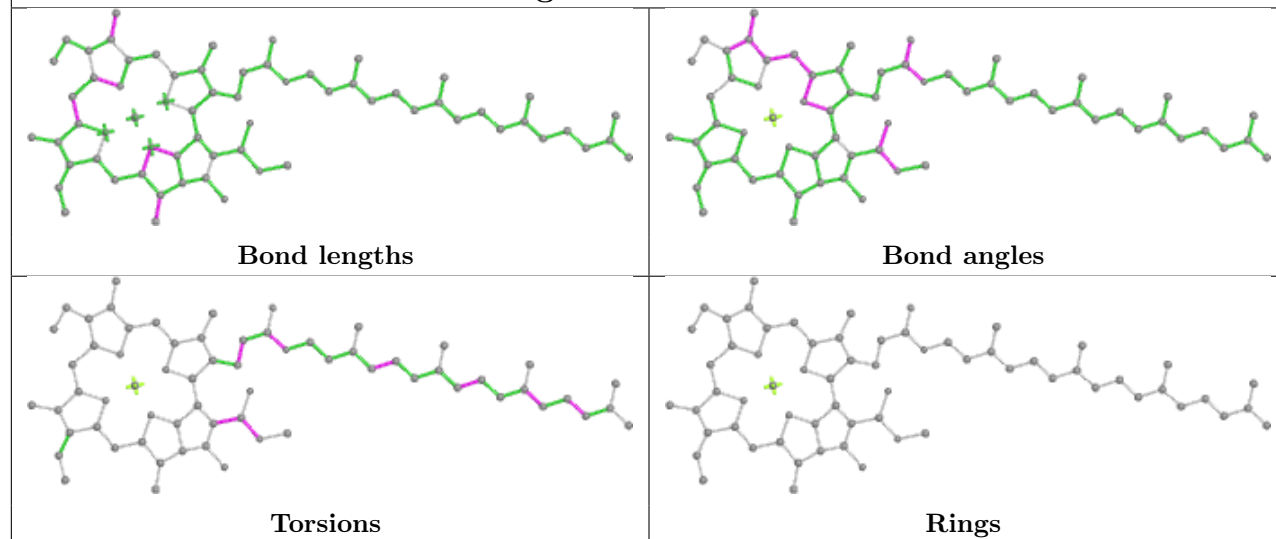
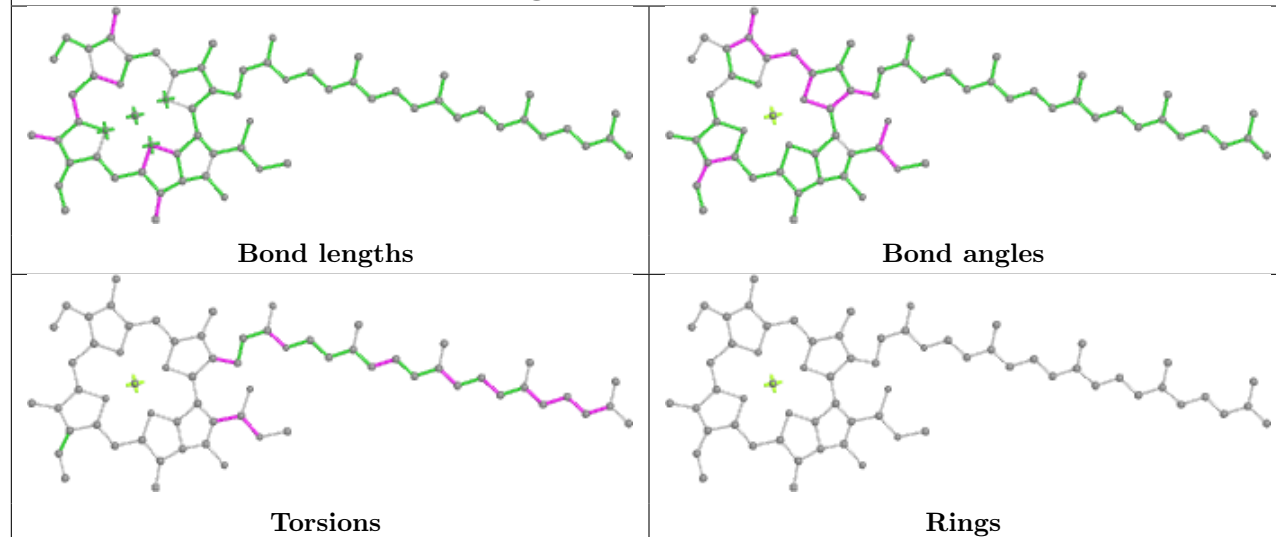
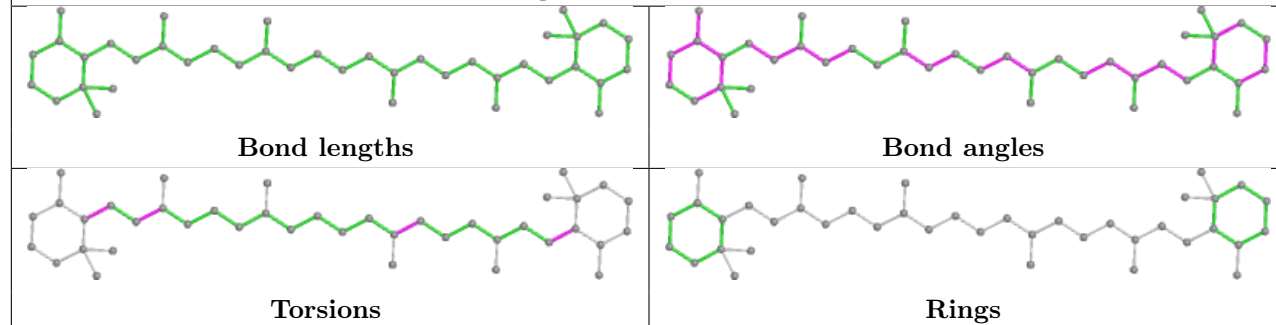


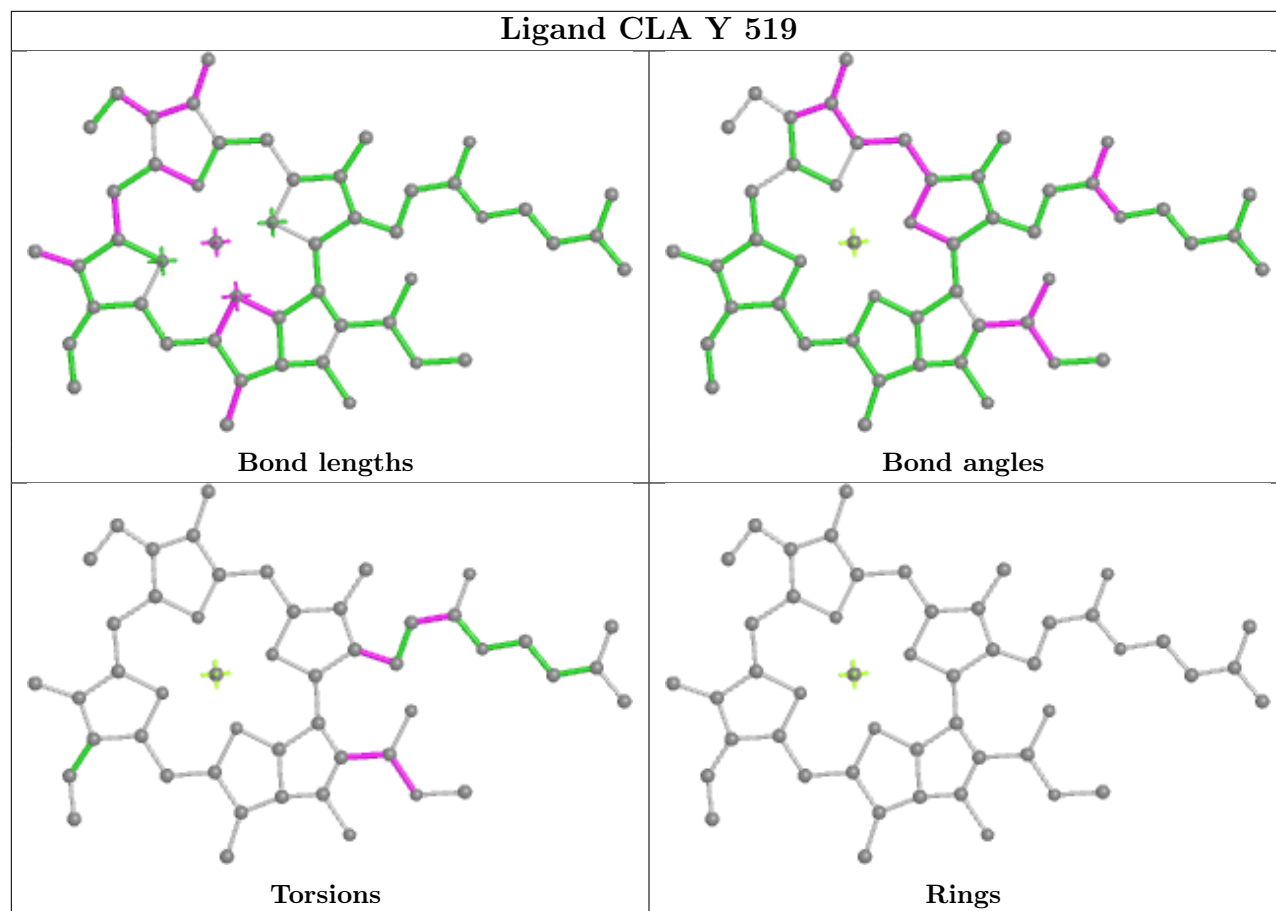
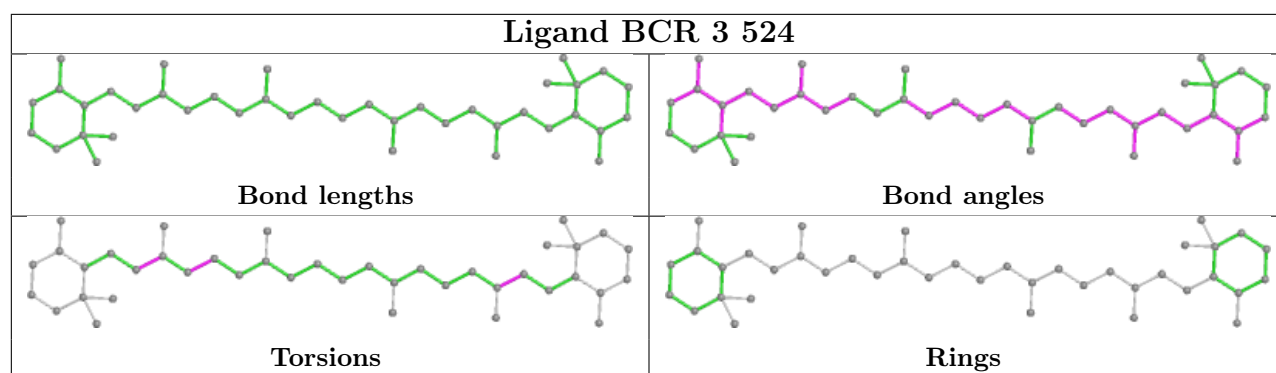
Ligand CLA d 511



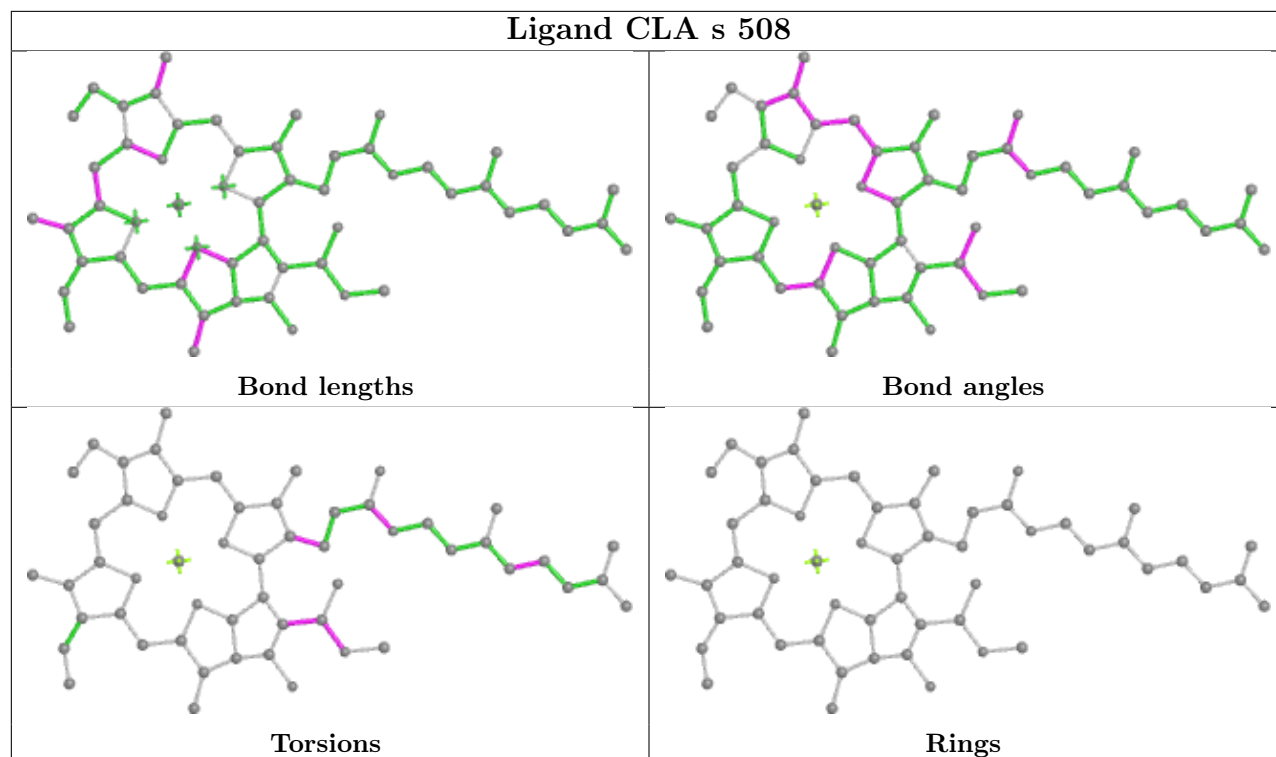
Ligand BCR s 524



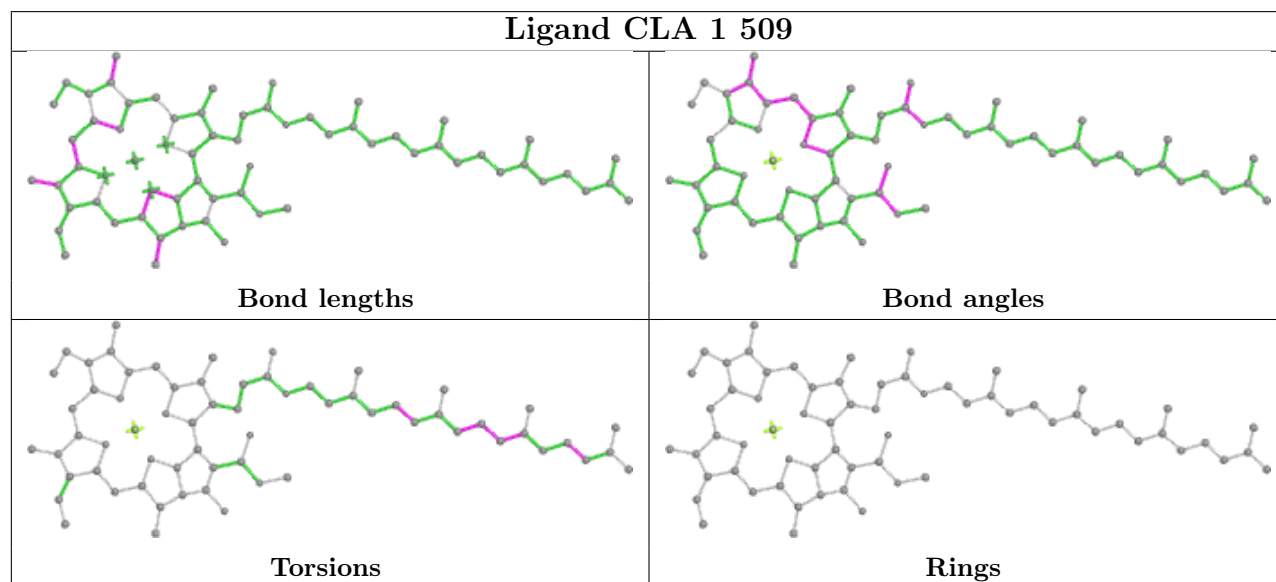
Ligand CLA 4 505**Ligand CLA e 1103****Ligand BCR 1 521**

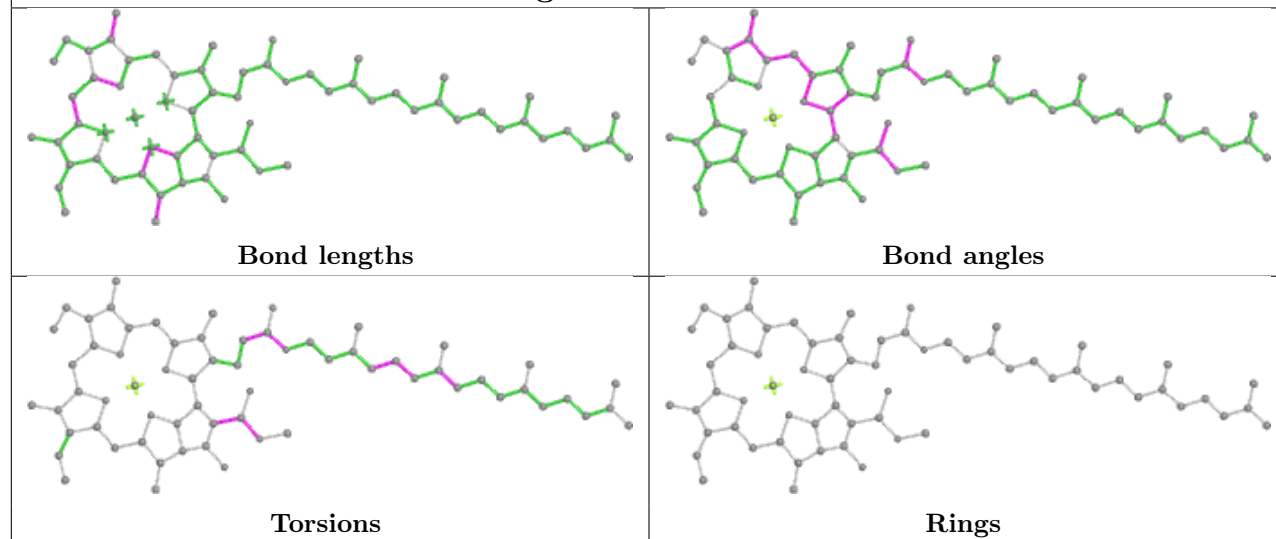
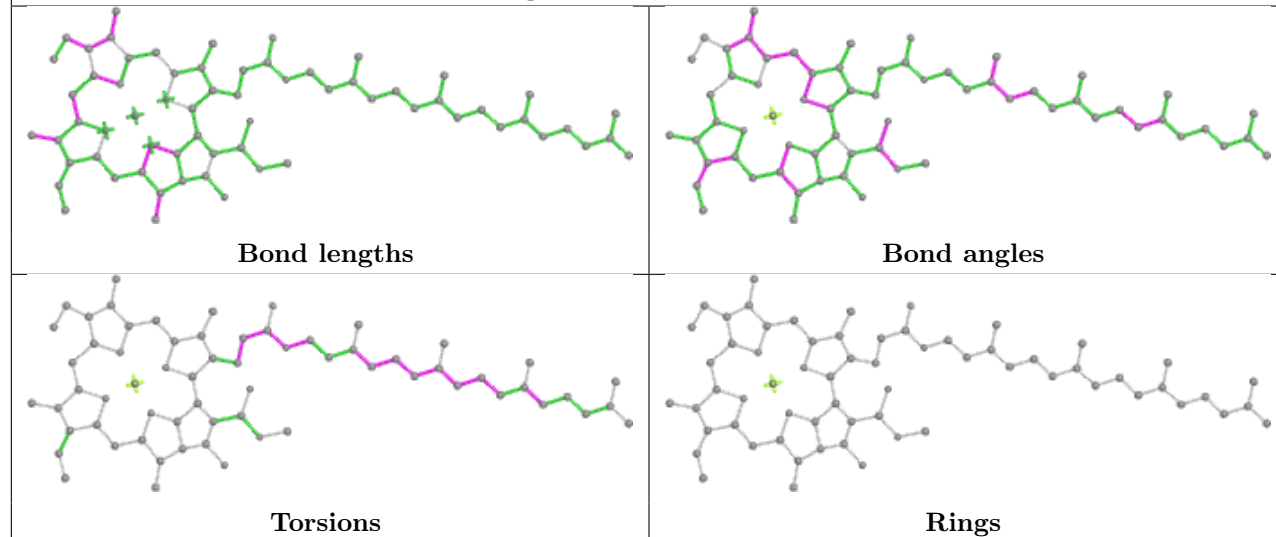


Ligand CLA s 508

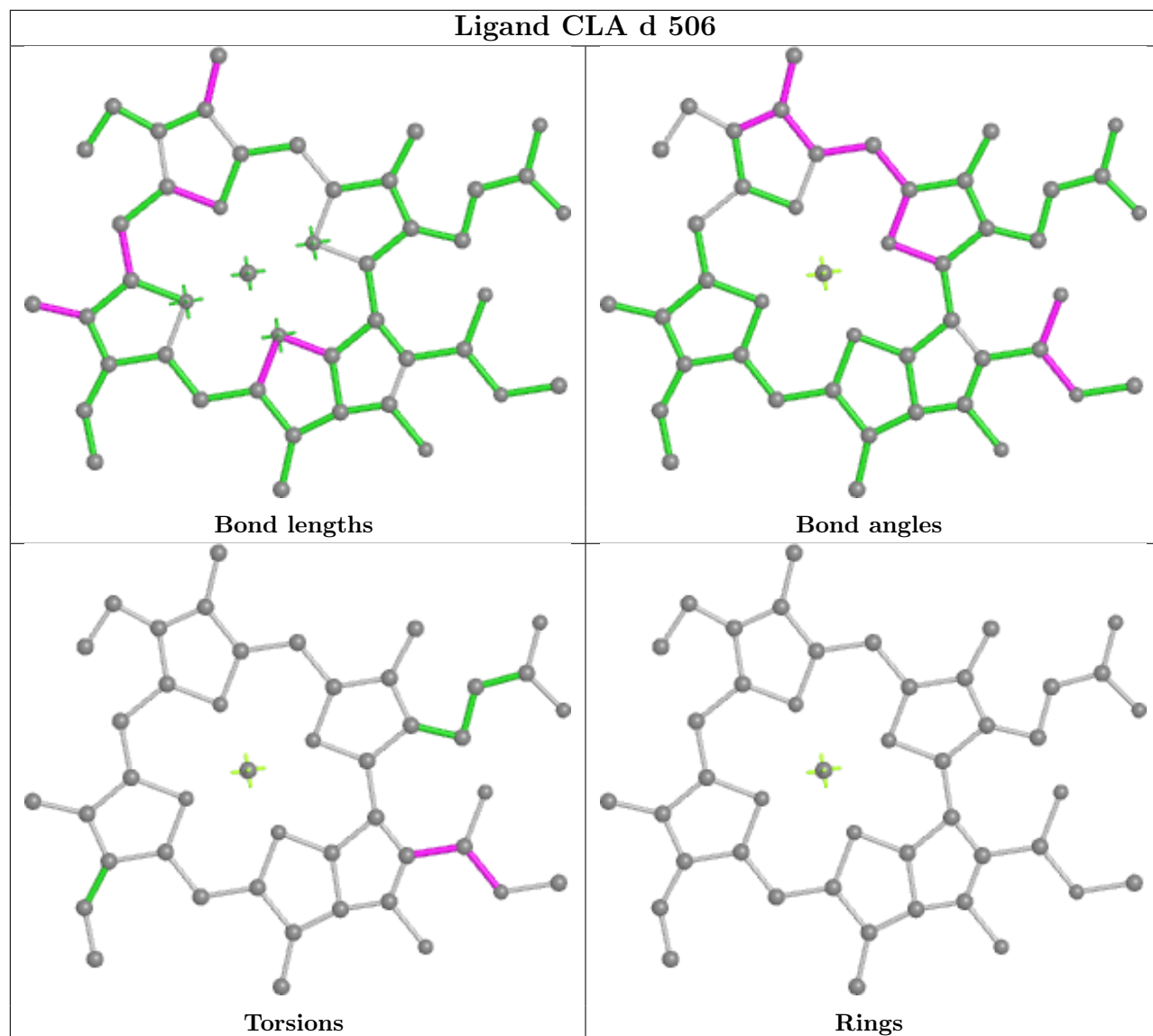


Ligand CLA 1 509

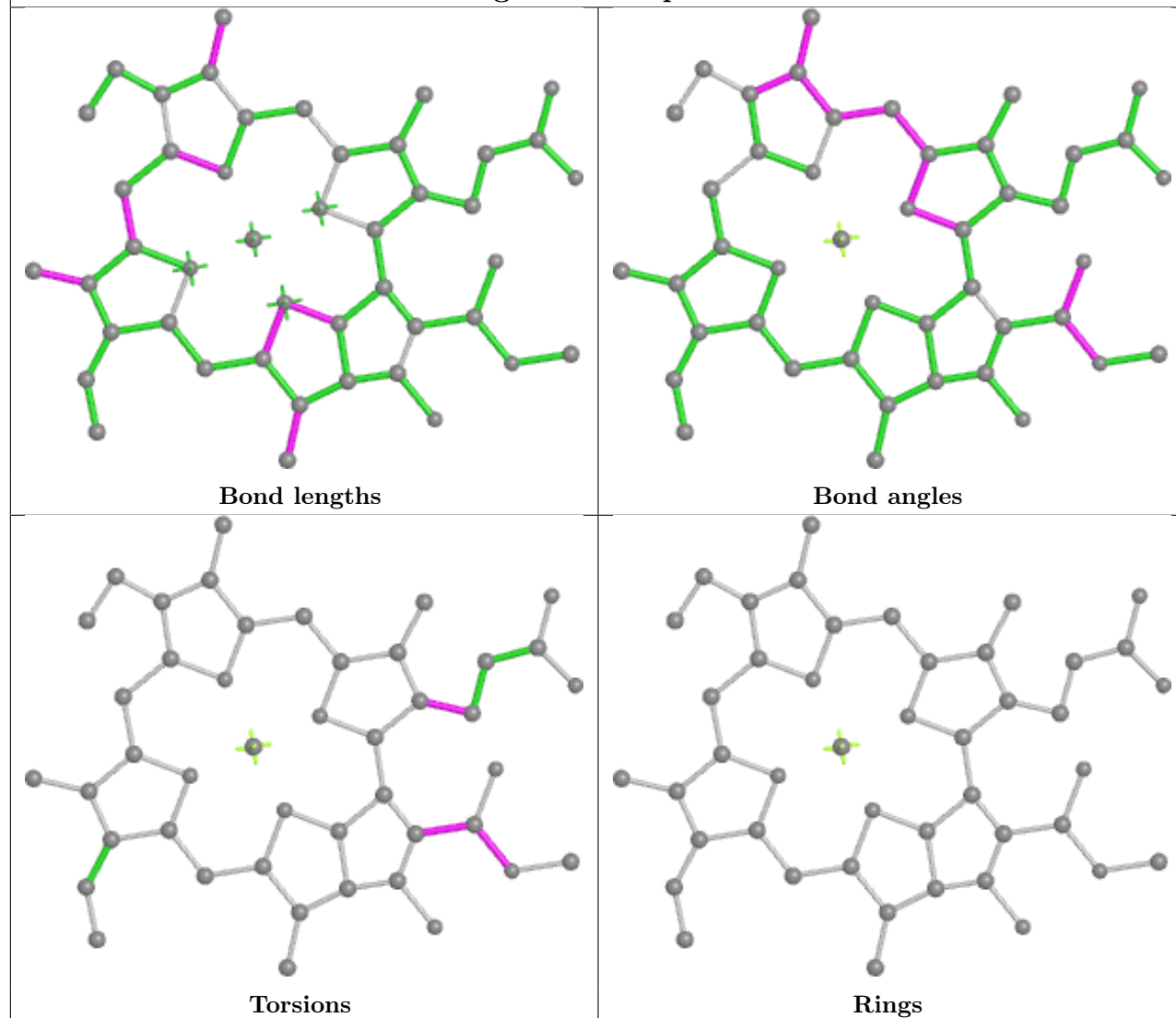


Ligand CLA a 507**Ligand CLA G 1237**

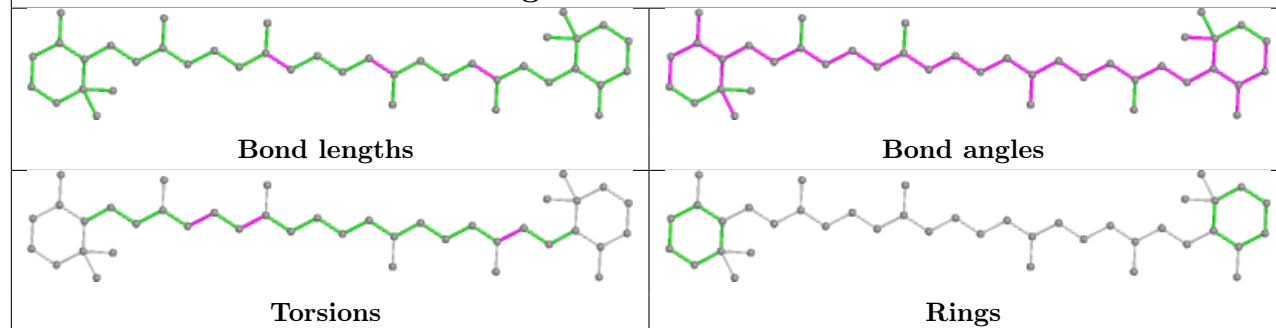
Ligand CLA d 506



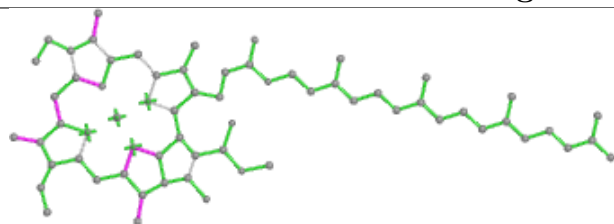
Ligand CLA q 506



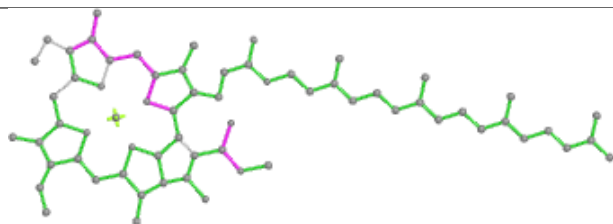
Ligand BCR B 4010



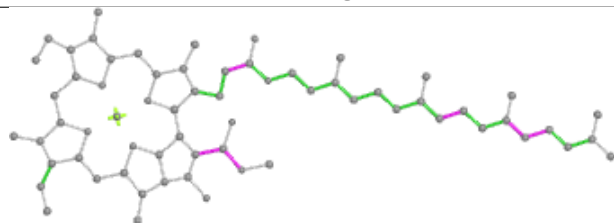
Ligand CLA Z 510



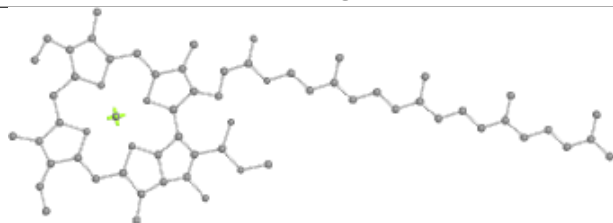
Bond lengths



Bond angles

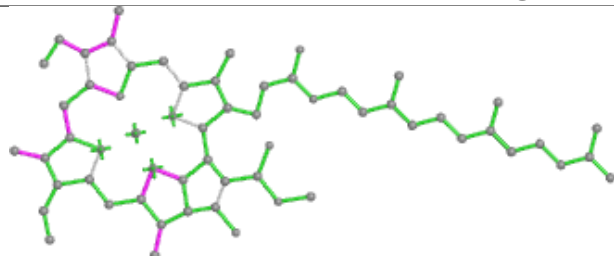


Torsions

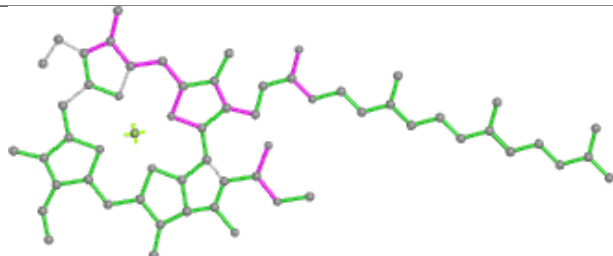


Rings

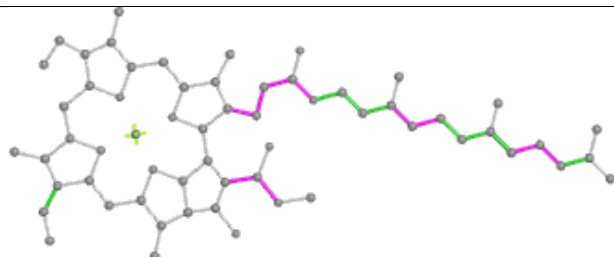
Ligand CLA Y 518



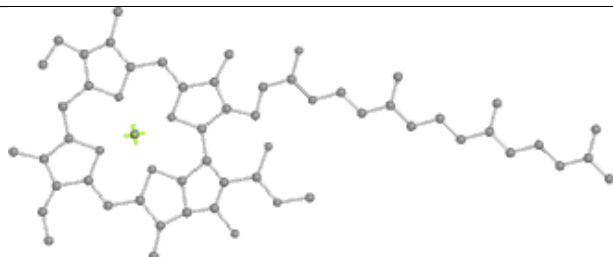
Bond lengths



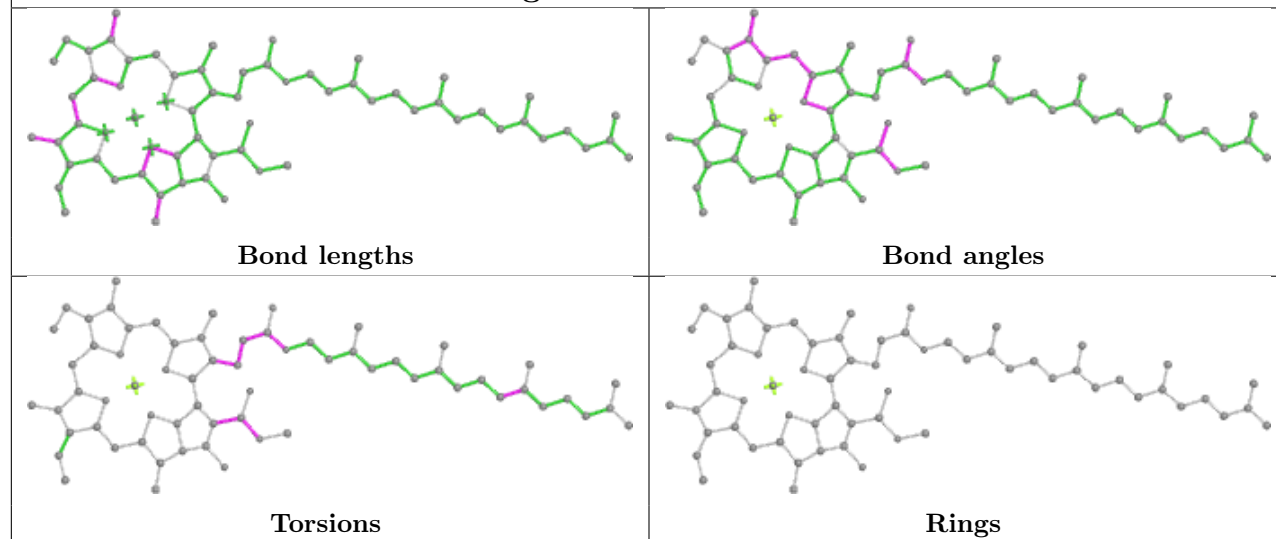
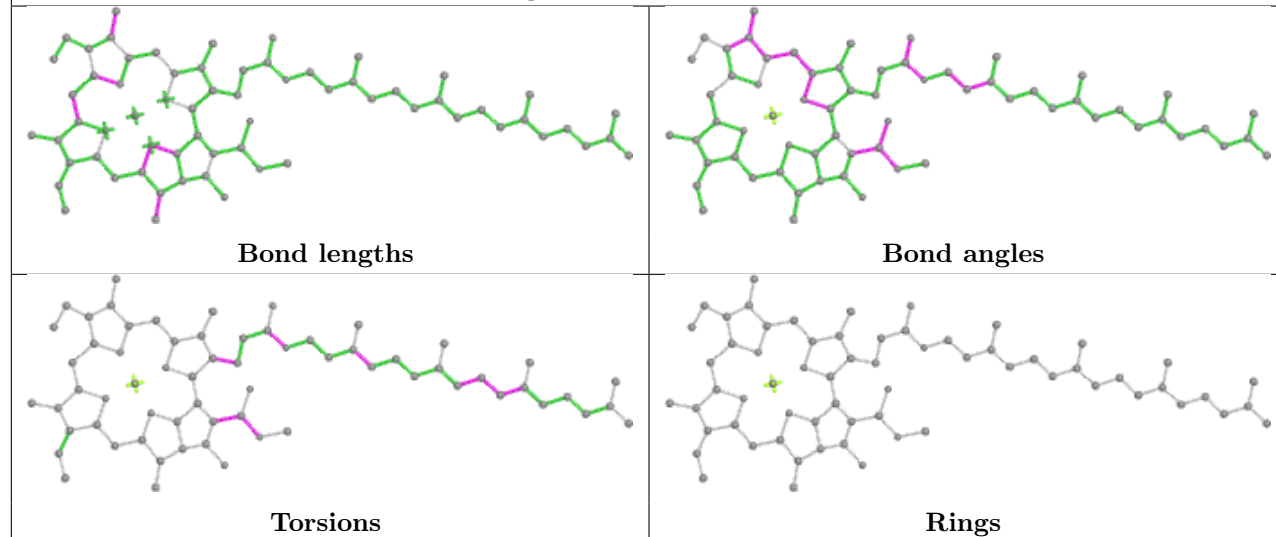
Bond angles



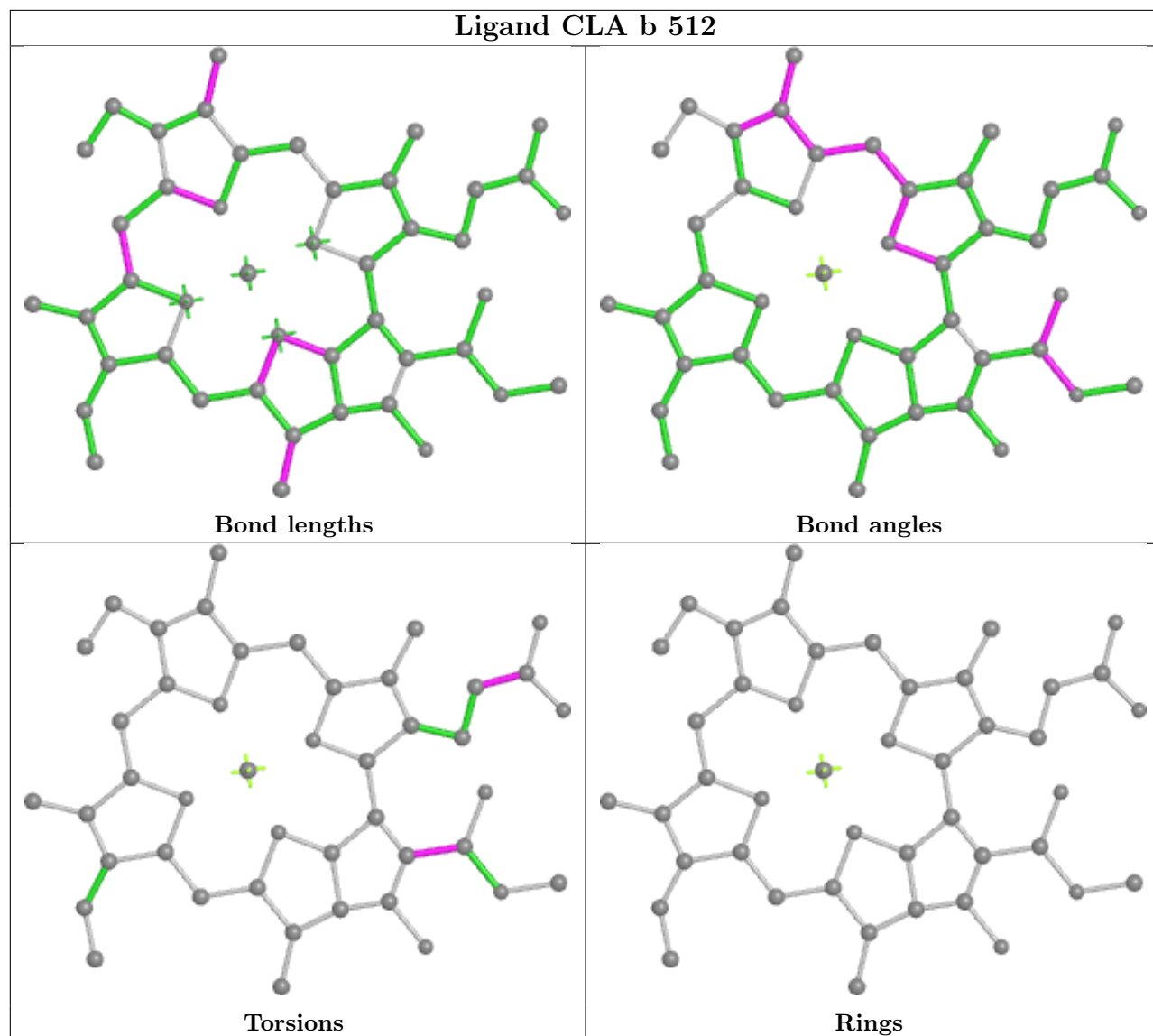
Torsions



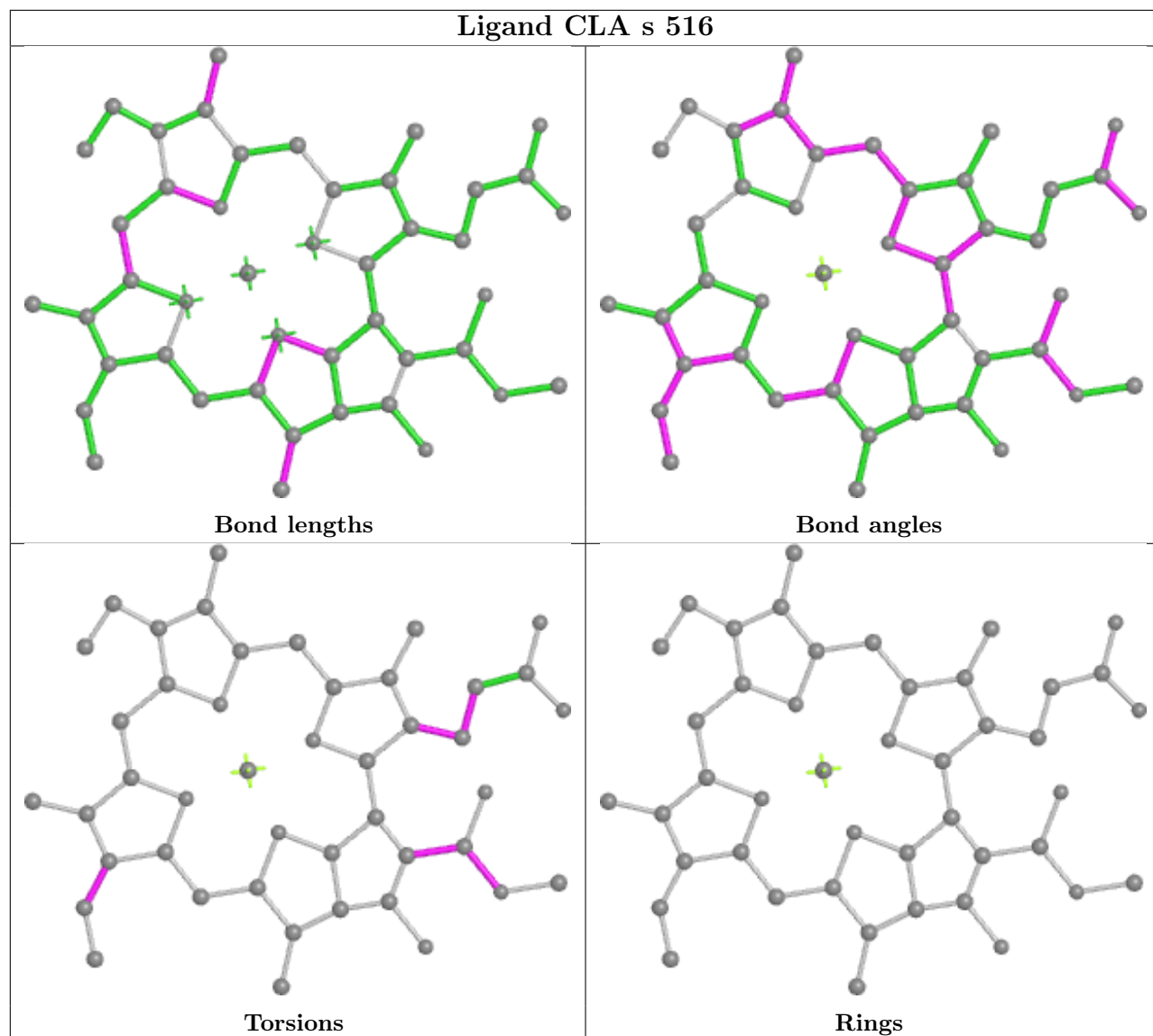
Rings

Ligand CLA A 1111**Ligand CLA H 1240**

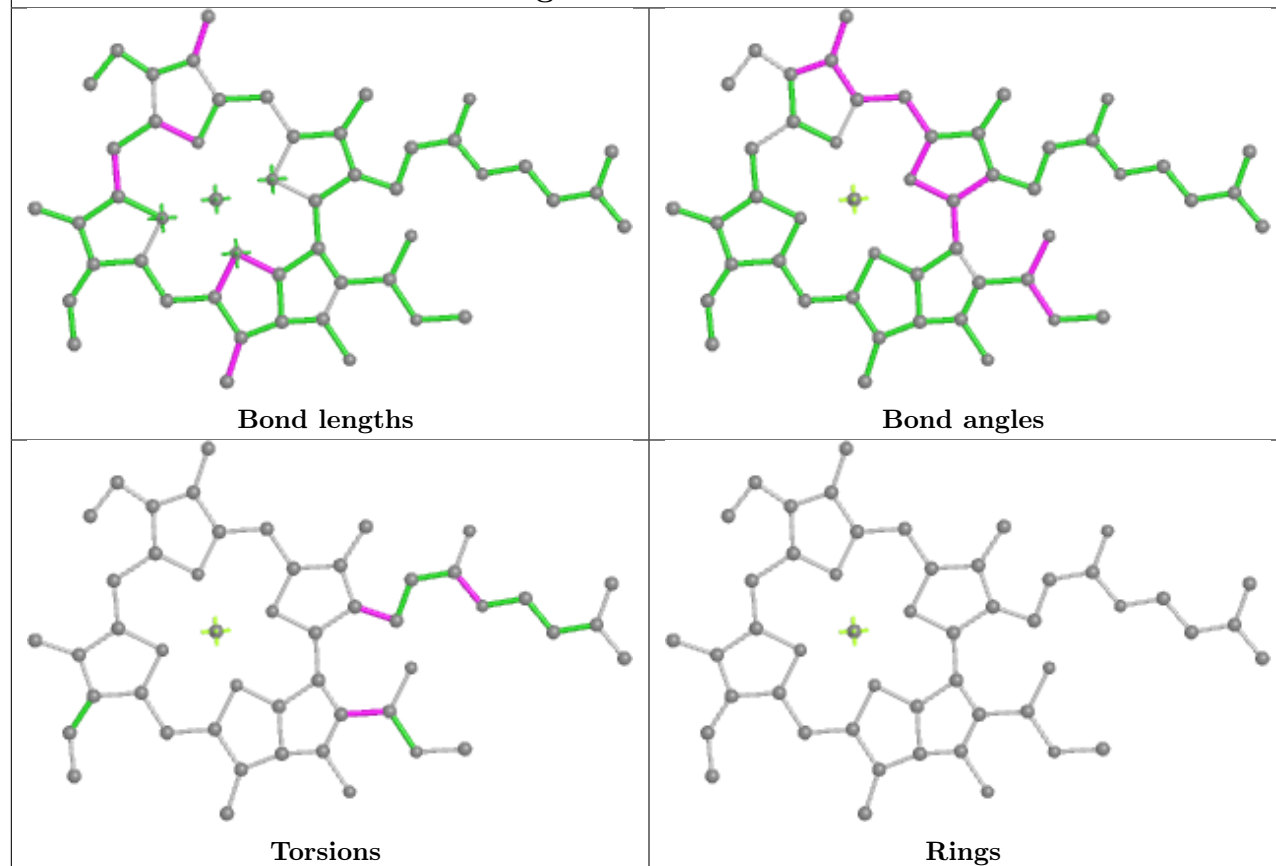
Ligand CLA b 512



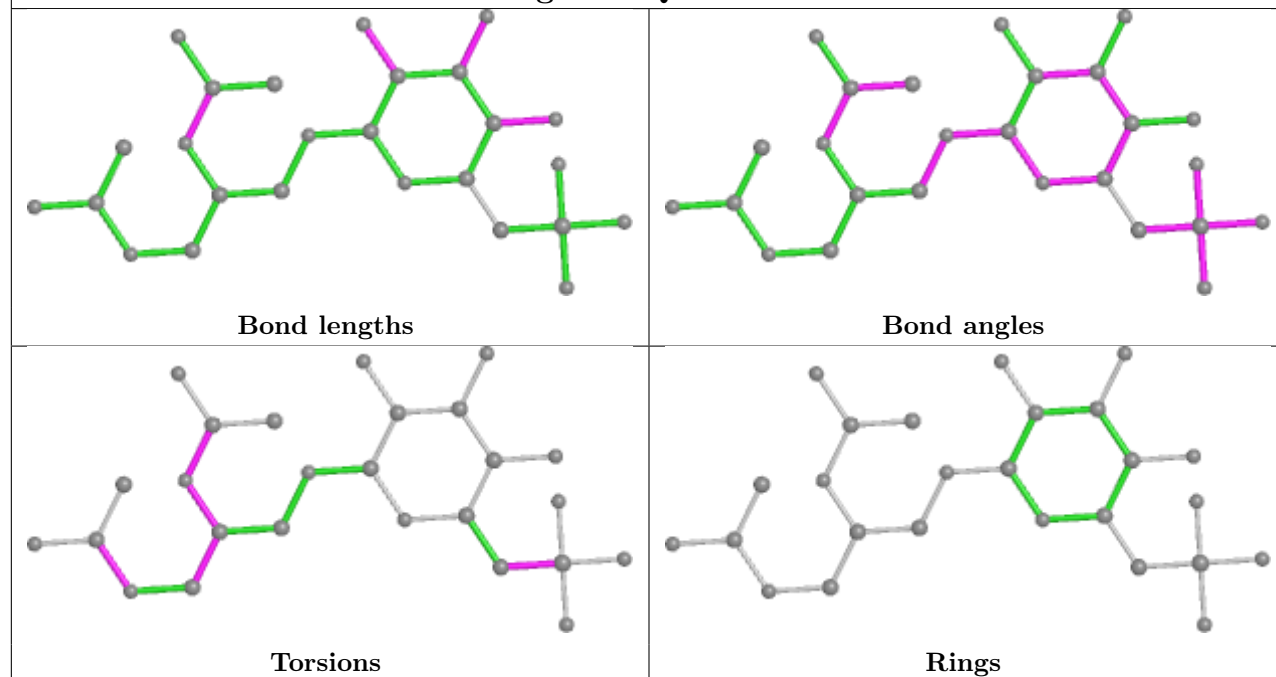
Ligand CLA s 516

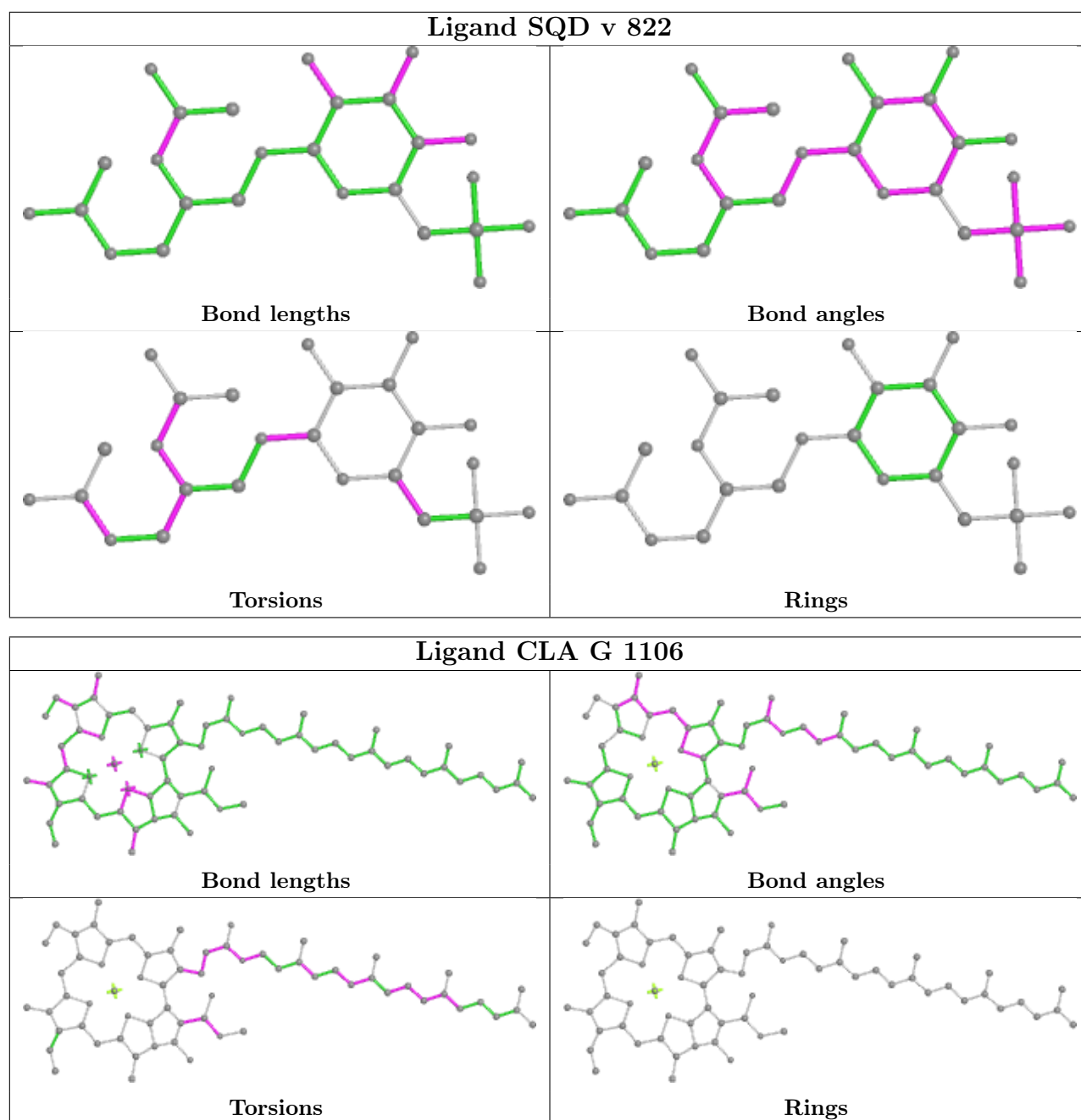


Ligand CLA 4 502

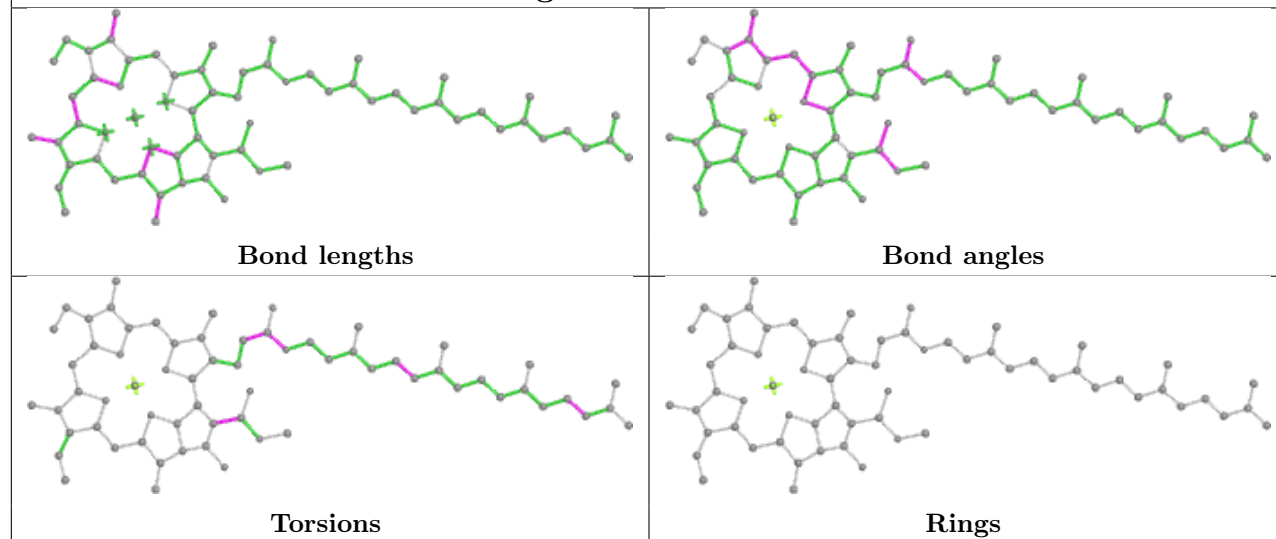


Ligand SQD 4 822

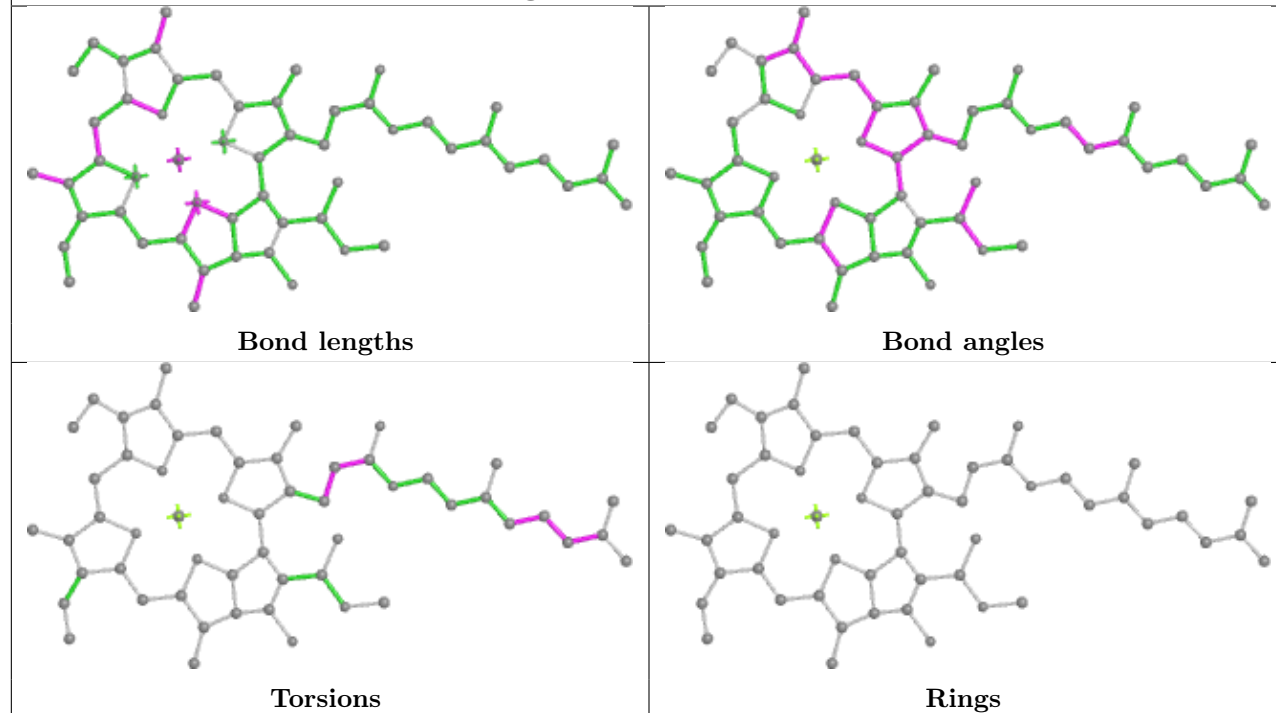




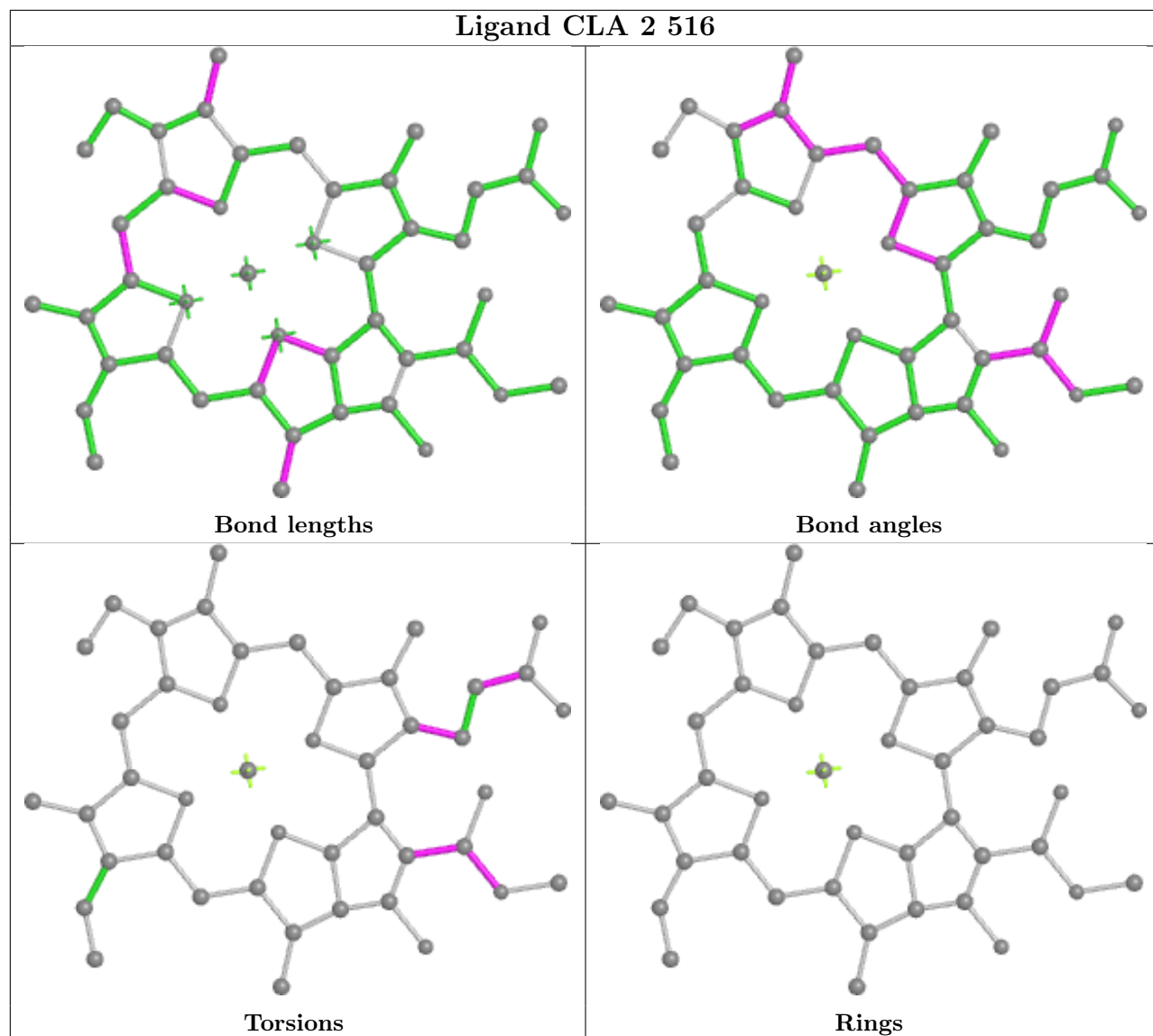
Ligand CLA 2 509



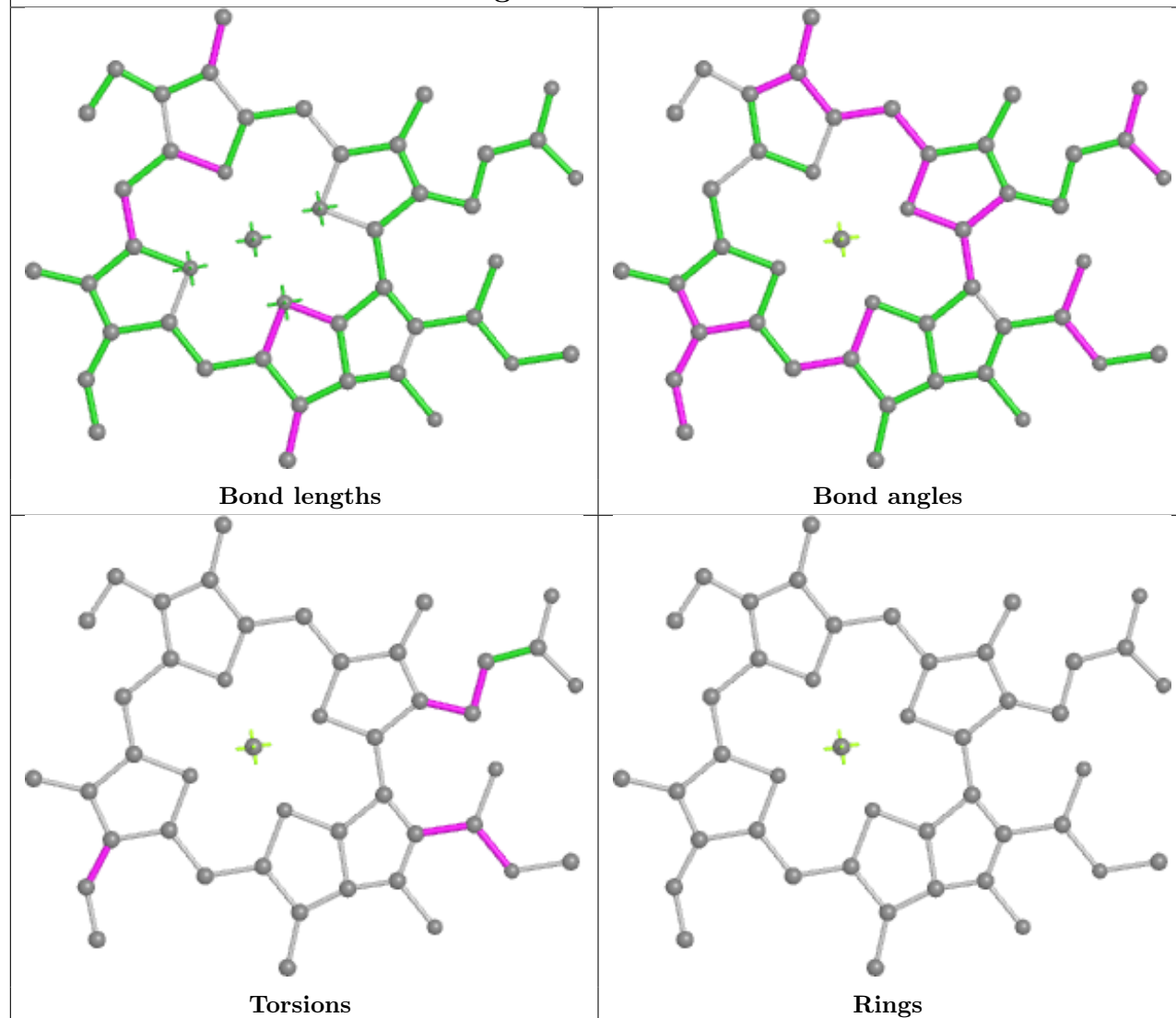
Ligand CLA G 1121



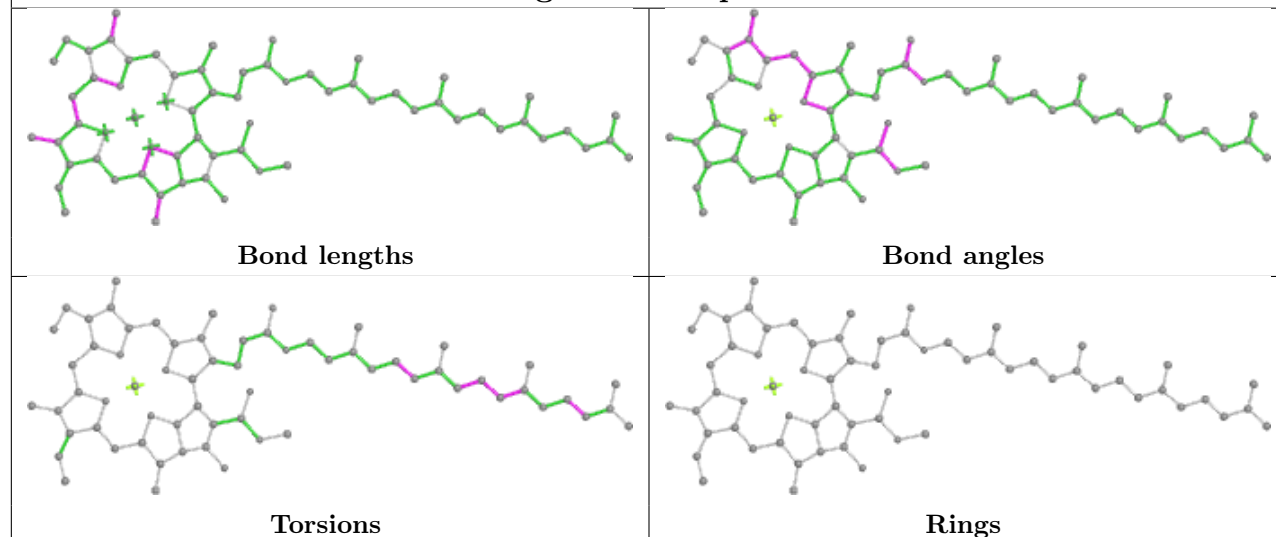
Ligand CLA 2 516



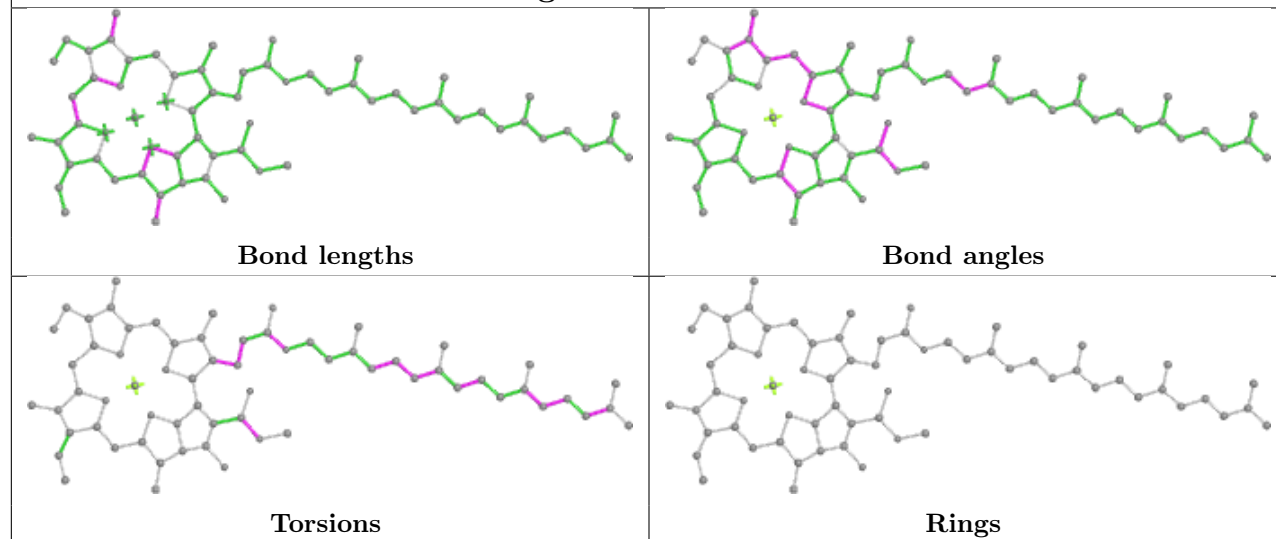
Ligand CLA 3 516



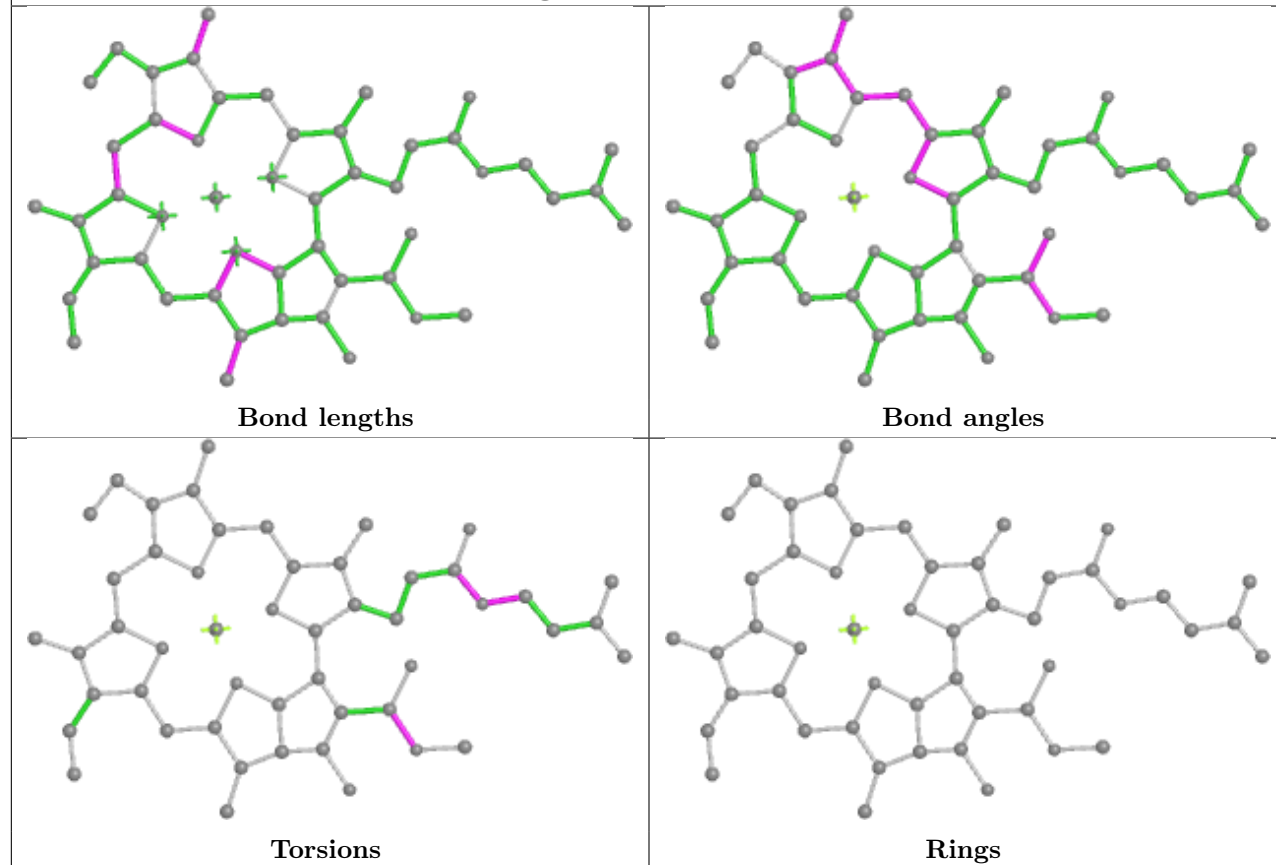
Ligand CLA q 509

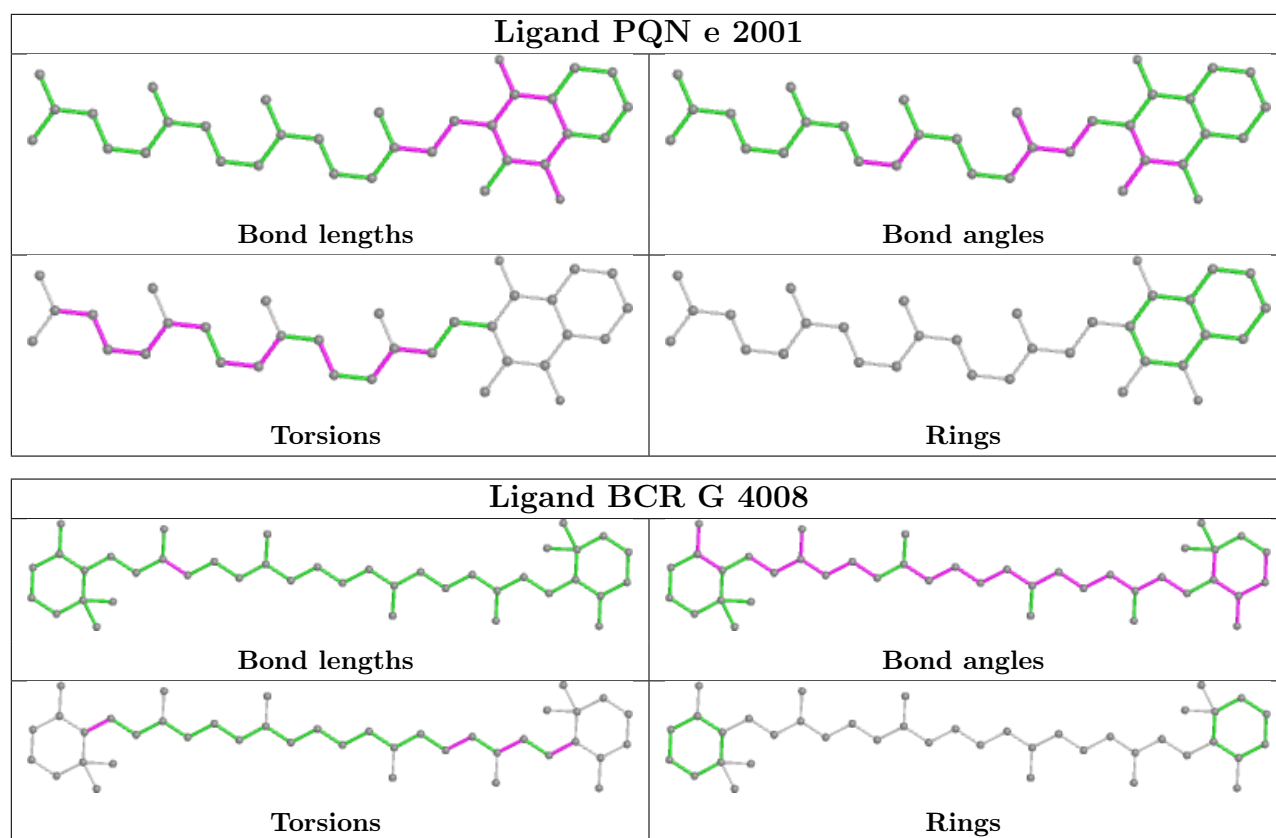


Ligand CLA r 505

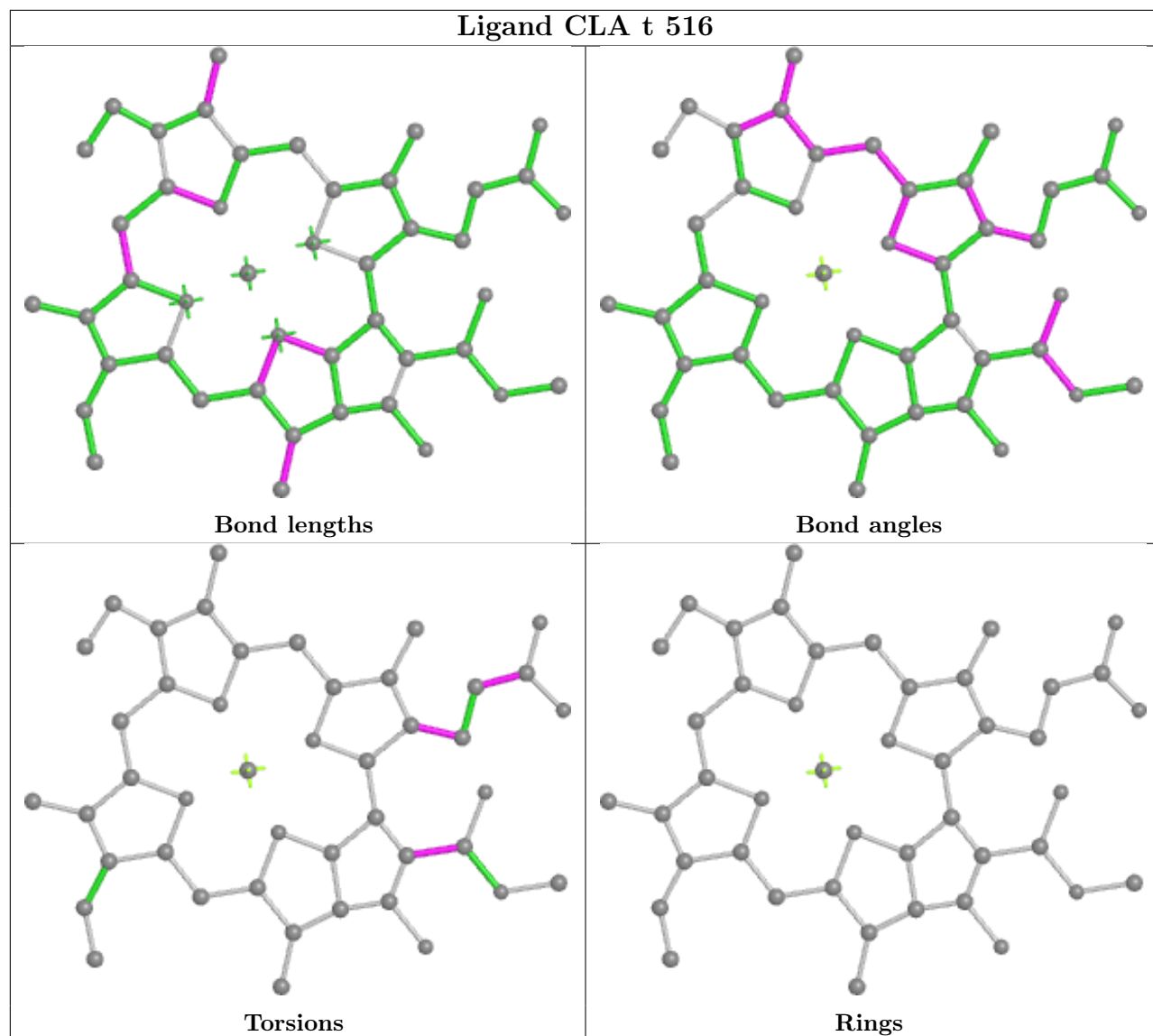


Ligand CLA a 511

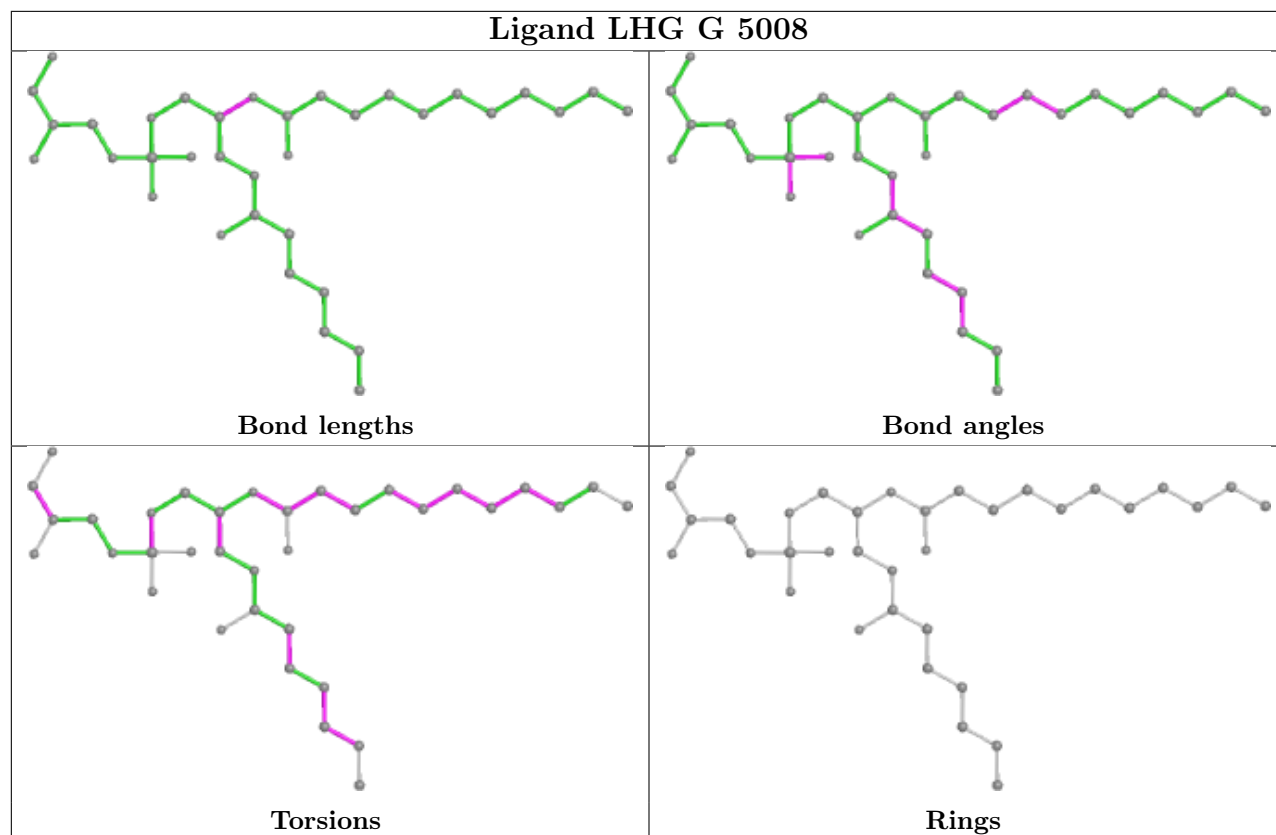




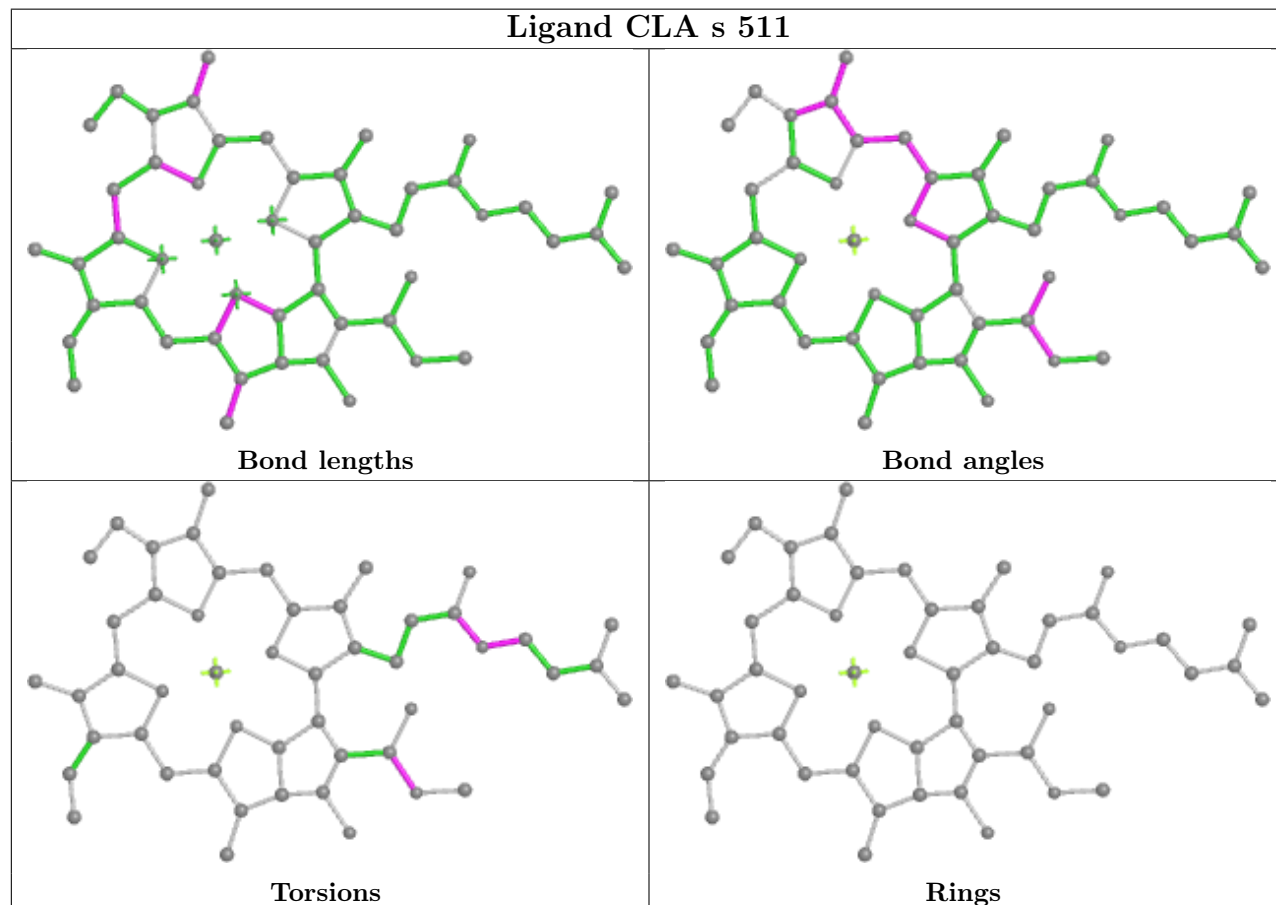
Ligand CLA t 516



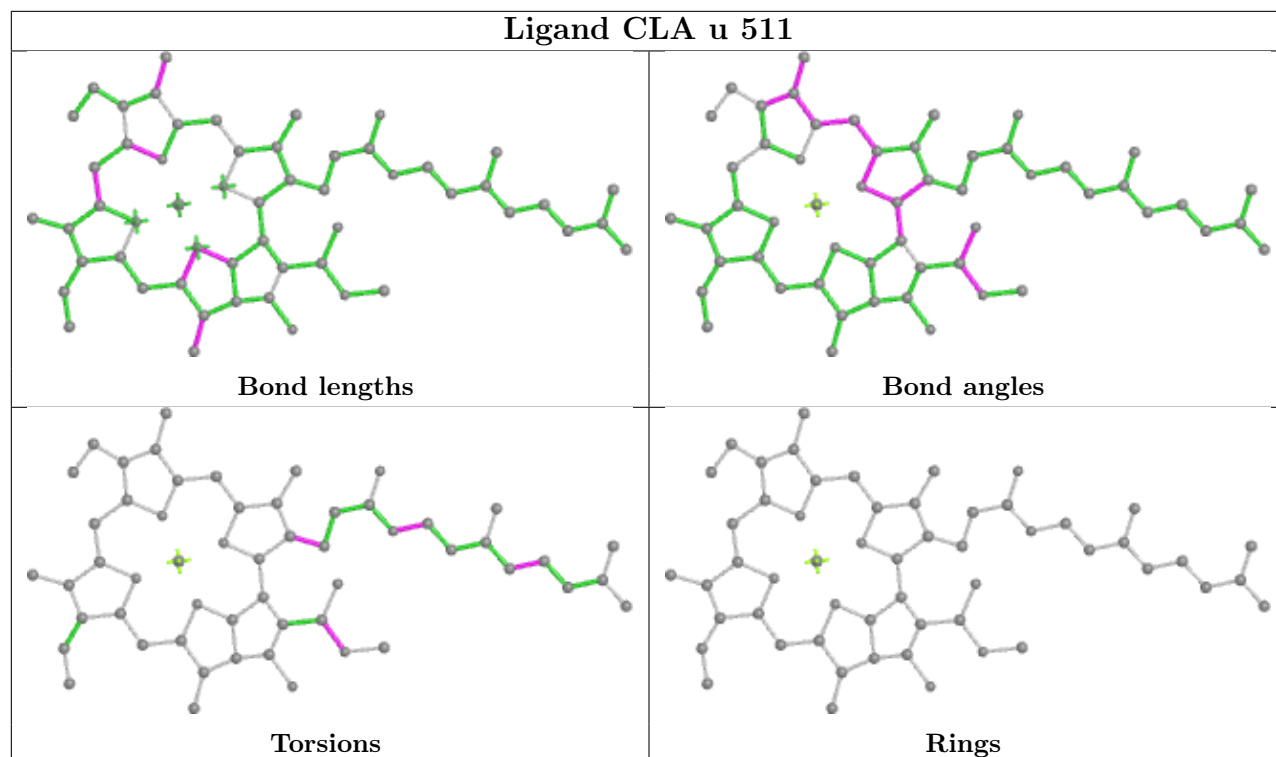
Ligand LHG G 5008



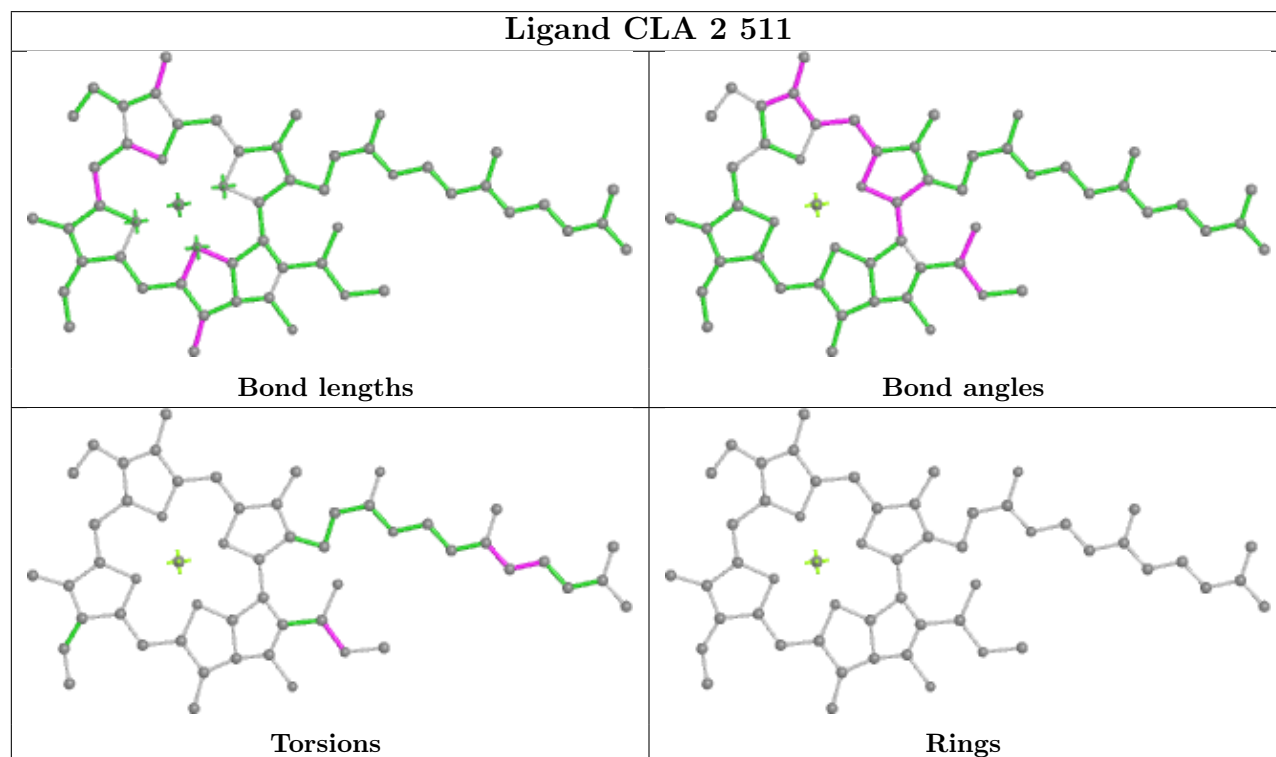
Ligand CLA s 511

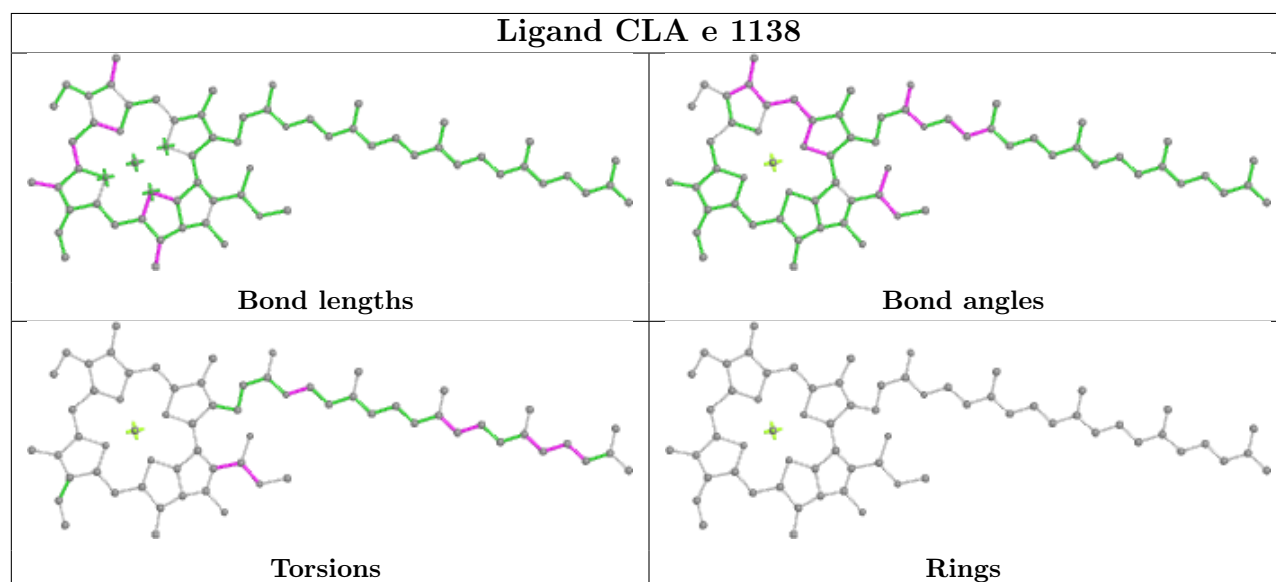
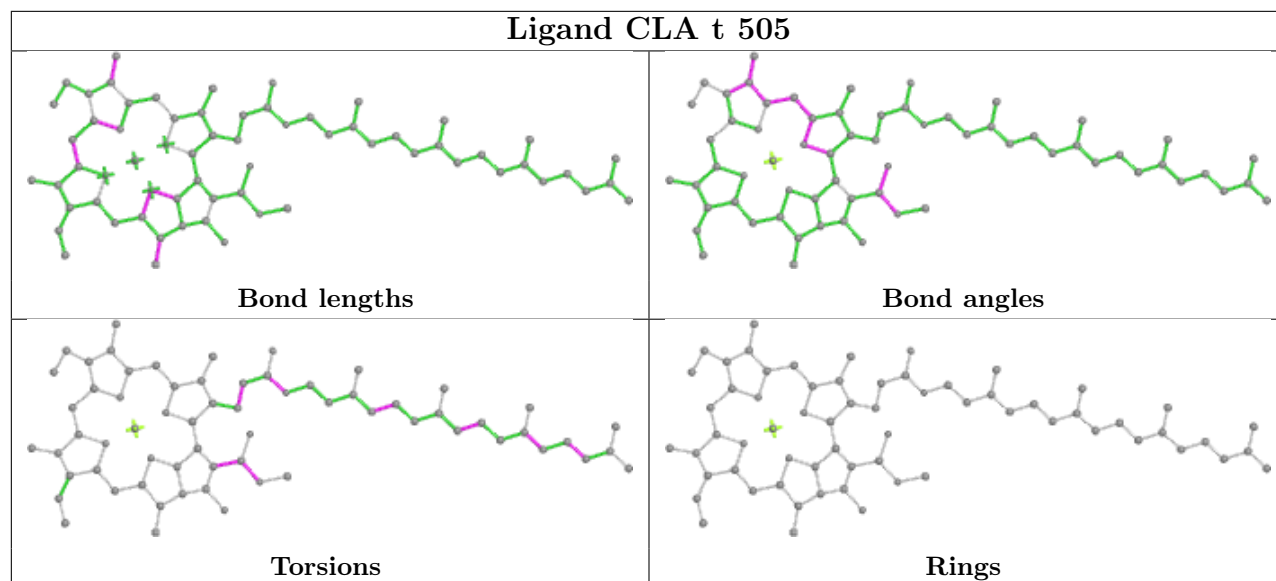
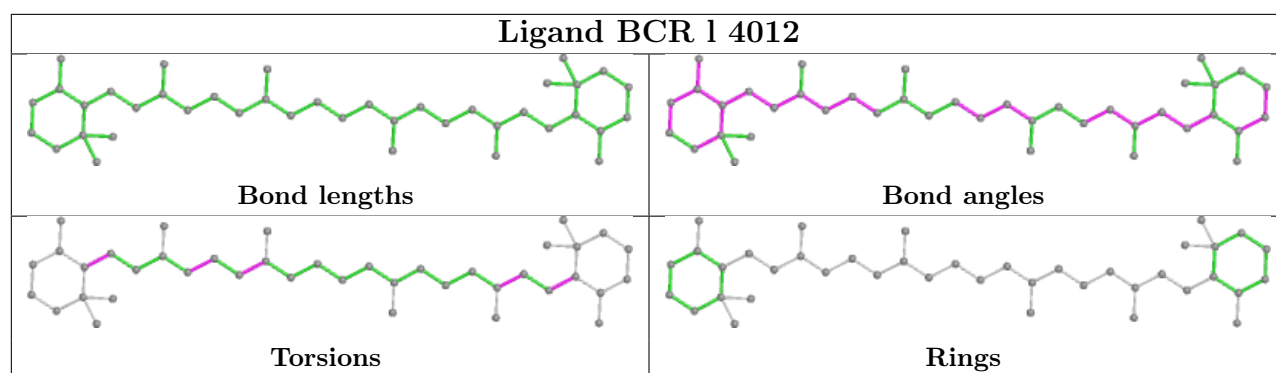


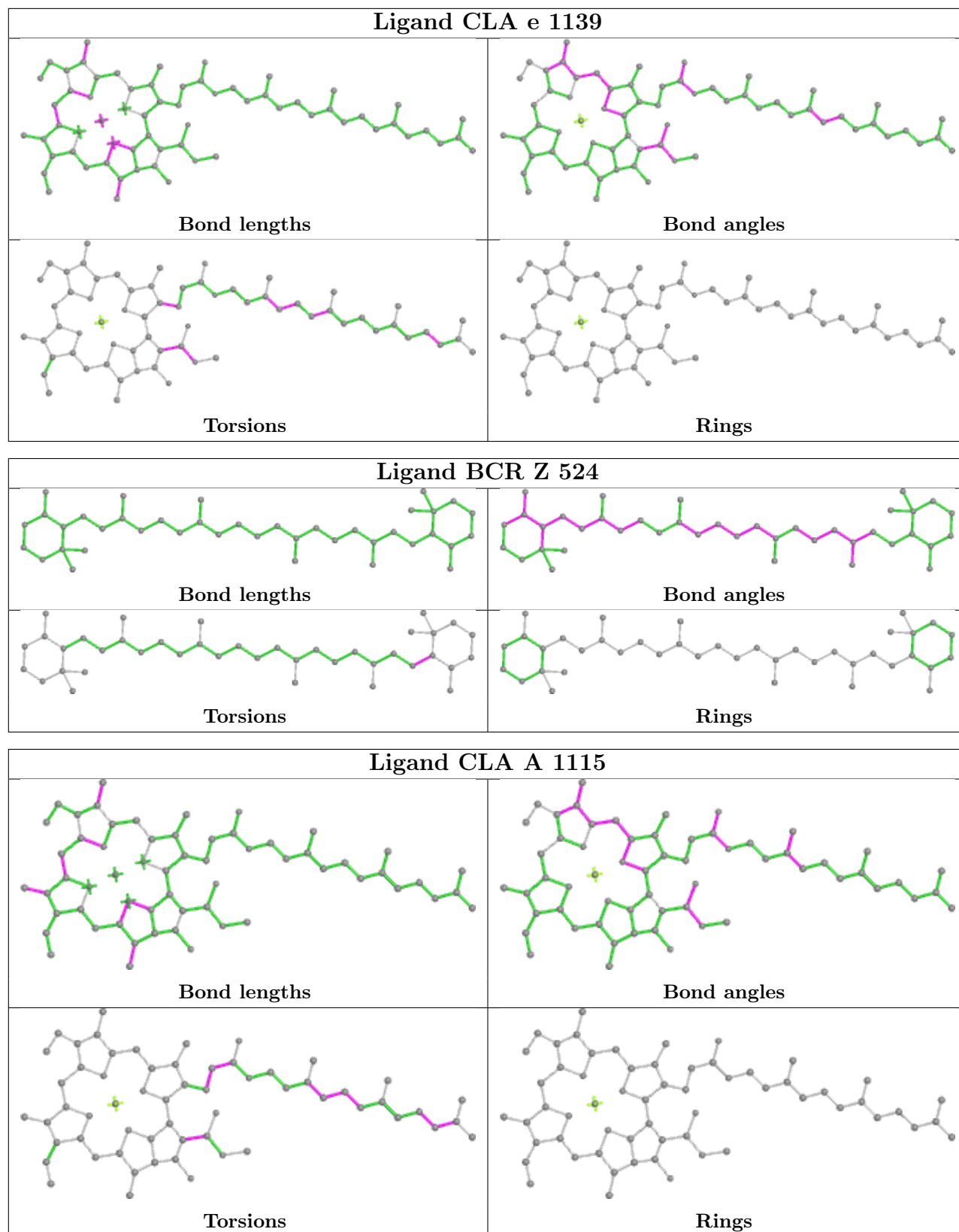
Ligand CLA u 511

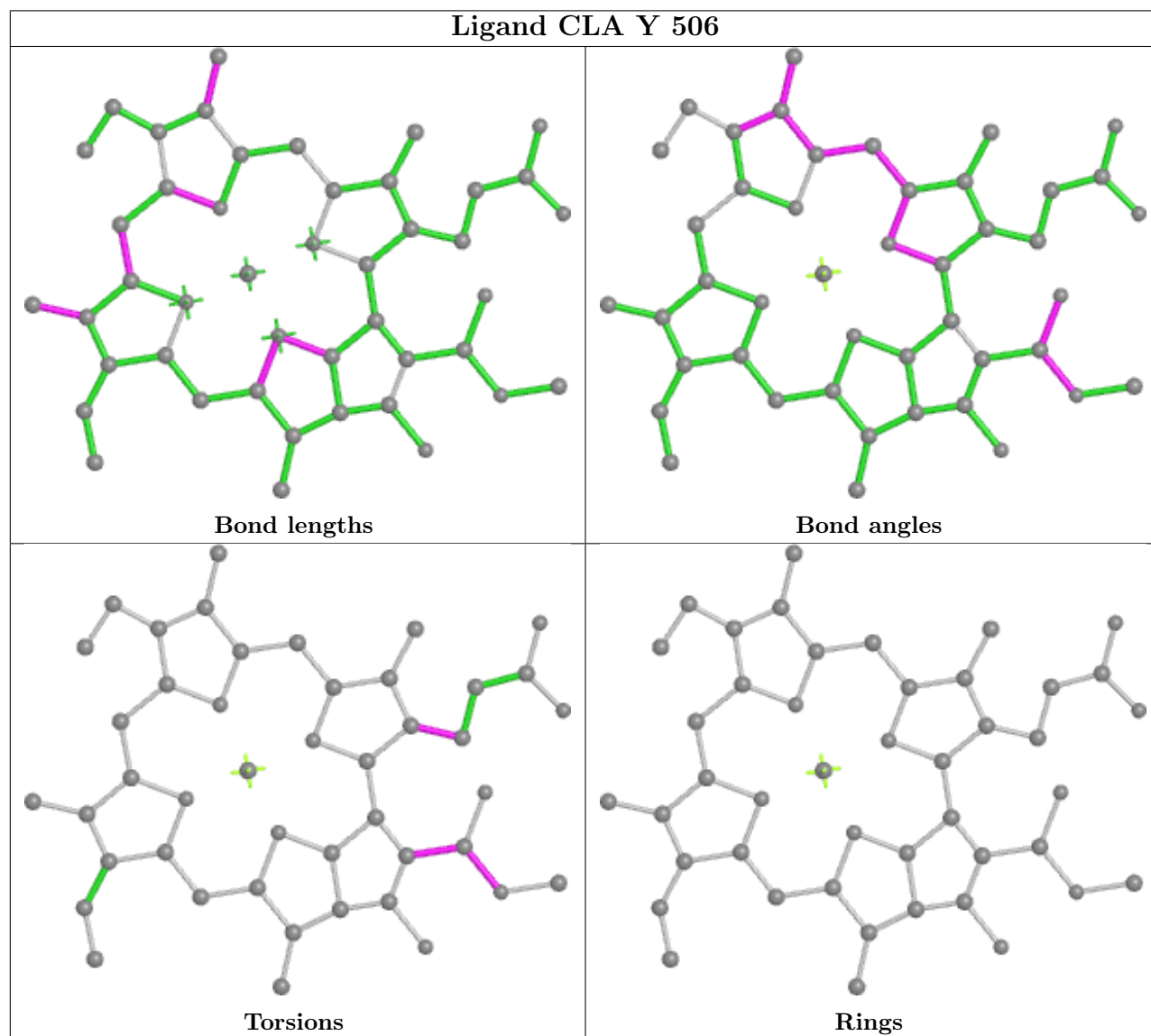
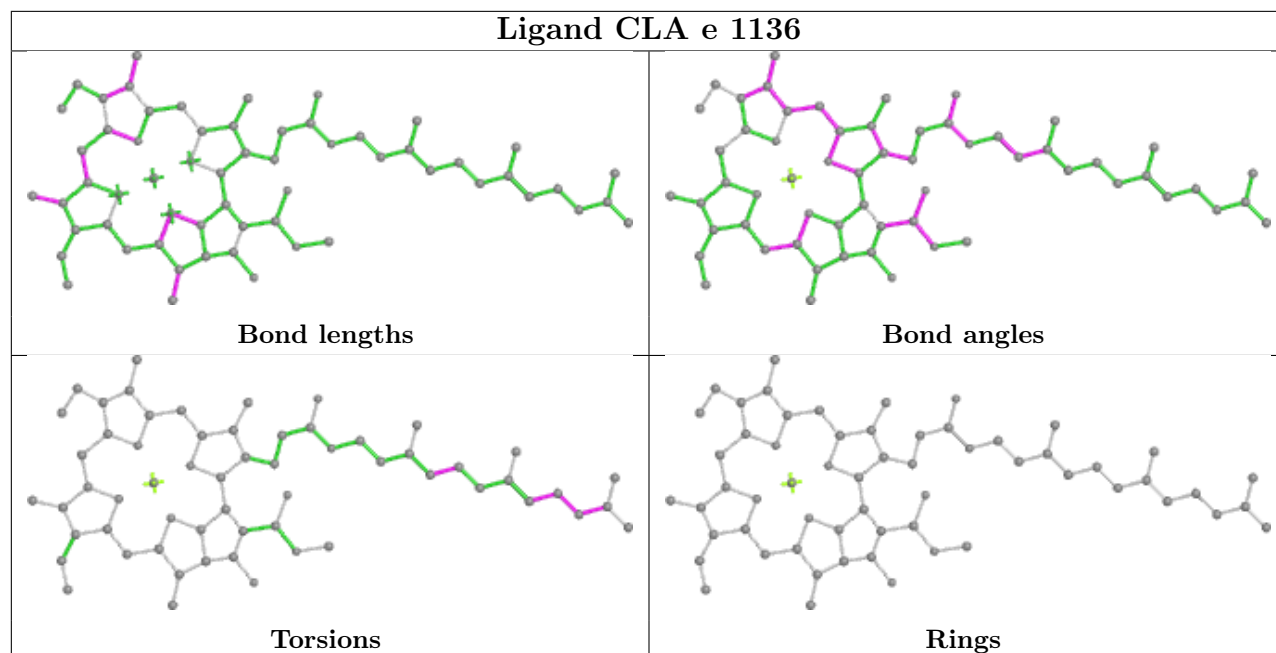


Ligand CLA 2 511

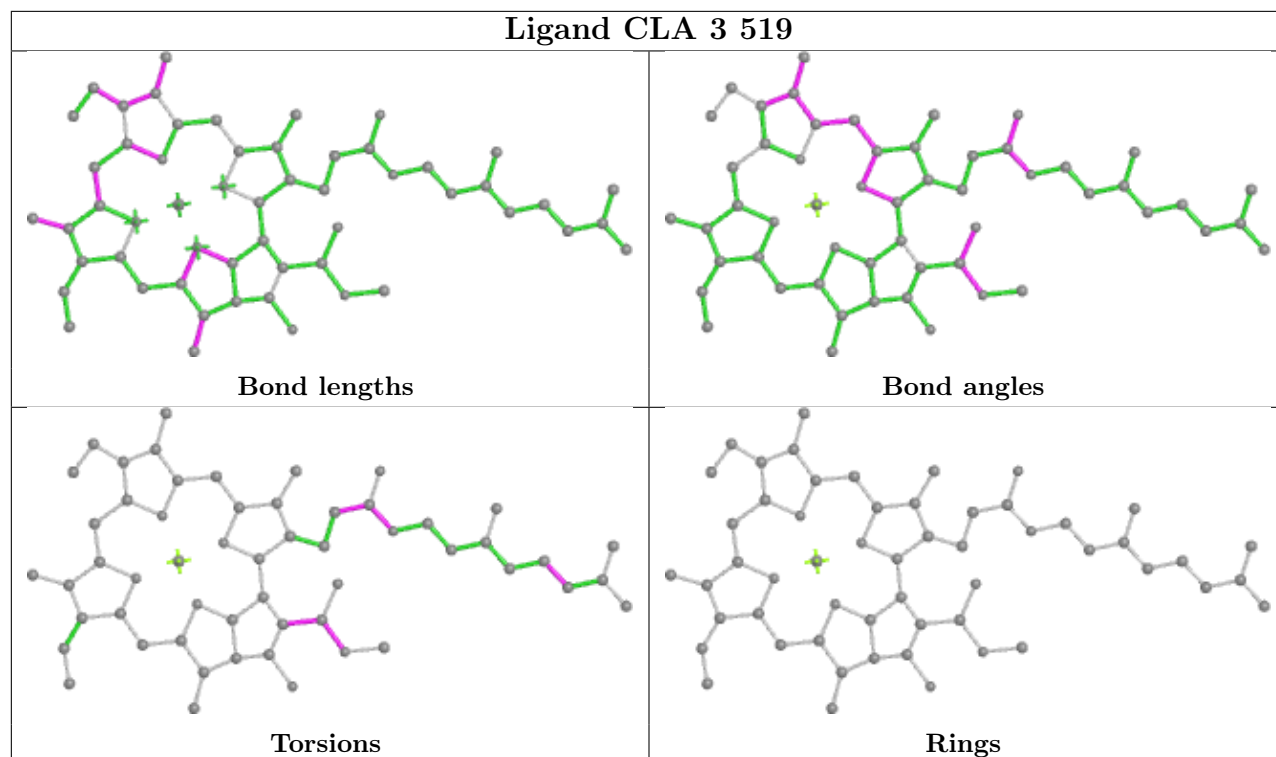




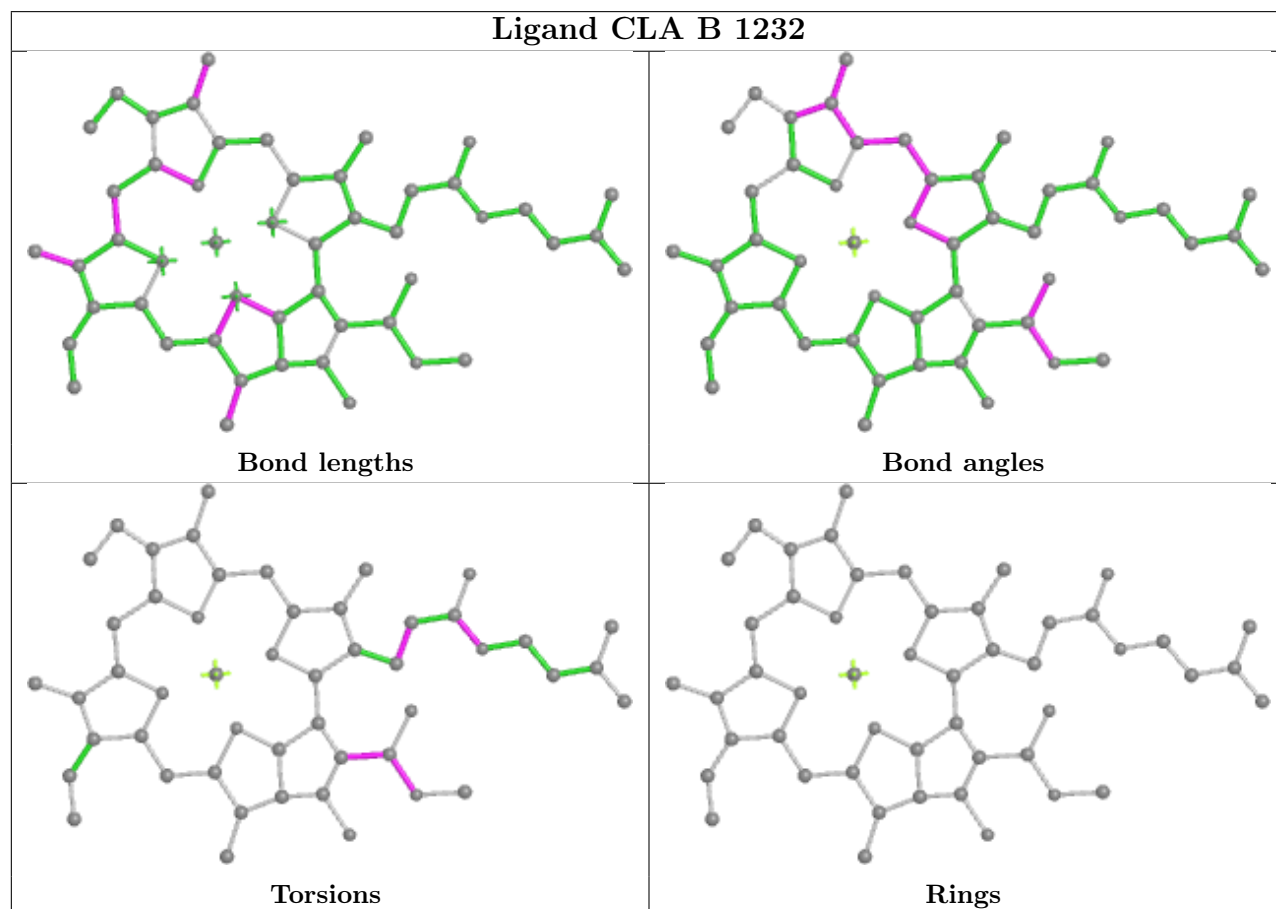




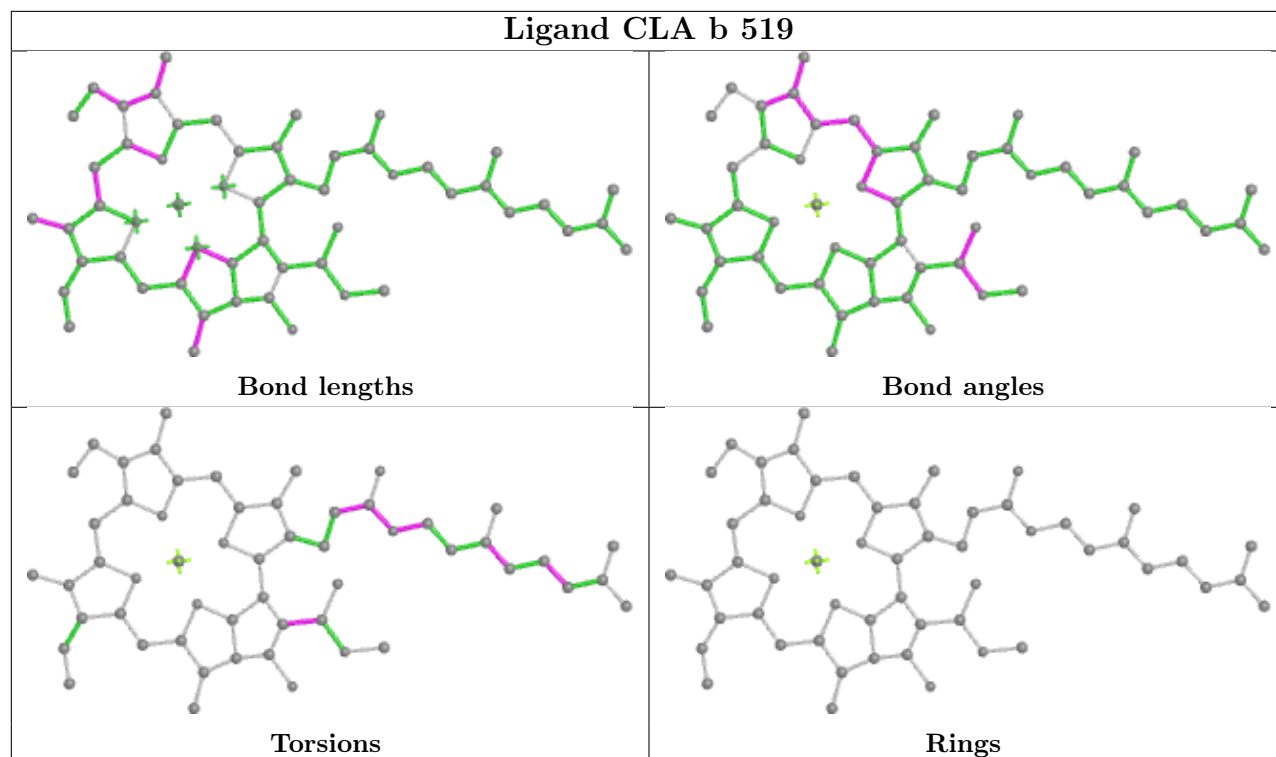
Ligand CLA 3 519



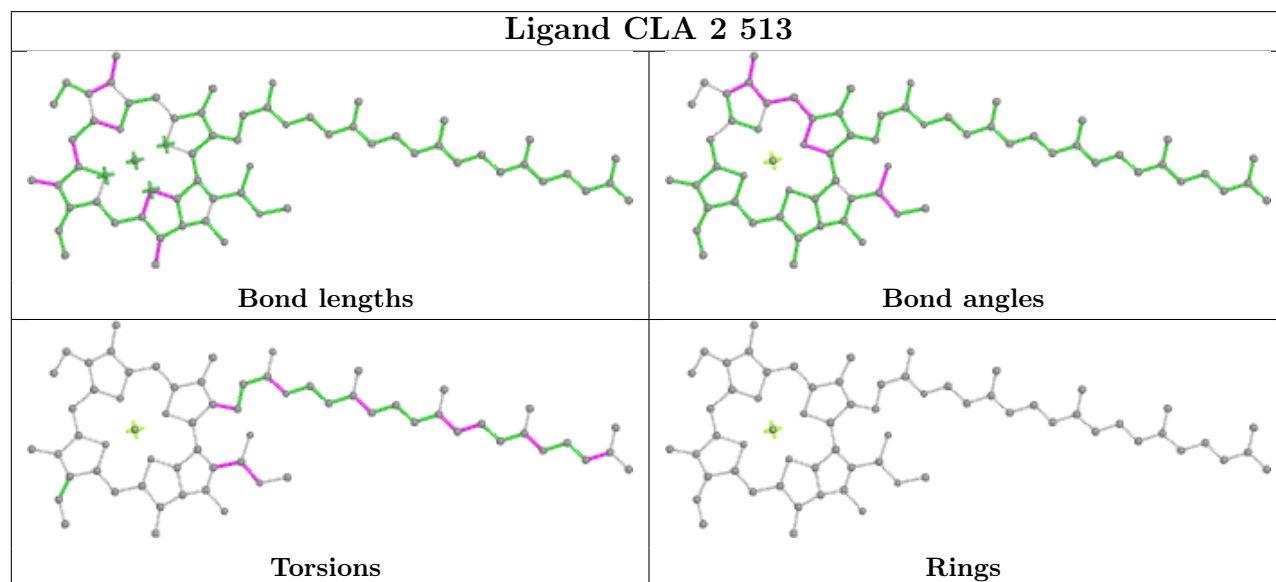
Ligand CLA B 1232



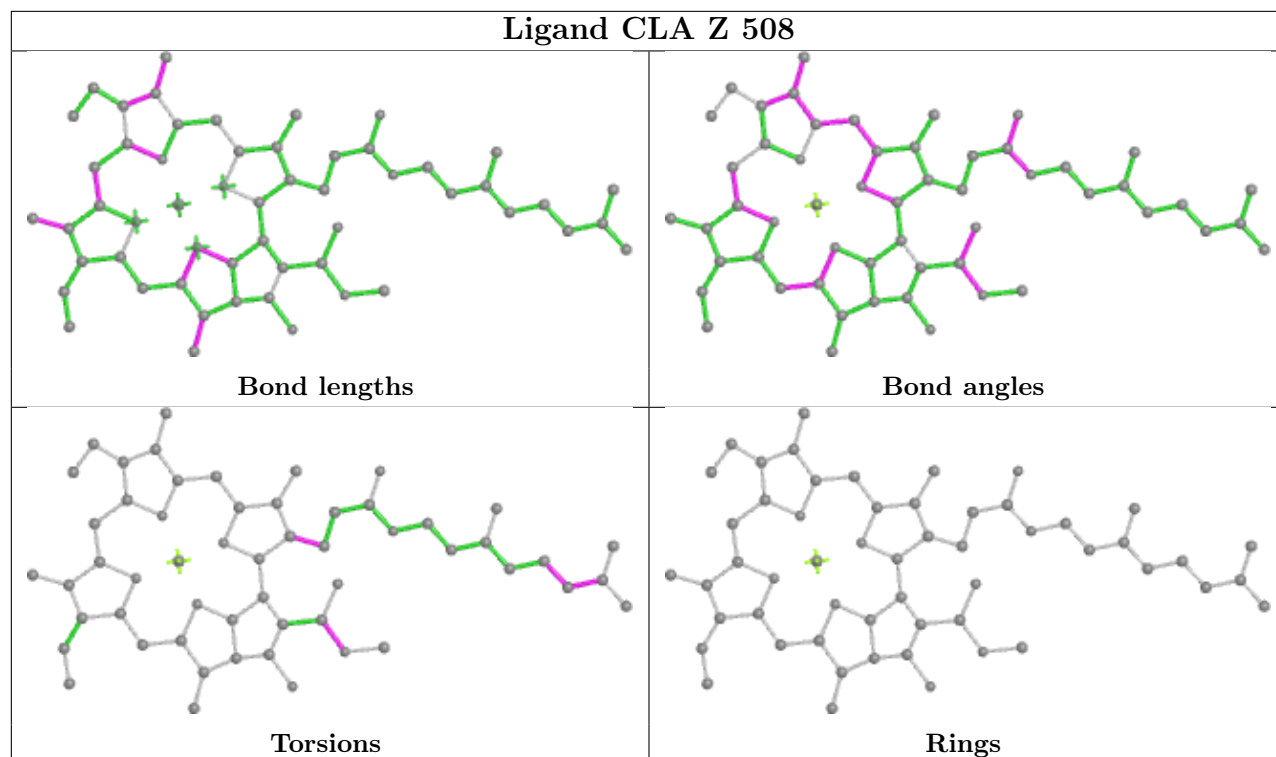
Ligand CLA b 519



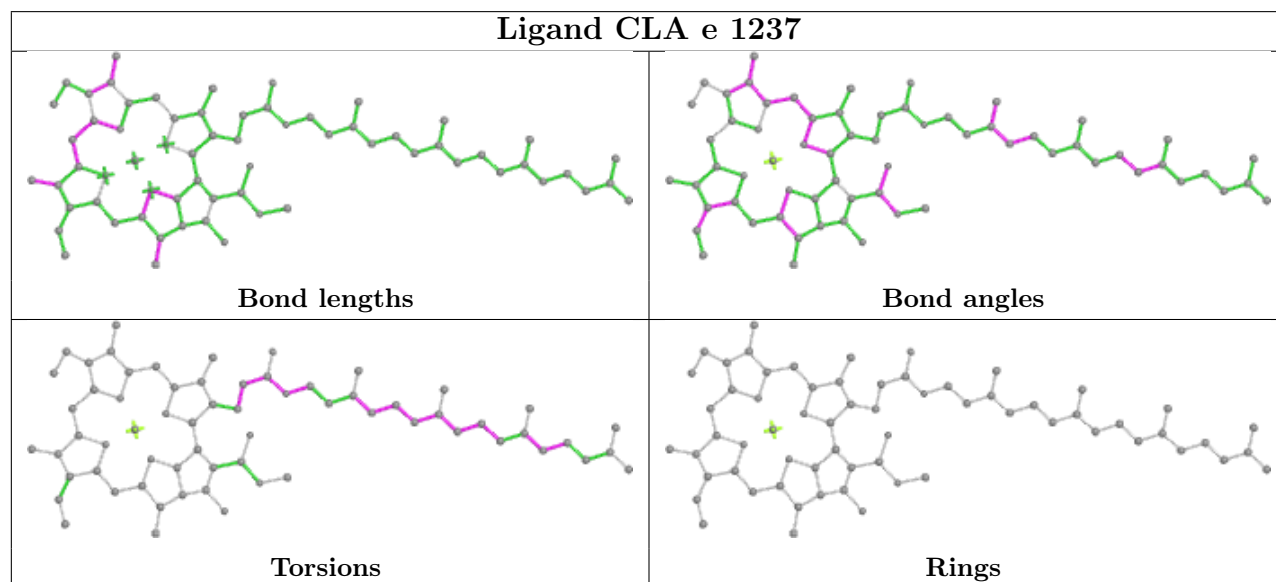
Ligand CLA 2 513



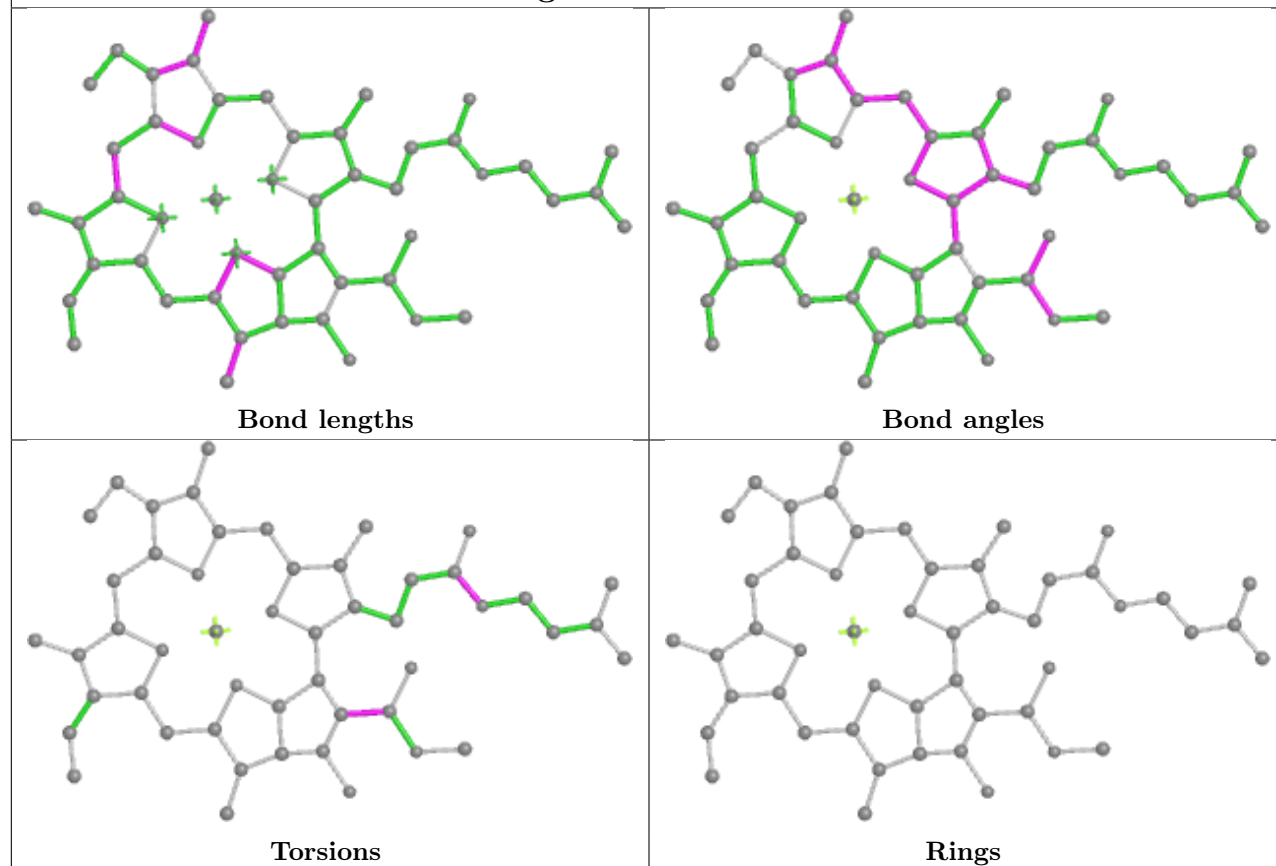
Ligand CLA Z 508



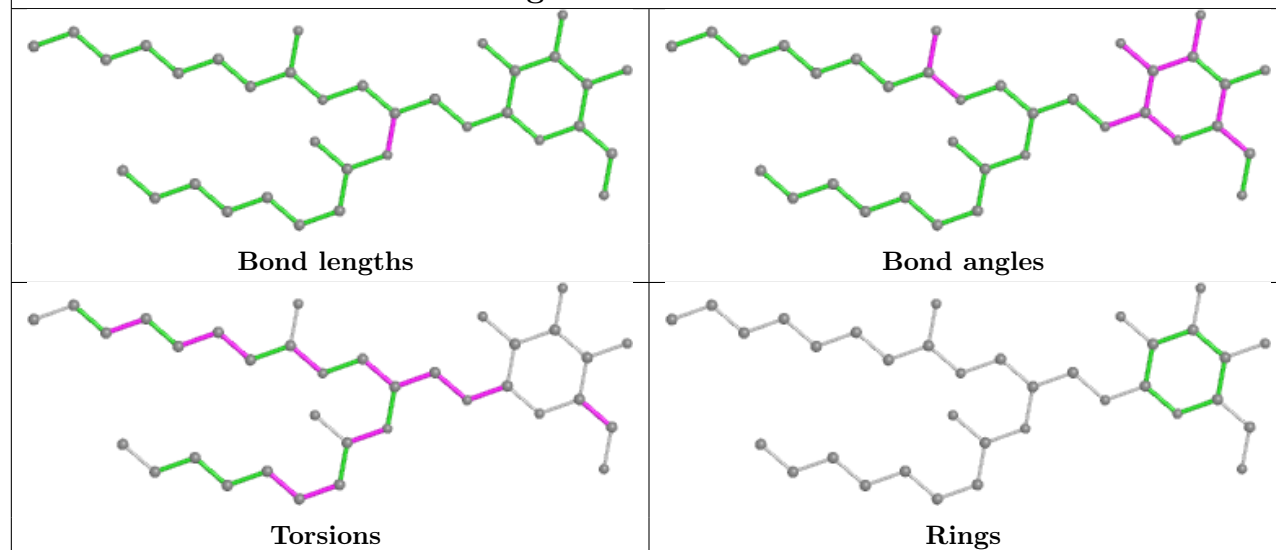
Ligand CLA e 1237

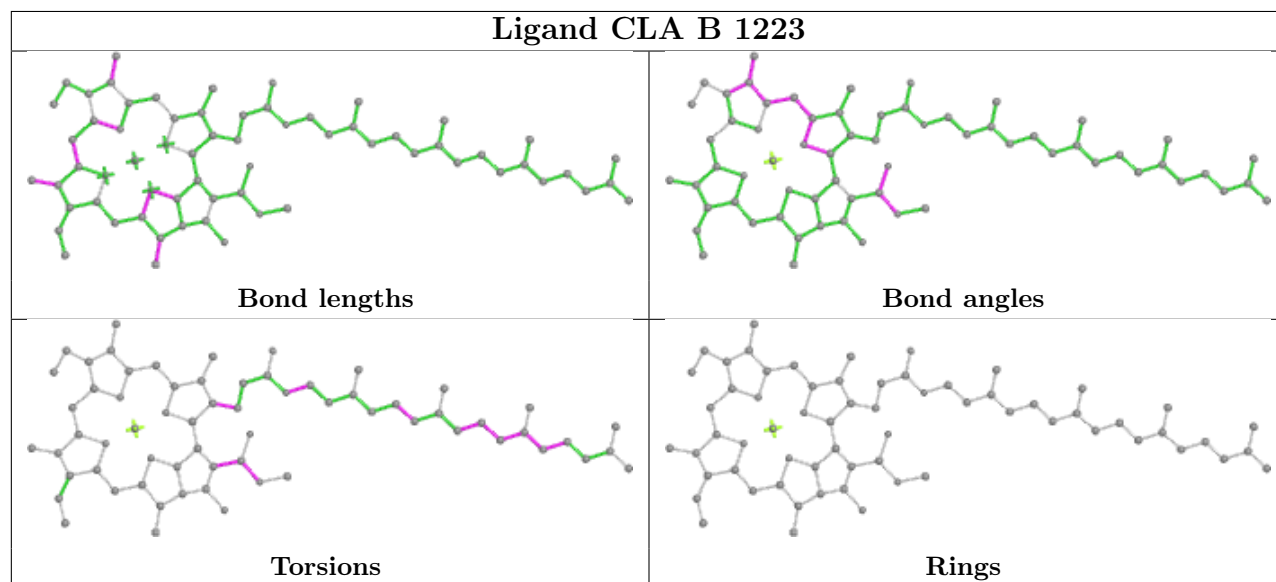
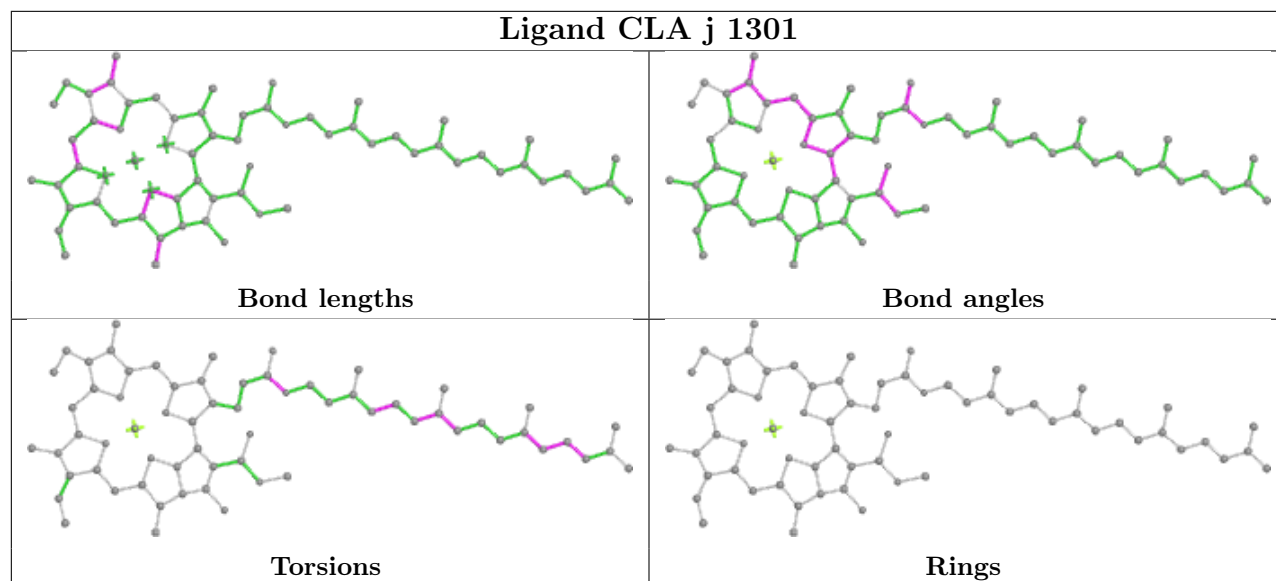
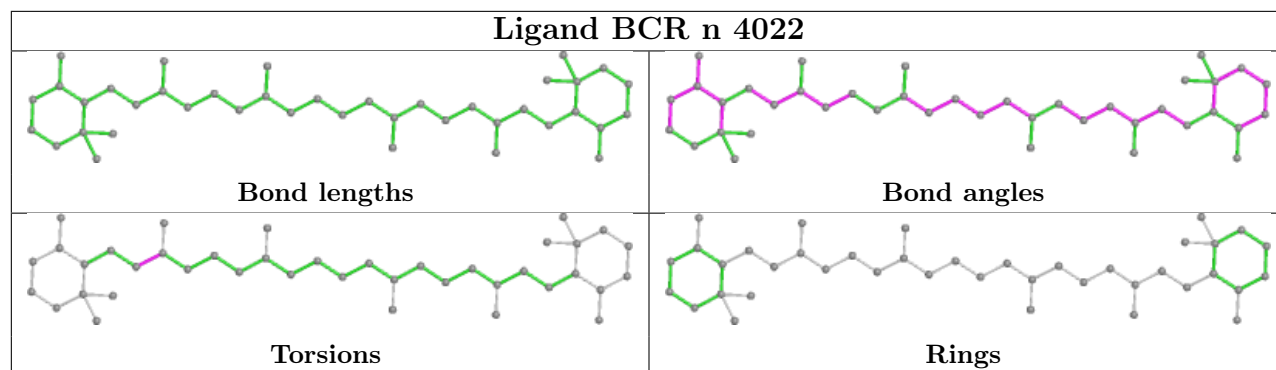


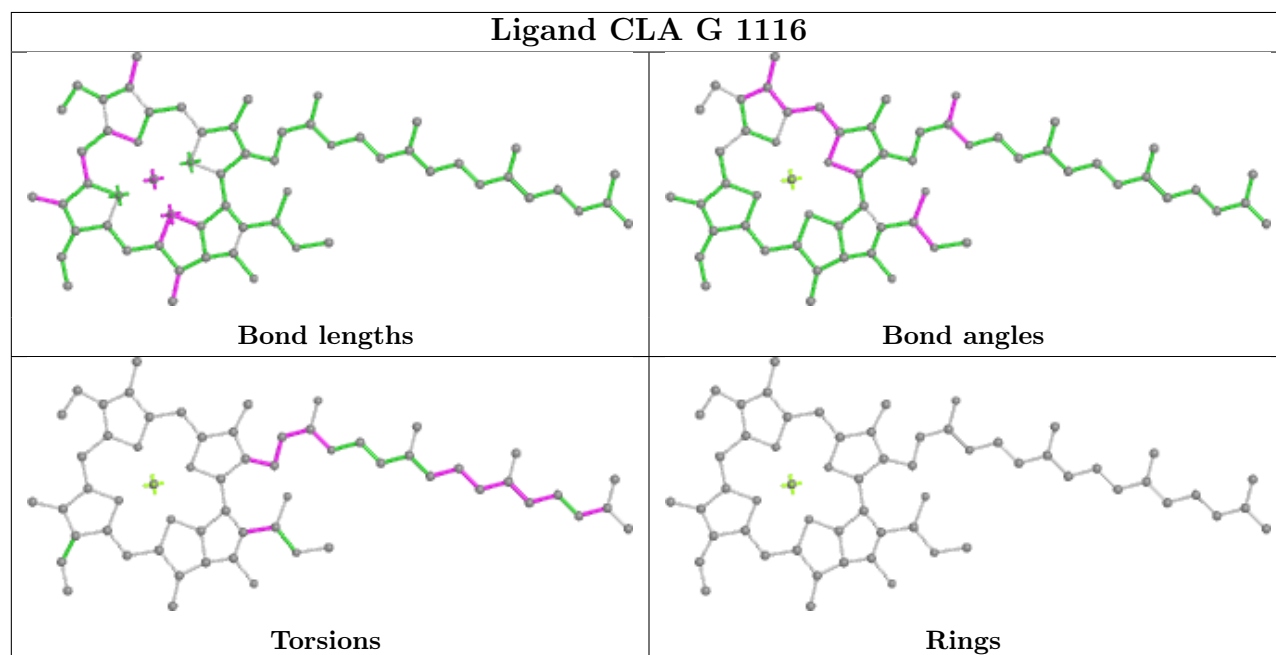
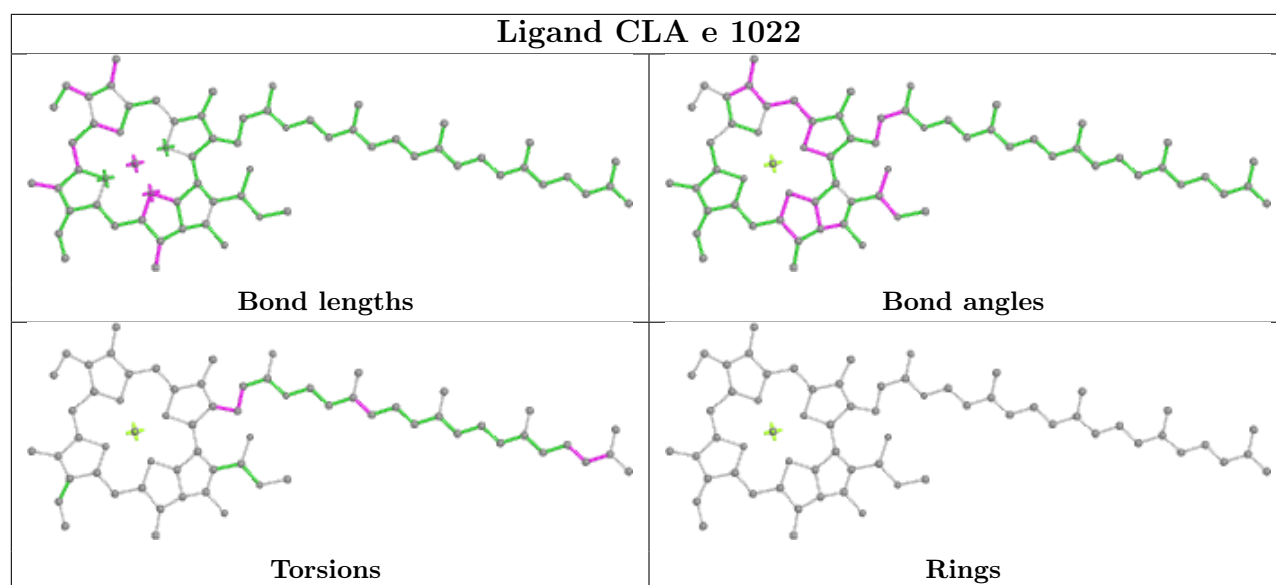
Ligand CLA s 502



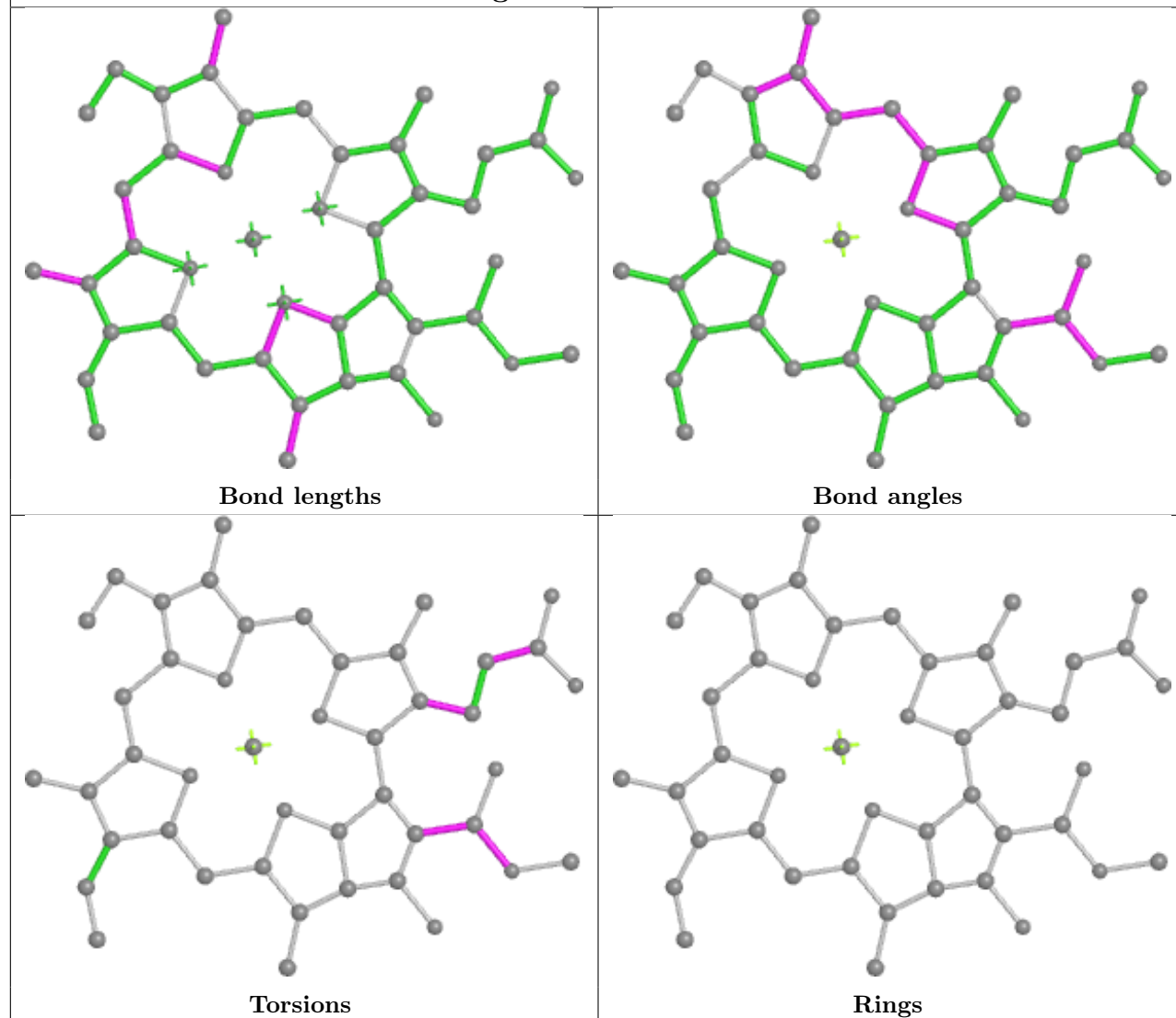
Ligand LMG 1 5104



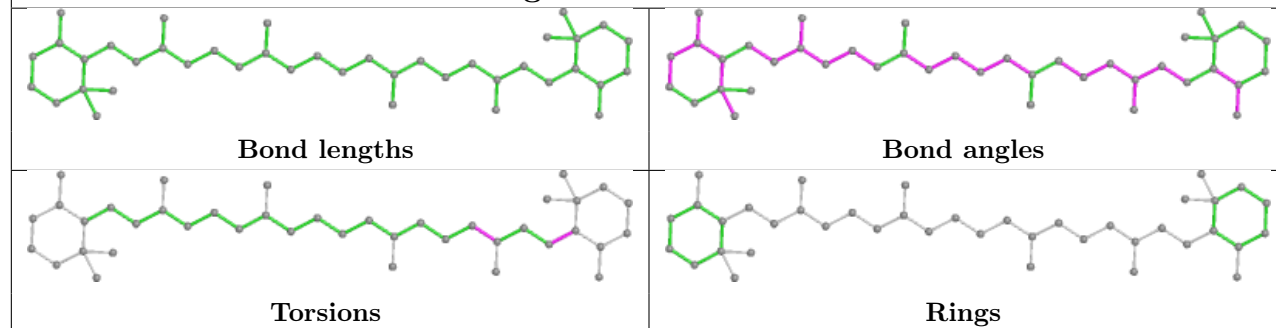


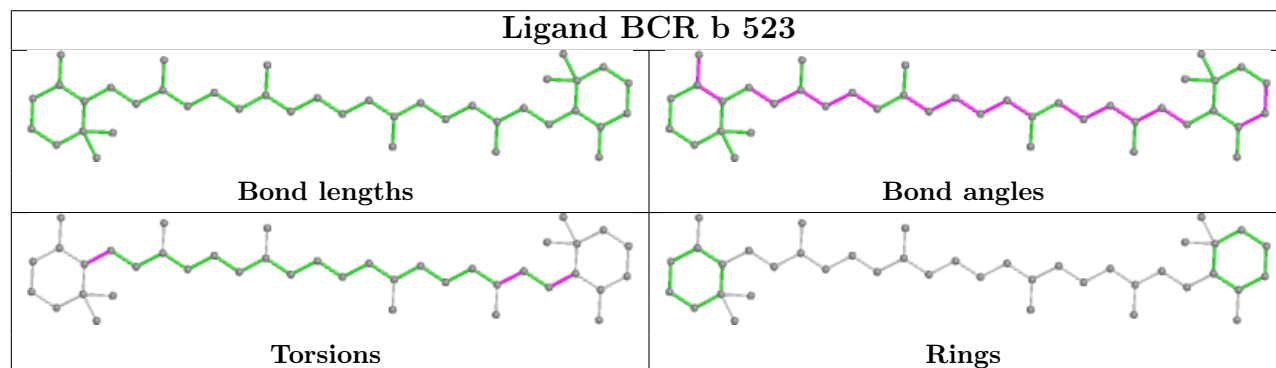
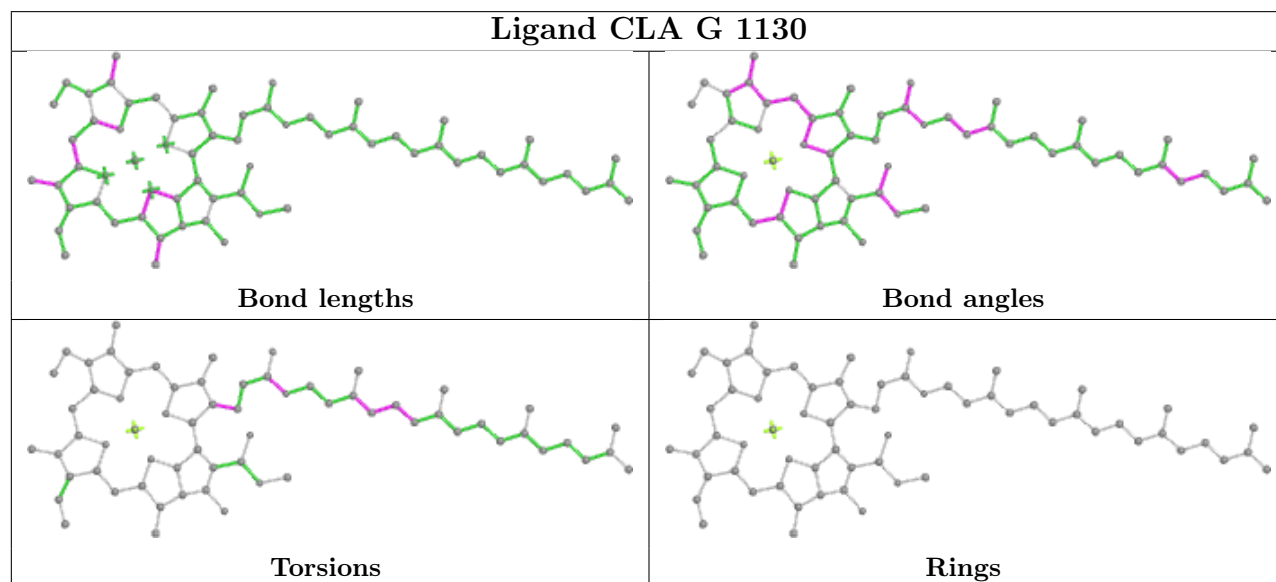
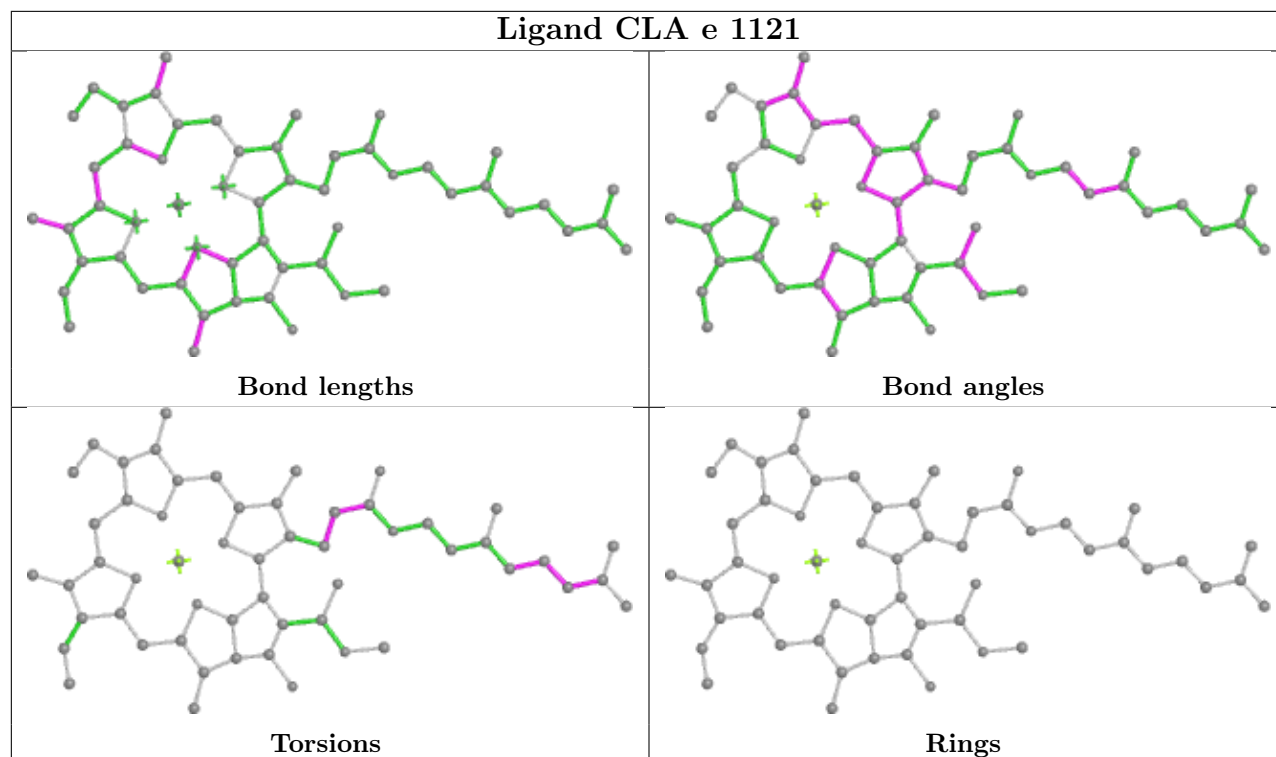


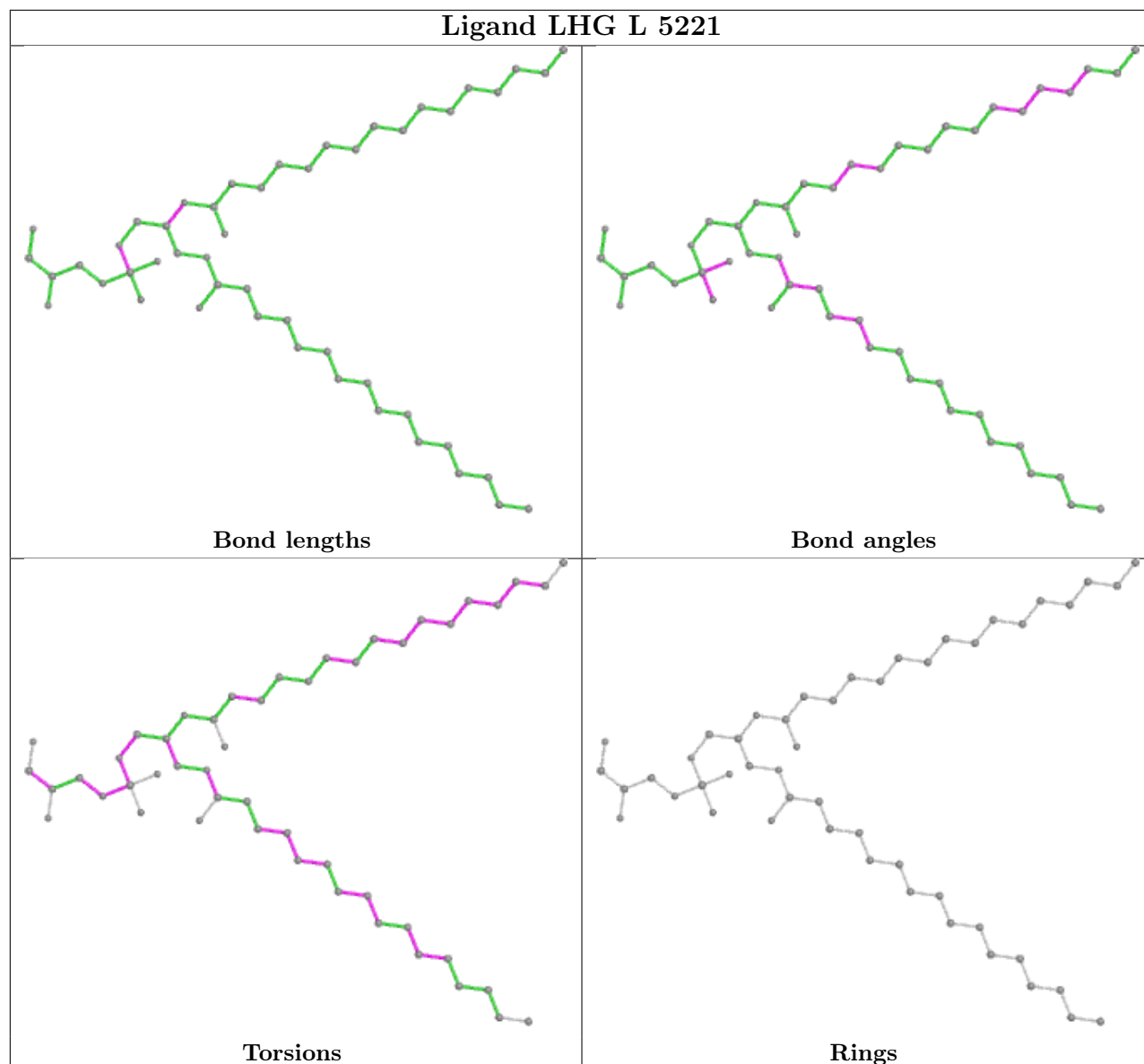
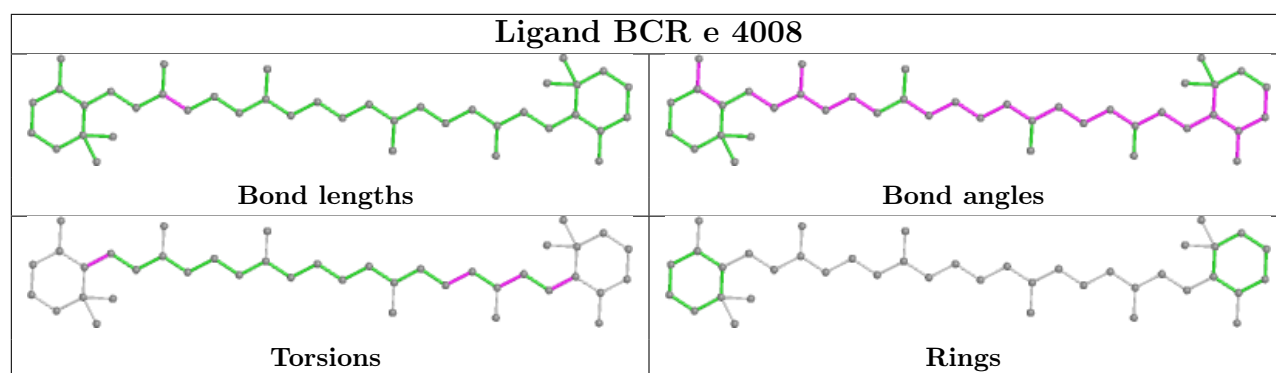
Ligand CLA Z 516

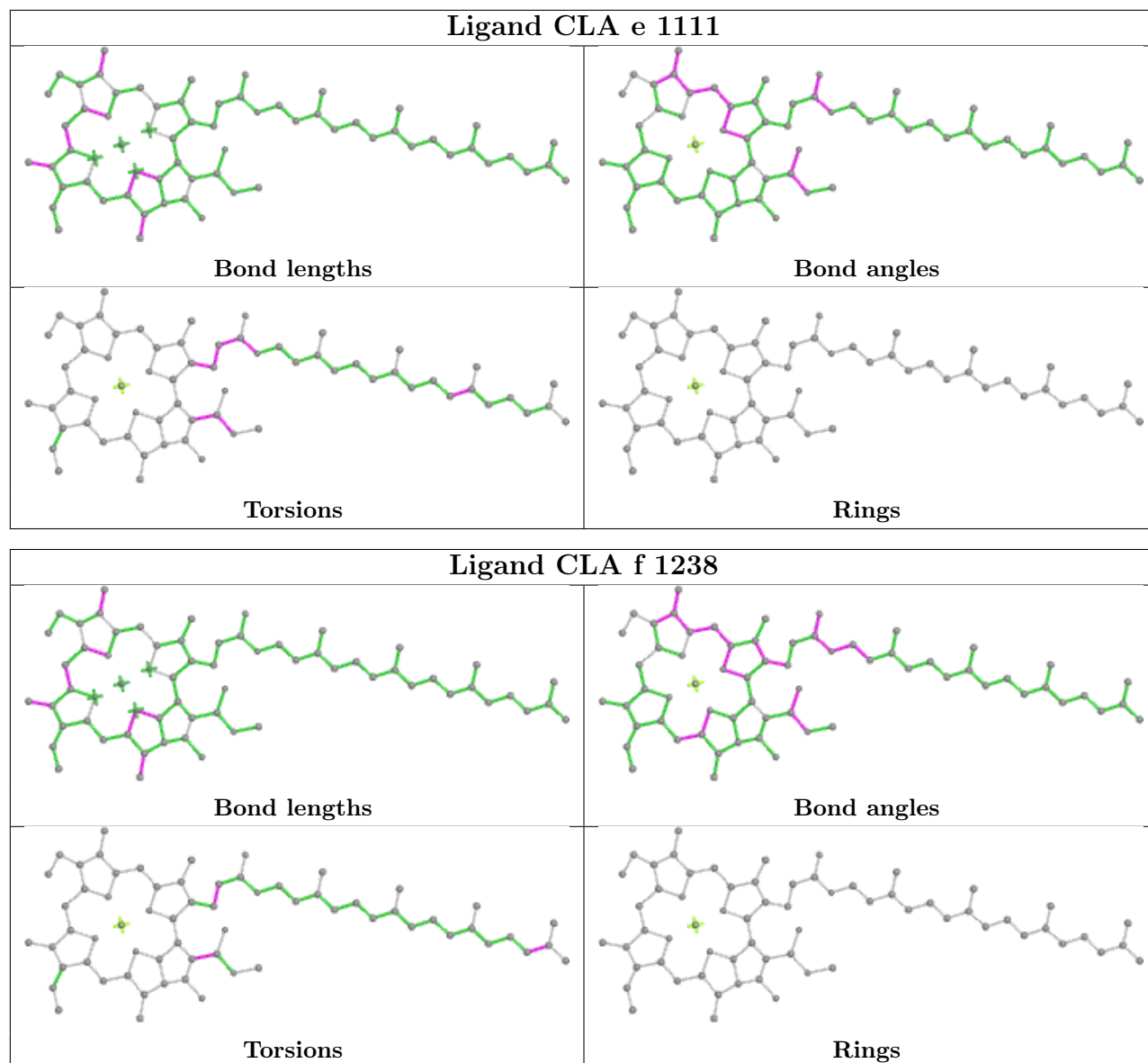


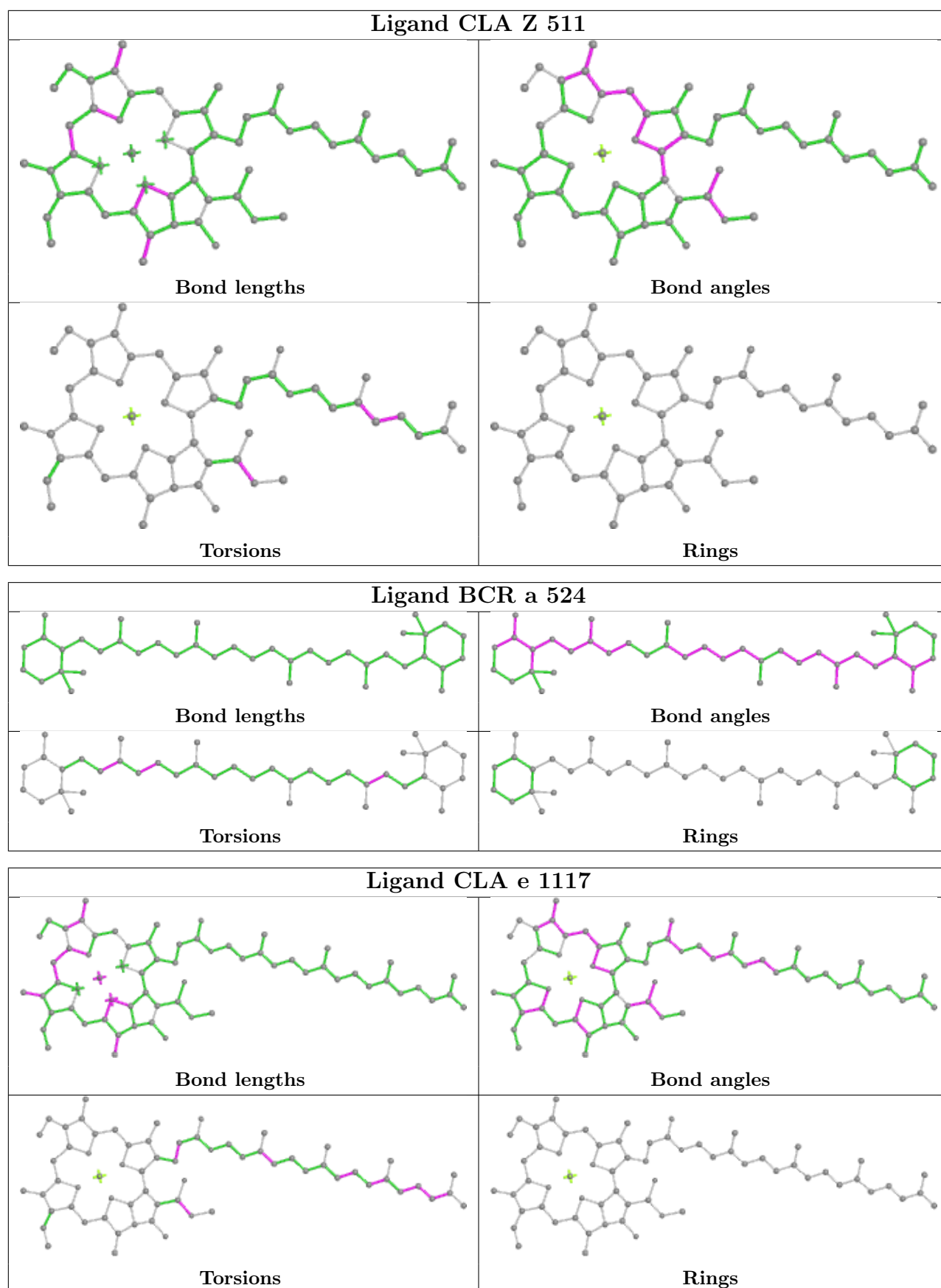
Ligand BCR L 4020

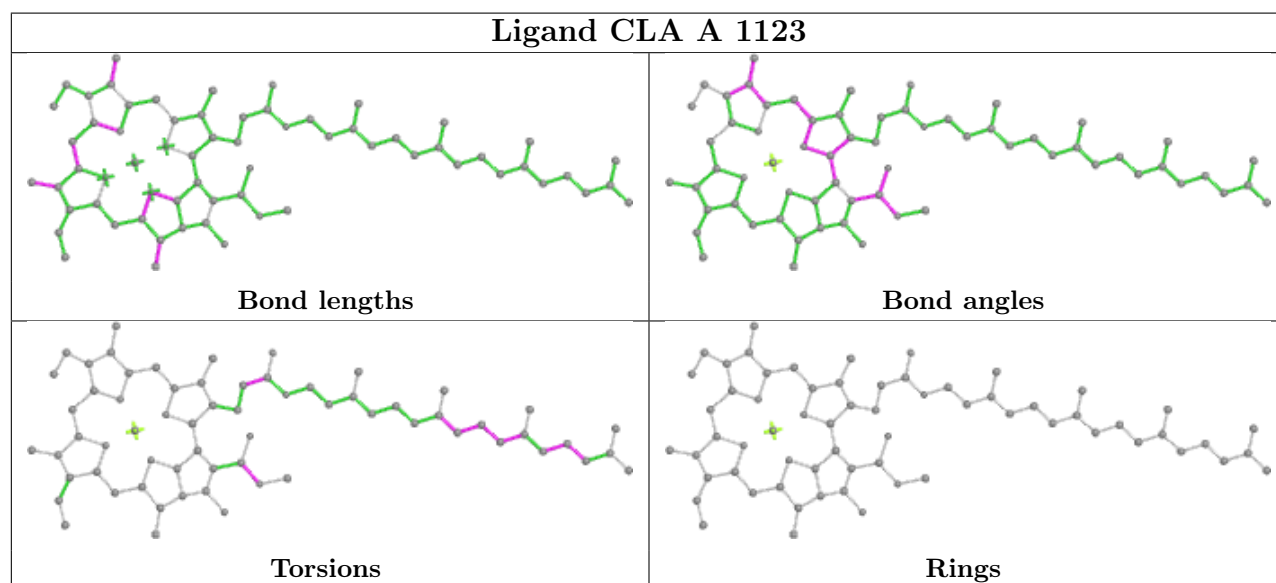
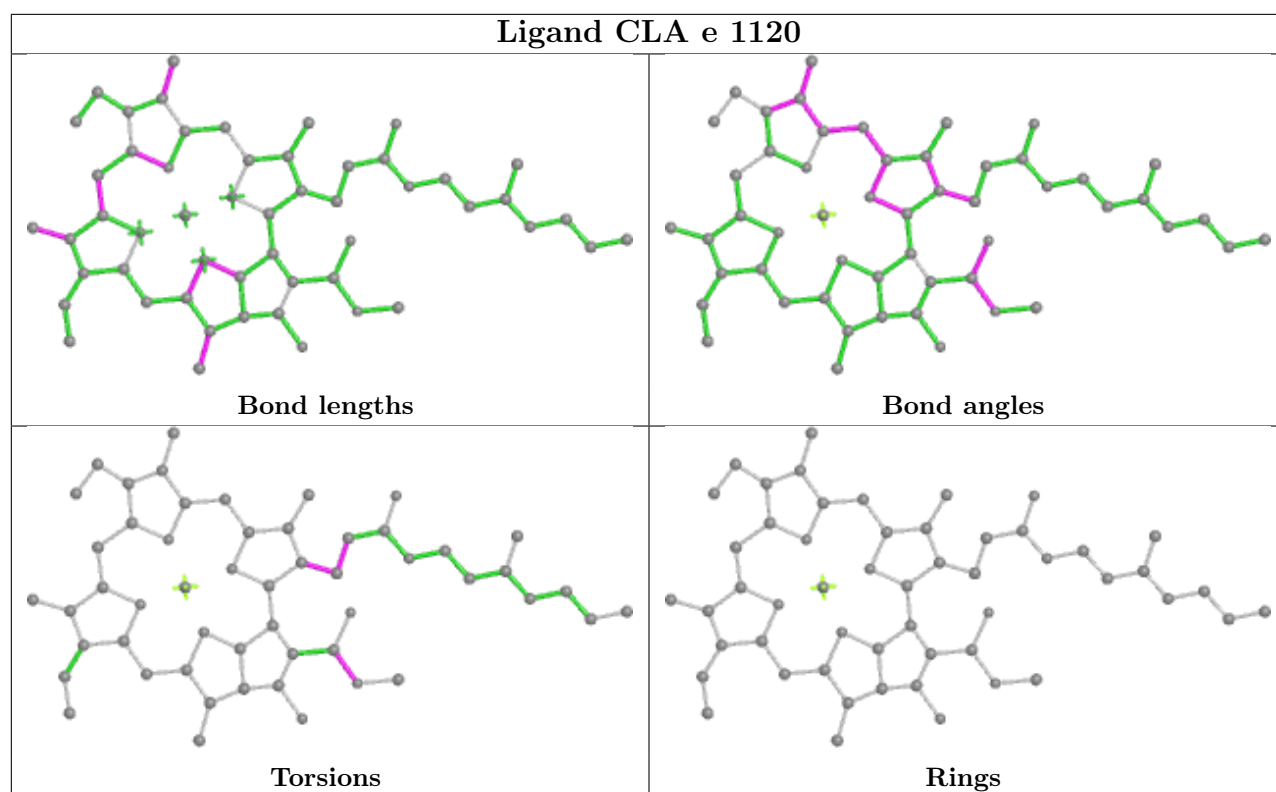


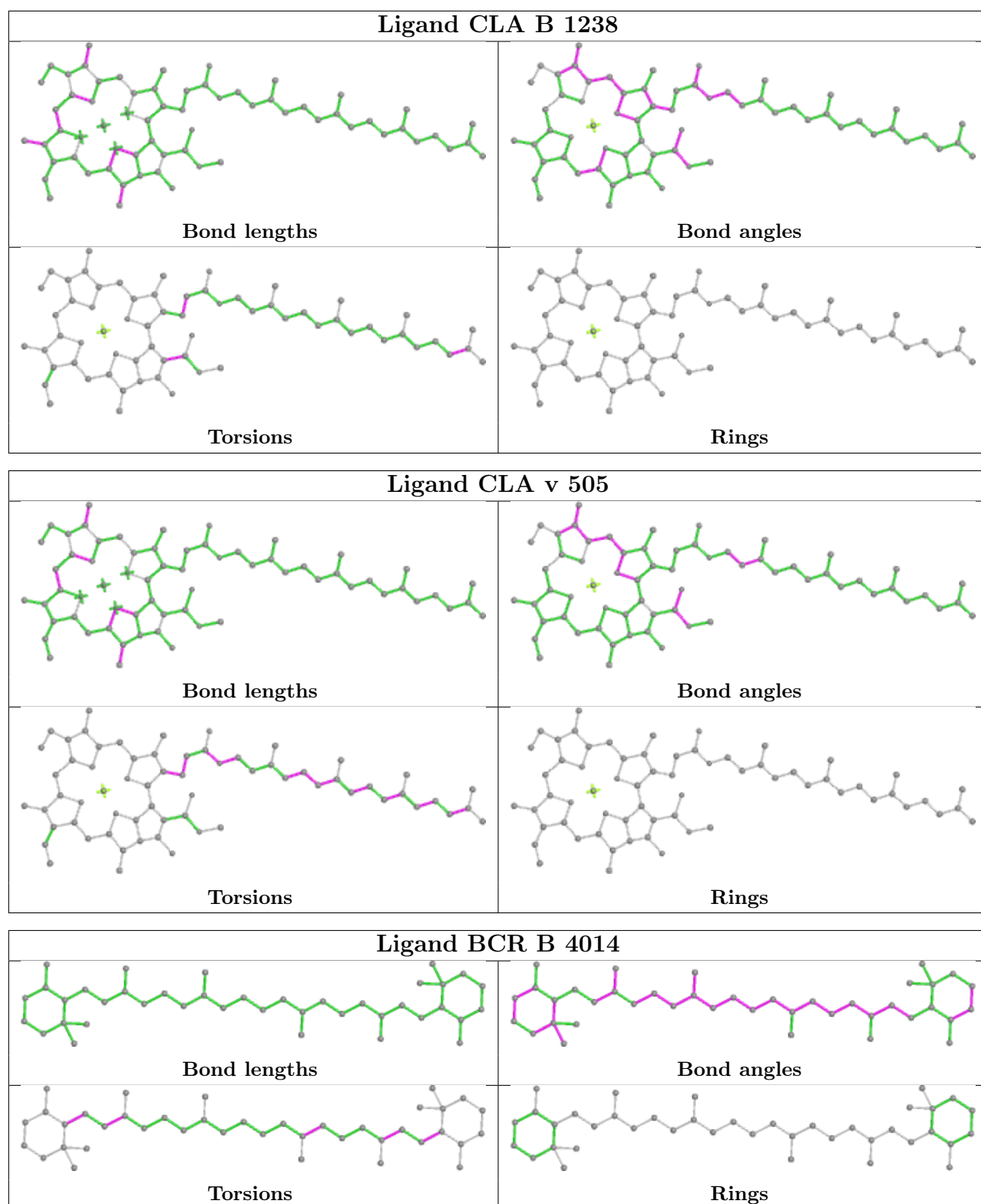


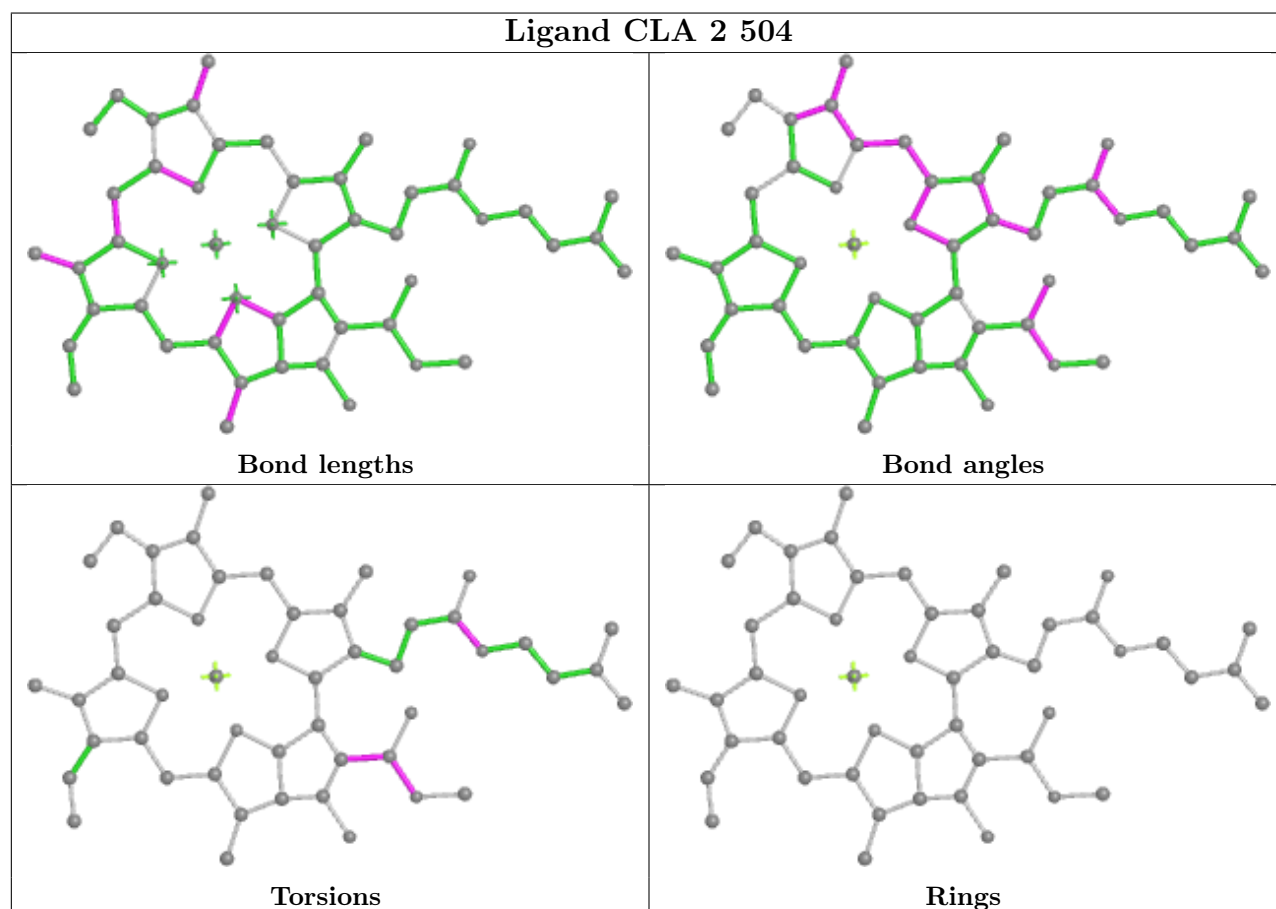
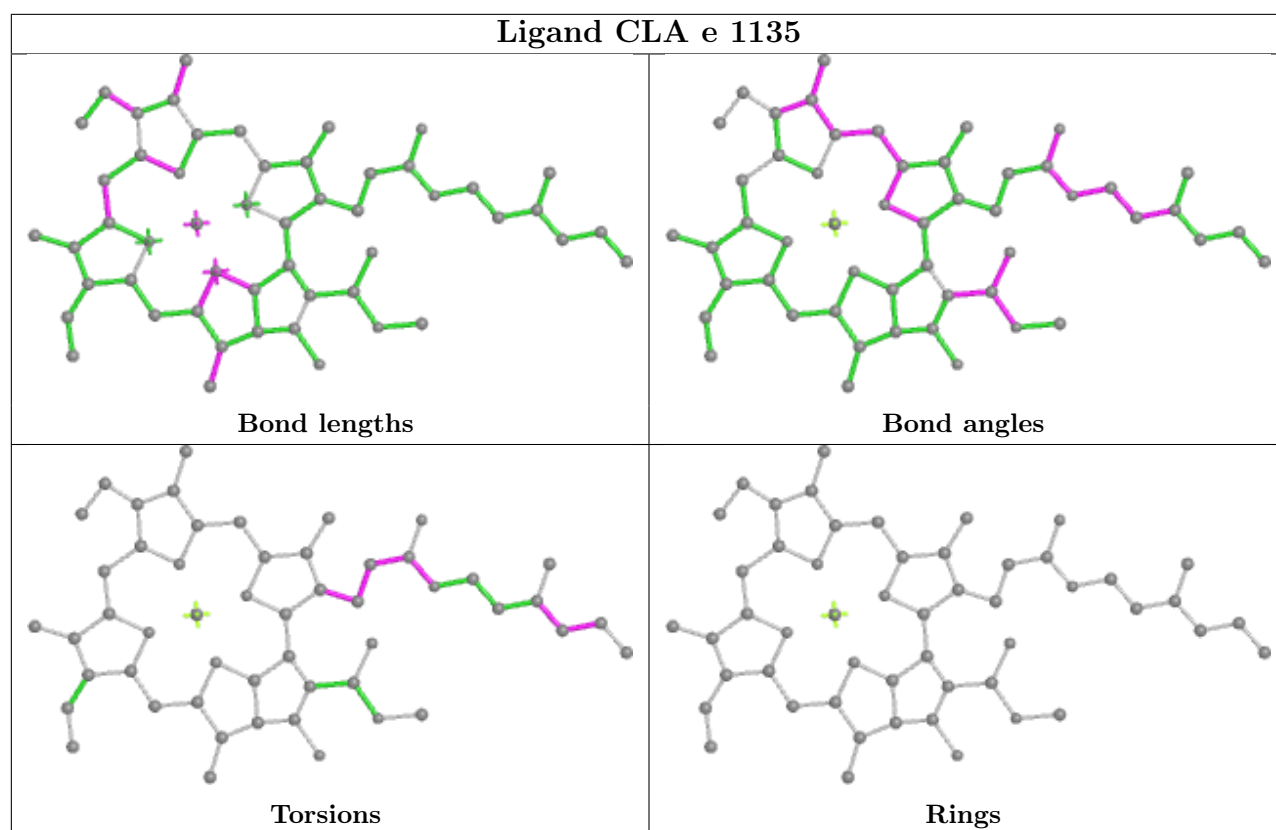




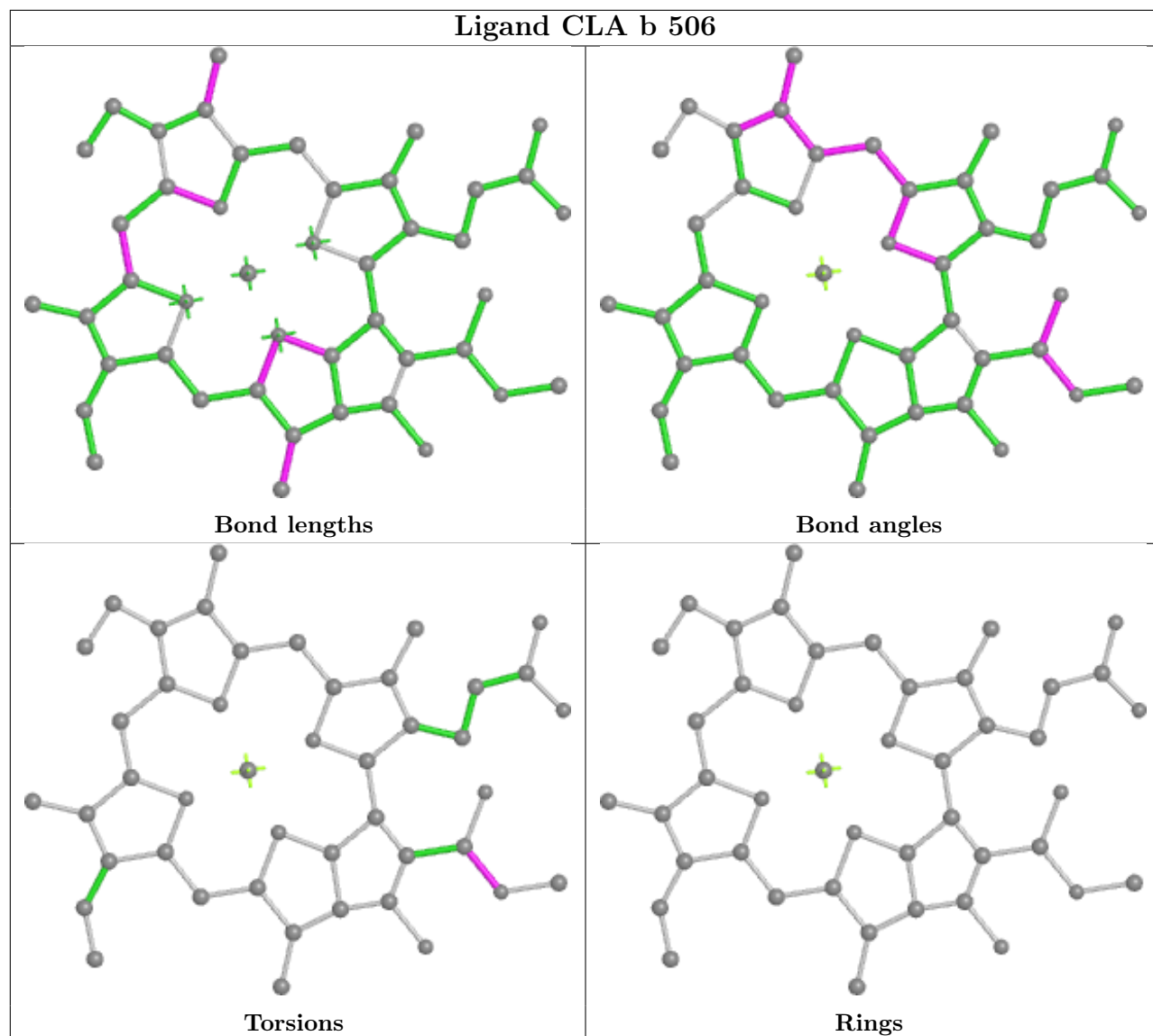


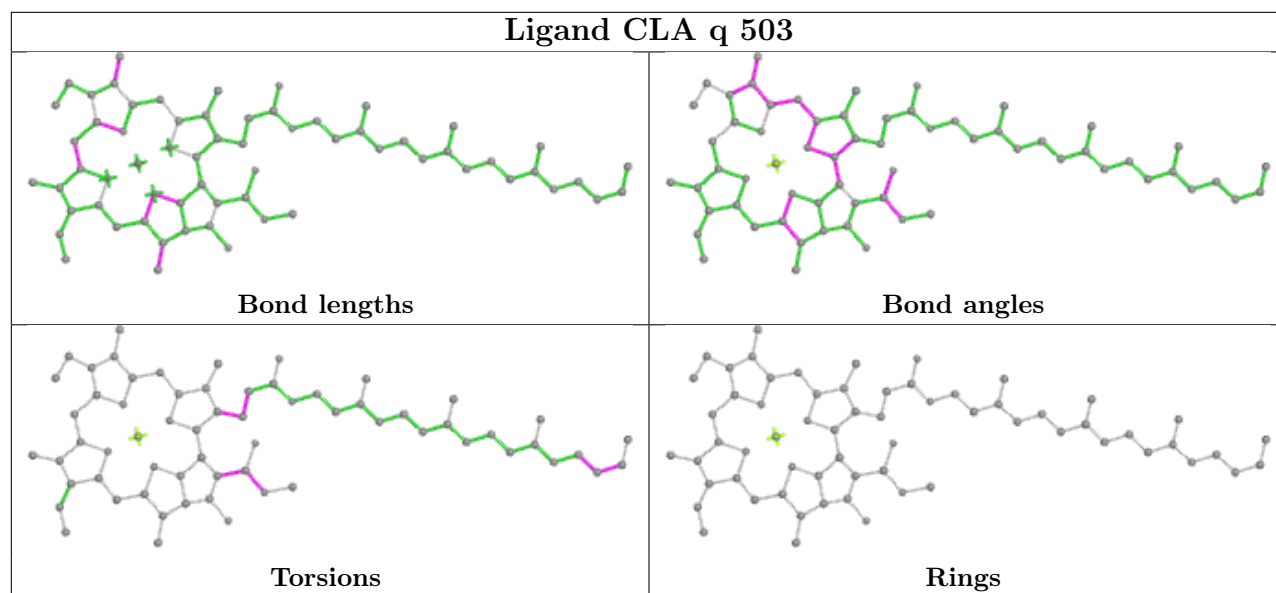
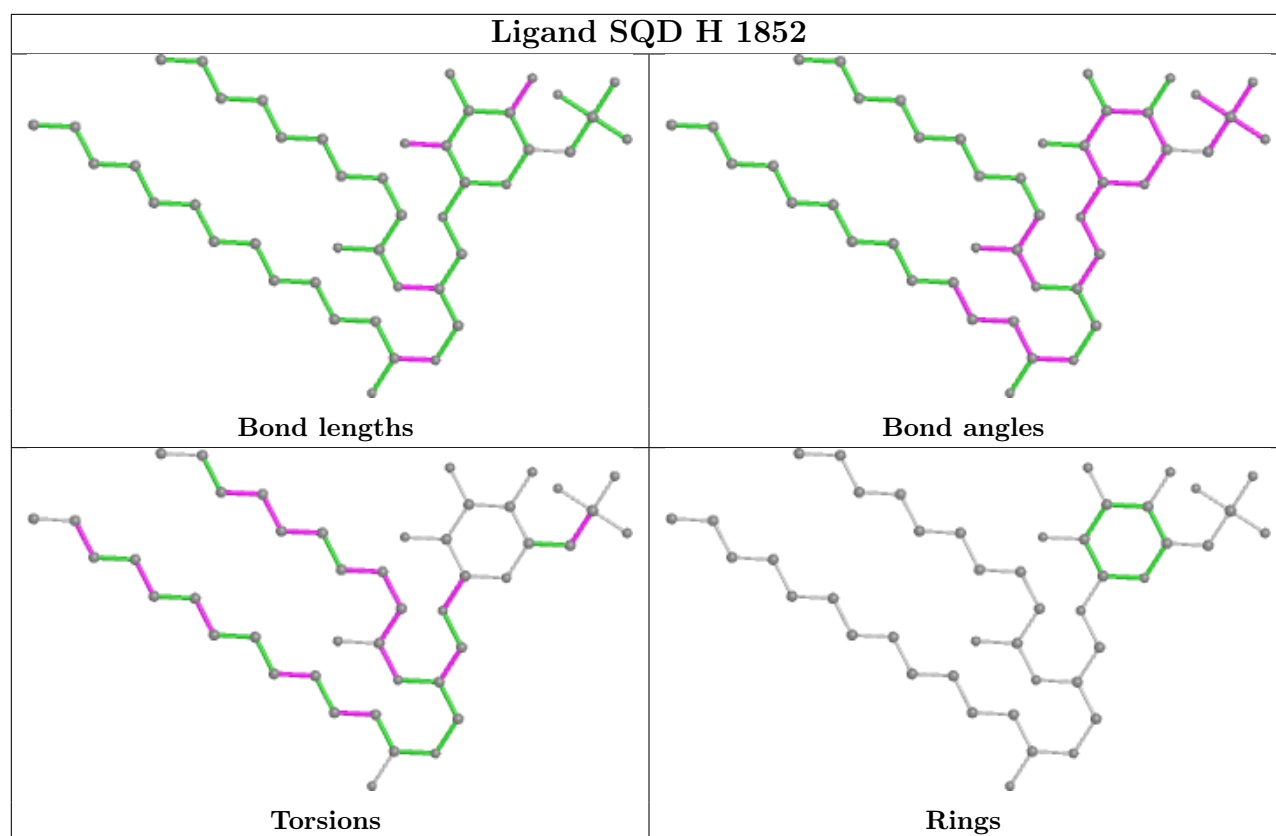




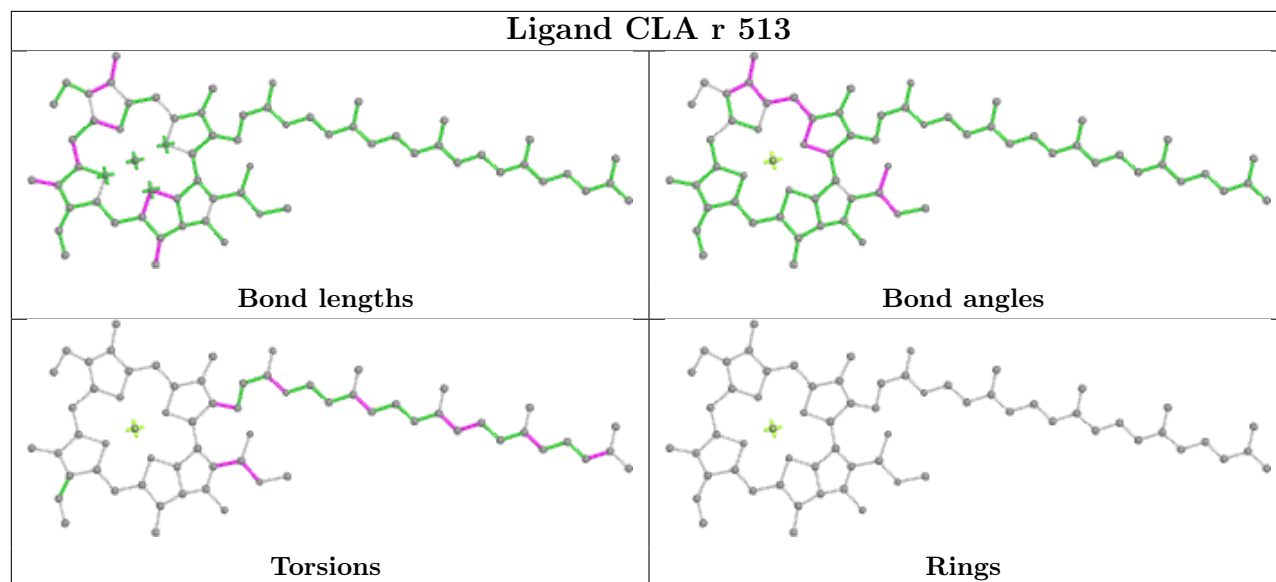


Ligand CLA b 506

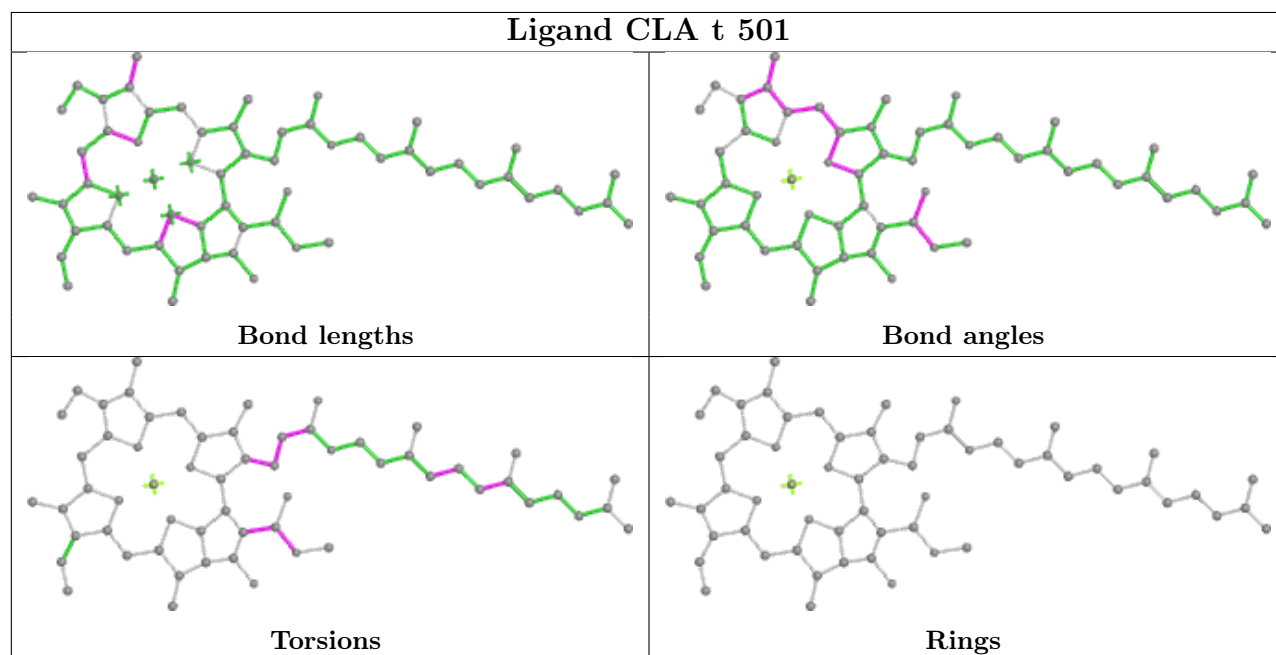


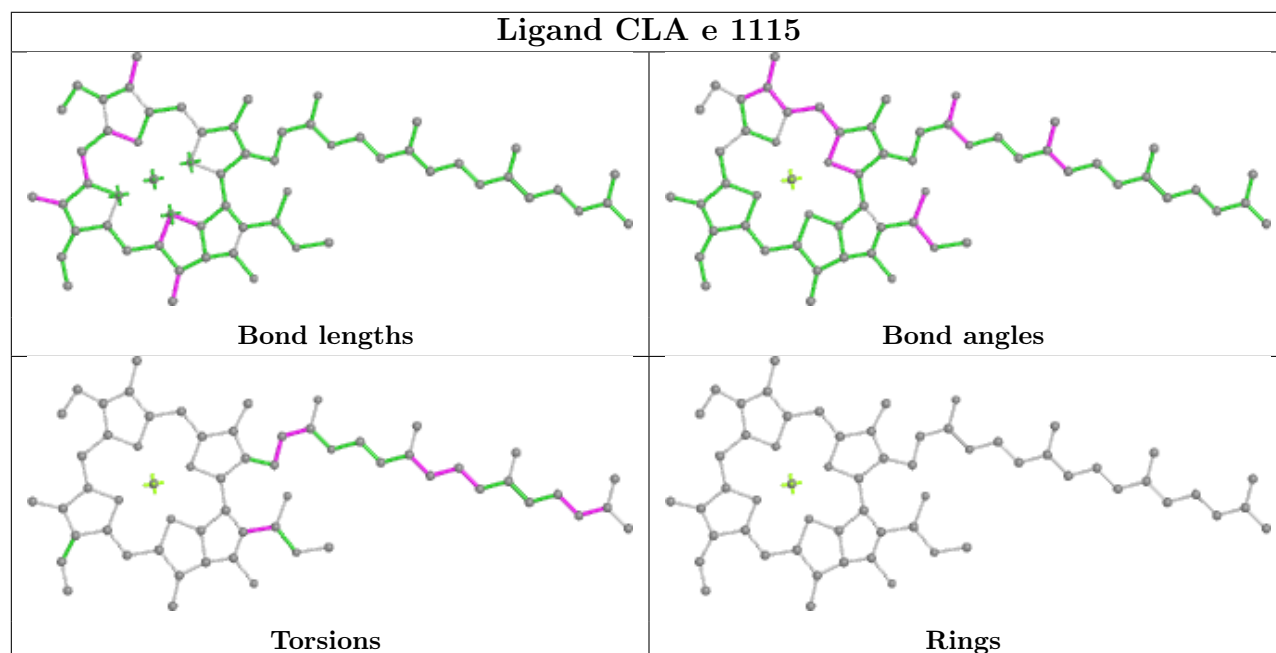
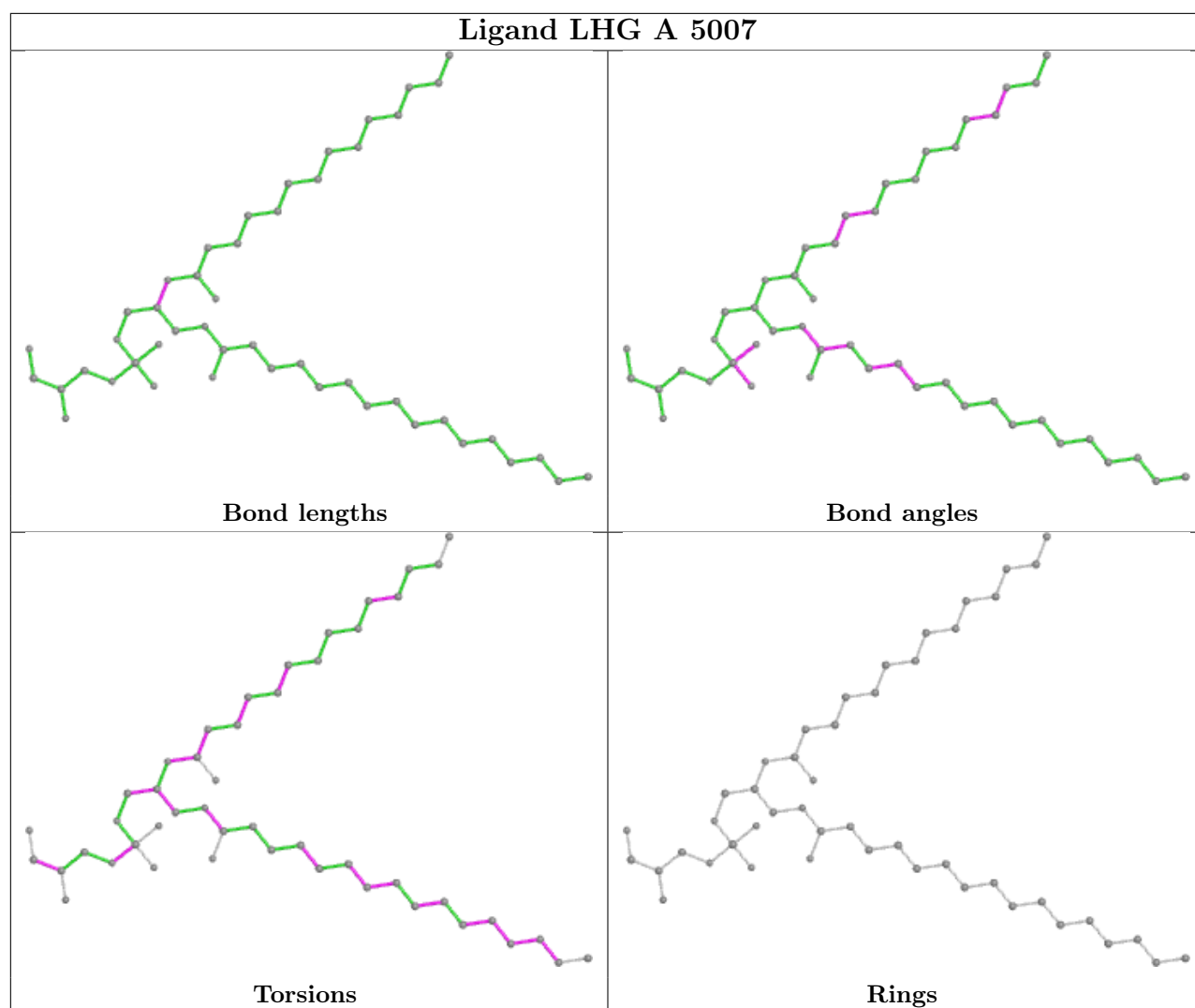


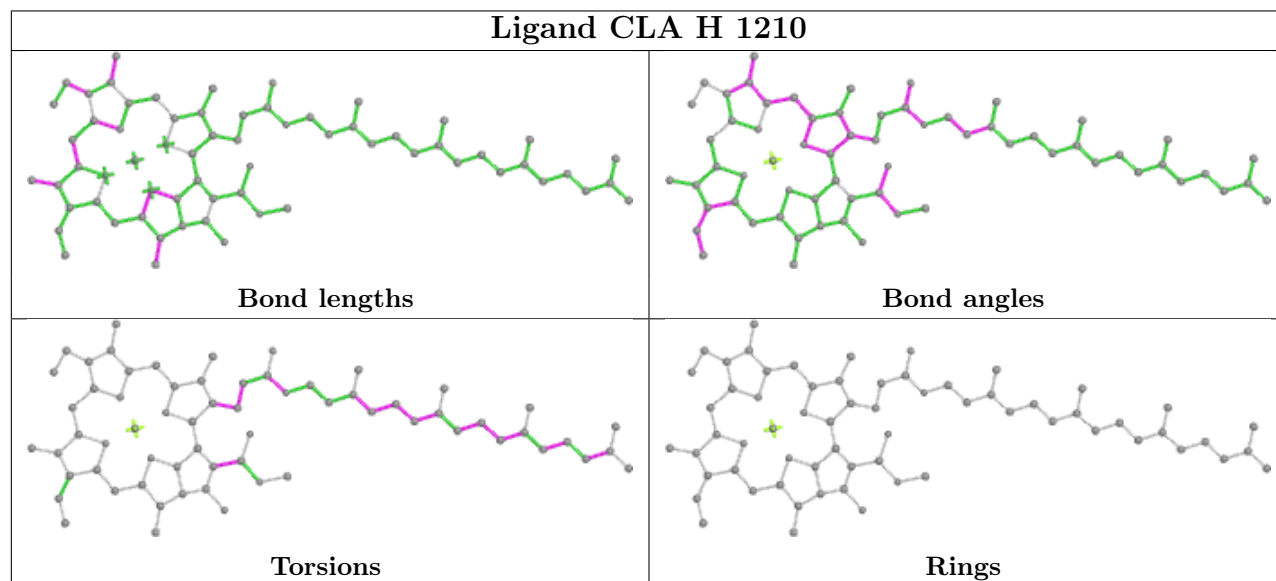
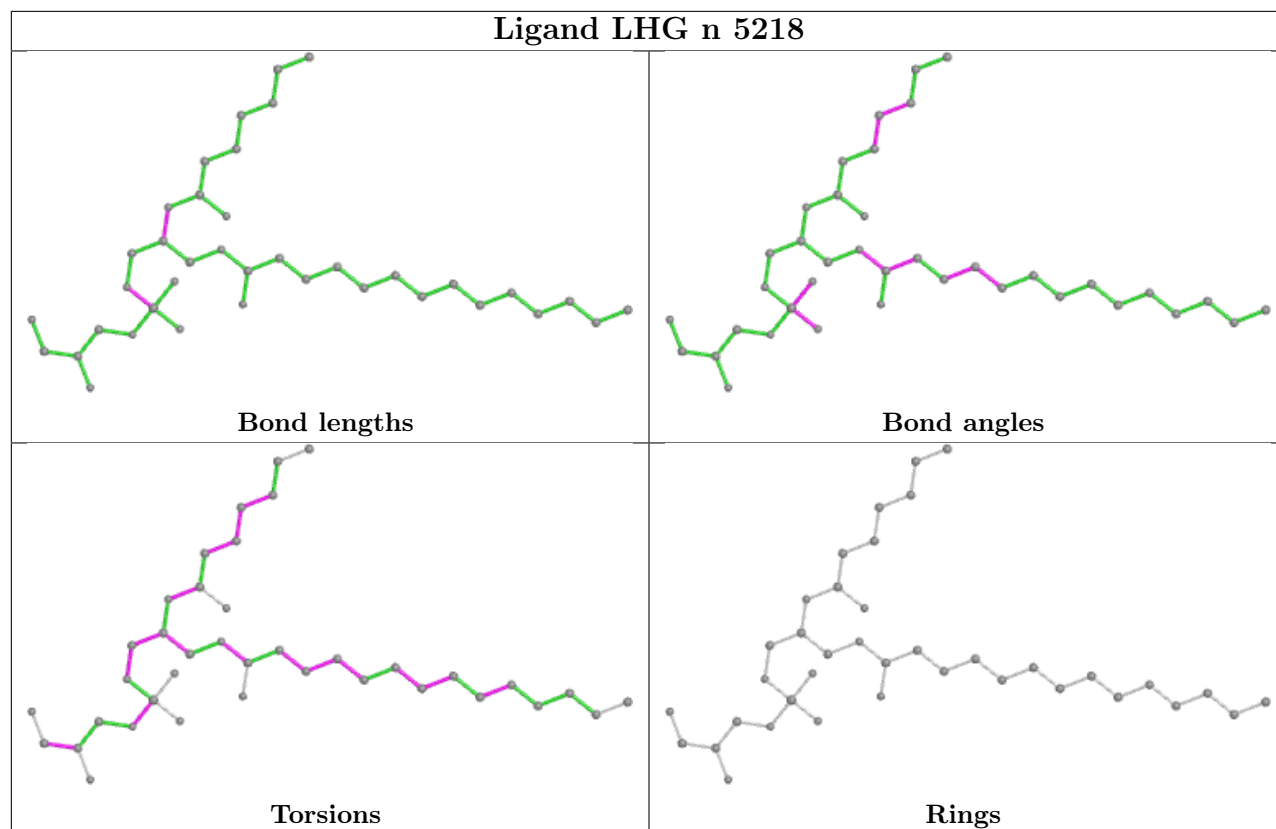
Ligand CLA r 513



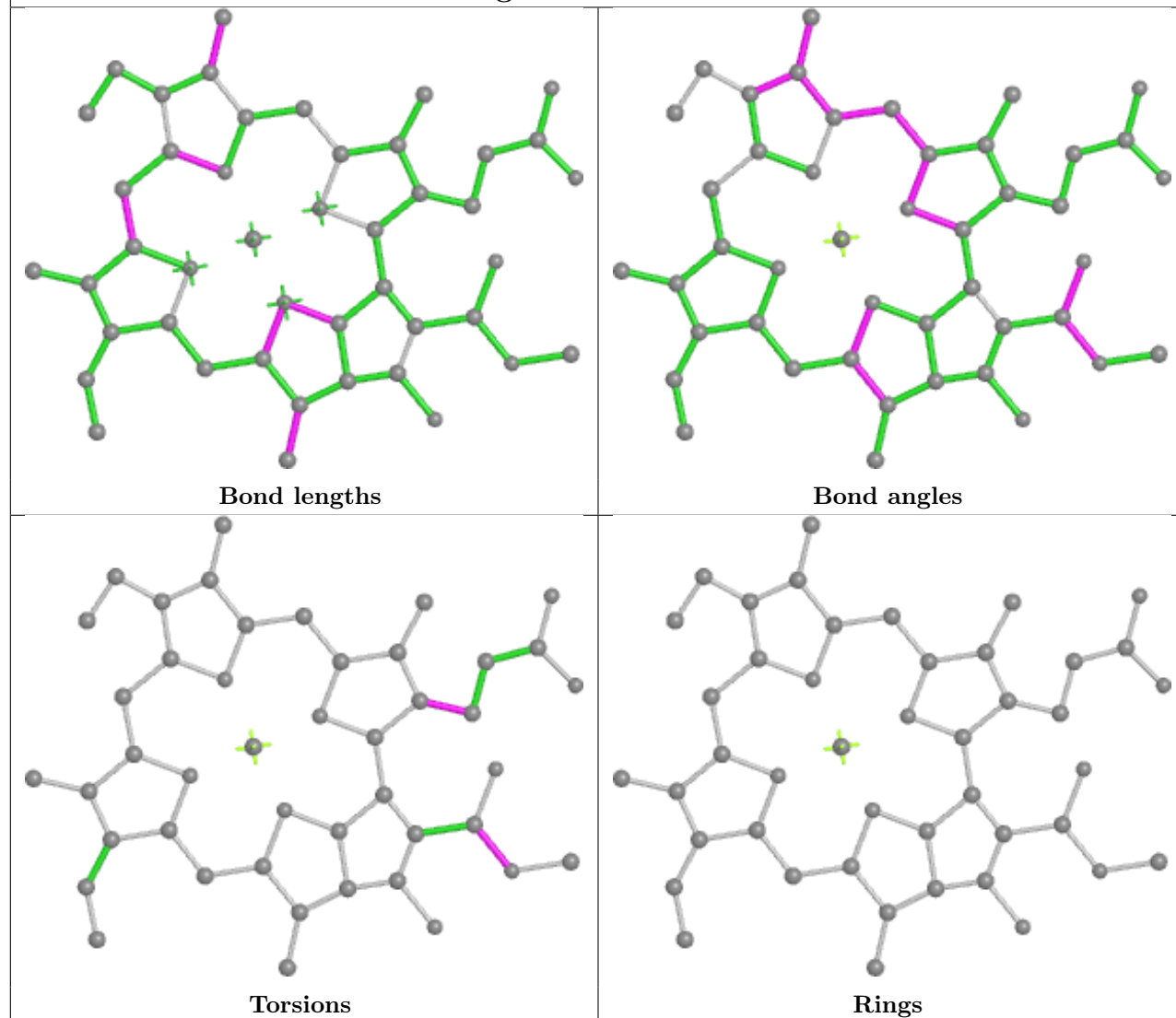
Ligand CLA t 501



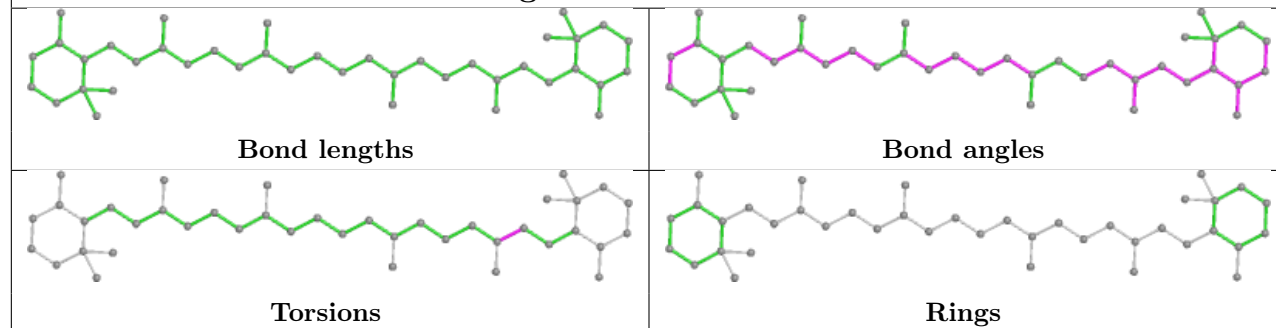


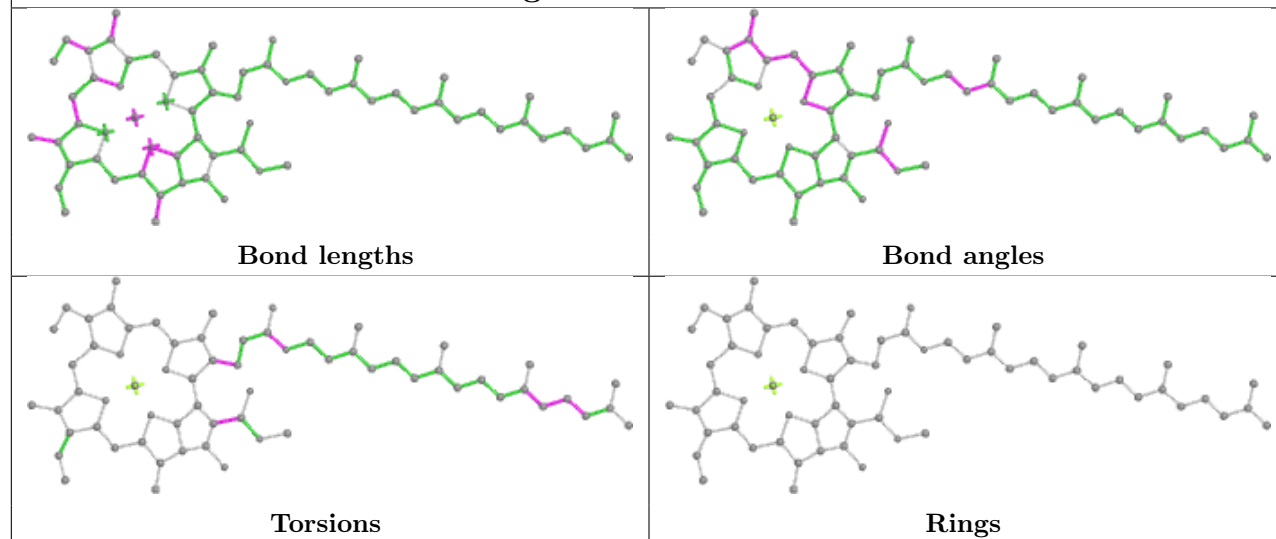
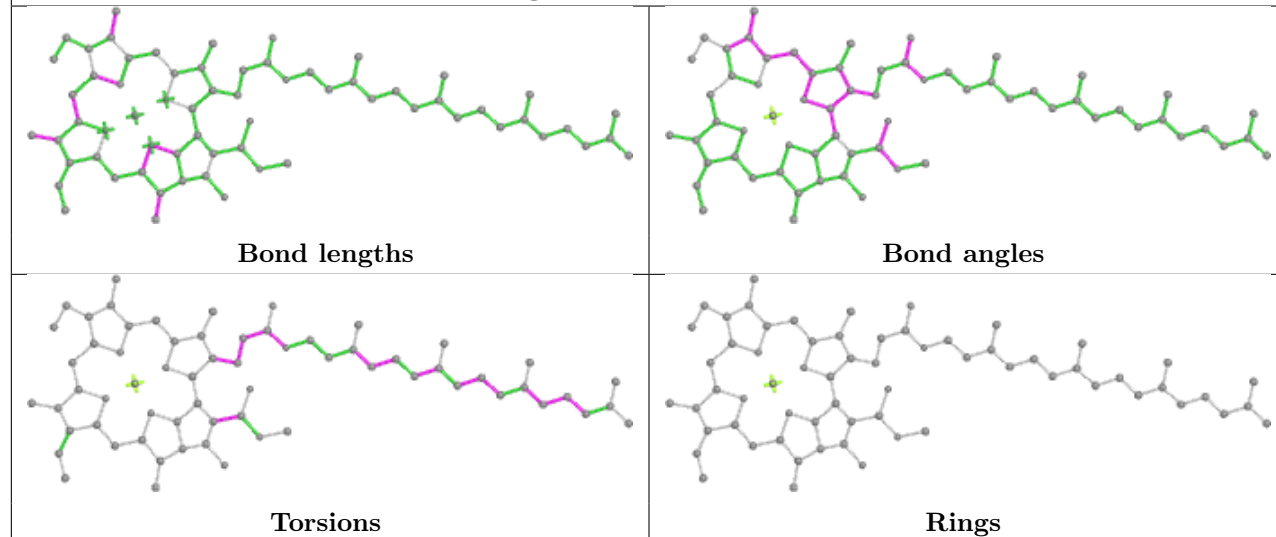


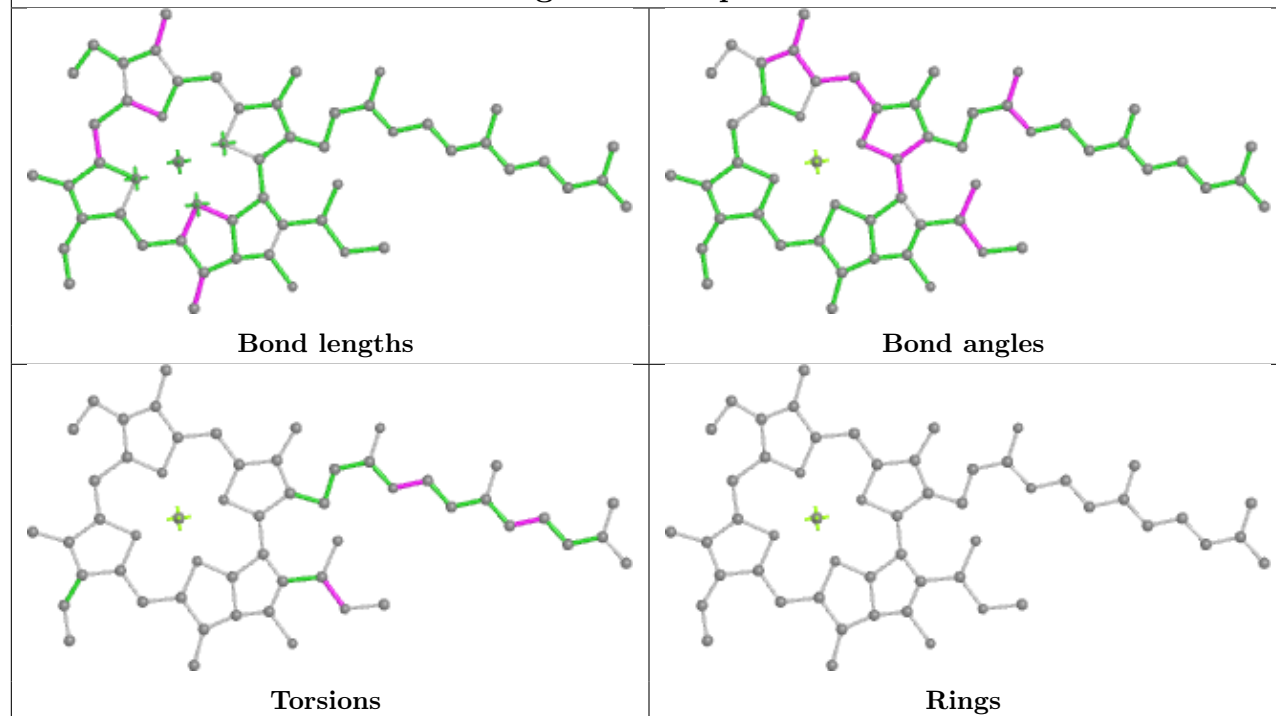
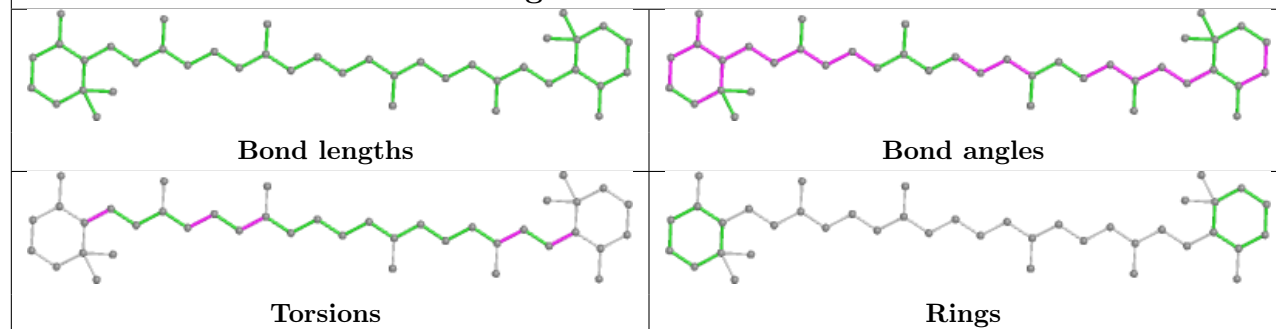
Ligand CLA t 511



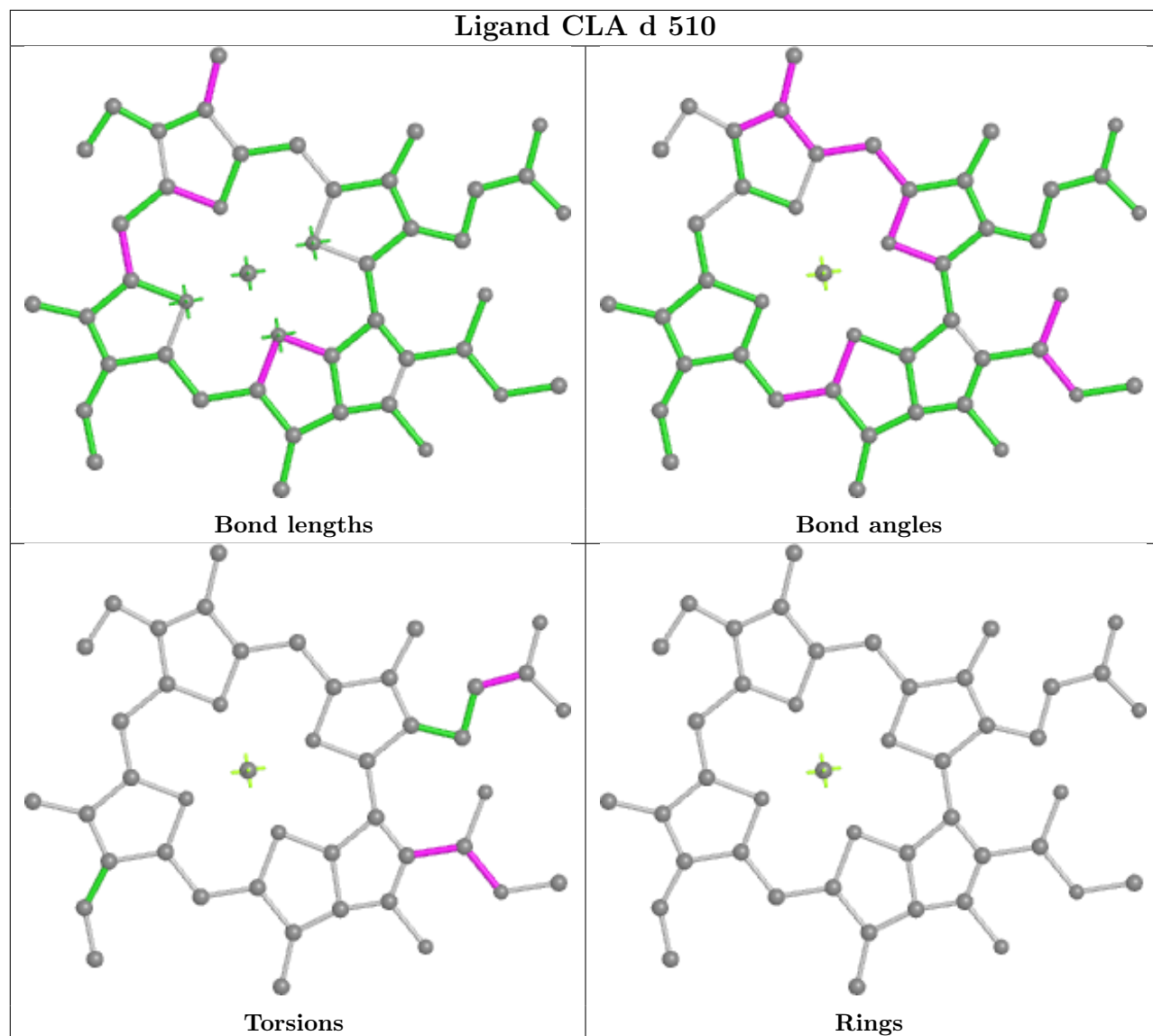
Ligand BCR m 4104

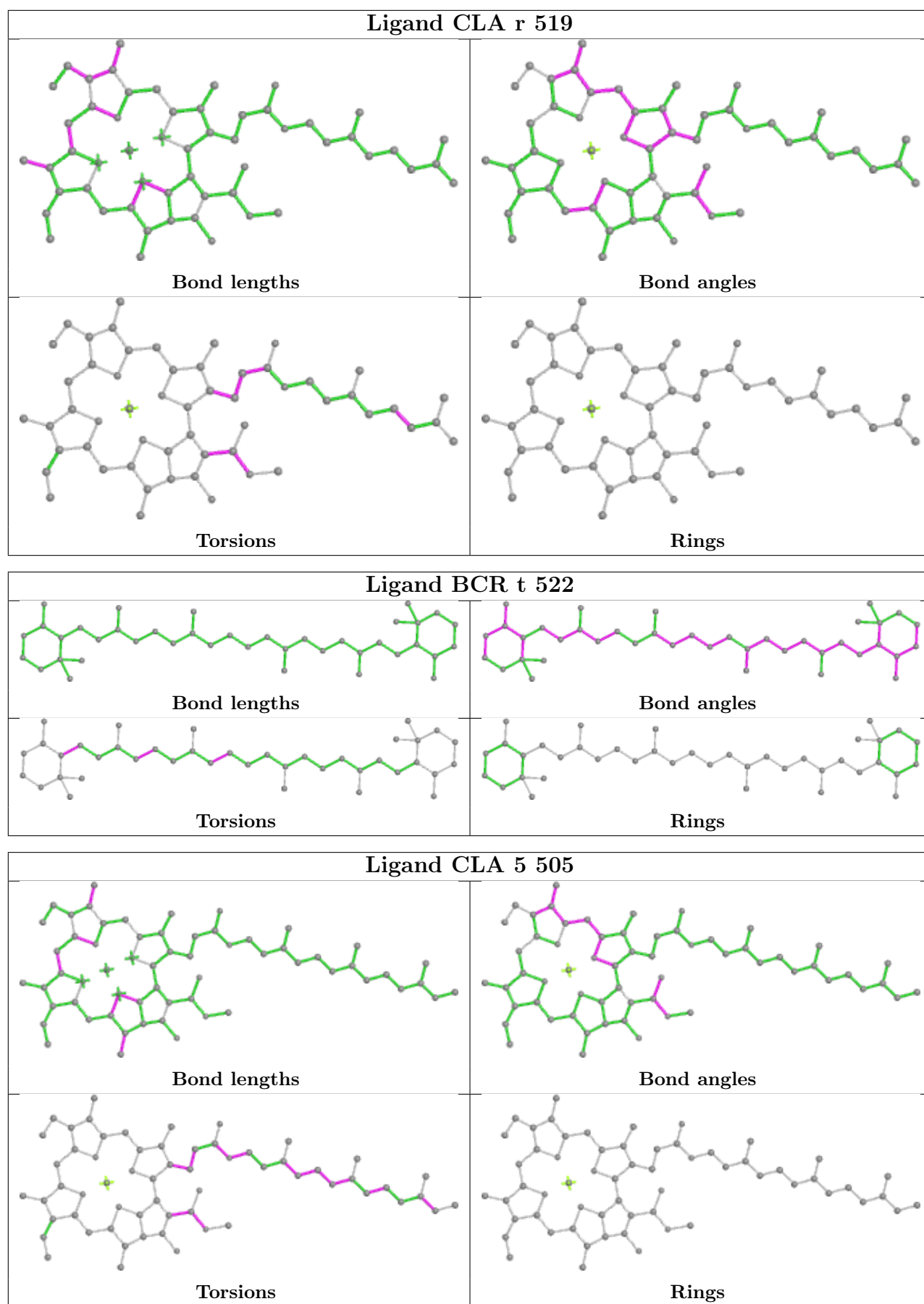


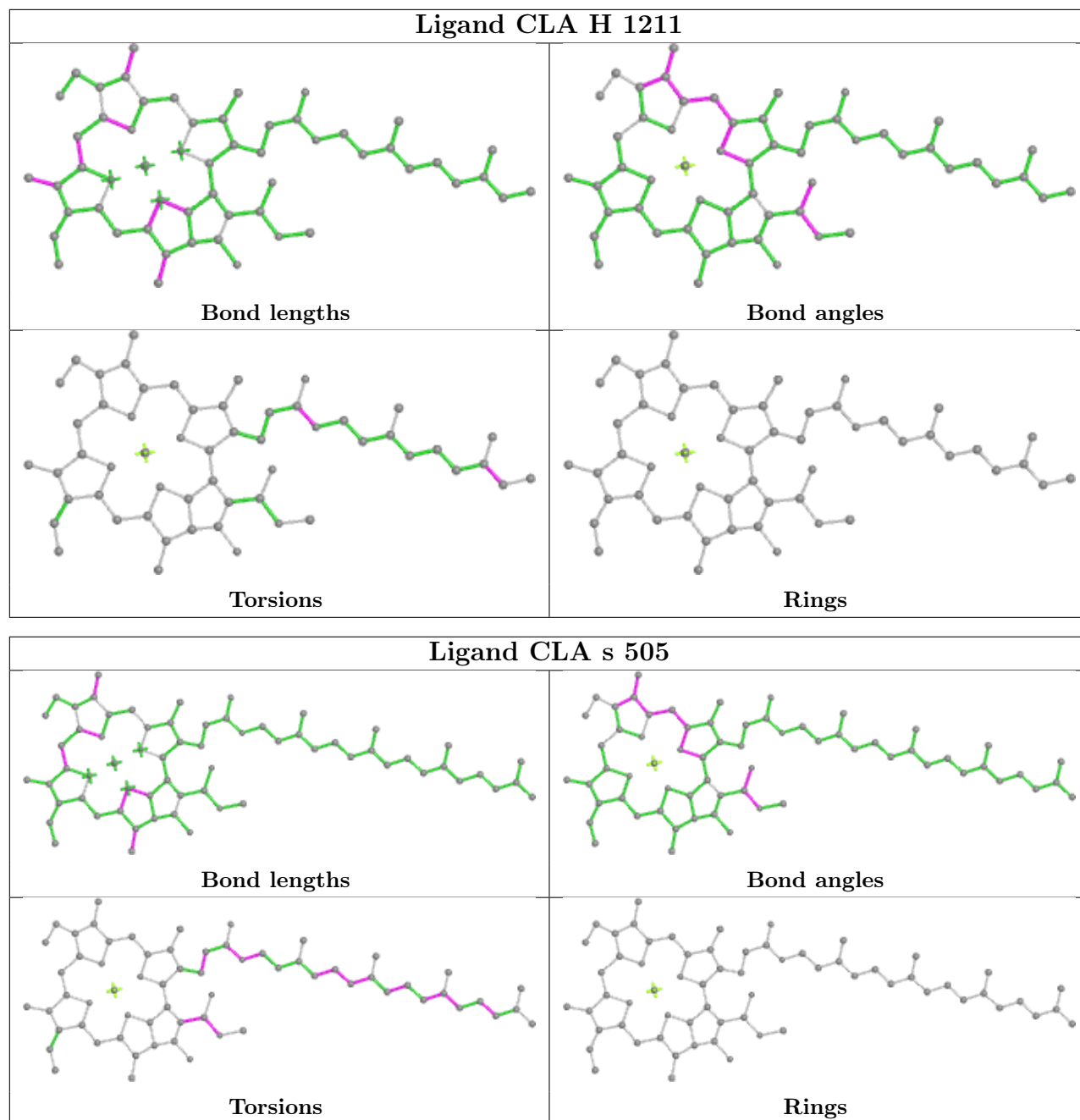
Ligand CLA B 1225**Ligand CLA L 1501**

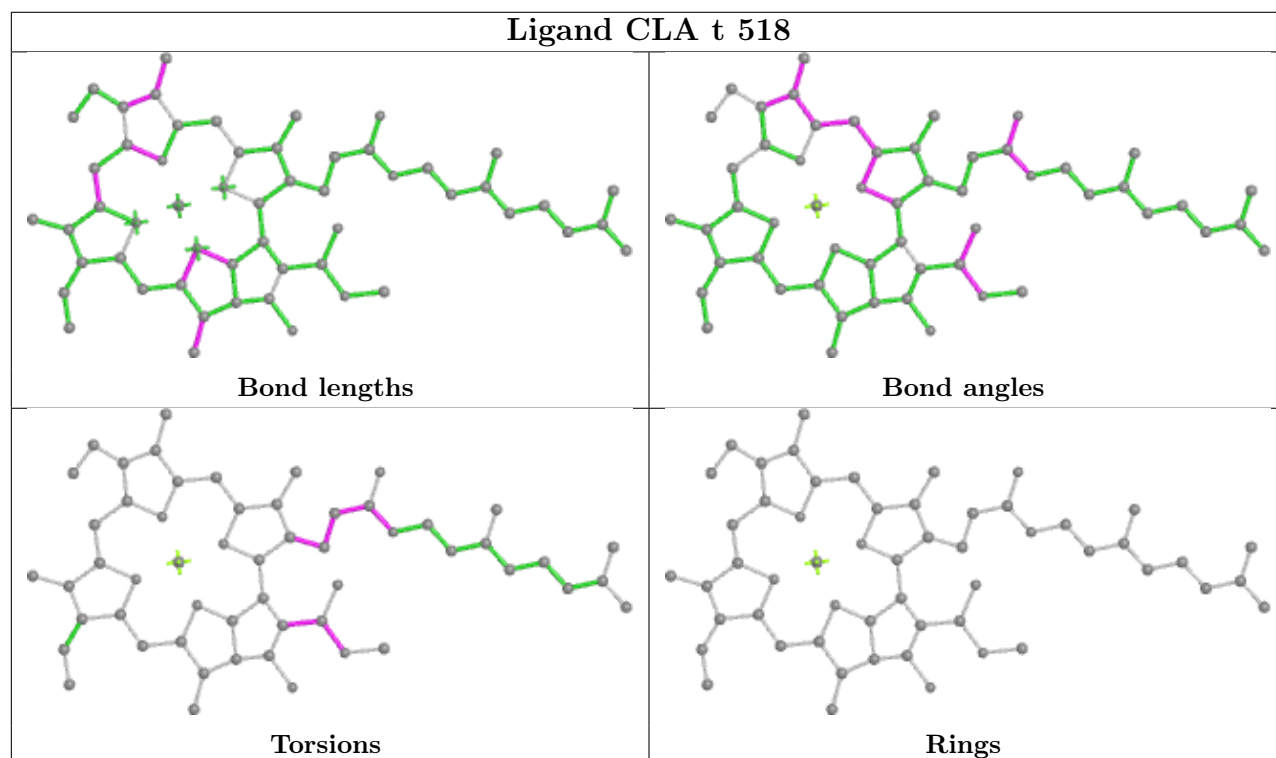
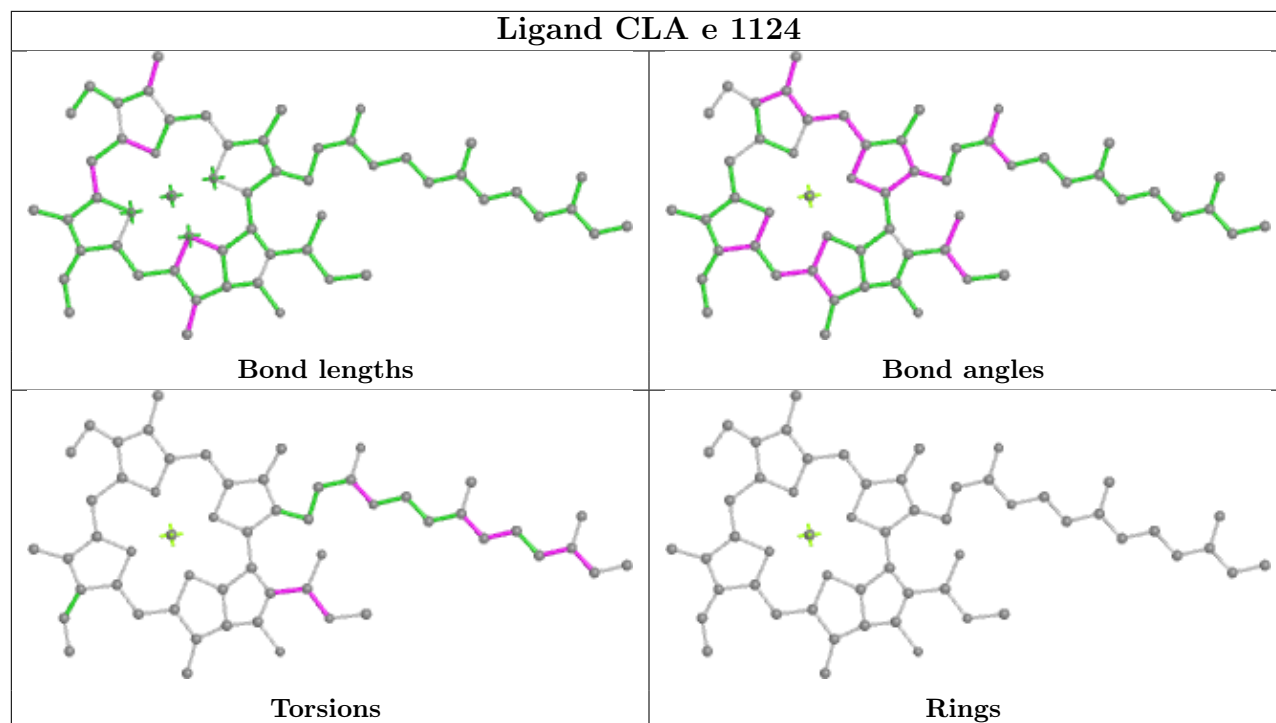
Ligand CLA q 511**Ligand BCR J 4012**

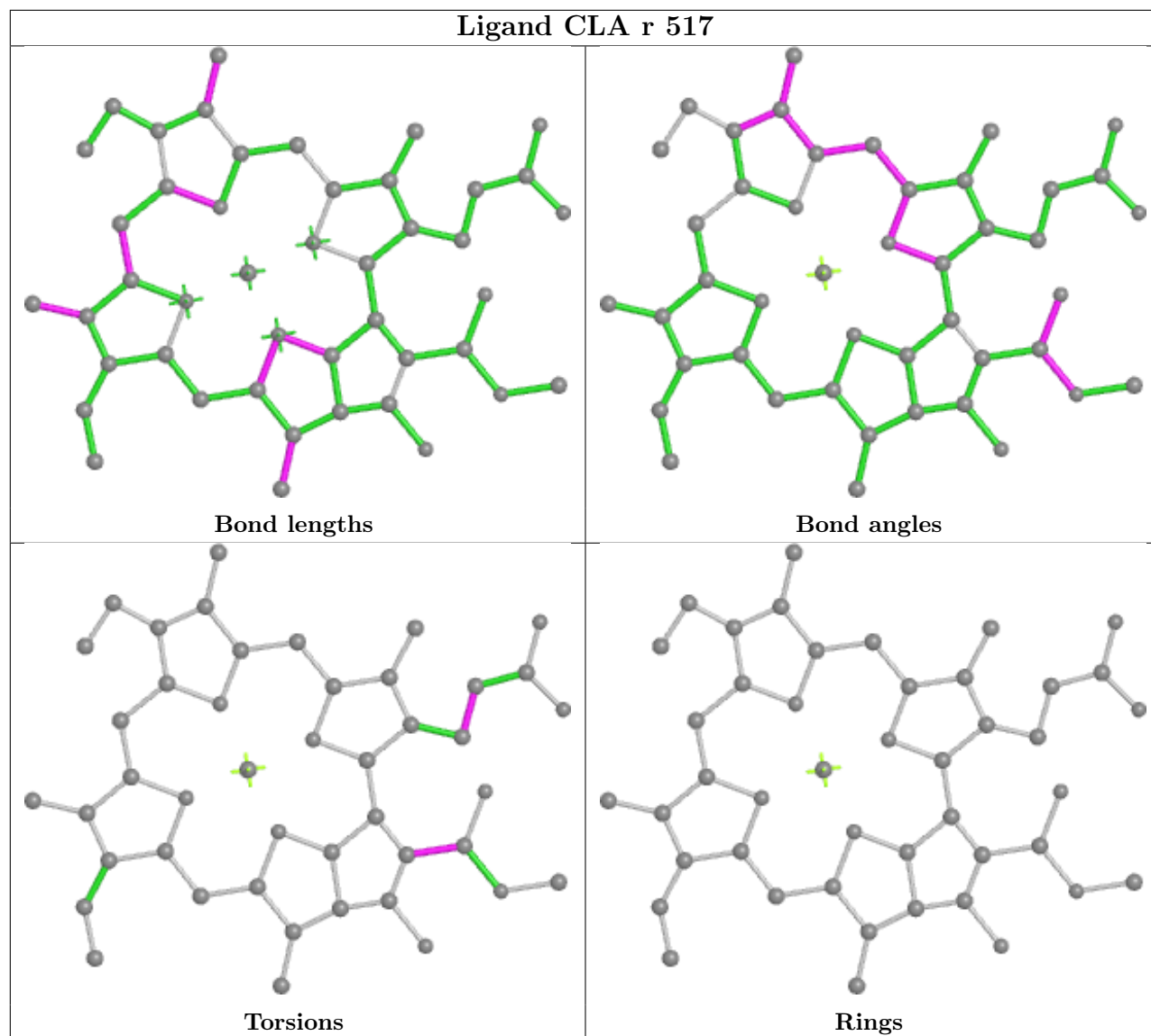
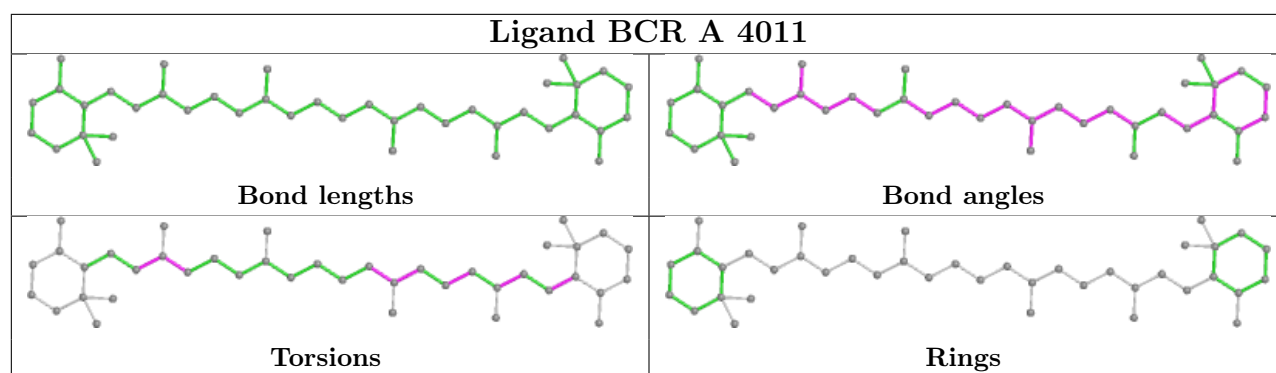
Ligand CLA d 510



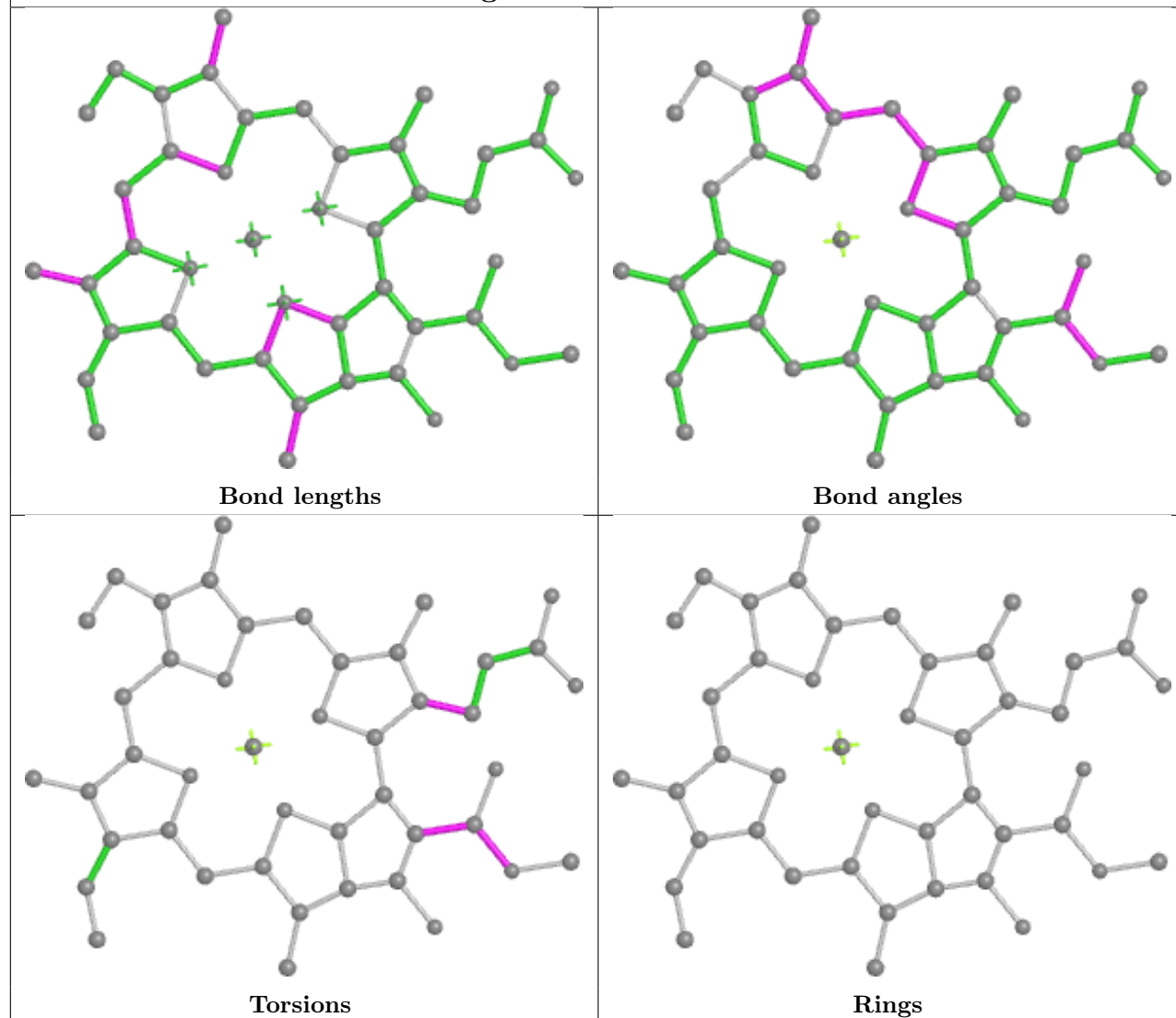




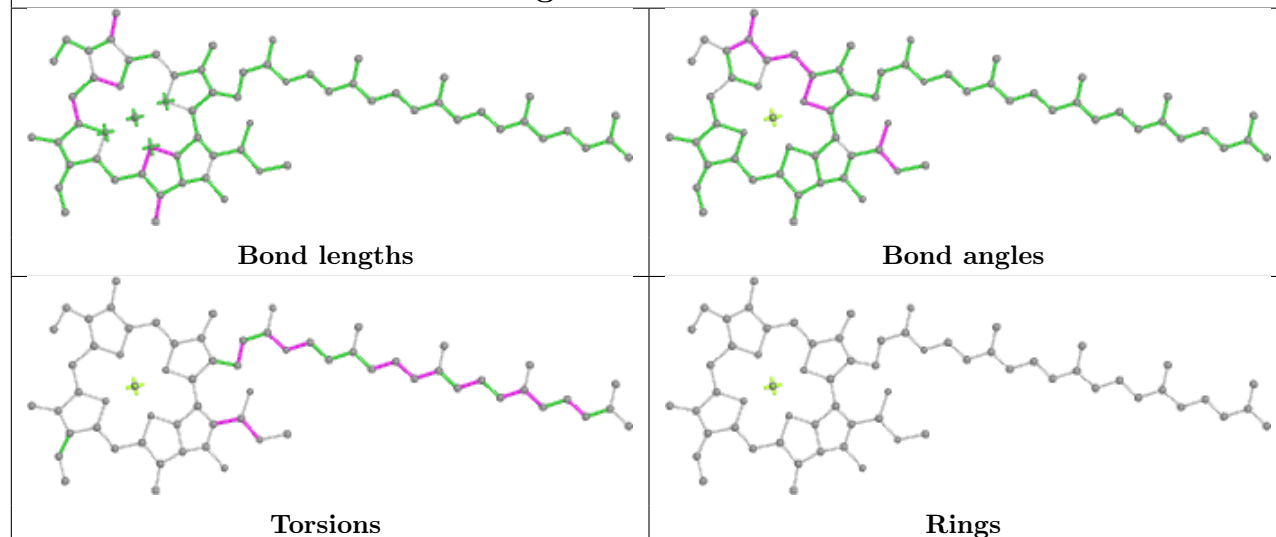


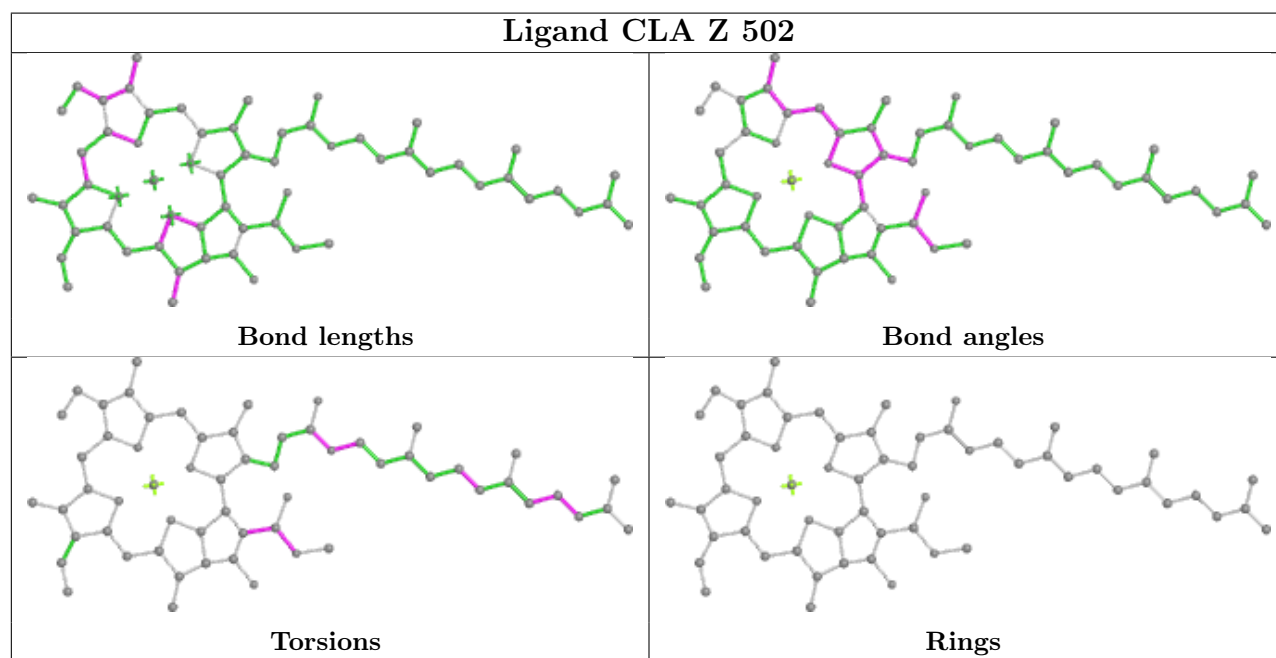
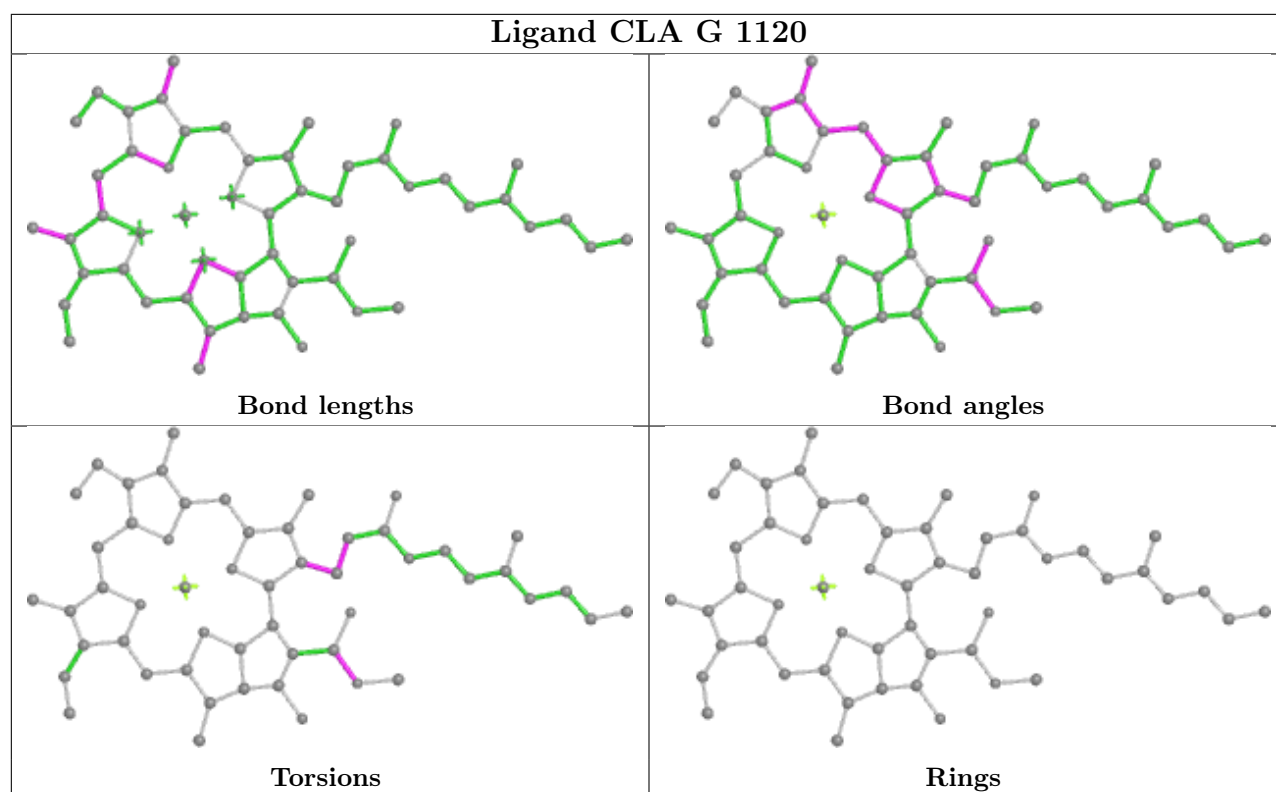


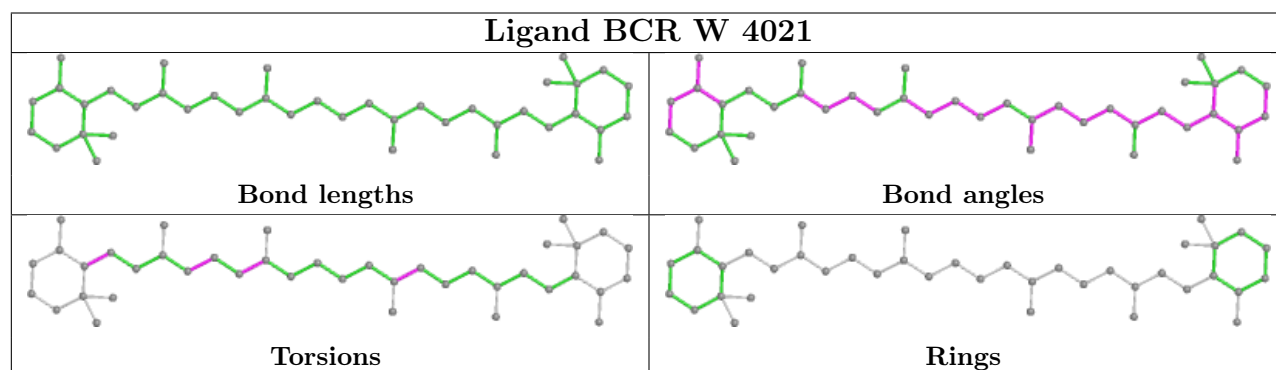
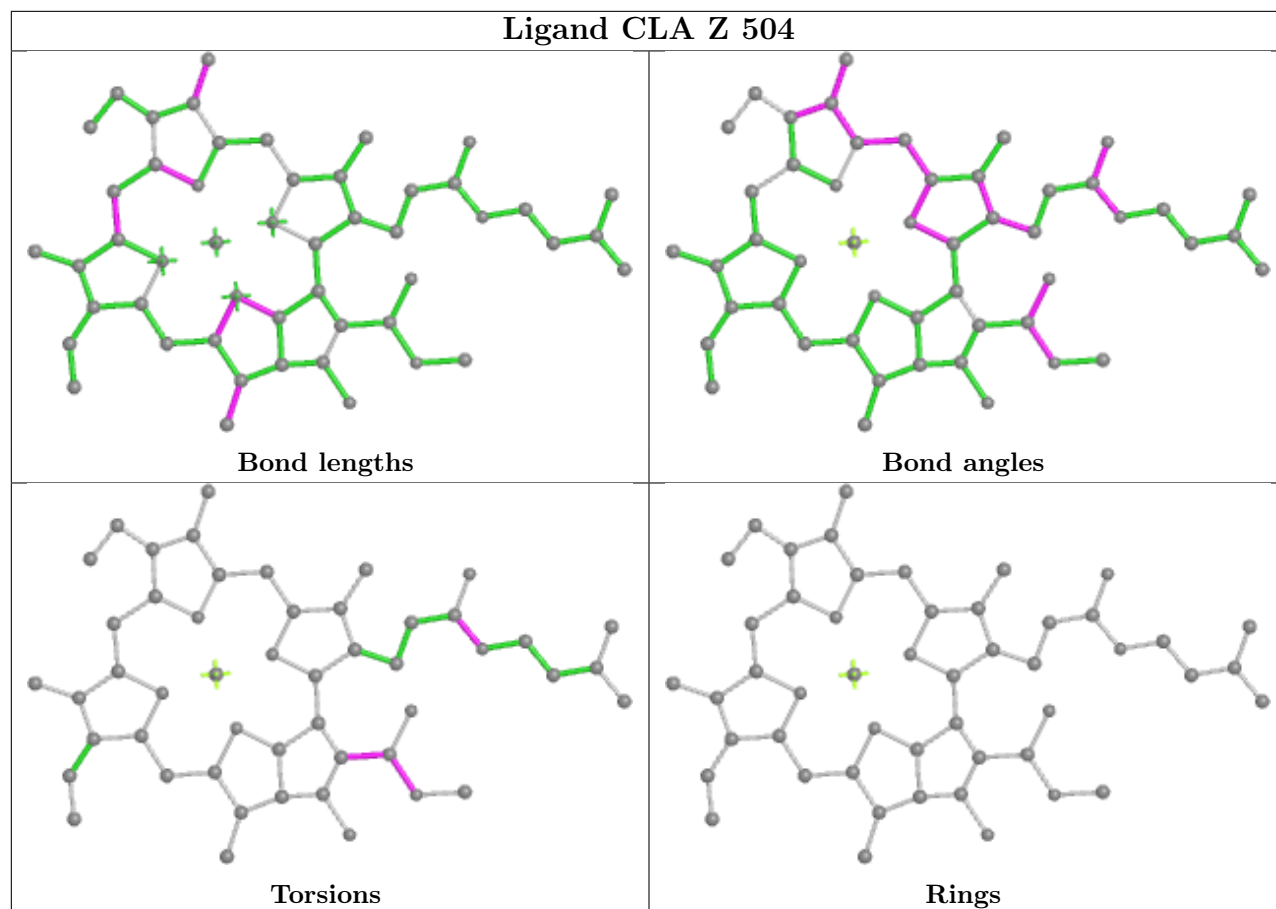
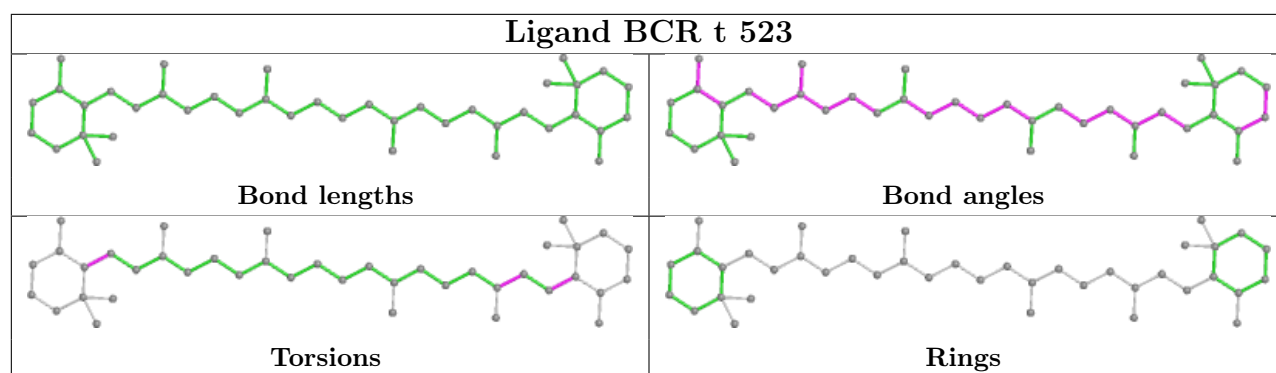
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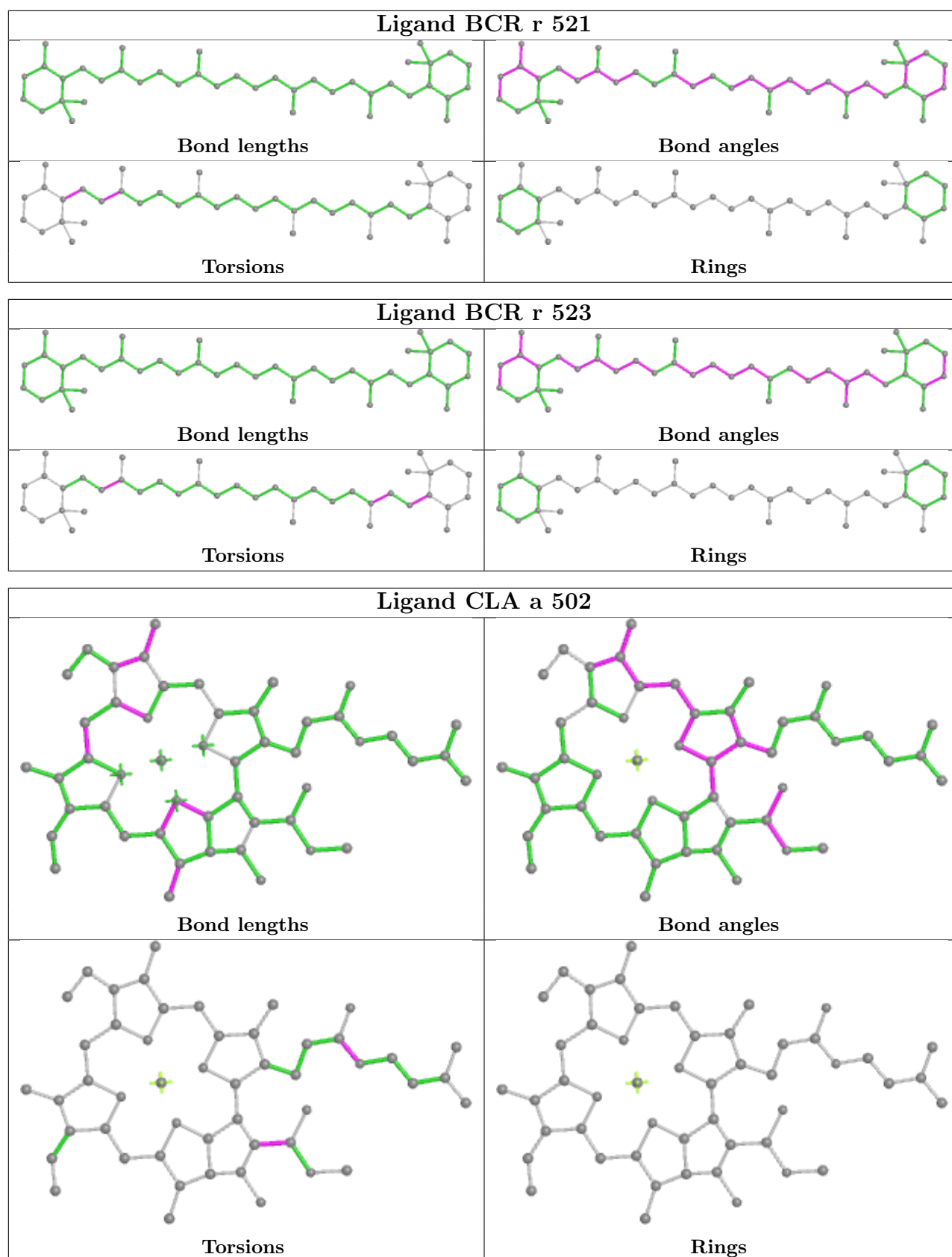


Ligand CLA 3 505

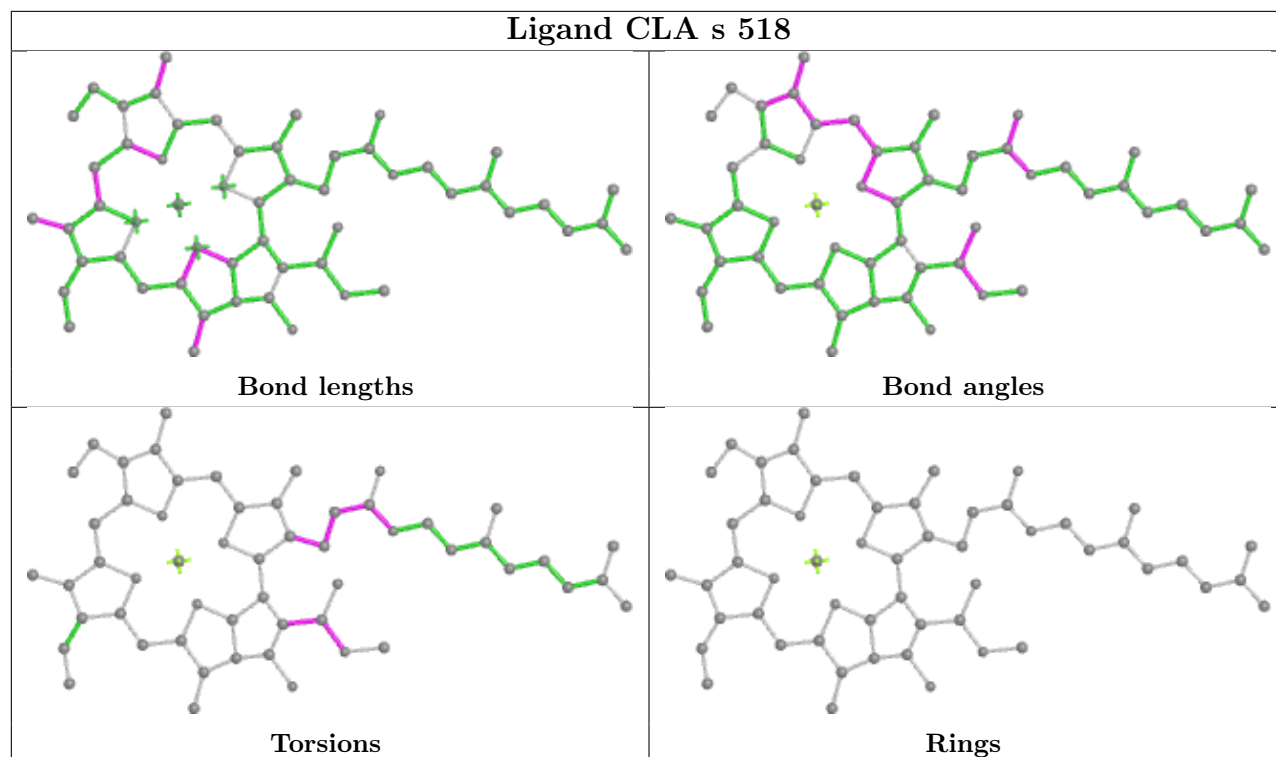




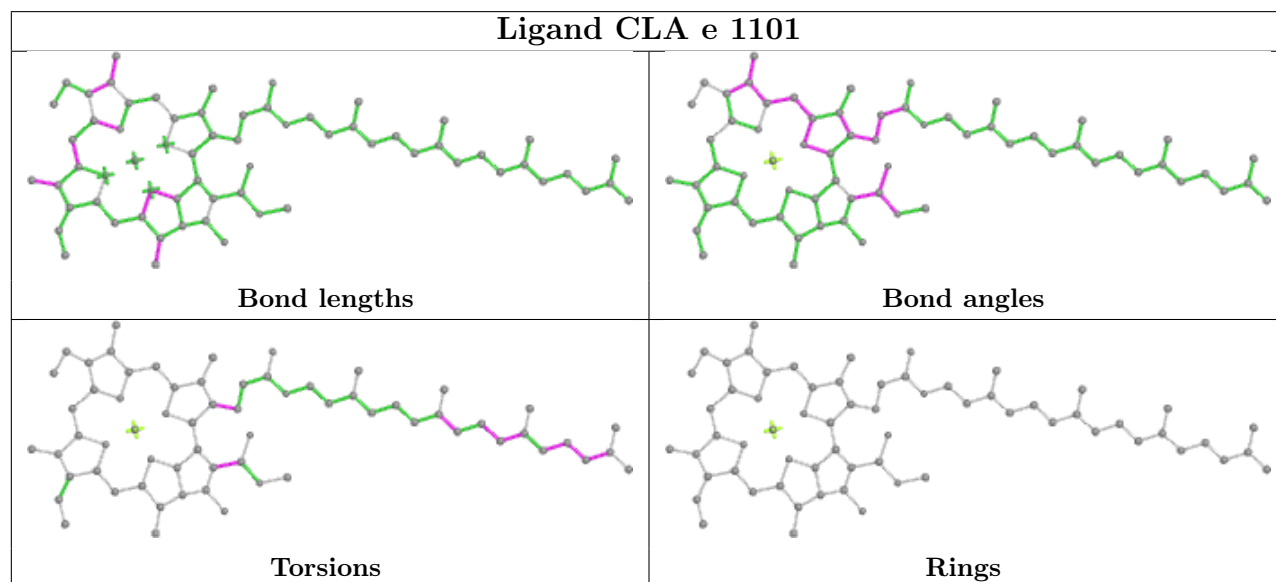




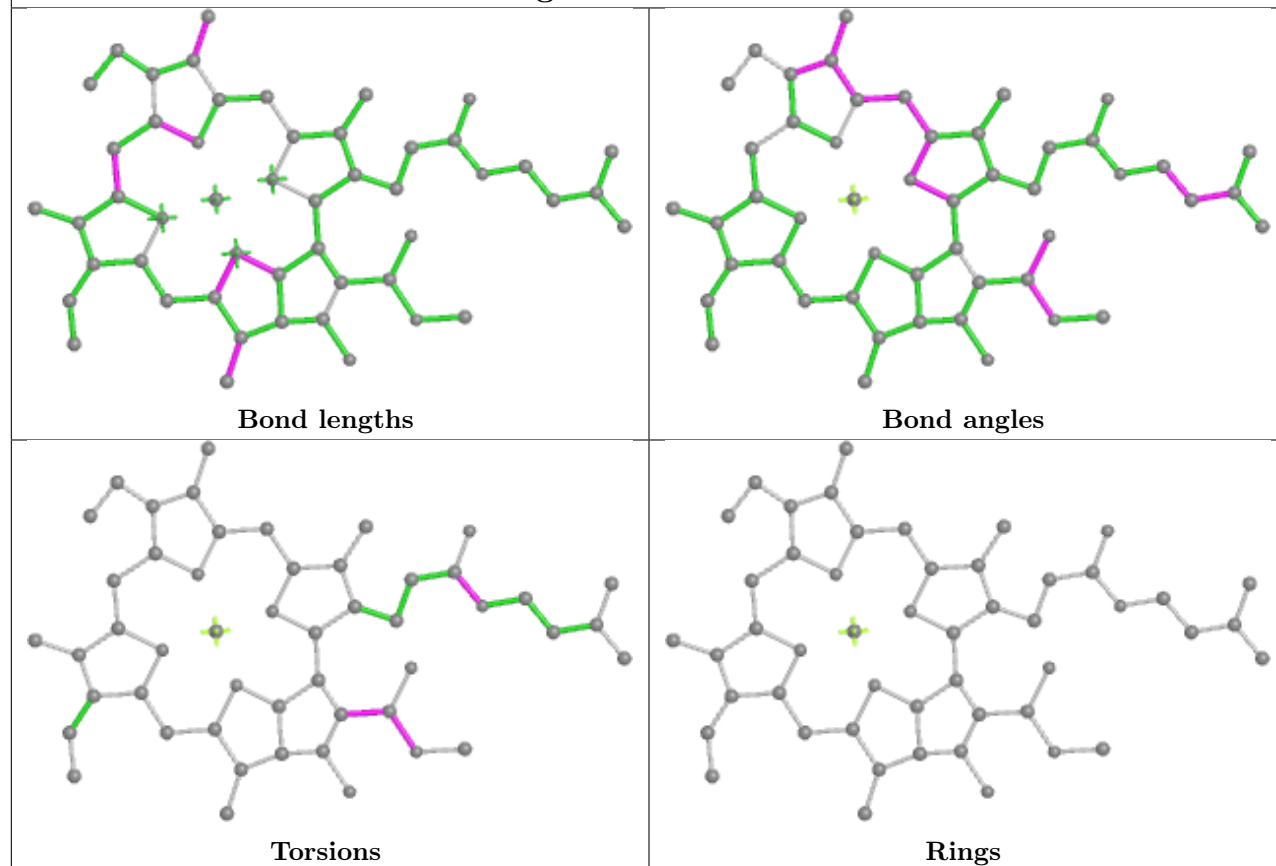
Ligand CLA s 518



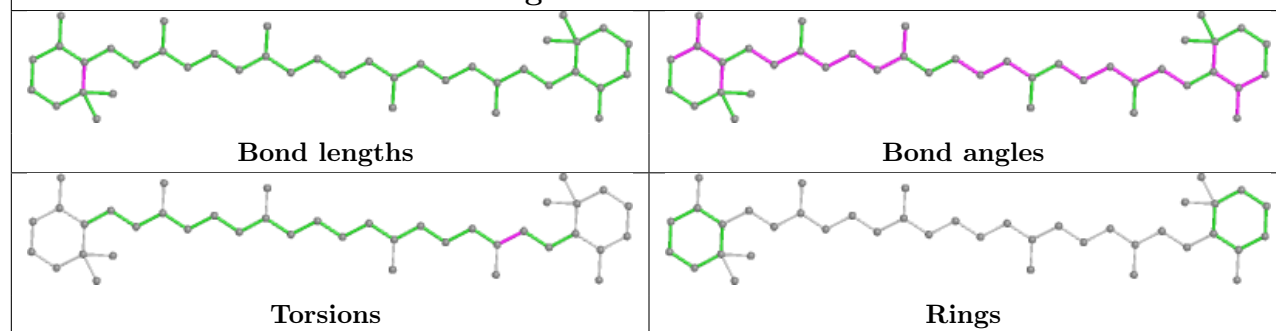
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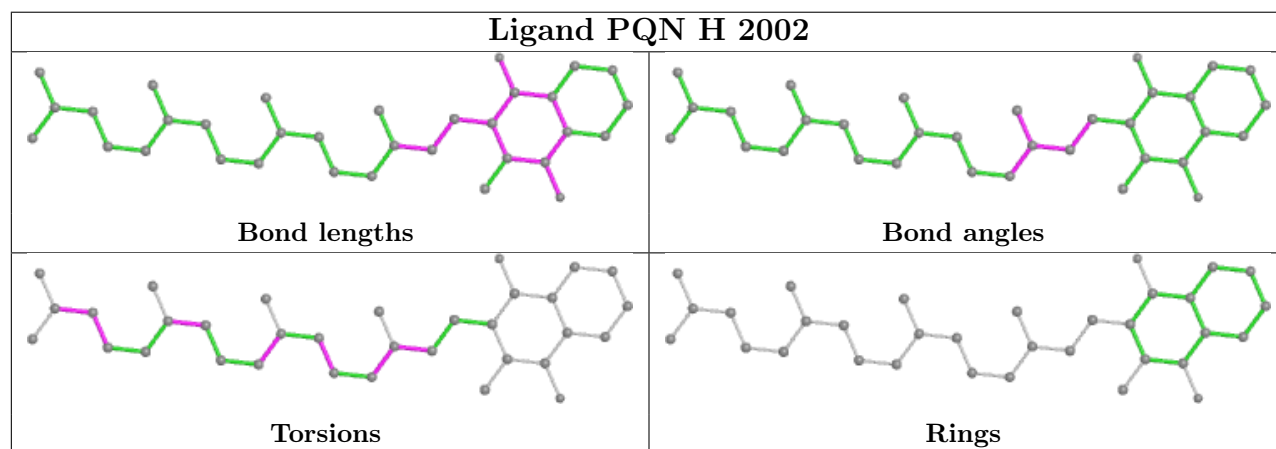
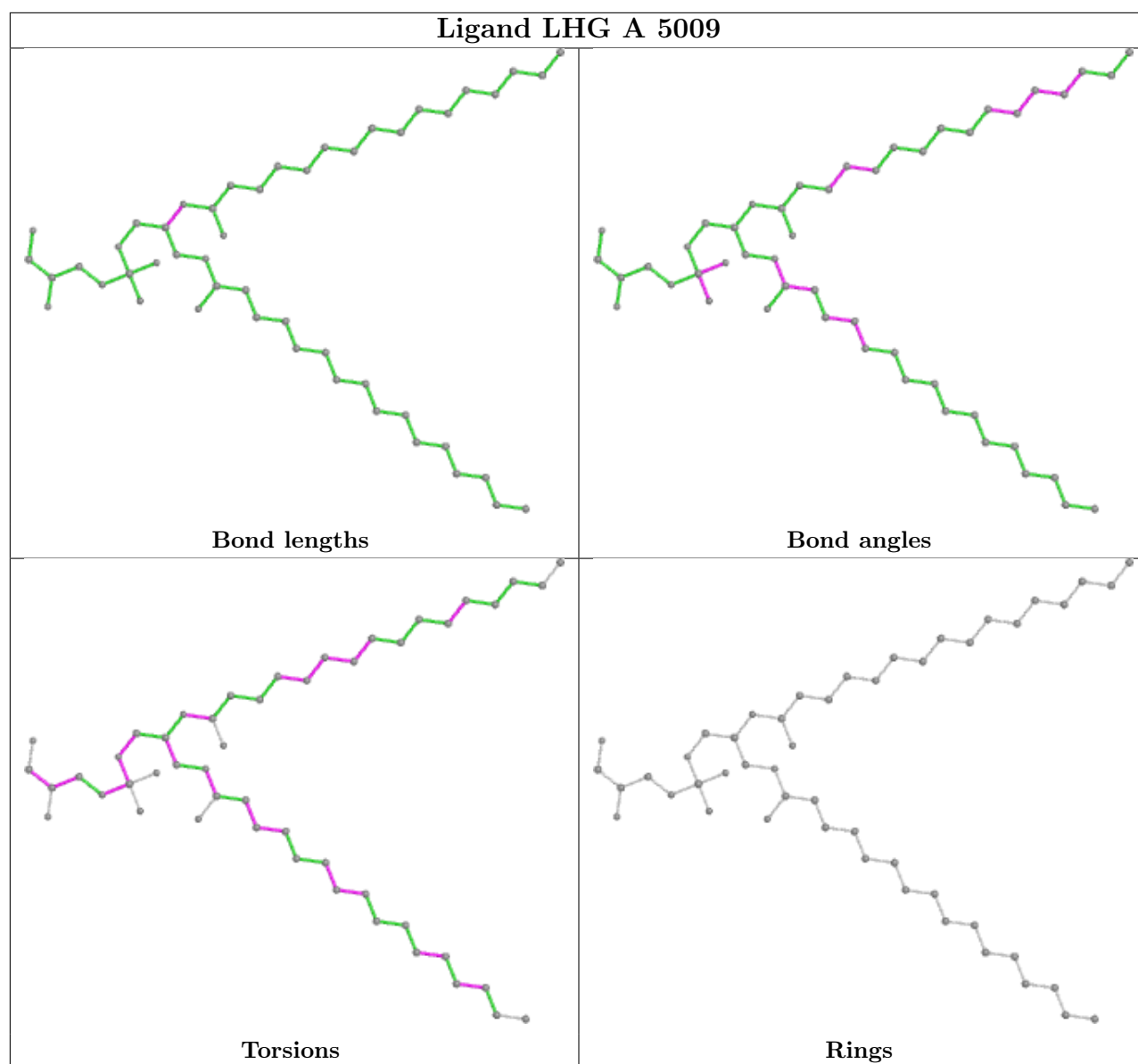


Ligand CLA 6 502

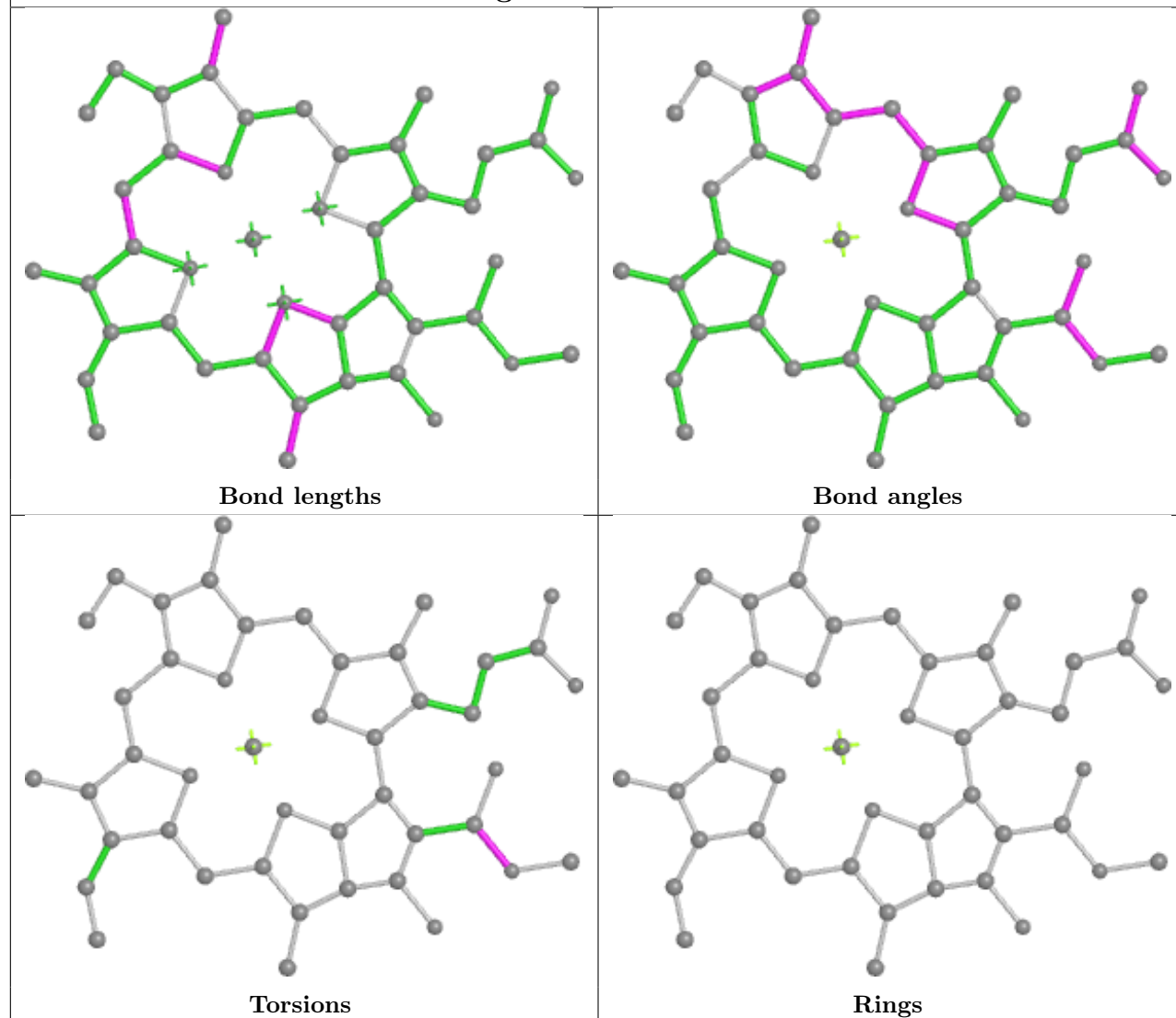


Ligand BCR k 4018

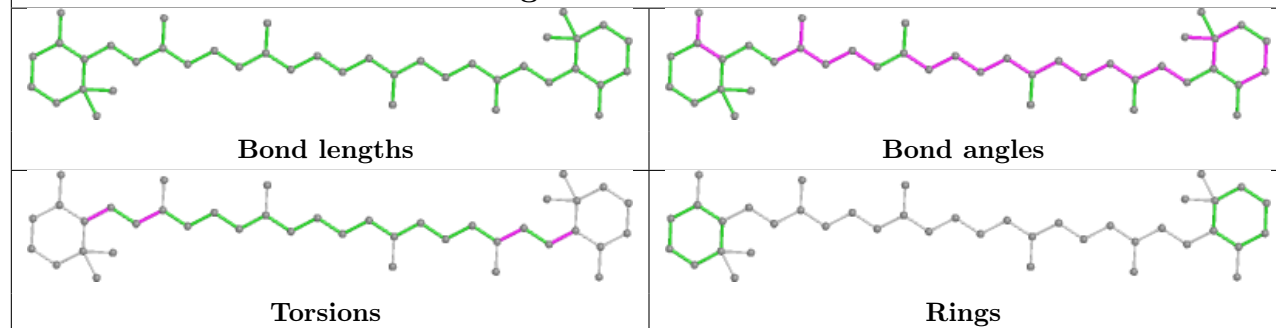


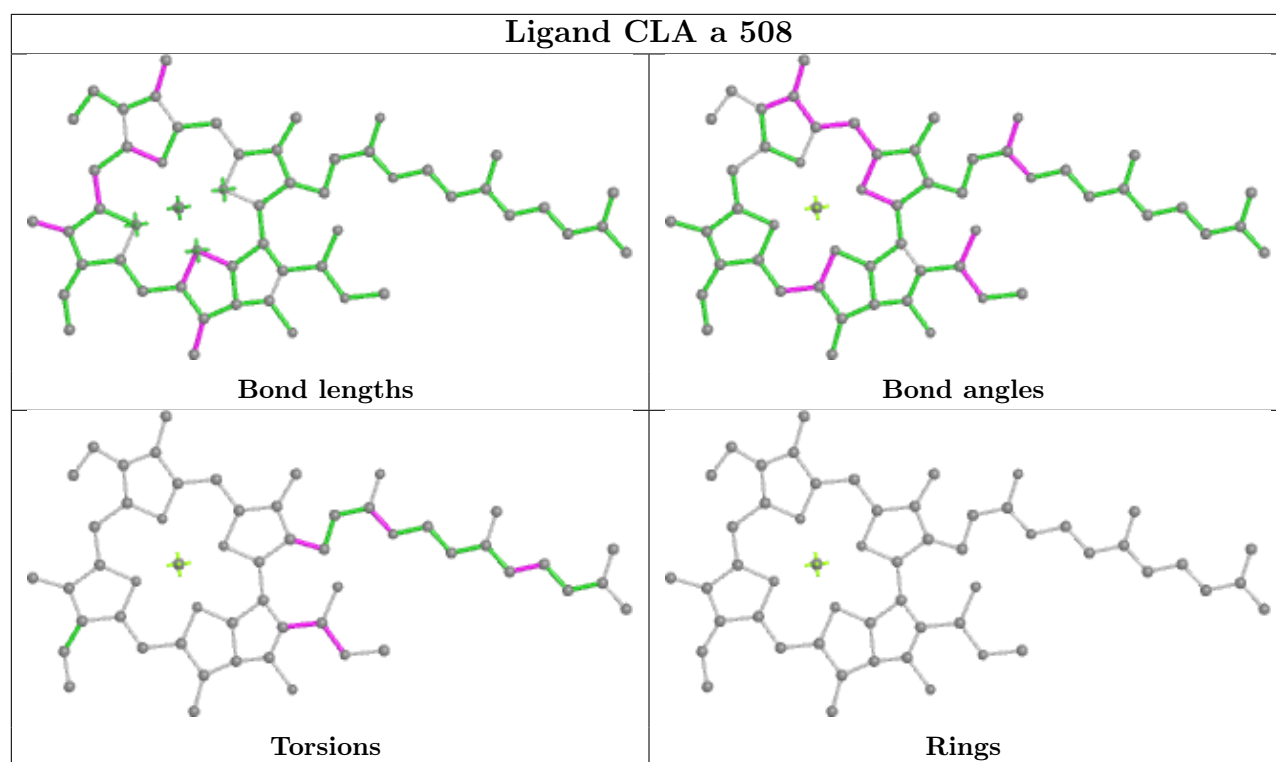


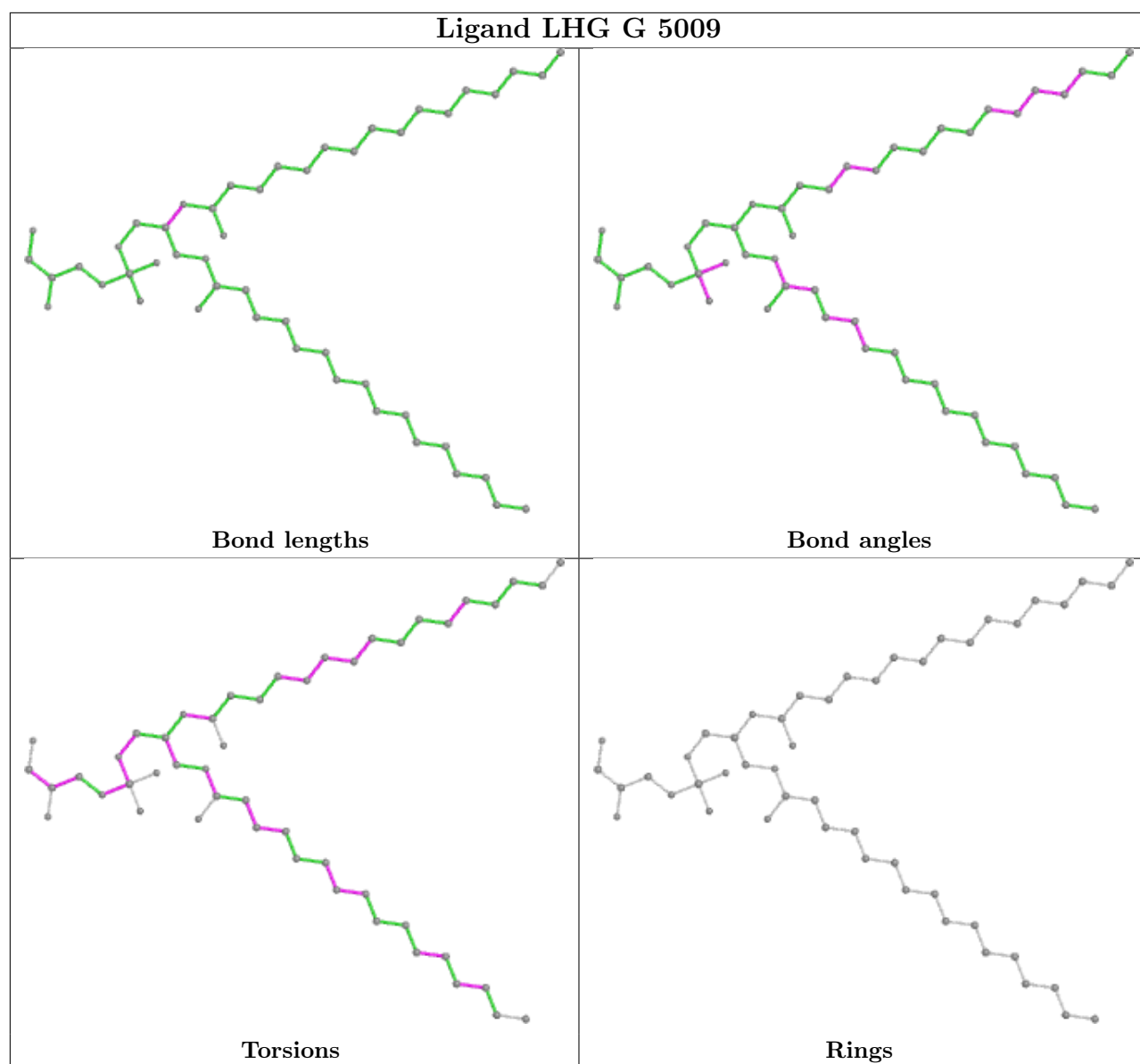
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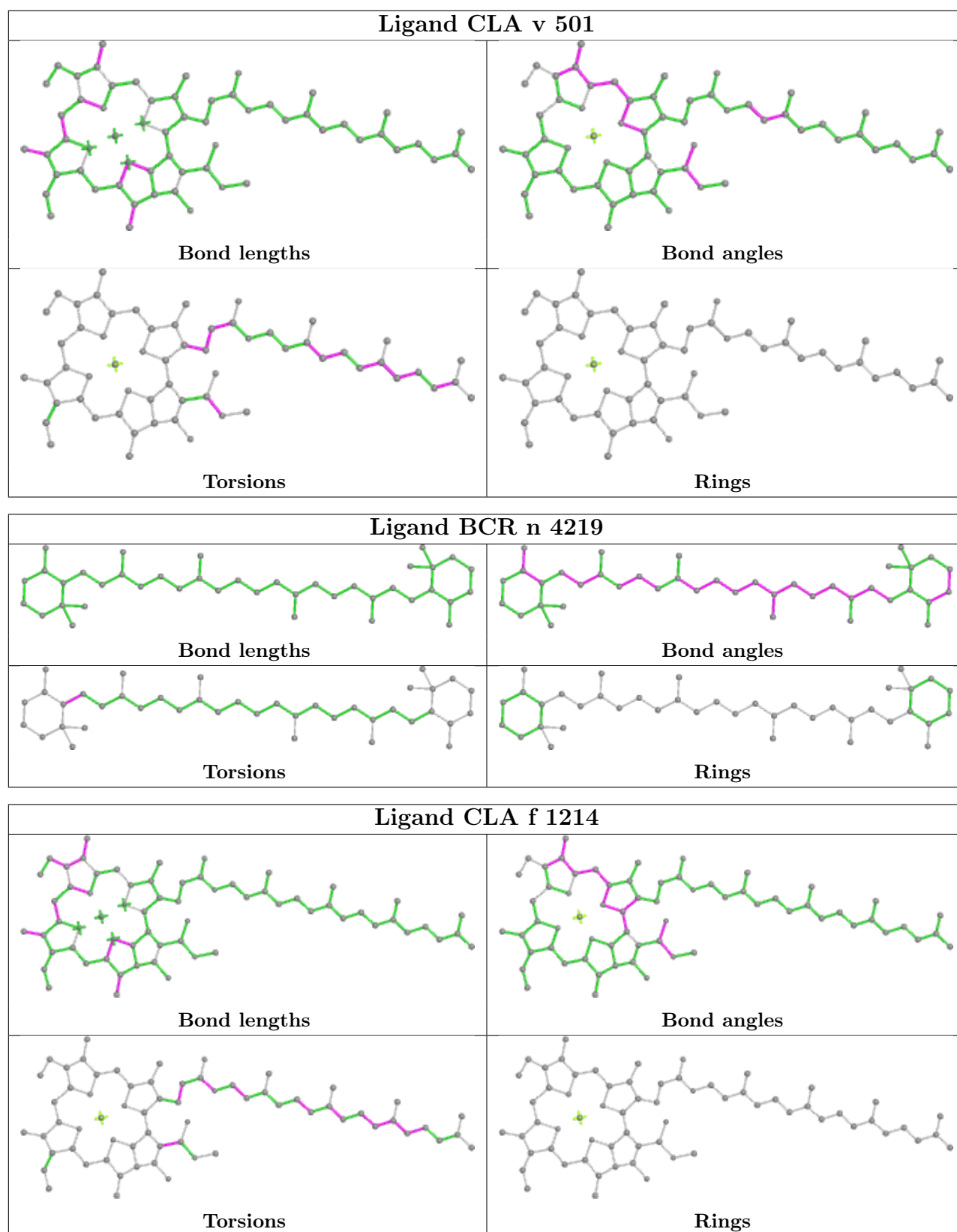


Ligand BCR H 4004

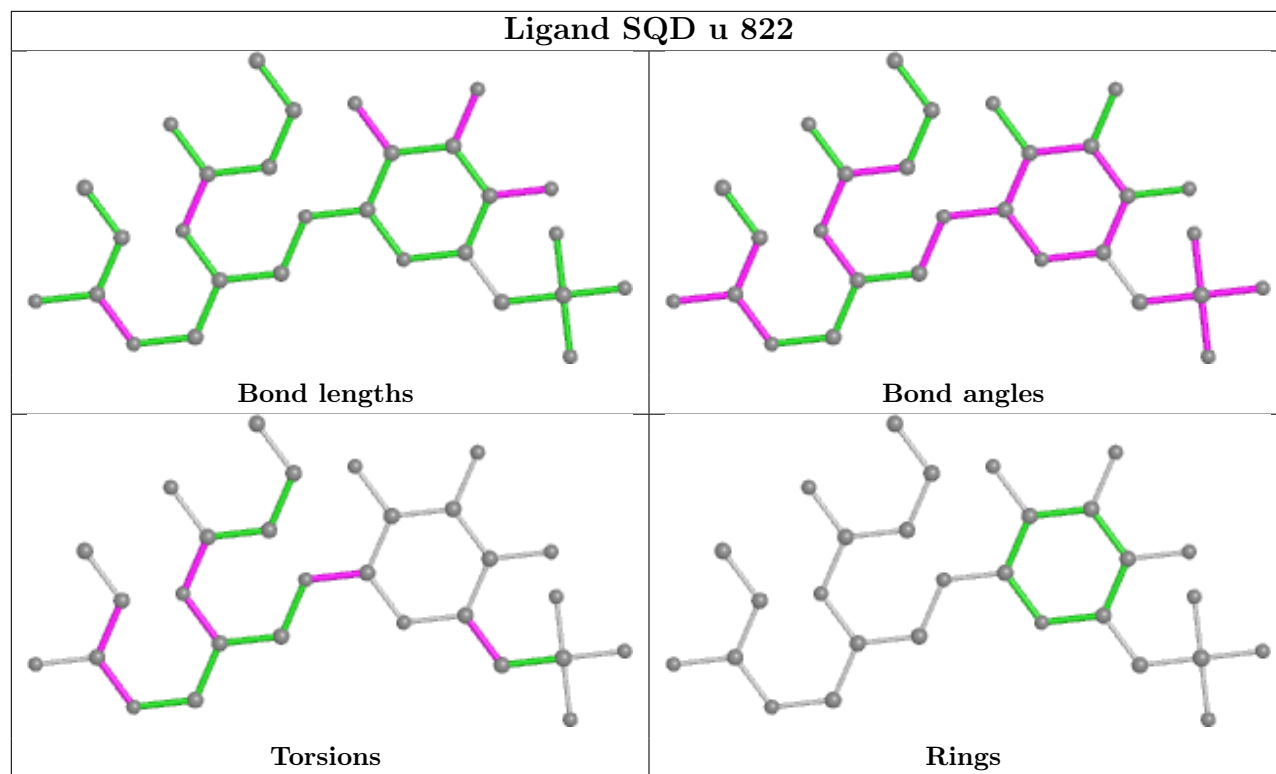




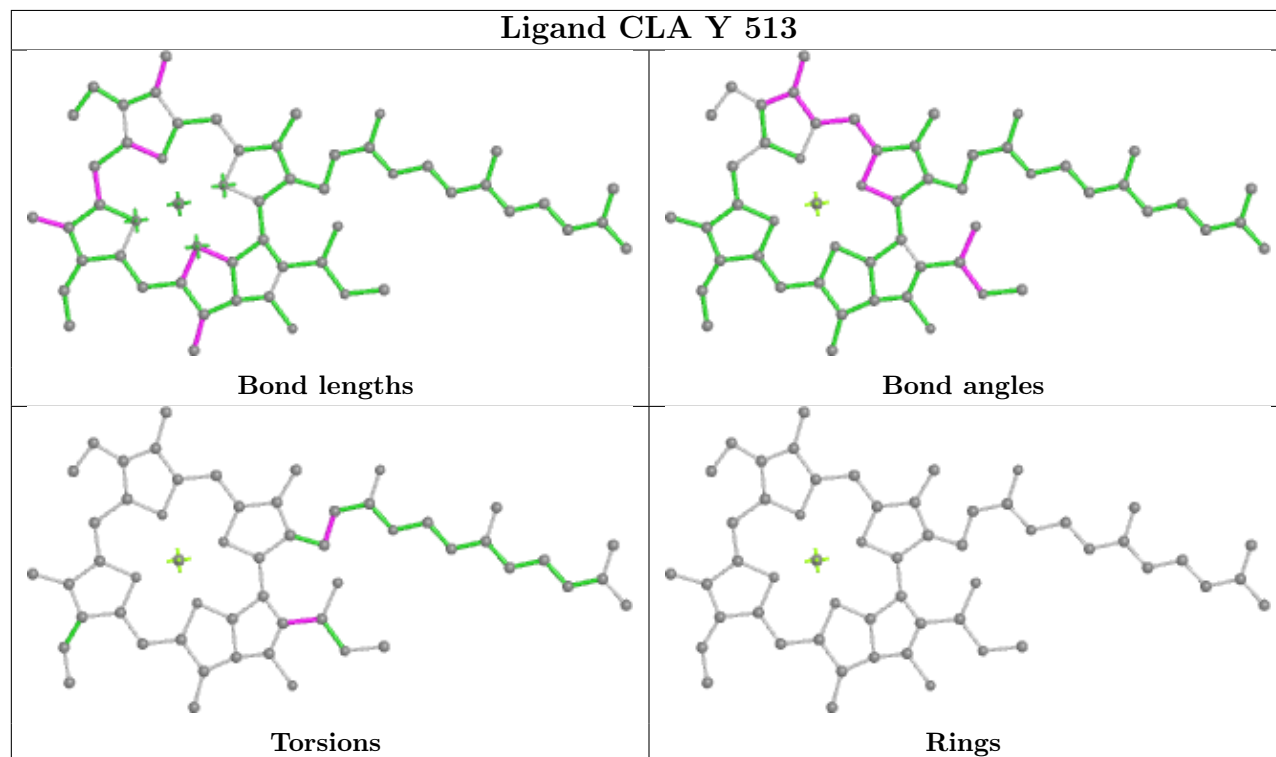


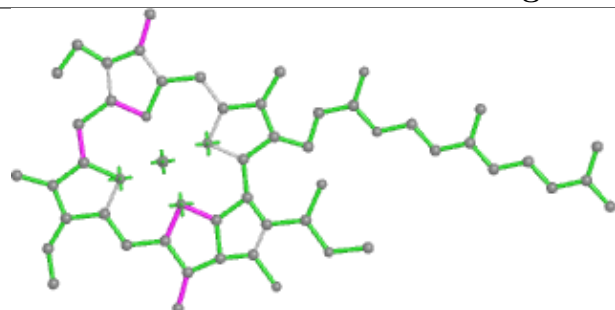
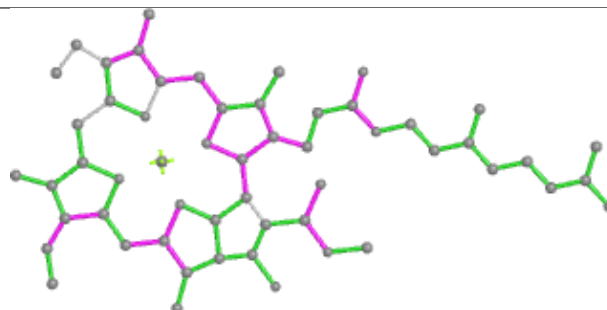
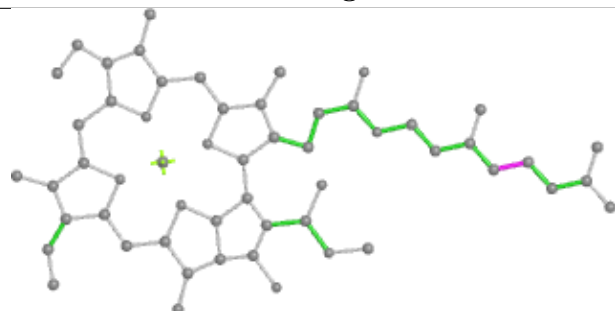
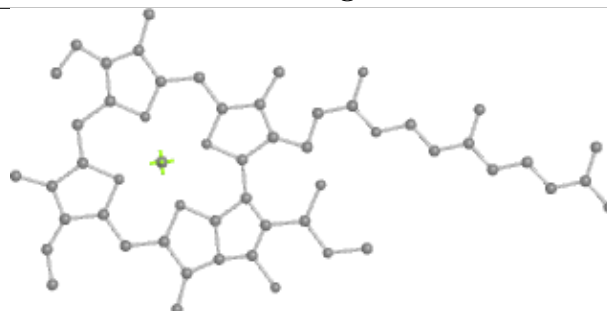
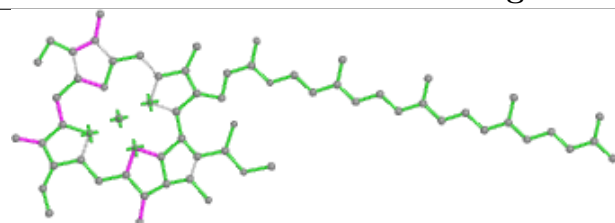
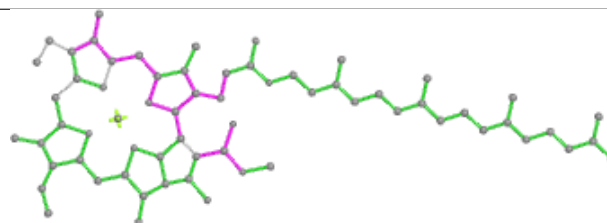
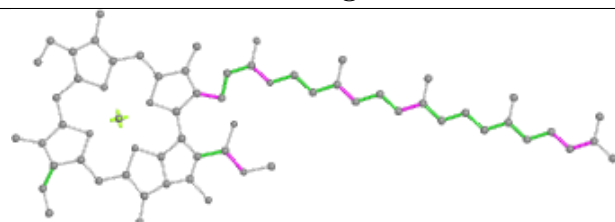
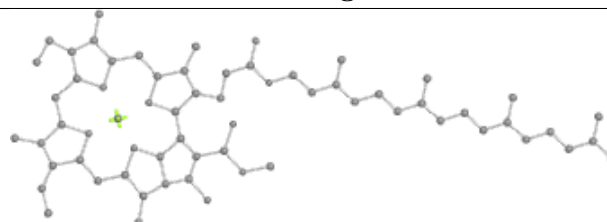


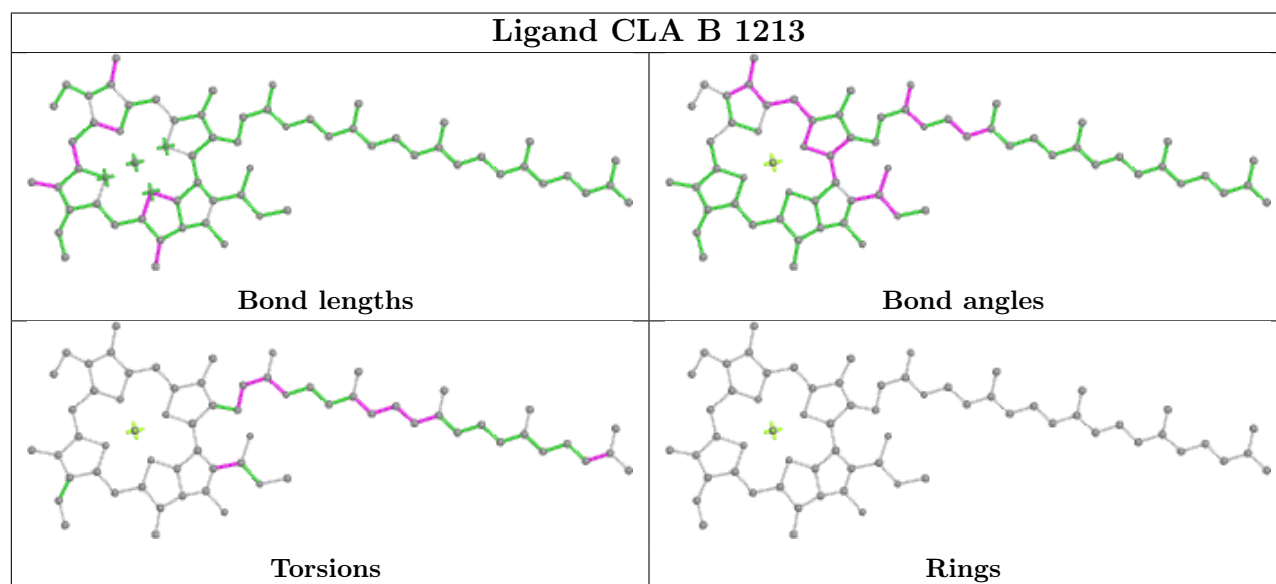
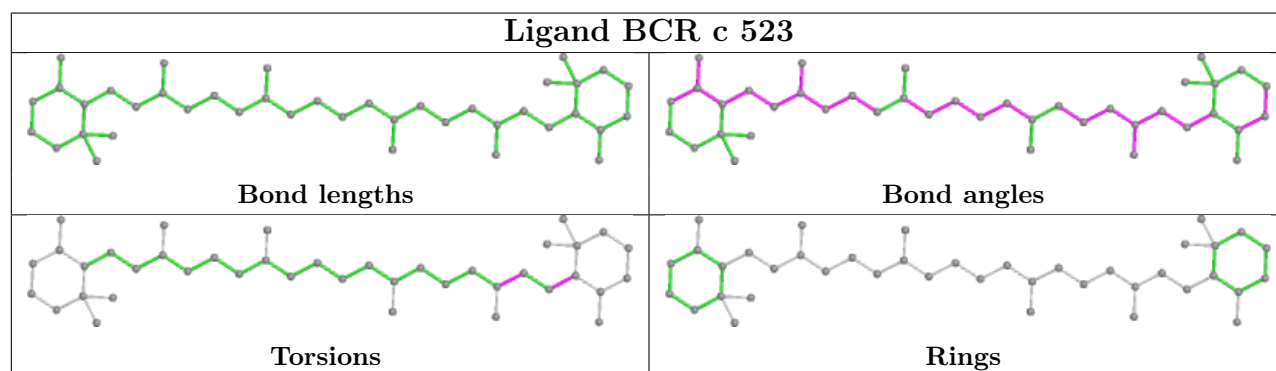
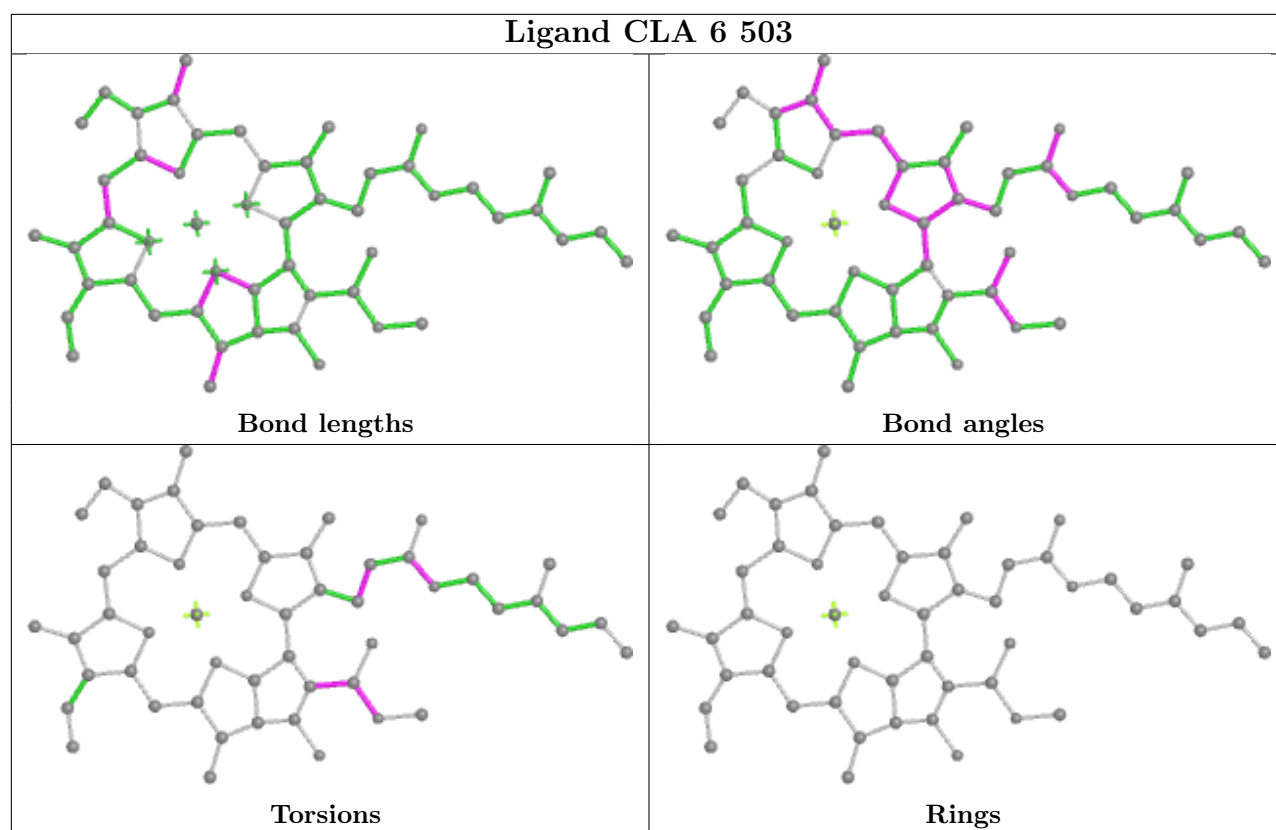
Ligand SQD u 822

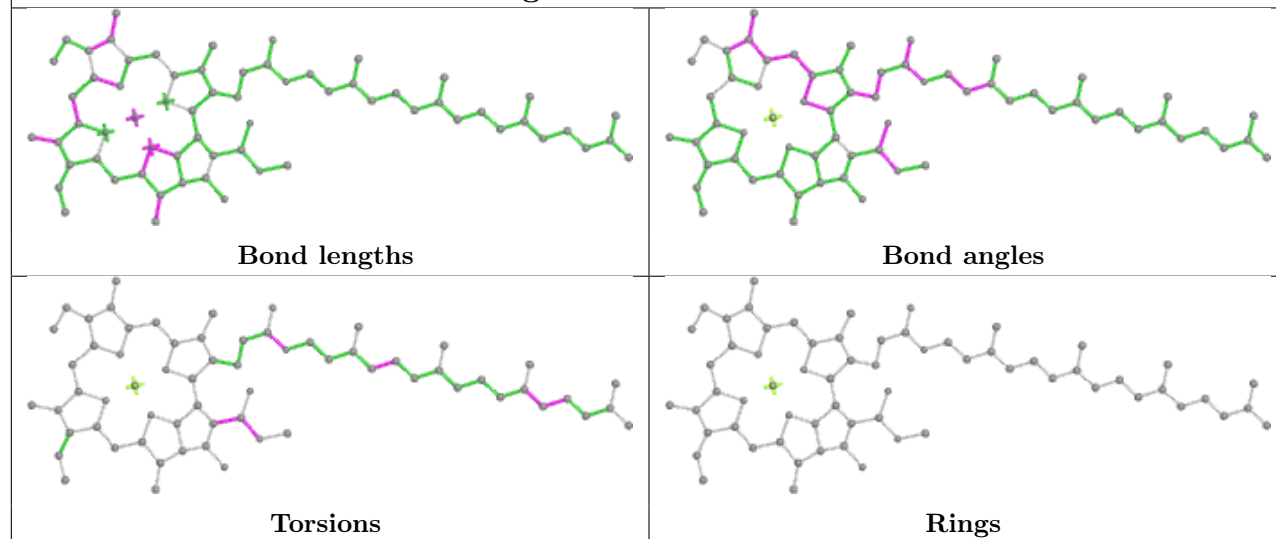
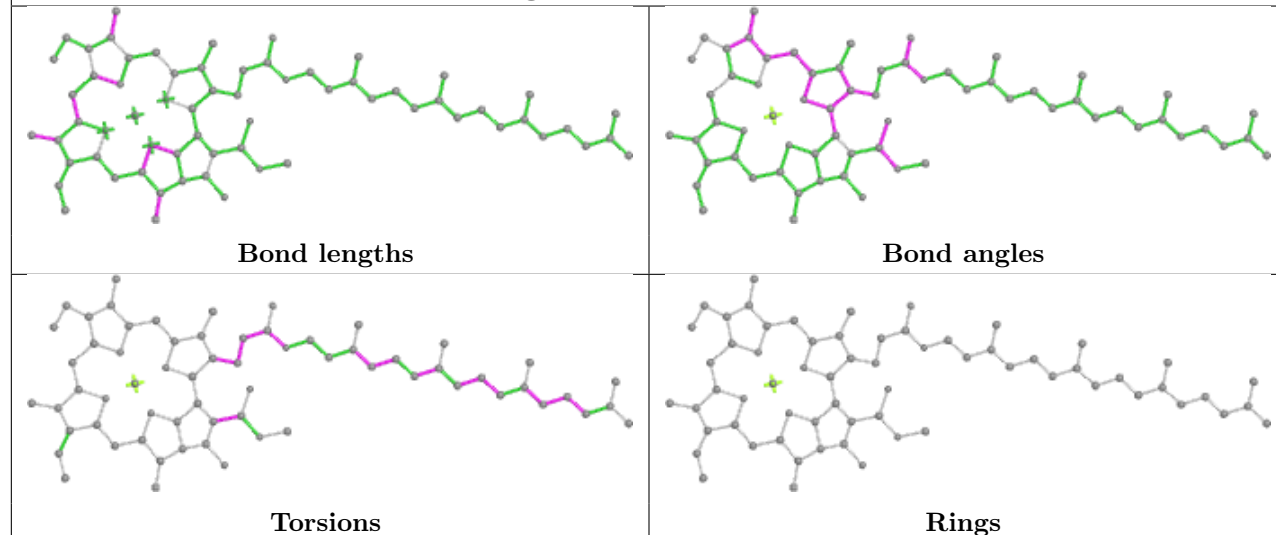
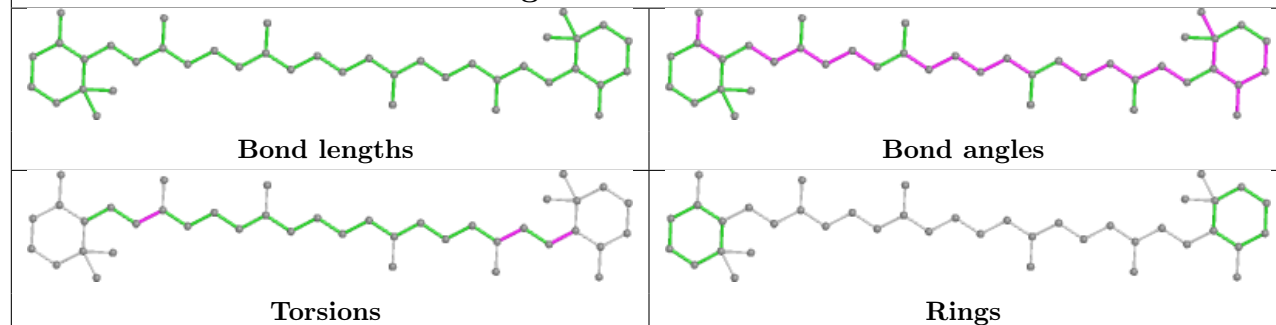


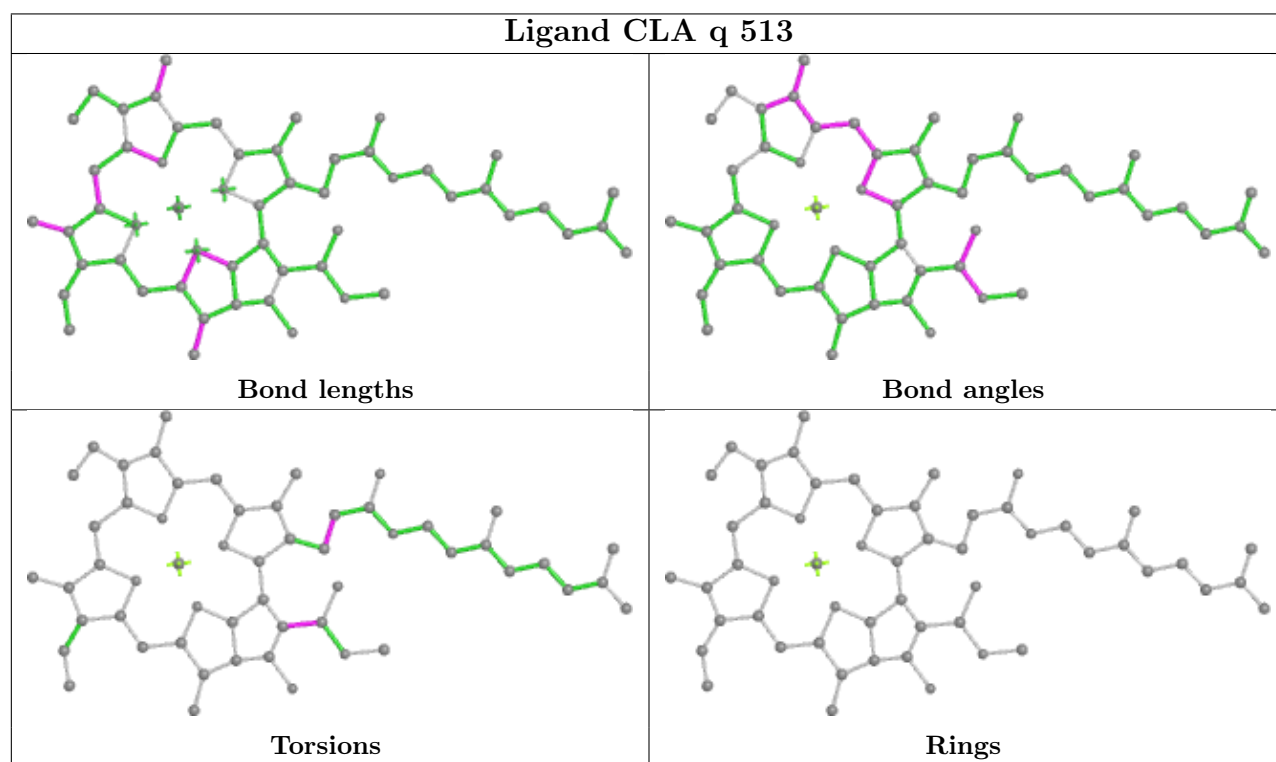
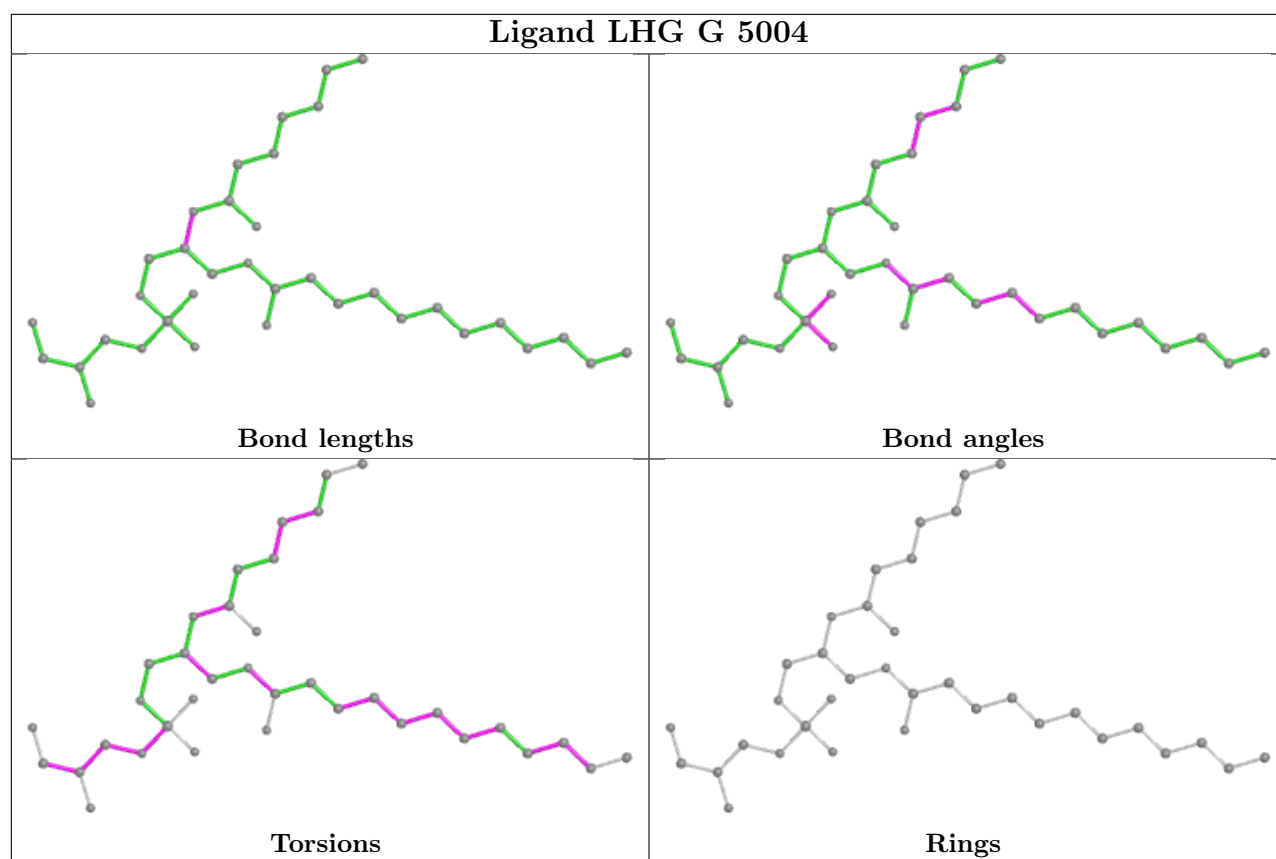
Ligand CLA Y 513

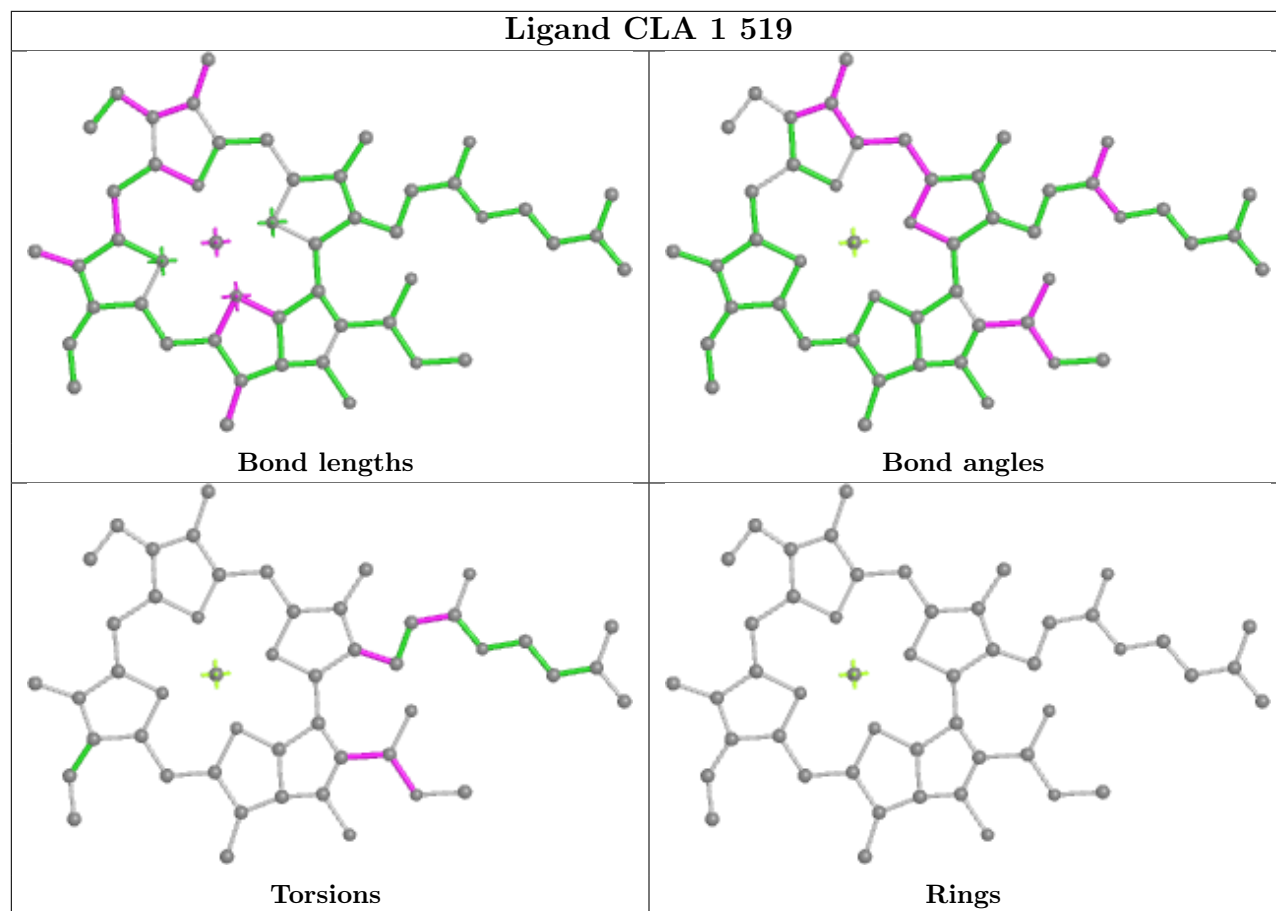
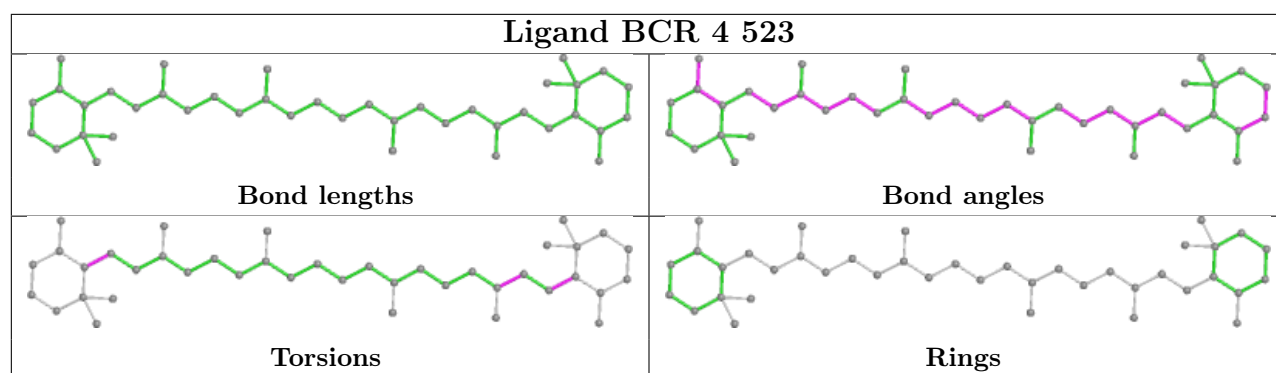


Ligand CLA t 503**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 1140****Bond lengths****Bond angles****Torsions****Rings**

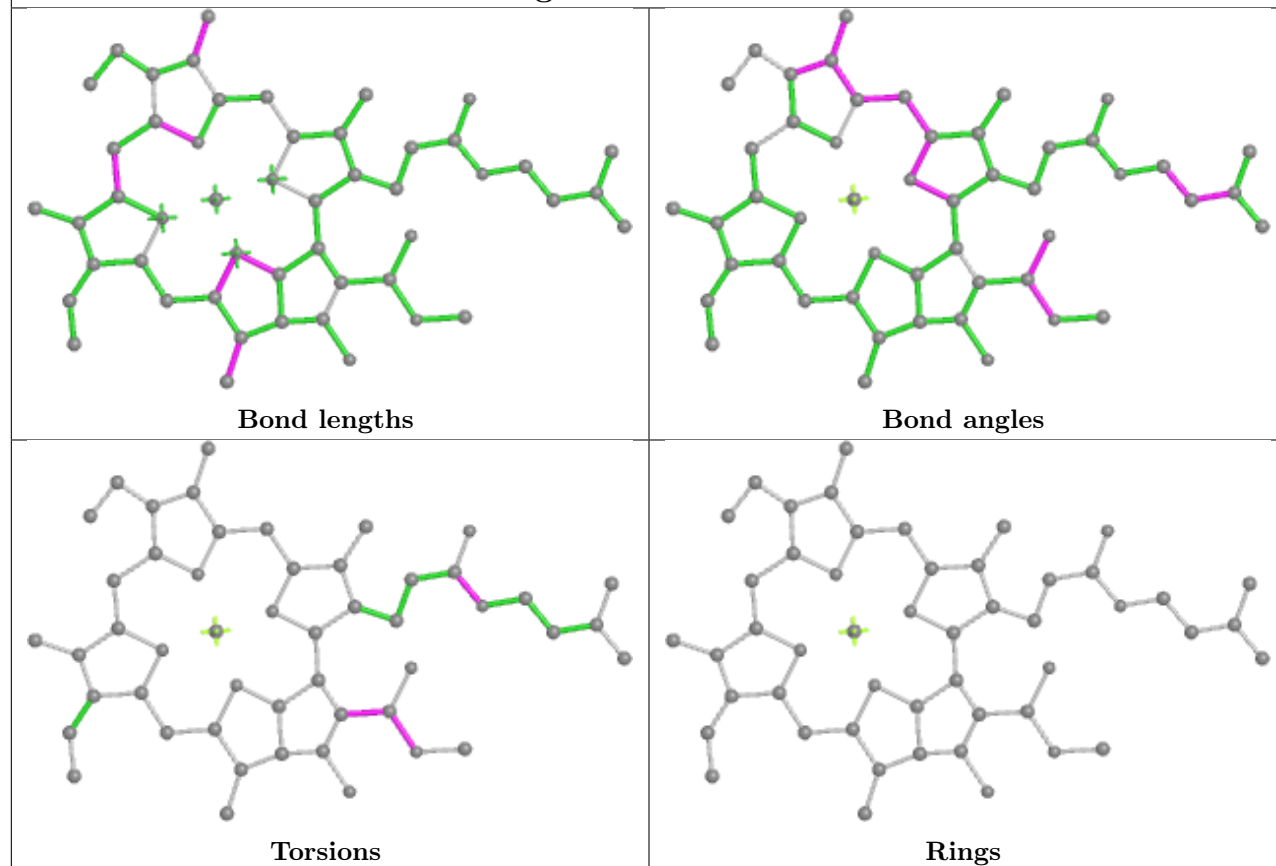


Ligand CLA H 1205**Ligand CLA V 1501****Ligand BCR V 4019**

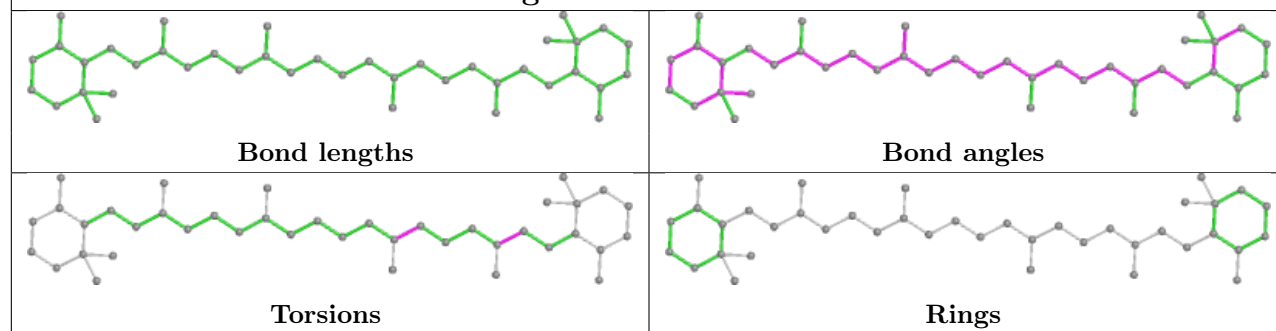




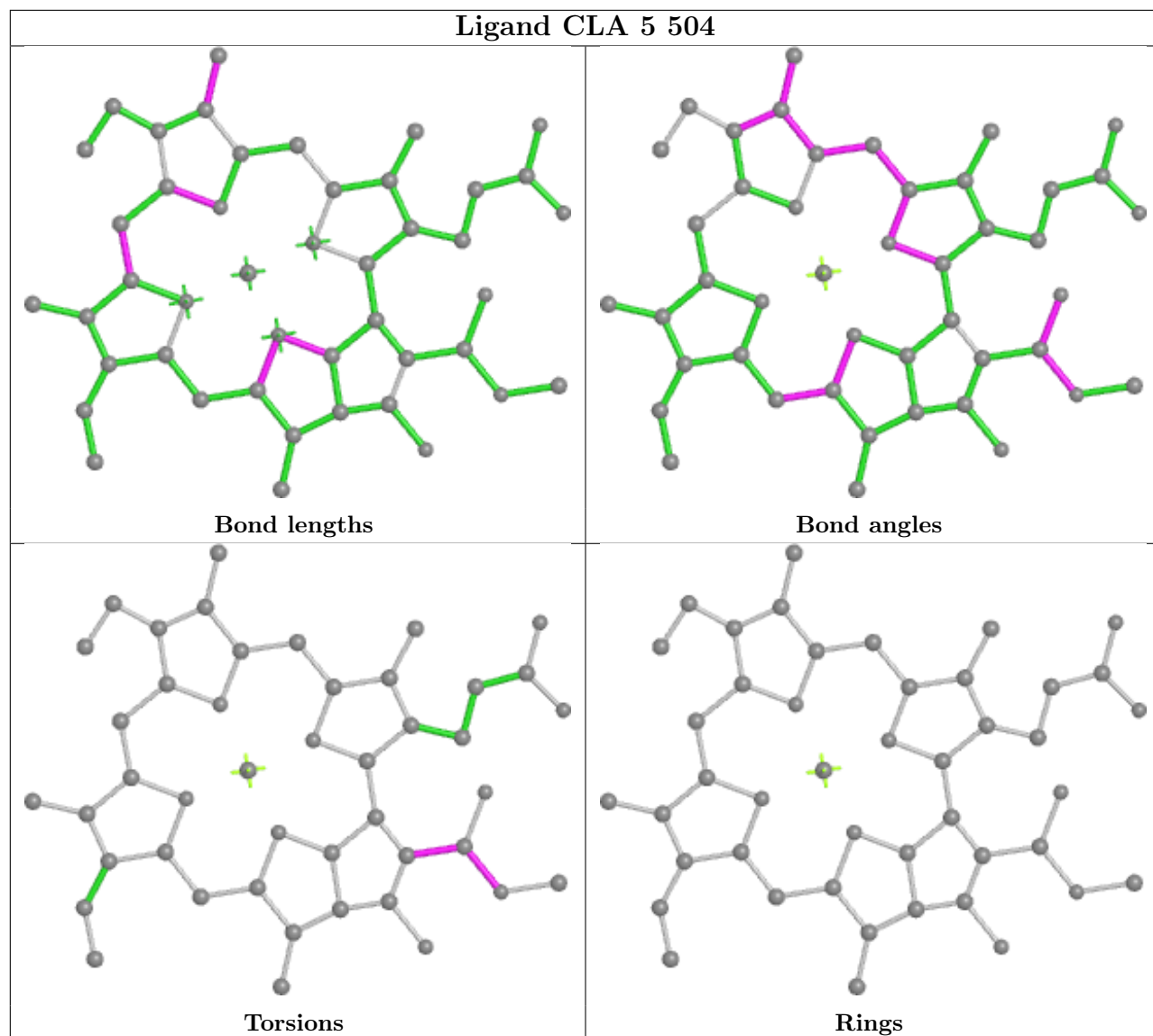
Ligand CLA d 502



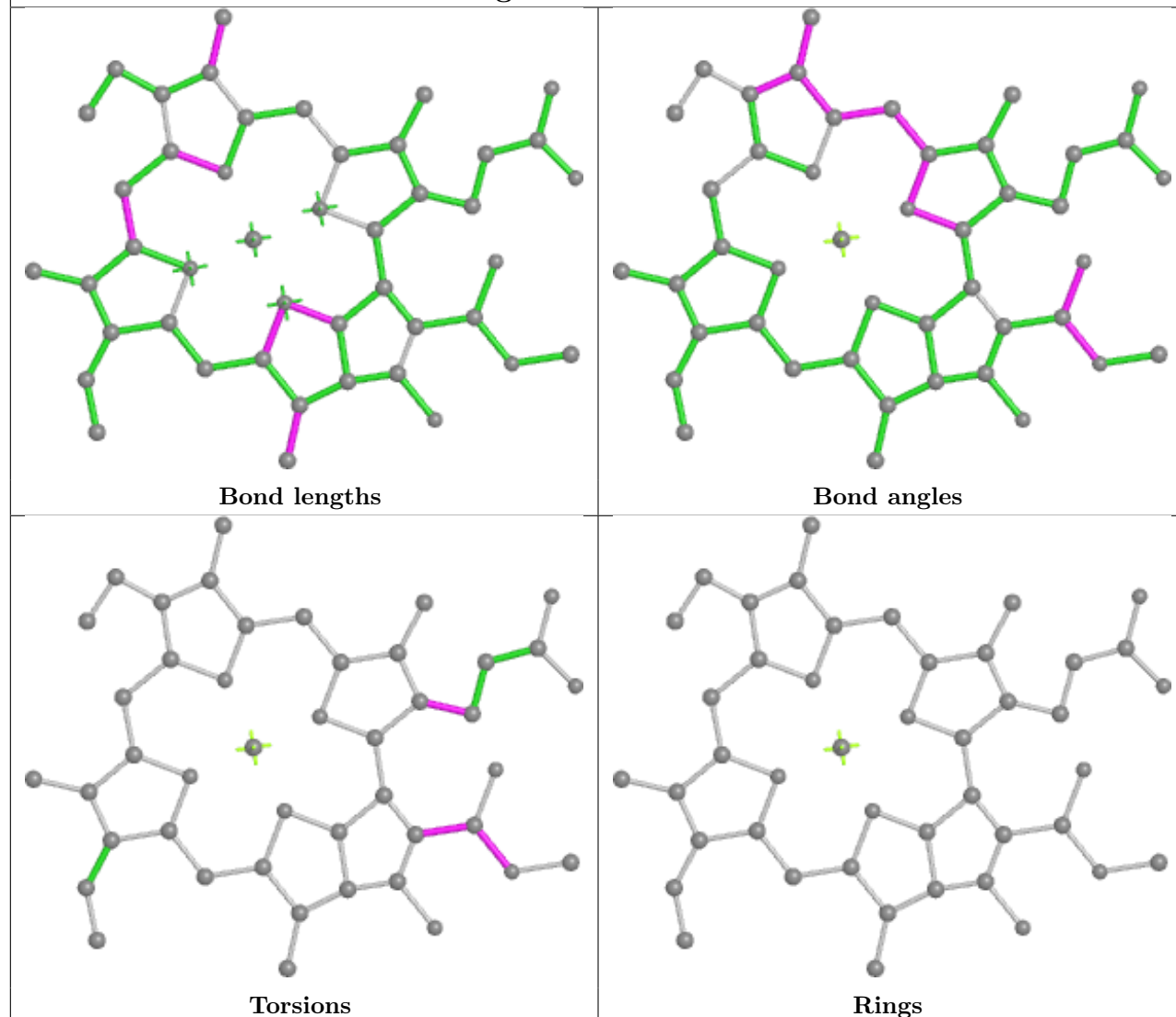
Ligand BCR T 4013



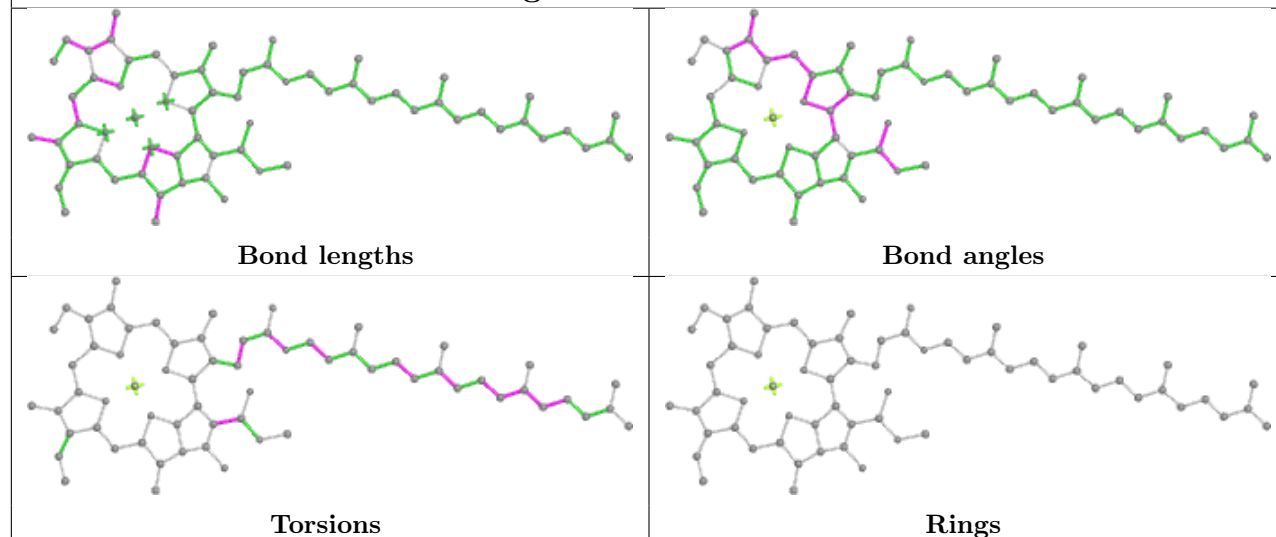
Ligand CLA 5 504

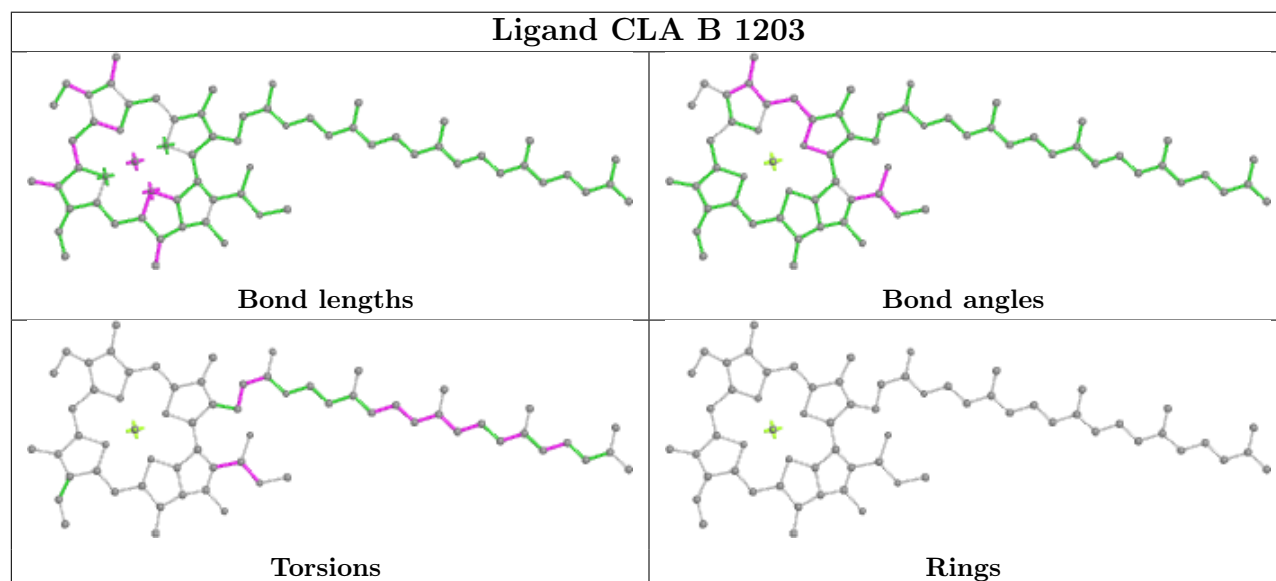
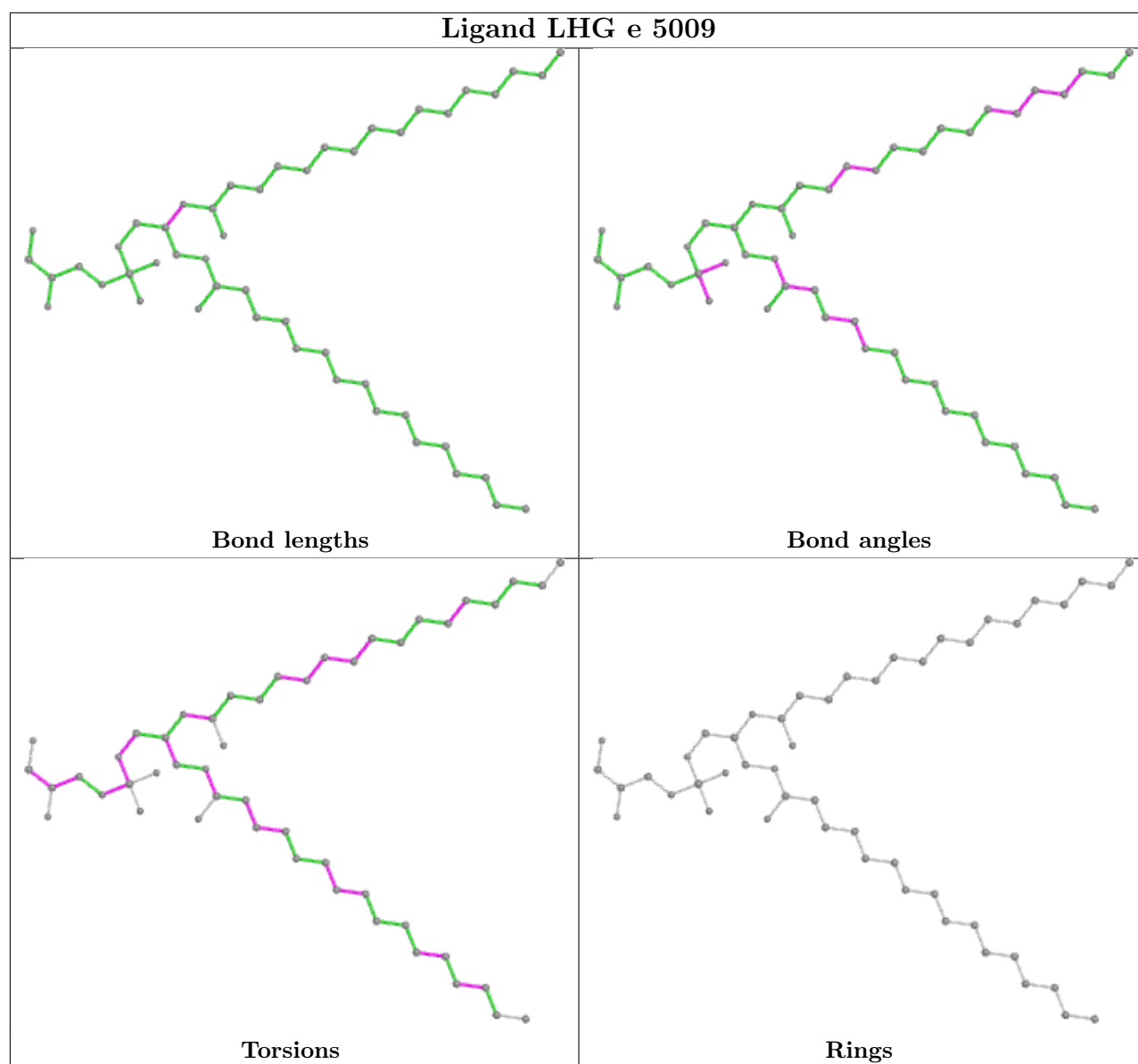


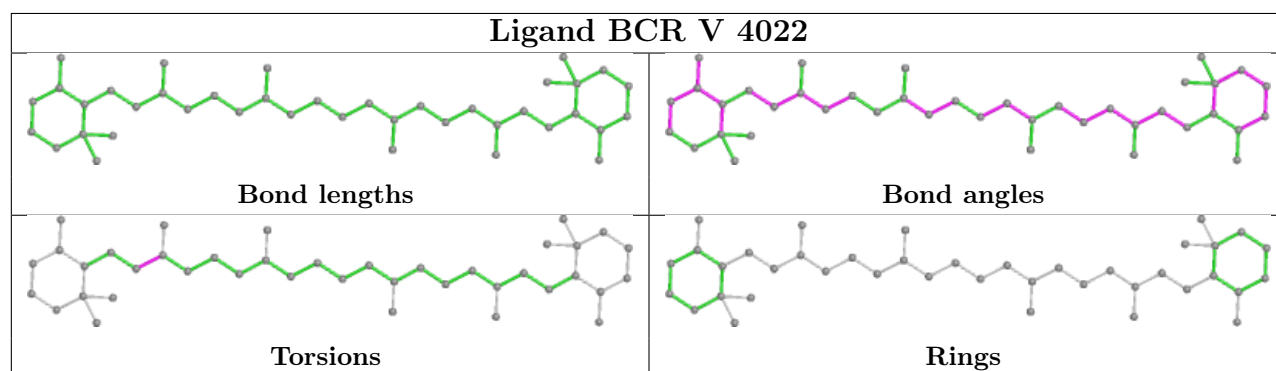
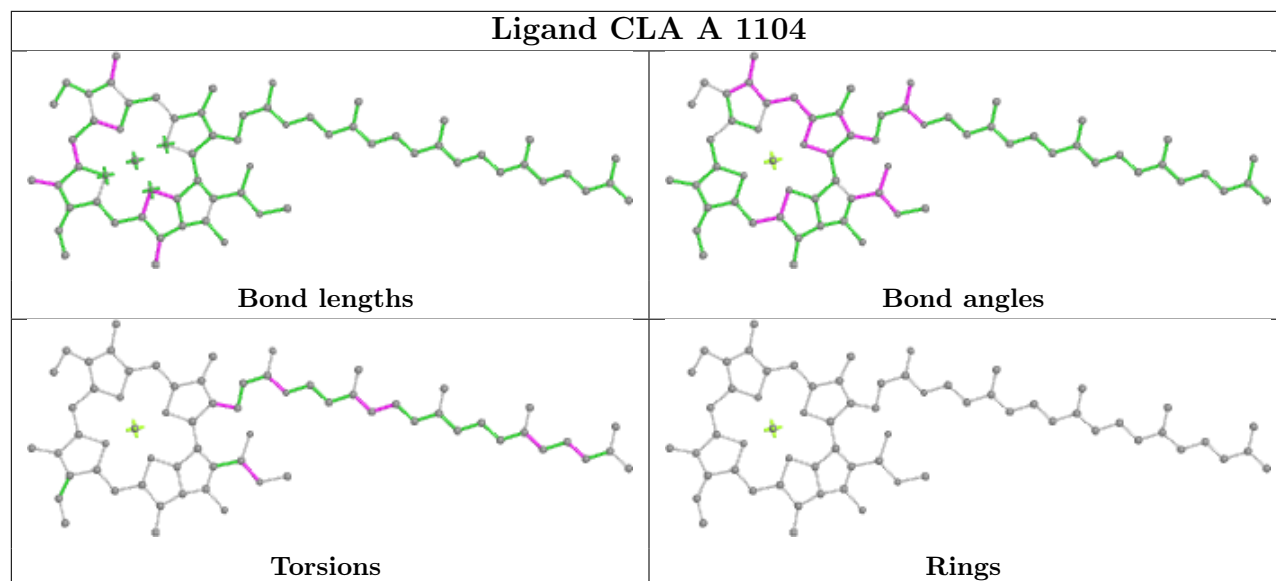
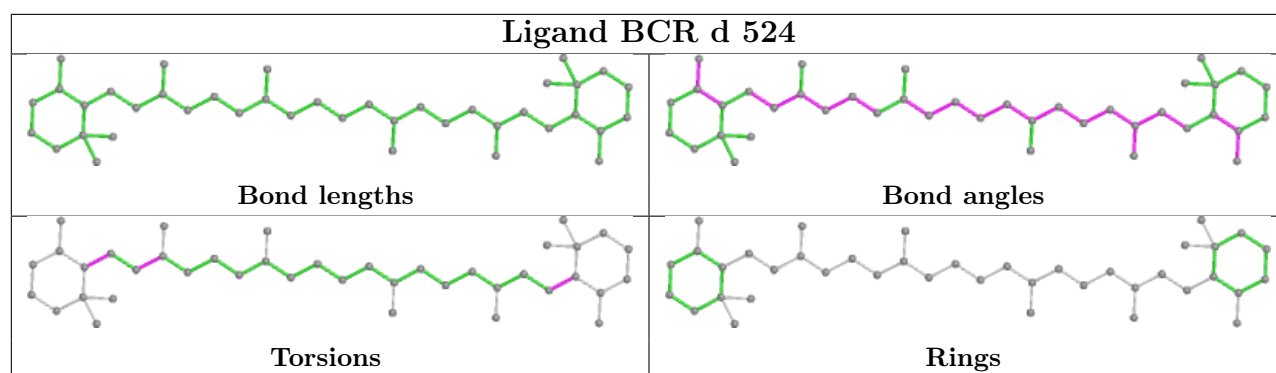
Ligand CLA s 504

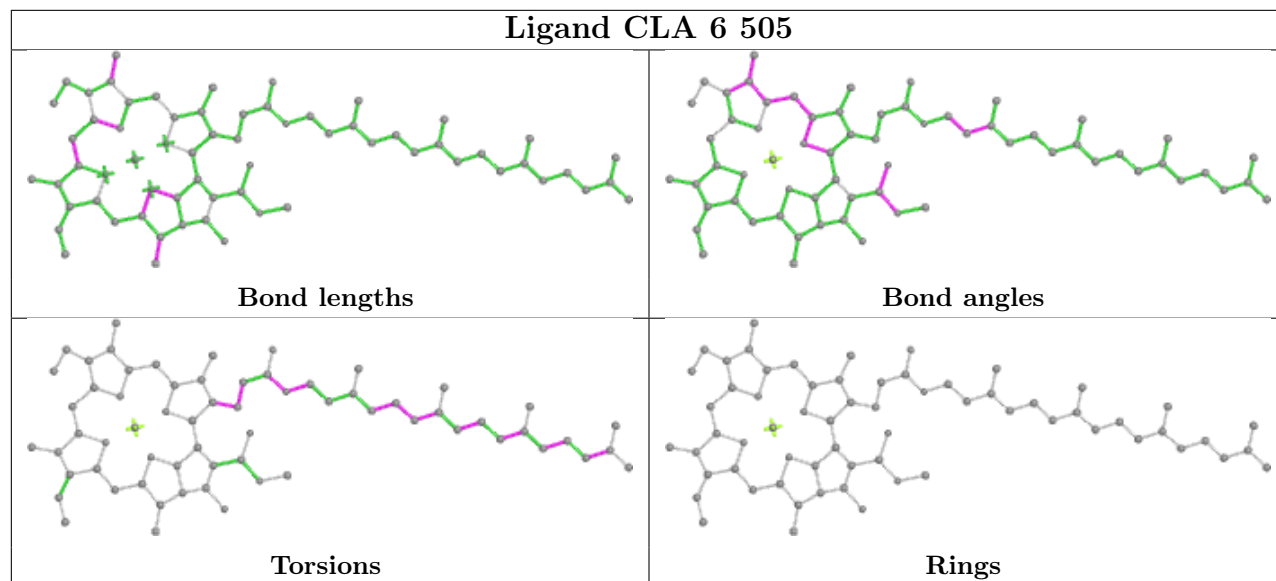
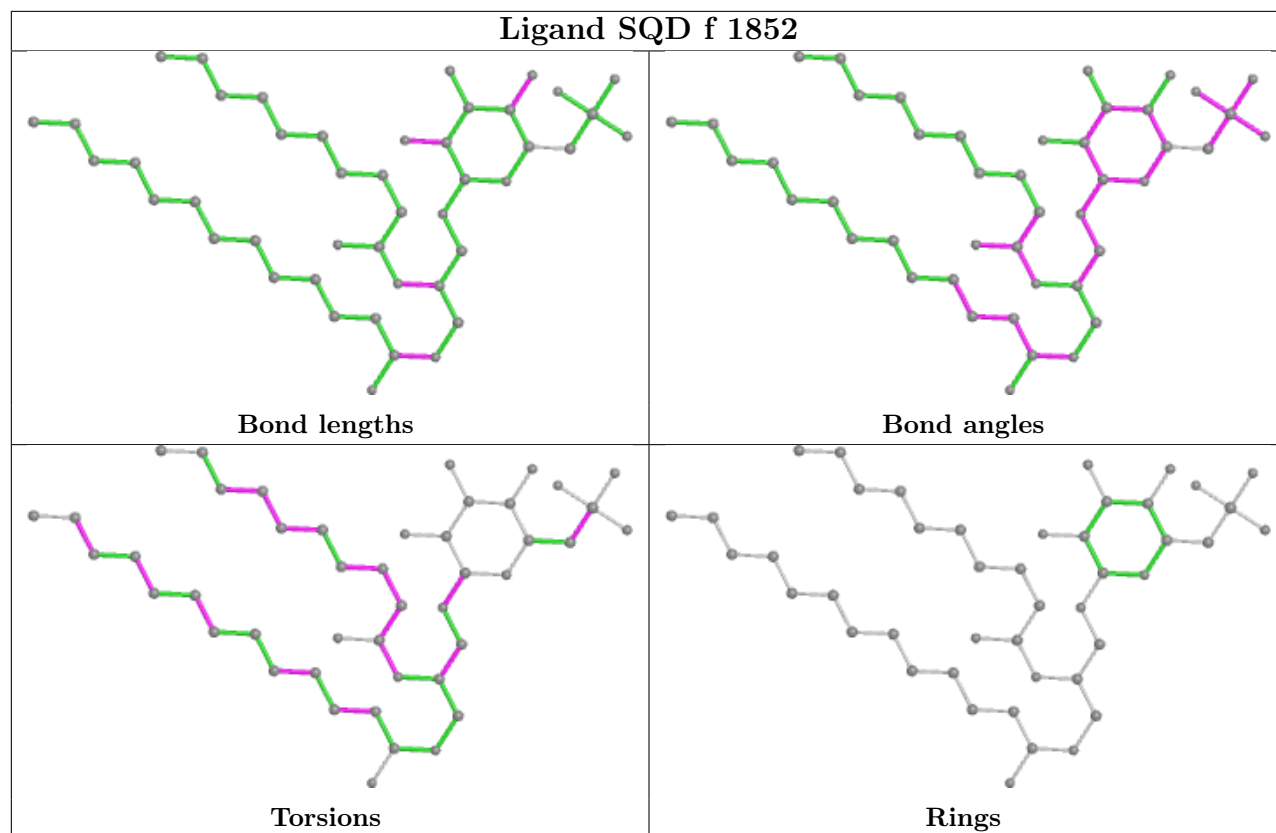


Ligand CLA B 1214

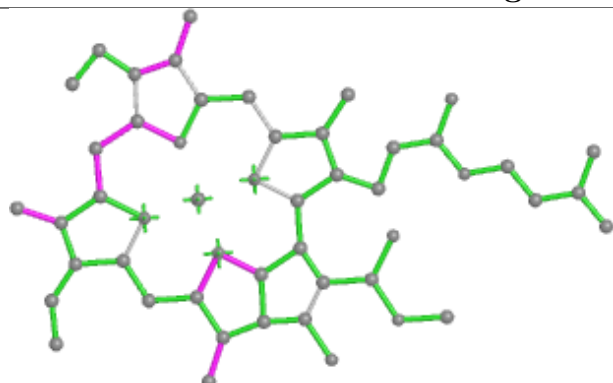




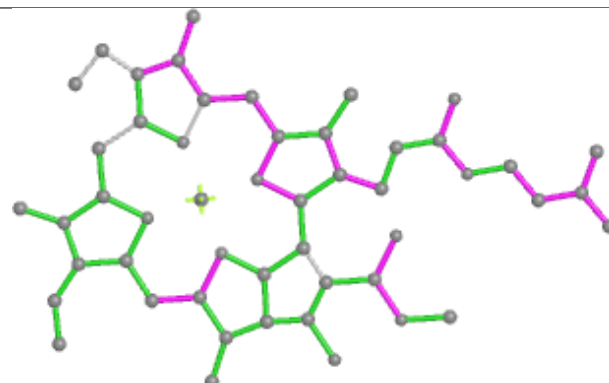




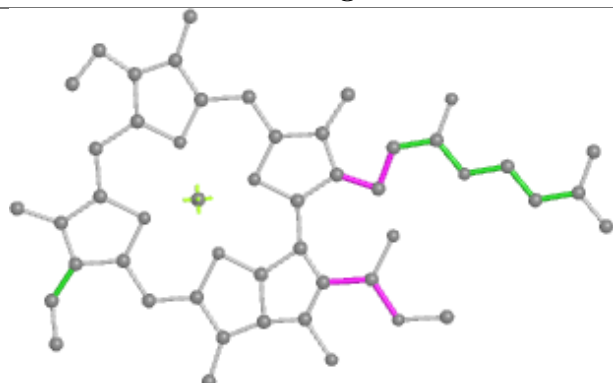
Ligand CLA U 1103



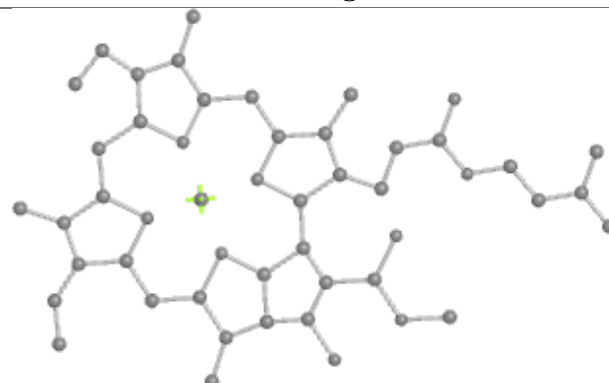
Bond lengths



Bond angles

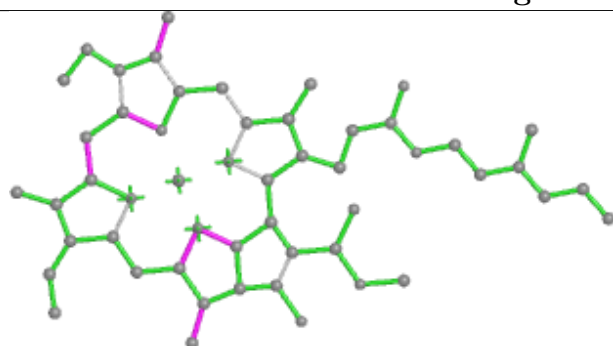


Torsions

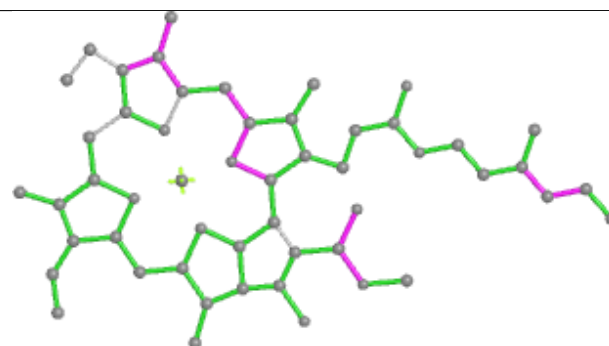


Rings

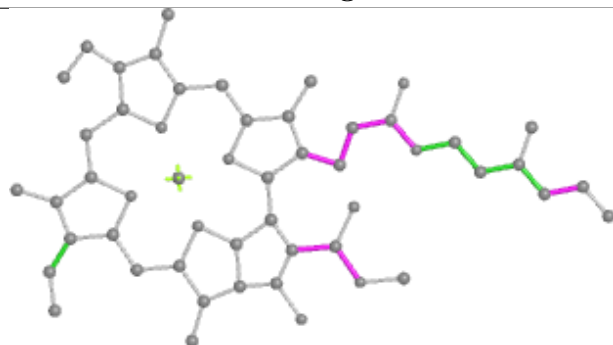
Ligand CLA Y 512



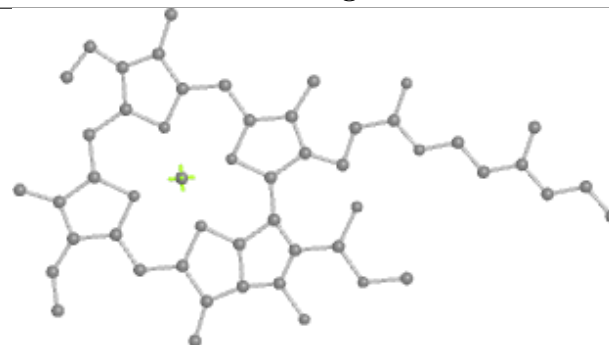
Bond lengths



Bond angles

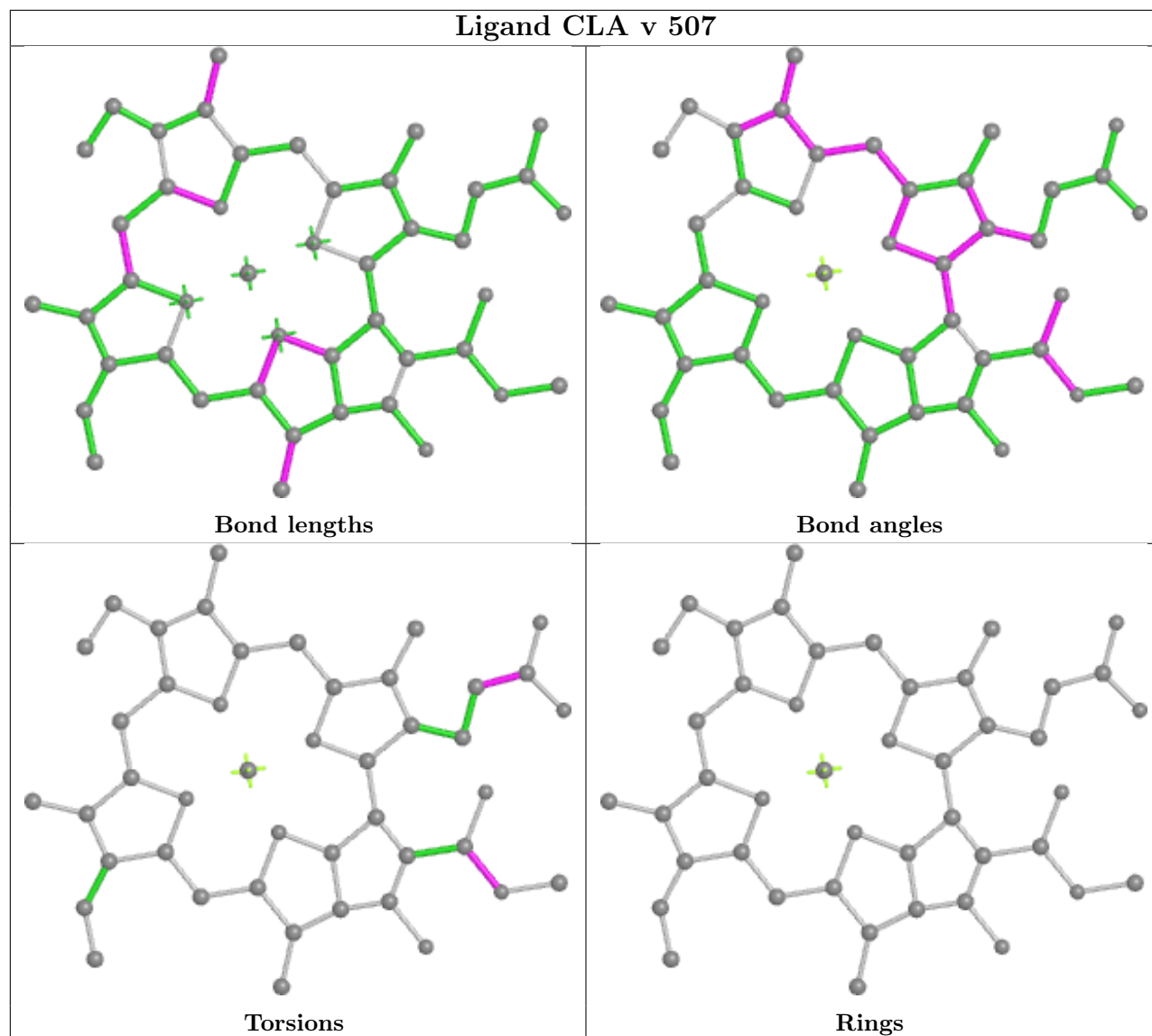


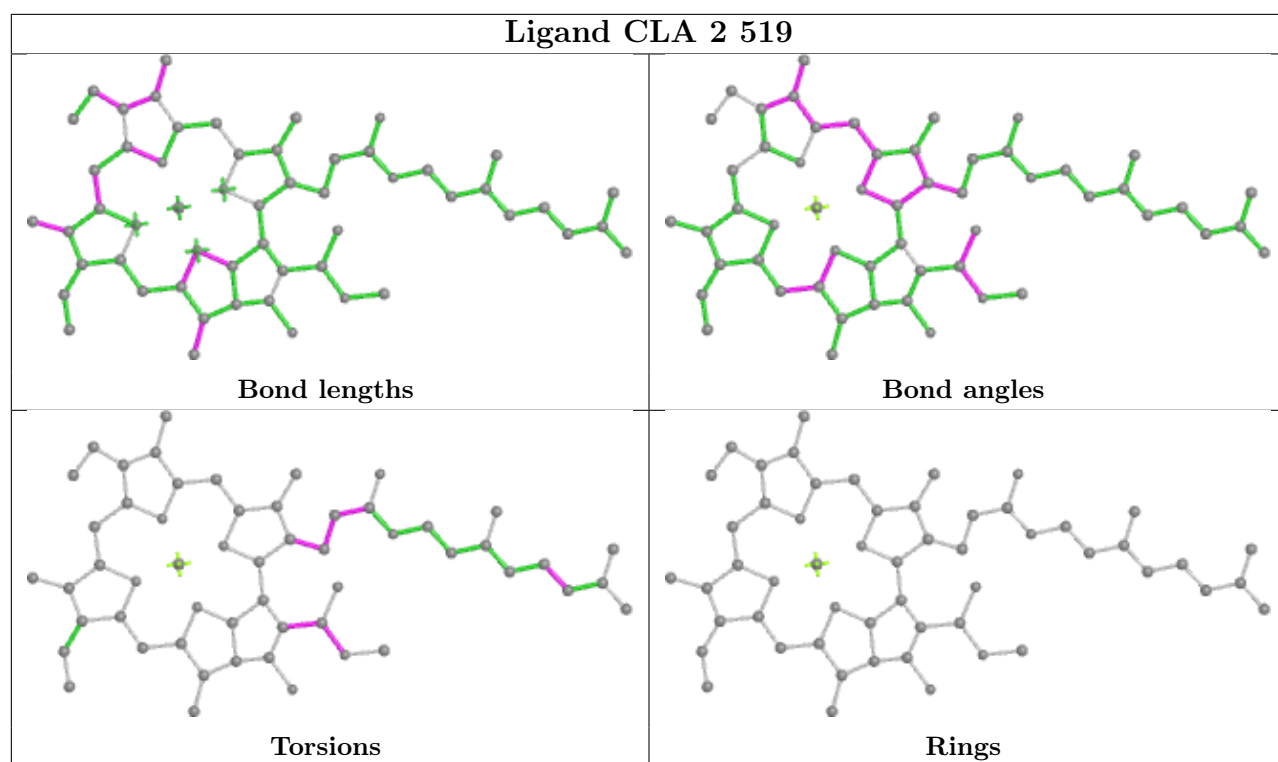
Torsions



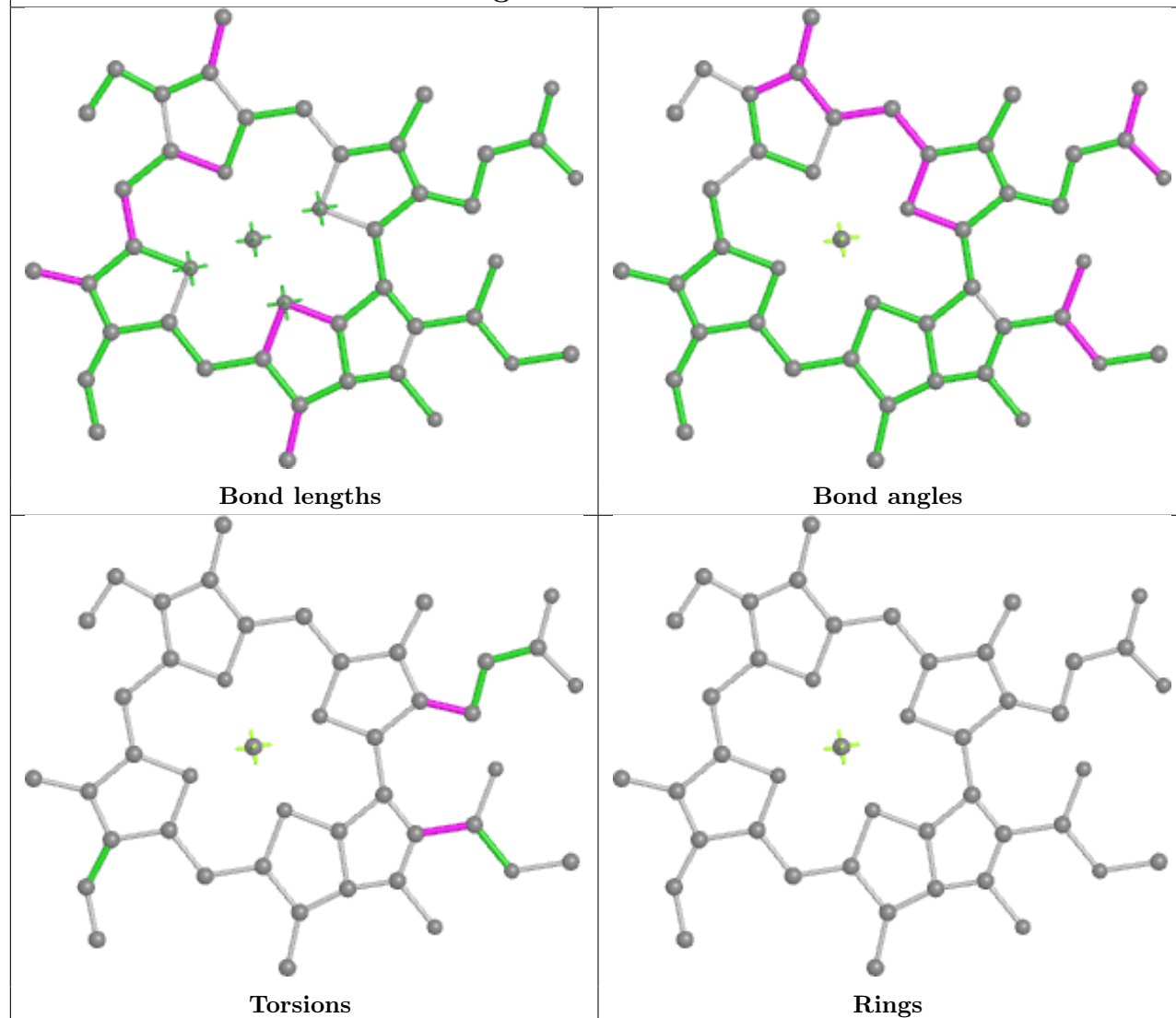
Rings

Ligand CLA v 507

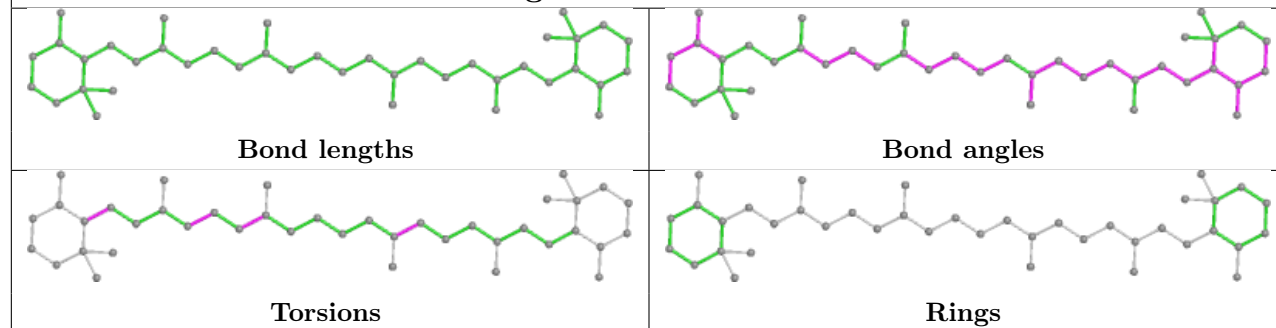


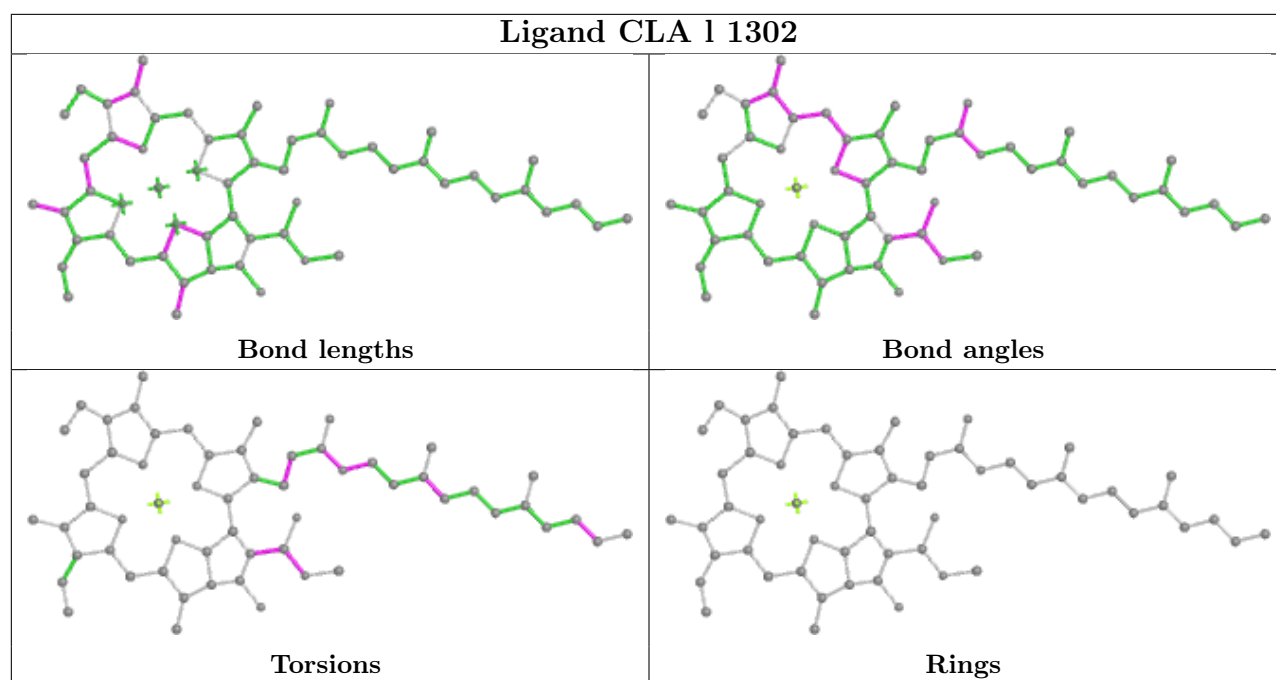


Ligand CLA d 508

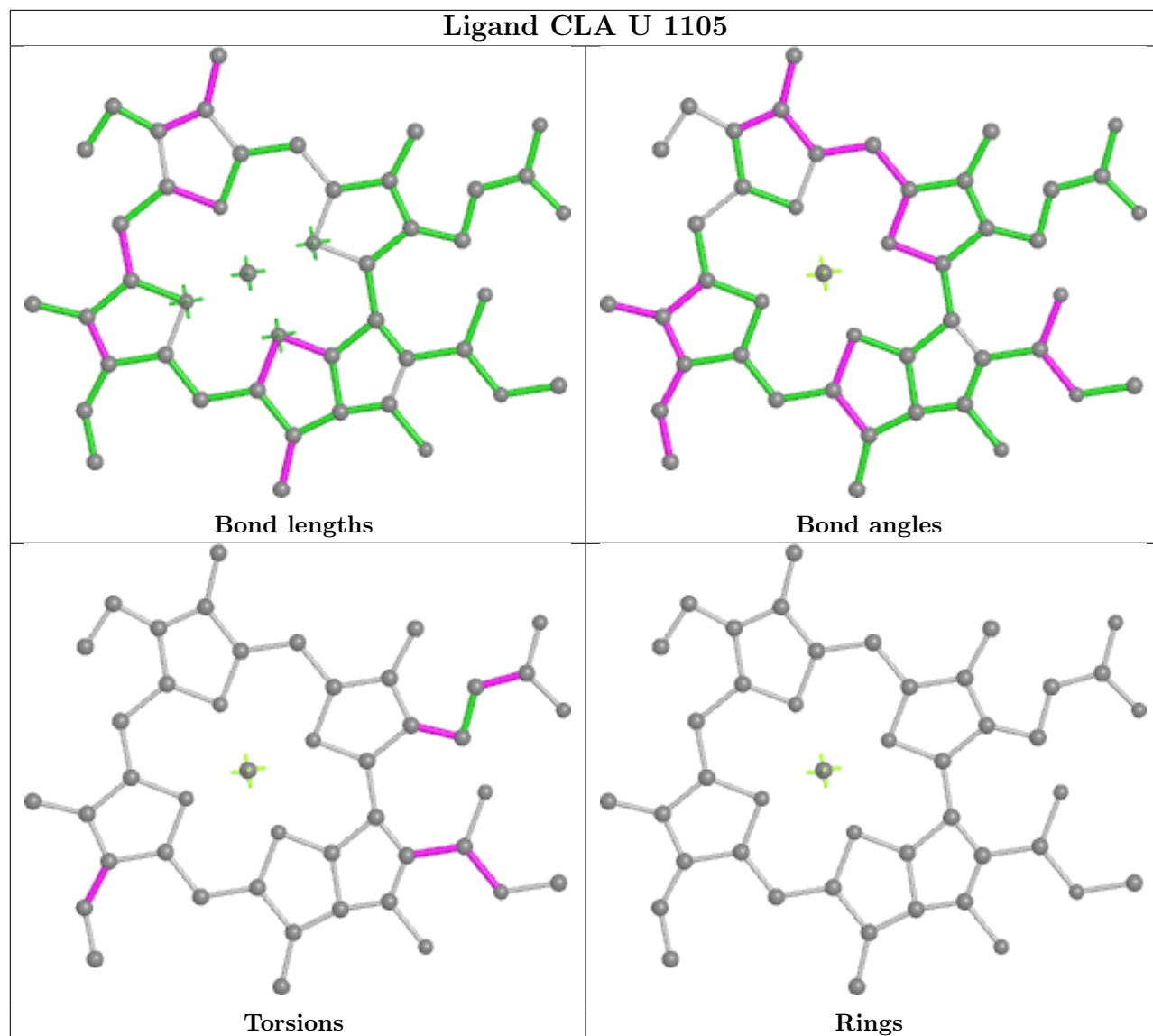


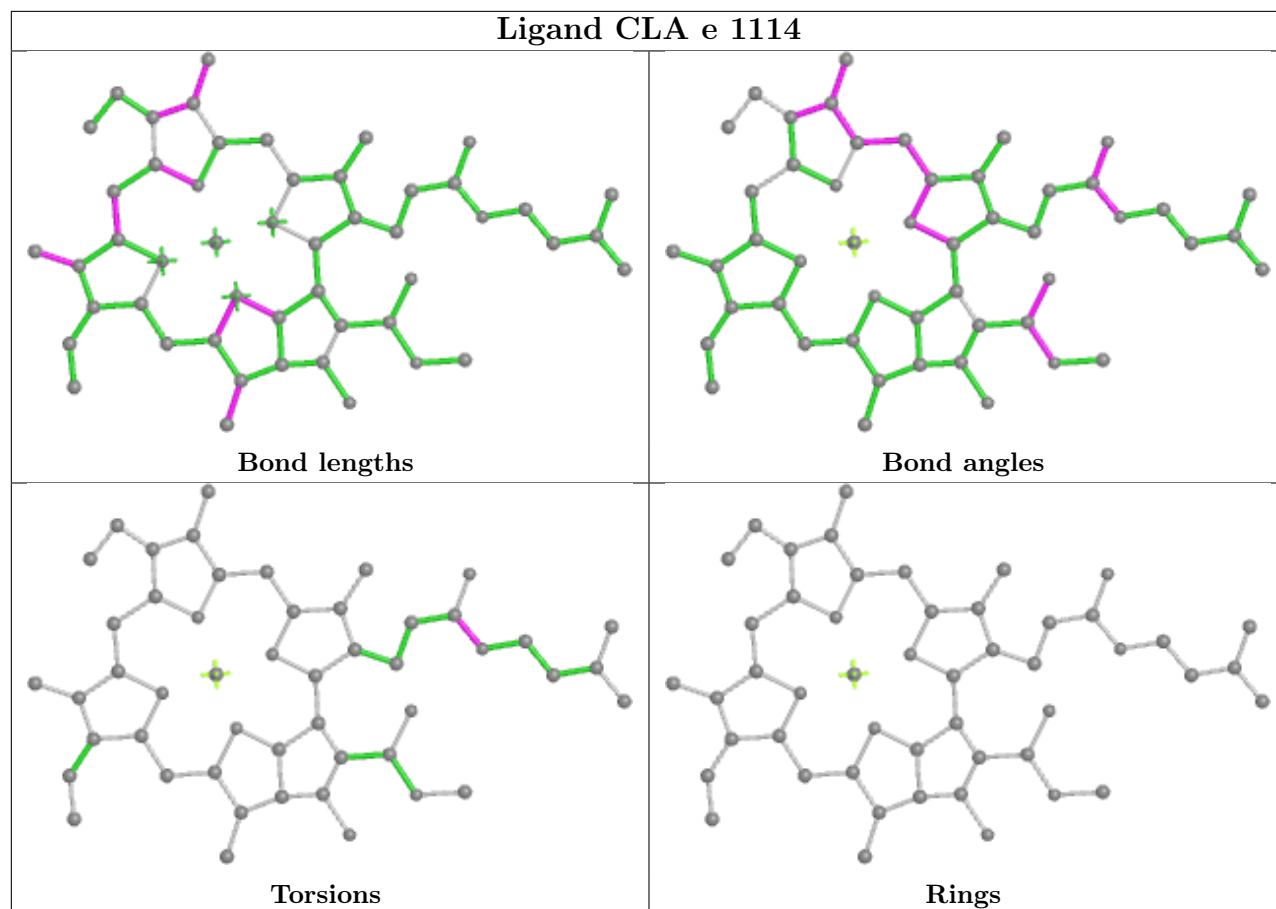
Ligand BCR o 4021

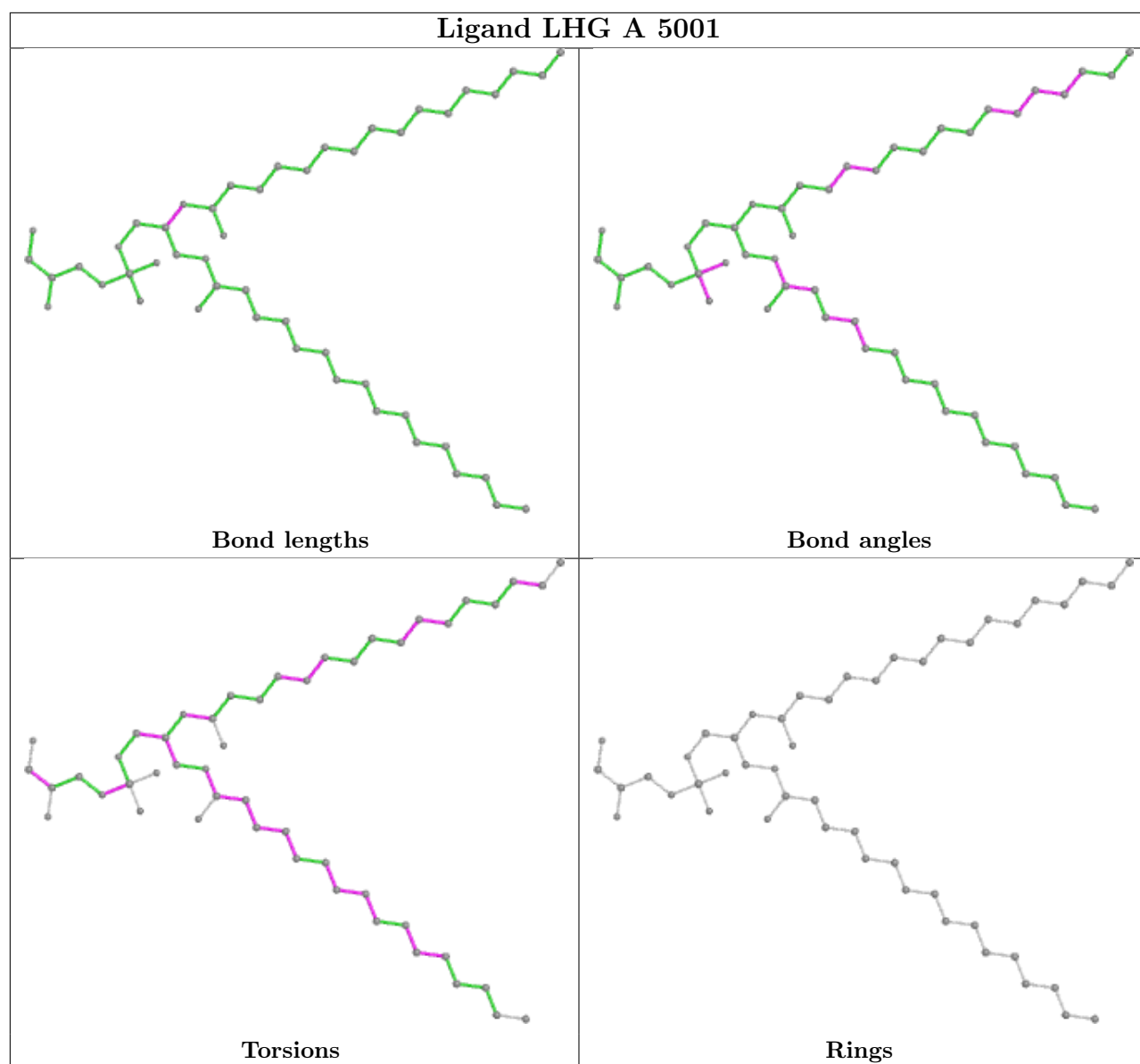




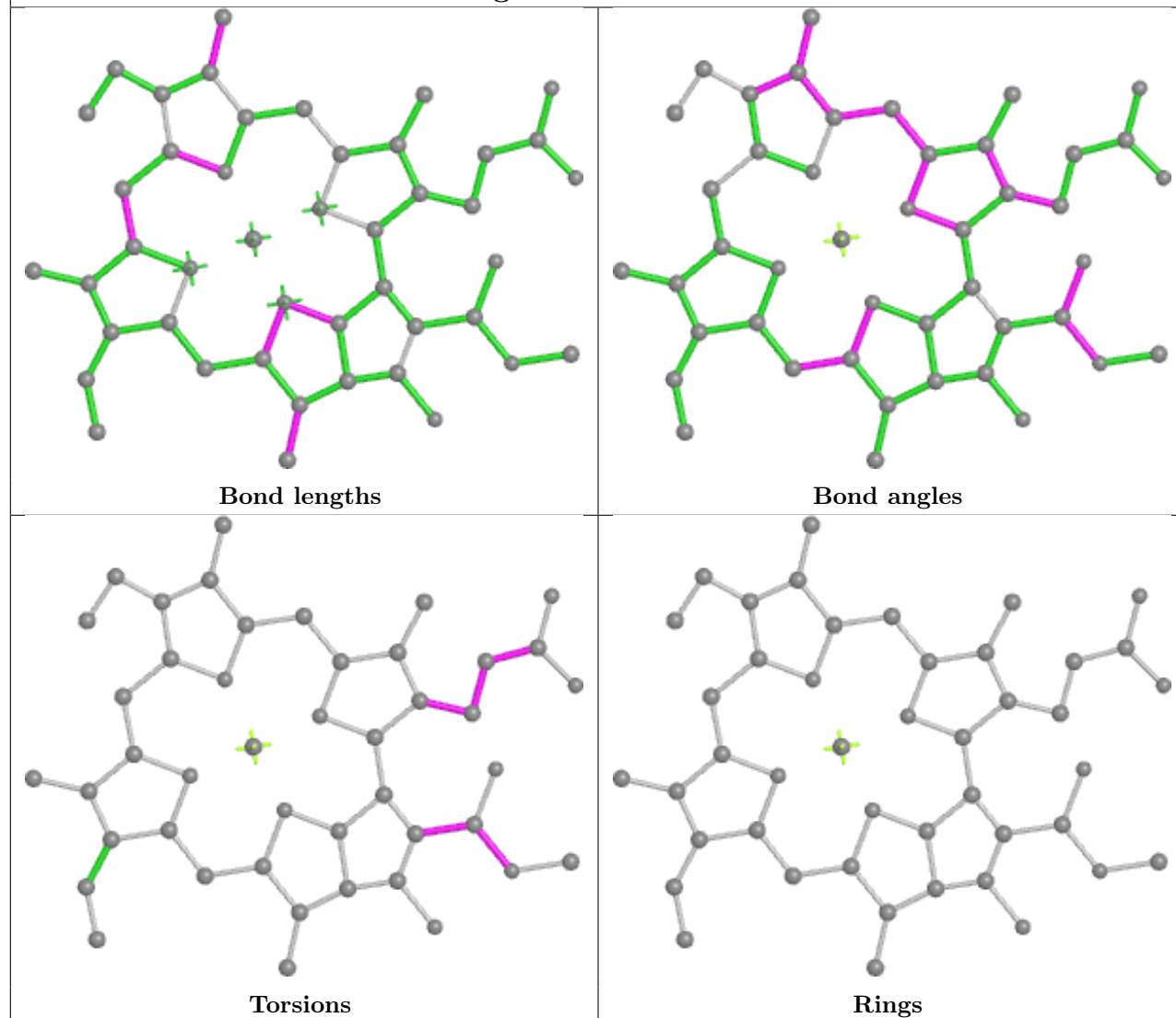
Ligand CLA U 1105



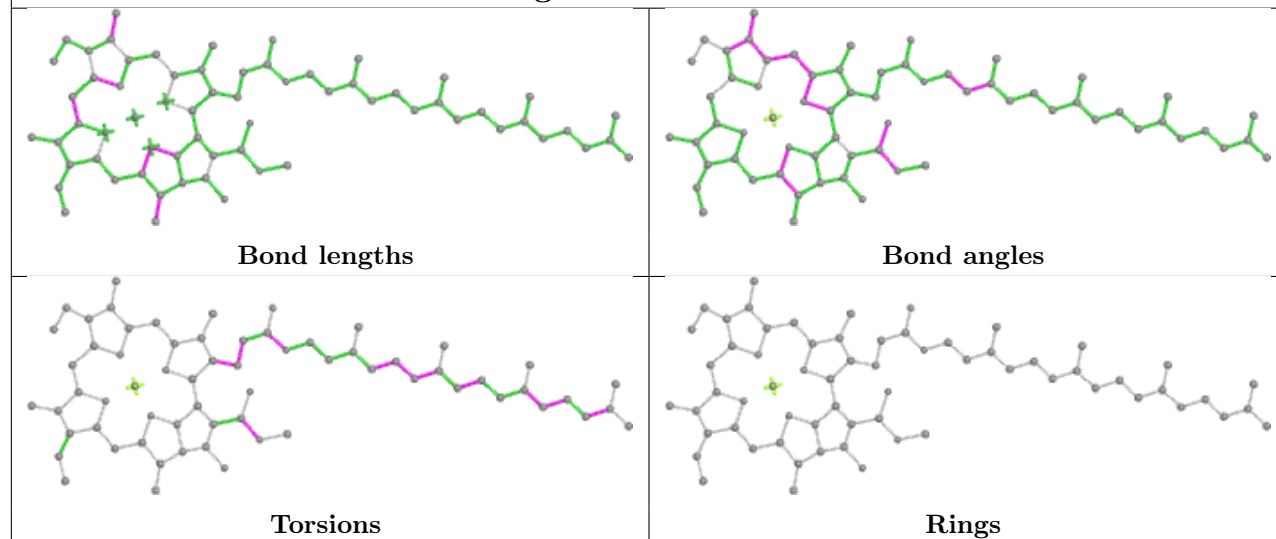




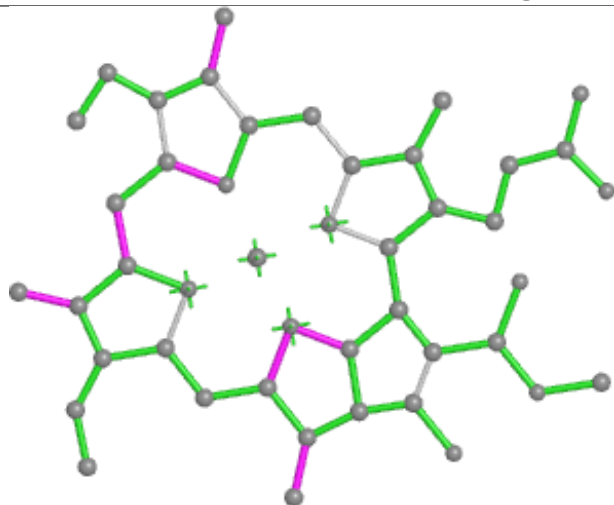
Ligand CLA d 516



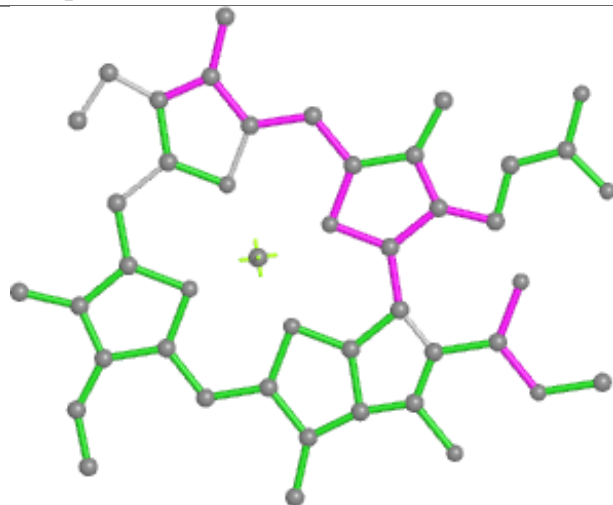
Ligand CLA Z 505



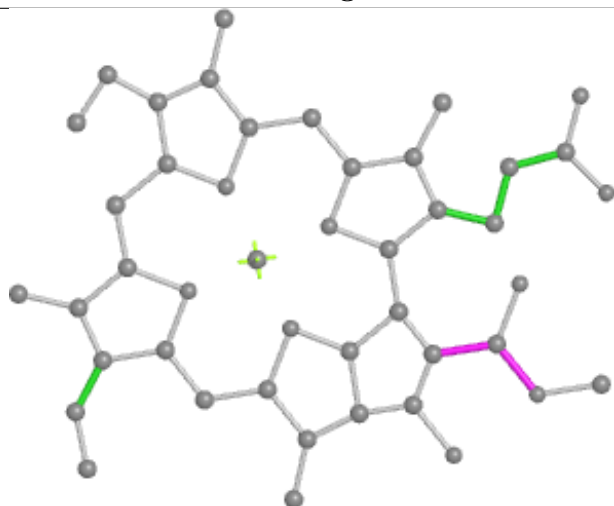
Ligand CLA q 504



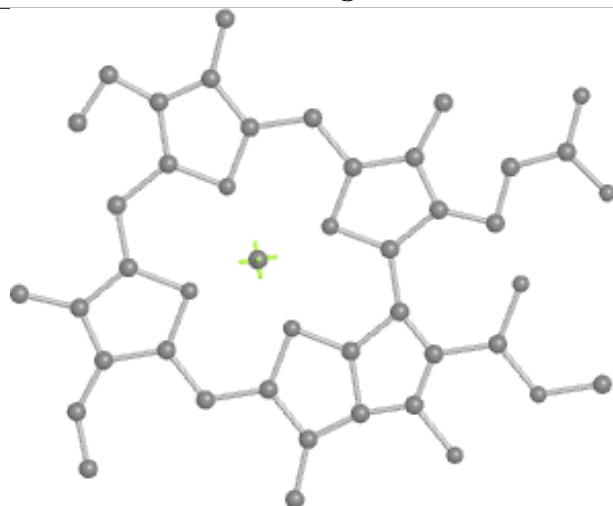
Bond lengths



Bond angles

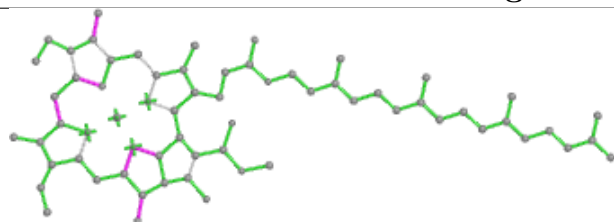


Torsions

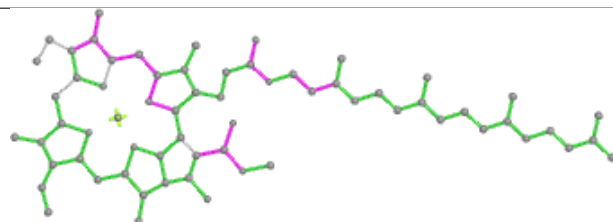


Rings

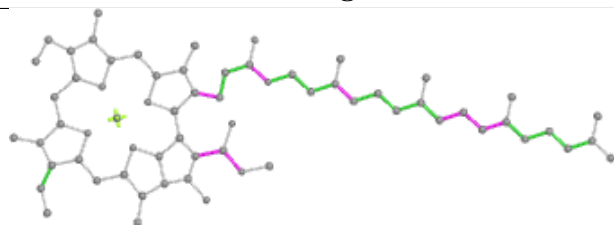
Ligand CLA B 1240



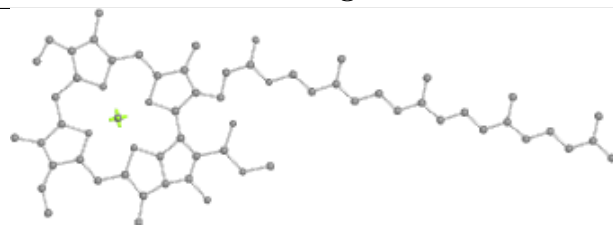
Bond lengths



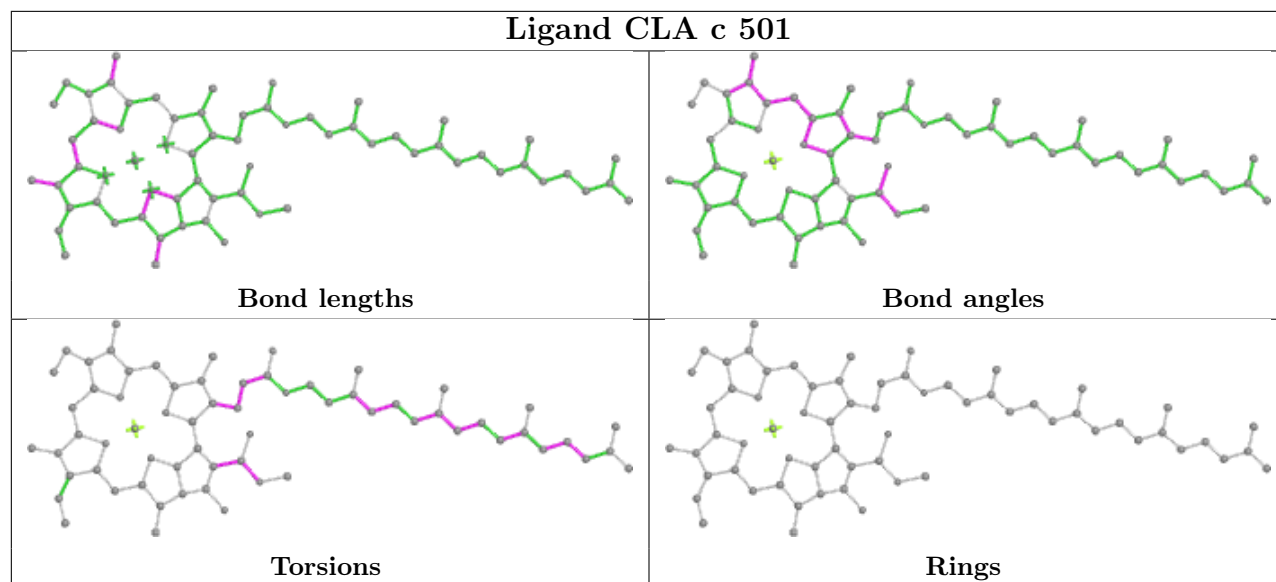
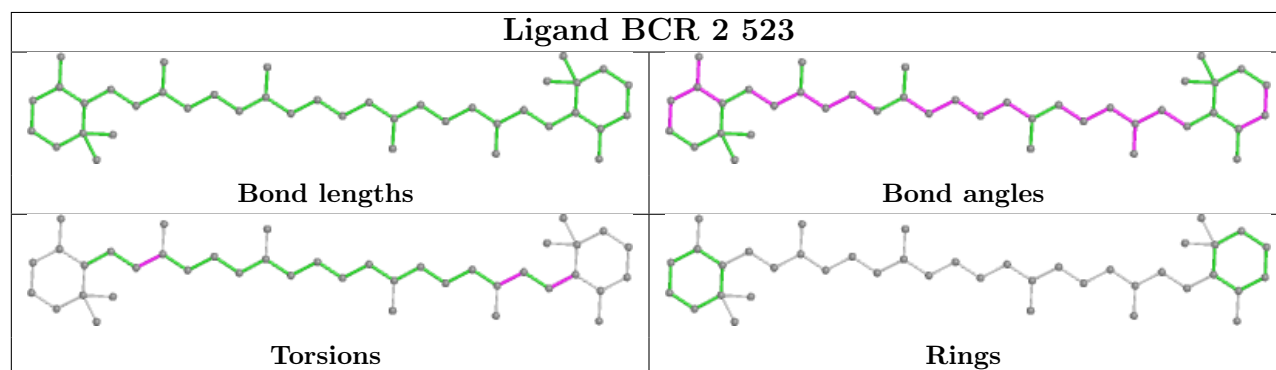
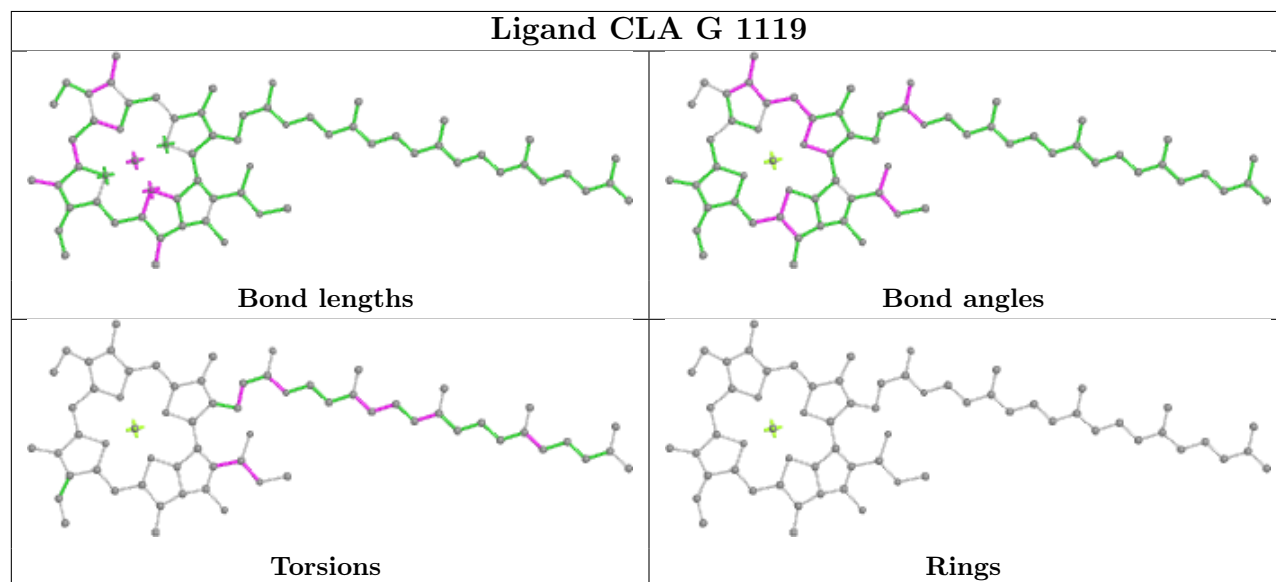
Bond angles



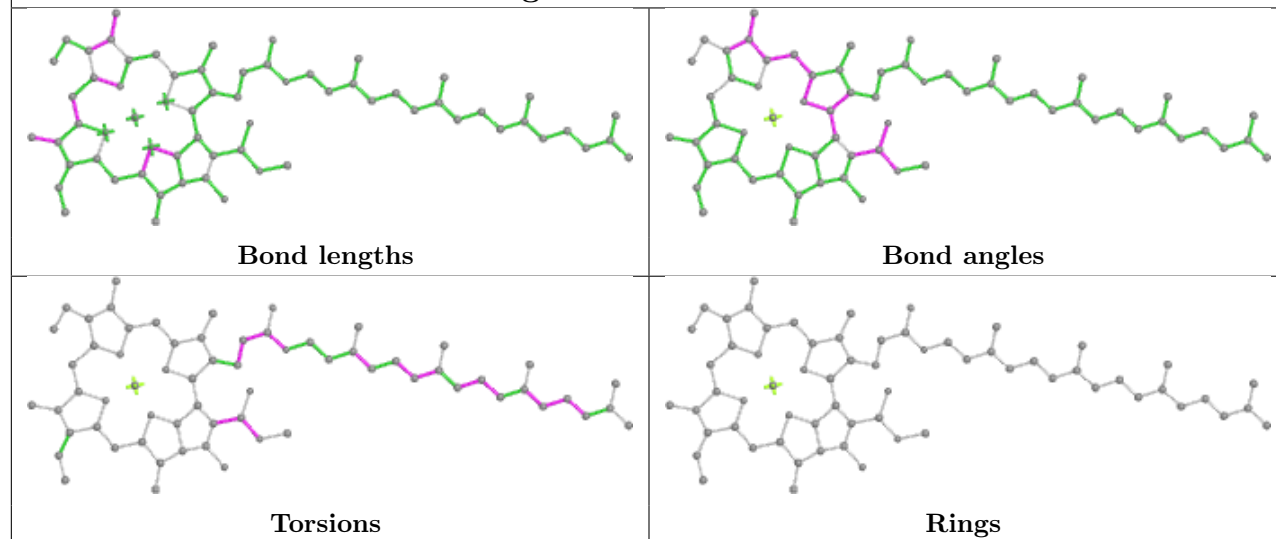
Torsions



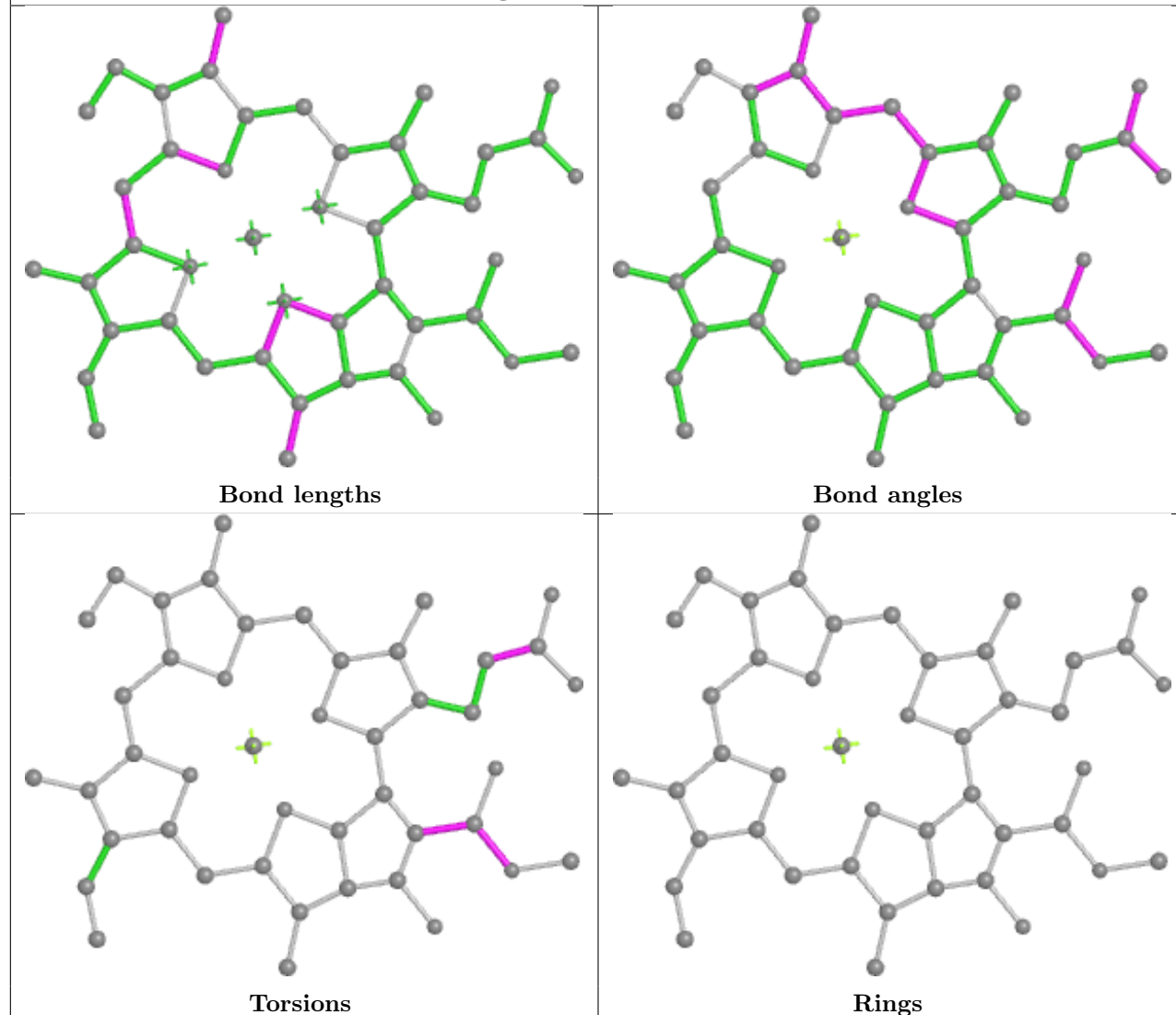
Rings

Ligand CLA c 501**Ligand BCR 2 523****Ligand CLA G 1119**

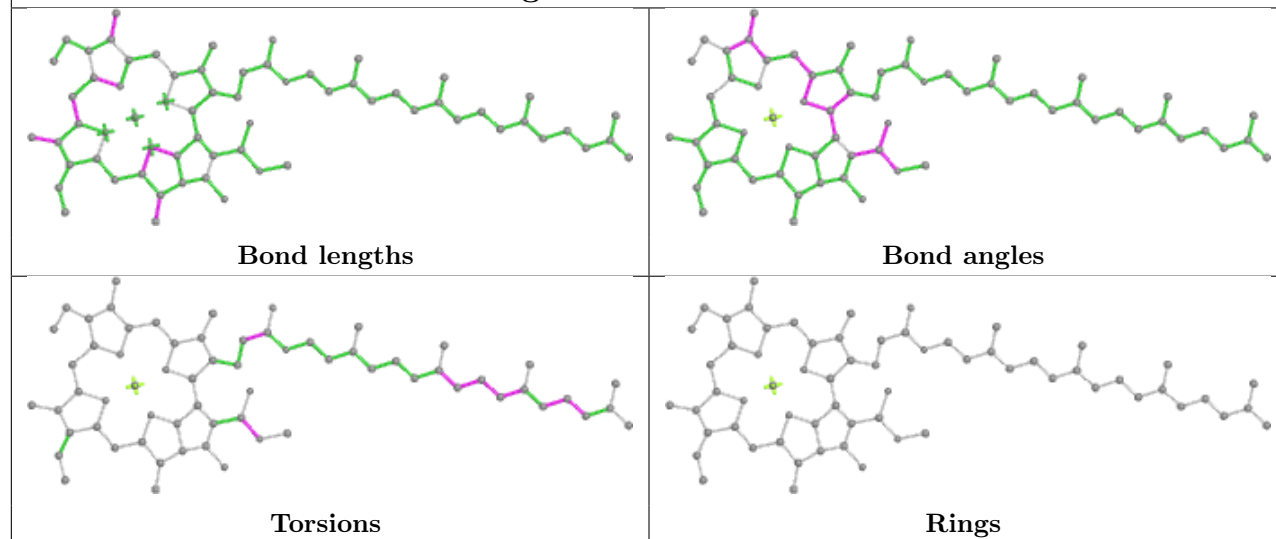
Ligand CLA G 1137



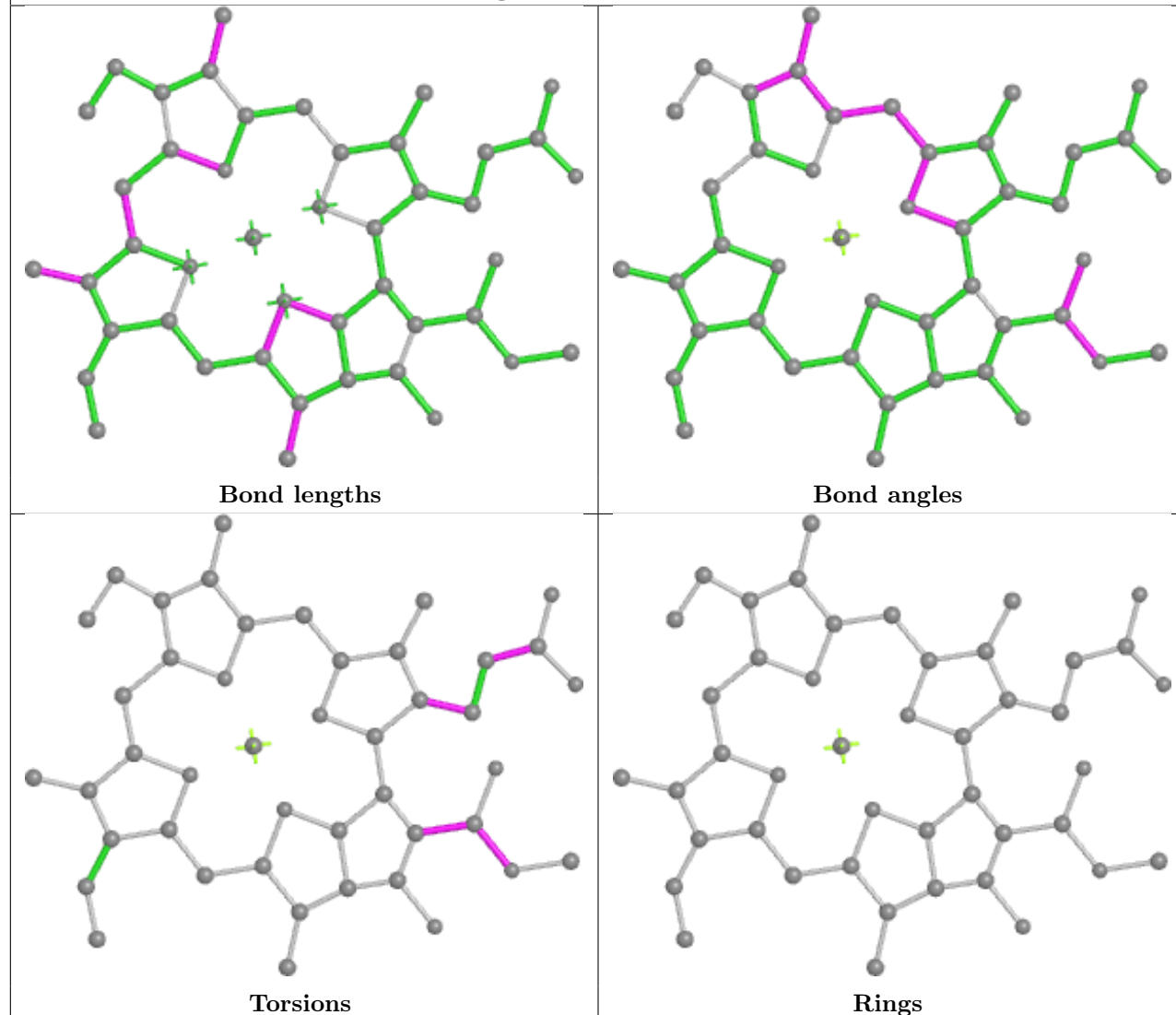
Ligand CLA c 512

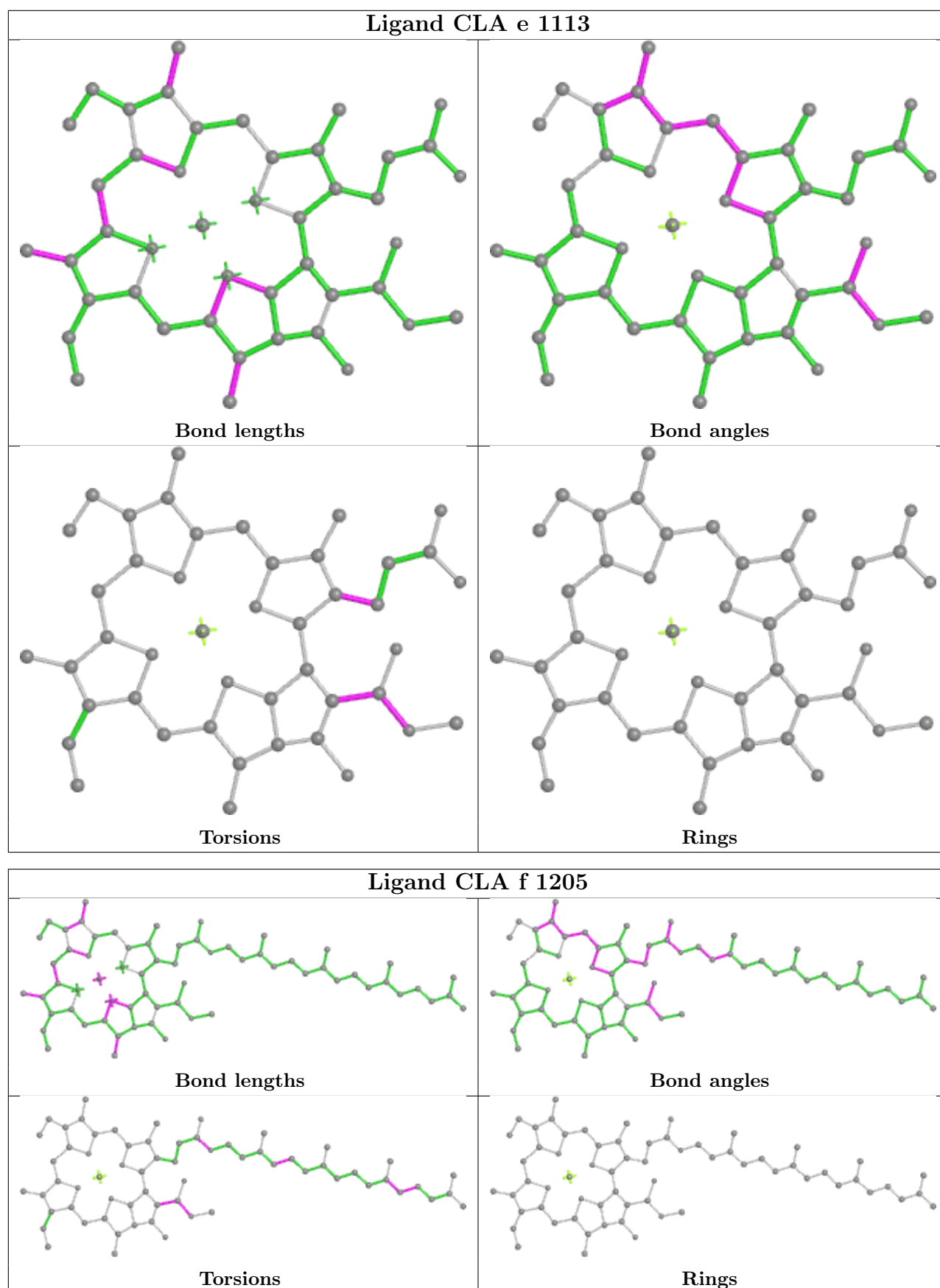


Ligand CLA G 1123

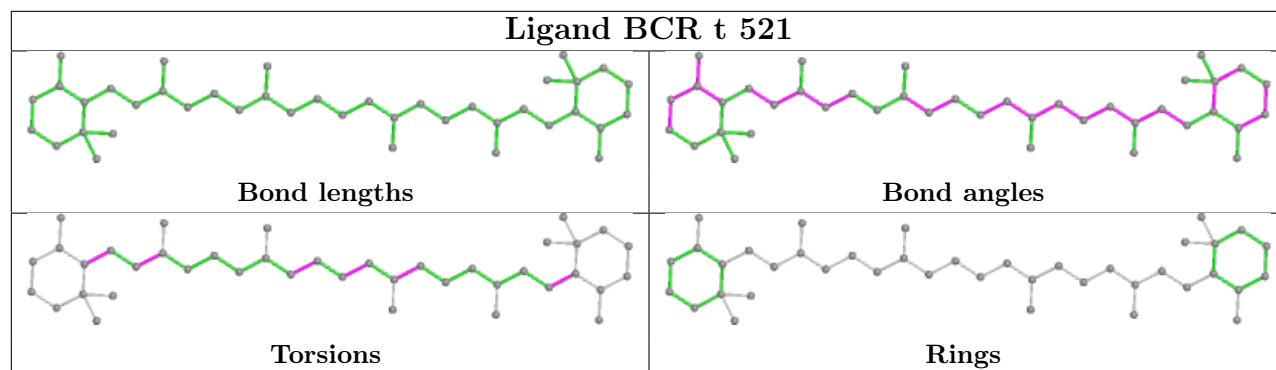


Ligand CLA v 517

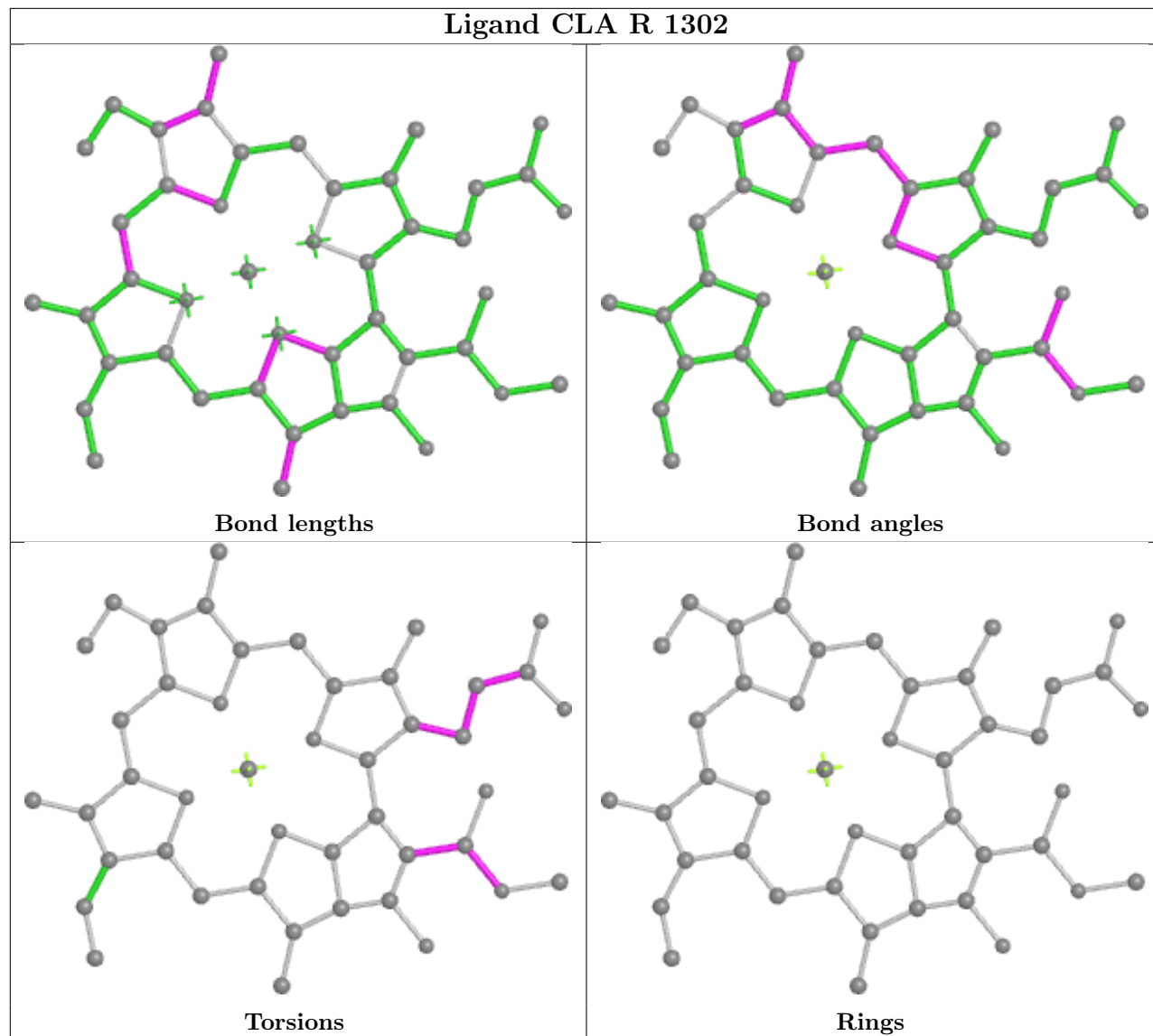




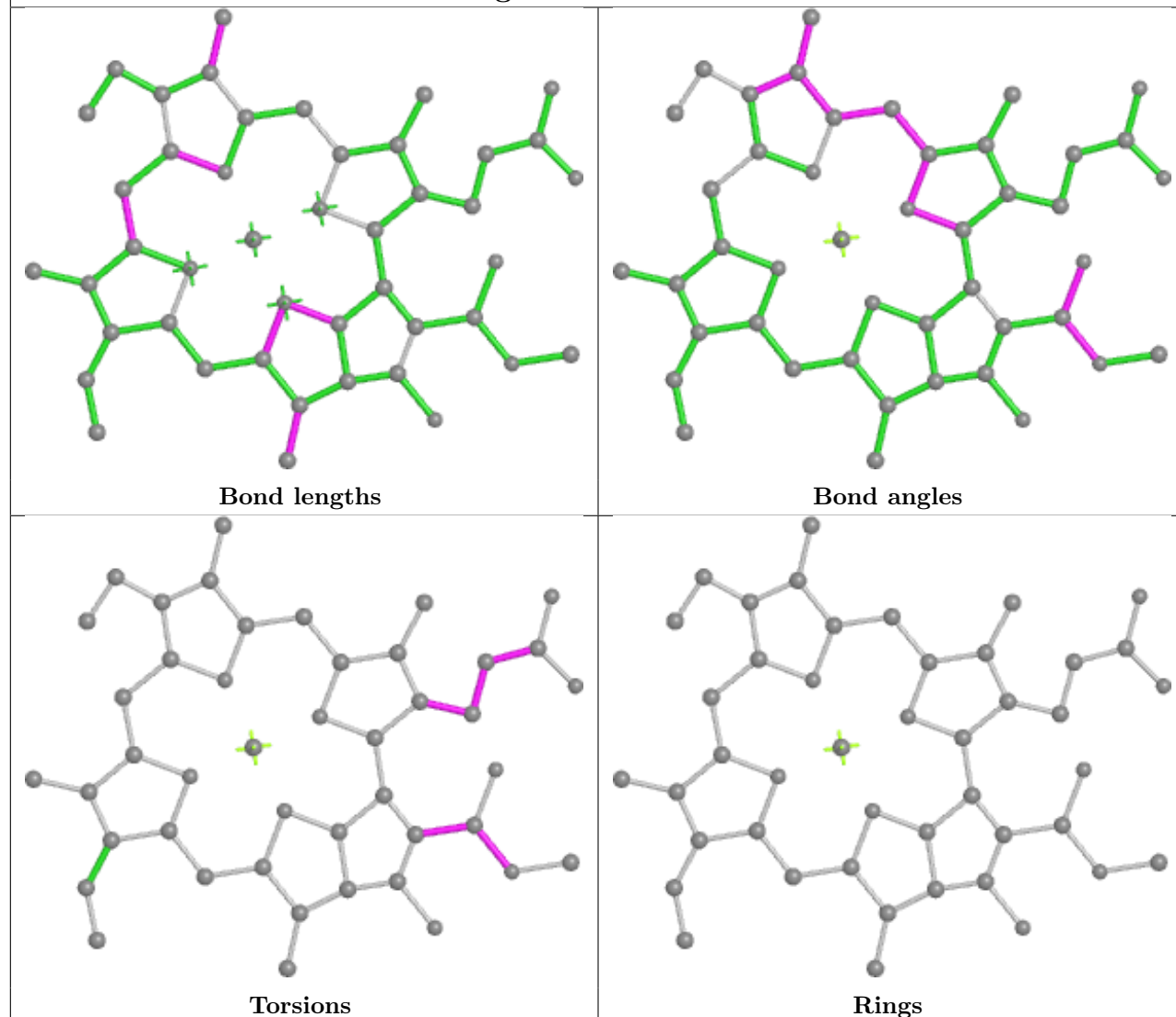
Ligand BCR t 521



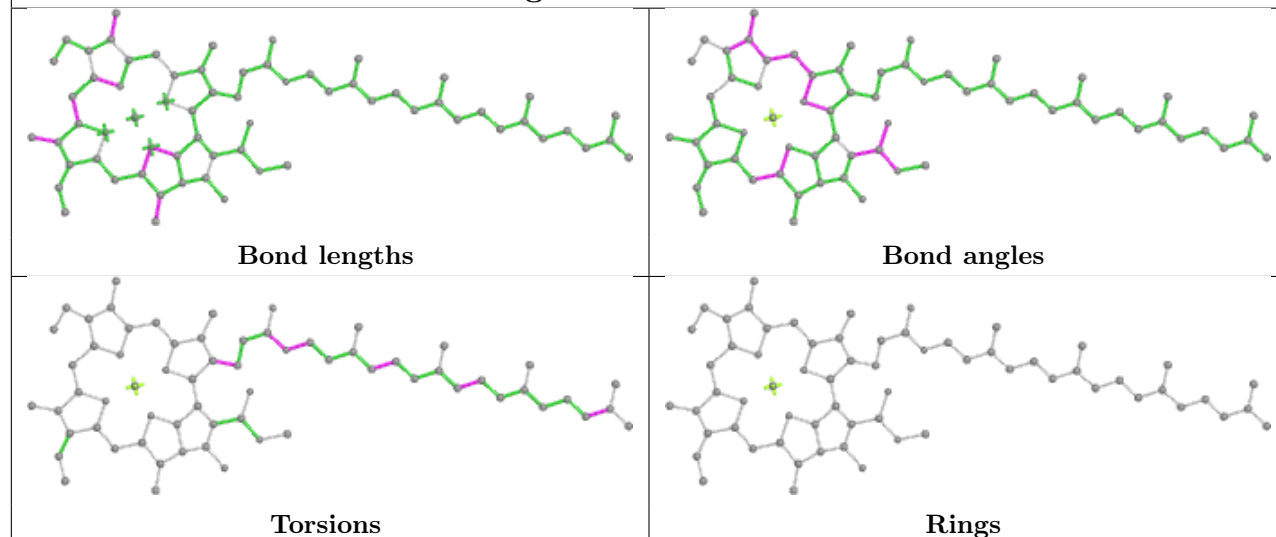
Ligand CLA R 1302

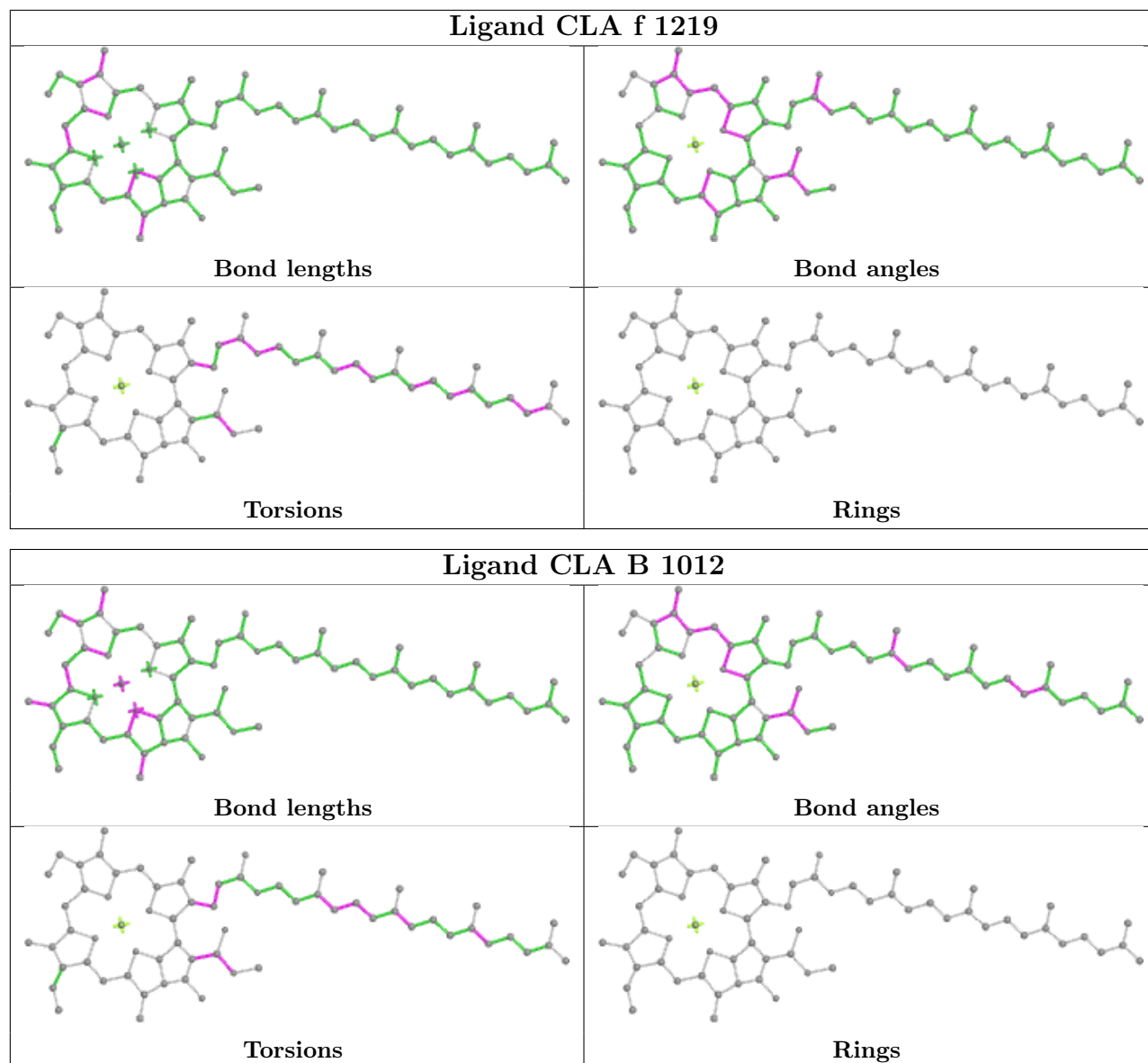


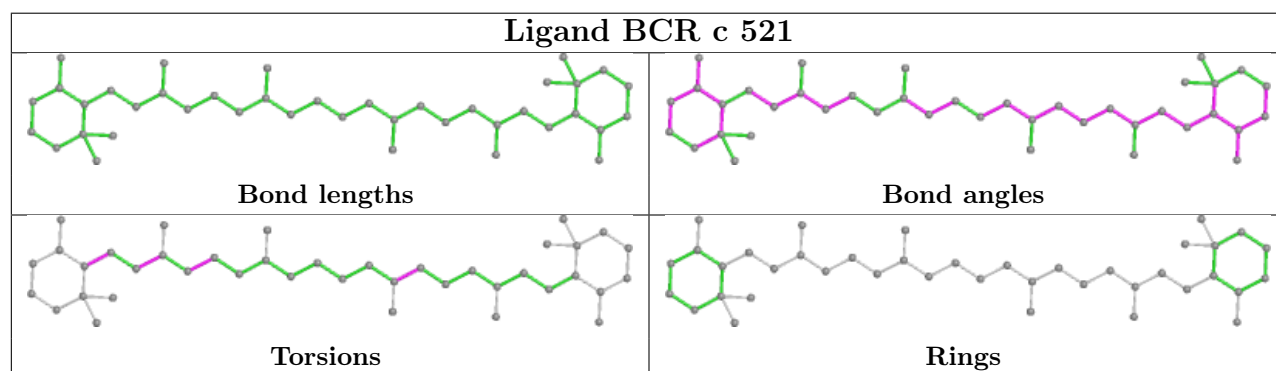
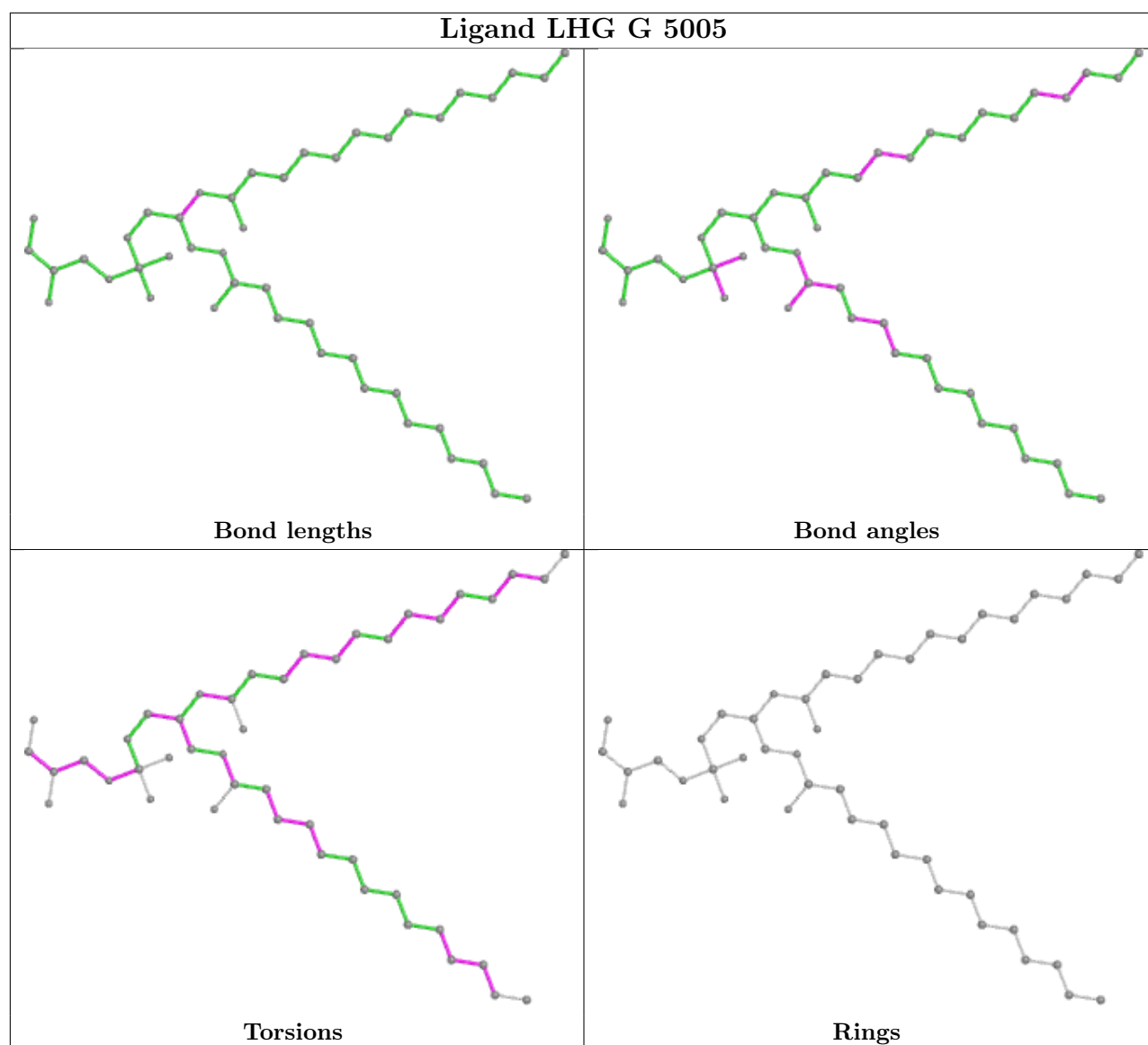
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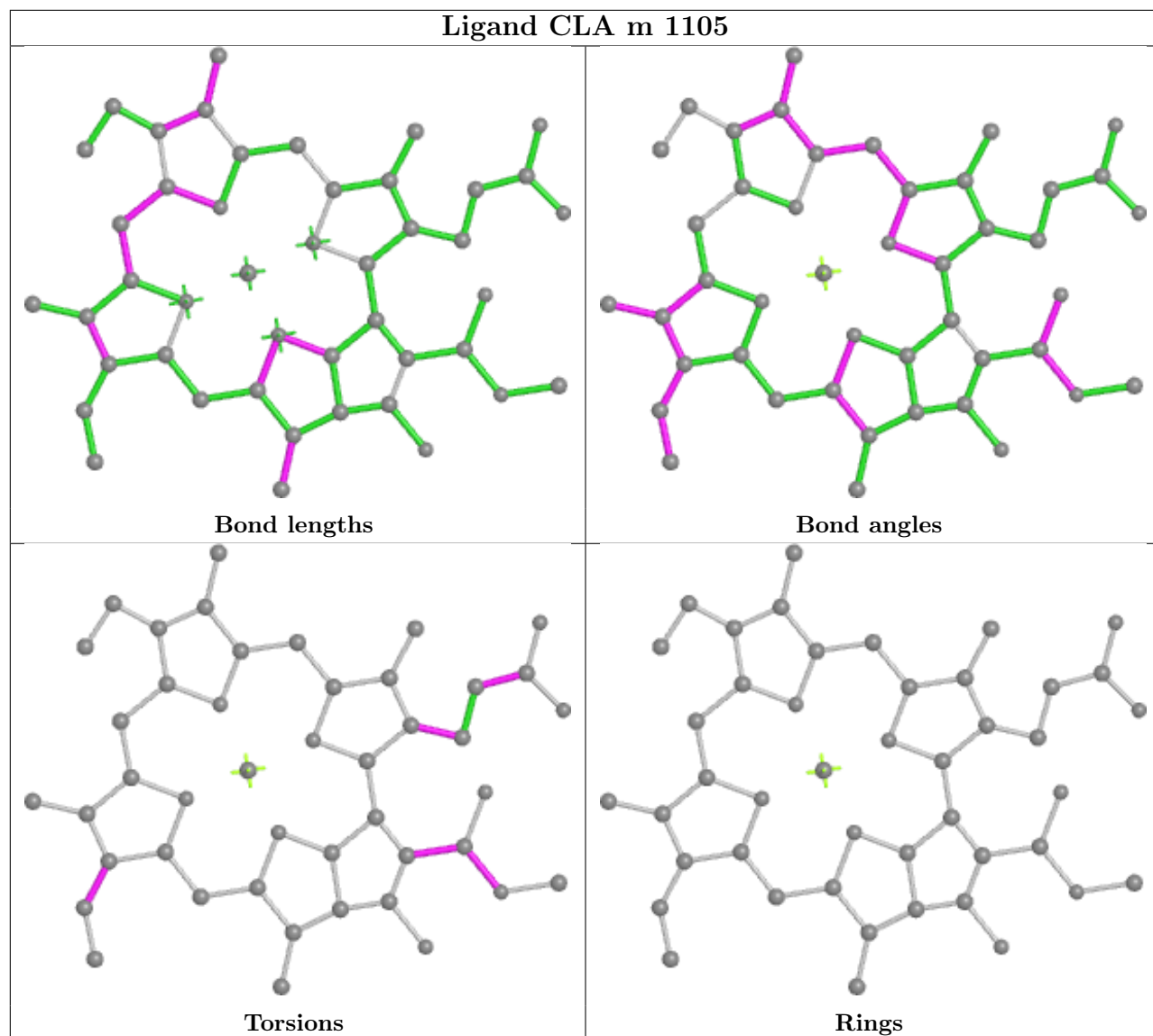
Ligand CLA L 1502



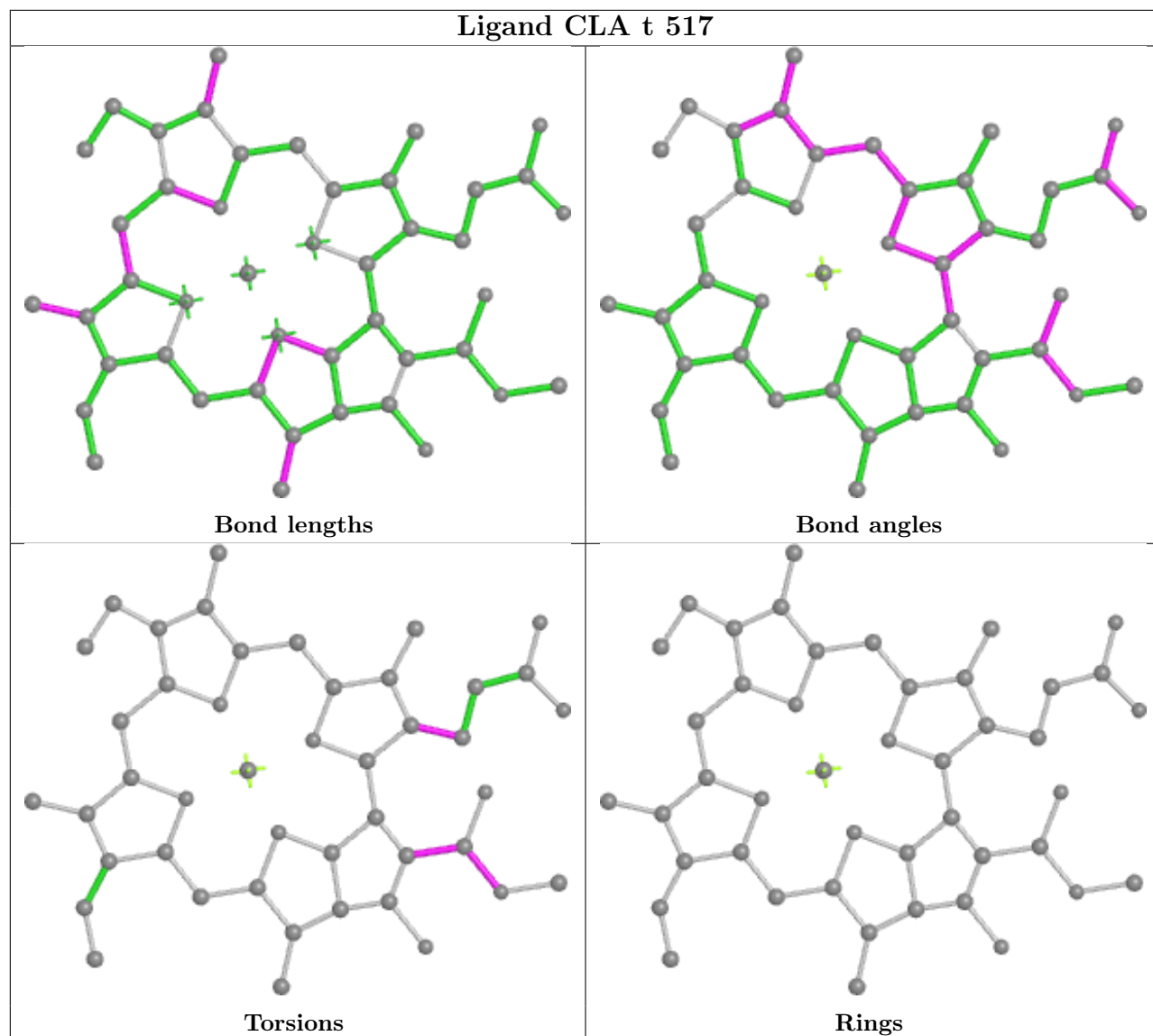




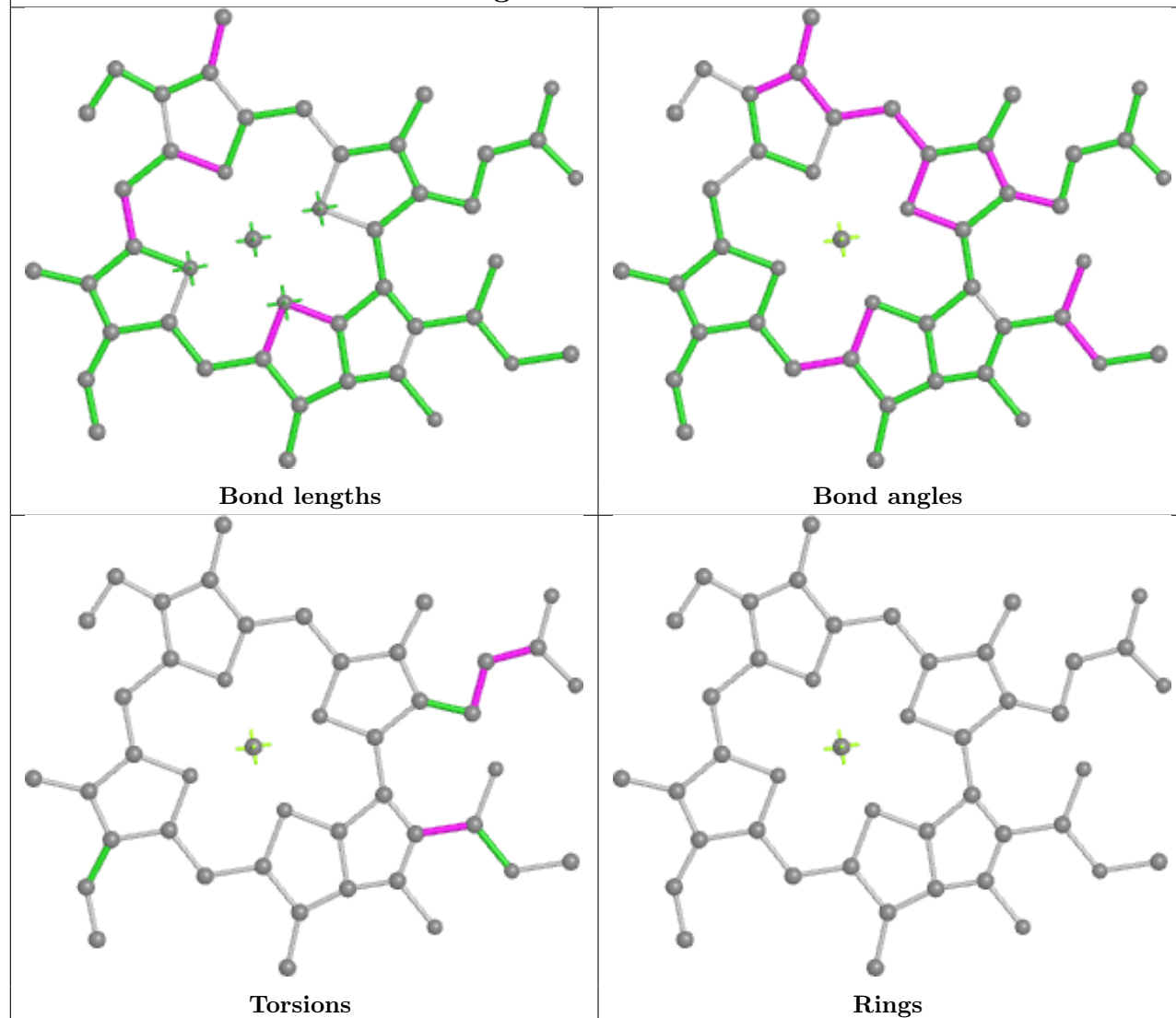
Ligand CLA m 1105



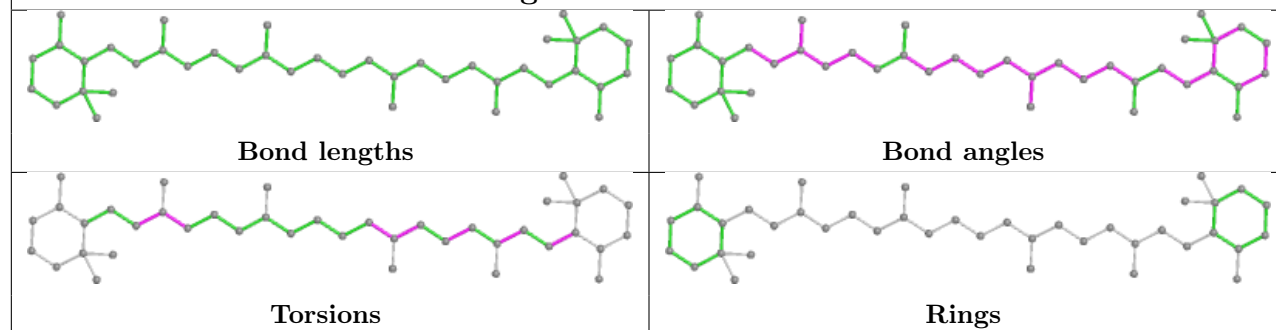
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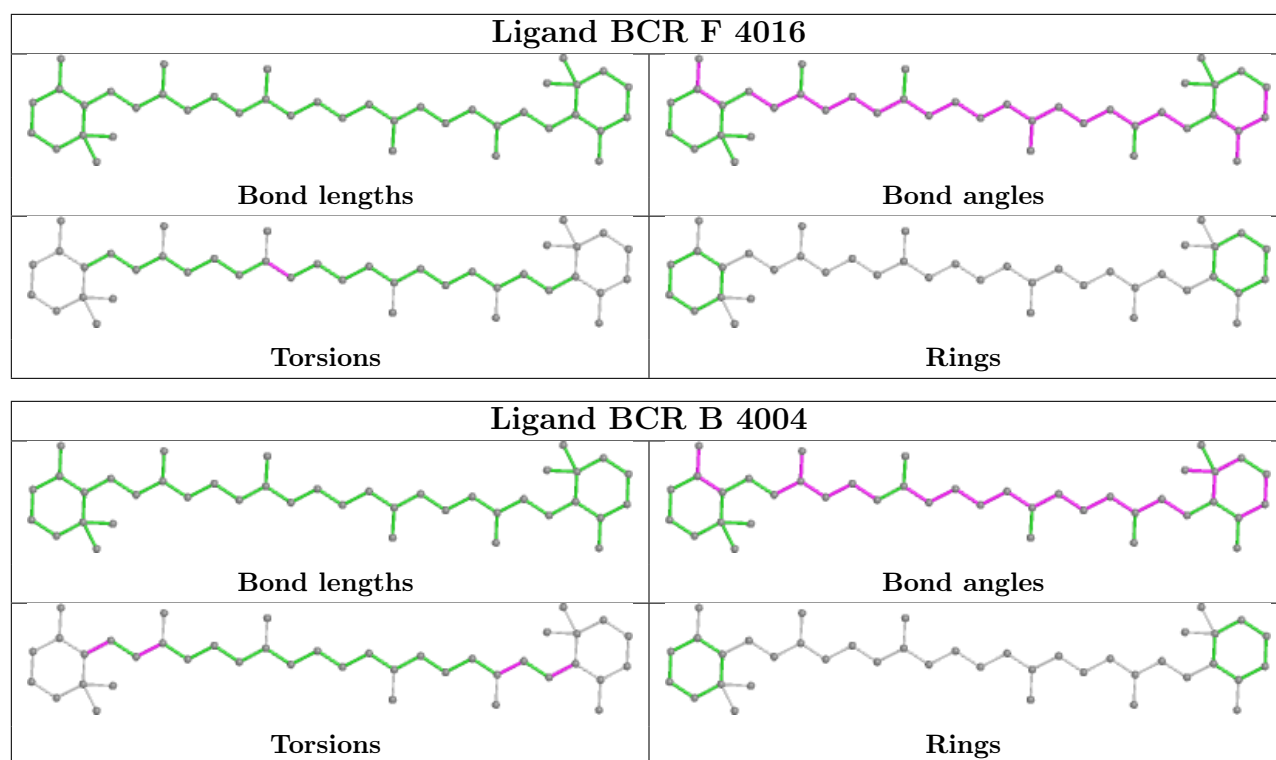


Ligand CLA v 504

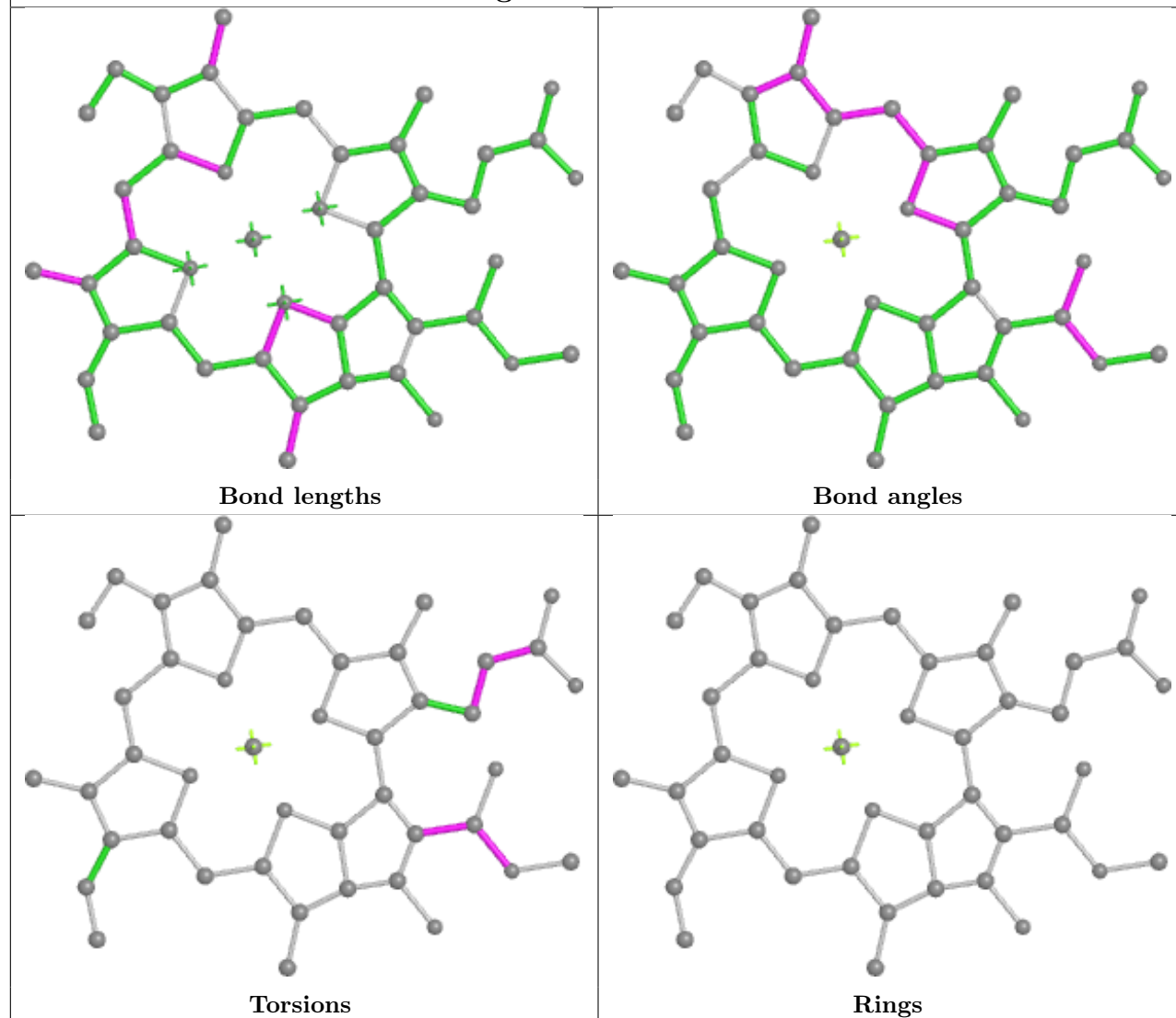


Ligand BCR G 4011

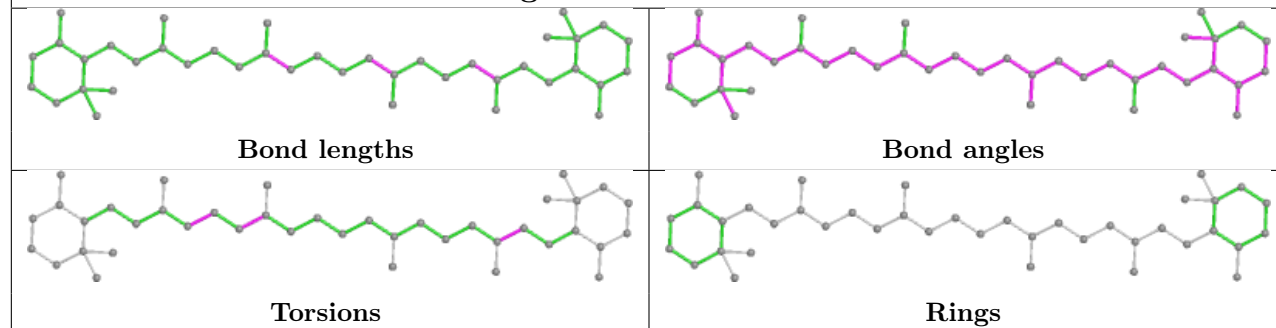




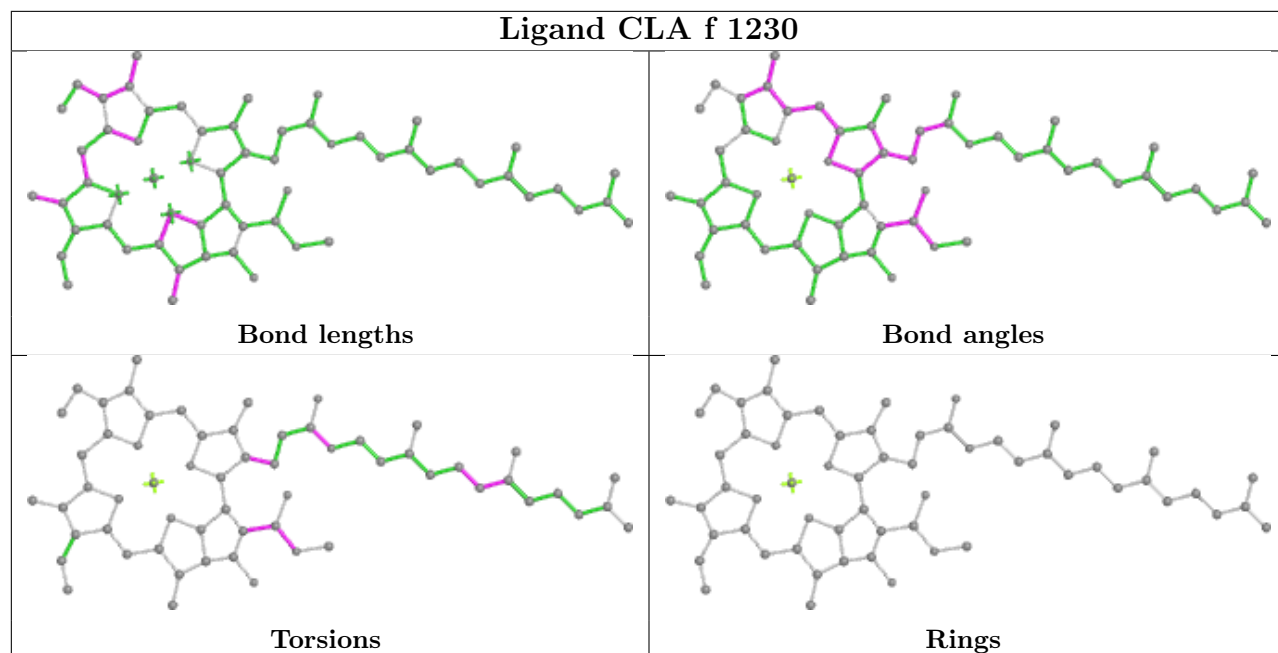
Ligand CLA t 513



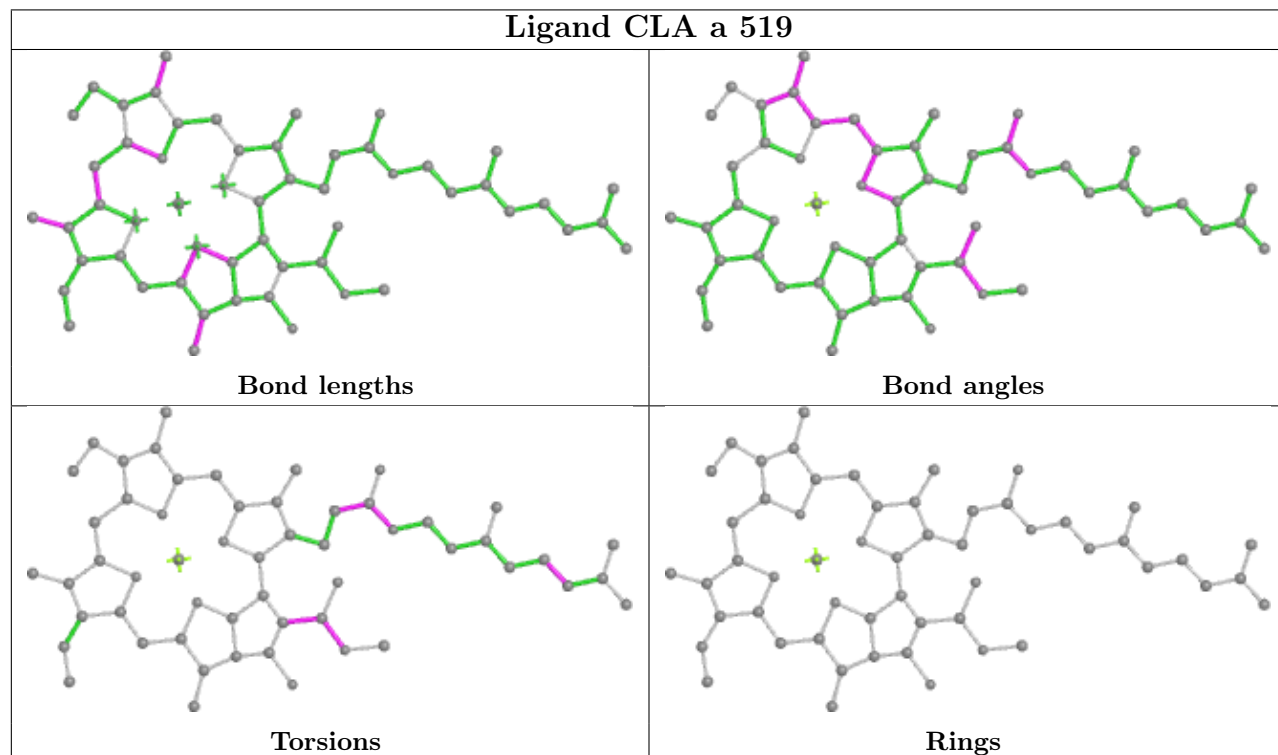
Ligand BCR H 4010



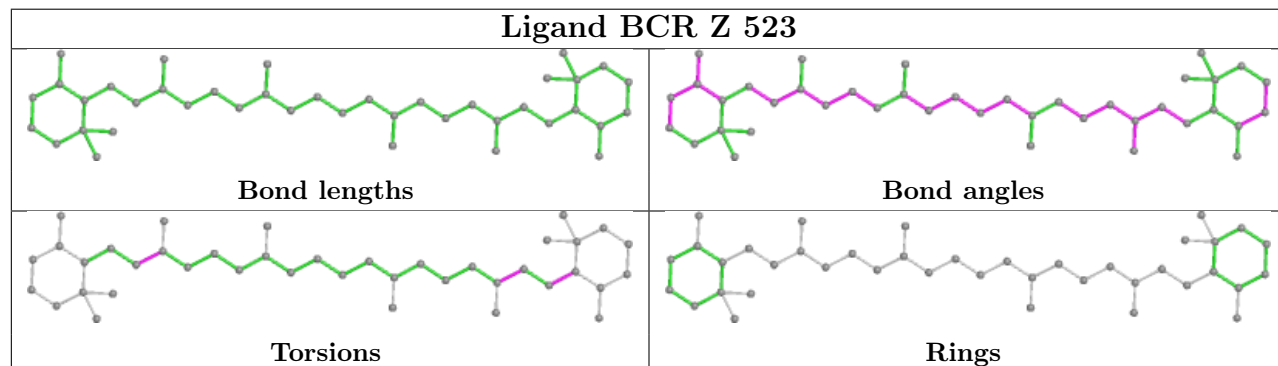
Ligand CLA f 1230

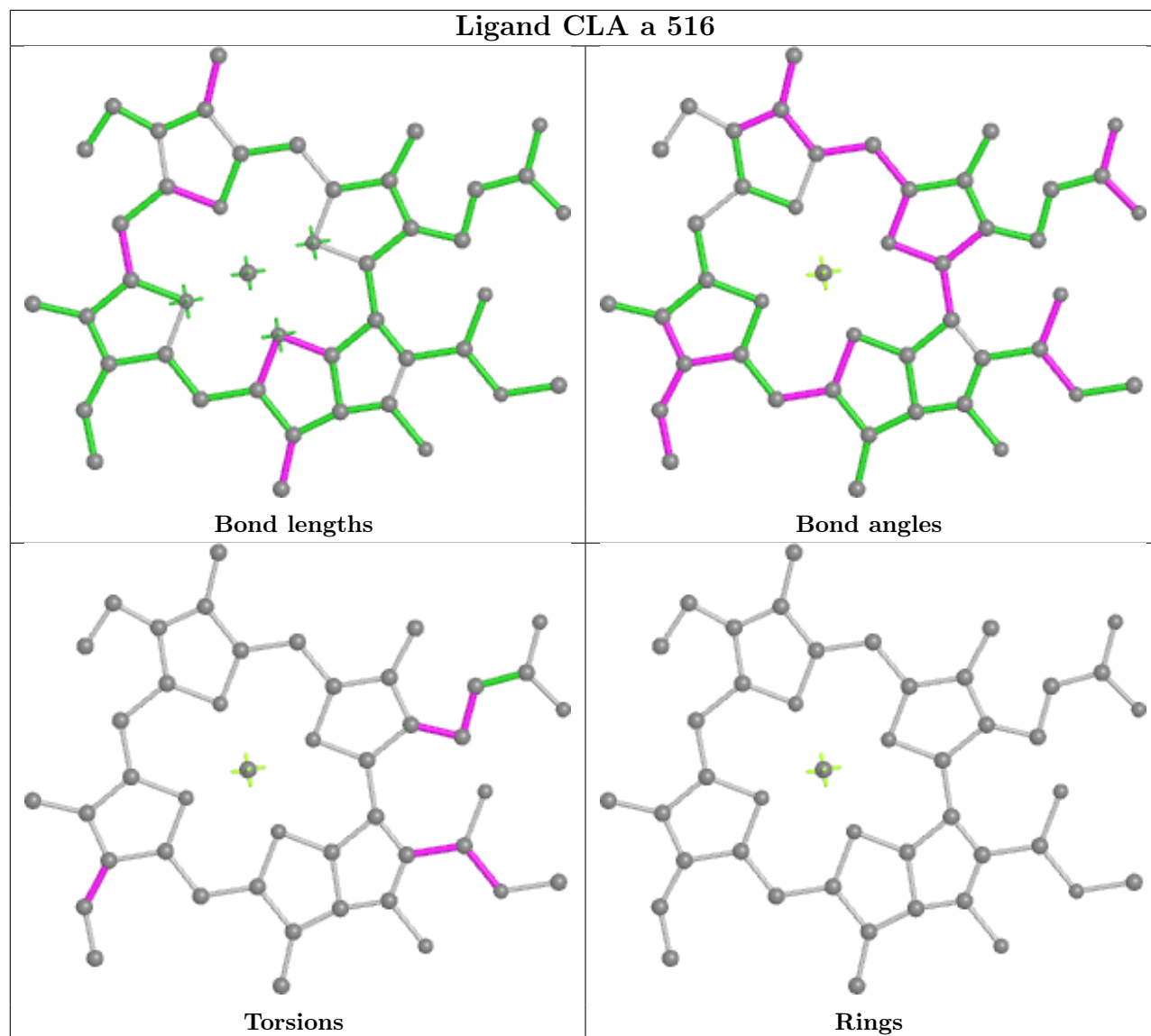
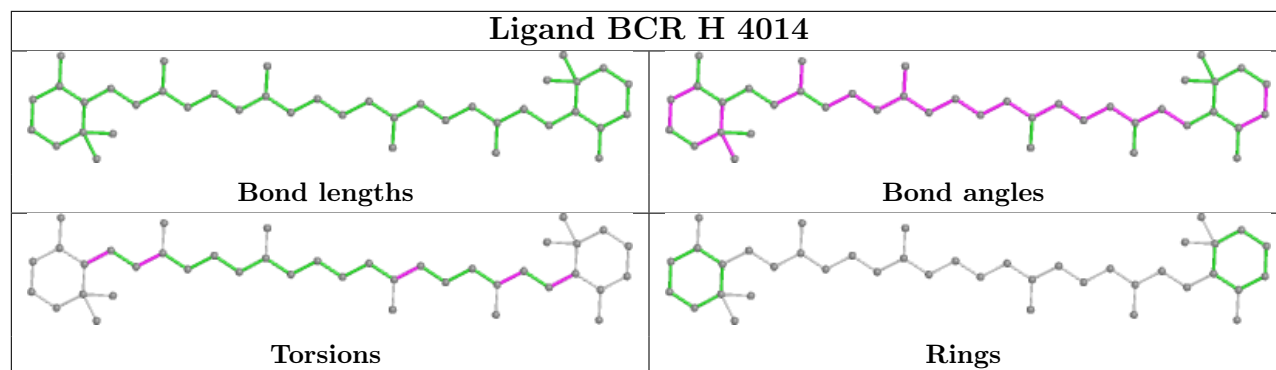


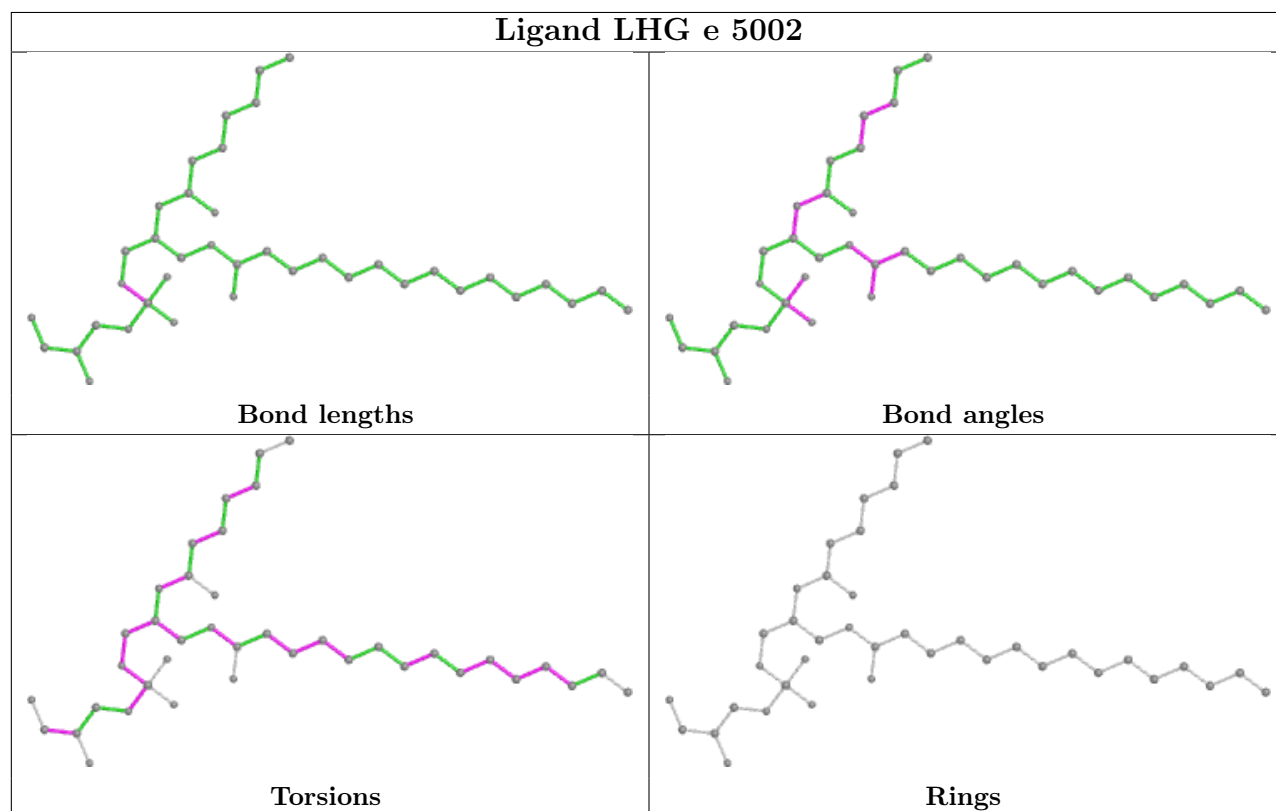
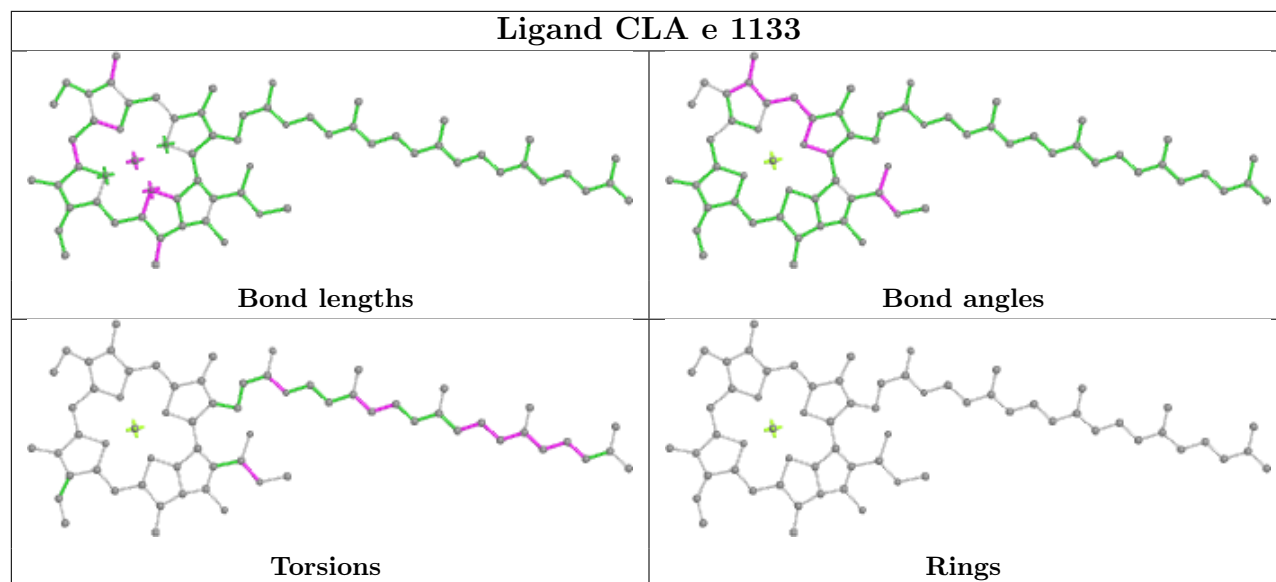
Ligand CLA a 519



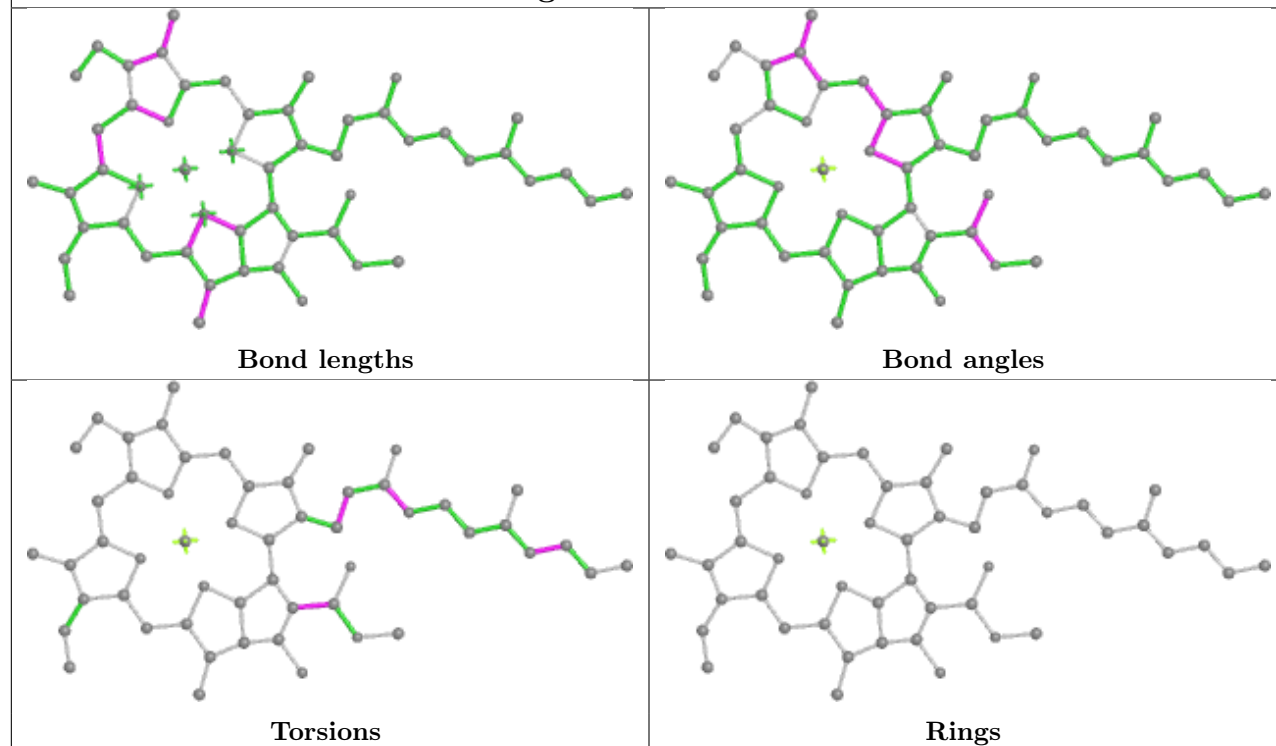
Ligand BCR Z 523



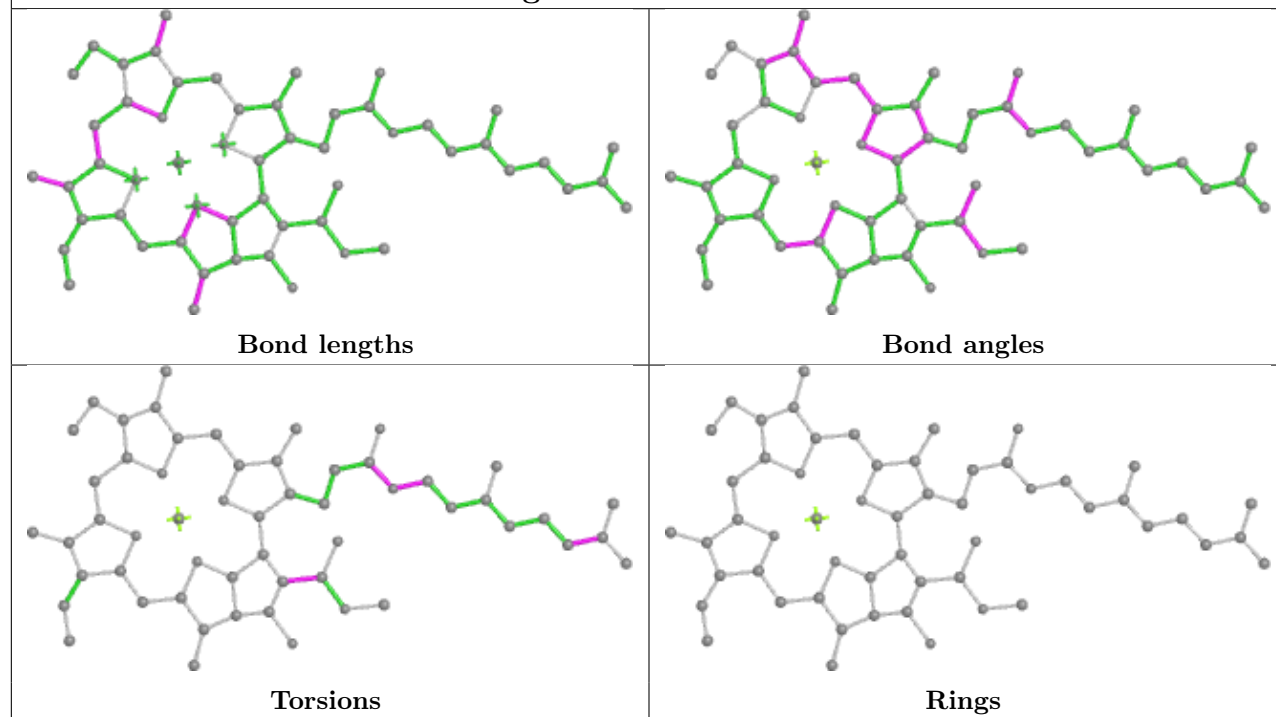


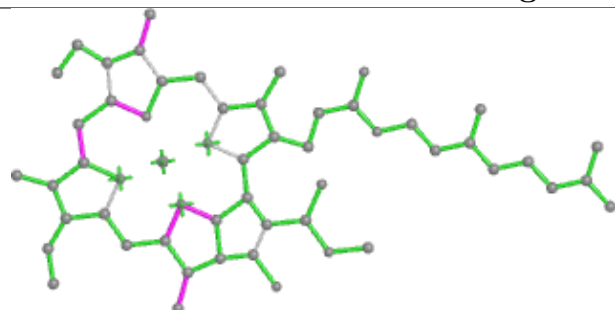


Ligand CLA r 512

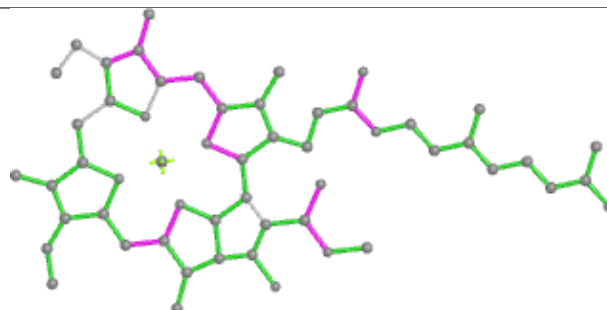


Ligand CLA A 1105

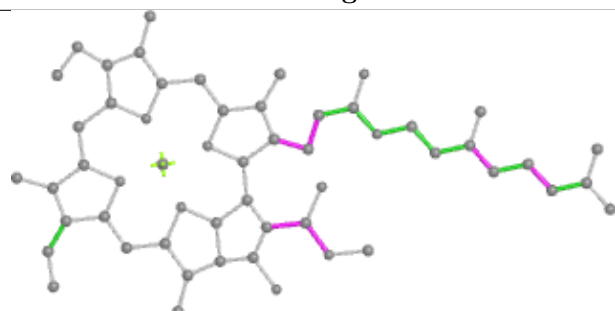


Ligand CLA u 503

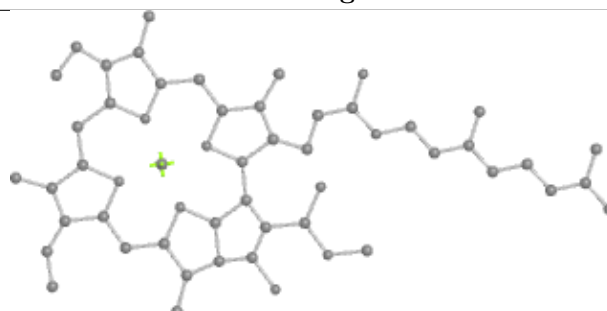
Bond lengths



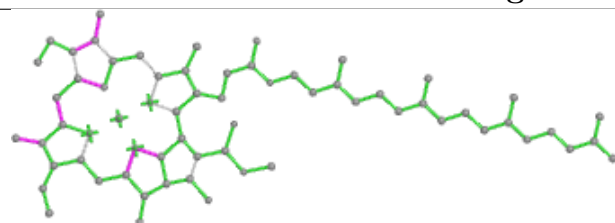
Bond angles



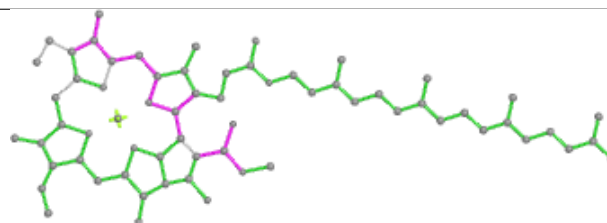
Torsions



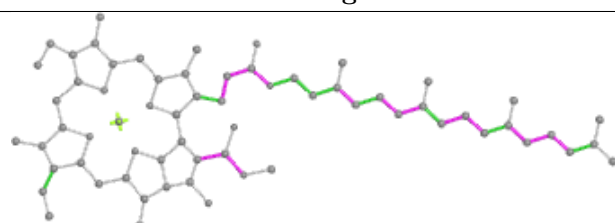
Rings

Ligand CLA A 1137

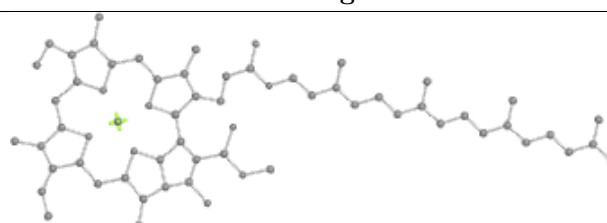
Bond lengths



Bond angles

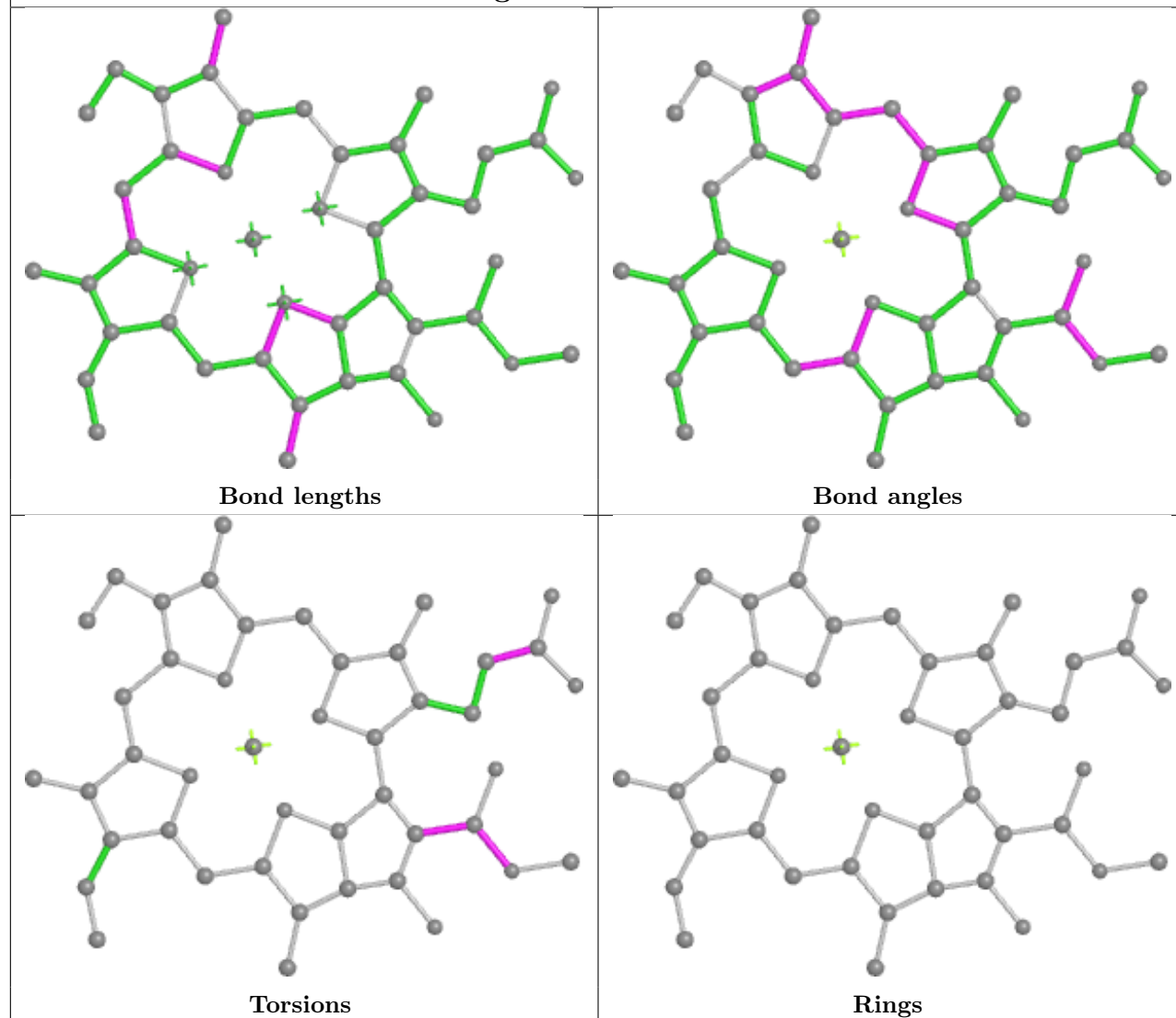


Torsions

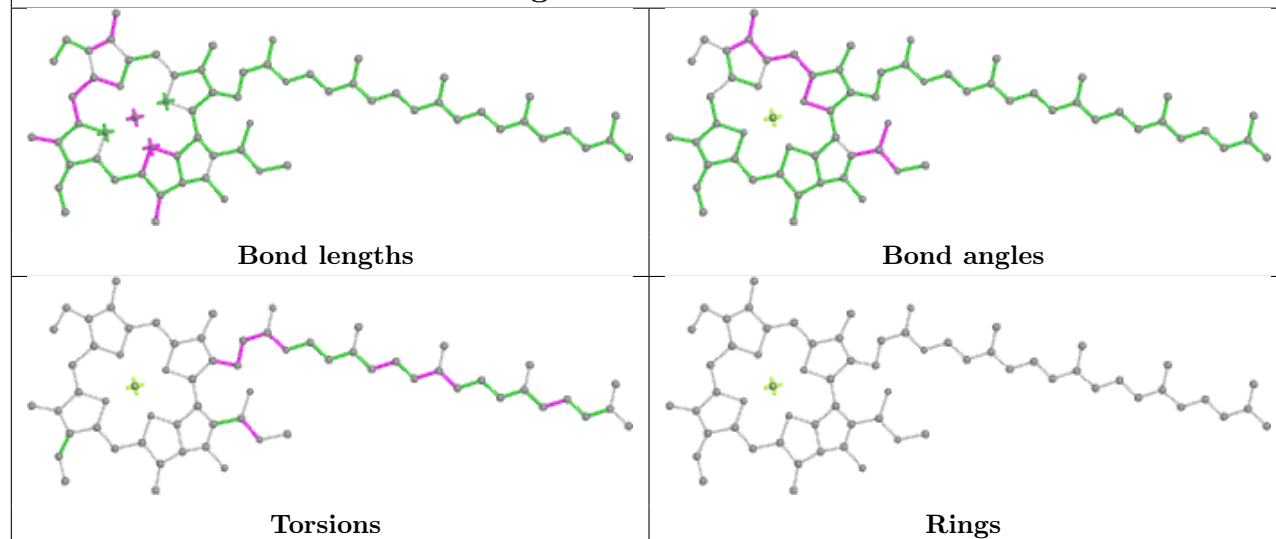


Rings

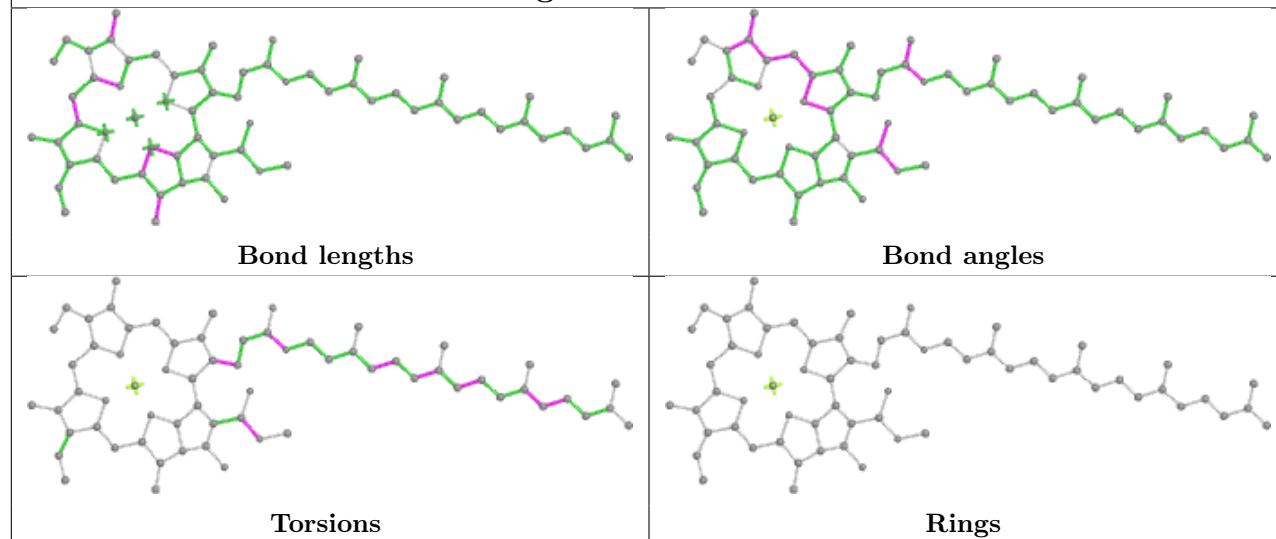
Ligand CLA 5 510



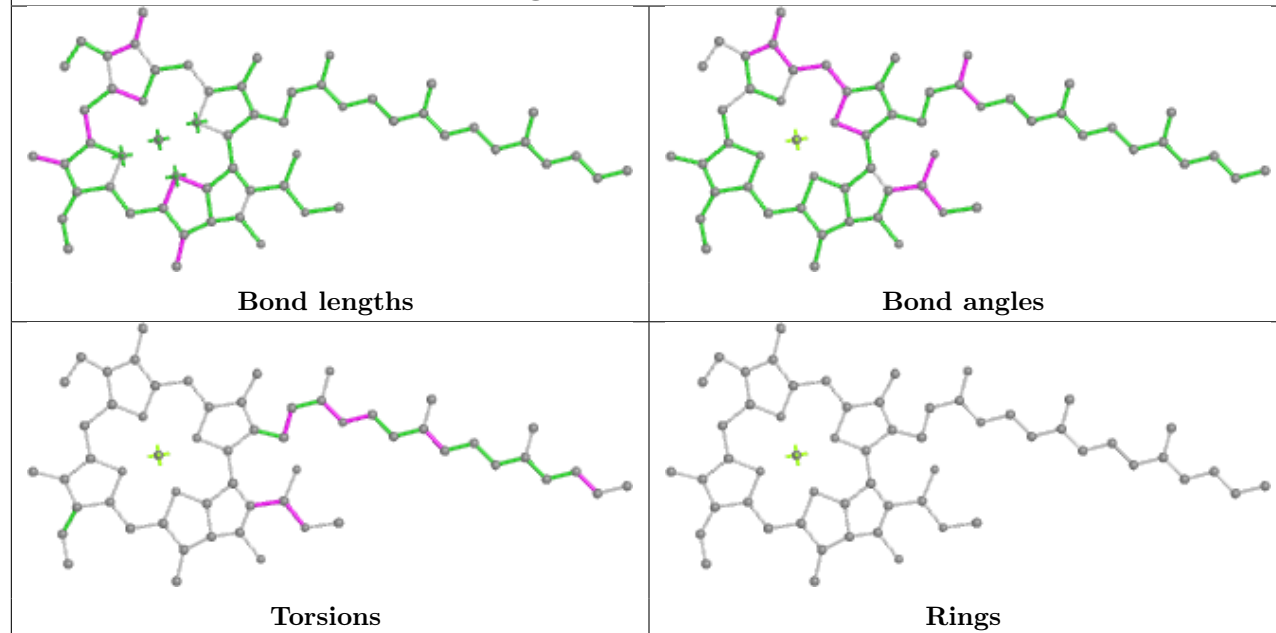
Ligand CLA f 1206

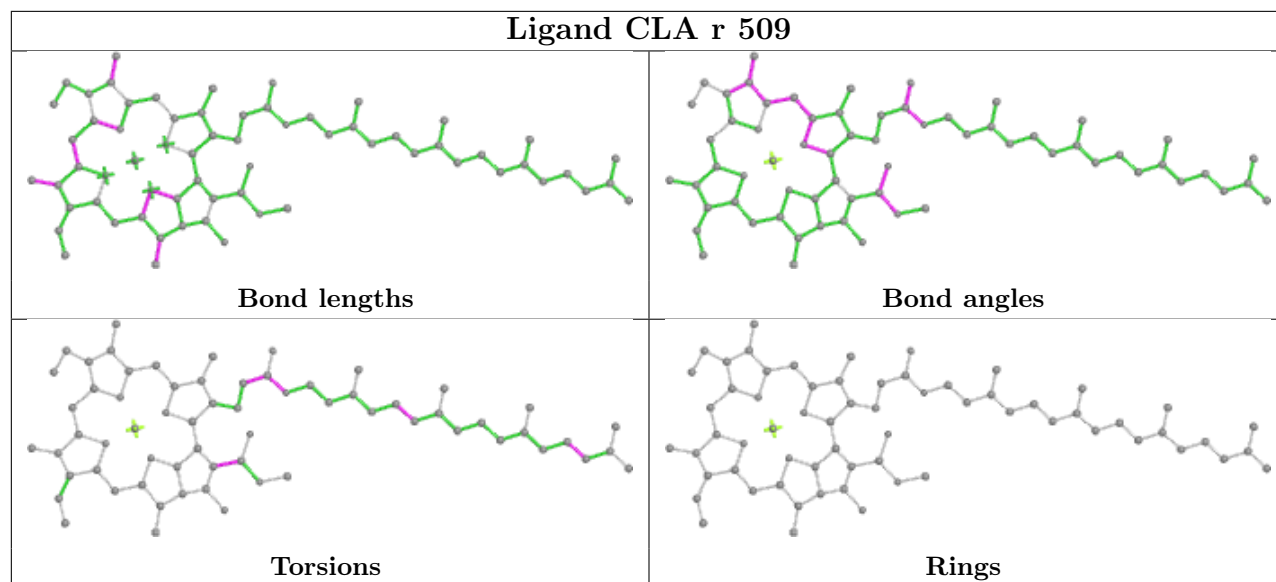
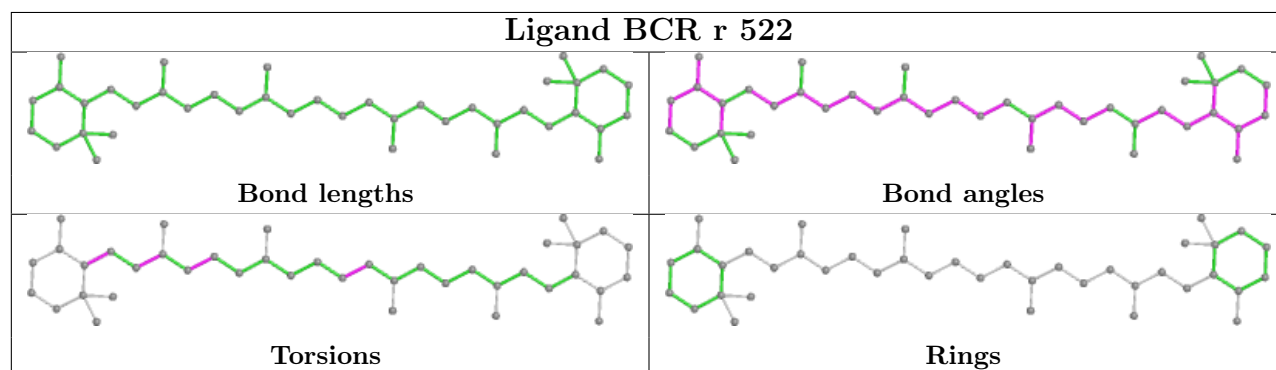


Ligand CLA a 513

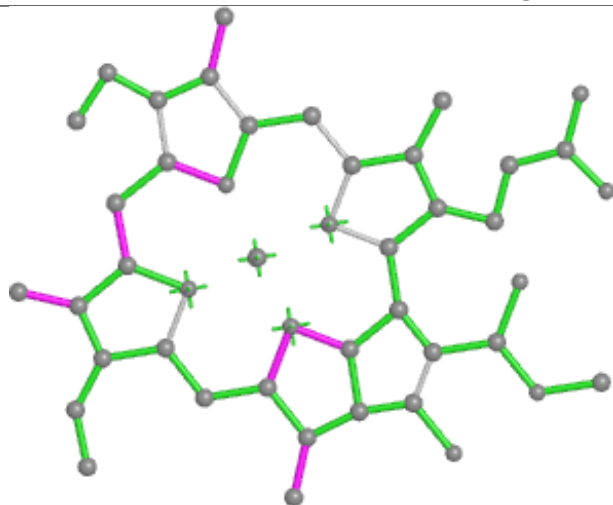


Ligand CLA J 1302

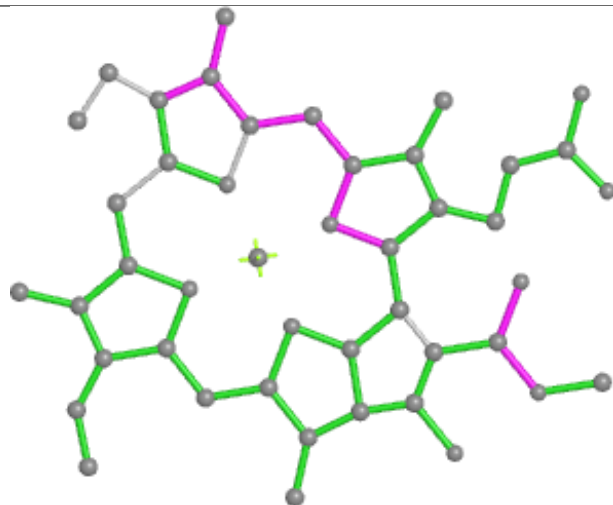


Ligand CLA r 509**Ligand BCR r 522**

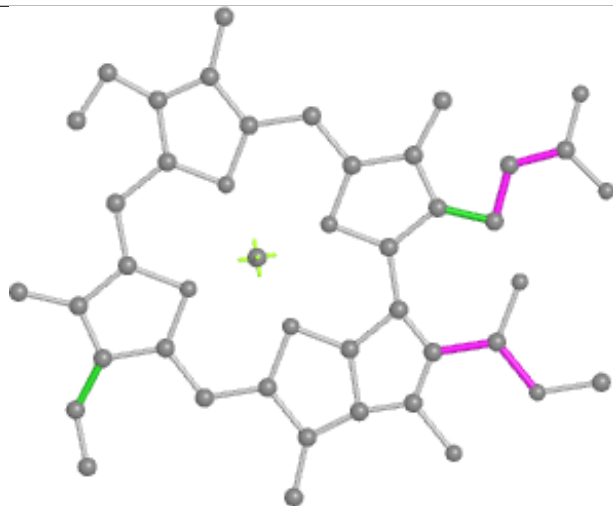
Ligand CLA b 513



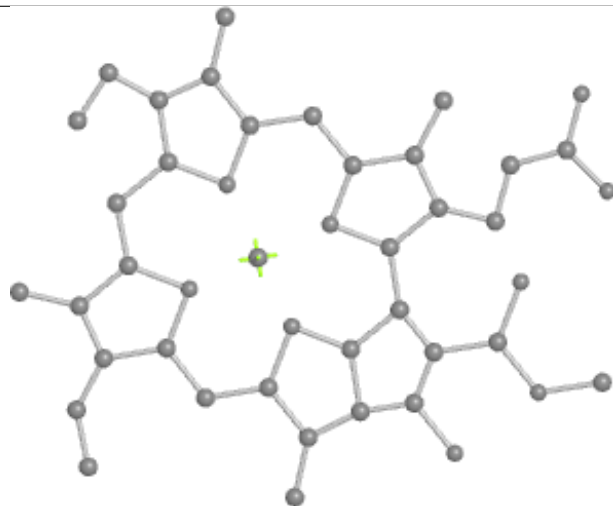
Bond lengths



Bond angles

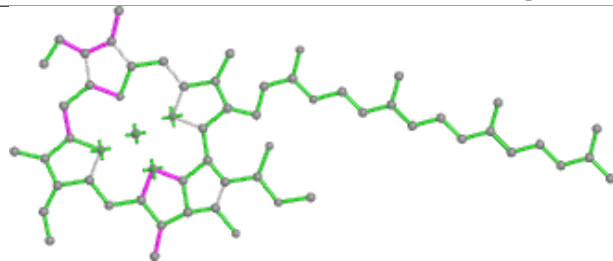


Torsions

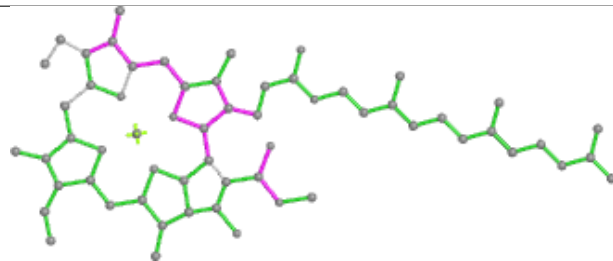


Rings

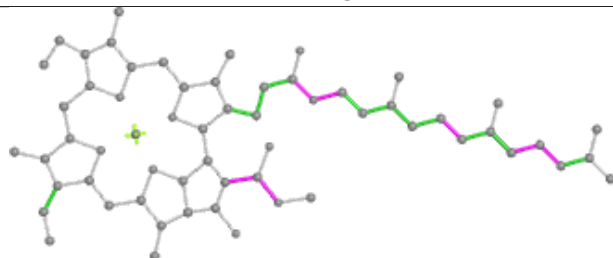
Ligand CLA r 502



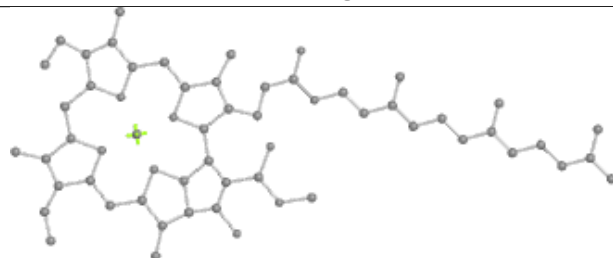
Bond lengths



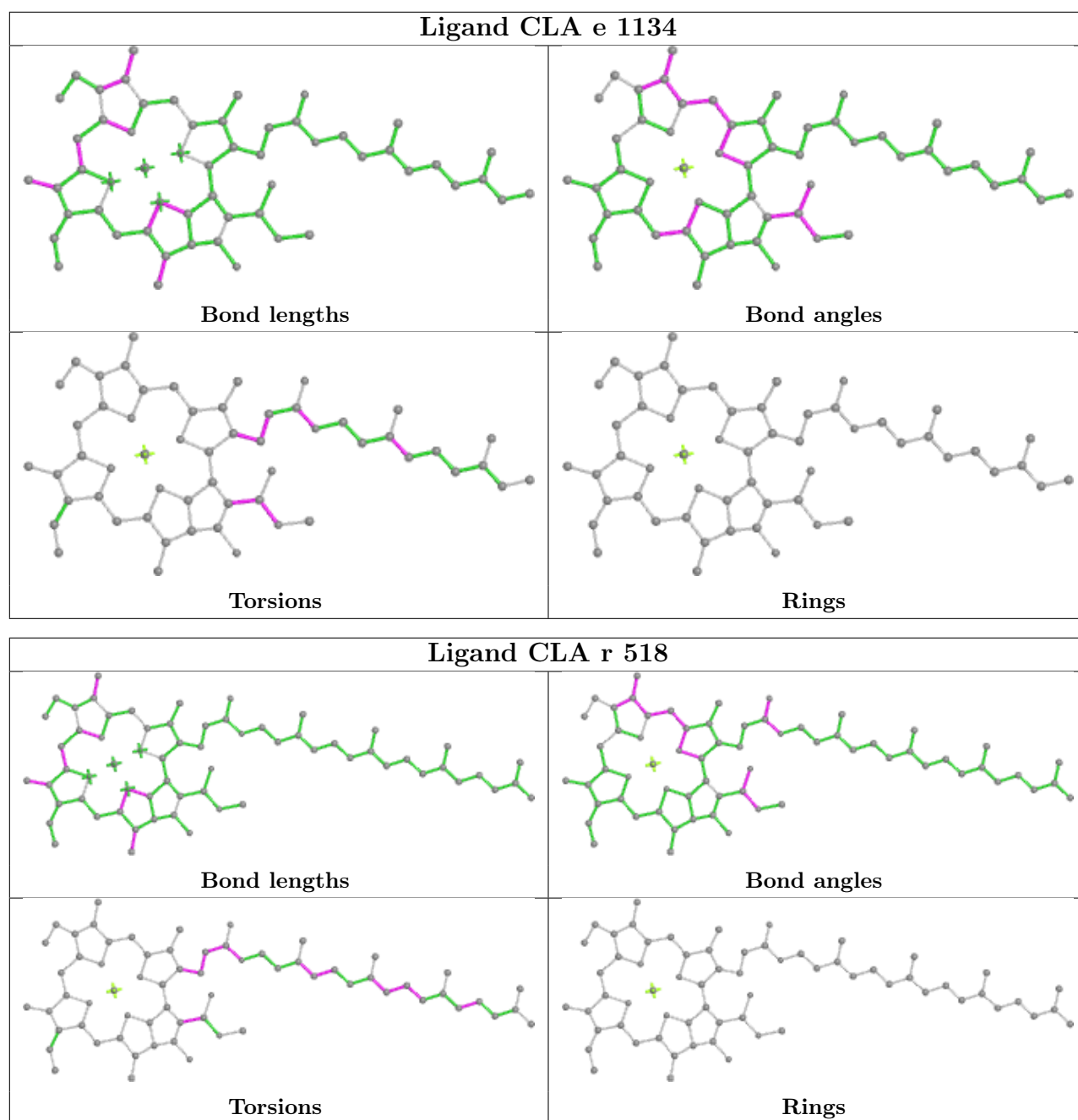
Bond angles

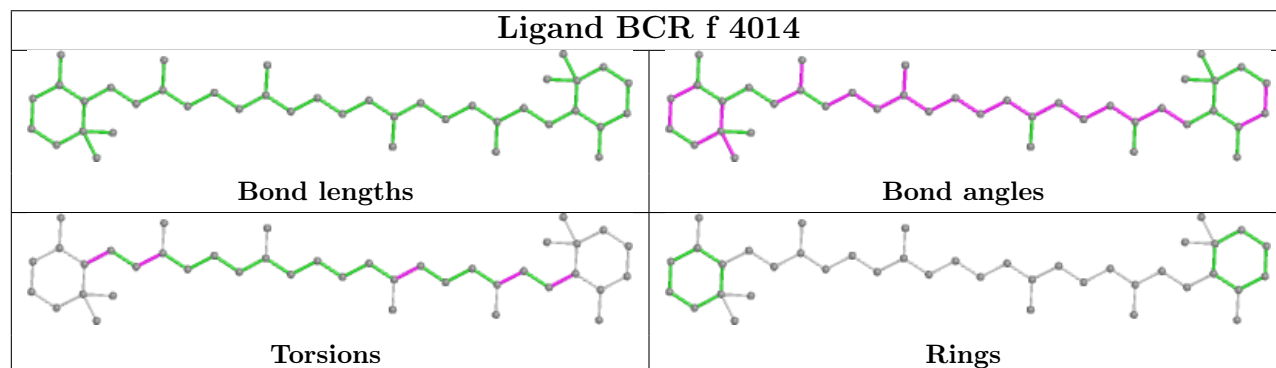
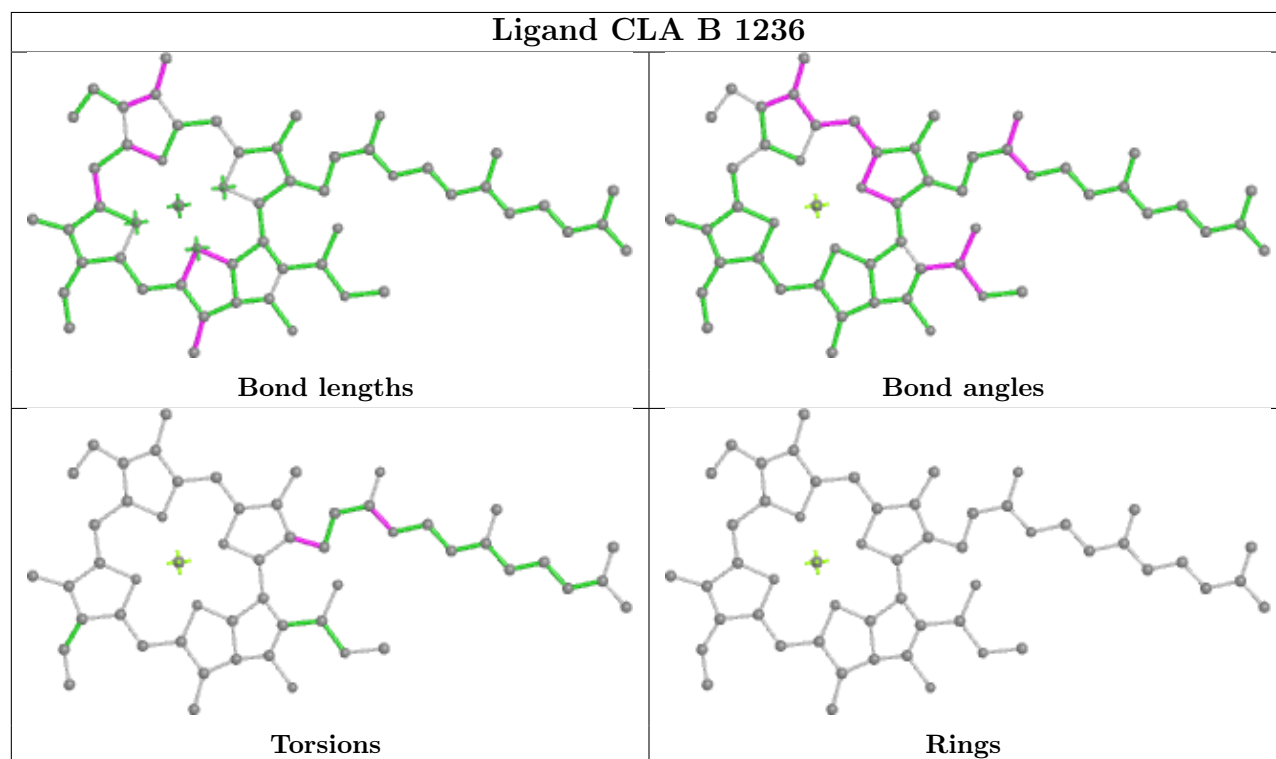
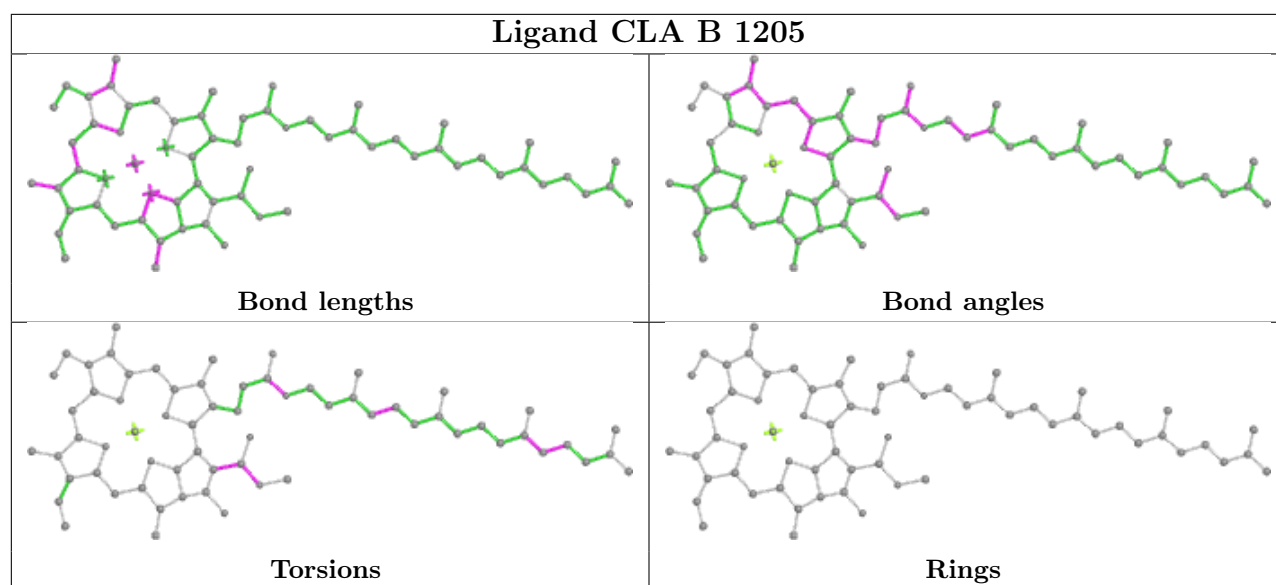


Torsions

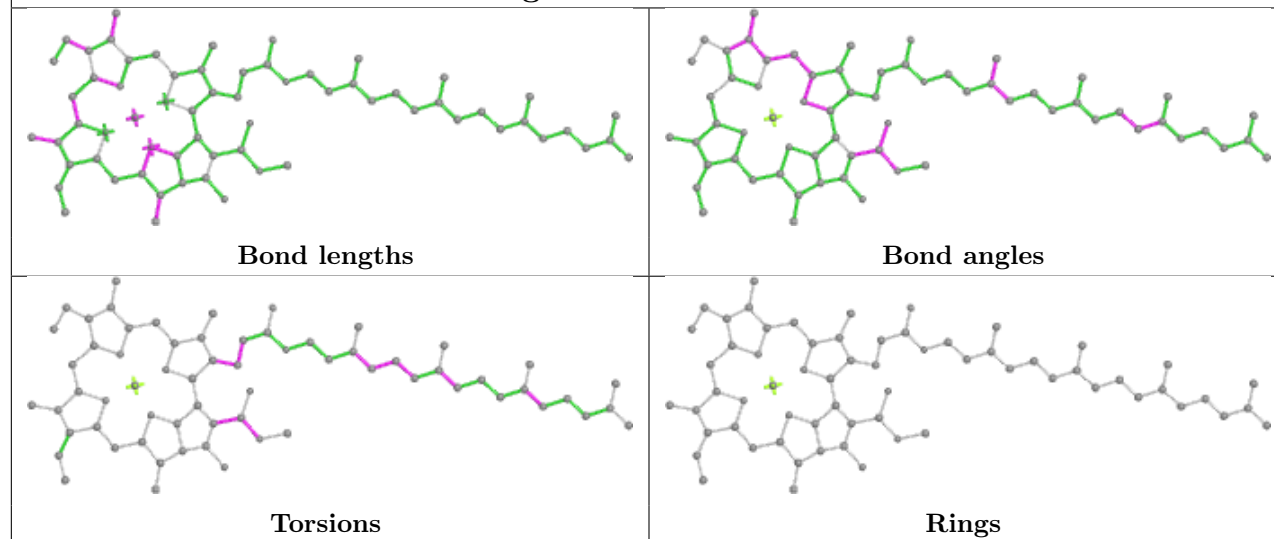


Rings

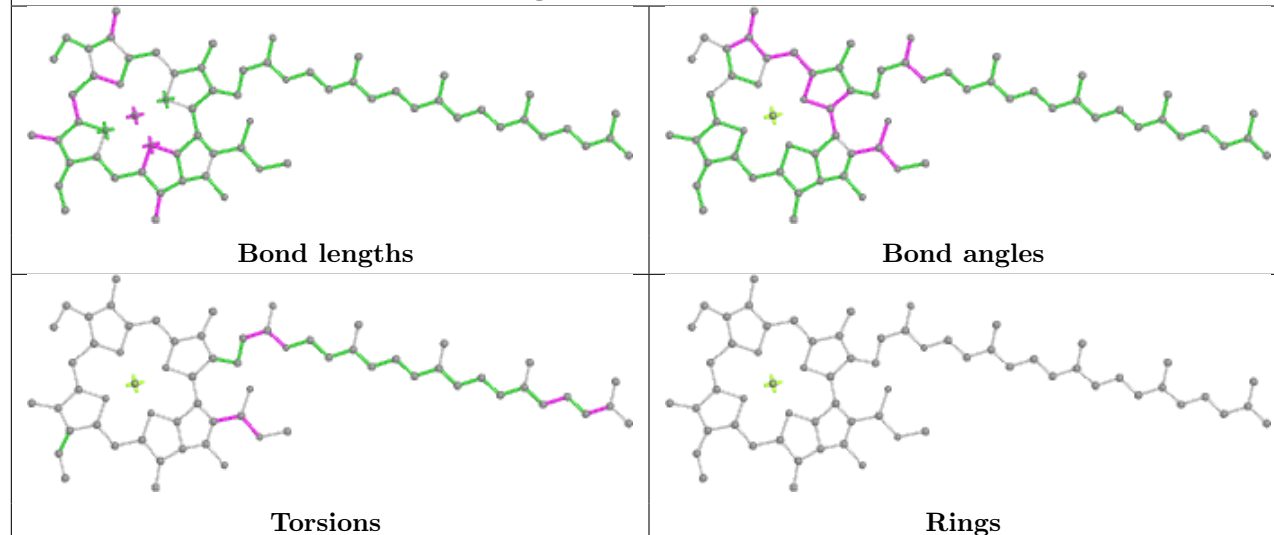




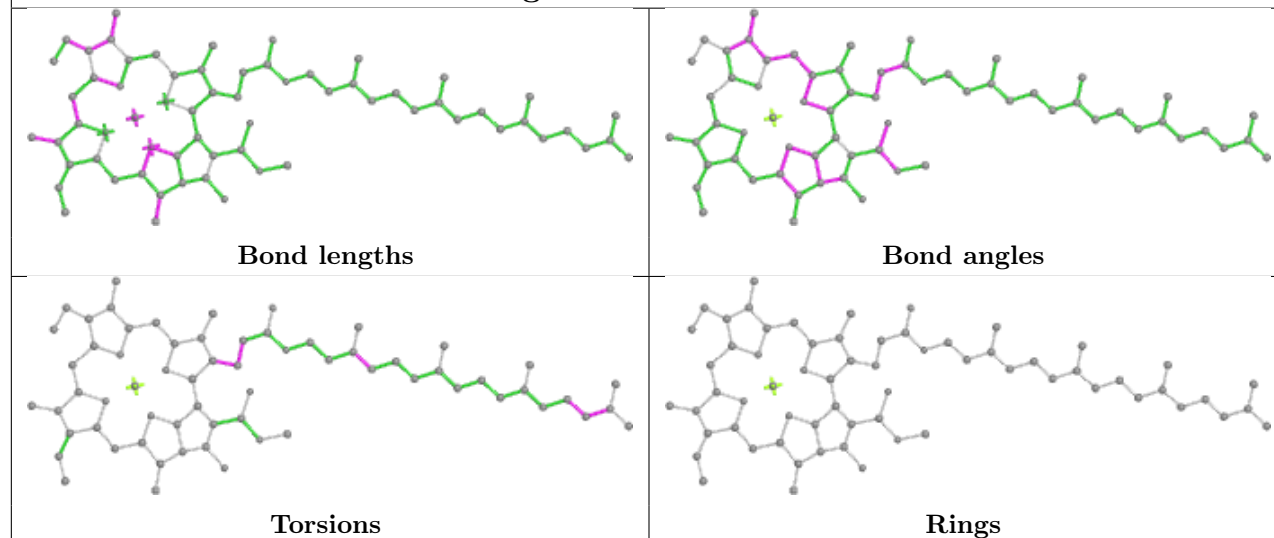
Ligand CLA H 1012



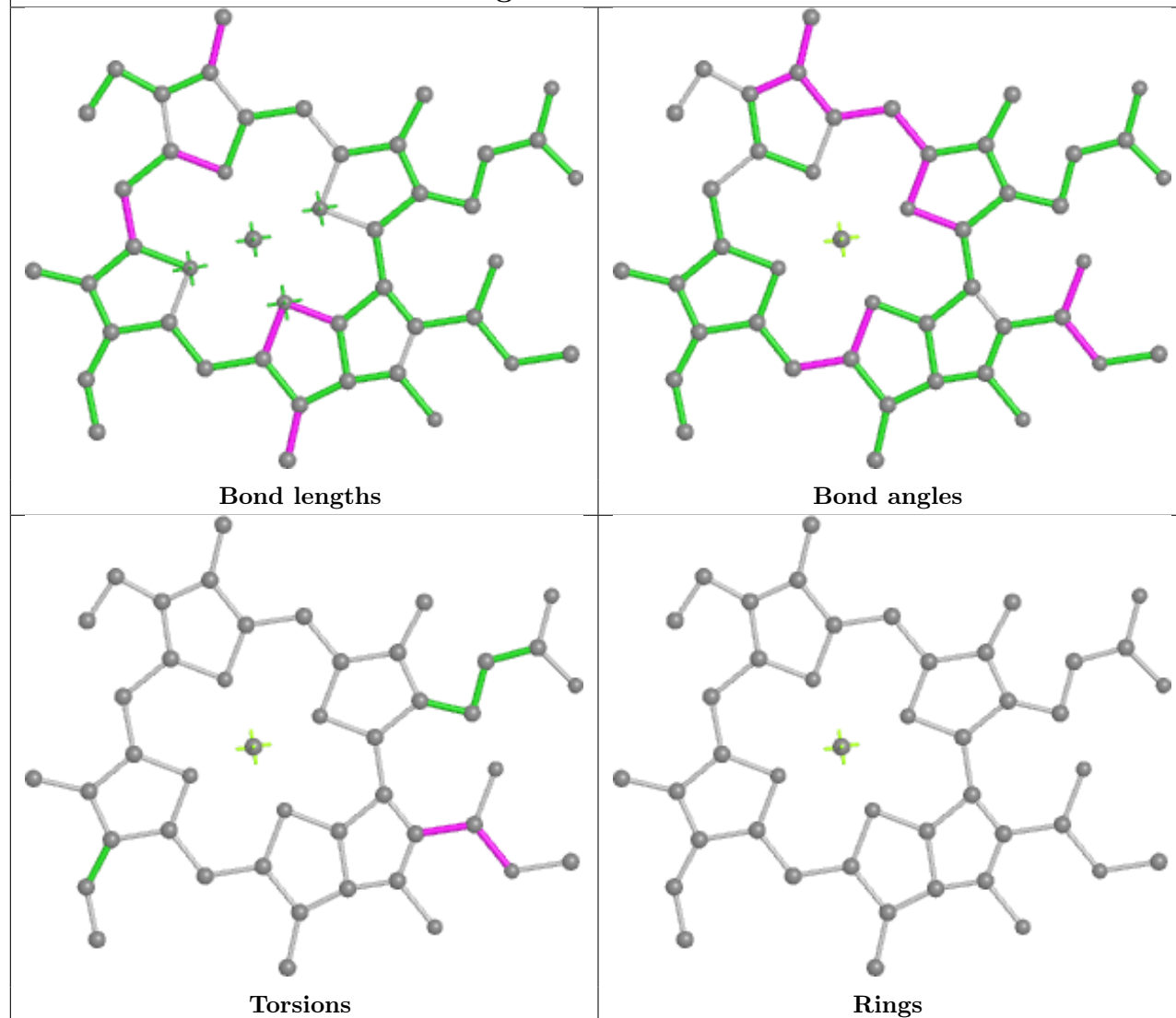
Ligand CLA f 1021



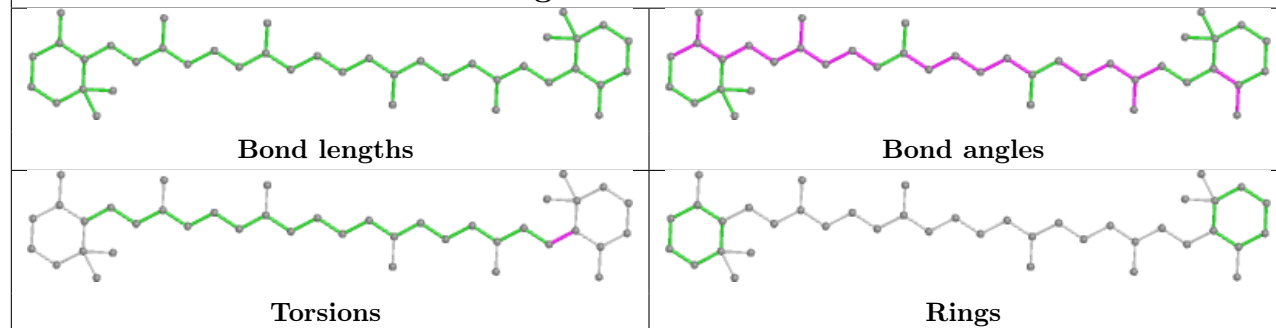
Ligand CLA A 1022

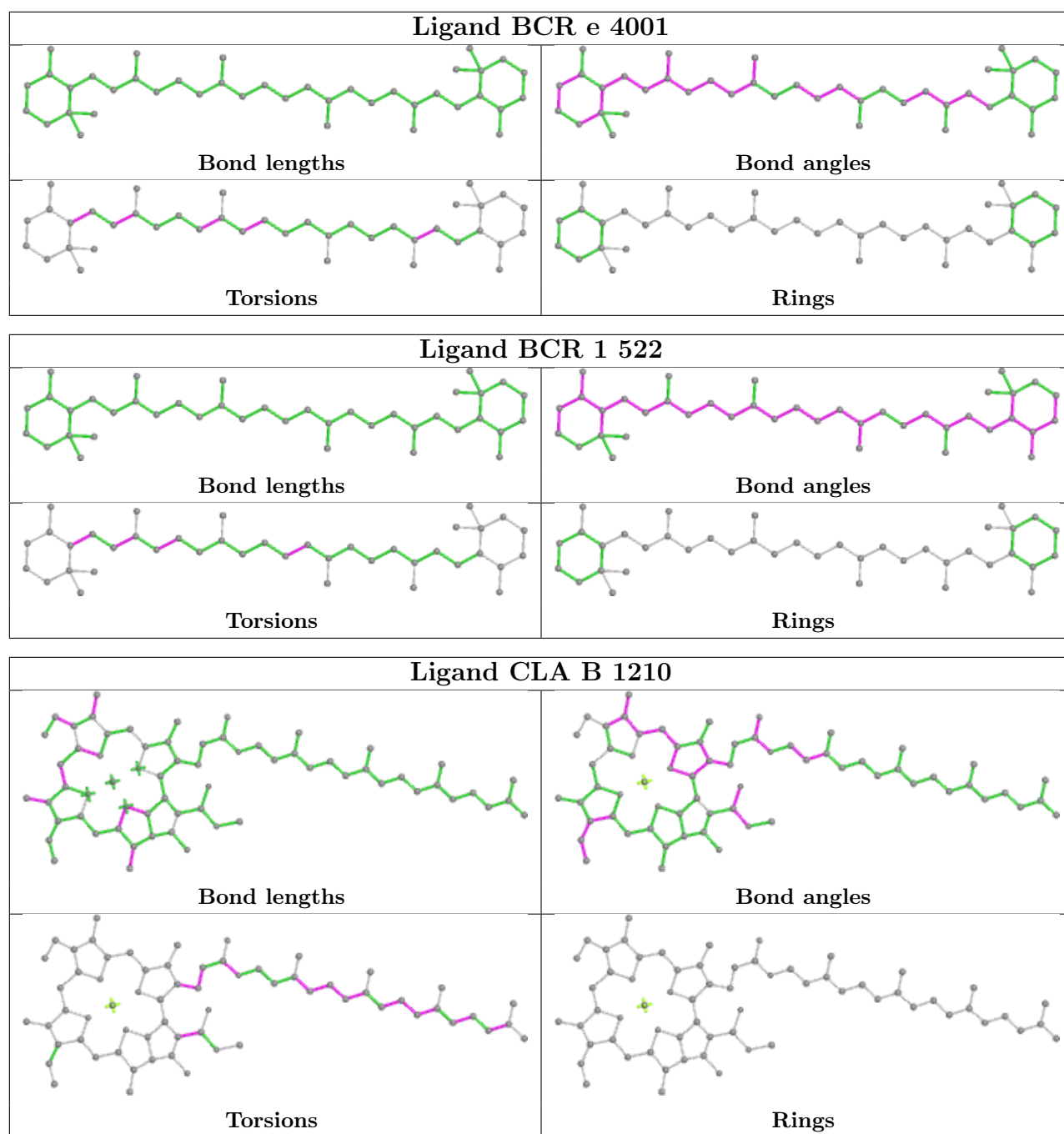


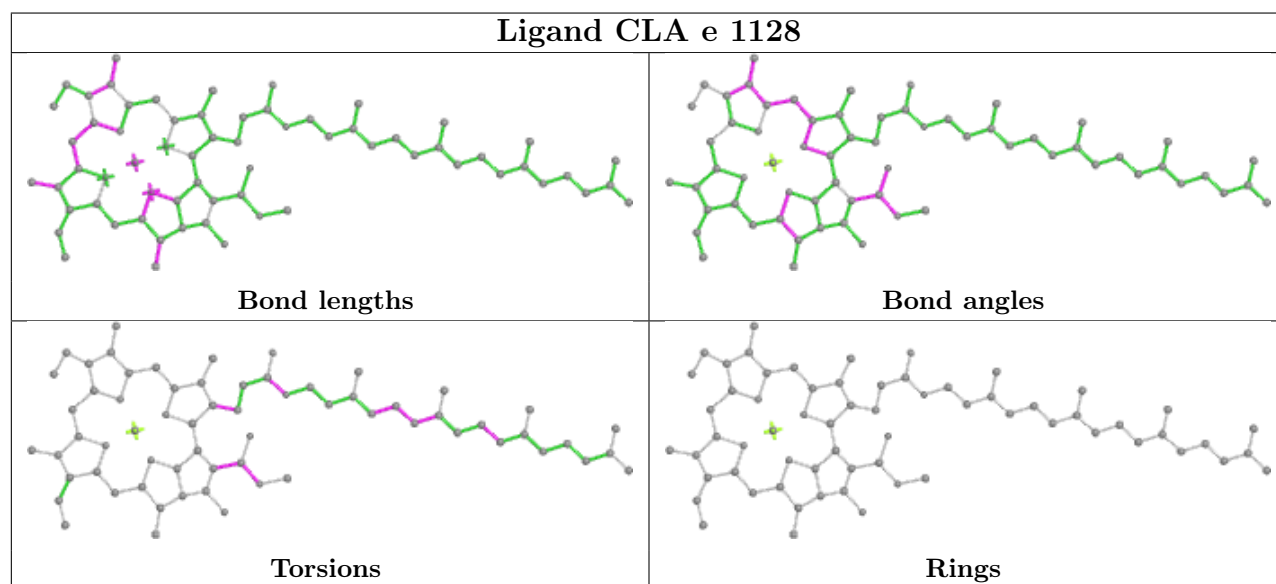
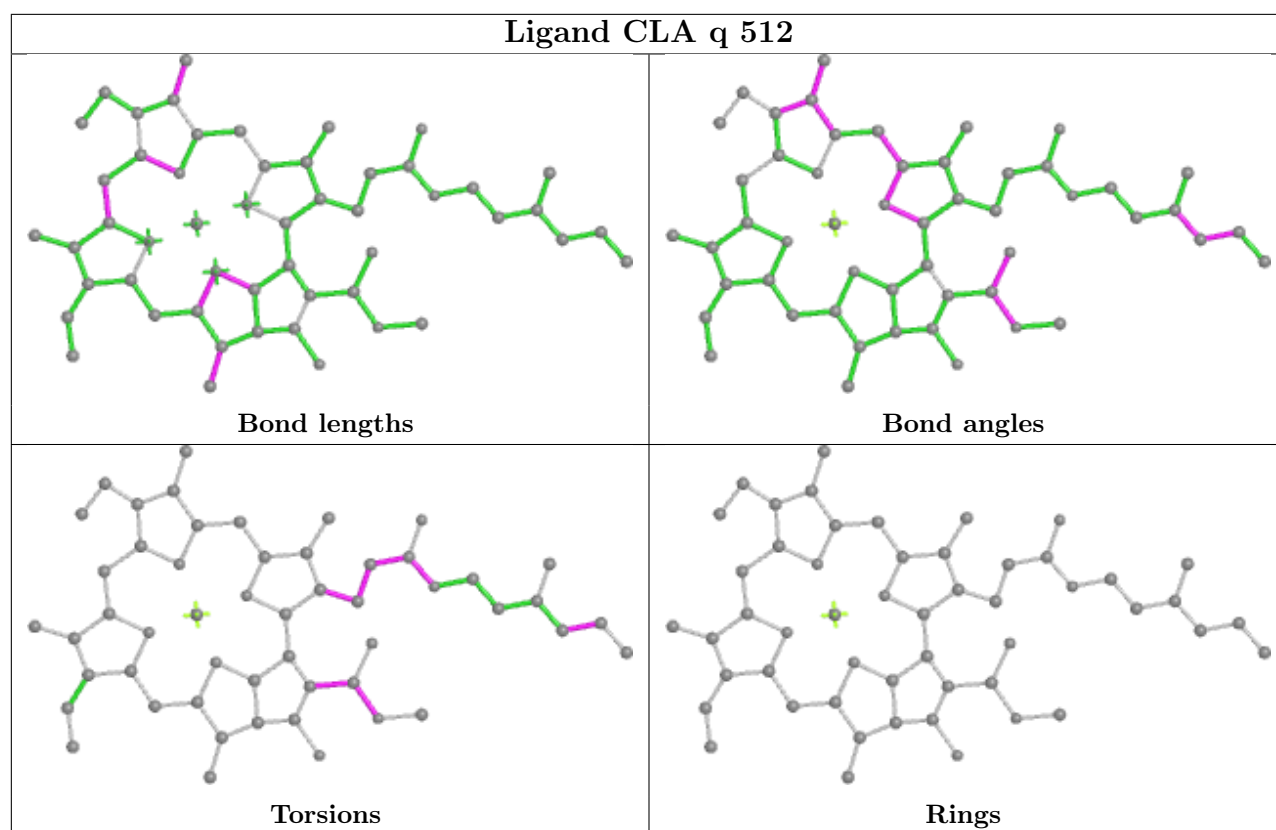
Ligand CLA t 504



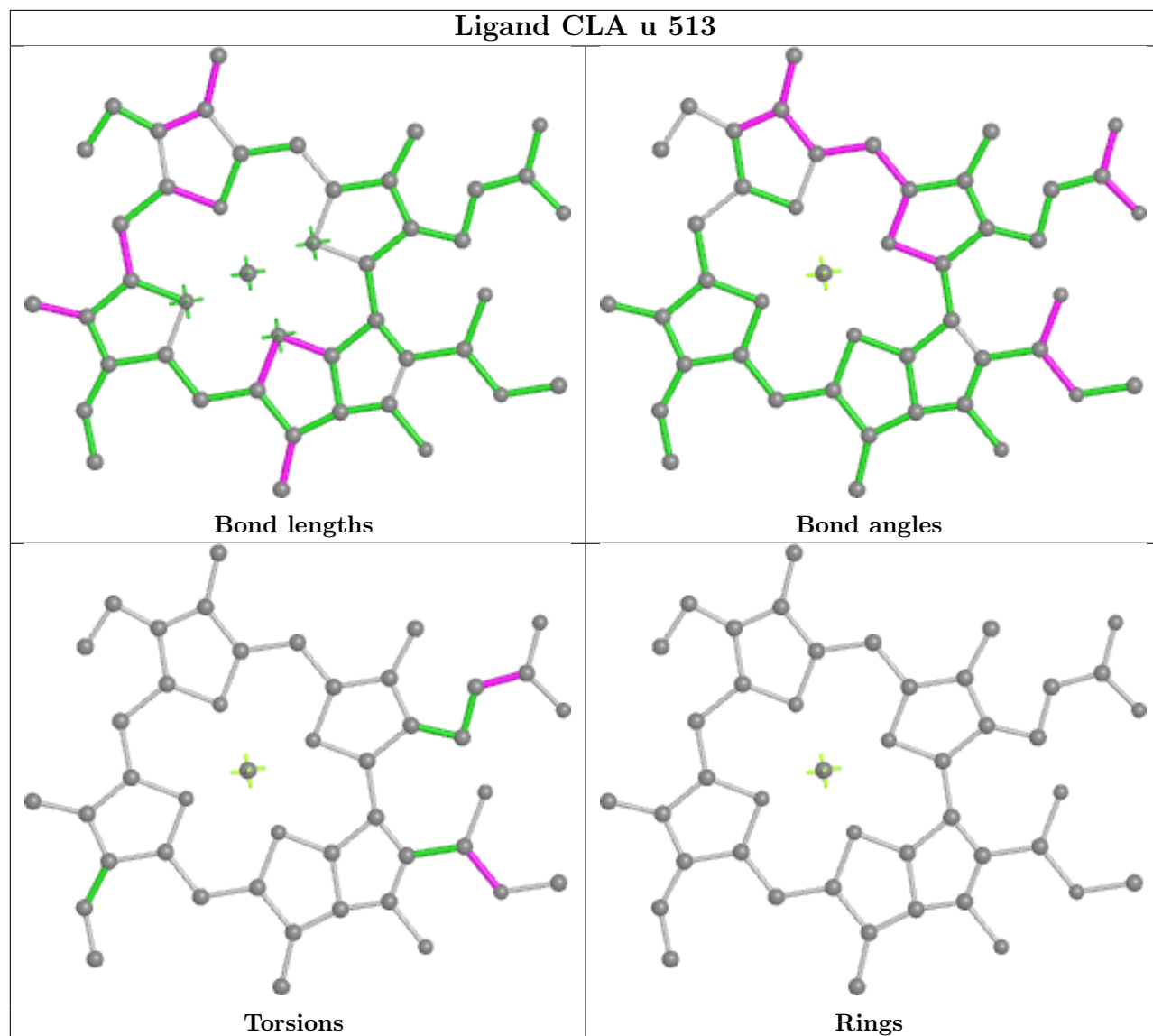
Ligand BCR 5 524



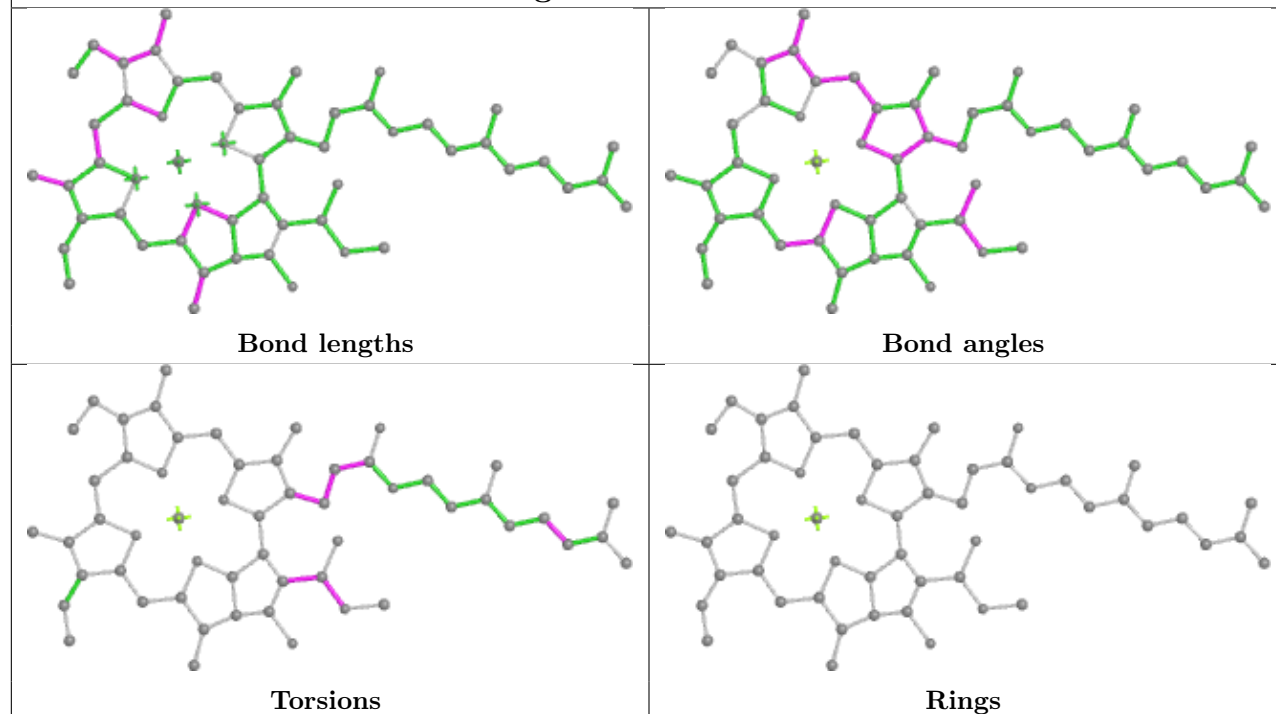




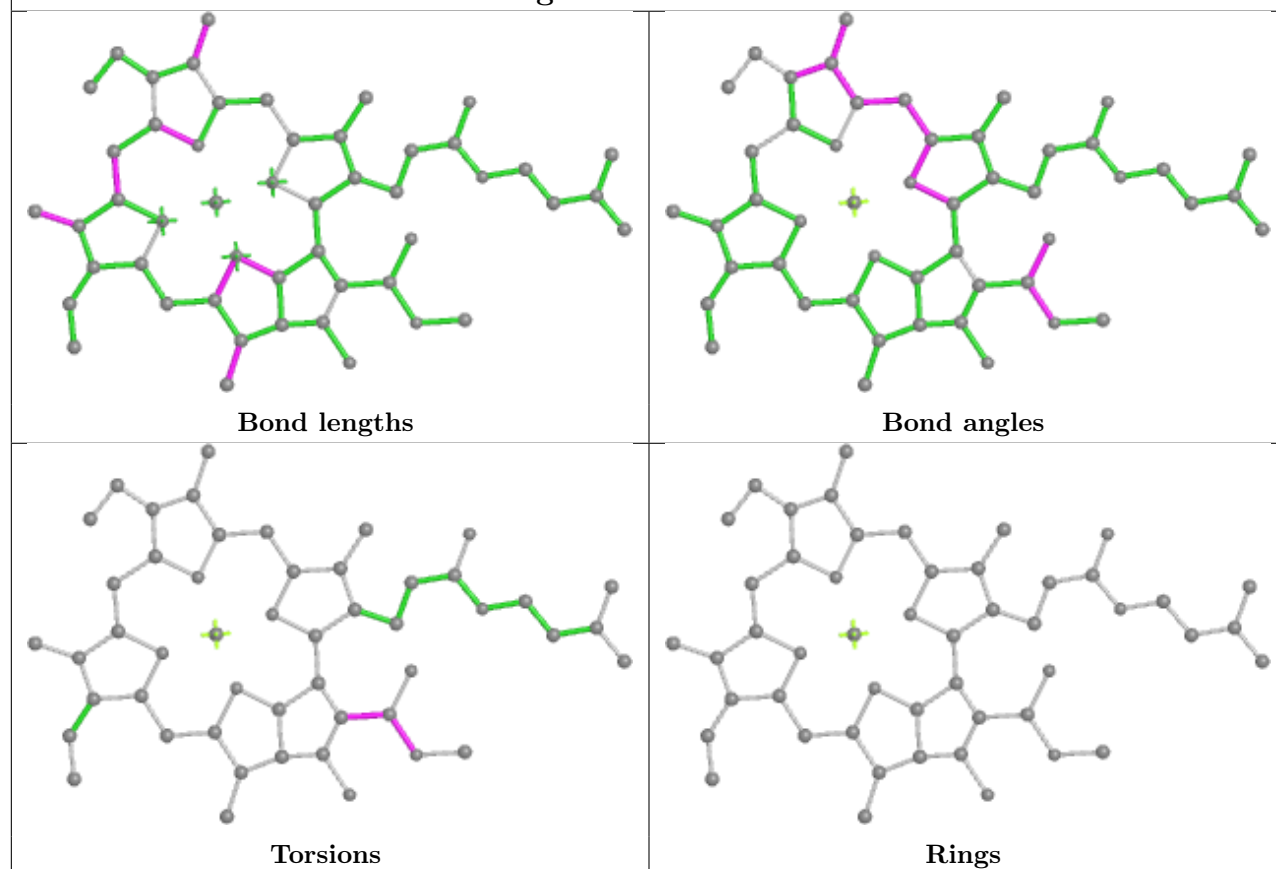
Ligand CLA u 513



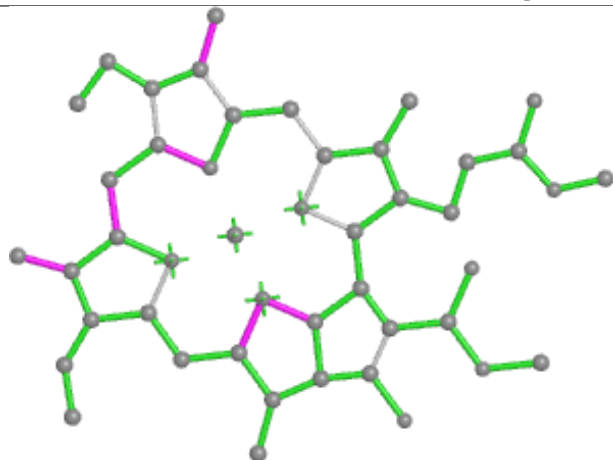
Ligand CLA Z 519



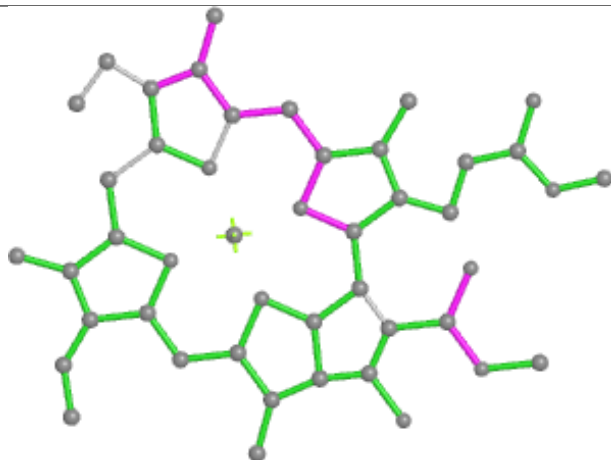
Ligand CLA a 506



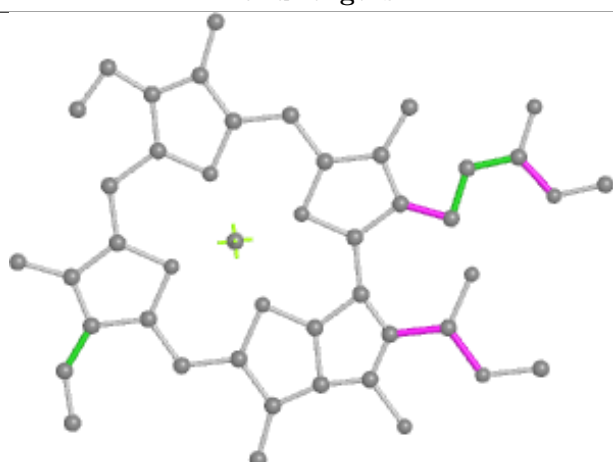
Ligand CLA 6 519



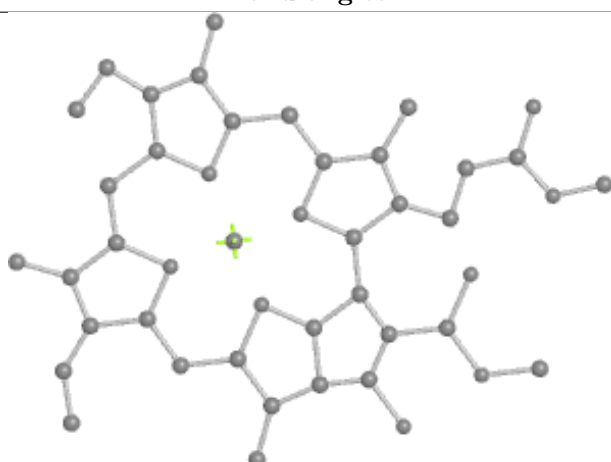
Bond lengths



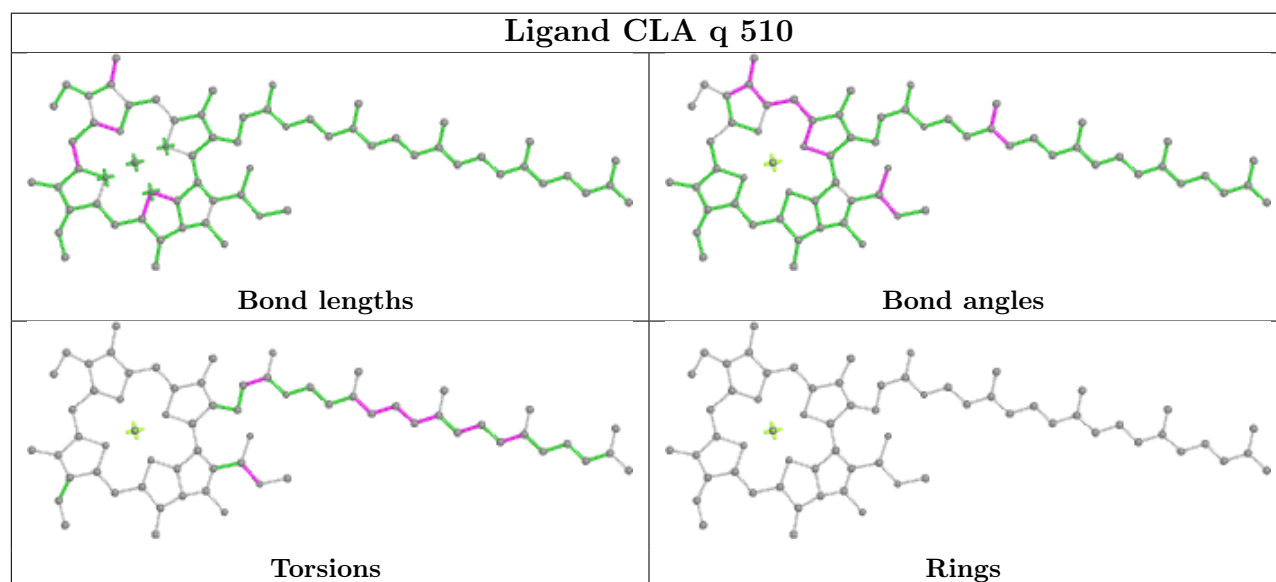
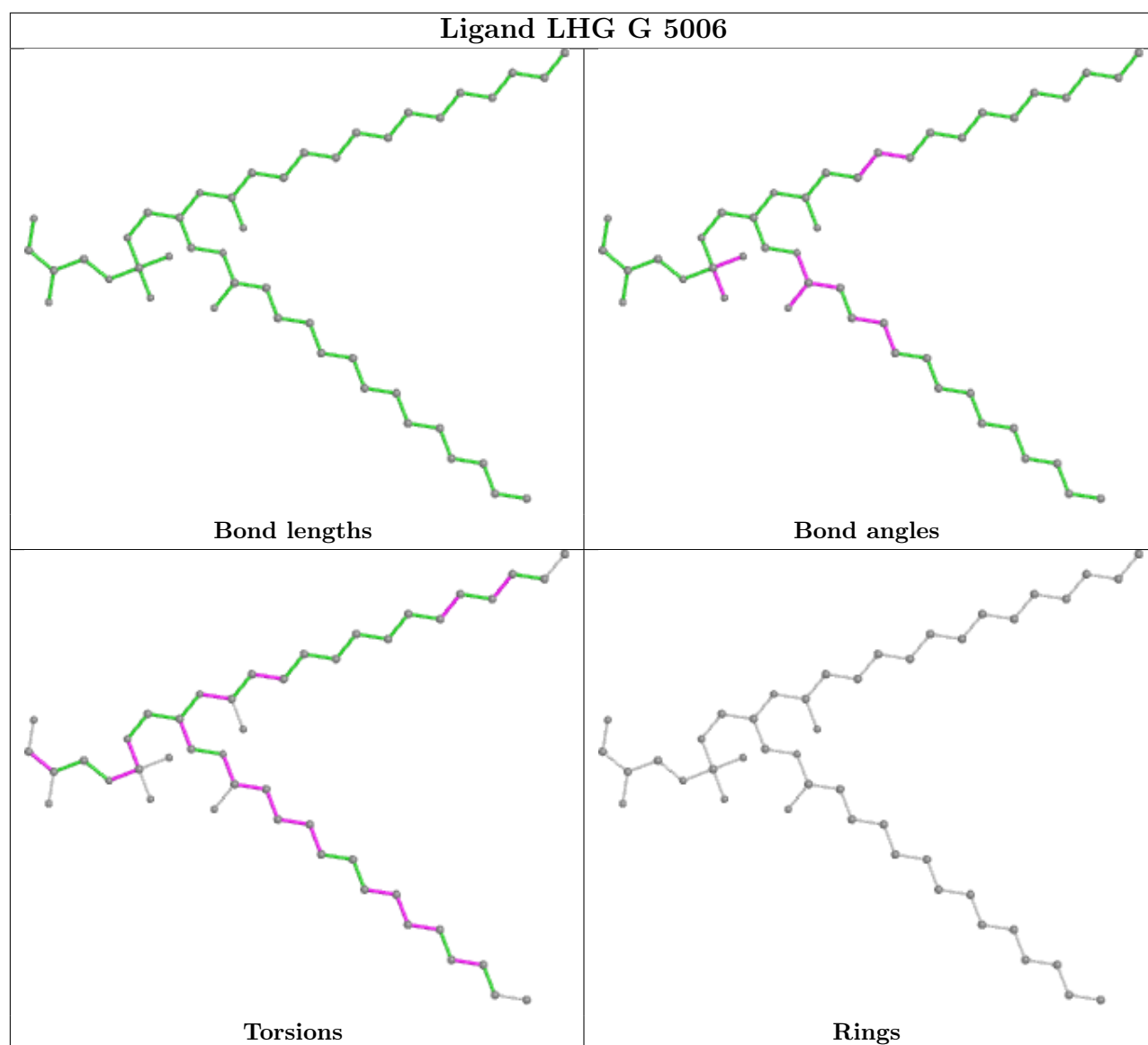
Bond angles

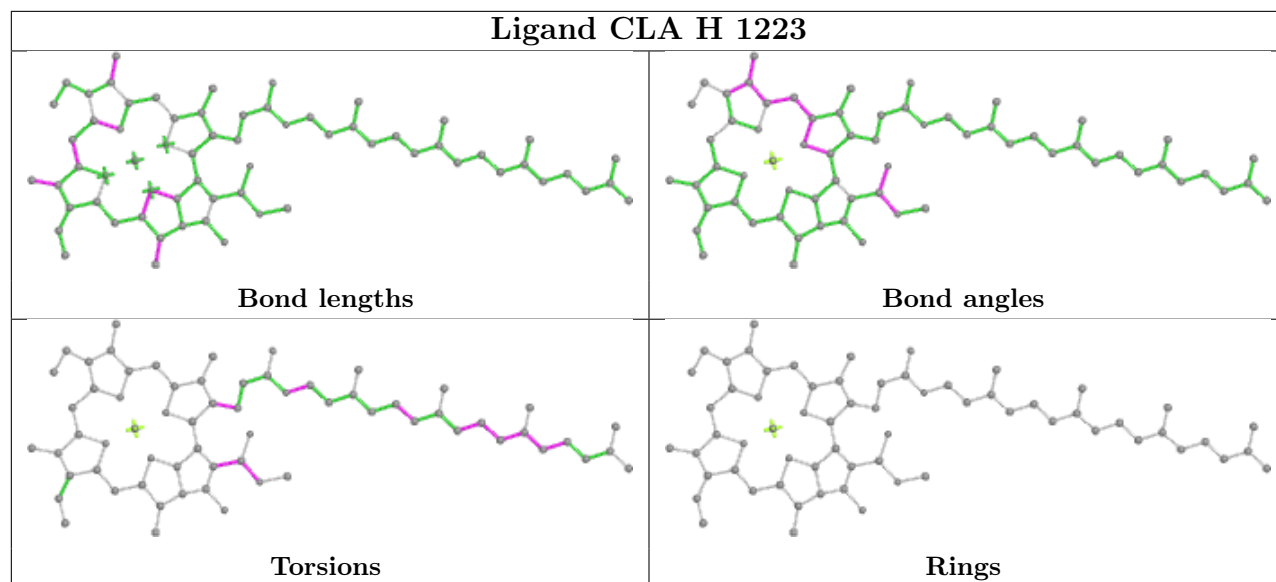
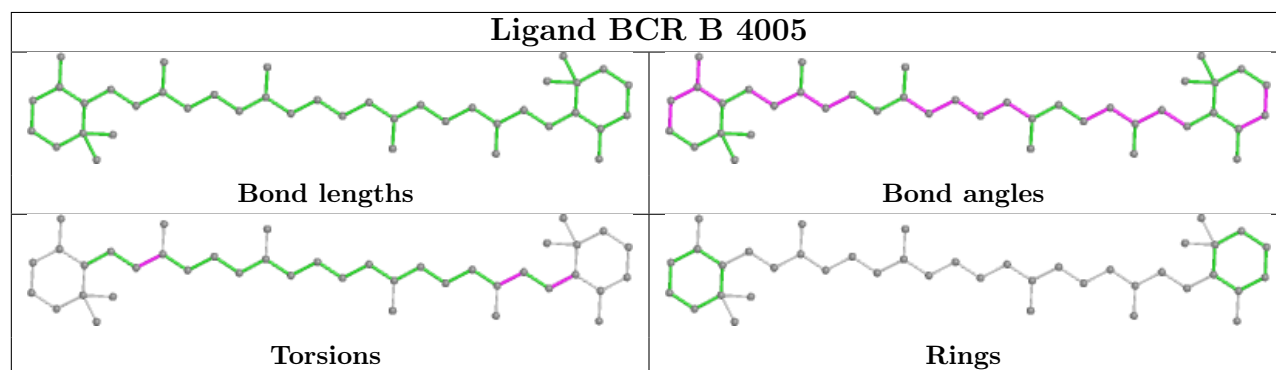


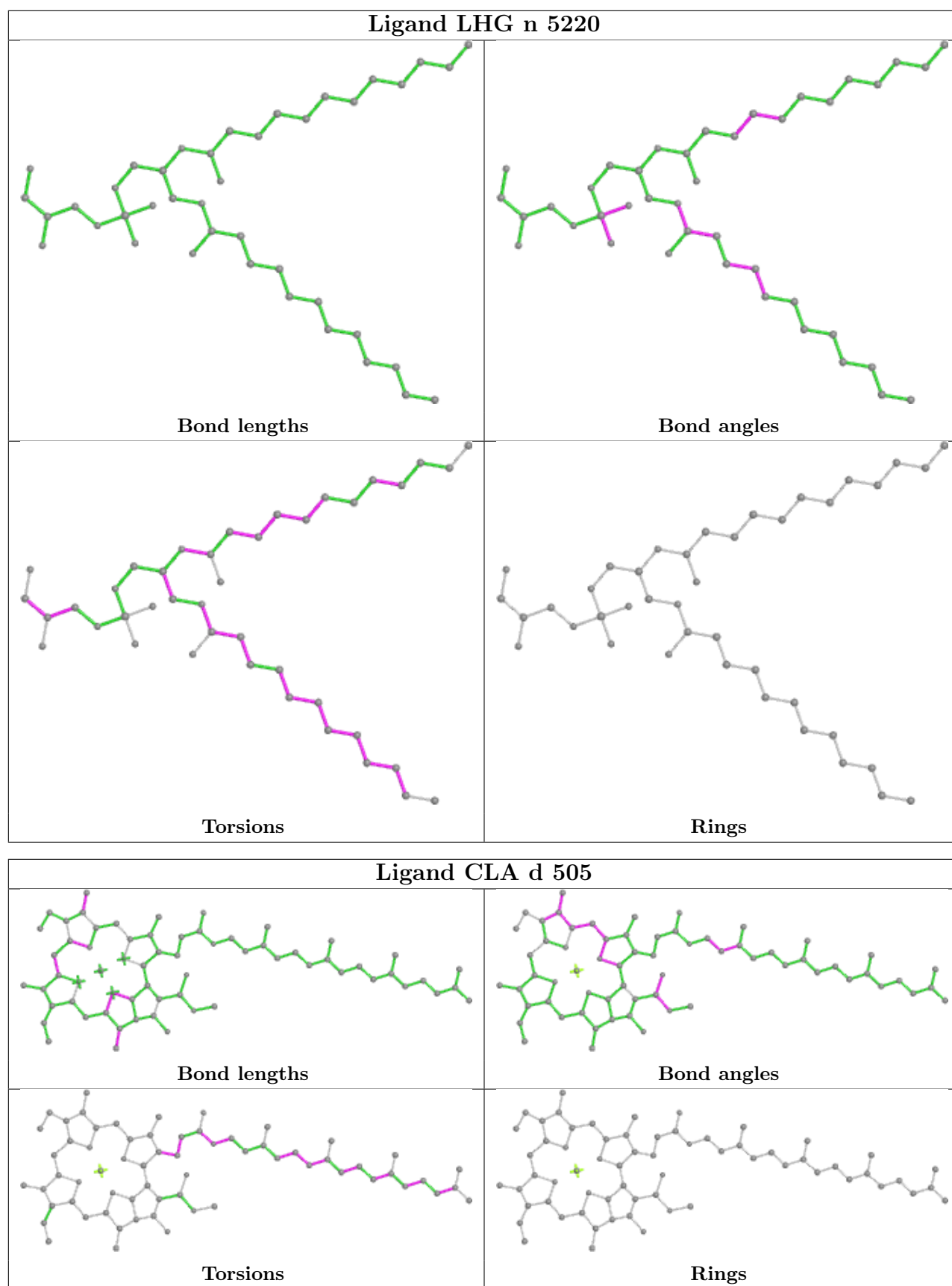
Torsions

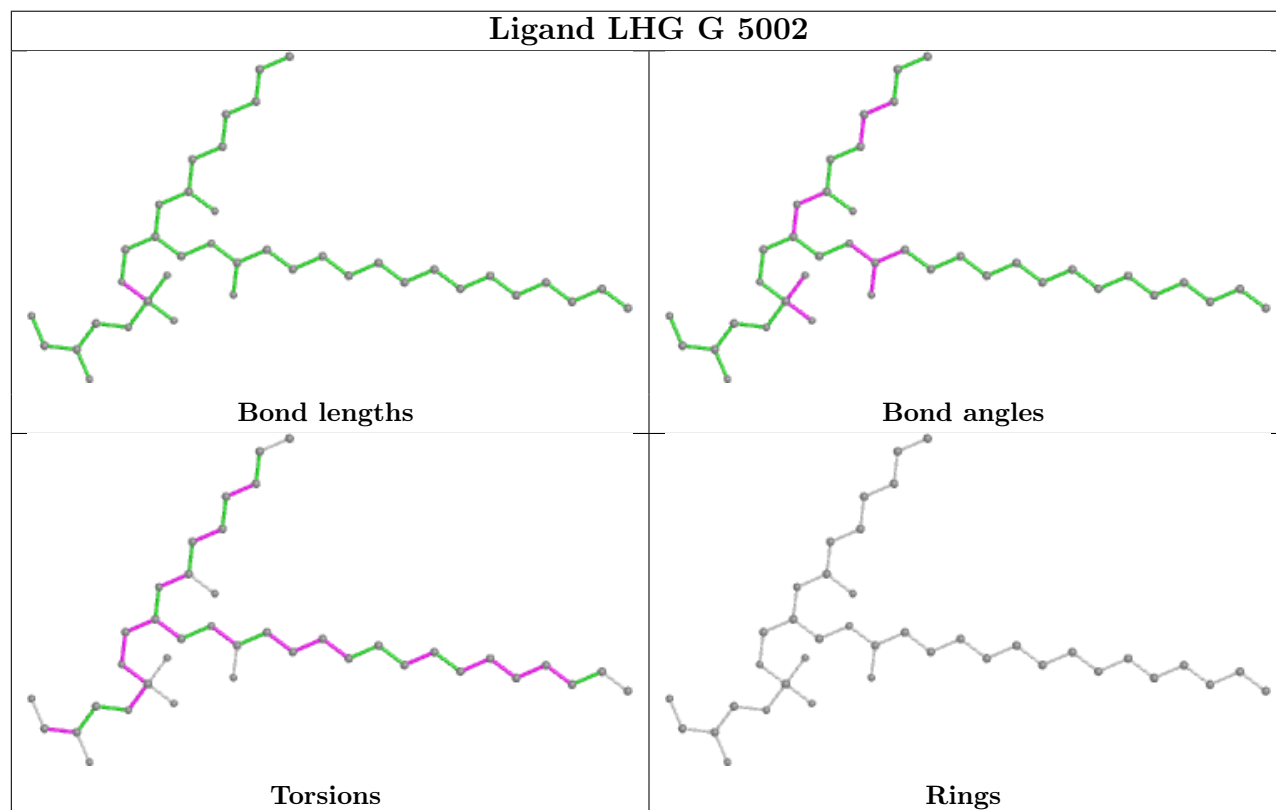
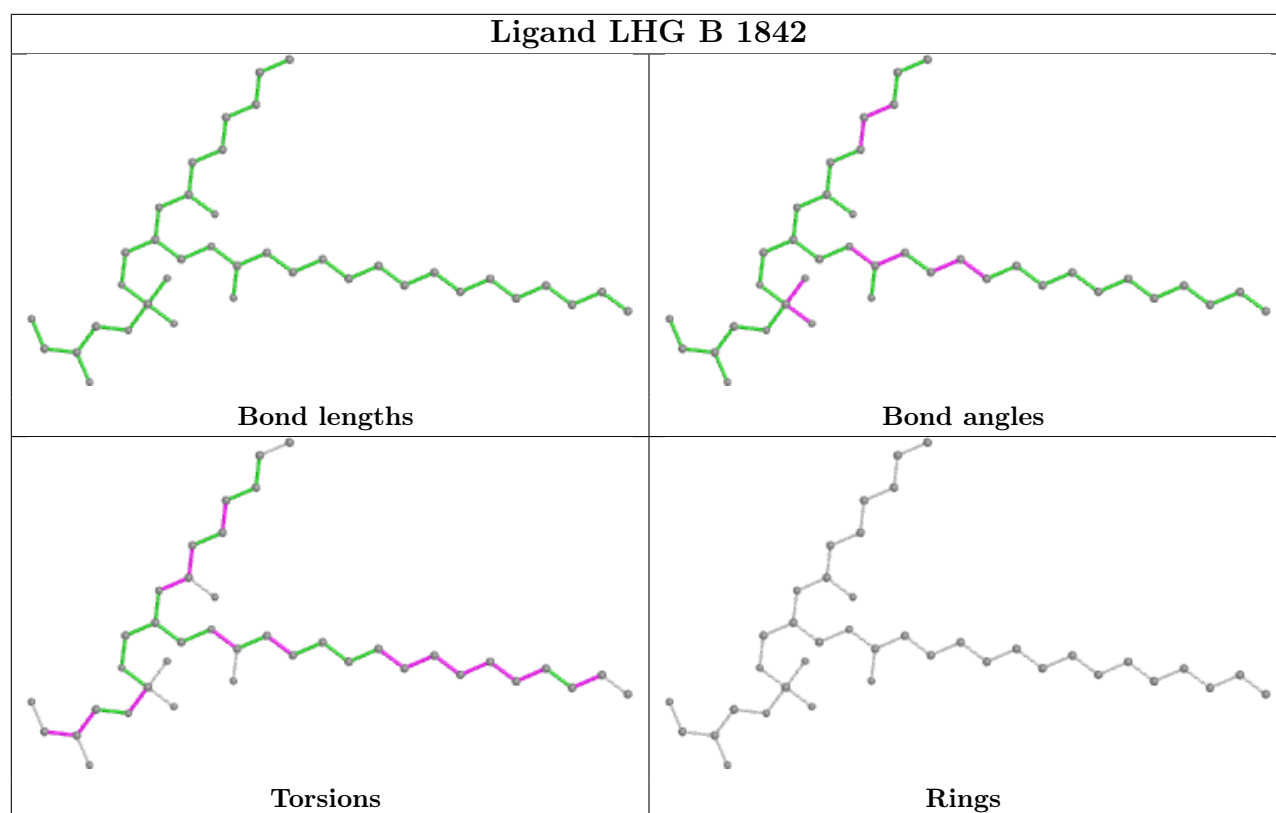


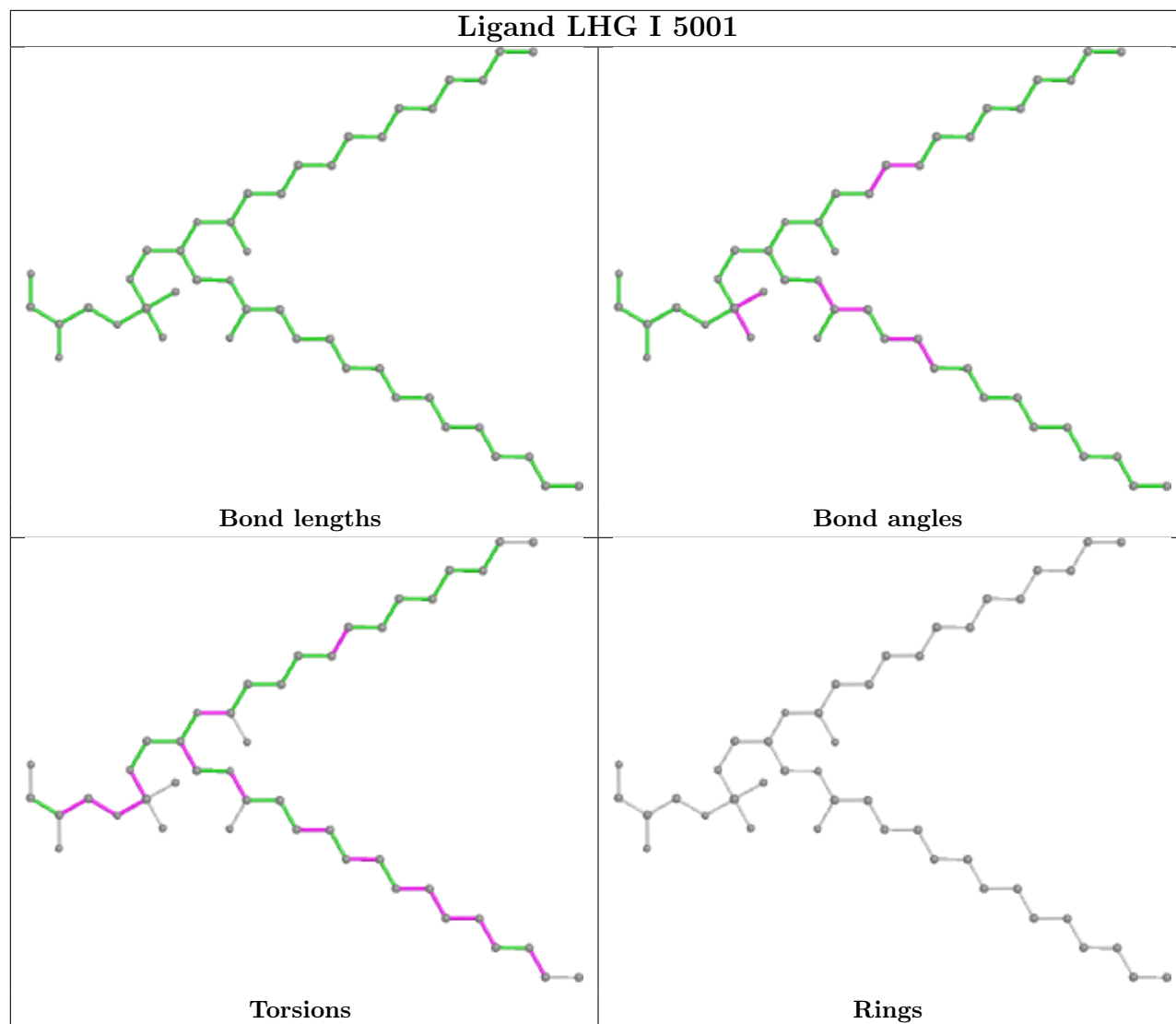
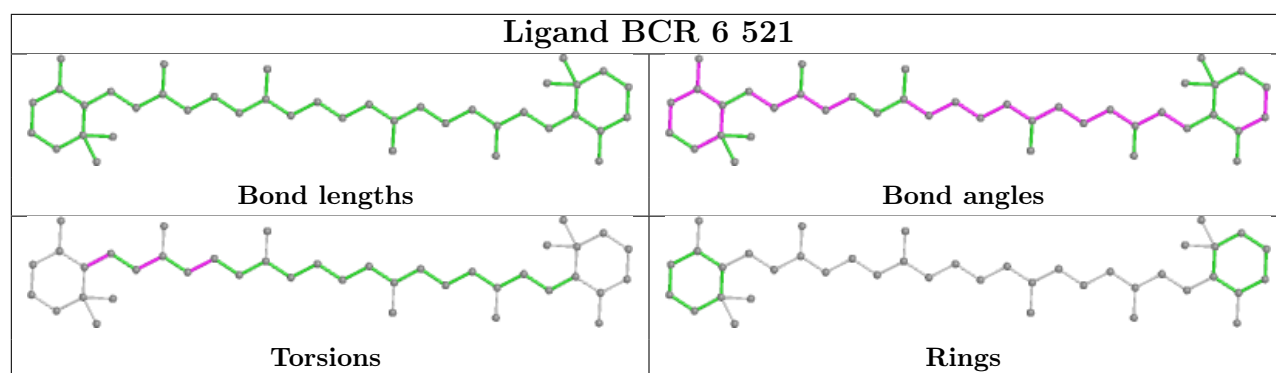
Rings



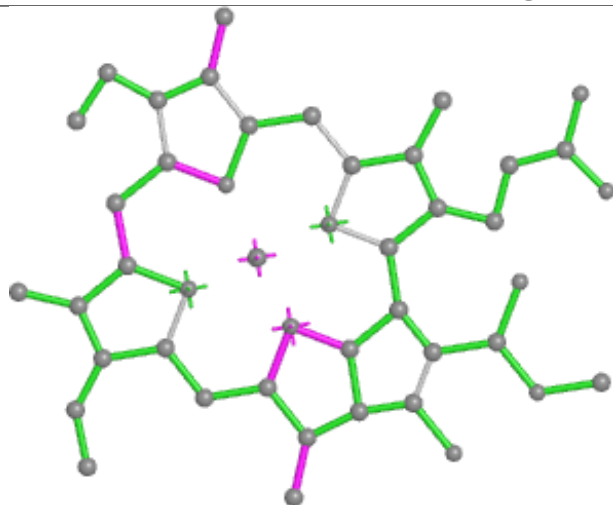
Ligand CLA H 1223**Ligand BCR B 4005**



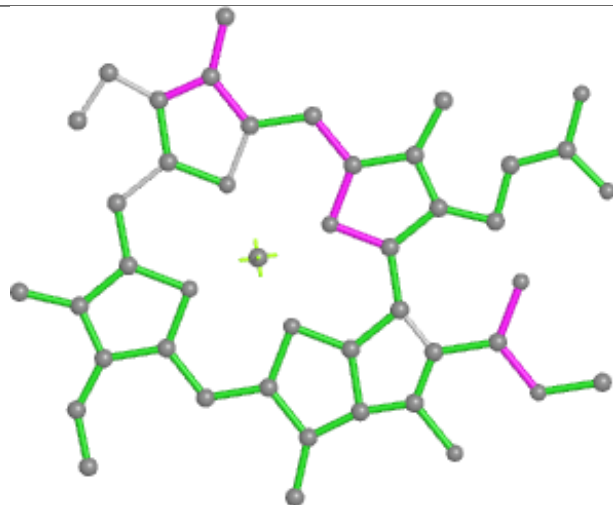




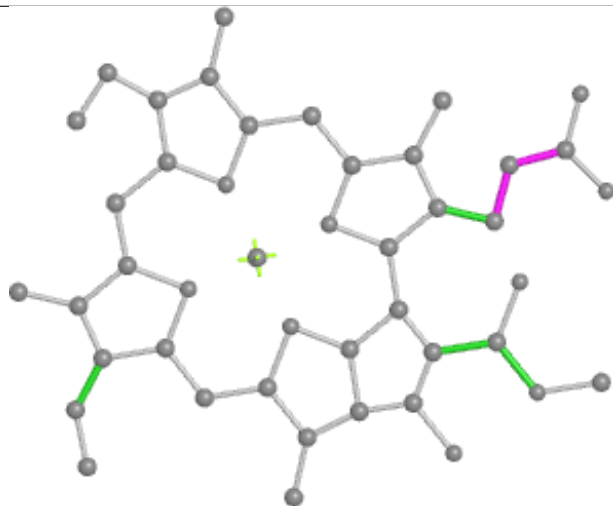
Ligand CLA s 512



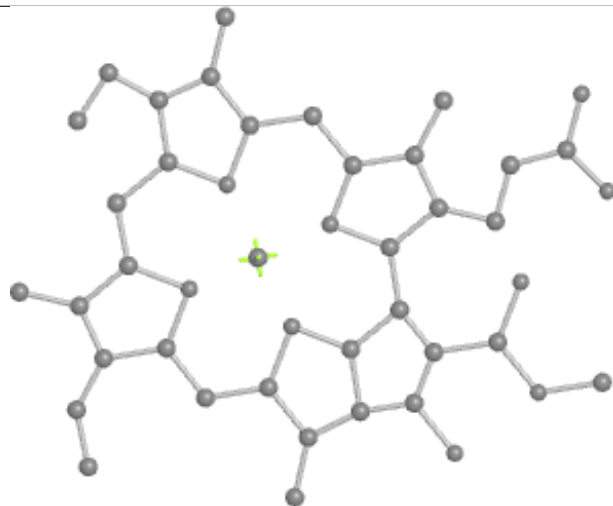
Bond lengths



Bond angles

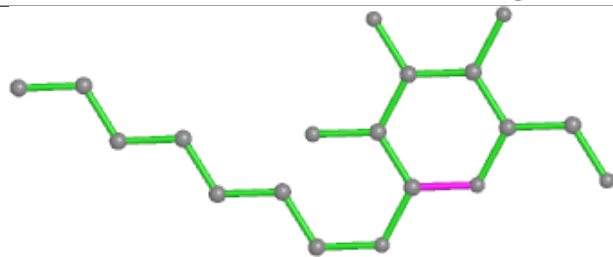


Torsions

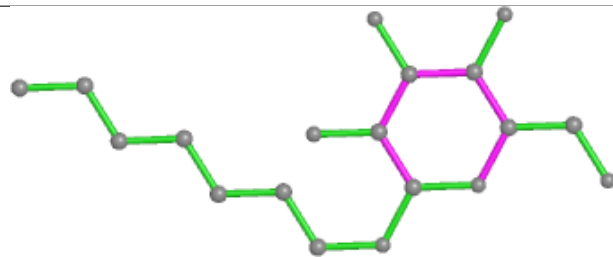


Rings

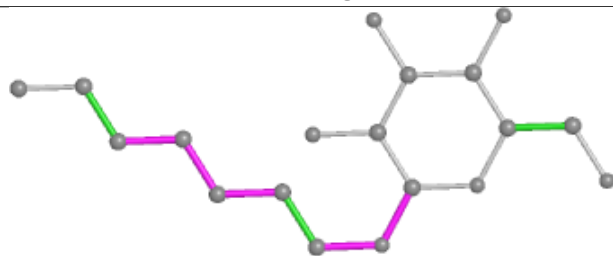
Ligand LMU Y 902



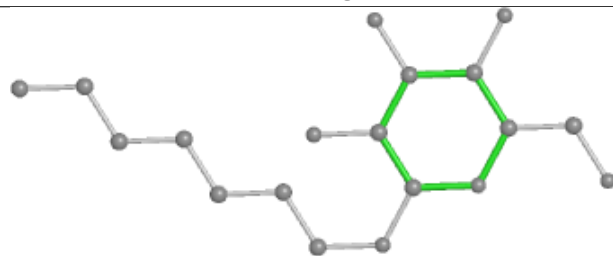
Bond lengths



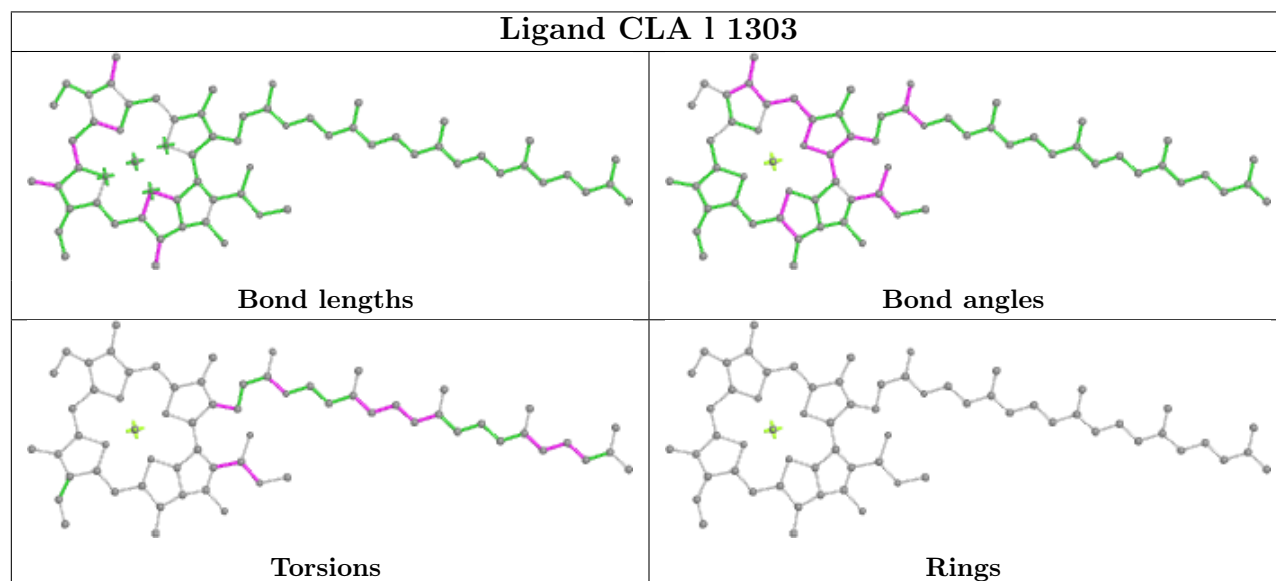
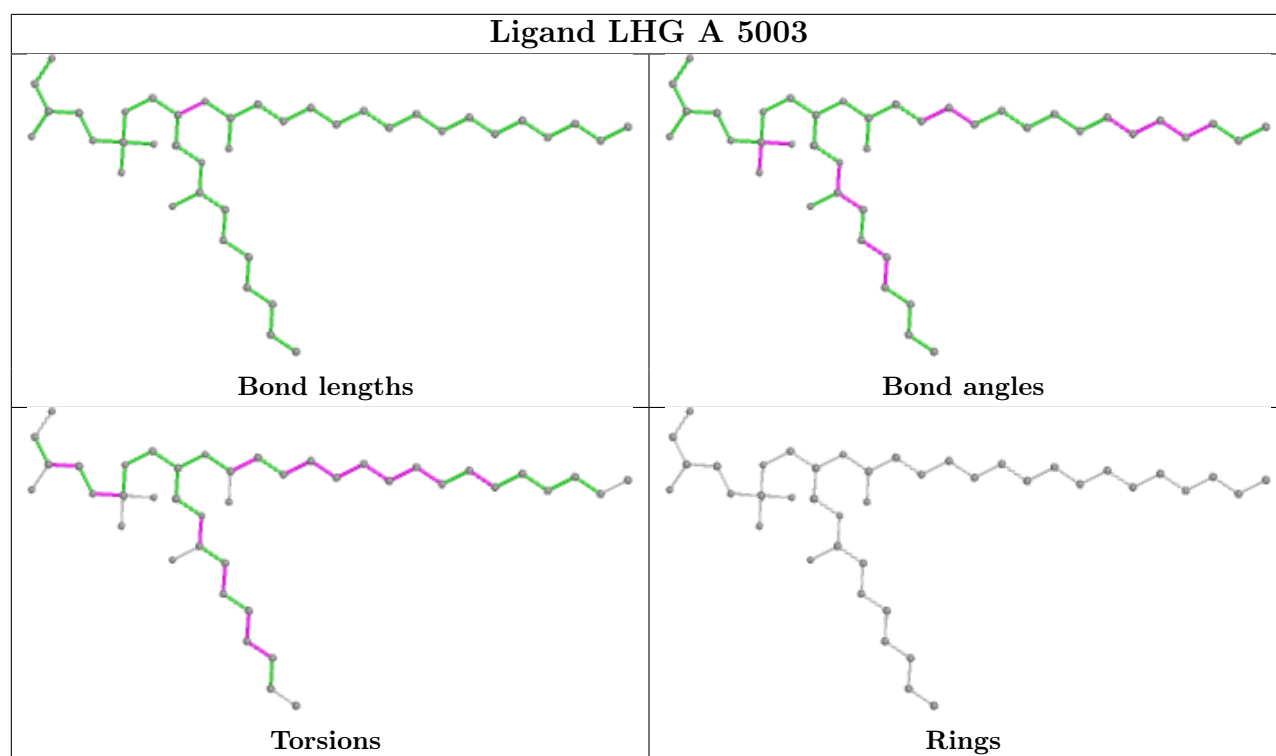
Bond angles



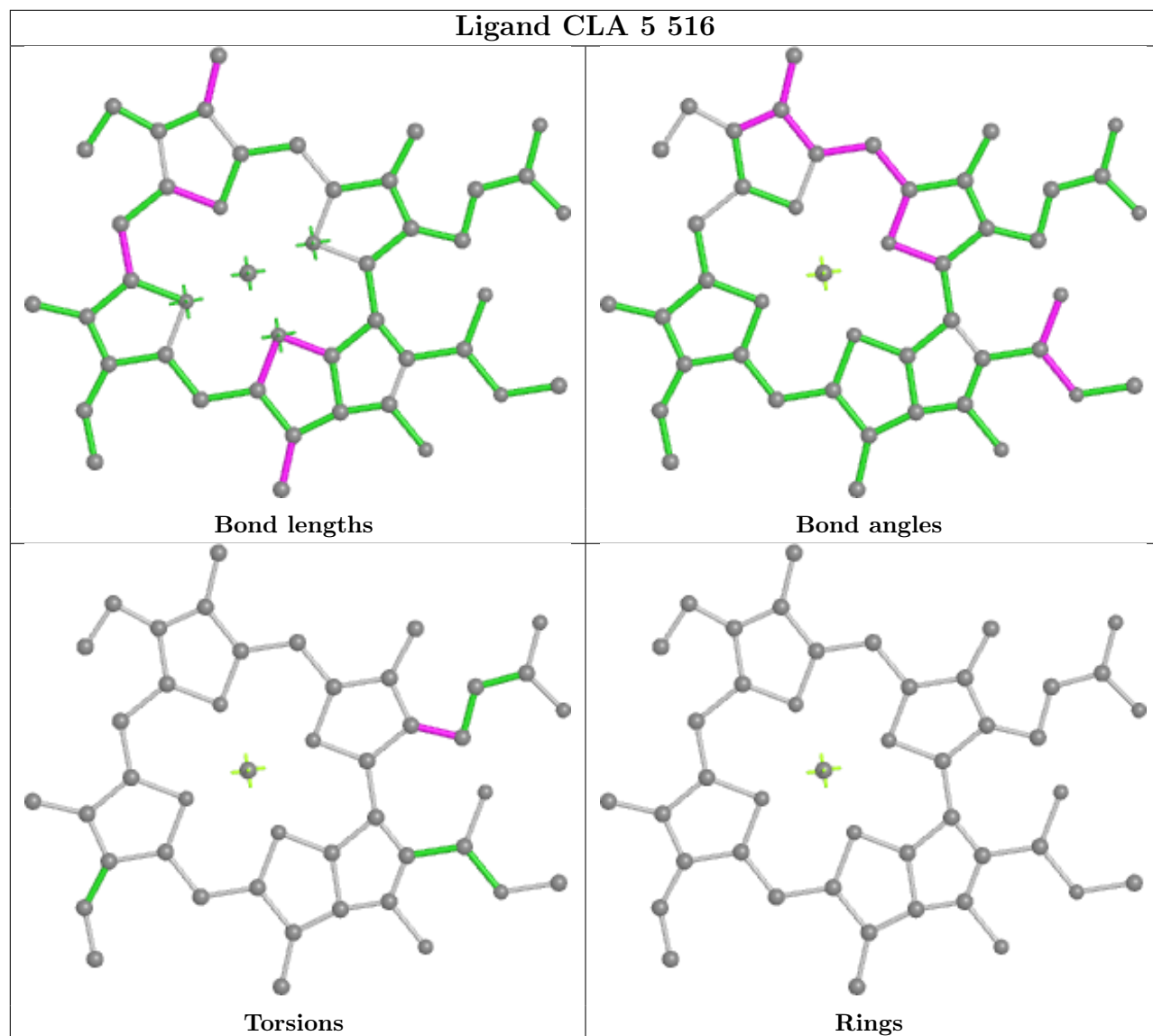
Torsions



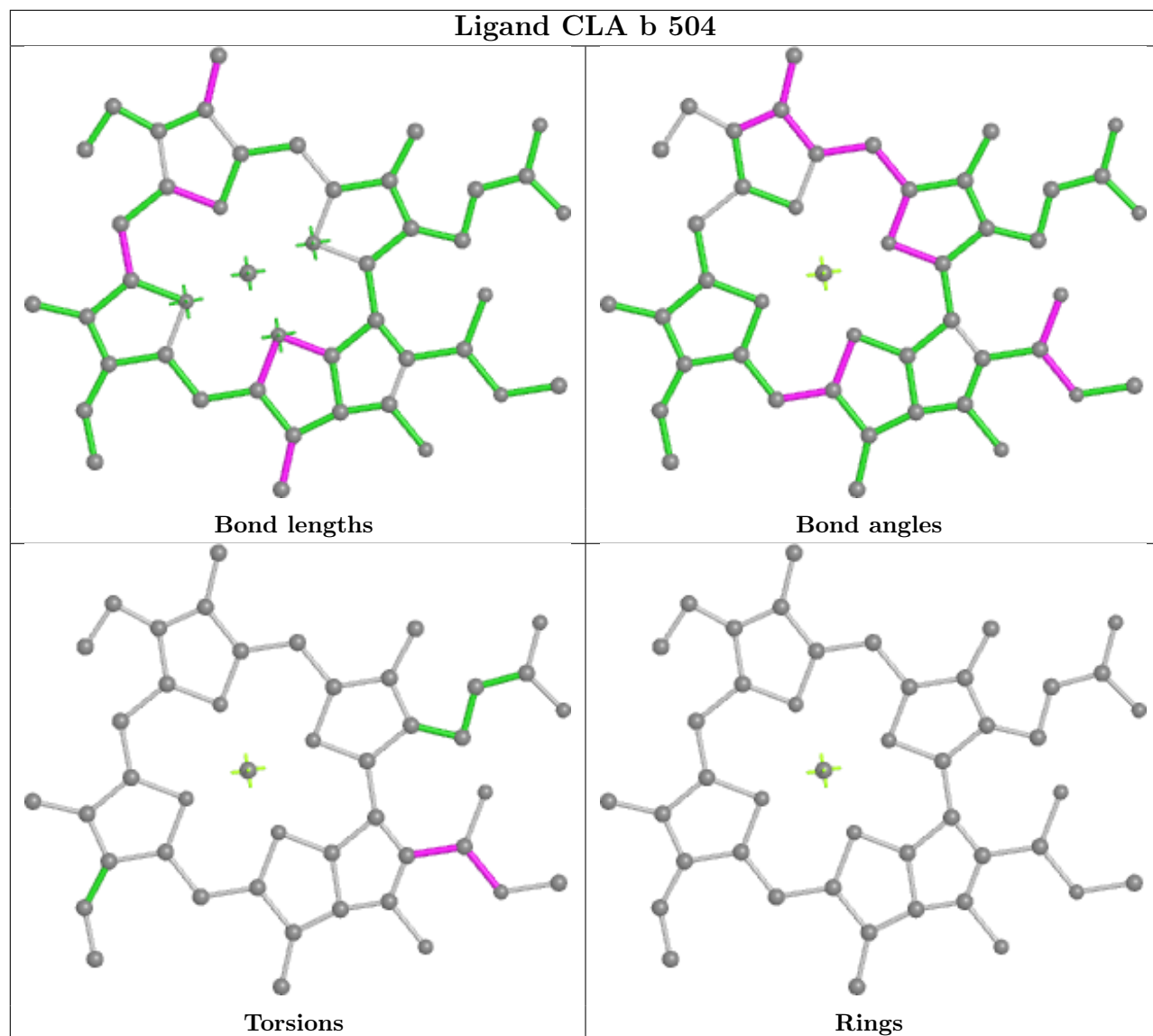
Rings

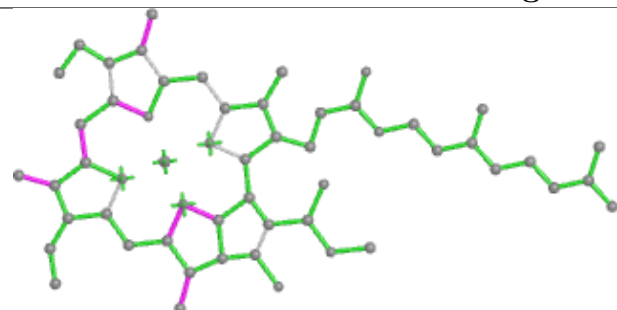


Ligand CLA 5 516

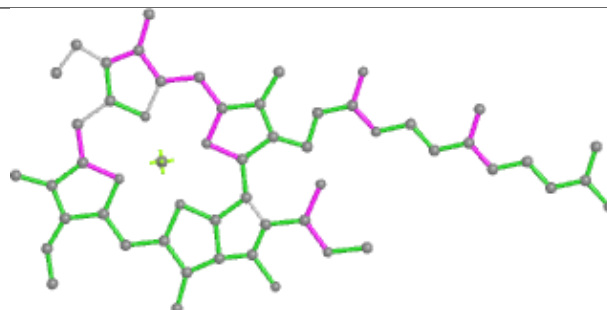


Ligand CLA b 504

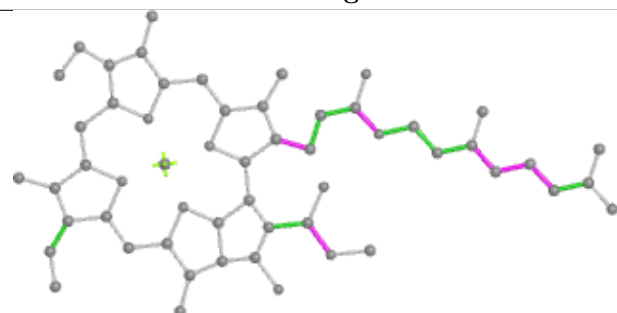


Ligand CLA 1 508

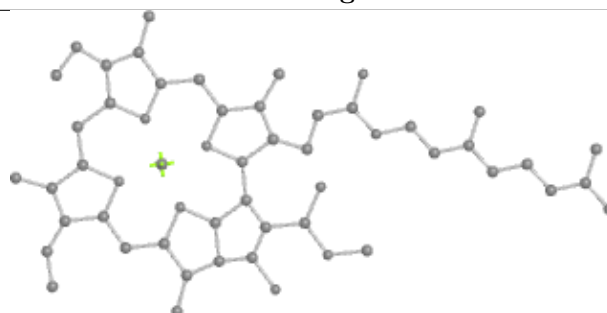
Bond lengths



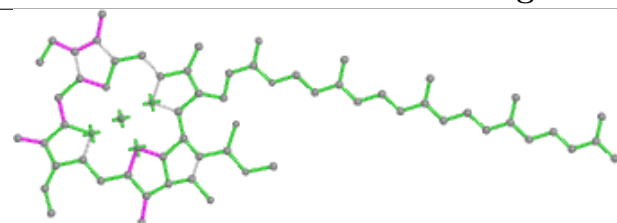
Bond angles



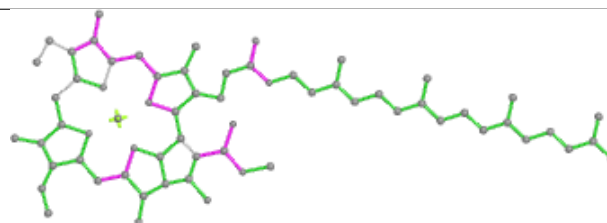
Torsions



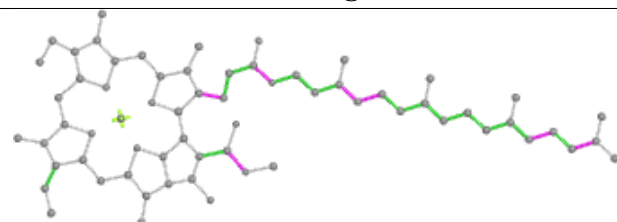
Rings

Ligand CLA f 1227

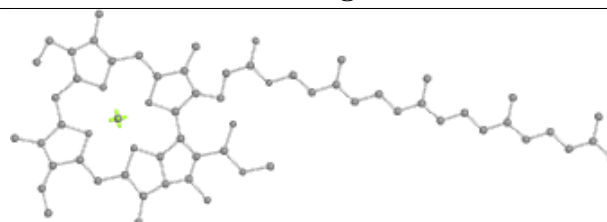
Bond lengths



Bond angles

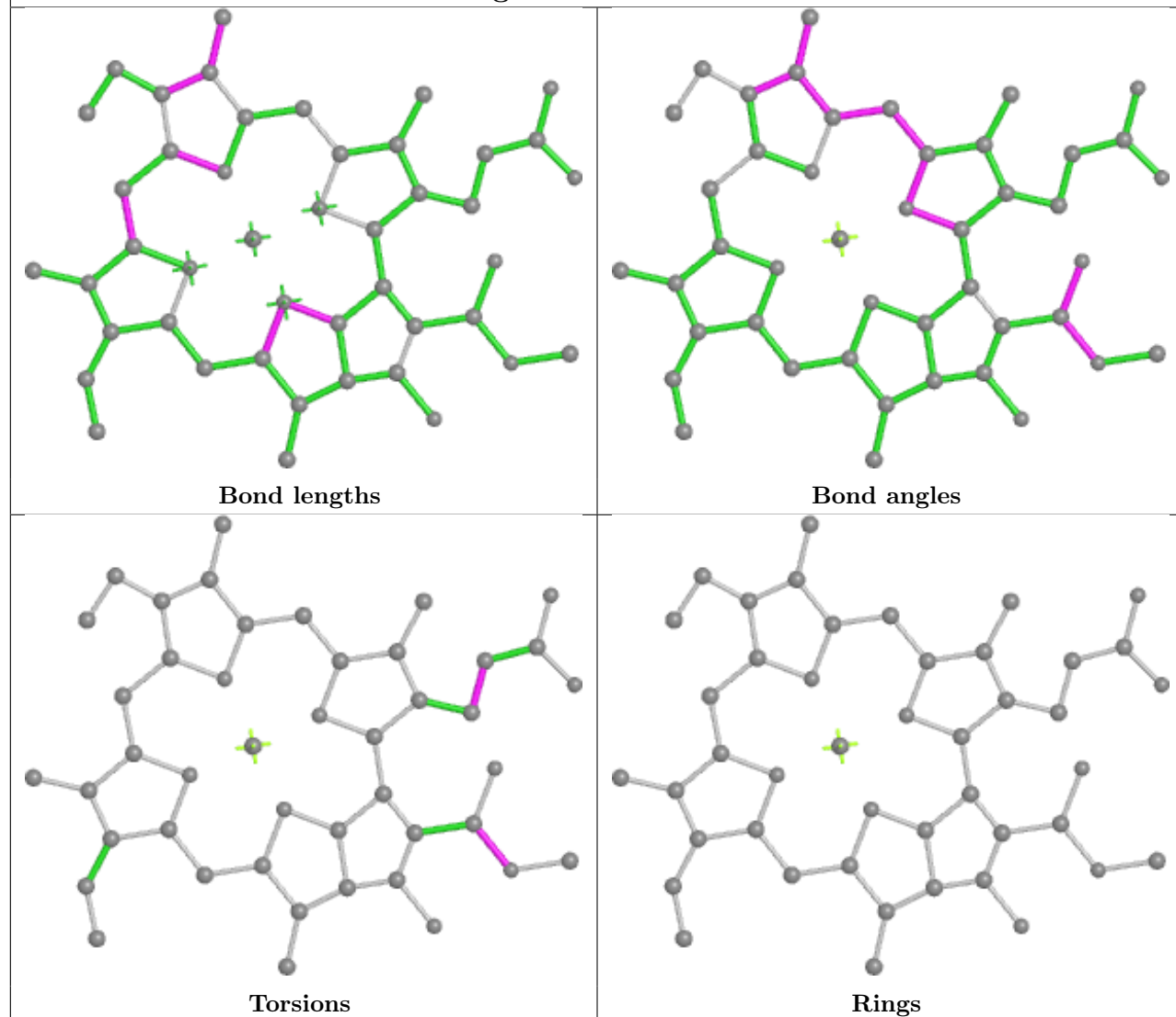


Torsions

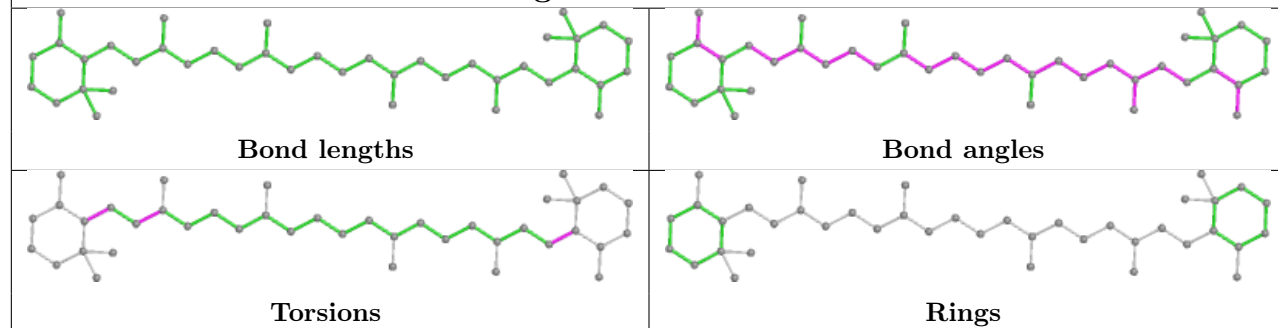


Rings

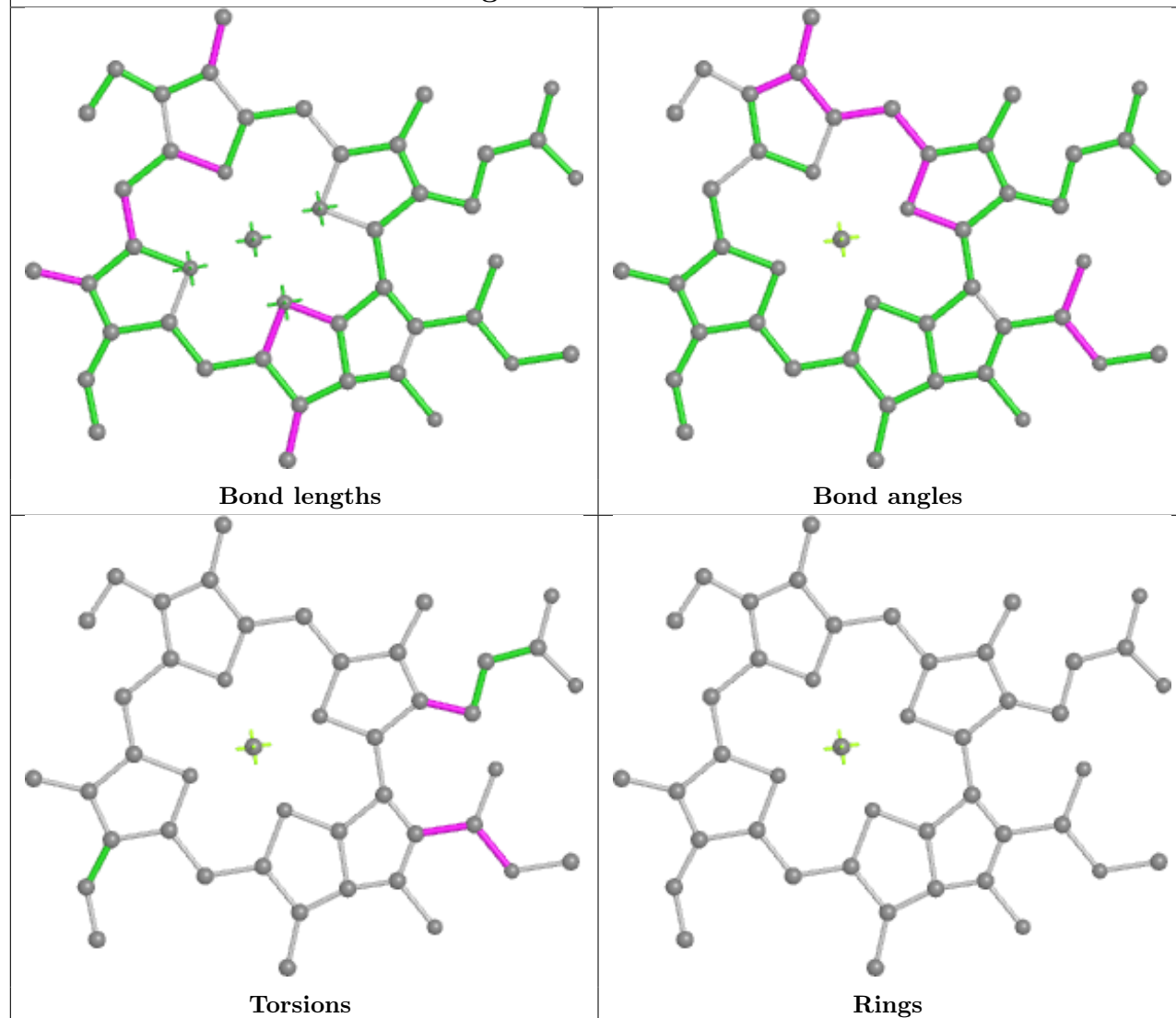
Ligand CLA v 513



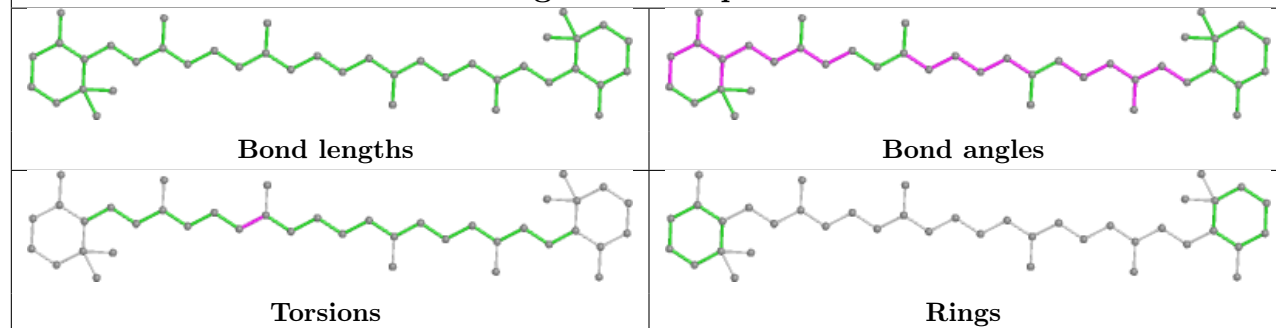
Ligand BCR v 524



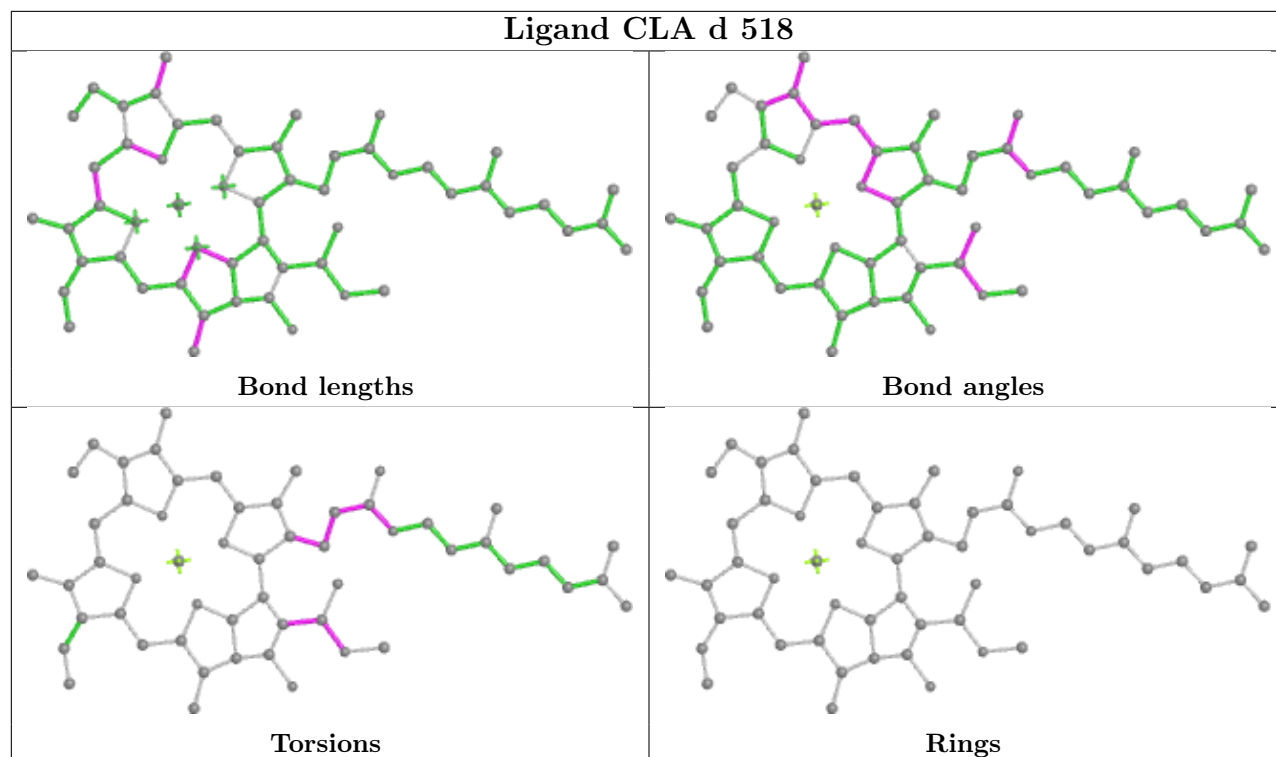
Ligand CLA A 1113



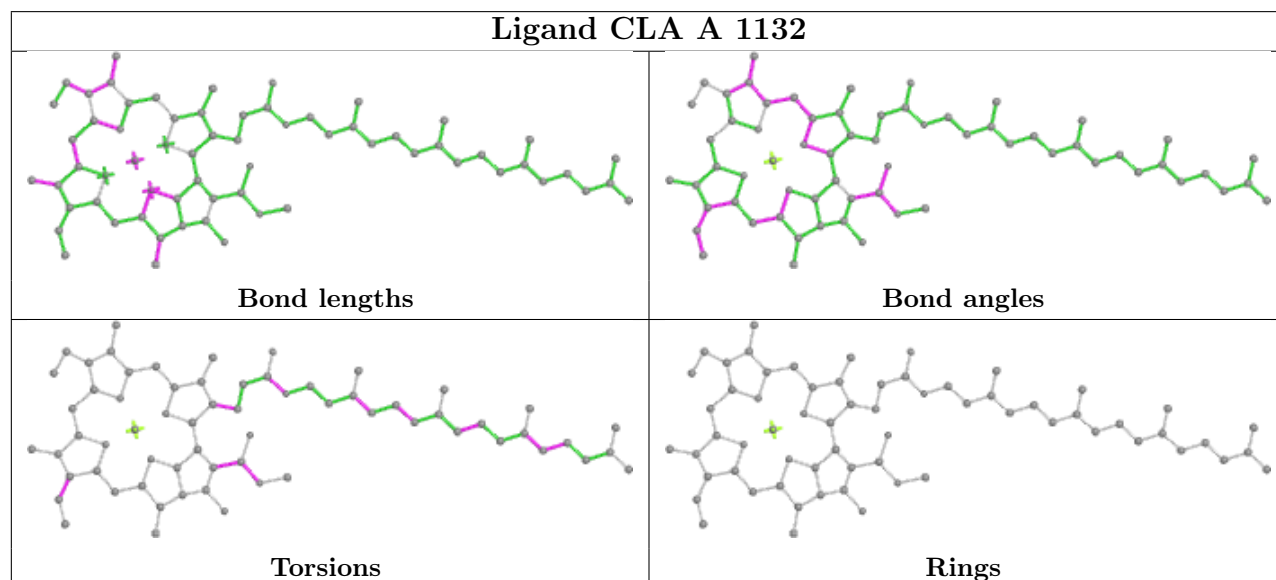
Ligand BCR q 524

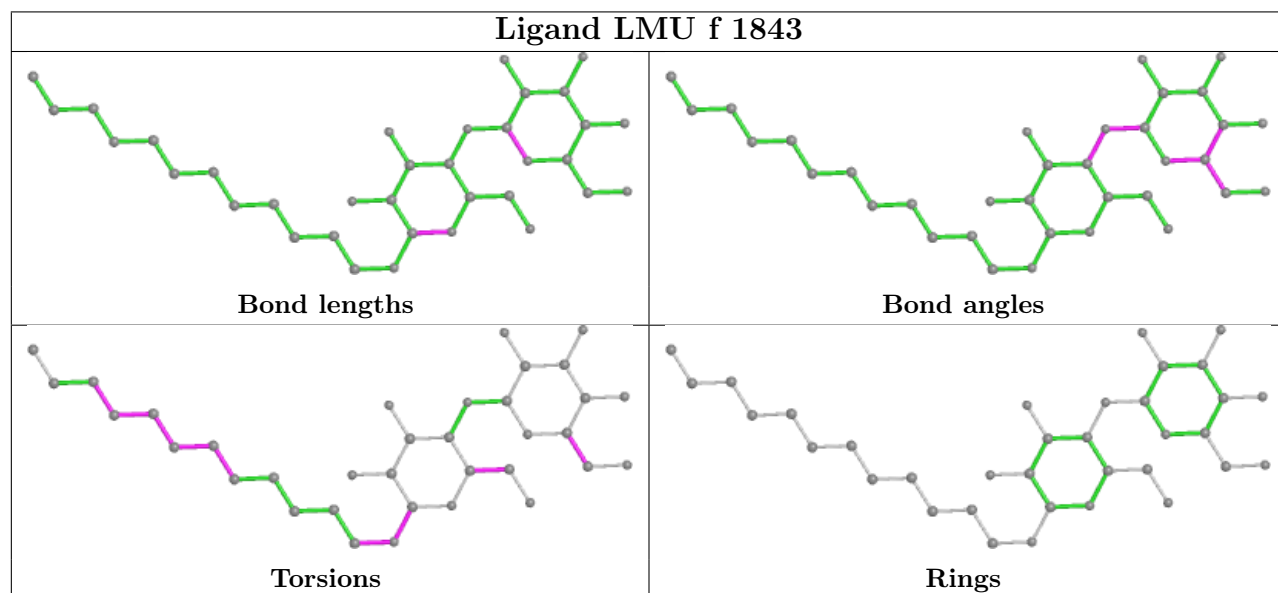
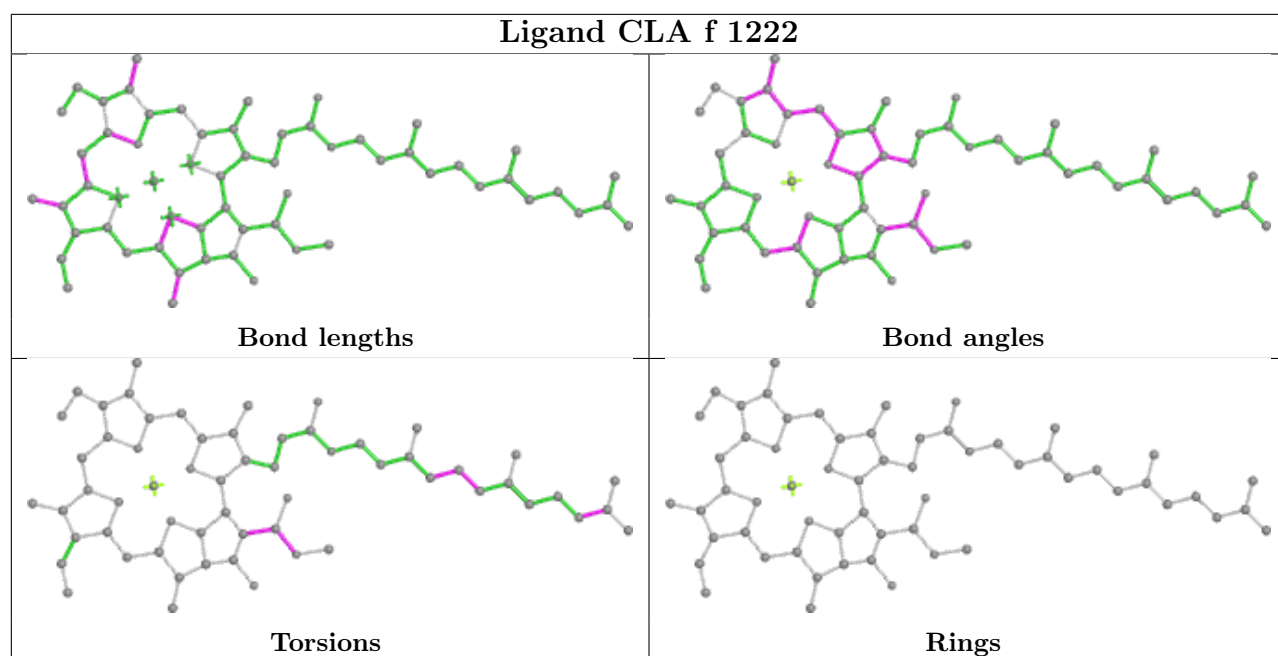


Ligand CLA d 518

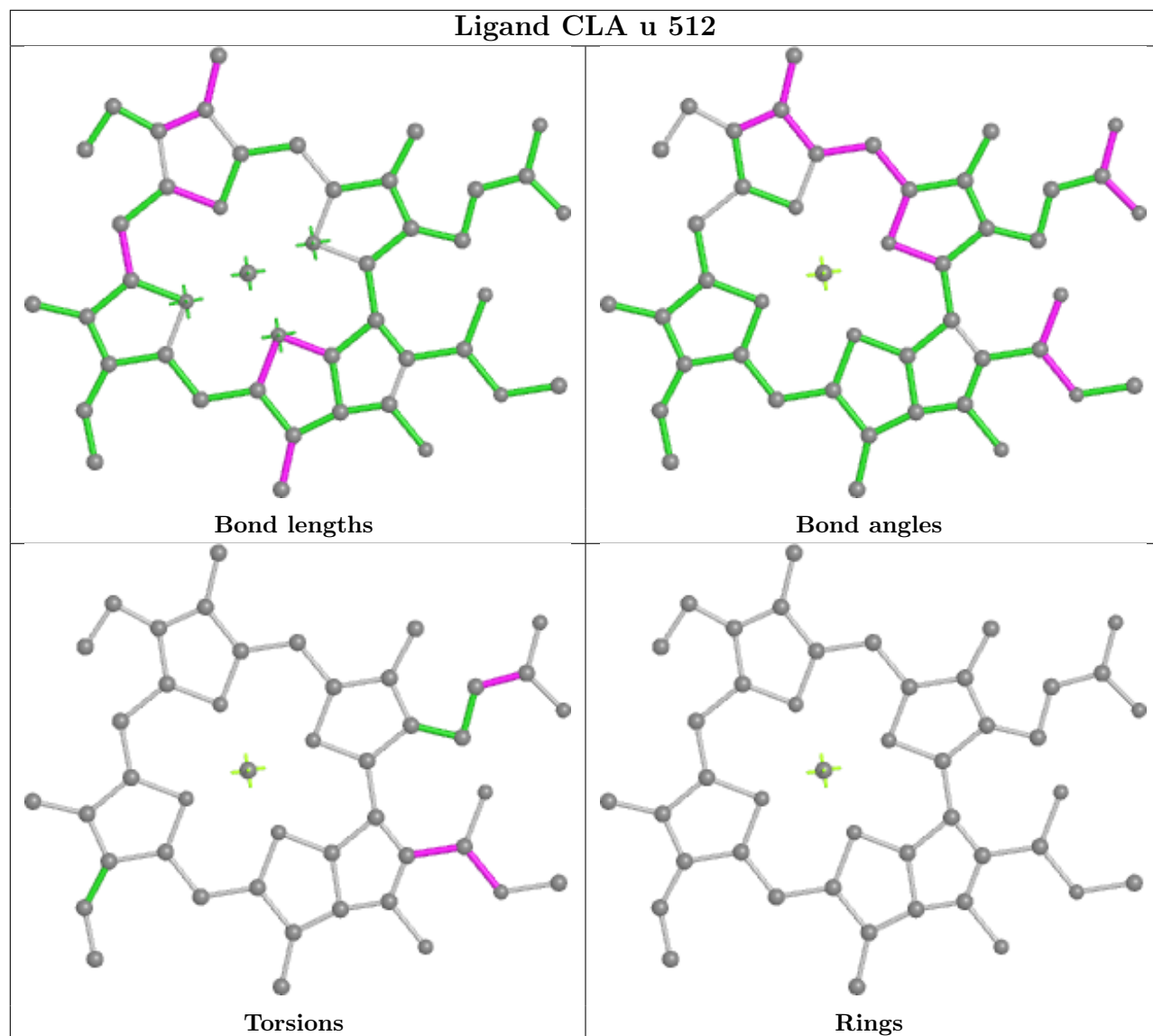


Ligand CLA A 1132

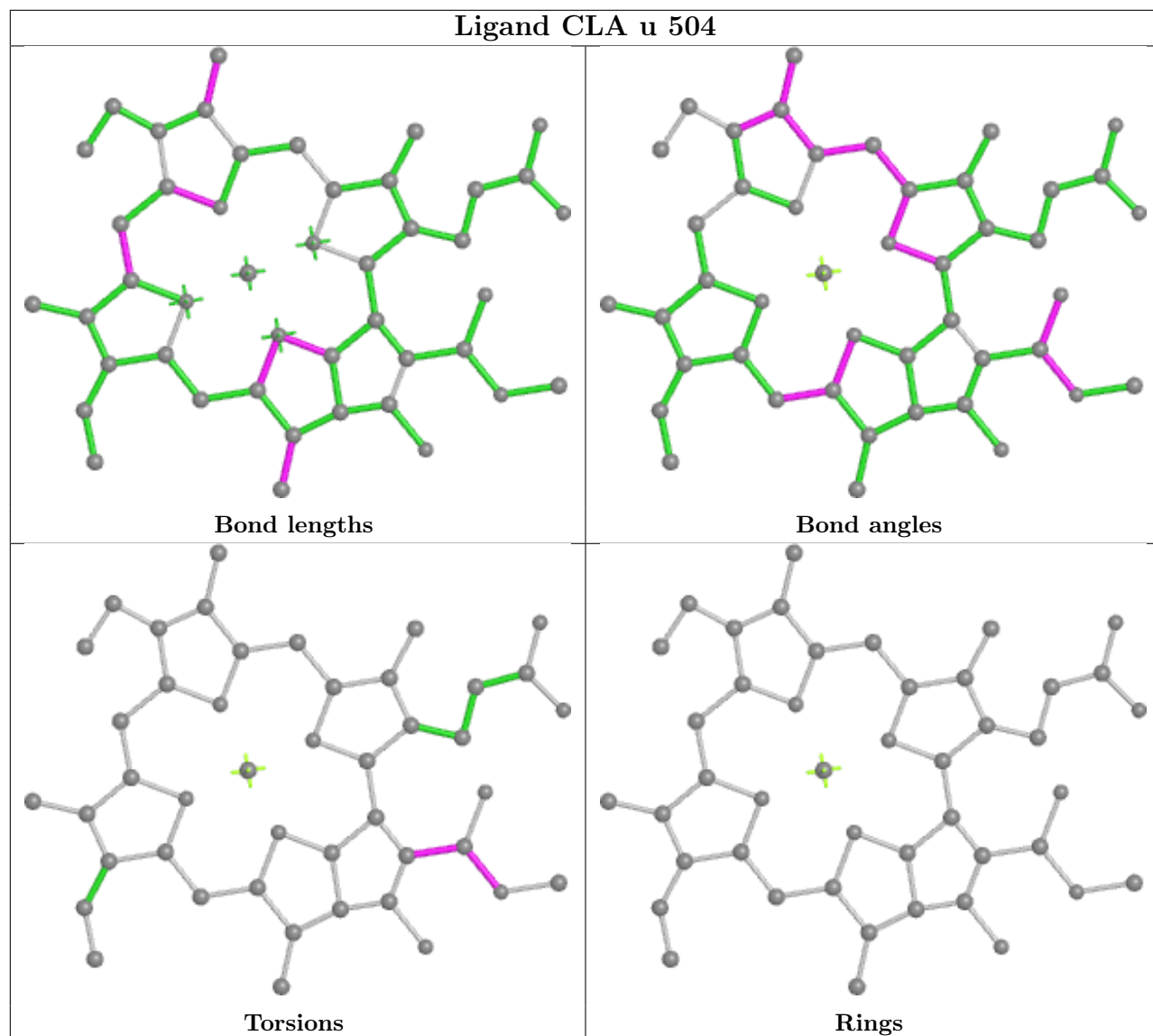




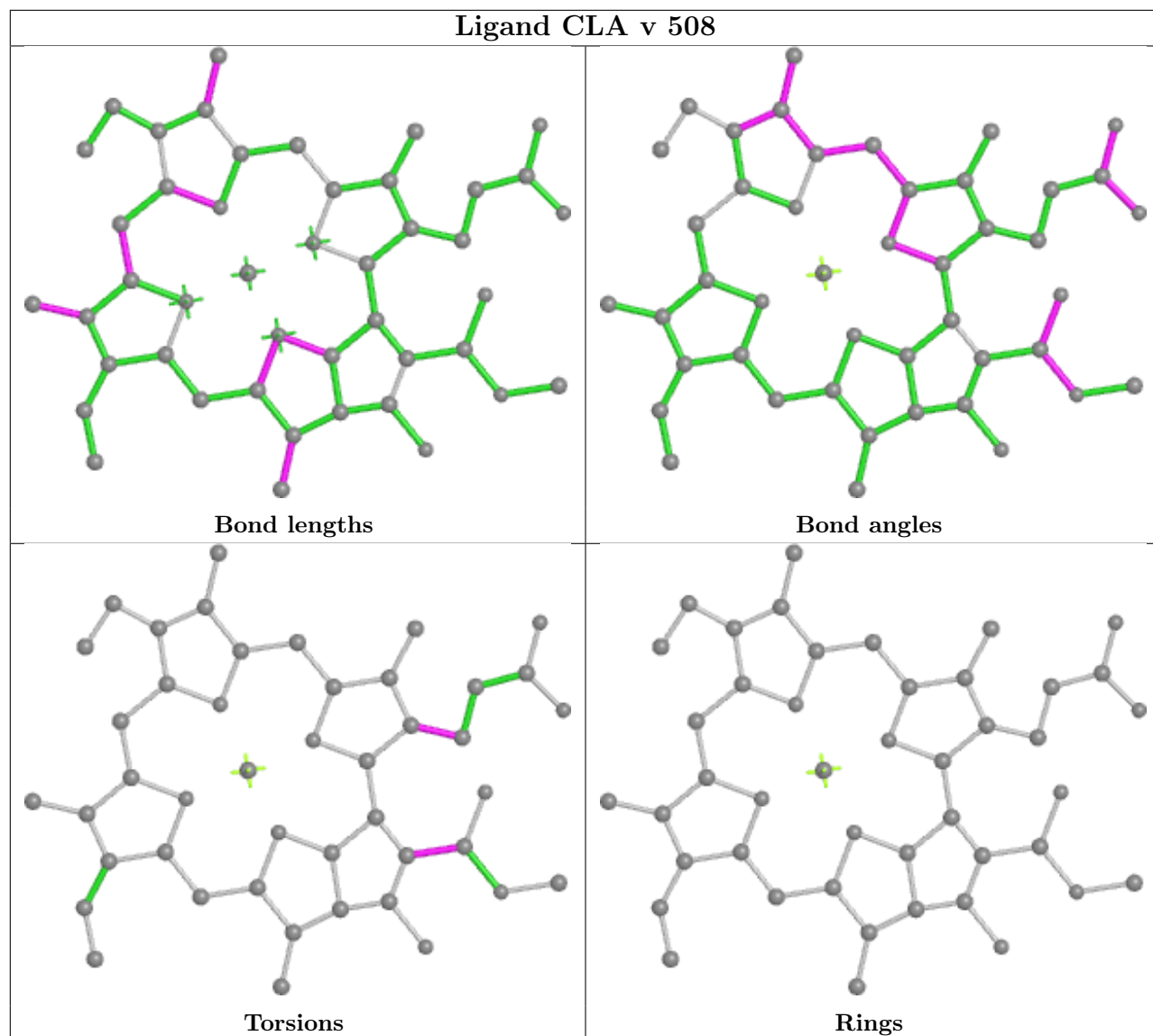
Ligand CLA u 512



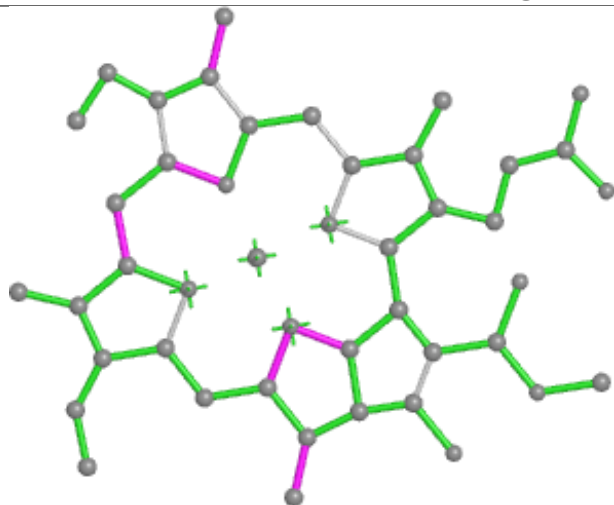
Ligand CLA u 504



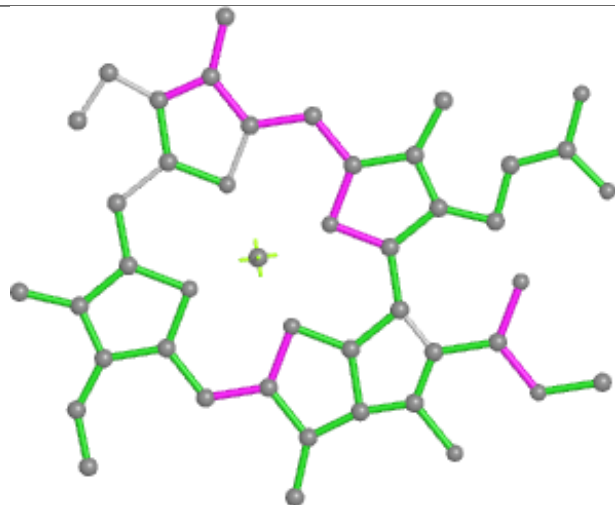
Ligand CLA v 508



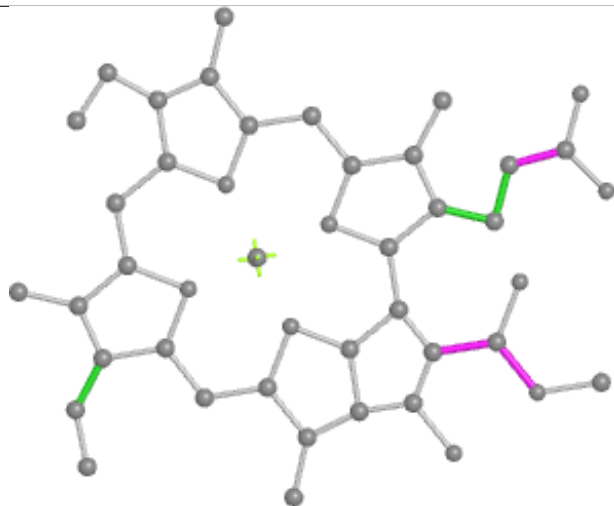
Ligand CLA u 510



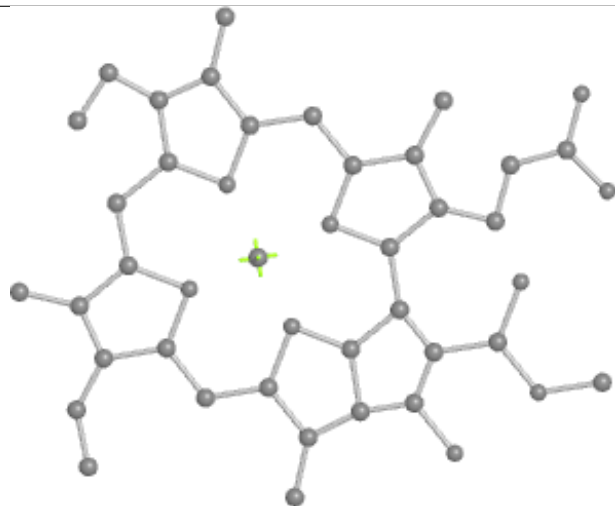
Bond lengths



Bond angles

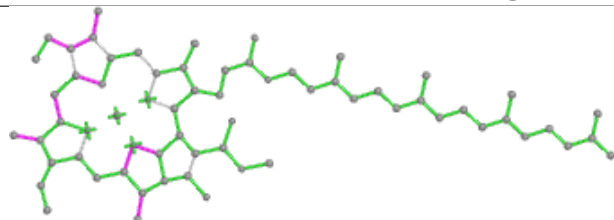


Torsions

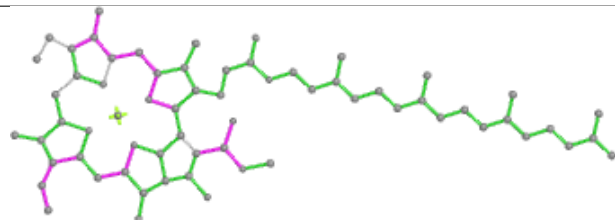


Rings

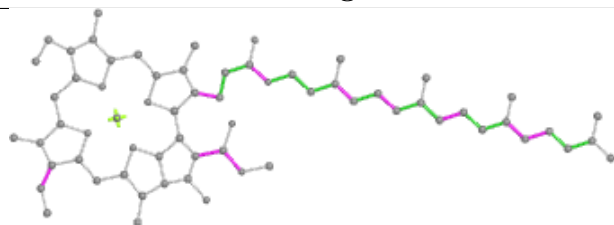
Ligand CLA G 1132



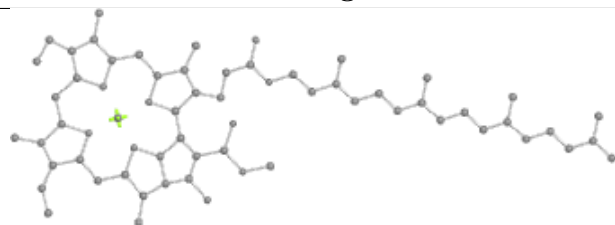
Bond lengths



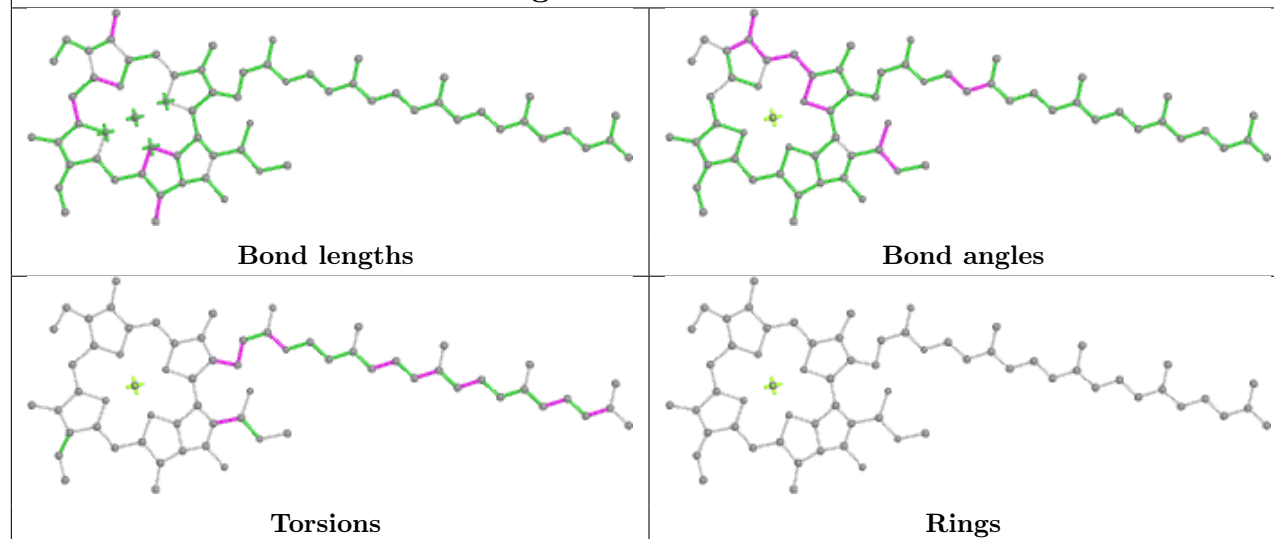
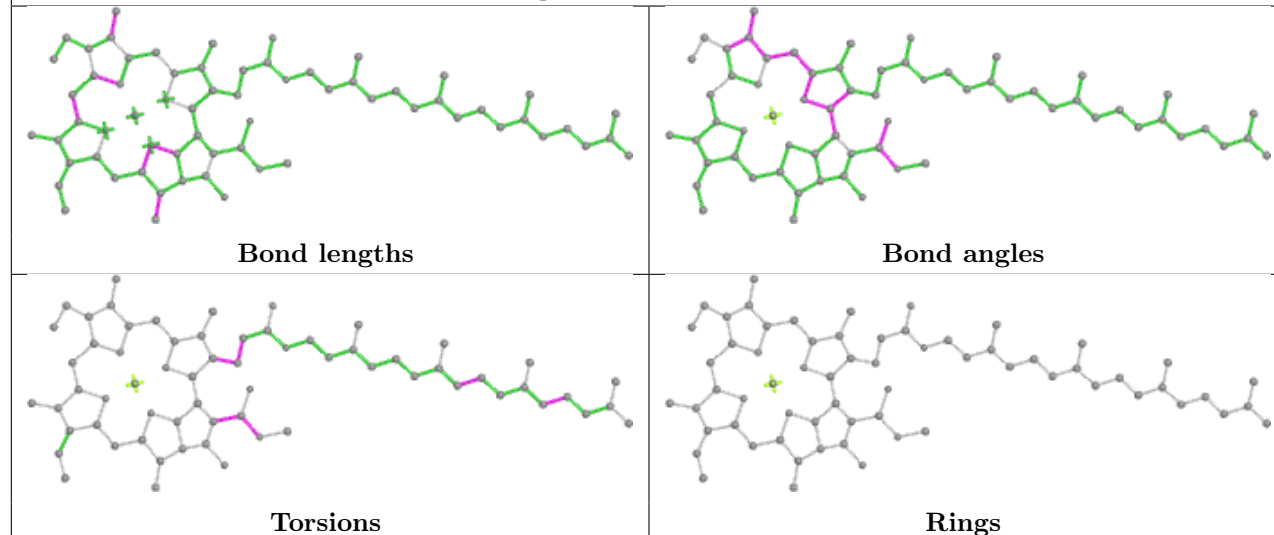
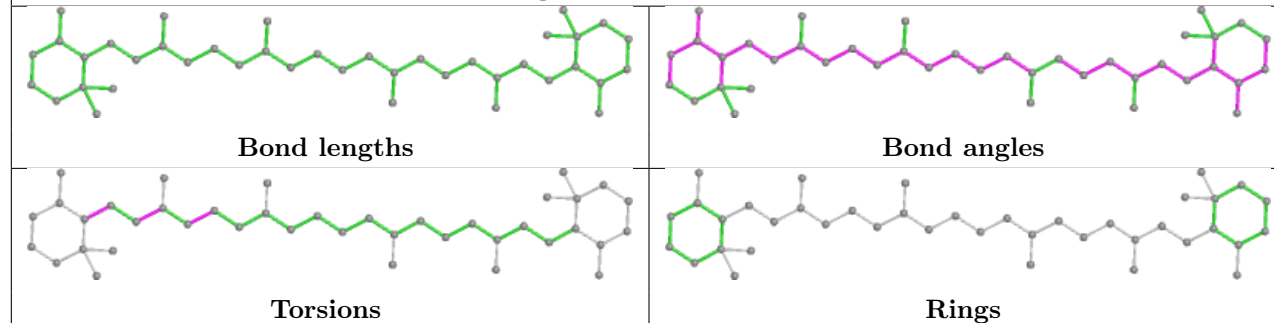
Bond angles

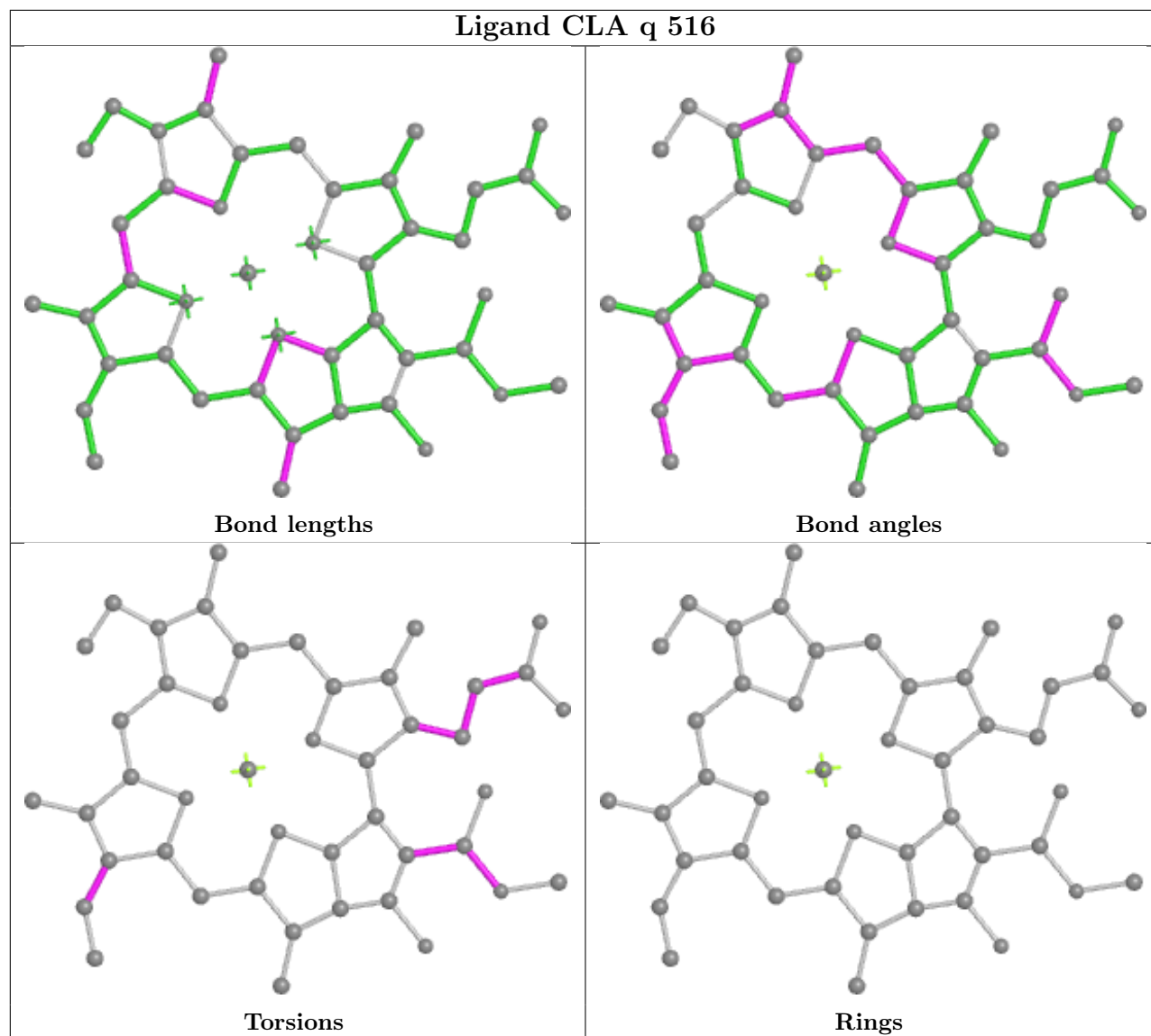
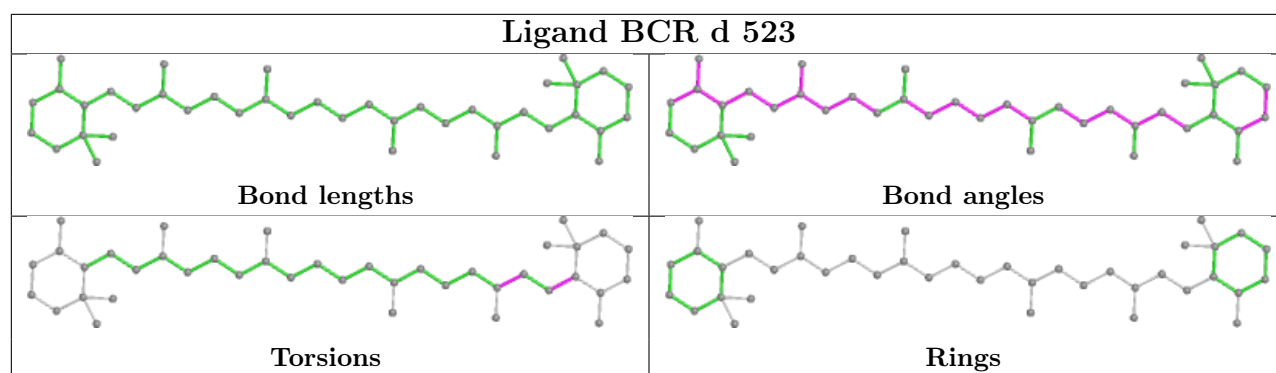


Torsions

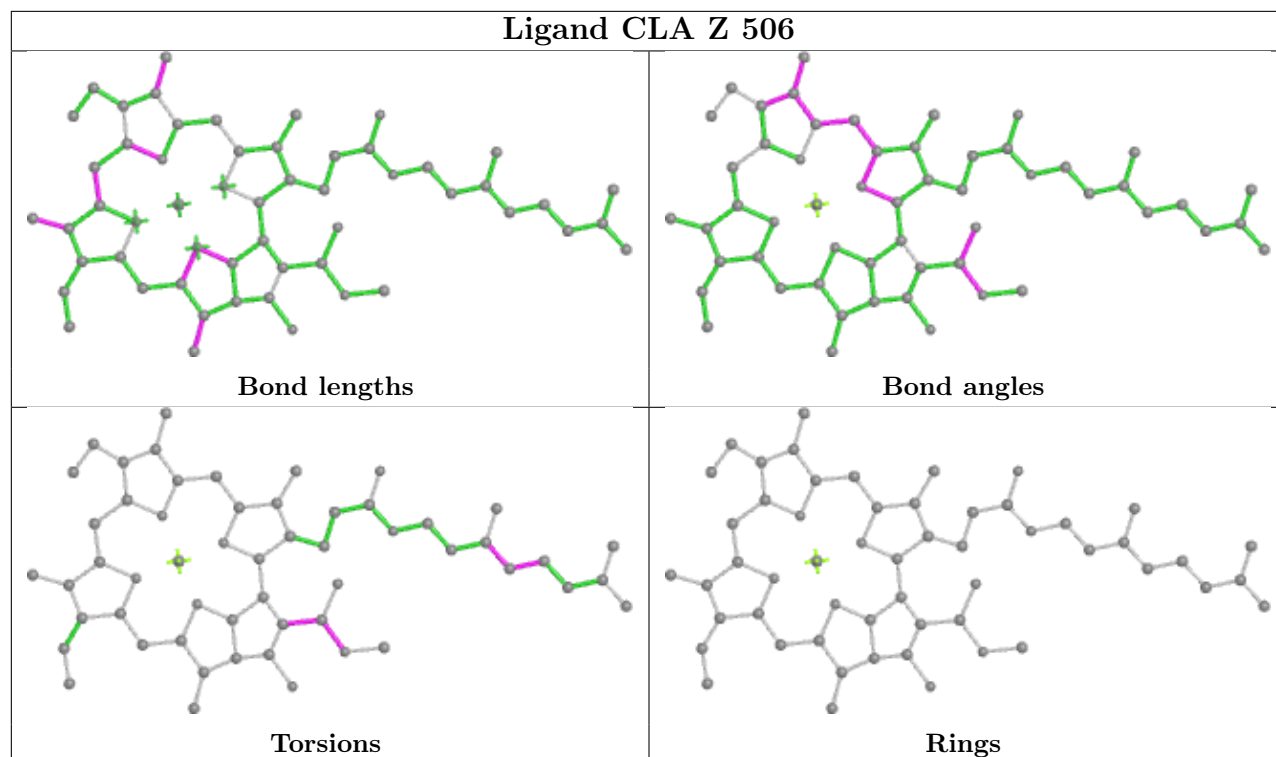


Rings

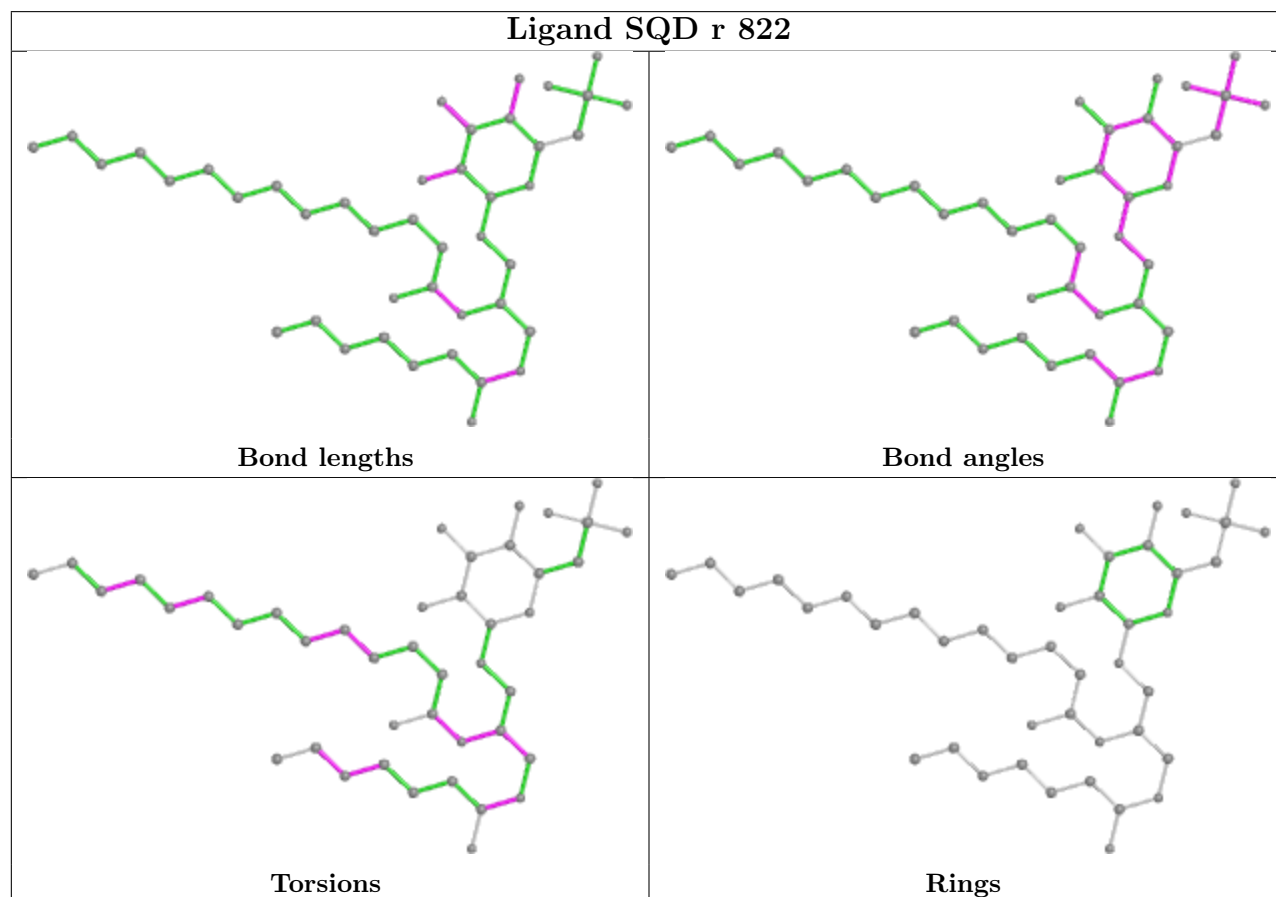
Ligand CLA Y 505**Ligand CLA Z 503****Ligand BCR 5 522**

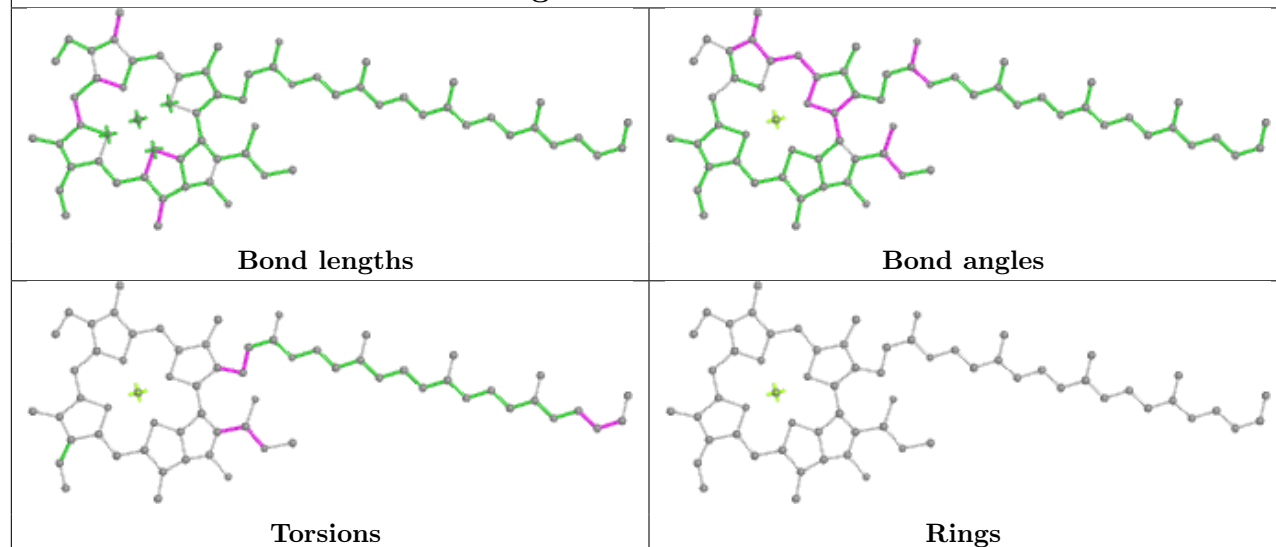
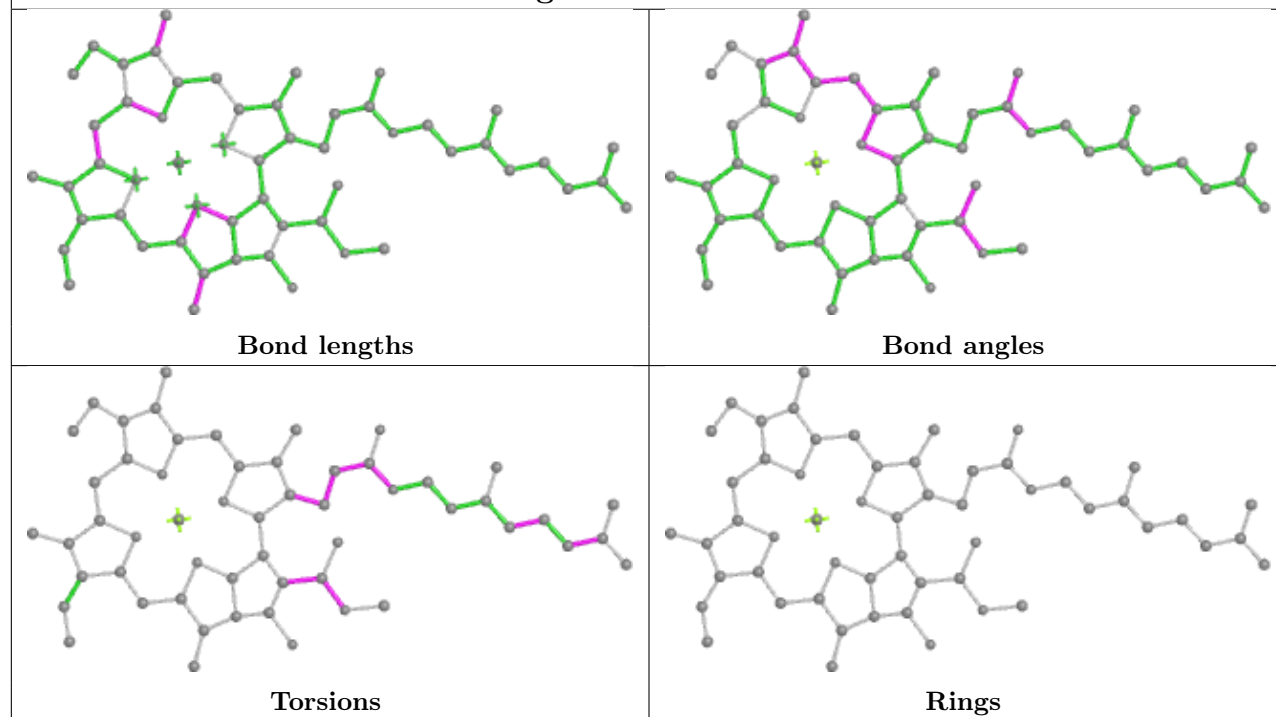


Ligand CLA Z 506

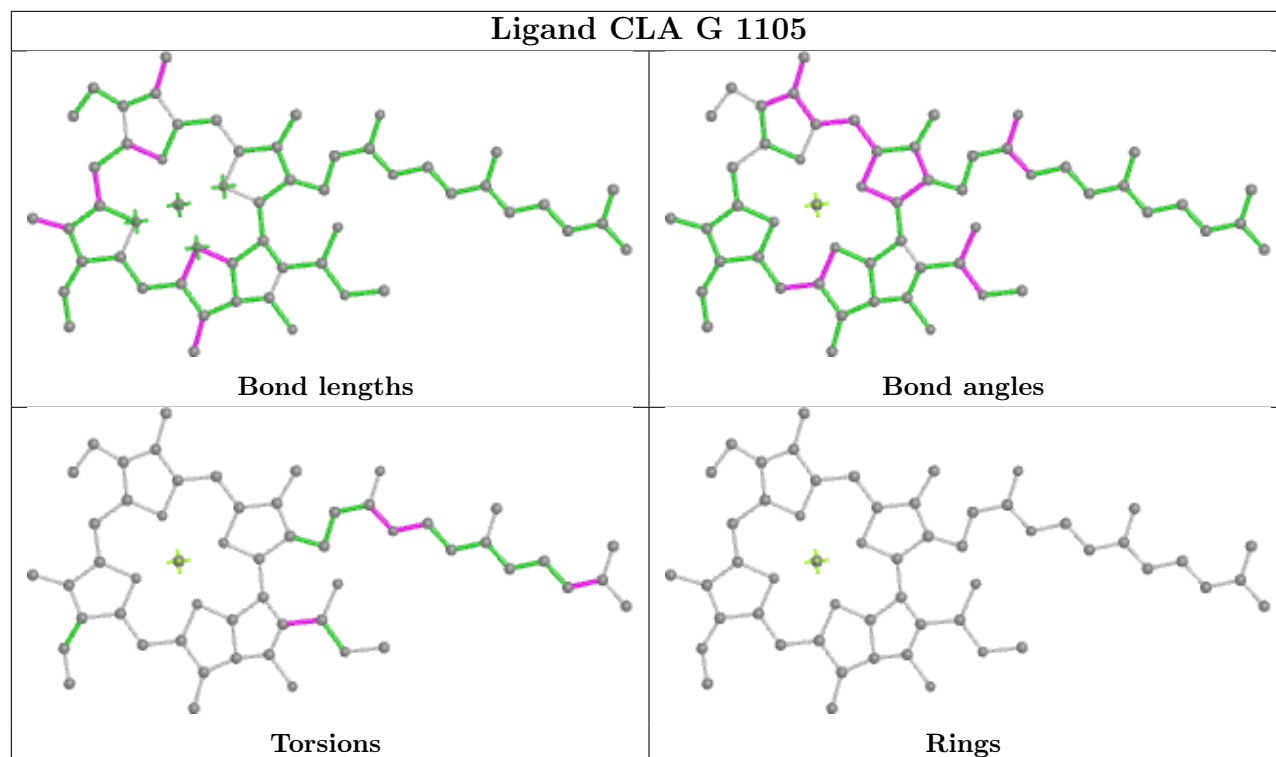


Ligand SQD r 822

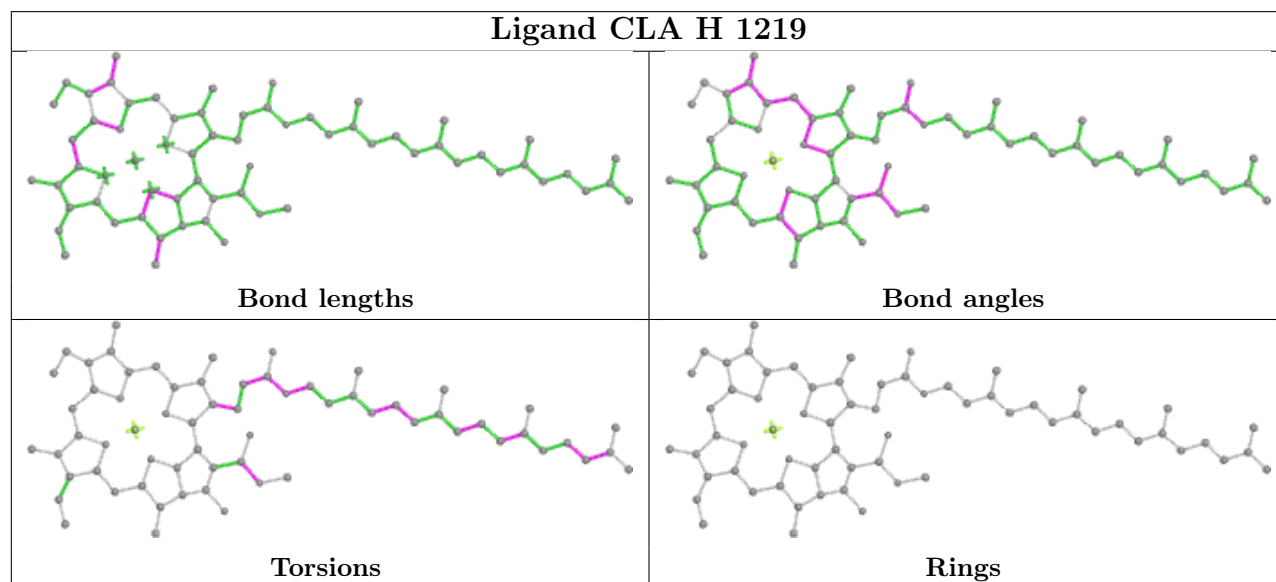


Ligand CLA Y 503**Ligand CLA 5 518**

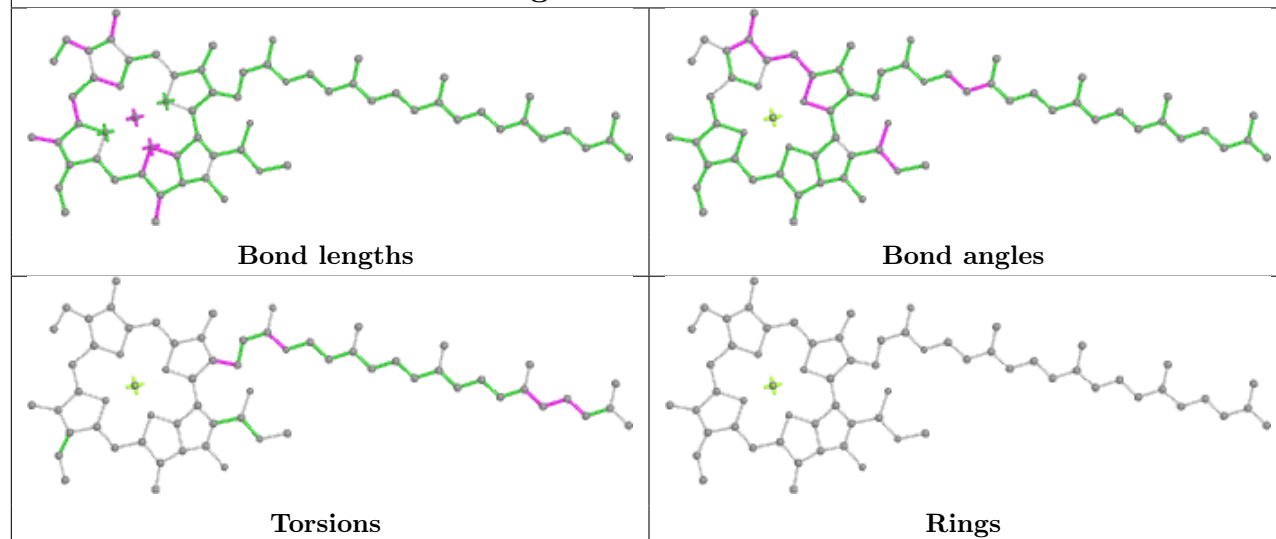
Ligand CLA G 1105



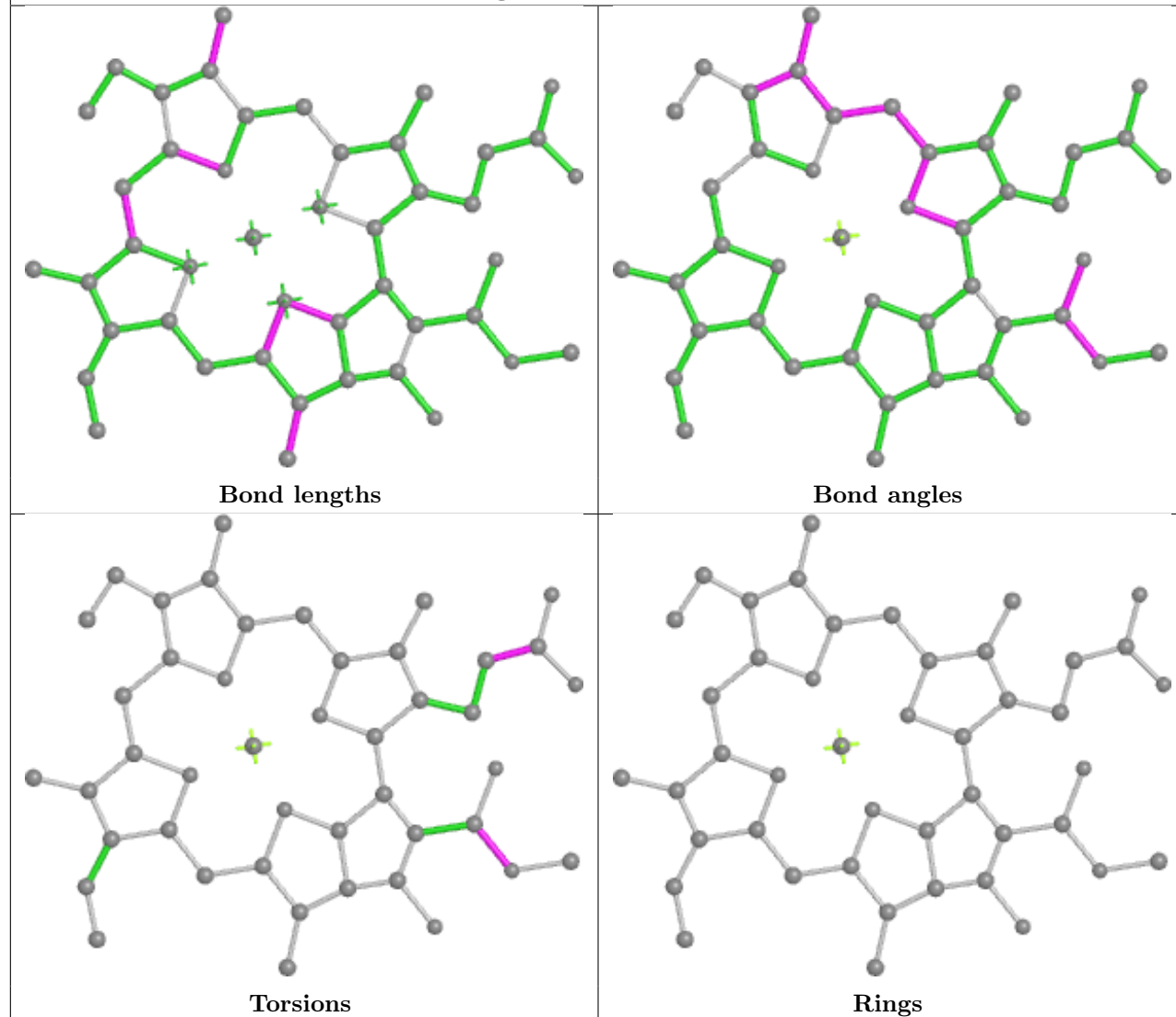
Ligand CLA H 1219



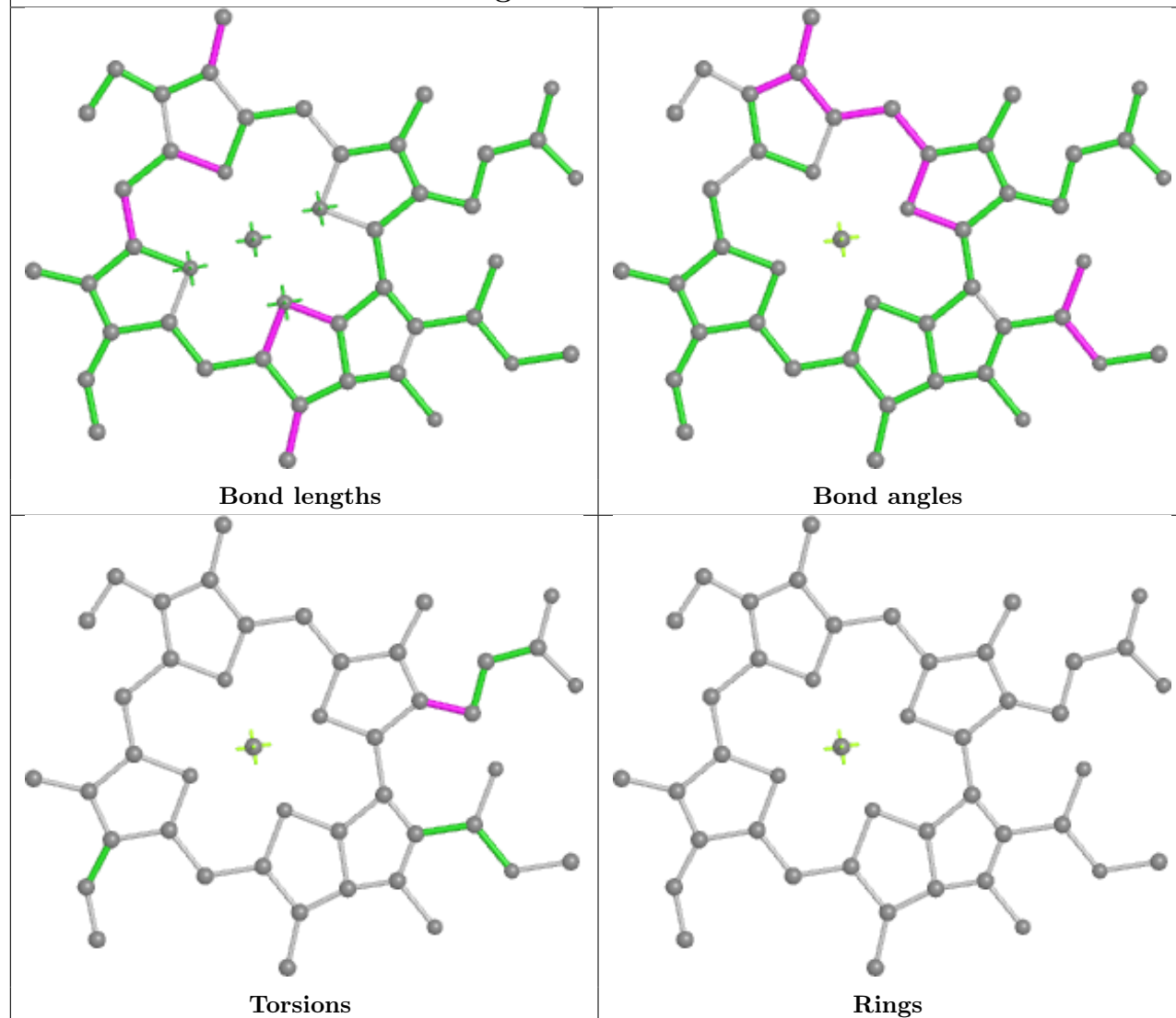
Ligand CLA f 1225



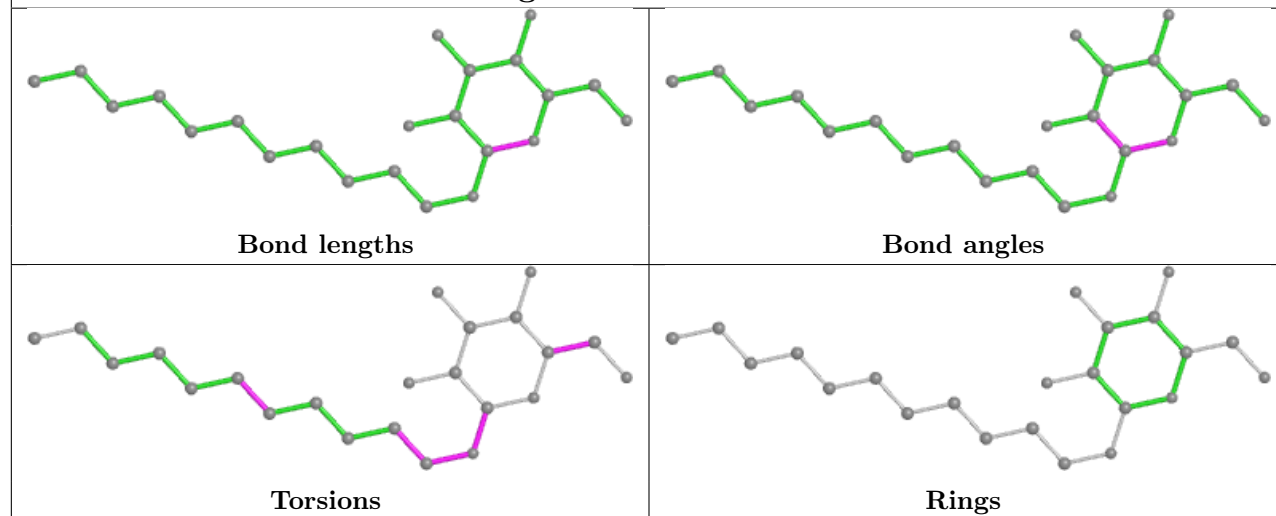
Ligand CLA v 511

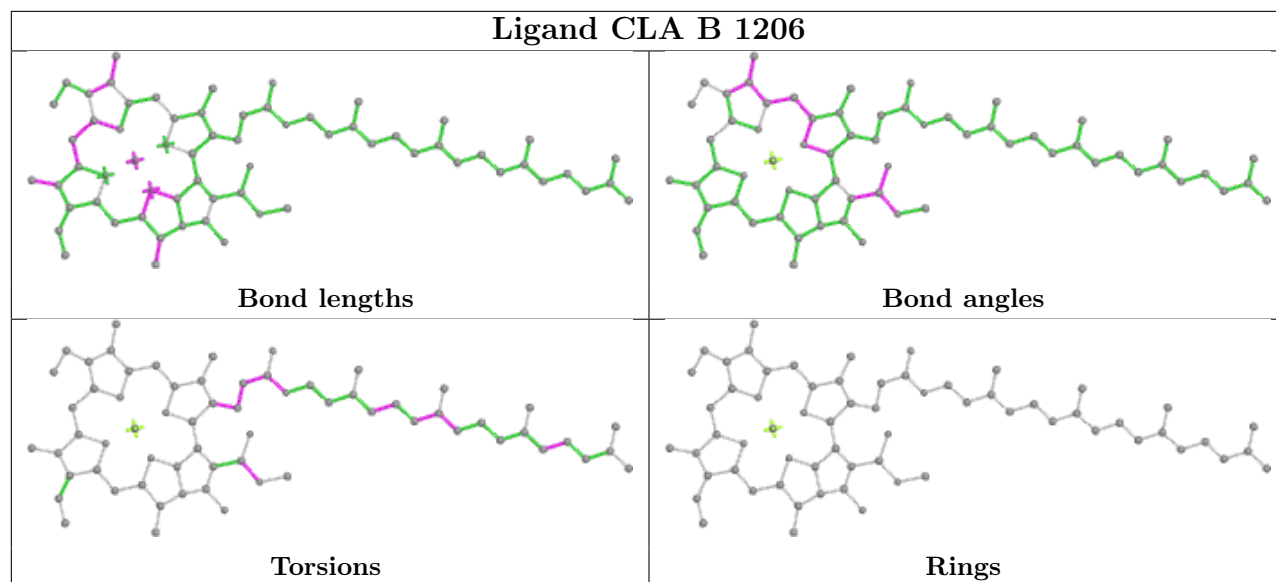
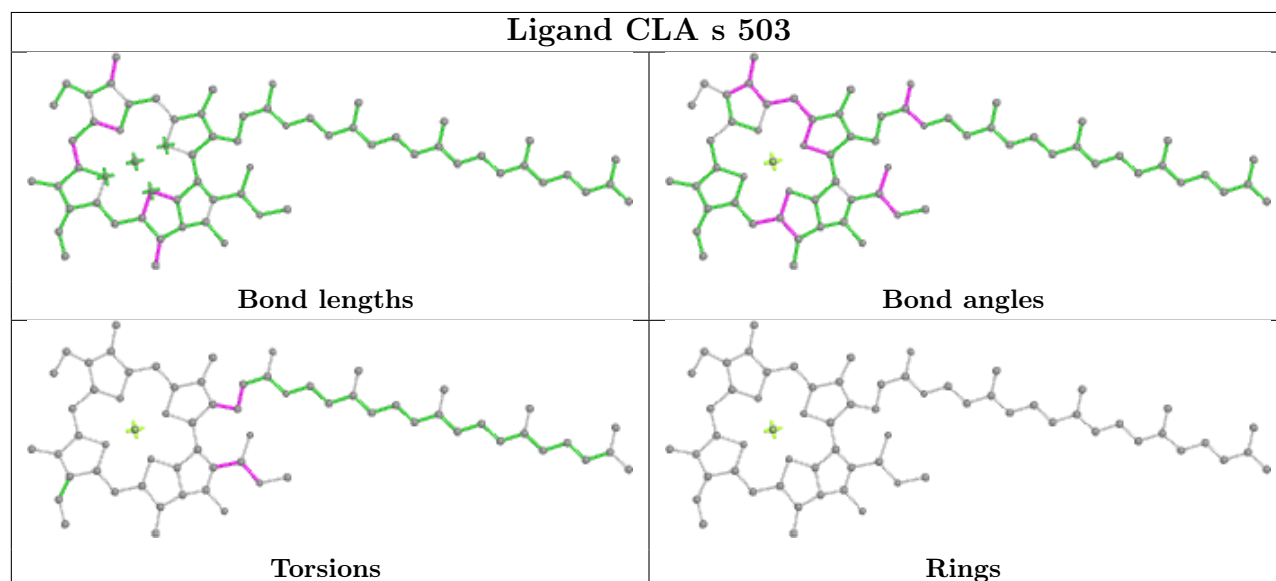
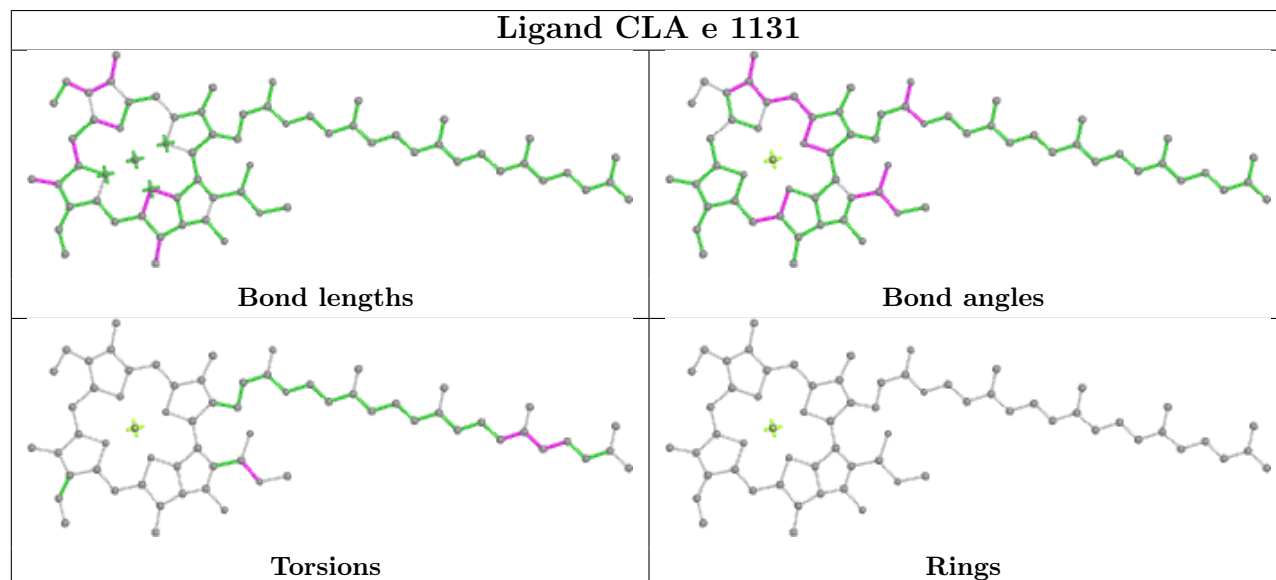


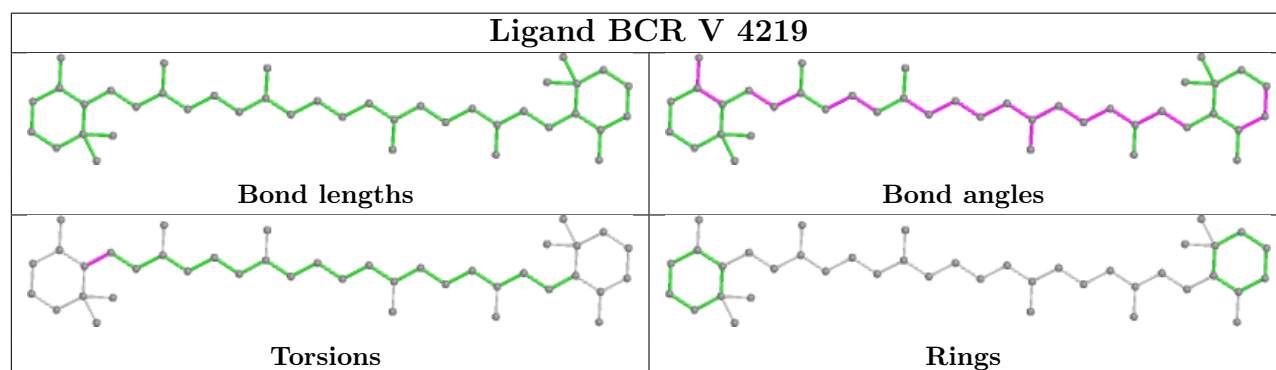
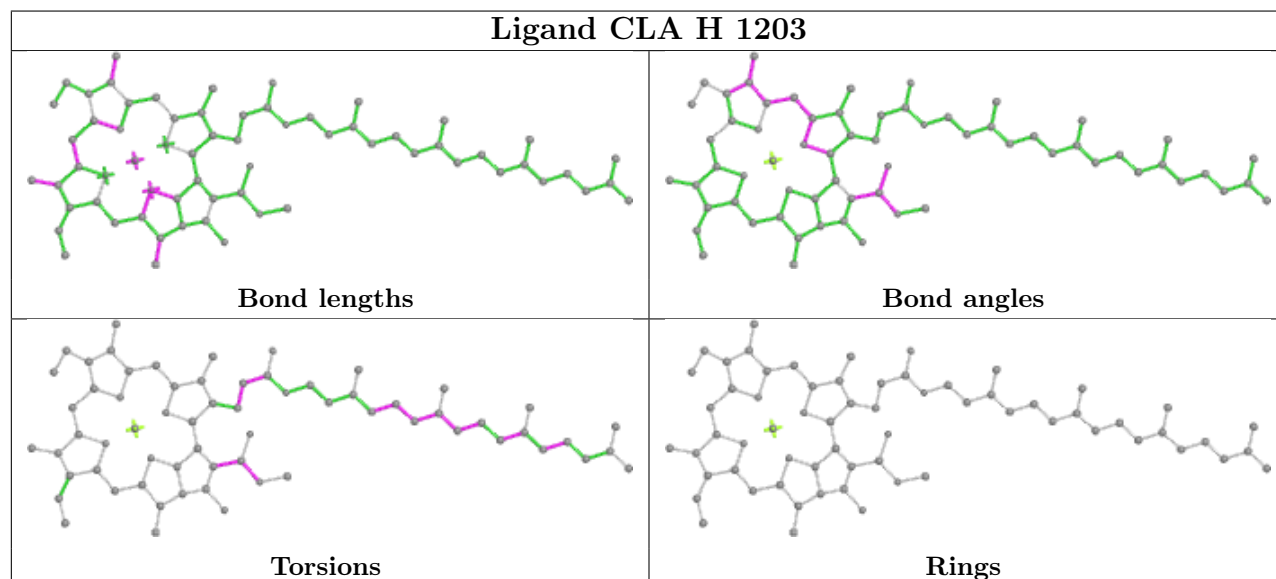
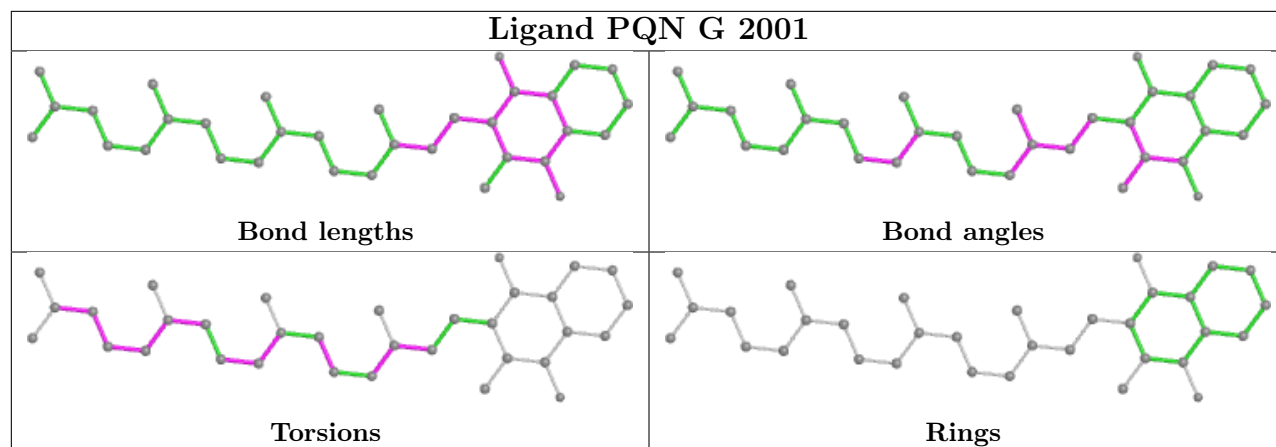
Ligand CLA c 516

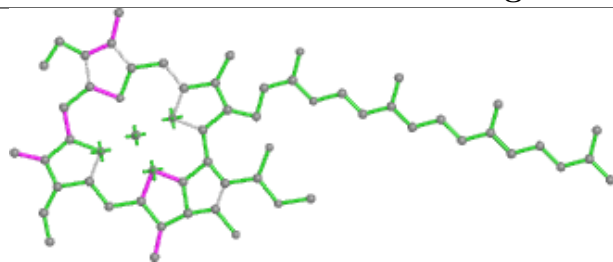


Ligand LMU A 1849

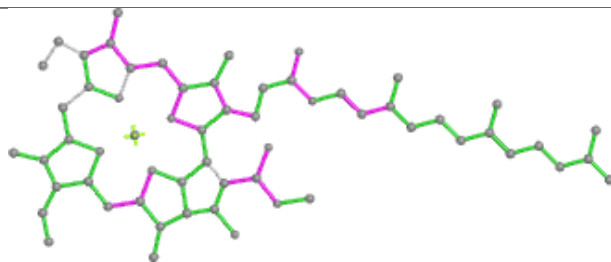


Ligand CLA B 1206**Ligand CLA s 503****Ligand CLA e 1131**

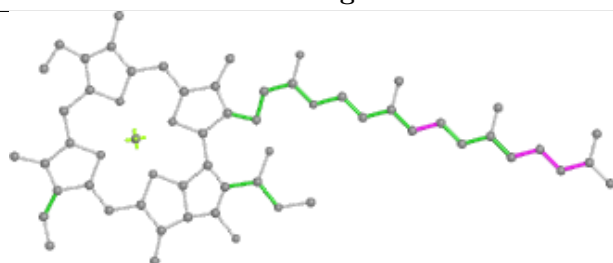


Ligand CLA A 1136

Bond lengths



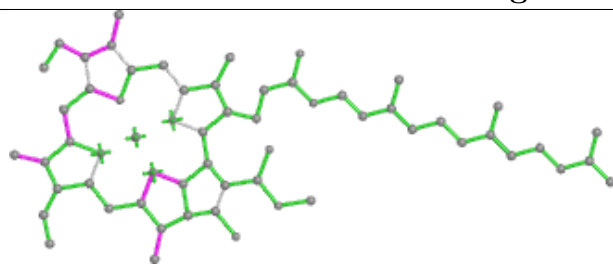
Bond angles



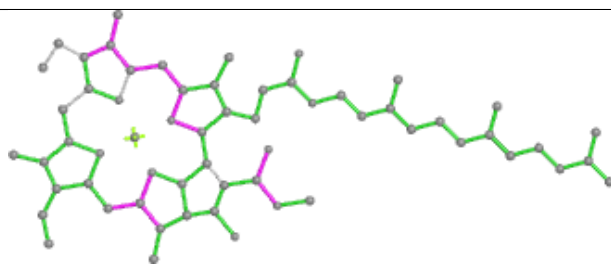
Torsions



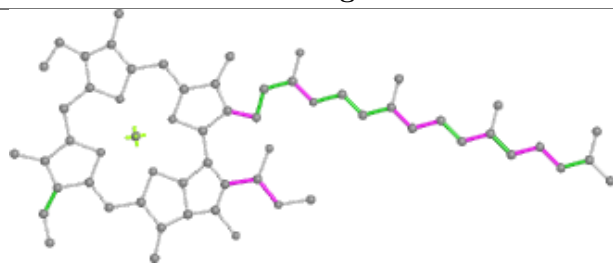
Rings

Ligand CLA e 1122

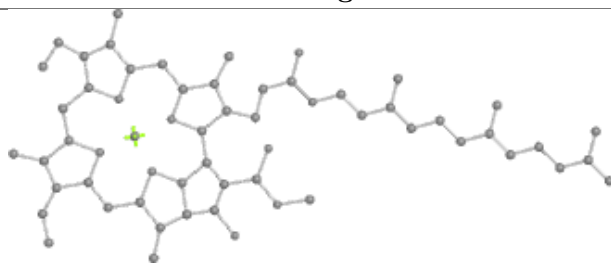
Bond lengths



Bond angles

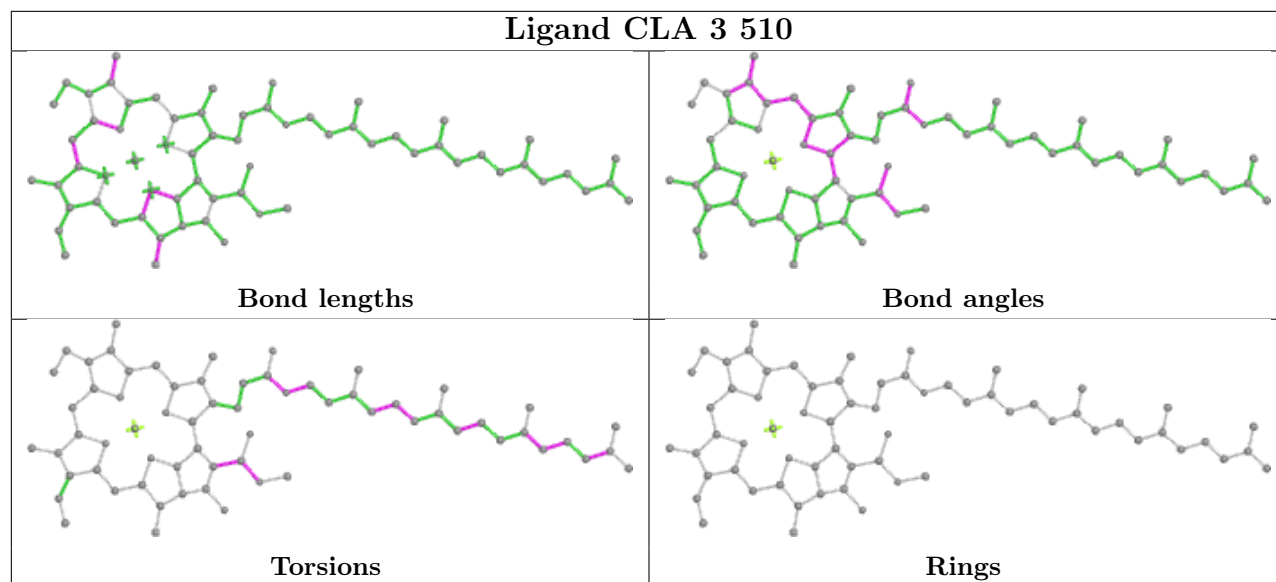


Torsions

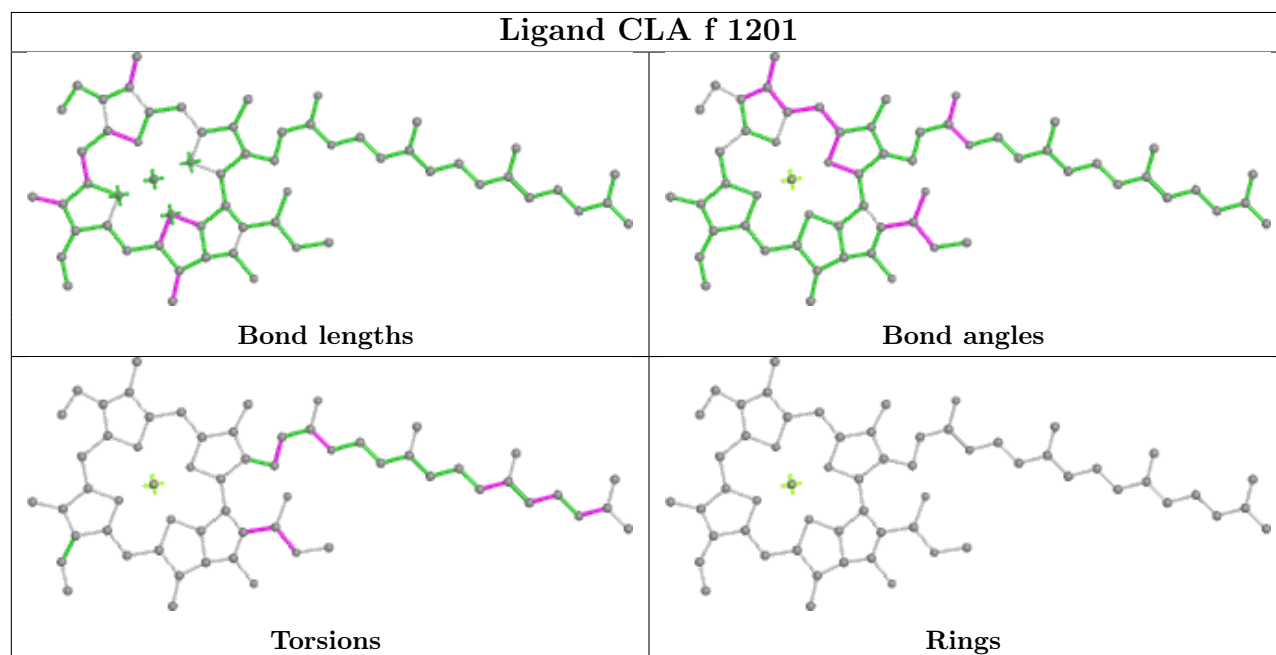


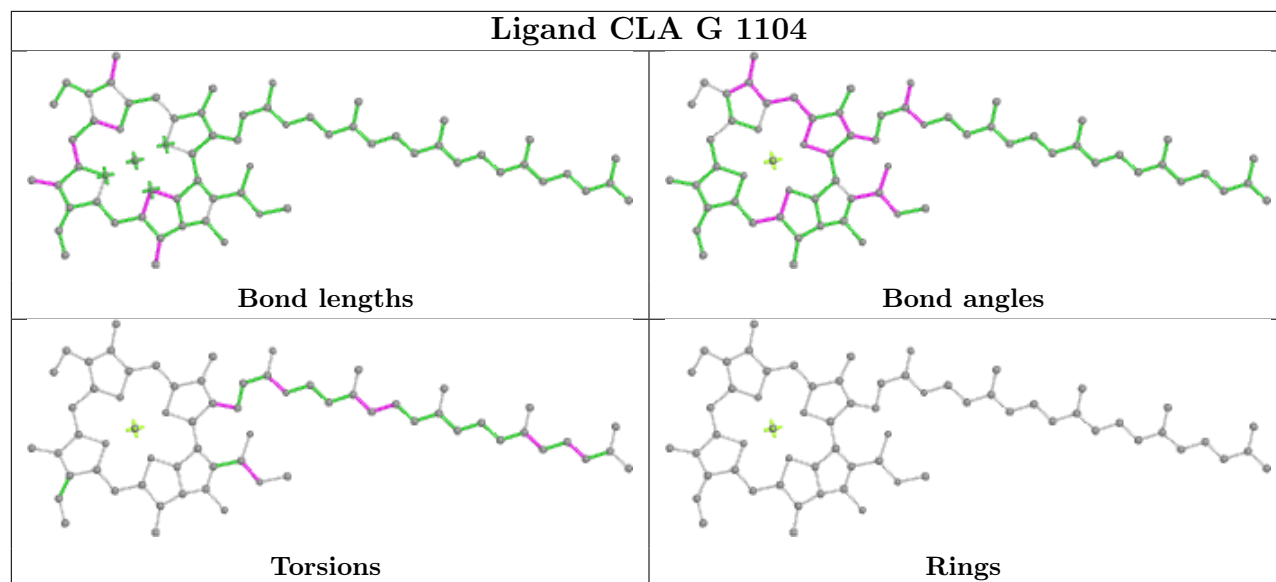
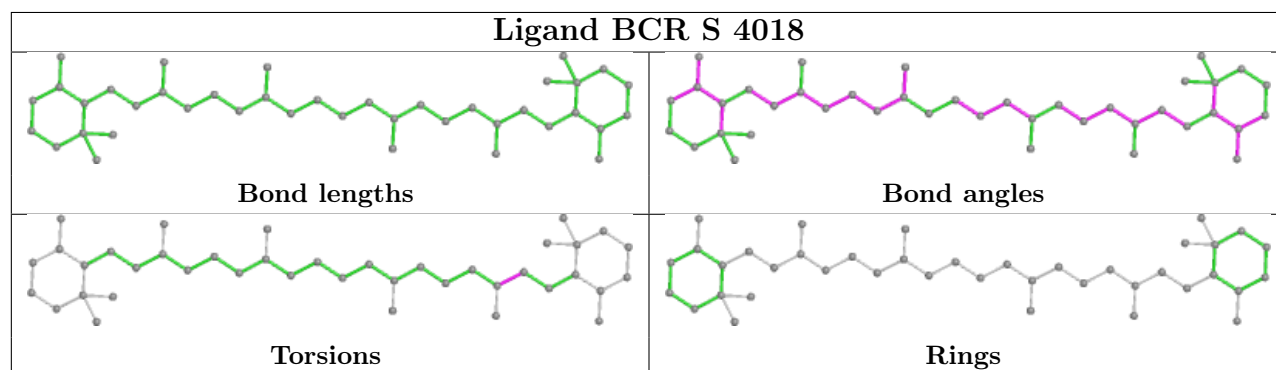
Rings

Ligand CLA 3 510

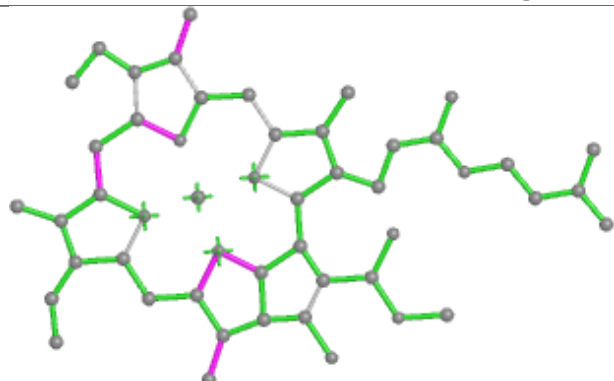


Ligand CLA f 1201

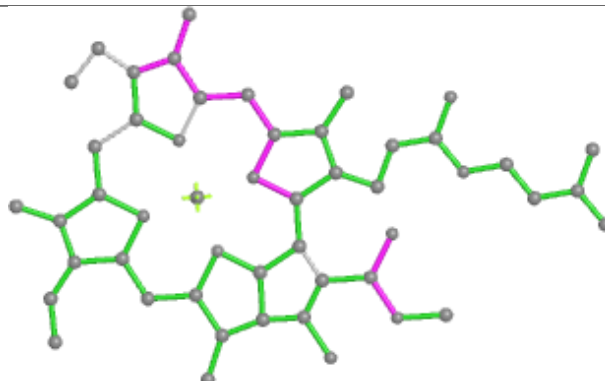


Ligand CLA G 1104**Ligand BCR S 4018**

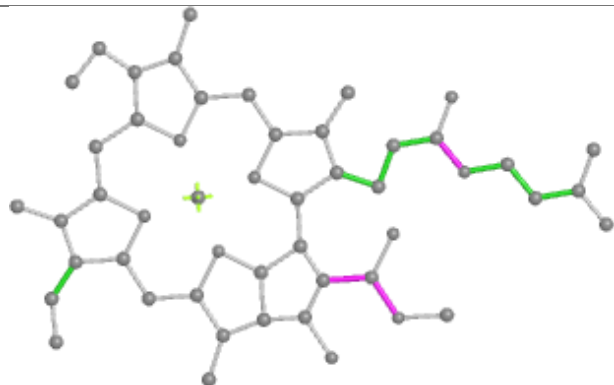
Ligand CLA v 502



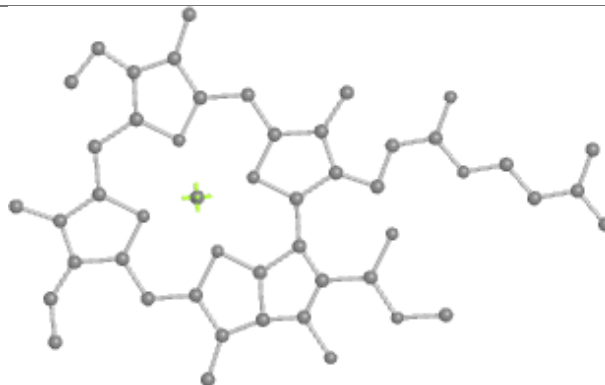
Bond lengths



Bond angles

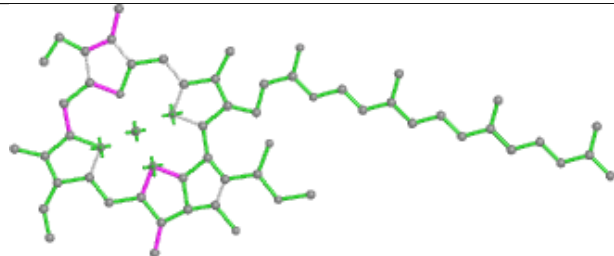


Torsions

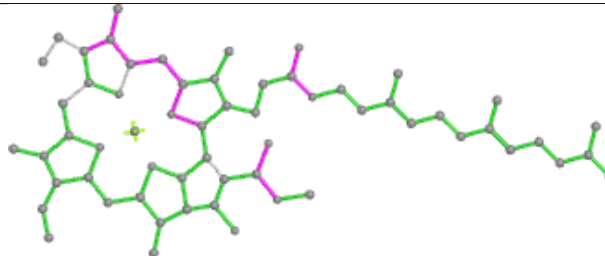


Rings

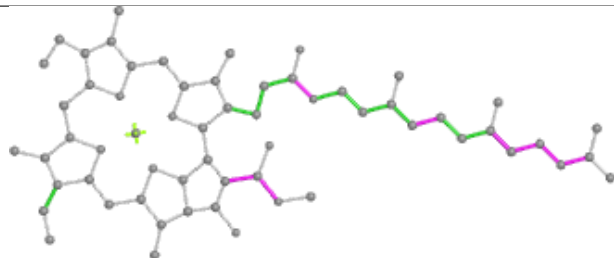
Ligand CLA q 502



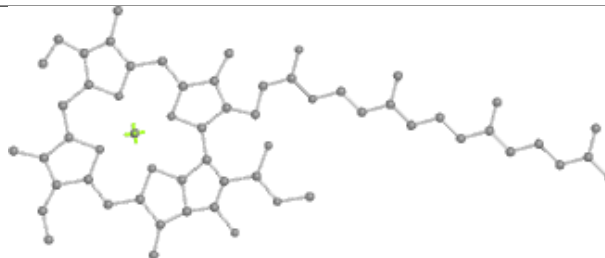
Bond lengths



Bond angles

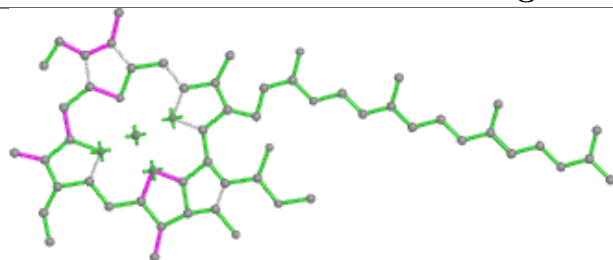


Torsions

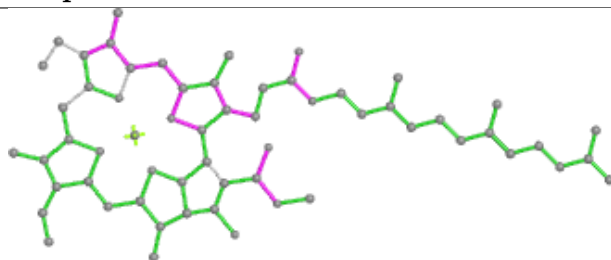


Rings

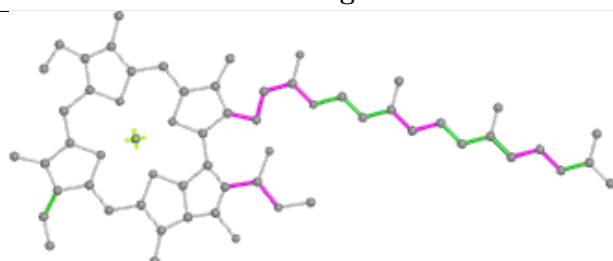
Ligand CLA q 518



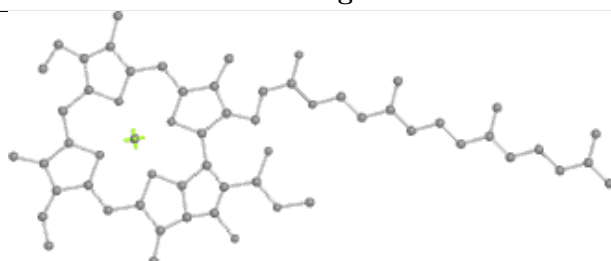
Bond lengths



Bond angles

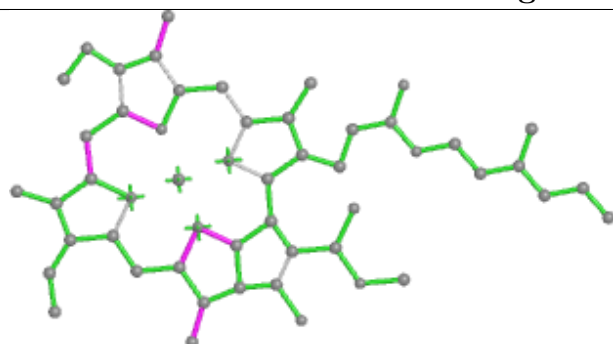


Torsions

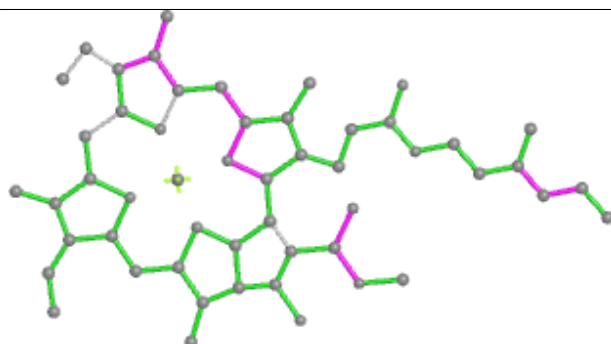


Rings

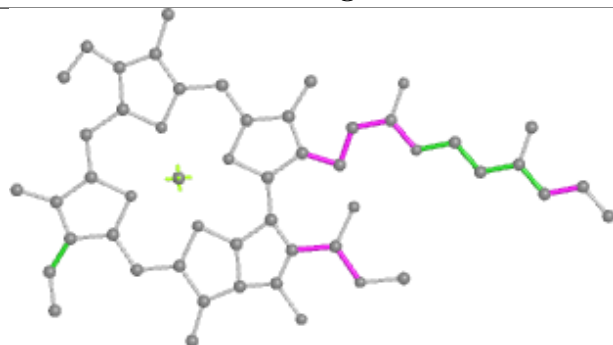
Ligand CLA 1 512



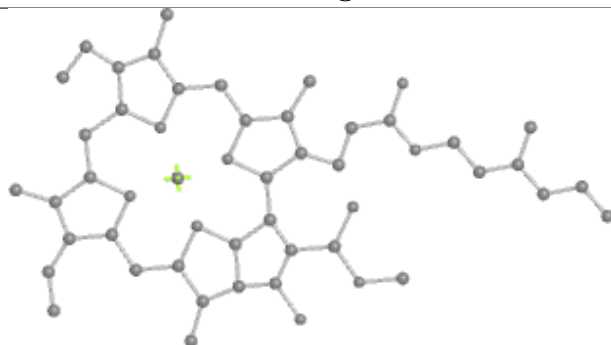
Bond lengths



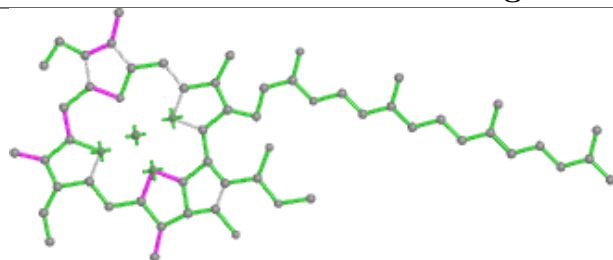
Bond angles



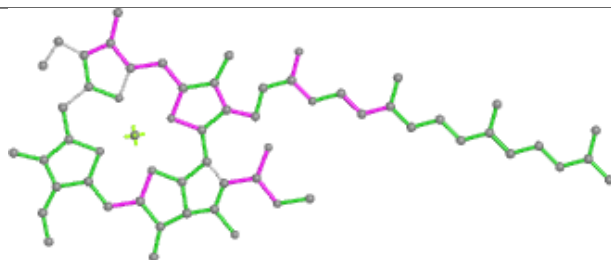
Torsions



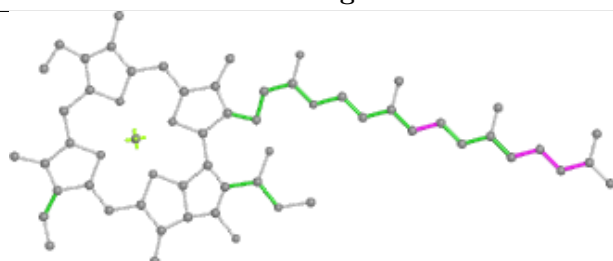
Rings

Ligand CLA G 1136

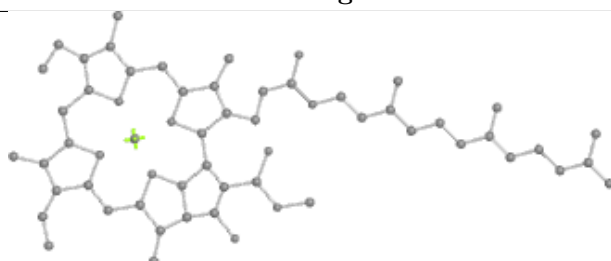
Bond lengths



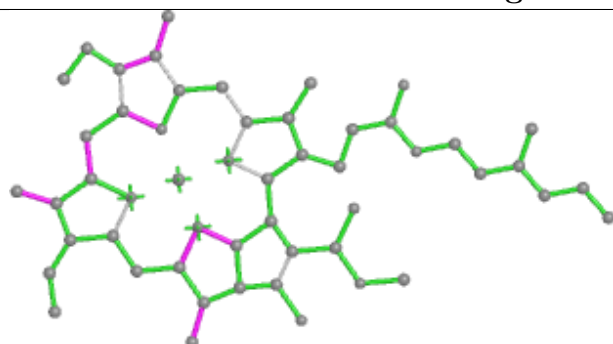
Bond angles



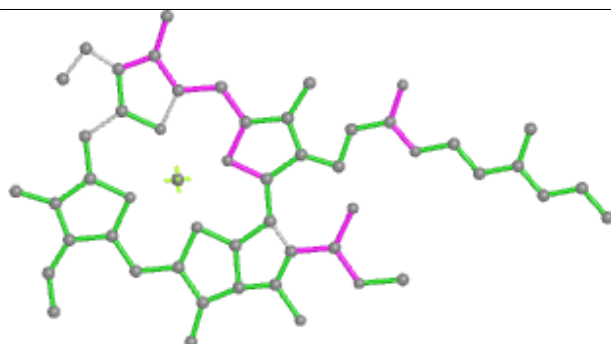
Torsions



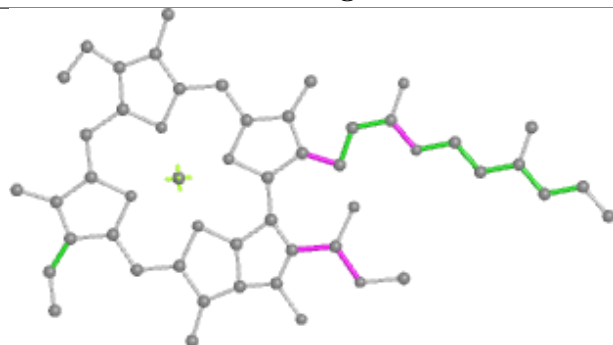
Rings

Ligand CLA B 1209

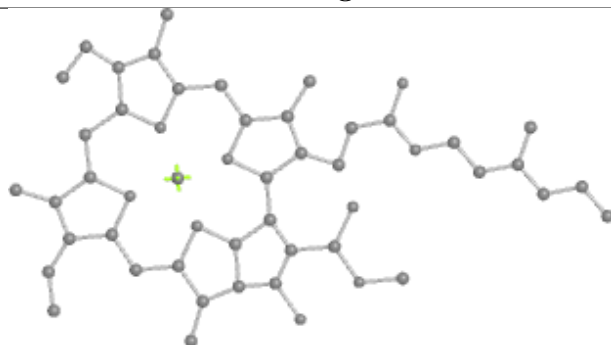
Bond lengths



Bond angles

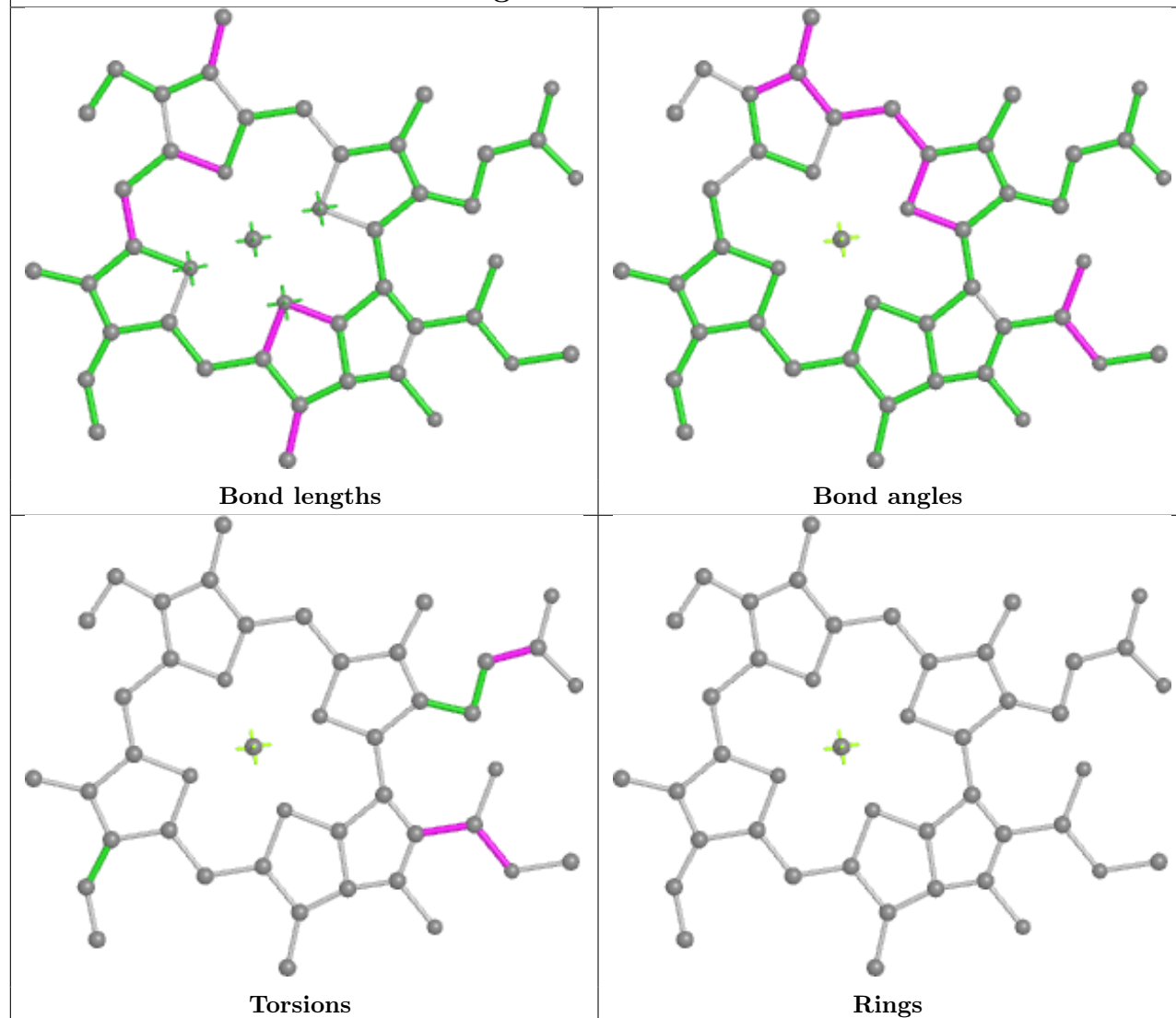


Torsions

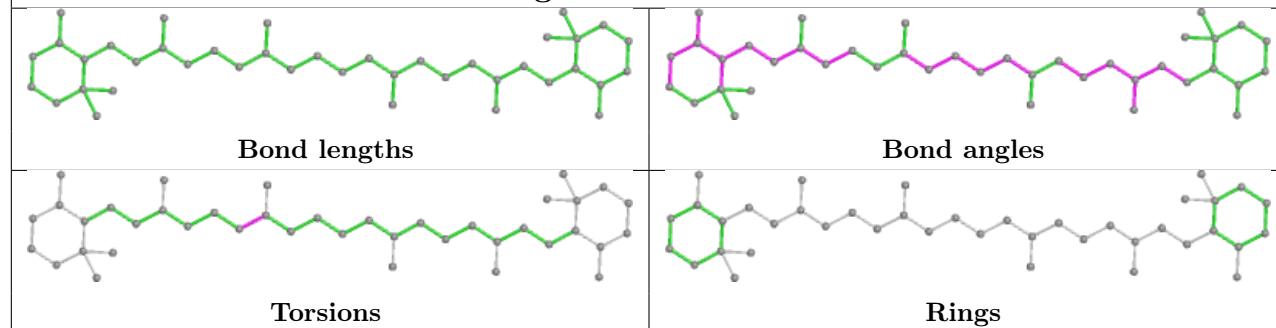


Rings

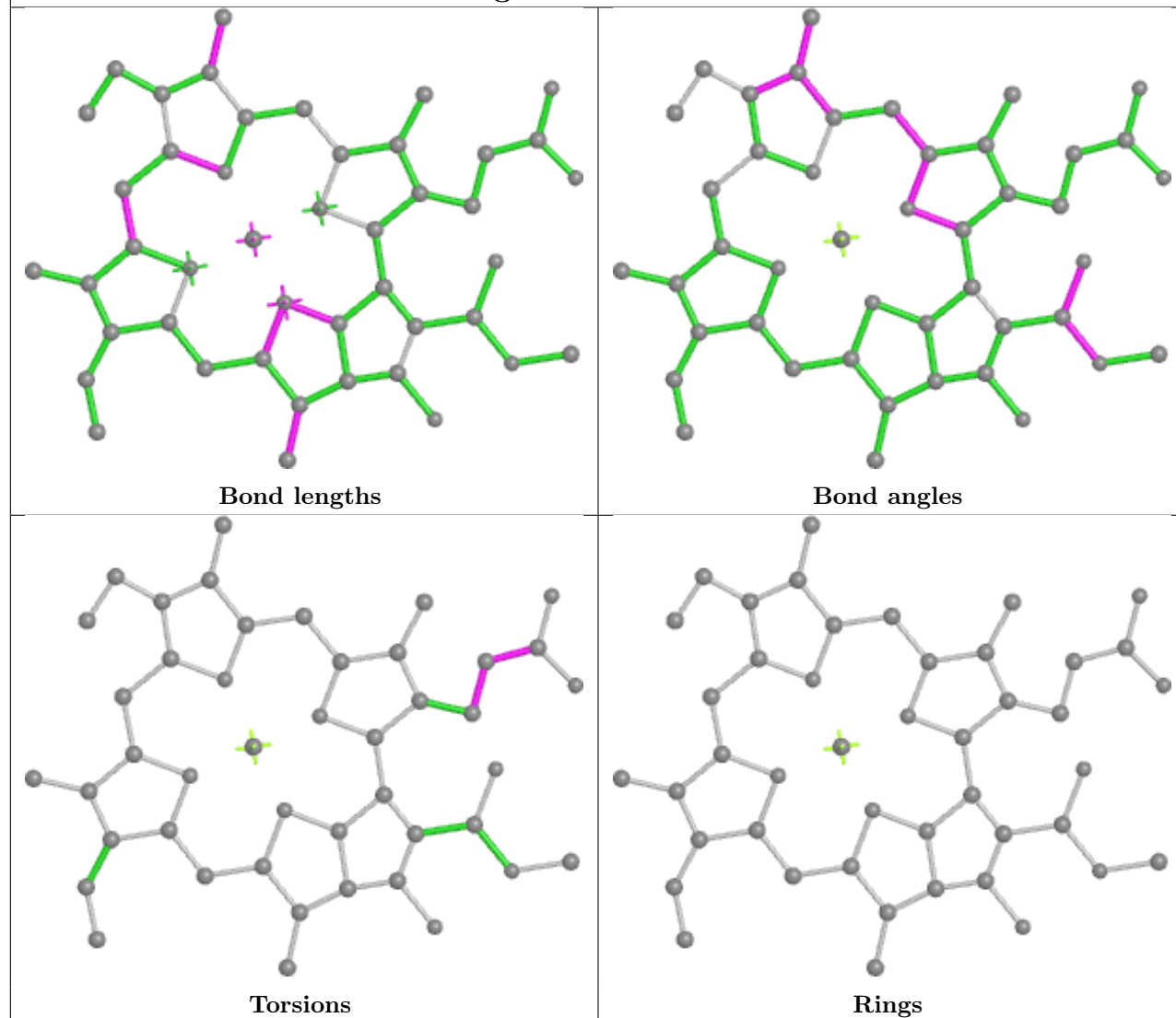
Ligand CLA v 509



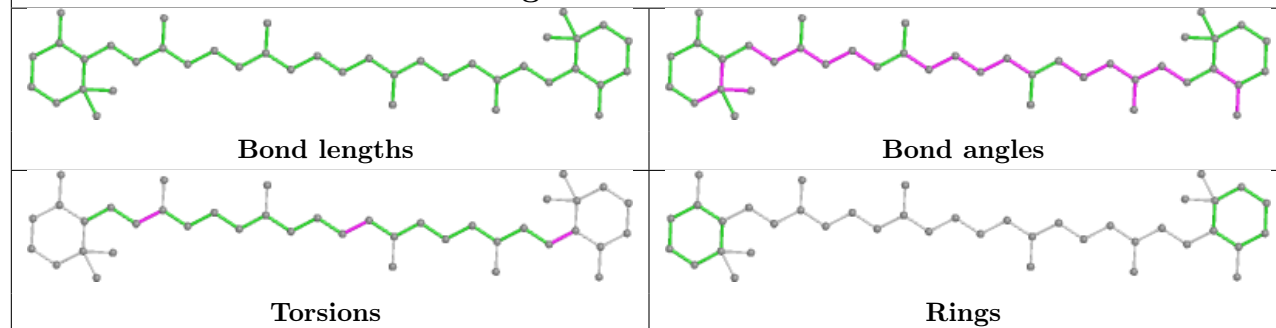
Ligand BCR 1 524



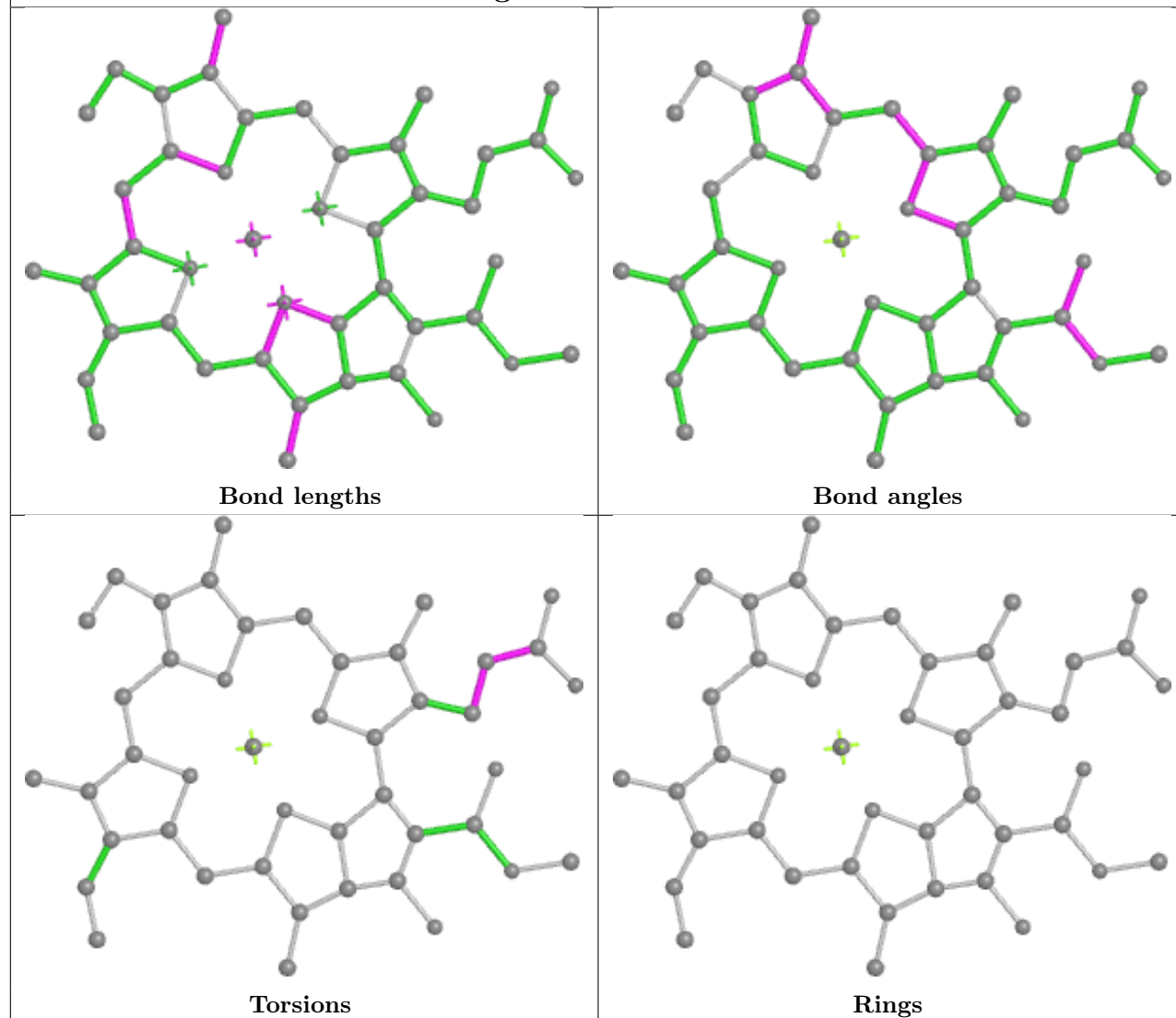
Ligand CLA a 512



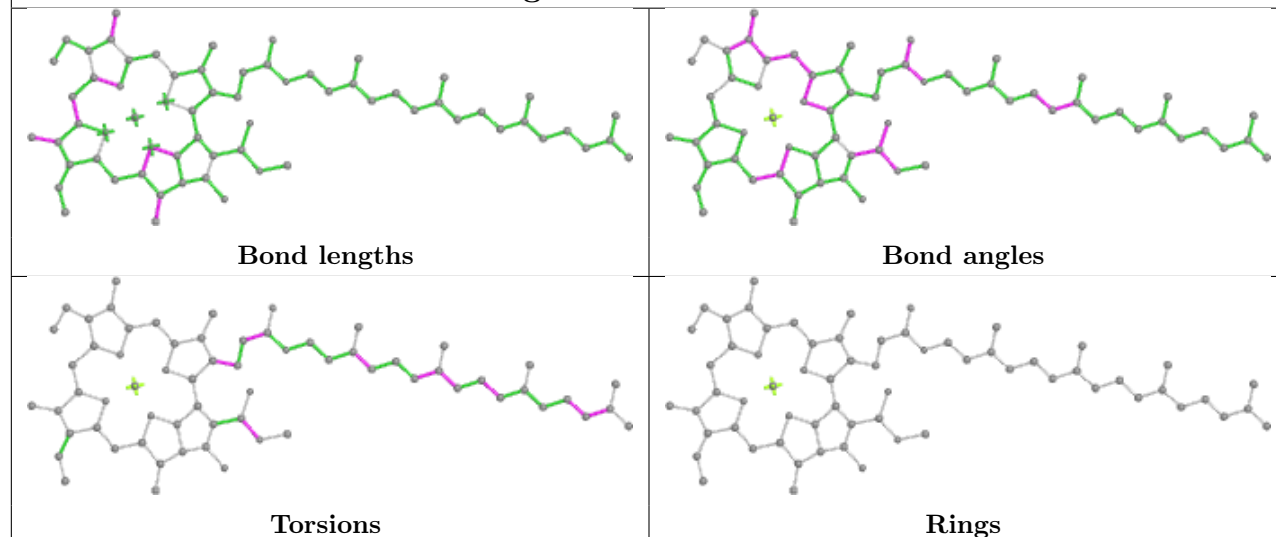
Ligand BCR T 4015



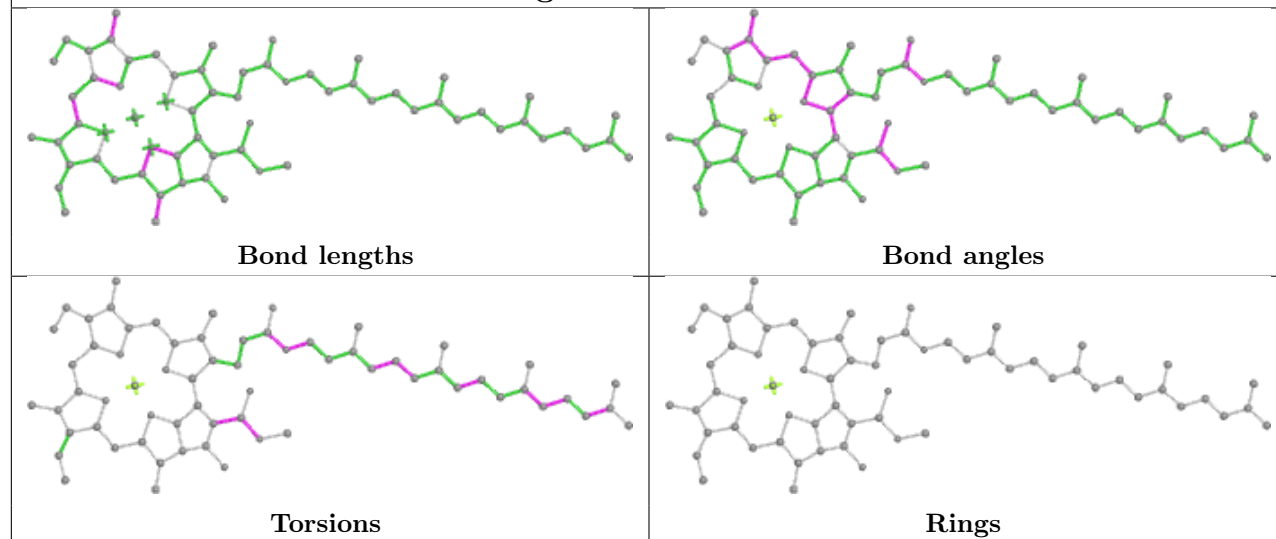
Ligand CLA 3 512



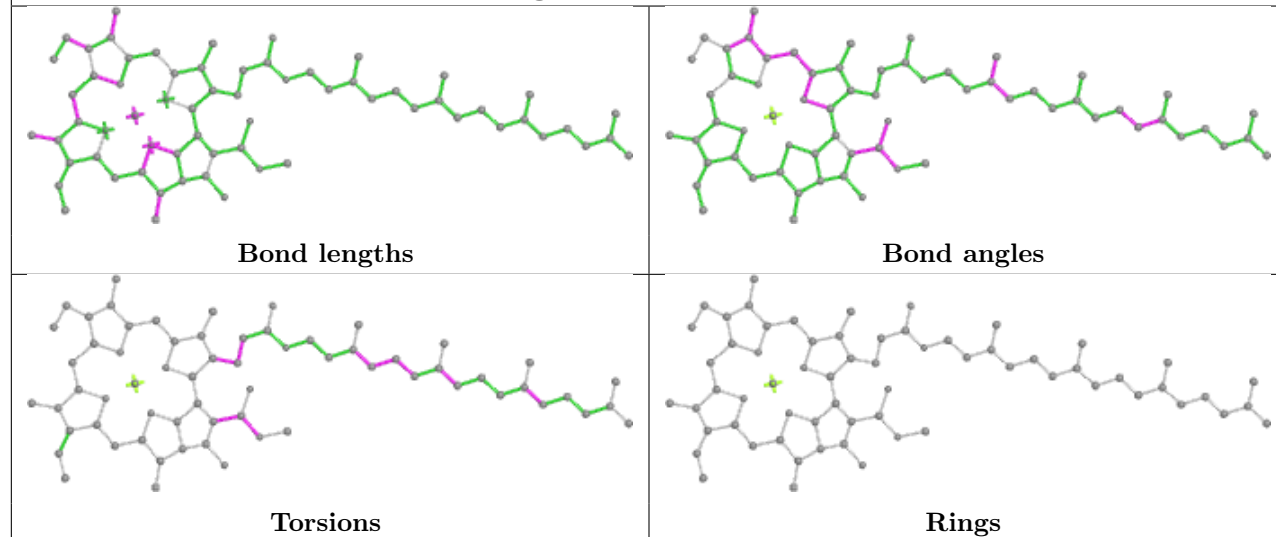
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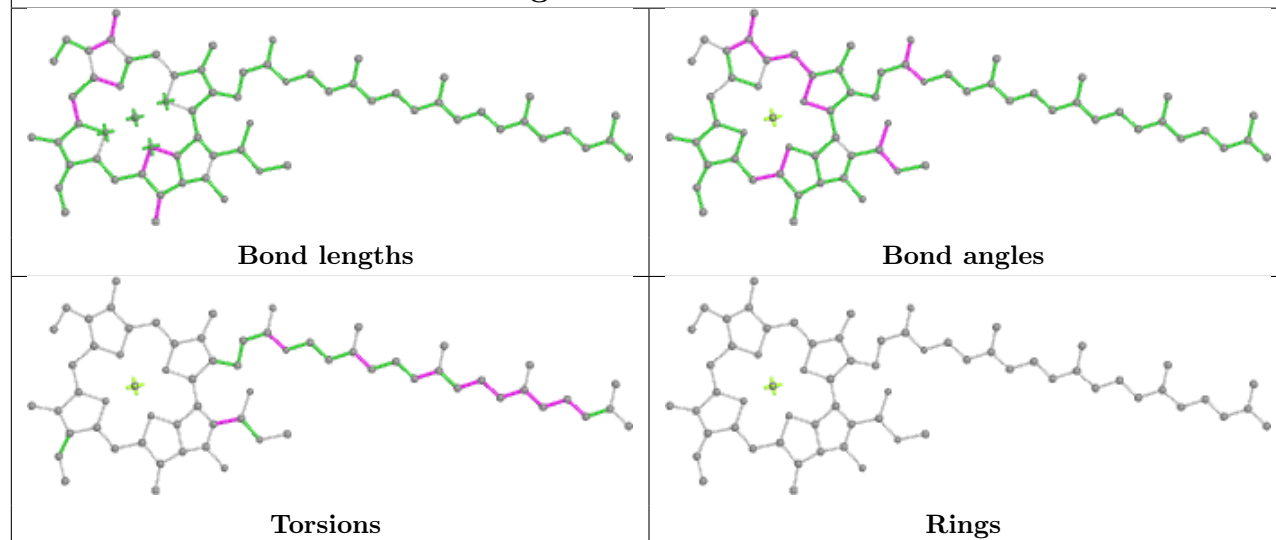
Ligand CLA a 510



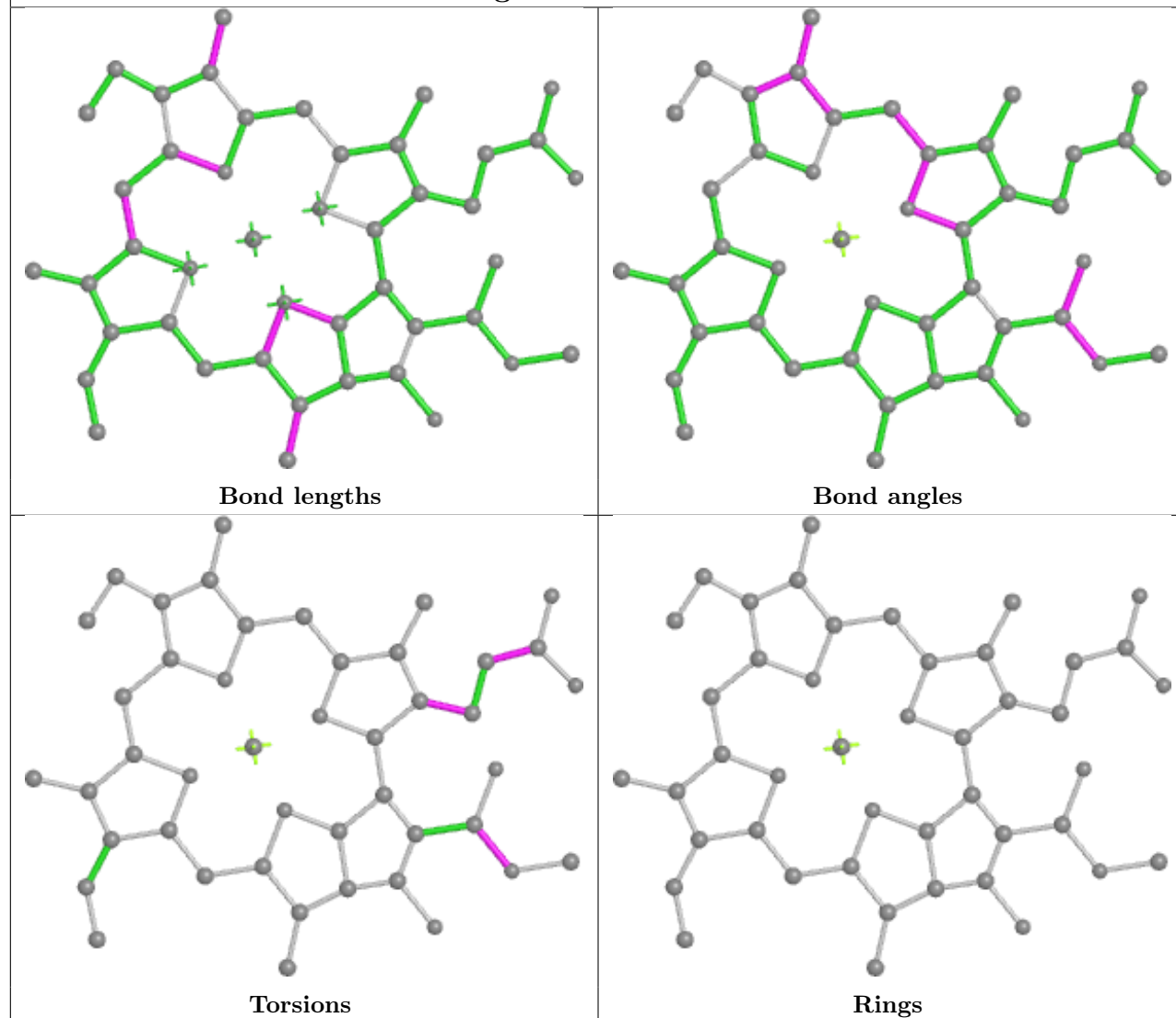
Ligand CLA f 1012



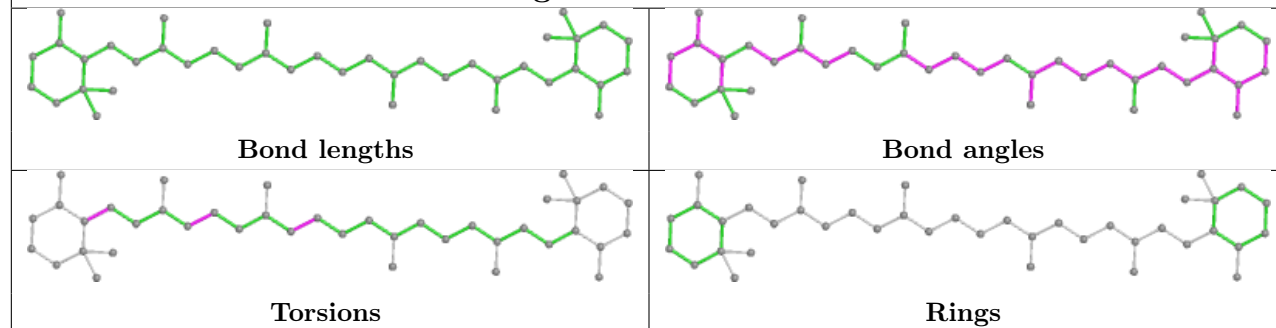
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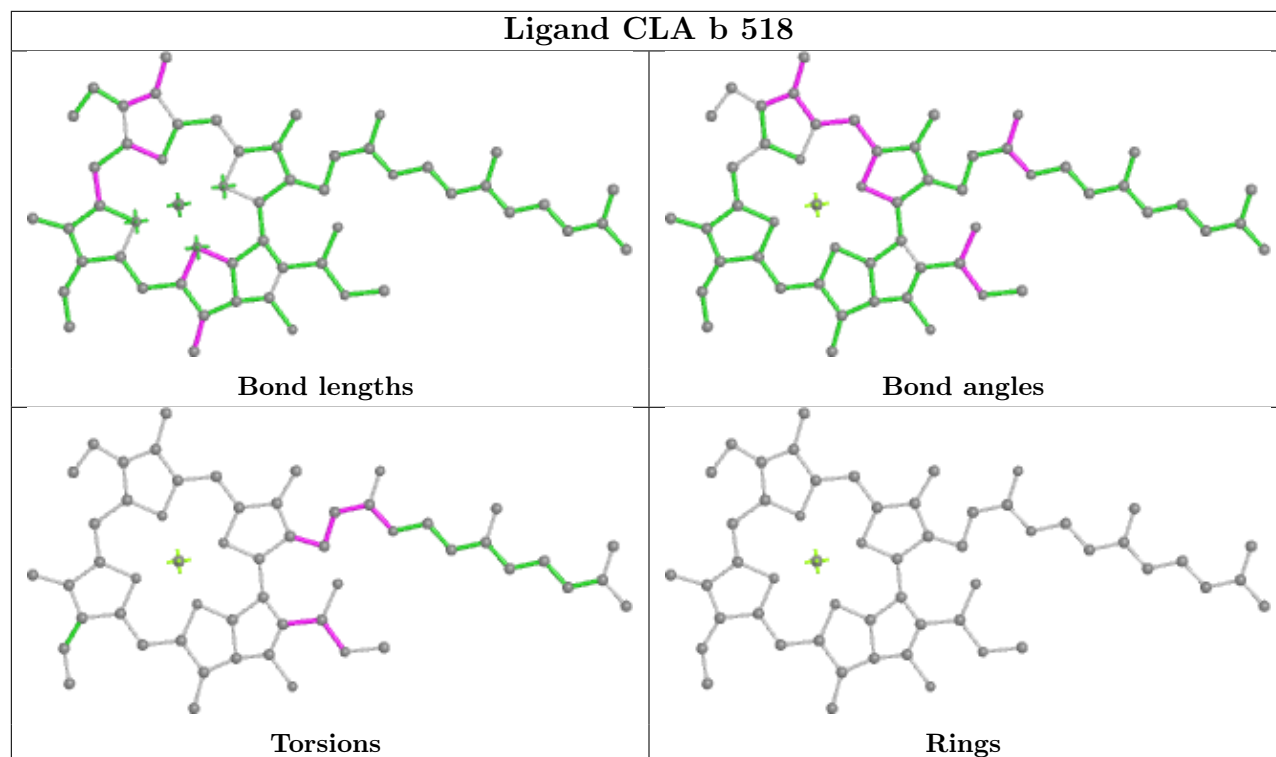
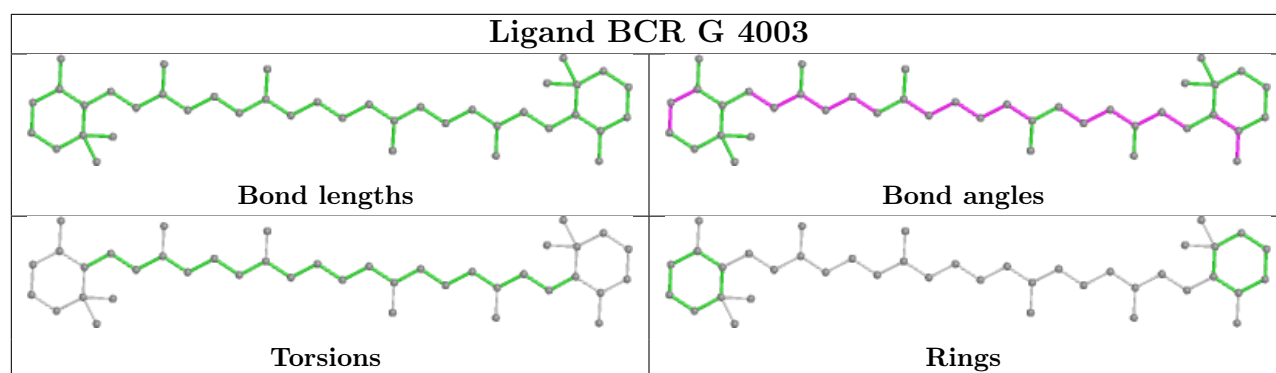


Ligand CLA 6 512

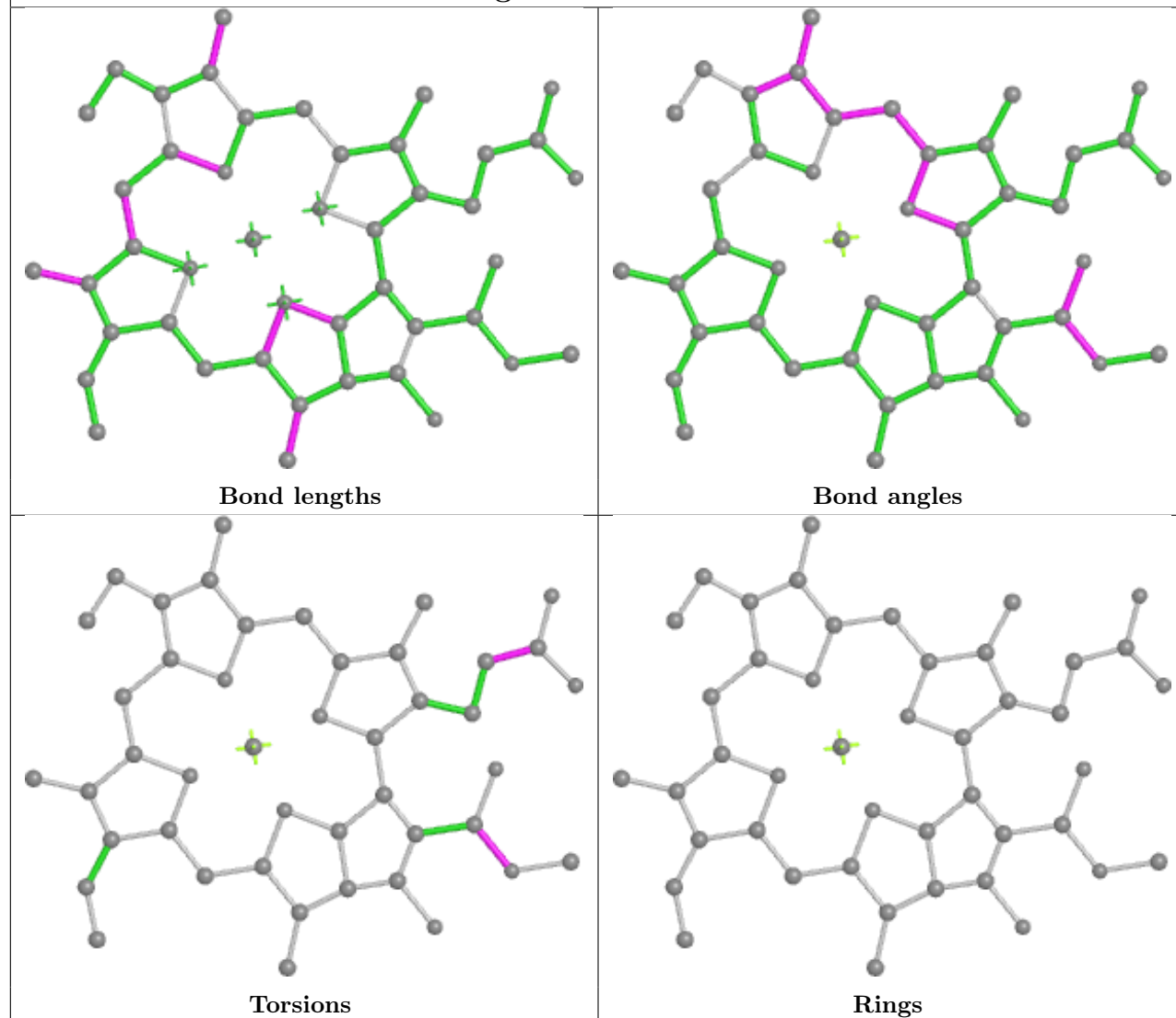


Ligand BCR b 522

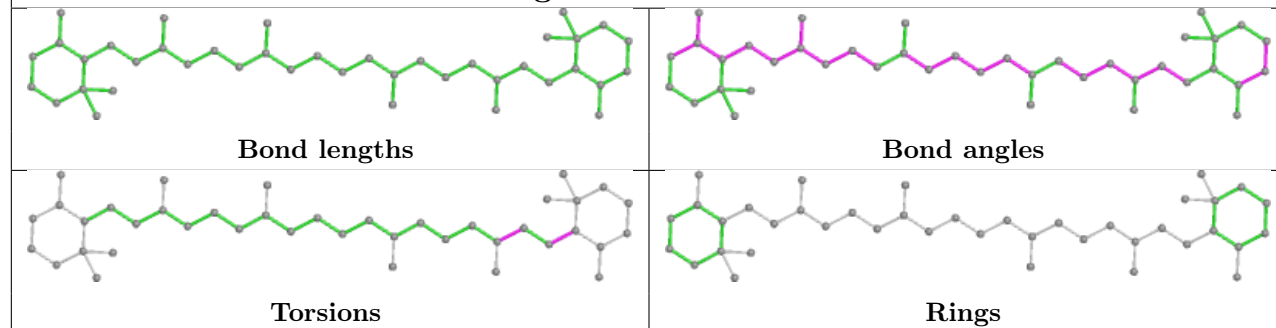




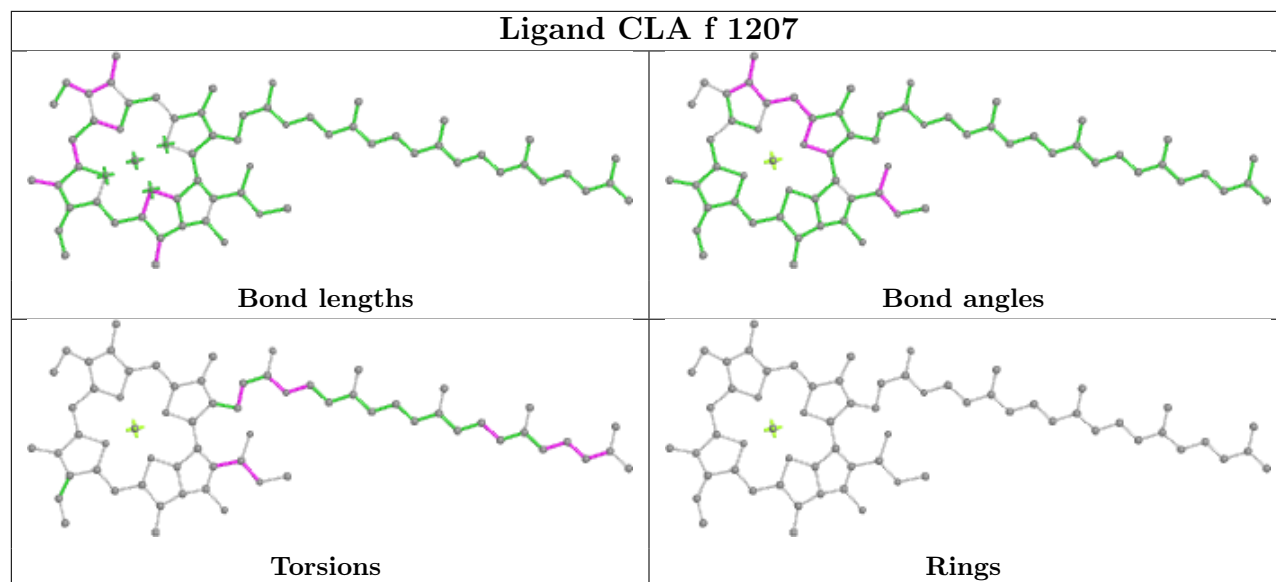
Ligand CLA c 508



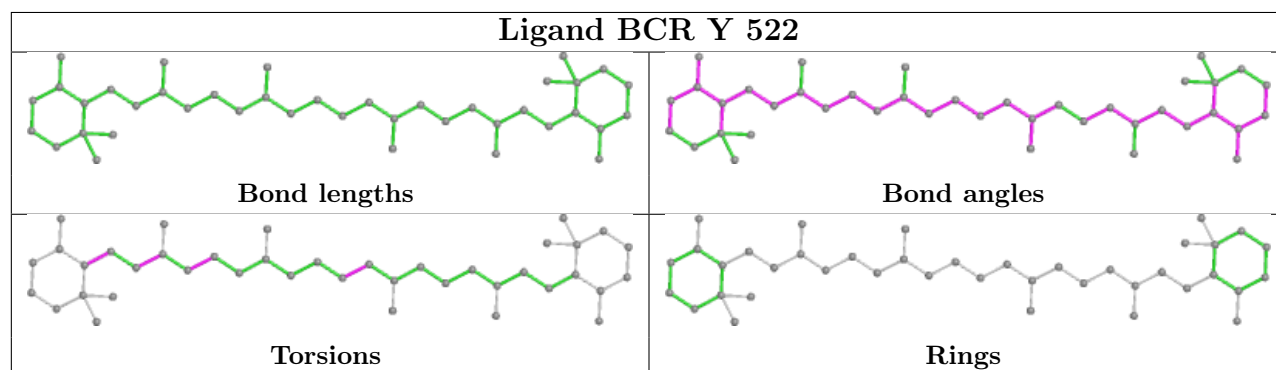
Ligand BCR v 523



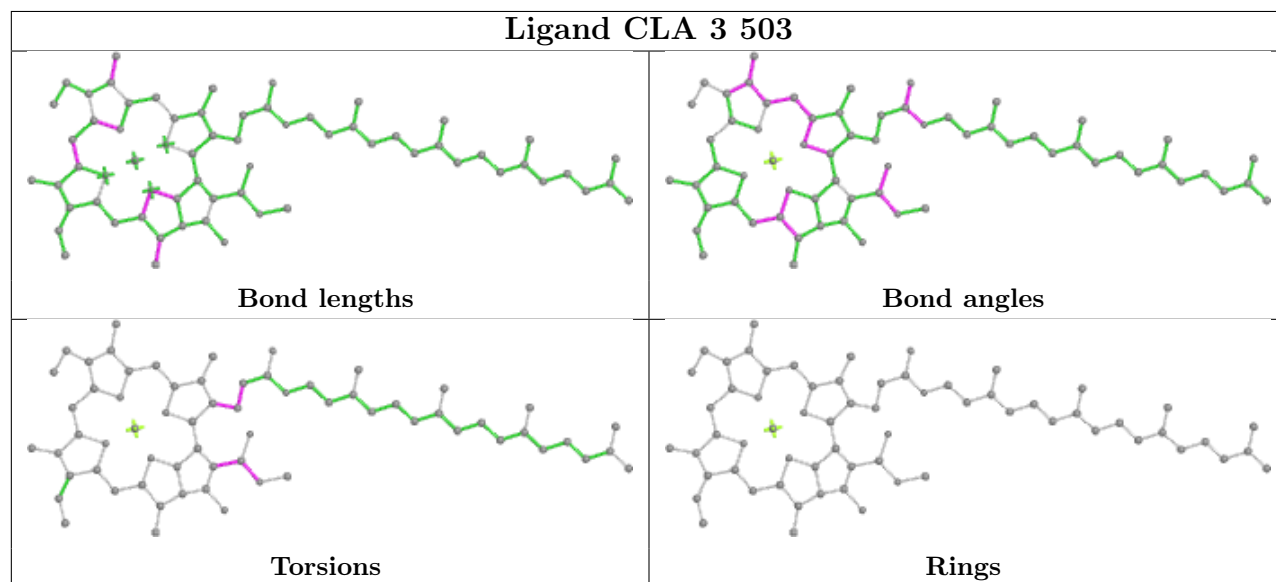
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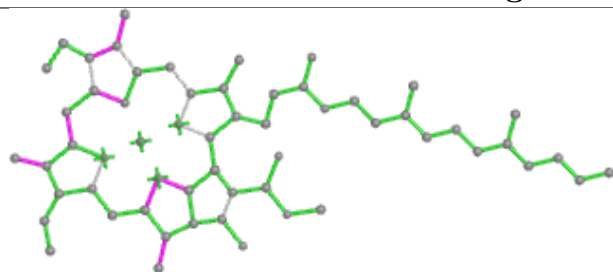
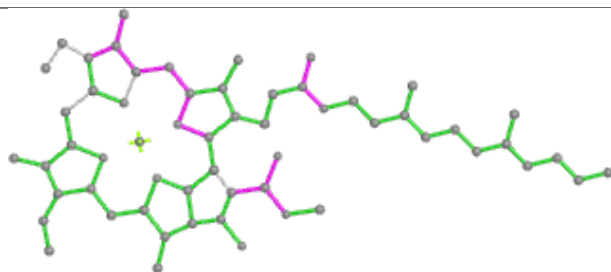
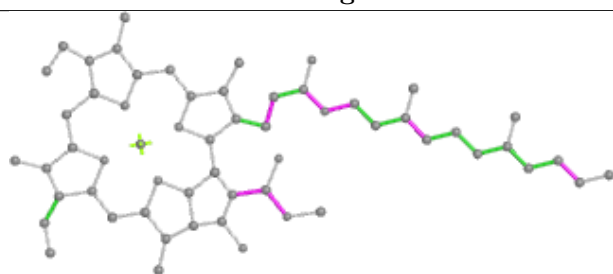
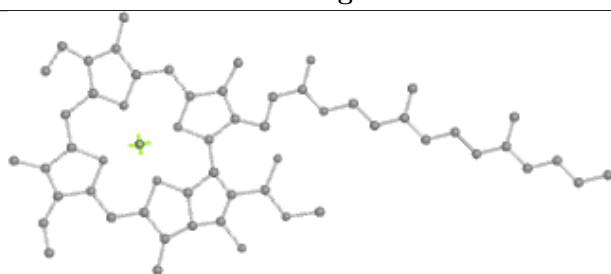
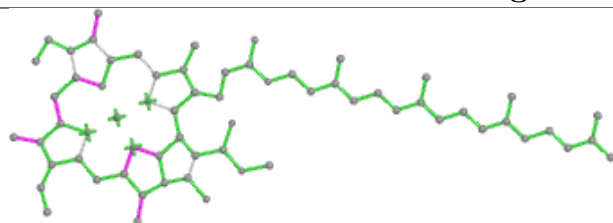
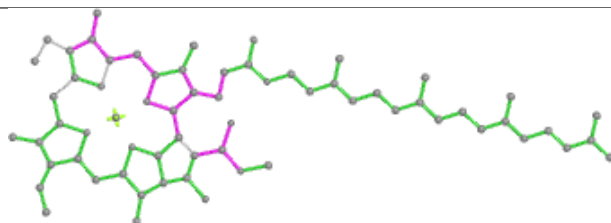
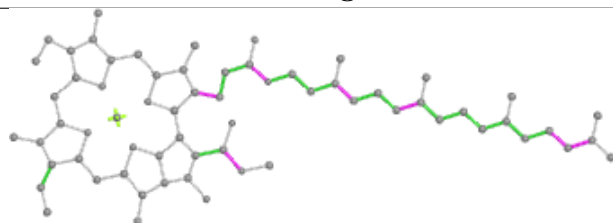
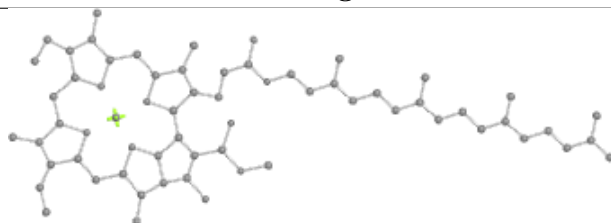


Ligand BCR Y 522

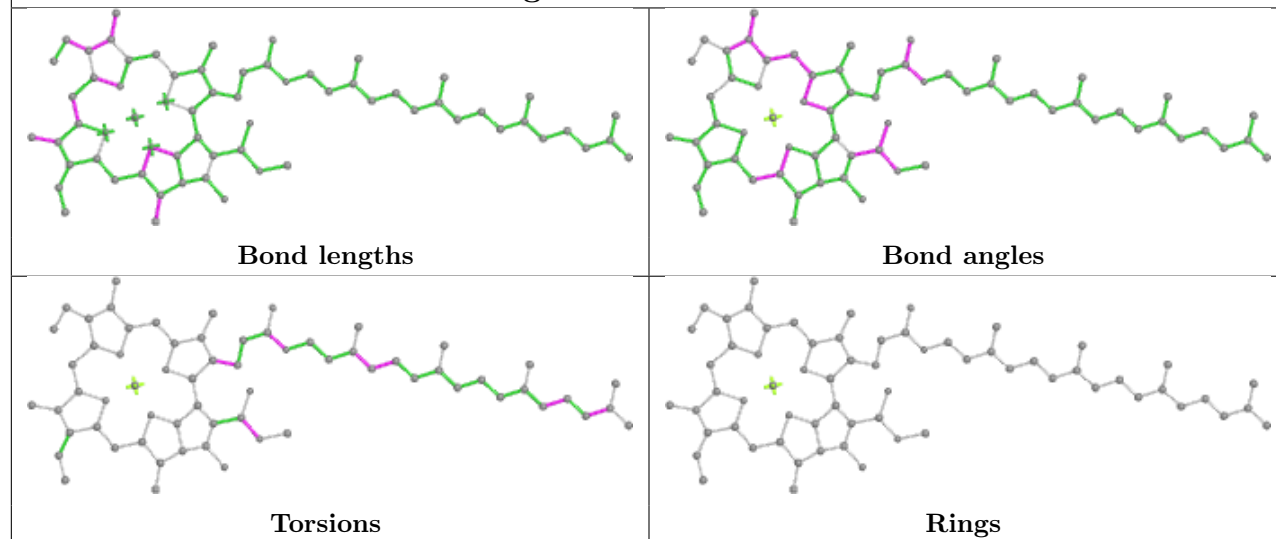


Ligand CLA 3 503

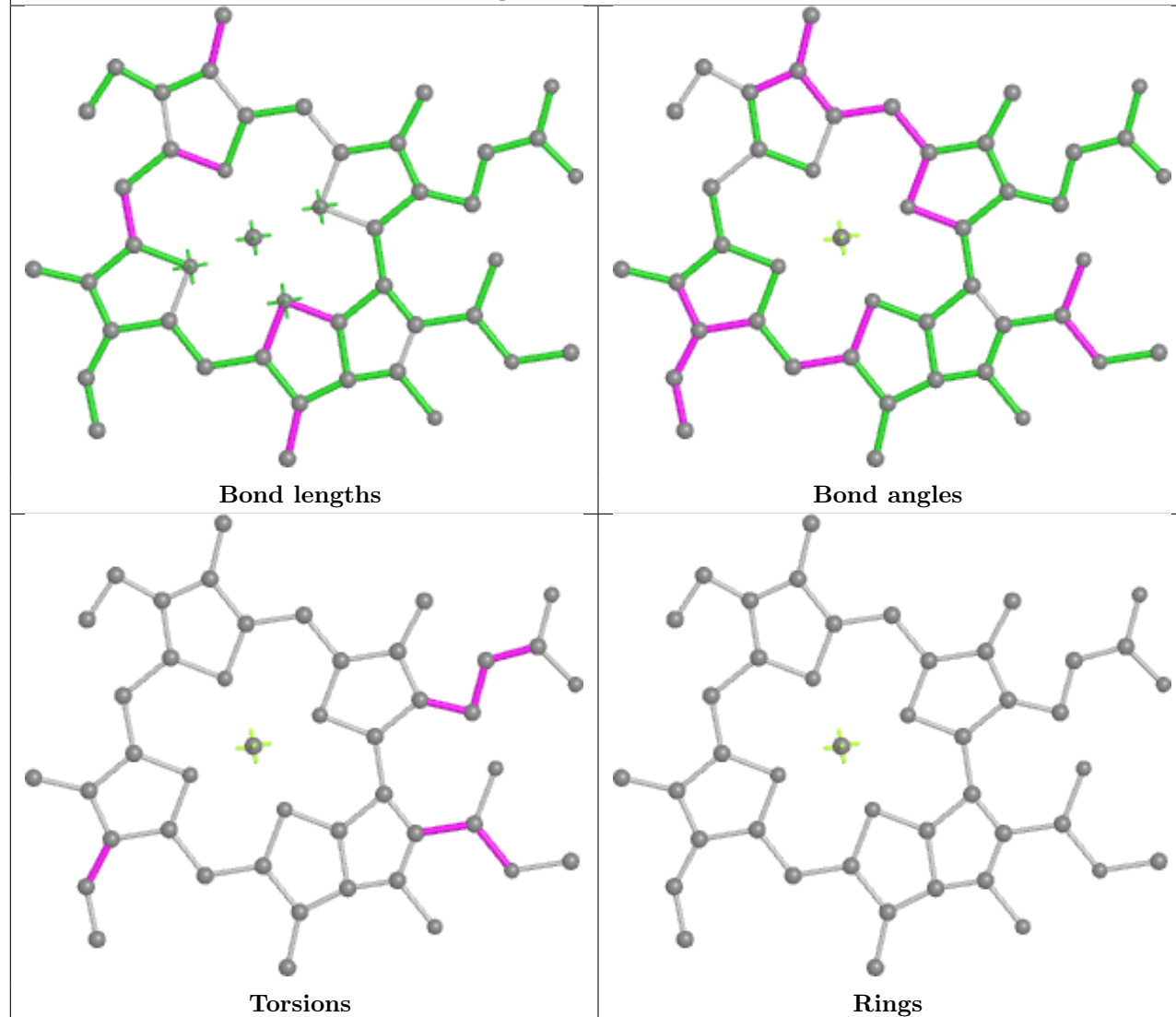


Ligand CLA T 1302**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA e 1140****Bond lengths****Bond angles****Torsions****Rings**

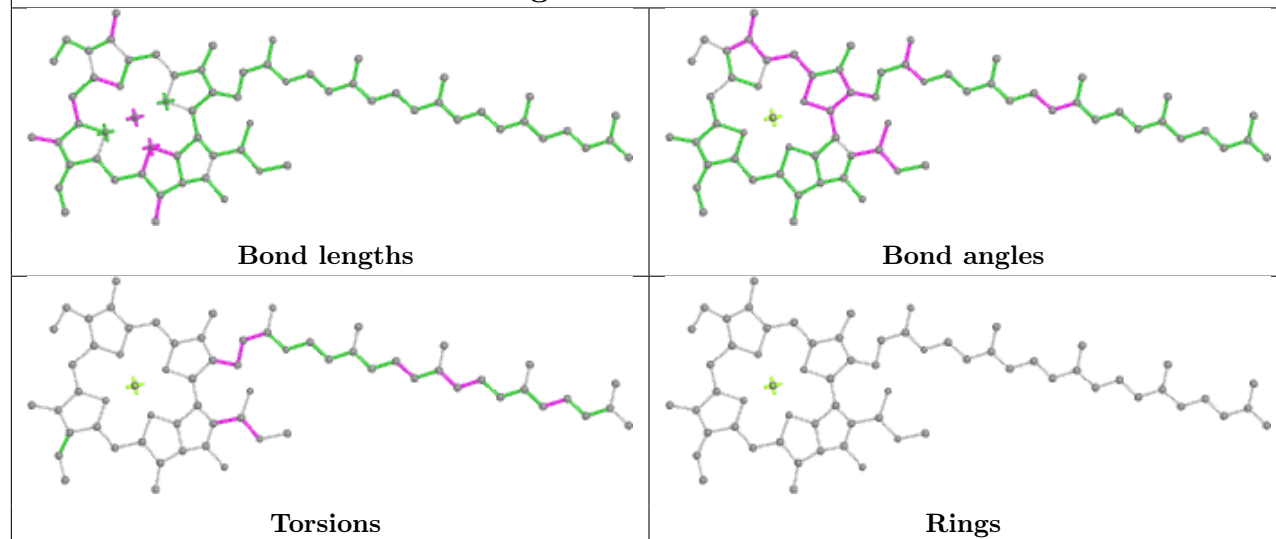
Ligand CLA B 1227



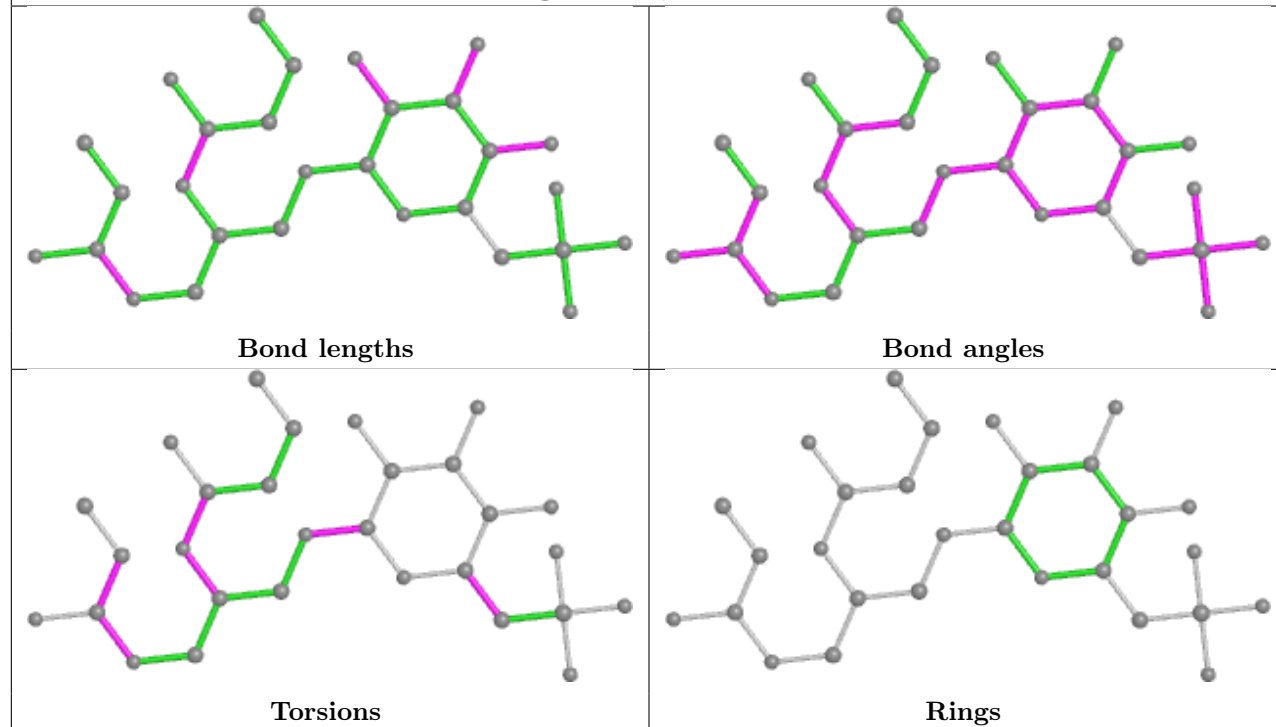
Ligand CLA 1 516

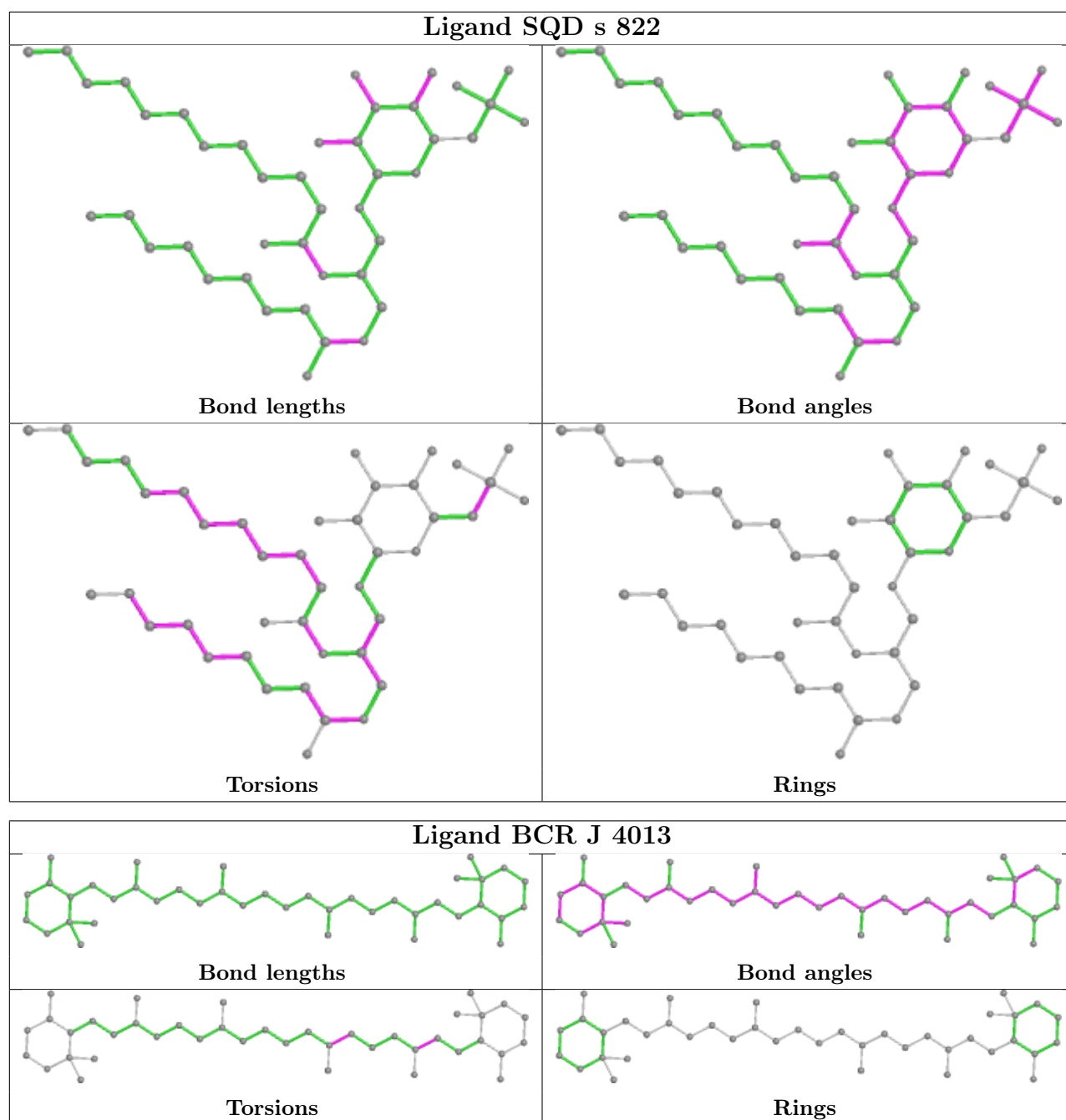


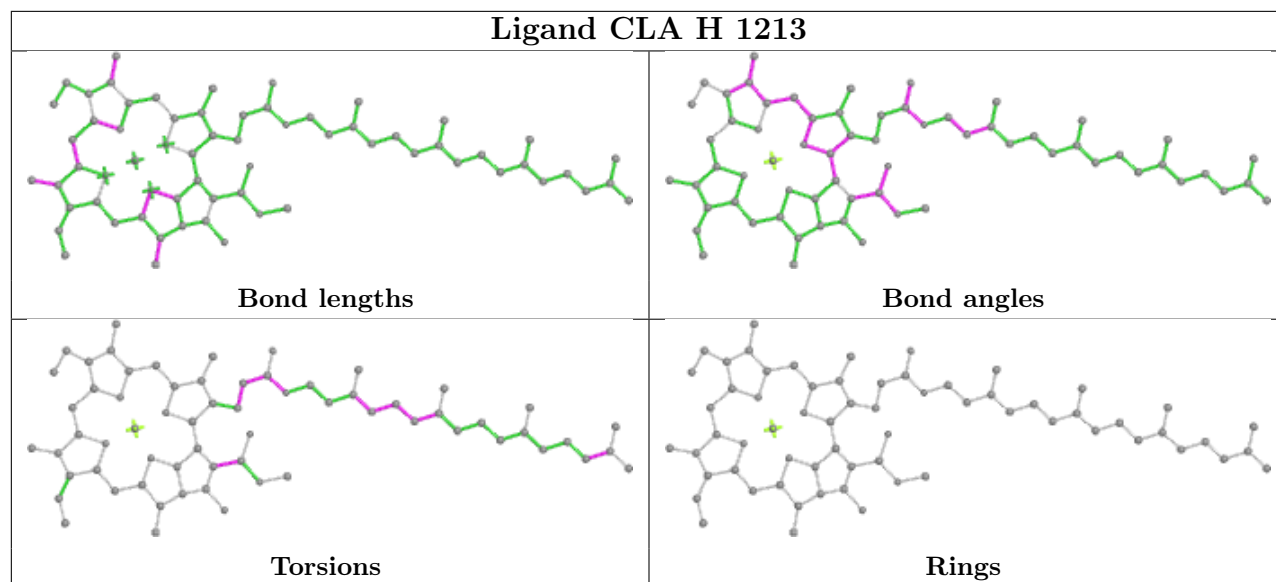
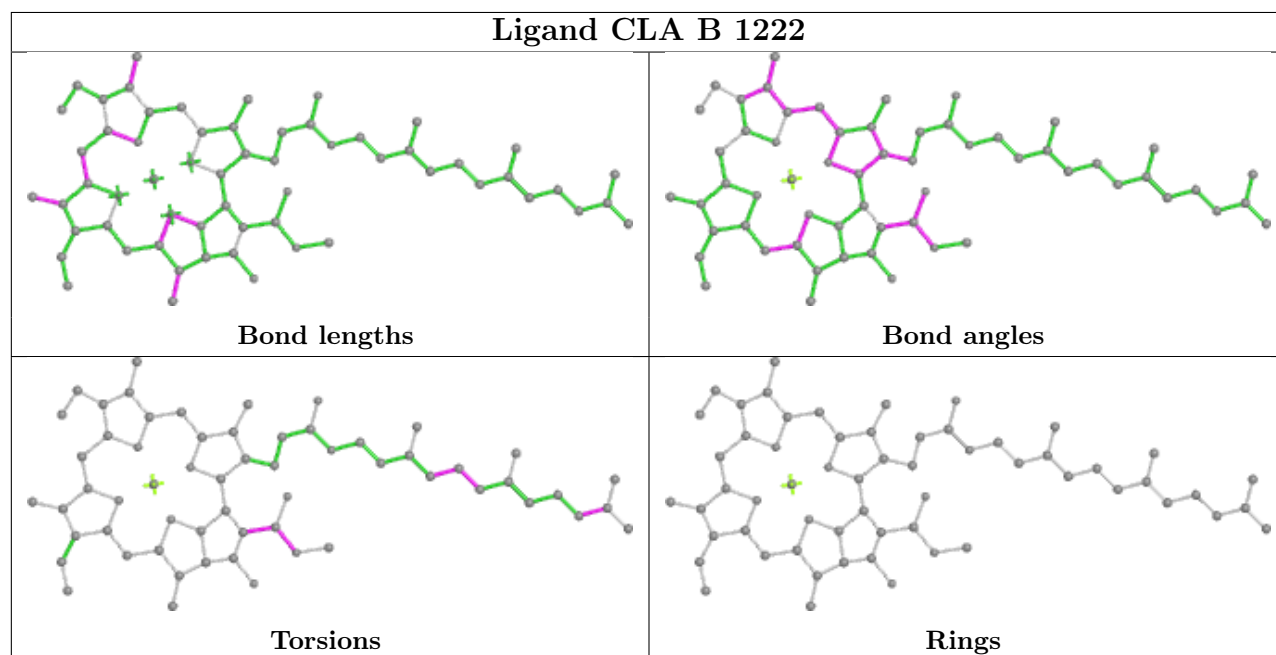
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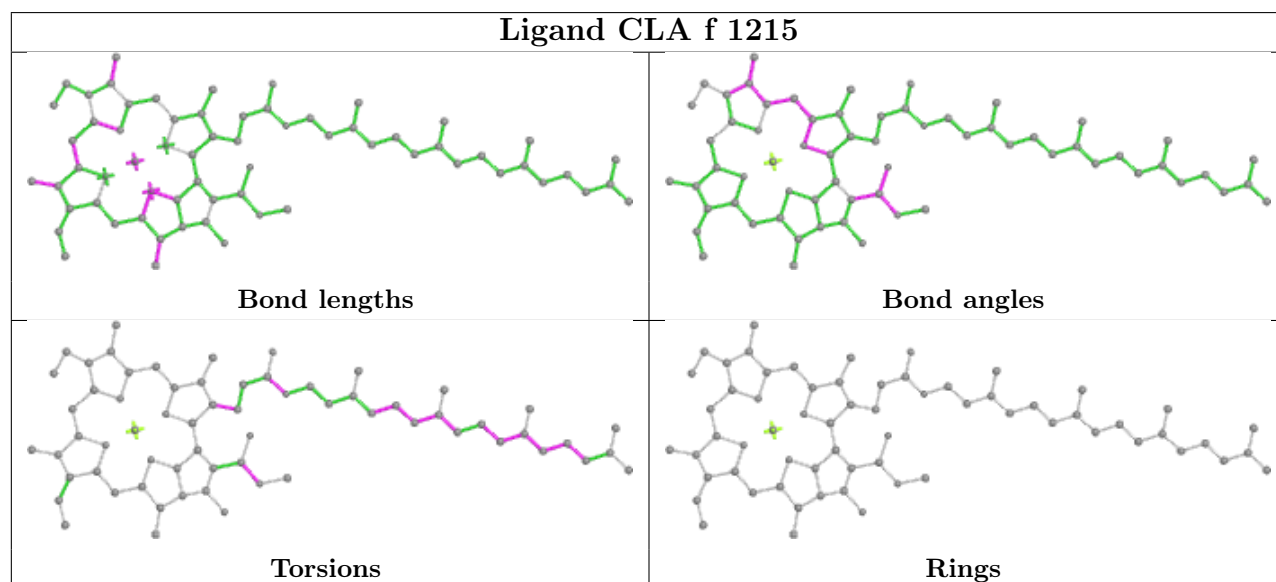
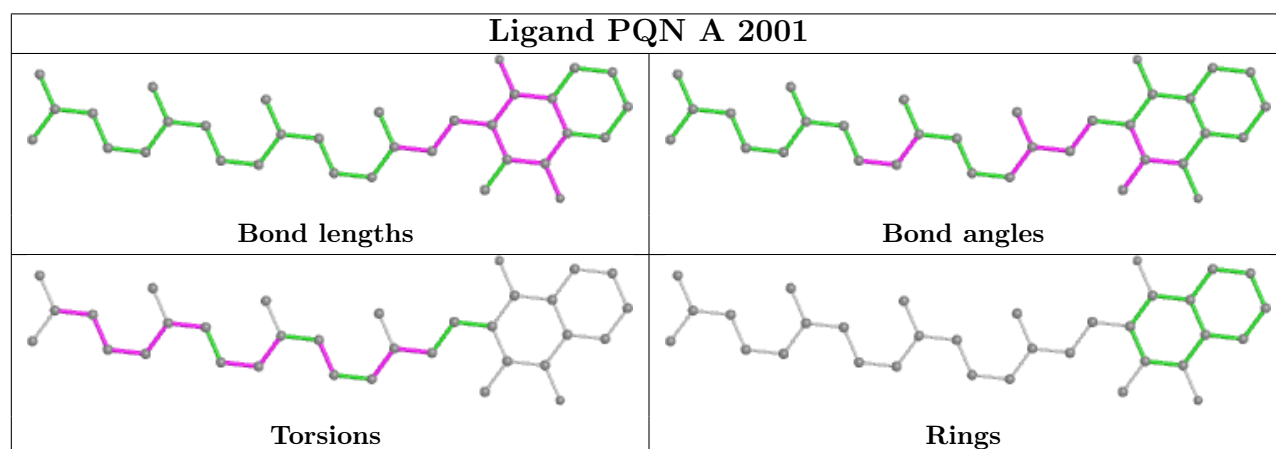
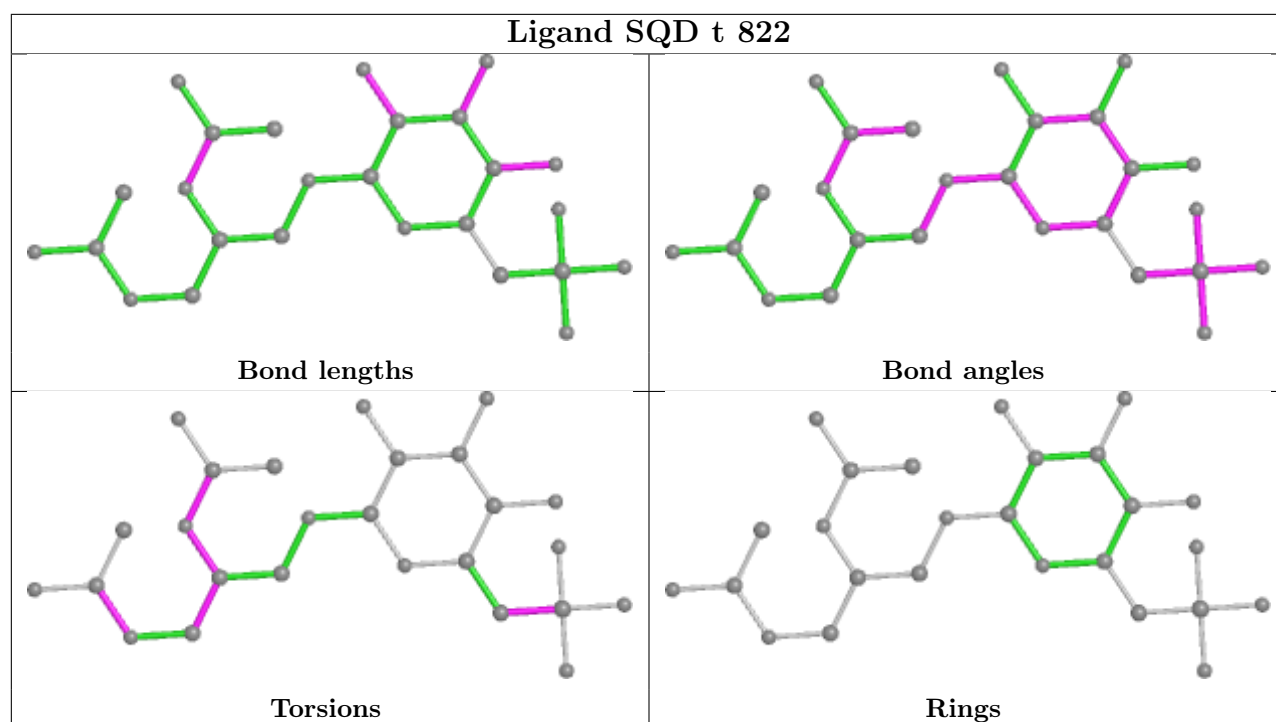


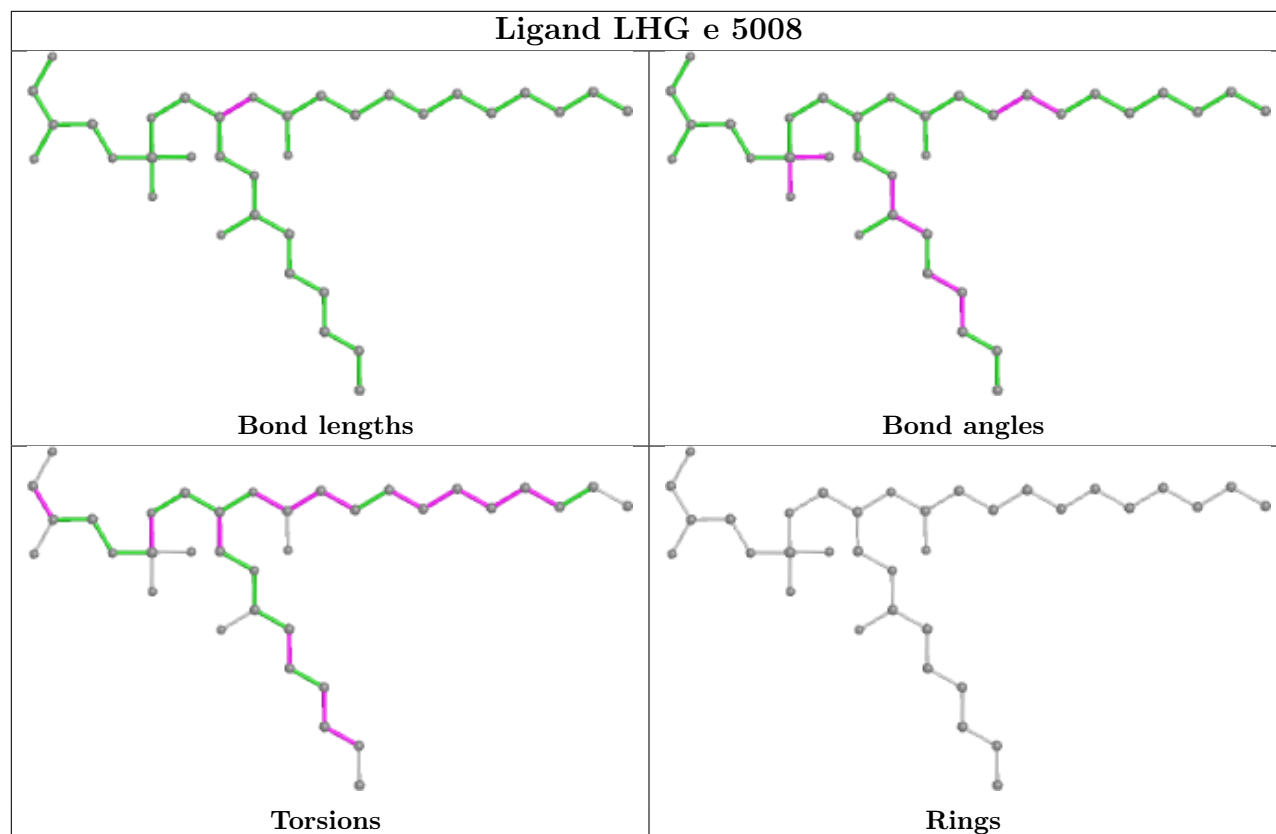
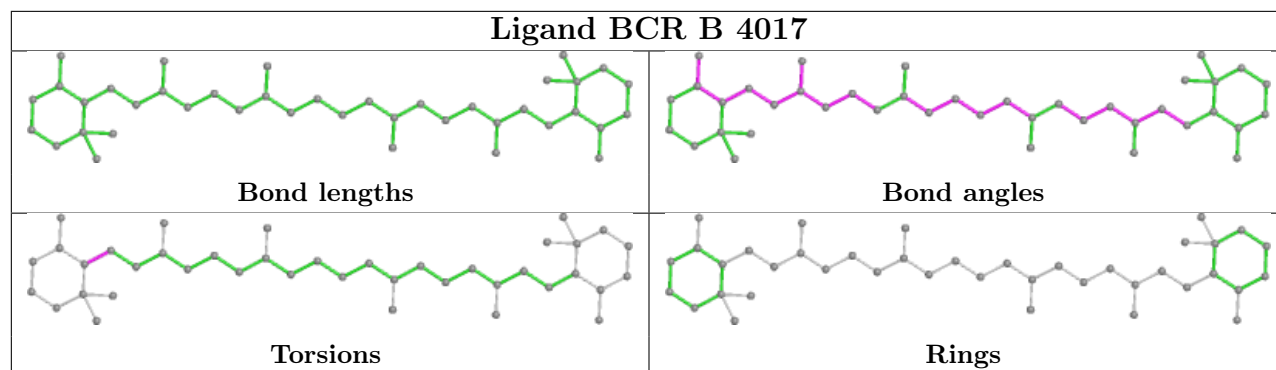
Ligand SQD 5 822

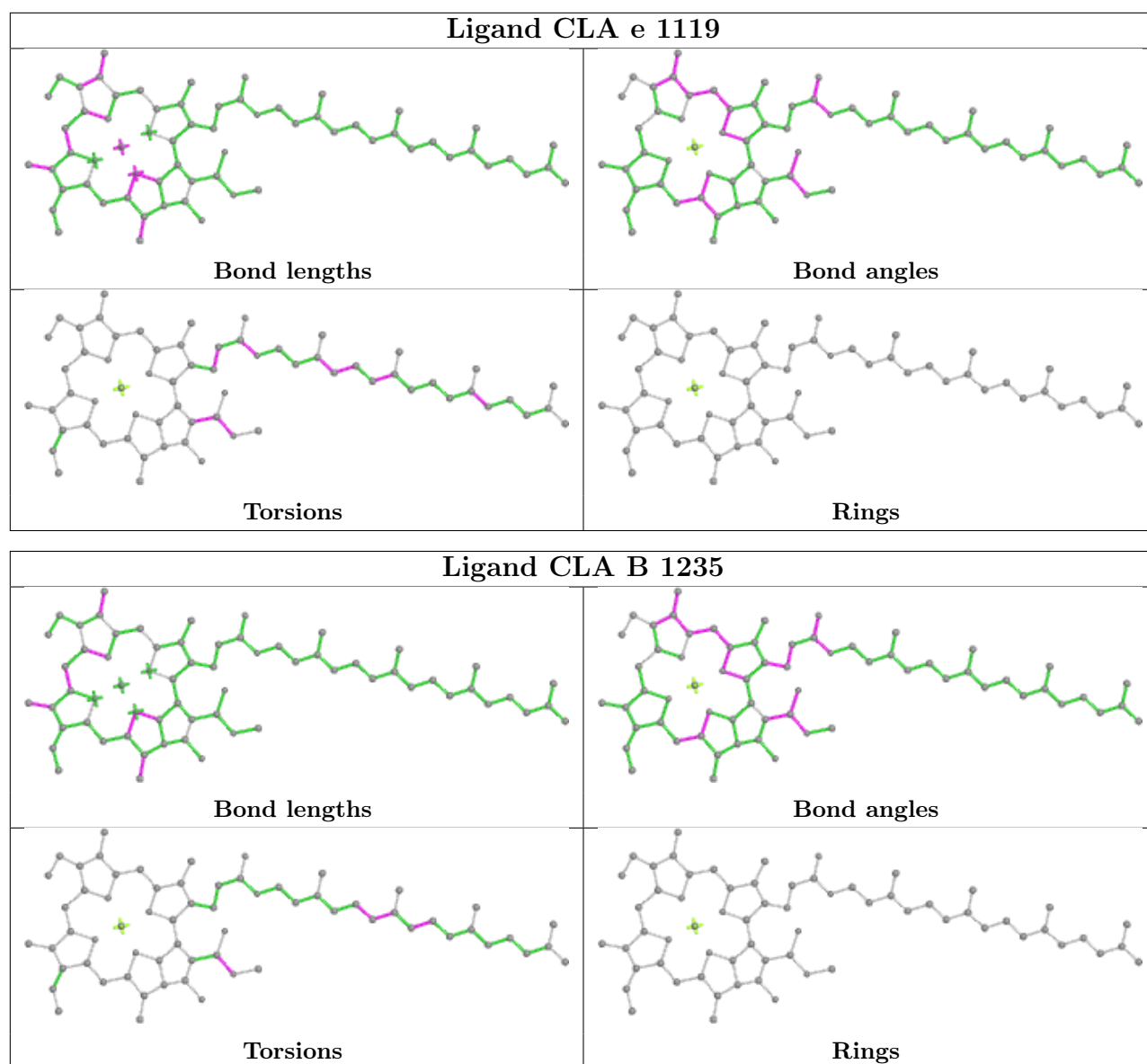




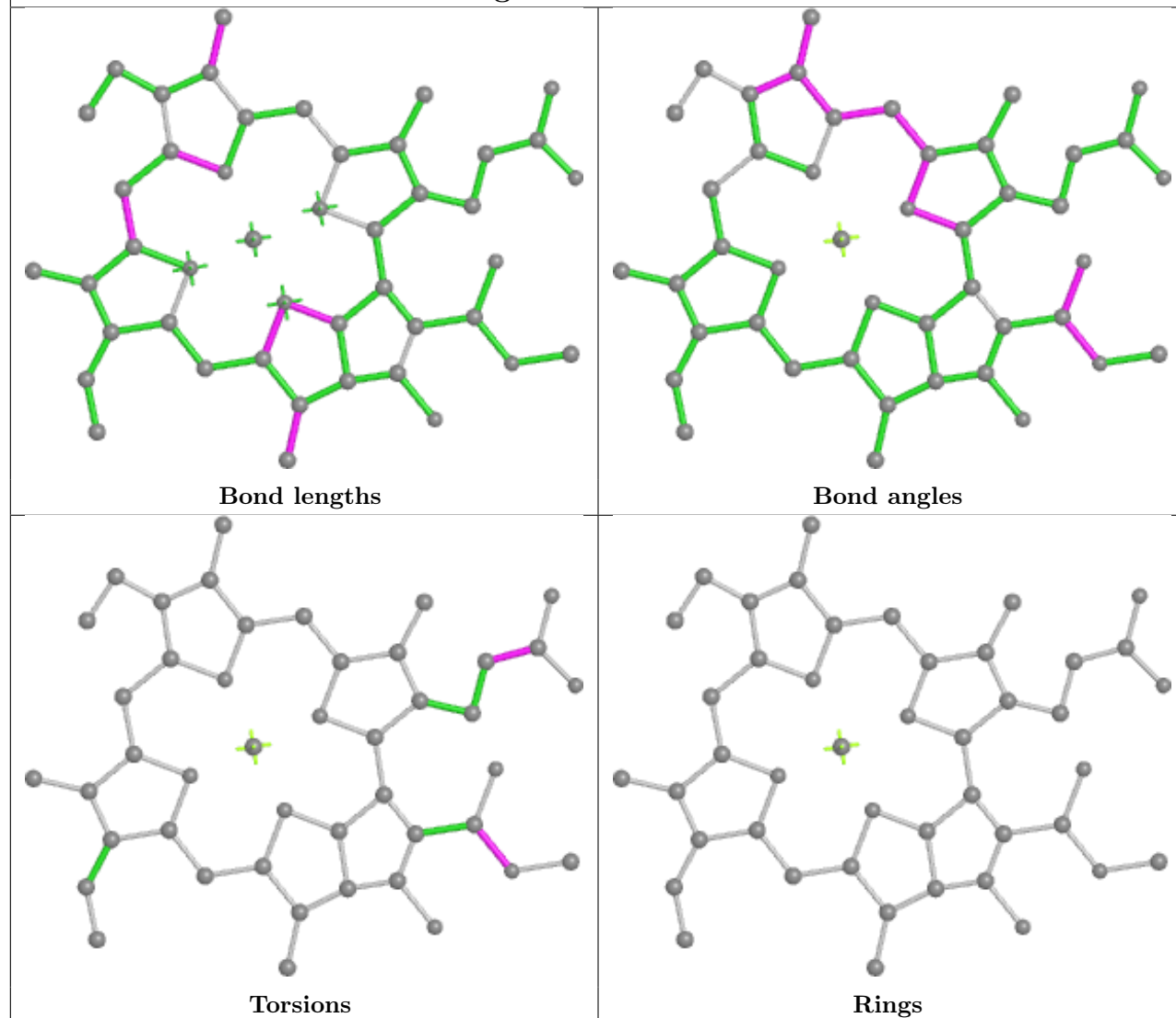
Ligand CLA H 1213**Ligand CLA B 1222**



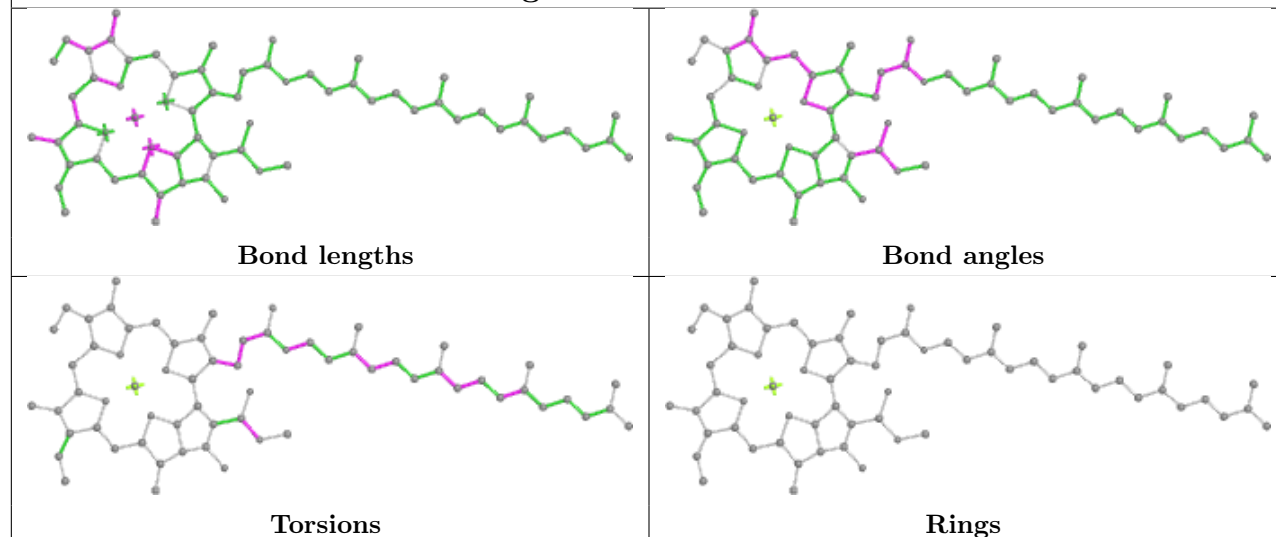




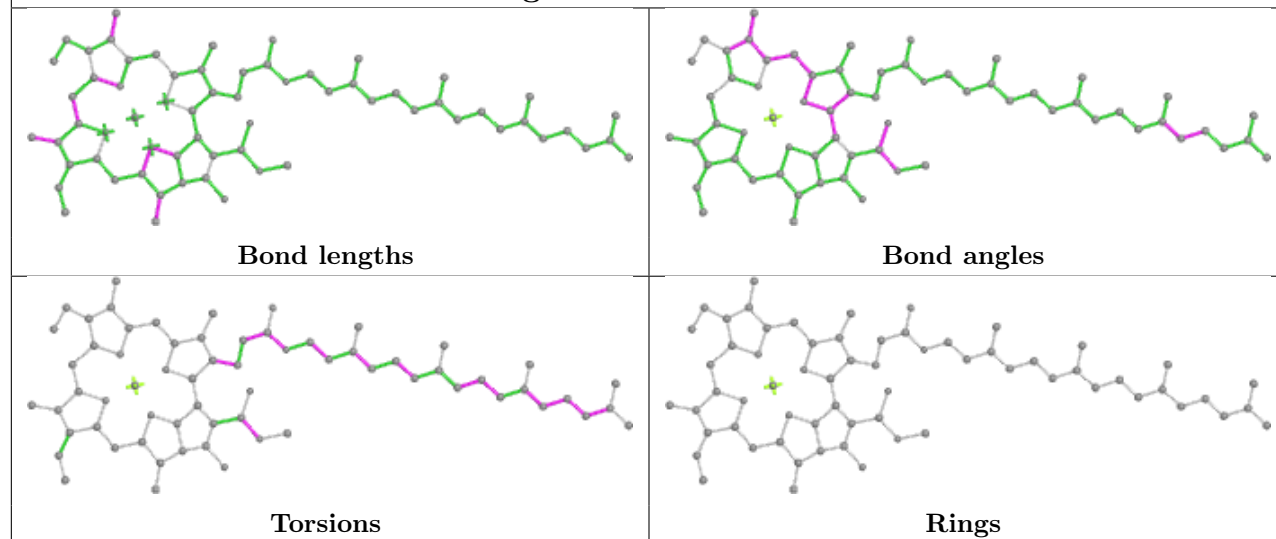
Ligand CLA 6 511



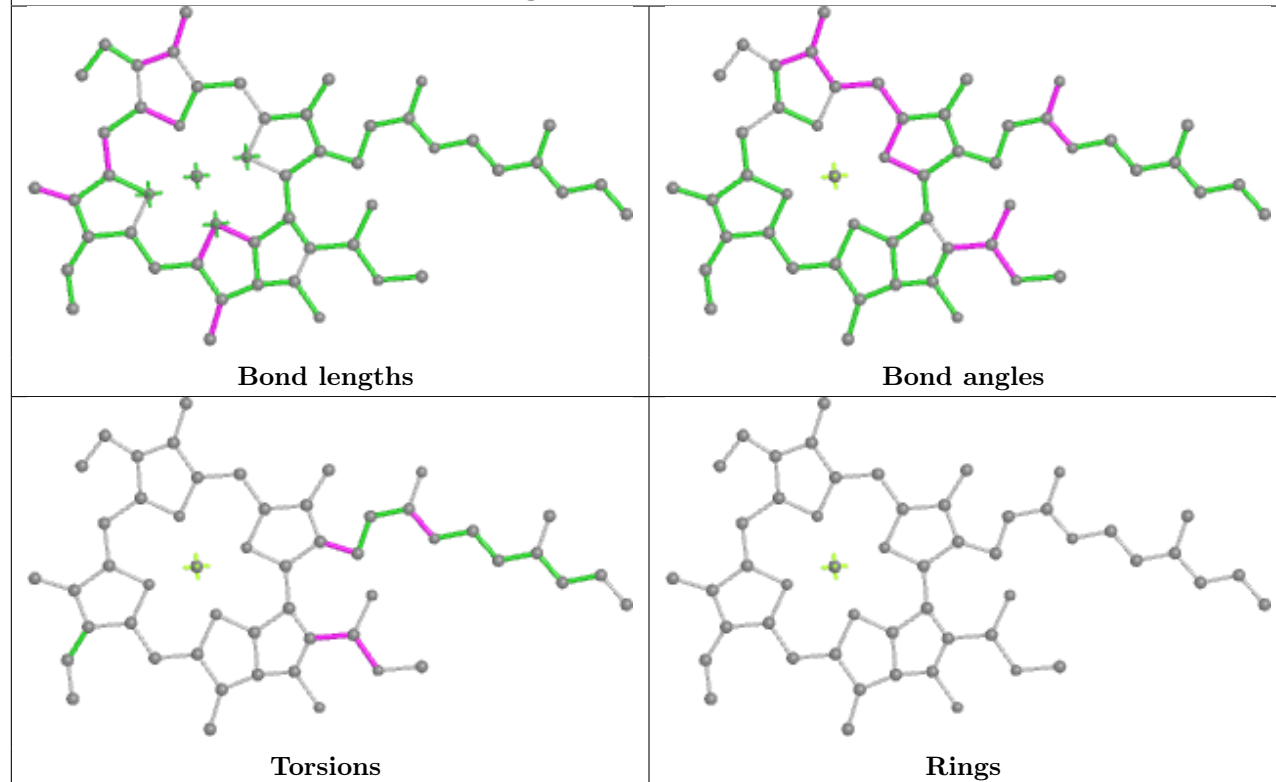
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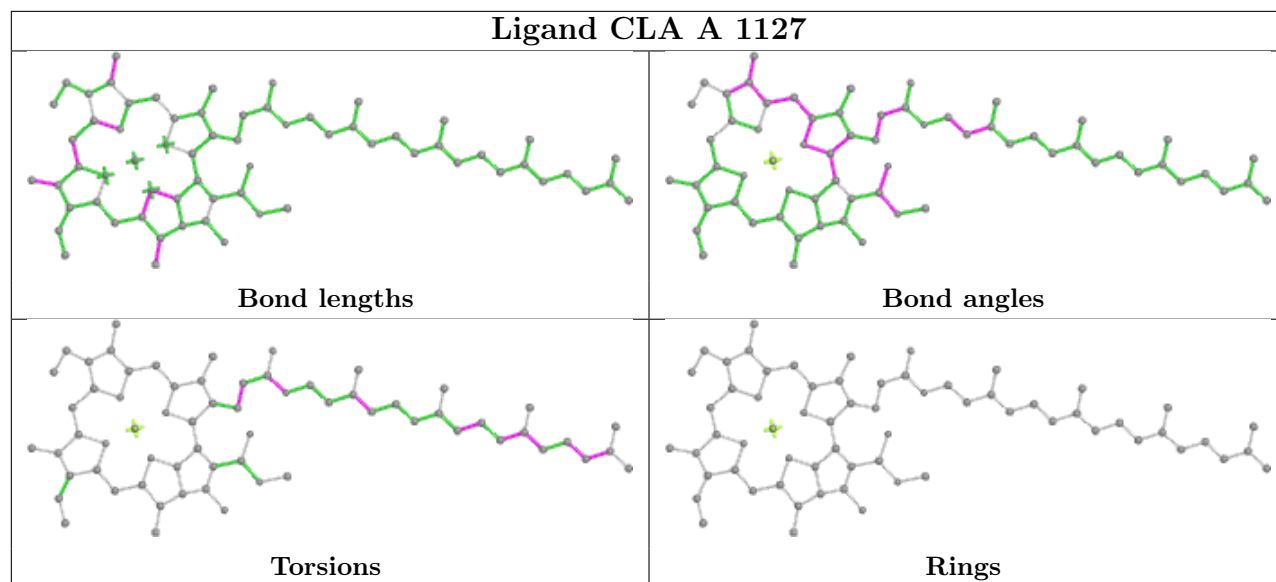
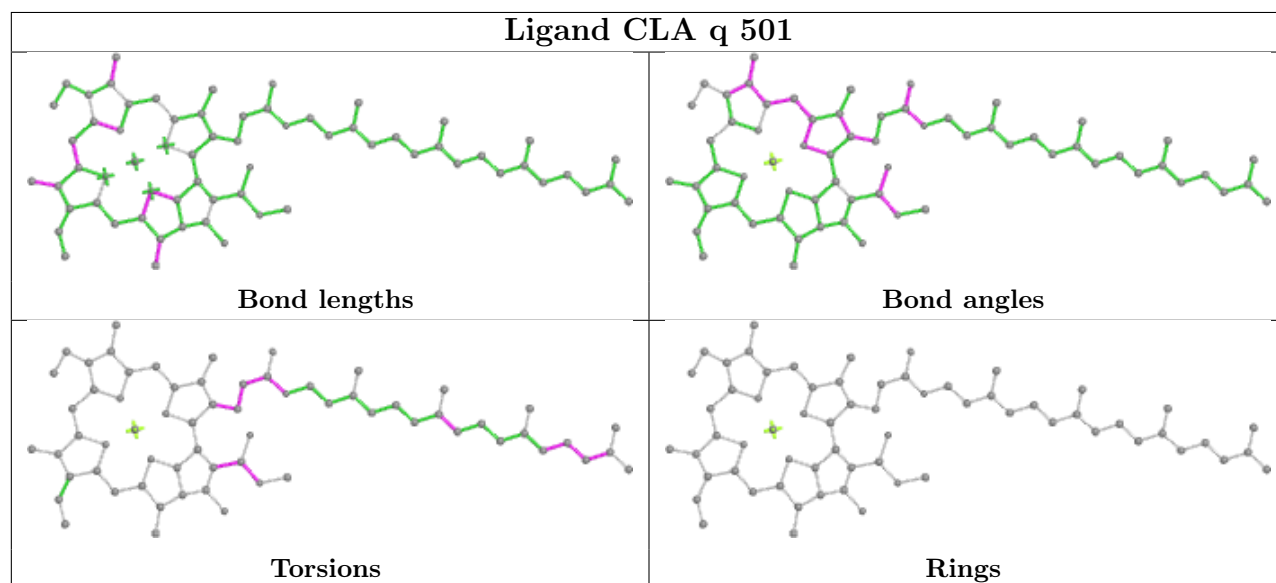


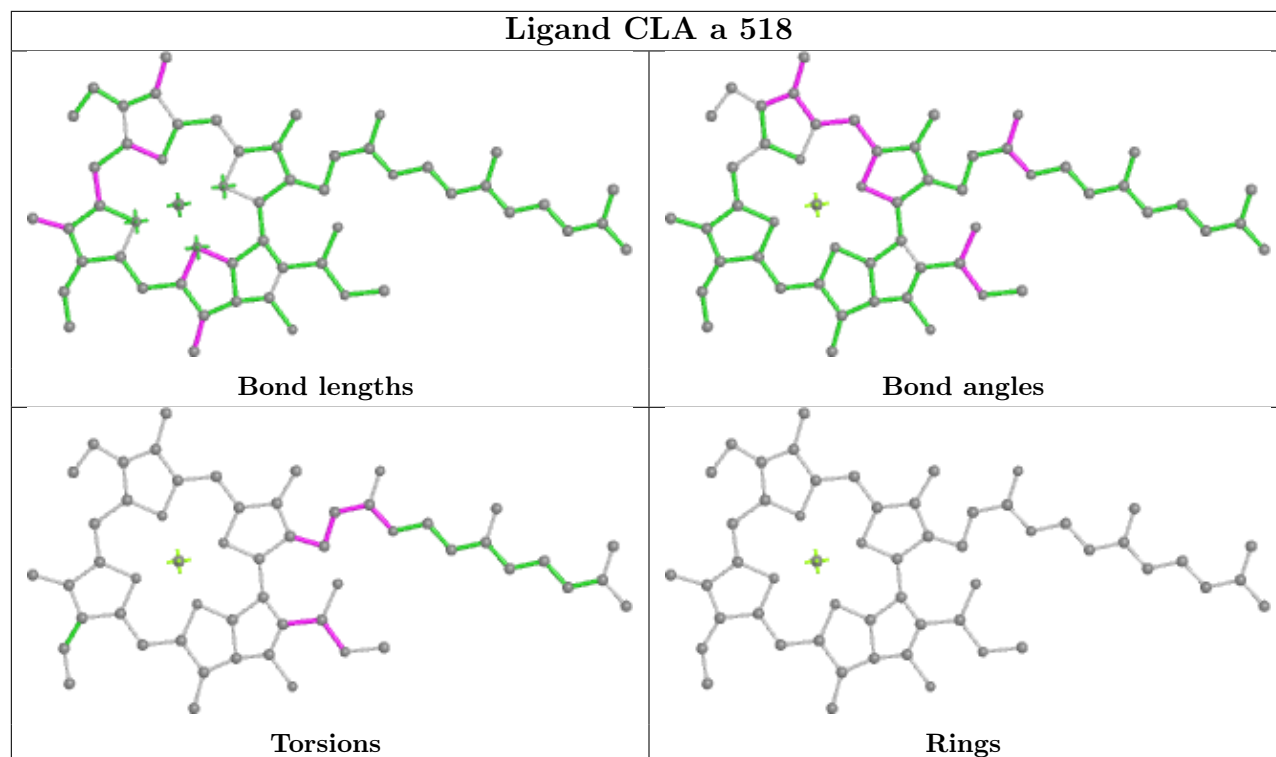
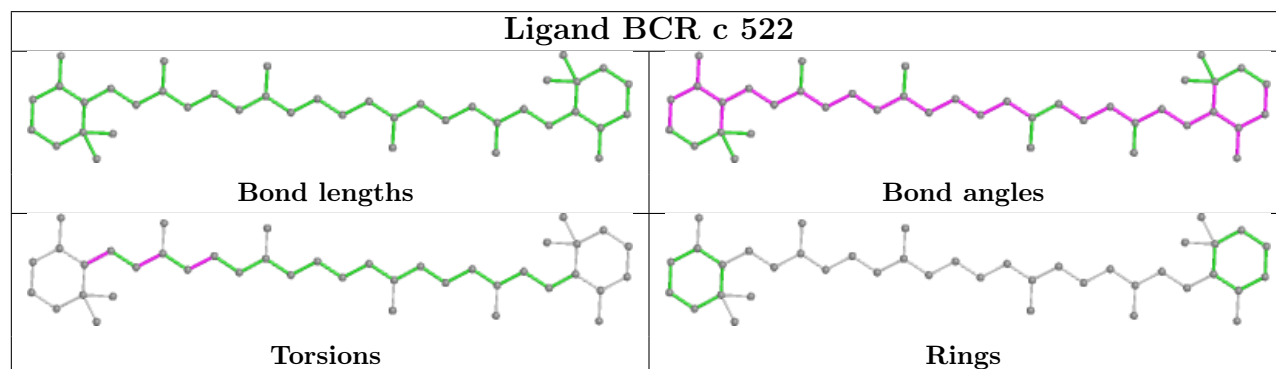
Ligand CLA A 1126

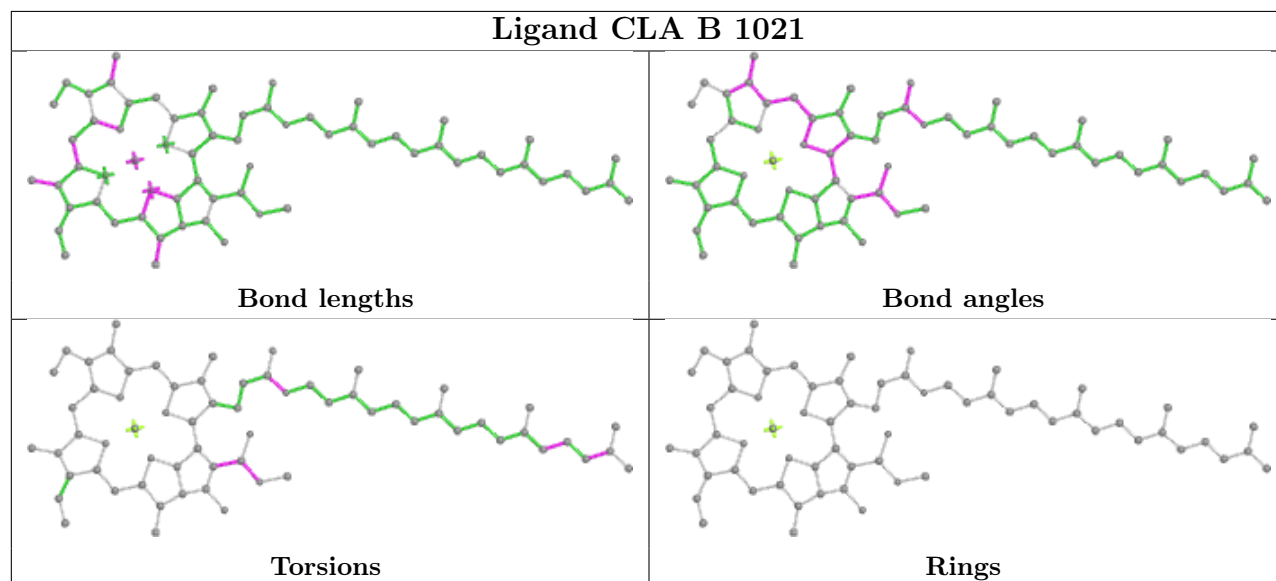
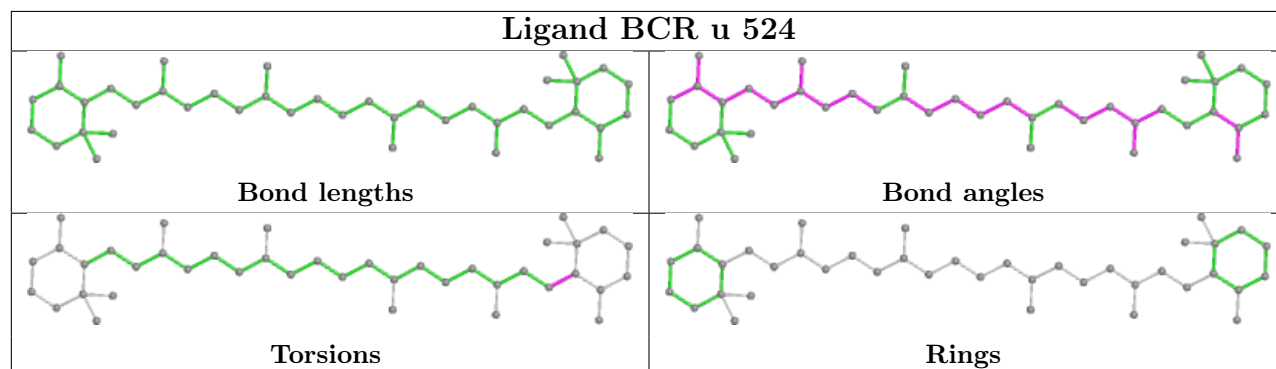
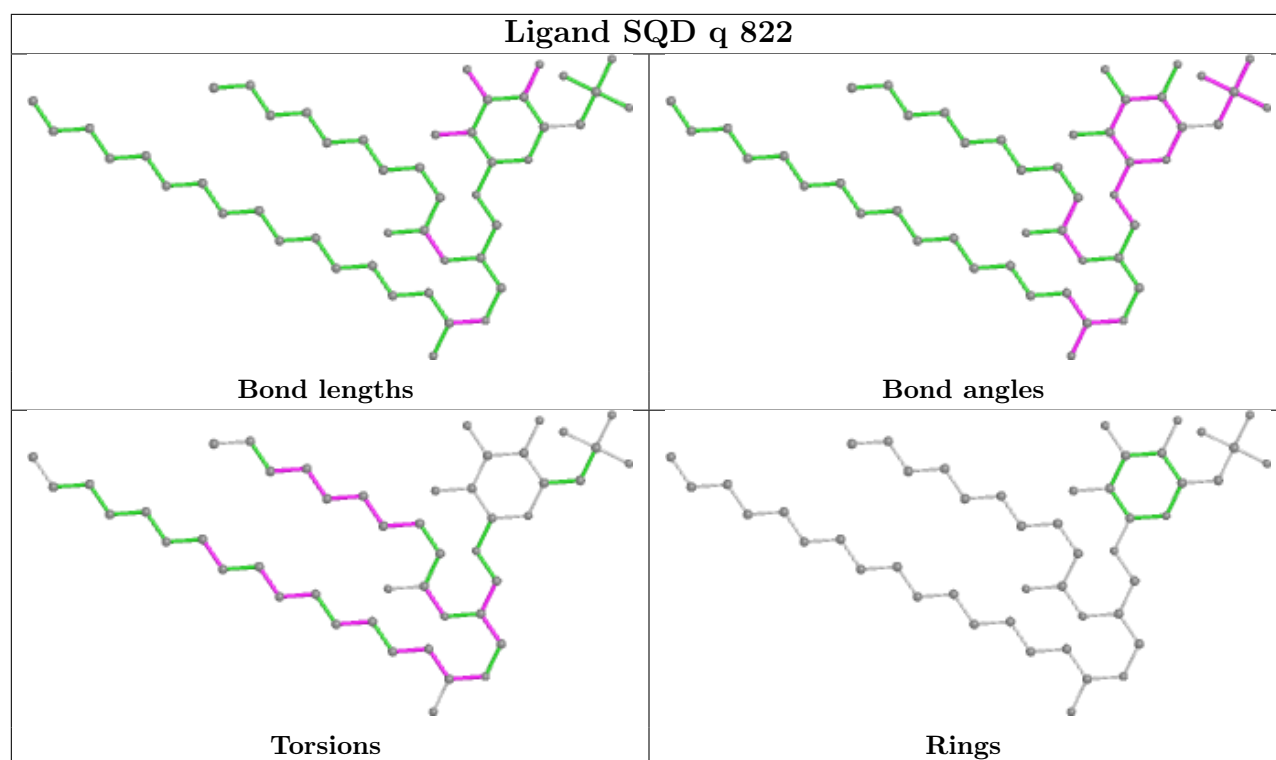


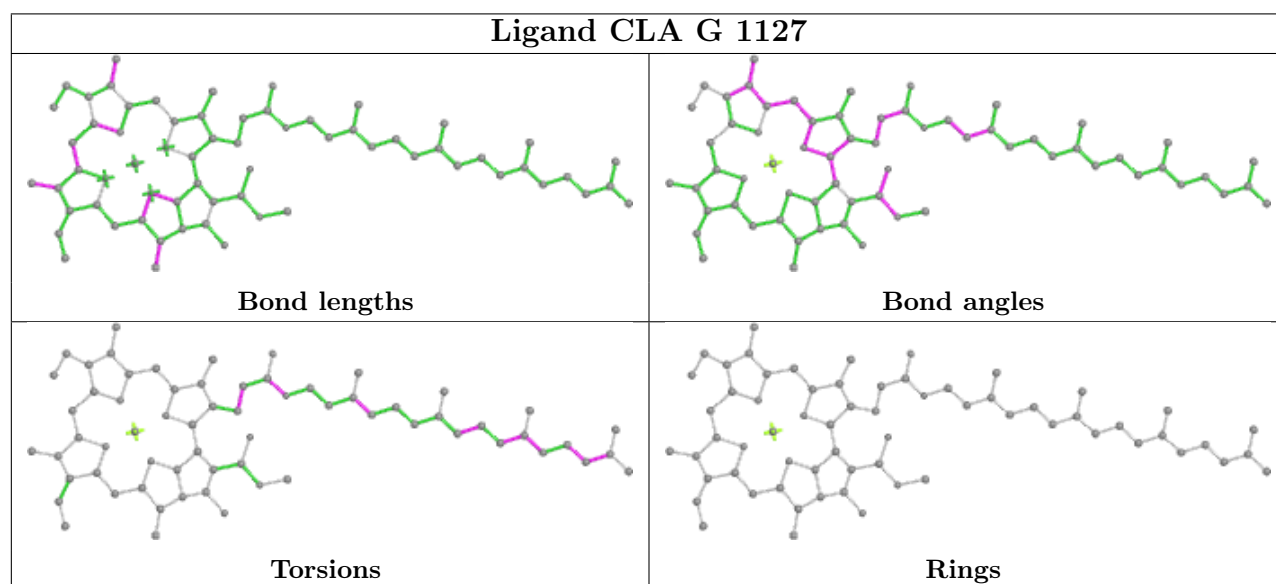
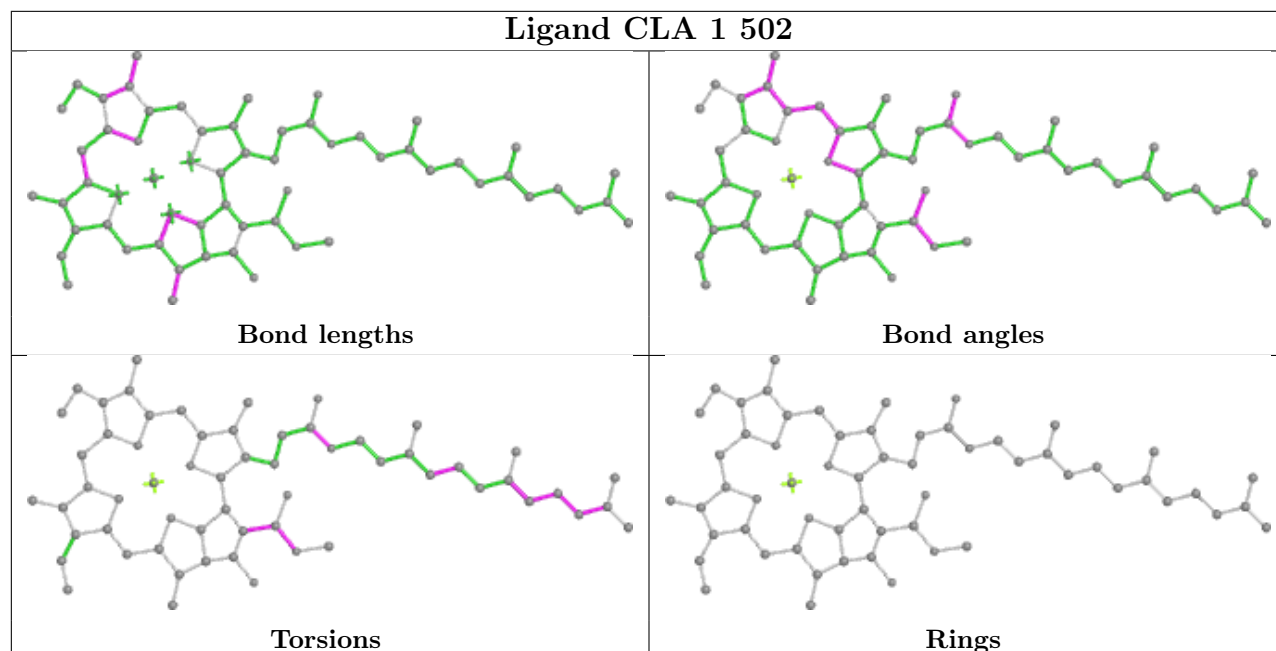
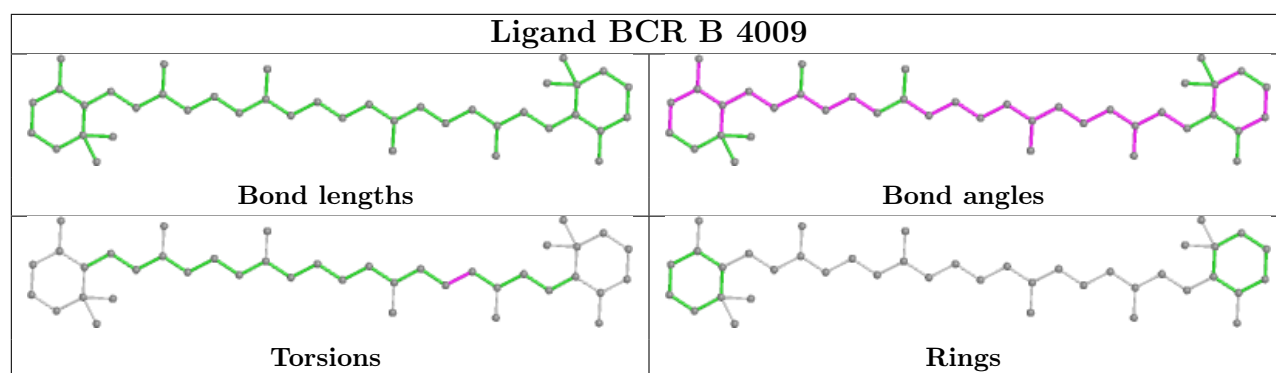
Ligand CLA H 1209



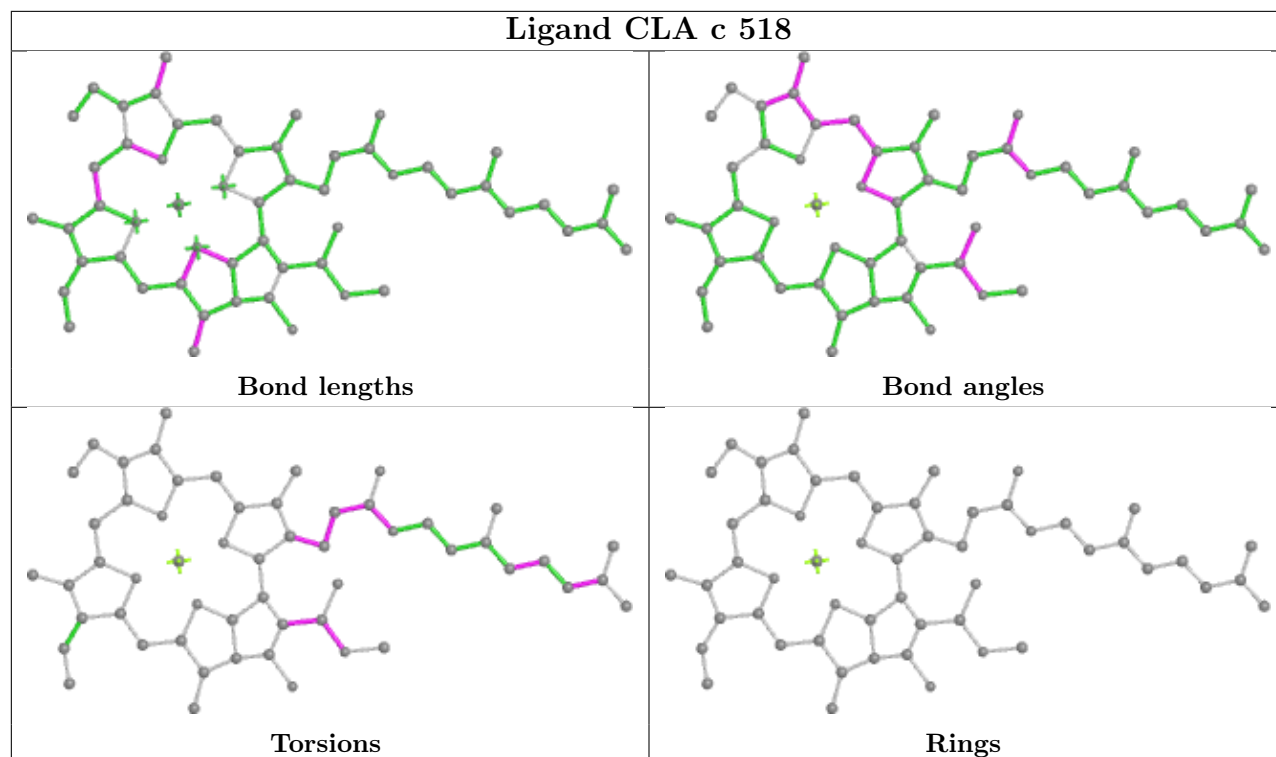
Ligand CLA A 1127**Ligand CLA q 501**

Ligand CLA a 518**Ligand BCR c 522**

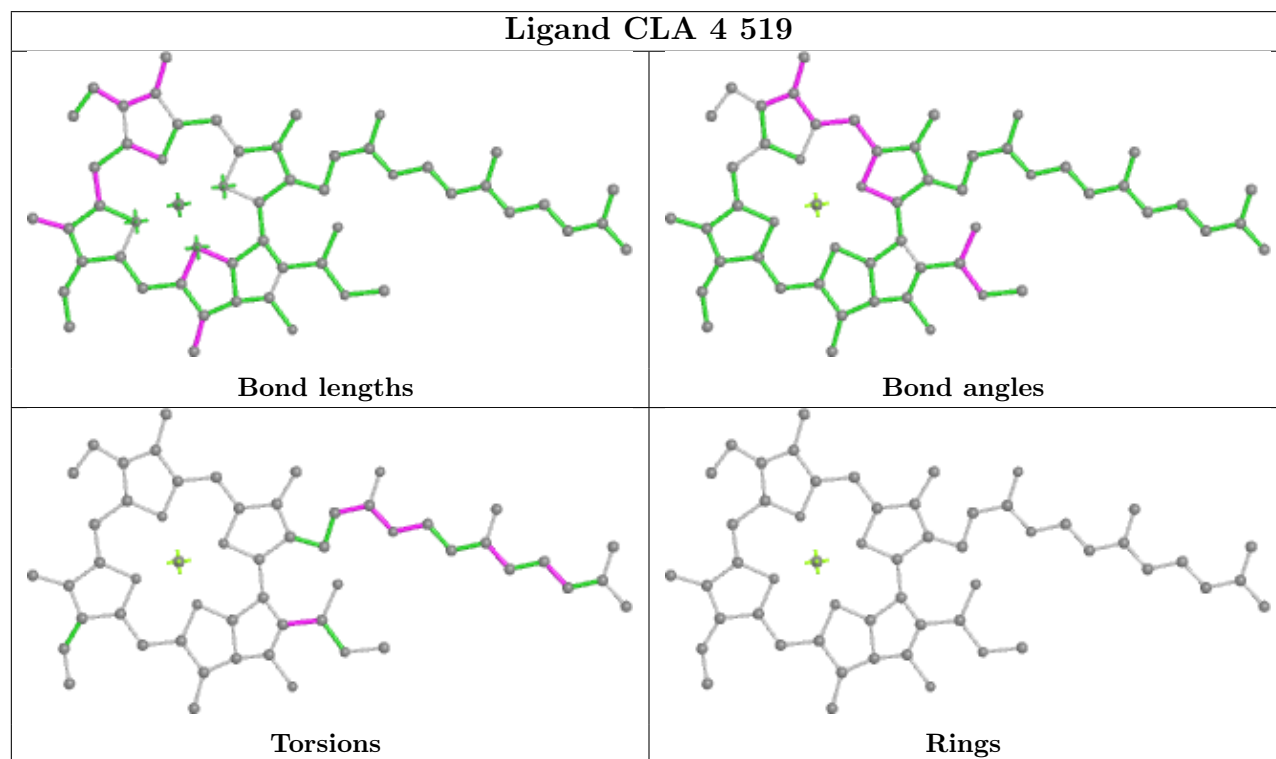


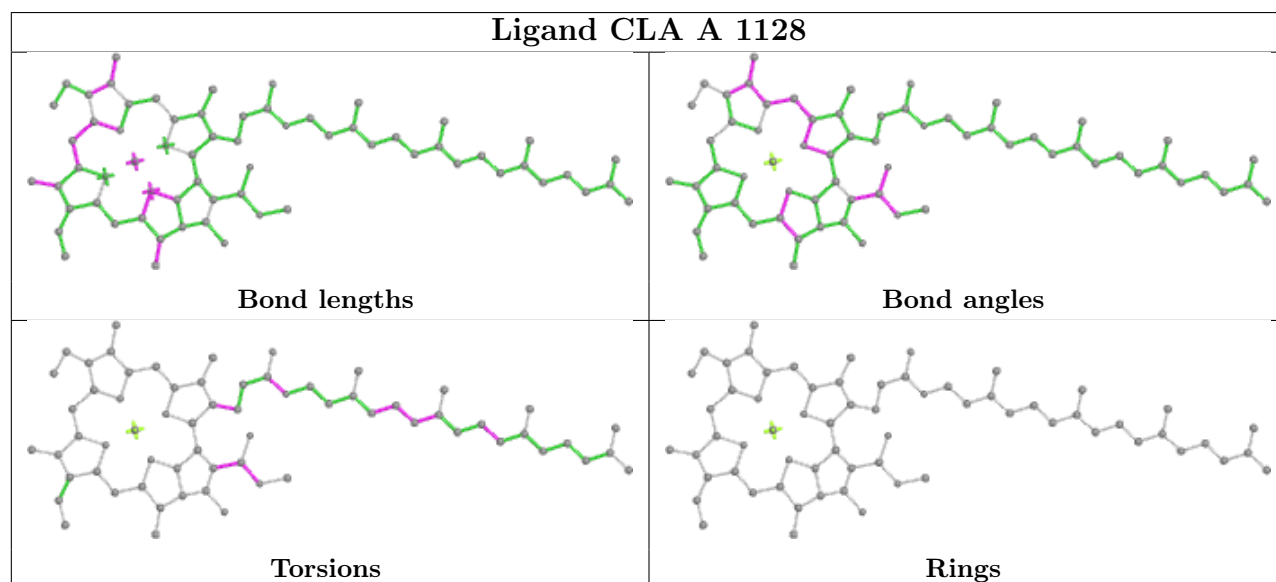
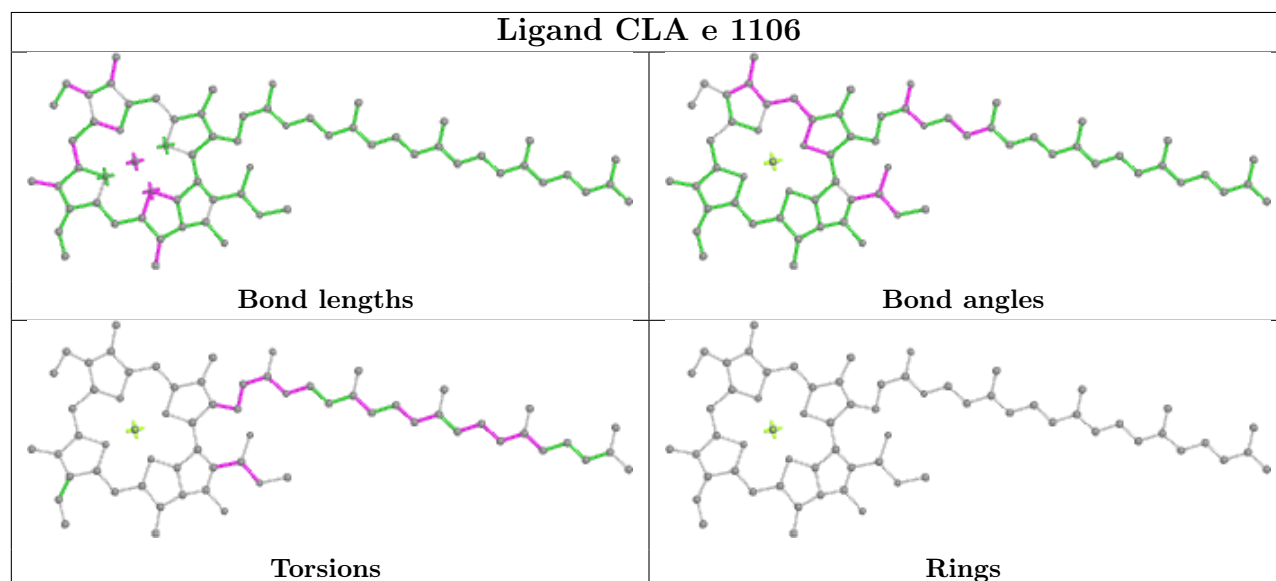
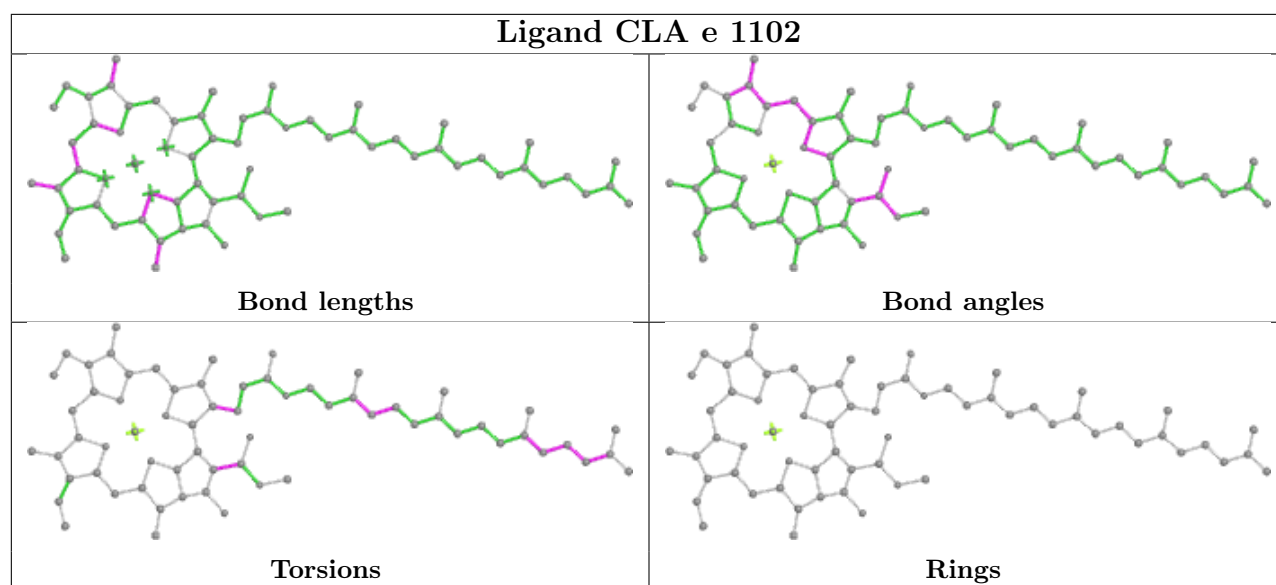


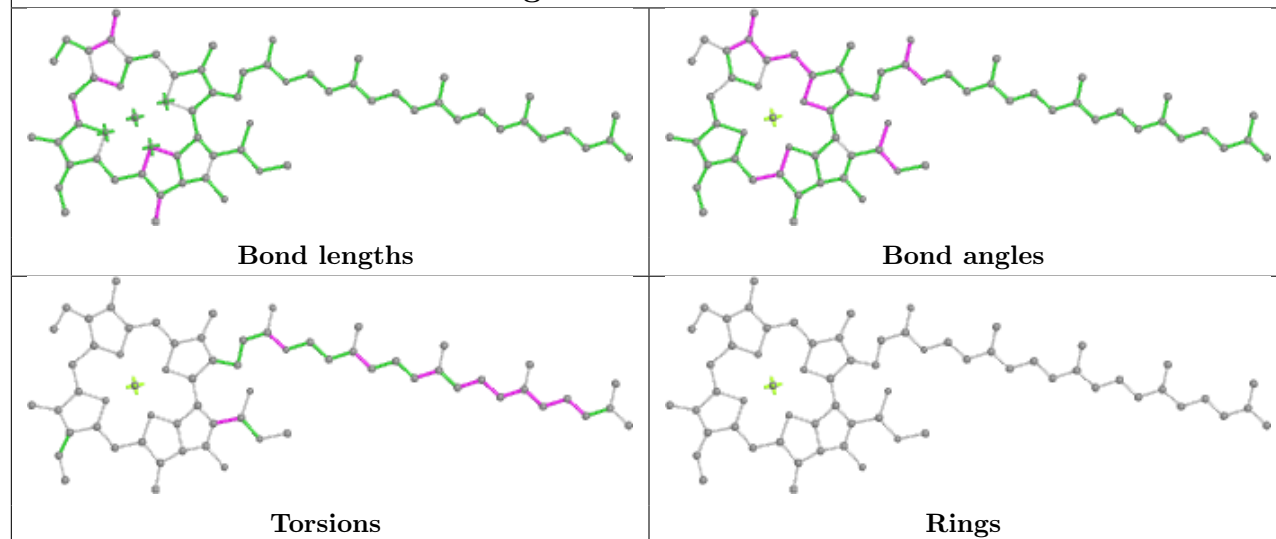
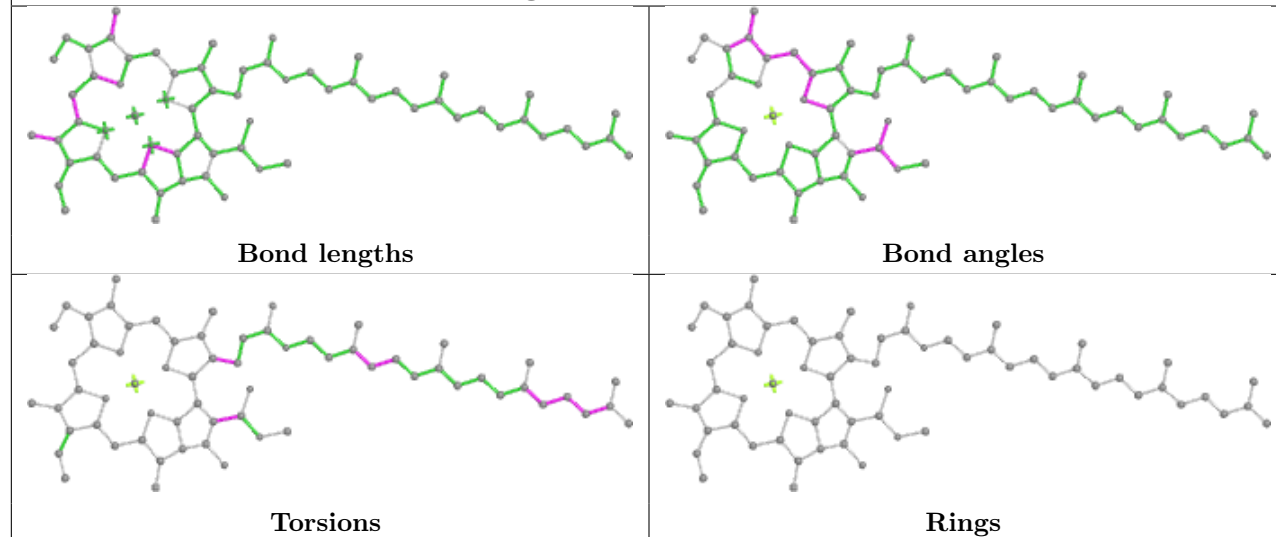
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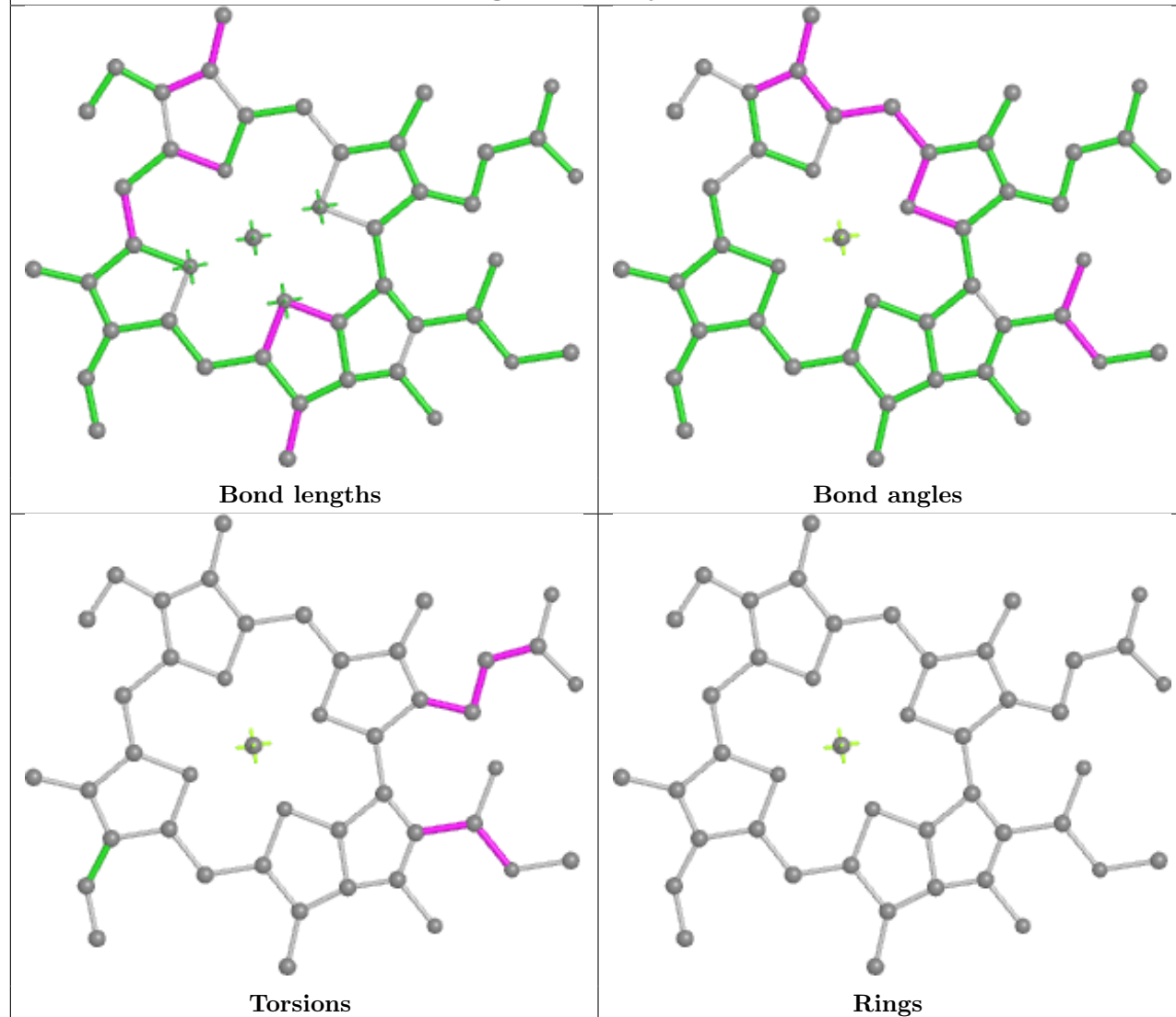
Ligand CLA 4 519



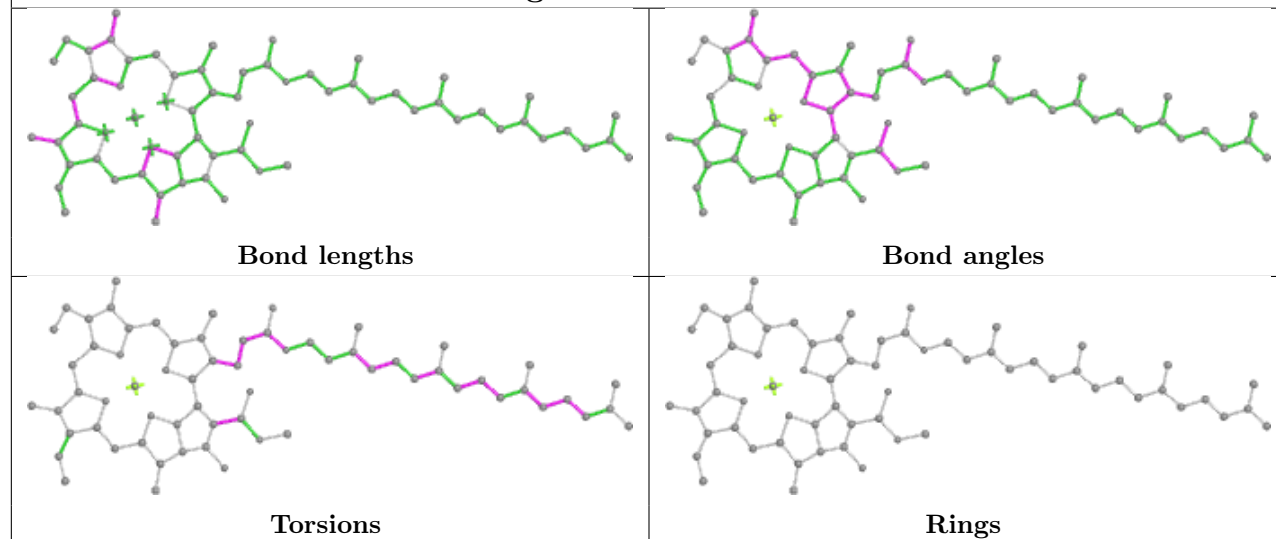


Ligand CLA B 1208**Ligand CLA A 1102**

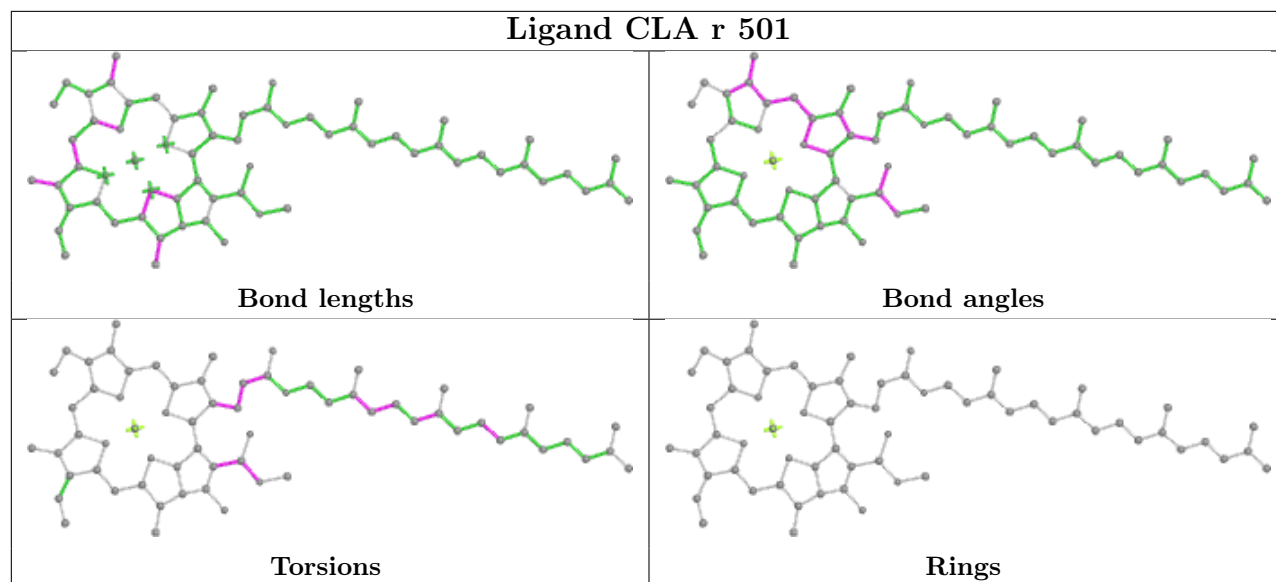
Ligand CLA j 1302



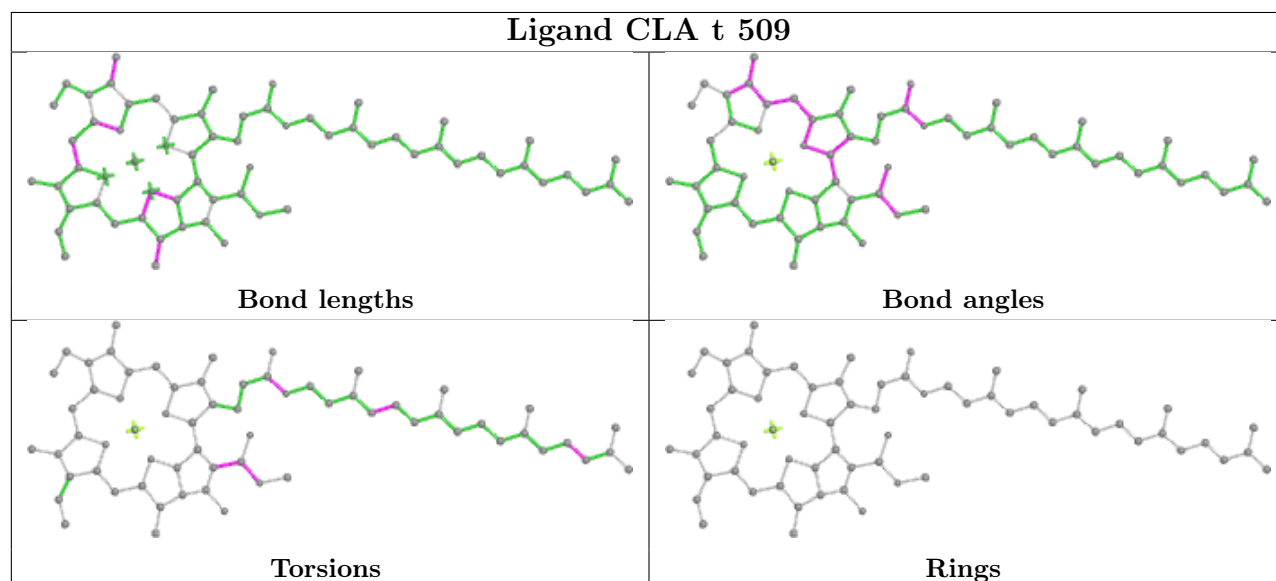
Ligand CLA n 1501



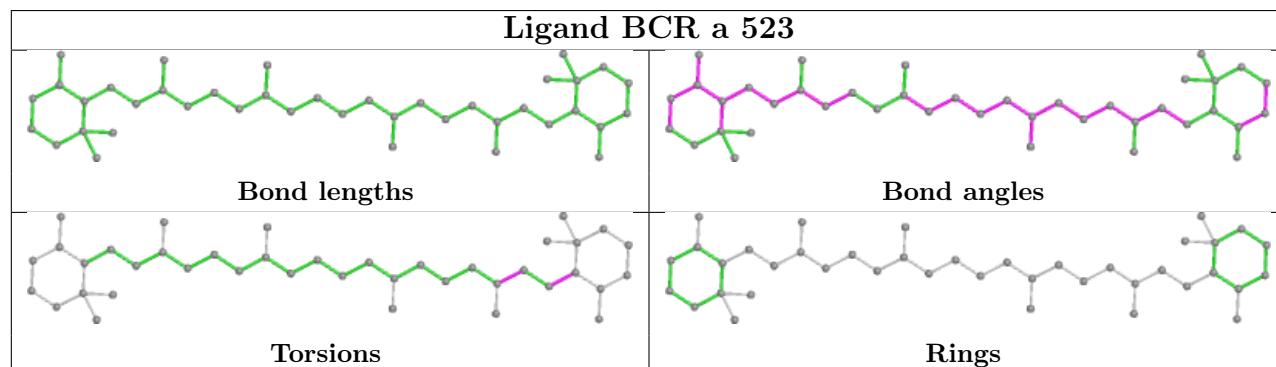
Ligand CLA r 501

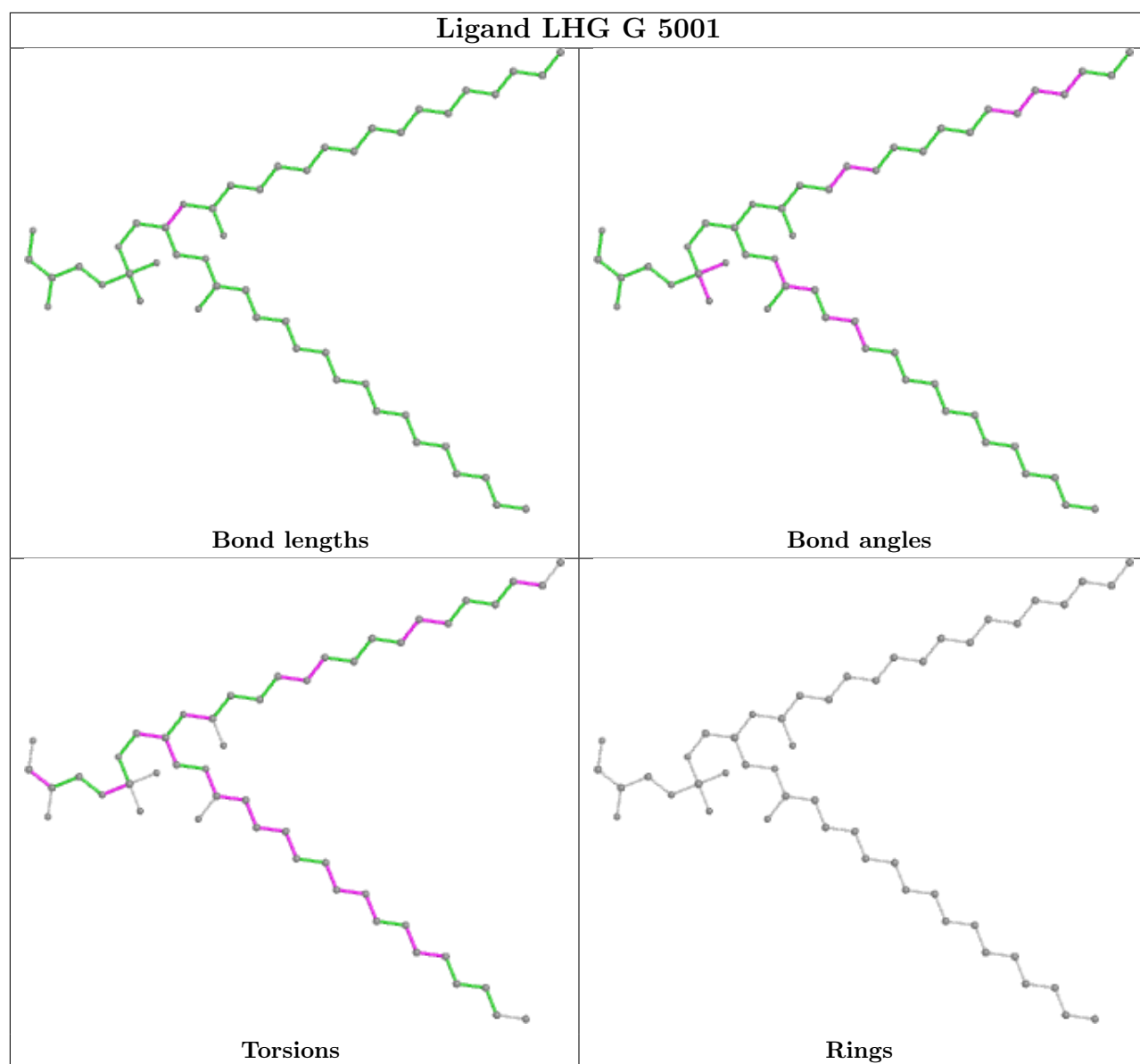


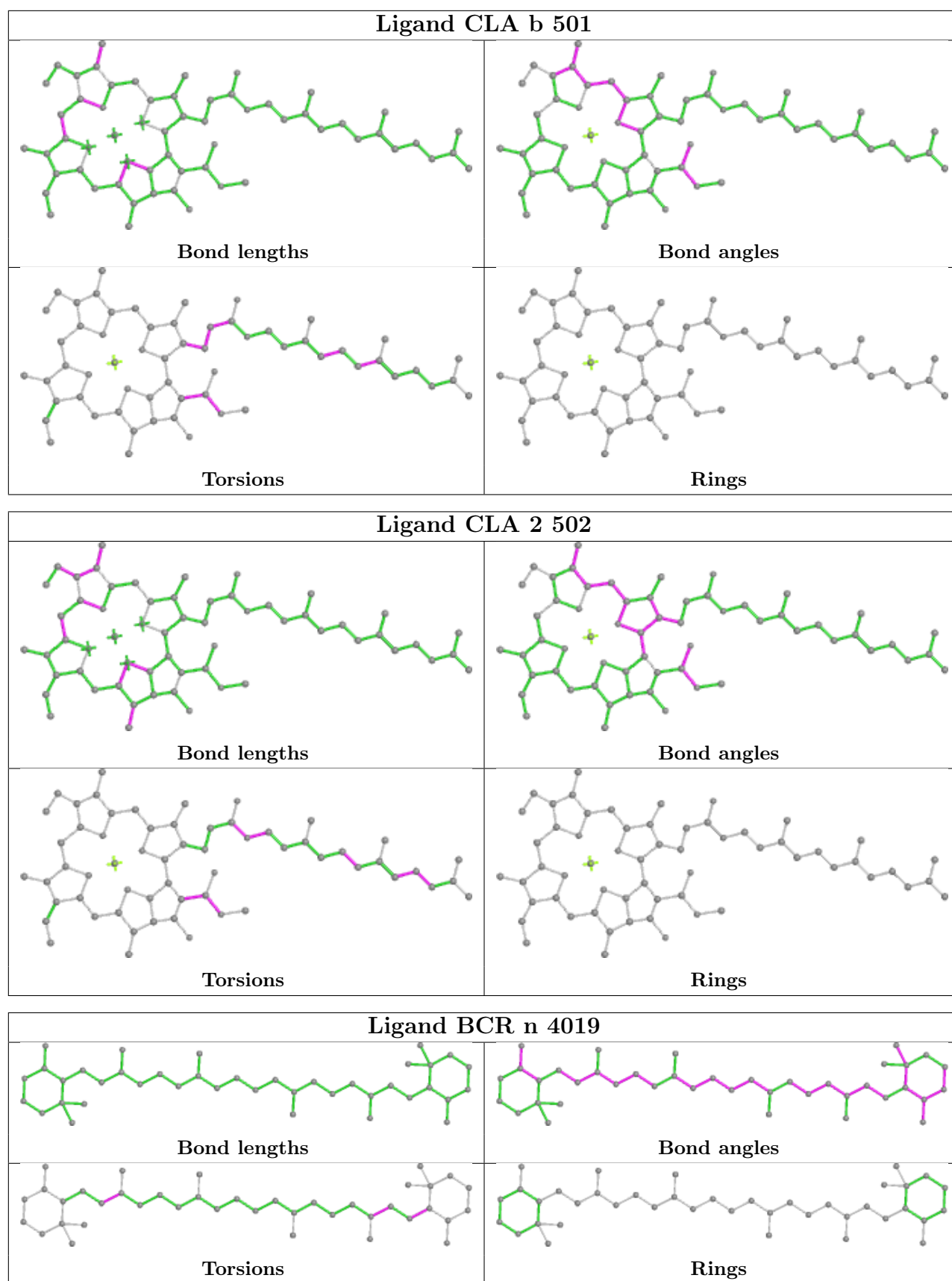
Ligand CLA t 509

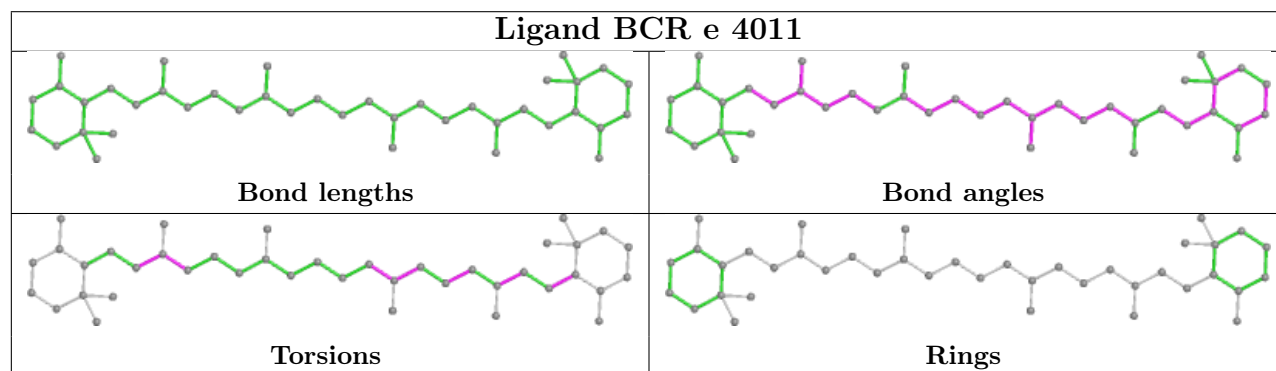
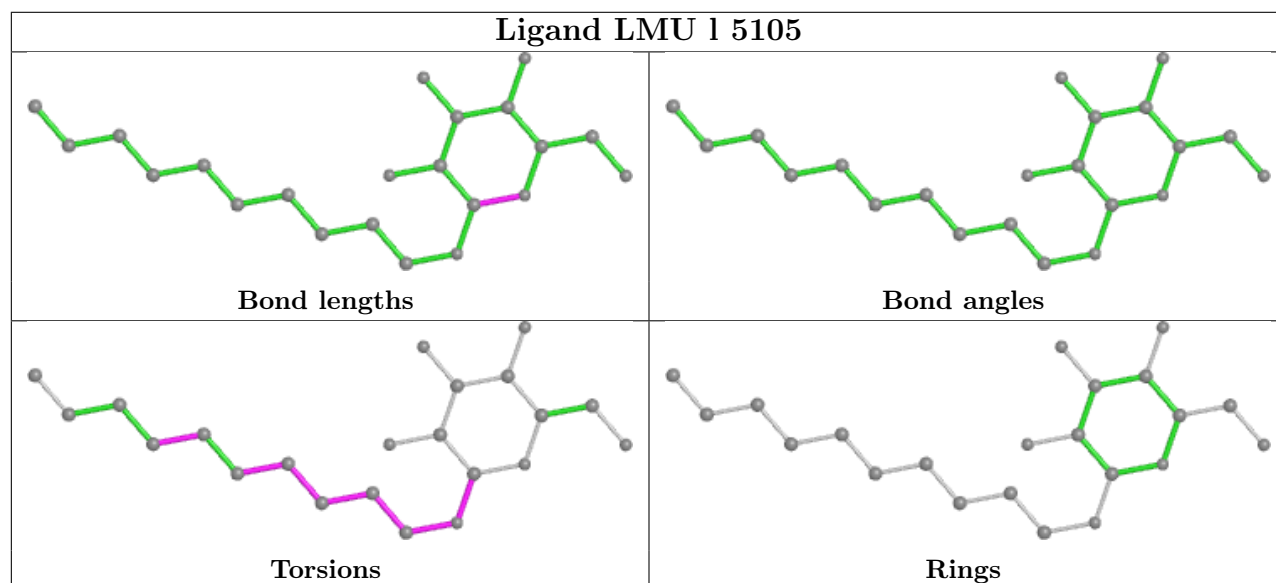
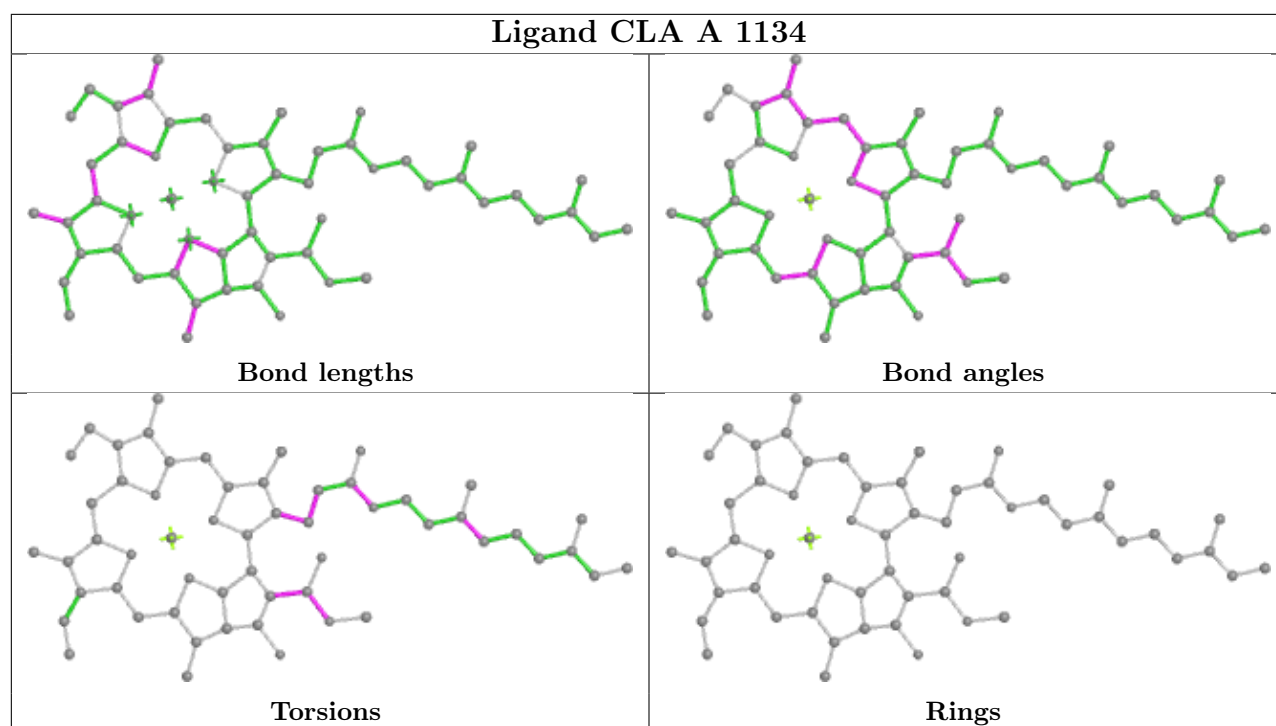


Ligand BCR a 523

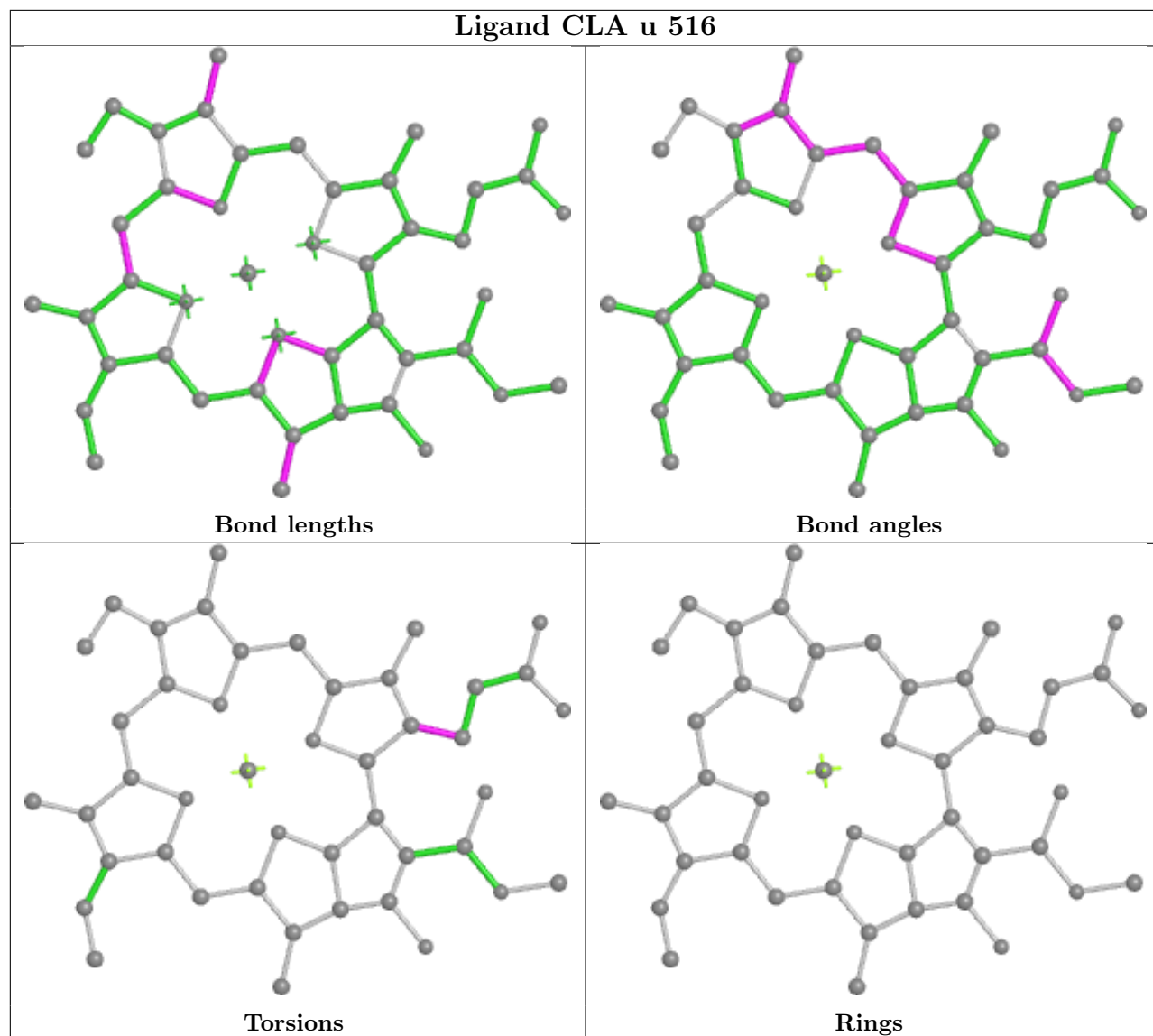


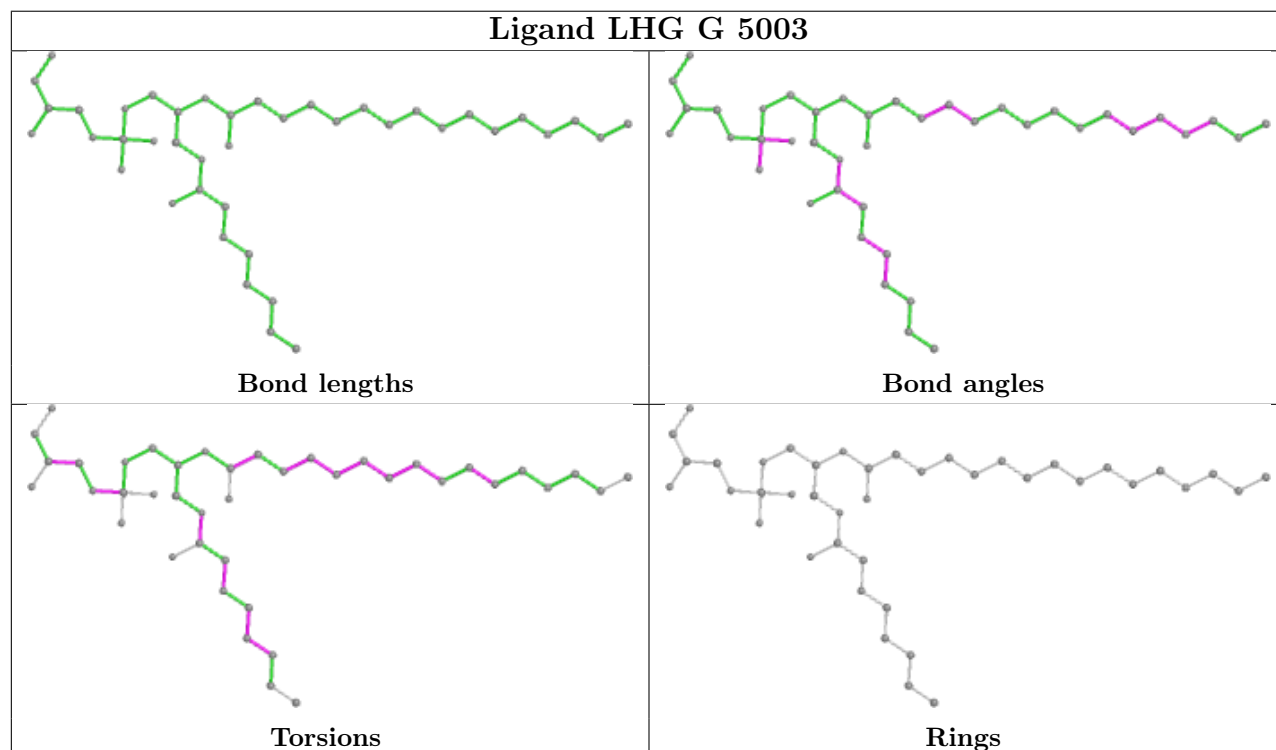
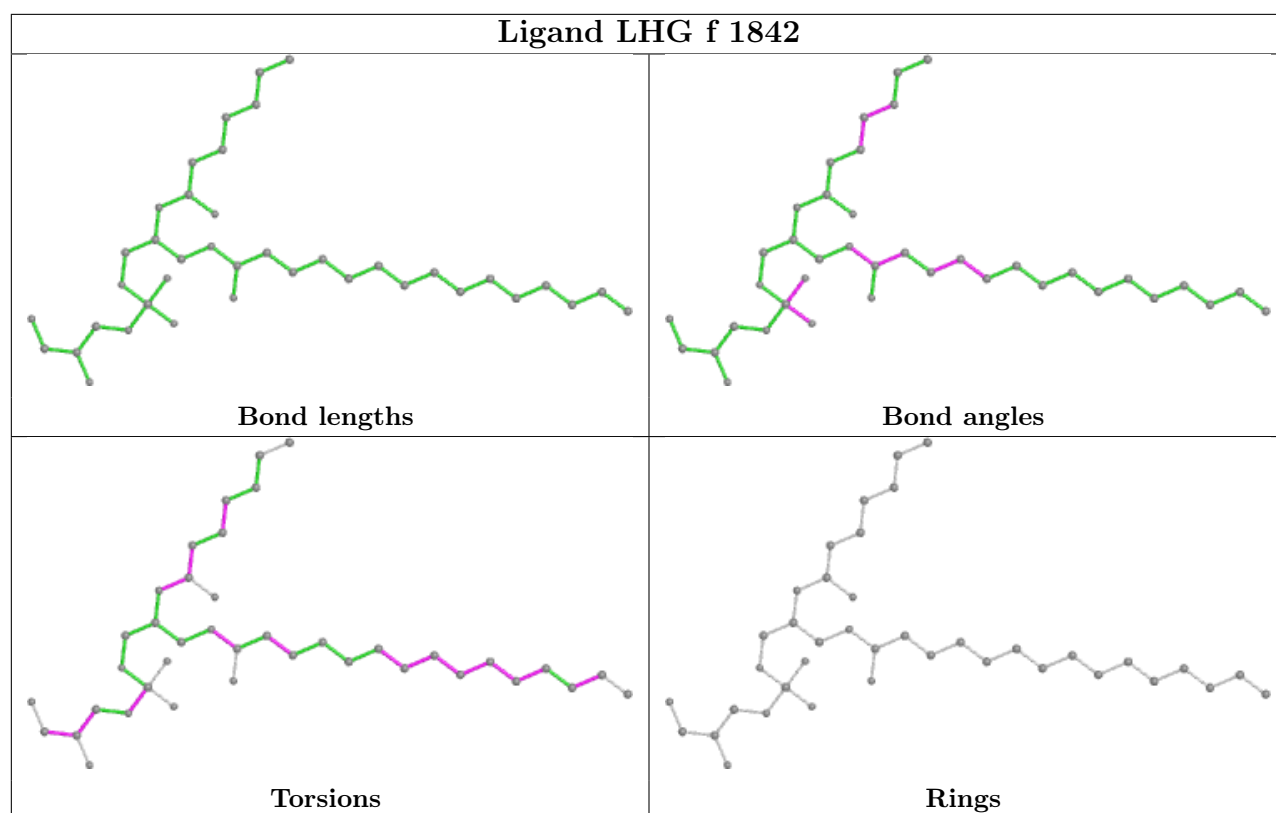




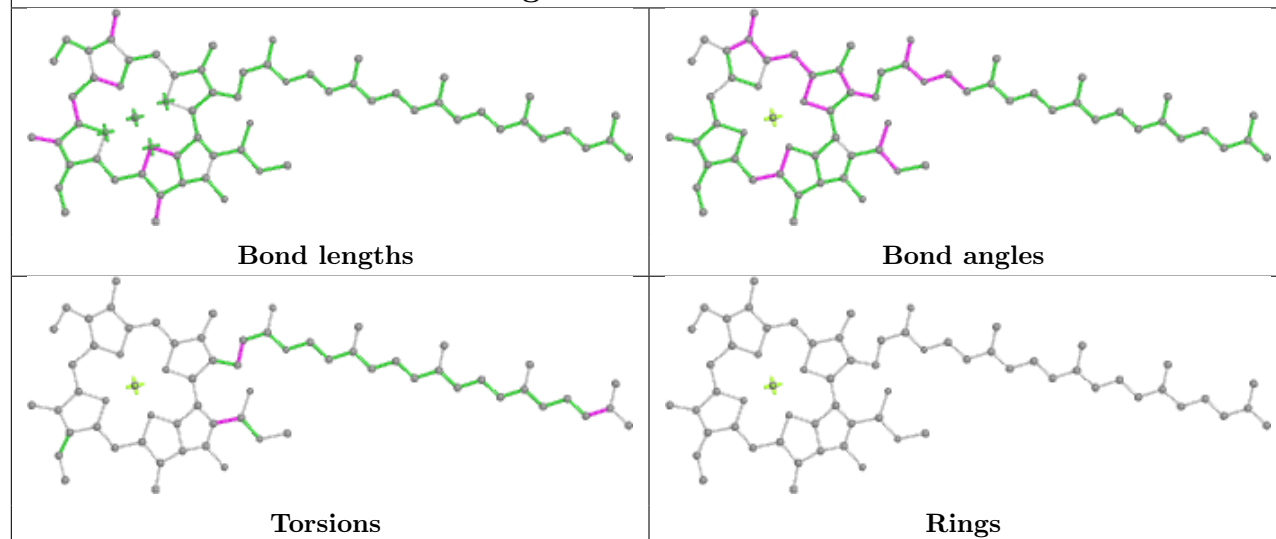


Ligand CLA u 516

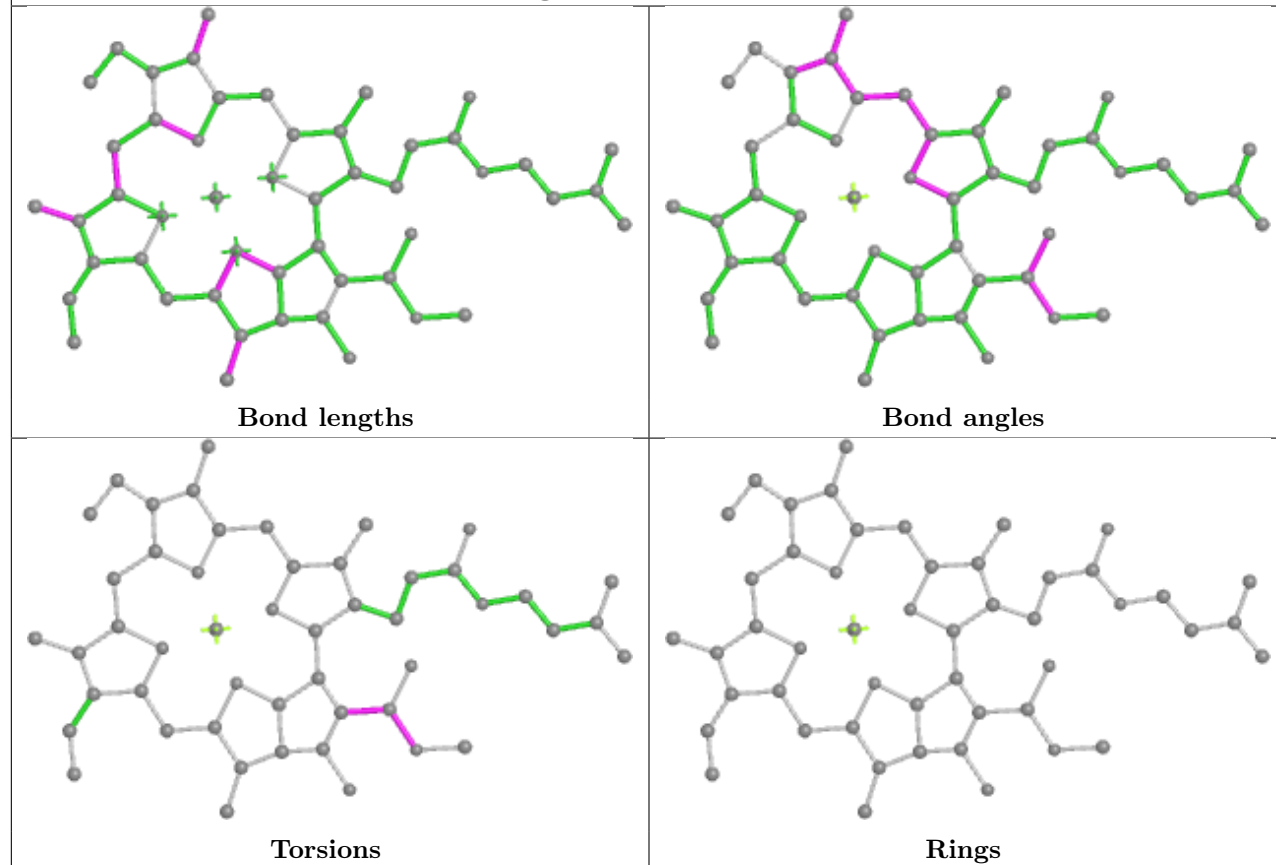


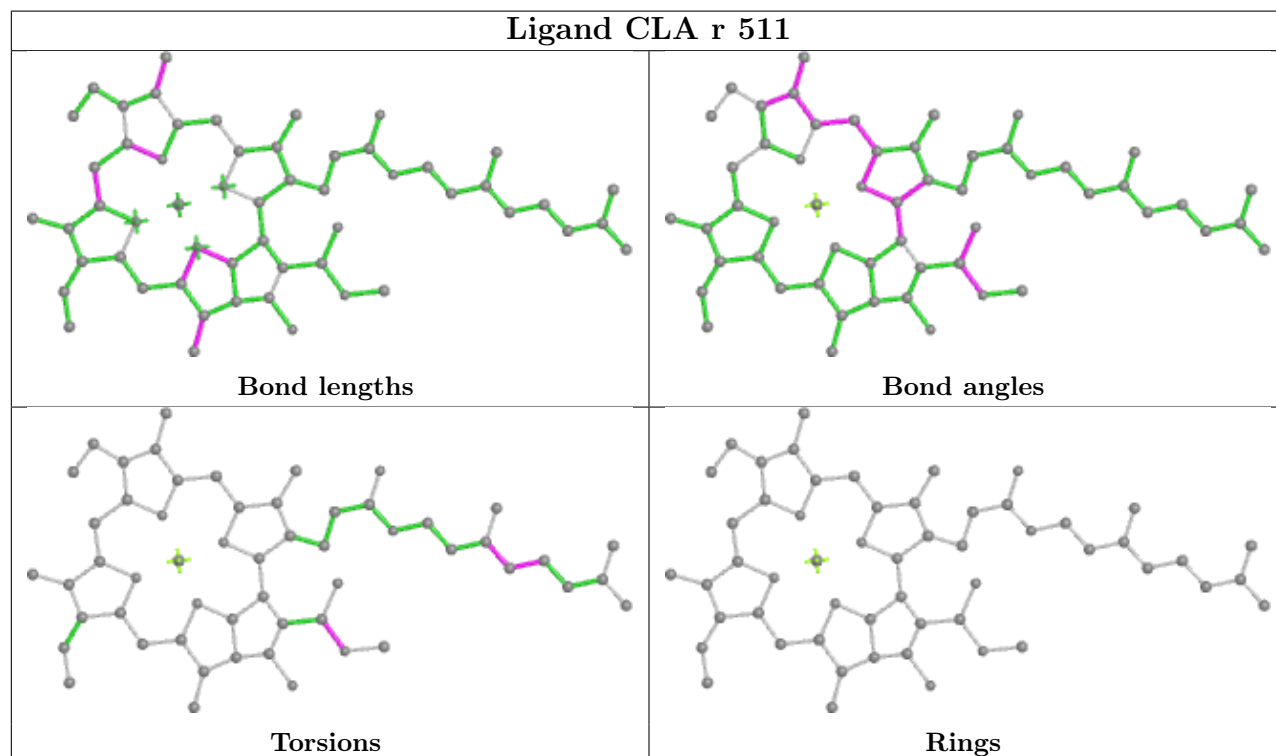
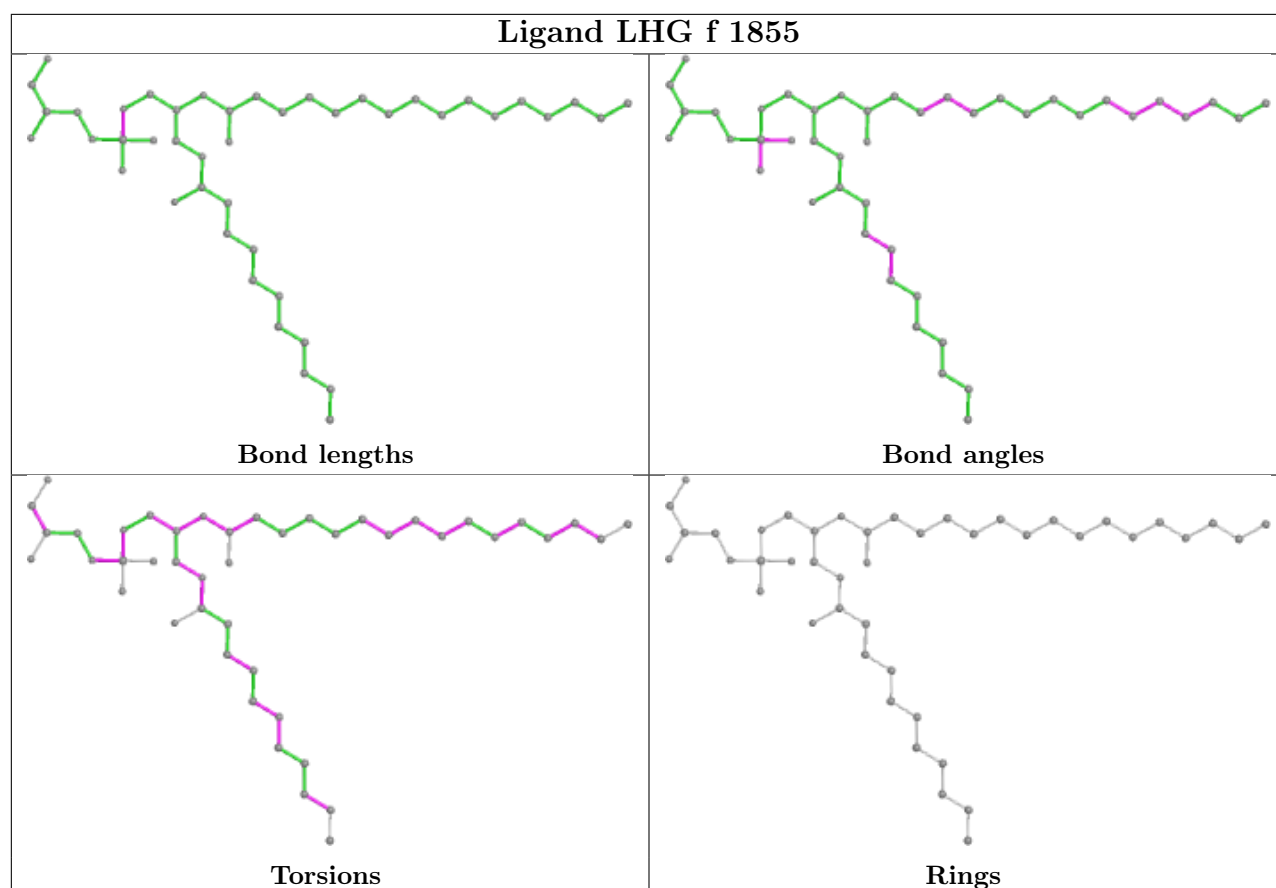


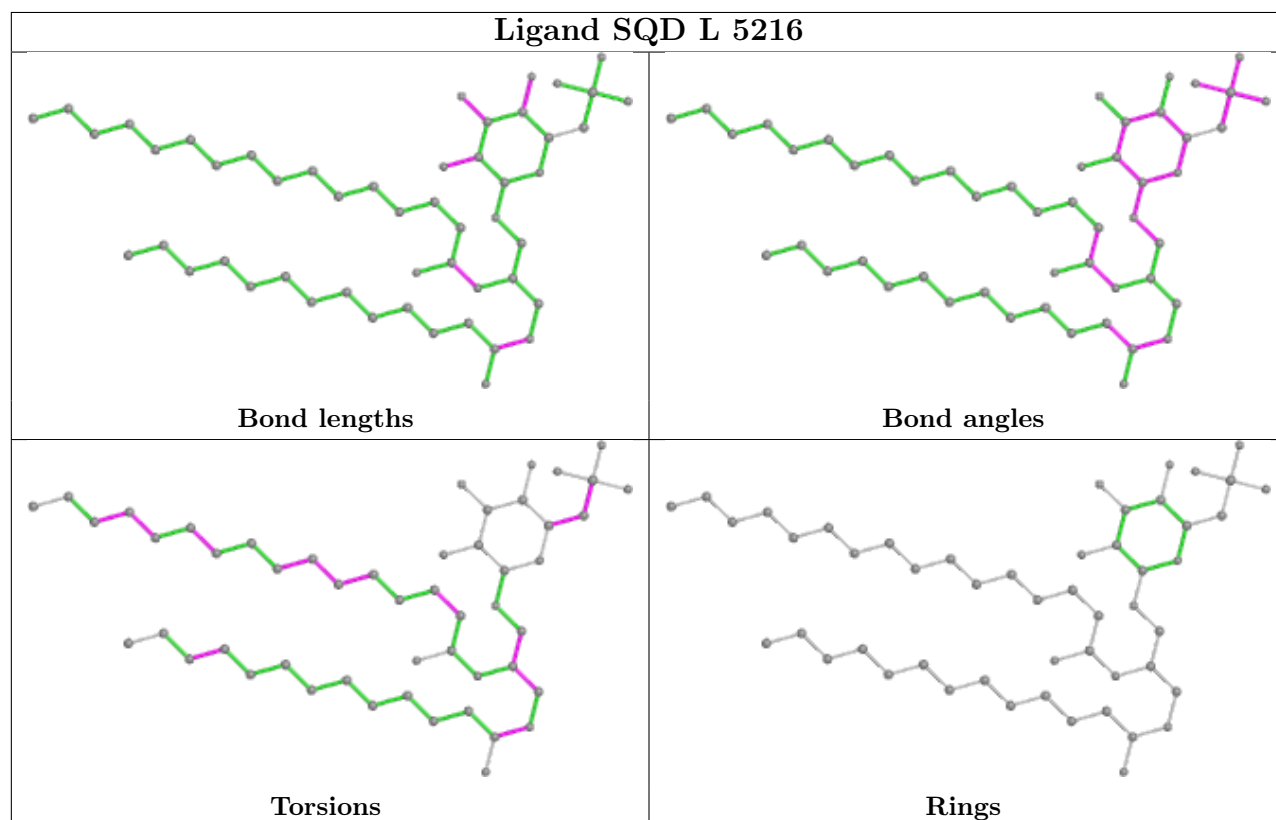
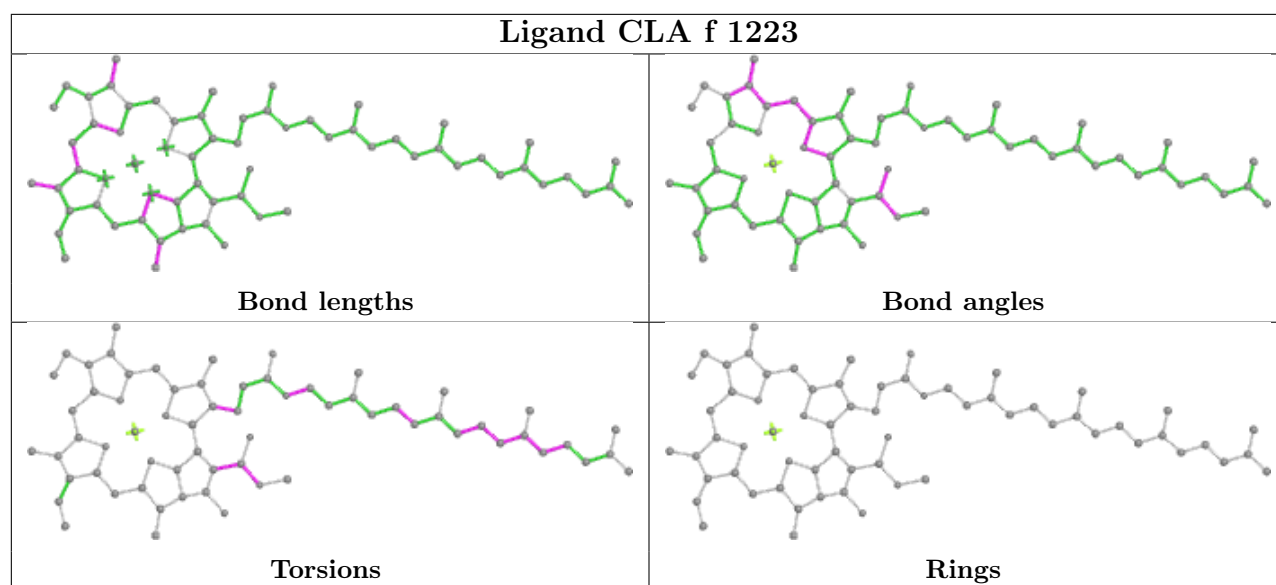
Ligand CLA H 1238



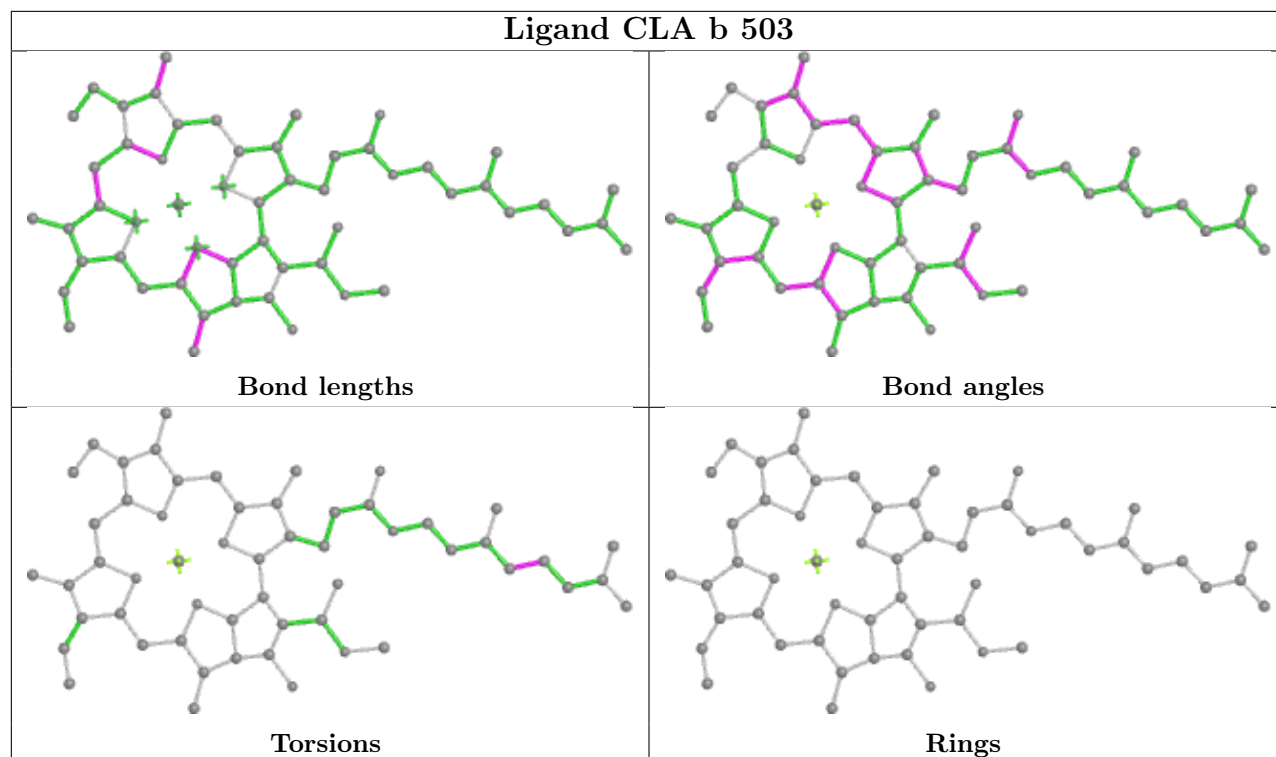
Ligand CLA 3 506



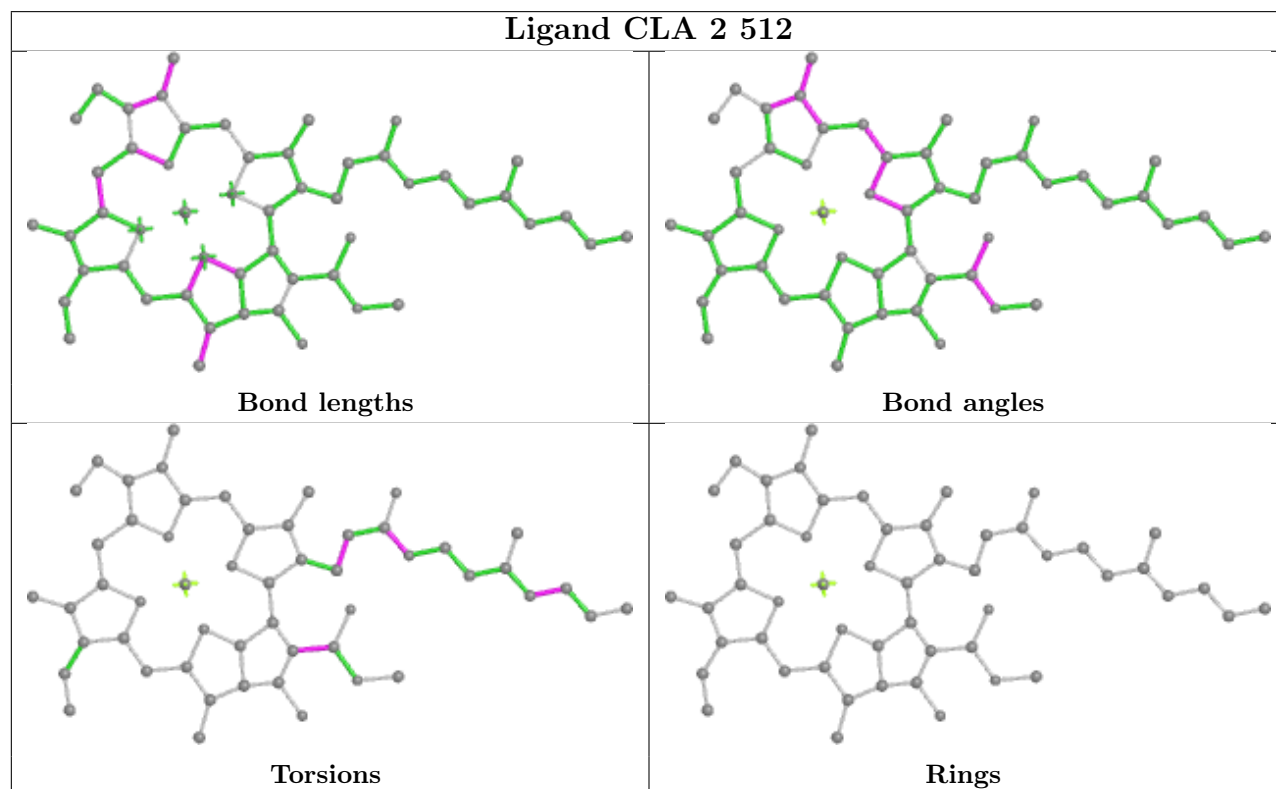


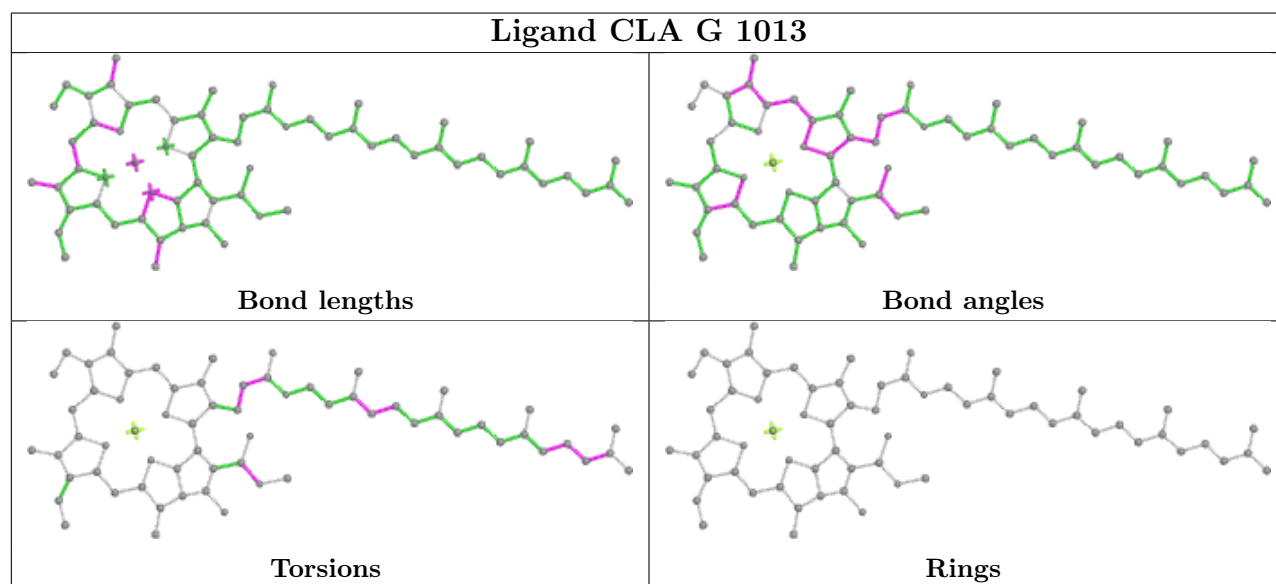
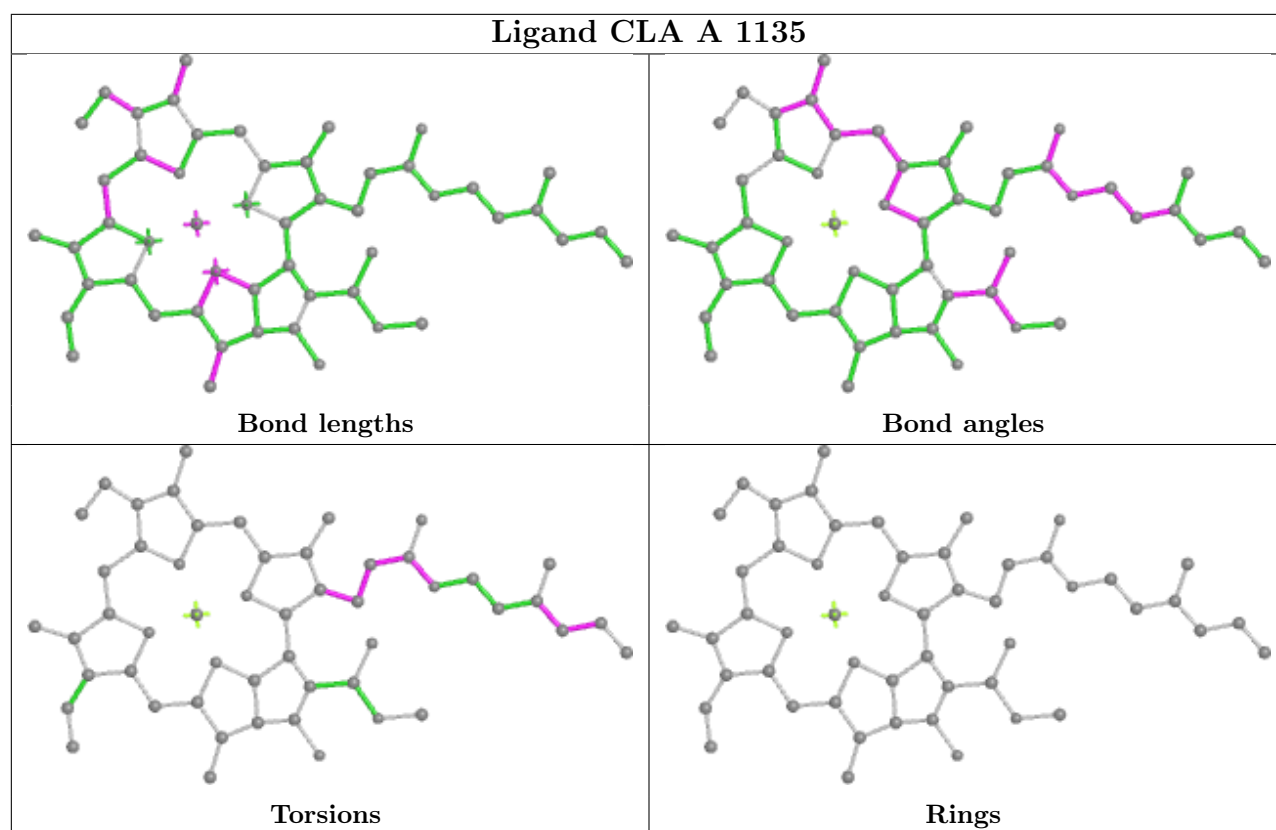


Ligand CLA b 503

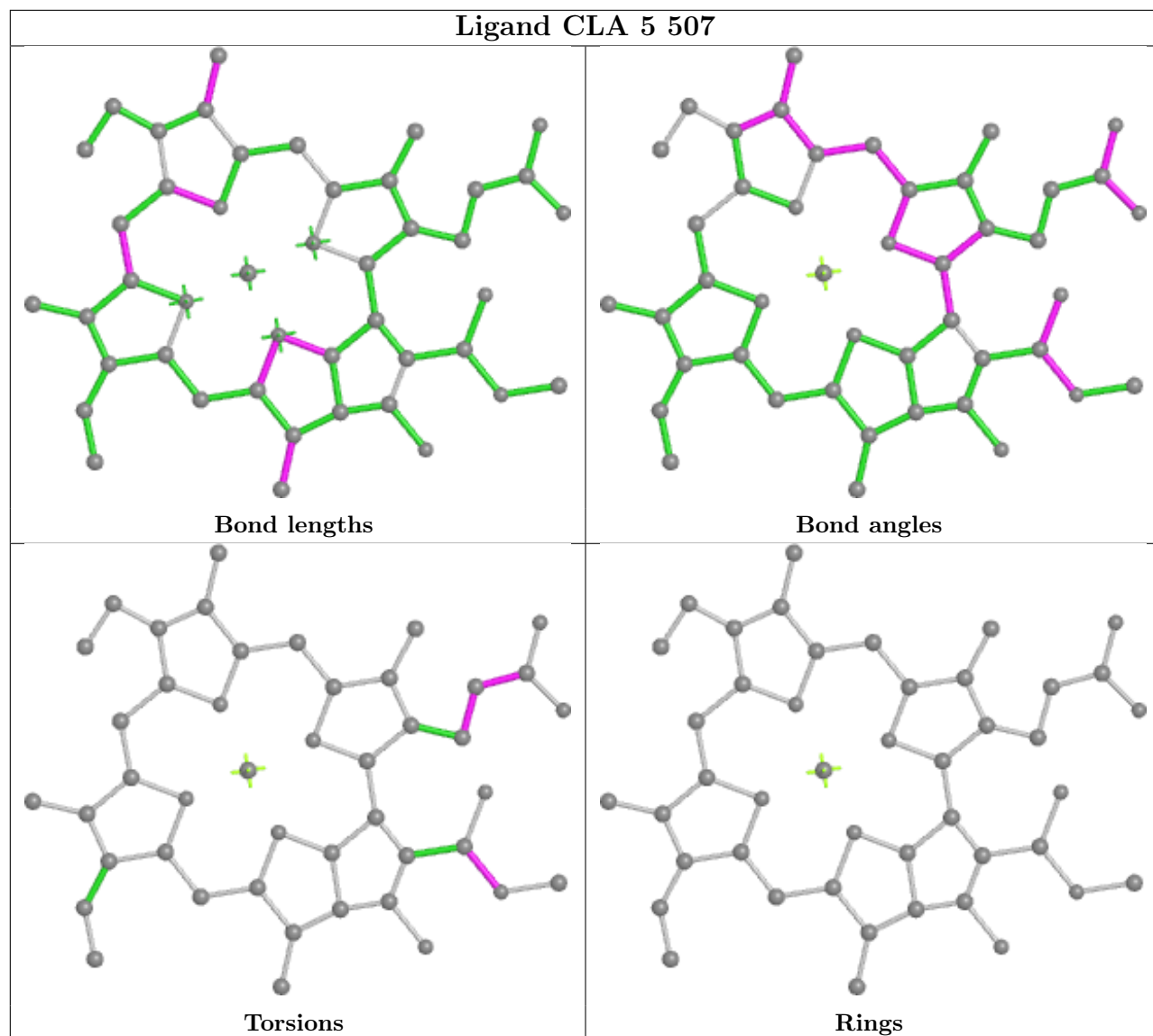


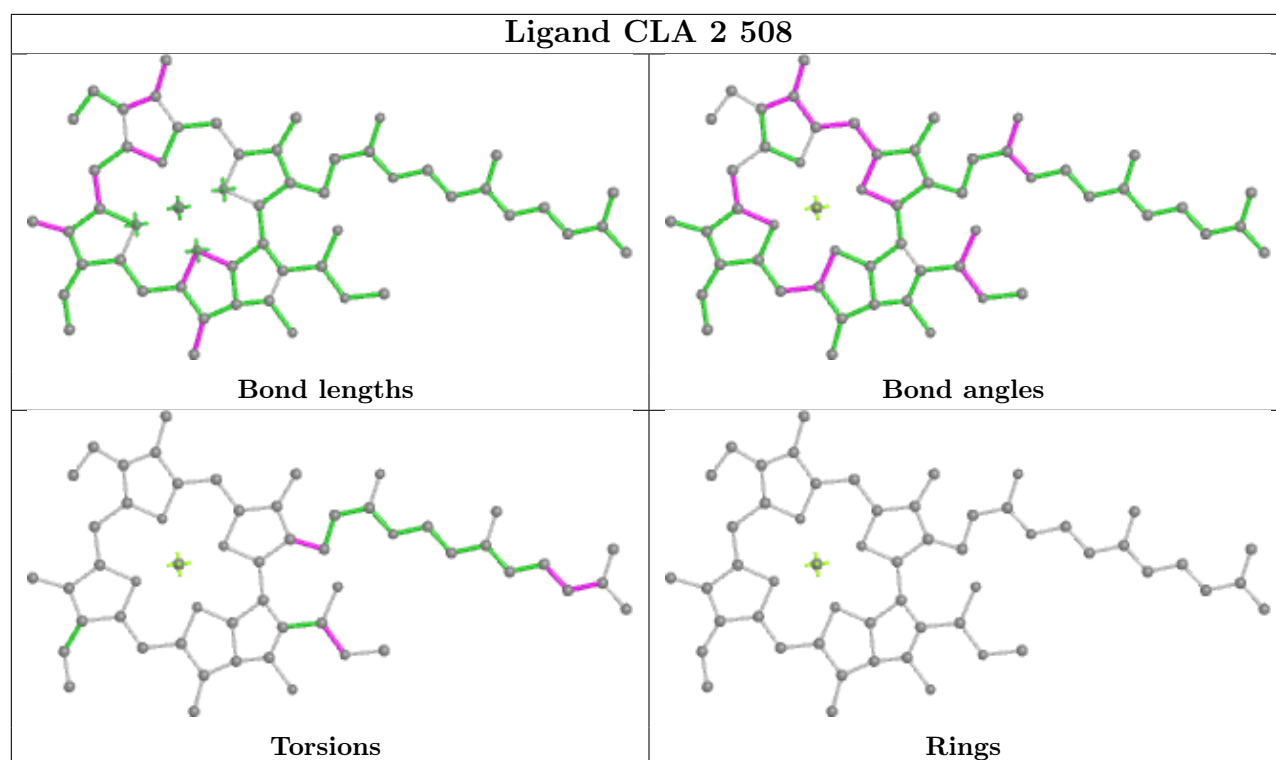
Ligand CLA 2 512

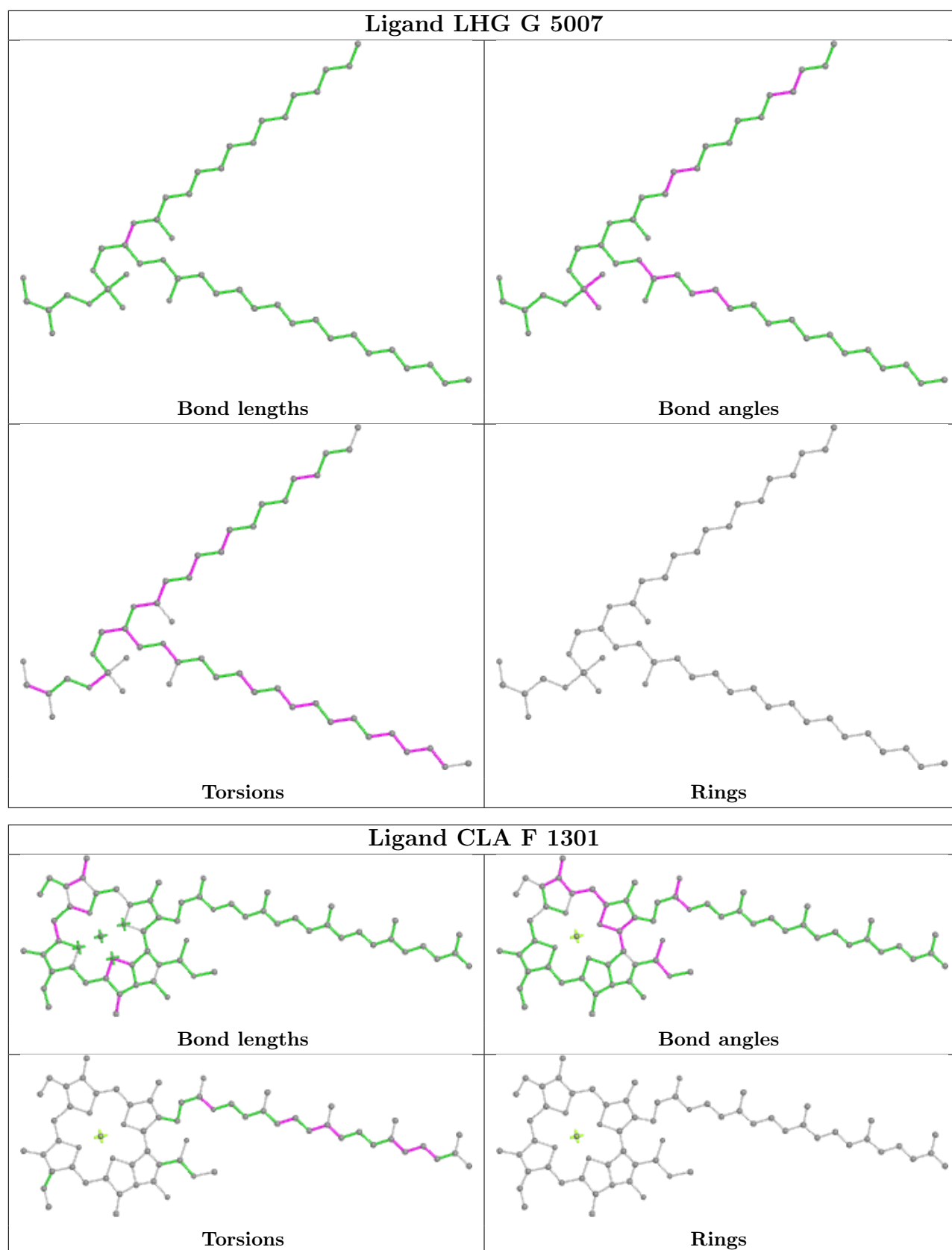




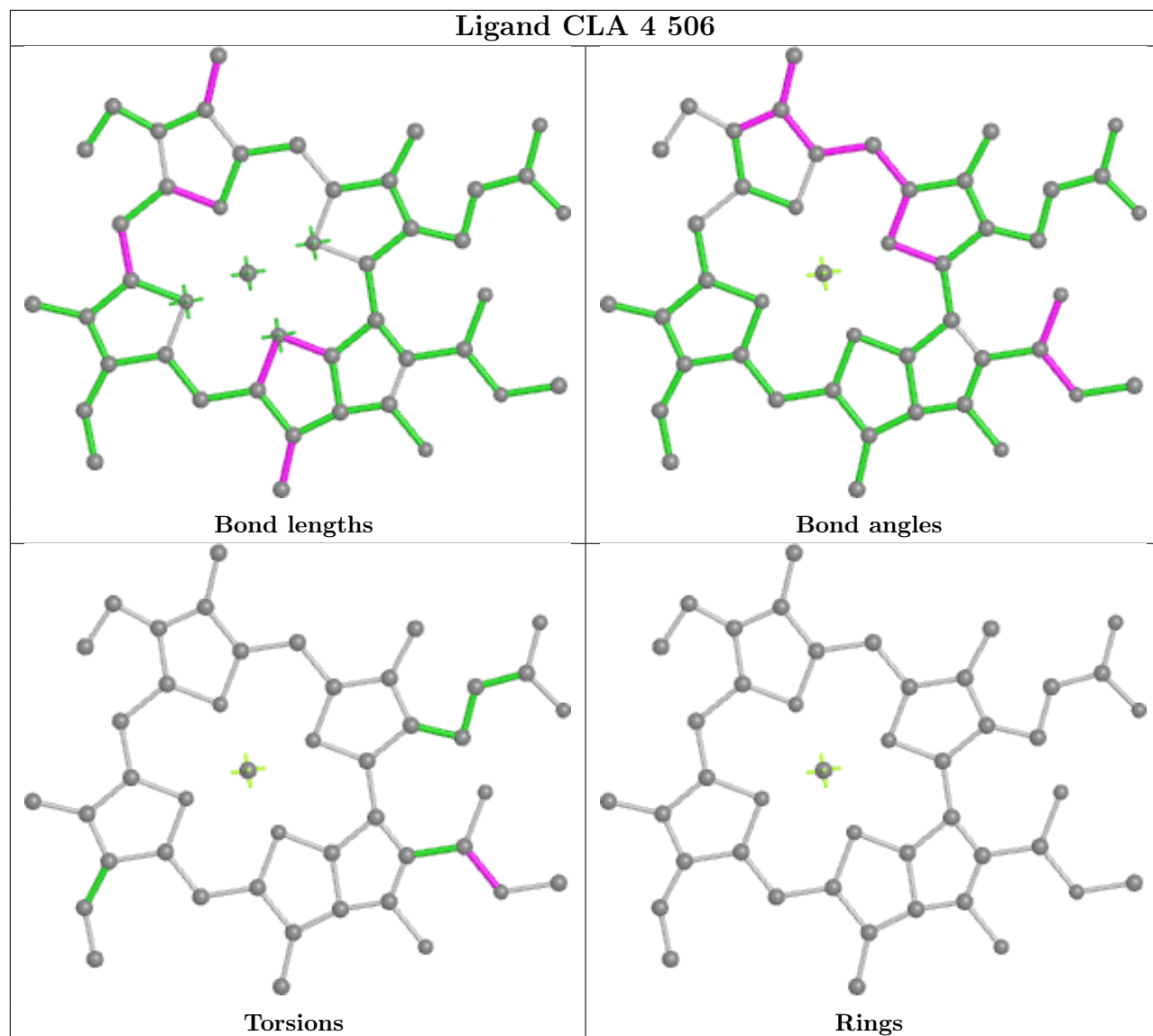
Ligand CLA 5 507



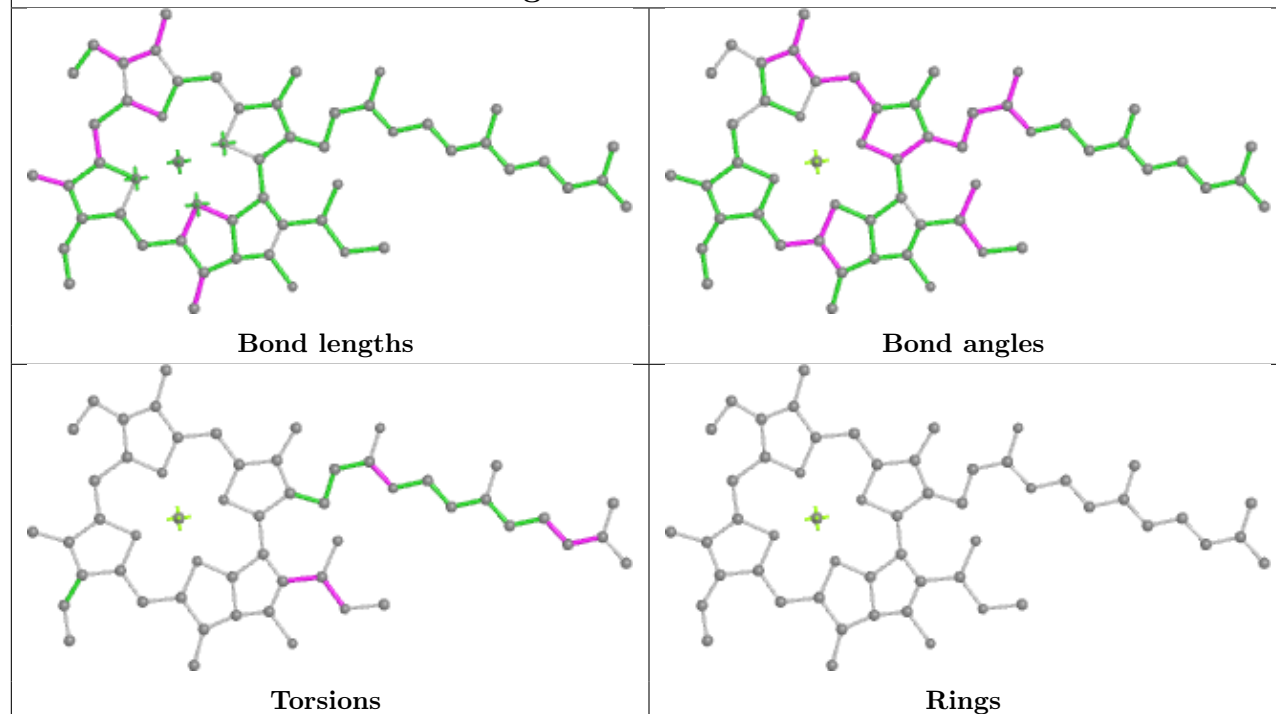




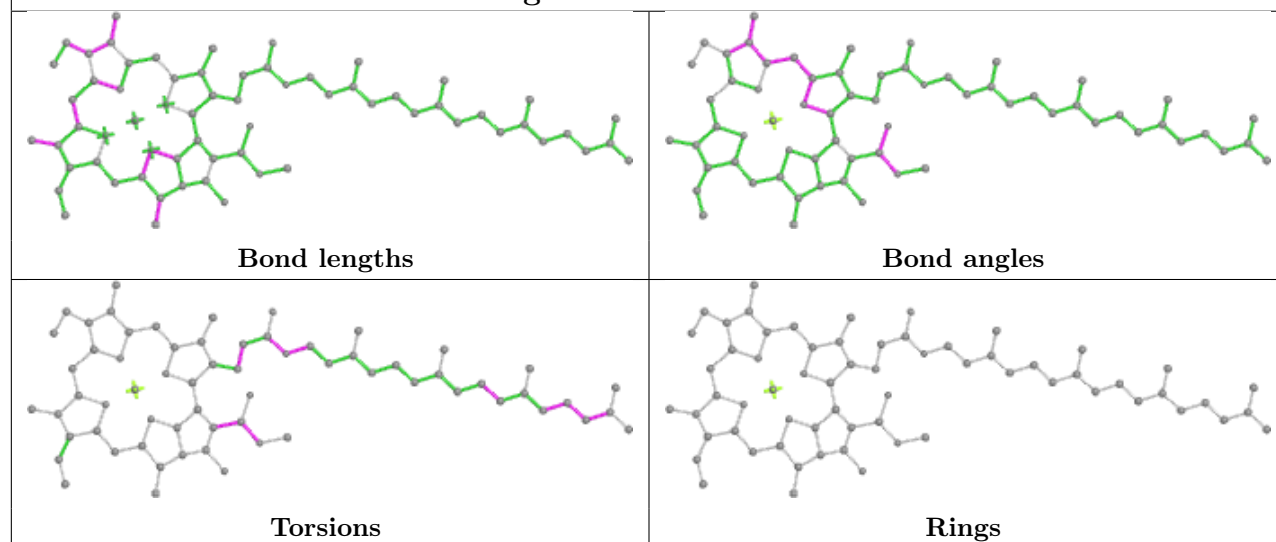
Ligand CLA 4 506

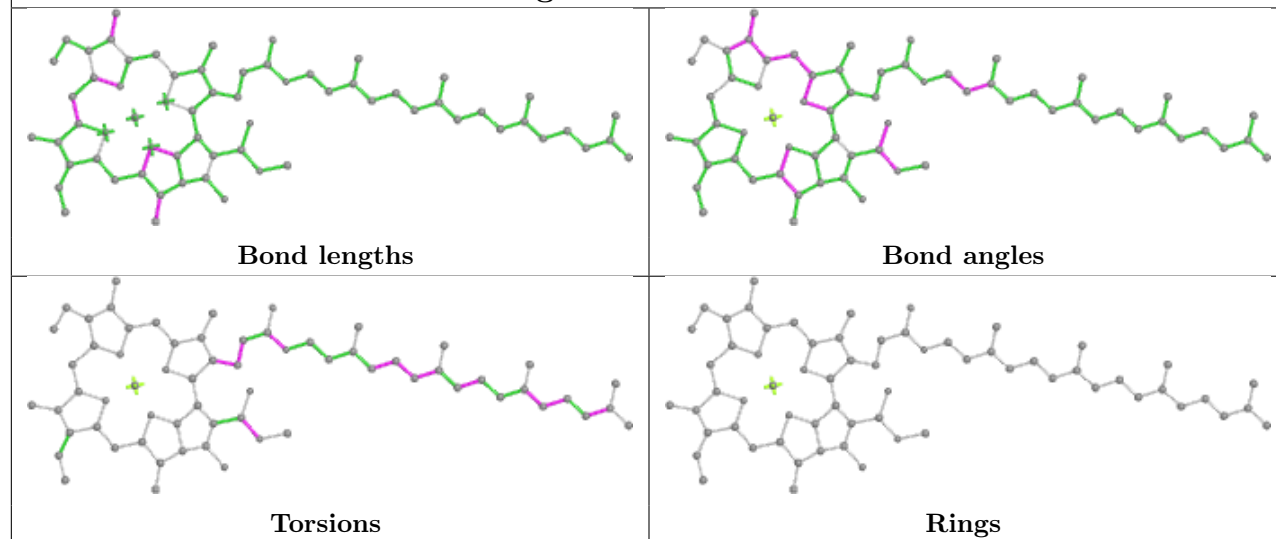
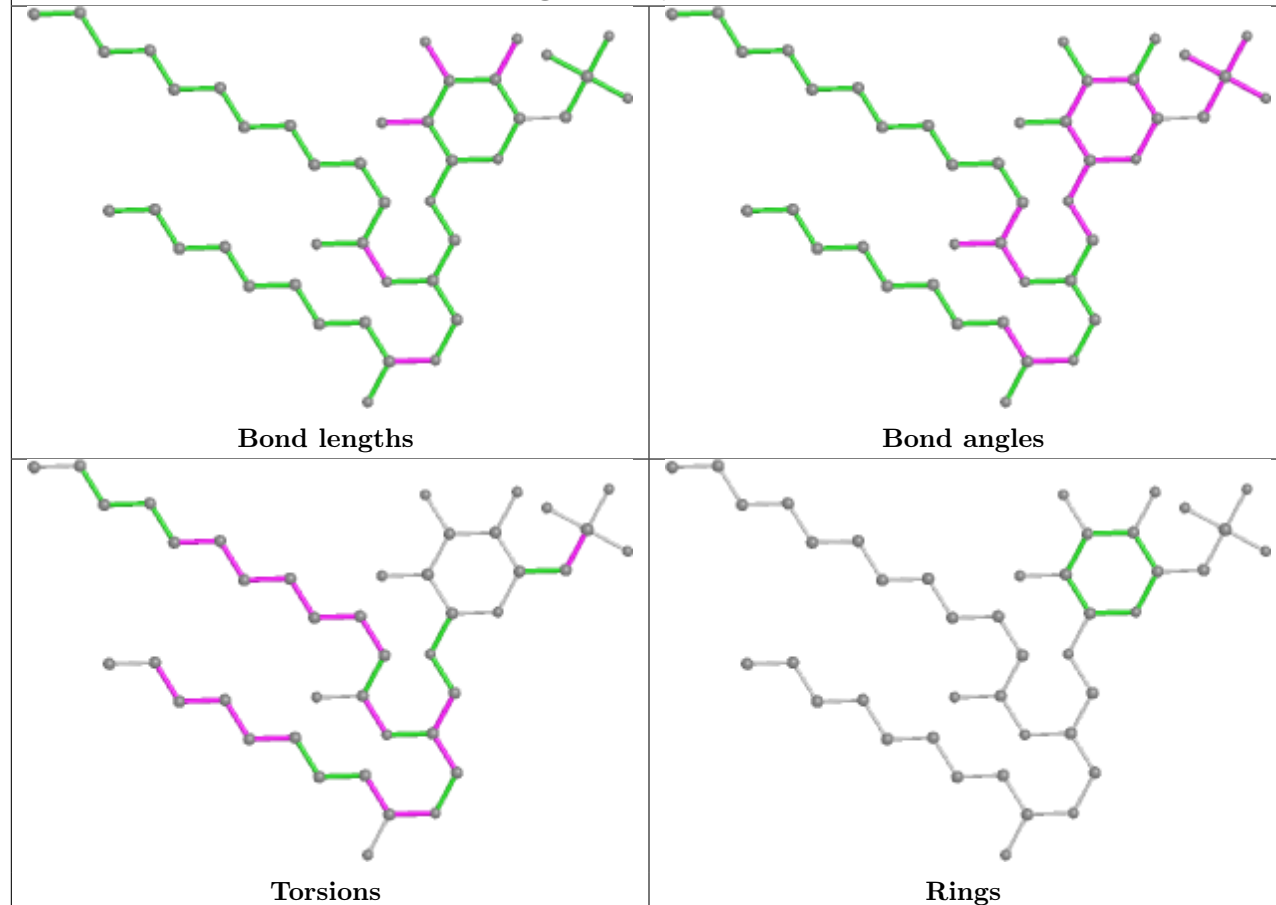


Ligand CLA B 1220

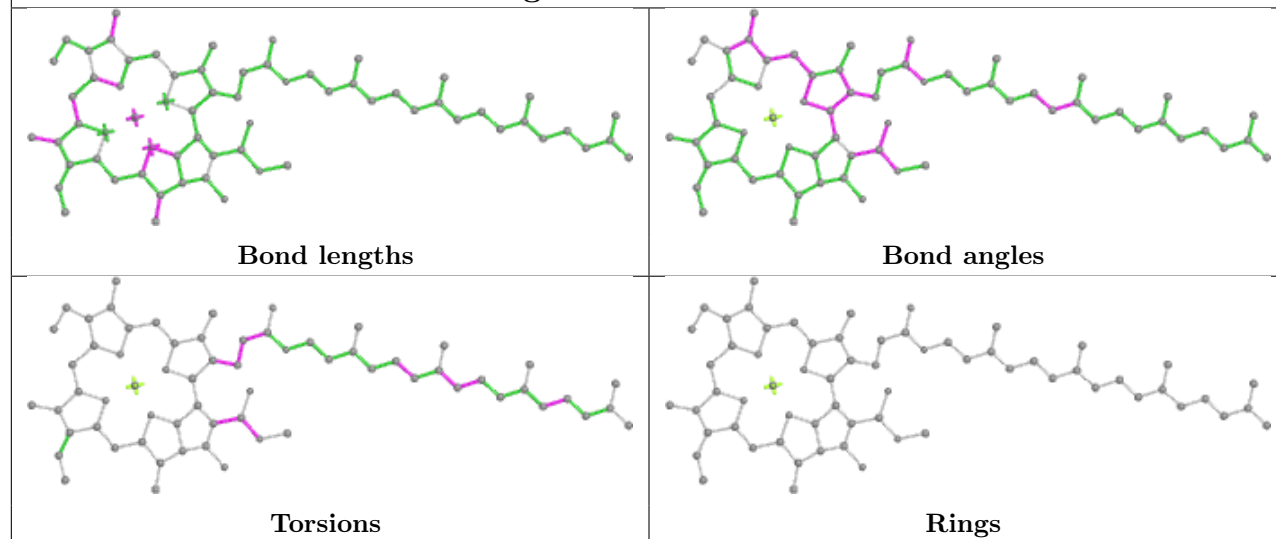


Ligand CLA B 1207

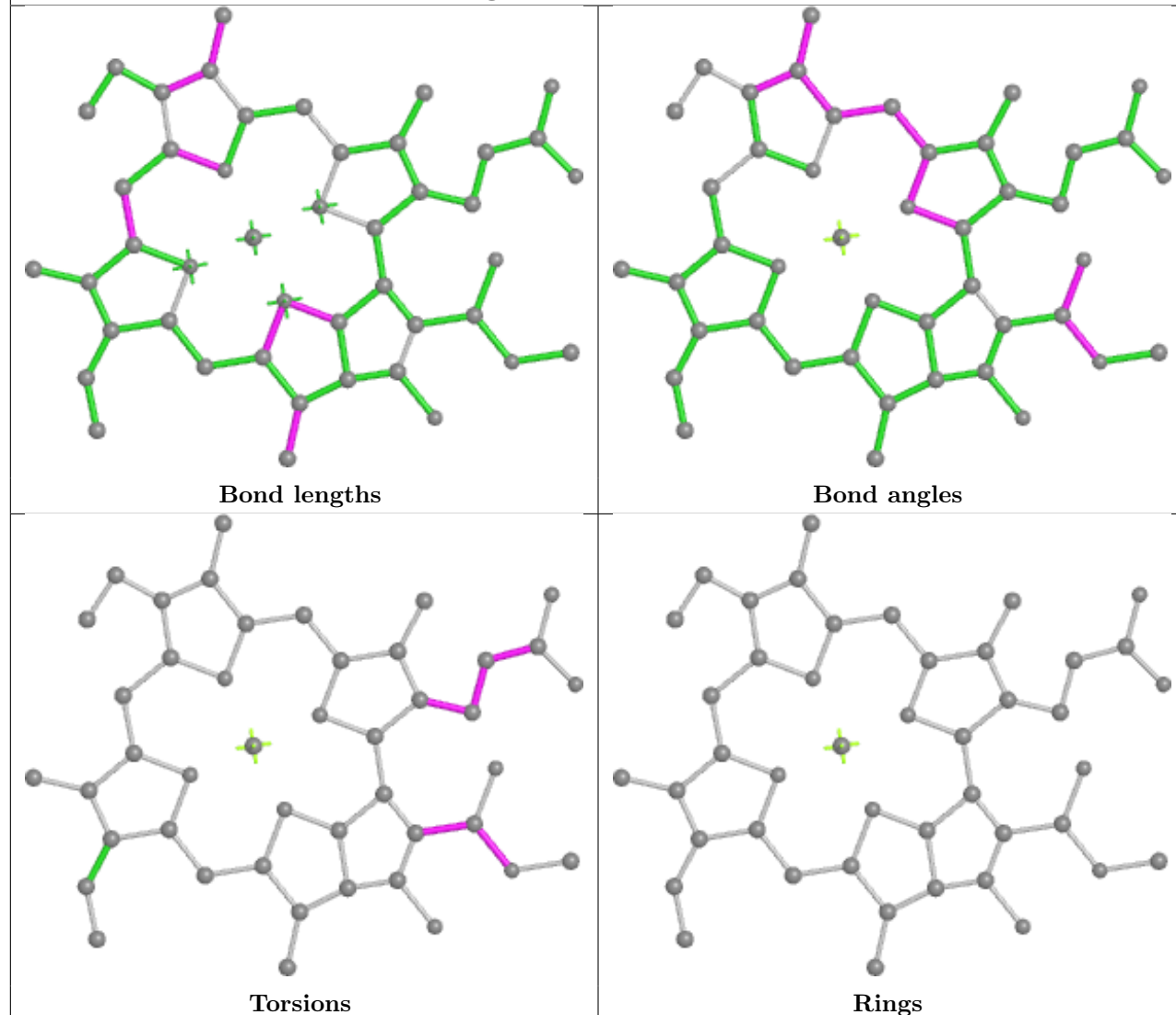


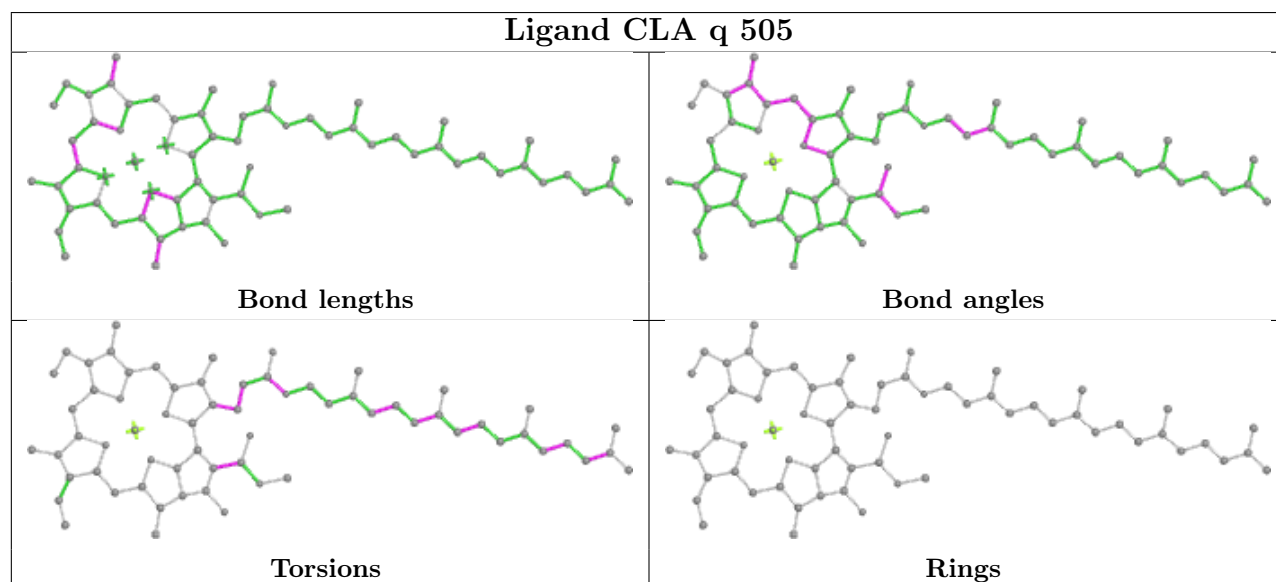
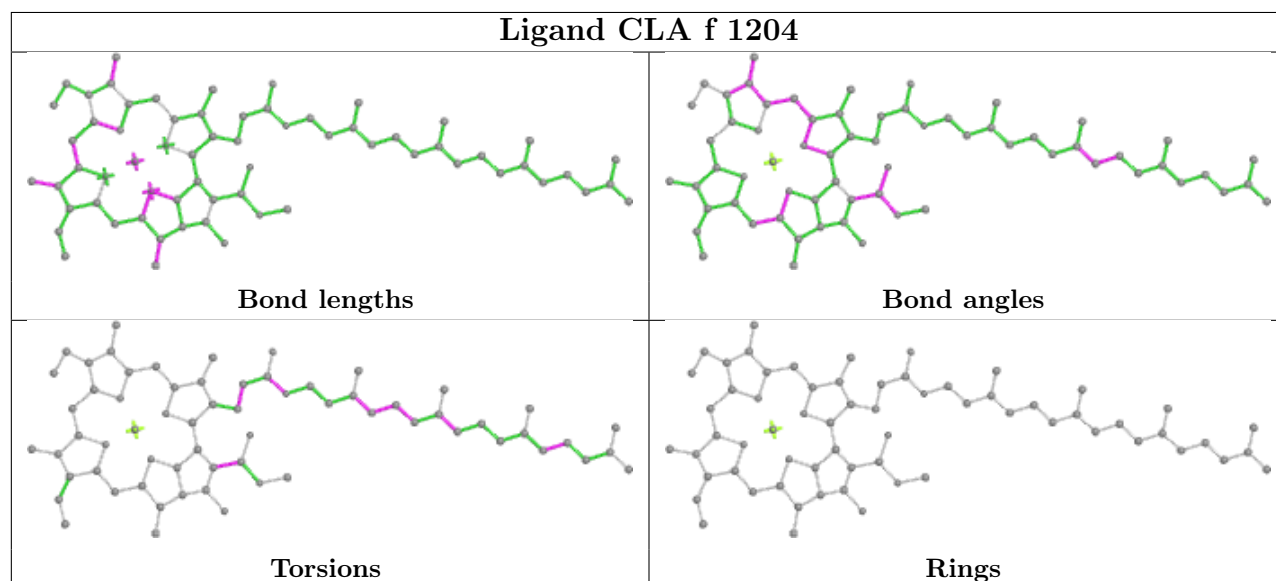
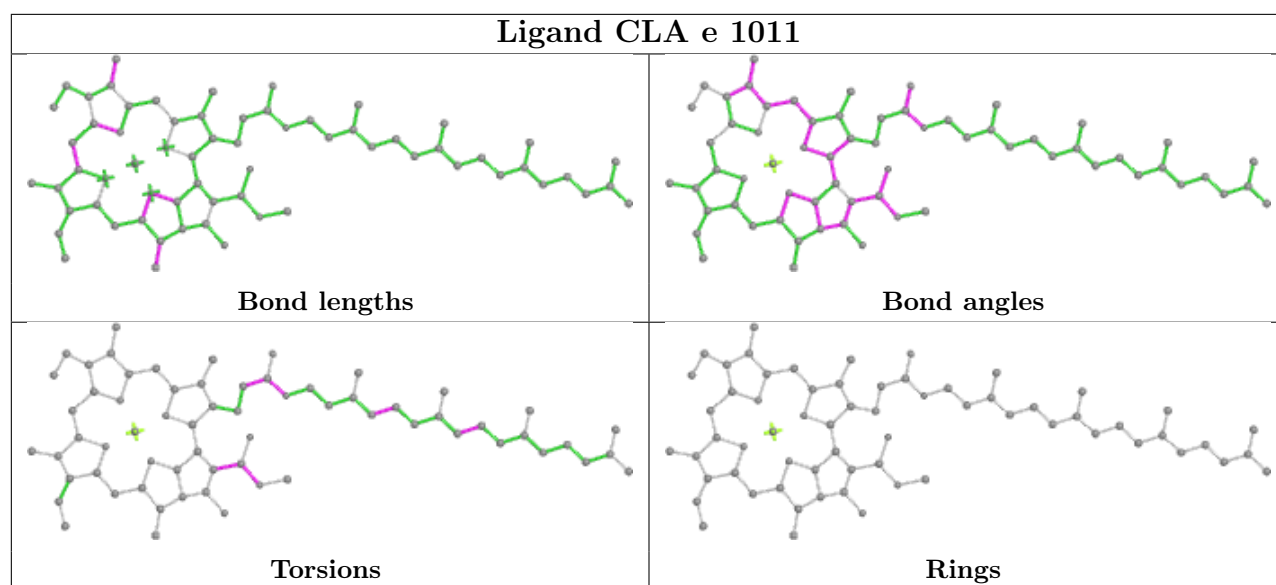
Ligand CLA 2 505**Ligand SQD 3 822**

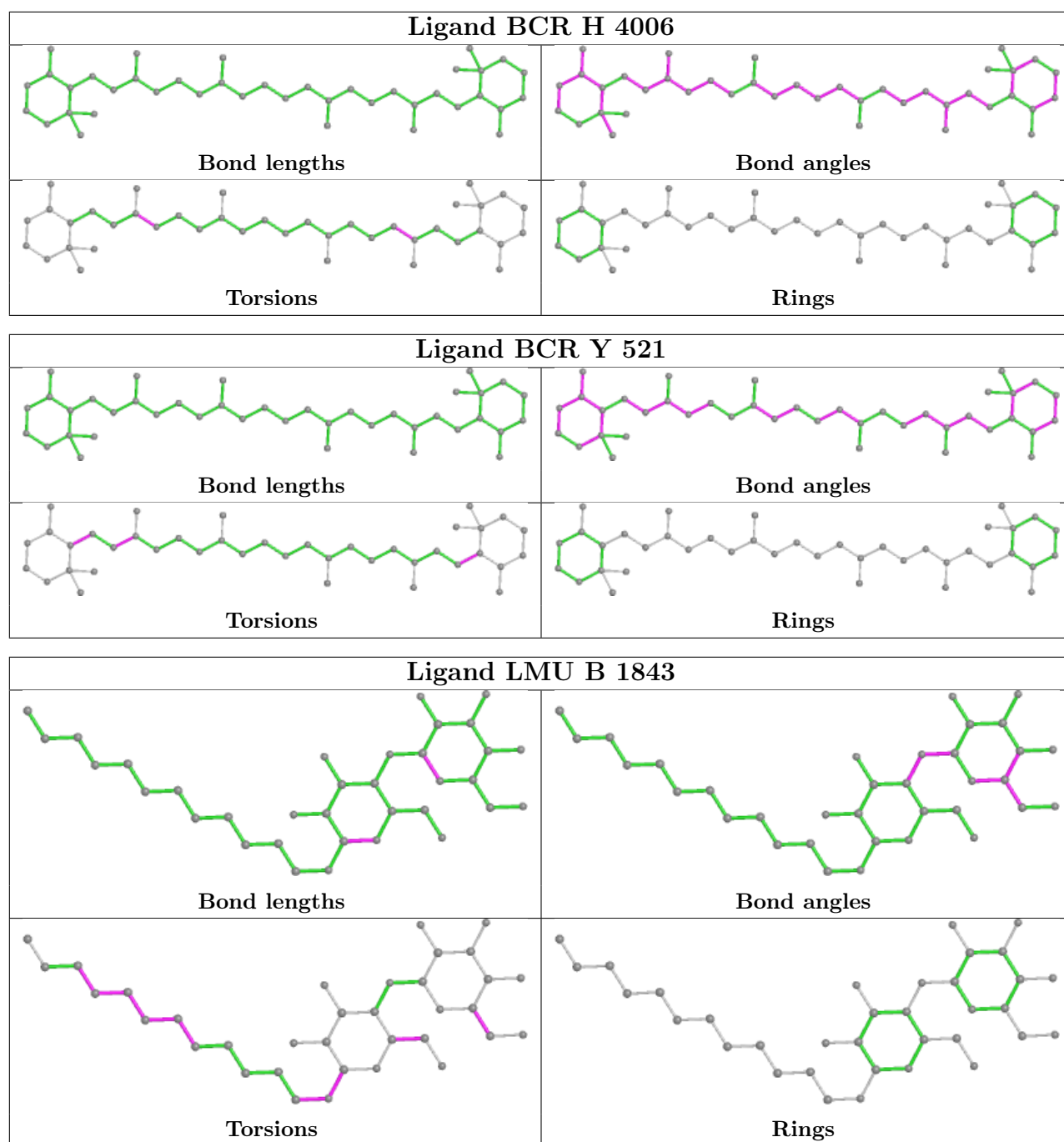
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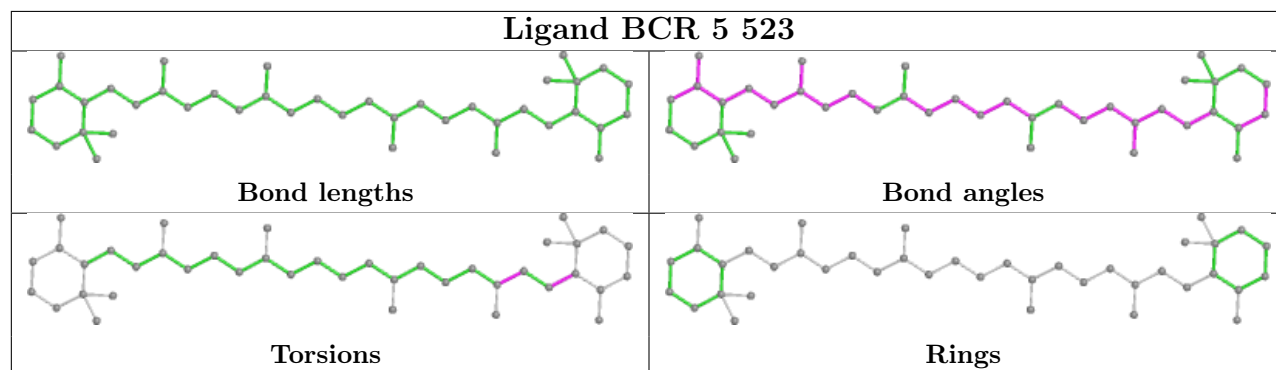
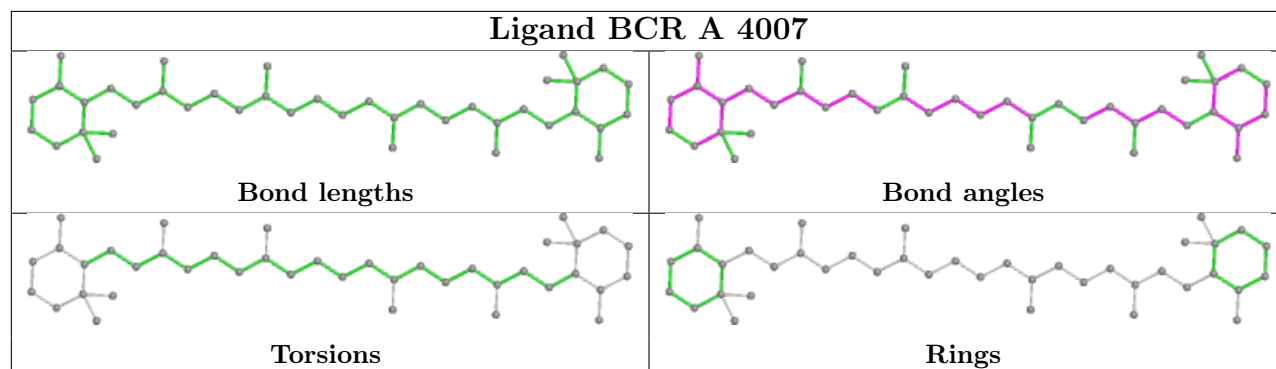
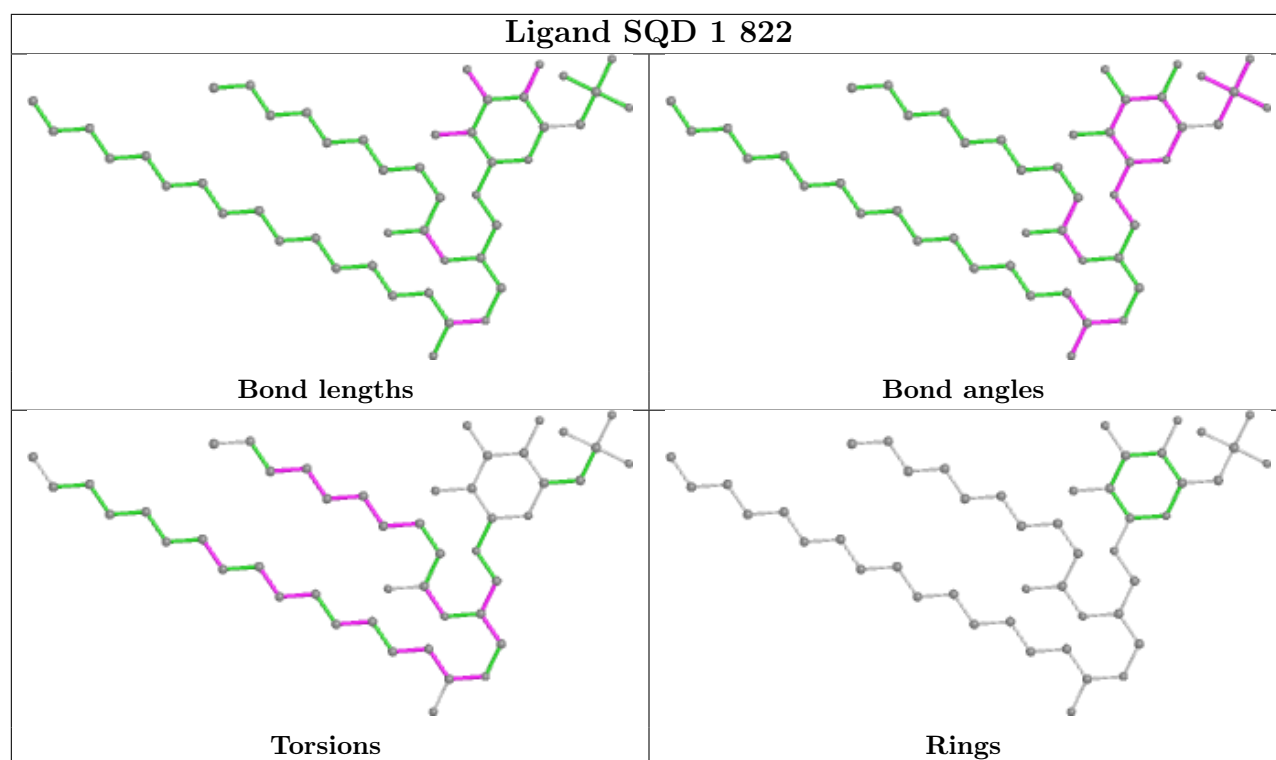


Ligand CLA F 1302

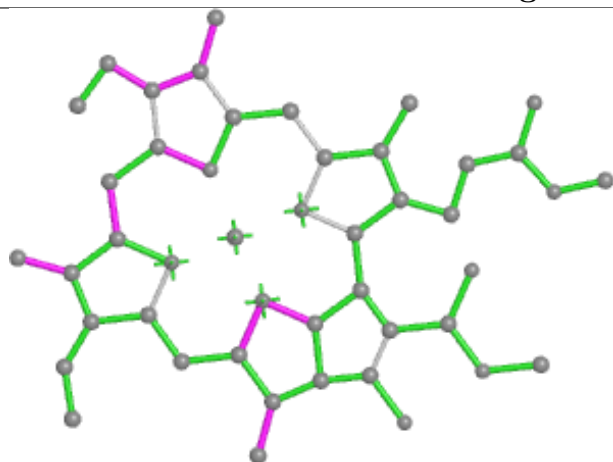




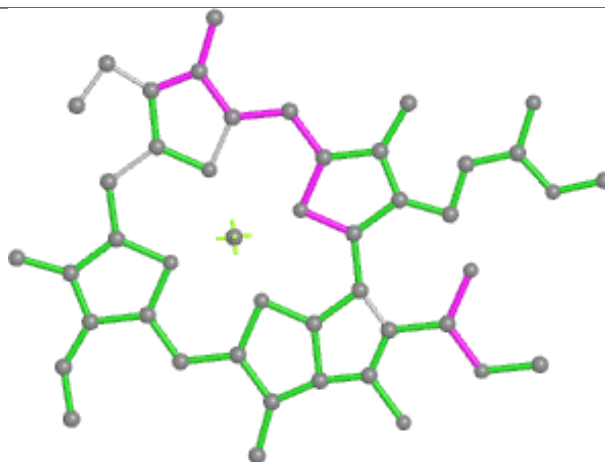




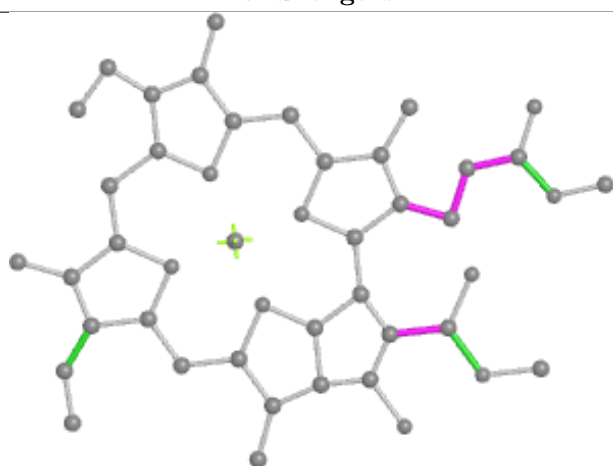
Ligand CLA c 519



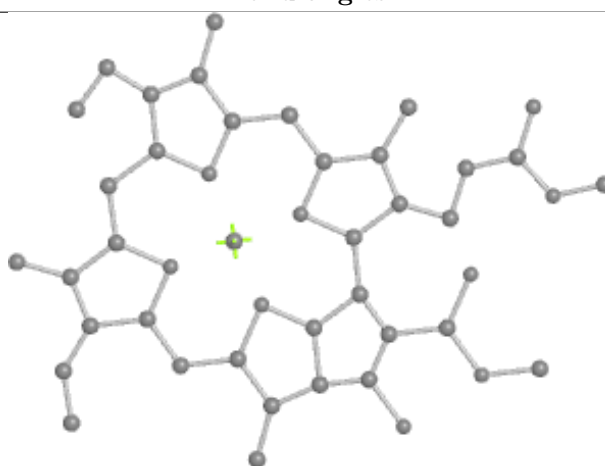
Bond lengths



Bond angles

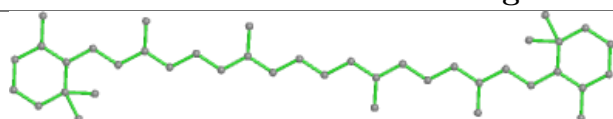


Torsions

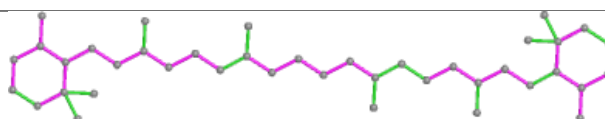


Rings

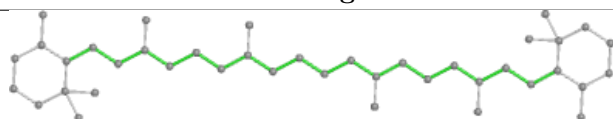
Ligand BCR G 4007



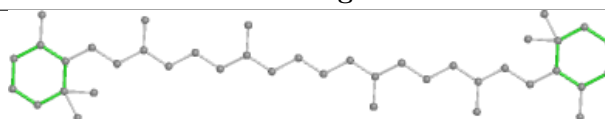
Bond lengths



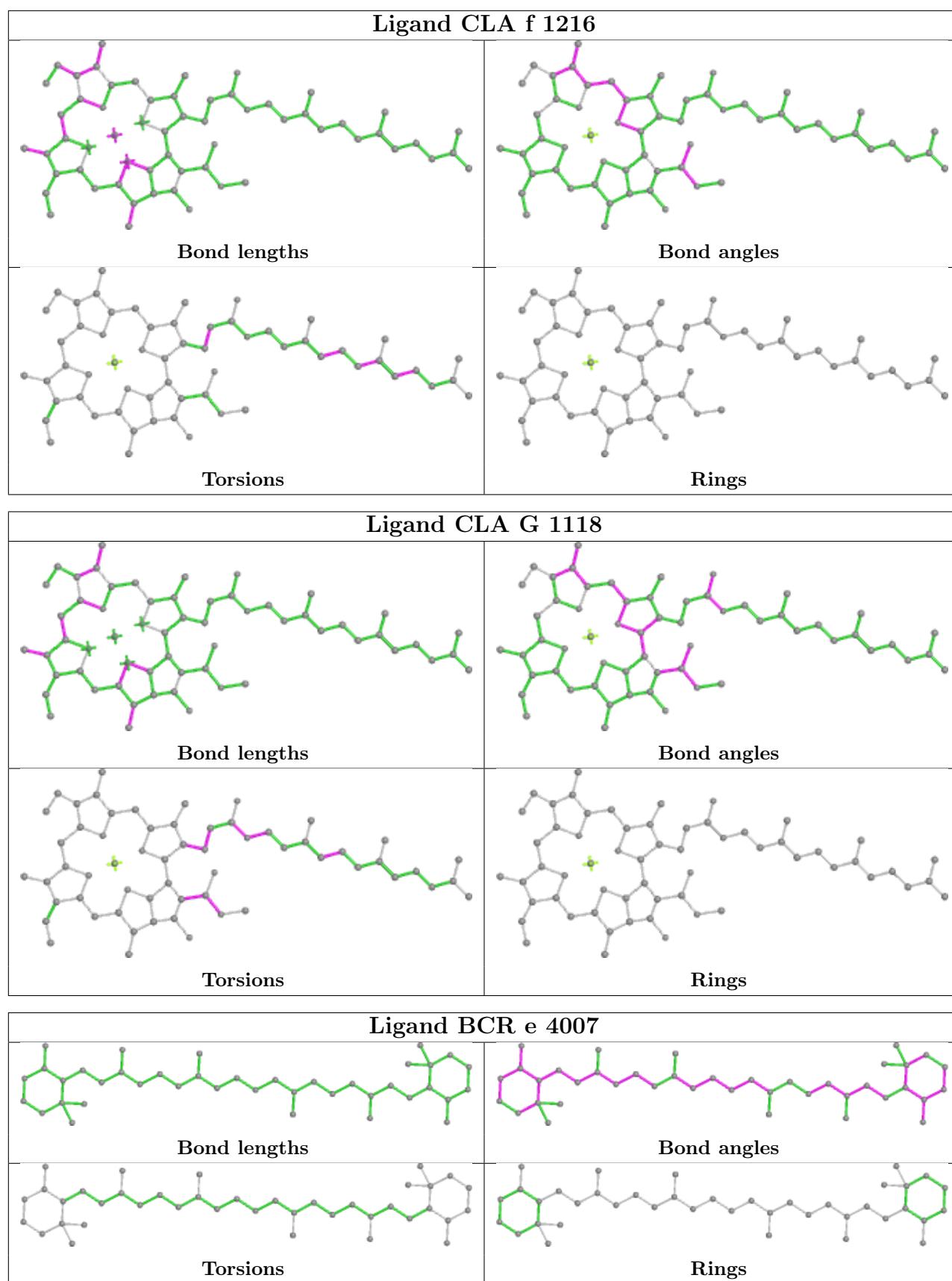
Bond angles

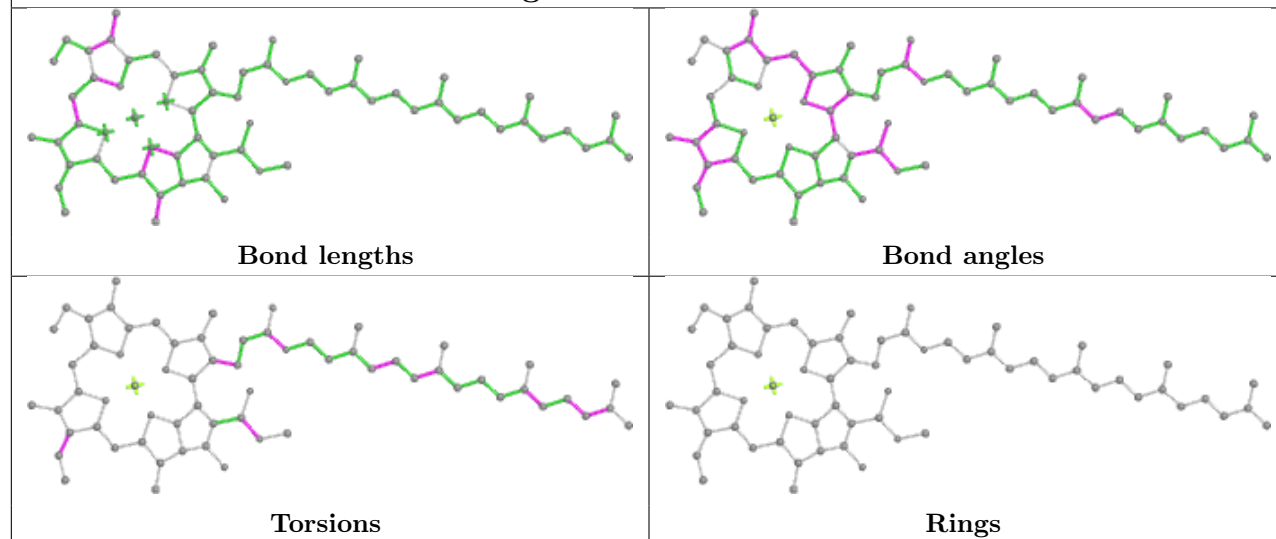
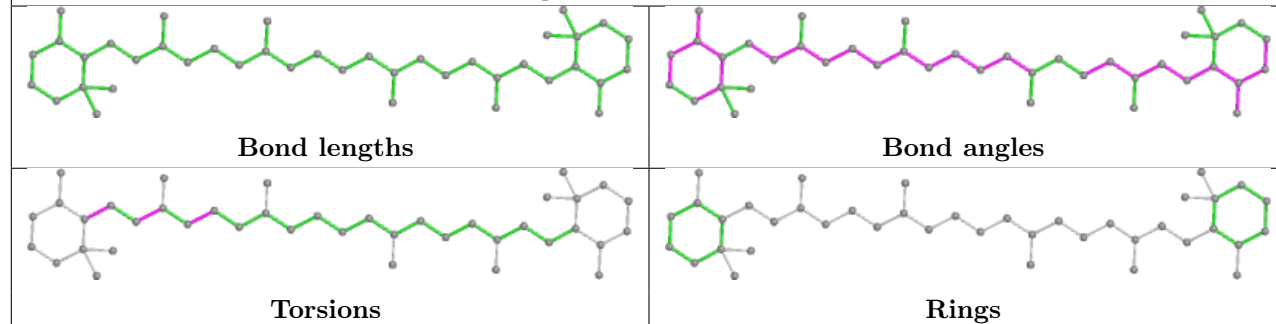
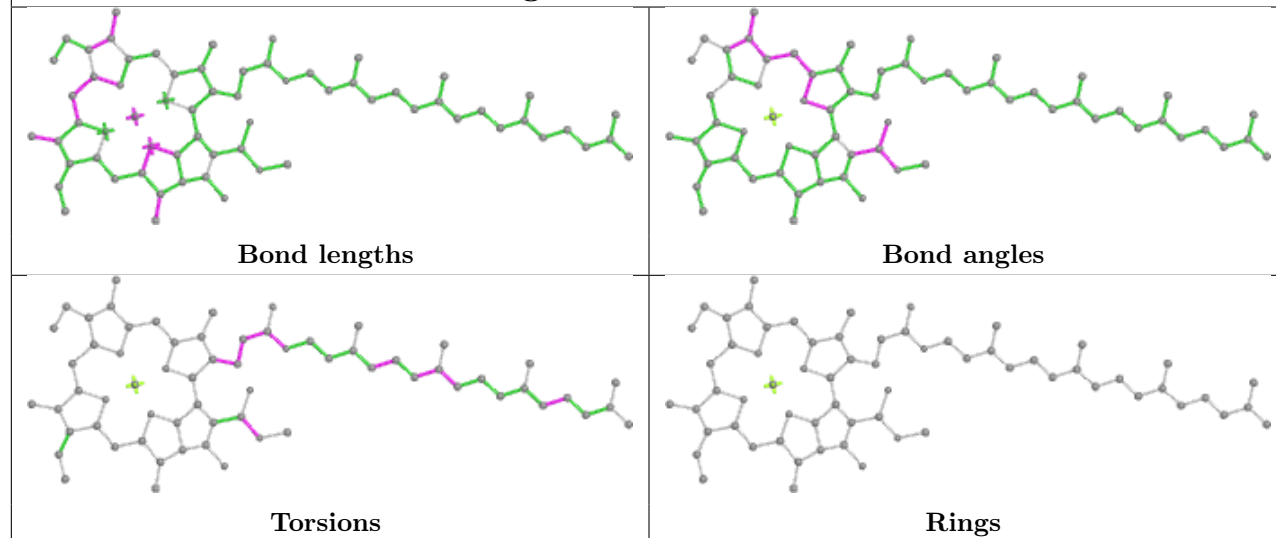


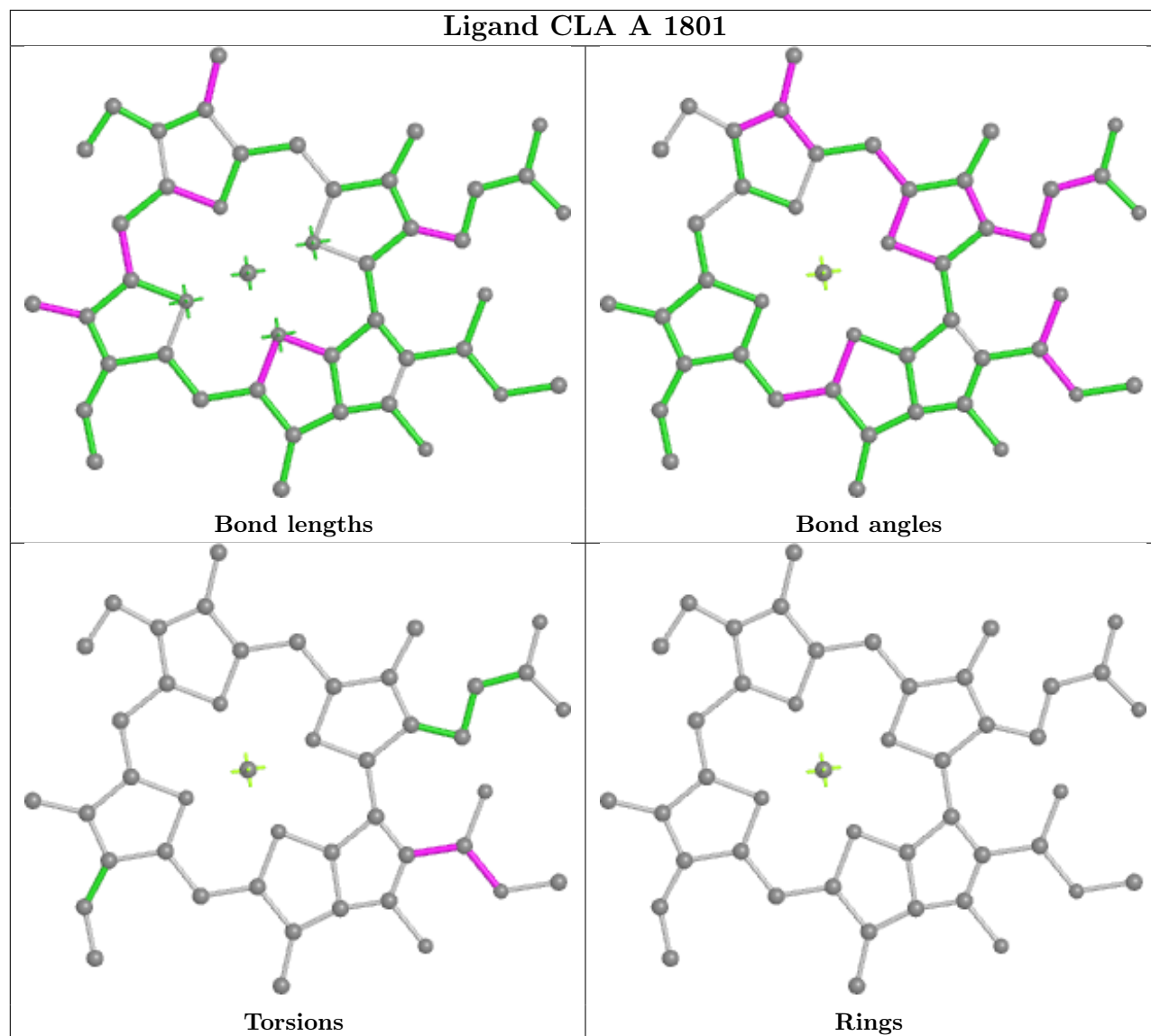
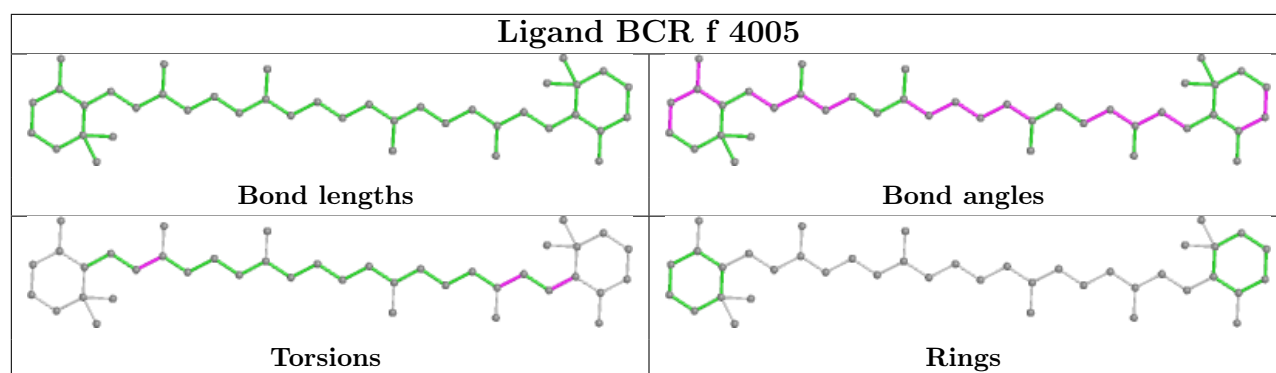
Torsions

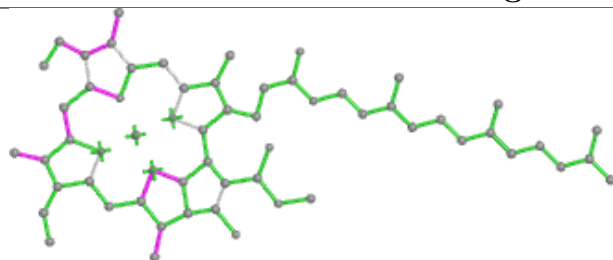


Rings

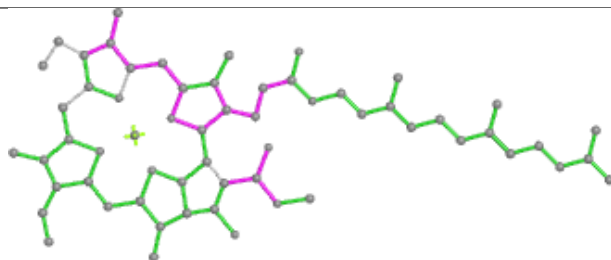


Ligand CLA H 1239**Ligand BCR s 522****Ligand CLA H 1206**

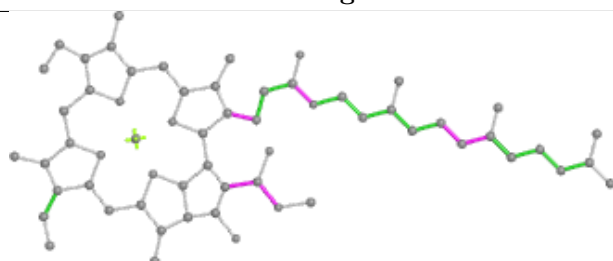


Ligand CLA H 1230

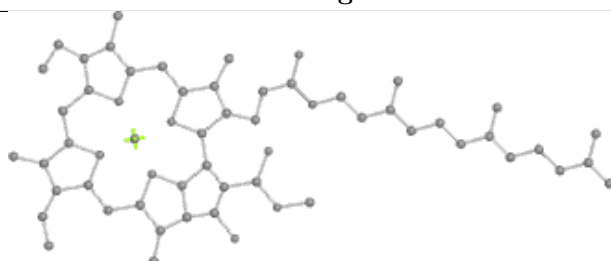
Bond lengths



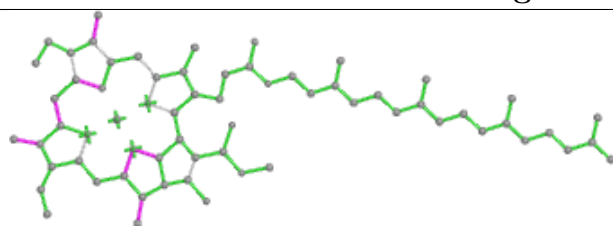
Bond angles



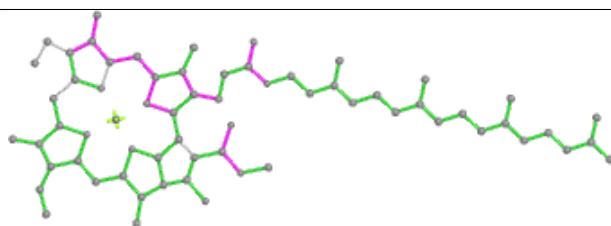
Torsions



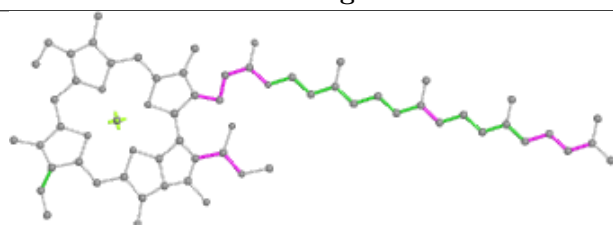
Rings

Ligand CLA Y 501

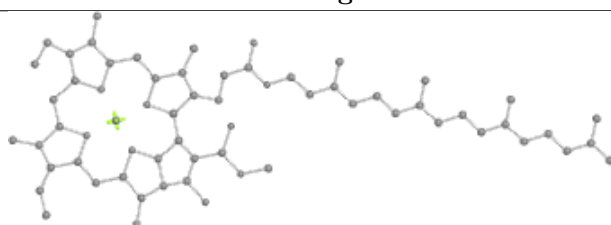
Bond lengths



Bond angles

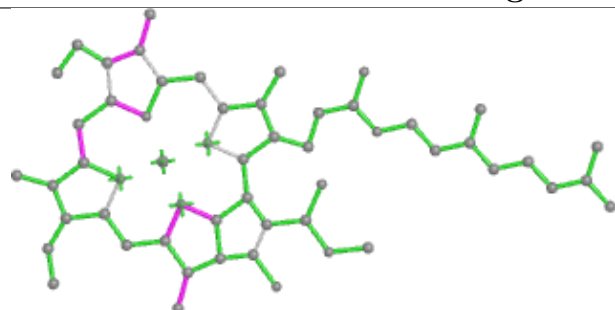


Torsions

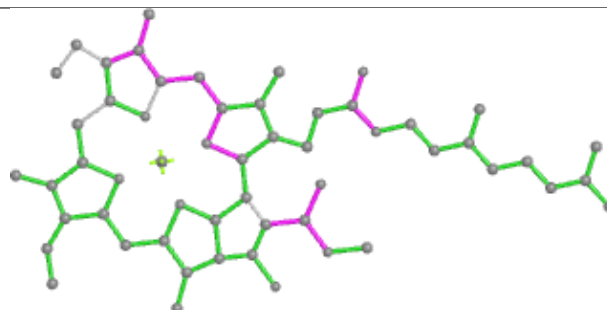


Rings

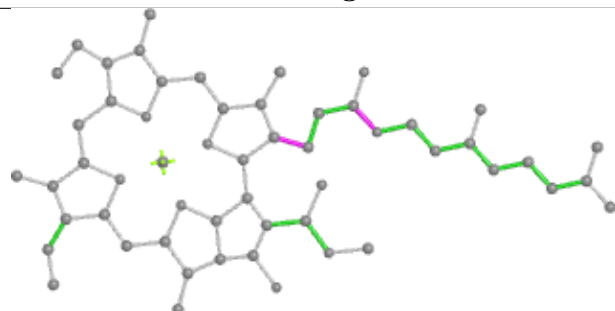
Ligand CLA H 1236



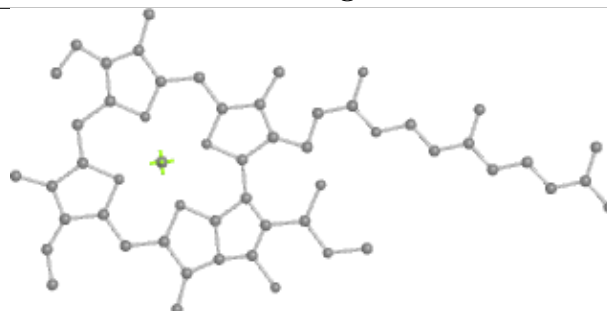
Bond lengths



Bond angles

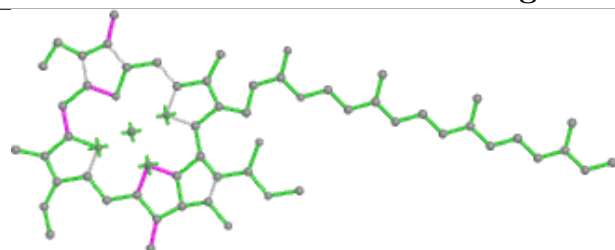


Torsions

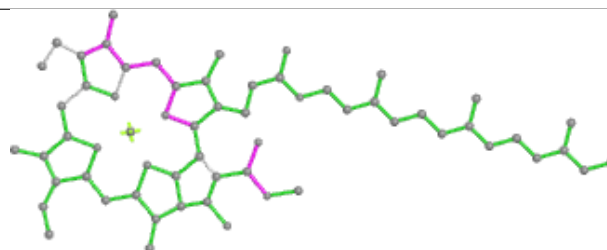


Rings

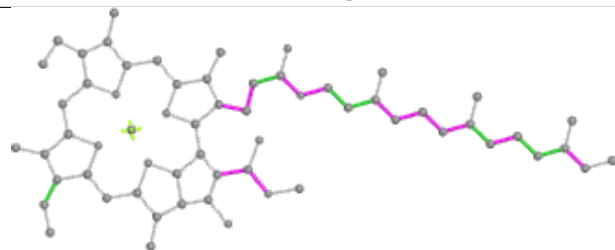
Ligand CLA u 505



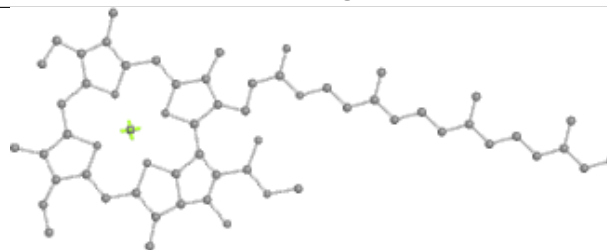
Bond lengths



Bond angles

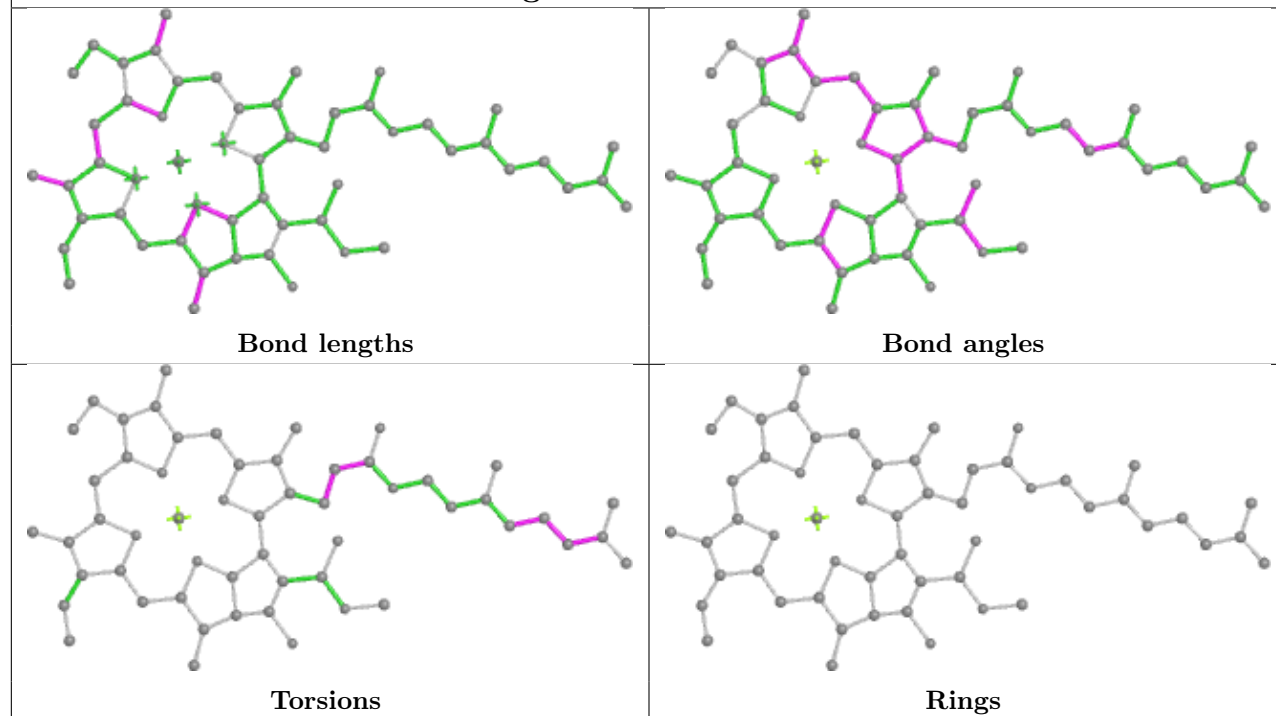


Torsions

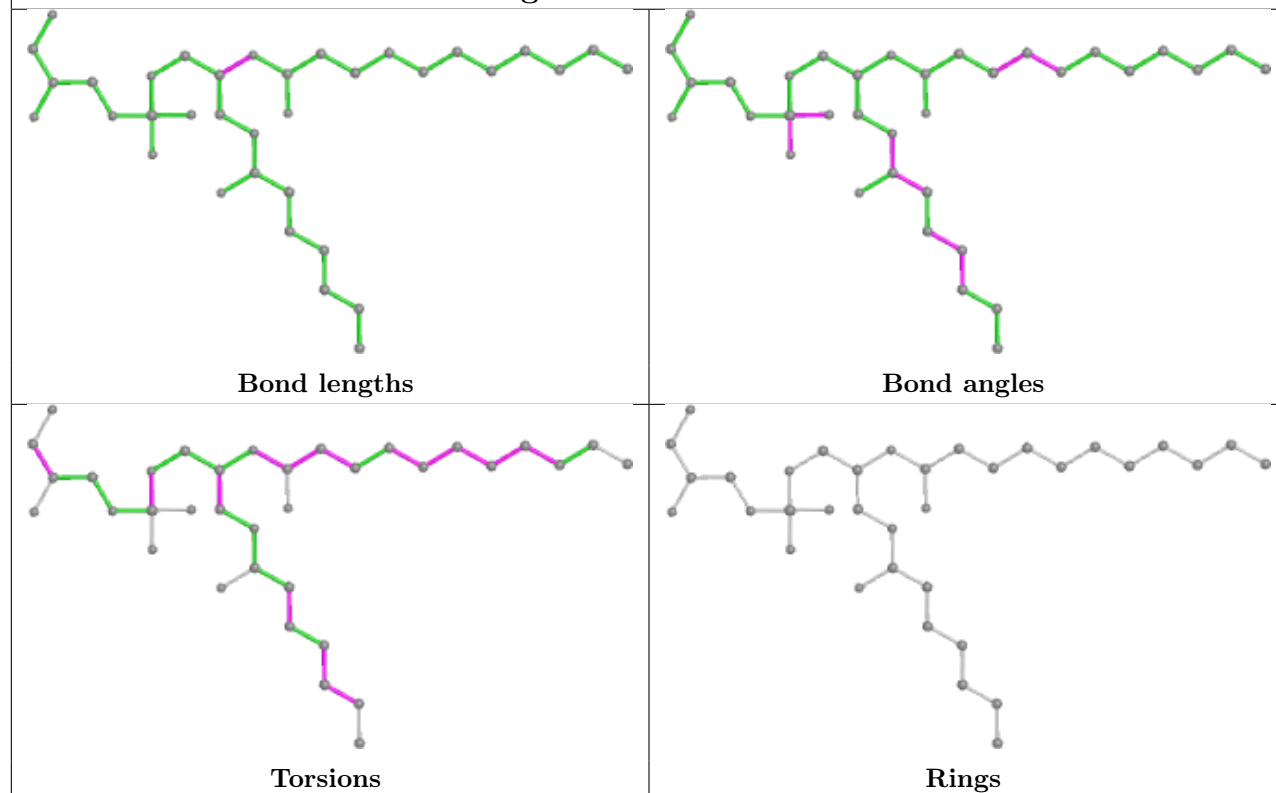


Rings

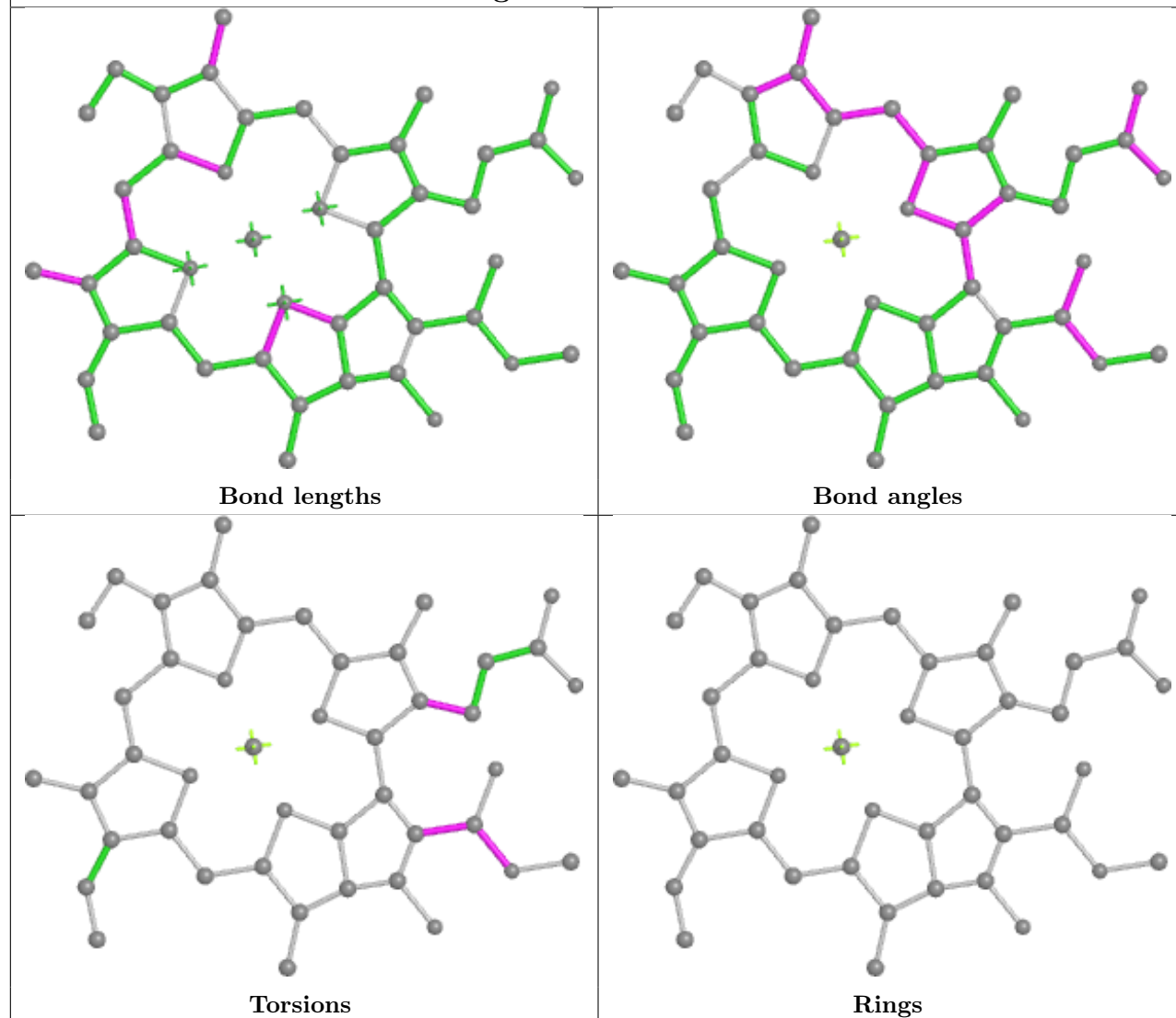
Ligand CLA A 1121



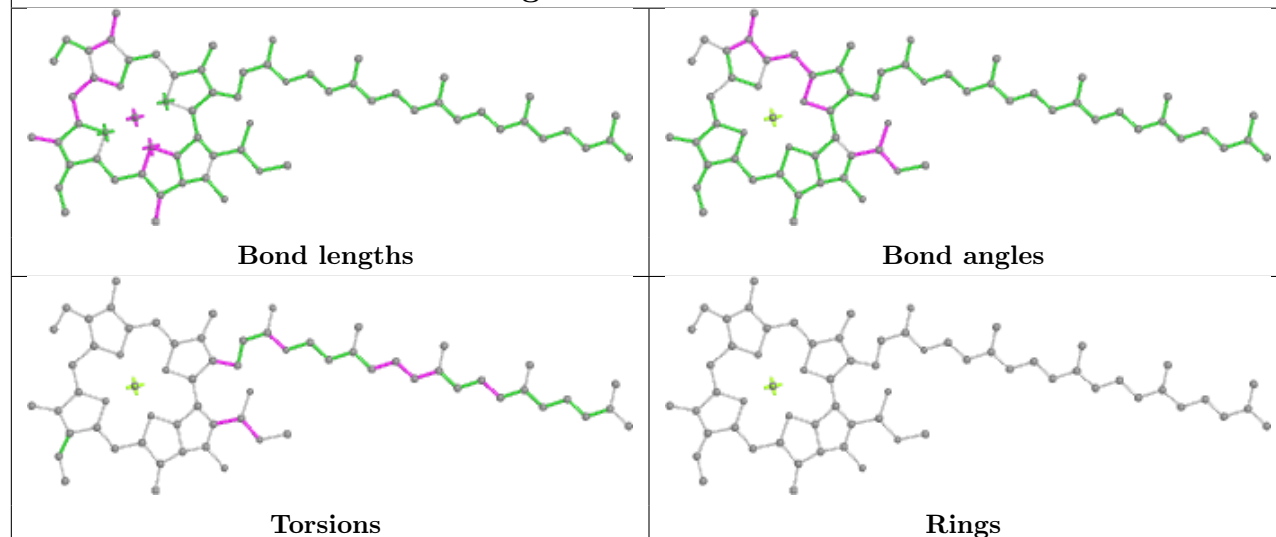
Ligand LHG A 5008

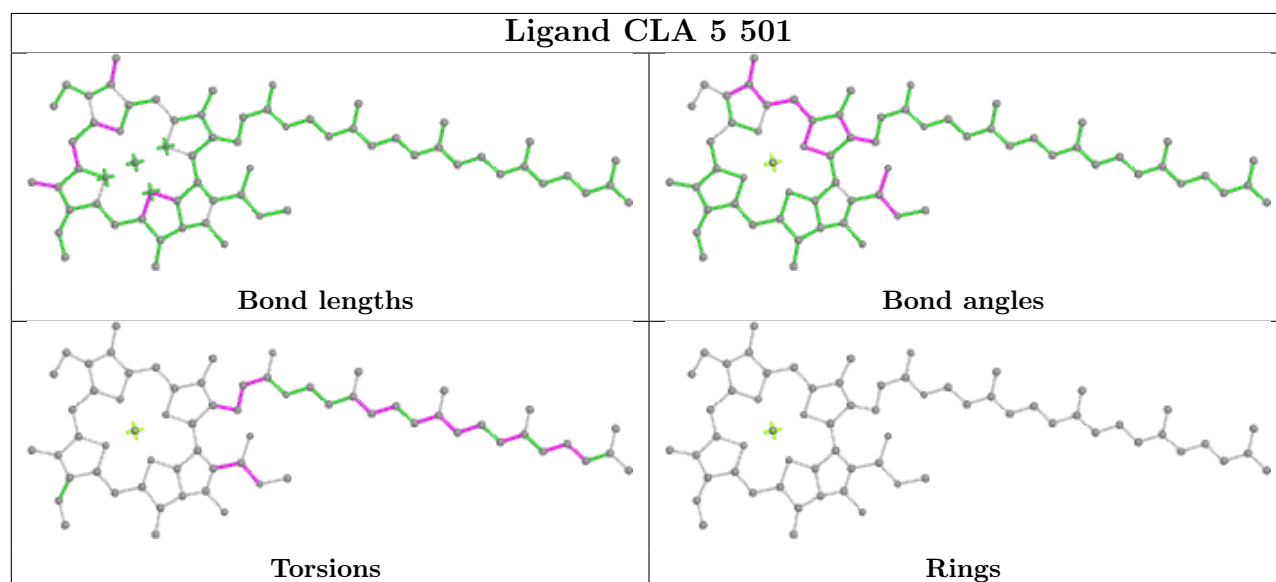
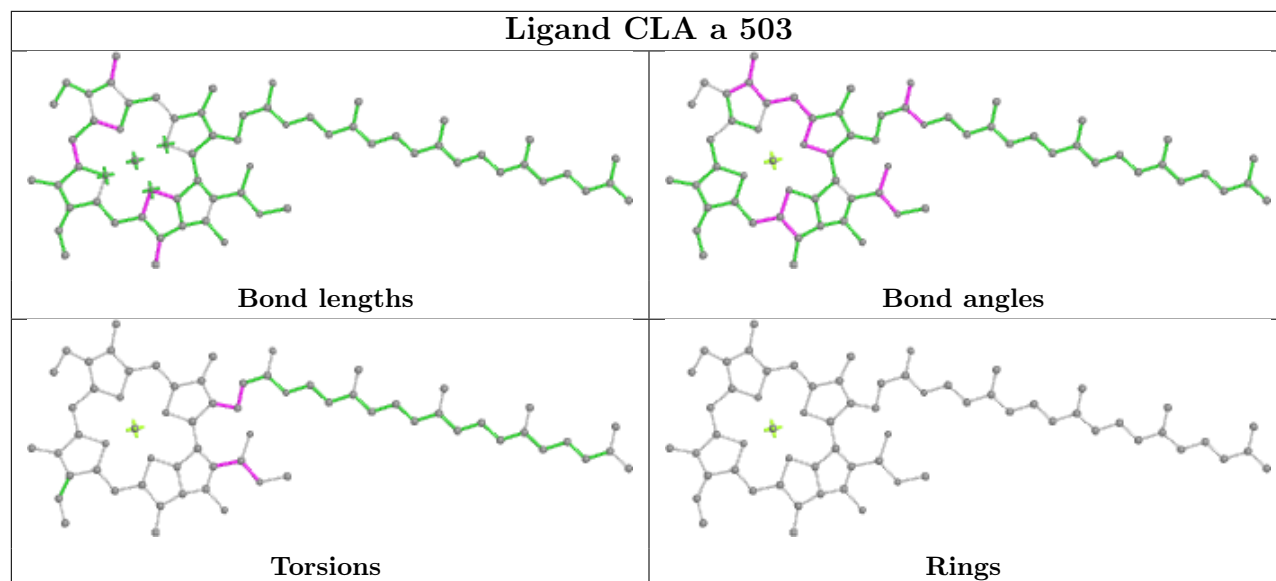
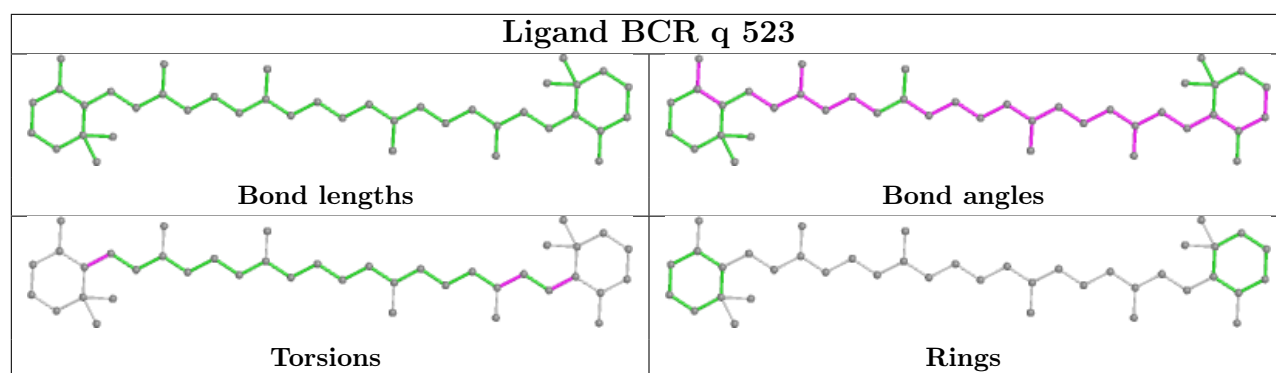


Ligand CLA b 517

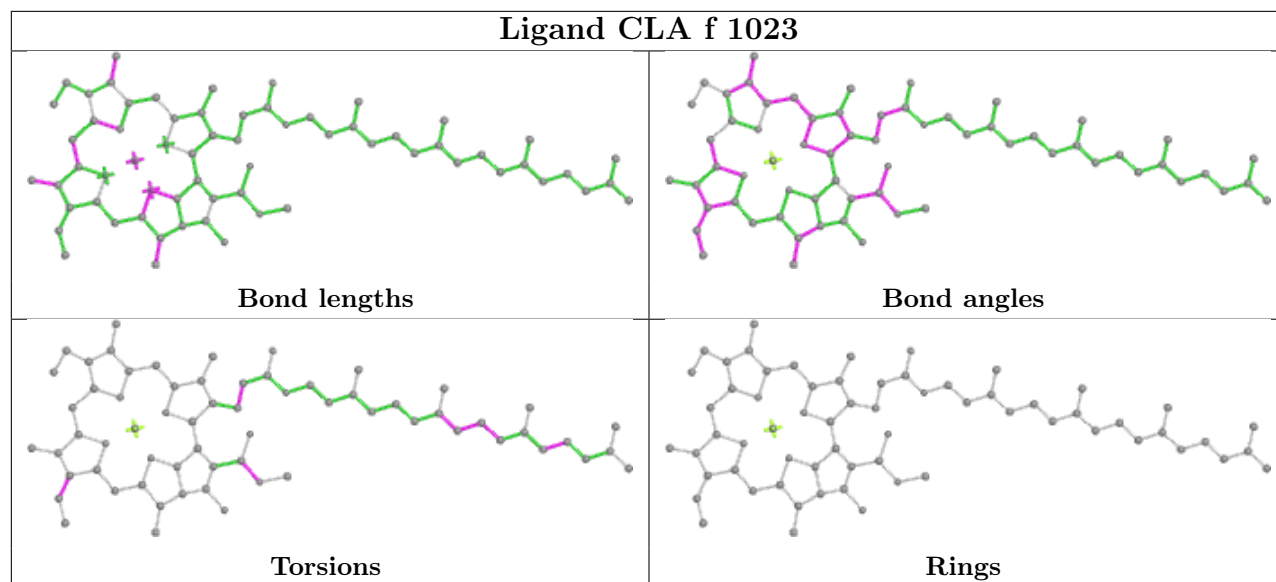


Ligand CLA G 1128

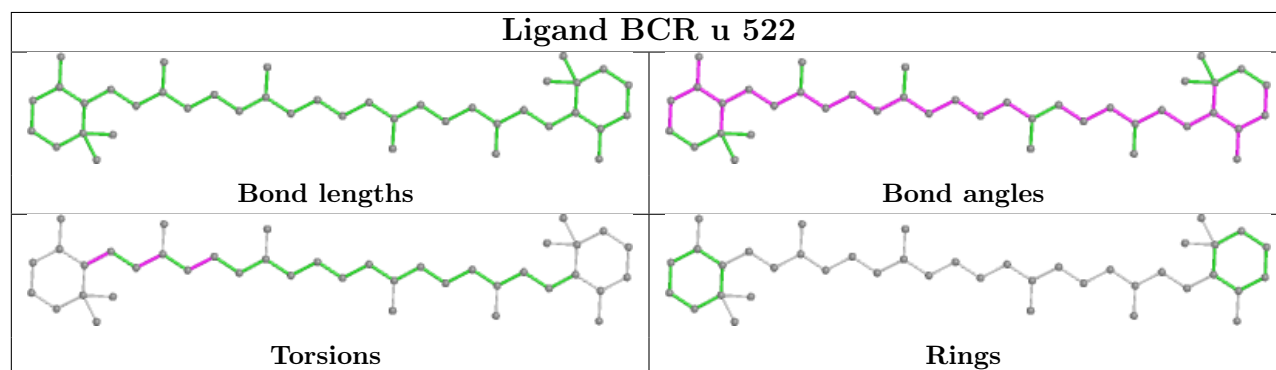




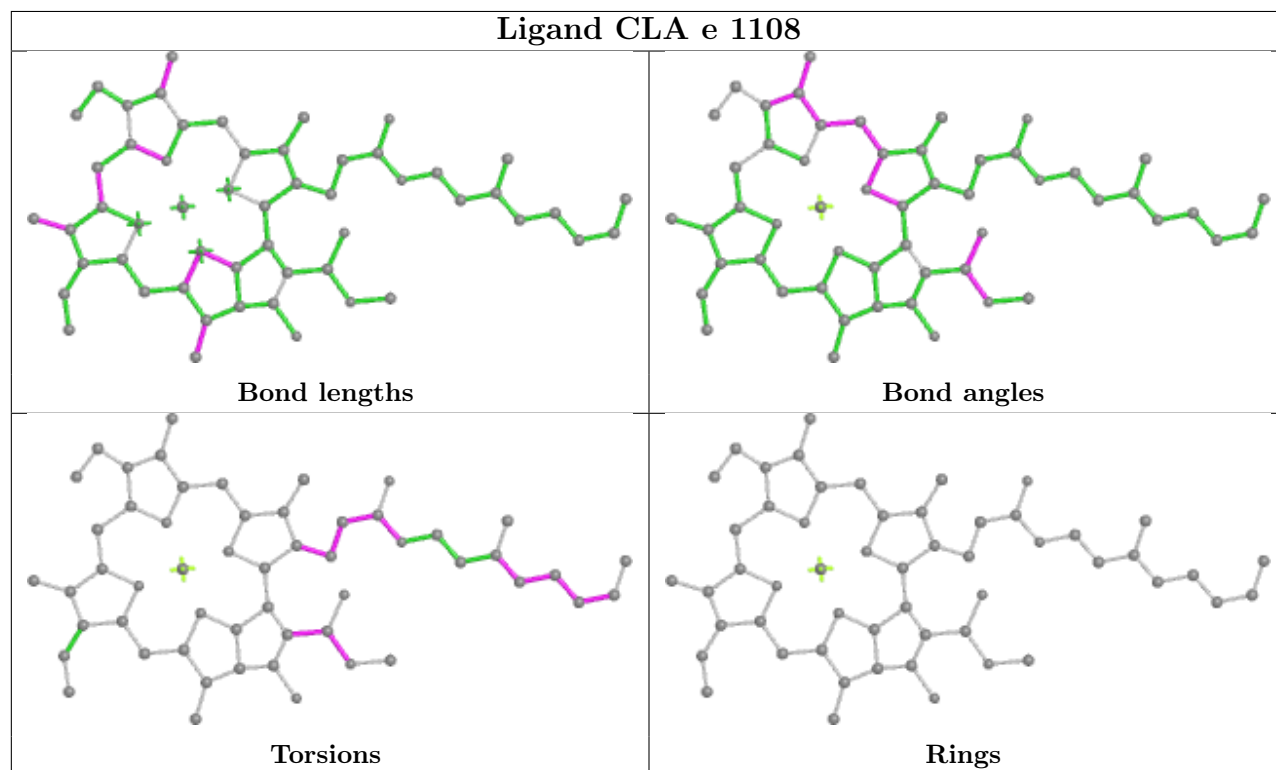
Ligand CLA f 1023

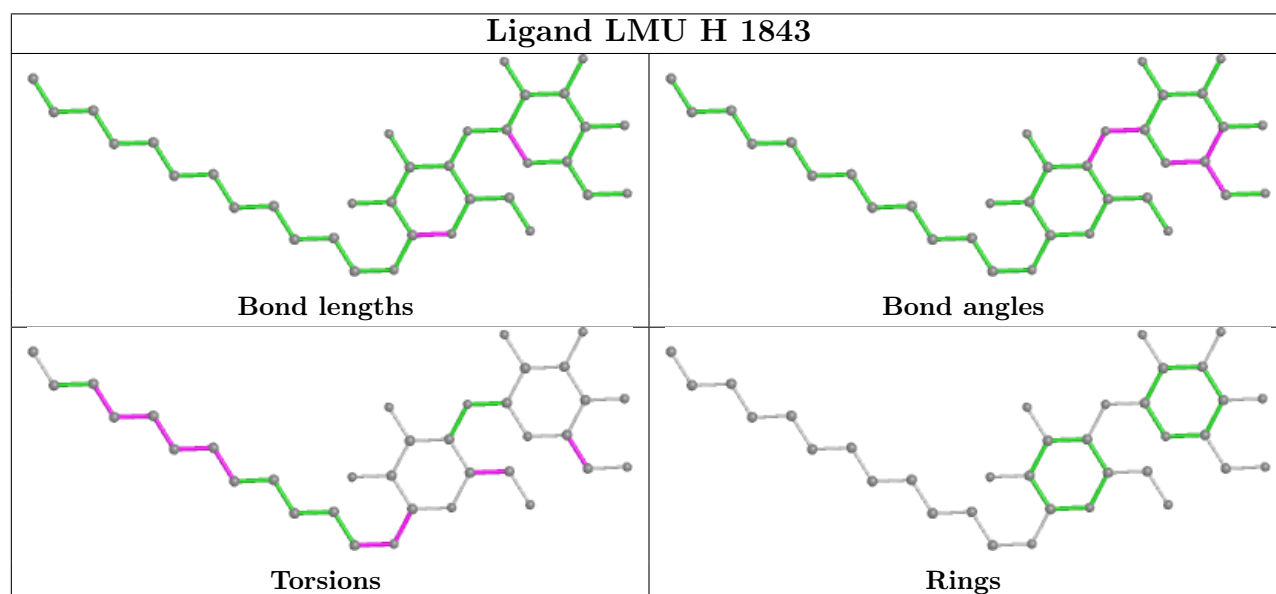
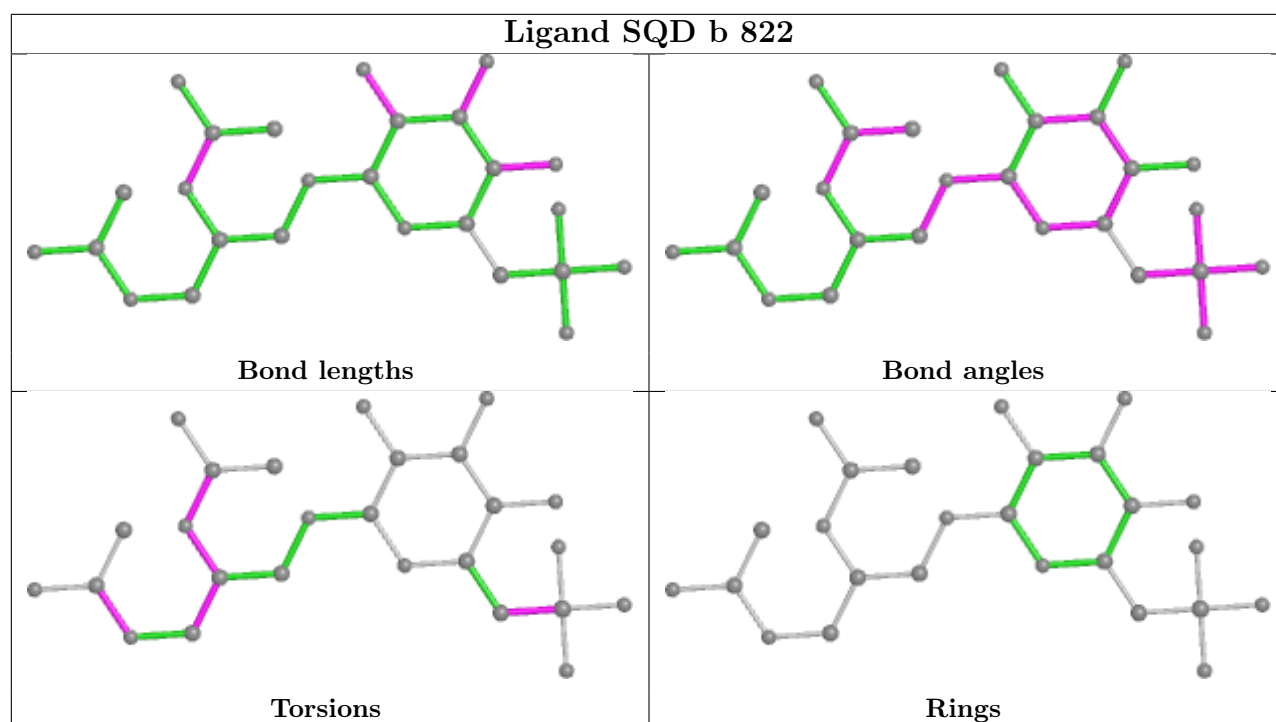


Ligand BCR u 522

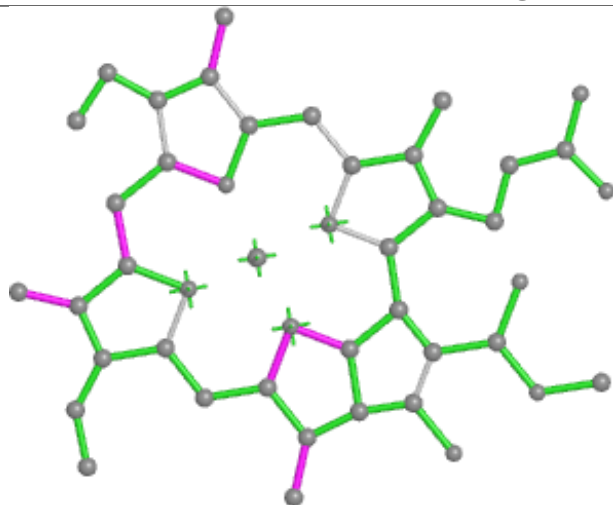


Ligand CLA e 1108

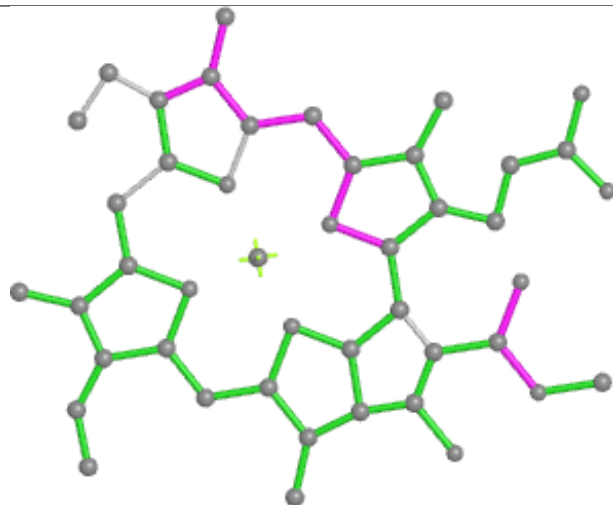




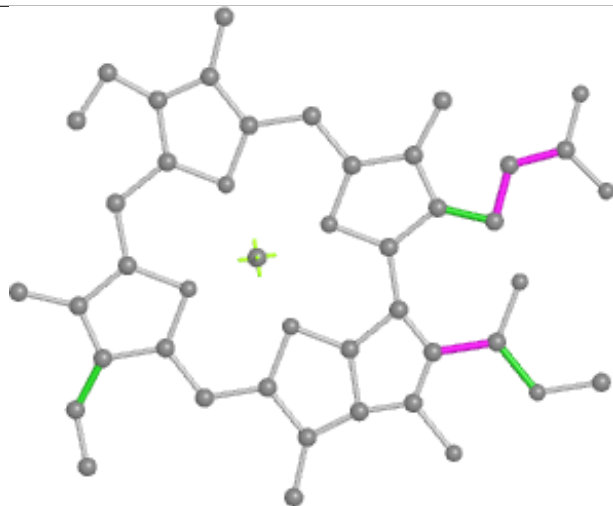
Ligand CLA Y 517



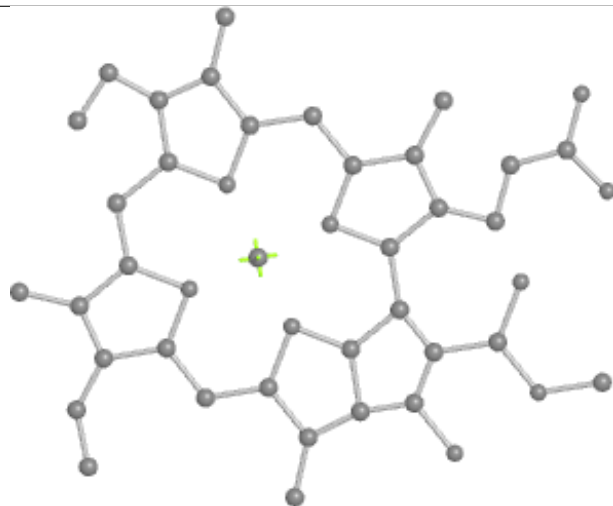
Bond lengths



Bond angles

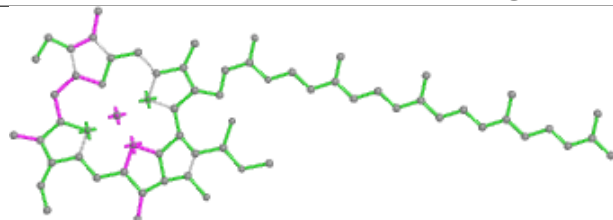


Torsions

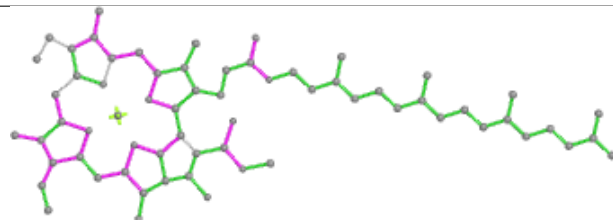


Rings

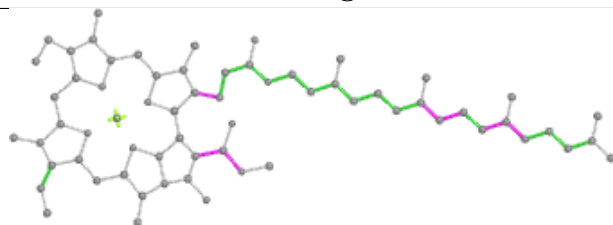
Ligand CLA B 1226



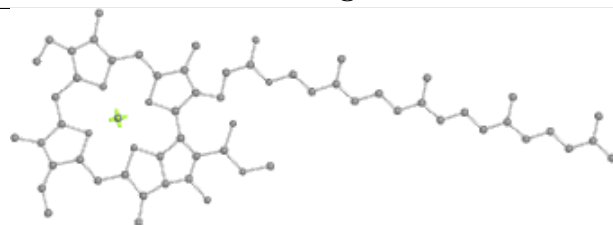
Bond lengths



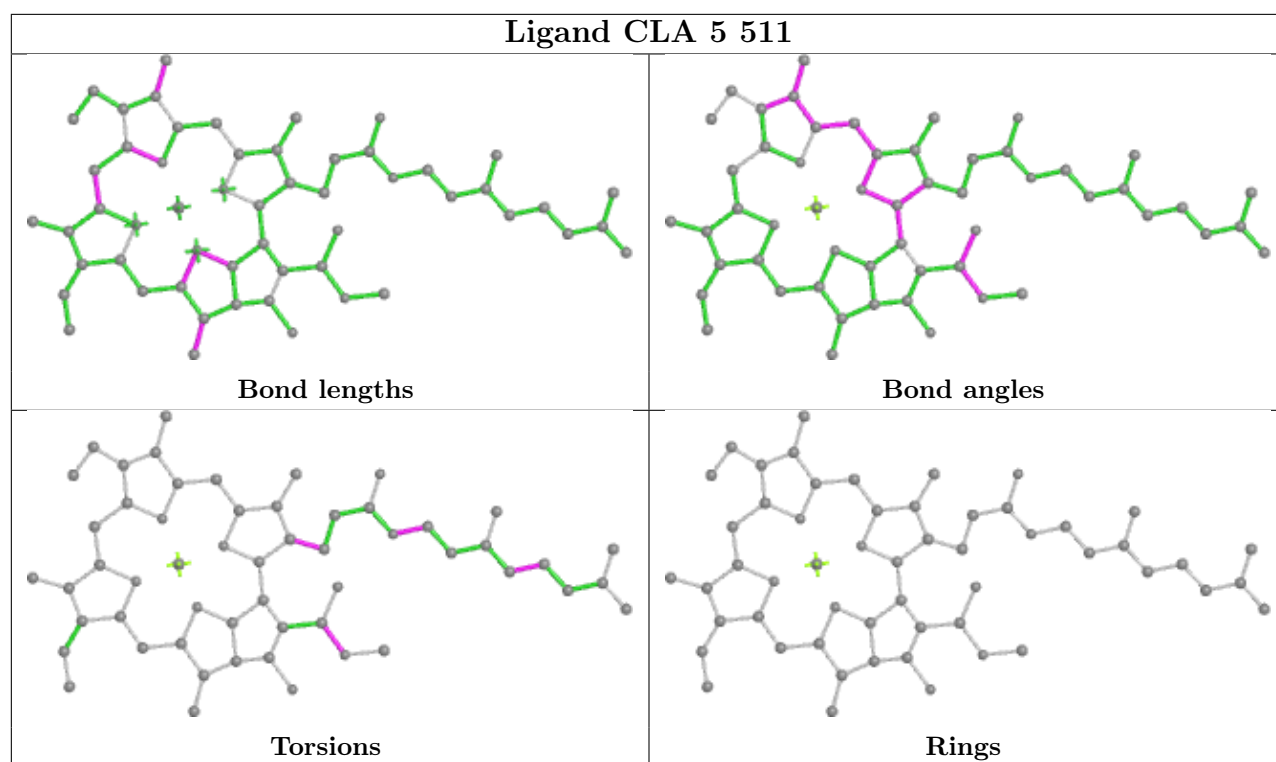
Bond angles



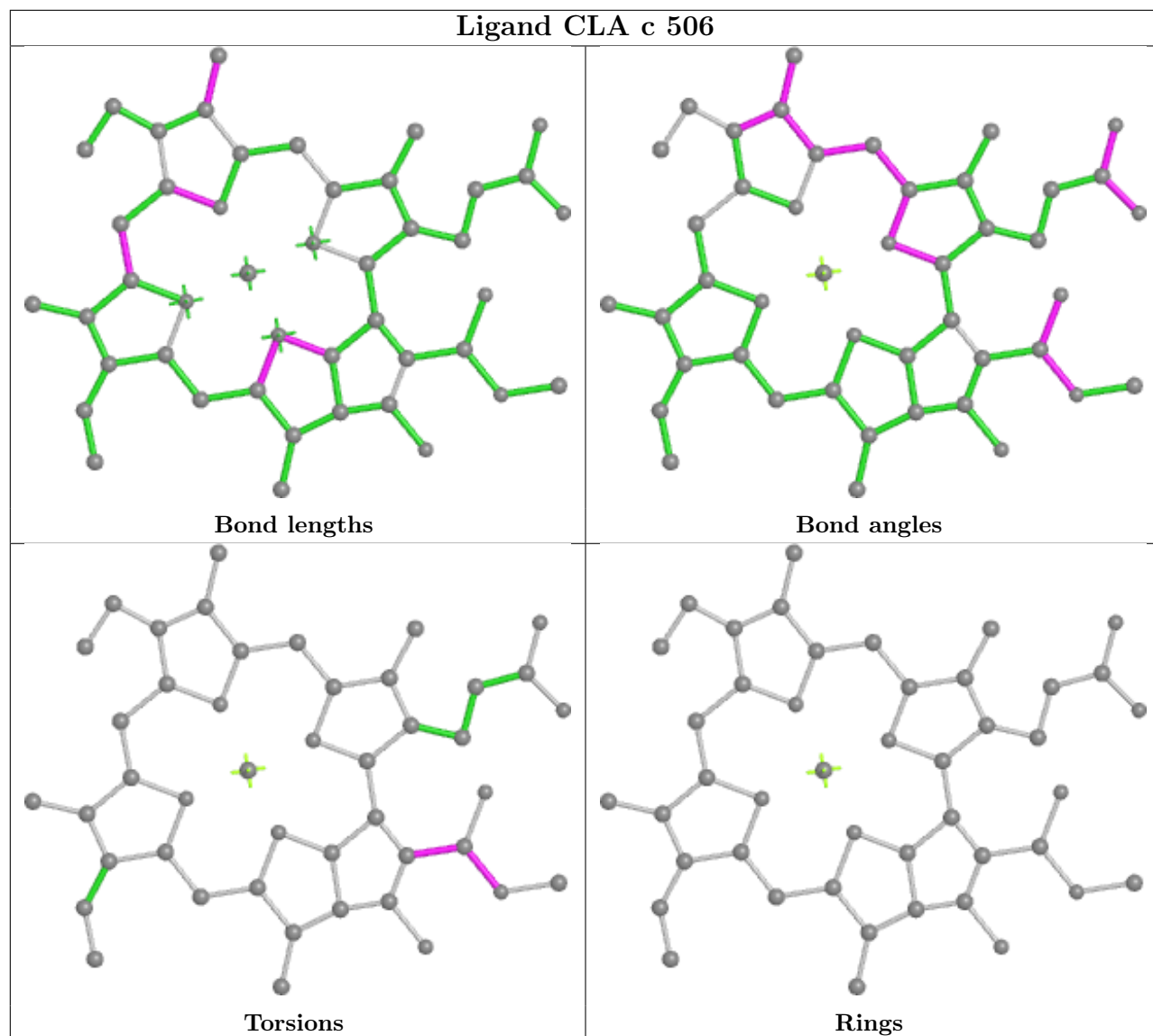
Torsions

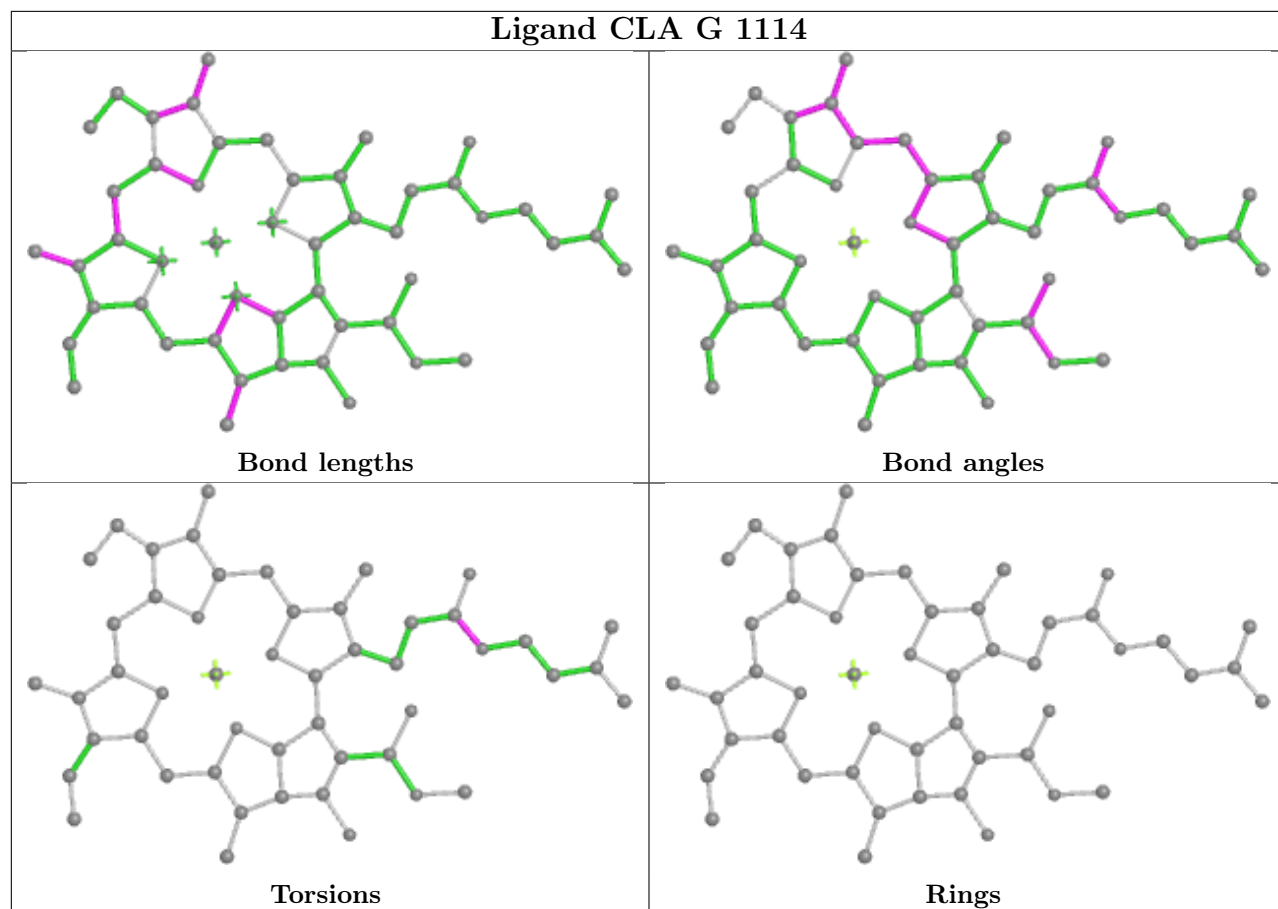


Rings

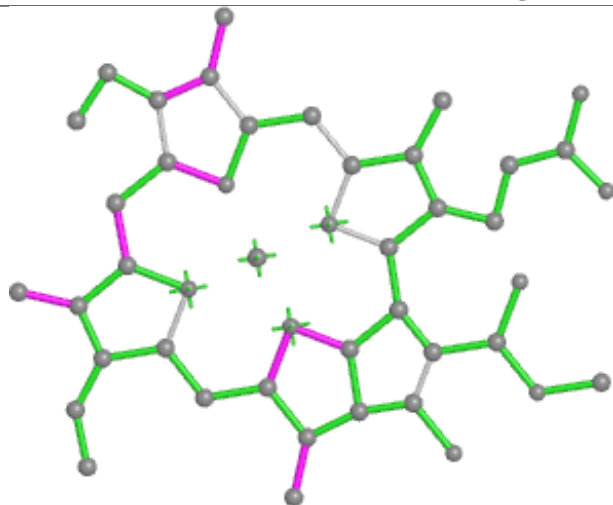


Ligand CLA c 506

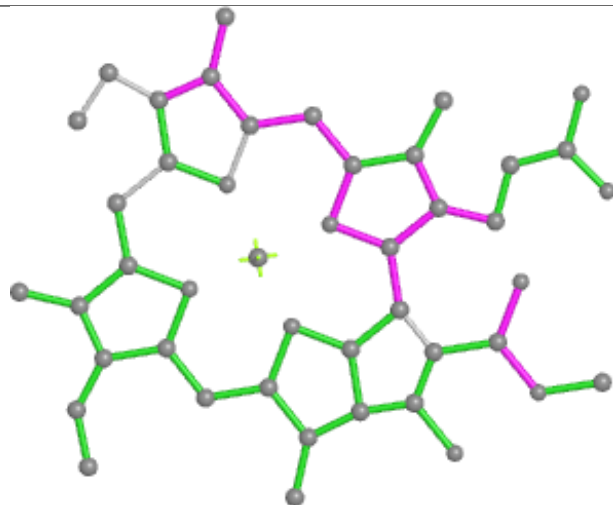




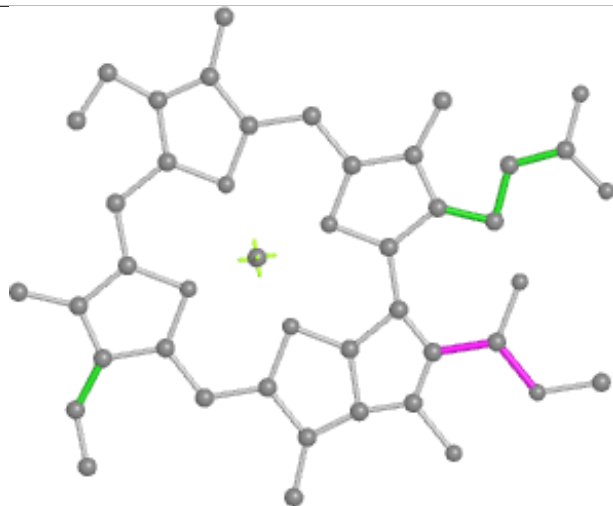
Ligand CLA Y 504



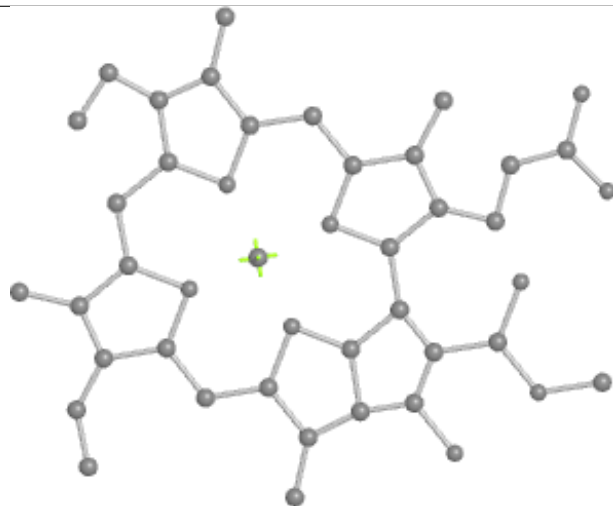
Bond lengths



Bond angles

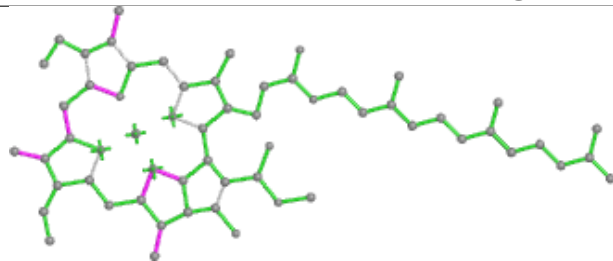


Torsions

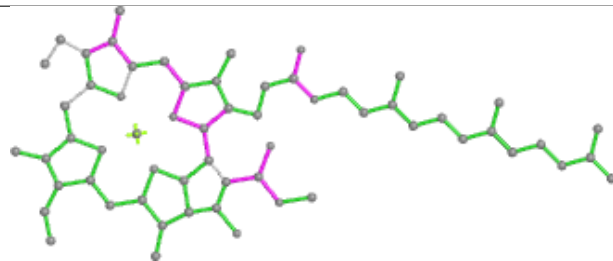


Rings

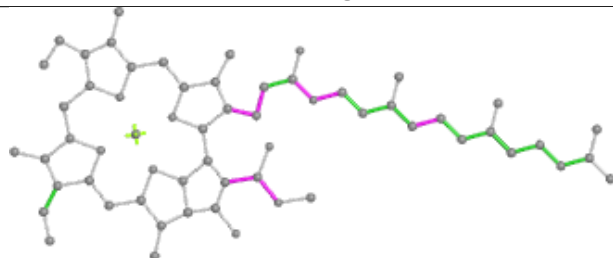
Ligand CLA e 1118



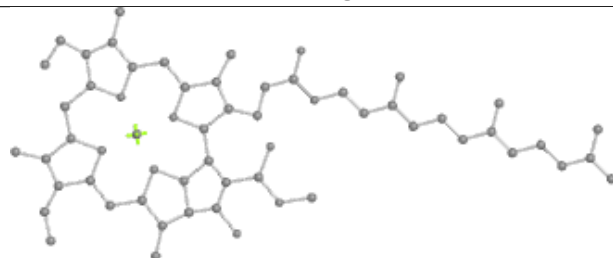
Bond lengths



Bond angles

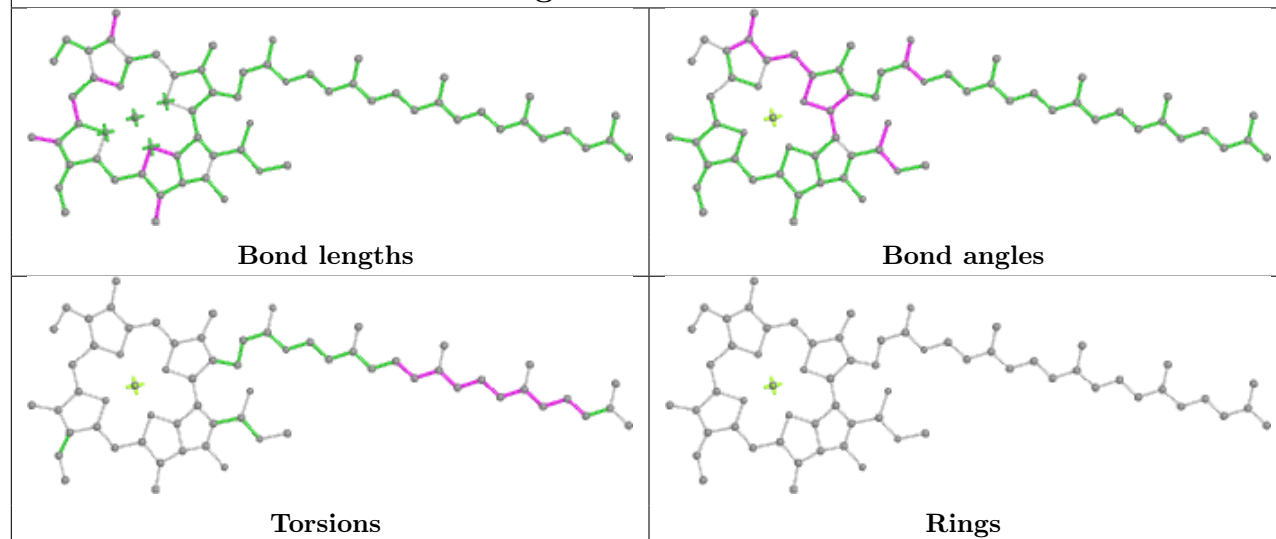


Torsions

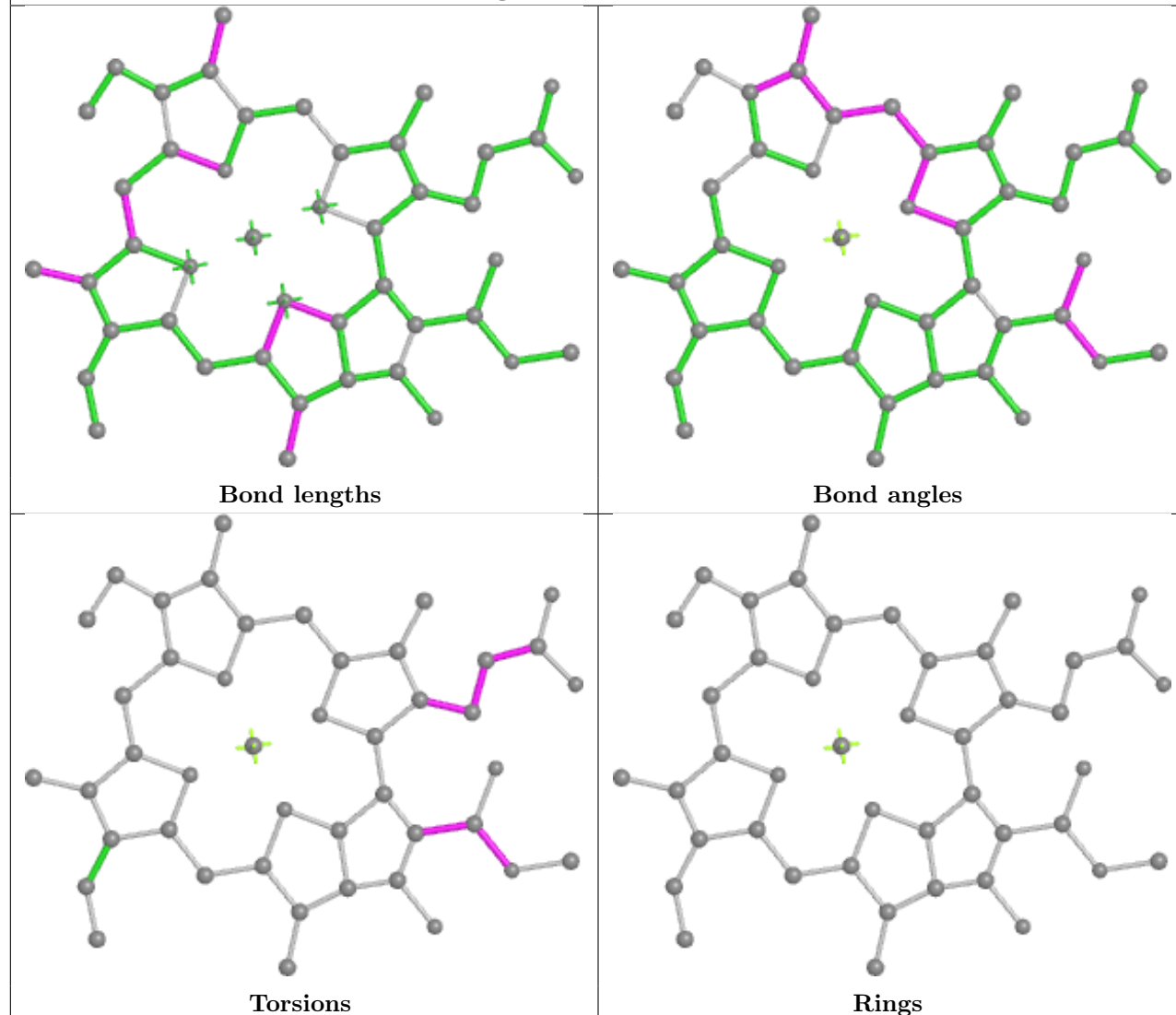


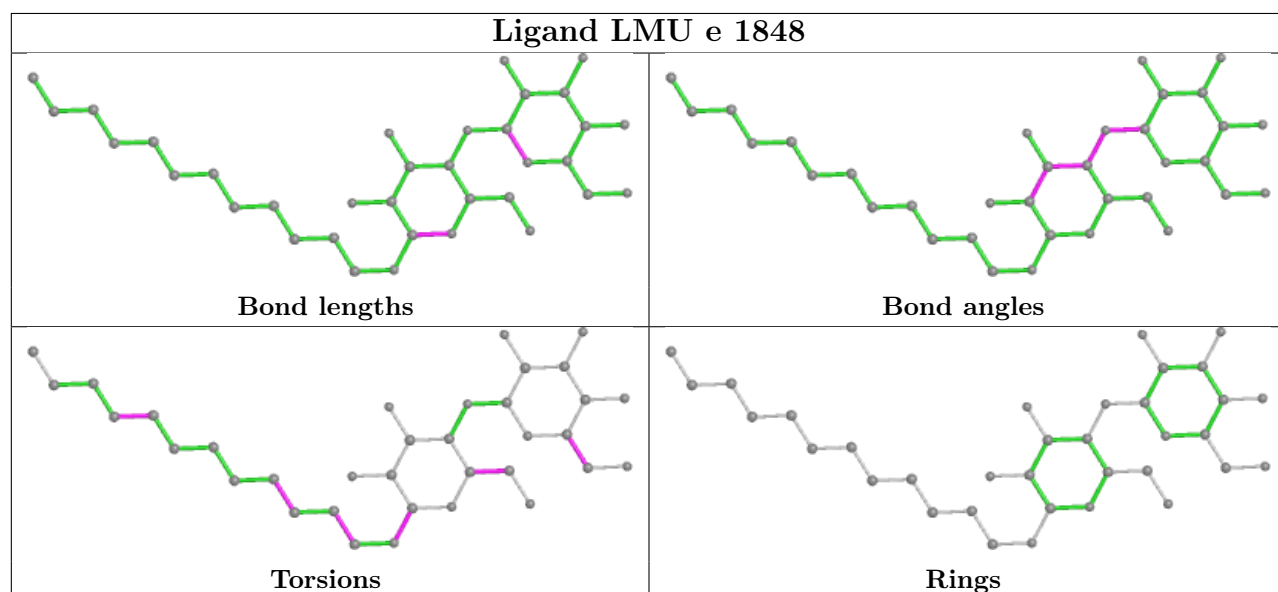
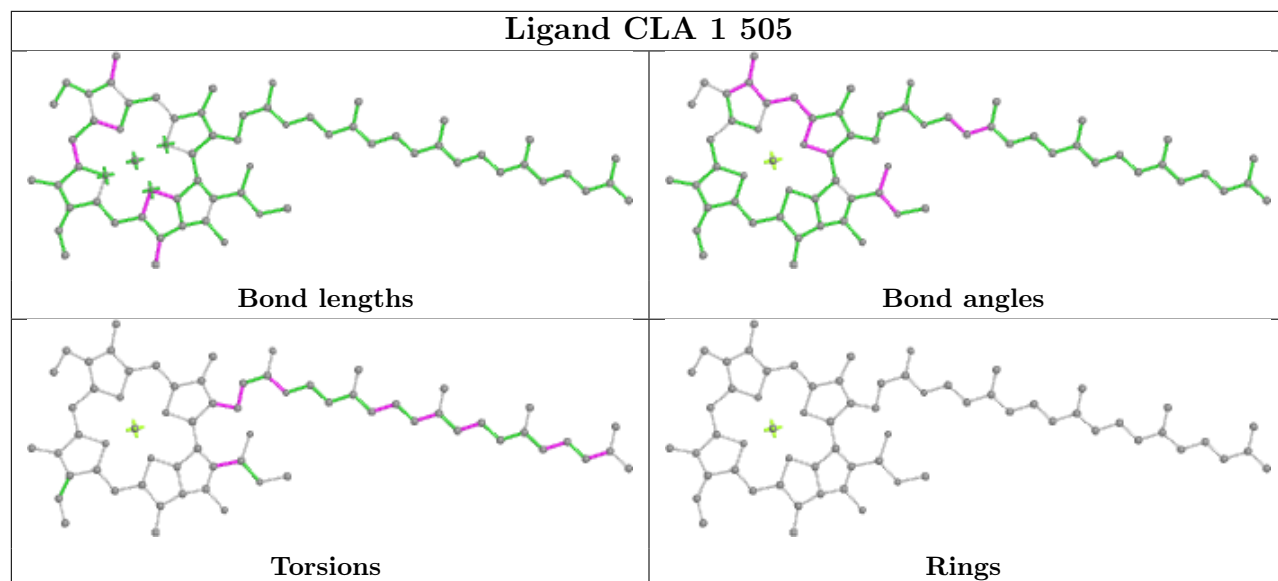
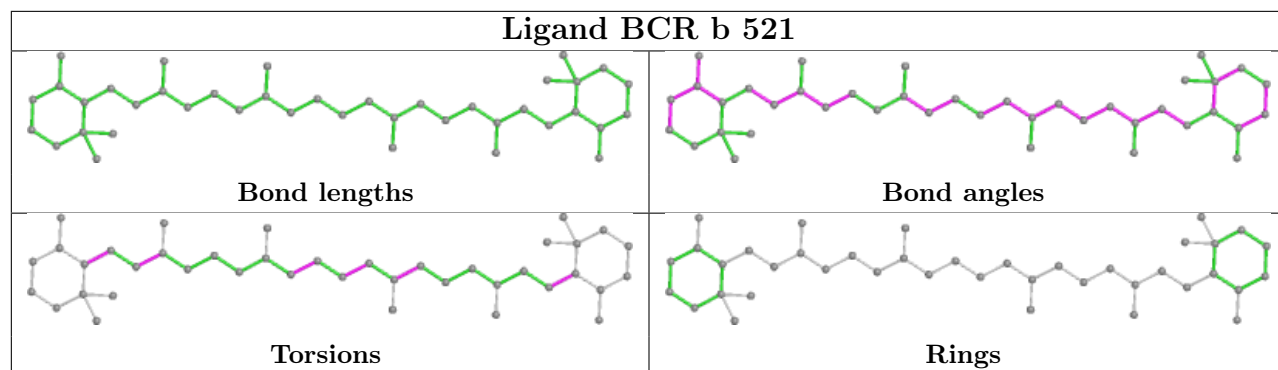
Rings

Ligand CLA u 509

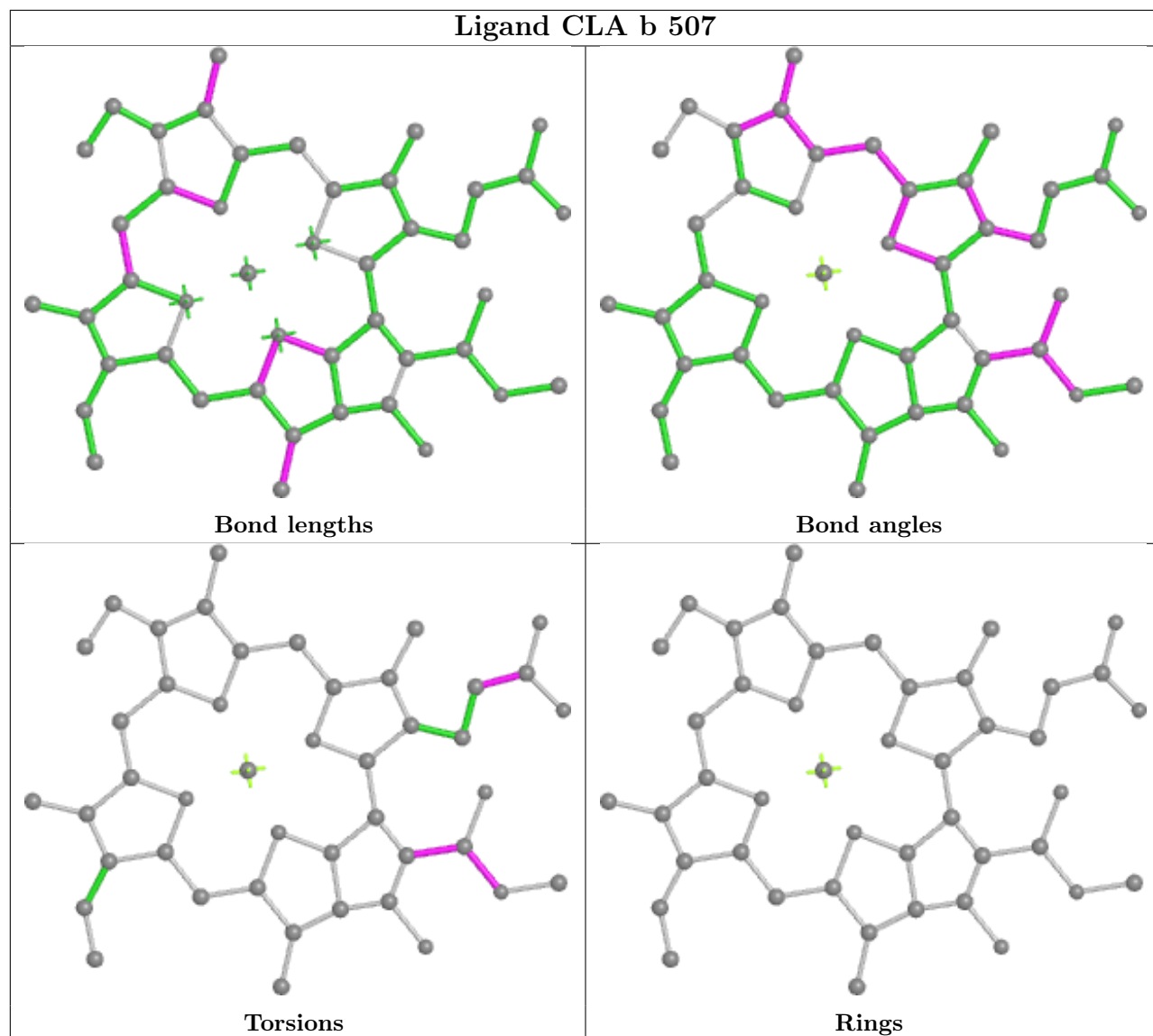


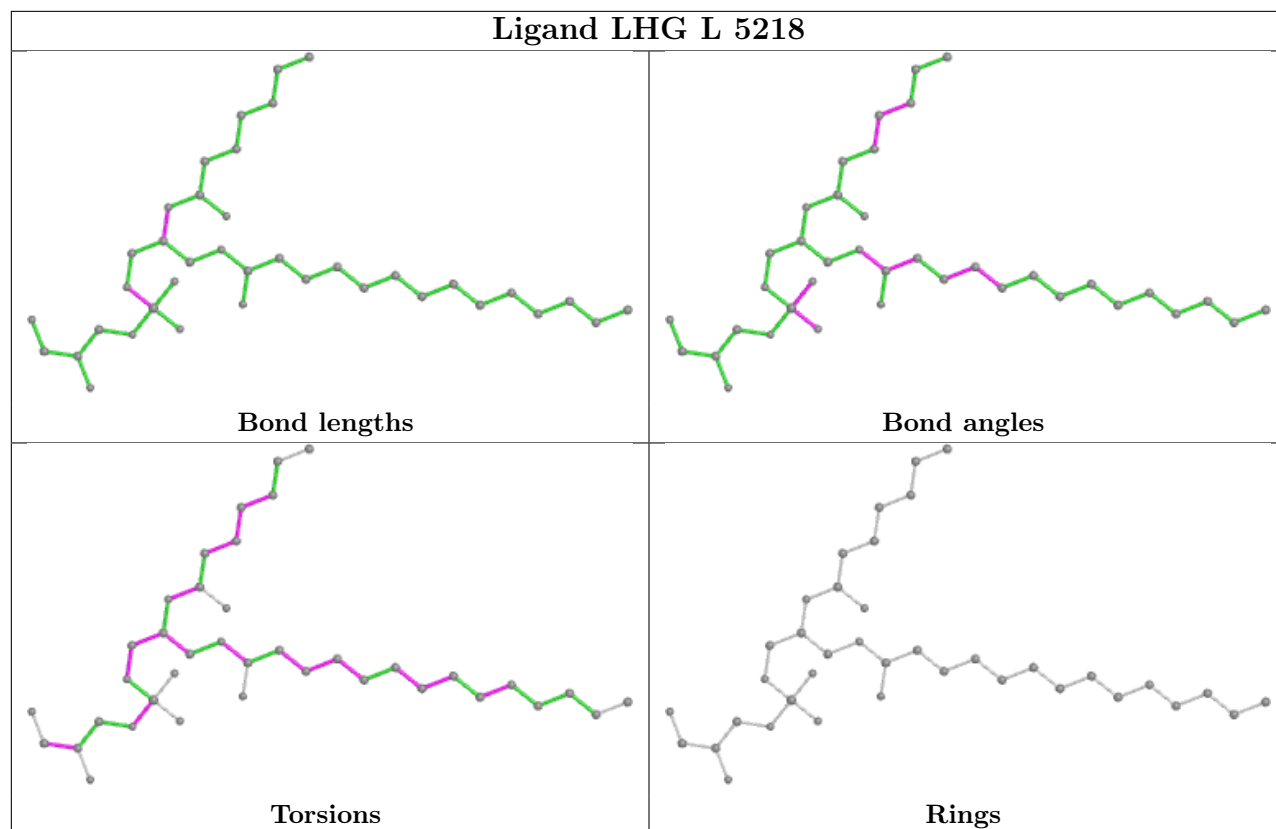
Ligand CLA 5 517

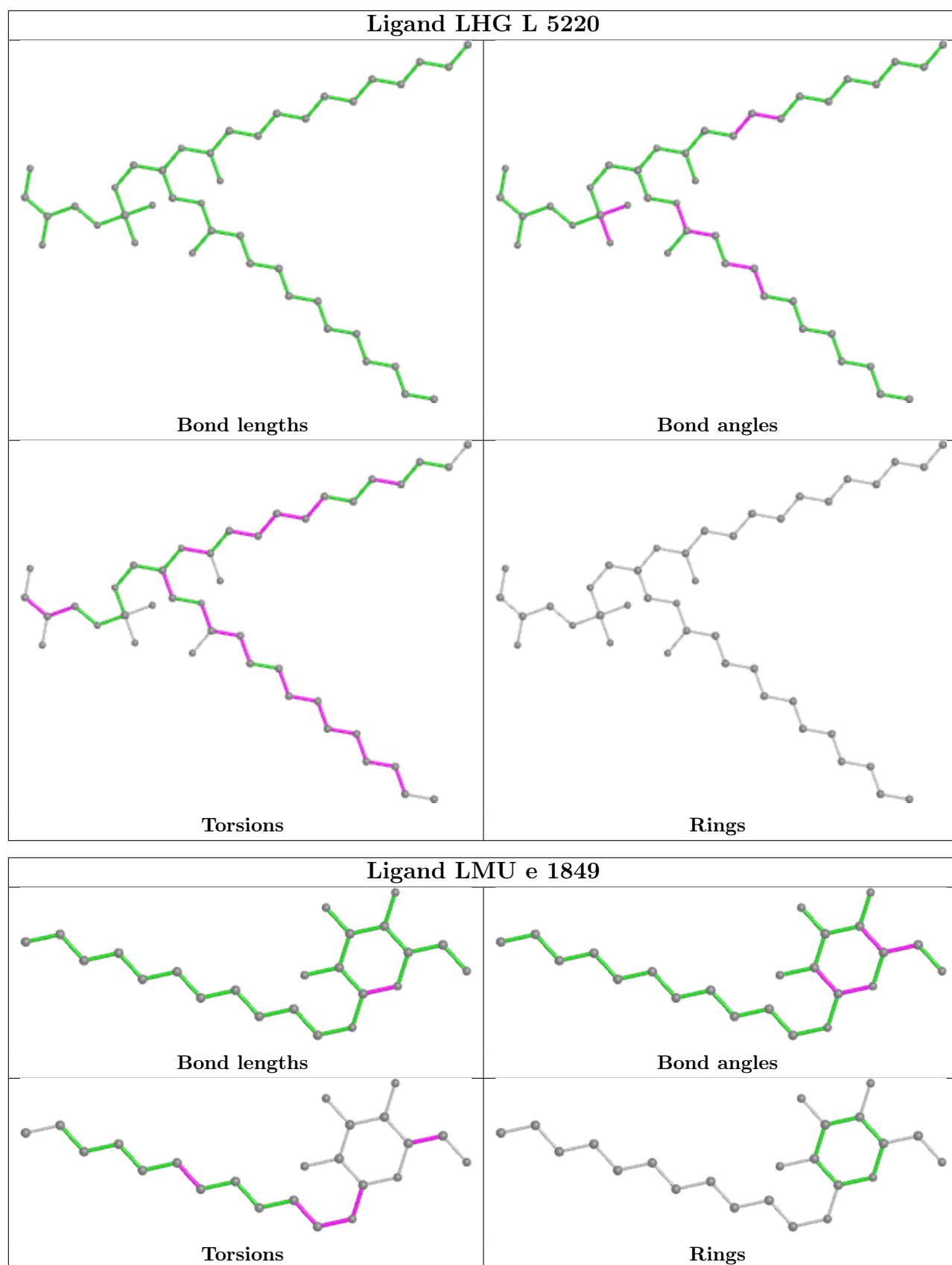




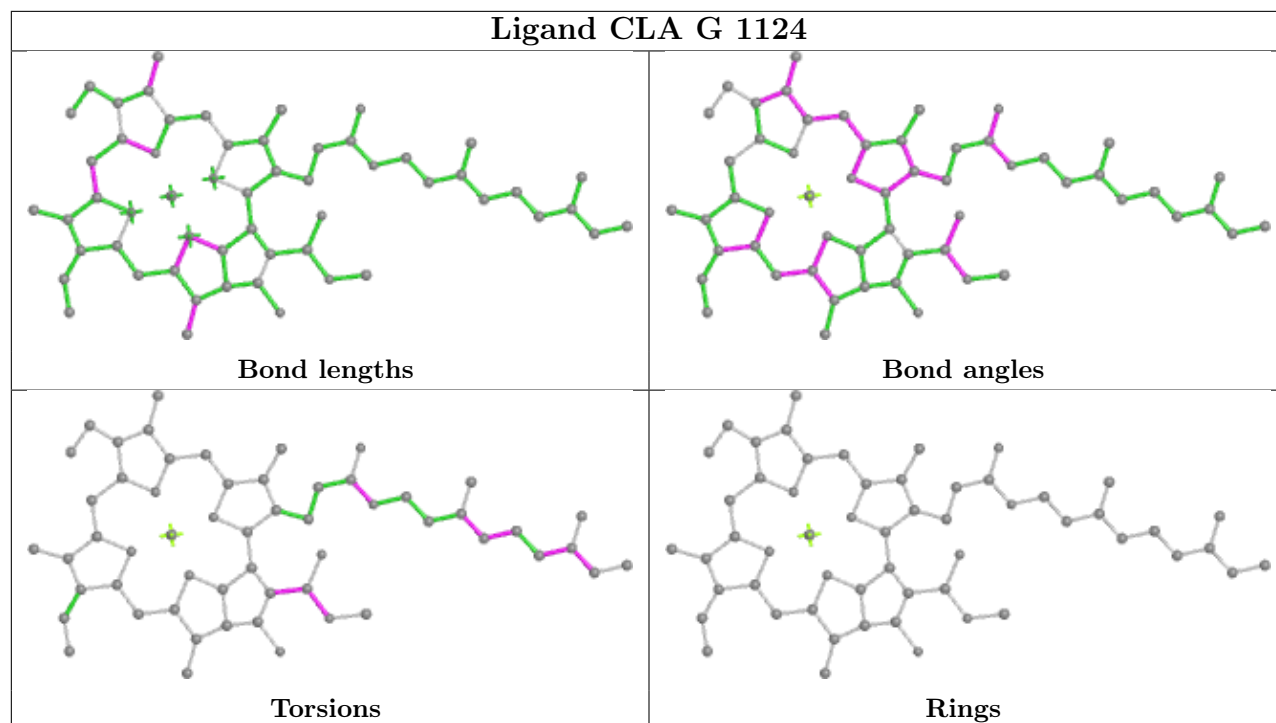
Ligand CLA b 507



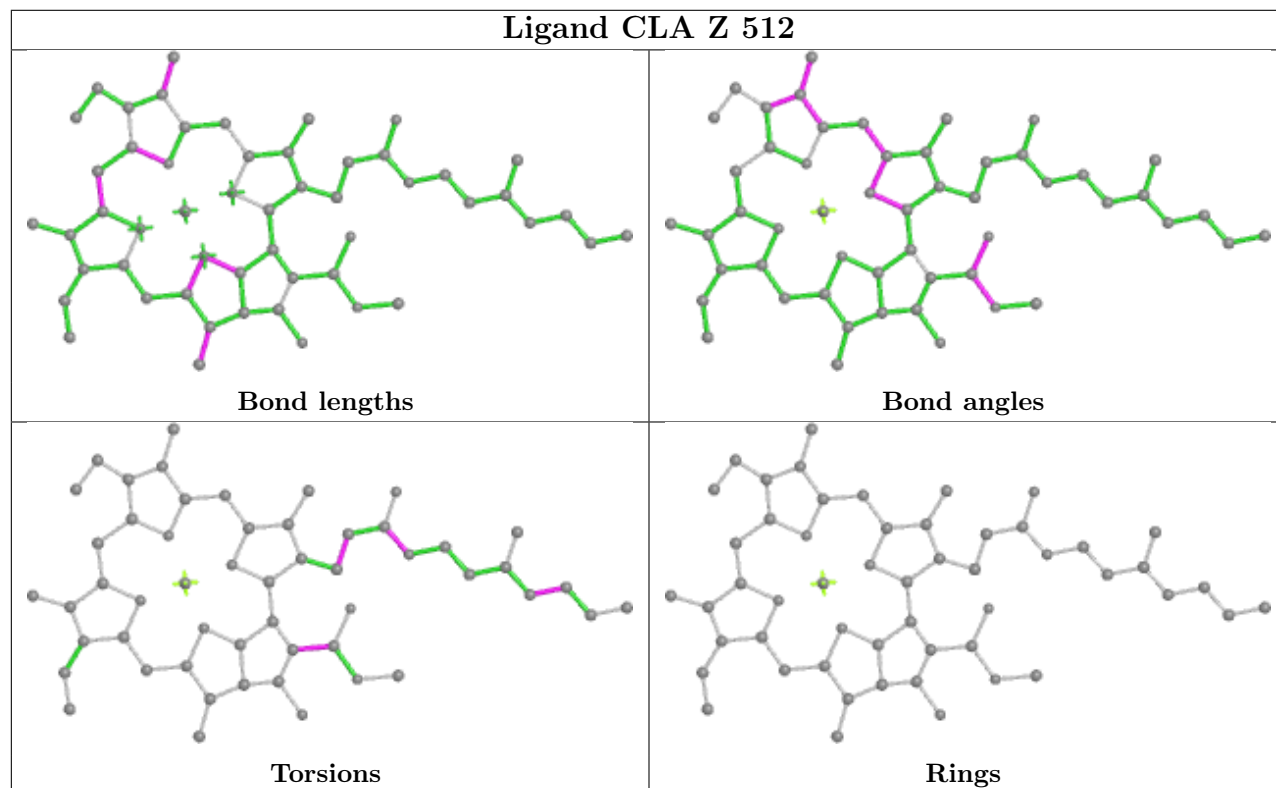


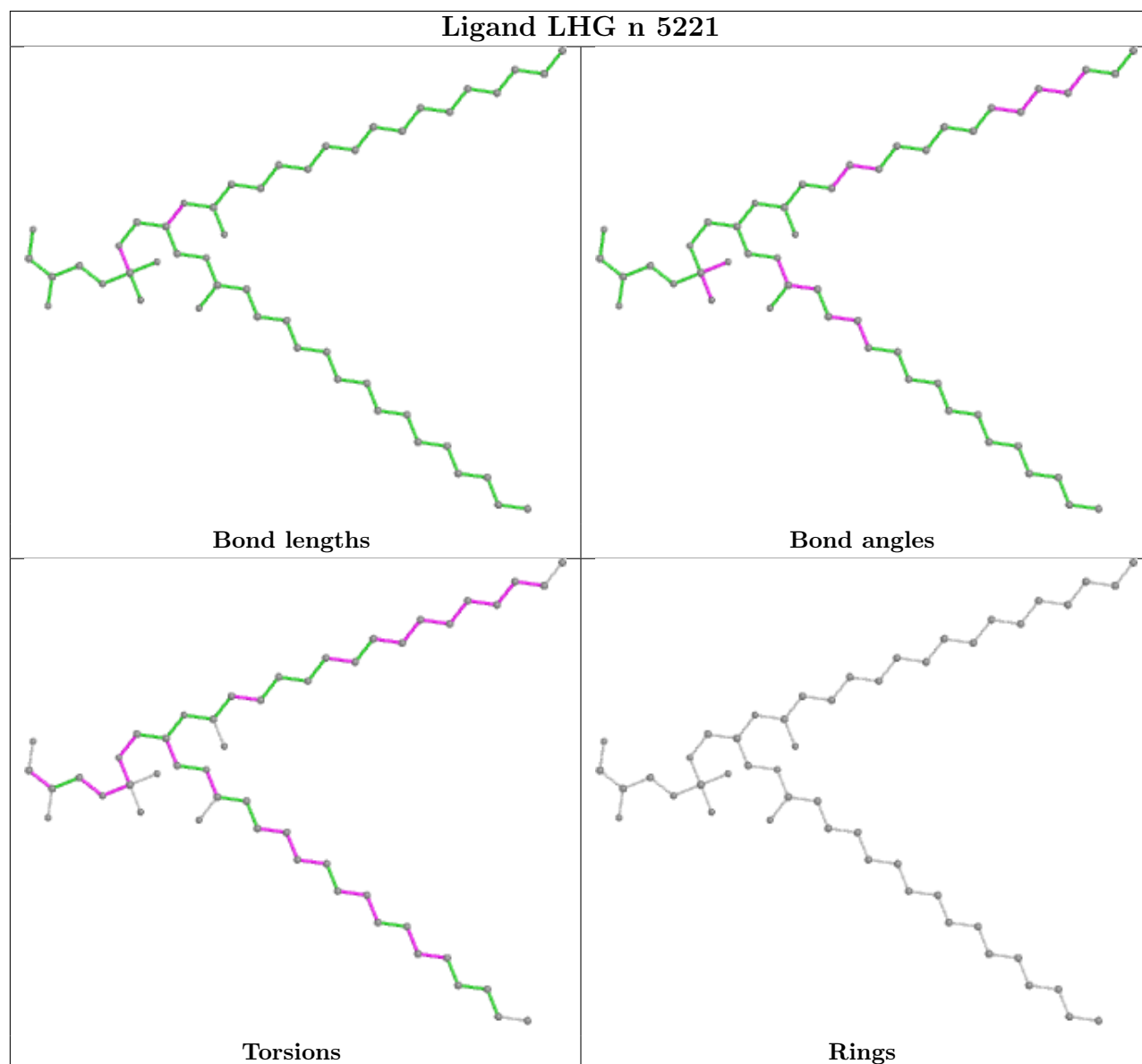
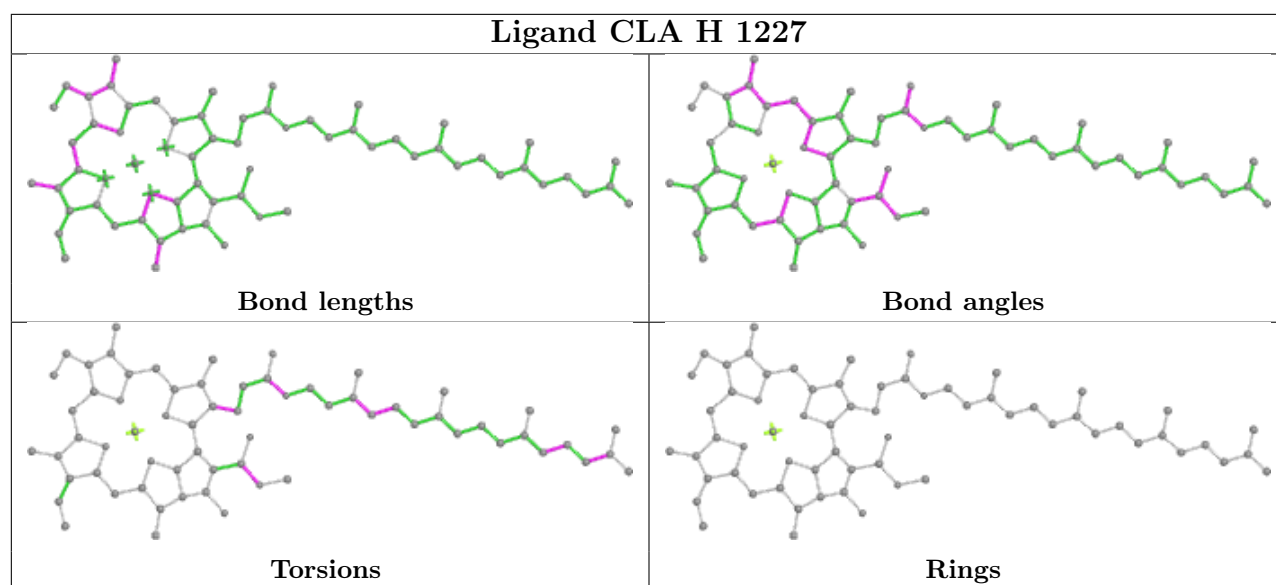


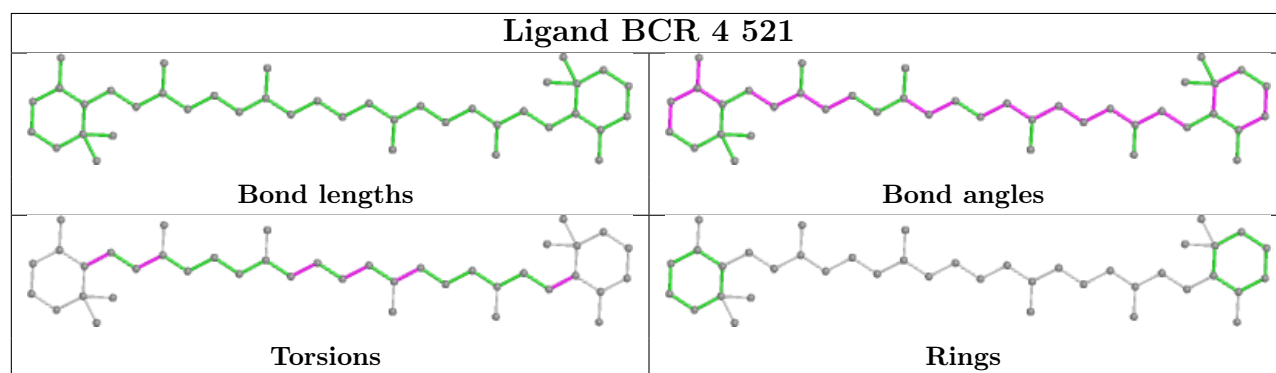
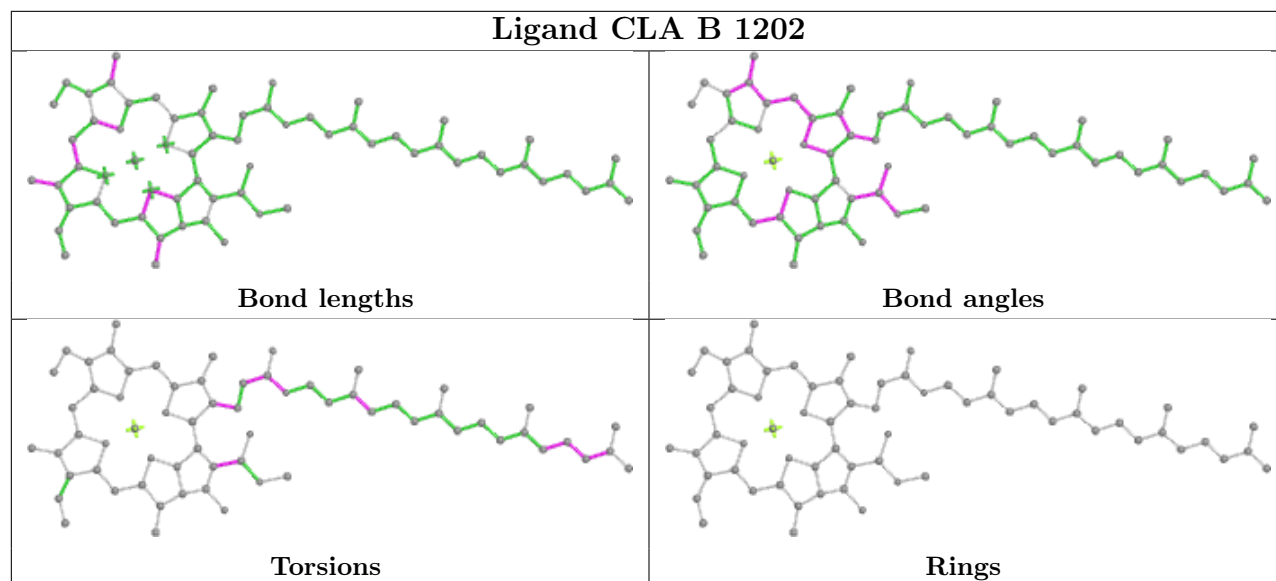
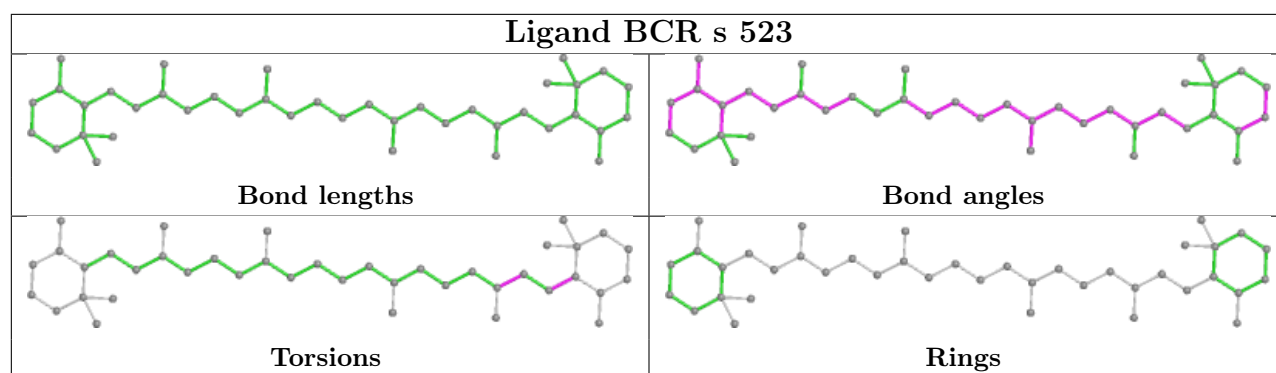
Ligand CLA G 1124

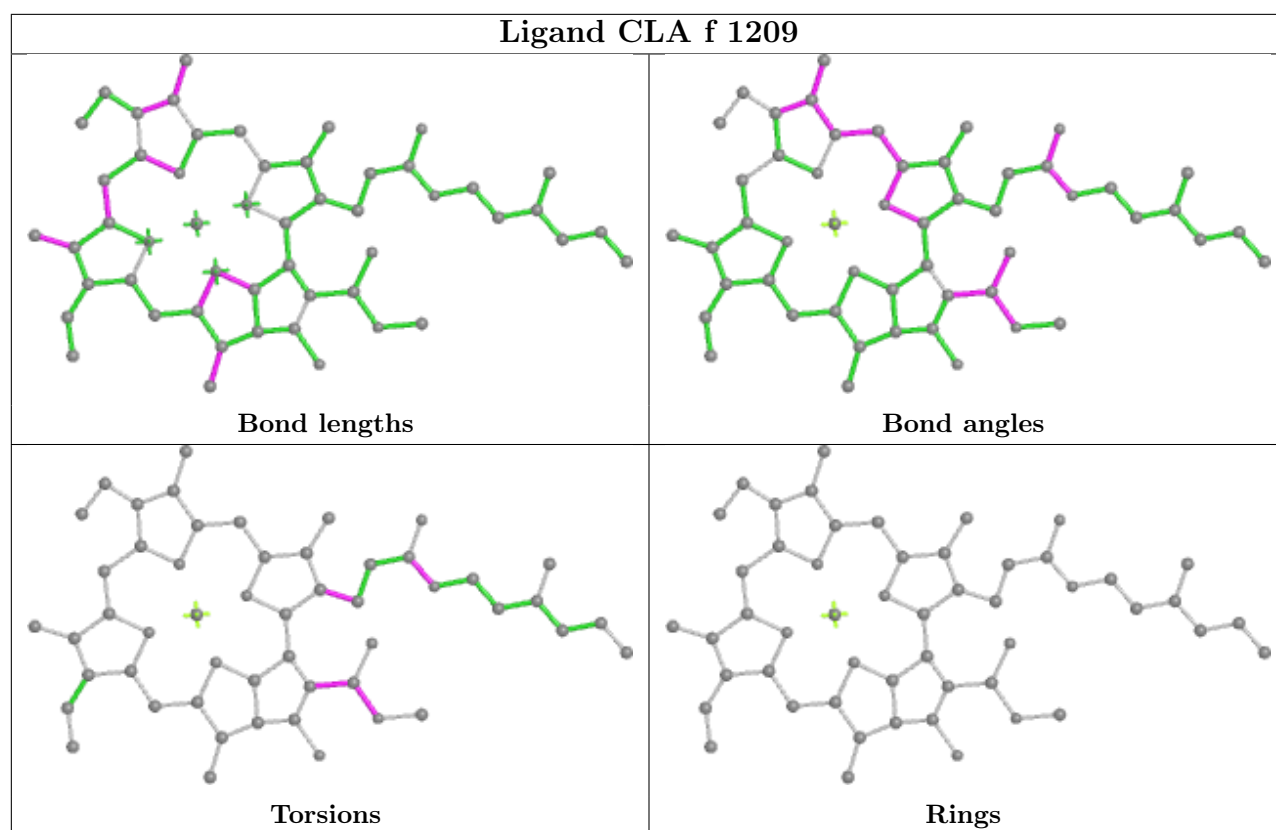


Ligand CLA Z 512

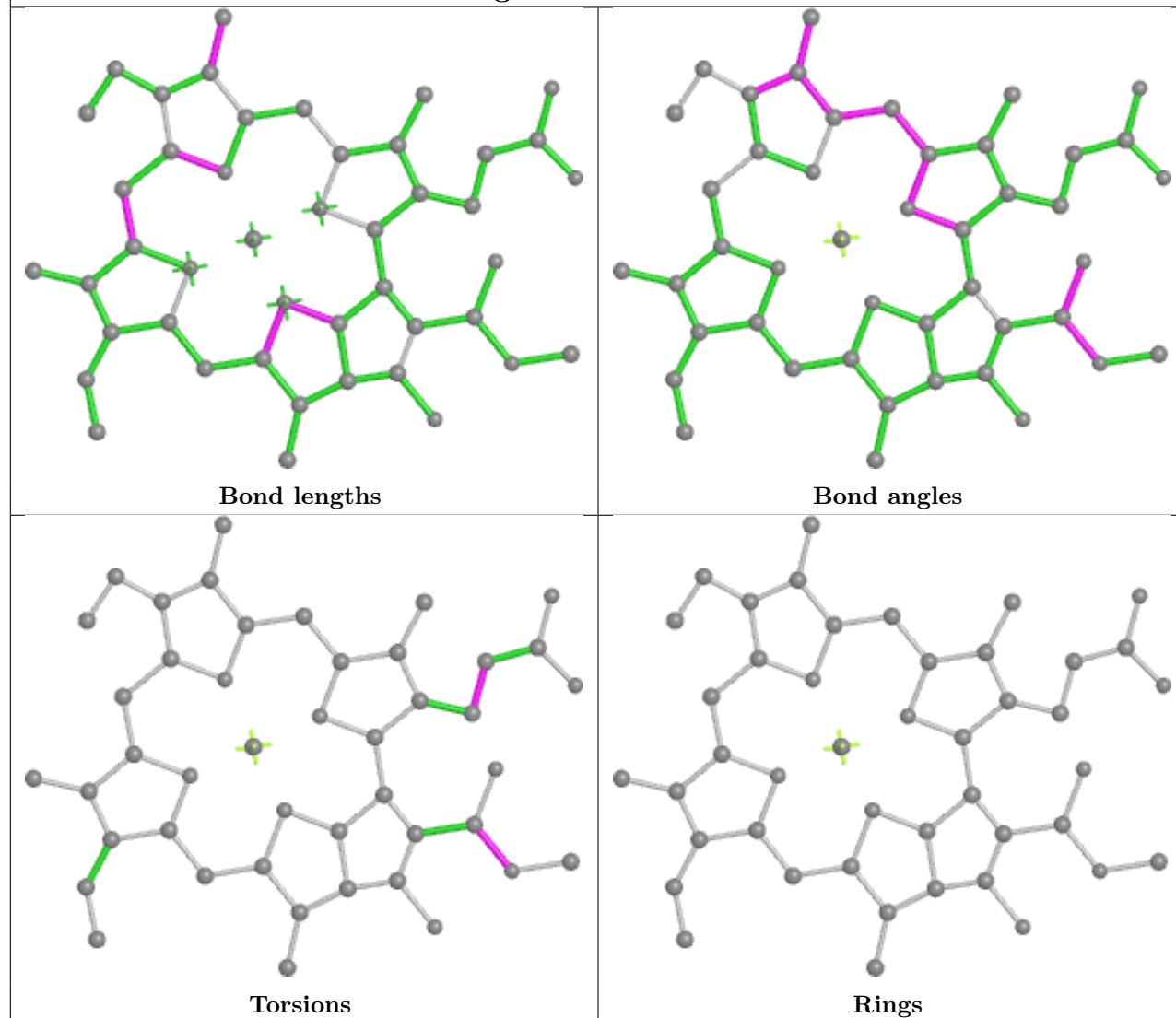




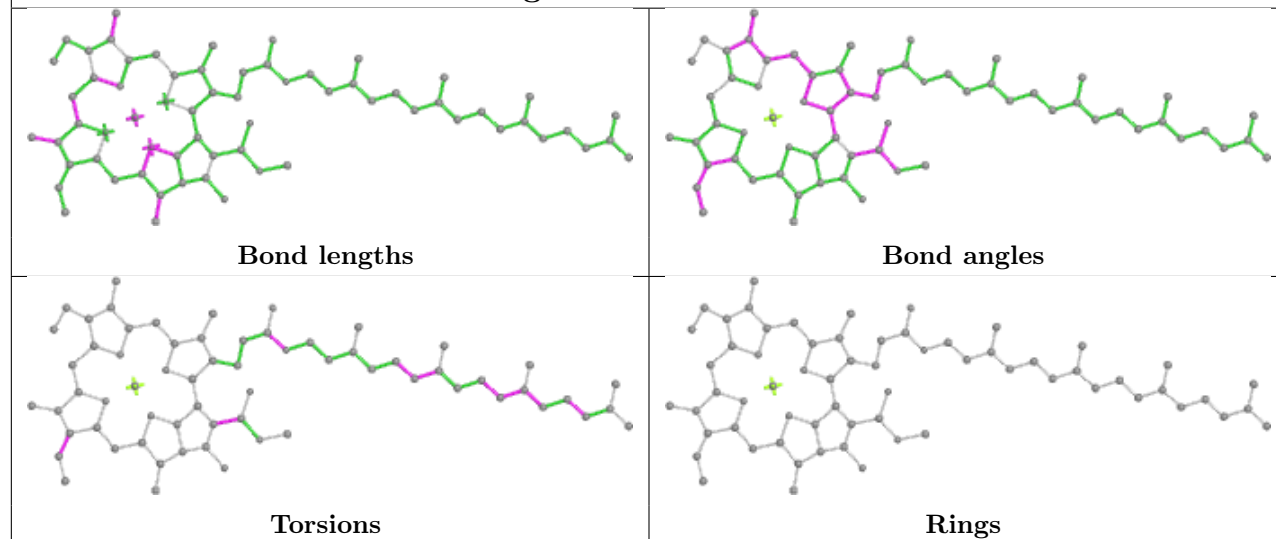


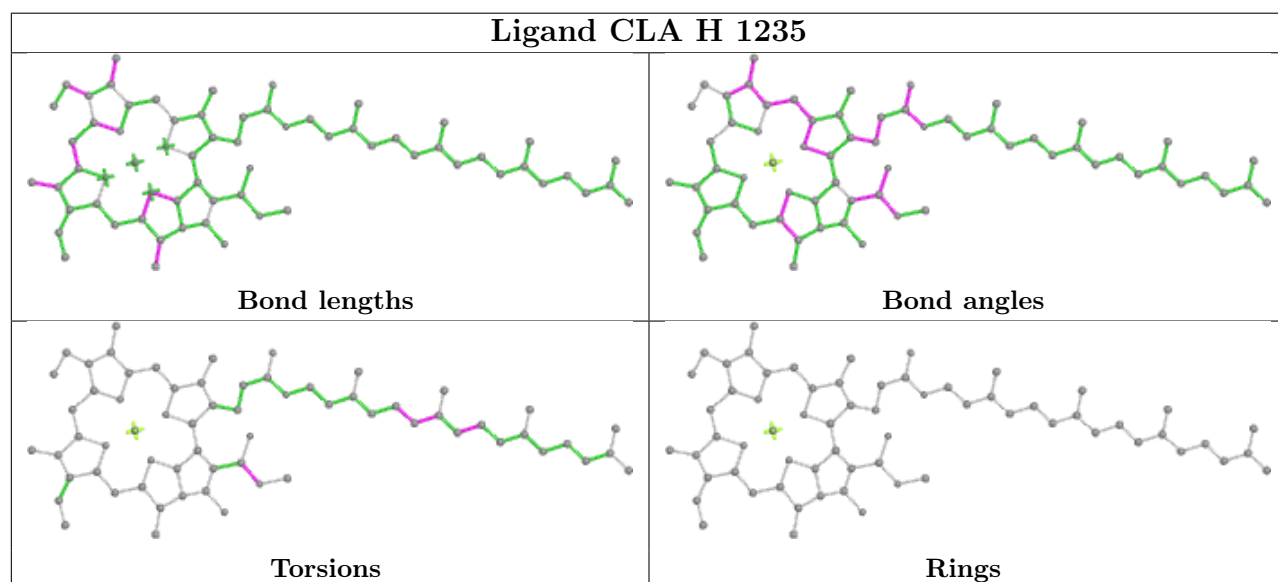
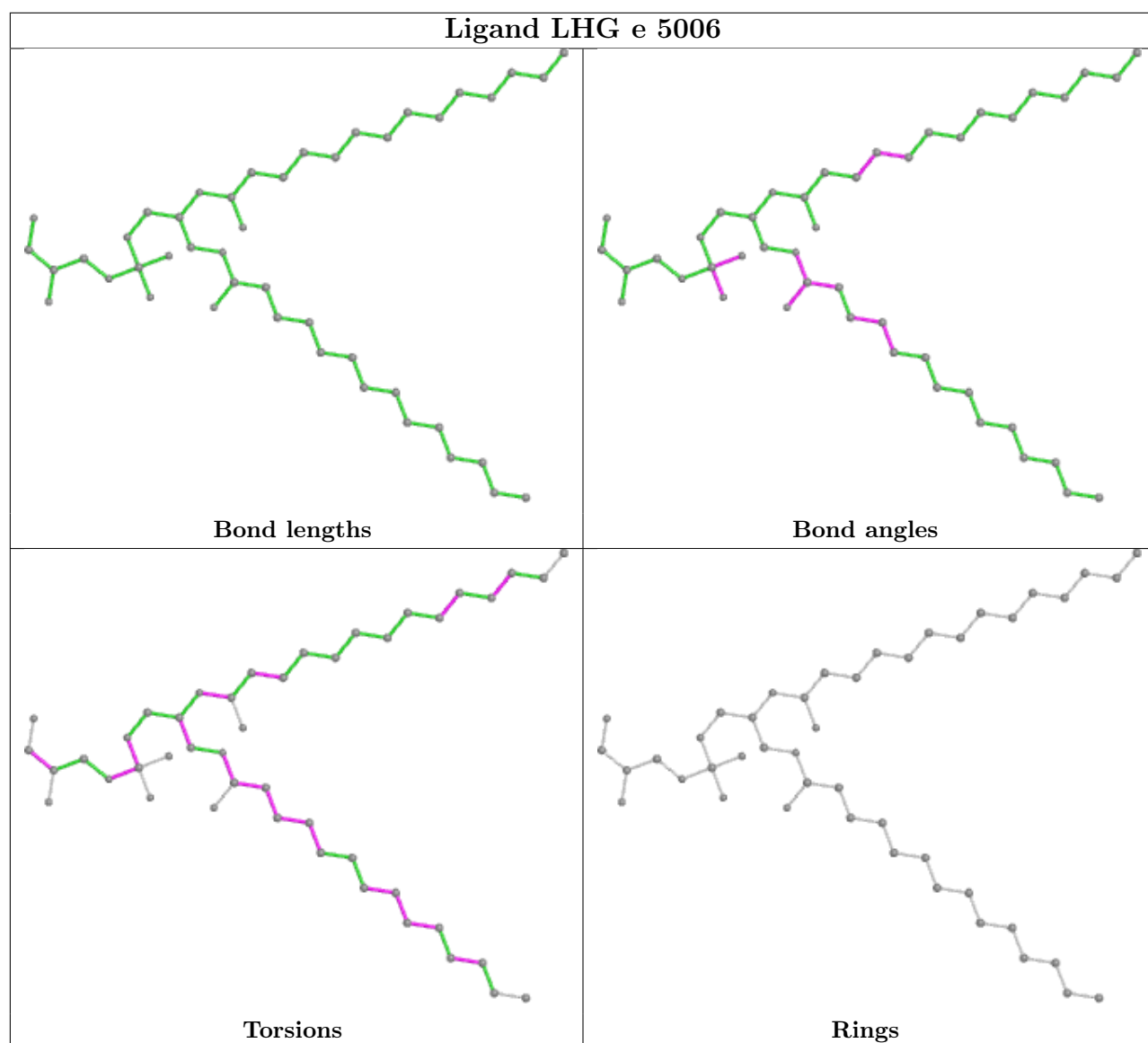


Ligand CLA 6 513

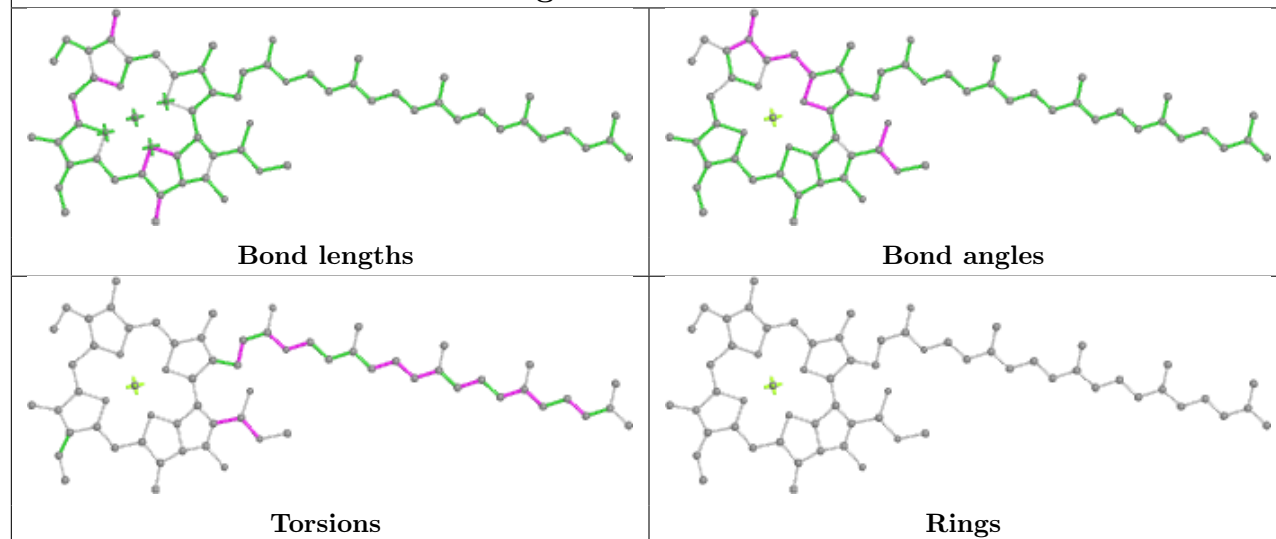


Ligand CLA B 1234

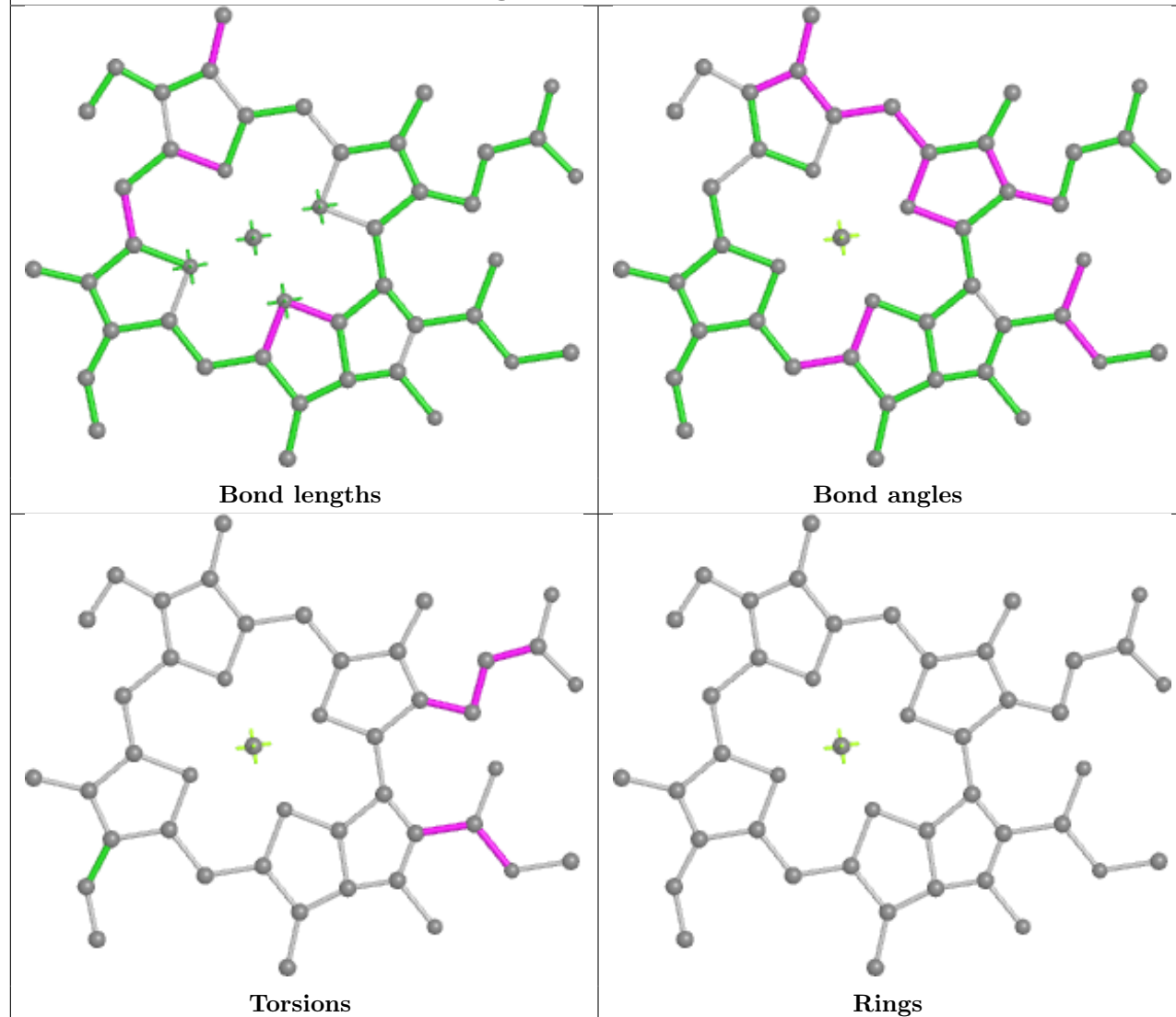




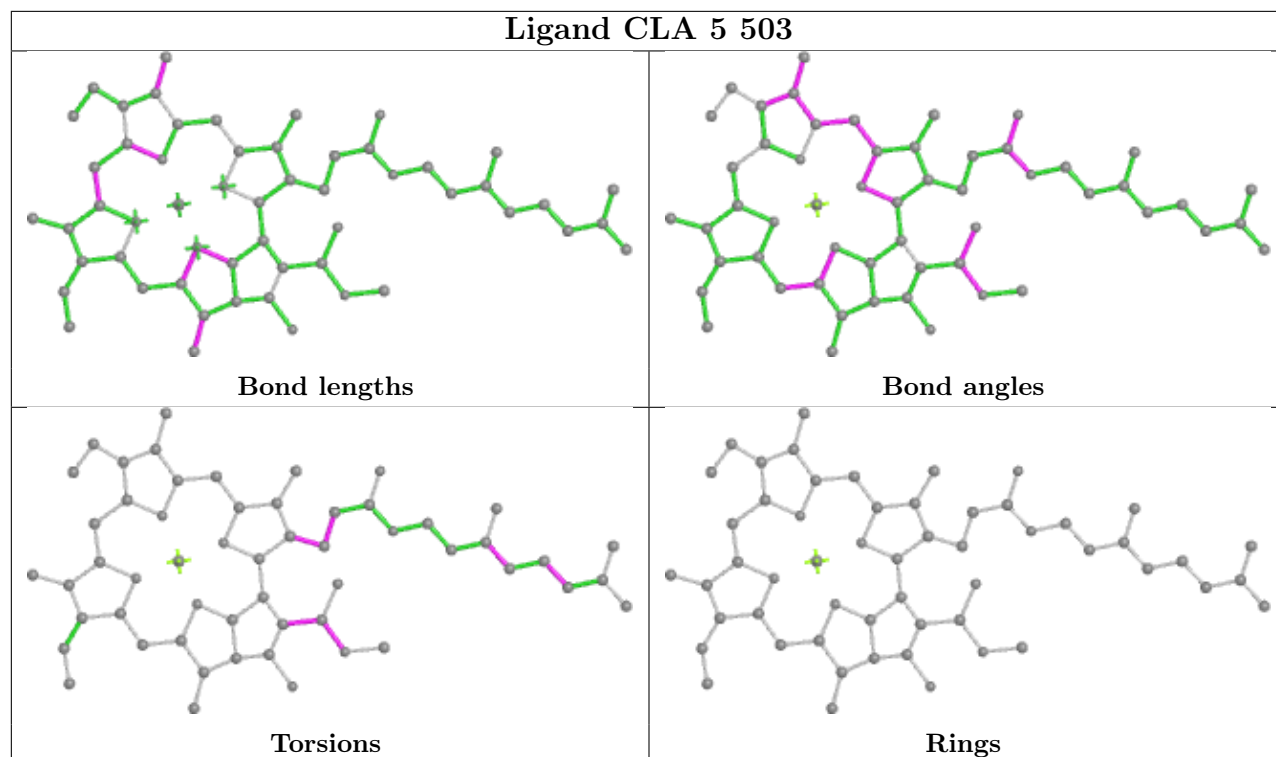
Ligand CLA a 505



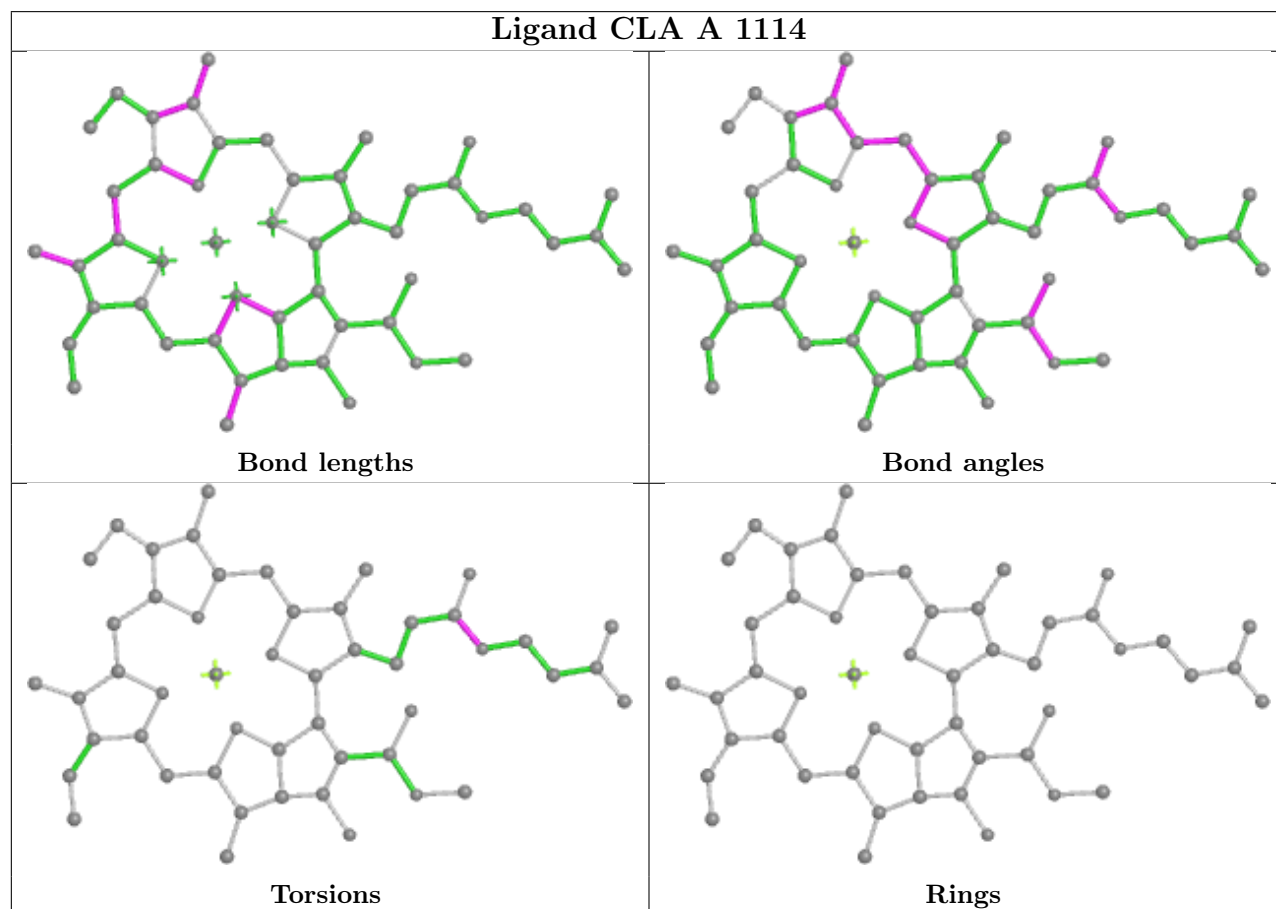
Ligand CLA v 516

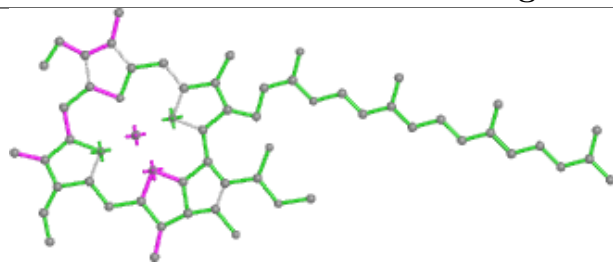


Ligand CLA 5 503

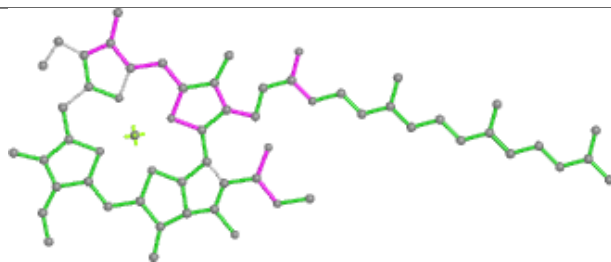


Ligand CLA A 1114

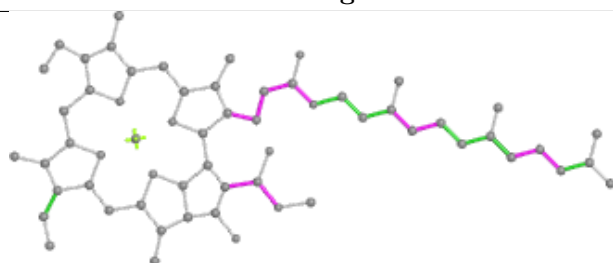


Ligand CLA 1 518

Bond lengths



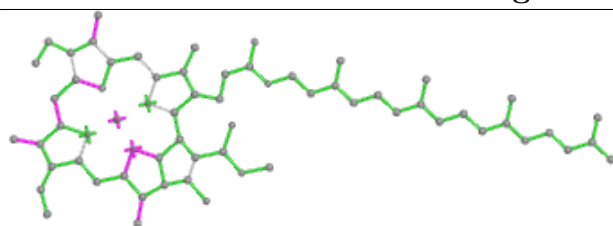
Bond angles



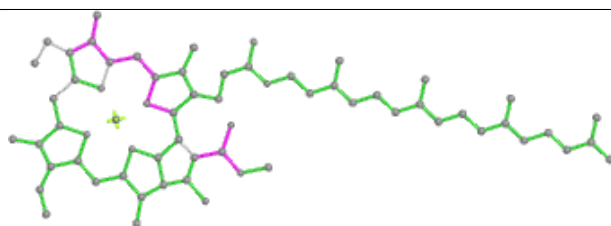
Torsions



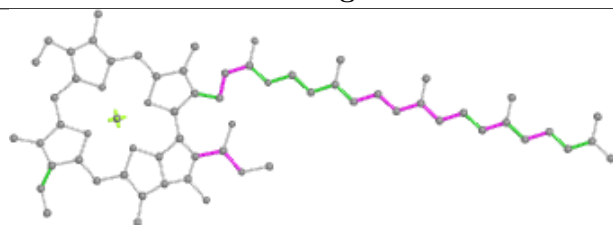
Rings

Ligand CLA f 1203

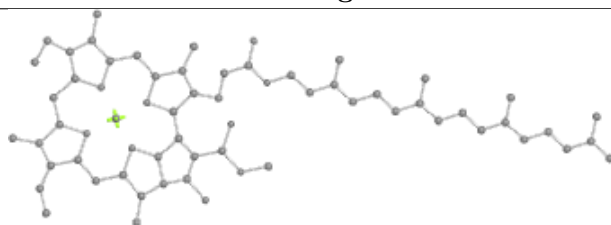
Bond lengths



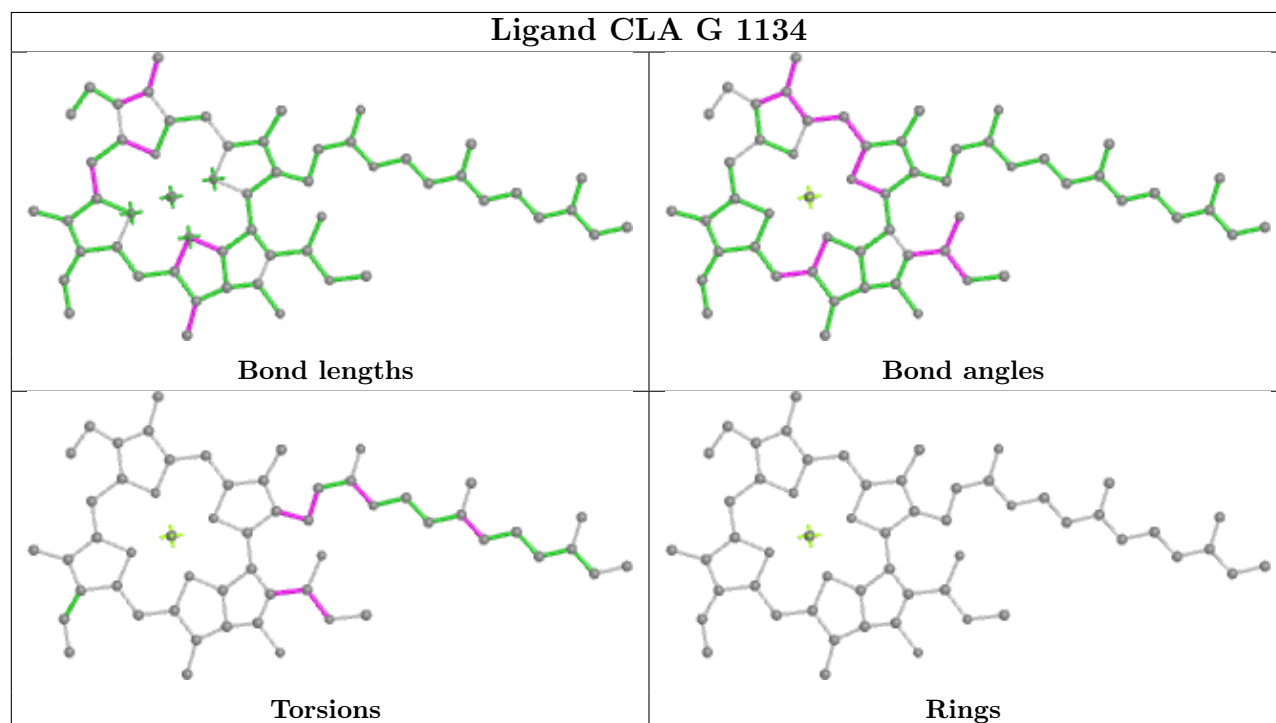
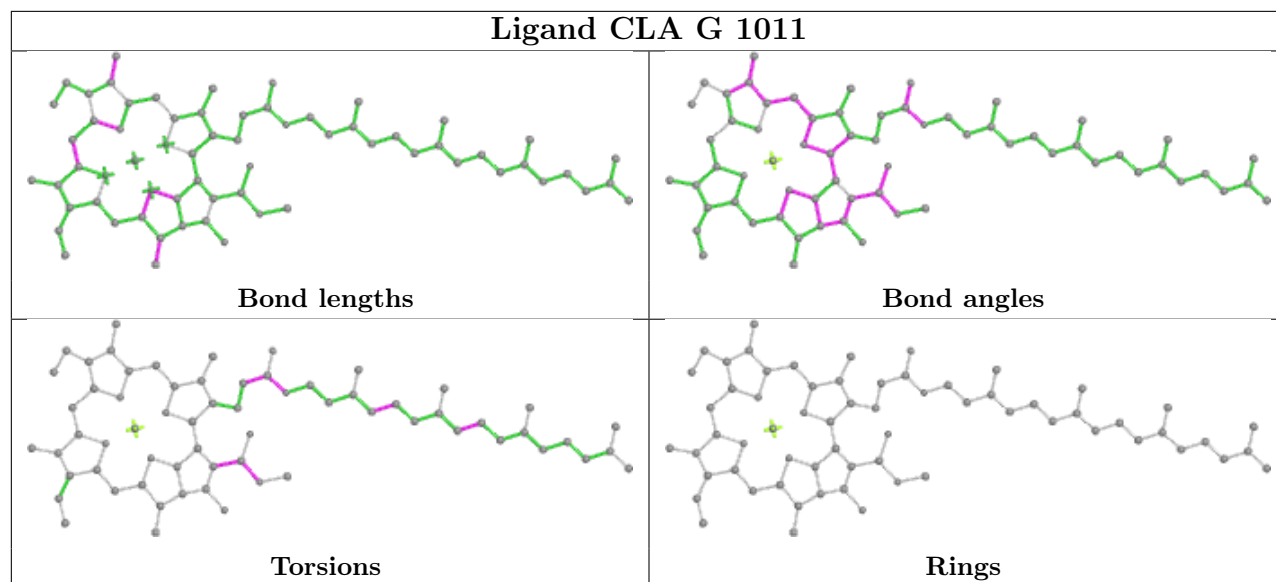
Bond angles

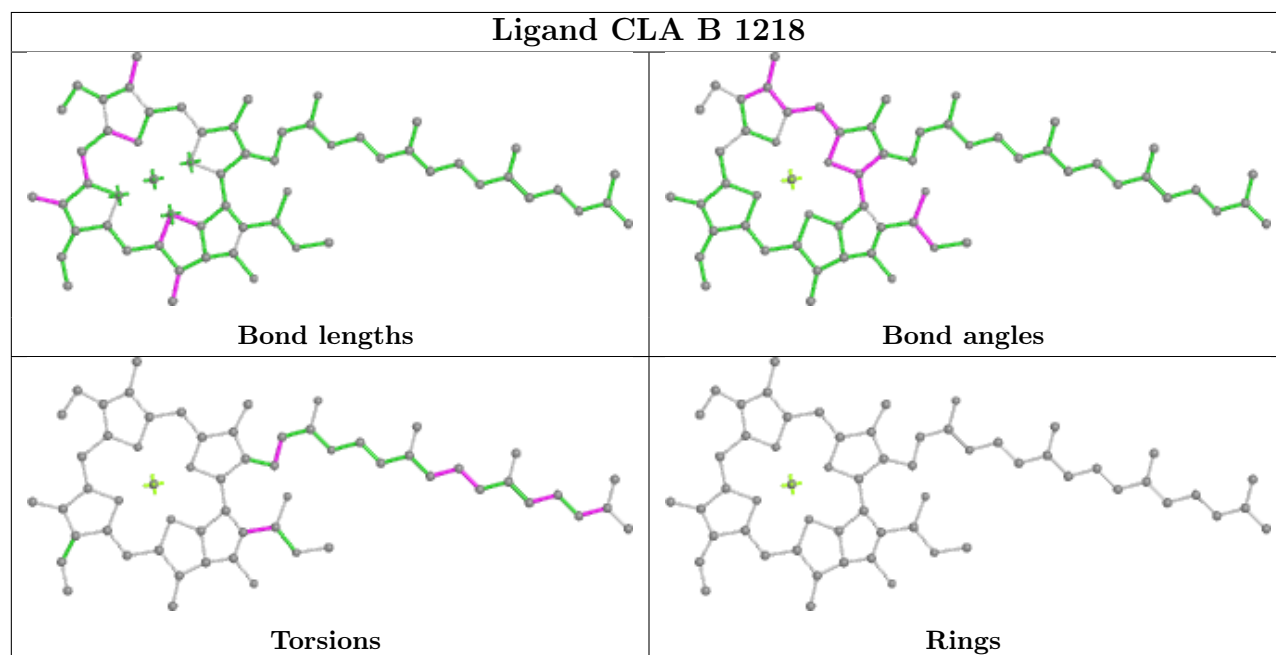
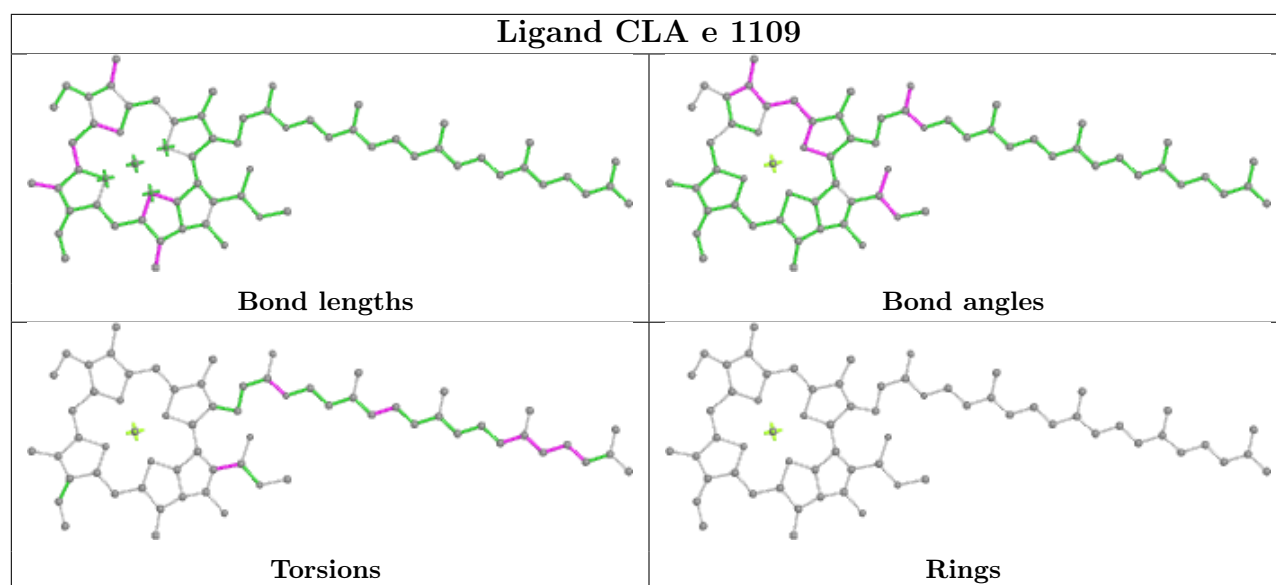


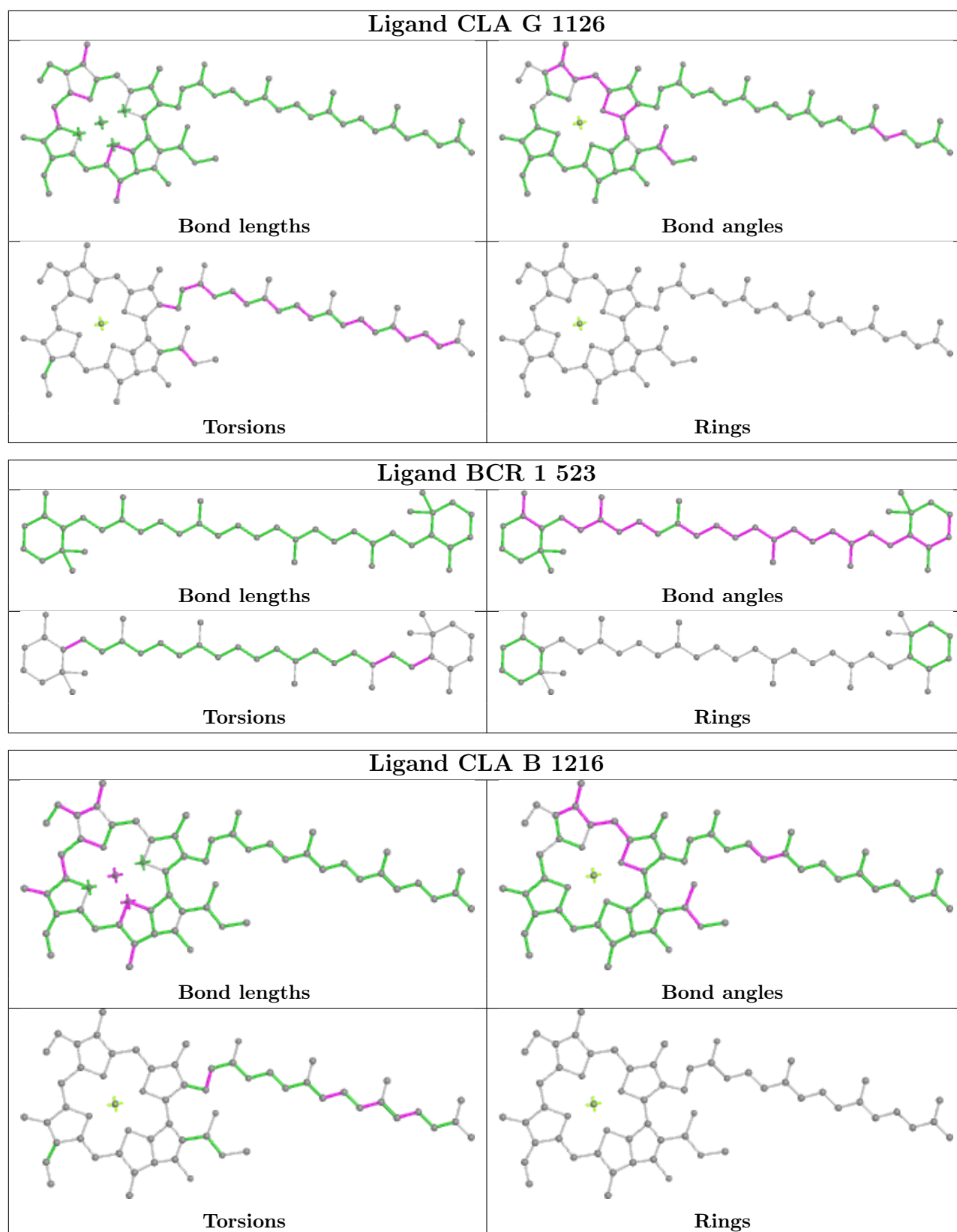
Torsions



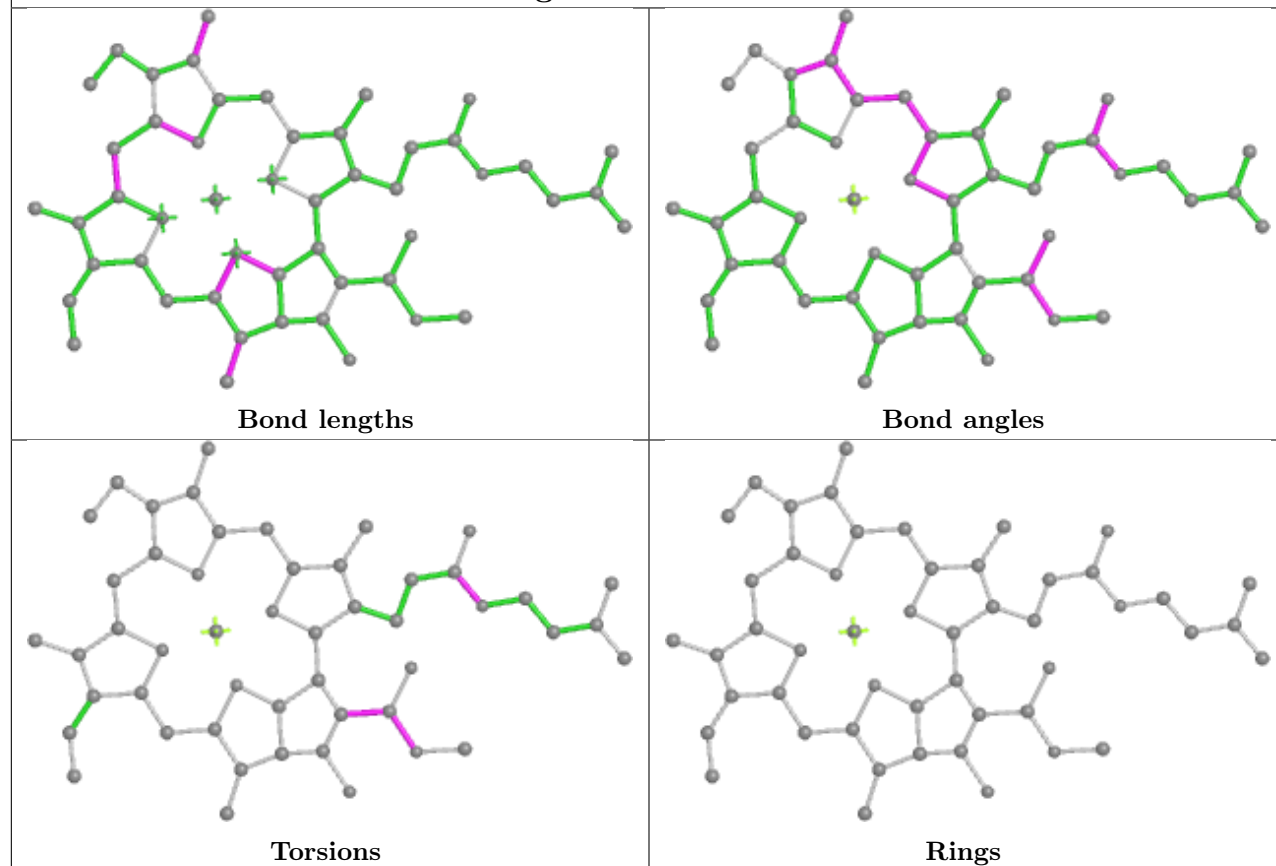
Rings



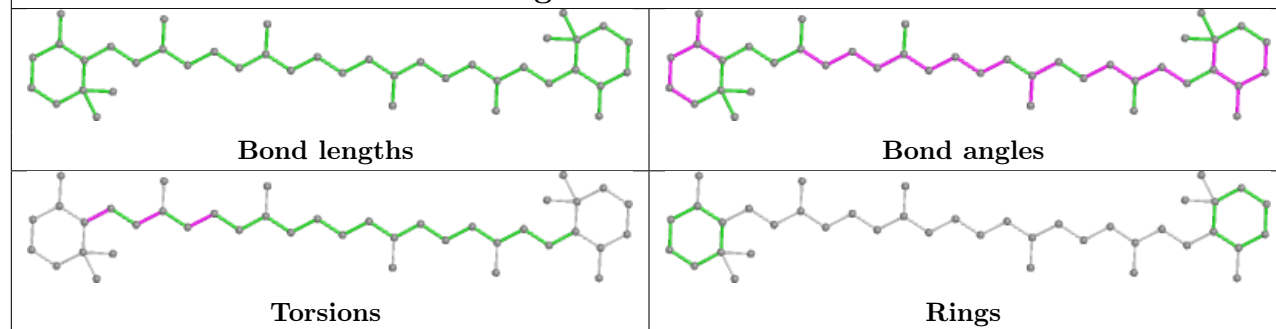


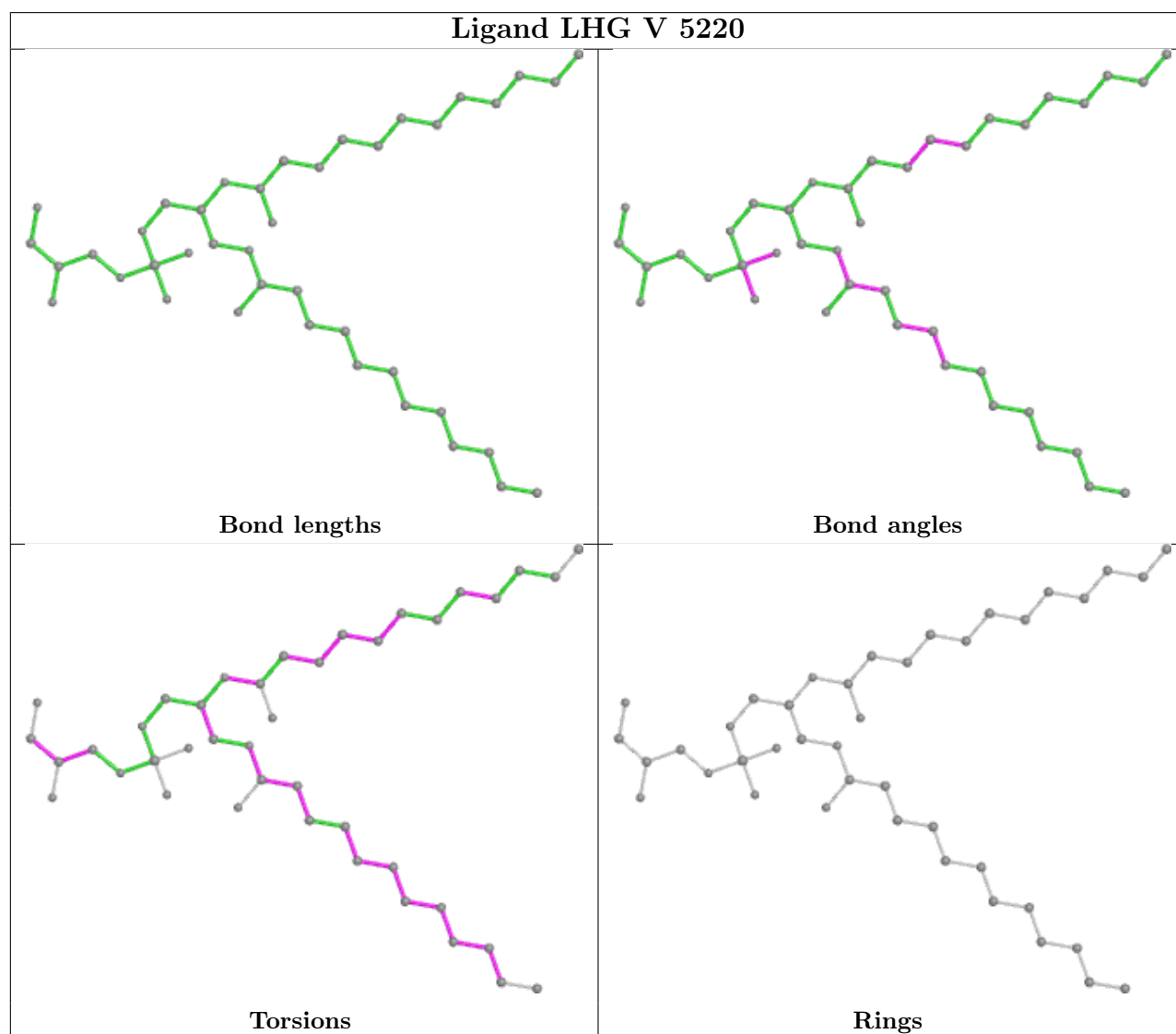
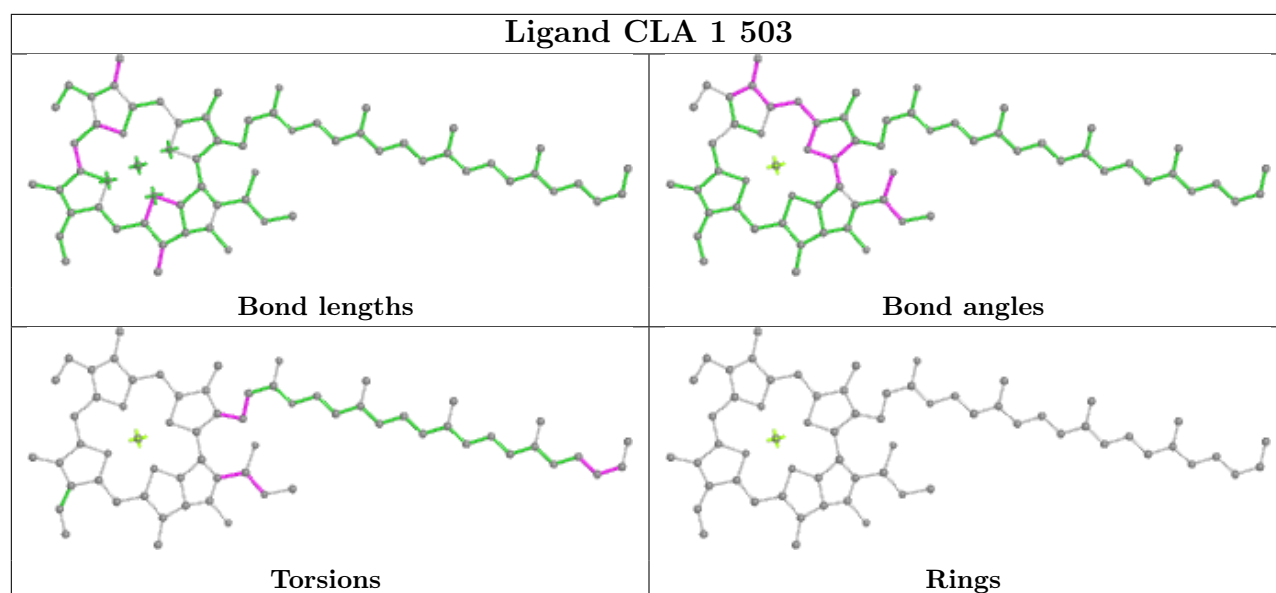


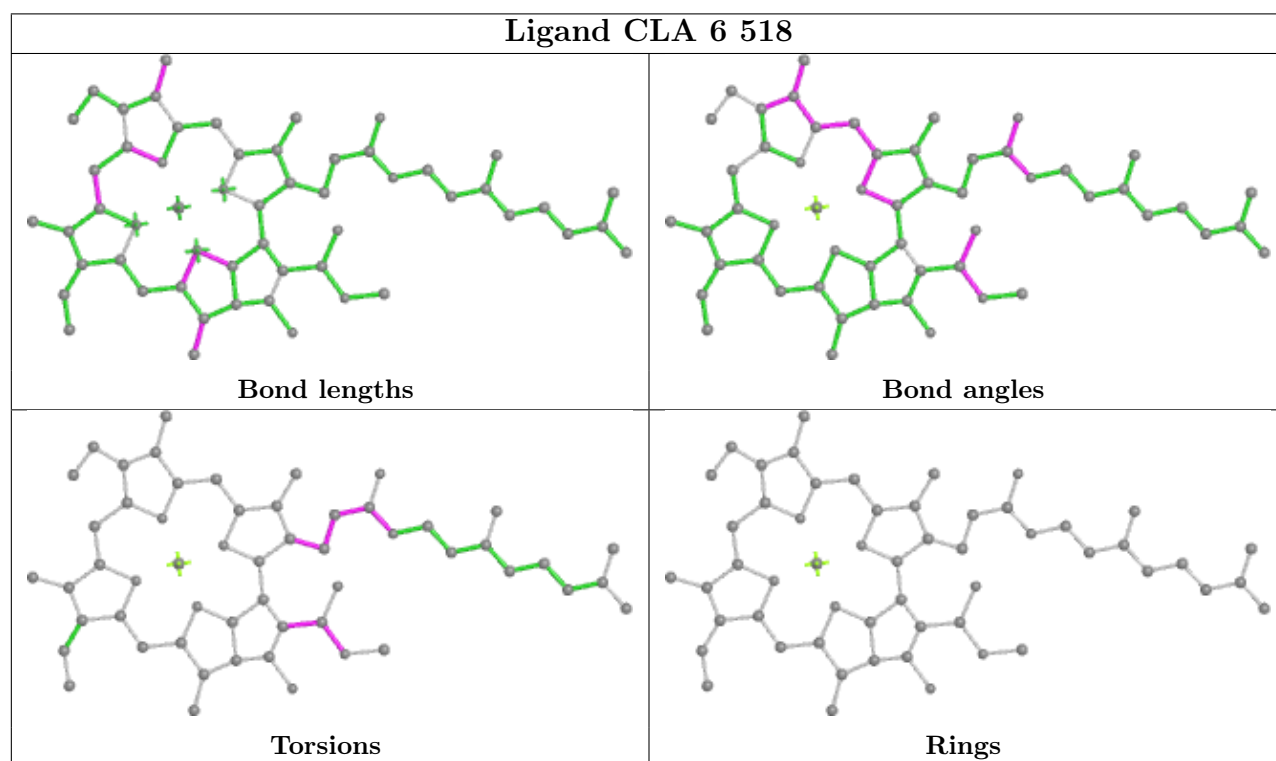
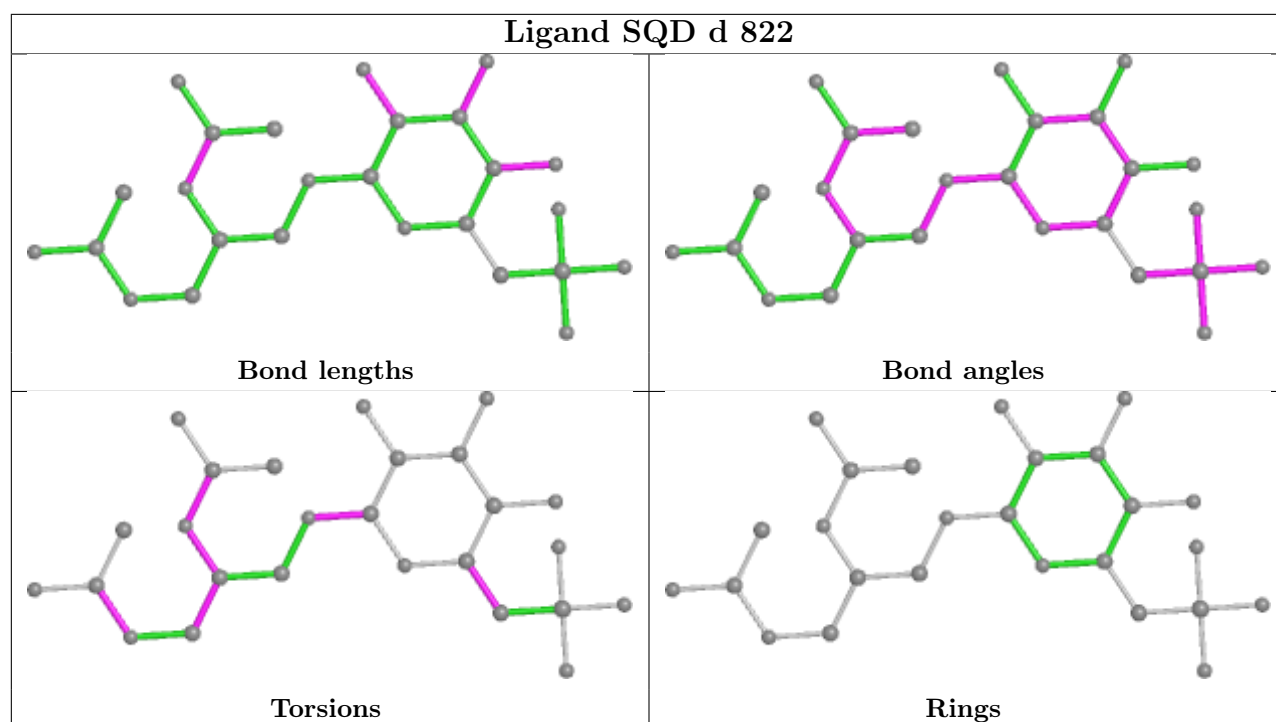
Ligand CLA b 510



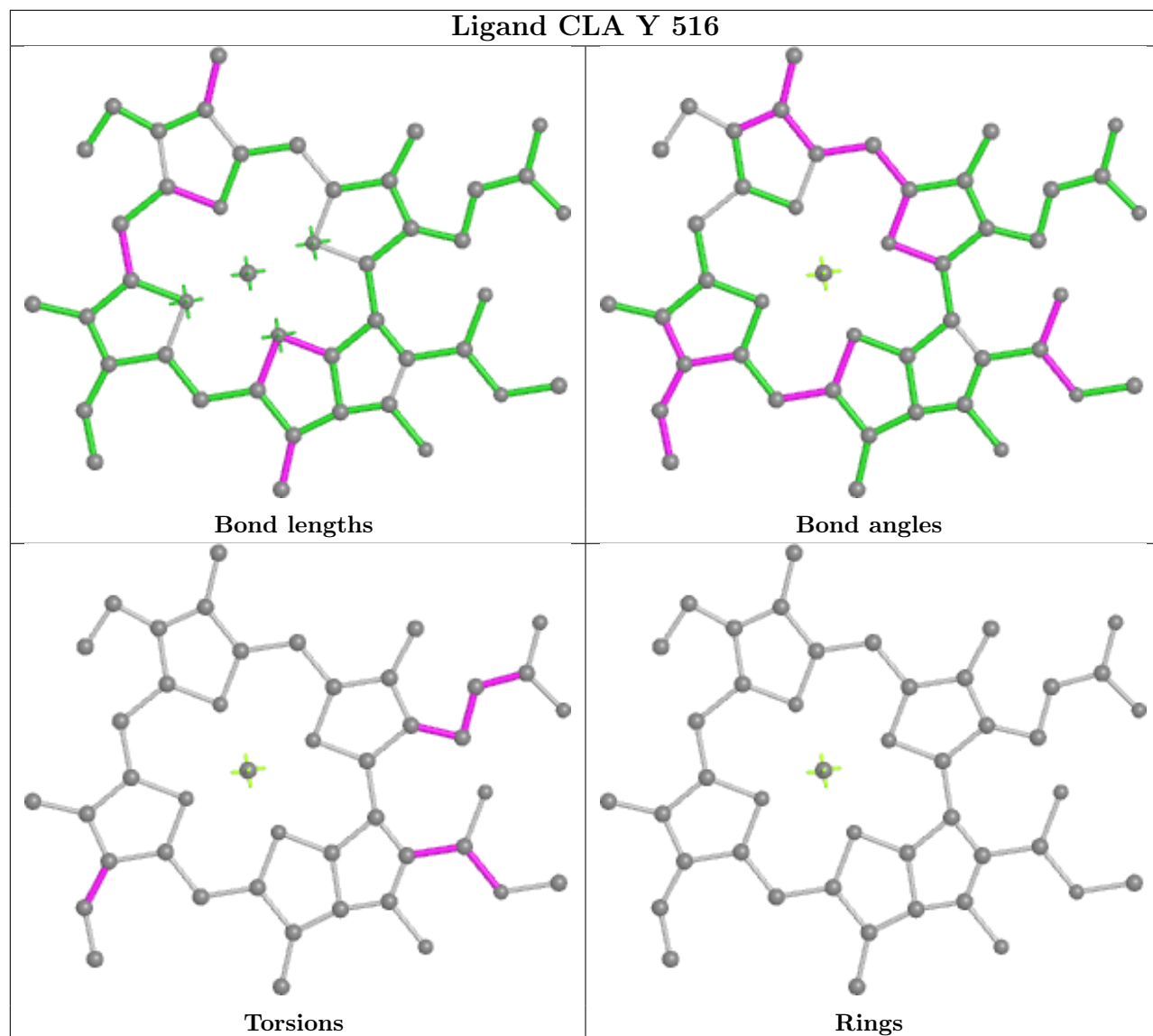
Ligand BCR 6 522

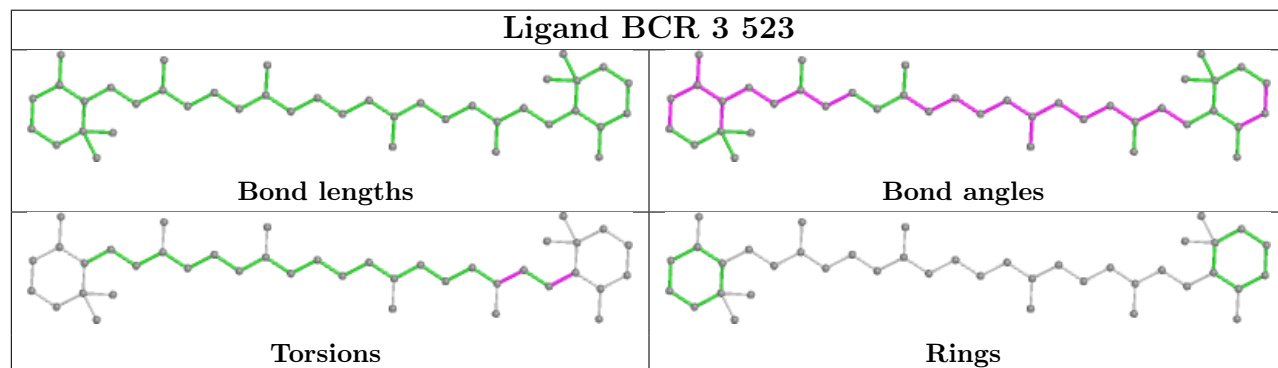
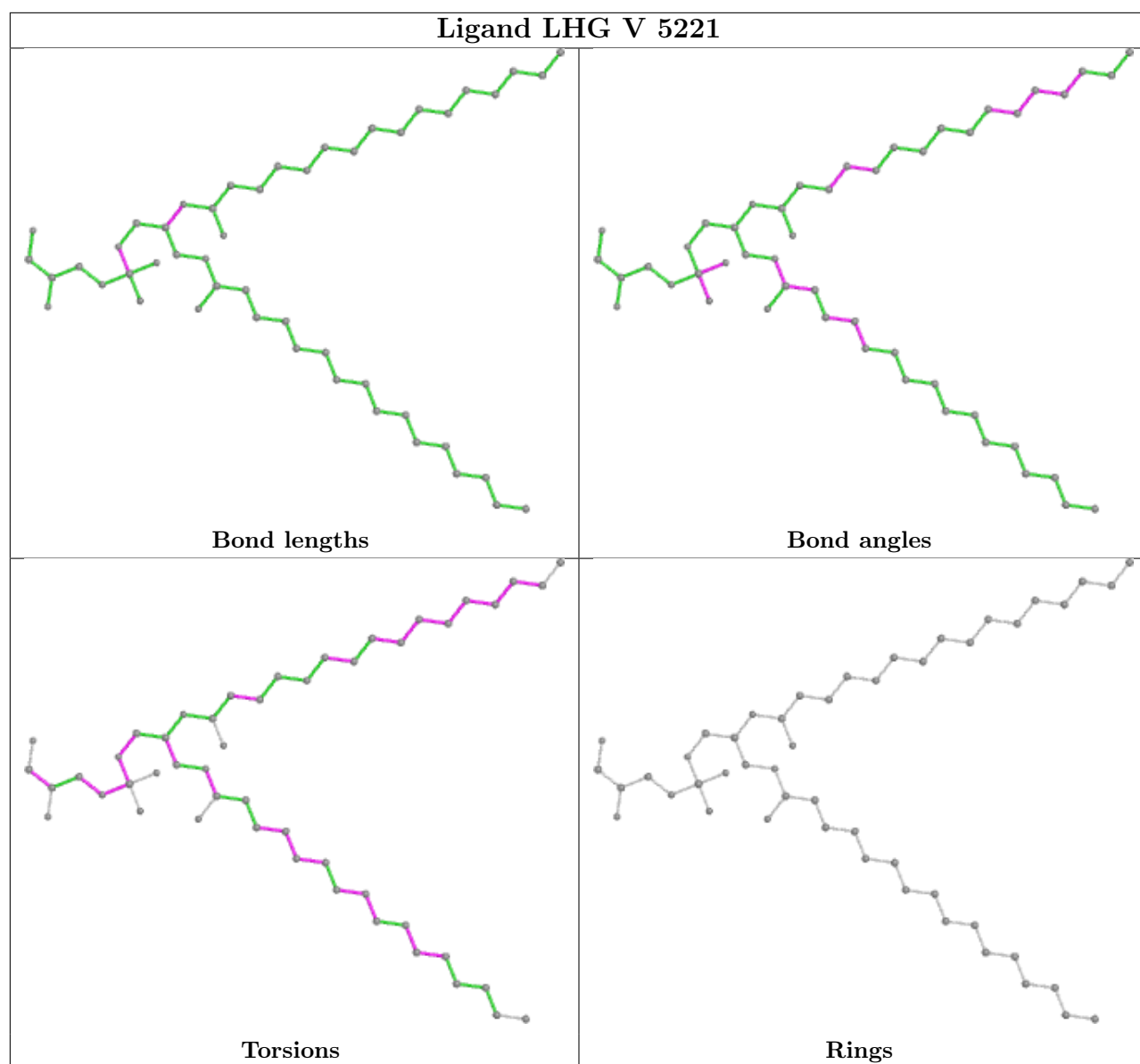


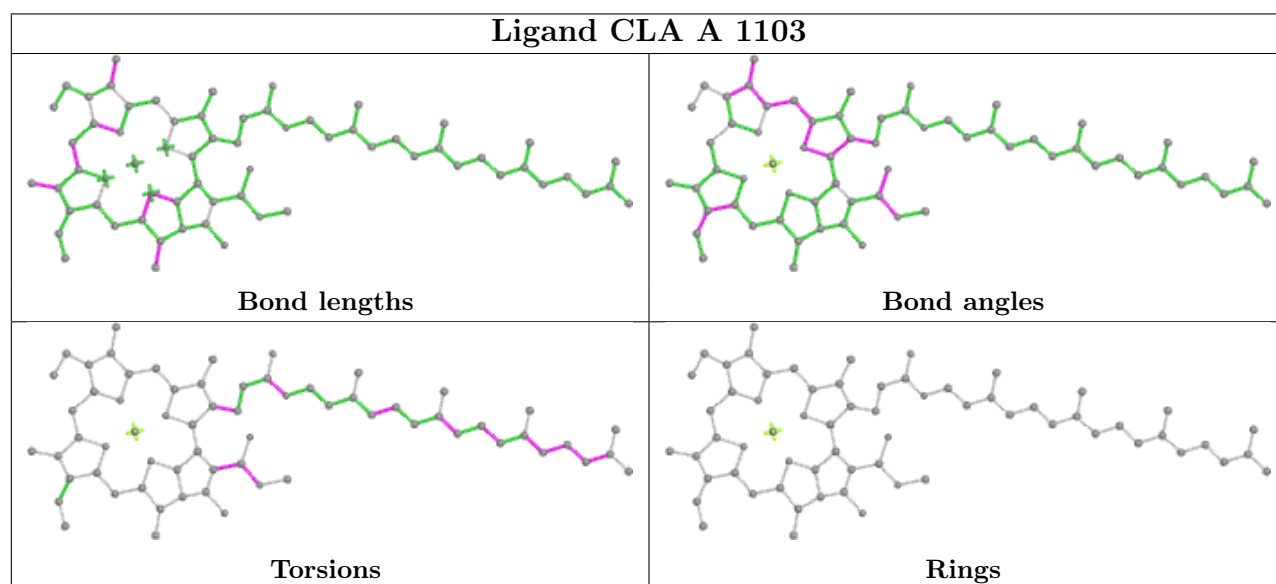
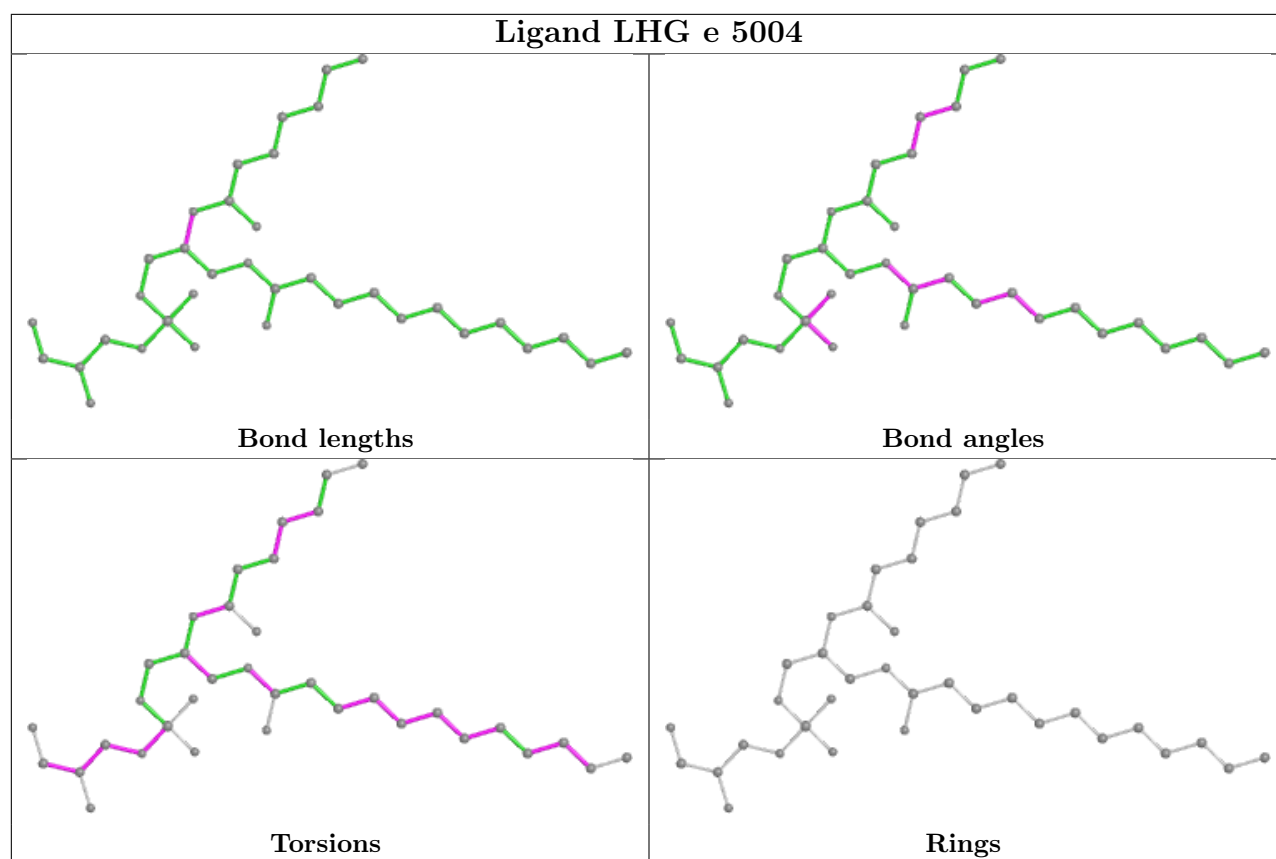


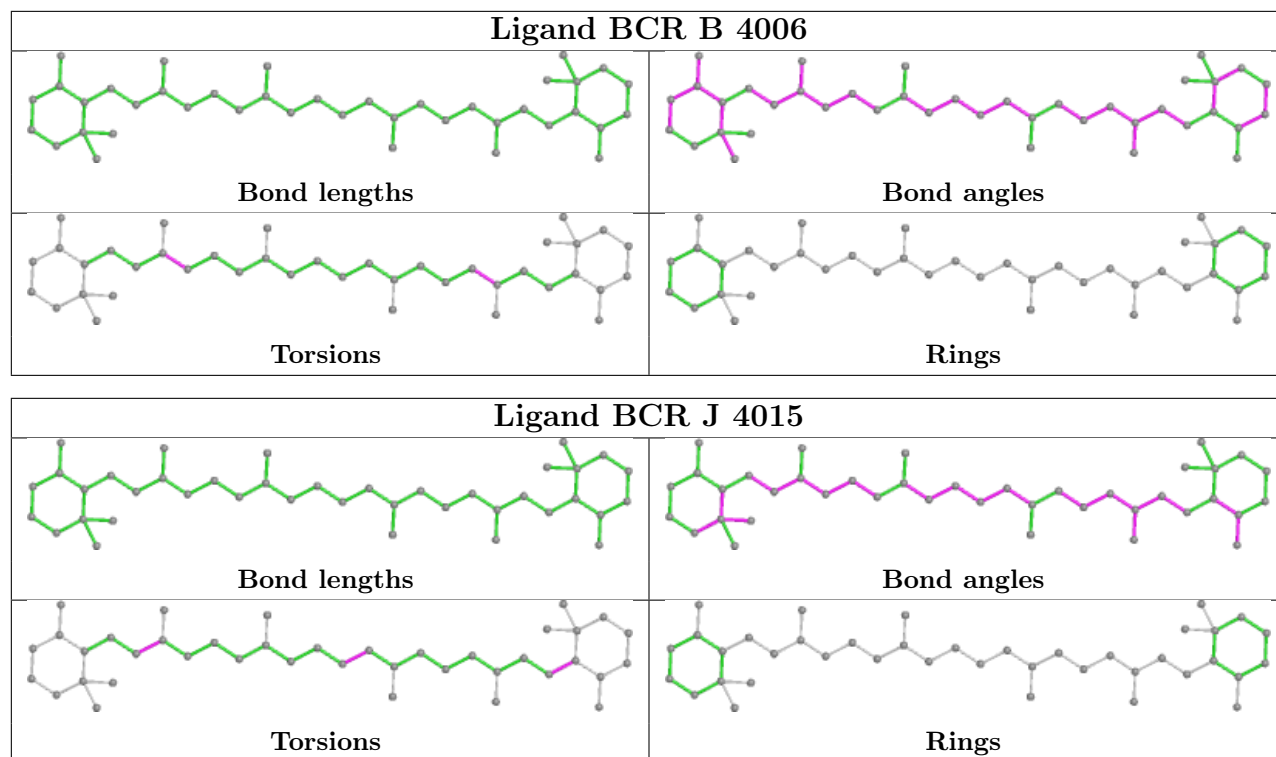


Ligand CLA Y 516

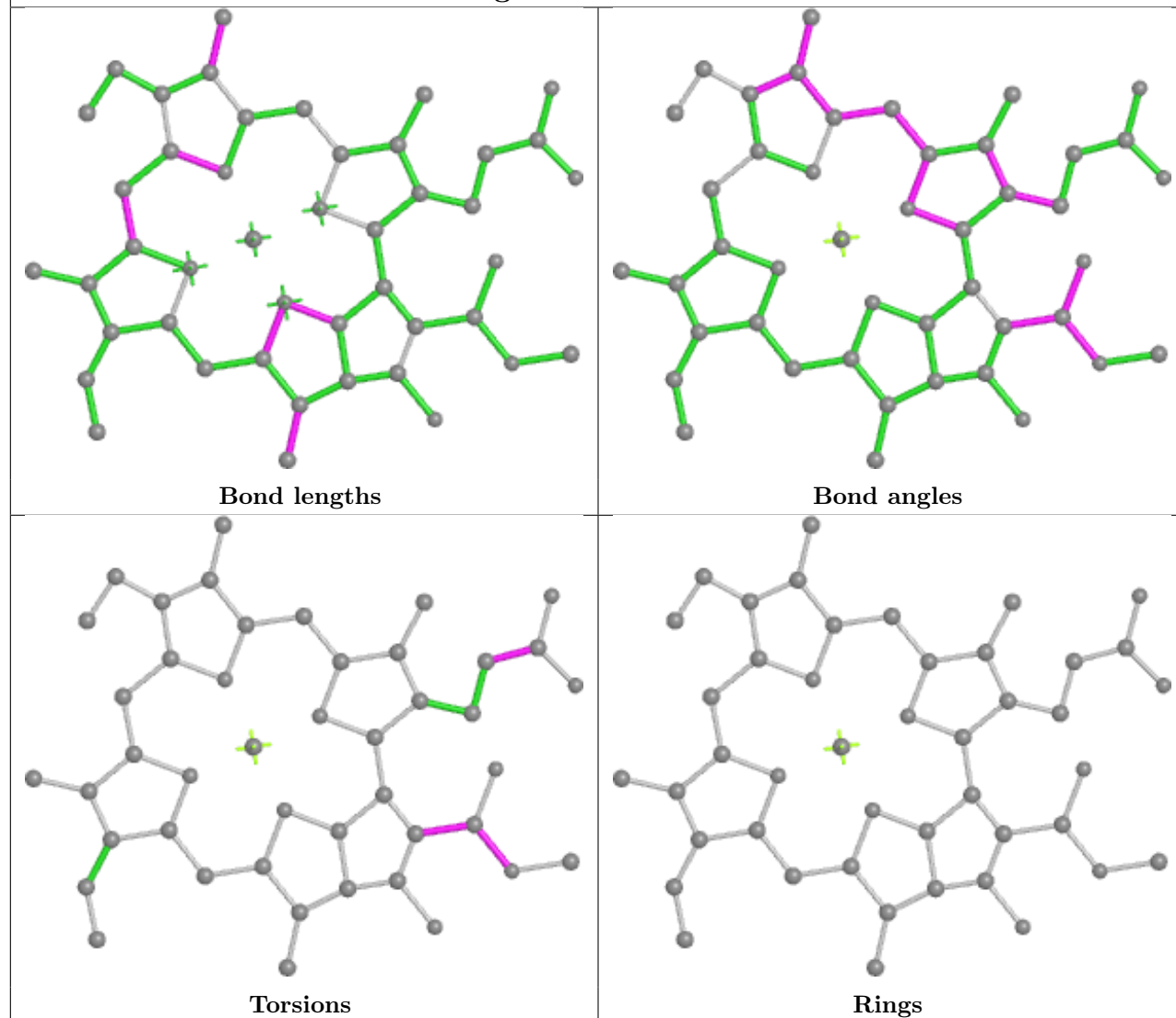




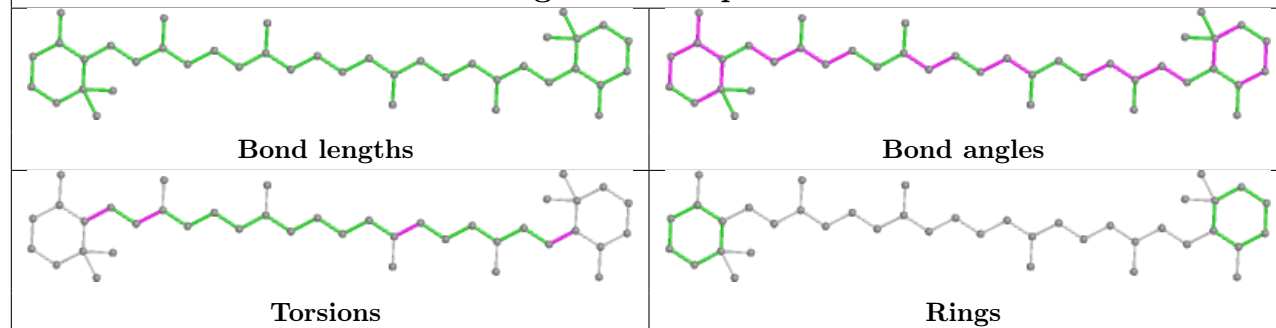


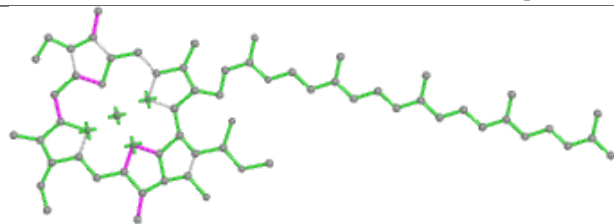


Ligand CLA 4 507

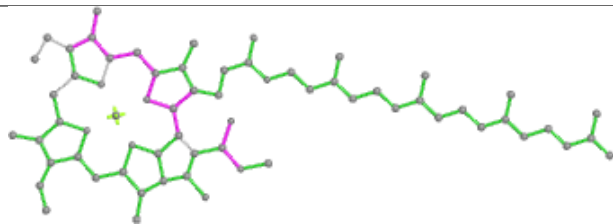


Ligand BCR q 521

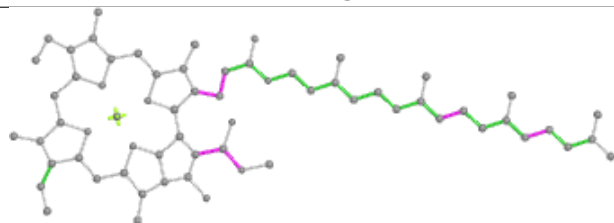


Ligand CLA 2 503

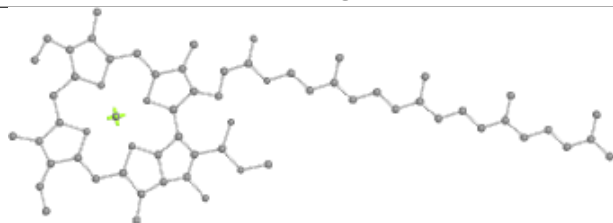
Bond lengths



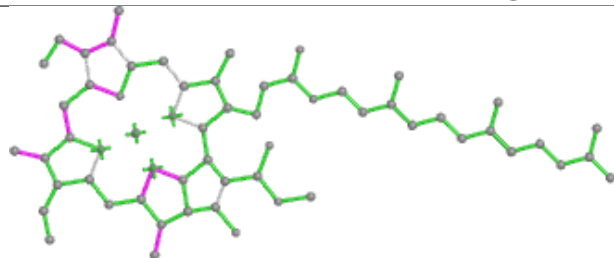
Bond angles



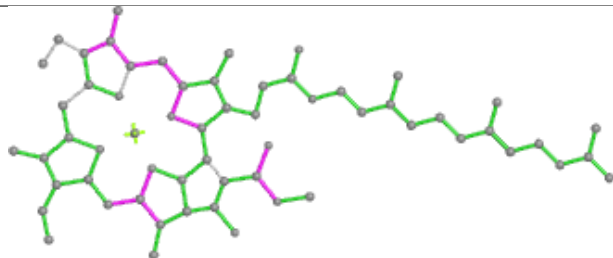
Torsions



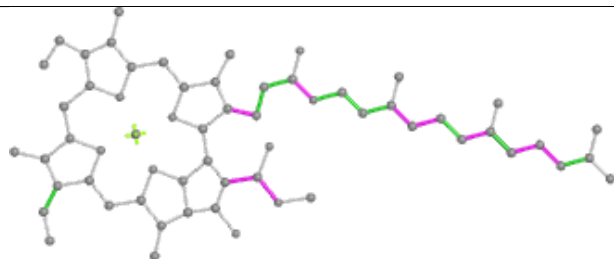
Rings

Ligand CLA A 1122

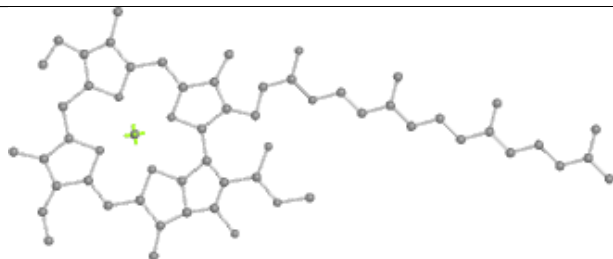
Bond lengths



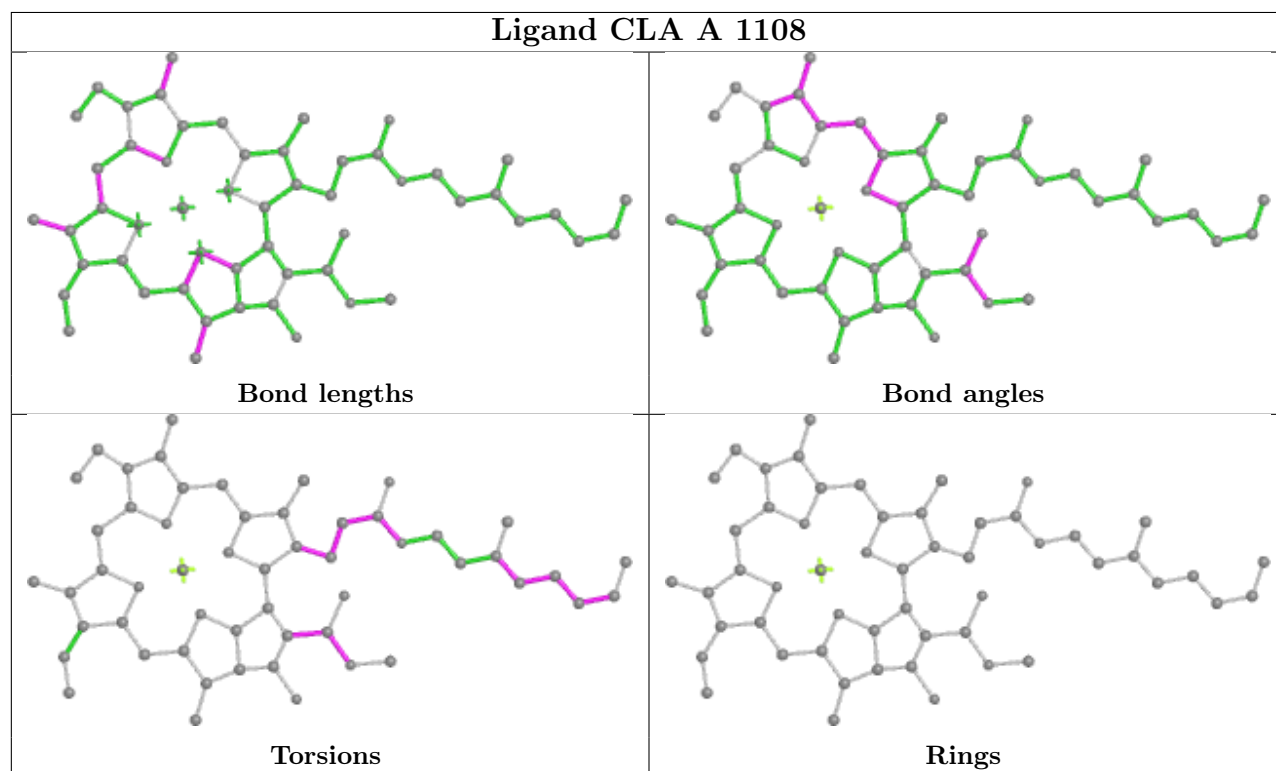
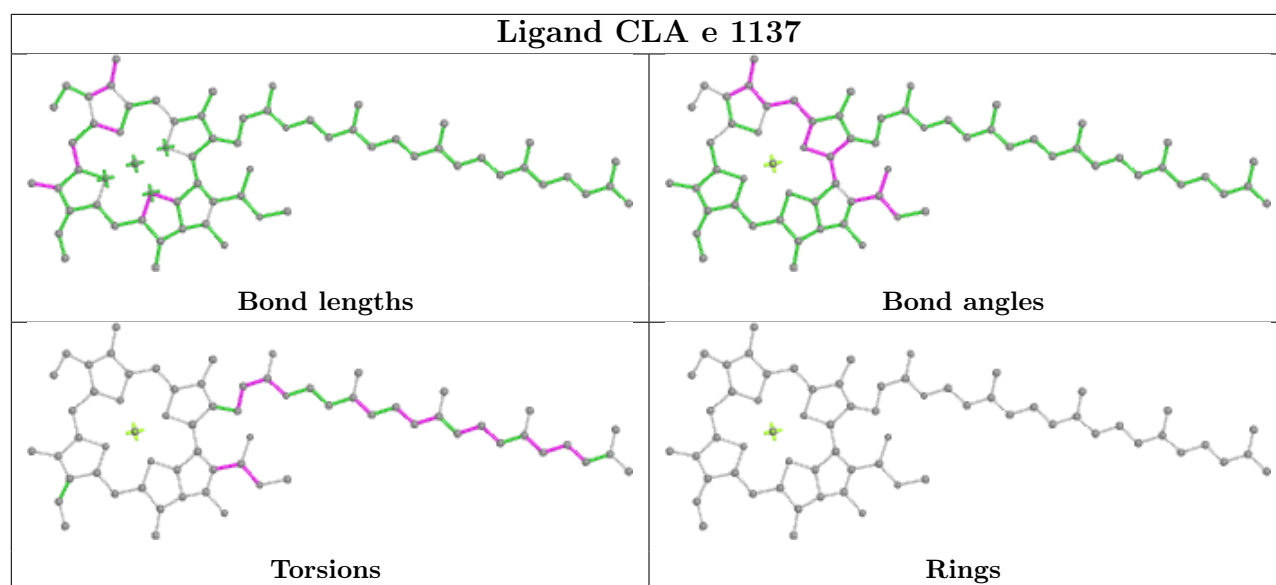
Bond angles



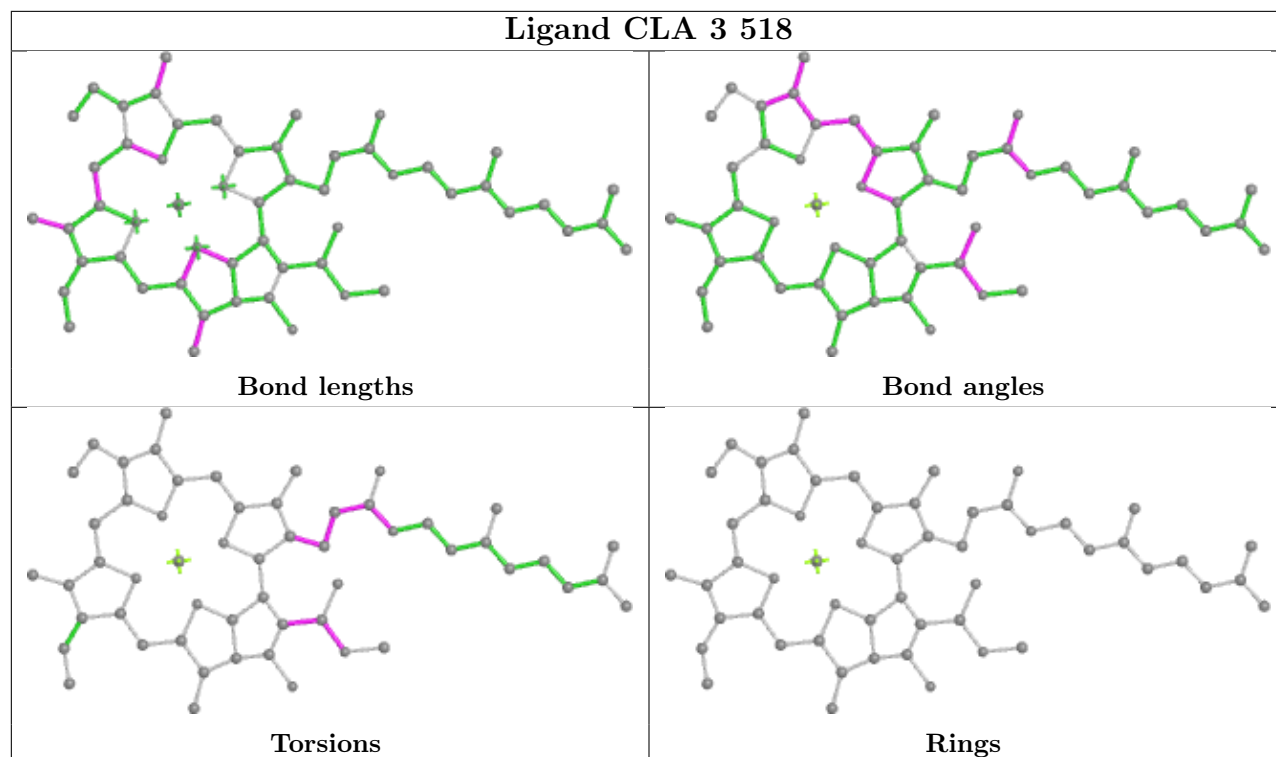
Torsions



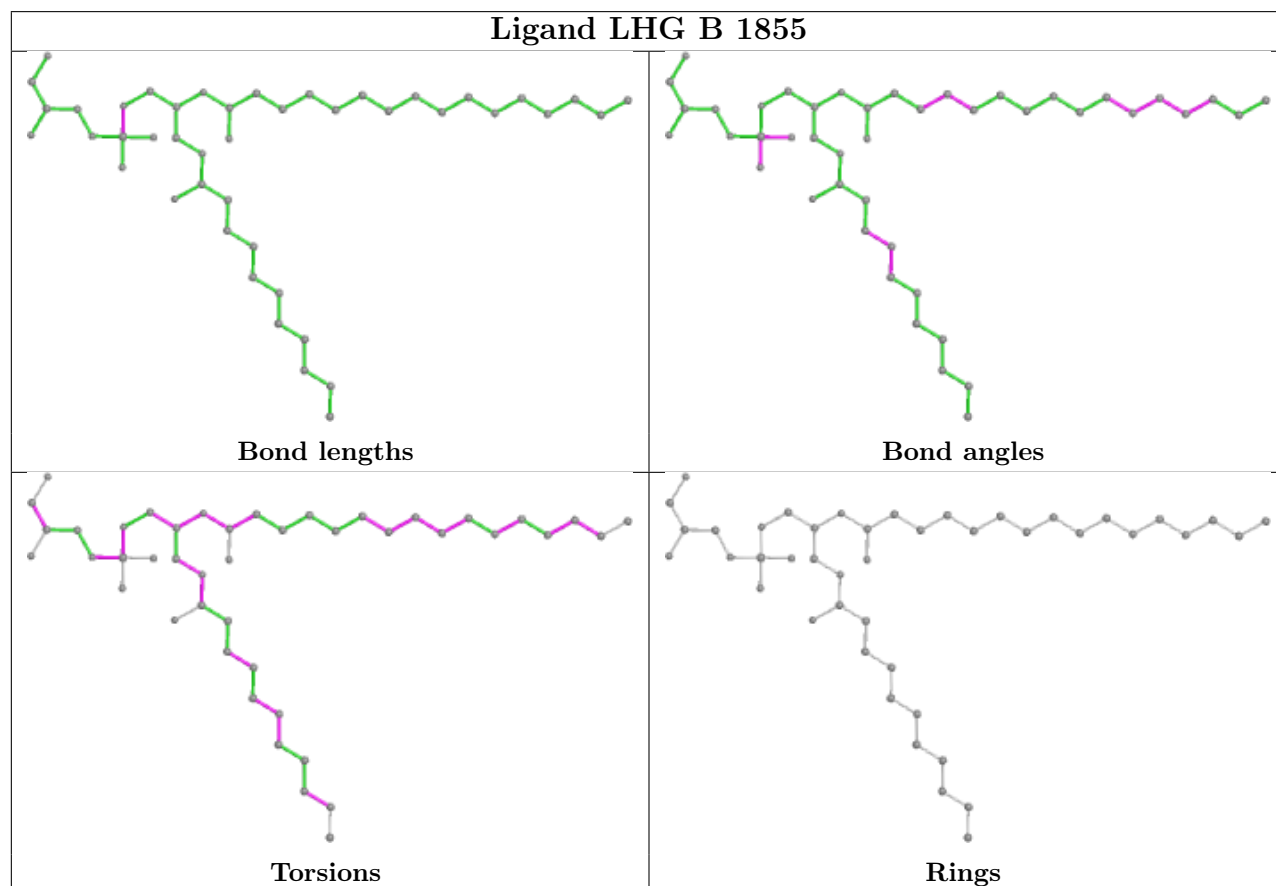
Rings



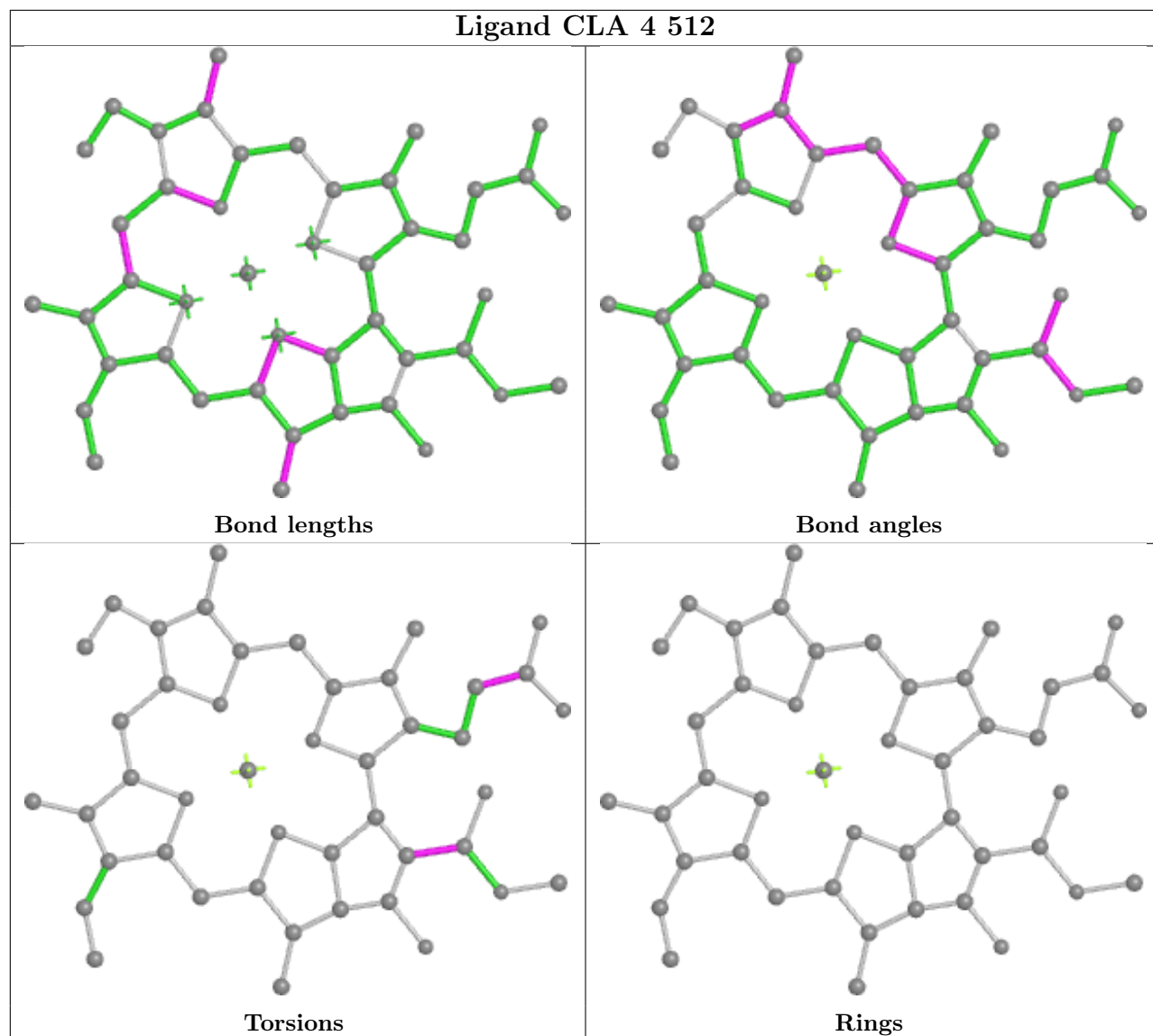
Ligand CLA 3 518



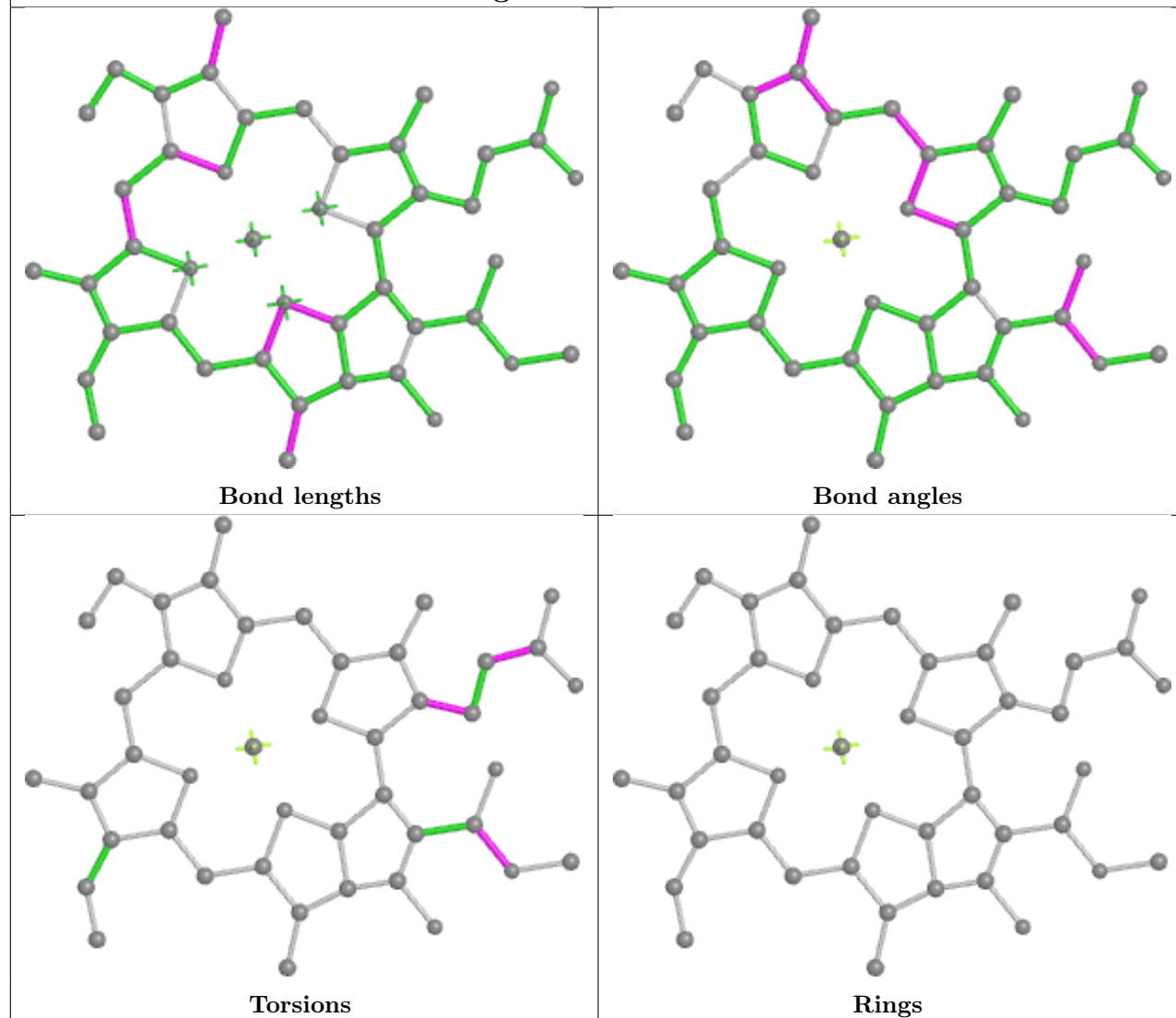
Ligand LHG B 1855



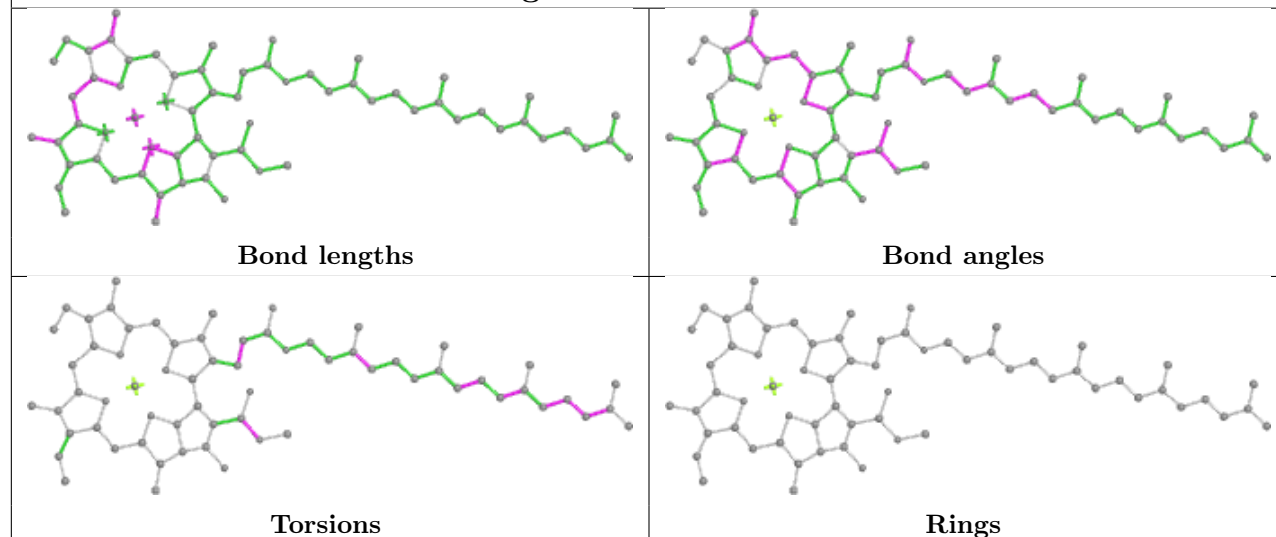
Ligand CLA 4 512



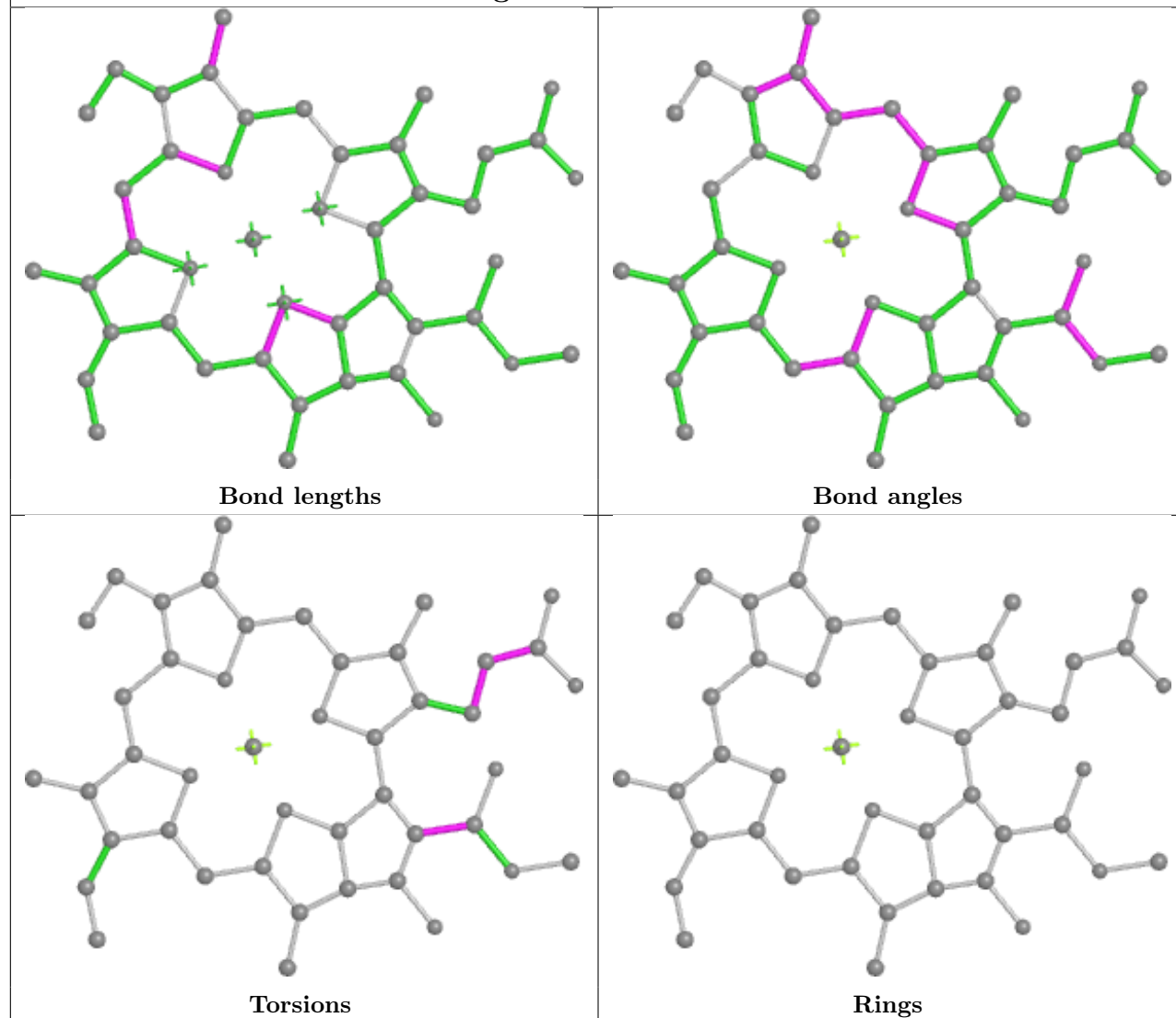
Ligand CLA d 512



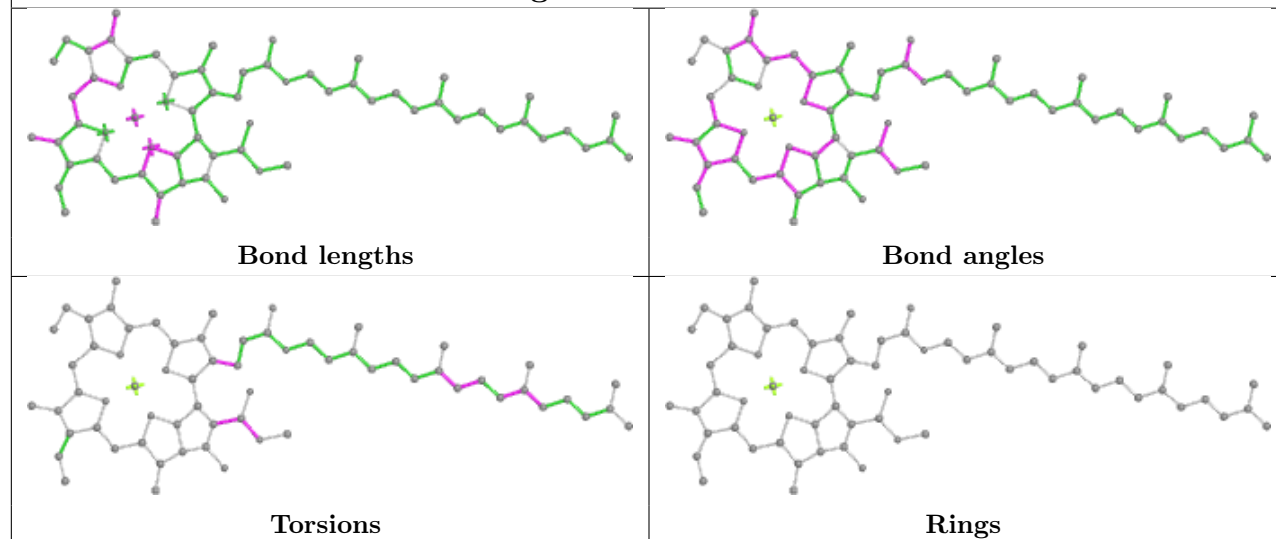
Ligand CLA G 1117



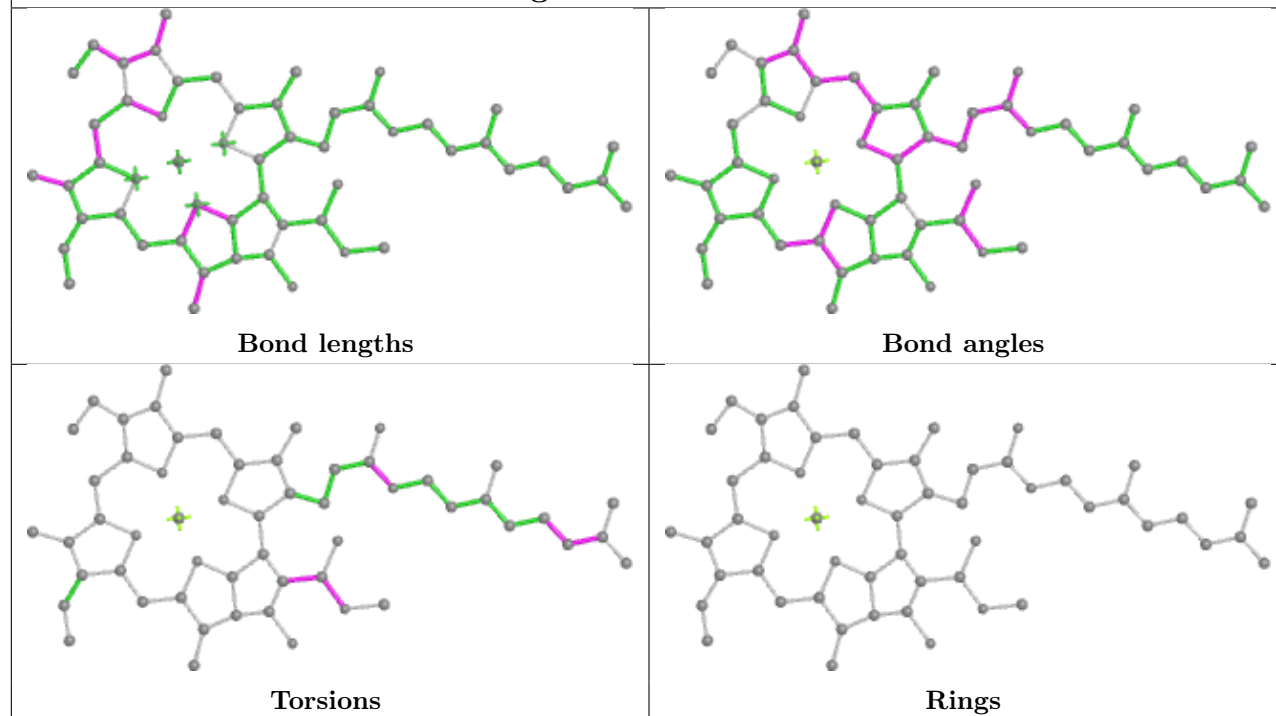
Ligand CLA d 504



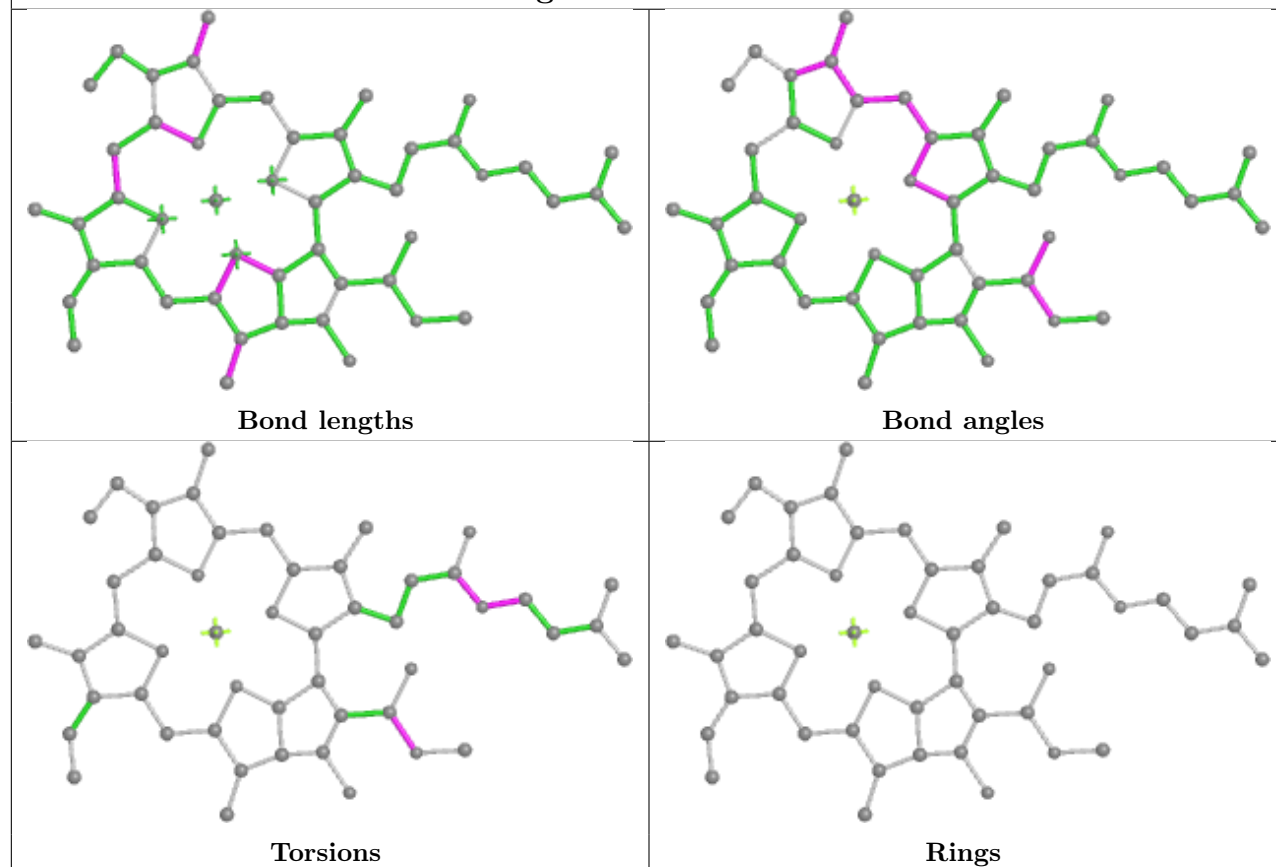
Ligand CLA f 1226



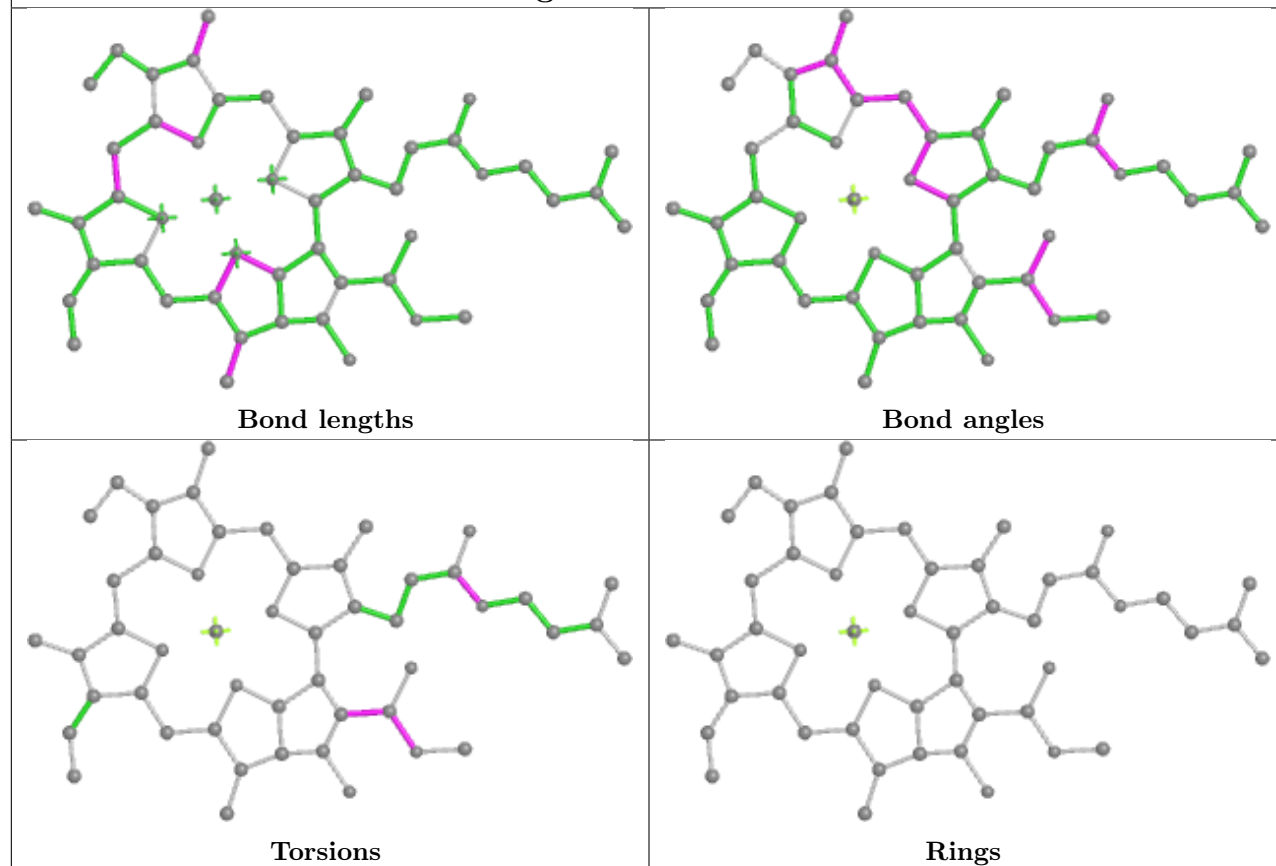
Ligand CLA f 1220



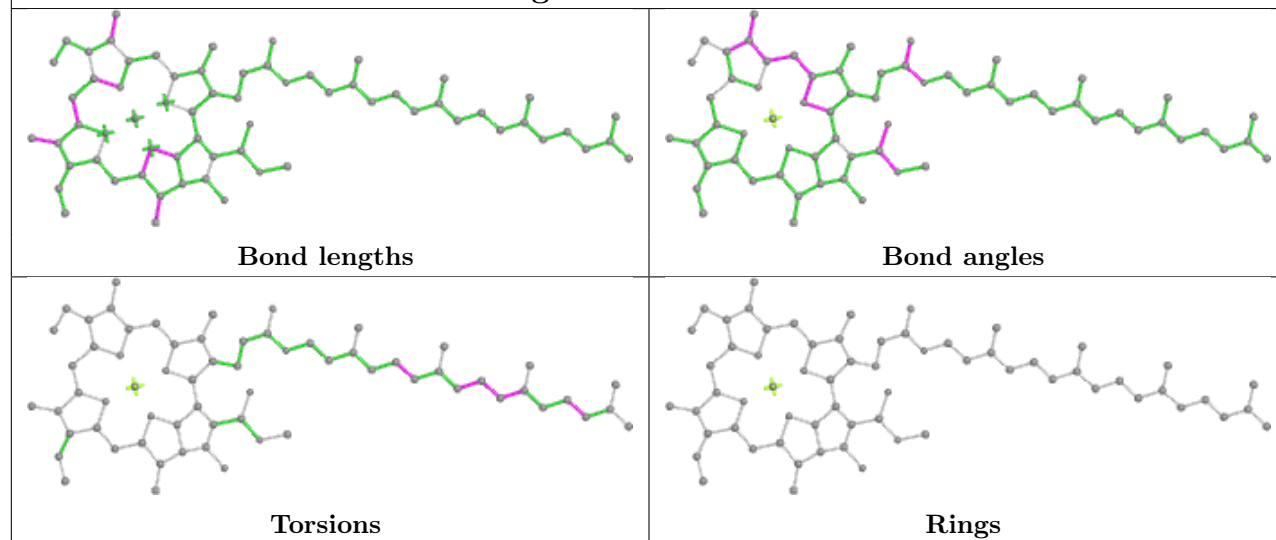
Ligand CLA 3 511

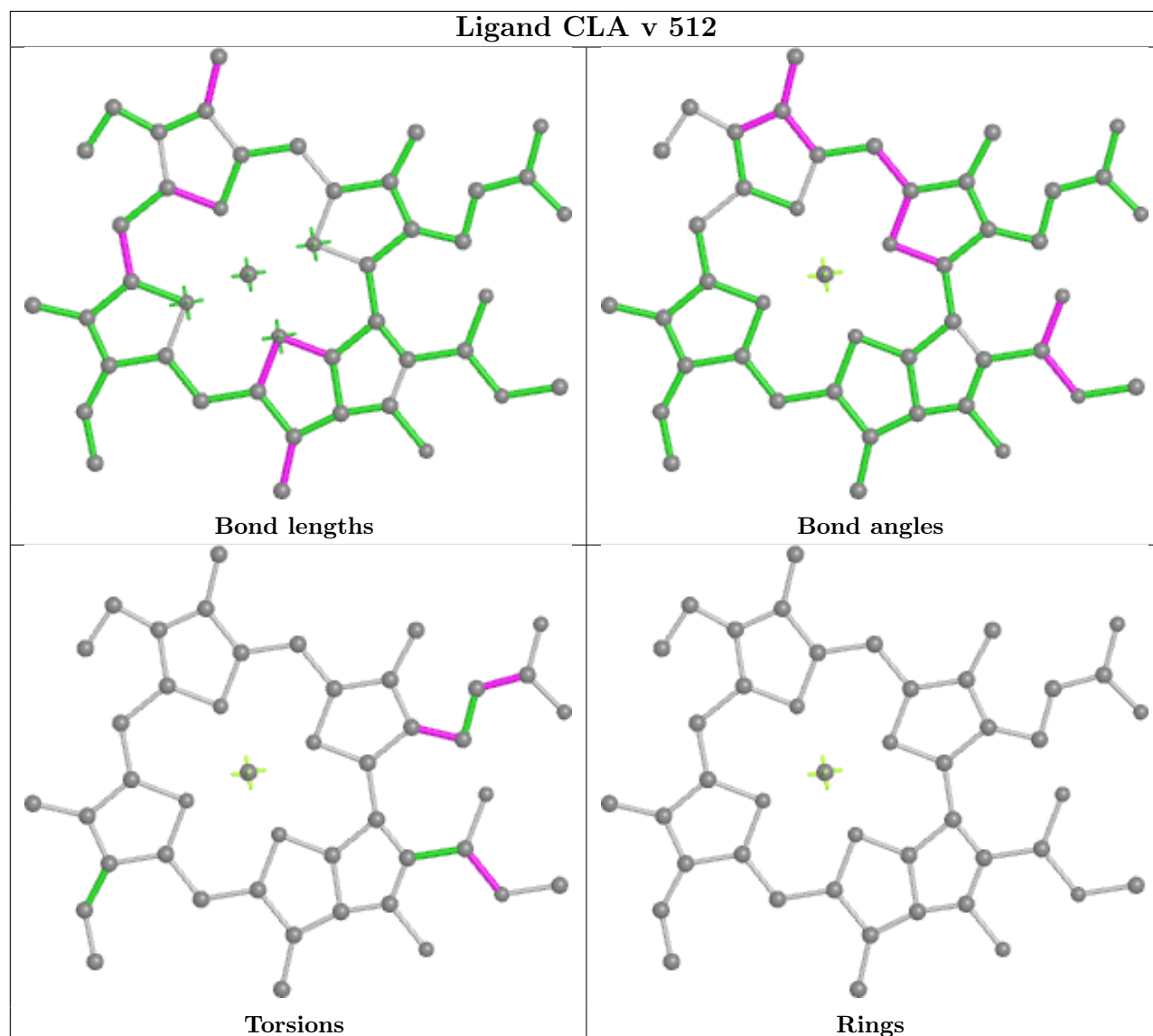
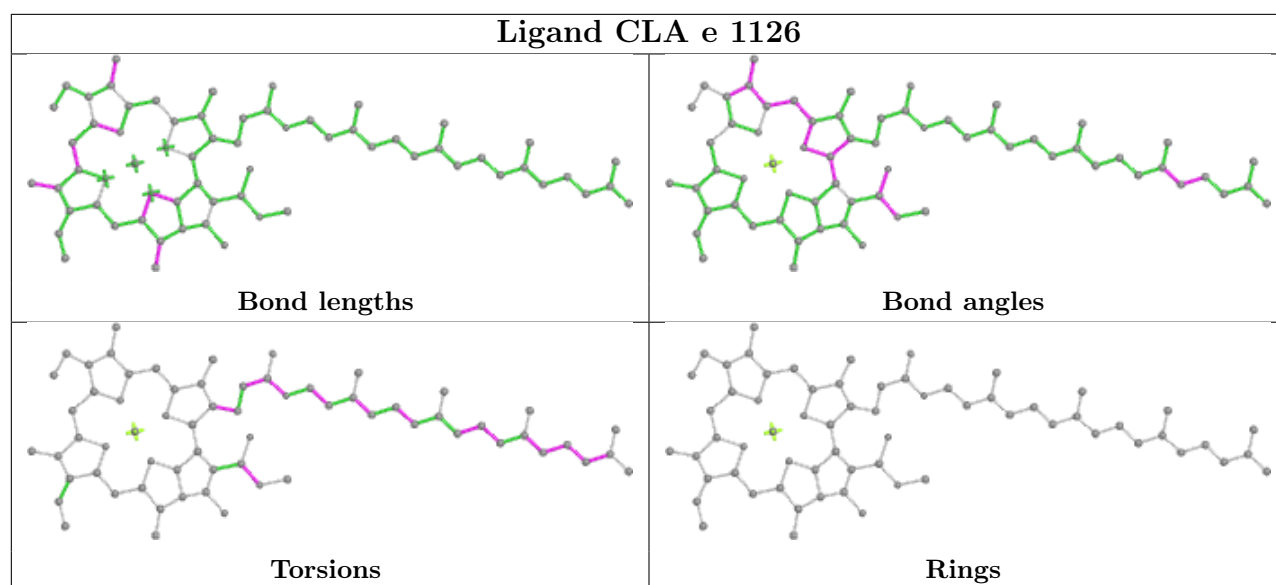


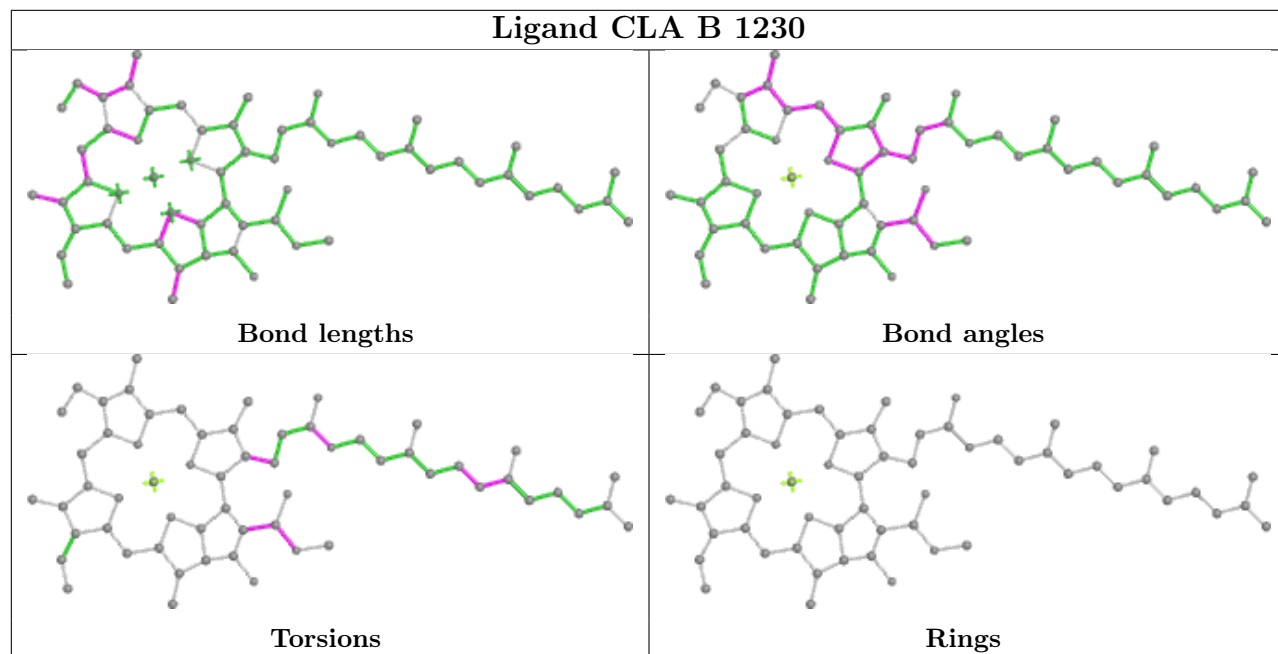
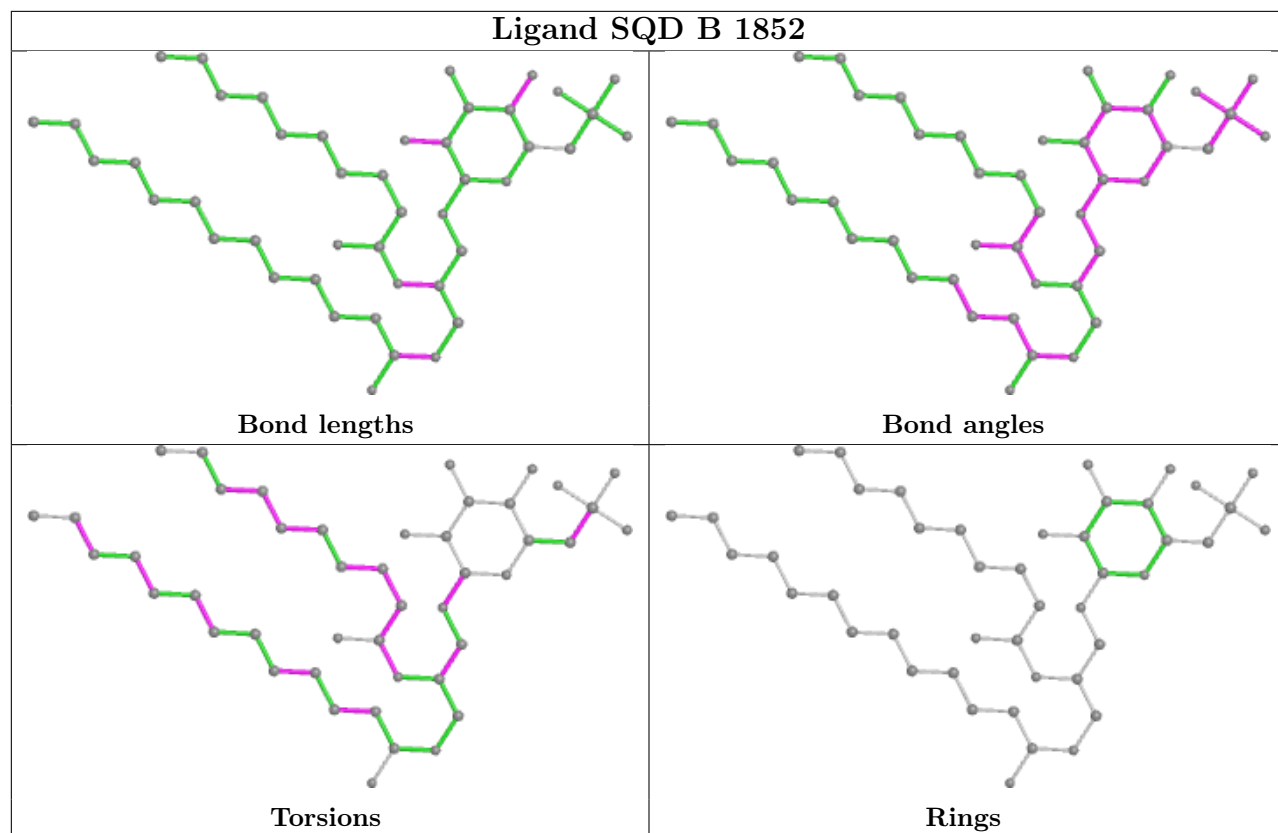
Ligand CLA 4 510

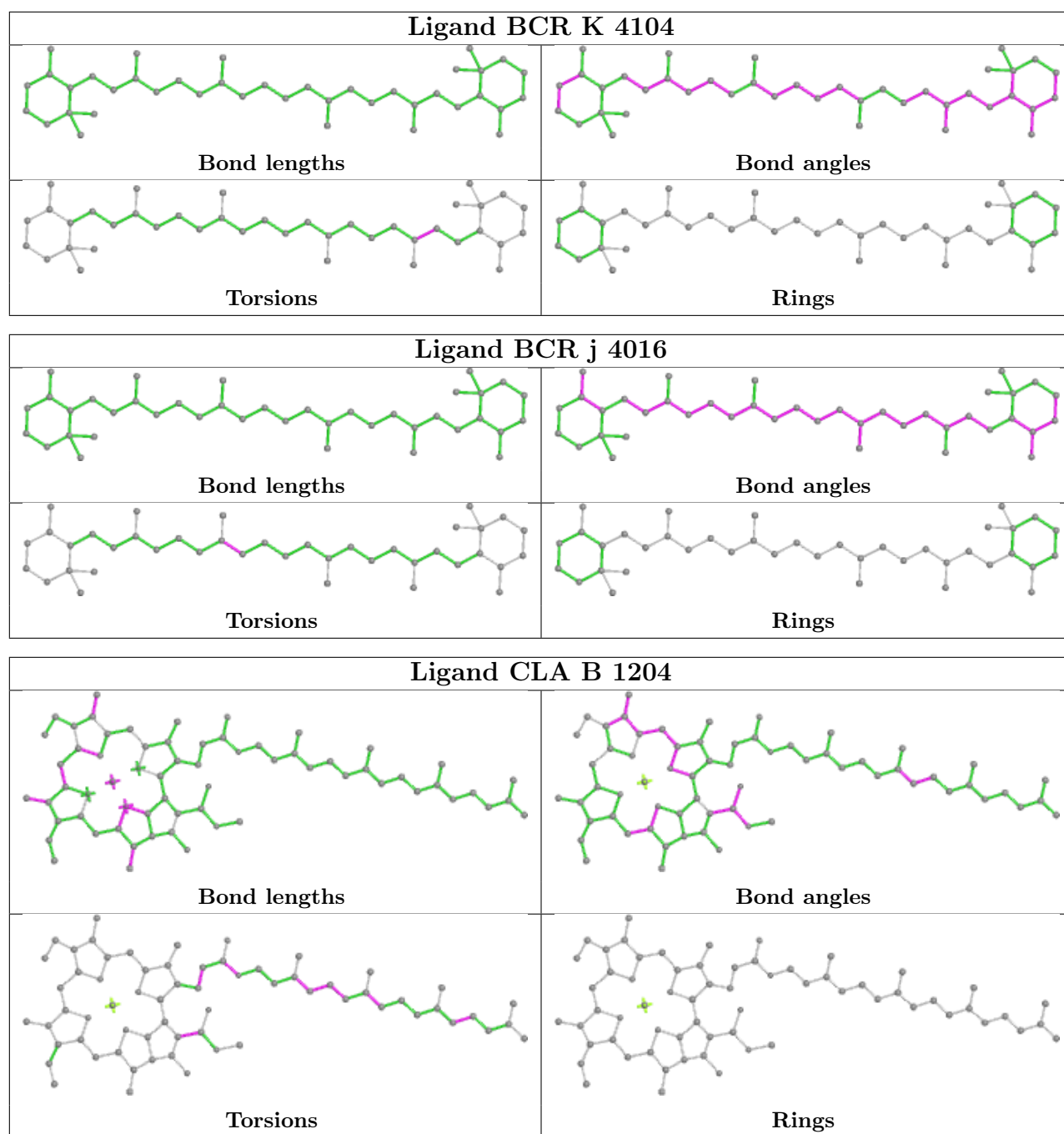


Ligand CLA Y 509

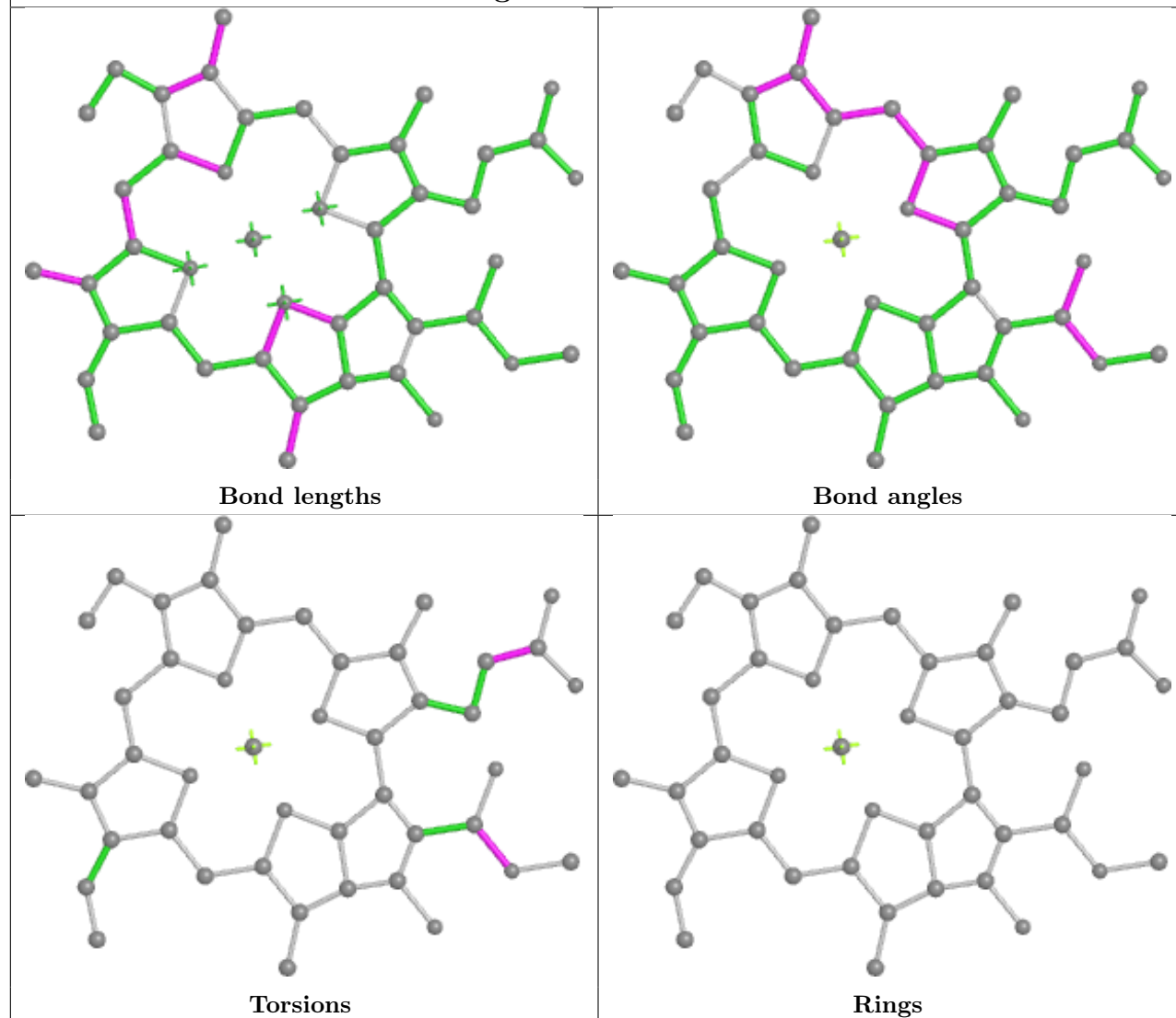




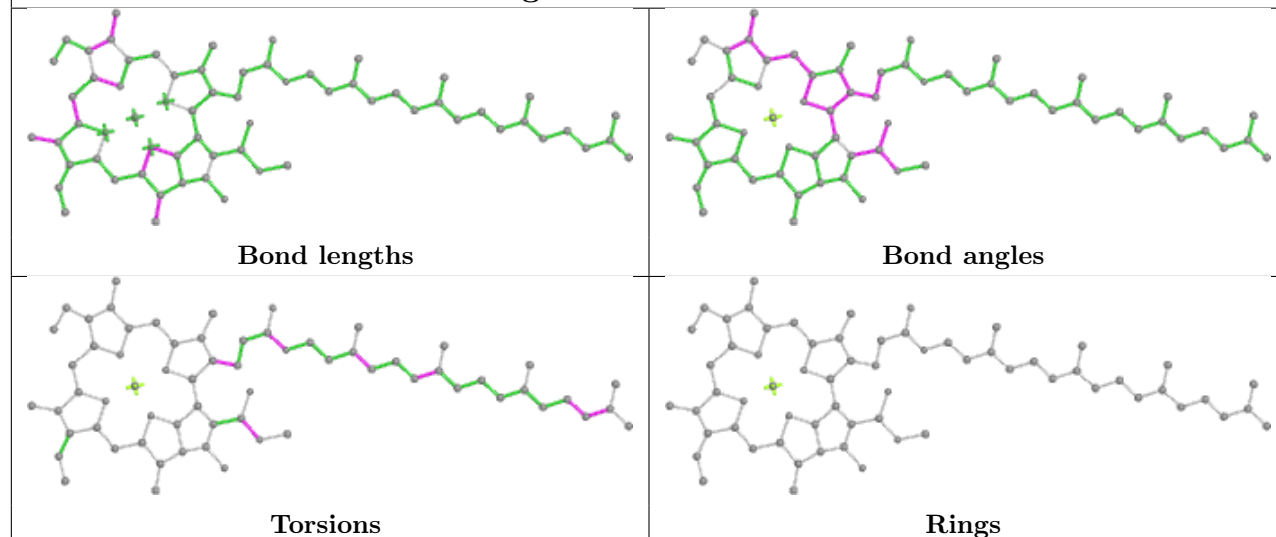


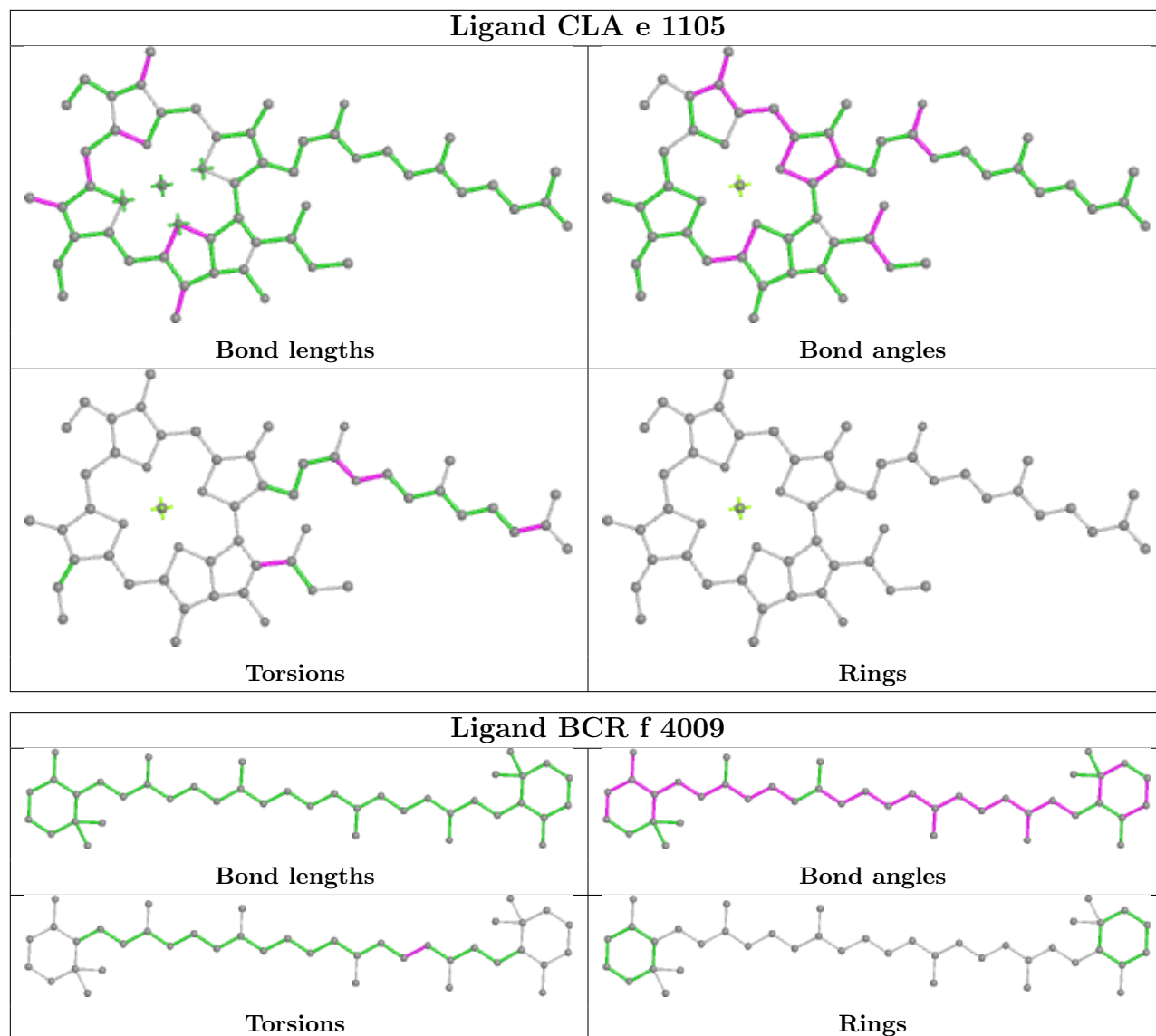


Ligand CLA 5 513

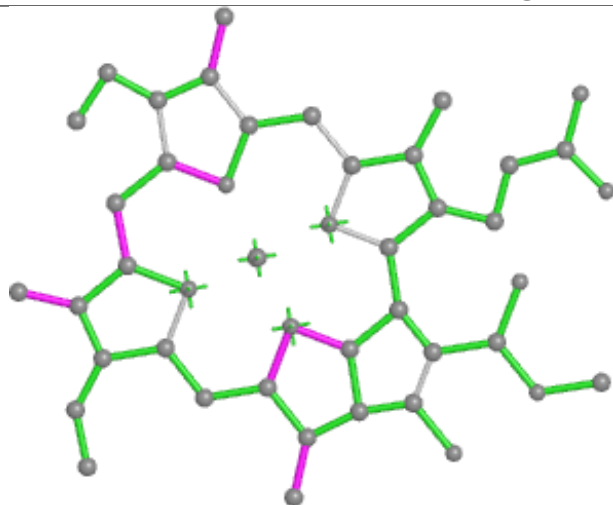


Ligand CLA G 1140

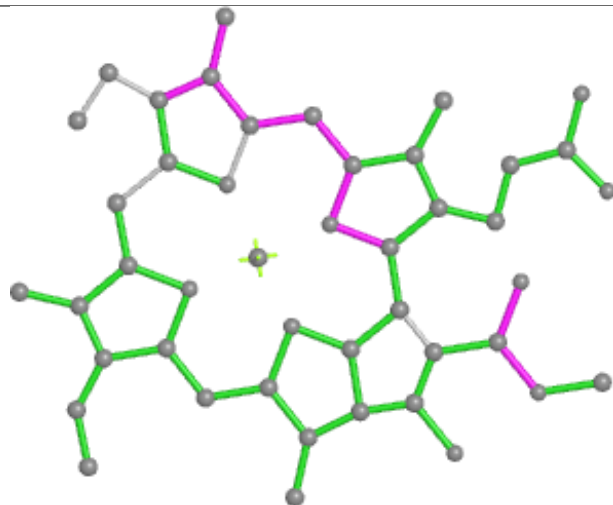




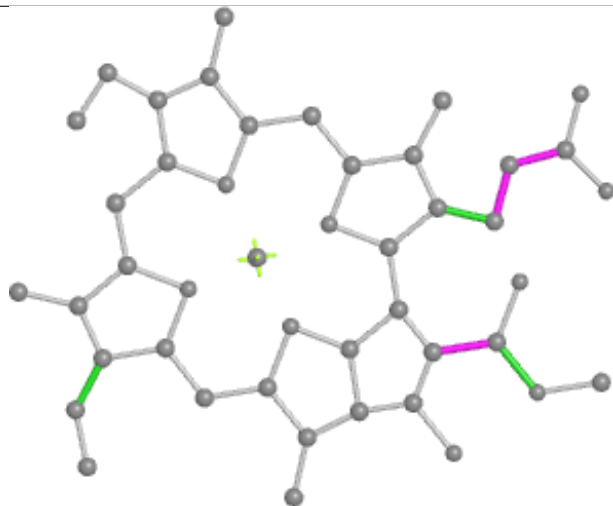
Ligand CLA 1 517



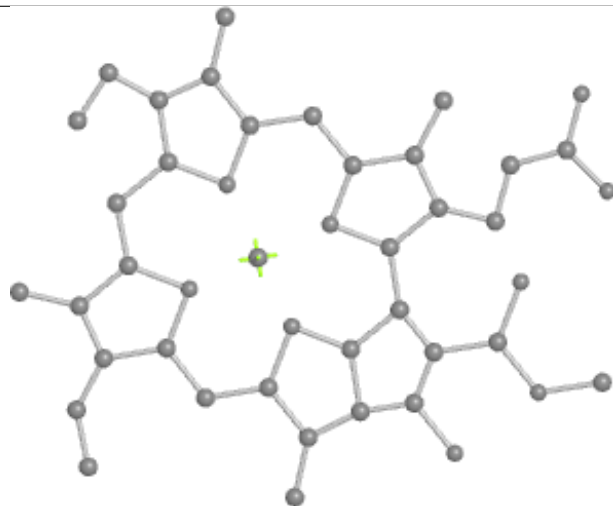
Bond lengths



Bond angles

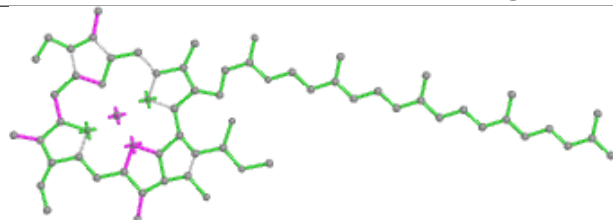


Torsions

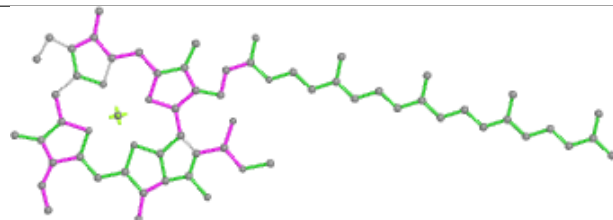


Rings

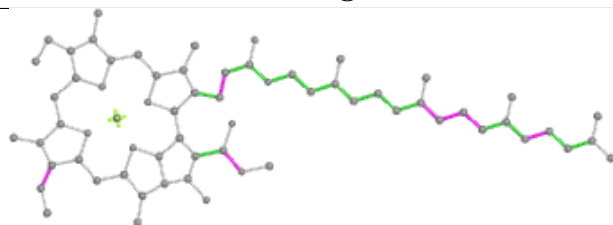
Ligand CLA H 1023



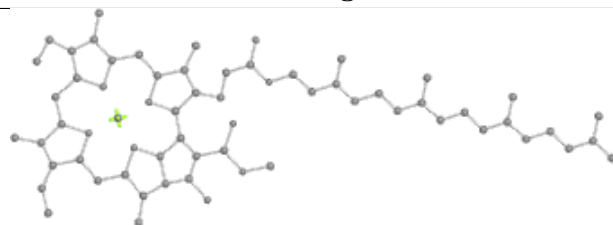
Bond lengths



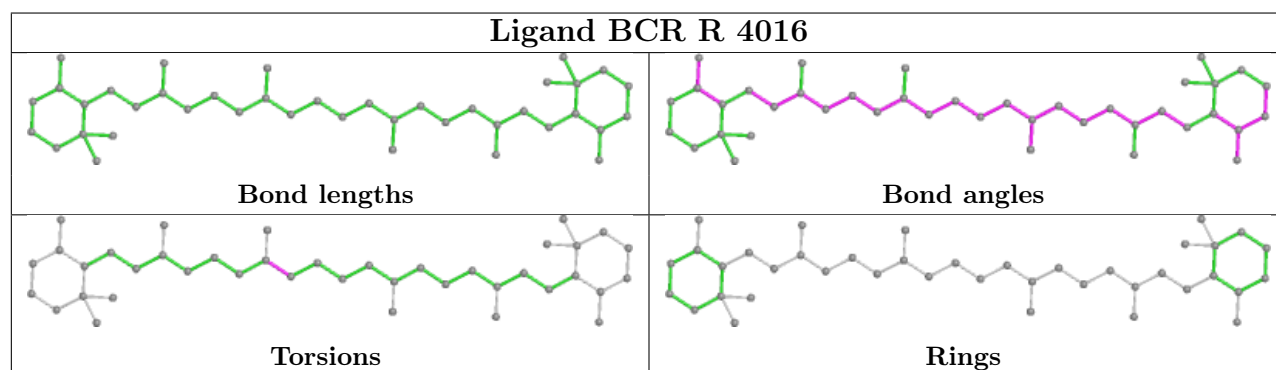
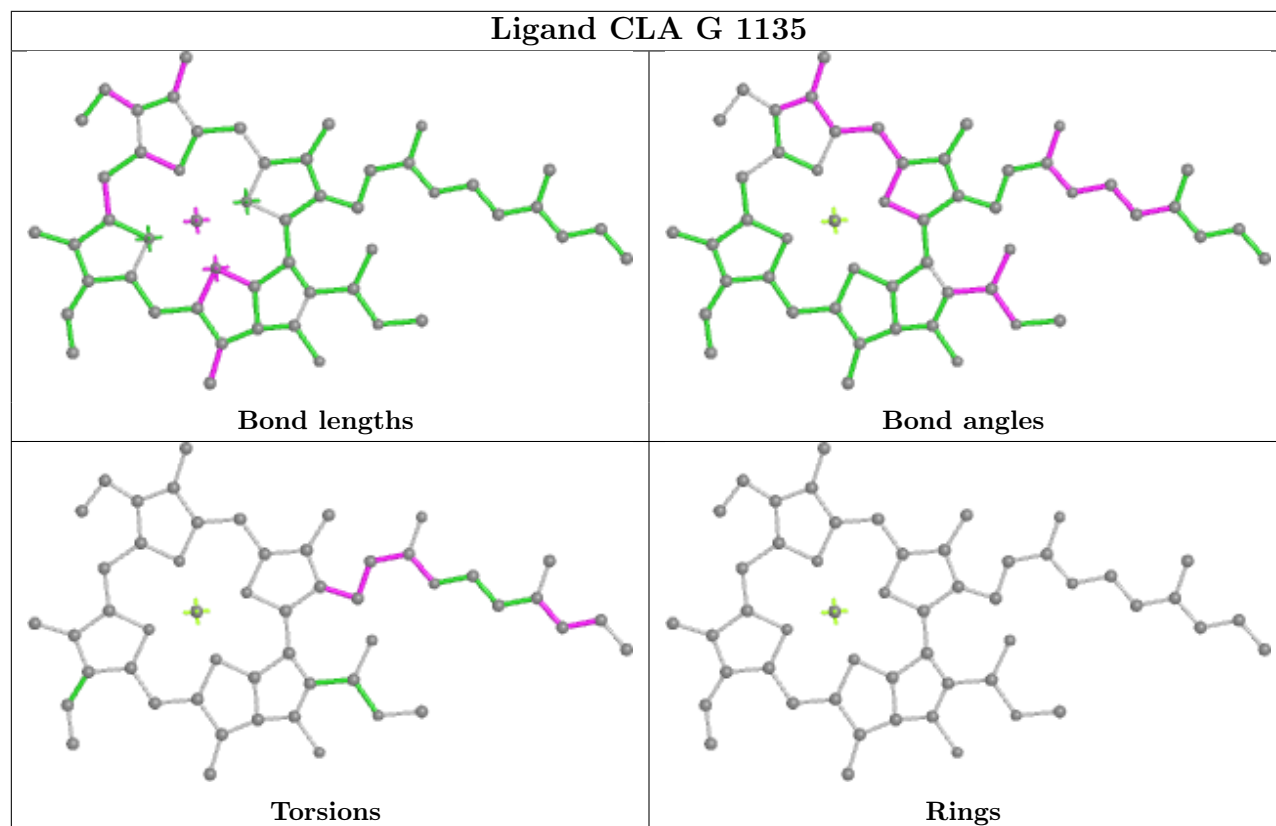
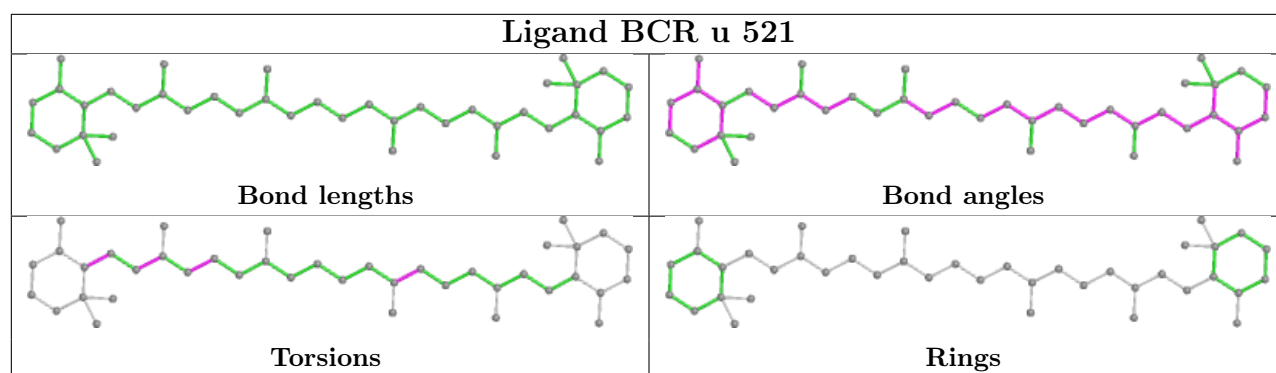
Bond angles

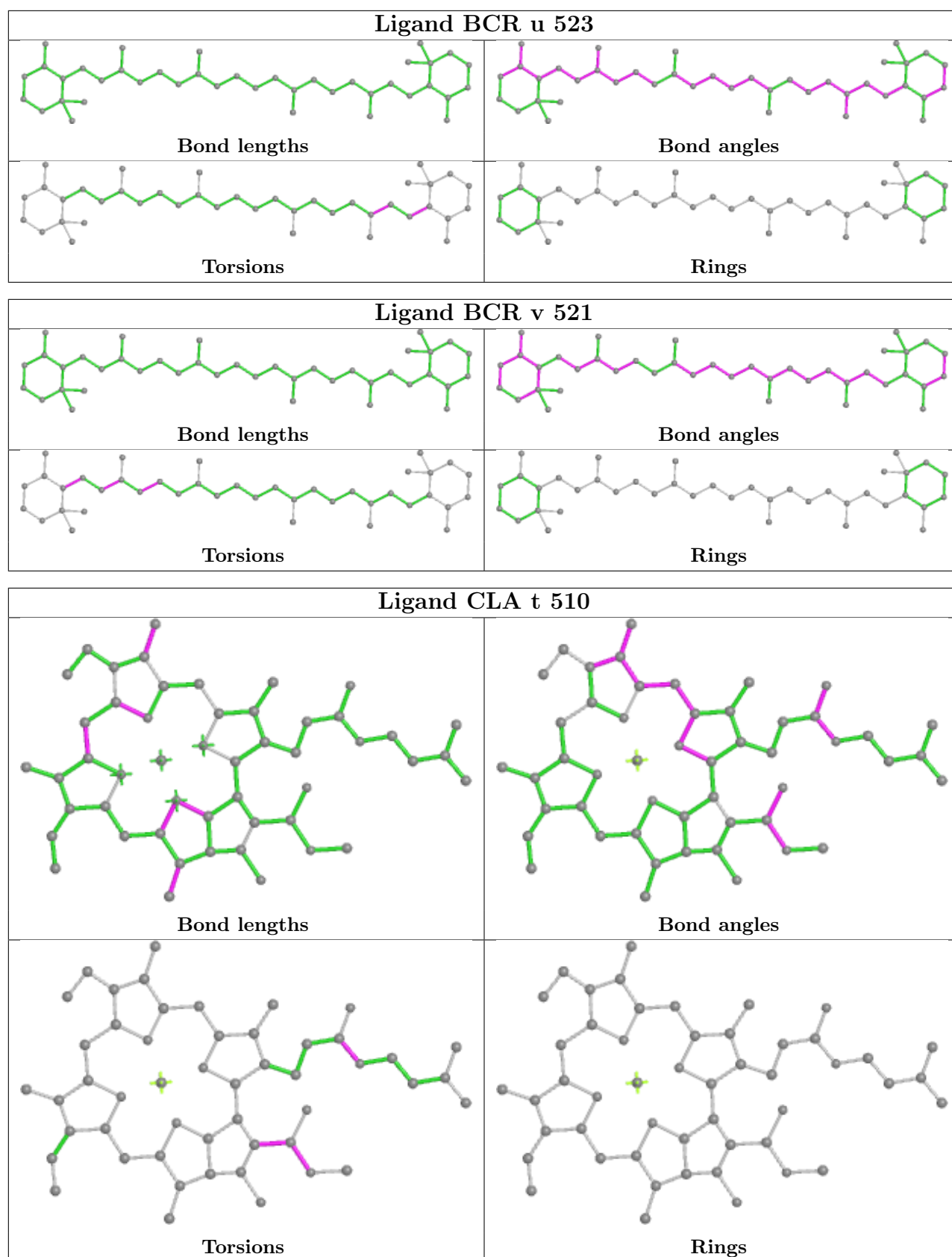


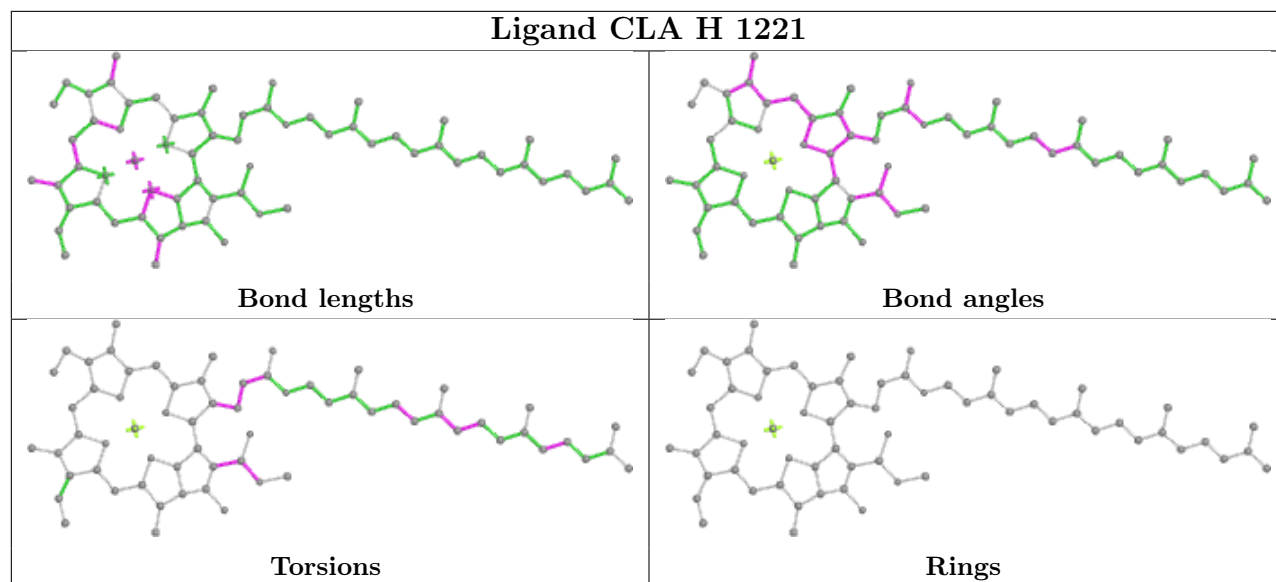
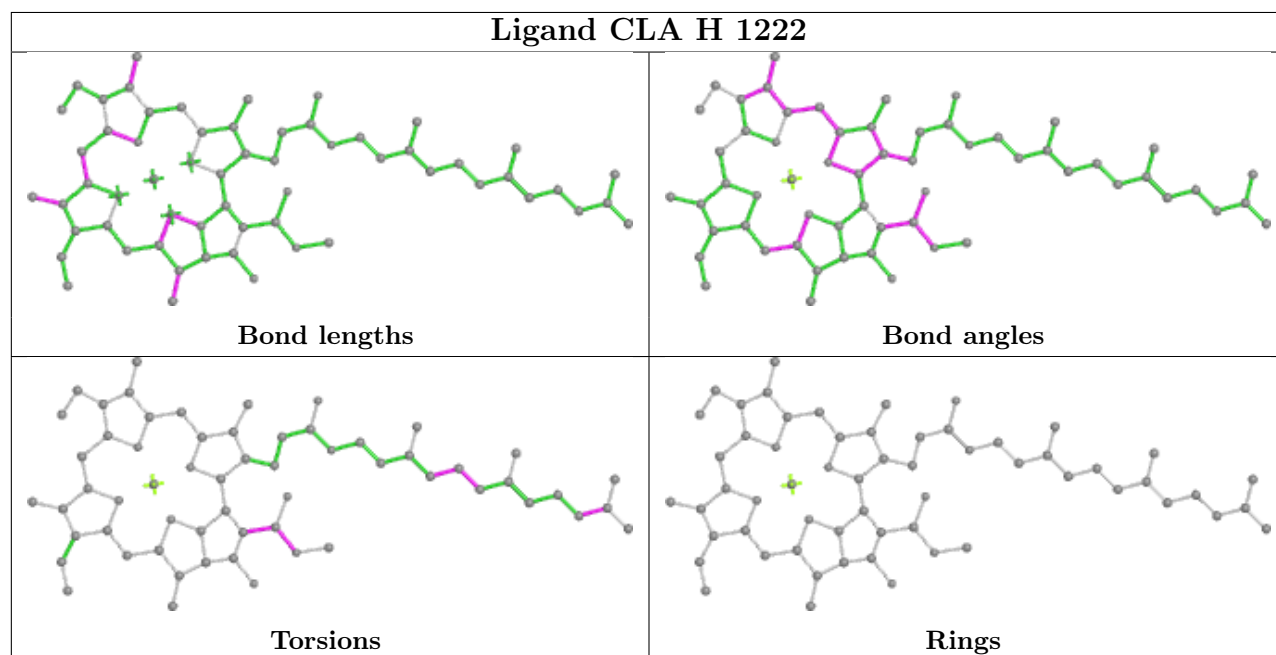
Torsions



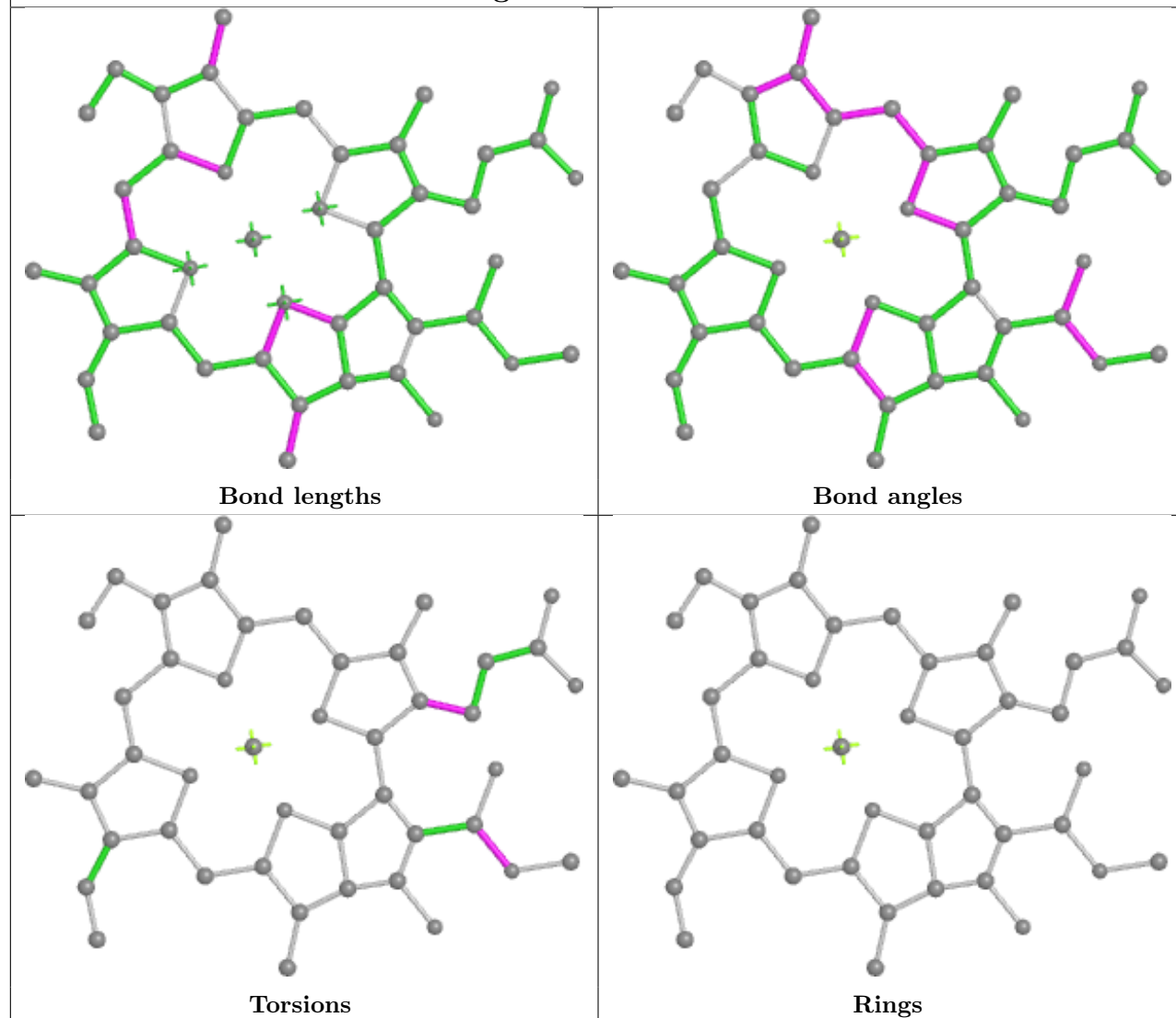
Rings

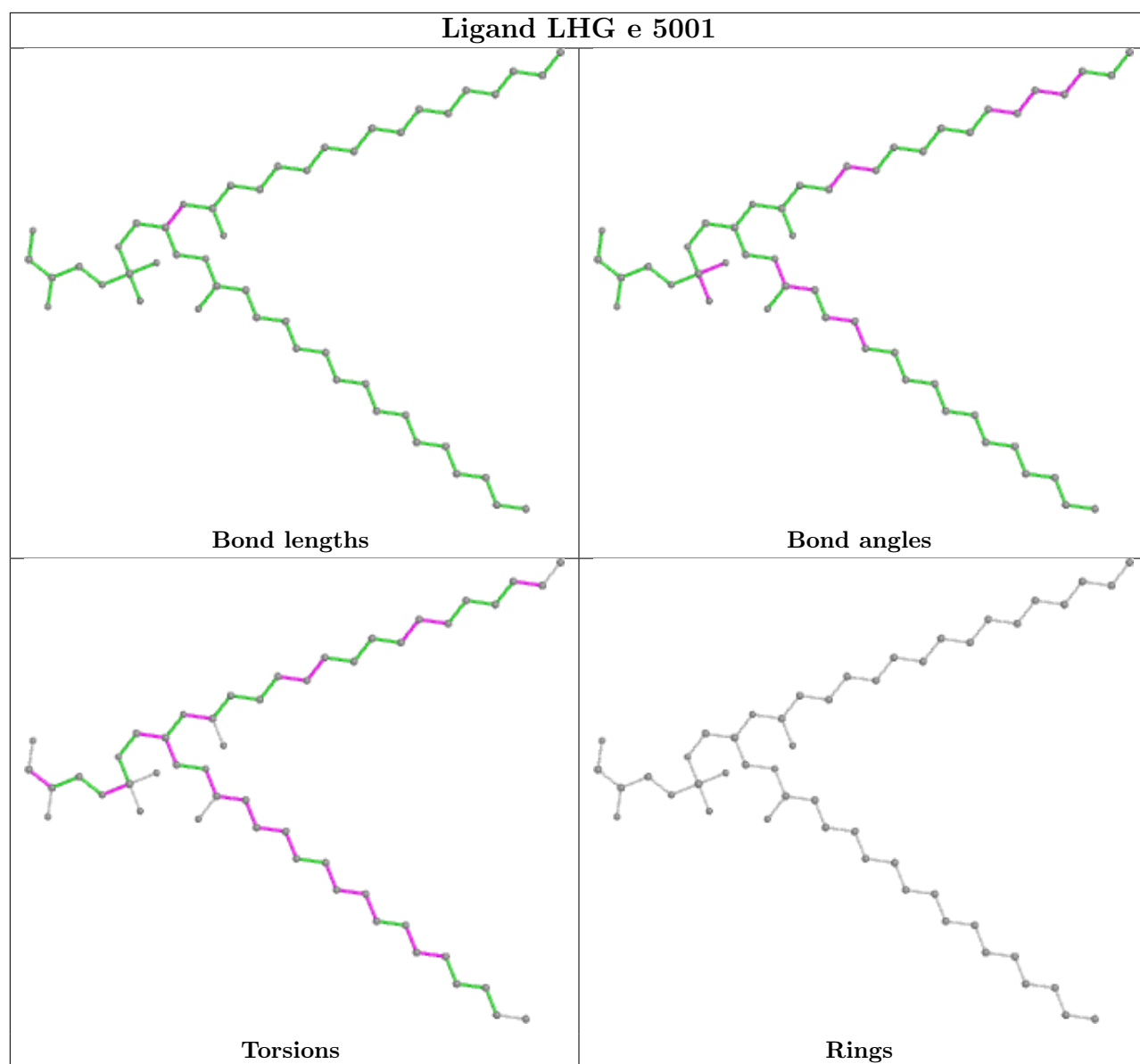




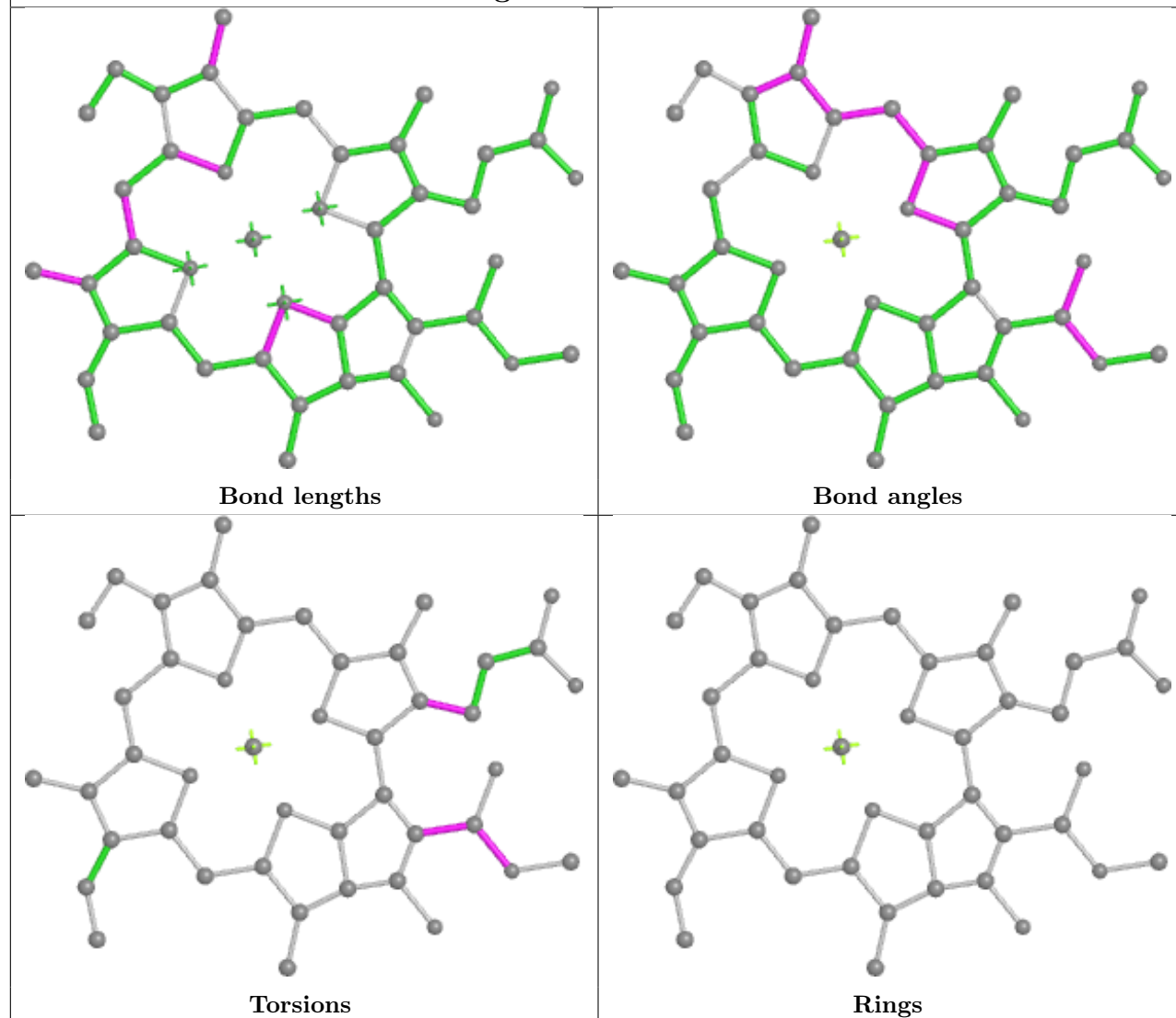
Ligand CLA H 1221**Ligand CLA H 1222**

Ligand CLA b 511

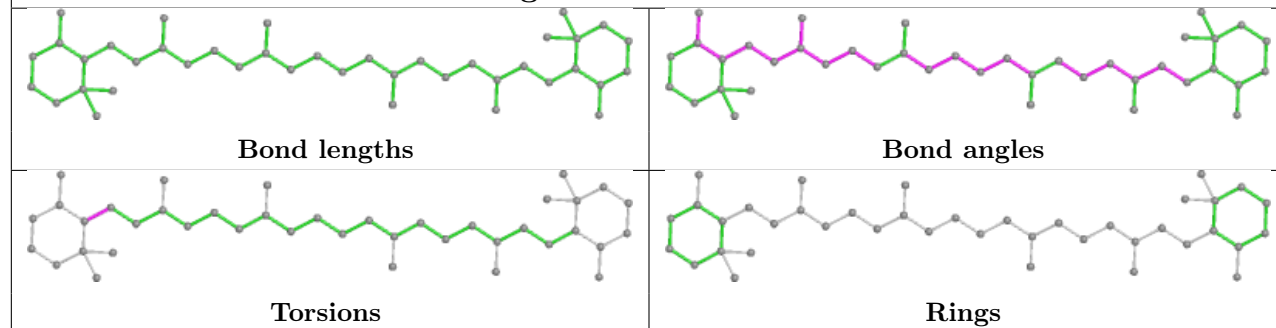


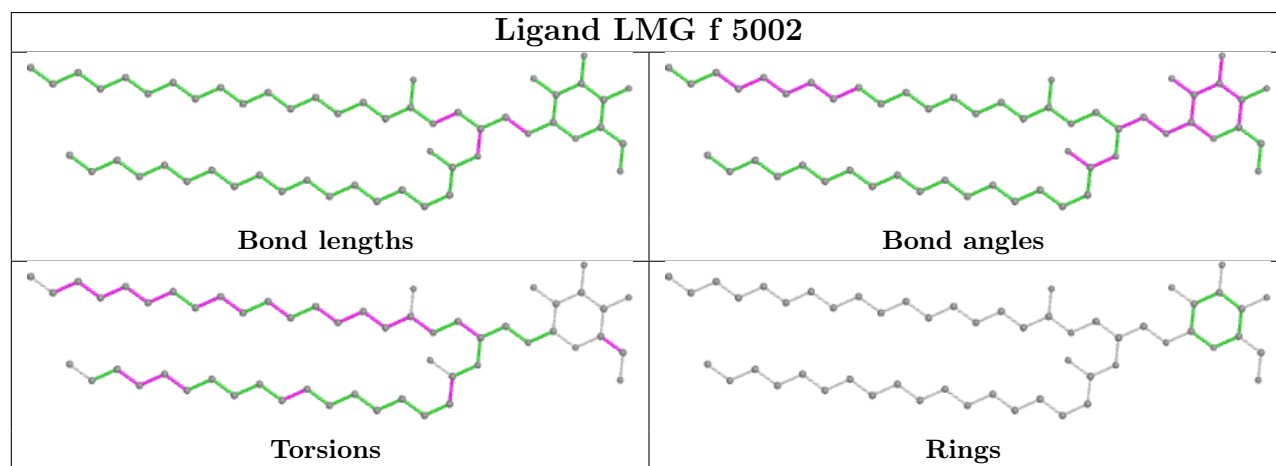
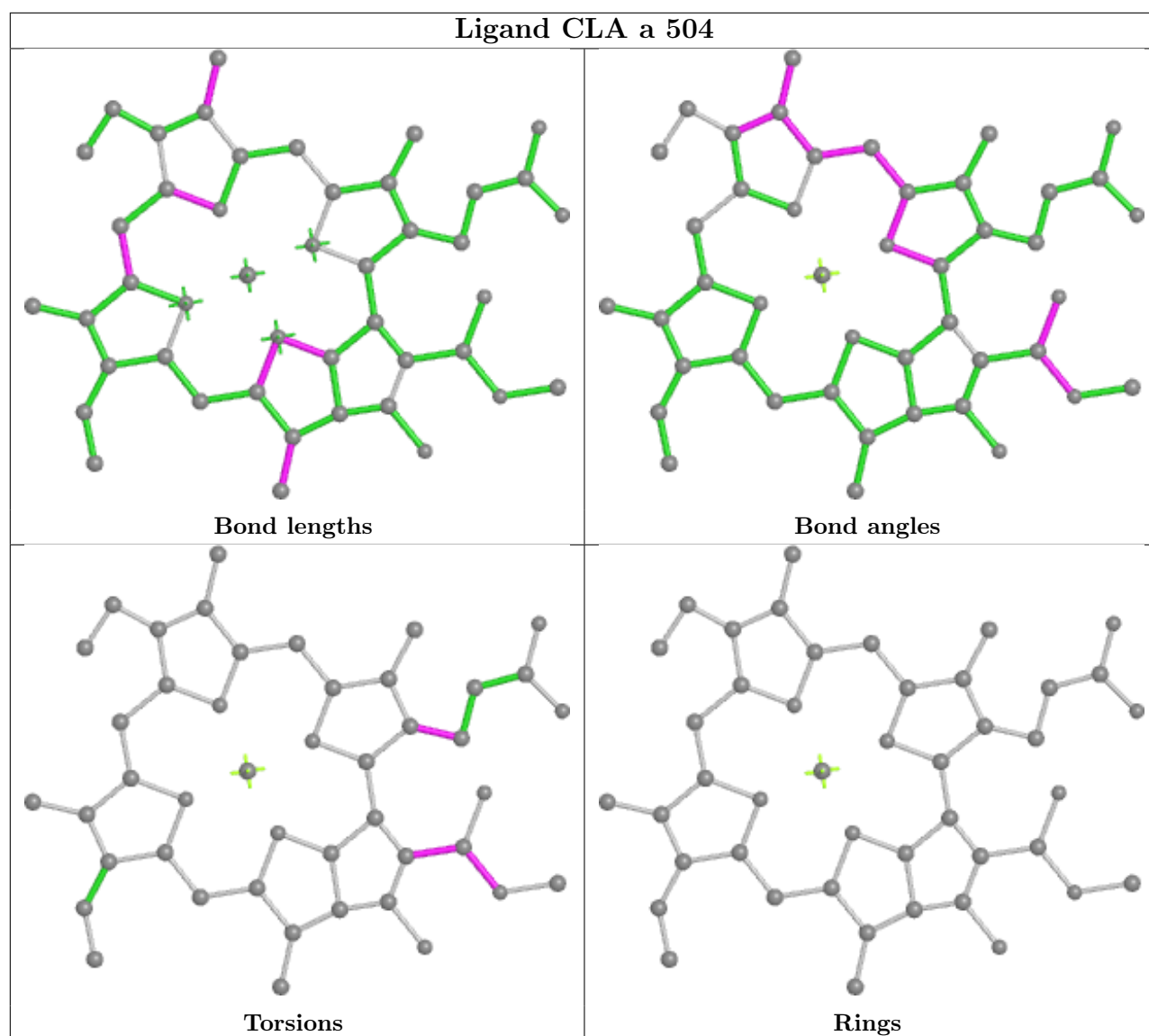


Ligand CLA 1 506

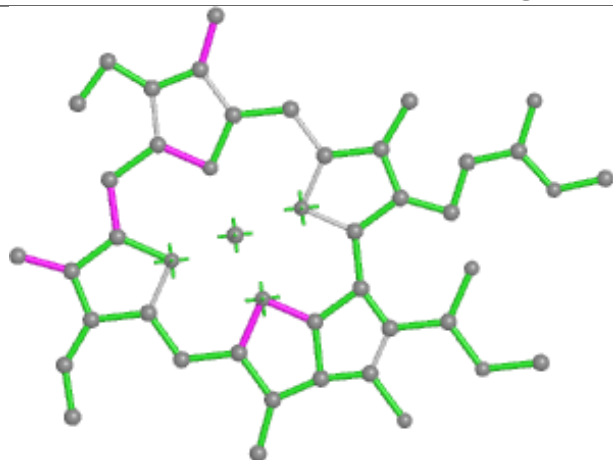


Ligand BCR H 4017

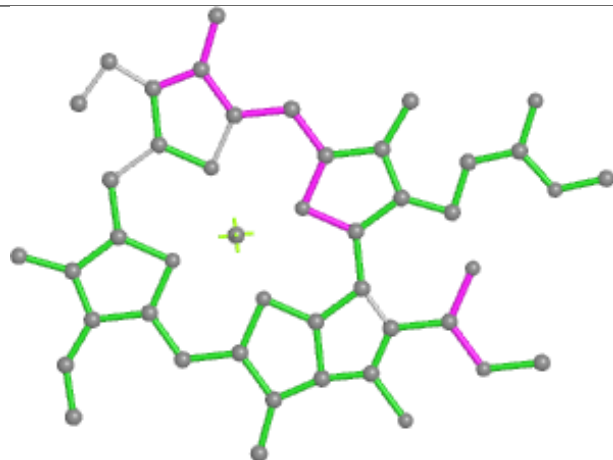




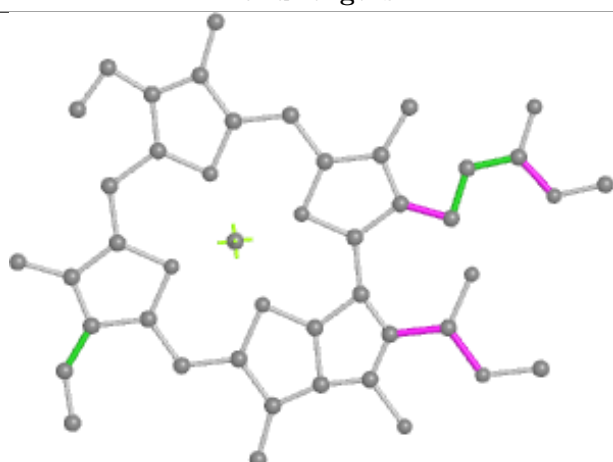
Ligand CLA d 519



Bond lengths



Bond angles

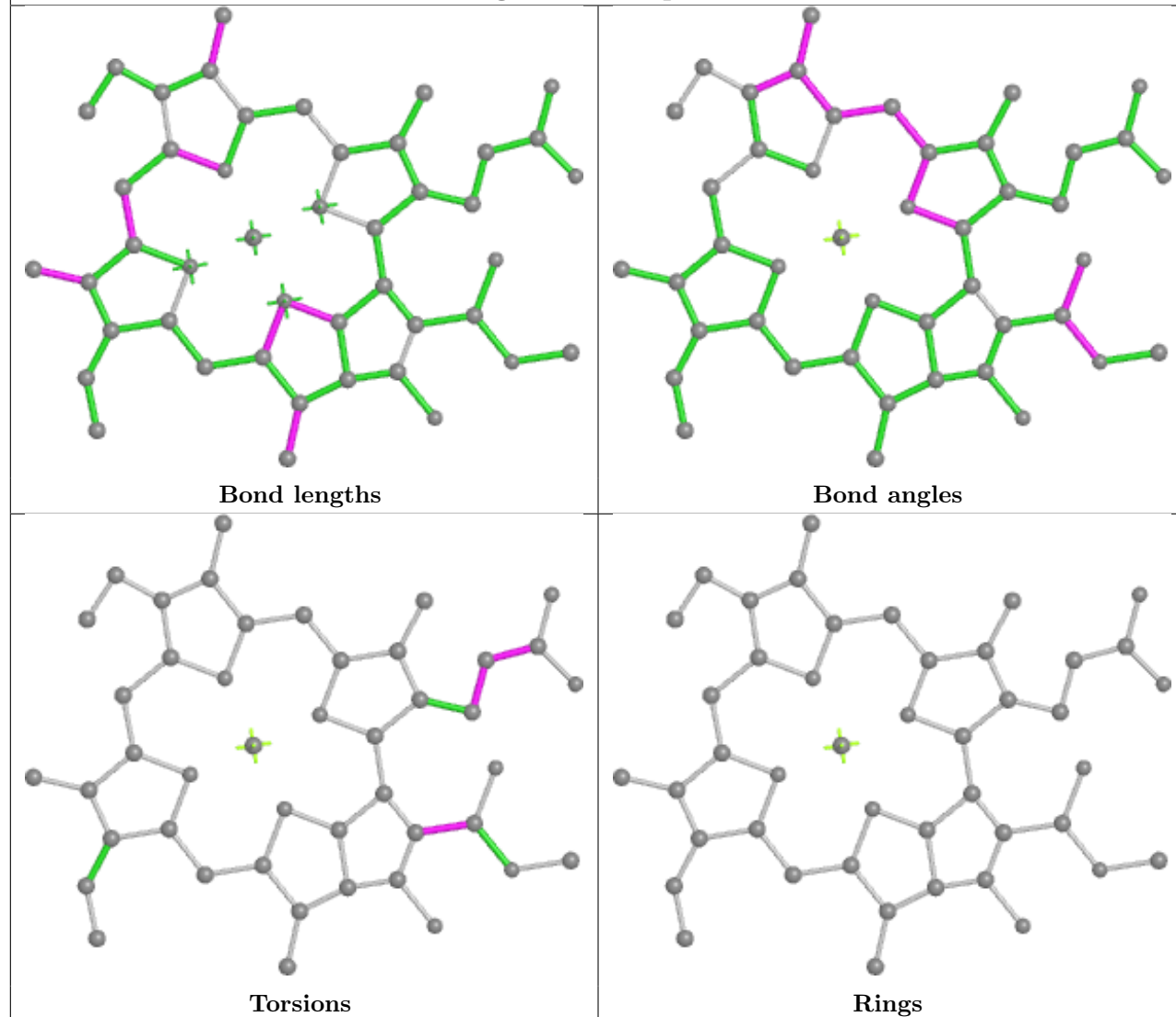


Torsions

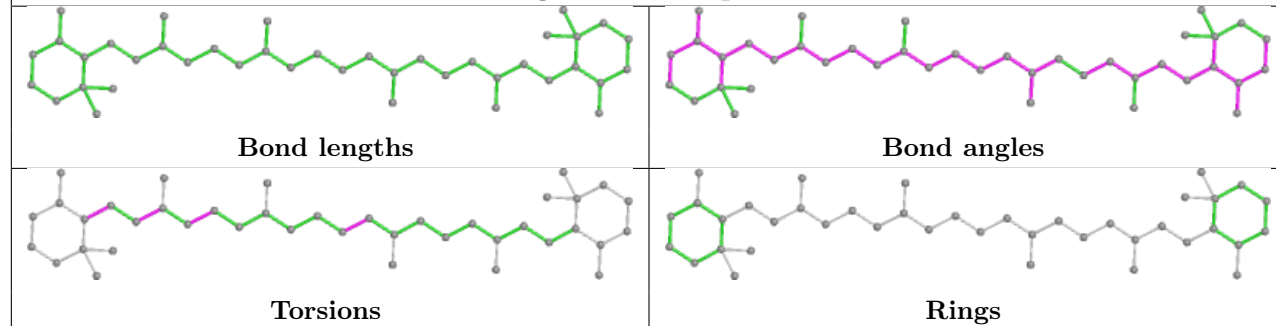


Rings

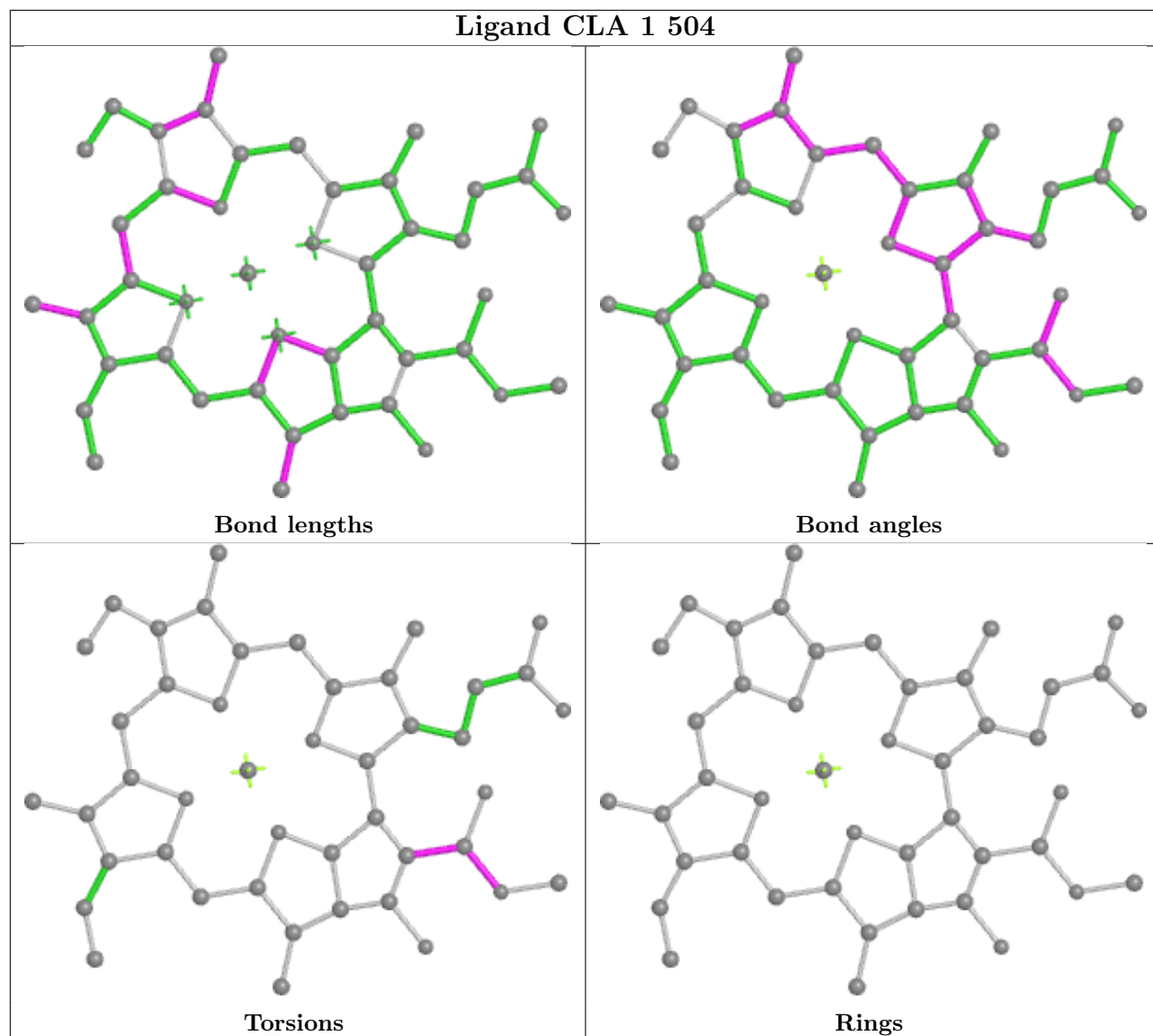
Ligand CLA q 517



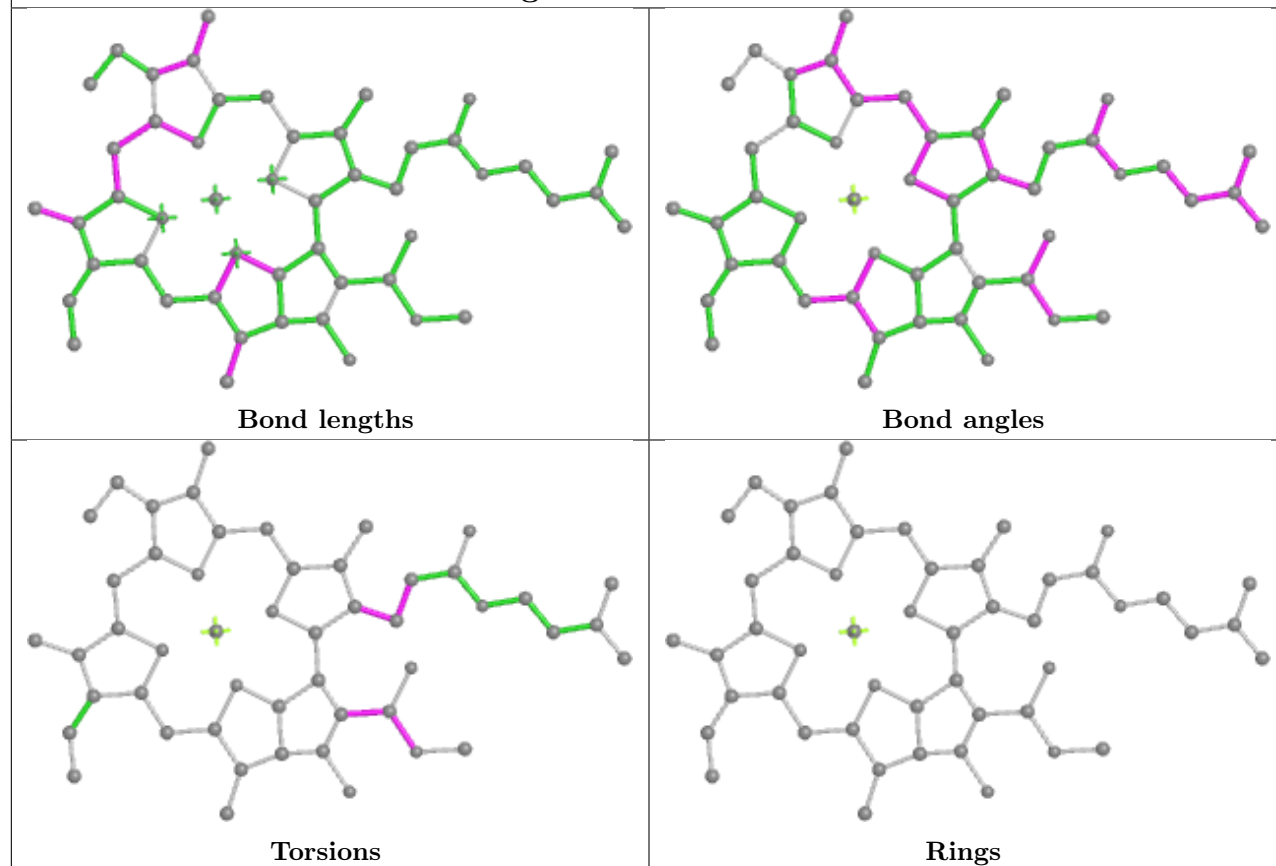
Ligand BCR q 522



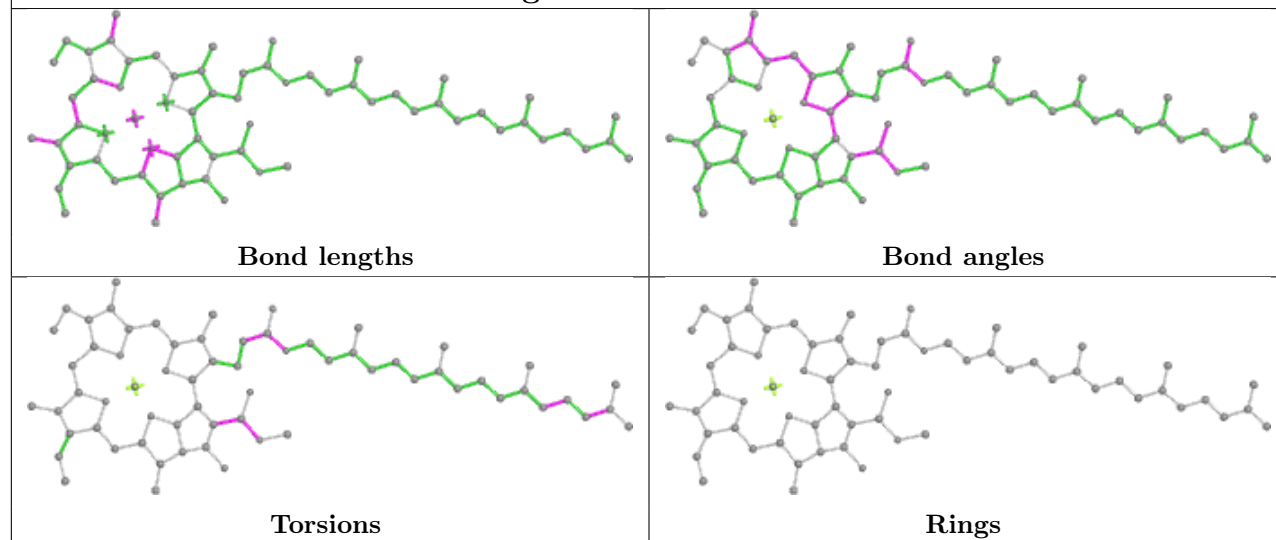
Ligand CLA 1 504



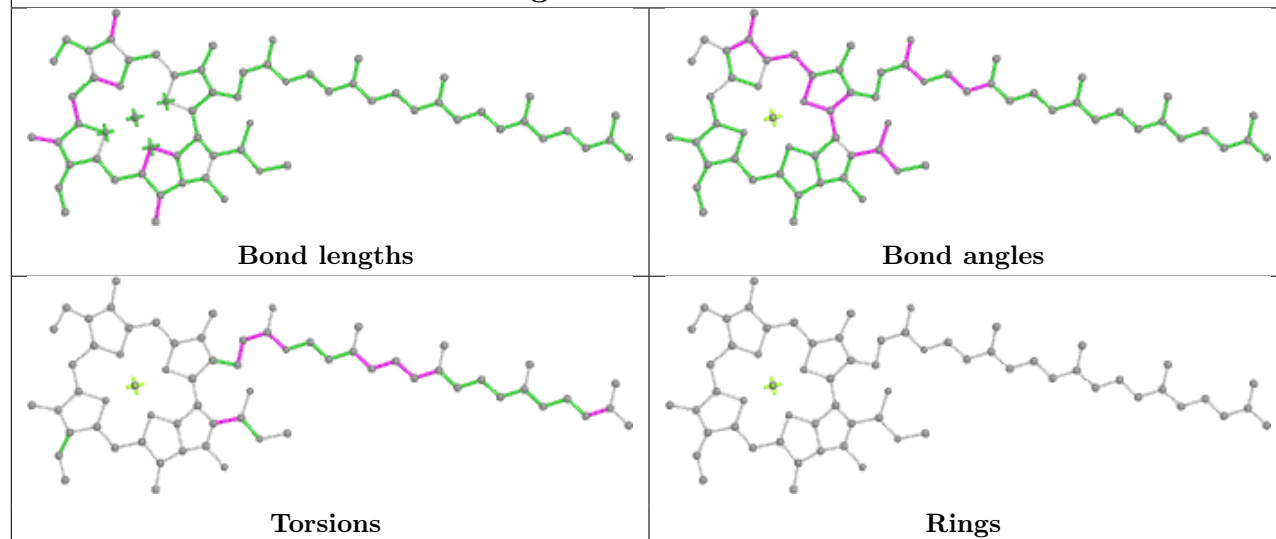
Ligand CLA m 1103



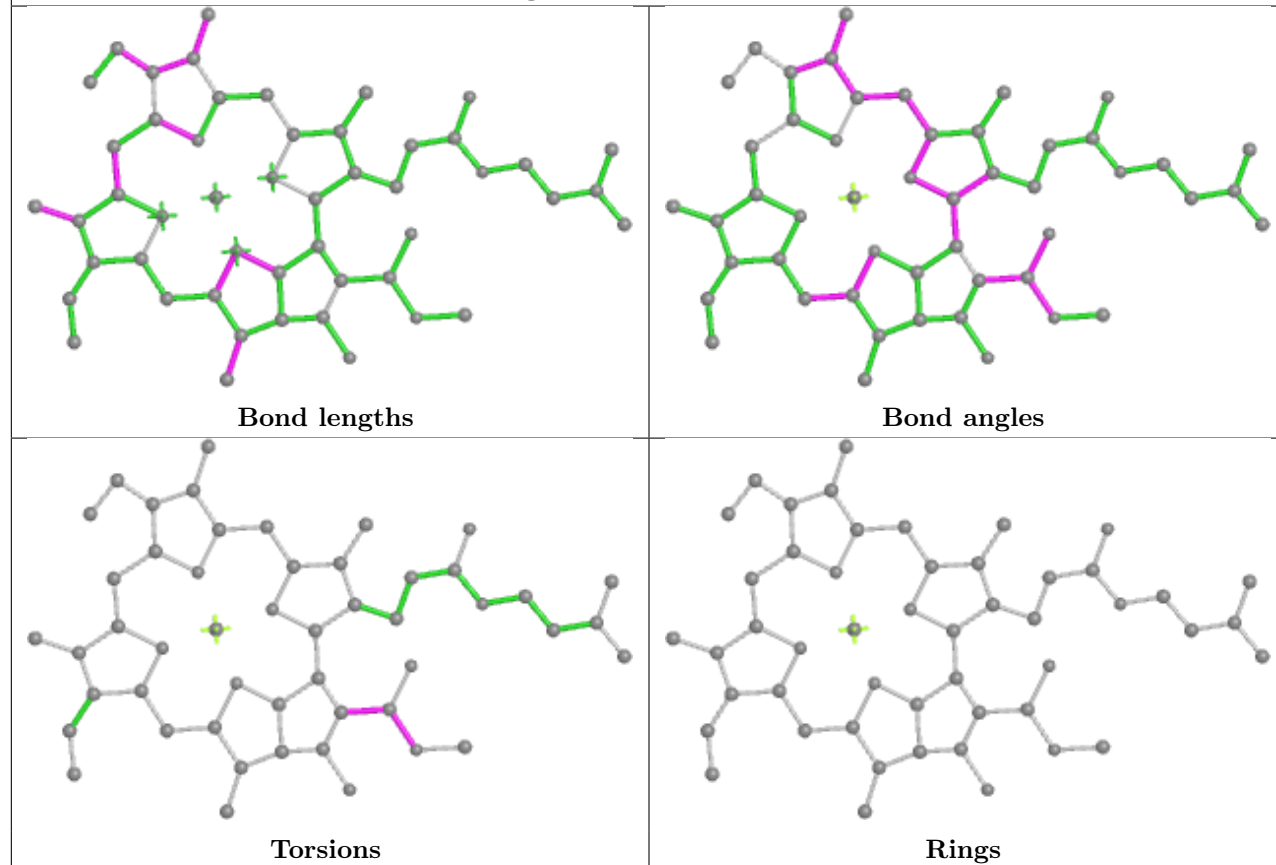
Ligand CLA H 1021

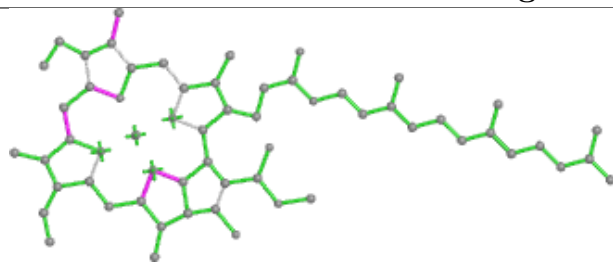
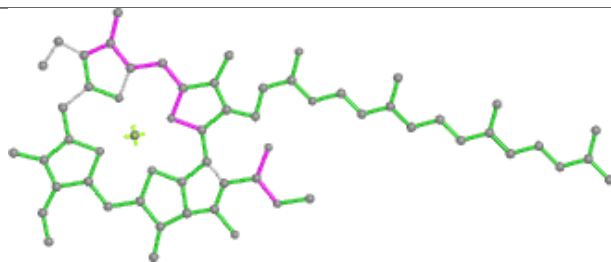
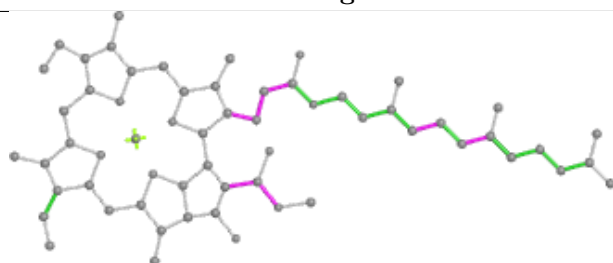
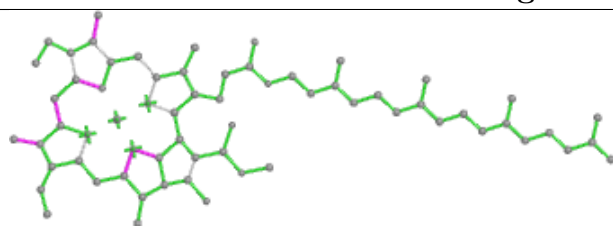
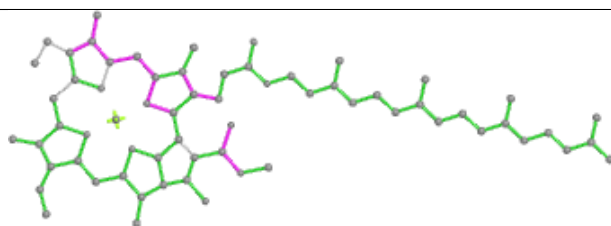
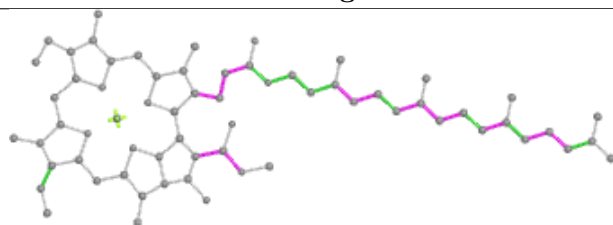
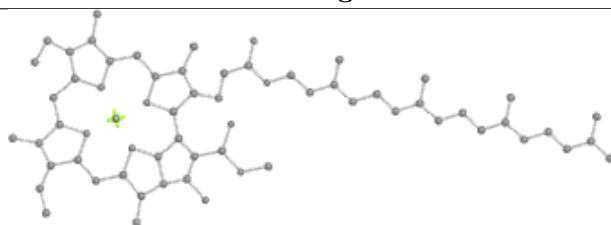


Ligand CLA f 1213

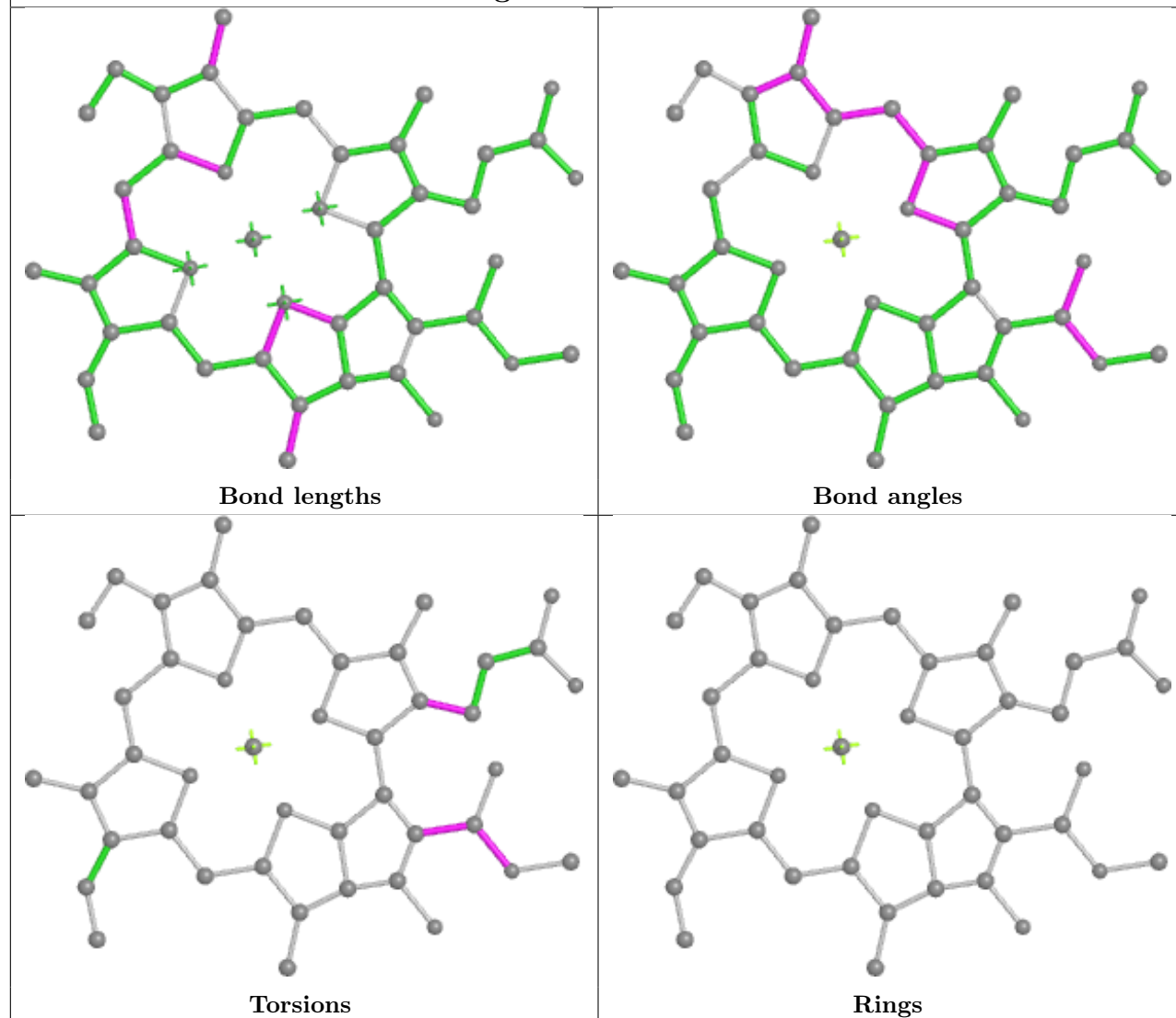


Ligand CLA A 1112

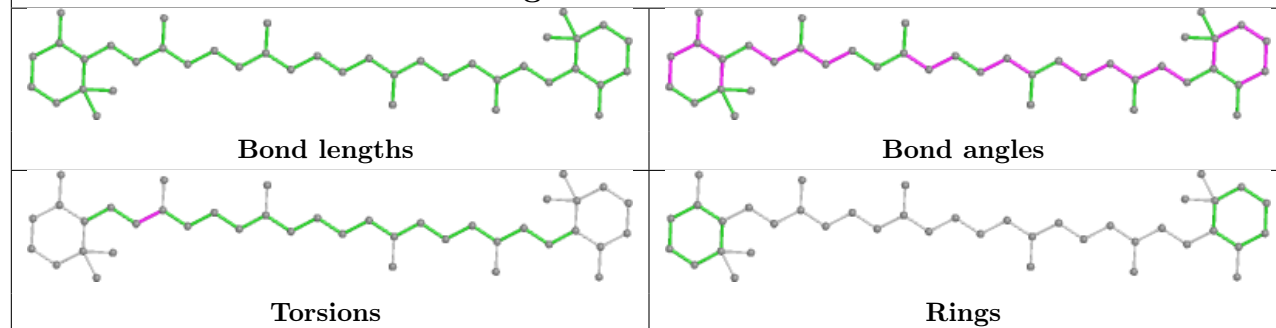


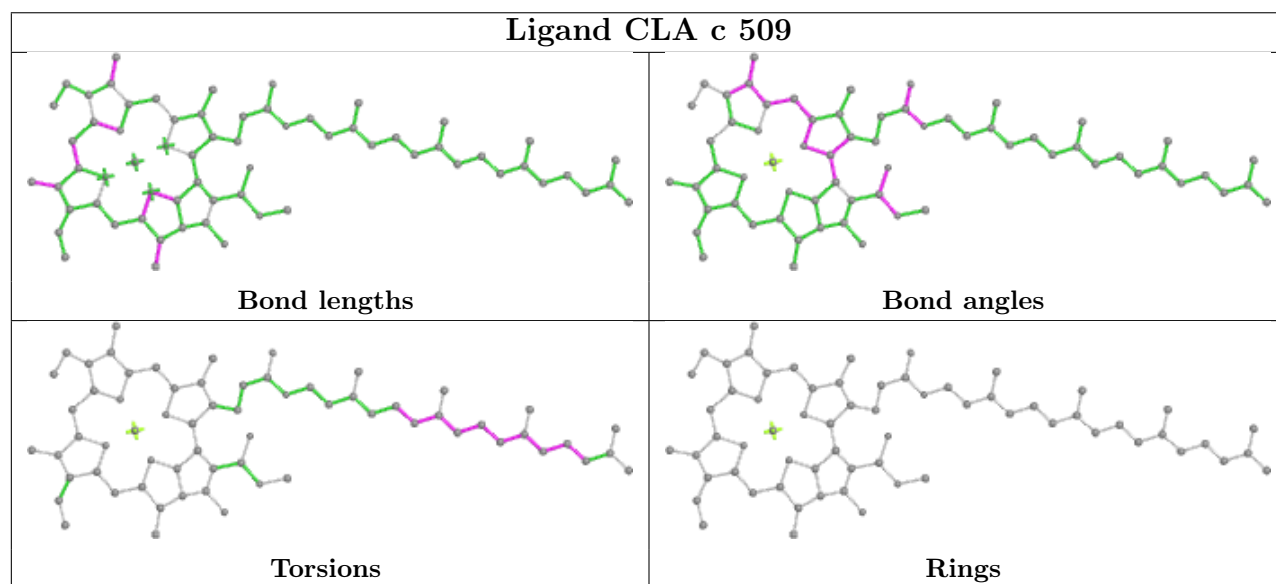
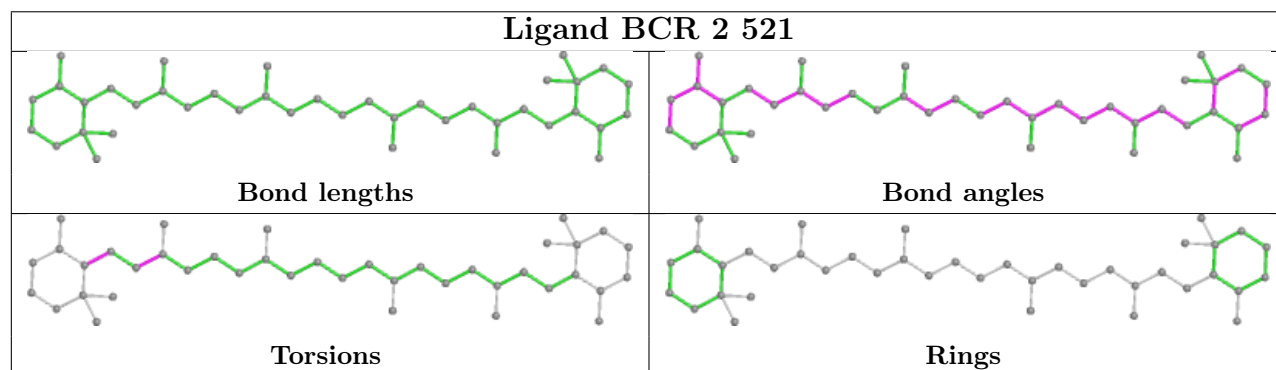
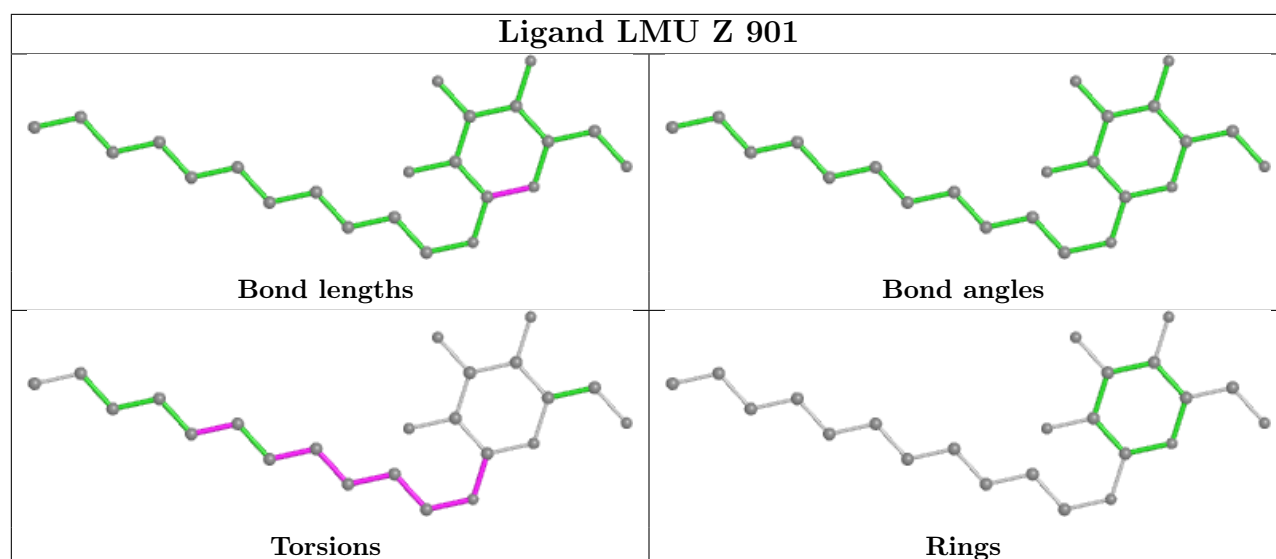
Ligand CLA 4 501**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA u 501****Bond lengths****Bond angles****Torsions****Rings**

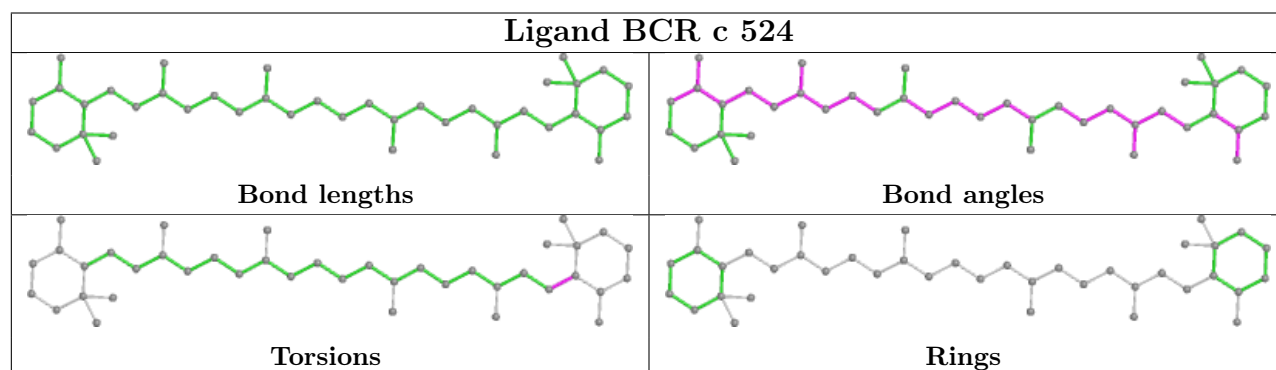
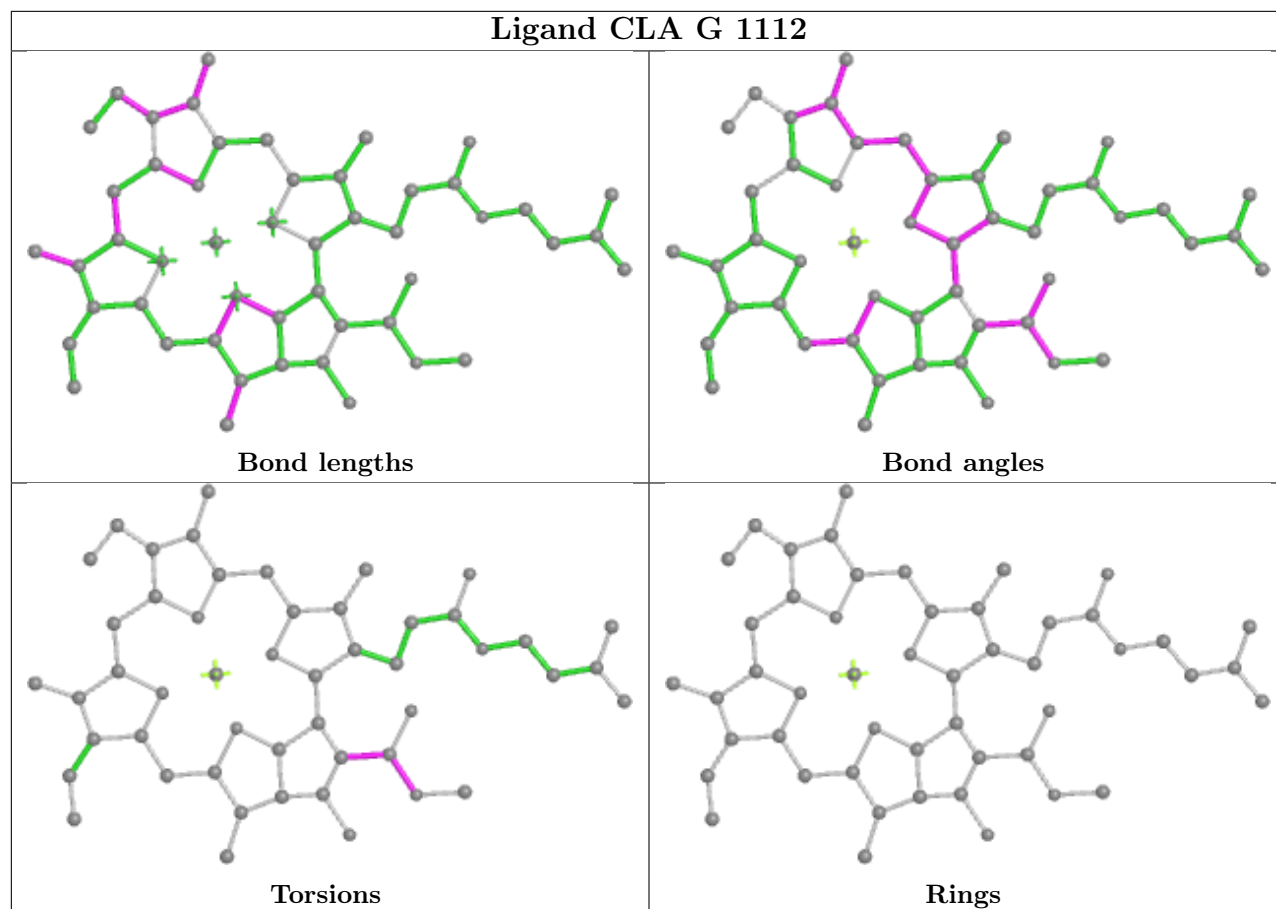
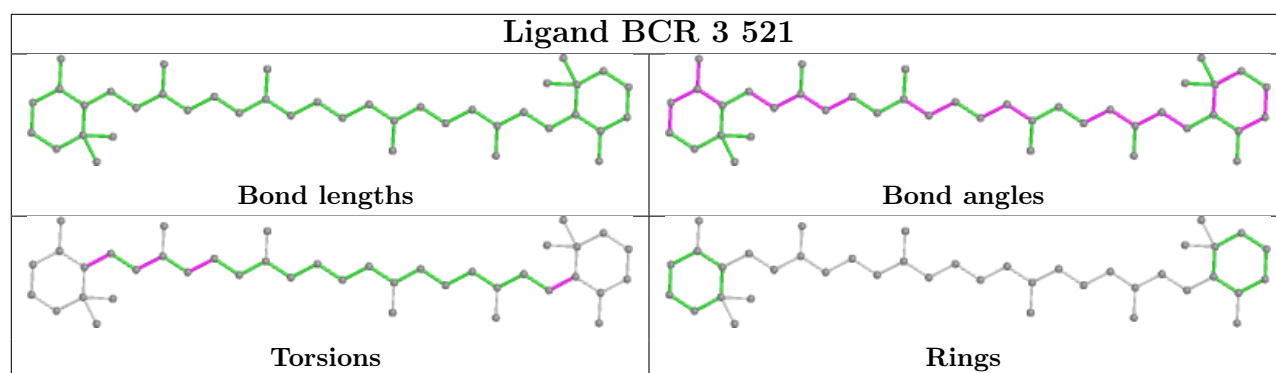
Ligand CLA 3 504

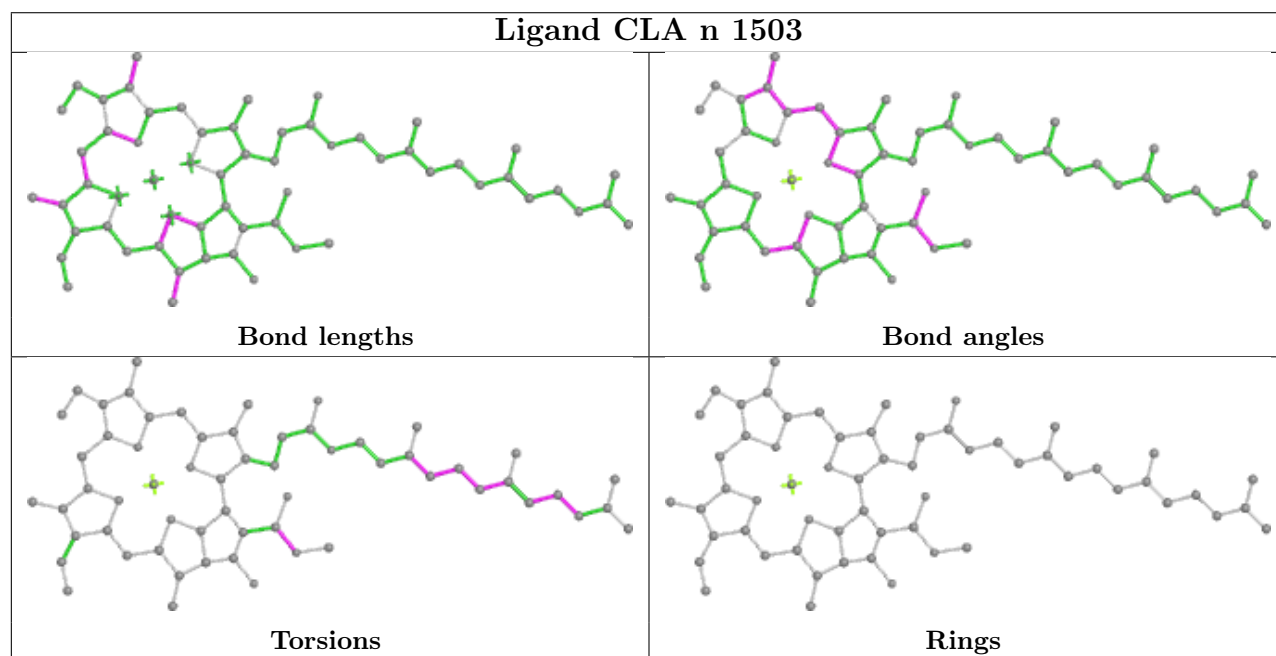
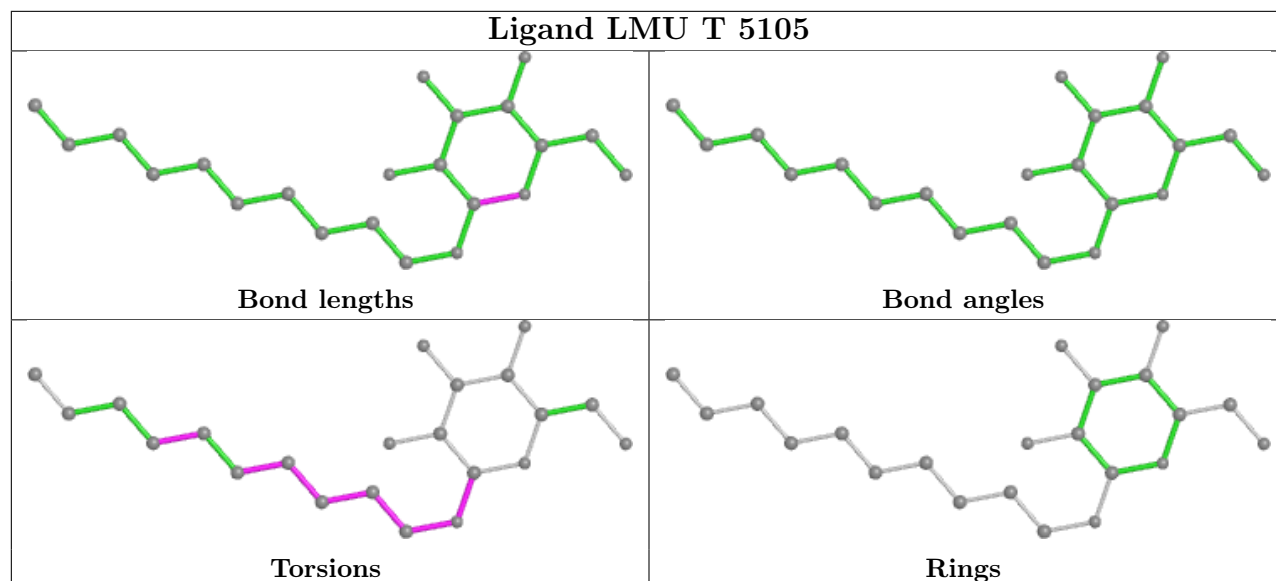
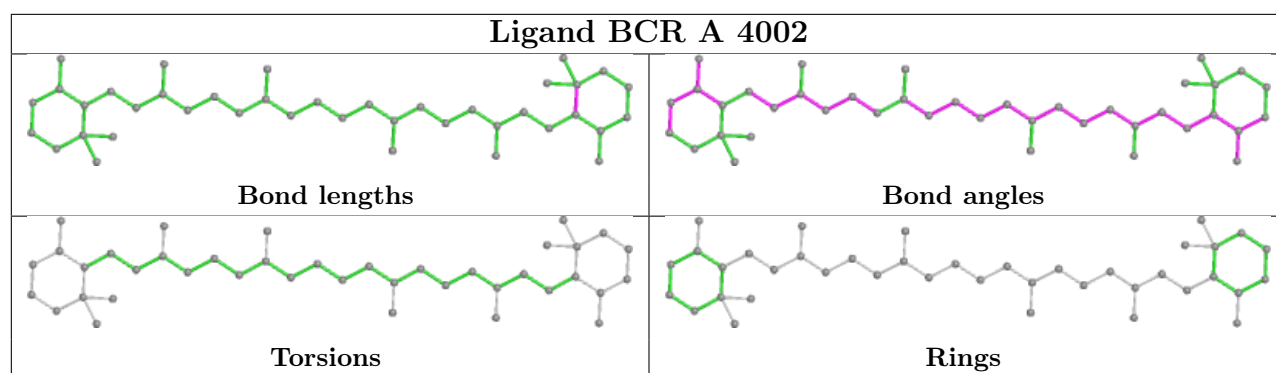


Ligand BCR L 4022

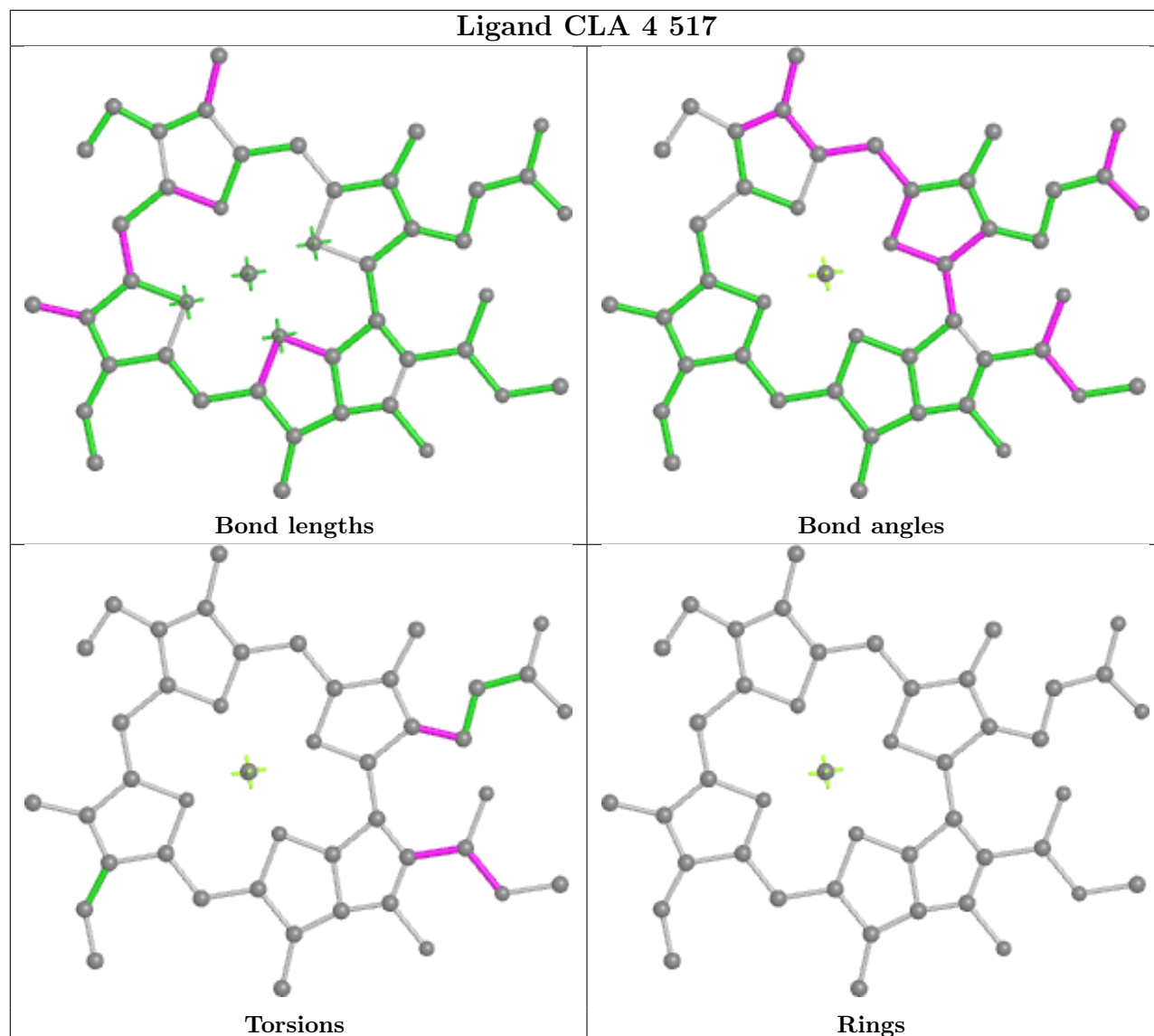




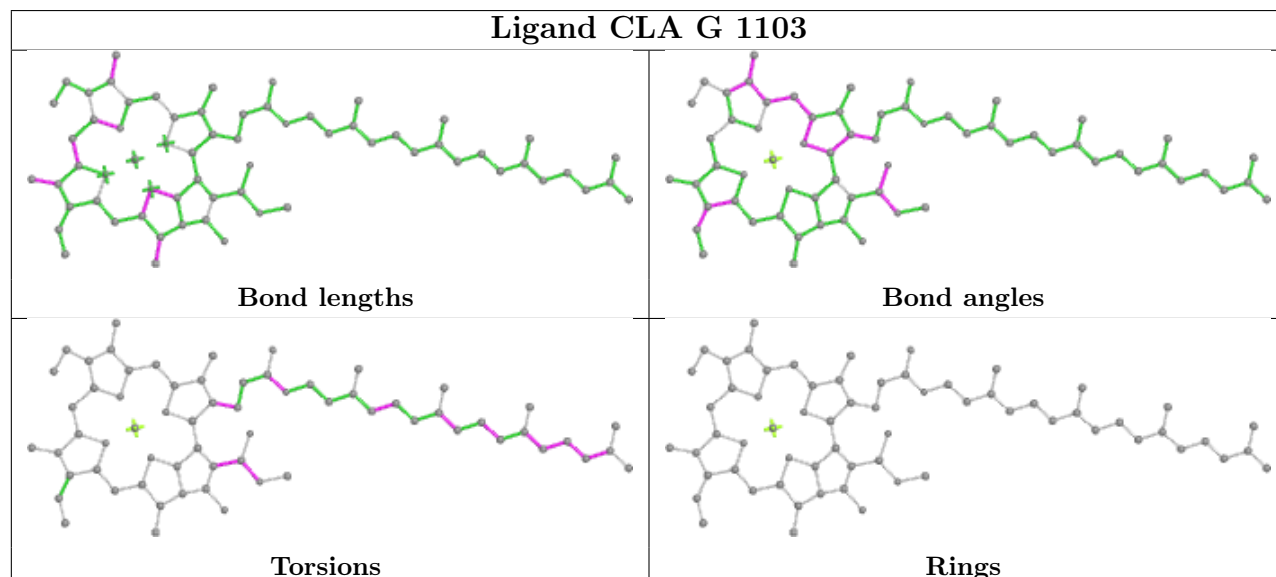




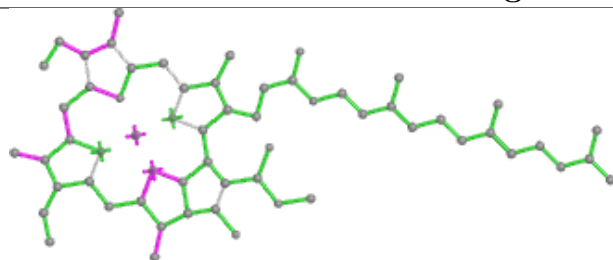
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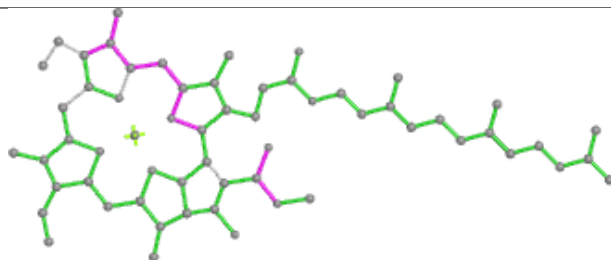
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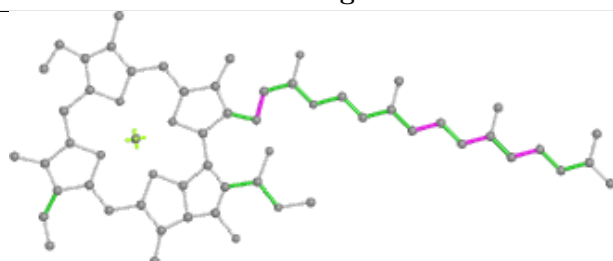
Ligand CLA H 1216



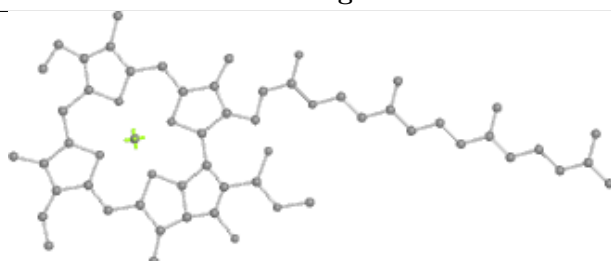
Bond lengths



Bond angles

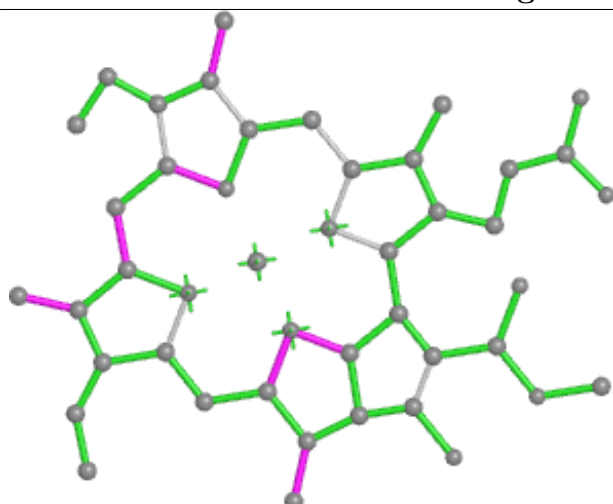


Torsions

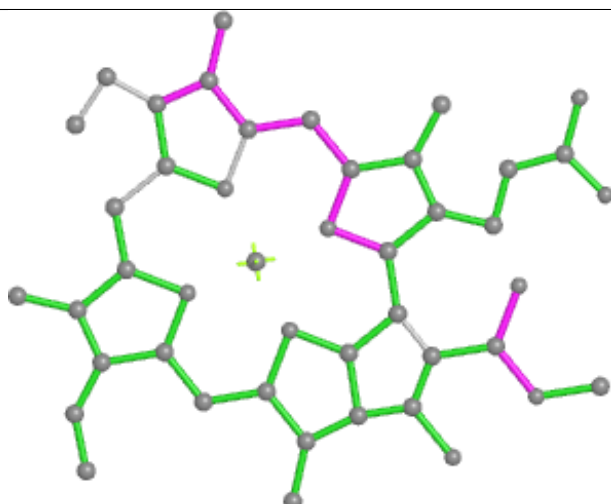


Rings

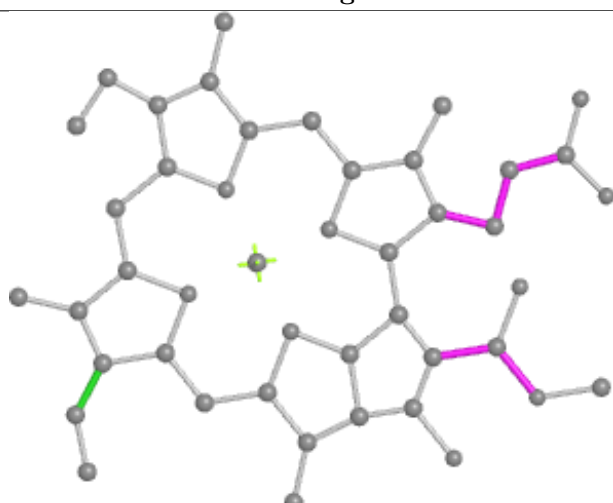
Ligand CLA u 517



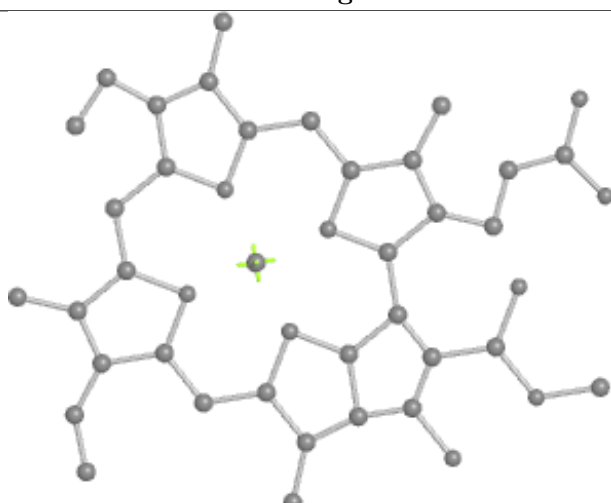
Bond lengths



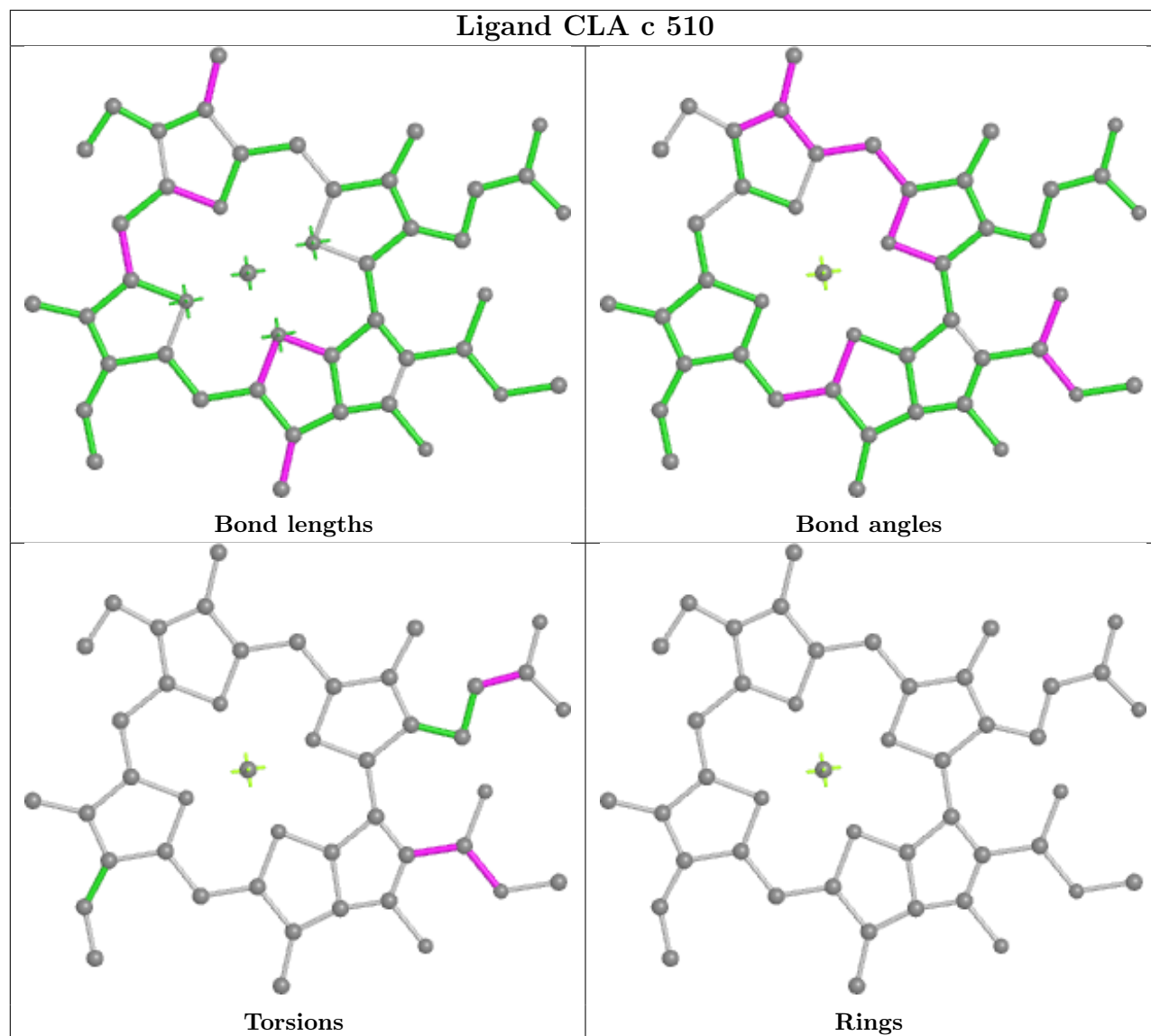
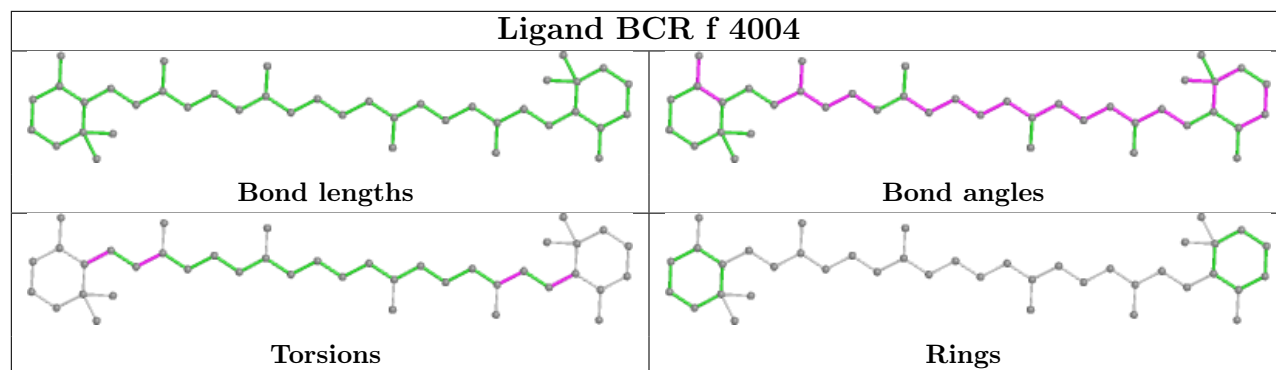
Bond angles

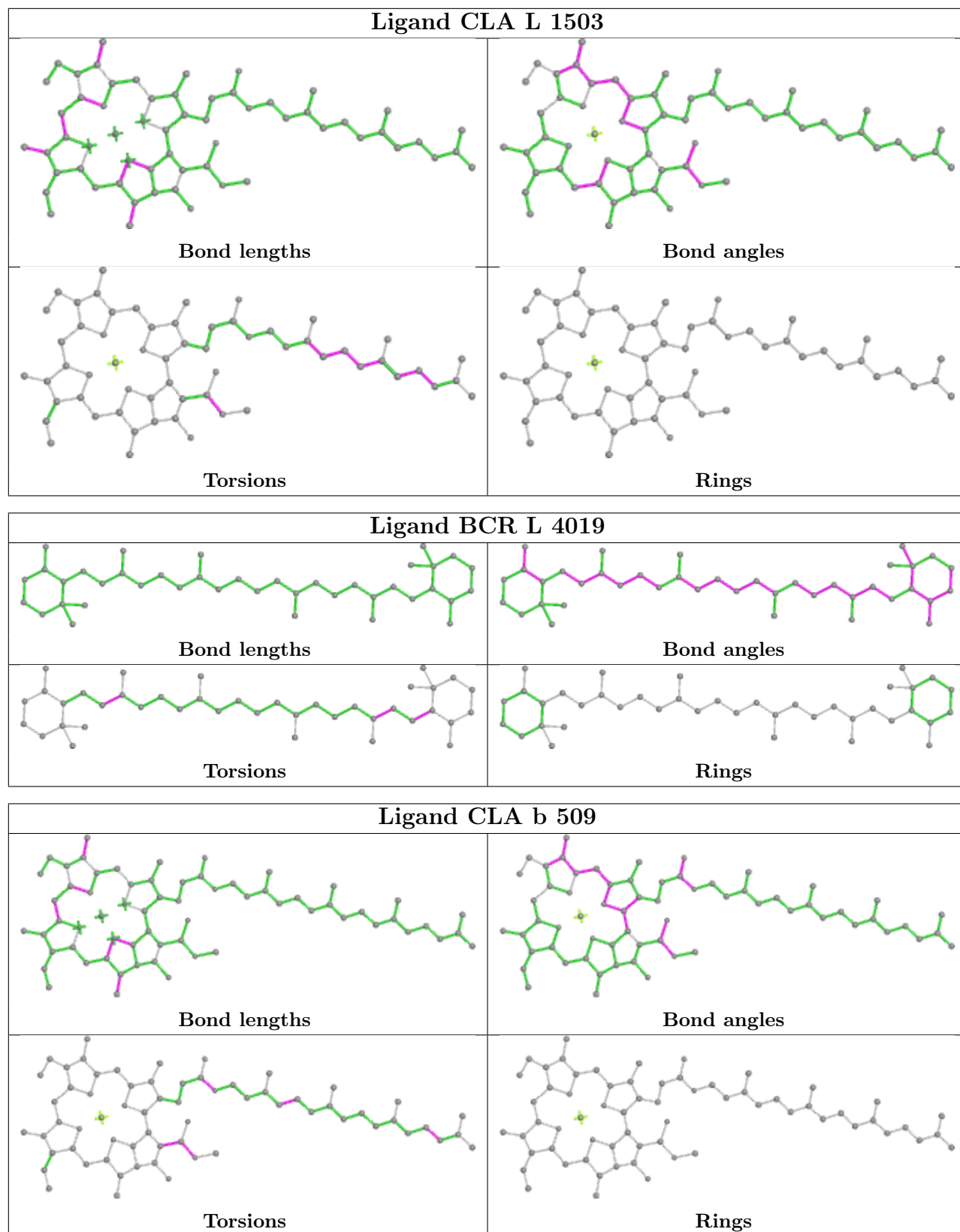


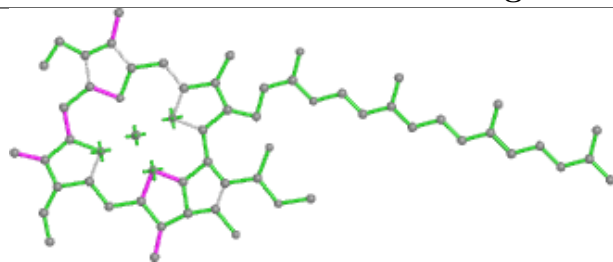
Torsions



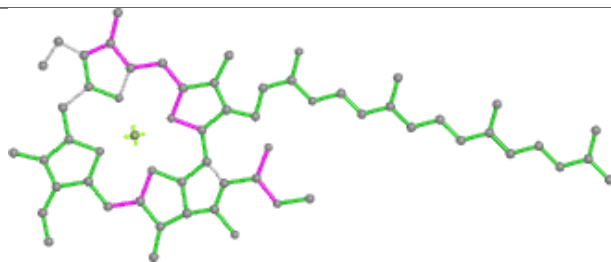
Rings



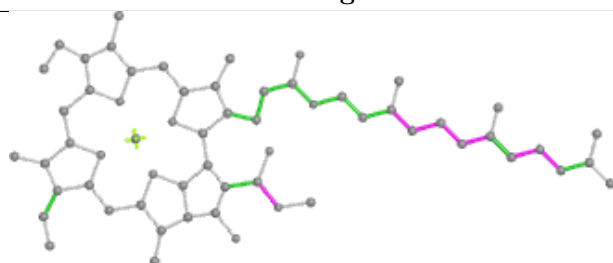


Ligand CLA V 1503

Bond lengths



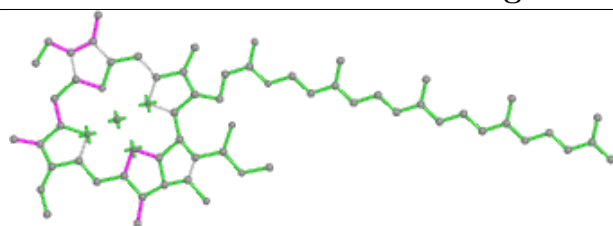
Bond angles



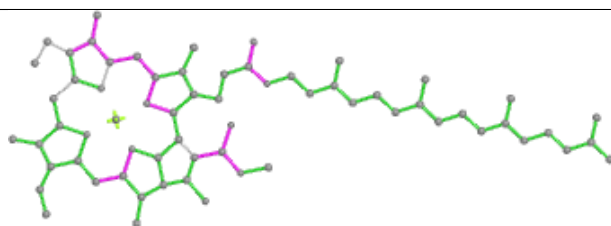
Torsions



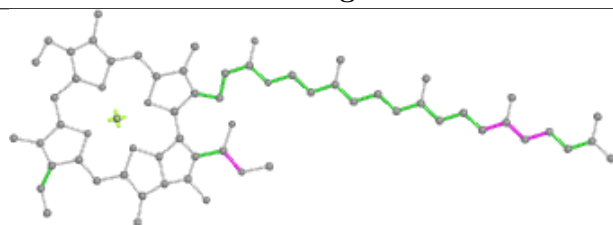
Rings

Ligand CLA G 1131

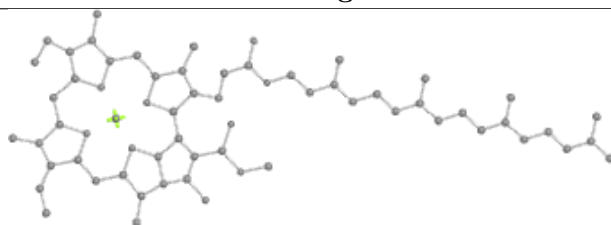
Bond lengths



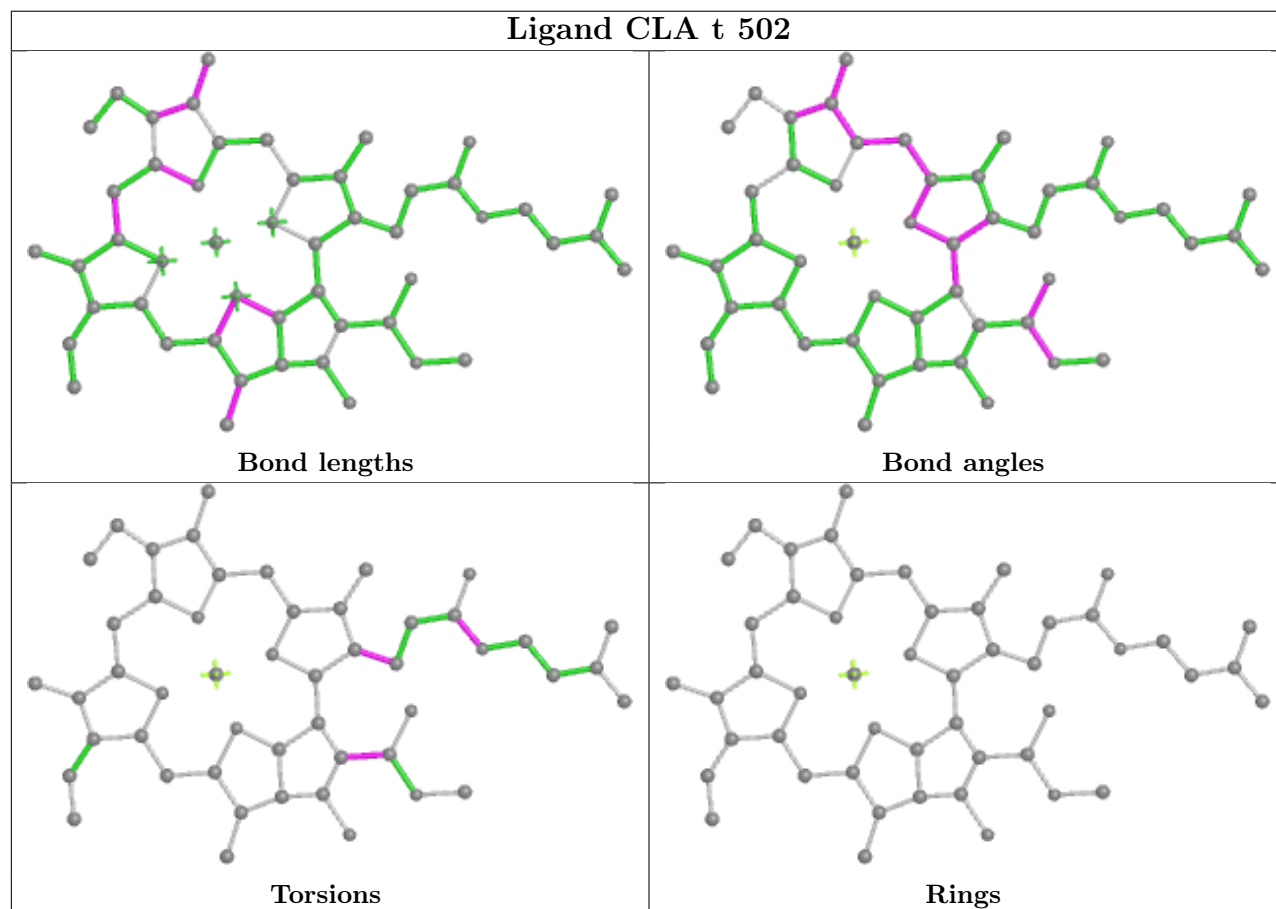
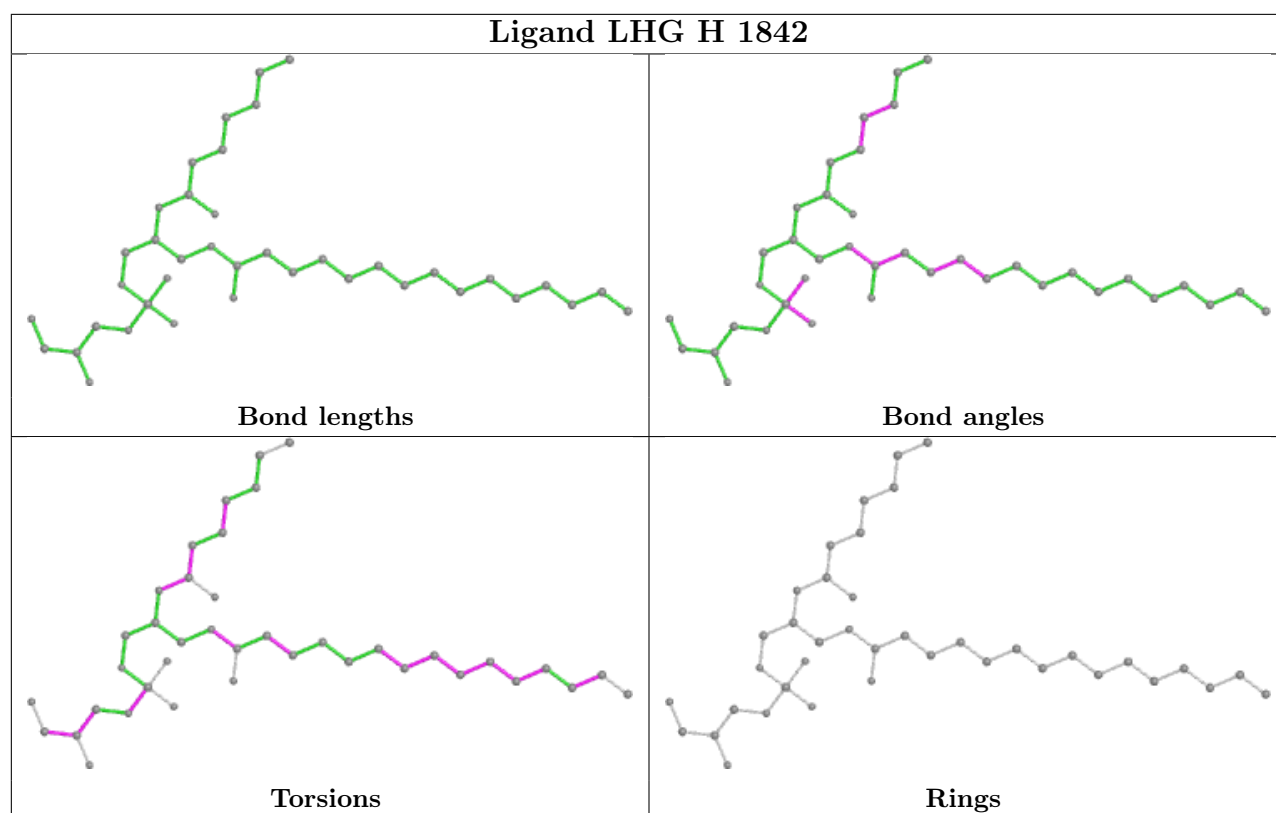
Bond angles

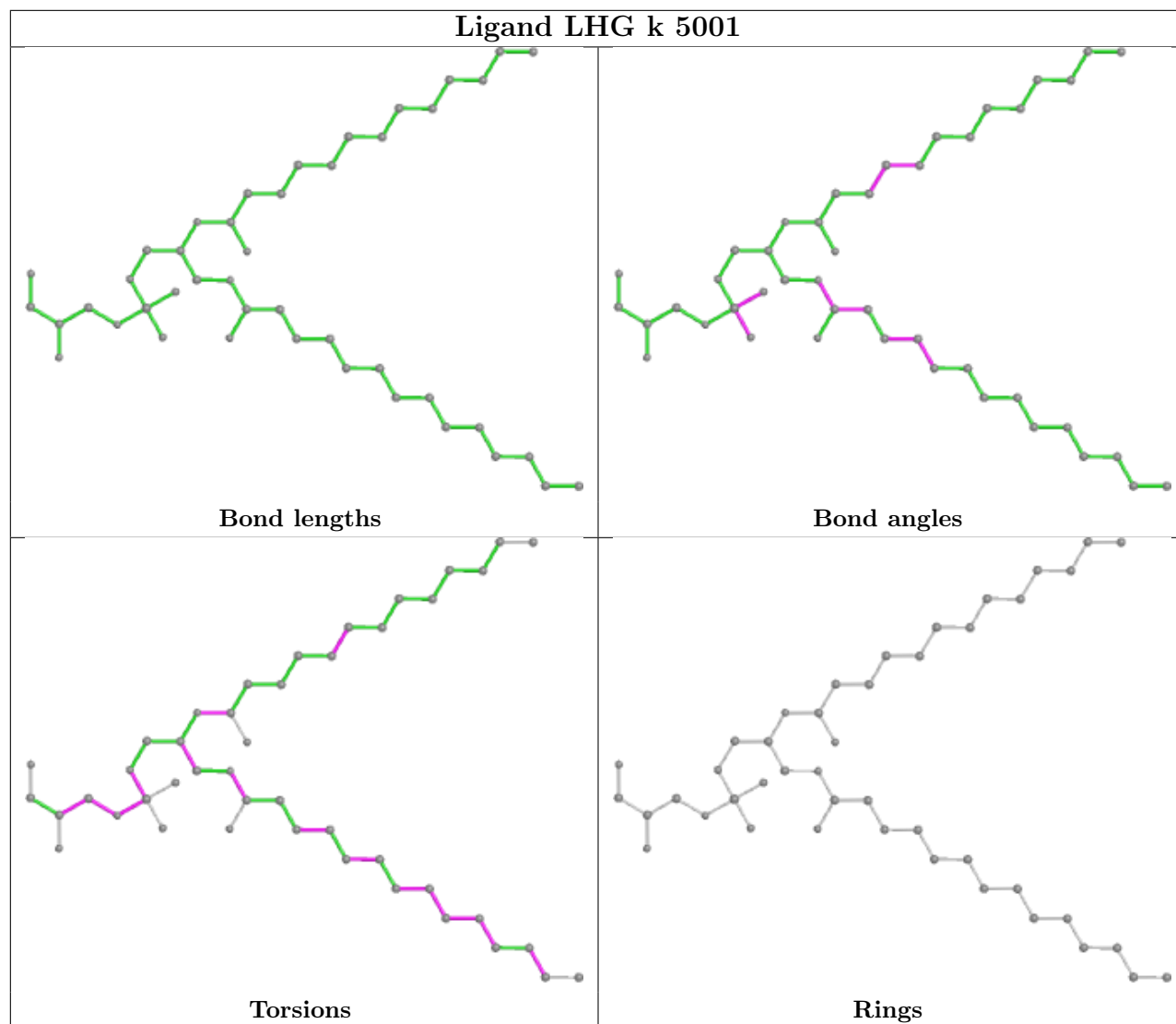
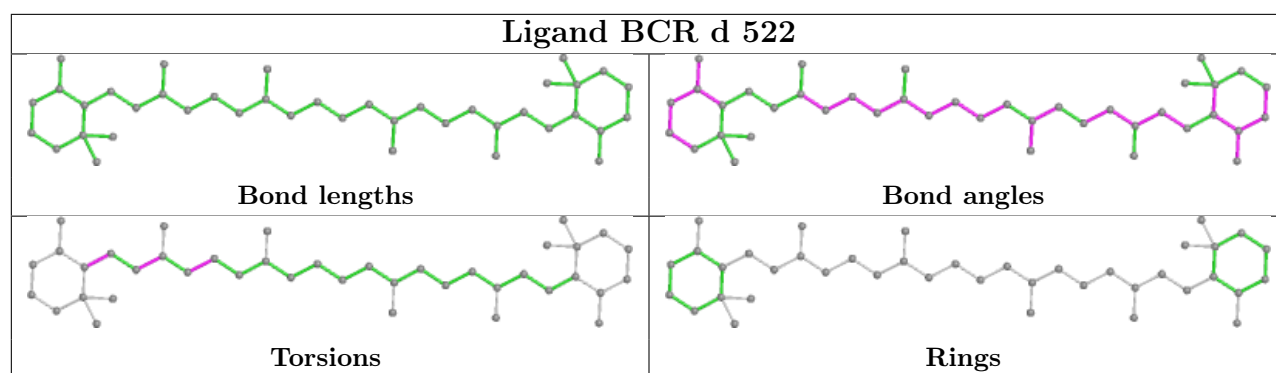


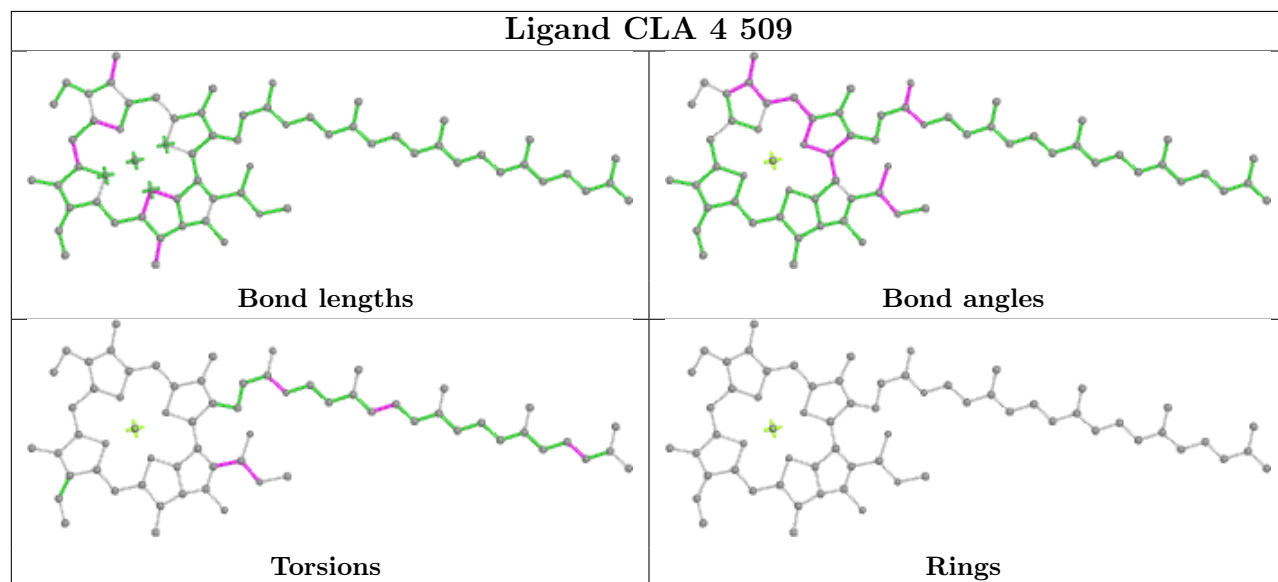
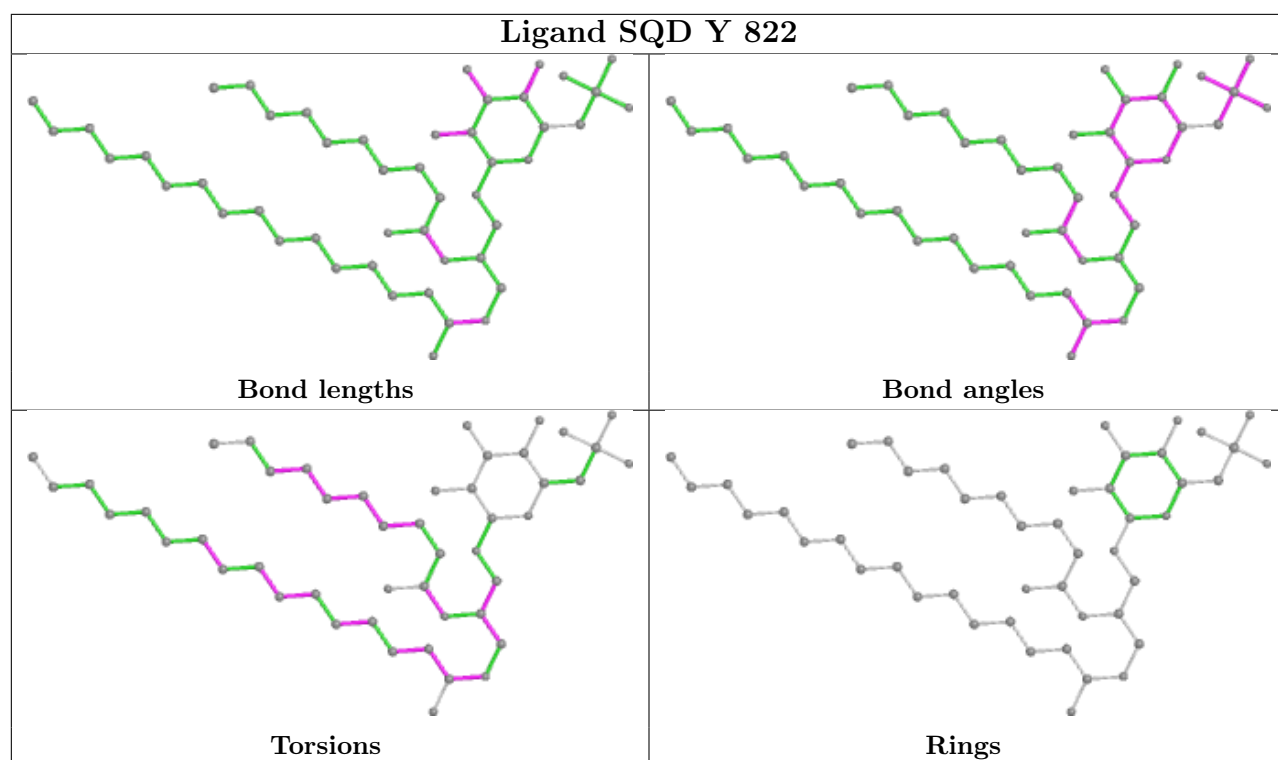
Torsions



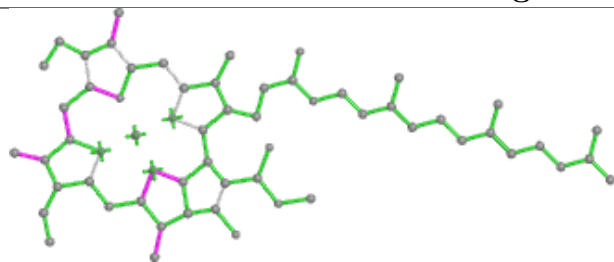
Rings



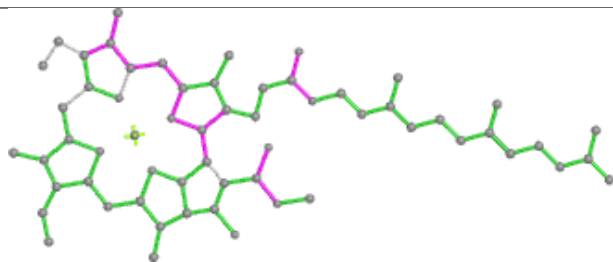




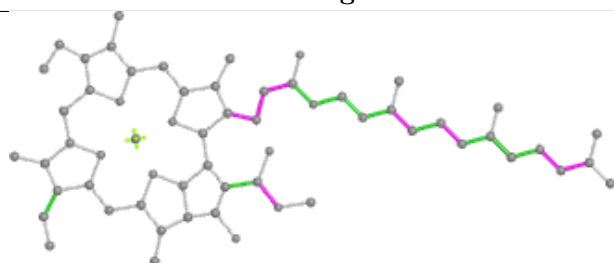
Ligand CLA f 1224



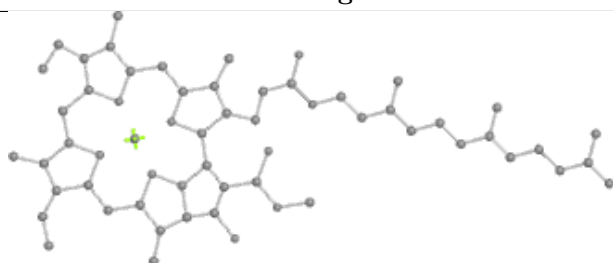
Bond lengths



Bond angles

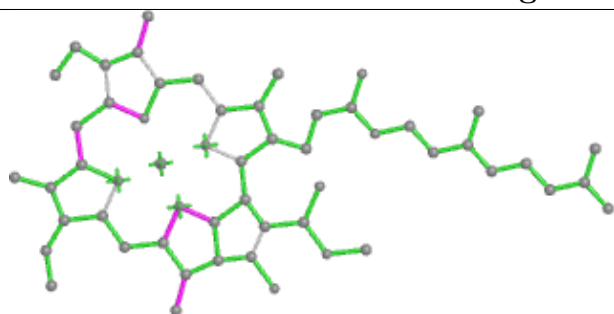


Torsions

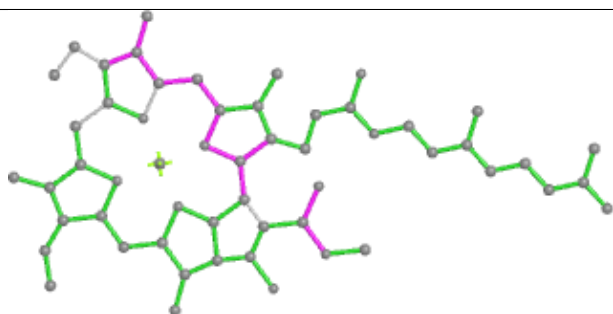


Rings

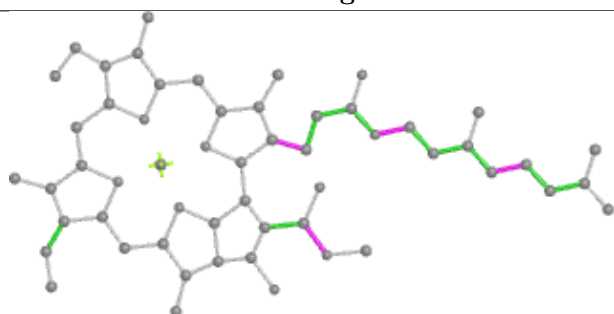
Ligand CLA c 511



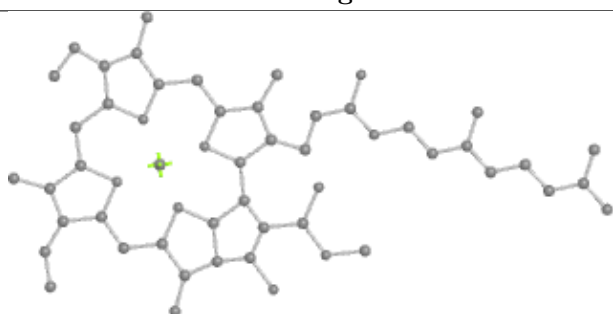
Bond lengths



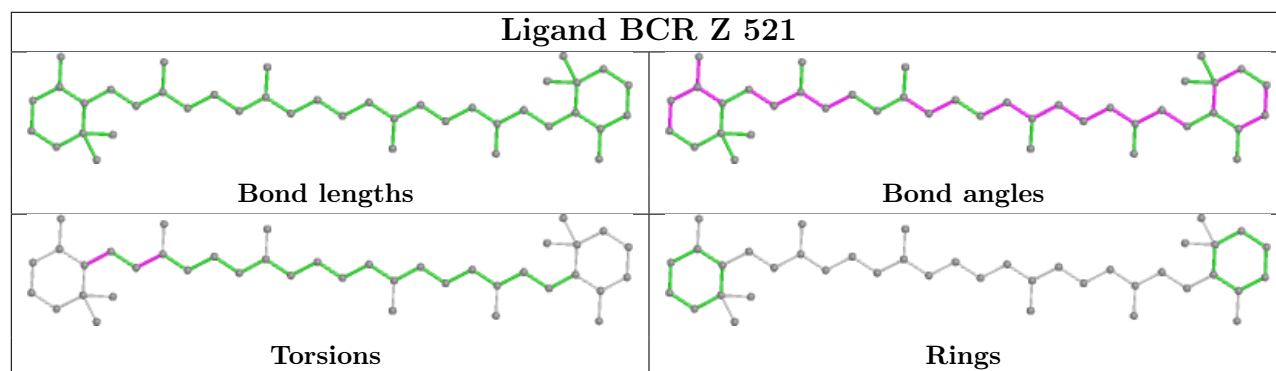
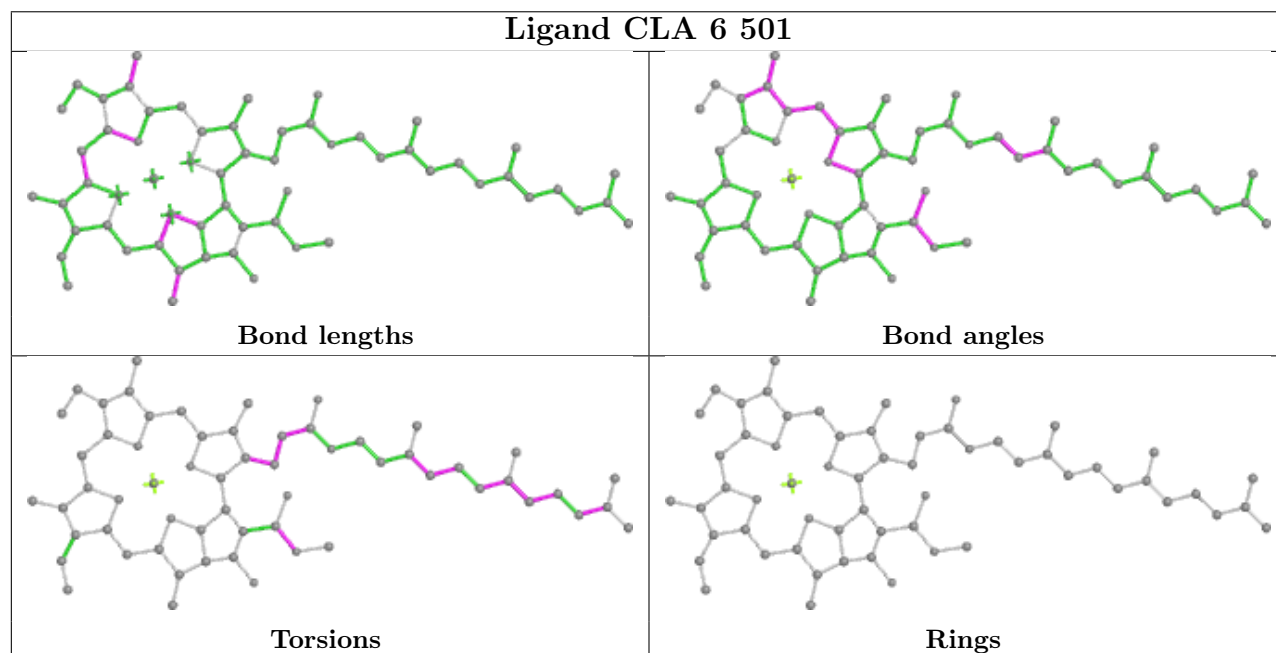
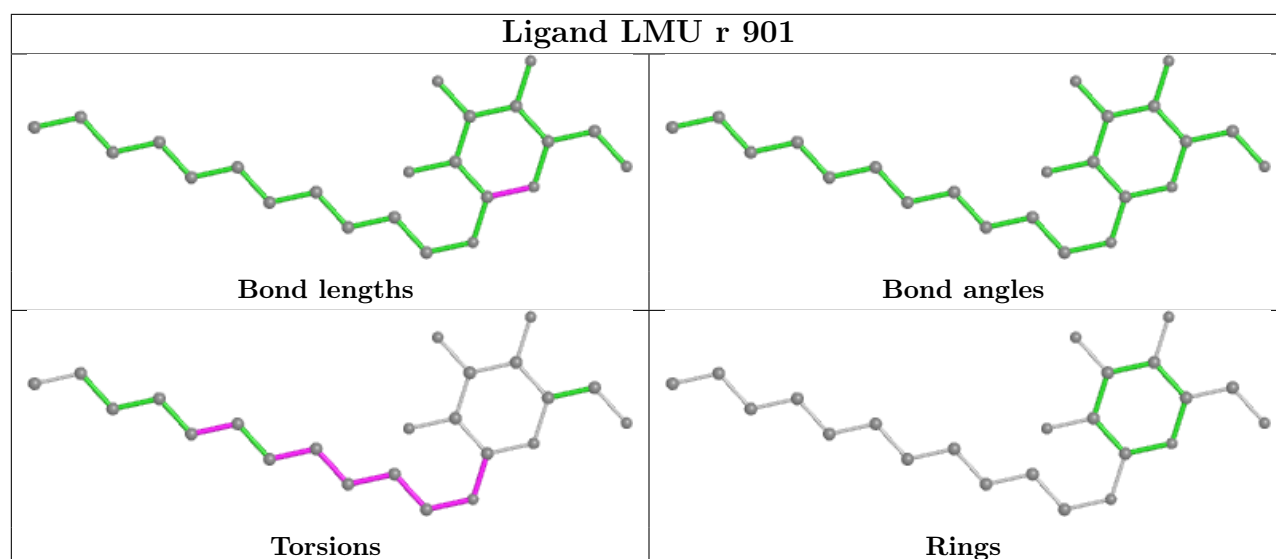
Bond angles



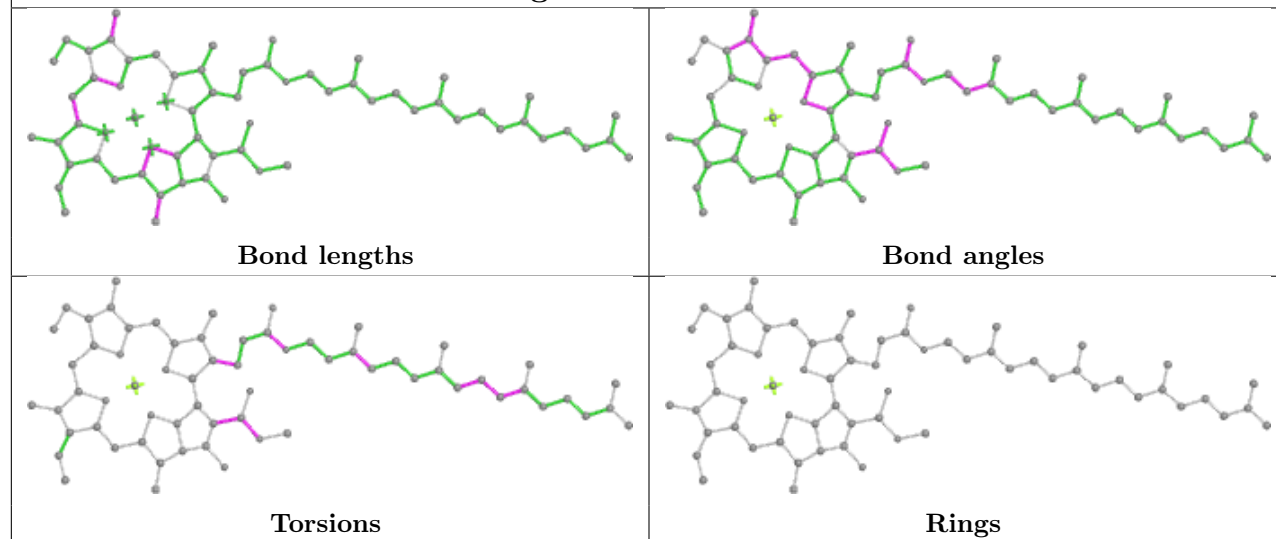
Torsions



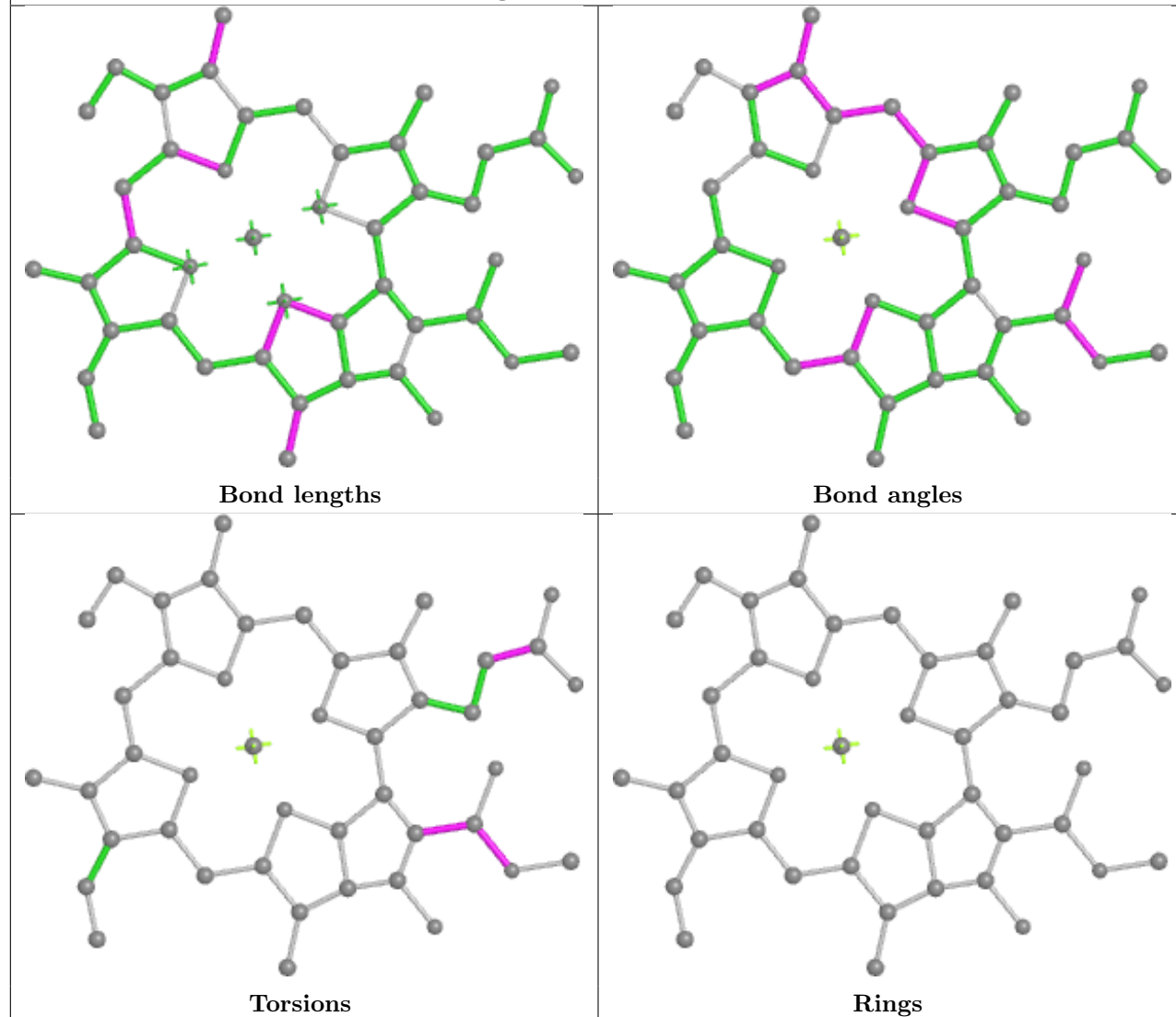
Rings

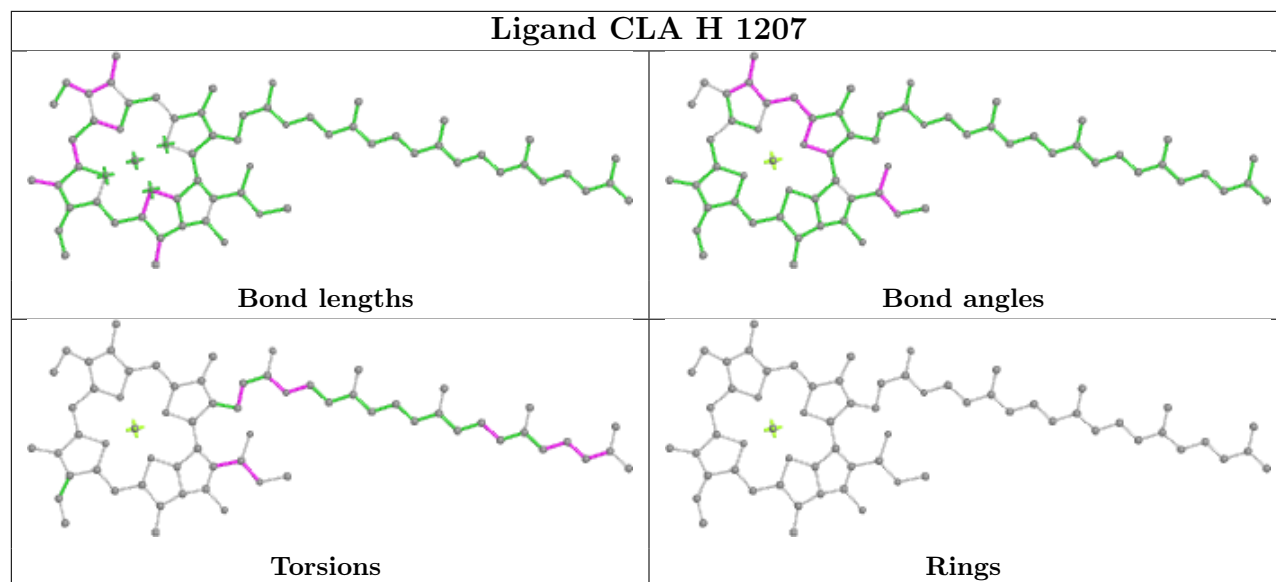
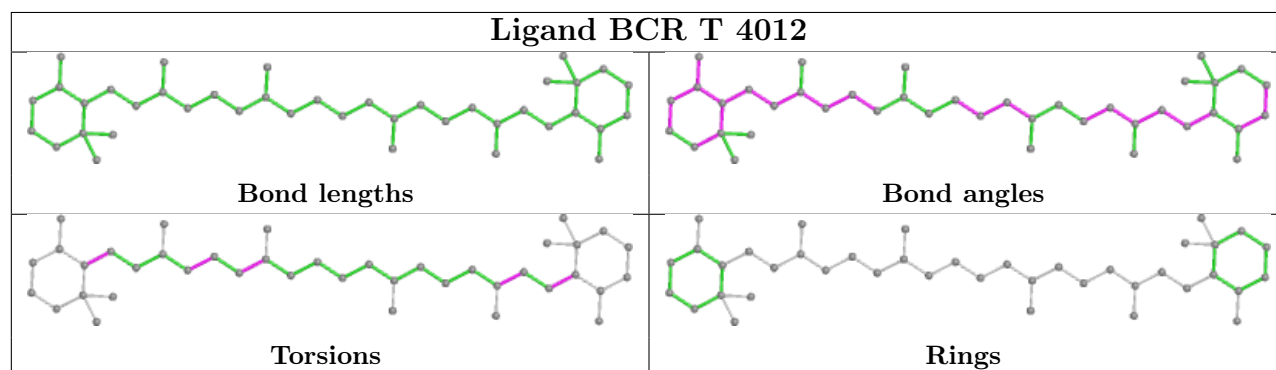
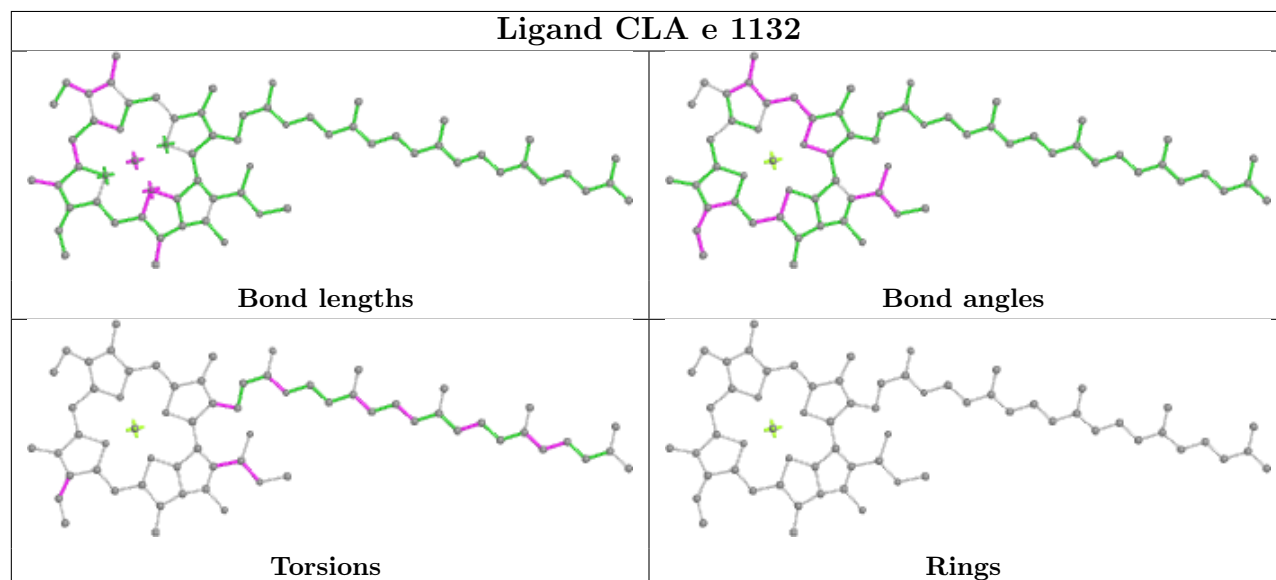


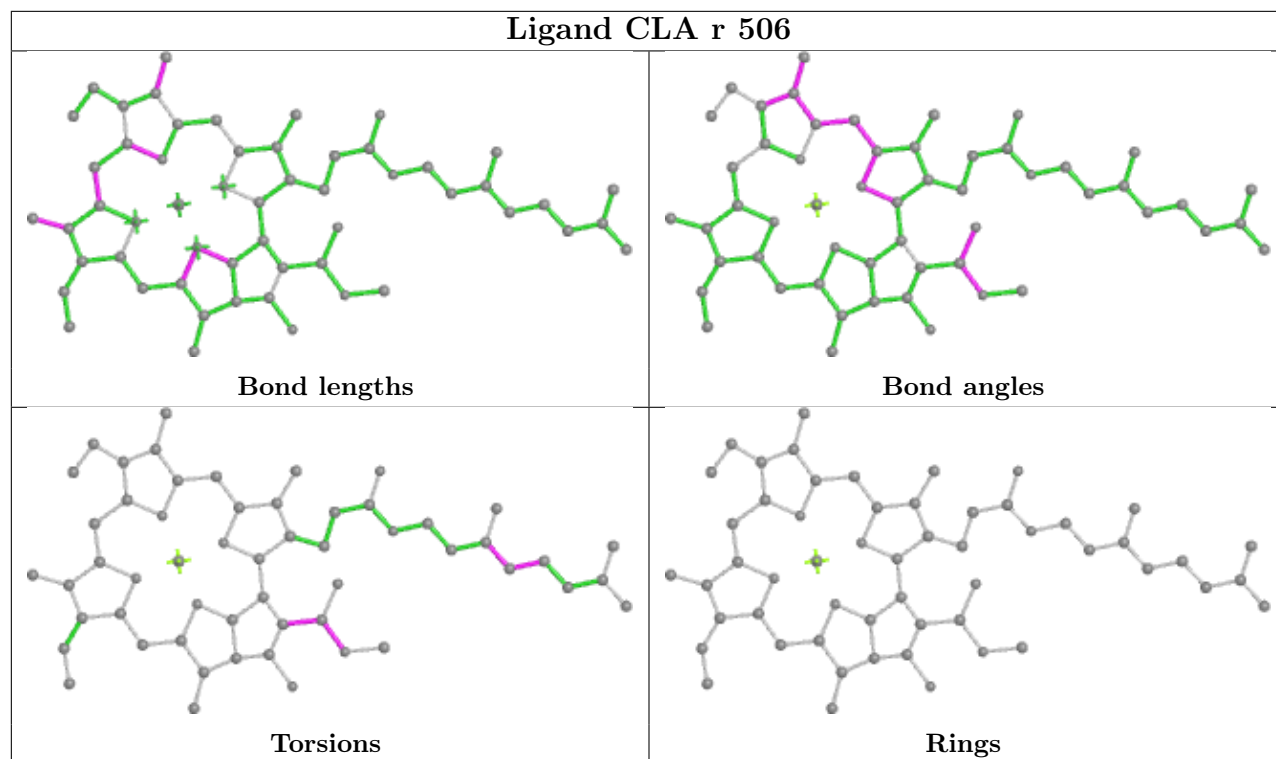
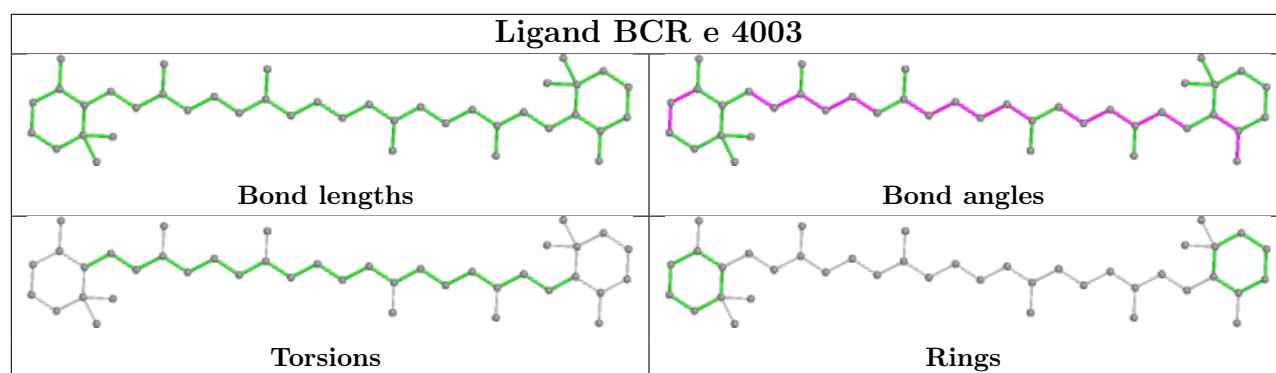
Ligand CLA f 1240

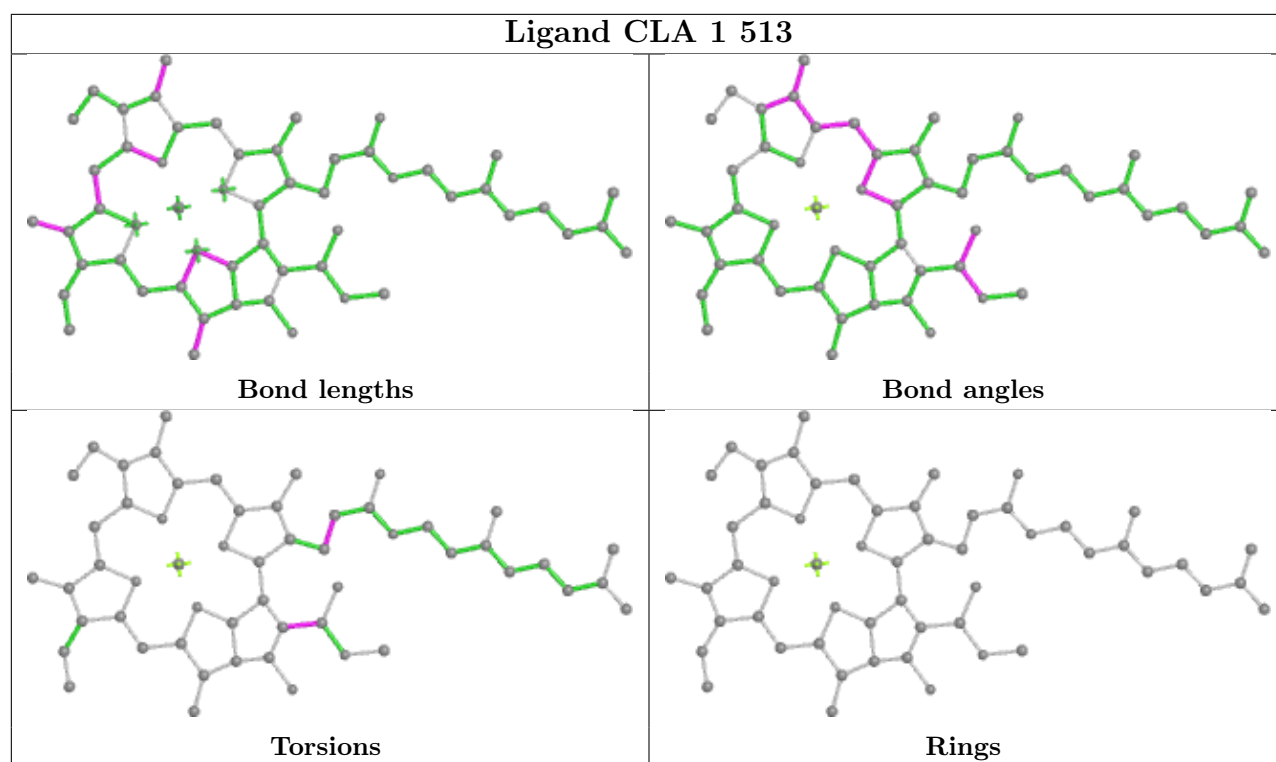


Ligand CLA 6 510

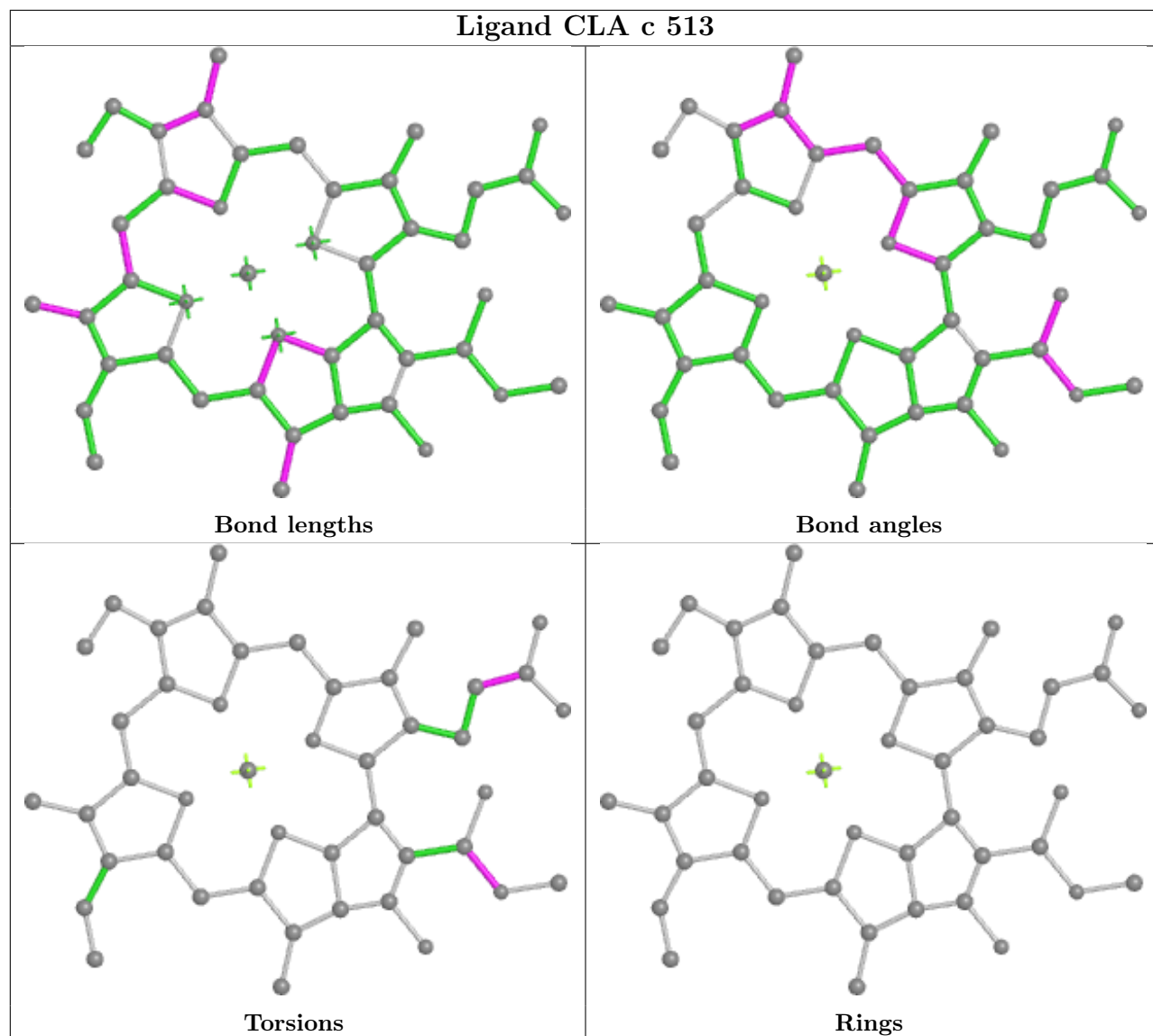


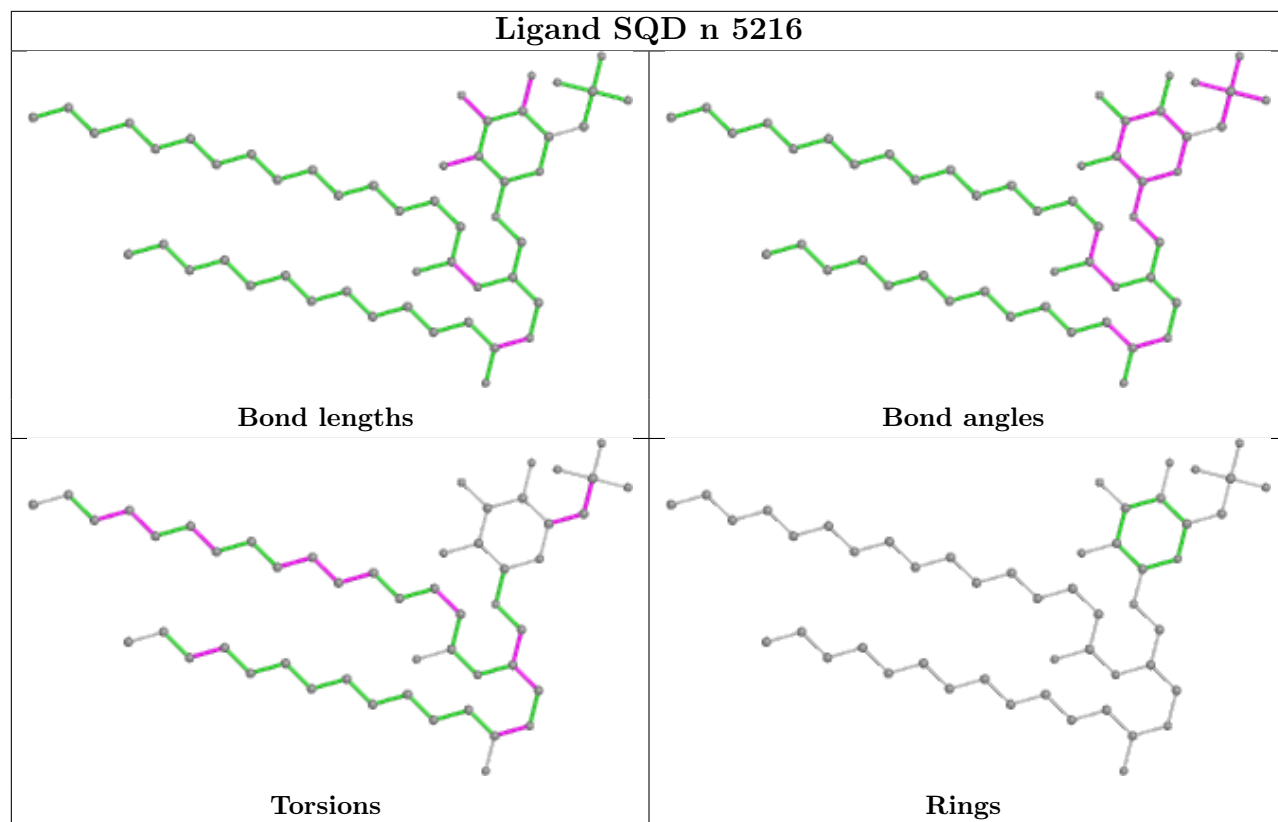
Ligand CLA H 1207**Ligand BCR T 4012****Ligand CLA e 1132**



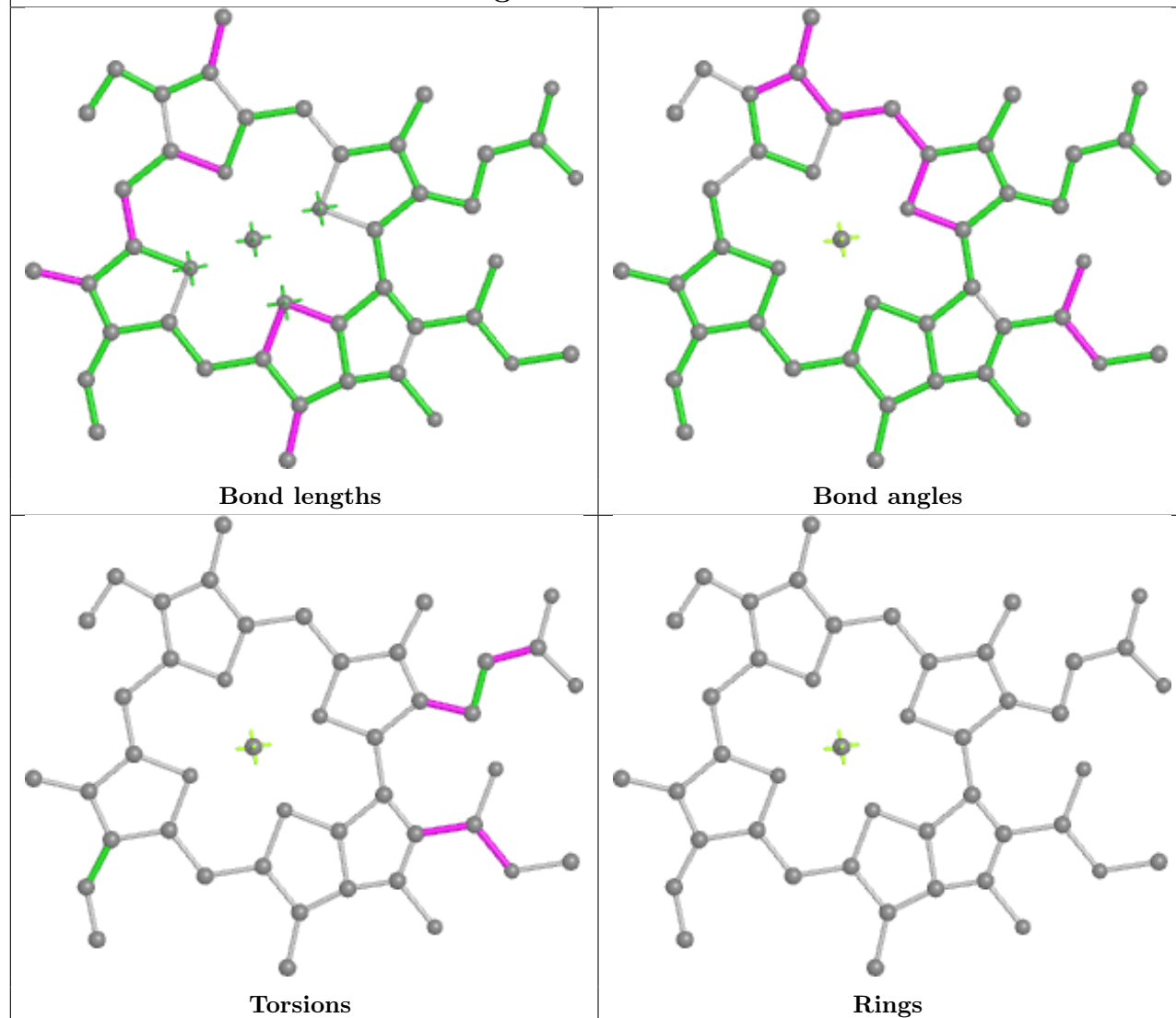


Ligand CLA c 513

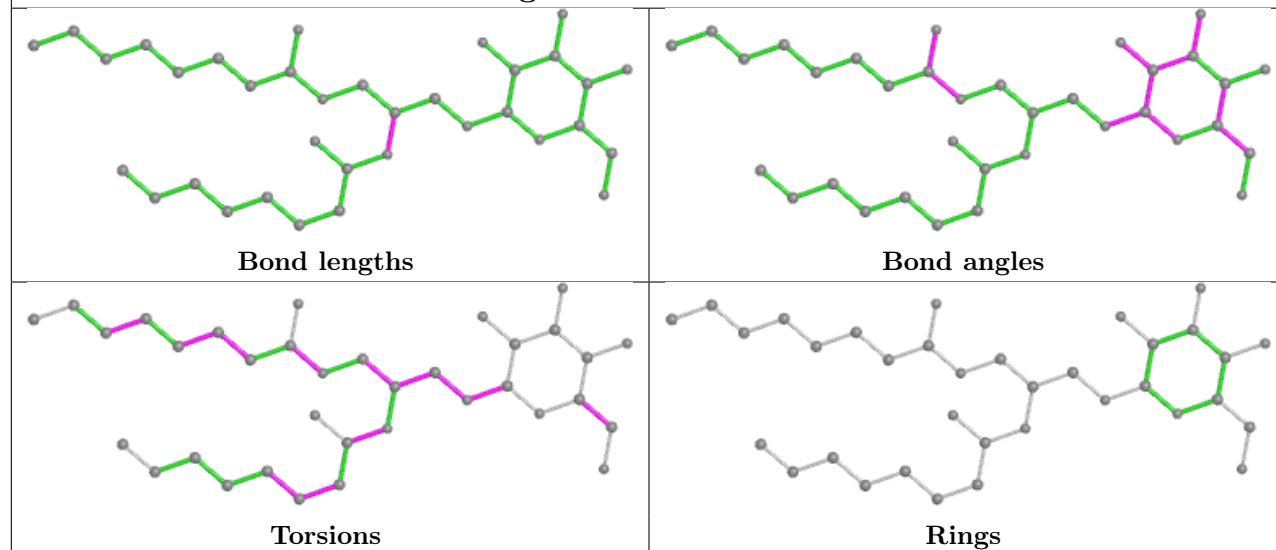


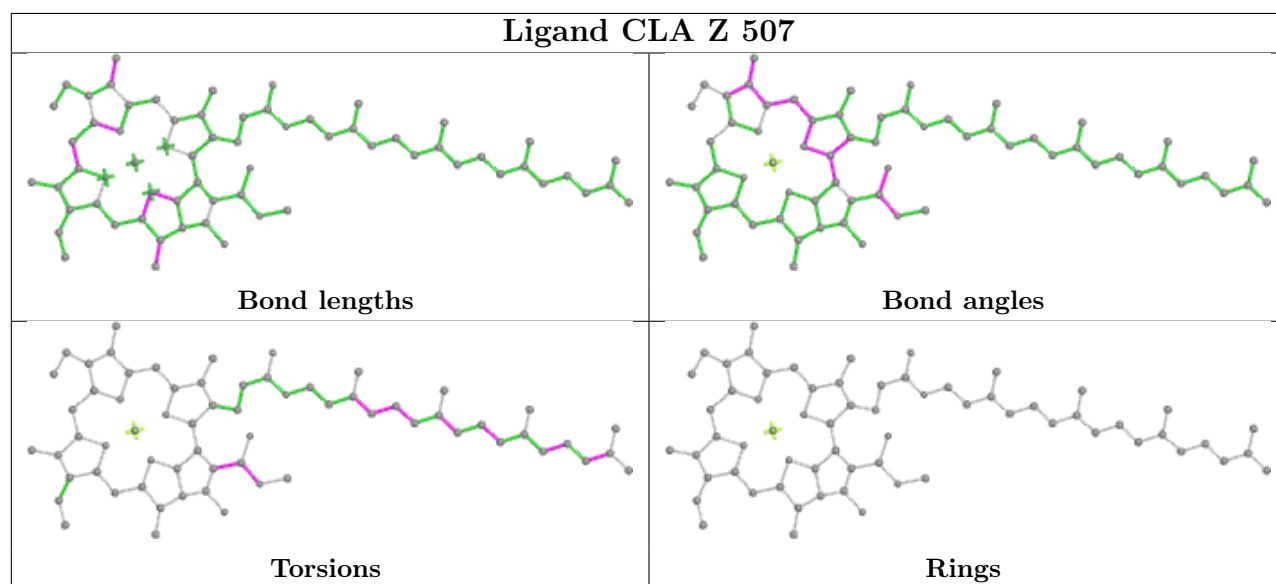
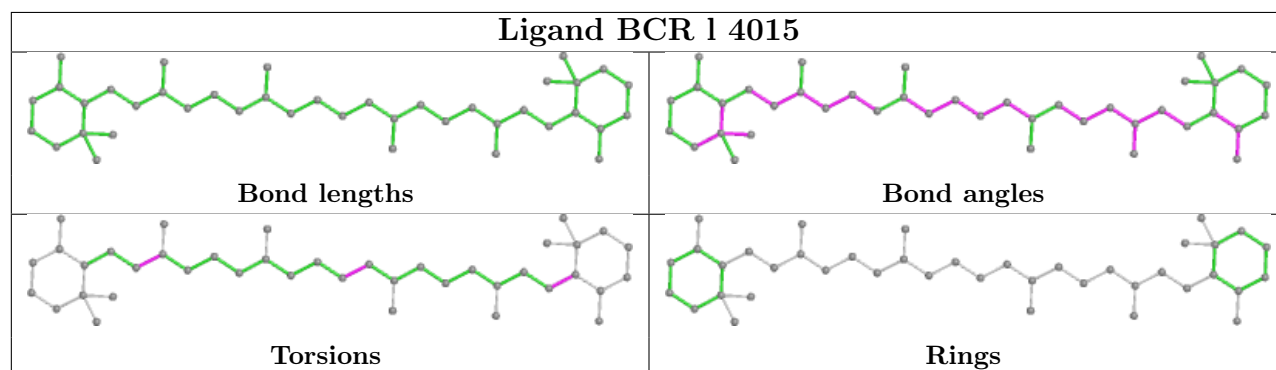
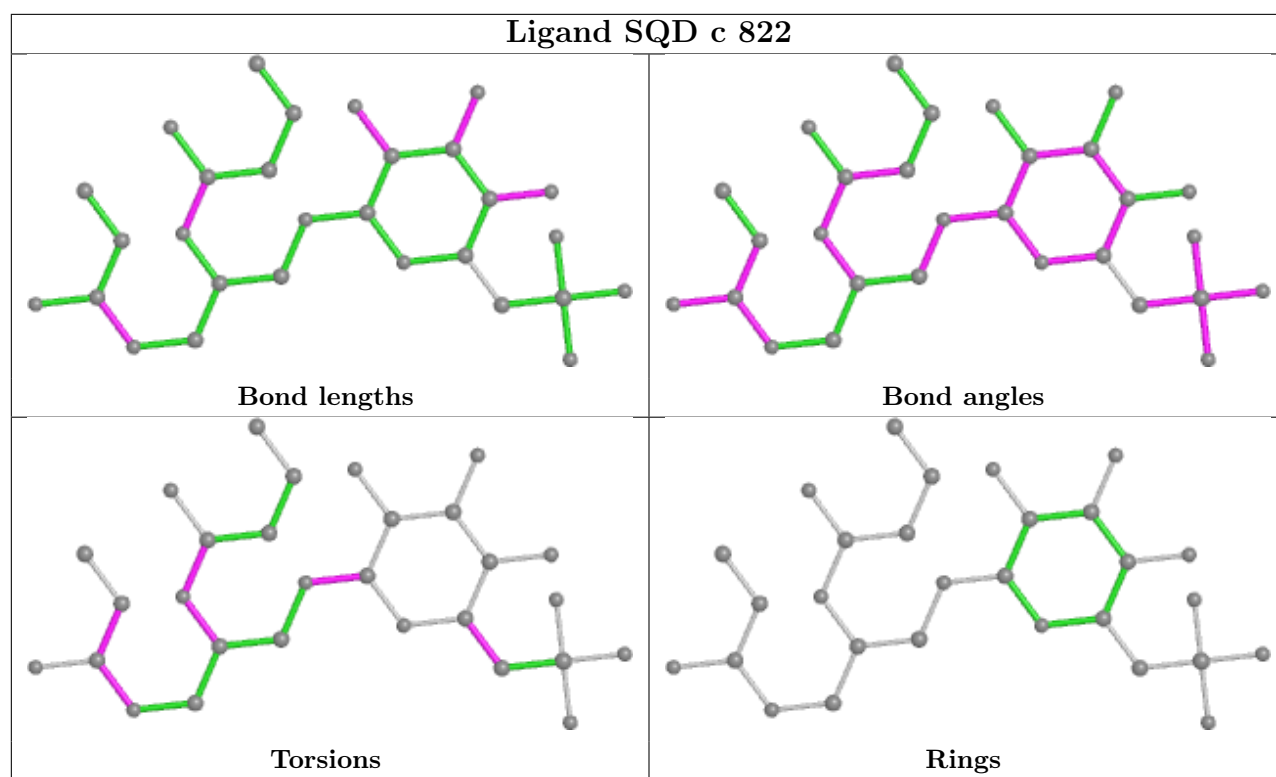


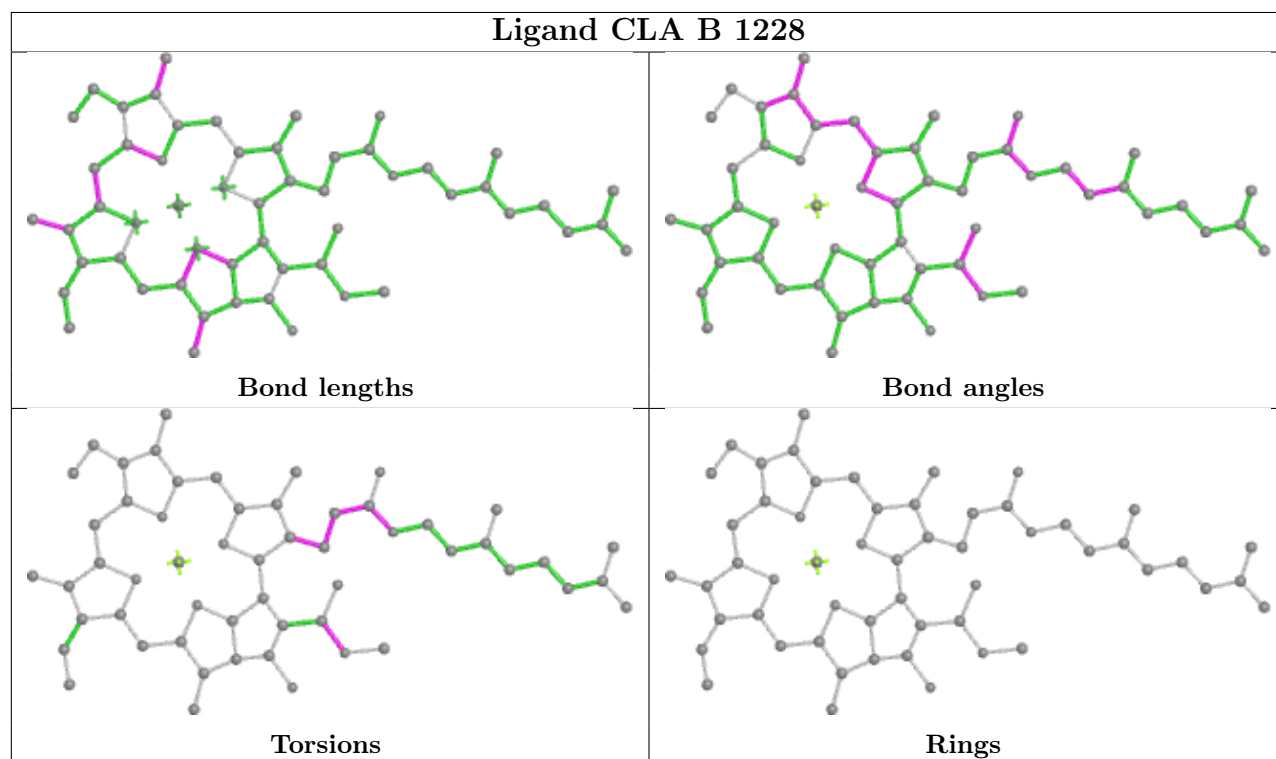
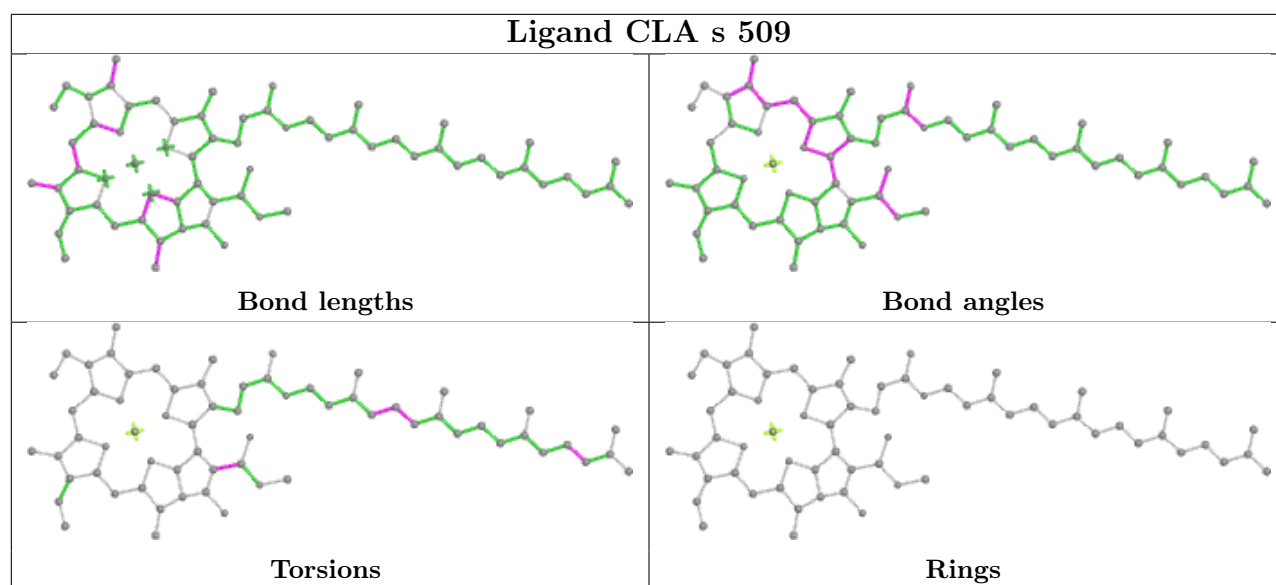
Ligand CLA 6 517

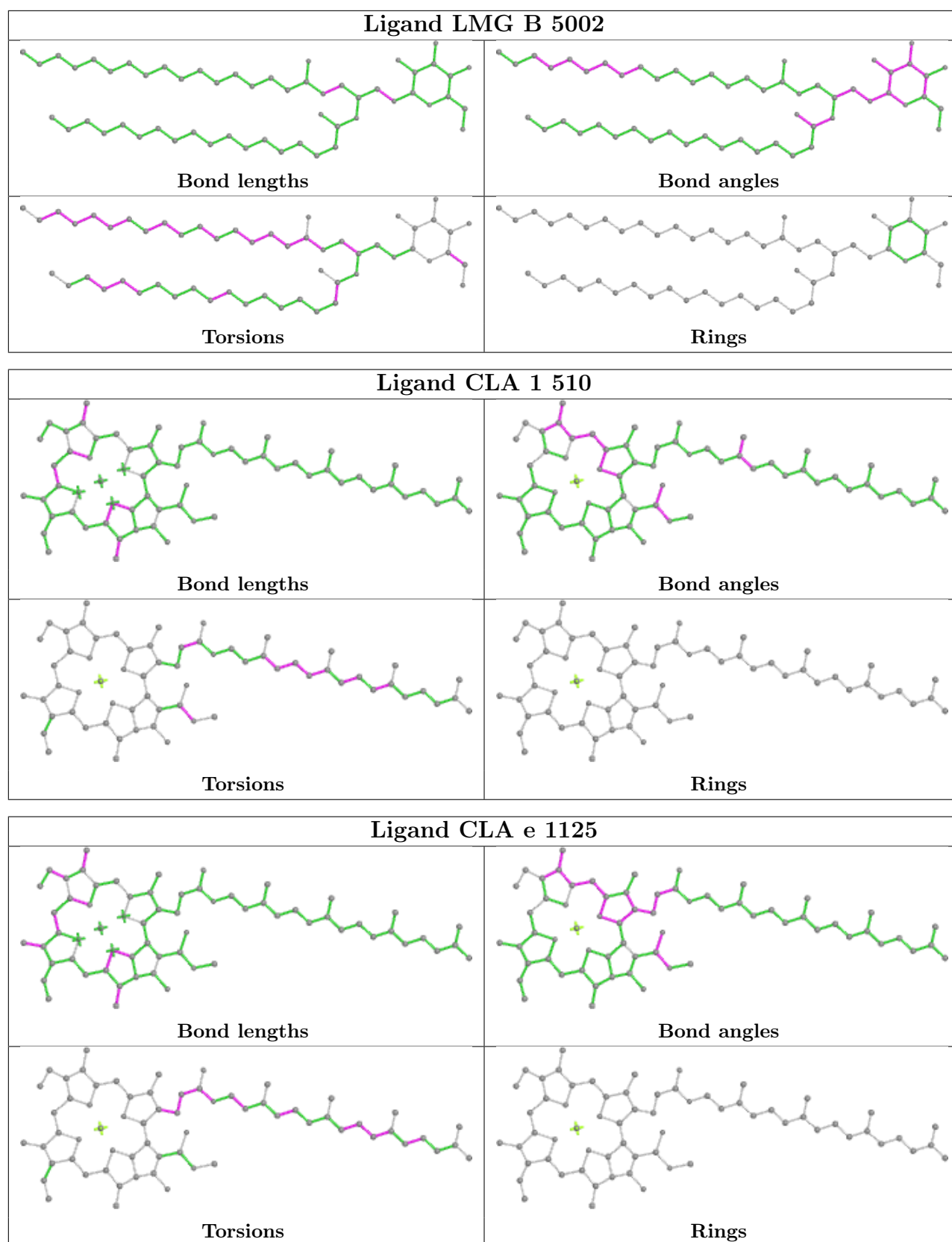


Ligand LMG T 5104

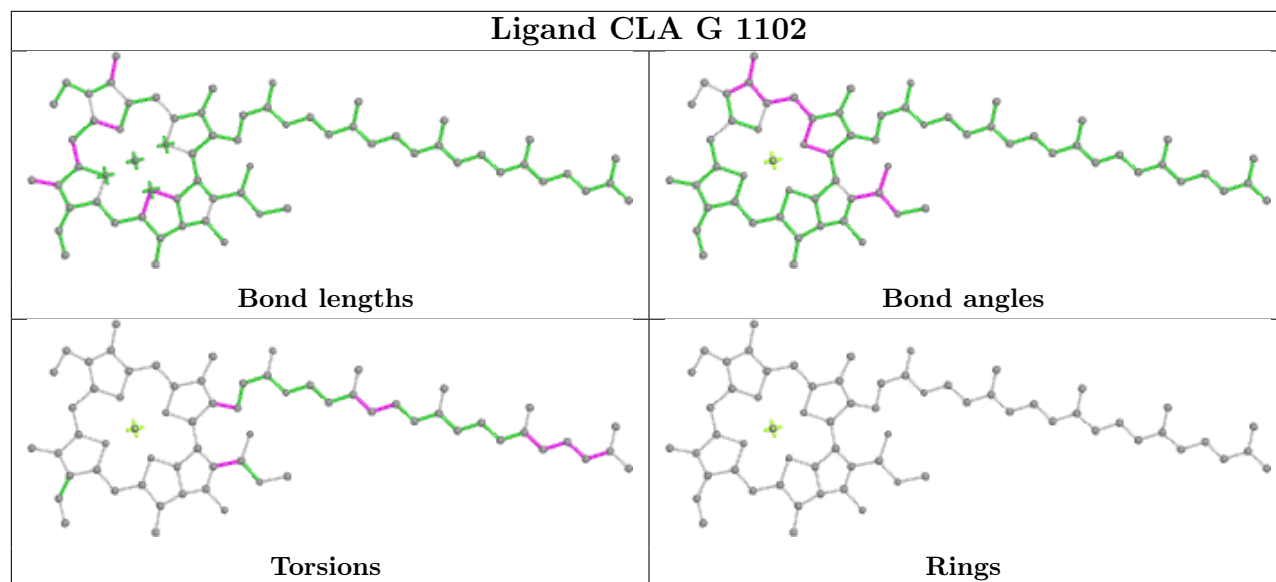




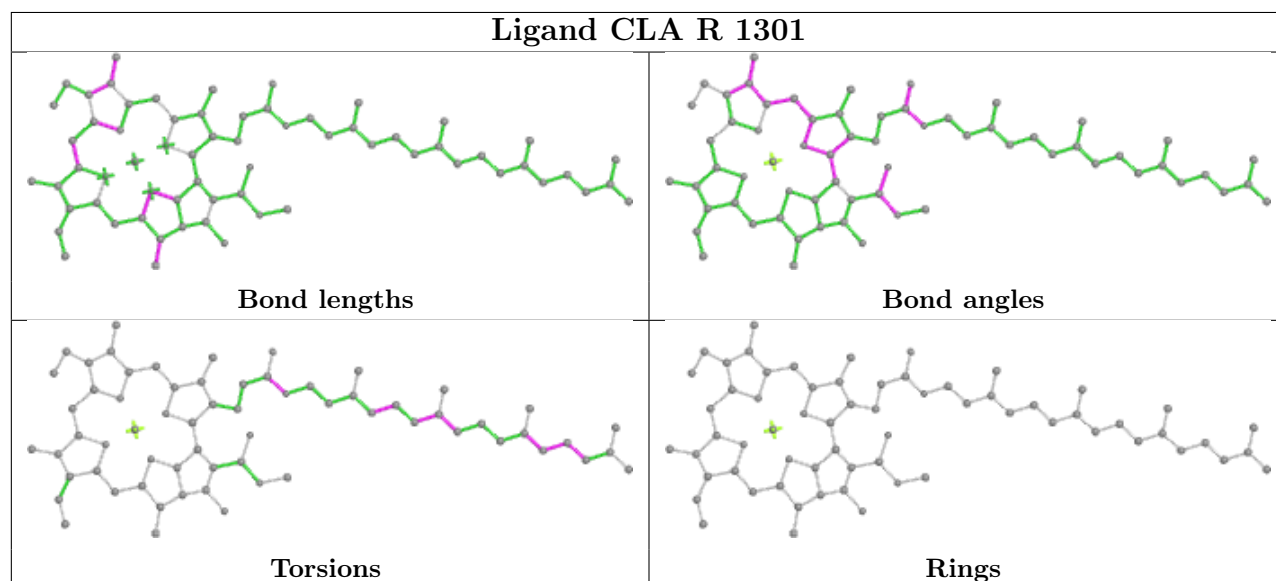




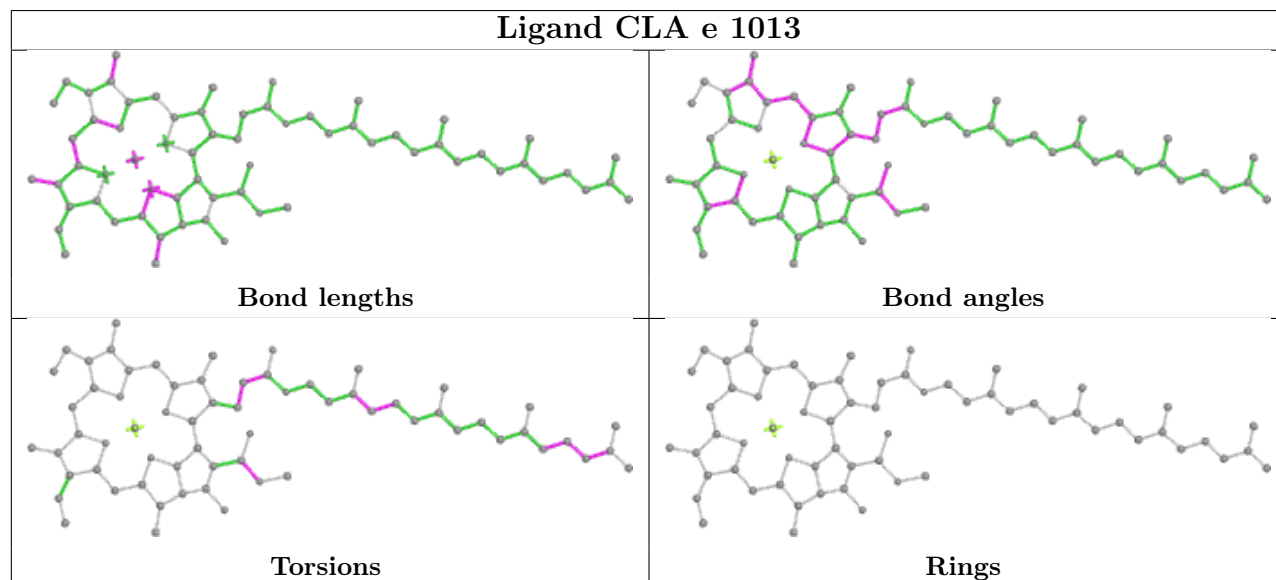
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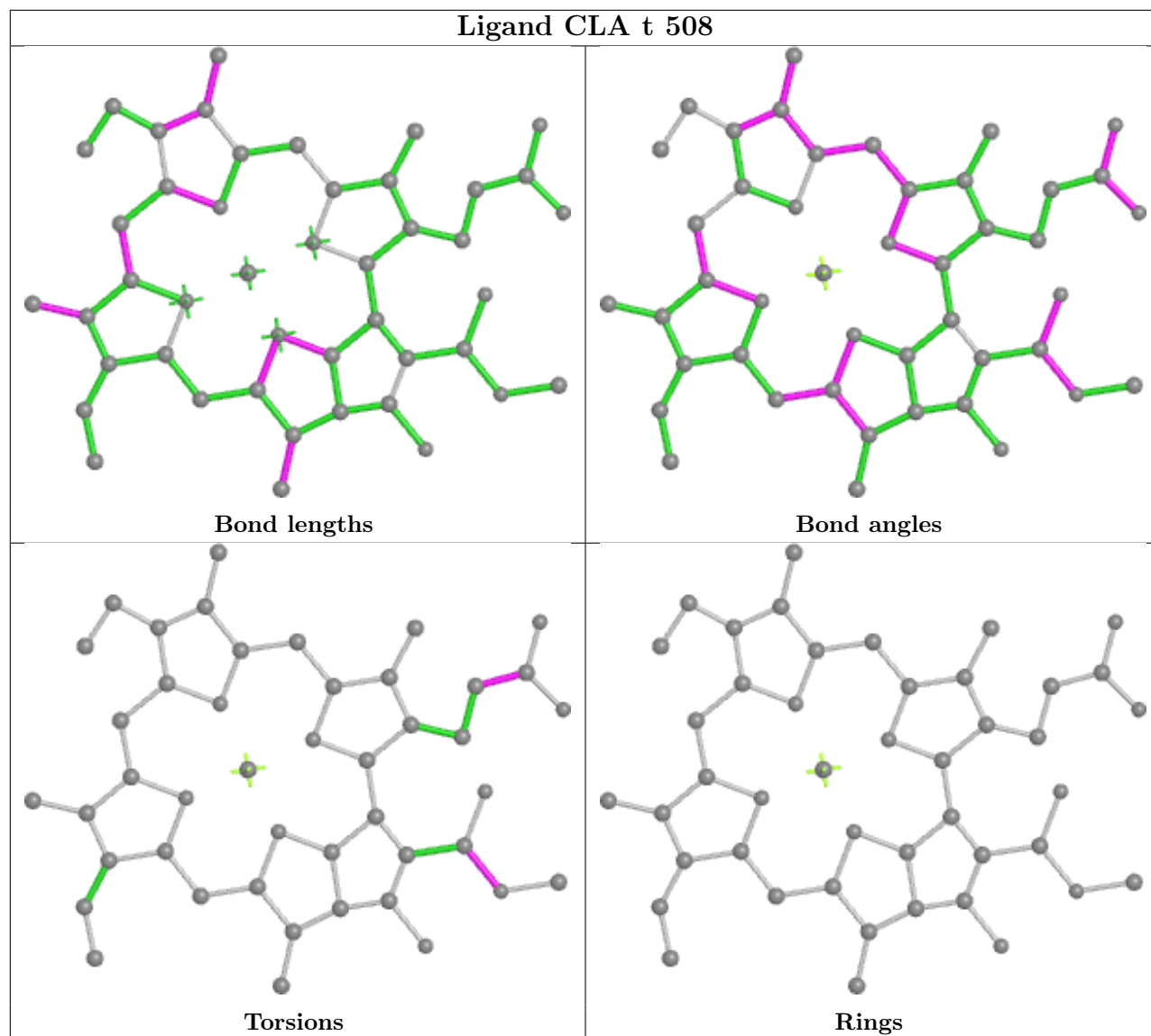
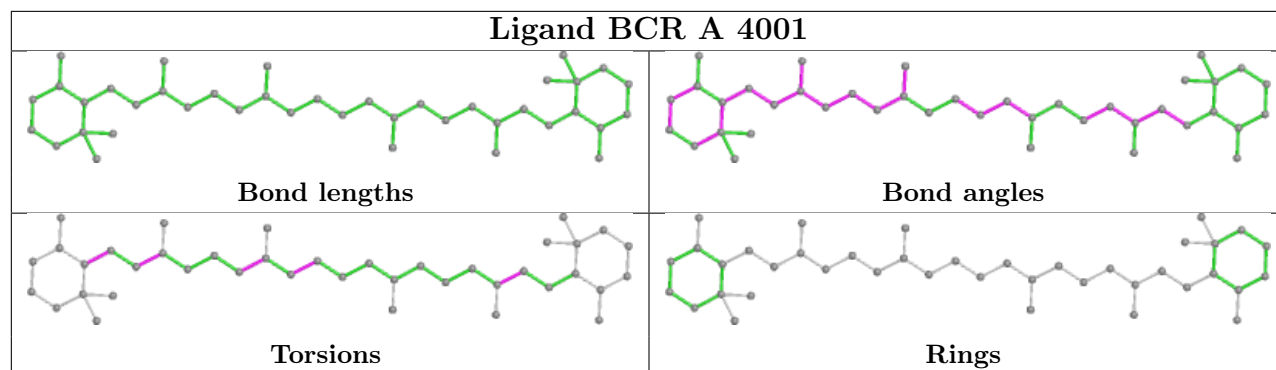


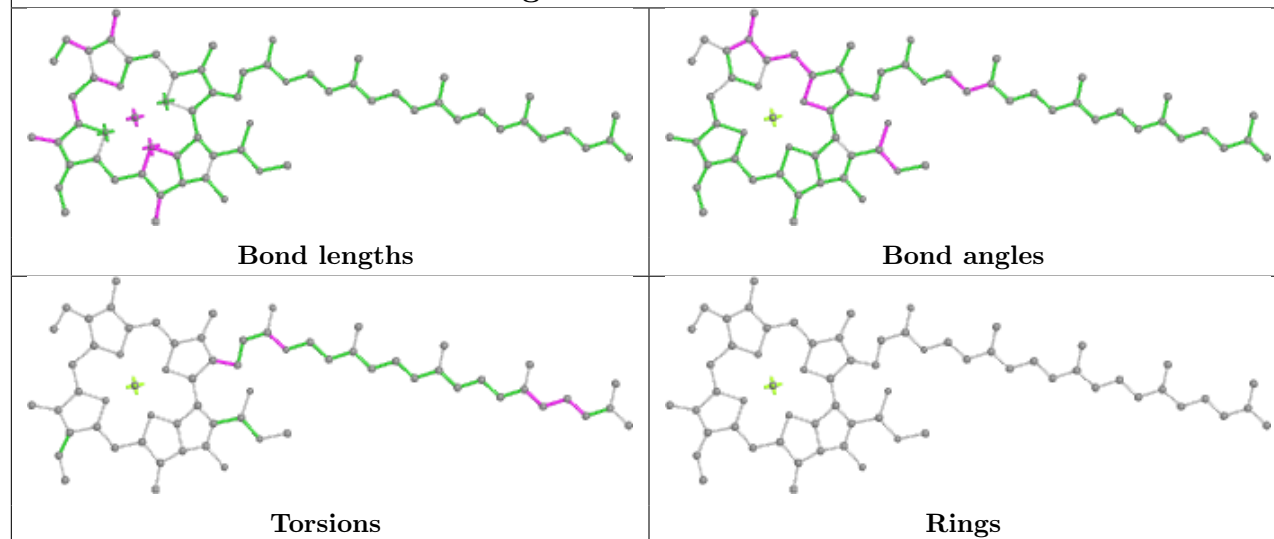
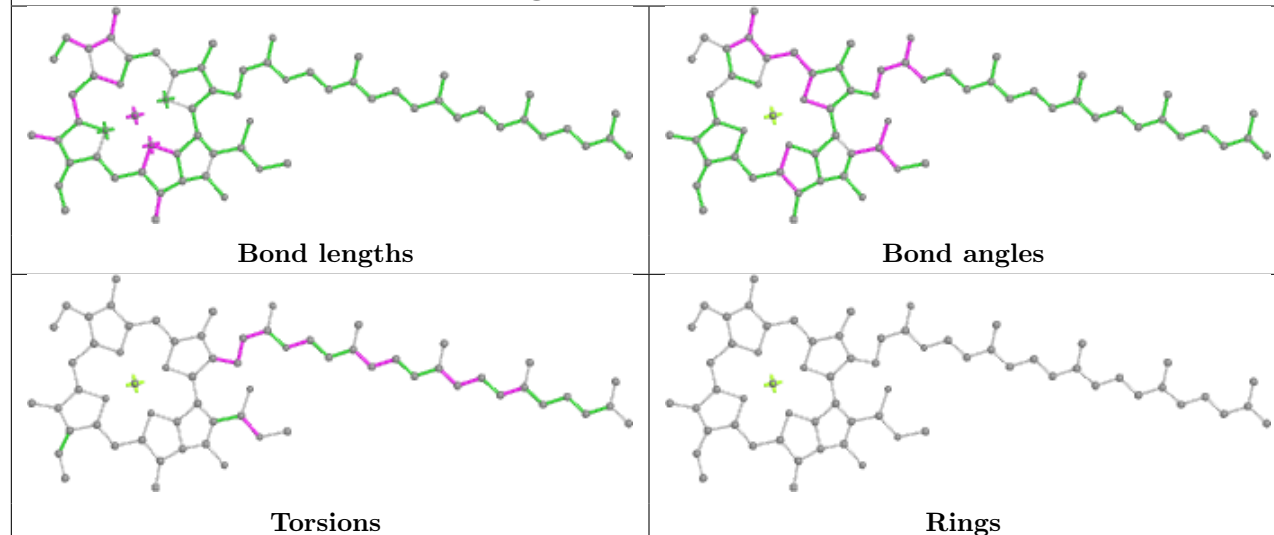
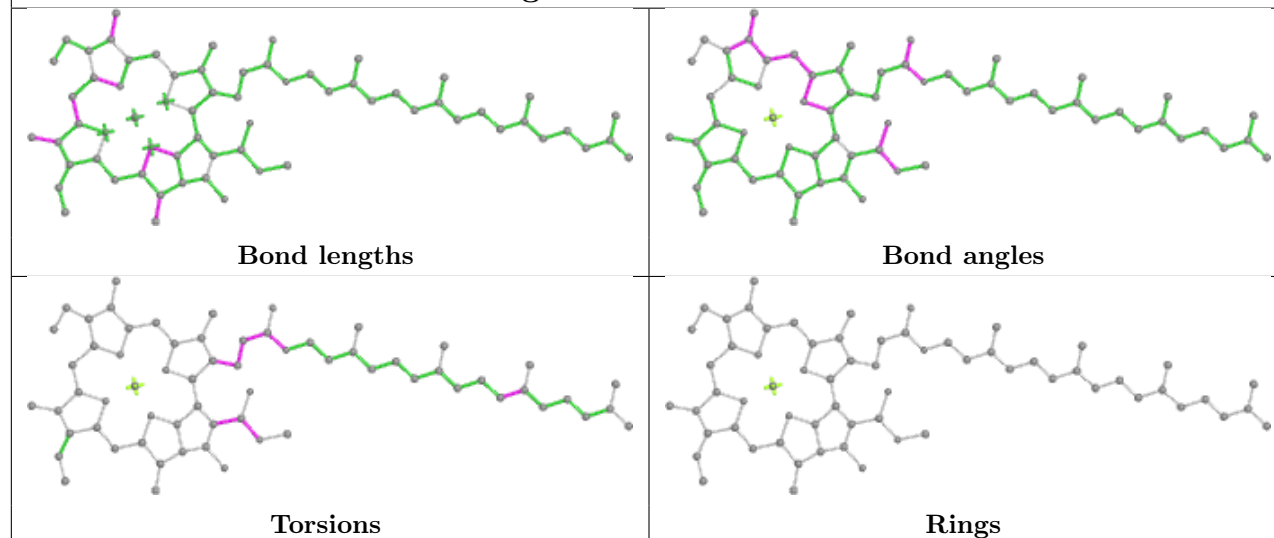
Ligand CLA R 1301



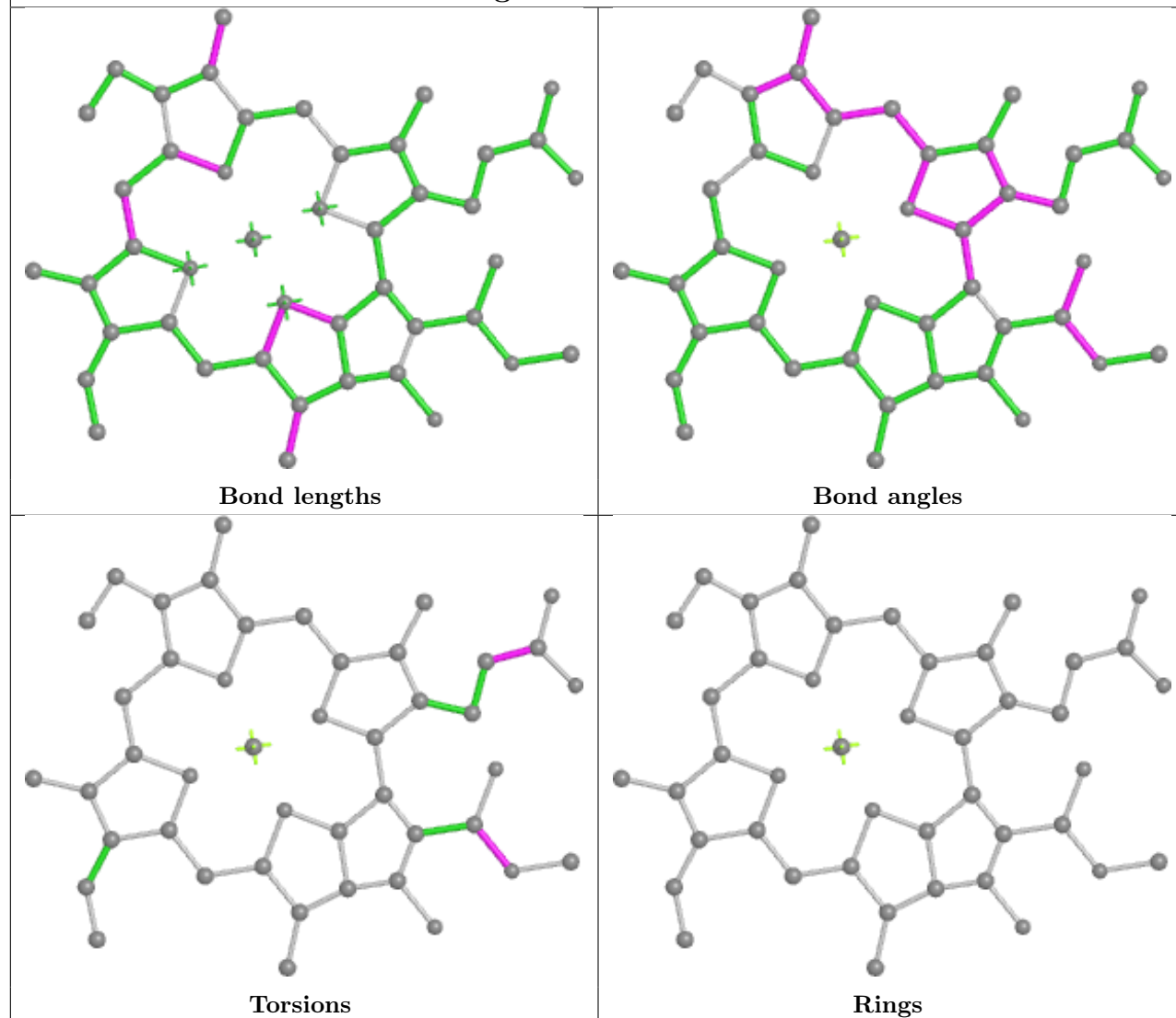
Ligand CLA e 1013



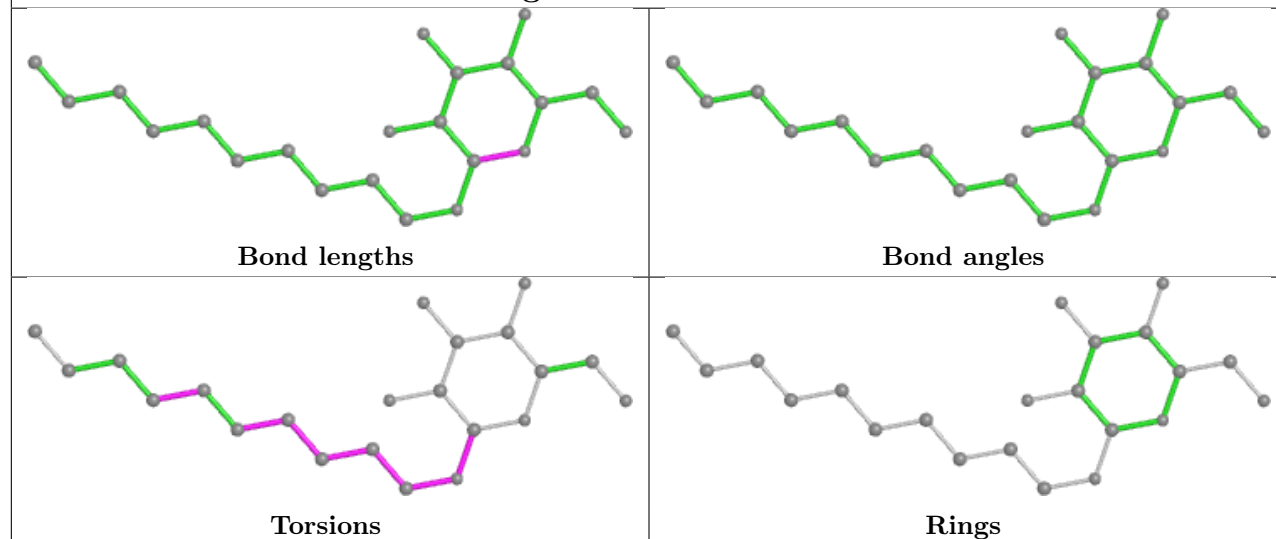


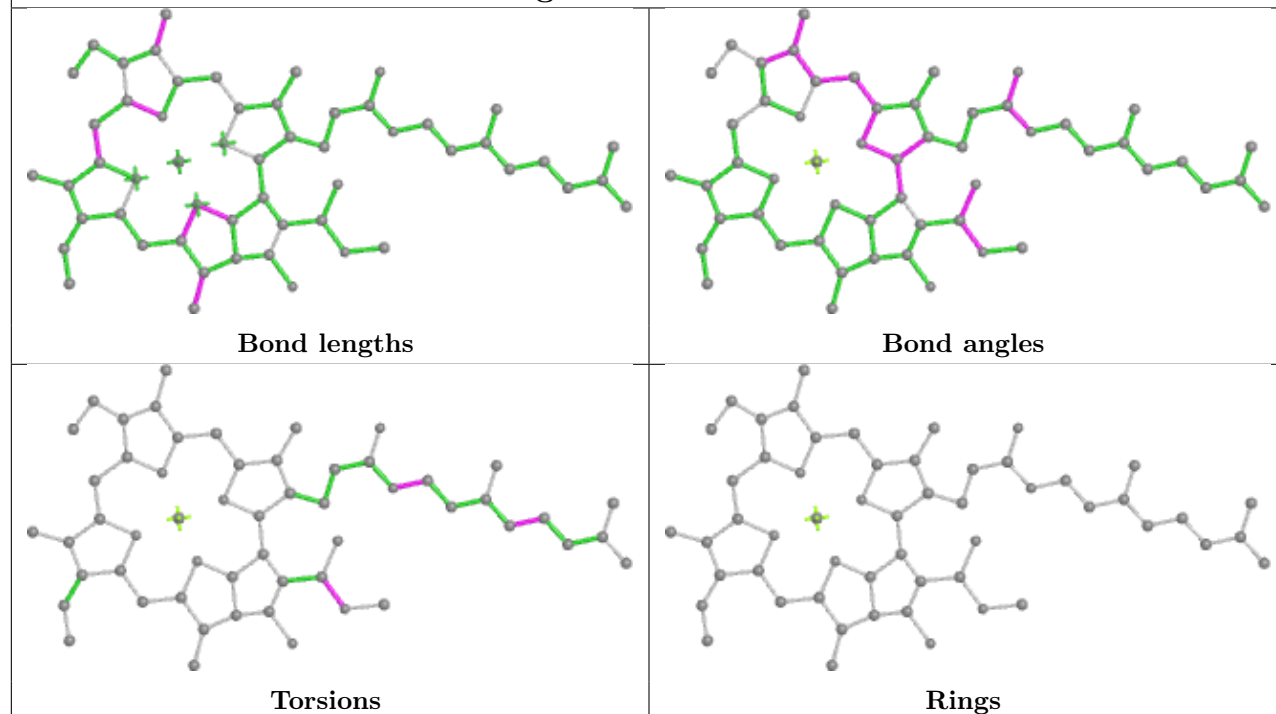
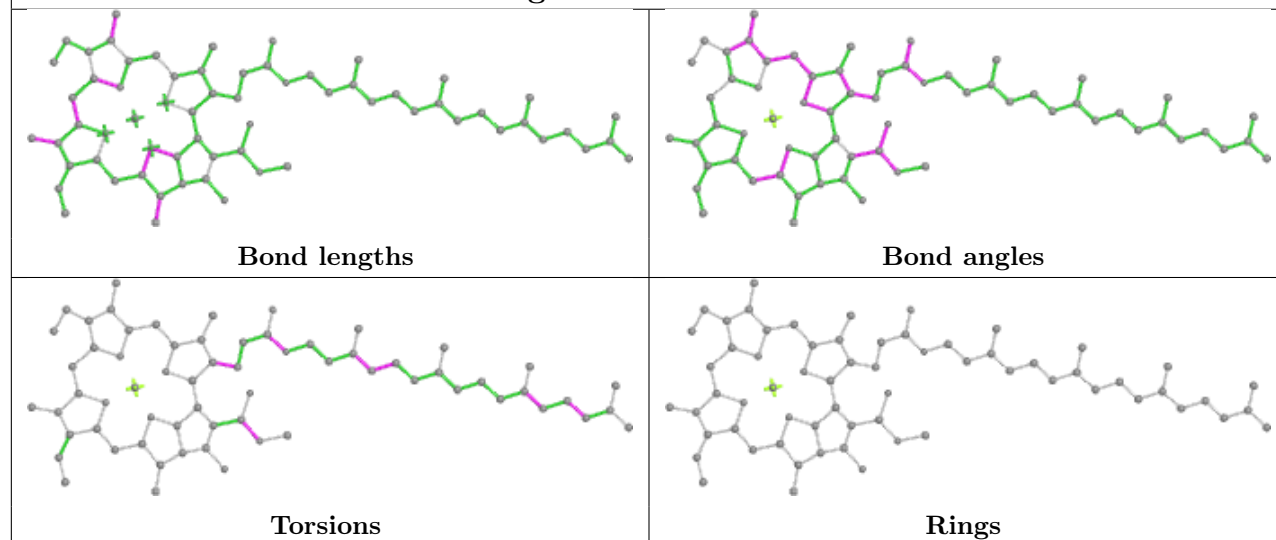
Ligand CLA H 1225**Ligand CLA e 1107****Ligand CLA G 1111**

Ligand CLA 6 507

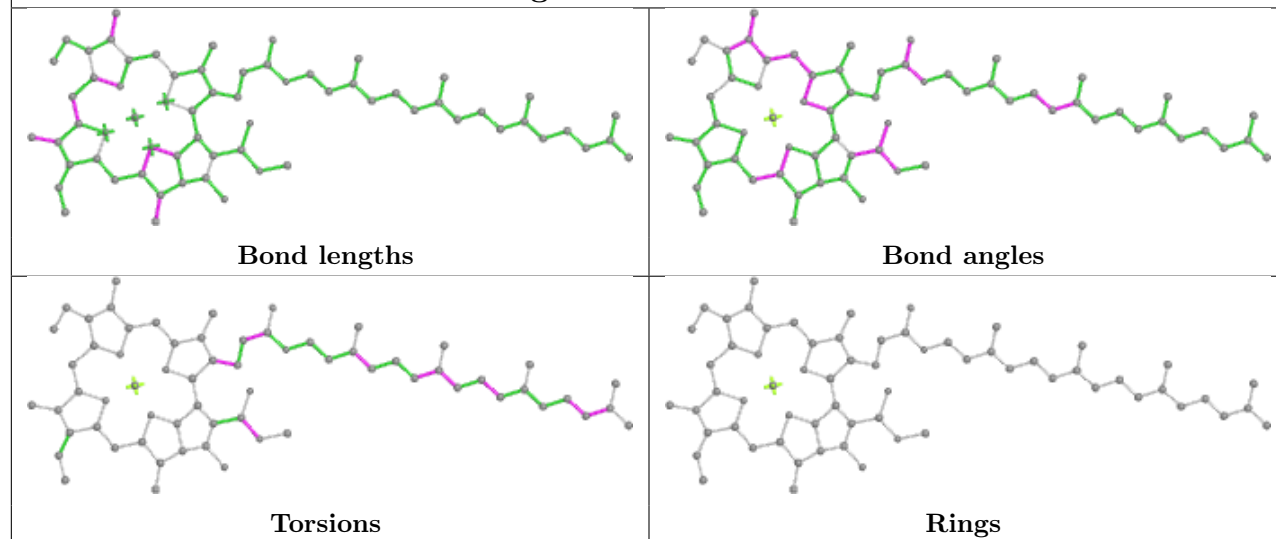


Ligand LMU J 5105

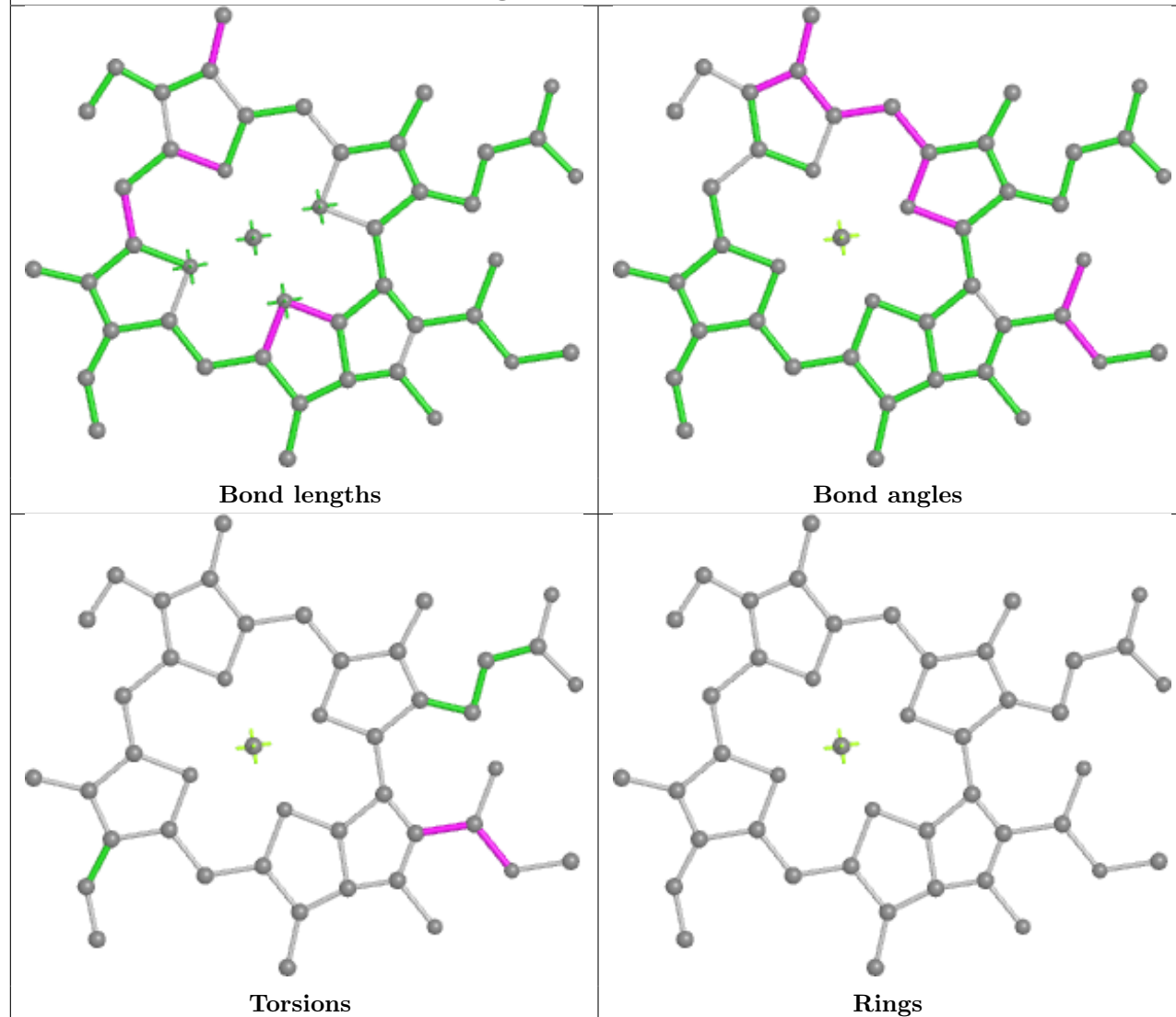


Ligand CLA 1 511**Ligand CLA e 1104**

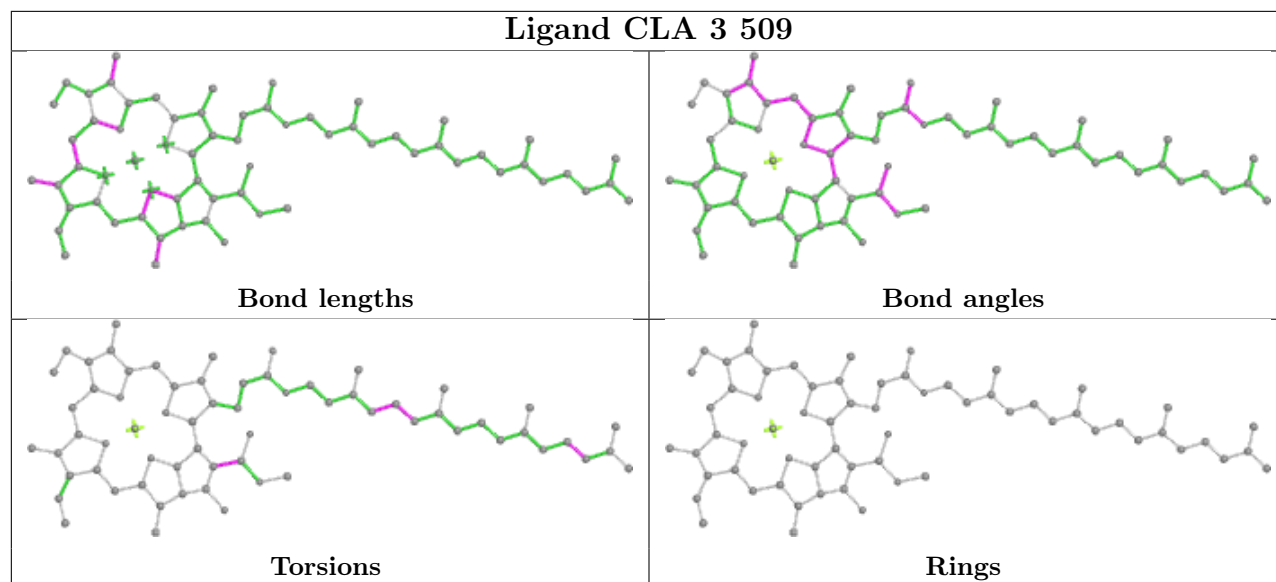
Ligand CLA f 1229



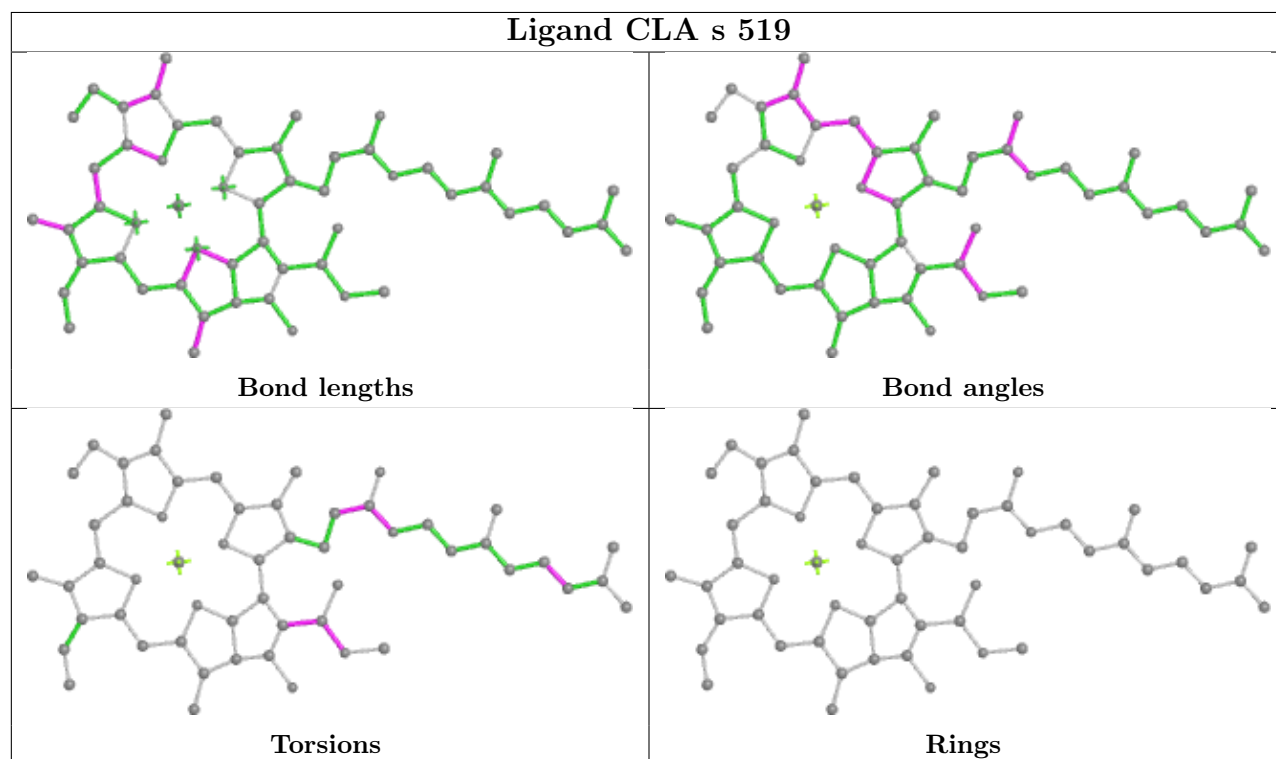
Ligand CLA 6 506



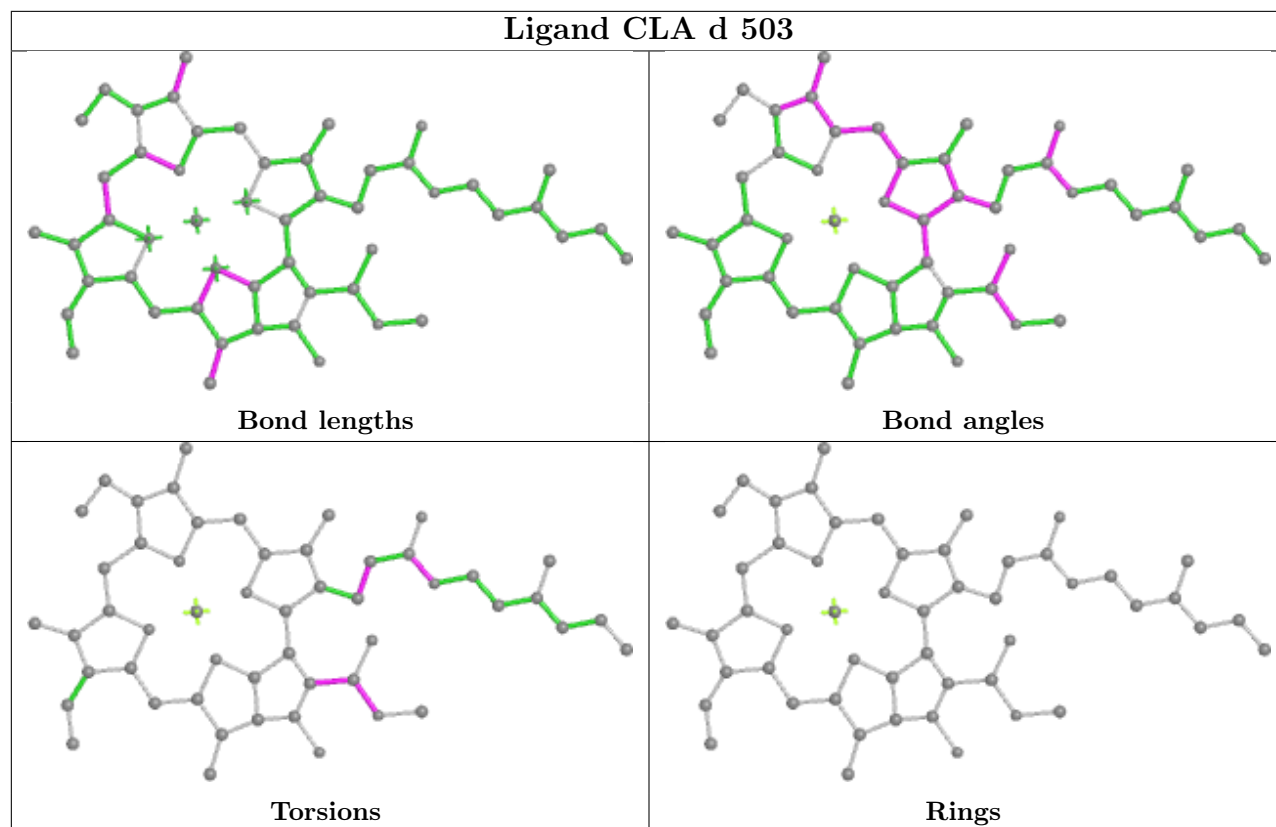
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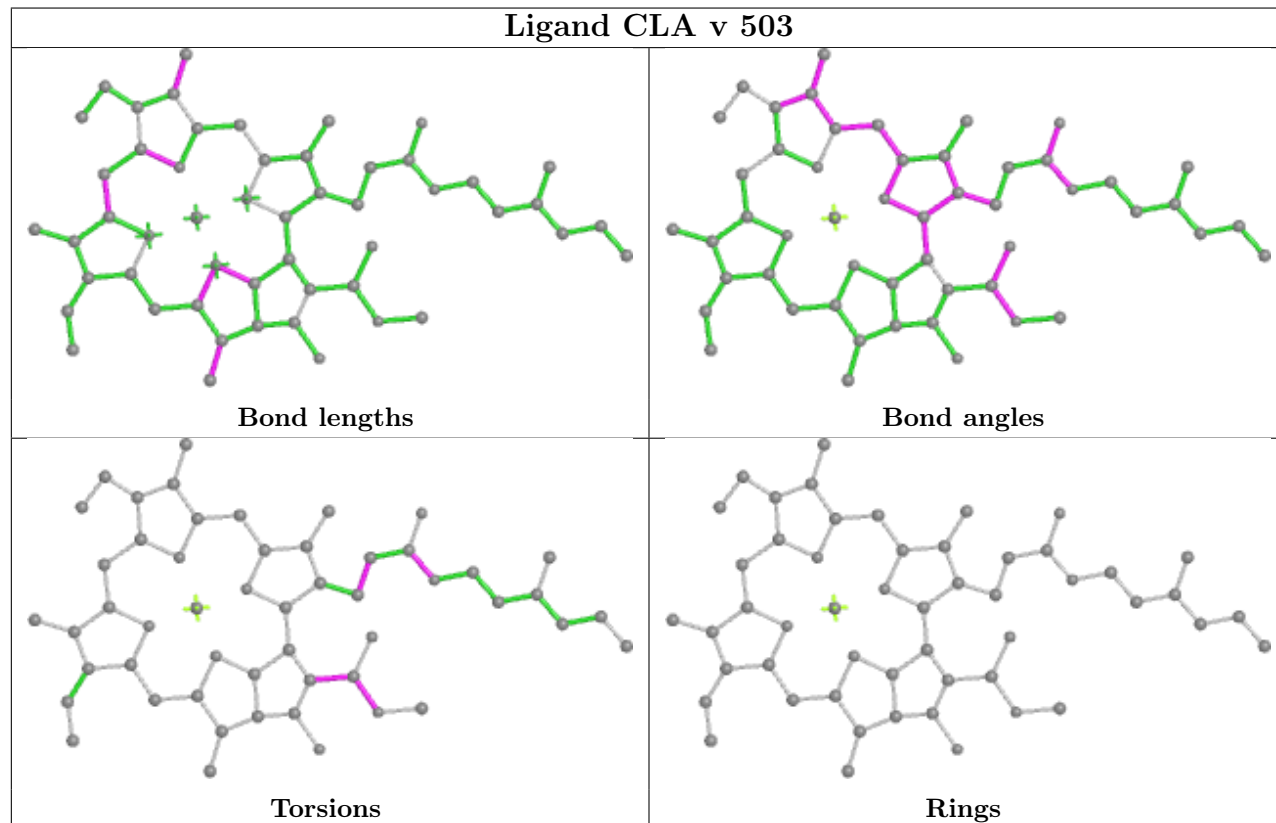
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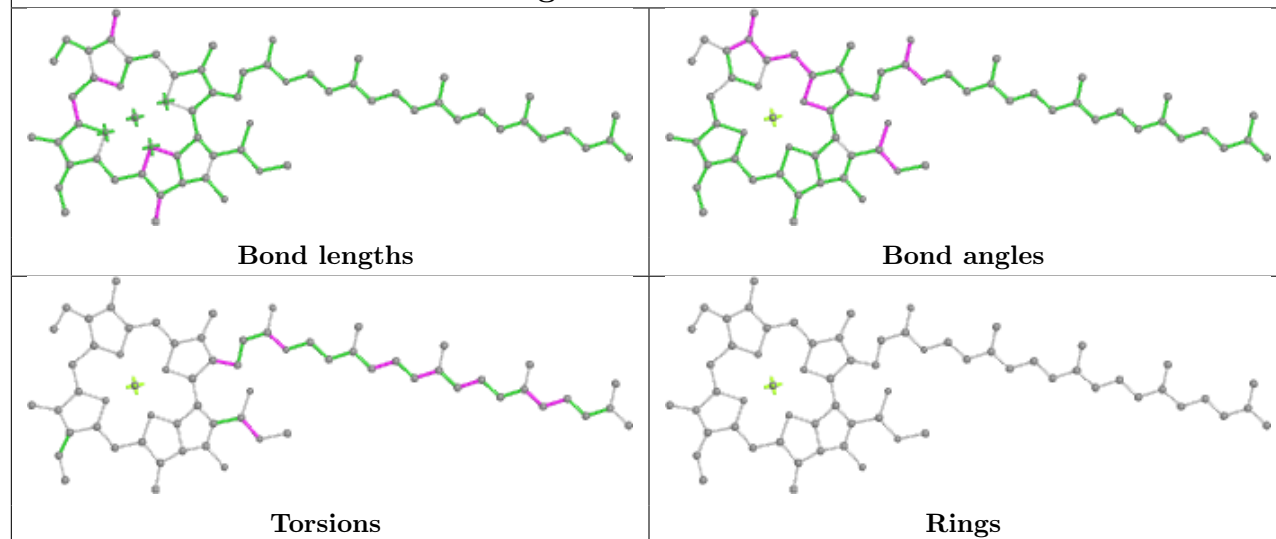
Ligand CLA d 503



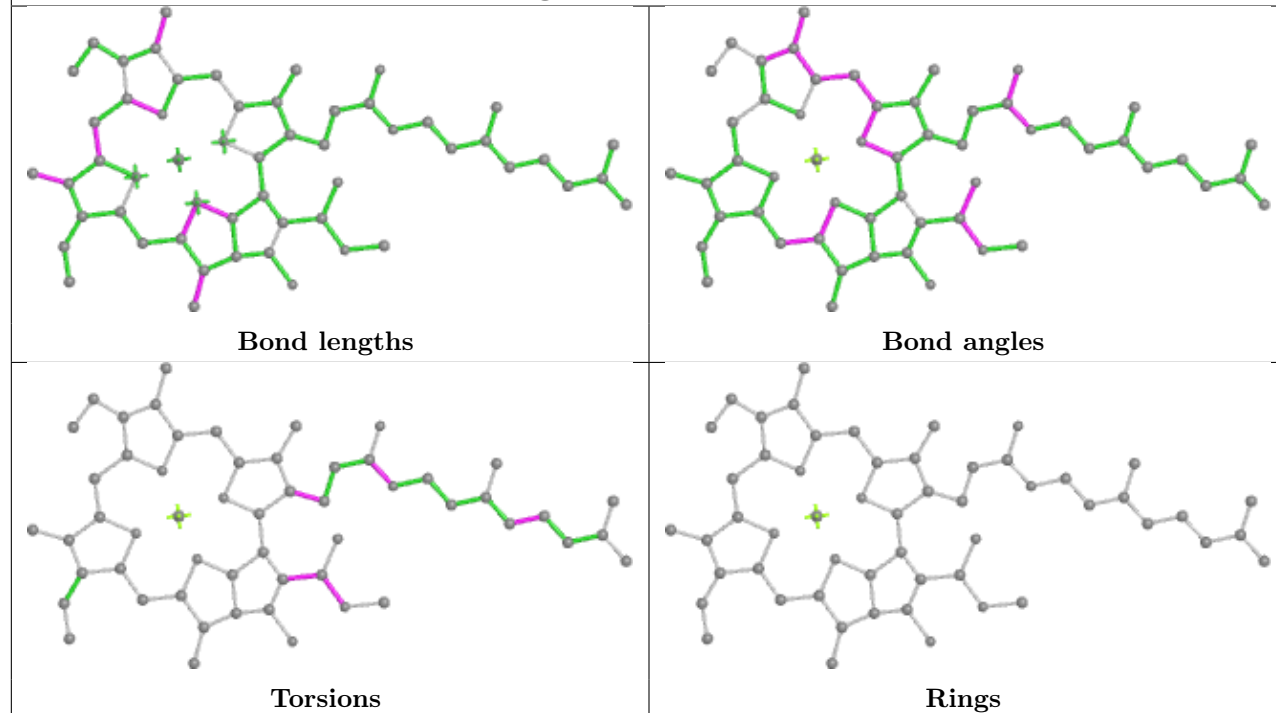
Ligand CLA v 503



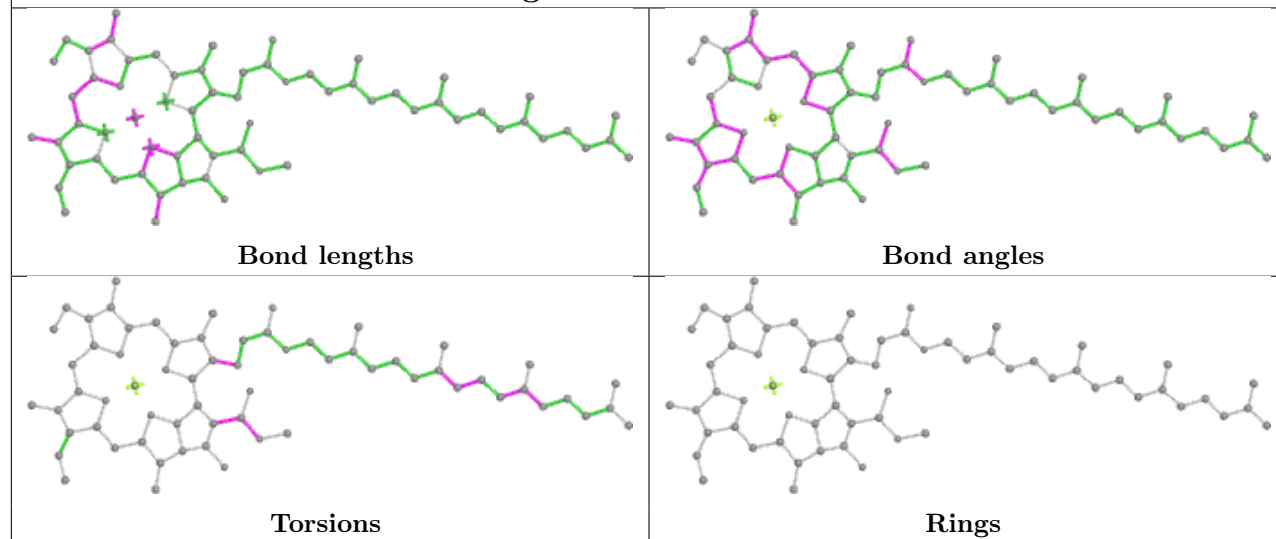
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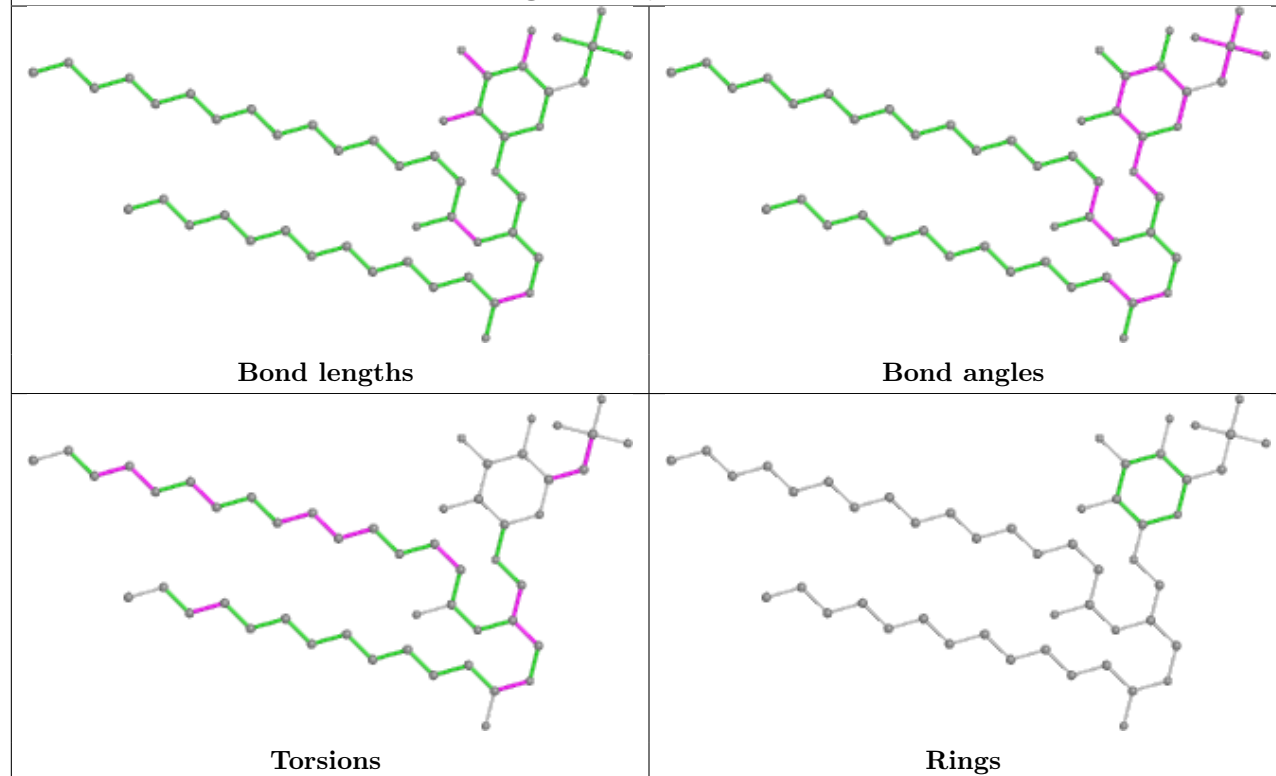
Ligand CLA 3 508

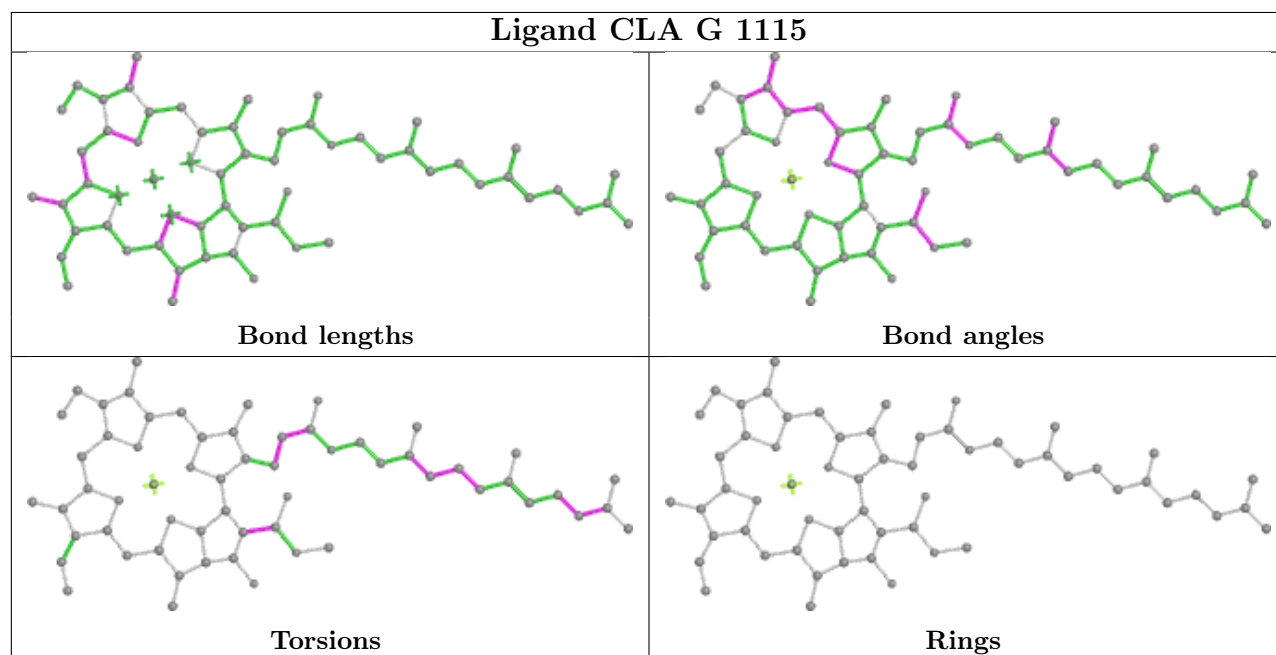
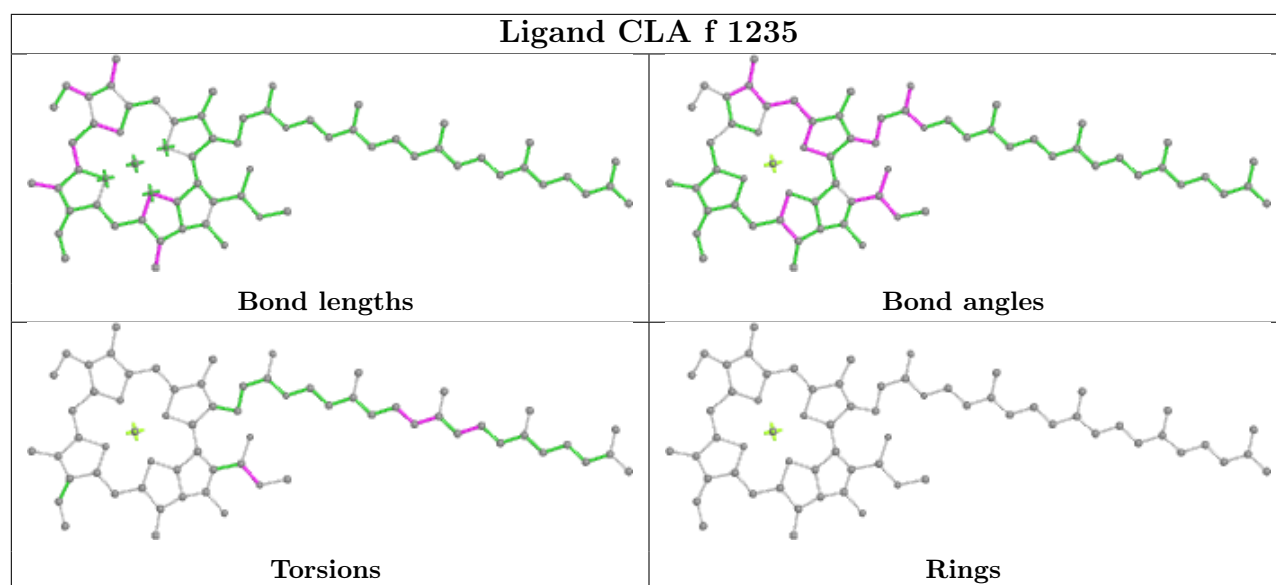


Ligand CLA H 1226

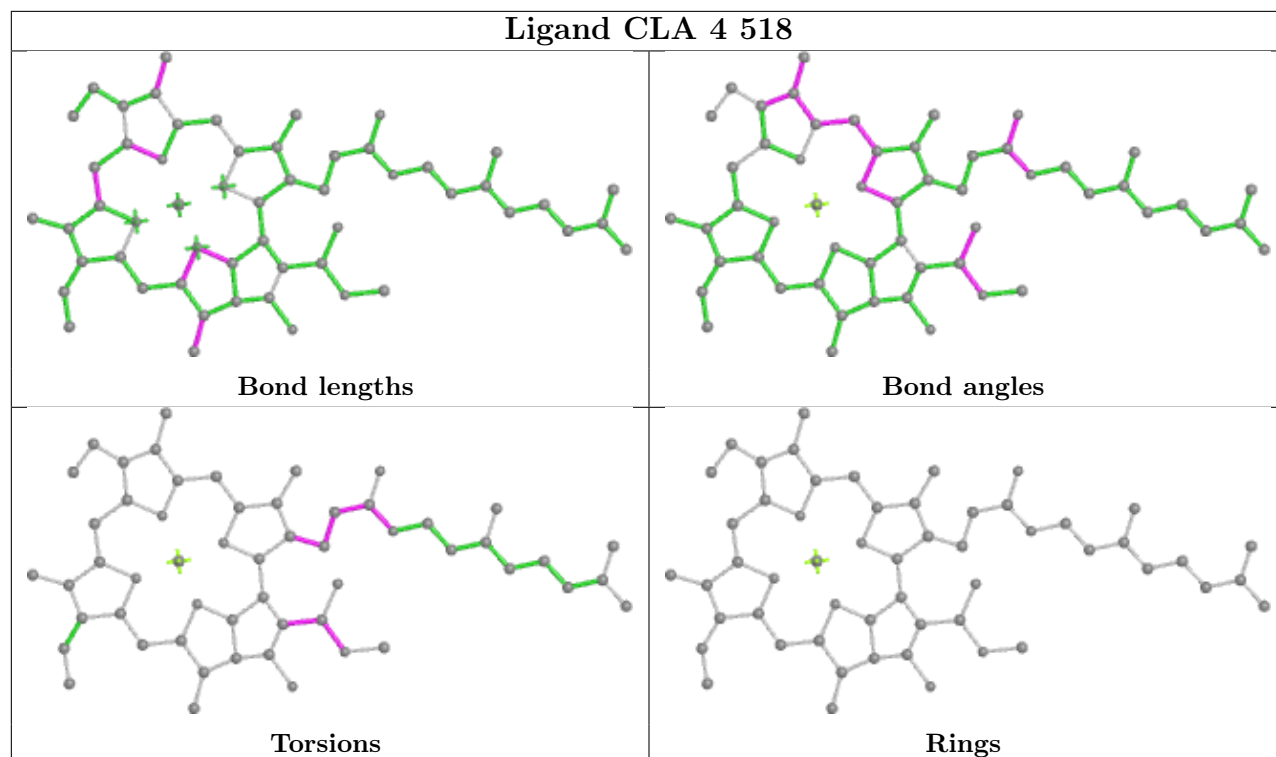


Ligand SQD V 5216

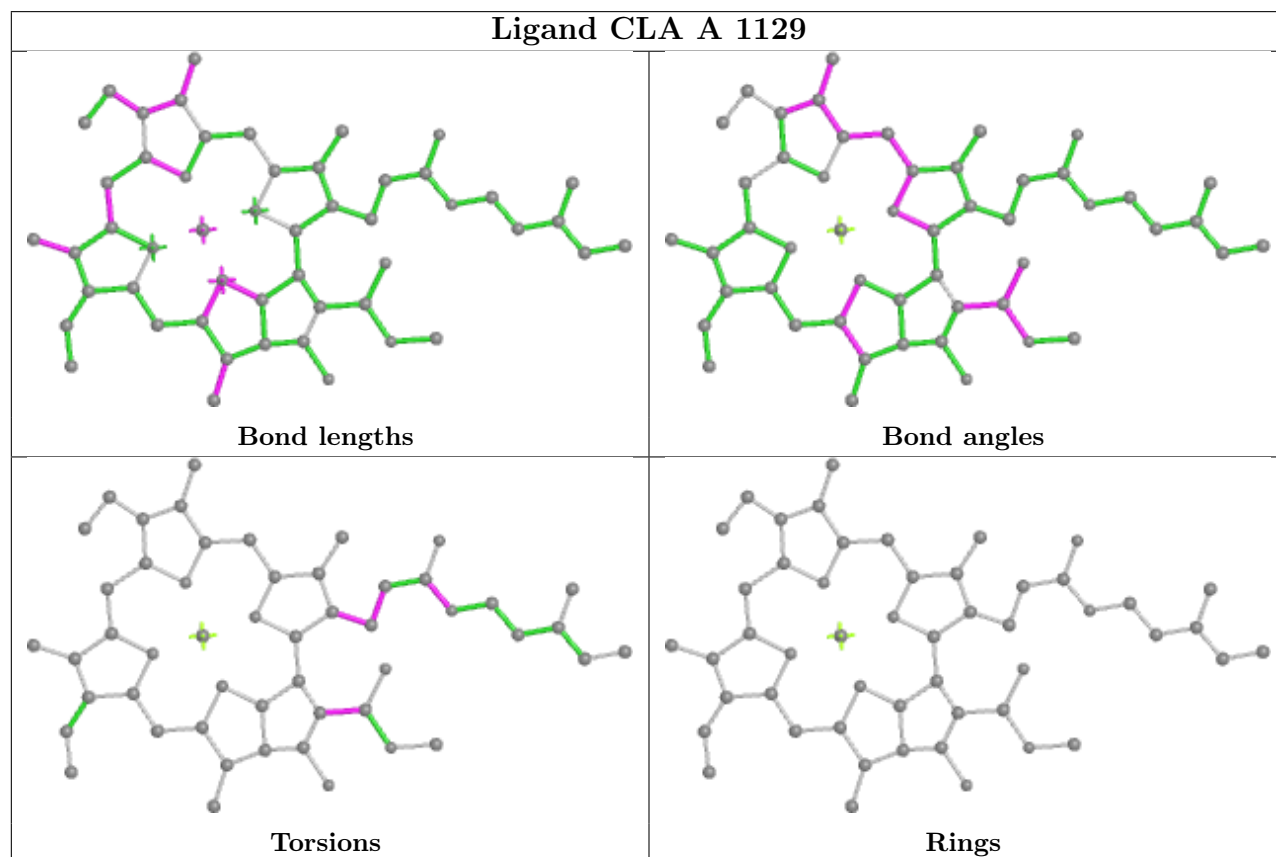


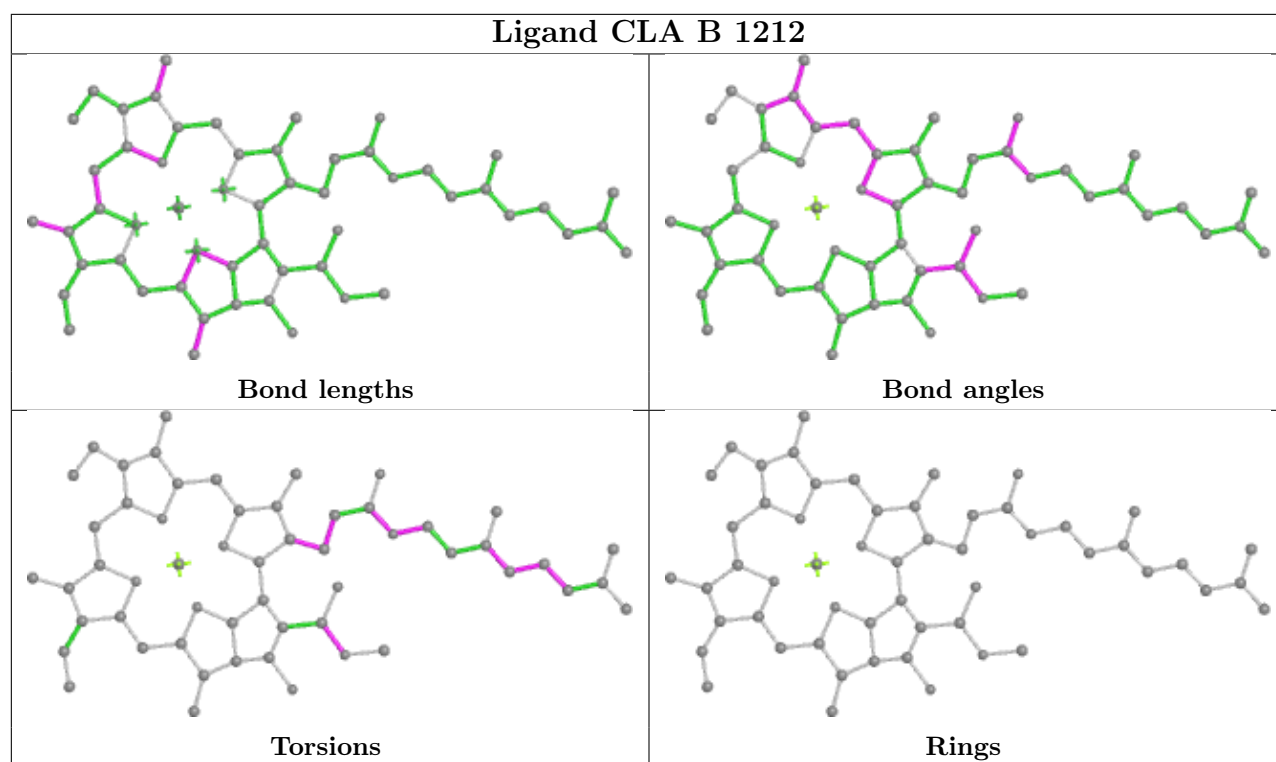


Ligand CLA 4 518

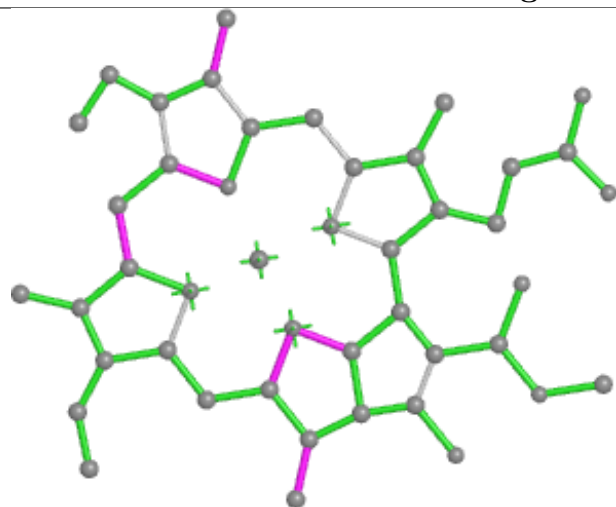


Ligand CLA A 1129

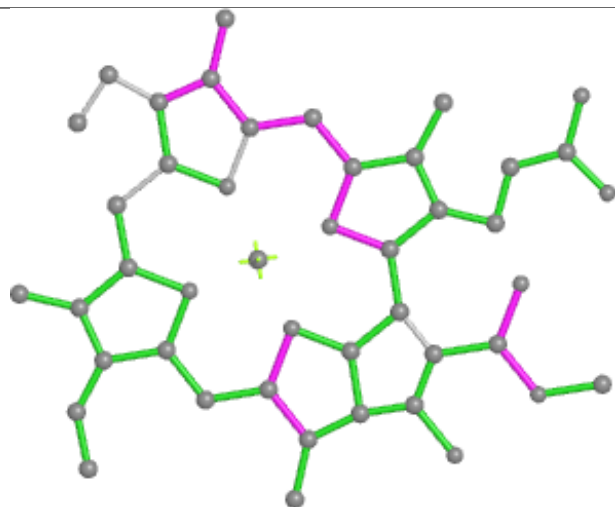




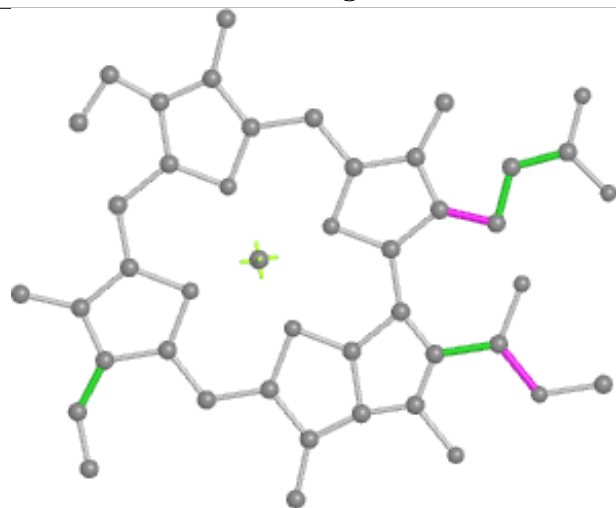
Ligand CLA 4 511



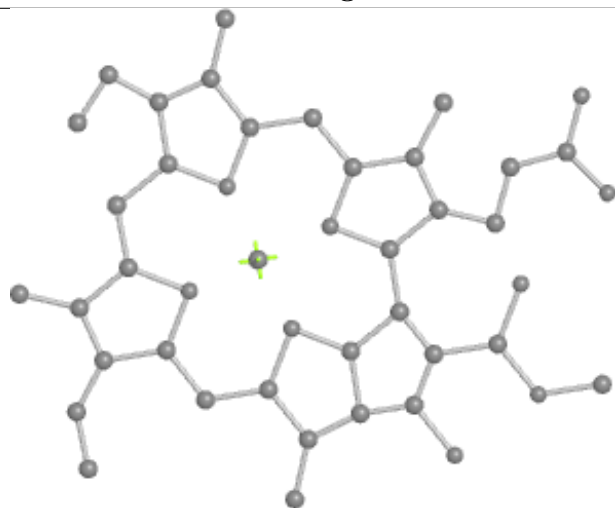
Bond lengths



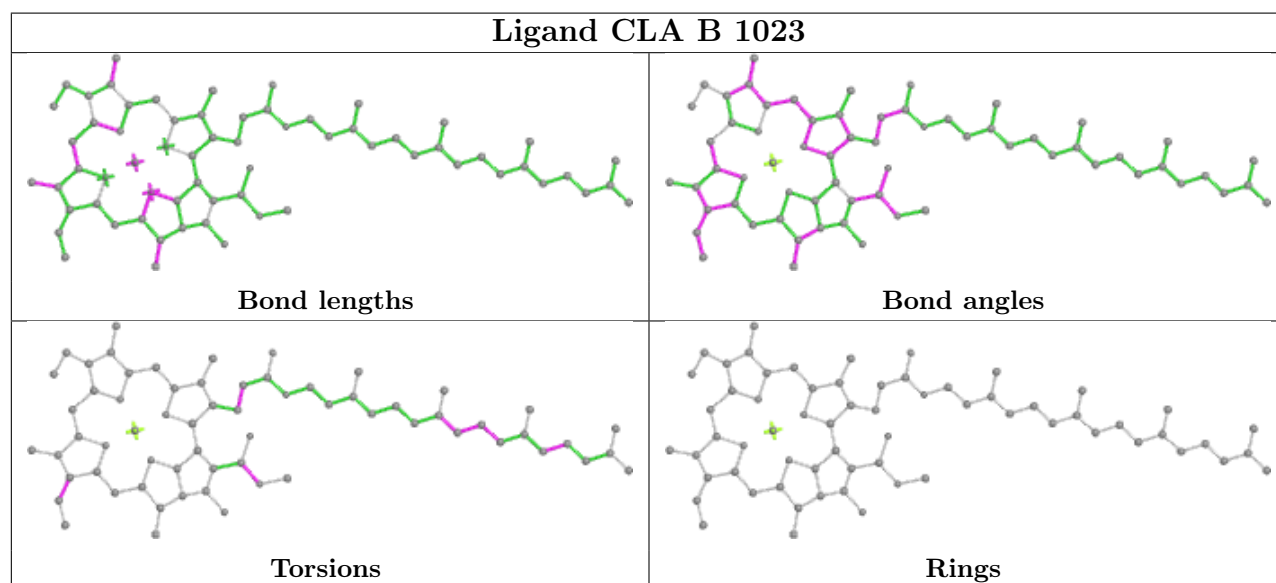
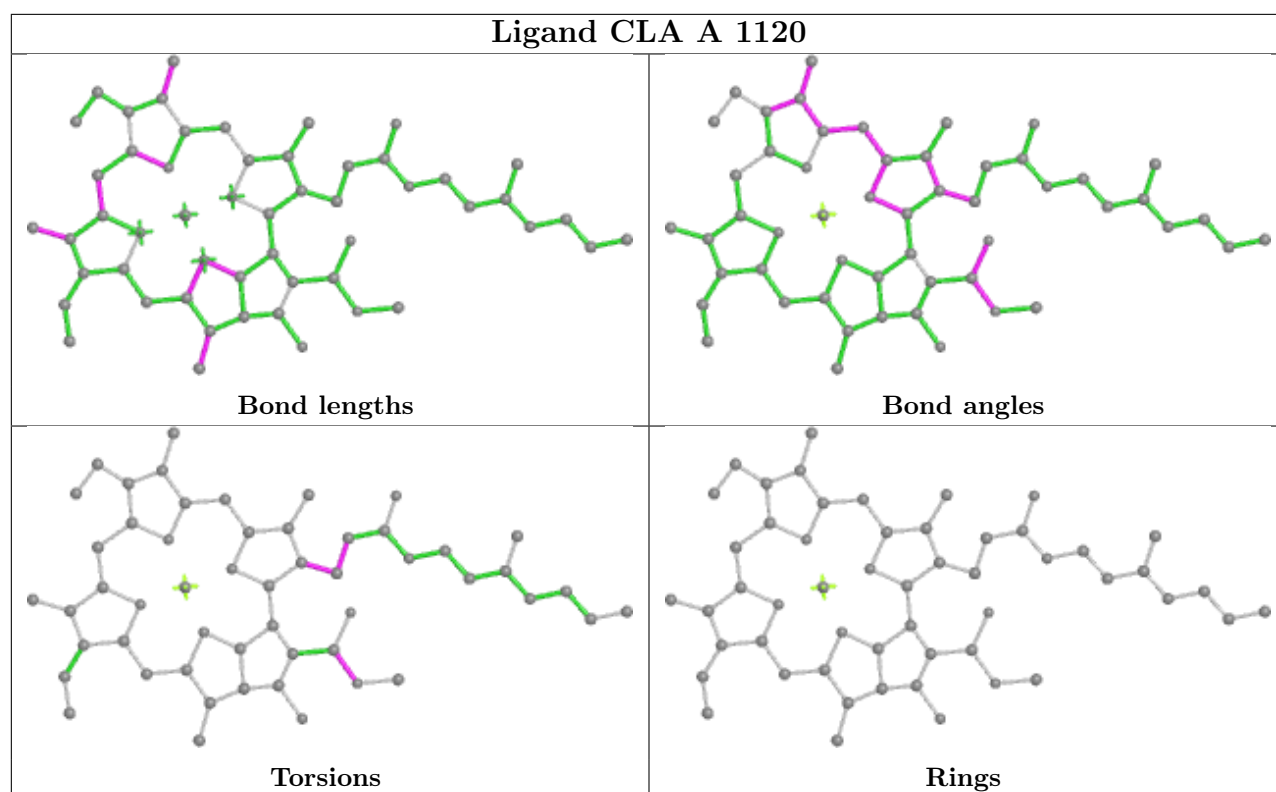
Bond angles



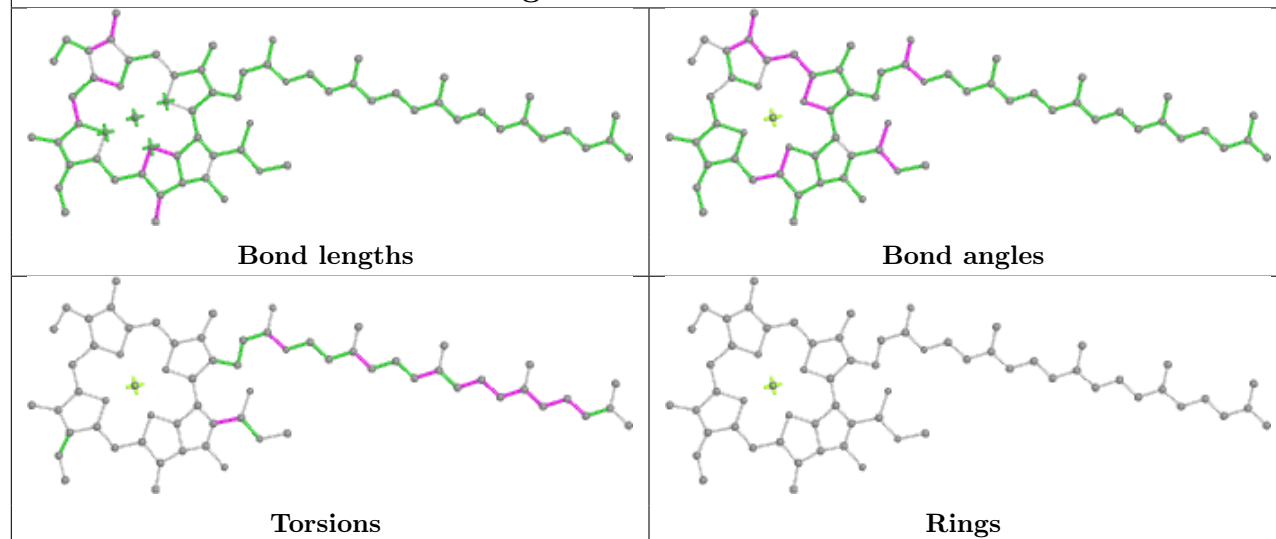
Torsions



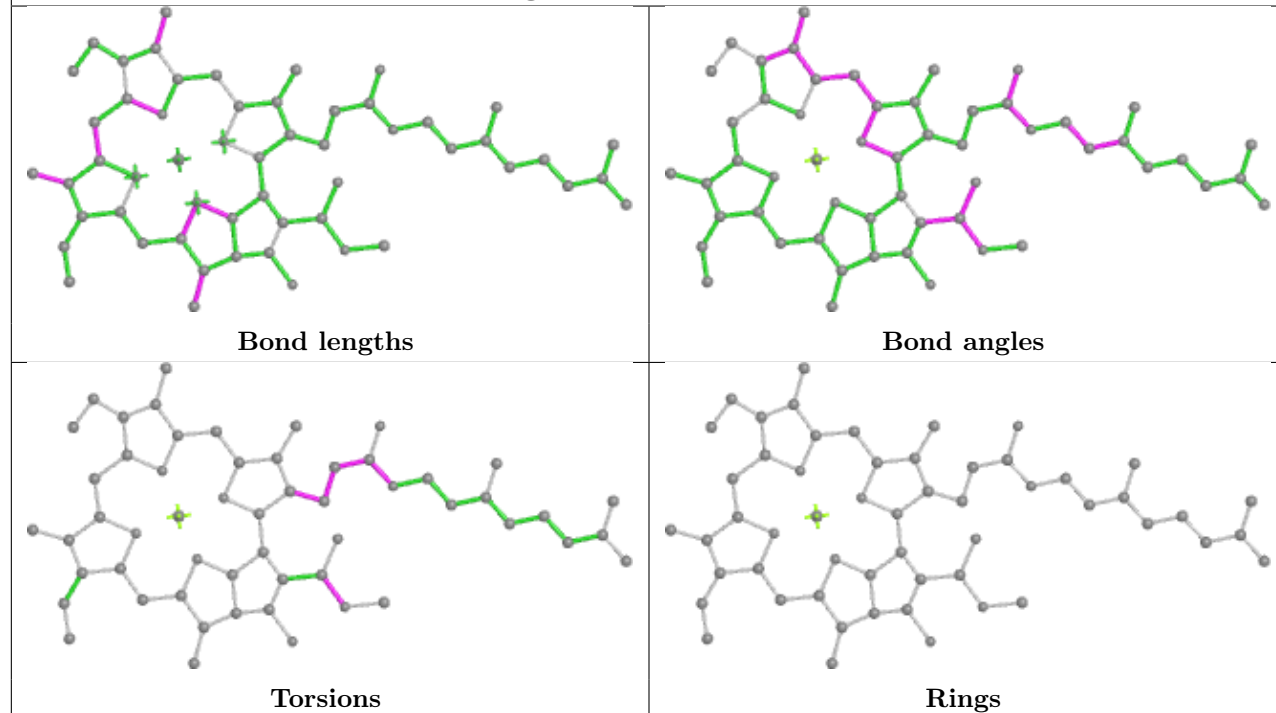
Rings

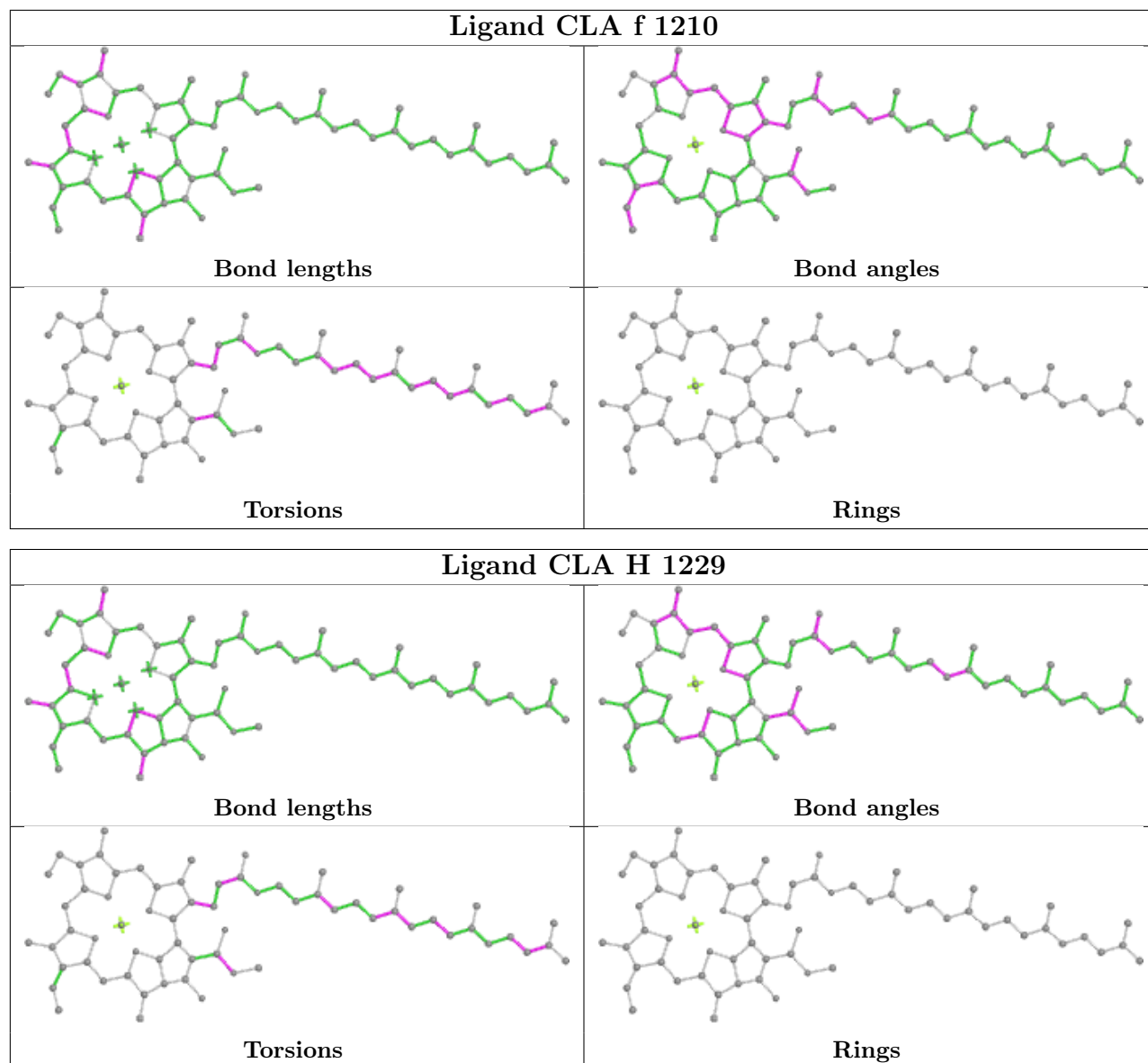


Ligand CLA H 1208

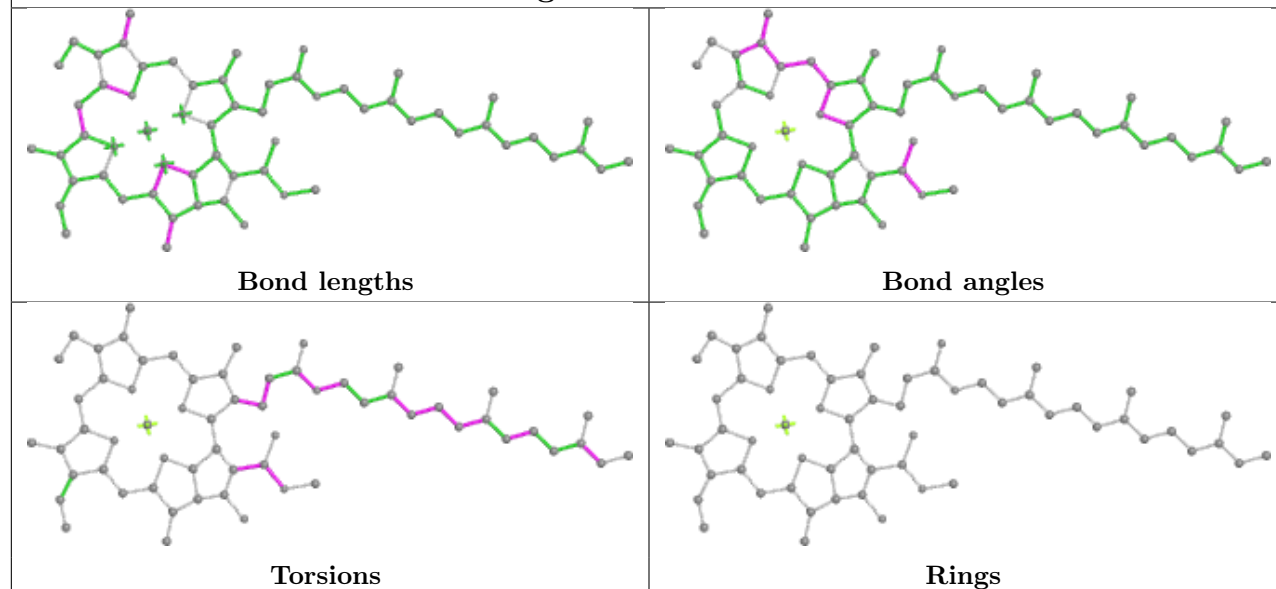


Ligand CLA H 1228

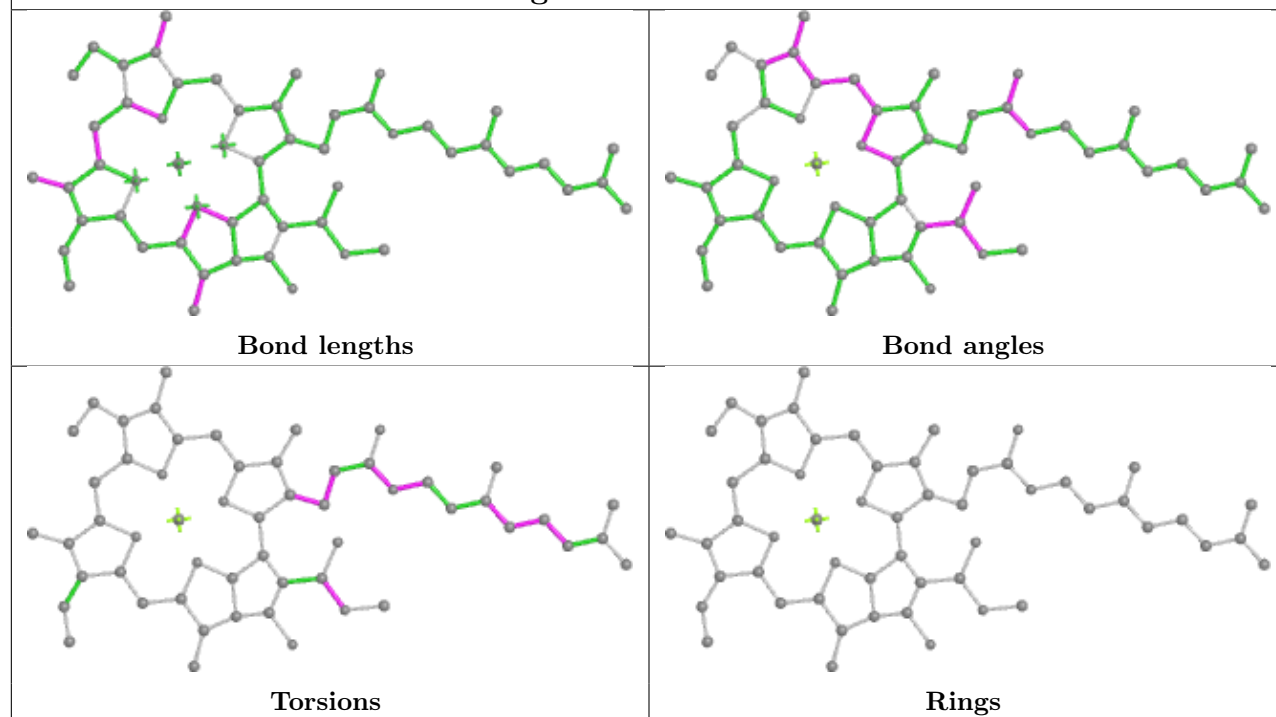


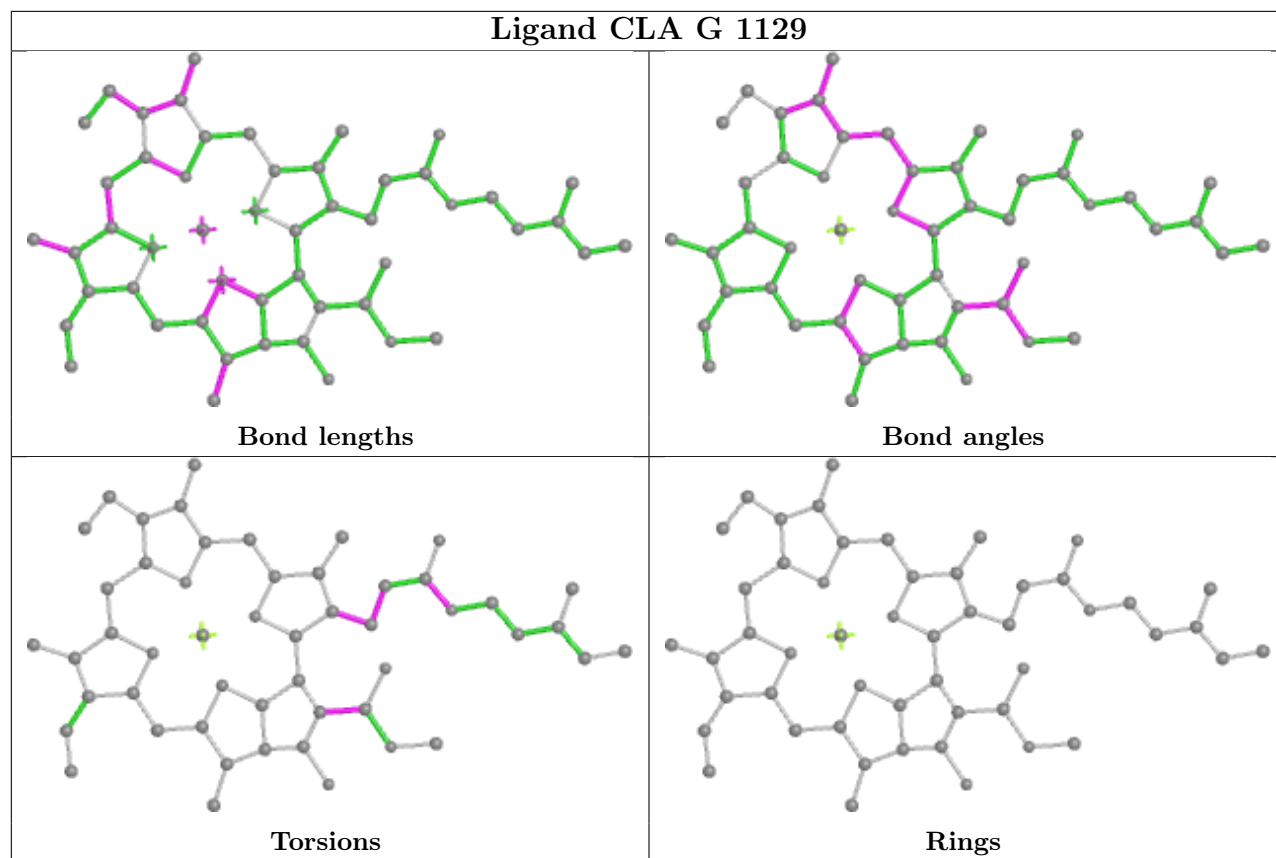


Ligand CLA c 505

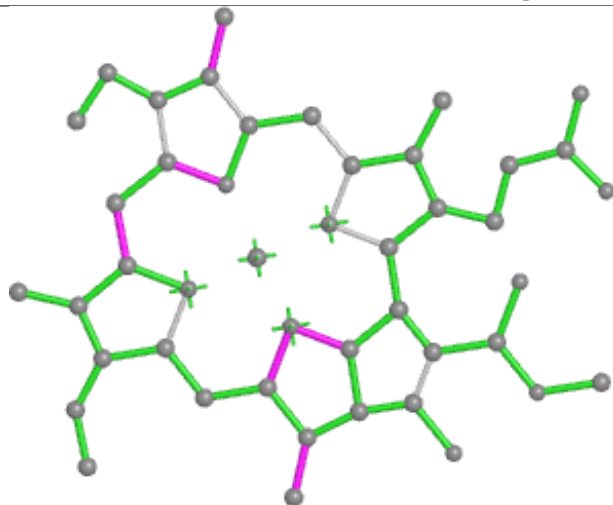


Ligand CLA f 1212

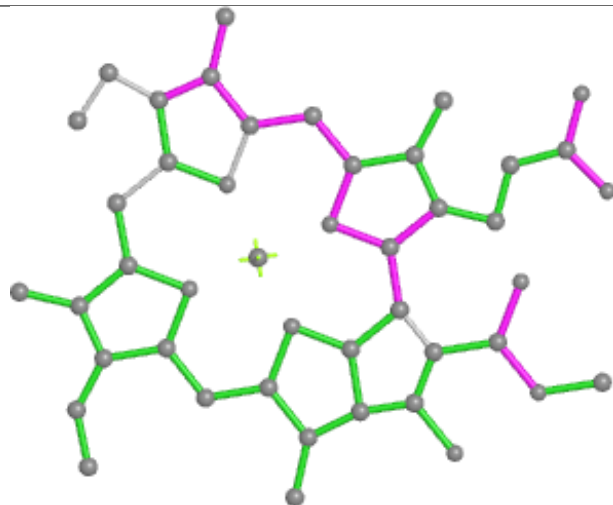




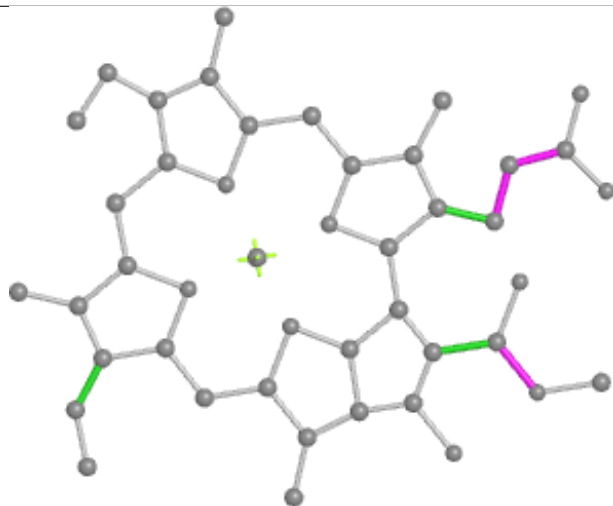
Ligand CLA u 507



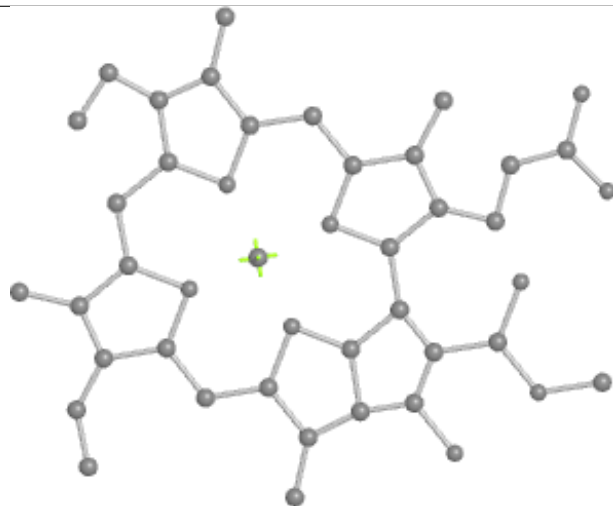
Bond lengths



Bond angles

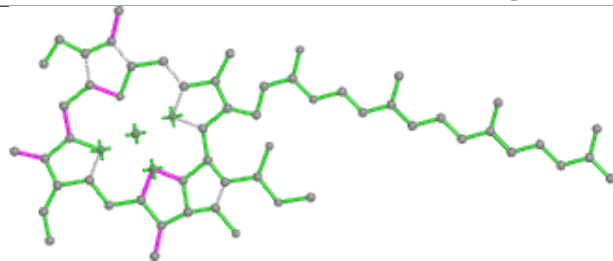


Torsions

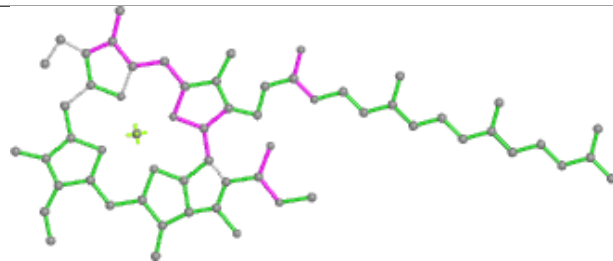


Rings

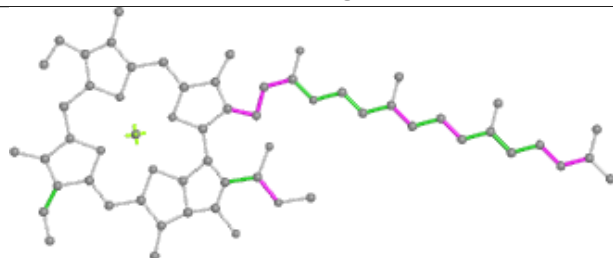
Ligand CLA B 1224



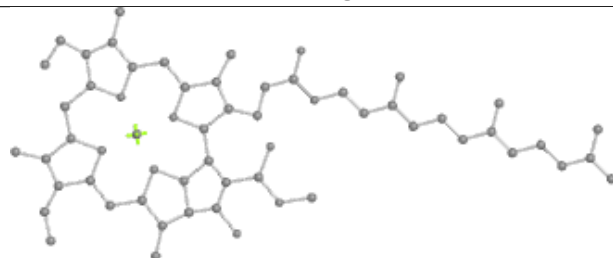
Bond lengths



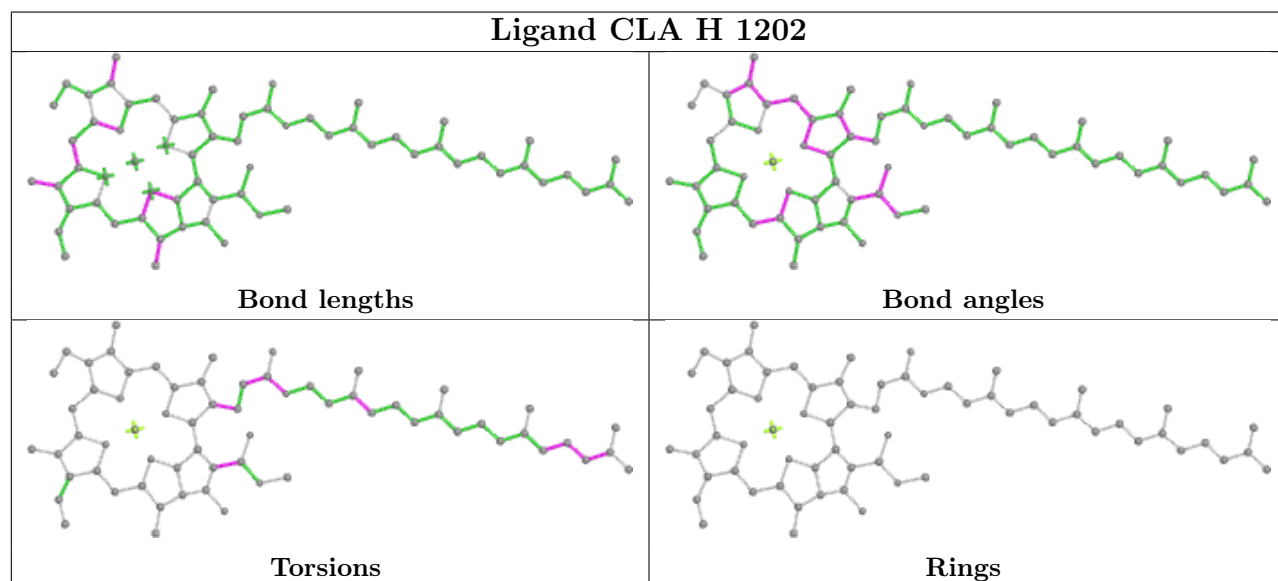
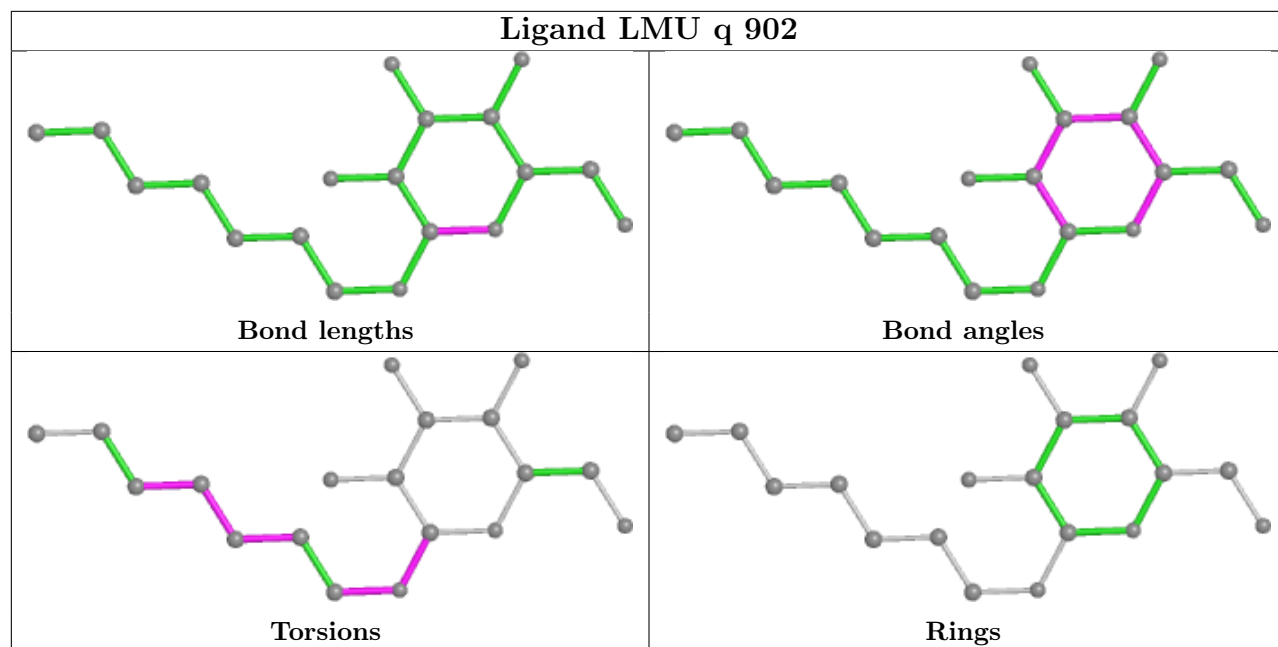
Bond angles

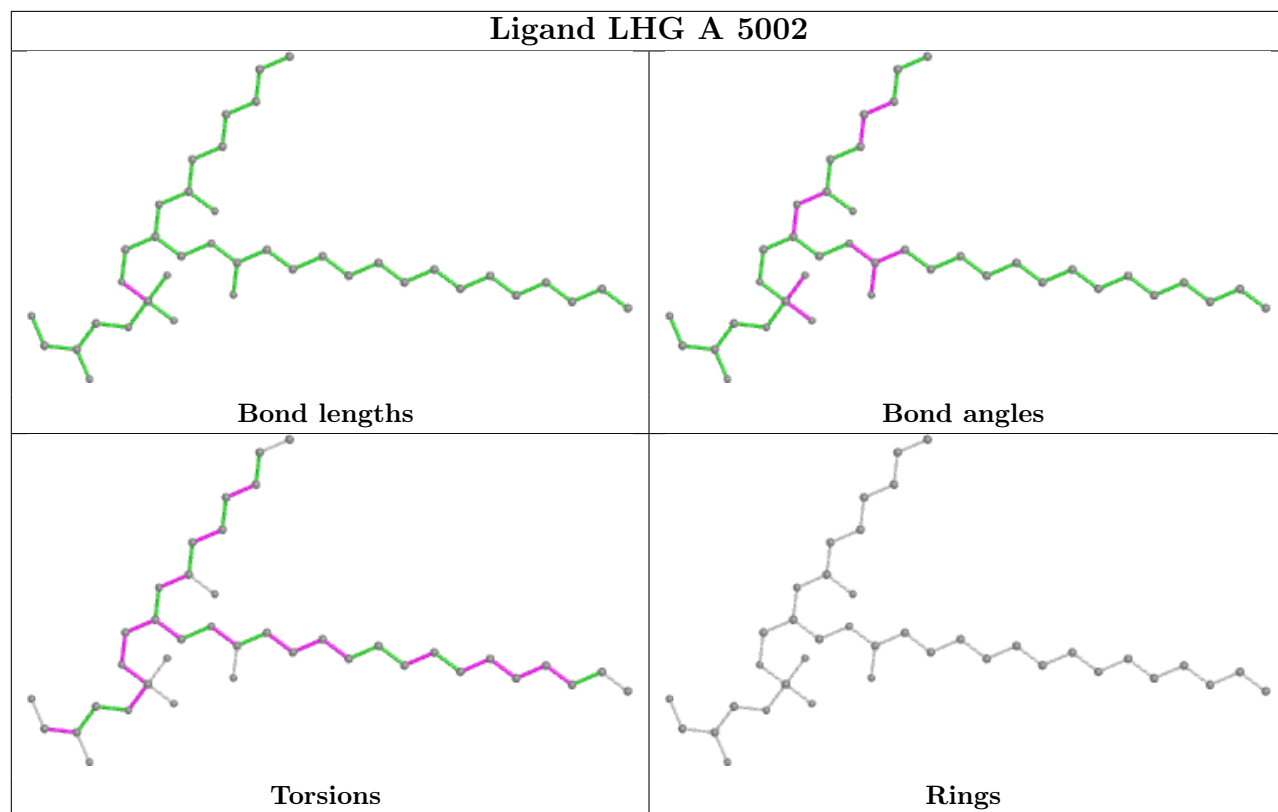


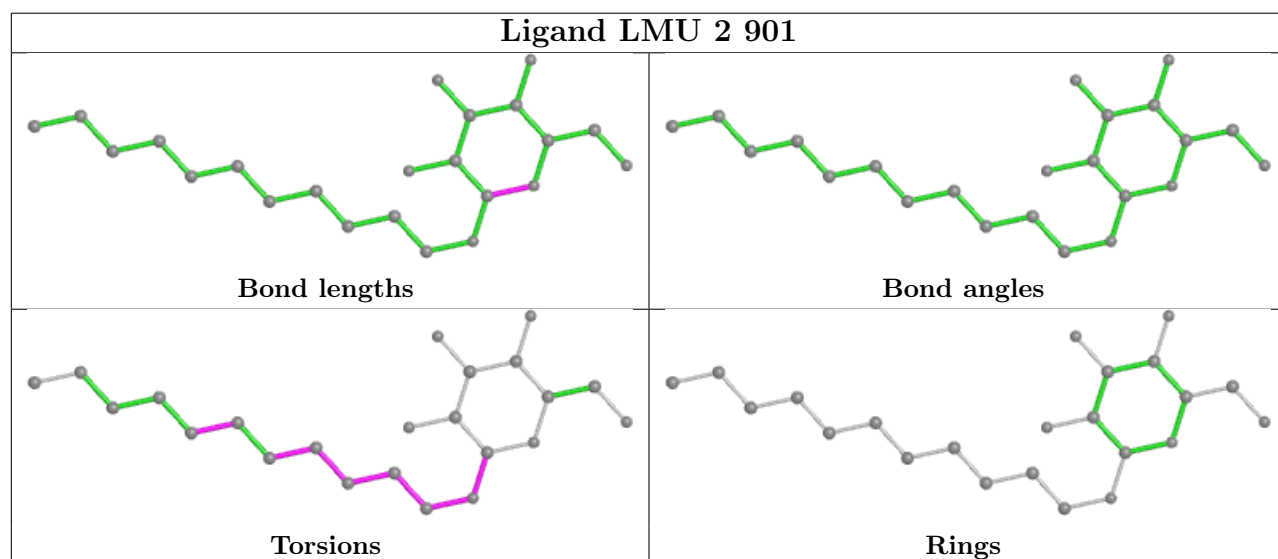
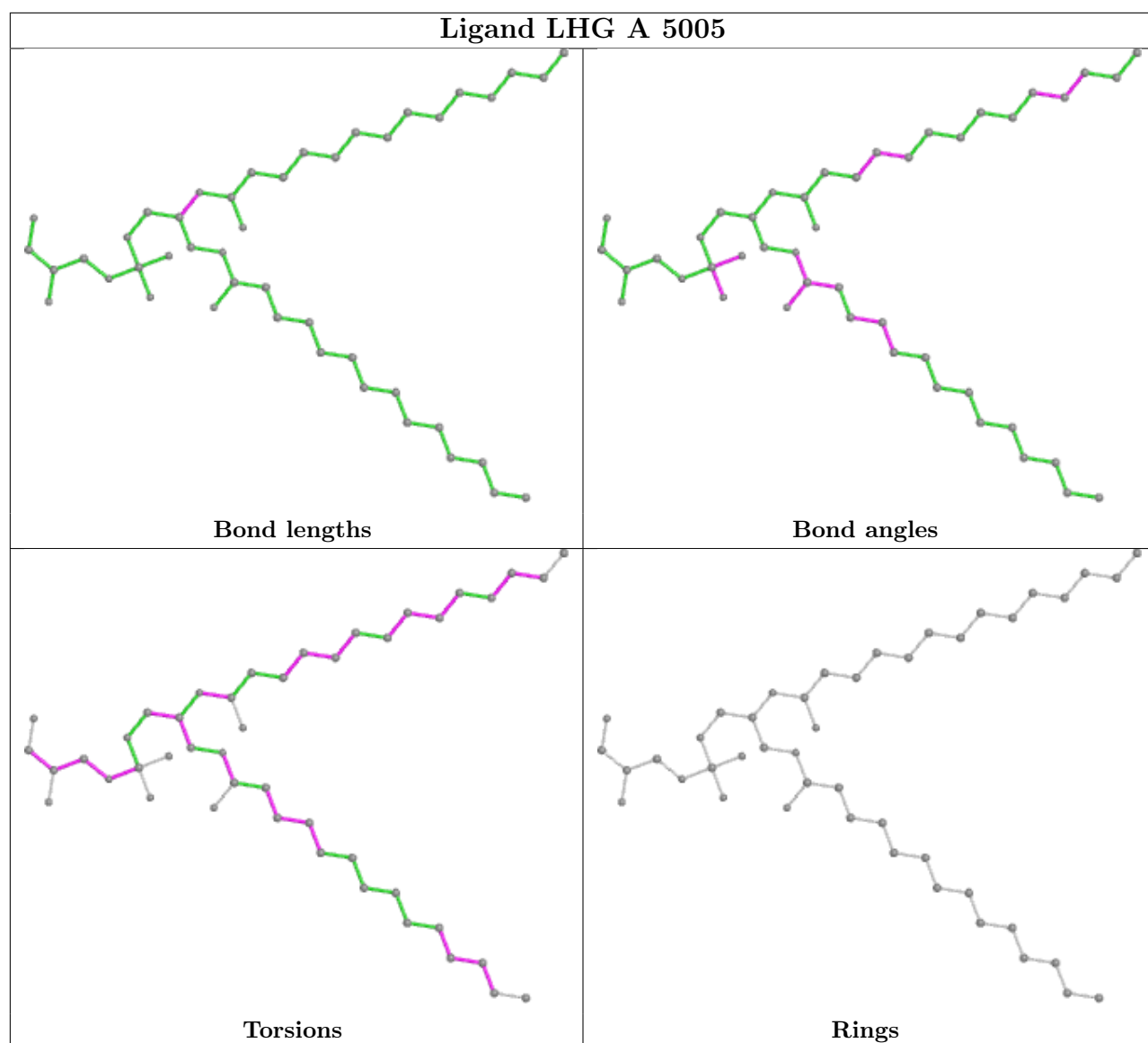
Torsions

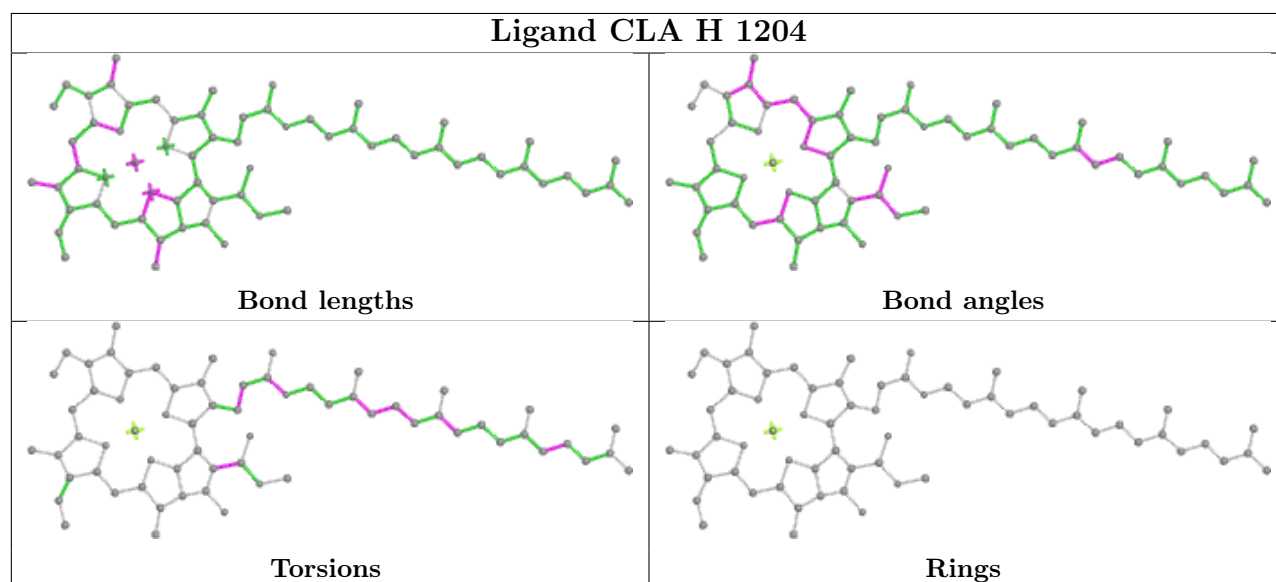
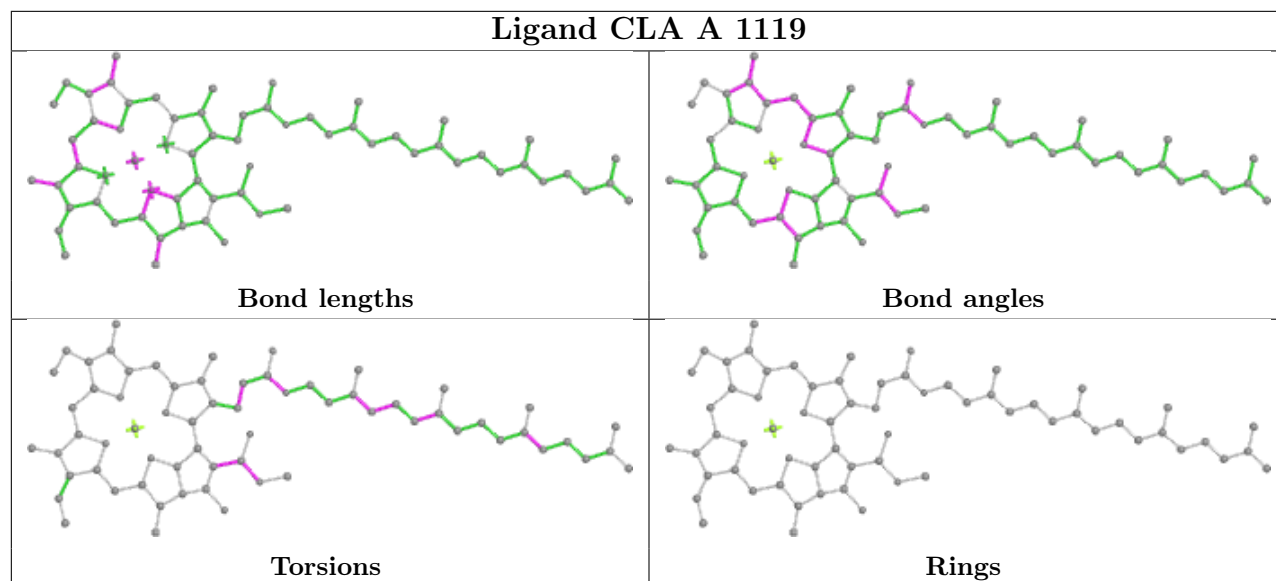
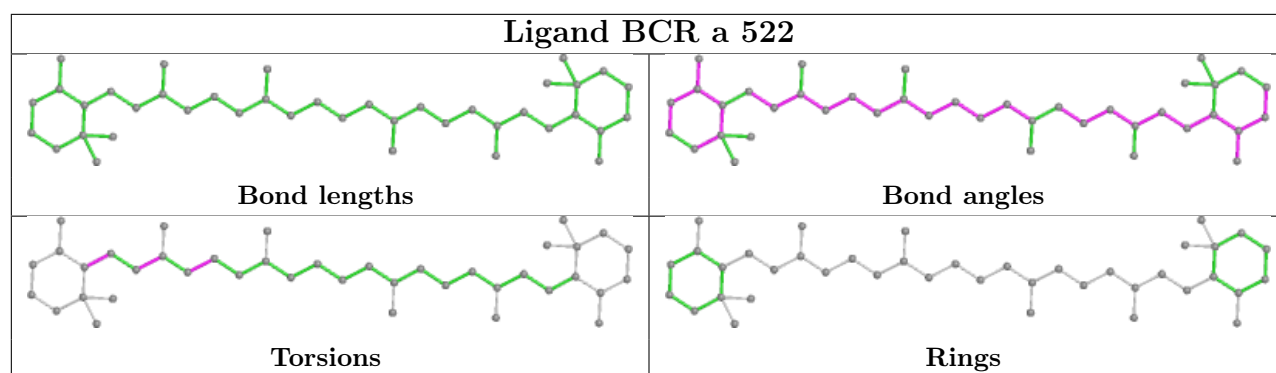


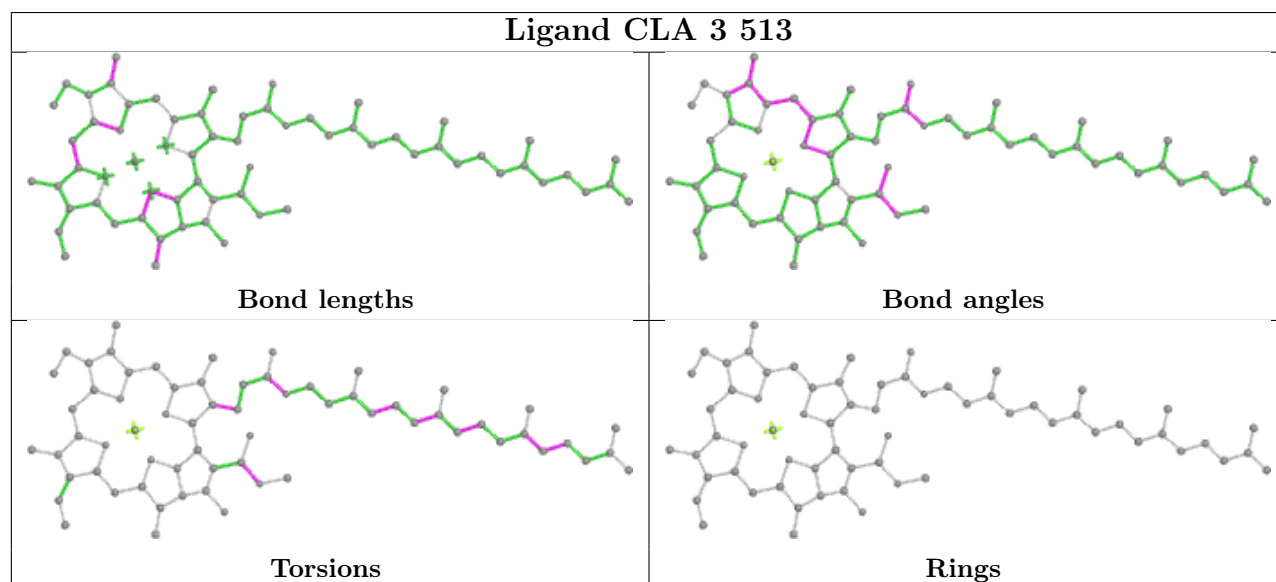
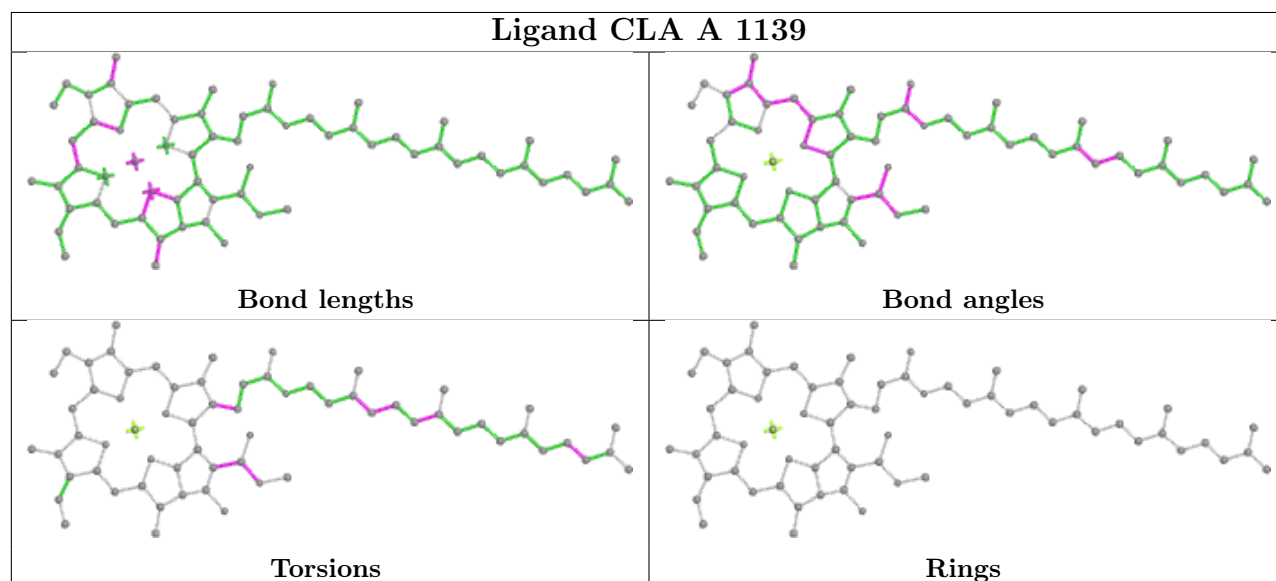
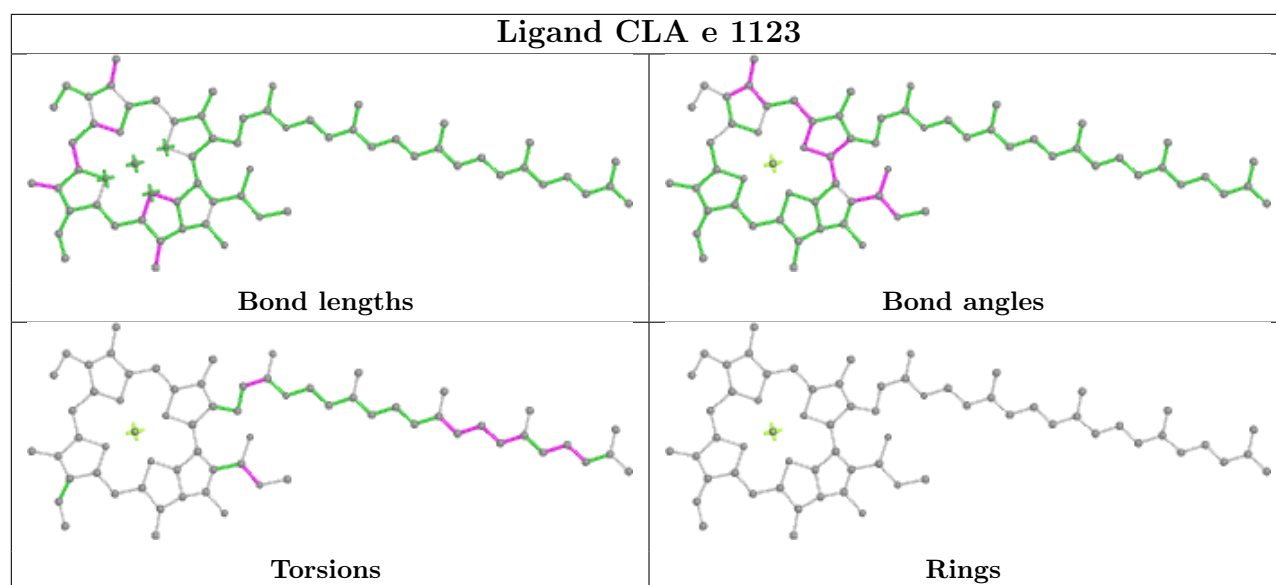
Rings



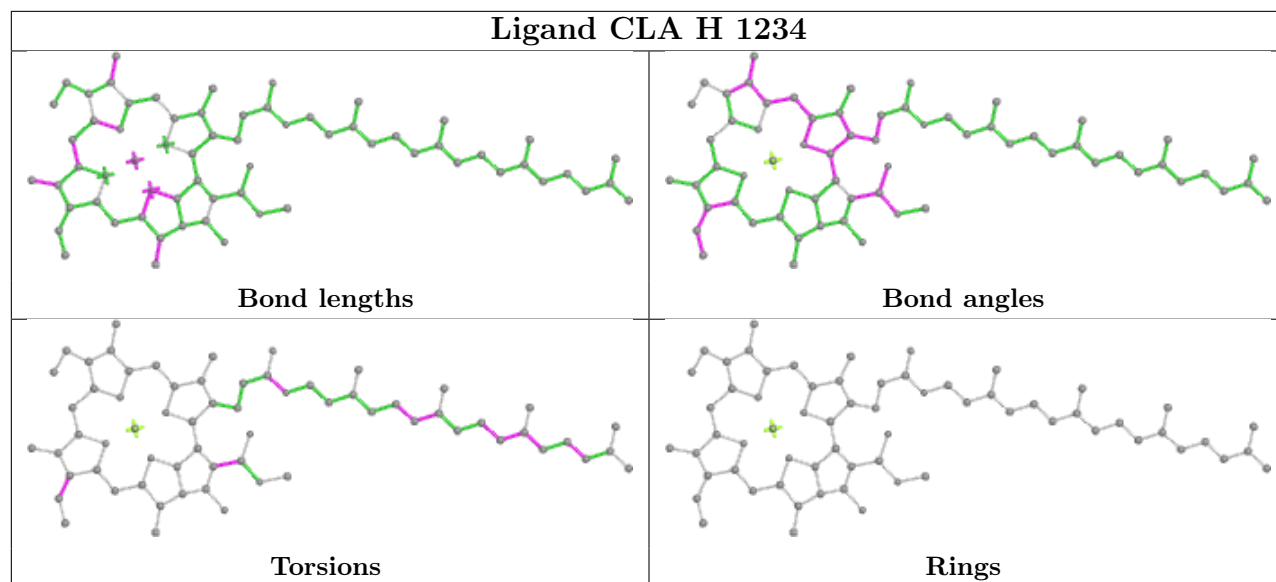




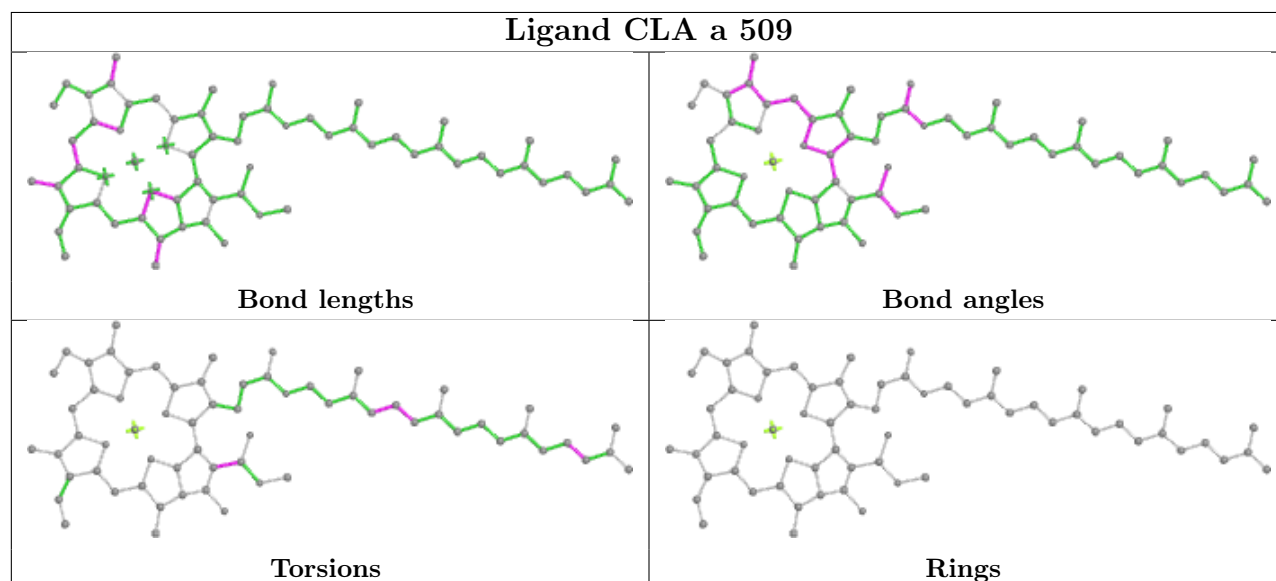




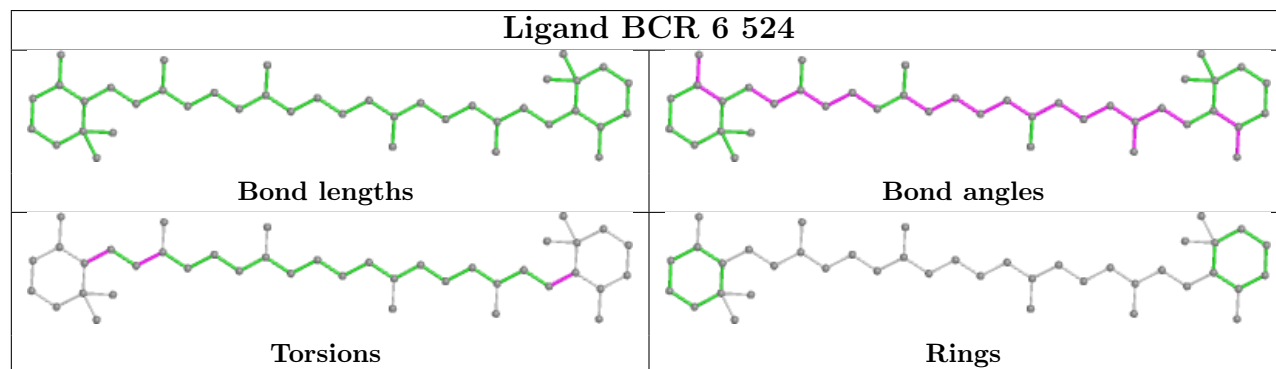
Ligand CLA H 1234



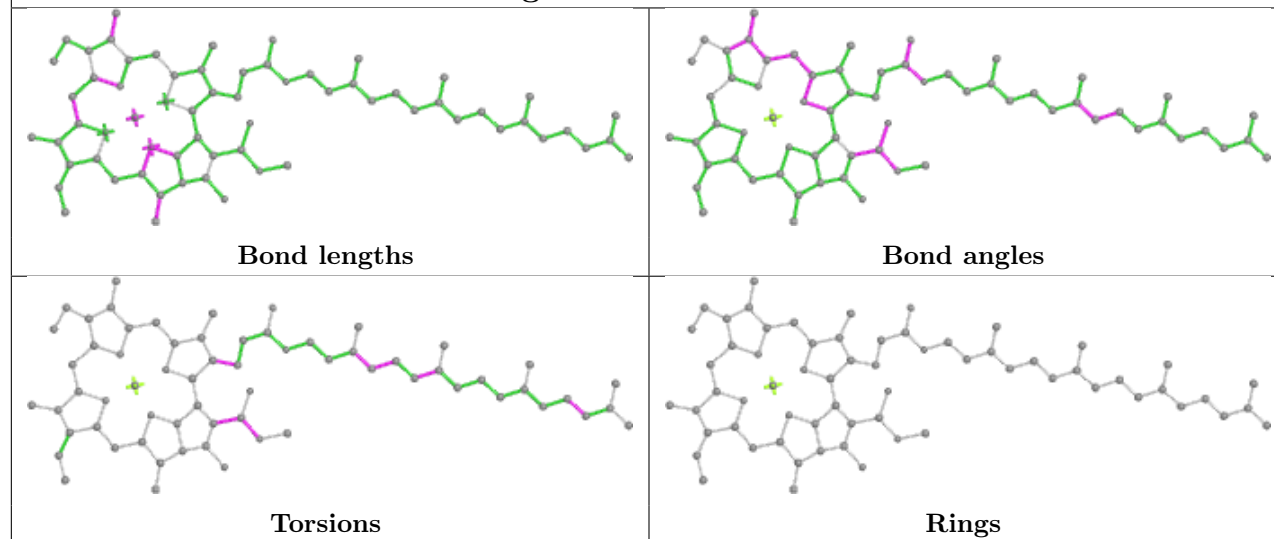
Ligand CLA a 509



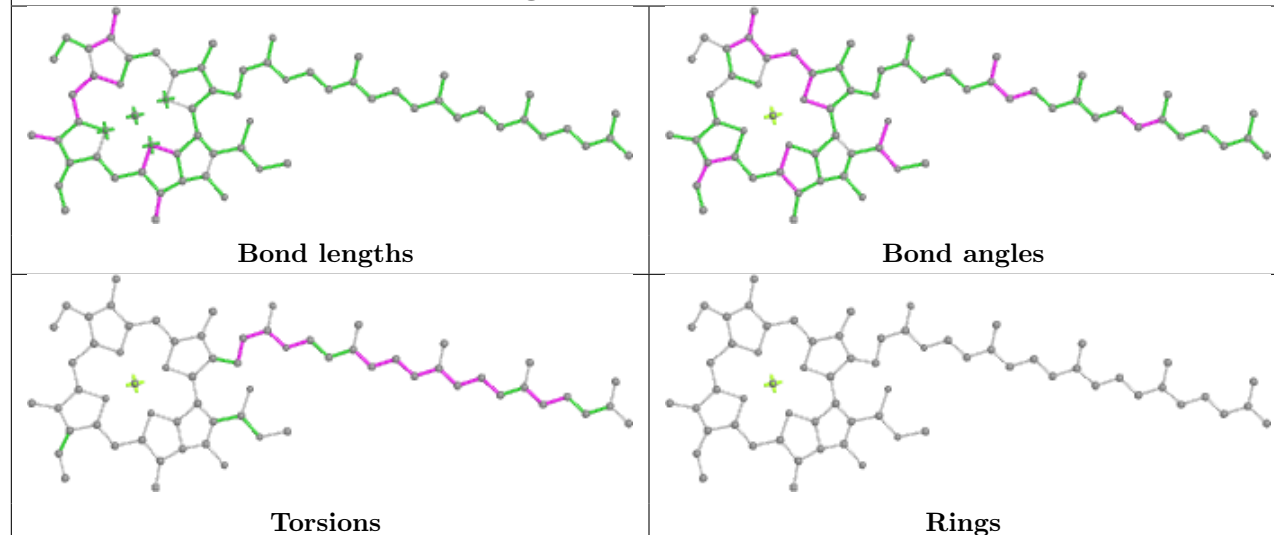
Ligand BCR 6 524



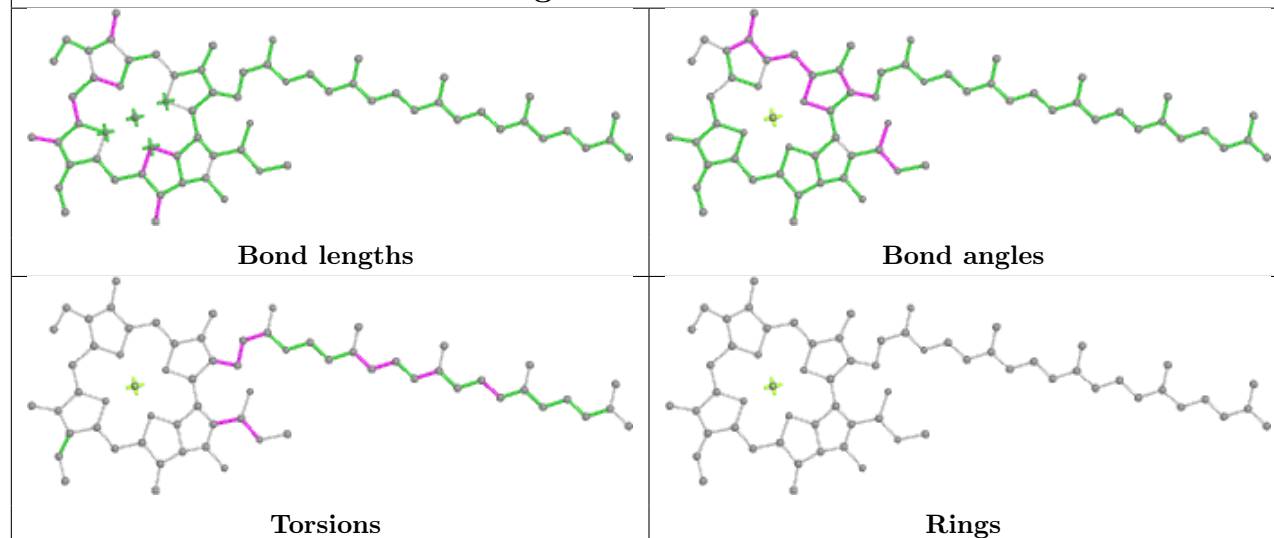
Ligand CLA G 1139

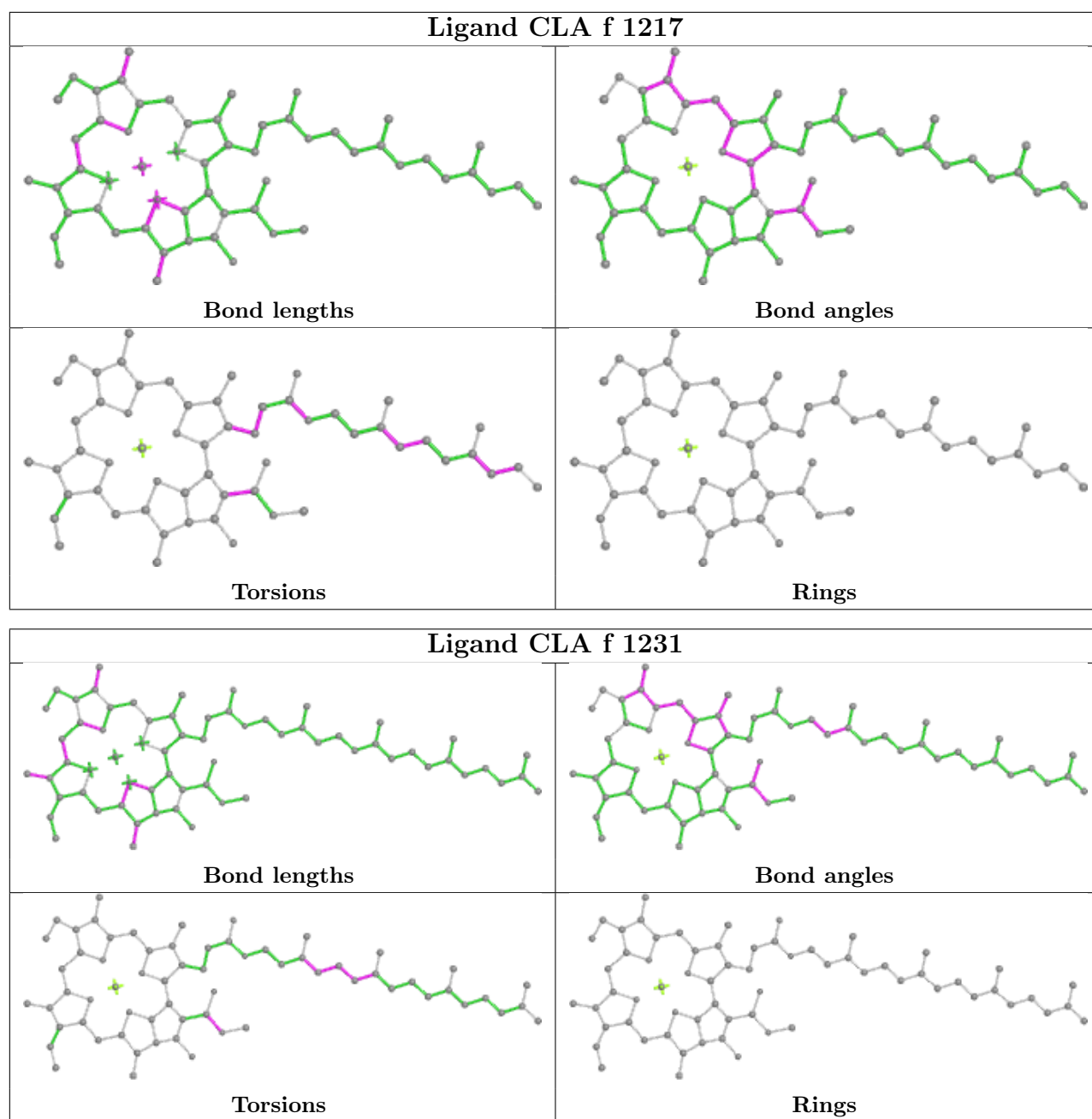


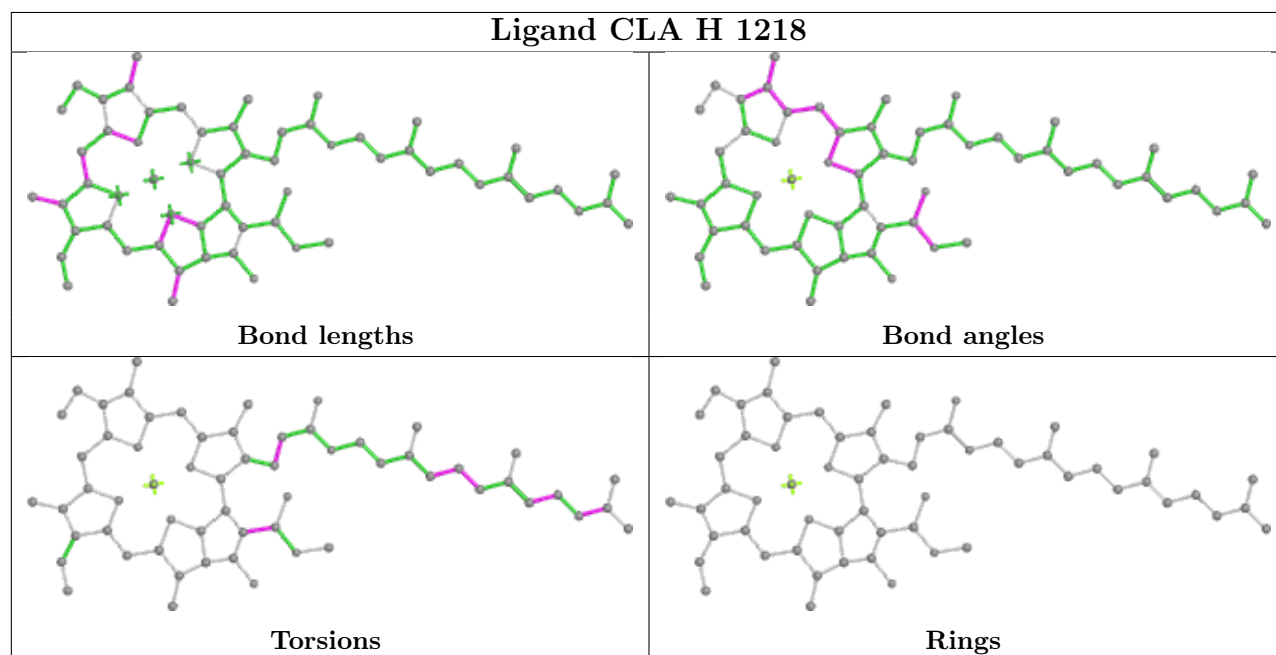
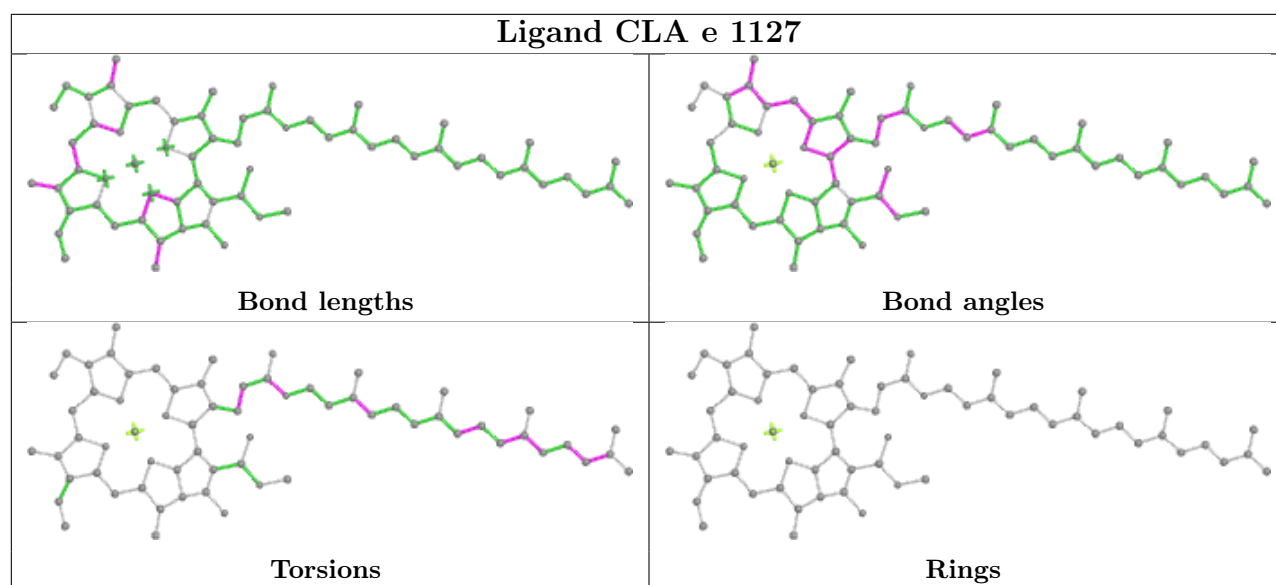
Ligand CLA A 1237

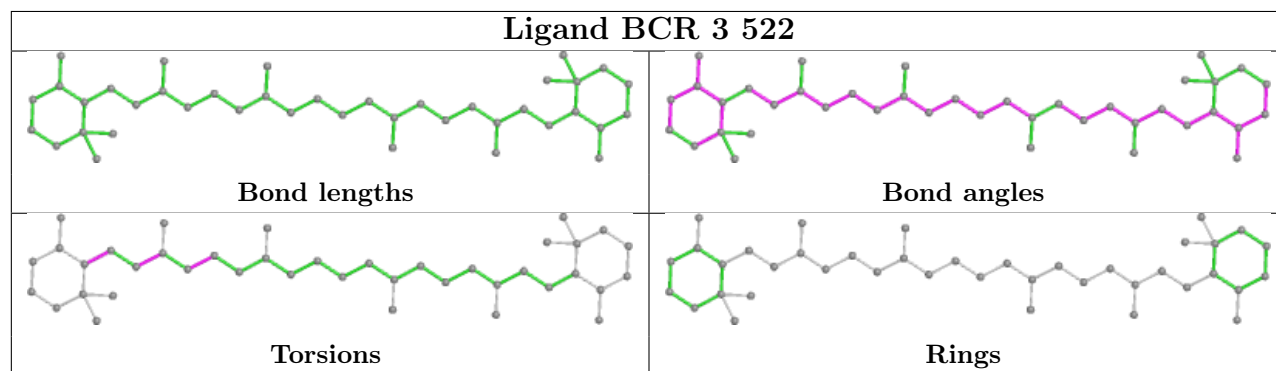
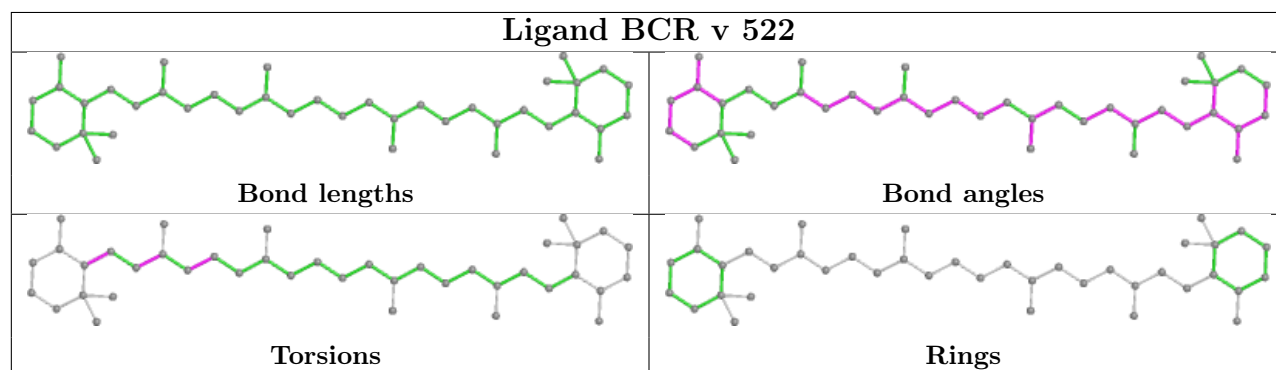
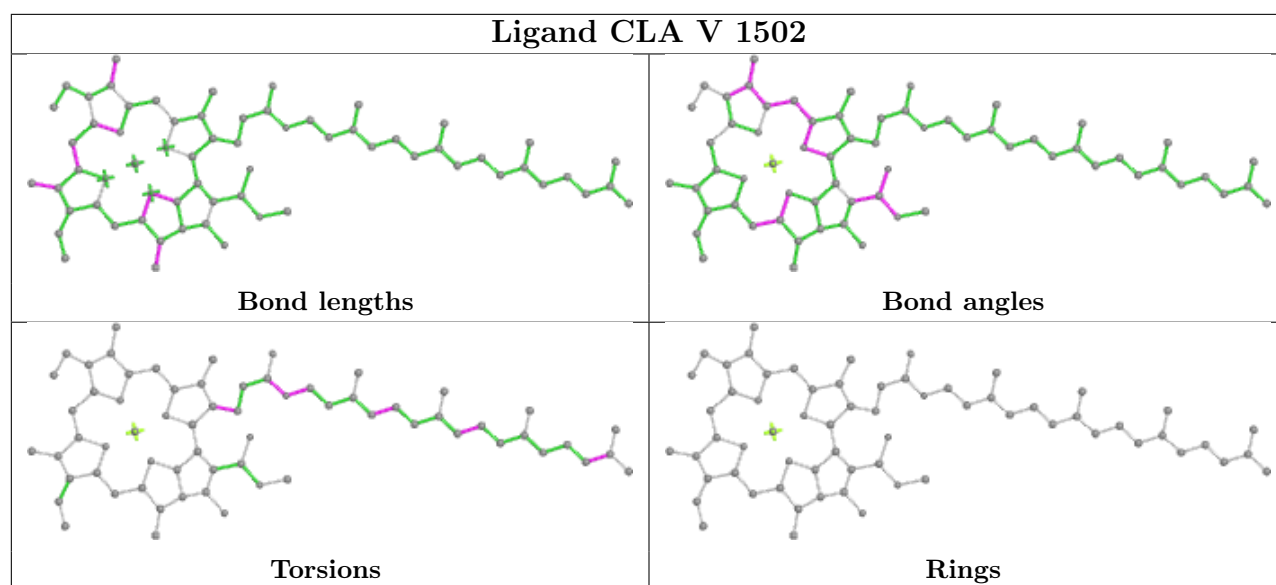


Ligand CLA Z 501

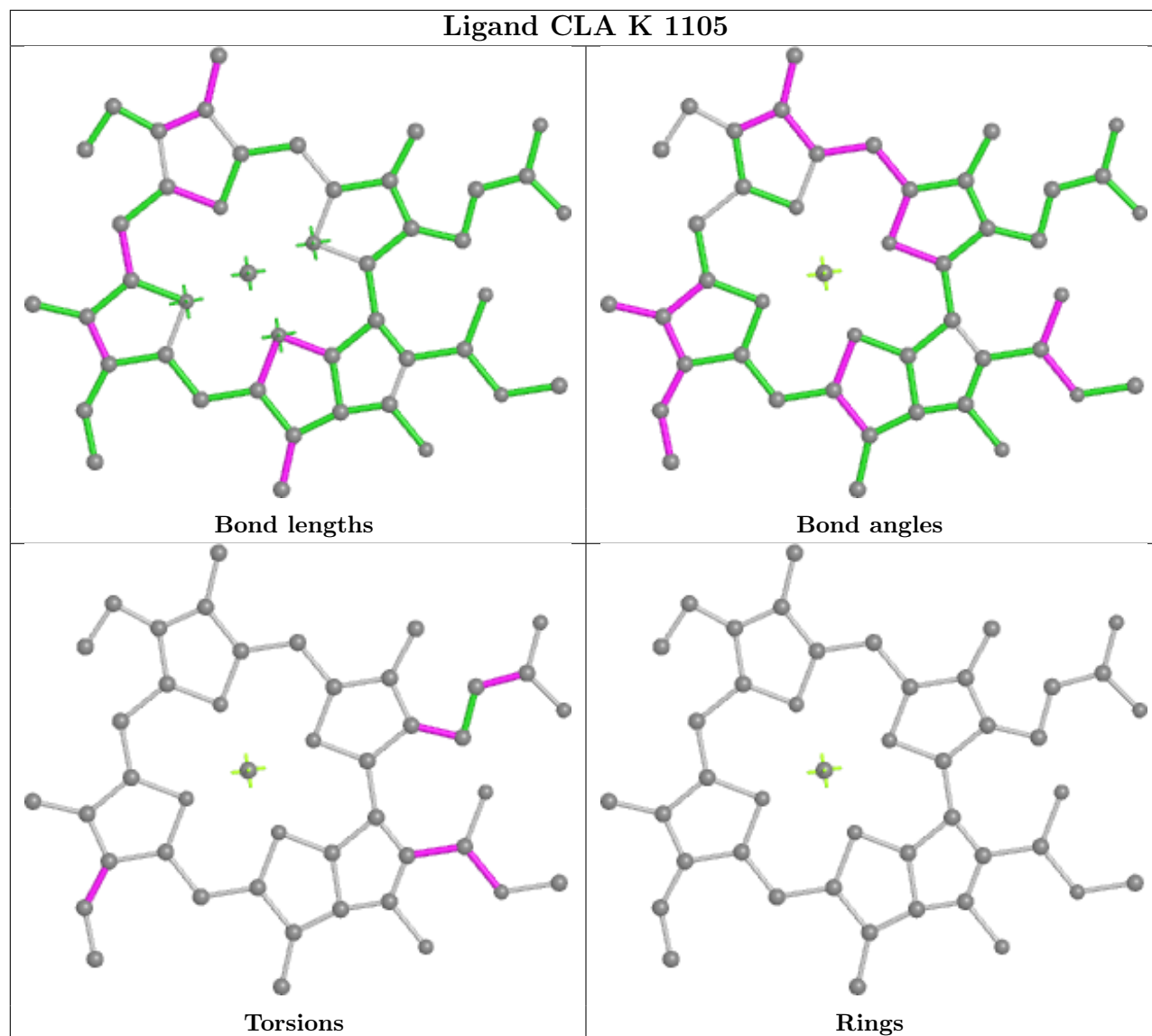


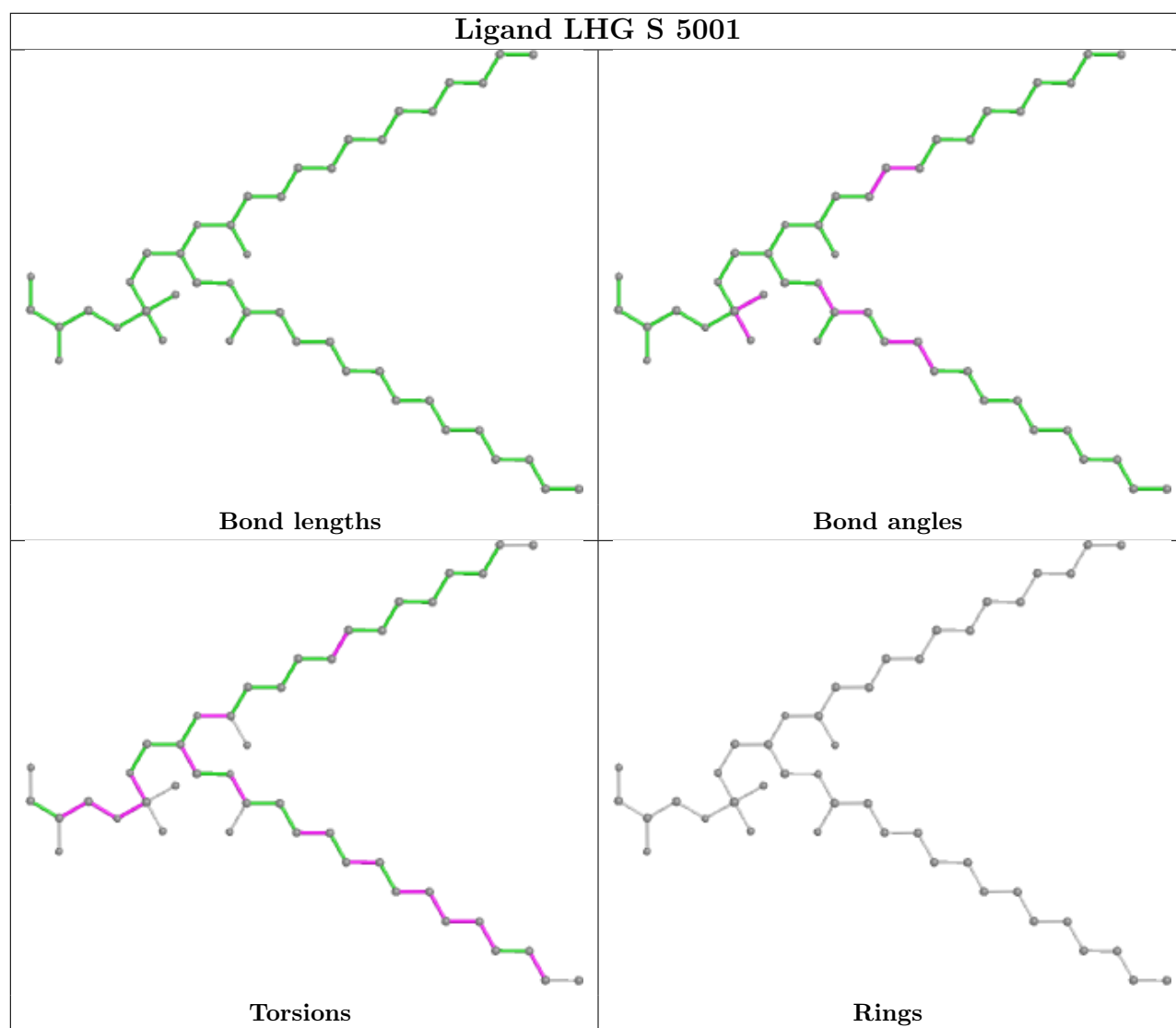


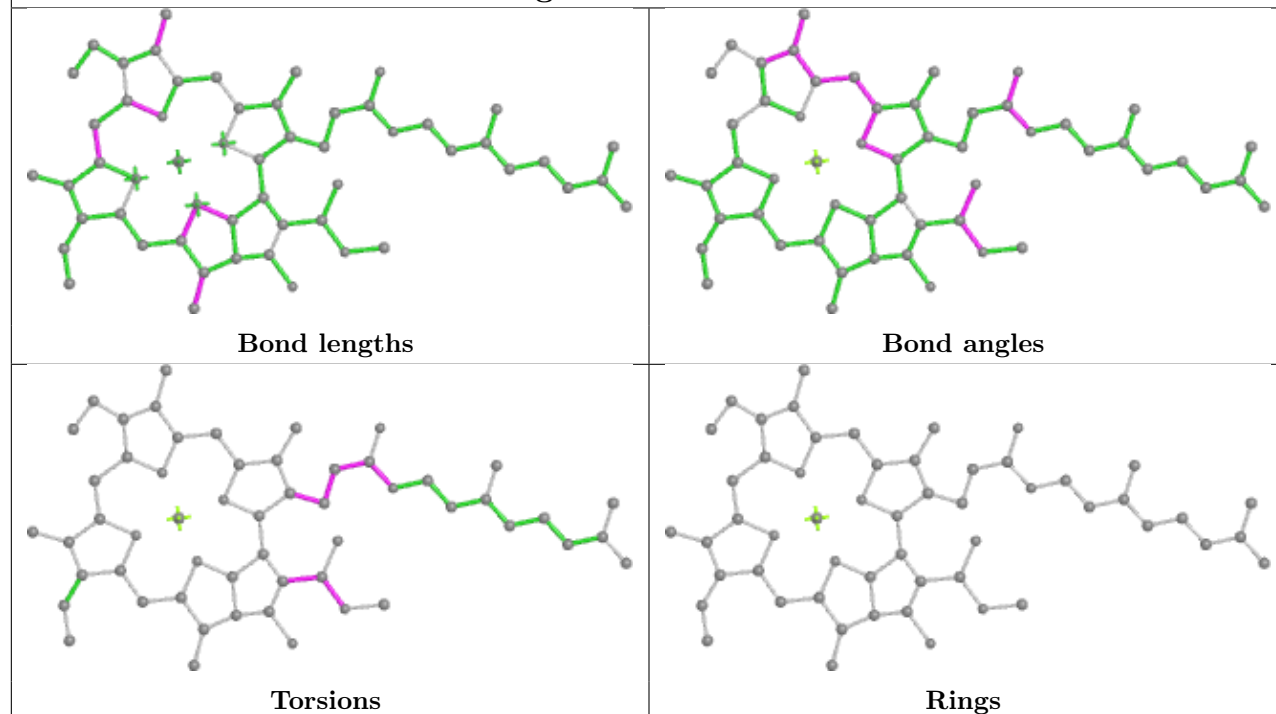
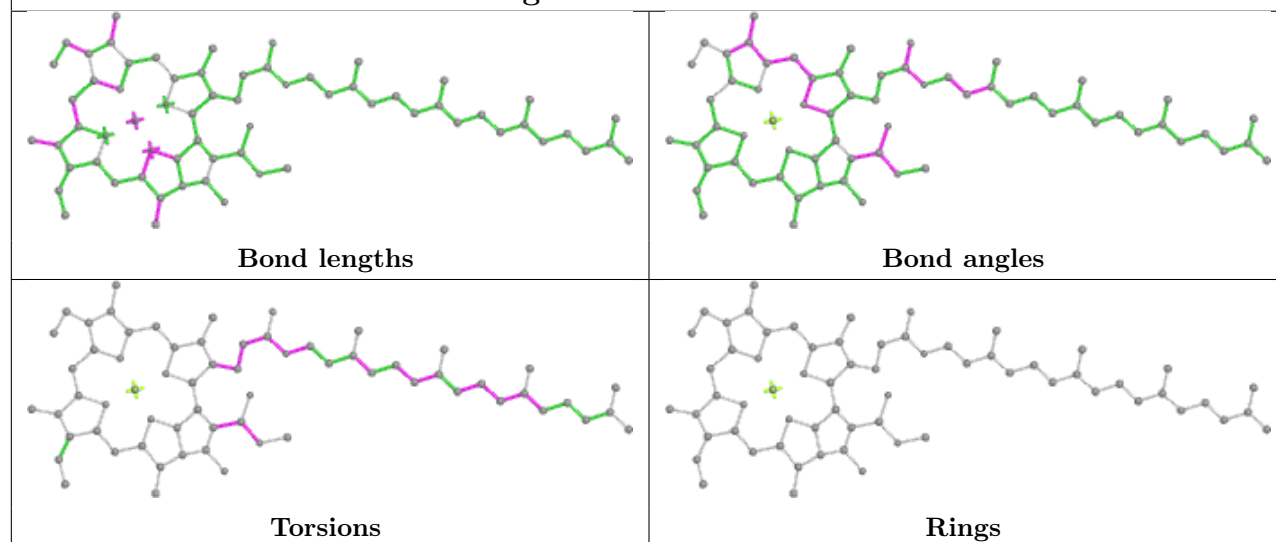


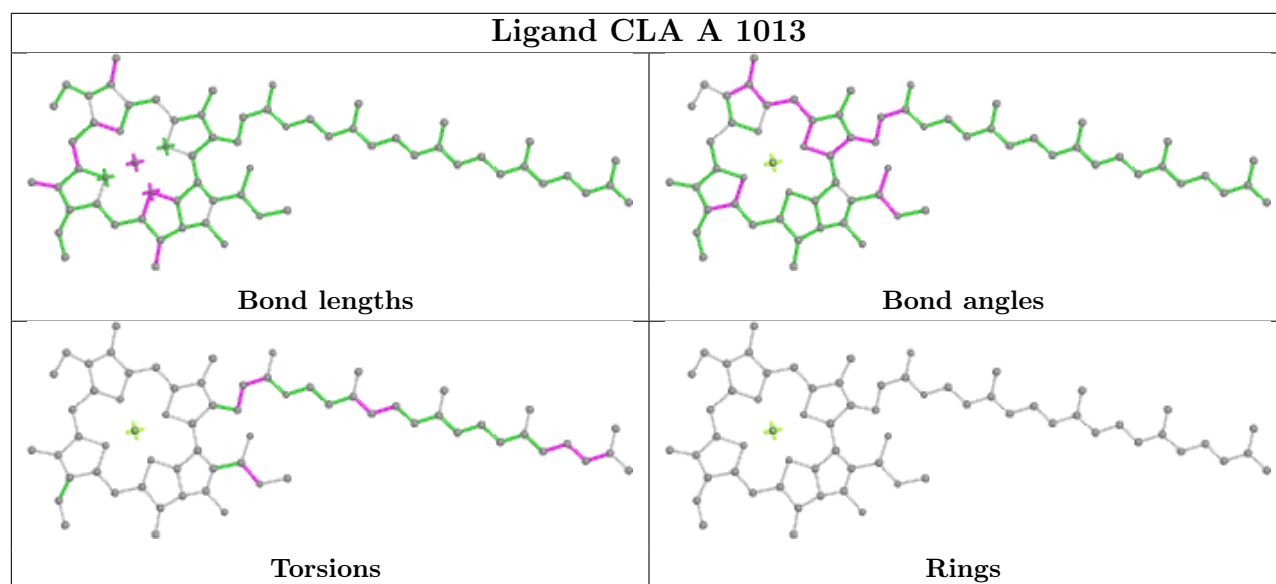
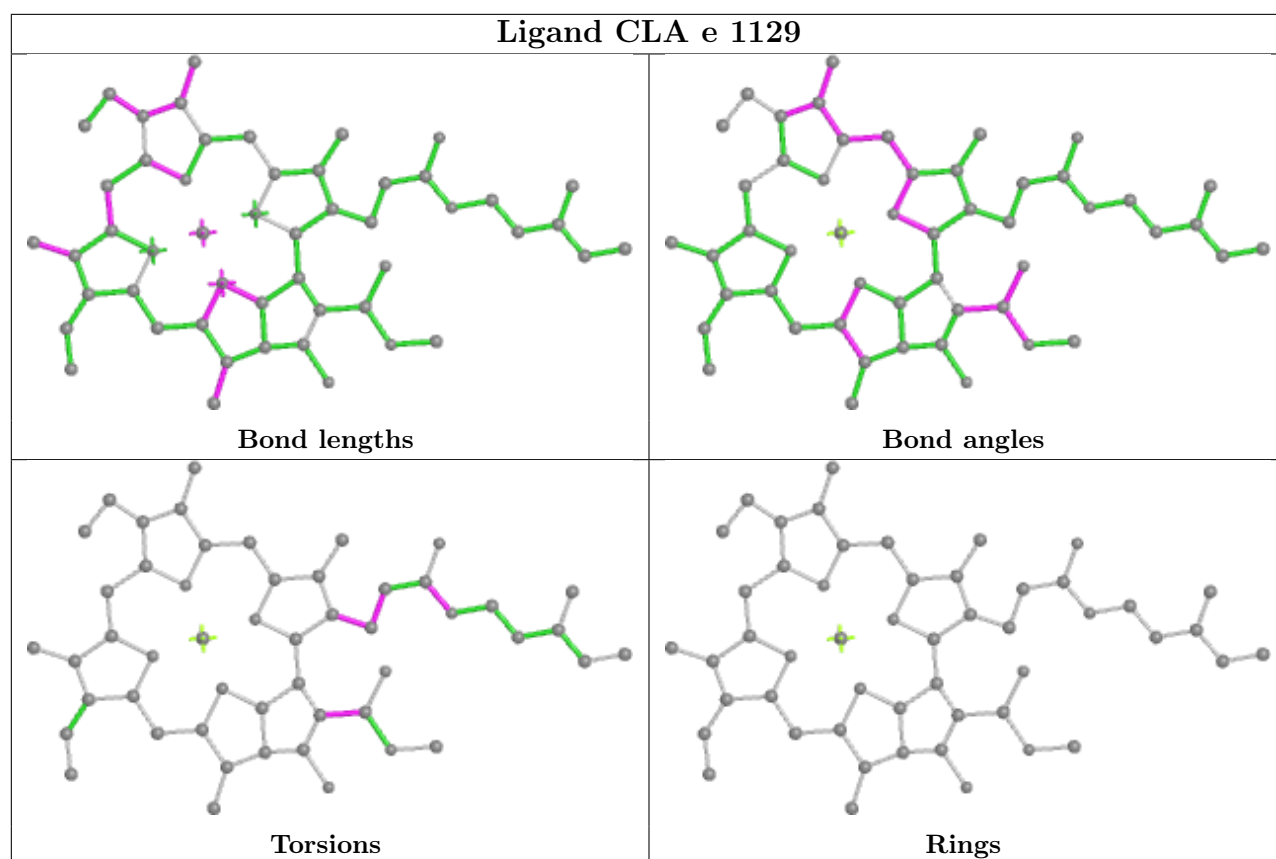


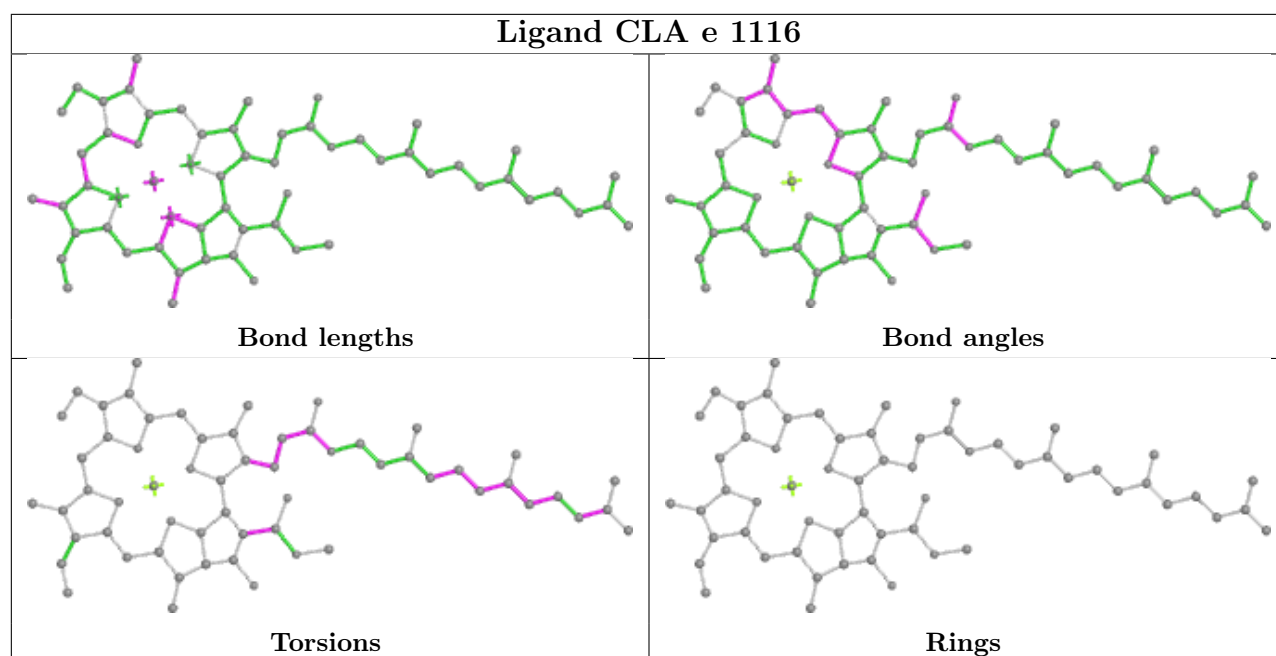
Ligand CLA K 1105





Ligand CLA v 518**Ligand CLA A 1106**





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.

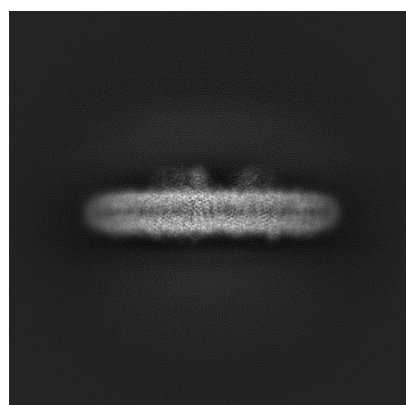
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9995. These allow visual inspection of the internal detail of the map and identification of artifacts.

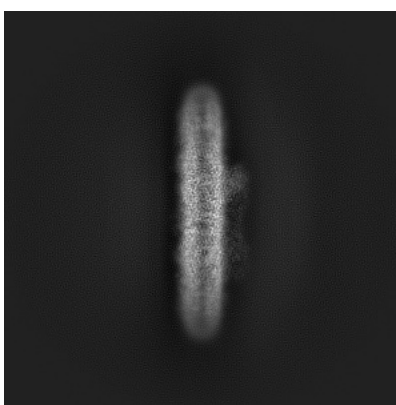
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

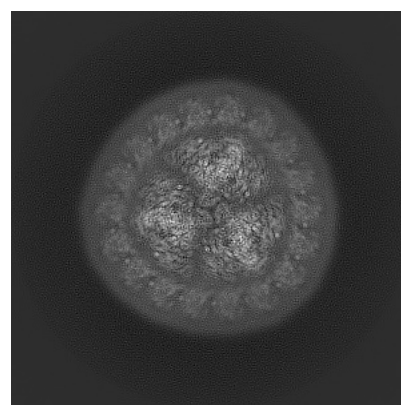
6.1.1 Primary map



X



Y

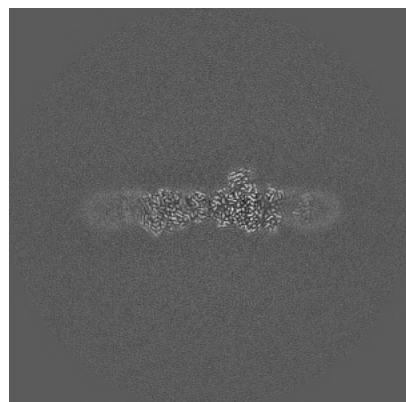


Z

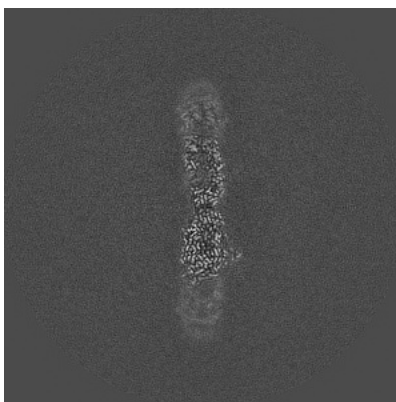
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

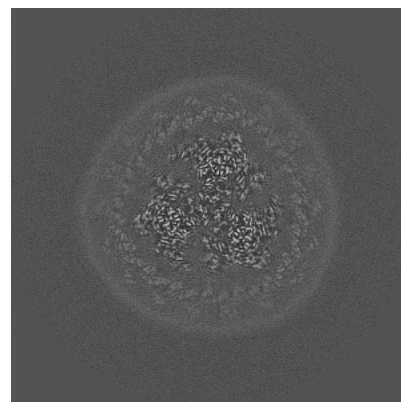
6.2.1 Primary map



X Index: 240



Y Index: 240

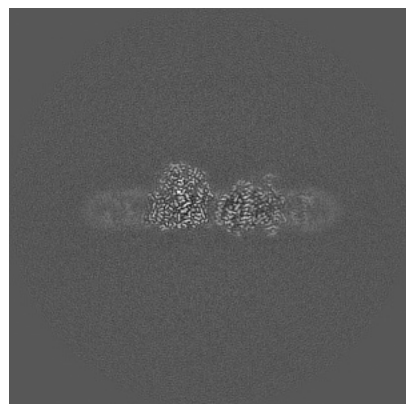


Z Index: 240

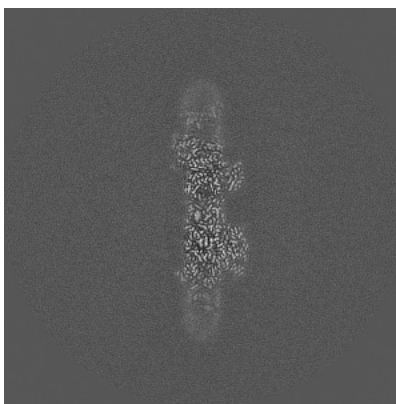
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

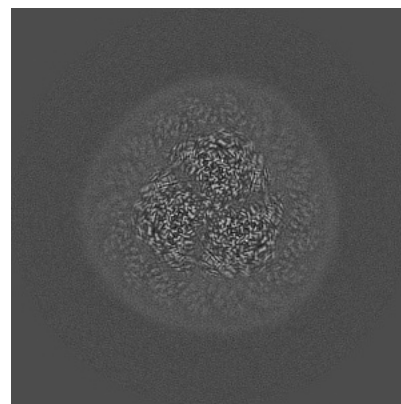
6.3.1 Primary map



X Index: 276



Y Index: 224

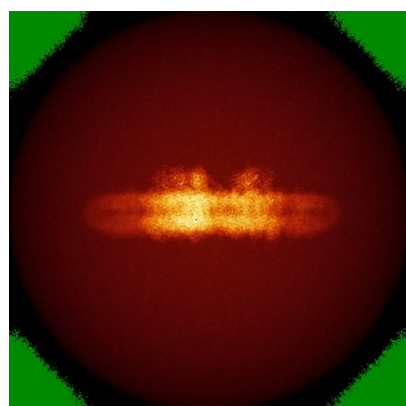


Z Index: 229

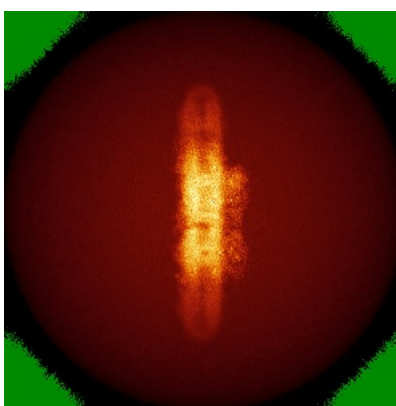
The images above show the largest variance slices of the map in three orthogonal directions.

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

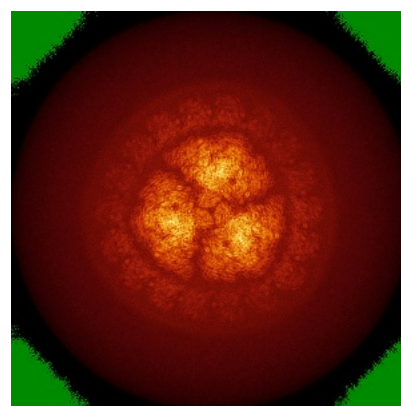
6.4.1 Primary map



X



Y

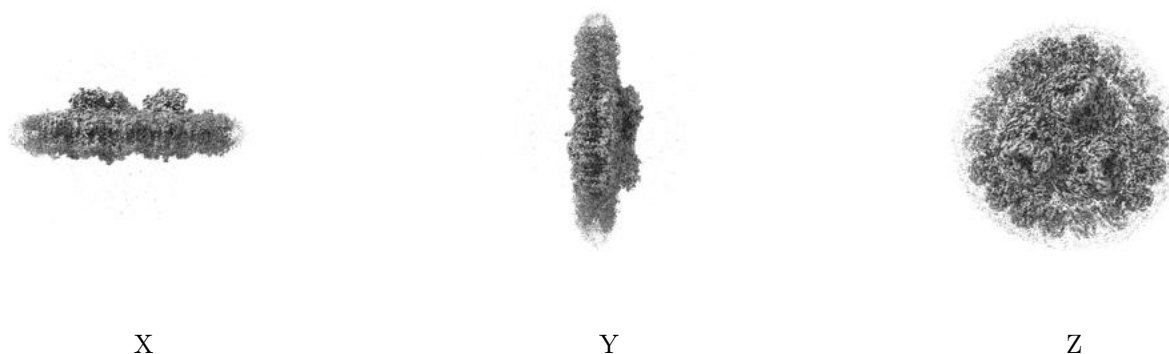


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

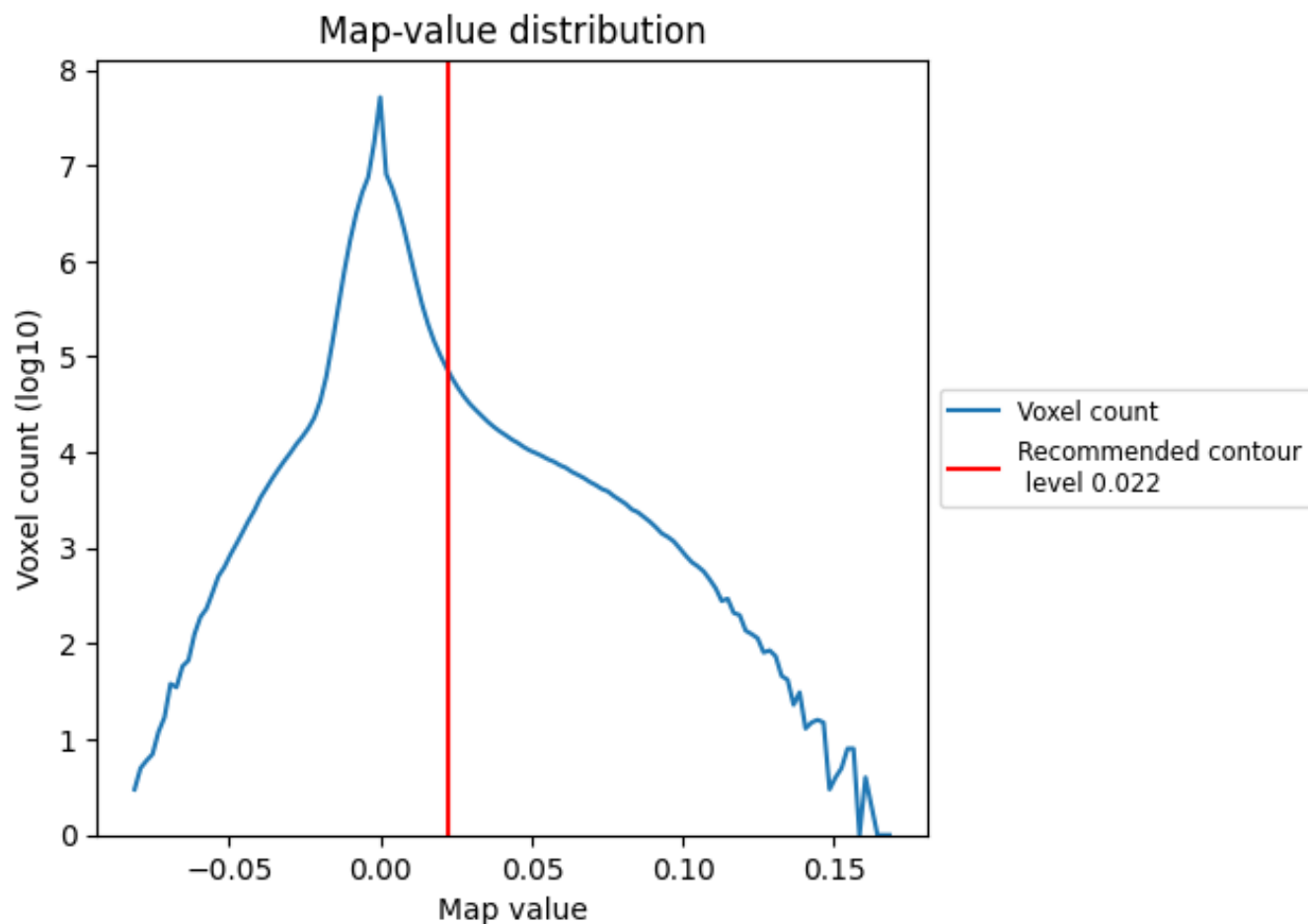
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

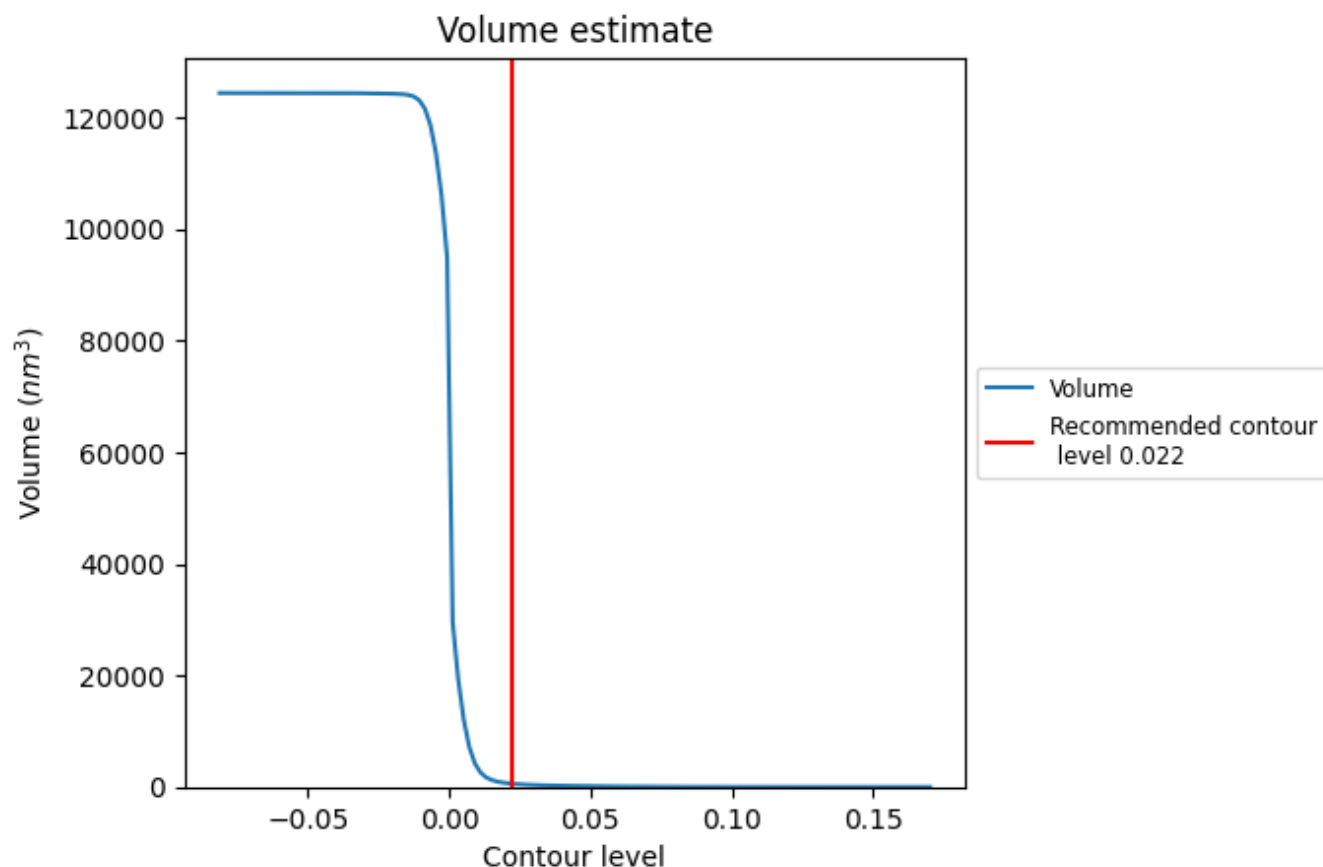
This section contains the results of statistical analysis of the map.

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.

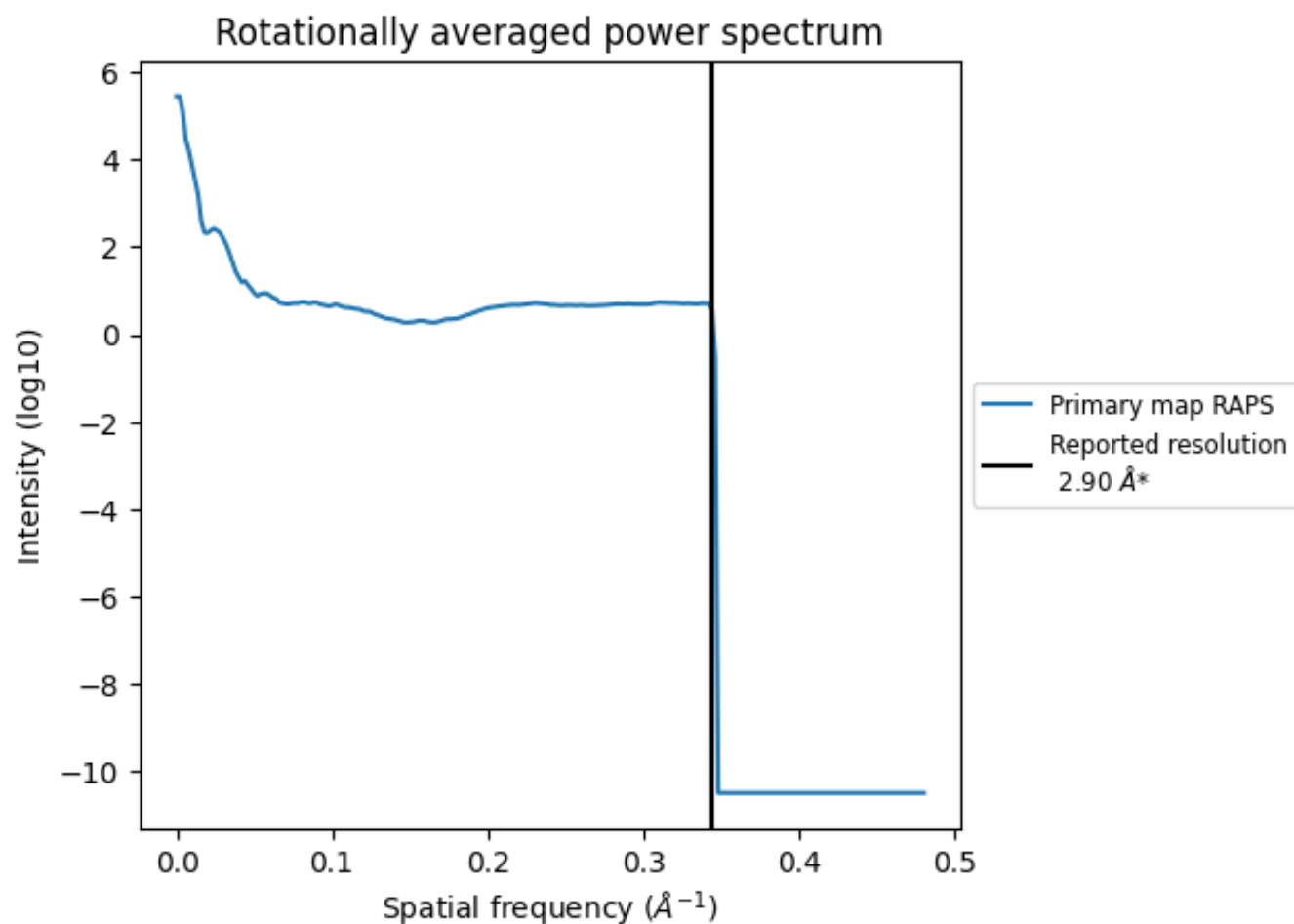
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 595 nm³; this corresponds to an approximate mass of 538 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 0.345 Å⁻¹

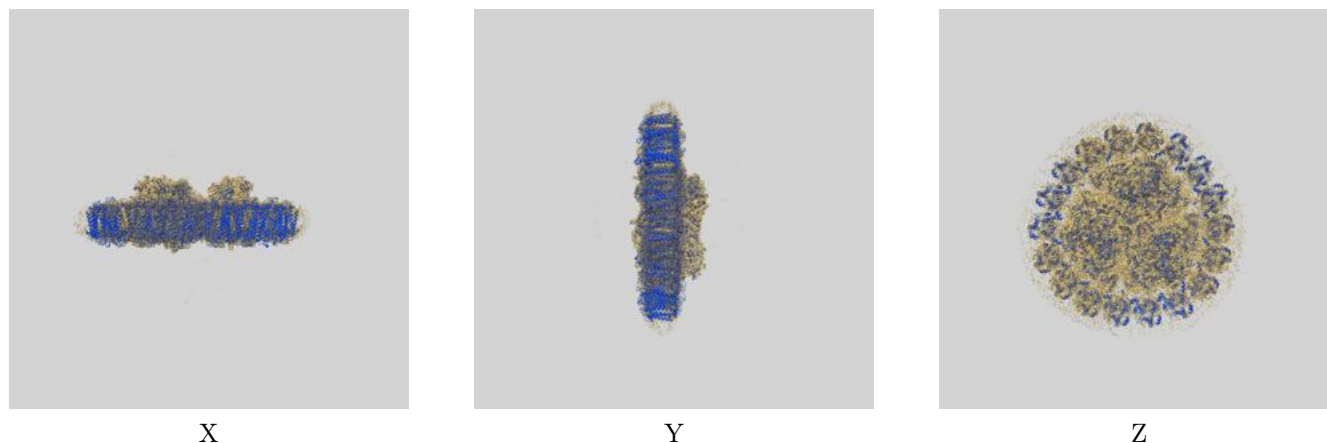
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

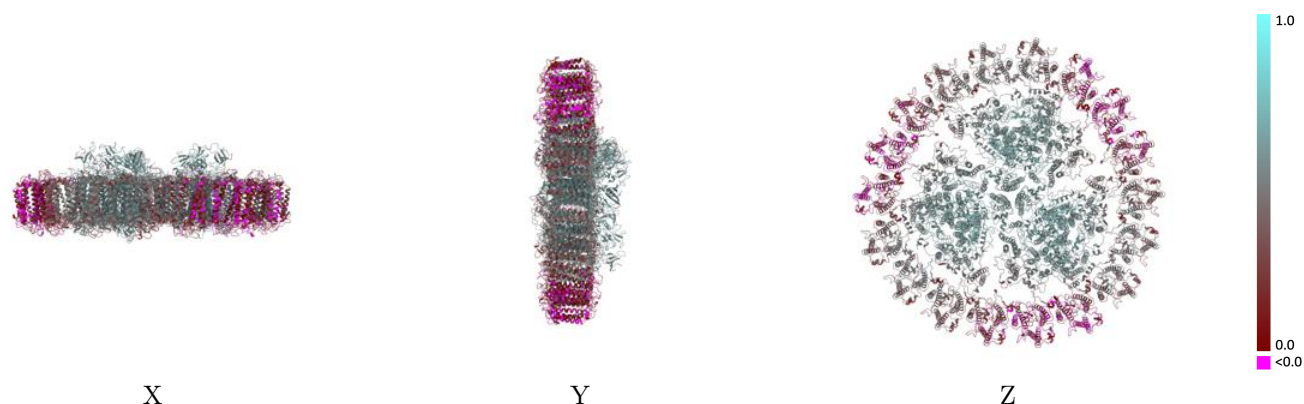
This section contains information regarding the fit between EMDB map EMD-9995 and PDB model 6KIG. Per-residue inclusion information can be found in section [3](#) on page [69](#).

9.1 Map-model overlay [i](#)



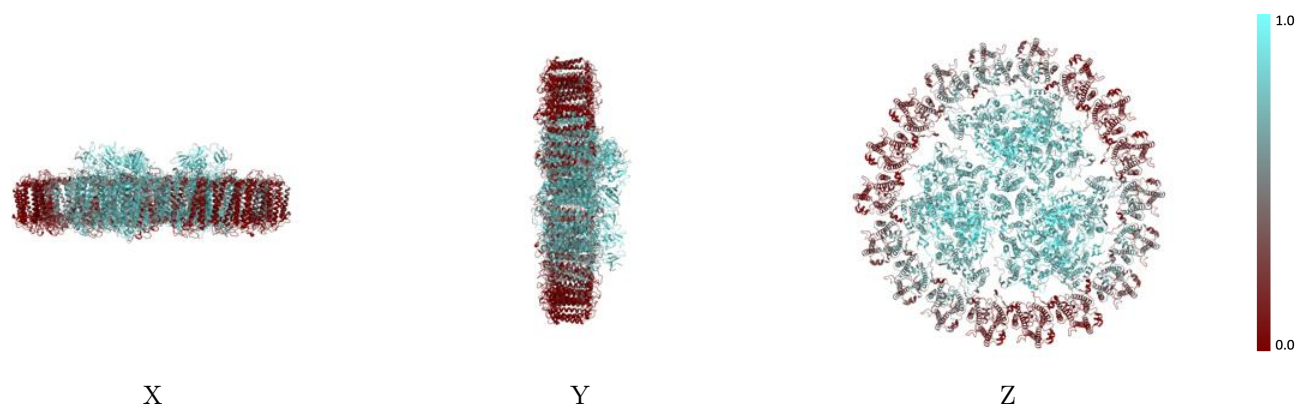
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



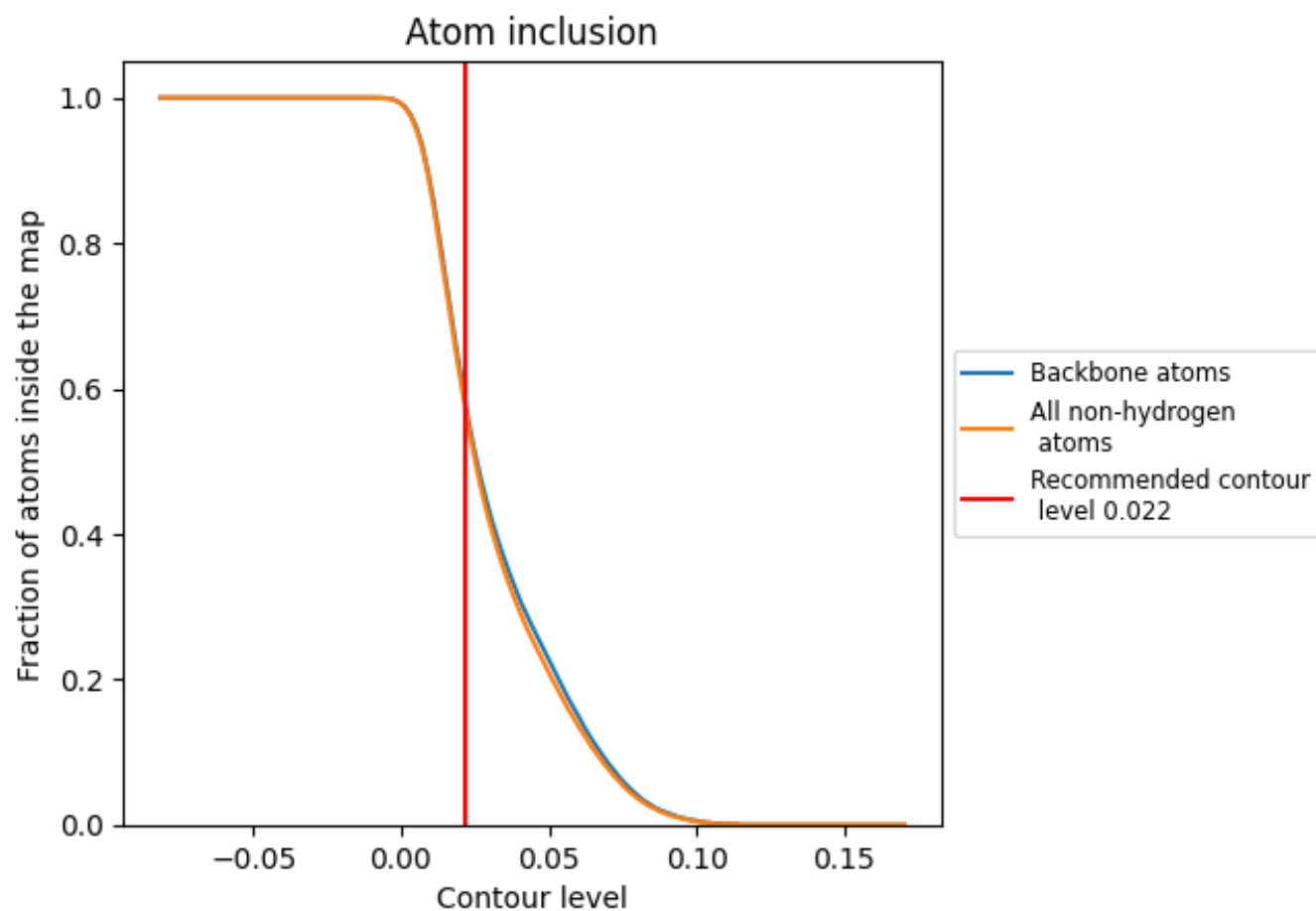
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



































The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5650	 0.4190
1	 0.4070	 0.3640
2	 0.4700	 0.4180
3	 0.3900	 0.3830
4	 0.1070	 0.1410
5	 0.0560	 0.0860
6	 0.1520	 0.1850
A	 0.8490	 0.5780
B	 0.8270	 0.5450
C	 0.9420	 0.6070
D	 0.8580	 0.5770
E	 0.7870	 0.5410
F	 0.7470	 0.5290
G	 0.8450	 0.5770
H	 0.8160	 0.5370
I	 0.8330	 0.5720
J	 0.7550	 0.5460
K	 0.5870	 0.3890
L	 0.8650	 0.5930
M	 0.7980	 0.5290
N	 0.9450	 0.6070
O	 0.8590	 0.5780
Q	 0.7810	 0.5500
R	 0.7440	 0.5230
S	 0.8250	 0.5780
T	 0.7360	 0.5460
U	 0.5810	 0.3860
V	 0.8690	 0.5940
W	 0.7790	 0.5320
Y	 0.4060	 0.3660
Z	 0.4670	 0.4160
a	 0.3870	 0.3780
b	 0.1040	 0.1380
c	 0.0530	 0.0780
d	 0.1450	 0.1710



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.8420	 0.5750
f	 0.8210	 0.5420
g	 0.9420	 0.6070
h	 0.8690	 0.5800
i	 0.7950	 0.5480
j	 0.7500	 0.5280
k	 0.8410	 0.5750
l	 0.7470	 0.5450
m	 0.5790	 0.3770
n	 0.8670	 0.5940
o	 0.7820	 0.5290
q	 0.3920	 0.3580
r	 0.4580	 0.4140
s	 0.3910	 0.3860
t	 0.1100	 0.1390
u	 0.0560	 0.0810
v	 0.1540	 0.1840