



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 04:44 AM UTC

PDB ID : 9LZJ / pdb_00009lj
EMDB ID : EMD-63527
Title : The PSI3-IsiA43 complex with a closed double ring of IsiA proteins bound to a trimeric PSI core
Authors : Si, L.; Cao, P.; Li, M.
Deposited on : 2025-02-21
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

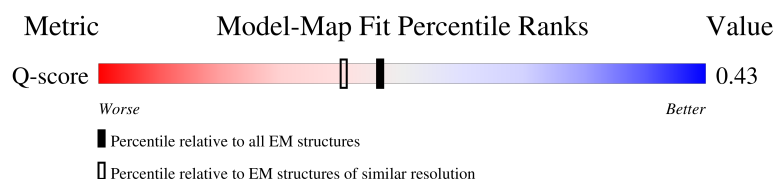
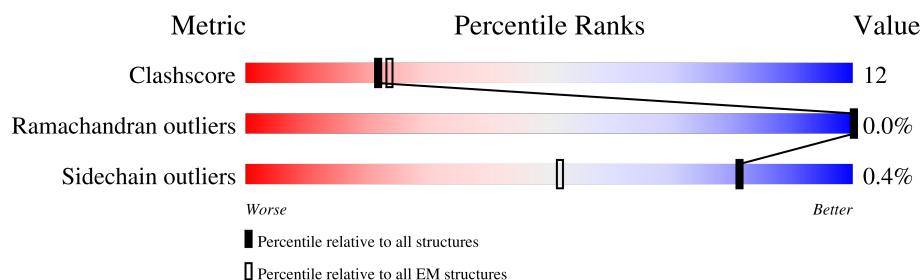
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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





The reported resolution of this entry is 3.40 Å.

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

















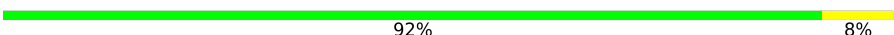

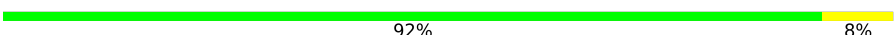








Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	aA	755	
1	bA	755	
1	cA	755	
2	aB	741	












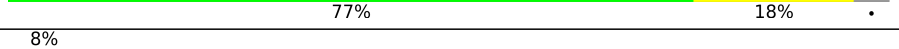



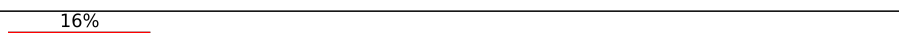
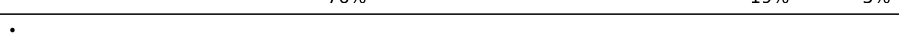








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Mol	Chain	Length	Quality of chain
2	bB	741	
2	cB	741	
3	aC	81	
3	bC	81	
3	cC	81	
4	aD	139	
4	bD	139	
4	cD	139	
5	aE	76	
5	bE	76	
5	cE	76	
6	aF	164	
6	bF	164	
6	cF	164	
7	aI	38	
7	bI	38	
7	cI	38	
8	aJ	41	
8	bJ	41	
8	cJ	41	
9	aK	83	
9	bK	83	
9	cK	83	
10	aL	155	
10	bL	155	







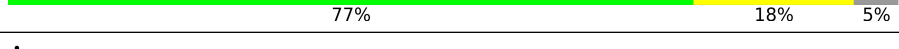
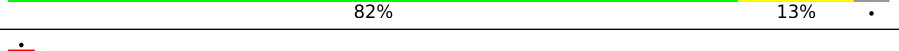
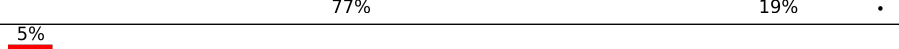
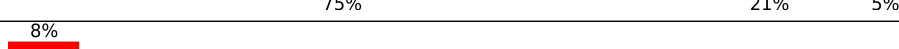
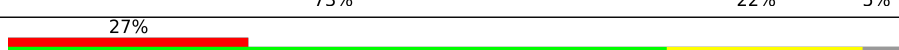

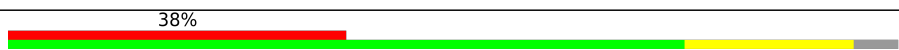

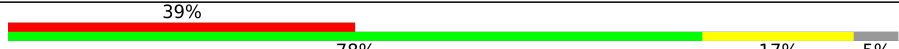





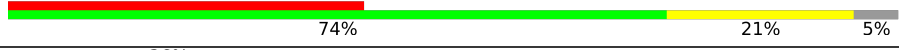
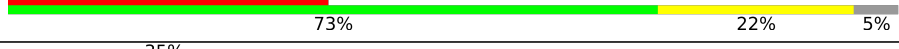



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Mol	Chain	Length	Quality of chain
10	cL	155	
11	aM	31	
11	bM	31	
11	cM	31	
12	aX	39	
12	bX	39	
12	cX	39	
13	S	358	
13	T	358	
13	U	358	
13	V	358	
13	W	358	
13	X	358	
13	Y	358	
13	Z	358	
13	a	358	
13	a1	358	
13	a2	358	
13	a3	358	
13	a4	358	
13	a5	358	
13	a6	358	
13	b	358	
13	b1	358	
13	b2	358	

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Mol	Chain	Length	Quality of chain
13	b3	358	
13	b4	358	
13	b5	358	
13	b6	358	
13	c	358	
13	c1	358	
13	c2	358	
13	c3	358	
13	c4	358	
13	c5	358	
13	c6	358	
13	d	358	
13	e	358	
13	f	358	
13	g	358	
13	h	358	
13	i	358	
13	j	358	
13	k	358	
13	l	358	
13	m	358	
13	n	358	
13	o	358	
13	p	358	
13	q	358	

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
14	CLA	S	501	X	-	-	-
14	CLA	S	502	X	-	-	-
14	CLA	S	503	X	-	-	-
14	CLA	S	504	X	-	-	-
14	CLA	S	505	X	-	-	-
14	CLA	S	506	X	-	-	-
14	CLA	S	507	X	-	-	-
14	CLA	S	508	X	-	-	-
14	CLA	S	509	X	-	-	-
14	CLA	S	510	X	-	-	-
14	CLA	S	511	X	-	-	-
14	CLA	S	512	X	-	-	-
14	CLA	S	513	X	-	-	-
14	CLA	S	516	X	-	-	-
14	CLA	S	517	X	-	-	-
14	CLA	S	518	X	-	-	-
14	CLA	S	519	X	-	-	-
14	CLA	T	501	X	-	-	-
14	CLA	T	502	X	-	-	-
14	CLA	T	503	X	-	-	-
14	CLA	T	504	X	-	-	-
14	CLA	T	505	X	-	-	-
14	CLA	T	506	X	-	-	-
14	CLA	T	507	X	-	-	-
14	CLA	T	508	X	-	-	-
14	CLA	T	509	X	-	-	-
14	CLA	T	510	X	-	-	-
14	CLA	T	511	X	-	-	-
14	CLA	T	512	X	-	-	-
14	CLA	T	513	X	-	-	-
14	CLA	T	516	X	-	-	-
14	CLA	T	517	X	-	-	-
14	CLA	T	518	X	-	-	-
14	CLA	T	519	X	-	-	-
14	CLA	U	501	X	-	-	-
14	CLA	U	502	X	-	-	-
14	CLA	U	503	X	-	-	-
14	CLA	U	504	X	-	-	-
14	CLA	U	505	X	-	-	-
14	CLA	U	506	X	-	-	-

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	Z	506	X	-	-	-
14	CLA	Z	507	X	-	-	-
14	CLA	Z	508	X	-	-	-
14	CLA	Z	509	X	-	-	-
14	CLA	Z	510	X	-	-	-
14	CLA	Z	511	X	-	-	-
14	CLA	Z	512	X	-	-	-
14	CLA	Z	513	X	-	-	-
14	CLA	Z	516	X	-	-	-
14	CLA	Z	517	X	-	-	-
14	CLA	Z	518	X	-	-	-
14	CLA	Z	519	X	-	-	-
14	CLA	a	501	X	-	-	-
14	CLA	a	502	X	-	-	-
14	CLA	a	503	X	-	-	-
14	CLA	a	504	X	-	-	-
14	CLA	a	505	X	-	-	-
14	CLA	a	506	X	-	-	-
14	CLA	a	507	X	-	-	-
14	CLA	a	508	X	-	-	-
14	CLA	a	509	X	-	-	-
14	CLA	a	510	X	-	-	-
14	CLA	a	511	X	-	-	-
14	CLA	a	512	X	-	-	-
14	CLA	a	513	X	-	-	-
14	CLA	a	516	X	-	-	-
14	CLA	a	517	X	-	-	-
14	CLA	a	518	X	-	-	-
14	CLA	a	519	X	-	-	-
14	CLA	a1	501	X	-	-	-
14	CLA	a1	502	X	-	-	-
14	CLA	a1	503	X	-	-	-
14	CLA	a1	504	X	-	-	-
14	CLA	a1	505	X	-	-	-
14	CLA	a1	506	X	-	-	-
14	CLA	a1	507	X	-	-	-
14	CLA	a1	508	X	-	-	-
14	CLA	a1	509	X	-	-	-
14	CLA	a1	510	X	-	-	-
14	CLA	a1	511	X	-	-	-
14	CLA	a1	512	X	-	-	-
14	CLA	a1	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a1	516	X	-	-	-
14	CLA	a1	517	X	-	-	-
14	CLA	a1	518	X	-	-	-
14	CLA	a1	519	X	-	-	-
14	CLA	a2	501	X	-	-	-
14	CLA	a2	502	X	-	-	-
14	CLA	a2	503	X	-	-	-
14	CLA	a2	504	X	-	-	-
14	CLA	a2	505	X	-	-	-
14	CLA	a2	506	X	-	-	-
14	CLA	a2	507	X	-	-	-
14	CLA	a2	508	X	-	-	-
14	CLA	a2	509	X	-	-	-
14	CLA	a2	510	X	-	-	-
14	CLA	a2	511	X	-	-	-
14	CLA	a2	512	X	-	-	-
14	CLA	a2	513	X	-	-	-
14	CLA	a2	516	X	-	-	-
14	CLA	a2	517	X	-	-	-
14	CLA	a2	518	X	-	-	-
14	CLA	a2	519	X	-	-	-
14	CLA	a3	501	X	-	-	-
14	CLA	a3	502	X	-	-	-
14	CLA	a3	503	X	-	-	-
14	CLA	a3	504	X	-	-	-
14	CLA	a3	505	X	-	-	-
14	CLA	a3	506	X	-	-	-
14	CLA	a3	507	X	-	-	-
14	CLA	a3	508	X	-	-	-
14	CLA	a3	509	X	-	-	-
14	CLA	a3	510	X	-	-	-
14	CLA	a3	511	X	-	-	-
14	CLA	a3	512	X	-	-	-
14	CLA	a3	513	X	-	-	-
14	CLA	a3	516	X	-	-	-
14	CLA	a3	517	X	-	-	-
14	CLA	a3	518	X	-	-	-
14	CLA	a3	519	X	-	-	-
14	CLA	a4	501	X	-	-	-
14	CLA	a4	502	X	-	-	-
14	CLA	a4	503	X	-	-	-
14	CLA	a4	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a4	505	X	-	-	-
14	CLA	a4	506	X	-	-	-
14	CLA	a4	507	X	-	-	-
14	CLA	a4	508	X	-	-	-
14	CLA	a4	509	X	-	-	-
14	CLA	a4	510	X	-	-	-
14	CLA	a4	511	X	-	-	-
14	CLA	a4	512	X	-	-	-
14	CLA	a4	513	X	-	-	-
14	CLA	a4	516	X	-	-	-
14	CLA	a4	517	X	-	-	-
14	CLA	a4	518	X	-	-	-
14	CLA	a4	519	X	-	-	-
14	CLA	a5	501	X	-	-	-
14	CLA	a5	502	X	-	-	-
14	CLA	a5	503	X	-	-	-
14	CLA	a5	504	X	-	-	-
14	CLA	a5	505	X	-	-	-
14	CLA	a5	506	X	-	-	-
14	CLA	a5	507	X	-	-	-
14	CLA	a5	508	X	-	-	-
14	CLA	a5	509	X	-	-	-
14	CLA	a5	510	X	-	-	-
14	CLA	a5	511	X	-	-	-
14	CLA	a5	512	X	-	-	-
14	CLA	a5	513	X	-	-	-
14	CLA	a5	516	X	-	-	-
14	CLA	a5	517	X	-	-	-
14	CLA	a5	518	X	-	-	-
14	CLA	a5	519	X	-	-	-
14	CLA	a6	501	X	-	-	-
14	CLA	a6	502	X	-	-	-
14	CLA	a6	503	X	-	-	-
14	CLA	a6	504	X	-	-	-
14	CLA	a6	505	X	-	-	-
14	CLA	a6	506	X	-	-	-
14	CLA	a6	507	X	-	-	-
14	CLA	a6	508	X	-	-	-
14	CLA	a6	509	X	-	-	-
14	CLA	a6	510	X	-	-	-
14	CLA	a6	511	X	-	-	-
14	CLA	a6	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a6	513	X	-	-	-
14	CLA	a6	516	X	-	-	-
14	CLA	a6	517	X	-	-	-
14	CLA	a6	518	X	-	-	-
14	CLA	a6	519	X	-	-	-
14	CLA	aA	1011	X	-	-	-
14	CLA	aA	1013	X	-	-	-
14	CLA	aA	1022	X	-	-	-
14	CLA	aA	1101	X	-	-	-
14	CLA	aA	1102	X	-	-	-
14	CLA	aA	1103	X	-	-	-
14	CLA	aA	1104	X	-	-	-
14	CLA	aA	1105	X	-	-	-
14	CLA	aA	1106	X	-	-	-
14	CLA	aA	1107	X	-	-	-
14	CLA	aA	1108	X	-	-	-
14	CLA	aA	1109	X	-	-	-
14	CLA	aA	1110	X	-	-	-
14	CLA	aA	1111	X	-	-	-
14	CLA	aA	1112	X	-	-	-
14	CLA	aA	1113	X	-	-	-
14	CLA	aA	1114	X	-	-	-
14	CLA	aA	1115	X	-	-	-
14	CLA	aA	1116	X	-	-	-
14	CLA	aA	1117	X	-	-	-
14	CLA	aA	1118	X	-	-	-
14	CLA	aA	1119	X	-	-	-
14	CLA	aA	1120	X	-	-	-
14	CLA	aA	1121	X	-	-	-
14	CLA	aA	1122	X	-	-	-
14	CLA	aA	1123	X	-	-	-
14	CLA	aA	1124	X	-	-	-
14	CLA	aA	1125	X	-	-	-
14	CLA	aA	1126	X	-	-	-
14	CLA	aA	1127	X	-	-	-
14	CLA	aA	1128	X	-	-	-
14	CLA	aA	1129	X	-	-	-
14	CLA	aA	1130	X	-	-	-
14	CLA	aA	1131	X	-	-	-
14	CLA	aA	1132	X	-	-	-
14	CLA	aA	1133	X	-	-	-
14	CLA	aA	1134	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	aA	1135	X	-	-	-
14	CLA	aA	1136	X	-	-	-
14	CLA	aA	1137	X	-	-	-
14	CLA	aA	1138	X	-	-	-
14	CLA	aA	1139	X	-	-	-
14	CLA	aA	1140	X	-	-	-
14	CLA	aA	1237	X	-	-	-
14	CLA	aA	1801	X	-	-	-
14	CLA	aB	1012	X	-	-	-
14	CLA	aB	1021	X	-	-	-
14	CLA	aB	1023	X	-	-	-
14	CLA	aB	1201	X	-	-	-
14	CLA	aB	1202	X	-	-	-
14	CLA	aB	1203	X	-	-	-
14	CLA	aB	1204	X	-	-	-
14	CLA	aB	1205	X	-	-	-
14	CLA	aB	1206	X	-	-	-
14	CLA	aB	1207	X	-	-	-
14	CLA	aB	1208	X	-	-	-
14	CLA	aB	1209	X	-	-	-
14	CLA	aB	1210	X	-	-	-
14	CLA	aB	1211	X	-	-	-
14	CLA	aB	1212	X	-	-	-
14	CLA	aB	1213	X	-	-	-
14	CLA	aB	1214	X	-	-	-
14	CLA	aB	1215	X	-	-	-
14	CLA	aB	1216	X	-	-	-
14	CLA	aB	1217	X	-	-	-
14	CLA	aB	1218	X	-	-	-
14	CLA	aB	1219	X	-	-	-
14	CLA	aB	1220	X	-	-	-
14	CLA	aB	1221	X	-	-	-
14	CLA	aB	1222	X	-	-	-
14	CLA	aB	1223	X	-	-	-
14	CLA	aB	1224	X	-	-	-
14	CLA	aB	1225	X	-	-	-
14	CLA	aB	1226	X	-	-	-
14	CLA	aB	1227	X	-	-	-
14	CLA	aB	1228	X	-	-	-
14	CLA	aB	1229	X	-	-	-
14	CLA	aB	1230	X	-	-	-
14	CLA	aB	1231	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	aB	1232	X	-	-	-
14	CLA	aB	1233	X	-	-	-
14	CLA	aB	1234	X	-	-	-
14	CLA	aB	1235	X	-	-	-
14	CLA	aB	1236	X	-	-	-
14	CLA	aB	1238	X	-	-	-
14	CLA	aB	1239	X	-	-	-
14	CLA	aF	1301	X	-	-	-
14	CLA	aJ	1302	X	-	-	-
14	CLA	aJ	1303	X	-	-	-
14	CLA	aK	1103	X	-	-	-
14	CLA	aK	1401	X	-	-	-
14	CLA	aL	1501	X	-	-	-
14	CLA	aL	1502	X	-	-	-
14	CLA	aL	1503	X	-	-	-
14	CLA	aX	1401	X	-	-	-
14	CLA	b	501	X	-	-	-
14	CLA	b	502	X	-	-	-
14	CLA	b	503	X	-	-	-
14	CLA	b	504	X	-	-	-
14	CLA	b	505	X	-	-	-
14	CLA	b	506	X	-	-	-
14	CLA	b	507	X	-	-	-
14	CLA	b	508	X	-	-	-
14	CLA	b	509	X	-	-	-
14	CLA	b	510	X	-	-	-
14	CLA	b	511	X	-	-	-
14	CLA	b	512	X	-	-	-
14	CLA	b	513	X	-	-	-
14	CLA	b	516	X	-	-	-
14	CLA	b	517	X	-	-	-
14	CLA	b	518	X	-	-	-
14	CLA	b	519	X	-	-	-
14	CLA	b1	501	X	-	-	-
14	CLA	b1	502	X	-	-	-
14	CLA	b1	503	X	-	-	-
14	CLA	b1	504	X	-	-	-
14	CLA	b1	505	X	-	-	-
14	CLA	b1	506	X	-	-	-
14	CLA	b1	507	X	-	-	-
14	CLA	b1	508	X	-	-	-
14	CLA	b1	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b1	510	X	-	-	-
14	CLA	b1	511	X	-	-	-
14	CLA	b1	512	X	-	-	-
14	CLA	b1	513	X	-	-	-
14	CLA	b1	516	X	-	-	-
14	CLA	b1	517	X	-	-	-
14	CLA	b1	518	X	-	-	-
14	CLA	b1	519	X	-	-	-
14	CLA	b2	501	X	-	-	-
14	CLA	b2	502	X	-	-	-
14	CLA	b2	503	X	-	-	-
14	CLA	b2	504	X	-	-	-
14	CLA	b2	505	X	-	-	-
14	CLA	b2	506	X	-	-	-
14	CLA	b2	507	X	-	-	-
14	CLA	b2	508	X	-	-	-
14	CLA	b2	509	X	-	-	-
14	CLA	b2	510	X	-	-	-
14	CLA	b2	511	X	-	-	-
14	CLA	b2	512	X	-	-	-
14	CLA	b2	513	X	-	-	-
14	CLA	b2	516	X	-	-	-
14	CLA	b2	517	X	-	-	-
14	CLA	b2	518	X	-	-	-
14	CLA	b2	519	X	-	-	-
14	CLA	b3	501	X	-	-	-
14	CLA	b3	502	X	-	-	-
14	CLA	b3	503	X	-	-	-
14	CLA	b3	504	X	-	-	-
14	CLA	b3	505	X	-	-	-
14	CLA	b3	506	X	-	-	-
14	CLA	b3	507	X	-	-	-
14	CLA	b3	508	X	-	-	-
14	CLA	b3	509	X	-	-	-
14	CLA	b3	510	X	-	-	-
14	CLA	b3	511	X	-	-	-
14	CLA	b3	512	X	-	-	-
14	CLA	b3	513	X	-	-	-
14	CLA	b3	516	X	-	-	-
14	CLA	b3	517	X	-	-	-
14	CLA	b3	518	X	-	-	-
14	CLA	b3	519	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b4	501	X	-	-	-
14	CLA	b4	502	X	-	-	-
14	CLA	b4	503	X	-	-	-
14	CLA	b4	504	X	-	-	-
14	CLA	b4	505	X	-	-	-
14	CLA	b4	506	X	-	-	-
14	CLA	b4	507	X	-	-	-
14	CLA	b4	508	X	-	-	-
14	CLA	b4	509	X	-	-	-
14	CLA	b4	510	X	-	-	-
14	CLA	b4	511	X	-	-	-
14	CLA	b4	512	X	-	-	-
14	CLA	b4	513	X	-	-	-
14	CLA	b4	516	X	-	-	-
14	CLA	b4	517	X	-	-	-
14	CLA	b4	518	X	-	-	-
14	CLA	b4	519	X	-	-	-
14	CLA	b5	501	X	-	-	-
14	CLA	b5	502	X	-	-	-
14	CLA	b5	503	X	-	-	-
14	CLA	b5	504	X	-	-	-
14	CLA	b5	505	X	-	-	-
14	CLA	b5	506	X	-	-	-
14	CLA	b5	507	X	-	-	-
14	CLA	b5	508	X	-	-	-
14	CLA	b5	509	X	-	-	-
14	CLA	b5	510	X	-	-	-
14	CLA	b5	511	X	-	-	-
14	CLA	b5	512	X	-	-	-
14	CLA	b5	513	X	-	-	-
14	CLA	b5	516	X	-	-	-
14	CLA	b5	517	X	-	-	-
14	CLA	b5	518	X	-	-	-
14	CLA	b5	519	X	-	-	-
14	CLA	b6	501	X	-	-	-
14	CLA	b6	502	X	-	-	-
14	CLA	b6	503	X	-	-	-
14	CLA	b6	504	X	-	-	-
14	CLA	b6	505	X	-	-	-
14	CLA	b6	506	X	-	-	-
14	CLA	b6	507	X	-	-	-
14	CLA	b6	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b6	509	X	-	-	-
14	CLA	b6	510	X	-	-	-
14	CLA	b6	511	X	-	-	-
14	CLA	b6	512	X	-	-	-
14	CLA	b6	513	X	-	-	-
14	CLA	b6	516	X	-	-	-
14	CLA	b6	517	X	-	-	-
14	CLA	b6	518	X	-	-	-
14	CLA	b6	519	X	-	-	-
14	CLA	bA	1011	X	-	-	-
14	CLA	bA	1013	X	-	-	-
14	CLA	bA	1022	X	-	-	-
14	CLA	bA	1101	X	-	-	-
14	CLA	bA	1102	X	-	-	-
14	CLA	bA	1103	X	-	-	-
14	CLA	bA	1104	X	-	-	-
14	CLA	bA	1105	X	-	-	-
14	CLA	bA	1106	X	-	-	-
14	CLA	bA	1107	X	-	-	-
14	CLA	bA	1108	X	-	-	-
14	CLA	bA	1109	X	-	-	-
14	CLA	bA	1110	X	-	-	-
14	CLA	bA	1111	X	-	-	-
14	CLA	bA	1112	X	-	-	-
14	CLA	bA	1113	X	-	-	-
14	CLA	bA	1114	X	-	-	-
14	CLA	bA	1115	X	-	-	-
14	CLA	bA	1116	X	-	-	-
14	CLA	bA	1117	X	-	-	-
14	CLA	bA	1118	X	-	-	-
14	CLA	bA	1119	X	-	-	-
14	CLA	bA	1120	X	-	-	-
14	CLA	bA	1121	X	-	-	-
14	CLA	bA	1122	X	-	-	-
14	CLA	bA	1123	X	-	-	-
14	CLA	bA	1124	X	-	-	-
14	CLA	bA	1125	X	-	-	-
14	CLA	bA	1126	X	-	-	-
14	CLA	bA	1127	X	-	-	-
14	CLA	bA	1128	X	-	-	-
14	CLA	bA	1129	X	-	-	-
14	CLA	bA	1130	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	bA	1131	X	-	-	-
14	CLA	bA	1132	X	-	-	-
14	CLA	bA	1133	X	-	-	-
14	CLA	bA	1134	X	-	-	-
14	CLA	bA	1135	X	-	-	-
14	CLA	bA	1136	X	-	-	-
14	CLA	bA	1137	X	-	-	-
14	CLA	bA	1138	X	-	-	-
14	CLA	bA	1139	X	-	-	-
14	CLA	bA	1140	X	-	-	-
14	CLA	bA	1237	X	-	-	-
14	CLA	bA	1801	X	-	-	-
14	CLA	bB	1012	X	-	-	-
14	CLA	bB	1021	X	-	-	-
14	CLA	bB	1023	X	-	-	-
14	CLA	bB	1201	X	-	-	-
14	CLA	bB	1202	X	-	-	-
14	CLA	bB	1203	X	-	-	-
14	CLA	bB	1204	X	-	-	-
14	CLA	bB	1205	X	-	-	-
14	CLA	bB	1206	X	-	-	-
14	CLA	bB	1207	X	-	-	-
14	CLA	bB	1208	X	-	-	-
14	CLA	bB	1209	X	-	-	-
14	CLA	bB	1210	X	-	-	-
14	CLA	bB	1211	X	-	-	-
14	CLA	bB	1212	X	-	-	-
14	CLA	bB	1213	X	-	-	-
14	CLA	bB	1214	X	-	-	-
14	CLA	bB	1215	X	-	-	-
14	CLA	bB	1216	X	-	-	-
14	CLA	bB	1217	X	-	-	-
14	CLA	bB	1218	X	-	-	-
14	CLA	bB	1219	X	-	-	-
14	CLA	bB	1220	X	-	-	-
14	CLA	bB	1221	X	-	-	-
14	CLA	bB	1222	X	-	-	-
14	CLA	bB	1223	X	-	-	-
14	CLA	bB	1224	X	-	-	-
14	CLA	bB	1225	X	-	-	-
14	CLA	bB	1226	X	-	-	-
14	CLA	bB	1227	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	bB	1228	X	-	-	-
14	CLA	bB	1229	X	-	-	-
14	CLA	bB	1230	X	-	-	-
14	CLA	bB	1231	X	-	-	-
14	CLA	bB	1232	X	-	-	-
14	CLA	bB	1233	X	-	-	-
14	CLA	bB	1234	X	-	-	-
14	CLA	bB	1235	X	-	-	-
14	CLA	bB	1236	X	-	-	-
14	CLA	bB	1238	X	-	-	-
14	CLA	bB	1239	X	-	-	-
14	CLA	bF	1301	X	-	-	-
14	CLA	bJ	1302	X	-	-	-
14	CLA	bJ	1303	X	-	-	-
14	CLA	bK	1103	X	-	-	-
14	CLA	bK	1401	X	-	-	-
14	CLA	bL	1501	X	-	-	-
14	CLA	bL	1502	X	-	-	-
14	CLA	bL	1503	X	-	-	-
14	CLA	bX	1401	X	-	-	-
14	CLA	c	501	X	-	-	-
14	CLA	c	502	X	-	-	-
14	CLA	c	503	X	-	-	-
14	CLA	c	504	X	-	-	-
14	CLA	c	505	X	-	-	-
14	CLA	c	506	X	-	-	-
14	CLA	c	507	X	-	-	-
14	CLA	c	508	X	-	-	-
14	CLA	c	509	X	-	-	-
14	CLA	c	510	X	-	-	-
14	CLA	c	511	X	-	-	-
14	CLA	c	512	X	-	-	-
14	CLA	c	513	X	-	-	-
14	CLA	c	516	X	-	-	-
14	CLA	c	517	X	-	-	-
14	CLA	c	518	X	-	-	-
14	CLA	c	519	X	-	-	-
14	CLA	c1	501	X	-	-	-
14	CLA	c1	502	X	-	-	-
14	CLA	c1	503	X	-	-	-
14	CLA	c1	504	X	-	-	-
14	CLA	c1	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	c1	506	X	-	-	-
14	CLA	c1	507	X	-	-	-
14	CLA	c1	508	X	-	-	-
14	CLA	c1	509	X	-	-	-
14	CLA	c1	510	X	-	-	-
14	CLA	c1	511	X	-	-	-
14	CLA	c1	512	X	-	-	-
14	CLA	c1	513	X	-	-	-
14	CLA	c1	516	X	-	-	-
14	CLA	c1	517	X	-	-	-
14	CLA	c1	518	X	-	-	-
14	CLA	c1	519	X	-	-	-
14	CLA	c2	501	X	-	-	-
14	CLA	c2	502	X	-	-	-
14	CLA	c2	503	X	-	-	-
14	CLA	c2	504	X	-	-	-
14	CLA	c2	505	X	-	-	-
14	CLA	c2	506	X	-	-	-
14	CLA	c2	507	X	-	-	-
14	CLA	c2	508	X	-	-	-
14	CLA	c2	509	X	-	-	-
14	CLA	c2	510	X	-	-	-
14	CLA	c2	511	X	-	-	-
14	CLA	c2	512	X	-	-	-
14	CLA	c2	513	X	-	-	-
14	CLA	c2	516	X	-	-	-
14	CLA	c2	517	X	-	-	-
14	CLA	c2	518	X	-	-	-
14	CLA	c2	519	X	-	-	-
14	CLA	c3	501	X	-	-	-
14	CLA	c3	502	X	-	-	-
14	CLA	c3	503	X	-	-	-
14	CLA	c3	504	X	-	-	-
14	CLA	c3	505	X	-	-	-
14	CLA	c3	506	X	-	-	-
14	CLA	c3	507	X	-	-	-
14	CLA	c3	508	X	-	-	-
14	CLA	c3	509	X	-	-	-
14	CLA	c3	510	X	-	-	-
14	CLA	c3	511	X	-	-	-
14	CLA	c3	512	X	-	-	-
14	CLA	c3	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	c3	516	X	-	-	-
14	CLA	c3	517	X	-	-	-
14	CLA	c3	518	X	-	-	-
14	CLA	c3	519	X	-	-	-
14	CLA	c4	501	X	-	-	-
14	CLA	c4	502	X	-	-	-
14	CLA	c4	503	X	-	-	-
14	CLA	c4	504	X	-	-	-
14	CLA	c4	505	X	-	-	-
14	CLA	c4	506	X	-	-	-
14	CLA	c4	507	X	-	-	-
14	CLA	c4	508	X	-	-	-
14	CLA	c4	509	X	-	-	-
14	CLA	c4	510	X	-	-	-
14	CLA	c4	511	X	-	-	-
14	CLA	c4	512	X	-	-	-
14	CLA	c4	513	X	-	-	-
14	CLA	c4	516	X	-	-	-
14	CLA	c4	517	X	-	-	-
14	CLA	c4	518	X	-	-	-
14	CLA	c4	519	X	-	-	-
14	CLA	c5	501	X	-	-	-
14	CLA	c5	502	X	-	-	-
14	CLA	c5	503	X	-	-	-
14	CLA	c5	504	X	-	-	-
14	CLA	c5	505	X	-	-	-
14	CLA	c5	506	X	-	-	-
14	CLA	c5	507	X	-	-	-
14	CLA	c5	508	X	-	-	-
14	CLA	c5	509	X	-	-	-
14	CLA	c5	510	X	-	-	-
14	CLA	c5	511	X	-	-	-
14	CLA	c5	512	X	-	-	-
14	CLA	c5	513	X	-	-	-
14	CLA	c5	516	X	-	-	-
14	CLA	c5	517	X	-	-	-
14	CLA	c5	518	X	-	-	-
14	CLA	c5	519	X	-	-	-
14	CLA	c6	501	X	-	-	-
14	CLA	c6	502	X	-	-	-
14	CLA	c6	503	X	-	-	-
14	CLA	c6	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	c6	505	X	-	-	-
14	CLA	c6	506	X	-	-	-
14	CLA	c6	507	X	-	-	-
14	CLA	c6	508	X	-	-	-
14	CLA	c6	509	X	-	-	-
14	CLA	c6	510	X	-	-	-
14	CLA	c6	511	X	-	-	-
14	CLA	c6	512	X	-	-	-
14	CLA	c6	513	X	-	-	-
14	CLA	c6	516	X	-	-	-
14	CLA	c6	517	X	-	-	-
14	CLA	c6	518	X	-	-	-
14	CLA	c6	519	X	-	-	-
14	CLA	cA	1011	X	-	-	-
14	CLA	cA	1013	X	-	-	-
14	CLA	cA	1022	X	-	-	-
14	CLA	cA	1101	X	-	-	-
14	CLA	cA	1102	X	-	-	-
14	CLA	cA	1103	X	-	-	-
14	CLA	cA	1104	X	-	-	-
14	CLA	cA	1105	X	-	-	-
14	CLA	cA	1106	X	-	-	-
14	CLA	cA	1107	X	-	-	-
14	CLA	cA	1108	X	-	-	-
14	CLA	cA	1109	X	-	-	-
14	CLA	cA	1110	X	-	-	-
14	CLA	cA	1111	X	-	-	-
14	CLA	cA	1112	X	-	-	-
14	CLA	cA	1113	X	-	-	-
14	CLA	cA	1114	X	-	-	-
14	CLA	cA	1115	X	-	-	-
14	CLA	cA	1116	X	-	-	-
14	CLA	cA	1117	X	-	-	-
14	CLA	cA	1118	X	-	-	-
14	CLA	cA	1119	X	-	-	-
14	CLA	cA	1120	X	-	-	-
14	CLA	cA	1121	X	-	-	-
14	CLA	cA	1122	X	-	-	-
14	CLA	cA	1123	X	-	-	-
14	CLA	cA	1124	X	-	-	-
14	CLA	cA	1125	X	-	-	-
14	CLA	cA	1126	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	cA	1127	X	-	-	-
14	CLA	cA	1128	X	-	-	-
14	CLA	cA	1129	X	-	-	-
14	CLA	cA	1130	X	-	-	-
14	CLA	cA	1131	X	-	-	-
14	CLA	cA	1132	X	-	-	-
14	CLA	cA	1133	X	-	-	-
14	CLA	cA	1134	X	-	-	-
14	CLA	cA	1135	X	-	-	-
14	CLA	cA	1136	X	-	-	-
14	CLA	cA	1137	X	-	-	-
14	CLA	cA	1138	X	-	-	-
14	CLA	cA	1139	X	-	-	-
14	CLA	cA	1140	X	-	-	-
14	CLA	cA	1237	X	-	-	-
14	CLA	cA	1801	X	-	-	-
14	CLA	cB	1012	X	-	-	-
14	CLA	cB	1021	X	-	-	-
14	CLA	cB	1023	X	-	-	-
14	CLA	cB	1201	X	-	-	-
14	CLA	cB	1202	X	-	-	-
14	CLA	cB	1203	X	-	-	-
14	CLA	cB	1204	X	-	-	-
14	CLA	cB	1205	X	-	-	-
14	CLA	cB	1206	X	-	-	-
14	CLA	cB	1207	X	-	-	-
14	CLA	cB	1208	X	-	-	-
14	CLA	cB	1209	X	-	-	-
14	CLA	cB	1210	X	-	-	-
14	CLA	cB	1211	X	-	-	-
14	CLA	cB	1212	X	-	-	-
14	CLA	cB	1213	X	-	-	-
14	CLA	cB	1214	X	-	-	-
14	CLA	cB	1215	X	-	-	-
14	CLA	cB	1216	X	-	-	-
14	CLA	cB	1217	X	-	-	-
14	CLA	cB	1218	X	-	-	-
14	CLA	cB	1219	X	-	-	-
14	CLA	cB	1220	X	-	-	-
14	CLA	cB	1221	X	-	-	-
14	CLA	cB	1222	X	-	-	-
14	CLA	cB	1223	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	cB	1224	X	-	-	-
14	CLA	cB	1225	X	-	-	-
14	CLA	cB	1226	X	-	-	-
14	CLA	cB	1227	X	-	-	-
14	CLA	cB	1228	X	-	-	-
14	CLA	cB	1229	X	-	-	-
14	CLA	cB	1230	X	-	-	-
14	CLA	cB	1231	X	-	-	-
14	CLA	cB	1232	X	-	-	-
14	CLA	cB	1233	X	-	-	-
14	CLA	cB	1234	X	-	-	-
14	CLA	cB	1235	X	-	-	-
14	CLA	cB	1236	X	-	-	-
14	CLA	cB	1238	X	-	-	-
14	CLA	cB	1239	X	-	-	-
14	CLA	cF	1301	X	-	-	-
14	CLA	cJ	1302	X	-	-	-
14	CLA	cJ	1303	X	-	-	-
14	CLA	cK	1103	X	-	-	-
14	CLA	cK	1401	X	-	-	-
14	CLA	cL	1501	X	-	-	-
14	CLA	cL	1502	X	-	-	-
14	CLA	cL	1503	X	-	-	-
14	CLA	cX	1401	X	-	-	-
14	CLA	d	501	X	-	-	-
14	CLA	d	502	X	-	-	-
14	CLA	d	503	X	-	-	-
14	CLA	d	504	X	-	-	-
14	CLA	d	505	X	-	-	-
14	CLA	d	506	X	-	-	-
14	CLA	d	507	X	-	-	-
14	CLA	d	508	X	-	-	-
14	CLA	d	509	X	-	-	-
14	CLA	d	510	X	-	-	-
14	CLA	d	511	X	-	-	-
14	CLA	d	512	X	-	-	-
14	CLA	d	513	X	-	-	-
14	CLA	d	516	X	-	-	-
14	CLA	d	517	X	-	-	-
14	CLA	d	518	X	-	-	-
14	CLA	d	519	X	-	-	-
14	CLA	e	501	X	-	-	-

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

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	n	519	X	-	-	-
14	CLA	o	501	X	-	-	-
14	CLA	o	502	X	-	-	-
14	CLA	o	503	X	-	-	-
14	CLA	o	504	X	-	-	-
14	CLA	o	505	X	-	-	-
14	CLA	o	506	X	-	-	-
14	CLA	o	507	X	-	-	-
14	CLA	o	508	X	-	-	-
14	CLA	o	509	X	-	-	-
14	CLA	o	510	X	-	-	-
14	CLA	o	511	X	-	-	-
14	CLA	o	512	X	-	-	-
14	CLA	o	513	X	-	-	-
14	CLA	o	516	X	-	-	-
14	CLA	o	517	X	-	-	-
14	CLA	o	518	X	-	-	-
14	CLA	o	519	X	-	-	-
14	CLA	p	501	X	-	-	-
14	CLA	p	502	X	-	-	-
14	CLA	p	503	X	-	-	-
14	CLA	p	504	X	-	-	-
14	CLA	p	505	X	-	-	-
14	CLA	p	506	X	-	-	-
14	CLA	p	507	X	-	-	-
14	CLA	p	508	X	-	-	-
14	CLA	p	509	X	-	-	-
14	CLA	p	510	X	-	-	-
14	CLA	p	511	X	-	-	-
14	CLA	p	512	X	-	-	-
14	CLA	p	513	X	-	-	-
14	CLA	p	516	X	-	-	-
14	CLA	p	517	X	-	-	-
14	CLA	p	518	X	-	-	-
14	CLA	p	519	X	-	-	-
14	CLA	q	501	X	-	-	-
14	CLA	q	502	X	-	-	-
14	CLA	q	503	X	-	-	-
14	CLA	q	504	X	-	-	-
14	CLA	q	505	X	-	-	-
14	CLA	q	506	X	-	-	-
14	CLA	q	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	q	508	X	-	-	-
14	CLA	q	509	X	-	-	-
14	CLA	q	510	X	-	-	-
14	CLA	q	511	X	-	-	-
14	CLA	q	512	X	-	-	-
14	CLA	q	513	X	-	-	-
14	CLA	q	516	X	-	-	-
14	CLA	q	517	X	-	-	-
14	CLA	q	518	X	-	-	-
14	CLA	q	519	X	-	-	-

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 235011 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	aA	745	Total	C	N	O	S	0	0
			5819	3818	994	981	26		
1	bA	745	Total	C	N	O	S	0	0
			5819	3818	994	981	26		
1	cA	745	Total	C	N	O	S	0	0
			5819	3818	994	981	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		
2	bB	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		
2	cB	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aC	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	bC	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	cC	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	137	Total	C	N	O	S	0	0
			1068	678	185	202	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	137	Total	C	N	O	S	0	0
			1068	678	185	202	3		
4	cD	137	Total	C	N	O	S	0	0
			1068	678	185	202	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	aE	69	Total	C	N	O		0	0
			539	342	93	104			
5	bE	69	Total	C	N	O		0	0
			539	342	93	104			
5	cE	69	Total	C	N	O		0	0
			539	342	93	104			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	bF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	cF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		
7	bI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		
7	cI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	aJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		
8	bJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	cJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	aK	62	Total	C	N	O	S	0	0
			452	298	71	82	1		
9	bK	62	Total	C	N	O	S	0	0
			452	298	71	82	1		
9	cK	62	Total	C	N	O	S	0	0
			452	298	71	82	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aL	152	Total	C	N	O	S	0	0
			1126	737	180	205	4		
10	bL	152	Total	C	N	O	S	0	0
			1126	737	180	205	4		
10	cL	152	Total	C	N	O	S	0	0
			1126	737	180	205	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	aM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	bM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	cM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

- Molecule 12 is a protein called Photosystem I 4.8K protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	aX	29	Total	C	N	O	0	0
			243	172	35	36		
12	bX	29	Total	C	N	O	0	0
			243	172	35	36		
12	cX	29	Total	C	N	O	0	0
			243	172	35	36		

- Molecule 13 is a protein called Iron stress-induced chlorophyll-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a1	340	Total	C	N	O	S	0	0
			2665	1780	438	443	4		
13	a2	339	Total	C	N	O	S	0	0
			2657	1774	437	442	4		
13	a3	343	Total	C	N	O	S	0	0
			2685	1792	442	447	4		
13	a4	343	Total	C	N	O	S	0	0
			2685	1792	442	447	4		
13	a5	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
13	a6	341	Total	C	N	O	S	0	0
			2673	1784	440	445	4		
13	b1	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
13	b2	341	Total	C	N	O	S	0	0
			2673	1784	440	445	4		
13	b3	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
13	b4	343	Total	C	N	O	S	0	0
			2685	1792	442	447	4		
13	b5	340	Total	C	N	O	S	0	0
			2665	1780	438	443	4		
13	b6	339	Total	C	N	O	S	0	0
			2657	1774	437	442	4		
13	c1	341	Total	C	N	O	S	0	0
			2673	1784	440	445	4		
13	c2	340	Total	C	N	O	S	0	0
			2665	1780	438	443	4		
13	c3	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
13	c4	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
13	c5	341	Total	C	N	O	S	0	0
			2673	1784	440	445	4		
13	c6	339	Total	C	N	O	S	0	0
			2657	1774	437	442	4		
13	S	341	Total	C	N	O	S	0	0
			2674	1786	440	444	4		
13	T	340	Total	C	N	O	S	0	0
			2665	1780	438	443	4		
13	U	340	Total	C	N	O	S	0	0
			2667	1781	439	443	4		

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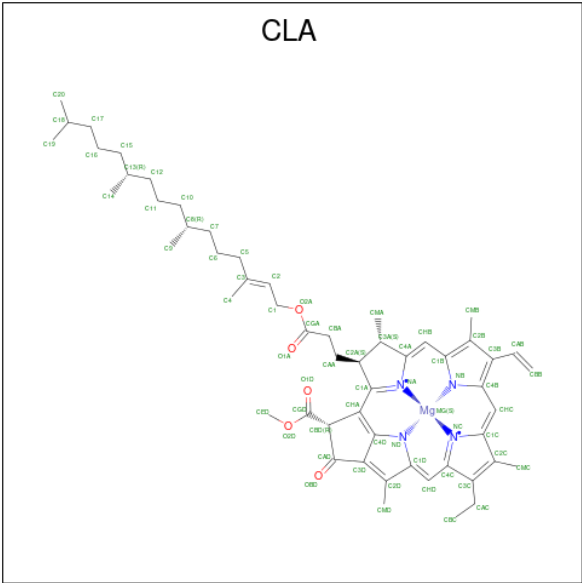
Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	341	Total	C	N	O	S	0	0
			2674	1786	440	444	4		
13	W	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
13	X	343	Total	C	N	O	S	0	0
			2687	1795	442	446	4		
13	Y	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
13	Z	340	Total	C	N	O	S	0	0
			2667	1781	439	443	4		
13	a	341	Total	C	N	O	S	0	0
			2673	1784	440	445	4		
13	b	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
13	c	341	Total	C	N	O	S	0	0
			2674	1786	440	444	4		
13	d	341	Total	C	N	O	S	0	0
			2674	1786	440	444	4		
13	e	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
13	f	341	Total	C	N	O	S	0	0
			2674	1786	440	444	4		
13	g	341	Total	C	N	O	S	0	0
			2673	1784	440	445	4		
13	h	341	Total	C	N	O	S	0	0
			2673	1784	440	445	4		
13	i	340	Total	C	N	O	S	0	0
			2667	1781	439	443	4		
13	j	339	Total	C	N	O	S	0	0
			2659	1777	437	441	4		
13	k	340	Total	C	N	O	S	0	0
			2667	1781	439	443	4		
13	l	340	Total	C	N	O	S	0	0
			2667	1781	439	443	4		
13	m	341	Total	C	N	O	S	0	0
			2674	1786	440	444	4		
13	n	340	Total	C	N	O	S	0	0
			2667	1781	439	443	4		
13	o	341	Total	C	N	O	S	0	0
			2674	1786	440	444	4		
13	p	339	Total	C	N	O	S	0	0
			2659	1777	437	441	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	q	343	Total	C	N	O	S	0	0
			2685	1792	442	447	4		

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



Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 57	C 47	Mg 1	N 4	O 5	0
14	aA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 57	C 47	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	aB	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 61	C 51	Mg 1	N 4	O 5	0
14	aB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	aB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	aB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	aB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	aB	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	aB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	aB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 57	C 47	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	aB	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	aB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	aB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aF	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aJ	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	aJ	1	Total 57	C 47	Mg 1	N 4	O 5	0
14	aK	1	Total 41	C 33	Mg 1	N 4	O 3	0
14	aK	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	aL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aL	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	aL	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	aX	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a1	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a1	1	Total 63	C 53	Mg 1	N 4	O 5	0
14	a1	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a1	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a1	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a1	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a1	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	a1	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	a1	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	a1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a1	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a2	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	a2	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a2	1	Total 61	C 51	Mg 1	N 4	O 5	0
14	a2	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a2	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	a2	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	a2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a2	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a2	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	a3	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a3	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a3	1	Total 63	C 53	Mg 1	N 4	O 5	0
14	a3	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	a3	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a3	1	Total 62	C 52	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	a3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	a3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a3	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	a3	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	a3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a3	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	a3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a4	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	a4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a4	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	a4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a4	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	a4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a4	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a4	1	Total 57	C 47	Mg 1	N 4	O 5	0
14	a4	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	a5	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a5	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a5	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a5	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	a5	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a5	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a5	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a5	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a5	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a5	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a5	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	a5	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a5	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	a5	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	a5	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
14	a5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	bA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bA	1	Total 48	C 38	Mg 1	N 4	O 5	0
14	bA	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	bA	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bA	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	bA	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 61	C 51	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 57	C 47	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bB	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	bB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bB	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	bB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	bB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bB	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	bB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	bB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 57	C 47	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	bB	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	bB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	bF	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bJ	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	bJ	1	Total 57	C 47	Mg 1	N 4	O 5	0
14	bK	1	Total 41	C 33	Mg 1	N 4	O 3	0
14	bK	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bL	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bX	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b1	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b1	1	Total 63	C 53	Mg 1	N 4	O 5	0
14	b1	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b1	1	Total 61	C 51	Mg 1	N 4	O 5	0
14	b1	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b1	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b1	1	Total 53	C 43	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	b1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	b2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
14	b3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	b4	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	b5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	b6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b6	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	b6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b6	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	b6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	cA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cA	1	Total 48	C 38	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
14	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 57	C 47	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	cB	1	Total 53	C 43	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	cB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	cB	1	Total 61	C 51	Mg 1	N 4	O 5	0
14	cB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cB	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	cB	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	cB	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	cB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	cB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	cB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	cB	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	cB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cF	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cJ	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	cJ	1	Total 57	C 47	Mg 1	N 4	O 5	0
14	cK	1	Total 41	C 33	Mg 1	N 4	O 3	0
14	cK	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cL	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	cL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cX	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c1	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	c1	1	Total 63	C 53	Mg 1	N 4	O 5	0
14	c1	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c1	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	c1	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c1	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	c1	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	c1	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	c1	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	c1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c1	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	c1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c2	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c2	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	c2	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c2	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	c2	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	c2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c2	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	c2	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	c3	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c3	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	c3	1	Total 63	C 53	Mg 1	N 4	O 5	0
14	c3	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	c3	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c3	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c3	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	c3	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	c3	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c3	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c3	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	c3	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	c3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	c4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	c5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	c6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c6	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c6	1	Total 57	C 47	Mg 1	N 4	O 5	0
14	c6	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	c6	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c6	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c6	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	S	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	S	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	S	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	S	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	S	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
14	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	T	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	T	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	U	1	Total 57	C 47	Mg 1	N 4	O 5	0
14	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	U	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	U	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	U	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	W	1	Total 63	C 53	Mg 1	N 4	O 5	0
14	W	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	W	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	W	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	W	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	W	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	X	1	Total 63	C 53	Mg 1	N 4	O 5	0
14	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	X	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	X	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	Y	1	Total 63	C 53	Mg 1	N 4	O 5	0
14	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	Y	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	Y	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Y	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	Z	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	Z	1	Total 61	C 51	Mg 1	N 4	O 5	0
14	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 63	C 53	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 57	C 47	Mg 1	N 4	O 5	0
14	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	c	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	d	1	Total 62	C 52	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	d	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	d	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	e	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	e	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	h	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	h	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	j	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	n	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	o	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	o	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	o	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	o	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	o	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	p	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	p	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	p	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	p	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	p	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
14	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).

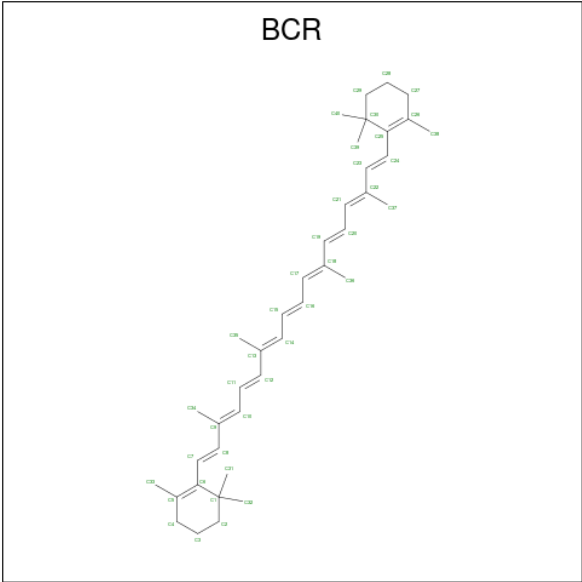


- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
16	aA	1	Total	Fe	S	0
			8	4	4	
16	aC	1	Total	Fe	S	0
			8	4	4	
16	aC	1	Total	Fe	S	0
			8	4	4	
16	bA	1	Total	Fe	S	0
			8	4	4	
16	bC	1	Total	Fe	S	0
			8	4	4	
16	bC	1	Total	Fe	S	0
			8	4	4	
16	cA	1	Total	Fe	S	0
			8	4	4	
16	cC	1	Total	Fe	S	0
			8	4	4	
16	cC	1	Total	Fe	S	0
			8	4	4	

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	
17	aB	1	Total	C	0
			40	40	
17	aB	1	Total	C	0
			40	40	
17	aB	1	Total	C	0
			40	40	
17	aB	1	Total	C	0
			40	40	
17	aB	1	Total	C	0
			40	40	
17	aF	1	Total	C	0
			40	40	
17	aF	1	Total	C	0
			40	40	
17	aF	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
17	aI	1	Total C 40 40	0
17	aI	1	Total C 40 40	0
17	aI	1	Total C 40 40	0
17	aJ	1	Total C 40 40	0
17	aJ	1	Total C 40 40	0
17	aK	1	Total C 40 40	0
17	aL	1	Total C 40 40	0
17	aM	1	Total C 40 40	0
17	a1	1	Total C 40 40	0
17	a1	1	Total C 40 40	0
17	a1	1	Total C 40 40	0
17	a1	1	Total C 40 40	0
17	a1	1	Total C 40 40	0
17	a2	1	Total C 40 40	0
17	a2	1	Total C 40 40	0
17	a2	1	Total C 40 40	0
17	a2	1	Total C 40 40	0
17	a3	1	Total C 40 40	0
17	a3	1	Total C 40 40	0
17	a3	1	Total C 40 40	0
17	a3	1	Total C 40 40	0
17	a4	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	a4	1	Total C 40 40	0
17	a4	1	Total C 40 40	0
17	a4	1	Total C 40 40	0
17	a5	1	Total C 40 40	0
17	a5	1	Total C 40 40	0
17	a5	1	Total C 40 40	0
17	a5	1	Total C 40 40	0
17	a6	1	Total C 40 40	0
17	a6	1	Total C 40 40	0
17	a6	1	Total C 40 40	0
17	a6	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	bB	1	Total C 40 40	0
17	bF	1	Total C 40 40	0
17	bF	1	Total C 40 40	0
17	bF	1	Total C 40 40	0
17	bI	1	Total C 40 40	0
17	bI	1	Total C 40 40	0
17	bI	1	Total C 40 40	0
17	bJ	1	Total C 40 40	0
17	bJ	1	Total C 40 40	0
17	bK	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	bM	1	Total C 40 40	0
17	b1	1	Total C 40 40	0
17	b1	1	Total C 40 40	0
17	b1	1	Total C 40 40	0
17	b1	1	Total C 40 40	0
17	b2	1	Total C 40 40	0
17	b2	1	Total C 40 40	0
17	b2	1	Total C 40 40	0
17	b2	1	Total C 40 40	0
17	b3	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	b3	1	Total C 40 40	0
17	b3	1	Total C 40 40	0
17	b3	1	Total C 40 40	0
17	b4	1	Total C 40 40	0
17	b4	1	Total C 40 40	0
17	b4	1	Total C 40 40	0
17	b4	1	Total C 40 40	0
17	b5	1	Total C 40 40	0
17	b5	1	Total C 40 40	0
17	b5	1	Total C 40 40	0
17	b5	1	Total C 40 40	0
17	b6	1	Total C 40 40	0
17	b6	1	Total C 40 40	0
17	b6	1	Total C 40 40	0
17	b6	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cB	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cF	1	Total C 40 40	0
17	cF	1	Total C 40 40	0
17	cF	1	Total C 40 40	0
17	cI	1	Total C 40 40	0
17	cI	1	Total C 40 40	0
17	cI	1	Total C 40 40	0
17	cJ	1	Total C 40 40	0
17	cJ	1	Total C 40 40	0
17	cK	1	Total C 40 40	0
17	cL	1	Total C 40 40	0
17	cM	1	Total C 40 40	0
17	c1	1	Total C 40 40	0
17	c1	1	Total C 40 40	0
17	c1	1	Total C 40 40	0
17	c1	1	Total C 40 40	0
17	c2	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	c2	1	Total C 40 40	0
17	c2	1	Total C 40 40	0
17	c2	1	Total C 40 40	0
17	c3	1	Total C 40 40	0
17	c3	1	Total C 40 40	0
17	c3	1	Total C 40 40	0
17	c3	1	Total C 40 40	0
17	c4	1	Total C 40 40	0
17	c4	1	Total C 40 40	0
17	c4	1	Total C 40 40	0
17	c4	1	Total C 40 40	0
17	c5	1	Total C 40 40	0
17	c5	1	Total C 40 40	0
17	c5	1	Total C 40 40	0
17	c5	1	Total C 40 40	0
17	c6	1	Total C 40 40	0
17	c6	1	Total C 40 40	0
17	c6	1	Total C 40 40	0
17	c6	1	Total C 40 40	0
17	S	1	Total C 40 40	0
17	S	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	S	1	Total C 40 40	0
17	S	1	Total C 40 40	0
17	T	1	Total C 40 40	0
17	T	1	Total C 40 40	0
17	T	1	Total C 40 40	0
17	T	1	Total C 40 40	0
17	U	1	Total C 40 40	0
17	U	1	Total C 40 40	0
17	U	1	Total C 40 40	0
17	U	1	Total C 40 40	0
17	V	1	Total C 40 40	0
17	V	1	Total C 40 40	0
17	V	1	Total C 40 40	0
17	V	1	Total C 40 40	0
17	W	1	Total C 40 40	0
17	W	1	Total C 40 40	0
17	W	1	Total C 40 40	0
17	W	1	Total C 40 40	0
17	X	1	Total C 40 40	0
17	X	1	Total C 40 40	0
17	X	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	X	1	Total C 40 40	0
17	Y	1	Total C 40 40	0
17	Y	1	Total C 40 40	0
17	Y	1	Total C 40 40	0
17	Y	1	Total C 40 40	0
17	Z	1	Total C 40 40	0
17	Z	1	Total C 40 40	0
17	Z	1	Total C 40 40	0
17	Z	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	c	1	Total C 40 40	0
17	c	1	Total C 40 40	0
17	c	1	Total C 40 40	0
17	c	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	d	1	Total C 40 40	0
17	d	1	Total C 40 40	0
17	d	1	Total C 40 40	0
17	d	1	Total C 40 40	0
17	e	1	Total C 40 40	0
17	e	1	Total C 40 40	0
17	e	1	Total C 40 40	0
17	e	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	g	1	Total C 40 40	0
17	g	1	Total C 40 40	0
17	g	1	Total C 40 40	0
17	g	1	Total C 40 40	0
17	h	1	Total C 40 40	0
17	h	1	Total C 40 40	0
17	h	1	Total C 40 40	0
17	h	1	Total C 40 40	0
17	i	1	Total C 40 40	0

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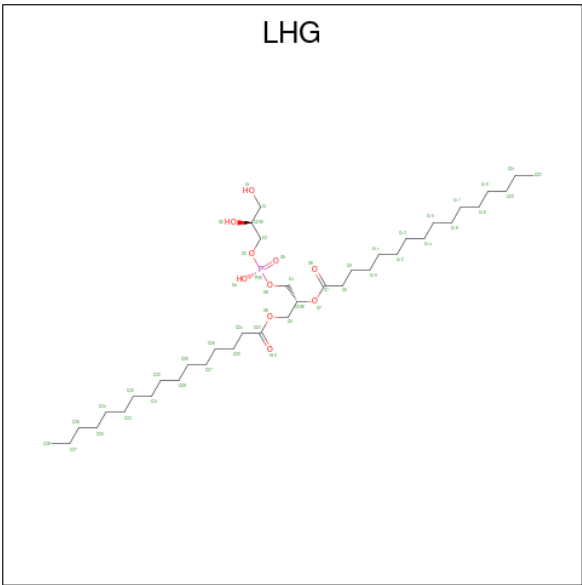
Mol	Chain	Residues	Atoms	AltConf
17	i	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	k	1	Total C 40 40	0
17	k	1	Total C 40 40	0
17	k	1	Total C 40 40	0
17	k	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	m	1	Total C 40 40	0
17	m	1	Total C 40 40	0
17	m	1	Total C 40 40	0
17	m	1	Total C 40 40	0
17	n	1	Total C 40 40	0
17	n	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	n	1	Total C 40 40	0
17	n	1	Total C 40 40	0
17	o	1	Total C 40 40	0
17	o	1	Total C 40 40	0
17	o	1	Total C 40 40	0
17	o	1	Total C 40 40	0
17	p	1	Total C 40 40	0
17	p	1	Total C 40 40	0
17	p	1	Total C 40 40	0
17	p	1	Total C 40 40	0
17	q	1	Total C 40 40	0
17	q	1	Total C 40 40	0
17	q	1	Total C 40 40	0
17	q	1	Total C 40 40	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



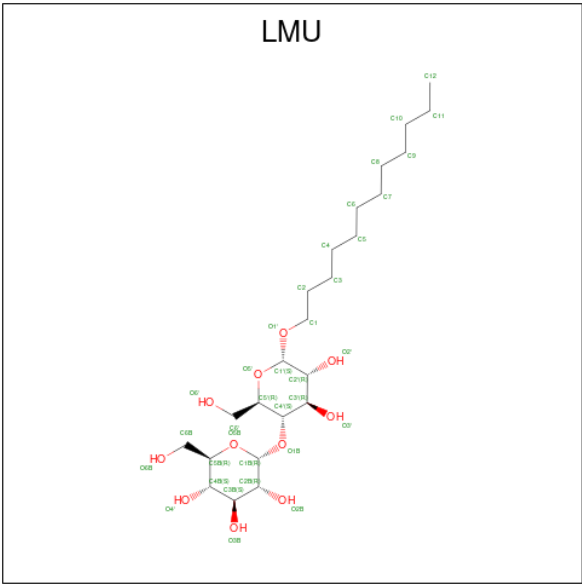
Mol	Chain	Residues	Atoms				AltConf
18	aA	1	Total	C	O	P	0
			48	37	10	1	
18	aA	1	Total	C	O	P	0
			41	30	10	1	
18	aA	1	Total	C	O	P	0
			41	30	10	1	
18	aA	1	Total	C	O	P	0
			33	22	10	1	
18	aA	1	Total	C	O	P	0
			45	34	10	1	
18	aX	1	Total	C	O	P	0
			39	28	10	1	
18	bA	1	Total	C	O	P	0
			49	38	10	1	
18	bA	1	Total	C	O	P	0
			42	31	10	1	
18	bA	1	Total	C	O	P	0
			41	30	10	1	
18	bA	1	Total	C	O	P	0
			39	28	10	1	
18	bA	1	Total	C	O	P	0
			39	28	10	1	
18	bX	1	Total	C	O	P	0
			39	28	10	1	
18	cA	1	Total	C	O	P	0
			48	37	10	1	
18	cA	1	Total	C	O	P	0
			42	31	10	1	

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Mol	Chain	Residues	Atoms				AltConf
18	cA	1	Total	C	O	P	0
			41	30	10	1	
18	cA	1	Total	C	O	P	0
			31	20	10	1	
18	cA	1	Total	C	O	P	0
			44	33	10	1	
18	cX	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 19 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



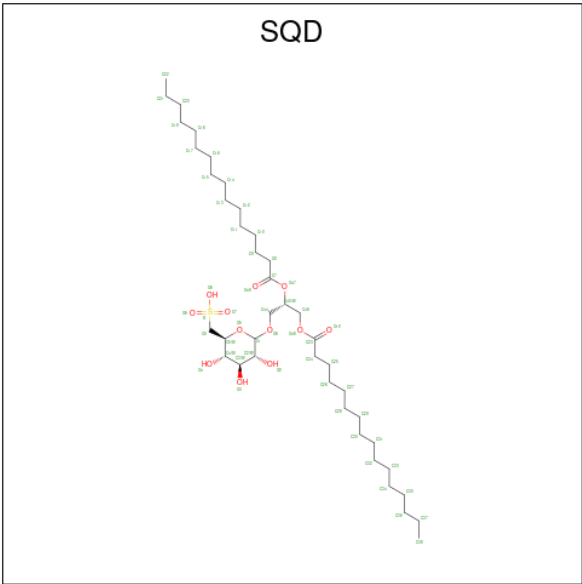
Mol	Chain	Residues	Atoms			AltConf
19	aA	1	Total	C	O	0
			24	18	6	
19	aA	1	Total	C	O	0
			23	17	6	
19	aB	1	Total	C	O	0
			35	24	11	
19	aJ	1	Total	C	O	0
			22	16	6	
19	bA	1	Total	C	O	0
			24	18	6	
19	bA	1	Total	C	O	0
			23	17	6	
19	bB	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
19	bJ	1	Total	C	O	0
			22	16	6	
19	cA	1	Total	C	O	0
			24	18	6	
19	cA	1	Total	C	O	0
			23	17	6	
19	cB	1	Total	C	O	0
			35	24	11	
19	cJ	1	Total	C	O	0
			21	15	6	

- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				AltConf
20	aB	1	Total	C	O	S	0
			42	29	12	1	
20	a1	1	Total	C	O	S	0
			31	18	12	1	
20	a2	1	Total	C	O	S	0
			33	20	12	1	
20	a3	1	Total	C	O	S	0
			38	25	12	1	
20	a4	1	Total	C	O	S	0
			36	23	12	1	
20	a5	1	Total	C	O	S	0
			33	20	12	1	

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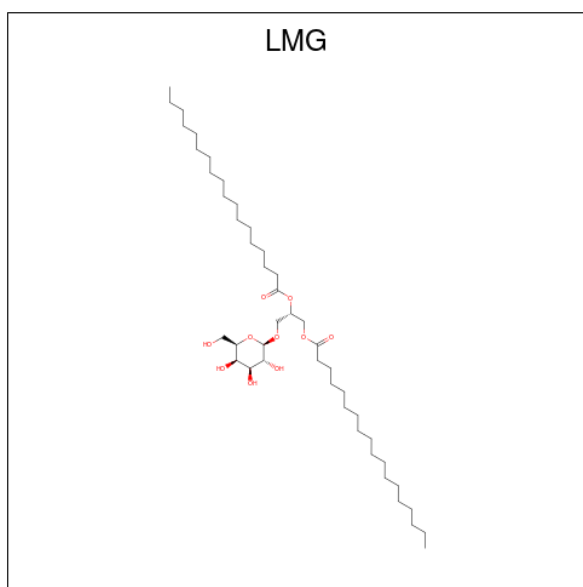
Mol	Chain	Residues	Atoms				AltConf
20	a6	1	Total 31	C 18	O 12	S 1	0
20	bB	1	Total 42	C 29	O 12	S 1	0
20	b1	1	Total 31	C 18	O 12	S 1	0
20	b2	1	Total 32	C 19	O 12	S 1	0
20	b3	1	Total 37	C 24	O 12	S 1	0
20	b4	1	Total 33	C 20	O 12	S 1	0
20	b5	1	Total 30	C 17	O 12	S 1	0
20	b6	1	Total 30	C 17	O 12	S 1	0
20	cB	1	Total 39	C 26	O 12	S 1	0
20	c1	1	Total 31	C 18	O 12	S 1	0
20	c2	1	Total 31	C 18	O 12	S 1	0
20	c3	1	Total 32	C 19	O 12	S 1	0
20	c4	1	Total 33	C 20	O 12	S 1	0
20	c5	1	Total 31	C 18	O 12	S 1	0
20	c6	1	Total 30	C 17	O 12	S 1	0
20	S	1	Total 31	C 18	O 12	S 1	0
20	T	1	Total 31	C 18	O 12	S 1	0
20	V	1	Total 31	C 18	O 12	S 1	0
20	W	1	Total 32	C 19	O 12	S 1	0
20	X	1	Total 36	C 23	O 12	S 1	0
20	Y	1	Total 33	C 20	O 12	S 1	0

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Mol	Chain	Residues	Atoms				AltConf
20	Z	1	Total	C	O	S	0
			29	16	12	1	
20	b	1	Total	C	O	S	0
			31	18	12	1	
20	c	1	Total	C	O	S	0
			31	18	12	1	
20	d	1	Total	C	O	S	0
			31	18	12	1	
20	e	1	Total	C	O	S	0
			32	19	12	1	
20	f	1	Total	C	O	S	0
			30	17	12	1	
20	g	1	Total	C	O	S	0
			30	17	12	1	
20	h	1	Total	C	O	S	0
			32	19	12	1	
20	i	1	Total	C	O	S	0
			30	17	12	1	
20	m	1	Total	C	O	S	0
			29	16	12	1	
20	n	1	Total	C	O	S	0
			31	18	12	1	
20	p	1	Total	C	O	S	0
			31	18	12	1	
20	q	1	Total	C	O	S	0
			26	13	12	1	

- Molecule 21 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
21	aB	1	Total	C	O	0
			49	39	10	
21	aJ	1	Total	C	O	0
			31	21	10	
21	a1	1	Total	C	O	0
			40	30	10	
21	a2	1	Total	C	O	0
			40	30	10	
21	a6	1	Total	C	O	0
			38	28	10	
21	bB	1	Total	C	O	0
			49	39	10	
21	bJ	1	Total	C	O	0
			29	19	10	
21	b1	1	Total	C	O	0
			35	25	10	
21	b2	1	Total	C	O	0
			40	30	10	
21	cB	1	Total	C	O	0
			49	39	10	
21	cJ	1	Total	C	O	0
			31	21	10	
21	c1	1	Total	C	O	0
			39	29	10	

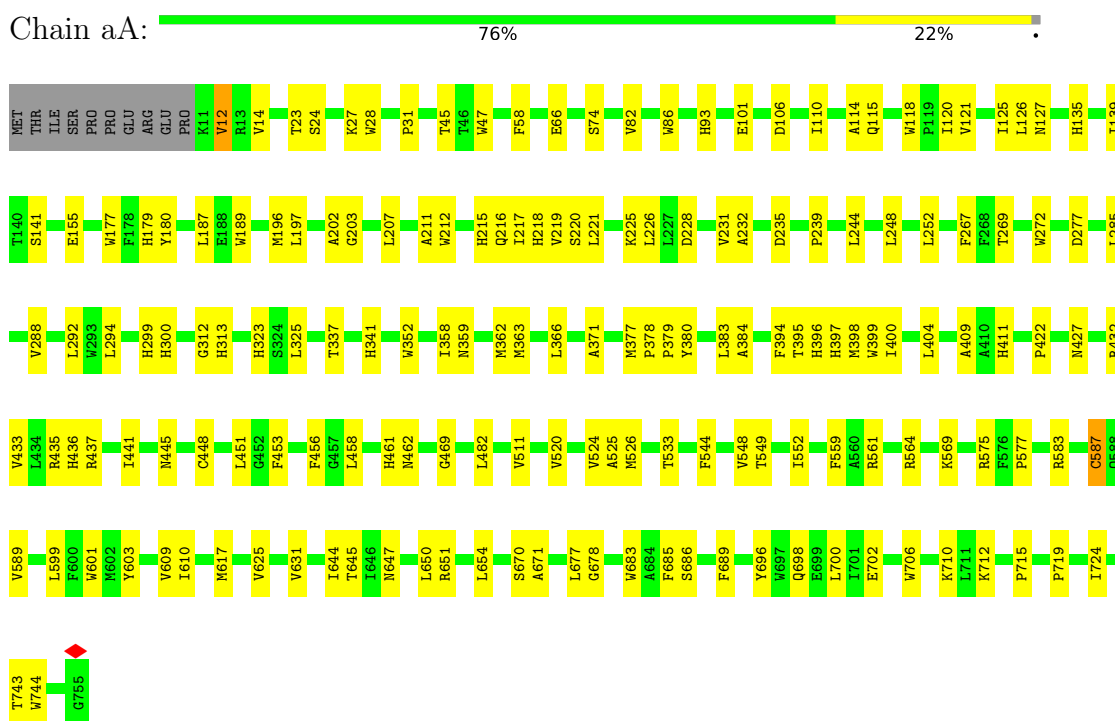
- Molecule 22 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
22	aL	1	Total 1	Ca 1	0
22	bL	1	Total 1	Ca 1	0
22	cL	1	Total 1	Ca 1	0

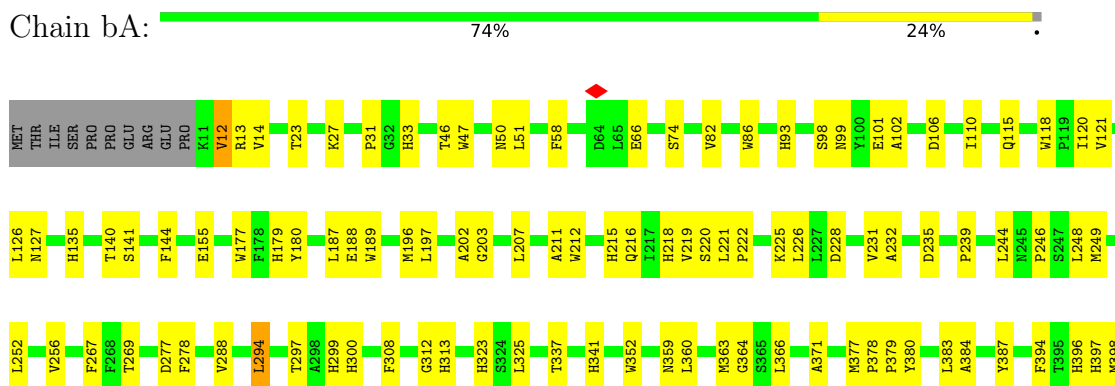
3 Residue-property plots

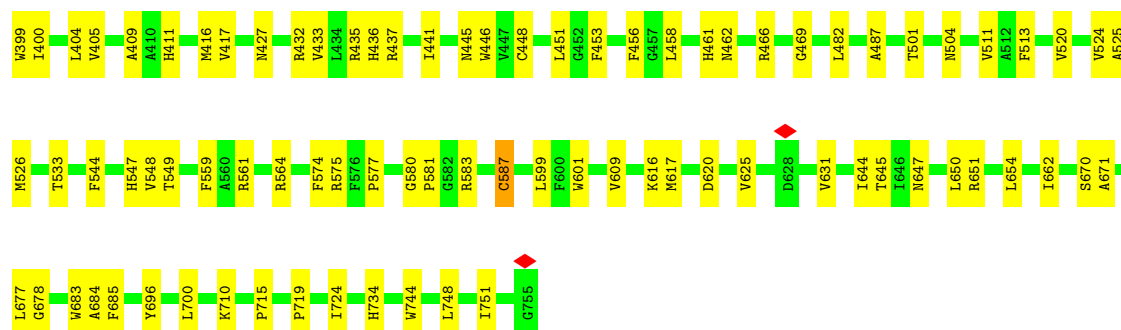
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

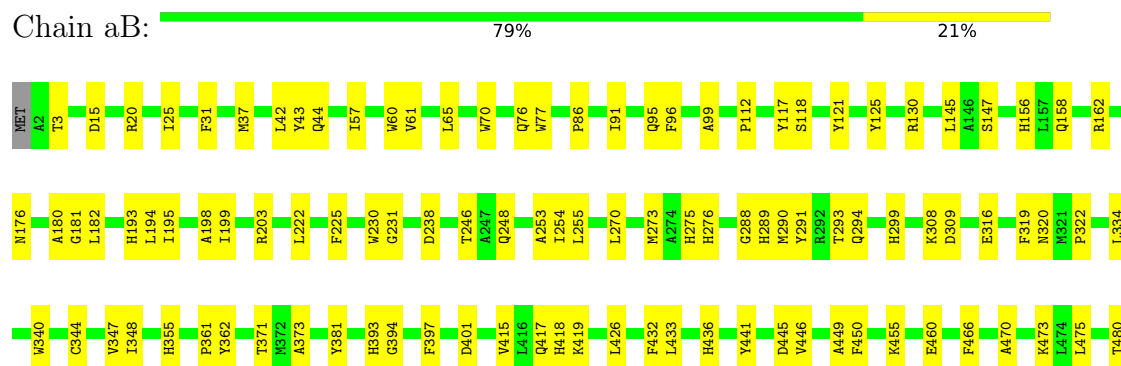


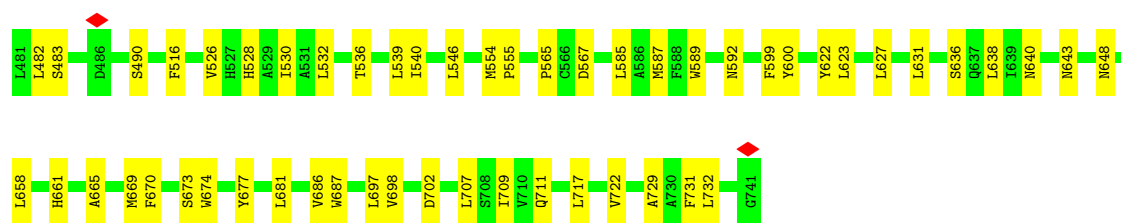


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



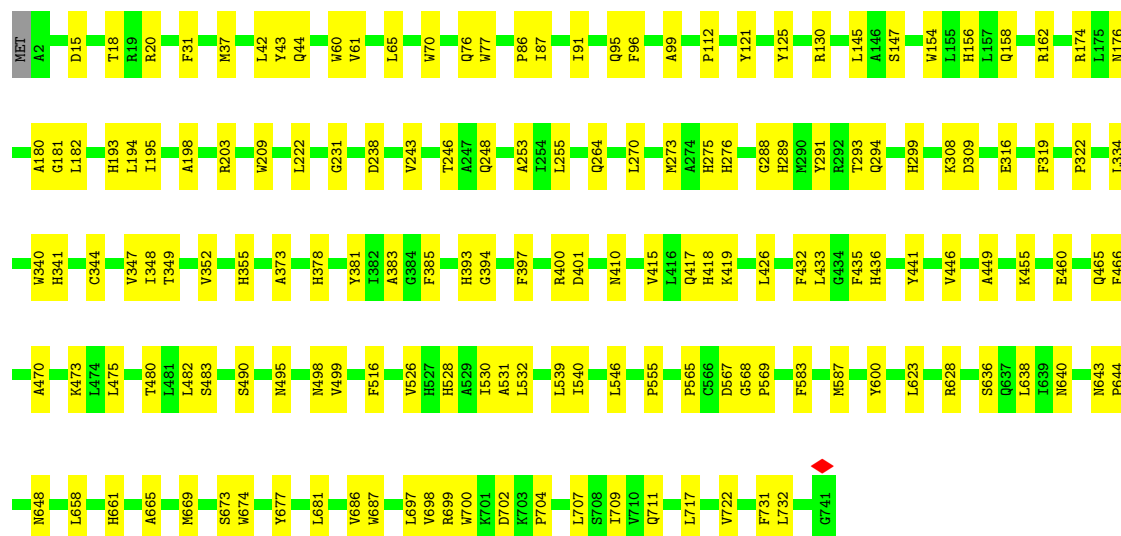
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





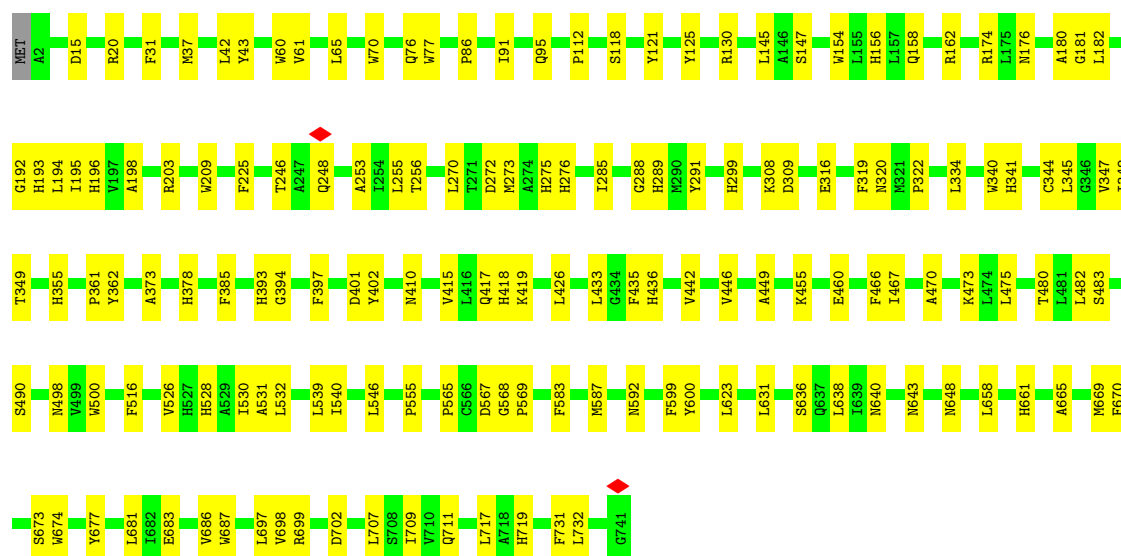
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain bB: 78% 21%



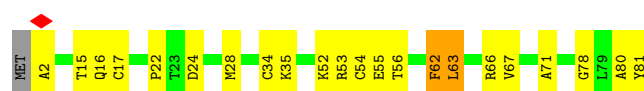
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain cB: 79% 21%




• Molecule 3: Photosystem I iron-sulfur center

Chain aC:  72% 25% ..




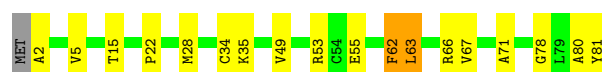
- Molecule 3: Photosystem I iron-sulfur center

Chain bC:  78% 19% ..




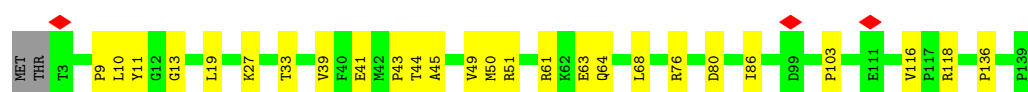
- Molecule 3: Photosystem I iron-sulfur center

Chain cC:  77% 20% ..




- Molecule 4: Photosystem I reaction center subunit II

Chain aD:  80% 19% .




- Molecule 4: Photosystem I reaction center subunit II

Chain bD:  75% 24% .



- Molecule 4: Photosystem I reaction center subunit II

Chain cD:  81% 18% .

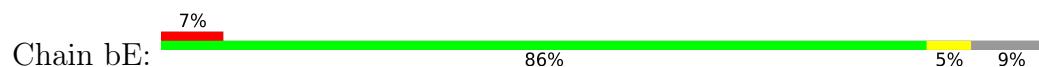


- Molecule 5: Photosystem I reaction center subunit IV

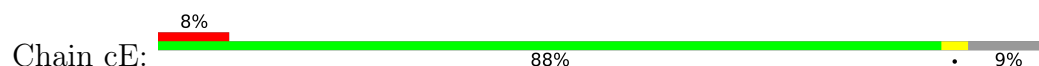
Chain aE:  74% 17% 9%



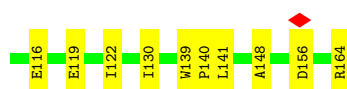
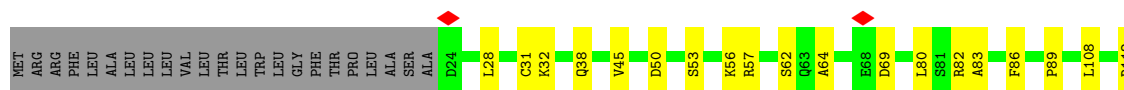
- Molecule 5: Photosystem I reaction center subunit IV



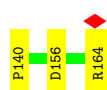
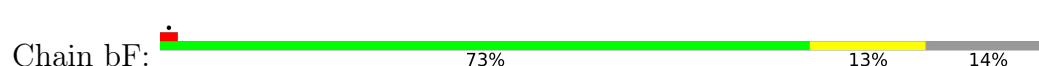
- Molecule 5: Photosystem I reaction center subunit IV



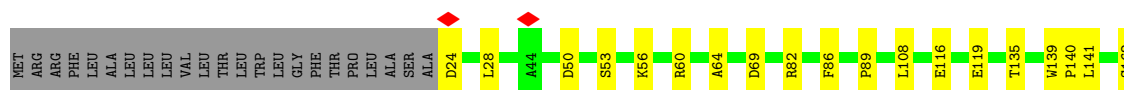
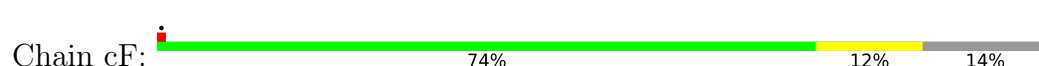
- Molecule 6: Photosystem I reaction center subunit III



- Molecule 6: Photosystem I reaction center subunit III



- Molecule 6: Photosystem I reaction center subunit III





- Molecule 7: Photosystem I reaction center subunit VIII

Chain aI: 92% 8%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain bI: 92% 8%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain cI: 92% 8%



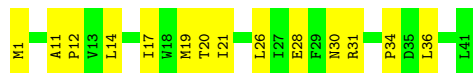
- Molecule 8: Photosystem I reaction center subunit IX

Chain aJ: 66% 34%



- Molecule 8: Photosystem I reaction center subunit IX

Chain bJ: 66% 34%



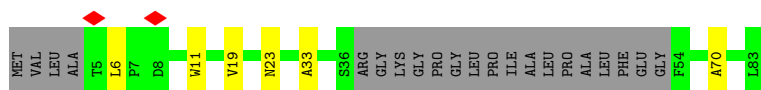
- Molecule 8: Photosystem I reaction center subunit IX

Chain cJ: 68% 32%

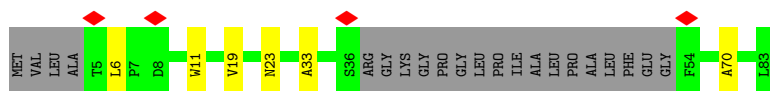


- Molecule 9: Photosystem I reaction center subunit Psak

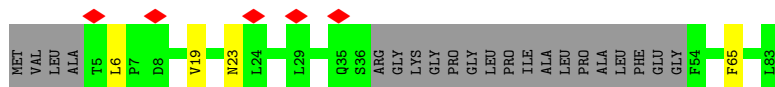
Chain aK: 67% 7% 25%



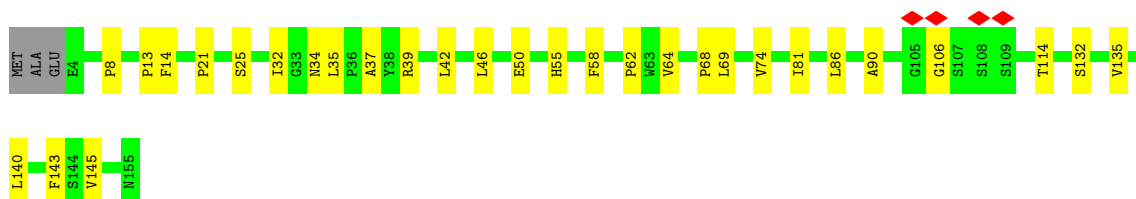
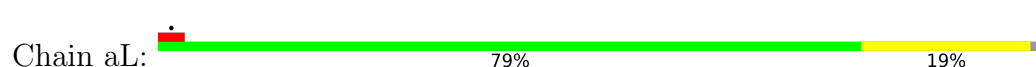
- Molecule 9: Photosystem I reaction center subunit PsaK



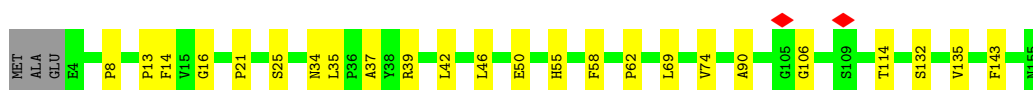
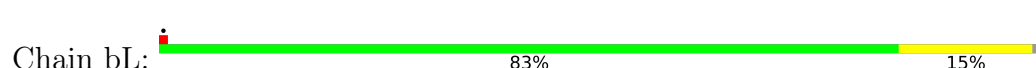
- Molecule 9: Photosystem I reaction center subunit PsaK



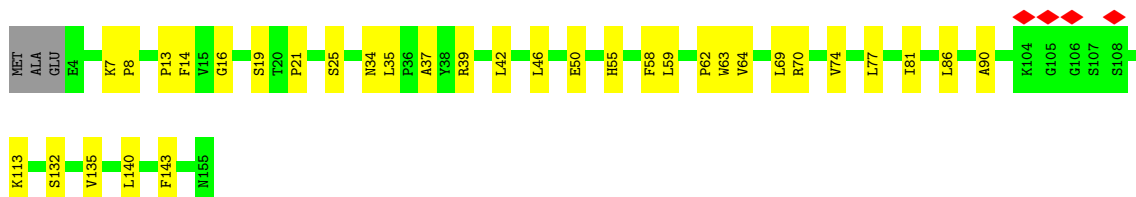
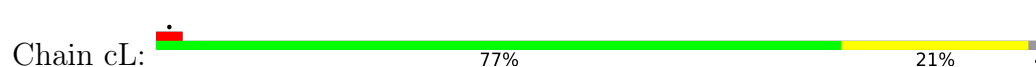
- Molecule 10: Photosystem I reaction center subunit XI




- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XI




- Molecule 11: Photosystem I reaction center subunit XII

Chain aM:  77% 23%




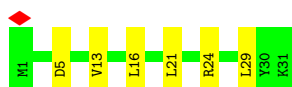
- Molecule 11: Photosystem I reaction center subunit XII

Chain bM:  77% 23%




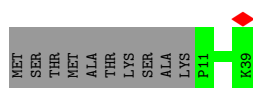
- Molecule 11: Photosystem I reaction center subunit XII

Chain cM:  81% 19%




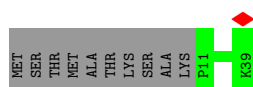
- Molecule 12: Photosystem I 4.8K protein

Chain aX:  74% 26%



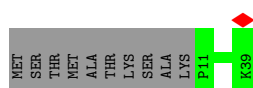
- Molecule 12: Photosystem I 4.8K protein

Chain bX:  74% 26%



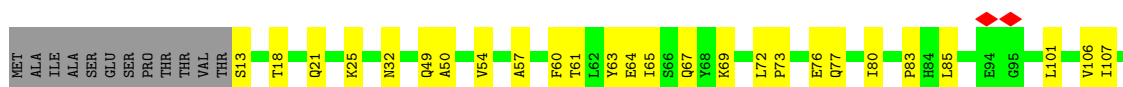
- Molecule 12: Photosystem I 4.8K protein

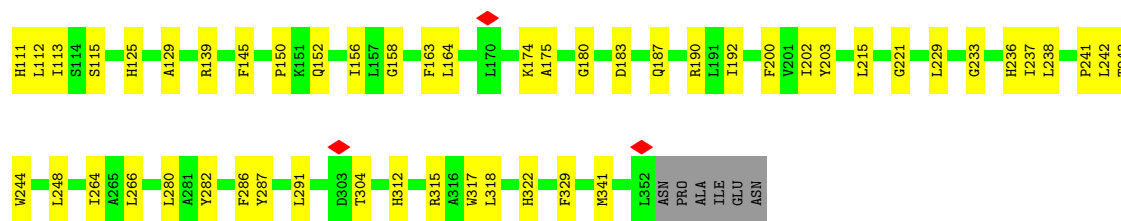
Chain cX:  74% 26%



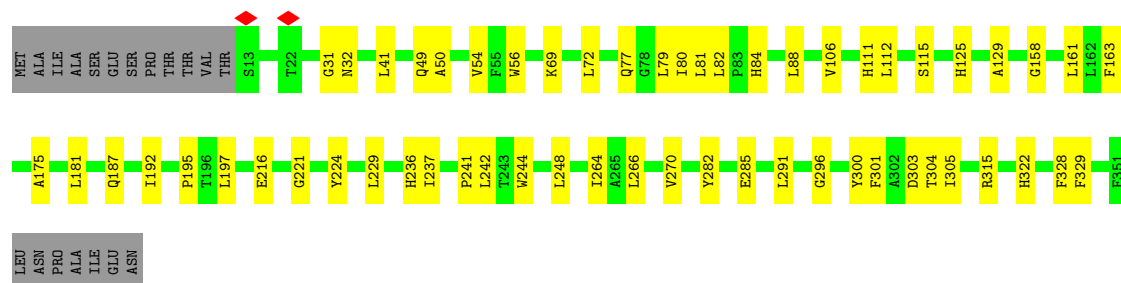
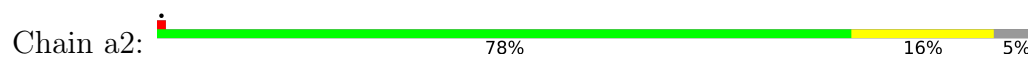
- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain a1:  73% 22% 5%

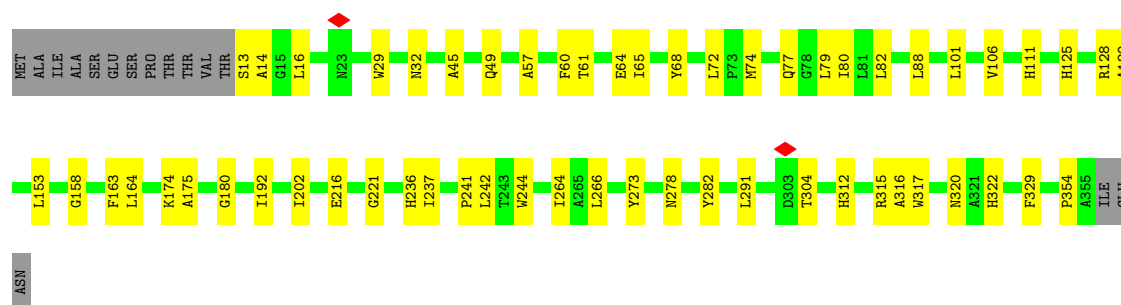
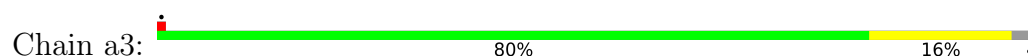




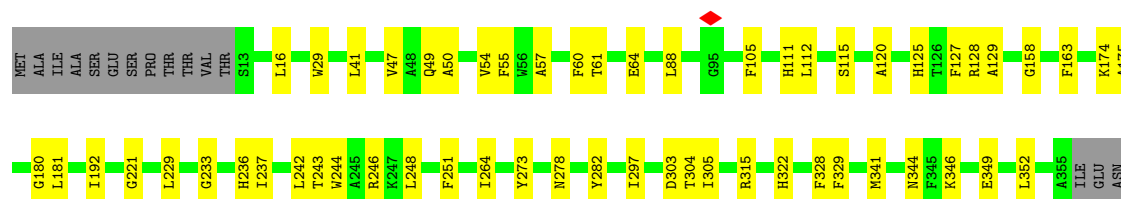
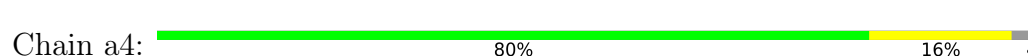
- Molecule 13: Iron stress-induced chlorophyll-binding protein



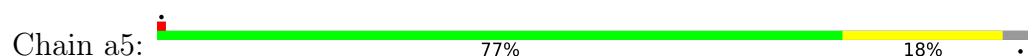
- Molecule 13: Iron stress-induced chlorophyll-binding protein

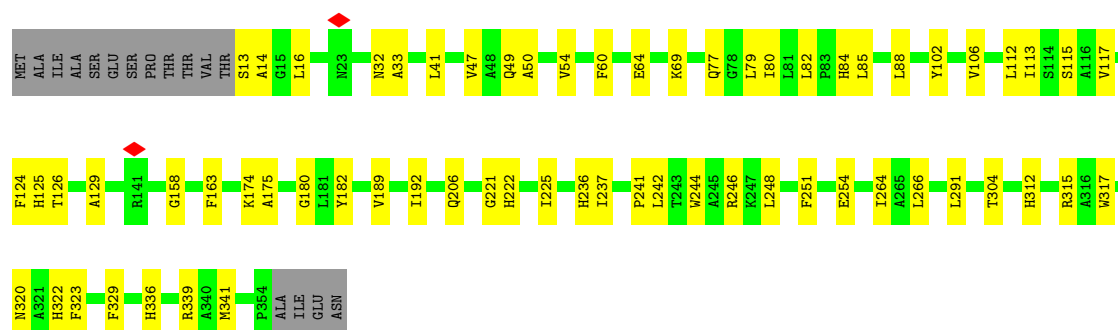


- Molecule 13: Iron stress-induced chlorophyll-binding protein



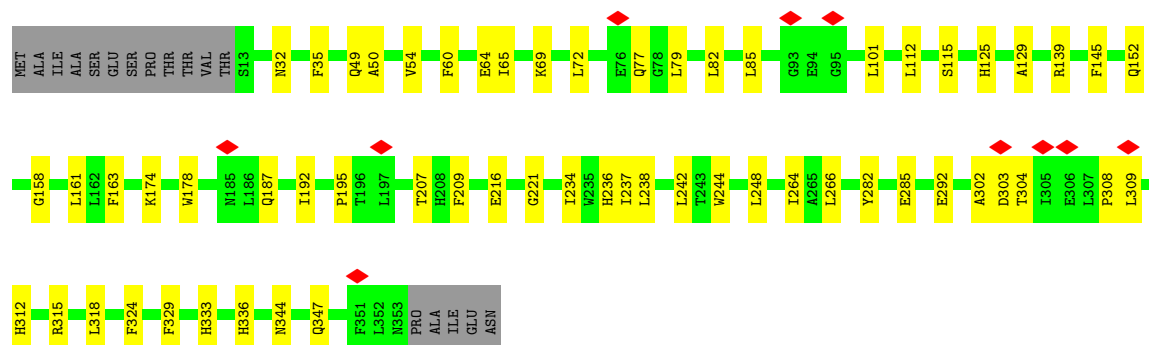
- Molecule 13: Iron stress-induced chlorophyll-binding protein





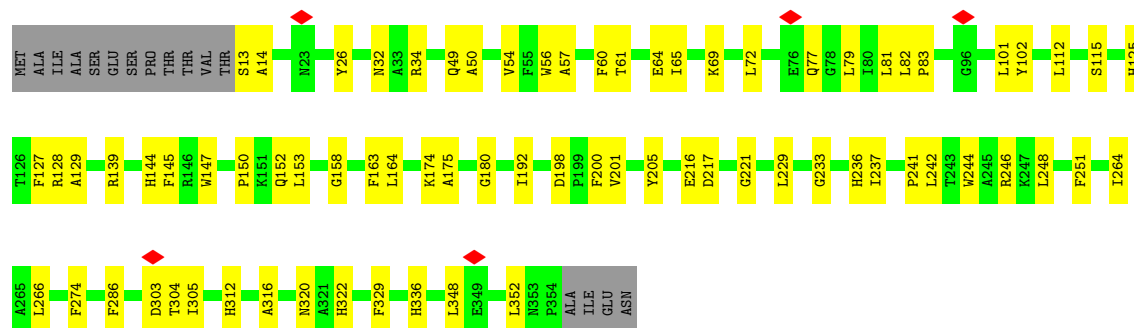
- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain a6: 78% 17% 5%



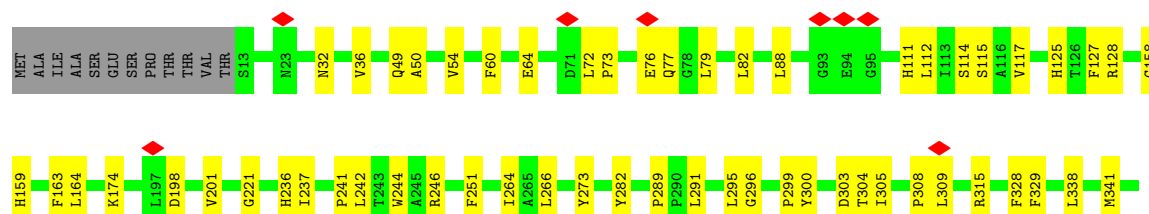
- Molecule 13: Iron stress-induced chlorophyll-binding protein

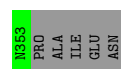
Chain b1: 75% 21% 4%




- Molecule 13: Iron stress-induced chlorophyll-binding protein

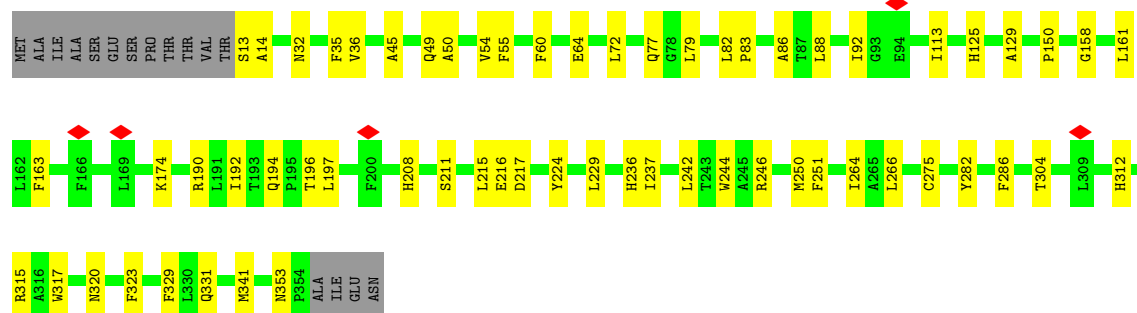
Chain b2: 79% 16% 5%






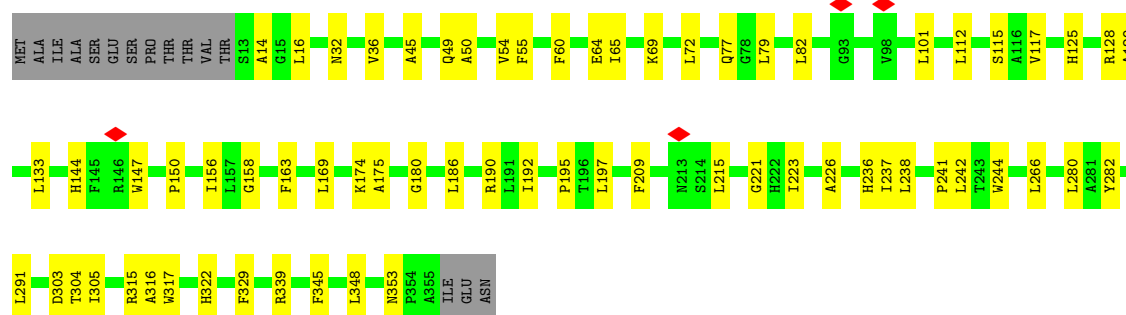
- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain b3:  78% 17%



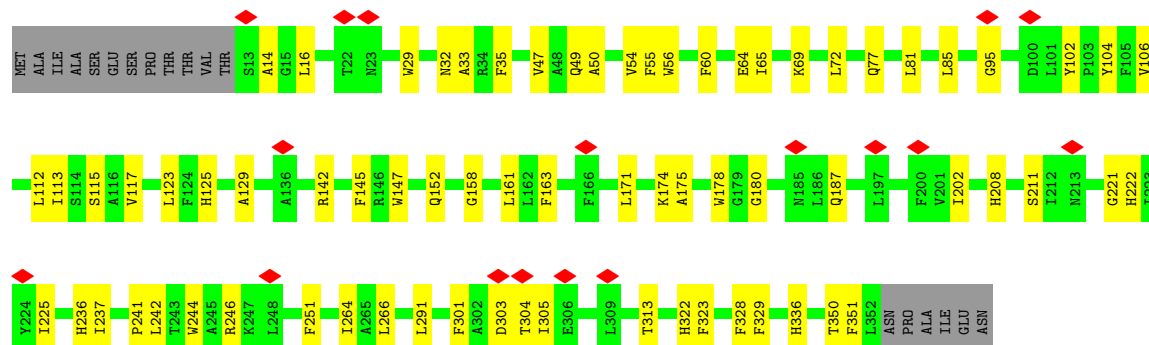
- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain b4:  77% 19%



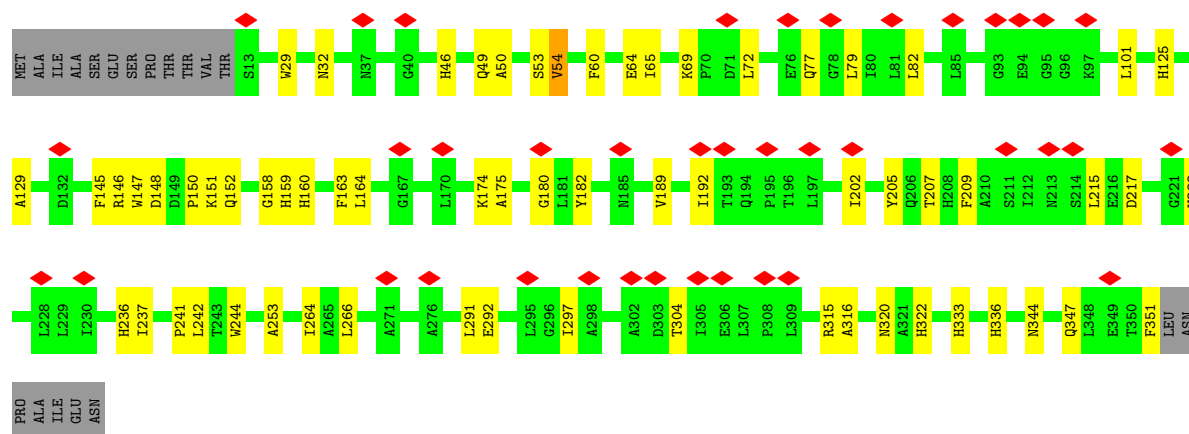
- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain b5:  5% 75% 20% 5%



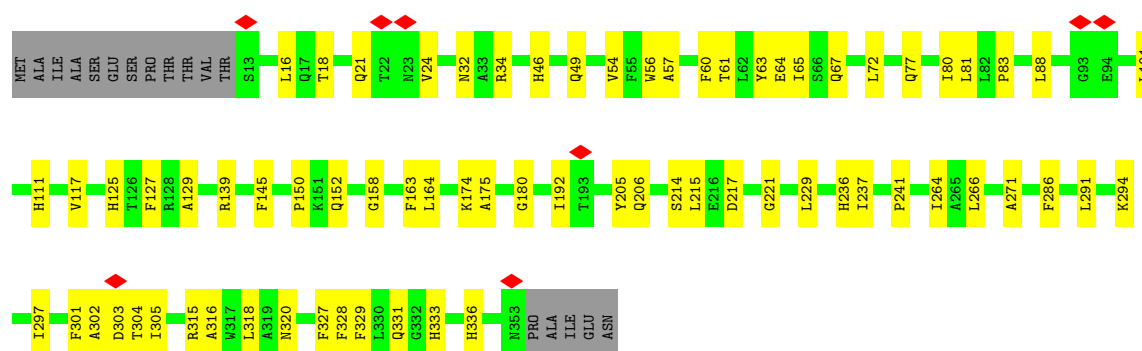
- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain b6:  11% 77% 18% 5%



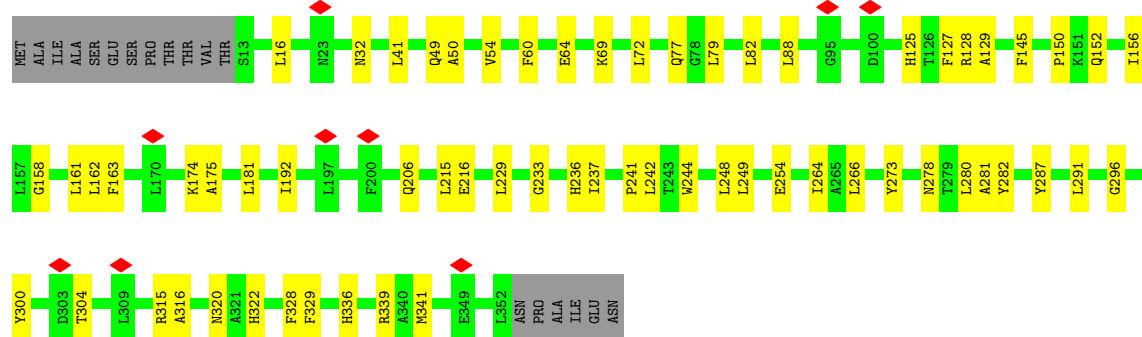
• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain c1: 75% 20% 5%



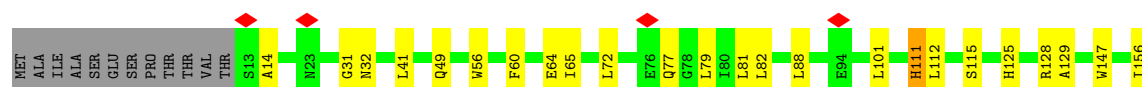
• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain c2: 77% 18% 5%



• Molecule 13: Iron stress-induced chlorophyll-binding protein

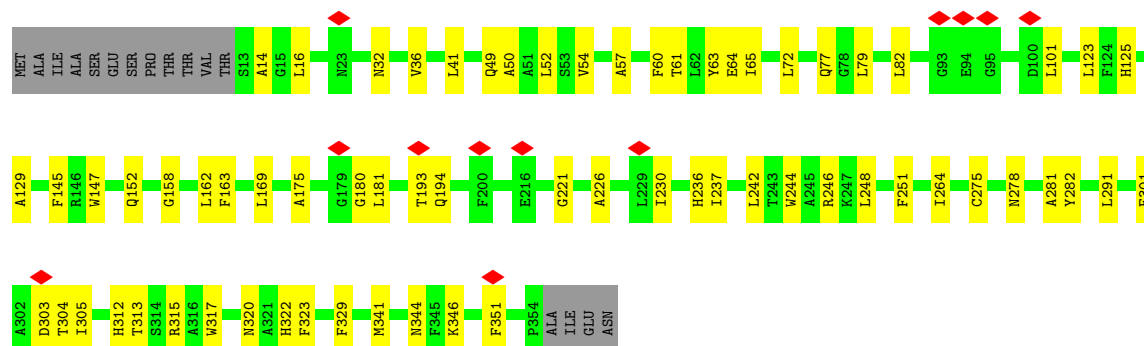
Chain c3: 82% 13% 5%





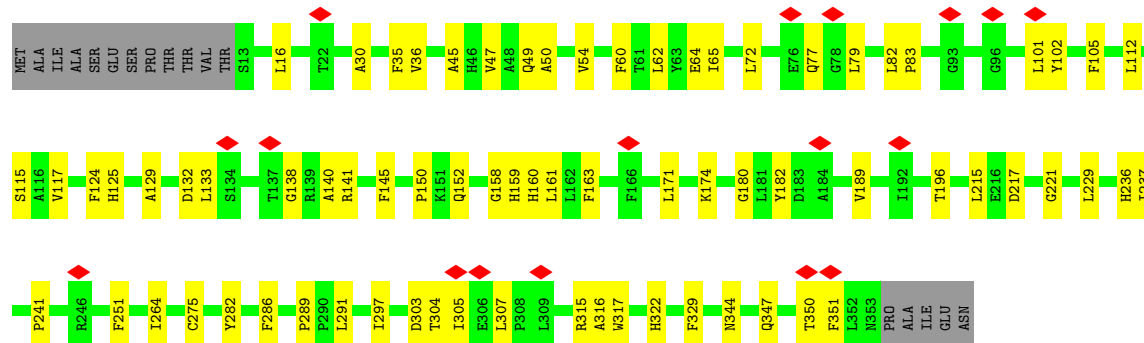
• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain c4: 77% 19%



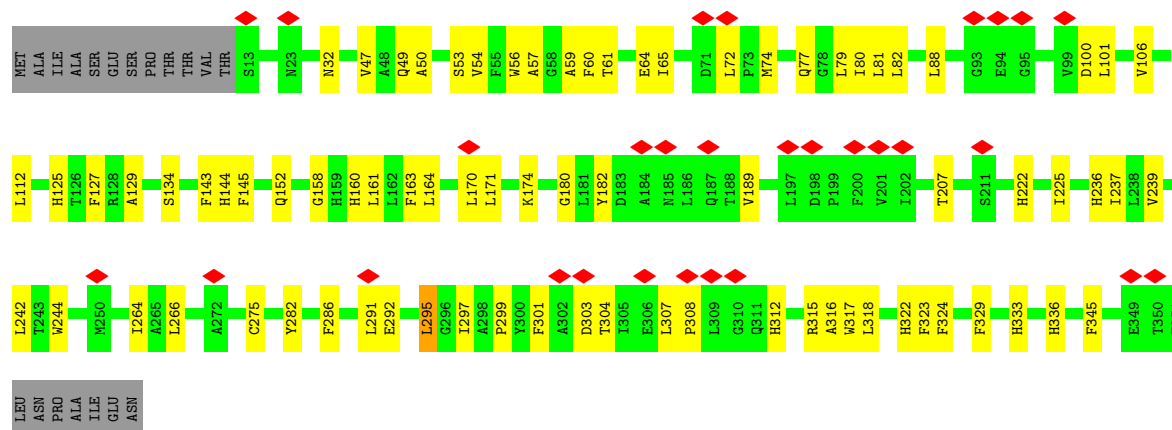
• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain c5: 5% 75% 21% 5%

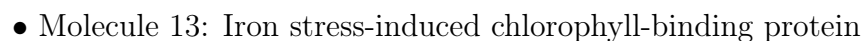


• Molecule 13: Iron stress-induced chlorophyll-binding protein

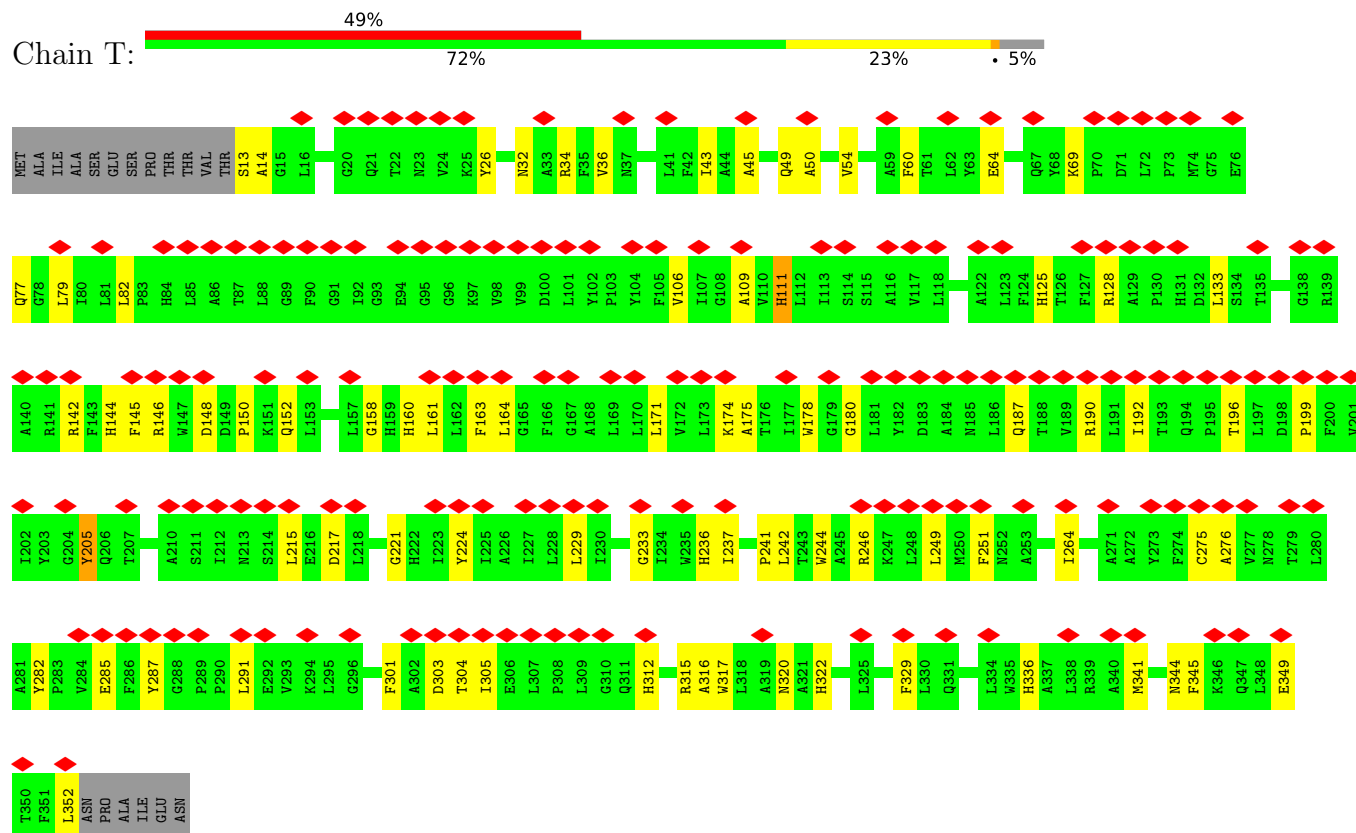
Chain c6: 8% 73% 22% 5%



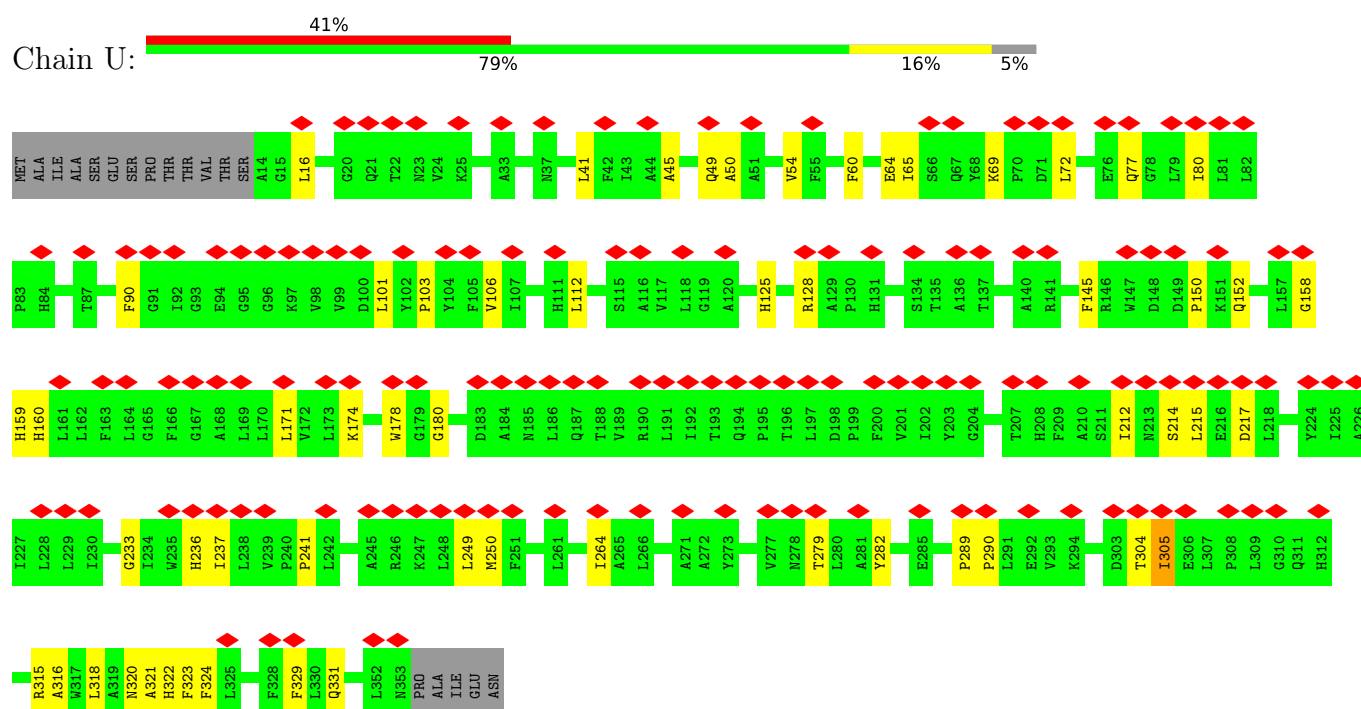
Chain S:



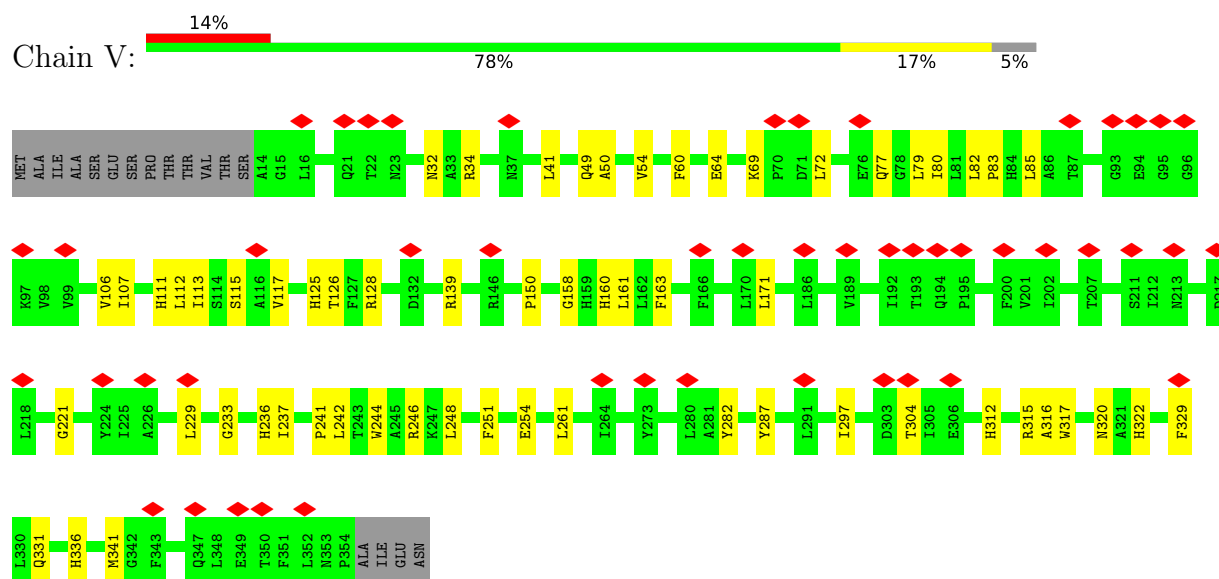
Chain T:



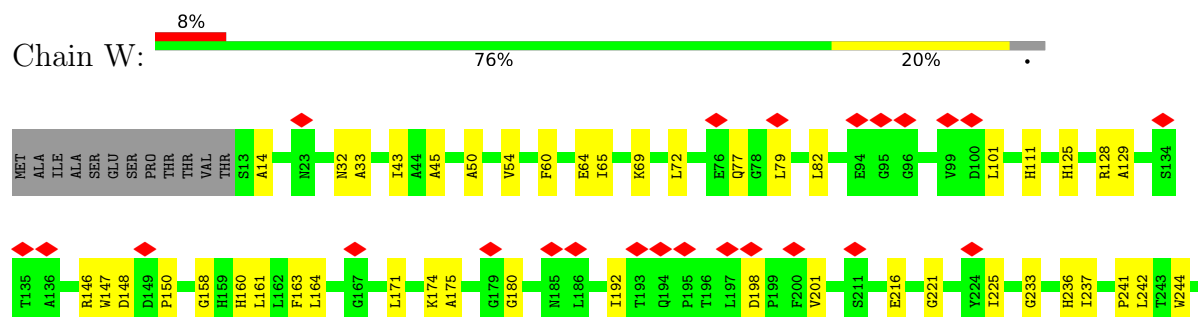
- Molecule 13: Iron stress-induced chlorophyll-binding protein

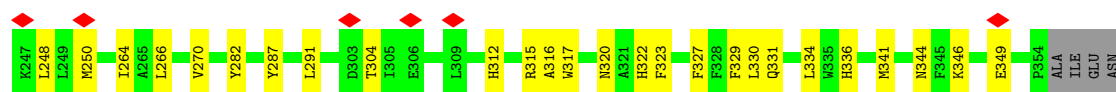


• Molecule 13: Iron stress-induced chlorophyll-binding protein



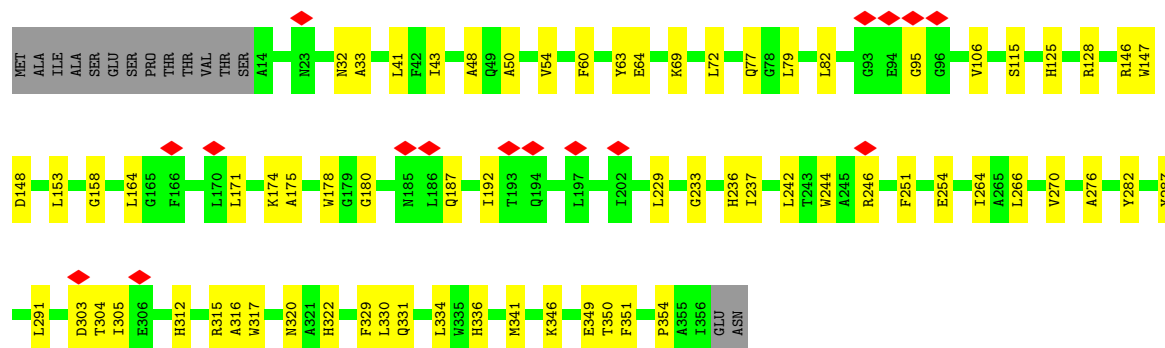
• Molecule 13: Iron stress-induced chlorophyll-binding protein





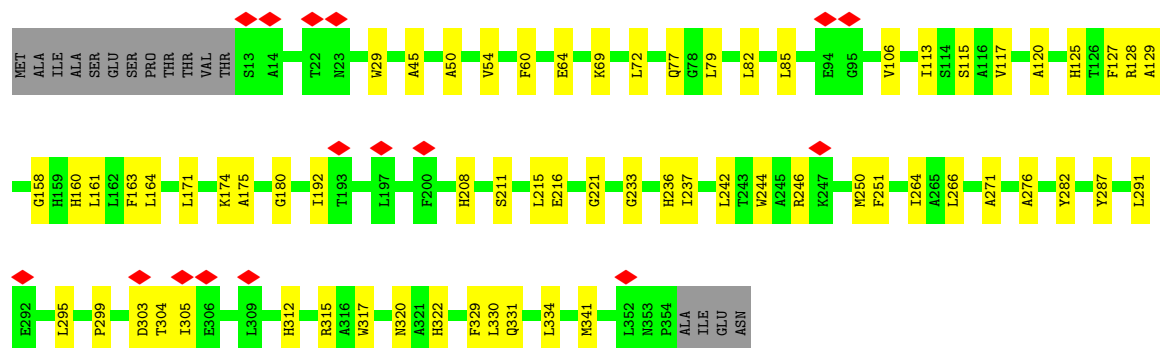
- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain X: 77% 19%



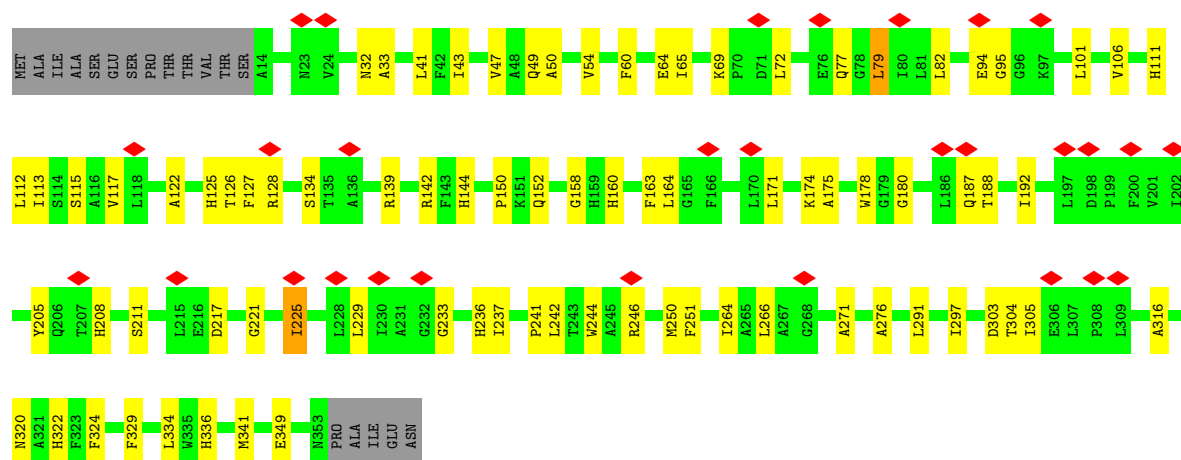
- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain Y: 77% 18%

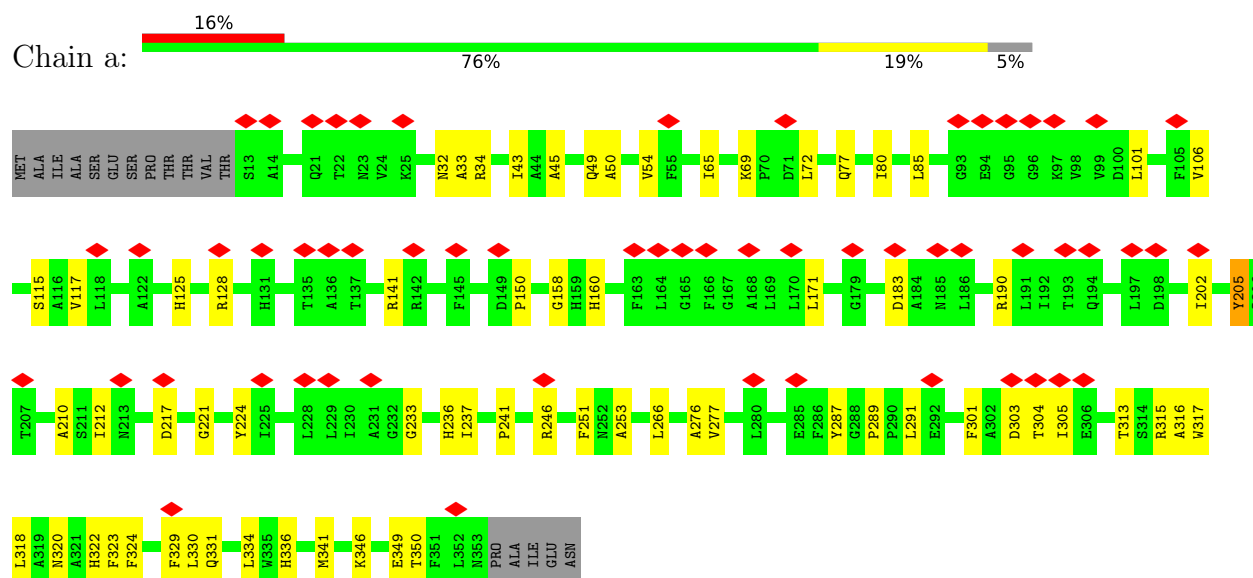


- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain Z: 8% 72% 22% 5%



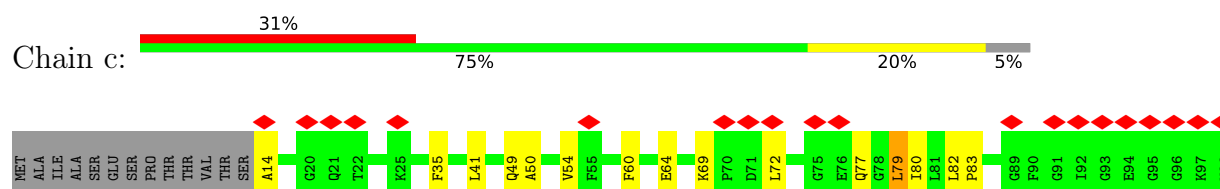
- Molecule 13: Iron stress-induced chlorophyll-binding protein

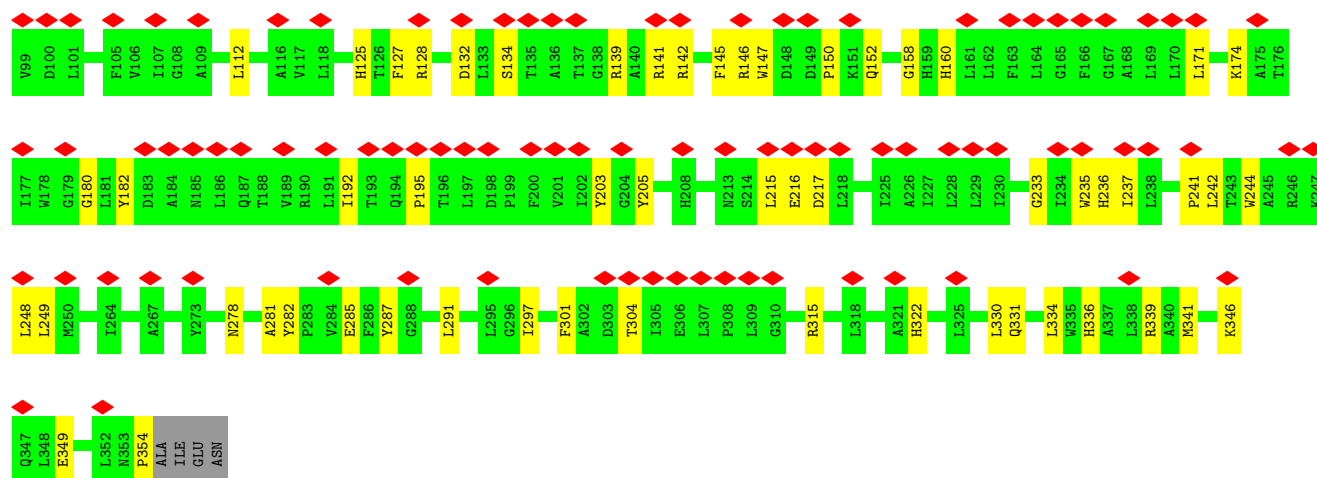


- Molecule 13: Iron stress-induced chlorophyll-binding protein

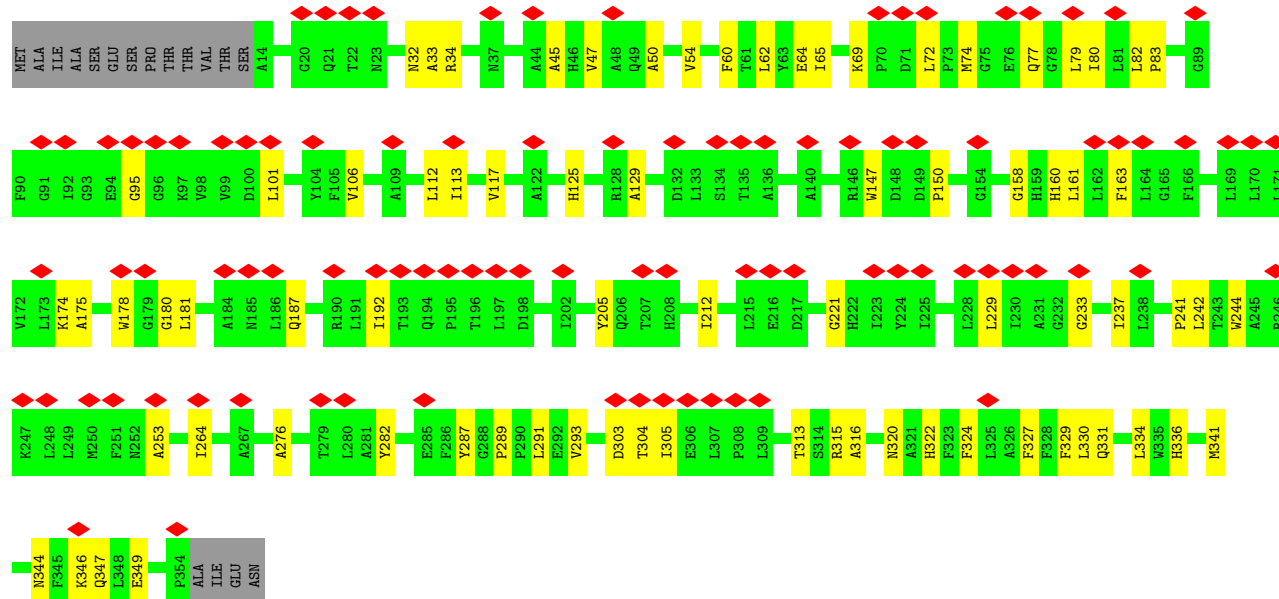
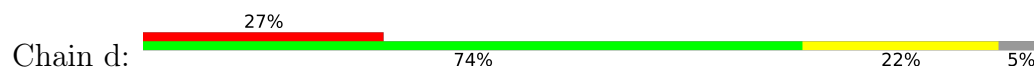


- Molecule 13: Iron stress-induced chlorophyll-binding protein

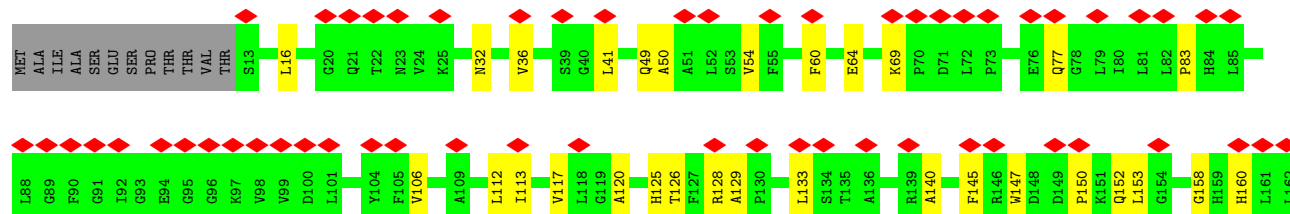
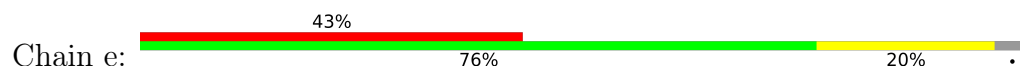


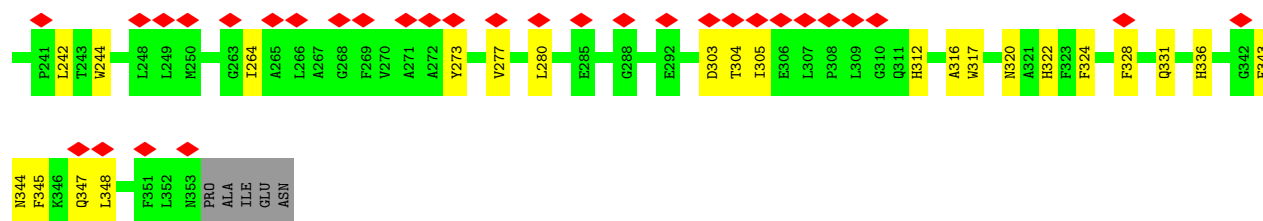


- Molecule 13: Iron stress-induced chlorophyll-binding protein



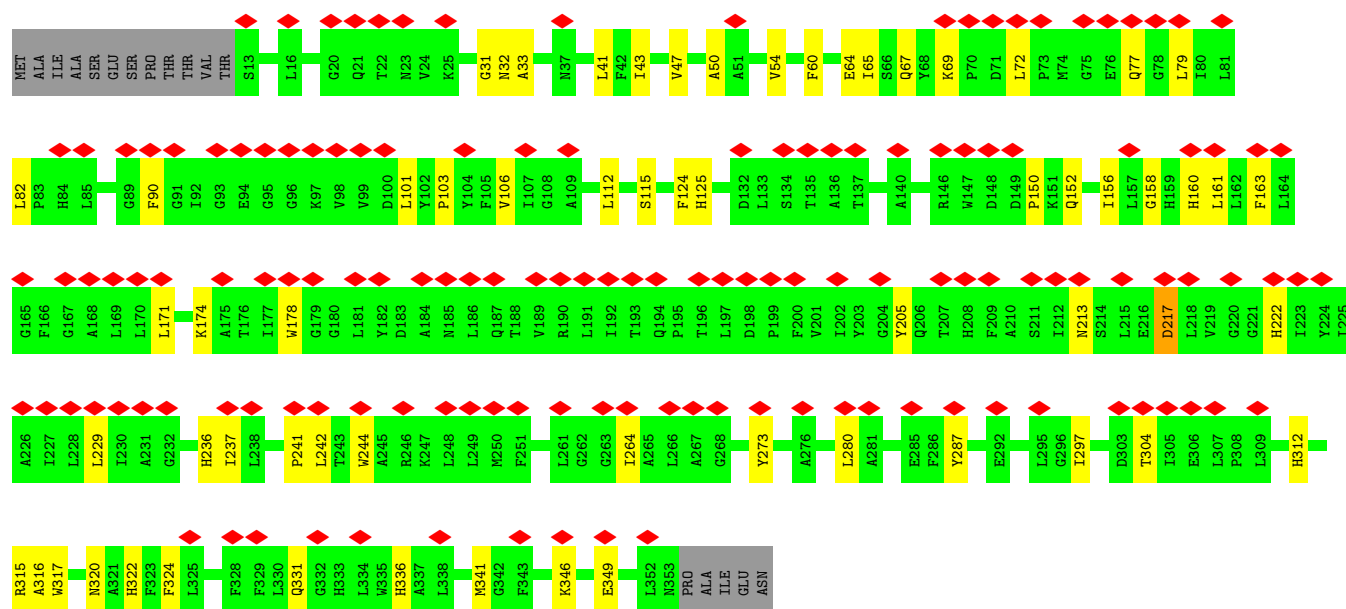
- Molecule 13: Iron stress-induced chlorophyll-binding protein





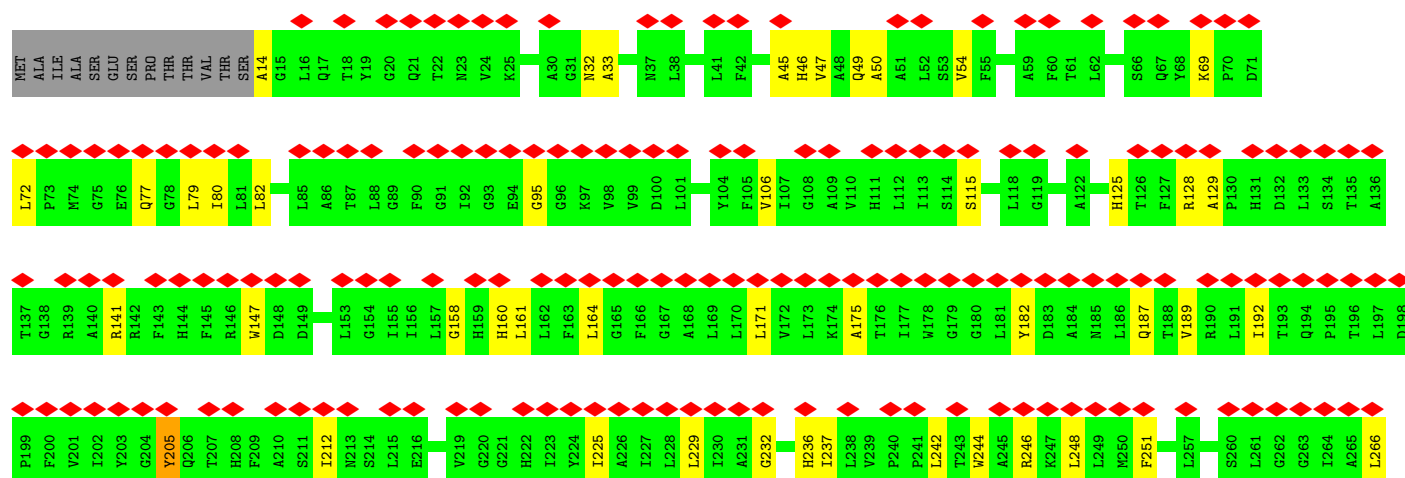
• Molecule 13: Iron stress-induced chlorophyll-binding protein

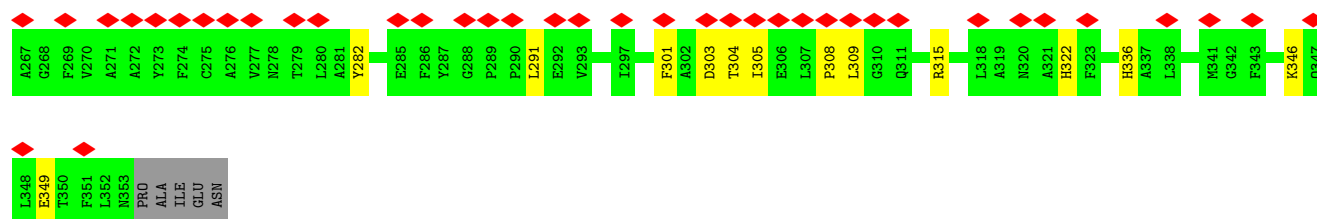
Chain h: 39% 78% 17% 5%



• Molecule 13: Iron stress-induced chlorophyll-binding protein

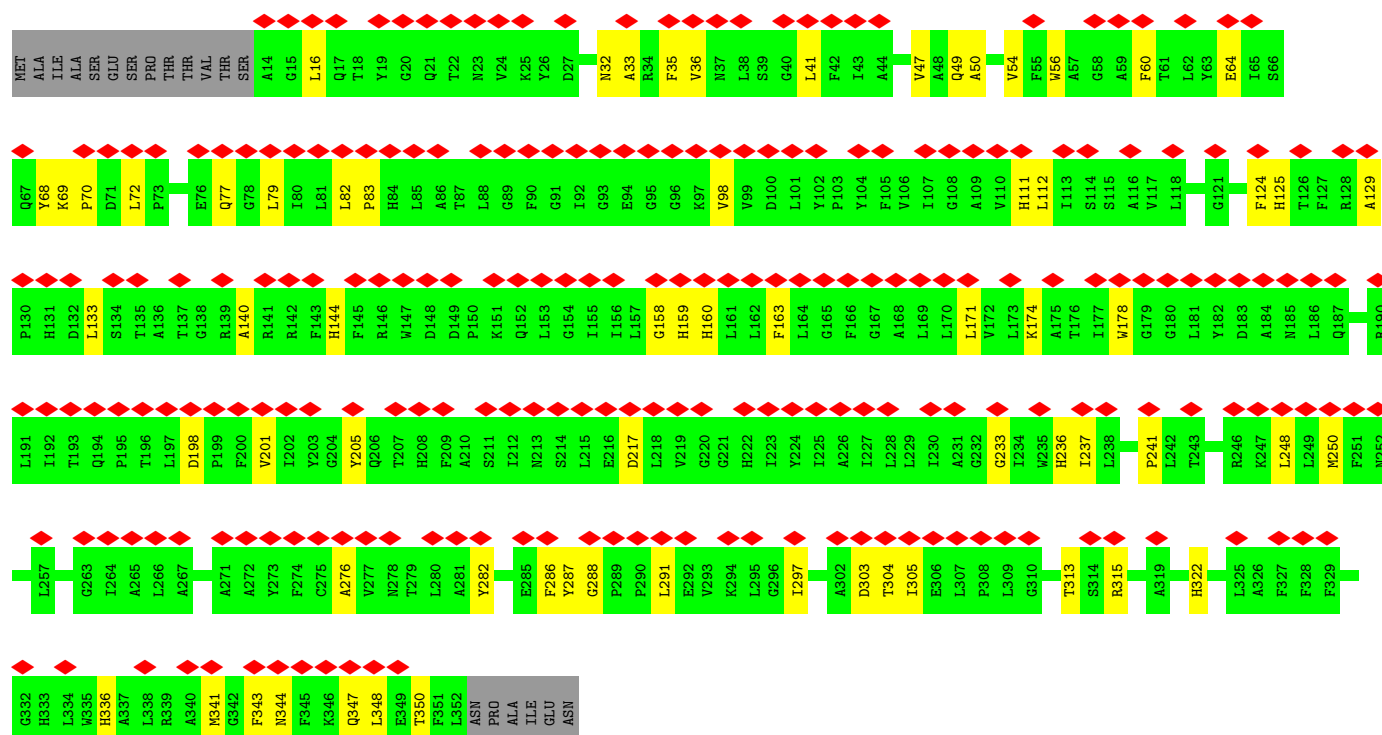
Chain i: 59% 78% 16% 5%





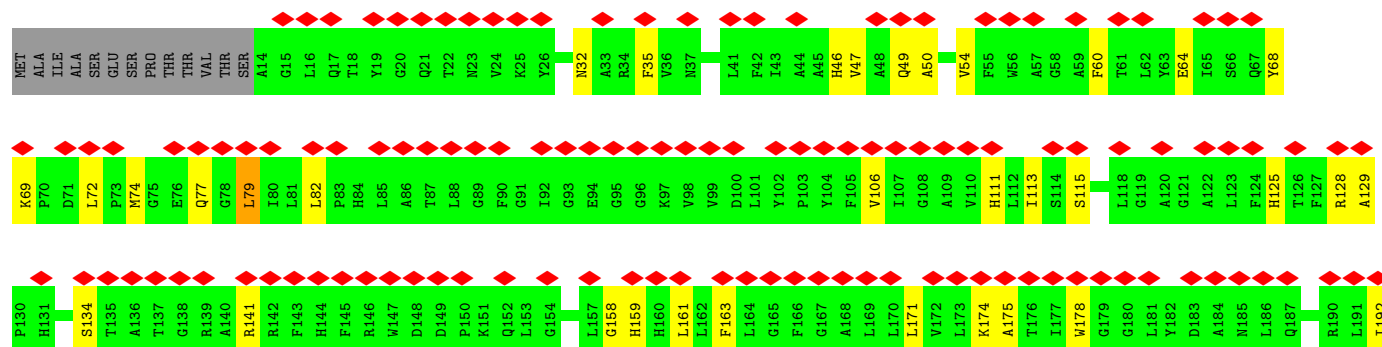
• Molecule 13: Iron stress-induced chlorophyll-binding protein

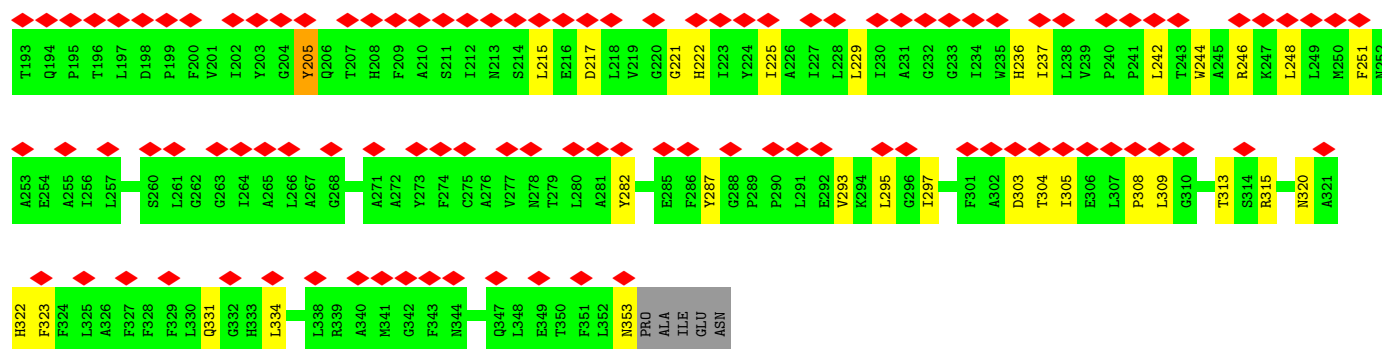
Chain j:



• Molecule 13: Iron stress-induced chlorophyll-binding protein

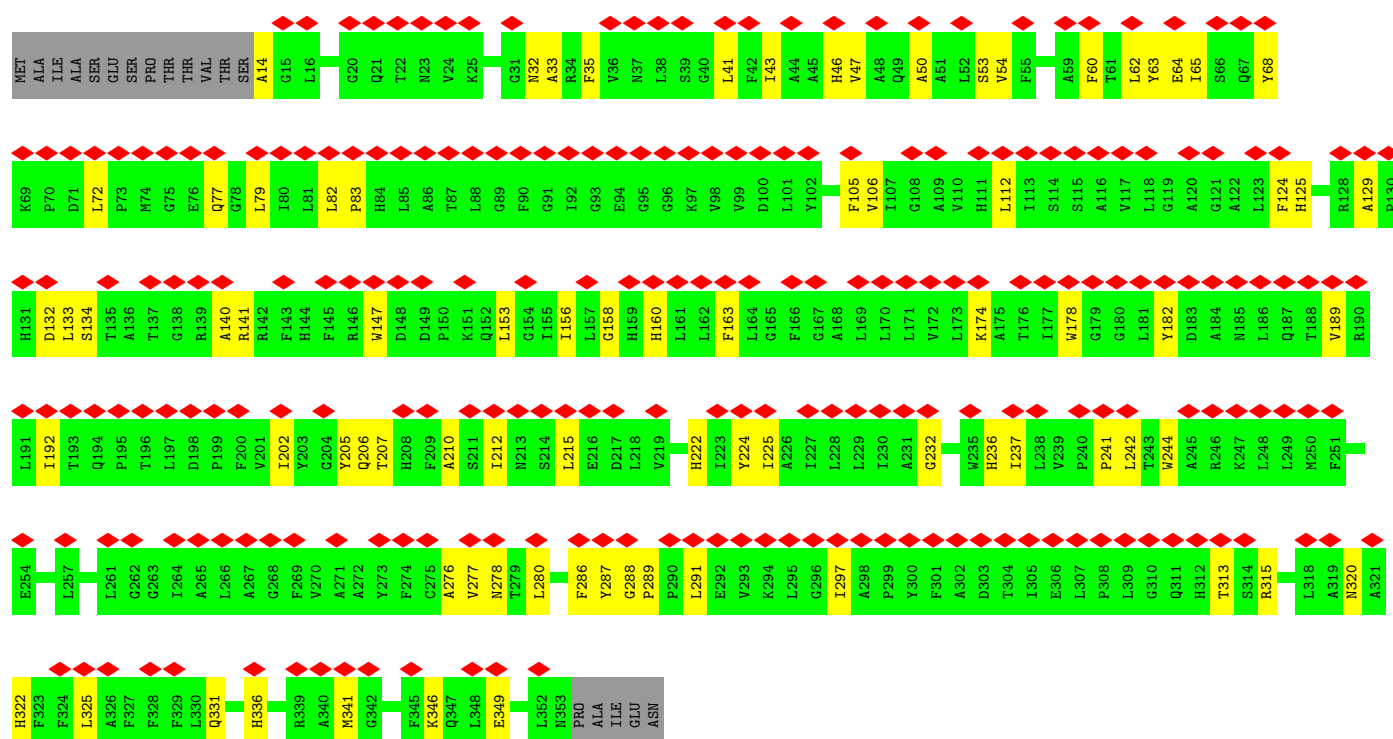
Chain k:





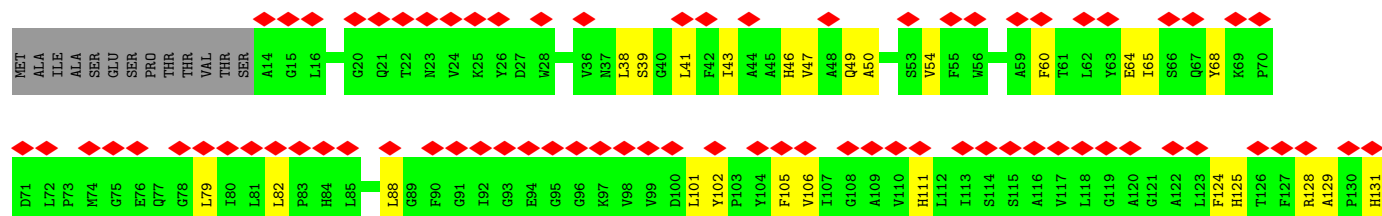
• Molecule 13: Iron stress-induced chlorophyll-binding protein

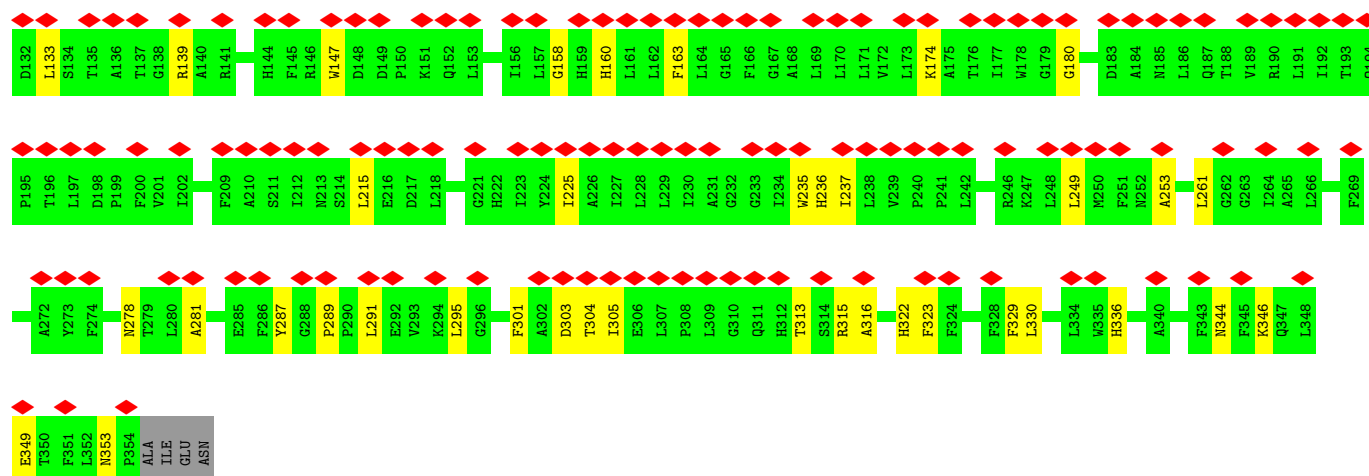
Chain l: 64% 73% 22% 5%



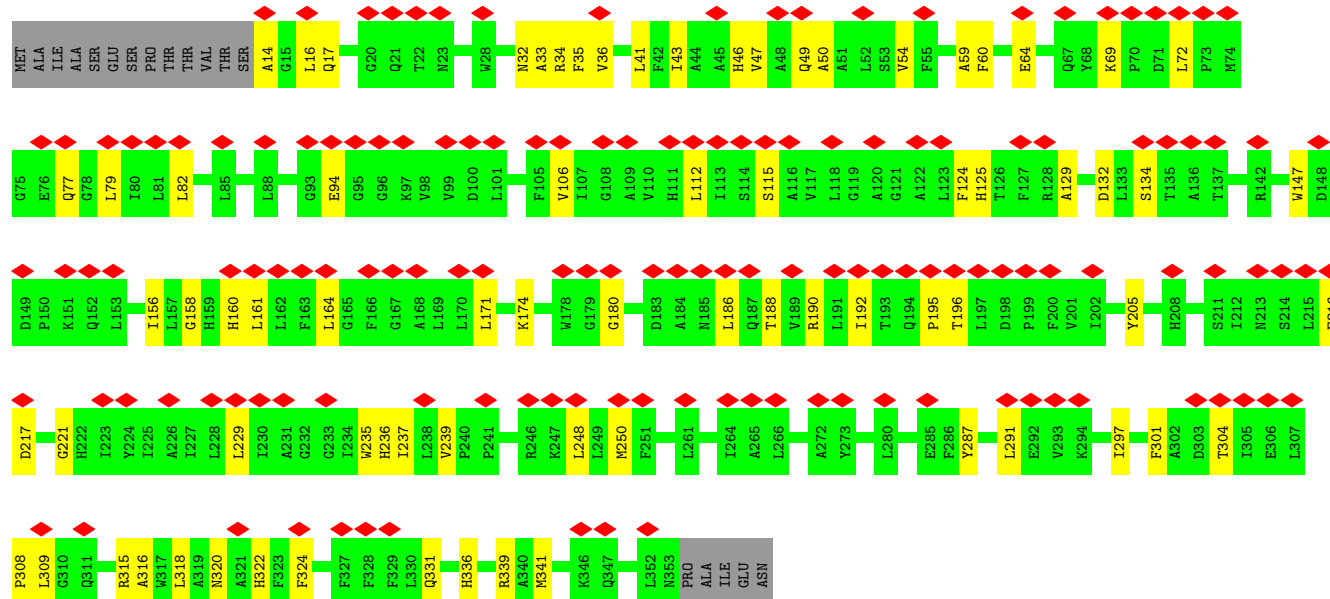
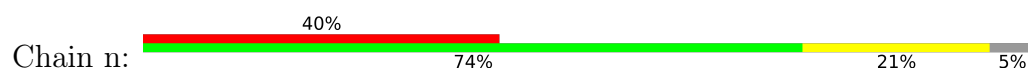
• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain m: 57% 77% 18% 5%

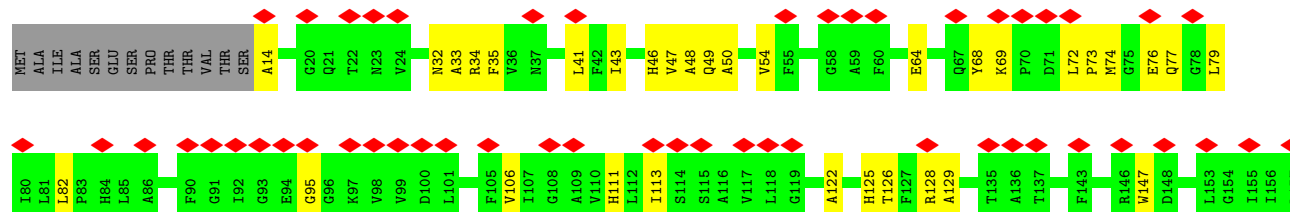


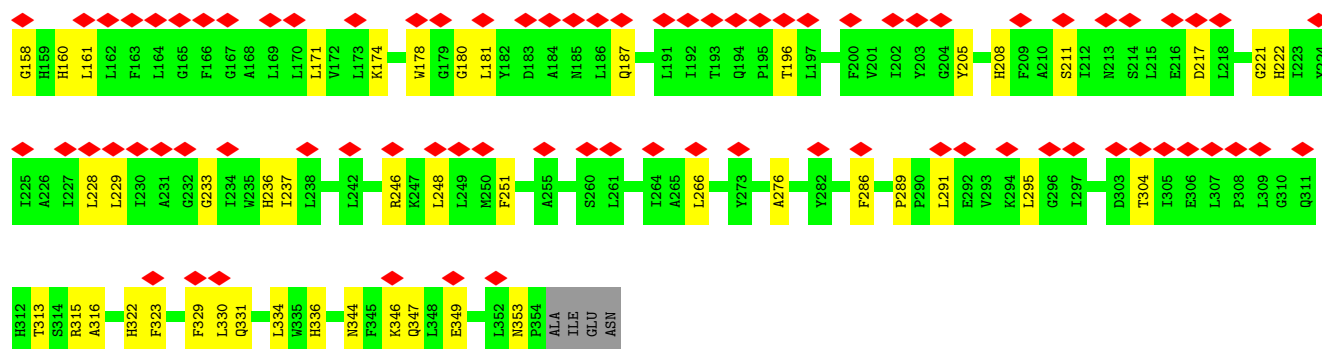


• Molecule 13: Iron stress-induced chlorophyll-binding protein

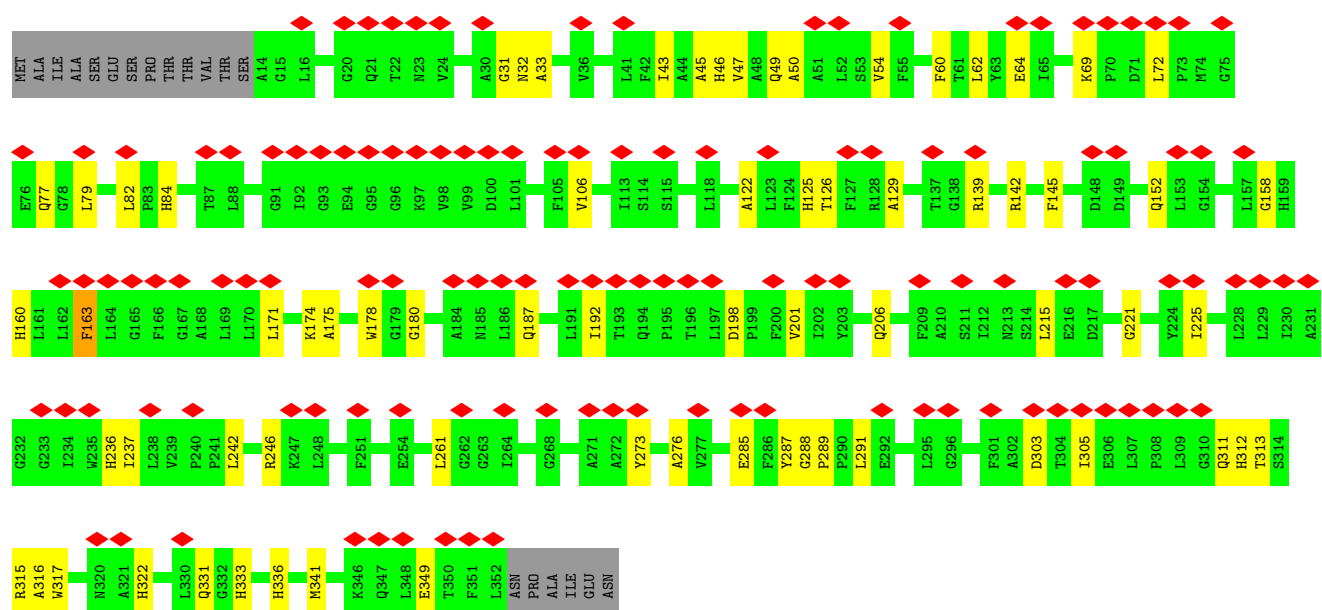
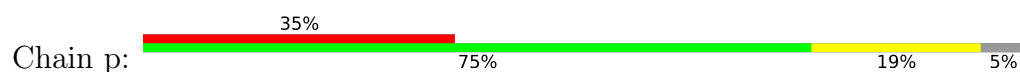


• Molecule 13: Iron stress-induced chlorophyll-binding protein

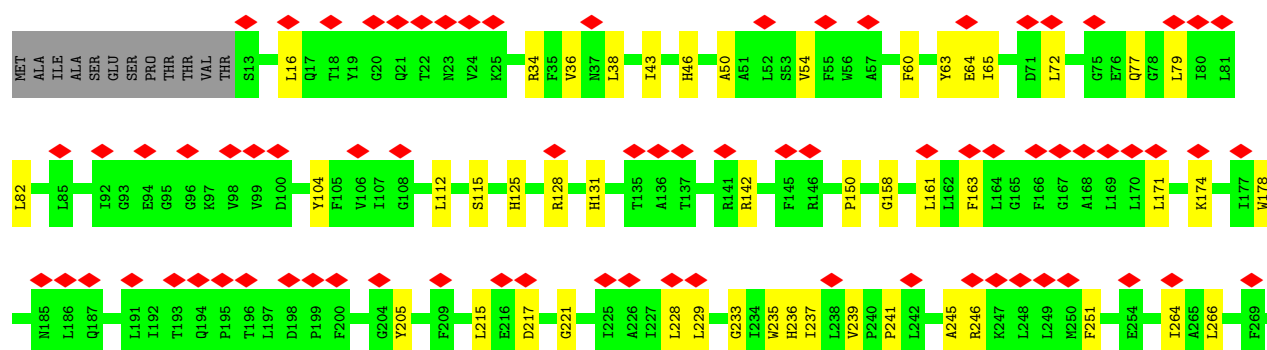
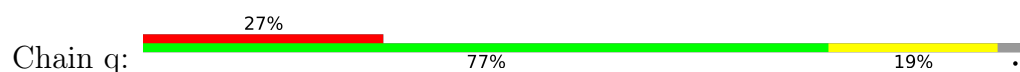


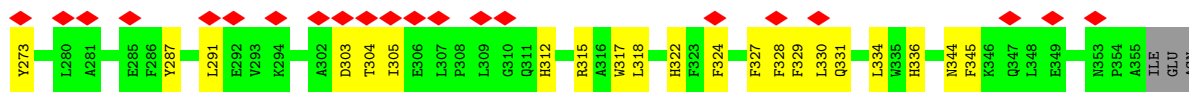


• Molecule 13: Iron stress-induced chlorophyll-binding protein



• Molecule 13: Iron stress-induced chlorophyll-binding protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95950	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	540.8, 540.8, 540.8	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	aA	0.08	0/6019	0.21	0/8209
1	bA	0.08	0/6019	0.20	0/8209
1	cA	0.08	0/6019	0.20	0/8209
2	aB	0.07	0/6112	0.21	0/8350
2	bB	0.07	0/6112	0.21	0/8350
2	cB	0.07	0/6112	0.21	0/8350
3	aC	0.09	0/608	0.30	0/824
3	bC	0.09	0/608	0.27	0/824
3	cC	0.08	0/608	0.27	0/824
4	aD	0.08	0/1094	0.21	0/1482
4	bD	0.08	0/1094	0.21	0/1482
4	cD	0.07	0/1094	0.21	0/1482
5	aE	0.06	0/551	0.20	0/750
5	bE	0.07	0/551	0.19	0/750
5	cE	0.07	0/551	0.20	0/750
6	aF	0.08	0/1087	0.23	0/1476
6	bF	0.08	0/1087	0.21	0/1476
6	cF	0.08	0/1087	0.20	0/1476
7	aI	0.09	0/312	0.25	0/425
7	bI	0.09	0/312	0.25	0/425
7	cI	0.09	0/312	0.24	0/425
8	aJ	0.07	0/350	0.20	0/477
8	bJ	0.07	0/350	0.19	0/477
8	cJ	0.07	0/350	0.19	0/477
9	aK	0.08	0/461	0.22	0/630
9	bK	0.07	0/461	0.22	0/630
9	cK	0.08	0/461	0.24	0/630
10	aL	0.07	0/1155	0.20	0/1567
10	bL	0.07	0/1155	0.22	0/1567
10	cL	0.07	0/1155	0.22	0/1567
11	aM	0.10	0/244	0.22	0/332
11	bM	0.07	0/244	0.19	0/332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	cM	0.07	0/244	0.19	0/332
12	aX	0.07	0/252	0.16	0/342
12	bX	0.07	0/252	0.17	0/342
12	cX	0.07	0/252	0.17	0/342
13	S	0.09	0/2764	0.21	0/3775
13	T	0.09	0/2754	0.21	0/3760
13	U	0.09	0/2756	0.23	0/3763
13	V	0.09	0/2764	0.22	0/3775
13	W	0.09	0/2770	0.22	0/3783
13	X	0.10	0/2777	0.24	0/3793
13	Y	0.09	0/2770	0.22	0/3783
13	Z	0.09	0/2756	0.24	1/3763 (0.0%)
13	a	0.09	0/2762	0.22	0/3771
13	a1	0.07	0/2754	0.21	0/3760
13	a2	0.07	0/2746	0.20	0/3749
13	a3	0.08	0/2775	0.20	0/3790
13	a4	0.07	0/2775	0.20	0/3790
13	a5	0.08	0/2770	0.21	0/3783
13	a6	0.07	0/2762	0.19	0/3771
13	b	0.09	0/2770	0.21	0/3783
13	b1	0.07	0/2770	0.21	0/3783
13	b2	0.07	0/2762	0.20	0/3771
13	b3	0.07	0/2770	0.19	0/3783
13	b4	0.07	0/2775	0.19	0/3790
13	b5	0.07	0/2754	0.20	0/3760
13	b6	0.08	0/2746	0.22	0/3749
13	c	0.08	0/2764	0.21	0/3775
13	c1	0.08	0/2762	0.24	1/3771 (0.0%)
13	c2	0.07	0/2754	0.21	0/3760
13	c3	0.07	0/2770	0.19	0/3783
13	c4	0.08	0/2770	0.19	0/3783
13	c5	0.09	0/2762	0.22	0/3771
13	c6	0.08	0/2746	0.22	0/3749
13	d	0.09	0/2764	0.21	0/3775
13	e	0.09	0/2770	0.22	0/3783
13	f	0.09	0/2764	0.23	0/3775
13	g	0.09	0/2762	0.23	0/3771
13	h	0.09	0/2762	0.22	0/3771
13	i	0.08	0/2756	0.21	0/3763
13	j	0.10	0/2748	0.23	0/3752
13	k	0.09	0/2756	0.21	0/3763
13	l	0.09	0/2756	0.23	0/3763
13	m	0.09	0/2764	0.21	0/3775

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
13	n	0.08	0/2756	0.21	0/3763
13	o	0.08	0/2764	0.21	0/3775
13	p	0.09	0/2748	0.23	0/3752
13	q	0.09	0/2775	0.22	0/3790
All	All	0.08	0/173510	0.21	2/236783 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	c1	297	ILE	N-CA-C	-6.16	107.86	113.71
13	Z	297	ILE	N-CA-C	-6.10	107.92	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	5819	0	5684	152	0
1	bA	5819	0	5684	157	0
1	cA	5819	0	5684	154	0
2	aB	5894	0	5650	134	0
2	bB	5894	0	5650	134	0
2	cB	5894	0	5650	135	0
3	aC	598	0	577	18	0
3	bC	598	0	577	12	0
3	cC	598	0	577	15	0
4	aD	1068	0	1067	23	0
4	bD	1068	0	1067	27	0
4	cD	1068	0	1067	22	0
5	aE	539	0	525	7	0
5	bE	539	0	525	2	0
5	cE	539	0	525	1	0
6	aF	1065	0	1074	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	bF	1065	0	1074	17	0
6	cF	1065	0	1074	16	0
7	aI	301	0	306	3	0
7	bI	301	0	306	3	0
7	cI	301	0	306	3	0
8	aJ	338	0	347	15	0
8	bJ	338	0	347	13	0
8	cJ	338	0	347	12	0
9	aK	452	0	464	5	0
9	bK	452	0	464	5	0
9	cK	452	0	464	3	0
10	aL	1126	0	1125	24	0
10	bL	1126	0	1125	19	0
10	cL	1126	0	1125	28	0
11	aM	241	0	264	6	0
11	bM	241	0	264	8	0
11	cM	241	0	264	6	0
12	aX	243	0	249	0	0
12	bX	243	0	249	0	0
12	cX	243	0	249	0	0
13	S	2674	0	2660	55	0
13	T	2665	0	2652	74	0
13	U	2667	0	2653	51	0
13	V	2674	0	2660	62	0
13	W	2680	0	2665	62	0
13	X	2687	0	2676	55	0
13	Y	2680	0	2665	59	0
13	Z	2667	0	2653	73	0
13	a	2673	0	2658	61	0
13	a1	2665	0	2652	63	0
13	a2	2657	0	2641	50	0
13	a3	2685	0	2670	51	0
13	a4	2685	0	2670	53	0
13	a5	2680	0	2665	58	0
13	a6	2673	0	2658	48	0
13	b	2680	0	2665	61	0
13	b1	2680	0	2665	59	0
13	b2	2673	0	2658	50	0
13	b3	2680	0	2665	52	0
13	b4	2685	0	2670	58	0
13	b5	2665	0	2652	64	0
13	b6	2657	0	2641	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	c	2674	0	2660	65	0
13	c1	2673	0	2658	62	0
13	c2	2665	0	2652	55	0
13	c3	2680	0	2665	45	0
13	c4	2680	0	2665	53	0
13	c5	2673	0	2658	63	0
13	c6	2657	0	2641	67	0
13	d	2674	0	2660	62	0
13	e	2680	0	2665	62	0
13	f	2674	0	2660	55	0
13	g	2673	0	2658	49	0
13	h	2673	0	2658	56	0
13	i	2667	0	2653	48	0
13	j	2659	0	2647	59	0
13	k	2667	0	2653	55	0
13	l	2667	0	2653	69	0
13	m	2674	0	2660	62	0
13	n	2667	0	2653	64	0
13	o	2674	0	2660	78	0
13	p	2659	0	2647	63	0
13	q	2685	0	2670	52	0
14	S	842	0	684	34	0
14	T	829	0	661	34	0
14	U	817	0	641	34	0
14	V	871	0	744	46	0
14	W	909	0	814	48	0
14	X	921	0	840	39	0
14	Y	918	0	836	42	0
14	Z	912	0	827	48	0
14	a	848	0	713	40	0
14	a1	959	0	905	41	0
14	a2	937	0	870	47	0
14	a3	972	0	932	52	0
14	a4	944	0	886	51	0
14	a5	949	0	890	49	0
14	a6	939	0	880	43	0
14	aA	2674	0	2682	187	0
14	aB	2443	0	2452	157	0
14	aF	45	0	33	3	0
14	aJ	106	0	92	1	0
14	aK	96	0	78	4	0
14	aL	190	0	203	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	aX	45	0	33	1	0
14	b	839	0	681	37	0
14	b1	947	0	885	46	0
14	b2	940	0	877	46	0
14	b3	963	0	913	46	0
14	b4	925	0	849	48	0
14	b5	959	0	906	46	0
14	b6	921	0	844	45	0
14	bA	2673	0	2680	174	0
14	bB	2431	0	2425	152	0
14	bF	45	0	33	3	0
14	bJ	104	0	88	1	0
14	bK	96	0	78	3	0
14	bL	190	0	203	12	0
14	bX	45	0	33	2	0
14	c	844	0	698	38	0
14	c1	953	0	893	56	0
14	c2	928	0	856	43	0
14	c3	953	0	897	49	0
14	c4	927	0	860	48	0
14	c5	950	0	894	48	0
14	c6	902	0	811	48	0
14	cA	2650	0	2635	174	0
14	cB	2410	0	2379	153	0
14	cF	45	0	33	2	0
14	cJ	106	0	92	3	0
14	cK	96	0	78	3	0
14	cL	190	0	203	9	0
14	cX	45	0	33	2	0
14	d	842	0	694	34	0
14	e	797	0	613	30	0
14	f	765	0	561	23	0
14	g	795	0	616	30	0
14	h	802	0	624	33	0
14	i	790	0	599	22	0
14	j	805	0	625	28	0
14	k	771	0	569	23	0
14	l	781	0	583	31	0
14	m	778	0	579	33	0
14	n	815	0	648	32	0
14	o	804	0	625	36	0
14	p	798	0	612	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	q	838	0	687	31	0
15	aA	33	0	46	7	0
15	aB	33	0	46	8	0
15	bA	33	0	46	4	0
15	bB	33	0	46	8	0
15	cA	33	0	46	7	0
15	cB	33	0	46	8	0
16	aA	8	0	0	1	0
16	aC	16	0	0	0	0
16	bA	8	0	0	0	0
16	bC	16	0	0	0	0
16	cA	8	0	0	0	0
16	cC	16	0	0	0	0
17	S	160	0	224	11	0
17	T	160	0	224	14	0
17	U	160	0	224	13	0
17	V	160	0	224	20	0
17	W	160	0	224	15	0
17	X	160	0	224	12	0
17	Y	160	0	224	15	0
17	Z	160	0	224	14	0
17	a	160	0	224	15	0
17	a1	160	0	224	12	0
17	a2	160	0	224	17	0
17	a3	160	0	224	17	0
17	a4	160	0	224	18	0
17	a5	160	0	224	20	0
17	a6	160	0	224	15	0
17	aA	200	0	280	26	0
17	aB	240	0	336	32	0
17	aF	120	0	168	14	0
17	aI	120	0	168	10	0
17	aJ	80	0	112	17	0
17	aK	40	0	56	6	0
17	aL	40	0	56	5	0
17	aM	40	0	56	5	0
17	b	160	0	224	14	0
17	b1	160	0	224	13	0
17	b2	160	0	224	16	0
17	b3	160	0	224	17	0
17	b4	160	0	224	14	0
17	b5	160	0	224	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	b6	160	0	224	10	0
17	bA	200	0	280	24	0
17	bB	240	0	336	36	0
17	bF	120	0	168	19	0
17	bI	120	0	168	9	0
17	bJ	80	0	112	15	0
17	bK	40	0	56	5	0
17	bL	40	0	56	7	0
17	bM	40	0	56	6	0
17	c	160	0	224	17	0
17	c1	160	0	224	19	0
17	c2	160	0	224	16	0
17	c3	160	0	224	14	0
17	c4	160	0	224	21	0
17	c5	160	0	224	14	0
17	c6	160	0	224	15	0
17	cA	200	0	280	25	0
17	cB	240	0	336	29	0
17	cF	120	0	168	17	0
17	cI	120	0	168	11	0
17	cJ	80	0	112	11	0
17	cK	40	0	56	5	0
17	cL	40	0	56	6	0
17	cM	40	0	56	4	0
17	d	160	0	224	18	0
17	e	160	0	224	20	0
17	f	160	0	224	13	0
17	g	160	0	224	22	0
17	h	160	0	224	19	0
17	i	160	0	224	15	0
17	j	160	0	224	14	0
17	k	160	0	224	17	0
17	l	160	0	224	17	0
17	m	160	0	224	17	0
17	n	160	0	224	21	0
17	o	160	0	224	18	0
17	p	160	0	224	14	0
17	q	160	0	224	15	0
18	aA	208	0	272	12	0
18	aX	39	0	48	3	0
18	bA	210	0	279	13	0
18	bX	39	0	48	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	cA	206	0	268	15	0
18	cX	39	0	48	2	0
19	aA	47	0	65	3	0
19	aB	35	0	46	2	0
19	aJ	22	0	28	1	0
19	bA	47	0	65	1	0
19	bB	35	0	46	2	0
19	bJ	22	0	28	1	0
19	cA	47	0	65	2	0
19	cB	35	0	46	1	0
19	cJ	21	0	26	1	0
20	S	31	0	26	1	0
20	T	31	0	26	0	0
20	V	31	0	26	0	0
20	W	32	0	28	1	0
20	X	36	0	35	0	0
20	Y	33	0	30	1	0
20	Z	29	0	22	1	0
20	a1	31	0	26	1	0
20	a2	33	0	30	0	0
20	a3	38	0	39	1	0
20	a4	36	0	36	2	0
20	a5	33	0	29	0	0
20	a6	31	0	25	0	0
20	aB	42	0	47	4	0
20	b	31	0	25	0	0
20	b1	31	0	26	0	0
20	b2	32	0	27	0	0
20	b3	37	0	38	1	0
20	b4	33	0	30	2	0
20	b5	30	0	24	0	0
20	b6	30	0	24	0	0
20	bB	42	0	48	3	0
20	c	31	0	26	1	0
20	c1	31	0	25	1	0
20	c2	31	0	26	0	0
20	c3	32	0	28	0	0
20	c4	33	0	30	1	0
20	c5	31	0	25	1	0
20	c6	30	0	24	1	0
20	cB	39	0	41	3	0
20	d	31	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	e	32	0	28	0	0
20	f	30	0	23	0	0
20	g	30	0	24	1	0
20	h	32	0	27	0	0
20	i	30	0	24	0	0
20	m	29	0	22	1	0
20	n	31	0	25	1	0
20	p	31	0	25	1	0
20	q	26	0	15	0	0
21	a1	40	0	50	1	0
21	a2	40	0	50	1	0
21	a6	38	0	46	0	0
21	aB	49	0	71	1	0
21	aJ	31	0	32	1	0
21	b1	35	0	40	1	0
21	b2	40	0	50	1	0
21	bB	49	0	71	3	0
21	bJ	29	0	28	1	0
21	c1	39	0	48	0	0
21	cB	49	0	71	1	0
21	cJ	31	0	32	0	0
22	aL	1	0	0	0	0
22	bL	1	0	0	0	0
22	cL	1	0	0	0	0
All	All	235011	0	232195	5433	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 5433 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:cA:1107:CLA:HBB1	17:cJ:4012:BCR:HC8	1.57	0.86
14:bA:1107:CLA:HBB1	17:bJ:4012:BCR:HC8	1.58	0.85
14:aA:1107:CLA:HBB1	17:aJ:4012:BCR:HC8	1.56	0.84
14:cA:1013:CLA:H111	17:cA:4011:BCR:H23C	1.59	0.83
1:aA:66:GLU:HG2	1:aA:187:LEU:HB2	1.61	0.83

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	743/755 (98%)	718 (97%)	25 (3%)	0	100	100
1	bA	743/755 (98%)	720 (97%)	23 (3%)	0	100	100
1	cA	743/755 (98%)	718 (97%)	25 (3%)	0	100	100
2	aB	738/741 (100%)	721 (98%)	17 (2%)	0	100	100
2	bB	738/741 (100%)	724 (98%)	14 (2%)	0	100	100
2	cB	738/741 (100%)	722 (98%)	16 (2%)	0	100	100
3	aC	78/81 (96%)	74 (95%)	3 (4%)	1 (1%)	9	33
3	bC	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	9	33
3	cC	78/81 (96%)	74 (95%)	3 (4%)	1 (1%)	9	33
4	aD	135/139 (97%)	133 (98%)	2 (2%)	0	100	100
4	bD	135/139 (97%)	133 (98%)	2 (2%)	0	100	100
4	cD	135/139 (97%)	134 (99%)	1 (1%)	0	100	100
5	aE	67/76 (88%)	66 (98%)	1 (2%)	0	100	100
5	bE	67/76 (88%)	67 (100%)	0	0	100	100
5	cE	67/76 (88%)	67 (100%)	0	0	100	100
6	aF	139/164 (85%)	134 (96%)	5 (4%)	0	100	100
6	bF	139/164 (85%)	135 (97%)	4 (3%)	0	100	100
6	cF	139/164 (85%)	135 (97%)	4 (3%)	0	100	100
7	aI	36/38 (95%)	36 (100%)	0	0	100	100
7	bI	36/38 (95%)	36 (100%)	0	0	100	100
7	cI	36/38 (95%)	36 (100%)	0	0	100	100
8	aJ	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
8	bJ	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
8	cJ	39/41 (95%)	39 (100%)	0	0	100	100
9	aK	58/83 (70%)	56 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	bK	58/83 (70%)	56 (97%)	2 (3%)	0	100	100
9	cK	58/83 (70%)	56 (97%)	2 (3%)	0	100	100
10	aL	150/155 (97%)	146 (97%)	4 (3%)	0	100	100
10	bL	150/155 (97%)	148 (99%)	2 (1%)	0	100	100
10	cL	150/155 (97%)	148 (99%)	2 (1%)	0	100	100
11	aM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	bM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	cM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
12	aX	27/39 (69%)	26 (96%)	1 (4%)	0	100	100
12	bX	27/39 (69%)	26 (96%)	1 (4%)	0	100	100
12	cX	27/39 (69%)	27 (100%)	0	0	100	100
13	S	339/358 (95%)	335 (99%)	4 (1%)	0	100	100
13	T	338/358 (94%)	334 (99%)	4 (1%)	0	100	100
13	U	338/358 (94%)	334 (99%)	4 (1%)	0	100	100
13	V	339/358 (95%)	333 (98%)	6 (2%)	0	100	100
13	W	340/358 (95%)	336 (99%)	4 (1%)	0	100	100
13	X	341/358 (95%)	332 (97%)	9 (3%)	0	100	100
13	Y	340/358 (95%)	335 (98%)	5 (2%)	0	100	100
13	Z	338/358 (94%)	333 (98%)	5 (2%)	0	100	100
13	a	339/358 (95%)	335 (99%)	4 (1%)	0	100	100
13	a1	338/358 (94%)	332 (98%)	6 (2%)	0	100	100
13	a2	337/358 (94%)	334 (99%)	3 (1%)	0	100	100
13	a3	341/358 (95%)	338 (99%)	3 (1%)	0	100	100
13	a4	341/358 (95%)	338 (99%)	3 (1%)	0	100	100
13	a5	340/358 (95%)	334 (98%)	6 (2%)	0	100	100
13	a6	339/358 (95%)	337 (99%)	2 (1%)	0	100	100
13	b	340/358 (95%)	334 (98%)	6 (2%)	0	100	100
13	b1	340/358 (95%)	334 (98%)	6 (2%)	0	100	100
13	b2	339/358 (95%)	334 (98%)	5 (2%)	0	100	100
13	b3	340/358 (95%)	336 (99%)	4 (1%)	0	100	100
13	b4	341/358 (95%)	338 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	b5	338/358 (94%)	331 (98%)	7 (2%)	0	100	100
13	b6	337/358 (94%)	331 (98%)	6 (2%)	0	100	100
13	c	339/358 (95%)	334 (98%)	5 (2%)	0	100	100
13	c1	339/358 (95%)	328 (97%)	11 (3%)	0	100	100
13	c2	338/358 (94%)	333 (98%)	5 (2%)	0	100	100
13	c3	340/358 (95%)	337 (99%)	3 (1%)	0	100	100
13	c4	340/358 (95%)	336 (99%)	4 (1%)	0	100	100
13	c5	339/358 (95%)	331 (98%)	8 (2%)	0	100	100
13	c6	337/358 (94%)	332 (98%)	5 (2%)	0	100	100
13	d	339/358 (95%)	335 (99%)	4 (1%)	0	100	100
13	e	340/358 (95%)	336 (99%)	4 (1%)	0	100	100
13	f	339/358 (95%)	336 (99%)	3 (1%)	0	100	100
13	g	339/358 (95%)	327 (96%)	12 (4%)	0	100	100
13	h	339/358 (95%)	336 (99%)	3 (1%)	0	100	100
13	i	338/358 (94%)	334 (99%)	4 (1%)	0	100	100
13	j	337/358 (94%)	332 (98%)	5 (2%)	0	100	100
13	k	338/358 (94%)	334 (99%)	4 (1%)	0	100	100
13	l	338/358 (94%)	336 (99%)	2 (1%)	0	100	100
13	m	339/358 (95%)	334 (98%)	5 (2%)	0	100	100
13	n	338/358 (94%)	333 (98%)	5 (2%)	0	100	100
13	o	339/358 (95%)	336 (99%)	3 (1%)	0	100	100
13	p	337/358 (94%)	332 (98%)	5 (2%)	0	100	100
13	q	341/358 (95%)	337 (99%)	4 (1%)	0	100	100
All	All	21293/22423 (95%)	20913 (98%)	377 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	aC	62	PHE
3	bC	62	PHE
3	cC	62	PHE

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	aA	593/603 (98%)	590 (100%)	3 (0%)	81	81
1	bA	593/603 (98%)	588 (99%)	5 (1%)	73	77
1	cA	593/603 (98%)	590 (100%)	3 (0%)	81	81
2	aB	597/598 (100%)	595 (100%)	2 (0%)	86	84
2	bB	597/598 (100%)	594 (100%)	3 (0%)	81	81
2	cB	597/598 (100%)	596 (100%)	1 (0%)	87	85
3	aC	67/68 (98%)	65 (97%)	2 (3%)	36	59
3	bC	67/68 (98%)	65 (97%)	2 (3%)	36	59
3	cC	67/68 (98%)	66 (98%)	1 (2%)	57	69
4	aD	114/116 (98%)	114 (100%)	0	100	100
4	bD	114/116 (98%)	114 (100%)	0	100	100
4	cD	114/116 (98%)	114 (100%)	0	100	100
5	aE	59/65 (91%)	59 (100%)	0	100	100
5	bE	59/65 (91%)	59 (100%)	0	100	100
5	cE	59/65 (91%)	59 (100%)	0	100	100
6	aF	109/128 (85%)	109 (100%)	0	100	100
6	bF	109/128 (85%)	109 (100%)	0	100	100
6	cF	109/128 (85%)	109 (100%)	0	100	100
7	aI	32/32 (100%)	32 (100%)	0	100	100
7	bI	32/32 (100%)	32 (100%)	0	100	100
7	cI	32/32 (100%)	32 (100%)	0	100	100
8	aJ	36/36 (100%)	36 (100%)	0	100	100
8	bJ	36/36 (100%)	36 (100%)	0	100	100
8	cJ	36/36 (100%)	36 (100%)	0	100	100
9	aK	47/61 (77%)	47 (100%)	0	100	100
9	bK	47/61 (77%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	cK	47/61 (77%)	47 (100%)	0	100	100
10	aL	118/120 (98%)	118 (100%)	0	100	100
10	bL	118/120 (98%)	118 (100%)	0	100	100
10	cL	118/120 (98%)	118 (100%)	0	100	100
11	aM	26/26 (100%)	25 (96%)	1 (4%)	29	54
11	bM	26/26 (100%)	26 (100%)	0	100	100
11	cM	26/26 (100%)	26 (100%)	0	100	100
12	aX	23/31 (74%)	23 (100%)	0	100	100
12	bX	23/31 (74%)	23 (100%)	0	100	100
12	cX	23/31 (74%)	23 (100%)	0	100	100
13	S	265/279 (95%)	264 (100%)	1 (0%)	84	83
13	T	264/279 (95%)	260 (98%)	4 (2%)	57	69
13	U	264/279 (95%)	262 (99%)	2 (1%)	73	77
13	V	265/279 (95%)	264 (100%)	1 (0%)	84	83
13	W	266/279 (95%)	266 (100%)	0	100	100
13	X	266/279 (95%)	265 (100%)	1 (0%)	84	83
13	Y	266/279 (95%)	266 (100%)	0	100	100
13	Z	264/279 (95%)	262 (99%)	2 (1%)	73	77
13	a	265/279 (95%)	263 (99%)	2 (1%)	73	77
13	a1	264/279 (95%)	264 (100%)	0	100	100
13	a2	263/279 (94%)	263 (100%)	0	100	100
13	a3	266/279 (95%)	266 (100%)	0	100	100
13	a4	266/279 (95%)	266 (100%)	0	100	100
13	a5	266/279 (95%)	266 (100%)	0	100	100
13	a6	265/279 (95%)	265 (100%)	0	100	100
13	b	266/279 (95%)	266 (100%)	0	100	100
13	b1	266/279 (95%)	265 (100%)	1 (0%)	84	83
13	b2	265/279 (95%)	264 (100%)	1 (0%)	84	83
13	b3	266/279 (95%)	266 (100%)	0	100	100
13	b4	266/279 (95%)	265 (100%)	1 (0%)	84	83
13	b5	264/279 (95%)	262 (99%)	2 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	b6	263/279 (94%)	261 (99%)	2 (1%)	73	77
13	c	265/279 (95%)	263 (99%)	2 (1%)	73	77
13	c1	265/279 (95%)	264 (100%)	1 (0%)	84	83
13	c2	264/279 (95%)	264 (100%)	0	100	100
13	c3	266/279 (95%)	265 (100%)	1 (0%)	84	83
13	c4	266/279 (95%)	266 (100%)	0	100	100
13	c5	265/279 (95%)	265 (100%)	0	100	100
13	c6	263/279 (94%)	262 (100%)	1 (0%)	84	83
13	d	265/279 (95%)	262 (99%)	3 (1%)	65	74
13	e	266/279 (95%)	265 (100%)	1 (0%)	84	83
13	f	265/279 (95%)	263 (99%)	2 (1%)	73	77
13	g	265/279 (95%)	263 (99%)	2 (1%)	73	77
13	h	265/279 (95%)	263 (99%)	2 (1%)	73	77
13	i	264/279 (95%)	261 (99%)	3 (1%)	65	74
13	j	263/279 (94%)	261 (99%)	2 (1%)	73	77
13	k	264/279 (95%)	260 (98%)	4 (2%)	57	69
13	l	264/279 (95%)	263 (100%)	1 (0%)	84	83
13	m	265/279 (95%)	265 (100%)	0	100	100
13	n	264/279 (95%)	264 (100%)	0	100	100
13	o	265/279 (95%)	265 (100%)	0	100	100
13	p	263/279 (94%)	262 (100%)	1 (0%)	84	83
13	q	266/279 (95%)	265 (100%)	1 (0%)	84	83
All	All	16852/17649 (96%)	16782 (100%)	70 (0%)	81	83

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	h	217	ASP
13	i	205	TYR
13	k	205	TYR
13	b6	351	PHE
13	b6	54	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 203 such sidechains are listed below:

Mol	Chain	Res	Type
13	c2	236	HIS
13	Y	236	HIS
13	p	336	HIS
13	c4	144	HIS
13	U	17	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](#)

Of 1354 ligands modelled in this entry, 3 are monoatomic - leaving 1351 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	CLA	bL	1503	-	69,73,73	1.18	6 (8%)	82,113,113	1.24	6 (7%)
14	CLA	a6	516	13	49,53,73	1.39	8 (16%)	58,89,113	1.45	6 (10%)
14	CLA	cA	1110	1	57,61,73	1.30	8 (14%)	67,98,113	1.34	5 (7%)
14	CLA	bB	1222	-	64,68,73	1.23	7 (10%)	76,107,113	1.30	7 (9%)
14	CLA	c3	513	13	54,58,73	1.33	6 (11%)	64,95,113	1.37	6 (9%)
17	BCR	aM	4021	-	41,41,41	0.67	0	56,56,56	2.21	15 (26%)
14	CLA	c	519	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
17	BCR	Y	521	-	41,41,41	0.64	0	56,56,56	2.06	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	aB	1223	2	69,73,73	1.17	8 (11%)	82,113,113	1.28	5 (6%)
17	BCR	l	524	-	41,41,41	0.70	0	56,56,56	2.16	15 (26%)
14	CLA	c	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
14	CLA	f	508	13	49,53,73	1.39	7 (14%)	58,89,113	1.43	4 (6%)
14	CLA	i	508	13	49,53,73	1.40	9 (18%)	58,89,113	1.41	5 (8%)
14	CLA	c4	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	p	502	13	59,63,73	1.29	8 (13%)	70,101,113	1.33	6 (8%)
14	CLA	cA	1139	-	64,68,73	1.23	8 (12%)	76,107,113	1.25	5 (6%)
14	CLA	cB	1235	2	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
17	BCR	bA	4003	-	41,41,41	0.67	0	56,56,56	2.10	15 (26%)
17	BCR	c2	522	-	41,41,41	0.68	0	56,56,56	2.08	17 (30%)
17	BCR	a4	522	-	41,41,41	0.67	0	56,56,56	2.03	17 (30%)
14	CLA	U	505	13	59,63,73	1.27	7 (11%)	70,101,113	1.31	8 (11%)
21	LMG	b1	5104	-	35,35,55	0.89	0	43,43,63	1.24	3 (6%)
14	CLA	bA	1102	1	69,73,73	1.18	7 (10%)	82,113,113	1.27	7 (8%)
14	CLA	bB	1215	2	64,68,73	1.22	6 (9%)	76,107,113	1.28	6 (7%)
14	CLA	aA	1119	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
14	CLA	a4	505	13	64,68,73	1.22	7 (10%)	76,107,113	1.26	6 (7%)
14	CLA	bA	1128	1	69,73,73	1.19	8 (11%)	82,113,113	1.28	7 (8%)
14	CLA	bB	1219	-	59,63,73	1.27	5 (8%)	70,101,113	1.36	8 (11%)
14	CLA	cB	1210	2	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
17	BCR	g	523	-	41,41,41	0.69	0	56,56,56	2.06	17 (30%)
14	CLA	e	508	13	49,53,73	1.39	9 (18%)	58,89,113	1.42	5 (8%)
21	LMG	cB	5002	-	49,49,55	0.73	1 (2%)	57,57,63	1.34	8 (14%)
14	CLA	aA	1133	1	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
14	CLA	q	516	13	49,53,73	1.41	8 (16%)	58,89,113	1.37	6 (10%)
14	CLA	b1	503	13	67,71,73	1.20	7 (10%)	79,110,113	1.28	5 (6%)
14	CLA	S	519	13	49,53,73	1.41	7 (14%)	58,89,113	1.40	4 (6%)
17	BCR	o	522	-	41,41,41	0.68	0	56,56,56	2.17	16 (28%)
14	CLA	W	502	13	64,68,73	1.22	8 (12%)	76,107,113	1.31	6 (7%)
14	CLA	a6	510	13	69,73,73	1.19	8 (11%)	82,113,113	1.25	6 (7%)
19	LMU	bJ	5105	-	22,22,36	1.13	1 (4%)	27,27,47	0.82	0
17	BCR	c3	521	-	41,41,41	0.64	0	56,56,56	2.02	15 (26%)
14	CLA	cA	1022	-	69,73,73	1.18	8 (11%)	82,113,113	1.18	4 (4%)
14	CLA	Y	504	-	59,63,73	1.28	7 (11%)	70,101,113	1.33	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	LHG	cA	5005	-	43,43,48	0.65	0	46,49,54	1.27	4 (8%)
17	BCR	b3	524	-	41,41,41	0.70	0	56,56,56	2.14	17 (30%)
20	SQD	a2	822	-	31,33,54	1.23	3 (9%)	41,44,65	1.64	9 (21%)
20	SQD	g	822	-	28,30,54	1.28	3 (10%)	38,41,65	1.71	8 (21%)
14	CLA	g	512	13	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	S	518	13	55,59,73	1.33	8 (14%)	64,96,113	1.36	6 (9%)
14	CLA	c	513	13	49,53,73	1.39	7 (14%)	58,89,113	1.40	5 (8%)
14	CLA	b	510	13	64,68,73	1.23	8 (12%)	76,107,113	1.28	6 (7%)
14	CLA	c1	509	13	69,73,73	1.18	6 (8%)	82,113,113	1.27	6 (7%)
14	CLA	b5	502	13	64,68,73	1.23	9 (14%)	76,107,113	1.31	6 (7%)
17	BCR	c2	523	-	41,41,41	0.72	1 (2%)	56,56,56	1.98	18 (32%)
17	BCR	bF	4014	-	41,41,41	0.68	0	56,56,56	2.20	15 (26%)
14	CLA	q	513	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	5 (8%)
14	CLA	c2	509	13	69,73,73	1.18	8 (11%)	82,113,113	1.26	4 (4%)
20	SQD	b	822	-	29,31,54	1.26	3 (10%)	39,42,65	1.69	9 (23%)
14	CLA	aA	1121	1	59,63,73	1.28	7 (11%)	70,101,113	1.31	5 (7%)
14	CLA	bA	1108	1	49,53,73	1.40	6 (12%)	58,89,113	1.38	4 (6%)
14	CLA	a2	518	13	59,63,73	1.28	8 (13%)	70,101,113	1.33	6 (8%)
14	CLA	d	513	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	5 (8%)
17	BCR	c3	523	-	41,41,41	0.69	0	56,56,56	2.01	15 (26%)
14	CLA	cA	1105	1	55,59,73	1.32	7 (12%)	64,96,113	1.39	6 (9%)
16	SF4	bA	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	U	519	13	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
14	CLA	T	507	-	49,53,73	1.39	6 (12%)	58,89,113	1.40	4 (6%)
17	BCR	cB	4004	-	41,41,41	0.66	0	56,56,56	2.15	13 (23%)
14	CLA	bB	1239	2	69,73,73	1.19	7 (10%)	82,113,113	1.26	6 (7%)
14	CLA	c2	505	13	69,73,73	1.17	7 (10%)	82,113,113	1.28	7 (8%)
19	LMU	bA	1848	-	24,24,36	1.11	1 (4%)	29,29,47	0.83	0
14	CLA	b4	504	-	57,61,73	1.32	9 (15%)	67,98,113	1.38	6 (8%)
14	CLA	cB	1221	2	64,68,73	1.22	8 (12%)	76,107,113	1.26	4 (5%)
14	CLA	i	504	-	49,53,73	1.41	7 (14%)	58,89,113	1.43	4 (6%)
18	LHG	bX	4021	-	38,38,48	0.70	1 (2%)	41,44,54	1.39	6 (14%)
17	BCR	bI	4018	-	41,41,41	0.74	1 (2%)	56,56,56	2.15	17 (30%)
14	CLA	q	503	13	66,70,73	1.20	6 (9%)	78,109,113	1.30	5 (6%)
14	CLA	m	502	13	49,53,73	1.41	8 (16%)	58,89,113	1.45	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a1	519	13	49,53,73	1.41	6 (12%)	58,89,113	1.42	4 (6%)
14	CLA	k	511	13	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
17	BCR	o	521	-	41,41,41	0.65	0	56,56,56	2.09	14 (25%)
14	CLA	Z	511	13	49,53,73	1.40	6 (12%)	58,89,113	1.41	4 (6%)
14	CLA	W	510	13	69,73,73	1.19	8 (11%)	82,113,113	1.25	5 (6%)
14	CLA	a2	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.26	7 (8%)
14	CLA	U	507	-	49,53,73	1.40	6 (12%)	58,89,113	1.39	4 (6%)
14	CLA	aA	1116	1	64,68,73	1.23	9 (14%)	76,107,113	1.28	6 (7%)
14	CLA	a6	501	13	69,73,73	1.19	8 (11%)	82,113,113	1.29	6 (7%)
14	CLA	cB	1239	2	69,73,73	1.19	7 (10%)	82,113,113	1.26	6 (7%)
14	CLA	c5	507	-	64,68,73	1.22	8 (12%)	76,107,113	1.30	6 (7%)
14	CLA	c1	501	13	69,73,73	1.19	8 (11%)	82,113,113	1.27	6 (7%)
14	CLA	g	518	13	49,53,73	1.39	7 (14%)	58,89,113	1.43	4 (6%)
14	CLA	l	508	13	50,54,73	1.37	8 (16%)	59,90,113	1.37	5 (8%)
14	CLA	cA	1113	1	49,53,73	1.39	7 (14%)	58,89,113	1.43	6 (10%)
14	CLA	o	507	-	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
17	BCR	g	521	-	41,41,41	0.65	0	56,56,56	2.13	14 (25%)
14	CLA	b1	516	13	49,53,73	1.40	8 (16%)	58,89,113	1.39	4 (6%)
14	CLA	c3	507	-	64,68,73	1.22	7 (10%)	76,107,113	1.29	5 (6%)
17	BCR	c	523	-	41,41,41	0.67	0	56,56,56	1.98	14 (25%)
14	CLA	f	512	13	49,53,73	1.41	8 (16%)	58,89,113	1.39	4 (6%)
17	BCR	b2	522	-	41,41,41	0.67	0	56,56,56	2.13	15 (26%)
14	CLA	b4	518	13	59,63,73	1.27	8 (13%)	70,101,113	1.35	6 (8%)
14	CLA	W	512	13	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	g	506	13	49,53,73	1.41	7 (14%)	58,89,113	1.40	4 (6%)
14	CLA	e	510	13	59,63,73	1.28	7 (11%)	70,101,113	1.32	7 (10%)
14	CLA	b	509	13	66,70,73	1.21	7 (10%)	78,109,113	1.30	6 (7%)
17	BCR	b5	523	-	41,41,41	0.69	0	56,56,56	1.90	15 (26%)
14	CLA	b2	508	13	59,63,73	1.28	7 (11%)	70,101,113	1.32	6 (8%)
14	CLA	b6	518	13	54,58,73	1.33	7 (12%)	64,95,113	1.36	6 (9%)
17	BCR	b6	521	-	41,41,41	0.66	0	56,56,56	2.15	14 (25%)
14	CLA	c4	517	-	49,53,73	1.40	6 (12%)	58,89,113	1.41	4 (6%)
14	CLA	aB	1012	-	66,70,73	1.20	7 (10%)	78,109,113	1.21	6 (7%)
14	CLA	a4	502	13	64,68,73	1.22	8 (12%)	76,107,113	1.30	6 (7%)
14	CLA	c	518	13	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b4	519	13	56,60,73	1.31	7 (12%)	65,97,113	1.34	5 (7%)
14	CLA	U	502	13	61,65,73	1.26	8 (13%)	72,103,113	1.32	6 (8%)
14	CLA	c3	510	13	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
14	CLA	q	509	13	66,70,73	1.20	7 (10%)	78,109,113	1.29	6 (7%)
14	CLA	bB	1213	2	64,68,73	1.23	7 (10%)	76,107,113	1.31	6 (7%)
14	CLA	c2	506	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	5 (8%)
14	CLA	aA	1134	1	61,65,73	1.26	7 (11%)	72,103,113	1.31	5 (6%)
17	BCR	b6	524	-	41,41,41	0.68	0	56,56,56	2.18	14 (25%)
14	CLA	l	510	13	49,53,73	1.40	7 (14%)	58,89,113	1.39	5 (8%)
20	SQD	c	822	-	29,31,54	1.26	3 (10%)	39,42,65	1.65	9 (23%)
14	CLA	a5	504	-	56,60,73	1.32	8 (14%)	65,97,113	1.37	6 (9%)
14	CLA	c	501	13	56,60,73	1.32	8 (14%)	65,97,113	1.36	5 (7%)
14	CLA	cB	1205	2	69,73,73	1.17	8 (11%)	82,113,113	1.31	7 (8%)
17	BCR	T	522	-	41,41,41	0.67	0	56,56,56	2.11	16 (28%)
14	CLA	Z	503	13	65,69,73	1.21	6 (9%)	77,108,113	1.29	5 (6%)
17	BCR	bF	4016	-	41,41,41	0.70	0	56,56,56	2.06	15 (26%)
14	CLA	c	516	13	49,53,73	1.39	5 (10%)	58,89,113	1.46	5 (8%)
14	CLA	n	518	13	51,55,73	1.36	8 (15%)	60,91,113	1.40	5 (8%)
14	CLA	aA	1111	1	59,63,73	1.28	7 (11%)	70,101,113	1.34	6 (8%)
14	CLA	cB	1224	2	62,66,73	1.24	8 (12%)	73,104,113	1.26	5 (6%)
14	CLA	a2	519	13	54,58,73	1.33	7 (12%)	64,95,113	1.37	6 (9%)
14	CLA	T	508	13	49,53,73	1.39	9 (18%)	58,89,113	1.42	4 (6%)
14	CLA	a1	509	13	69,73,73	1.18	7 (10%)	82,113,113	1.26	5 (6%)
17	BCR	h	523	-	41,41,41	0.68	0	56,56,56	1.96	14 (25%)
14	CLA	k	501	13	55,59,73	1.33	7 (12%)	64,96,113	1.37	6 (9%)
14	CLA	bA	1110	1	57,61,73	1.30	8 (14%)	67,98,113	1.33	5 (7%)
14	CLA	cB	1203	2	69,73,73	1.17	7 (10%)	82,113,113	1.25	5 (6%)
17	BCR	d	524	-	41,41,41	0.70	0	56,56,56	2.18	18 (32%)
14	CLA	cA	1121	1	55,59,73	1.33	7 (12%)	64,96,113	1.35	5 (7%)
14	CLA	l	512	13	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	o	503	13	66,70,73	1.21	7 (10%)	78,109,113	1.30	6 (7%)
14	CLA	S	513	13	51,55,73	1.36	6 (11%)	60,91,113	1.36	5 (8%)
14	CLA	k	516	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	6 (10%)
17	BCR	p	521	-	41,41,41	0.66	0	56,56,56	2.17	13 (23%)
20	SQD	d	822	-	29,31,54	1.27	3 (10%)	39,42,65	1.65	9 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	bB	1226	2	69,73,73	1.19	8 (11%)	82,113,113	1.30	7 (8%)
14	CLA	S	502	13	50,54,73	1.38	8 (16%)	59,90,113	1.40	4 (6%)
14	CLA	b3	510	13	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
14	CLA	m	512	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
14	CLA	d	516	13	49,53,73	1.40	6 (12%)	58,89,113	1.40	4 (6%)
14	CLA	c3	506	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
14	CLA	a	502	13	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
14	CLA	c1	502	13	64,68,73	1.23	8 (12%)	76,107,113	1.30	6 (7%)
14	CLA	c	510	13	64,68,73	1.23	8 (12%)	76,107,113	1.28	7 (9%)
14	CLA	bB	1227	2	58,62,73	1.28	6 (10%)	68,99,113	1.33	6 (8%)
14	CLA	l	516	13	49,53,73	1.38	6 (12%)	58,89,113	1.45	4 (6%)
14	CLA	g	519	13	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
14	CLA	W	506	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
18	LHG	bA	5001	-	48,48,48	0.62	1 (2%)	51,54,54	1.30	6 (11%)
14	CLA	aB	1239	2	69,73,73	1.19	8 (11%)	82,113,113	1.25	6 (7%)
15	PQN	cA	2001	-	34,34,34	3.05	12 (35%)	43,45,45	1.95	6 (13%)
14	CLA	c	512	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
20	SQD	V	822	-	29,31,54	1.28	3 (10%)	39,42,65	1.65	9 (23%)
14	CLA	f	519	13	49,53,73	1.40	6 (12%)	58,89,113	1.38	4 (6%)
14	CLA	aL	1503	-	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
14	CLA	i	517	-	49,53,73	1.41	7 (14%)	58,89,113	1.39	4 (6%)
17	BCR	aB	4006	-	41,41,41	0.68	0	56,56,56	2.08	14 (25%)
14	CLA	bJ	1303	8	61,65,73	1.27	7 (11%)	72,103,113	1.40	5 (6%)
14	CLA	c4	501	13	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)
14	CLA	b6	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
17	BCR	Z	524	-	41,41,41	0.69	0	56,56,56	2.07	17 (30%)
14	CLA	b5	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	5 (8%)
14	CLA	cB	1209	2	57,61,73	1.30	7 (12%)	67,98,113	1.41	7 (10%)
17	BCR	j	523	-	41,41,41	0.69	0	56,56,56	2.01	15 (26%)
17	BCR	k	521	-	41,41,41	0.65	0	56,56,56	2.10	14 (25%)
14	CLA	i	511	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	p	510	13	50,54,73	1.37	7 (14%)	59,90,113	1.37	5 (8%)
14	CLA	n	513	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	5 (8%)
14	CLA	c	506	13	49,53,73	1.40	9 (18%)	58,89,113	1.41	5 (8%)
20	SQD	i	822	-	28,30,54	1.28	3 (10%)	38,41,65	1.70	10 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	m	523	-	41,41,41	0.68	0	56,56,56	1.99	15 (26%)
17	BCR	Y	522	-	41,41,41	0.67	0	56,56,56	2.02	16 (28%)
14	CLA	cA	1138	1	69,73,73	1.18	7 (10%)	82,113,113	1.24	5 (6%)
14	CLA	a4	512	13	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
17	BCR	cB	4010	-	41,41,41	0.69	0	56,56,56	2.07	16 (28%)
14	CLA	b2	512	13	58,62,73	1.29	7 (12%)	68,99,113	1.32	5 (7%)
17	BCR	U	523	-	41,41,41	0.70	0	56,56,56	1.98	15 (26%)
17	BCR	X	521	-	41,41,41	0.64	0	56,56,56	2.06	14 (25%)
17	BCR	cA	4002	-	41,41,41	0.67	0	56,56,56	2.08	14 (25%)
17	BCR	j	524	-	41,41,41	0.72	0	56,56,56	2.20	17 (30%)
14	CLA	cB	1207	2	69,73,73	1.18	6 (8%)	82,113,113	1.26	5 (6%)
14	CLA	aA	1129	1	57,61,73	1.29	8 (14%)	67,98,113	1.34	5 (7%)
17	BCR	bB	4009	-	41,41,41	0.70	0	56,56,56	2.07	16 (28%)
14	CLA	X	516	13	49,53,73	1.41	6 (12%)	58,89,113	1.41	5 (8%)
14	CLA	bA	1122	1	64,68,73	1.23	7 (10%)	76,107,113	1.28	5 (6%)
14	CLA	l	511	13	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
14	CLA	c2	516	13	49,53,73	1.41	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	a4	516	13	49,53,73	1.39	6 (12%)	58,89,113	1.44	4 (6%)
17	BCR	c5	521	-	41,41,41	0.64	0	56,56,56	2.10	14 (25%)
14	CLA	T	510	13	60,64,73	1.27	7 (11%)	71,102,113	1.33	5 (7%)
14	CLA	n	516	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
17	BCR	b4	523	-	41,41,41	0.67	0	56,56,56	1.93	16 (28%)
14	CLA	a	519	13	49,53,73	1.40	7 (14%)	58,89,113	1.37	4 (6%)
14	CLA	p	506	13	49,53,73	1.41	8 (16%)	58,89,113	1.41	5 (8%)
14	CLA	aA	1115	1	64,68,73	1.22	7 (10%)	76,107,113	1.31	6 (7%)
14	CLA	h	509	13	69,73,73	1.18	8 (11%)	82,113,113	1.29	6 (7%)
14	CLA	j	516	13	49,53,73	1.40	6 (12%)	58,89,113	1.37	4 (6%)
17	BCR	a3	524	-	41,41,41	0.68	0	56,56,56	2.11	17 (30%)
17	BCR	c1	523	-	41,41,41	0.69	0	56,56,56	1.98	14 (25%)
18	LHG	cA	5003	14	40,40,48	0.69	2 (5%)	43,46,54	1.33	6 (13%)
14	CLA	p	505	13	51,55,73	1.35	7 (13%)	60,91,113	1.36	5 (8%)
14	CLA	bA	1116	1	64,68,73	1.23	9 (14%)	76,107,113	1.28	6 (7%)
14	CLA	b	517	-	49,53,73	1.40	8 (16%)	58,89,113	1.41	5 (8%)
14	CLA	bA	1130	1	59,63,73	1.27	7 (11%)	70,101,113	1.34	7 (10%)
14	CLA	f	517	-	49,53,73	1.41	7 (14%)	58,89,113	1.39	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	k	510	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	5 (8%)
14	CLA	c5	516	13	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
21	LMG	bJ	5104	-	29,29,55	0.98	0	37,37,63	1.23	4 (10%)
14	CLA	a4	510	13	69,73,73	1.19	7 (10%)	82,113,113	1.23	7 (8%)
14	CLA	aA	1135	1	55,59,73	1.32	7 (12%)	64,96,113	1.39	6 (9%)
14	CLA	aB	1233	-	49,53,73	1.40	6 (12%)	58,89,113	1.40	4 (6%)
14	CLA	U	516	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	5 (8%)
14	CLA	aB	1211	2	69,73,73	1.18	7 (10%)	82,113,113	1.28	9 (10%)
18	LHG	cA	5004	-	30,30,48	0.78	1 (3%)	33,36,54	1.35	4 (12%)
14	CLA	a5	519	13	55,59,73	1.32	8 (14%)	64,96,113	1.36	4 (6%)
17	BCR	b	521	-	41,41,41	0.65	0	56,56,56	2.10	13 (23%)
17	BCR	aJ	4012	-	41,41,41	0.66	0	56,56,56	2.05	18 (32%)
14	CLA	U	504	-	54,58,73	1.33	6 (11%)	64,95,113	1.40	6 (9%)
14	CLA	o	510	13	60,64,73	1.26	6 (10%)	71,102,113	1.30	6 (8%)
14	CLA	b3	511	13	66,70,73	1.21	8 (12%)	78,109,113	1.27	5 (6%)
17	BCR	bL	4022	-	41,41,41	0.65	0	56,56,56	2.13	13 (23%)
14	CLA	h	508	13	49,53,73	1.39	8 (16%)	58,89,113	1.41	5 (8%)
14	CLA	S	507	-	51,55,73	1.35	6 (11%)	60,91,113	1.38	5 (8%)
14	CLA	c6	507	-	61,65,73	1.26	7 (11%)	72,103,113	1.30	5 (6%)
14	CLA	f	502	13	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
14	CLA	b5	519	13	56,60,73	1.31	7 (12%)	65,97,113	1.36	5 (7%)
17	BCR	cK	4001	-	41,41,41	0.68	0	56,56,56	1.93	15 (26%)
17	BCR	c2	524	-	41,41,41	0.68	0	56,56,56	2.06	16 (28%)
14	CLA	c6	519	13	49,53,73	1.41	7 (14%)	58,89,113	1.39	4 (6%)
14	CLA	a1	502	13	64,68,73	1.23	9 (14%)	76,107,113	1.33	5 (6%)
14	CLA	e	501	13	49,53,73	1.41	9 (18%)	58,89,113	1.42	4 (6%)
14	CLA	cA	1801	18	49,53,73	1.40	8 (16%)	58,89,113	1.39	4 (6%)
14	CLA	c1	516	13	59,63,73	1.29	5 (8%)	70,101,113	1.36	6 (8%)
14	CLA	c4	503	13	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
14	CLA	T	503	13	49,53,73	1.41	6 (12%)	58,89,113	1.44	4 (6%)
14	CLA	W	516	13	49,53,73	1.39	7 (14%)	58,89,113	1.38	4 (6%)
17	BCR	aA	4011	-	41,41,41	0.70	1 (2%)	56,56,56	2.18	18 (32%)
14	CLA	i	506	13	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
17	BCR	aB	4009	-	41,41,41	0.71	0	56,56,56	2.12	16 (28%)
18	LHG	bA	5004	-	38,38,48	0.70	2 (5%)	41,44,54	1.25	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	cB	1228	2	59,63,73	1.28	8 (13%)	70,101,113	1.32	6 (8%)
14	CLA	n	503	13	50,54,73	1.38	7 (14%)	59,90,113	1.40	4 (6%)
17	BCR	e	524	-	41,41,41	0.69	0	56,56,56	2.17	18 (32%)
14	CLA	e	507	-	54,58,73	1.33	7 (12%)	64,95,113	1.40	6 (9%)
14	CLA	cA	1118	1	64,68,73	1.22	7 (10%)	76,107,113	1.29	5 (6%)
14	CLA	o	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
14	CLA	c3	518	13	59,63,73	1.28	8 (13%)	70,101,113	1.33	6 (8%)
14	CLA	o	502	13	49,53,73	1.41	8 (16%)	58,89,113	1.45	4 (6%)
14	CLA	g	501	13	59,63,73	1.28	7 (11%)	70,101,113	1.35	6 (8%)
14	CLA	c5	505	13	69,73,73	1.17	7 (10%)	82,113,113	1.27	6 (7%)
17	BCR	Z	521	-	41,41,41	0.65	0	56,56,56	2.04	13 (23%)
14	CLA	a	509	13	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
14	CLA	bB	1212	2	49,53,73	1.39	7 (14%)	58,89,113	1.44	6 (10%)
14	CLA	c3	502	13	64,68,73	1.23	8 (12%)	76,107,113	1.31	5 (6%)
17	BCR	b1	521	-	41,41,41	0.65	0	56,56,56	2.09	16 (28%)
14	CLA	cA	1133	1	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
14	CLA	c1	510	13	69,73,73	1.18	6 (8%)	82,113,113	1.26	5 (6%)
14	CLA	i	510	13	54,58,73	1.33	7 (12%)	64,95,113	1.36	6 (9%)
14	CLA	p	518	13	52,56,73	1.35	7 (13%)	61,92,113	1.39	5 (8%)
14	CLA	c3	503	13	67,71,73	1.20	5 (7%)	79,110,113	1.27	5 (6%)
14	CLA	n	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
16	SF4	bC	3003	3	0,12,12	-	-	-	-	-
14	CLA	e	517	-	49,53,73	1.40	7 (14%)	58,89,113	1.43	5 (8%)
14	CLA	h	501	13	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)
20	SQD	a1	822	-	29,31,54	1.27	3 (10%)	39,42,65	1.68	8 (20%)
14	CLA	bB	1206	2	69,73,73	1.19	8 (11%)	82,113,113	1.25	6 (7%)
17	BCR	W	524	-	41,41,41	0.70	0	56,56,56	2.04	17 (30%)
16	SF4	aC	3003	3	0,12,12	-	-	-	-	-
14	CLA	a6	519	13	49,53,73	1.39	6 (12%)	58,89,113	1.48	4 (6%)
14	CLA	g	516	13	49,53,73	1.39	6 (12%)	58,89,113	1.51	6 (10%)
14	CLA	a5	512	13	56,60,73	1.31	7 (12%)	65,97,113	1.34	6 (9%)
14	CLA	c1	506	13	49,53,73	1.40	9 (18%)	58,89,113	1.43	5 (8%)
14	CLA	aB	1219	-	59,63,73	1.27	5 (8%)	70,101,113	1.36	8 (11%)
14	CLA	aA	1128	1	69,73,73	1.19	8 (11%)	82,113,113	1.28	7 (8%)
14	CLA	a3	508	13	59,63,73	1.27	8 (13%)	70,101,113	1.32	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	q	510	13	66,70,73	1.21	7 (10%)	78,109,113	1.29	7 (8%)
14	CLA	c1	507	-	64,68,73	1.23	8 (12%)	76,107,113	1.28	6 (7%)
14	CLA	cA	1116	1	64,68,73	1.22	9 (14%)	76,107,113	1.26	6 (7%)
14	CLA	l	517	-	49,53,73	1.38	9 (18%)	58,89,113	1.57	6 (10%)
14	CLA	a5	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	5 (8%)
14	CLA	a1	504	-	59,63,73	1.29	7 (11%)	70,101,113	1.34	6 (8%)
14	CLA	o	512	13	49,53,73	1.40	8 (16%)	58,89,113	1.39	4 (6%)
17	BCR	bB	4004	-	41,41,41	0.66	0	56,56,56	2.14	13 (23%)
17	BCR	c1	522	-	41,41,41	0.68	0	56,56,56	2.11	15 (26%)
14	CLA	c6	512	13	49,53,73	1.40	7 (14%)	58,89,113	1.38	4 (6%)
21	LMG	c1	5104	-	39,39,55	0.85	1 (2%)	47,47,63	1.24	4 (8%)
14	CLA	a4	511	13	49,53,73	1.41	8 (16%)	58,89,113	1.42	4 (6%)
17	BCR	cB	4006	-	41,41,41	0.68	0	56,56,56	2.11	15 (26%)
20	SQD	f	822	-	28,30,54	1.28	3 (10%)	38,41,65	1.66	9 (23%)
14	CLA	h	510	13	59,63,73	1.28	7 (11%)	70,101,113	1.31	7 (10%)
14	CLA	k	518	13	49,53,73	1.39	7 (14%)	58,89,113	1.40	4 (6%)
14	CLA	i	503	13	49,53,73	1.40	6 (12%)	58,89,113	1.44	4 (6%)
14	CLA	bB	1012	-	65,69,73	1.21	7 (10%)	77,108,113	1.22	6 (7%)
14	CLA	T	516	13	49,53,73	1.39	6 (12%)	58,89,113	1.46	5 (8%)
17	BCR	b4	521	-	41,41,41	0.65	0	56,56,56	2.07	15 (26%)
14	CLA	b5	508	13	59,63,73	1.28	9 (15%)	70,101,113	1.31	6 (8%)
14	CLA	p	509	13	66,70,73	1.21	7 (10%)	78,109,113	1.30	6 (7%)
14	CLA	l	502	13	59,63,73	1.29	8 (13%)	70,101,113	1.35	6 (8%)
21	LMG	aB	5002	-	49,49,55	0.74	1 (2%)	57,57,63	1.32	6 (10%)
14	CLA	p	512	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
17	BCR	g	524	-	41,41,41	0.69	0	56,56,56	2.03	16 (28%)
14	CLA	a3	509	13	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	a2	503	13	69,73,73	1.18	7 (10%)	82,113,113	1.28	7 (8%)
14	CLA	bA	1125	1	69,73,73	1.18	9 (13%)	82,113,113	1.25	6 (7%)
14	CLA	b2	511	13	55,59,73	1.33	8 (14%)	64,96,113	1.39	6 (9%)
14	CLA	c2	508	13	59,63,73	1.27	8 (13%)	70,101,113	1.31	5 (7%)
20	SQD	aB	1852	-	40,42,54	1.08	3 (7%)	50,53,65	1.60	11 (22%)
14	CLA	X	507	-	64,68,73	1.23	7 (10%)	76,107,113	1.30	6 (7%)
14	CLA	aA	1109	1	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
14	CLA	Z	507	-	64,68,73	1.22	8 (12%)	76,107,113	1.29	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	c	508	13	59,63,73	1.28	8 (13%)	70,101,113	1.32	6 (8%)
14	CLA	a	513	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	b2	502	13	64,68,73	1.23	8 (12%)	76,107,113	1.31	6 (7%)
17	BCR	b3	521	-	41,41,41	0.64	0	56,56,56	2.07	15 (26%)
14	CLA	U	501	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	cA	1119	-	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
14	CLA	aB	1206	2	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
17	BCR	U	522	-	41,41,41	0.68	0	56,56,56	2.18	16 (28%)
14	CLA	V	511	13	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
17	BCR	V	521	-	41,41,41	0.64	0	56,56,56	2.05	12 (21%)
14	CLA	bA	1120	1	59,63,73	1.28	6 (10%)	70,101,113	1.36	6 (8%)
14	CLA	bA	1801	18	49,53,73	1.39	8 (16%)	58,89,113	1.39	4 (6%)
14	CLA	b6	513	13	54,58,73	1.33	7 (12%)	64,95,113	1.36	6 (9%)
19	LMU	aA	1848	-	24,24,36	1.10	1 (4%)	29,29,47	0.81	0
17	BCR	a	524	-	41,41,41	0.69	0	56,56,56	2.09	14 (25%)
14	CLA	aA	1114	-	49,53,73	1.41	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	X	517	-	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
14	CLA	b	519	13	49,53,73	1.41	7 (14%)	58,89,113	1.41	4 (6%)
14	CLA	cL	1503	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
14	CLA	h	503	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	T	511	13	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	c4	518	13	60,64,73	1.27	8 (13%)	71,102,113	1.33	6 (8%)
14	CLA	e	504	-	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
14	CLA	i	509	13	49,53,73	1.40	7 (14%)	58,89,113	1.43	5 (8%)
17	BCR	aA	4003	-	41,41,41	0.68	0	56,56,56	2.09	15 (26%)
14	CLA	bB	1233	-	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
14	CLA	c6	518	13	54,58,73	1.33	7 (12%)	64,95,113	1.39	6 (9%)
14	CLA	bB	1205	2	69,73,73	1.18	9 (13%)	82,113,113	1.29	7 (8%)
19	LMU	cB	1843	-	36,36,36	1.18	2 (5%)	47,47,47	0.97	1 (2%)
14	CLA	c2	510	13	69,73,73	1.18	7 (10%)	82,113,113	1.26	5 (6%)
14	CLA	g	507	-	49,53,73	1.40	6 (12%)	58,89,113	1.42	4 (6%)
14	CLA	bB	1211	2	69,73,73	1.17	7 (10%)	82,113,113	1.27	7 (8%)
16	SF4	bC	3002	3	0,12,12	-	-	-	-	-
14	CLA	aA	1139	-	64,68,73	1.23	8 (12%)	76,107,113	1.25	5 (6%)
14	CLA	k	502	13	49,53,73	1.40	8 (16%)	58,89,113	1.45	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	X	502	13	64,68,73	1.23	9 (14%)	76,107,113	1.32	6 (7%)
17	BCR	T	524	-	41,41,41	0.69	0	56,56,56	2.10	15 (26%)
14	CLA	W	505	13	69,73,73	1.17	7 (10%)	82,113,113	1.27	7 (8%)
14	CLA	Z	502	13	60,64,73	1.27	8 (13%)	71,102,113	1.33	5 (7%)
14	CLA	m	518	13	49,53,73	1.39	6 (12%)	58,89,113	1.44	5 (8%)
16	SF4	aC	3002	3	0,12,12	-	-	-		
14	CLA	a4	509	13	69,73,73	1.18	7 (10%)	82,113,113	1.28	6 (7%)
14	CLA	n	502	13	61,65,73	1.26	8 (13%)	72,103,113	1.34	5 (6%)
14	CLA	aB	1222	-	64,68,73	1.23	7 (10%)	76,107,113	1.32	8 (10%)
14	CLA	bA	1101	1	64,68,73	1.23	8 (12%)	76,107,113	1.28	5 (6%)
14	CLA	Y	501	13	69,73,73	1.19	9 (13%)	82,113,113	1.28	6 (7%)
14	CLA	b4	505	13	64,68,73	1.22	7 (10%)	76,107,113	1.27	6 (7%)
20	SQD	c2	822	-	29,31,54	1.26	3 (10%)	39,42,65	1.69	9 (23%)
14	CLA	g	504	-	49,53,73	1.41	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	bB	1238	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
14	CLA	cB	1211	2	69,73,73	1.18	7 (10%)	82,113,113	1.27	7 (8%)
17	BCR	b1	523	-	41,41,41	0.69	0	56,56,56	1.89	14 (25%)
14	CLA	q	511	13	49,53,73	1.41	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	a4	518	13	61,65,73	1.26	8 (13%)	72,103,113	1.35	6 (8%)
17	BCR	aA	4002	-	41,41,41	0.68	0	56,56,56	2.07	15 (26%)
14	CLA	a3	518	13	63,67,73	1.23	7 (11%)	74,105,113	1.34	5 (6%)
17	BCR	aL	4022	-	41,41,41	0.65	0	56,56,56	2.13	14 (25%)
14	CLA	g	509	13	49,53,73	1.40	7 (14%)	58,89,113	1.43	5 (8%)
14	CLA	p	513	13	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)
17	BCR	aI	4019	-	41,41,41	0.69	0	56,56,56	2.02	12 (21%)
17	BCR	aK	4001	-	41,41,41	0.68	0	56,56,56	1.93	15 (26%)
14	CLA	a6	508	13	59,63,73	1.28	9 (15%)	70,101,113	1.32	6 (8%)
14	CLA	bA	1011	1	69,73,73	1.18	6 (8%)	82,113,113	1.23	7 (8%)
17	BCR	cF	4015	-	41,41,41	0.67	0	56,56,56	2.12	16 (28%)
17	BCR	c	521	-	41,41,41	0.66	0	56,56,56	2.10	13 (23%)
14	CLA	j	502	13	49,53,73	1.41	8 (16%)	58,89,113	1.42	4 (6%)
14	CLA	Y	507	-	64,68,73	1.22	7 (10%)	76,107,113	1.28	5 (6%)
20	SQD	b1	822	-	29,31,54	1.27	4 (13%)	39,42,65	1.63	9 (23%)
14	CLA	aA	1124	-	60,64,73	1.25	7 (11%)	71,102,113	1.35	7 (9%)
14	CLA	a1	507	-	64,68,73	1.22	7 (10%)	76,107,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	cA	1104	1	69,73,73	1.17	6 (8%)	82,113,113	1.25	6 (7%)
21	LMG	bB	5002	-	49,49,55	0.74	1 (2%)	57,57,63	1.33	8 (14%)
14	CLA	bA	1124	-	60,64,73	1.26	7 (11%)	71,102,113	1.34	6 (8%)
14	CLA	cB	1222	-	64,68,73	1.22	7 (10%)	76,107,113	1.30	7 (9%)
14	CLA	cB	1217	2	59,63,73	1.28	7 (11%)	70,101,113	1.33	6 (8%)
14	CLA	cB	1238	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
14	CLA	U	508	13	54,58,73	1.33	8 (14%)	64,95,113	1.36	6 (9%)
15	PQN	bA	2001	-	34,34,34	3.05	12 (35%)	43,45,45	1.97	6 (13%)
14	CLA	aJ	1303	8	61,65,73	1.28	6 (9%)	72,103,113	1.38	6 (8%)
20	SQD	c4	822	-	31,33,54	1.22	3 (9%)	41,44,65	1.66	10 (24%)
14	CLA	a6	518	13	54,58,73	1.33	8 (14%)	64,95,113	1.38	6 (9%)
17	BCR	cA	4003	-	41,41,41	0.69	0	56,56,56	2.09	14 (25%)
14	CLA	cB	1232	-	49,53,73	1.41	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	p	503	13	49,53,73	1.40	6 (12%)	58,89,113	1.42	4 (6%)
21	LMG	aJ	5104	-	31,31,55	0.91	0	39,39,63	1.22	4 (10%)
14	CLA	b3	519	13	56,60,73	1.32	6 (10%)	65,97,113	1.35	6 (9%)
14	CLA	a3	504	-	62,66,73	1.26	8 (12%)	73,104,113	1.35	5 (6%)
20	SQD	p	822	-	29,31,54	1.17	2 (6%)	39,42,65	1.64	9 (23%)
14	CLA	c1	518	13	59,63,73	1.27	7 (11%)	70,101,113	1.34	6 (8%)
14	CLA	k	513	13	49,53,73	1.40	6 (12%)	58,89,113	1.37	4 (6%)
17	BCR	c3	522	-	41,41,41	0.67	0	56,56,56	2.08	15 (26%)
18	LHG	aA	5001	-	47,47,48	0.62	1 (2%)	50,53,54	1.28	6 (12%)
14	CLA	i	513	13	49,53,73	1.40	7 (14%)	58,89,113	1.38	4 (6%)
14	CLA	X	504	-	59,63,73	1.27	8 (13%)	70,101,113	1.37	6 (8%)
14	CLA	T	506	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
14	CLA	Y	502	13	64,68,73	1.23	9 (14%)	76,107,113	1.31	6 (7%)
14	CLA	a1	513	13	54,58,73	1.33	7 (12%)	64,95,113	1.37	7 (10%)
17	BCR	k	523	-	41,41,41	0.71	0	56,56,56	1.95	16 (28%)
14	CLA	aB	1238	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
14	CLA	o	501	13	50,54,73	1.38	8 (16%)	59,90,113	1.39	4 (6%)
14	CLA	c1	503	13	67,71,73	1.20	6 (8%)	79,110,113	1.30	5 (6%)
14	CLA	bA	1119	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
14	CLA	a3	517	-	49,53,73	1.40	7 (14%)	58,89,113	1.44	6 (10%)
17	BCR	bA	4011	-	41,41,41	0.69	0	56,56,56	2.18	15 (26%)
14	CLA	aB	1216	-	64,68,73	1.23	8 (12%)	76,107,113	1.28	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	bB	1214	2	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
14	CLA	bB	1204	2	64,68,73	1.22	7 (10%)	76,107,113	1.26	5 (6%)
14	CLA	T	512	13	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
17	BCR	bF	4015	-	41,41,41	0.67	0	56,56,56	2.05	16 (28%)
14	CLA	a4	513	13	54,58,73	1.33	7 (12%)	64,95,113	1.37	7 (10%)
14	CLA	d	511	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
17	BCR	b4	522	-	41,41,41	0.68	0	56,56,56	2.06	16 (28%)
14	CLA	m	519	13	49,53,73	1.41	6 (12%)	58,89,113	1.37	4 (6%)
14	CLA	a1	517	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	5 (8%)
20	SQD	q	822	-	24,26,54	1.33	2 (8%)	34,37,65	1.75	8 (23%)
14	CLA	c2	511	13	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
17	BCR	c4	522	-	41,41,41	0.68	0	56,56,56	2.12	15 (26%)
14	CLA	c5	513	13	59,63,73	1.28	6 (10%)	70,101,113	1.31	5 (7%)
14	CLA	Z	518	13	59,63,73	1.28	7 (11%)	70,101,113	1.33	6 (8%)
14	CLA	bK	1103	9	45,49,73	1.46	9 (20%)	54,83,113	1.37	3 (5%)
14	CLA	b5	504	-	59,63,73	1.28	7 (11%)	70,101,113	1.32	5 (7%)
14	CLA	b1	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.40	5 (8%)
14	CLA	X	508	13	49,53,73	1.40	9 (18%)	58,89,113	1.41	5 (8%)
14	CLA	b4	513	13	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
14	CLA	aA	1131	1	69,73,73	1.19	7 (10%)	82,113,113	1.24	6 (7%)
14	CLA	b1	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.25	7 (8%)
14	CLA	a	510	13	49,53,73	1.40	7 (14%)	58,89,113	1.39	5 (8%)
14	CLA	V	519	13	49,53,73	1.40	6 (12%)	58,89,113	1.38	4 (6%)
17	BCR	bJ	4013	-	41,41,41	0.66	0	56,56,56	2.19	19 (33%)
17	BCR	e	522	-	41,41,41	0.68	0	56,56,56	2.20	15 (26%)
17	BCR	a2	521	-	41,41,41	0.65	0	56,56,56	2.03	14 (25%)
14	CLA	b	518	13	54,58,73	1.33	7 (12%)	64,95,113	1.39	6 (9%)
14	CLA	cA	1013	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	7 (8%)
14	CLA	aB	1209	2	57,61,73	1.31	7 (12%)	67,98,113	1.40	7 (10%)
14	CLA	b3	518	13	60,64,73	1.27	6 (10%)	71,102,113	1.32	6 (8%)
14	CLA	b4	502	13	64,68,73	1.23	8 (12%)	76,107,113	1.31	6 (7%)
14	CLA	c6	504	-	49,53,73	1.40	7 (14%)	58,89,113	1.43	4 (6%)
14	CLA	h	507	-	49,53,73	1.40	7 (14%)	58,89,113	1.39	5 (8%)
14	CLA	S	503	13	64,68,73	1.23	7 (10%)	76,107,113	1.29	5 (6%)
14	CLA	cA	1136	1	69,73,73	1.17	7 (10%)	82,113,113	1.25	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	Z	510	13	69,73,73	1.19	8 (11%)	82,113,113	1.24	6 (7%)
14	CLA	aB	1232	-	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	j	505	13	49,53,73	1.40	6 (12%)	58,89,113	1.38	4 (6%)
14	CLA	aB	1227	2	58,62,73	1.28	8 (13%)	68,99,113	1.35	7 (10%)
14	CLA	f	503	13	49,53,73	1.40	6 (12%)	58,89,113	1.42	4 (6%)
17	BCR	X	523	-	41,41,41	0.69	0	56,56,56	1.89	18 (32%)
14	CLA	n	510	13	49,53,73	1.40	7 (14%)	58,89,113	1.38	4 (6%)
14	CLA	bB	1236	2	54,58,73	1.32	6 (11%)	64,95,113	1.35	6 (9%)
14	CLA	e	513	13	49,53,73	1.41	8 (16%)	58,89,113	1.37	4 (6%)
17	BCR	Z	523	-	41,41,41	0.71	1 (2%)	56,56,56	2.01	18 (32%)
14	CLA	T	509	13	65,69,73	1.21	7 (10%)	77,108,113	1.30	5 (6%)
14	CLA	bA	1118	1	64,68,73	1.23	7 (10%)	76,107,113	1.29	5 (6%)
17	BCR	cA	4008	-	41,41,41	0.71	0	56,56,56	2.02	12 (21%)
14	CLA	aB	1207	2	69,73,73	1.18	7 (10%)	82,113,113	1.28	5 (6%)
14	CLA	W	511	13	49,53,73	1.41	8 (16%)	58,89,113	1.43	4 (6%)
14	CLA	aB	1204	2	64,68,73	1.22	7 (10%)	76,107,113	1.27	5 (6%)
14	CLA	aA	1130	1	59,63,73	1.27	7 (11%)	70,101,113	1.35	8 (11%)
14	CLA	b2	504	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
17	BCR	o	523	-	41,41,41	0.70	0	56,56,56	1.94	16 (28%)
14	CLA	aB	1213	2	69,73,73	1.17	6 (8%)	82,113,113	1.29	7 (8%)
14	CLA	b4	501	13	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
14	CLA	cB	1219	-	56,60,73	1.30	5 (8%)	65,97,113	1.40	7 (10%)
14	CLA	V	517	-	49,53,73	1.41	8 (16%)	58,89,113	1.33	6 (10%)
14	CLA	m	509	13	49,53,73	1.40	7 (14%)	58,89,113	1.43	4 (6%)
14	CLA	bB	1210	2	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
14	CLA	bA	1103	1	69,73,73	1.18	6 (8%)	82,113,113	1.29	6 (7%)
17	BCR	h	522	-	41,41,41	0.68	0	56,56,56	2.04	16 (28%)
14	CLA	Y	512	13	49,53,73	1.39	8 (16%)	58,89,113	1.40	4 (6%)
17	BCR	cJ	4013	-	41,41,41	0.66	0	56,56,56	2.21	17 (30%)
14	CLA	i	512	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	b2	509	13	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
18	LHG	cA	5002	-	41,41,48	0.67	1 (2%)	44,47,54	1.22	4 (9%)
14	CLA	Z	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
17	BCR	c5	523	-	41,41,41	0.70	0	56,56,56	2.00	16 (28%)
14	CLA	q	506	13	49,53,73	1.41	8 (16%)	58,89,113	1.45	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	U	503	13	49,53,73	1.41	6 (12%)	58,89,113	1.43	4 (6%)
14	CLA	f	505	13	49,53,73	1.39	6 (12%)	58,89,113	1.46	9 (15%)
14	CLA	V	501	13	66,70,73	1.21	8 (12%)	78,109,113	1.28	6 (7%)
14	CLA	b	504	-	54,58,73	1.34	7 (12%)	64,95,113	1.39	6 (9%)
14	CLA	cB	1012	-	66,70,73	1.20	7 (10%)	78,109,113	1.21	6 (7%)
14	CLA	j	507	-	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)
14	CLA	aB	1226	2	69,73,73	1.19	8 (11%)	82,113,113	1.31	6 (7%)
14	CLA	g	517	-	49,53,73	1.40	7 (14%)	58,89,113	1.38	4 (6%)
14	CLA	a5	502	13	64,68,73	1.23	9 (14%)	76,107,113	1.31	6 (7%)
14	CLA	T	517	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	5 (8%)
14	CLA	b	513	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	5 (8%)
14	CLA	bB	1201	2	61,65,73	1.25	6 (9%)	72,103,113	1.31	5 (6%)
14	CLA	m	507	-	49,53,73	1.40	6 (12%)	58,89,113	1.41	4 (6%)
14	CLA	b4	510	13	69,73,73	1.18	6 (8%)	82,113,113	1.27	6 (7%)
14	CLA	bA	1132	1	69,73,73	1.17	8 (11%)	82,113,113	1.28	7 (8%)
14	CLA	b5	517	-	49,53,73	1.40	7 (14%)	58,89,113	1.44	4 (6%)
14	CLA	cA	1107	1	59,63,73	1.27	7 (11%)	70,101,113	1.32	6 (8%)
14	CLA	b6	510	13	69,73,73	1.18	7 (10%)	82,113,113	1.24	7 (8%)
14	CLA	a3	507	-	66,70,73	1.21	7 (10%)	78,109,113	1.27	5 (6%)
14	CLA	aB	1236	2	54,58,73	1.33	7 (12%)	64,95,113	1.36	6 (9%)
14	CLA	Y	510	13	69,73,73	1.18	7 (10%)	82,113,113	1.26	4 (4%)
20	SQD	S	822	-	29,31,54	1.25	3 (10%)	39,42,65	1.66	10 (25%)
14	CLA	cB	1226	2	69,73,73	1.19	8 (11%)	82,113,113	1.31	7 (8%)
17	BCR	b6	523	-	41,41,41	0.69	0	56,56,56	2.00	14 (25%)
14	CLA	d	508	13	59,63,73	1.28	9 (15%)	70,101,113	1.33	6 (8%)
14	CLA	c2	517	-	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	h	512	13	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	a5	510	13	69,73,73	1.19	7 (10%)	82,113,113	1.26	6 (7%)
14	CLA	aB	1221	2	64,68,73	1.22	7 (10%)	76,107,113	1.27	5 (6%)
14	CLA	o	504	-	49,53,73	1.41	8 (16%)	58,89,113	1.42	4 (6%)
17	BCR	j	522	-	41,41,41	0.68	0	56,56,56	2.17	15 (26%)
14	CLA	a2	510	13	69,73,73	1.18	7 (10%)	82,113,113	1.28	7 (8%)
17	BCR	aI	4018	-	41,41,41	0.74	1 (2%)	56,56,56	2.12	15 (26%)
14	CLA	a	511	13	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
14	CLA	c3	516	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	c2	521	-	41,41,41	0.66	0	56,56,56	2.06	13 (23%)
14	CLA	cA	1237	-	69,73,73	1.19	8 (11%)	82,113,113	1.28	6 (7%)
17	BCR	a5	522	-	41,41,41	0.68	0	56,56,56	2.09	16 (28%)
17	BCR	bA	4007	-	41,41,41	0.69	0	56,56,56	2.05	15 (26%)
14	CLA	cB	1234	2	64,68,73	1.24	8 (12%)	76,107,113	1.30	6 (7%)
14	CLA	c	511	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
20	SQD	a5	822	-	31,33,54	1.23	3 (9%)	41,44,65	1.65	9 (21%)
14	CLA	U	509	13	49,53,73	1.40	6 (12%)	58,89,113	1.41	4 (6%)
14	CLA	p	516	13	49,53,73	1.39	6 (12%)	58,89,113	1.40	4 (6%)
14	CLA	cB	1233	-	49,53,73	1.40	6 (12%)	58,89,113	1.41	4 (6%)
14	CLA	a	504	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	cB	1225	2	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
14	CLA	b1	509	13	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
14	CLA	m	501	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
17	BCR	b5	522	-	41,41,41	0.69	0	56,56,56	2.09	16 (28%)
14	CLA	n	511	13	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
14	CLA	b4	503	13	69,73,73	1.18	7 (10%)	82,113,113	1.24	5 (6%)
14	CLA	S	510	13	59,63,73	1.27	7 (11%)	70,101,113	1.32	7 (10%)
14	CLA	b1	512	13	57,61,73	1.30	8 (14%)	67,98,113	1.34	6 (8%)
17	BCR	cF	4016	-	41,41,41	0.69	0	56,56,56	2.07	15 (26%)
20	SQD	b5	822	-	28,30,54	1.29	3 (10%)	38,41,65	1.68	9 (23%)
14	CLA	bB	1207	2	69,73,73	1.18	7 (10%)	82,113,113	1.29	5 (6%)
14	CLA	bA	1109	1	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
17	BCR	cA	4011	-	41,41,41	0.69	0	56,56,56	2.16	16 (28%)
14	CLA	Y	503	13	67,71,73	1.20	6 (8%)	79,110,113	1.27	5 (6%)
14	CLA	c4	511	13	49,53,73	1.41	8 (16%)	58,89,113	1.43	4 (6%)
14	CLA	V	518	13	49,53,73	1.39	6 (12%)	58,89,113	1.43	5 (8%)
14	CLA	n	509	13	64,68,73	1.23	7 (10%)	76,107,113	1.29	6 (7%)
14	CLA	b3	513	13	54,58,73	1.33	7 (12%)	64,95,113	1.39	6 (9%)
14	CLA	cA	1108	1	49,53,73	1.40	8 (16%)	58,89,113	1.39	4 (6%)
14	CLA	j	509	13	64,68,73	1.22	7 (10%)	76,107,113	1.29	6 (7%)
14	CLA	cA	1103	1	69,73,73	1.18	6 (8%)	82,113,113	1.29	5 (6%)
17	BCR	X	522	-	41,41,41	0.68	0	56,56,56	2.06	17 (30%)
17	BCR	cL	4022	-	41,41,41	0.64	0	56,56,56	2.15	13 (23%)
14	CLA	cB	1201	2	61,65,73	1.26	6 (9%)	72,103,113	1.32	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a4	508	13	69,73,73	1.18	9 (13%)	82,113,113	1.31	6 (7%)
14	CLA	c6	513	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	5 (8%)
17	BCR	aJ	4013	-	41,41,41	0.67	0	56,56,56	2.13	18 (32%)
14	CLA	S	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
14	CLA	i	516	13	49,53,73	1.38	8 (16%)	58,89,113	1.44	5 (8%)
14	CLA	cB	1223	2	69,73,73	1.18	8 (11%)	82,113,113	1.28	7 (8%)
17	BCR	c5	522	-	41,41,41	0.66	0	56,56,56	2.12	15 (26%)
20	SQD	b2	822	-	30,32,54	1.26	4 (13%)	40,43,65	1.70	10 (25%)
14	CLA	b6	512	13	49,53,73	1.41	8 (16%)	58,89,113	1.39	4 (6%)
14	CLA	d	504	-	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	a2	507	-	65,69,73	1.21	7 (10%)	77,108,113	1.27	6 (7%)
20	SQD	m	822	-	27,29,54	1.22	3 (11%)	37,40,65	1.66	8 (21%)
14	CLA	bB	1224	2	61,65,73	1.25	9 (14%)	72,103,113	1.27	6 (8%)
17	BCR	cI	4020	-	41,41,41	0.68	0	56,56,56	1.98	15 (26%)
14	CLA	b4	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	Y	513	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	5 (8%)
14	CLA	e	512	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
17	BCR	b1	522	-	41,41,41	0.69	0	56,56,56	2.02	17 (30%)
14	CLA	bA	1104	1	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
14	CLA	b6	506	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
14	CLA	b6	502	13	64,68,73	1.23	9 (14%)	76,107,113	1.29	6 (7%)
14	CLA	k	512	13	49,53,73	1.40	7 (14%)	58,89,113	1.43	4 (6%)
14	CLA	bB	1231	2	59,63,73	1.29	7 (11%)	70,101,113	1.31	6 (8%)
17	BCR	a4	523	-	41,41,41	0.71	1 (2%)	56,56,56	1.97	16 (28%)
17	BCR	bA	4008	-	41,41,41	0.70	0	56,56,56	2.05	16 (28%)
14	CLA	b2	517	-	49,53,73	1.40	8 (16%)	58,89,113	1.42	5 (8%)
14	CLA	h	504	-	49,53,73	1.40	8 (16%)	58,89,113	1.42	5 (8%)
14	CLA	c2	519	13	54,58,73	1.33	6 (11%)	64,95,113	1.38	6 (9%)
14	CLA	a2	517	-	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	bJ	1302	8	51,55,73	1.37	7 (13%)	60,91,113	1.38	4 (6%)
17	BCR	c	524	-	41,41,41	0.70	0	56,56,56	2.13	17 (30%)
17	BCR	cF	4014	-	41,41,41	0.69	0	56,56,56	2.21	16 (28%)
14	CLA	V	504	-	59,63,73	1.29	8 (13%)	70,101,113	1.33	5 (7%)
14	CLA	d	512	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	bA	1115	1	64,68,73	1.22	7 (10%)	76,107,113	1.31	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	c4	521	-	41,41,41	0.66	0	56,56,56	2.09	17 (30%)
14	CLA	b1	513	13	54,58,73	1.33	7 (12%)	64,95,113	1.38	6 (9%)
14	CLA	q	502	13	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
14	CLA	bB	1217	2	59,63,73	1.27	7 (11%)	70,101,113	1.33	5 (7%)
14	CLA	a2	511	13	55,59,73	1.33	8 (14%)	64,96,113	1.40	5 (7%)
21	LMG	cJ	5104	-	31,31,55	0.90	0	39,39,63	1.22	4 (10%)
14	CLA	m	517	-	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
20	SQD	T	822	-	29,31,54	1.25	3 (10%)	39,42,65	1.70	11 (28%)
14	CLA	o	519	13	49,53,73	1.40	7 (14%)	58,89,113	1.36	4 (6%)
17	BCR	q	524	-	41,41,41	0.70	0	56,56,56	2.12	18 (32%)
14	CLA	m	503	13	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)
14	CLA	X	501	13	69,73,73	1.19	7 (10%)	82,113,113	1.27	6 (7%)
17	BCR	b1	524	-	41,41,41	0.70	0	56,56,56	2.03	17 (30%)
14	CLA	c4	516	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	Y	516	13	49,53,73	1.40	5 (10%)	58,89,113	1.43	4 (6%)
14	CLA	k	505	13	49,53,73	1.40	6 (12%)	58,89,113	1.38	4 (6%)
17	BCR	m	521	-	41,41,41	0.64	0	56,56,56	2.17	15 (26%)
14	CLA	aA	1122	1	64,68,73	1.23	7 (10%)	76,107,113	1.29	6 (7%)
14	CLA	k	504	-	49,53,73	1.41	6 (12%)	58,89,113	1.42	4 (6%)
14	CLA	bB	1216	-	59,63,73	1.28	8 (13%)	70,101,113	1.32	5 (7%)
20	SQD	a4	822	-	34,36,54	1.17	3 (8%)	44,47,65	1.61	10 (22%)
14	CLA	Z	505	13	69,73,73	1.17	7 (10%)	82,113,113	1.24	5 (6%)
14	CLA	j	513	13	54,58,73	1.33	6 (11%)	64,95,113	1.39	6 (9%)
15	PQN	cB	2002	-	34,34,34	3.04	11 (32%)	43,45,45	2.00	6 (13%)
14	CLA	S	509	13	69,73,73	1.18	6 (8%)	82,113,113	1.27	5 (6%)
14	CLA	aA	1013	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
14	CLA	T	504	-	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	S	511	13	54,58,73	1.34	7 (12%)	64,95,113	1.39	6 (9%)
14	CLA	c5	501	13	69,73,73	1.19	7 (10%)	82,113,113	1.26	6 (7%)
14	CLA	bA	1022	-	69,73,73	1.18	8 (11%)	82,113,113	1.18	4 (4%)
18	LHG	bA	5005	-	38,38,48	0.69	0	41,44,54	1.29	4 (9%)
15	PQN	aA	2001	-	34,34,34	3.04	12 (35%)	43,45,45	1.97	6 (13%)
20	SQD	c3	822	-	30,32,54	1.25	3 (10%)	40,43,65	1.62	10 (25%)
14	CLA	cA	1135	1	55,59,73	1.32	8 (14%)	64,96,113	1.39	7 (10%)
14	CLA	c3	501	13	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	g	503	13	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)
14	CLA	S	512	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
17	BCR	Z	522	-	41,41,41	0.67	0	56,56,56	2.15	15 (26%)
14	CLA	c5	508	13	59,63,73	1.28	9 (15%)	70,101,113	1.31	6 (8%)
14	CLA	o	516	13	49,53,73	1.40	5 (10%)	58,89,113	1.45	5 (8%)
14	CLA	aA	1123	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	8 (9%)
17	BCR	bB	4005	-	41,41,41	0.72	0	56,56,56	1.95	13 (23%)
21	LMG	a1	5104	-	40,40,55	0.85	1 (2%)	48,48,63	1.22	4 (8%)
14	CLA	cJ	1303	8	61,65,73	1.28	7 (11%)	72,103,113	1.39	6 (8%)
20	SQD	W	822	-	30,32,54	1.24	3 (10%)	40,43,65	1.66	9 (22%)
14	CLA	bB	1220	2	54,58,73	1.33	8 (14%)	64,95,113	1.39	6 (9%)
14	CLA	b6	503	13	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)
17	BCR	c1	521	-	41,41,41	0.67	0	56,56,56	2.12	15 (26%)
14	CLA	a5	503	13	69,73,73	1.19	6 (8%)	82,113,113	1.25	5 (6%)
14	CLA	q	501	13	61,65,73	1.26	8 (13%)	72,103,113	1.32	6 (8%)
17	BCR	b2	523	-	41,41,41	0.68	0	56,56,56	1.91	12 (21%)
17	BCR	b3	522	-	41,41,41	0.68	0	56,56,56	2.08	17 (30%)
14	CLA	Z	513	13	54,58,73	1.33	7 (12%)	64,95,113	1.37	5 (7%)
14	CLA	b5	507	-	65,69,73	1.21	8 (12%)	77,108,113	1.31	5 (6%)
17	BCR	a2	523	-	41,41,41	0.69	0	56,56,56	1.92	15 (26%)
14	CLA	a5	511	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	cF	1301	-	49,53,73	1.41	8 (16%)	58,89,113	1.38	4 (6%)
14	CLA	b	508	13	49,53,73	1.39	7 (14%)	58,89,113	1.42	5 (8%)
14	CLA	c2	518	13	59,63,73	1.28	8 (13%)	70,101,113	1.32	6 (8%)
14	CLA	c	509	13	66,70,73	1.21	8 (12%)	78,109,113	1.30	6 (7%)
14	CLA	o	517	-	49,53,73	1.41	8 (16%)	58,89,113	1.40	4 (6%)
17	BCR	c6	521	-	41,41,41	0.66	0	56,56,56	2.14	16 (28%)
17	BCR	b4	524	-	41,41,41	0.71	0	56,56,56	2.07	14 (25%)
14	CLA	cA	1106	1	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
14	CLA	aB	1021	2	69,73,73	1.18	6 (8%)	82,113,113	1.19	6 (7%)
14	CLA	S	505	13	59,63,73	1.28	7 (11%)	70,101,113	1.32	8 (11%)
14	CLA	c6	505	13	64,68,73	1.23	7 (10%)	76,107,113	1.28	6 (7%)
17	BCR	q	523	-	41,41,41	0.68	0	56,56,56	1.95	14 (25%)
14	CLA	c6	503	13	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)
19	LMU	aA	1849	-	23,23,36	1.13	1 (4%)	28,28,47	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	c5	512	13	56,60,73	1.32	8 (14%)	65,97,113	1.35	6 (9%)
17	BCR	a2	524	-	41,41,41	0.69	0	56,56,56	2.03	14 (25%)
14	CLA	Y	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.42	5 (8%)
14	CLA	d	519	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
14	CLA	k	503	13	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)
14	CLA	a1	506	13	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
14	CLA	U	512	13	49,53,73	1.42	8 (16%)	58,89,113	1.41	5 (8%)
14	CLA	Y	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
14	CLA	a5	513	13	59,63,73	1.27	7 (11%)	70,101,113	1.31	5 (7%)
14	CLA	b2	519	13	54,58,73	1.33	7 (12%)	64,95,113	1.38	5 (7%)
14	CLA	b4	517	-	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
14	CLA	aB	1214	2	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
14	CLA	cA	1011	1	69,73,73	1.18	7 (10%)	82,113,113	1.24	7 (8%)
17	BCR	b3	523	-	41,41,41	0.69	0	56,56,56	1.98	12 (21%)
14	CLA	cA	1137	1	59,63,73	1.29	7 (11%)	70,101,113	1.32	5 (7%)
14	CLA	a4	506	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	6 (10%)
14	CLA	cA	1124	-	60,64,73	1.26	7 (11%)	71,102,113	1.35	7 (9%)
14	CLA	bA	1137	1	59,63,73	1.29	8 (13%)	70,101,113	1.32	5 (7%)
14	CLA	b2	507	-	67,71,73	1.20	7 (10%)	79,110,113	1.26	5 (6%)
14	CLA	p	511	13	49,53,73	1.41	6 (12%)	58,89,113	1.43	4 (6%)
18	LHG	aX	4021	-	38,38,48	0.70	0	41,44,54	1.38	6 (14%)
14	CLA	a3	511	13	66,70,73	1.21	7 (10%)	78,109,113	1.28	5 (6%)
14	CLA	q	508	13	49,53,73	1.40	8 (16%)	58,89,113	1.42	5 (8%)
14	CLA	a5	517	-	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	c	504	-	49,53,73	1.40	7 (14%)	58,89,113	1.43	4 (6%)
14	CLA	j	503	13	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)
14	CLA	f	518	13	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
14	CLA	c1	512	13	57,61,73	1.30	8 (14%)	67,98,113	1.34	6 (8%)
14	CLA	aB	1220	2	54,58,73	1.33	7 (12%)	64,95,113	1.39	6 (9%)
14	CLA	bA	1127	1	69,73,73	1.18	7 (10%)	82,113,113	1.22	6 (7%)
17	BCR	h	524	-	41,41,41	0.71	0	56,56,56	2.06	16 (28%)
14	CLA	bA	1113	1	54,58,73	1.33	7 (12%)	64,95,113	1.41	8 (12%)
14	CLA	f	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	aK	1401	-	59,63,73	1.29	8 (13%)	70,101,113	1.33	5 (7%)
14	CLA	bB	1228	2	60,64,73	1.27	7 (11%)	71,102,113	1.32	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	c6	502	13	64,68,73	1.23	7 (10%)	76,107,113	1.31	6 (7%)
14	CLA	o	508	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
20	SQD	h	822	-	30,32,54	1.24	3 (10%)	40,43,65	1.66	9 (22%)
14	CLA	aA	1120	1	59,63,73	1.28	7 (11%)	70,101,113	1.33	6 (8%)
14	CLA	cL	1502	10	64,68,73	1.22	8 (12%)	76,107,113	1.30	6 (7%)
20	SQD	b3	822	-	35,37,54	1.15	3 (8%)	45,48,65	1.64	12 (26%)
14	CLA	aA	1801	18	49,53,73	1.39	8 (16%)	58,89,113	1.39	4 (6%)
14	CLA	k	509	13	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
14	CLA	i	505	13	59,63,73	1.27	7 (11%)	70,101,113	1.32	7 (10%)
17	BCR	a6	521	-	41,41,41	0.66	0	56,56,56	2.09	14 (25%)
14	CLA	cA	1117	1	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
14	CLA	c1	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.26	5 (6%)
14	CLA	b	516	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
14	CLA	bB	1218	2	64,68,73	1.23	7 (10%)	76,107,113	1.31	5 (6%)
14	CLA	a2	504	-	51,55,73	1.36	8 (15%)	60,91,113	1.43	6 (10%)
14	CLA	d	501	13	49,53,73	1.40	6 (12%)	58,89,113	1.41	4 (6%)
14	CLA	b3	516	13	49,53,73	1.40	7 (14%)	58,89,113	1.45	5 (8%)
17	BCR	S	522	-	41,41,41	0.67	0	56,56,56	2.09	16 (28%)
14	CLA	e	502	13	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
14	CLA	aA	1118	1	64,68,73	1.23	8 (12%)	76,107,113	1.29	5 (6%)
19	LMU	bA	1849	-	23,23,36	1.12	1 (4%)	28,28,47	0.82	0
14	CLA	bB	1021	2	69,73,73	1.18	7 (10%)	82,113,113	1.19	6 (7%)
17	BCR	q	521	-	41,41,41	0.65	0	56,56,56	2.03	15 (26%)
14	CLA	bB	1235	2	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
14	CLA	b3	504	-	61,65,73	1.27	8 (13%)	72,103,113	1.33	6 (8%)
14	CLA	cK	1103	9	45,49,73	1.45	9 (20%)	54,83,113	1.37	3 (5%)
14	CLA	a1	512	13	57,61,73	1.30	6 (10%)	67,98,113	1.34	6 (8%)
14	CLA	X	503	13	67,71,73	1.20	7 (10%)	79,110,113	1.29	5 (6%)
17	BCR	aF	4015	-	41,41,41	0.67	0	56,56,56	2.05	14 (25%)
14	CLA	U	506	13	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	S	501	13	49,53,73	1.41	9 (18%)	58,89,113	1.37	4 (6%)
14	CLA	k	508	13	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
17	BCR	bJ	4012	-	41,41,41	0.66	0	56,56,56	2.03	17 (30%)
17	BCR	cI	4018	-	41,41,41	0.73	1 (2%)	56,56,56	2.14	15 (26%)
14	CLA	aA	1103	1	69,73,73	1.18	7 (10%)	82,113,113	1.28	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	g	513	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	5 (8%)
14	CLA	p	501	13	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)
14	CLA	a	501	13	64,68,73	1.23	8 (12%)	76,107,113	1.29	5 (6%)
17	BCR	bI	4019	-	41,41,41	0.69	0	56,56,56	2.02	14 (25%)
14	CLA	b6	508	13	55,59,73	1.32	8 (14%)	64,96,113	1.37	5 (7%)
14	CLA	a3	519	13	59,63,73	1.28	7 (11%)	70,101,113	1.32	6 (8%)
14	CLA	W	508	13	55,59,73	1.32	9 (16%)	64,96,113	1.35	5 (7%)
14	CLA	a6	517	-	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	cA	1101	1	64,68,73	1.23	7 (10%)	76,107,113	1.29	5 (6%)
19	LMU	cA	1848	-	24,24,36	1.10	1 (4%)	29,29,47	0.81	0
14	CLA	c5	503	13	69,73,73	1.19	8 (11%)	82,113,113	1.25	5 (6%)
14	CLA	b6	501	13	69,73,73	1.19	8 (11%)	82,113,113	1.28	6 (7%)
17	BCR	p	524	-	41,41,41	0.70	0	56,56,56	2.11	15 (26%)
14	CLA	aB	1228	2	60,64,73	1.27	8 (13%)	71,102,113	1.30	6 (8%)
17	BCR	V	522	-	41,41,41	0.68	0	56,56,56	2.14	16 (28%)
14	CLA	h	505	13	49,53,73	1.40	7 (14%)	58,89,113	1.37	4 (6%)
14	CLA	bA	1114	-	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
14	CLA	aK	1103	9	45,49,73	1.45	9 (20%)	54,83,113	1.37	3 (5%)
14	CLA	a	507	-	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
14	CLA	a1	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.27	6 (7%)
14	CLA	a5	501	13	69,73,73	1.19	8 (11%)	82,113,113	1.27	6 (7%)
17	BCR	d	523	-	41,41,41	0.69	0	56,56,56	1.94	15 (26%)
14	CLA	V	508	13	56,60,73	1.31	8 (14%)	65,97,113	1.34	6 (9%)
14	CLA	cJ	1302	8	53,57,73	1.32	7 (13%)	61,93,113	1.42	6 (9%)
17	BCR	c6	523	-	41,41,41	0.72	1 (2%)	56,56,56	2.04	14 (25%)
14	CLA	a5	505	13	69,73,73	1.17	7 (10%)	82,113,113	1.24	6 (7%)
14	CLA	cB	1212	2	49,53,73	1.39	7 (14%)	58,89,113	1.43	4 (6%)
17	BCR	l	523	-	41,41,41	0.68	0	56,56,56	1.98	14 (25%)
14	CLA	bB	1225	2	69,73,73	1.18	7 (10%)	82,113,113	1.23	6 (7%)
14	CLA	W	519	13	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
17	BCR	W	523	-	41,41,41	0.69	0	56,56,56	2.01	13 (23%)
14	CLA	b	503	13	61,65,73	1.26	6 (9%)	72,103,113	1.31	5 (6%)
14	CLA	V	513	13	54,58,73	1.34	7 (12%)	64,95,113	1.34	5 (7%)
14	CLA	b5	501	13	69,73,73	1.19	8 (11%)	82,113,113	1.27	6 (7%)
14	CLA	c4	509	13	69,73,73	1.18	8 (11%)	82,113,113	1.28	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	SQD	c6	822	-	28,30,54	1.28	3 (10%)	38,41,65	1.71	9 (23%)
14	CLA	b4	512	13	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	Y	509	13	66,70,73	1.21	7 (10%)	78,109,113	1.29	8 (10%)
14	CLA	p	517	-	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
14	CLA	a4	517	-	49,53,73	1.40	6 (12%)	58,89,113	1.39	4 (6%)
14	CLA	a3	502	13	64,68,73	1.23	8 (12%)	76,107,113	1.31	5 (6%)
14	CLA	aA	1127	1	69,73,73	1.18	8 (11%)	82,113,113	1.22	6 (7%)
14	CLA	Y	518	13	60,64,73	1.27	8 (13%)	71,102,113	1.31	6 (8%)
17	BCR	V	523	-	41,41,41	0.67	0	56,56,56	1.91	13 (23%)
14	CLA	a6	507	-	66,70,73	1.20	7 (10%)	78,109,113	1.28	5 (6%)
14	CLA	cB	1227	2	58,62,73	1.29	8 (13%)	68,99,113	1.33	6 (8%)
17	BCR	bK	4001	-	41,41,41	0.67	0	56,56,56	1.93	15 (26%)
17	BCR	e	523	-	41,41,41	0.69	0	56,56,56	2.00	15 (26%)
14	CLA	a4	503	13	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
14	CLA	e	503	13	49,53,73	1.41	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	a2	512	13	57,61,73	1.30	7 (12%)	67,98,113	1.33	5 (7%)
14	CLA	b2	518	13	59,63,73	1.28	7 (11%)	70,101,113	1.33	6 (8%)
14	CLA	aB	1218	2	64,68,73	1.23	7 (10%)	76,107,113	1.30	4 (5%)
14	CLA	aB	1210	2	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
14	CLA	bB	1230	2	62,66,73	1.25	8 (12%)	73,104,113	1.35	6 (8%)
14	CLA	bL	1501	10	69,73,73	1.17	7 (10%)	82,113,113	1.28	7 (8%)
14	CLA	b2	501	13	69,73,73	1.17	7 (10%)	82,113,113	1.27	6 (7%)
17	BCR	aA	4007	-	41,41,41	0.69	0	56,56,56	2.02	17 (30%)
14	CLA	cB	1204	2	64,68,73	1.22	8 (12%)	76,107,113	1.27	6 (7%)
14	CLA	V	512	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
20	SQD	e	822	-	30,32,54	1.24	3 (10%)	40,43,65	1.67	9 (22%)
14	CLA	cA	1134	1	55,59,73	1.32	7 (12%)	64,96,113	1.37	6 (9%)
14	CLA	o	509	13	49,53,73	1.40	7 (14%)	58,89,113	1.43	5 (8%)
19	LMU	cA	1849	-	23,23,36	1.12	1 (4%)	28,28,47	0.79	0
14	CLA	o	511	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	T	513	13	54,58,73	1.33	7 (12%)	64,95,113	1.36	6 (9%)
17	BCR	S	523	-	41,41,41	0.68	0	56,56,56	2.00	14 (25%)
14	CLA	c3	509	13	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
14	CLA	c2	504	-	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
14	CLA	a6	511	13	49,53,73	1.41	7 (14%)	58,89,113	1.42	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	c5	502	13	64,68,73	1.23	8 (12%)	76,107,113	1.29	6 (7%)
14	CLA	cK	1401	-	59,63,73	1.29	8 (13%)	70,101,113	1.32	5 (7%)
14	CLA	m	516	13	49,53,73	1.40	8 (16%)	58,89,113	1.38	5 (8%)
14	CLA	cA	1129	1	56,60,73	1.31	8 (14%)	65,97,113	1.34	4 (6%)
17	BCR	n	522	-	41,41,41	0.69	0	56,56,56	2.20	15 (26%)
14	CLA	f	509	13	49,53,73	1.40	8 (16%)	58,89,113	1.44	5 (8%)
14	CLA	b4	509	13	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	a6	502	13	64,68,73	1.23	8 (12%)	76,107,113	1.30	6 (7%)
14	CLA	cA	1140	1	69,73,73	1.18	7 (10%)	82,113,113	1.22	5 (6%)
14	CLA	n	508	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	5 (8%)
14	CLA	b6	509	13	69,73,73	1.19	7 (10%)	82,113,113	1.27	6 (7%)
17	BCR	a1	522	-	41,41,41	0.68	0	56,56,56	2.06	16 (28%)
14	CLA	W	509	13	66,70,73	1.20	7 (10%)	78,109,113	1.29	5 (6%)
14	CLA	m	510	13	49,53,73	1.39	7 (14%)	58,89,113	1.41	6 (10%)
14	CLA	j	508	13	49,53,73	1.39	8 (16%)	58,89,113	1.43	5 (8%)
14	CLA	bB	1229	2	69,73,73	1.19	7 (10%)	82,113,113	1.23	6 (7%)
14	CLA	b	501	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	g	505	13	69,73,73	1.17	7 (10%)	82,113,113	1.23	6 (7%)
20	SQD	c1	822	-	29,31,54	1.27	3 (10%)	39,42,65	1.65	9 (23%)
14	CLA	T	501	13	54,58,73	1.33	9 (16%)	64,95,113	1.40	6 (9%)
17	BCR	cI	4019	-	41,41,41	0.69	0	56,56,56	2.03	13 (23%)
14	CLA	b3	501	13	69,73,73	1.18	6 (8%)	82,113,113	1.26	6 (7%)
14	CLA	d	506	13	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	aB	1205	2	69,73,73	1.17	9 (13%)	82,113,113	1.29	7 (8%)
17	BCR	a3	523	-	41,41,41	0.70	0	56,56,56	2.00	12 (21%)
14	CLA	c4	513	13	49,53,73	1.40	6 (12%)	58,89,113	1.41	4 (6%)
17	BCR	a5	521	-	41,41,41	0.66	0	56,56,56	2.09	14 (25%)
14	CLA	cA	1114	-	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	c6	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.42	5 (8%)
14	CLA	bX	1401	12	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
14	CLA	c3	517	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
14	CLA	e	509	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	cB	1220	2	51,55,73	1.36	7 (13%)	60,91,113	1.38	5 (8%)
14	CLA	aB	1224	2	61,65,73	1.25	9 (14%)	72,103,113	1.27	6 (8%)
17	BCR	n	523	-	41,41,41	0.69	0	56,56,56	1.97	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	S	504	-	49,53,73	1.41	8 (16%)	58,89,113	1.42	4 (6%)
14	CLA	b	507	-	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
14	CLA	a4	501	13	69,73,73	1.19	8 (11%)	82,113,113	1.26	6 (7%)
14	CLA	f	507	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	p	504	-	49,53,73	1.41	8 (16%)	58,89,113	1.42	4 (6%)
14	CLA	cA	1112	1	52,56,73	1.36	7 (13%)	61,92,113	1.39	5 (8%)
14	CLA	b3	507	-	64,68,73	1.22	7 (10%)	76,107,113	1.28	6 (7%)
17	BCR	X	524	-	41,41,41	0.69	0	56,56,56	2.03	15 (26%)
14	CLA	l	503	13	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
14	CLA	m	513	13	56,60,73	1.32	7 (12%)	65,97,113	1.34	6 (9%)
14	CLA	aA	1104	1	69,73,73	1.18	6 (8%)	82,113,113	1.26	7 (8%)
14	CLA	m	506	13	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	n	512	13	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
17	BCR	U	524	-	41,41,41	0.70	0	56,56,56	2.09	17 (30%)
14	CLA	cA	1111	1	59,63,73	1.28	7 (11%)	70,101,113	1.34	6 (8%)
14	CLA	V	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	cB	1023	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	7 (8%)
14	CLA	b6	504	-	59,63,73	1.29	6 (10%)	70,101,113	1.37	5 (7%)
14	CLA	b2	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
14	CLA	bB	1202	2	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
14	CLA	l	509	13	49,53,73	1.40	6 (12%)	58,89,113	1.42	4 (6%)
14	CLA	b2	503	13	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
14	CLA	h	517	-	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
20	SQD	Z	822	-	27,29,54	1.27	3 (11%)	37,40,65	1.82	11 (29%)
19	LMU	cJ	5105	-	21,21,36	1.14	1 (4%)	26,26,47	0.81	0
17	BCR	a	523	-	41,41,41	0.68	0	56,56,56	1.91	16 (28%)
17	BCR	c5	524	-	41,41,41	0.69	0	56,56,56	2.08	15 (26%)
14	CLA	bA	1131	1	69,73,73	1.19	8 (11%)	82,113,113	1.24	6 (7%)
14	CLA	a	503	13	67,71,73	1.20	6 (8%)	79,110,113	1.28	5 (6%)
17	BCR	d	521	-	41,41,41	0.64	0	56,56,56	2.06	15 (26%)
14	CLA	b3	517	-	49,53,73	1.40	8 (16%)	58,89,113	1.46	5 (8%)
20	SQD	n	822	-	29,31,54	1.18	2 (6%)	39,42,65	1.62	8 (20%)
17	BCR	bB	4017	-	41,41,41	0.68	0	56,56,56	2.07	15 (26%)
14	CLA	a1	518	13	59,63,73	1.27	6 (10%)	70,101,113	1.34	6 (8%)
17	BCR	b2	521	-	41,41,41	0.65	0	56,56,56	2.07	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	Z	516	13	49,53,73	1.40	7 (14%)	58,89,113	1.38	4 (6%)
14	CLA	l	507	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	q	504	-	49,53,73	1.41	6 (12%)	58,89,113	1.42	4 (6%)
14	CLA	bA	1237	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
14	CLA	f	504	-	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
14	CLA	j	512	13	49,53,73	1.41	7 (14%)	58,89,113	1.41	4 (6%)
14	CLA	cA	1109	1	69,73,73	1.18	6 (8%)	82,113,113	1.22	5 (6%)
14	CLA	a6	504	-	66,70,73	1.21	8 (12%)	78,109,113	1.29	4 (5%)
14	CLA	bB	1209	2	57,61,73	1.31	8 (14%)	67,98,113	1.41	7 (10%)
14	CLA	aX	1401	12	49,53,73	1.40	5 (10%)	58,89,113	1.40	4 (6%)
16	SF4	aA	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	V	503	13	49,53,73	1.40	6 (12%)	58,89,113	1.42	4 (6%)
17	BCR	a2	522	-	41,41,41	0.68	0	56,56,56	2.06	18 (32%)
17	BCR	cB	4009	-	41,41,41	0.71	0	56,56,56	2.08	16 (28%)
14	CLA	b	502	13	49,53,73	1.41	7 (14%)	58,89,113	1.44	4 (6%)
14	CLA	a5	518	13	61,65,73	1.25	8 (13%)	72,103,113	1.32	6 (8%)
14	CLA	a2	508	13	59,63,73	1.27	9 (15%)	70,101,113	1.33	6 (8%)
14	CLA	c1	513	13	56,60,73	1.31	6 (10%)	65,97,113	1.34	6 (9%)
14	CLA	b3	502	13	64,68,73	1.23	8 (12%)	76,107,113	1.28	5 (6%)
14	CLA	bA	1138	1	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
14	CLA	T	505	13	56,60,73	1.31	6 (10%)	65,97,113	1.35	6 (9%)
14	CLA	a4	504	-	57,61,73	1.32	7 (12%)	67,98,113	1.39	5 (7%)
14	CLA	Z	517	-	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	aA	1022	-	69,73,73	1.18	8 (11%)	82,113,113	1.18	4 (4%)
19	LMU	aJ	5105	-	22,22,36	1.12	1 (4%)	27,27,47	0.82	0
14	CLA	cA	1130	1	56,60,73	1.31	7 (12%)	65,97,113	1.38	8 (12%)
17	BCR	Y	523	-	41,41,41	0.69	0	56,56,56	1.90	15 (26%)
14	CLA	b5	518	13	59,63,73	1.28	8 (13%)	70,101,113	1.32	6 (8%)
14	CLA	q	517	-	49,53,73	1.40	6 (12%)	58,89,113	1.40	4 (6%)
14	CLA	h	511	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
17	BCR	aB	4010	-	41,41,41	0.69	0	56,56,56	2.09	16 (28%)
14	CLA	aA	1117	1	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
14	CLA	a1	510	13	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
14	CLA	X	509	13	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	m	511	13	49,53,73	1.41	7 (14%)	58,89,113	1.44	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	c	507	-	49,53,73	1.40	6 (12%)	58,89,113	1.40	4 (6%)
14	CLA	l	501	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	a3	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.39	4 (6%)
14	CLA	aB	1202	2	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
14	CLA	aB	1215	2	65,69,73	1.21	7 (10%)	77,108,113	1.28	6 (7%)
14	CLA	q	505	13	59,63,73	1.27	7 (11%)	70,101,113	1.31	6 (8%)
17	BCR	Y	524	-	41,41,41	0.70	0	56,56,56	2.03	16 (28%)
16	SF4	cC	3002	3	0,12,12	-	-	-		
20	SQD	Y	822	-	31,33,54	1.22	3 (9%)	41,44,65	1.77	11 (26%)
14	CLA	e	518	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	b4	516	13	49,53,73	1.39	6 (12%)	58,89,113	1.43	4 (6%)
14	CLA	a4	507	-	66,70,73	1.21	7 (10%)	78,109,113	1.28	5 (6%)
17	BCR	a4	521	-	41,41,41	0.65	0	56,56,56	2.12	16 (28%)
14	CLA	b1	511	13	59,63,73	1.28	7 (11%)	70,101,113	1.36	6 (8%)
14	CLA	c5	509	13	69,73,73	1.18	7 (10%)	82,113,113	1.27	6 (7%)
17	BCR	aI	4020	-	41,41,41	0.69	0	56,56,56	1.99	13 (23%)
14	CLA	X	506	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	5 (8%)
14	CLA	c4	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
14	CLA	b6	516	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
17	BCR	a3	521	-	41,41,41	0.64	0	56,56,56	2.01	14 (25%)
14	CLA	cA	1122	1	64,68,73	1.23	6 (9%)	76,107,113	1.30	6 (7%)
14	CLA	W	504	-	56,60,73	1.32	6 (10%)	65,97,113	1.35	5 (7%)
14	CLA	X	505	13	69,73,73	1.17	7 (10%)	82,113,113	1.26	6 (7%)
14	CLA	d	507	-	49,53,73	1.39	7 (14%)	58,89,113	1.41	4 (6%)
14	CLA	c6	517	-	49,53,73	1.41	7 (14%)	58,89,113	1.40	4 (6%)
14	CLA	aA	1136	1	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
14	CLA	n	506	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	5 (8%)
17	BCR	bM	4021	-	41,41,41	0.67	0	56,56,56	2.27	15 (26%)
14	CLA	f	510	13	49,53,73	1.39	6 (12%)	58,89,113	1.41	5 (8%)
20	SQD	cB	1852	-	37,39,54	1.13	3 (8%)	47,50,65	1.60	10 (21%)
17	BCR	cB	4017	-	41,41,41	0.68	0	56,56,56	2.11	15 (26%)
14	CLA	bB	1208	2	59,63,73	1.28	7 (11%)	70,101,113	1.29	6 (8%)
14	CLA	b5	509	13	69,73,73	1.18	6 (8%)	82,113,113	1.27	6 (7%)
14	CLA	aA	1137	1	59,63,73	1.29	6 (10%)	70,101,113	1.33	5 (7%)
14	CLA	k	517	-	49,53,73	1.43	7 (14%)	58,89,113	1.39	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	p	519	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	bB	1234	2	64,68,73	1.23	9 (14%)	76,107,113	1.30	6 (7%)
14	CLA	j	511	13	49,53,73	1.40	6 (12%)	58,89,113	1.41	4 (6%)
14	CLA	c6	509	13	69,73,73	1.19	8 (11%)	82,113,113	1.27	5 (6%)
14	CLA	m	505	13	55,59,73	1.32	7 (12%)	64,96,113	1.36	7 (10%)
14	CLA	b5	512	13	56,60,73	1.31	8 (14%)	65,97,113	1.34	6 (9%)
14	CLA	V	516	13	49,53,73	1.42	5 (10%)	58,89,113	1.34	4 (6%)
14	CLA	c6	511	13	49,53,73	1.41	7 (14%)	58,89,113	1.43	4 (6%)
14	CLA	aF	1301	-	49,53,73	1.41	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	a1	503	13	67,71,73	1.20	6 (8%)	79,110,113	1.26	5 (6%)
14	CLA	W	518	13	59,63,73	1.27	7 (11%)	70,101,113	1.33	6 (8%)
14	CLA	g	508	13	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	b6	519	13	49,53,73	1.41	5 (10%)	58,89,113	1.38	4 (6%)
17	BCR	S	524	-	41,41,41	0.69	0	56,56,56	2.10	18 (32%)
14	CLA	aA	1132	1	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	X	510	13	66,70,73	1.21	7 (10%)	78,109,113	1.28	6 (7%)
17	BCR	W	521	-	41,41,41	0.65	0	56,56,56	2.09	14 (25%)
14	CLA	cA	1120	1	59,63,73	1.29	5 (8%)	70,101,113	1.36	5 (7%)
14	CLA	V	507	-	49,53,73	1.40	6 (12%)	58,89,113	1.40	4 (6%)
17	BCR	a1	521	-	41,41,41	0.66	0	56,56,56	2.11	16 (28%)
14	CLA	aA	1113	1	54,58,73	1.33	7 (12%)	64,95,113	1.38	6 (9%)
14	CLA	bA	1106	1	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
14	CLA	aB	1235	2	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
14	CLA	aB	1231	2	59,63,73	1.29	8 (13%)	70,101,113	1.32	6 (8%)
17	BCR	a	522	-	41,41,41	0.68	0	56,56,56	2.16	15 (26%)
14	CLA	aL	1502	10	64,68,73	1.21	8 (12%)	76,107,113	1.29	6 (7%)
14	CLA	bA	1139	-	64,68,73	1.23	8 (12%)	76,107,113	1.25	6 (7%)
17	BCR	f	521	-	41,41,41	0.67	0	56,56,56	2.19	16 (28%)
14	CLA	c5	504	-	61,65,73	1.26	7 (11%)	72,103,113	1.33	4 (5%)
17	BCR	c4	524	-	41,41,41	0.70	0	56,56,56	2.01	15 (26%)
17	BCR	i	521	-	41,41,41	0.67	0	56,56,56	2.15	16 (28%)
17	BCR	aB	4017	-	41,41,41	0.68	0	56,56,56	2.07	15 (26%)
14	CLA	S	516	13	49,53,73	1.41	5 (10%)	58,89,113	1.43	4 (6%)
20	SQD	b4	822	-	31,33,54	1.22	3 (9%)	41,44,65	1.67	11 (26%)
17	BCR	b6	522	-	41,41,41	0.68	0	56,56,56	2.10	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	cA	1128	1	69,73,73	1.19	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	e	511	13	49,53,73	1.41	8 (16%)	58,89,113	1.42	4 (6%)
14	CLA	p	508	13	49,53,73	1.40	8 (16%)	58,89,113	1.42	5 (8%)
14	CLA	bA	1140	1	69,73,73	1.19	8 (11%)	82,113,113	1.22	5 (6%)
14	CLA	X	512	13	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
14	CLA	d	502	13	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
14	CLA	c3	504	-	60,64,73	1.27	6 (10%)	71,102,113	1.35	5 (7%)
14	CLA	aB	1217	2	59,63,73	1.28	7 (11%)	70,101,113	1.34	5 (7%)
21	LMG	a6	5104	-	38,38,55	0.87	1 (2%)	46,46,63	1.22	3 (6%)
20	SQD	b6	822	-	28,30,54	1.28	3 (10%)	38,41,65	1.69	9 (23%)
14	CLA	k	507	-	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
14	CLA	f	516	13	49,53,73	1.40	7 (14%)	58,89,113	1.55	7 (12%)
14	CLA	U	510	13	59,63,73	1.29	7 (11%)	70,101,113	1.32	5 (7%)
14	CLA	cB	1208	2	56,60,73	1.31	7 (12%)	65,97,113	1.35	6 (9%)
14	CLA	cB	1236	2	54,58,73	1.32	7 (12%)	64,95,113	1.35	6 (9%)
14	CLA	i	507	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
17	BCR	bA	4002	-	41,41,41	0.67	0	56,56,56	2.07	15 (26%)
17	BCR	m	524	-	41,41,41	0.70	0	56,56,56	2.19	18 (32%)
14	CLA	k	519	13	49,53,73	1.40	6 (12%)	58,89,113	1.44	6 (10%)
14	CLA	q	519	13	49,53,73	1.40	6 (12%)	58,89,113	1.39	4 (6%)
14	CLA	g	510	13	49,53,73	1.40	6 (12%)	58,89,113	1.41	4 (6%)
14	CLA	i	519	13	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
14	CLA	bA	1135	1	55,59,73	1.32	7 (12%)	64,96,113	1.39	7 (10%)
14	CLA	b1	501	13	69,73,73	1.19	8 (11%)	82,113,113	1.26	5 (6%)
14	CLA	j	519	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
14	CLA	S	517	-	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	a6	509	13	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
14	CLA	h	502	13	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
14	CLA	bB	1221	-	64,68,73	1.22	6 (9%)	76,107,113	1.27	5 (6%)
17	BCR	d	522	-	41,41,41	0.69	0	56,56,56	2.20	15 (26%)
17	BCR	l	521	-	41,41,41	0.64	0	56,56,56	2.16	14 (25%)
17	BCR	c6	522	-	41,41,41	0.67	0	56,56,56	2.02	16 (28%)
14	CLA	V	502	13	64,68,73	1.23	9 (14%)	76,107,113	1.30	5 (6%)
14	CLA	c3	512	13	56,60,73	1.31	7 (12%)	65,97,113	1.35	6 (9%)
14	CLA	Z	512	13	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	c1	517	-	49,53,73	1.40	6 (12%)	58,89,113	1.41	4 (6%)
14	CLA	c4	508	13	64,68,73	1.22	9 (14%)	76,107,113	1.28	5 (6%)
14	CLA	cB	1214	2	64,68,73	1.23	8 (12%)	76,107,113	1.30	7 (9%)
14	CLA	Y	508	13	56,60,73	1.30	8 (14%)	65,97,113	1.36	6 (9%)
14	CLA	q	507	-	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
14	CLA	aA	1108	1	49,53,73	1.39	8 (16%)	58,89,113	1.39	4 (6%)
14	CLA	e	505	13	66,70,73	1.20	7 (10%)	78,109,113	1.27	6 (7%)
14	CLA	cA	1102	1	69,73,73	1.18	6 (8%)	82,113,113	1.26	6 (7%)
14	CLA	a3	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.27	6 (7%)
17	BCR	h	521	-	41,41,41	0.66	0	56,56,56	2.07	15 (26%)
14	CLA	c6	501	13	69,73,73	1.19	8 (11%)	82,113,113	1.26	6 (7%)
14	CLA	b5	513	13	59,63,73	1.28	7 (11%)	70,101,113	1.34	6 (8%)
17	BCR	aB	4005	-	41,41,41	0.71	0	56,56,56	1.95	13 (23%)
14	CLA	a6	506	13	49,53,73	1.41	8 (16%)	58,89,113	1.42	5 (8%)
14	CLA	a	518	13	59,63,73	1.27	7 (11%)	70,101,113	1.34	8 (11%)
21	LMG	b2	5104	-	40,40,55	0.83	1 (2%)	48,48,63	1.31	5 (10%)
17	BCR	c1	524	-	41,41,41	0.70	0	56,56,56	2.08	19 (33%)
14	CLA	c2	513	13	50,54,73	1.38	5 (10%)	59,90,113	1.38	4 (6%)
17	BCR	c4	523	-	41,41,41	0.73	1 (2%)	56,56,56	2.04	16 (28%)
14	CLA	cA	1132	1	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
17	BCR	aF	4014	-	41,41,41	0.69	0	56,56,56	2.23	15 (26%)
14	CLA	T	502	13	64,68,73	1.24	8 (12%)	76,107,113	1.31	5 (6%)
14	CLA	aA	1138	1	69,73,73	1.19	8 (11%)	82,113,113	1.25	6 (7%)
14	CLA	c5	517	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	l	504	-	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)
14	CLA	a5	507	-	64,68,73	1.22	7 (10%)	76,107,113	1.28	6 (7%)
14	CLA	b1	517	-	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	a3	513	13	54,58,73	1.33	7 (12%)	64,95,113	1.37	6 (9%)
14	CLA	m	504	-	49,53,73	1.41	7 (14%)	58,89,113	1.41	4 (6%)
17	BCR	T	521	-	41,41,41	0.65	0	56,56,56	2.06	14 (25%)
17	BCR	p	523	-	41,41,41	0.68	0	56,56,56	2.00	16 (28%)
17	BCR	a6	522	-	41,41,41	0.68	0	56,56,56	2.01	17 (30%)
14	CLA	S	508	13	55,59,73	1.32	8 (14%)	64,96,113	1.37	6 (9%)
14	CLA	X	511	13	59,63,73	1.28	8 (13%)	70,101,113	1.33	4 (5%)
14	CLA	Z	509	13	69,73,73	1.18	8 (11%)	82,113,113	1.28	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	c2	503	13	69,73,73	1.18	7 (10%)	82,113,113	1.26	5 (6%)
14	CLA	c1	508	13	59,63,73	1.27	8 (13%)	70,101,113	1.32	5 (7%)
14	CLA	a4	519	13	56,60,73	1.32	8 (14%)	65,97,113	1.37	6 (9%)
14	CLA	e	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
17	BCR	b	522	-	41,41,41	0.66	0	56,56,56	1.99	17 (30%)
18	LHG	bA	5003	14	40,40,48	0.69	2 (5%)	43,46,54	1.32	6 (13%)
14	CLA	aA	1110	1	57,61,73	1.30	8 (14%)	67,98,113	1.32	5 (7%)
14	CLA	a6	513	13	59,63,73	1.28	7 (11%)	70,101,113	1.32	7 (10%)
14	CLA	c5	511	13	49,53,73	1.40	7 (14%)	58,89,113	1.43	5 (8%)
14	CLA	b3	509	13	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
14	CLA	a	512	13	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
14	CLA	bA	1133	1	69,73,73	1.18	8 (11%)	82,113,113	1.27	4 (4%)
14	CLA	aA	1101	1	64,68,73	1.23	7 (10%)	76,107,113	1.28	5 (6%)
17	BCR	n	524	-	41,41,41	0.71	0	56,56,56	2.11	16 (28%)
14	CLA	aB	1230	2	62,66,73	1.26	9 (14%)	73,104,113	1.35	7 (9%)
14	CLA	U	511	13	59,63,73	1.28	7 (11%)	70,101,113	1.33	4 (5%)
14	CLA	bA	1013	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	7 (8%)
14	CLA	c3	511	13	66,70,73	1.21	7 (10%)	78,109,113	1.29	6 (7%)
14	CLA	c2	507	-	64,68,73	1.22	7 (10%)	76,107,113	1.30	6 (7%)
14	CLA	l	505	13	49,53,73	1.40	7 (14%)	58,89,113	1.37	4 (6%)
17	BCR	a6	523	-	41,41,41	0.69	0	56,56,56	1.92	14 (25%)
14	CLA	a	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.42	5 (8%)
18	LHG	bA	5002	-	41,41,48	0.70	2 (4%)	44,47,54	1.20	4 (9%)
14	CLA	c	517	-	49,53,73	1.40	9 (18%)	58,89,113	1.41	4 (6%)
14	CLA	bA	1112	1	52,56,73	1.35	9 (17%)	61,92,113	1.41	5 (8%)
14	CLA	g	511	13	49,53,73	1.40	6 (12%)	58,89,113	1.41	4 (6%)
17	BCR	a3	522	-	41,41,41	0.66	0	56,56,56	2.03	17 (30%)
14	CLA	cA	1123	-	69,73,73	1.18	7 (10%)	82,113,113	1.29	7 (8%)
14	CLA	cA	1125	1	64,68,73	1.23	9 (14%)	76,107,113	1.27	6 (7%)
14	CLA	b2	516	13	49,53,73	1.40	8 (16%)	58,89,113	1.39	5 (8%)
14	CLA	bA	1123	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	7 (8%)
14	CLA	a2	516	13	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	h	519	13	49,53,73	1.40	6 (12%)	58,89,113	1.41	4 (6%)
17	BCR	i	523	-	41,41,41	0.69	0	56,56,56	2.00	15 (26%)
14	CLA	cA	1115	1	64,68,73	1.22	7 (10%)	76,107,113	1.31	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	d	510	13	64,68,73	1.23	7 (10%)	76,107,113	1.28	7 (9%)
17	BCR	c3	524	-	41,41,41	0.68	0	56,56,56	2.02	19 (33%)
20	SQD	c5	822	-	29,31,54	1.26	4 (13%)	39,42,65	1.69	8 (20%)
17	BCR	b	523	-	41,41,41	0.68	0	56,56,56	1.95	13 (23%)
14	CLA	c6	510	13	69,73,73	1.18	7 (10%)	82,113,113	1.26	4 (4%)
14	CLA	cX	1401	12	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
14	CLA	b5	503	13	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
14	CLA	bA	1126	1	69,73,73	1.18	7 (10%)	82,113,113	1.22	5 (6%)
14	CLA	a	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
14	CLA	U	513	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	5 (8%)
14	CLA	c4	512	13	49,53,73	1.41	7 (14%)	58,89,113	1.40	4 (6%)
17	BCR	a6	524	-	41,41,41	0.70	0	56,56,56	2.07	18 (32%)
14	CLA	b2	510	13	69,73,73	1.18	6 (8%)	82,113,113	1.27	8 (9%)
14	CLA	Y	517	-	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
17	BCR	aB	4004	-	41,41,41	0.66	0	56,56,56	2.12	15 (26%)
14	CLA	c	502	13	59,63,73	1.28	8 (13%)	70,101,113	1.35	6 (8%)
14	CLA	a1	508	13	59,63,73	1.27	9 (15%)	70,101,113	1.32	6 (8%)
14	CLA	Z	501	13	69,73,73	1.19	8 (11%)	82,113,113	1.26	6 (7%)
14	CLA	i	501	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
15	PQN	aB	2002	-	34,34,34	3.03	11 (32%)	43,45,45	1.99	6 (13%)
14	CLA	bA	1121	1	56,60,73	1.31	8 (14%)	65,97,113	1.36	5 (7%)
14	CLA	e	519	13	49,53,73	1.41	6 (12%)	58,89,113	1.39	4 (6%)
17	BCR	W	522	-	41,41,41	0.68	0	56,56,56	2.03	17 (30%)
18	LHG	cX	4021	-	38,38,48	0.71	1 (2%)	41,44,54	1.36	6 (14%)
14	CLA	c	503	13	49,53,73	1.41	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	b6	511	13	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
14	CLA	aA	1105	1	55,59,73	1.32	7 (12%)	64,96,113	1.40	6 (9%)
14	CLA	Y	511	13	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
14	CLA	i	518	13	59,63,73	1.28	8 (13%)	70,101,113	1.33	6 (8%)
14	CLA	b5	505	13	69,73,73	1.17	7 (10%)	82,113,113	1.25	7 (8%)
14	CLA	V	510	13	64,68,73	1.23	7 (10%)	76,107,113	1.28	5 (6%)
14	CLA	n	501	13	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
14	CLA	W	507	-	55,59,73	1.31	7 (12%)	64,96,113	1.37	6 (9%)
14	CLA	j	501	13	49,53,73	1.42	7 (14%)	58,89,113	1.37	4 (6%)
14	CLA	a1	501	13	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	bB	4010	-	41,41,41	0.69	0	56,56,56	2.10	16 (28%)
14	CLA	cB	1218	2	60,64,73	1.28	6 (10%)	71,102,113	1.35	4 (5%)
14	CLA	c1	504	-	59,63,73	1.29	7 (11%)	70,101,113	1.33	5 (7%)
14	CLA	a3	512	13	57,61,73	1.30	7 (12%)	67,98,113	1.32	5 (7%)
14	CLA	aJ	1302	8	53,57,73	1.33	7 (13%)	61,93,113	1.39	6 (9%)
14	CLA	l	519	13	49,53,73	1.39	5 (10%)	58,89,113	1.40	4 (6%)
14	CLA	a2	513	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
14	CLA	b2	506	13	49,53,73	1.41	7 (14%)	58,89,113	1.43	5 (8%)
14	CLA	d	503	13	54,58,73	1.34	7 (12%)	64,95,113	1.38	6 (9%)
14	CLA	a2	502	13	64,68,73	1.23	8 (12%)	76,107,113	1.28	4 (5%)
14	CLA	bA	1136	1	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
17	BCR	aA	4008	-	41,41,41	0.70	0	56,56,56	2.10	15 (26%)
17	BCR	a5	523	-	41,41,41	0.70	1 (2%)	56,56,56	1.88	16 (28%)
19	LMU	aB	1843	-	36,36,36	1.18	2 (5%)	47,47,47	0.96	1 (2%)
14	CLA	W	517	-	49,53,73	1.41	8 (16%)	58,89,113	1.43	5 (8%)
19	LMU	bB	1843	-	36,36,36	1.18	2 (5%)	47,47,47	0.97	1 (2%)
17	BCR	o	524	-	41,41,41	0.70	0	56,56,56	2.13	16 (28%)
14	CLA	cB	1230	2	62,66,73	1.25	8 (12%)	73,104,113	1.35	7 (9%)
17	BCR	l	522	-	41,41,41	0.67	0	56,56,56	2.28	15 (26%)
14	CLA	a6	512	13	49,53,73	1.40	8 (16%)	58,89,113	1.39	4 (6%)
17	BCR	b5	524	-	41,41,41	0.69	0	56,56,56	2.09	16 (28%)
14	CLA	cB	1229	2	64,68,73	1.24	7 (10%)	76,107,113	1.27	6 (7%)
14	CLA	h	518	13	51,55,73	1.36	7 (13%)	60,91,113	1.39	5 (8%)
14	CLA	j	510	13	64,68,73	1.23	7 (10%)	76,107,113	1.29	7 (9%)
14	CLA	cL	1501	10	69,73,73	1.18	7 (10%)	82,113,113	1.28	7 (8%)
14	CLA	W	501	13	69,73,73	1.18	9 (13%)	82,113,113	1.27	6 (7%)
14	CLA	b	512	13	54,58,73	1.34	8 (14%)	64,95,113	1.38	5 (7%)
14	CLA	a6	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
18	LHG	aA	5004	-	32,32,48	0.76	1 (3%)	35,38,54	1.27	4 (11%)
14	CLA	aA	1237	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
14	CLA	a6	503	13	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
14	CLA	cA	1126	1	69,73,73	1.17	7 (10%)	82,113,113	1.21	5 (6%)
14	CLA	a5	508	13	59,63,73	1.27	8 (13%)	70,101,113	1.30	6 (8%)
14	CLA	c2	501	13	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
14	CLA	bB	1203	2	69,73,73	1.18	7 (10%)	82,113,113	1.24	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	516	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
14	CLA	a3	510	13	69,73,73	1.18	6 (8%)	82,113,113	1.26	6 (7%)
14	CLA	b	506	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	5 (8%)
14	CLA	c4	519	13	55,59,73	1.32	7 (12%)	64,96,113	1.38	6 (9%)
14	CLA	T	519	13	49,53,73	1.40	6 (12%)	58,89,113	1.41	4 (6%)
17	BCR	bB	4006	-	41,41,41	0.68	0	56,56,56	2.11	15 (26%)
14	CLA	b	505	13	64,68,73	1.22	7 (10%)	76,107,113	1.31	7 (9%)
14	CLA	X	519	13	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
14	CLA	o	518	13	59,63,73	1.27	7 (11%)	70,101,113	1.33	6 (8%)
14	CLA	b1	508	13	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
14	CLA	V	509	13	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	c3	508	13	59,63,73	1.27	9 (15%)	70,101,113	1.32	6 (8%)
14	CLA	b4	511	13	49,53,73	1.41	6 (12%)	58,89,113	1.43	4 (6%)
14	CLA	c5	510	13	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
14	CLA	cB	1206	2	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
14	CLA	c6	508	13	59,63,73	1.28	8 (13%)	70,101,113	1.32	5 (7%)
14	CLA	a5	516	13	51,55,73	1.34	8 (15%)	60,91,113	1.41	5 (8%)
14	CLA	j	506	13	49,53,73	1.41	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	c5	519	13	55,59,73	1.32	6 (10%)	64,96,113	1.36	5 (7%)
20	SQD	bB	1852	-	40,42,54	1.09	3 (7%)	50,53,65	1.56	10 (20%)
14	CLA	c5	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	5 (8%)
14	CLA	bA	1107	1	59,63,73	1.27	7 (11%)	70,101,113	1.32	5 (7%)
14	CLA	aA	1107	1	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
14	CLA	a	517	-	49,53,73	1.41	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	b1	507	-	65,69,73	1.22	7 (10%)	77,108,113	1.27	6 (7%)
14	CLA	b5	516	13	53,57,73	1.35	7 (13%)	61,93,113	1.39	5 (8%)
14	CLA	n	507	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
17	BCR	n	521	-	41,41,41	0.67	0	56,56,56	2.18	14 (25%)
14	CLA	o	505	13	49,53,73	1.39	7 (14%)	58,89,113	1.36	4 (6%)
14	CLA	c3	519	13	49,53,73	1.40	6 (12%)	58,89,113	1.40	4 (6%)
14	CLA	bL	1502	10	64,68,73	1.22	7 (10%)	76,107,113	1.28	6 (7%)
14	CLA	c6	516	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	5 (8%)
20	SQD	X	822	-	34,36,54	1.17	3 (8%)	44,47,65	1.58	8 (18%)
17	BCR	j	521	-	41,41,41	0.67	0	56,56,56	2.14	16 (28%)
14	CLA	b1	519	13	49,53,73	1.40	6 (12%)	58,89,113	1.39	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	f	501	13	49,53,73	1.41	9 (18%)	58,89,113	1.40	4 (6%)
14	CLA	c3	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
14	CLA	aA	1102	1	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
14	CLA	b6	517	-	49,53,73	1.41	8 (16%)	58,89,113	1.40	4 (6%)
17	BCR	m	522	-	41,41,41	0.69	0	56,56,56	2.06	14 (25%)
14	CLA	c4	507	-	64,68,73	1.22	7 (10%)	76,107,113	1.29	5 (6%)
14	CLA	W	513	13	54,58,73	1.33	7 (12%)	64,95,113	1.35	7 (10%)
14	CLA	a3	503	13	67,71,73	1.20	6 (8%)	79,110,113	1.26	5 (6%)
14	CLA	m	508	13	49,53,73	1.39	9 (18%)	58,89,113	1.42	5 (8%)
16	SF4	cA	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	b3	512	13	57,61,73	1.30	7 (12%)	67,98,113	1.34	6 (8%)
14	CLA	aL	1501	10	69,73,73	1.17	7 (10%)	82,113,113	1.30	8 (9%)
14	CLA	bF	1301	-	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
14	CLA	h	516	13	49,53,73	1.41	5 (10%)	58,89,113	1.46	5 (8%)
14	CLA	bA	1134	1	59,63,73	1.29	7 (11%)	70,101,113	1.32	6 (8%)
14	CLA	c2	502	13	64,68,73	1.23	8 (12%)	76,107,113	1.28	5 (6%)
14	CLA	aB	1203	2	69,73,73	1.18	7 (10%)	82,113,113	1.24	5 (6%)
14	CLA	f	513	13	49,53,73	1.39	6 (12%)	58,89,113	1.42	6 (10%)
14	CLA	aB	1229	2	69,73,73	1.19	6 (8%)	82,113,113	1.22	6 (7%)
17	BCR	a5	524	-	41,41,41	0.69	0	56,56,56	2.03	14 (25%)
14	CLA	e	516	13	49,53,73	1.40	8 (16%)	58,89,113	1.49	6 (10%)
14	CLA	p	507	-	49,53,73	1.40	5 (10%)	58,89,113	1.40	4 (6%)
14	CLA	aB	1023	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	6 (7%)
14	CLA	b3	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
14	CLA	bA	1111	1	59,63,73	1.28	7 (11%)	70,101,113	1.34	6 (8%)
14	CLA	b3	508	13	59,63,73	1.27	8 (13%)	70,101,113	1.33	6 (8%)
14	CLA	c1	511	13	54,58,73	1.33	8 (14%)	64,95,113	1.40	6 (9%)
14	CLA	W	503	13	67,71,73	1.20	5 (7%)	79,110,113	1.28	5 (6%)
14	CLA	j	517	-	49,53,73	1.40	8 (16%)	58,89,113	1.39	4 (6%)
14	CLA	cA	1127	1	69,73,73	1.18	8 (11%)	82,113,113	1.22	6 (7%)
14	CLA	b1	502	13	64,68,73	1.23	8 (12%)	76,107,113	1.31	6 (7%)
14	CLA	Y	519	13	49,53,73	1.41	8 (16%)	58,89,113	1.40	4 (6%)
17	BCR	b5	521	-	41,41,41	0.66	0	56,56,56	2.14	16 (28%)
17	BCR	c6	524	-	41,41,41	0.69	0	56,56,56	2.11	16 (28%)
14	CLA	d	518	13	59,63,73	1.28	7 (11%)	70,101,113	1.33	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	PQN	bB	2002	-	34,34,34	3.03	12 (35%)	43,45,45	1.99	6 (13%)
17	BCR	k	524	-	41,41,41	0.70	0	56,56,56	2.04	17 (30%)
14	CLA	c4	502	13	64,68,73	1.23	9 (14%)	76,107,113	1.31	6 (7%)
14	CLA	l	518	13	54,58,73	1.32	7 (12%)	64,95,113	1.39	6 (9%)
14	CLA	b4	507	-	64,68,73	1.23	7 (10%)	76,107,113	1.28	5 (6%)
17	BCR	aF	4016	-	41,41,41	0.69	0	56,56,56	2.07	15 (26%)
17	BCR	cA	4007	-	41,41,41	0.69	0	56,56,56	2.06	16 (28%)
14	CLA	l	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
17	BCR	b2	524	-	41,41,41	0.69	0	56,56,56	2.09	17 (30%)
14	CLA	aA	1125	1	69,73,73	1.19	9 (13%)	82,113,113	1.25	5 (6%)
17	BCR	c	522	-	41,41,41	0.69	0	56,56,56	2.17	15 (26%)
17	BCR	cM	4021	-	41,41,41	0.67	0	56,56,56	2.29	15 (26%)
14	CLA	h	513	13	54,58,73	1.33	7 (12%)	64,95,113	1.38	7 (10%)
17	BCR	e	521	-	41,41,41	0.68	0	56,56,56	2.13	17 (30%)
17	BCR	T	523	-	41,41,41	0.69	0	56,56,56	1.99	14 (25%)
14	CLA	b5	510	13	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
14	CLA	cB	1202	2	69,73,73	1.17	6 (8%)	82,113,113	1.26	5 (6%)
14	CLA	cB	1215	2	65,69,73	1.21	7 (10%)	77,108,113	1.27	6 (7%)
14	CLA	cB	1021	2	69,73,73	1.17	7 (10%)	82,113,113	1.19	6 (7%)
17	BCR	V	524	-	41,41,41	0.70	0	56,56,56	2.14	16 (28%)
14	CLA	d	517	-	49,53,73	1.40	7 (14%)	58,89,113	1.37	4 (6%)
14	CLA	a3	501	13	69,73,73	1.18	9 (13%)	82,113,113	1.26	6 (7%)
14	CLA	a2	506	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	5 (8%)
17	BCR	S	521	-	41,41,41	0.66	0	56,56,56	2.14	14 (25%)
14	CLA	h	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	a3	516	13	49,53,73	1.39	6 (12%)	58,89,113	1.42	4 (6%)
14	CLA	Z	508	13	49,53,73	1.40	9 (18%)	58,89,113	1.40	4 (6%)
14	CLA	b	511	13	49,53,73	1.41	8 (16%)	58,89,113	1.42	4 (6%)
14	CLA	f	511	13	49,53,73	1.40	5 (10%)	58,89,113	1.44	4 (6%)
14	CLA	b3	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.42	5 (8%)
17	BCR	p	522	-	41,41,41	0.67	0	56,56,56	2.16	15 (26%)
14	CLA	T	518	13	54,58,73	1.33	8 (14%)	64,95,113	1.39	6 (9%)
21	LMG	a2	5104	-	40,40,55	0.83	1 (2%)	48,48,63	1.25	5 (10%)
14	CLA	a	508	13	49,53,73	1.39	7 (14%)	58,89,113	1.43	5 (8%)
14	CLA	i	502	13	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	X	518	13	59,63,73	1.28	8 (13%)	70,101,113	1.32	6 (8%)
14	CLA	aB	1225	2	69,73,73	1.18	7 (10%)	82,113,113	1.25	8 (9%)
14	CLA	b1	504	-	59,63,73	1.28	7 (11%)	70,101,113	1.32	5 (7%)
14	CLA	c2	512	13	56,60,73	1.32	7 (12%)	65,97,113	1.36	6 (9%)
17	BCR	b	524	-	41,41,41	0.70	0	56,56,56	2.04	17 (30%)
14	CLA	bB	1023	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	6 (7%)
14	CLA	cB	1231	2	59,63,73	1.30	7 (11%)	70,101,113	1.31	6 (8%)
14	CLA	aA	1106	1	69,73,73	1.17	7 (10%)	82,113,113	1.26	6 (7%)
14	CLA	b3	503	13	67,71,73	1.20	8 (11%)	79,110,113	1.28	5 (6%)
17	BCR	cJ	4012	-	41,41,41	0.67	0	56,56,56	2.02	16 (28%)
14	CLA	bA	1129	1	59,63,73	1.27	8 (13%)	70,101,113	1.35	5 (7%)
14	CLA	a2	501	13	69,73,73	1.18	7 (10%)	82,113,113	1.27	6 (7%)
18	LHG	cA	5001	-	47,47,48	0.62	1 (2%)	50,53,54	1.28	6 (12%)
14	CLA	l	513	13	49,53,73	1.40	6 (12%)	58,89,113	1.41	4 (6%)
14	CLA	a2	509	13	69,73,73	1.18	7 (10%)	82,113,113	1.29	6 (7%)
14	CLA	U	517	-	49,53,73	1.41	7 (14%)	58,89,113	1.40	4 (6%)
14	CLA	Z	519	13	49,53,73	1.40	8 (16%)	58,89,113	1.38	4 (6%)
14	CLA	cB	1213	2	64,68,73	1.22	7 (10%)	76,107,113	1.32	6 (7%)
14	CLA	c5	518	13	59,63,73	1.28	7 (11%)	70,101,113	1.35	6 (8%)
16	SF4	cC	3003	3	0,12,12	-	-	-	-	-
17	BCR	a4	524	-	41,41,41	0.69	0	56,56,56	1.99	14 (25%)
14	CLA	d	505	13	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
14	CLA	U	518	13	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)
14	CLA	q	518	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	aB	1212	2	49,53,73	1.40	7 (14%)	58,89,113	1.44	5 (8%)
17	BCR	U	521	-	41,41,41	0.66	0	56,56,56	2.06	13 (23%)
14	CLA	b2	513	13	51,55,73	1.35	7 (13%)	60,91,113	1.36	5 (8%)
14	CLA	b1	518	13	59,63,73	1.28	8 (13%)	70,101,113	1.33	6 (8%)
14	CLA	aA	1011	1	69,73,73	1.17	6 (8%)	82,113,113	1.24	7 (8%)
17	BCR	k	522	-	41,41,41	0.66	0	56,56,56	2.13	18 (32%)
17	BCR	q	522	-	41,41,41	0.68	0	56,56,56	2.13	16 (28%)
17	BCR	a1	523	-	41,41,41	0.70	0	56,56,56	1.91	16 (28%)
20	SQD	a3	822	-	36,38,54	1.14	3 (8%)	46,49,65	1.56	9 (19%)
17	BCR	f	522	-	41,41,41	0.67	0	56,56,56	2.10	15 (26%)
14	CLA	n	519	13	49,53,73	1.41	7 (14%)	58,89,113	1.41	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	aB	1201	2	61,65,73	1.25	6 (9%)	72,103,113	1.31	4 (5%)
17	BCR	i	522	-	41,41,41	0.69	0	56,56,56	2.05	16 (28%)
14	CLA	bB	1223	2	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
14	CLA	cB	1216	-	59,63,73	1.28	8 (13%)	70,101,113	1.31	4 (5%)
18	LHG	aA	5003	14	40,40,48	0.71	2 (5%)	43,46,54	1.34	6 (13%)
14	CLA	a1	511	13	59,63,73	1.28	8 (13%)	70,101,113	1.34	6 (8%)
14	CLA	b4	508	13	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
14	CLA	aB	1208	2	59,63,73	1.28	7 (11%)	70,101,113	1.31	6 (8%)
14	CLA	aA	1140	1	69,73,73	1.19	8 (11%)	82,113,113	1.22	4 (4%)
14	CLA	aB	1234	2	64,68,73	1.24	8 (12%)	76,107,113	1.29	6 (7%)
14	CLA	g	502	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	a5	509	13	69,73,73	1.18	7 (10%)	82,113,113	1.27	4 (4%)
17	BCR	bI	4020	-	41,41,41	0.69	0	56,56,56	2.00	15 (26%)
14	CLA	V	505	13	66,70,73	1.20	7 (10%)	78,109,113	1.29	5 (6%)
14	CLA	j	518	13	54,58,73	1.33	7 (12%)	64,95,113	1.41	6 (9%)
14	CLA	c4	504	-	49,53,73	1.40	7 (14%)	58,89,113	1.43	4 (6%)
14	CLA	cA	1131	1	69,73,73	1.19	8 (11%)	82,113,113	1.24	6 (7%)
14	CLA	bA	1117	1	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
14	CLA	bB	1232	-	49,53,73	1.41	8 (16%)	58,89,113	1.39	4 (6%)
17	BCR	a1	524	-	41,41,41	0.69	0	56,56,56	2.08	19 (33%)
14	CLA	Z	504	-	59,63,73	1.29	8 (13%)	70,101,113	1.36	6 (8%)
17	BCR	a	521	-	41,41,41	0.66	0	56,56,56	2.07	14 (25%)
14	CLA	n	504	-	49,53,73	1.41	8 (16%)	58,89,113	1.42	4 (6%)
17	BCR	f	524	-	41,41,41	0.71	0	56,56,56	2.09	18 (32%)
14	CLA	X	513	13	50,54,73	1.37	6 (12%)	59,90,113	1.36	4 (6%)
17	BCR	i	524	-	41,41,41	0.69	0	56,56,56	2.20	17 (30%)
17	BCR	f	523	-	41,41,41	0.67	0	56,56,56	1.90	16 (28%)
14	CLA	c4	510	13	69,73,73	1.18	6 (8%)	82,113,113	1.25	6 (7%)
14	CLA	bA	1105	1	57,61,73	1.30	8 (14%)	67,98,113	1.37	7 (10%)
14	CLA	b5	511	13	54,58,73	1.33	8 (14%)	64,95,113	1.38	6 (9%)
14	CLA	k	506	13	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	c1	519	13	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
14	CLA	a1	516	13	62,66,73	1.25	8 (12%)	73,104,113	1.40	8 (10%)
14	CLA	b6	507	-	64,68,73	1.23	8 (12%)	76,107,113	1.27	4 (5%)
18	LHG	aA	5002	-	40,40,48	0.69	2 (5%)	43,46,54	1.24	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b1	510	13	69,73,73	1.19	8 (11%)	82,113,113	1.25	6 (7%)
14	CLA	n	517	-	49,53,73	1.42	8 (16%)	58,89,113	1.38	4 (6%)
14	CLA	bK	1401	-	59,63,73	1.29	8 (13%)	70,101,113	1.32	5 (7%)
14	CLA	aA	1112	1	52,56,73	1.35	9 (17%)	61,92,113	1.40	5 (8%)
14	CLA	aA	1126	1	69,73,73	1.18	8 (11%)	82,113,113	1.23	4 (4%)
18	LHG	aA	5005	-	44,44,48	0.63	1 (2%)	47,50,54	1.28	5 (10%)
17	BCR	cB	4005	-	41,41,41	0.71	0	56,56,56	1.97	13 (23%)
14	CLA	q	512	13	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
14	CLA	j	504	-	49,53,73	1.41	7 (14%)	58,89,113	1.44	4 (6%)
14	CLA	o	513	13	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
20	SQD	a6	822	-	29,31,54	1.28	3 (10%)	39,42,65	1.65	8 (20%)
14	CLA	d	509	13	66,70,73	1.20	7 (10%)	78,109,113	1.31	6 (7%)
17	BCR	g	522	-	41,41,41	0.68	0	56,56,56	2.12	16 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	bL	1503	-	1/1/15/20	10/39/115/115	-
14	CLA	a6	516	13	1/1/11/20	7/15/91/115	-
14	CLA	cA	1110	1	1/1/12/20	7/25/101/115	-
14	CLA	bB	1222	-	1/1/14/20	4/33/109/115	-
14	CLA	c3	513	13	1/1/12/20	3/21/97/115	-
17	BCR	aM	4021	-	-	7/29/63/63	0/2/2/2
14	CLA	c	519	13	1/1/11/20	7/15/91/115	-
17	BCR	Y	521	-	-	4/29/63/63	0/2/2/2
14	CLA	aB	1223	2	1/1/15/20	8/39/115/115	-
17	BCR	l	524	-	-	0/29/63/63	0/2/2/2
14	CLA	c	505	13	1/1/15/20	14/39/115/115	-
14	CLA	f	508	13	1/1/11/20	1/15/91/115	-
14	CLA	i	508	13	1/1/11/20	2/15/91/115	-
14	CLA	c4	506	13	1/1/11/20	7/15/91/115	-
14	CLA	p	502	13	1/1/13/20	9/27/103/115	-
14	CLA	cA	1139	-	1/1/14/20	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cB	1235	2	1/1/15/20	11/39/115/115	-
17	BCR	bA	4003	-	-	4/29/63/63	0/2/2/2
17	BCR	c2	522	-	-	5/29/63/63	0/2/2/2
17	BCR	a4	522	-	-	4/29/63/63	0/2/2/2
14	CLA	U	505	13	1/1/13/20	6/27/103/115	-
21	LMG	b1	5104	-	-	6/30/50/70	0/1/1/1
14	CLA	bA	1102	1	1/1/15/20	8/39/115/115	-
14	CLA	bB	1215	2	1/1/14/20	6/33/109/115	-
14	CLA	aA	1119	-	1/1/15/20	10/39/115/115	-
14	CLA	a4	505	13	1/1/14/20	12/33/109/115	-
14	CLA	bA	1128	1	1/1/15/20	9/39/115/115	-
14	CLA	bB	1219	-	1/1/13/20	9/27/103/115	-
14	CLA	cB	1210	2	1/1/15/20	17/39/115/115	-
17	BCR	g	523	-	-	2/29/63/63	0/2/2/2
14	CLA	e	508	13	1/1/11/20	4/15/91/115	-
21	LMG	cB	5002	-	-	15/44/64/70	0/1/1/1
14	CLA	aA	1133	1	1/1/15/20	14/39/115/115	-
14	CLA	q	516	13	1/1/11/20	11/15/91/115	-
14	CLA	b1	503	13	1/1/14/20	8/37/113/115	-
14	CLA	S	519	13	1/1/11/20	7/15/91/115	-
17	BCR	o	522	-	-	4/29/63/63	0/2/2/2
14	CLA	W	502	13	1/1/14/20	10/33/109/115	-
14	CLA	a6	510	13	1/1/15/20	12/39/115/115	-
19	LMU	bJ	5105	-	-	5/13/33/61	0/1/1/2
17	BCR	c3	521	-	-	7/29/63/63	0/2/2/2
14	CLA	cA	1022	-	1/1/15/20	10/39/115/115	-
14	CLA	Y	504	-	1/1/13/20	10/27/103/115	-
18	LHG	cA	5005	-	-	17/48/48/53	-
17	BCR	b3	524	-	-	2/29/63/63	0/2/2/2
20	SQD	a2	822	-	-	8/28/48/69	0/1/1/1
20	SQD	g	822	-	-	6/25/45/69	0/1/1/1
14	CLA	g	512	13	1/1/11/20	3/15/91/115	-
14	CLA	S	518	13	1/1/12/20	11/23/99/115	-
14	CLA	c	513	13	1/1/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	510	13	1/1/14/20	10/33/109/115	-
14	CLA	c1	509	13	1/1/15/20	9/39/115/115	-
14	CLA	b5	502	13	1/1/14/20	12/33/109/115	-
17	BCR	c2	523	-	-	0/29/63/63	0/2/2/2
17	BCR	bF	4014	-	-	4/29/63/63	0/2/2/2
14	CLA	q	513	13	1/1/11/20	0/15/91/115	-
14	CLA	c2	509	13	1/1/15/20	6/39/115/115	-
20	SQD	b	822	-	-	7/26/46/69	0/1/1/1
14	CLA	aA	1121	1	1/1/13/20	13/27/103/115	-
14	CLA	bA	1108	1	1/1/11/20	3/15/91/115	-
14	CLA	a2	518	13	1/1/13/20	8/27/103/115	-
14	CLA	d	513	13	1/1/11/20	5/15/91/115	-
17	BCR	c3	523	-	-	3/29/63/63	0/2/2/2
14	CLA	cA	1105	1	1/1/12/20	5/23/99/115	-
16	SF4	bA	3001	2,1	-	-	0/6/5/5
14	CLA	U	519	13	1/1/11/20	6/15/91/115	-
14	CLA	T	507	-	1/1/11/20	4/15/91/115	-
17	BCR	cB	4004	-	-	7/29/63/63	0/2/2/2
14	CLA	bB	1239	2	1/1/15/20	12/39/115/115	-
14	CLA	c2	505	13	1/1/15/20	14/39/115/115	-
19	LMU	bA	1848	-	-	5/15/35/61	0/1/1/2
14	CLA	b4	504	-	1/1/12/20	11/25/101/115	-
14	CLA	cB	1221	2	1/1/14/20	13/33/109/115	-
14	CLA	i	504	-	1/1/11/20	5/15/91/115	-
18	LHG	bX	4021	-	-	13/43/43/53	-
17	BCR	bI	4018	-	-	6/29/63/63	0/2/2/2
14	CLA	q	503	13	1/1/14/20	8/36/112/115	-
14	CLA	m	502	13	1/1/11/20	3/15/91/115	-
14	CLA	a1	519	13	1/1/11/20	8/15/91/115	-
14	CLA	k	511	13	1/1/11/20	5/15/91/115	-
17	BCR	o	521	-	-	5/29/63/63	0/2/2/2
14	CLA	Z	511	13	1/1/11/20	5/15/91/115	-
14	CLA	W	510	13	1/1/15/20	11/39/115/115	-
14	CLA	a2	505	13	1/1/15/20	12/39/115/115	-
14	CLA	U	507	-	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	aA	1116	1	1/1/14/20	10/33/109/115	-
14	CLA	a6	501	13	1/1/15/20	9/39/115/115	-
14	CLA	cB	1239	2	1/1/15/20	13/39/115/115	-
14	CLA	c5	507	-	1/1/14/20	8/33/109/115	-
14	CLA	c1	501	13	1/1/15/20	13/39/115/115	-
14	CLA	g	518	13	1/1/11/20	5/15/91/115	-
14	CLA	l	508	13	1/1/11/20	5/17/93/115	-
14	CLA	cA	1113	1	1/1/11/20	4/15/91/115	-
14	CLA	o	507	-	1/1/11/20	4/15/91/115	-
17	BCR	g	521	-	-	4/29/63/63	0/2/2/2
14	CLA	b1	516	13	1/1/11/20	10/15/91/115	-
14	CLA	c3	507	-	1/1/14/20	4/33/109/115	-
17	BCR	c	523	-	-	2/29/63/63	0/2/2/2
14	CLA	f	512	13	1/1/11/20	6/15/91/115	-
17	BCR	b2	522	-	-	4/29/63/63	0/2/2/2
14	CLA	b4	518	13	1/1/13/20	10/27/103/115	-
14	CLA	W	512	13	1/1/11/20	8/15/91/115	-
14	CLA	g	506	13	1/1/11/20	6/15/91/115	-
14	CLA	e	510	13	1/1/13/20	10/27/103/115	-
14	CLA	b	509	13	1/1/14/20	4/36/112/115	-
17	BCR	b5	523	-	-	2/29/63/63	0/2/2/2
14	CLA	b2	508	13	1/1/13/20	2/27/103/115	-
14	CLA	b6	518	13	1/1/12/20	11/21/97/115	-
17	BCR	b6	521	-	-	2/29/63/63	0/2/2/2
14	CLA	c4	517	-	1/1/11/20	11/15/91/115	-
14	CLA	aB	1012	-	1/1/14/20	13/36/112/115	-
14	CLA	a4	502	13	1/1/14/20	11/33/109/115	-
14	CLA	c	518	13	1/1/11/20	5/15/91/115	-
14	CLA	b4	519	13	1/1/12/20	6/24/100/115	-
14	CLA	U	502	13	1/1/13/20	6/30/106/115	-
14	CLA	c3	510	13	1/1/15/20	8/39/115/115	-
14	CLA	q	509	13	1/1/14/20	12/36/112/115	-
14	CLA	bB	1213	2	1/1/14/20	7/33/109/115	-
14	CLA	c2	506	13	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	aA	1134	1	1/1/13/20	13/30/106/115	-
17	BCR	b6	524	-	-	0/29/63/63	0/2/2/2
14	CLA	l	510	13	1/1/11/20	4/15/91/115	-
20	SQD	c	822	-	-	7/26/46/69	0/1/1/1
14	CLA	a5	504	-	1/1/12/20	6/24/100/115	-
14	CLA	c	501	13	1/1/12/20	12/24/100/115	-
14	CLA	cB	1205	2	1/1/15/20	11/39/115/115	-
17	BCR	T	522	-	-	5/29/63/63	0/2/2/2
14	CLA	Z	503	13	1/1/14/20	13/35/111/115	-
17	BCR	bF	4016	-	-	2/29/63/63	0/2/2/2
14	CLA	c	516	13	1/1/11/20	6/15/91/115	-
14	CLA	n	518	13	1/1/11/20	8/18/94/115	-
14	CLA	aA	1111	1	1/1/13/20	9/27/103/115	-
14	CLA	cB	1224	2	1/1/13/20	14/31/107/115	-
14	CLA	a2	519	13	1/1/12/20	4/21/97/115	-
14	CLA	T	508	13	1/1/11/20	4/15/91/115	-
14	CLA	a1	509	13	1/1/15/20	5/39/115/115	-
17	BCR	h	523	-	-	4/29/63/63	0/2/2/2
14	CLA	k	501	13	1/1/12/20	12/23/99/115	-
14	CLA	bA	1110	1	1/1/12/20	5/25/101/115	-
14	CLA	cB	1203	2	1/1/15/20	18/39/115/115	-
17	BCR	d	524	-	-	0/29/63/63	0/2/2/2
14	CLA	cA	1121	1	1/1/12/20	8/23/99/115	-
14	CLA	l	512	13	1/1/11/20	3/15/91/115	-
14	CLA	o	503	13	1/1/14/20	9/36/112/115	-
14	CLA	S	513	13	1/1/11/20	3/18/94/115	-
14	CLA	k	516	13	1/1/11/20	4/15/91/115	-
17	BCR	p	521	-	-	5/29/63/63	0/2/2/2
20	SQD	d	822	-	-	10/26/46/69	0/1/1/1
14	CLA	bB	1226	2	1/1/15/20	9/39/115/115	-
14	CLA	S	502	13	1/1/11/20	6/17/93/115	-
14	CLA	b3	510	13	1/1/15/20	10/39/115/115	-
14	CLA	m	512	13	1/1/11/20	7/15/91/115	-
14	CLA	d	516	13	1/1/11/20	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	c3	506	13	1/1/11/20	5/15/91/115	-
14	CLA	a	502	13	1/1/11/20	6/15/91/115	-
14	CLA	c1	502	13	1/1/14/20	6/33/109/115	-
14	CLA	c	510	13	1/1/14/20	9/33/109/115	-
14	CLA	bB	1227	2	1/1/12/20	12/26/102/115	-
14	CLA	l	516	13	1/1/11/20	7/15/91/115	-
14	CLA	g	519	13	1/1/11/20	8/15/91/115	-
14	CLA	W	506	13	1/1/11/20	5/15/91/115	-
18	LHG	bA	5001	-	-	17/53/53/53	-
14	CLA	aB	1239	2	1/1/15/20	12/39/115/115	-
15	PQN	cA	2001	-	-	10/23/43/43	0/2/2/2
14	CLA	c	512	13	1/1/11/20	8/15/91/115	-
20	SQD	V	822	-	-	10/26/46/69	0/1/1/1
14	CLA	f	519	13	1/1/11/20	4/15/91/115	-
14	CLA	aL	1503	-	1/1/15/20	11/39/115/115	-
14	CLA	i	517	-	1/1/11/20	11/15/91/115	-
17	BCR	aB	4006	-	-	4/29/63/63	0/2/2/2
14	CLA	bJ	1303	8	1/1/13/20	6/30/106/115	-
14	CLA	c4	501	13	1/1/15/20	16/39/115/115	-
14	CLA	b6	505	13	1/1/15/20	11/39/115/115	-
17	BCR	Z	524	-	-	0/29/63/63	0/2/2/2
14	CLA	b5	506	13	1/1/11/20	4/15/91/115	-
14	CLA	cB	1209	2	1/1/12/20	11/25/101/115	-
17	BCR	j	523	-	-	2/29/63/63	0/2/2/2
17	BCR	k	521	-	-	2/29/63/63	0/2/2/2
14	CLA	i	511	13	1/1/11/20	5/15/91/115	-
14	CLA	p	510	13	1/1/11/20	4/17/93/115	-
14	CLA	n	513	13	1/1/11/20	3/15/91/115	-
14	CLA	c	506	13	1/1/11/20	4/15/91/115	-
20	SQD	i	822	-	-	8/25/45/69	0/1/1/1
17	BCR	m	523	-	-	2/29/63/63	0/2/2/2
17	BCR	Y	522	-	-	5/29/63/63	0/2/2/2
14	CLA	cA	1138	1	1/1/15/20	11/39/115/115	-
14	CLA	a4	512	13	1/1/11/20	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	cB	4010	-	-	2/29/63/63	0/2/2/2
14	CLA	b2	512	13	1/1/12/20	11/26/102/115	-
17	BCR	U	523	-	-	2/29/63/63	0/2/2/2
17	BCR	X	521	-	-	5/29/63/63	0/2/2/2
17	BCR	cA	4002	-	-	4/29/63/63	0/2/2/2
17	BCR	j	524	-	-	2/29/63/63	0/2/2/2
14	CLA	cB	1207	2	1/1/15/20	12/39/115/115	-
14	CLA	aA	1129	1	1/1/12/20	11/25/101/115	-
17	BCR	bB	4009	-	-	4/29/63/63	0/2/2/2
14	CLA	X	516	13	1/1/11/20	6/15/91/115	-
14	CLA	bA	1122	1	1/1/14/20	9/33/109/115	-
14	CLA	l	511	13	1/1/11/20	5/15/91/115	-
14	CLA	c2	516	13	1/1/11/20	9/15/91/115	-
14	CLA	a4	516	13	1/1/11/20	5/15/91/115	-
17	BCR	c5	521	-	-	2/29/63/63	0/2/2/2
14	CLA	T	510	13	1/1/13/20	10/29/105/115	-
14	CLA	n	516	13	1/1/11/20	6/15/91/115	-
17	BCR	b4	523	-	-	2/29/63/63	0/2/2/2
14	CLA	a	519	13	1/1/11/20	6/15/91/115	-
14	CLA	p	506	13	1/1/11/20	4/15/91/115	-
14	CLA	aA	1115	1	1/1/14/20	13/33/109/115	-
14	CLA	h	509	13	1/1/15/20	8/39/115/115	-
14	CLA	j	516	13	1/1/11/20	3/15/91/115	-
17	BCR	a3	524	-	-	0/29/63/63	0/2/2/2
17	BCR	c1	523	-	-	3/29/63/63	0/2/2/2
18	LHG	cA	5003	14	-	10/45/45/53	-
14	CLA	p	505	13	1/1/11/20	3/18/94/115	-
14	CLA	bA	1116	1	1/1/14/20	13/33/109/115	-
14	CLA	b	517	-	1/1/11/20	6/15/91/115	-
14	CLA	bA	1130	1	1/1/13/20	5/27/103/115	-
14	CLA	f	517	-	1/1/11/20	6/15/91/115	-
14	CLA	k	510	13	1/1/11/20	6/15/91/115	-
14	CLA	c5	516	13	1/1/11/20	7/15/91/115	-
21	LMG	bJ	5104	-	-	8/24/44/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a4	510	13	1/1/15/20	10/39/115/115	-
14	CLA	aA	1135	1	1/1/12/20	10/23/99/115	-
14	CLA	aB	1233	-	1/1/11/20	2/15/91/115	-
14	CLA	U	516	13	1/1/11/20	9/15/91/115	-
14	CLA	aB	1211	2	1/1/15/20	9/39/115/115	-
18	LHG	cA	5004	-	-	10/35/35/53	-
14	CLA	a5	519	13	1/1/12/20	4/23/99/115	-
17	BCR	b	521	-	-	7/29/63/63	0/2/2/2
17	BCR	aJ	4012	-	-	4/29/63/63	0/2/2/2
14	CLA	U	504	-	1/1/12/20	8/21/97/115	-
14	CLA	o	510	13	1/1/13/20	10/29/105/115	-
14	CLA	b3	511	13	1/1/14/20	16/36/112/115	-
17	BCR	bL	4022	-	-	3/29/63/63	0/2/2/2
14	CLA	h	508	13	1/1/11/20	4/15/91/115	-
14	CLA	S	507	-	1/1/11/20	6/18/94/115	-
14	CLA	c6	507	-	1/1/13/20	3/30/106/115	-
14	CLA	f	502	13	1/1/11/20	4/15/91/115	-
14	CLA	b5	519	13	1/1/12/20	6/24/100/115	-
17	BCR	cK	4001	-	-	2/29/63/63	0/2/2/2
17	BCR	c2	524	-	-	0/29/63/63	0/2/2/2
14	CLA	c6	519	13	1/1/11/20	7/15/91/115	-
14	CLA	a1	502	13	1/1/14/20	14/33/109/115	-
14	CLA	e	501	13	1/1/11/20	9/15/91/115	-
14	CLA	cA	1801	18	1/1/11/20	8/15/91/115	-
14	CLA	c1	516	13	1/1/13/20	8/27/103/115	-
14	CLA	c4	503	13	1/1/15/20	13/39/115/115	-
14	CLA	T	503	13	1/1/11/20	2/15/91/115	-
14	CLA	W	516	13	1/1/11/20	9/15/91/115	-
17	BCR	aA	4011	-	-	7/29/63/63	0/2/2/2
14	CLA	i	506	13	1/1/11/20	6/15/91/115	-
17	BCR	aB	4009	-	-	7/29/63/63	0/2/2/2
18	LHG	bA	5004	-	-	16/43/43/53	-
14	CLA	cB	1228	2	1/1/13/20	4/27/103/115	-
14	CLA	n	503	13	1/1/11/20	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	e	524	-	-	0/29/63/63	0/2/2/2
14	CLA	e	507	-	1/1/12/20	5/21/97/115	-
14	CLA	cA	1118	1	1/1/14/20	15/33/109/115	-
14	CLA	o	506	13	1/1/11/20	6/15/91/115	-
14	CLA	c3	518	13	1/1/13/20	14/27/103/115	-
14	CLA	o	502	13	1/1/11/20	2/15/91/115	-
14	CLA	g	501	13	1/1/13/20	15/27/103/115	-
14	CLA	c5	505	13	1/1/15/20	16/39/115/115	-
17	BCR	Z	521	-	-	7/29/63/63	0/2/2/2
14	CLA	a	509	13	1/1/15/20	6/39/115/115	-
14	CLA	bB	1212	2	1/1/11/20	2/15/91/115	-
14	CLA	c3	502	13	1/1/14/20	8/33/109/115	-
17	BCR	b1	521	-	-	7/29/63/63	0/2/2/2
14	CLA	cA	1133	1	1/1/15/20	12/39/115/115	-
14	CLA	c1	510	13	1/1/15/20	8/39/115/115	-
14	CLA	i	510	13	1/1/12/20	2/21/97/115	-
14	CLA	p	518	13	1/1/11/20	10/19/95/115	-
14	CLA	c3	503	13	1/1/14/20	5/37/113/115	-
14	CLA	n	505	13	1/1/15/20	9/39/115/115	-
16	SF4	bC	3003	3	-	-	0/6/5/5
14	CLA	e	517	-	1/1/11/20	9/15/91/115	-
14	CLA	h	501	13	1/1/11/20	8/15/91/115	-
20	SQD	a1	822	-	-	6/26/46/69	0/1/1/1
14	CLA	bB	1206	2	1/1/15/20	10/39/115/115	-
17	BCR	W	524	-	-	0/29/63/63	0/2/2/2
16	SF4	aC	3003	3	-	-	0/6/5/5
14	CLA	a6	519	13	1/1/11/20	7/15/91/115	-
14	CLA	g	516	13	1/1/11/20	11/15/91/115	-
14	CLA	a5	512	13	1/1/12/20	9/24/100/115	-
14	CLA	c1	506	13	1/1/11/20	6/15/91/115	-
14	CLA	aB	1219	-	1/1/13/20	8/27/103/115	-
14	CLA	aA	1128	1	1/1/15/20	8/39/115/115	-
14	CLA	a3	508	13	1/1/13/20	4/27/103/115	-
14	CLA	q	510	13	1/1/14/20	8/36/112/115	-
14	CLA	c1	507	-	1/1/14/20	6/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cA	1116	1	1/1/14/20	8/33/109/115	-
14	CLA	l	517	-	1/1/11/20	8/15/91/115	-
14	CLA	a5	506	13	1/1/11/20	6/15/91/115	-
14	CLA	a1	504	-	1/1/13/20	9/27/103/115	-
14	CLA	o	512	13	1/1/11/20	5/15/91/115	-
17	BCR	bB	4004	-	-	6/29/63/63	0/2/2/2
17	BCR	c1	522	-	-	4/29/63/63	0/2/2/2
14	CLA	c6	512	13	1/1/11/20	10/15/91/115	-
21	LMG	c1	5104	-	-	7/34/54/70	0/1/1/1
14	CLA	a4	511	13	1/1/11/20	3/15/91/115	-
17	BCR	cB	4006	-	-	4/29/63/63	0/2/2/2
20	SQD	f	822	-	-	12/25/45/69	0/1/1/1
14	CLA	h	510	13	1/1/13/20	10/27/103/115	-
14	CLA	k	518	13	1/1/11/20	7/15/91/115	-
14	CLA	i	503	13	1/1/11/20	3/15/91/115	-
14	CLA	bB	1012	-	1/1/14/20	14/35/111/115	-
14	CLA	T	516	13	1/1/11/20	4/15/91/115	-
17	BCR	b4	521	-	-	7/29/63/63	0/2/2/2
14	CLA	b5	508	13	1/1/13/20	1/27/103/115	-
14	CLA	p	509	13	1/1/14/20	11/36/112/115	-
14	CLA	l	502	13	1/1/13/20	10/27/103/115	-
21	LMG	aB	5002	-	-	16/44/64/70	0/1/1/1
14	CLA	p	512	13	1/1/11/20	5/15/91/115	-
17	BCR	g	524	-	-	0/29/63/63	0/2/2/2
14	CLA	a3	509	13	1/1/15/20	3/39/115/115	-
14	CLA	a2	503	13	1/1/15/20	8/39/115/115	-
14	CLA	bA	1125	1	1/1/15/20	16/39/115/115	-
14	CLA	b2	511	13	1/1/12/20	2/23/99/115	-
14	CLA	c2	508	13	1/1/13/20	2/27/103/115	-
20	SQD	aB	1852	-	-	9/37/57/69	0/1/1/1
14	CLA	X	507	-	1/1/14/20	7/33/109/115	-
14	CLA	aA	1109	1	1/1/15/20	11/39/115/115	-
14	CLA	Z	507	-	1/1/14/20	6/33/109/115	-
14	CLA	c	508	13	1/1/13/20	6/27/103/115	-
14	CLA	a	513	13	1/1/11/20	1/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b2	502	13	1/1/14/20	8/33/109/115	-
17	BCR	b3	521	-	-	5/29/63/63	0/2/2/2
14	CLA	U	501	13	1/1/11/20	10/15/91/115	-
14	CLA	cA	1119	-	1/1/15/20	11/39/115/115	-
14	CLA	aB	1206	2	1/1/15/20	9/39/115/115	-
17	BCR	U	522	-	-	4/29/63/63	0/2/2/2
14	CLA	V	511	13	1/1/11/20	4/15/91/115	-
17	BCR	V	521	-	-	2/29/63/63	0/2/2/2
14	CLA	bA	1120	1	1/1/13/20	13/27/103/115	-
14	CLA	bA	1801	18	1/1/11/20	8/15/91/115	-
14	CLA	b6	513	13	1/1/12/20	3/21/97/115	-
19	LMU	aA	1848	-	-	5/15/35/61	0/1/1/2
17	BCR	a	524	-	-	0/29/63/63	0/2/2/2
14	CLA	aA	1114	-	1/1/11/20	6/15/91/115	-
14	CLA	X	517	-	1/1/11/20	9/15/91/115	-
14	CLA	b	519	13	1/1/11/20	8/15/91/115	-
14	CLA	cL	1503	-	1/1/15/20	9/39/115/115	-
14	CLA	h	503	13	1/1/11/20	2/15/91/115	-
14	CLA	T	511	13	1/1/11/20	5/15/91/115	-
14	CLA	c4	518	13	1/1/13/20	11/29/105/115	-
14	CLA	e	504	-	1/1/11/20	8/15/91/115	-
14	CLA	i	509	13	1/1/11/20	6/15/91/115	-
17	BCR	aA	4003	-	-	4/29/63/63	0/2/2/2
14	CLA	bB	1233	-	1/1/11/20	2/15/91/115	-
14	CLA	c6	518	13	1/1/12/20	9/21/97/115	-
14	CLA	bB	1205	2	1/1/15/20	14/39/115/115	-
19	LMU	cB	1843	-	-	9/21/61/61	0/2/2/2
14	CLA	c2	510	13	1/1/15/20	3/39/115/115	-
14	CLA	g	507	-	1/1/11/20	7/15/91/115	-
14	CLA	bB	1211	2	1/1/15/20	6/39/115/115	-
16	SF4	bC	3002	3	-	-	0/6/5/5
14	CLA	aA	1139	-	1/1/14/20	10/33/109/115	-
14	CLA	k	502	13	1/1/11/20	4/15/91/115	-
14	CLA	X	502	13	1/1/14/20	8/33/109/115	-
17	BCR	T	524	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	W	505	13	1/1/15/20	12/39/115/115	-
14	CLA	Z	502	13	1/1/13/20	6/29/105/115	-
14	CLA	m	518	13	1/1/11/20	5/15/91/115	-
16	SF4	aC	3002	3	-	-	0/6/5/5
14	CLA	a4	509	13	1/1/15/20	9/39/115/115	-
14	CLA	n	502	13	1/1/13/20	12/30/106/115	-
14	CLA	aB	1222	-	1/1/14/20	5/33/109/115	-
14	CLA	bA	1101	1	1/1/14/20	10/33/109/115	-
14	CLA	Y	501	13	1/1/15/20	15/39/115/115	-
14	CLA	b4	505	13	1/1/14/20	10/33/109/115	-
20	SQD	c2	822	-	-	10/26/46/69	0/1/1/1
14	CLA	g	504	-	1/1/11/20	6/15/91/115	-
14	CLA	bB	1238	-	1/1/15/20	5/39/115/115	-
14	CLA	cB	1211	2	1/1/15/20	11/39/115/115	-
17	BCR	b1	523	-	-	2/29/63/63	0/2/2/2
14	CLA	q	511	13	1/1/11/20	8/15/91/115	-
14	CLA	a4	518	13	1/1/13/20	15/30/106/115	-
17	BCR	aA	4002	-	-	4/29/63/63	0/2/2/2
14	CLA	a3	518	13	1/1/13/20	12/32/108/115	-
17	BCR	aL	4022	-	-	3/29/63/63	0/2/2/2
14	CLA	g	509	13	1/1/11/20	4/15/91/115	-
14	CLA	p	513	13	1/1/11/20	8/15/91/115	-
17	BCR	aI	4019	-	-	4/29/63/63	0/2/2/2
17	BCR	aK	4001	-	-	4/29/63/63	0/2/2/2
14	CLA	a6	508	13	1/1/13/20	6/27/103/115	-
14	CLA	bA	1011	1	1/1/15/20	6/39/115/115	-
17	BCR	cF	4015	-	-	1/29/63/63	0/2/2/2
17	BCR	c	521	-	-	4/29/63/63	0/2/2/2
14	CLA	j	502	13	1/1/11/20	2/15/91/115	-
14	CLA	Y	507	-	1/1/14/20	4/33/109/115	-
20	SQD	b1	822	-	-	6/26/46/69	0/1/1/1
14	CLA	aA	1124	-	1/1/13/20	5/29/105/115	-
14	CLA	a1	507	-	1/1/14/20	11/33/109/115	-
14	CLA	cA	1104	1	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMG	bB	5002	-	-	15/44/64/70	0/1/1/1
14	CLA	bA	1124	-	1/1/13/20	4/29/105/115	-
14	CLA	cB	1222	-	1/1/14/20	4/33/109/115	-
14	CLA	cB	1217	2	1/1/13/20	12/27/103/115	-
14	CLA	cB	1238	-	1/1/15/20	4/39/115/115	-
14	CLA	U	508	13	1/1/12/20	4/21/97/115	-
15	PQN	bA	2001	-	-	11/23/43/43	0/2/2/2
14	CLA	aJ	1303	8	1/1/13/20	11/30/106/115	-
20	SQD	c4	822	-	-	17/28/48/69	0/1/1/1
14	CLA	a6	518	13	1/1/12/20	6/21/97/115	-
17	BCR	cA	4003	-	-	4/29/63/63	0/2/2/2
14	CLA	cB	1232	-	1/1/11/20	9/15/91/115	-
14	CLA	p	503	13	1/1/11/20	2/15/91/115	-
21	LMG	aJ	5104	-	-	6/26/46/70	0/1/1/1
14	CLA	b3	519	13	1/1/12/20	3/24/100/115	-
14	CLA	a3	504	-	1/1/13/20	12/31/107/115	-
20	SQD	p	822	-	-	14/25/45/69	0/1/1/1
14	CLA	c1	518	13	1/1/13/20	9/27/103/115	-
14	CLA	k	513	13	1/1/11/20	3/15/91/115	-
17	BCR	c3	522	-	-	4/29/63/63	0/2/2/2
18	LHG	aA	5001	-	-	17/52/52/53	-
14	CLA	i	513	13	1/1/11/20	3/15/91/115	-
14	CLA	X	504	-	1/1/13/20	13/27/103/115	-
14	CLA	T	506	13	1/1/11/20	4/15/91/115	-
14	CLA	Y	502	13	1/1/14/20	9/33/109/115	-
14	CLA	a1	513	13	1/1/12/20	3/21/97/115	-
17	BCR	k	523	-	-	2/29/63/63	0/2/2/2
14	CLA	aB	1238	-	1/1/15/20	7/39/115/115	-
14	CLA	o	501	13	1/1/11/20	11/17/93/115	-
14	CLA	c1	503	13	1/1/14/20	10/37/113/115	-
14	CLA	bA	1119	-	1/1/15/20	12/39/115/115	-
14	CLA	a3	517	-	1/1/11/20	9/15/91/115	-
17	BCR	bA	4011	-	-	6/29/63/63	0/2/2/2
14	CLA	aB	1216	-	1/1/14/20	9/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	bB	1214	2	1/1/15/20	15/39/115/115	-
14	CLA	bB	1204	2	1/1/14/20	1/33/109/115	-
14	CLA	T	512	13	1/1/11/20	6/15/91/115	-
17	BCR	bF	4015	-	-	1/29/63/63	0/2/2/2
14	CLA	a4	513	13	1/1/12/20	2/21/97/115	-
14	CLA	d	511	13	1/1/11/20	2/15/91/115	-
17	BCR	b4	522	-	-	4/29/63/63	0/2/2/2
14	CLA	m	519	13	1/1/11/20	5/15/91/115	-
14	CLA	a1	517	-	1/1/11/20	9/15/91/115	-
20	SQD	q	822	-	-	7/19/39/69	0/1/1/1
14	CLA	c2	511	13	1/1/11/20	2/15/91/115	-
17	BCR	c4	522	-	-	4/29/63/63	0/2/2/2
14	CLA	c5	513	13	1/1/13/20	5/27/103/115	-
14	CLA	Z	518	13	1/1/13/20	7/27/103/115	-
14	CLA	bK	1103	9	1/1/9/20	7/9/81/115	-
14	CLA	b5	504	-	1/1/13/20	11/27/103/115	-
14	CLA	b1	506	13	1/1/11/20	6/15/91/115	-
14	CLA	X	508	13	1/1/11/20	4/15/91/115	-
14	CLA	b4	513	13	1/1/11/20	4/15/91/115	-
14	CLA	aA	1131	1	1/1/15/20	13/39/115/115	-
14	CLA	b1	505	13	1/1/15/20	15/39/115/115	-
14	CLA	a	510	13	1/1/11/20	6/15/91/115	-
14	CLA	V	519	13	1/1/11/20	6/15/91/115	-
17	BCR	bJ	4013	-	-	8/29/63/63	0/2/2/2
17	BCR	e	522	-	-	4/29/63/63	0/2/2/2
17	BCR	a2	521	-	-	7/29/63/63	0/2/2/2
14	CLA	b	518	13	1/1/12/20	7/21/97/115	-
14	CLA	cA	1013	-	1/1/15/20	9/39/115/115	-
14	CLA	aB	1209	2	1/1/12/20	12/25/101/115	-
14	CLA	b3	518	13	1/1/13/20	15/29/105/115	-
14	CLA	b4	502	13	1/1/14/20	12/33/109/115	-
14	CLA	c6	504	-	1/1/11/20	5/15/91/115	-
14	CLA	h	507	-	1/1/11/20	4/15/91/115	-
14	CLA	S	503	13	1/1/14/20	3/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cA	1136	1	1/1/15/20	11/39/115/115	-
14	CLA	Z	510	13	1/1/15/20	6/39/115/115	-
14	CLA	aB	1232	-	1/1/11/20	9/15/91/115	-
14	CLA	j	505	13	1/1/11/20	5/15/91/115	-
14	CLA	aB	1227	2	1/1/12/20	10/26/102/115	-
14	CLA	f	503	13	1/1/11/20	3/15/91/115	-
17	BCR	X	523	-	-	2/29/63/63	0/2/2/2
14	CLA	n	510	13	1/1/11/20	4/15/91/115	-
14	CLA	bB	1236	2	1/1/12/20	4/21/97/115	-
14	CLA	e	513	13	1/1/11/20	5/15/91/115	-
17	BCR	Z	523	-	-	5/29/63/63	0/2/2/2
14	CLA	T	509	13	1/1/14/20	7/35/111/115	-
14	CLA	bA	1118	1	1/1/14/20	12/33/109/115	-
17	BCR	cA	4008	-	-	2/29/63/63	0/2/2/2
14	CLA	aB	1207	2	1/1/15/20	12/39/115/115	-
14	CLA	W	511	13	1/1/11/20	8/15/91/115	-
14	CLA	aB	1204	2	1/1/14/20	1/33/109/115	-
14	CLA	aA	1130	1	1/1/13/20	5/27/103/115	-
14	CLA	b2	504	-	1/1/11/20	3/15/91/115	-
17	BCR	o	523	-	-	4/29/63/63	0/2/2/2
14	CLA	aB	1213	2	1/1/15/20	11/39/115/115	-
14	CLA	b4	501	13	1/1/15/20	16/39/115/115	-
14	CLA	cB	1219	-	1/1/12/20	7/24/100/115	-
14	CLA	V	517	-	1/1/11/20	11/15/91/115	-
14	CLA	m	509	13	1/1/11/20	4/15/91/115	-
14	CLA	bB	1210	2	1/1/15/20	19/39/115/115	-
14	CLA	bA	1103	1	1/1/15/20	10/39/115/115	-
17	BCR	h	522	-	-	5/29/63/63	0/2/2/2
14	CLA	Y	512	13	1/1/11/20	7/15/91/115	-
17	BCR	cJ	4013	-	-	6/29/63/63	0/2/2/2
14	CLA	i	512	13	1/1/11/20	6/15/91/115	-
14	CLA	b2	509	13	1/1/15/20	5/39/115/115	-
18	LHG	cA	5002	-	-	14/46/46/53	-
14	CLA	Z	506	13	1/1/11/20	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	c5	523	-	-	0/29/63/63	0/2/2/2
14	CLA	q	506	13	1/1/11/20	4/15/91/115	-
14	CLA	U	503	13	1/1/11/20	2/15/91/115	-
14	CLA	f	505	13	1/1/11/20	3/15/91/115	-
14	CLA	V	501	13	1/1/14/20	13/36/112/115	-
14	CLA	b	504	-	1/1/12/20	9/21/97/115	-
14	CLA	cB	1012	-	1/1/14/20	16/36/112/115	-
14	CLA	j	507	-	1/1/11/20	4/15/91/115	-
14	CLA	aB	1226	2	1/1/15/20	9/39/115/115	-
14	CLA	g	517	-	1/1/11/20	11/15/91/115	-
14	CLA	a5	502	13	1/1/14/20	13/33/109/115	-
14	CLA	T	517	-	1/1/11/20	11/15/91/115	-
14	CLA	b	513	13	1/1/11/20	3/15/91/115	-
14	CLA	bB	1201	2	1/1/13/20	6/30/106/115	-
14	CLA	m	507	-	1/1/11/20	8/15/91/115	-
14	CLA	b4	510	13	1/1/15/20	10/39/115/115	-
14	CLA	bA	1132	1	1/1/15/20	13/39/115/115	-
14	CLA	b5	517	-	1/1/11/20	3/15/91/115	-
14	CLA	cA	1107	1	1/1/13/20	9/27/103/115	-
14	CLA	b6	510	13	1/1/15/20	8/39/115/115	-
14	CLA	a3	507	-	1/1/14/20	11/36/112/115	-
14	CLA	aB	1236	2	1/1/12/20	4/21/97/115	-
14	CLA	Y	510	13	1/1/15/20	8/39/115/115	-
20	SQD	S	822	-	-	8/26/46/69	0/1/1/1
14	CLA	cB	1226	2	1/1/15/20	10/39/115/115	-
17	BCR	b6	523	-	-	1/29/63/63	0/2/2/2
14	CLA	d	508	13	1/1/13/20	3/27/103/115	-
14	CLA	c2	517	-	1/1/11/20	9/15/91/115	-
14	CLA	h	512	13	1/1/11/20	8/15/91/115	-
14	CLA	a5	510	13	1/1/15/20	8/39/115/115	-
14	CLA	aB	1221	2	1/1/14/20	10/33/109/115	-
14	CLA	o	504	-	1/1/11/20	5/15/91/115	-
17	BCR	j	522	-	-	2/29/63/63	0/2/2/2
14	CLA	a2	510	13	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	aI	4018	-	-	6/29/63/63	0/2/2/2
14	CLA	a	511	13	1/1/11/20	4/15/91/115	-
14	CLA	c3	516	13	1/1/11/20	2/15/91/115	-
17	BCR	c2	521	-	-	5/29/63/63	0/2/2/2
14	CLA	cA	1237	-	1/1/15/20	14/39/115/115	-
17	BCR	a5	522	-	-	5/29/63/63	0/2/2/2
17	BCR	bA	4007	-	-	2/29/63/63	0/2/2/2
14	CLA	cB	1234	2	1/1/14/20	9/33/109/115	-
14	CLA	c	511	13	1/1/11/20	6/15/91/115	-
20	SQD	a5	822	-	-	15/28/48/69	0/1/1/1
14	CLA	U	509	13	1/1/11/20	2/15/91/115	-
14	CLA	p	516	13	1/1/11/20	2/15/91/115	-
14	CLA	cB	1233	-	1/1/11/20	2/15/91/115	-
14	CLA	a	504	-	1/1/11/20	9/15/91/115	-
14	CLA	cB	1225	2	1/1/15/20	14/39/115/115	-
14	CLA	b1	509	13	1/1/15/20	3/39/115/115	-
14	CLA	m	501	13	1/1/11/20	10/15/91/115	-
17	BCR	b5	522	-	-	5/29/63/63	0/2/2/2
14	CLA	n	511	13	1/1/11/20	7/15/91/115	-
14	CLA	b4	503	13	1/1/15/20	4/39/115/115	-
14	CLA	S	510	13	1/1/13/20	10/27/103/115	-
14	CLA	b1	512	13	1/1/12/20	7/25/101/115	-
17	BCR	cF	4016	-	-	2/29/63/63	0/2/2/2
20	SQD	b5	822	-	-	8/25/45/69	0/1/1/1
14	CLA	bB	1207	2	1/1/15/20	10/39/115/115	-
14	CLA	bA	1109	1	1/1/15/20	11/39/115/115	-
17	BCR	cA	4011	-	-	8/29/63/63	0/2/2/2
14	CLA	Y	503	13	1/1/14/20	6/37/113/115	-
14	CLA	c4	511	13	1/1/11/20	5/15/91/115	-
14	CLA	V	518	13	1/1/11/20	5/15/91/115	-
14	CLA	n	509	13	1/1/14/20	11/33/109/115	-
14	CLA	b3	513	13	1/1/12/20	3/21/97/115	-
14	CLA	cA	1108	1	1/1/11/20	2/15/91/115	-
14	CLA	j	509	13	1/1/14/20	4/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cA	1103	1	1/1/15/20	13/39/115/115	-
17	BCR	X	522	-	-	5/29/63/63	0/2/2/2
17	BCR	cL	4022	-	-	3/29/63/63	0/2/2/2
14	CLA	cB	1201	2	1/1/13/20	7/30/106/115	-
14	CLA	a4	508	13	1/1/15/20	8/39/115/115	-
14	CLA	c6	513	13	1/1/11/20	3/15/91/115	-
17	BCR	aJ	4013	-	-	7/29/63/63	0/2/2/2
14	CLA	S	506	13	1/1/11/20	4/15/91/115	-
14	CLA	i	516	13	1/1/11/20	8/15/91/115	-
14	CLA	cB	1223	2	1/1/15/20	8/39/115/115	-
17	BCR	c5	522	-	-	3/29/63/63	0/2/2/2
20	SQD	b2	822	-	-	8/27/47/69	0/1/1/1
14	CLA	b6	512	13	1/1/11/20	8/15/91/115	-
14	CLA	d	504	-	1/1/11/20	2/15/91/115	-
14	CLA	a2	507	-	1/1/14/20	7/35/111/115	-
20	SQD	m	822	-	-	9/23/43/69	0/1/1/1
14	CLA	bB	1224	2	1/1/13/20	13/30/106/115	-
17	BCR	cI	4020	-	-	3/29/63/63	0/2/2/2
14	CLA	b4	506	13	1/1/11/20	4/15/91/115	-
14	CLA	Y	513	13	1/1/11/20	1/15/91/115	-
14	CLA	e	512	13	1/1/11/20	9/15/91/115	-
17	BCR	b1	522	-	-	5/29/63/63	0/2/2/2
14	CLA	bA	1104	1	1/1/15/20	12/39/115/115	-
14	CLA	b6	506	13	1/1/11/20	6/15/91/115	-
14	CLA	b6	502	13	1/1/14/20	10/33/109/115	-
14	CLA	k	512	13	1/1/11/20	8/15/91/115	-
14	CLA	bB	1231	2	1/1/13/20	10/27/103/115	-
17	BCR	a4	523	-	-	4/29/63/63	0/2/2/2
17	BCR	bA	4008	-	-	2/29/63/63	0/2/2/2
14	CLA	b2	517	-	1/1/11/20	10/15/91/115	-
14	CLA	h	504	-	1/1/11/20	4/15/91/115	-
14	CLA	c2	519	13	1/1/12/20	4/21/97/115	-
14	CLA	a2	517	-	1/1/11/20	8/15/91/115	-
14	CLA	bJ	1302	8	1/1/11/20	7/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	c	524	-	-	0/29/63/63	0/2/2/2
17	BCR	cF	4014	-	-	5/29/63/63	0/2/2/2
14	CLA	V	504	-	1/1/13/20	10/27/103/115	-
14	CLA	d	512	13	1/1/11/20	4/15/91/115	-
14	CLA	bA	1115	1	1/1/14/20	11/33/109/115	-
17	BCR	c4	521	-	-	5/29/63/63	0/2/2/2
14	CLA	b1	513	13	1/1/12/20	4/21/97/115	-
14	CLA	q	502	13	1/1/11/20	6/15/91/115	-
14	CLA	bB	1217	2	1/1/13/20	11/27/103/115	-
14	CLA	a2	511	13	1/1/12/20	5/23/99/115	-
21	LMG	cJ	5104	-	-	6/26/46/70	0/1/1/1
14	CLA	m	517	-	1/1/11/20	8/15/91/115	-
20	SQD	T	822	-	-	7/26/46/69	0/1/1/1
14	CLA	o	519	13	1/1/11/20	0/15/91/115	-
17	BCR	q	524	-	-	0/29/63/63	0/2/2/2
14	CLA	m	503	13	1/1/11/20	6/15/91/115	-
14	CLA	X	501	13	1/1/15/20	14/39/115/115	-
17	BCR	b1	524	-	-	0/29/63/63	0/2/2/2
14	CLA	c4	516	13	1/1/11/20	5/15/91/115	-
14	CLA	Y	516	13	1/1/11/20	7/15/91/115	-
14	CLA	k	505	13	1/1/11/20	5/15/91/115	-
17	BCR	m	521	-	-	2/29/63/63	0/2/2/2
14	CLA	aA	1122	1	1/1/14/20	9/33/109/115	-
14	CLA	k	504	-	1/1/11/20	6/15/91/115	-
14	CLA	bB	1216	-	1/1/13/20	7/27/103/115	-
20	SQD	a4	822	-	-	14/31/51/69	0/1/1/1
14	CLA	Z	505	13	1/1/15/20	13/39/115/115	-
14	CLA	j	513	13	1/1/12/20	7/21/97/115	-
15	PQN	cB	2002	-	-	9/23/43/43	0/2/2/2
14	CLA	S	509	13	1/1/15/20	8/39/115/115	-
14	CLA	aA	1013	-	1/1/15/20	8/39/115/115	-
14	CLA	T	504	-	1/1/11/20	9/15/91/115	-
14	CLA	S	511	13	1/1/12/20	6/21/97/115	-
14	CLA	c5	501	13	1/1/15/20	19/39/115/115	-
14	CLA	bA	1022	-	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LHG	bA	5005	-	-	17/43/43/53	-
15	PQN	aA	2001	-	-	12/23/43/43	0/2/2/2
20	SQD	c3	822	-	-	13/27/47/69	0/1/1/1
14	CLA	cA	1135	1	1/1/12/20	11/23/99/115	-
14	CLA	c3	501	13	1/1/15/20	14/39/115/115	-
14	CLA	g	503	13	1/1/11/20	2/15/91/115	-
14	CLA	S	512	13	1/1/11/20	4/15/91/115	-
17	BCR	Z	522	-	-	4/29/63/63	0/2/2/2
14	CLA	c5	508	13	1/1/13/20	7/27/103/115	-
14	CLA	o	516	13	1/1/11/20	10/15/91/115	-
14	CLA	aA	1123	-	1/1/15/20	11/39/115/115	-
17	BCR	bB	4005	-	-	2/29/63/63	0/2/2/2
21	LMG	a1	5104	-	-	5/35/55/70	0/1/1/1
14	CLA	cJ	1303	8	1/1/13/20	12/30/106/115	-
20	SQD	W	822	-	-	8/27/47/69	0/1/1/1
14	CLA	bB	1220	2	1/1/12/20	2/21/97/115	-
14	CLA	b6	503	13	1/1/15/20	13/39/115/115	-
17	BCR	c1	521	-	-	5/29/63/63	0/2/2/2
14	CLA	a5	503	13	1/1/15/20	14/39/115/115	-
14	CLA	q	501	13	1/1/13/20	14/30/106/115	-
17	BCR	b2	523	-	-	1/29/63/63	0/2/2/2
17	BCR	b3	522	-	-	4/29/63/63	0/2/2/2
14	CLA	Z	513	13	1/1/12/20	3/21/97/115	-
14	CLA	b5	507	-	1/1/14/20	5/35/111/115	-
17	BCR	a2	523	-	-	0/29/63/63	0/2/2/2
14	CLA	a5	511	13	1/1/11/20	3/15/91/115	-
14	CLA	cF	1301	-	1/1/11/20	2/15/91/115	-
14	CLA	b	508	13	1/1/11/20	4/15/91/115	-
14	CLA	c2	518	13	1/1/13/20	5/27/103/115	-
14	CLA	c	509	13	1/1/14/20	7/36/112/115	-
14	CLA	o	517	-	1/1/11/20	6/15/91/115	-
17	BCR	c6	521	-	-	5/29/63/63	0/2/2/2
17	BCR	b4	524	-	-	0/29/63/63	0/2/2/2
14	CLA	cA	1106	1	1/1/15/20	21/39/115/115	-
14	CLA	aB	1021	2	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	S	505	13	1/1/13/20	6/27/103/115	-
14	CLA	c6	505	13	1/1/14/20	8/33/109/115	-
17	BCR	q	523	-	-	4/29/63/63	0/2/2/2
14	CLA	c6	503	13	1/1/15/20	14/39/115/115	-
19	LMU	aA	1849	-	-	7/14/34/61	0/1/1/2
14	CLA	c5	512	13	1/1/12/20	12/24/100/115	-
17	BCR	a2	524	-	-	0/29/63/63	0/2/2/2
14	CLA	Y	506	13	1/1/11/20	6/15/91/115	-
14	CLA	d	519	13	1/1/11/20	4/15/91/115	-
14	CLA	k	503	13	1/1/11/20	0/15/91/115	-
14	CLA	a1	506	13	1/1/11/20	4/15/91/115	-
14	CLA	U	512	13	1/1/11/20	6/15/91/115	-
14	CLA	Y	505	13	1/1/15/20	16/39/115/115	-
14	CLA	a5	513	13	1/1/13/20	3/27/103/115	-
14	CLA	b2	519	13	1/1/12/20	6/21/97/115	-
14	CLA	b4	517	-	1/1/11/20	8/15/91/115	-
14	CLA	aB	1214	2	1/1/15/20	15/39/115/115	-
14	CLA	cA	1011	1	1/1/15/20	9/39/115/115	-
17	BCR	b3	523	-	-	1/29/63/63	0/2/2/2
14	CLA	cA	1137	1	1/1/13/20	9/27/103/115	-
14	CLA	a4	506	13	1/1/11/20	6/15/91/115	-
14	CLA	cA	1124	-	1/1/13/20	4/29/105/115	-
14	CLA	bA	1137	1	1/1/13/20	10/27/103/115	-
14	CLA	b2	507	-	1/1/14/20	9/37/113/115	-
14	CLA	p	511	13	1/1/11/20	4/15/91/115	-
18	LHG	aX	4021	-	-	12/43/43/53	-
14	CLA	a3	511	13	1/1/14/20	14/36/112/115	-
14	CLA	q	508	13	1/1/11/20	2/15/91/115	-
14	CLA	a5	517	-	1/1/11/20	7/15/91/115	-
14	CLA	c	504	-	1/1/11/20	4/15/91/115	-
14	CLA	j	503	13	1/1/11/20	2/15/91/115	-
14	CLA	f	518	13	1/1/11/20	8/15/91/115	-
14	CLA	c1	512	13	1/1/12/20	9/25/101/115	-
14	CLA	aB	1220	2	1/1/12/20	2/21/97/115	-
14	CLA	bA	1127	1	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	h	524	-	-	0/29/63/63	0/2/2/2
14	CLA	bA	1113	1	1/1/12/20	5/21/97/115	-
14	CLA	f	506	13	1/1/11/20	4/15/91/115	-
14	CLA	aK	1401	-	1/1/13/20	9/27/103/115	-
14	CLA	bB	1228	2	1/1/13/20	5/29/105/115	-
14	CLA	c6	502	13	1/1/14/20	11/33/109/115	-
14	CLA	o	508	13	1/1/11/20	3/15/91/115	-
20	SQD	h	822	-	-	11/27/47/69	0/1/1/1
14	CLA	aA	1120	1	1/1/13/20	9/27/103/115	-
14	CLA	cL	1502	10	1/1/14/20	7/33/109/115	-
20	SQD	b3	822	-	-	17/32/52/69	0/1/1/1
14	CLA	aA	1801	18	1/1/11/20	8/15/91/115	-
14	CLA	k	509	13	1/1/11/20	5/15/91/115	-
14	CLA	i	505	13	1/1/13/20	7/27/103/115	-
17	BCR	a6	521	-	-	5/29/63/63	0/2/2/2
14	CLA	cA	1117	1	1/1/15/20	13/39/115/115	-
14	CLA	c1	505	13	1/1/15/20	12/39/115/115	-
14	CLA	b	516	13	1/1/11/20	4/15/91/115	-
14	CLA	bB	1218	2	1/1/14/20	11/33/109/115	-
14	CLA	a2	504	-	1/1/11/20	4/18/94/115	-
14	CLA	d	501	13	1/1/11/20	10/15/91/115	-
14	CLA	b3	516	13	1/1/11/20	5/15/91/115	-
17	BCR	S	522	-	-	5/29/63/63	0/2/2/2
14	CLA	e	502	13	1/1/11/20	4/15/91/115	-
14	CLA	aA	1118	1	1/1/14/20	12/33/109/115	-
19	LMU	bA	1849	-	-	7/14/34/61	0/1/1/2
14	CLA	bB	1021	2	1/1/15/20	14/39/115/115	-
17	BCR	q	521	-	-	4/29/63/63	0/2/2/2
14	CLA	bB	1235	2	1/1/15/20	10/39/115/115	-
14	CLA	b3	504	-	1/1/13/20	15/30/106/115	-
14	CLA	cK	1103	9	1/1/9/20	7/9/81/115	-
14	CLA	a1	512	13	1/1/12/20	10/25/101/115	-
14	CLA	X	503	13	1/1/14/20	9/37/113/115	-
17	BCR	aF	4015	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	U	506	13	1/1/11/20	6/15/91/115	-
14	CLA	S	501	13	1/1/11/20	5/15/91/115	-
14	CLA	k	508	13	1/1/11/20	3/15/91/115	-
17	BCR	bJ	4012	-	-	4/29/63/63	0/2/2/2
17	BCR	cI	4018	-	-	6/29/63/63	0/2/2/2
14	CLA	aA	1103	1	1/1/15/20	12/39/115/115	-
14	CLA	g	513	13	1/1/11/20	4/15/91/115	-
14	CLA	p	501	13	1/1/11/20	9/15/91/115	-
14	CLA	a	501	13	1/1/14/20	9/33/109/115	-
17	BCR	bI	4019	-	-	4/29/63/63	0/2/2/2
14	CLA	b6	508	13	1/1/12/20	4/23/99/115	-
14	CLA	a3	519	13	1/1/13/20	11/27/103/115	-
14	CLA	W	508	13	1/1/12/20	2/23/99/115	-
14	CLA	a6	517	-	1/1/11/20	8/15/91/115	-
14	CLA	cA	1101	1	1/1/14/20	10/33/109/115	-
19	LMU	cA	1848	-	-	4/15/35/61	0/1/1/2
14	CLA	c5	503	13	1/1/15/20	15/39/115/115	-
14	CLA	b6	501	13	1/1/15/20	14/39/115/115	-
17	BCR	p	524	-	-	0/29/63/63	0/2/2/2
14	CLA	aB	1228	2	1/1/13/20	4/29/105/115	-
17	BCR	V	522	-	-	5/29/63/63	0/2/2/2
14	CLA	h	505	13	1/1/11/20	3/15/91/115	-
14	CLA	bA	1114	-	1/1/11/20	6/15/91/115	-
14	CLA	aK	1103	9	1/1/9/20	7/9/81/115	-
14	CLA	a	507	-	1/1/11/20	4/15/91/115	-
14	CLA	a1	505	13	1/1/15/20	12/39/115/115	-
14	CLA	a5	501	13	1/1/15/20	13/39/115/115	-
17	BCR	d	523	-	-	7/29/63/63	0/2/2/2
14	CLA	V	508	13	1/1/12/20	4/24/100/115	-
14	CLA	cJ	1302	8	1/1/11/20	12/20/96/115	-
17	BCR	c6	523	-	-	6/29/63/63	0/2/2/2
14	CLA	a5	505	13	1/1/15/20	14/39/115/115	-
14	CLA	cB	1212	2	1/1/11/20	2/15/91/115	-
17	BCR	l	523	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	bB	1225	2	1/1/15/20	13/39/115/115	-
14	CLA	W	519	13	1/1/11/20	2/15/91/115	-
17	BCR	W	523	-	-	7/29/63/63	0/2/2/2
14	CLA	b	503	13	1/1/13/20	6/30/106/115	-
14	CLA	V	513	13	1/1/12/20	5/21/97/115	-
14	CLA	b5	501	13	1/1/15/20	13/39/115/115	-
14	CLA	c4	509	13	1/1/15/20	6/39/115/115	-
20	SQD	c6	822	-	-	9/25/45/69	0/1/1/1
14	CLA	b4	512	13	1/1/11/20	5/15/91/115	-
14	CLA	Y	509	13	1/1/14/20	9/36/112/115	-
14	CLA	p	517	-	1/1/11/20	6/15/91/115	-
14	CLA	a4	517	-	1/1/11/20	6/15/91/115	-
14	CLA	a3	502	13	1/1/14/20	9/33/109/115	-
14	CLA	aA	1127	1	1/1/15/20	4/39/115/115	-
14	CLA	Y	518	13	1/1/13/20	16/29/105/115	-
17	BCR	V	523	-	-	4/29/63/63	0/2/2/2
14	CLA	a6	507	-	1/1/14/20	7/36/112/115	-
14	CLA	cB	1227	2	1/1/12/20	11/26/102/115	-
17	BCR	bK	4001	-	-	3/29/63/63	0/2/2/2
17	BCR	e	523	-	-	0/29/63/63	0/2/2/2
14	CLA	a4	503	13	1/1/15/20	7/39/115/115	-
14	CLA	e	503	13	1/1/11/20	6/15/91/115	-
14	CLA	a2	512	13	1/1/12/20	8/25/101/115	-
14	CLA	b2	518	13	1/1/13/20	5/27/103/115	-
14	CLA	aB	1218	2	1/1/14/20	13/33/109/115	-
14	CLA	aB	1210	2	1/1/15/20	18/39/115/115	-
14	CLA	bB	1230	2	1/1/13/20	10/31/107/115	-
14	CLA	bL	1501	10	1/1/15/20	12/39/115/115	-
14	CLA	b2	501	13	1/1/15/20	16/39/115/115	-
17	BCR	aA	4007	-	-	2/29/63/63	0/2/2/2
14	CLA	cB	1204	2	1/1/14/20	3/33/109/115	-
14	CLA	V	512	13	1/1/11/20	8/15/91/115	-
20	SQD	e	822	-	-	12/27/47/69	0/1/1/1
14	CLA	cA	1134	1	1/1/12/20	7/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	o	509	13	1/1/11/20	2/15/91/115	-
19	LMU	cA	1849	-	-	7/14/34/61	0/1/1/2
14	CLA	o	511	13	1/1/11/20	7/15/91/115	-
14	CLA	T	513	13	1/1/12/20	3/21/97/115	-
17	BCR	S	523	-	-	4/29/63/63	0/2/2/2
14	CLA	c3	509	13	1/1/15/20	6/39/115/115	-
14	CLA	c2	504	-	1/1/11/20	2/15/91/115	-
14	CLA	a6	511	13	1/1/11/20	6/15/91/115	-
14	CLA	c5	502	13	1/1/14/20	11/33/109/115	-
14	CLA	cK	1401	-	1/1/13/20	7/27/103/115	-
14	CLA	m	516	13	1/1/11/20	5/15/91/115	-
14	CLA	cA	1129	1	1/1/12/20	9/24/100/115	-
17	BCR	n	522	-	-	3/29/63/63	0/2/2/2
14	CLA	f	509	13	1/1/11/20	2/15/91/115	-
14	CLA	b4	509	13	1/1/15/20	8/39/115/115	-
14	CLA	a6	502	13	1/1/14/20	11/33/109/115	-
14	CLA	cA	1140	1	1/1/15/20	15/39/115/115	-
14	CLA	n	508	13	1/1/11/20	0/15/91/115	-
14	CLA	b6	509	13	1/1/15/20	2/39/115/115	-
17	BCR	a1	522	-	-	5/29/63/63	0/2/2/2
14	CLA	W	509	13	1/1/14/20	5/36/112/115	-
14	CLA	m	510	13	1/1/11/20	4/15/91/115	-
14	CLA	j	508	13	1/1/11/20	0/15/91/115	-
14	CLA	bB	1229	2	1/1/15/20	11/39/115/115	-
14	CLA	b	501	13	1/1/11/20	9/15/91/115	-
14	CLA	g	505	13	1/1/15/20	14/39/115/115	-
20	SQD	c1	822	-	-	7/26/46/69	0/1/1/1
14	CLA	T	501	13	1/1/12/20	12/21/97/115	-
17	BCR	cI	4019	-	-	4/29/63/63	0/2/2/2
14	CLA	b3	501	13	1/1/15/20	12/39/115/115	-
14	CLA	d	506	13	1/1/11/20	6/15/91/115	-
14	CLA	aB	1205	2	1/1/15/20	13/39/115/115	-
17	BCR	a3	523	-	-	5/29/63/63	0/2/2/2
14	CLA	c4	513	13	1/1/11/20	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	a5	521	-	-	3/29/63/63	0/2/2/2
14	CLA	cA	1114	-	1/1/11/20	6/15/91/115	-
14	CLA	c6	506	13	1/1/11/20	8/15/91/115	-
14	CLA	bX	1401	12	1/1/11/20	7/15/91/115	-
14	CLA	c3	517	-	1/1/11/20	9/15/91/115	-
14	CLA	e	509	13	1/1/11/20	2/15/91/115	-
14	CLA	cB	1220	2	1/1/11/20	2/18/94/115	-
14	CLA	aB	1224	2	1/1/13/20	14/30/106/115	-
17	BCR	n	523	-	-	4/29/63/63	0/2/2/2
14	CLA	S	504	-	1/1/11/20	8/15/91/115	-
14	CLA	b	507	-	1/1/11/20	6/15/91/115	-
14	CLA	a4	501	13	1/1/15/20	16/39/115/115	-
14	CLA	f	507	-	1/1/11/20	4/15/91/115	-
14	CLA	p	504	-	1/1/11/20	9/15/91/115	-
14	CLA	cA	1112	1	1/1/11/20	4/19/95/115	-
14	CLA	b3	507	-	1/1/14/20	5/33/109/115	-
17	BCR	X	524	-	-	0/29/63/63	0/2/2/2
14	CLA	l	503	13	1/1/11/20	2/15/91/115	-
14	CLA	m	513	13	1/1/12/20	7/24/100/115	-
14	CLA	aA	1104	1	1/1/15/20	10/39/115/115	-
14	CLA	m	506	13	1/1/11/20	6/15/91/115	-
14	CLA	n	512	13	1/1/11/20	6/15/91/115	-
17	BCR	U	524	-	-	2/29/63/63	0/2/2/2
14	CLA	cA	1111	1	1/1/13/20	11/27/103/115	-
14	CLA	V	506	13	1/1/11/20	4/15/91/115	-
14	CLA	cB	1023	-	1/1/15/20	10/39/115/115	-
14	CLA	b6	504	-	1/1/13/20	7/27/103/115	-
14	CLA	b2	505	13	1/1/15/20	15/39/115/115	-
14	CLA	bB	1202	2	1/1/15/20	11/39/115/115	-
14	CLA	l	509	13	1/1/11/20	4/15/91/115	-
14	CLA	b2	503	13	1/1/15/20	4/39/115/115	-
14	CLA	h	517	-	1/1/11/20	11/15/91/115	-
20	SQD	Z	822	-	-	9/24/44/69	0/1/1/1
19	LMU	cJ	5105	-	-	4/12/32/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	a	523	-	-	4/29/63/63	0/2/2/2
17	BCR	c5	524	-	-	0/29/63/63	0/2/2/2
14	CLA	bA	1131	1	1/1/15/20	9/39/115/115	-
14	CLA	a	503	13	1/1/14/20	6/37/113/115	-
17	BCR	d	521	-	-	4/29/63/63	0/2/2/2
14	CLA	b3	517	-	1/1/11/20	6/15/91/115	-
20	SQD	n	822	-	-	16/25/45/69	0/1/1/1
17	BCR	bB	4017	-	-	2/29/63/63	0/2/2/2
14	CLA	a1	518	13	1/1/13/20	10/27/103/115	-
17	BCR	b2	521	-	-	7/29/63/63	0/2/2/2
14	CLA	Z	516	13	1/1/11/20	9/15/91/115	-
14	CLA	l	507	-	1/1/11/20	6/15/91/115	-
14	CLA	q	504	-	1/1/11/20	9/15/91/115	-
14	CLA	bA	1237	-	1/1/15/20	14/39/115/115	-
14	CLA	f	504	-	1/1/11/20	9/15/91/115	-
14	CLA	j	512	13	1/1/11/20	6/15/91/115	-
14	CLA	cA	1109	1	1/1/15/20	11/39/115/115	-
14	CLA	a6	504	-	1/1/14/20	16/36/112/115	-
14	CLA	bB	1209	2	1/1/12/20	12/25/101/115	-
14	CLA	aX	1401	12	1/1/11/20	7/15/91/115	-
16	SF4	aA	3001	2,1	-	-	0/6/5/5
14	CLA	V	503	13	1/1/11/20	4/15/91/115	-
17	BCR	a2	522	-	-	6/29/63/63	0/2/2/2
17	BCR	cB	4009	-	-	6/29/63/63	0/2/2/2
14	CLA	b	502	13	1/1/11/20	4/15/91/115	-
14	CLA	a5	518	13	1/1/13/20	10/30/106/115	-
14	CLA	a2	508	13	1/1/13/20	5/27/103/115	-
14	CLA	c1	513	13	1/1/12/20	1/24/100/115	-
14	CLA	b3	502	13	1/1/14/20	13/33/109/115	-
14	CLA	bA	1138	1	1/1/15/20	11/39/115/115	-
14	CLA	T	505	13	1/1/12/20	6/24/100/115	-
14	CLA	a4	504	-	1/1/12/20	4/25/101/115	-
14	CLA	Z	517	-	1/1/11/20	8/15/91/115	-
14	CLA	aA	1022	-	1/1/15/20	8/39/115/115	-
19	LMU	aJ	5105	-	-	5/13/33/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cA	1130	1	1/1/12/20	6/24/100/115	-
17	BCR	Y	523	-	-	2/29/63/63	0/2/2/2
14	CLA	b5	518	13	1/1/13/20	5/27/103/115	-
14	CLA	q	517	-	1/1/11/20	8/15/91/115	-
14	CLA	h	511	13	1/1/11/20	5/15/91/115	-
17	BCR	aB	4010	-	-	0/29/63/63	0/2/2/2
14	CLA	aA	1117	1	1/1/15/20	14/39/115/115	-
14	CLA	a1	510	13	1/1/15/20	8/39/115/115	-
14	CLA	X	509	13	1/1/15/20	6/39/115/115	-
14	CLA	m	511	13	1/1/11/20	4/15/91/115	-
14	CLA	c	507	-	1/1/11/20	4/15/91/115	-
14	CLA	l	501	13	1/1/11/20	9/15/91/115	-
14	CLA	a3	506	13	1/1/11/20	6/15/91/115	-
14	CLA	aB	1202	2	1/1/15/20	11/39/115/115	-
14	CLA	aB	1215	2	1/1/14/20	7/35/111/115	-
14	CLA	q	505	13	1/1/13/20	7/27/103/115	-
17	BCR	Y	524	-	-	0/29/63/63	0/2/2/2
16	SF4	cC	3002	3	-	-	0/6/5/5
20	SQD	Y	822	-	-	10/28/48/69	0/1/1/1
14	CLA	e	518	13	1/1/11/20	5/15/91/115	-
14	CLA	b4	516	13	1/1/11/20	5/15/91/115	-
14	CLA	a4	507	-	1/1/14/20	9/36/112/115	-
17	BCR	a4	521	-	-	8/29/63/63	0/2/2/2
14	CLA	b1	511	13	1/1/13/20	9/27/103/115	-
14	CLA	c5	509	13	1/1/15/20	12/39/115/115	-
17	BCR	aI	4020	-	-	2/29/63/63	0/2/2/2
14	CLA	X	506	13	1/1/11/20	6/15/91/115	-
14	CLA	c4	505	13	1/1/15/20	11/39/115/115	-
14	CLA	b6	516	13	1/1/11/20	8/15/91/115	-
17	BCR	a3	521	-	-	9/29/63/63	0/2/2/2
14	CLA	cA	1122	1	1/1/14/20	10/33/109/115	-
14	CLA	W	504	-	1/1/12/20	10/24/100/115	-
14	CLA	X	505	13	1/1/15/20	16/39/115/115	-
14	CLA	d	507	-	1/1/11/20	4/15/91/115	-
14	CLA	c6	517	-	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	aA	1136	1	1/1/15/20	10/39/115/115	-
14	CLA	n	506	13	1/1/11/20	6/15/91/115	-
17	BCR	bM	4021	-	-	5/29/63/63	0/2/2/2
14	CLA	f	510	13	1/1/11/20	6/15/91/115	-
20	SQD	cB	1852	-	-	8/34/54/69	0/1/1/1
17	BCR	cB	4017	-	-	2/29/63/63	0/2/2/2
14	CLA	bB	1208	2	1/1/13/20	5/27/103/115	-
14	CLA	b5	509	13	1/1/15/20	7/39/115/115	-
14	CLA	aA	1137	1	1/1/13/20	8/27/103/115	-
14	CLA	k	517	-	1/1/11/20	10/15/91/115	-
14	CLA	p	519	13	1/1/11/20	6/15/91/115	-
14	CLA	bB	1234	2	1/1/14/20	7/33/109/115	-
14	CLA	j	511	13	1/1/11/20	5/15/91/115	-
14	CLA	c6	509	13	1/1/15/20	9/39/115/115	-
14	CLA	m	505	13	1/1/12/20	6/23/99/115	-
14	CLA	b5	512	13	1/1/12/20	10/24/100/115	-
14	CLA	V	516	13	1/1/11/20	7/15/91/115	-
14	CLA	c6	511	13	1/1/11/20	6/15/91/115	-
14	CLA	aF	1301	-	1/1/11/20	2/15/91/115	-
14	CLA	a1	503	13	1/1/14/20	5/37/113/115	-
14	CLA	W	518	13	1/1/13/20	12/27/103/115	-
14	CLA	g	508	13	1/1/11/20	4/15/91/115	-
14	CLA	b6	519	13	1/1/11/20	8/15/91/115	-
17	BCR	S	524	-	-	0/29/63/63	0/2/2/2
14	CLA	aA	1132	1	1/1/15/20	13/39/115/115	-
14	CLA	X	510	13	1/1/14/20	11/36/112/115	-
17	BCR	W	521	-	-	5/29/63/63	0/2/2/2
14	CLA	cA	1120	1	1/1/13/20	13/27/103/115	-
14	CLA	V	507	-	1/1/11/20	4/15/91/115	-
17	BCR	a1	521	-	-	5/29/63/63	0/2/2/2
14	CLA	aA	1113	1	1/1/12/20	9/21/97/115	-
14	CLA	bA	1106	1	1/1/15/20	18/39/115/115	-
14	CLA	aB	1235	2	1/1/15/20	10/39/115/115	-
14	CLA	aB	1231	2	1/1/13/20	11/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	a	522	-	-	4/29/63/63	0/2/2/2
14	CLA	aL	1502	10	1/1/14/20	7/33/109/115	-
14	CLA	bA	1139	-	1/1/14/20	5/33/109/115	-
17	BCR	f	521	-	-	0/29/63/63	0/2/2/2
14	CLA	c5	504	-	1/1/13/20	9/30/106/115	-
17	BCR	c4	524	-	-	0/29/63/63	0/2/2/2
17	BCR	i	521	-	-	2/29/63/63	0/2/2/2
17	BCR	aB	4017	-	-	2/29/63/63	0/2/2/2
14	CLA	S	516	13	1/1/11/20	3/15/91/115	-
20	SQD	b4	822	-	-	17/28/48/69	0/1/1/1
17	BCR	b6	522	-	-	4/29/63/63	0/2/2/2
14	CLA	cA	1128	1	1/1/15/20	7/39/115/115	-
14	CLA	e	511	13	1/1/11/20	3/15/91/115	-
14	CLA	p	508	13	1/1/11/20	4/15/91/115	-
14	CLA	bA	1140	1	1/1/15/20	16/39/115/115	-
14	CLA	X	512	13	1/1/11/20	8/15/91/115	-
14	CLA	d	502	13	1/1/11/20	6/15/91/115	-
14	CLA	c3	504	-	1/1/13/20	10/29/105/115	-
14	CLA	aB	1217	2	1/1/13/20	12/27/103/115	-
21	LMG	a6	5104	-	-	3/33/53/70	0/1/1/1
20	SQD	b6	822	-	-	8/25/45/69	0/1/1/1
14	CLA	k	507	-	1/1/11/20	4/15/91/115	-
14	CLA	f	516	13	1/1/11/20	9/15/91/115	-
14	CLA	U	510	13	1/1/13/20	8/27/103/115	-
14	CLA	cB	1208	2	1/1/12/20	5/24/100/115	-
14	CLA	cB	1236	2	1/1/12/20	5/21/97/115	-
14	CLA	i	507	-	1/1/11/20	6/15/91/115	-
17	BCR	bA	4002	-	-	4/29/63/63	0/2/2/2
17	BCR	m	524	-	-	0/29/63/63	0/2/2/2
14	CLA	k	519	13	1/1/11/20	6/15/91/115	-
14	CLA	q	519	13	1/1/11/20	11/15/91/115	-
14	CLA	g	510	13	1/1/11/20	6/15/91/115	-
14	CLA	i	519	13	1/1/11/20	4/15/91/115	-
14	CLA	bA	1135	1	1/1/12/20	11/23/99/115	-
14	CLA	b1	501	13	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	j	519	13	1/1/11/20	5/15/91/115	-
14	CLA	S	517	-	1/1/11/20	8/15/91/115	-
14	CLA	a6	509	13	1/1/15/20	9/39/115/115	-
14	CLA	h	502	13	1/1/11/20	4/15/91/115	-
14	CLA	bB	1221	-	1/1/14/20	12/33/109/115	-
17	BCR	d	522	-	-	5/29/63/63	0/2/2/2
17	BCR	l	521	-	-	5/29/63/63	0/2/2/2
17	BCR	c6	522	-	-	5/29/63/63	0/2/2/2
14	CLA	V	502	13	1/1/14/20	10/33/109/115	-
14	CLA	c3	512	13	1/1/12/20	7/24/100/115	-
14	CLA	Z	512	13	1/1/11/20	8/15/91/115	-
14	CLA	c1	517	-	1/1/11/20	10/15/91/115	-
14	CLA	c4	508	13	1/1/14/20	7/33/109/115	-
14	CLA	cB	1214	2	1/1/14/20	11/33/109/115	-
14	CLA	Y	508	13	1/1/12/20	0/24/100/115	-
14	CLA	q	507	-	1/1/11/20	6/15/91/115	-
14	CLA	aA	1108	1	1/1/11/20	3/15/91/115	-
14	CLA	e	505	13	1/1/14/20	10/36/112/115	-
14	CLA	cA	1102	1	1/1/15/20	7/39/115/115	-
17	BCR	h	521	-	-	4/29/63/63	0/2/2/2
14	CLA	a3	505	13	1/1/15/20	11/39/115/115	-
14	CLA	c6	501	13	1/1/15/20	15/39/115/115	-
14	CLA	b5	513	13	1/1/13/20	4/27/103/115	-
17	BCR	aB	4005	-	-	2/29/63/63	0/2/2/2
14	CLA	a6	506	13	1/1/11/20	6/15/91/115	-
14	CLA	a	518	13	1/1/13/20	10/27/103/115	-
21	LMG	b2	5104	-	-	4/35/55/70	0/1/1/1
17	BCR	c1	524	-	-	0/29/63/63	0/2/2/2
14	CLA	c2	513	13	1/1/11/20	4/17/93/115	-
17	BCR	c4	523	-	-	7/29/63/63	0/2/2/2
14	CLA	cA	1132	1	1/1/15/20	10/39/115/115	-
17	BCR	aF	4014	-	-	4/29/63/63	0/2/2/2
14	CLA	T	502	13	1/1/14/20	11/33/109/115	-
14	CLA	aA	1138	1	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	c5	517	-	1/1/11/20	8/15/91/115	-
14	CLA	l	504	-	1/1/11/20	5/15/91/115	-
14	CLA	a5	507	-	1/1/14/20	8/33/109/115	-
14	CLA	b1	517	-	1/1/11/20	11/15/91/115	-
14	CLA	a3	513	13	1/1/12/20	5/21/97/115	-
14	CLA	m	504	-	1/1/11/20	7/15/91/115	-
17	BCR	T	521	-	-	5/29/63/63	0/2/2/2
17	BCR	p	523	-	-	2/29/63/63	0/2/2/2
17	BCR	a6	522	-	-	4/29/63/63	0/2/2/2
14	CLA	S	508	13	1/1/12/20	2/23/99/115	-
14	CLA	X	511	13	1/1/13/20	5/27/103/115	-
14	CLA	Z	509	13	1/1/15/20	5/39/115/115	-
14	CLA	c2	503	13	1/1/15/20	4/39/115/115	-
14	CLA	c1	508	13	1/1/13/20	4/27/103/115	-
14	CLA	a4	519	13	1/1/12/20	4/24/100/115	-
14	CLA	e	506	13	1/1/11/20	5/15/91/115	-
17	BCR	b	522	-	-	6/29/63/63	0/2/2/2
18	LHG	bA	5003	14	-	9/45/45/53	-
14	CLA	aA	1110	1	1/1/12/20	5/25/101/115	-
14	CLA	a6	513	13	1/1/13/20	7/27/103/115	-
14	CLA	c5	511	13	1/1/11/20	2/15/91/115	-
14	CLA	b3	509	13	1/1/15/20	10/39/115/115	-
14	CLA	a	512	13	1/1/11/20	7/15/91/115	-
14	CLA	bA	1133	1	1/1/15/20	12/39/115/115	-
14	CLA	aA	1101	1	1/1/14/20	9/33/109/115	-
17	BCR	n	524	-	-	0/29/63/63	0/2/2/2
14	CLA	aB	1230	2	1/1/13/20	10/31/107/115	-
14	CLA	U	511	13	1/1/13/20	4/27/103/115	-
14	CLA	bA	1013	-	1/1/15/20	8/39/115/115	-
14	CLA	c3	511	13	1/1/14/20	14/36/112/115	-
14	CLA	c2	507	-	1/1/14/20	5/33/109/115	-
14	CLA	l	505	13	1/1/11/20	5/15/91/115	-
17	BCR	a6	523	-	-	0/29/63/63	0/2/2/2
14	CLA	a	506	13	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LHG	bA	5002	-	-	18/46/46/53	-
14	CLA	c	517	-	1/1/11/20	6/15/91/115	-
14	CLA	bA	1112	1	1/1/11/20	3/19/95/115	-
14	CLA	g	511	13	1/1/11/20	3/15/91/115	-
17	BCR	a3	522	-	-	2/29/63/63	0/2/2/2
14	CLA	cA	1123	-	1/1/15/20	11/39/115/115	-
14	CLA	cA	1125	1	1/1/14/20	14/33/109/115	-
14	CLA	b2	516	13	1/1/11/20	7/15/91/115	-
14	CLA	bA	1123	-	1/1/15/20	7/39/115/115	-
14	CLA	a2	516	13	1/1/11/20	3/15/91/115	-
14	CLA	h	519	13	1/1/11/20	5/15/91/115	-
17	BCR	i	523	-	-	0/29/63/63	0/2/2/2
14	CLA	cA	1115	1	1/1/14/20	14/33/109/115	-
14	CLA	d	510	13	1/1/14/20	11/33/109/115	-
17	BCR	c3	524	-	-	2/29/63/63	0/2/2/2
20	SQD	c5	822	-	-	13/26/46/69	0/1/1/1
17	BCR	b	523	-	-	4/29/63/63	0/2/2/2
14	CLA	c6	510	13	1/1/15/20	11/39/115/115	-
14	CLA	cX	1401	12	1/1/11/20	7/15/91/115	-
14	CLA	b5	503	13	1/1/15/20	10/39/115/115	-
14	CLA	bA	1126	1	1/1/15/20	14/39/115/115	-
14	CLA	a	505	13	1/1/15/20	12/39/115/115	-
14	CLA	U	513	13	1/1/11/20	5/15/91/115	-
14	CLA	c4	512	13	1/1/11/20	7/15/91/115	-
17	BCR	a6	524	-	-	0/29/63/63	0/2/2/2
14	CLA	b2	510	13	1/1/15/20	10/39/115/115	-
14	CLA	Y	517	-	1/1/11/20	9/15/91/115	-
17	BCR	aB	4004	-	-	7/29/63/63	0/2/2/2
14	CLA	c	502	13	1/1/13/20	5/27/103/115	-
14	CLA	a1	508	13	1/1/13/20	7/27/103/115	-
14	CLA	Z	501	13	1/1/15/20	20/39/115/115	-
14	CLA	i	501	13	1/1/11/20	9/15/91/115	-
15	PQN	aB	2002	-	-	9/23/43/43	0/2/2/2
14	CLA	bA	1121	1	1/1/12/20	9/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	e	519	13	1/1/11/20	4/15/91/115	-
17	BCR	W	522	-	-	5/29/63/63	0/2/2/2
18	LHG	cX	4021	-	-	14/43/43/53	-
14	CLA	c	503	13	1/1/11/20	5/15/91/115	-
14	CLA	b6	511	13	1/1/11/20	4/15/91/115	-
14	CLA	aA	1105	1	1/1/12/20	2/23/99/115	-
14	CLA	Y	511	13	1/1/11/20	6/15/91/115	-
14	CLA	i	518	13	1/1/13/20	10/27/103/115	-
14	CLA	b5	505	13	1/1/15/20	10/39/115/115	-
14	CLA	V	510	13	1/1/14/20	10/33/109/115	-
14	CLA	n	501	13	1/1/11/20	8/15/91/115	-
14	CLA	W	507	-	1/1/12/20	2/23/99/115	-
14	CLA	j	501	13	1/1/11/20	9/15/91/115	-
14	CLA	a1	501	13	1/1/15/20	15/39/115/115	-
17	BCR	bB	4010	-	-	0/29/63/63	0/2/2/2
14	CLA	cB	1218	2	1/1/13/20	11/29/105/115	-
14	CLA	c1	504	-	1/1/13/20	8/27/103/115	-
14	CLA	a3	512	13	1/1/12/20	11/25/101/115	-
14	CLA	aJ	1302	8	1/1/11/20	9/20/96/115	-
14	CLA	l	519	13	1/1/11/20	5/15/91/115	-
14	CLA	a2	513	13	1/1/11/20	4/15/91/115	-
14	CLA	b2	506	13	1/1/11/20	7/15/91/115	-
14	CLA	d	503	13	1/1/12/20	4/21/97/115	-
14	CLA	a2	502	13	1/1/14/20	8/33/109/115	-
14	CLA	bA	1136	1	1/1/15/20	9/39/115/115	-
17	BCR	aA	4008	-	-	3/29/63/63	0/2/2/2
17	BCR	a5	523	-	-	2/29/63/63	0/2/2/2
19	LMU	aB	1843	-	-	11/21/61/61	0/2/2/2
14	CLA	W	517	-	1/1/11/20	8/15/91/115	-
19	LMU	bB	1843	-	-	9/21/61/61	0/2/2/2
17	BCR	o	524	-	-	0/29/63/63	0/2/2/2
14	CLA	cB	1230	2	1/1/13/20	10/31/107/115	-
17	BCR	l	522	-	-	2/29/63/63	0/2/2/2
14	CLA	a6	512	13	1/1/11/20	8/15/91/115	-
17	BCR	b5	524	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cB	1229	2	1/1/14/20	11/33/109/115	-
14	CLA	h	518	13	1/1/11/20	9/18/94/115	-
14	CLA	j	510	13	1/1/14/20	11/33/109/115	-
14	CLA	cL	1501	10	1/1/15/20	10/39/115/115	-
14	CLA	W	501	13	1/1/15/20	15/39/115/115	-
14	CLA	b	512	13	1/1/12/20	8/21/97/115	-
14	CLA	a6	505	13	1/1/15/20	12/39/115/115	-
18	LHG	aA	5004	-	-	13/37/37/53	-
14	CLA	aA	1237	-	1/1/15/20	15/39/115/115	-
14	CLA	a6	503	13	1/1/15/20	12/39/115/115	-
14	CLA	cA	1126	1	1/1/15/20	13/39/115/115	-
14	CLA	a5	508	13	1/1/13/20	4/27/103/115	-
14	CLA	c2	501	13	1/1/15/20	10/39/115/115	-
14	CLA	bB	1203	2	1/1/15/20	21/39/115/115	-
14	CLA	a	516	13	1/1/11/20	6/15/91/115	-
14	CLA	a3	510	13	1/1/15/20	7/39/115/115	-
14	CLA	b	506	13	1/1/11/20	6/15/91/115	-
14	CLA	c4	519	13	1/1/12/20	6/23/99/115	-
14	CLA	T	519	13	1/1/11/20	6/15/91/115	-
17	BCR	bB	4006	-	-	4/29/63/63	0/2/2/2
14	CLA	b	505	13	1/1/14/20	9/33/109/115	-
14	CLA	X	519	13	1/1/11/20	10/15/91/115	-
14	CLA	o	518	13	1/1/13/20	8/27/103/115	-
14	CLA	b1	508	13	1/1/13/20	8/27/103/115	-
14	CLA	V	509	13	1/1/15/20	10/39/115/115	-
14	CLA	c3	508	13	1/1/13/20	7/27/103/115	-
14	CLA	b4	511	13	1/1/11/20	5/15/91/115	-
14	CLA	c5	510	13	1/1/15/20	8/39/115/115	-
14	CLA	cB	1206	2	1/1/15/20	9/39/115/115	-
14	CLA	c6	508	13	1/1/13/20	4/27/103/115	-
14	CLA	a5	516	13	1/1/11/20	8/18/94/115	-
14	CLA	j	506	13	1/1/11/20	4/15/91/115	-
14	CLA	c5	519	13	1/1/12/20	4/23/99/115	-
20	SQD	bB	1852	-	-	11/37/57/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	c5	506	13	1/1/11/20	4/15/91/115	-
14	CLA	bA	1107	1	1/1/13/20	9/27/103/115	-
14	CLA	aA	1107	1	1/1/13/20	11/27/103/115	-
14	CLA	a	517	-	1/1/11/20	8/15/91/115	-
14	CLA	b1	507	-	1/1/14/20	5/35/111/115	-
14	CLA	b5	516	13	1/1/11/20	11/20/96/115	-
14	CLA	n	507	-	1/1/11/20	4/15/91/115	-
17	BCR	n	521	-	-	3/29/63/63	0/2/2/2
14	CLA	o	505	13	1/1/11/20	3/15/91/115	-
14	CLA	c3	519	13	1/1/11/20	4/15/91/115	-
14	CLA	bL	1502	10	1/1/14/20	9/33/109/115	-
14	CLA	c6	516	13	1/1/11/20	6/15/91/115	-
20	SQD	X	822	-	-	12/31/51/69	0/1/1/1
17	BCR	j	521	-	-	8/29/63/63	0/2/2/2
14	CLA	b1	519	13	1/1/11/20	6/15/91/115	-
14	CLA	f	501	13	1/1/11/20	8/15/91/115	-
14	CLA	c3	505	13	1/1/15/20	14/39/115/115	-
14	CLA	aA	1102	1	1/1/15/20	10/39/115/115	-
14	CLA	b6	517	-	1/1/11/20	4/15/91/115	-
17	BCR	m	522	-	-	2/29/63/63	0/2/2/2
14	CLA	c4	507	-	1/1/14/20	6/33/109/115	-
14	CLA	W	513	13	1/1/12/20	1/21/97/115	-
14	CLA	a3	503	13	1/1/14/20	3/37/113/115	-
14	CLA	m	508	13	1/1/11/20	3/15/91/115	-
16	SF4	cA	3001	2,1	-	-	0/6/5/5
14	CLA	b3	512	13	1/1/12/20	9/25/101/115	-
14	CLA	aL	1501	10	1/1/15/20	10/39/115/115	-
14	CLA	bF	1301	-	1/1/11/20	2/15/91/115	-
14	CLA	h	516	13	1/1/11/20	4/15/91/115	-
14	CLA	bA	1134	1	1/1/13/20	7/27/103/115	-
14	CLA	c2	502	13	1/1/14/20	10/33/109/115	-
14	CLA	aB	1203	2	1/1/15/20	18/39/115/115	-
14	CLA	f	513	13	1/1/11/20	5/15/91/115	-
14	CLA	aB	1229	2	1/1/15/20	14/39/115/115	-
17	BCR	a5	524	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	e	516	13	1/1/11/20	6/15/91/115	-
14	CLA	p	507	-	1/1/11/20	4/15/91/115	-
14	CLA	aB	1023	-	1/1/15/20	11/39/115/115	-
14	CLA	b3	505	13	1/1/15/20	14/39/115/115	-
14	CLA	bA	1111	1	1/1/13/20	9/27/103/115	-
14	CLA	b3	508	13	1/1/13/20	5/27/103/115	-
14	CLA	c1	511	13	1/1/12/20	2/21/97/115	-
14	CLA	W	503	13	1/1/14/20	5/37/113/115	-
14	CLA	j	517	-	1/1/11/20	4/15/91/115	-
14	CLA	cA	1127	1	1/1/15/20	4/39/115/115	-
14	CLA	b1	502	13	1/1/14/20	5/33/109/115	-
14	CLA	Y	519	13	1/1/11/20	9/15/91/115	-
17	BCR	b5	521	-	-	3/29/63/63	0/2/2/2
17	BCR	c6	524	-	-	0/29/63/63	0/2/2/2
14	CLA	d	518	13	1/1/13/20	7/27/103/115	-
15	PQN	bB	2002	-	-	11/23/43/43	0/2/2/2
17	BCR	k	524	-	-	0/29/63/63	0/2/2/2
14	CLA	c4	502	13	1/1/14/20	14/33/109/115	-
14	CLA	l	518	13	1/1/12/20	7/21/97/115	-
14	CLA	b4	507	-	1/1/14/20	6/33/109/115	-
17	BCR	aF	4016	-	-	2/29/63/63	0/2/2/2
17	BCR	cA	4007	-	-	2/29/63/63	0/2/2/2
14	CLA	l	506	13	1/1/11/20	4/15/91/115	-
17	BCR	b2	524	-	-	0/29/63/63	0/2/2/2
14	CLA	aA	1125	1	1/1/15/20	16/39/115/115	-
17	BCR	c	522	-	-	4/29/63/63	0/2/2/2
17	BCR	cM	4021	-	-	7/29/63/63	0/2/2/2
14	CLA	h	513	13	1/1/12/20	5/21/97/115	-
17	BCR	e	521	-	-	4/29/63/63	0/2/2/2
17	BCR	T	523	-	-	2/29/63/63	0/2/2/2
14	CLA	b5	510	13	1/1/15/20	9/39/115/115	-
14	CLA	cB	1202	2	1/1/15/20	10/39/115/115	-
14	CLA	cB	1215	2	1/1/14/20	6/35/111/115	-
14	CLA	cB	1021	2	1/1/15/20	13/39/115/115	-
17	BCR	V	524	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	d	517	-	1/1/11/20	10/15/91/115	-
14	CLA	a3	501	13	1/1/15/20	12/39/115/115	-
14	CLA	a2	506	13	1/1/11/20	4/15/91/115	-
17	BCR	S	521	-	-	3/29/63/63	0/2/2/2
14	CLA	h	506	13	1/1/11/20	4/15/91/115	-
14	CLA	a3	516	13	1/1/11/20	5/15/91/115	-
14	CLA	Z	508	13	1/1/11/20	4/15/91/115	-
14	CLA	b	511	13	1/1/11/20	3/15/91/115	-
14	CLA	f	511	13	1/1/11/20	7/15/91/115	-
14	CLA	b3	506	13	1/1/11/20	4/15/91/115	-
17	BCR	p	522	-	-	2/29/63/63	0/2/2/2
14	CLA	T	518	13	1/1/12/20	8/21/97/115	-
21	LMG	a2	5104	-	-	5/35/55/70	0/1/1/1
14	CLA	a	508	13	1/1/11/20	4/15/91/115	-
14	CLA	i	502	13	1/1/11/20	1/15/91/115	-
14	CLA	X	518	13	1/1/13/20	7/27/103/115	-
14	CLA	aB	1225	2	1/1/15/20	13/39/115/115	-
14	CLA	b1	504	-	1/1/13/20	9/27/103/115	-
14	CLA	c2	512	13	1/1/12/20	12/24/100/115	-
17	BCR	b	524	-	-	0/29/63/63	0/2/2/2
14	CLA	bB	1023	-	1/1/15/20	6/39/115/115	-
14	CLA	cB	1231	2	1/1/13/20	13/27/103/115	-
14	CLA	aA	1106	1	1/1/15/20	19/39/115/115	-
14	CLA	b3	503	13	1/1/14/20	3/37/113/115	-
17	BCR	cJ	4012	-	-	4/29/63/63	0/2/2/2
14	CLA	bA	1129	1	1/1/13/20	14/27/103/115	-
14	CLA	a2	501	13	1/1/15/20	16/39/115/115	-
18	LHG	cA	5001	-	-	18/52/52/53	-
14	CLA	l	513	13	1/1/11/20	2/15/91/115	-
14	CLA	a2	509	13	1/1/15/20	9/39/115/115	-
14	CLA	U	517	-	1/1/11/20	11/15/91/115	-
14	CLA	Z	519	13	1/1/11/20	4/15/91/115	-
14	CLA	cB	1213	2	1/1/14/20	7/33/109/115	-
14	CLA	c5	518	13	1/1/13/20	9/27/103/115	-
16	SF4	cC	3003	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	a4	524	-	-	0/29/63/63	0/2/2/2
14	CLA	d	505	13	1/1/15/20	16/39/115/115	-
14	CLA	U	518	13	1/1/11/20	5/15/91/115	-
14	CLA	q	518	13	1/1/11/20	5/15/91/115	-
14	CLA	aB	1212	2	1/1/11/20	2/15/91/115	-
17	BCR	U	521	-	-	5/29/63/63	0/2/2/2
14	CLA	b2	513	13	1/1/11/20	3/18/94/115	-
14	CLA	b1	518	13	1/1/13/20	9/27/103/115	-
14	CLA	aA	1011	1	1/1/15/20	8/39/115/115	-
17	BCR	k	522	-	-	2/29/63/63	0/2/2/2
17	BCR	q	522	-	-	3/29/63/63	0/2/2/2
17	BCR	a1	523	-	-	2/29/63/63	0/2/2/2
20	SQD	a3	822	-	-	15/33/53/69	0/1/1/1
17	BCR	f	522	-	-	4/29/63/63	0/2/2/2
14	CLA	n	519	13	1/1/11/20	4/15/91/115	-
14	CLA	aB	1201	2	1/1/13/20	7/30/106/115	-
17	BCR	i	522	-	-	5/29/63/63	0/2/2/2
14	CLA	bB	1223	2	1/1/15/20	8/39/115/115	-
14	CLA	cB	1216	-	1/1/13/20	6/27/103/115	-
18	LHG	aA	5003	14	-	6/45/45/53	-
14	CLA	a1	511	13	1/1/13/20	8/27/103/115	-
14	CLA	b4	508	13	1/1/13/20	4/27/103/115	-
14	CLA	aB	1208	2	1/1/13/20	4/27/103/115	-
14	CLA	aA	1140	1	1/1/15/20	17/39/115/115	-
14	CLA	aB	1234	2	1/1/14/20	10/33/109/115	-
14	CLA	g	502	13	1/1/11/20	6/15/91/115	-
14	CLA	a5	509	13	1/1/15/20	7/39/115/115	-
17	BCR	bI	4020	-	-	4/29/63/63	0/2/2/2
14	CLA	V	505	13	1/1/14/20	12/36/112/115	-
14	CLA	j	518	13	1/1/12/20	8/21/97/115	-
14	CLA	c4	504	-	1/1/11/20	7/15/91/115	-
14	CLA	cA	1131	1	1/1/15/20	8/39/115/115	-
14	CLA	bA	1117	1	1/1/15/20	13/39/115/115	-
14	CLA	bB	1232	-	1/1/11/20	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	a1	524	-	-	0/29/63/63	0/2/2/2
14	CLA	Z	504	-	1/1/13/20	11/27/103/115	-
17	BCR	a	521	-	-	6/29/63/63	0/2/2/2
14	CLA	n	504	-	1/1/11/20	6/15/91/115	-
17	BCR	f	524	-	-	0/29/63/63	0/2/2/2
14	CLA	X	513	13	1/1/11/20	3/17/93/115	-
17	BCR	i	524	-	-	0/29/63/63	0/2/2/2
17	BCR	f	523	-	-	4/29/63/63	0/2/2/2
14	CLA	c4	510	13	1/1/15/20	11/39/115/115	-
14	CLA	bA	1105	1	1/1/12/20	5/25/101/115	-
14	CLA	b5	511	13	1/1/12/20	3/21/97/115	-
14	CLA	k	506	13	1/1/11/20	5/15/91/115	-
14	CLA	c1	519	13	1/1/11/20	6/15/91/115	-
14	CLA	a1	516	13	1/1/13/20	9/31/107/115	-
14	CLA	b6	507	-	1/1/14/20	9/33/109/115	-
18	LHG	aA	5002	-	-	19/45/45/53	-
14	CLA	b1	510	13	1/1/15/20	9/39/115/115	-
14	CLA	n	517	-	1/1/11/20	7/15/91/115	-
14	CLA	bK	1401	-	1/1/13/20	9/27/103/115	-
14	CLA	aA	1112	1	1/1/11/20	5/19/95/115	-
14	CLA	aA	1126	1	1/1/15/20	14/39/115/115	-
18	LHG	aA	5005	-	-	21/49/49/53	-
17	BCR	cB	4005	-	-	2/29/63/63	0/2/2/2
14	CLA	q	512	13	1/1/11/20	4/15/91/115	-
14	CLA	j	504	-	1/1/11/20	4/15/91/115	-
14	CLA	o	513	13	1/1/11/20	3/15/91/115	-
20	SQD	a6	822	-	-	14/26/46/69	0/1/1/1
14	CLA	d	509	13	1/1/14/20	7/36/112/115	-
17	BCR	g	522	-	-	5/29/63/63	0/2/2/2

The worst 5 of 7652 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	2001	PQN	C12-C13	9.50	1.54	1.33
15	bA	2001	PQN	C12-C13	9.47	1.54	1.33
15	cB	2002	PQN	C12-C13	9.45	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	2001	PQN	C12-C13	9.42	1.54	1.33
15	bB	2002	PQN	C12-C13	9.42	1.54	1.33

The worst 5 of 9477 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	cB	2002	PQN	C11-C12-C13	-8.37	112.41	126.83
15	bB	2002	PQN	C11-C12-C13	-8.32	112.50	126.83
15	aB	2002	PQN	C11-C12-C13	-8.32	112.50	126.83
15	aA	2001	PQN	C11-C12-C13	-8.23	112.66	126.83
15	bA	2001	PQN	C11-C12-C13	-8.17	112.76	126.83

5 of 1016 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	aA	1022	CLA	ND
14	aA	1101	CLA	ND
14	aA	1102	CLA	ND
14	aA	1103	CLA	ND
14	aA	1104	CLA	ND

5 of 9482 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	aA	1101	CLA	C3A-C2A-CAA-CBA
14	aA	1101	CLA	CHA-CBD-CGD-O1D
14	aA	1101	CLA	CHA-CBD-CGD-O2D
14	aA	1102	CLA	C1A-C2A-CAA-CBA
14	aA	1102	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

1185 monomers are involved in 3625 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	bL	1503	CLA	3	0
14	cA	1110	CLA	5	0
14	bB	1222	CLA	7	0
14	c3	513	CLA	2	0
17	aM	4021	BCR	5	0
14	c	519	CLA	2	0
17	Y	521	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	aB	1223	CLA	8	0
17	l	524	BCR	2	0
14	c	505	CLA	4	0
14	f	508	CLA	4	0
14	i	508	CLA	3	0
14	c4	506	CLA	4	0
14	p	502	CLA	3	0
14	cA	1139	CLA	3	0
14	cB	1235	CLA	3	0
17	bA	4003	BCR	2	0
17	c2	522	BCR	3	0
17	a4	522	BCR	3	0
14	U	505	CLA	4	0
21	b1	5104	LMG	1	0
14	bA	1102	CLA	5	0
14	aA	1119	CLA	9	0
14	a4	505	CLA	1	0
14	bA	1128	CLA	8	0
14	bB	1219	CLA	1	0
14	cB	1210	CLA	3	0
17	g	523	BCR	4	0
14	e	508	CLA	3	0
21	cB	5002	LMG	1	0
14	aA	1133	CLA	3	0
14	q	516	CLA	1	0
14	b1	503	CLA	7	0
17	o	522	BCR	4	0
14	W	502	CLA	5	0
14	a6	510	CLA	5	0
19	bJ	5105	LMU	1	0
17	c3	521	BCR	4	0
14	cA	1022	CLA	6	0
18	cA	5005	LHG	3	0
17	b3	524	BCR	3	0
20	g	822	SQD	1	0
14	g	512	CLA	4	0
14	S	518	CLA	2	0
14	c	513	CLA	3	0
14	b	510	CLA	3	0
14	c1	509	CLA	6	0
14	b5	502	CLA	6	0
17	c2	523	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	bF	4014	BCR	8	0
14	q	513	CLA	2	0
14	c2	509	CLA	3	0
14	aA	1121	CLA	1	0
14	bA	1108	CLA	2	0
14	a2	518	CLA	2	0
14	d	513	CLA	2	0
17	c3	523	BCR	2	0
14	cA	1105	CLA	4	0
17	cB	4004	BCR	2	0
14	bB	1239	CLA	1	0
14	c2	505	CLA	3	0
19	bA	1848	LMU	1	0
14	b4	504	CLA	2	0
14	cB	1221	CLA	9	0
18	bX	4021	LHG	1	0
17	bI	4018	BCR	4	0
14	q	503	CLA	2	0
14	m	502	CLA	3	0
14	k	511	CLA	1	0
17	o	521	BCR	4	0
14	Z	511	CLA	2	0
14	W	510	CLA	3	0
14	a2	505	CLA	6	0
14	U	507	CLA	1	0
14	aA	1116	CLA	8	0
14	a6	501	CLA	3	0
14	cB	1239	CLA	2	0
14	c5	507	CLA	3	0
14	c1	501	CLA	3	0
14	g	518	CLA	1	0
14	l	508	CLA	3	0
14	cA	1113	CLA	4	0
17	g	521	BCR	7	0
14	b1	516	CLA	1	0
14	c3	507	CLA	3	0
17	c	523	BCR	1	0
14	f	512	CLA	1	0
17	b2	522	BCR	3	0
14	b4	518	CLA	3	0
14	W	512	CLA	5	0
14	g	506	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	e	510	CLA	2	0
14	b	509	CLA	3	0
17	b5	523	BCR	5	0
14	b2	508	CLA	3	0
14	b6	518	CLA	1	0
17	b6	521	BCR	1	0
14	c4	517	CLA	2	0
14	aB	1012	CLA	9	0
14	a4	502	CLA	5	0
14	c	518	CLA	2	0
14	b4	519	CLA	2	0
14	U	502	CLA	3	0
14	c3	510	CLA	6	0
14	q	509	CLA	2	0
14	bB	1213	CLA	3	0
14	c2	506	CLA	4	0
14	aA	1134	CLA	2	0
17	b6	524	BCR	4	0
14	l	510	CLA	1	0
20	c	822	SQD	1	0
14	c	501	CLA	1	0
14	cB	1205	CLA	6	0
17	T	522	BCR	2	0
14	Z	503	CLA	3	0
17	bF	4016	BCR	5	0
14	c	516	CLA	1	0
14	n	518	CLA	1	0
14	aA	1111	CLA	2	0
14	cB	1224	CLA	4	0
14	a2	519	CLA	1	0
14	T	508	CLA	4	0
14	a1	509	CLA	3	0
17	h	523	BCR	5	0
14	k	501	CLA	2	0
14	bA	1110	CLA	3	0
14	cB	1203	CLA	5	0
17	d	524	BCR	6	0
14	l	512	CLA	5	0
14	o	503	CLA	3	0
14	S	513	CLA	3	0
17	p	521	BCR	2	0
14	bB	1226	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	S	502	CLA	2	0
14	b3	510	CLA	4	0
14	m	512	CLA	5	0
14	d	516	CLA	1	0
14	c3	506	CLA	5	0
14	a	502	CLA	2	0
14	c1	502	CLA	4	0
14	c	510	CLA	3	0
14	bB	1227	CLA	5	0
14	W	506	CLA	5	0
18	bA	5001	LHG	4	0
14	aB	1239	CLA	2	0
15	cA	2001	PQN	7	0
14	c	512	CLA	2	0
14	aL	1503	CLA	4	0
14	i	517	CLA	1	0
17	aB	4006	BCR	4	0
14	c4	501	CLA	4	0
14	b6	505	CLA	4	0
17	Z	524	BCR	3	0
14	b5	506	CLA	4	0
14	cB	1209	CLA	3	0
17	j	523	BCR	2	0
17	k	521	BCR	3	0
14	i	511	CLA	2	0
14	p	510	CLA	1	0
14	n	513	CLA	3	0
14	c	506	CLA	5	0
17	m	523	BCR	4	0
17	Y	522	BCR	2	0
14	cA	1138	CLA	3	0
14	a4	512	CLA	5	0
17	cB	4010	BCR	9	0
14	b2	512	CLA	4	0
17	U	523	BCR	4	0
17	X	521	BCR	3	0
17	cA	4002	BCR	6	0
17	j	524	BCR	5	0
14	cB	1207	CLA	7	0
14	aA	1129	CLA	2	0
17	bB	4009	BCR	5	0
14	X	516	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	bA	1122	CLA	5	0
14	l	511	CLA	2	0
14	c2	516	CLA	1	0
17	c5	521	BCR	3	0
17	b4	523	BCR	2	0
14	a	519	CLA	2	0
14	p	506	CLA	2	0
14	aA	1115	CLA	6	0
14	h	509	CLA	3	0
14	j	516	CLA	1	0
17	a3	524	BCR	6	0
17	c1	523	BCR	4	0
18	cA	5003	LHG	1	0
14	p	505	CLA	2	0
14	bA	1116	CLA	3	0
14	b	517	CLA	1	0
14	bA	1130	CLA	2	0
14	f	517	CLA	1	0
14	c5	516	CLA	1	0
21	bJ	5104	LMG	1	0
14	a4	510	CLA	8	0
14	aA	1135	CLA	1	0
14	U	516	CLA	3	0
14	aB	1211	CLA	4	0
18	cA	5004	LHG	4	0
14	a5	519	CLA	3	0
17	b	521	BCR	3	0
17	aJ	4012	BCR	6	0
14	U	504	CLA	1	0
14	o	510	CLA	3	0
14	b3	511	CLA	4	0
17	bL	4022	BCR	7	0
14	h	508	CLA	2	0
14	c6	507	CLA	1	0
14	f	502	CLA	2	0
14	b5	519	CLA	1	0
17	cK	4001	BCR	5	0
17	c2	524	BCR	6	0
14	c6	519	CLA	2	0
14	a1	502	CLA	7	0
14	e	501	CLA	3	0
14	cA	1801	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	c1	516	CLA	3	0
14	c4	503	CLA	7	0
14	T	503	CLA	2	0
17	aA	4011	BCR	4	0
14	i	506	CLA	2	0
17	aB	4009	BCR	6	0
18	bA	5004	LHG	3	0
14	cB	1228	CLA	4	0
17	e	524	BCR	5	0
14	e	507	CLA	1	0
14	cA	1118	CLA	5	0
14	o	506	CLA	5	0
14	c3	518	CLA	1	0
14	o	502	CLA	3	0
14	g	501	CLA	3	0
14	c5	505	CLA	3	0
17	Z	521	BCR	6	0
14	a	509	CLA	3	0
14	bB	1212	CLA	1	0
14	c3	502	CLA	7	0
17	b1	521	BCR	2	0
14	cA	1133	CLA	1	0
14	c1	510	CLA	5	0
14	i	510	CLA	1	0
14	p	518	CLA	2	0
14	c3	503	CLA	7	0
14	n	505	CLA	1	0
14	e	517	CLA	2	0
14	h	501	CLA	3	0
20	a1	822	SQD	1	0
14	bB	1206	CLA	2	0
17	W	524	BCR	8	0
14	g	516	CLA	1	0
14	a5	512	CLA	5	0
14	c1	506	CLA	7	0
14	aA	1128	CLA	8	0
14	a3	508	CLA	6	0
14	q	510	CLA	3	0
14	c1	507	CLA	3	0
14	cA	1116	CLA	4	0
14	l	517	CLA	4	0
14	a5	506	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	o	512	CLA	3	0
17	bB	4004	BCR	4	0
17	c1	522	BCR	3	0
14	c6	512	CLA	4	0
14	a4	511	CLA	2	0
17	cB	4006	BCR	5	0
14	h	510	CLA	2	0
14	k	518	CLA	1	0
14	bB	1012	CLA	7	0
14	T	516	CLA	1	0
17	b4	521	BCR	3	0
14	b5	508	CLA	6	0
14	p	509	CLA	5	0
14	l	502	CLA	4	0
21	aB	5002	LMG	1	0
14	p	512	CLA	5	0
17	g	524	BCR	6	0
14	a3	509	CLA	4	0
14	a2	503	CLA	7	0
14	bA	1125	CLA	4	0
14	b2	511	CLA	2	0
14	c2	508	CLA	4	0
20	aB	1852	SQD	4	0
14	X	507	CLA	3	0
14	aA	1109	CLA	8	0
14	Z	507	CLA	4	0
14	c	508	CLA	4	0
14	a	513	CLA	4	0
14	b2	502	CLA	4	0
17	b3	521	BCR	3	0
14	U	501	CLA	2	0
14	cA	1119	CLA	7	0
14	aB	1206	CLA	3	0
17	U	522	BCR	2	0
14	V	511	CLA	4	0
17	V	521	BCR	2	0
14	bA	1120	CLA	4	0
14	b6	513	CLA	4	0
19	aA	1848	LMU	1	0
17	a	524	BCR	5	0
14	cL	1503	CLA	2	0
14	T	511	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	c4	518	CLA	1	0
14	i	509	CLA	3	0
17	aA	4003	BCR	2	0
14	c6	518	CLA	1	0
14	bB	1205	CLA	6	0
19	cB	1843	LMU	1	0
14	c2	510	CLA	7	0
14	bB	1211	CLA	5	0
14	aA	1139	CLA	6	0
14	k	502	CLA	1	0
14	X	502	CLA	5	0
17	T	524	BCR	6	0
14	W	505	CLA	6	0
14	Z	502	CLA	3	0
14	a4	509	CLA	7	0
14	n	502	CLA	2	0
14	aB	1222	CLA	6	0
14	bA	1101	CLA	3	0
14	Y	501	CLA	8	0
14	b4	505	CLA	2	0
14	bB	1238	CLA	7	0
14	cB	1211	CLA	6	0
17	b1	523	BCR	3	0
14	q	511	CLA	1	0
14	a4	518	CLA	6	0
17	aA	4002	BCR	8	0
14	a3	518	CLA	3	0
17	aL	4022	BCR	5	0
14	p	513	CLA	2	0
17	aI	4019	BCR	6	0
17	aK	4001	BCR	6	0
14	a6	508	CLA	4	0
14	bA	1011	CLA	5	0
17	cF	4015	BCR	7	0
17	c	521	BCR	6	0
14	j	502	CLA	1	0
14	Y	507	CLA	2	0
14	aA	1124	CLA	3	0
14	a1	507	CLA	5	0
14	cA	1104	CLA	6	0
21	bB	5002	LMG	3	0
14	bA	1124	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	cB	1222	CLA	7	0
14	cB	1217	CLA	3	0
14	cB	1238	CLA	3	0
14	U	508	CLA	3	0
15	bA	2001	PQN	4	0
20	c4	822	SQD	1	0
14	a6	518	CLA	2	0
17	cA	4003	BCR	3	0
14	cB	1232	CLA	3	0
21	aJ	5104	LMG	1	0
14	a3	504	CLA	2	0
20	p	822	SQD	1	0
14	c1	518	CLA	2	0
14	k	513	CLA	4	0
17	c3	522	BCR	2	0
18	aA	5001	LHG	2	0
14	i	513	CLA	3	0
14	X	504	CLA	2	0
14	T	506	CLA	4	0
14	Y	502	CLA	8	0
14	a1	513	CLA	3	0
17	k	523	BCR	4	0
14	aB	1238	CLA	5	0
14	o	501	CLA	3	0
14	c1	503	CLA	6	0
14	bA	1119	CLA	6	0
17	bA	4011	BCR	4	0
14	aB	1216	CLA	3	0
14	bB	1214	CLA	6	0
14	bB	1204	CLA	2	0
14	T	512	CLA	4	0
17	bF	4015	BCR	7	0
14	a4	513	CLA	3	0
14	d	511	CLA	3	0
17	b4	522	BCR	5	0
14	m	519	CLA	3	0
14	c2	511	CLA	2	0
17	c4	522	BCR	4	0
14	c5	513	CLA	2	0
14	Z	518	CLA	1	0
14	bK	1103	CLA	1	0
14	b5	504	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b1	506	CLA	6	0
14	X	508	CLA	2	0
14	b4	513	CLA	2	0
14	aA	1131	CLA	5	0
14	b1	505	CLA	4	0
14	a	510	CLA	1	0
14	V	519	CLA	3	0
17	bJ	4013	BCR	10	0
17	e	522	BCR	5	0
17	a2	521	BCR	4	0
14	b	518	CLA	1	0
14	cA	1013	CLA	7	0
14	aB	1209	CLA	3	0
14	b3	518	CLA	2	0
14	b4	502	CLA	7	0
14	S	503	CLA	5	0
14	cA	1136	CLA	2	0
14	Z	510	CLA	5	0
14	aB	1232	CLA	2	0
14	aB	1227	CLA	6	0
14	f	503	CLA	1	0
17	X	523	BCR	3	0
14	n	510	CLA	1	0
14	bB	1236	CLA	4	0
14	e	513	CLA	2	0
17	Z	523	BCR	2	0
14	T	509	CLA	6	0
14	bA	1118	CLA	6	0
17	cA	4008	BCR	9	0
14	aB	1207	CLA	7	0
14	W	511	CLA	2	0
14	aB	1204	CLA	3	0
14	aA	1130	CLA	3	0
17	o	523	BCR	4	0
14	aB	1213	CLA	5	0
14	b4	501	CLA	5	0
14	V	517	CLA	1	0
14	m	509	CLA	5	0
14	bB	1210	CLA	3	0
14	bA	1103	CLA	7	0
17	h	522	BCR	2	0
14	Y	512	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	cJ	4013	BCR	8	0
14	i	512	CLA	2	0
14	b2	509	CLA	5	0
18	cA	5002	LHG	4	0
14	Z	506	CLA	7	0
17	c5	523	BCR	4	0
14	q	506	CLA	5	0
14	f	505	CLA	1	0
14	V	501	CLA	2	0
14	b	504	CLA	1	0
14	cB	1012	CLA	9	0
14	aB	1226	CLA	3	0
14	g	517	CLA	1	0
14	a5	502	CLA	3	0
14	T	517	CLA	2	0
14	b	513	CLA	3	0
14	bB	1201	CLA	5	0
14	m	507	CLA	2	0
14	b4	510	CLA	6	0
14	bA	1132	CLA	3	0
14	b5	517	CLA	1	0
14	cA	1107	CLA	6	0
14	b6	510	CLA	4	0
14	a3	507	CLA	6	0
14	aB	1236	CLA	3	0
14	Y	510	CLA	5	0
20	S	822	SQD	1	0
14	cB	1226	CLA	4	0
17	b6	523	BCR	2	0
14	d	508	CLA	4	0
14	c2	517	CLA	2	0
14	h	512	CLA	6	0
14	a5	510	CLA	10	0
14	aB	1221	CLA	10	0
17	j	522	BCR	4	0
14	a2	510	CLA	7	0
17	aI	4018	BCR	3	0
14	a	511	CLA	3	0
17	c2	521	BCR	5	0
14	cA	1237	CLA	7	0
17	a5	522	BCR	2	0
17	bA	4007	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	cB	1234	CLA	3	0
14	c	511	CLA	1	0
14	U	509	CLA	4	0
14	p	516	CLA	1	0
14	a	504	CLA	2	0
14	cB	1225	CLA	5	0
14	b1	509	CLA	3	0
14	m	501	CLA	1	0
17	b5	522	BCR	3	0
14	n	511	CLA	4	0
14	b4	503	CLA	6	0
14	S	510	CLA	3	0
14	b1	512	CLA	4	0
17	cF	4016	BCR	6	0
14	bB	1207	CLA	6	0
14	bA	1109	CLA	7	0
17	cA	4011	BCR	4	0
14	Y	503	CLA	9	0
14	c4	511	CLA	3	0
14	V	518	CLA	1	0
14	n	509	CLA	7	0
14	b3	513	CLA	5	0
14	cA	1108	CLA	2	0
14	j	509	CLA	5	0
14	cA	1103	CLA	4	0
17	X	522	BCR	2	0
17	cL	4022	BCR	6	0
14	cB	1201	CLA	3	0
14	a4	508	CLA	5	0
14	c6	513	CLA	4	0
17	aJ	4013	BCR	11	0
14	S	506	CLA	4	0
14	cB	1223	CLA	8	0
17	c5	522	BCR	1	0
14	b6	512	CLA	4	0
14	a2	507	CLA	2	0
20	m	822	SQD	1	0
14	bB	1224	CLA	5	0
17	cI	4020	BCR	1	0
14	b4	506	CLA	5	0
14	Y	513	CLA	2	0
14	e	512	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	b1	522	BCR	3	0
14	bA	1104	CLA	7	0
14	b6	506	CLA	3	0
14	b6	502	CLA	7	0
14	k	512	CLA	4	0
14	bB	1231	CLA	3	0
17	a4	523	BCR	5	0
17	bA	4008	BCR	10	0
14	b2	517	CLA	1	0
14	h	504	CLA	2	0
14	a2	517	CLA	1	0
14	bJ	1302	CLA	1	0
17	c	524	BCR	6	0
17	cF	4014	BCR	4	0
14	V	504	CLA	1	0
14	d	512	CLA	4	0
14	bA	1115	CLA	4	0
17	c4	521	BCR	6	0
14	b1	513	CLA	4	0
14	q	502	CLA	4	0
14	bB	1217	CLA	2	0
14	a2	511	CLA	3	0
14	m	517	CLA	1	0
17	q	524	BCR	5	0
14	X	501	CLA	4	0
17	b1	524	BCR	5	0
14	k	505	CLA	1	0
17	m	521	BCR	4	0
14	aA	1122	CLA	8	0
14	bB	1216	CLA	2	0
20	a4	822	SQD	2	0
14	Z	505	CLA	5	0
14	j	513	CLA	2	0
15	cB	2002	PQN	8	0
14	S	509	CLA	3	0
14	aA	1013	CLA	9	0
14	S	511	CLA	3	0
14	c5	501	CLA	4	0
14	bA	1022	CLA	6	0
18	bA	5005	LHG	3	0
15	aA	2001	PQN	7	0
14	cA	1135	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	c3	501	CLA	5	0
14	S	512	CLA	2	0
17	Z	522	BCR	3	0
14	c5	508	CLA	4	0
14	aA	1123	CLA	5	0
17	bB	4005	BCR	4	0
21	a1	5104	LMG	1	0
14	cJ	1303	CLA	2	0
20	W	822	SQD	1	0
14	bB	1220	CLA	3	0
14	b6	503	CLA	5	0
17	c1	521	BCR	5	0
14	a5	503	CLA	8	0
14	q	501	CLA	3	0
17	b2	523	BCR	4	0
17	b3	522	BCR	5	0
14	Z	513	CLA	3	0
14	b5	507	CLA	1	0
17	a2	523	BCR	3	0
14	a5	511	CLA	3	0
14	cF	1301	CLA	2	0
14	b	508	CLA	4	0
14	c2	518	CLA	2	0
14	c	509	CLA	8	0
17	c6	521	BCR	4	0
17	b4	524	BCR	4	0
14	cA	1106	CLA	5	0
14	aB	1021	CLA	6	0
14	S	505	CLA	2	0
14	c6	505	CLA	4	0
17	q	523	BCR	3	0
14	c6	503	CLA	6	0
19	aA	1849	LMU	2	0
14	c5	512	CLA	8	0
17	a2	524	BCR	8	0
14	Y	506	CLA	4	0
14	d	519	CLA	1	0
14	k	503	CLA	1	0
14	a1	506	CLA	6	0
14	U	512	CLA	5	0
14	Y	505	CLA	2	0
14	a5	513	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b2	519	CLA	1	0
14	b4	517	CLA	1	0
14	aB	1214	CLA	8	0
14	cA	1011	CLA	6	0
17	b3	523	BCR	6	0
14	cA	1137	CLA	7	0
14	a4	506	CLA	3	0
14	cA	1124	CLA	3	0
14	bA	1137	CLA	7	0
14	b2	507	CLA	4	0
14	p	511	CLA	4	0
18	aX	4021	LHG	3	0
14	a3	511	CLA	5	0
14	q	508	CLA	2	0
14	a5	517	CLA	1	0
14	j	503	CLA	1	0
14	c1	512	CLA	3	0
14	aB	1220	CLA	3	0
14	bA	1127	CLA	7	0
17	h	524	BCR	5	0
14	bA	1113	CLA	4	0
14	f	506	CLA	4	0
14	aK	1401	CLA	3	0
14	bB	1228	CLA	2	0
14	c6	502	CLA	6	0
14	o	508	CLA	4	0
14	aA	1120	CLA	5	0
14	cL	1502	CLA	1	0
20	b3	822	SQD	1	0
14	k	509	CLA	3	0
14	i	505	CLA	1	0
17	a6	521	BCR	4	0
14	cA	1117	CLA	10	0
14	c1	505	CLA	6	0
14	b	516	CLA	2	0
14	bB	1218	CLA	4	0
14	d	501	CLA	1	0
17	S	522	BCR	3	0
14	e	502	CLA	4	0
14	aA	1118	CLA	6	0
14	bB	1021	CLA	5	0
17	q	521	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	bB	1235	CLA	3	0
14	b3	504	CLA	2	0
14	cK	1103	CLA	1	0
14	a1	512	CLA	5	0
14	X	503	CLA	8	0
17	aF	4015	BCR	5	0
14	U	506	CLA	4	0
14	S	501	CLA	2	0
14	k	508	CLA	1	0
17	bJ	4012	BCR	5	0
17	cI	4018	BCR	5	0
14	aA	1103	CLA	3	0
14	g	513	CLA	1	0
14	p	501	CLA	1	0
14	a	501	CLA	2	0
17	bI	4019	BCR	2	0
14	b6	508	CLA	2	0
14	a3	519	CLA	1	0
14	W	508	CLA	4	0
14	cA	1101	CLA	5	0
19	cA	1848	LMU	1	0
14	c5	503	CLA	5	0
14	b6	501	CLA	1	0
17	p	524	BCR	6	0
14	aB	1228	CLA	3	0
17	V	522	BCR	7	0
14	aK	1103	CLA	1	0
14	a	507	CLA	1	0
14	a1	505	CLA	2	0
14	a5	501	CLA	4	0
17	d	523	BCR	4	0
14	V	508	CLA	6	0
14	cJ	1302	CLA	1	0
17	c6	523	BCR	5	0
14	a5	505	CLA	3	0
14	cB	1212	CLA	2	0
17	l	523	BCR	4	0
14	bB	1225	CLA	7	0
17	W	523	BCR	3	0
14	b	503	CLA	1	0
14	V	513	CLA	5	0
14	b5	501	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	c4	509	CLA	7	0
20	c6	822	SQD	1	0
14	b4	512	CLA	4	0
14	Y	509	CLA	4	0
14	p	517	CLA	2	0
14	a4	517	CLA	1	0
14	a3	502	CLA	7	0
14	aA	1127	CLA	5	0
14	Y	518	CLA	2	0
17	V	523	BCR	3	0
14	a6	507	CLA	3	0
14	cB	1227	CLA	6	0
17	bK	4001	BCR	5	0
17	e	523	BCR	6	0
14	a4	503	CLA	7	0
14	a2	512	CLA	3	0
14	b2	518	CLA	2	0
14	aB	1218	CLA	2	0
14	aB	1210	CLA	3	0
14	bB	1230	CLA	4	0
14	bL	1501	CLA	7	0
14	b2	501	CLA	6	0
17	aA	4007	BCR	5	0
14	cB	1204	CLA	2	0
14	V	512	CLA	4	0
14	cA	1134	CLA	2	0
14	o	509	CLA	2	0
19	cA	1849	LMU	1	0
14	o	511	CLA	4	0
14	T	513	CLA	2	0
17	S	523	BCR	2	0
14	c3	509	CLA	5	0
14	a6	511	CLA	3	0
14	c5	502	CLA	5	0
14	cK	1401	CLA	2	0
14	cA	1129	CLA	5	0
17	n	522	BCR	6	0
14	f	509	CLA	1	0
14	b4	509	CLA	6	0
14	a6	502	CLA	2	0
14	cA	1140	CLA	12	0
14	n	508	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b6	509	CLA	5	0
17	a1	522	BCR	1	0
14	W	509	CLA	3	0
14	j	508	CLA	4	0
14	bB	1229	CLA	6	0
14	b	501	CLA	2	0
14	g	505	CLA	5	0
20	c1	822	SQD	1	0
14	T	501	CLA	1	0
17	cI	4019	BCR	5	0
14	b3	501	CLA	7	0
14	aB	1205	CLA	6	0
17	a3	523	BCR	3	0
14	c4	513	CLA	3	0
17	a5	521	BCR	4	0
14	c6	506	CLA	5	0
14	bX	1401	CLA	2	0
14	e	509	CLA	3	0
14	cB	1220	CLA	3	0
14	aB	1224	CLA	6	0
17	n	523	BCR	3	0
14	b	507	CLA	1	0
14	a4	501	CLA	6	0
14	cA	1112	CLA	3	0
14	b3	507	CLA	5	0
17	X	524	BCR	4	0
14	m	513	CLA	2	0
14	aA	1104	CLA	4	0
14	m	506	CLA	4	0
14	n	512	CLA	5	0
17	U	524	BCR	5	0
14	cA	1111	CLA	2	0
14	V	506	CLA	5	0
14	cB	1023	CLA	8	0
14	b2	505	CLA	2	0
14	bB	1202	CLA	2	0
14	l	509	CLA	4	0
14	b2	503	CLA	8	0
14	h	517	CLA	1	0
20	Z	822	SQD	1	0
19	cJ	5105	LMU	1	0
17	a	523	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	c5	524	BCR	6	0
14	bA	1131	CLA	2	0
14	a	503	CLA	5	0
17	d	521	BCR	4	0
14	b3	517	CLA	2	0
20	n	822	SQD	1	0
17	bB	4017	BCR	8	0
14	a1	518	CLA	1	0
17	b2	521	BCR	5	0
14	Z	516	CLA	1	0
14	q	504	CLA	1	0
14	bA	1237	CLA	4	0
14	f	504	CLA	2	0
14	j	512	CLA	3	0
14	cA	1109	CLA	7	0
14	a6	504	CLA	2	0
14	bB	1209	CLA	4	0
14	aX	1401	CLA	1	0
16	aA	3001	SF4	1	0
14	V	503	CLA	3	0
17	a2	522	BCR	2	0
17	cB	4009	BCR	5	0
14	b	502	CLA	5	0
14	a2	508	CLA	2	0
14	c1	513	CLA	4	0
14	b3	502	CLA	4	0
14	bA	1138	CLA	6	0
14	T	505	CLA	1	0
14	aA	1022	CLA	7	0
19	aJ	5105	LMU	1	0
14	cA	1130	CLA	2	0
17	Y	523	BCR	5	0
14	b5	518	CLA	2	0
14	q	517	CLA	2	0
14	h	511	CLA	4	0
17	aB	4010	BCR	10	0
14	aA	1117	CLA	9	0
14	a1	510	CLA	2	0
14	X	509	CLA	2	0
14	m	511	CLA	1	0
14	a3	506	CLA	6	0
14	aB	1202	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	aB	1215	CLA	3	0
14	q	505	CLA	2	0
17	Y	524	BCR	5	0
20	Y	822	SQD	1	0
14	a4	507	CLA	3	0
17	a4	521	BCR	2	0
14	b1	511	CLA	4	0
14	c5	509	CLA	5	0
17	aI	4020	BCR	1	0
14	X	506	CLA	4	0
14	c4	505	CLA	2	0
14	b6	516	CLA	2	0
17	a3	521	BCR	4	0
14	cA	1122	CLA	6	0
14	W	504	CLA	1	0
14	X	505	CLA	4	0
14	aA	1136	CLA	1	0
14	n	506	CLA	2	0
17	bM	4021	BCR	6	0
14	f	510	CLA	1	0
20	cB	1852	SQD	3	0
17	cB	4017	BCR	6	0
14	bB	1208	CLA	7	0
14	b5	509	CLA	2	0
14	aA	1137	CLA	7	0
14	k	517	CLA	1	0
14	bB	1234	CLA	4	0
14	j	511	CLA	3	0
14	c6	509	CLA	3	0
14	m	505	CLA	2	0
14	b5	512	CLA	6	0
14	V	516	CLA	1	0
14	c6	511	CLA	2	0
14	aF	1301	CLA	3	0
14	a1	503	CLA	7	0
14	W	518	CLA	3	0
14	g	508	CLA	3	0
14	b6	519	CLA	4	0
17	S	524	BCR	3	0
14	aA	1132	CLA	4	0
14	X	510	CLA	3	0
17	W	521	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	cA	1120	CLA	5	0
17	a1	521	BCR	2	0
14	aA	1113	CLA	3	0
14	bA	1106	CLA	6	0
14	aB	1235	CLA	4	0
14	aB	1231	CLA	3	0
17	a	522	BCR	2	0
14	aL	1502	CLA	1	0
14	bA	1139	CLA	4	0
17	f	521	BCR	4	0
14	c5	504	CLA	3	0
17	c4	524	BCR	9	0
17	i	521	BCR	4	0
17	aB	4017	BCR	6	0
20	b4	822	SQD	2	0
17	b6	522	BCR	3	0
14	cA	1128	CLA	7	0
14	e	511	CLA	2	0
14	p	508	CLA	5	0
14	bA	1140	CLA	11	0
14	X	512	CLA	2	0
14	d	502	CLA	3	0
14	c3	504	CLA	2	0
14	aB	1217	CLA	2	0
14	f	516	CLA	1	0
14	U	510	CLA	2	0
14	cB	1208	CLA	4	0
14	cB	1236	CLA	6	0
14	i	507	CLA	1	0
17	bA	4002	BCR	5	0
17	m	524	BCR	6	0
14	k	519	CLA	1	0
14	q	519	CLA	1	0
14	g	510	CLA	2	0
14	bA	1135	CLA	3	0
14	b1	501	CLA	5	0
14	j	519	CLA	2	0
14	S	517	CLA	1	0
14	a6	509	CLA	5	0
14	h	502	CLA	2	0
14	bB	1221	CLA	12	0
17	d	522	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	l	521	BCR	4	0
17	c6	522	BCR	3	0
14	V	502	CLA	3	0
14	c3	512	CLA	5	0
14	Z	512	CLA	6	0
14	c1	517	CLA	2	0
14	c4	508	CLA	7	0
14	cB	1214	CLA	5	0
14	Y	508	CLA	1	0
14	aA	1108	CLA	2	0
14	e	505	CLA	3	0
14	cA	1102	CLA	7	0
14	a3	505	CLA	2	0
17	h	521	BCR	7	0
14	c6	501	CLA	7	0
14	b5	513	CLA	2	0
17	aB	4005	BCR	4	0
14	a6	506	CLA	5	0
14	a	518	CLA	4	0
21	b2	5104	LMG	1	0
17	c1	524	BCR	7	0
14	c2	513	CLA	2	0
17	c4	523	BCR	2	0
14	cA	1132	CLA	3	0
17	aF	4014	BCR	4	0
14	T	502	CLA	4	0
14	aA	1138	CLA	4	0
14	a5	507	CLA	4	0
14	b1	517	CLA	1	0
14	a3	513	CLA	2	0
17	T	521	BCR	2	0
17	p	523	BCR	2	0
17	a6	522	BCR	1	0
14	S	508	CLA	7	0
14	X	511	CLA	2	0
14	Z	509	CLA	6	0
14	c2	503	CLA	5	0
14	c1	508	CLA	6	0
14	a4	519	CLA	3	0
14	e	506	CLA	4	0
17	b	522	BCR	4	0
18	bA	5003	LHG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	aA	1110	CLA	3	0
14	a6	513	CLA	3	0
14	c5	511	CLA	2	0
14	b3	509	CLA	4	0
14	a	512	CLA	2	0
14	bA	1133	CLA	2	0
14	aA	1101	CLA	5	0
17	n	524	BCR	6	0
14	aB	1230	CLA	5	0
14	U	511	CLA	1	0
14	bA	1013	CLA	9	0
14	c3	511	CLA	5	0
14	c2	507	CLA	2	0
14	l	505	CLA	2	0
17	a6	523	BCR	3	0
14	a	506	CLA	4	0
18	bA	5002	LHG	2	0
14	c	517	CLA	1	0
14	bA	1112	CLA	3	0
14	g	511	CLA	3	0
17	a3	522	BCR	4	0
14	cA	1123	CLA	2	0
14	cA	1125	CLA	3	0
14	b2	516	CLA	2	0
14	bA	1123	CLA	5	0
14	h	519	CLA	2	0
17	i	523	BCR	3	0
14	cA	1115	CLA	3	0
14	d	510	CLA	4	0
17	c3	524	BCR	6	0
20	c5	822	SQD	1	0
17	b	523	BCR	3	0
14	c6	510	CLA	8	0
14	cX	1401	CLA	2	0
14	b5	503	CLA	9	0
14	bA	1126	CLA	11	0
14	a	505	CLA	5	0
14	U	513	CLA	3	0
14	c4	512	CLA	4	0
17	a6	524	BCR	7	0
14	b2	510	CLA	5	0
17	aB	4004	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	c	502	CLA	2	0
14	a1	508	CLA	3	0
14	Z	501	CLA	4	0
14	i	501	CLA	1	0
15	aB	2002	PQN	8	0
17	W	522	BCR	1	0
18	cX	4021	LHG	2	0
14	b6	511	CLA	2	0
14	aA	1105	CLA	4	0
14	Y	511	CLA	1	0
14	i	518	CLA	1	0
14	b5	505	CLA	4	0
14	V	510	CLA	3	0
14	n	501	CLA	2	0
14	j	501	CLA	1	0
14	a1	501	CLA	3	0
17	bB	4010	BCR	11	0
14	cB	1218	CLA	3	0
14	c1	504	CLA	1	0
14	a3	512	CLA	3	0
14	aJ	1302	CLA	1	0
14	l	519	CLA	2	0
14	a2	513	CLA	3	0
14	b2	506	CLA	5	0
14	d	503	CLA	2	0
14	a2	502	CLA	6	0
14	bA	1136	CLA	2	0
17	aA	4008	BCR	8	0
17	a5	523	BCR	5	0
19	aB	1843	LMU	2	0
19	bB	1843	LMU	2	0
17	o	524	BCR	6	0
14	cB	1230	CLA	4	0
17	l	522	BCR	7	0
14	a6	512	CLA	3	0
17	b5	524	BCR	6	0
14	cB	1229	CLA	5	0
14	h	518	CLA	1	0
14	j	510	CLA	1	0
14	cL	1501	CLA	6	0
14	W	501	CLA	6	0
14	b	512	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a6	505	CLA	5	0
18	aA	5004	LHG	4	0
14	aA	1237	CLA	6	0
14	a6	503	CLA	3	0
14	cA	1126	CLA	9	0
14	a5	508	CLA	7	0
14	c2	501	CLA	4	0
14	bB	1203	CLA	6	0
14	a3	510	CLA	4	0
14	b	506	CLA	2	0
14	c4	519	CLA	1	0
17	bB	4006	BCR	6	0
14	b	505	CLA	3	0
14	X	519	CLA	1	0
14	o	518	CLA	2	0
14	b1	508	CLA	6	0
14	V	509	CLA	2	0
14	c3	508	CLA	4	0
14	b4	511	CLA	2	0
14	c5	510	CLA	3	0
14	cB	1206	CLA	6	0
14	c6	508	CLA	5	0
14	j	506	CLA	4	0
14	c5	519	CLA	3	0
20	bB	1852	SQD	3	0
14	c5	506	CLA	5	0
14	bA	1107	CLA	6	0
14	aA	1107	CLA	9	0
14	b1	507	CLA	4	0
17	n	521	BCR	6	0
14	o	505	CLA	1	0
14	bL	1502	CLA	2	0
17	j	521	BCR	3	0
14	f	501	CLA	2	0
14	c3	505	CLA	4	0
14	aA	1102	CLA	6	0
17	m	522	BCR	3	0
14	c4	507	CLA	3	0
14	W	513	CLA	4	0
14	a3	503	CLA	7	0
14	m	508	CLA	4	0
14	b3	512	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	aL	1501	CLA	6	0
14	bF	1301	CLA	3	0
14	bA	1134	CLA	3	0
14	c2	502	CLA	5	0
14	aB	1203	CLA	5	0
14	f	513	CLA	1	0
14	aB	1229	CLA	4	0
17	a5	524	BCR	9	0
14	p	507	CLA	1	0
14	aB	1023	CLA	9	0
14	b3	505	CLA	4	0
14	bA	1111	CLA	3	0
14	b3	508	CLA	4	0
14	c1	511	CLA	3	0
14	W	503	CLA	7	0
14	cA	1127	CLA	6	0
14	b1	502	CLA	6	0
17	b5	521	BCR	3	0
17	c6	524	BCR	3	0
14	d	518	CLA	3	0
15	bB	2002	PQN	8	0
17	k	524	BCR	7	0
14	c4	502	CLA	5	0
14	l	518	CLA	1	0
14	b4	507	CLA	3	0
17	aF	4016	BCR	5	0
17	cA	4007	BCR	4	0
14	l	506	CLA	1	0
17	b2	524	BCR	4	0
14	aA	1125	CLA	5	0
17	c	522	BCR	4	0
17	cM	4021	BCR	4	0
14	h	513	CLA	3	0
17	e	521	BCR	4	0
17	T	523	BCR	4	0
14	b5	510	CLA	4	0
14	cB	1202	CLA	2	0
14	cB	1215	CLA	3	0
14	cB	1021	CLA	5	0
17	V	524	BCR	8	0
14	d	517	CLA	1	0
14	a3	501	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a2	506	CLA	4	0
17	S	521	BCR	3	0
14	h	506	CLA	3	0
14	Z	508	CLA	5	0
14	b	511	CLA	3	0
14	f	511	CLA	1	0
14	b3	506	CLA	4	0
17	p	522	BCR	4	0
14	T	518	CLA	1	0
21	a2	5104	LMG	1	0
14	a	508	CLA	4	0
14	i	502	CLA	1	0
14	X	518	CLA	1	0
14	aB	1225	CLA	9	0
14	c2	512	CLA	5	0
17	b	524	BCR	4	0
14	bB	1023	CLA	7	0
14	cB	1231	CLA	4	0
14	aA	1106	CLA	8	0
14	b3	503	CLA	7	0
17	cJ	4012	BCR	3	0
14	bA	1129	CLA	2	0
14	a2	501	CLA	6	0
18	cA	5001	LHG	4	0
14	l	513	CLA	2	0
14	a2	509	CLA	3	0
14	cB	1213	CLA	3	0
14	c5	518	CLA	1	0
17	a4	524	BCR	8	0
14	d	505	CLA	4	0
14	U	518	CLA	1	0
14	q	518	CLA	1	0
14	aB	1212	CLA	1	0
17	U	521	BCR	2	0
14	b2	513	CLA	2	0
14	b1	518	CLA	2	0
14	aA	1011	CLA	6	0
17	k	522	BCR	3	0
17	q	522	BCR	3	0
17	a1	523	BCR	3	0
20	a3	822	SQD	1	0
17	f	522	BCR	5	0

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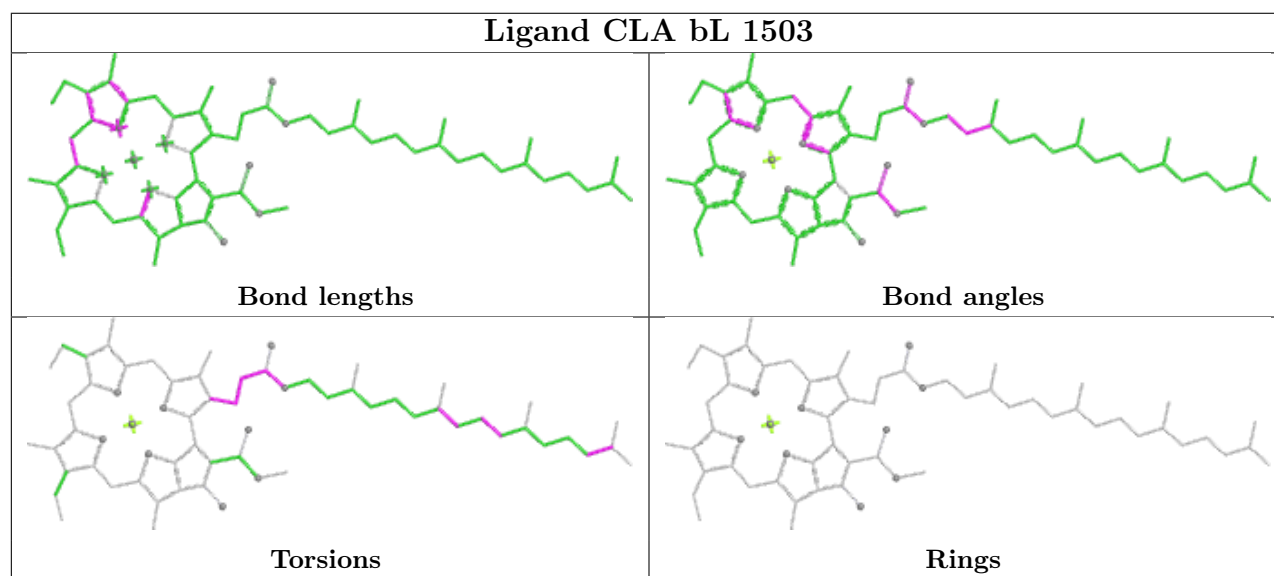
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	n	519	CLA	2	0
14	aB	1201	CLA	4	0
17	i	522	BCR	4	0
14	bB	1223	CLA	7	0
14	cB	1216	CLA	2	0
18	aA	5003	LHG	2	0
14	a1	511	CLA	3	0
14	b4	508	CLA	3	0
14	aB	1208	CLA	6	0
14	aA	1140	CLA	11	0
14	aB	1234	CLA	2	0
14	g	502	CLA	3	0
14	a5	509	CLA	2	0
17	bI	4020	BCR	3	0
14	V	505	CLA	6	0
14	j	518	CLA	1	0
14	cA	1131	CLA	2	0
14	bA	1117	CLA	7	0
14	bB	1232	CLA	3	0
17	a1	524	BCR	6	0
17	a	521	BCR	4	0
14	n	504	CLA	1	0
17	f	524	BCR	3	0
14	X	513	CLA	3	0
17	i	524	BCR	4	0
17	f	523	BCR	1	0
14	c4	510	CLA	4	0
14	bA	1105	CLA	3	0
14	b5	511	CLA	3	0
14	k	506	CLA	3	0
14	c1	519	CLA	1	0
14	a1	516	CLA	3	0
14	b6	507	CLA	2	0
18	aA	5002	LHG	3	0
14	b1	510	CLA	3	0
14	bK	1401	CLA	2	0
14	aA	1112	CLA	3	0
14	aA	1126	CLA	11	0
18	aA	5005	LHG	2	0
17	cB	4005	BCR	3	0
14	q	512	CLA	1	0
14	o	513	CLA	3	0

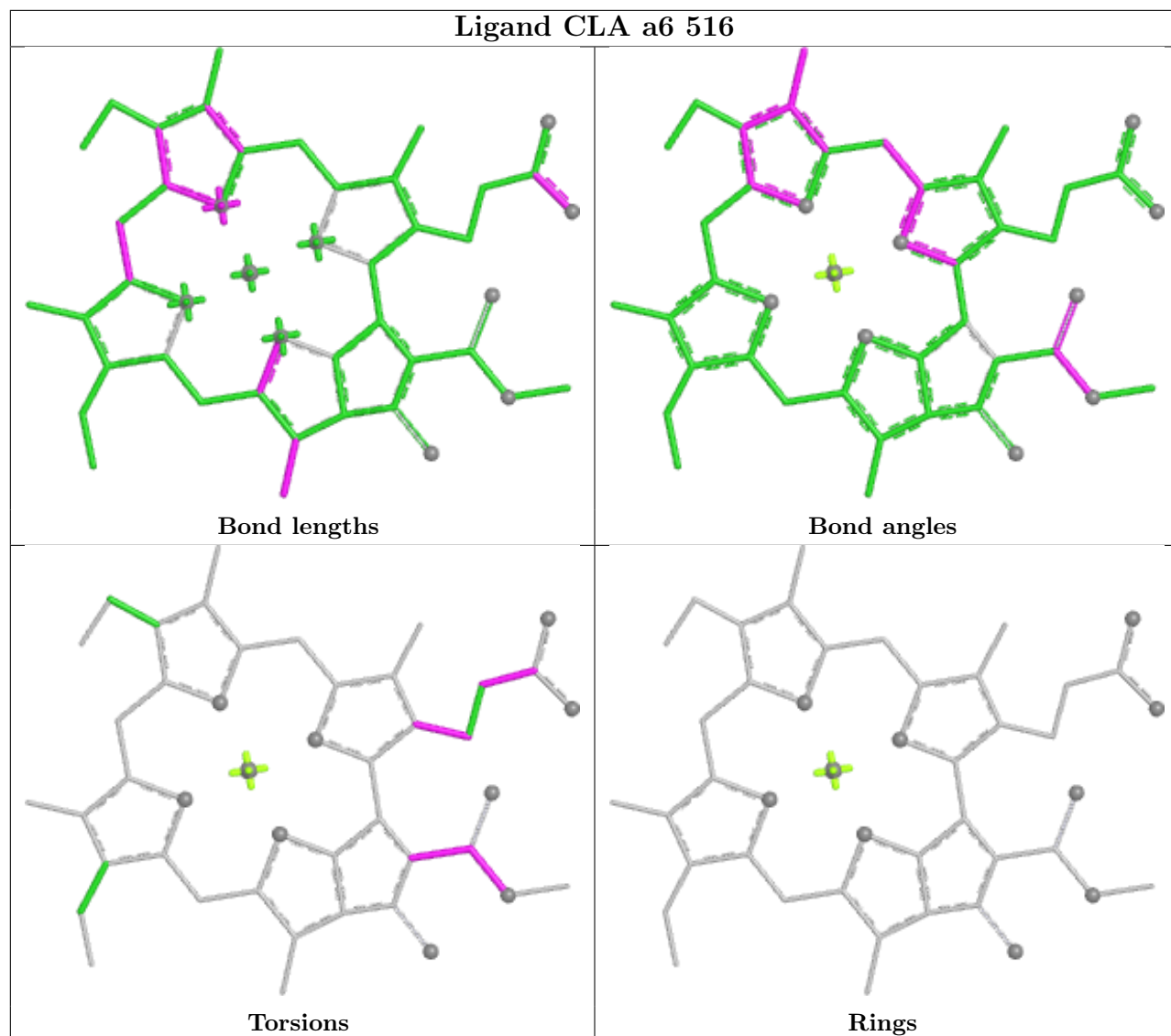
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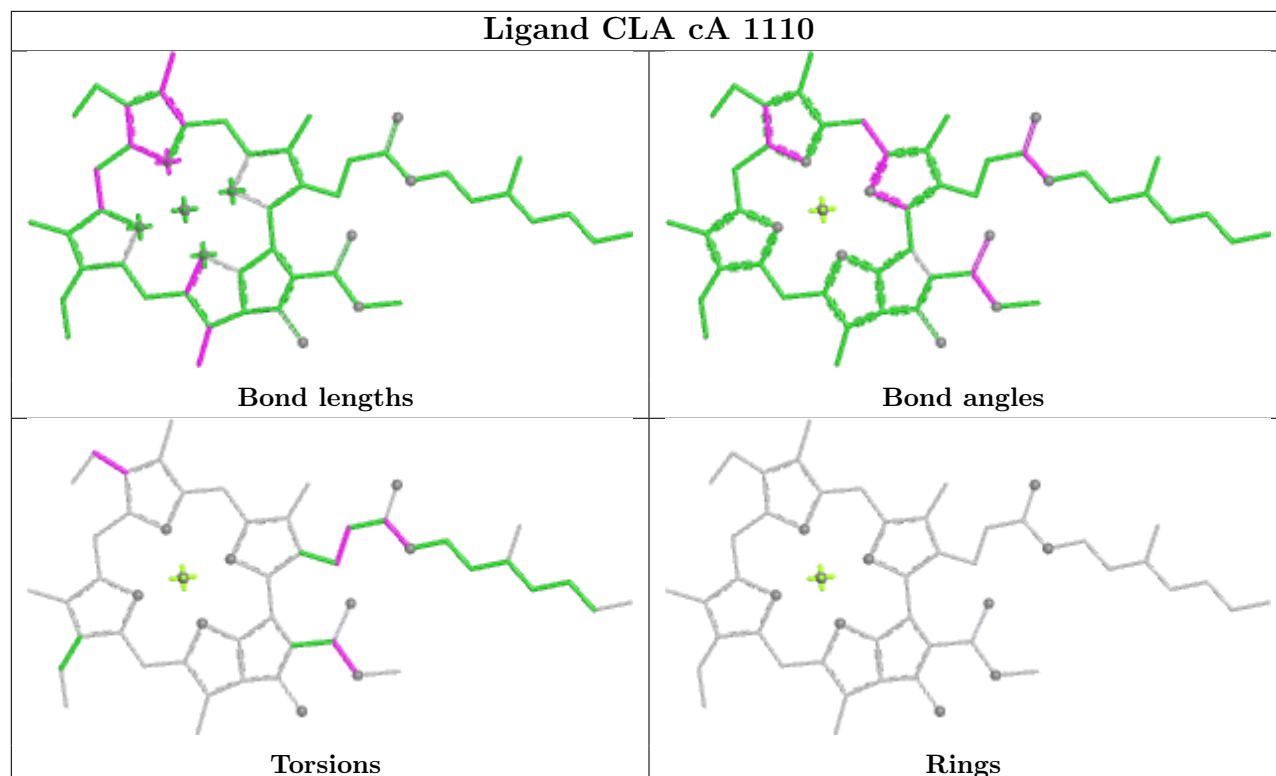
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	d	509	CLA	4	0
17	g	522	BCR	5	0

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

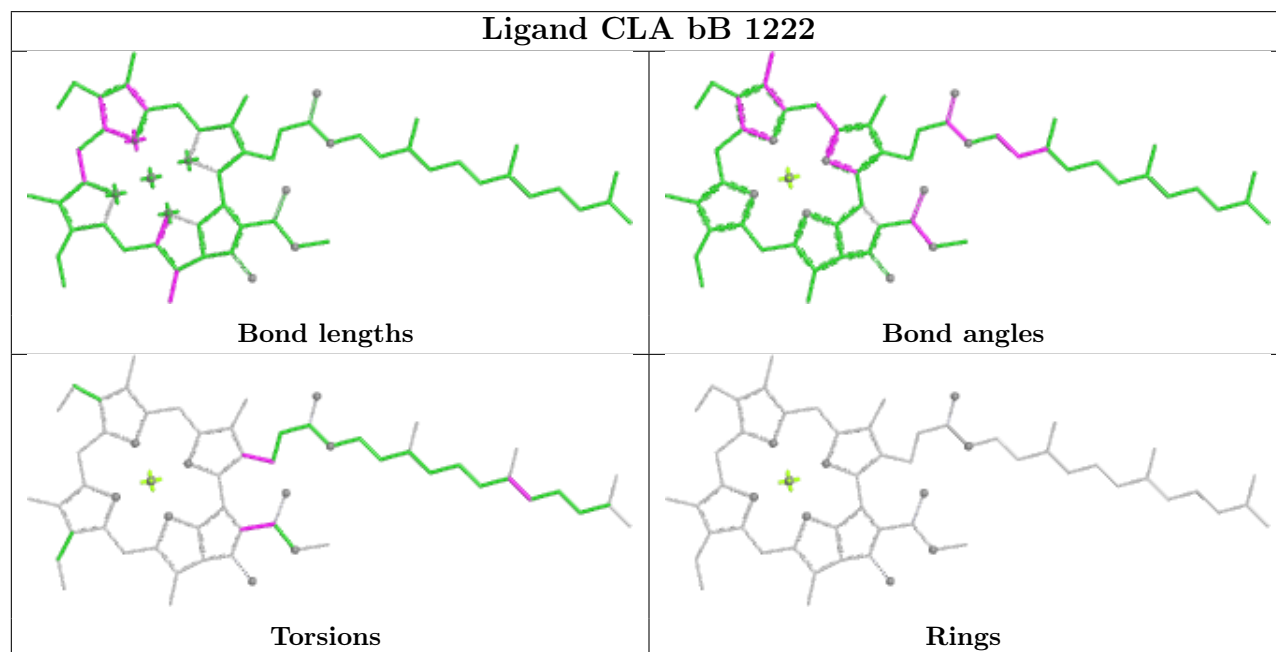


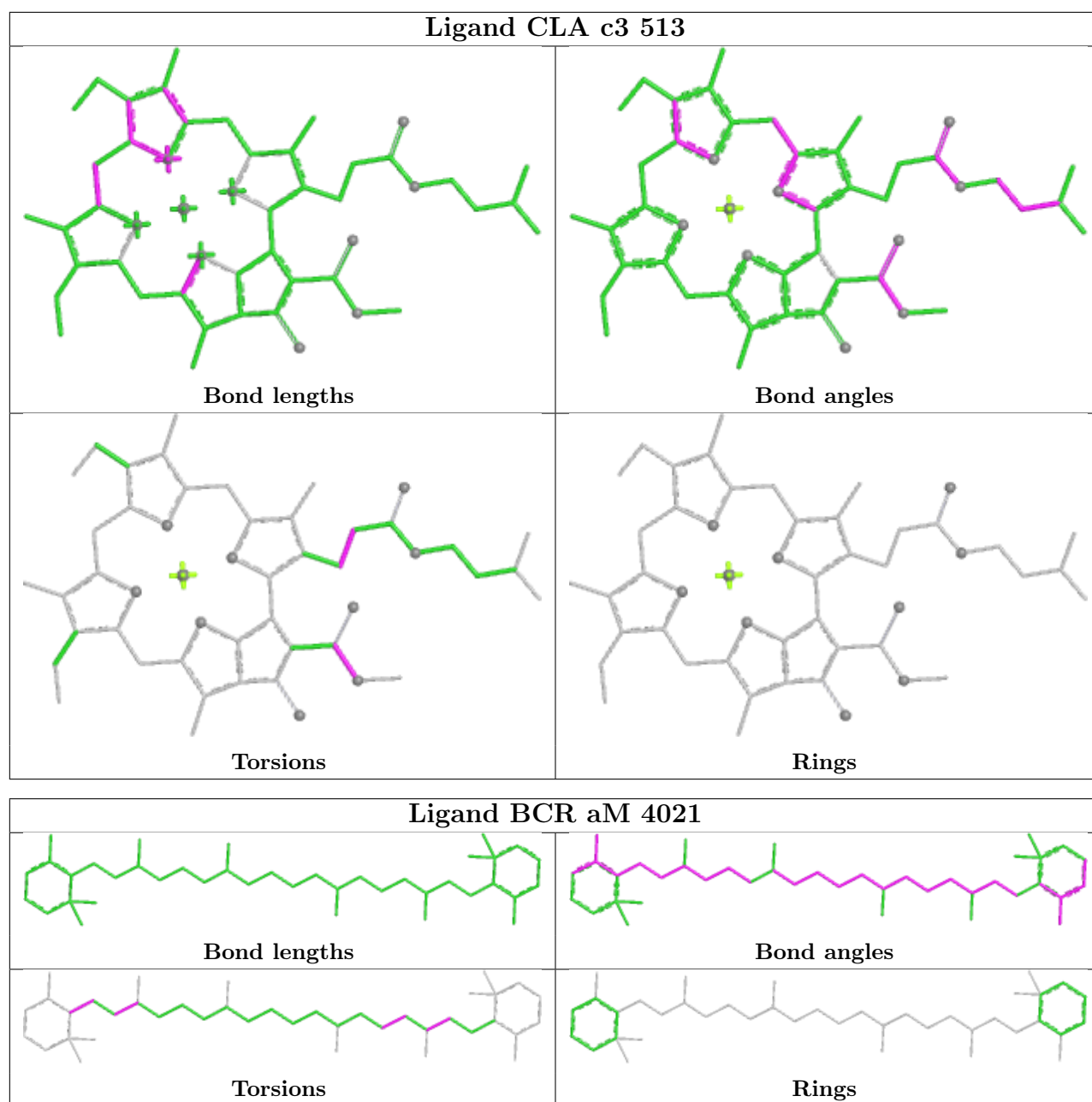


Ligand CLA cA 1110

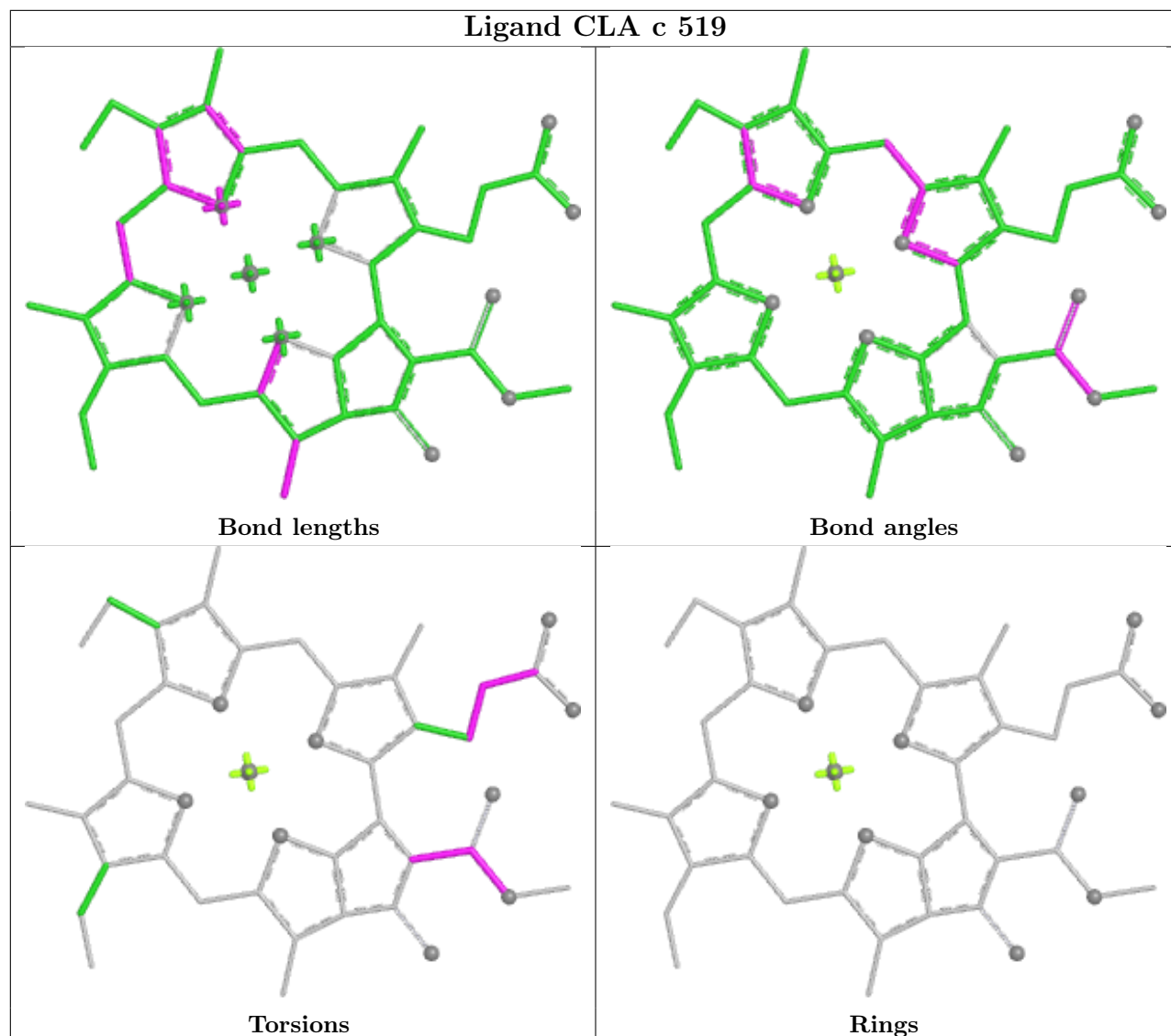


Ligand CLA bB 1222

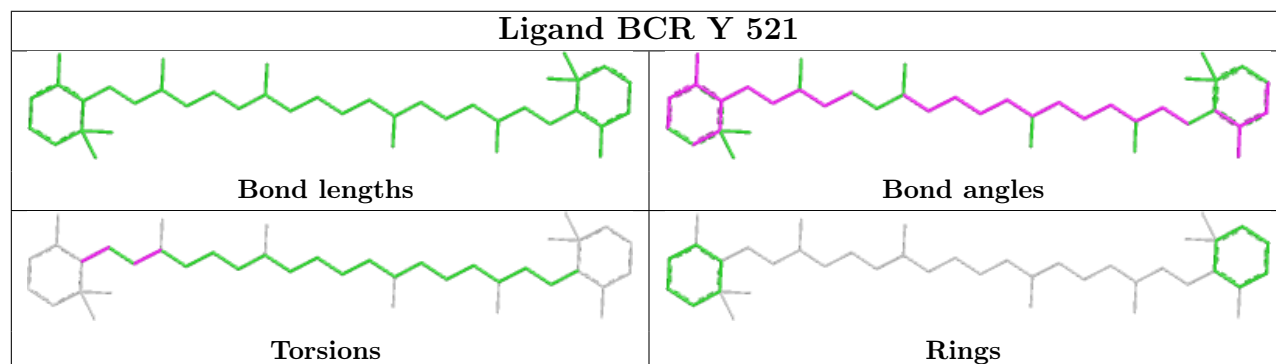


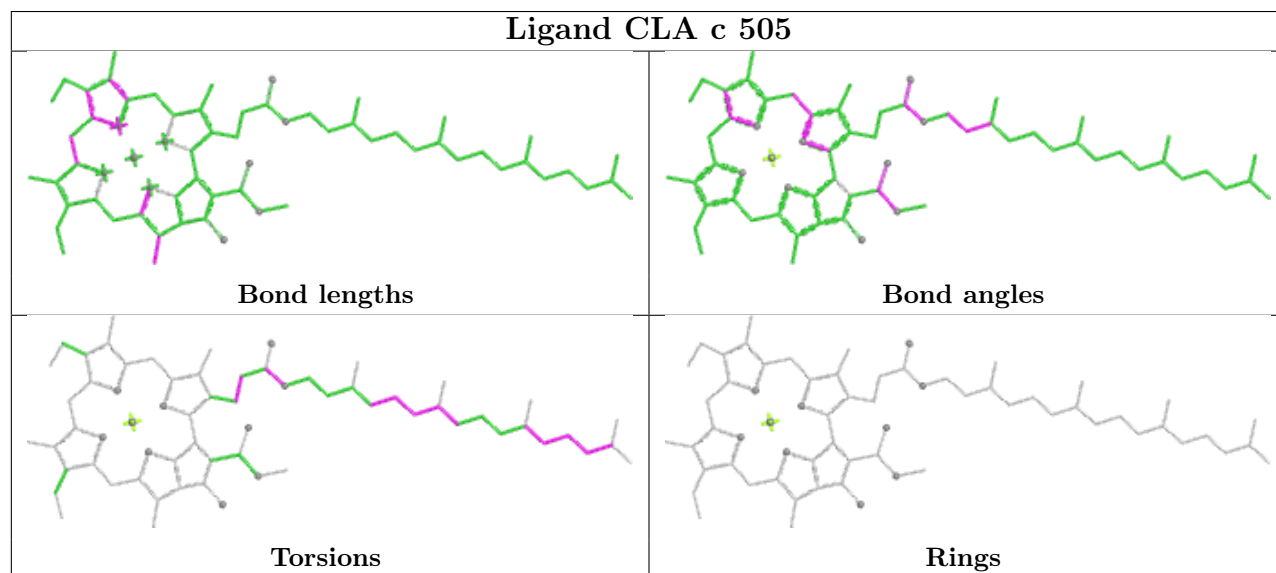
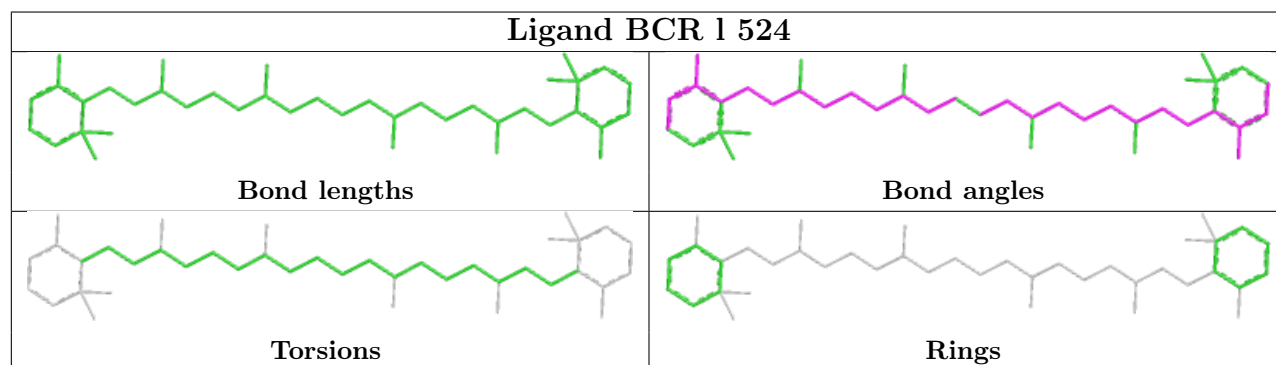
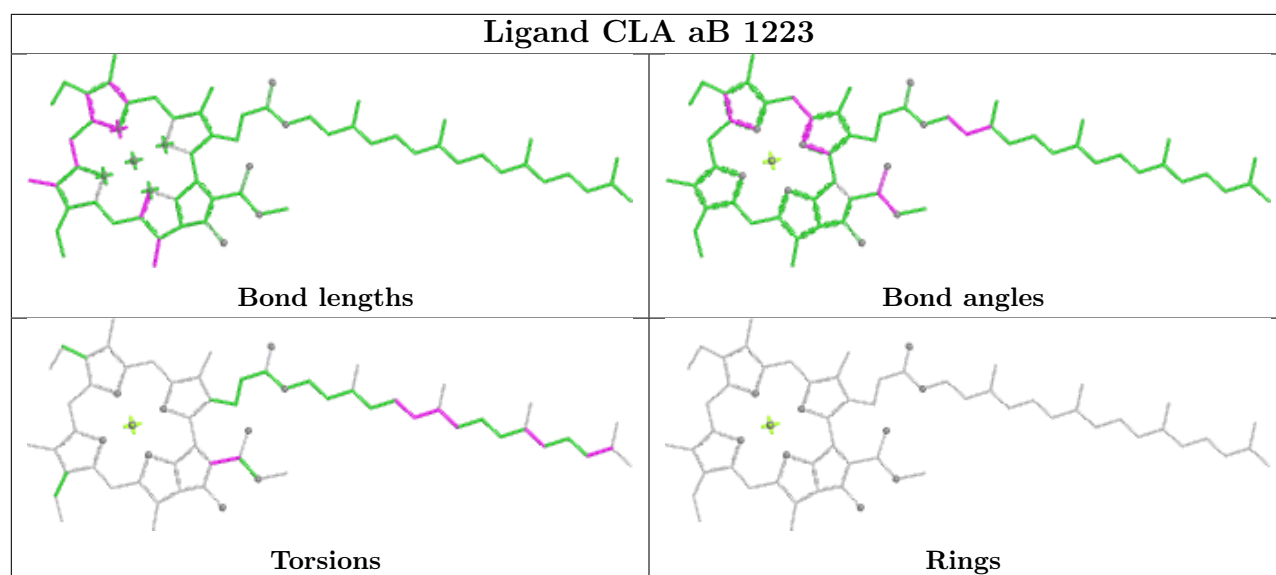


Ligand CLA c 519

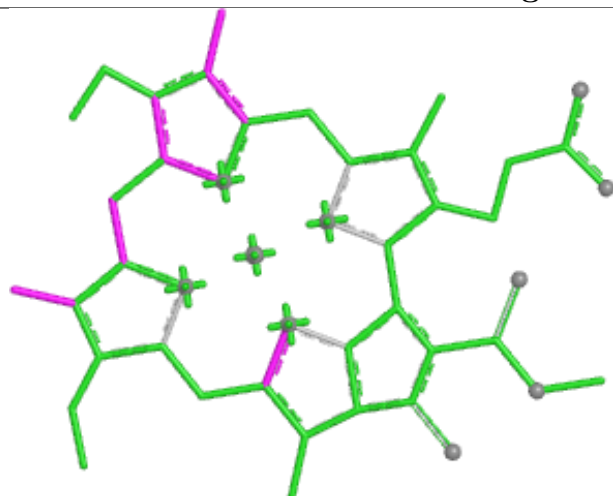


Ligand BCR Y 521

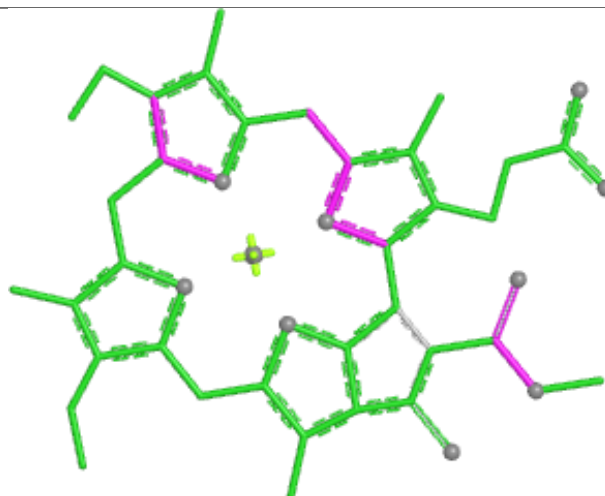




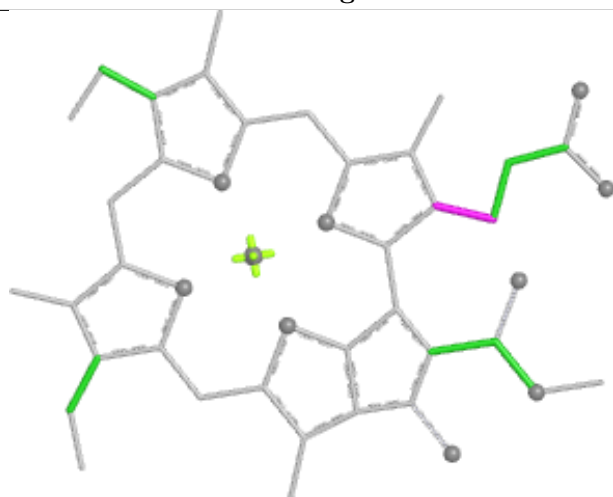
Ligand CLA f 508



Bond lengths



Bond angles

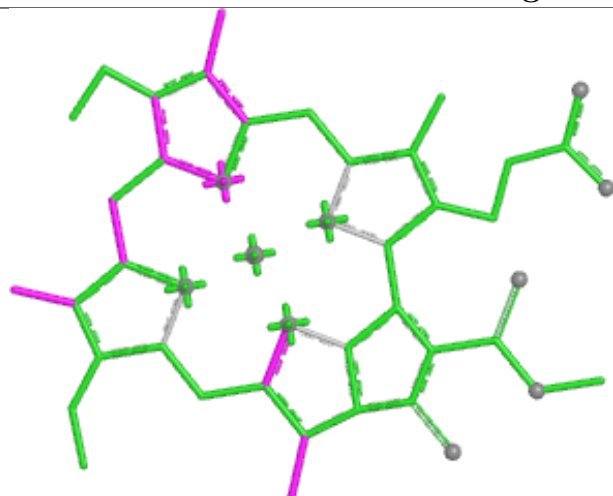


Torsions

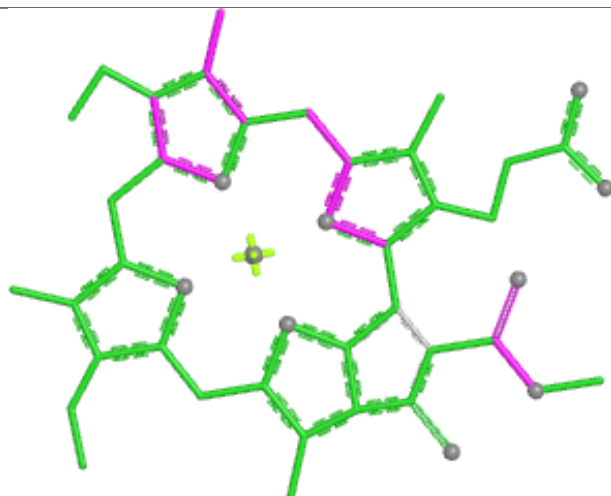


Rings

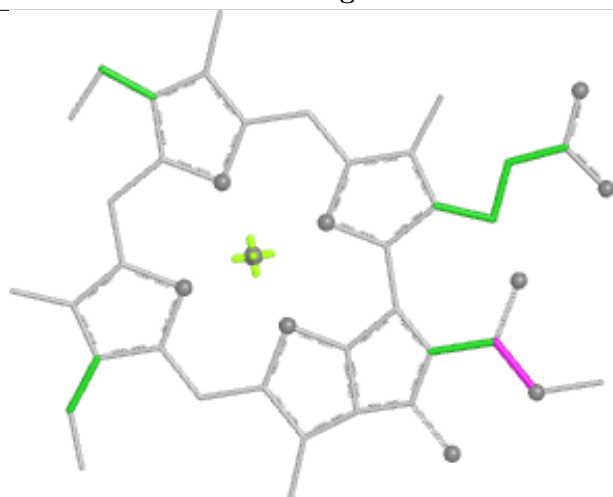
Ligand CLA i 508



Bond lengths



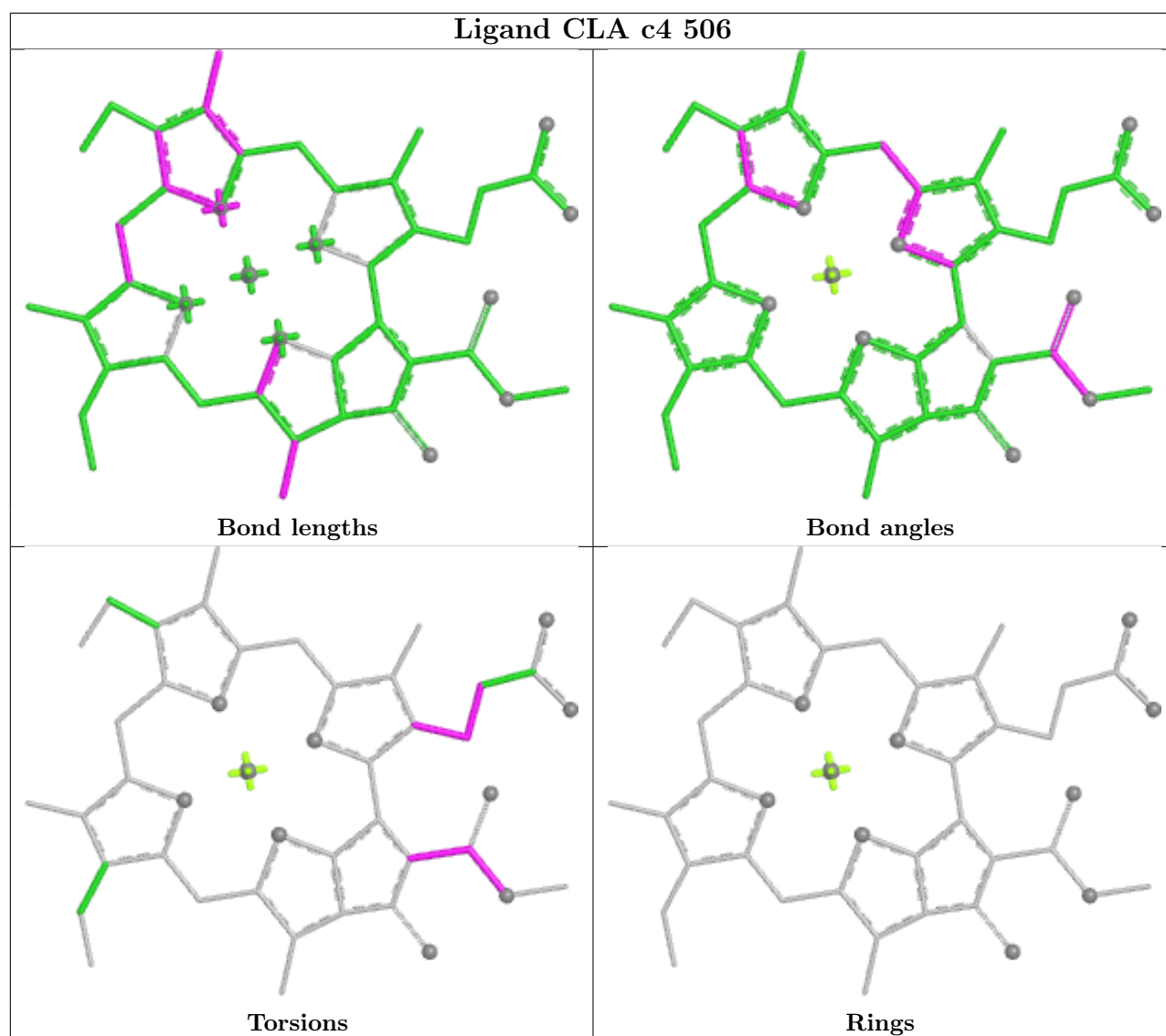
Bond angles



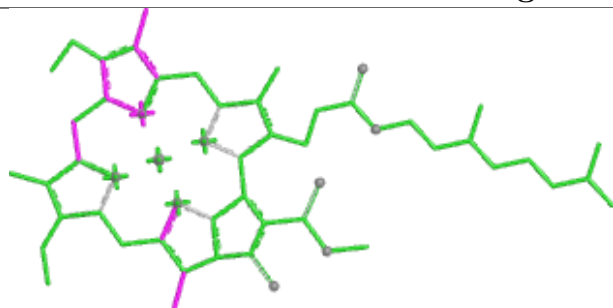
Torsions



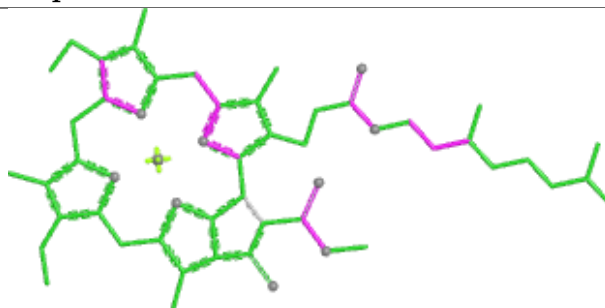
Rings



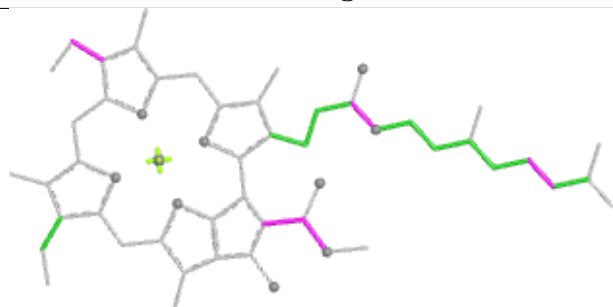
Ligand CLA p 502



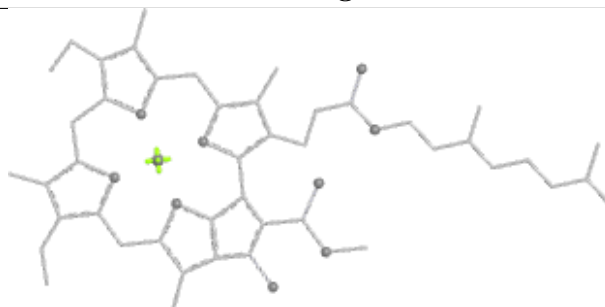
Bond lengths



Bond angles

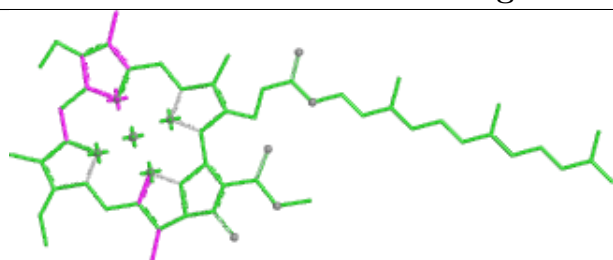


Torsions

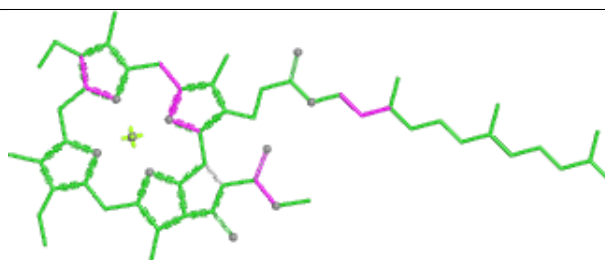


Rings

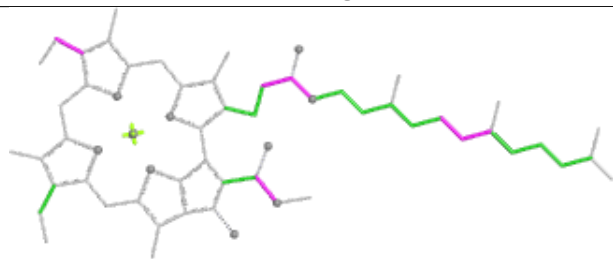
Ligand CLA cA 1139



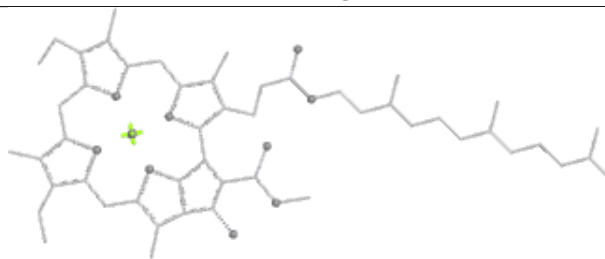
Bond lengths



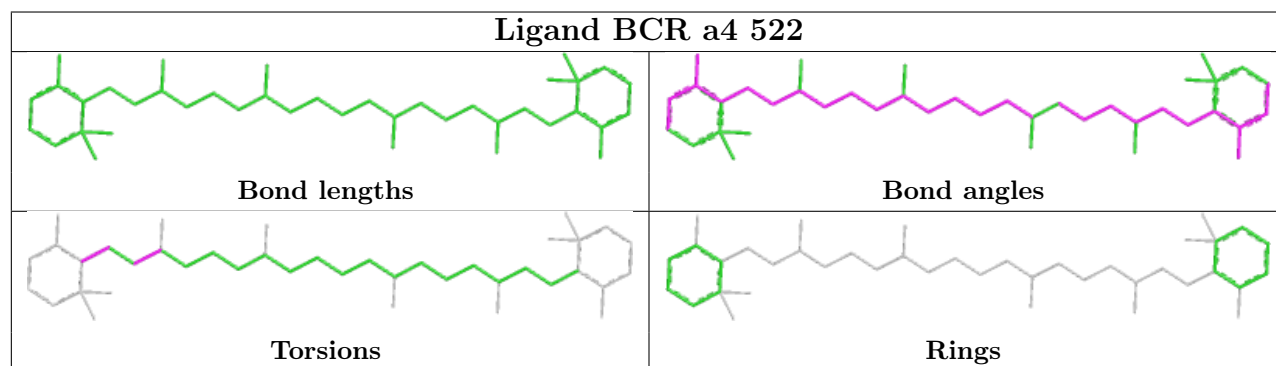
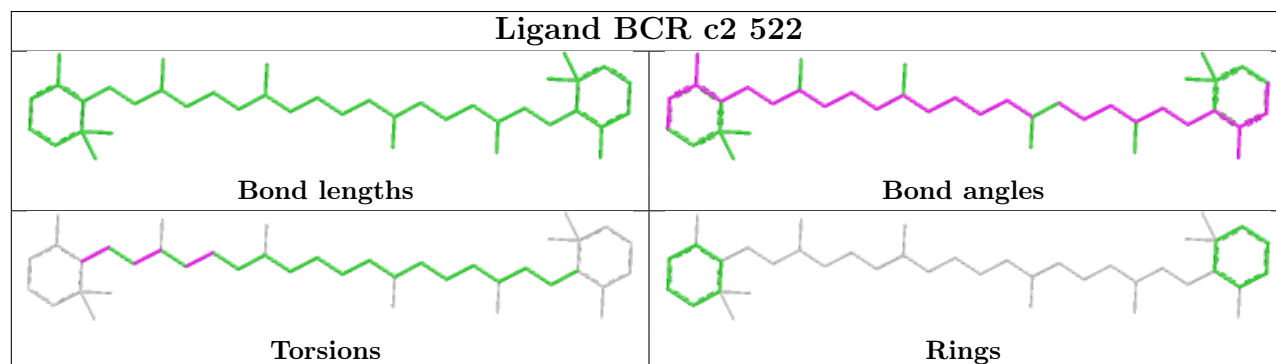
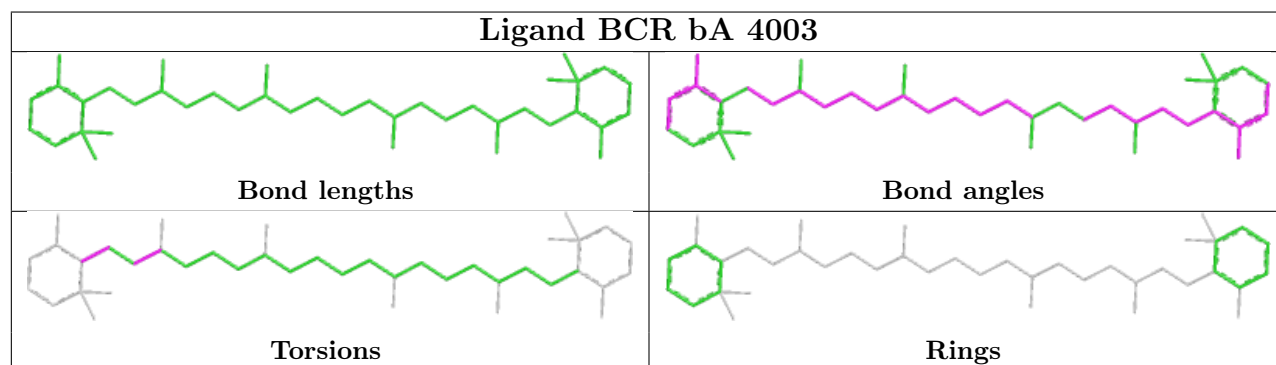
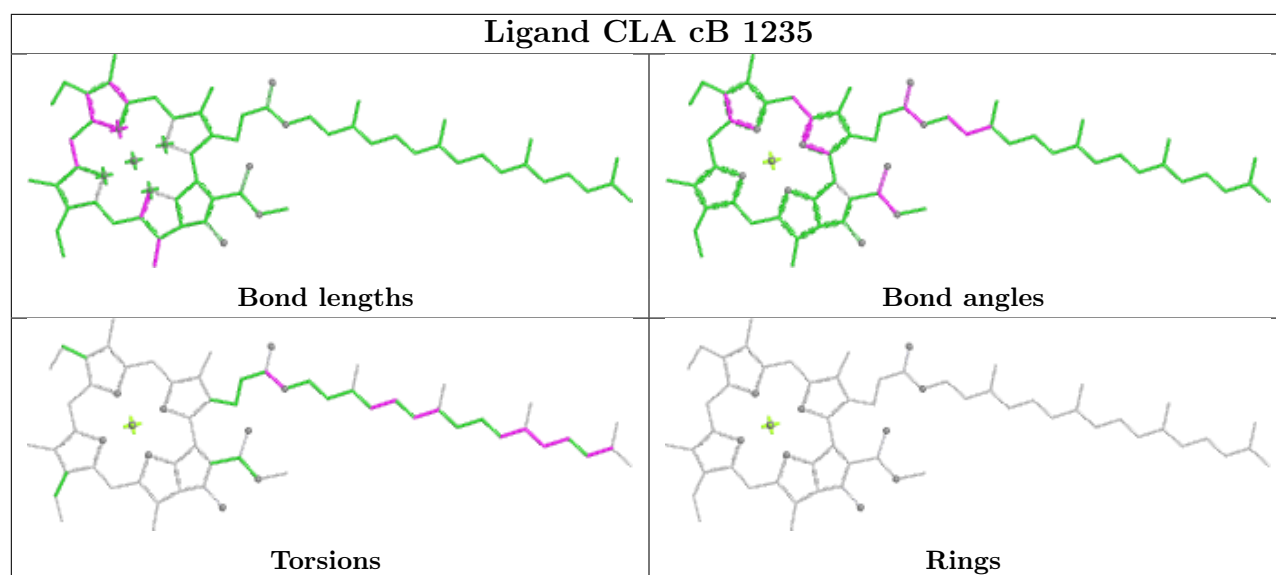
Bond angles

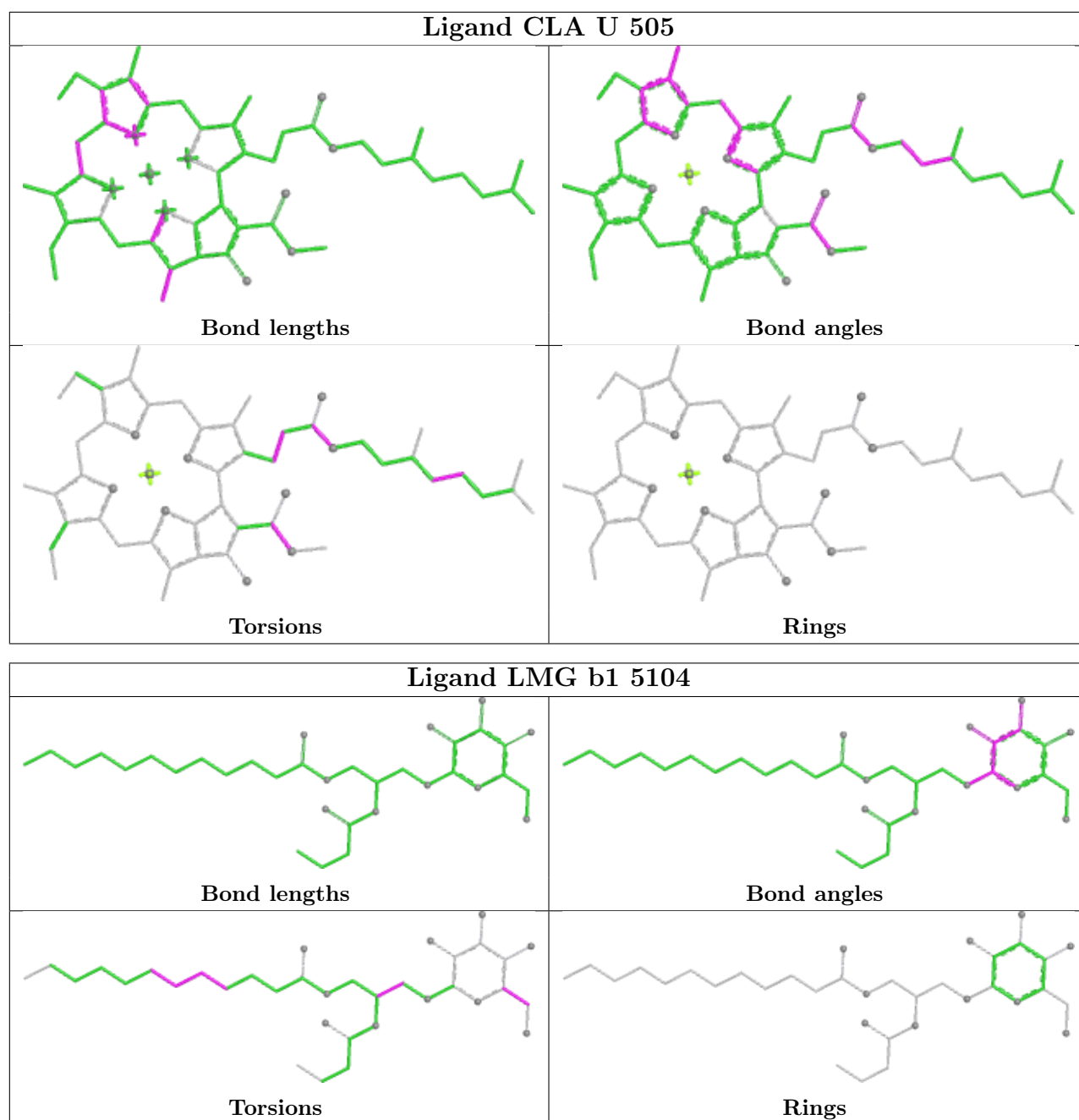


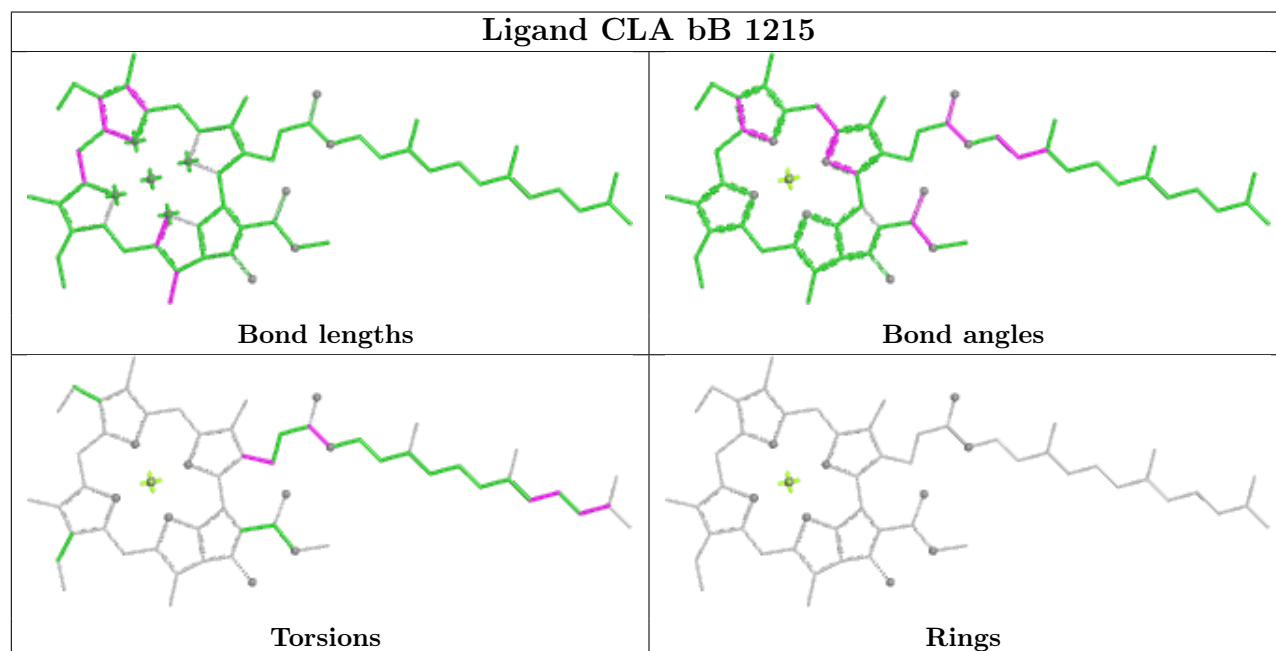
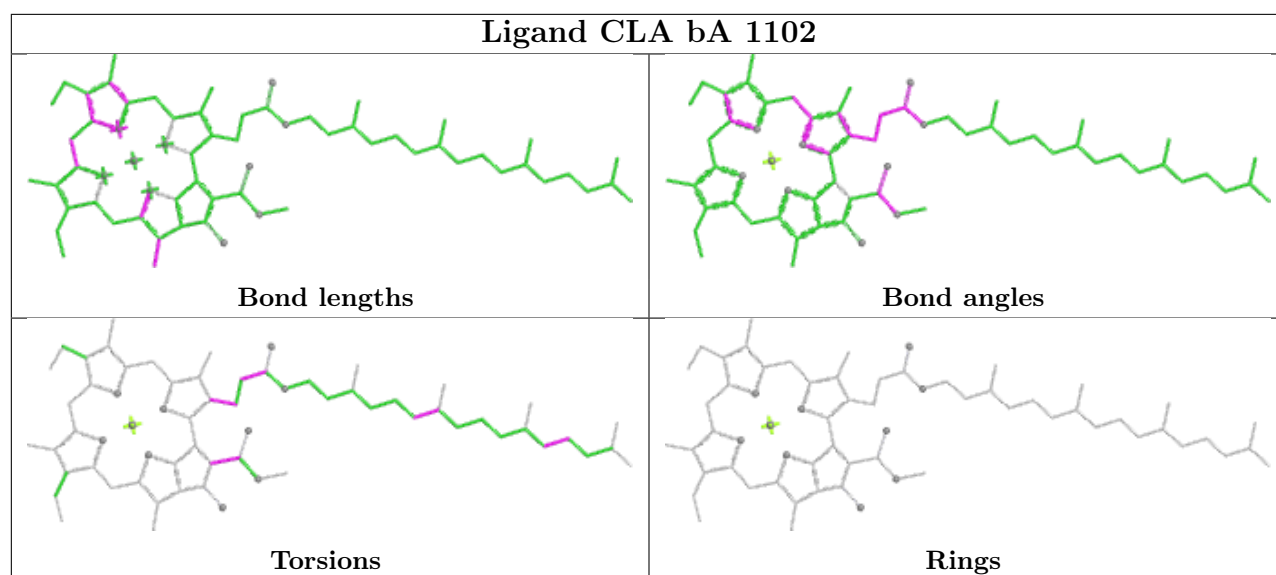
Torsions

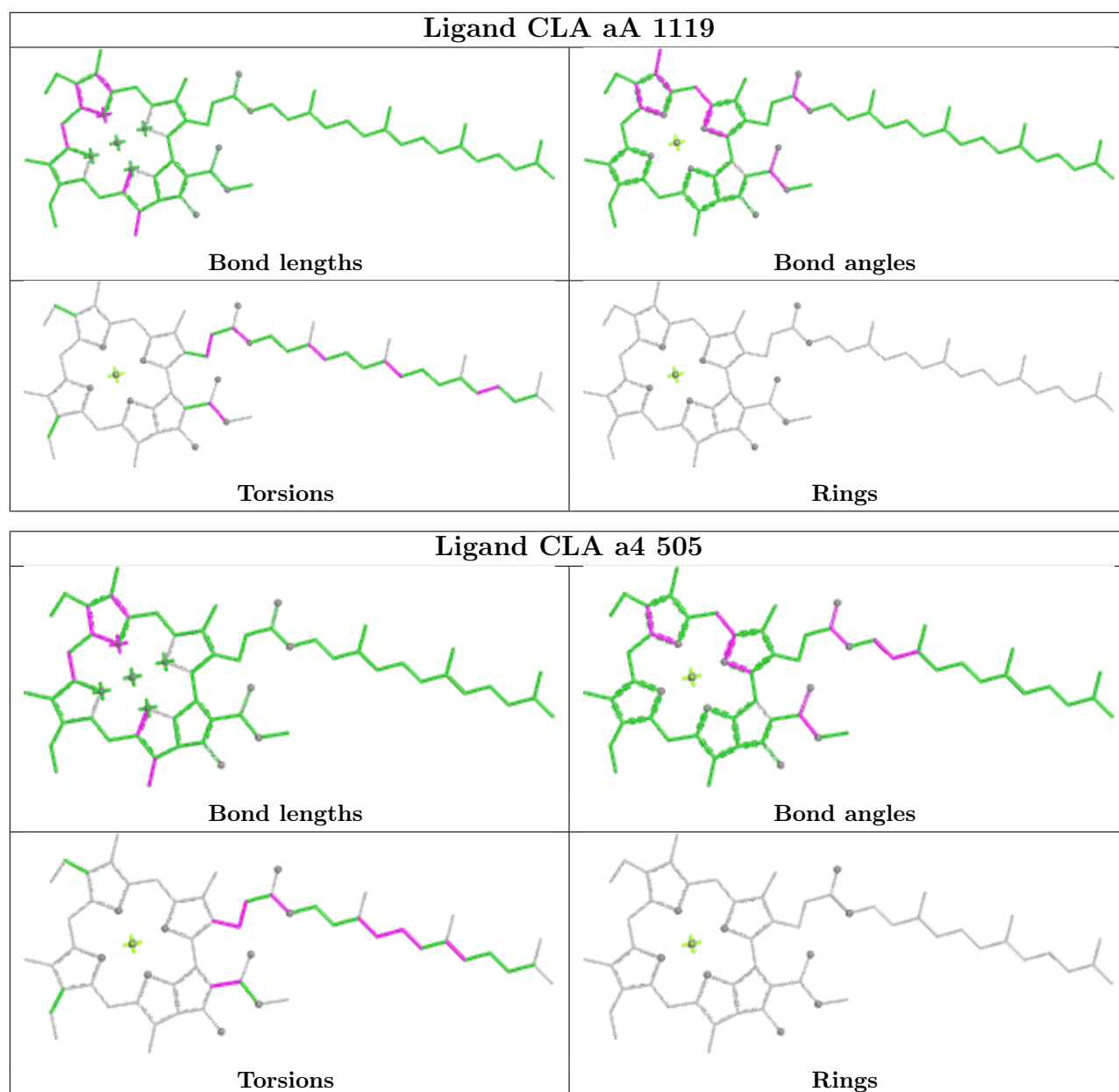


Rings

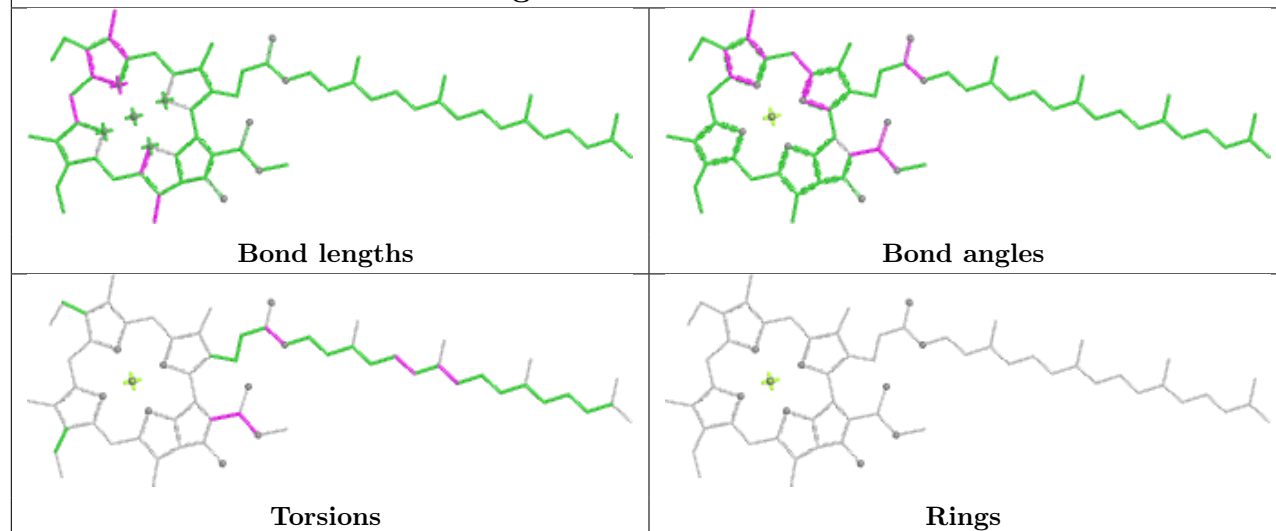




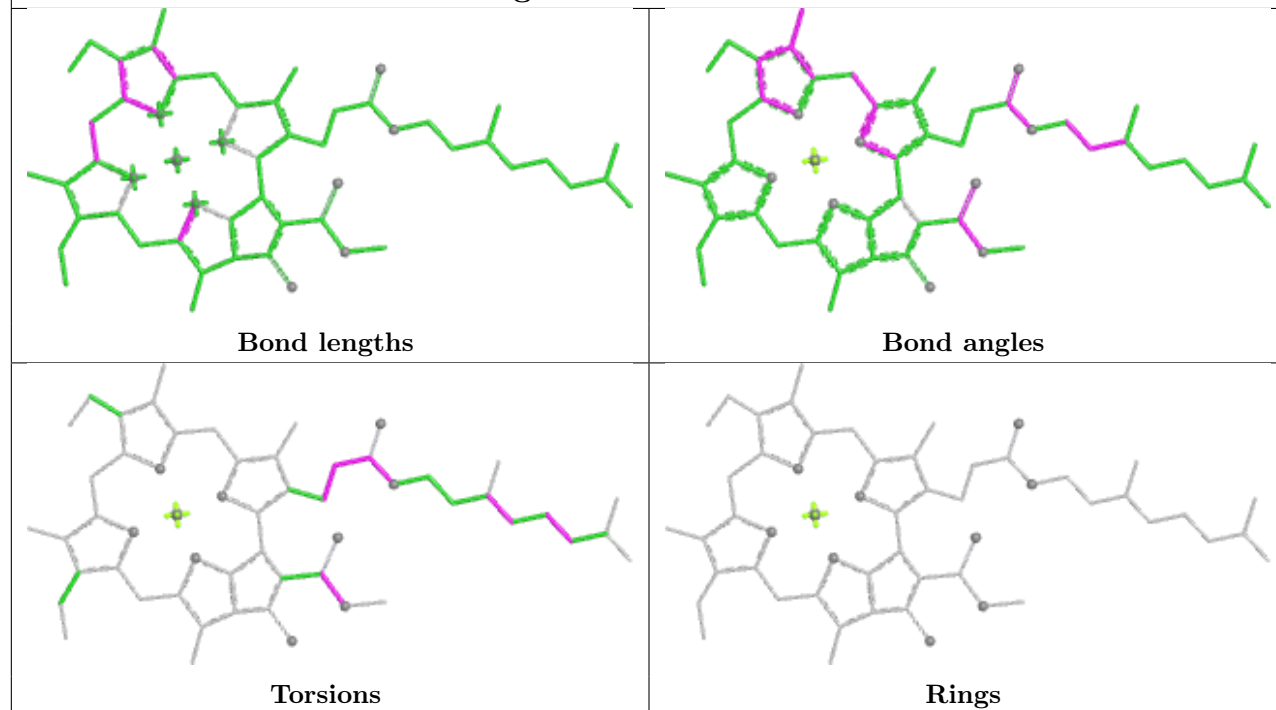


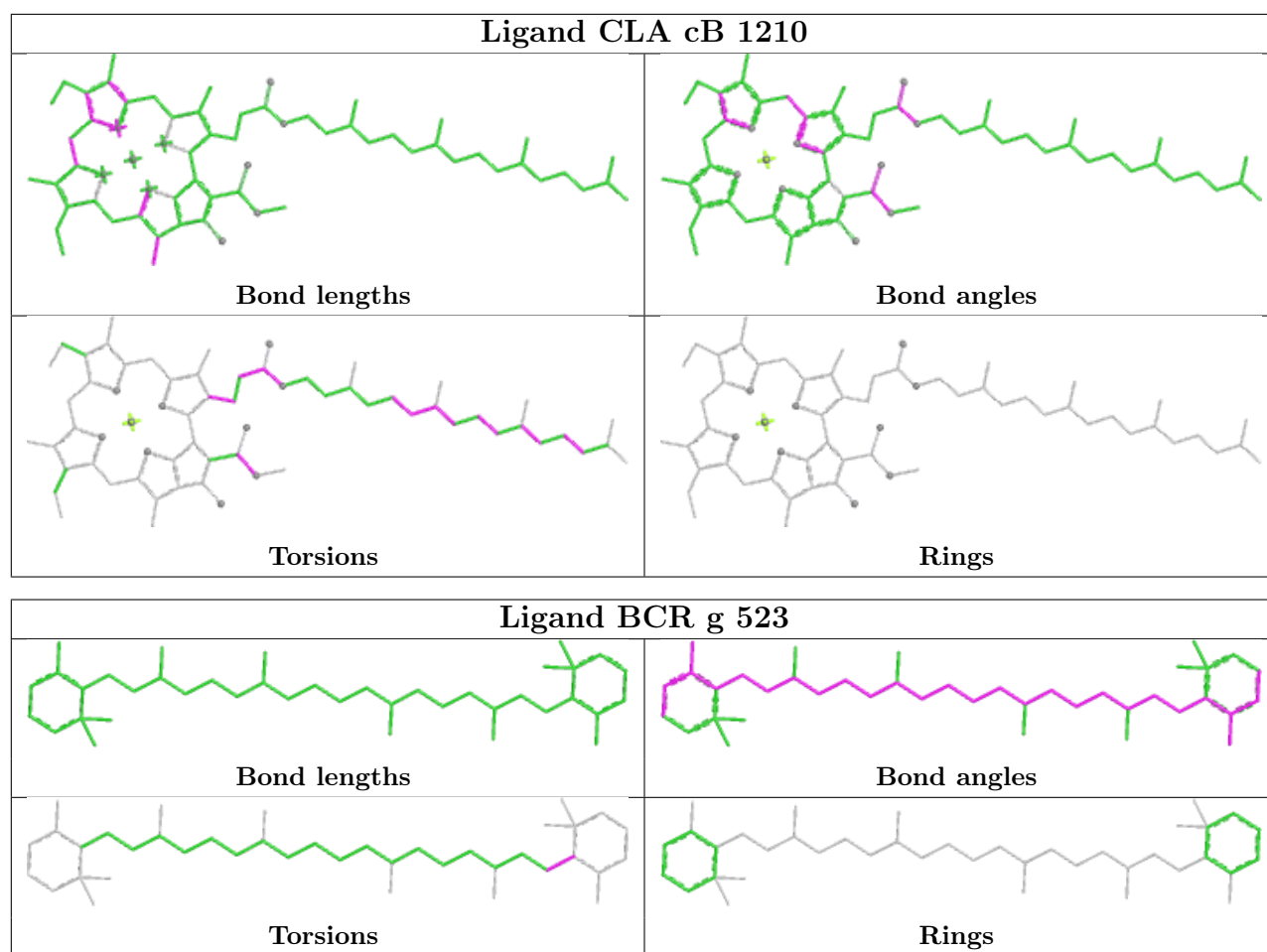


Ligand CLA bA 1128

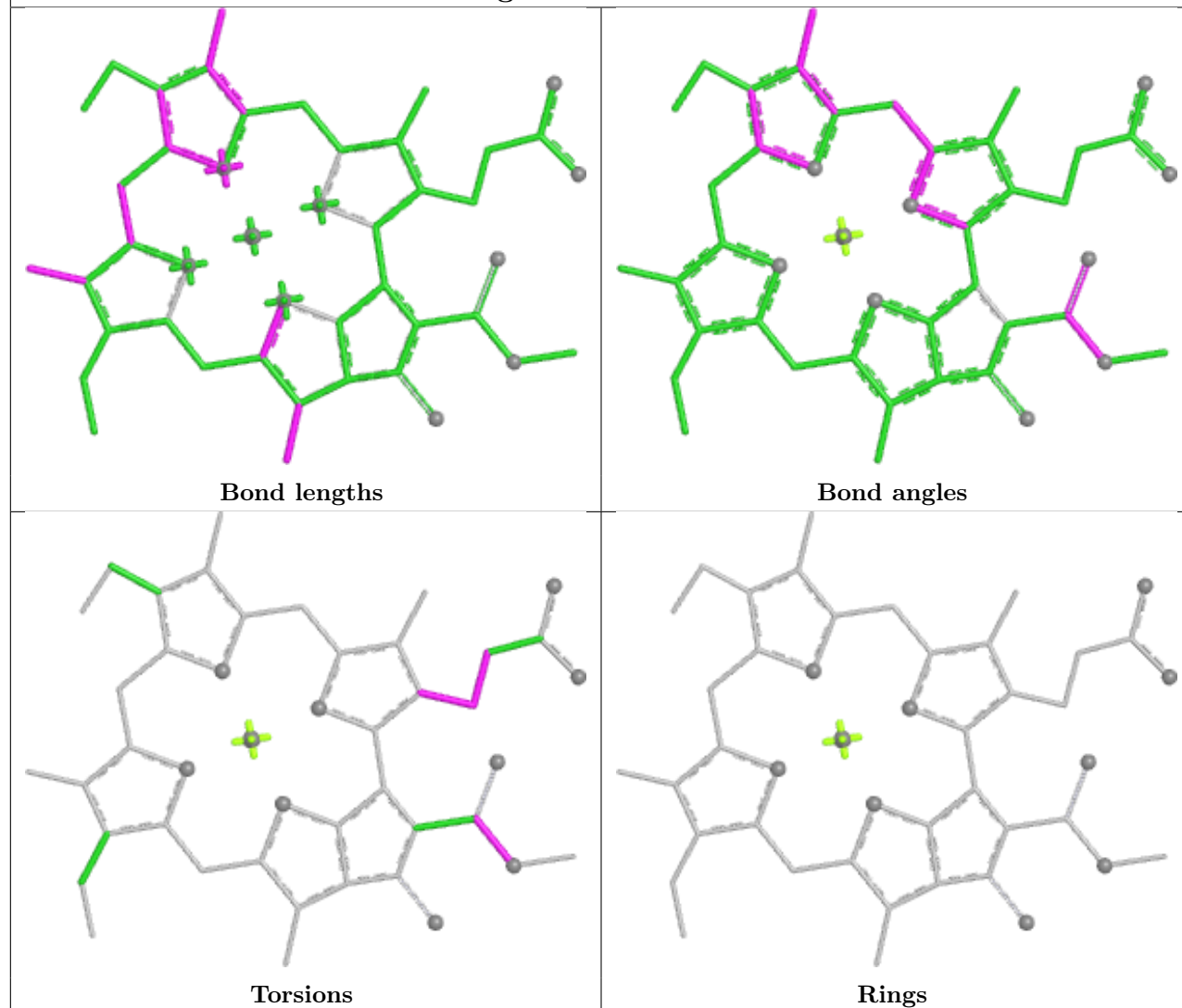


Ligand CLA bB 1219

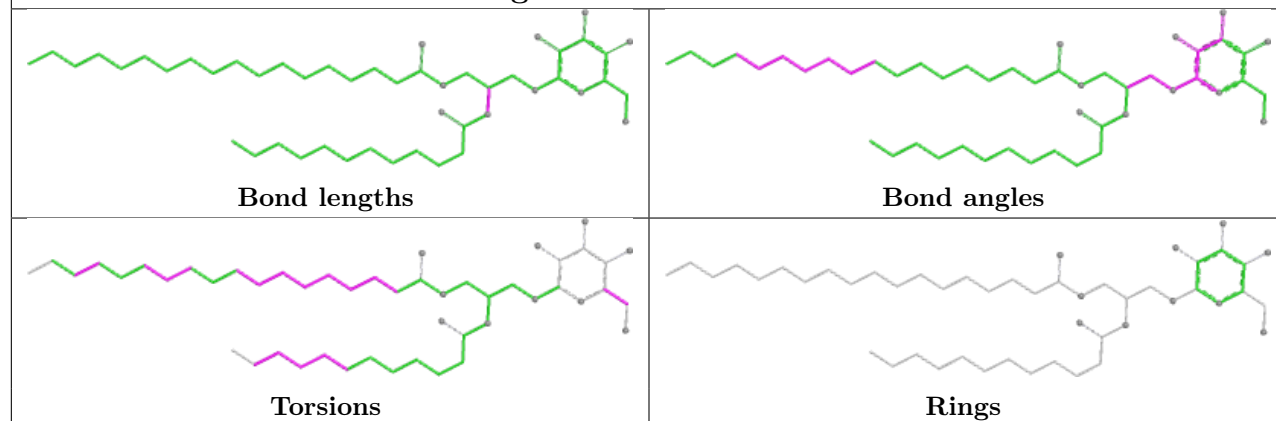




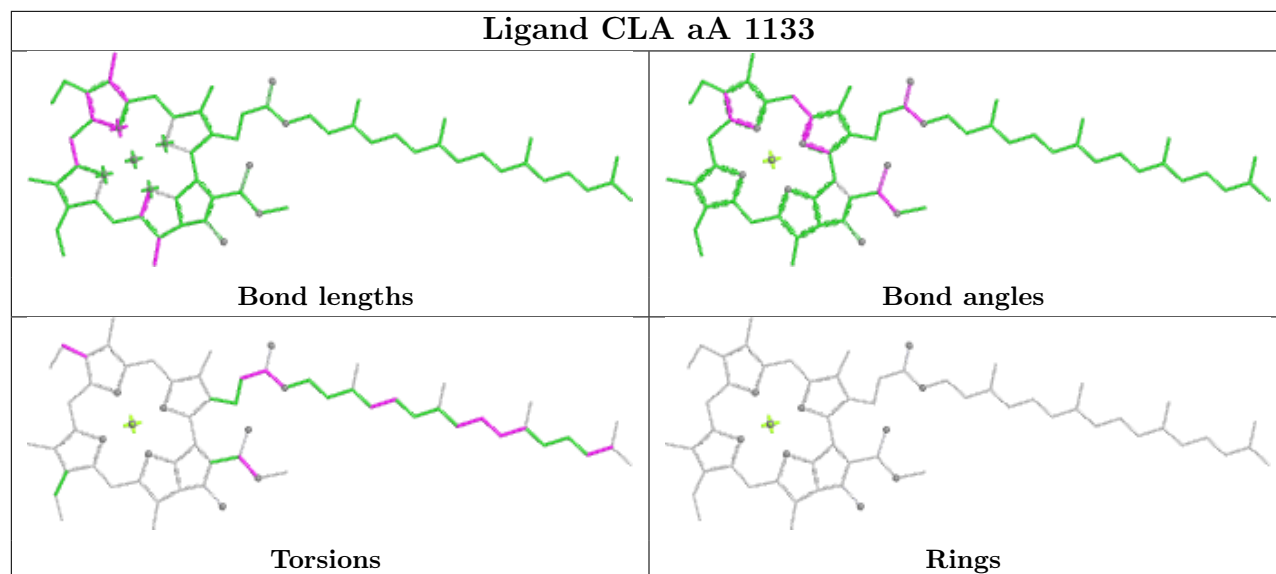
Ligand CLA e 508



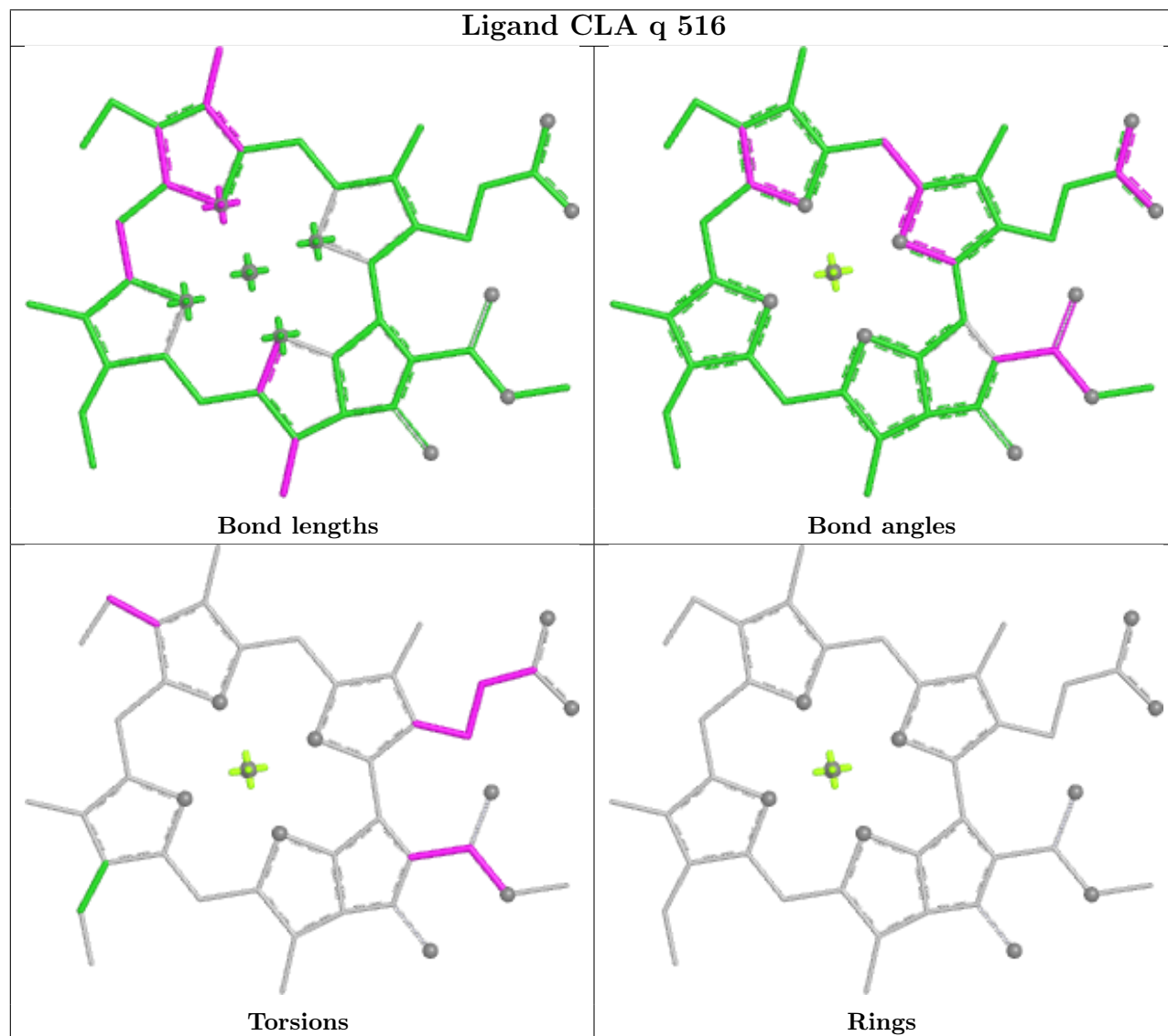
Ligand LMG cB 5002

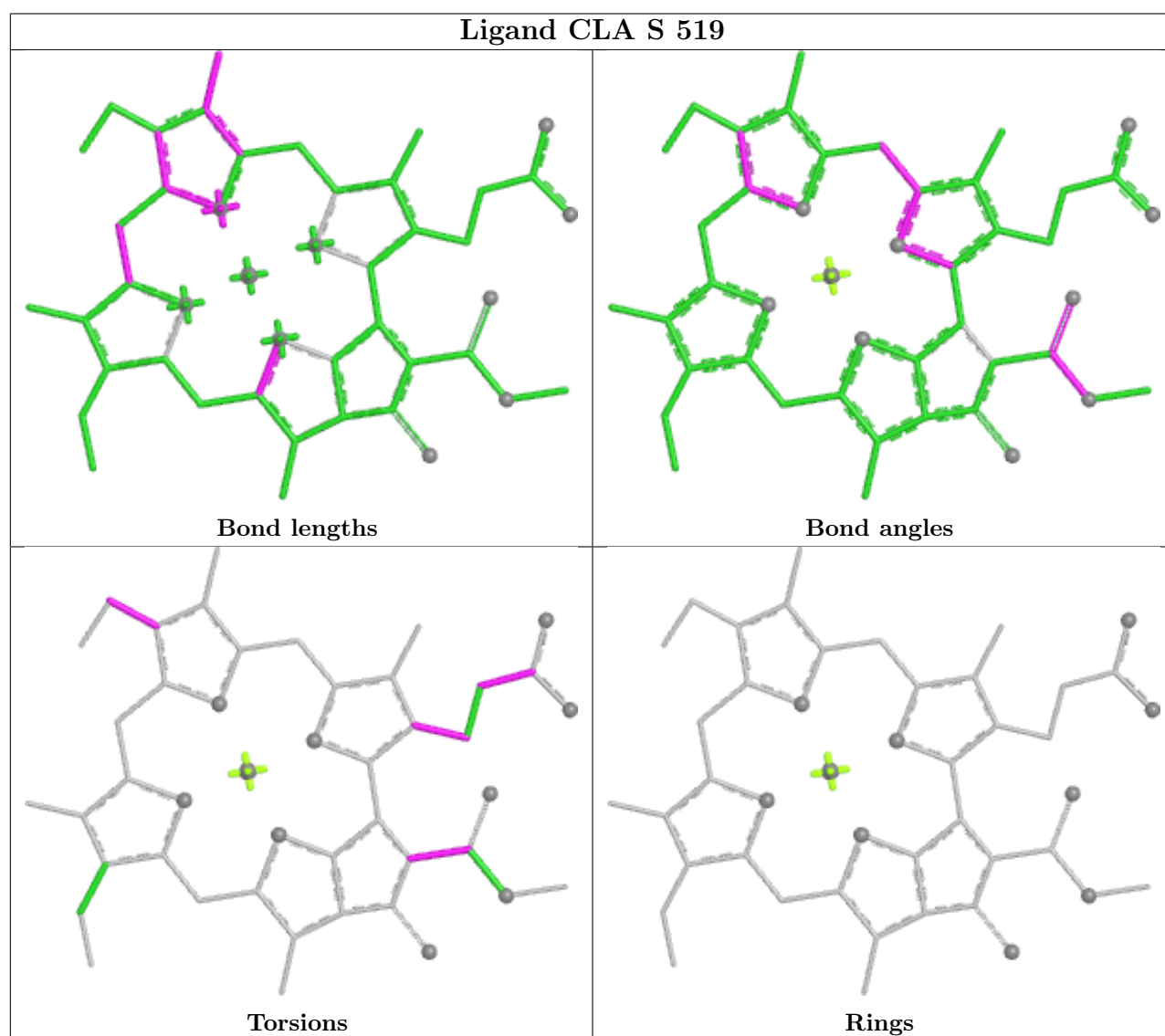
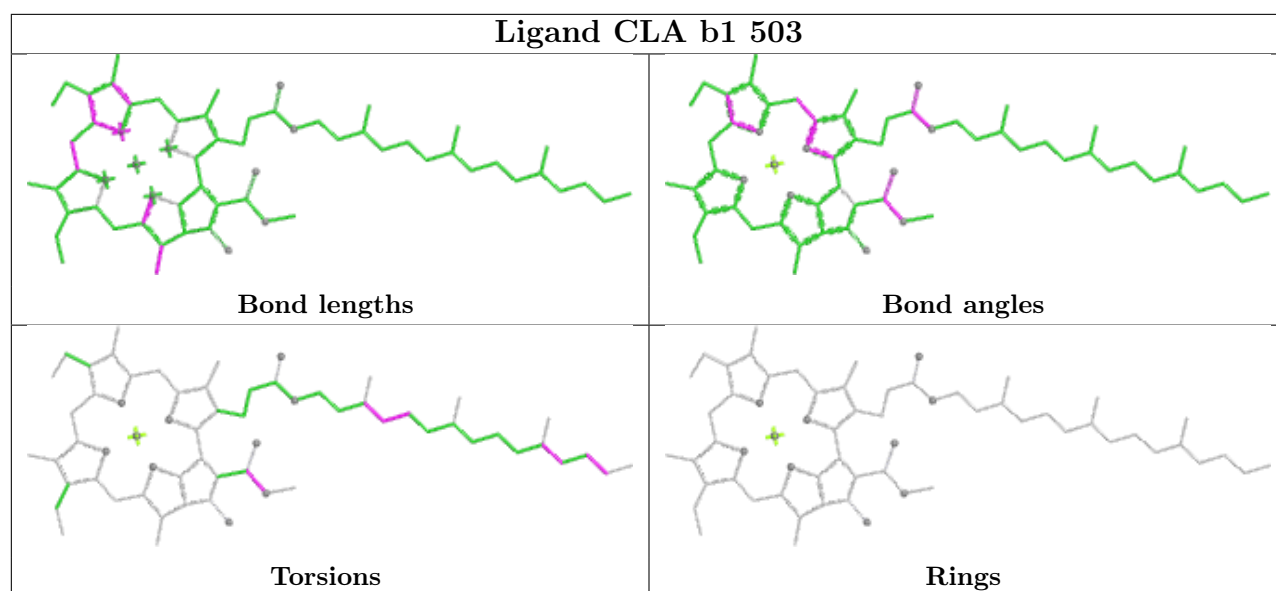


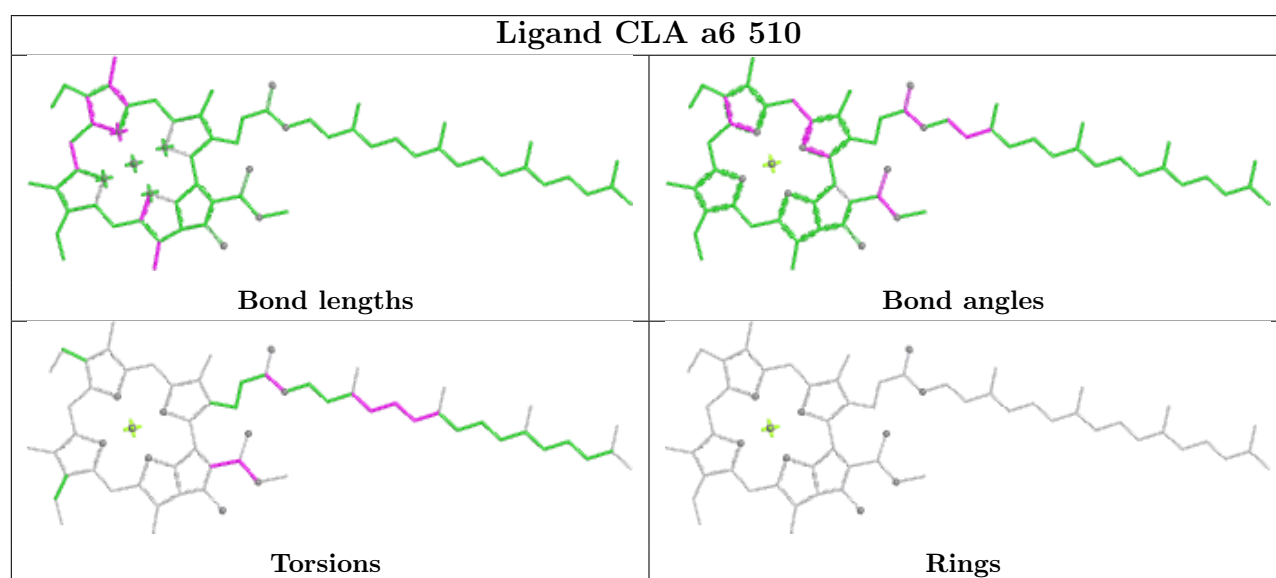
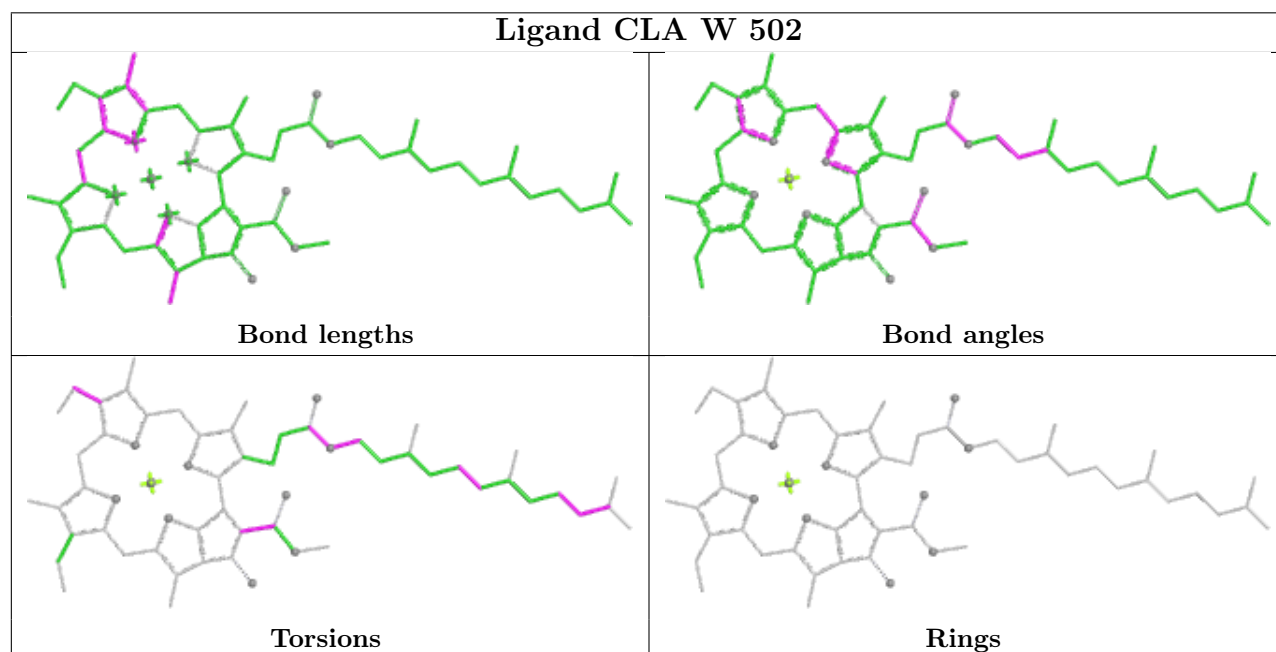
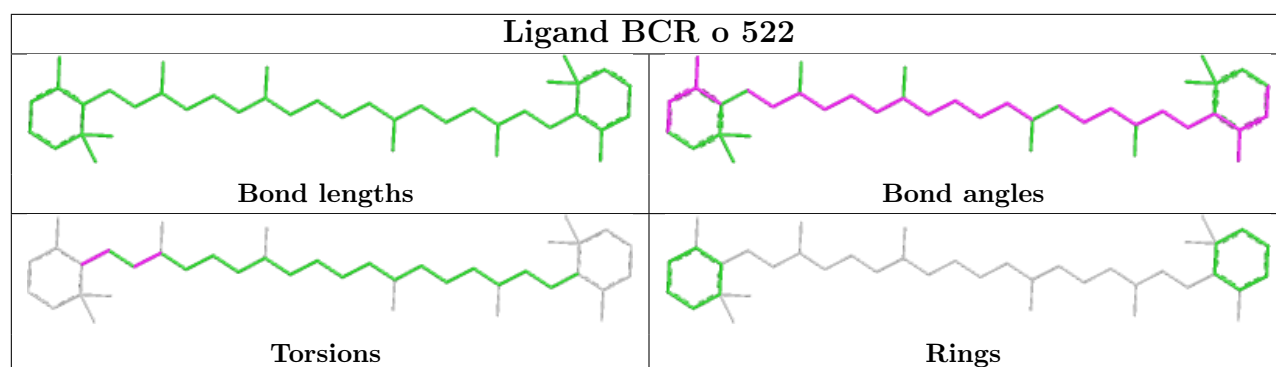
Ligand CLA aA 1133

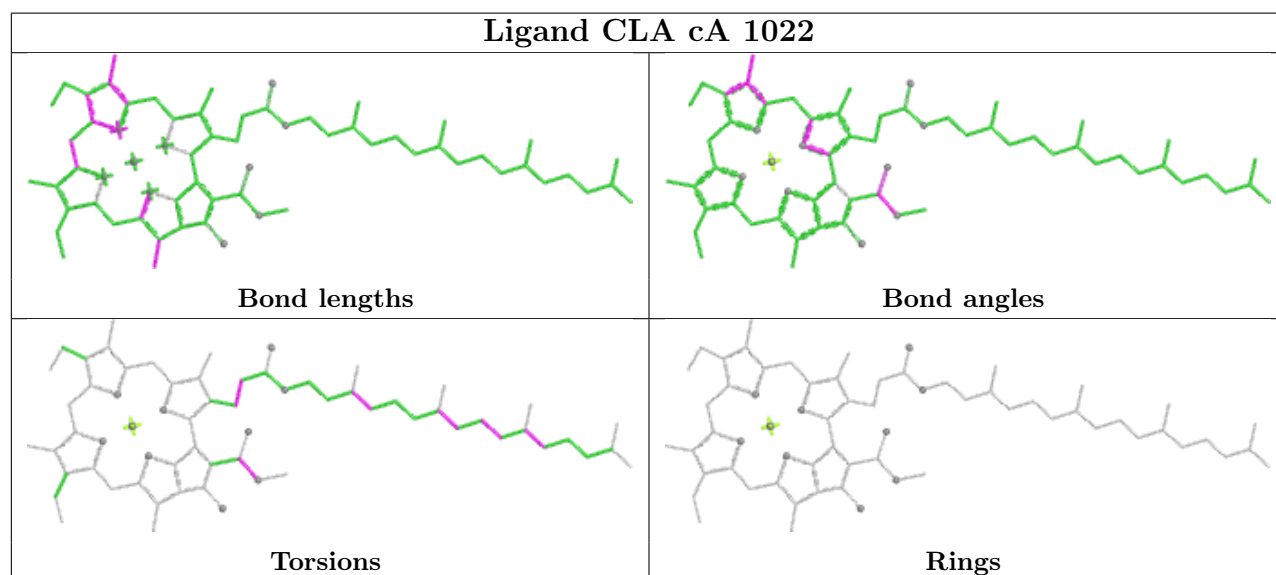
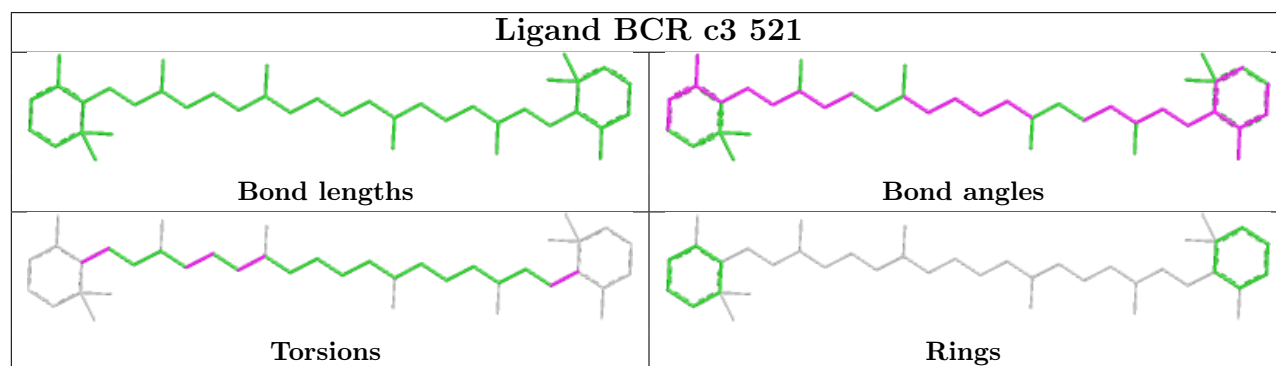
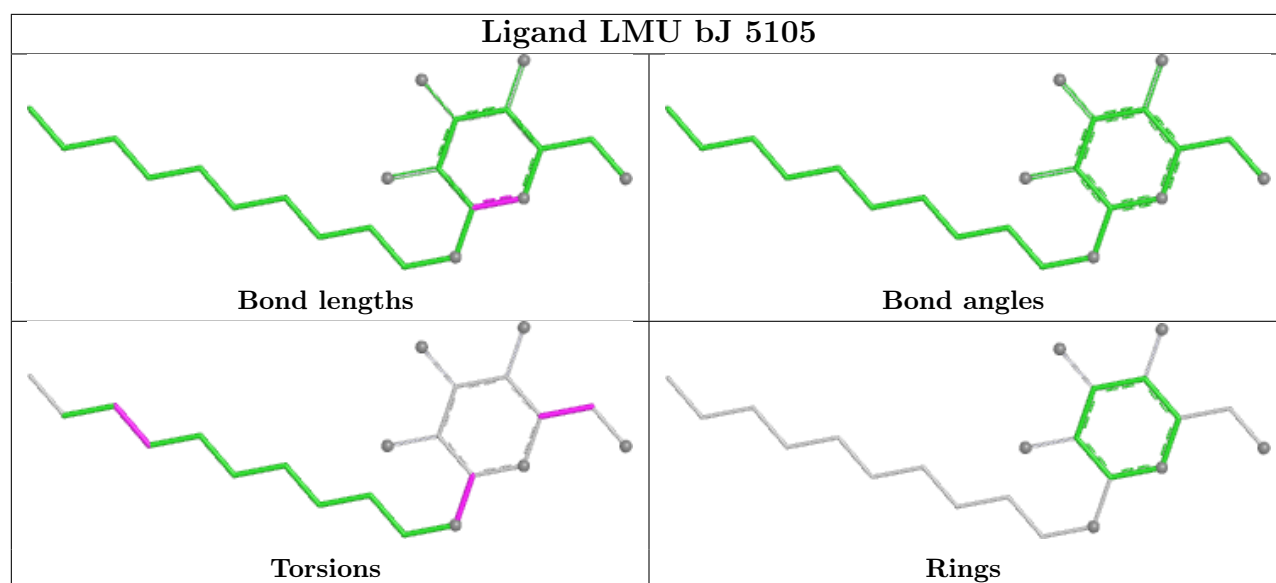


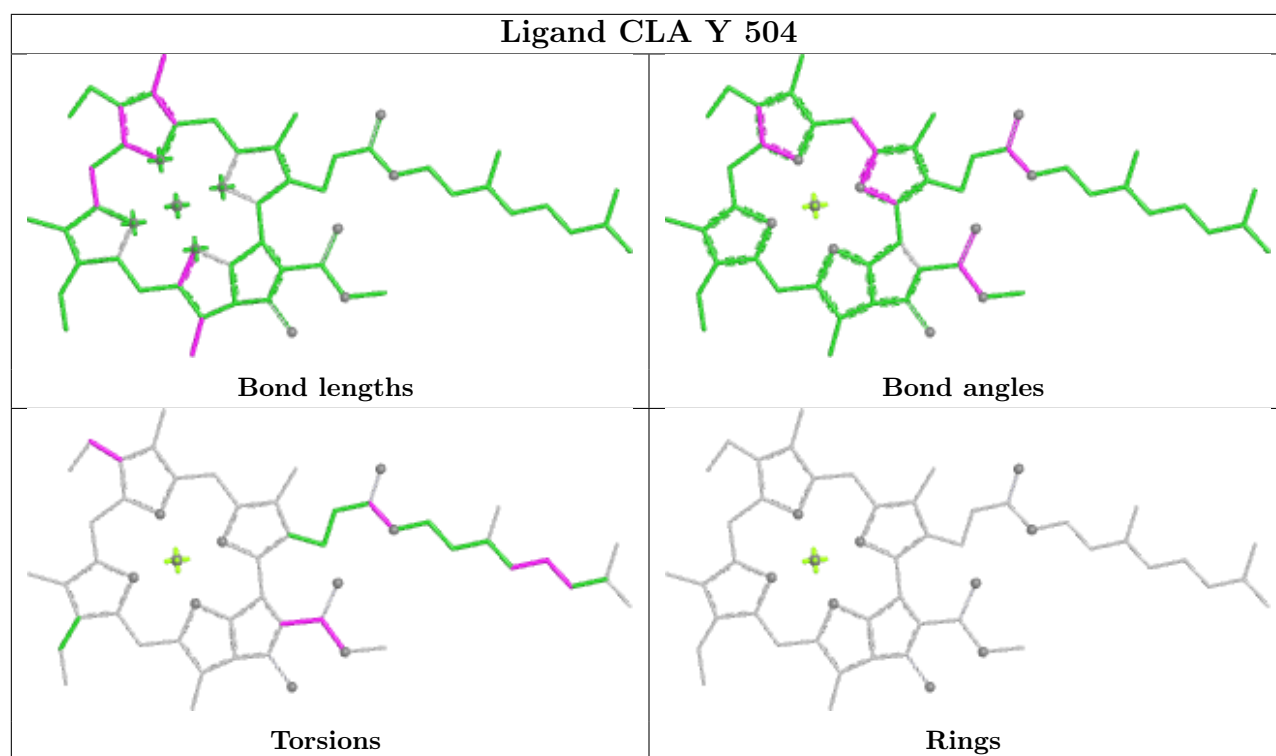
Ligand CLA q 516

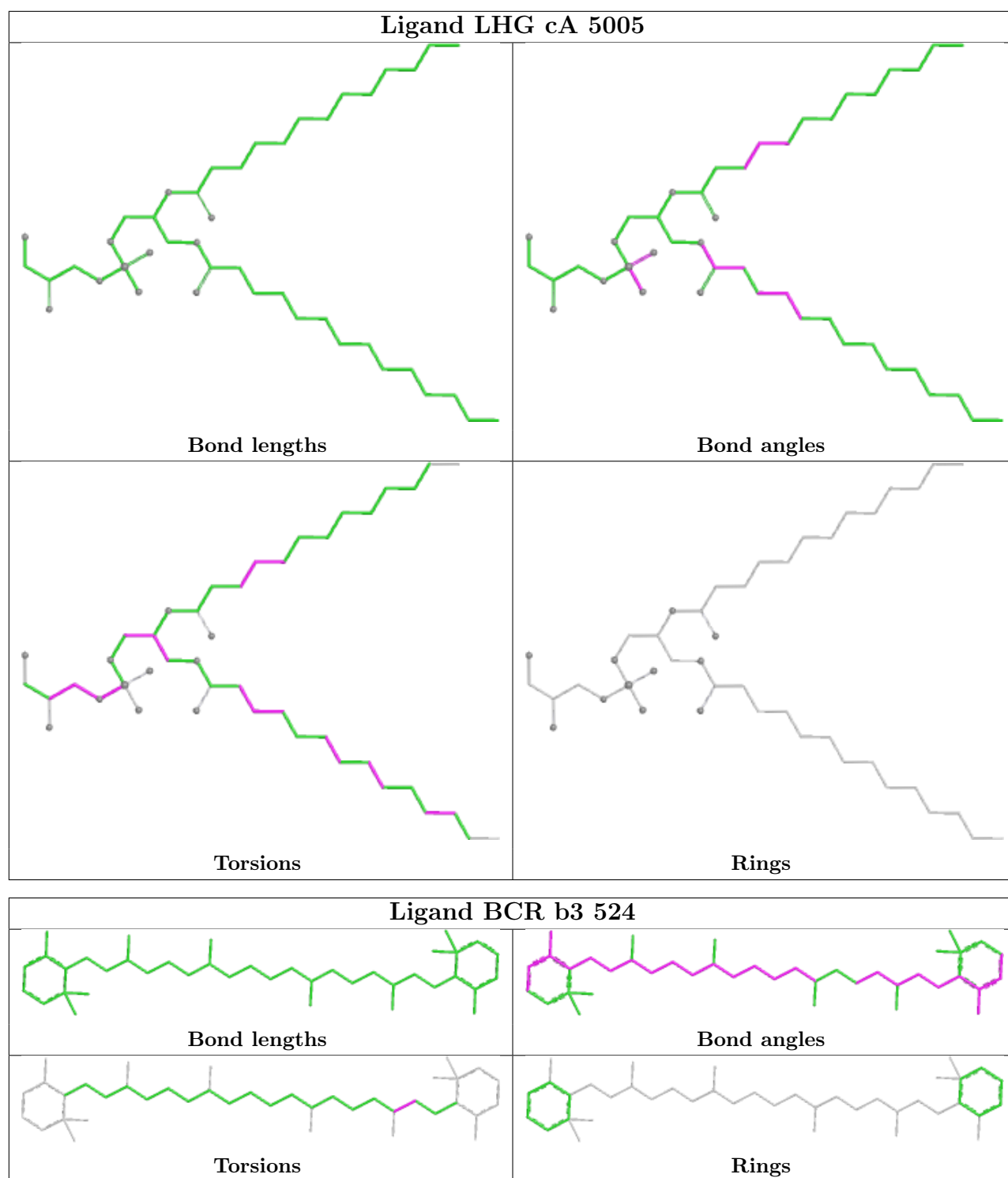


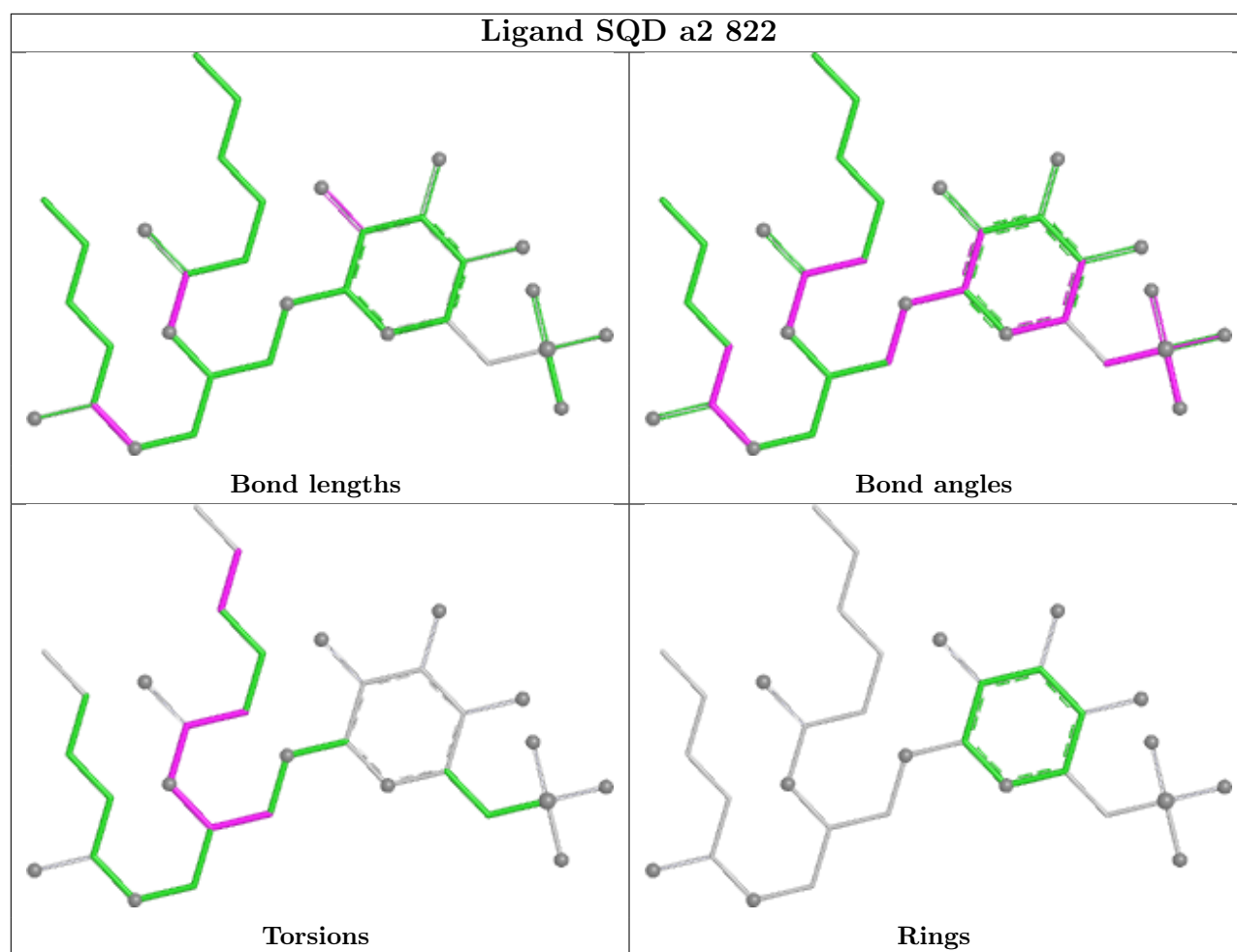


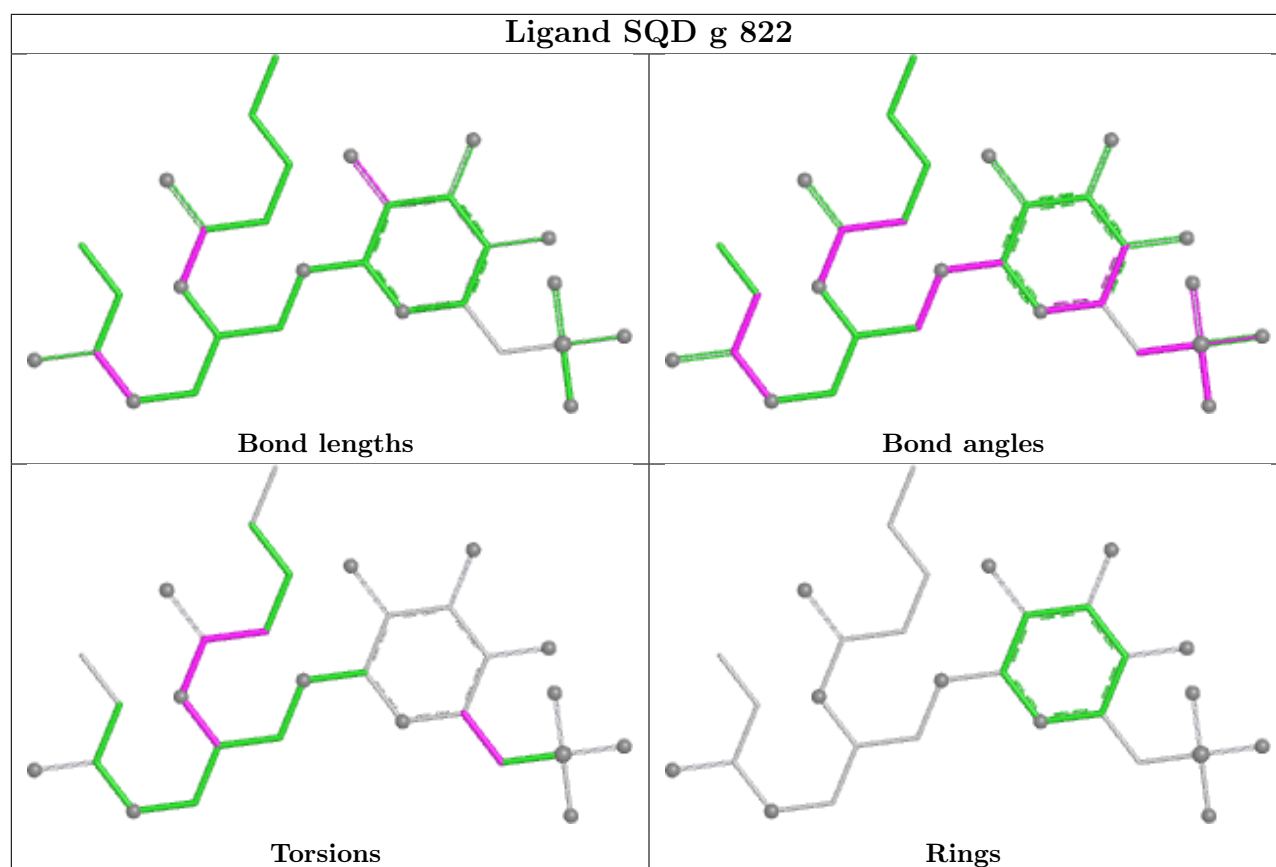




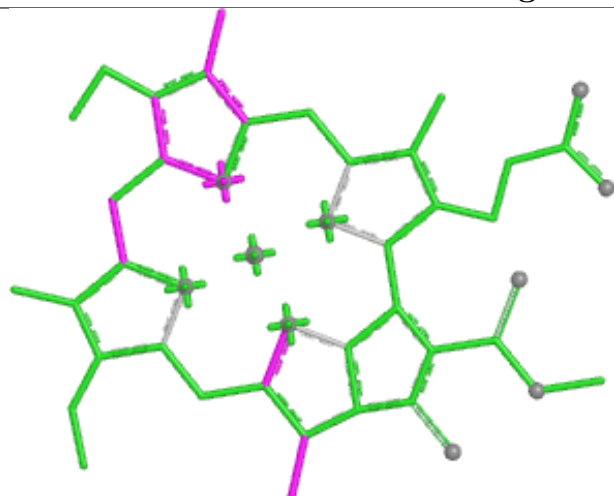




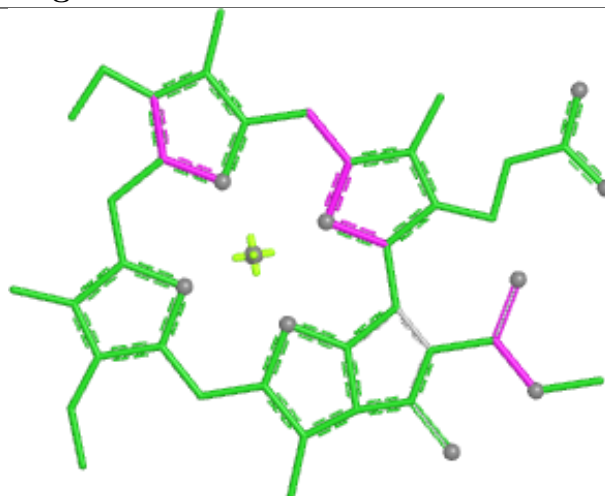




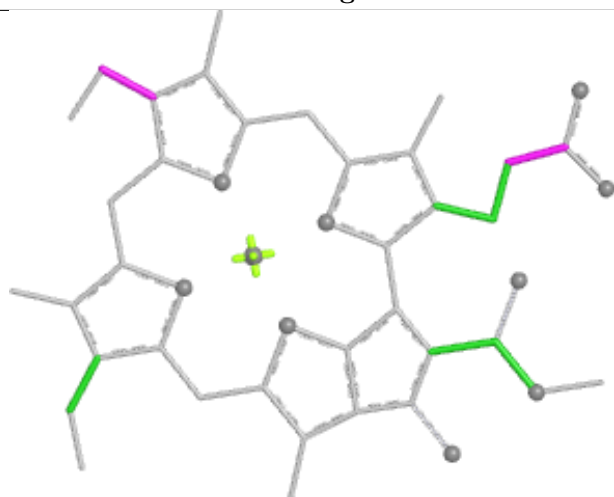
Ligand CLA g 512



Bond lengths



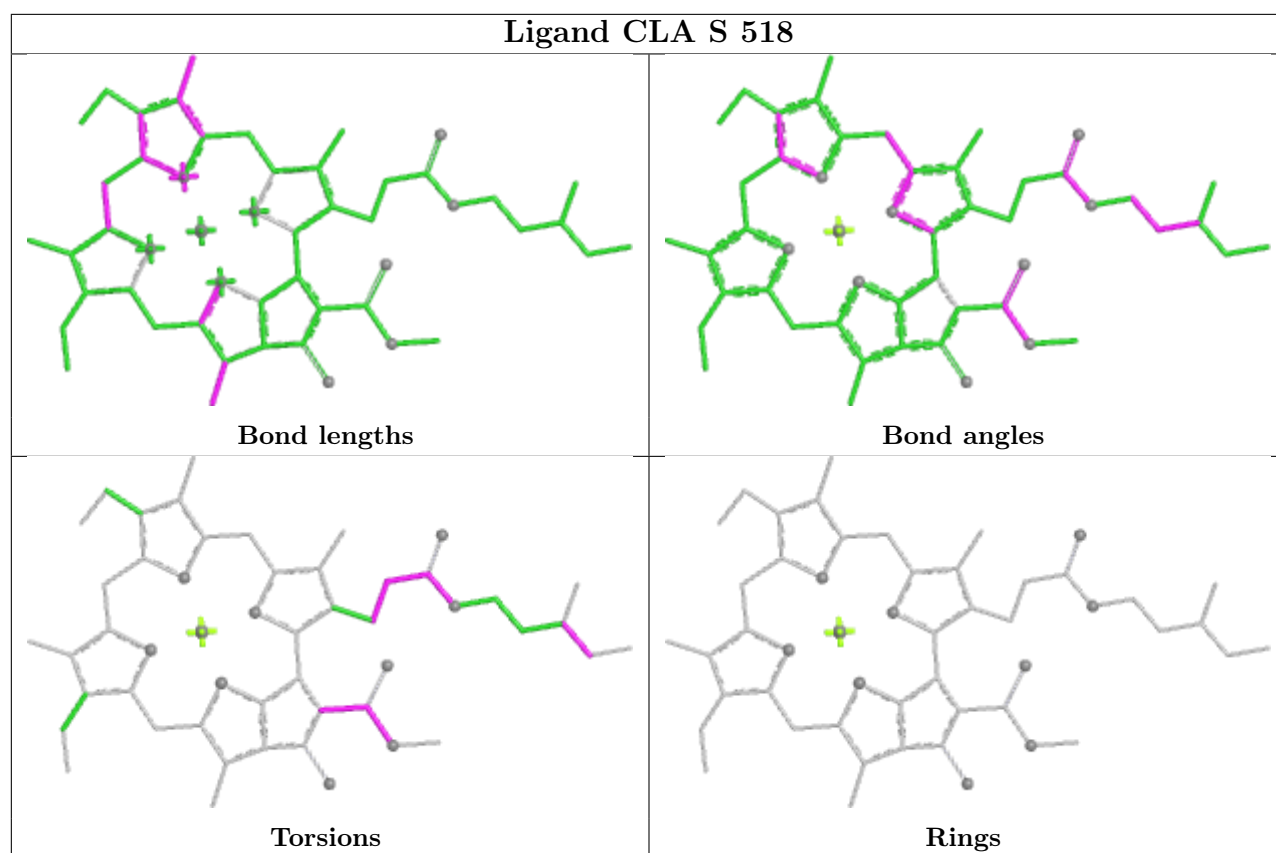
Bond angles



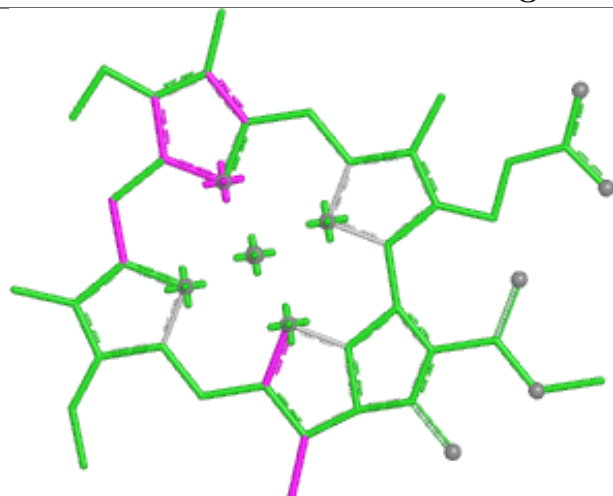
Torsions



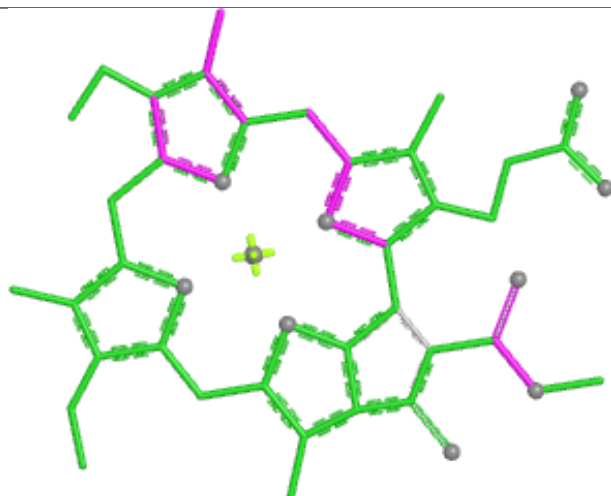
Rings



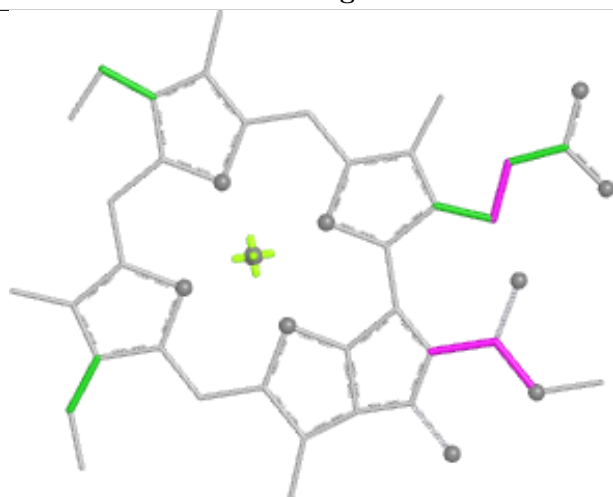
Ligand CLA c 513



Bond lengths



Bond angles

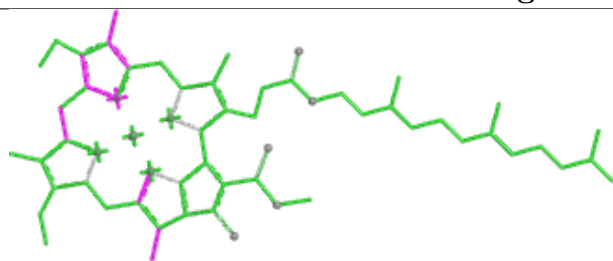


Torsions

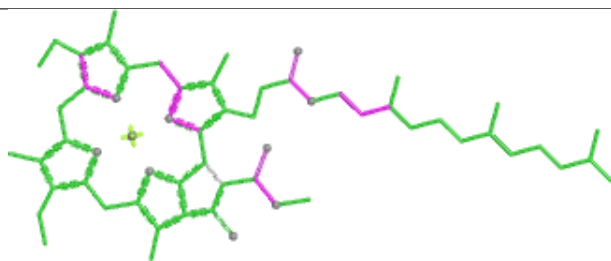


Rings

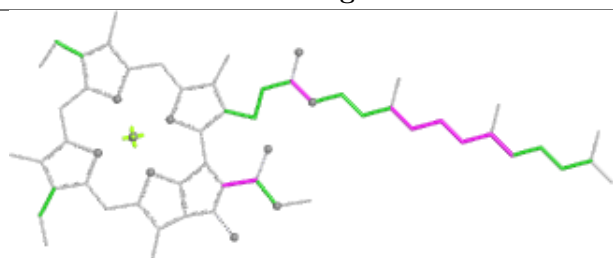
Ligand CLA b 510



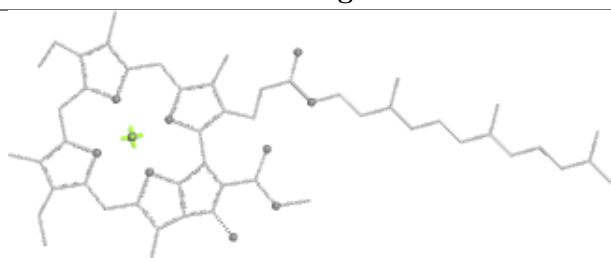
Bond lengths



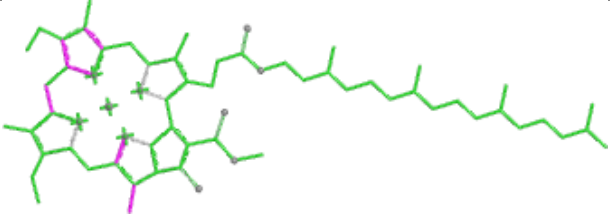
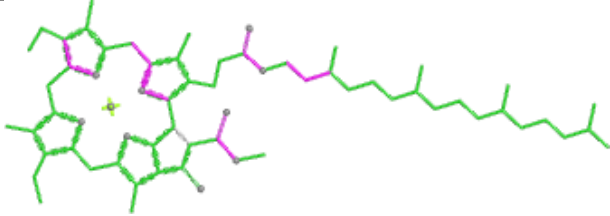
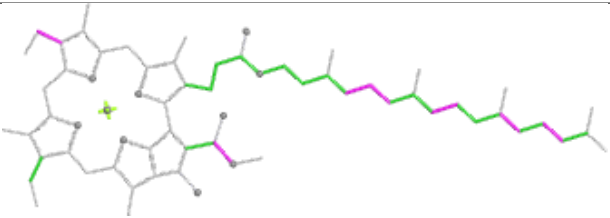
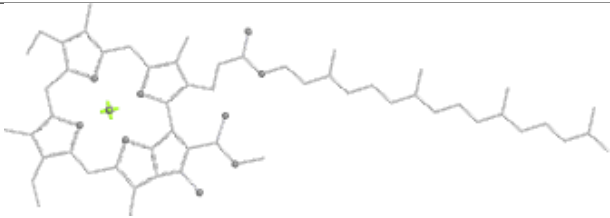
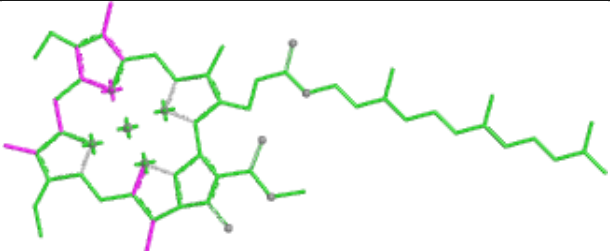
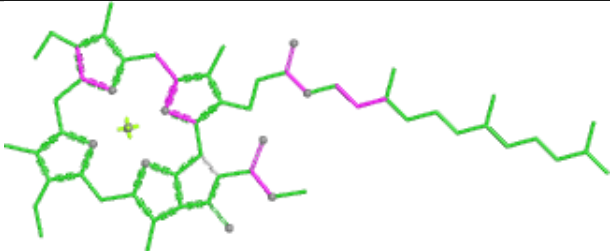
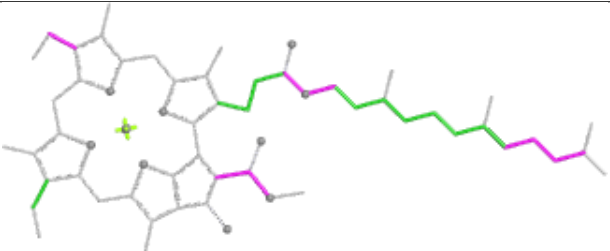
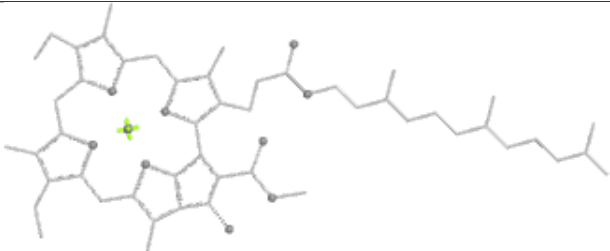


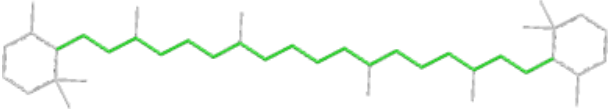
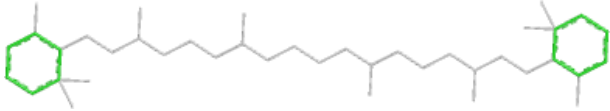
Bond angles

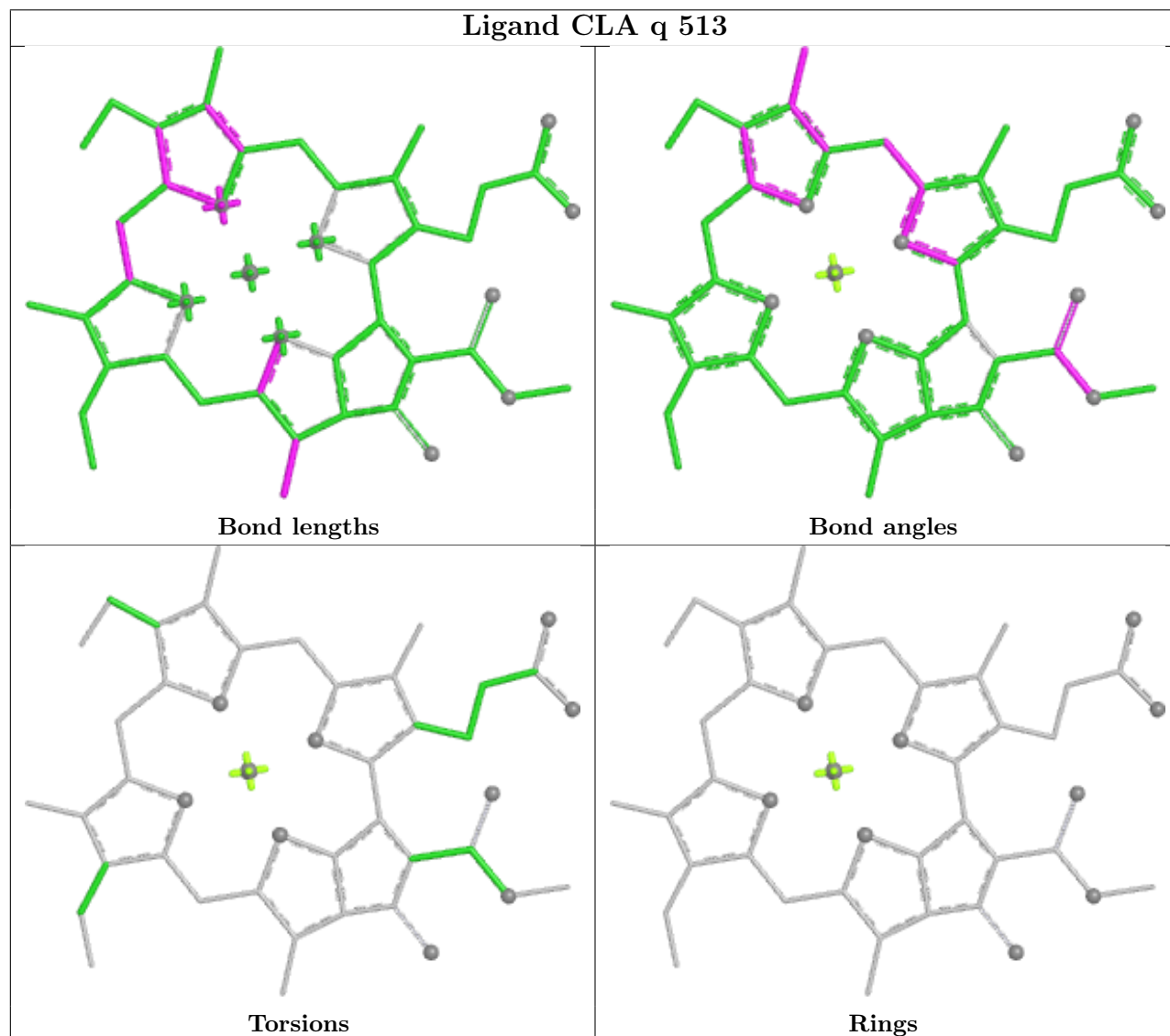
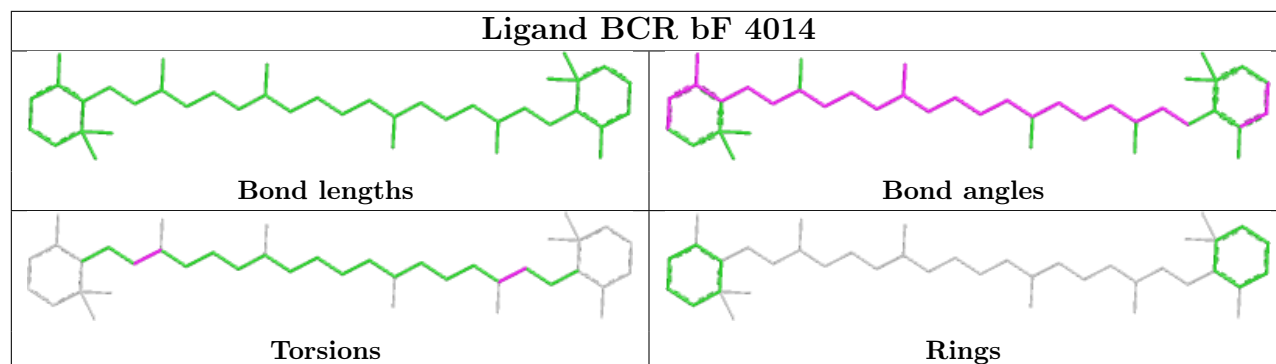


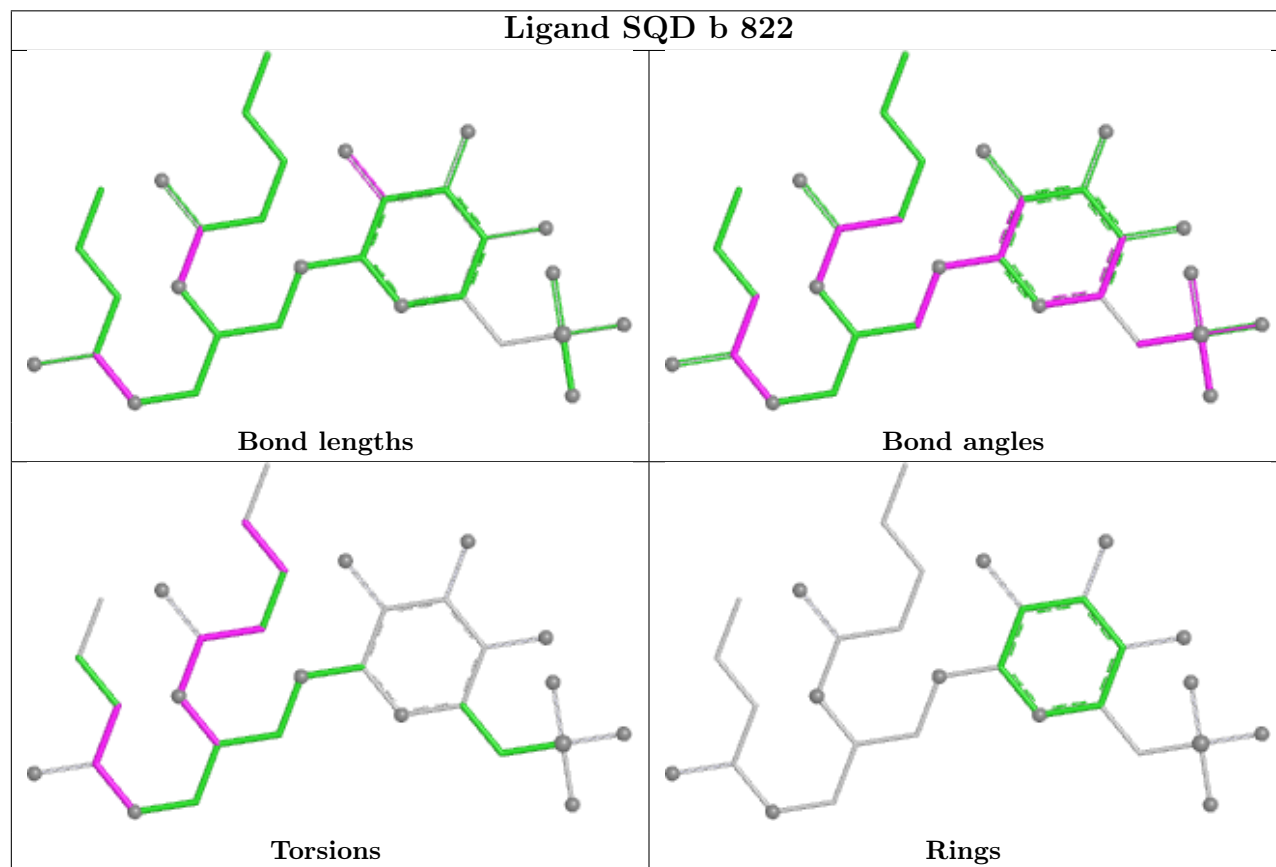
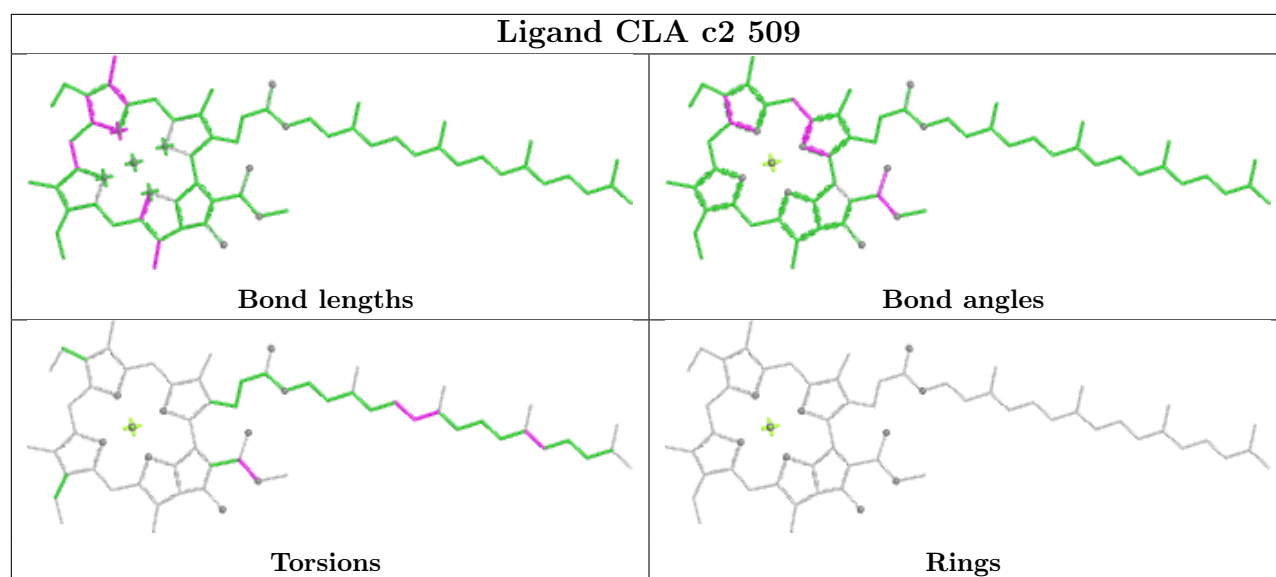
Torsions

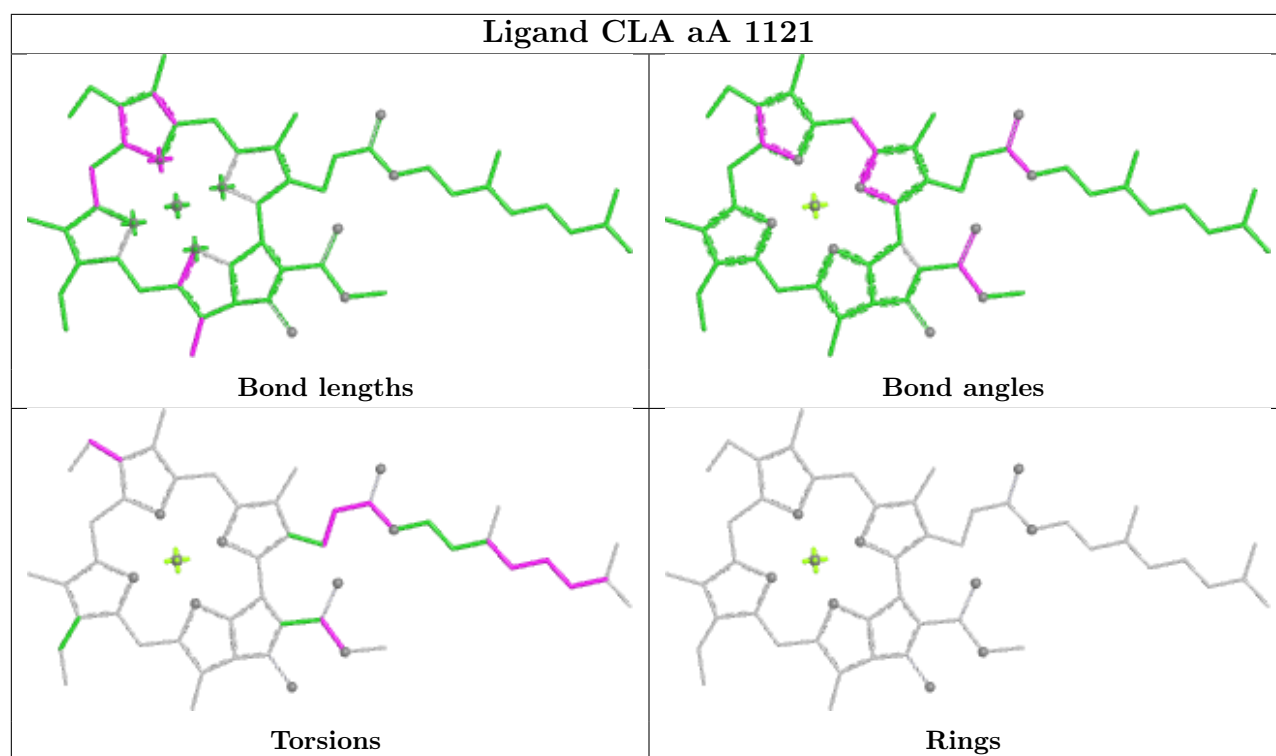


Rings

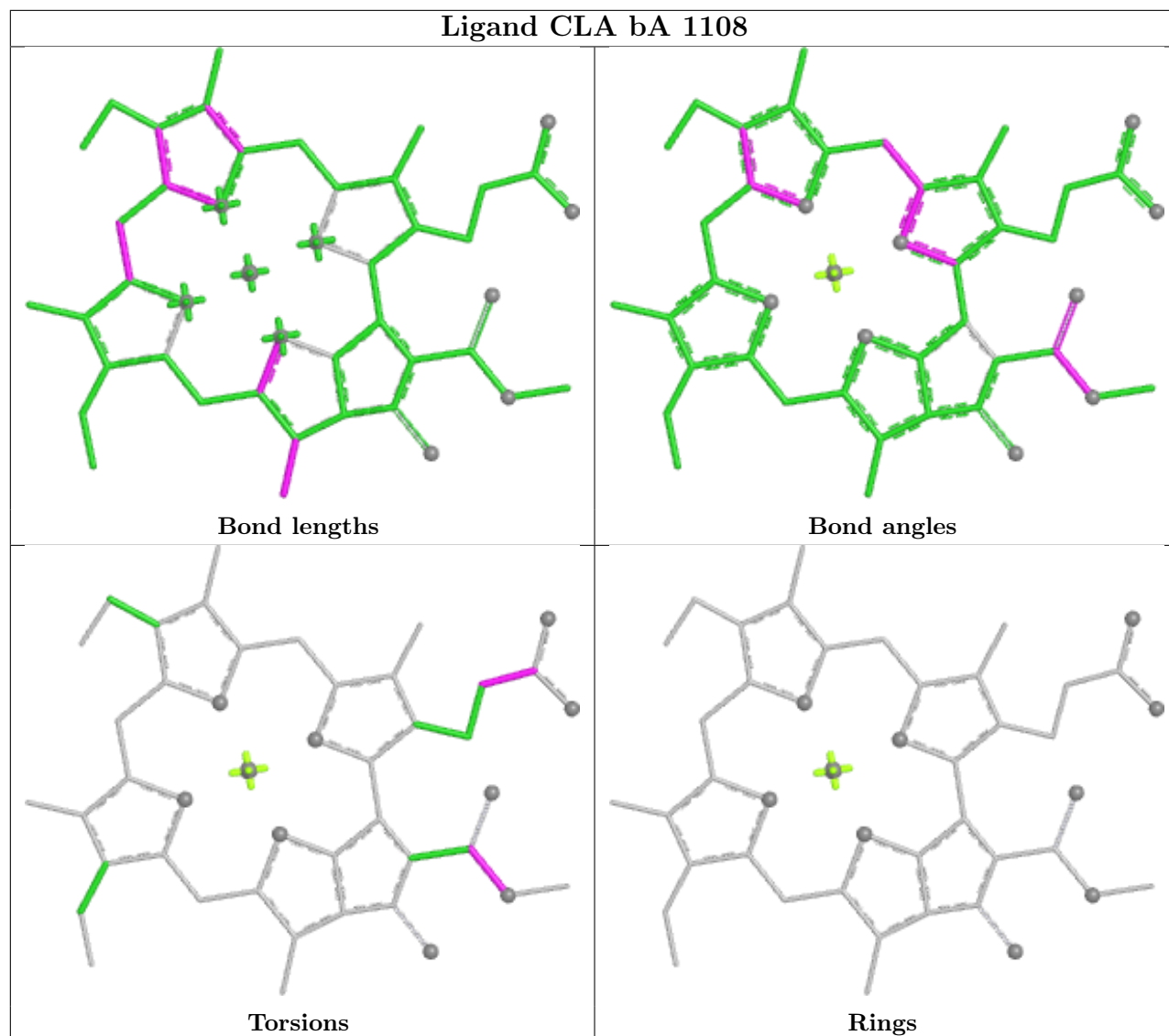
Ligand CLA c1 509	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA b5 502	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR c2 523	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

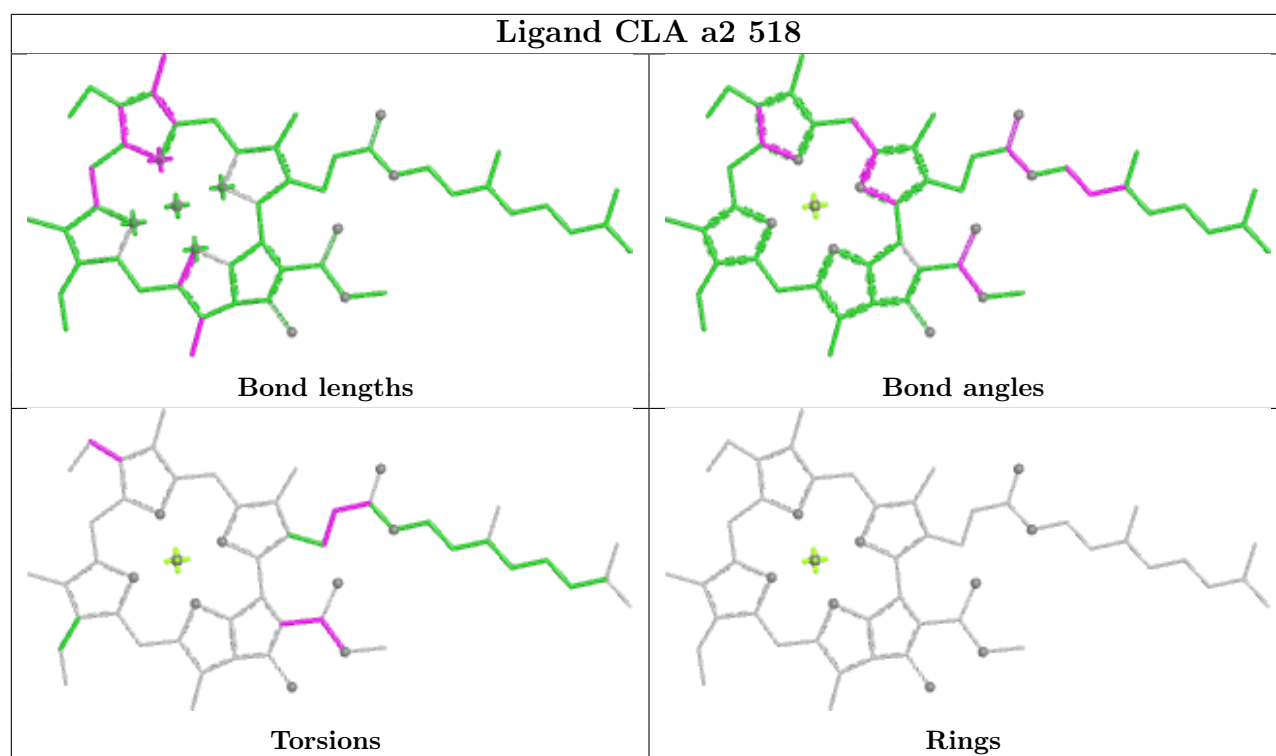




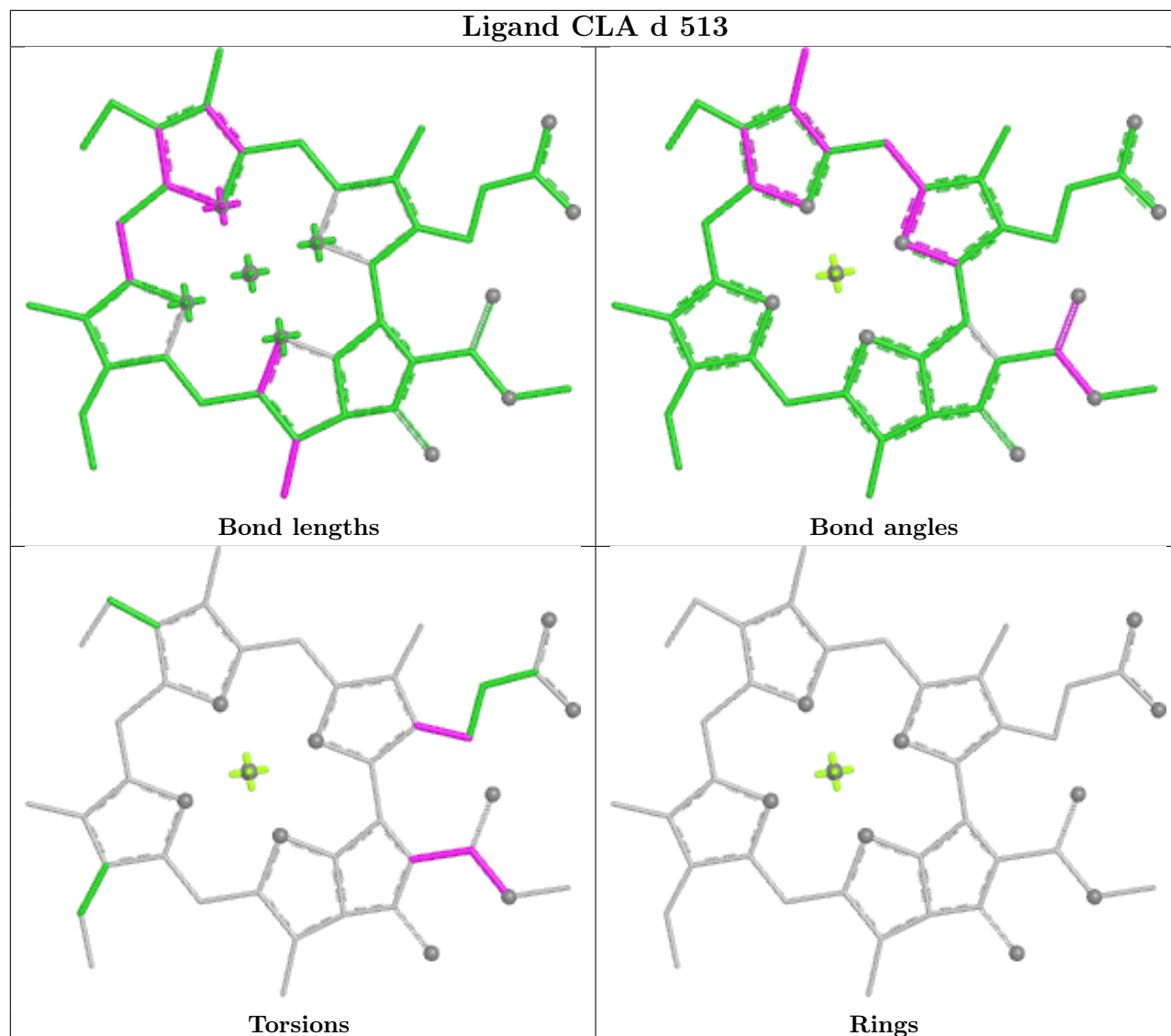


Ligand CLA bA 1108

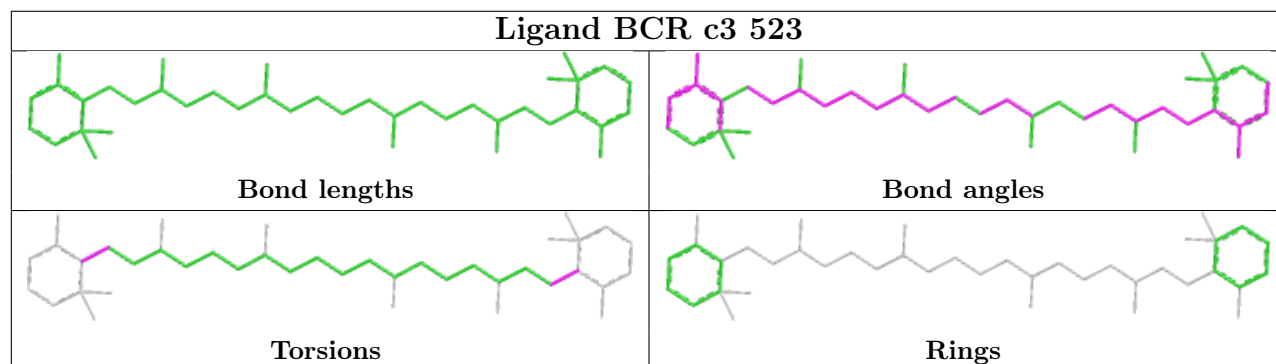


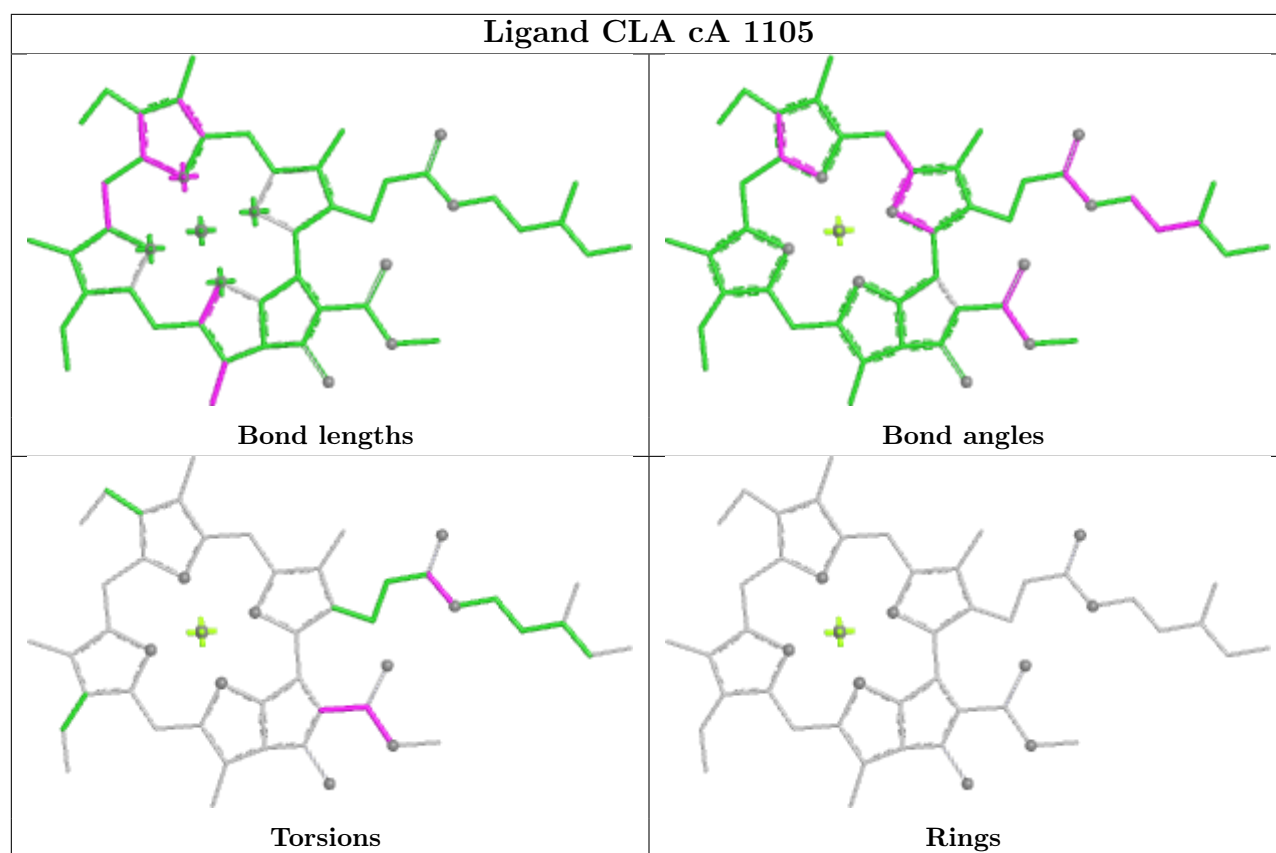


Ligand CLA d 513

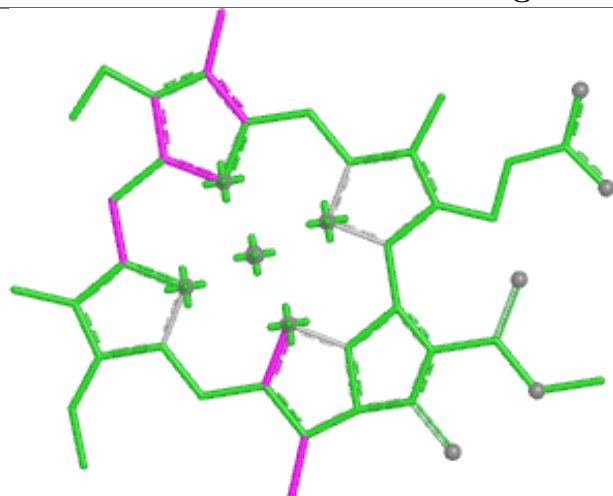


Ligand BCR c3 523





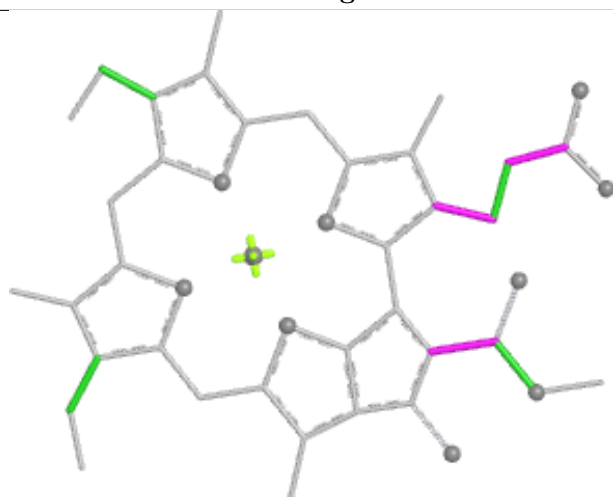
Ligand CLA U 519



Bond lengths



Bond angles

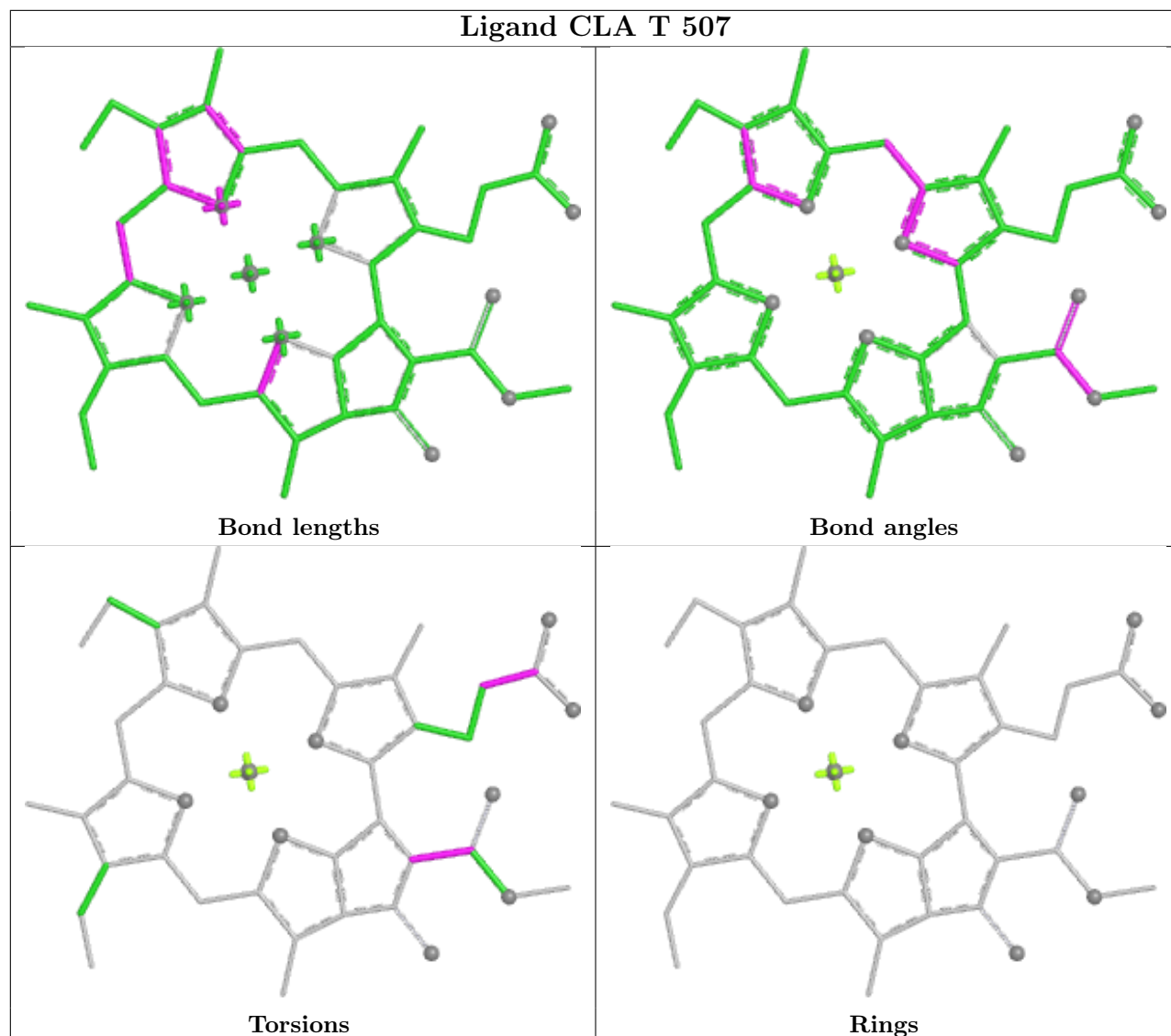


Torsions

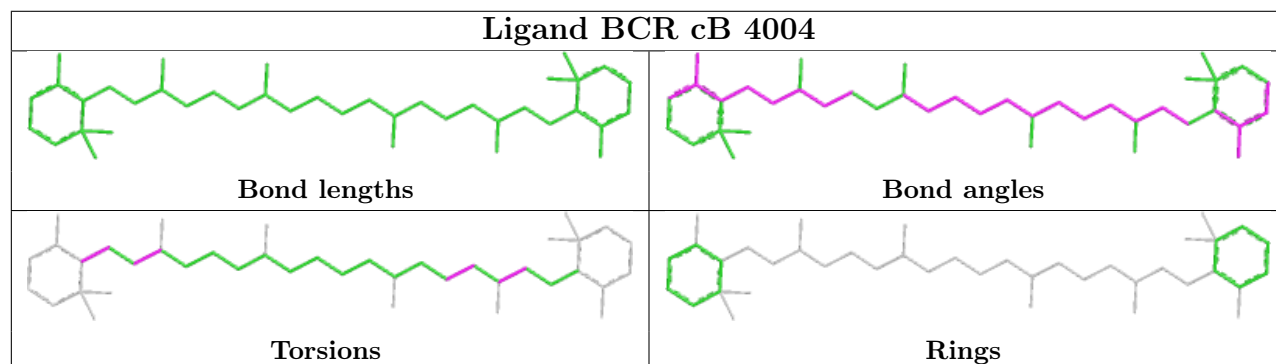


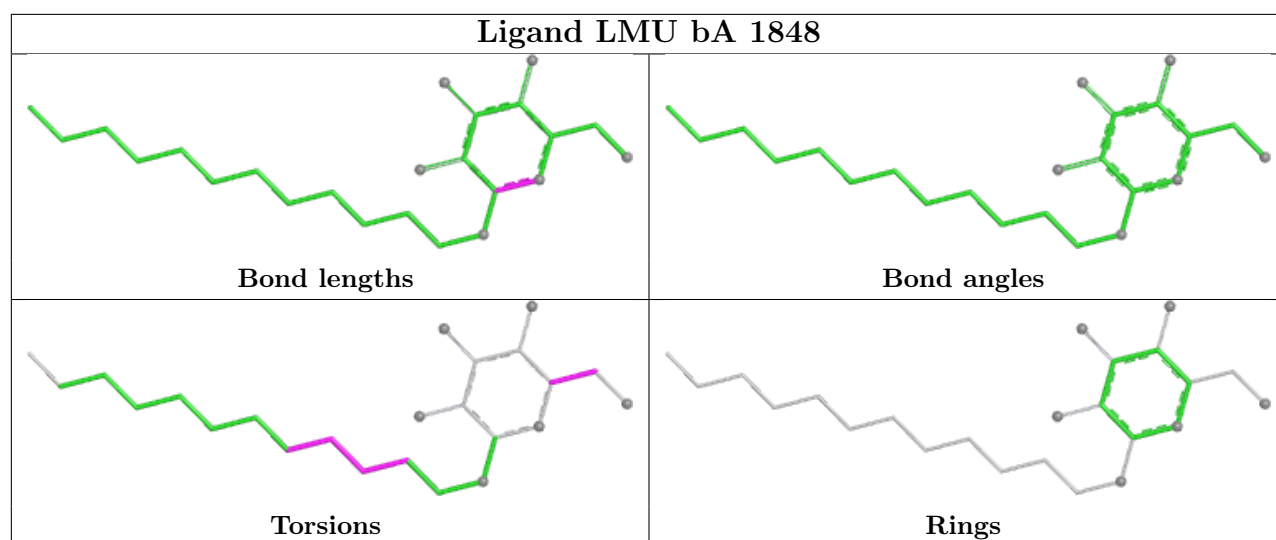
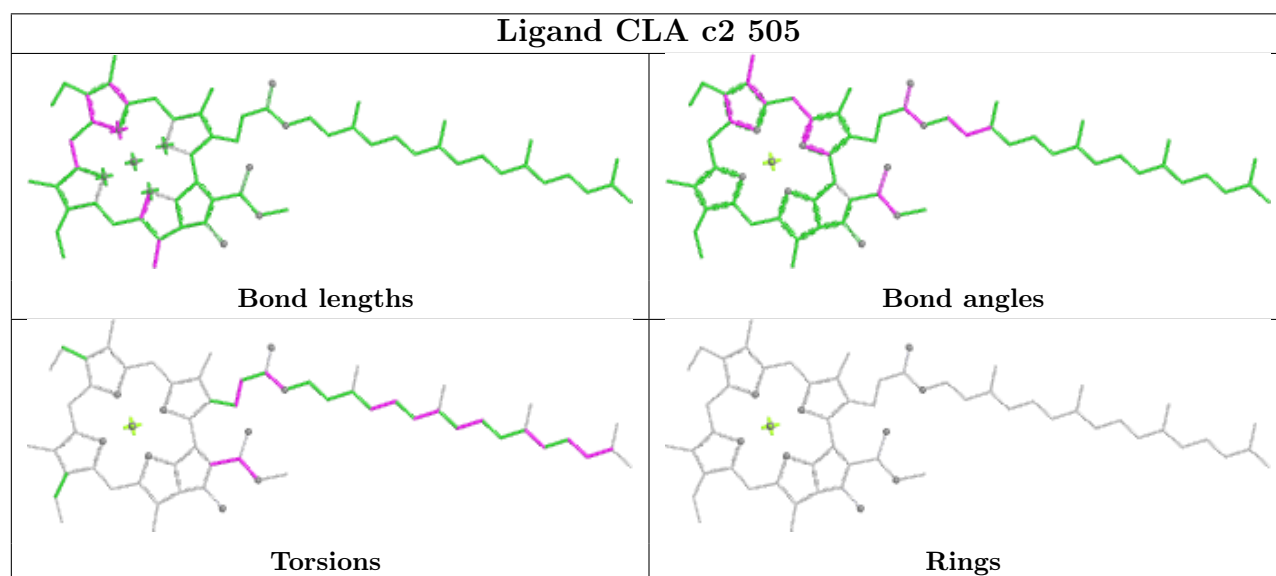
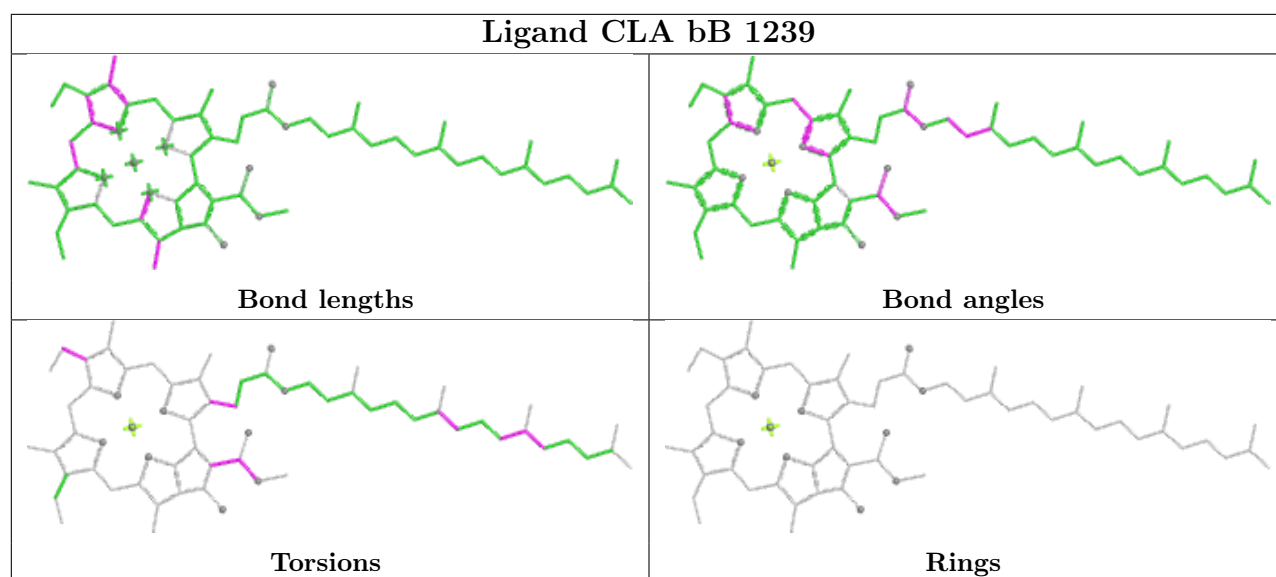
Rings

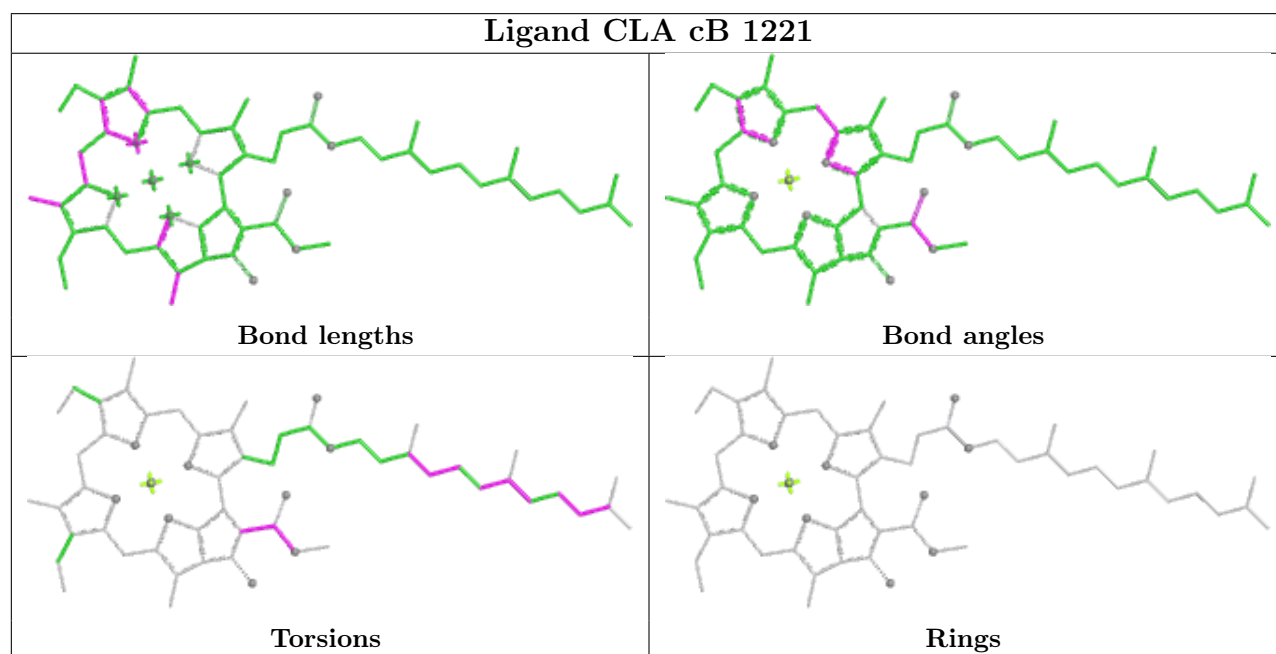
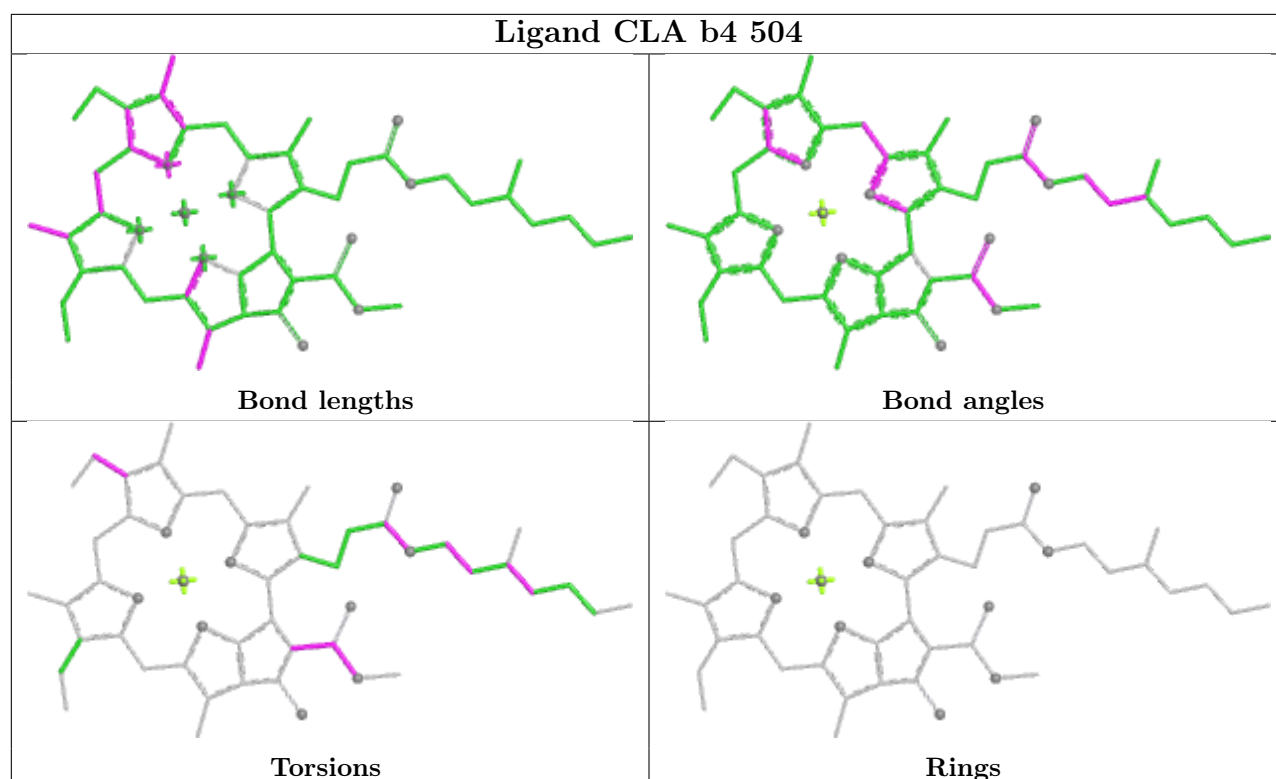
Ligand CLA T 507



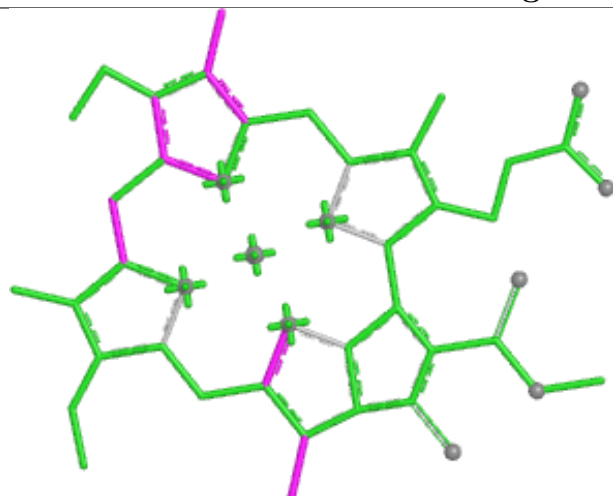
Ligand BCR cB 4004







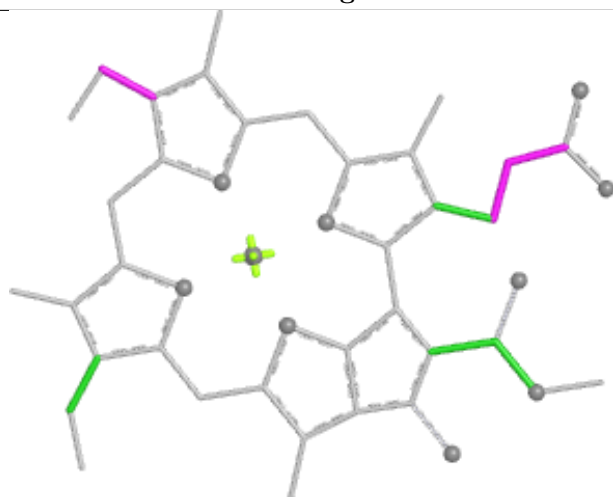
Ligand CLA i 504



Bond lengths



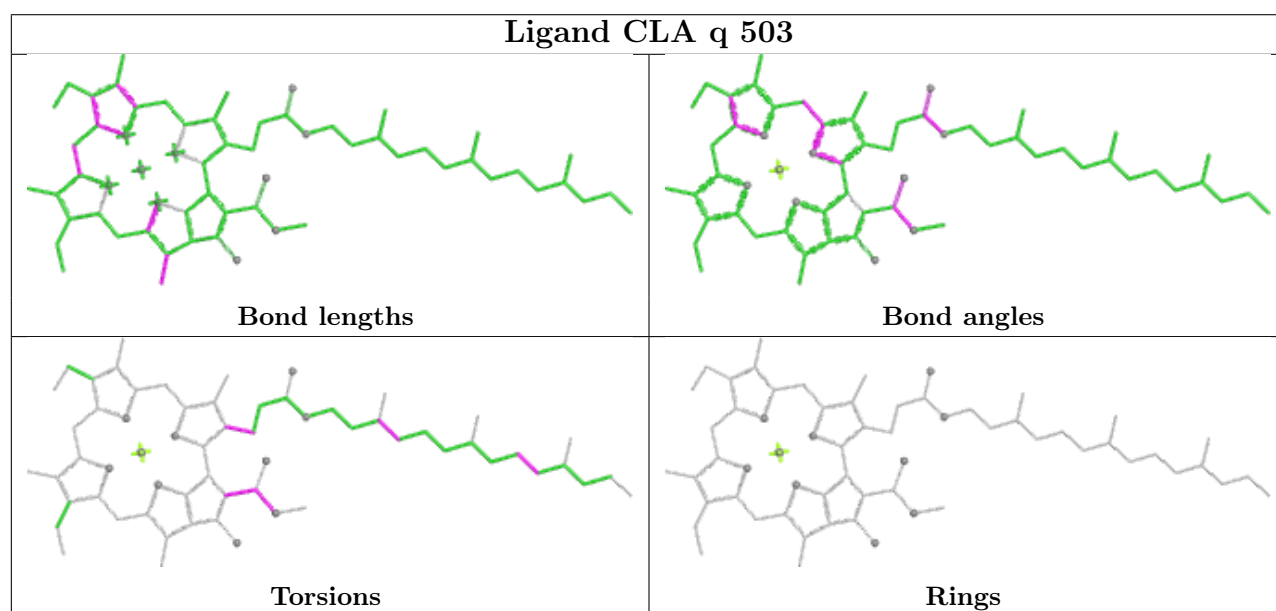
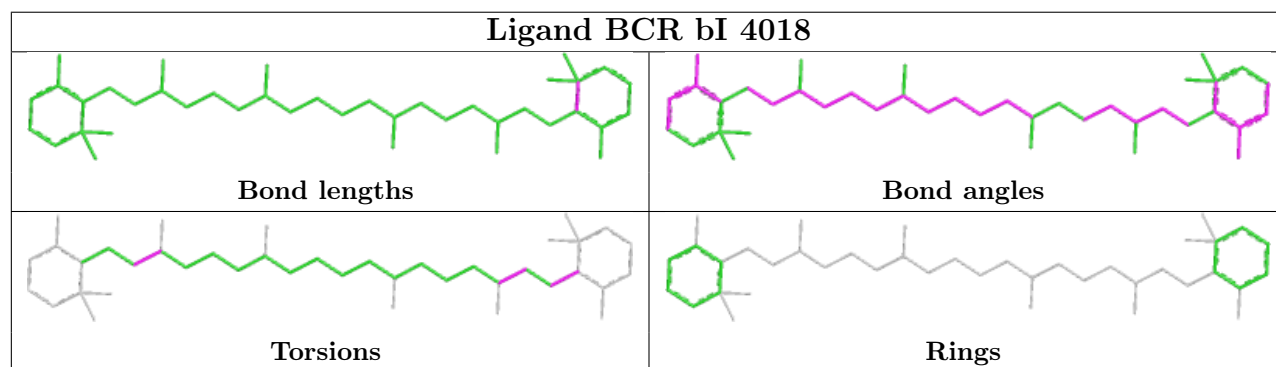
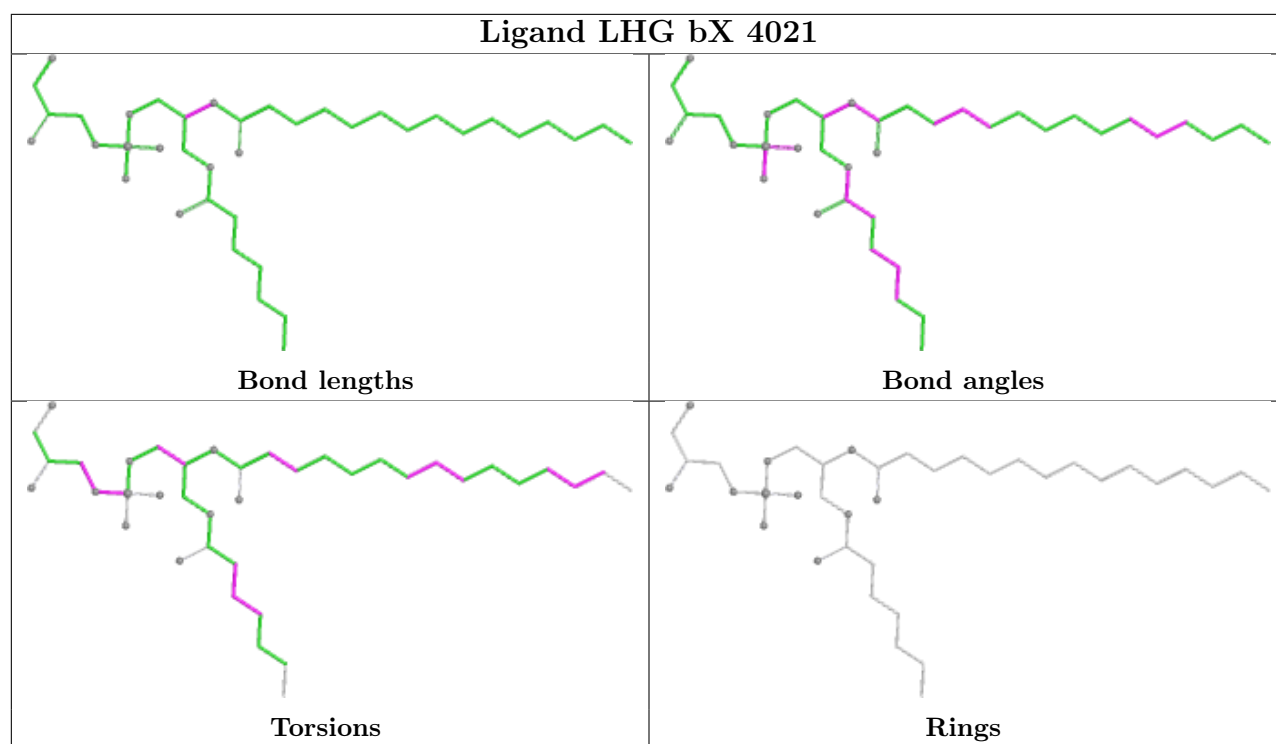
Bond angles

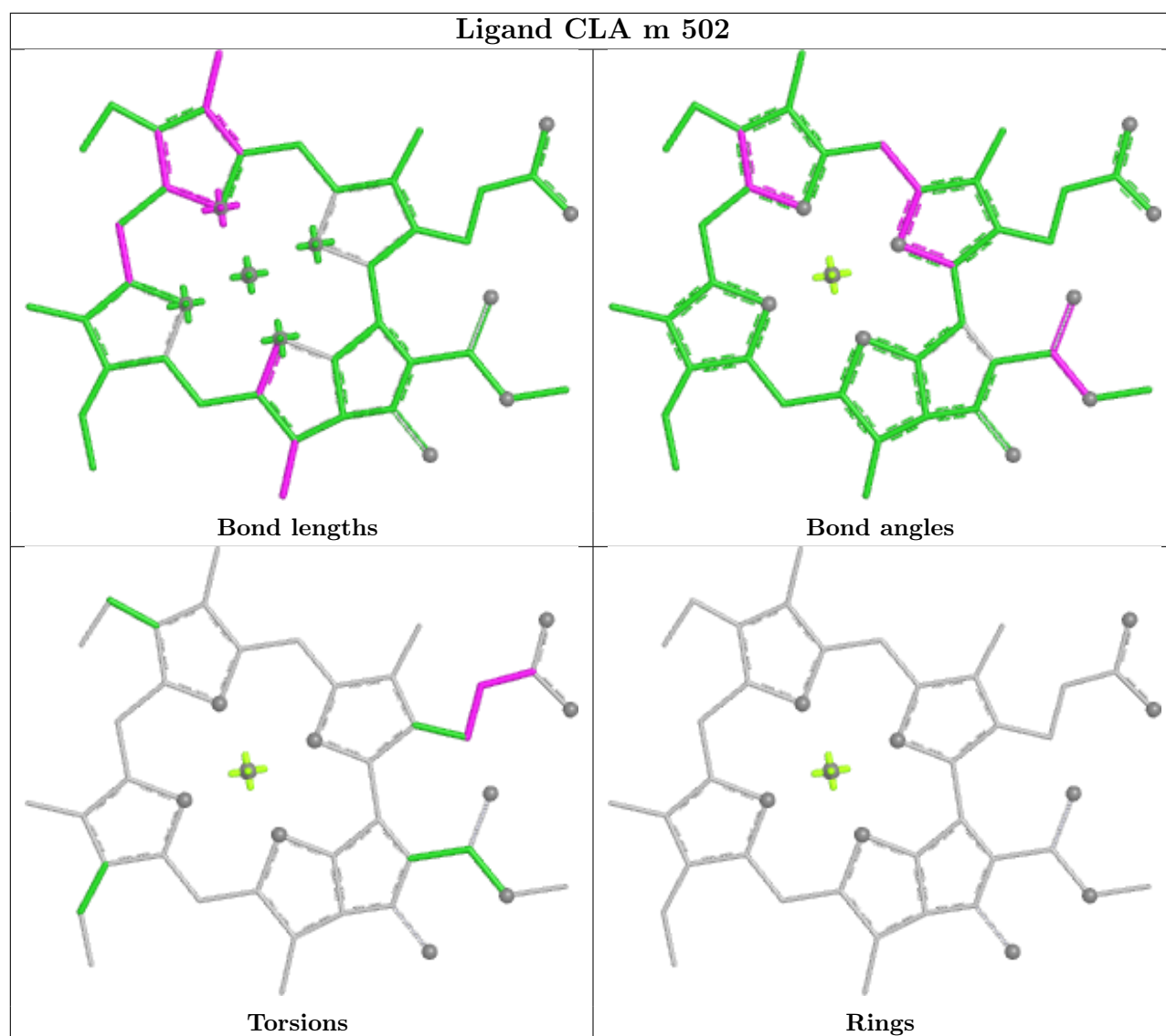


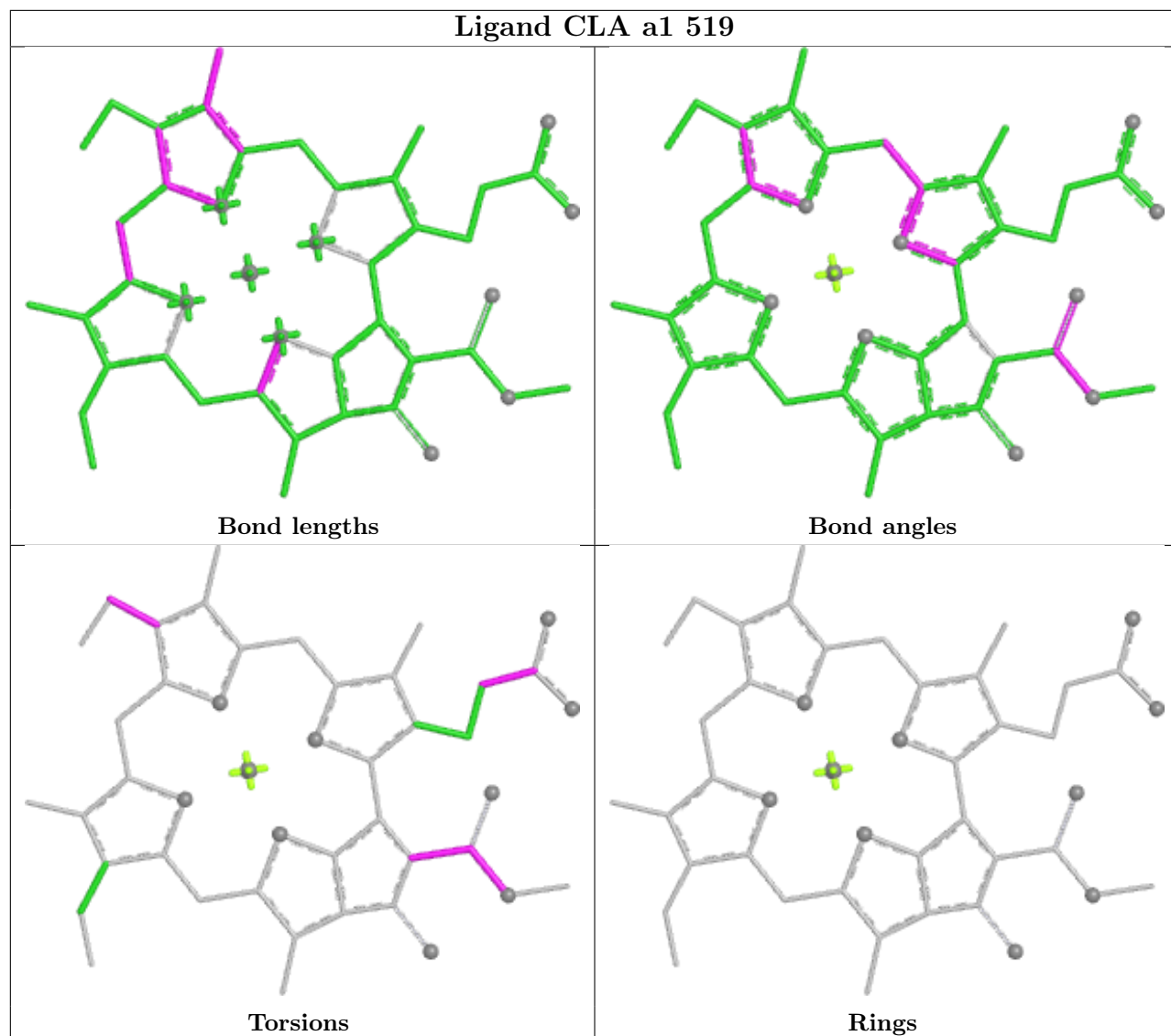
Torsions



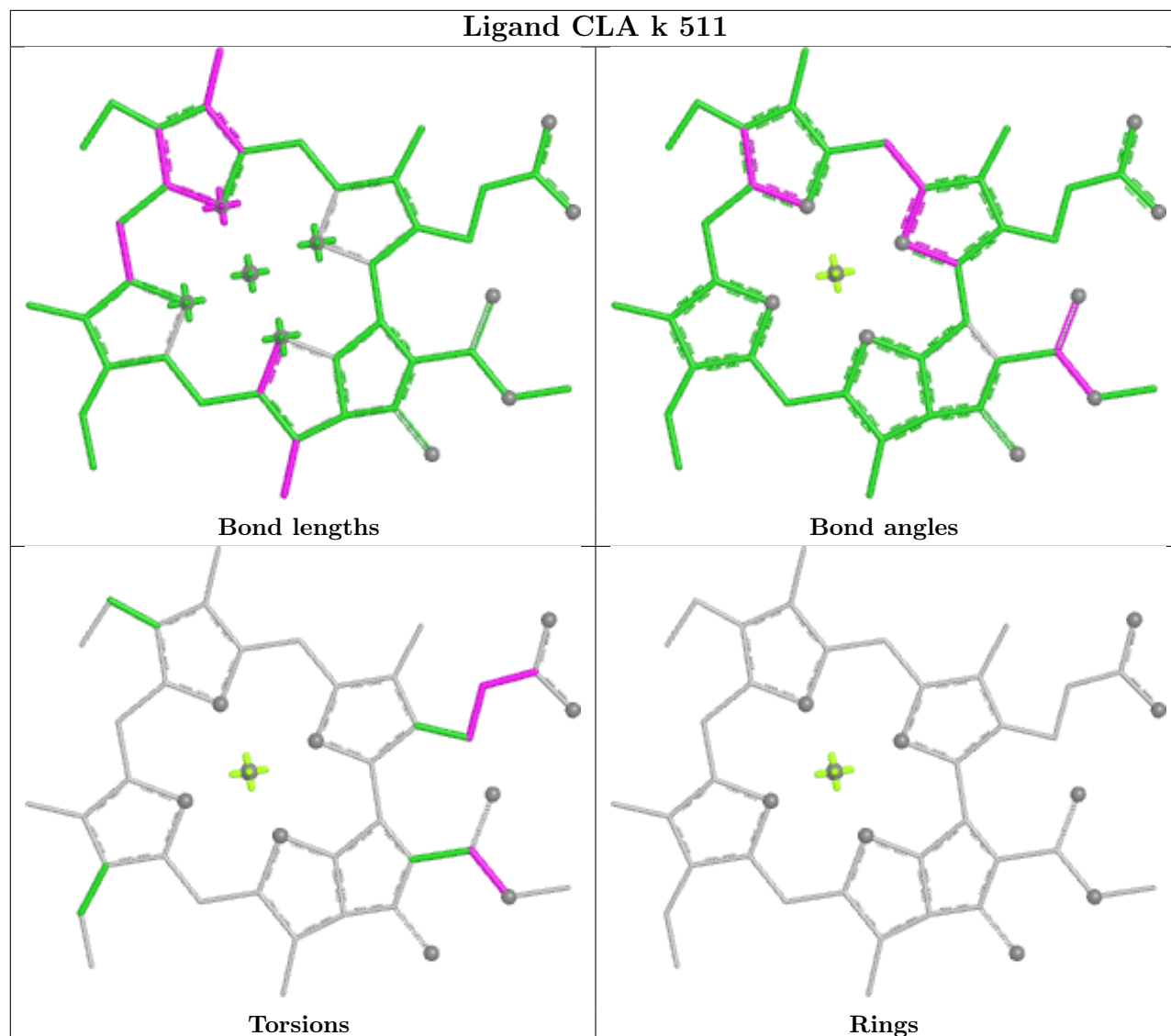
Rings



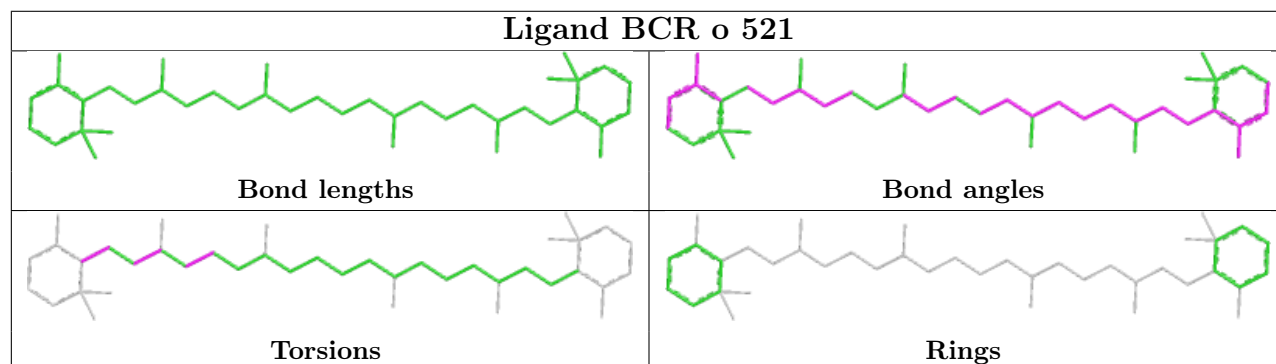




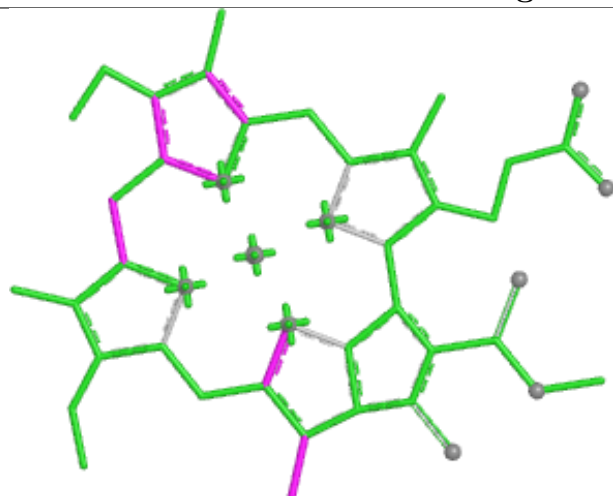
Ligand CLA k 511



Ligand BCR o 521



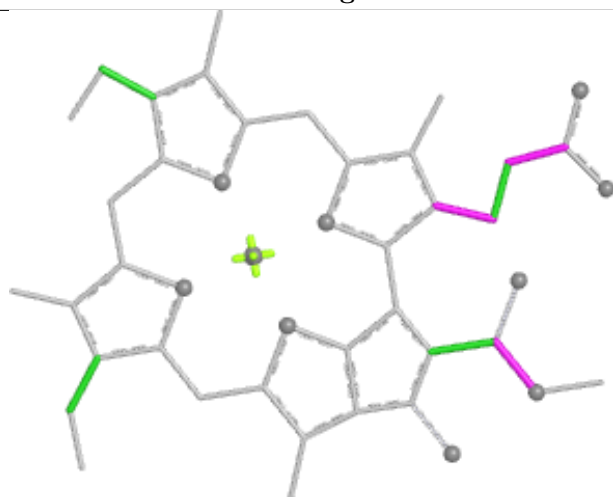
Ligand CLA Z 511



Bond lengths



Bond angles

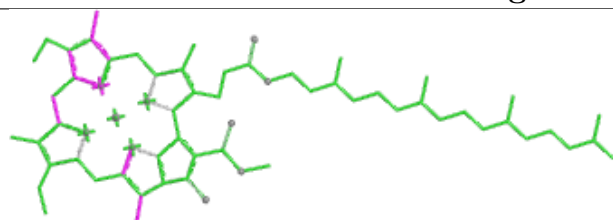


Torsions

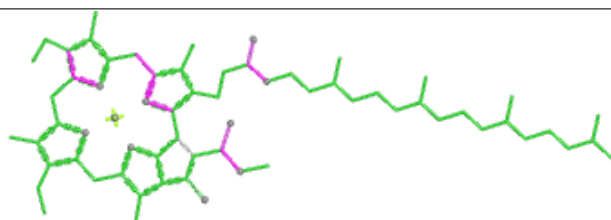


Rings

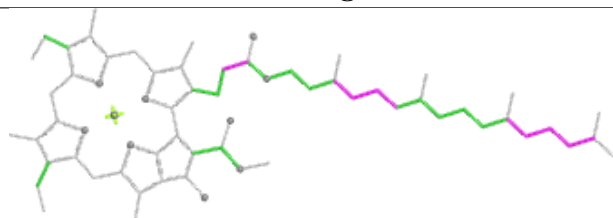
Ligand CLA W 510



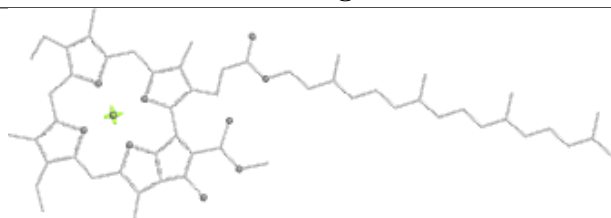
Bond lengths



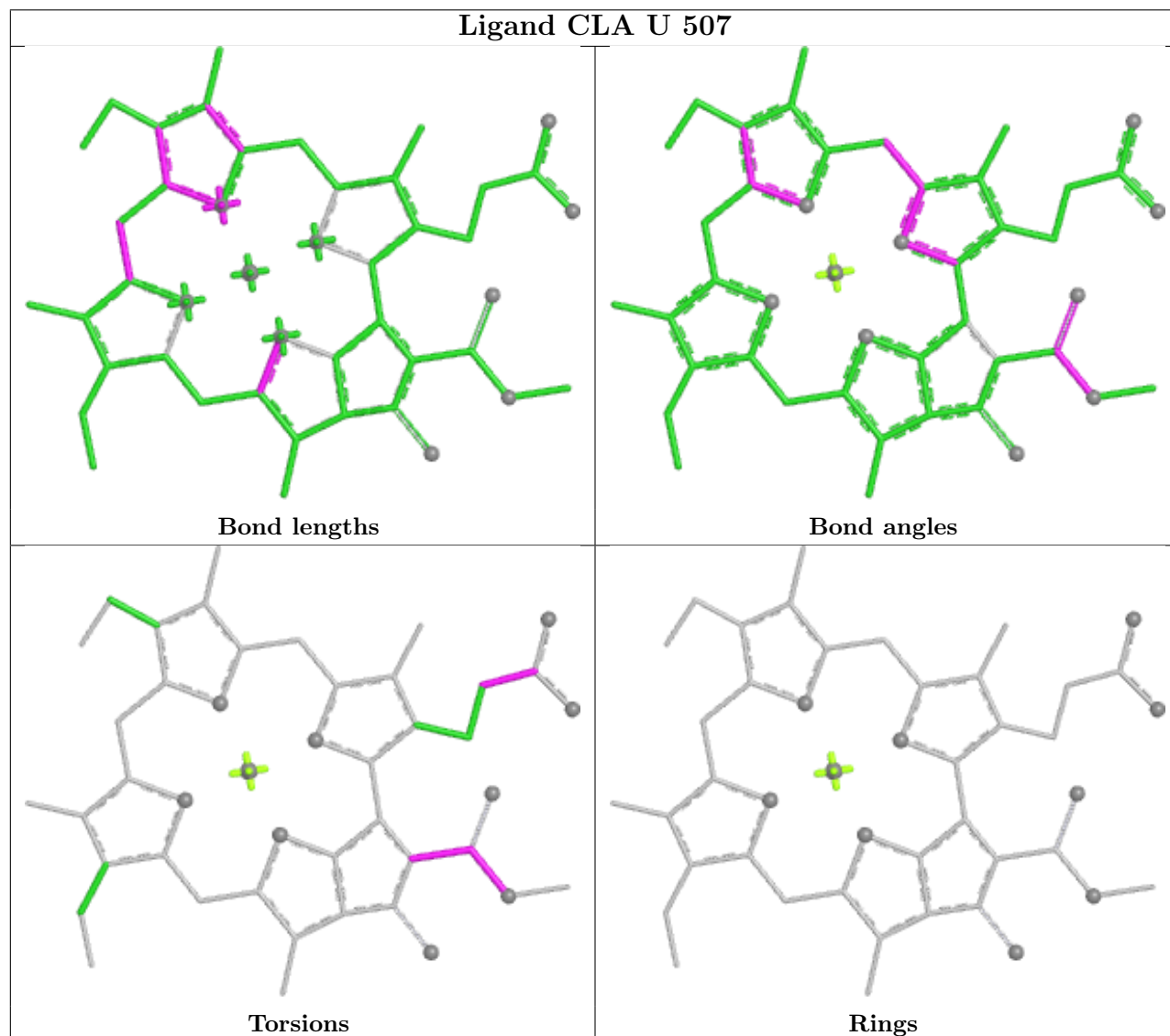
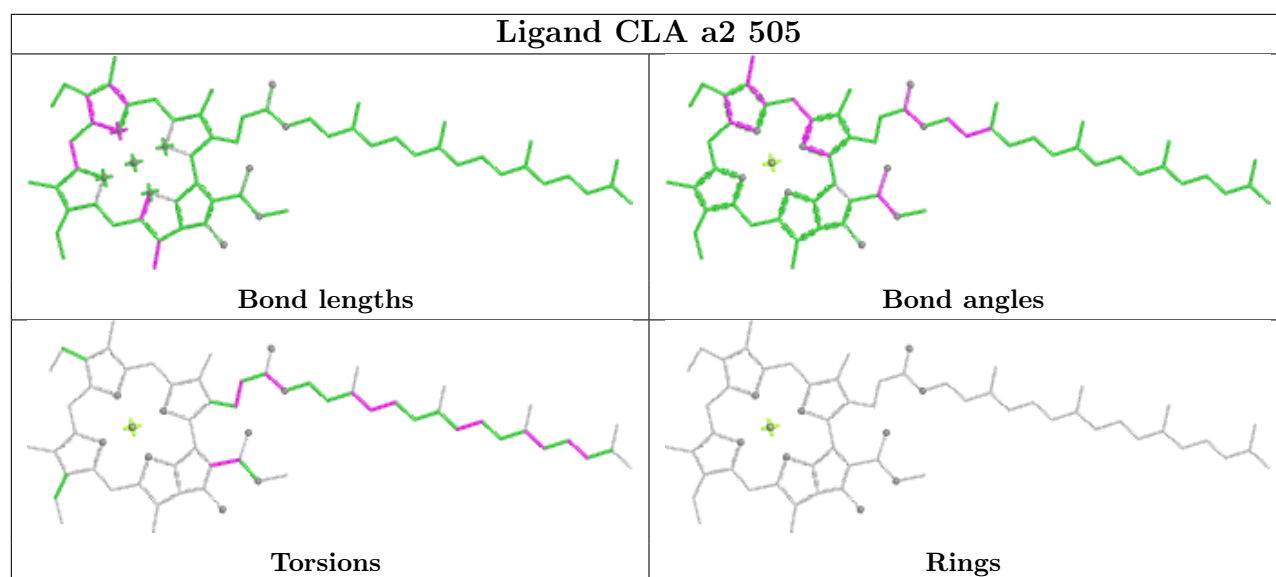
Bond angles



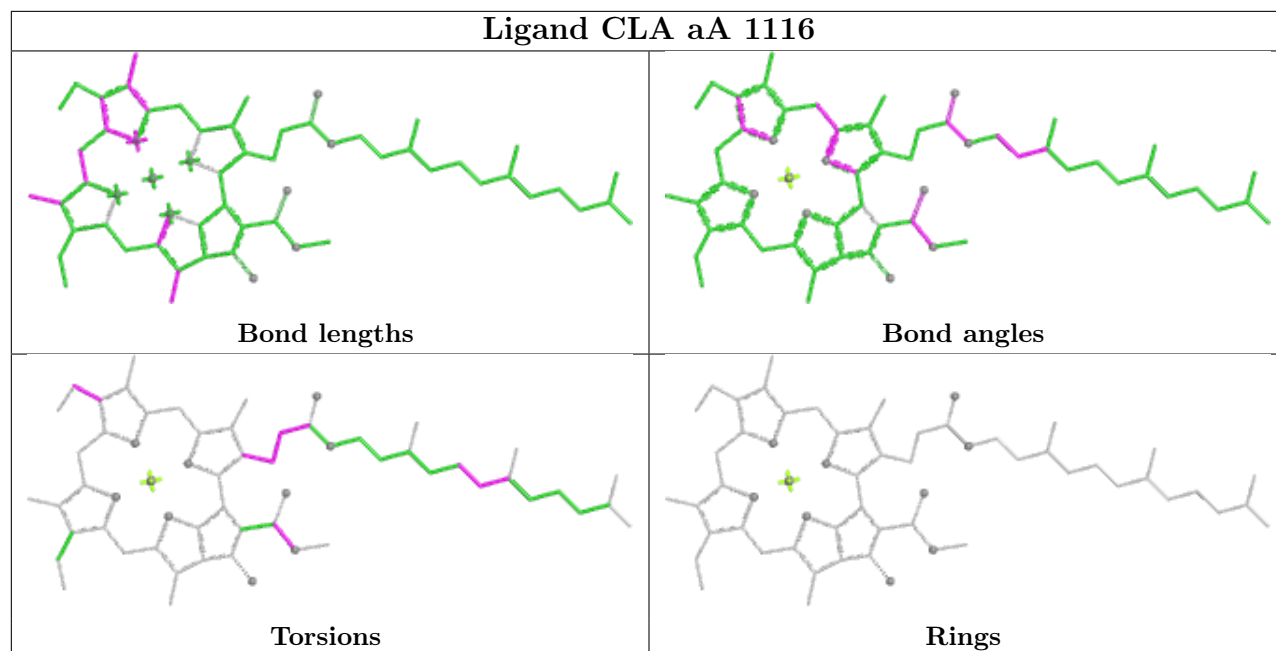
Torsions



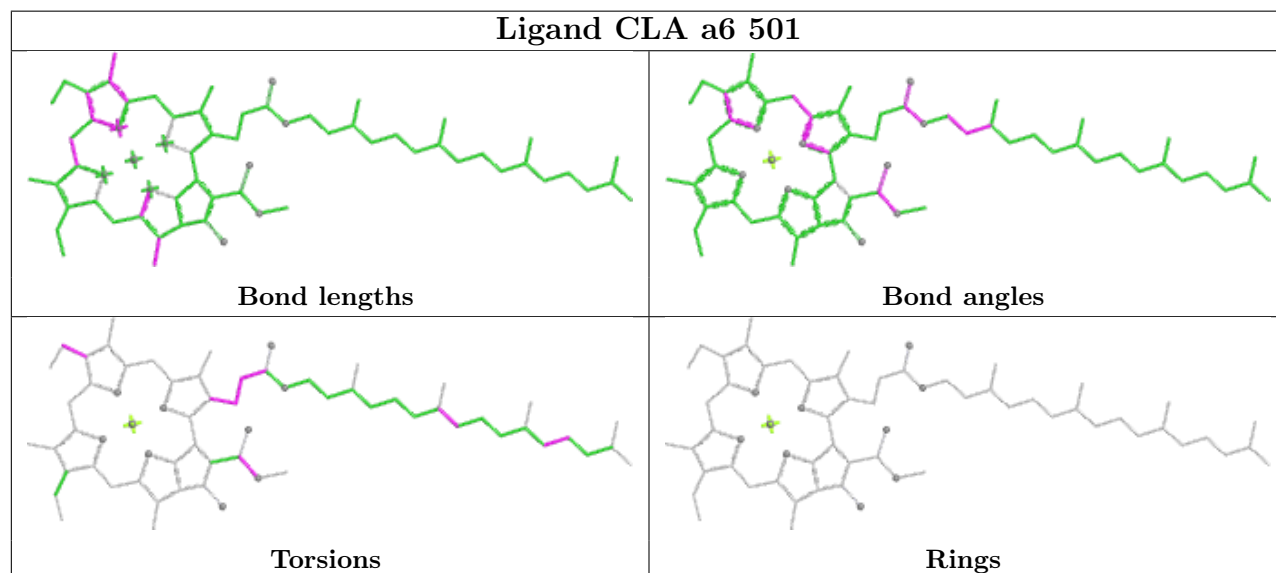
Rings

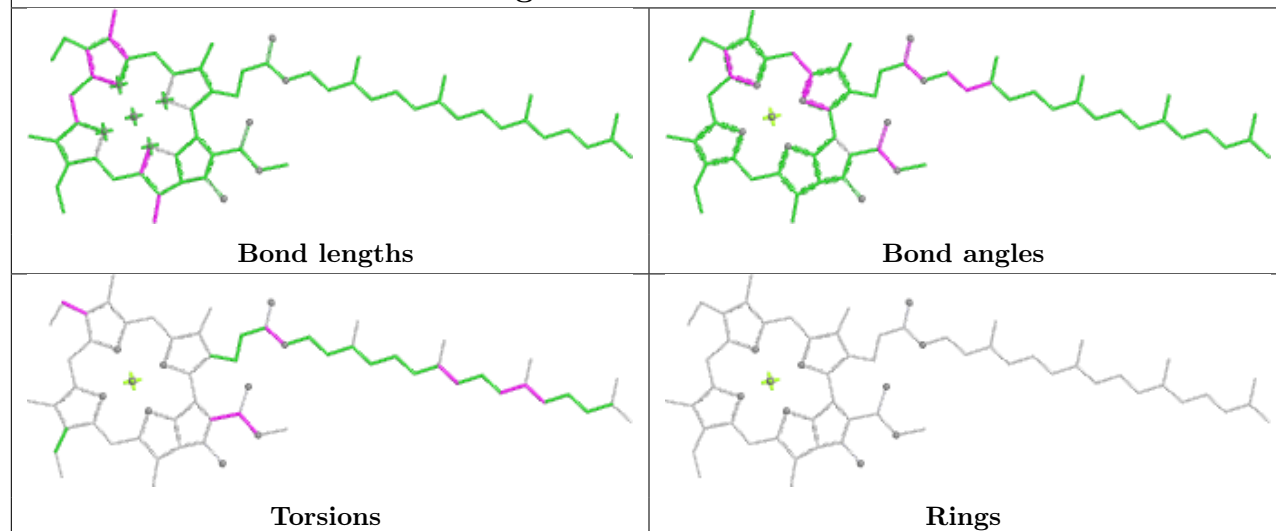
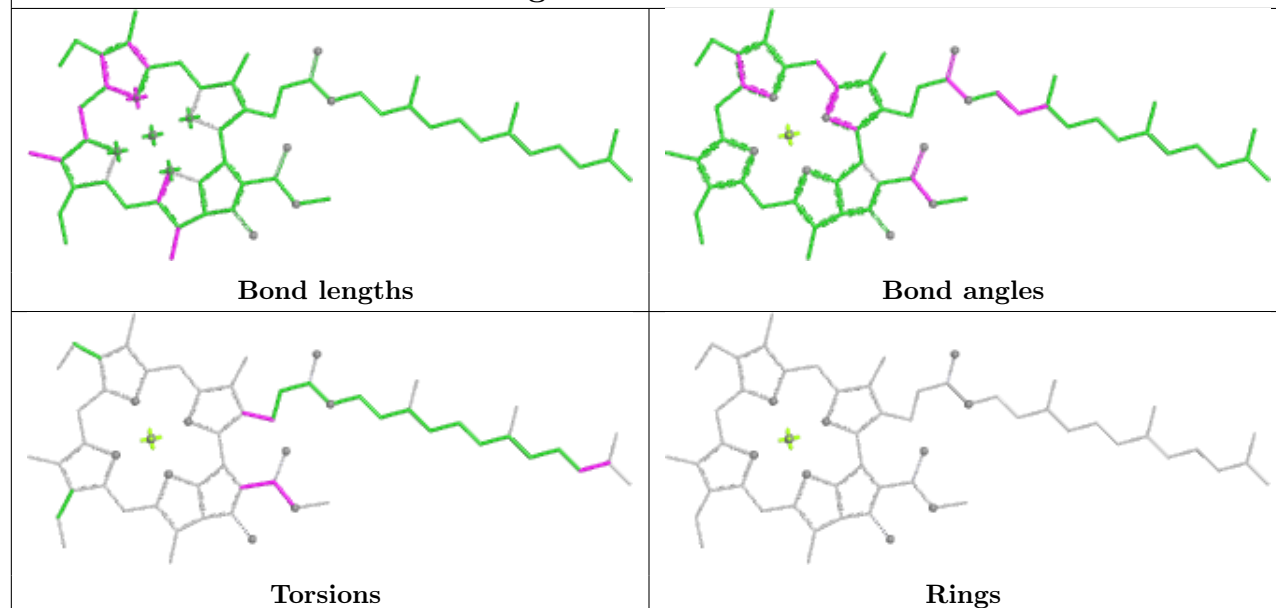


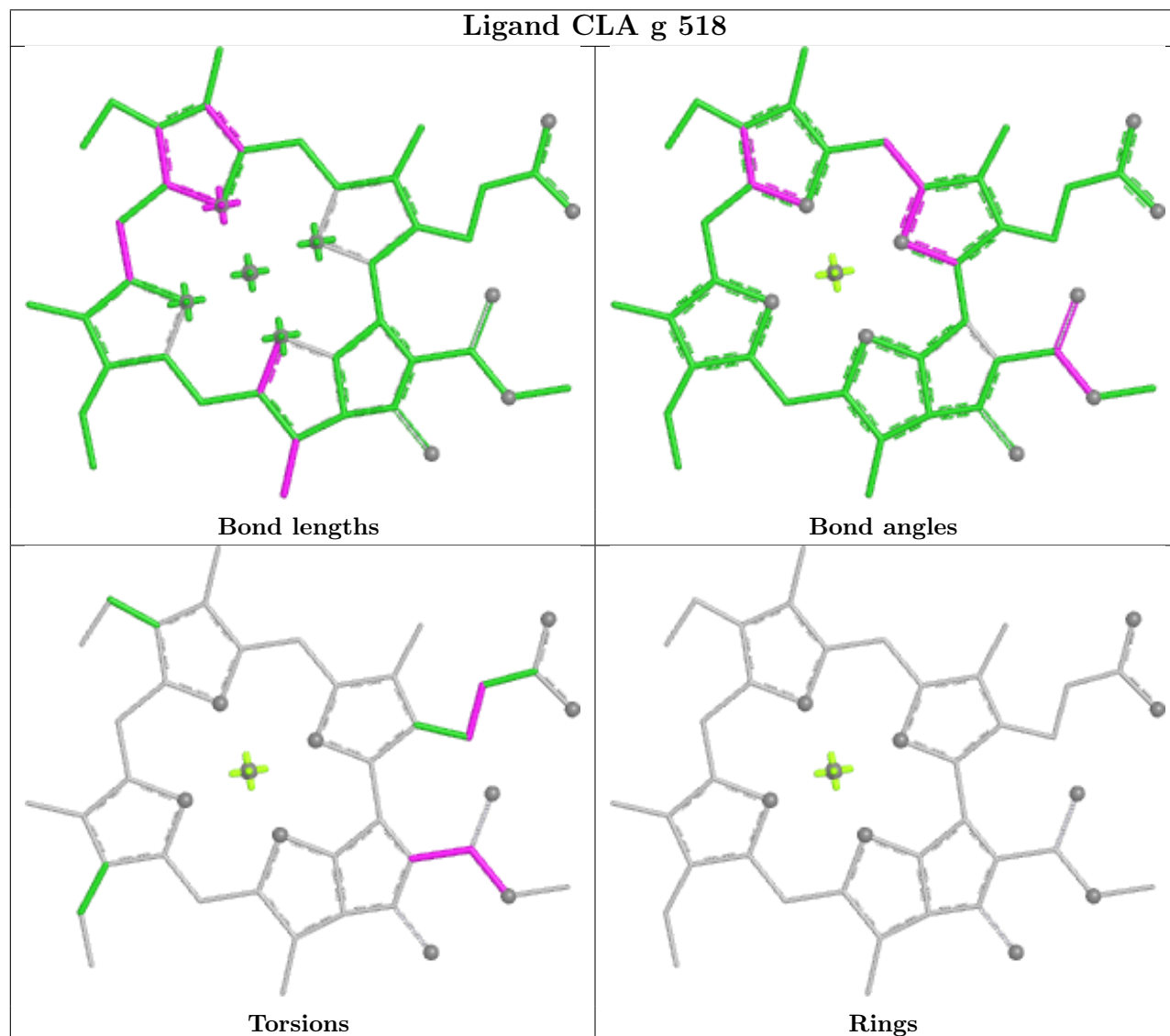
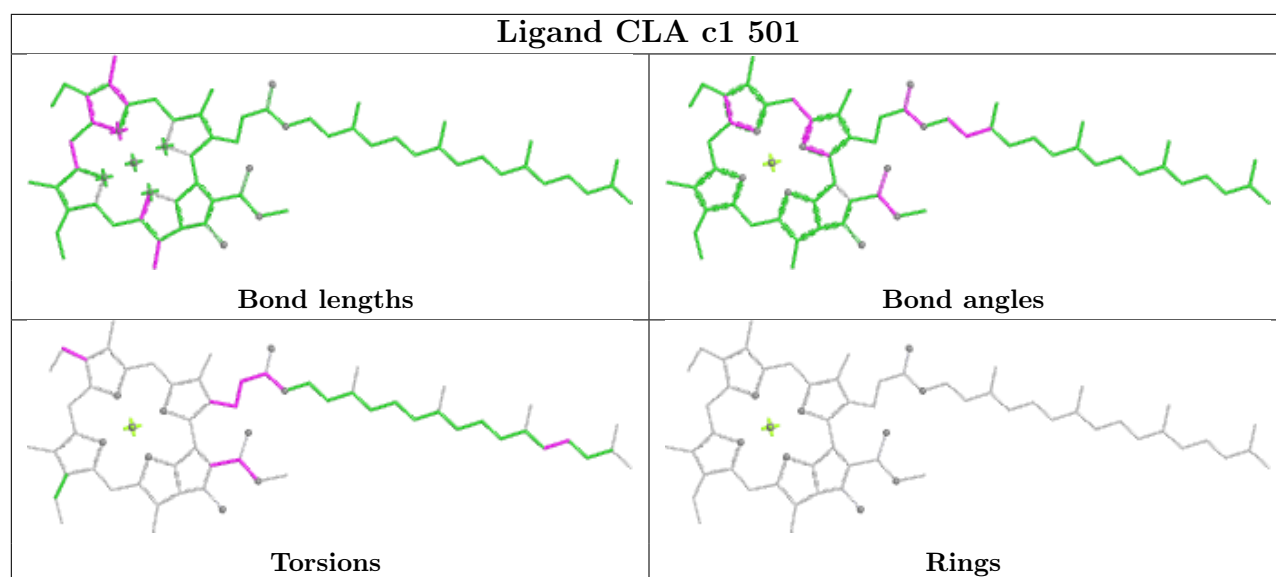
Ligand CLA aA 1116



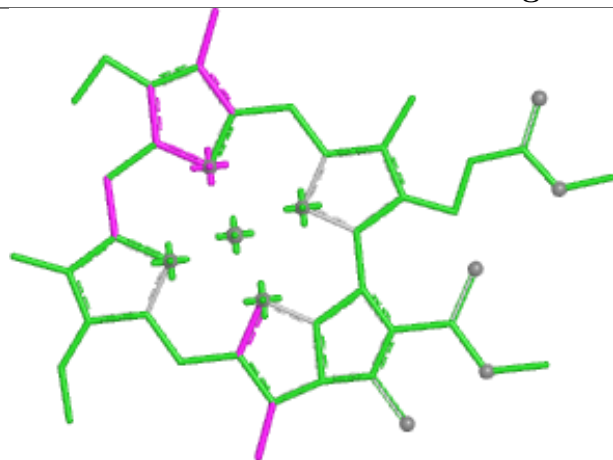
Ligand CLA a6 501



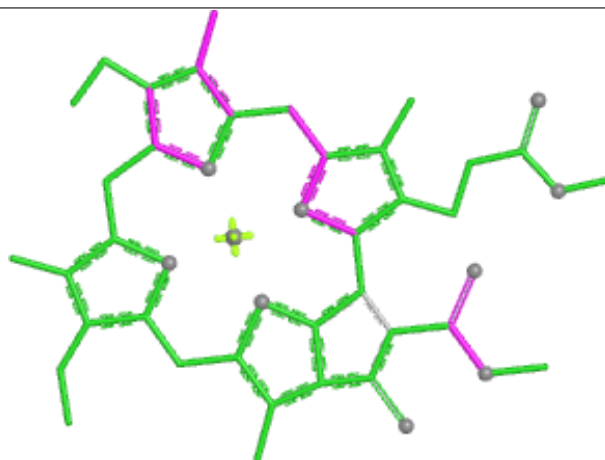
Ligand CLA cB 1239**Ligand CLA c5 507**



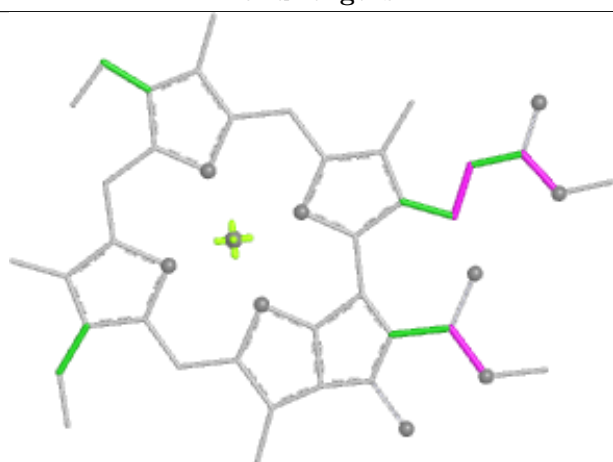
Ligand CLA 1 508



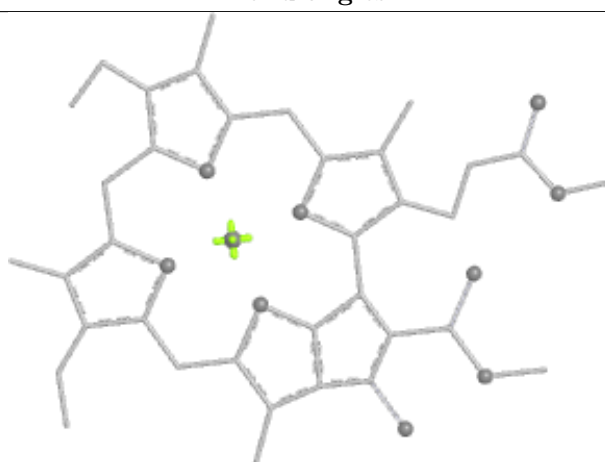
Bond lengths



Bond angles

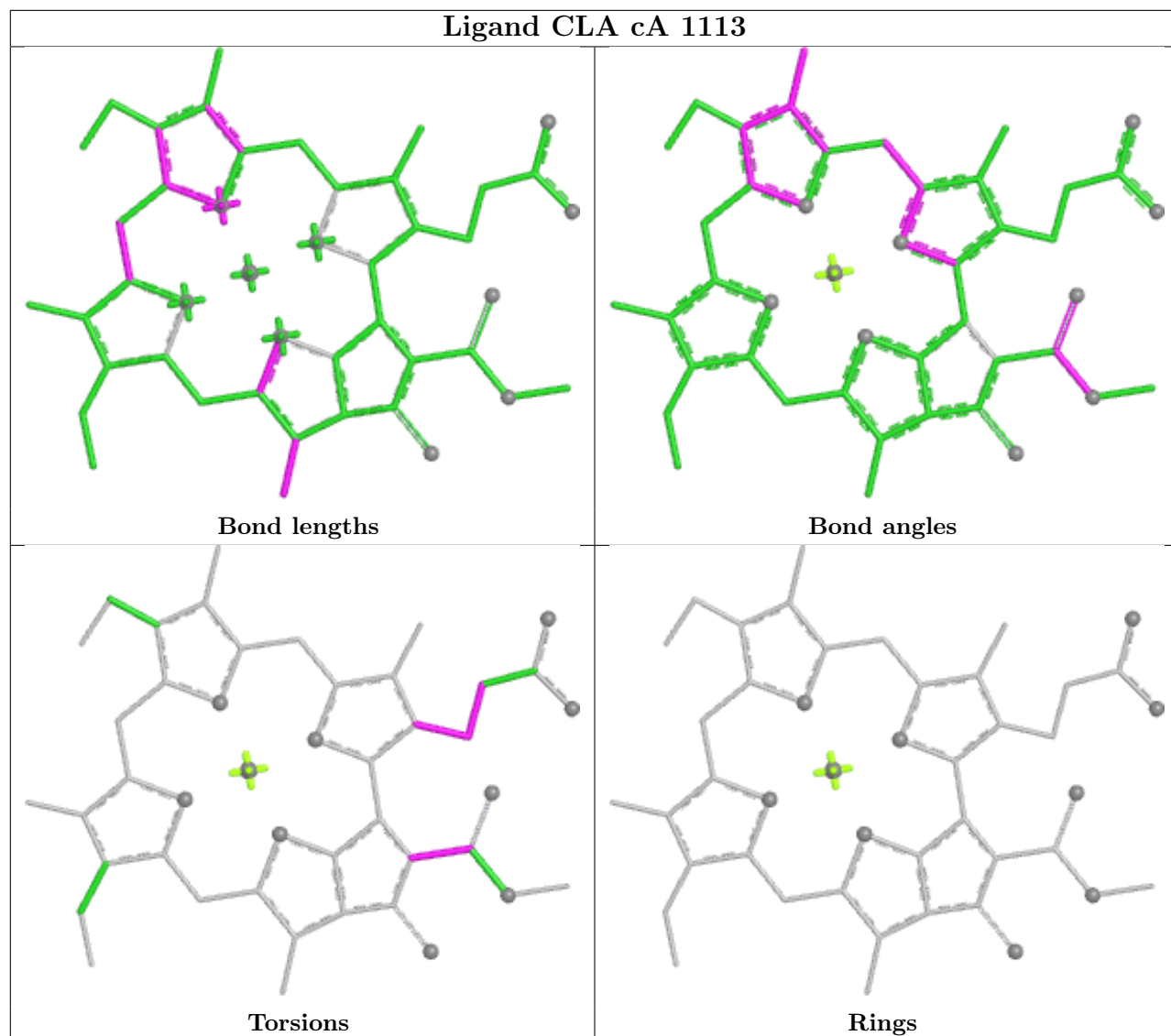


Torsions

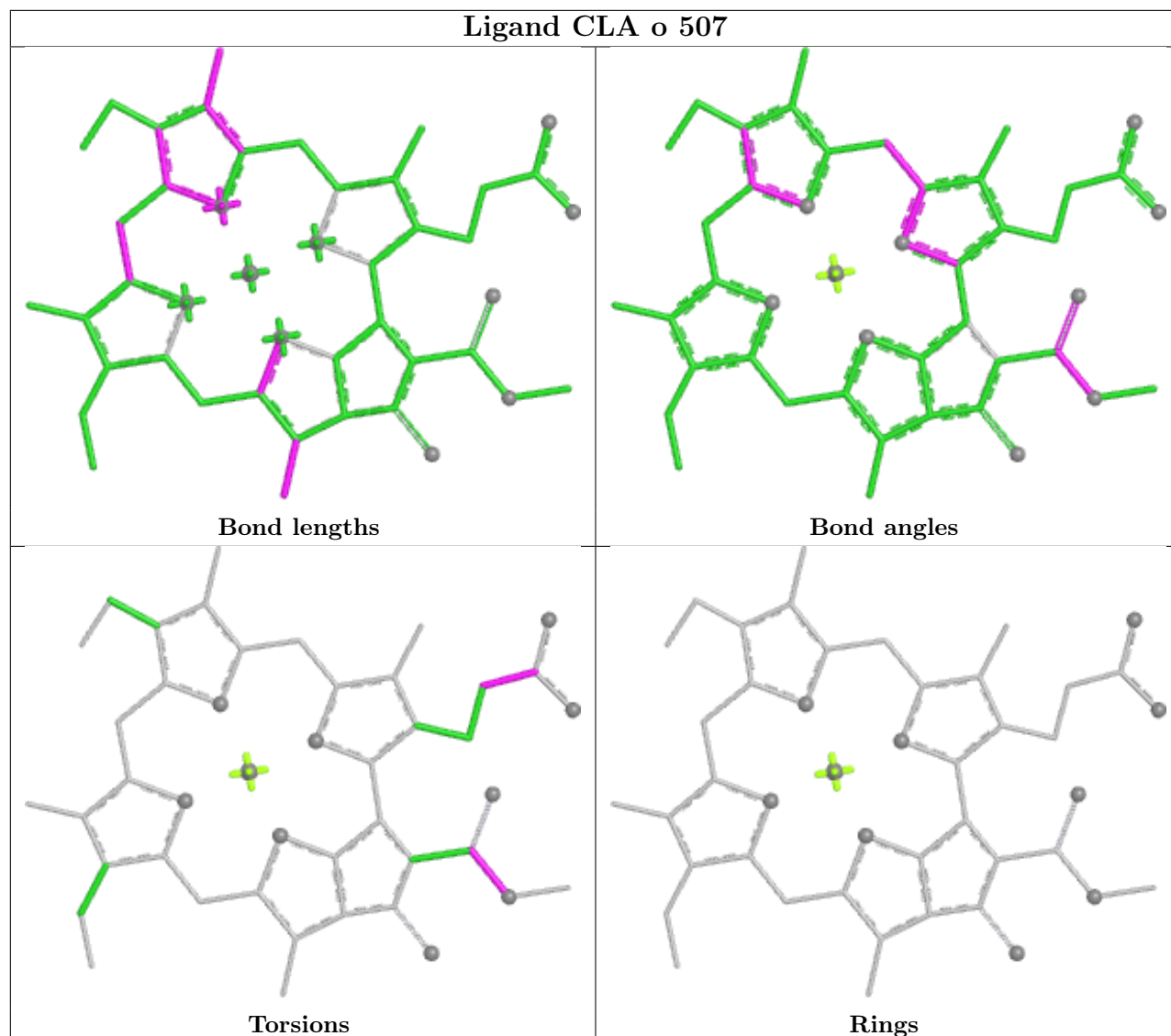


Rings

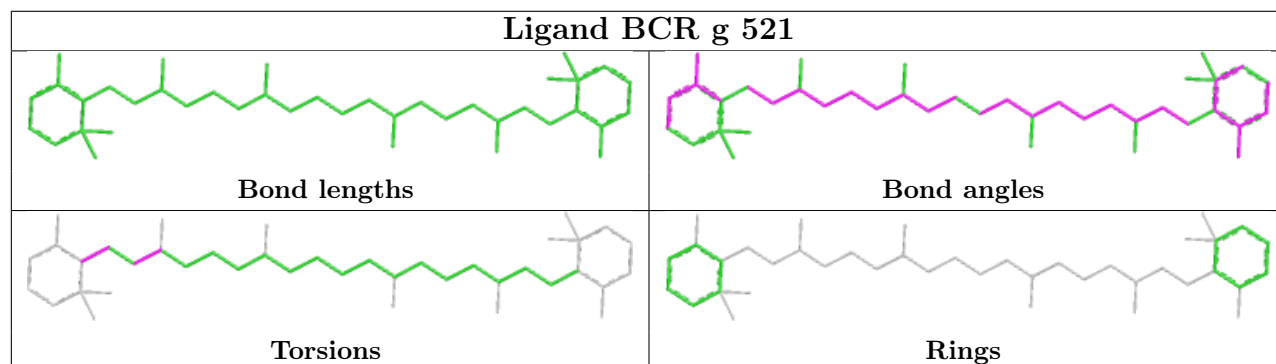
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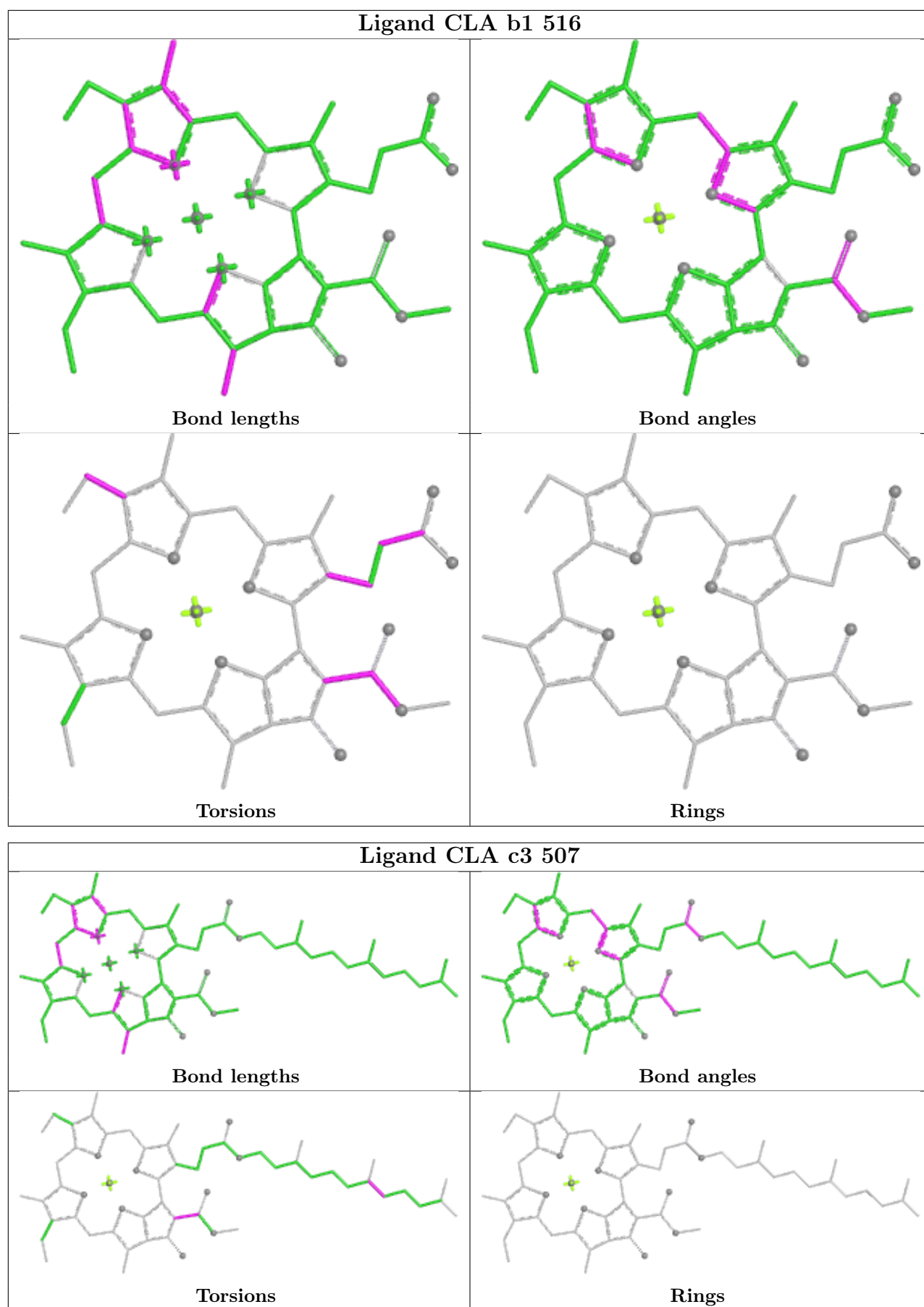


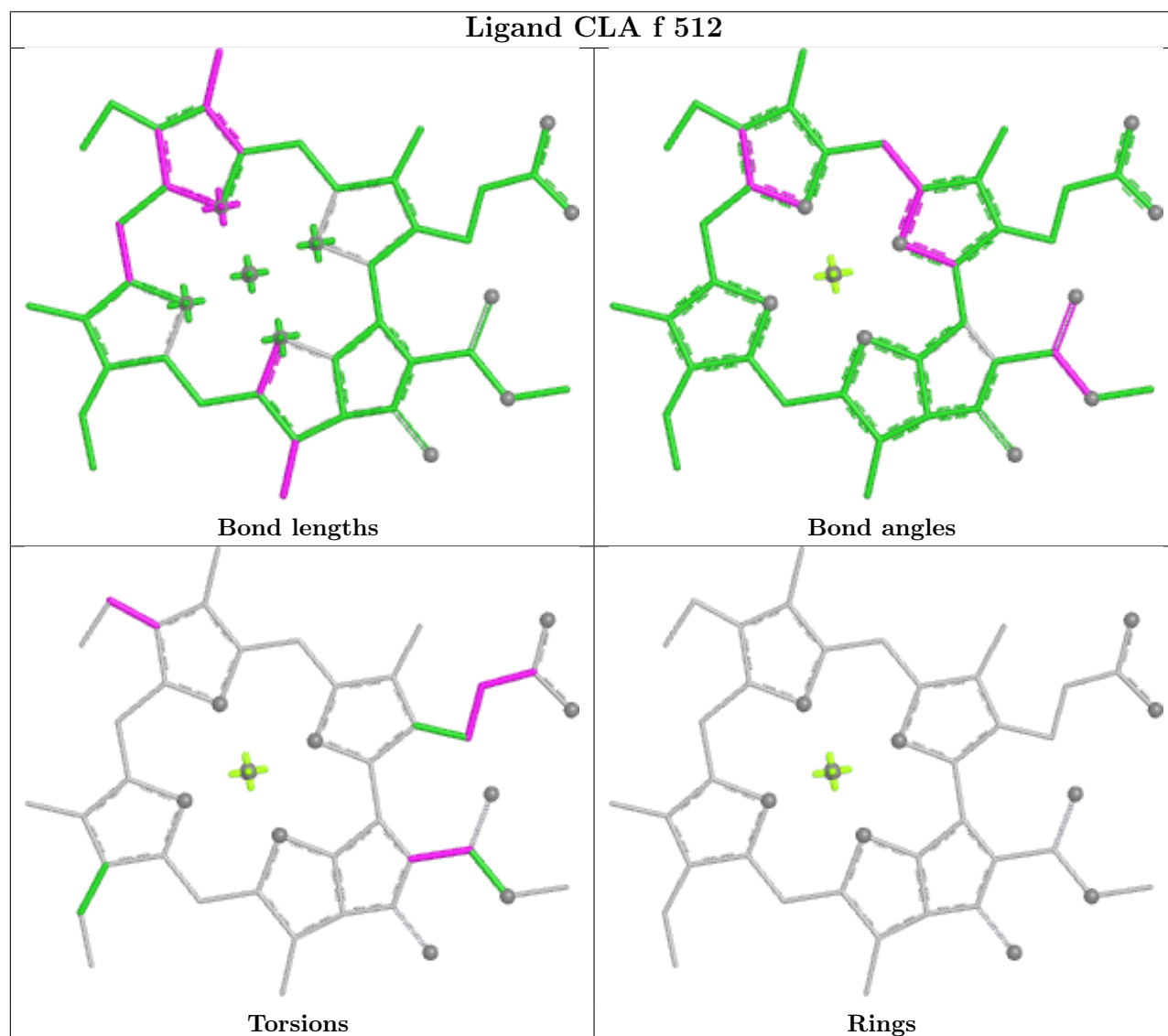
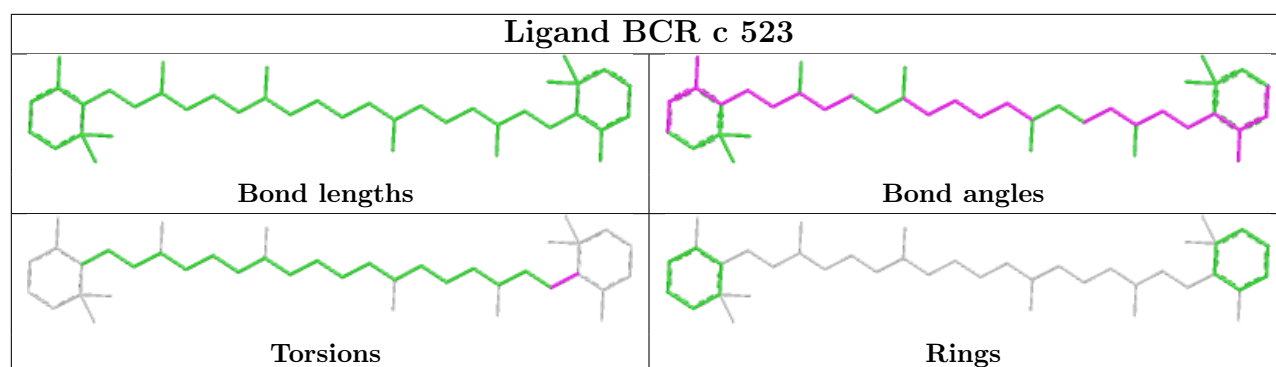
Ligand CLA o 507

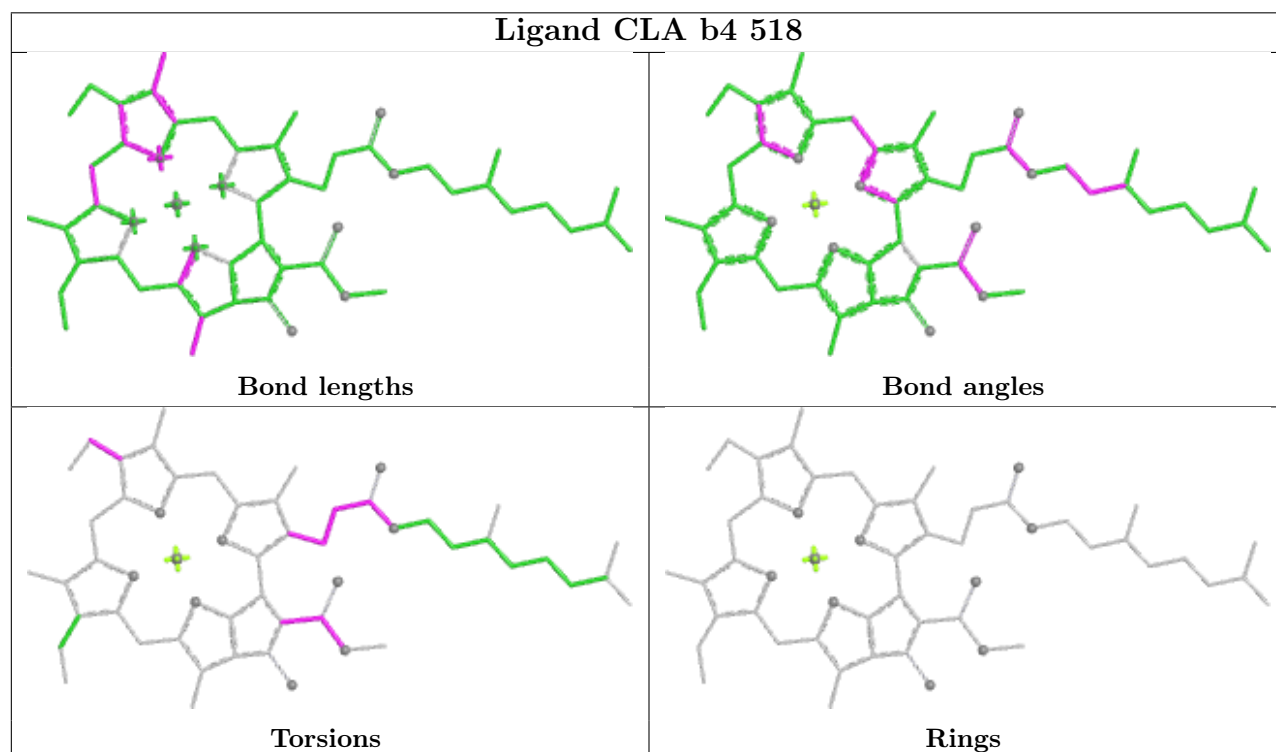
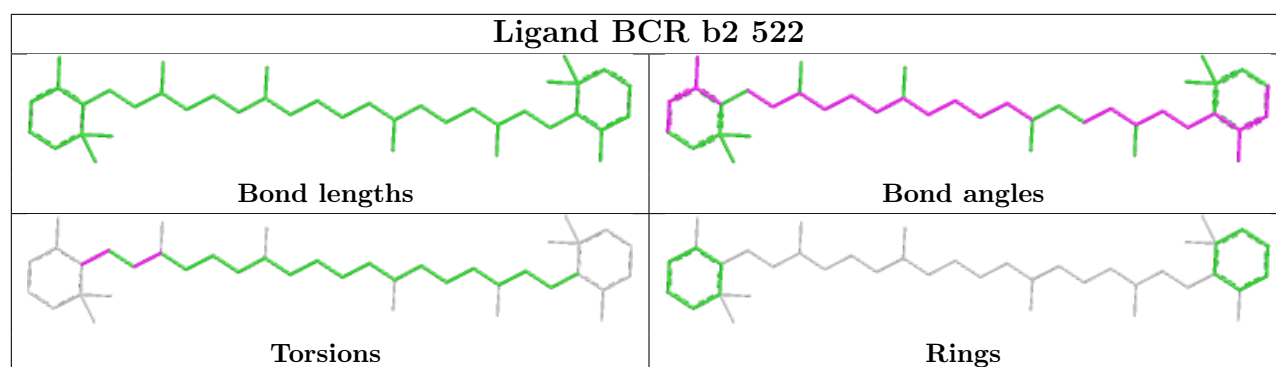


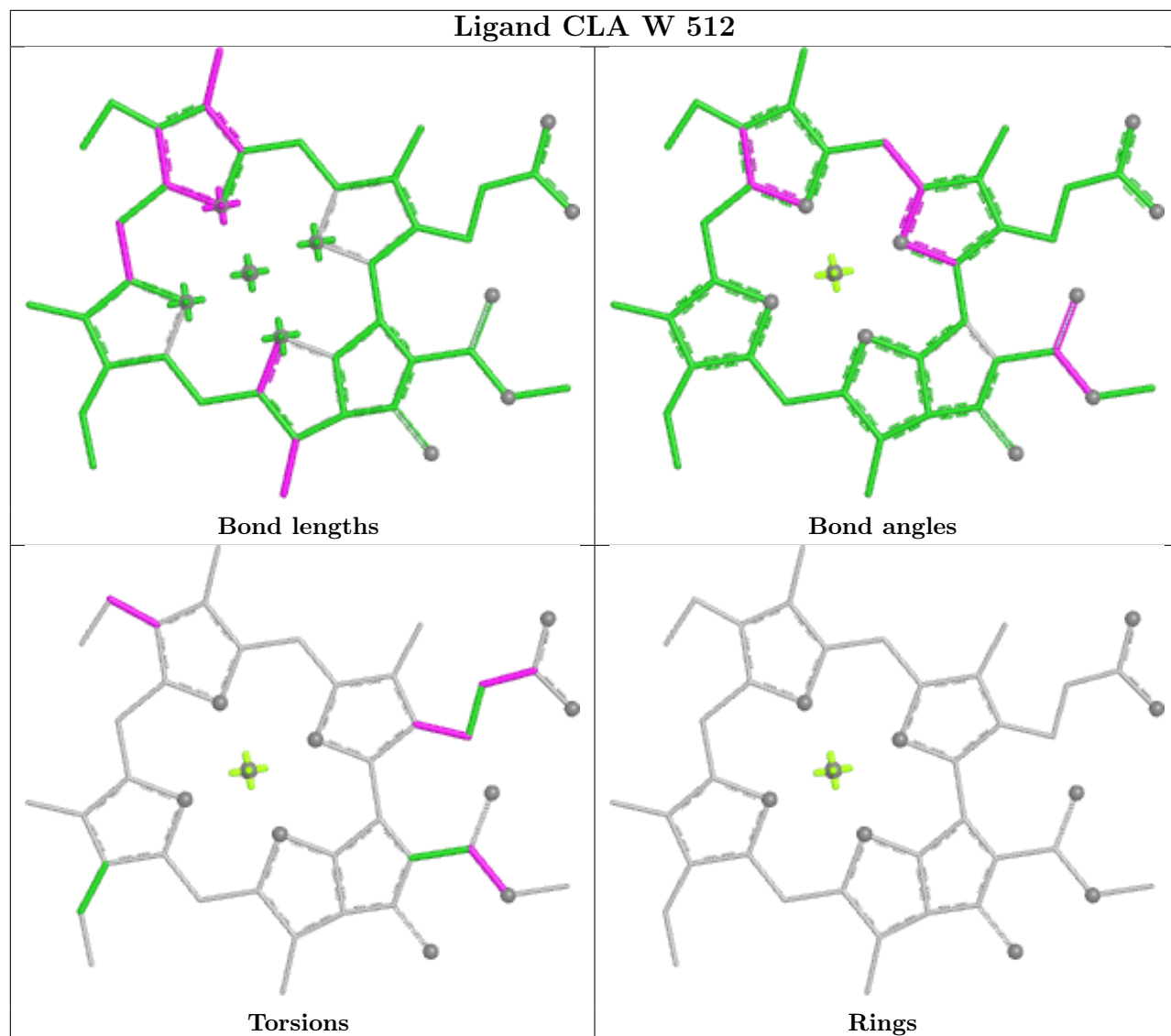
Ligand BCR g 521



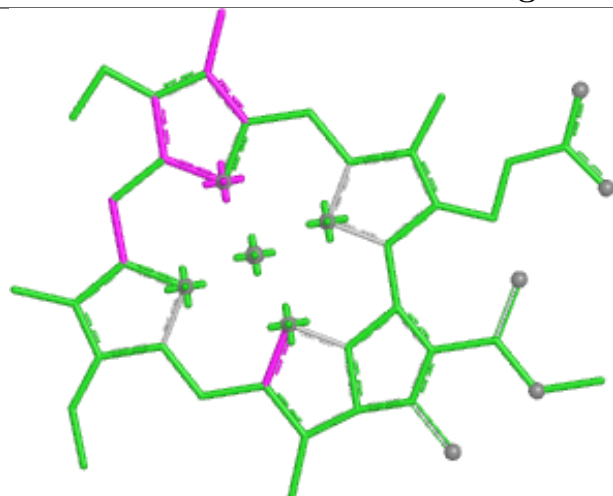




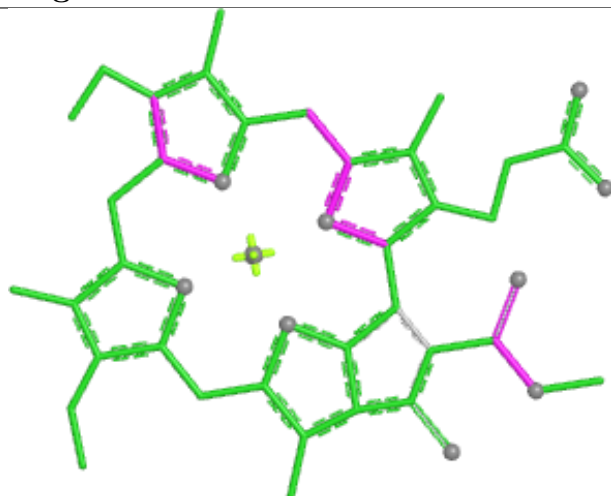




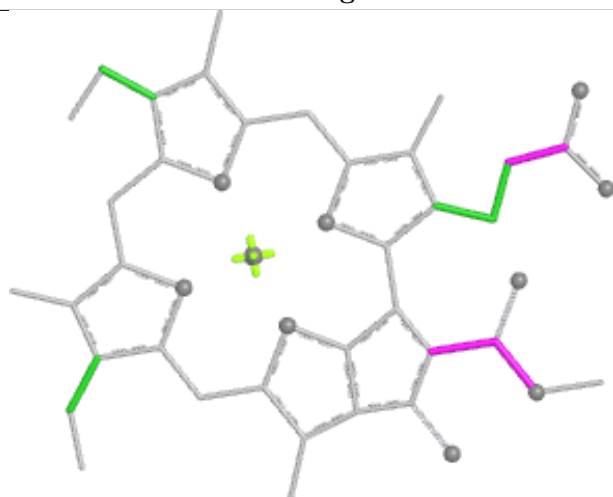
Ligand CLA g 506



Bond lengths



Bond angles

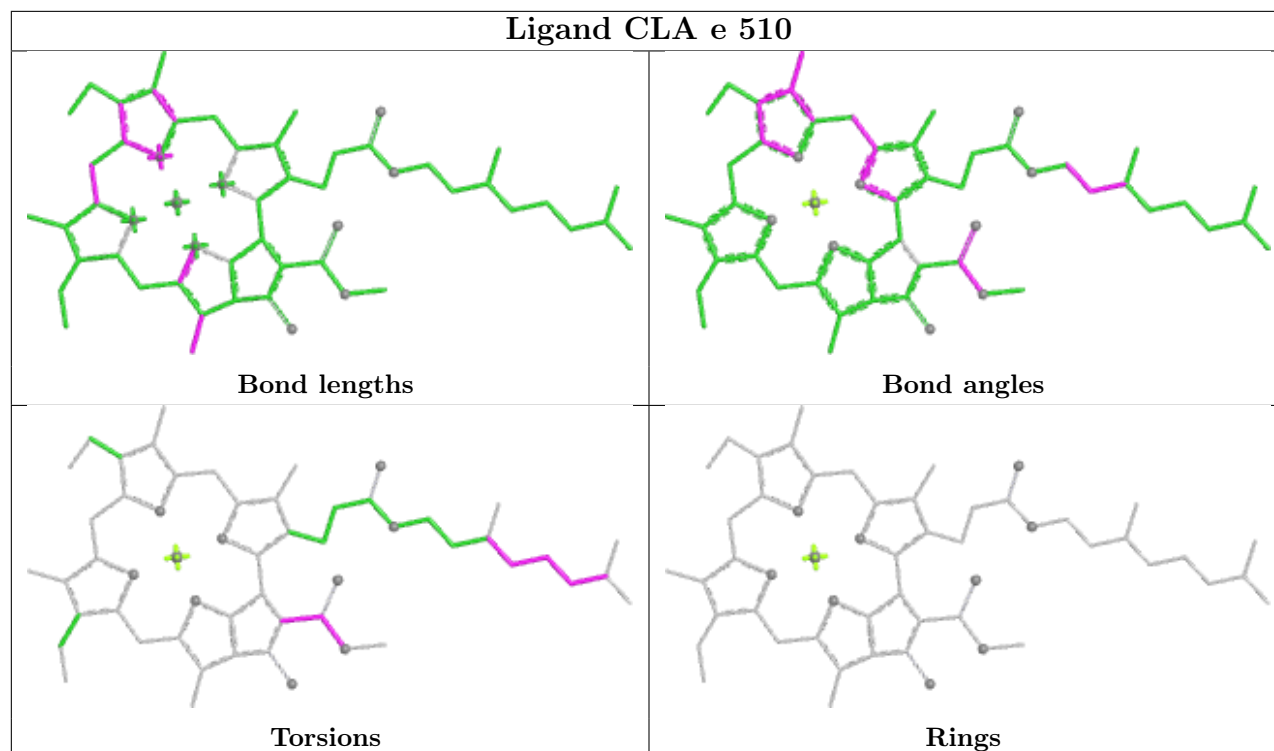


Torsions

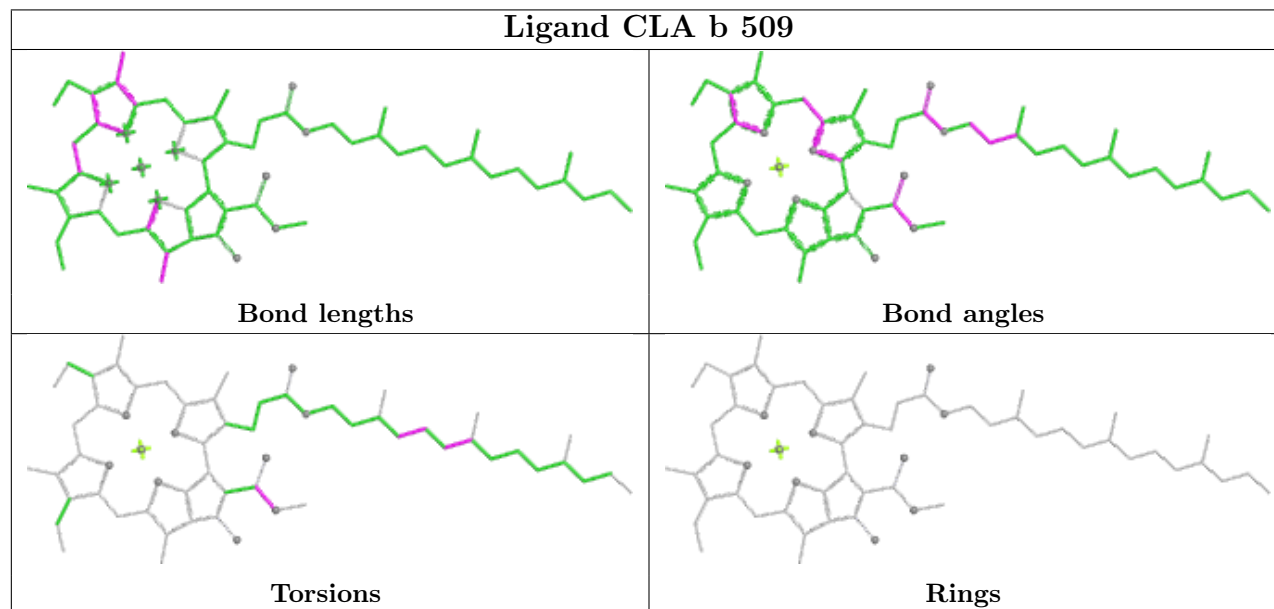


Rings

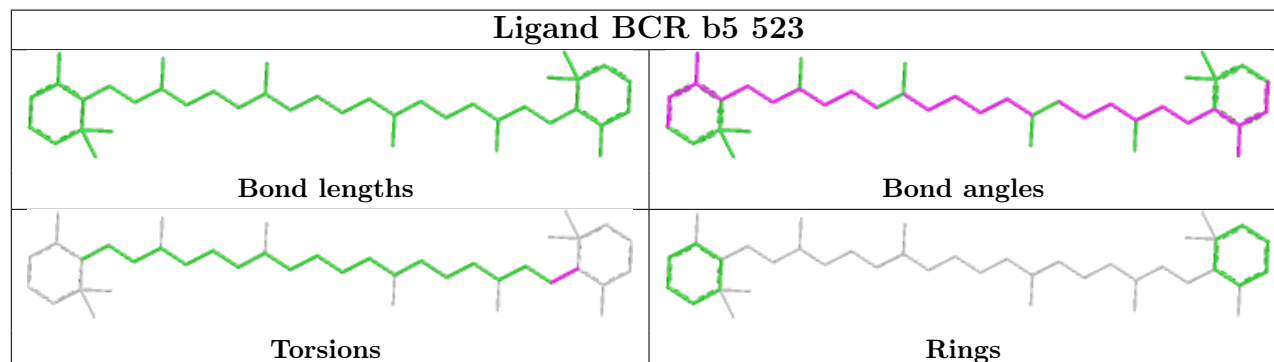
Ligand CLA e 510

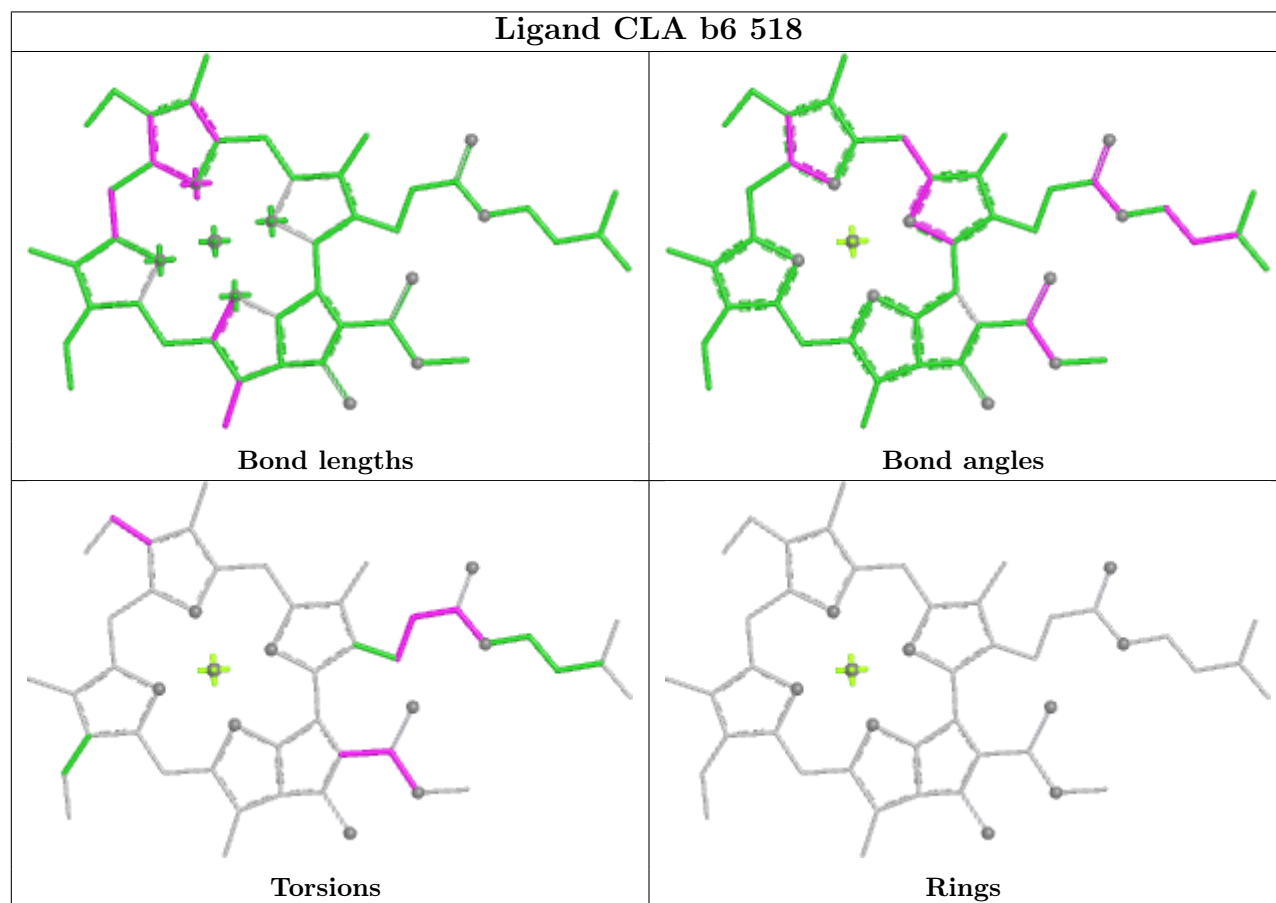
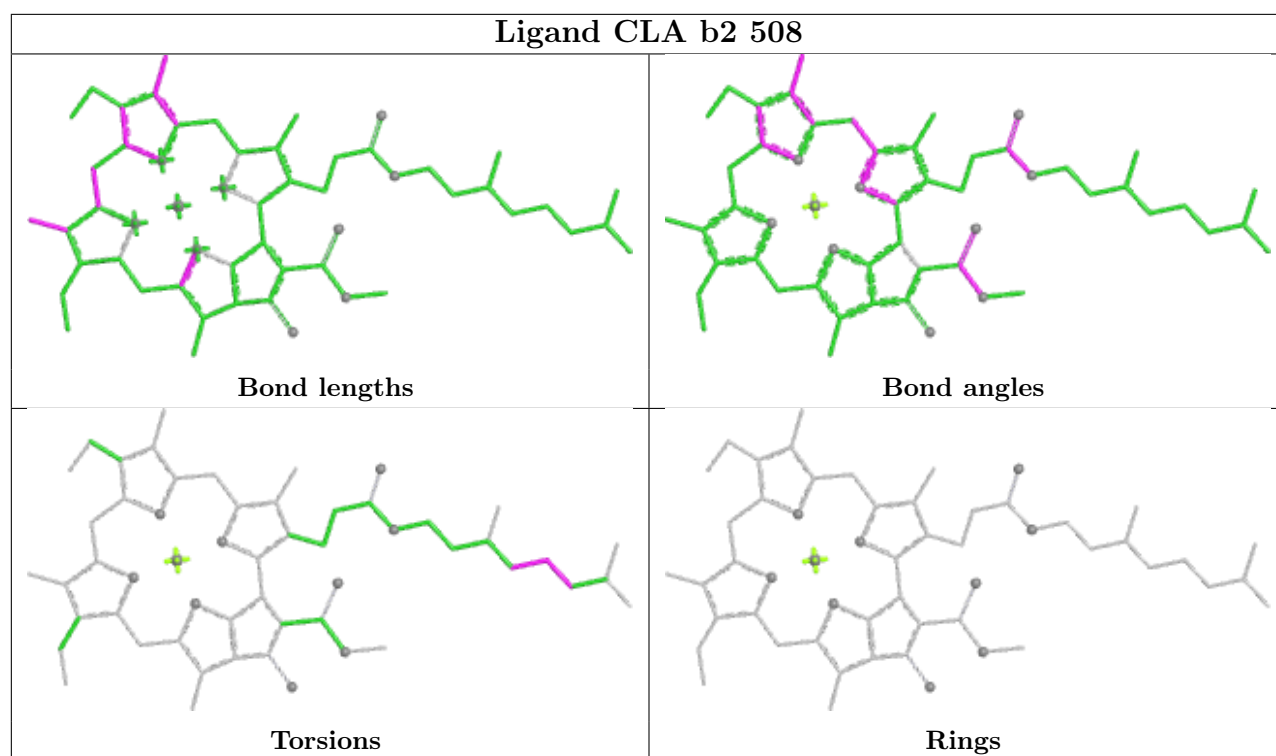


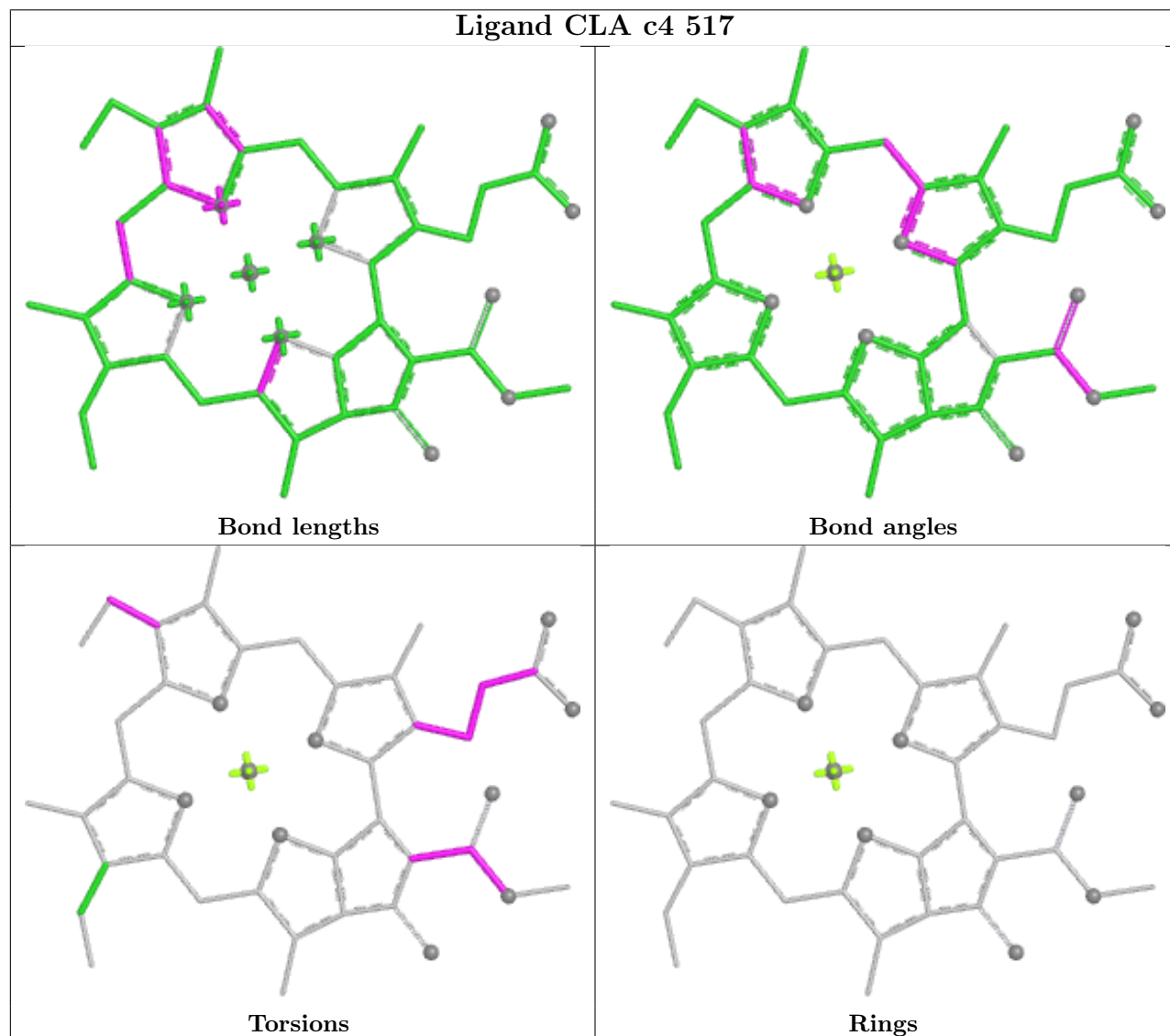
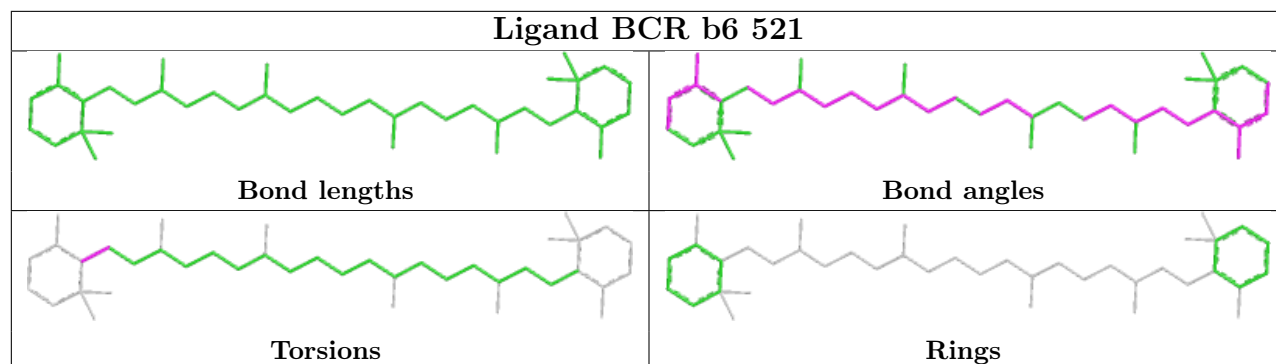
Ligand CLA b 509



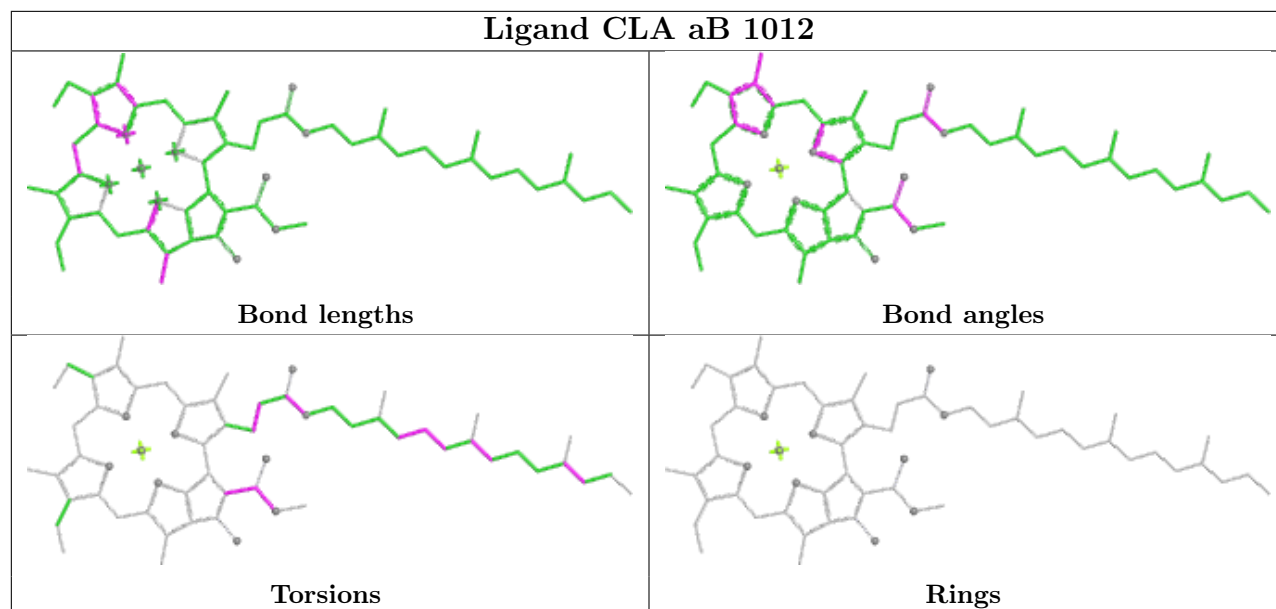
Ligand BCR b5 523



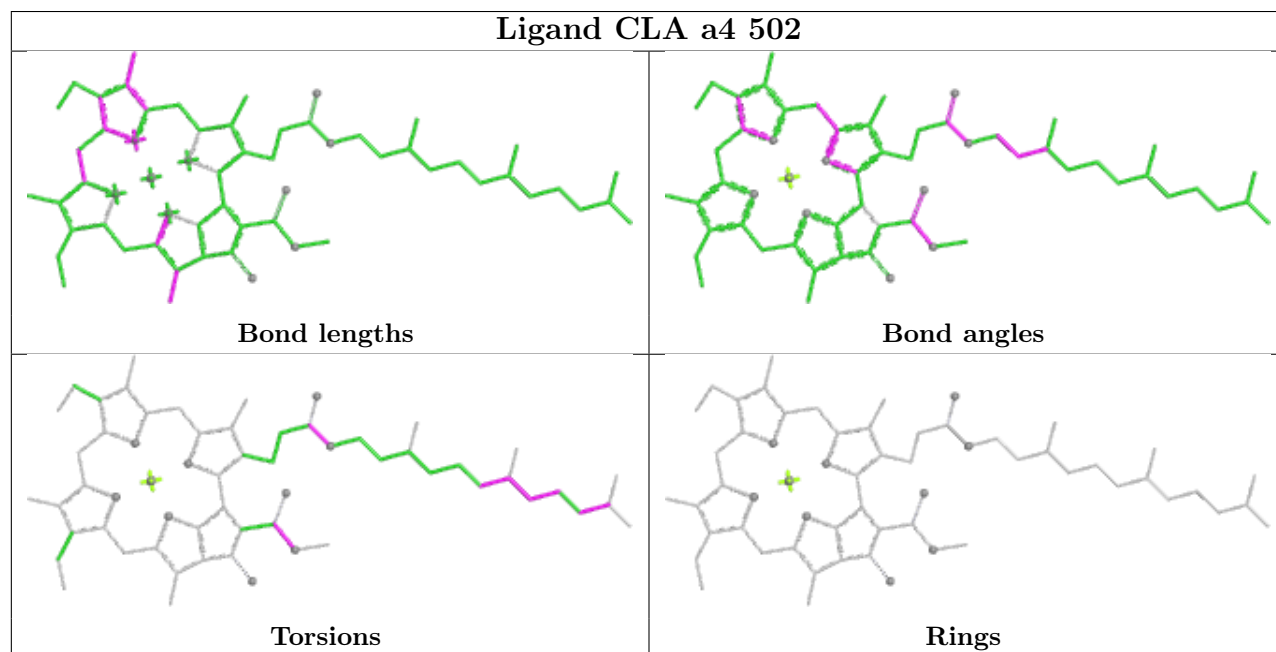




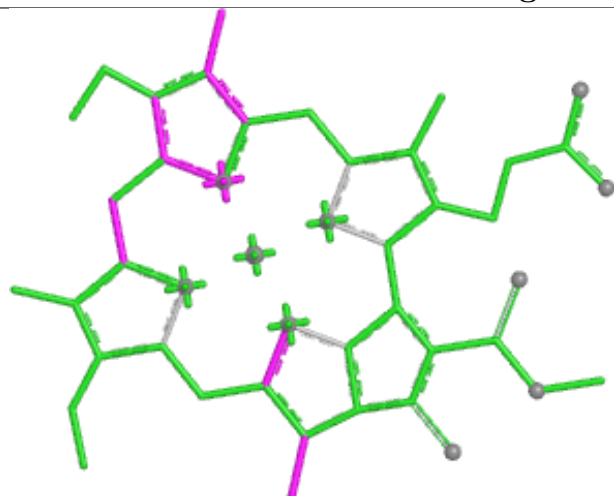
Ligand CLA aB 1012



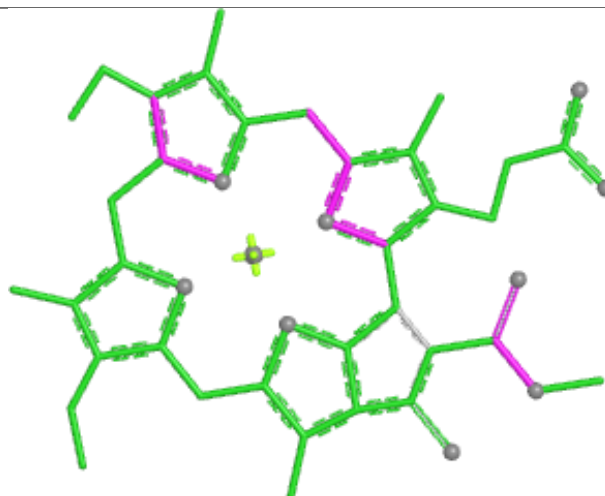
Ligand CLA a4 502



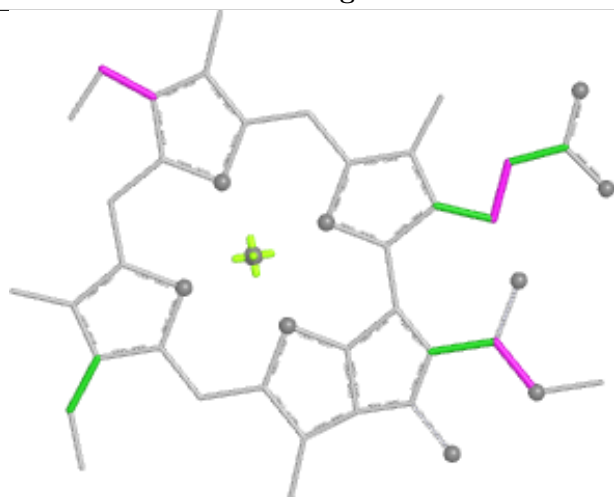
Ligand CLA c 518



Bond lengths



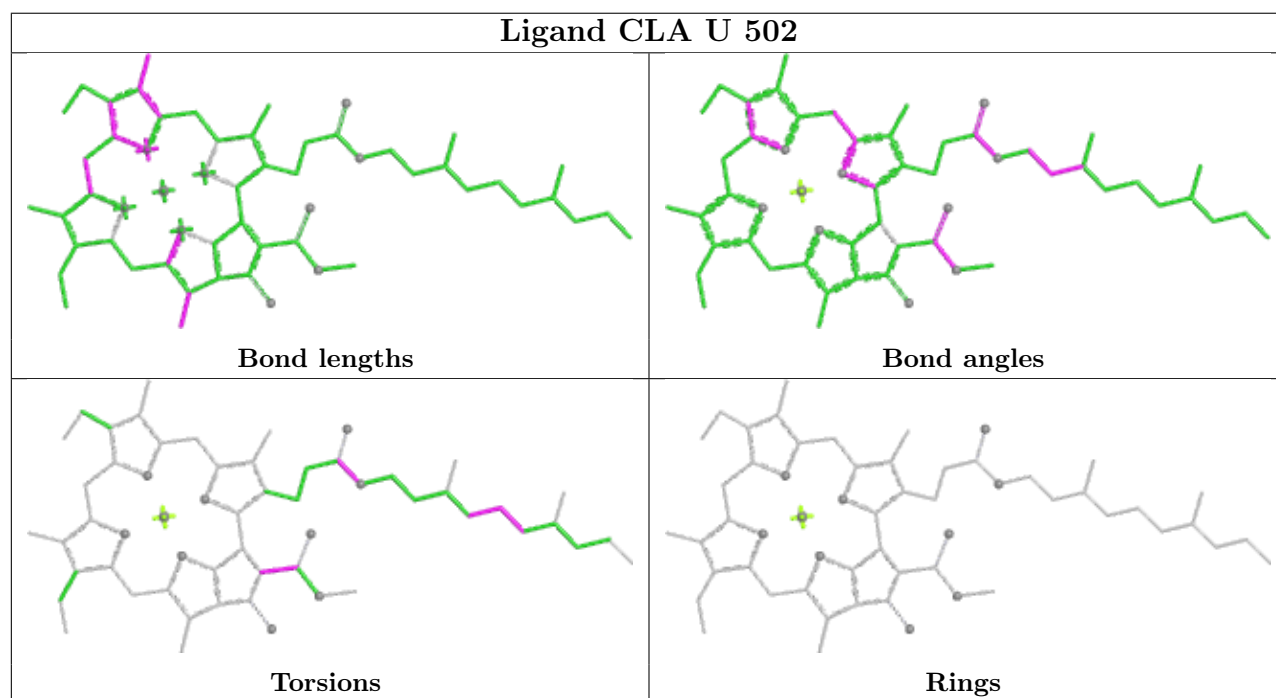
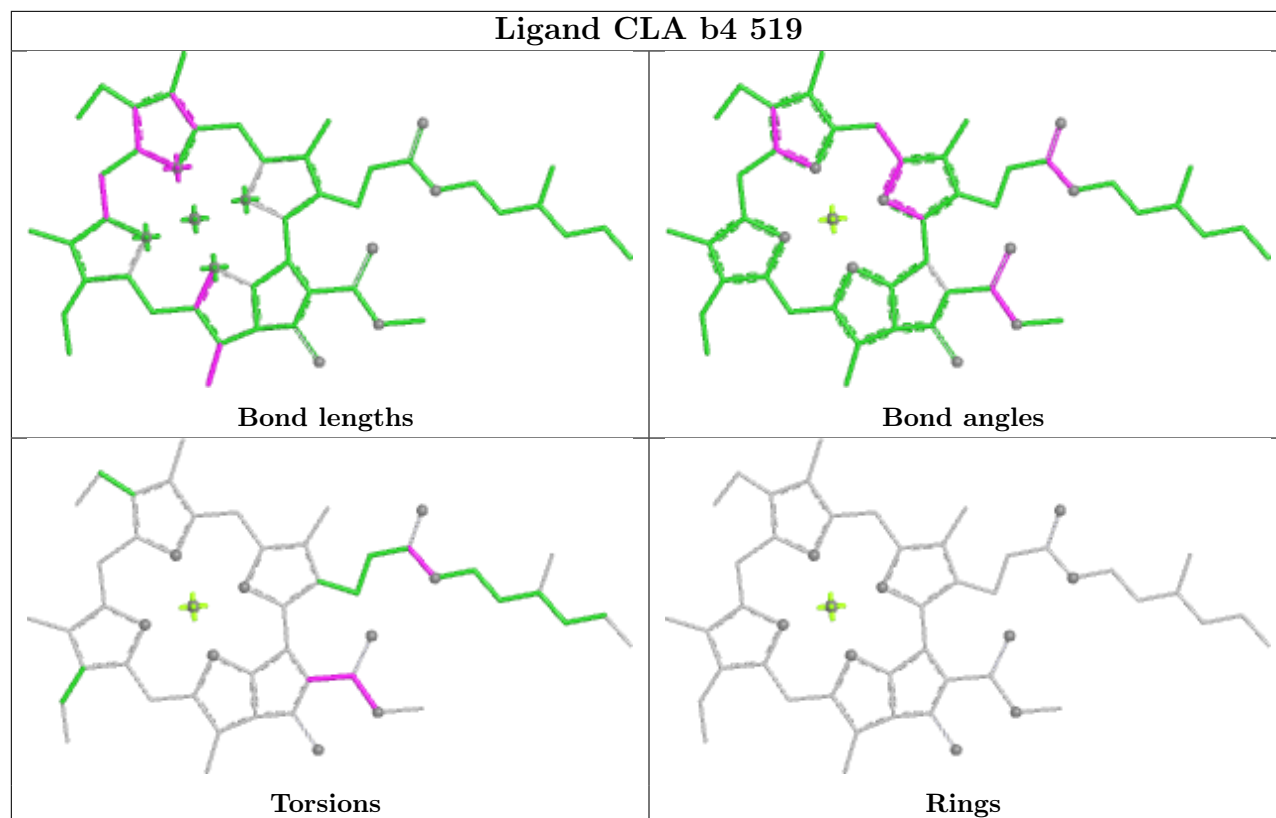
Bond angles

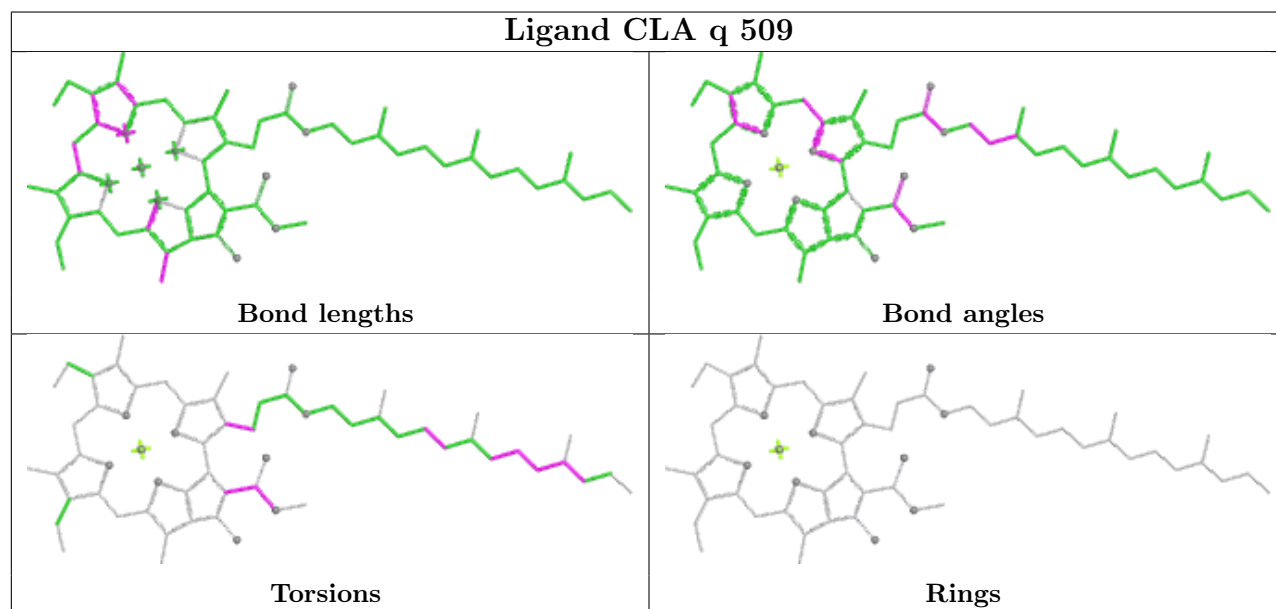
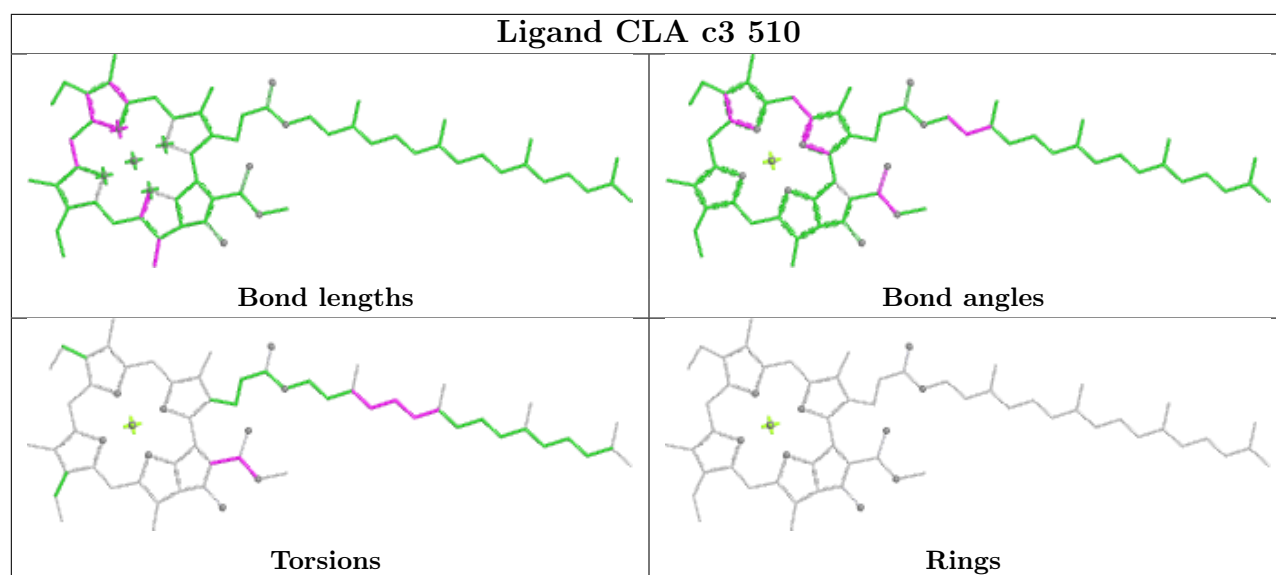


Torsions

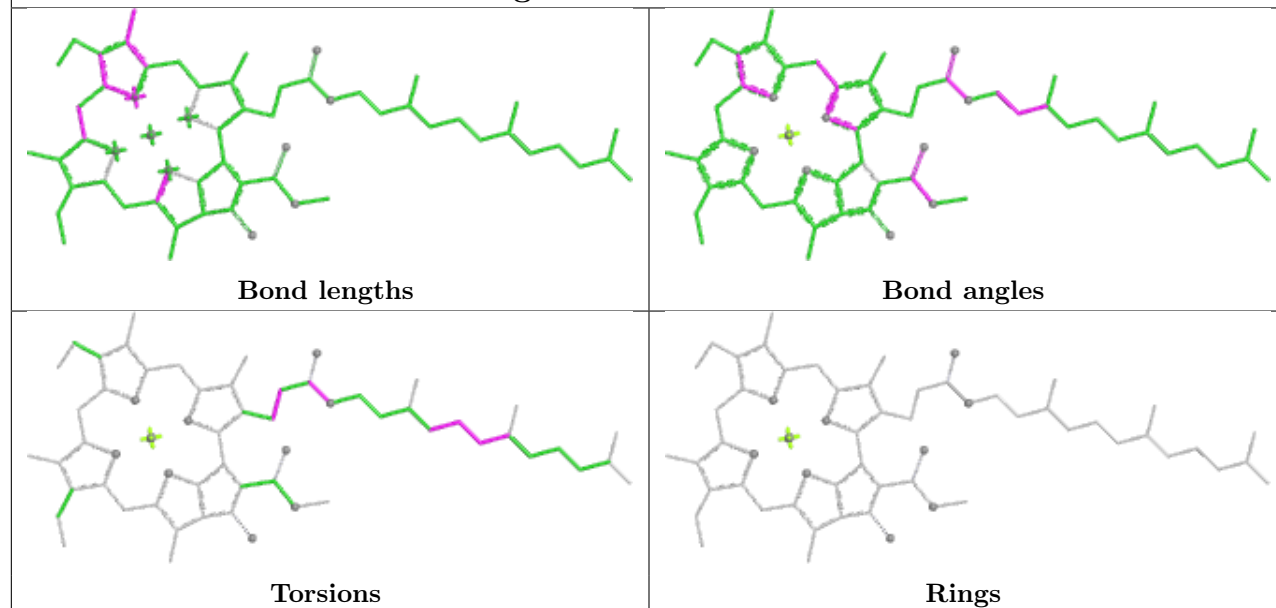


Rings

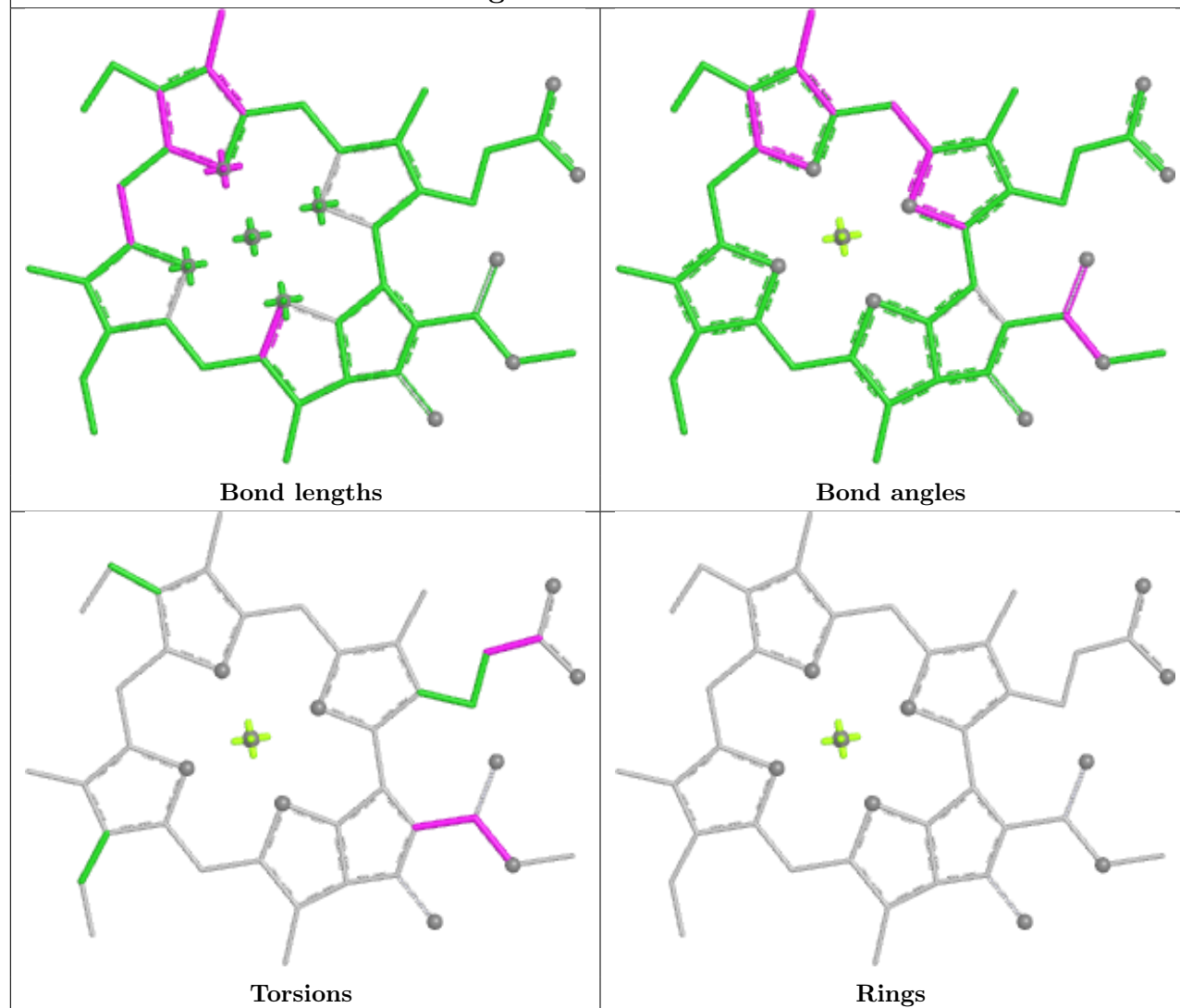


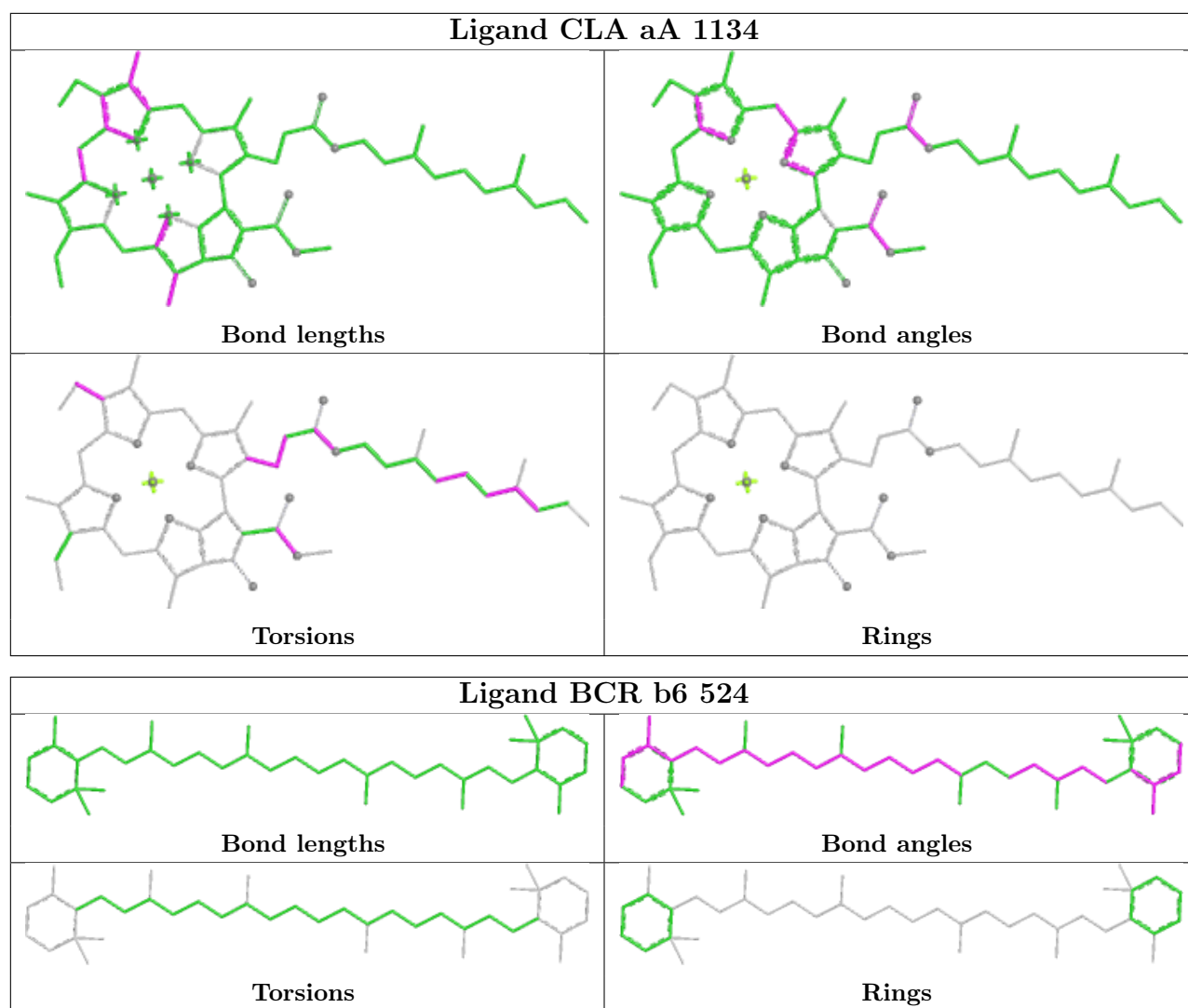


Ligand CLA bB 1213

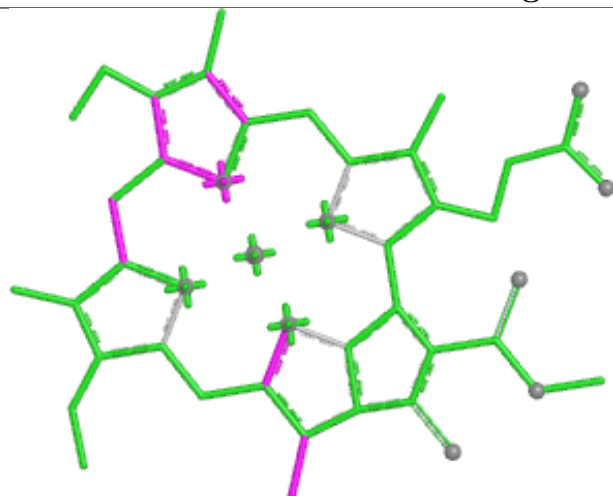


Ligand CLA c2 506

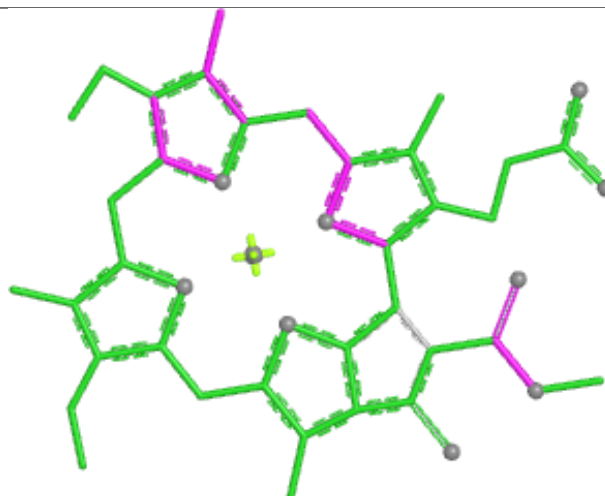




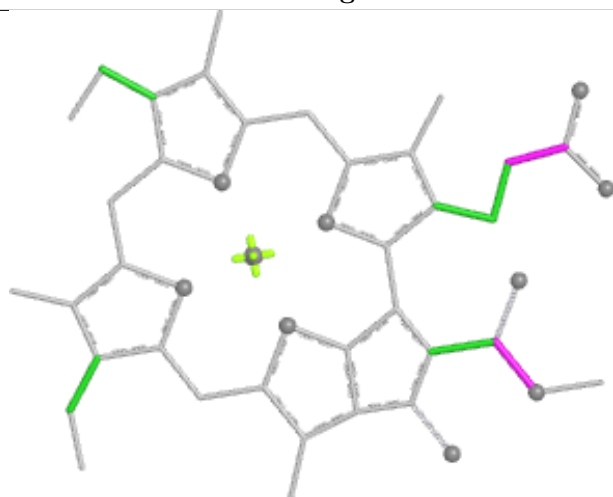
Ligand CLA 1 510



Bond lengths



Bond angles

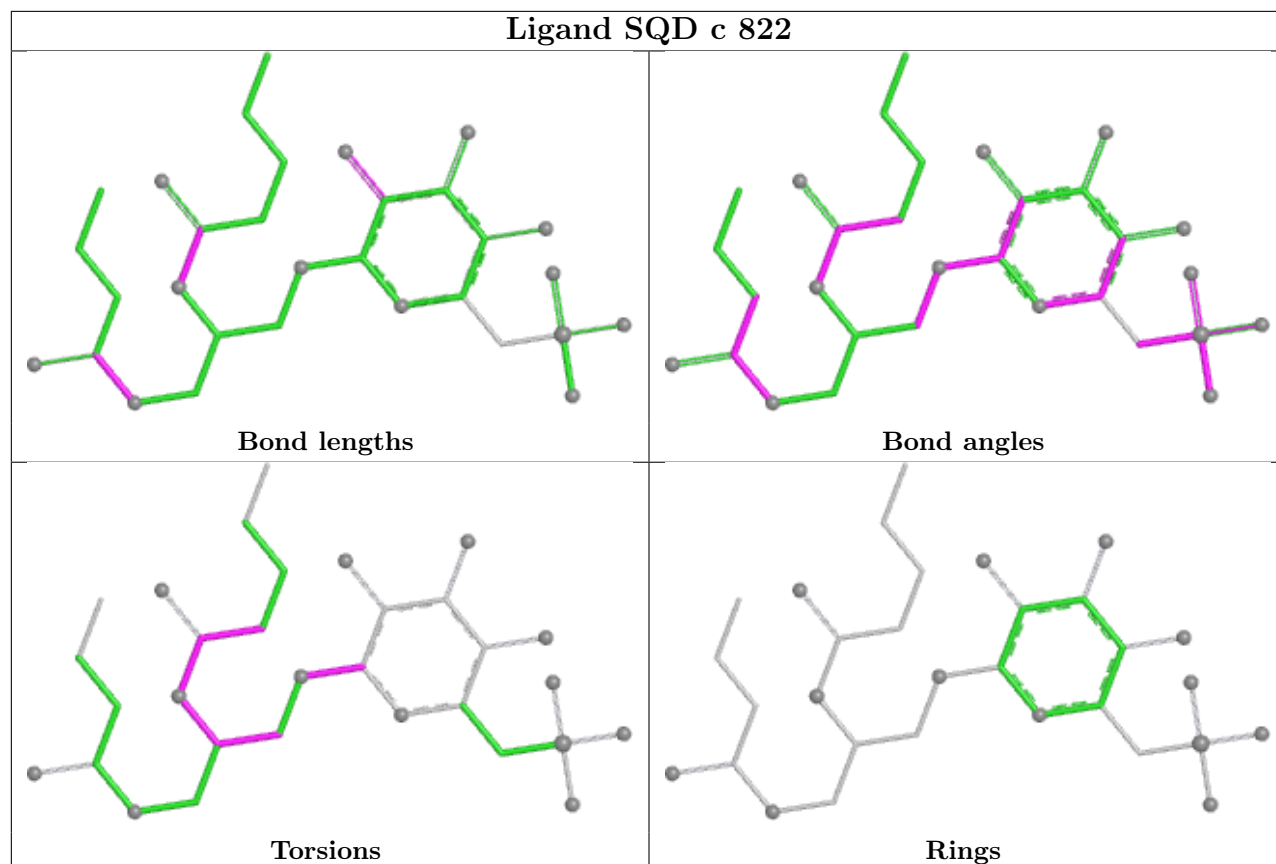


Torsions

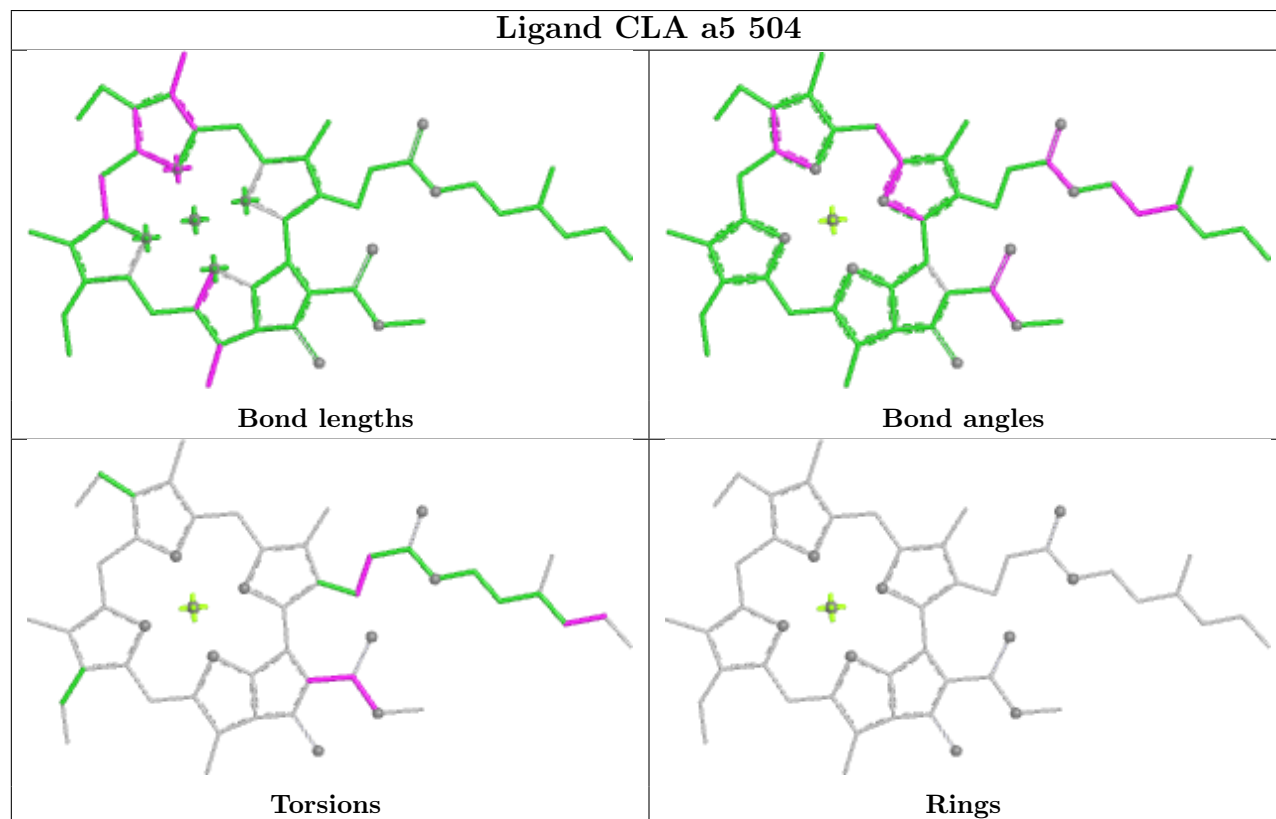


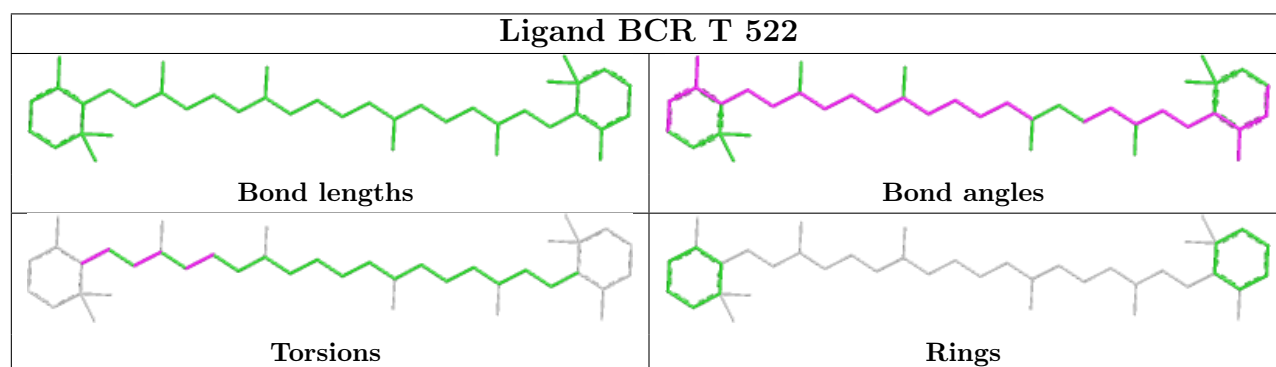
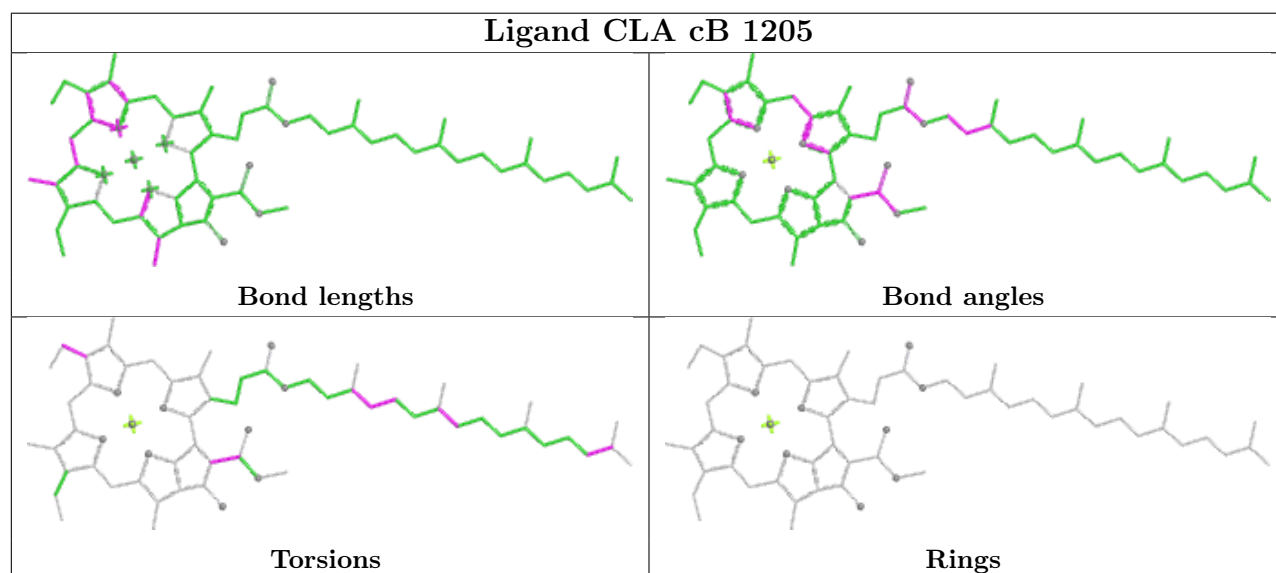
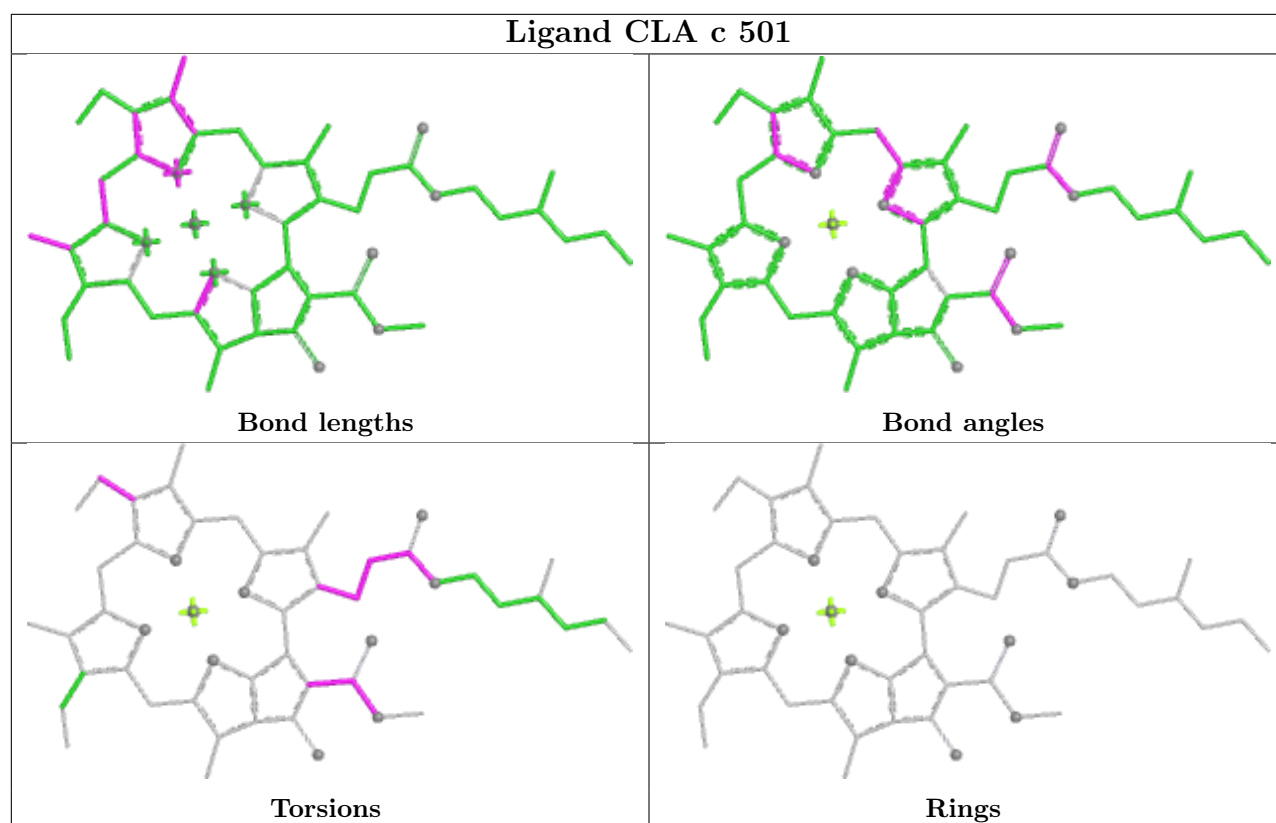
Rings

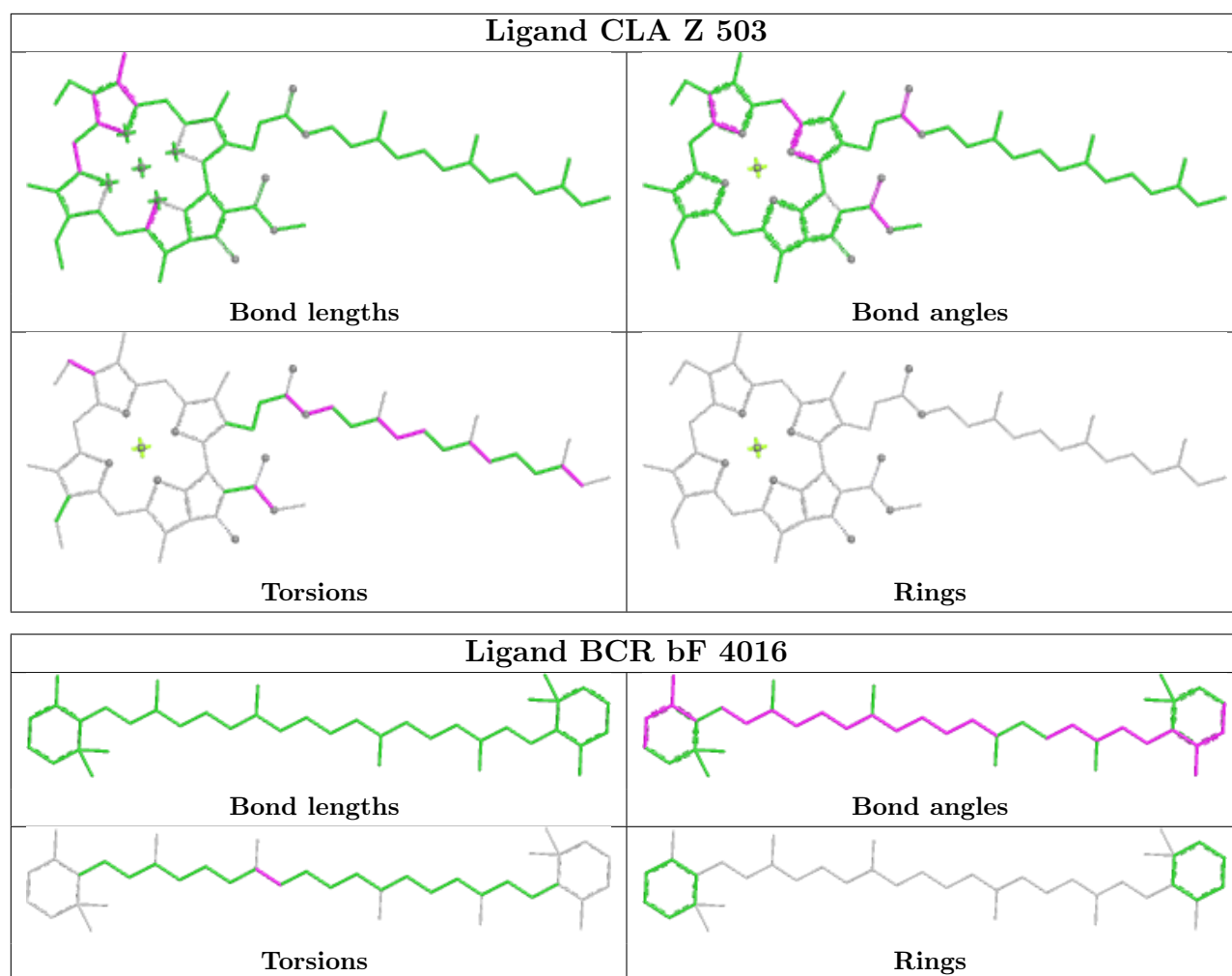
Ligand SQD c 822



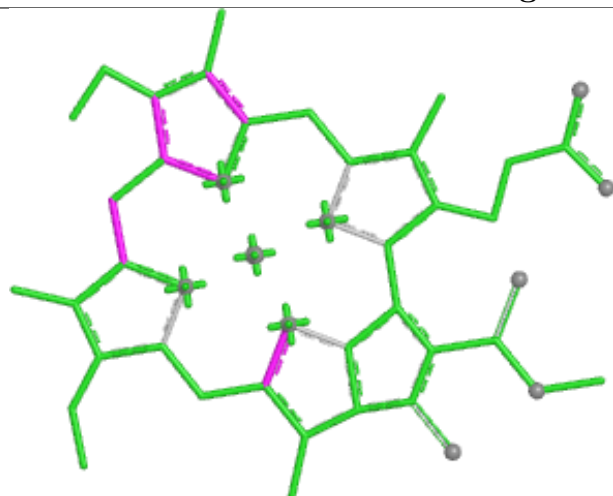
Ligand CLA a5 504



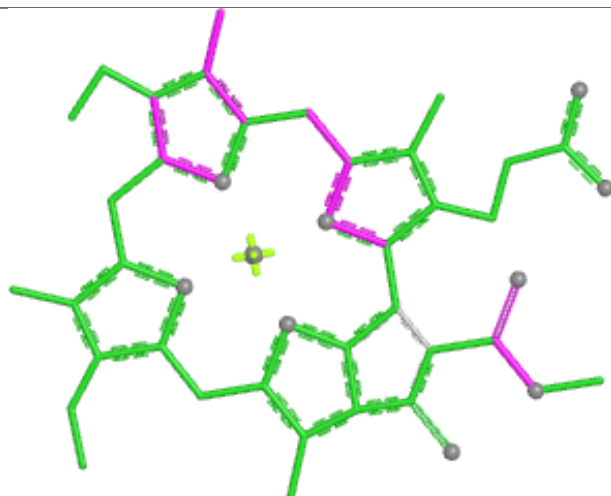




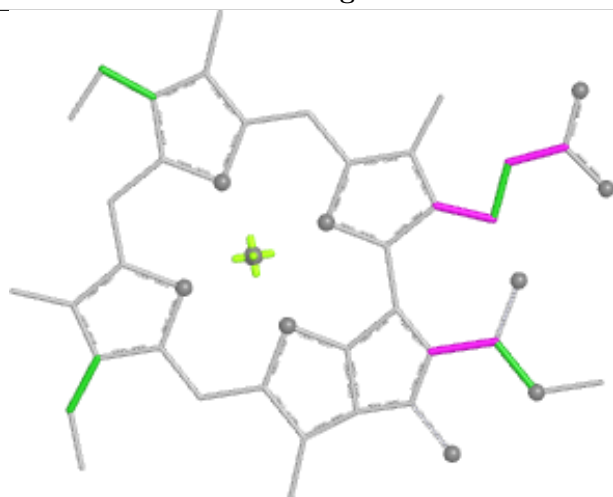
Ligand CLA c 516



Bond lengths



Bond angles

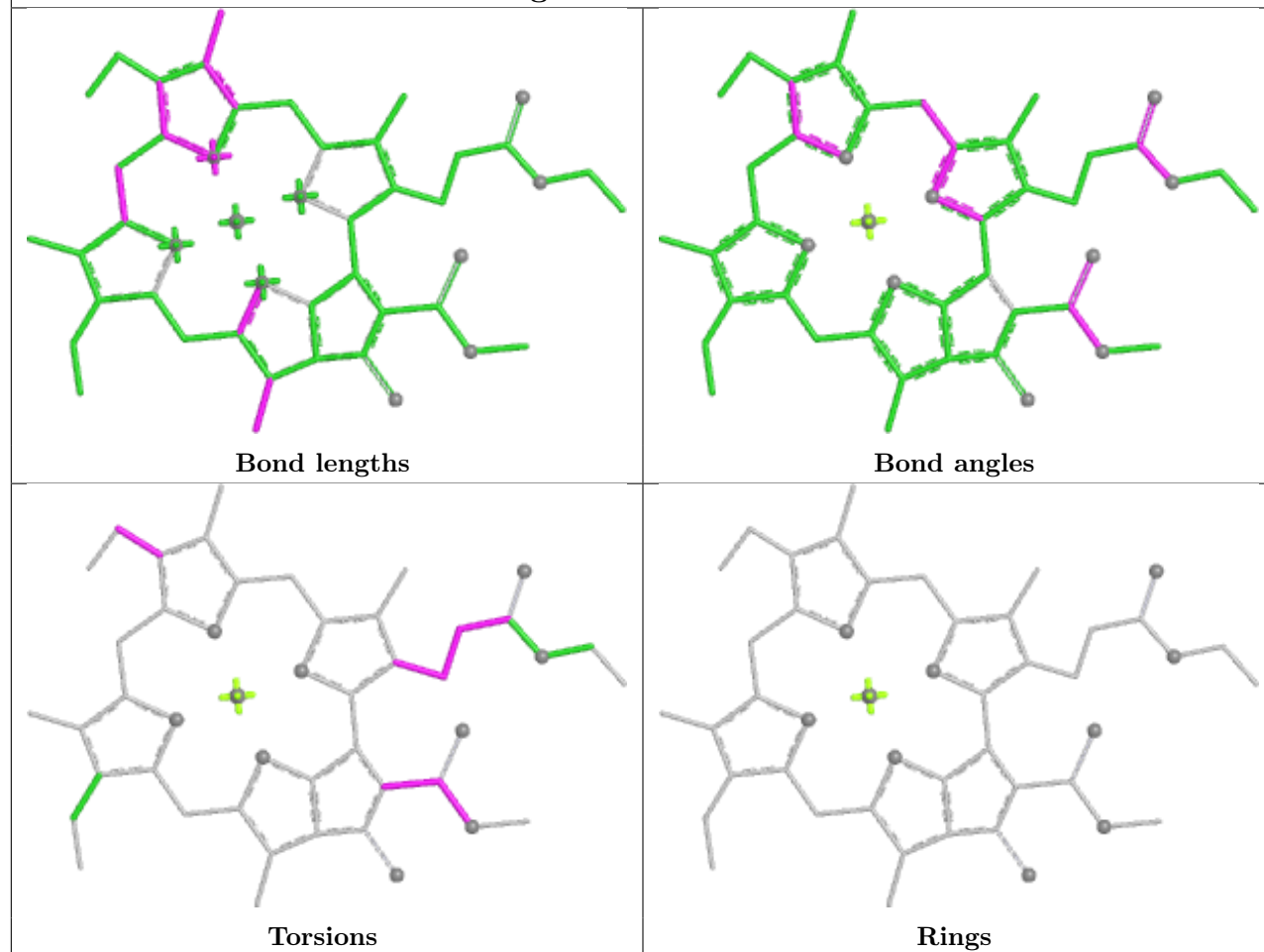


Torsions

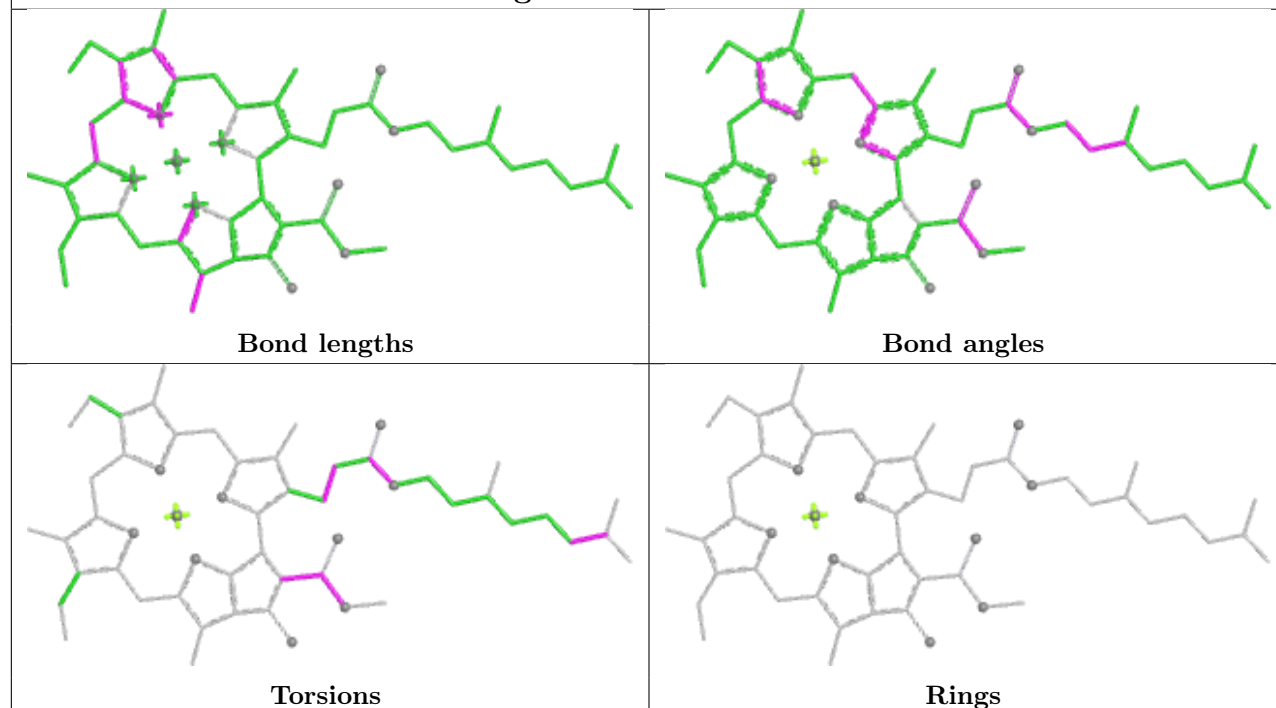


Rings

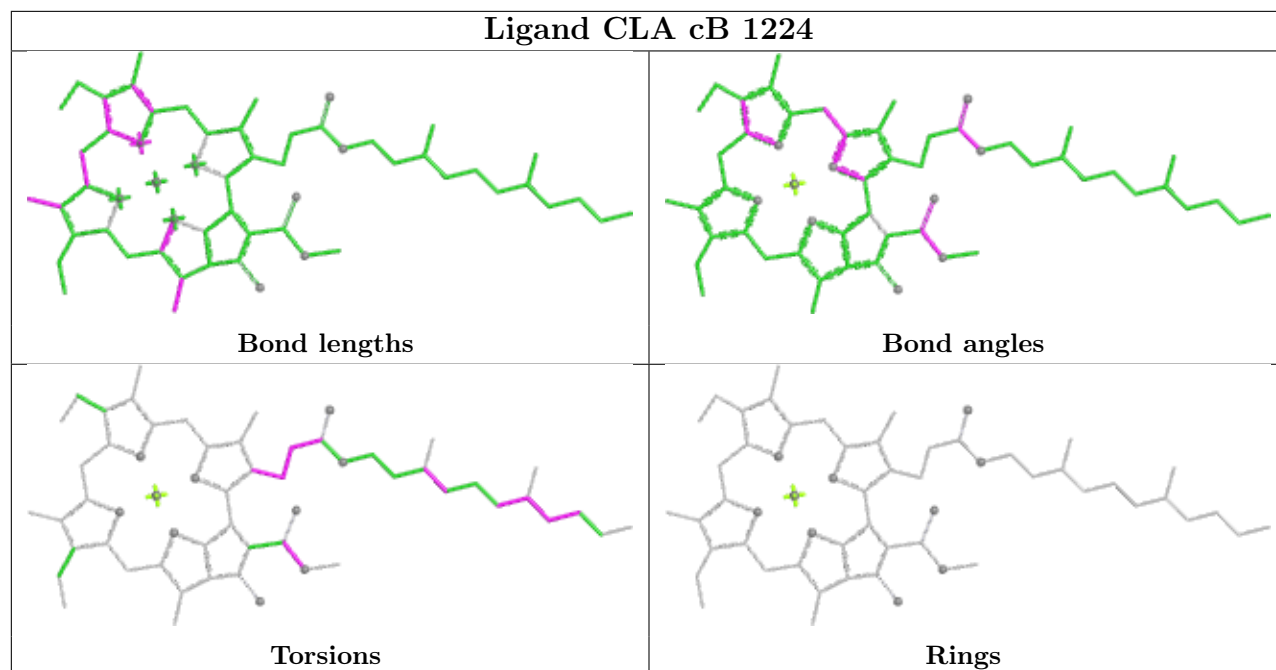
Ligand CLA n 518



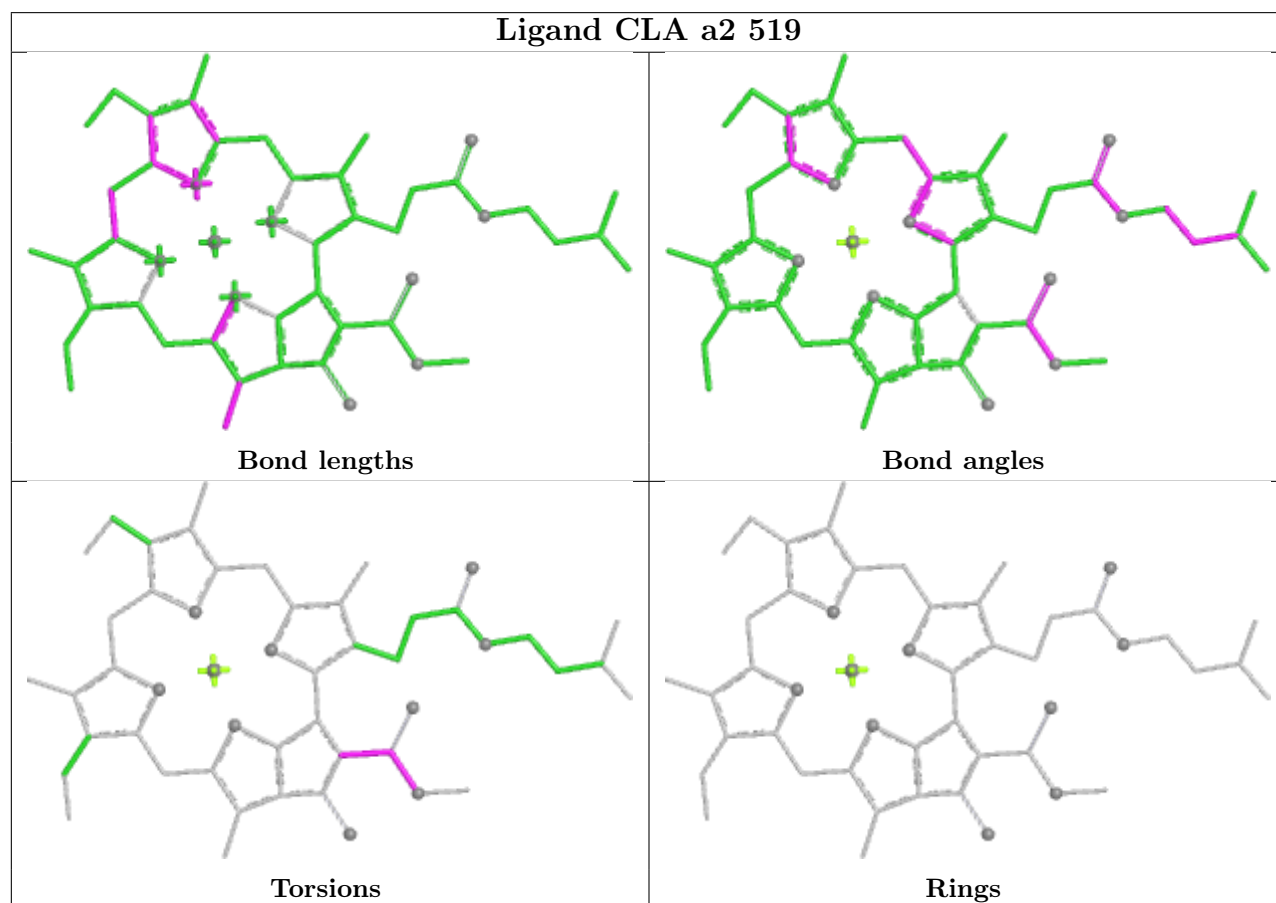
Ligand CLA aA 1111



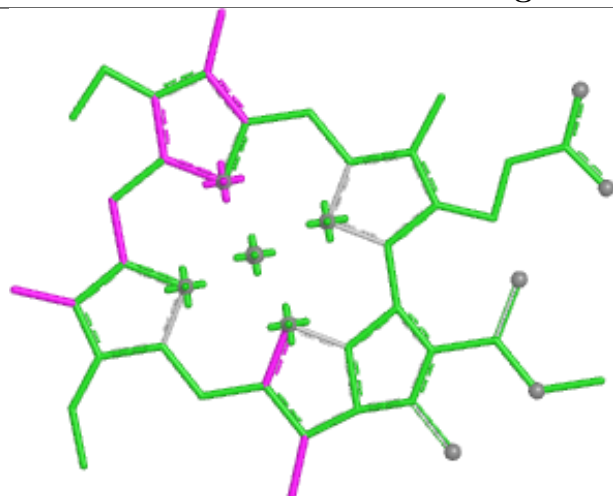
Ligand CLA cB 1224



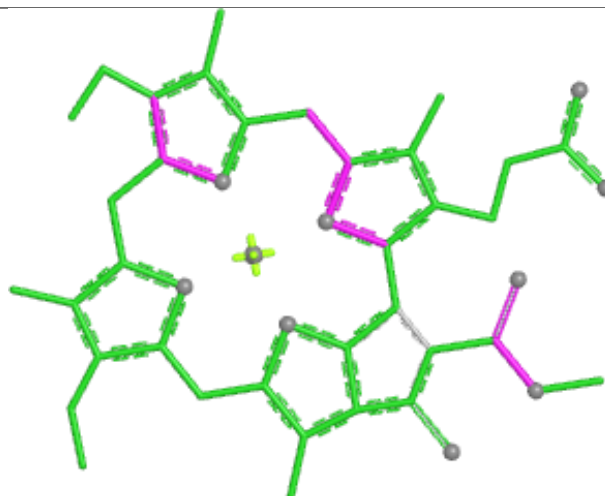
Ligand CLA a2 519



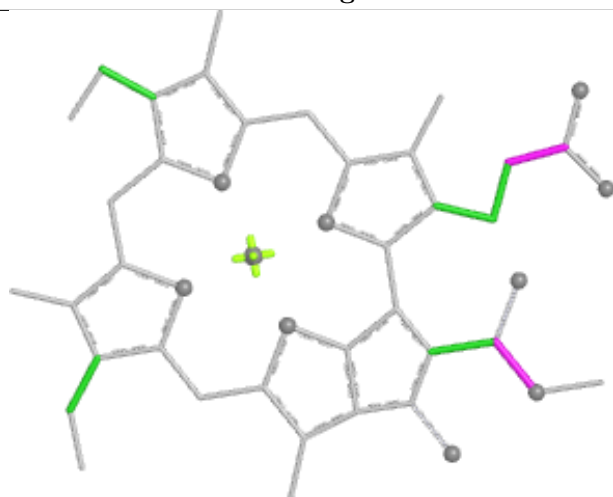
Ligand CLA T 508



Bond lengths



Bond angles

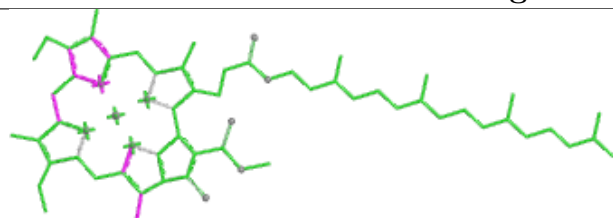


Torsions

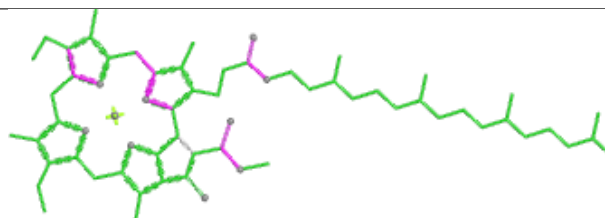


Rings

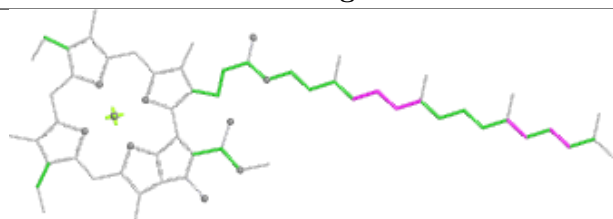
Ligand CLA a1 509



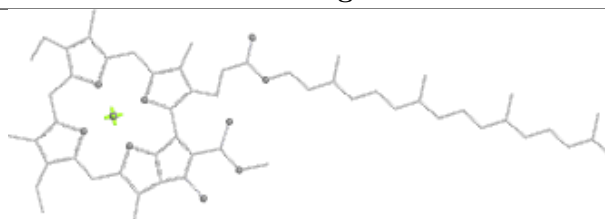
Bond lengths



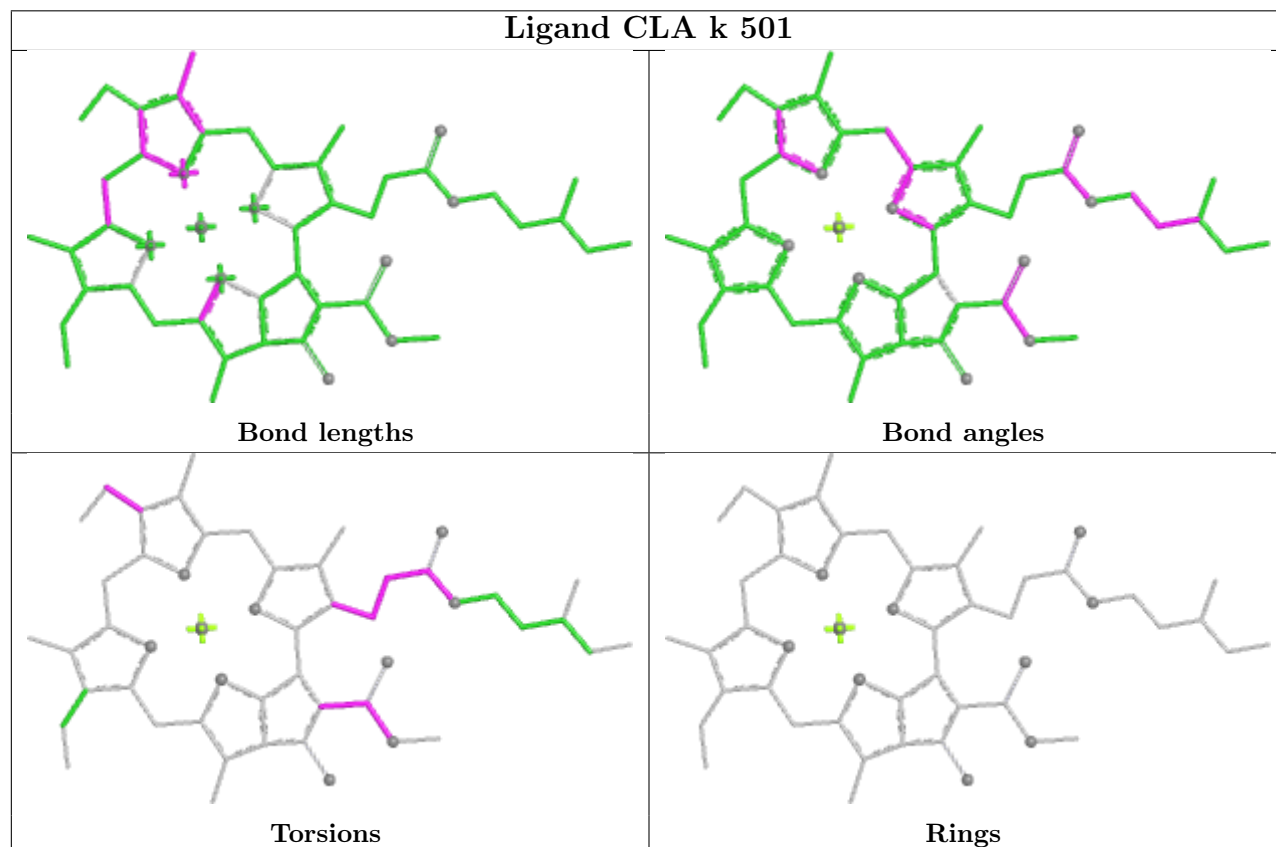
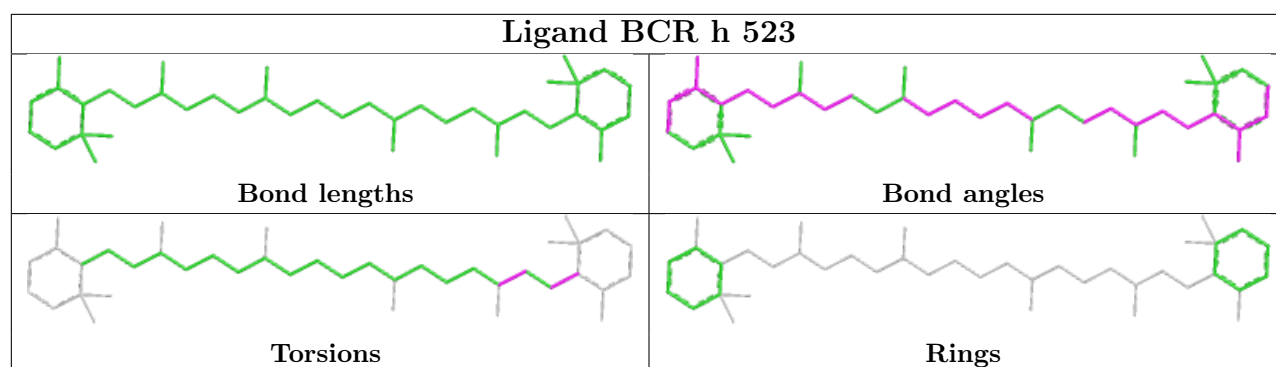
Bond angles

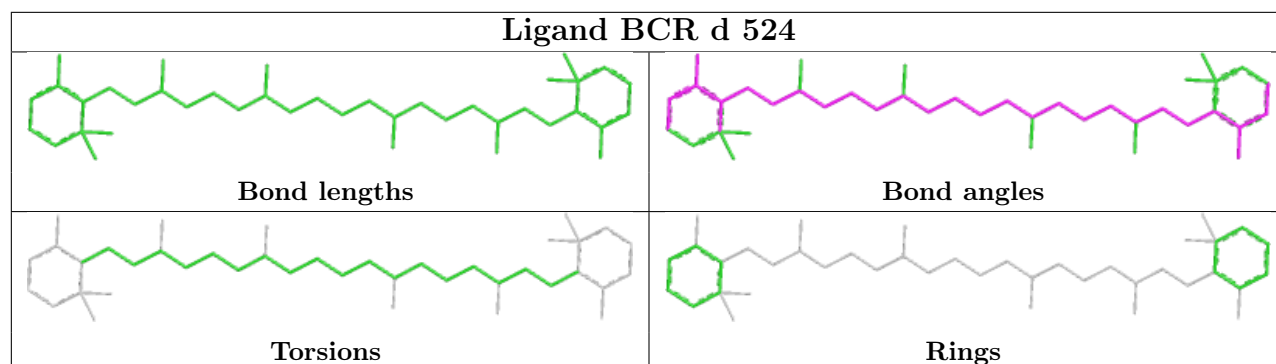
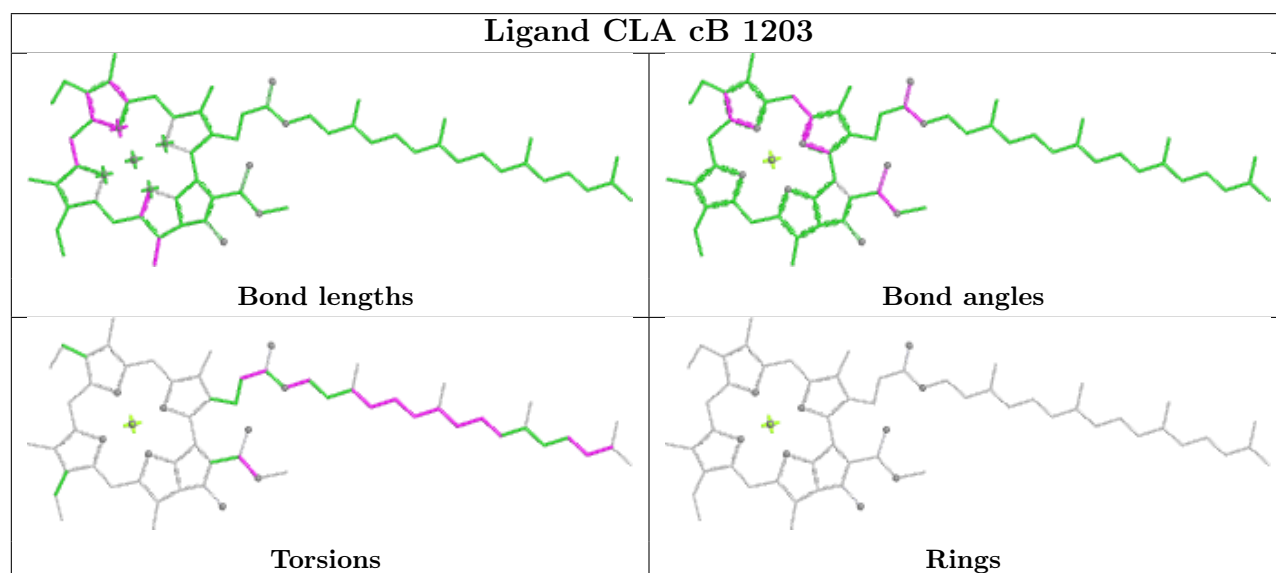
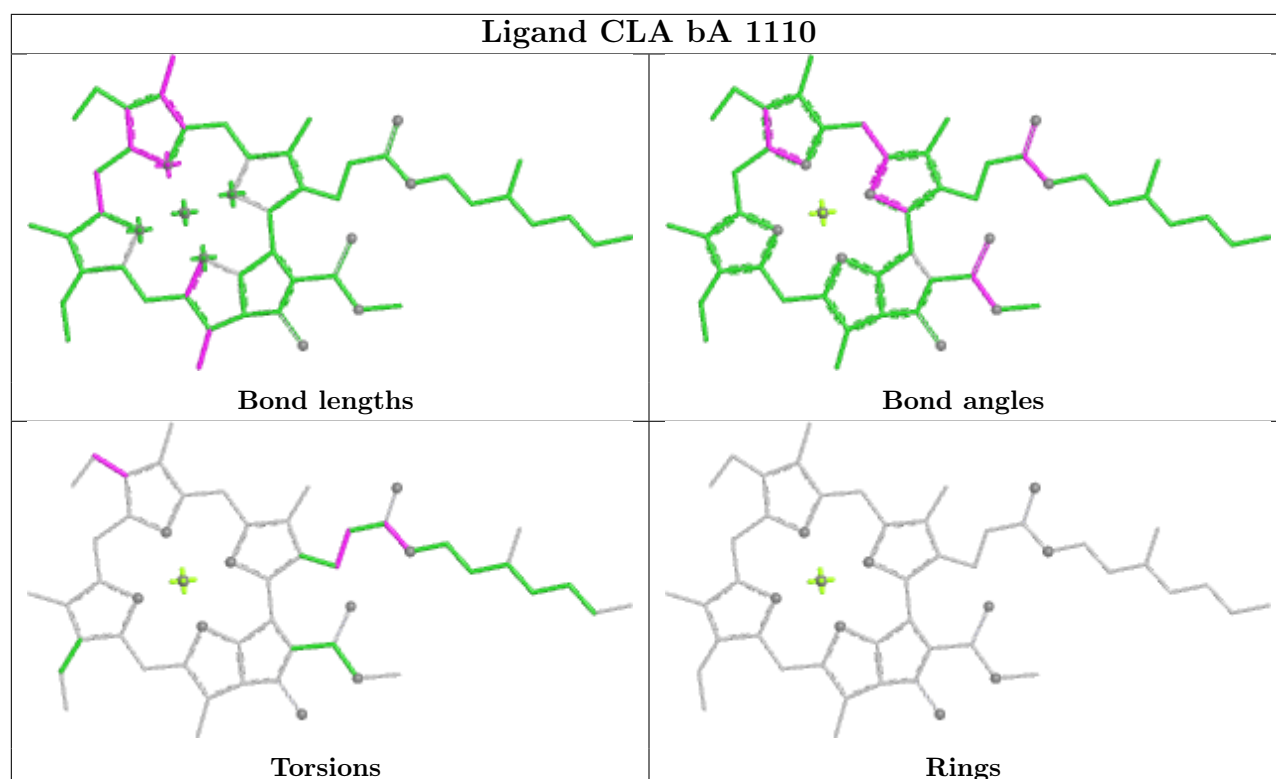


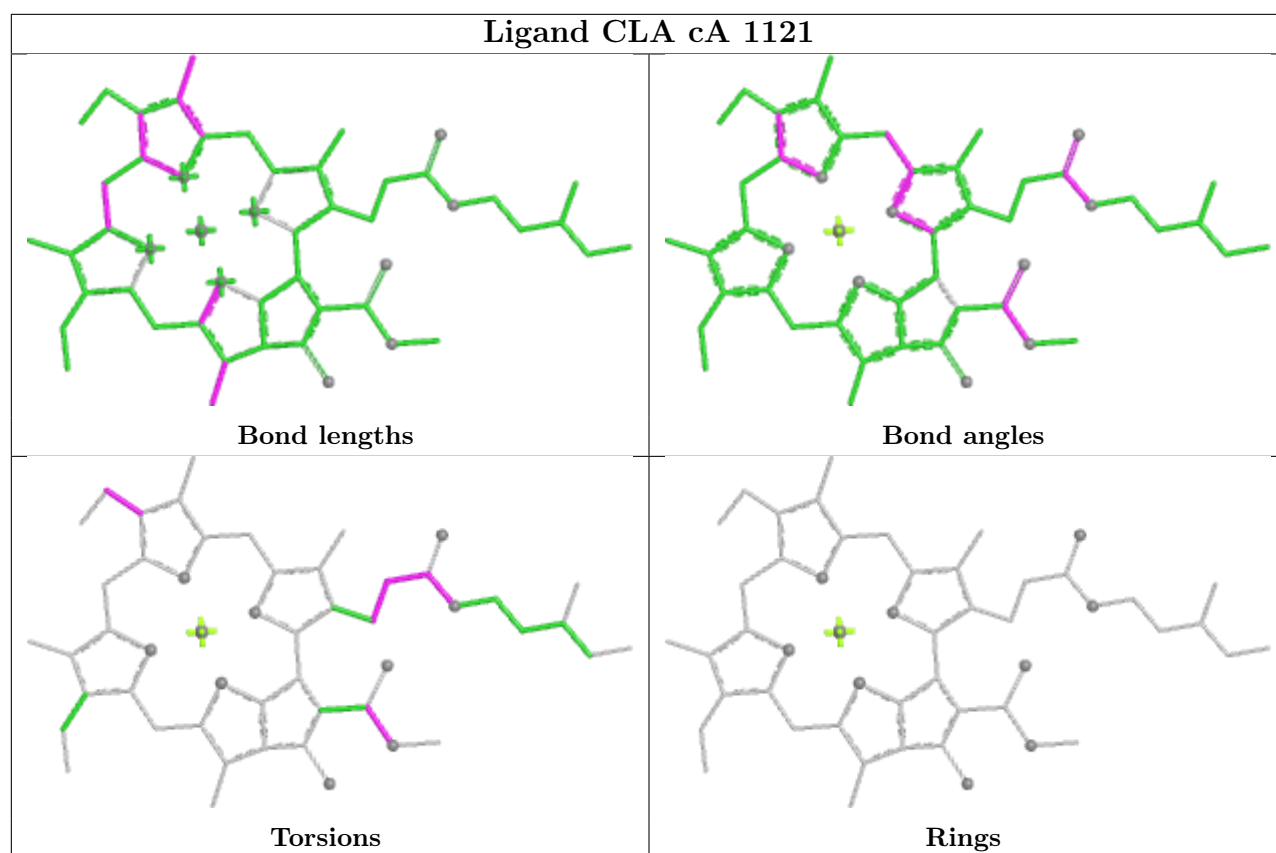
Torsions



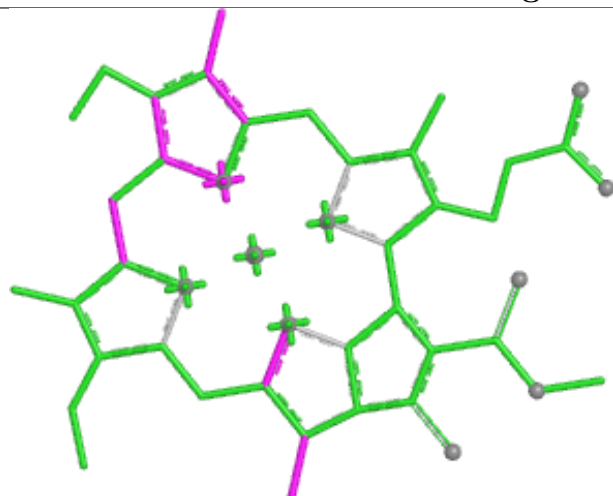
Rings







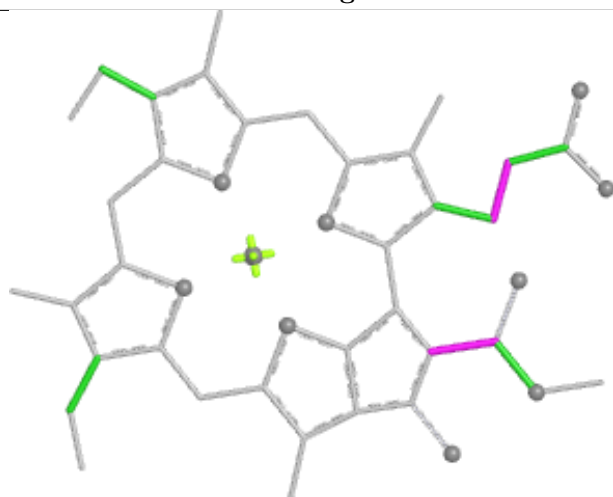
Ligand CLA l 512



Bond lengths



Bond angles

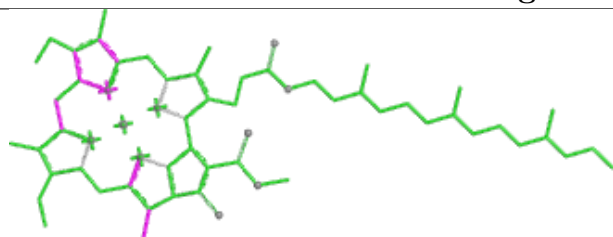


Torsions

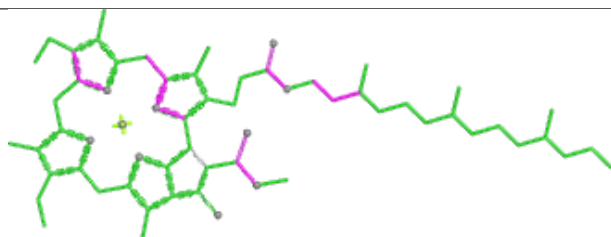


Rings

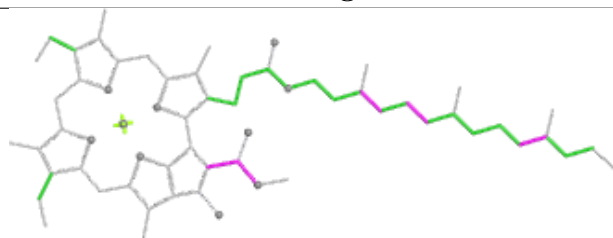
Ligand CLA o 503



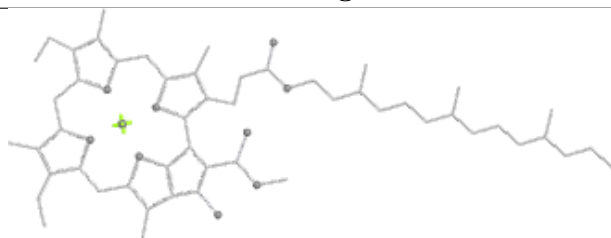
Bond lengths



Bond angles

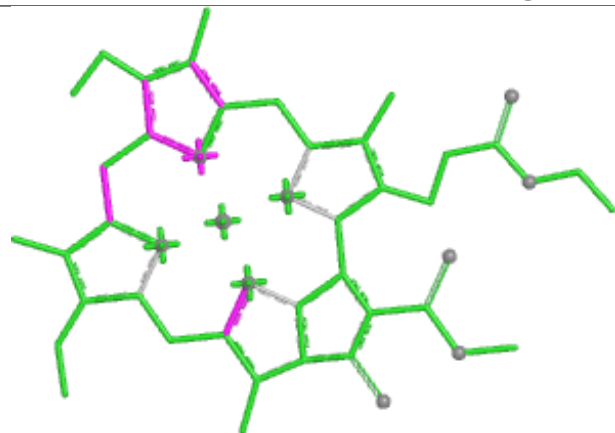


Torsions

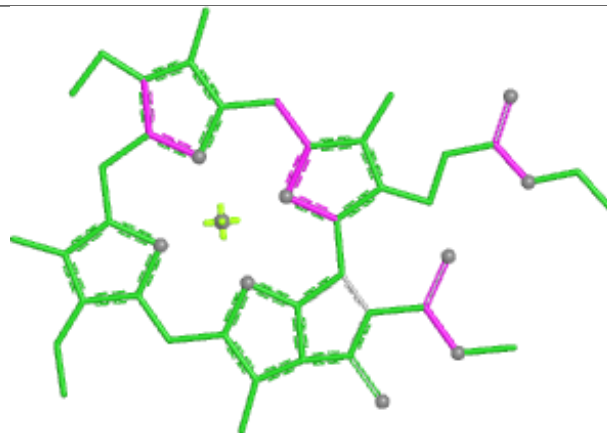


Rings

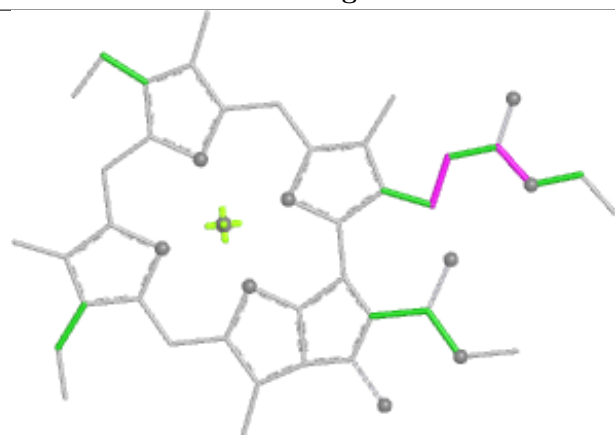
Ligand CLA S 513



Bond lengths



Bond angles

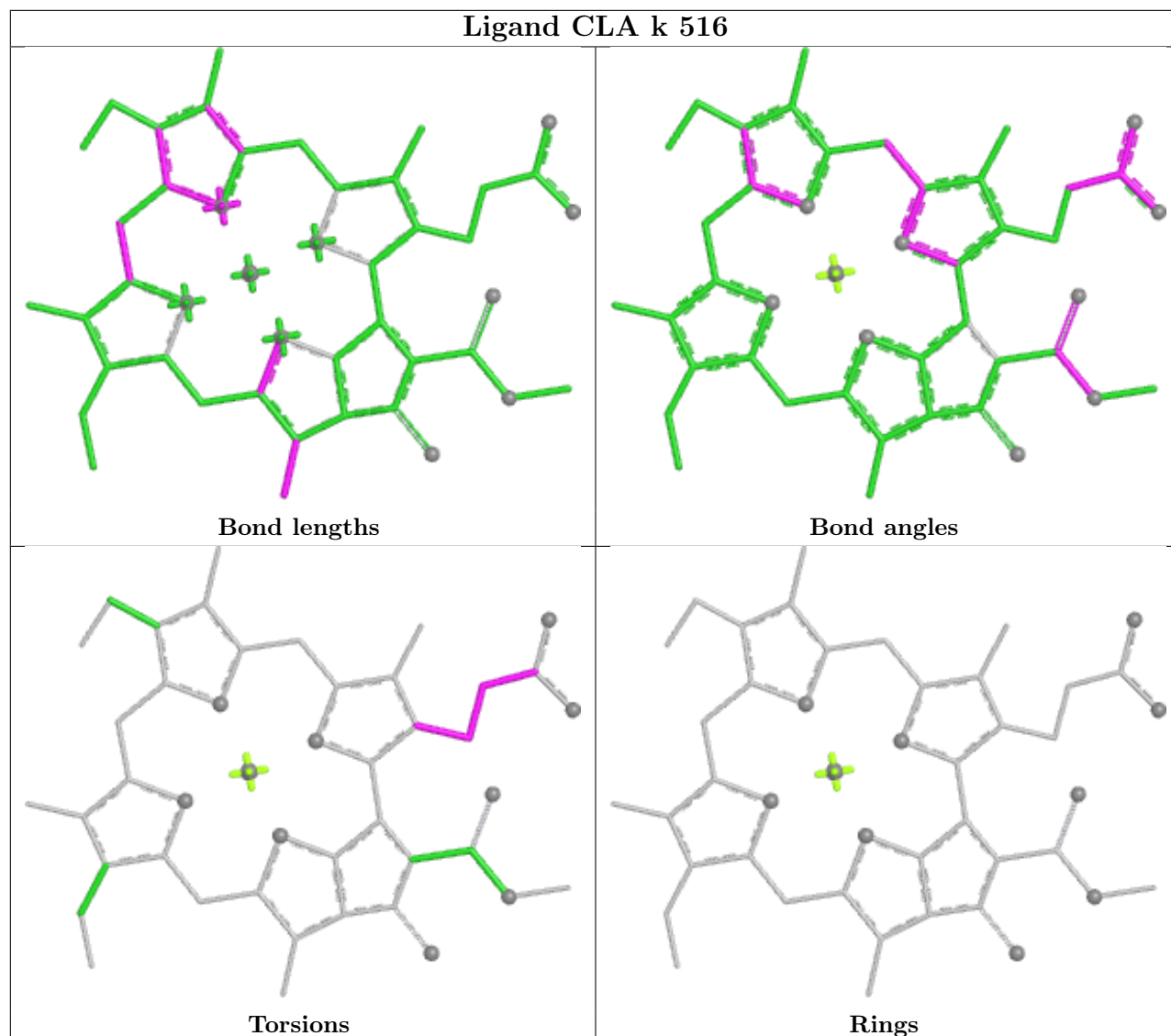


Torsions

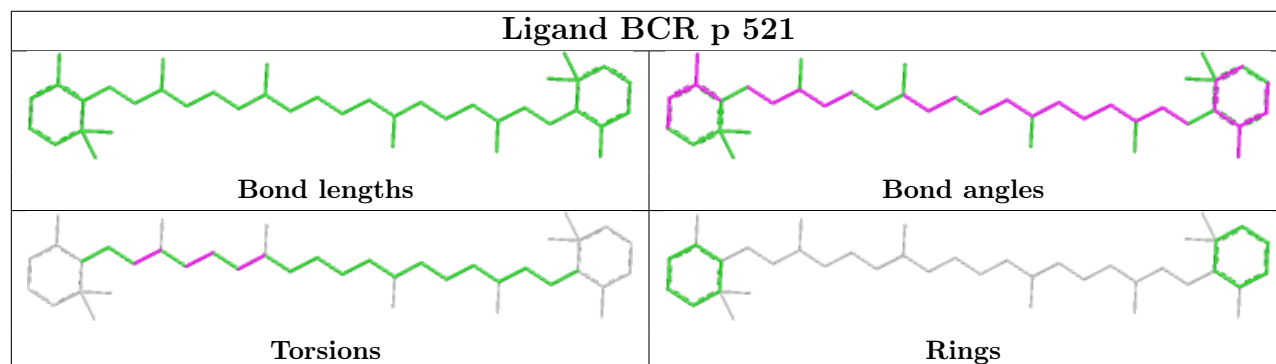


Rings

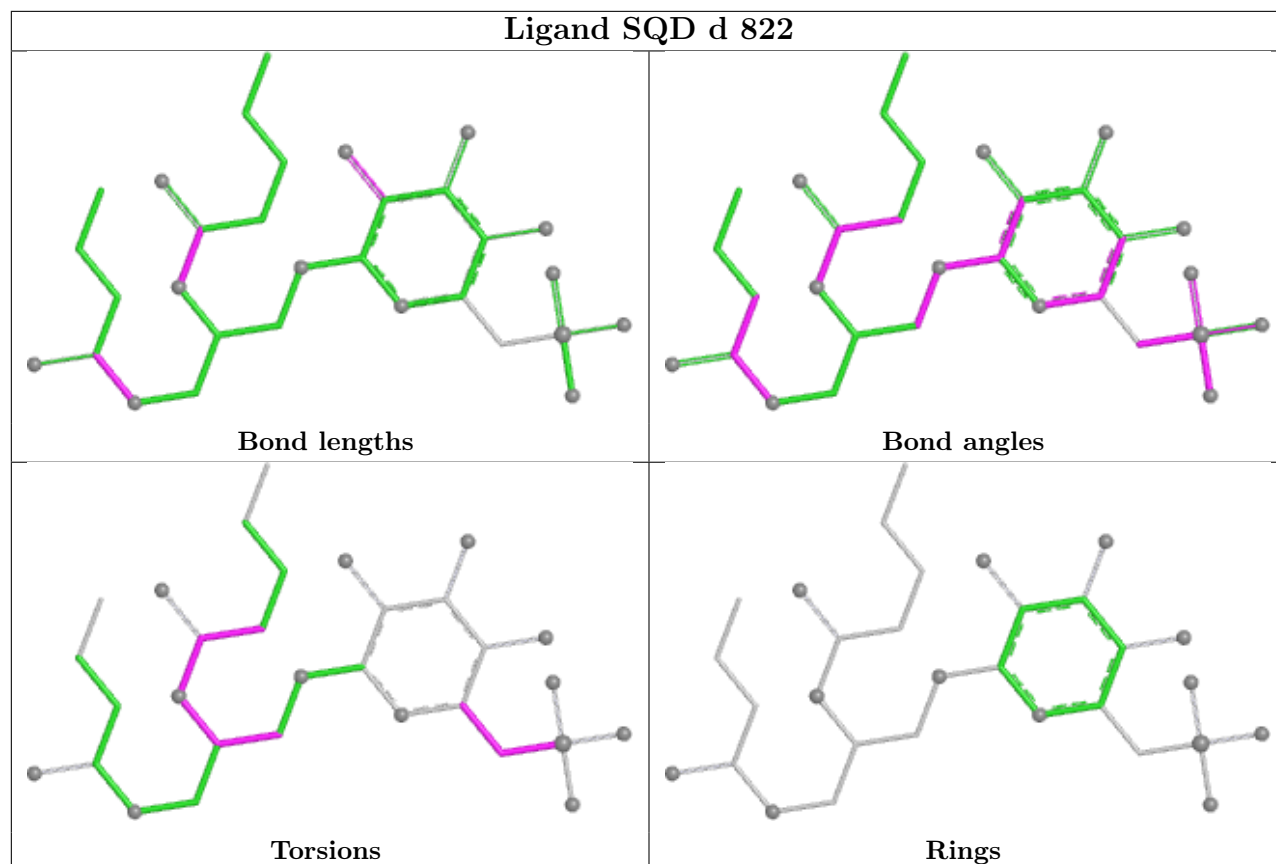
Ligand CLA k 516



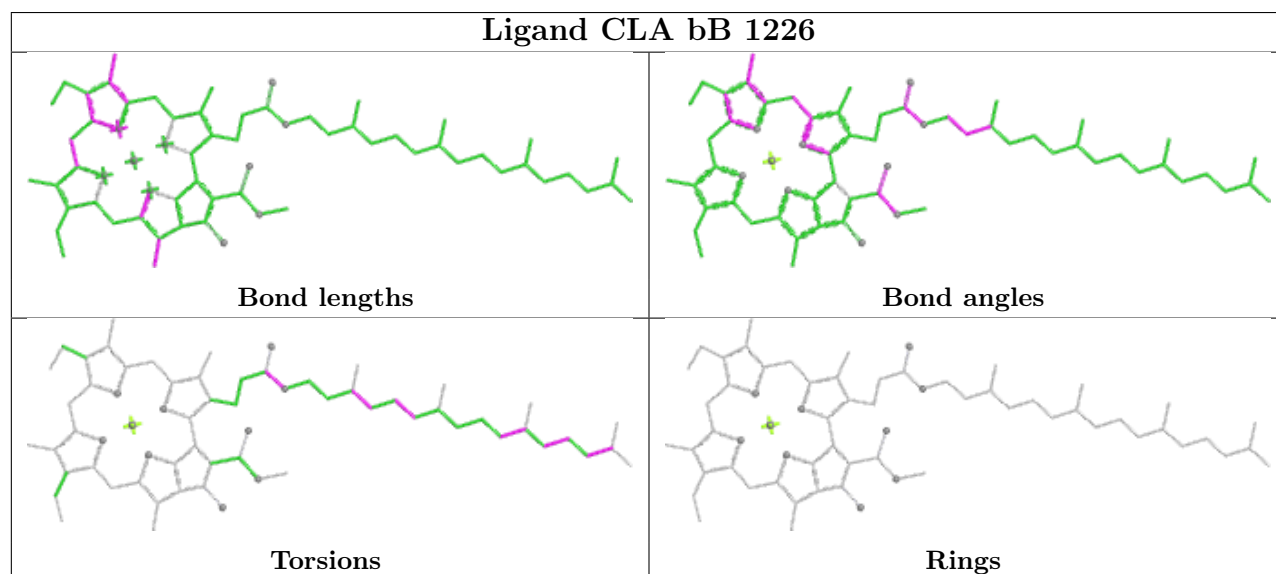
Ligand BCR p 521



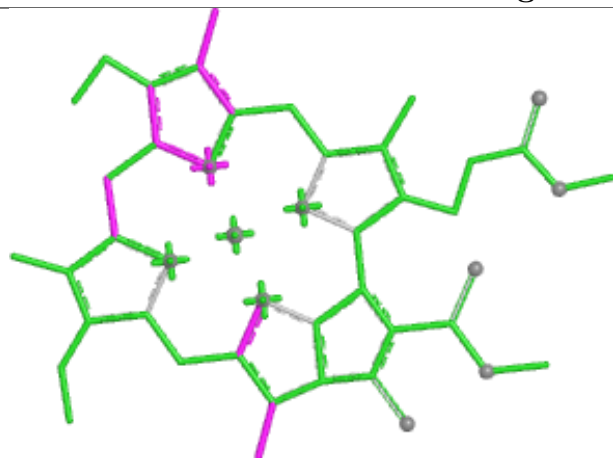
Ligand SQD d 822



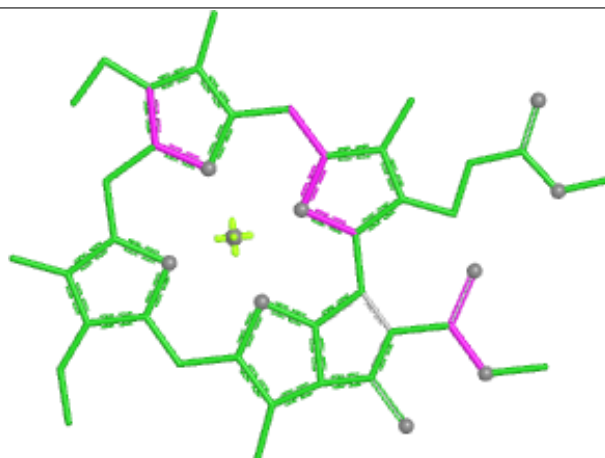
Ligand CLA bB 1226



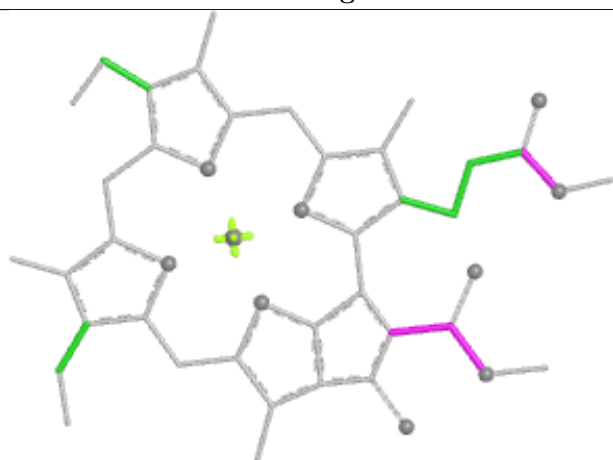
Ligand CLA S 502



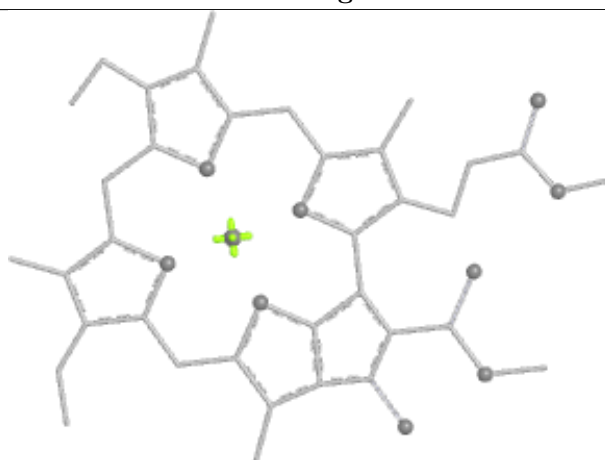
Bond lengths



Bond angles

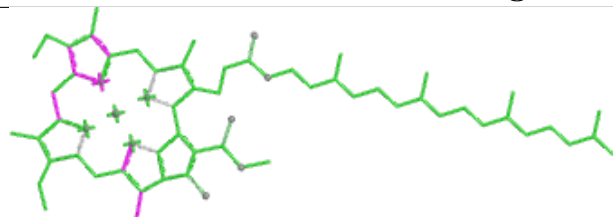


Torsions

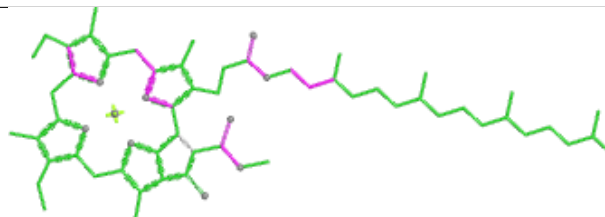


Rings

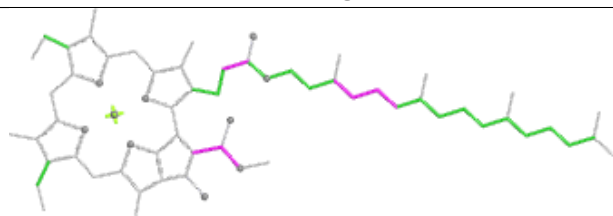
Ligand CLA b3 510



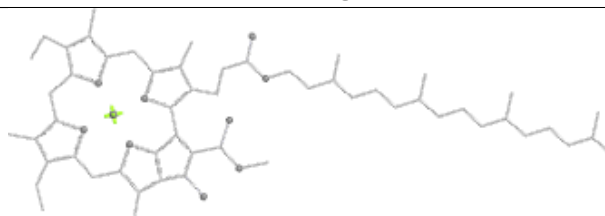
Bond lengths



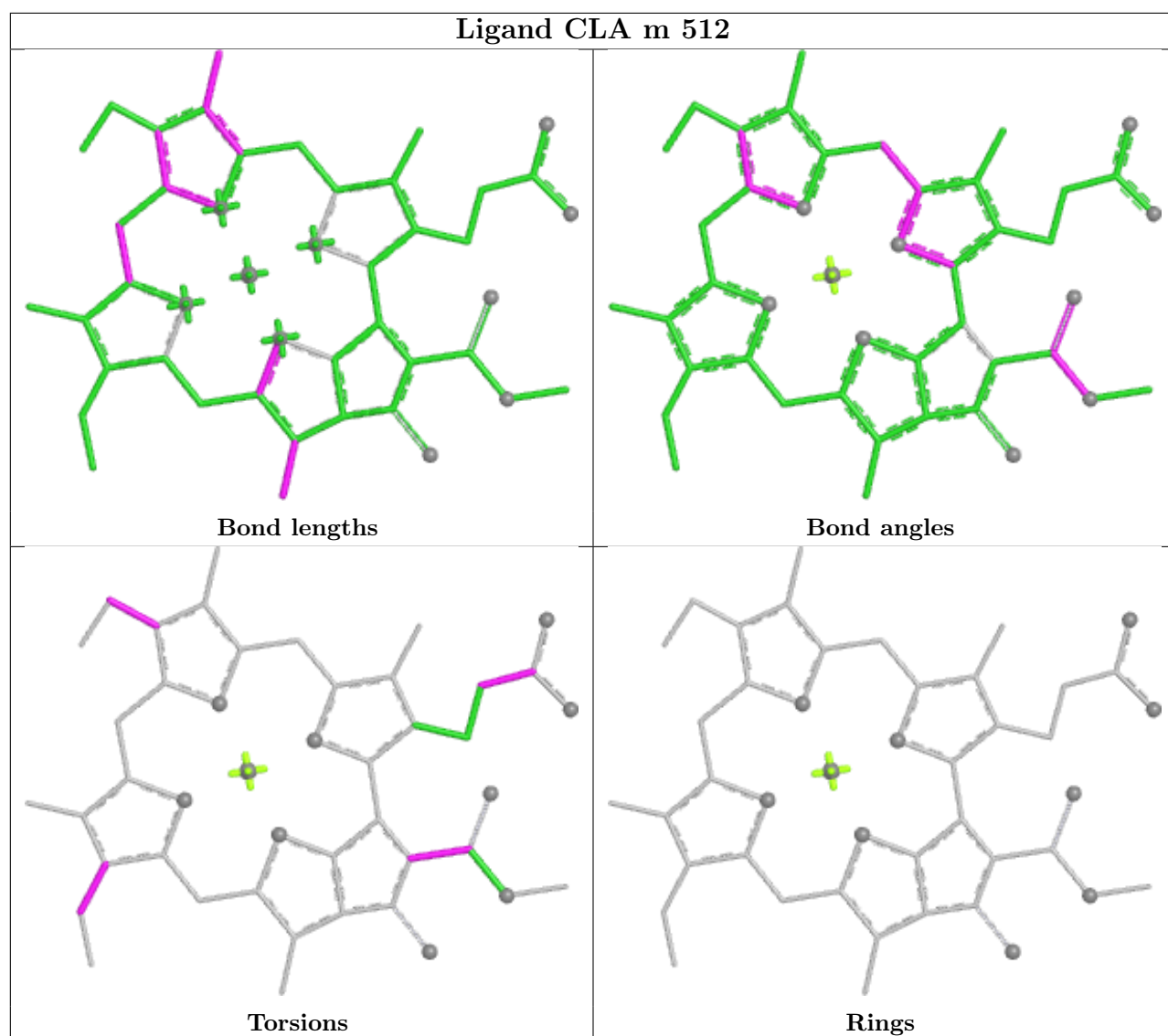
Bond angles



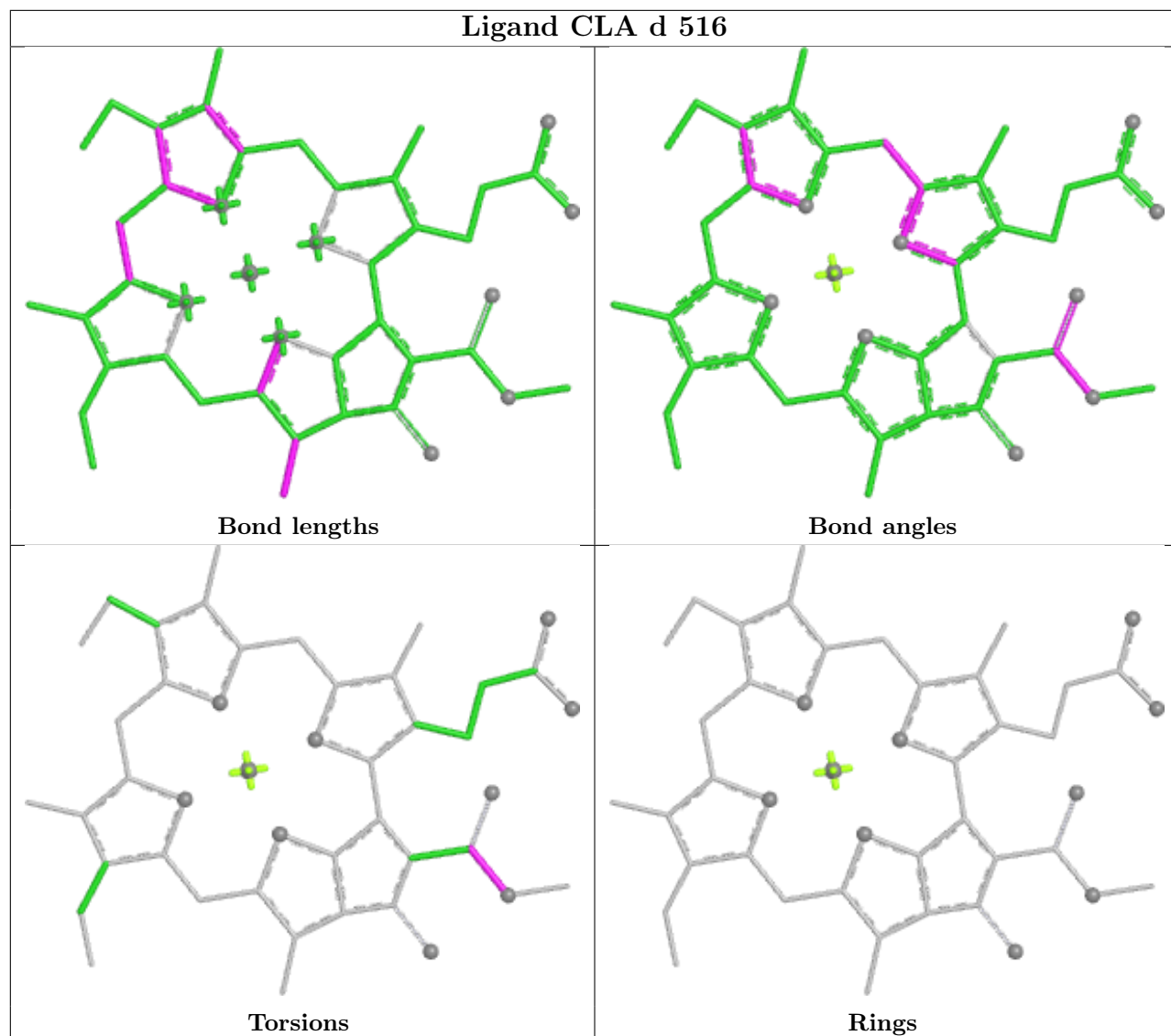
Torsions

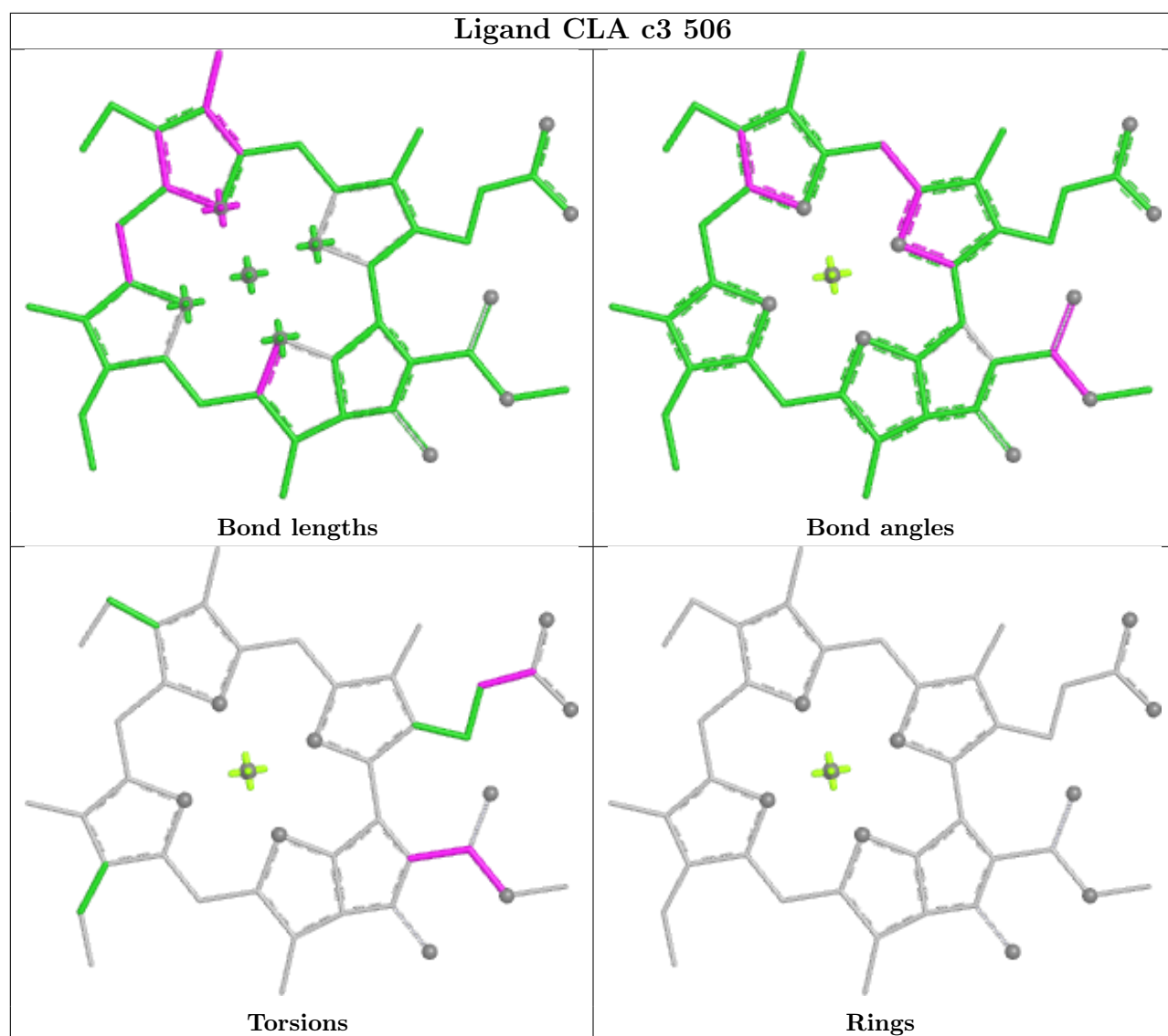


Rings

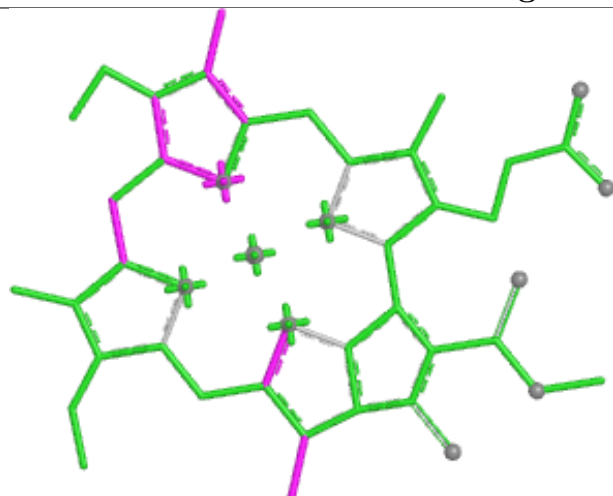


Ligand CLA d 516

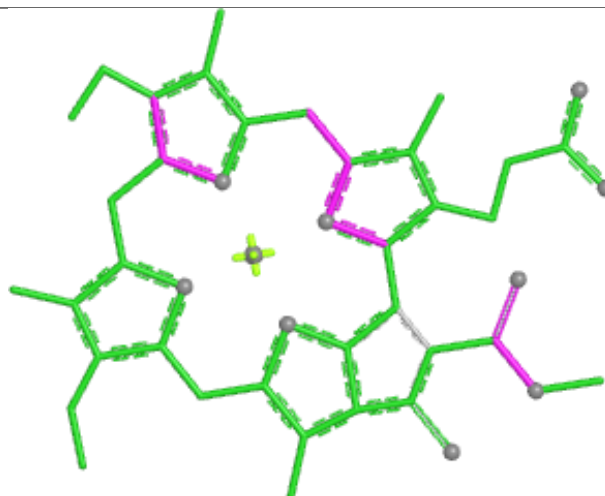




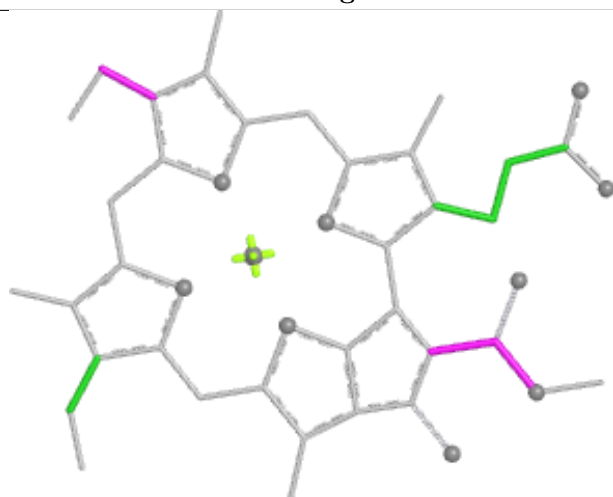
Ligand CLA a 502



Bond lengths



Bond angles

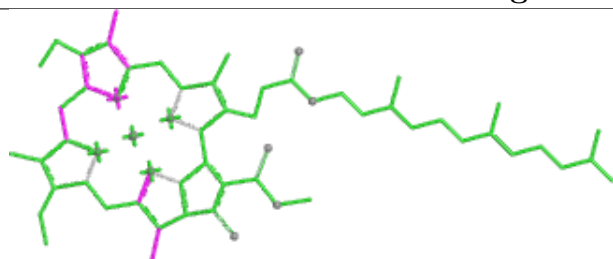


Torsions

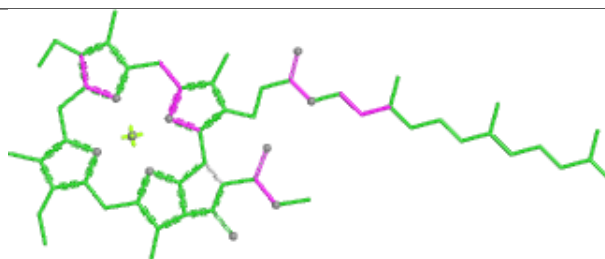


Rings

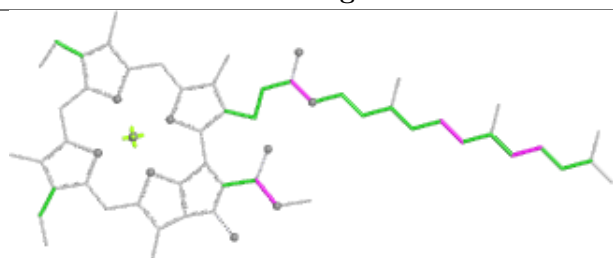
Ligand CLA c1 502



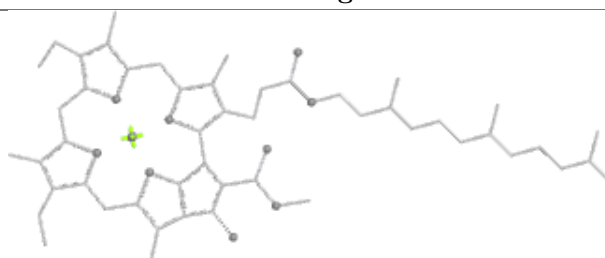
Bond lengths



Bond angles

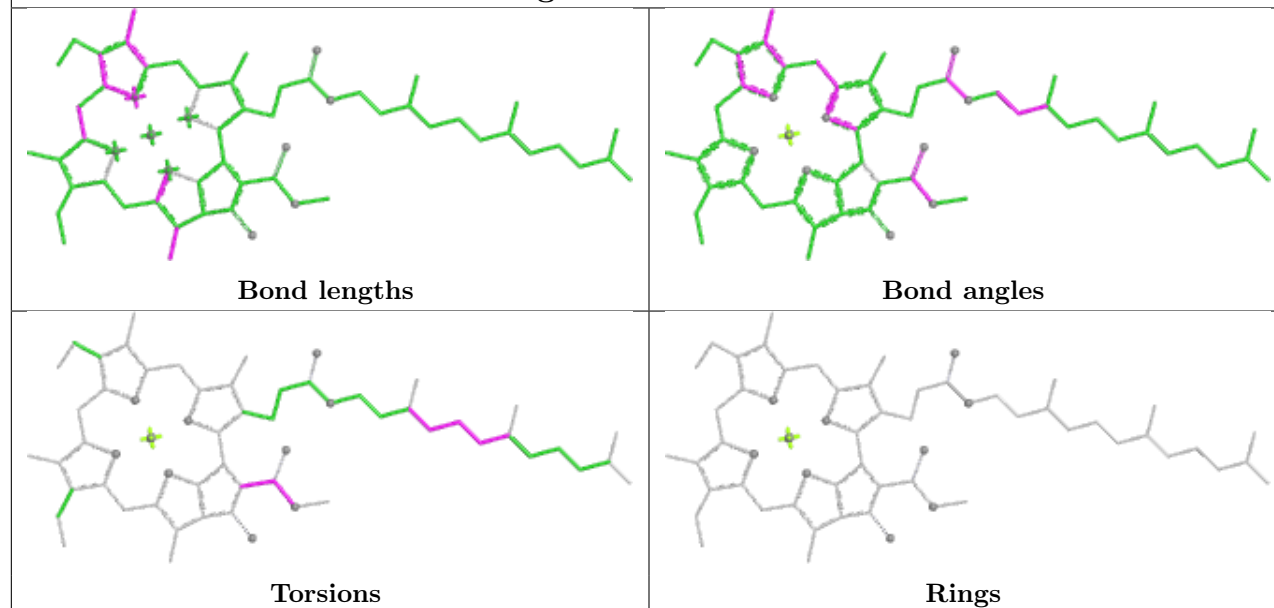


Torsions

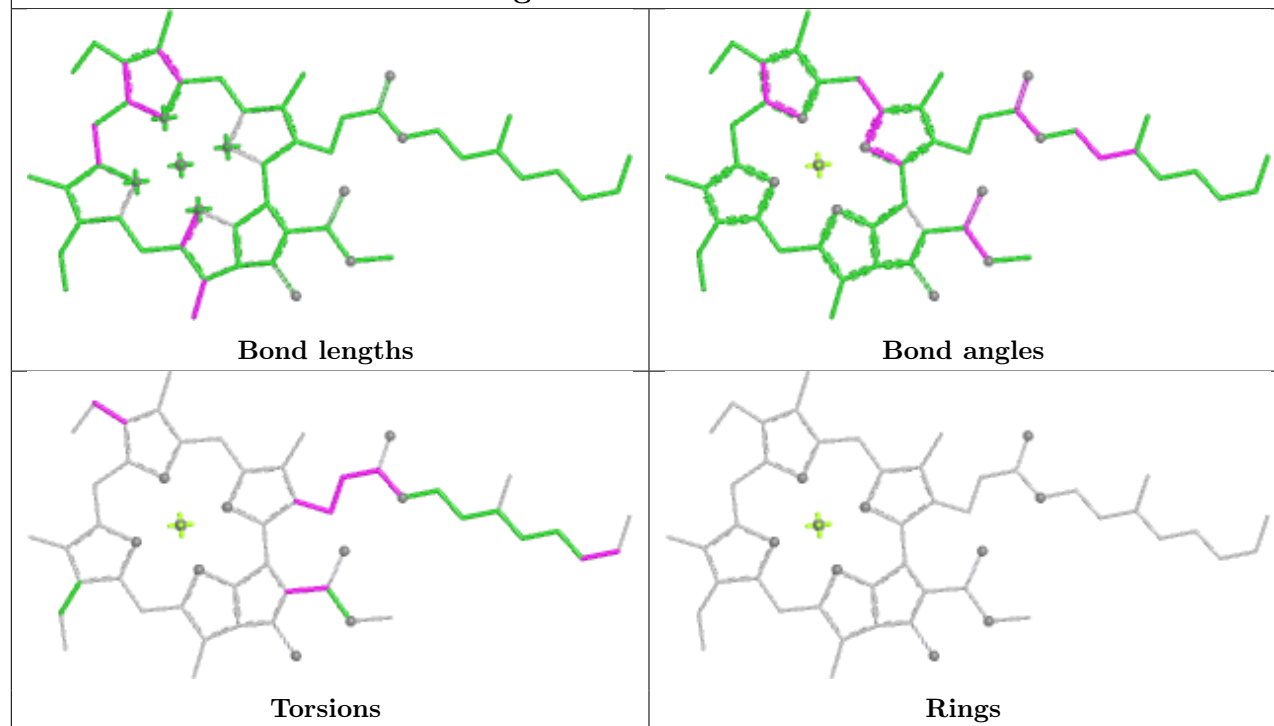


Rings

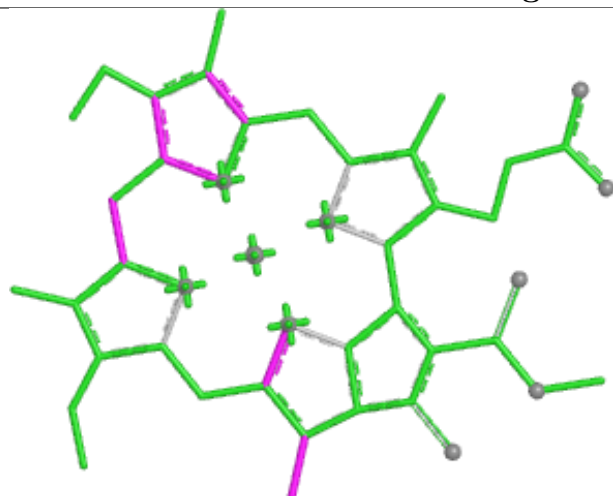
Ligand CLA c 510



Ligand CLA bB 1227



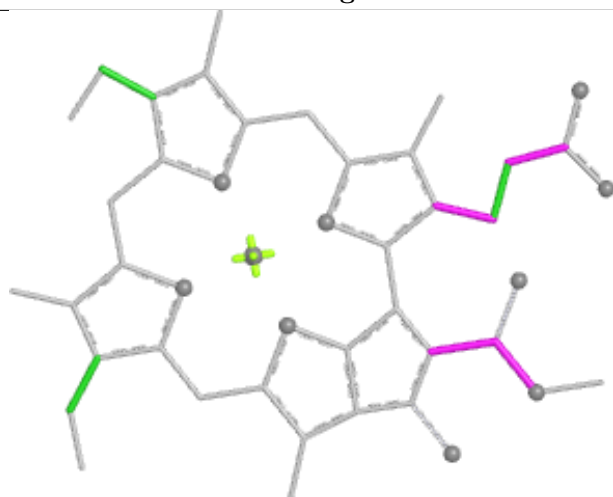
Ligand CLA 1 516



Bond lengths



Bond angles

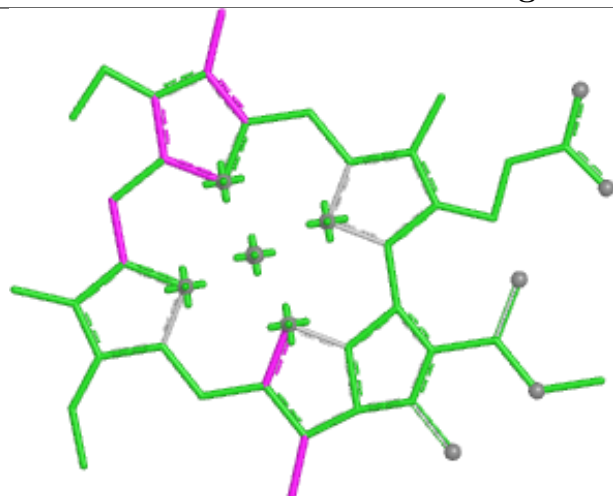


Torsions

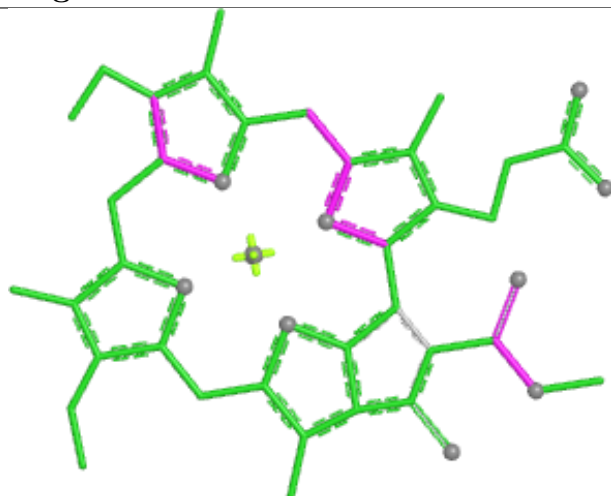


Rings

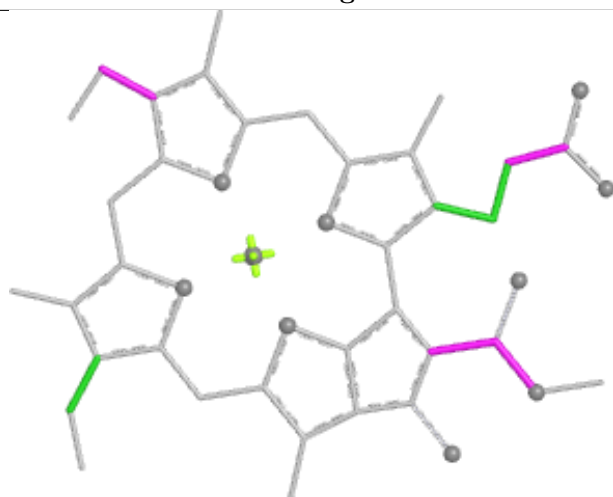
Ligand CLA g 519



Bond lengths



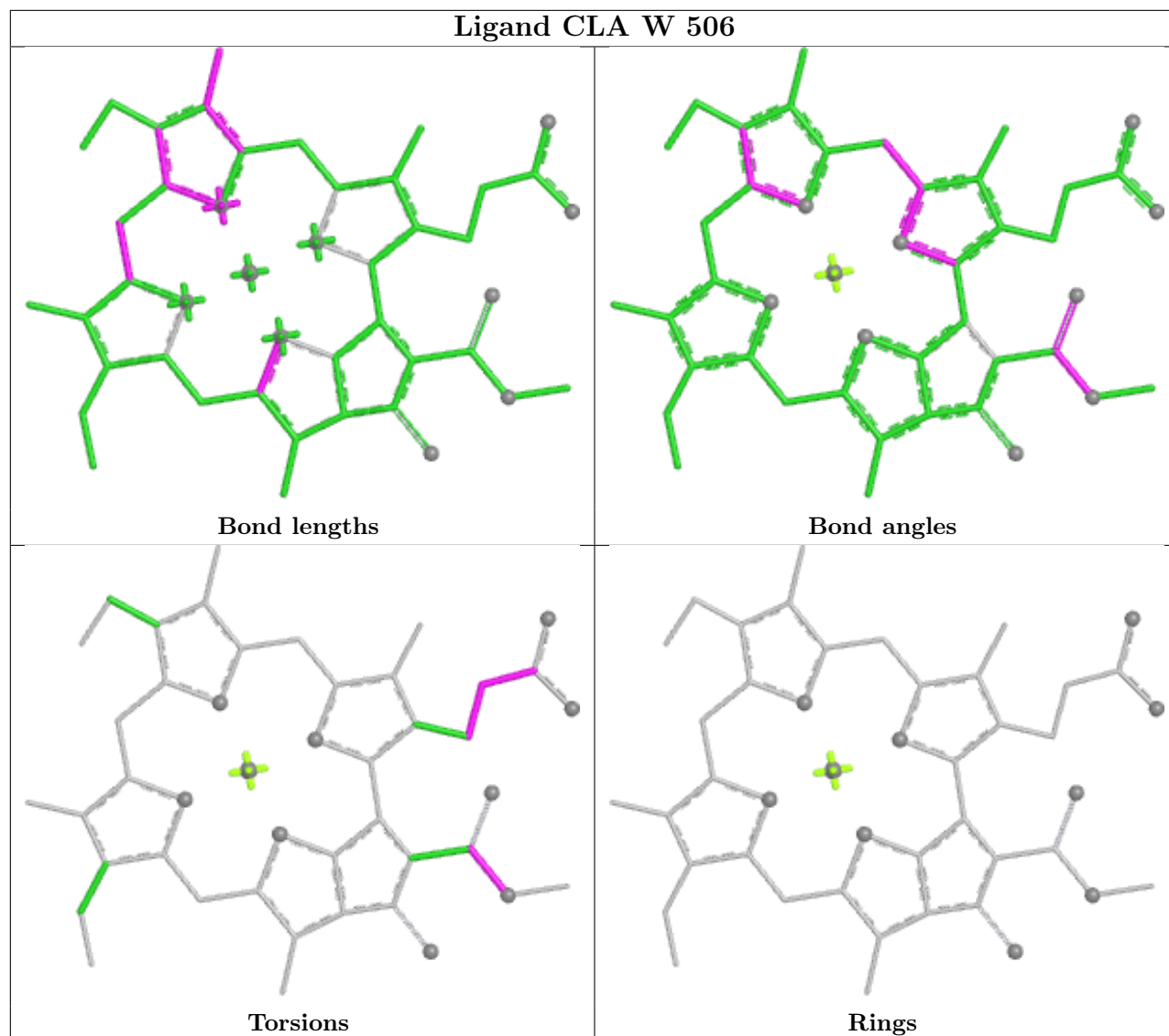
Bond angles

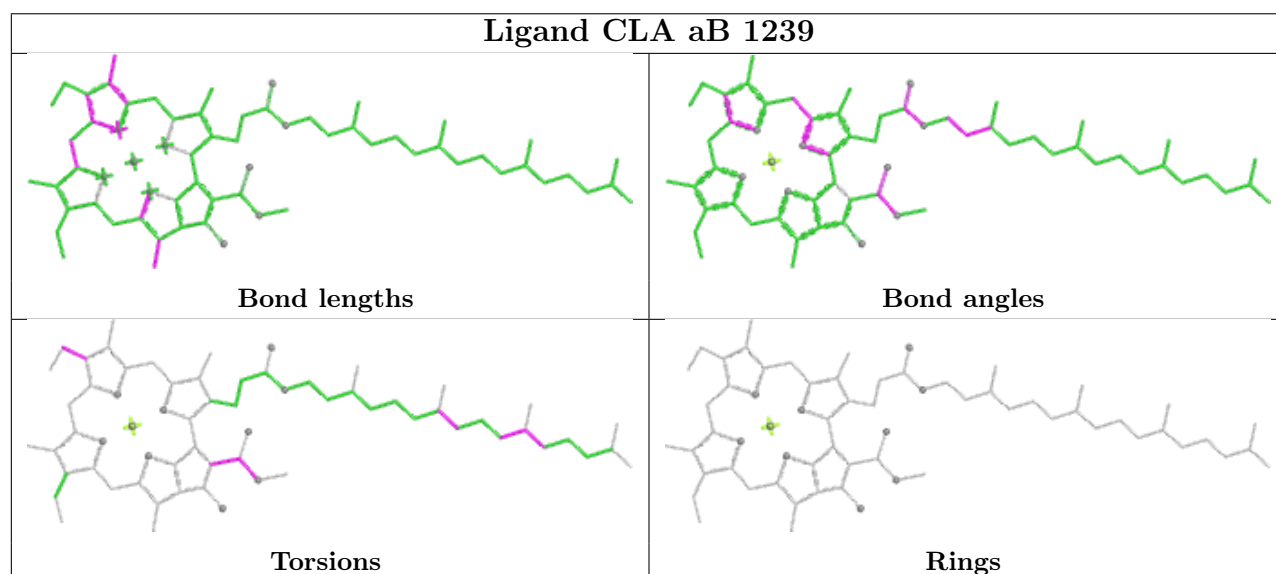
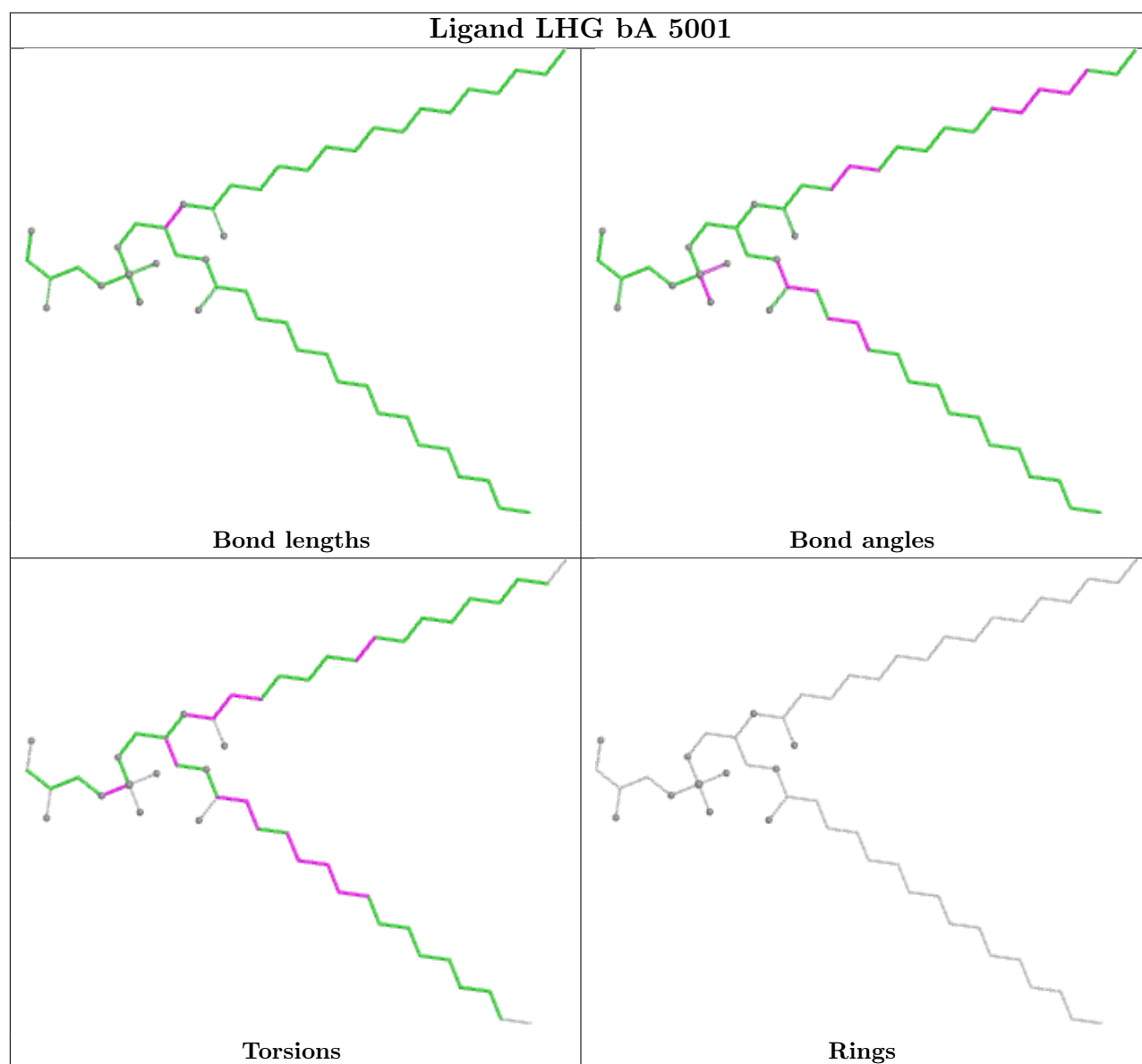


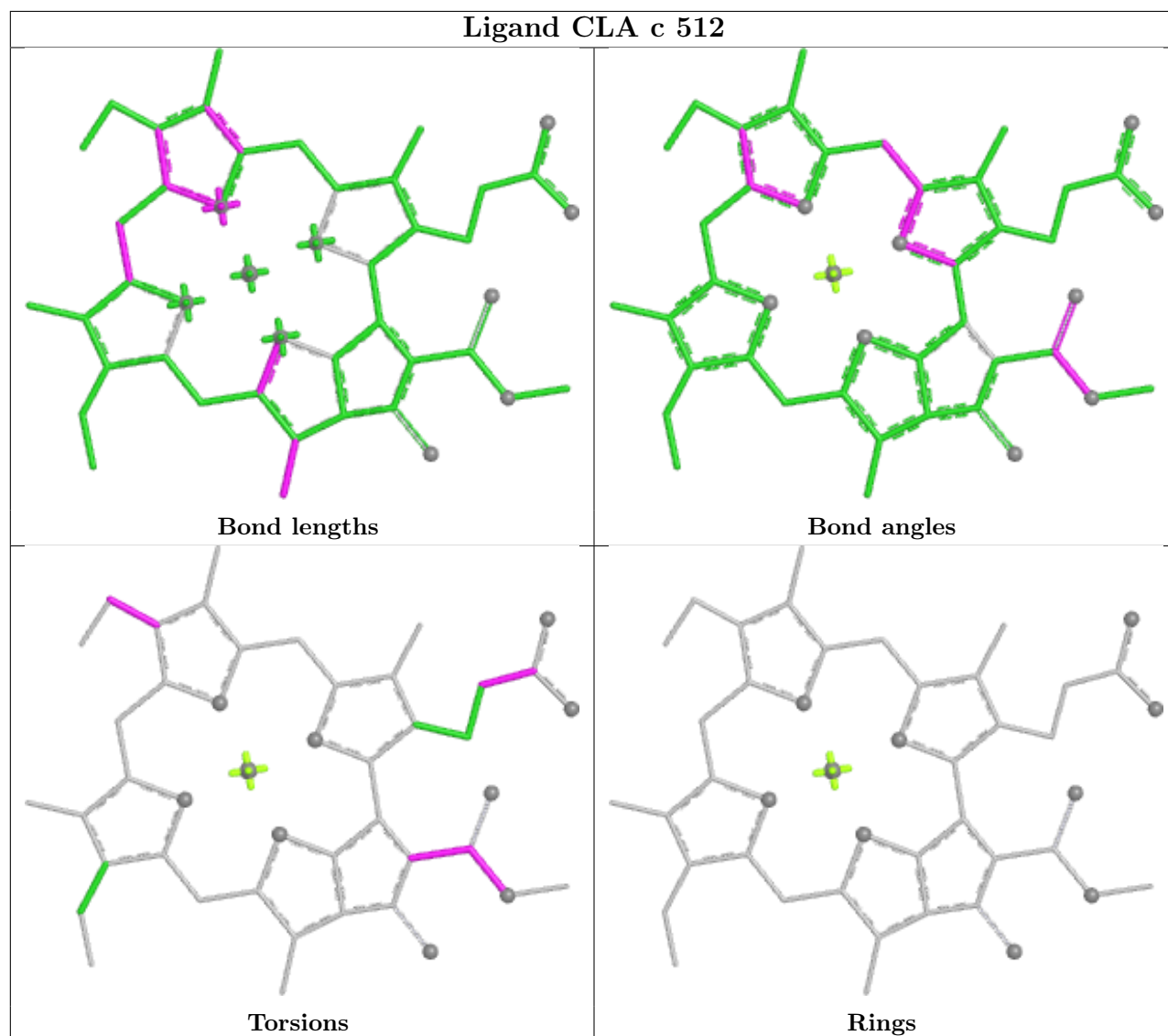
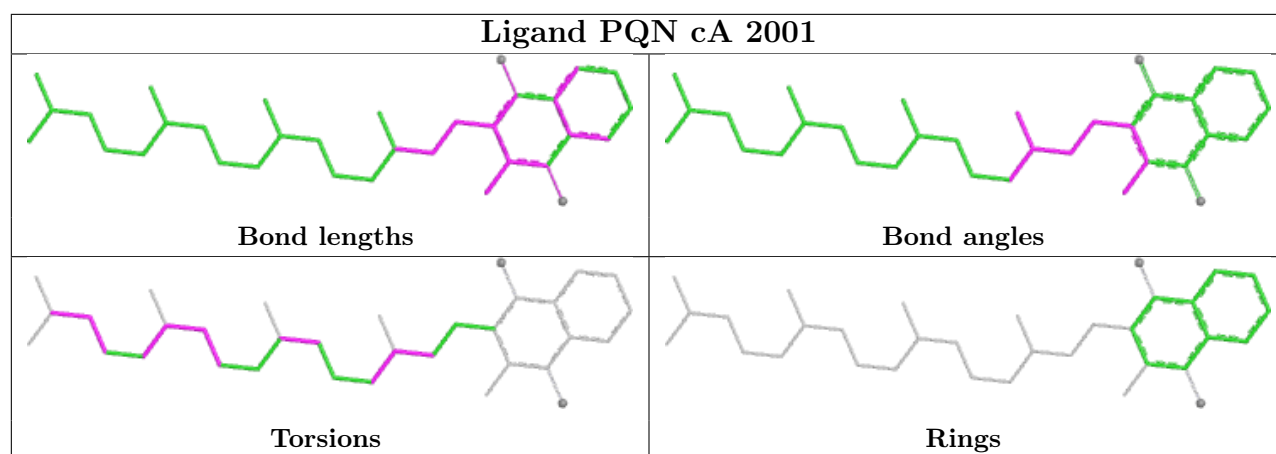
Torsions

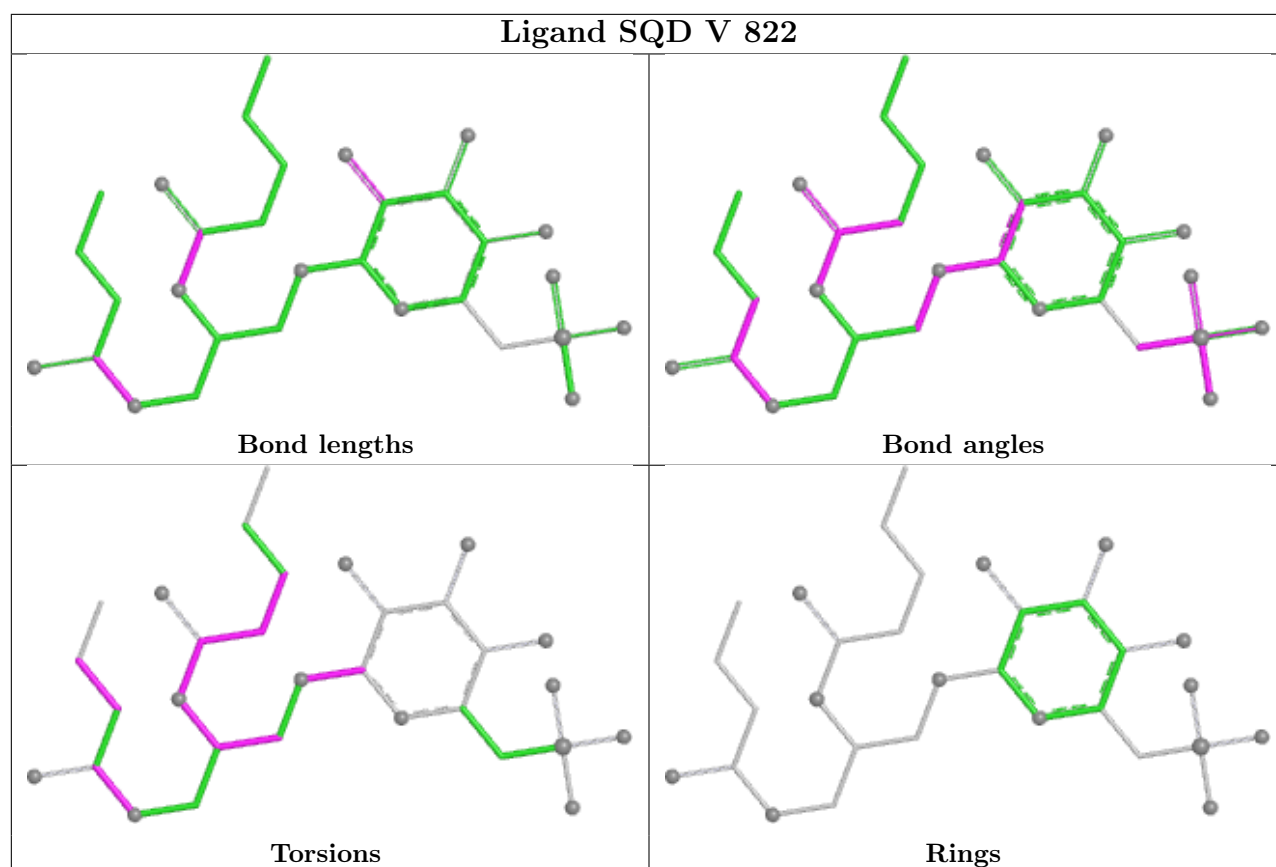


Rings

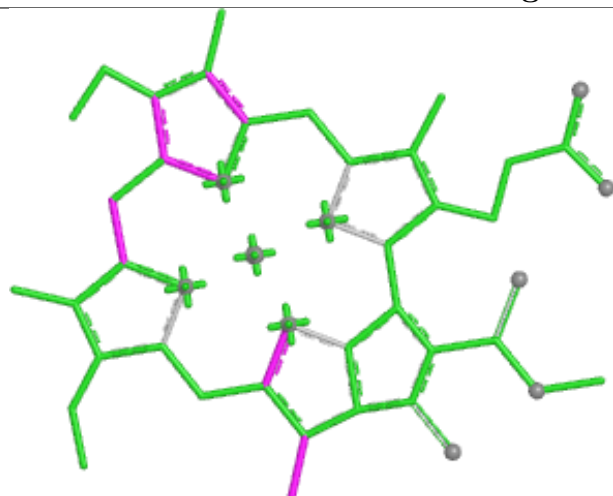




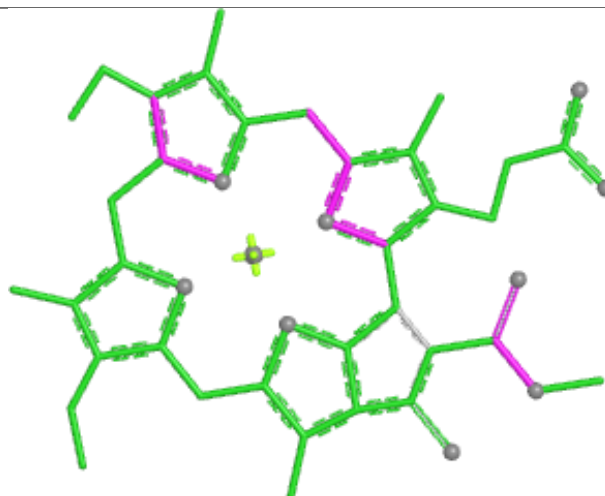




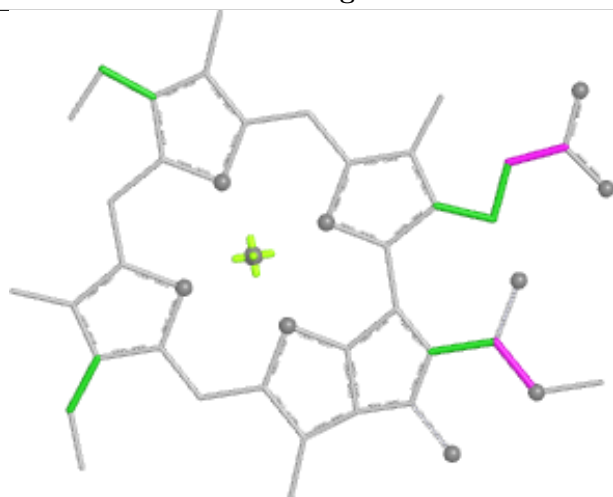
Ligand CLA f 519



Bond lengths



Bond angles

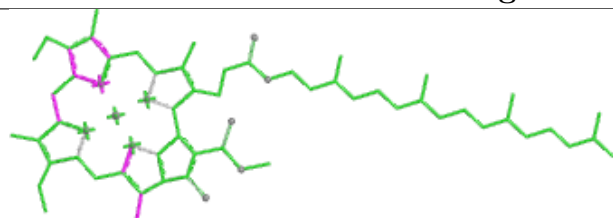


Torsions

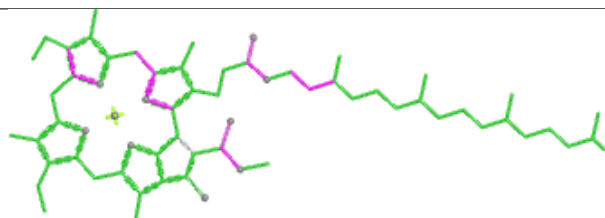


Rings

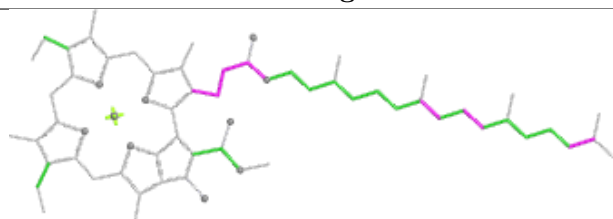
Ligand CLA aL 1503



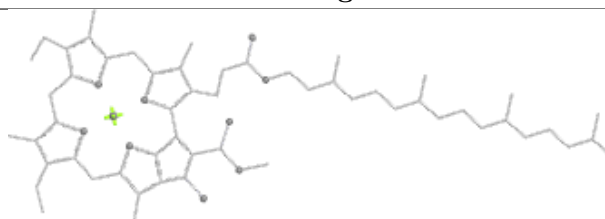
Bond lengths



Bond angles

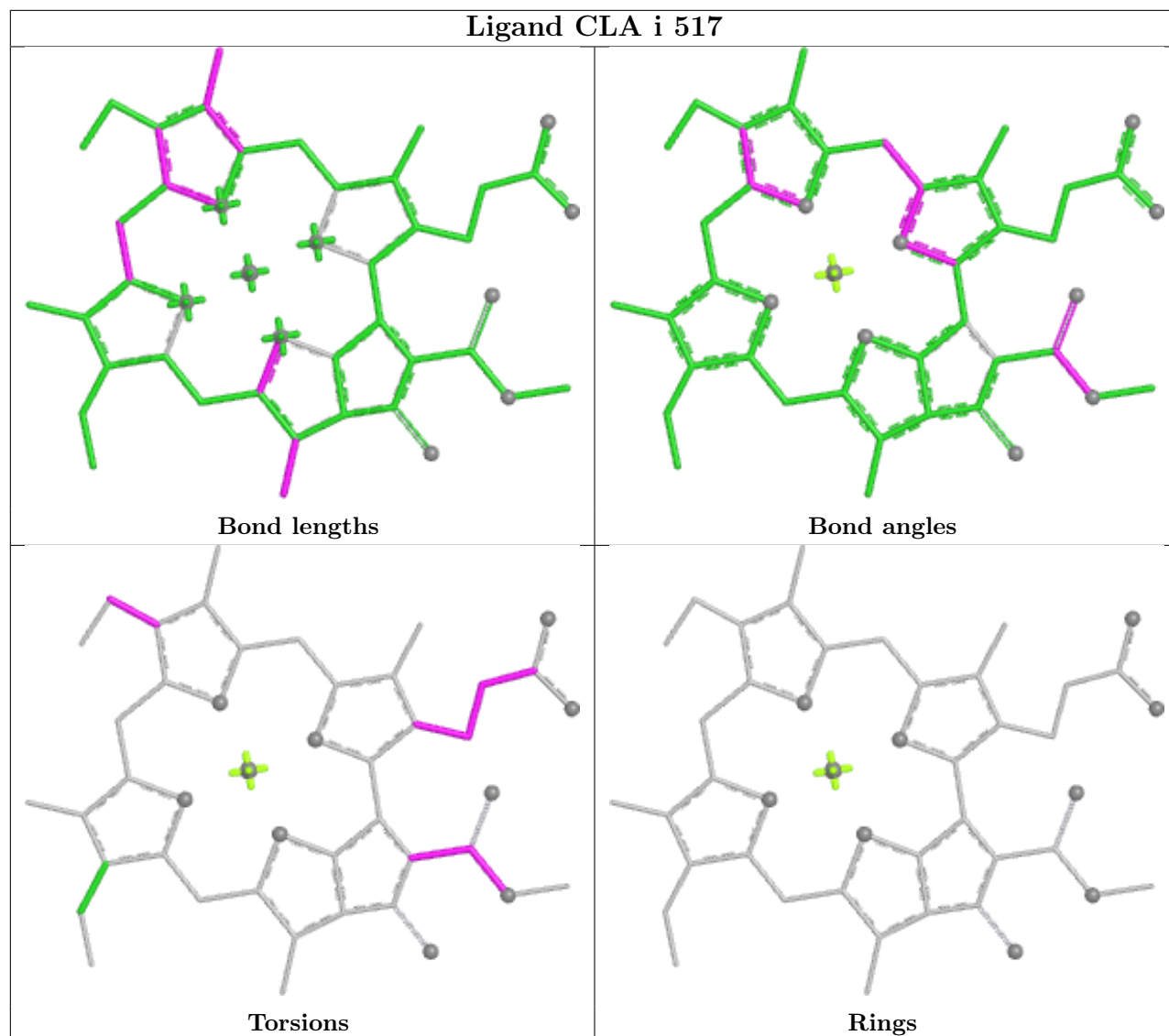


Torsions

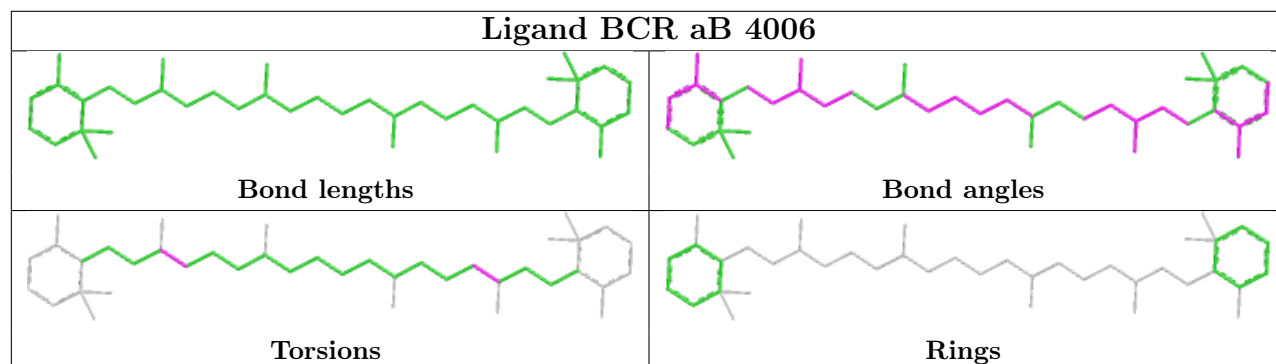


Rings

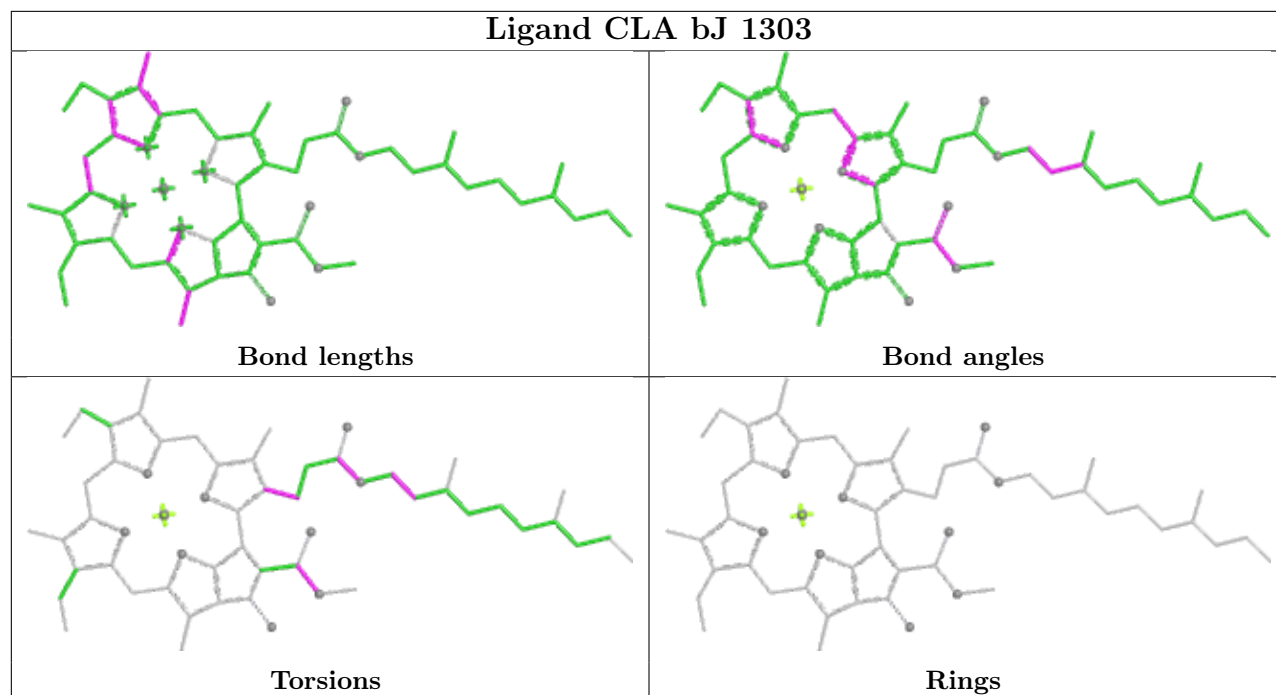
Ligand CLA i 517



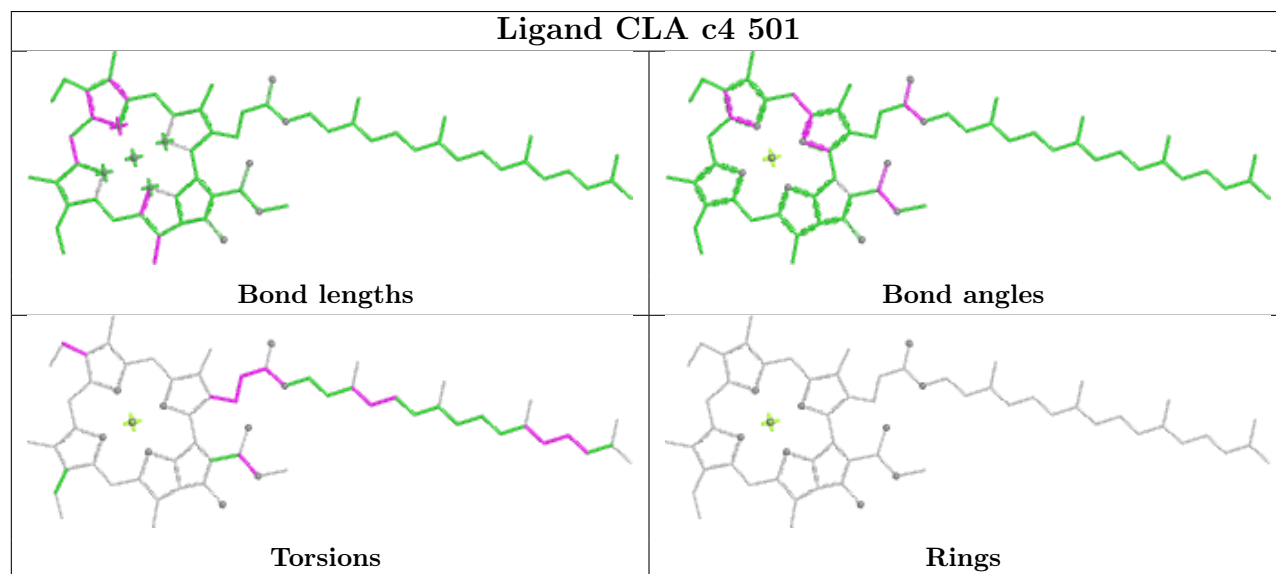
Ligand BCR aB 4006

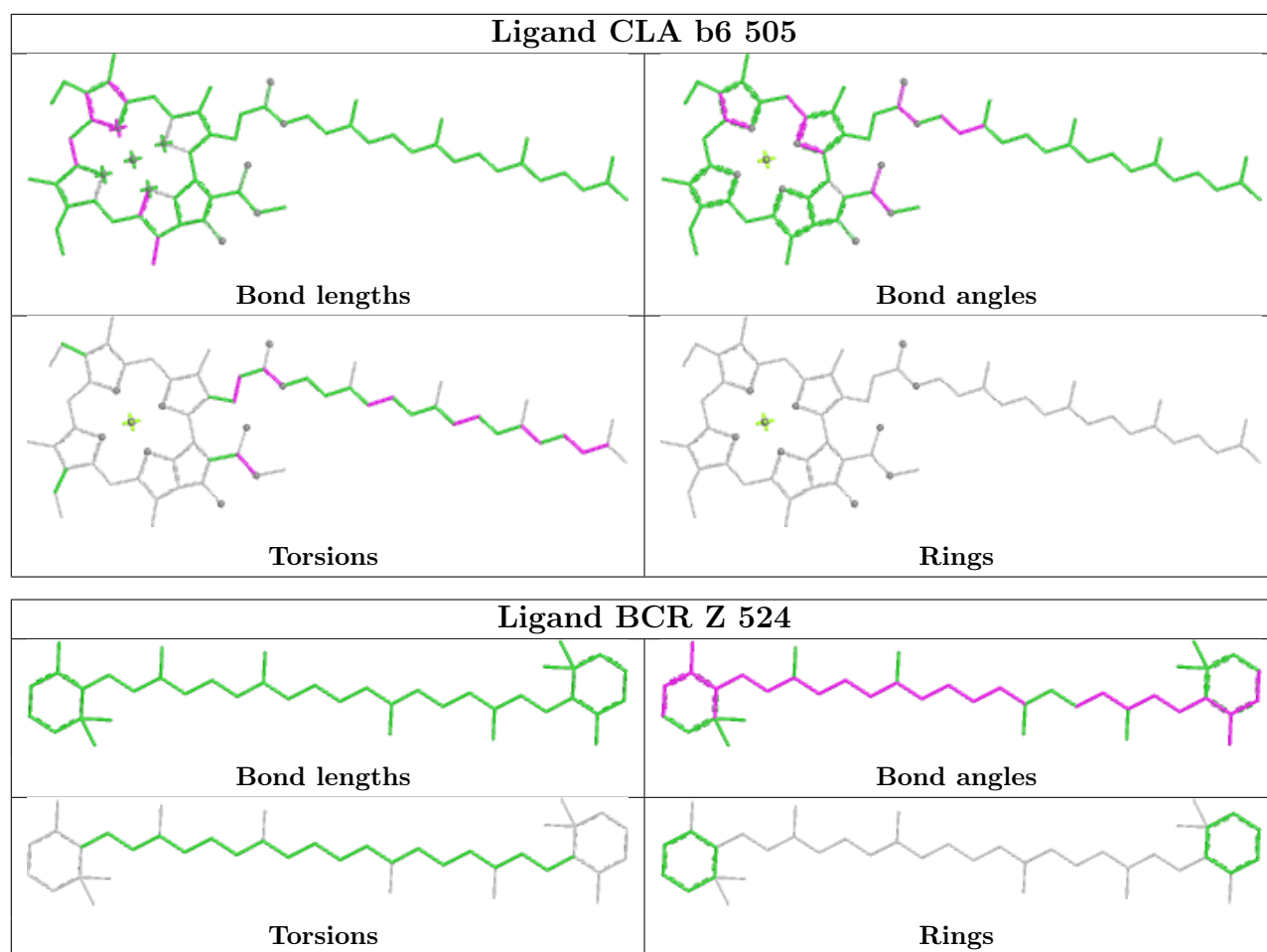


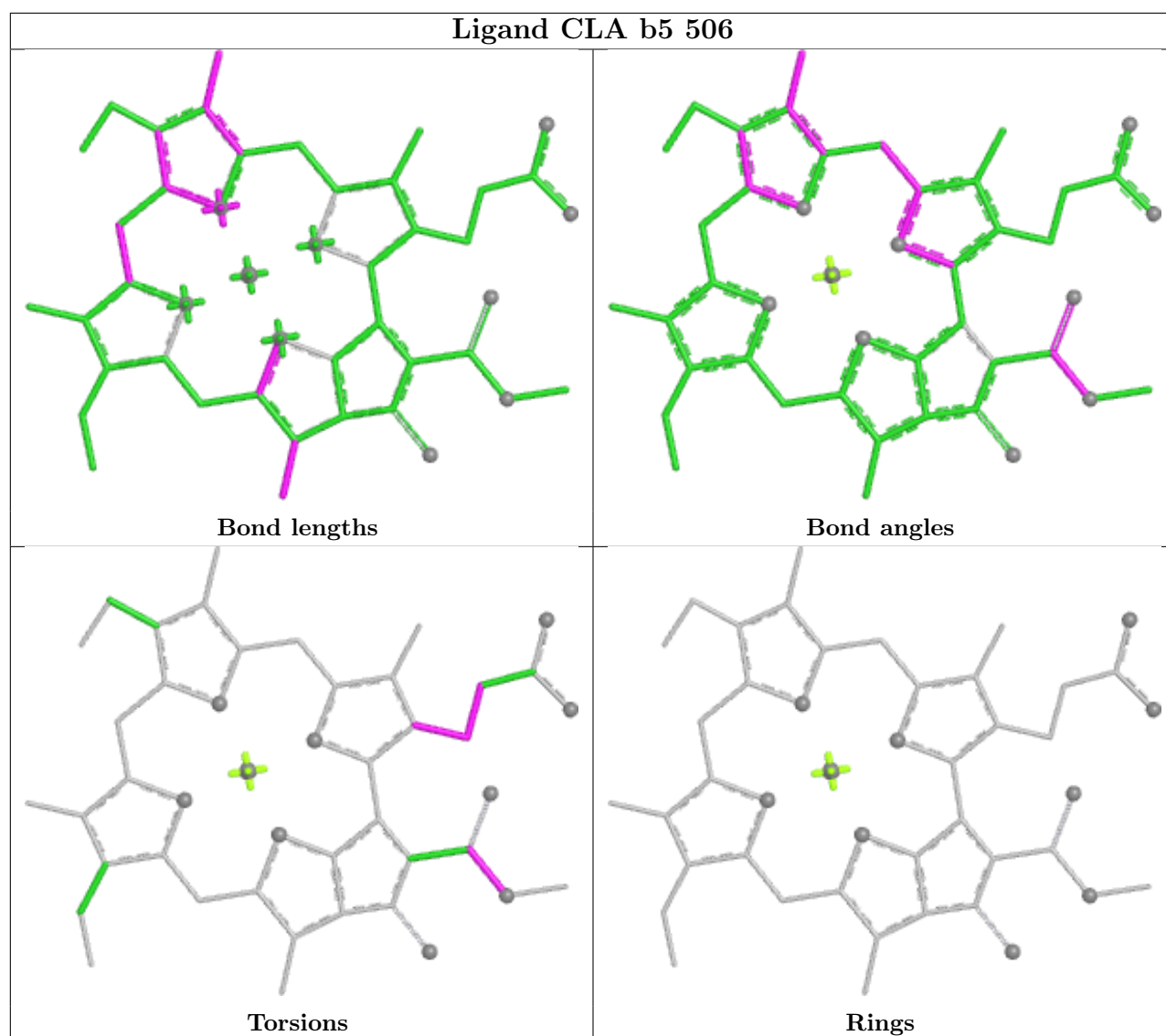
Ligand CLA bJ 1303

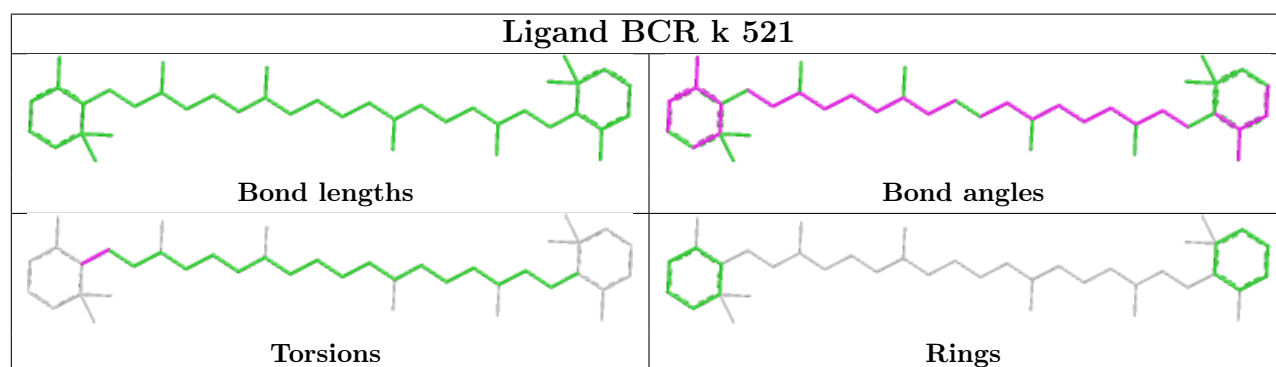
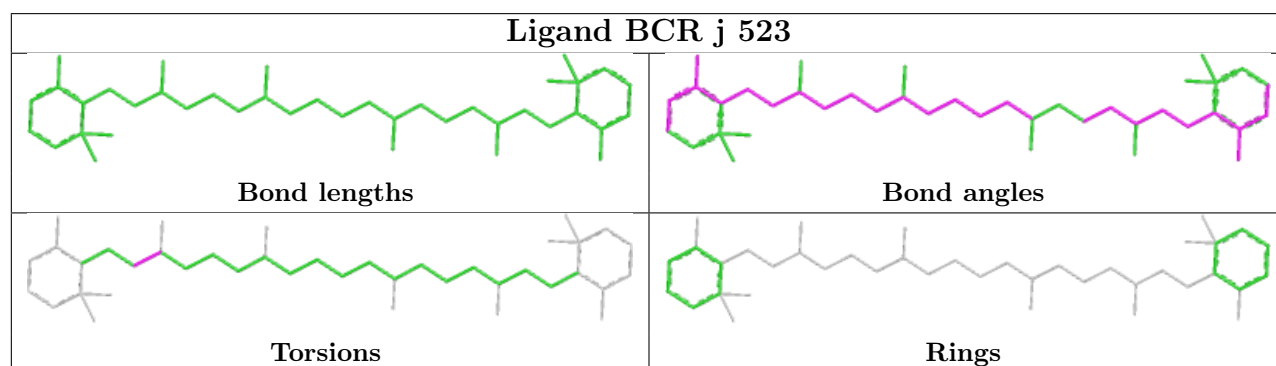
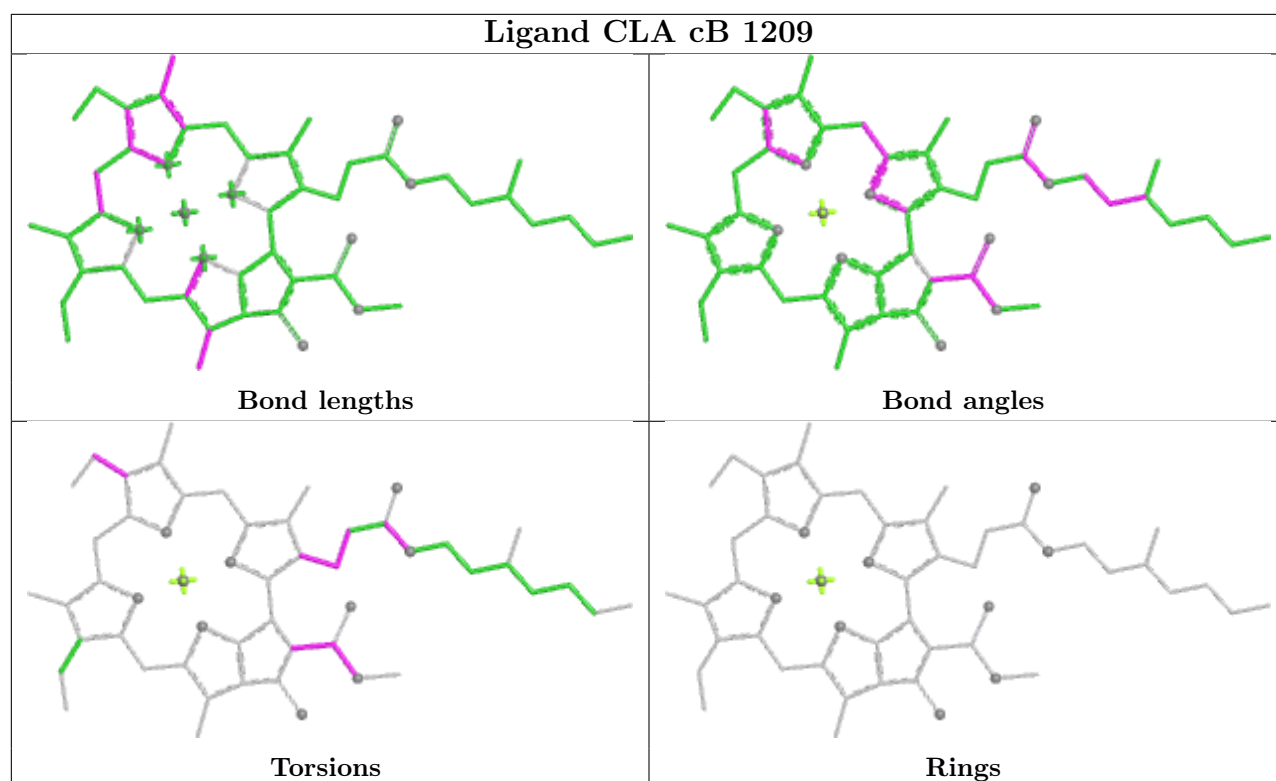


Ligand CLA c4 501

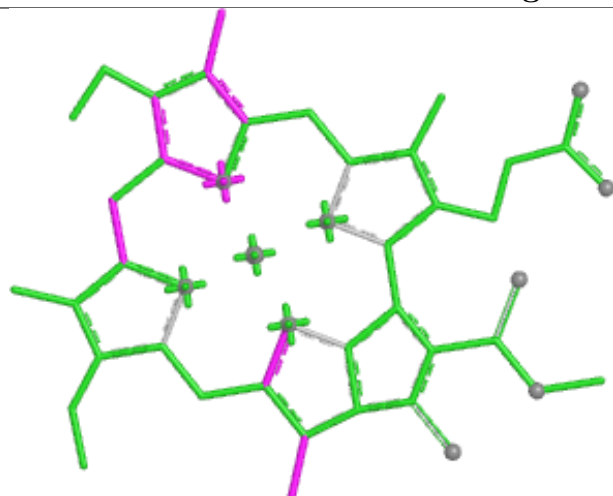








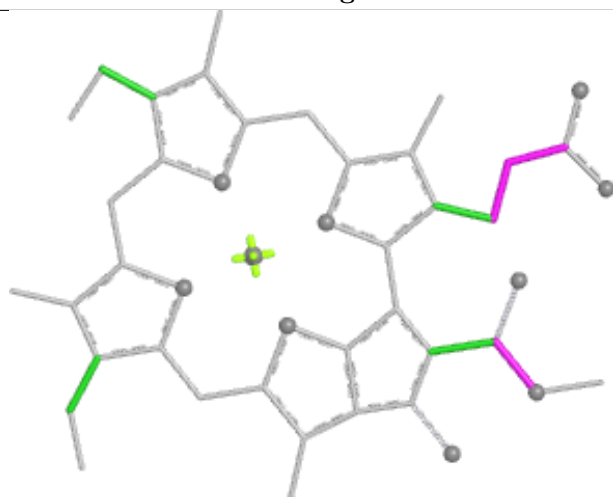
Ligand CLA i 511



Bond lengths



Bond angles

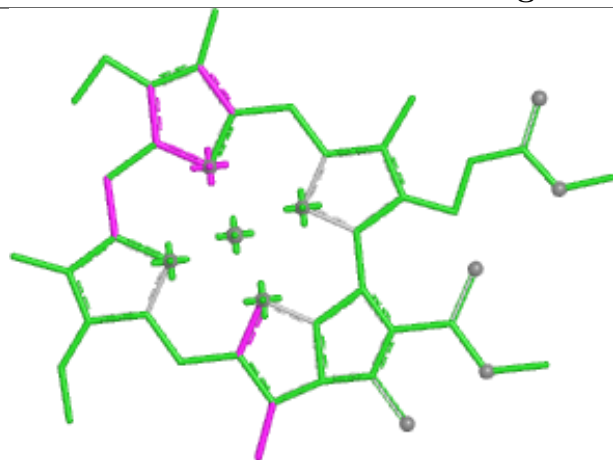


Torsions

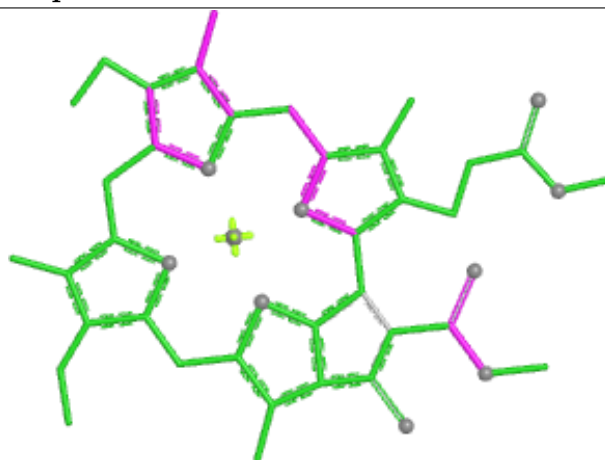


Rings

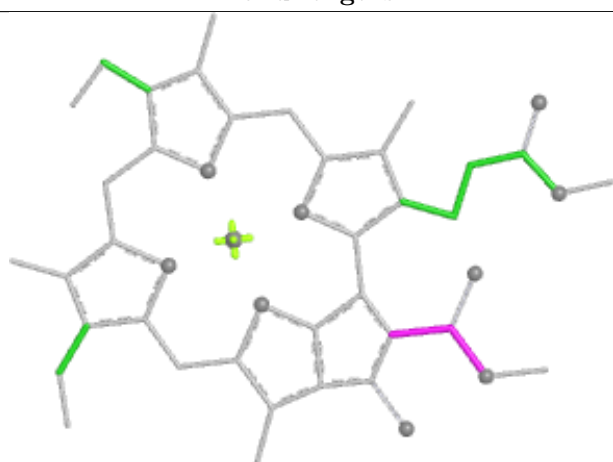
Ligand CLA p 510



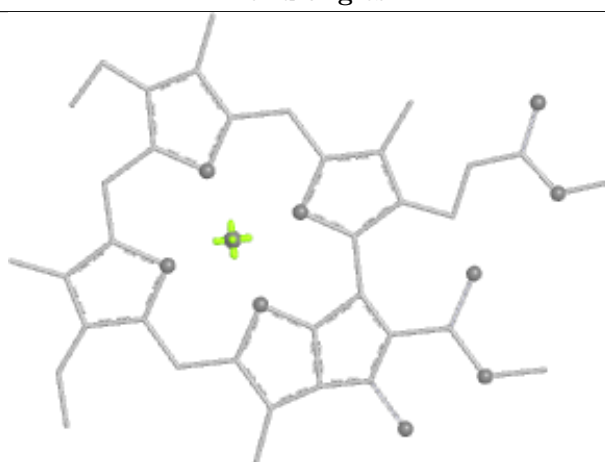
Bond lengths



Bond angles

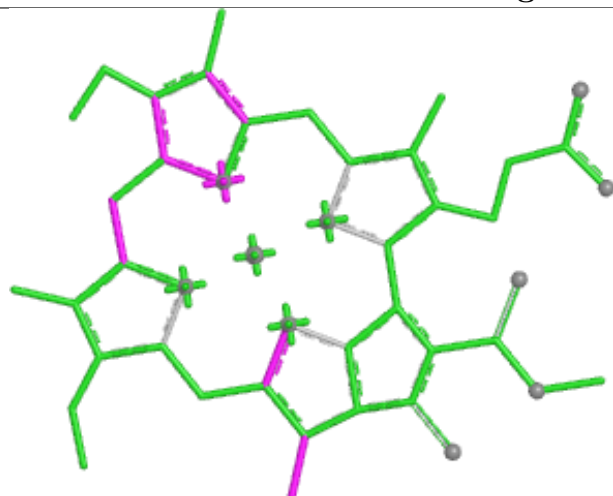


Torsions

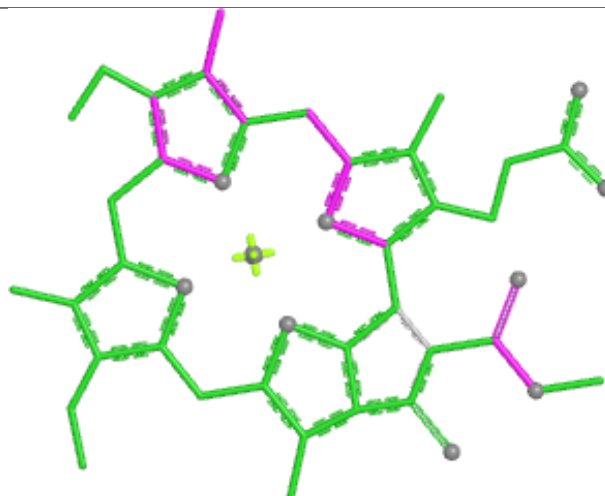


Rings

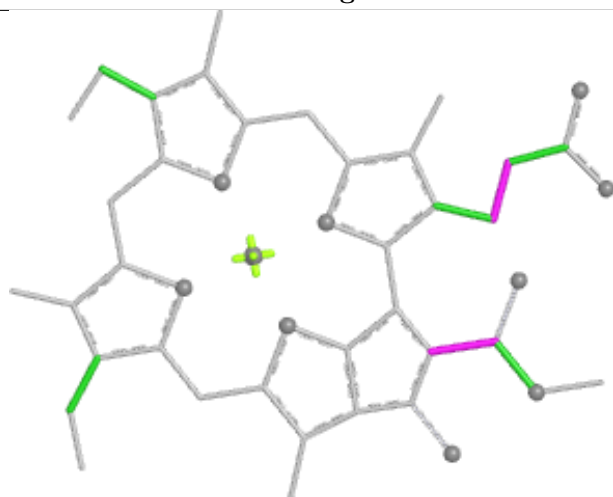
Ligand CLA n 513



Bond lengths



Bond angles

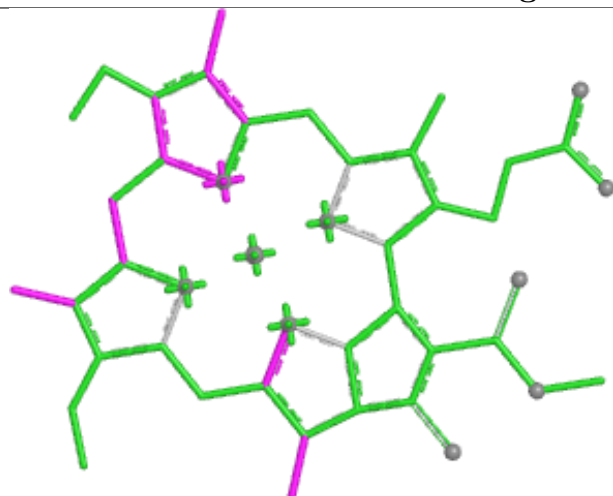


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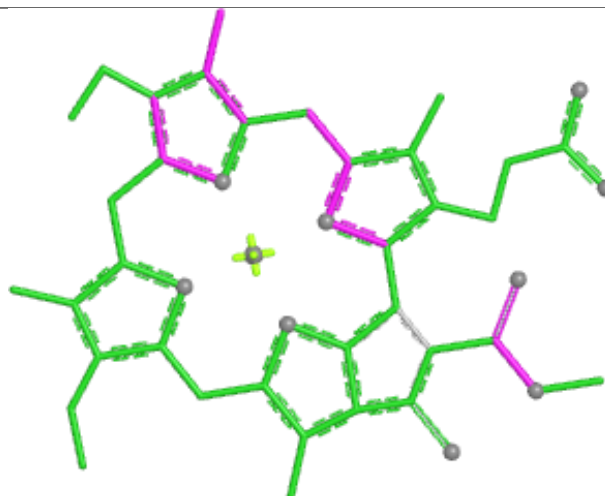


Rings

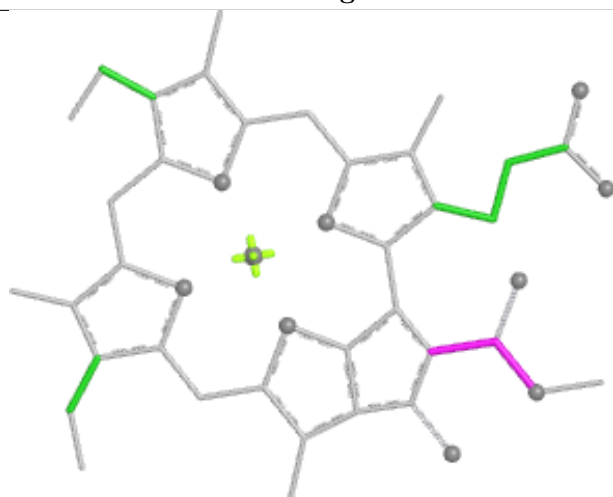
Ligand CLA c 506



Bond lengths



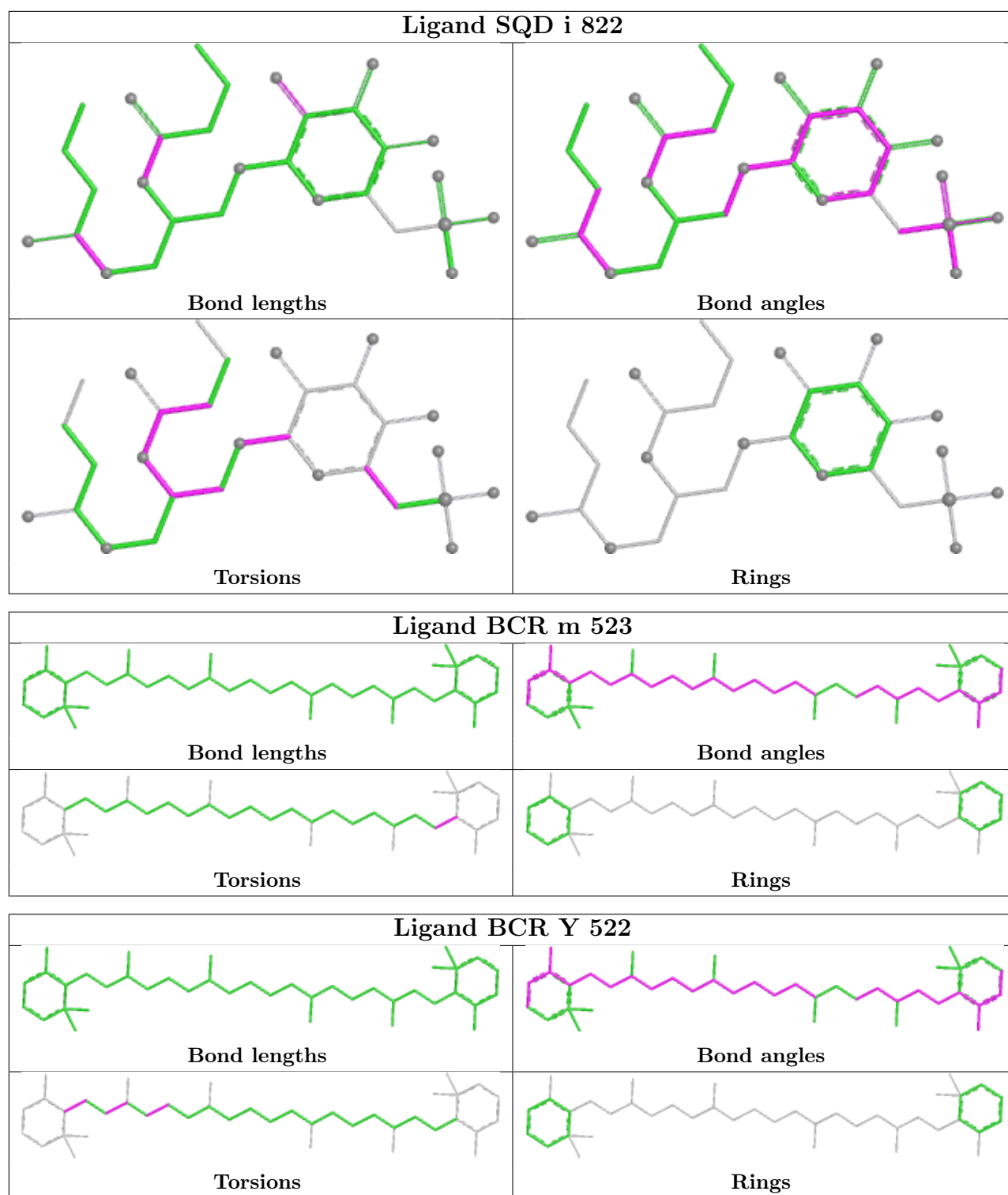
Bond angles



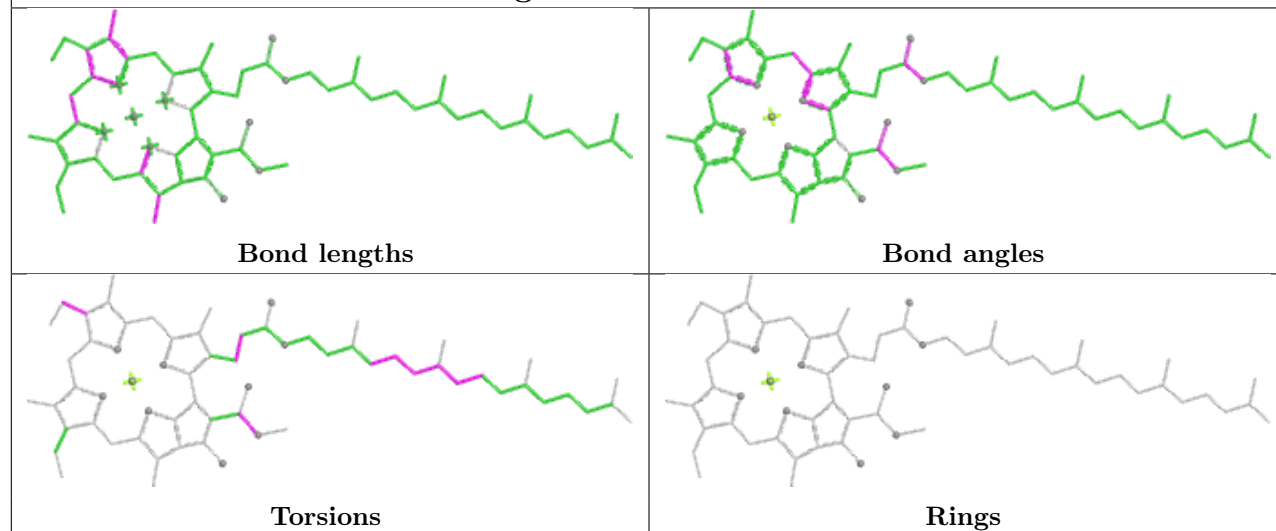
Torsions



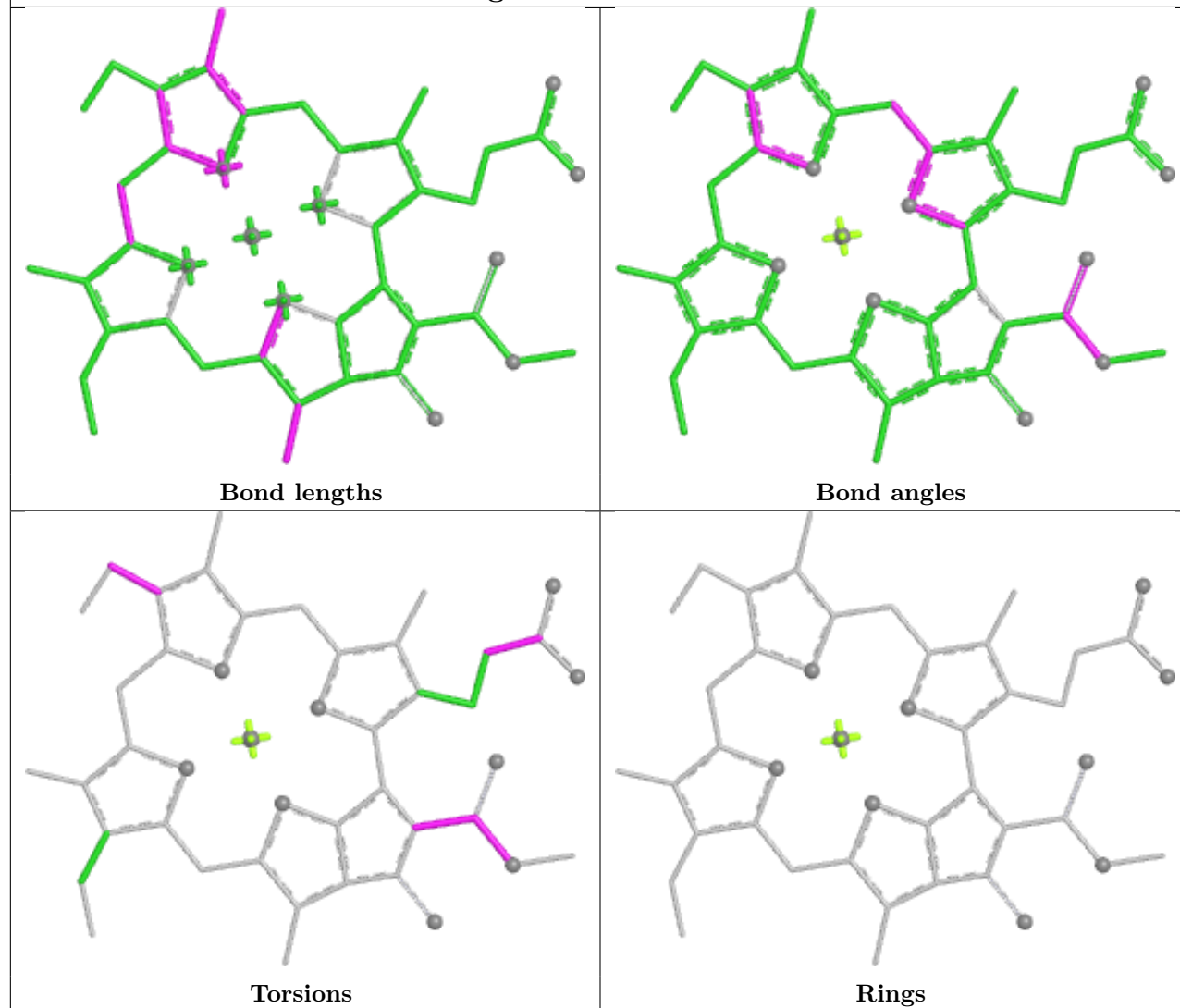
Rings

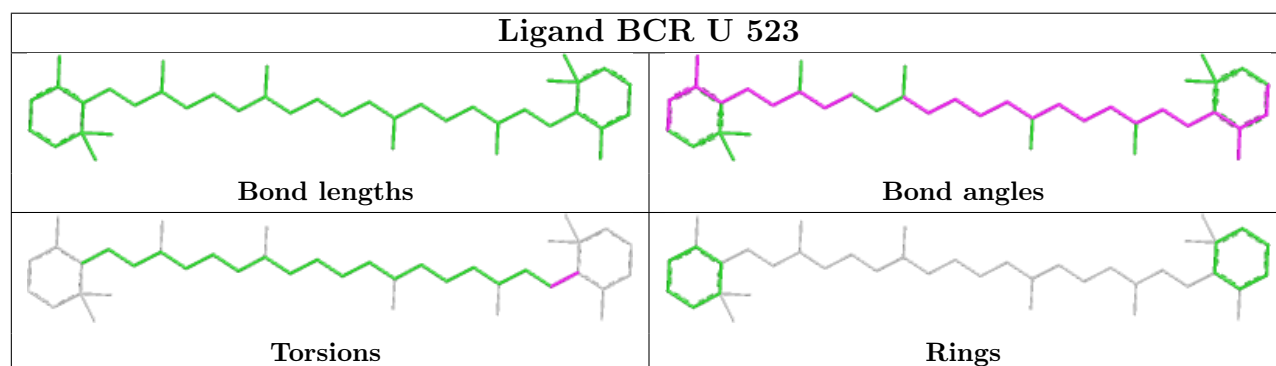
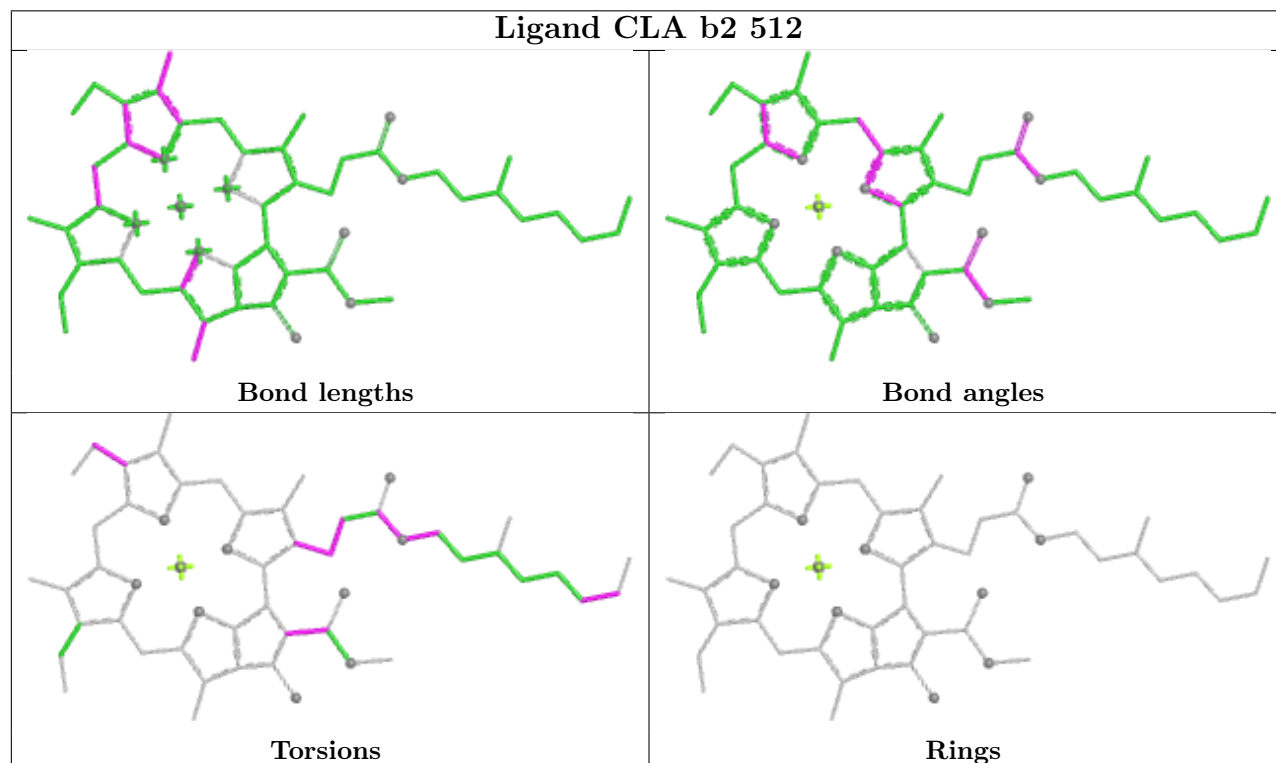
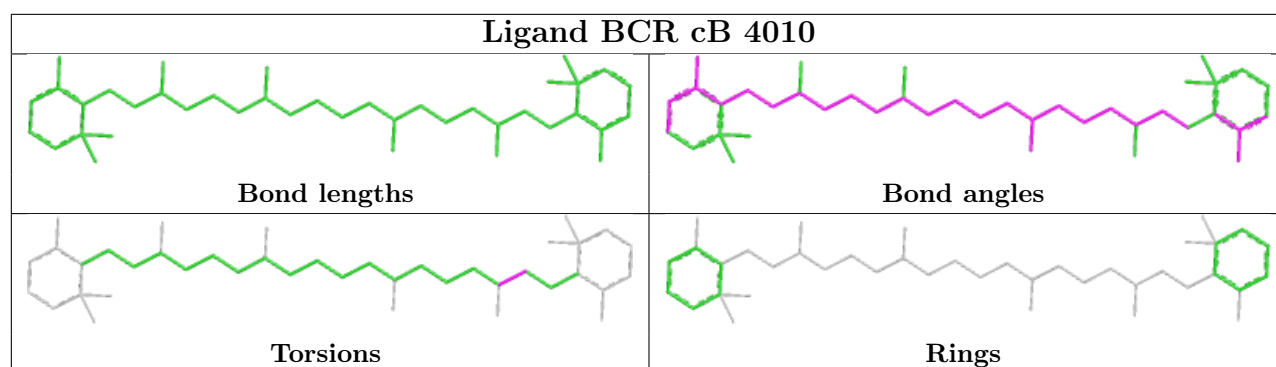


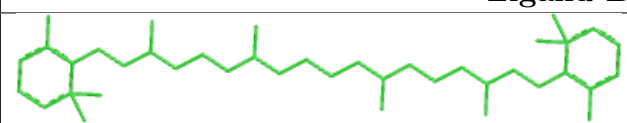
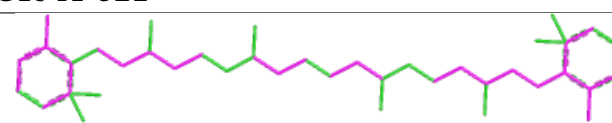
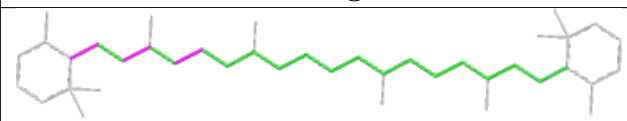
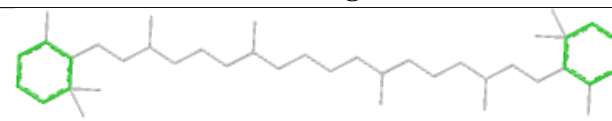
Ligand CLA cA 1138


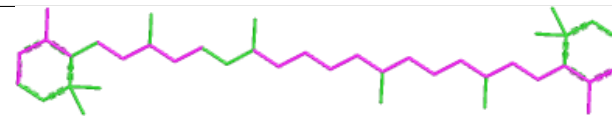
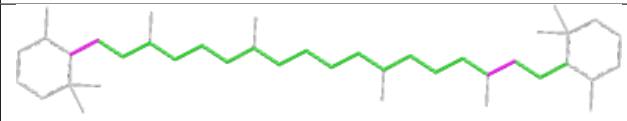
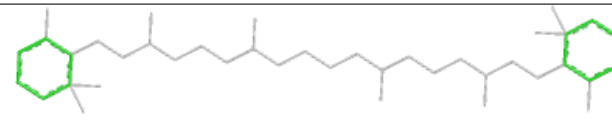


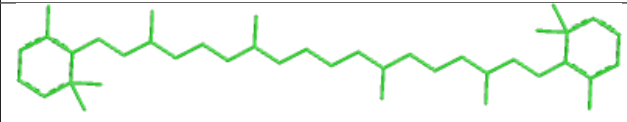
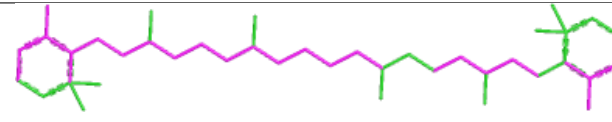
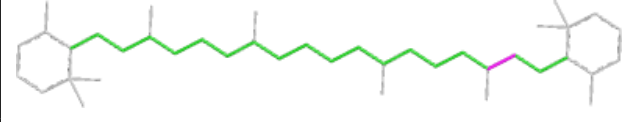
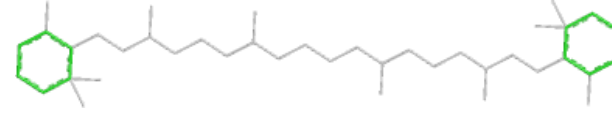
Ligand CLA a4 512

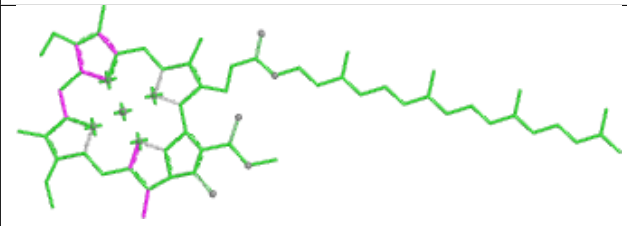
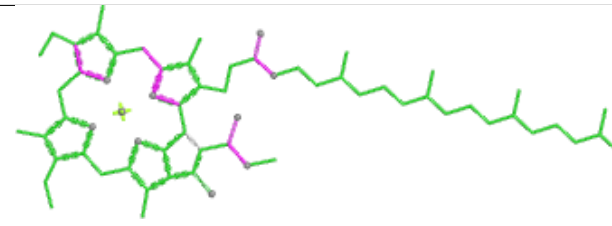
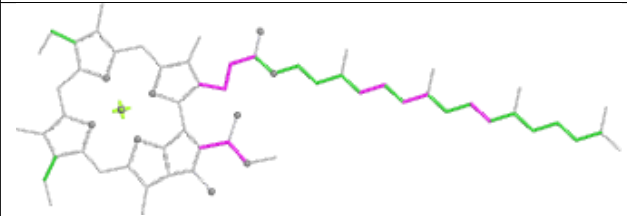
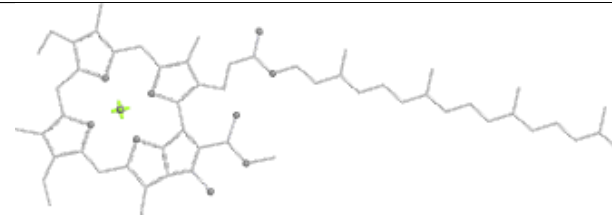


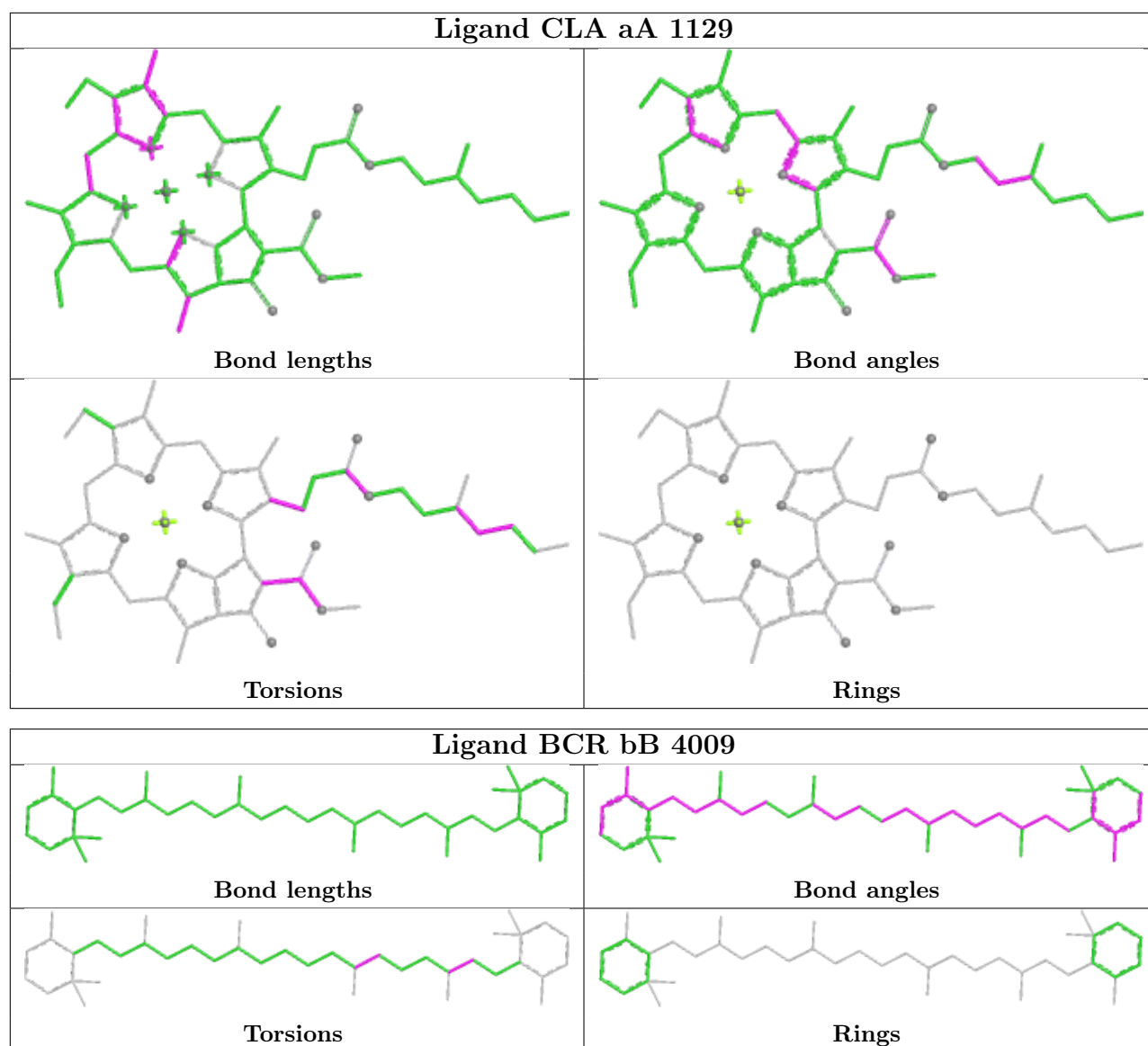


Ligand BCR X 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

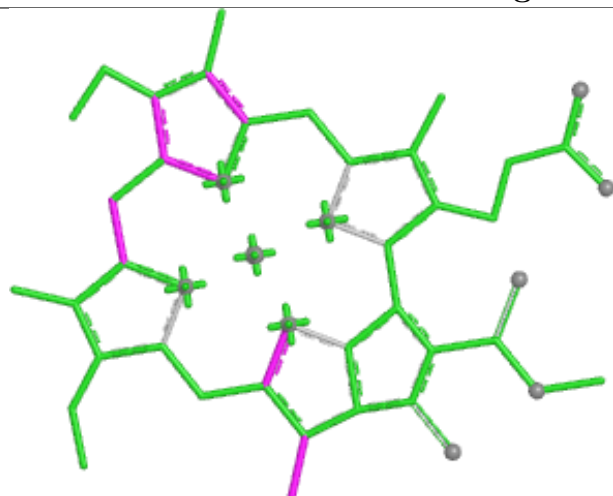
Ligand BCR cA 4002	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR j 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

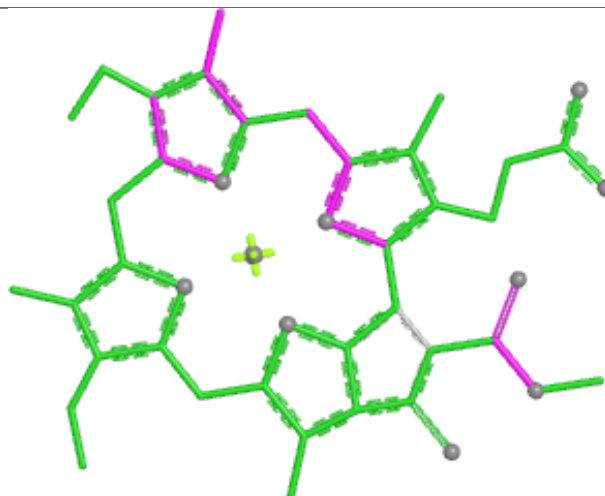
Ligand CLA cB 1207	
	
Bond lengths	Bond angles
	
Torsions	Rings



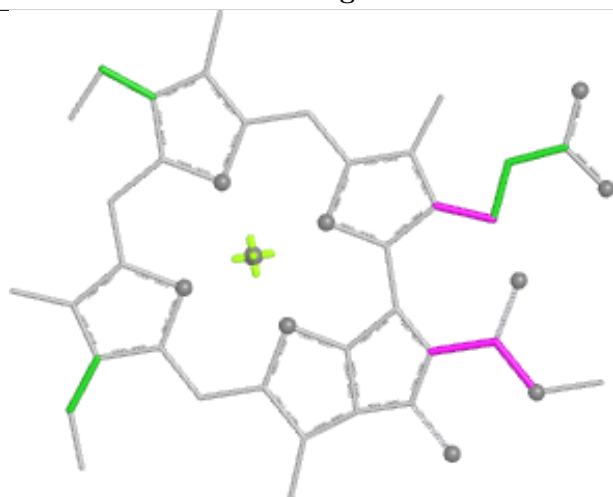
Ligand CLA X 516



Bond lengths



Bond angles

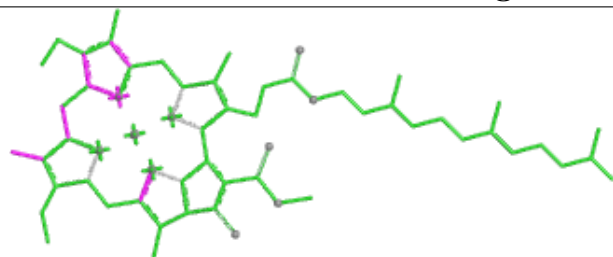


Torsions

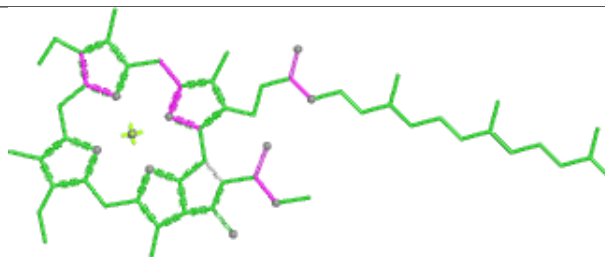


Rings

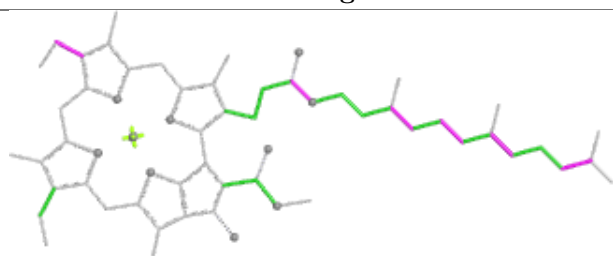
Ligand CLA bA 1122



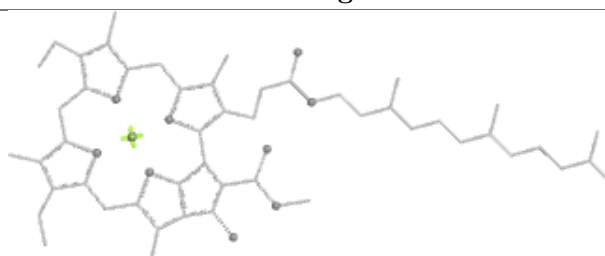
Bond lengths



Bond angles

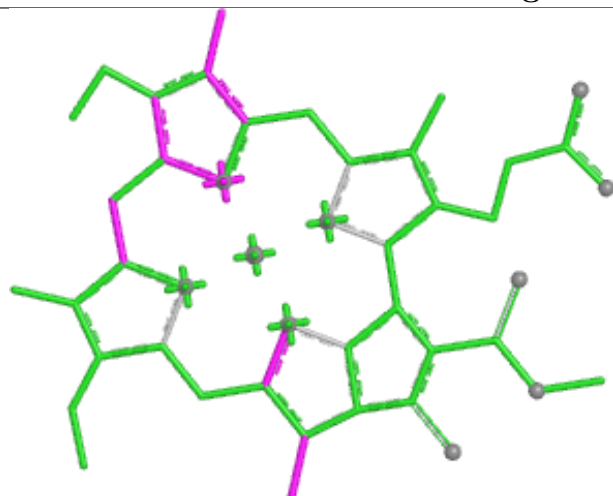


Torsions



Rings

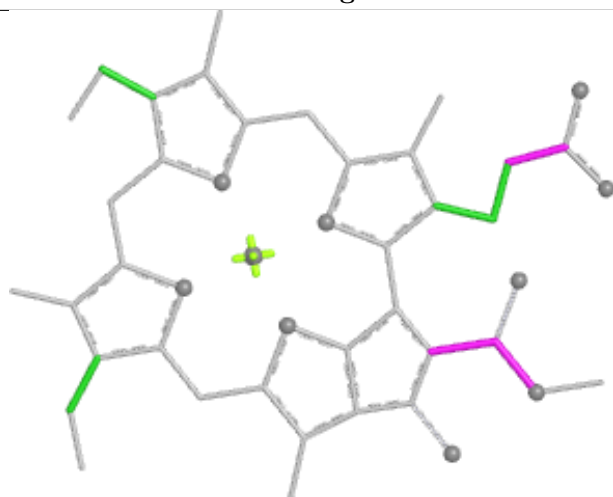
Ligand CLA 1 511



Bond lengths



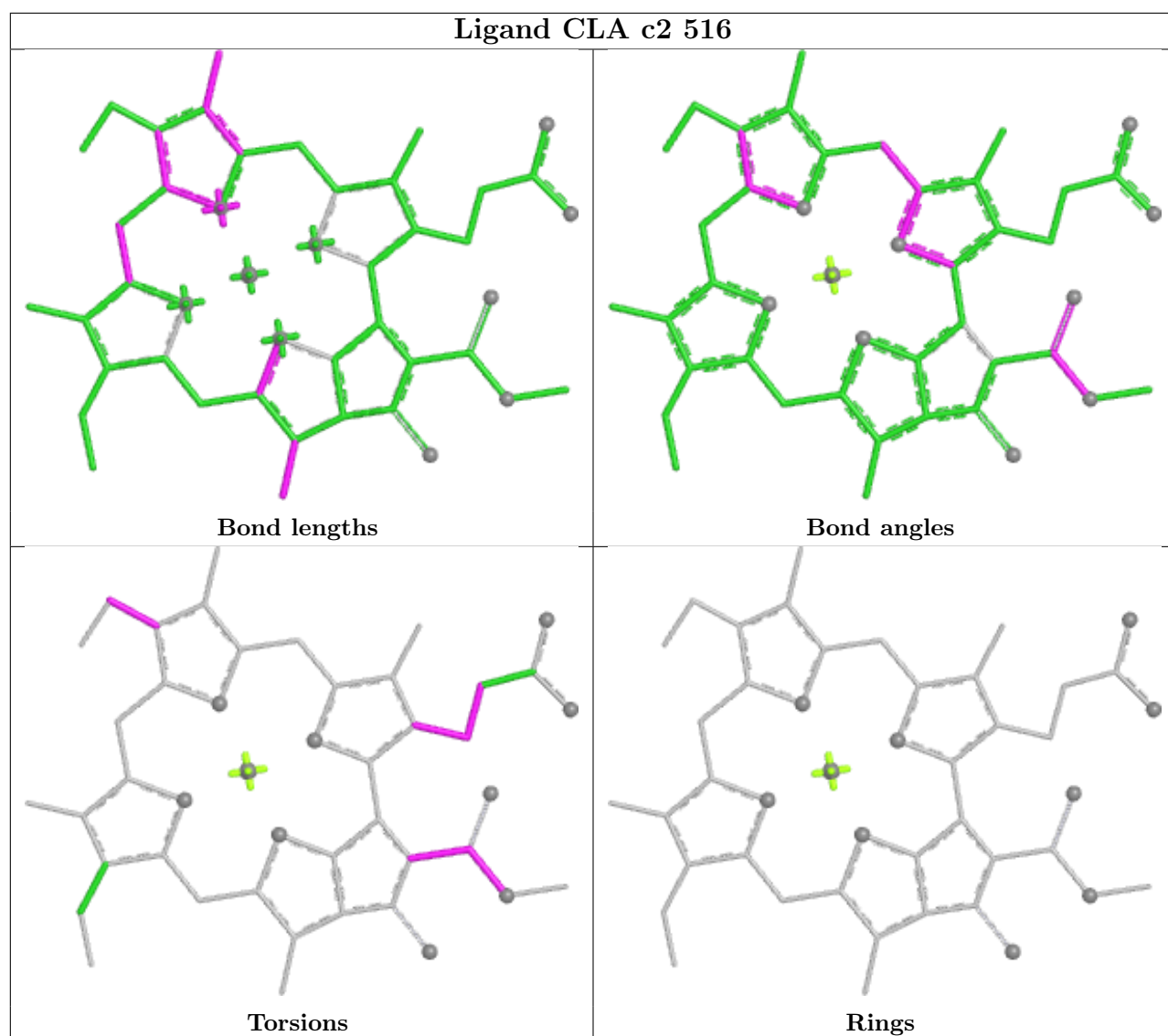
Bond angles

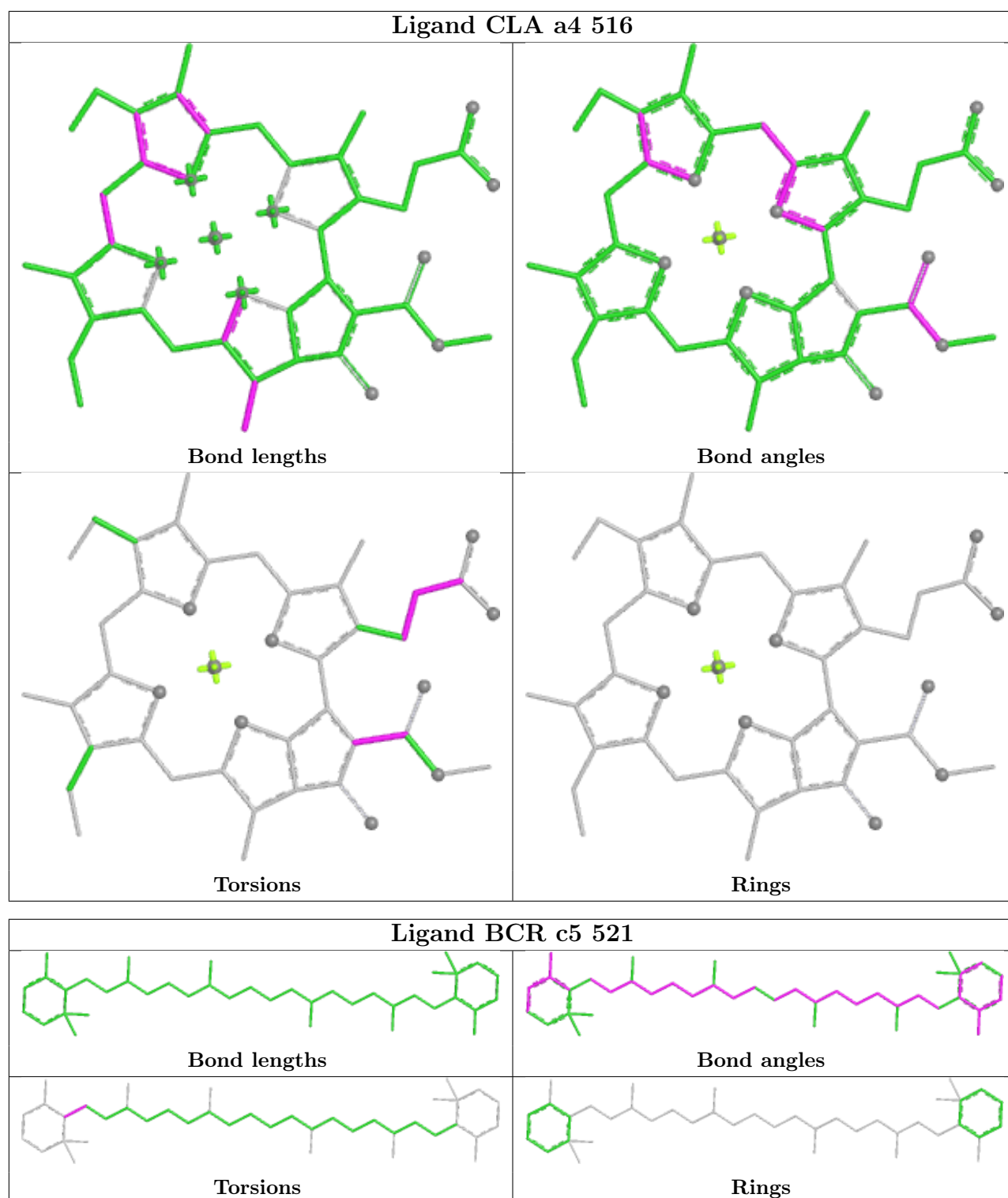


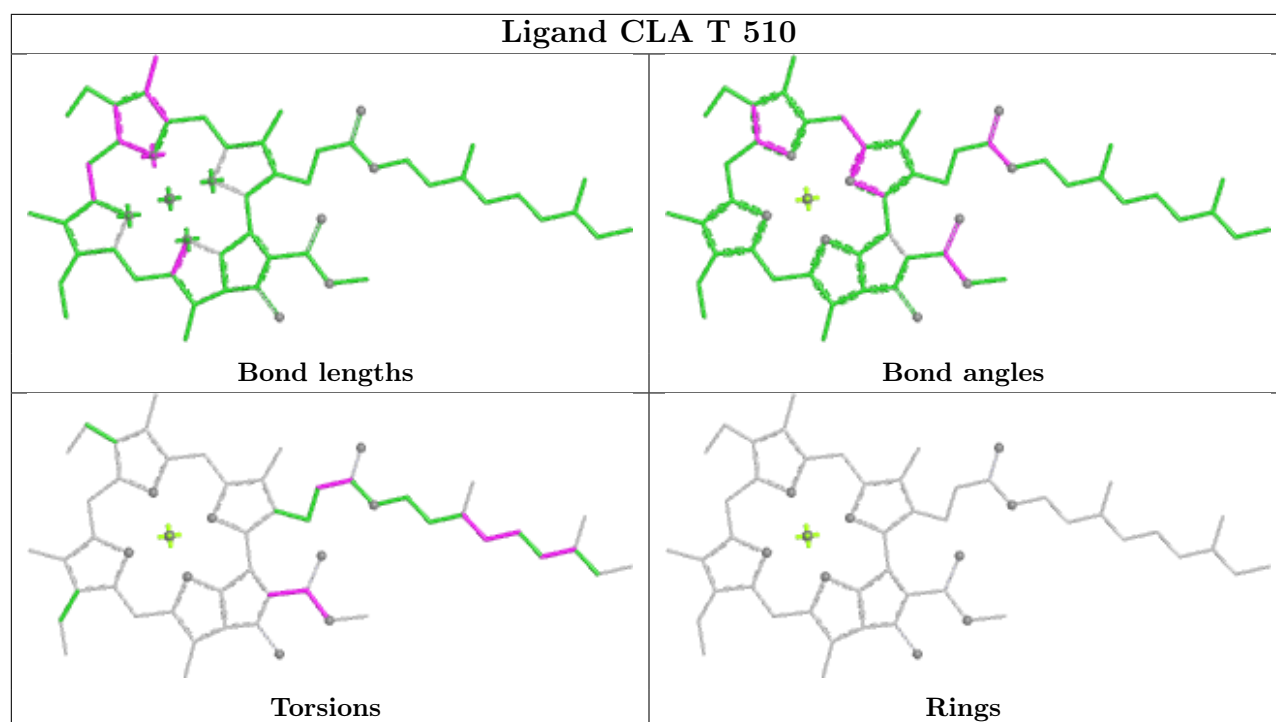
Torsions



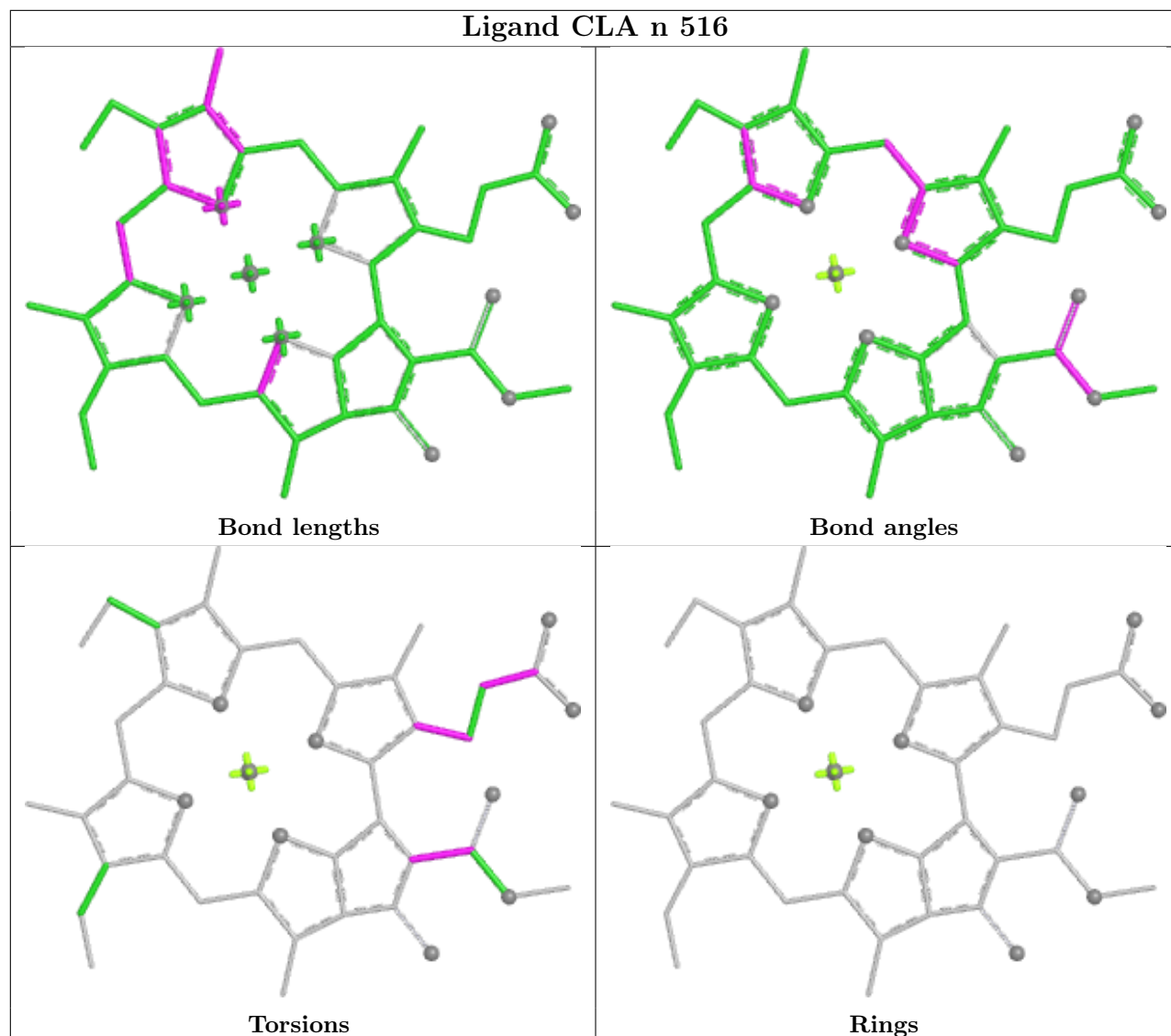
Rings



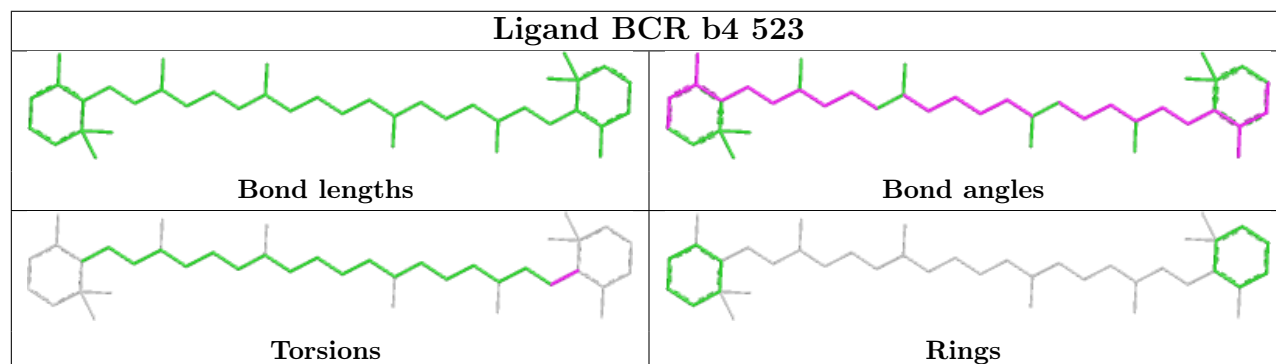




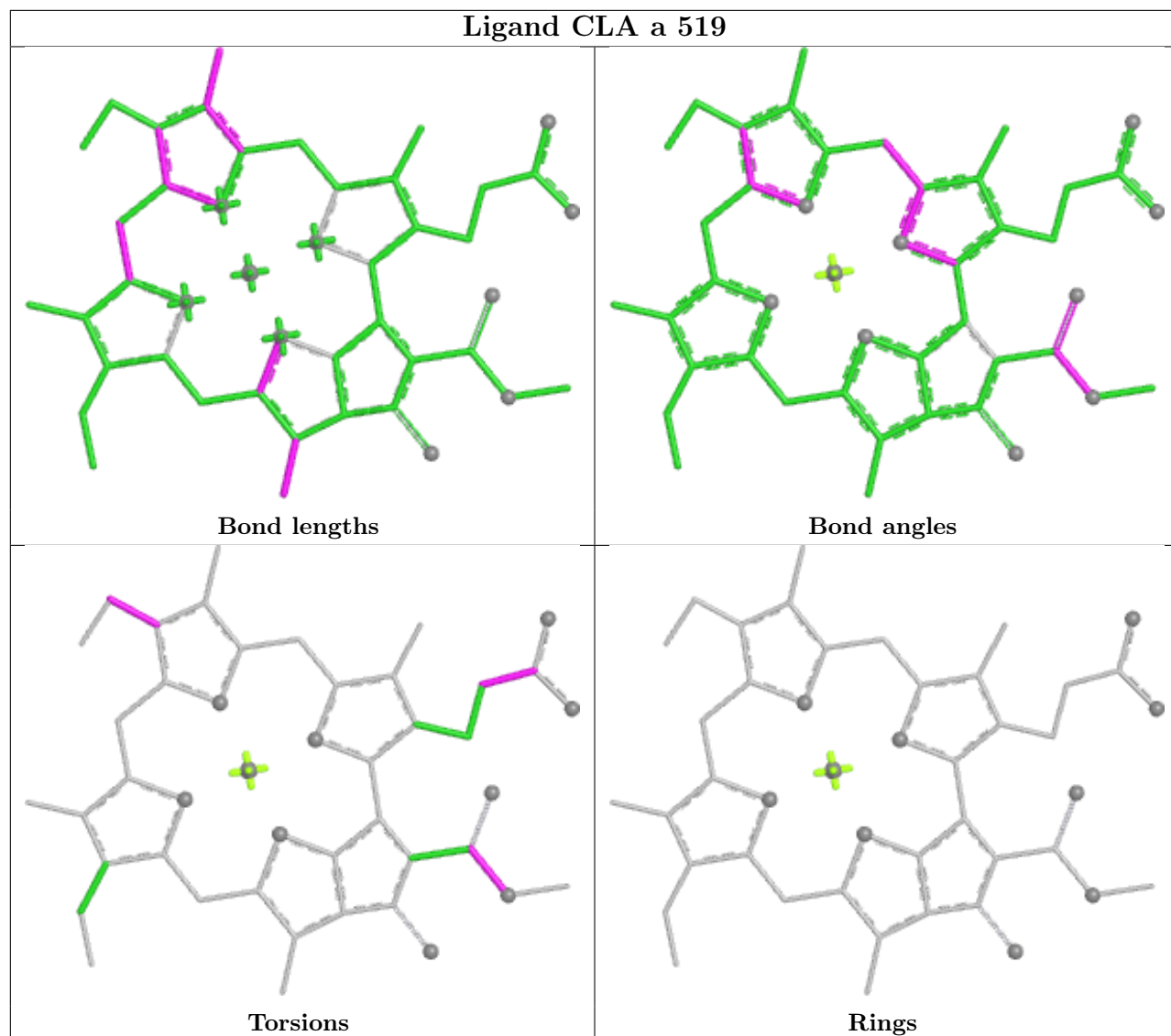
Ligand CLA n 516



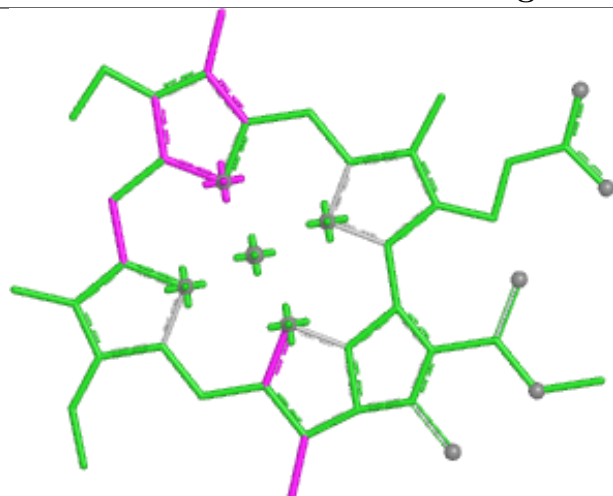
Ligand BCR b4 523



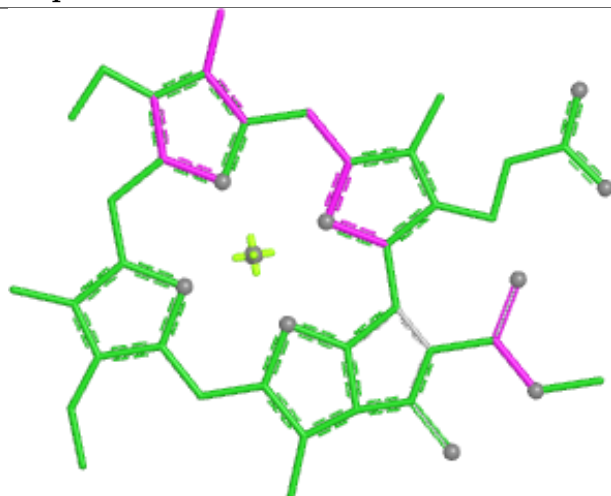
Ligand CLA a 519



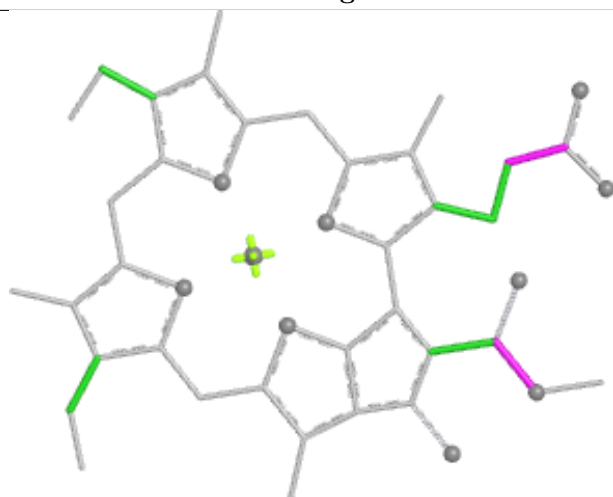
Ligand CLA p 506



Bond lengths



Bond angles

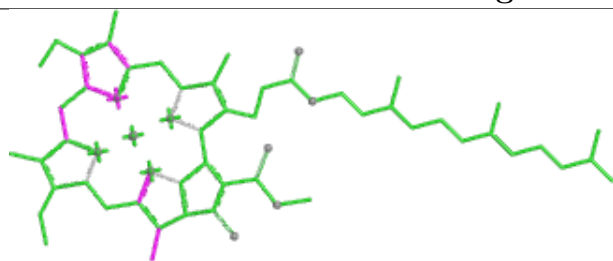


Torsions

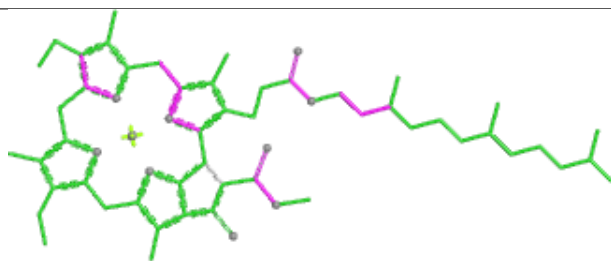


Rings

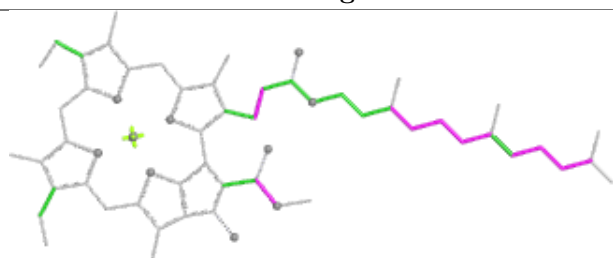
Ligand CLA aA 1115



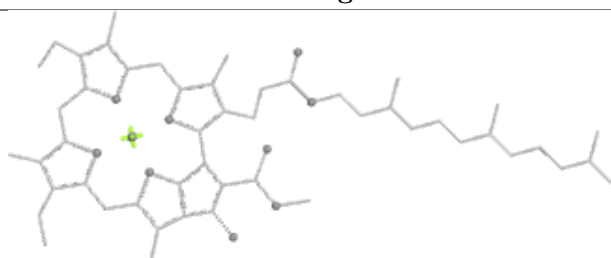
Bond lengths



Bond angles

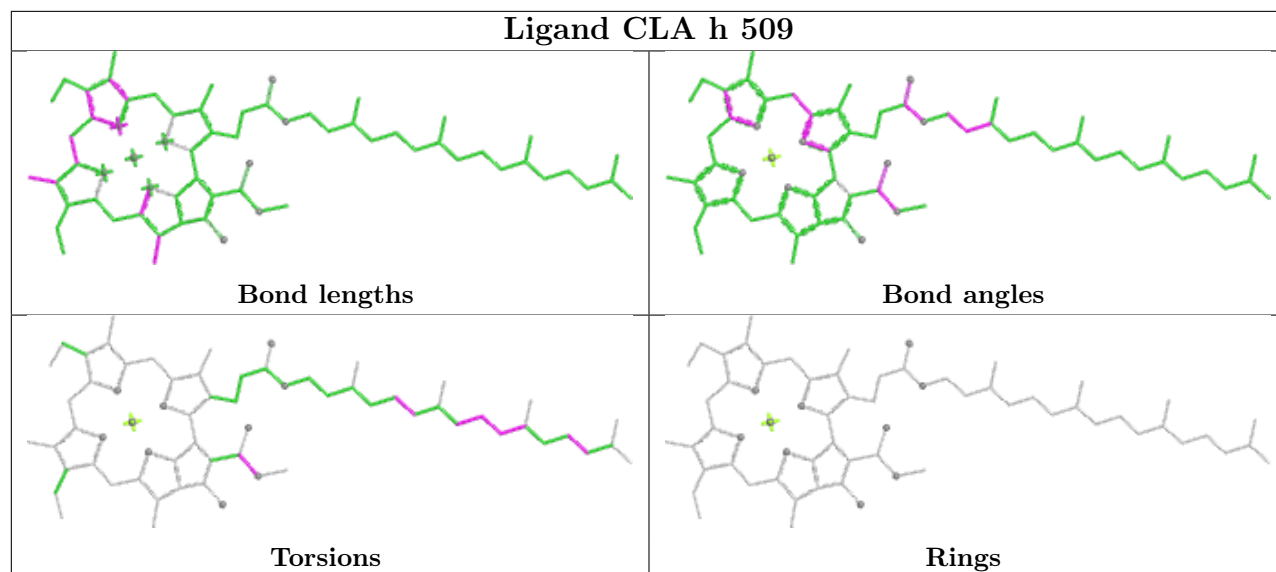


Torsions

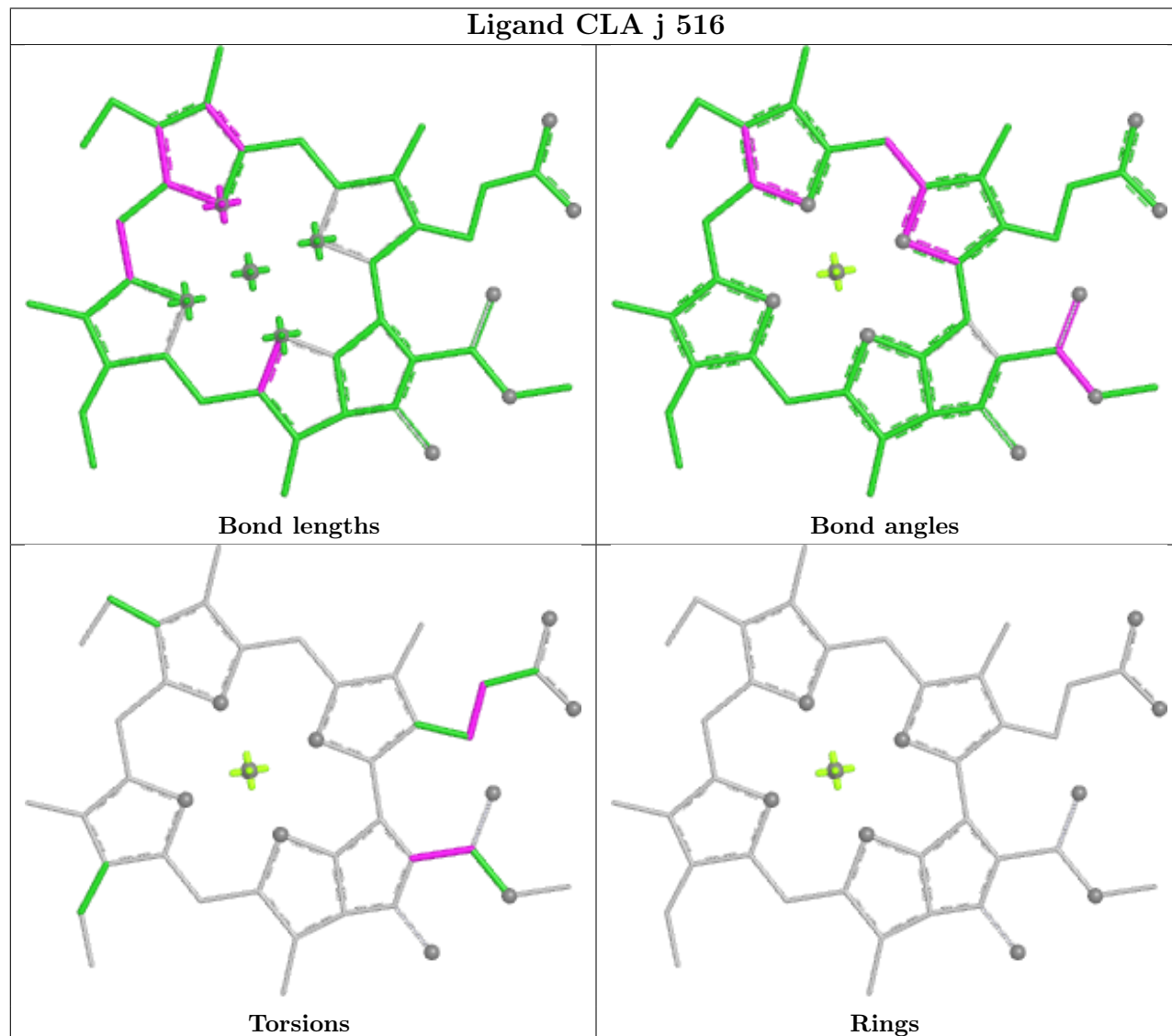


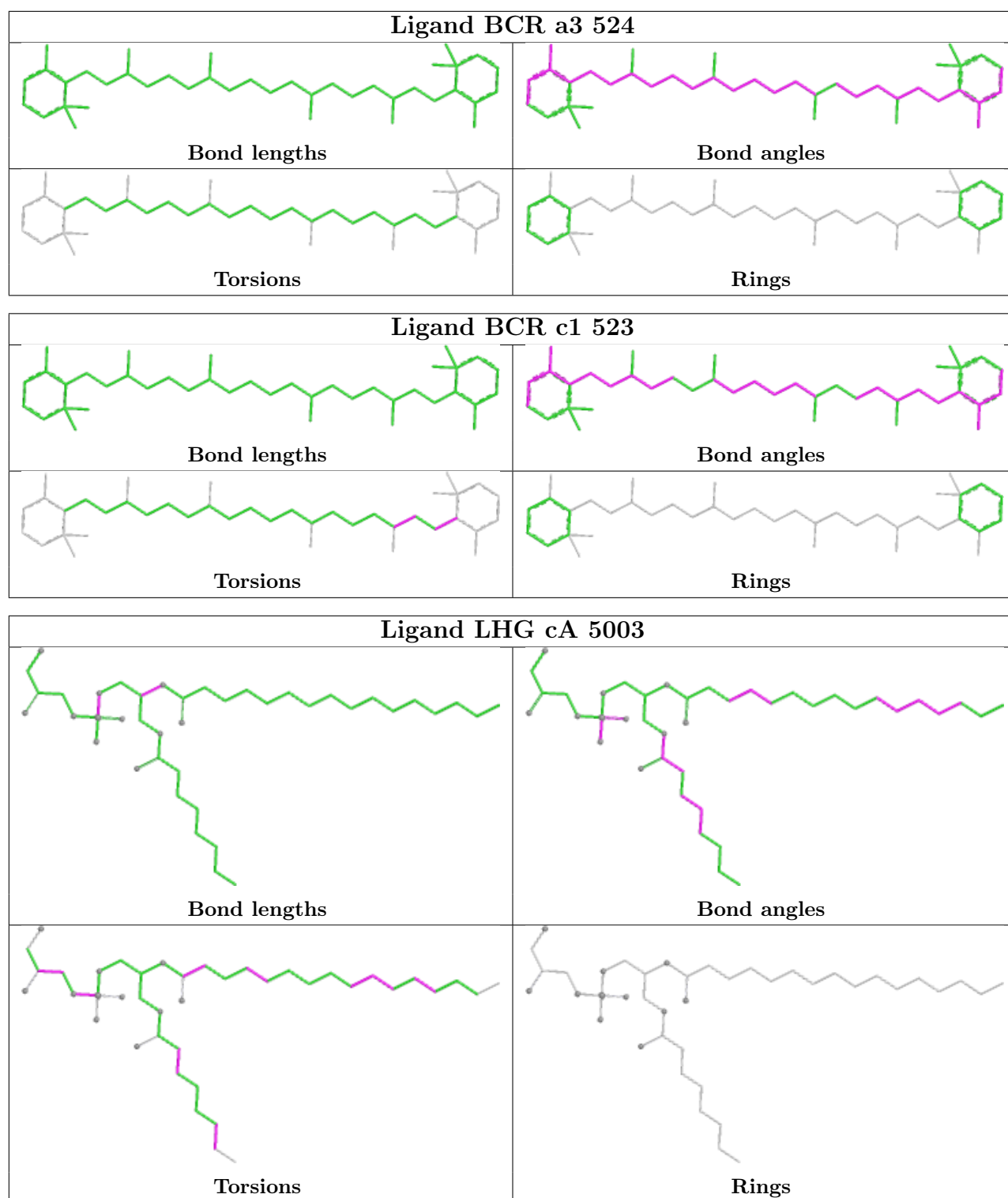
Rings

Ligand CLA h 509

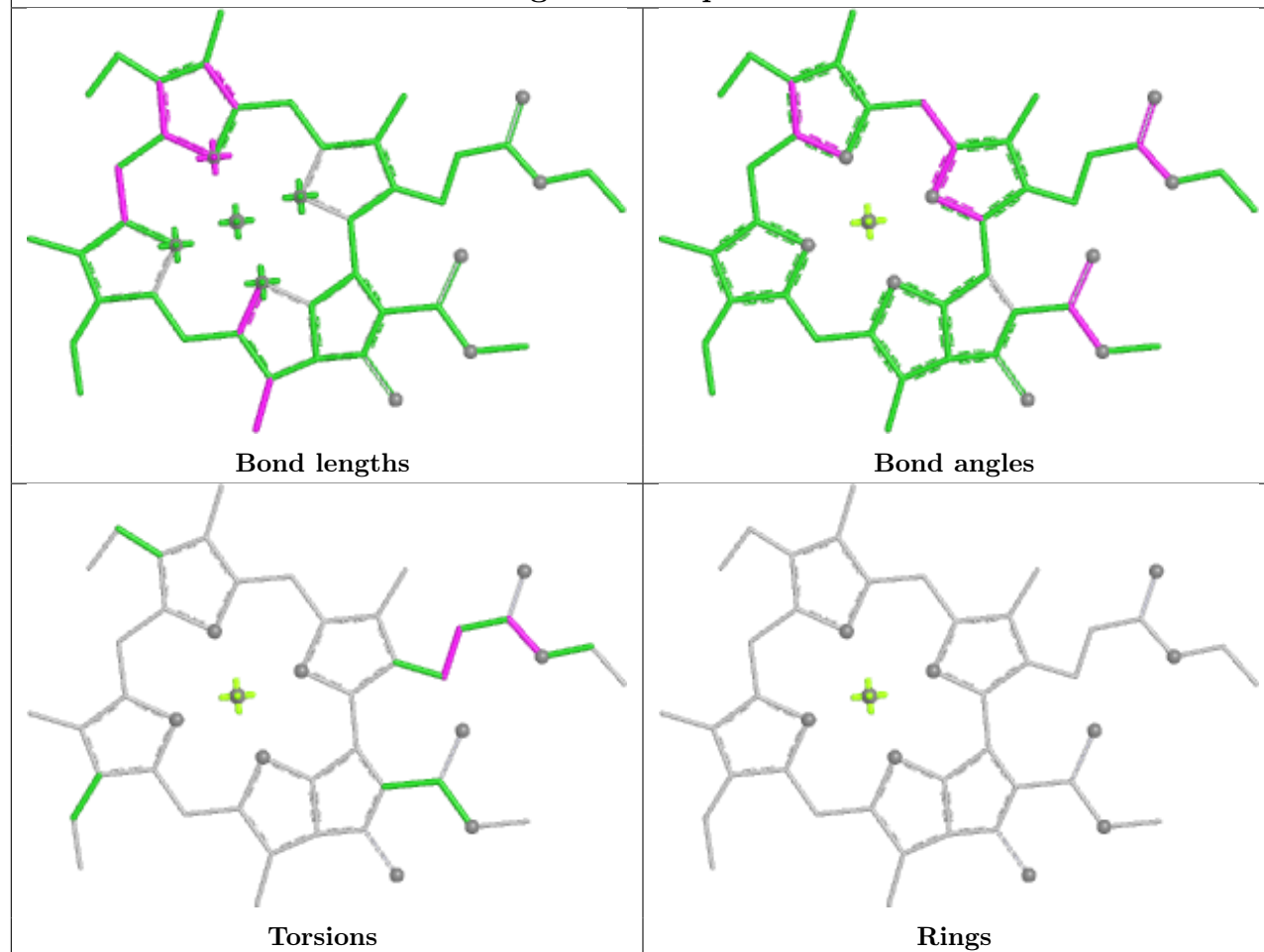


Ligand CLA j 516

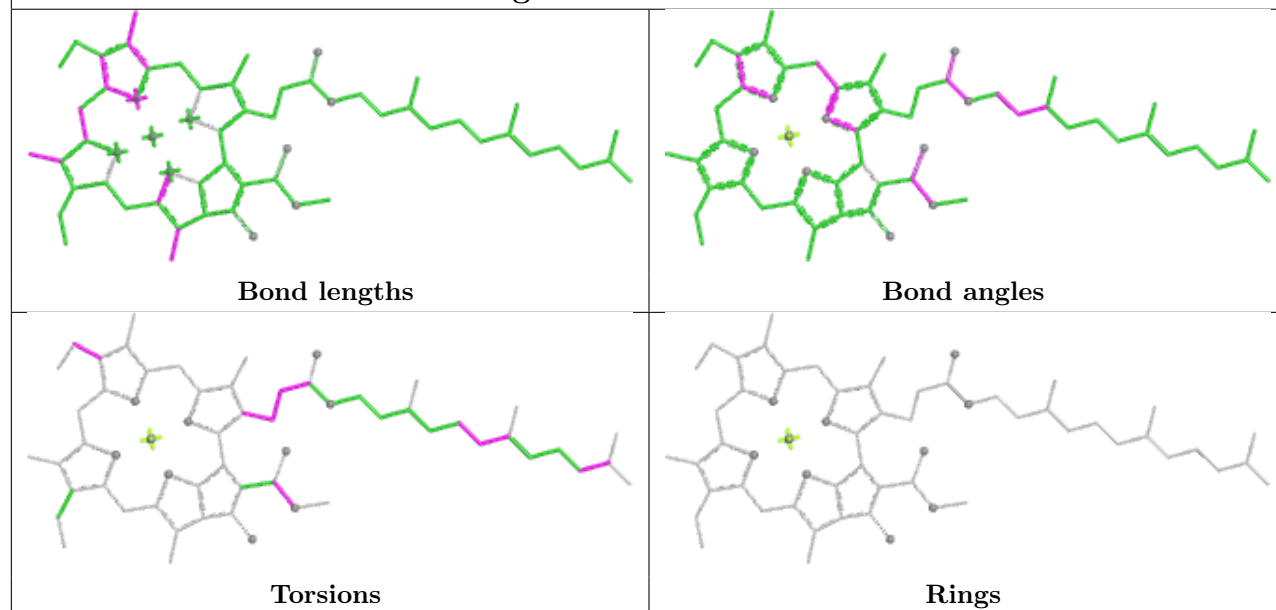




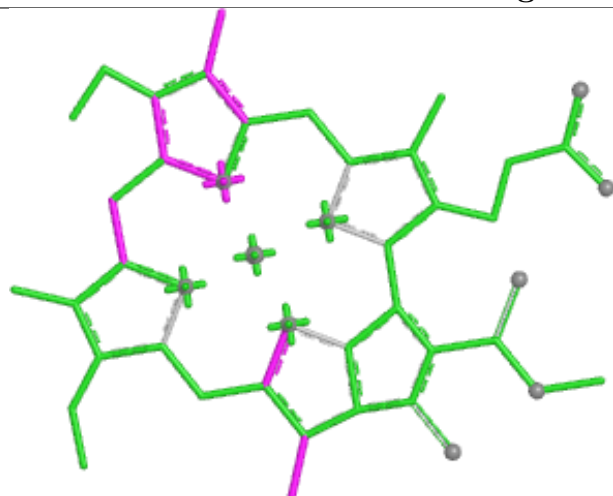
Ligand CLA p 505



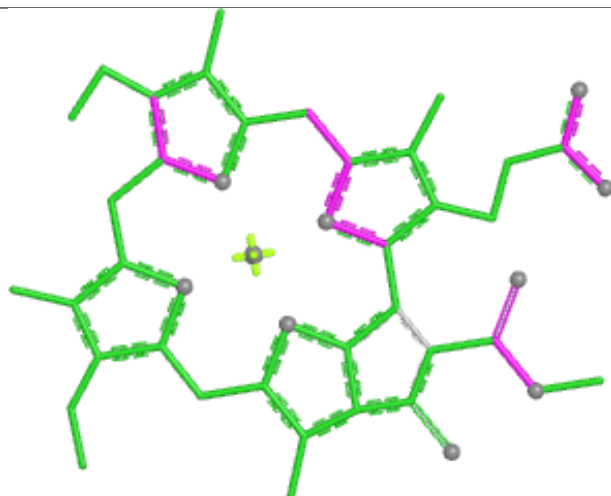
Ligand CLA ba 1116



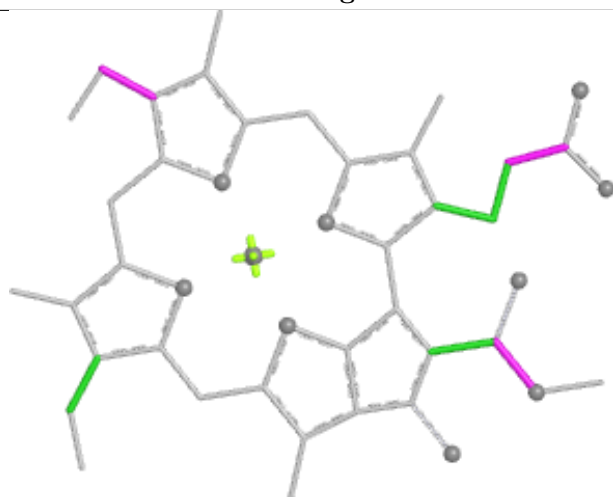
Ligand CLA b 517



Bond lengths



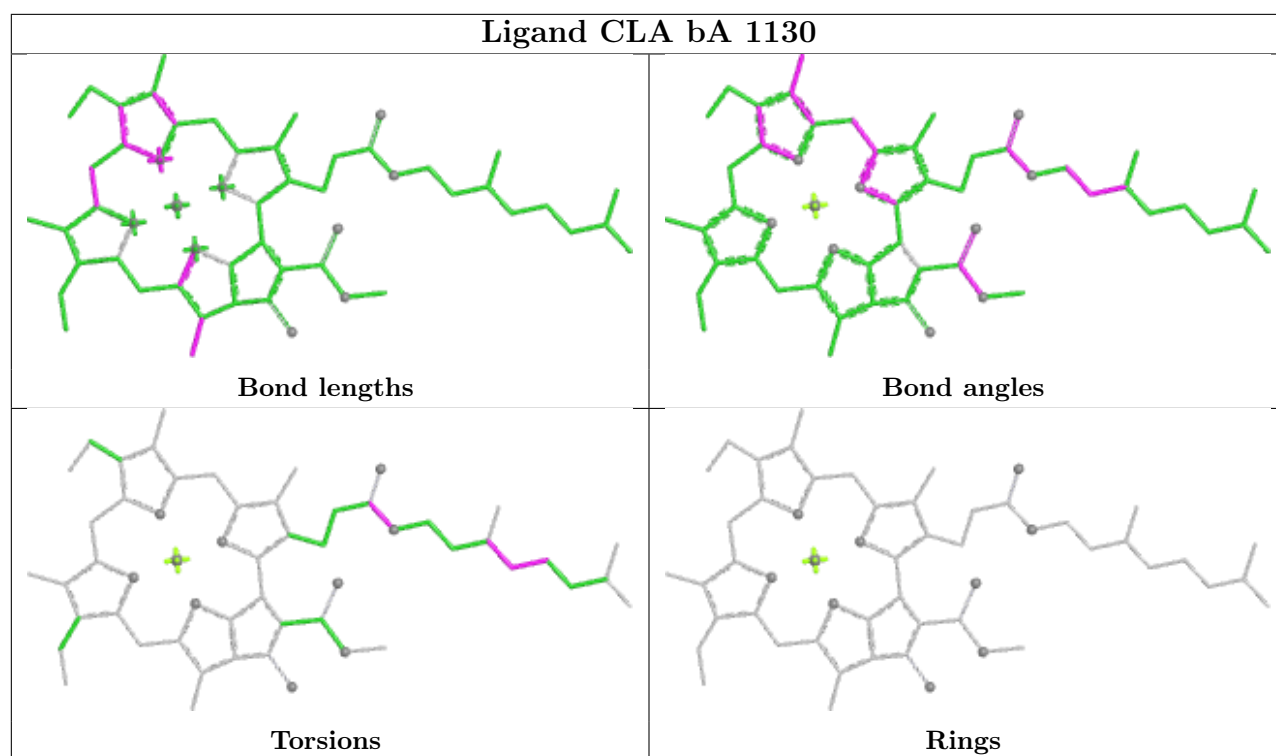
Bond angles



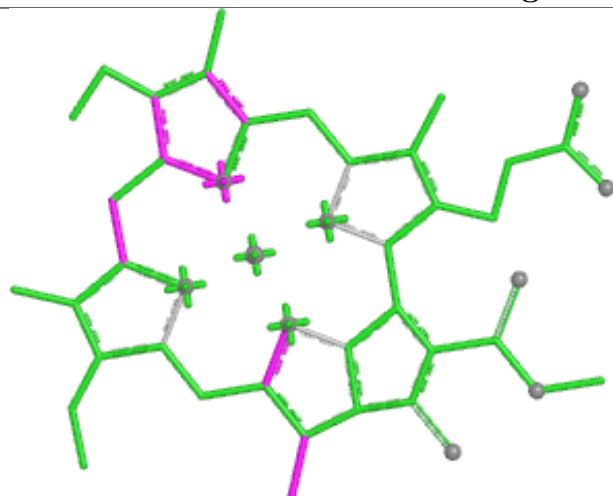
Torsions



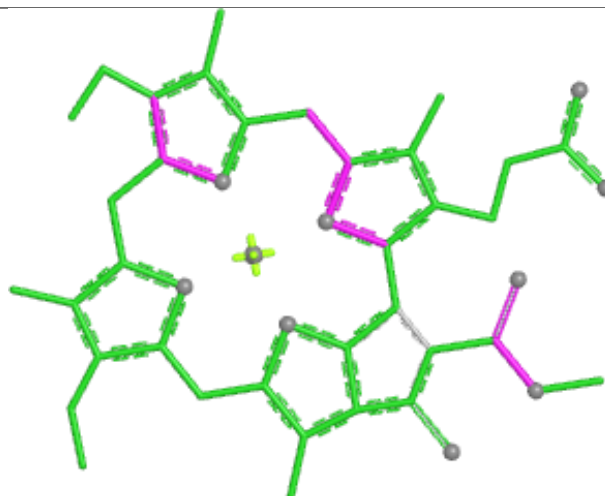
Rings



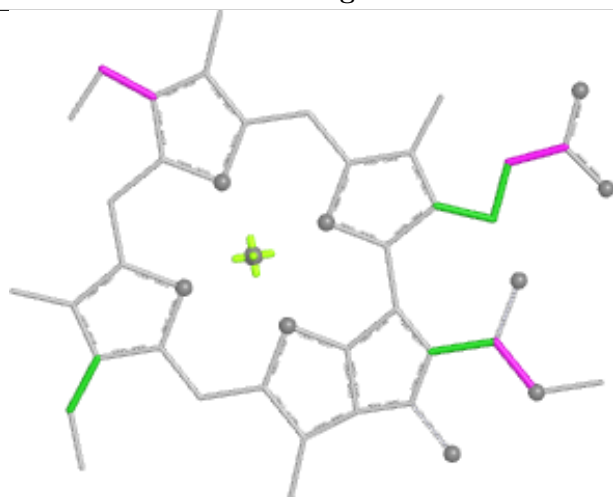
Ligand CLA f 517



Bond lengths



Bond angles

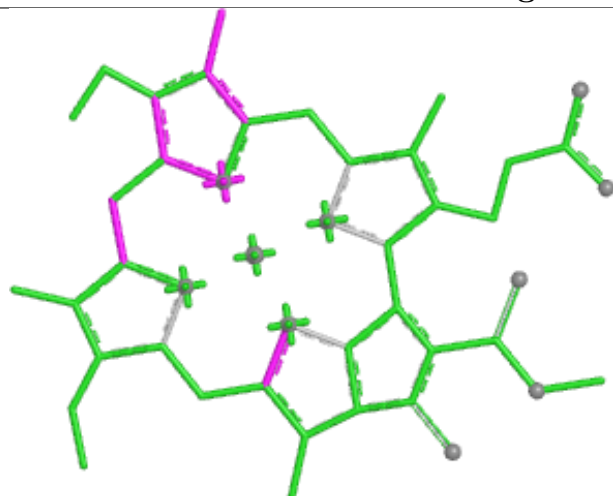


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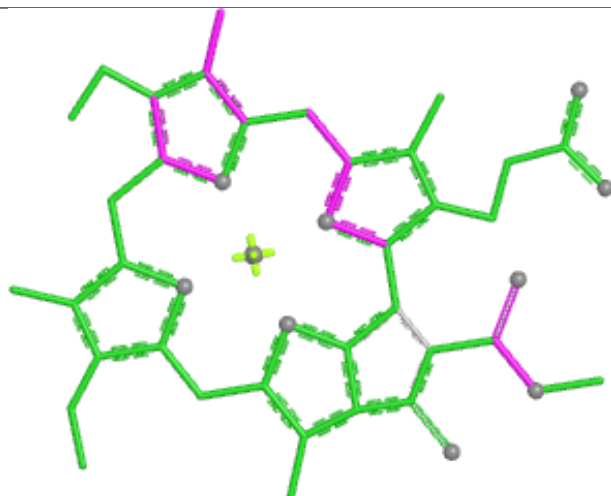


Rings

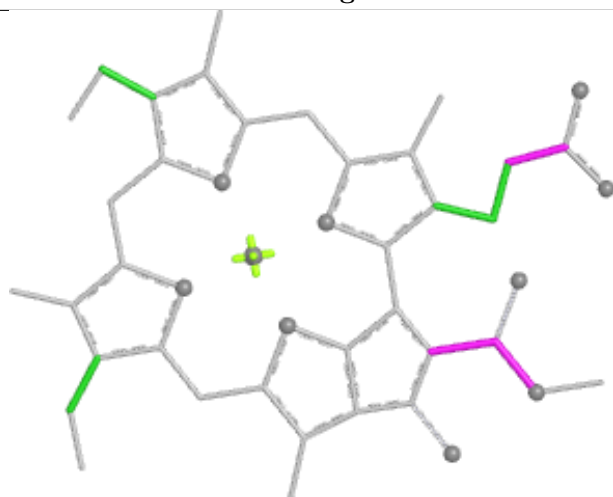
Ligand CLA k 510



Bond lengths



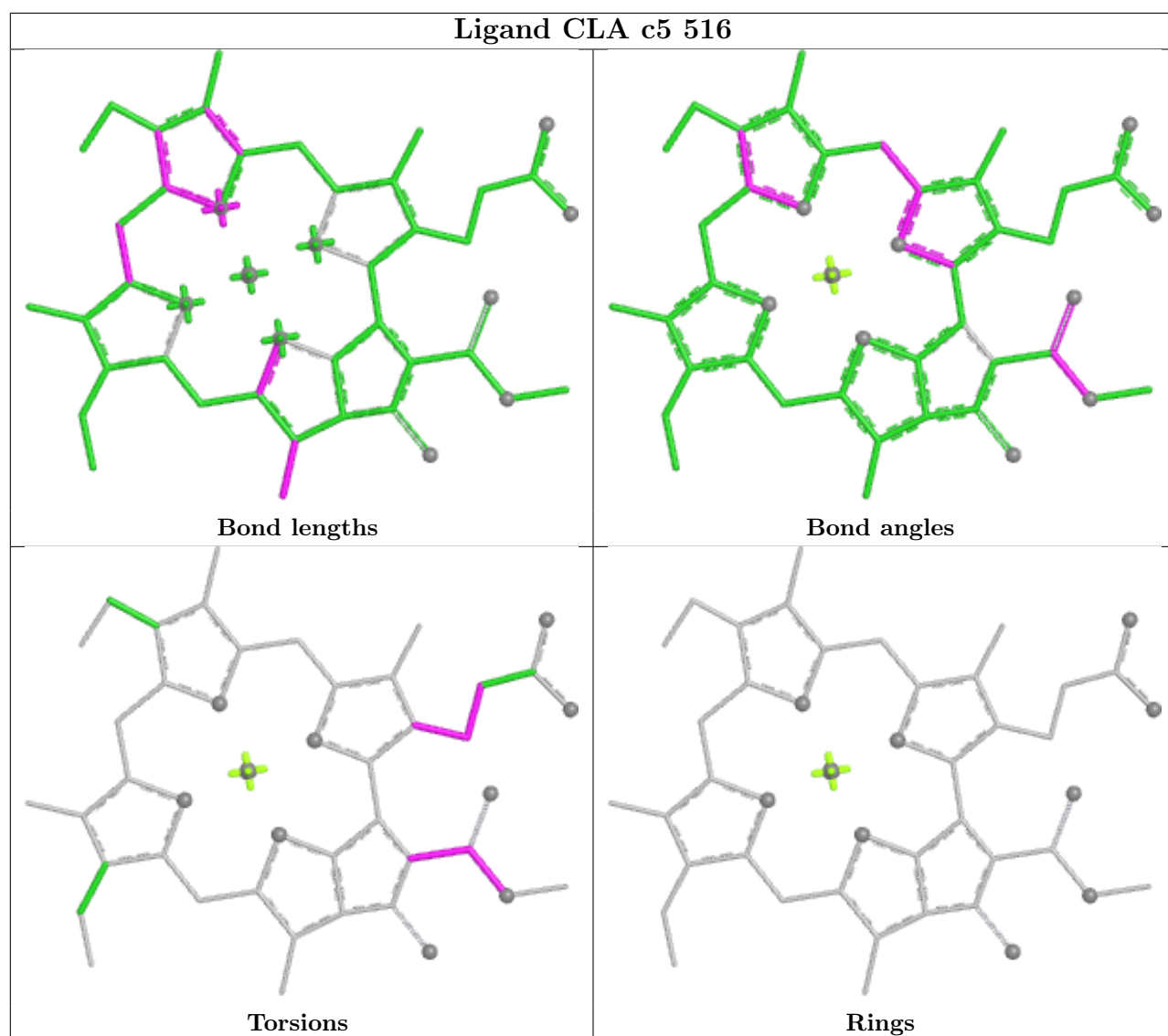
Bond angles

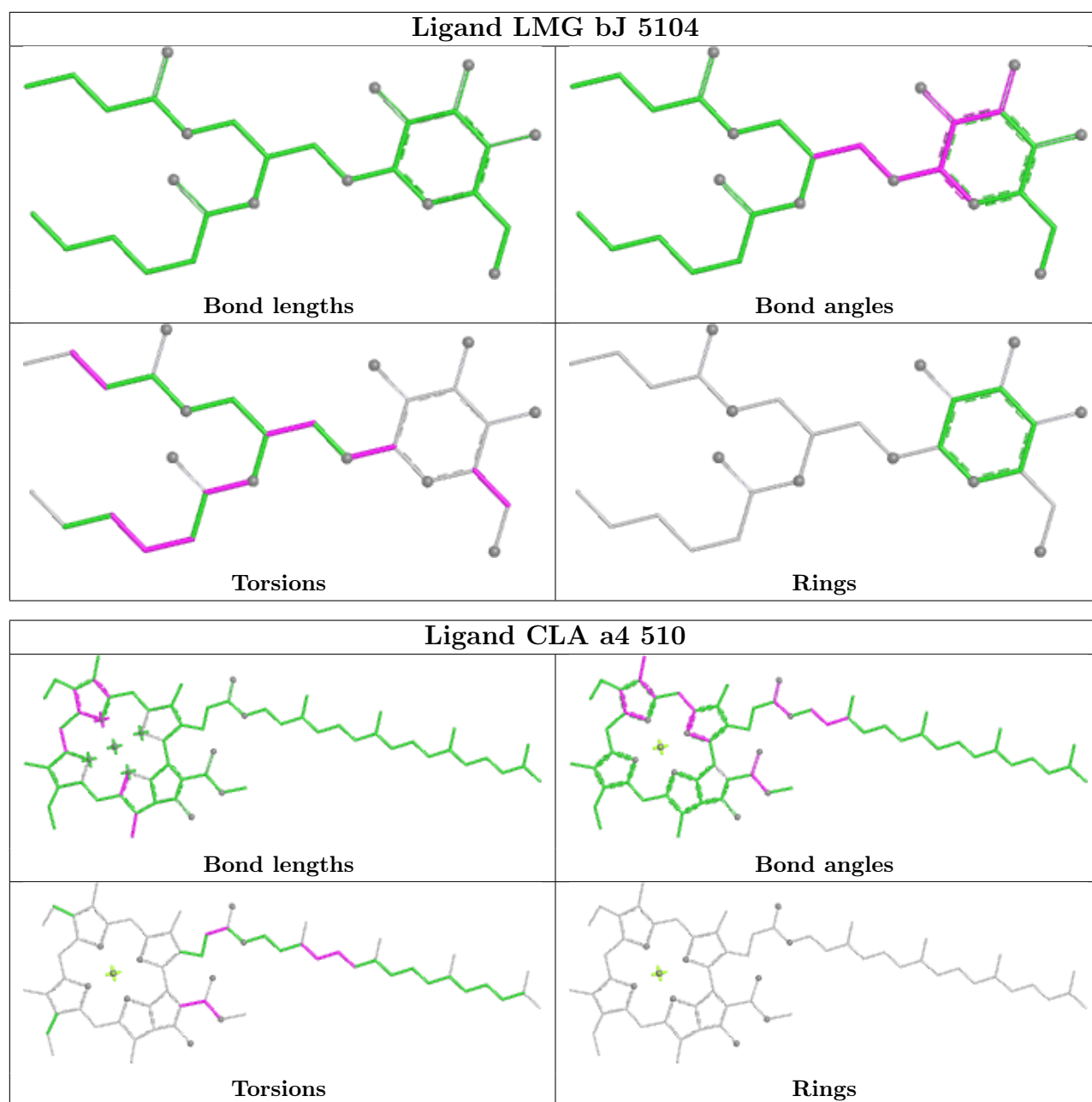


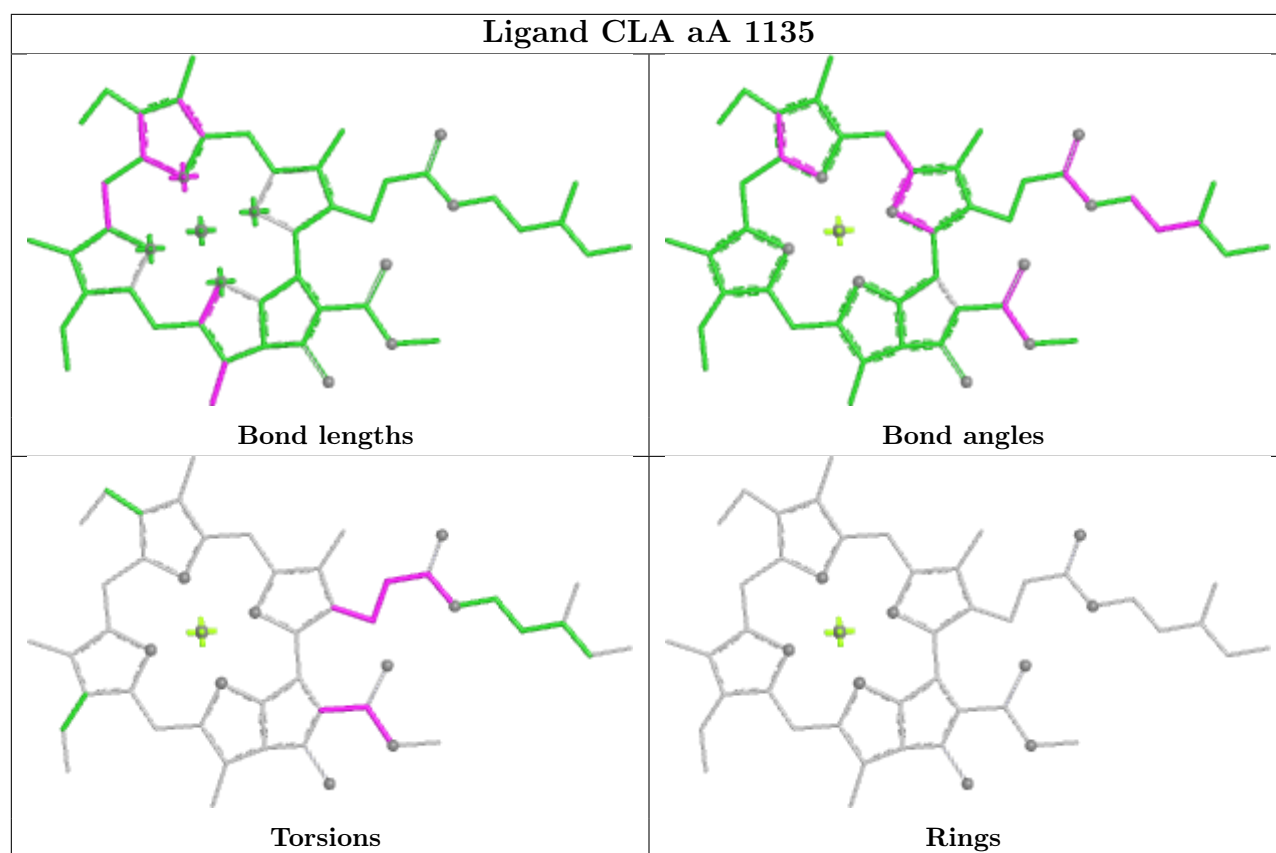
Torsions



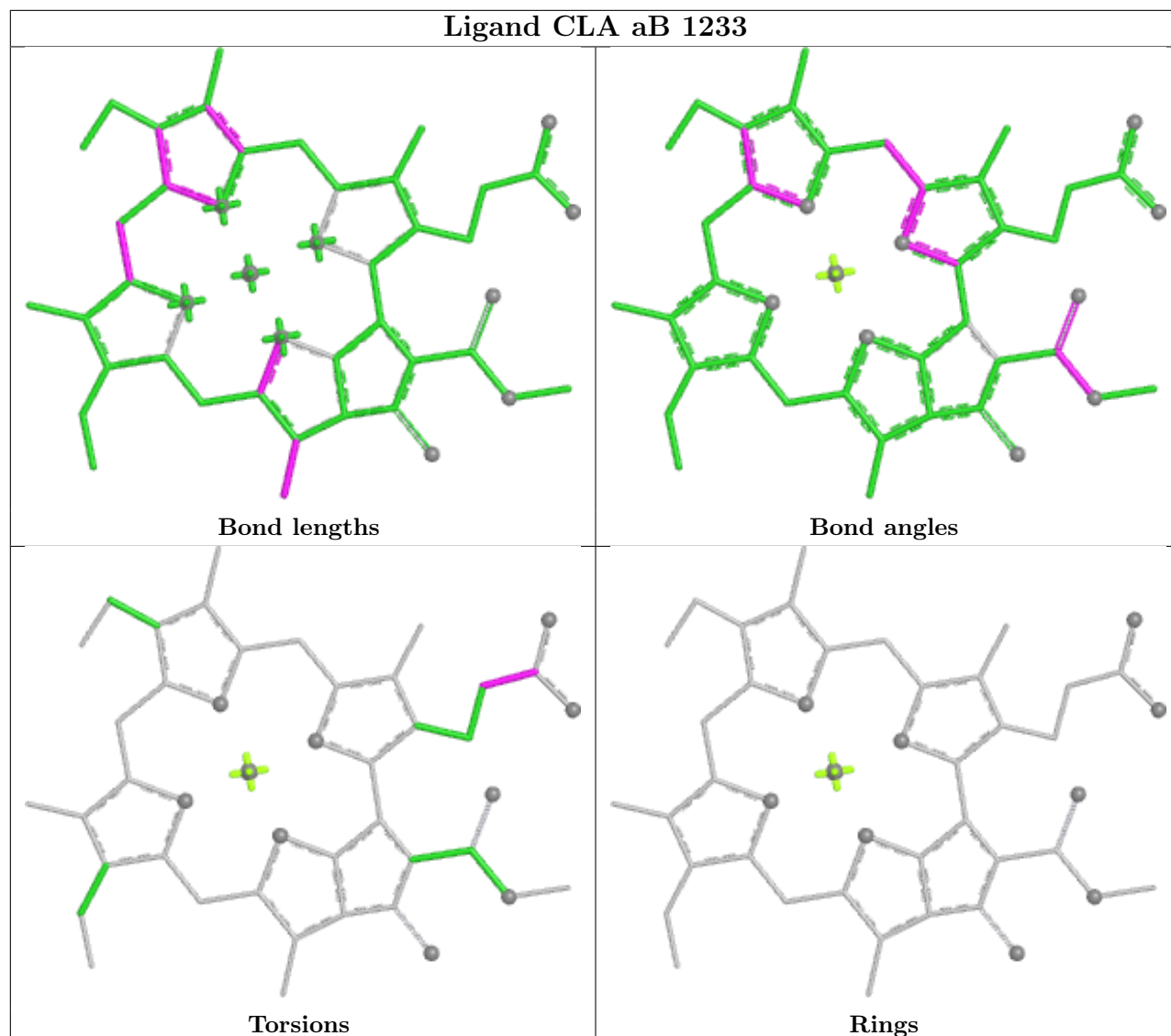
Rings



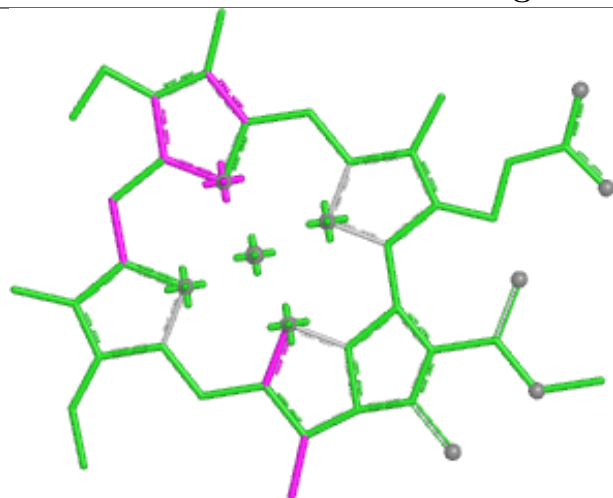




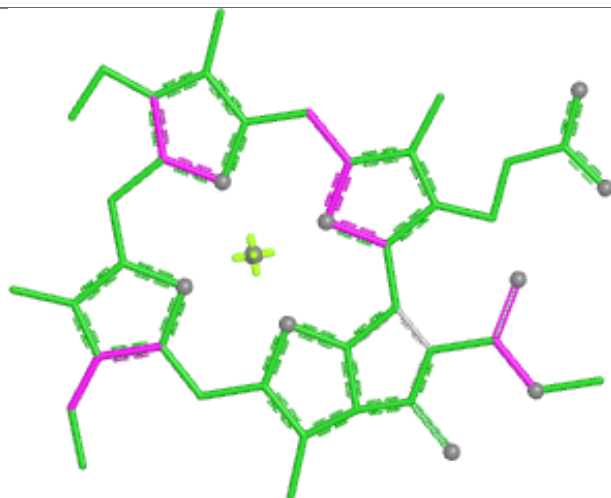
Ligand CLA aB 1233



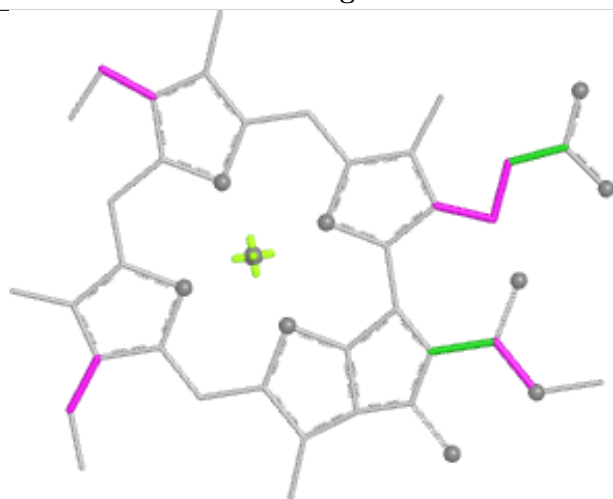
Ligand CLA U 516



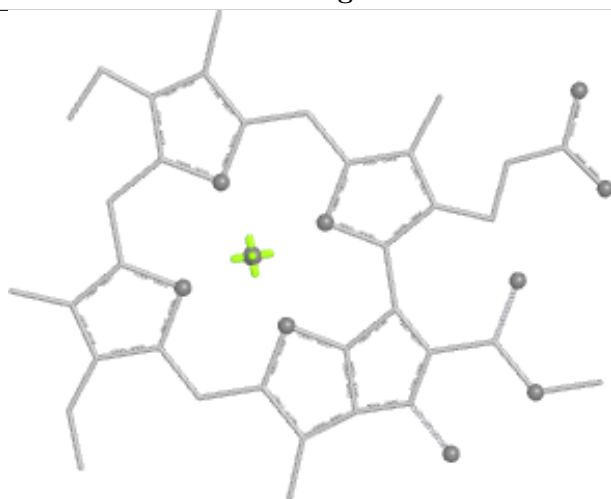
Bond lengths



Bond angles

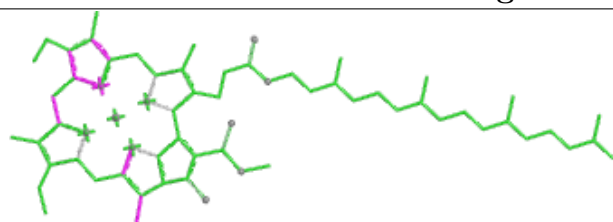


Torsions

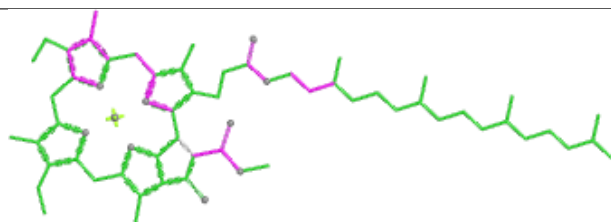


Rings

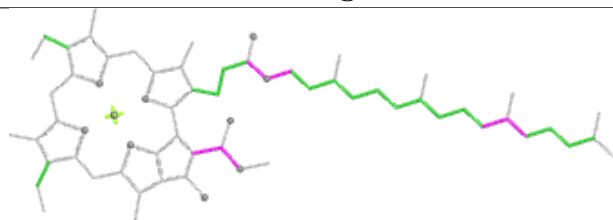
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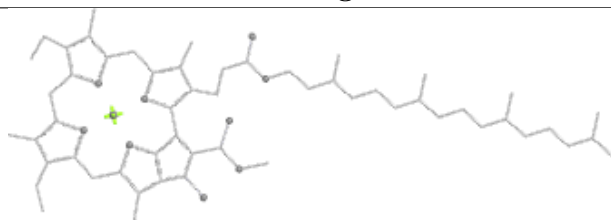
Bond lengths



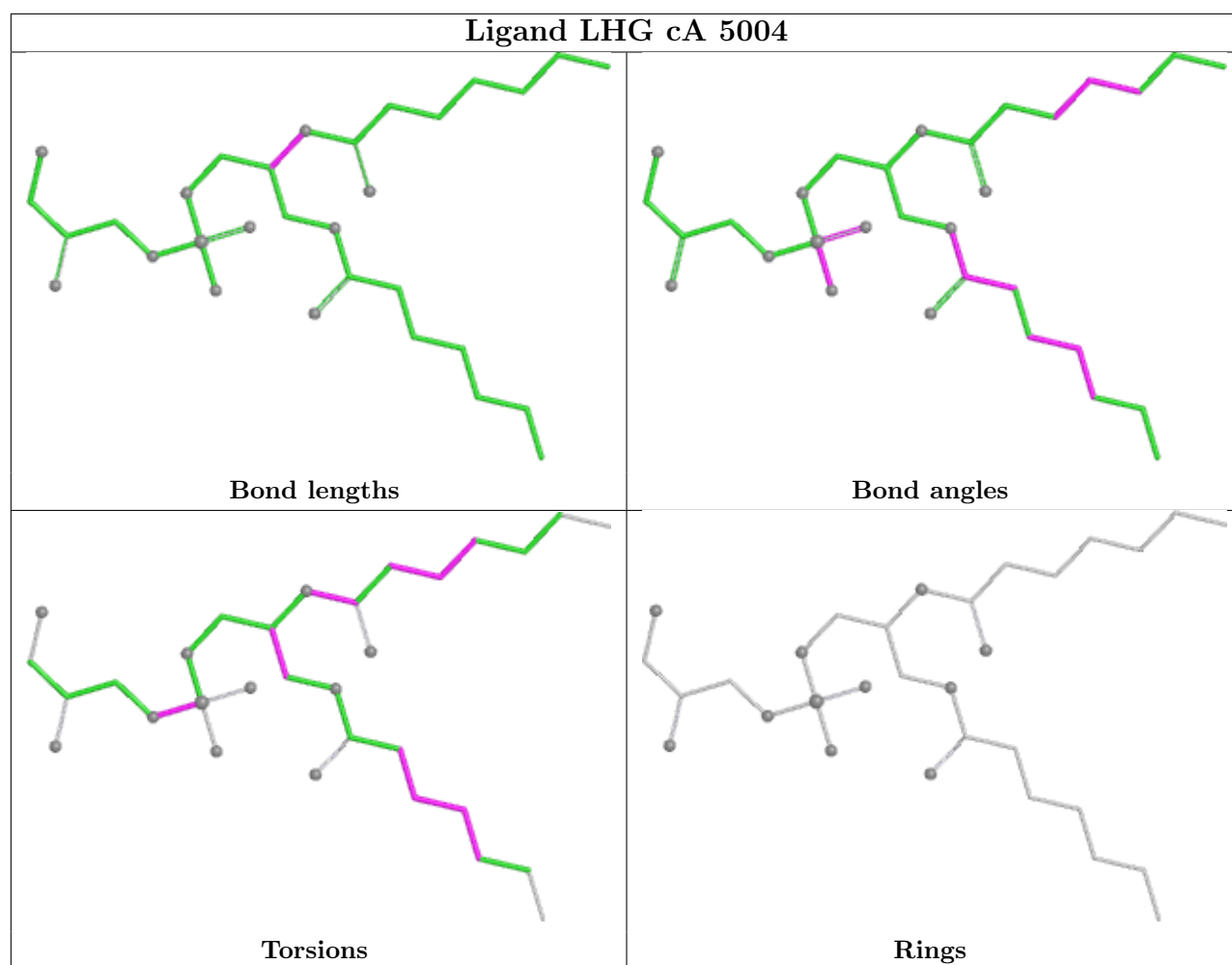
Bond angles

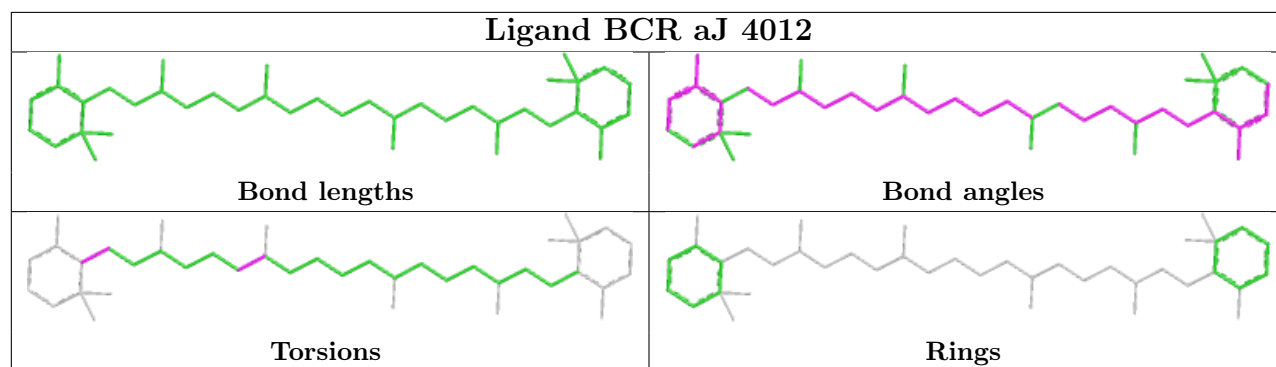
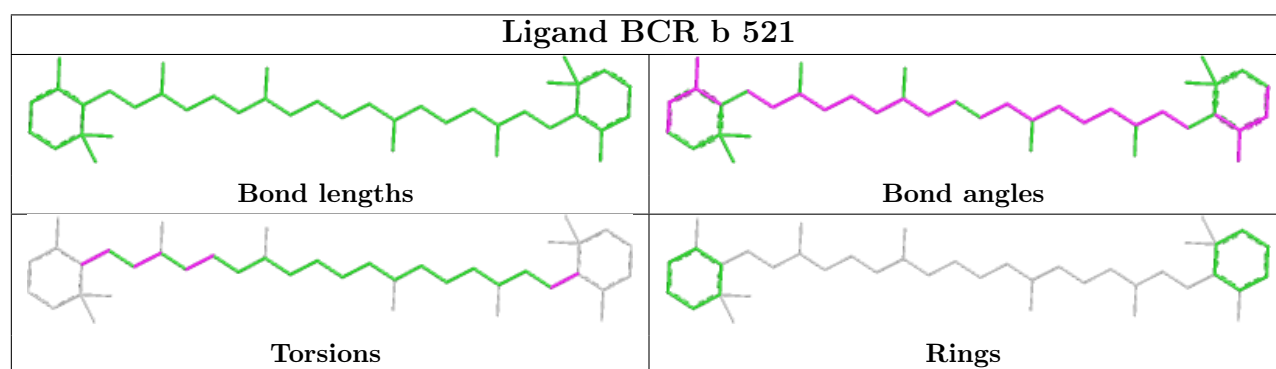
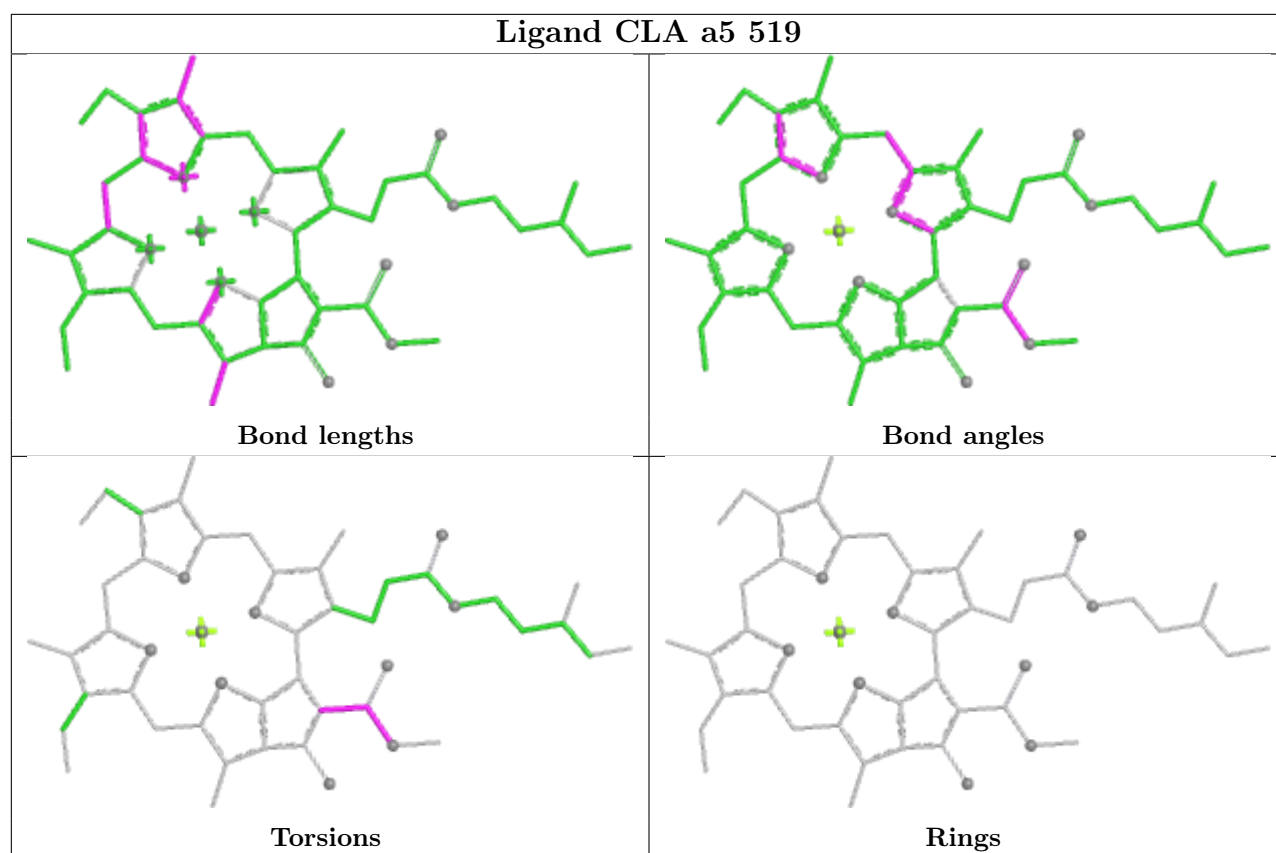


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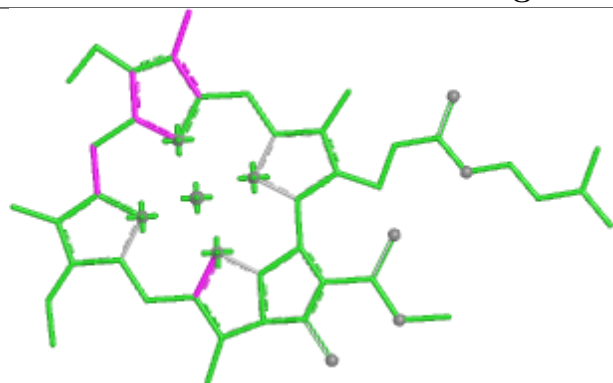


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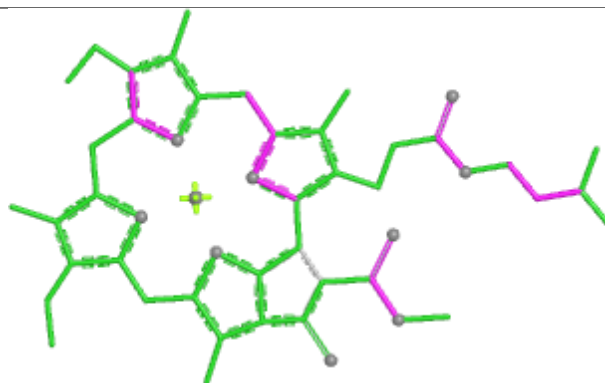




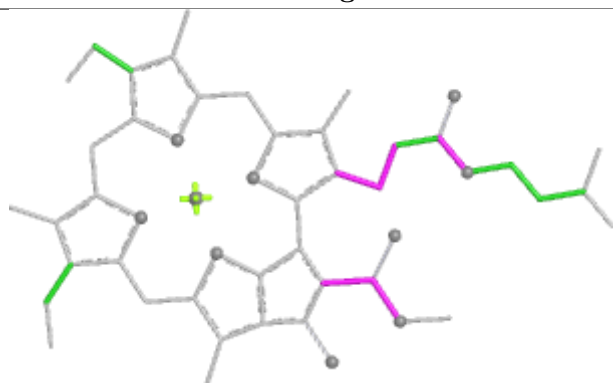
Ligand CLA U 504



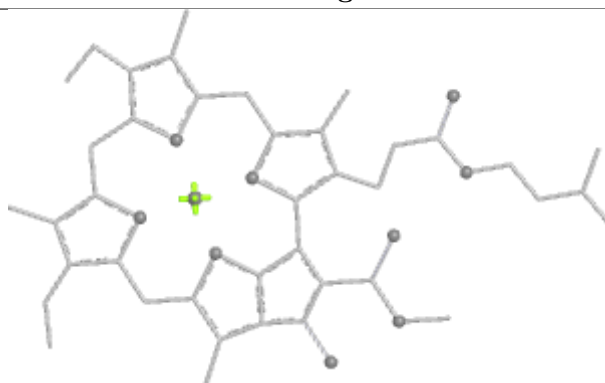
Bond lengths



Bond angles

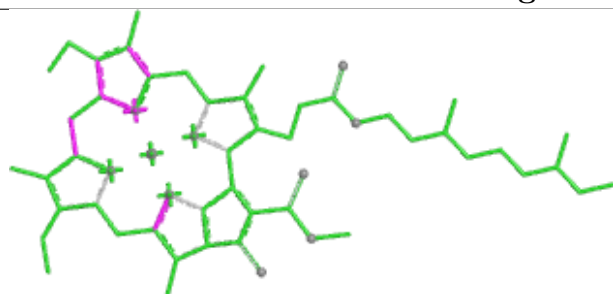


Torsions

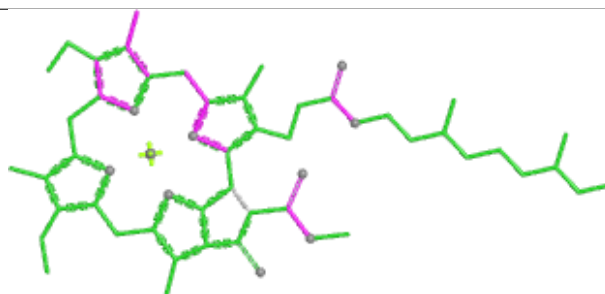


Rings

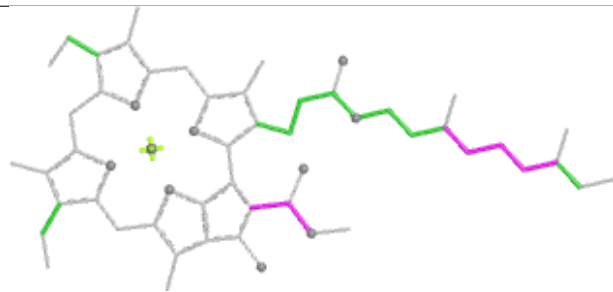
Ligand CLA o 510



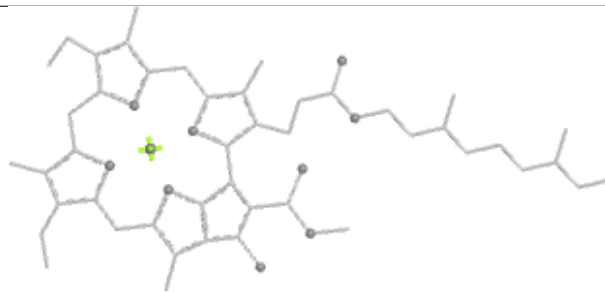
Bond lengths



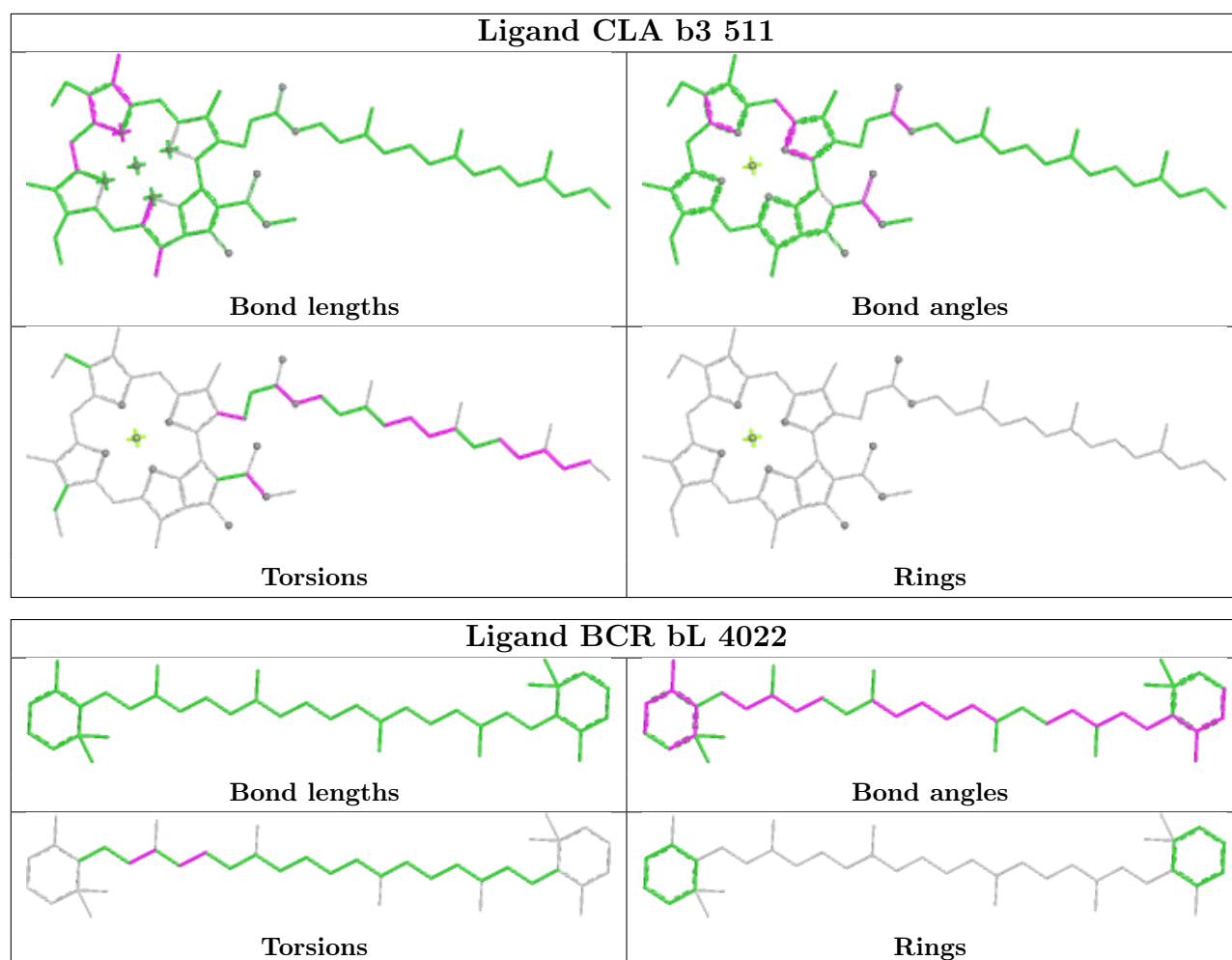
Bond angles



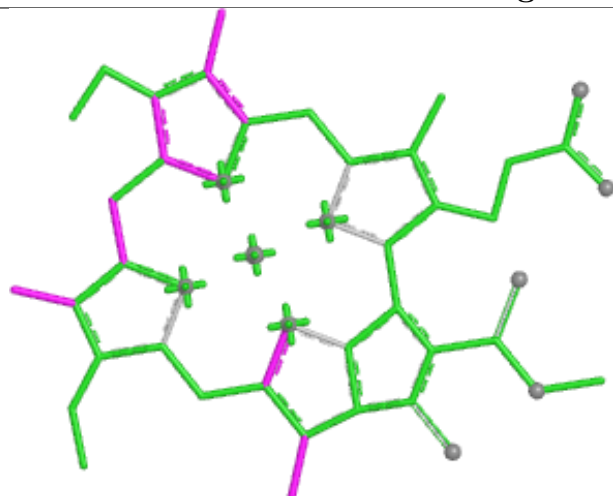
Torsions



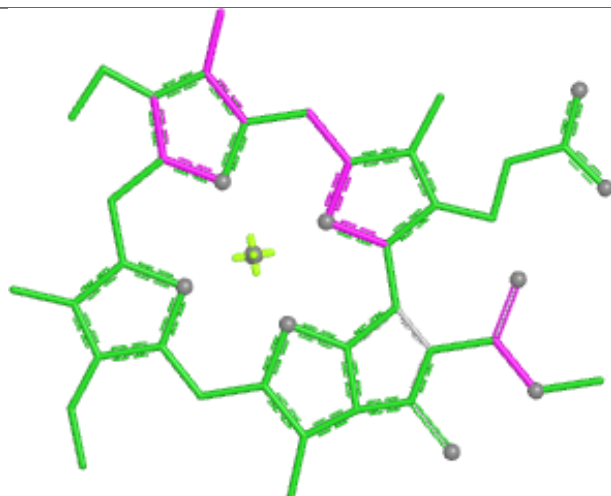
Rings



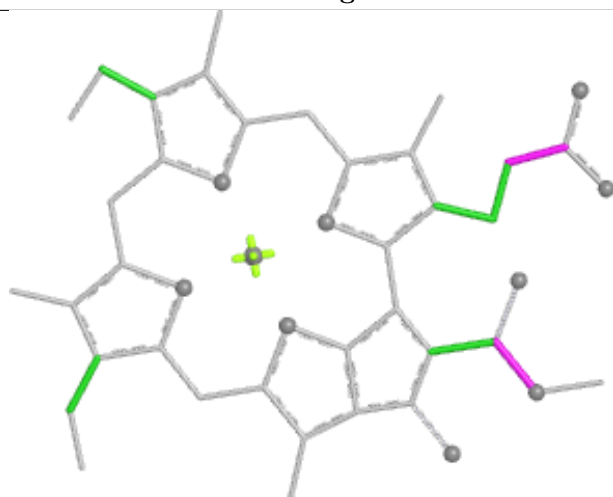
Ligand CLA h 508



Bond lengths



Bond angles

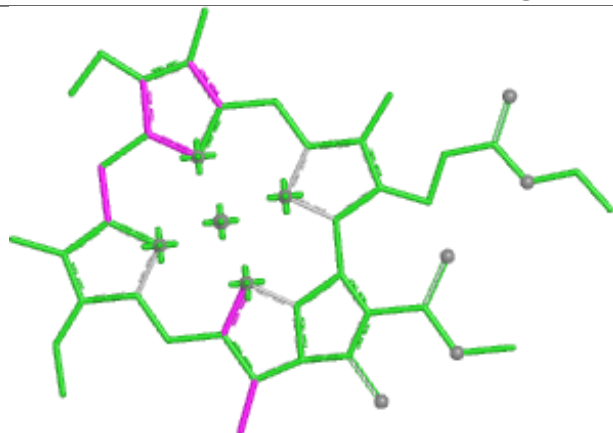


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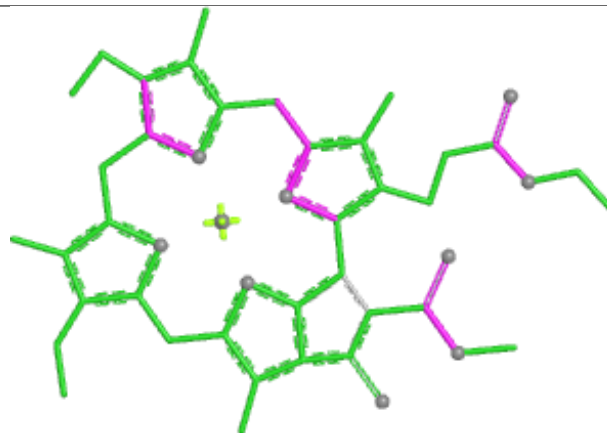


Rings

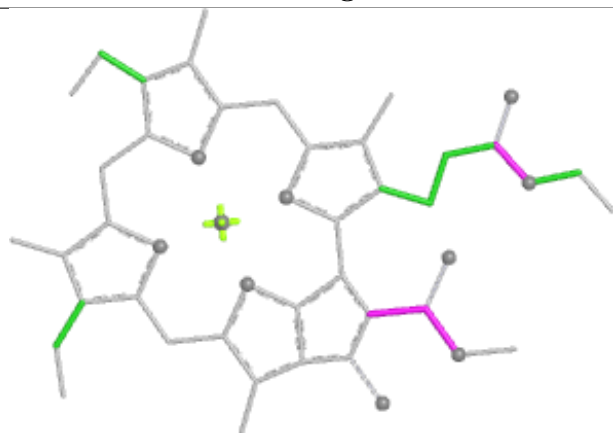
Ligand CLA S 507



Bond lengths



Bond angles

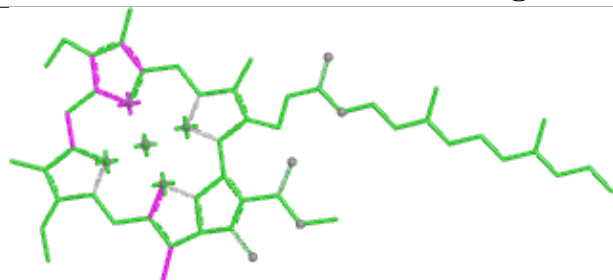


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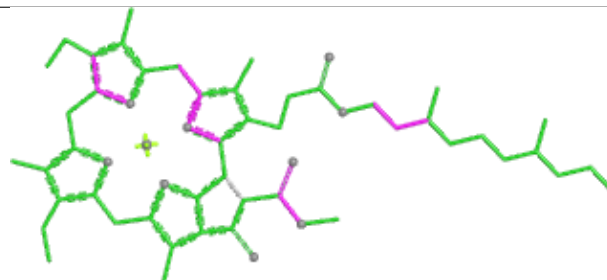


Rings

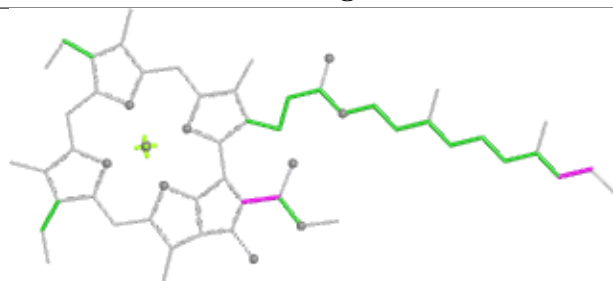
Ligand CLA c6 507



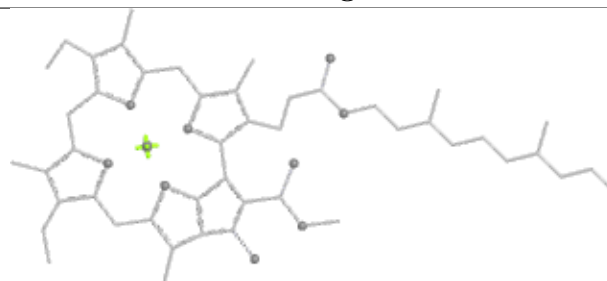
Bond lengths



Bond angles

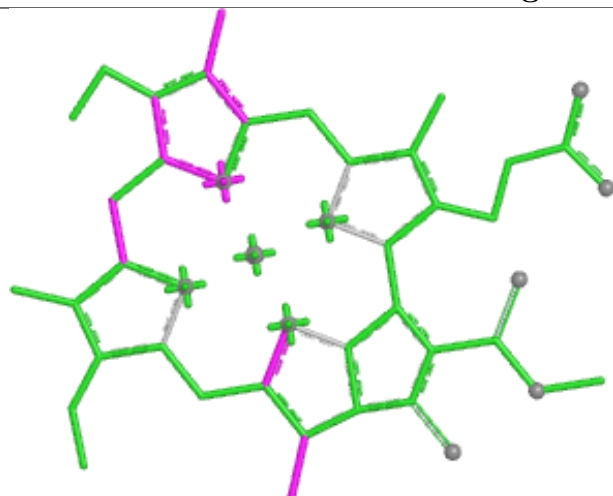


Torsions

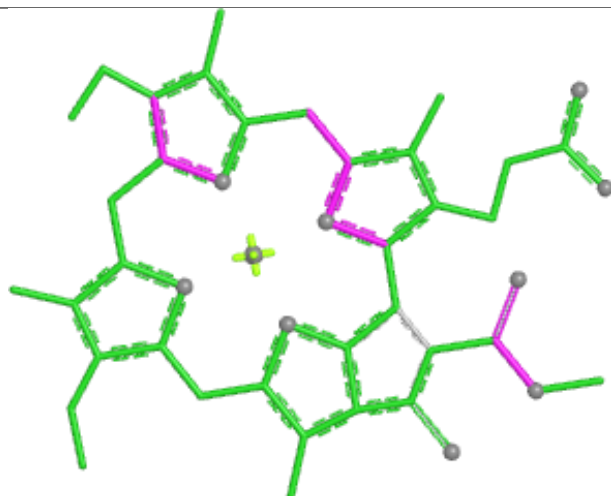


Rings

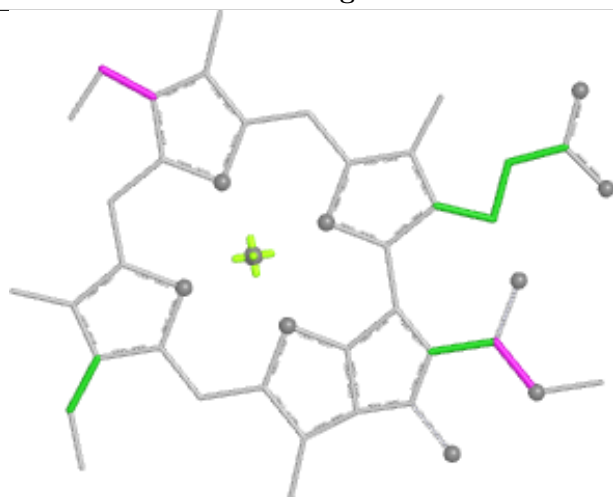
Ligand CLA f 502



Bond lengths



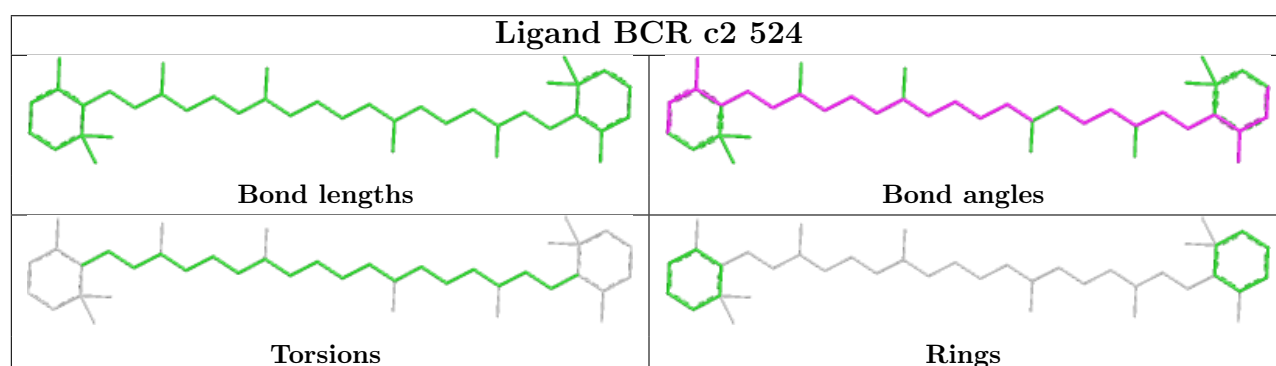
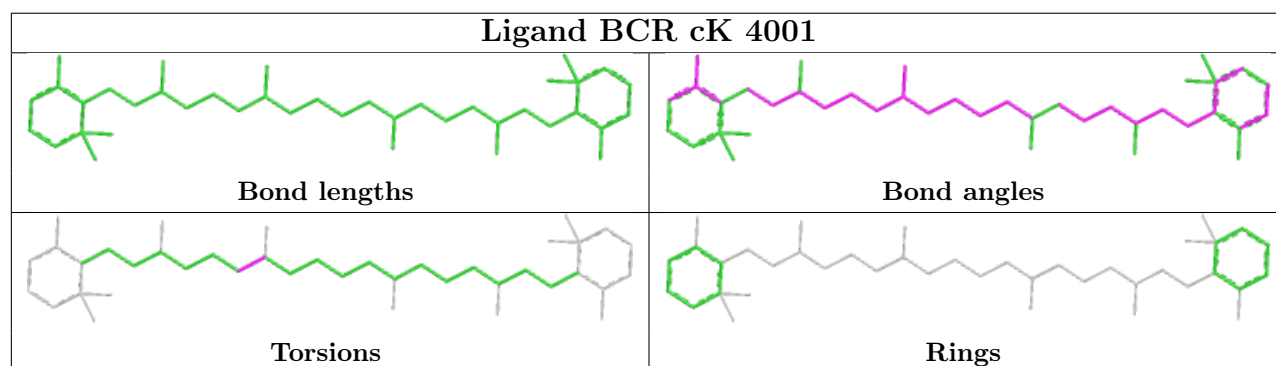
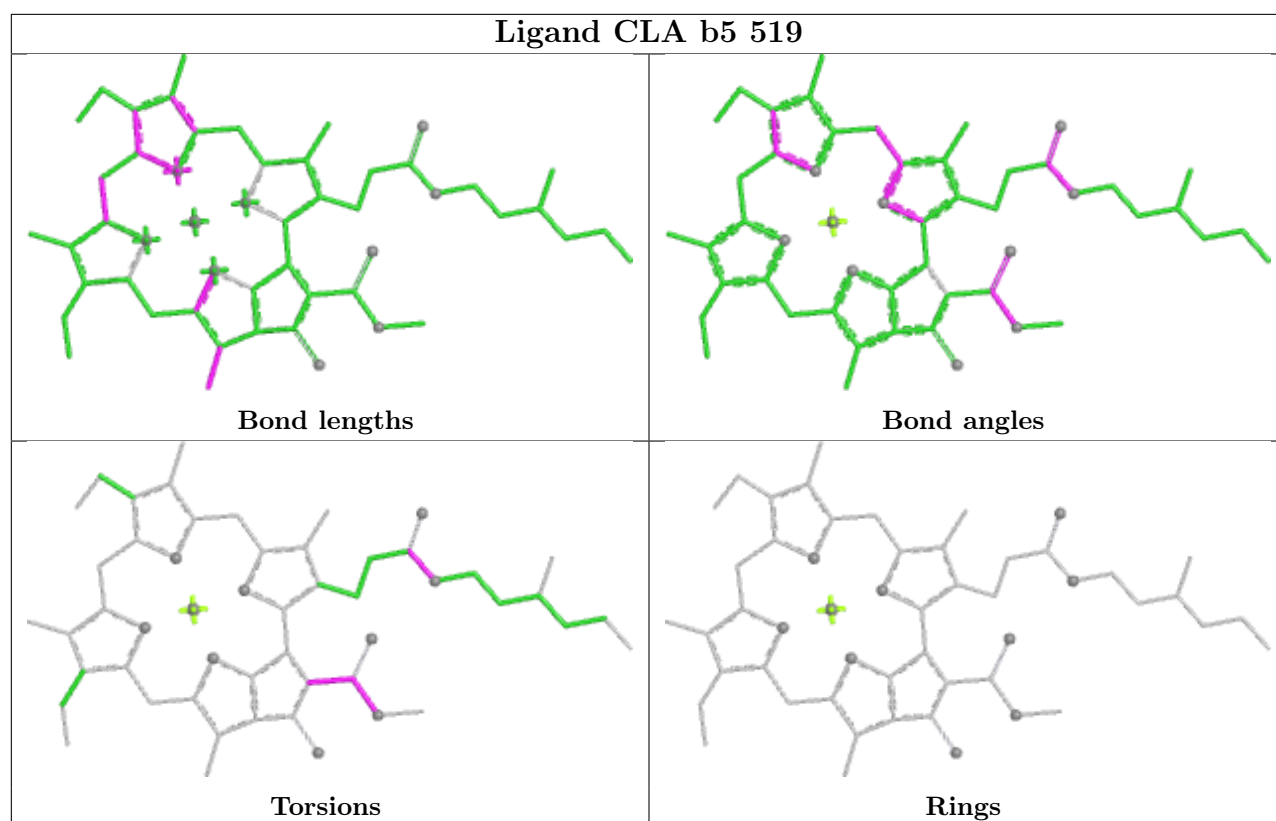
Bond angles

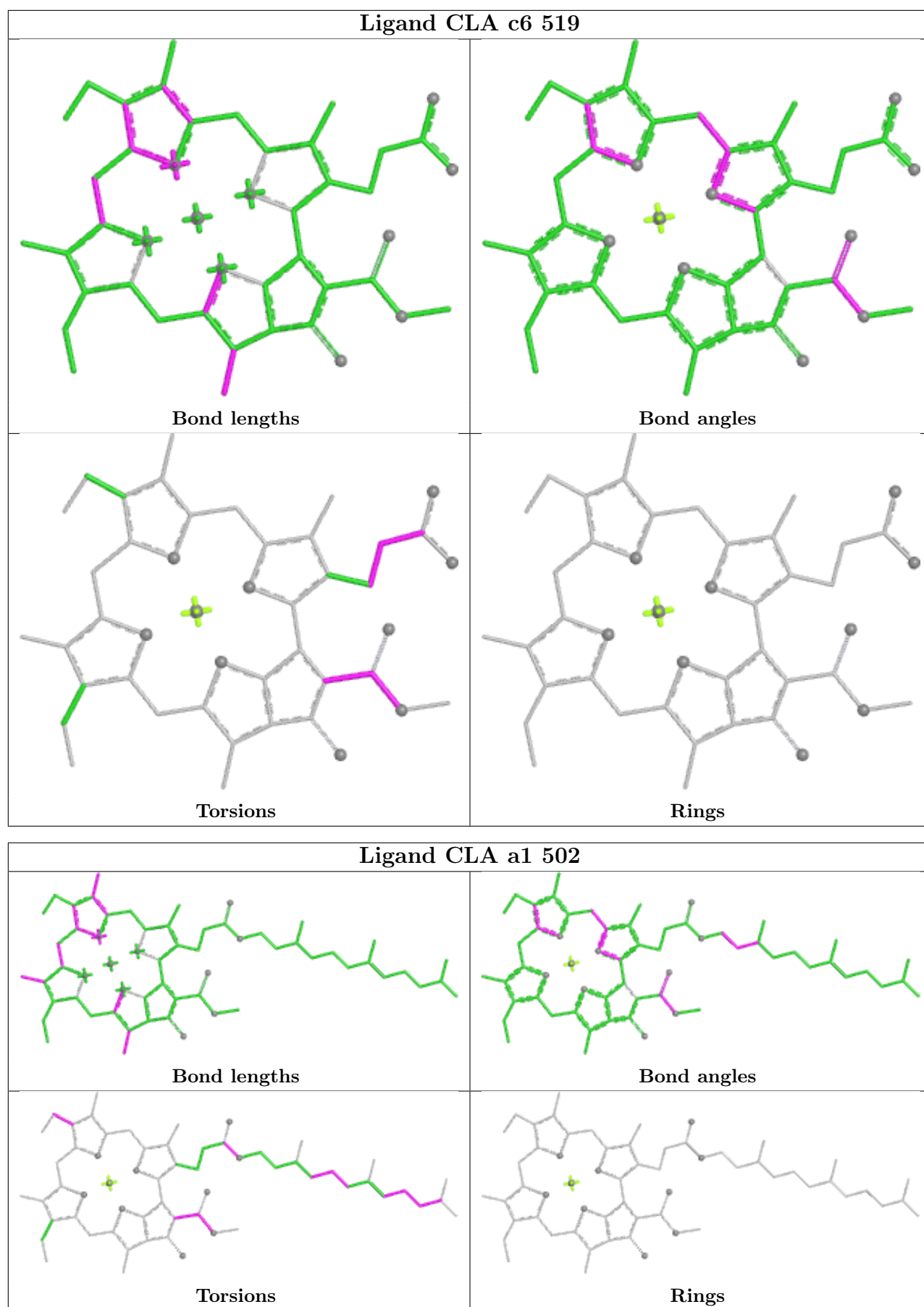


Torsions

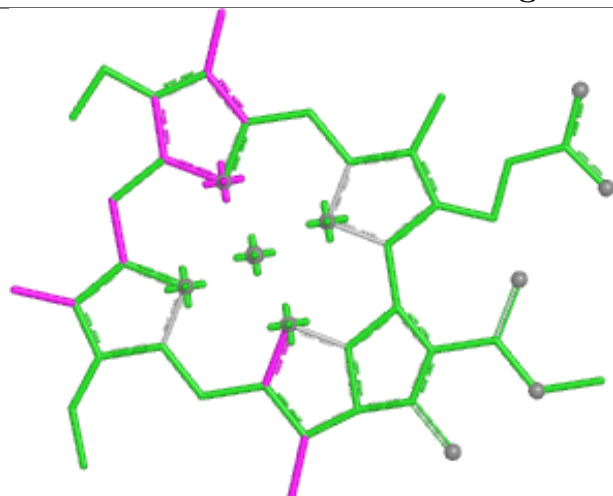


Rings





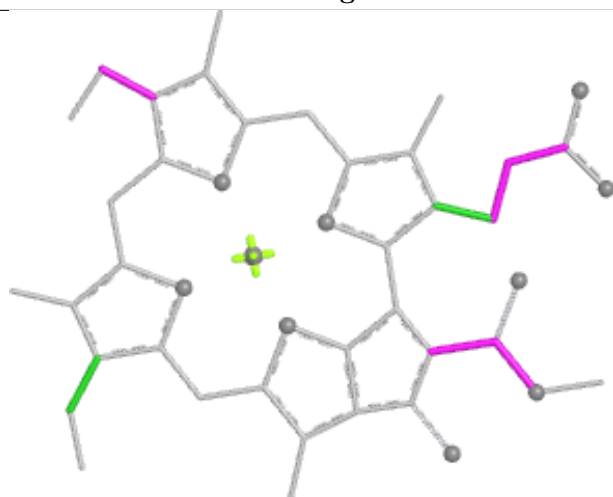
Ligand CLA e 501



Bond lengths



Bond angles

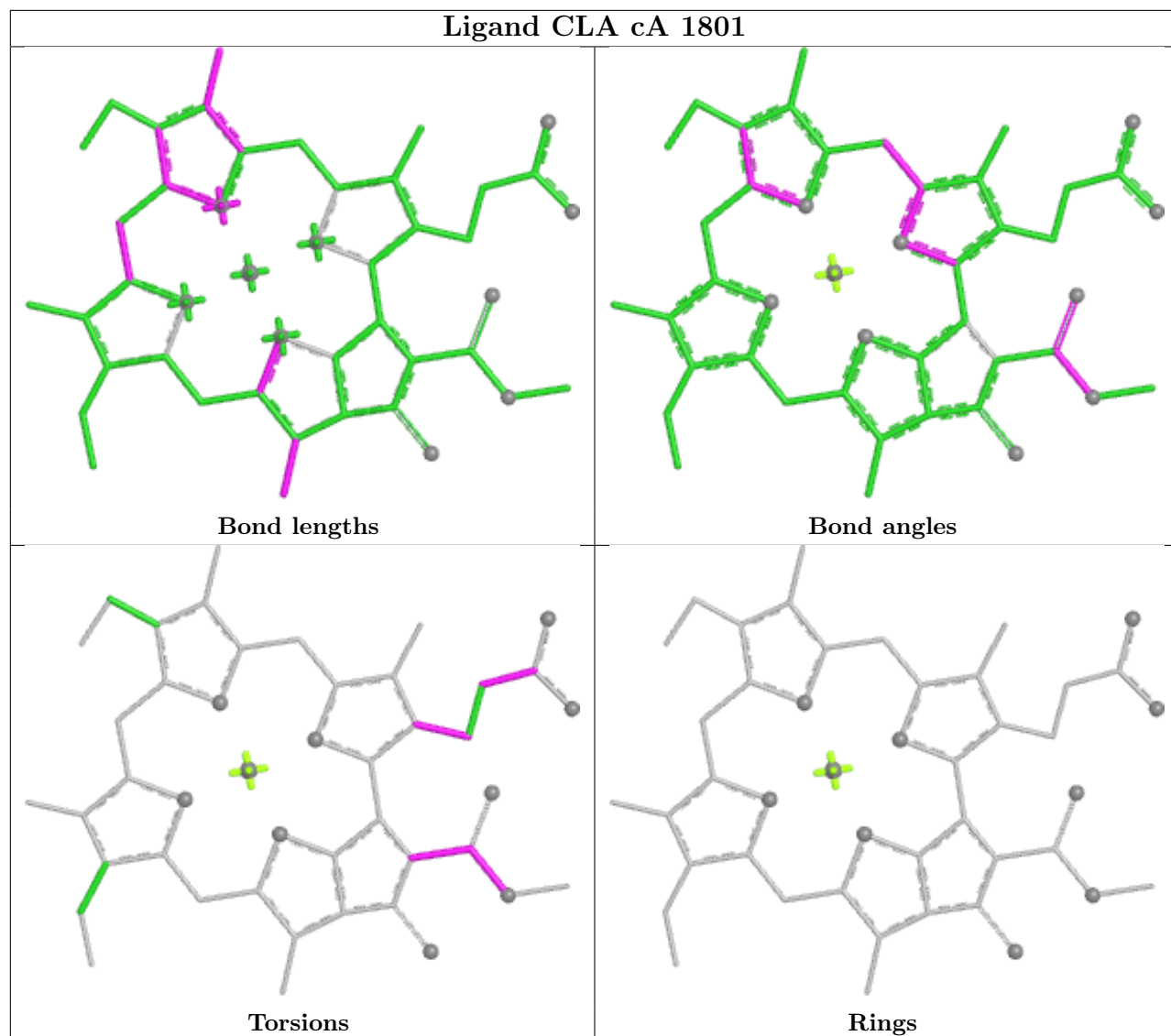


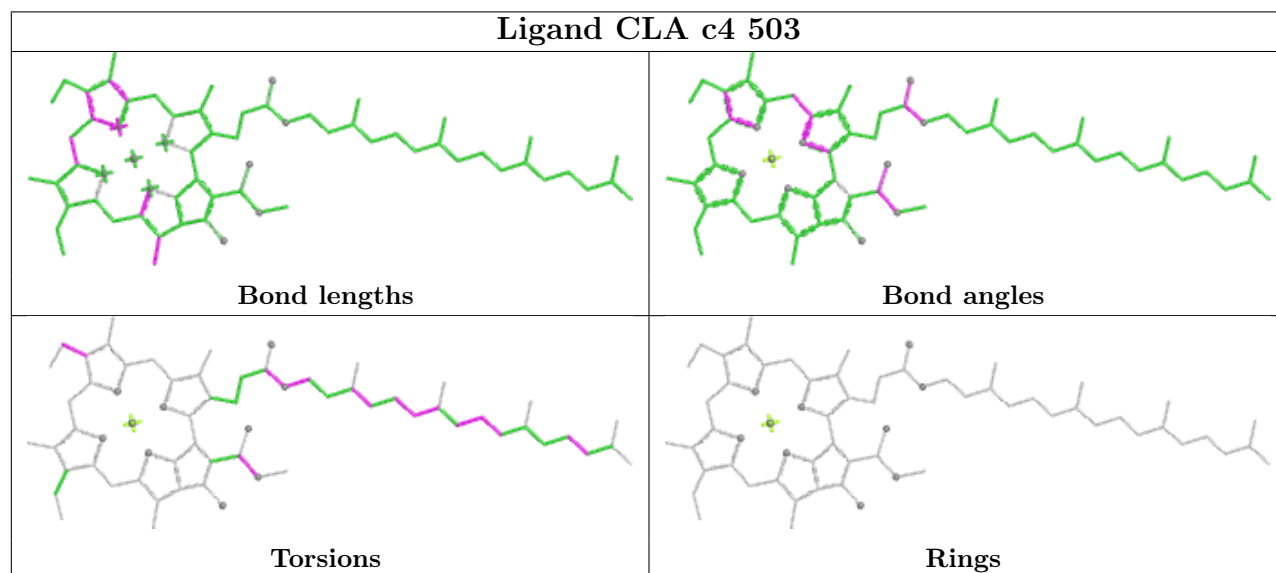
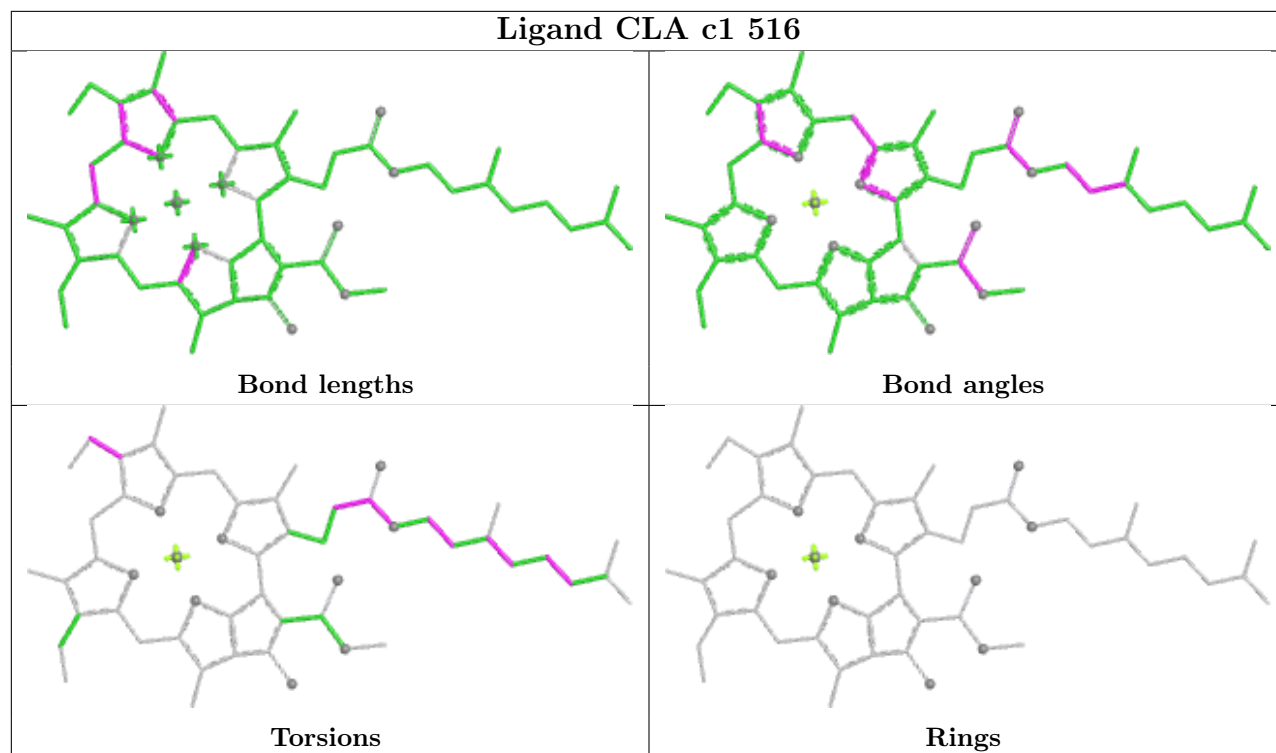
Torsions



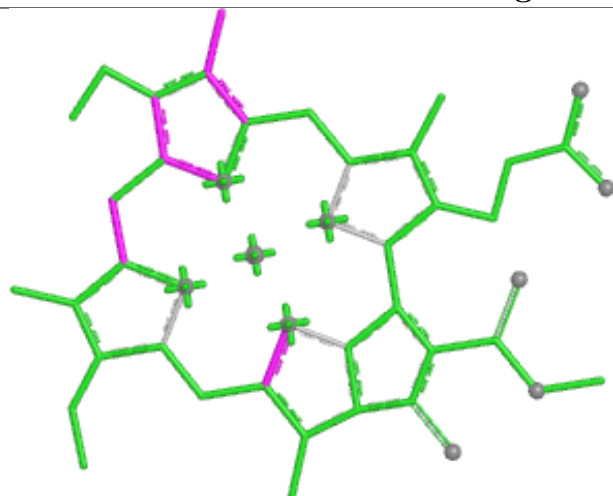
Rings

Ligand CLA cA 1801

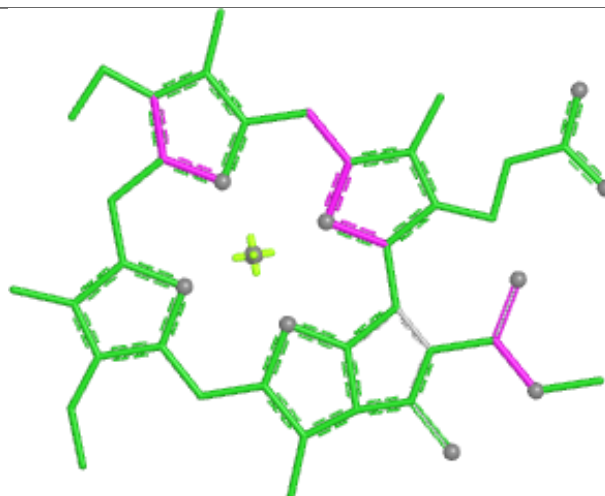




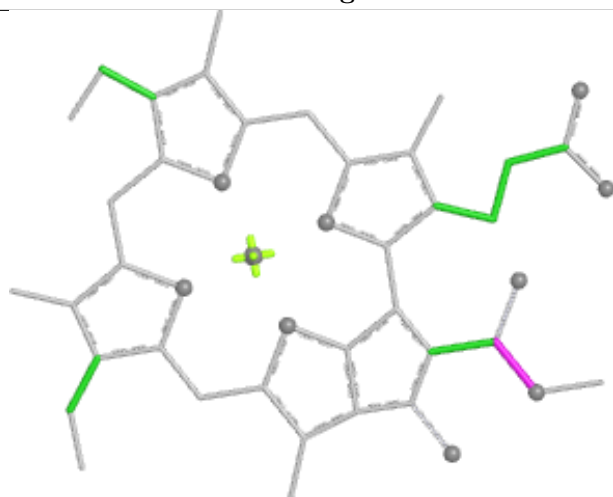
Ligand CLA T 503



Bond lengths



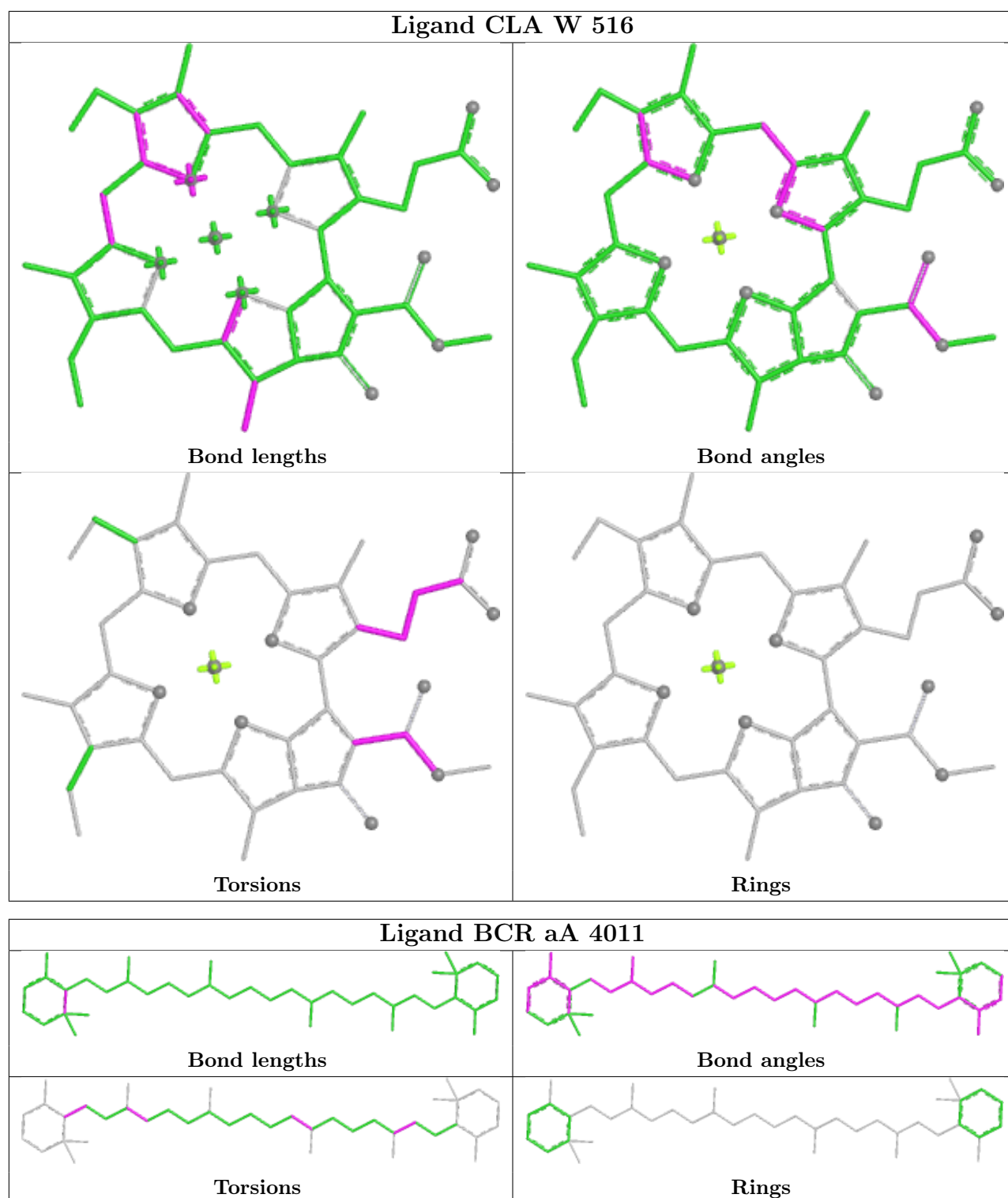
Bond angles



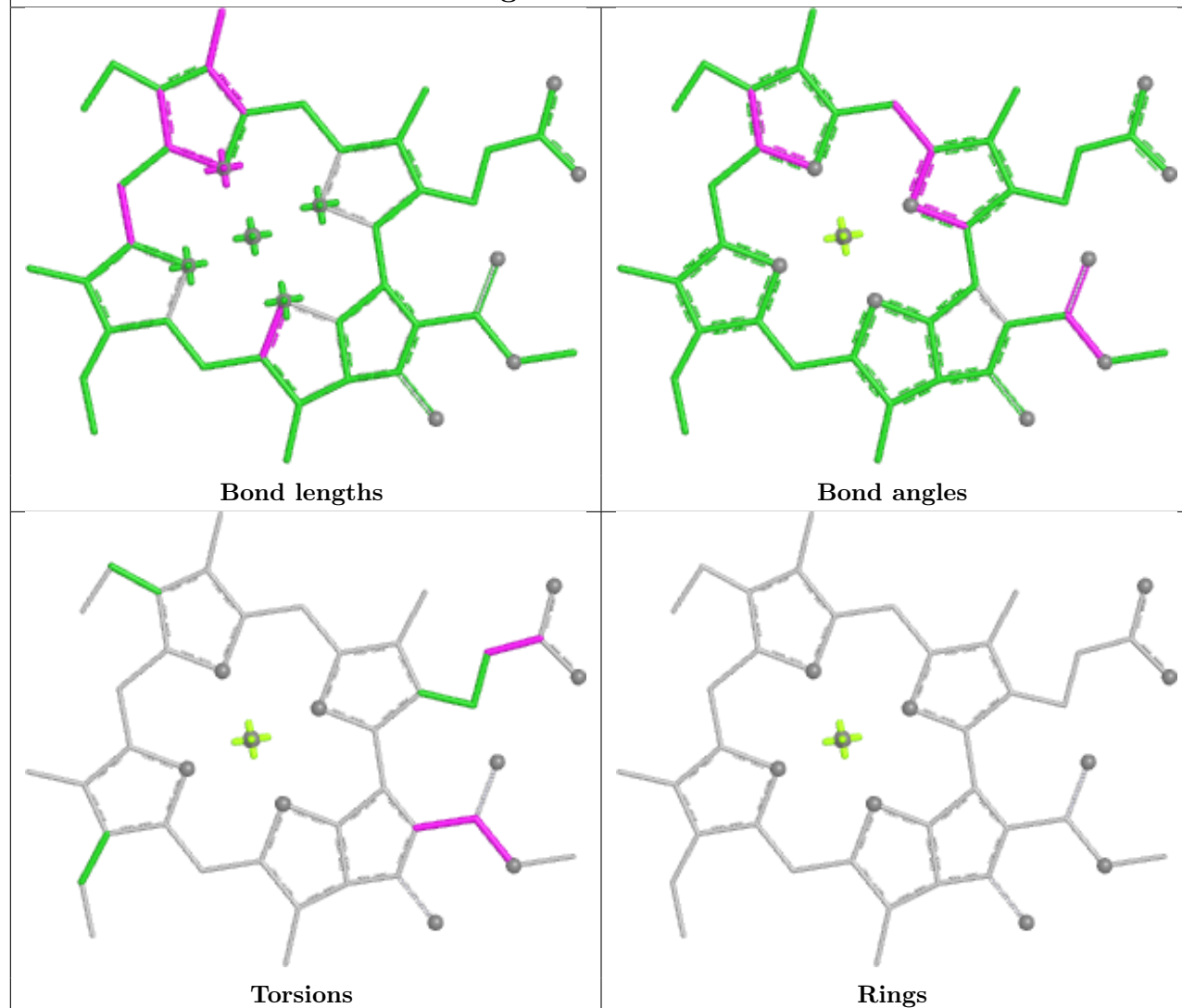
Torsions



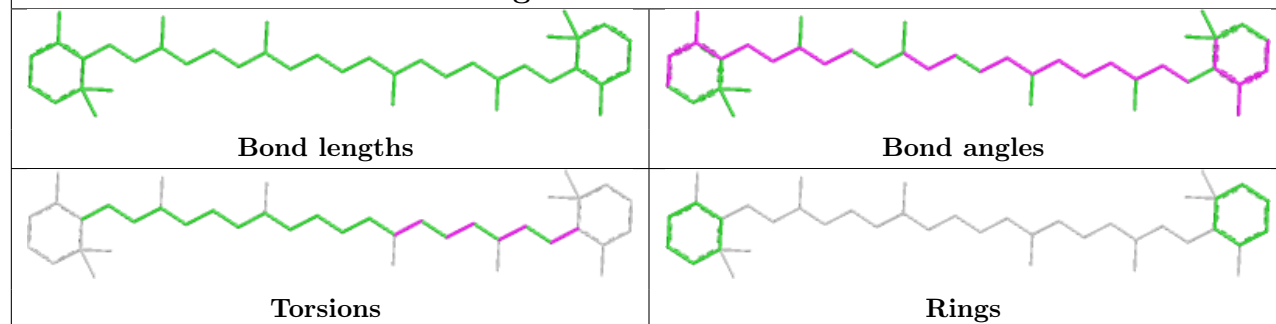
Rings

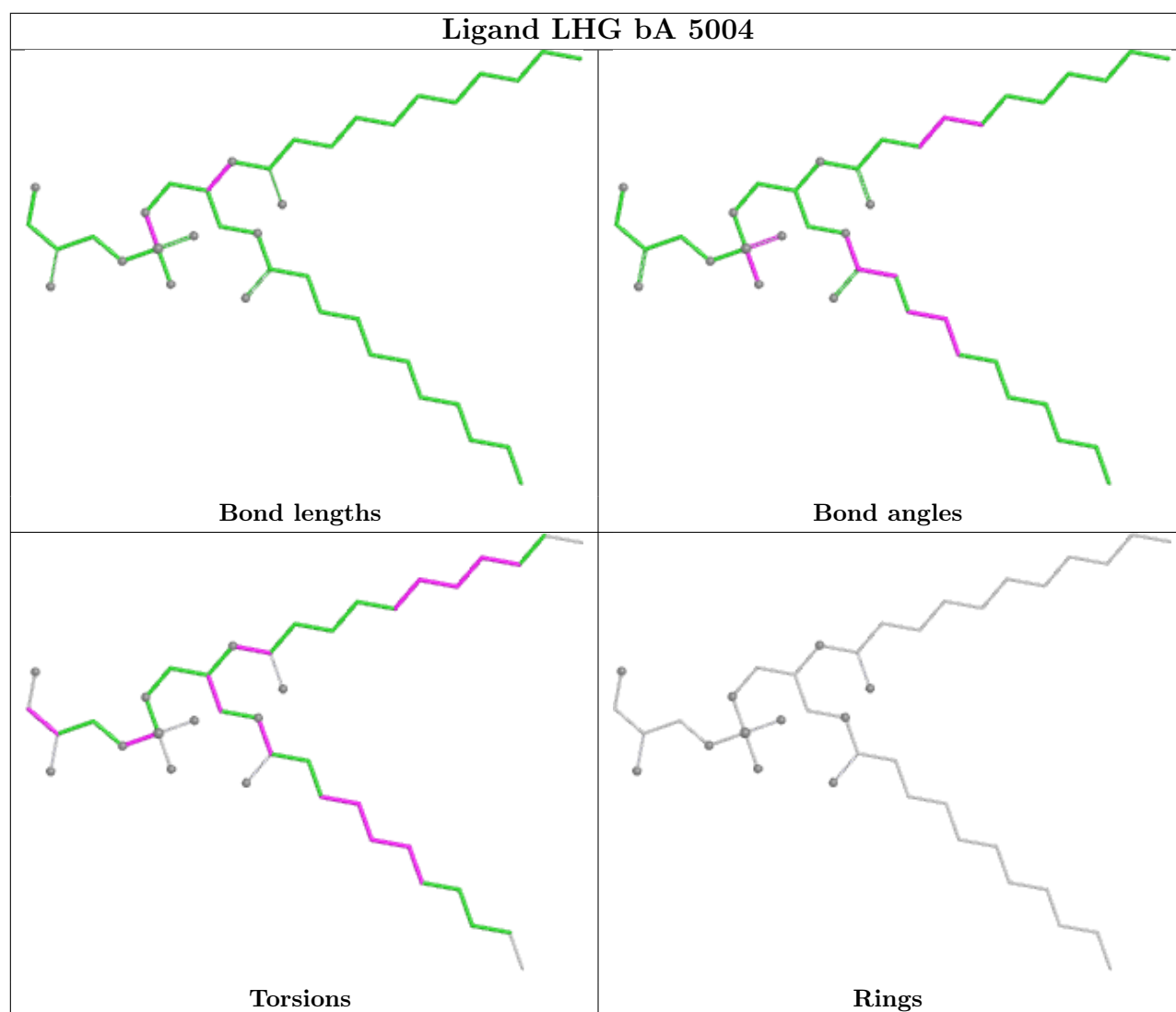


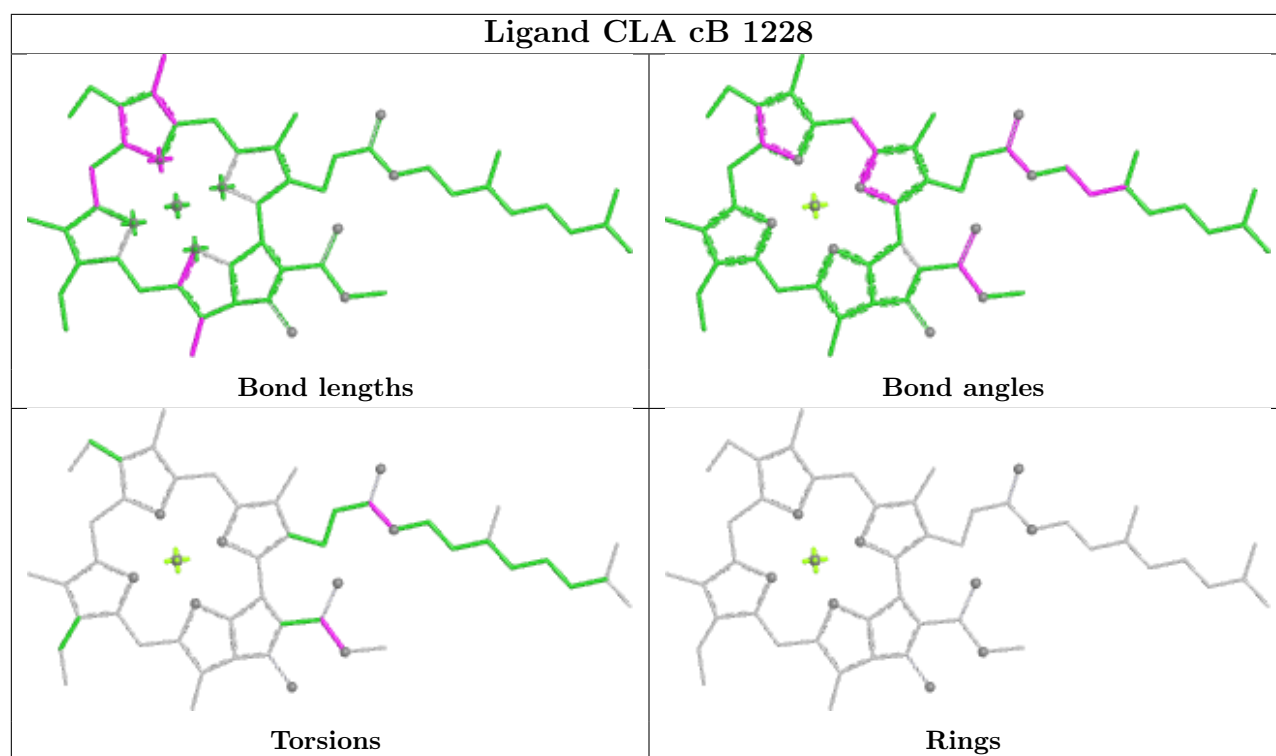
Ligand CLA i 506

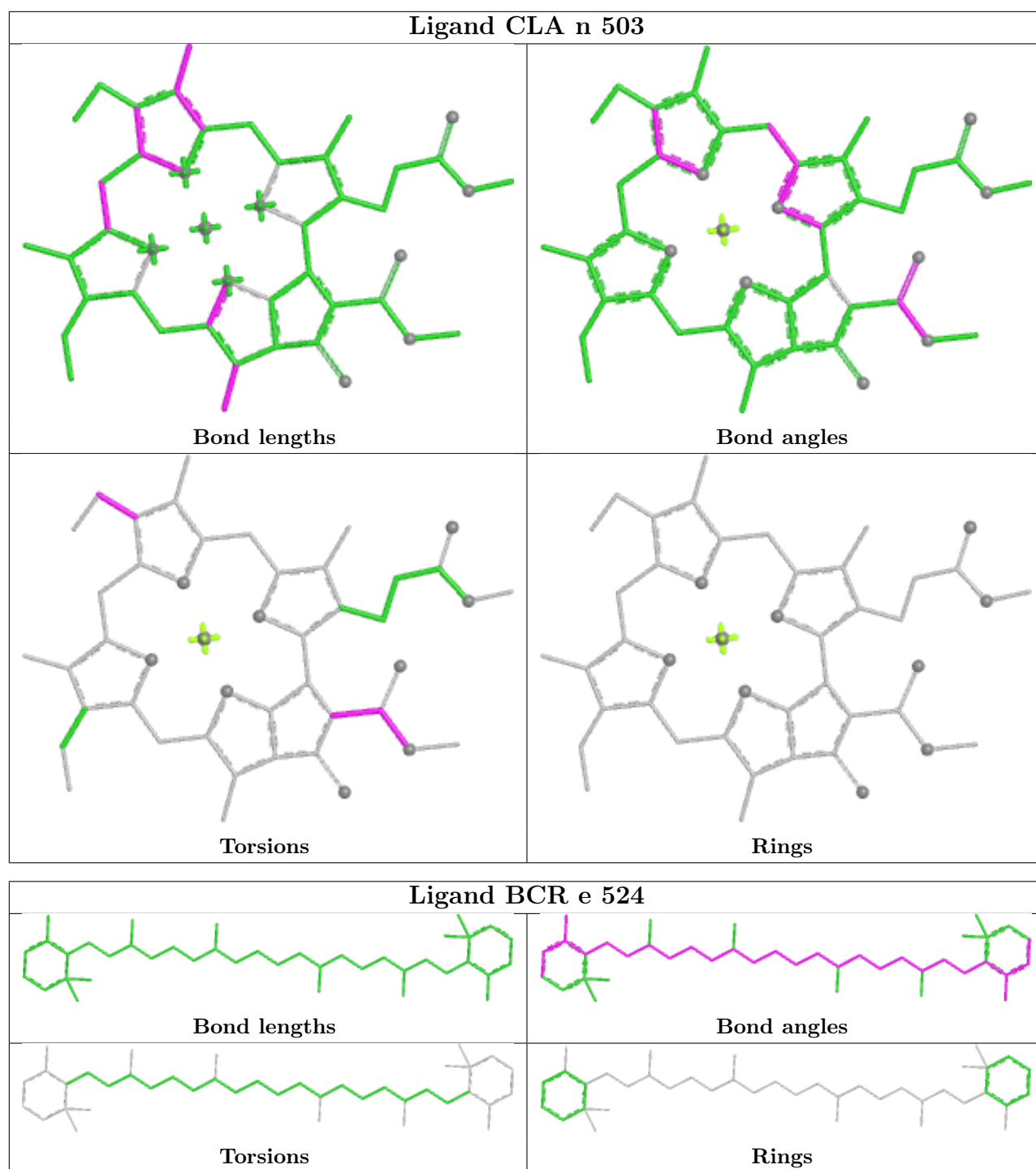


Ligand BCR aB 4009

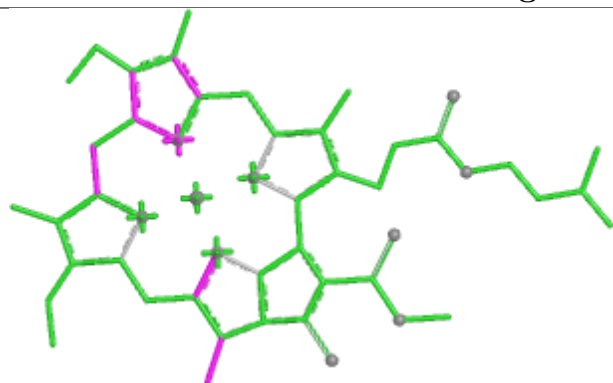




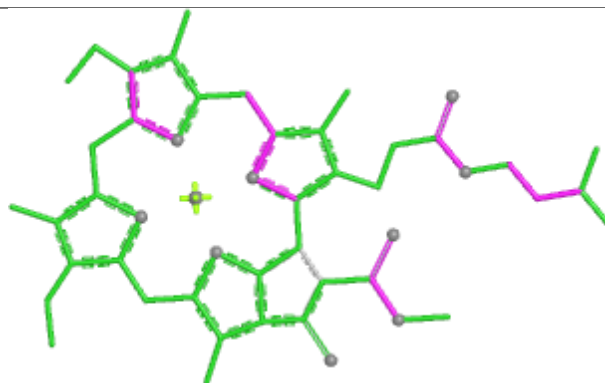




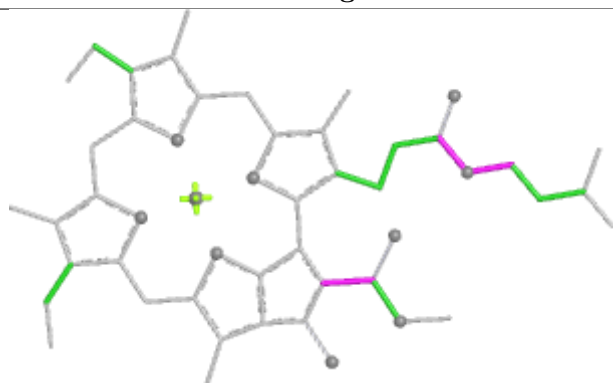
Ligand CLA e 507



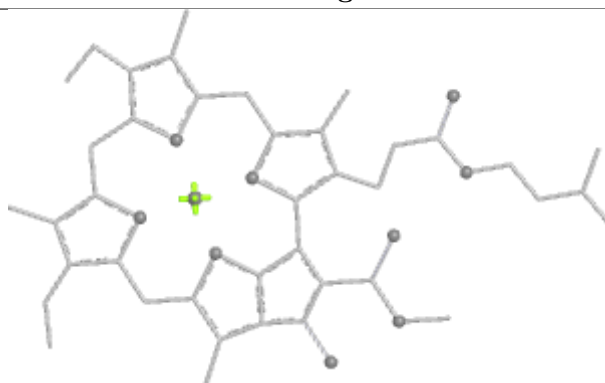
Bond lengths



Bond angles

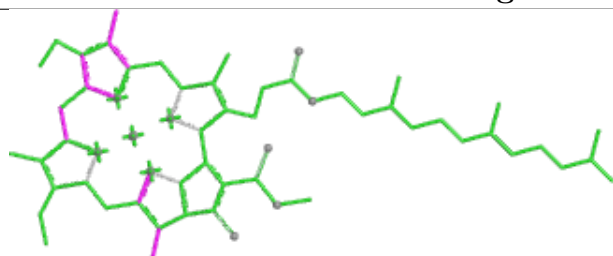


Torsions

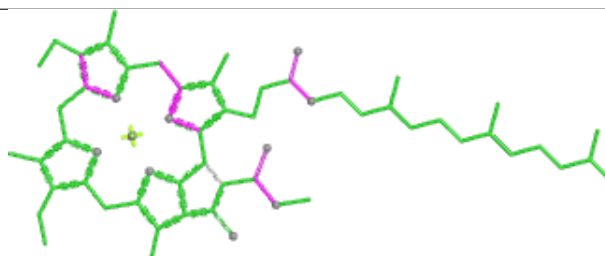


Rings

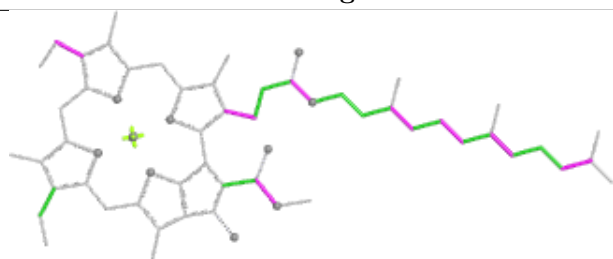
Ligand CLA cA 1118



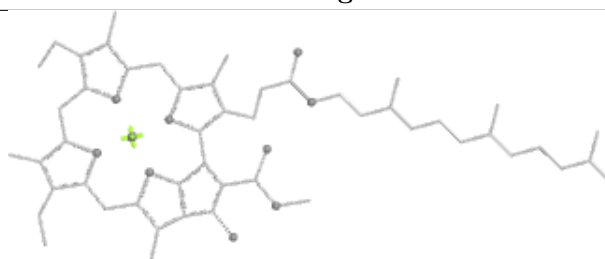
Bond lengths



Bond angles

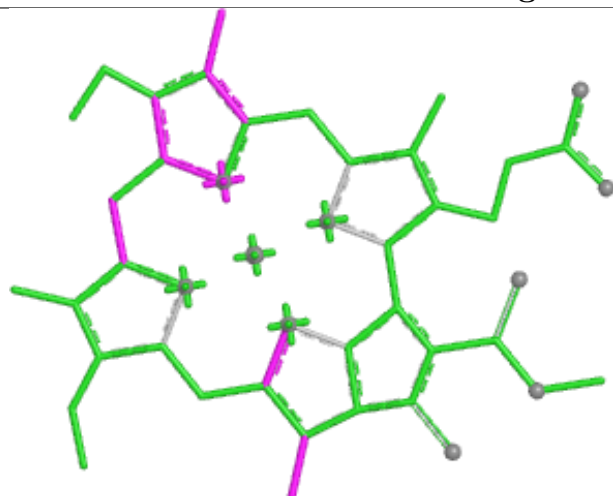


Torsions



Rings

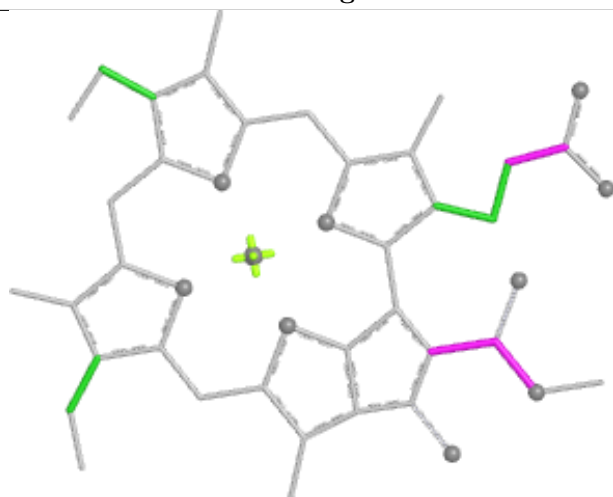
Ligand CLA o 506



Bond lengths



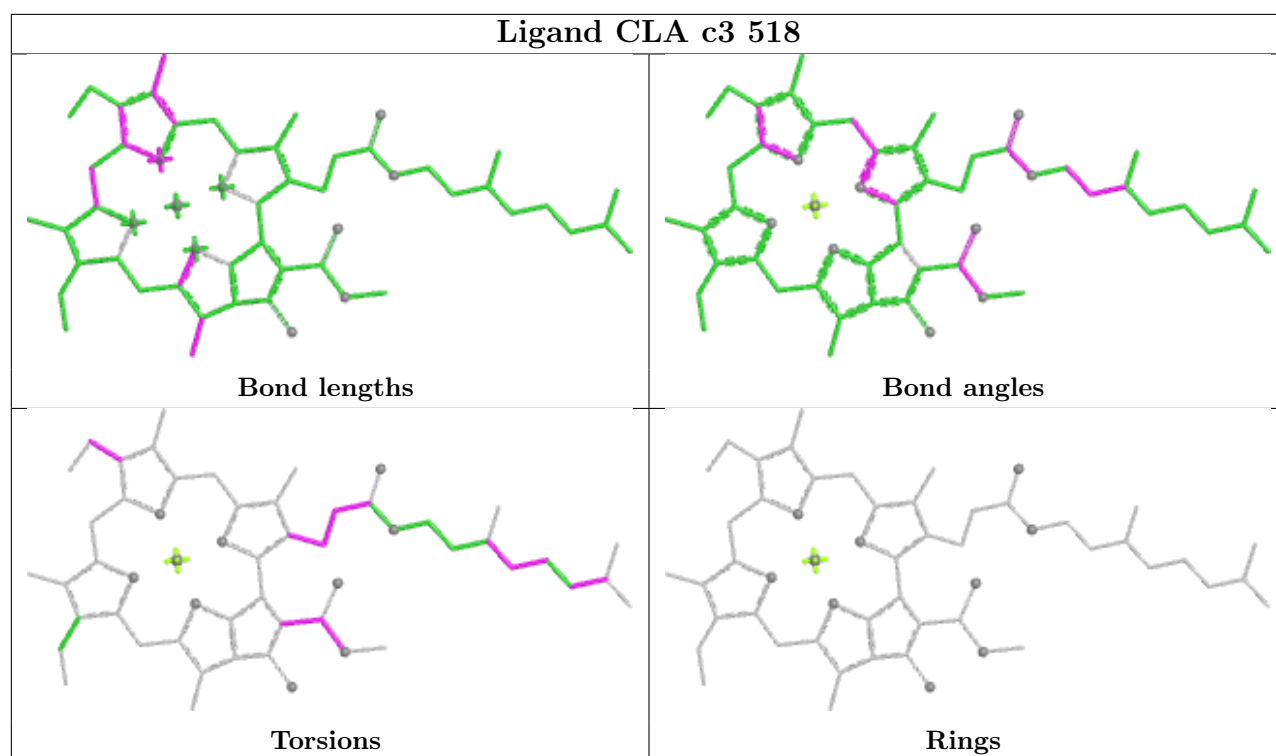
Bond angles



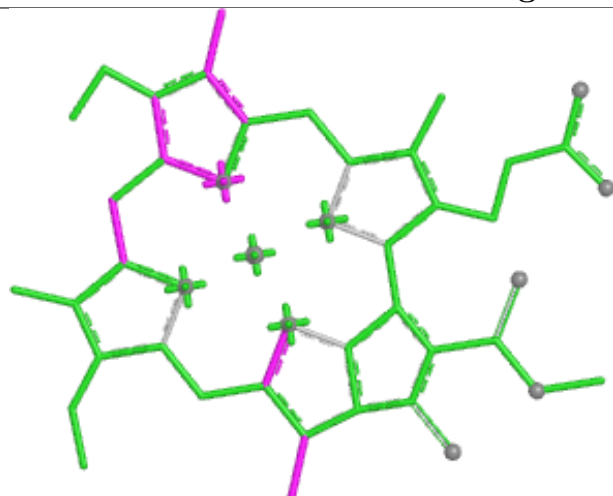
Torsions



Rings



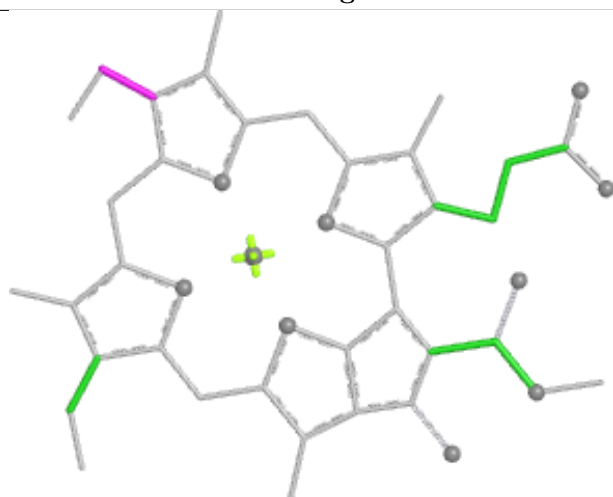
Ligand CLA o 502



Bond lengths



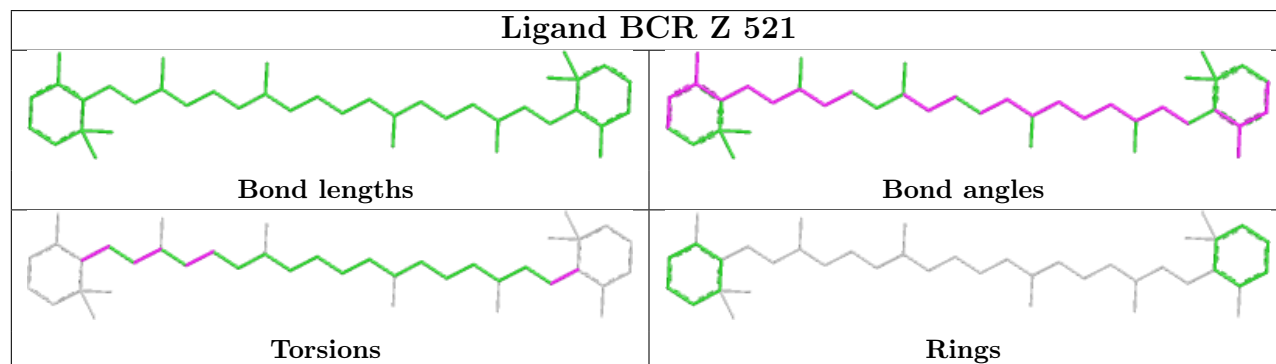
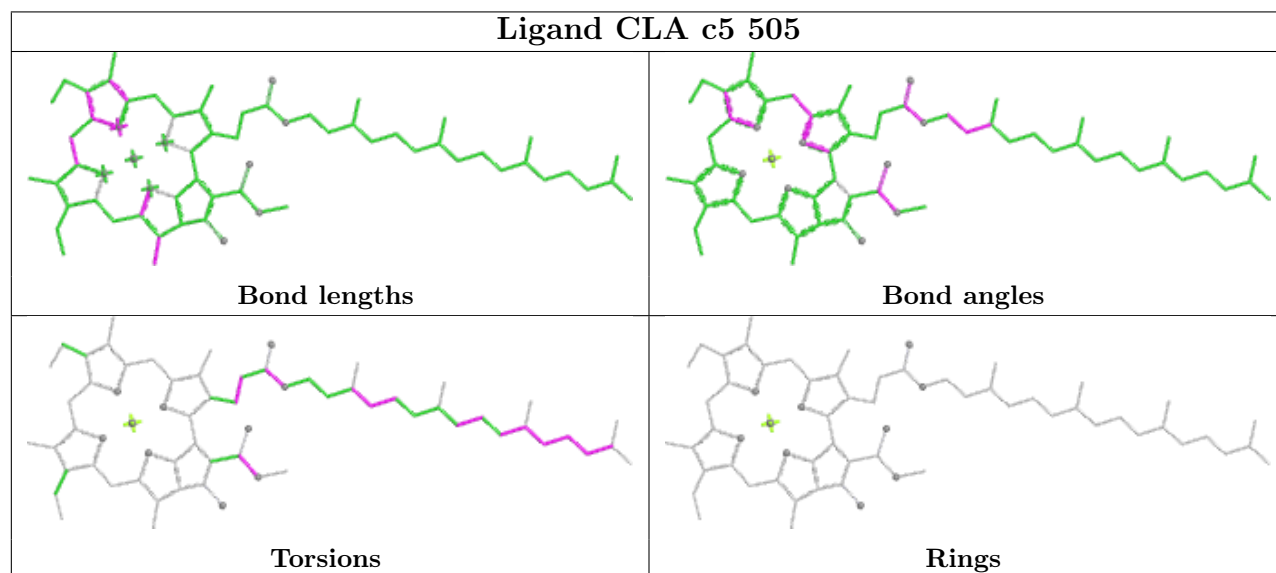
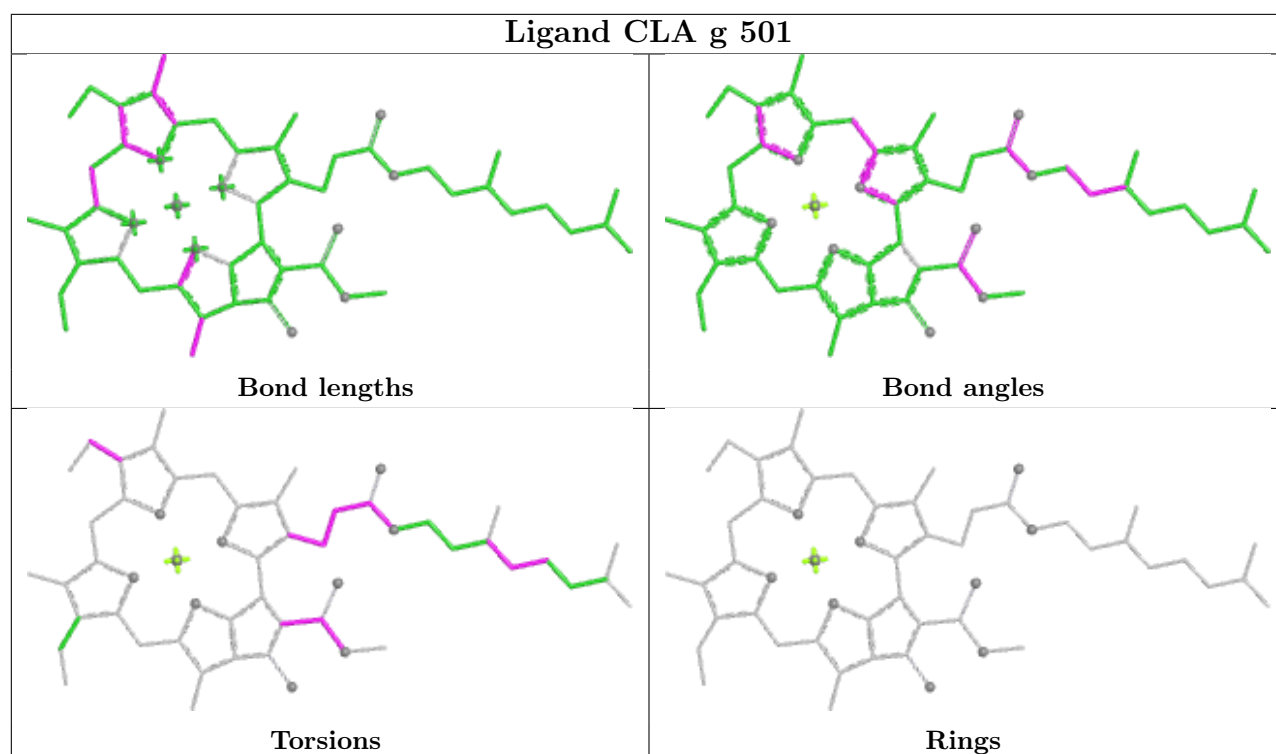
Bond angles

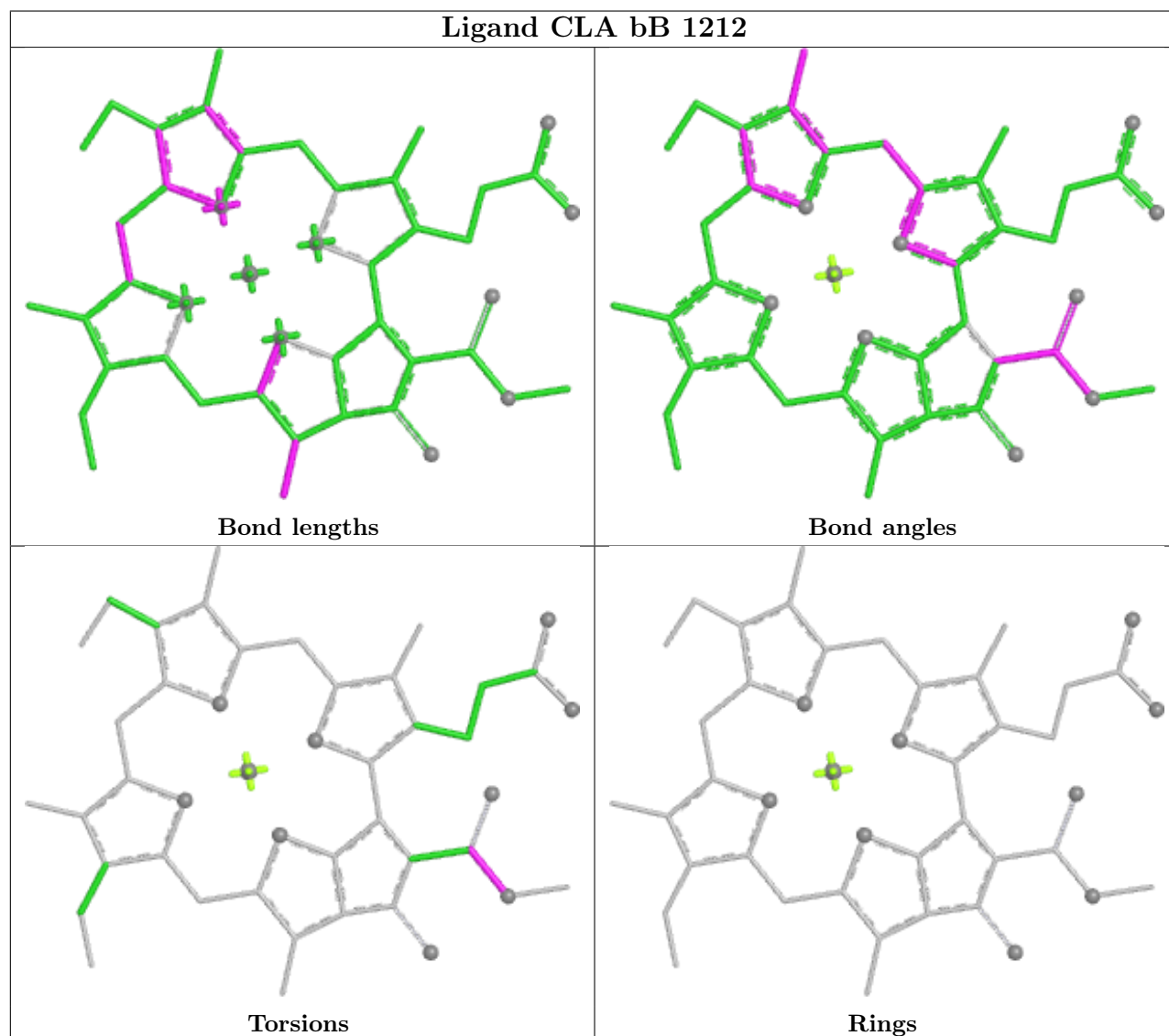
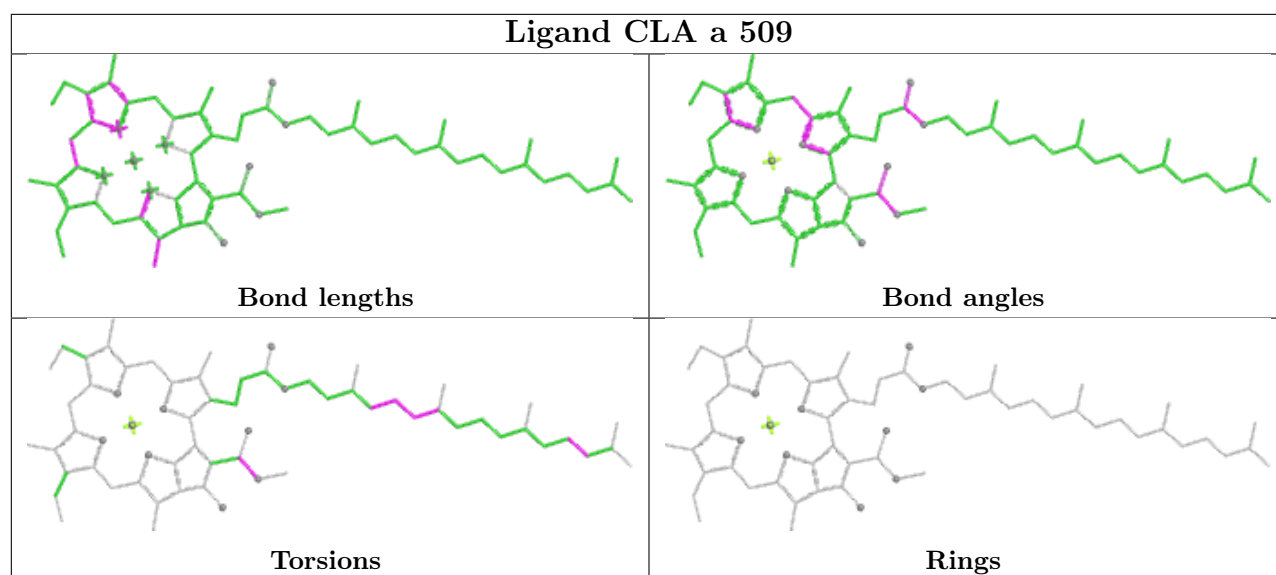


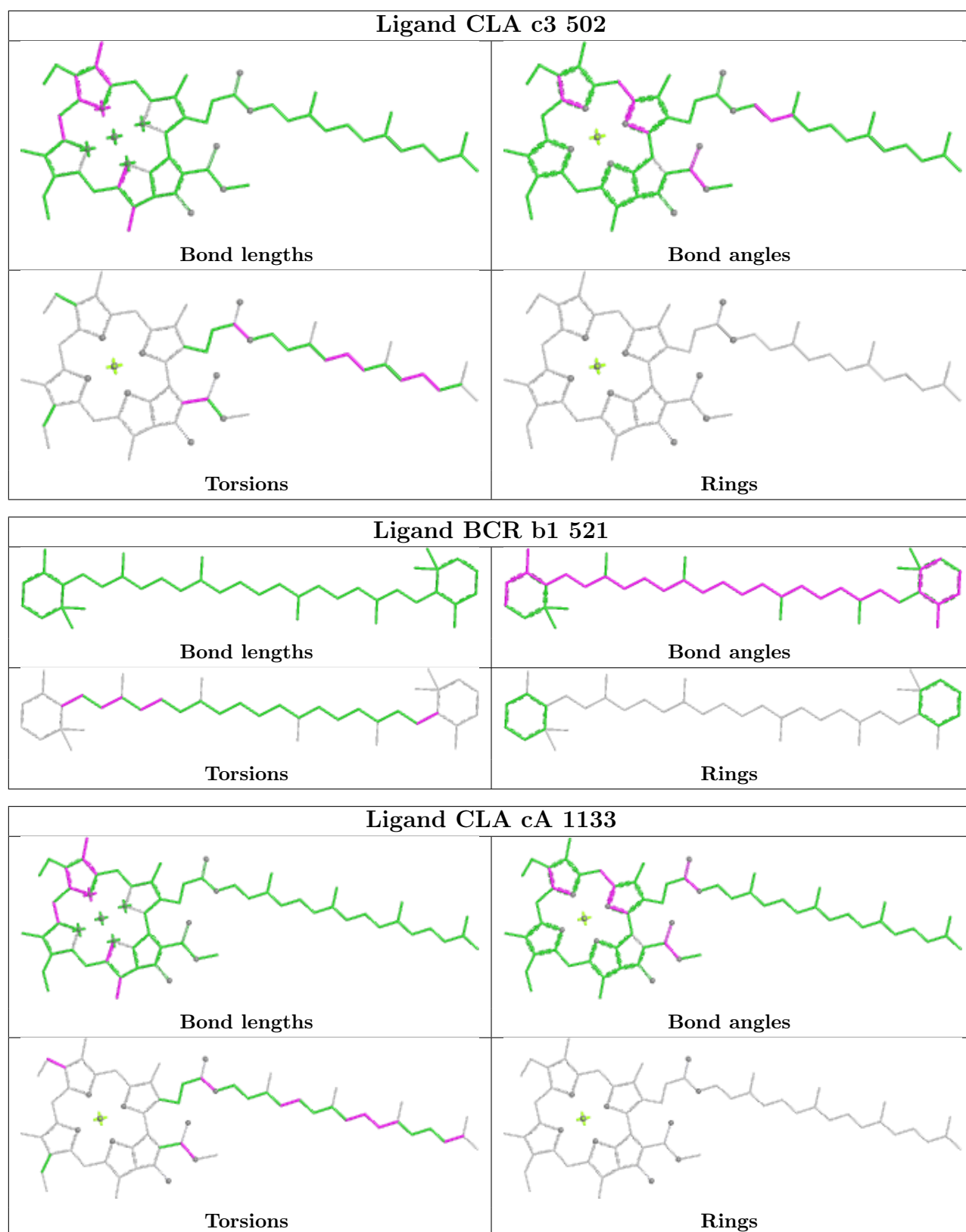
Torsions

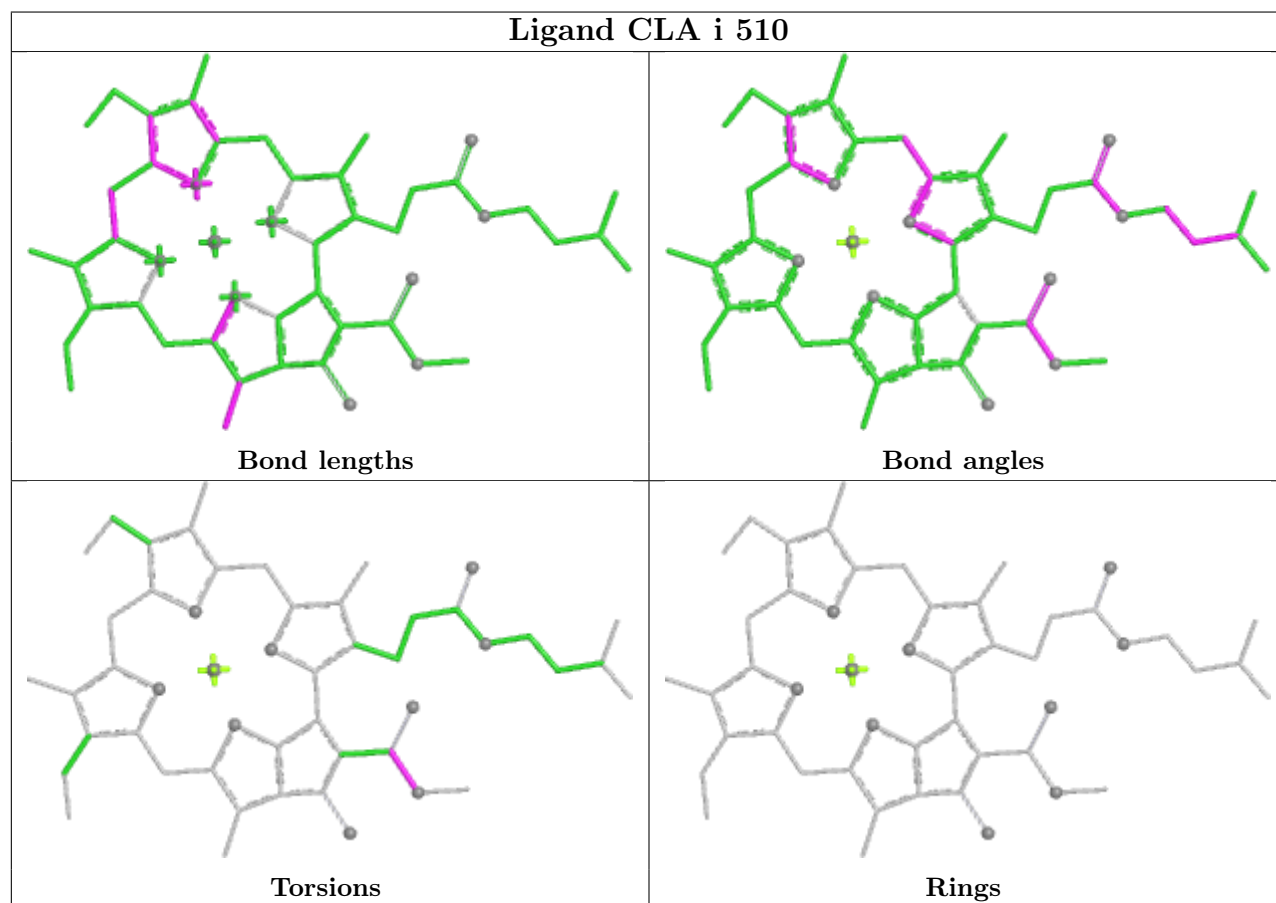
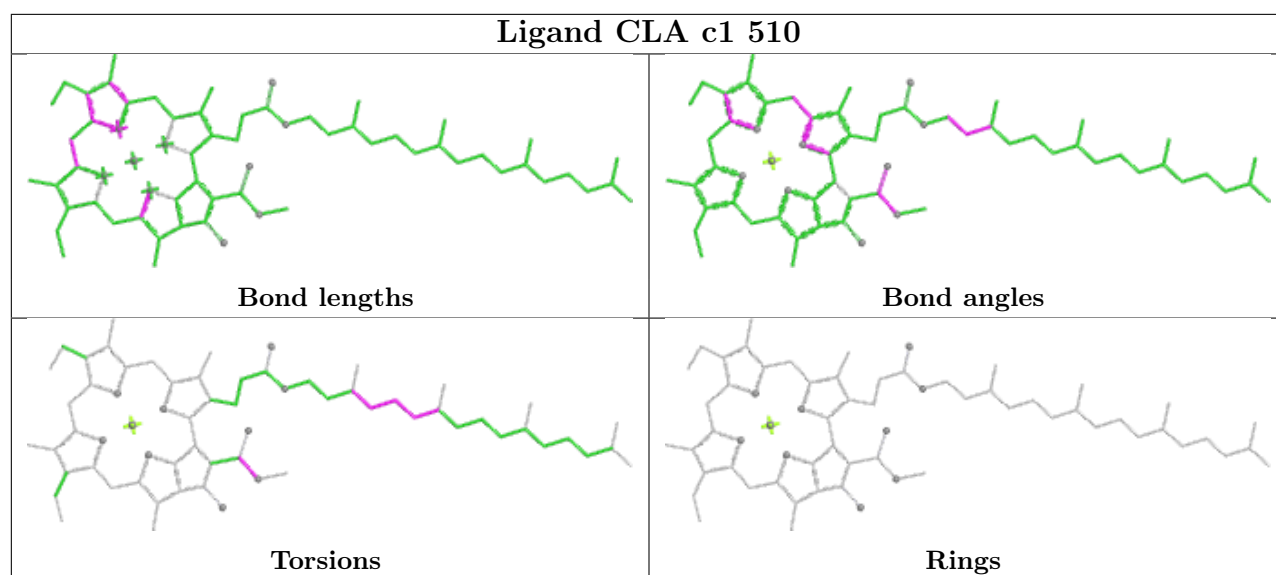


Rings

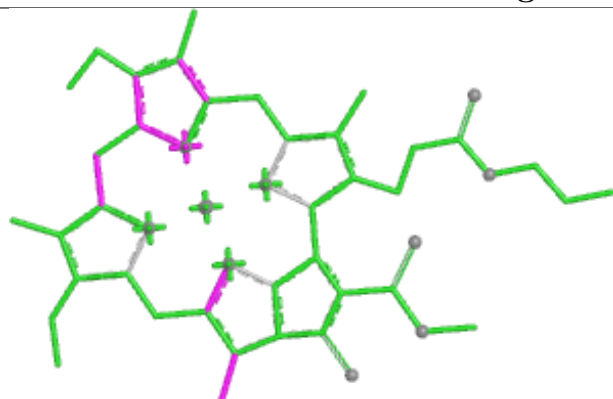




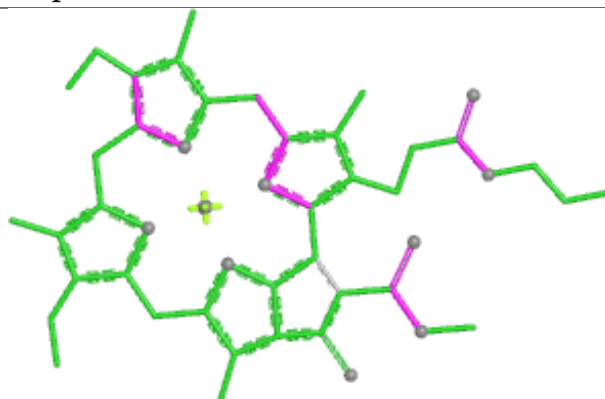




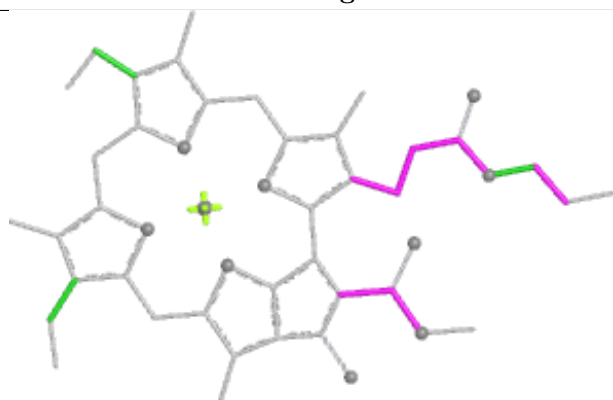
Ligand CLA p 518



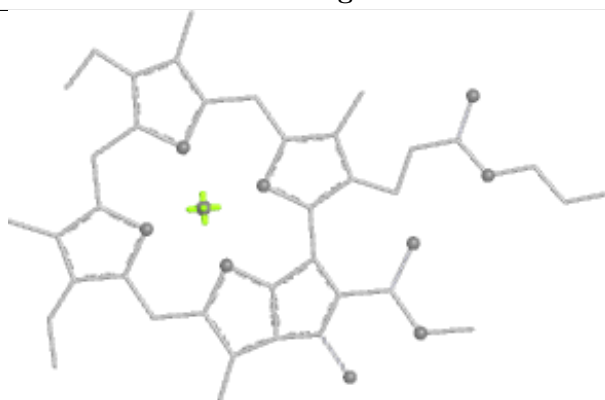
Bond lengths



Bond angles

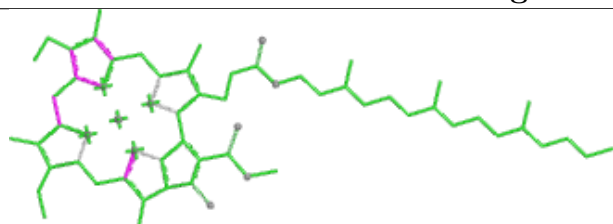


Torsions

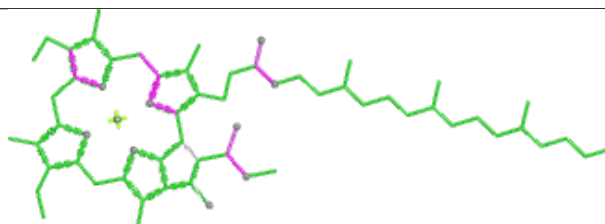


Rings

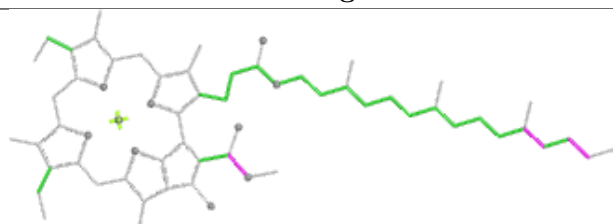
Ligand CLA c3 503



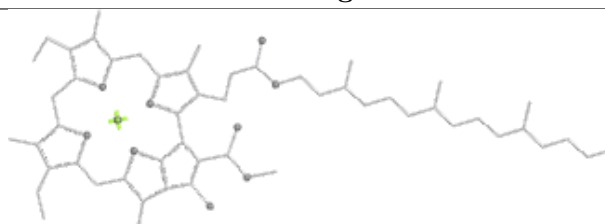
Bond lengths



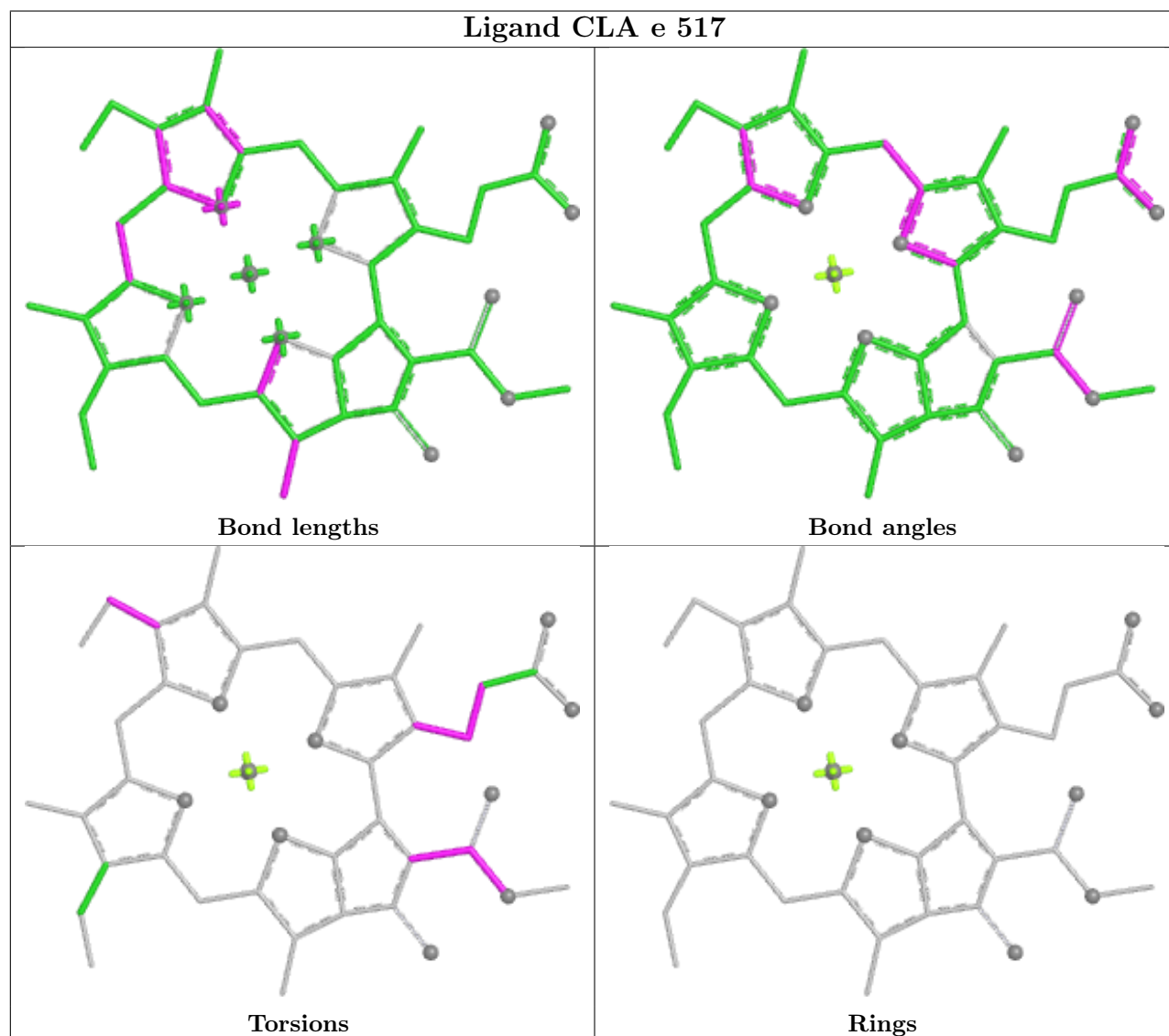
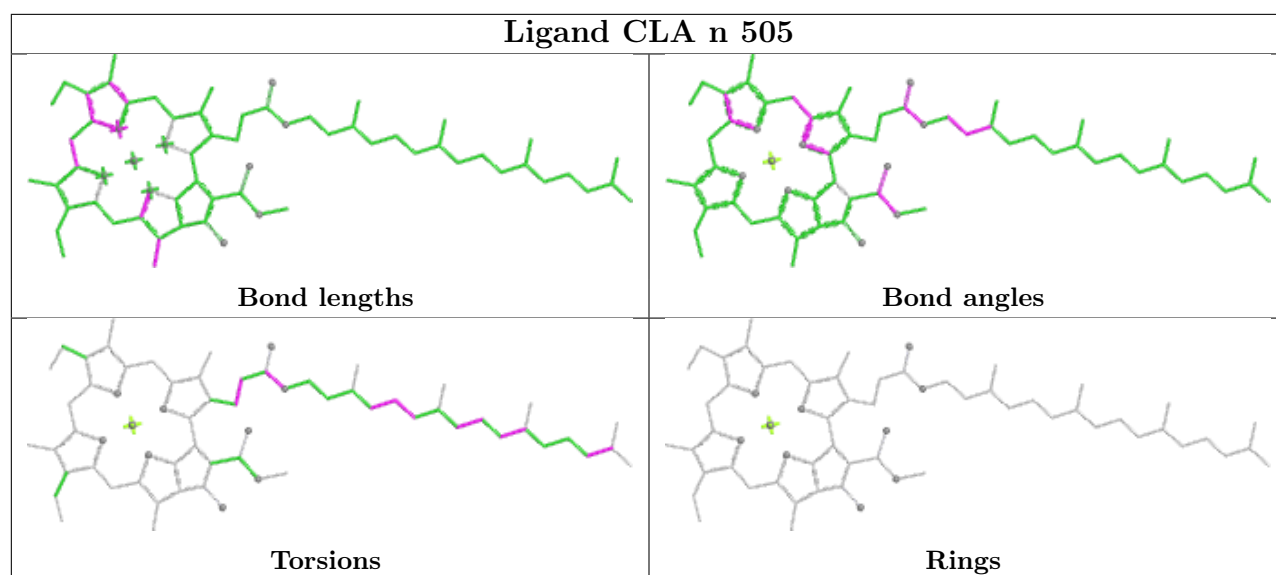
Bond angles



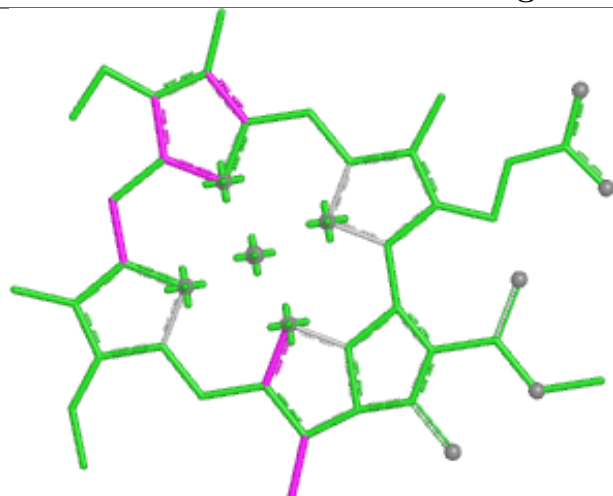
Torsions



Rings



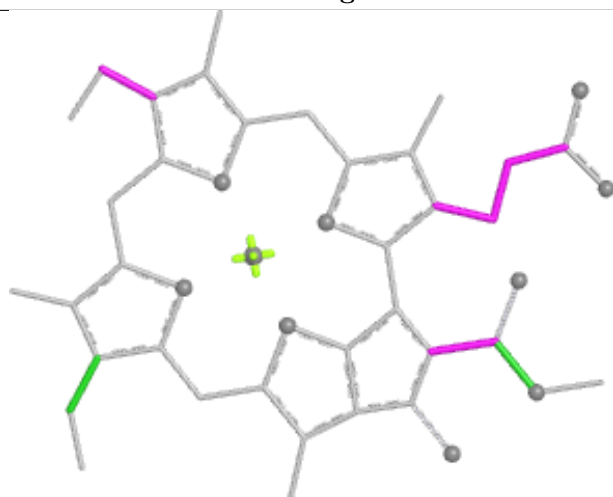
Ligand CLA h 501



Bond lengths



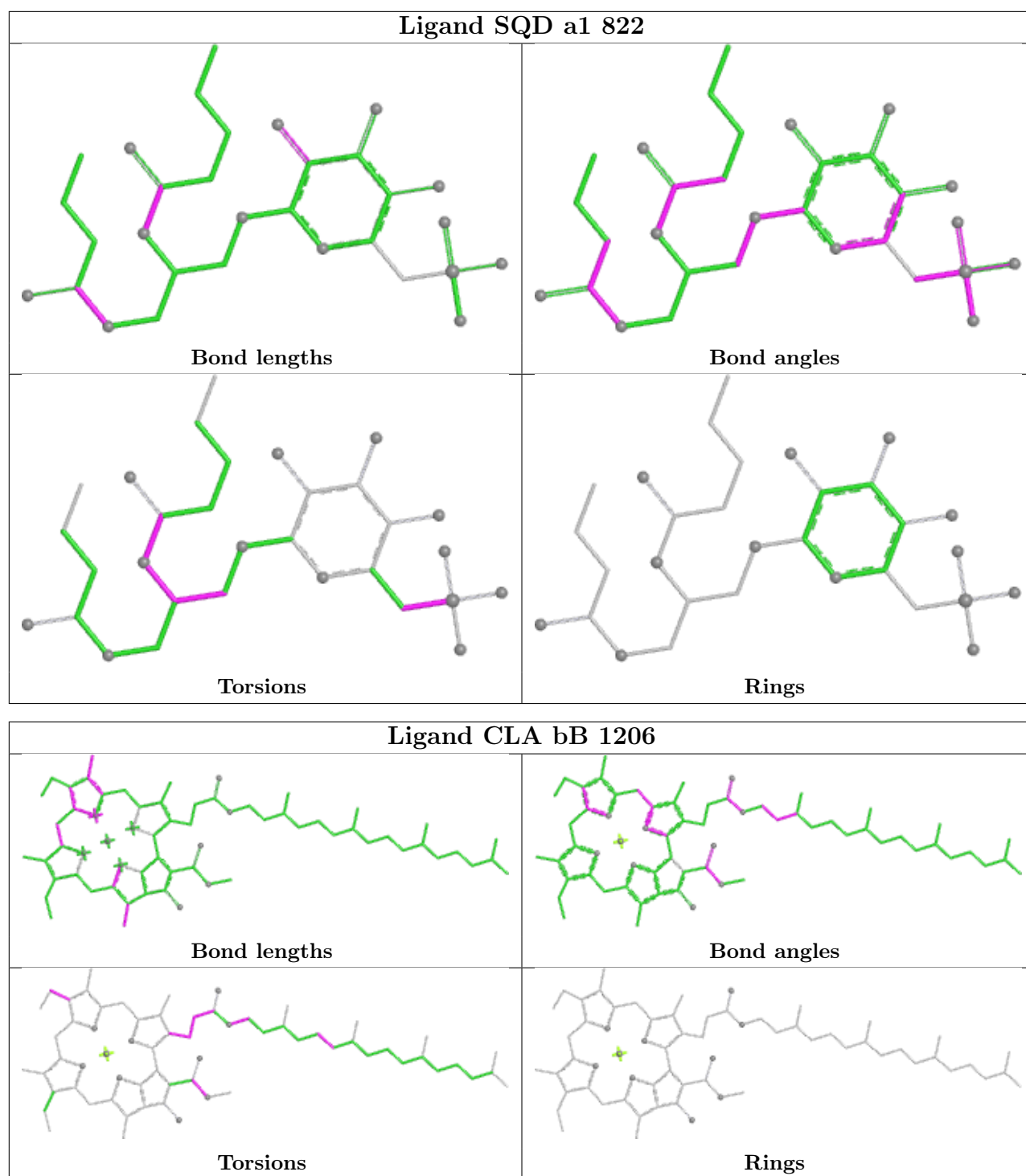
Bond angles

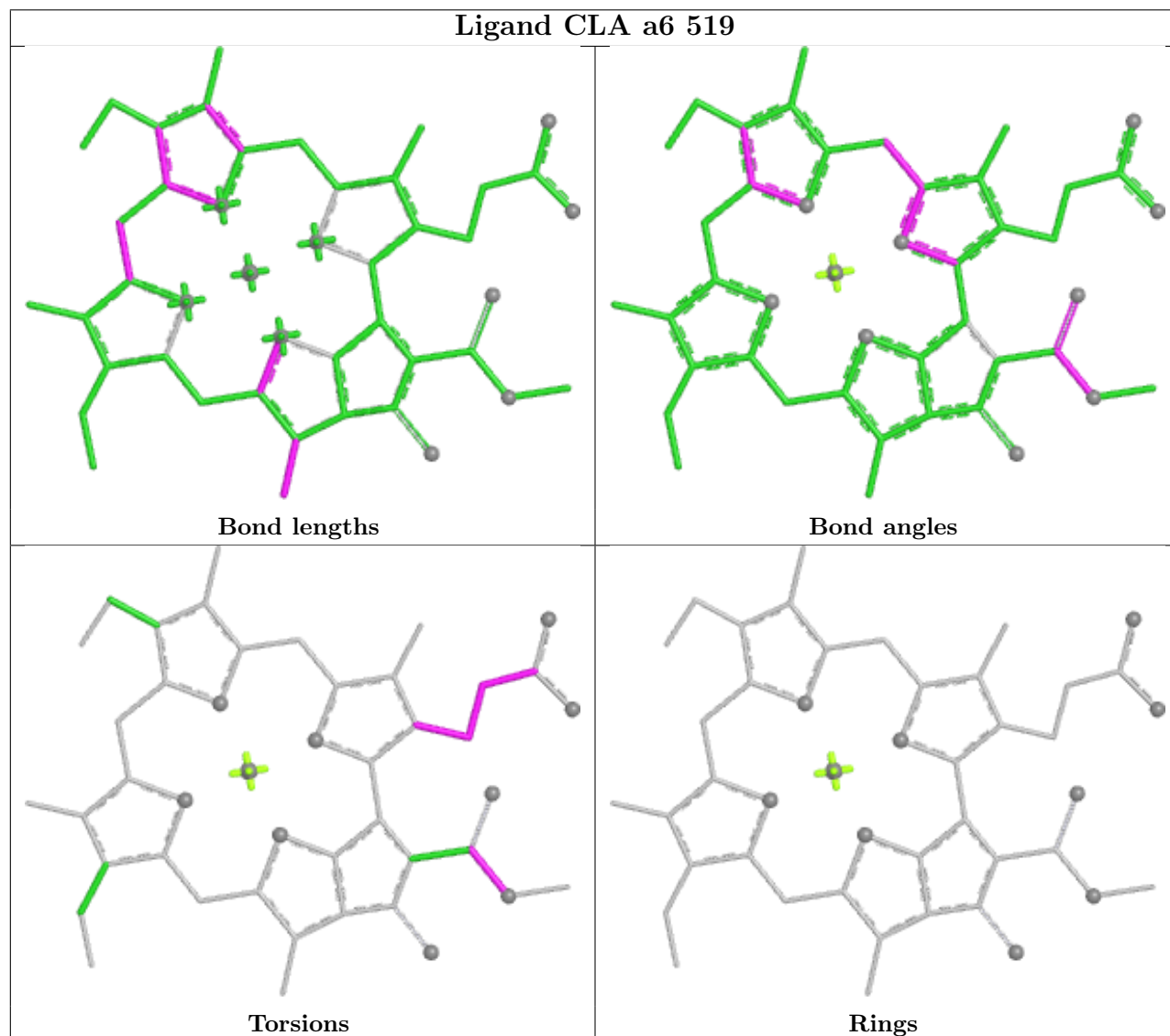
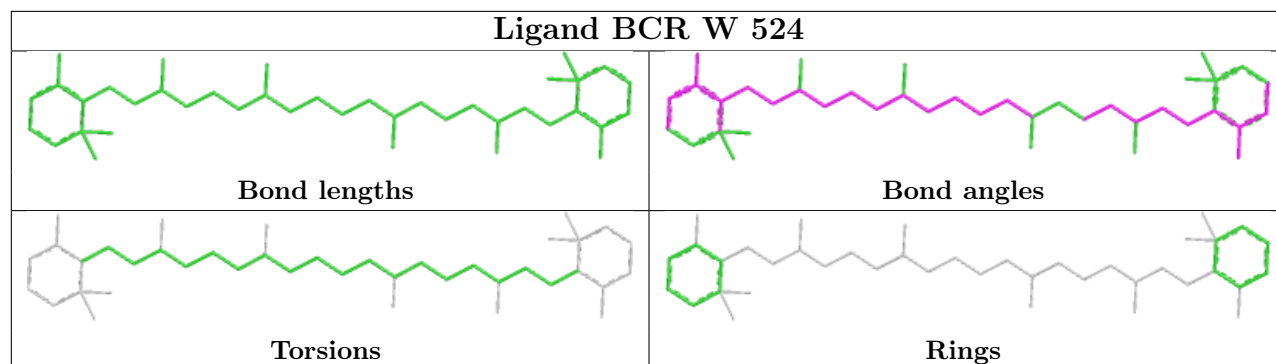


Torsions

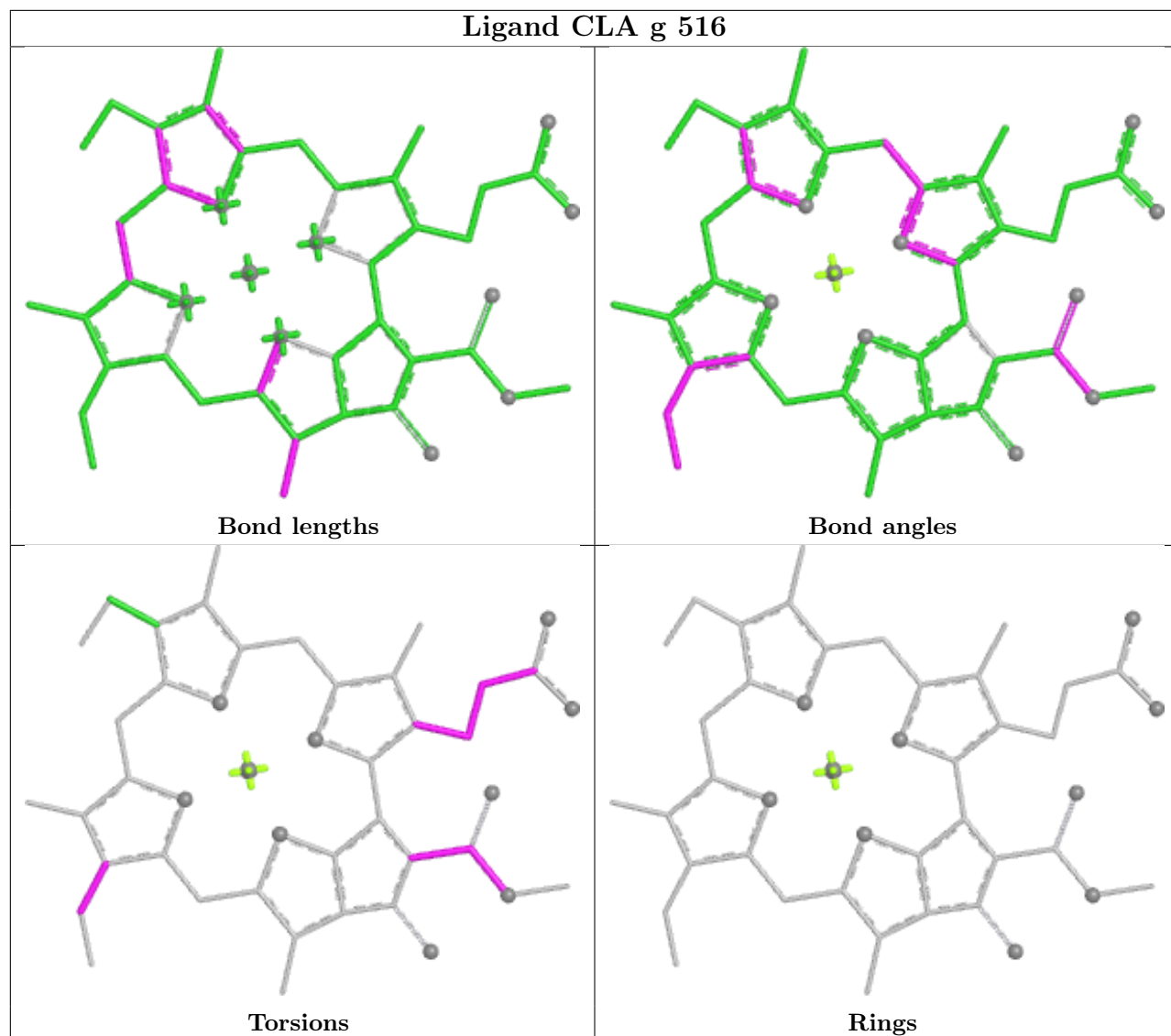


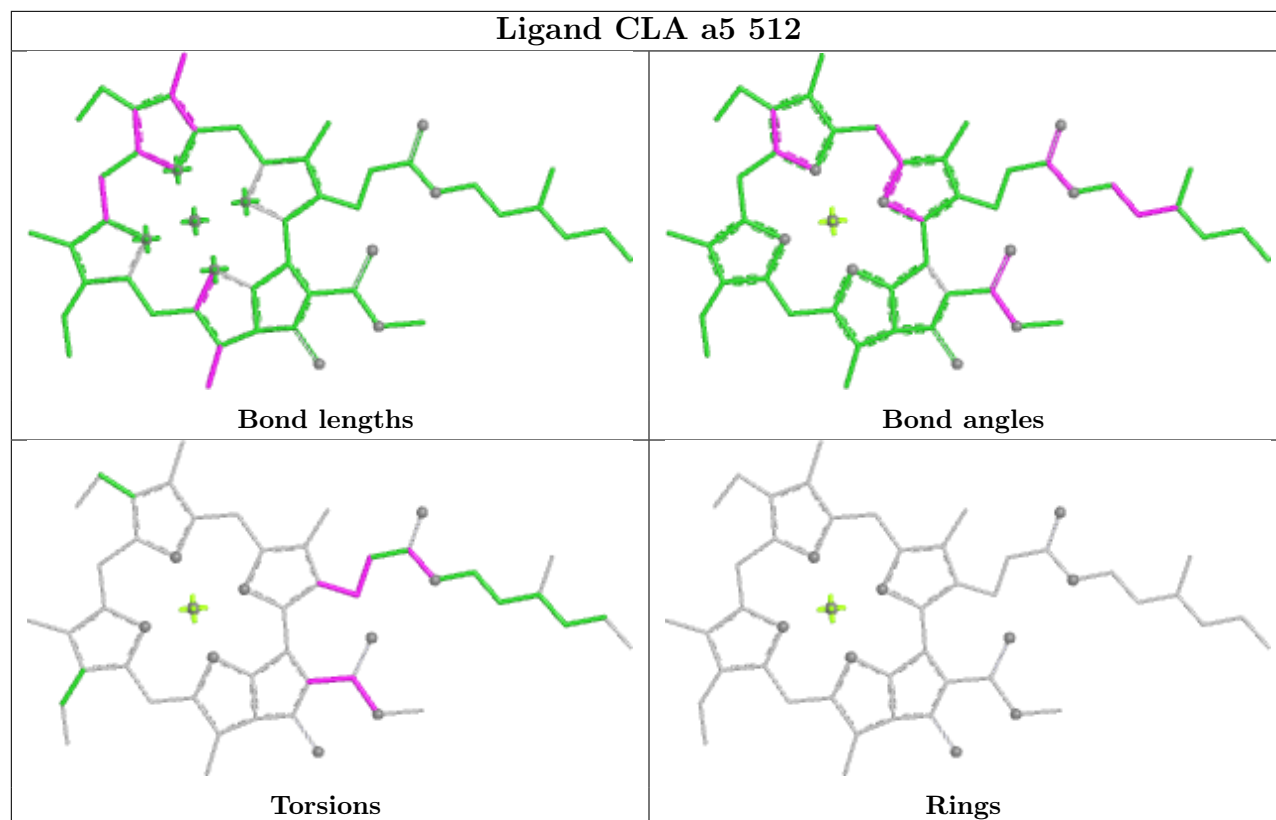
Rings

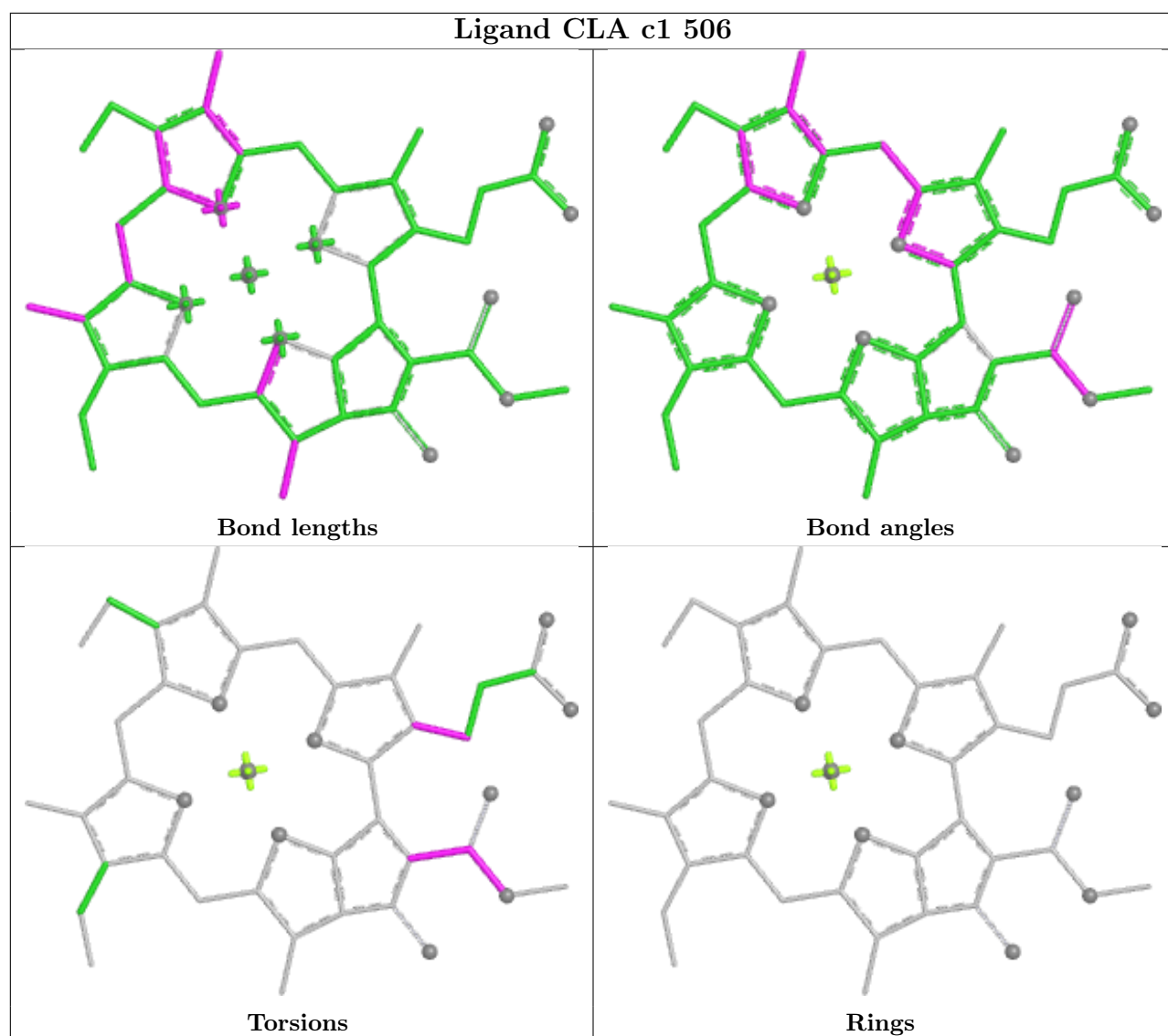




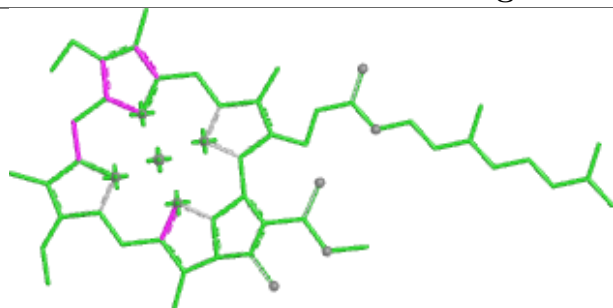
Ligand CLA g 516



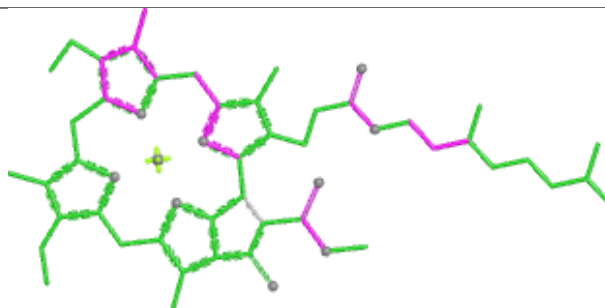




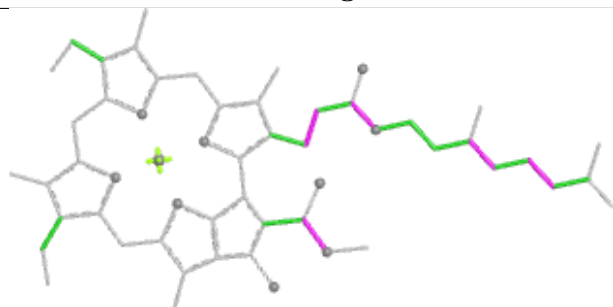
Ligand CLA aB 1219



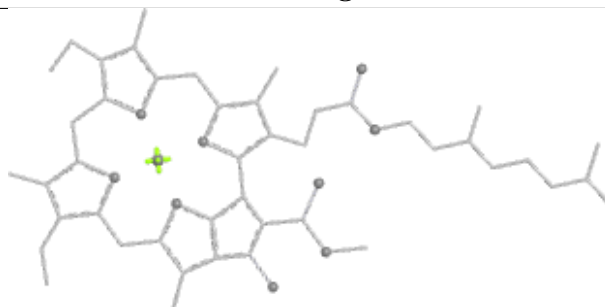
Bond lengths



Bond angles

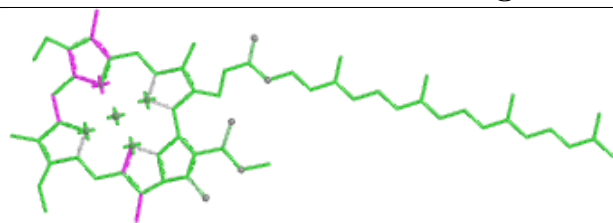


Torsions

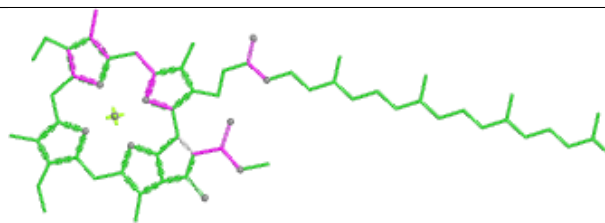


Rings

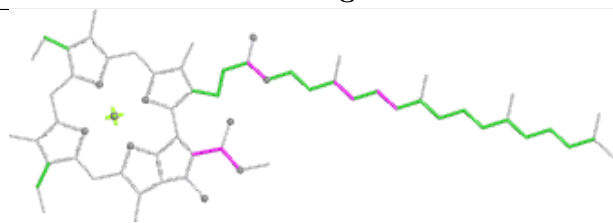
Ligand CLA aA 1128



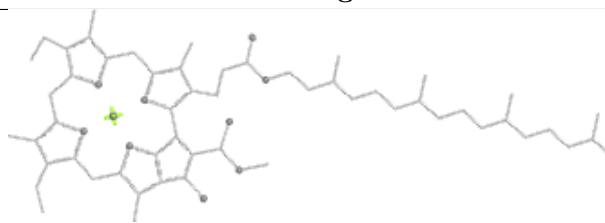
Bond lengths



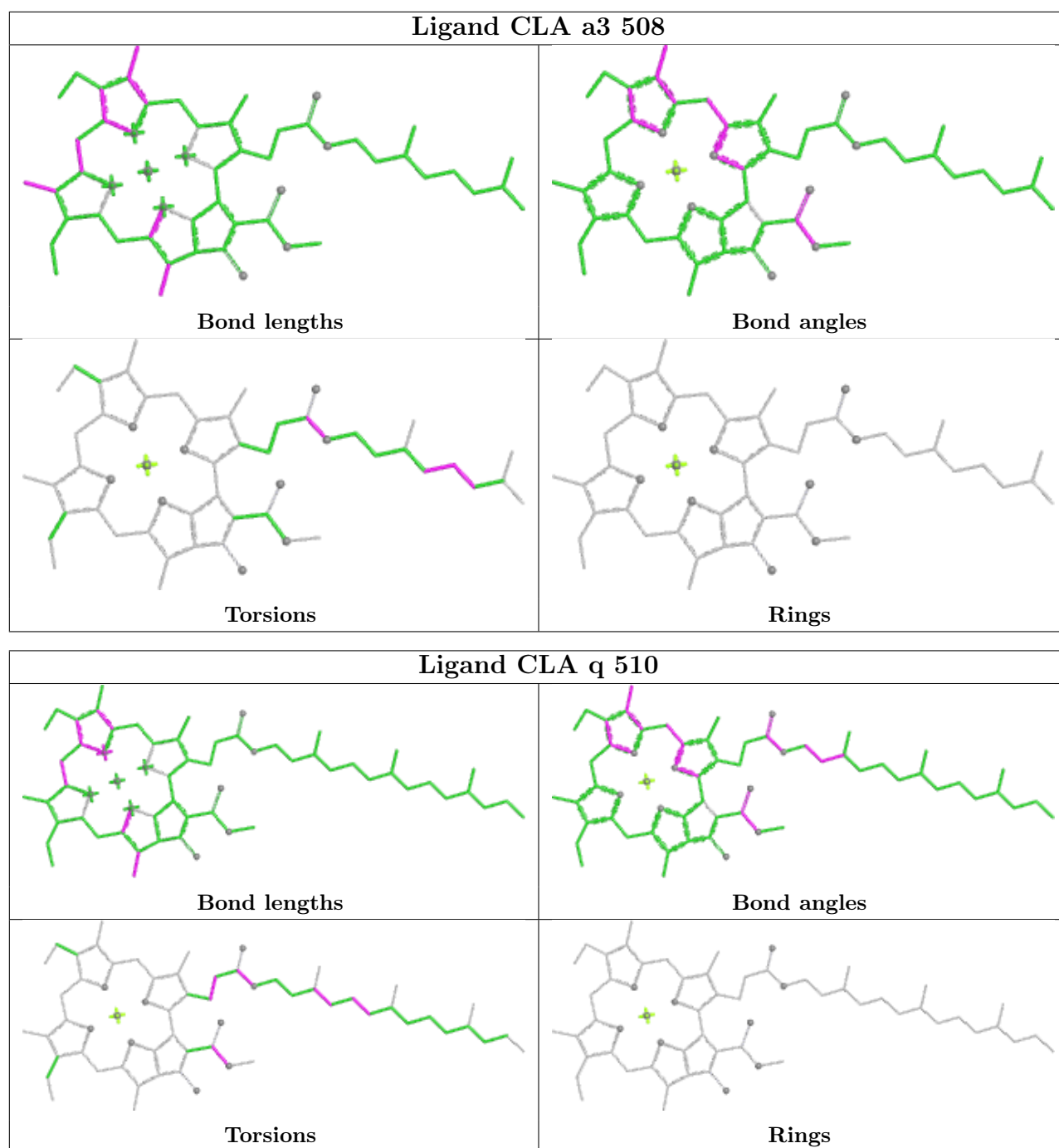
Bond angles

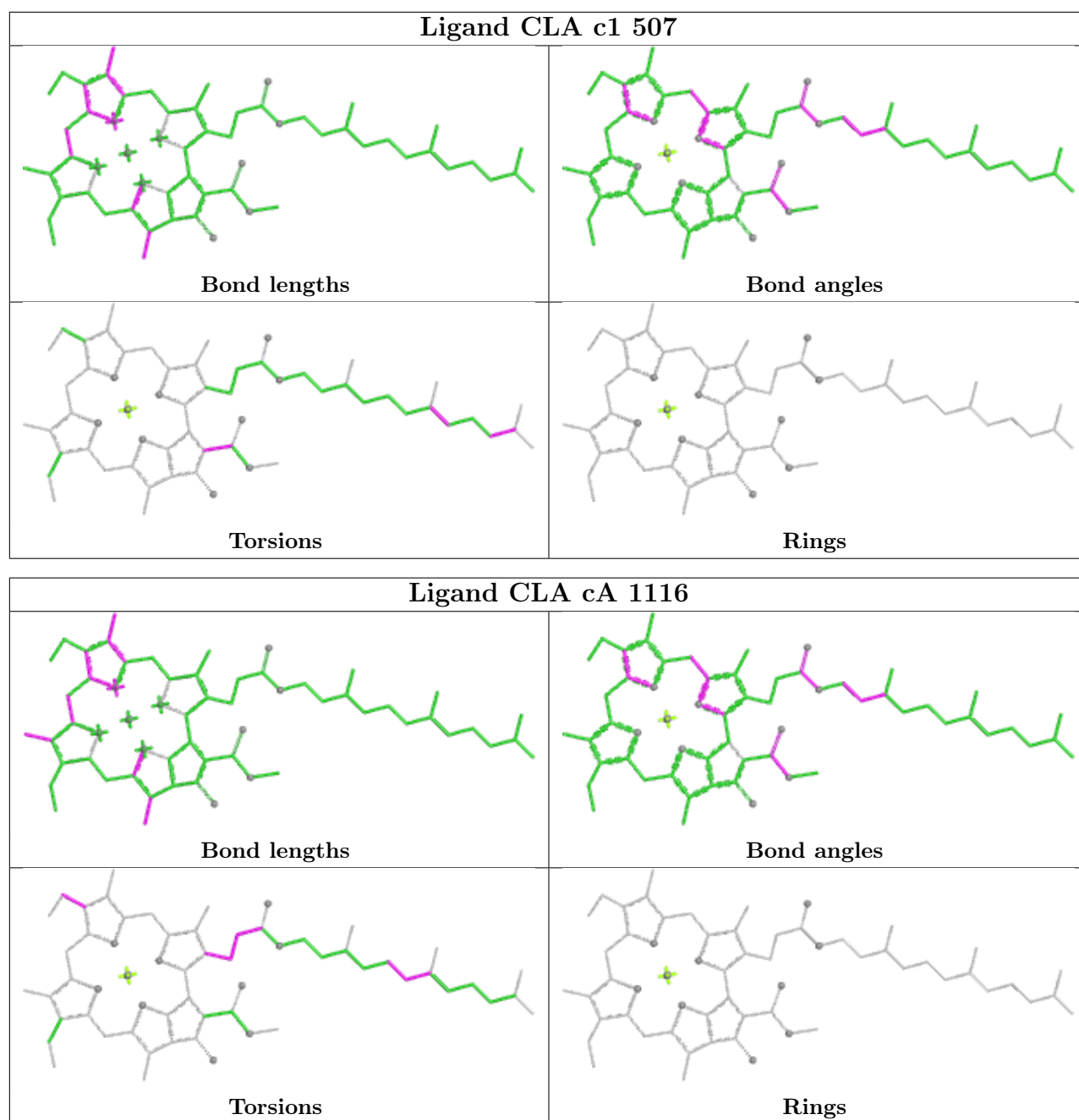


Torsions

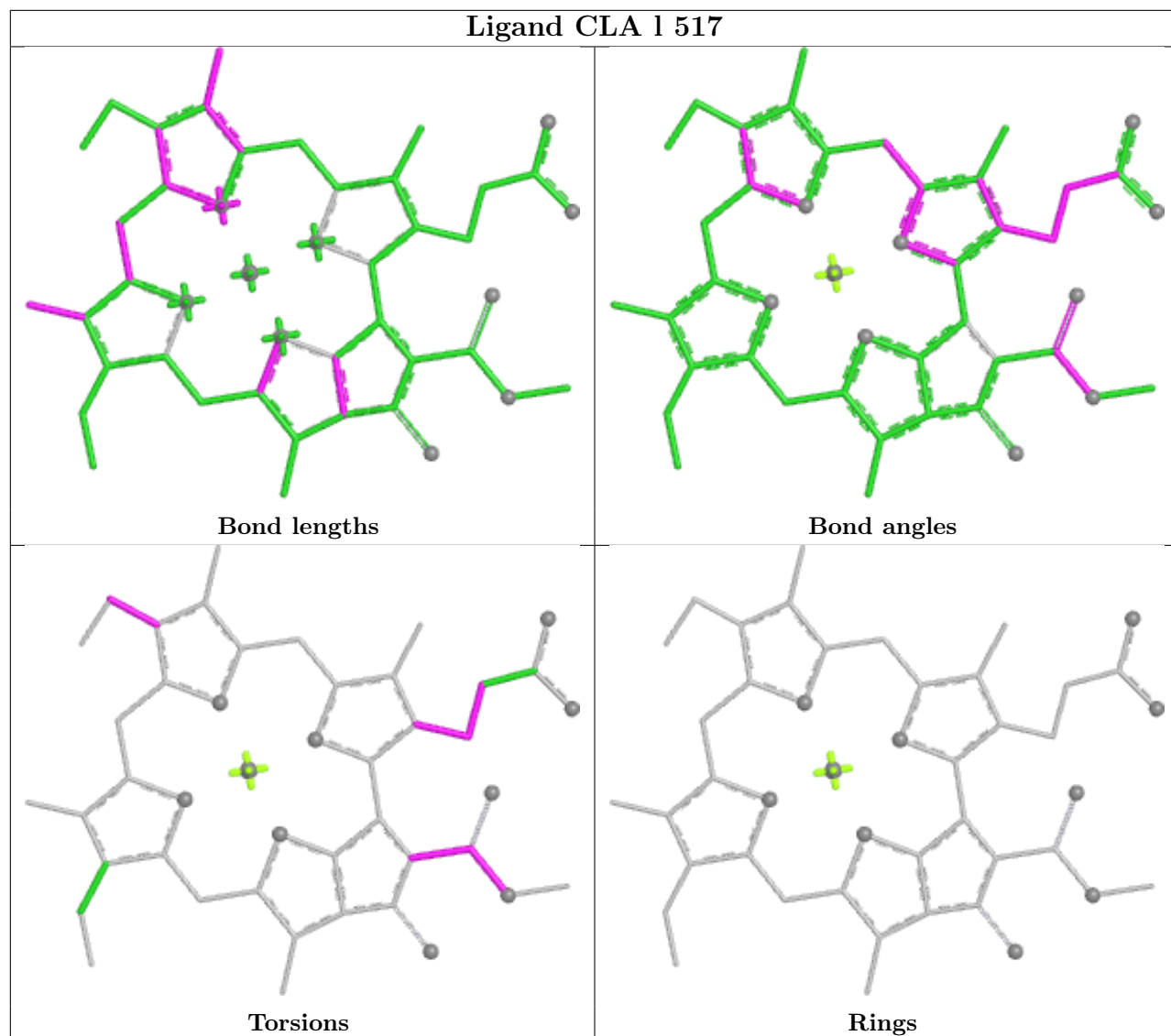


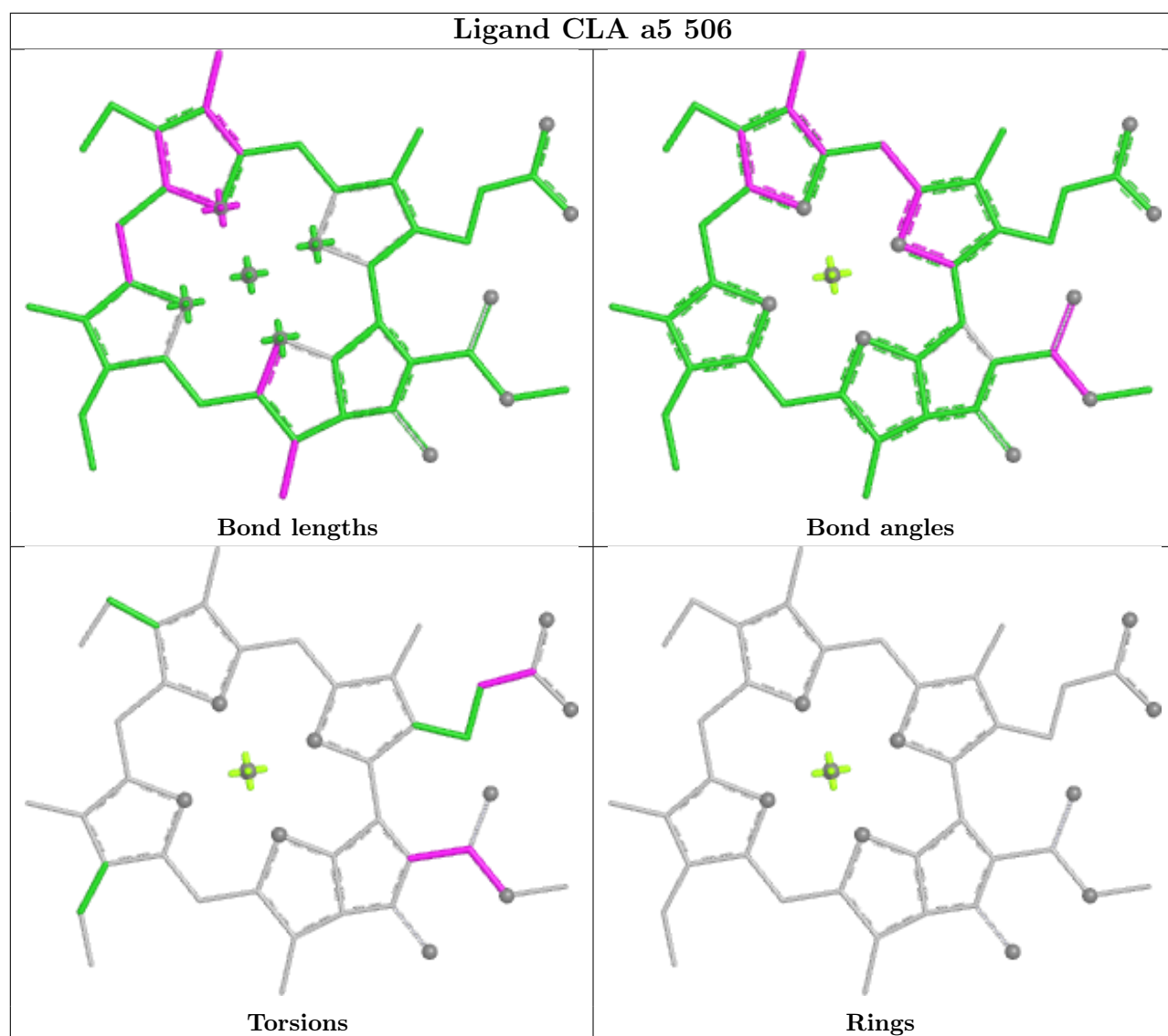
Rings

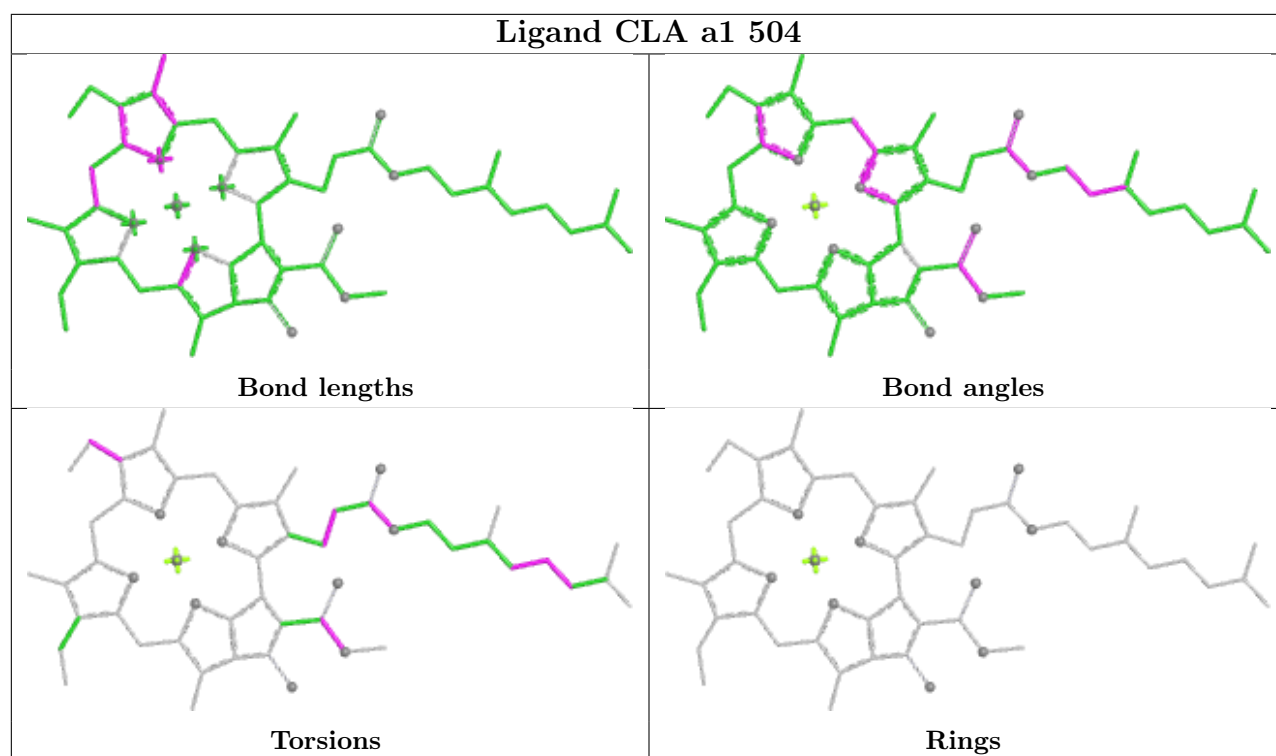




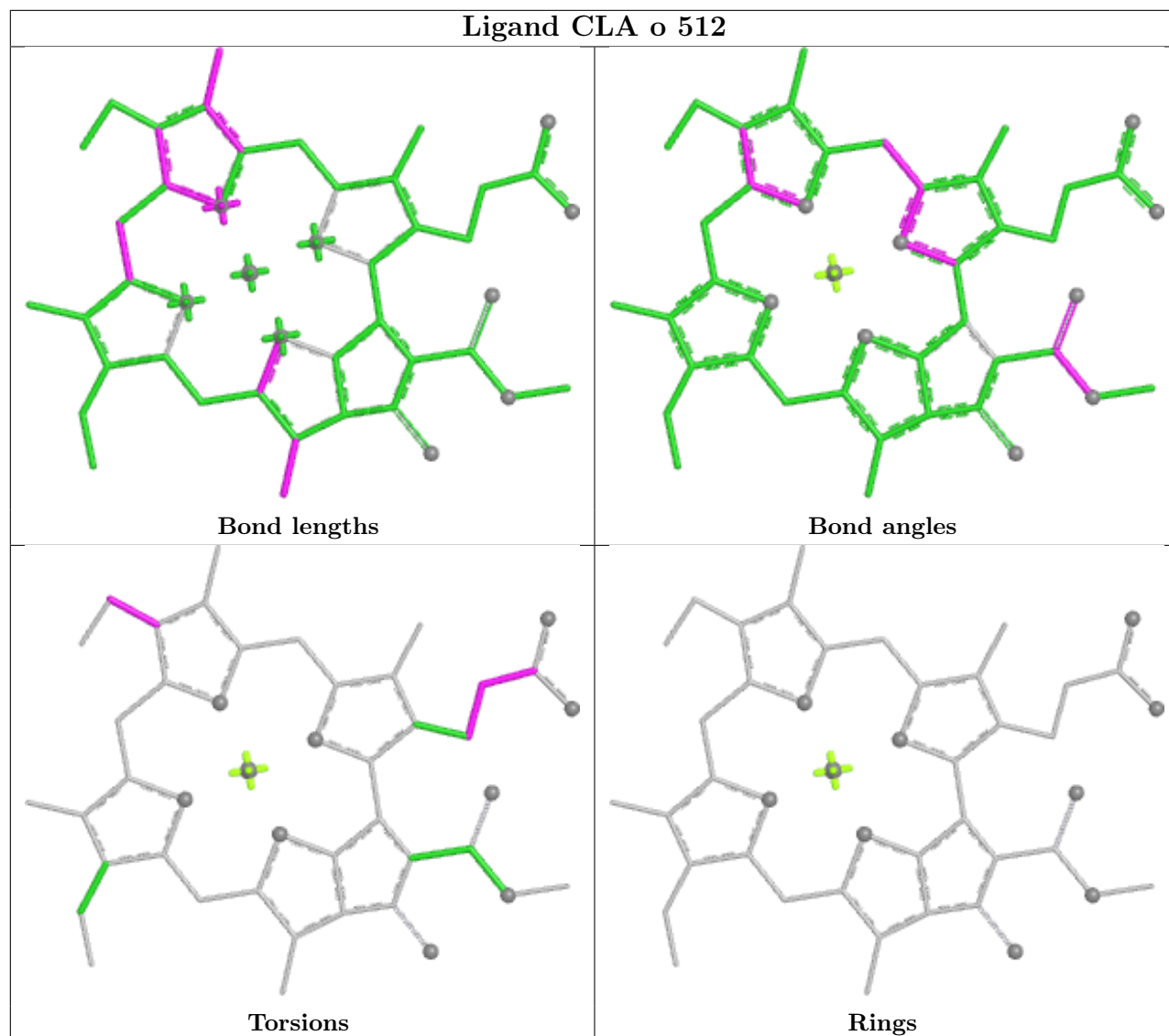
Ligand CLA 1 517



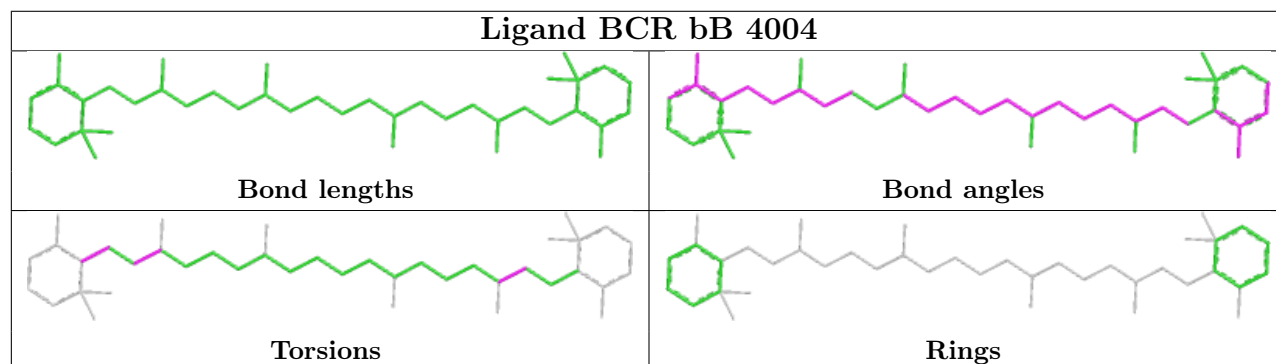


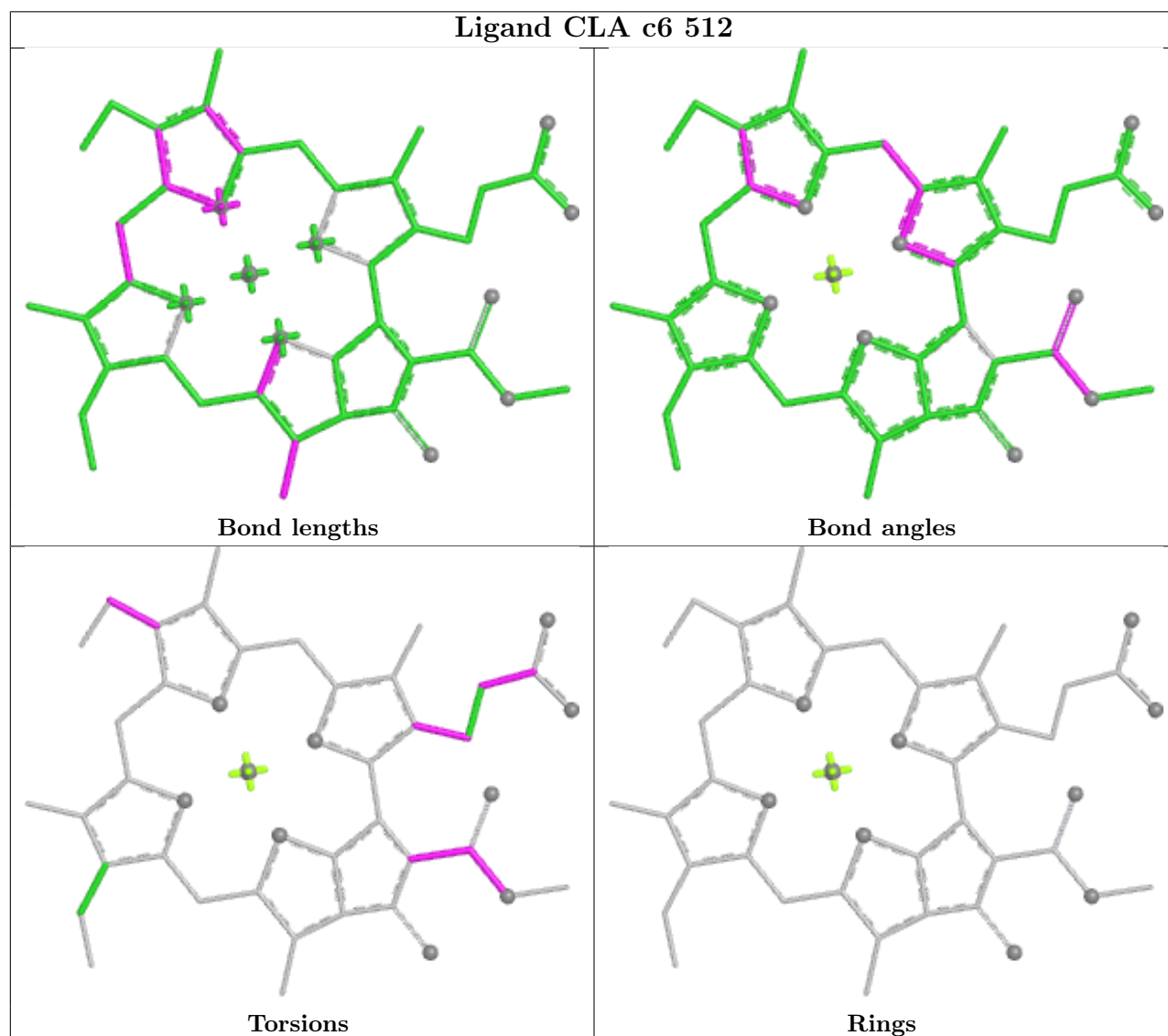
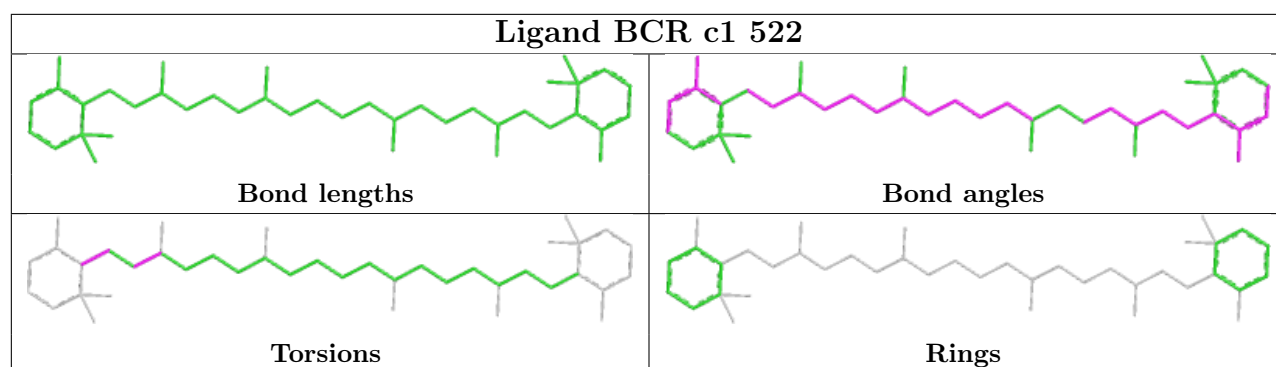


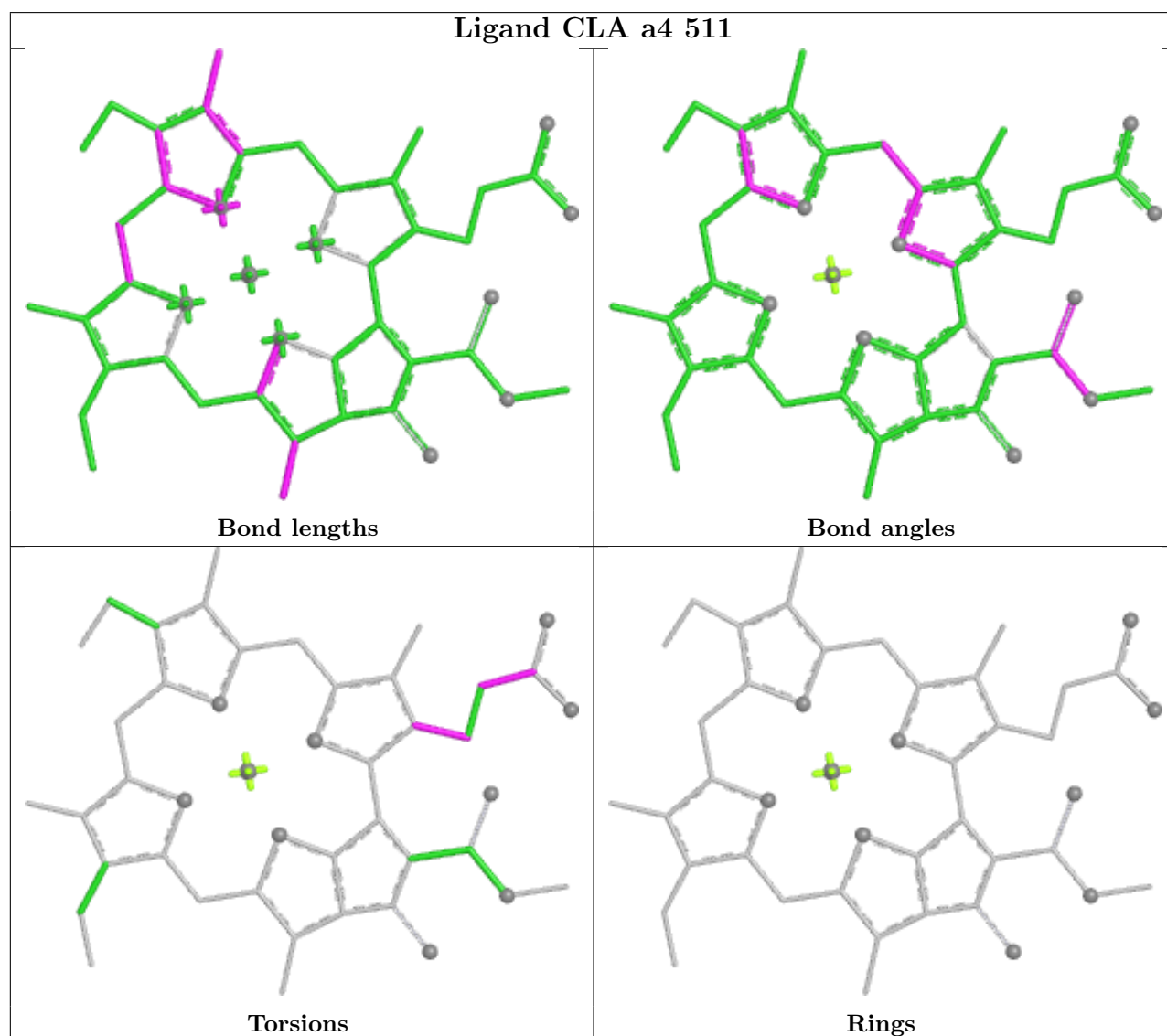
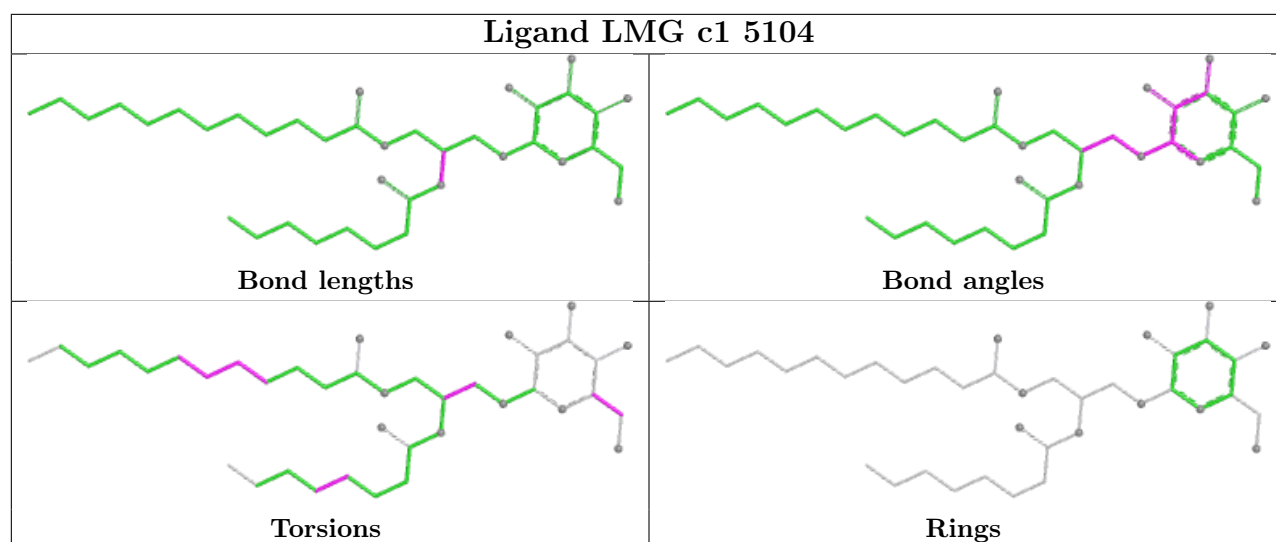
Ligand CLA o 512

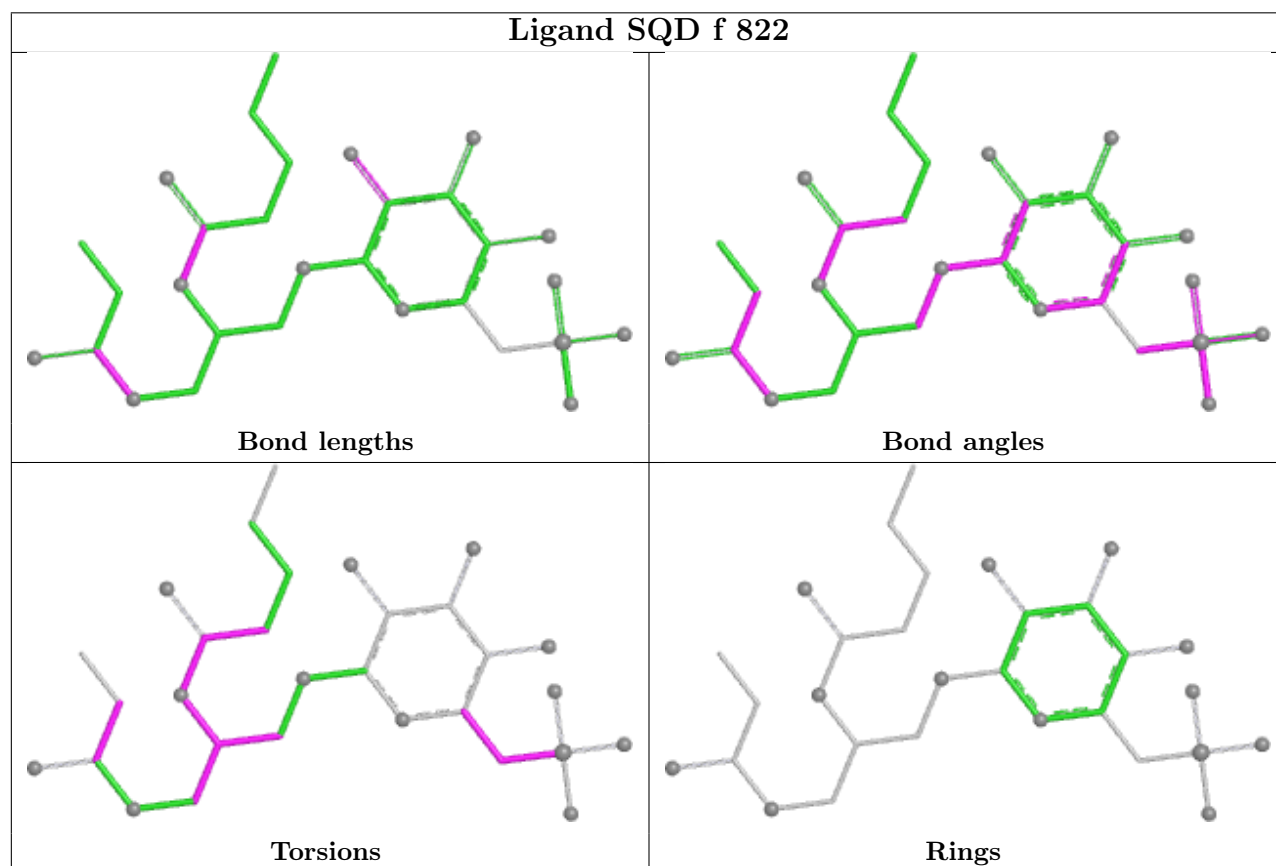
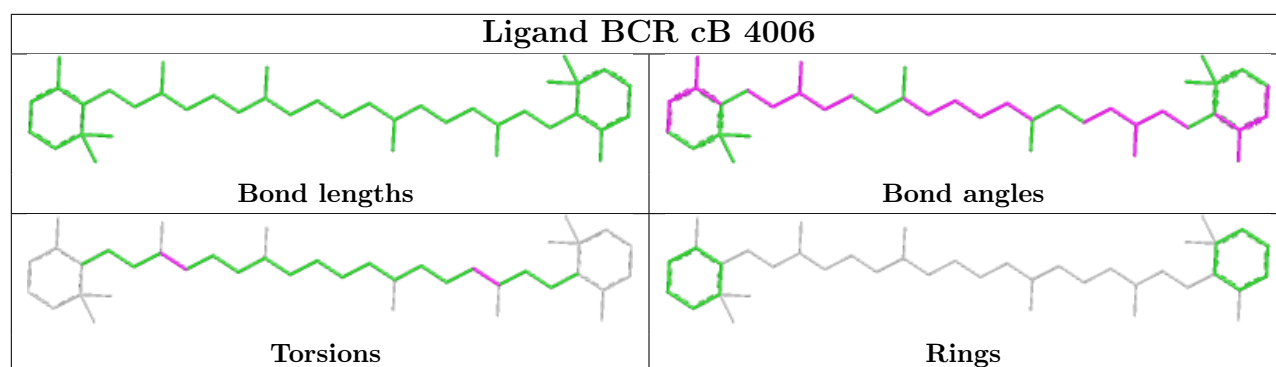


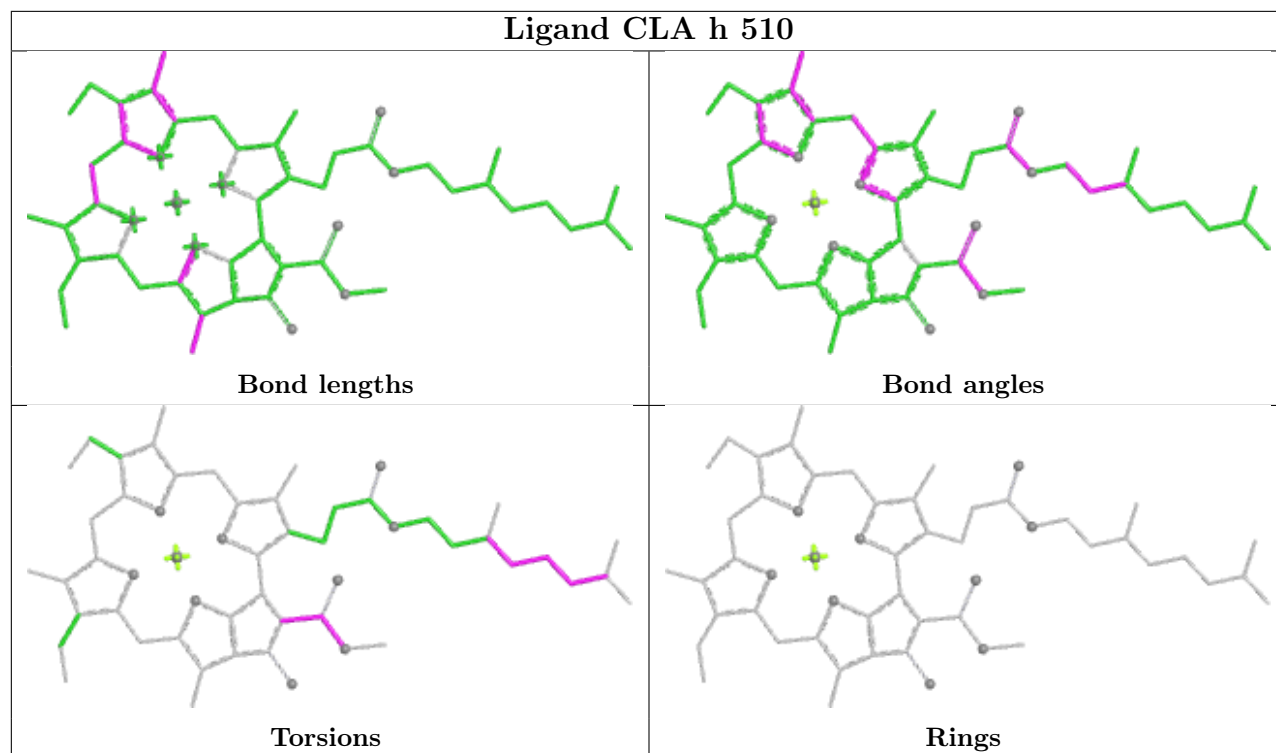
Ligand BCR bB 4004



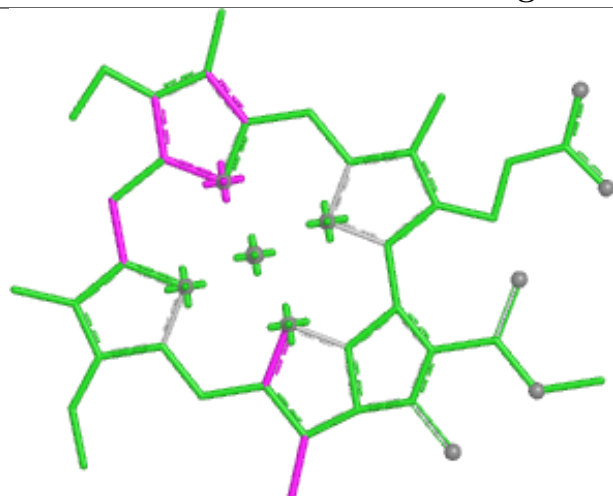








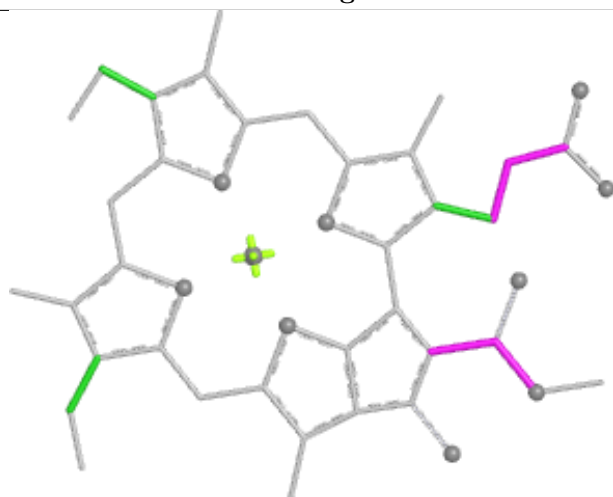
Ligand CLA k 518



Bond lengths



Bond angles

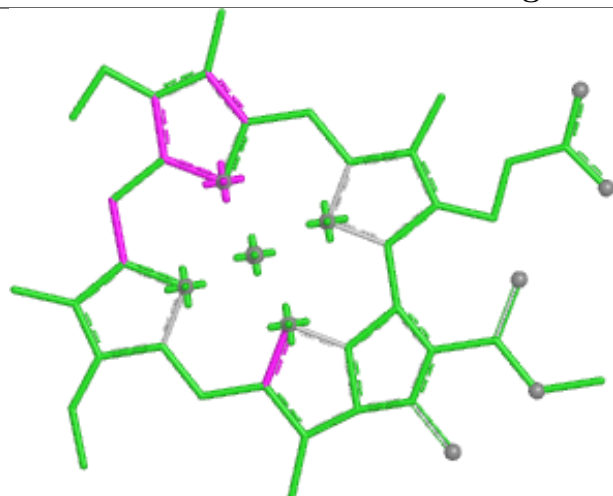


Torsions

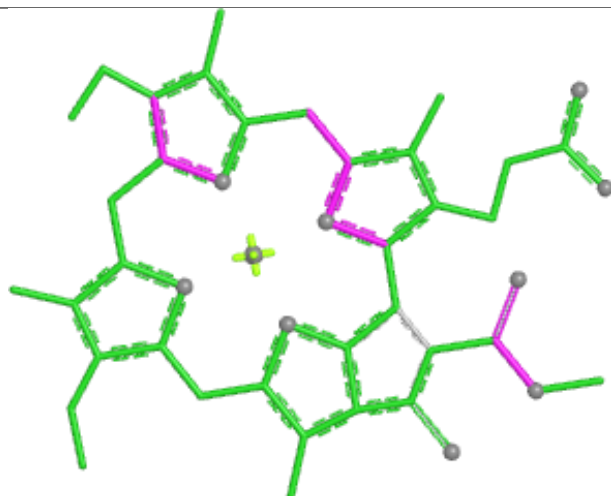


Rings

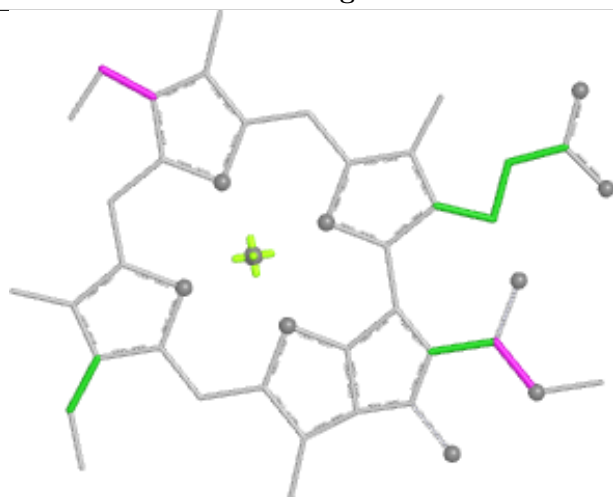
Ligand CLA i 503



Bond lengths



Bond angles

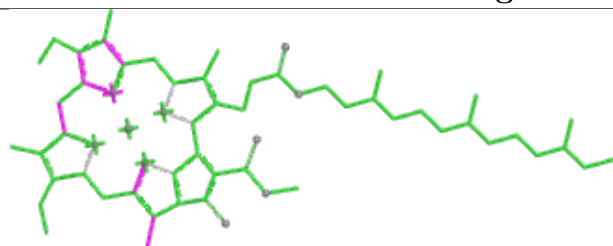


Torsions

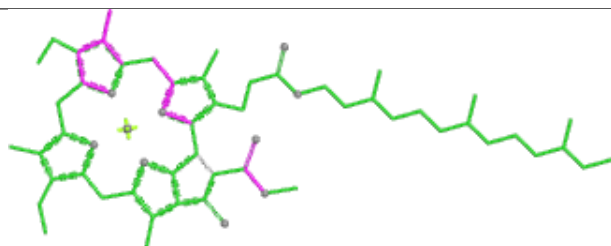


Rings

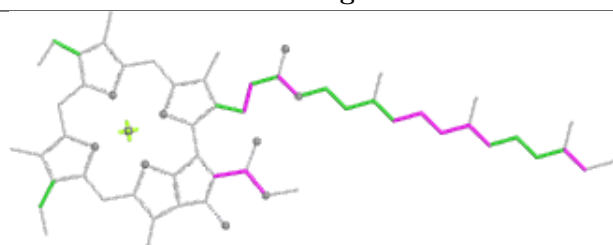
Ligand CLA bB 1012



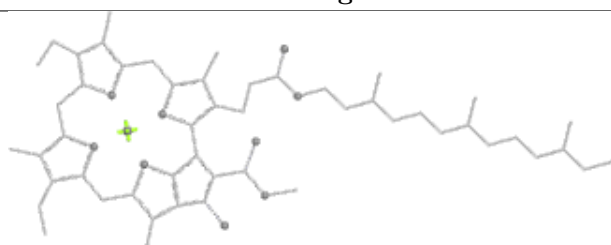
Bond lengths



Bond angles

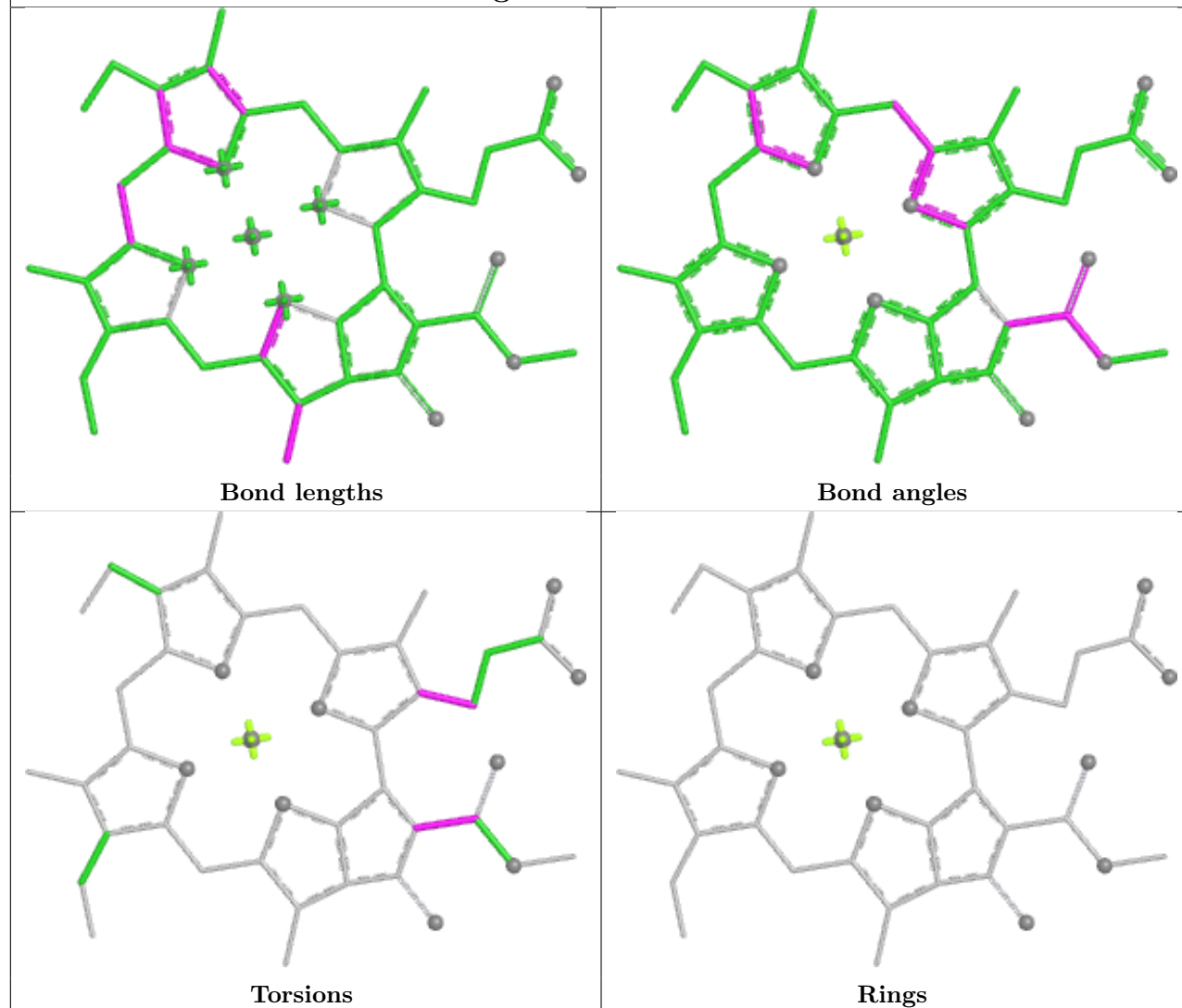


Torsions

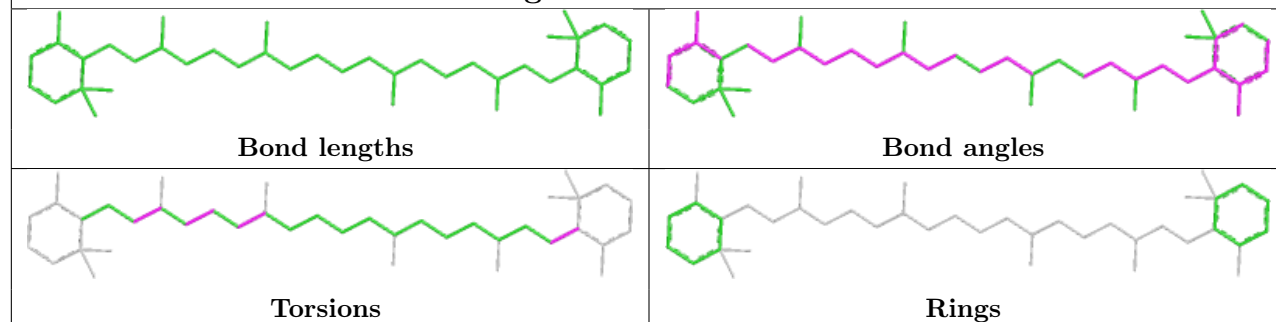


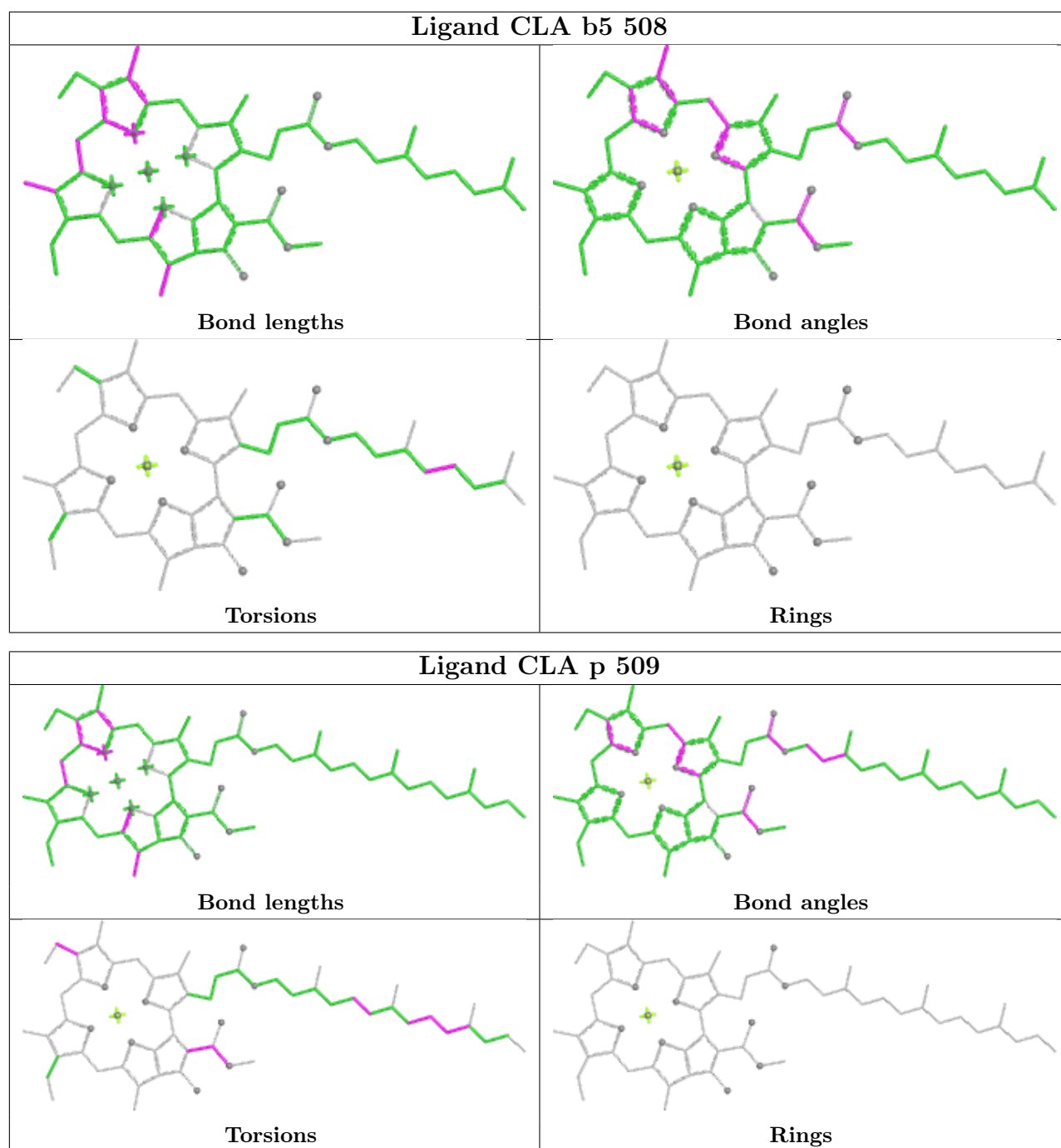
Rings

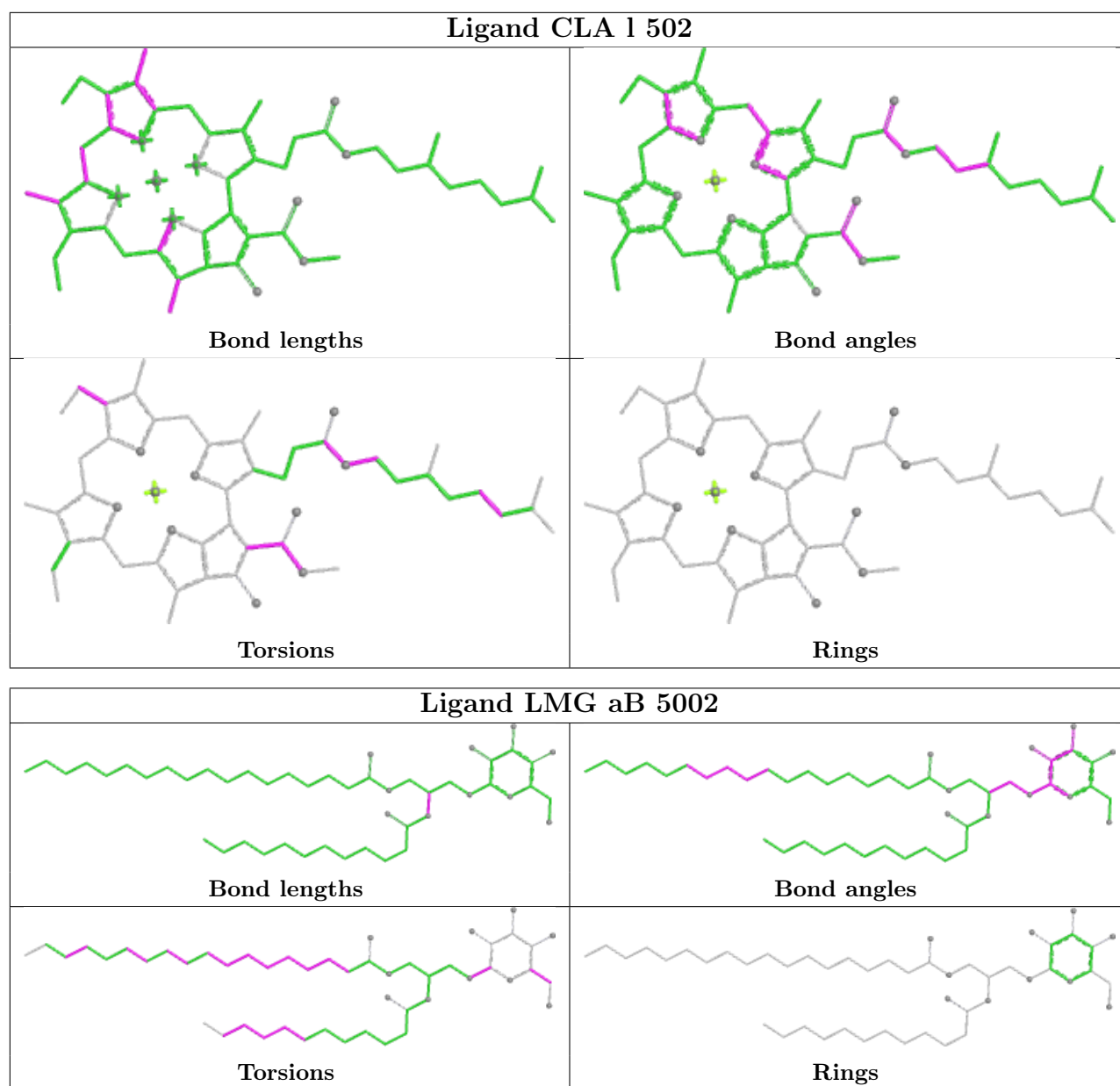
Ligand CLA T 516



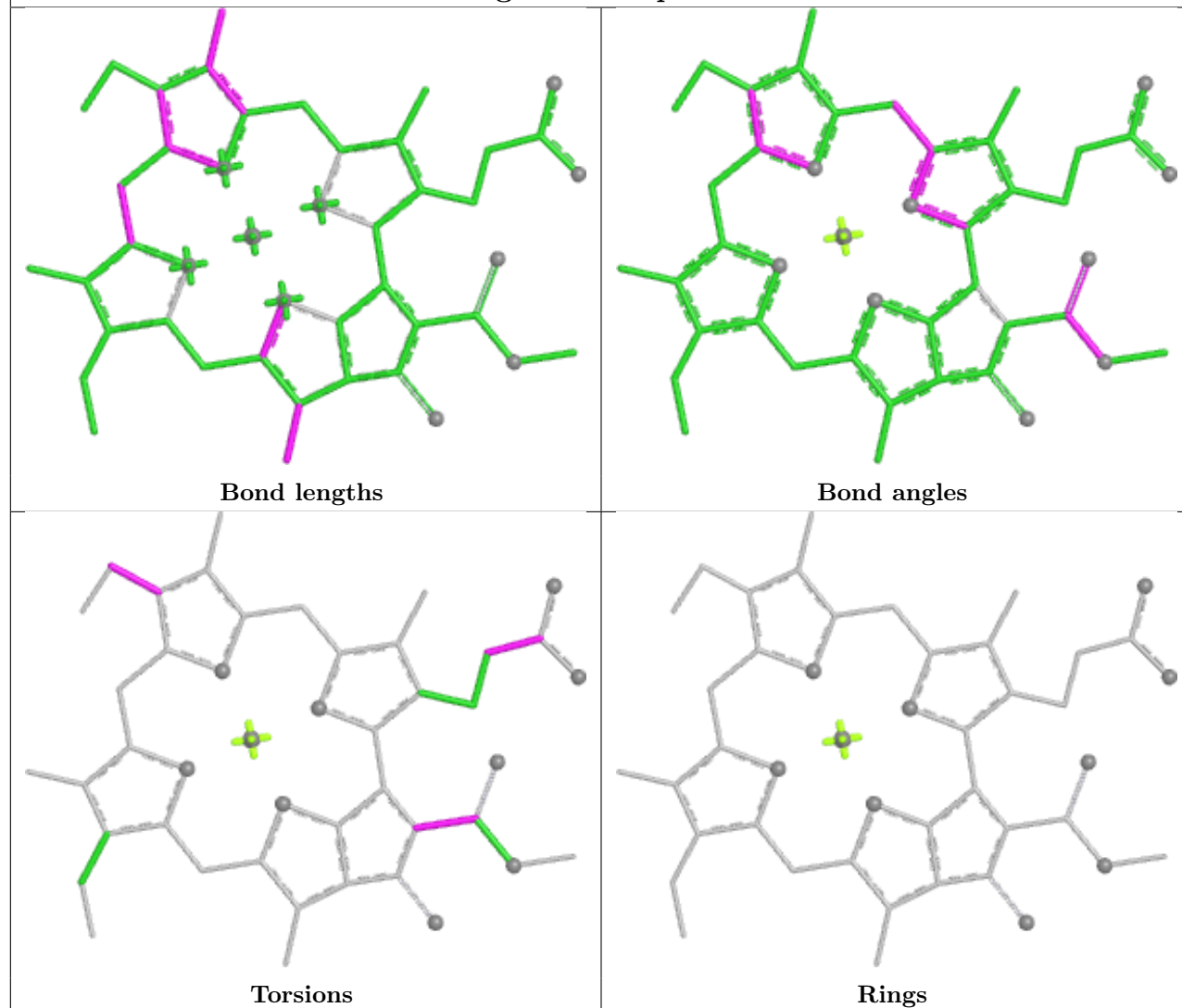
Ligand BCR b4 521



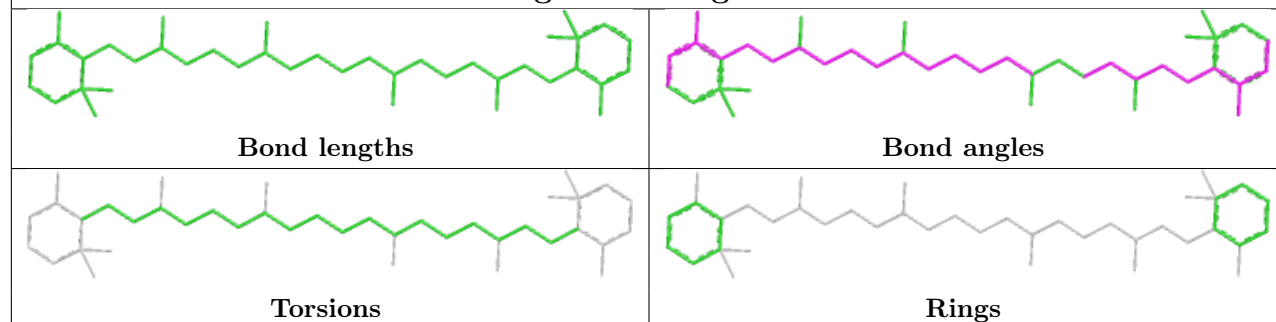


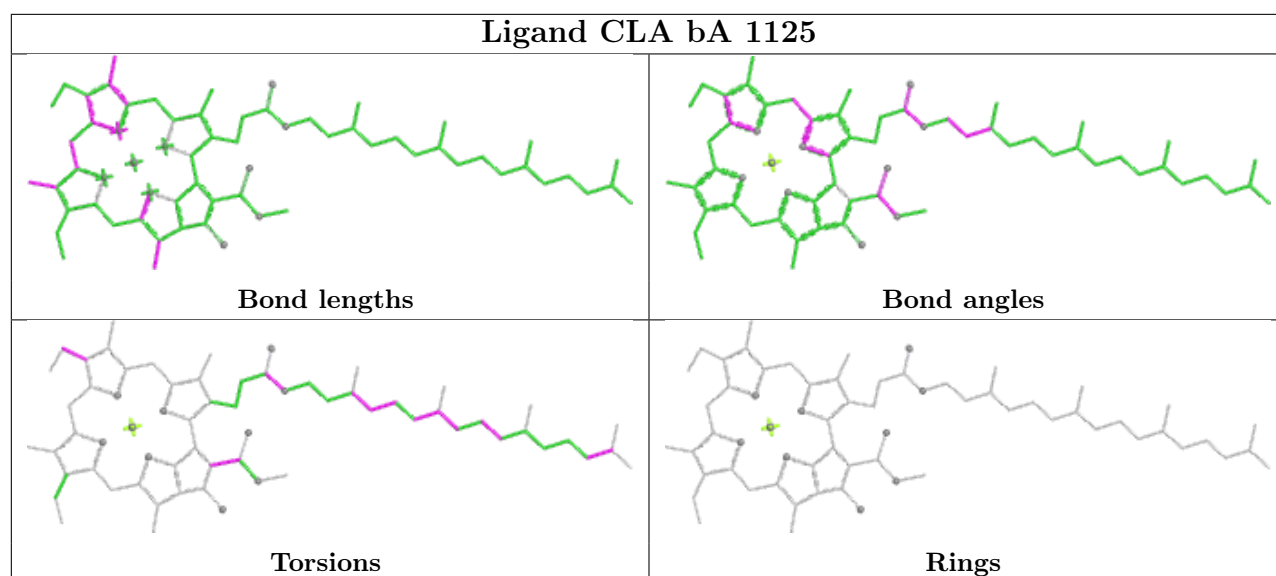
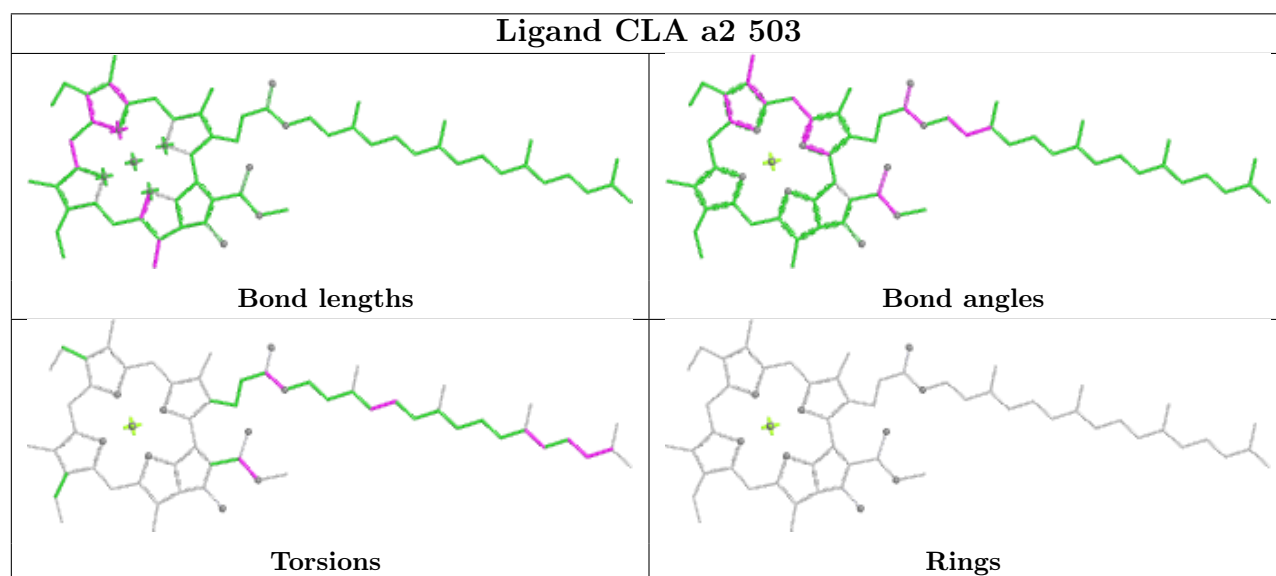
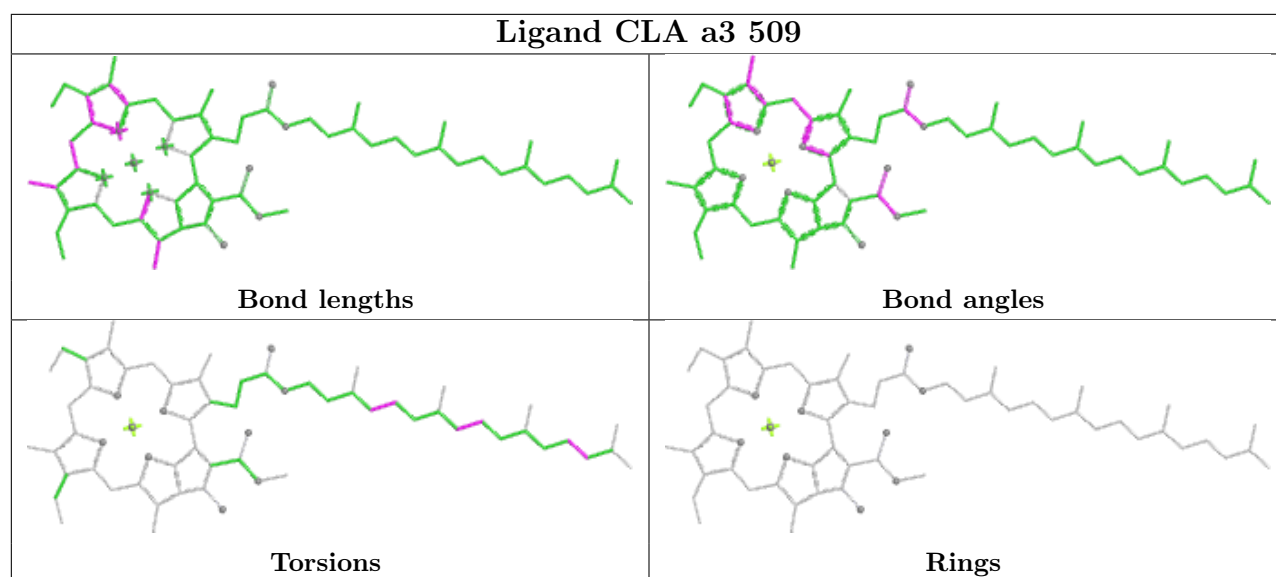


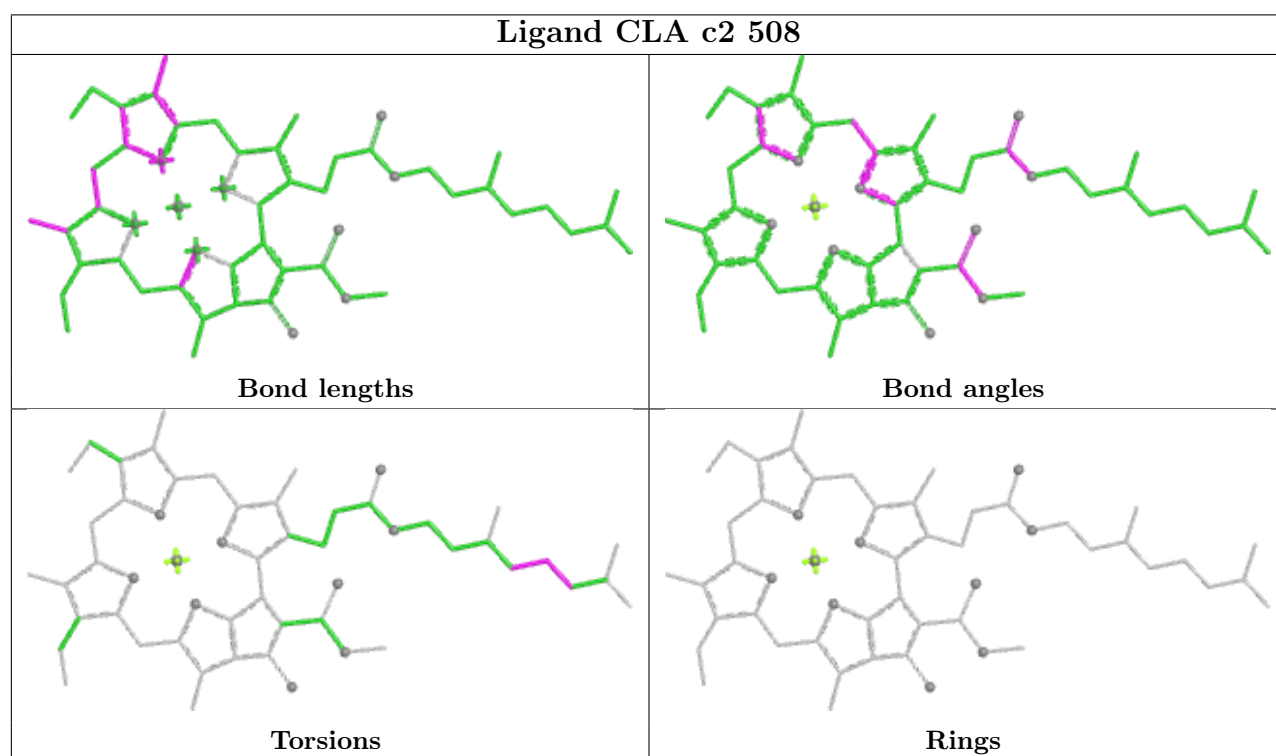
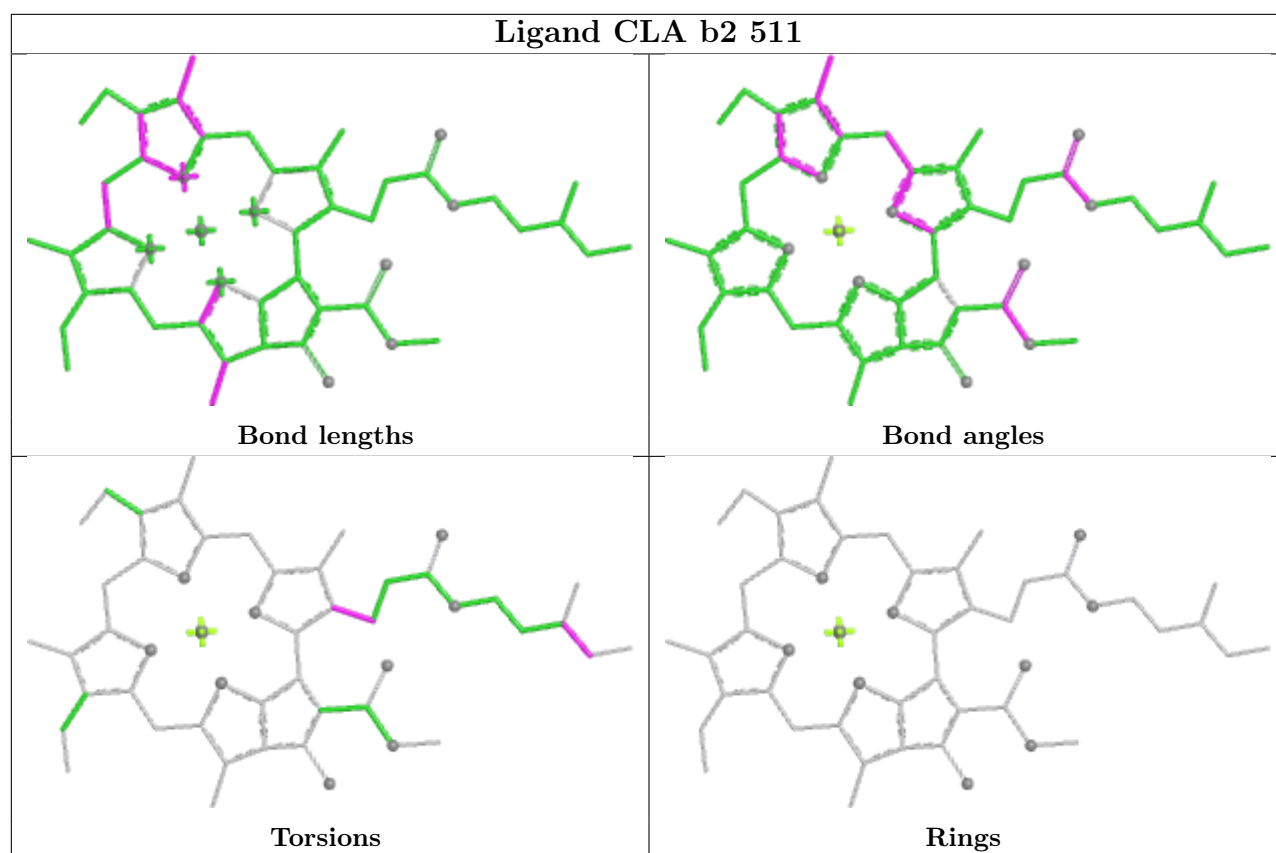
Ligand CLA p 512

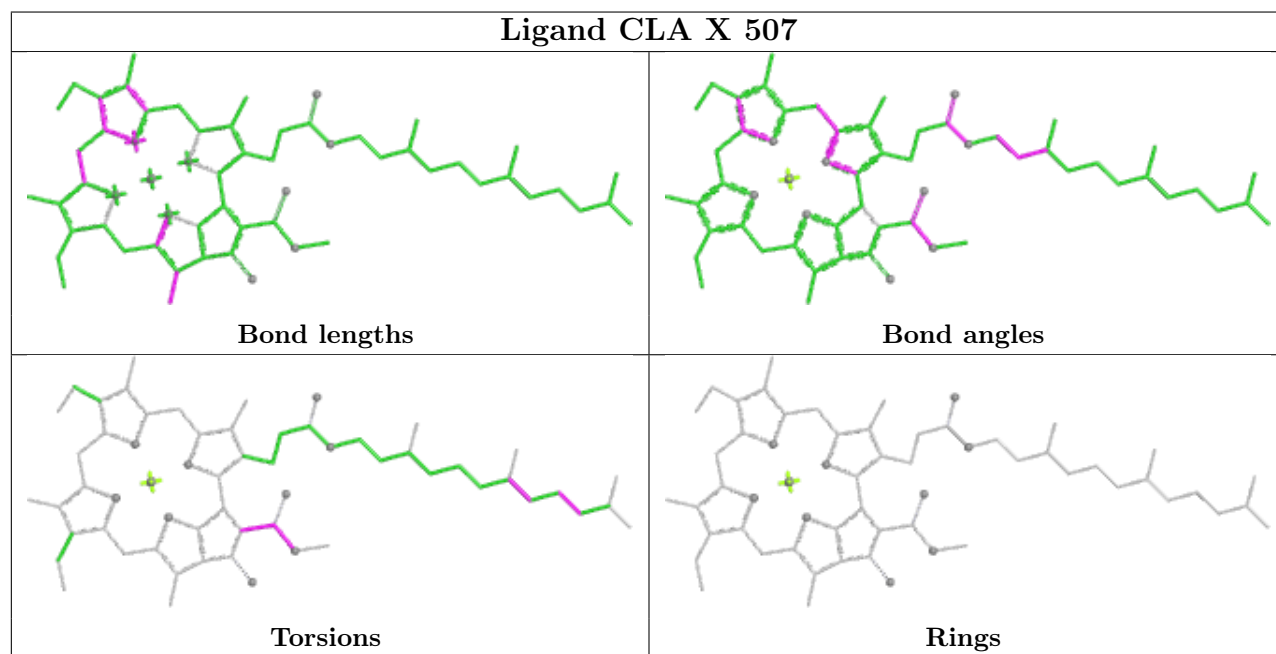
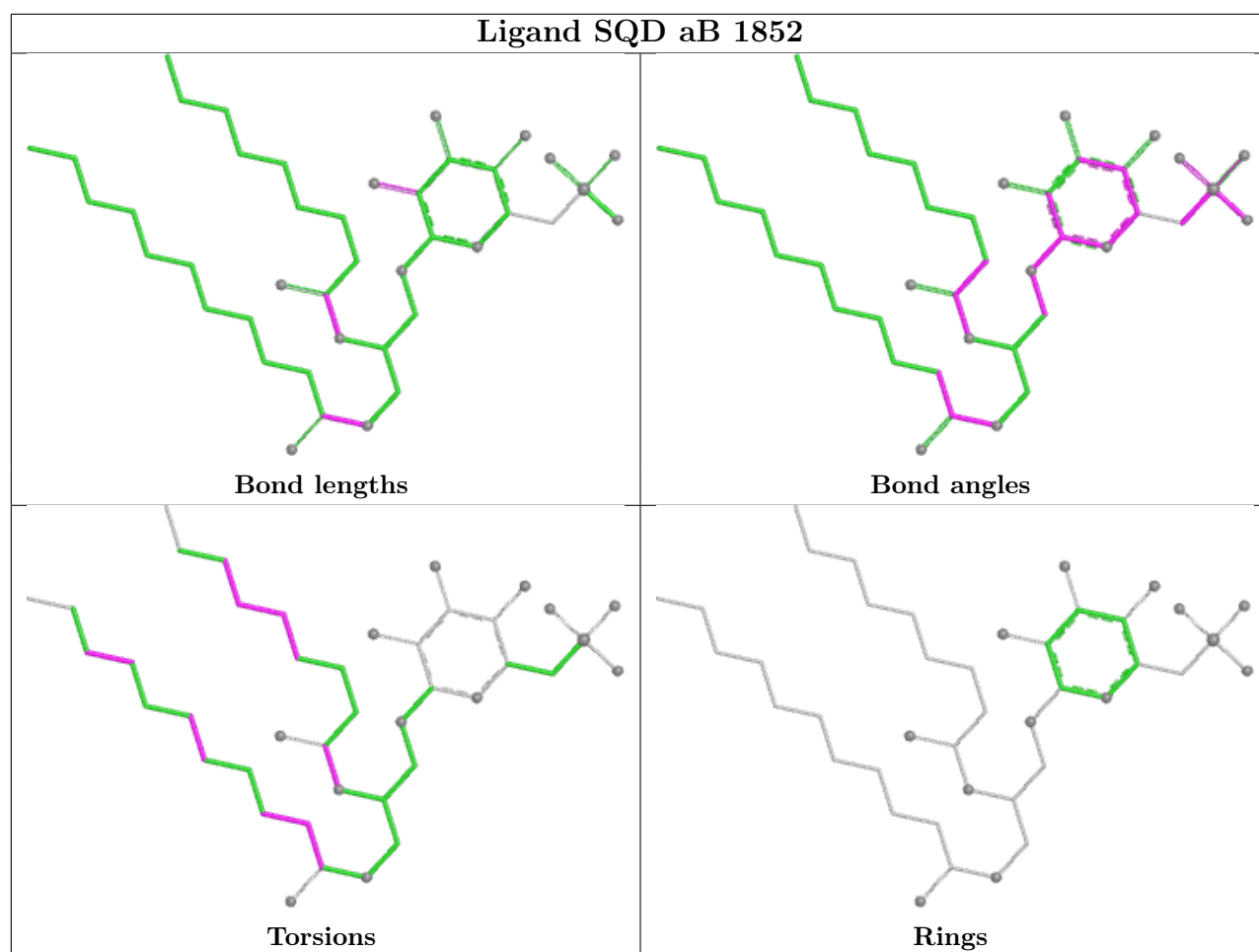


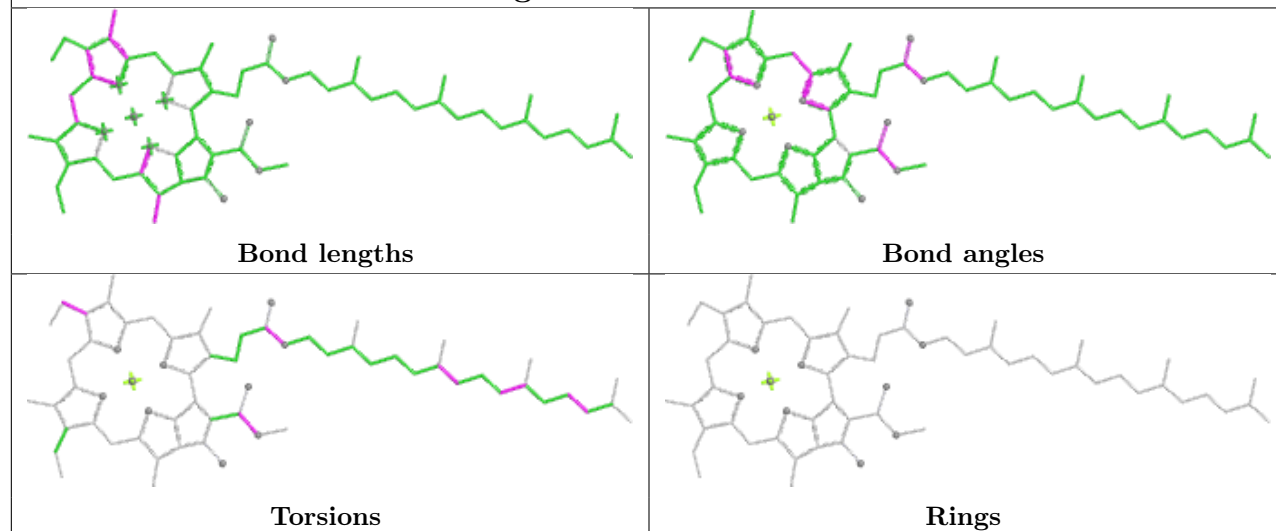
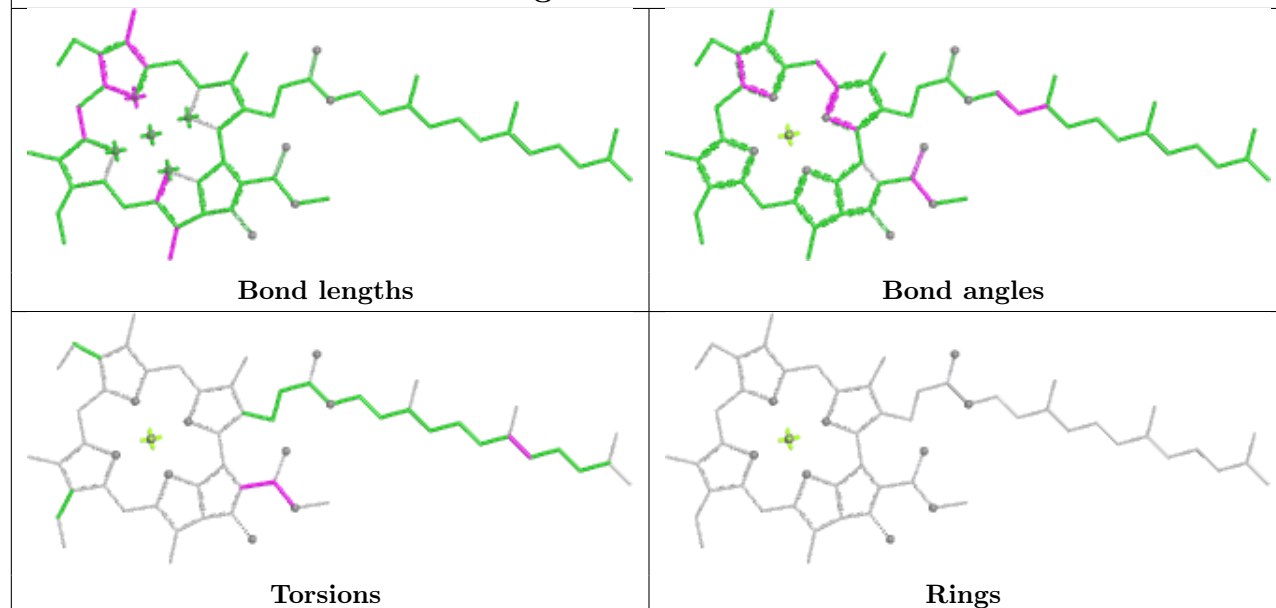
Ligand BCR g 524

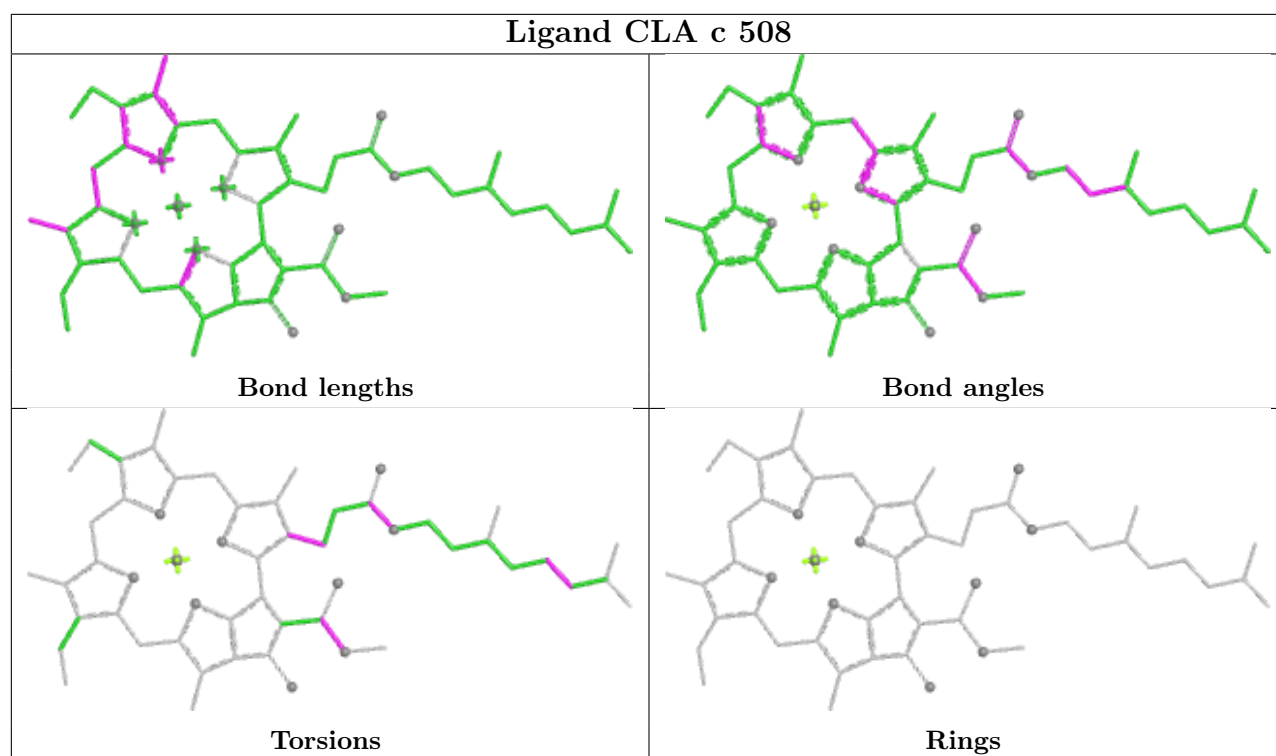




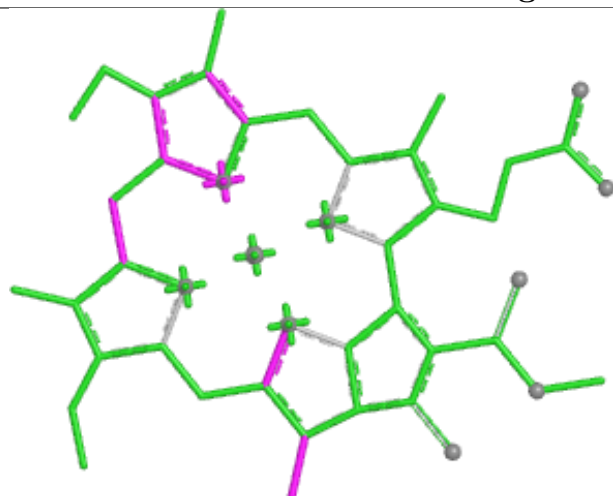




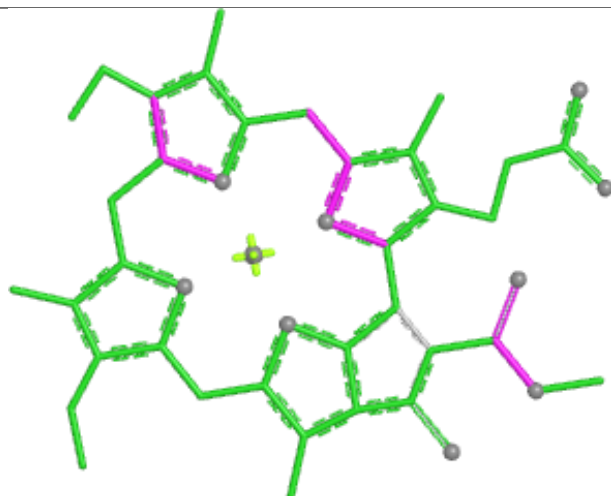
Ligand CLA aA 1109**Ligand CLA Z 507**



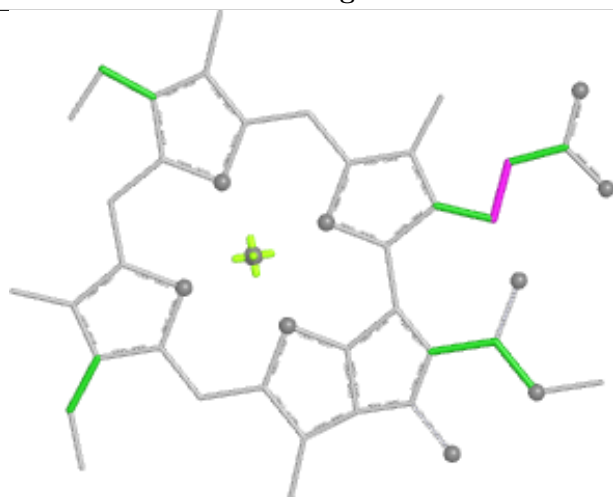
Ligand CLA a 513



Bond lengths



Bond angles

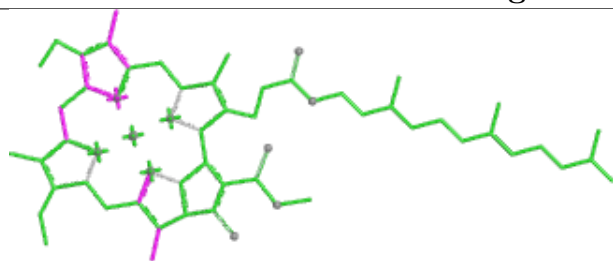


Torsions

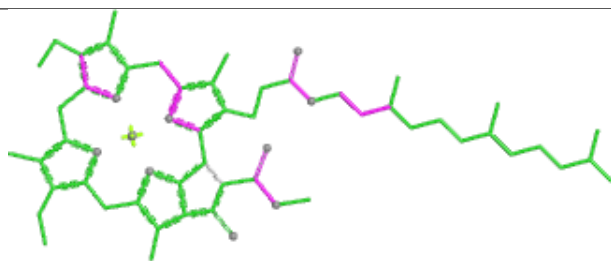


Rings

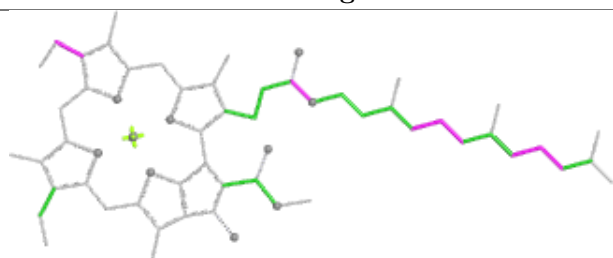
Ligand CLA b2 502



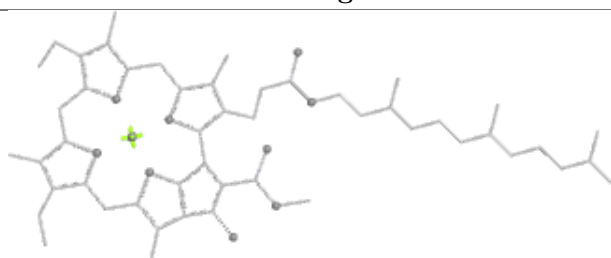
Bond lengths



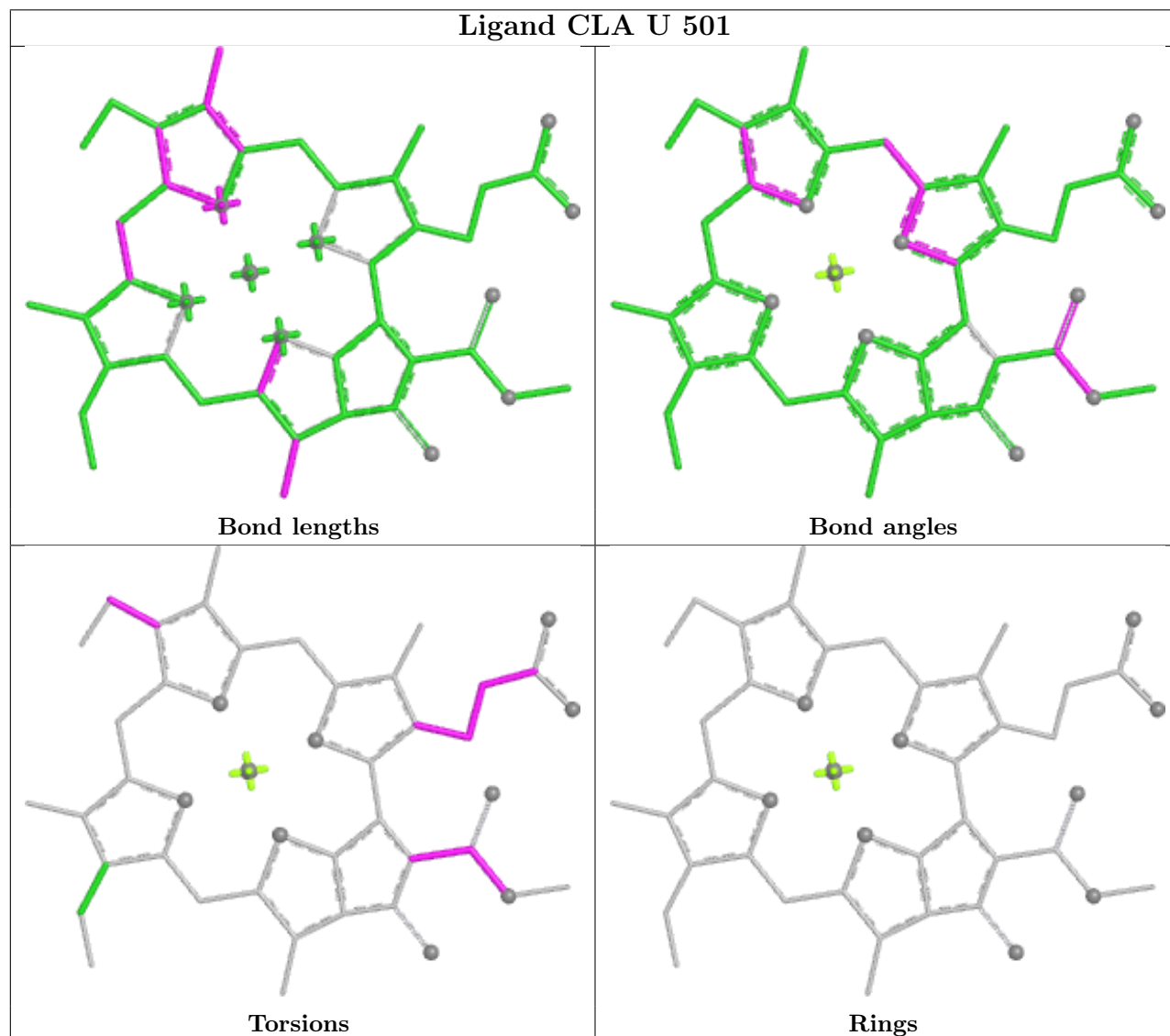
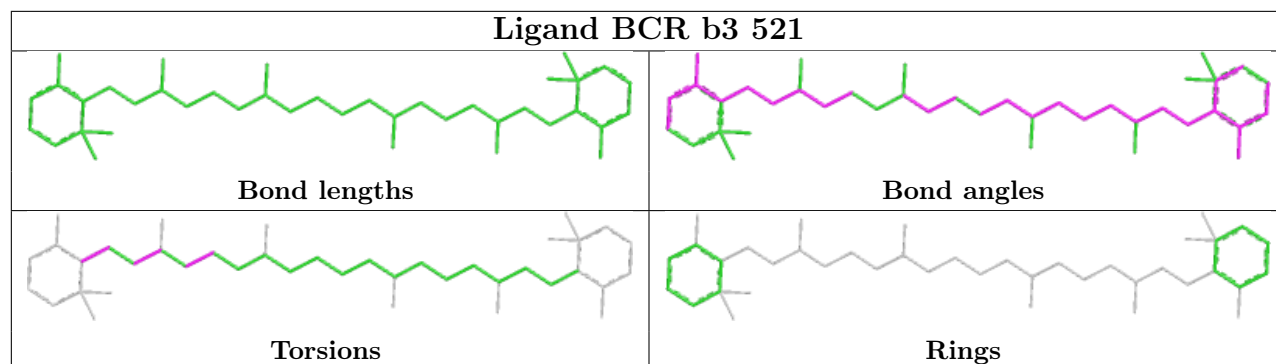
Bond angles

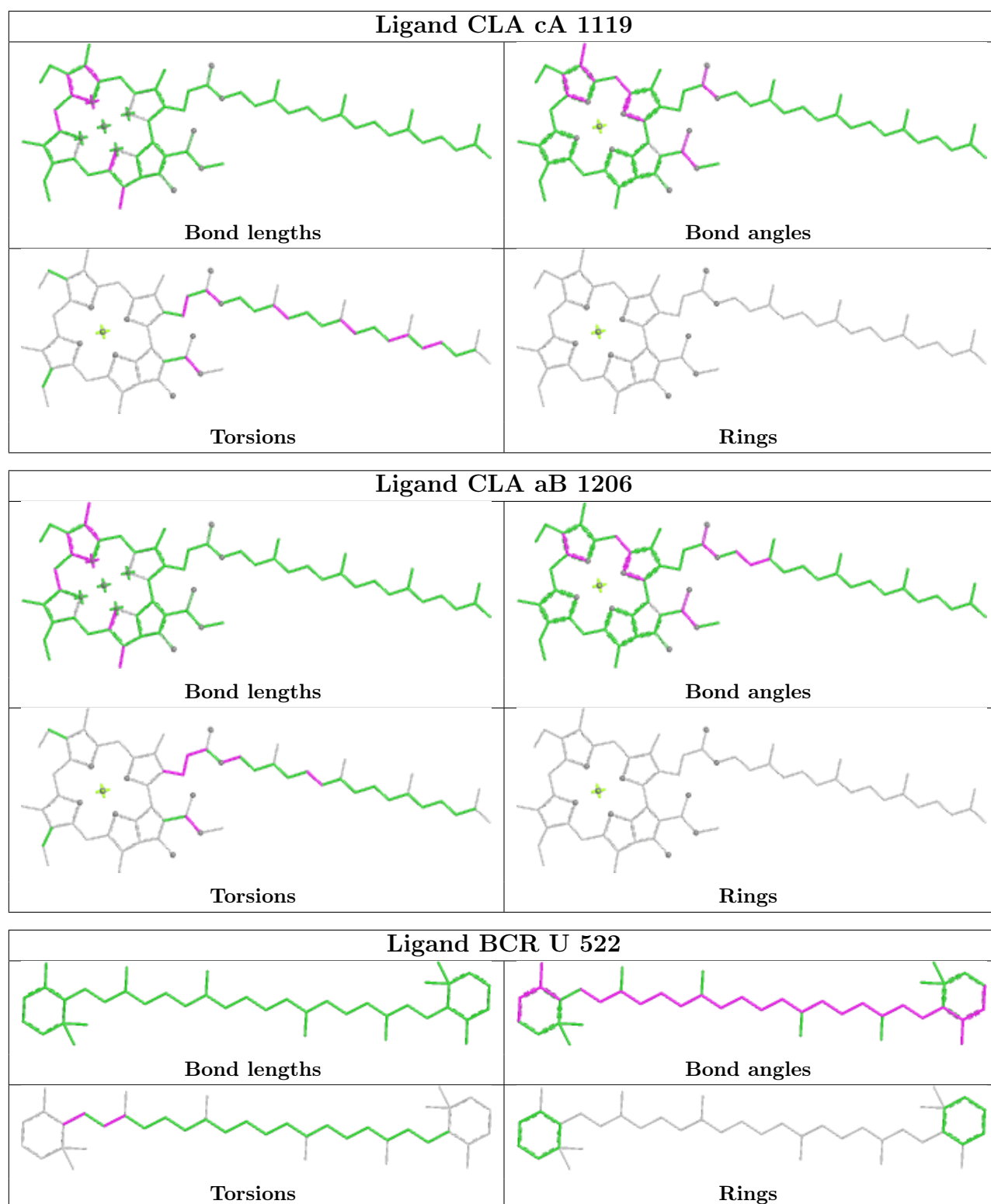


Torsions

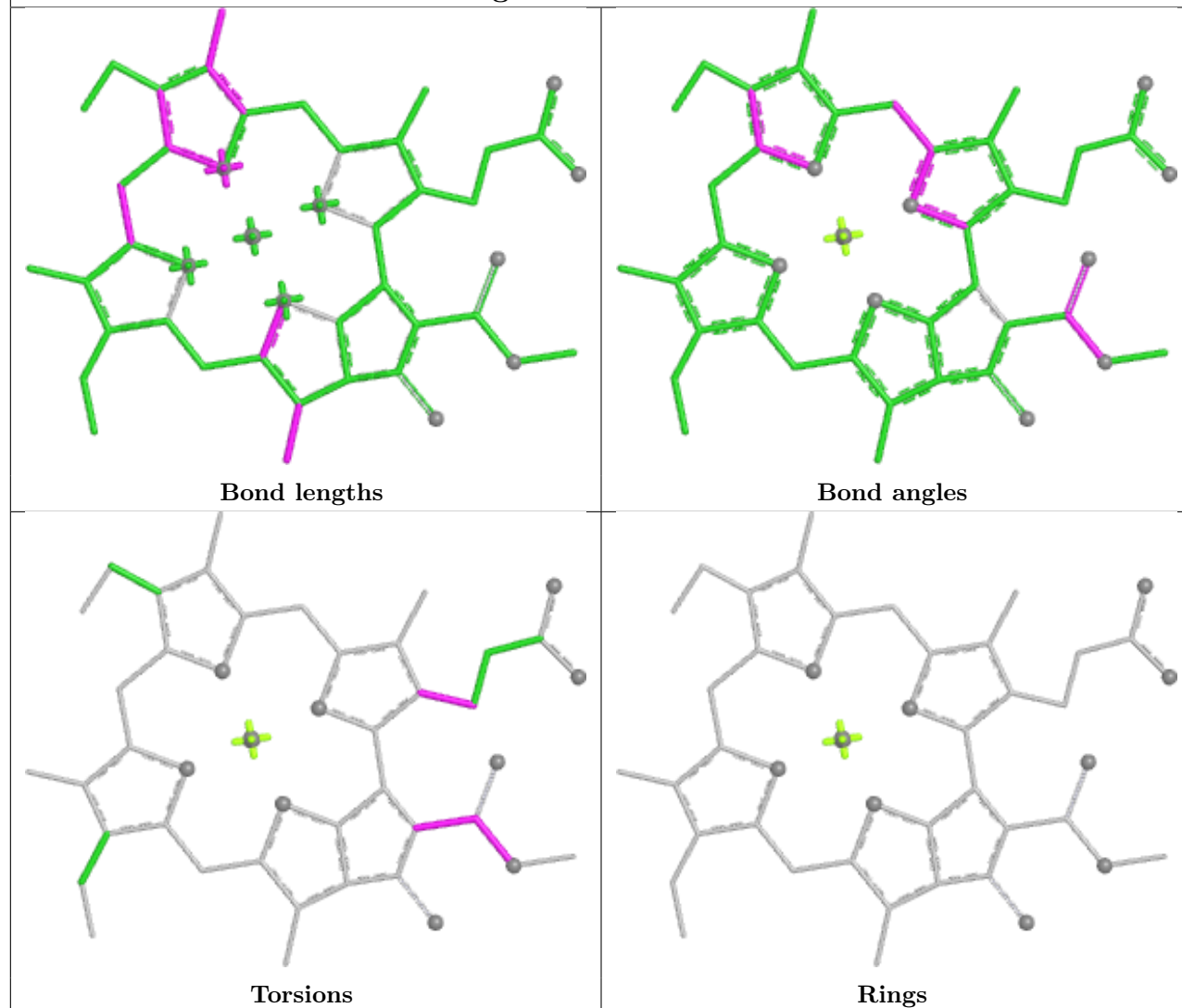


Rings

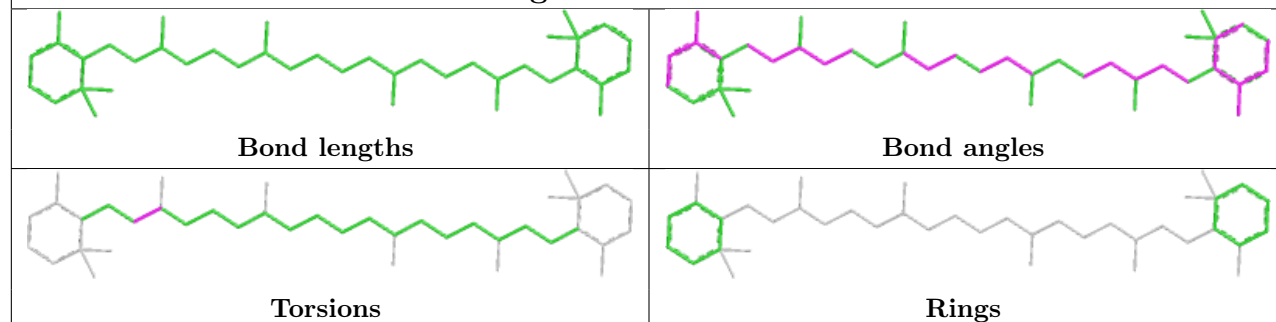


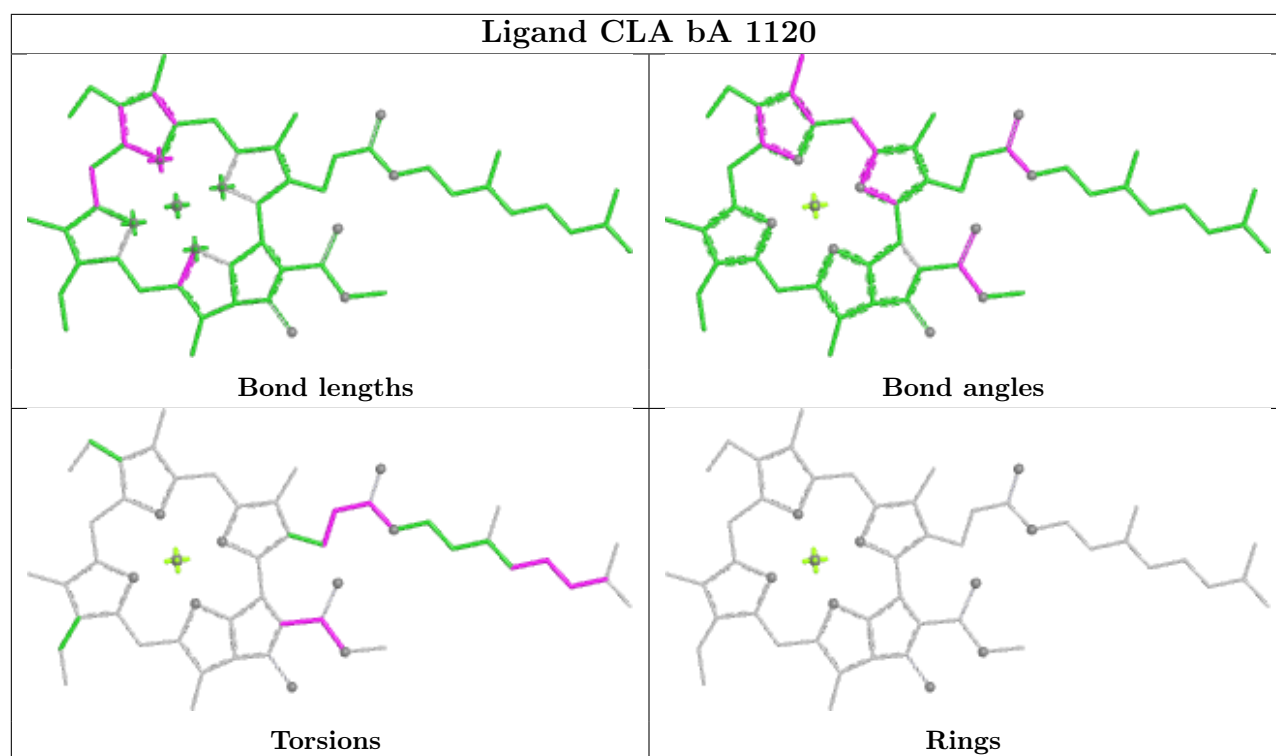


Ligand CLA V 511

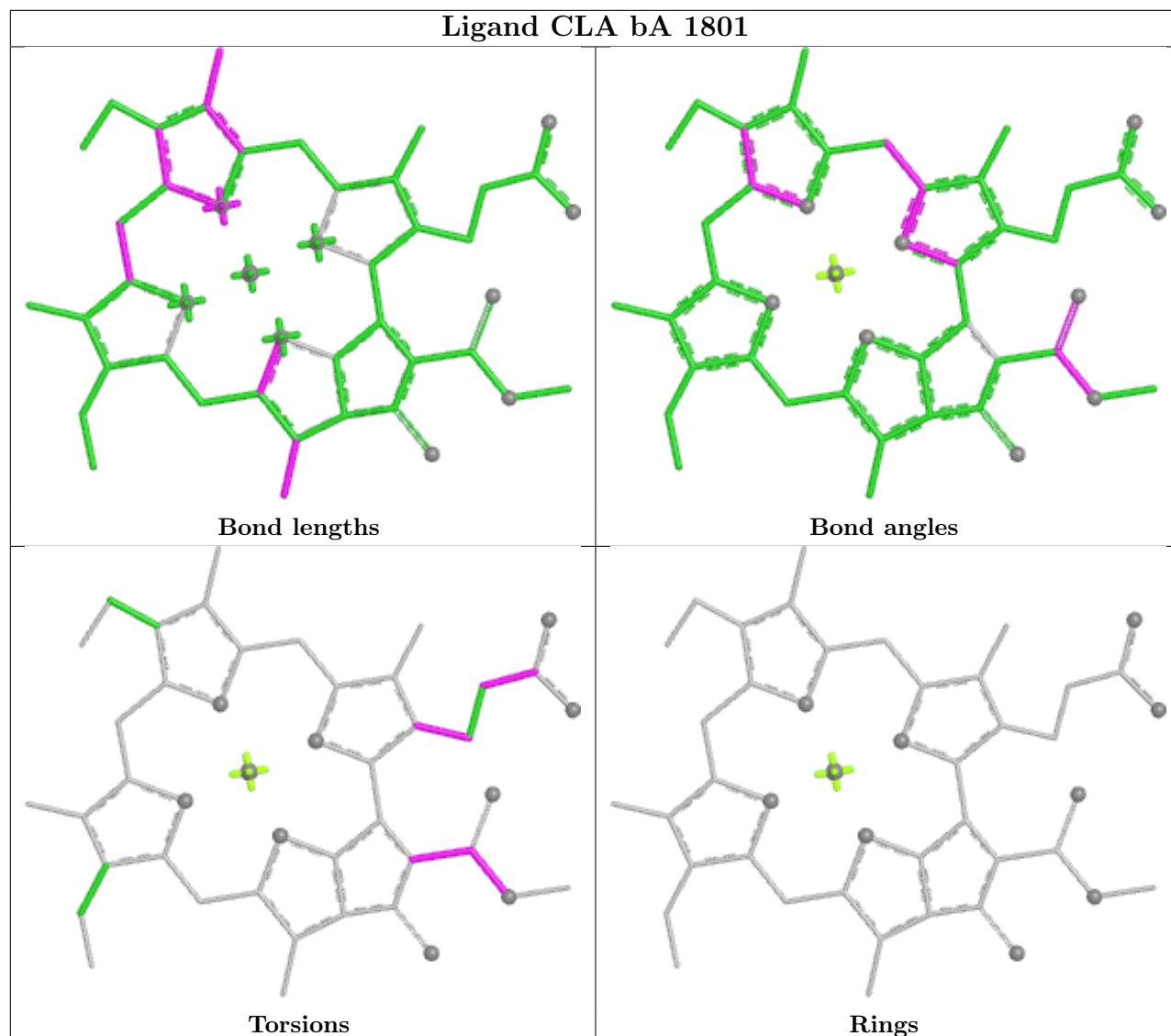


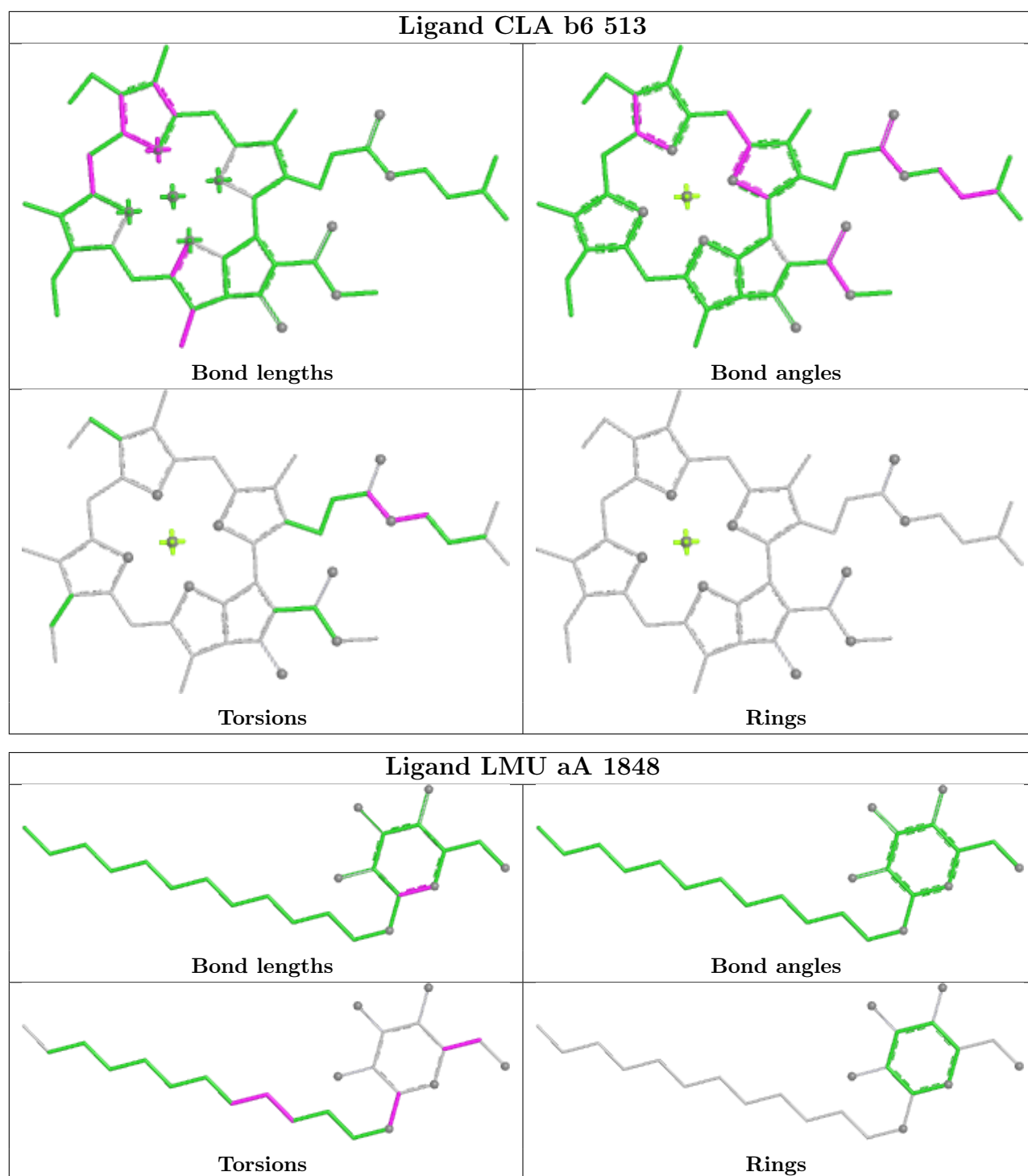
Ligand BCR V 521

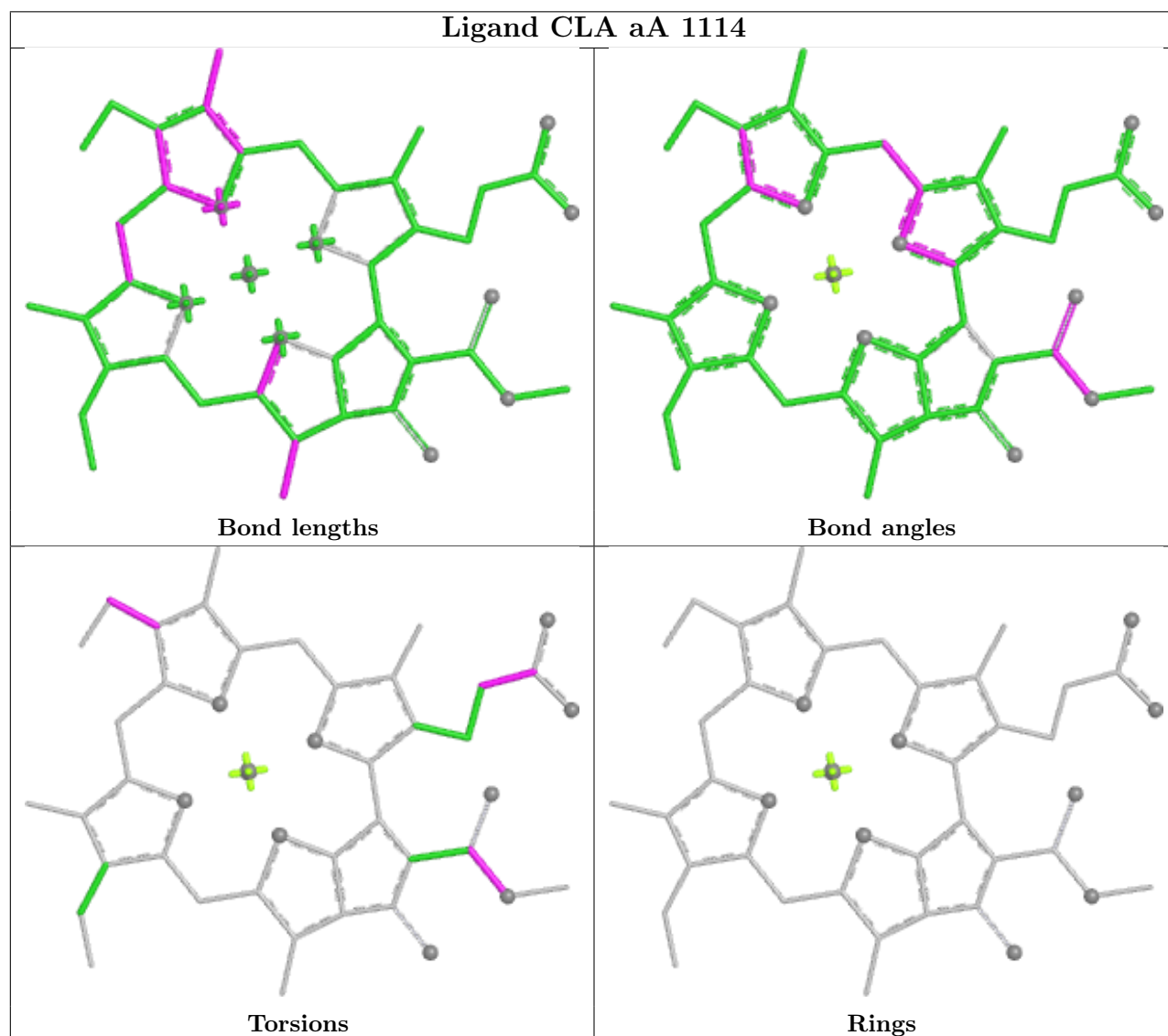
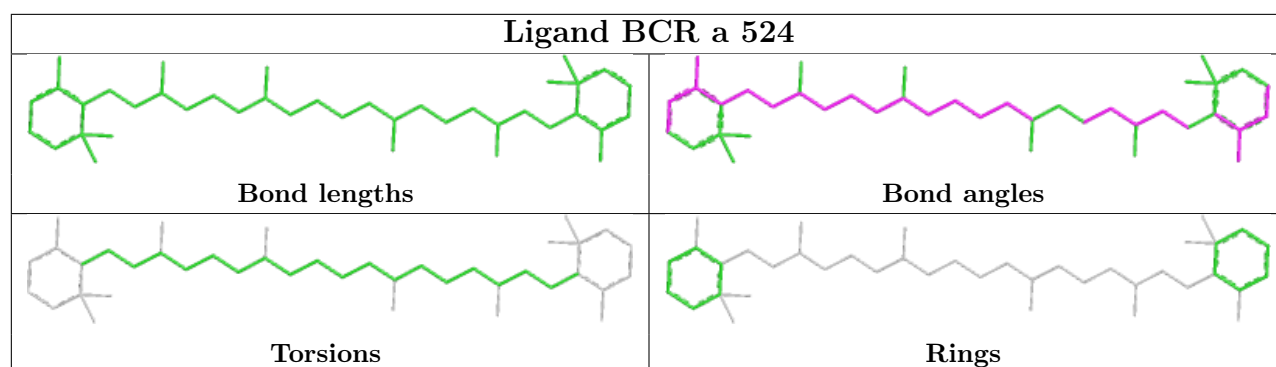




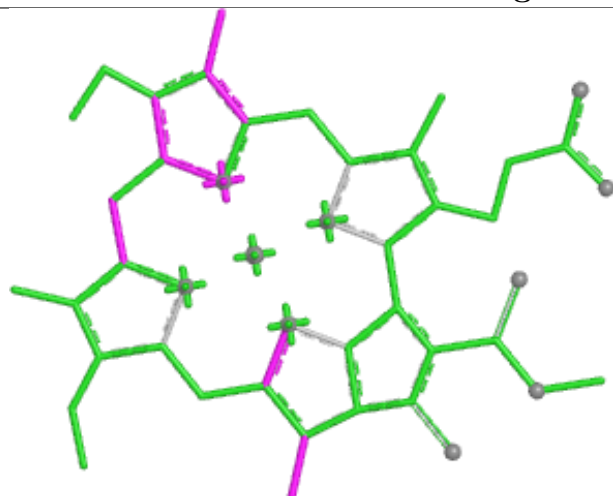
Ligand CLA bA 1801



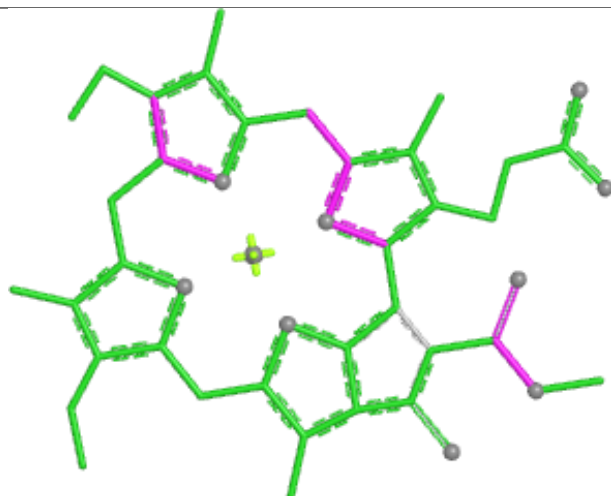




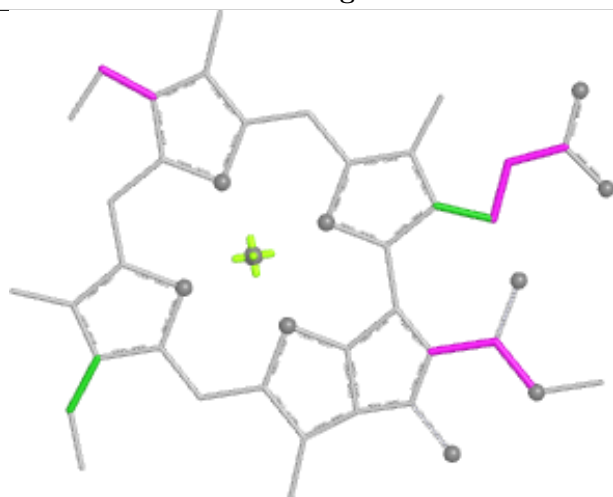
Ligand CLA X 517



Bond lengths



Bond angles

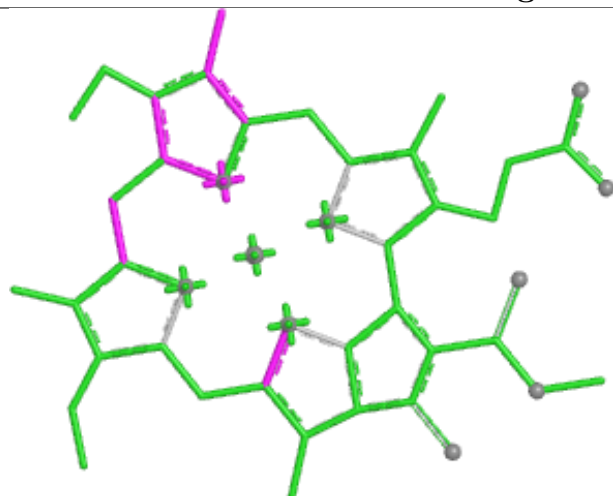


Torsions

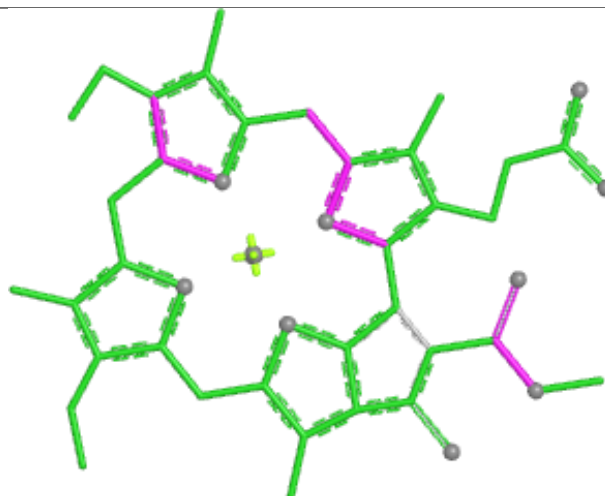


Rings

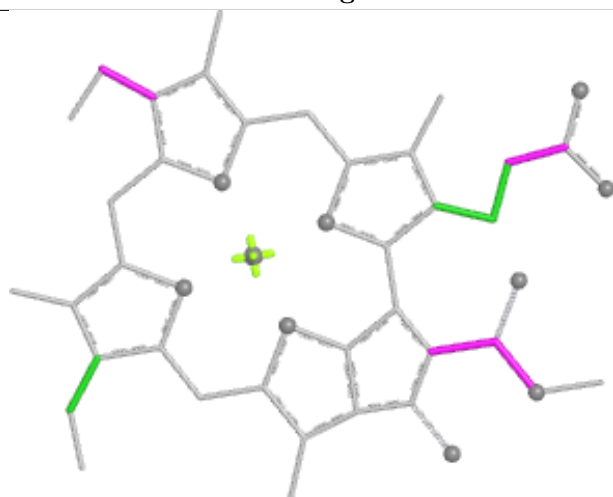
Ligand CLA b 519



Bond lengths



Bond angles

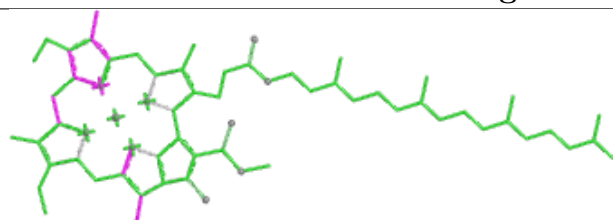


Torsions

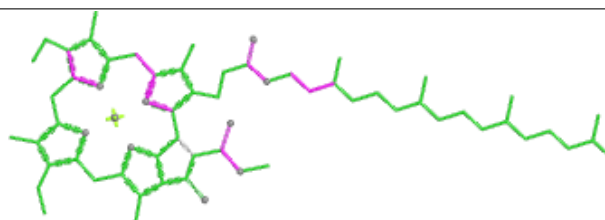


Rings

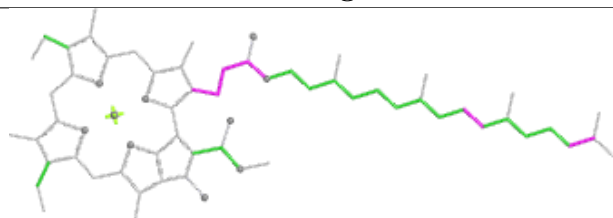
Ligand CLA cL 1503



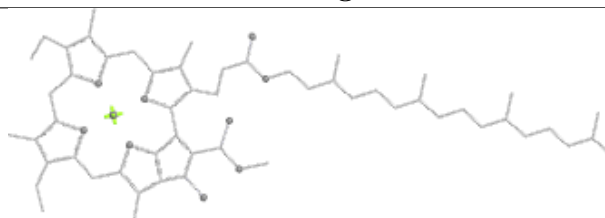
Bond lengths



Bond angles

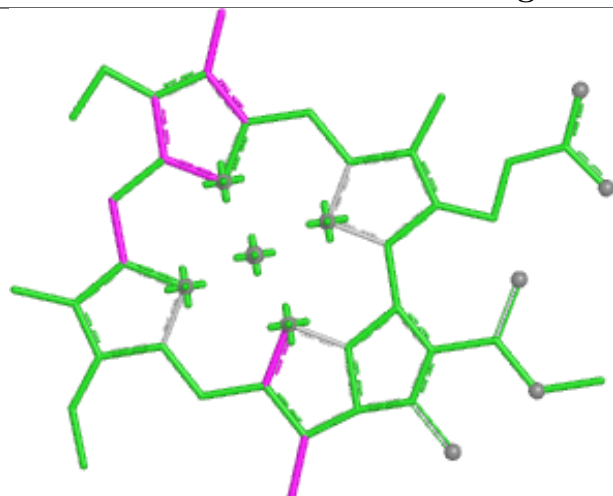


Torsions

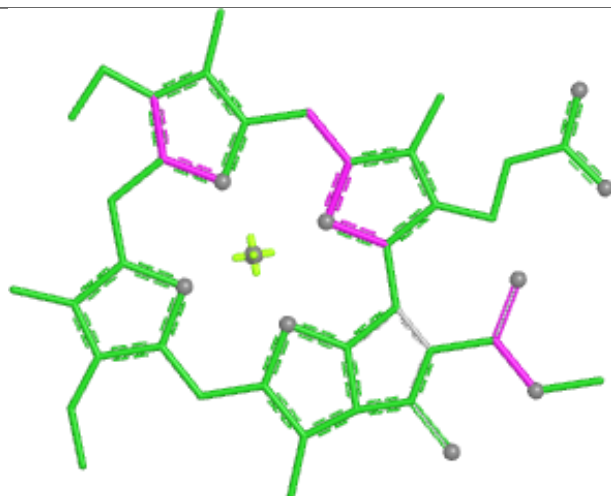


Rings

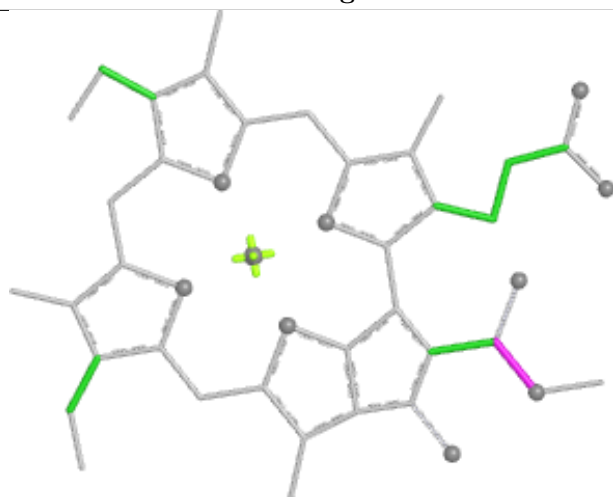
Ligand CLA h 503



Bond lengths



Bond angles

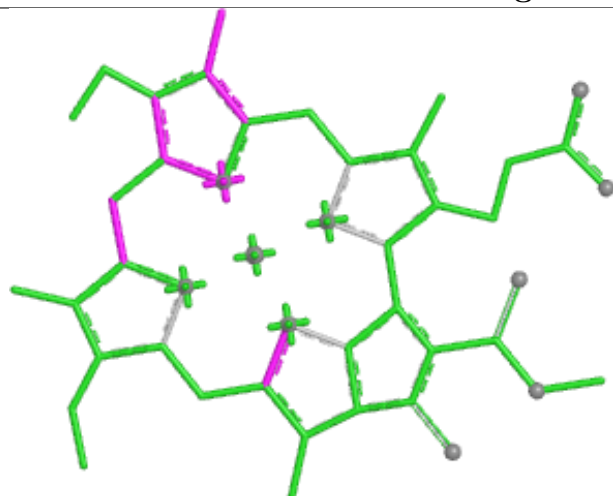


Torsions



Rings

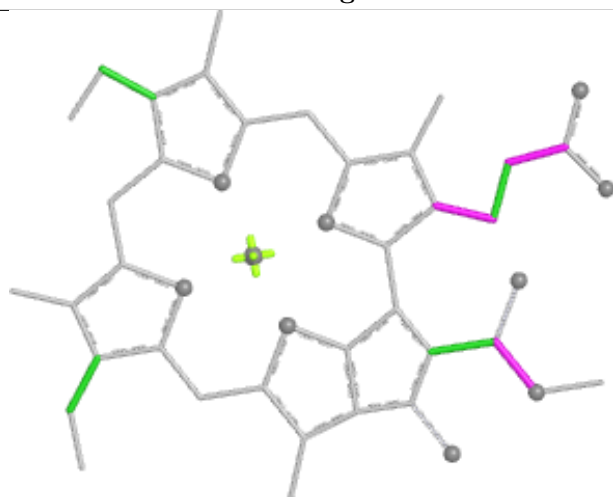
Ligand CLA T 511



Bond lengths



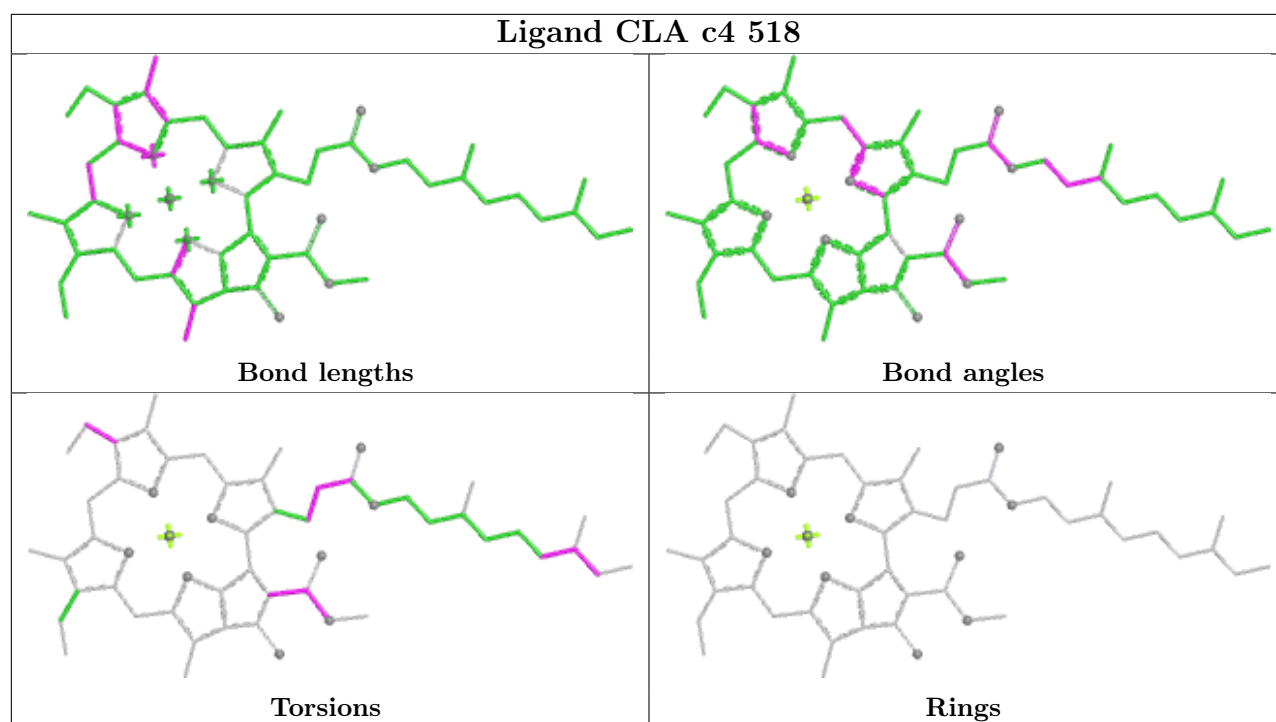
Bond angles



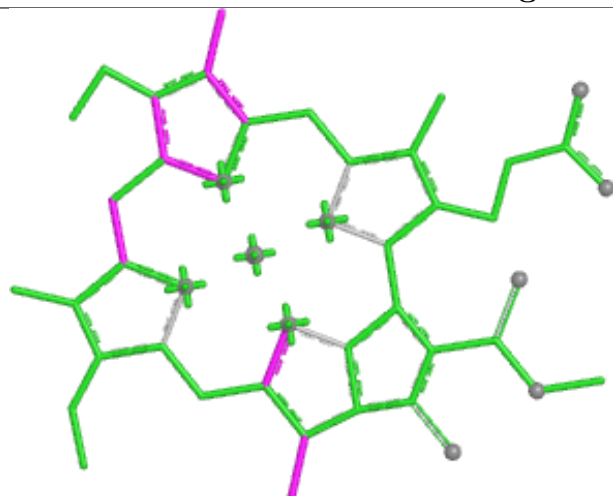
Torsions



Rings



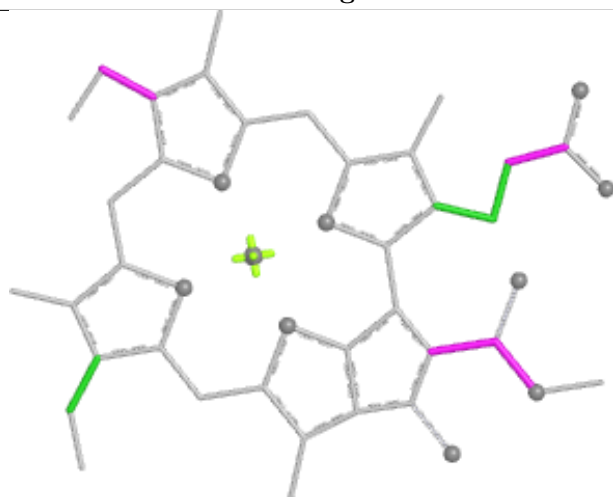
Ligand CLA e 504



Bond lengths



Bond angles

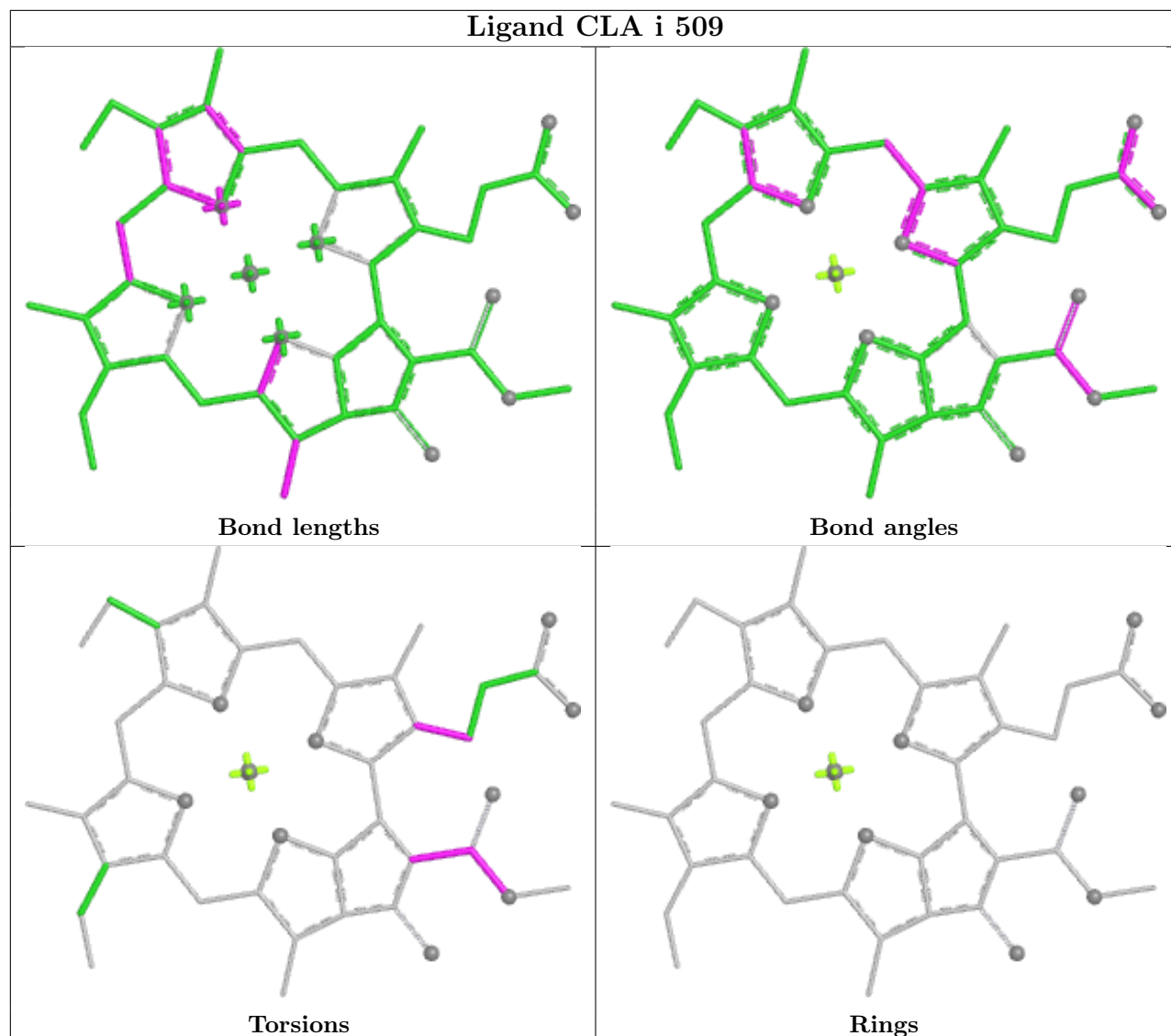


Torsions

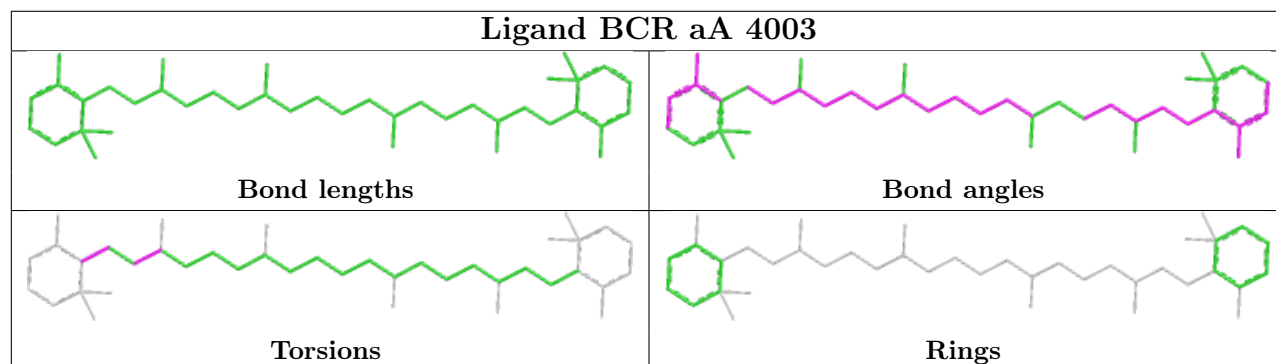


Rings

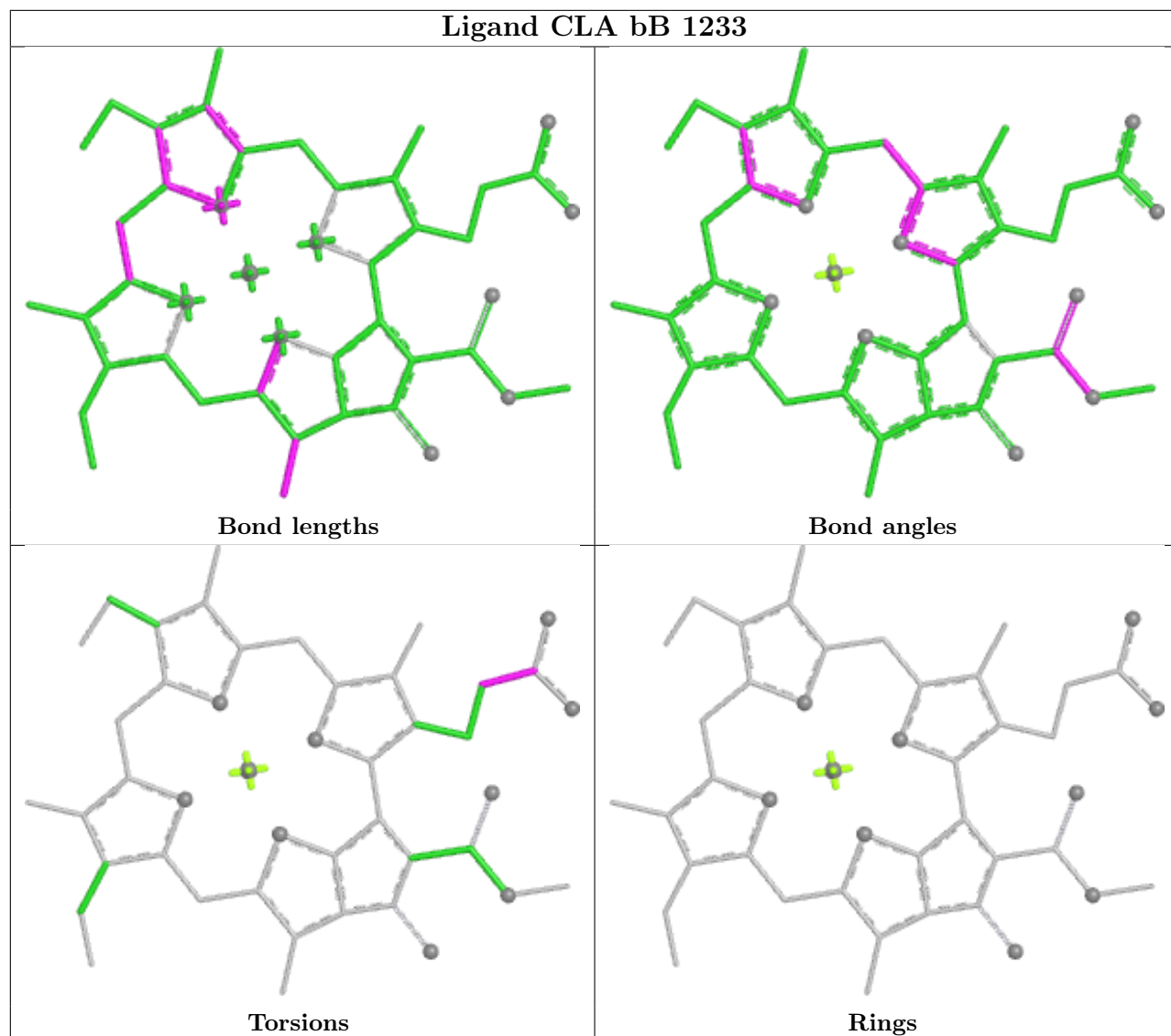
Ligand CLA i 509

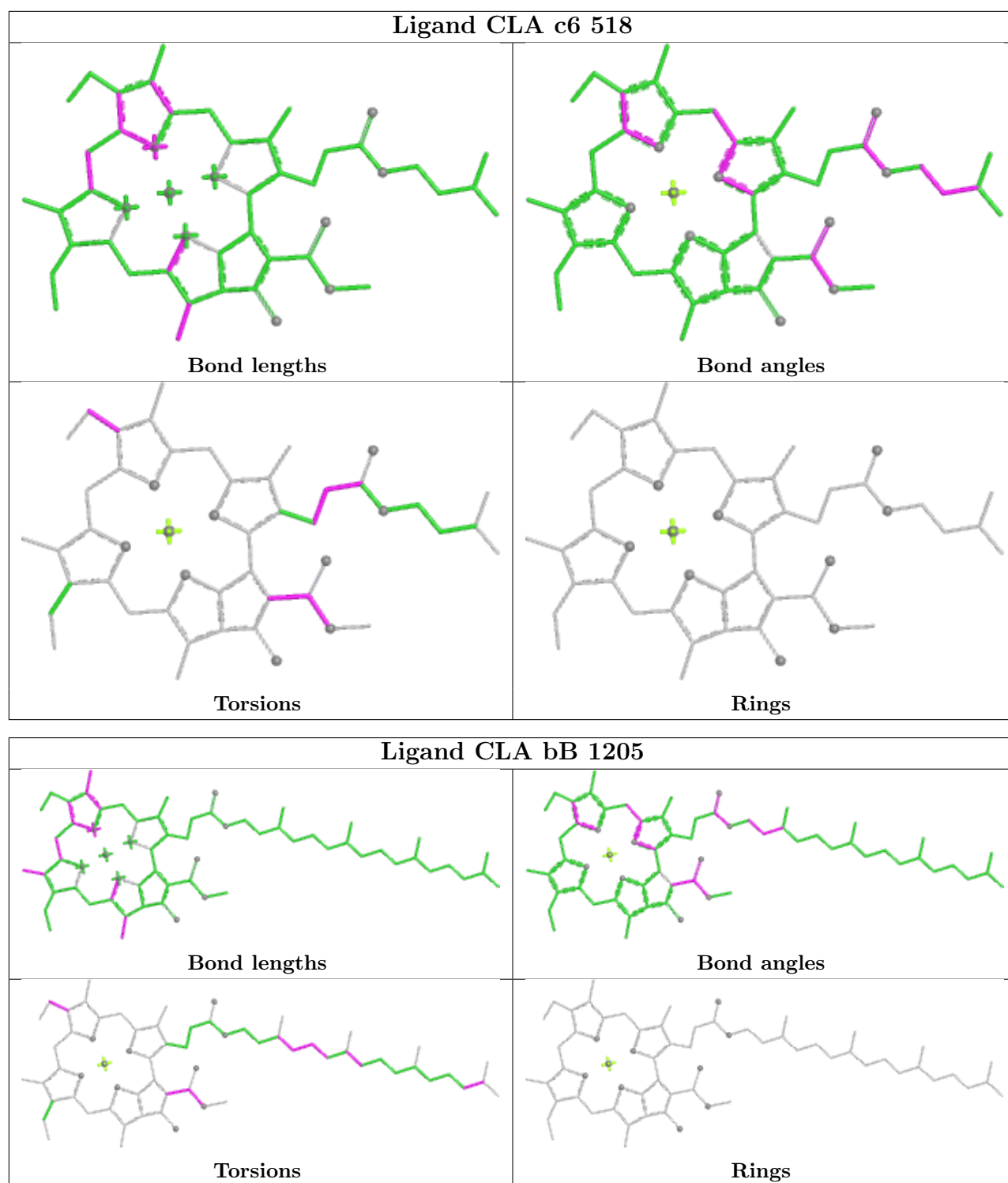


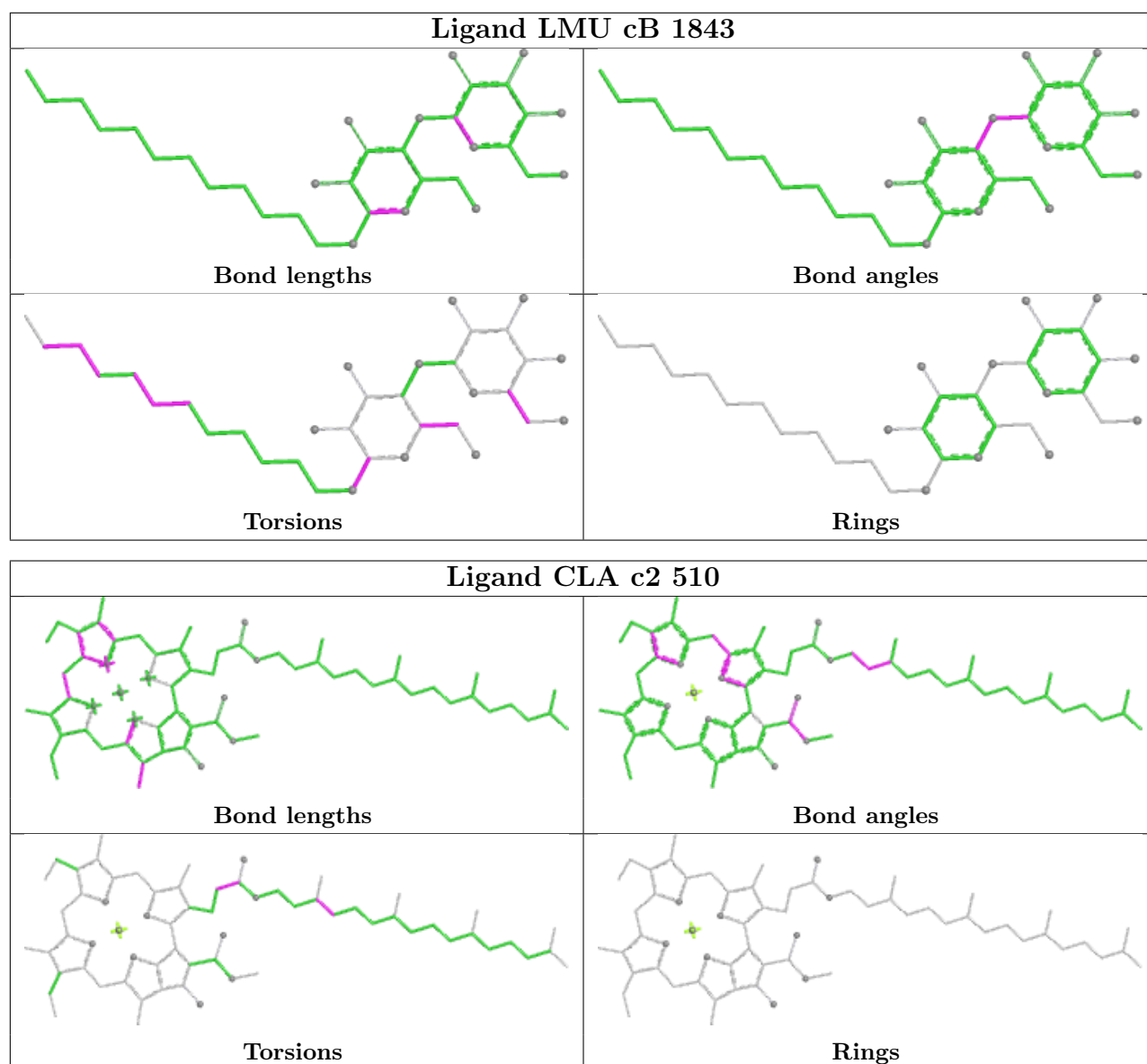
Ligand BCR aA 4003



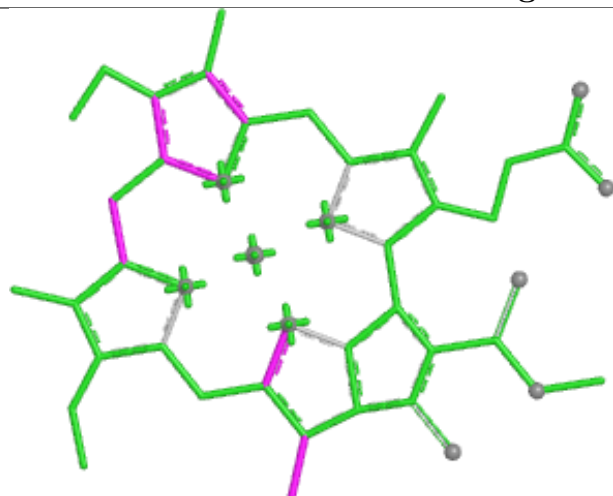
Ligand CLA bB 1233



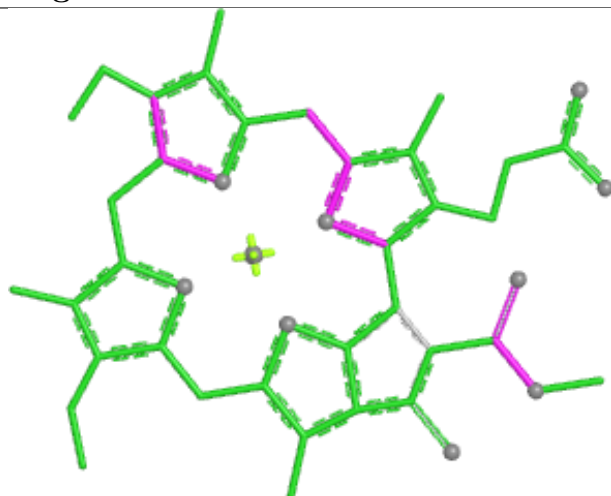




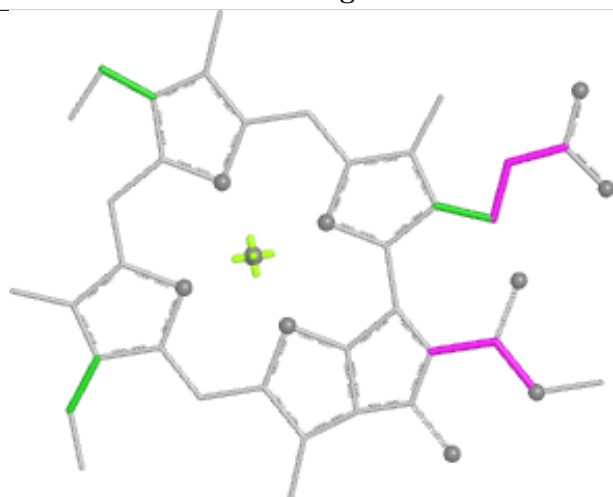
Ligand CLA g 507



Bond lengths



Bond angles

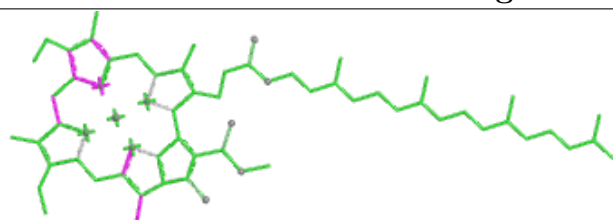


Torsions

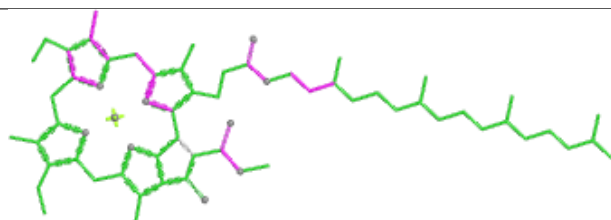


Rings

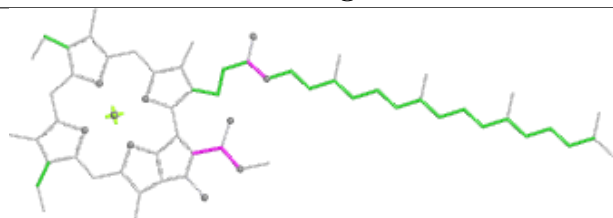
Ligand CLA bB 1211



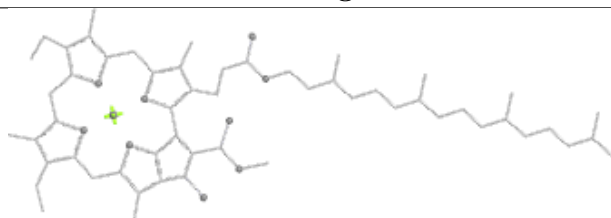
Bond lengths



Bond angles

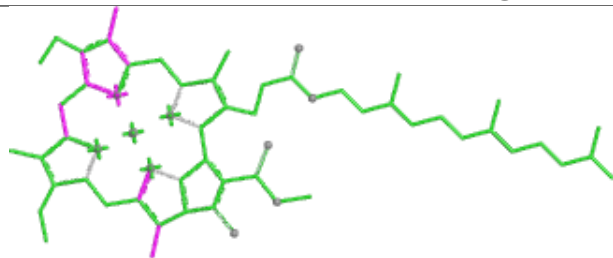


Torsions

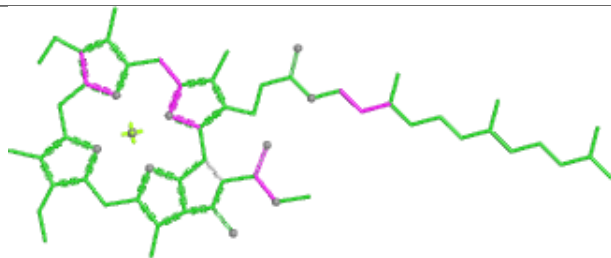


Rings

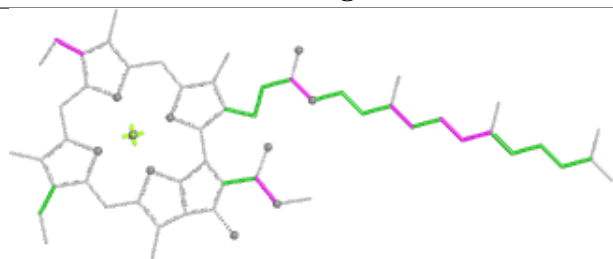
Ligand CLA aA 1139



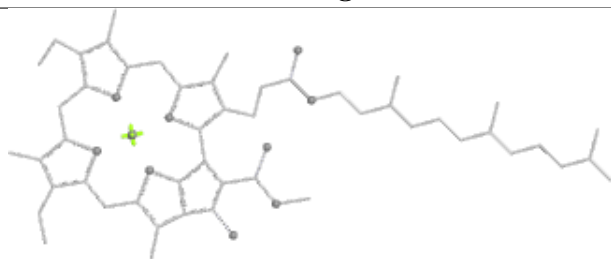
Bond lengths



Bond angles

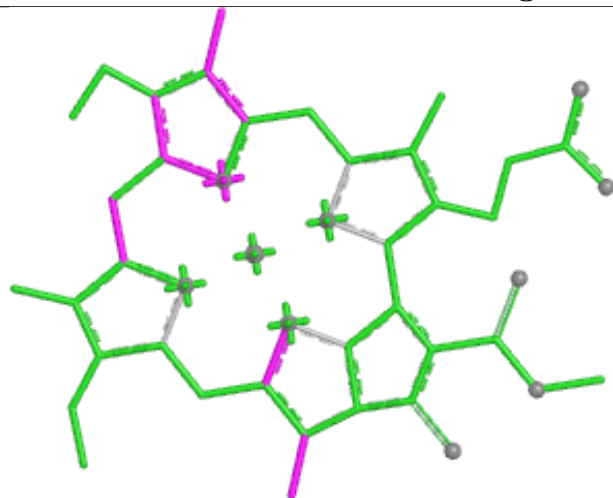


Torsions

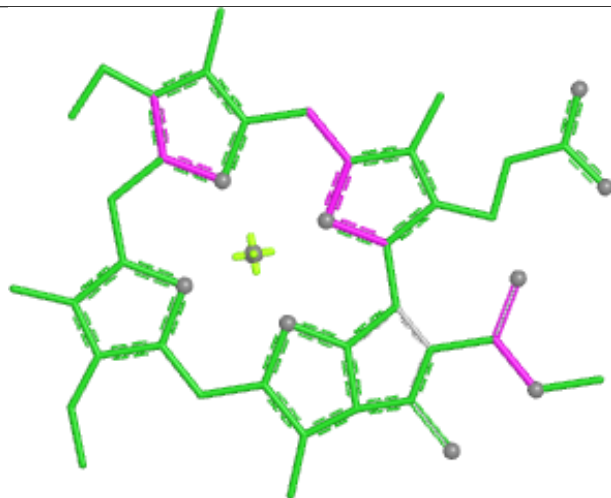


Rings

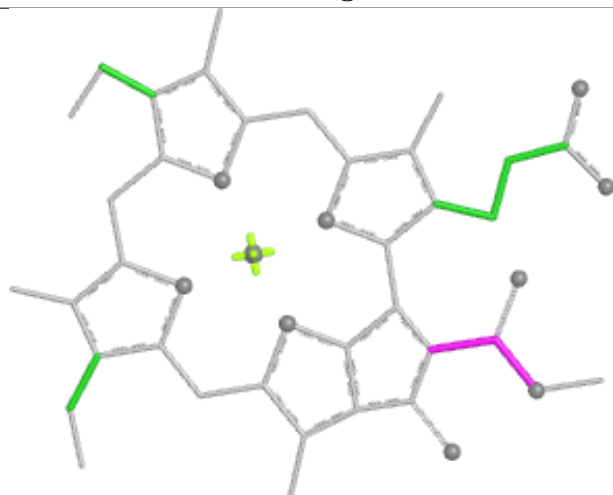
Ligand CLA k 502



Bond lengths



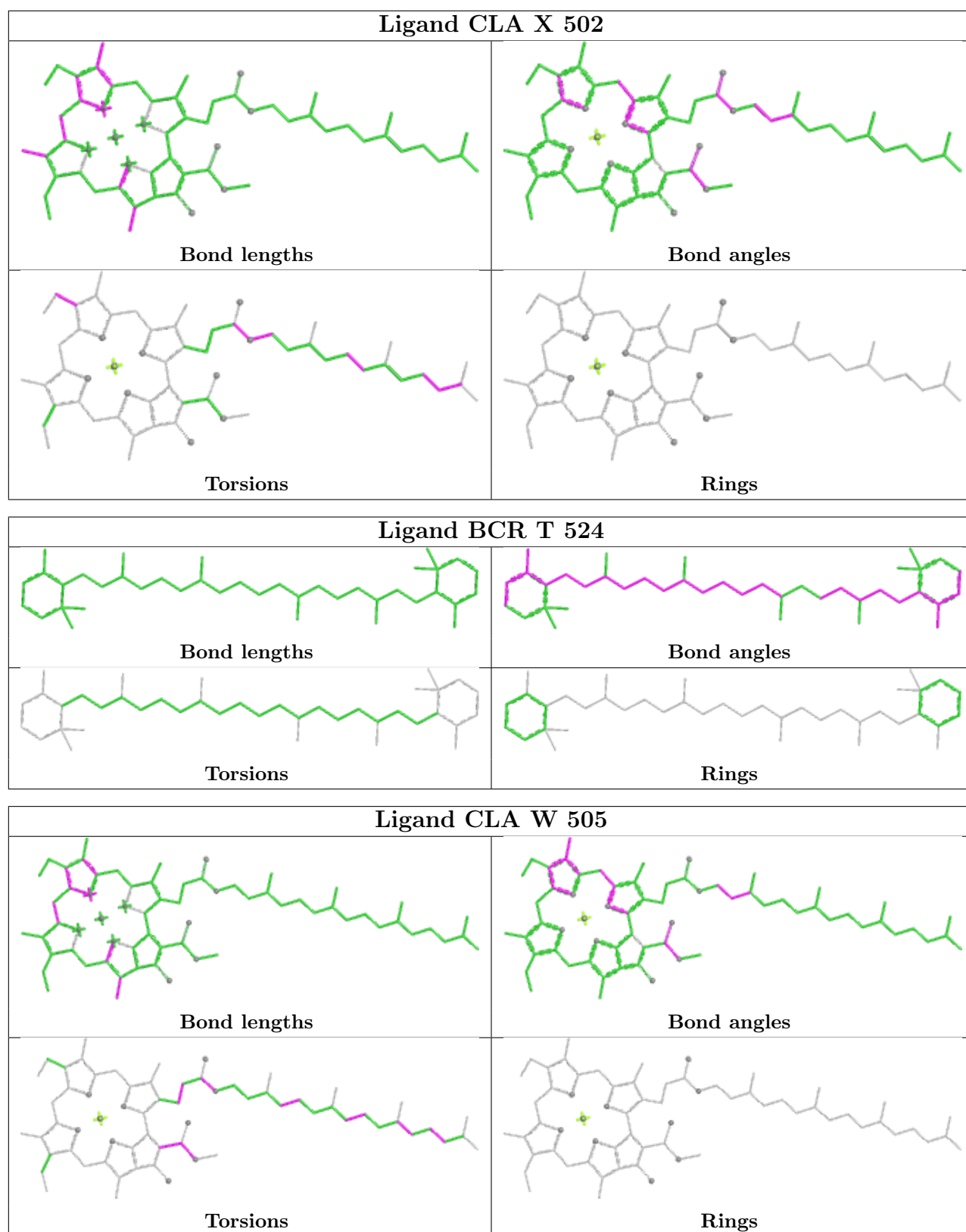
Bond angles

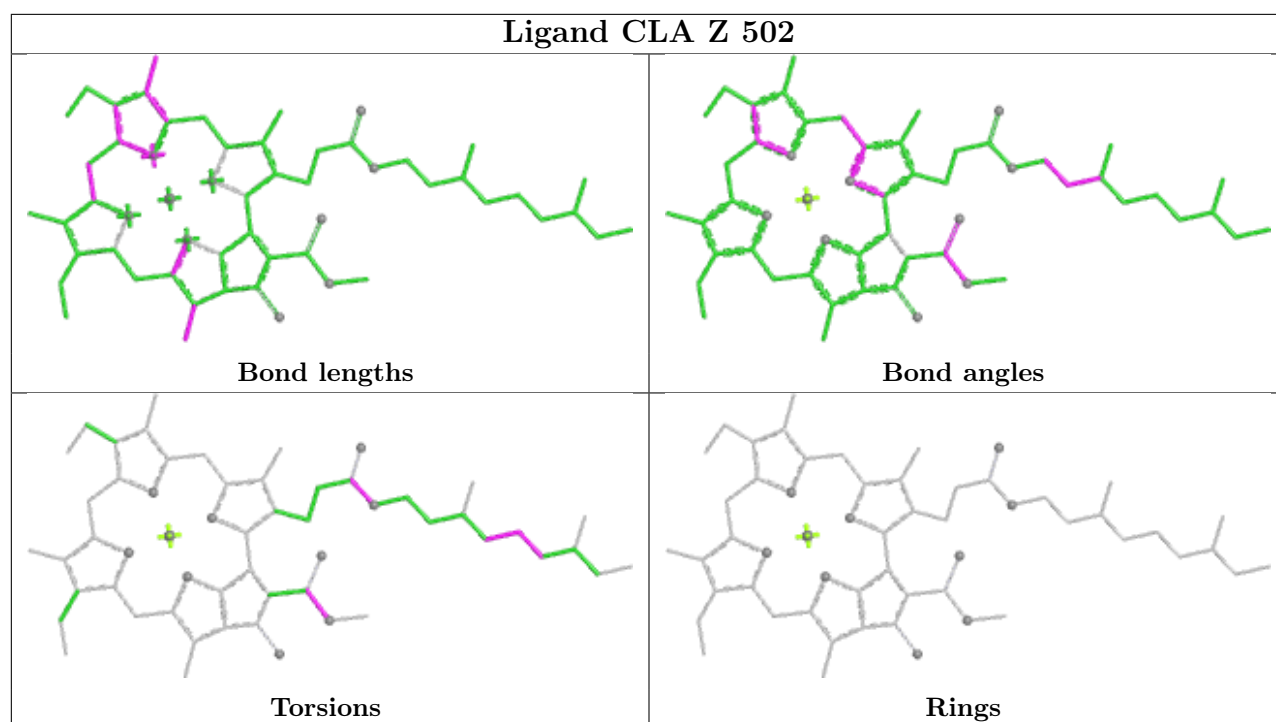


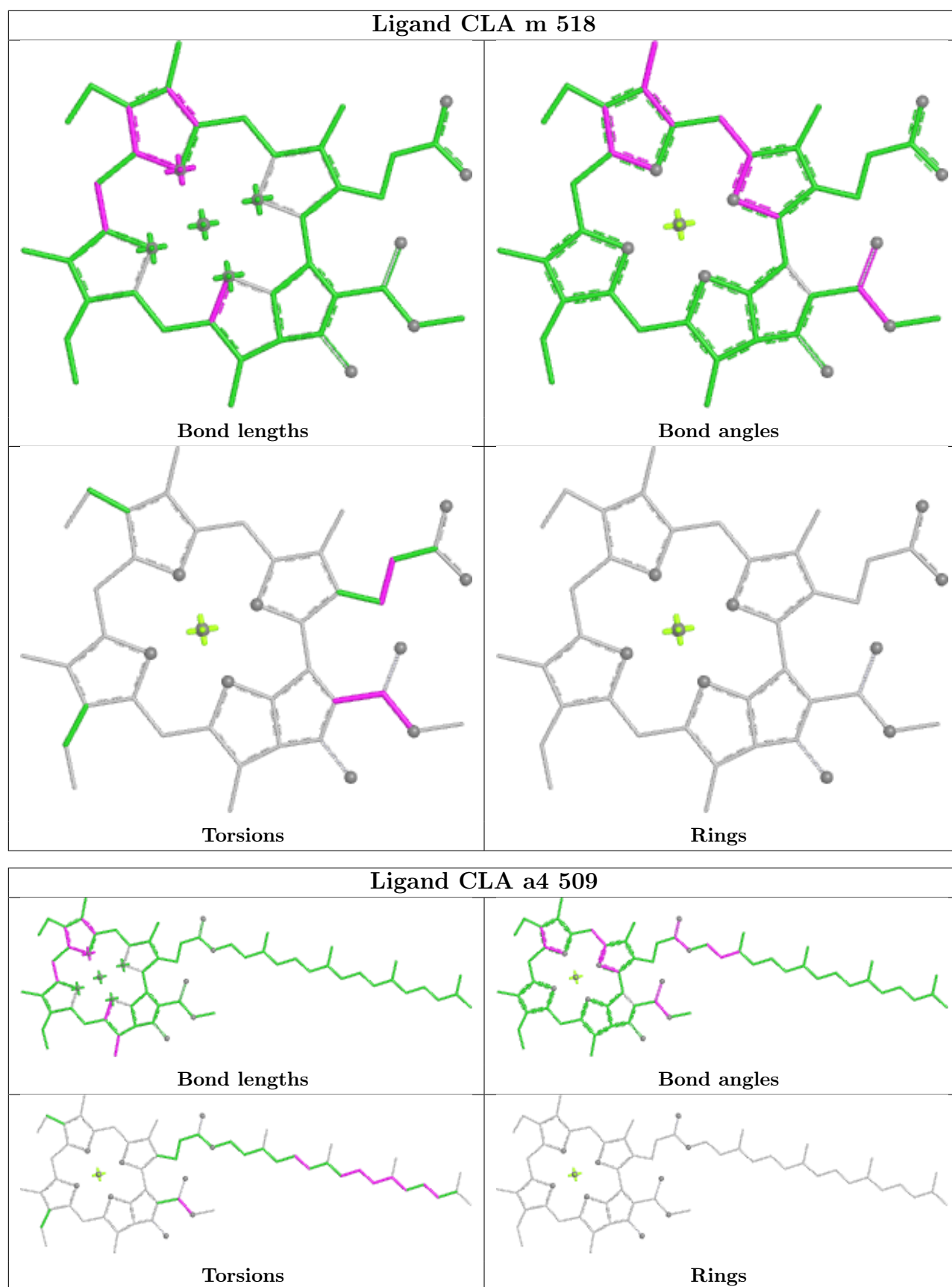
Torsions



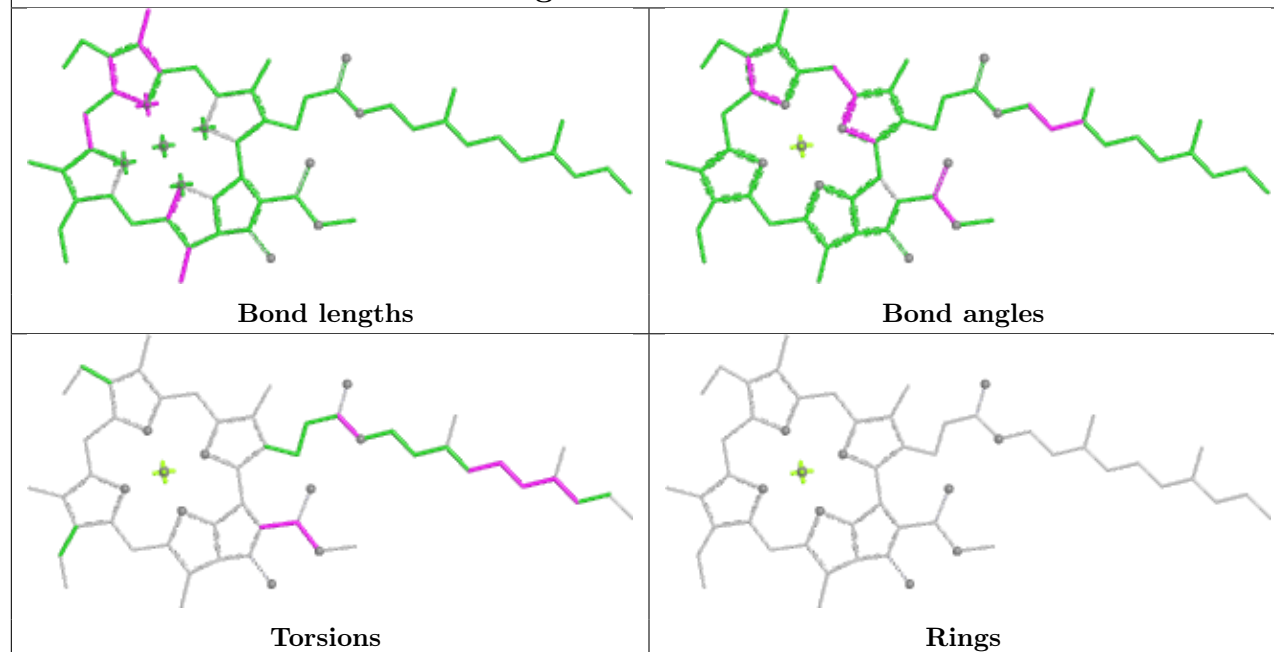
Rings



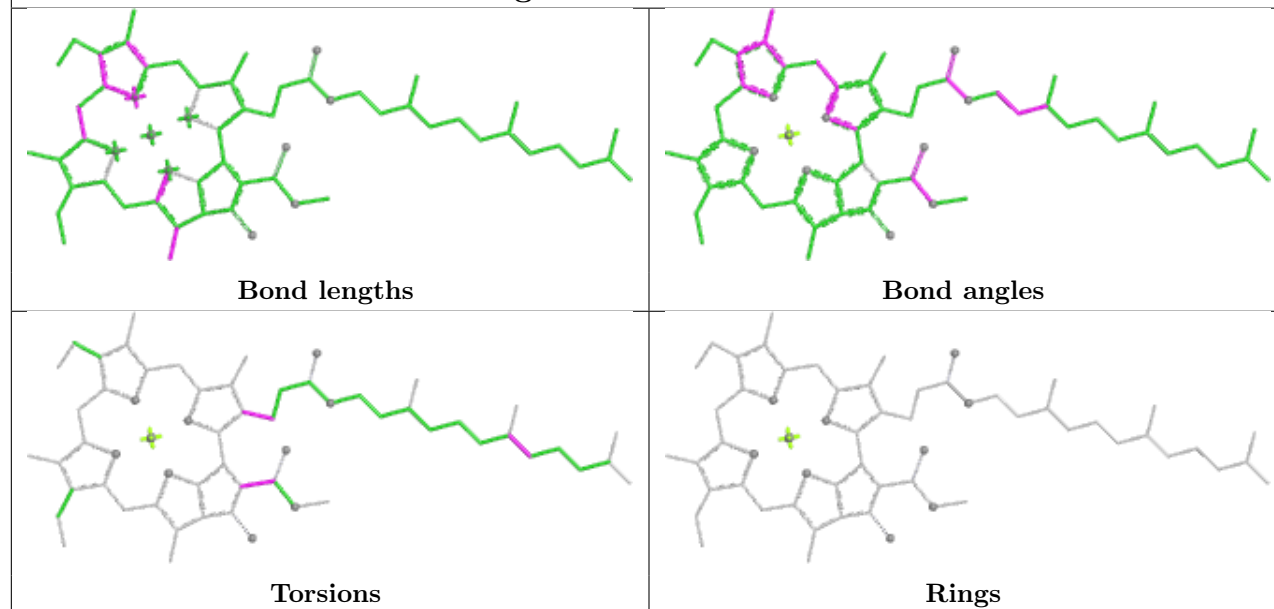




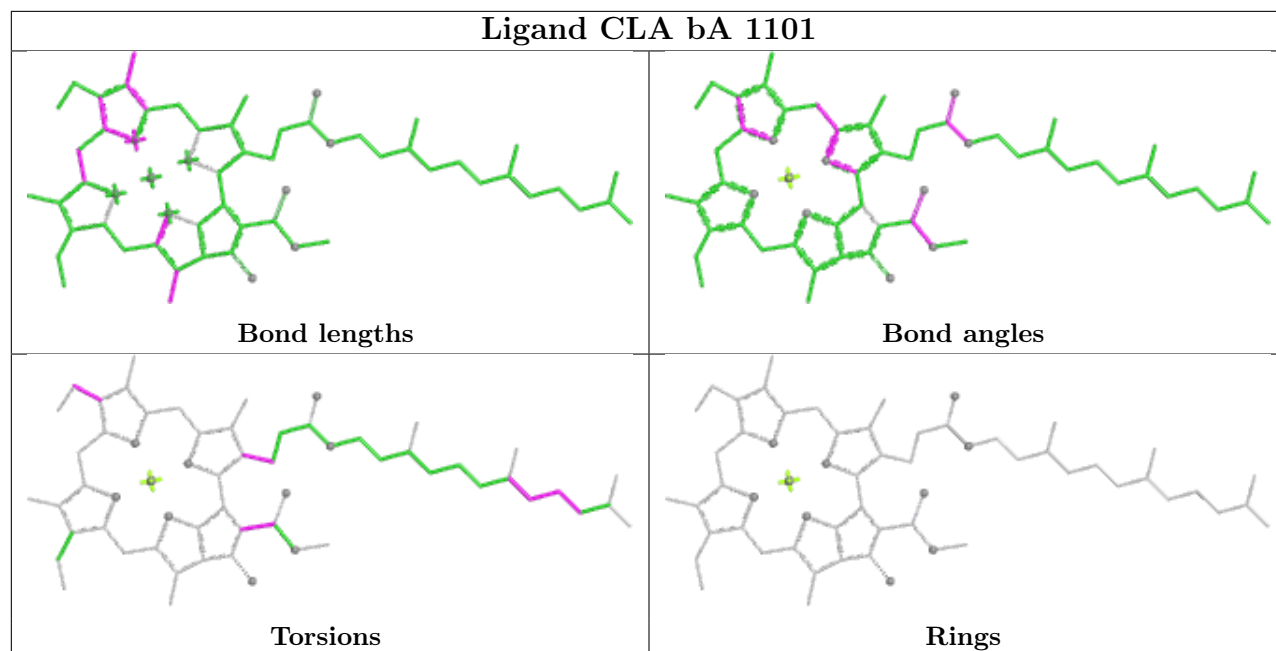
Ligand CLA n 502



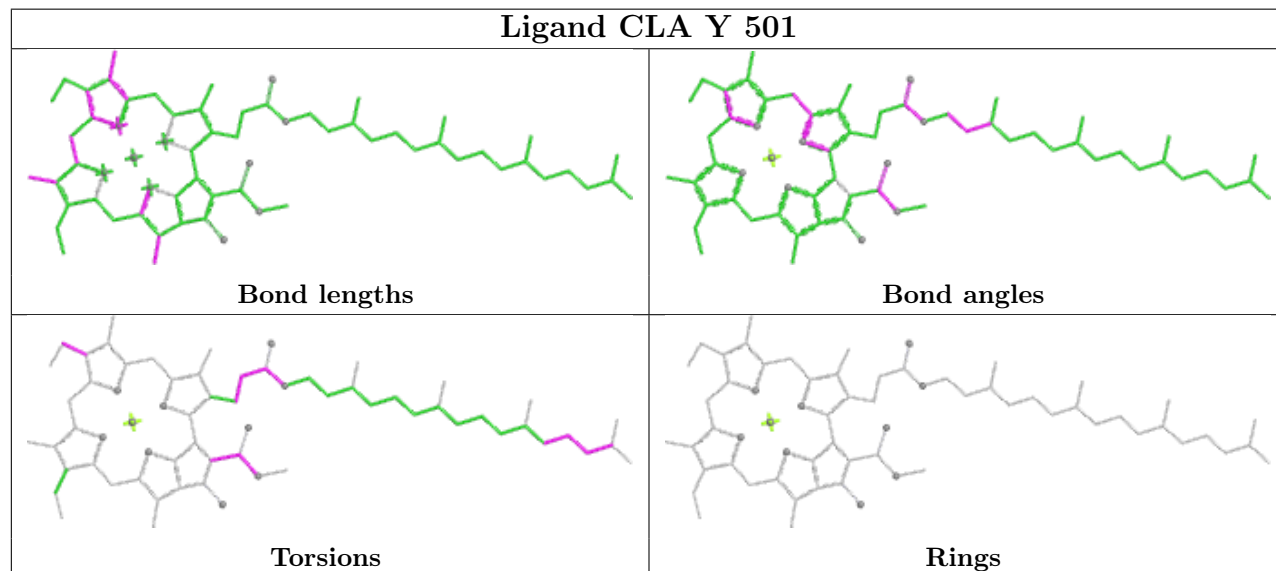
Ligand CLA aB 1222

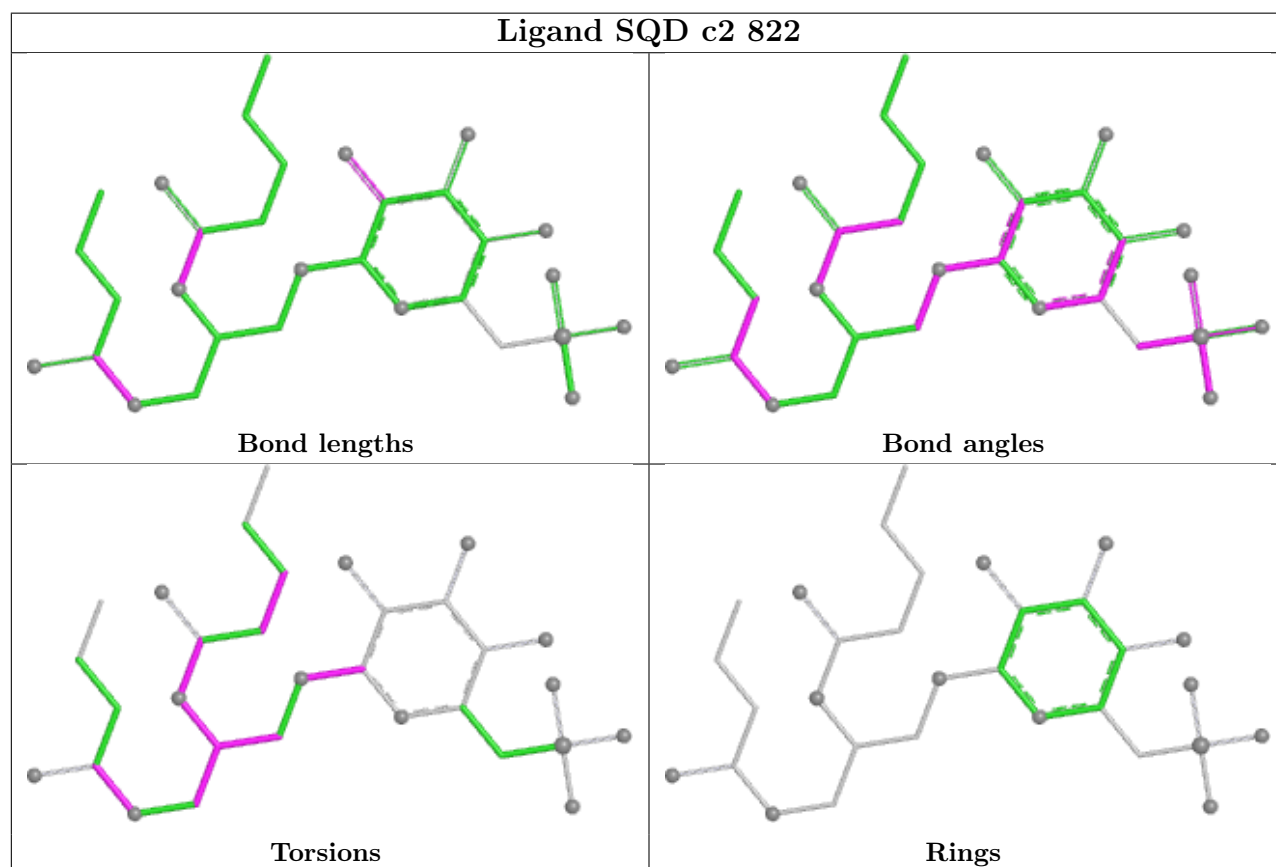
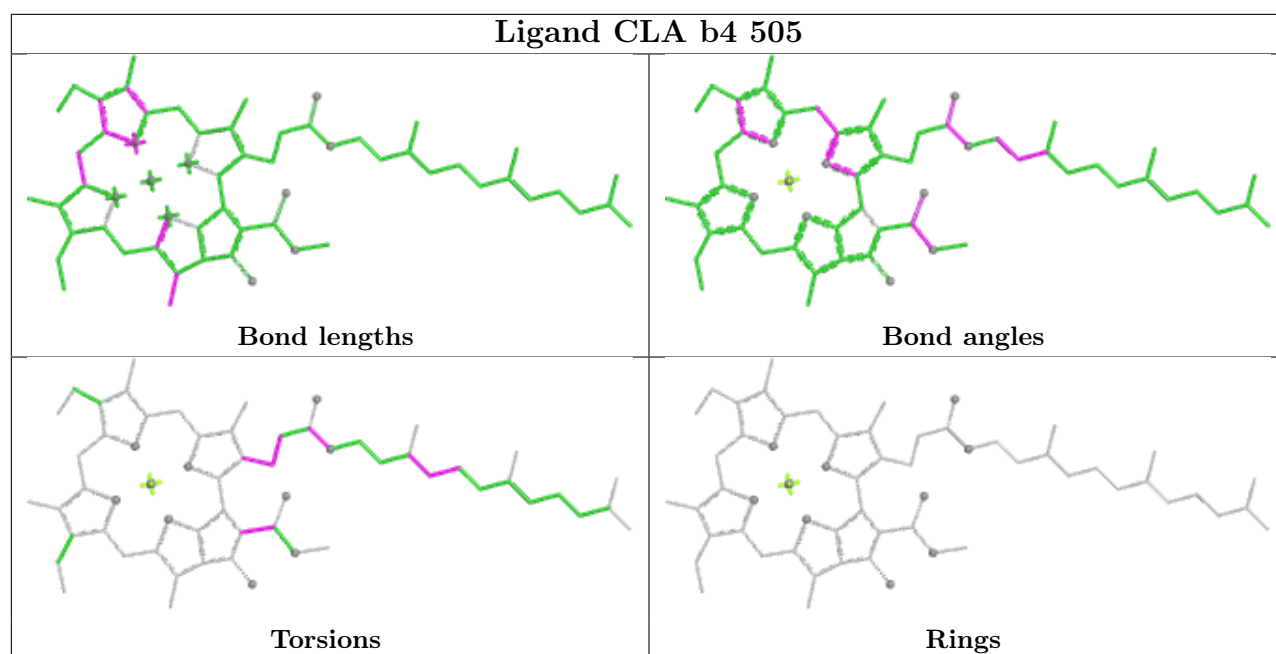


Ligand CLA bA 1101

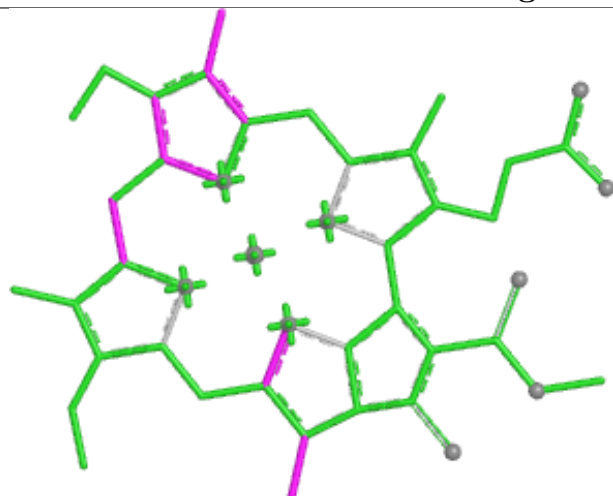


Ligand CLA Y 501

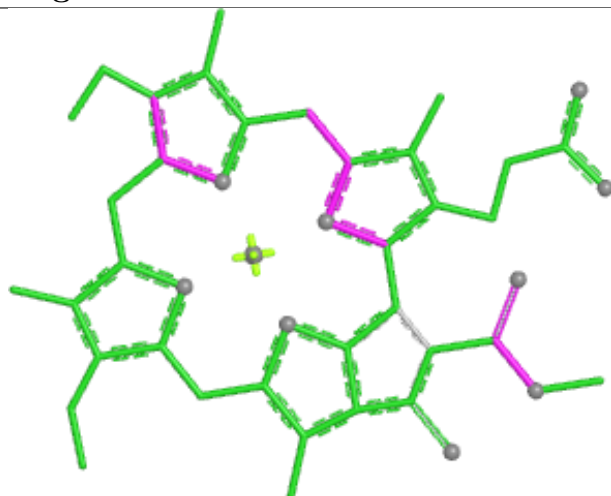




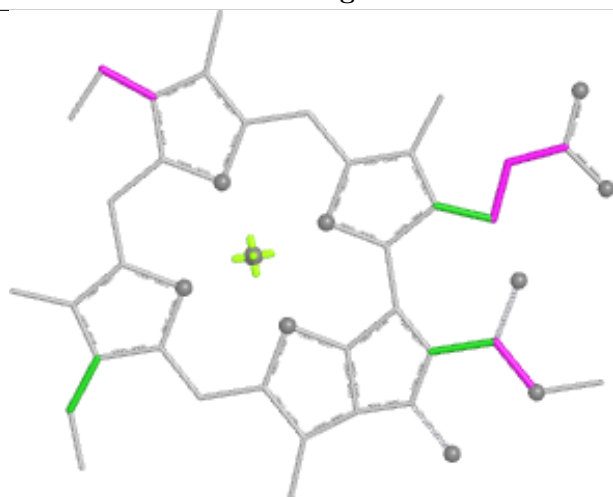
Ligand CLA g 504



Bond lengths



Bond angles

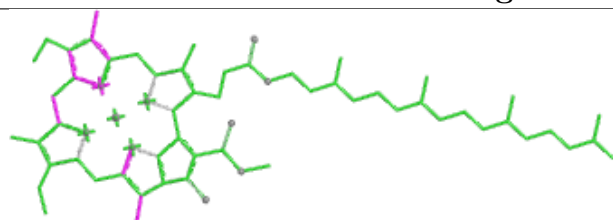


Torsions

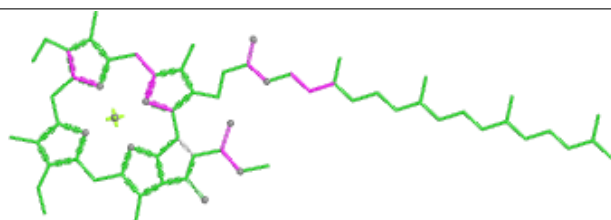


Rings

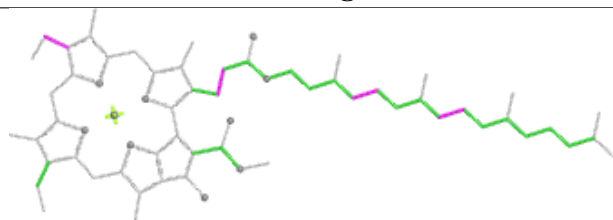
Ligand CLA bB 1238



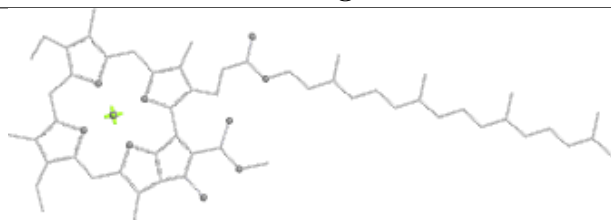
Bond lengths



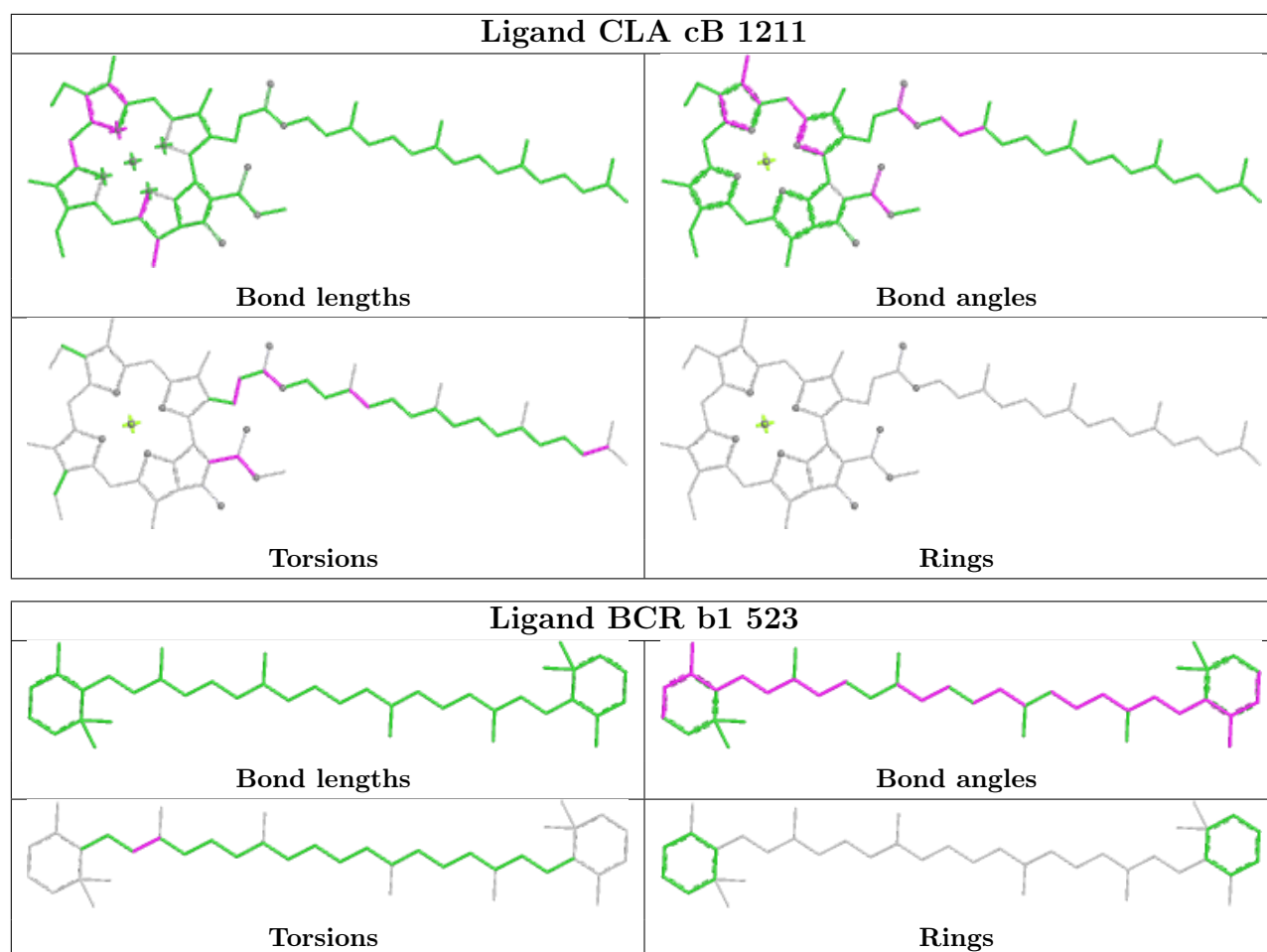
Bond angles



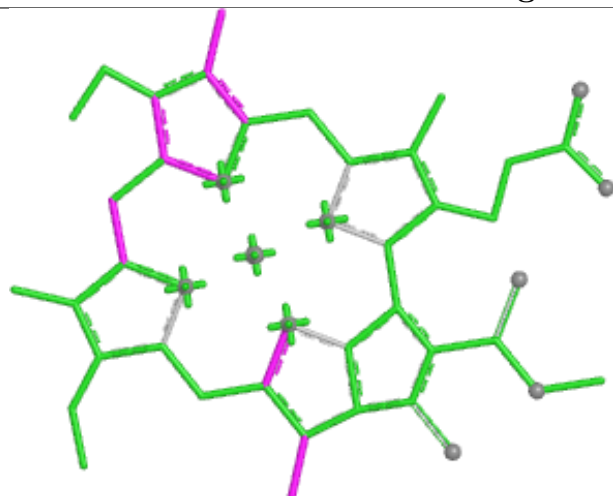
Torsions



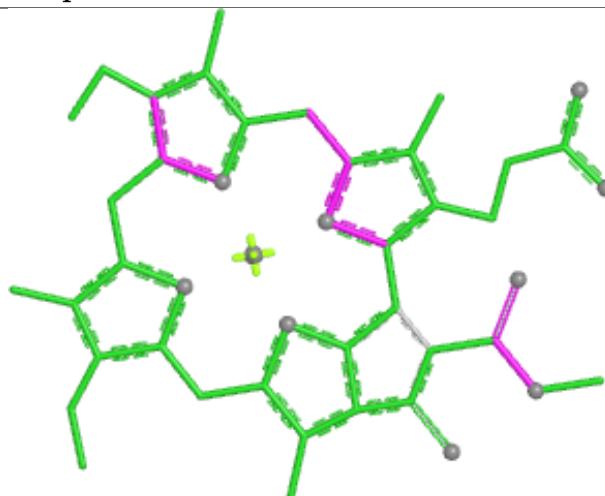
Rings



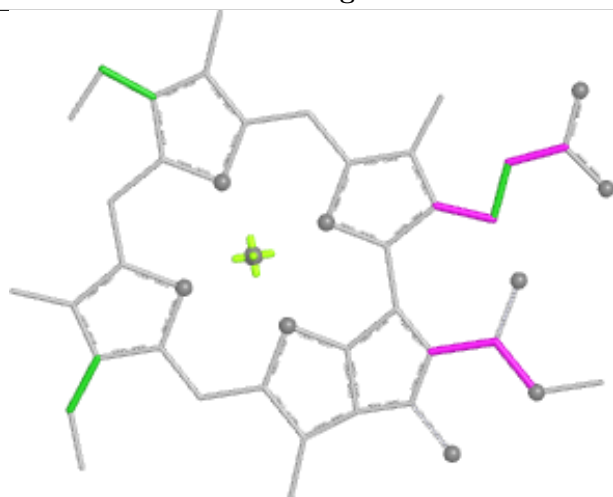
Ligand CLA q 511



Bond lengths



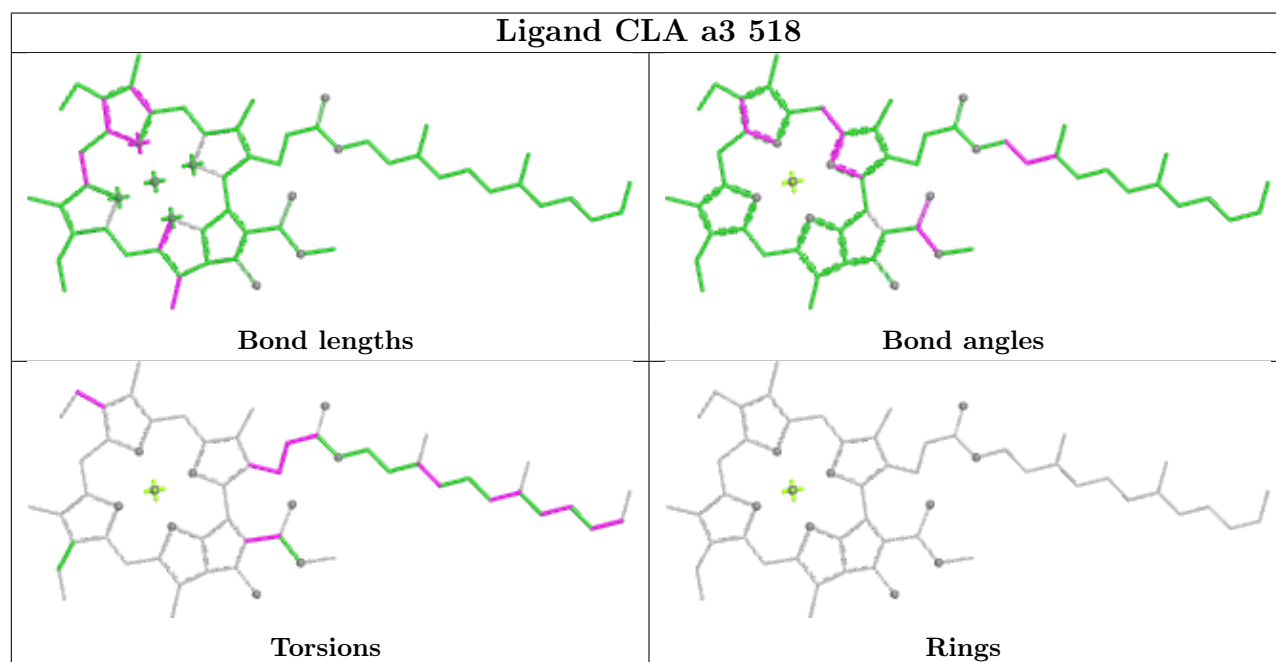
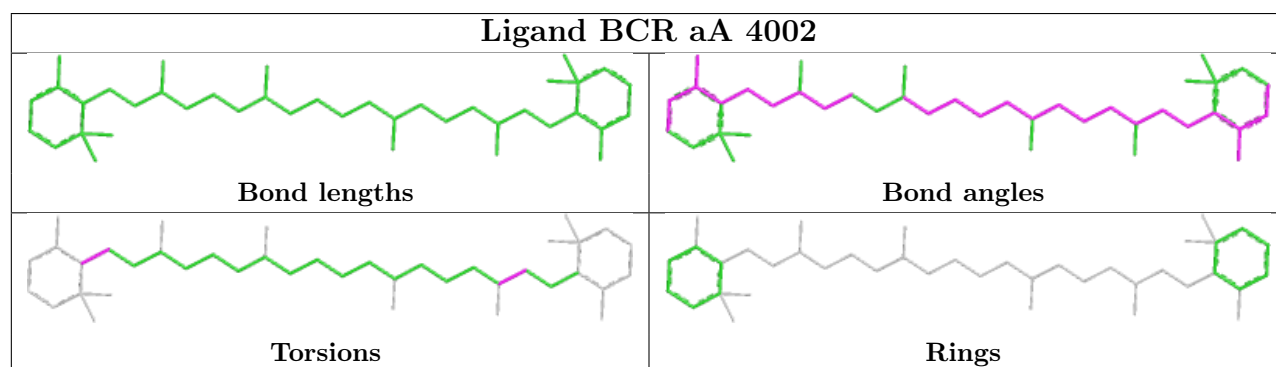
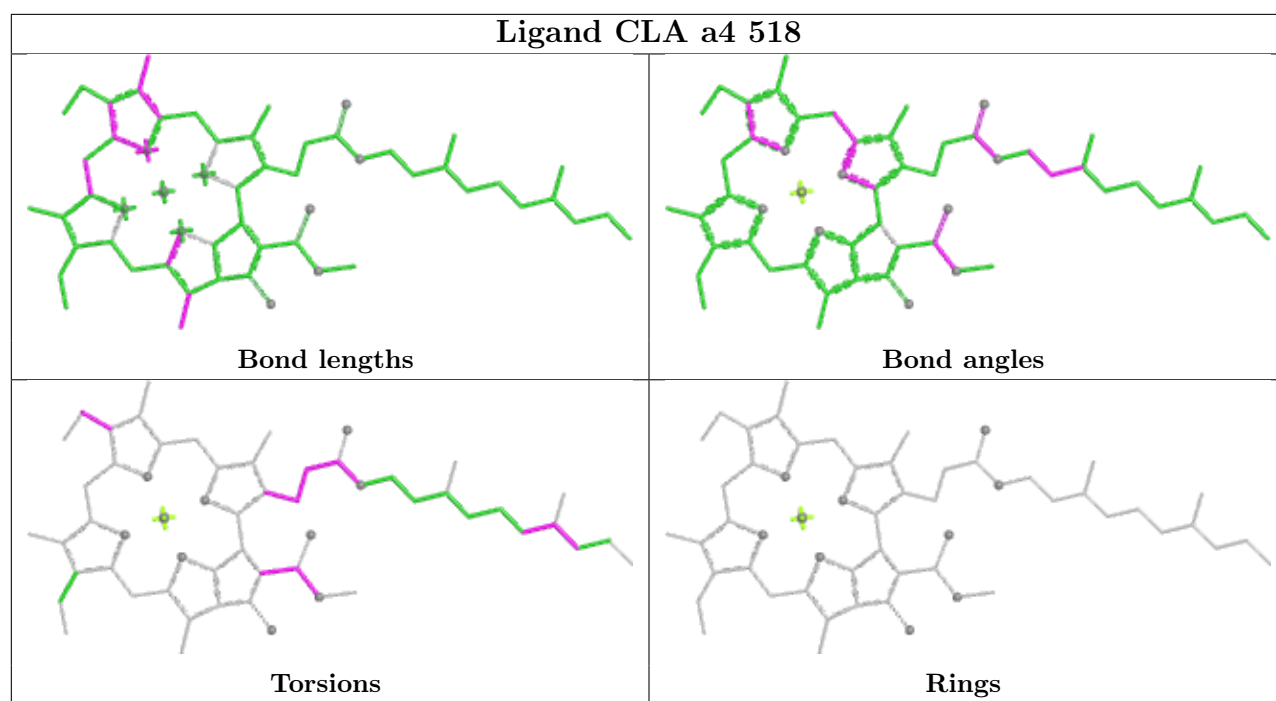
Bond angles

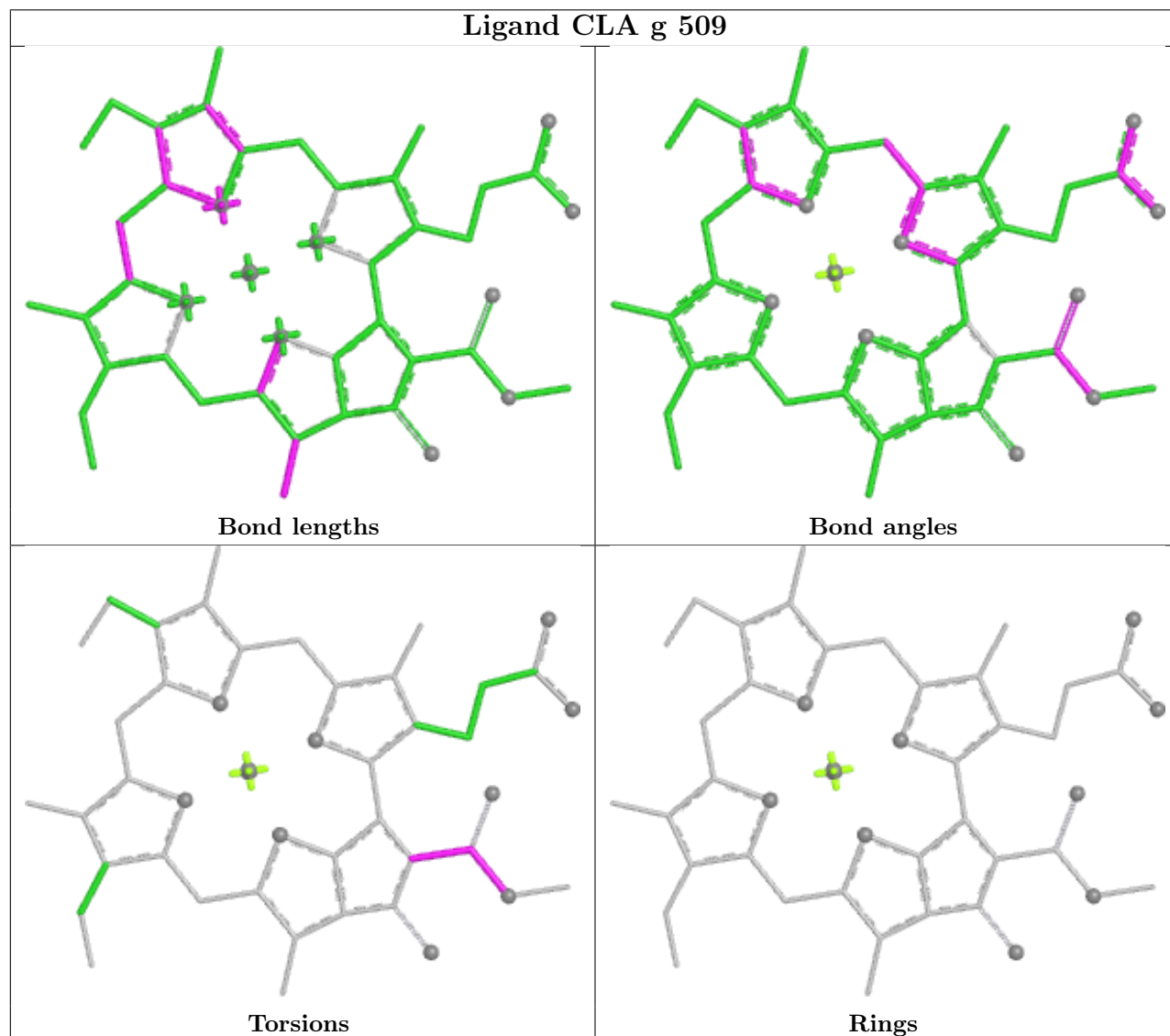
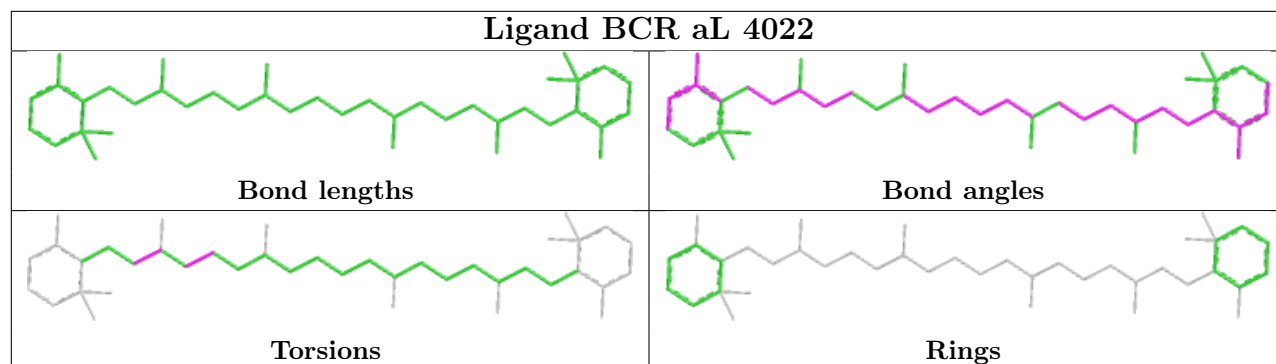


Torsions

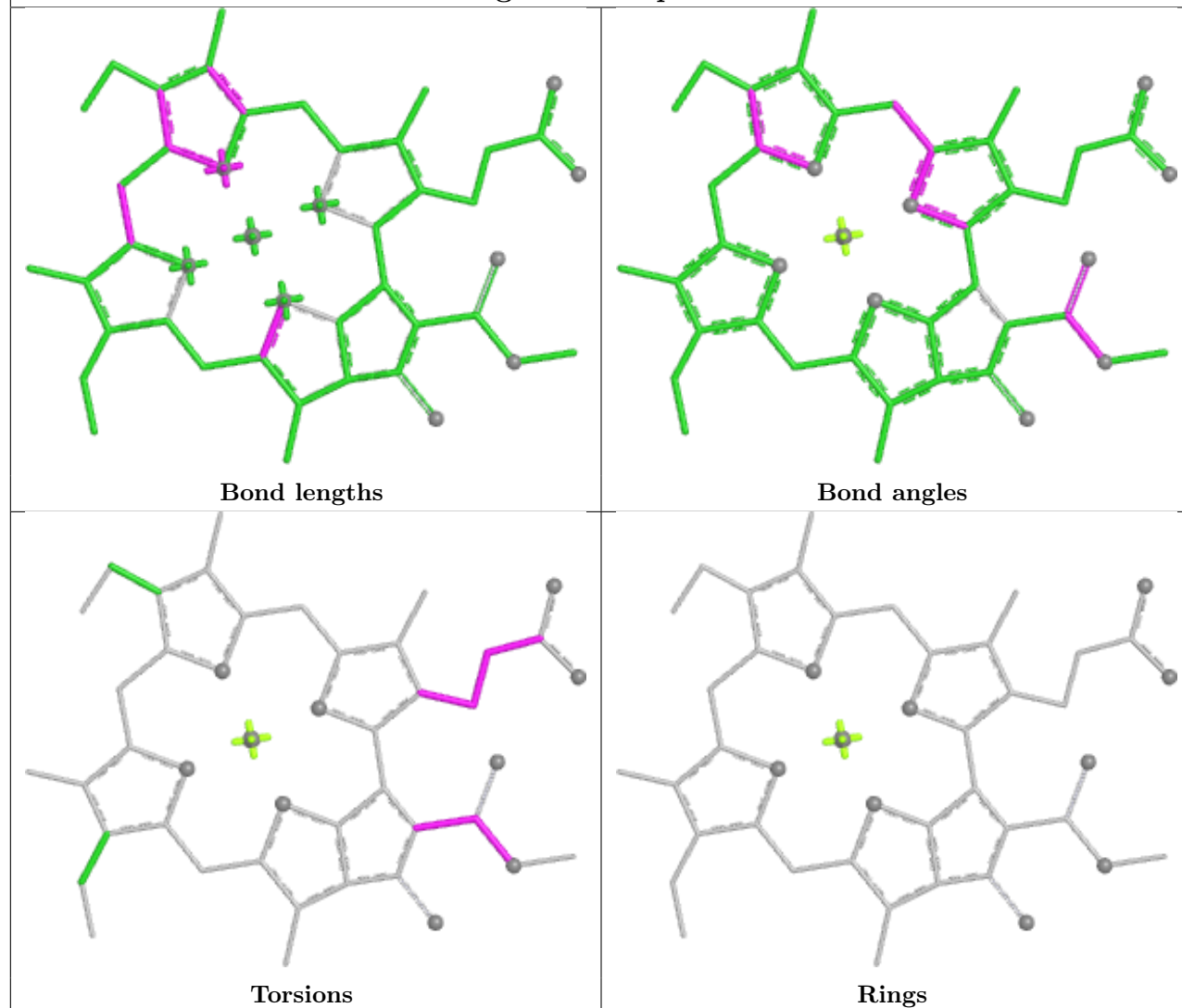


Rings

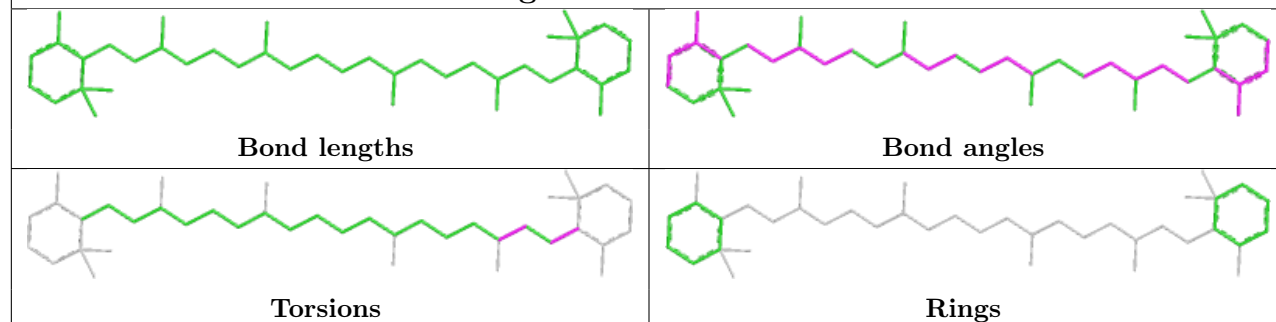


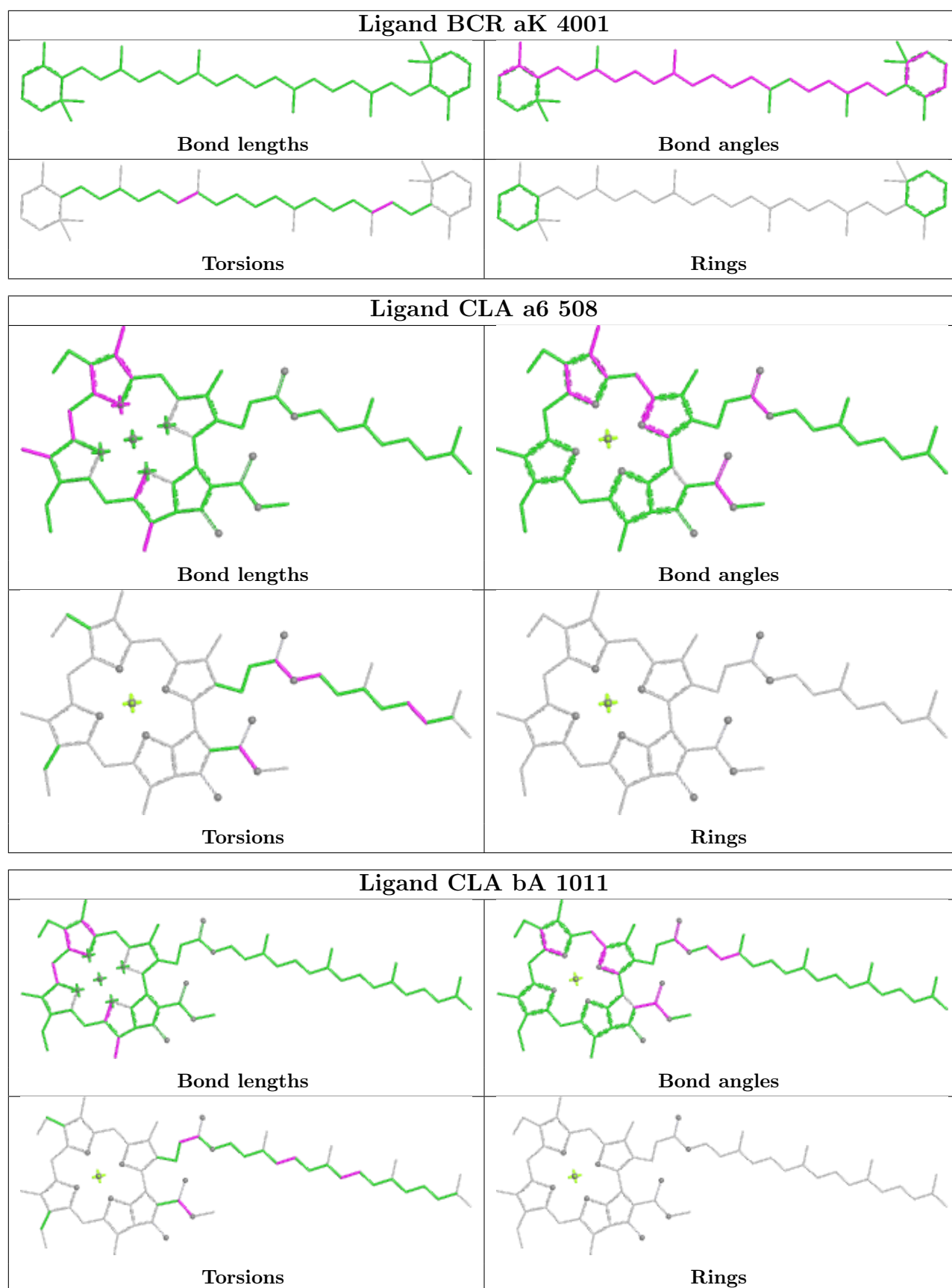


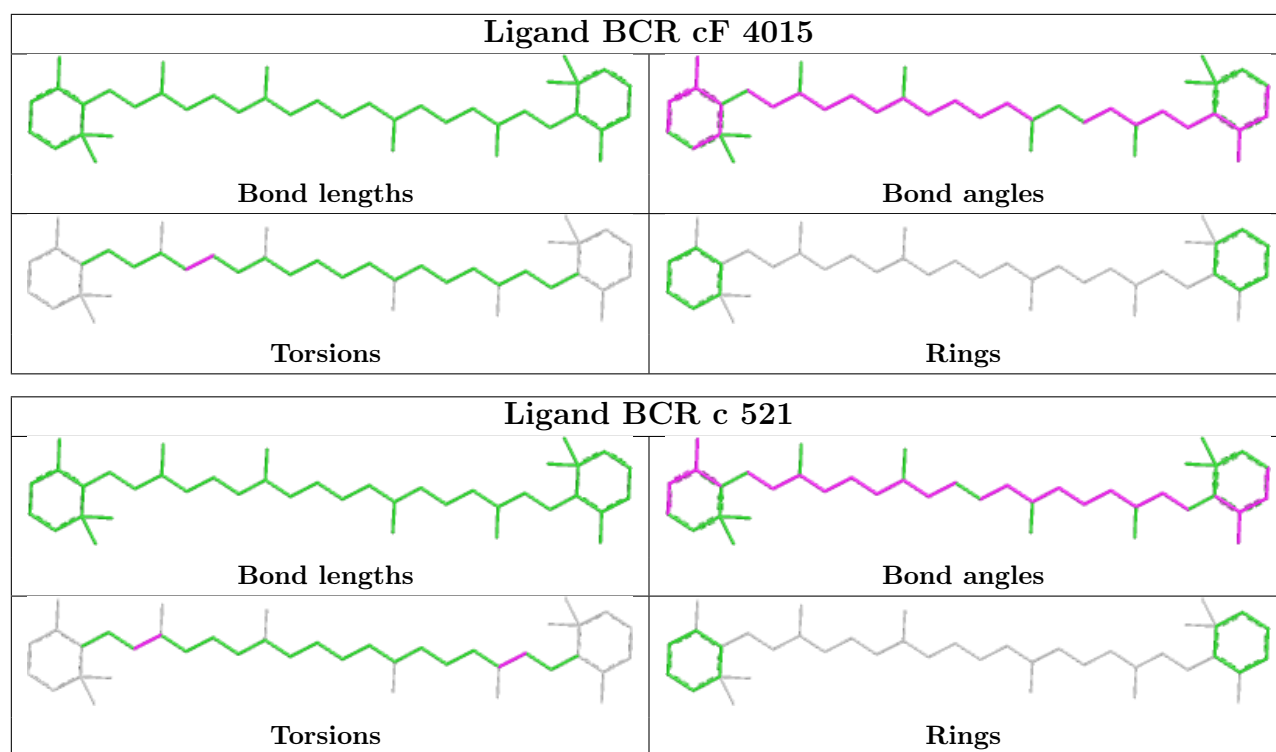
Ligand CLA p 513



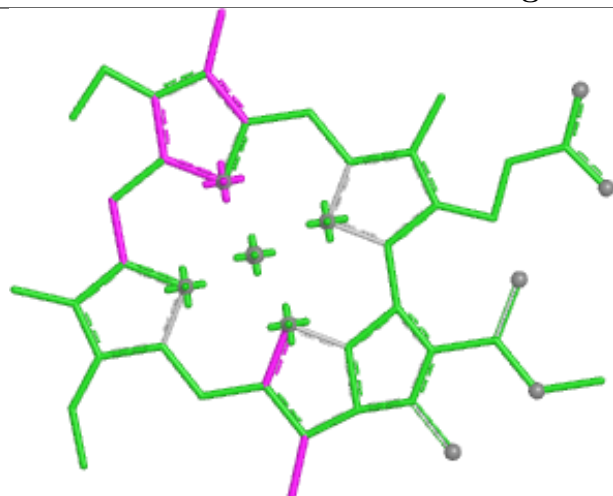
Ligand BCR aI 4019



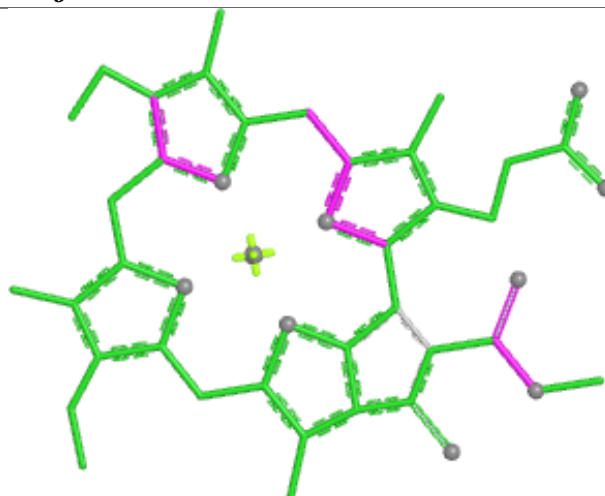




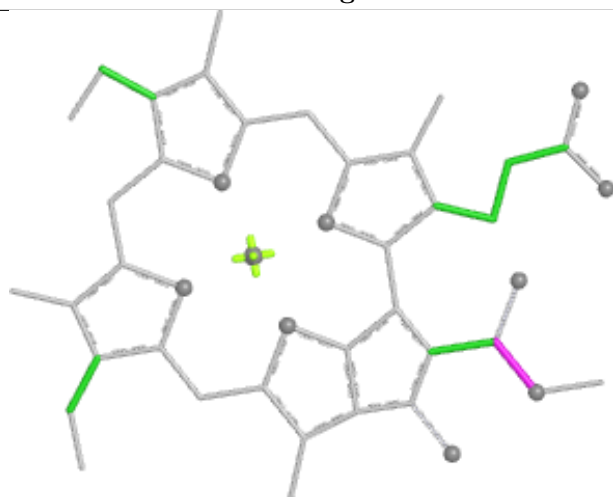
Ligand CLA j 502



Bond lengths



Bond angles

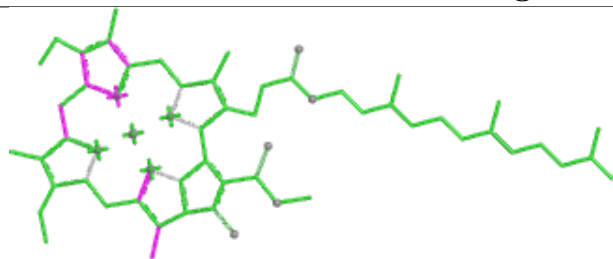


Torsions

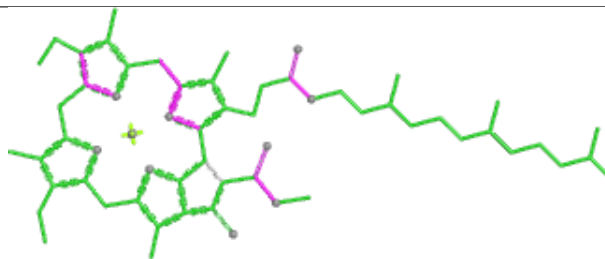


Rings

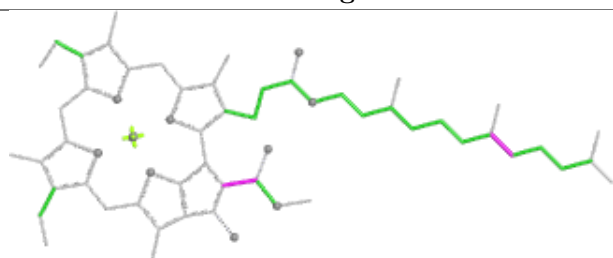
Ligand CLA Y 507



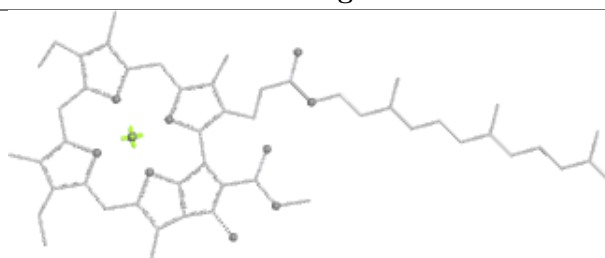
Bond lengths



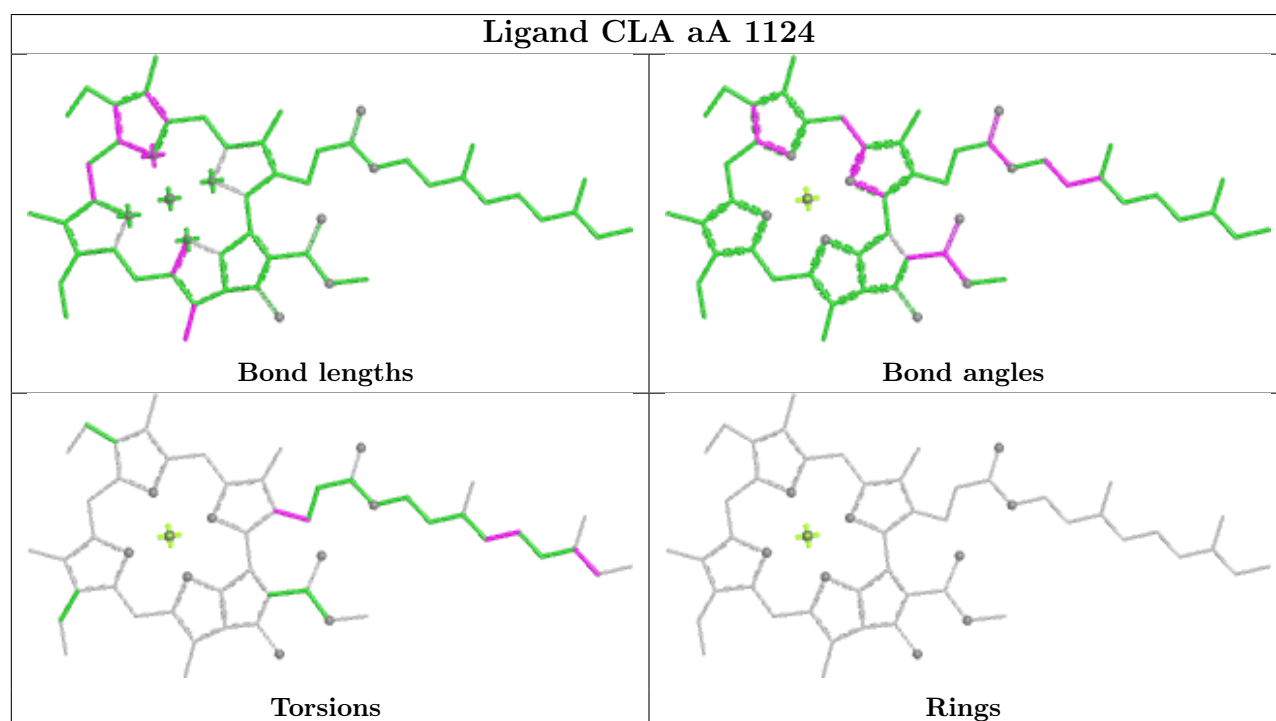
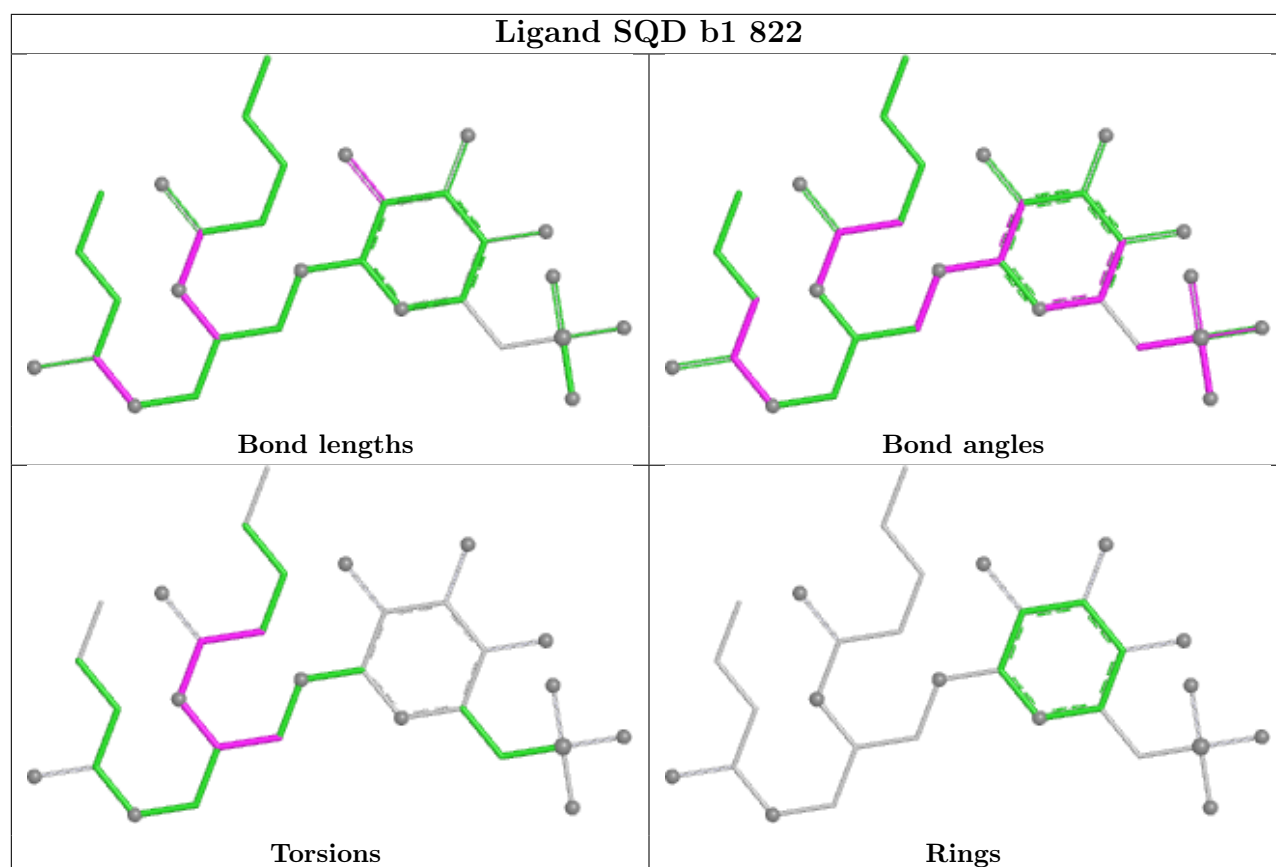
Bond angles

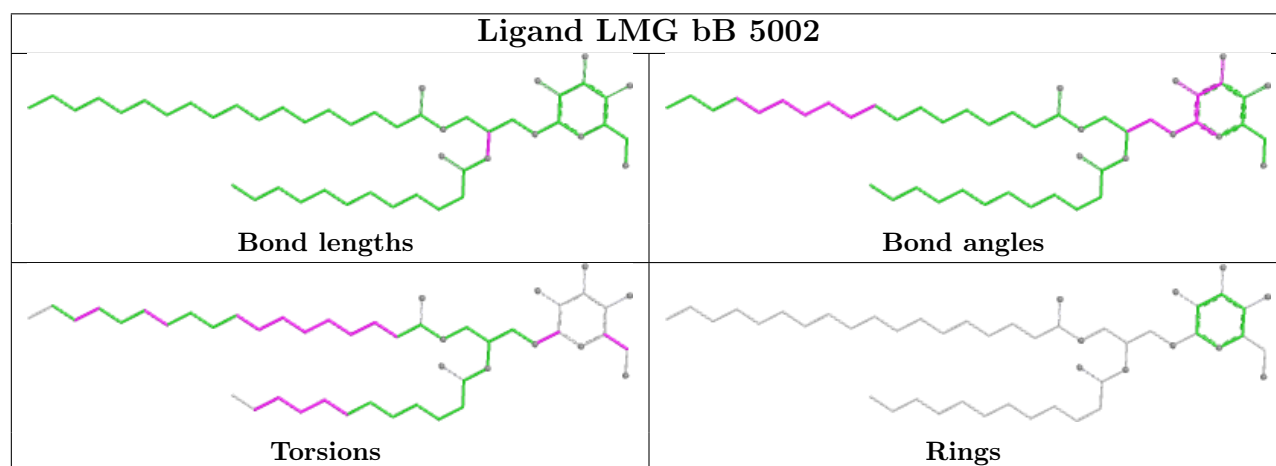
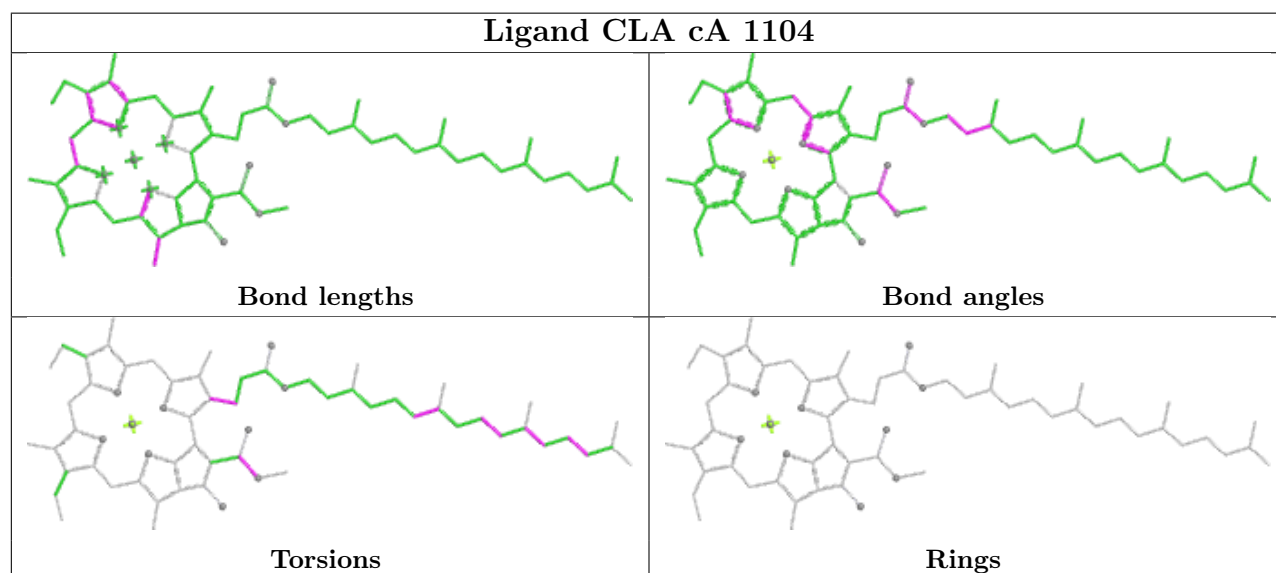
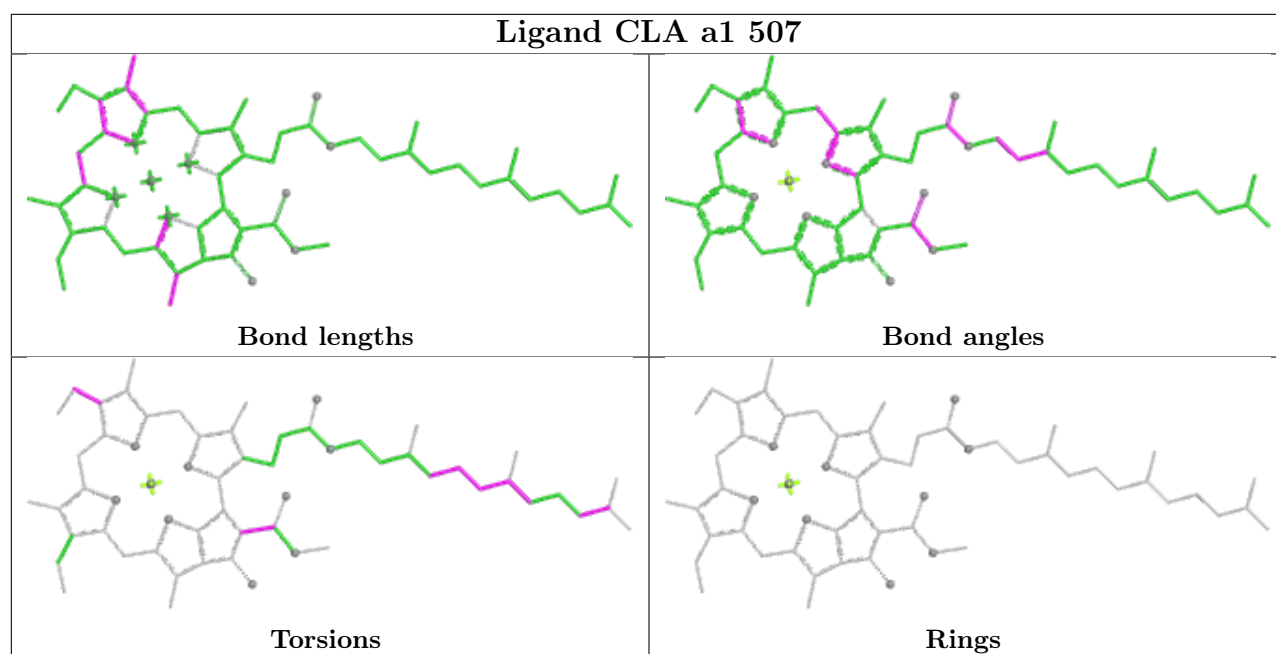


Torsions

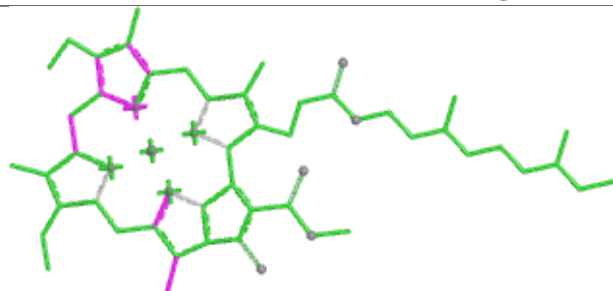


Rings

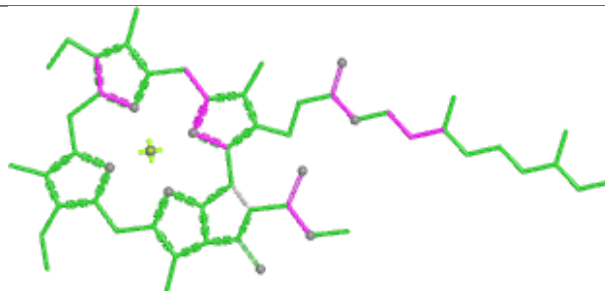




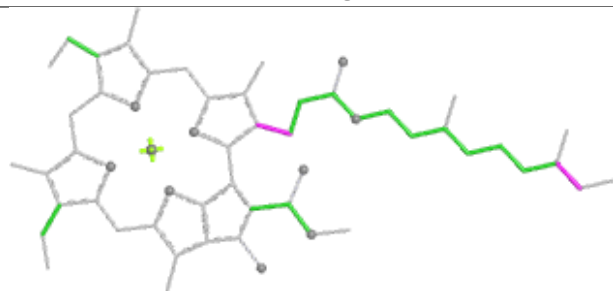
Ligand CLA bA 1124



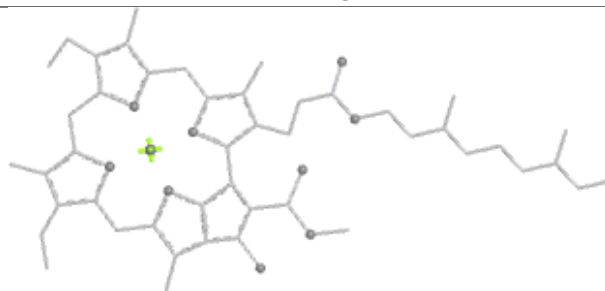
Bond lengths



Bond angles

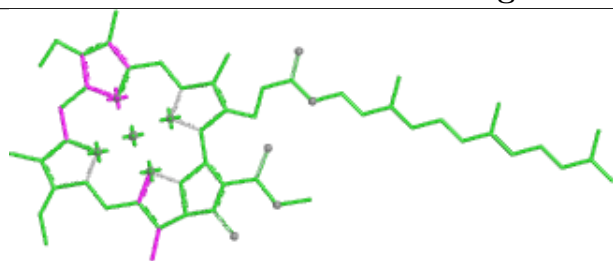


Torsions

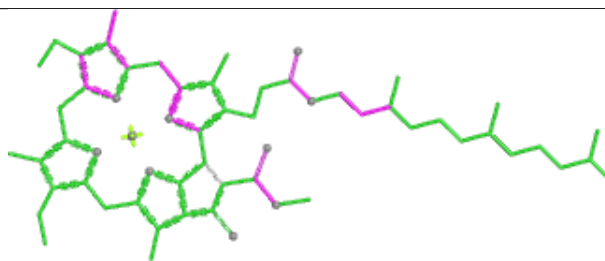


Rings

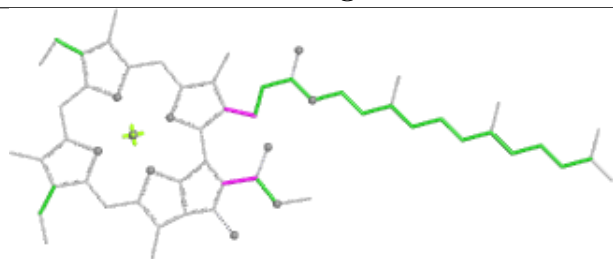
Ligand CLA cB 1222



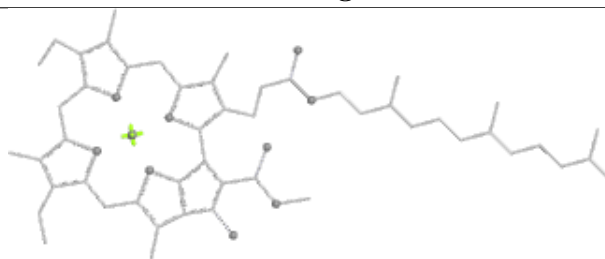
Bond lengths



Bond angles

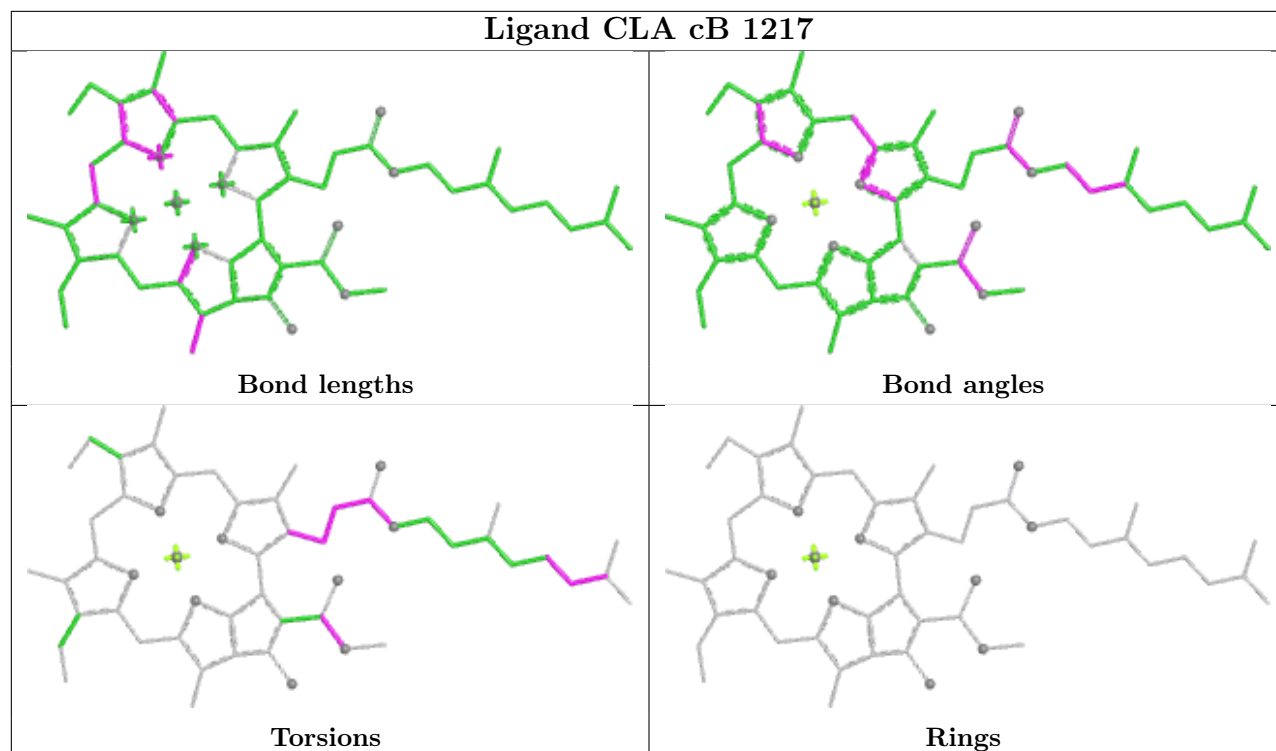


Torsions

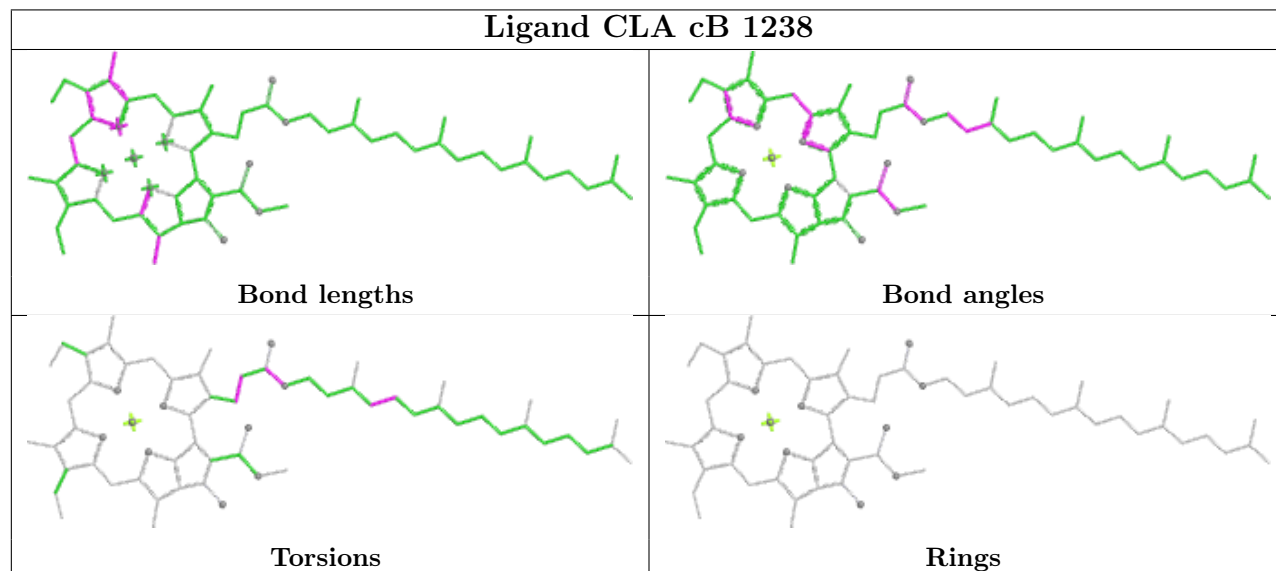


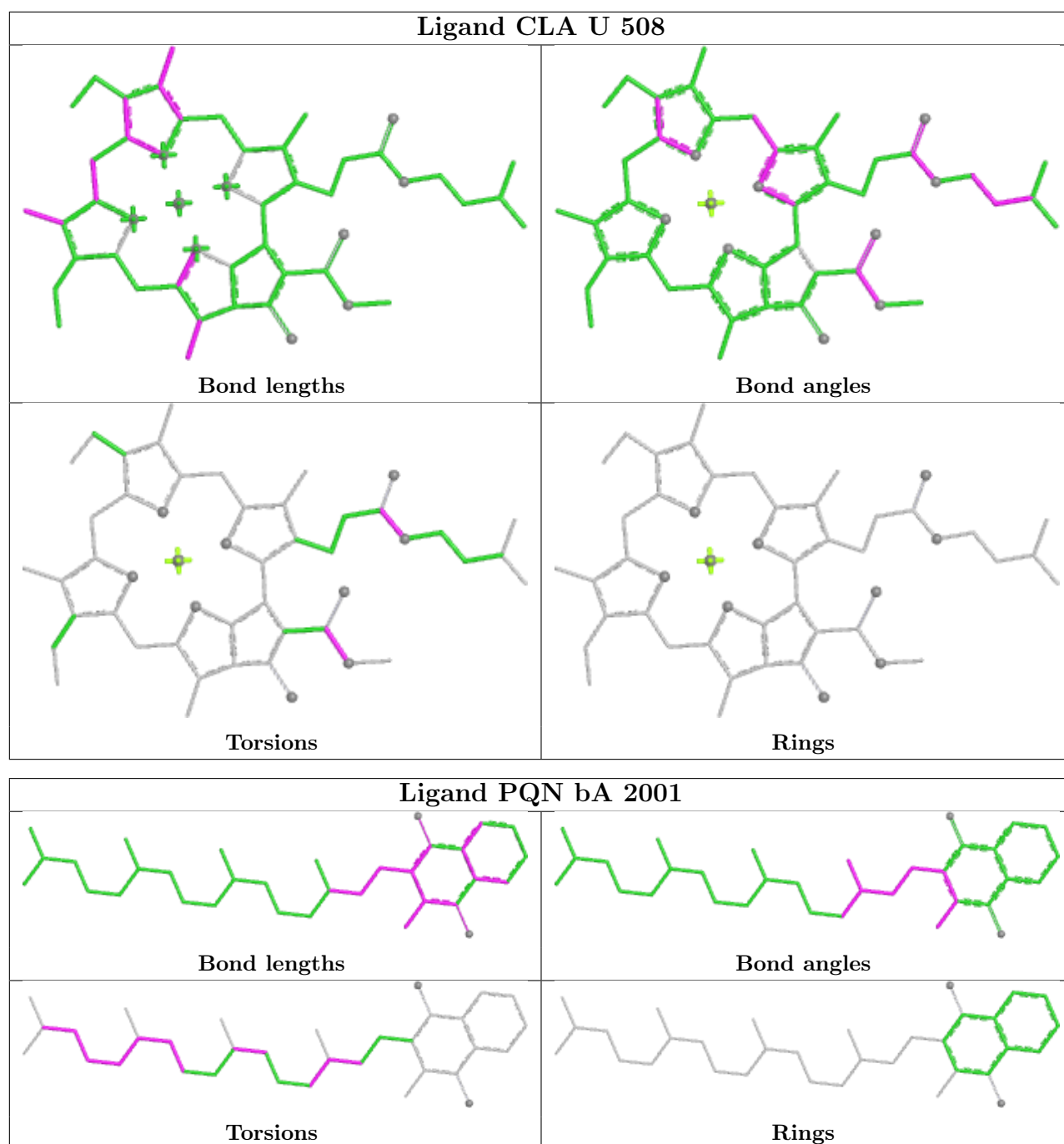
Rings

Ligand CLA cB 1217

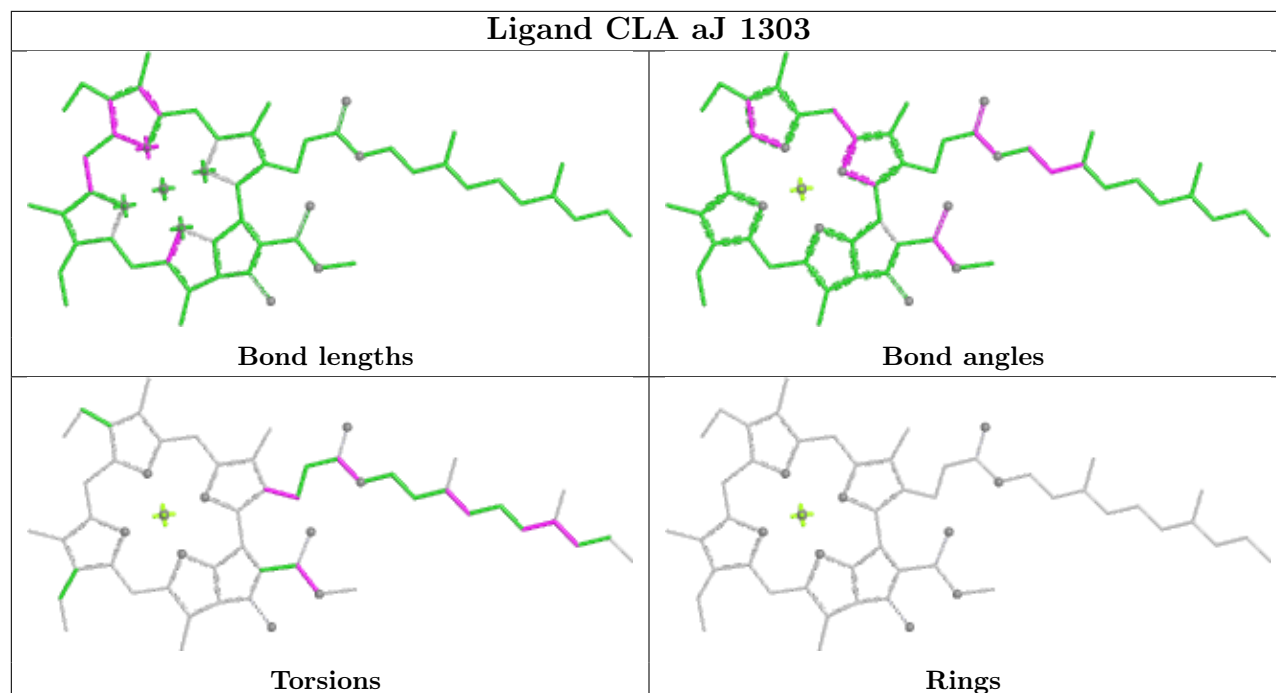


Ligand CLA cB 1238

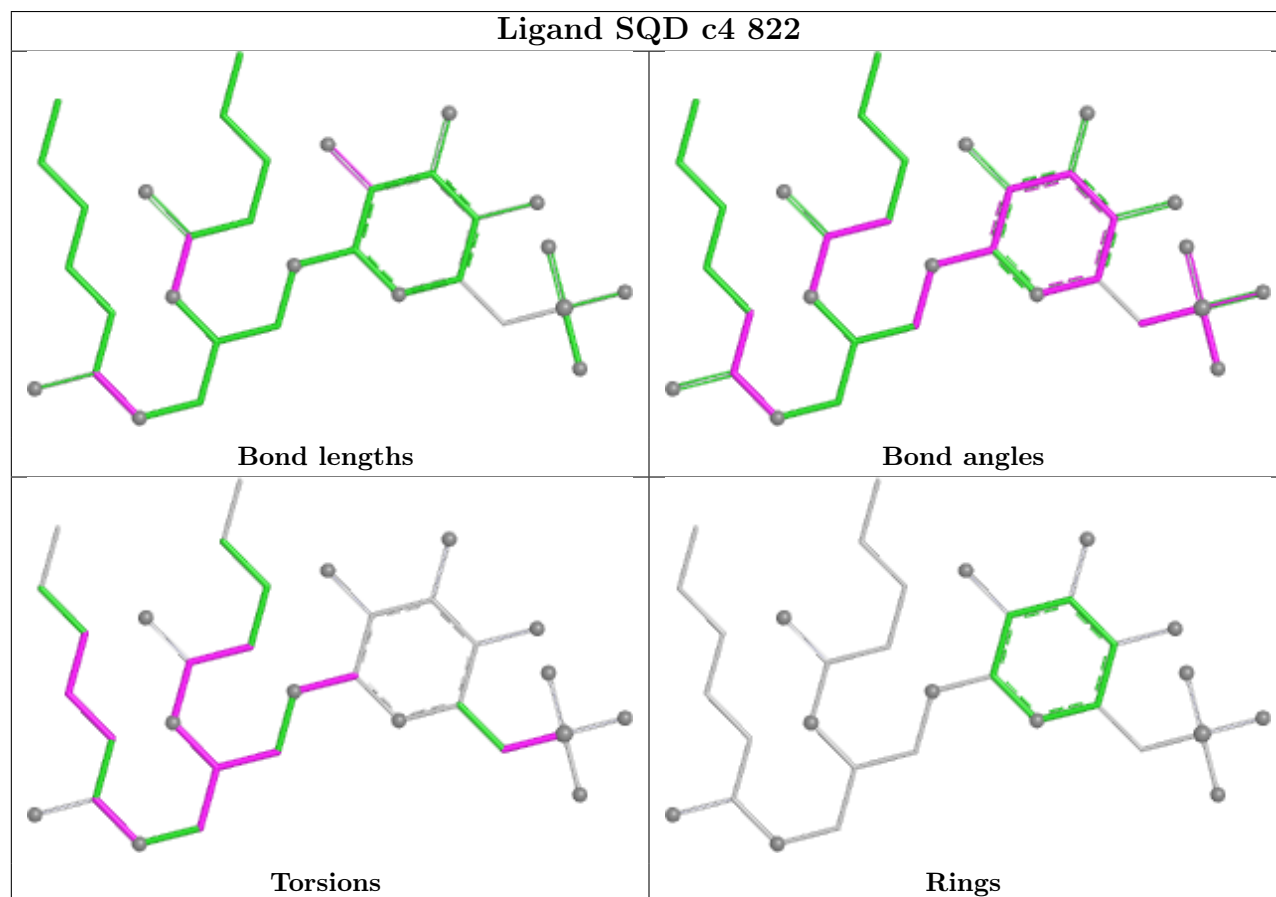


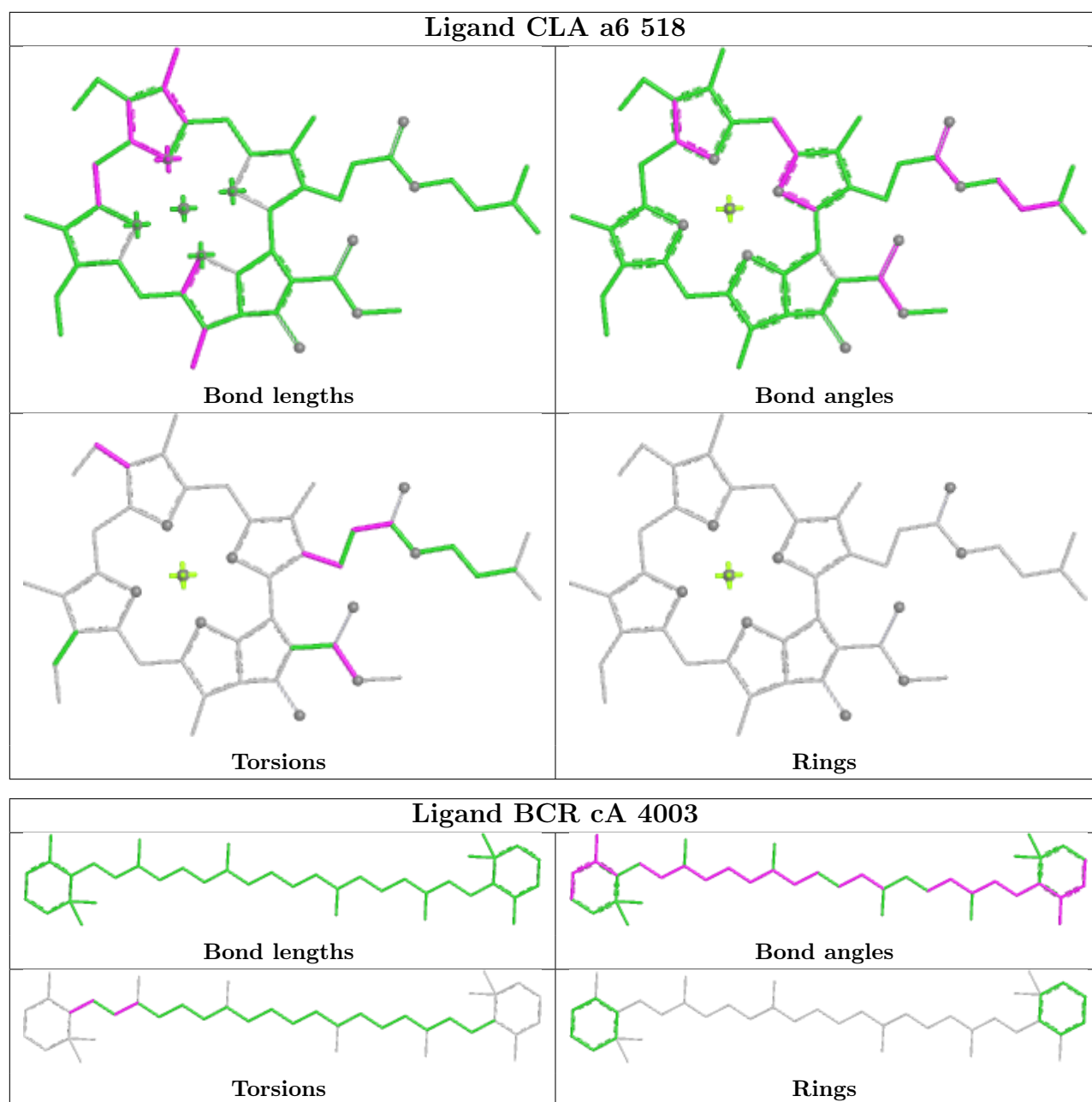


Ligand CLA aJ 1303

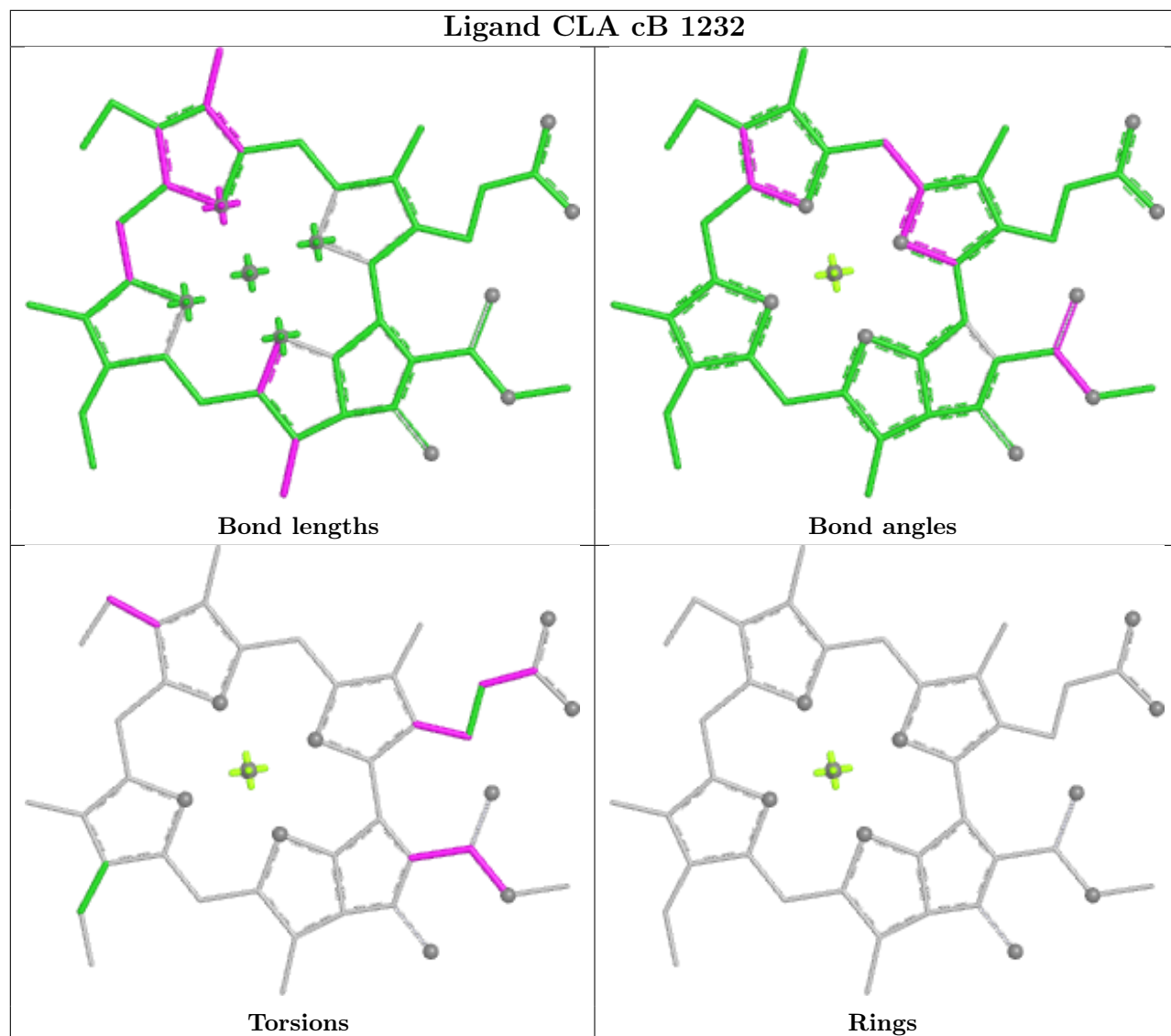


Ligand SQD c4 822

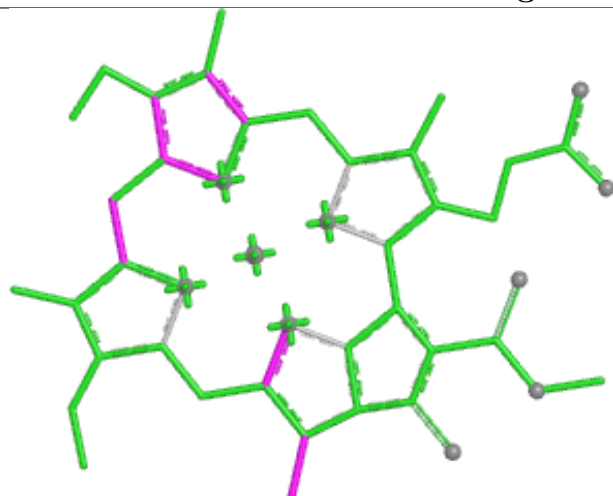




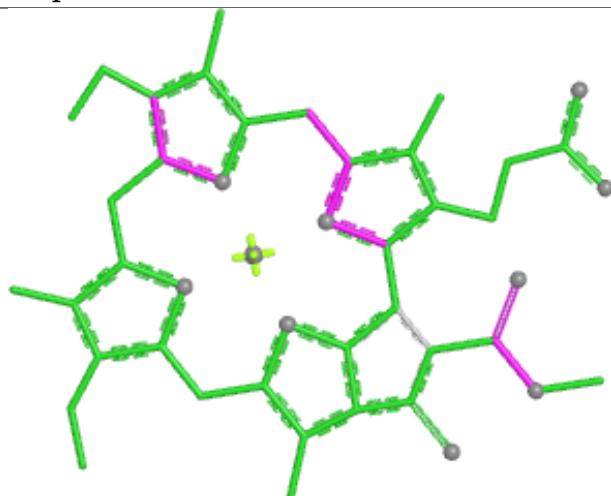
Ligand CLA cB 1232



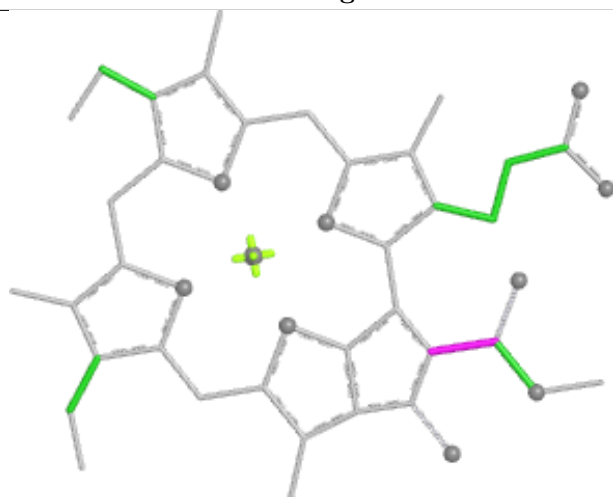
Ligand CLA p 503



Bond lengths



Bond angles

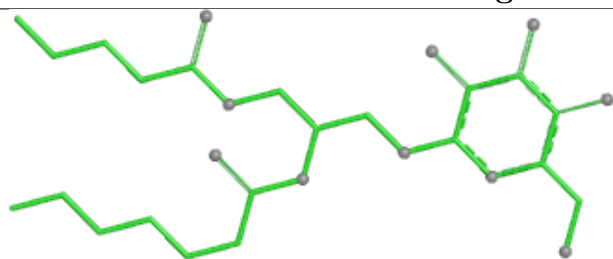


Torsions

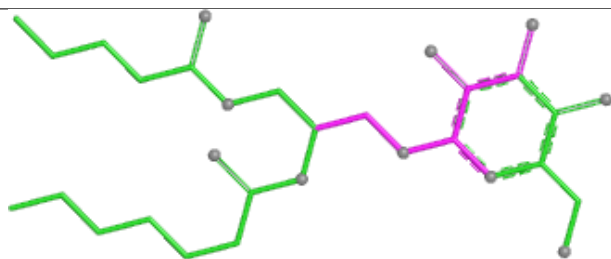


Rings

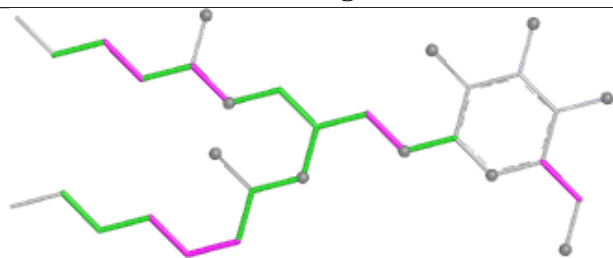
Ligand LMG aJ 5104



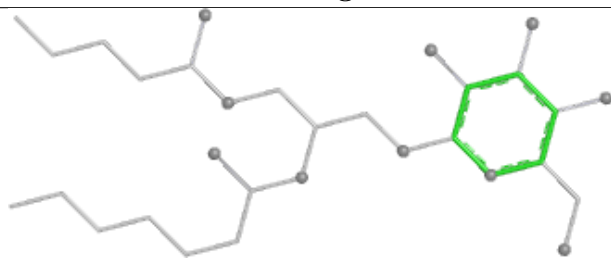
Bond lengths



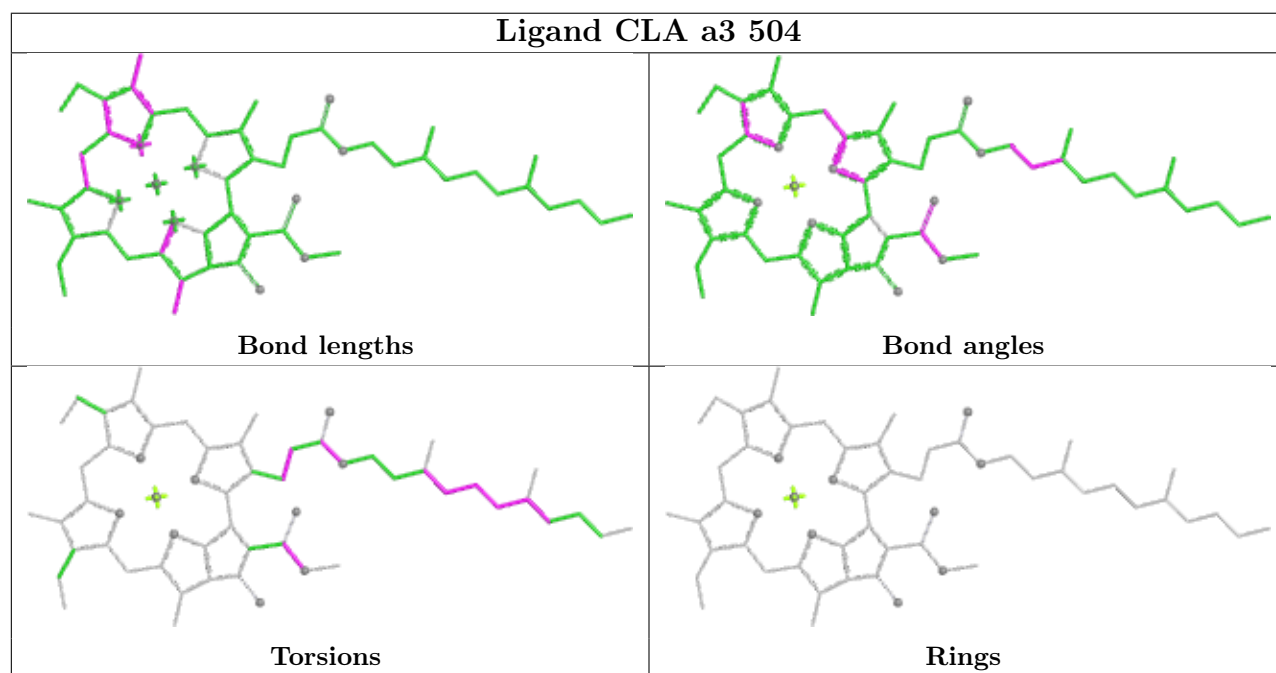
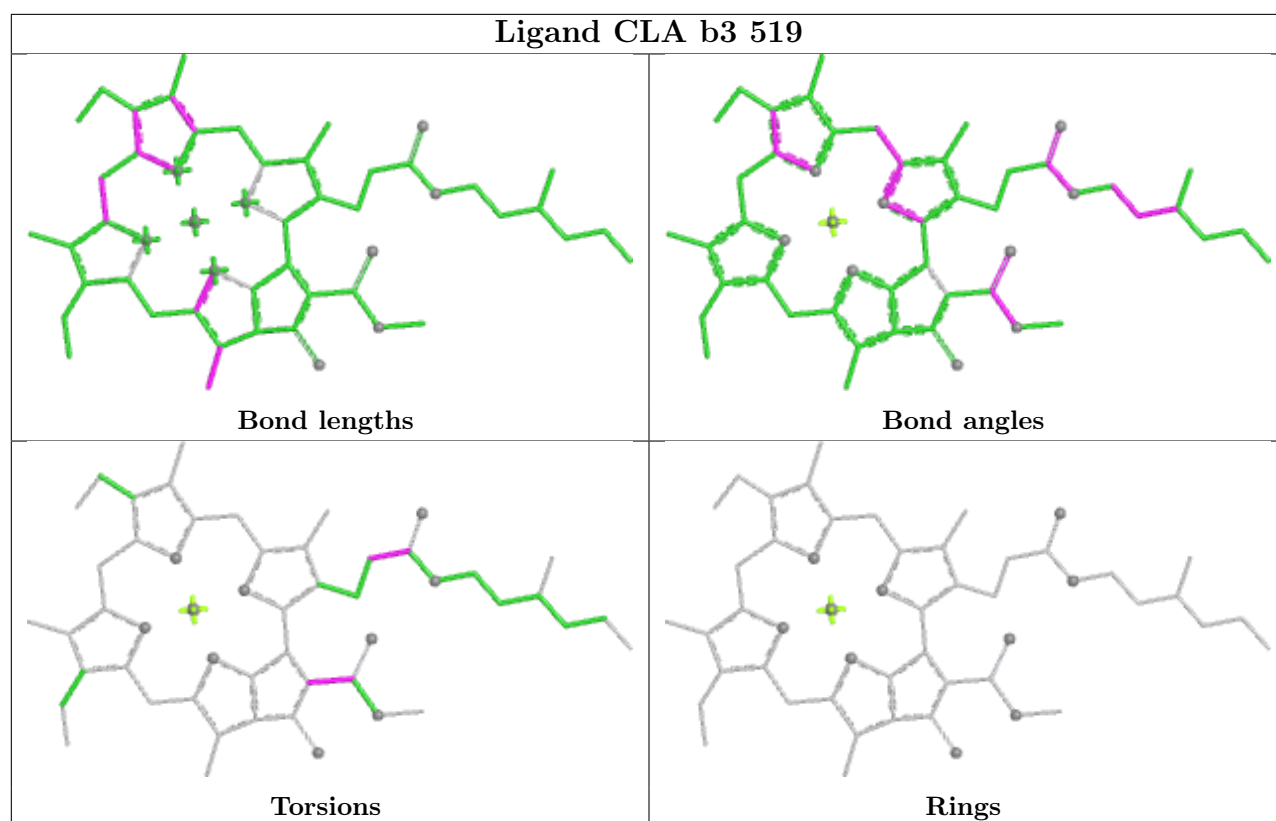
Bond angles



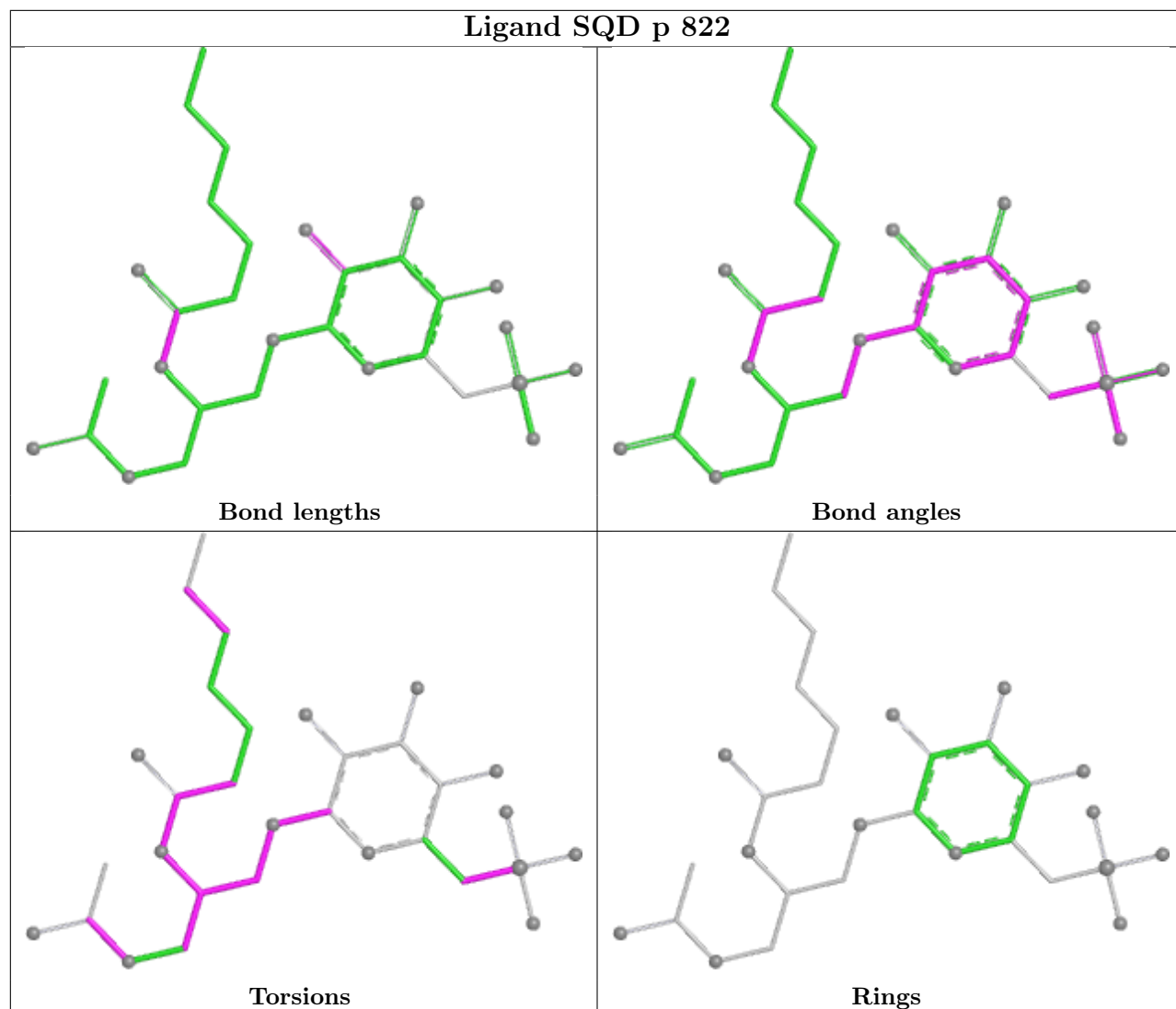
Torsions

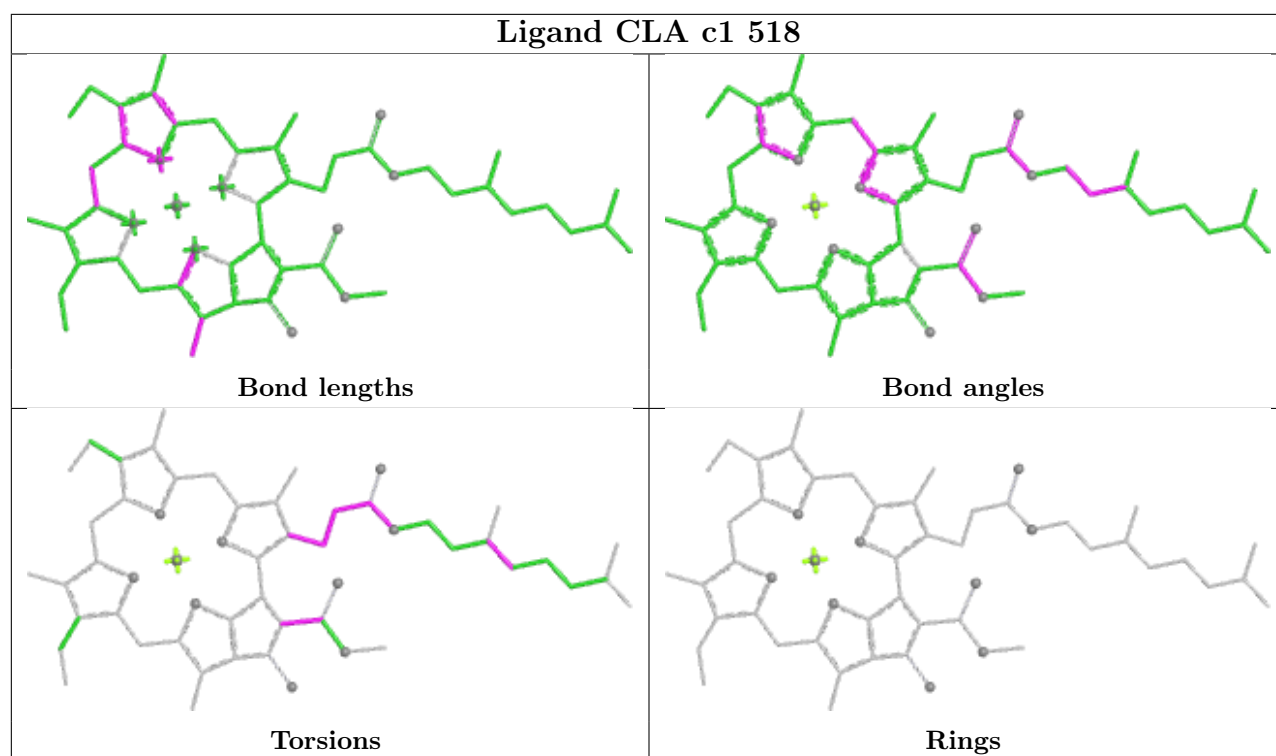


Rings

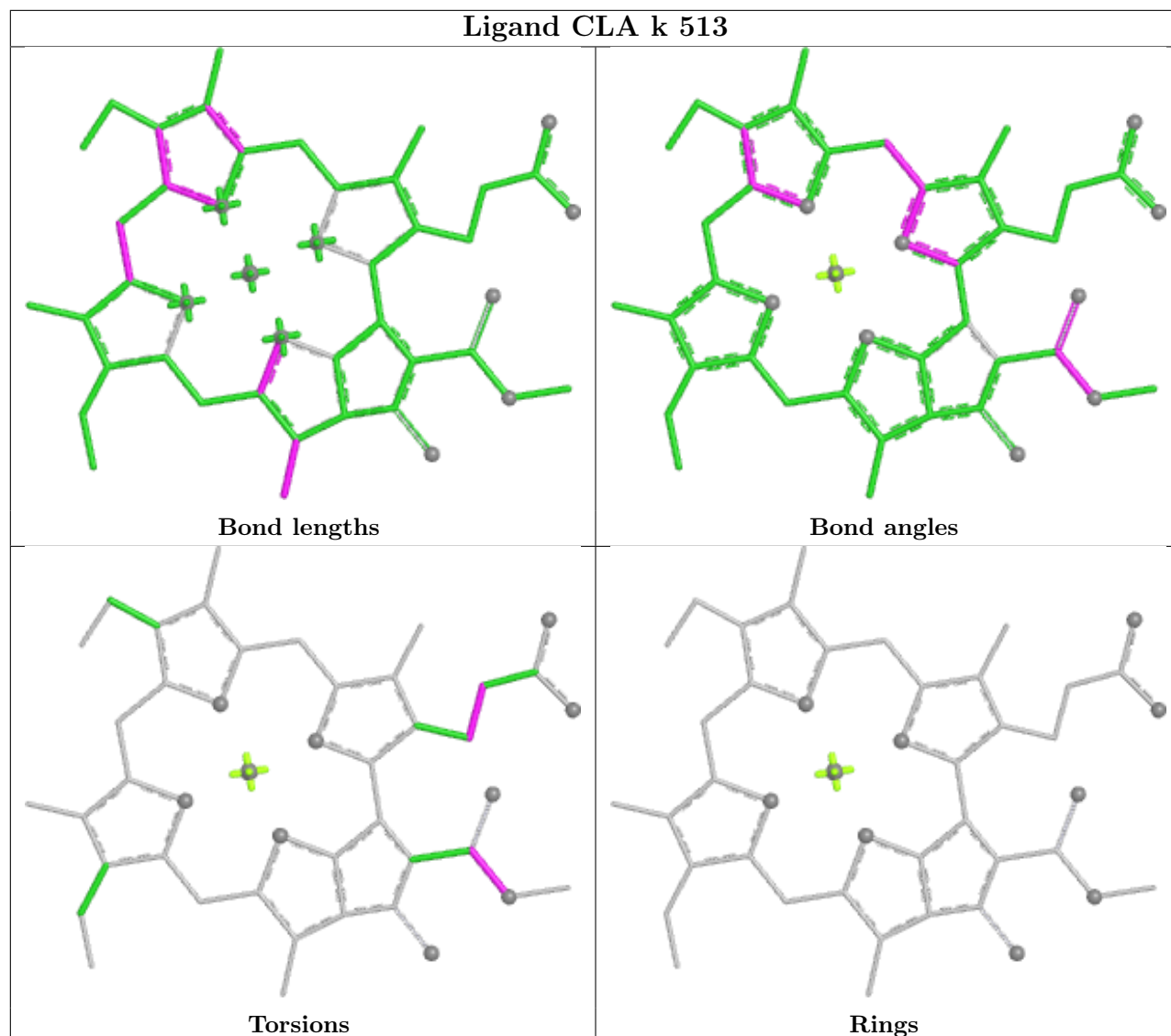


Ligand SQD p 822

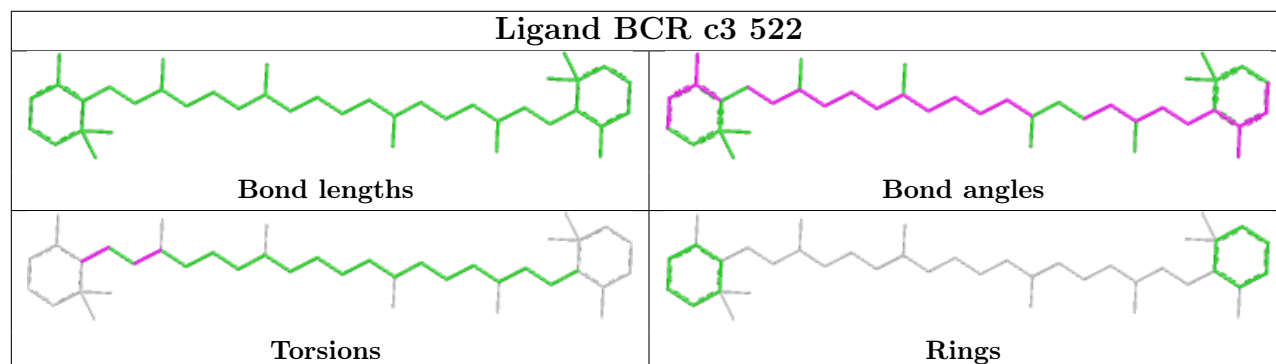


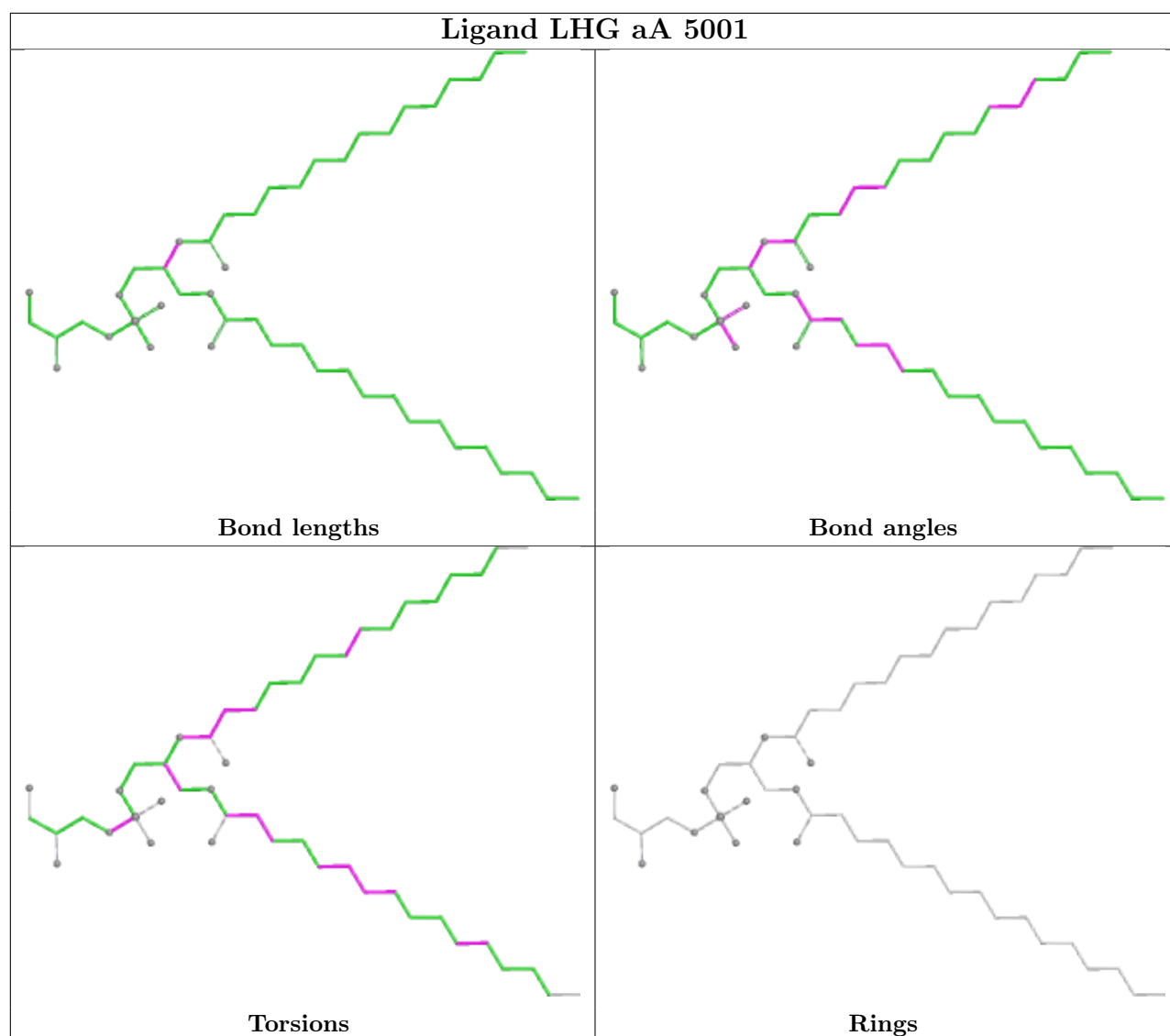


Ligand CLA k 513

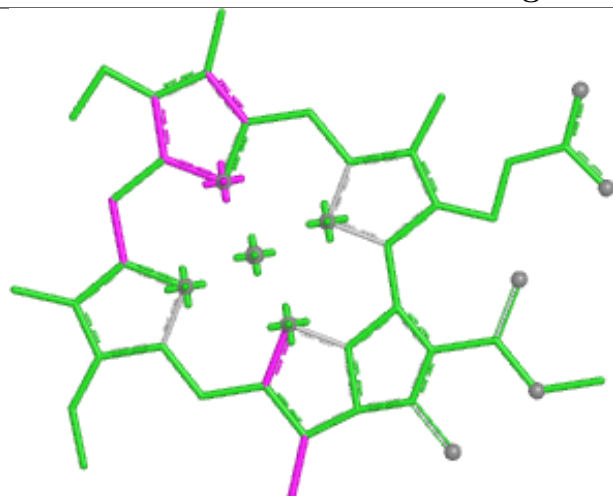


Ligand BCR c3 522

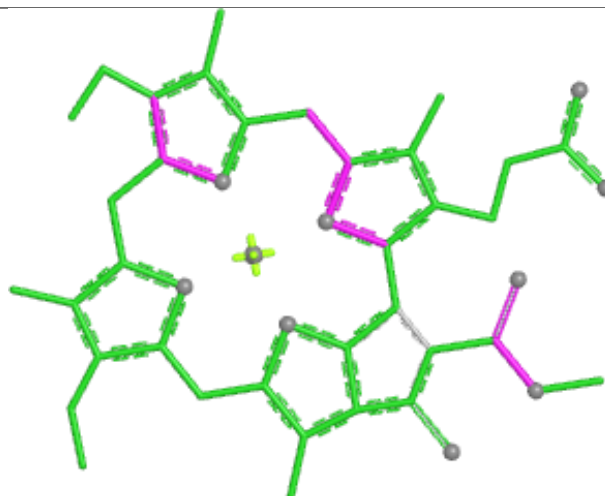




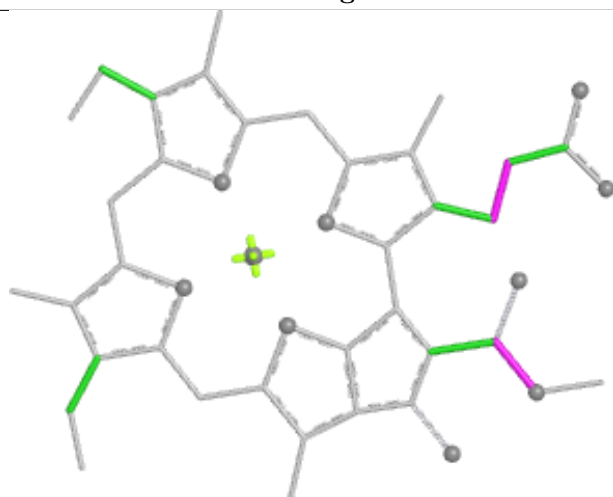
Ligand CLA i 513



Bond lengths



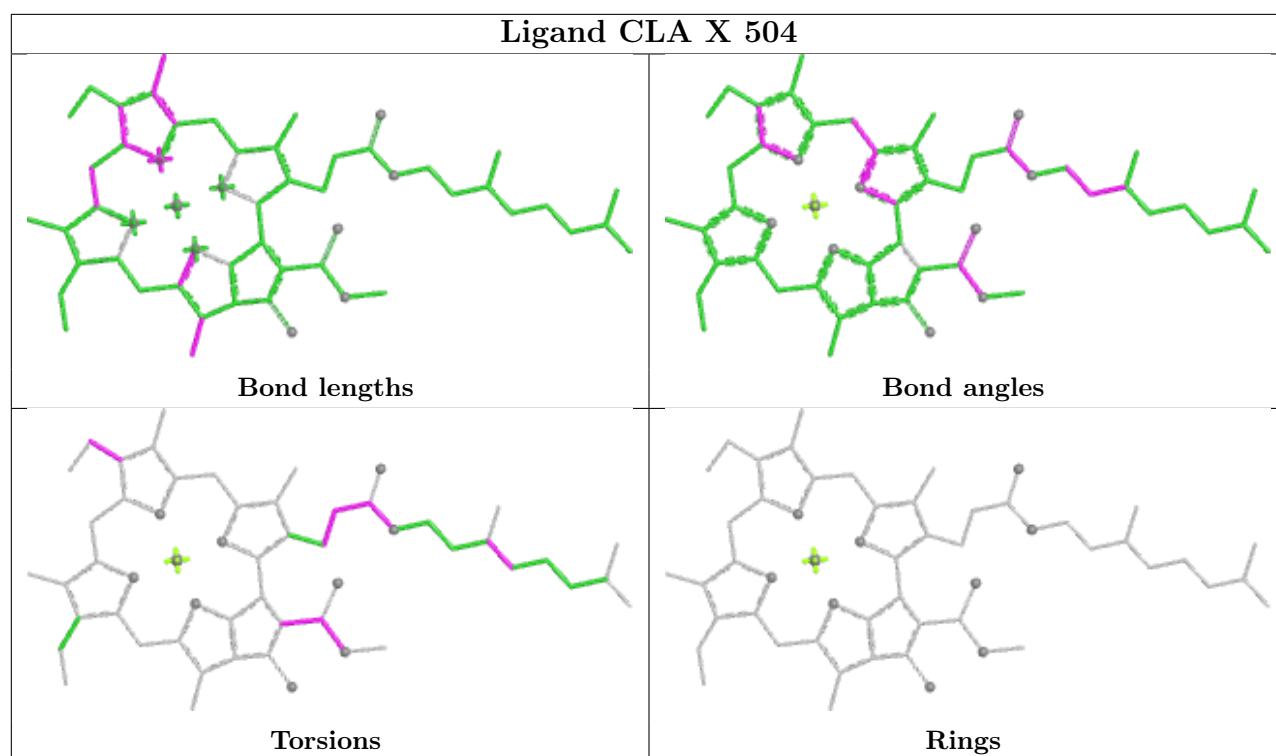
Bond angles



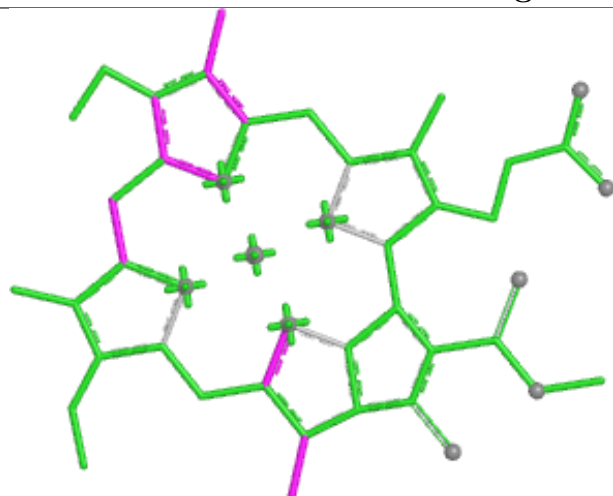
Torsions



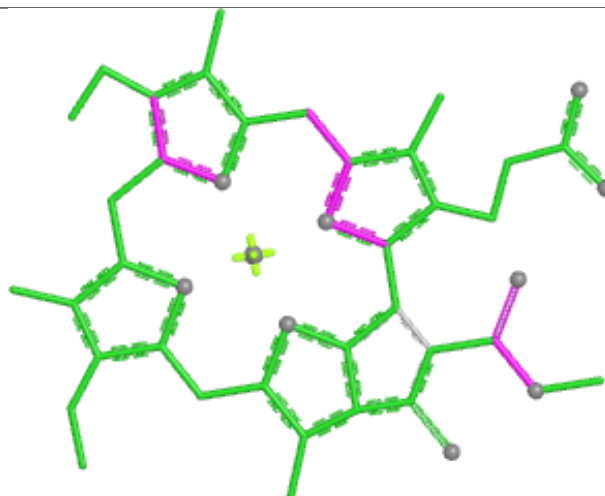
Rings



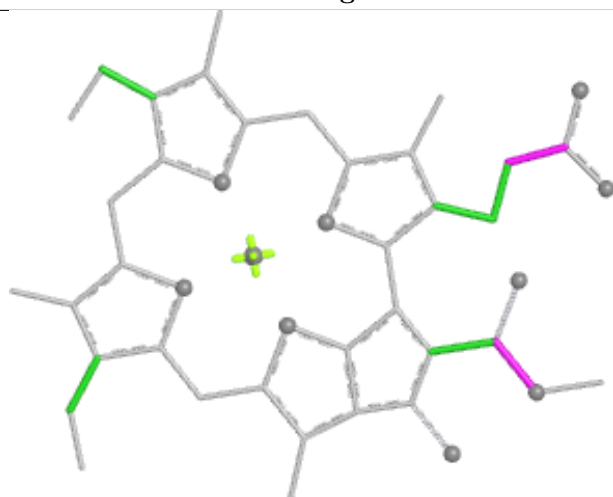
Ligand CLA T 506



Bond lengths



Bond angles

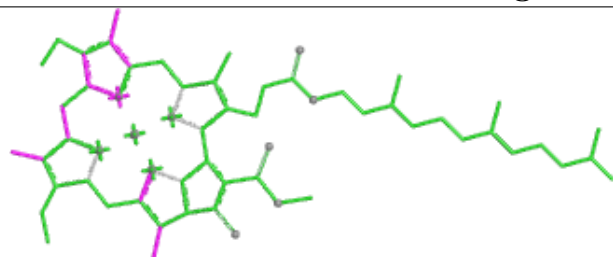


Torsions

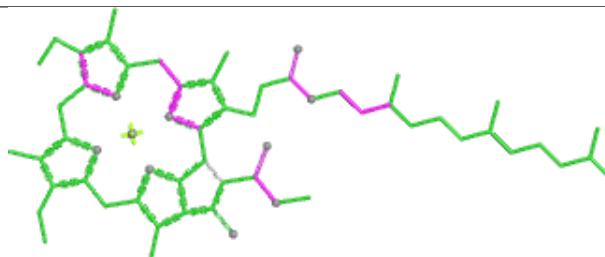


Rings

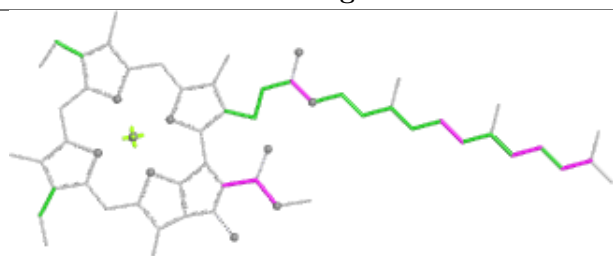
Ligand CLA Y 502



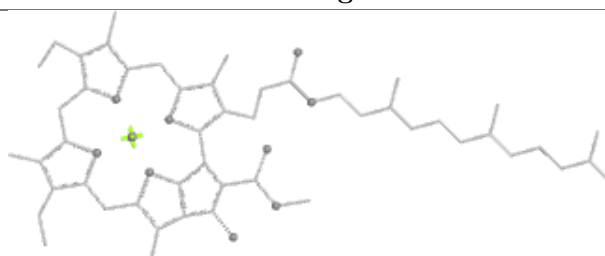
Bond lengths



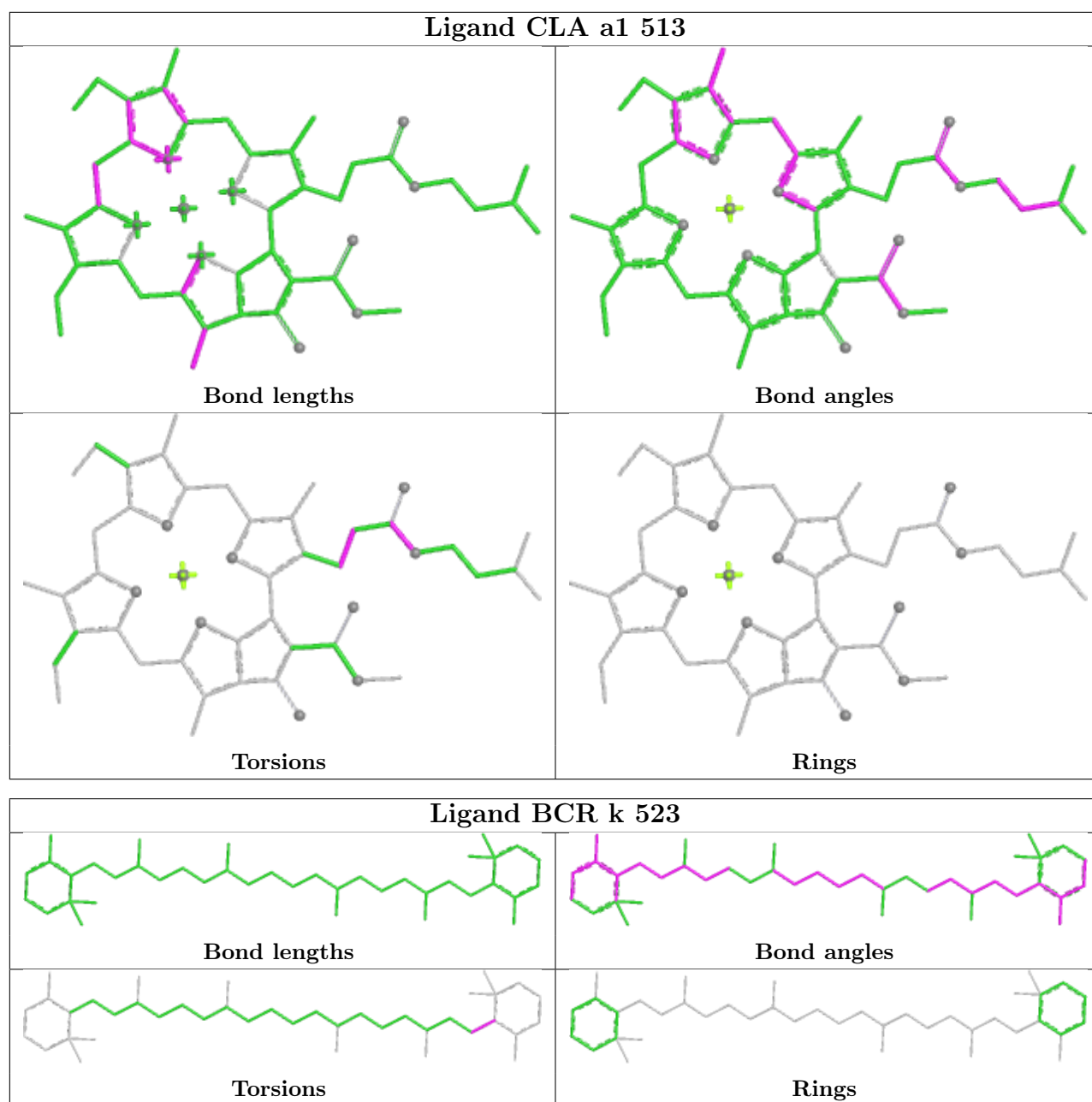
Bond angles



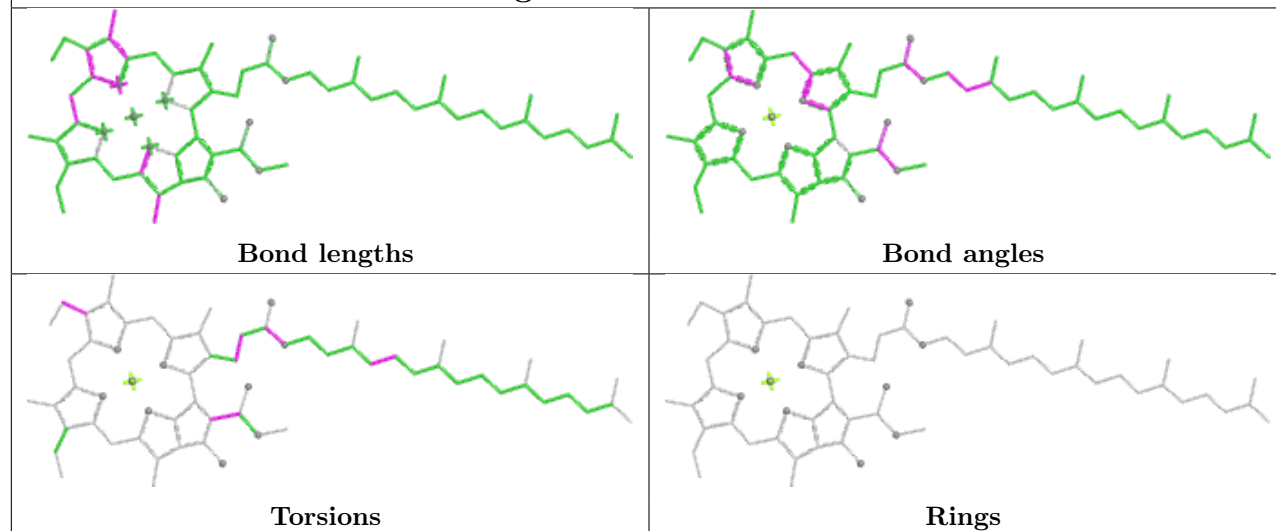
Torsions



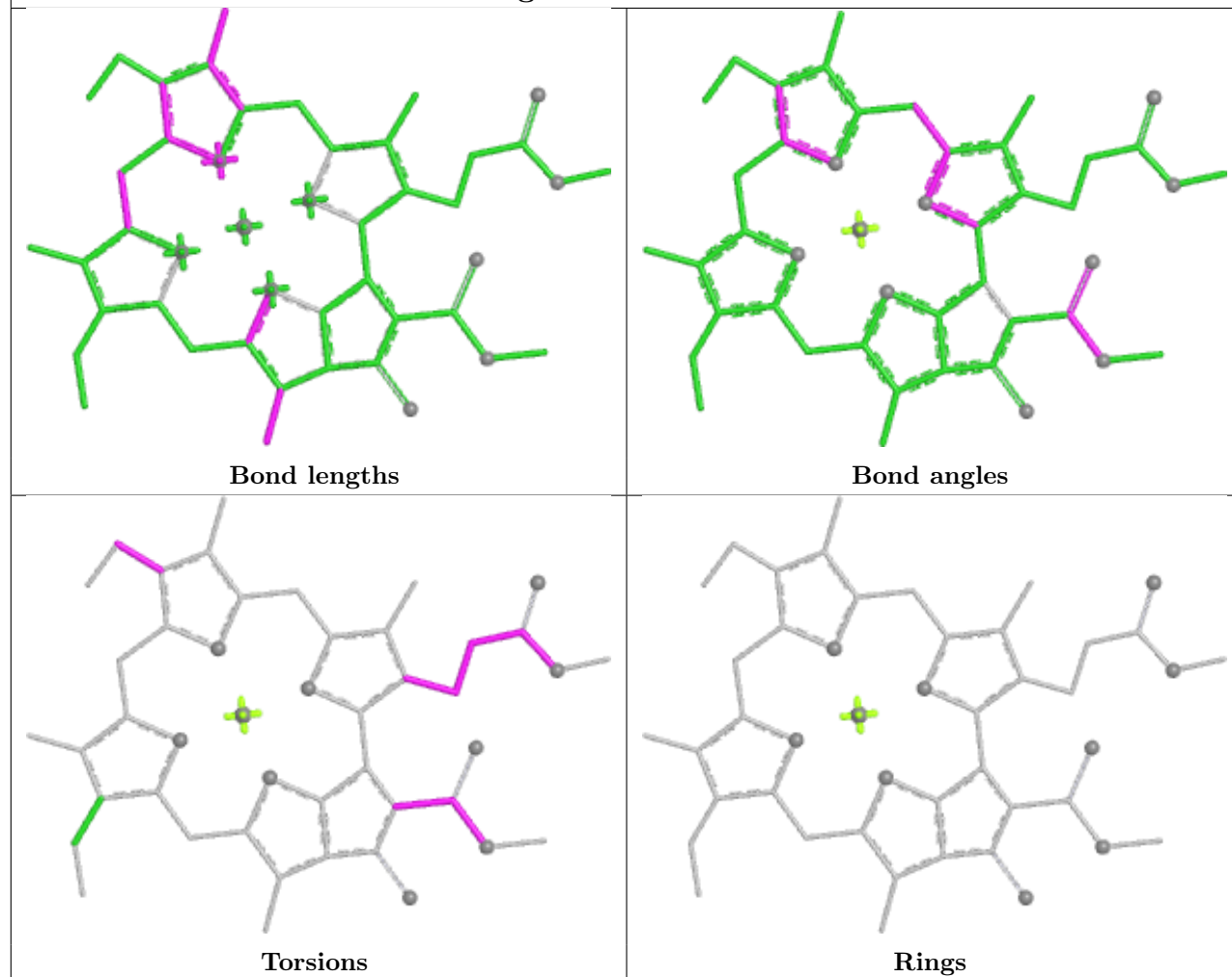
Rings

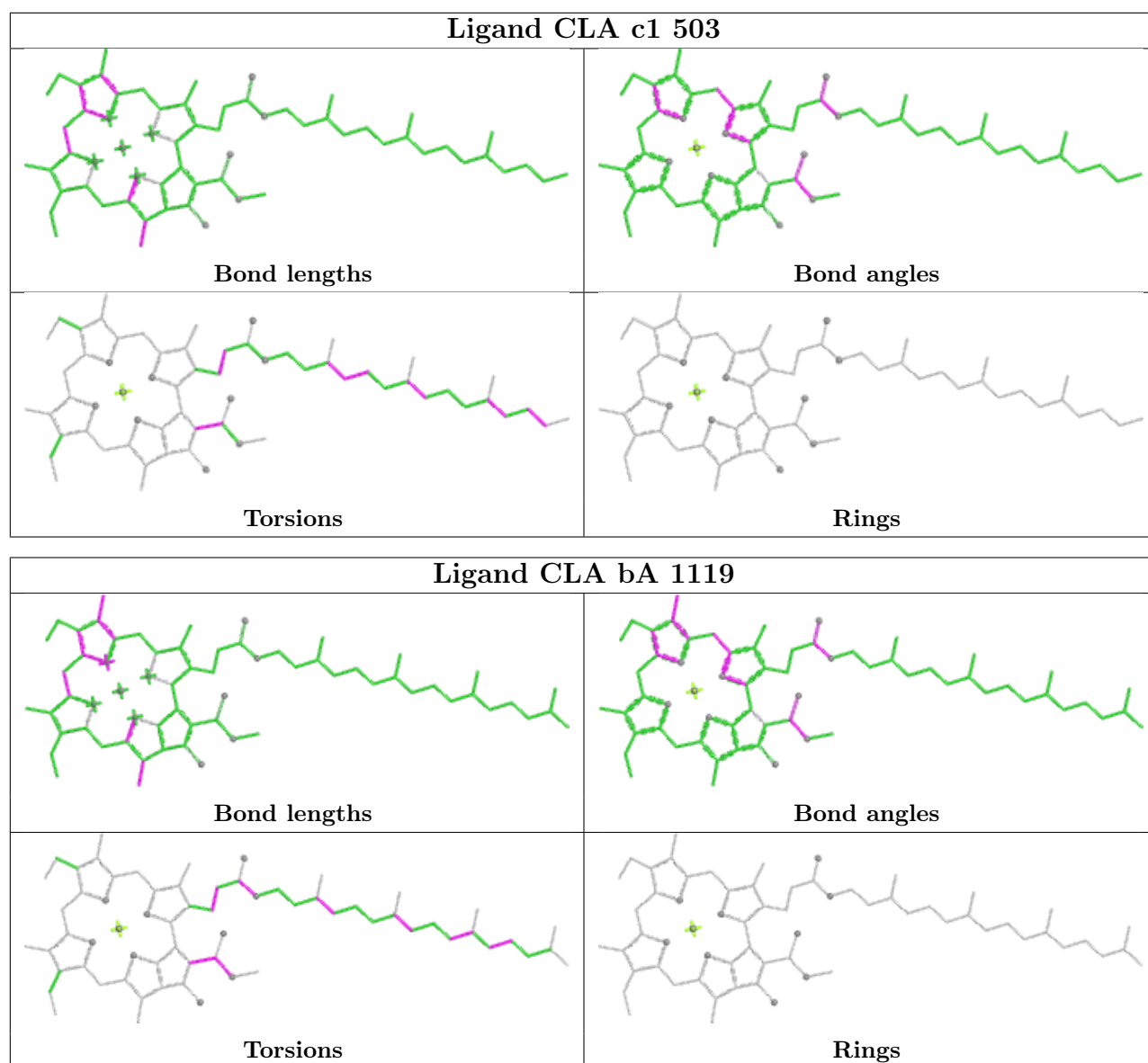


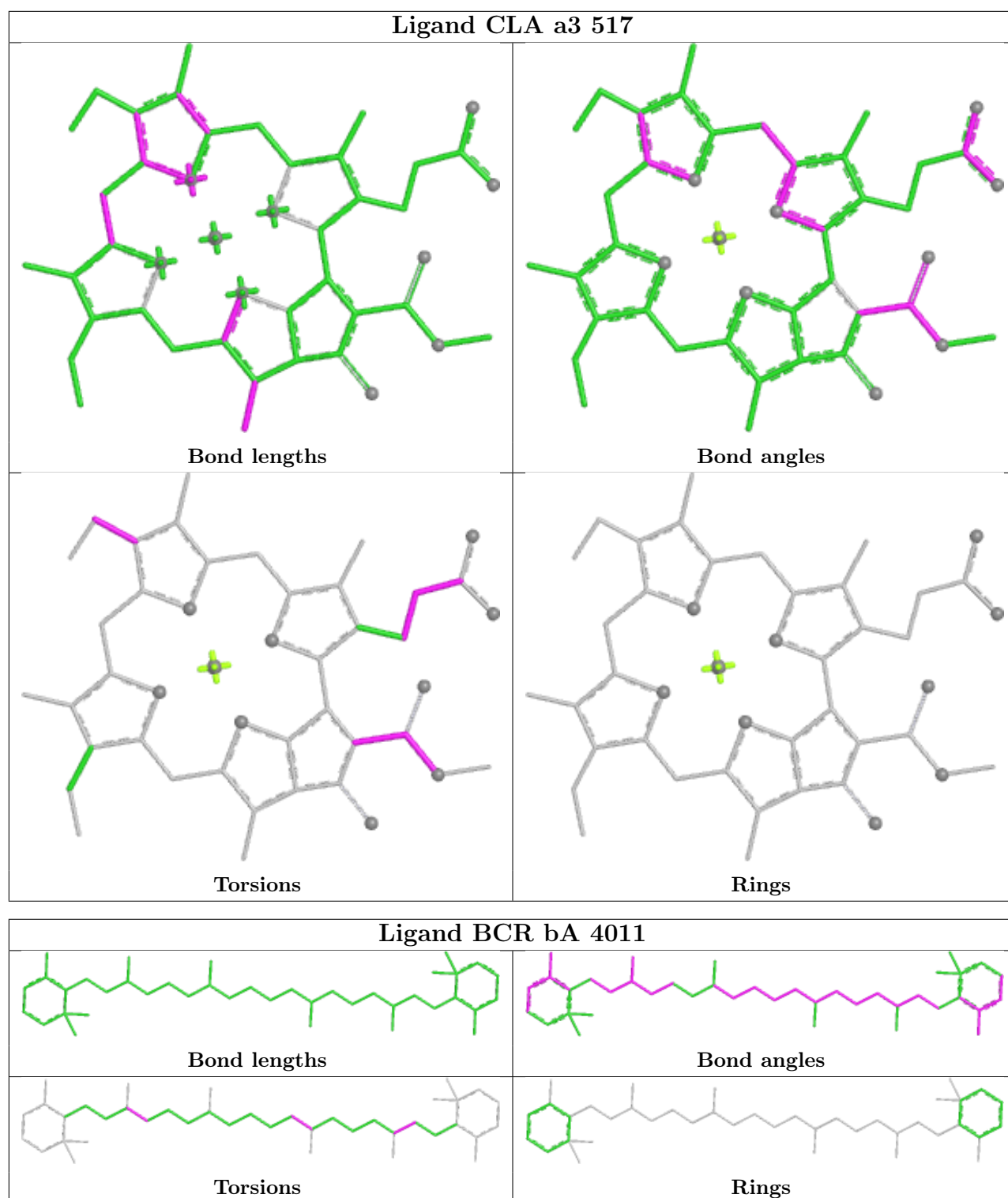
Ligand CLA aB 1238

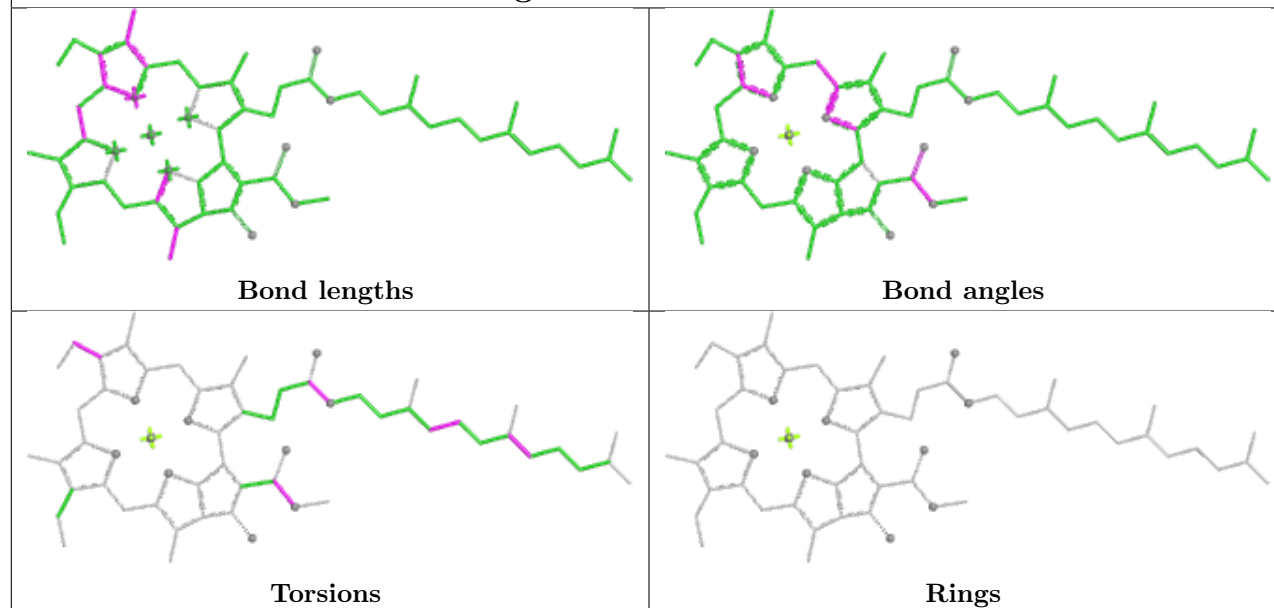
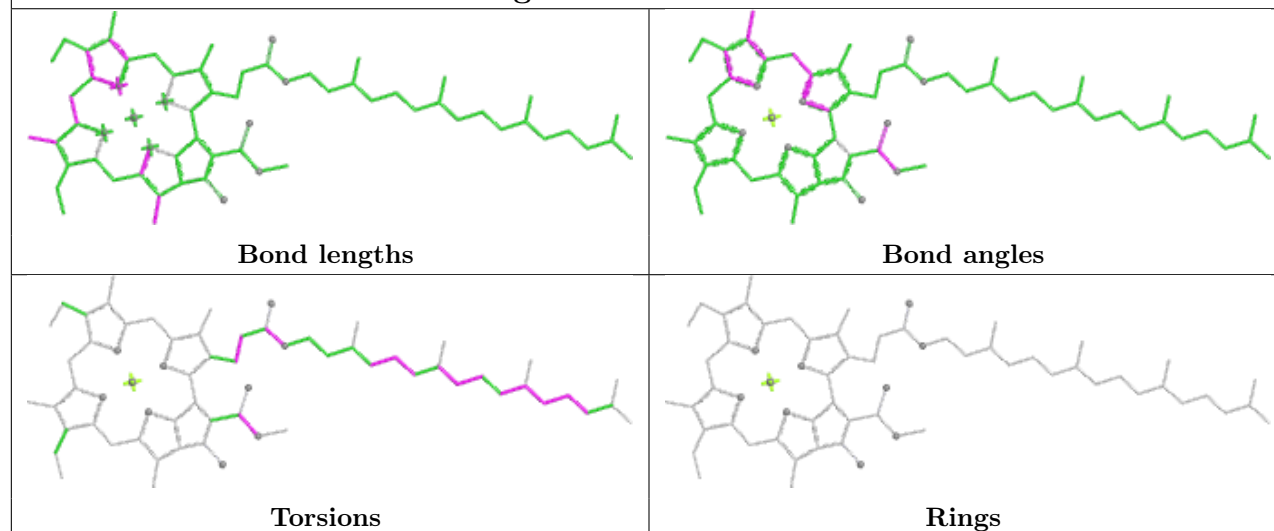


Ligand CLA o 501

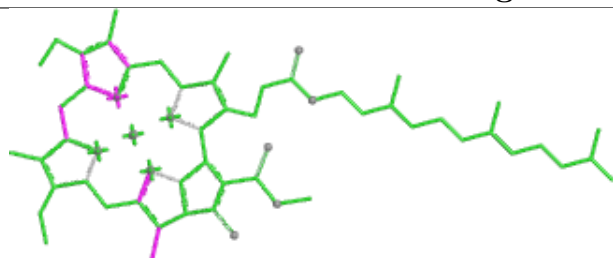




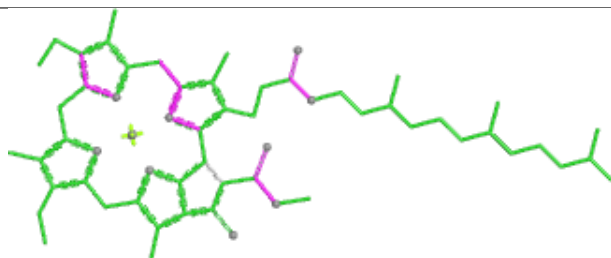


Ligand CLA aB 1216**Ligand CLA bB 1214**

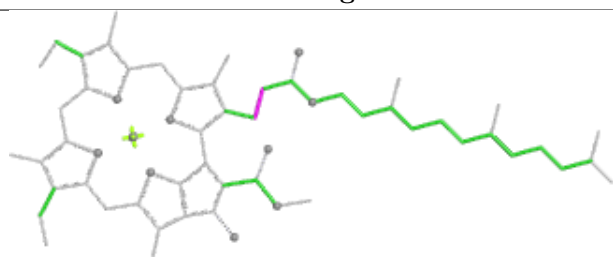
Ligand CLA bB 1204



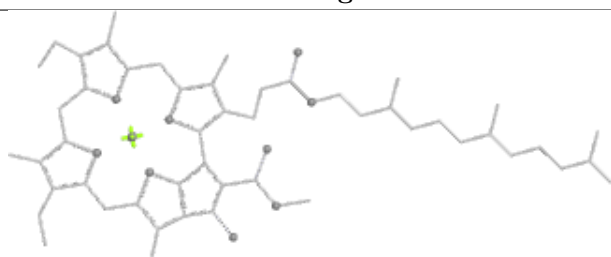
Bond lengths



Bond angles

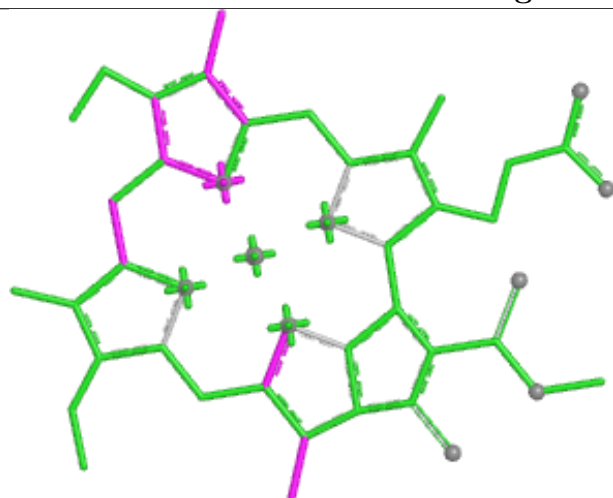


Torsions

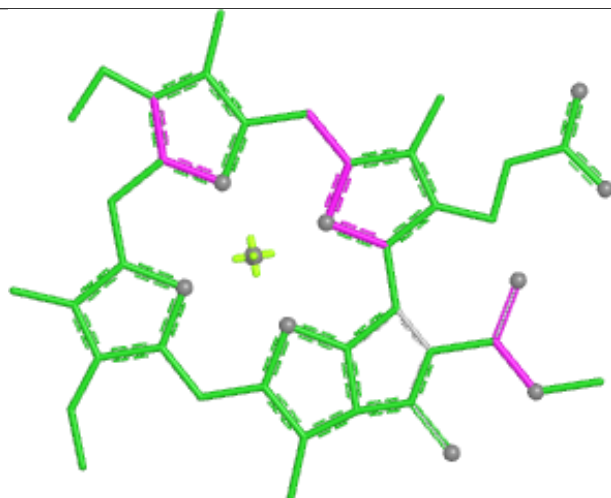


Rings

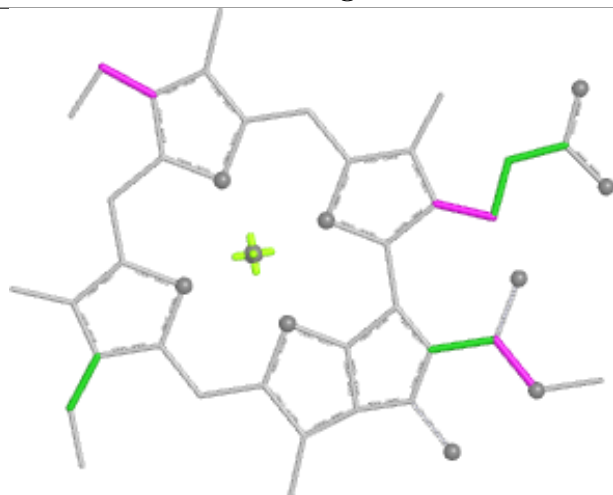
Ligand CLA T 512



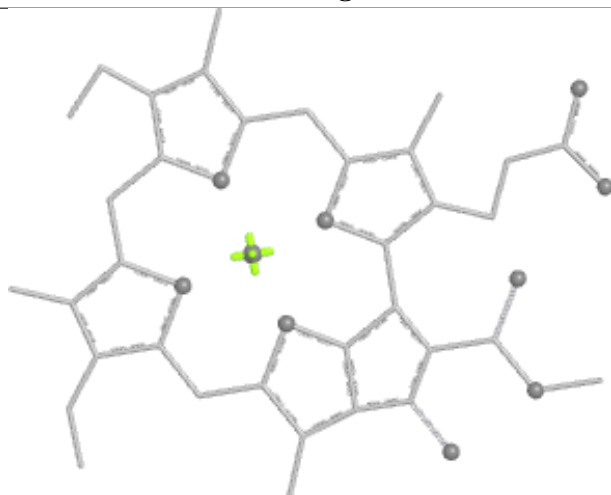
Bond lengths



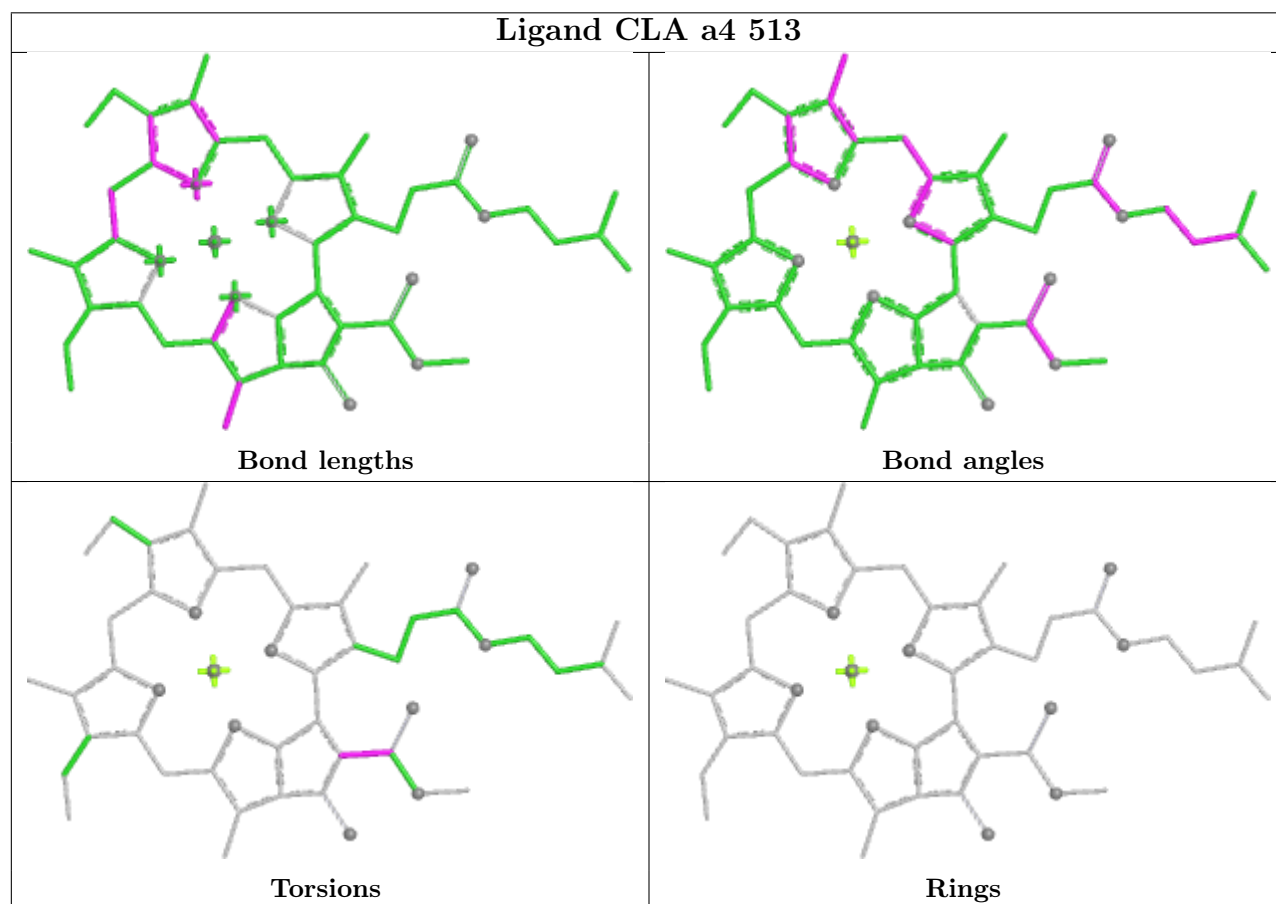
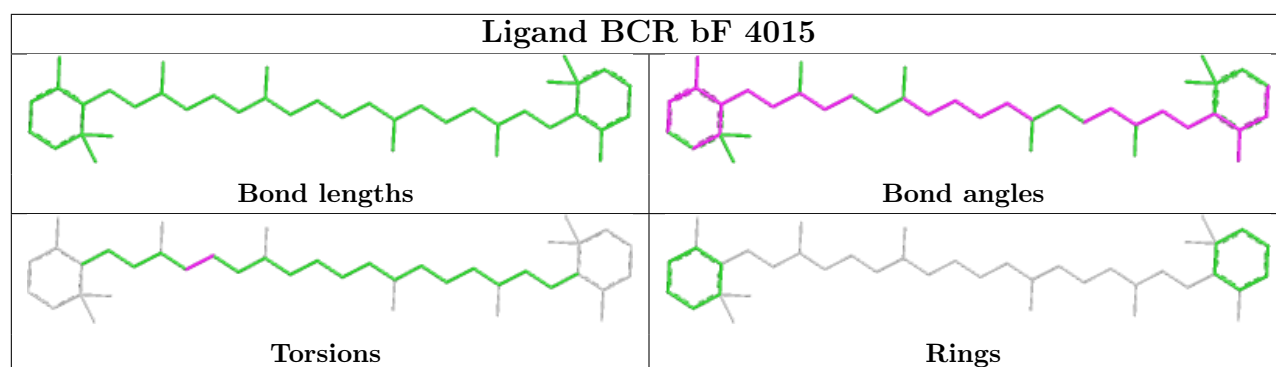
Bond angles



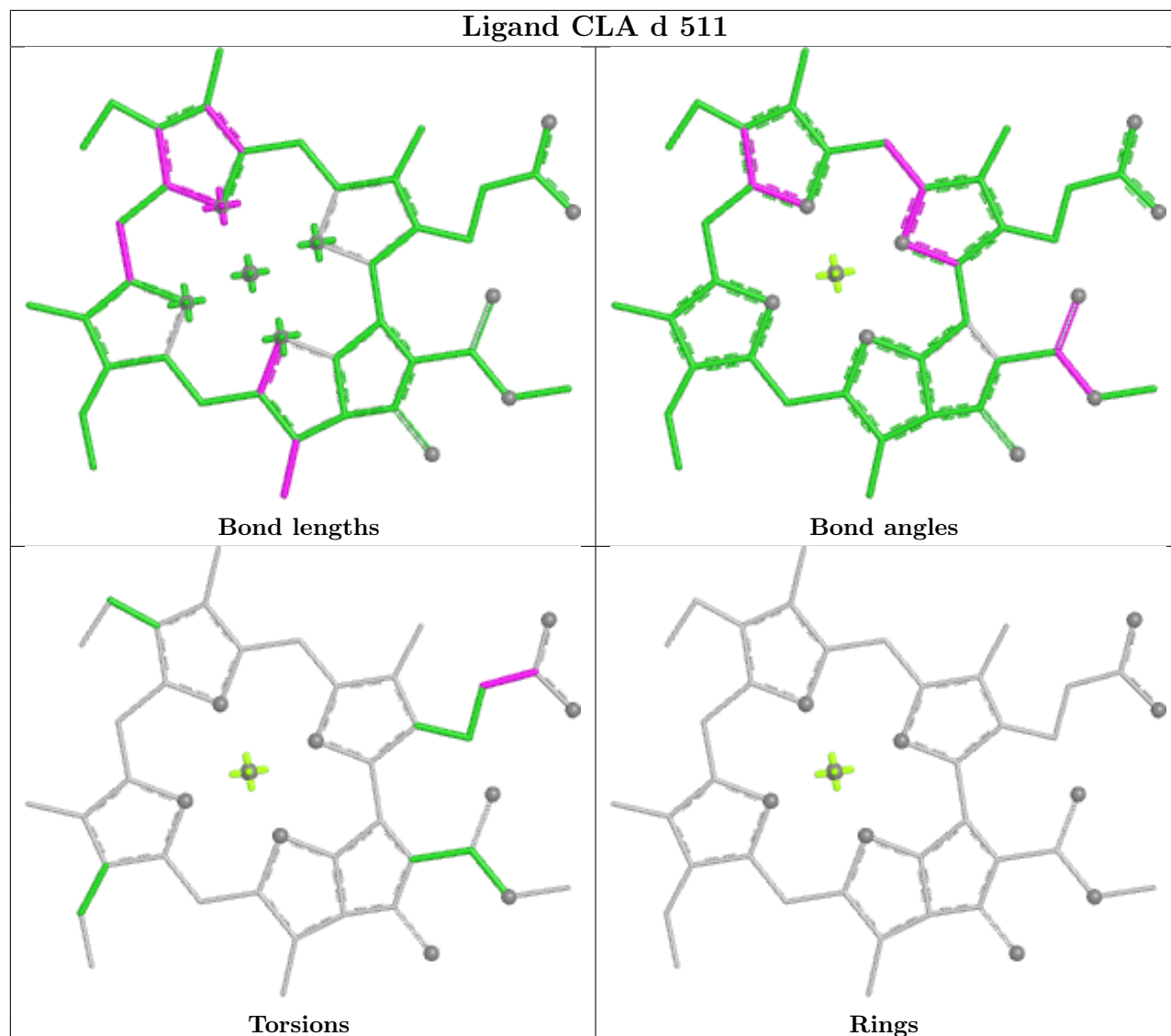
Torsions



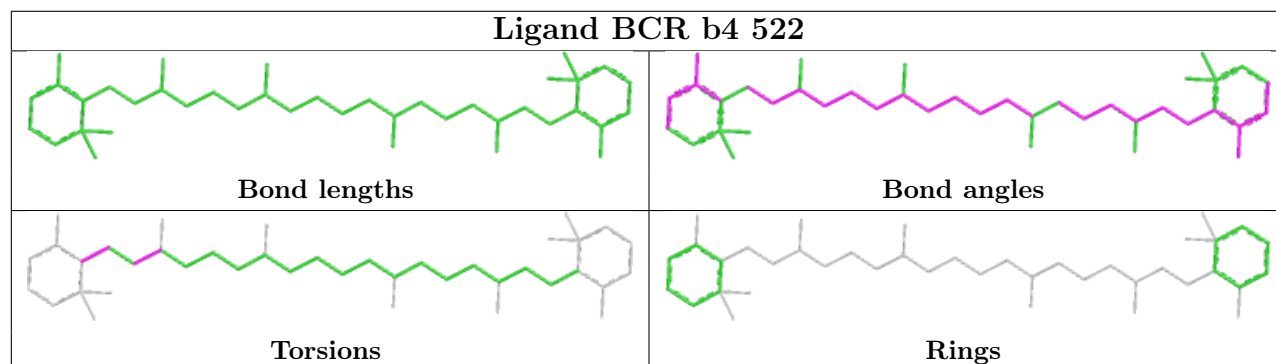
Rings

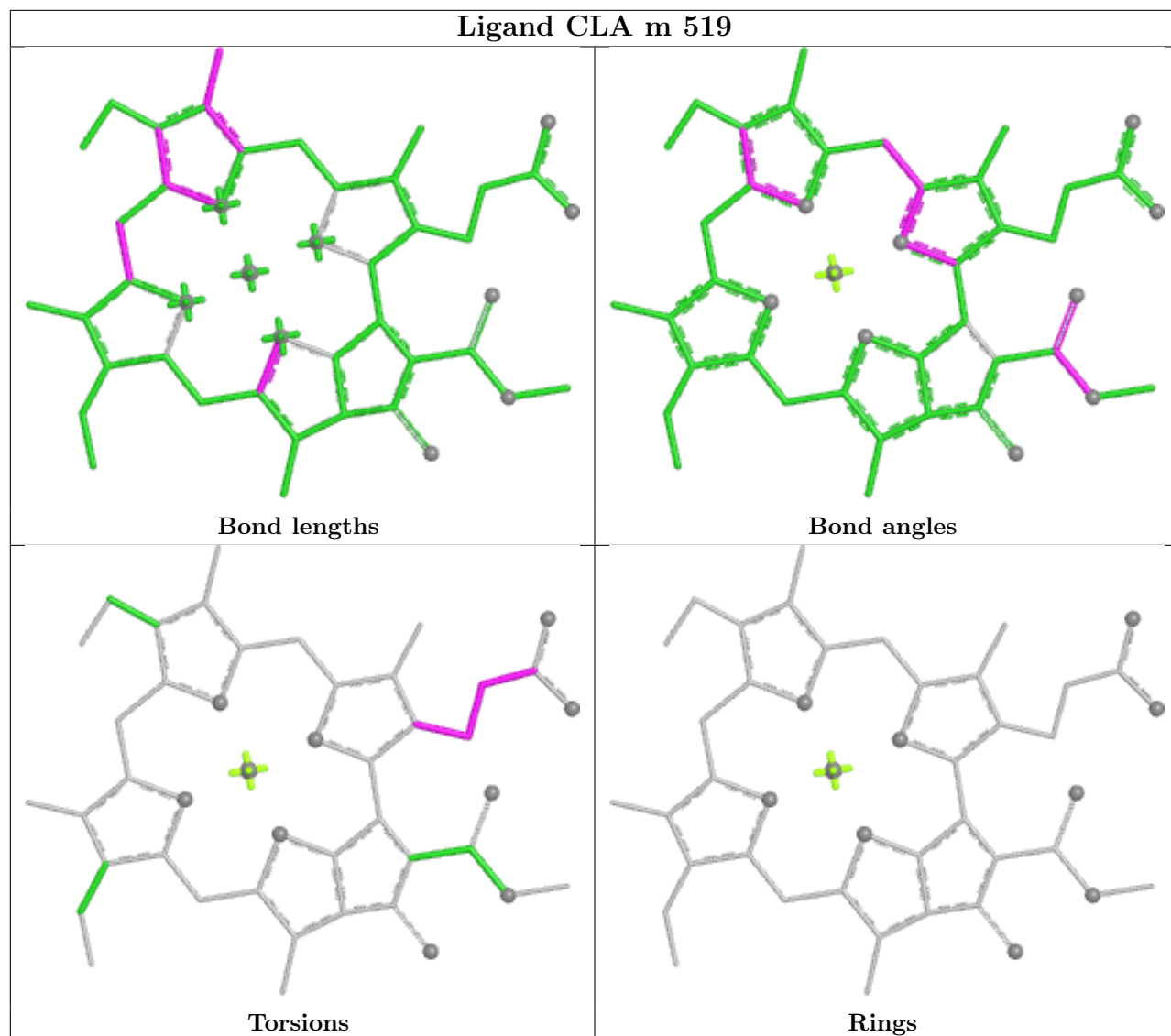


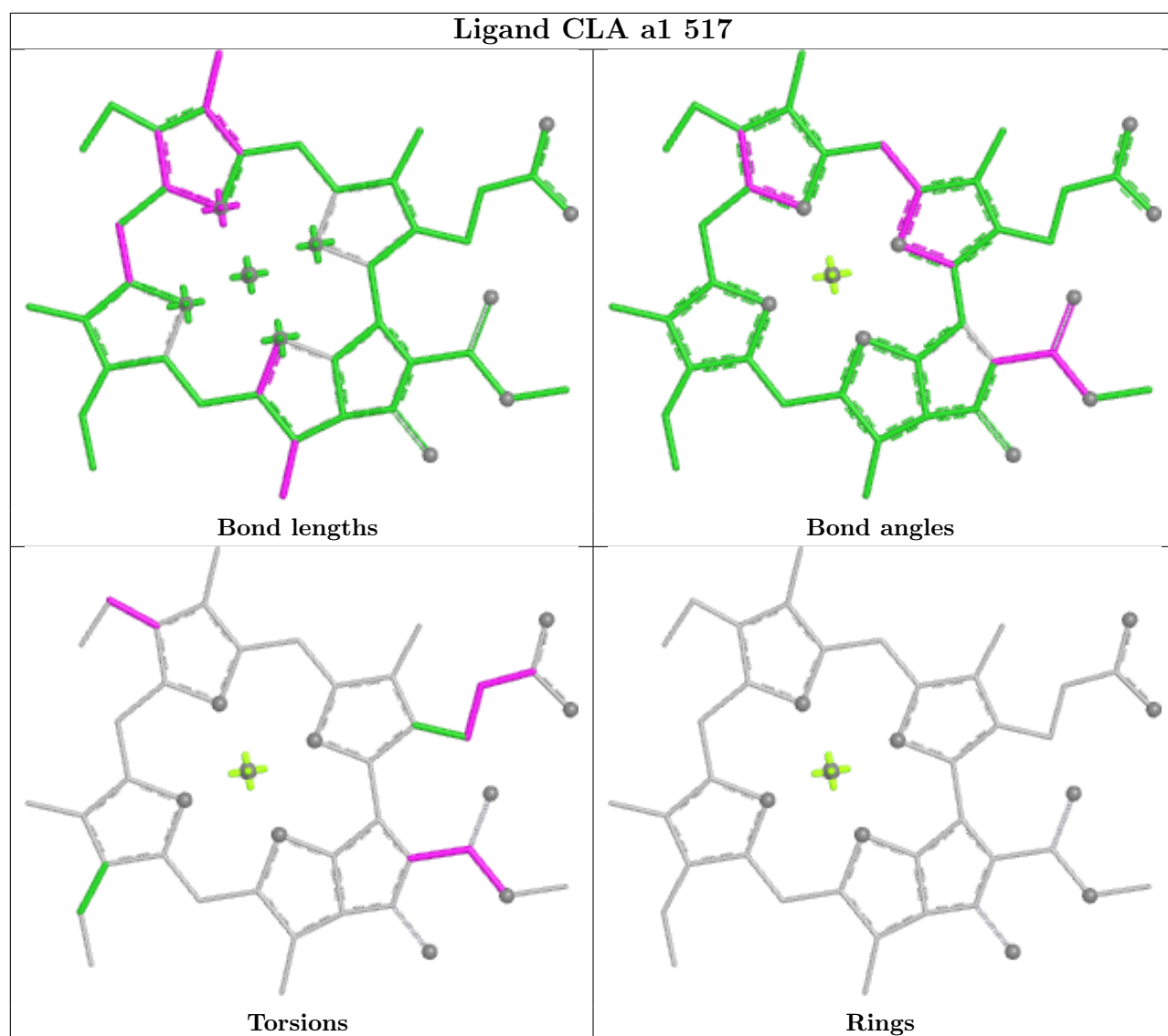
Ligand CLA d 511

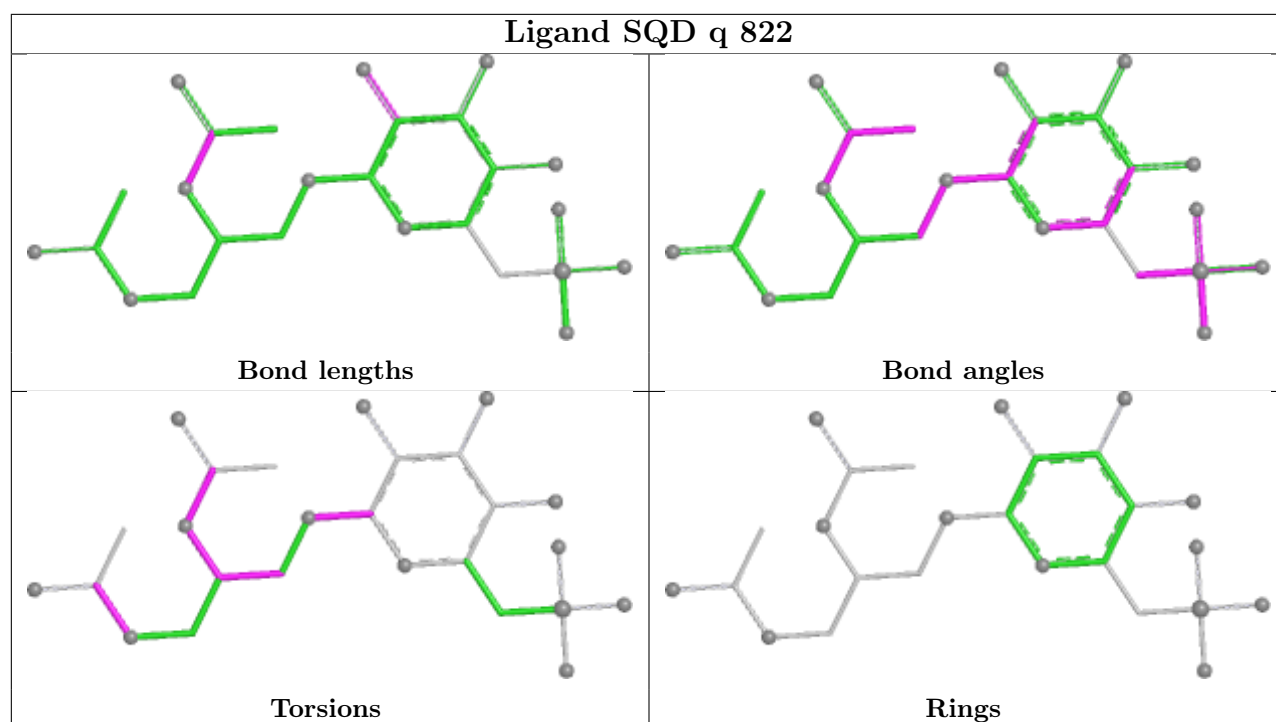


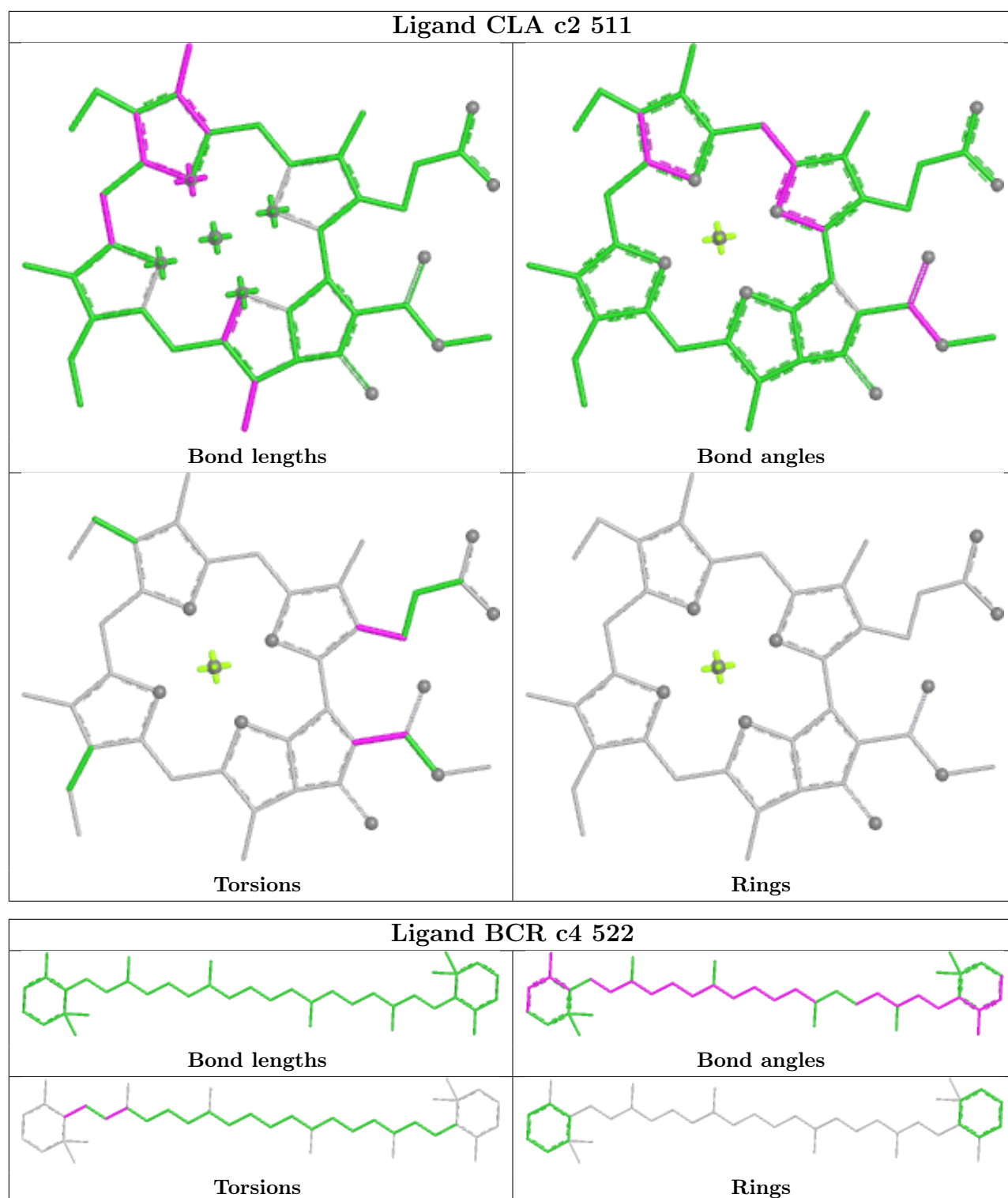
Ligand BCR b4 522

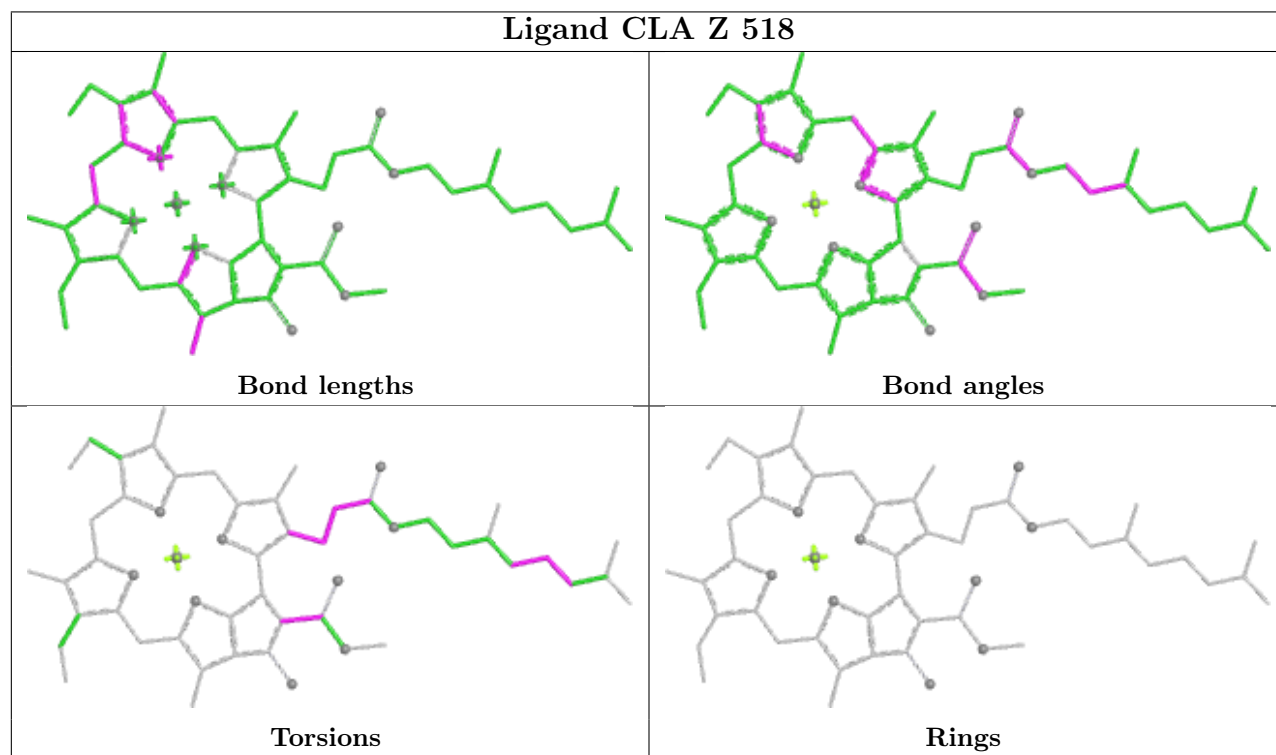
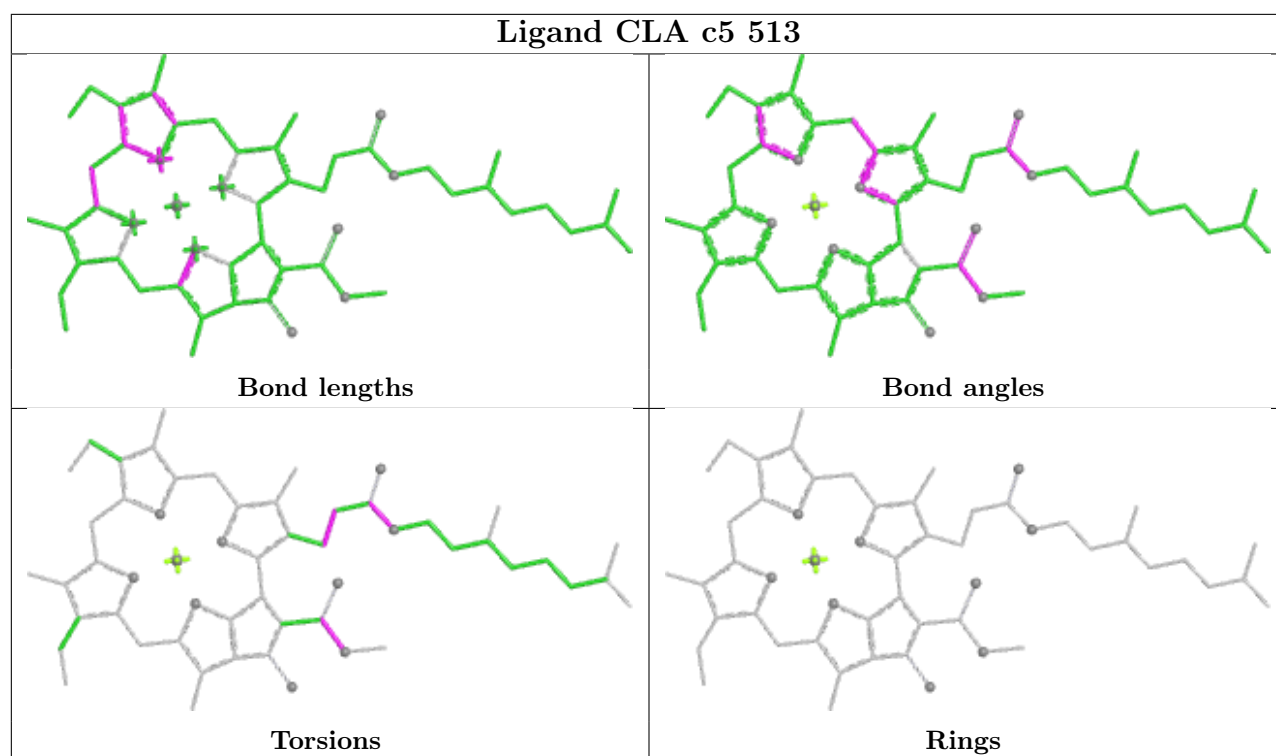




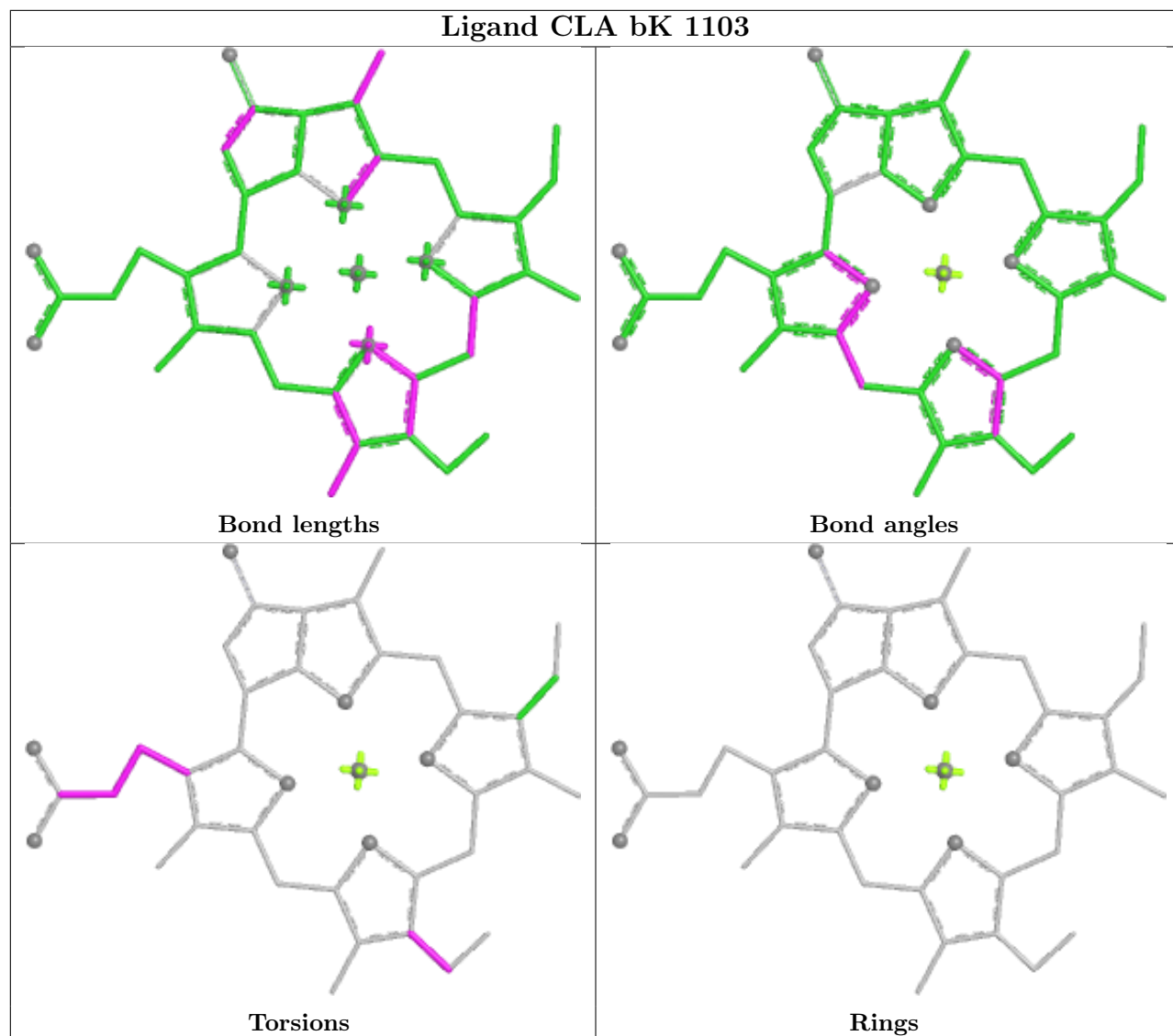


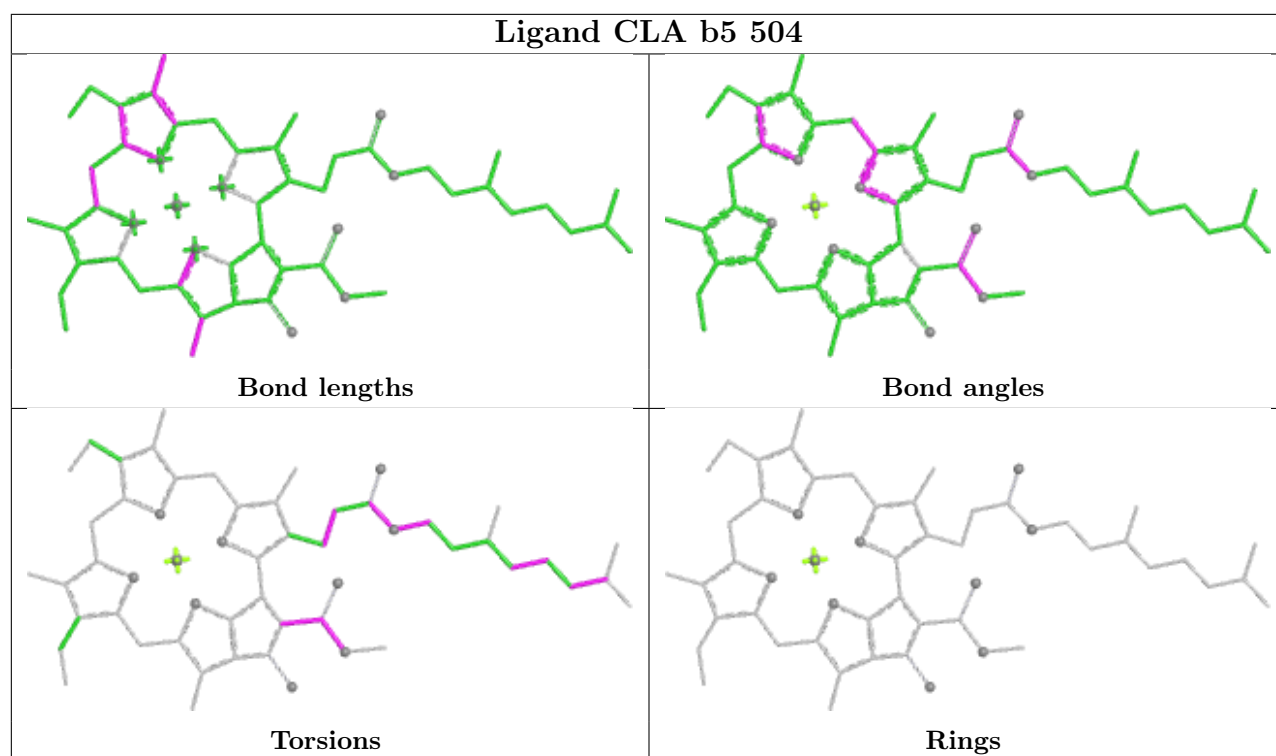


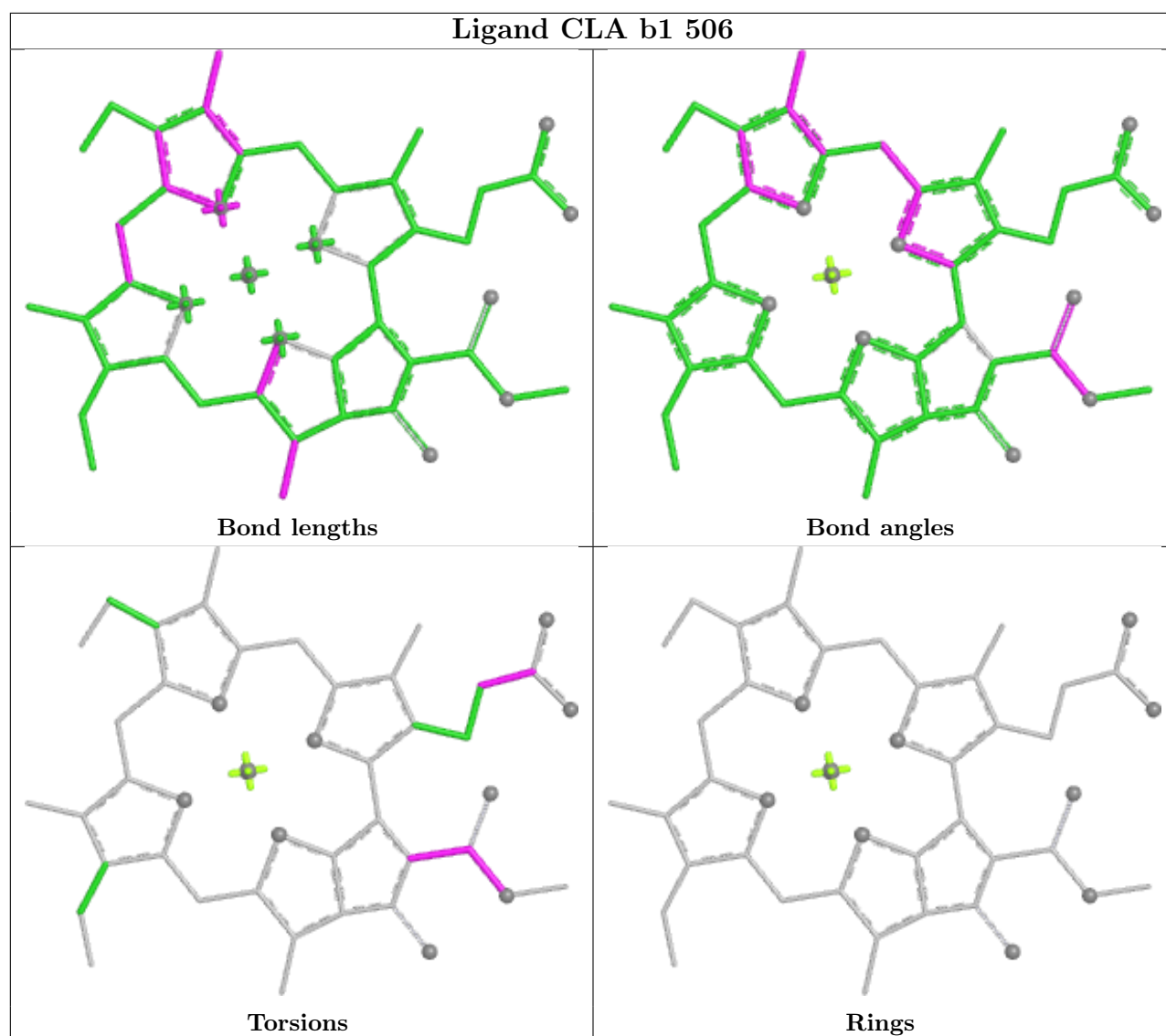




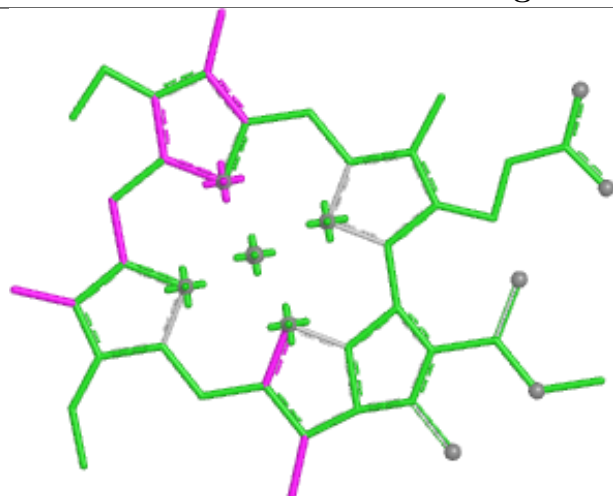
Ligand CLA bK 1103



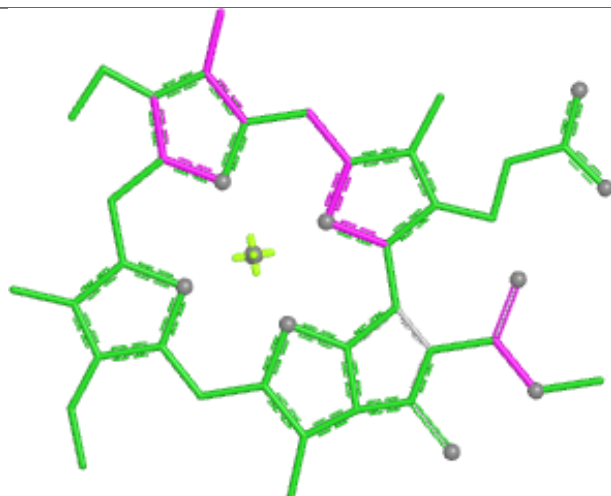




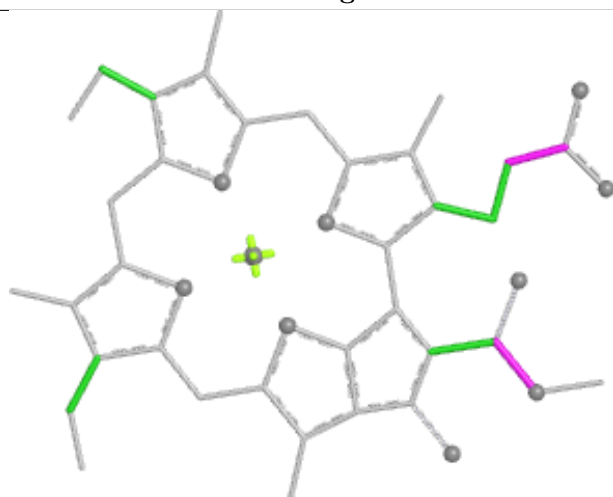
Ligand CLA X 508



Bond lengths



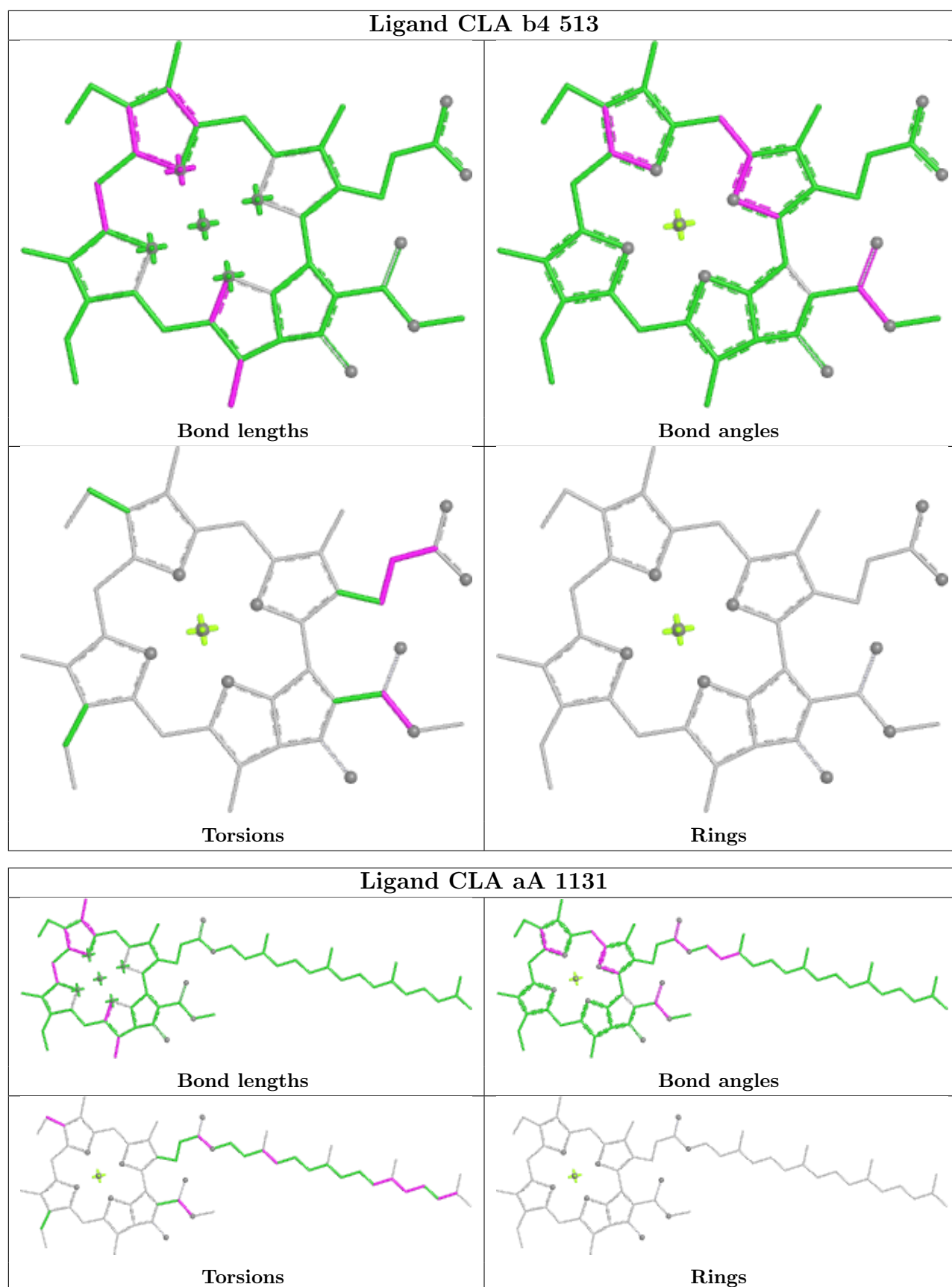
Bond angles

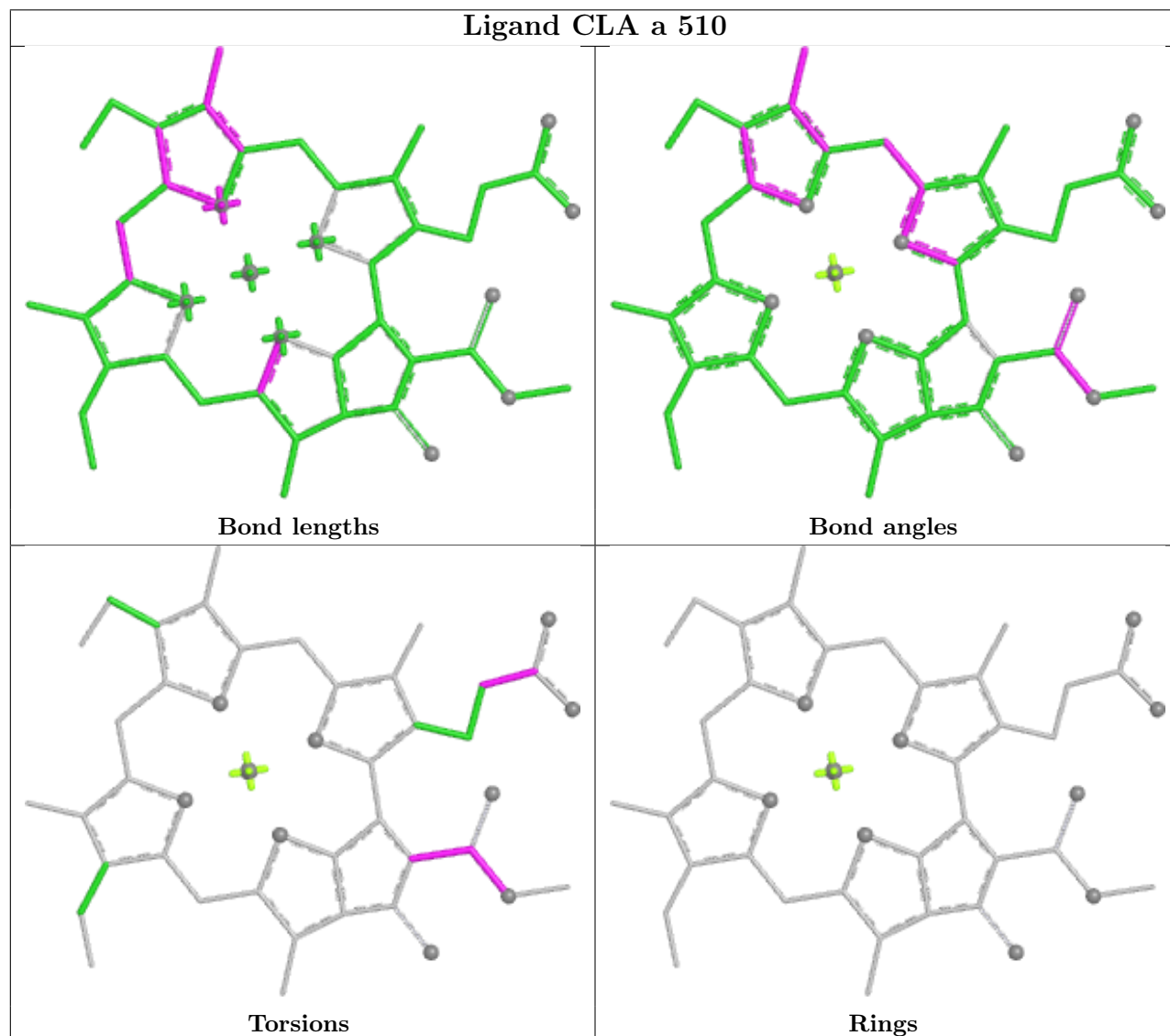
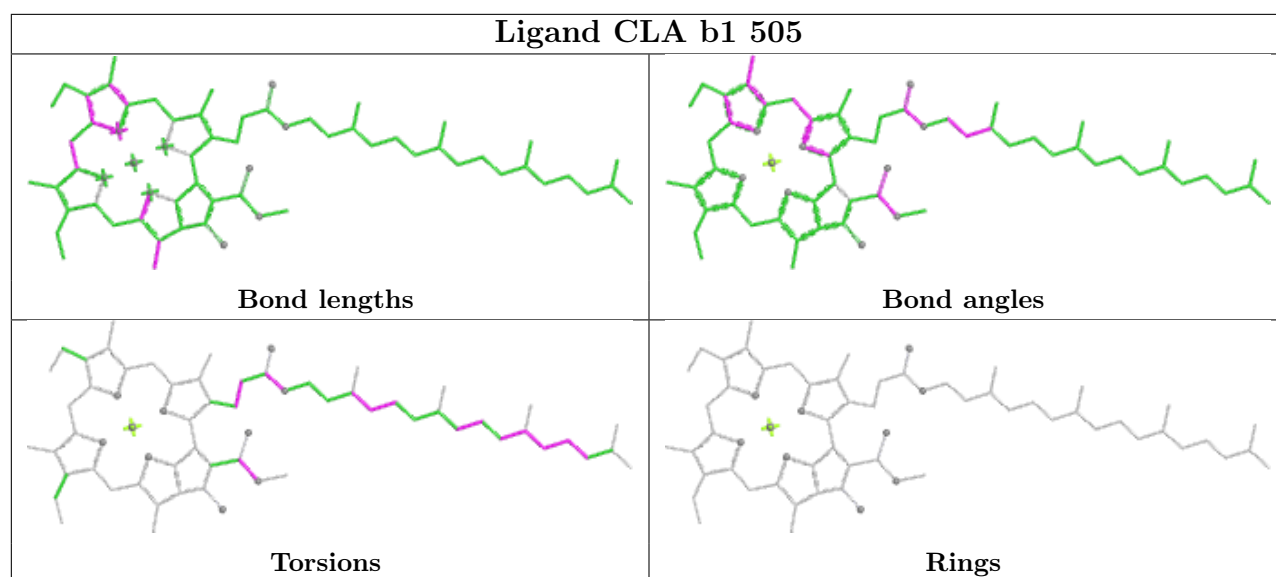


Torsions

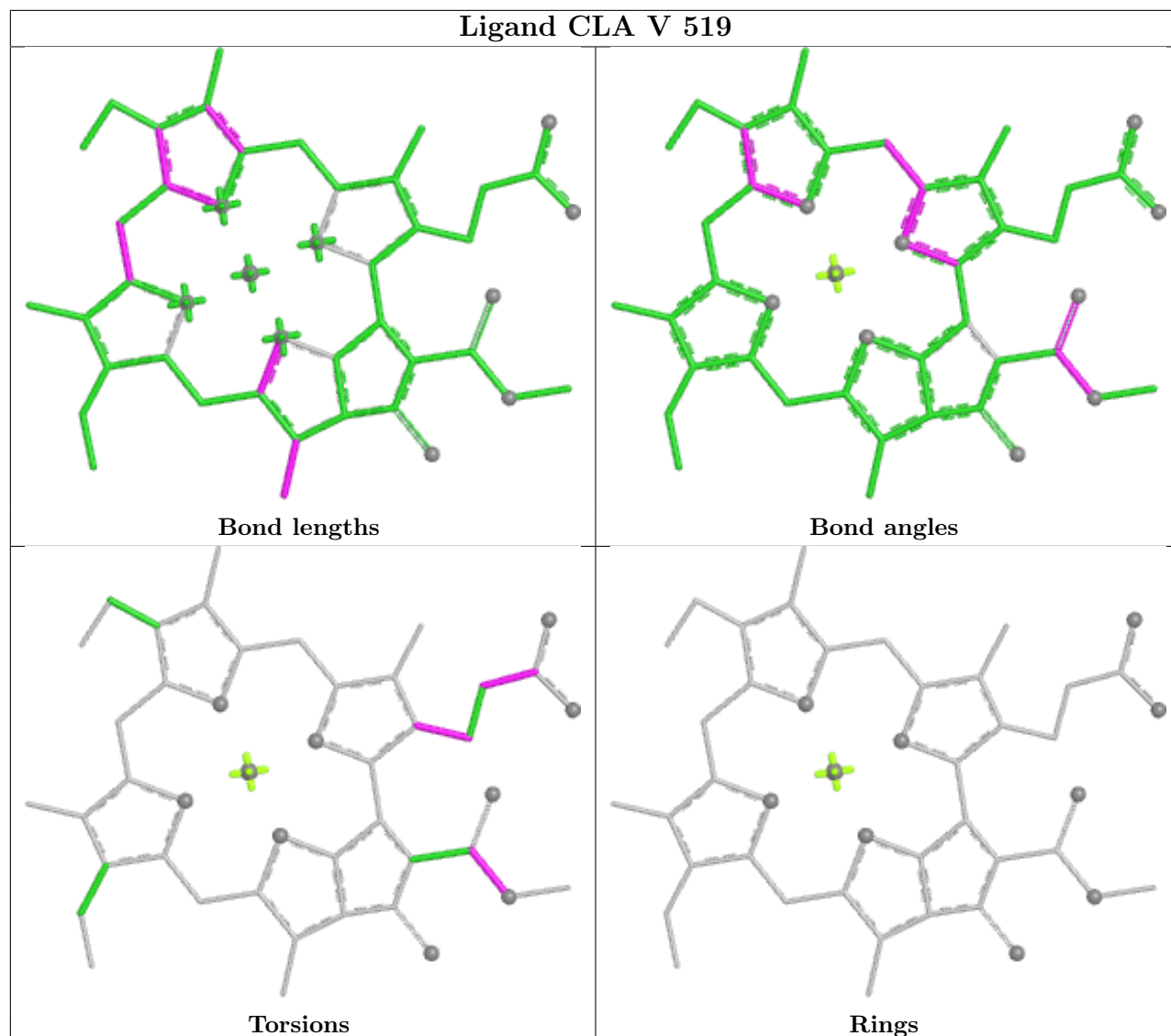


Rings

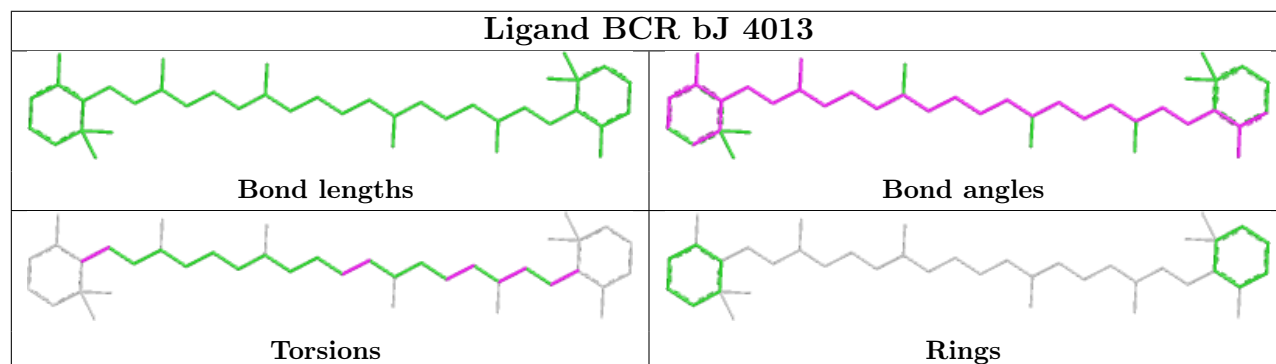


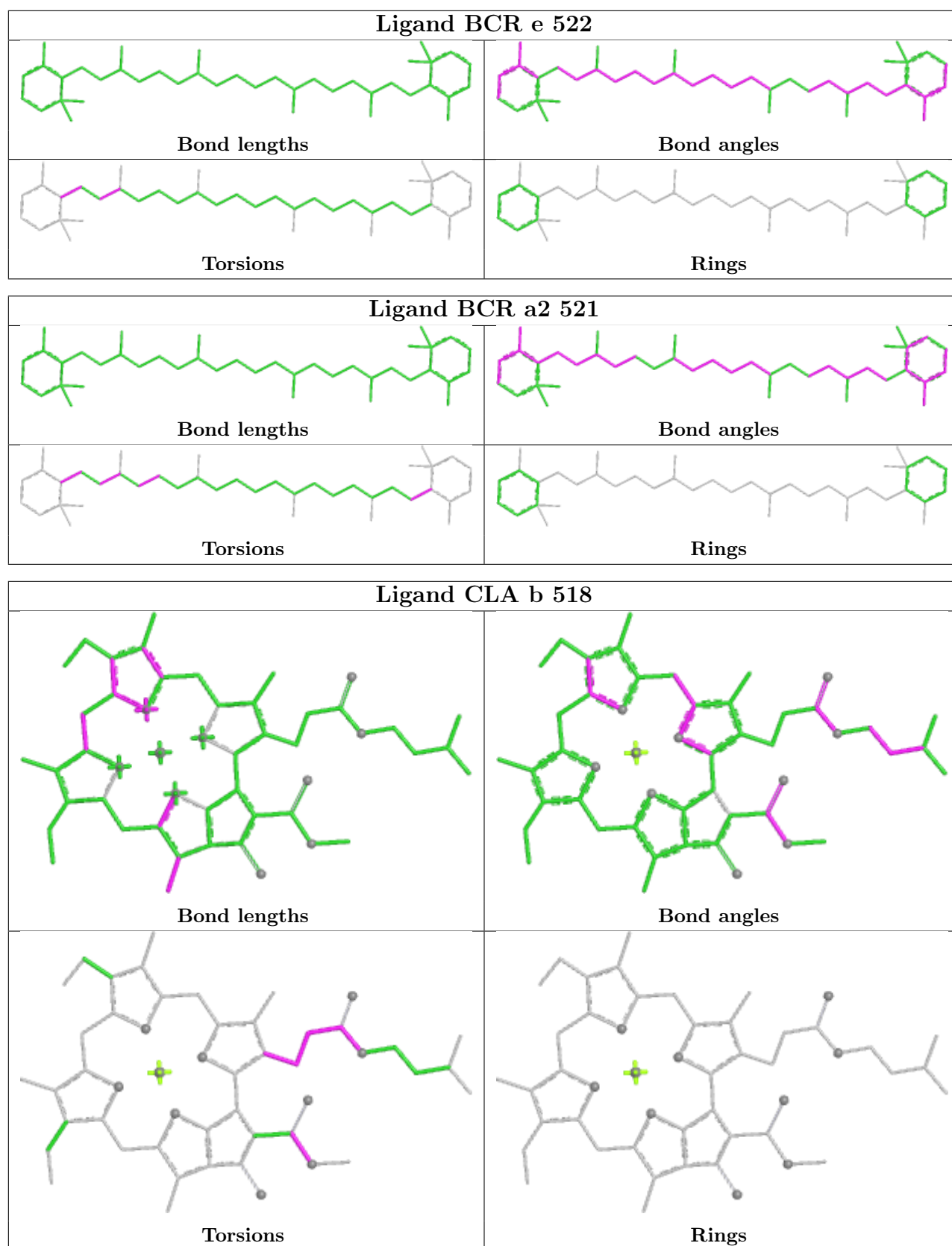


Ligand CLA V 519

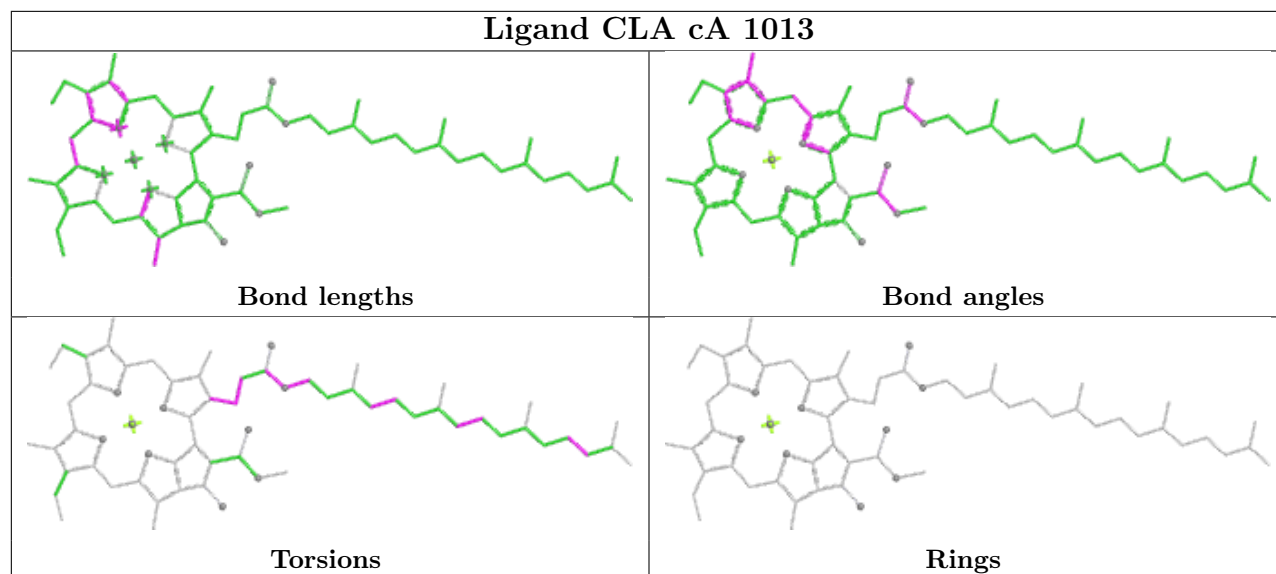


Ligand BCR bJ 4013

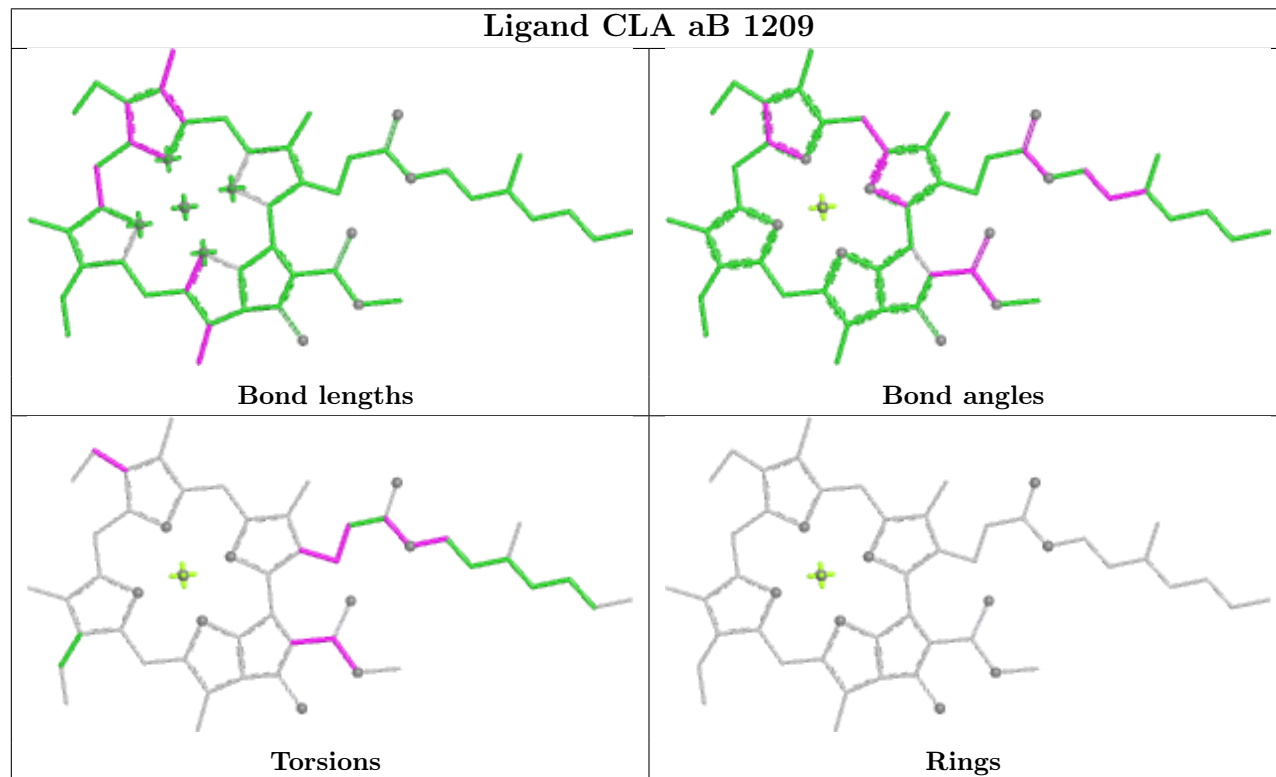


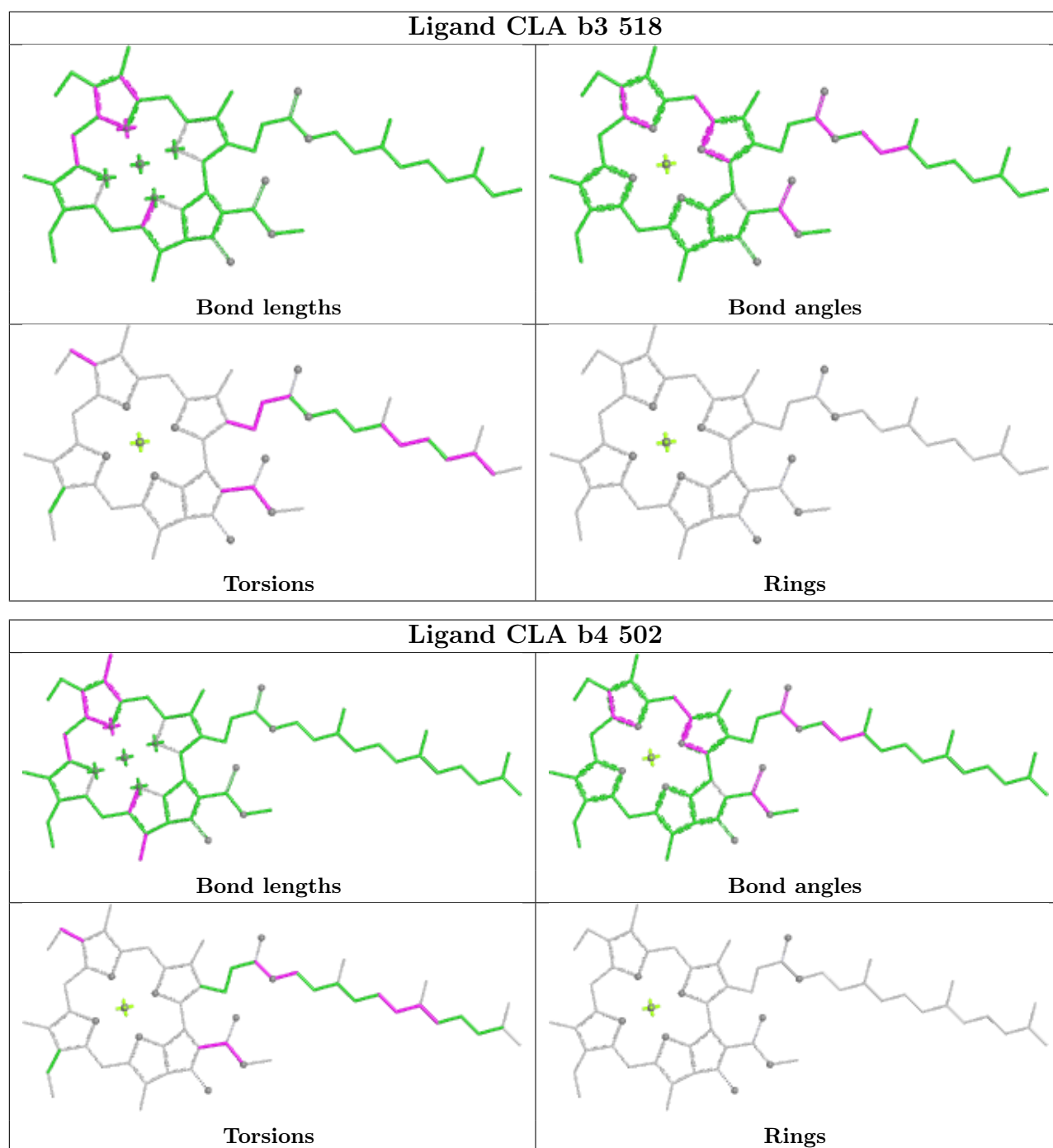


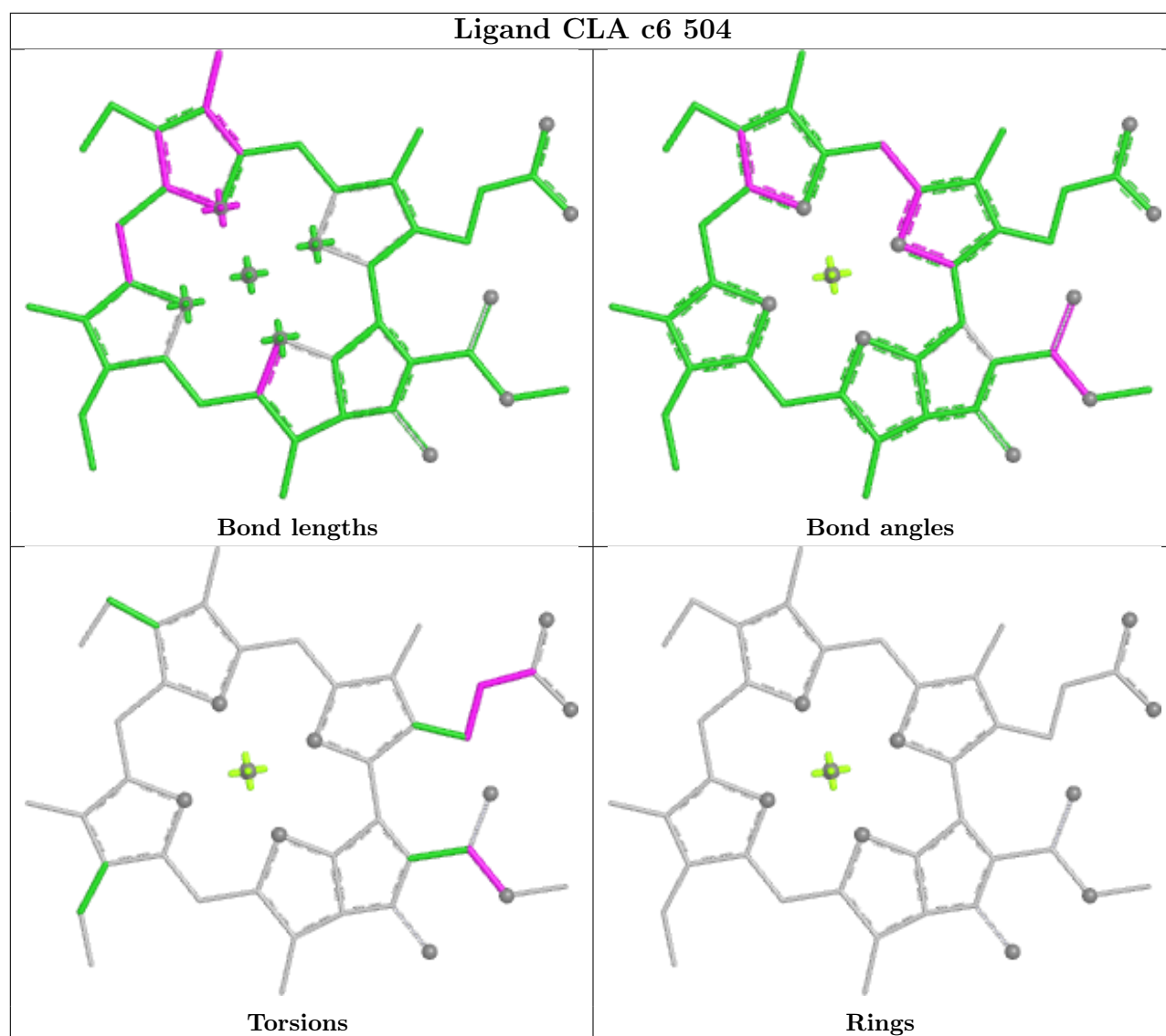
Ligand CLA cA 1013



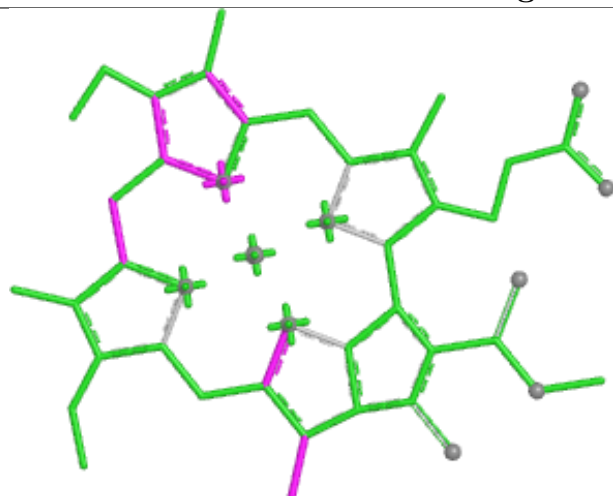
Ligand CLA aB 1209



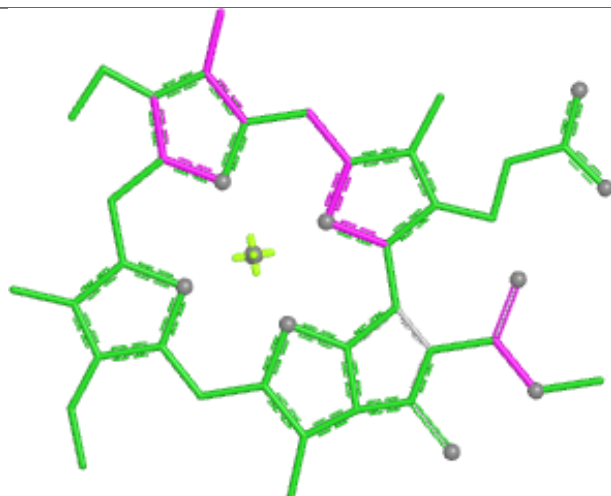




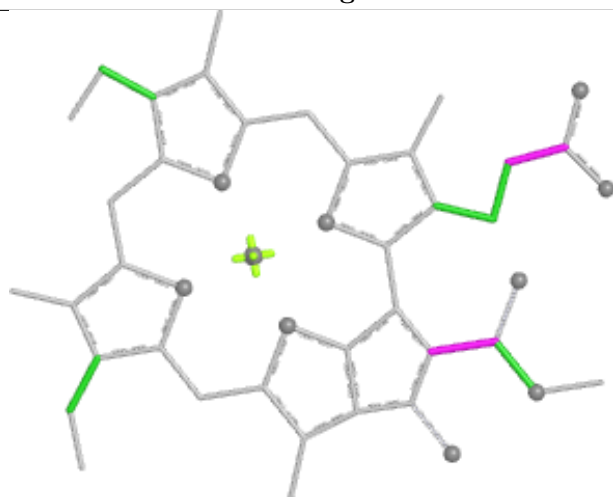
Ligand CLA h 507



Bond lengths



Bond angles

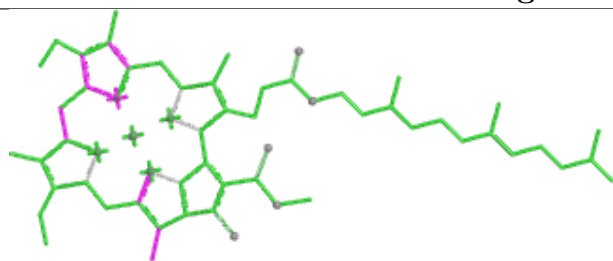


Torsions

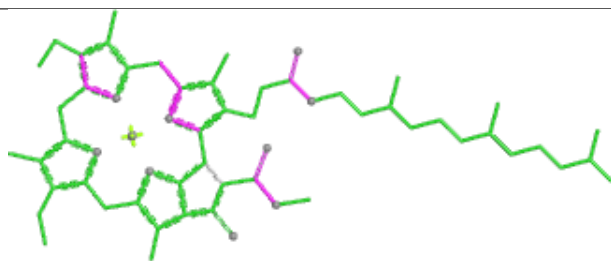


Rings

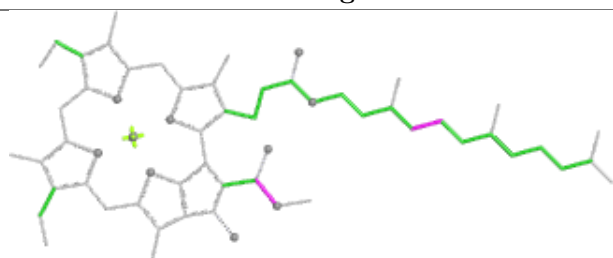
Ligand CLA S 503



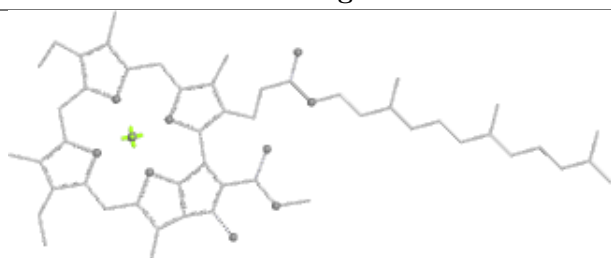
Bond lengths



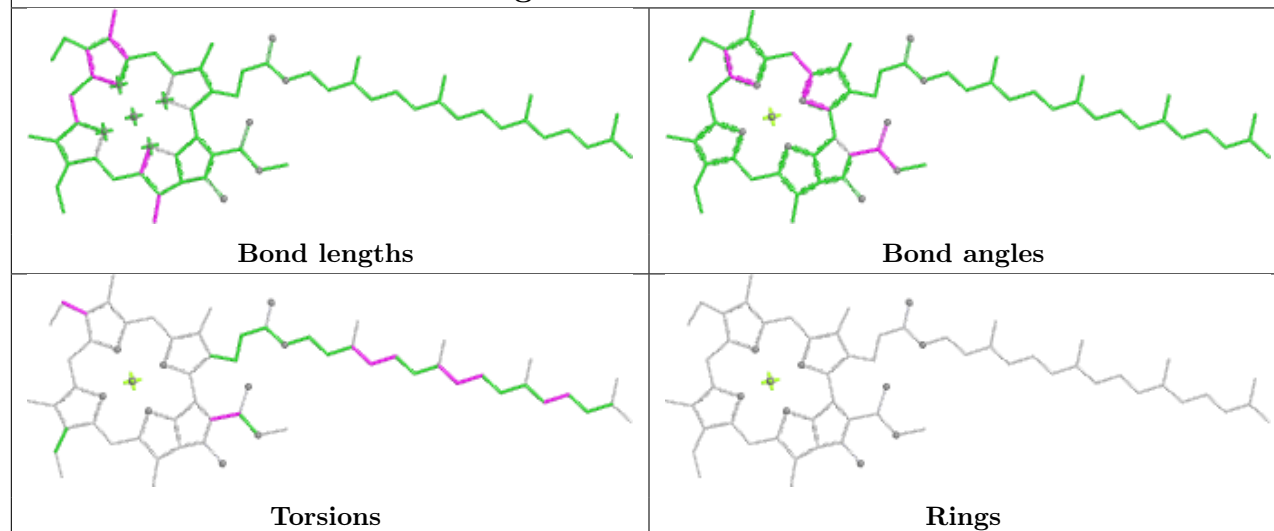
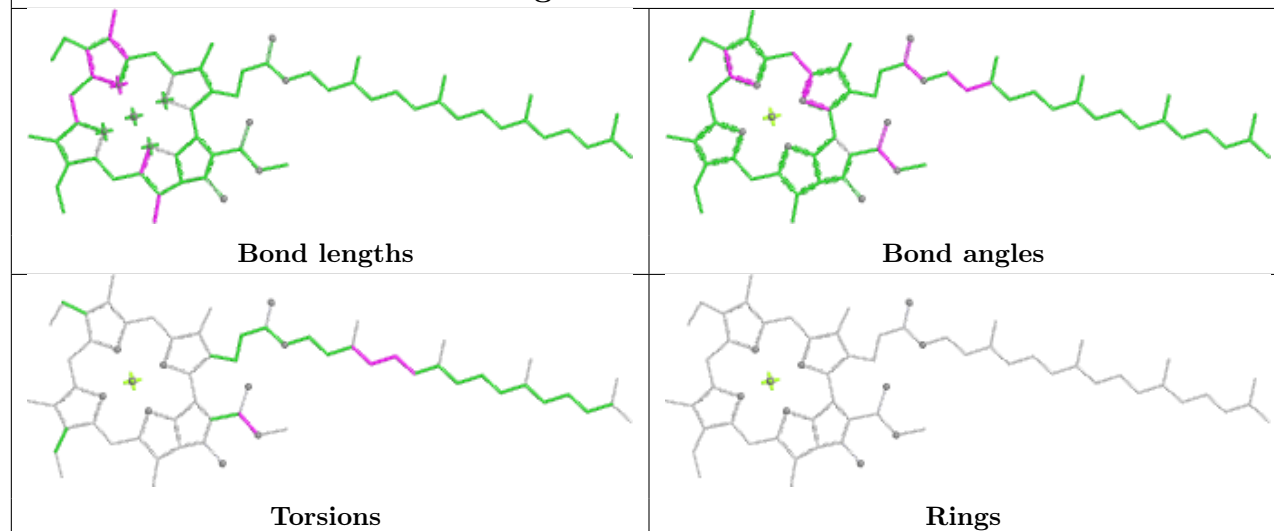
Bond angles



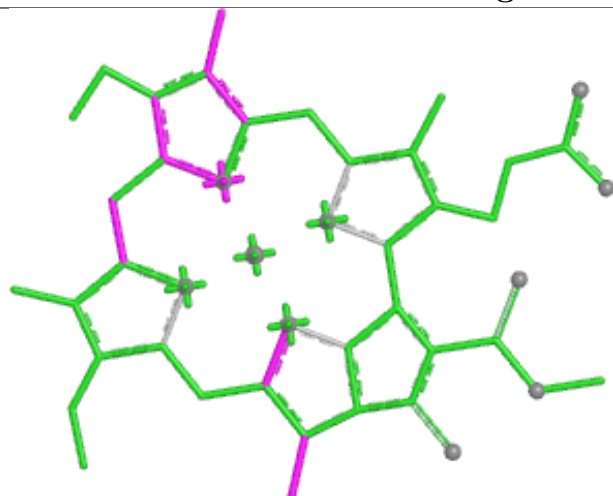
Torsions



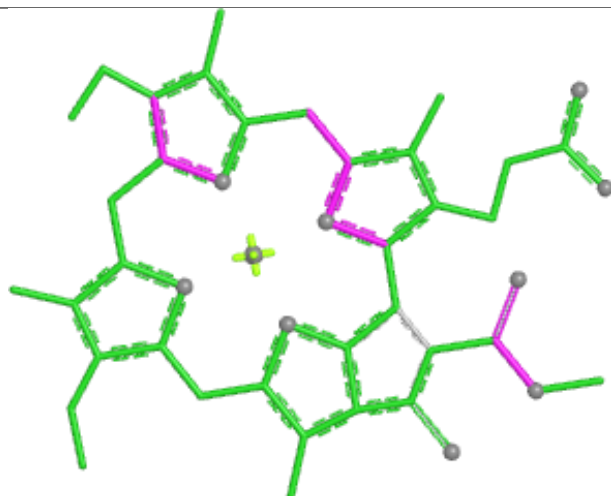
Rings

Ligand CLA cA 1136**Ligand CLA Z 510**

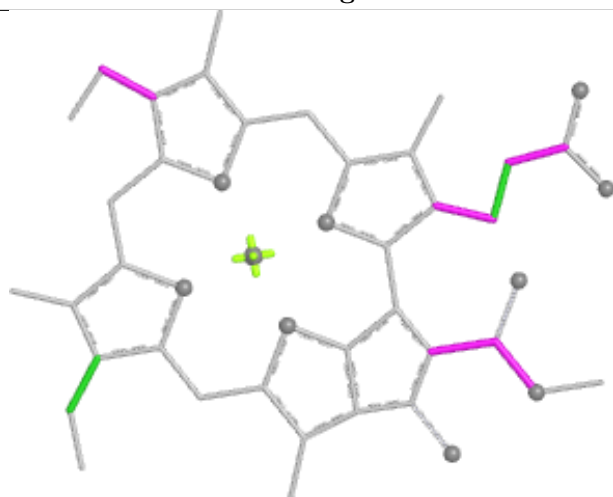
Ligand CLA aB 1232



Bond lengths



Bond angles

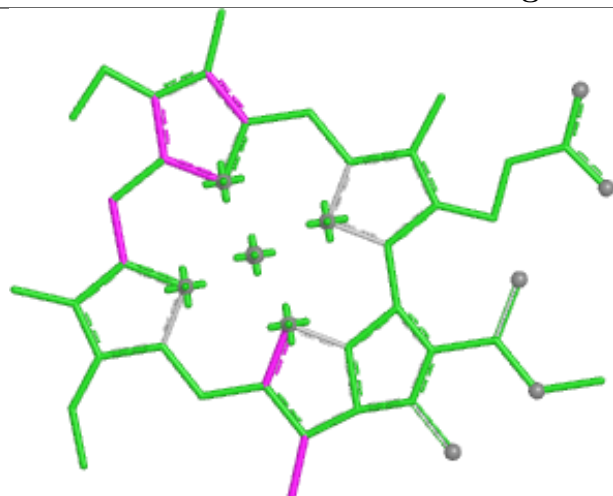


Torsions

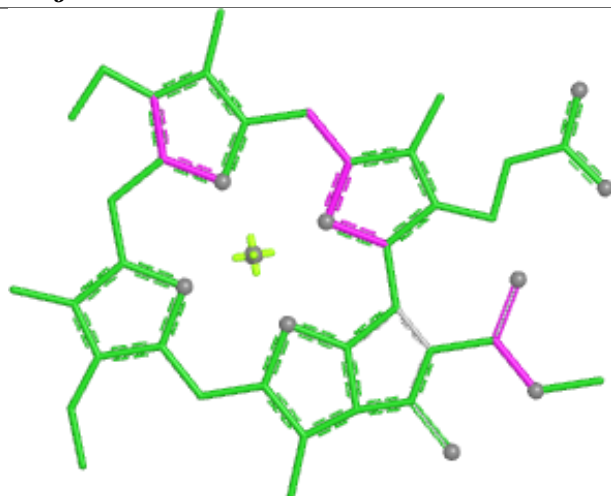


Rings

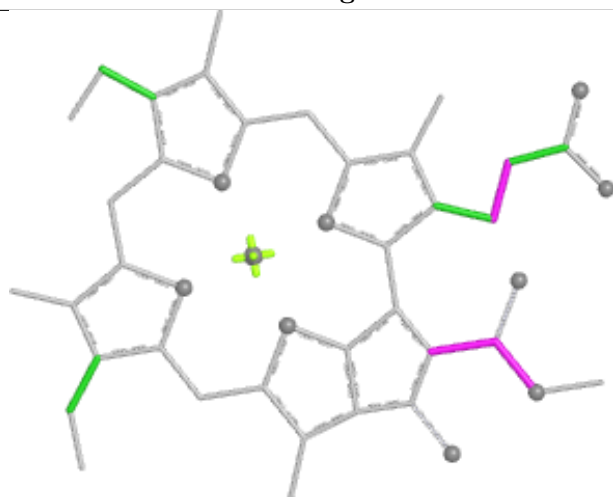
Ligand CLA j 505



Bond lengths



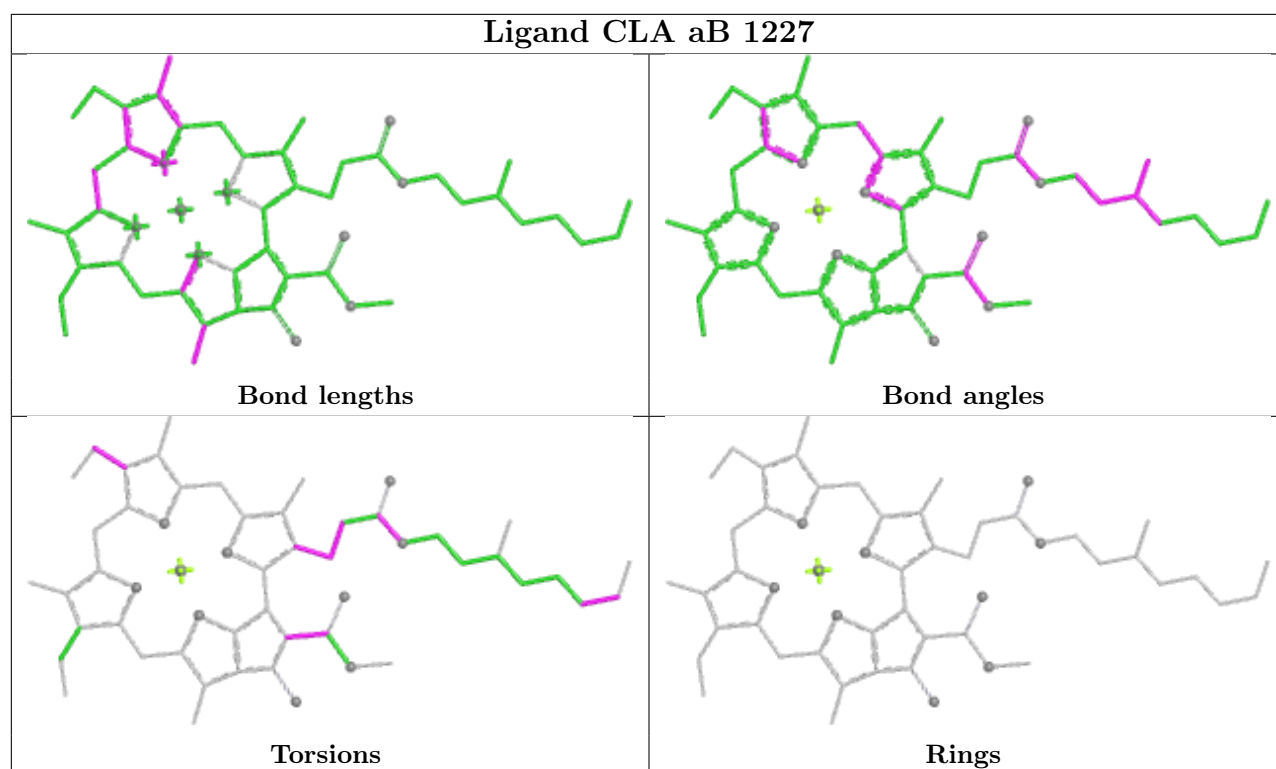
Bond angles



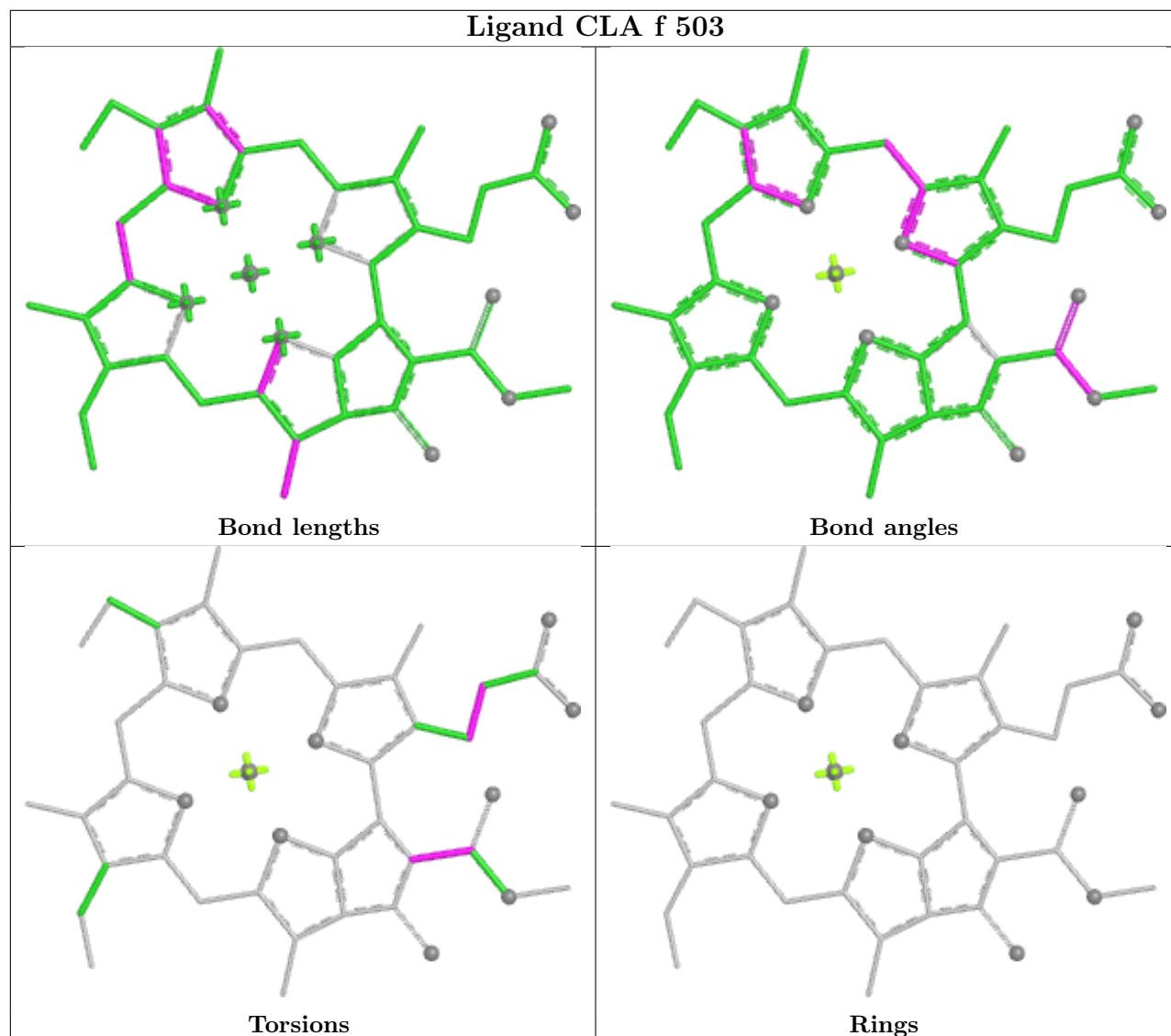
Torsions



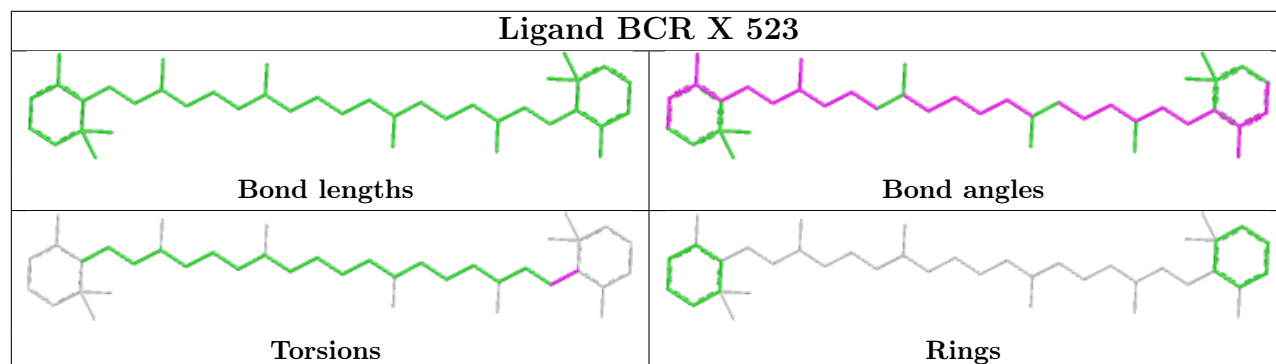
Rings



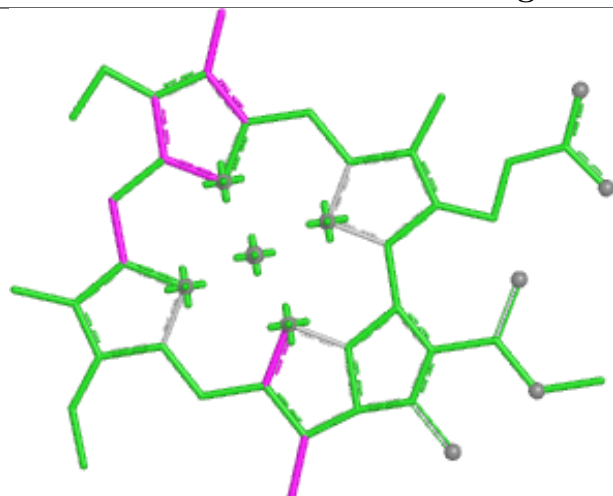
Ligand CLA f 503



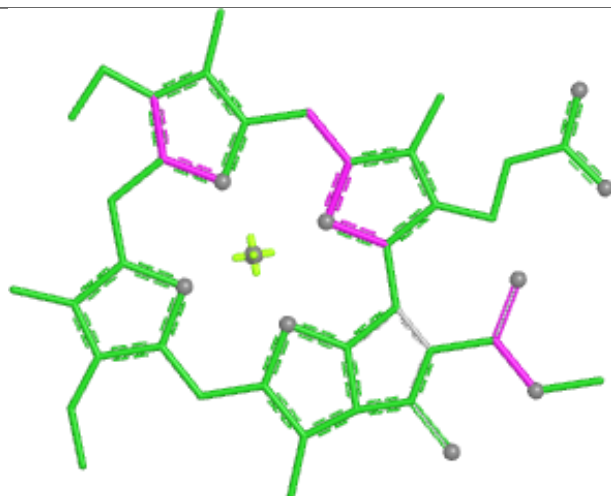
Ligand BCR X 523



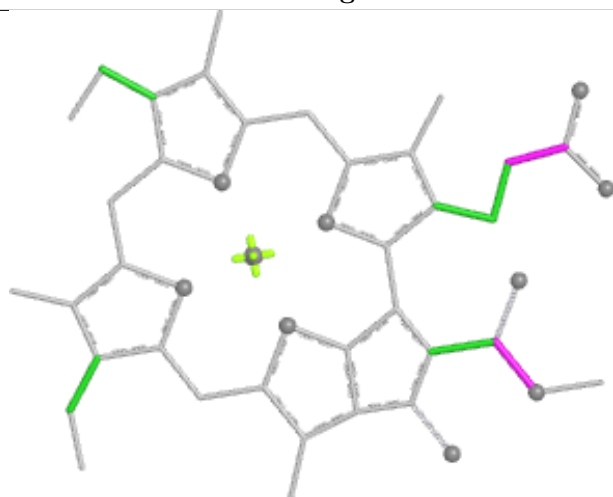
Ligand CLA n 510



Bond lengths



Bond angles

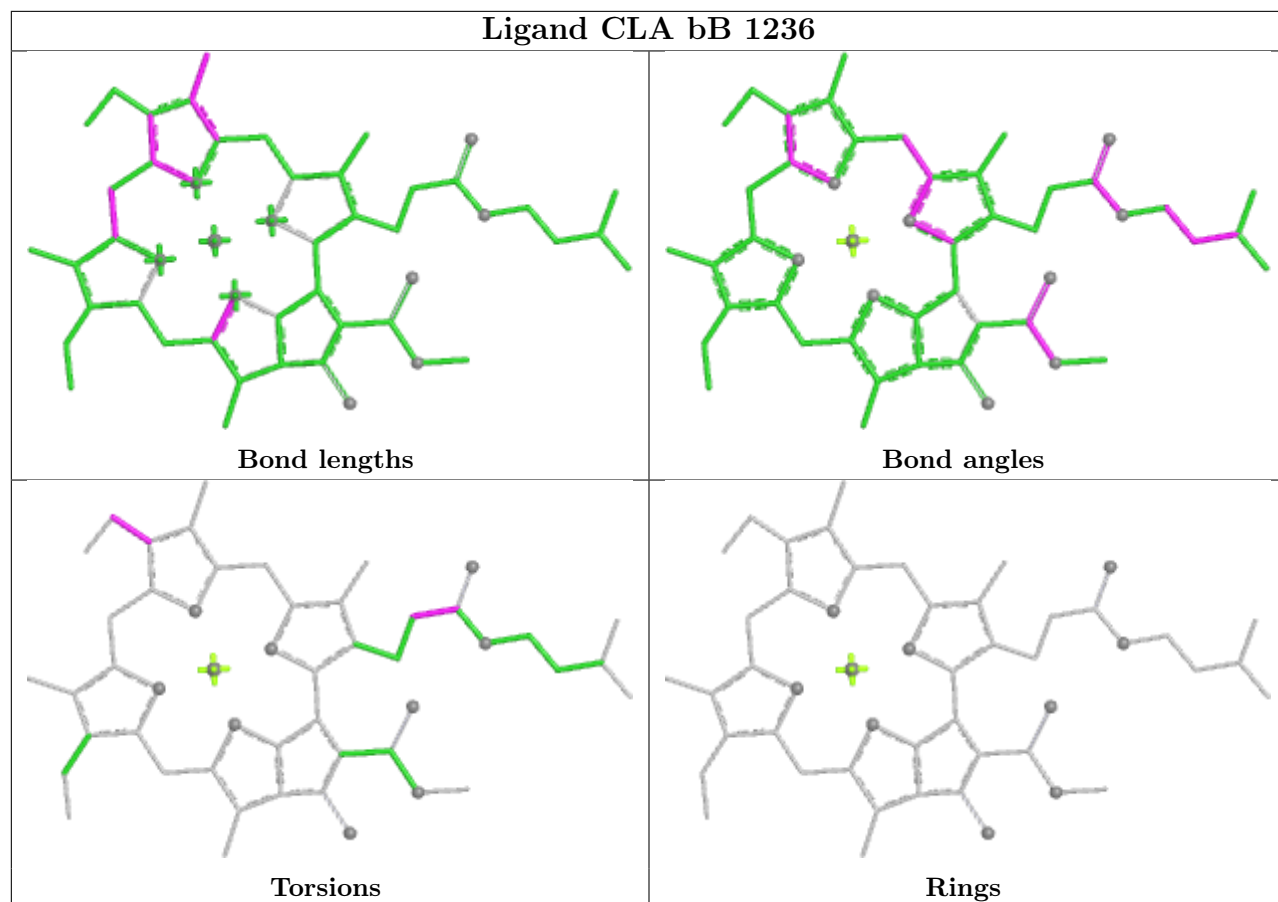


Torsions

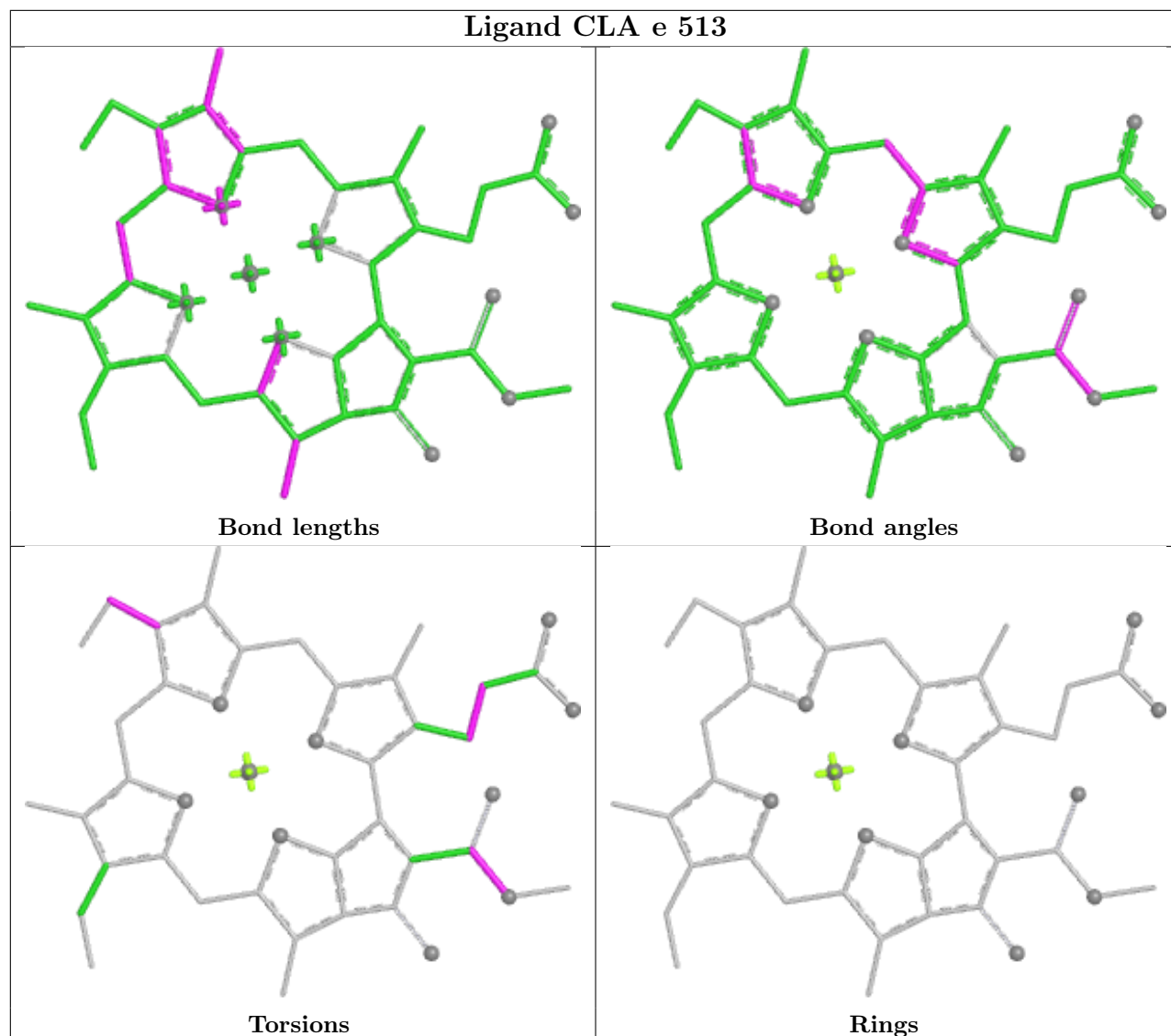


Rings

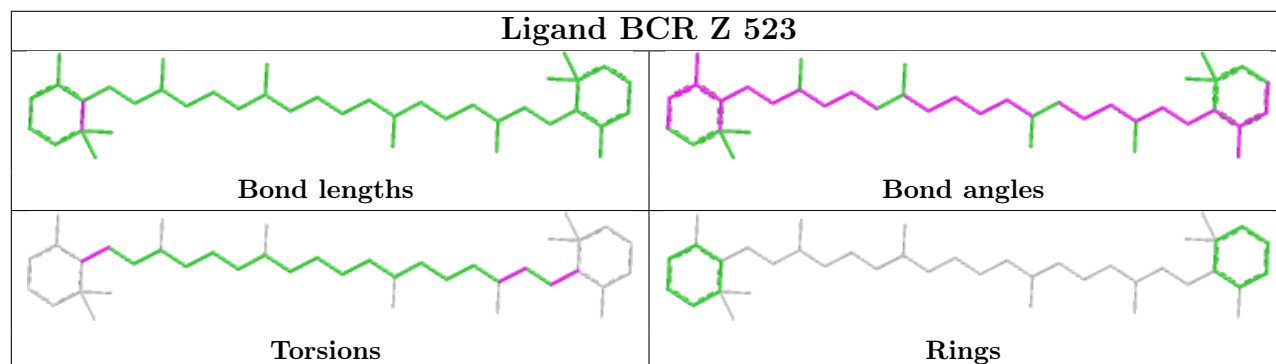
Ligand CLA bB 1236

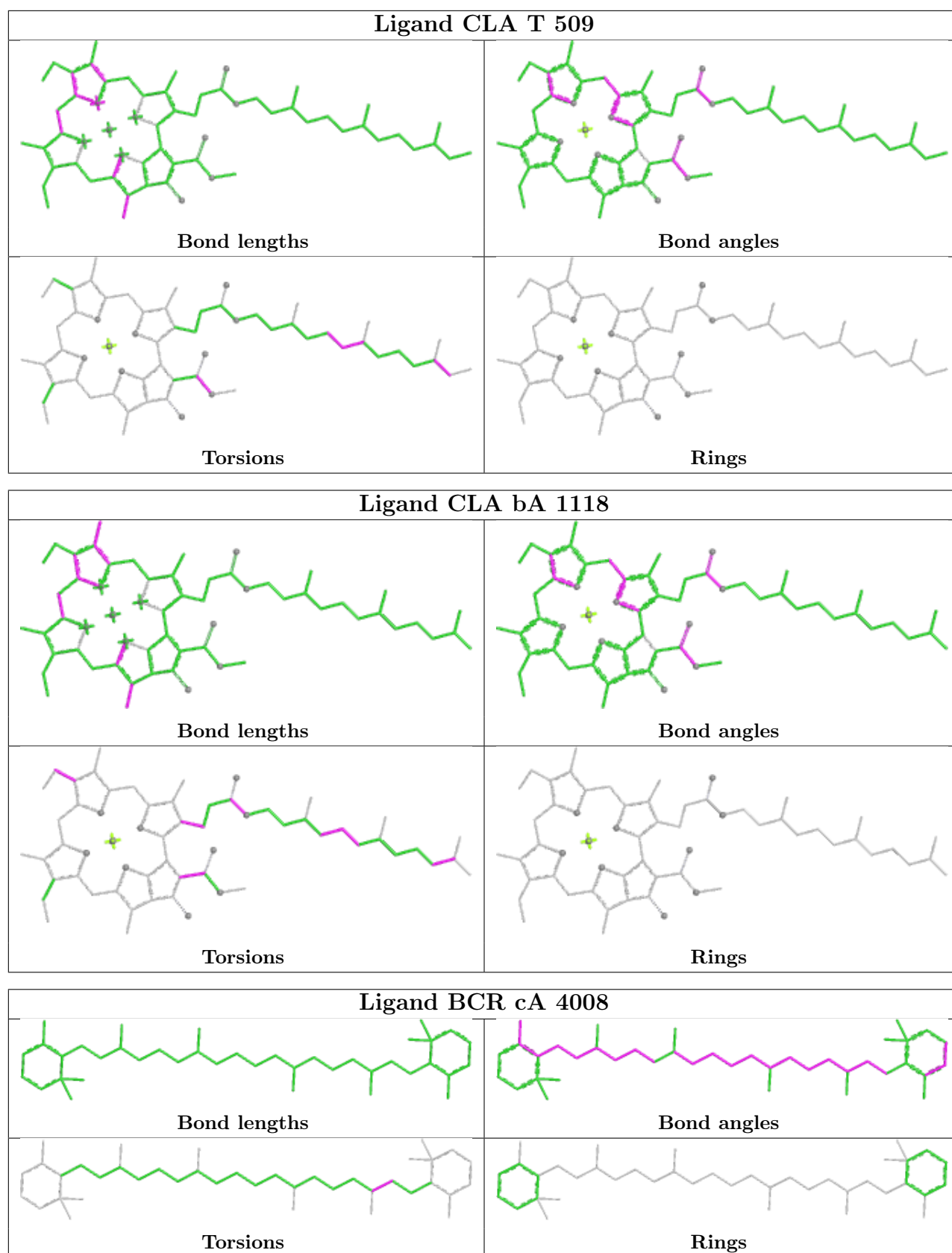


Ligand CLA e 513

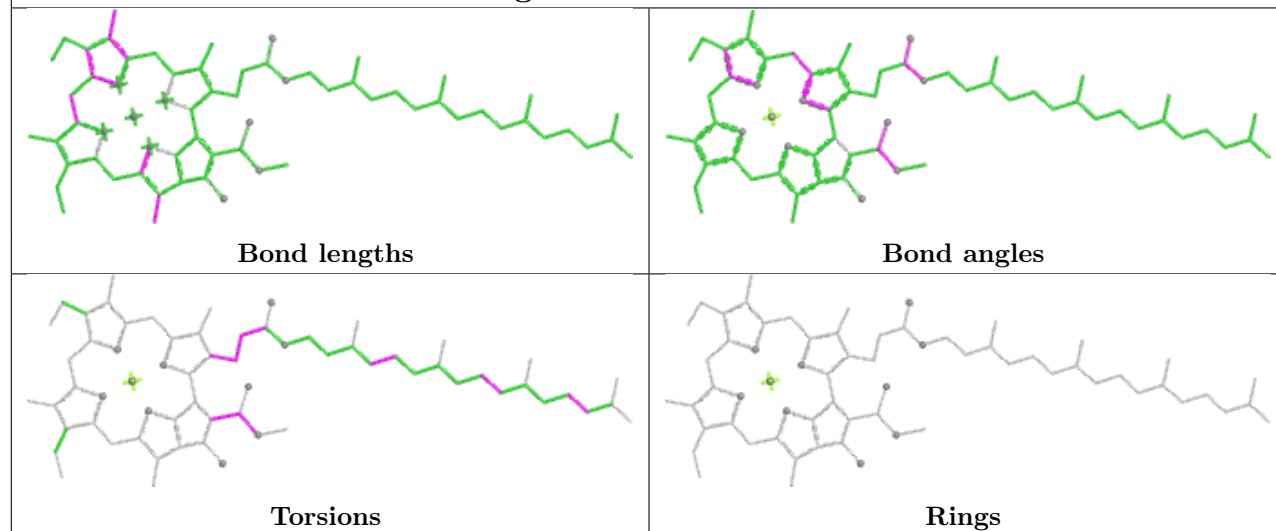


Ligand BCR Z 523

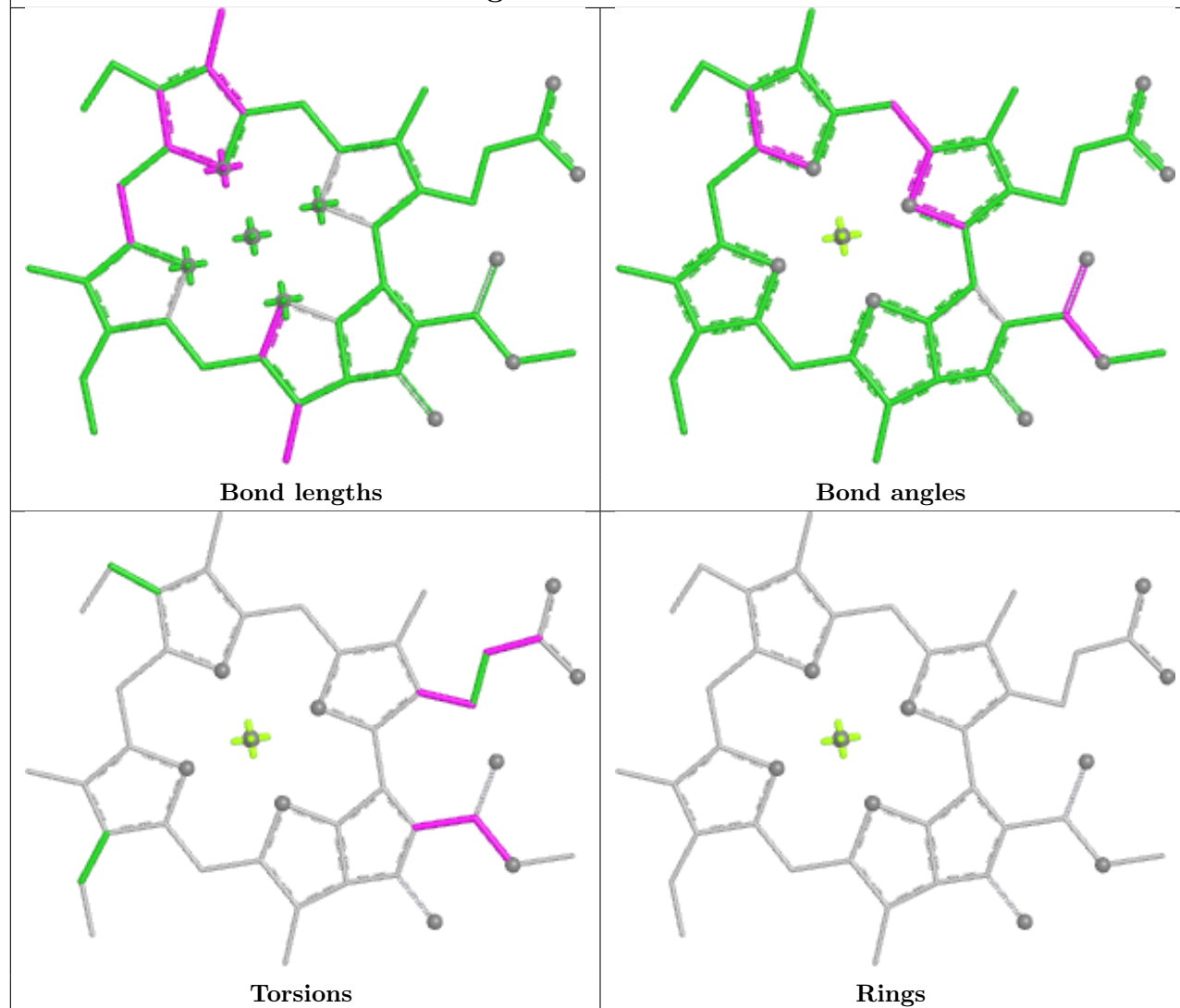




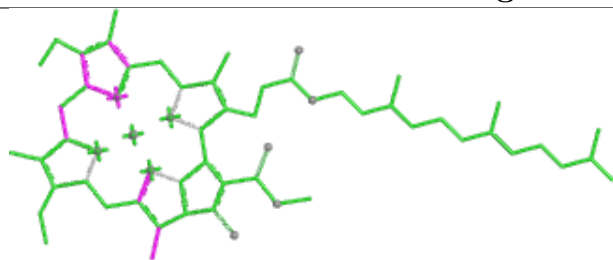
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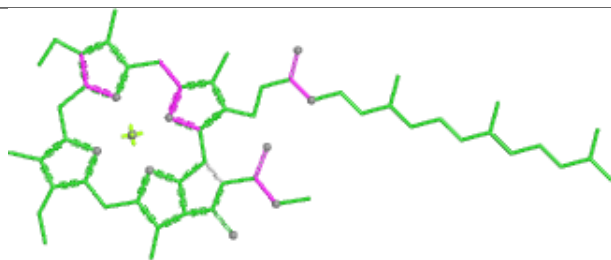
Ligand CLA W 511



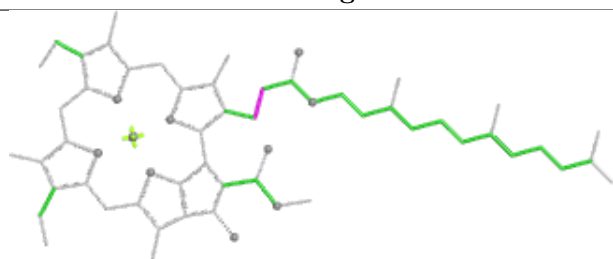
Ligand CLA aB 1204



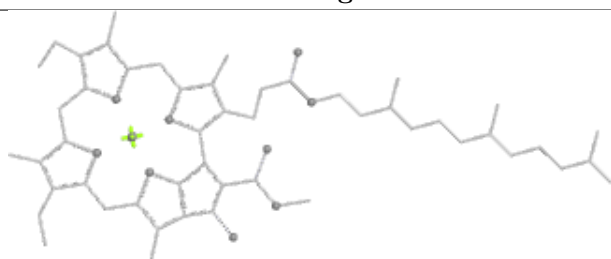
Bond lengths



Bond angles

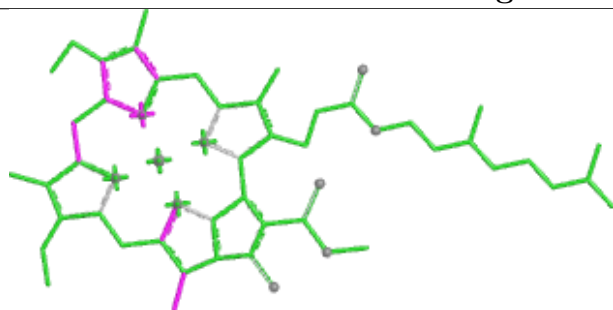


Torsions

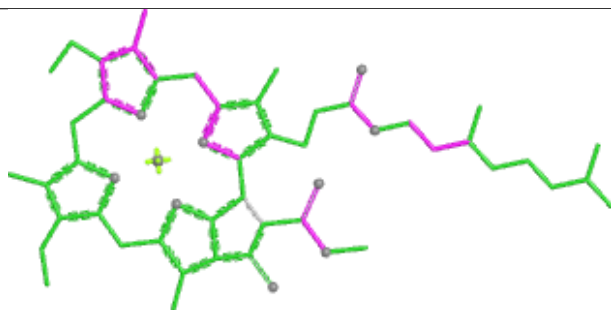


Rings

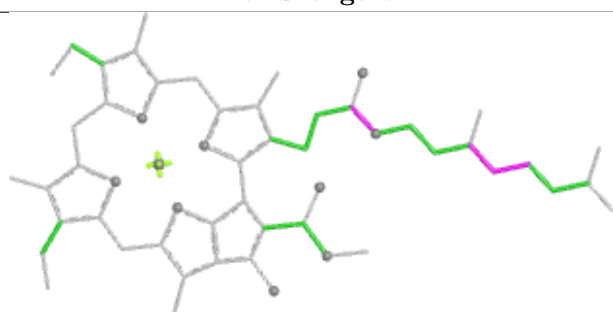
Ligand CLA aA 1130



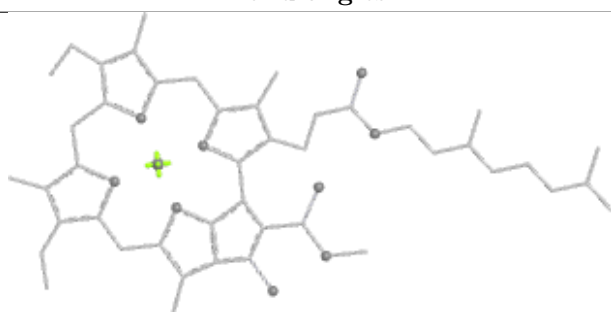
Bond lengths



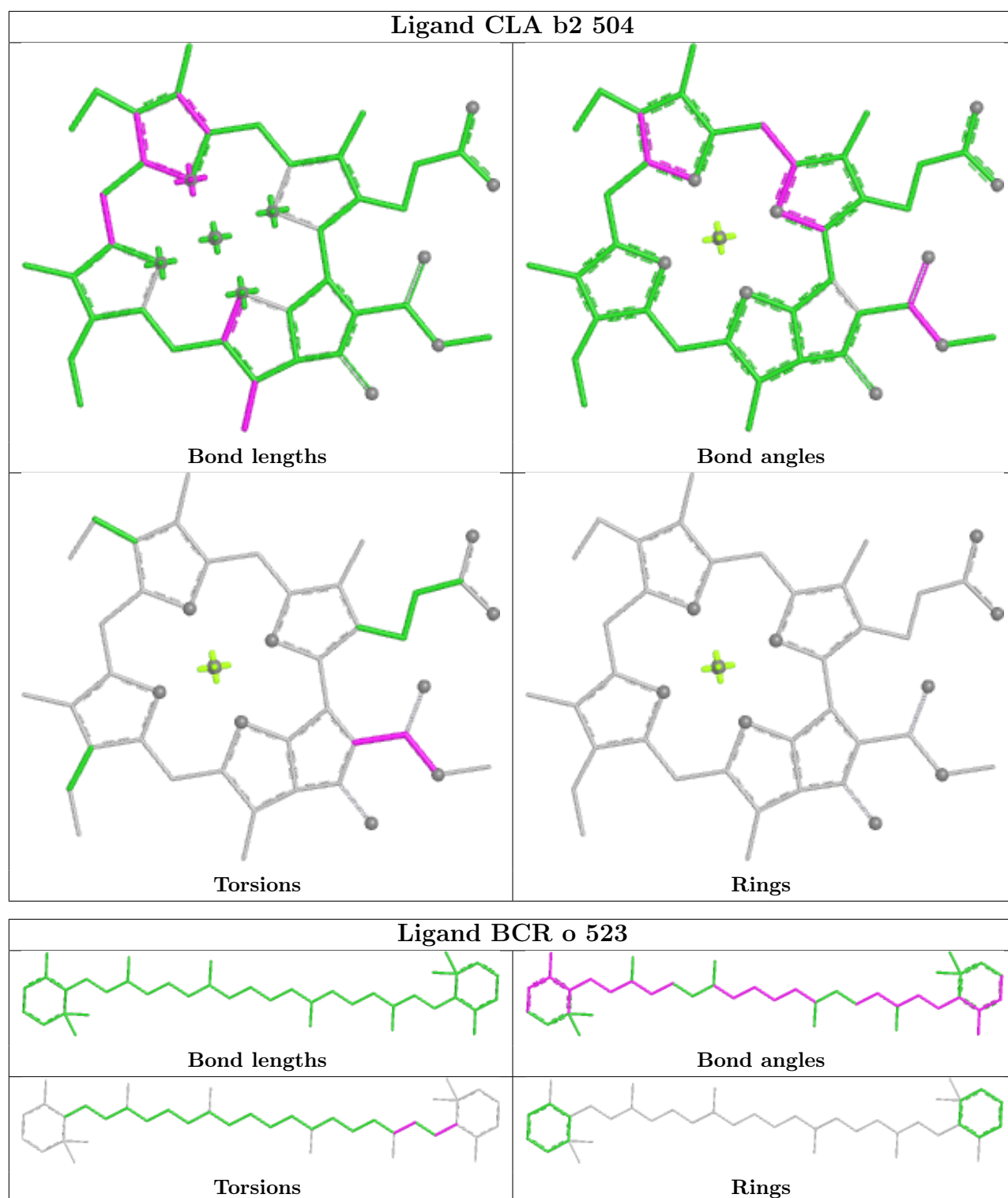
Bond angles

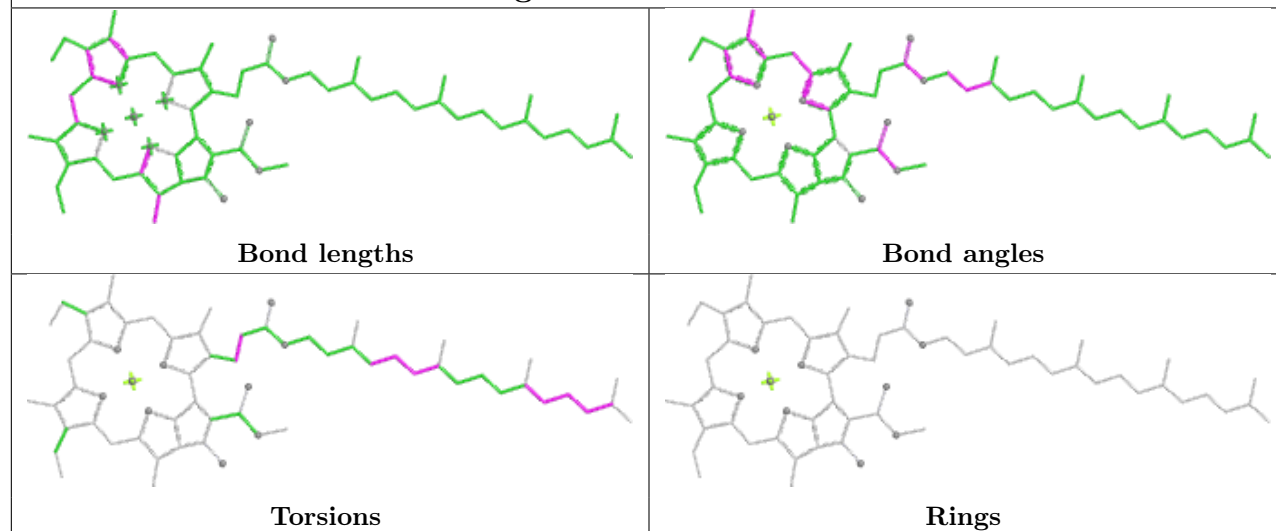
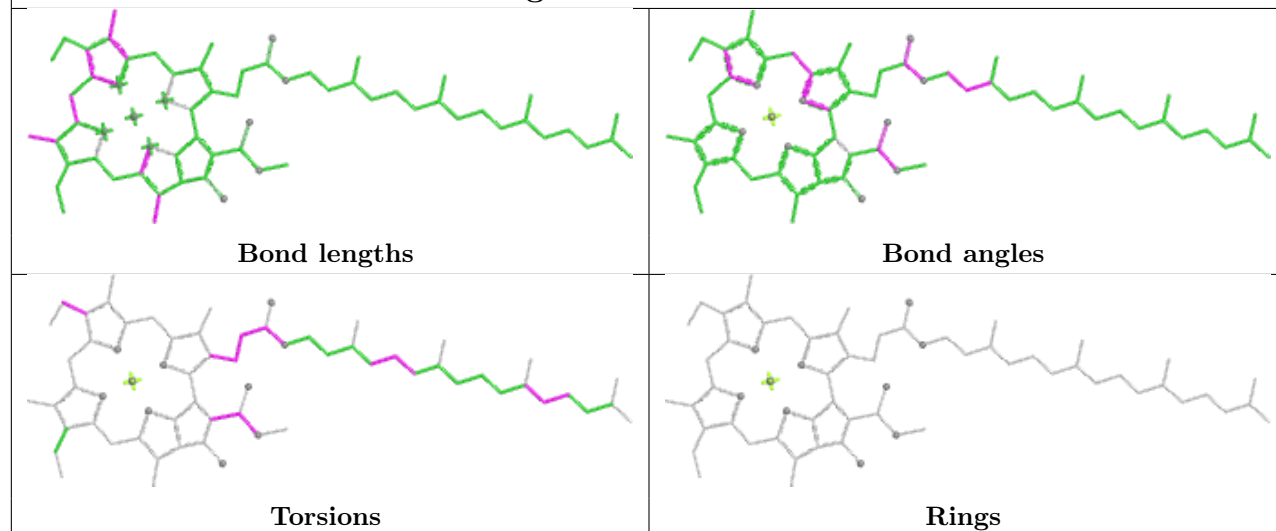


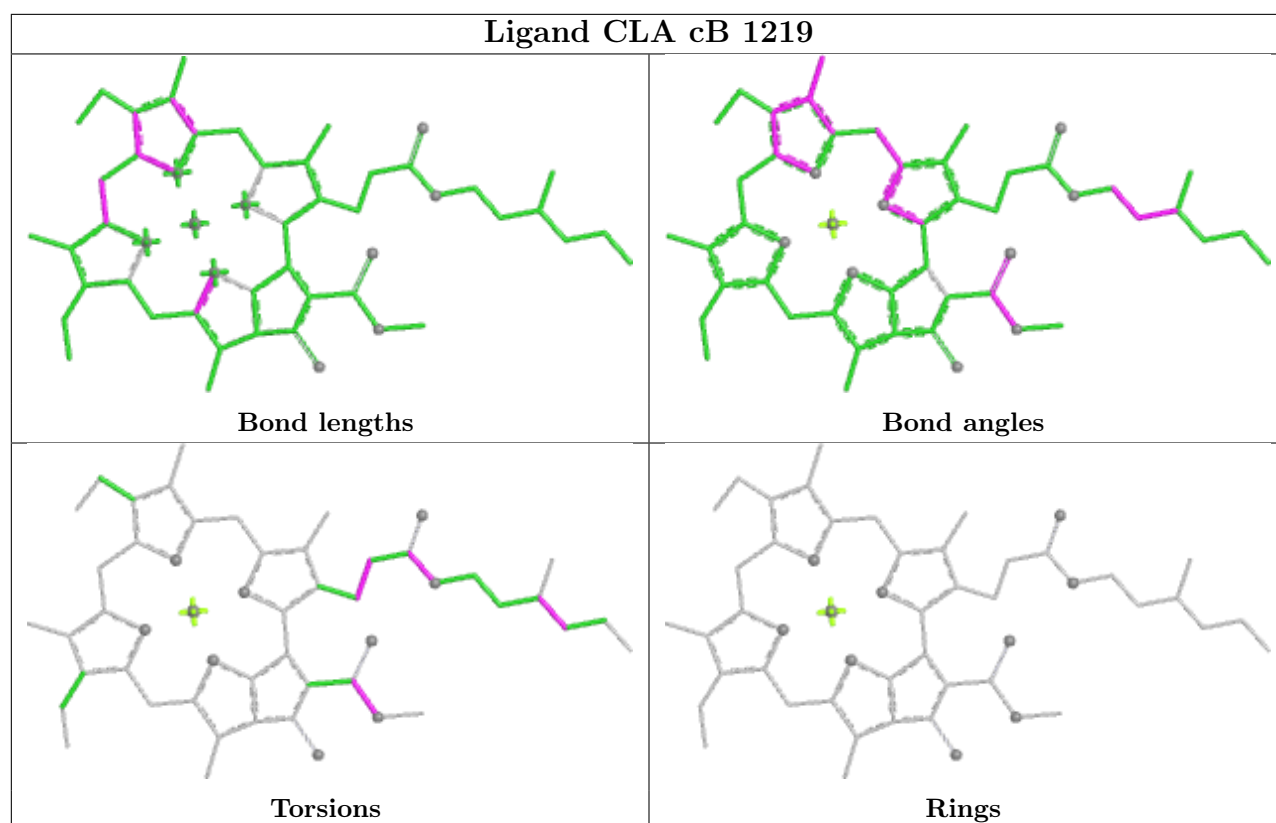
Torsions



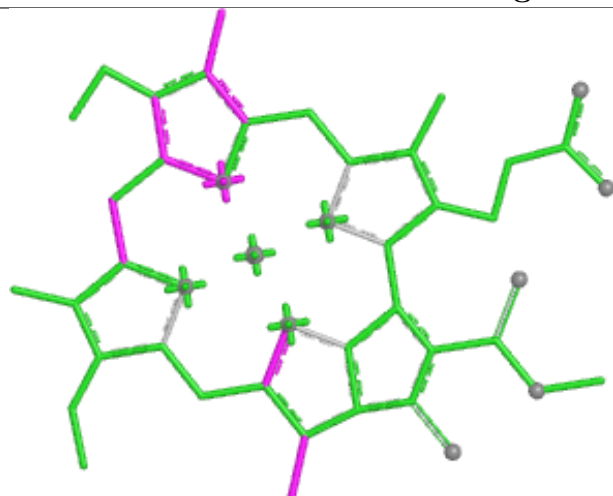
Rings



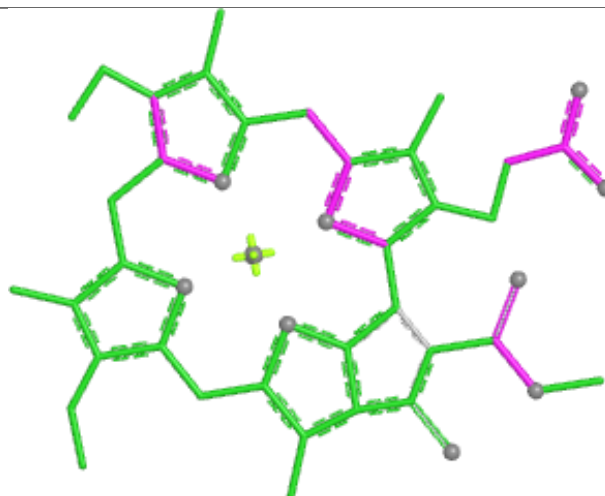
Ligand CLA aB 1213**Ligand CLA b4 501**



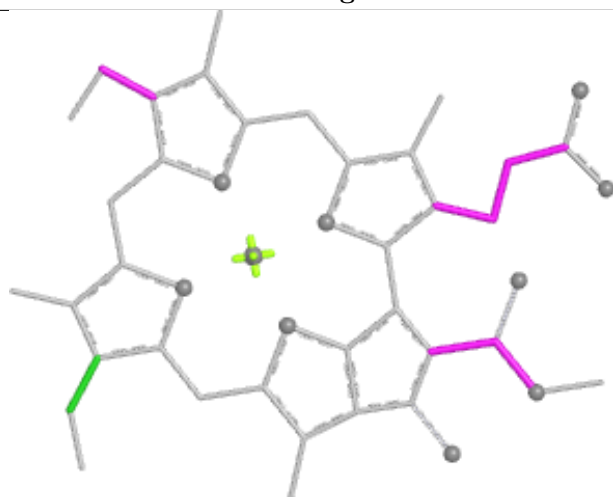
Ligand CLA V 517



Bond lengths



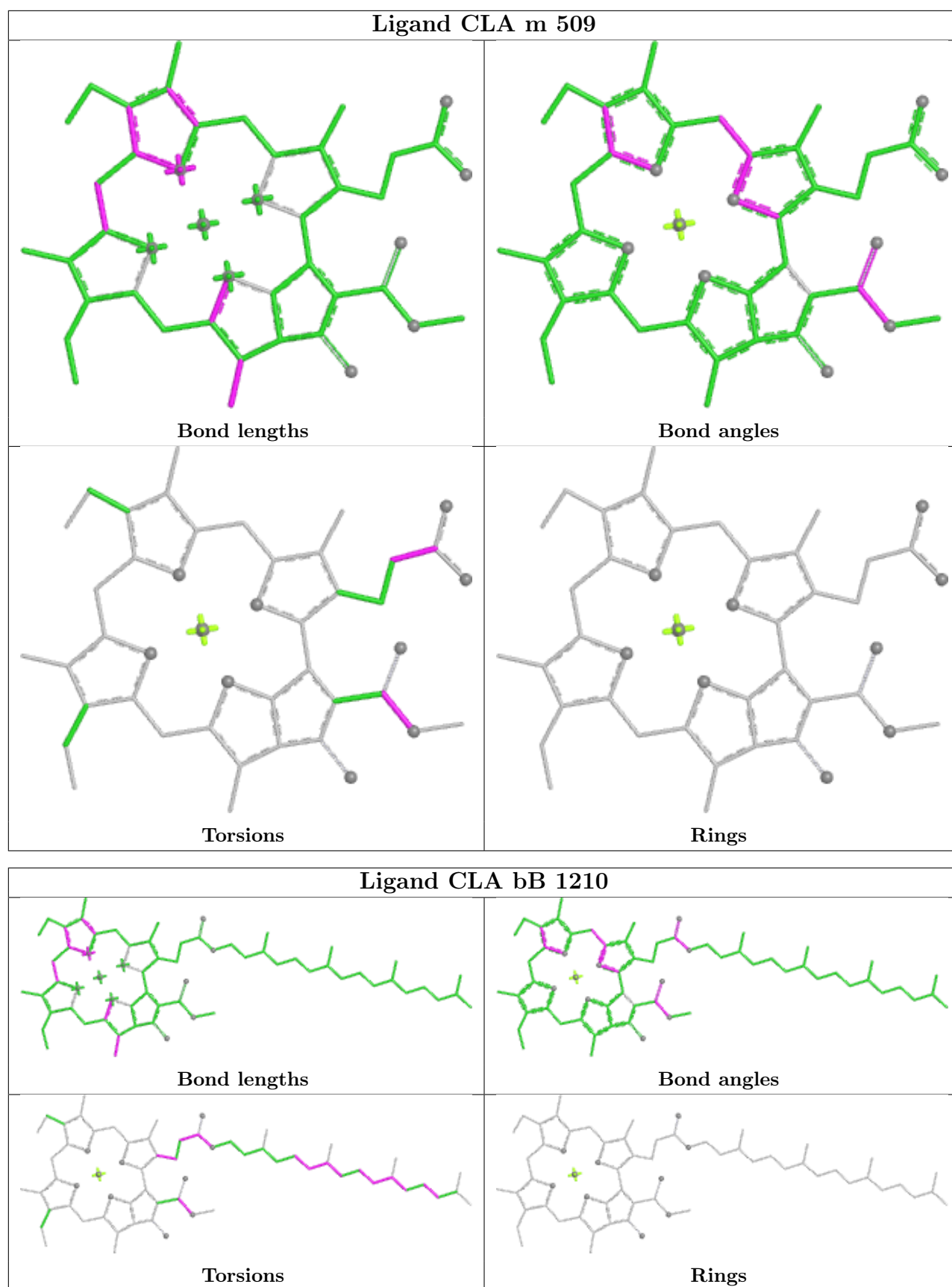
Bond angles

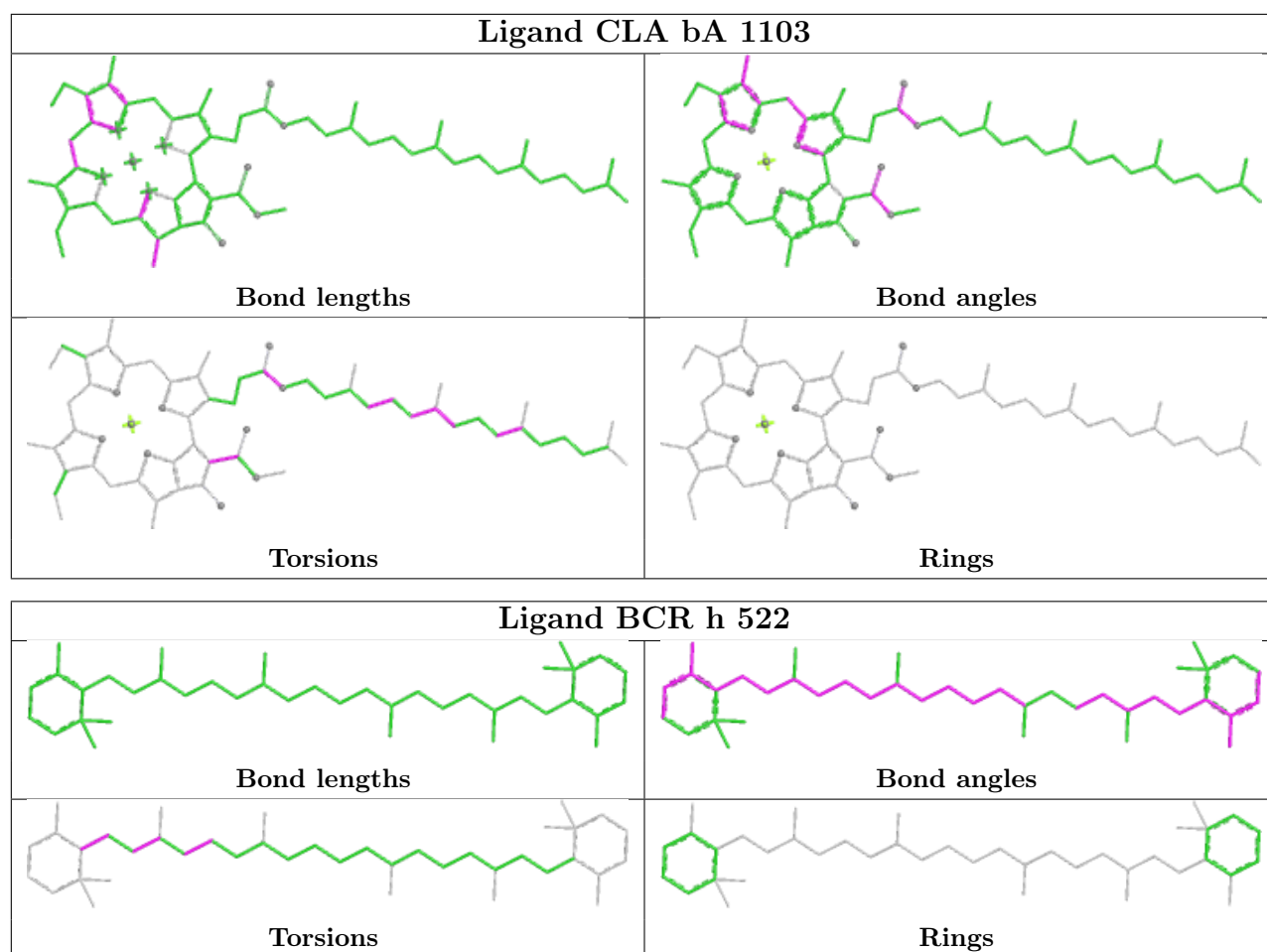


Torsions

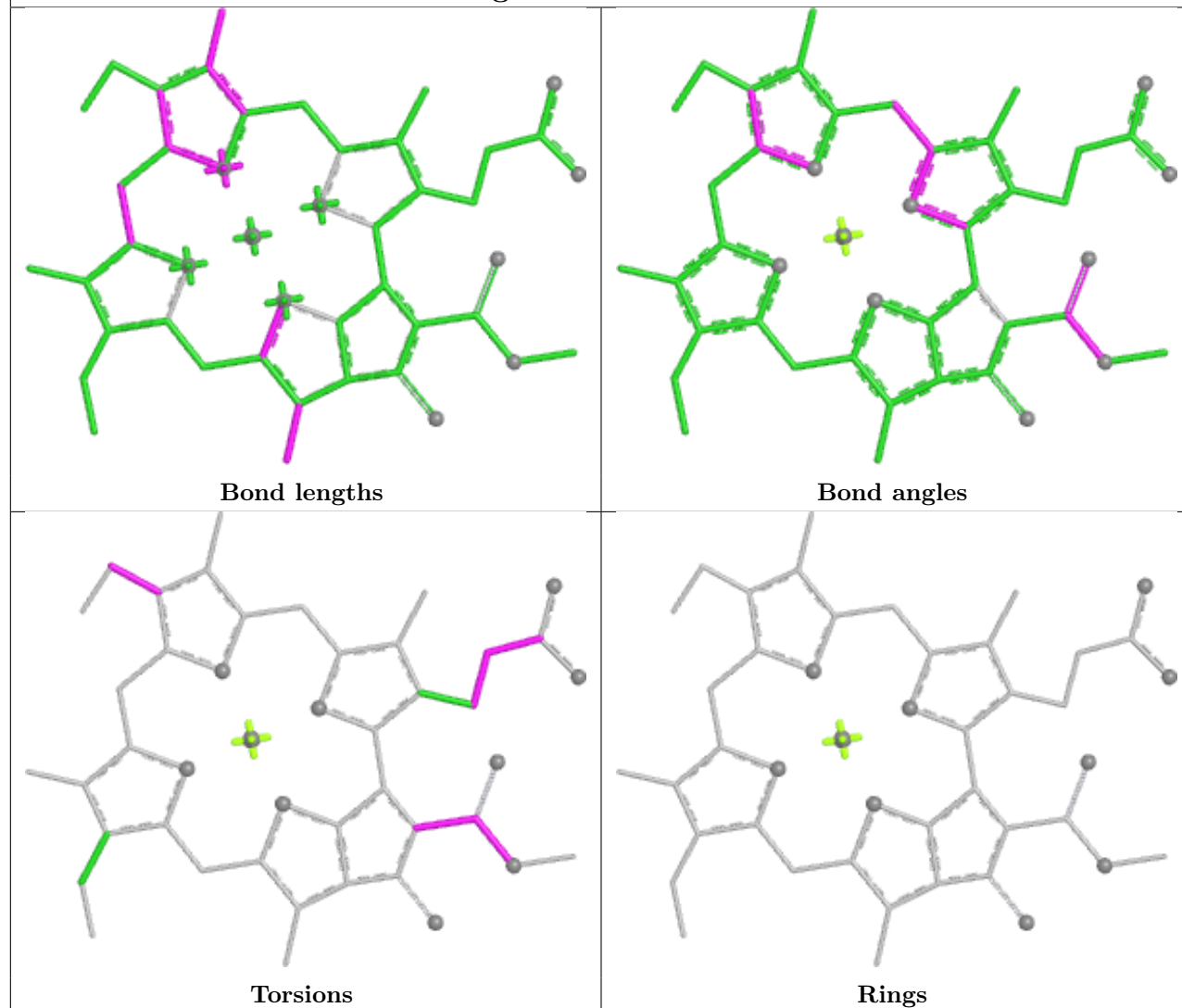


Rings

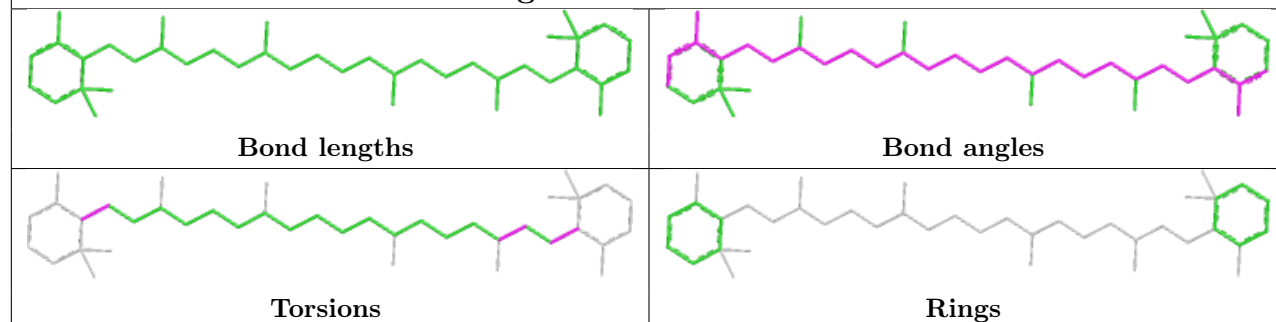




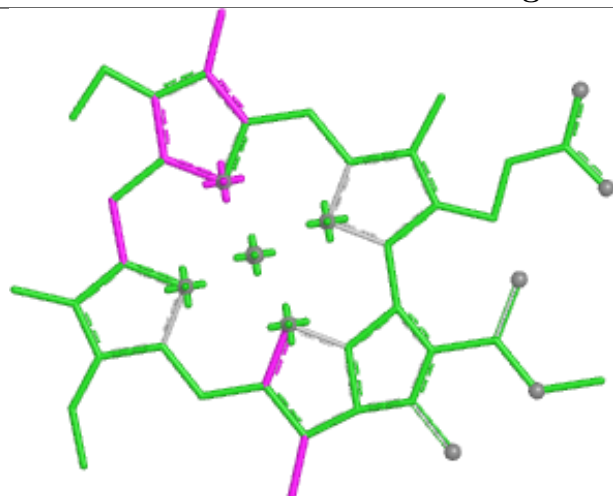
Ligand CLA Y 512



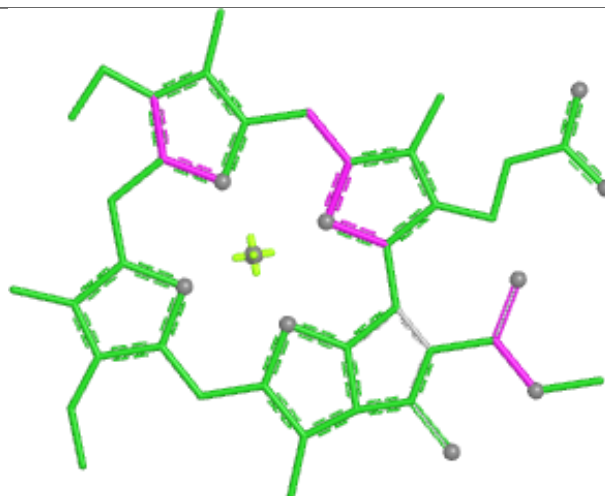
Ligand BCR cJ 4013



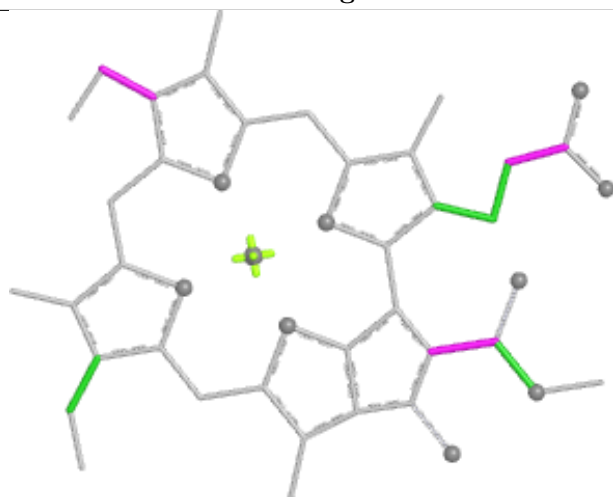
Ligand CLA i 512



Bond lengths



Bond angles

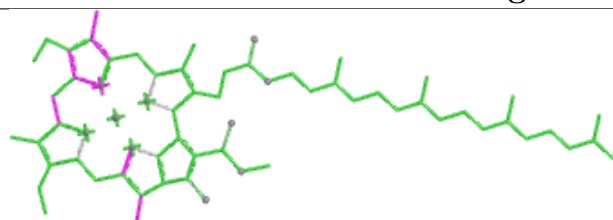


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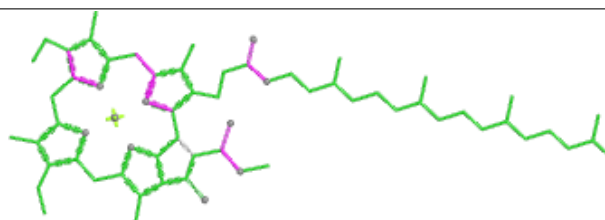


Rings

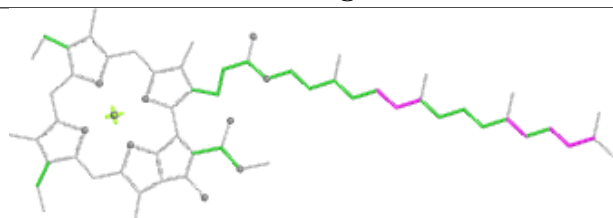
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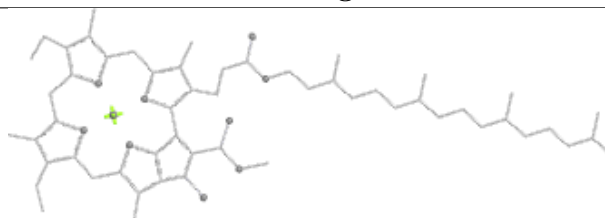
Bond lengths



Bond angles

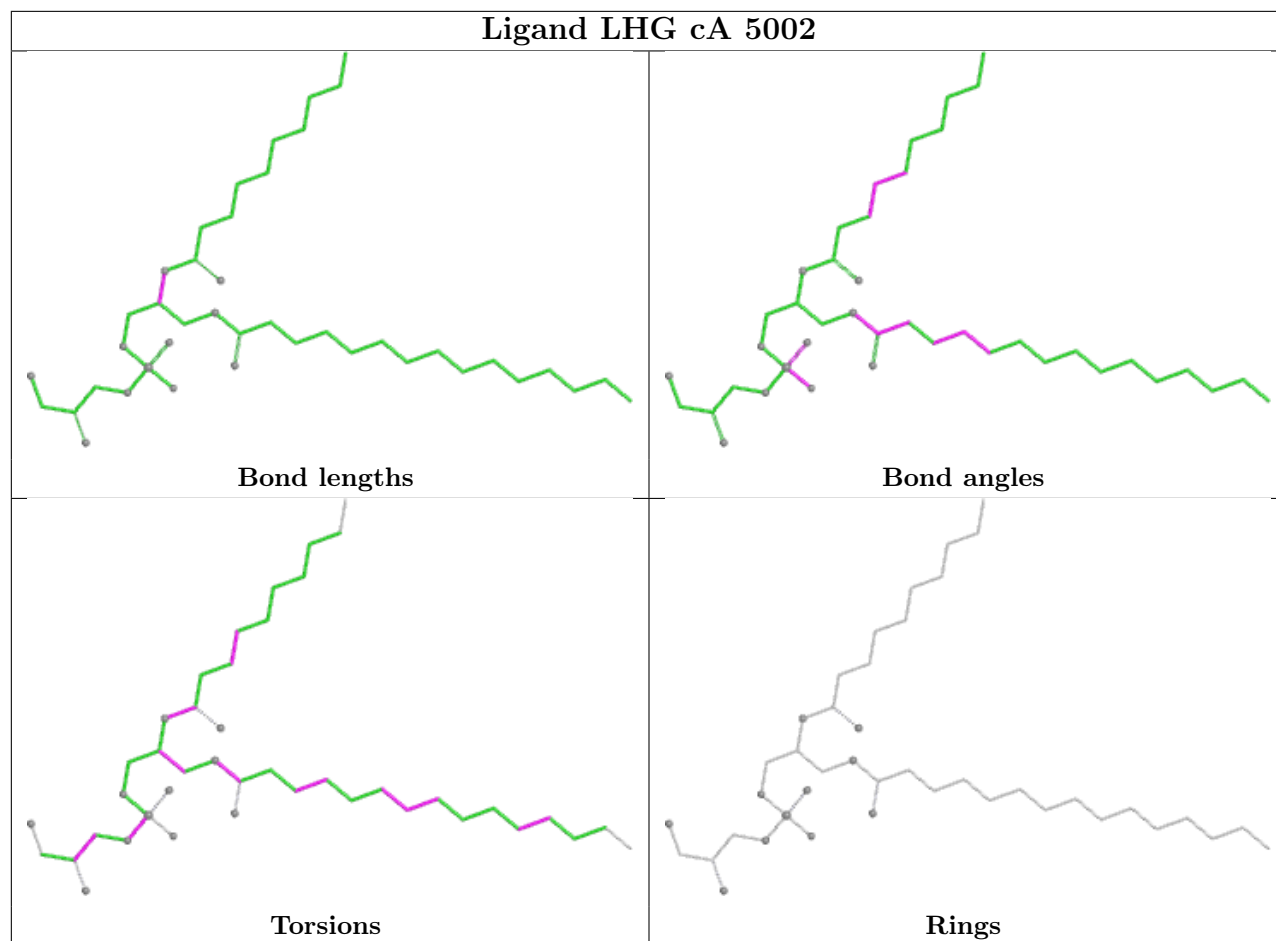


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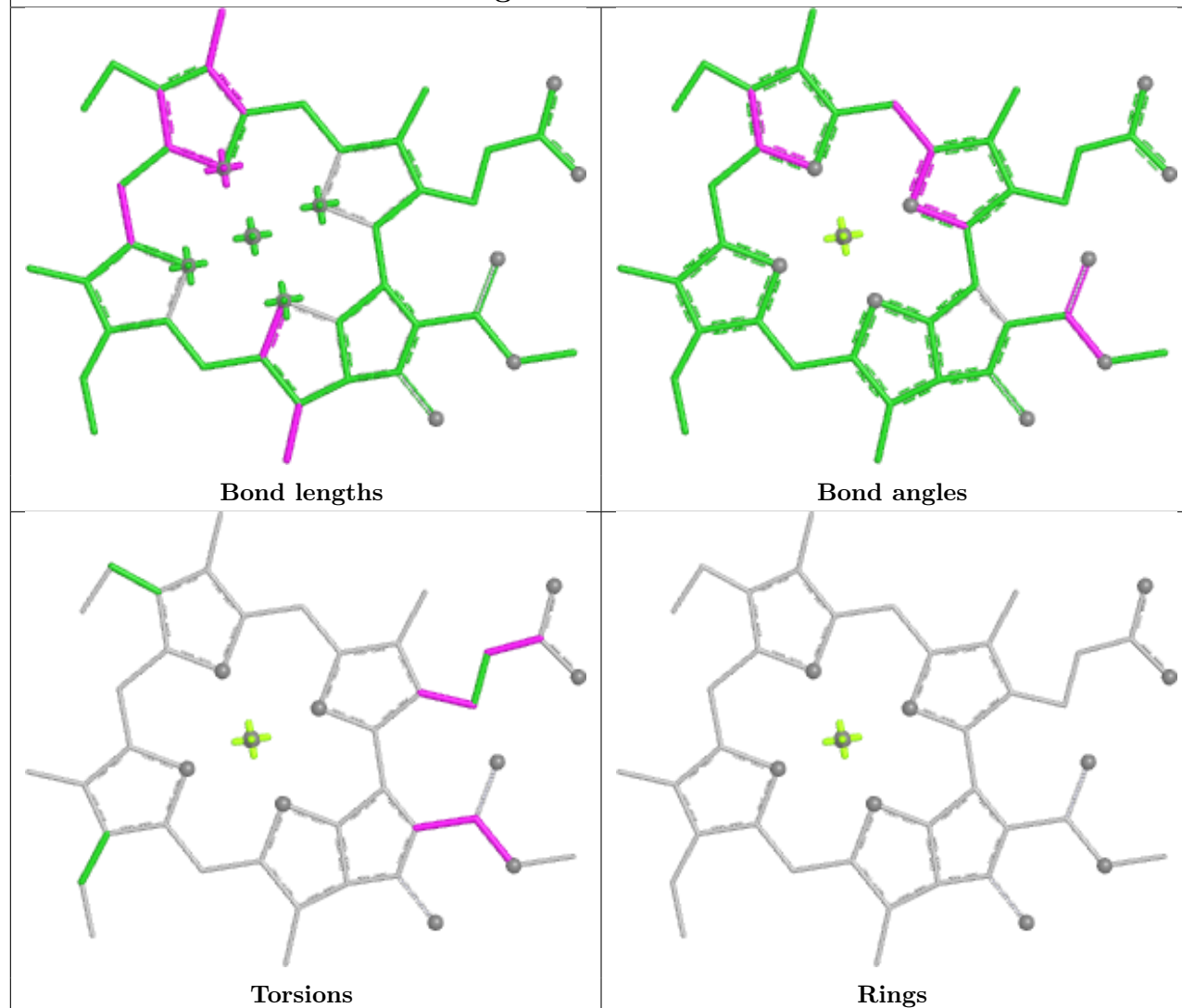


Rings

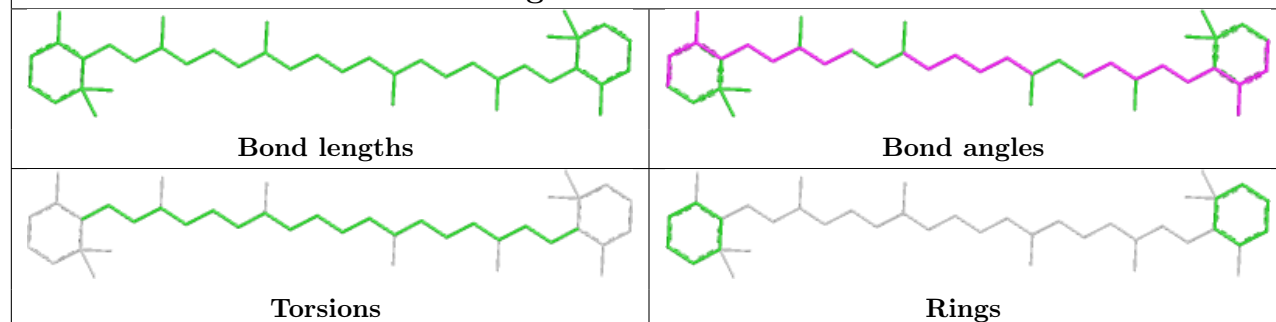
Ligand LHG cA 5002



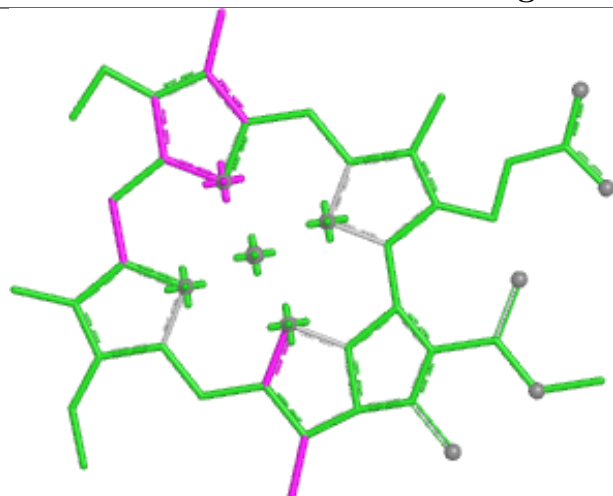
Ligand CLA Z 506



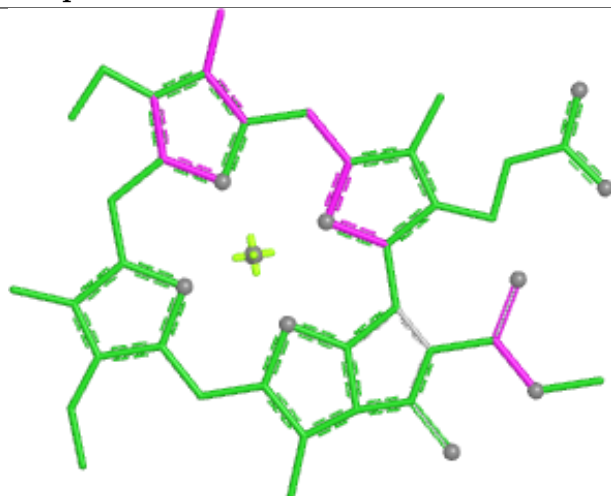
Ligand BCR c5 523



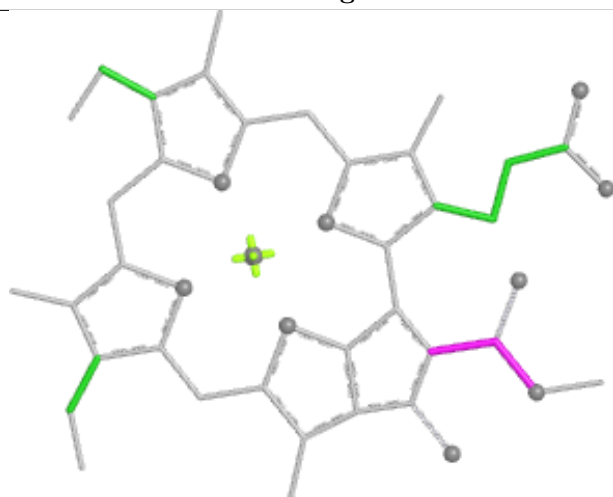
Ligand CLA q 506



Bond lengths



Bond angles

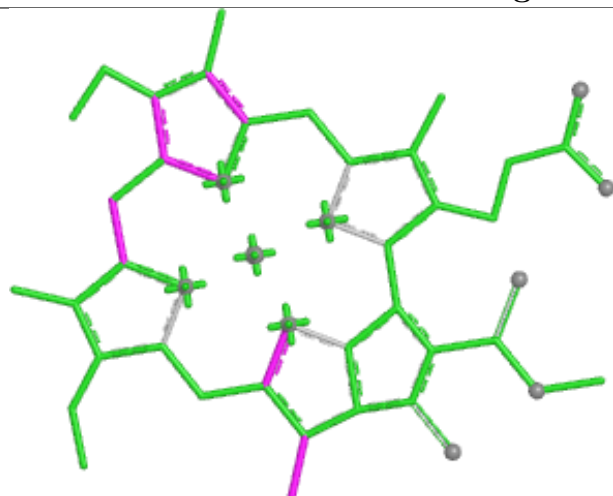


Torsions



Rings

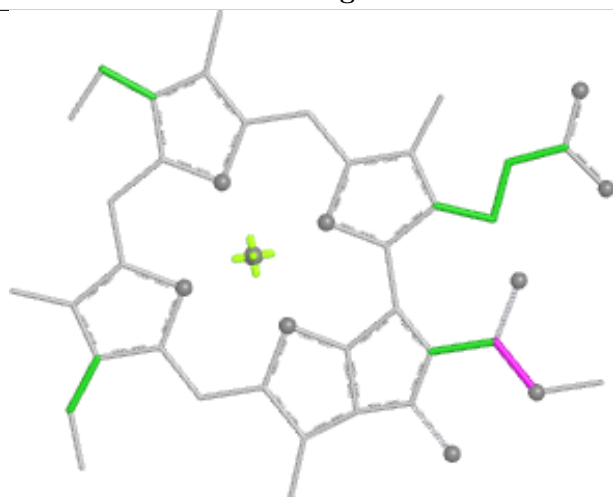
Ligand CLA U 503



Bond lengths



Bond angles

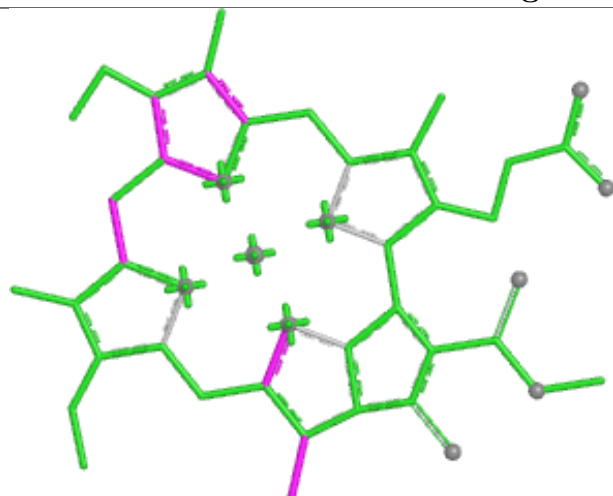


Torsions

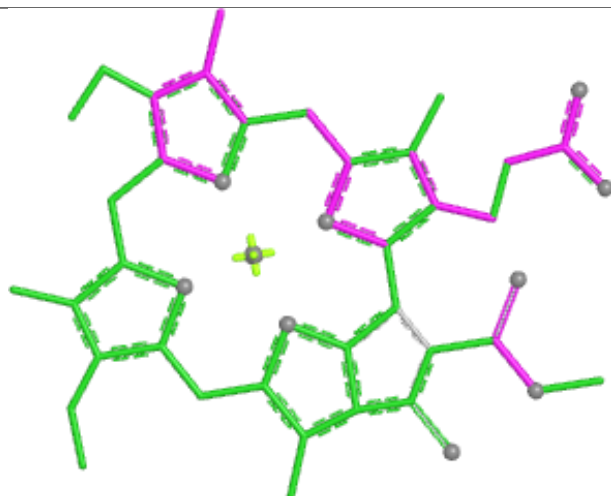


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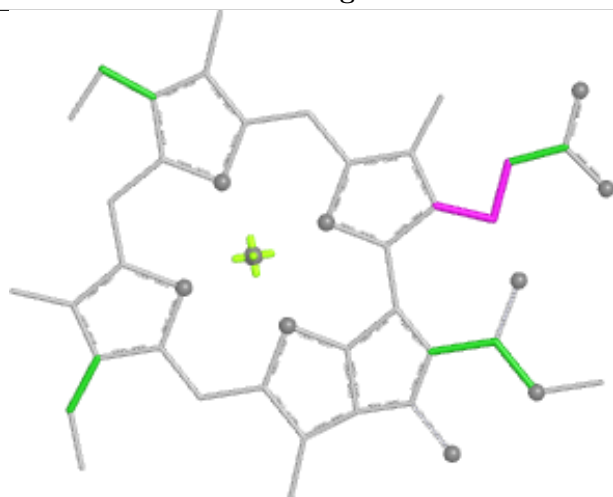
Ligand CLA f 505



Bond lengths



Bond angles

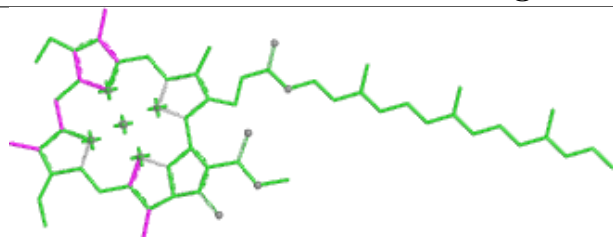


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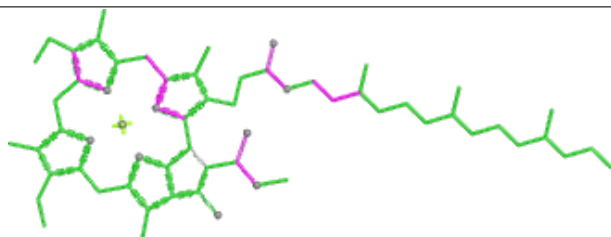


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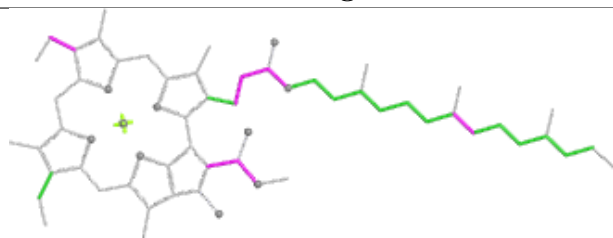
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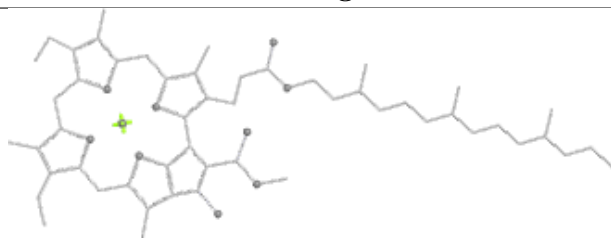
Bond lengths



Bond angles

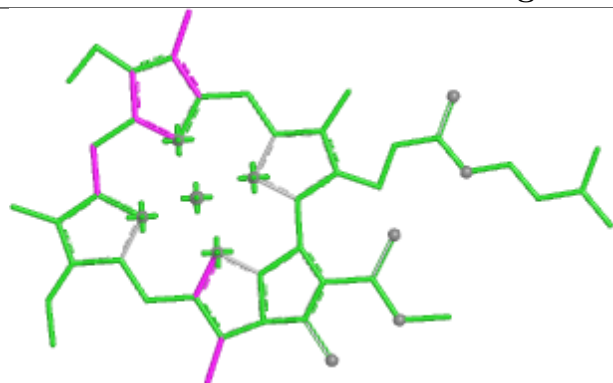


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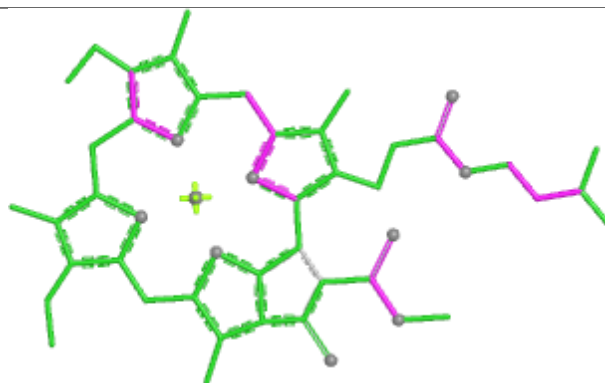


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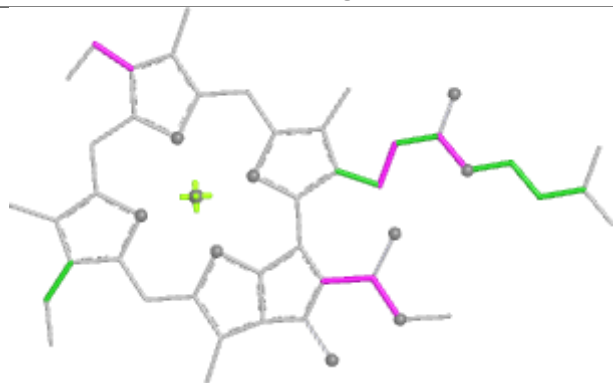
Ligand CLA b 504



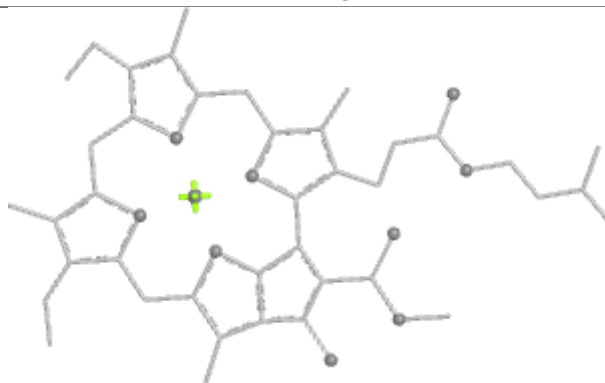
Bond lengths



Bond angles

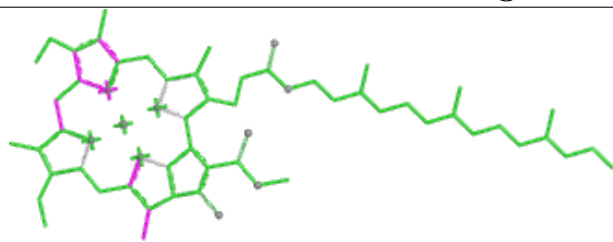


Torsions

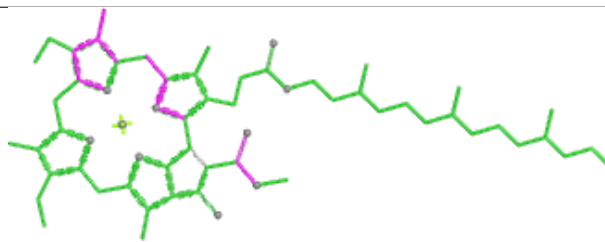


Rings

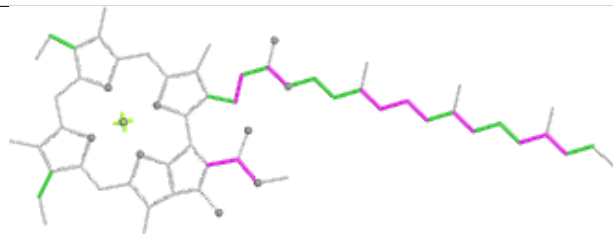
Ligand CLA cB 1012



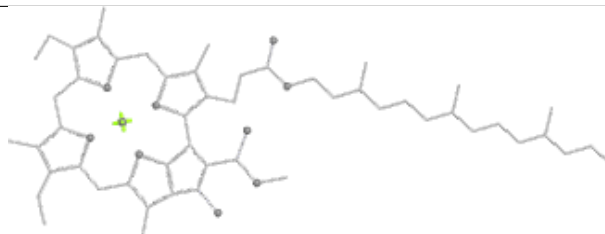
Bond lengths



Bond angles

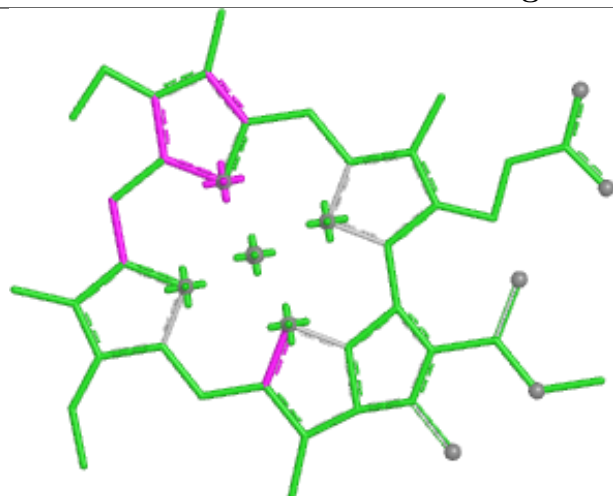


Torsions

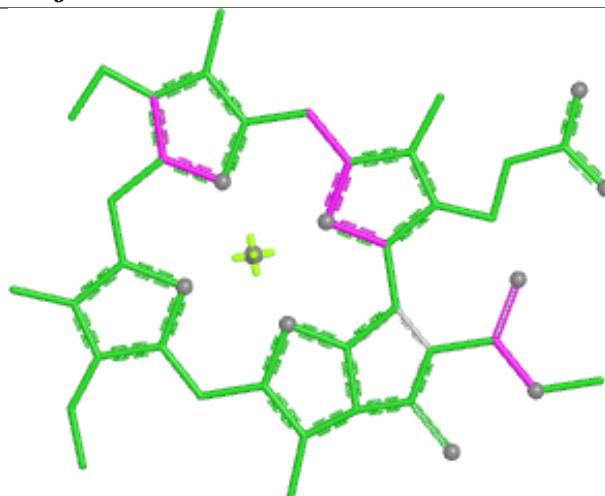


Rings

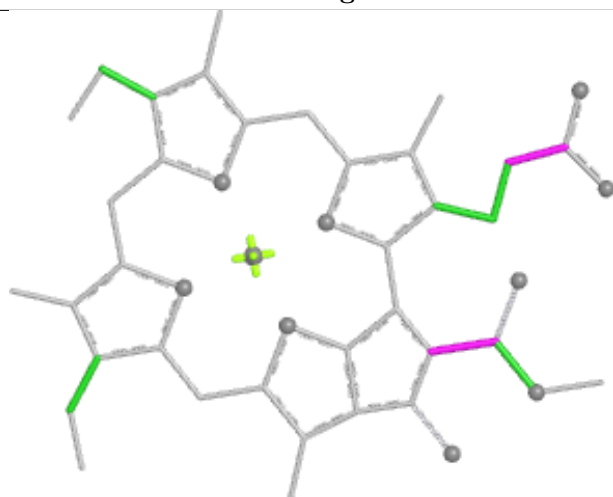
Ligand CLA j 507



Bond lengths



Bond angles

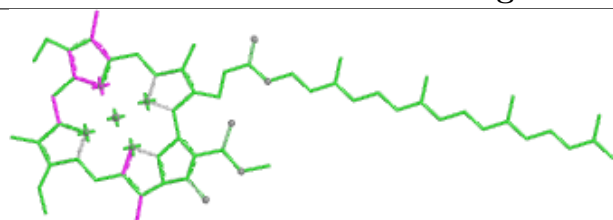


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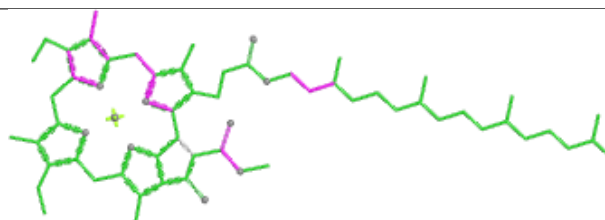


Rings

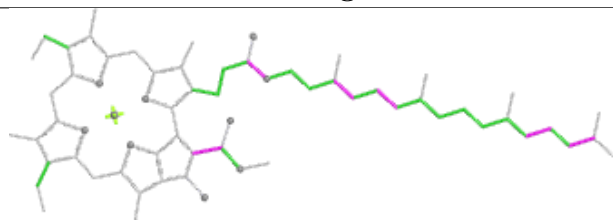
Ligand CLA aB 1226



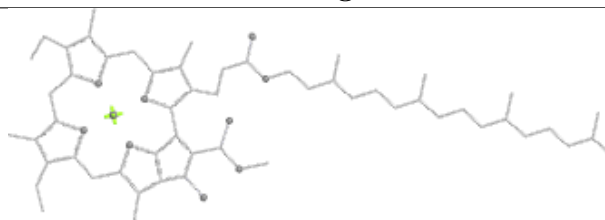
Bond lengths



Bond angles

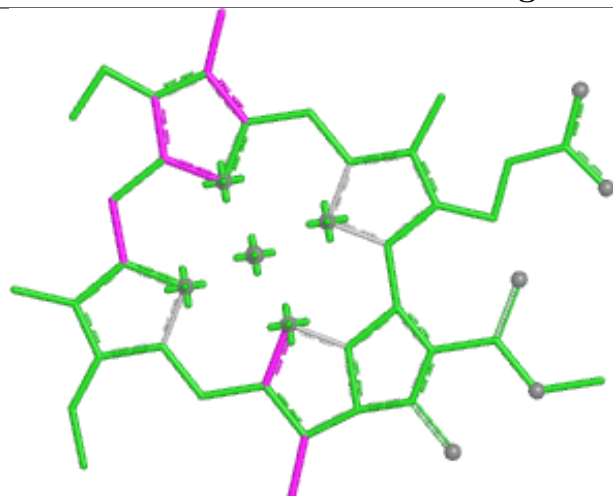


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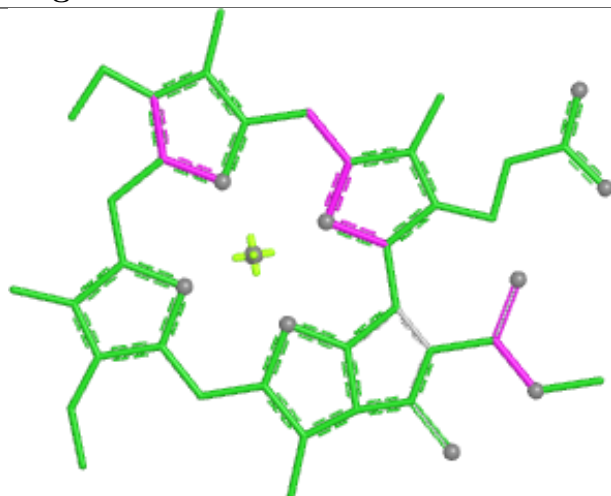


Rings

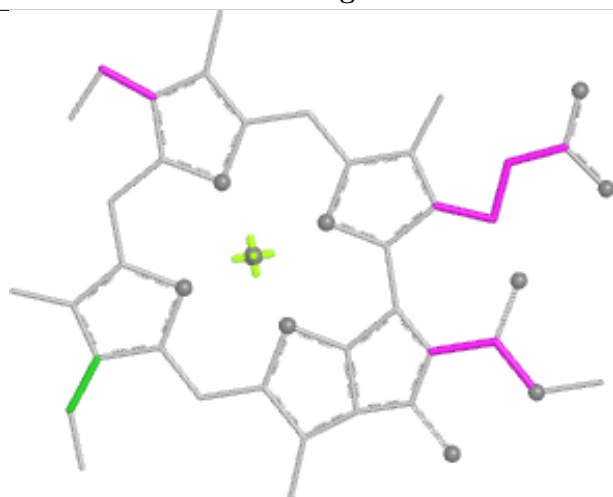
Ligand CLA g 517



Bond lengths



Bond angles

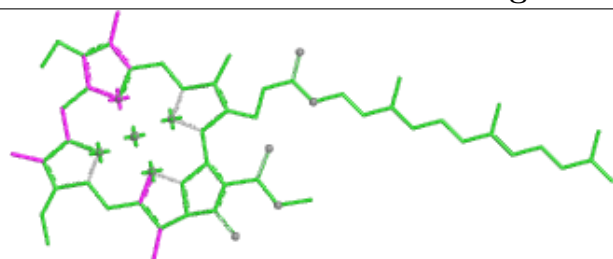


Torsions

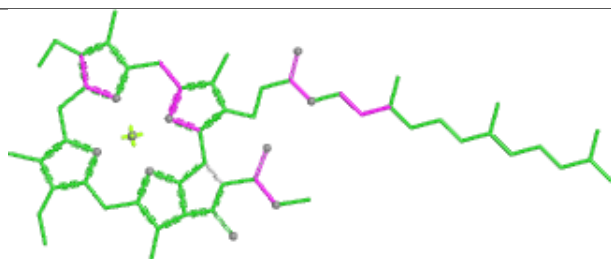


Rings

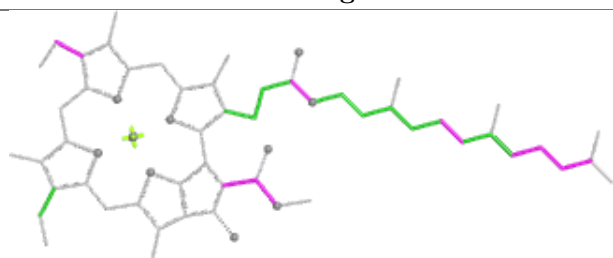
Ligand CLA a5 502



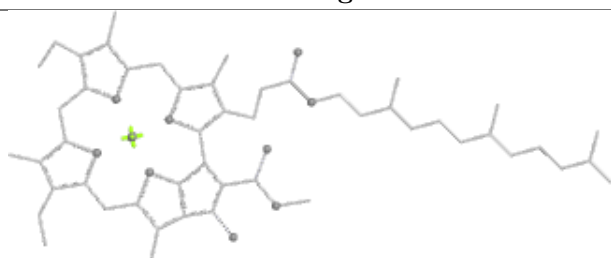
Bond lengths



Bond angles

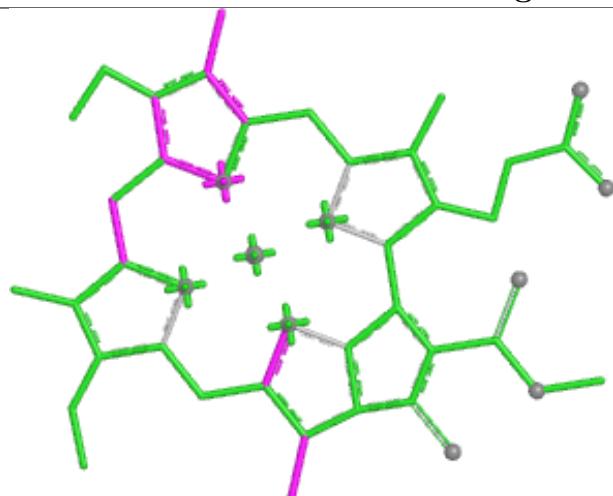


Torsions

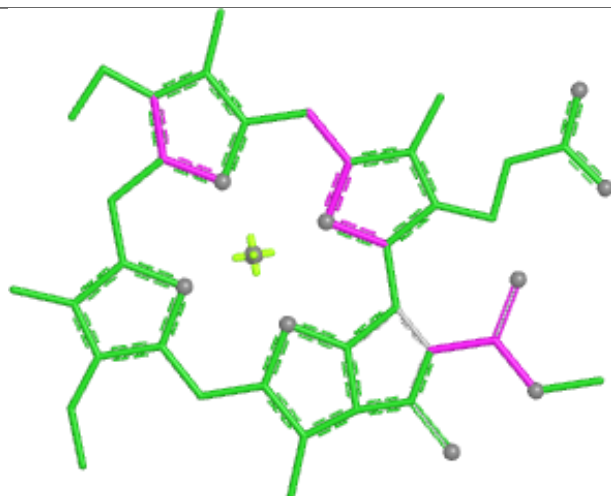


Rings

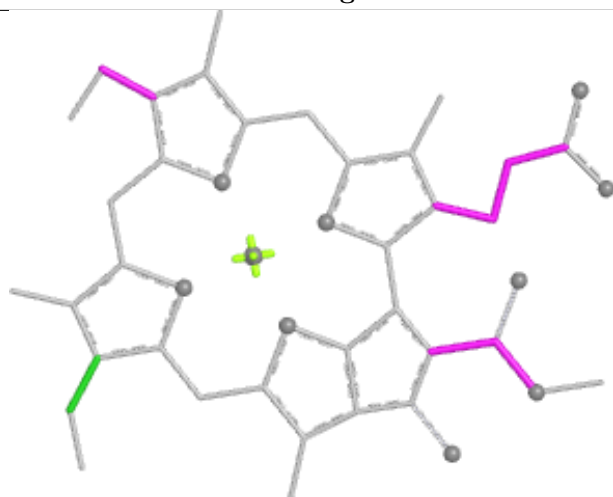
Ligand CLA T 517



Bond lengths



Bond angles

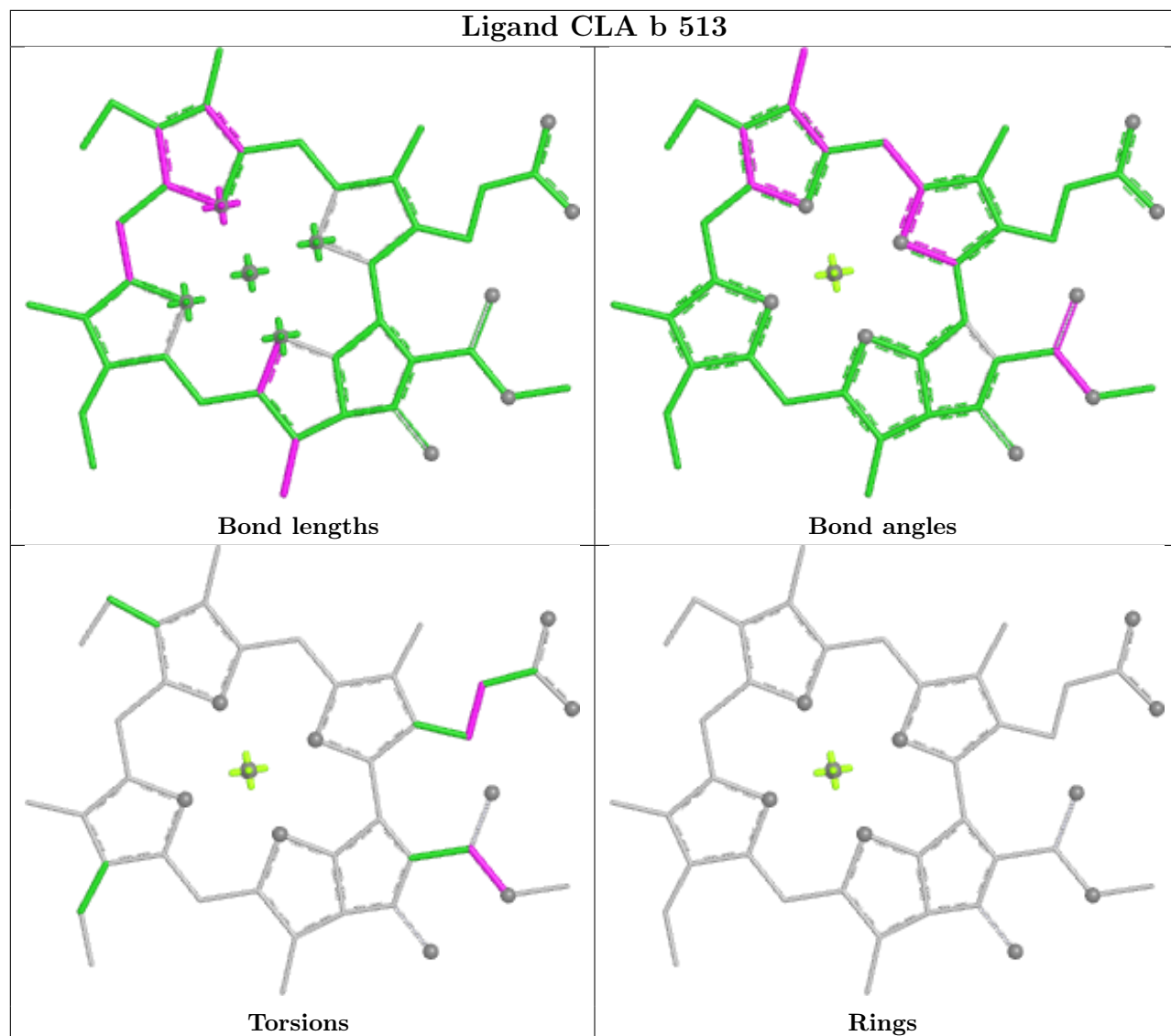


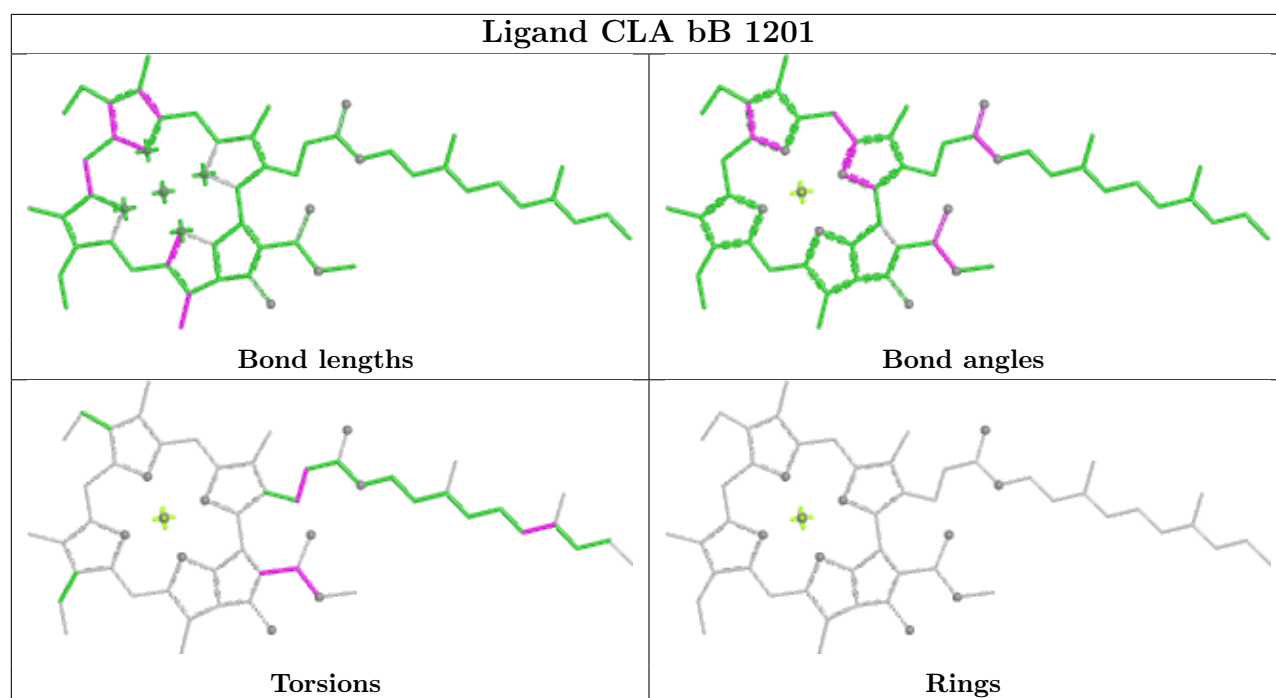
Torsions

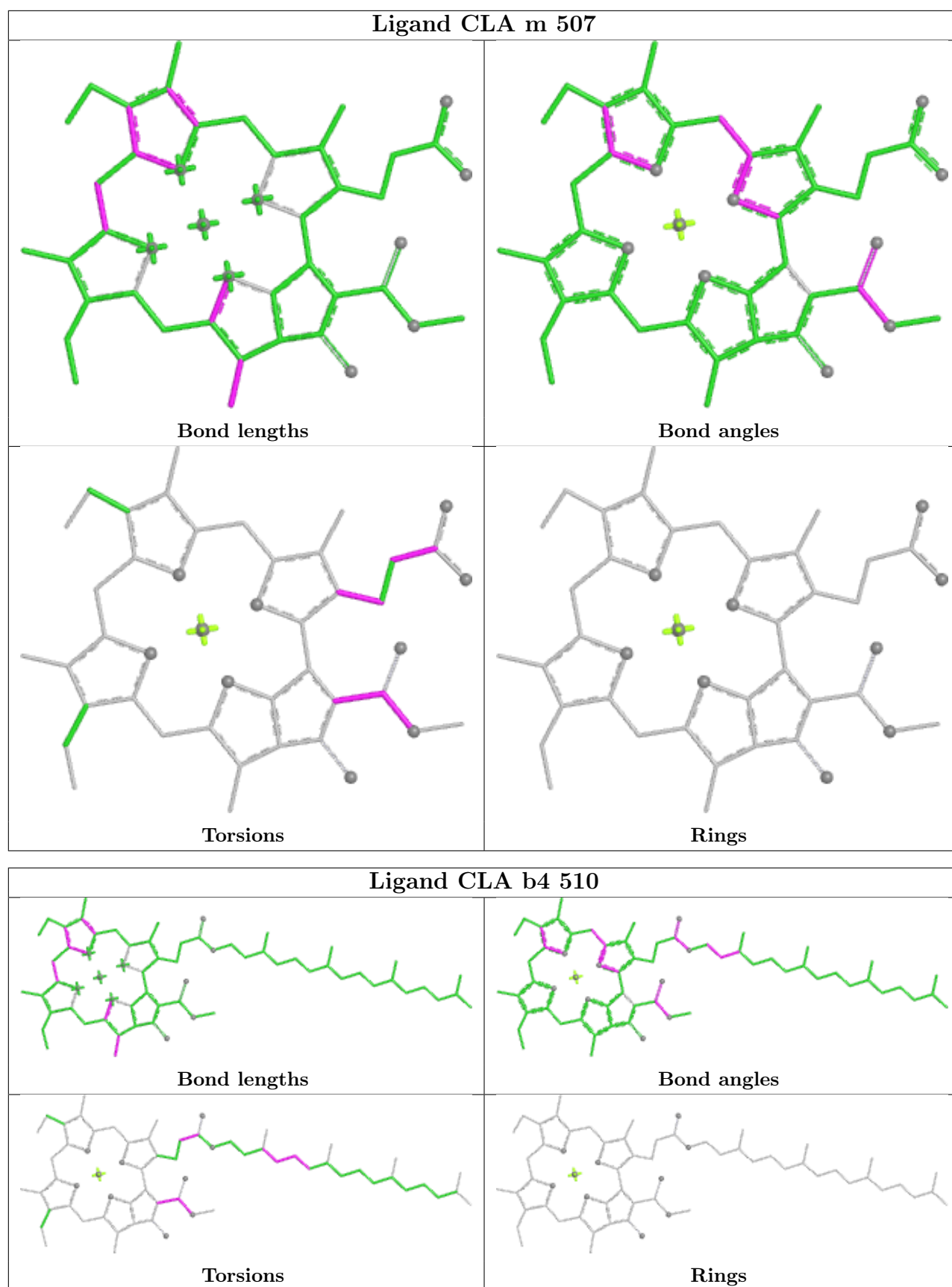


Rings

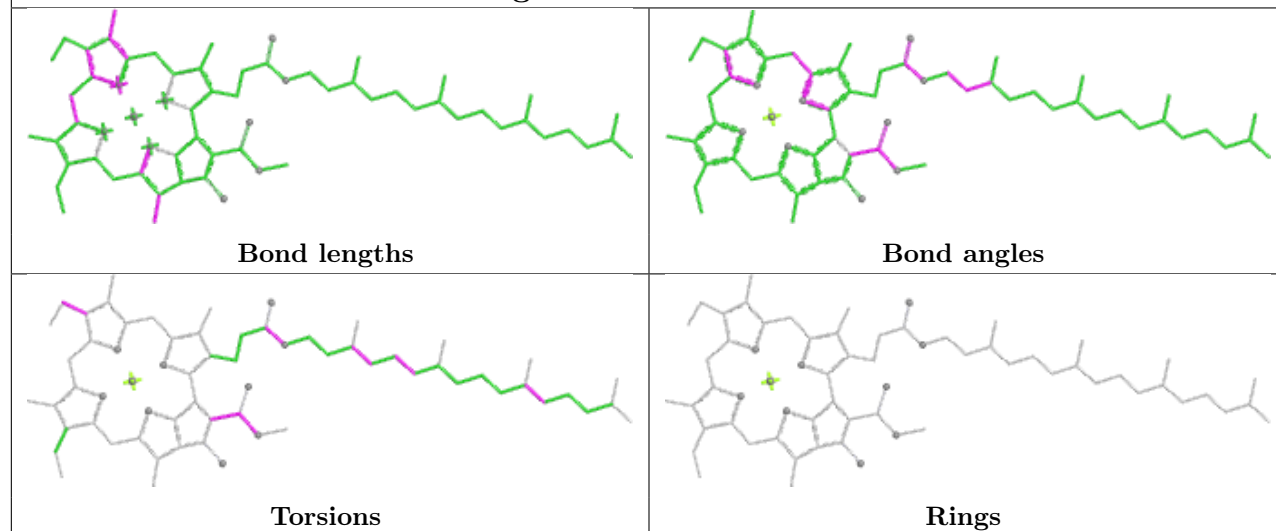
Ligand CLA b 513



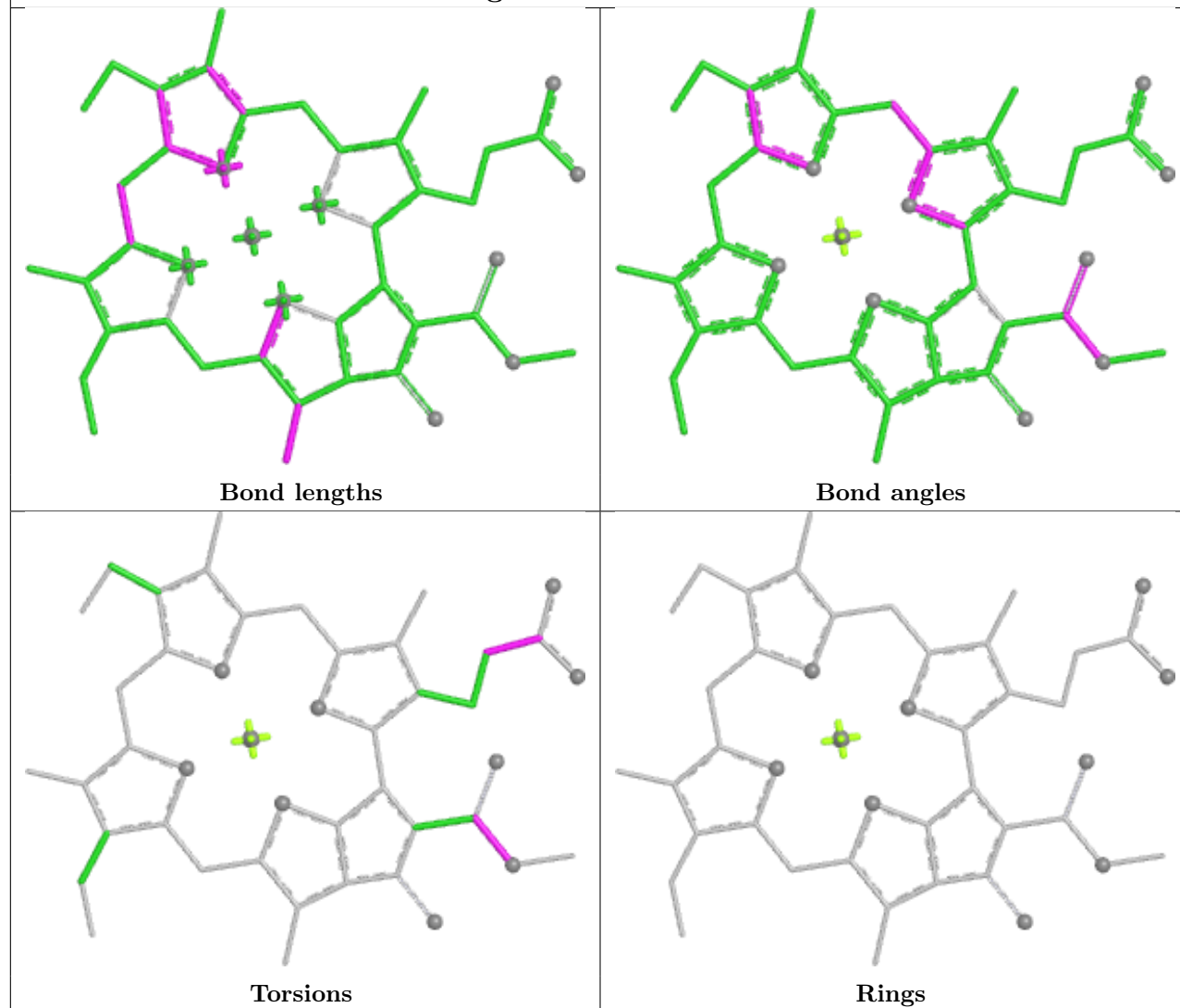




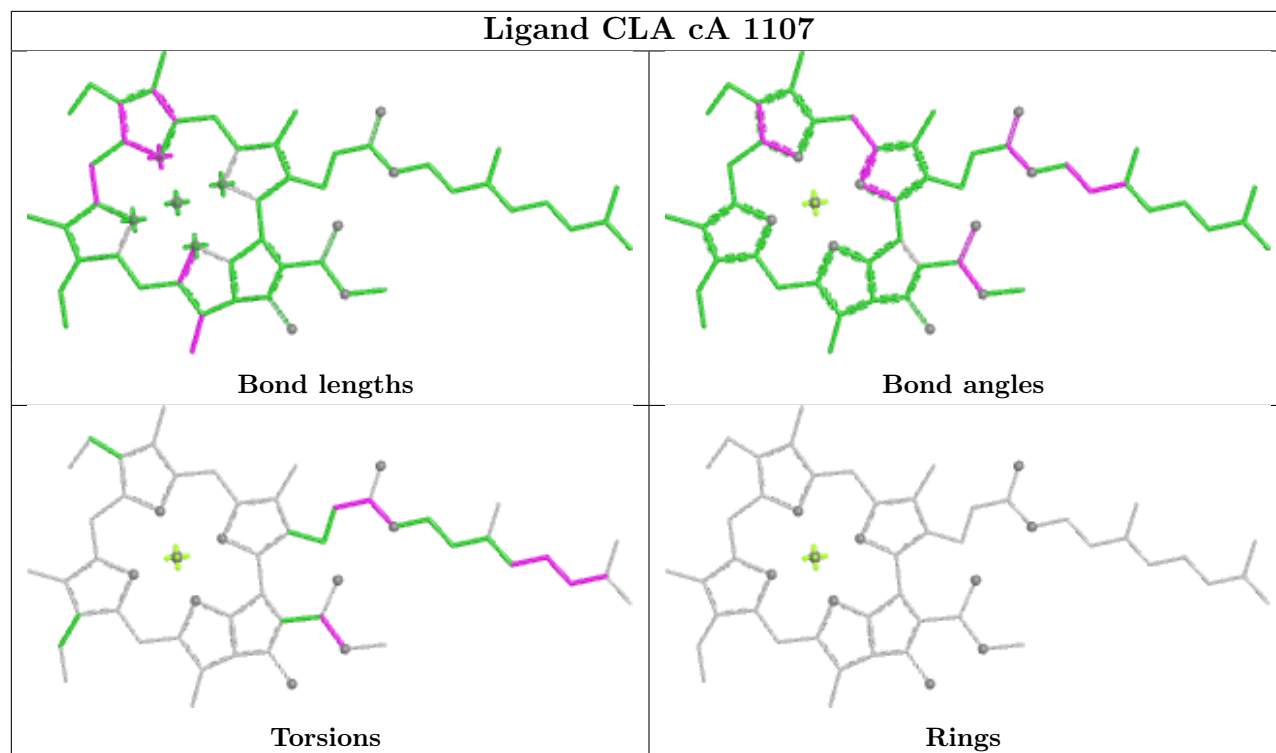
Ligand CLA bA 1132



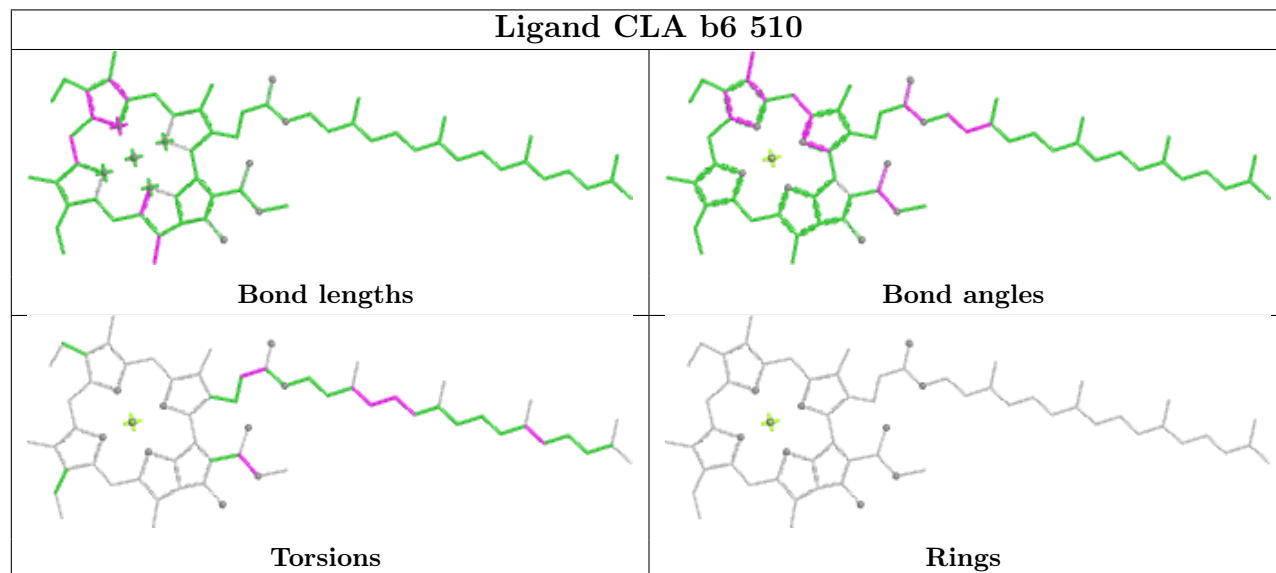
Ligand CLA b5 517

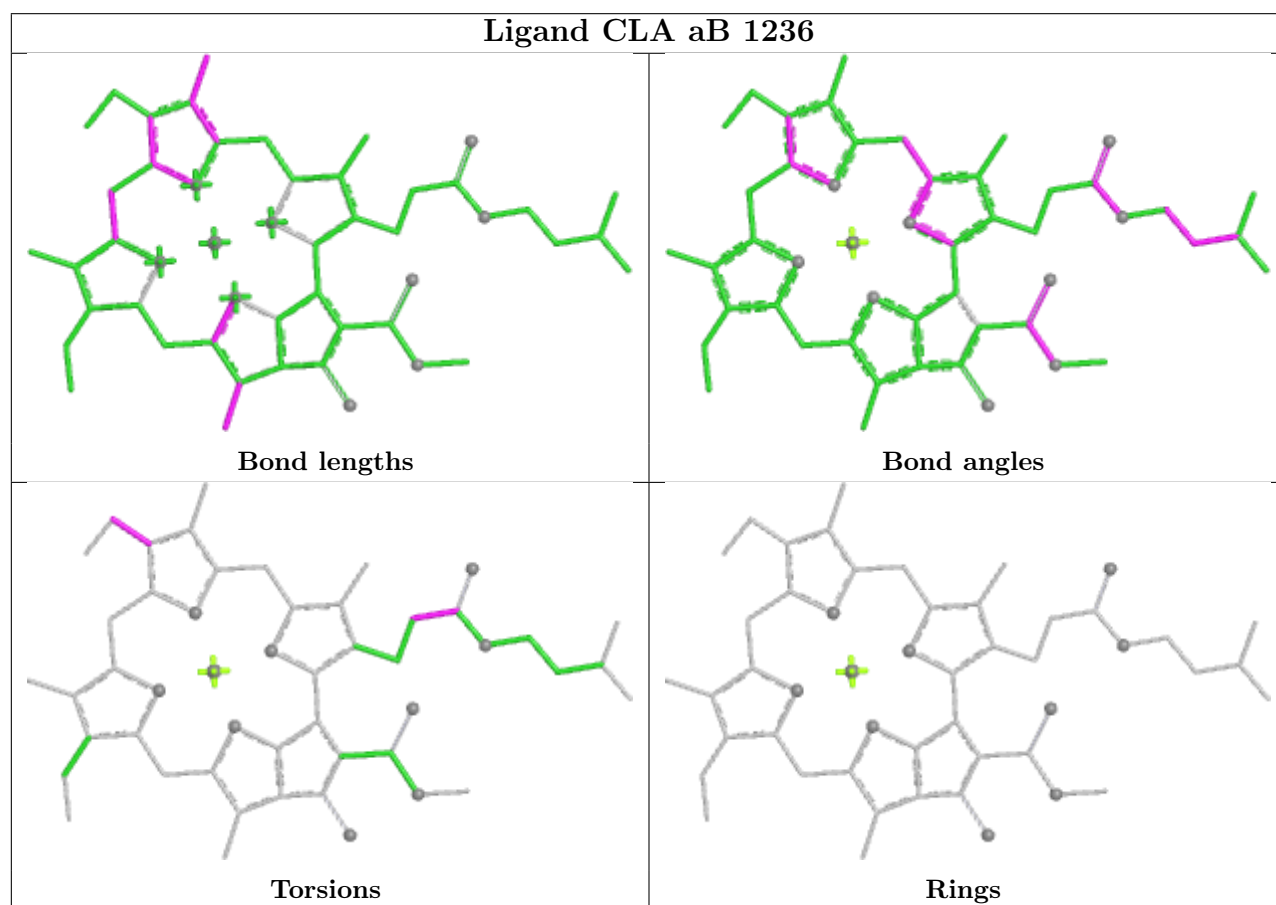
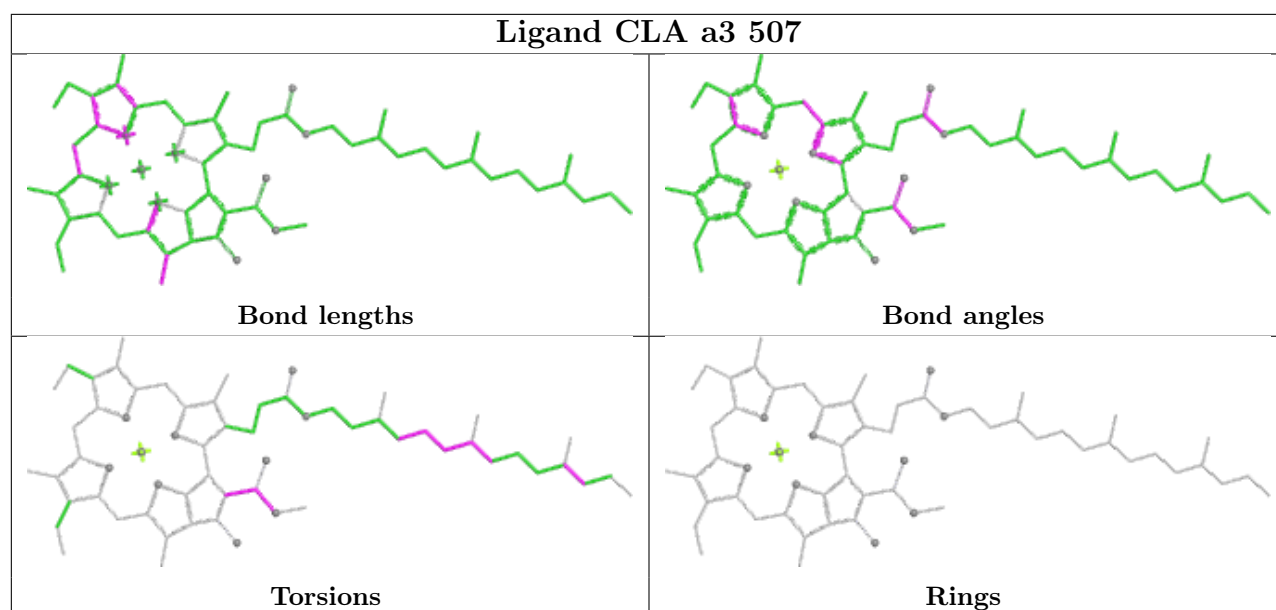


Ligand CLA cA 1107

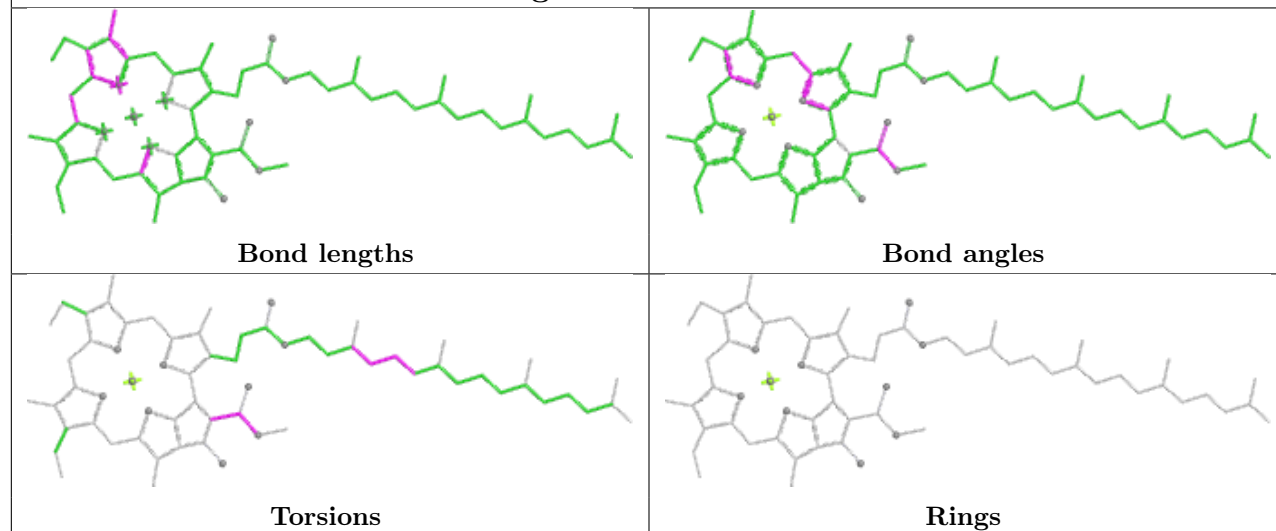


Ligand CLA b6 510

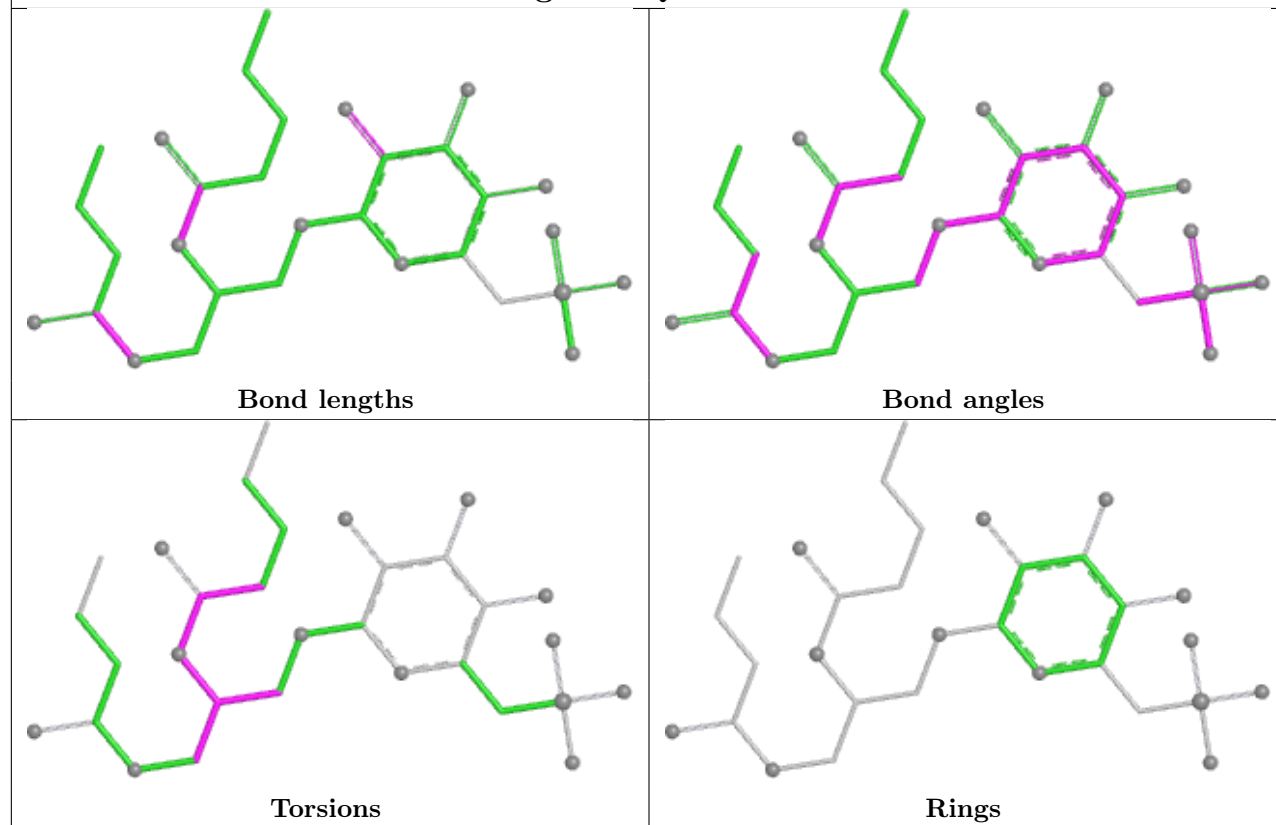




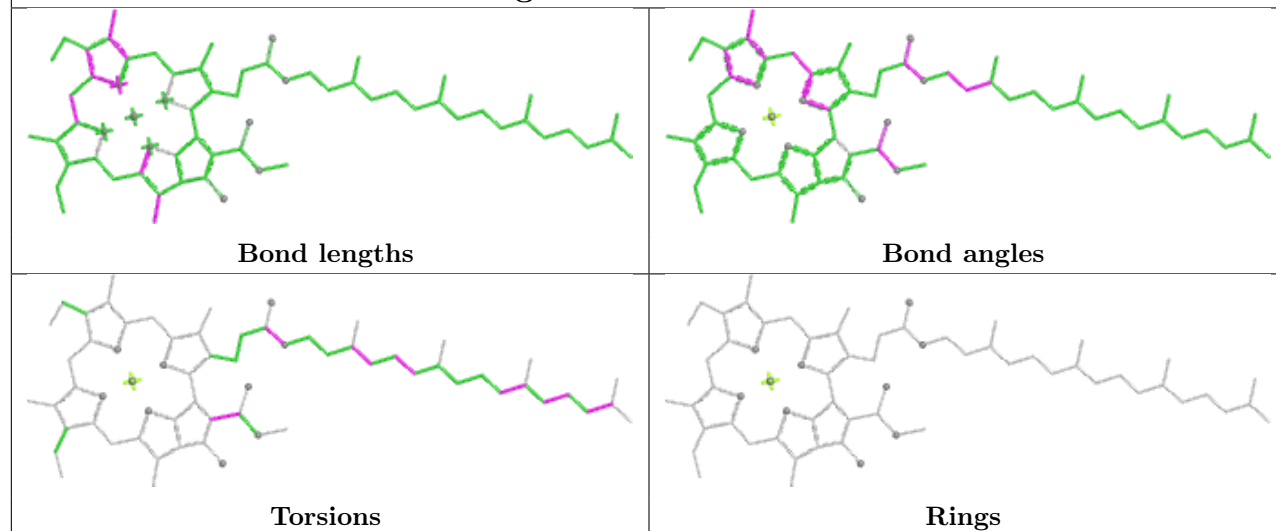
Ligand CLA Y 510



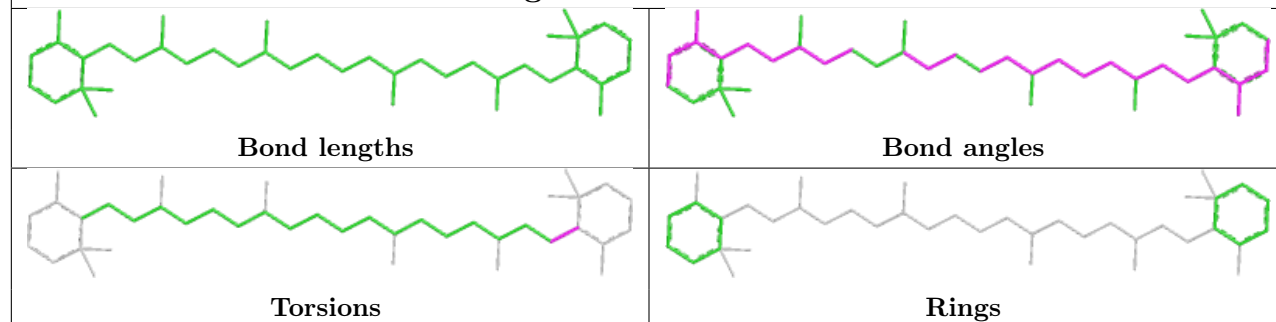
Ligand SQD S 822



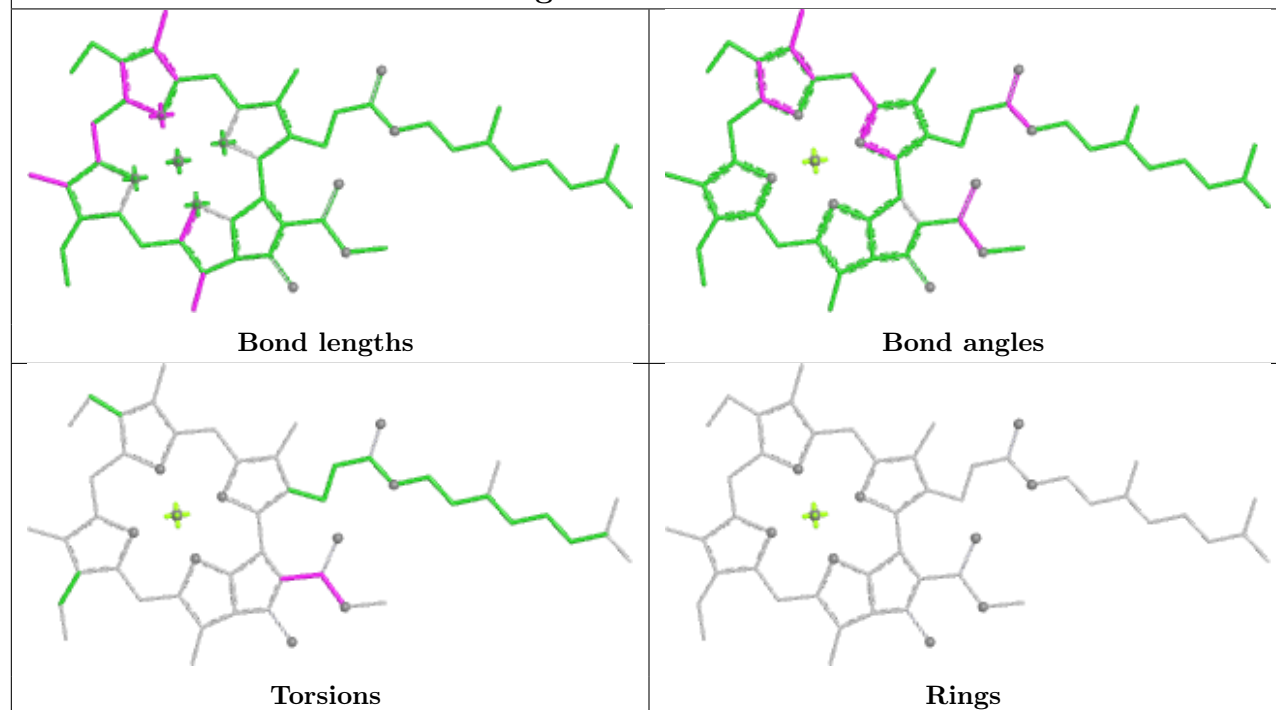
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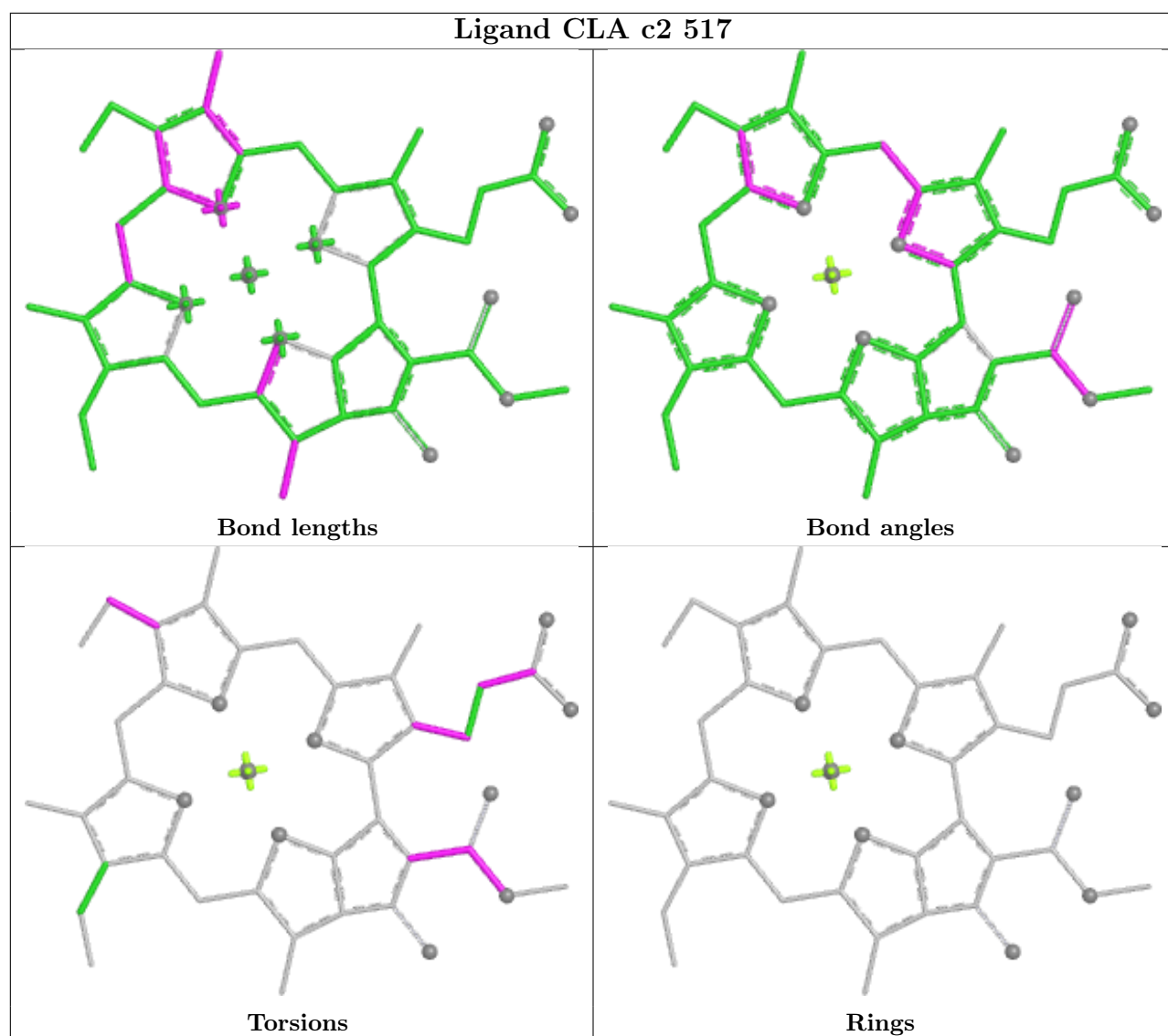


Ligand BCR b6 523

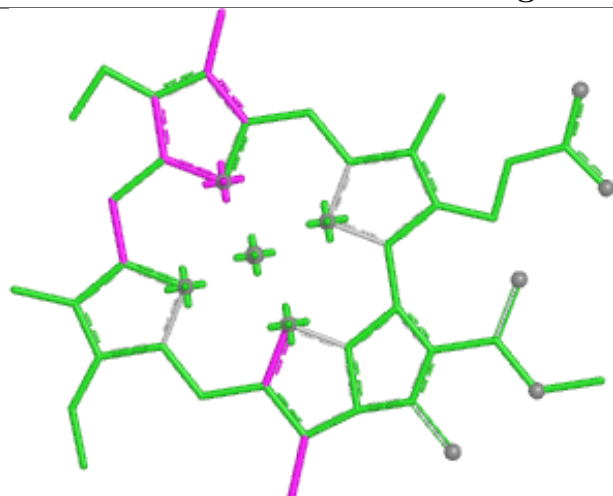


Ligand CLA d 508

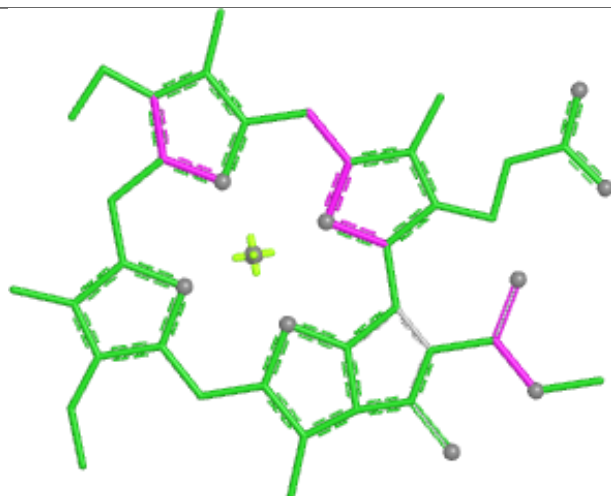




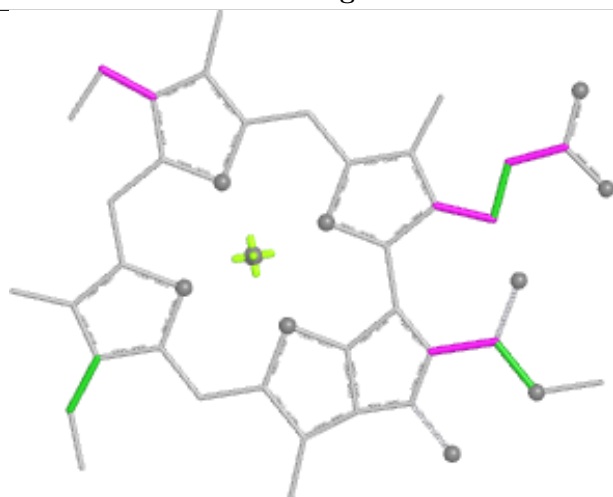
Ligand CLA h 512



Bond lengths



Bond angles

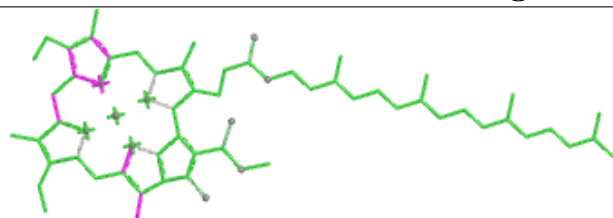


Torsions

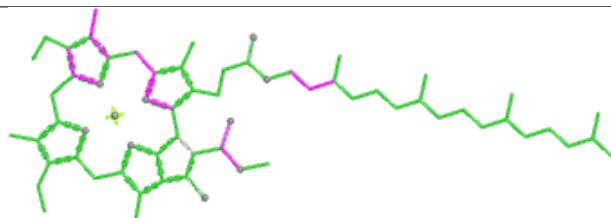


Rings

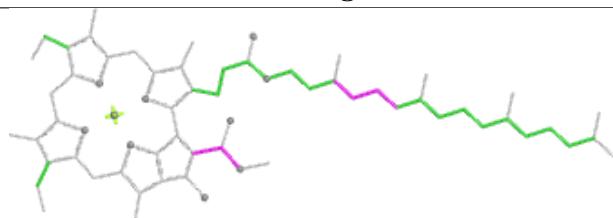
Ligand CLA a5 510



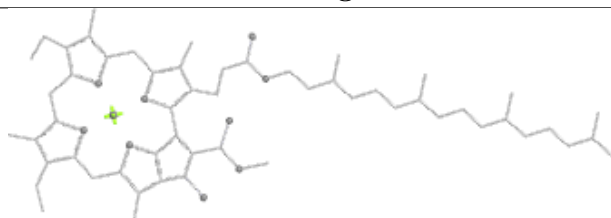
Bond lengths



Bond angles

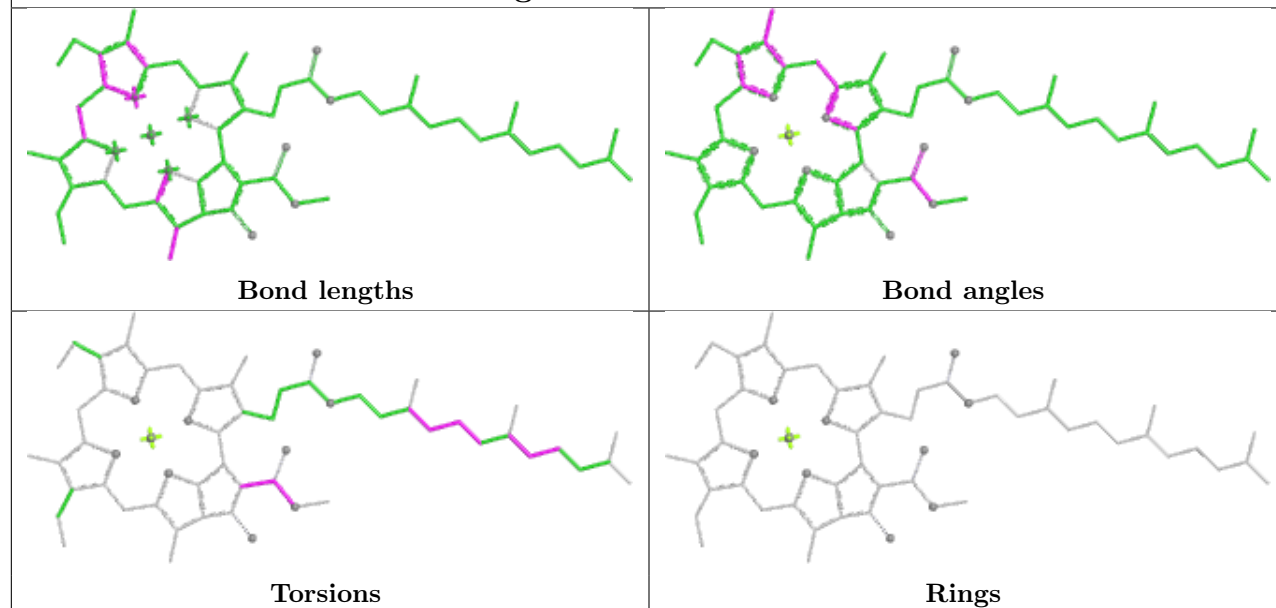


Torsions

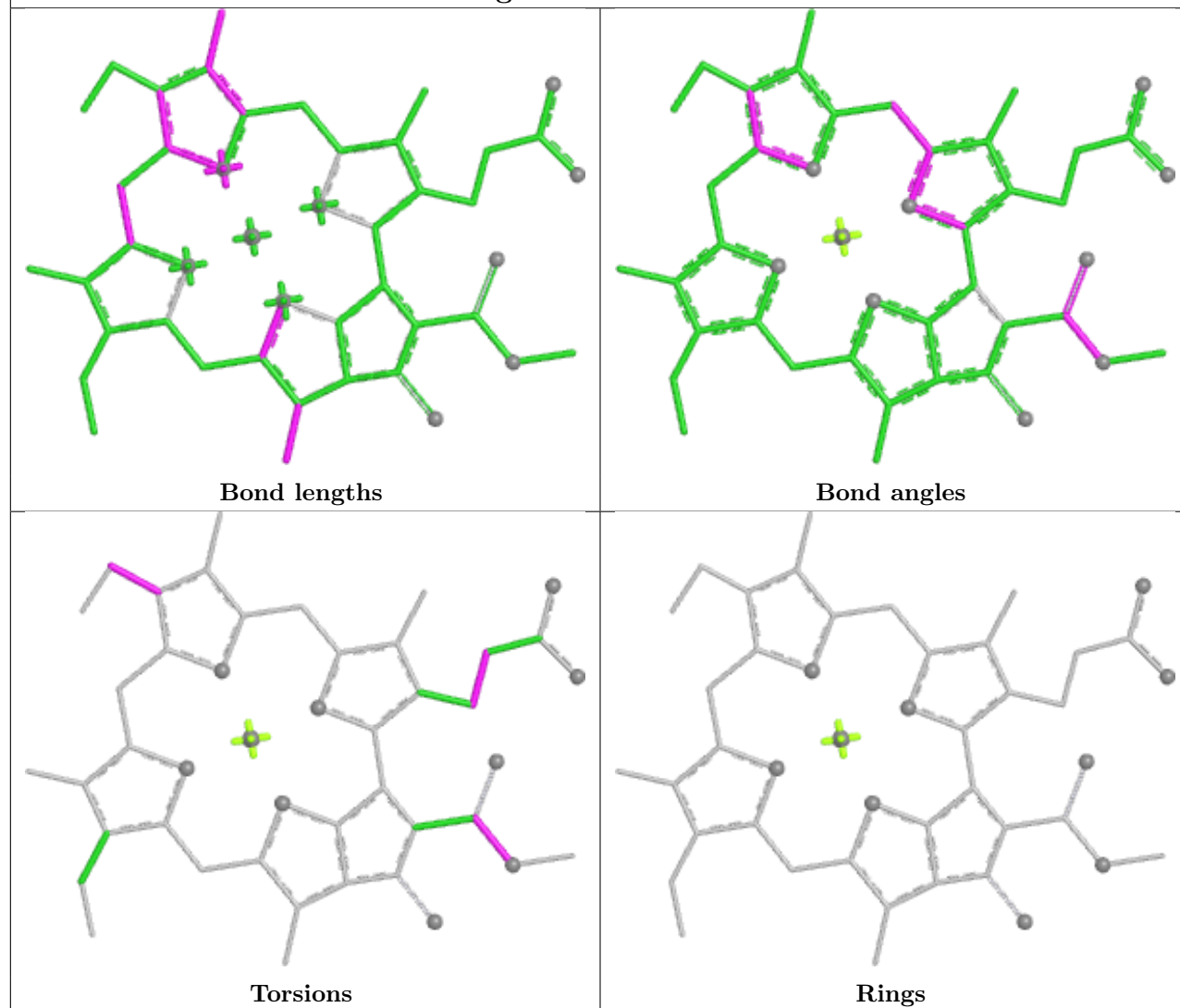


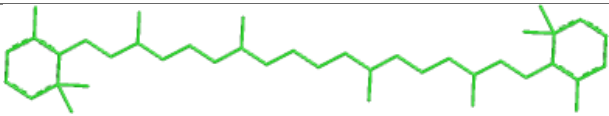
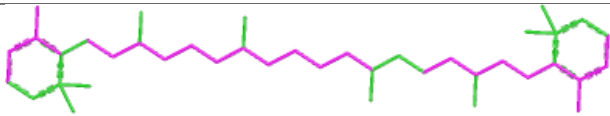
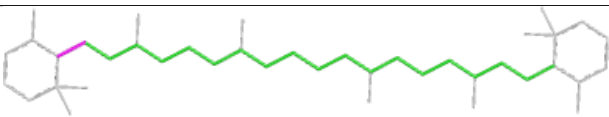
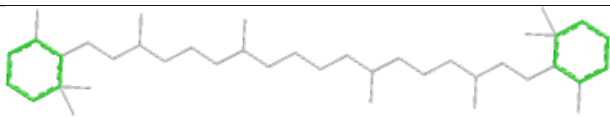
Rings

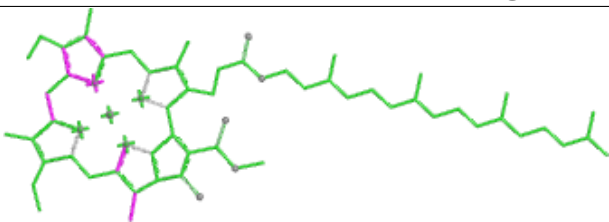
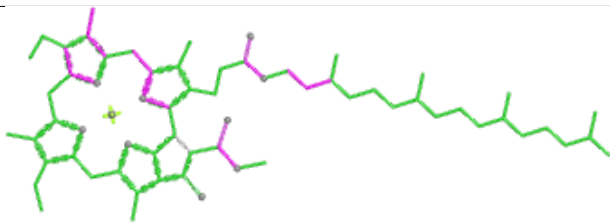
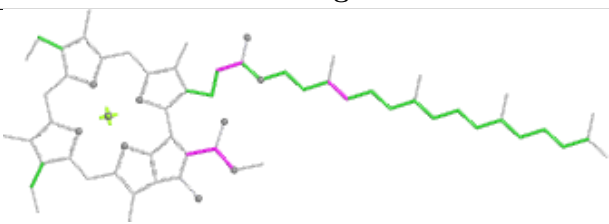
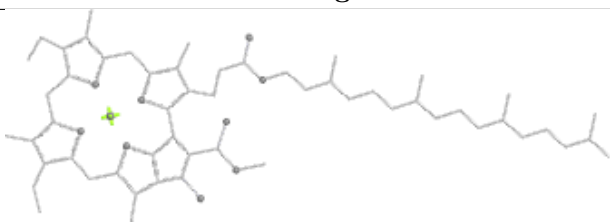
Ligand CLA aB 1221

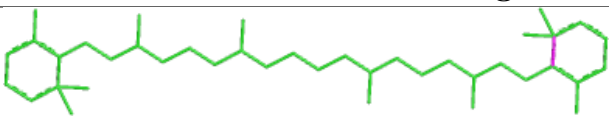
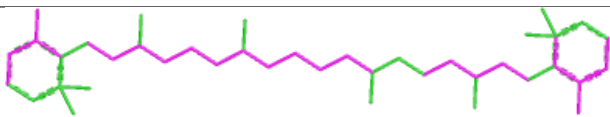
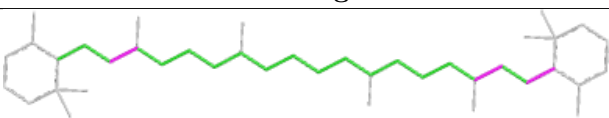
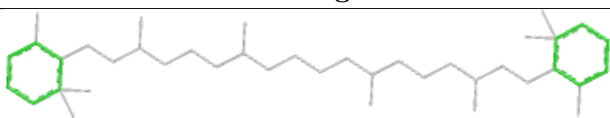


Ligand CLA o 504

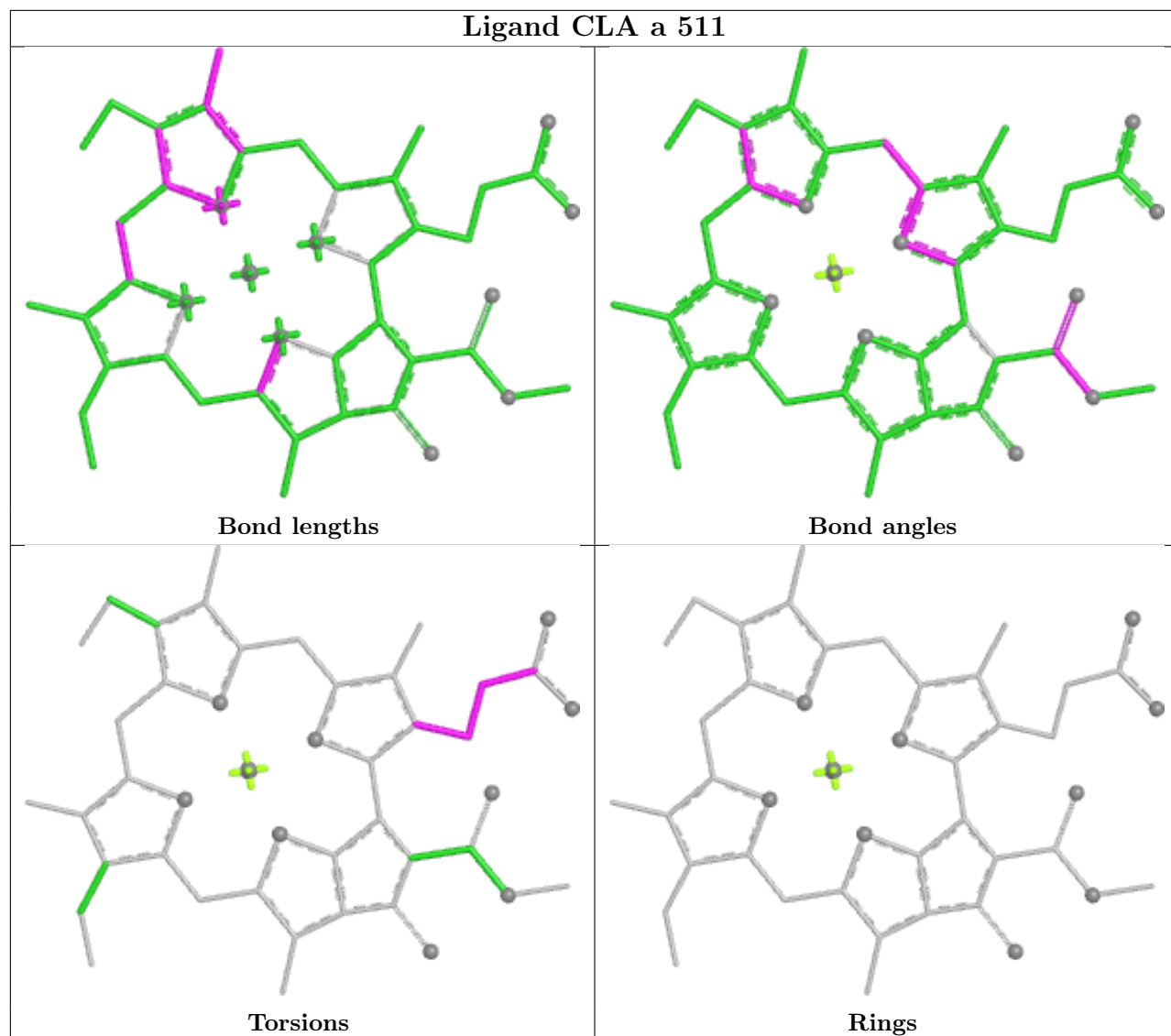


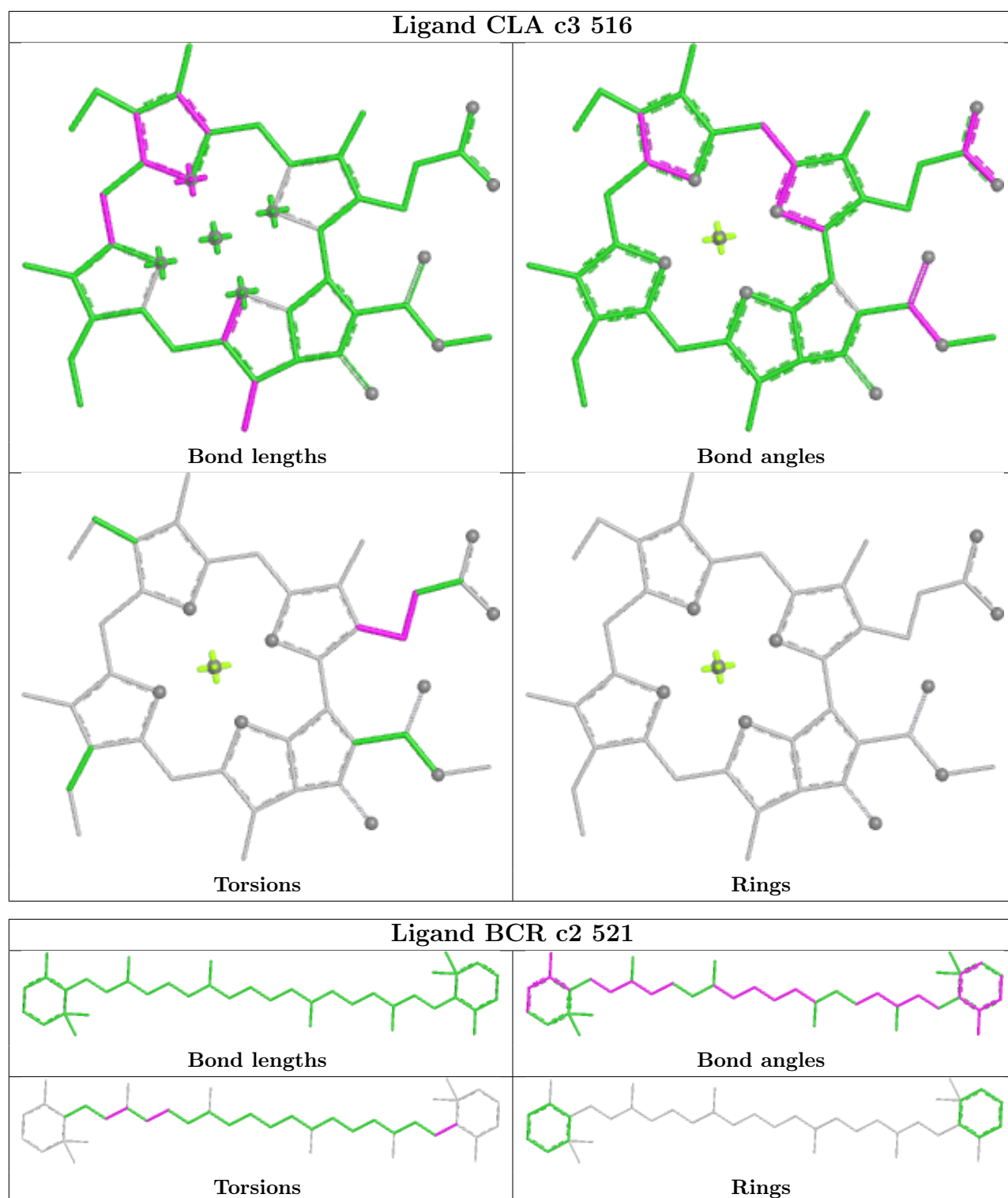
Ligand BCR j 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

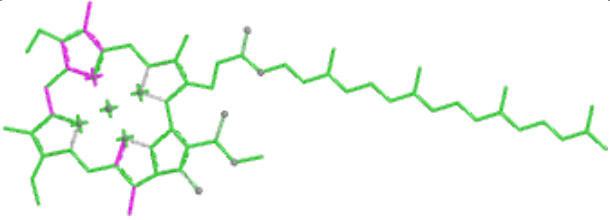
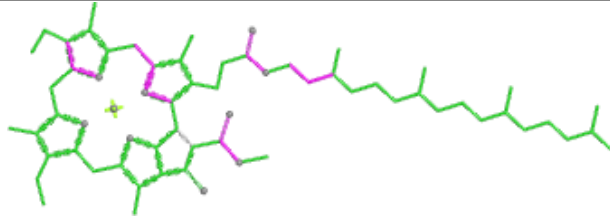
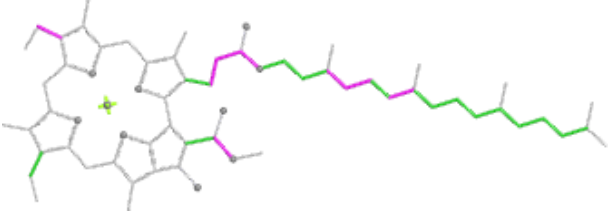
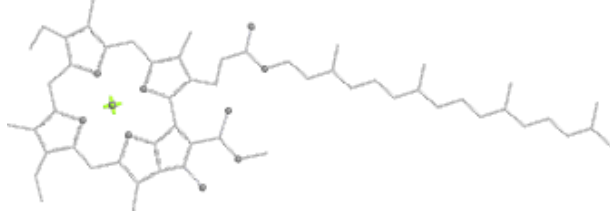
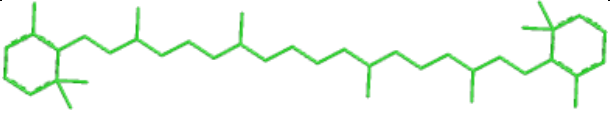
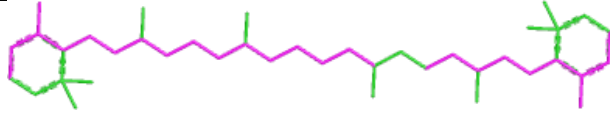
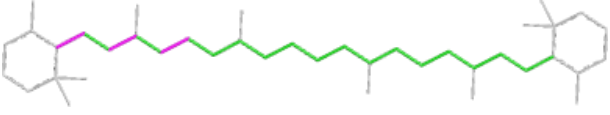
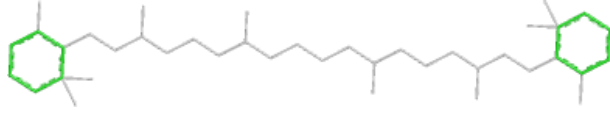
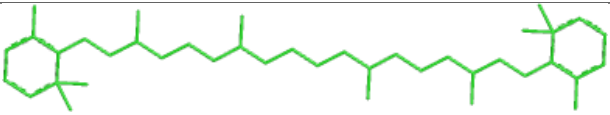
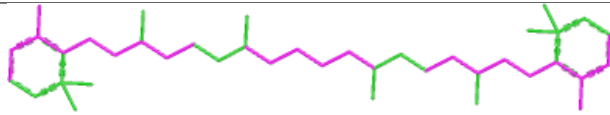
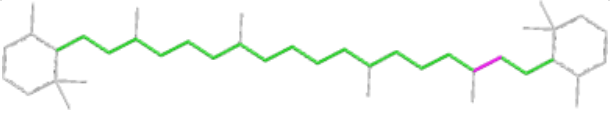
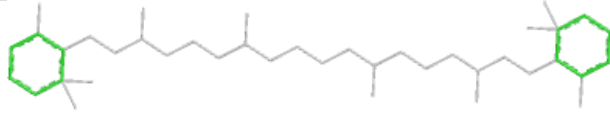
Ligand CLA a2 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR aI 4018	
	
Bond lengths	Bond angles
	
Torsions	Rings

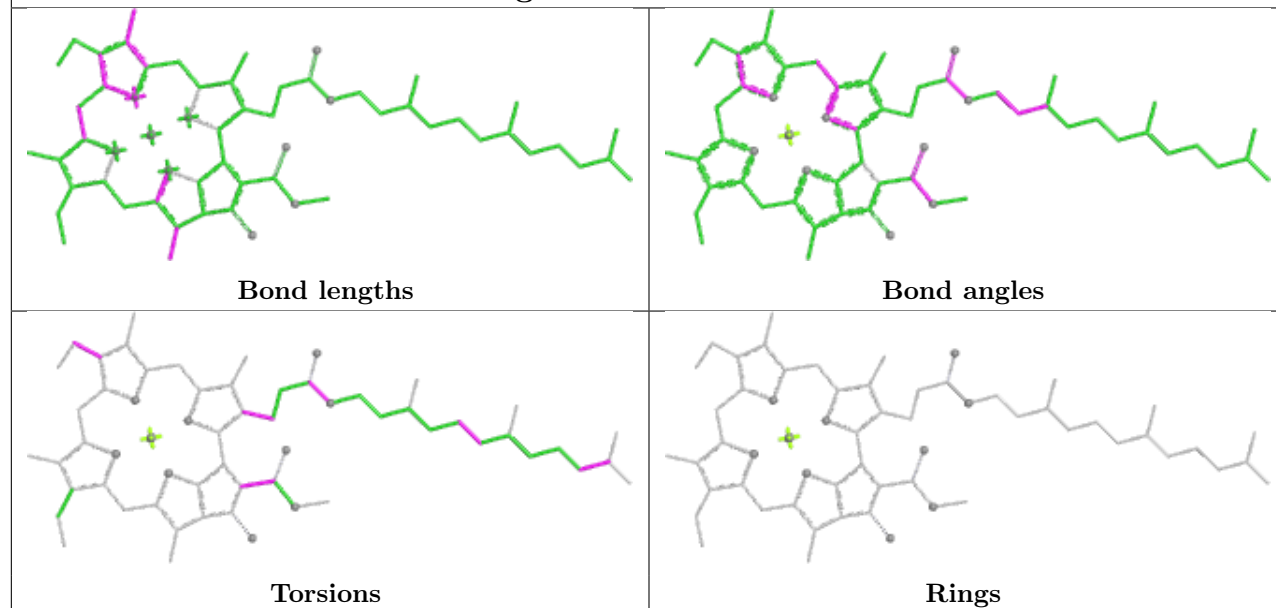
Ligand CLA a 511



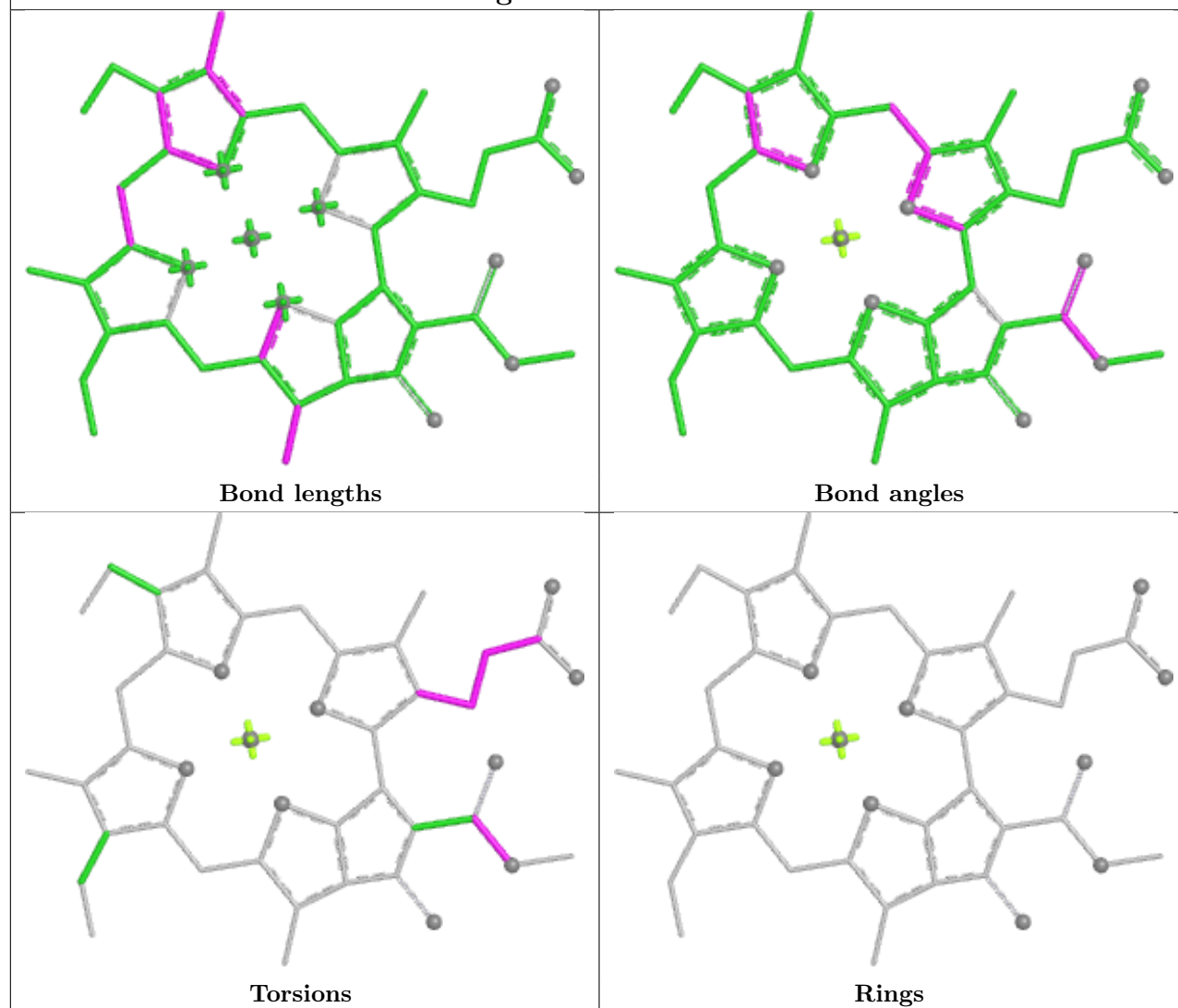


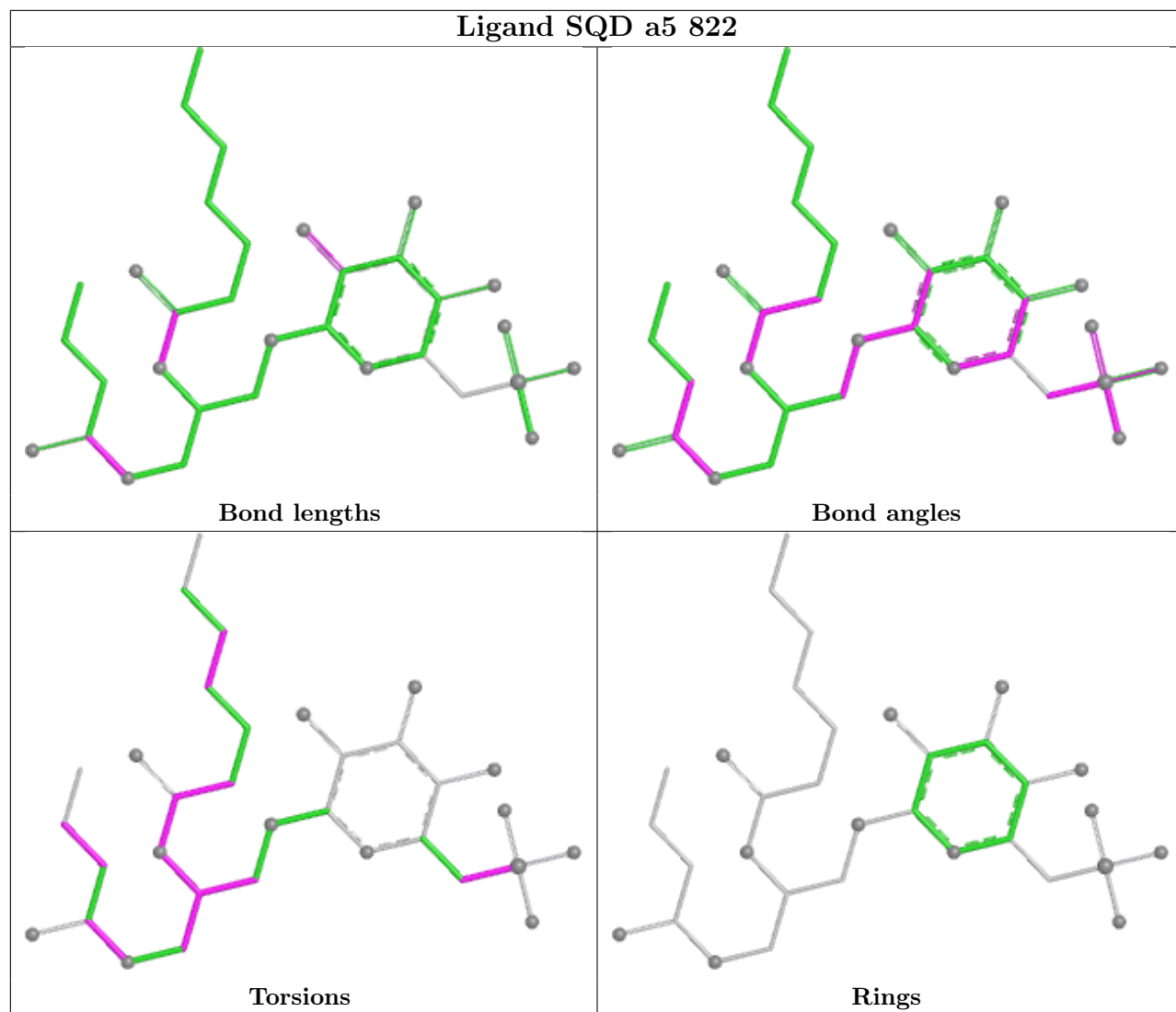
Ligand CLA cA 1237	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR a5 522	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR bA 4007	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand CLA cB 1234

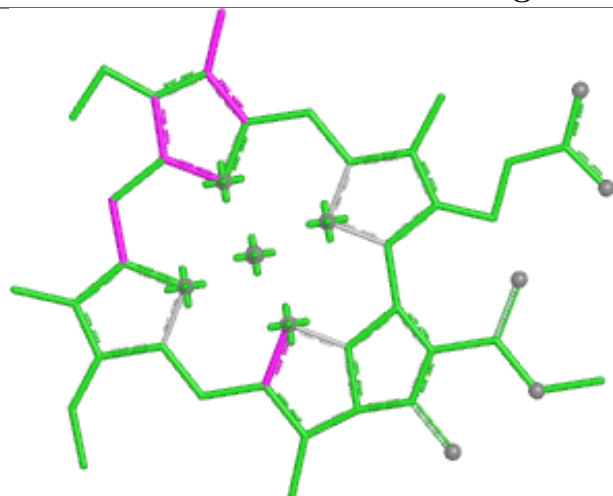


Ligand CLA c 511

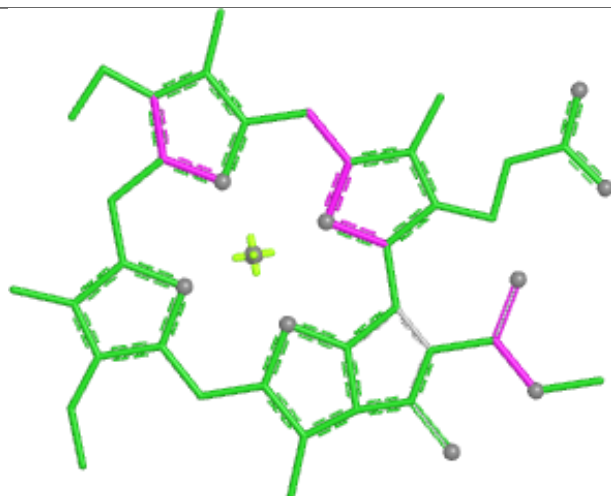




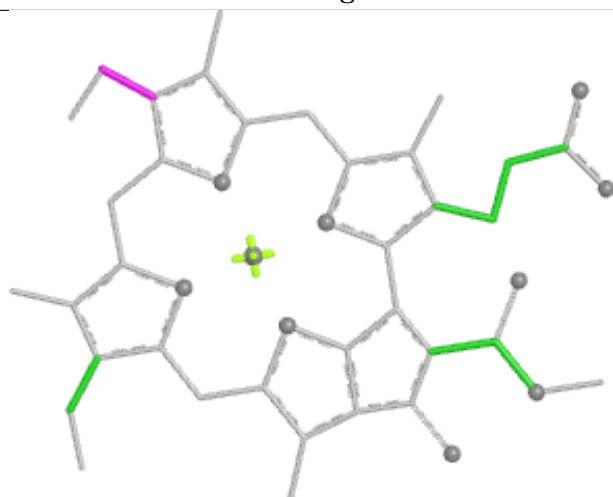
Ligand CLA U 509



Bond lengths



Bond angles

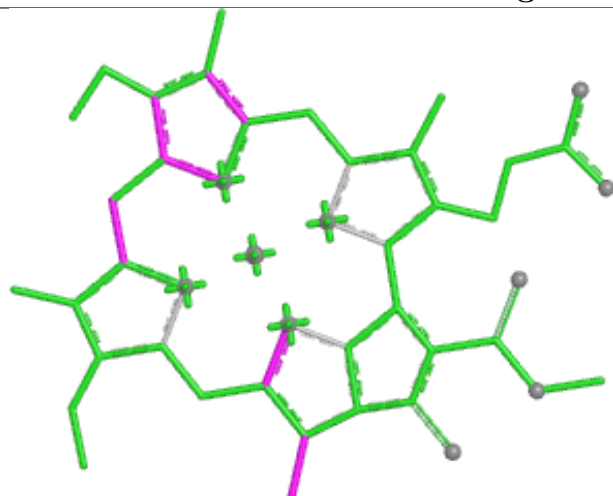


Torsions

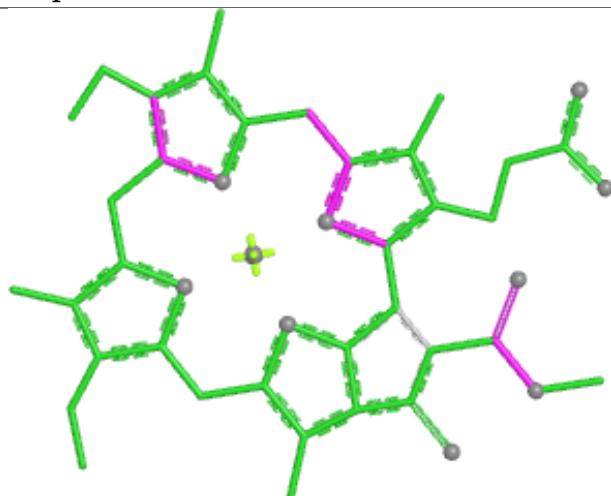


Rings

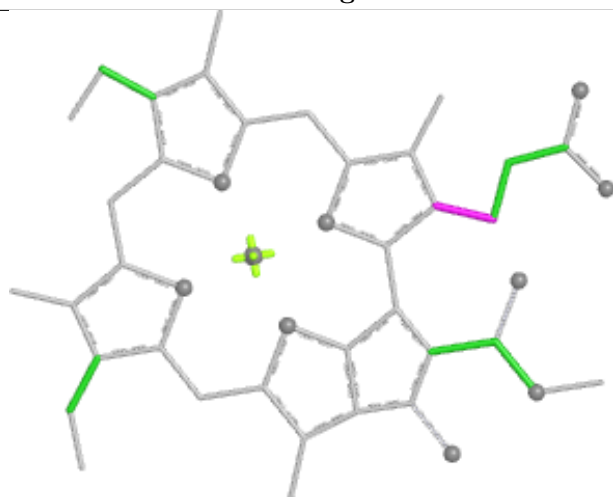
Ligand CLA p 516



Bond lengths



Bond angles

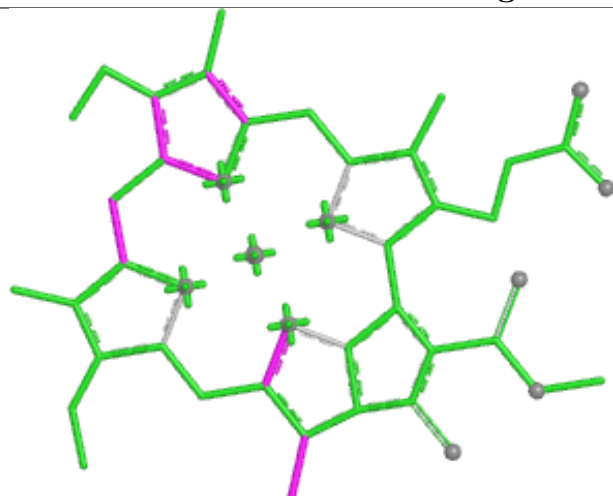


Torsions



Rings

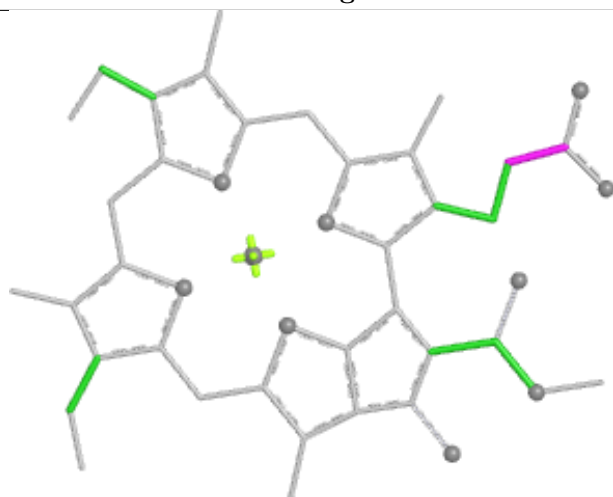
Ligand CLA cB 1233



Bond lengths



Bond angles

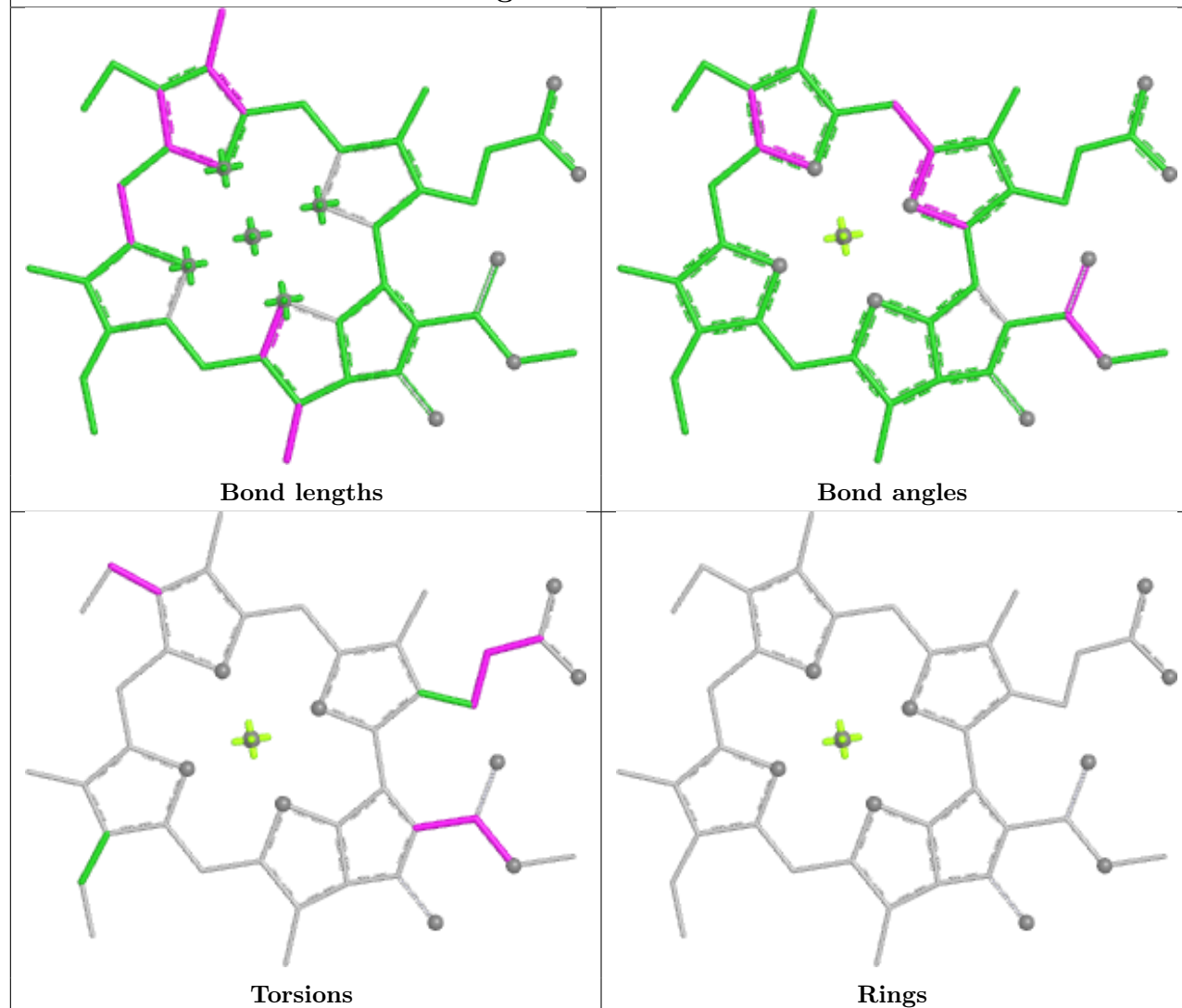


Torsions

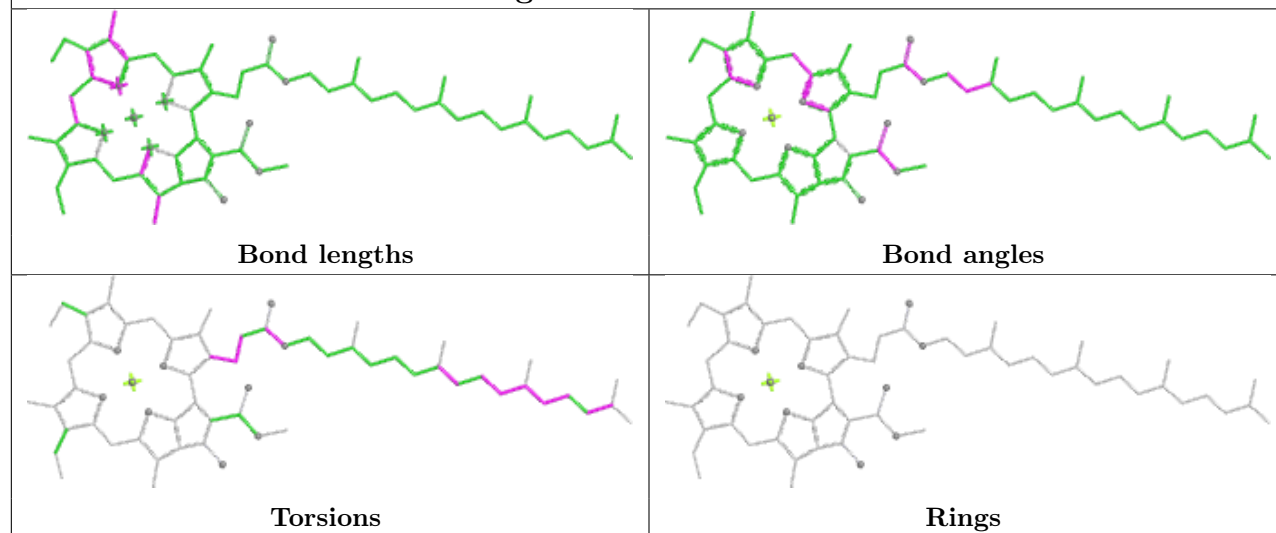


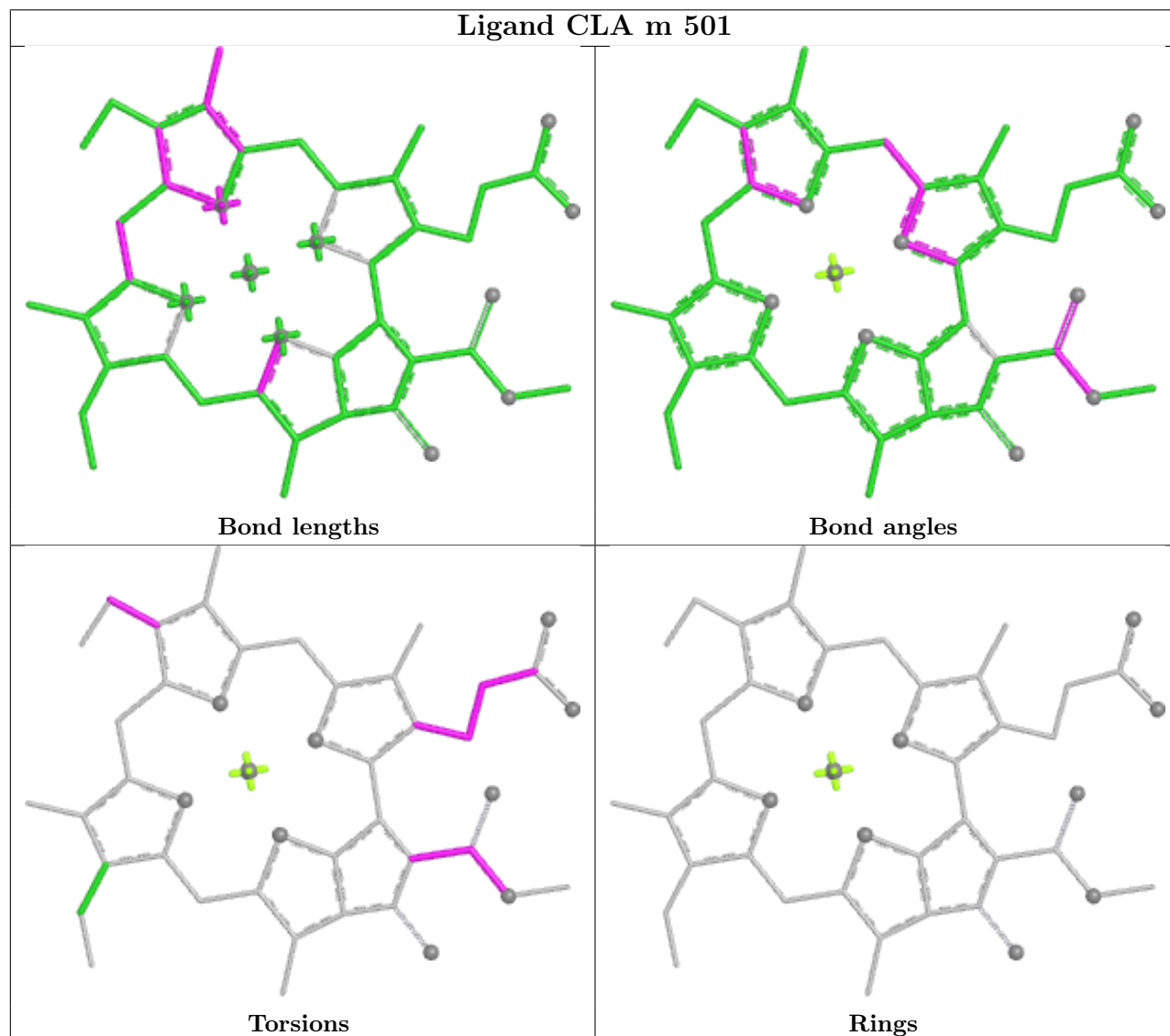
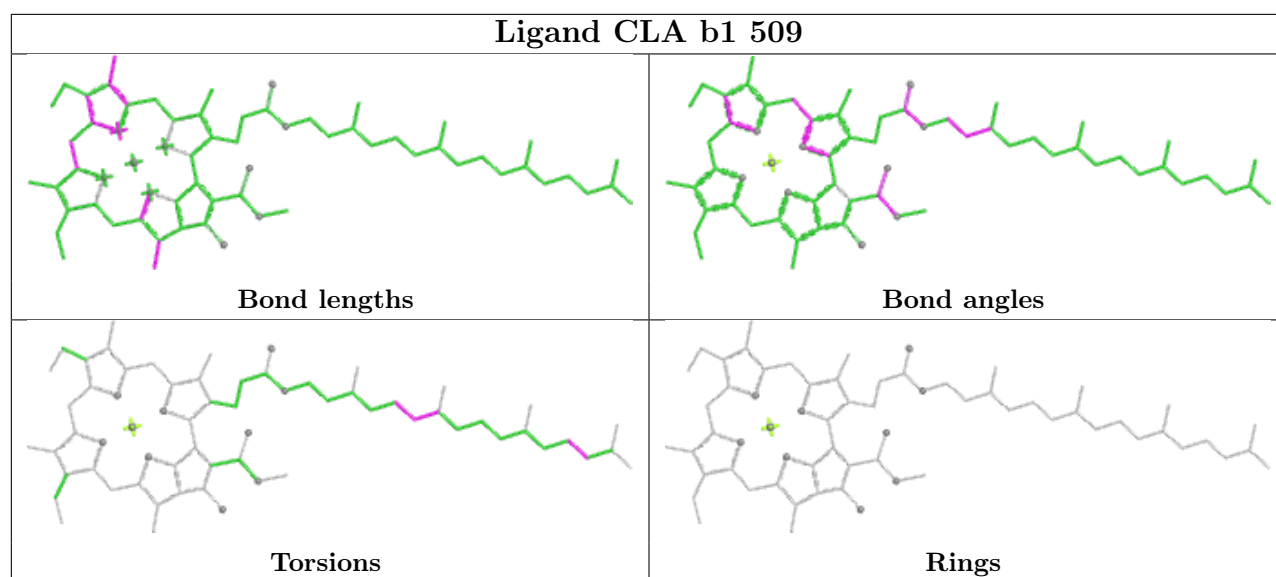
Rings

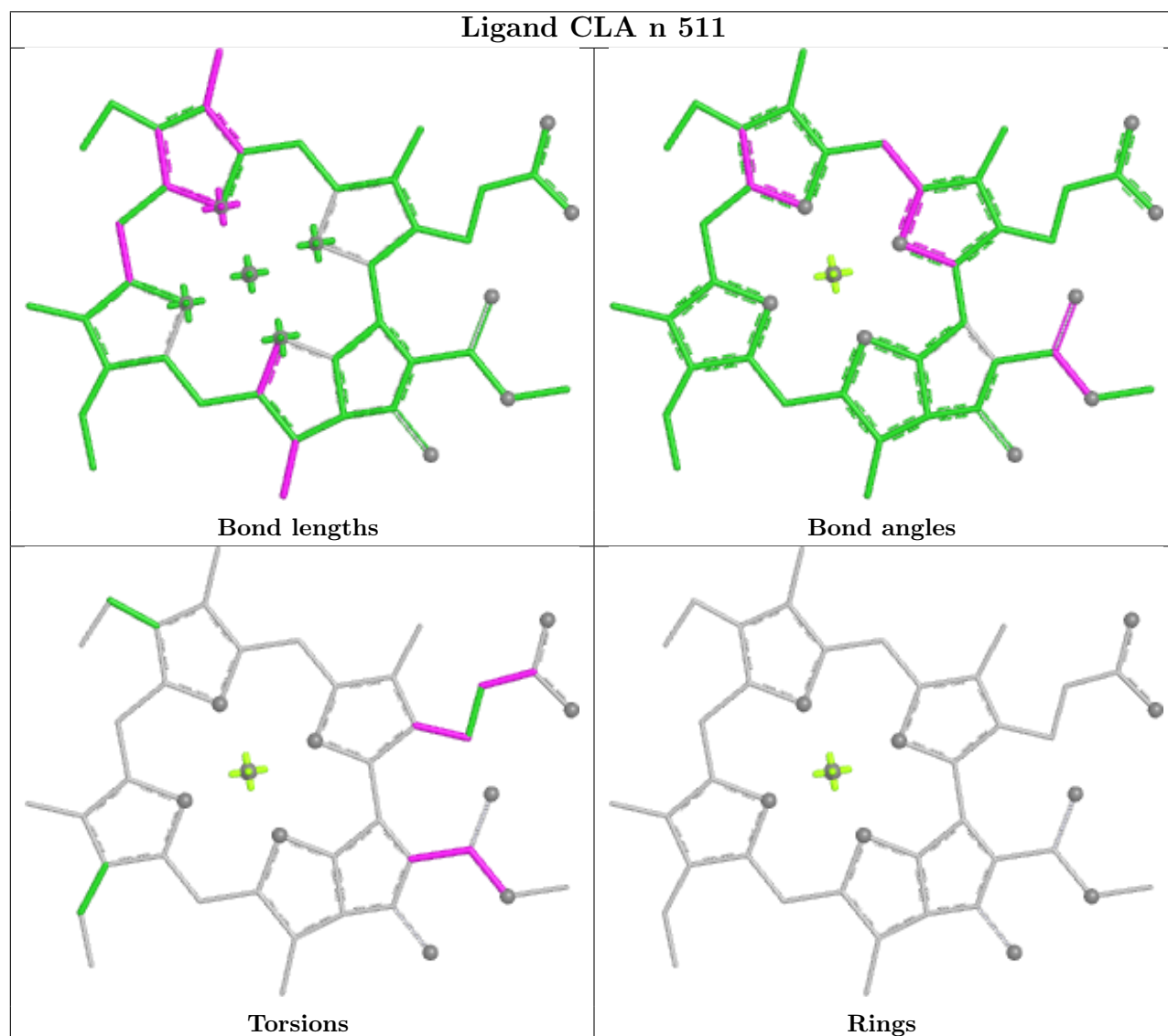
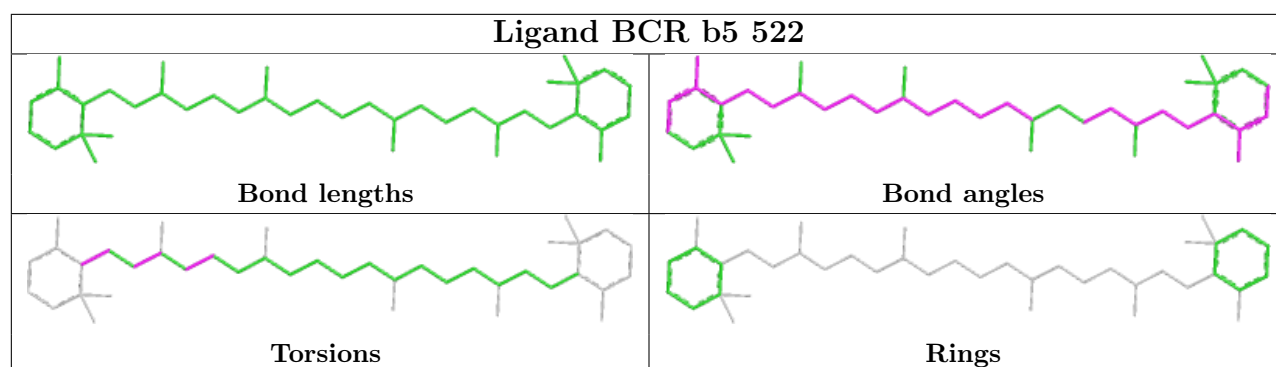
Ligand CLA a 504

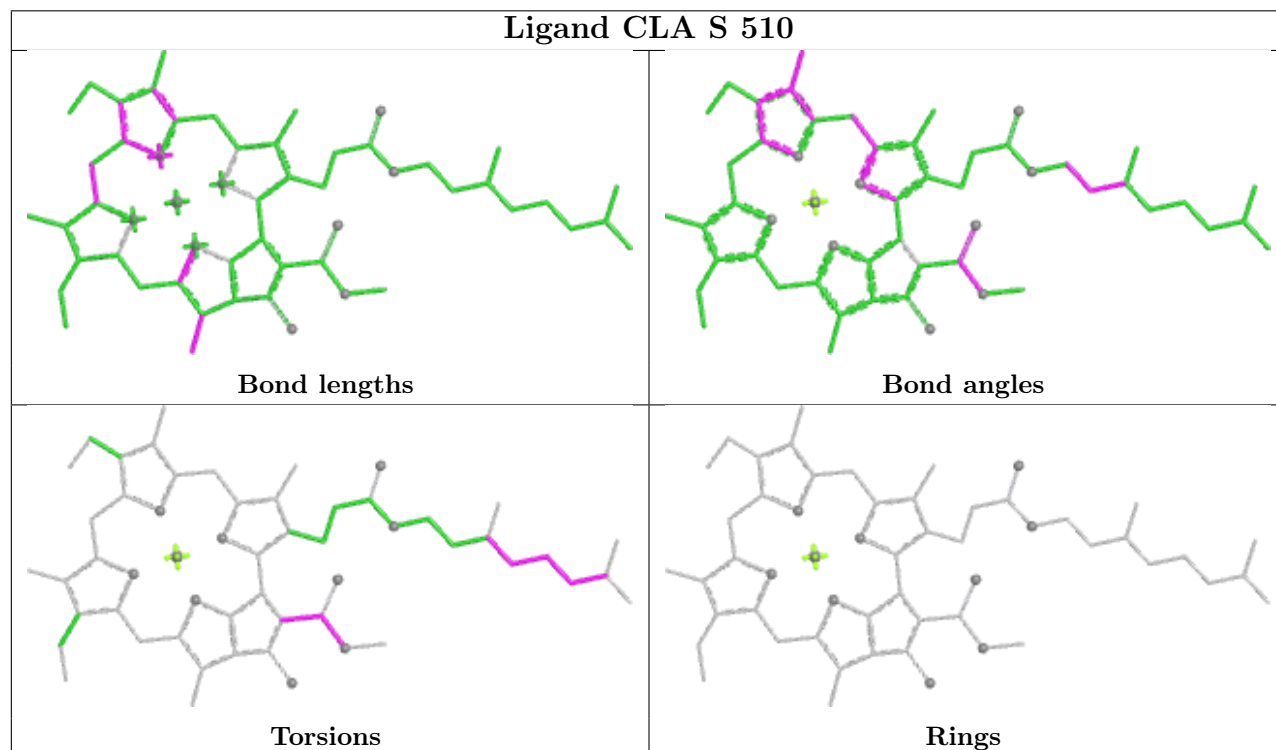
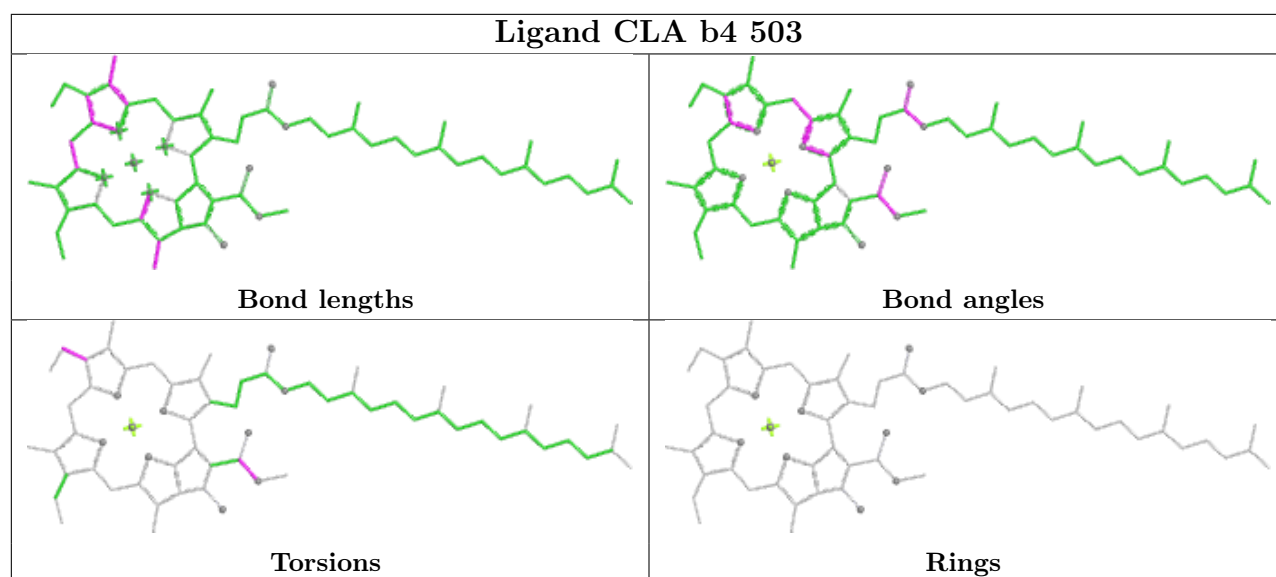


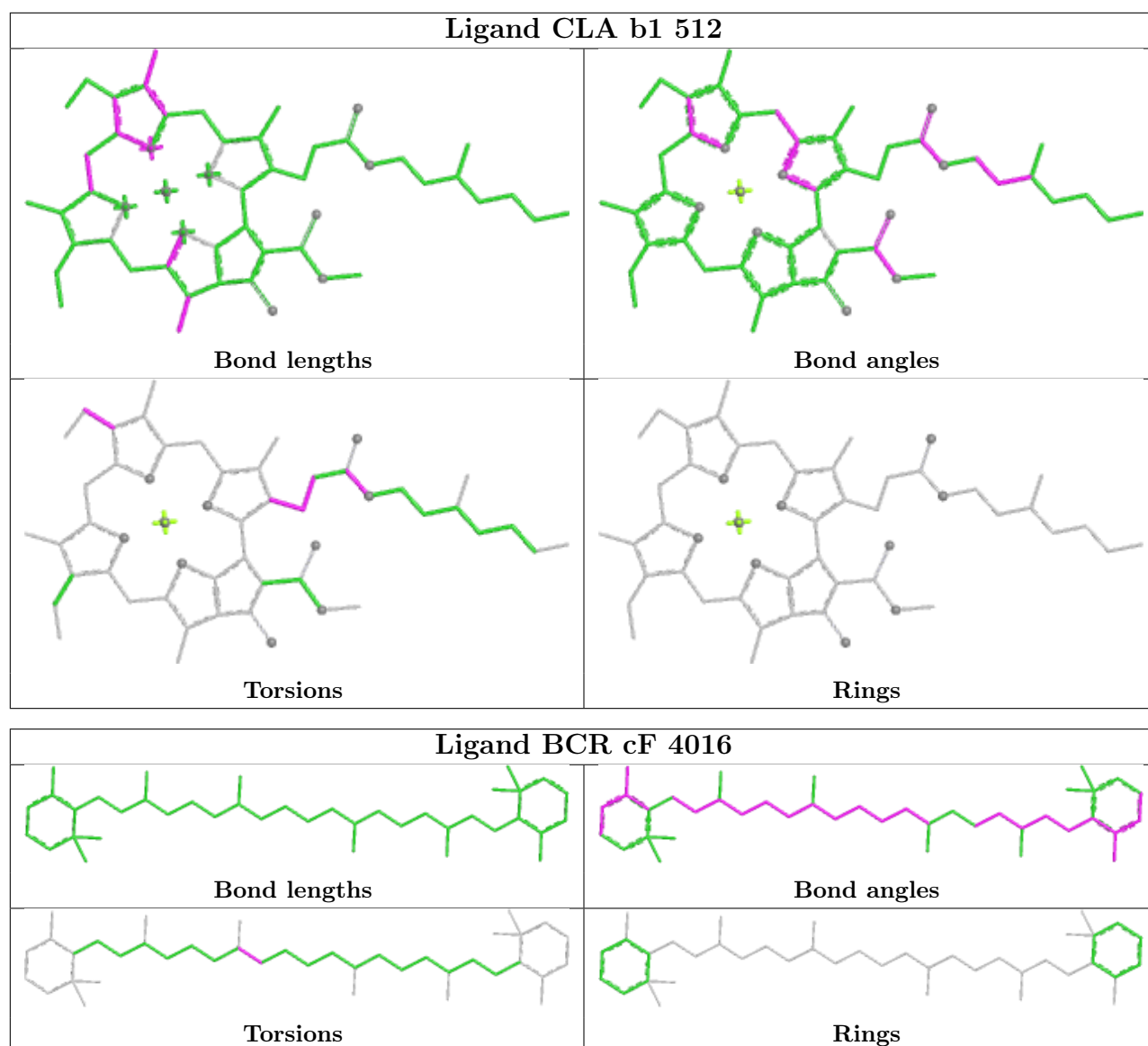
Ligand CLA cB 1225

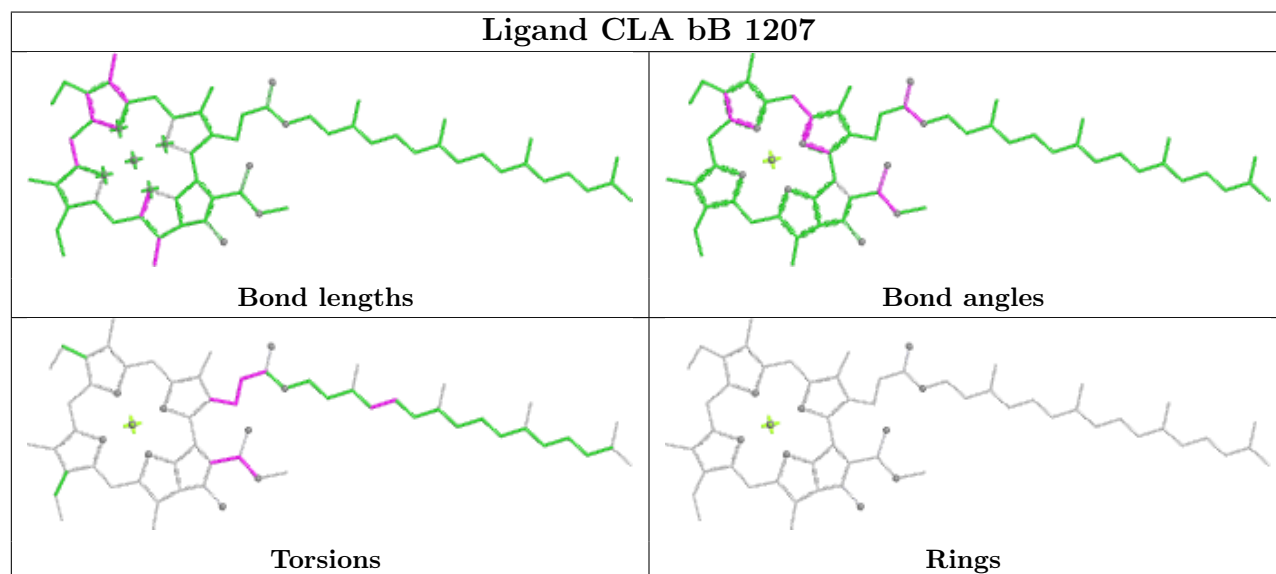
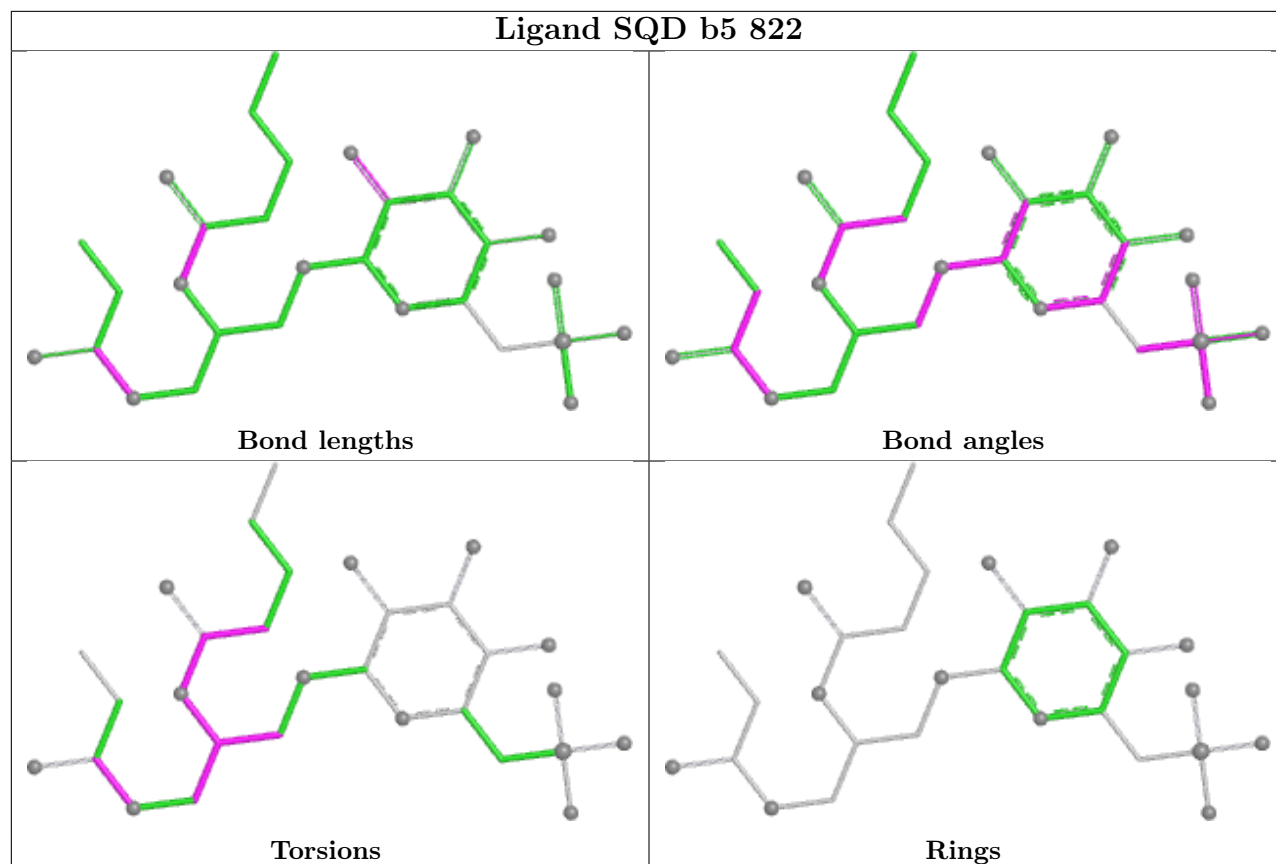


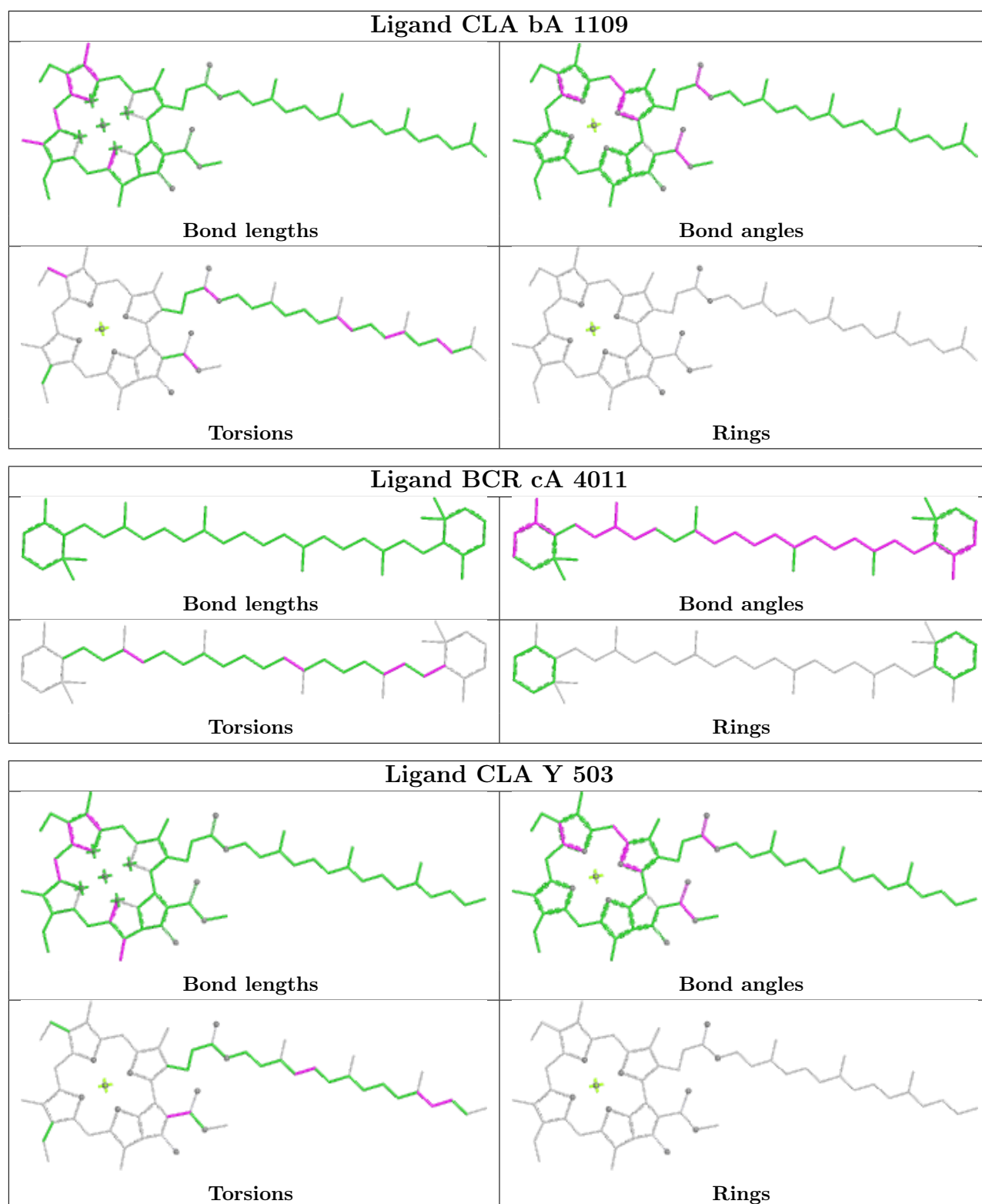


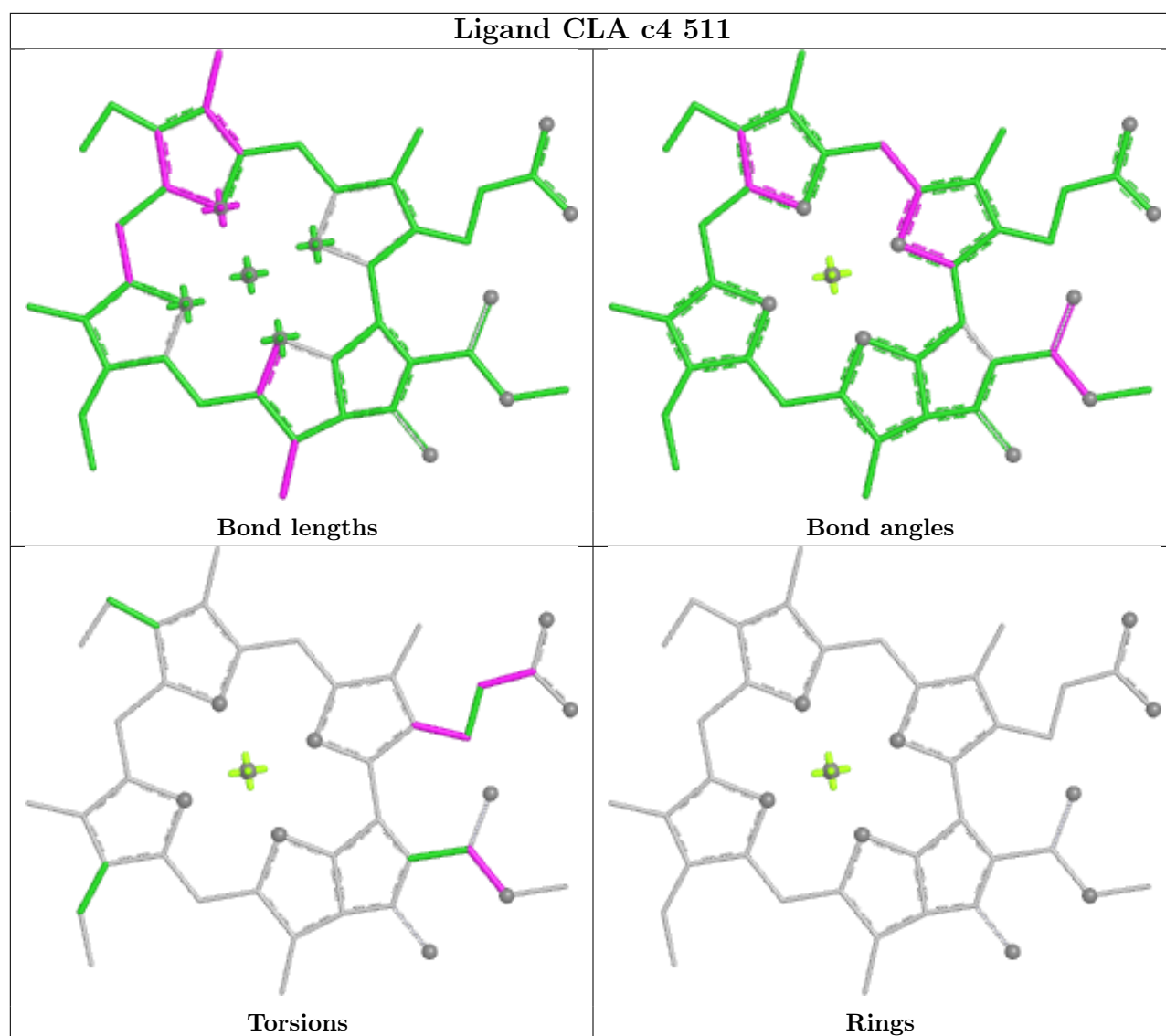




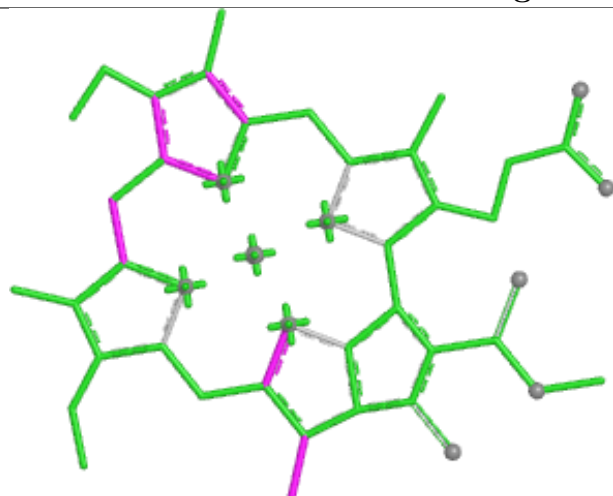




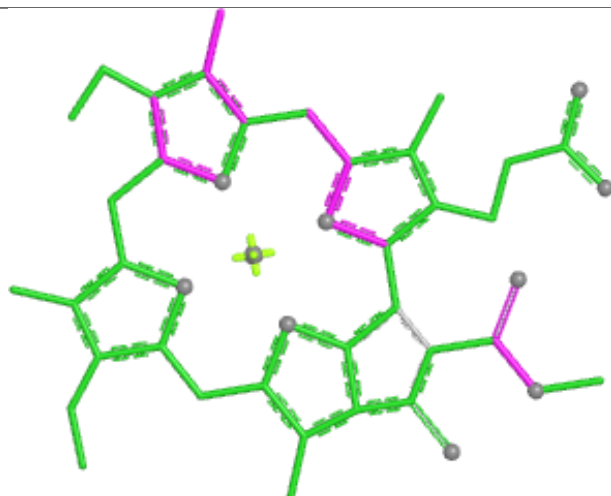




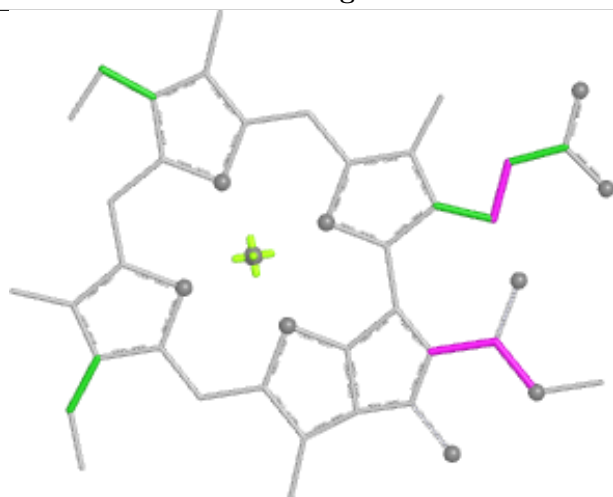
Ligand CLA V 518



Bond lengths



Bond angles

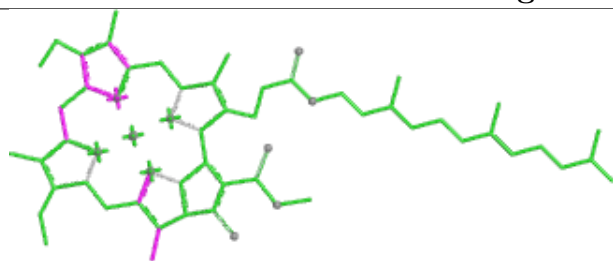


Torsions

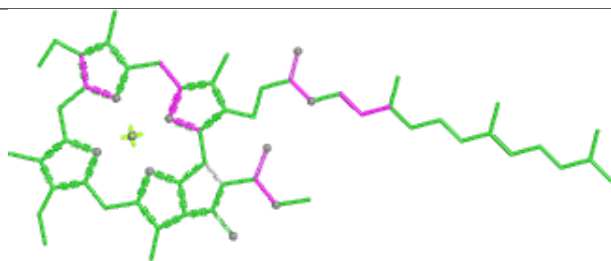


Rings

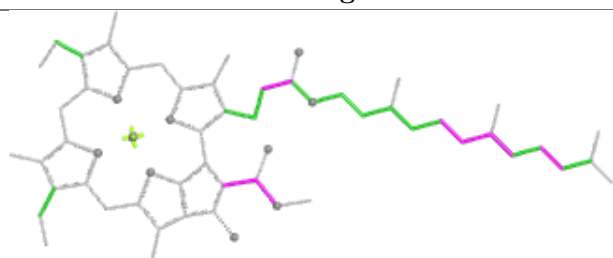
Ligand CLA n 509



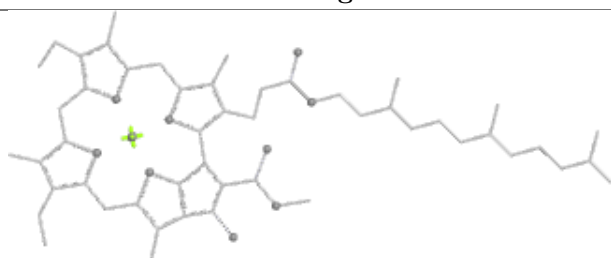
Bond lengths



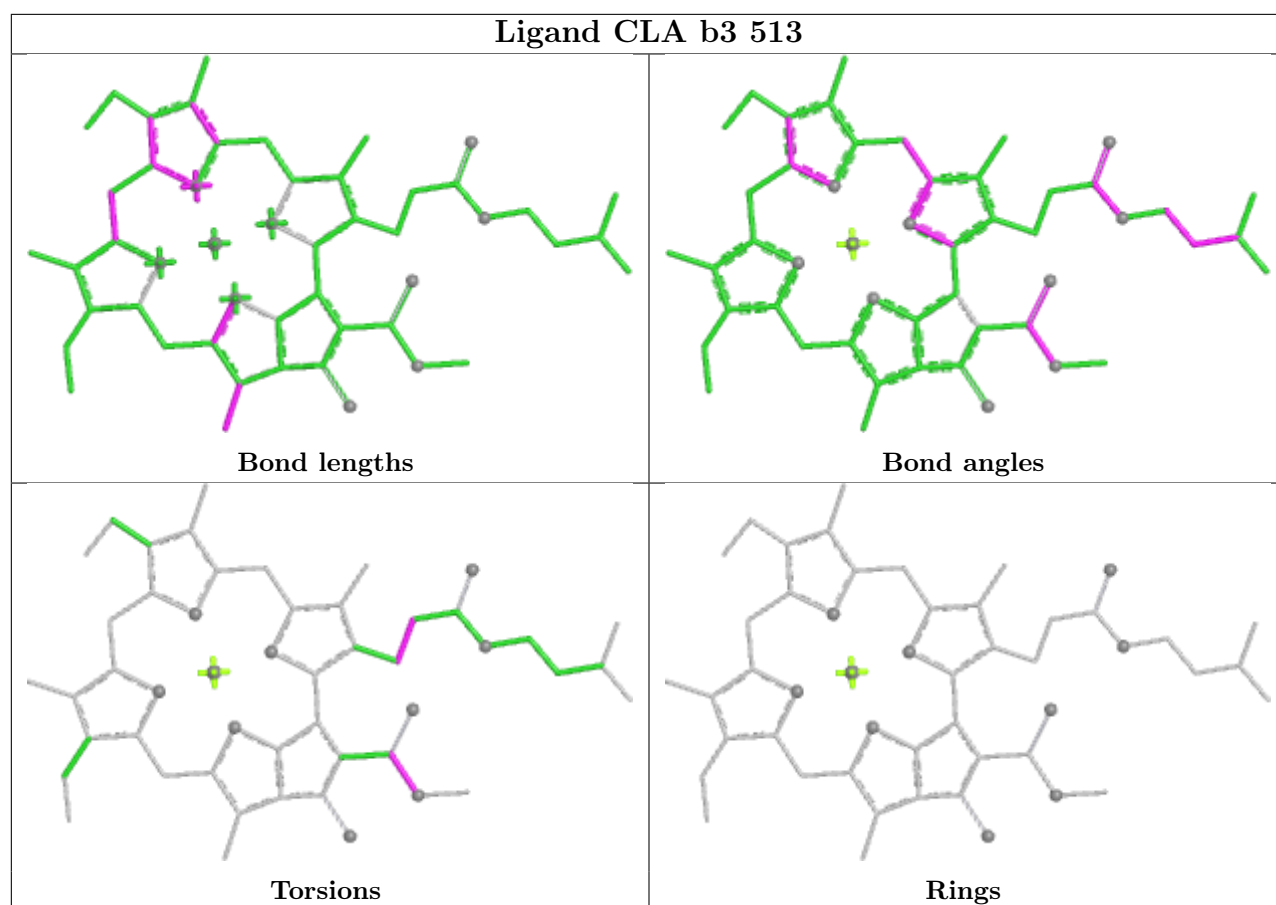
Bond angles



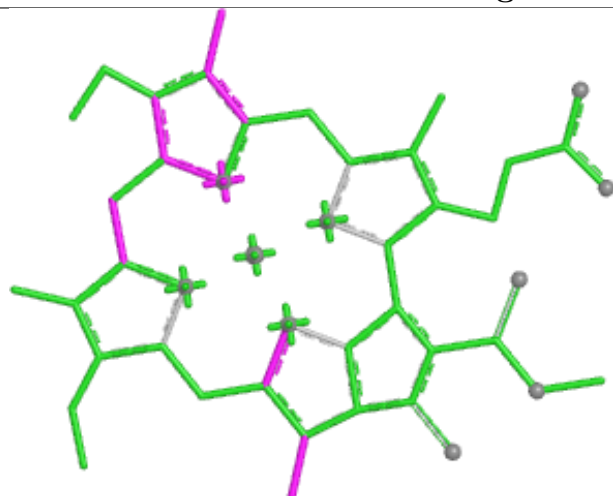
Torsions



Rings



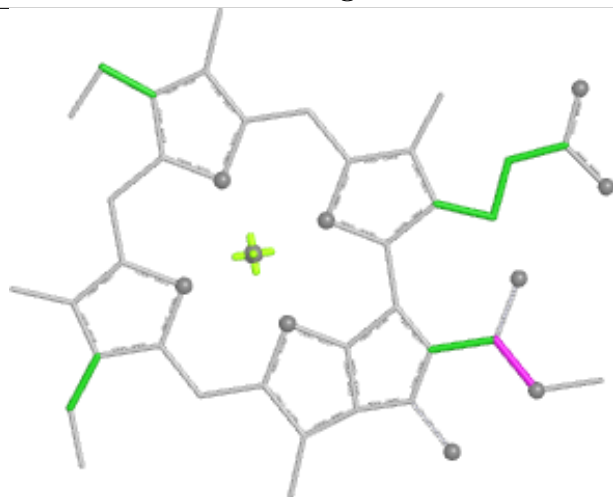
Ligand CLA cA 1108



Bond lengths



Bond angles

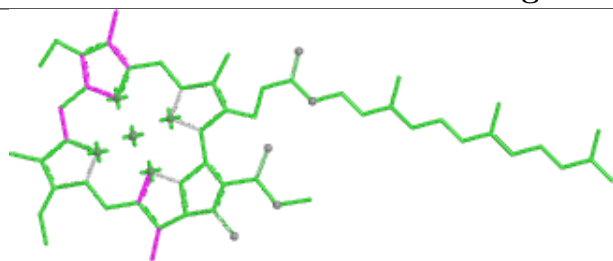


Torsions

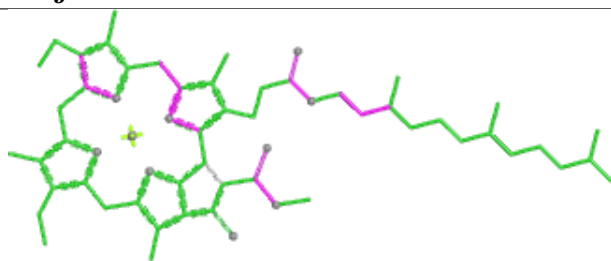


Rings

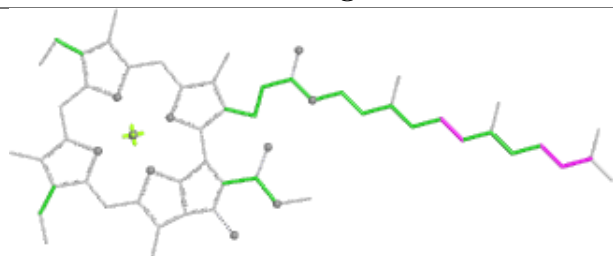
Ligand CLA j 509



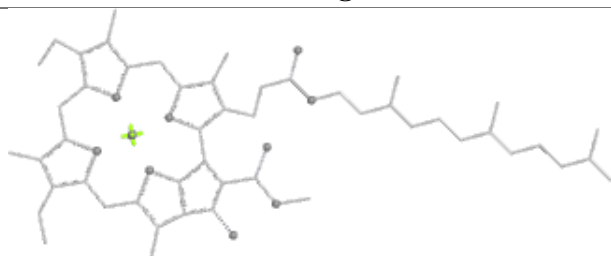
Bond lengths



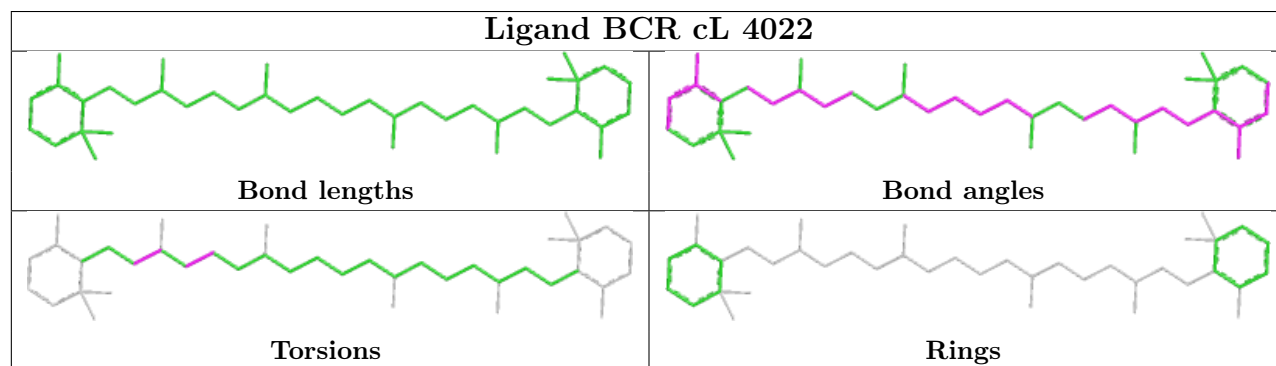
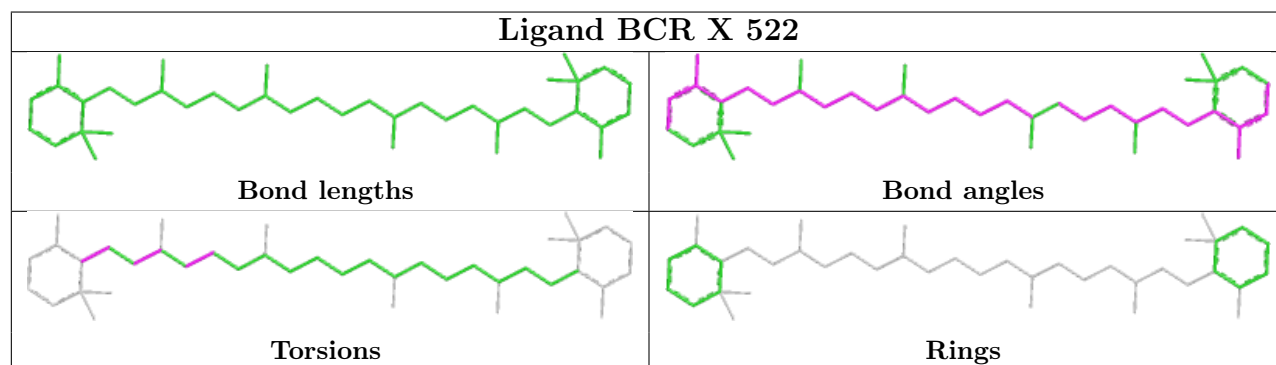
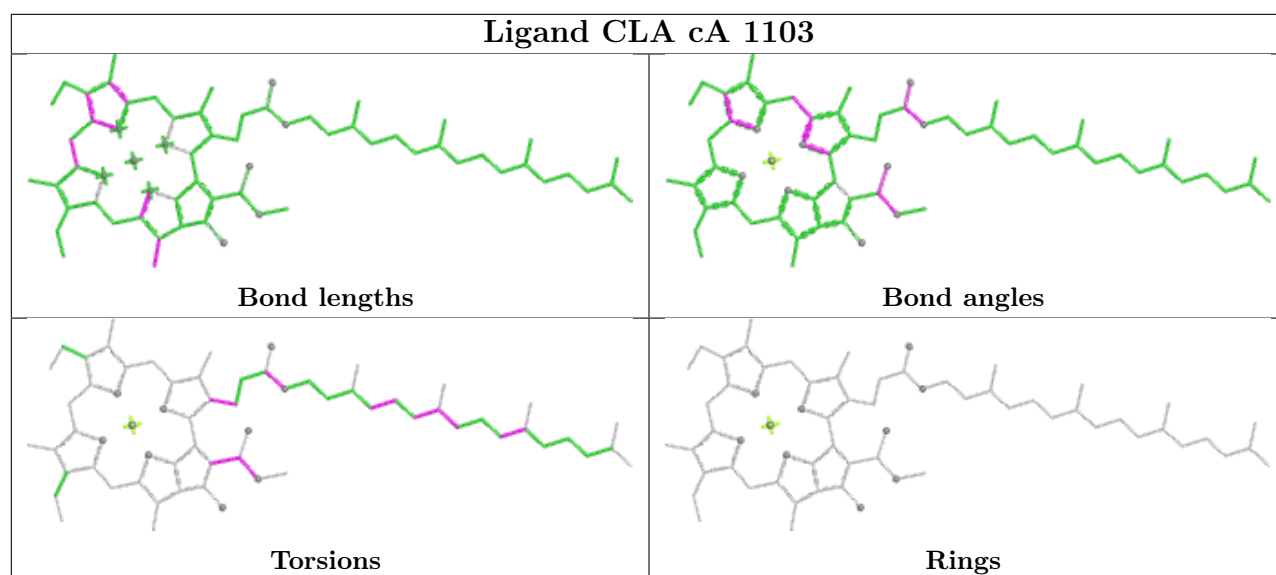
Bond angles



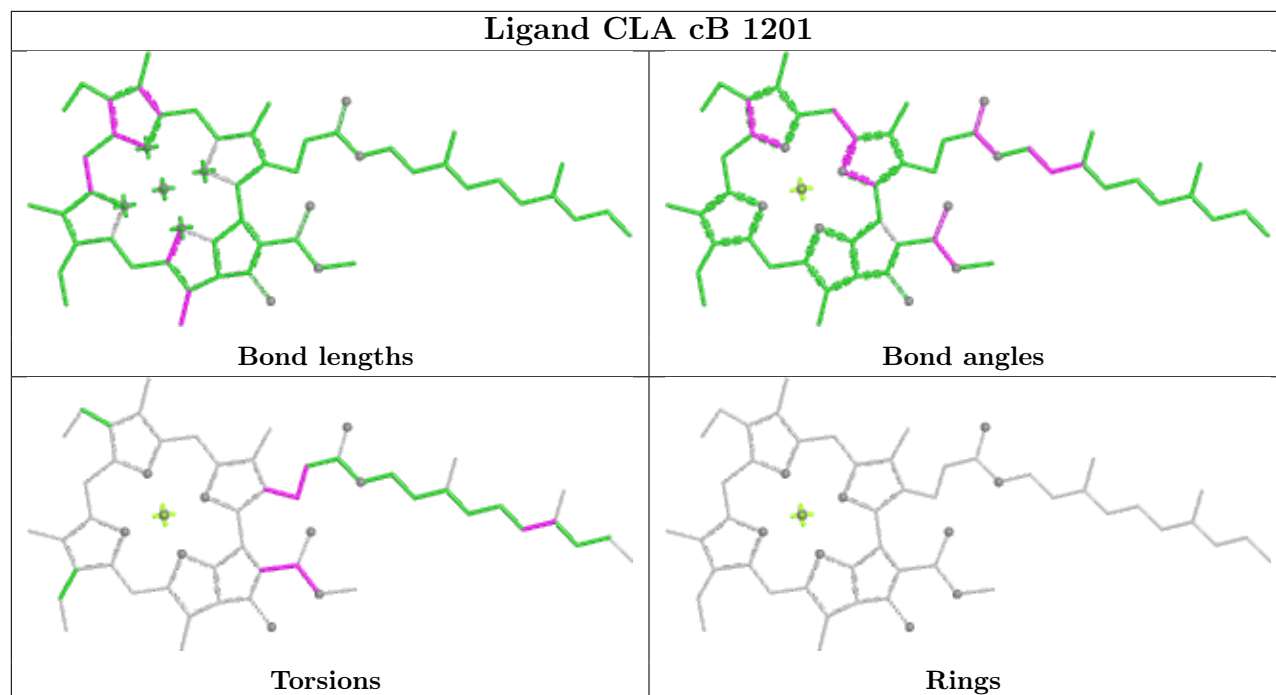
Torsions



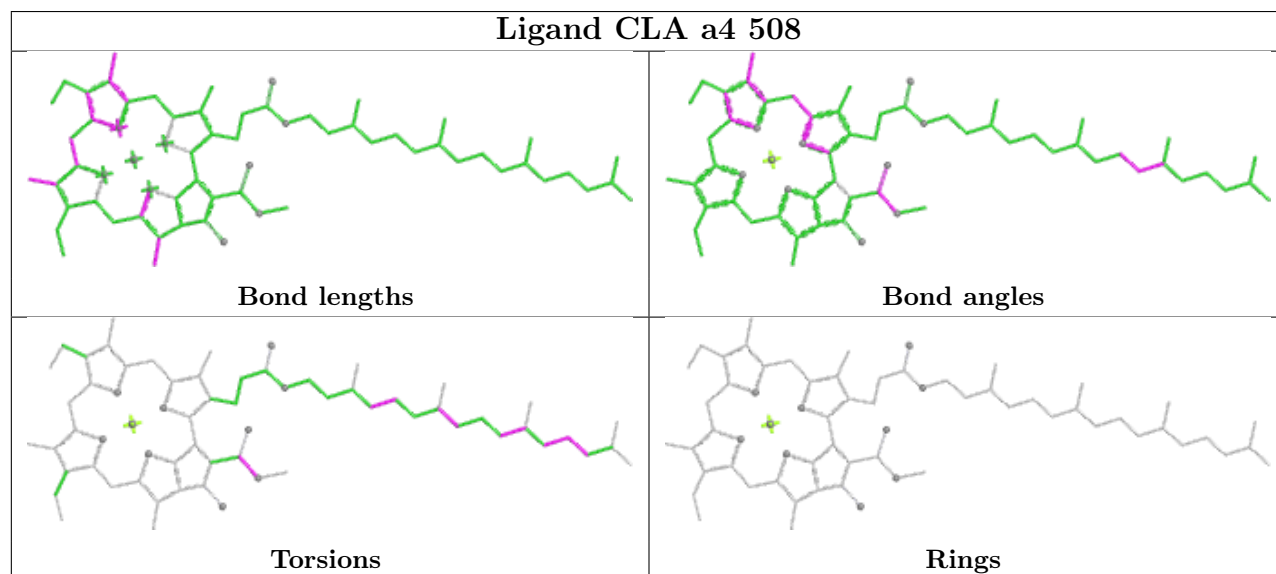
Rings

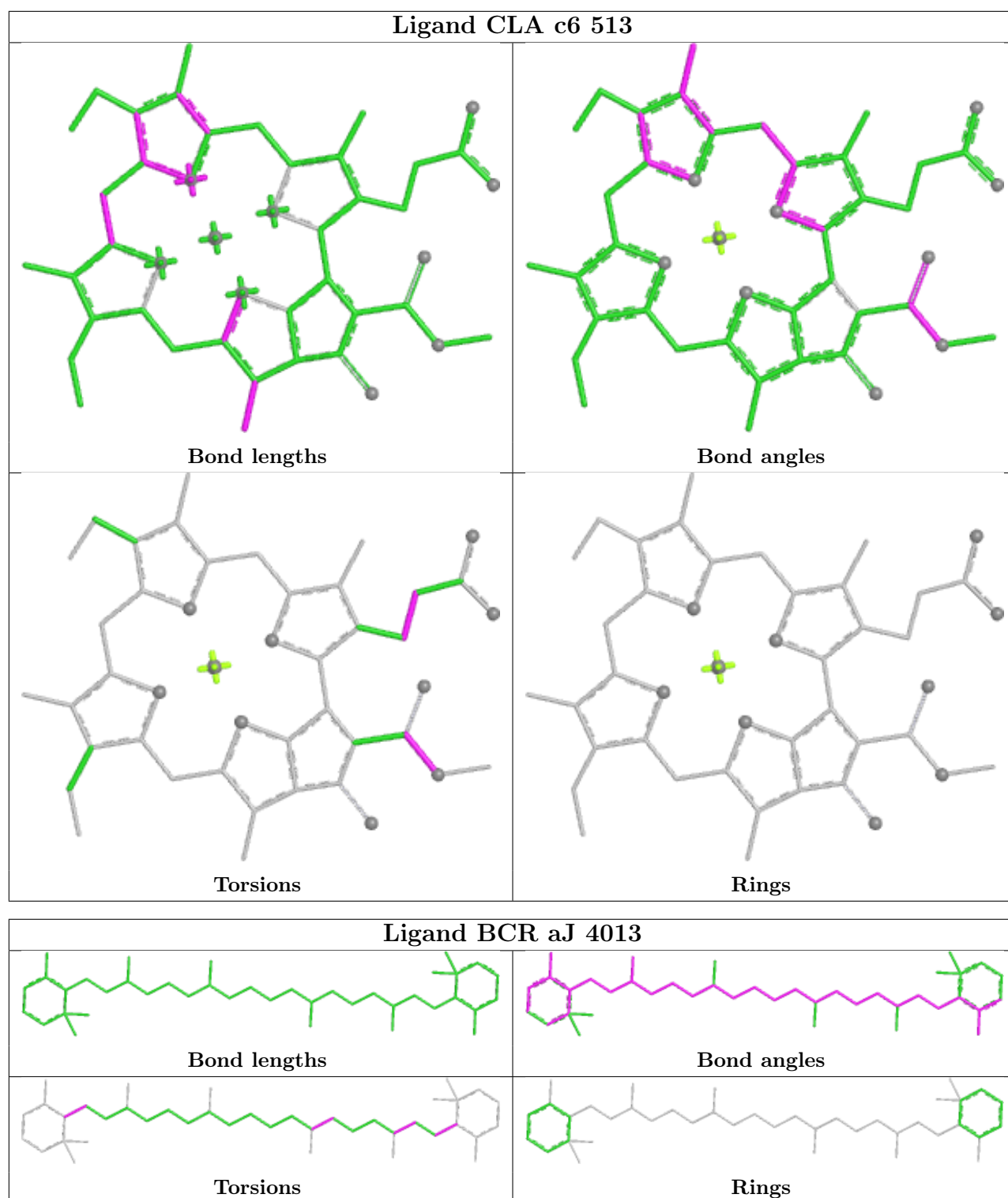


Ligand CLA cB 1201

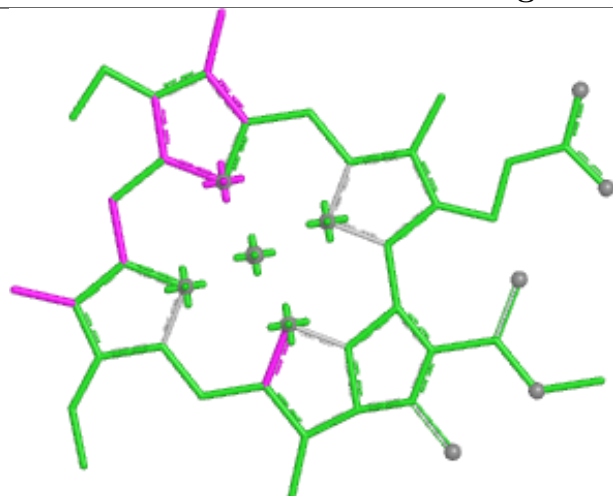


Ligand CLA a4 508





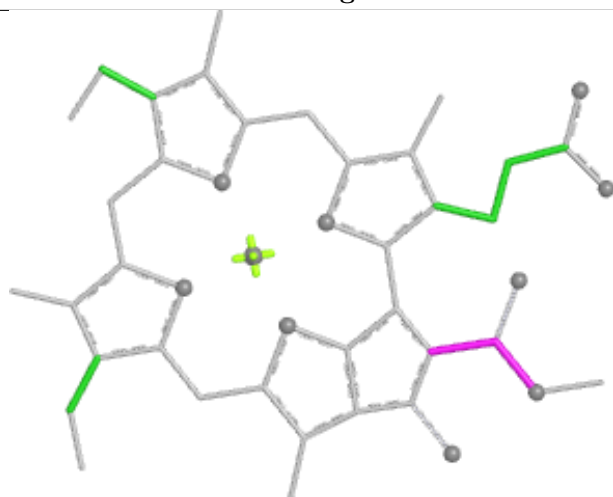
Ligand CLA S 506



Bond lengths



Bond angles

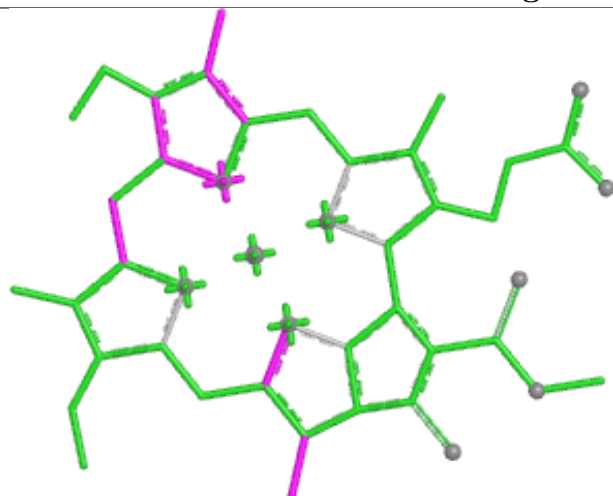


Torsions

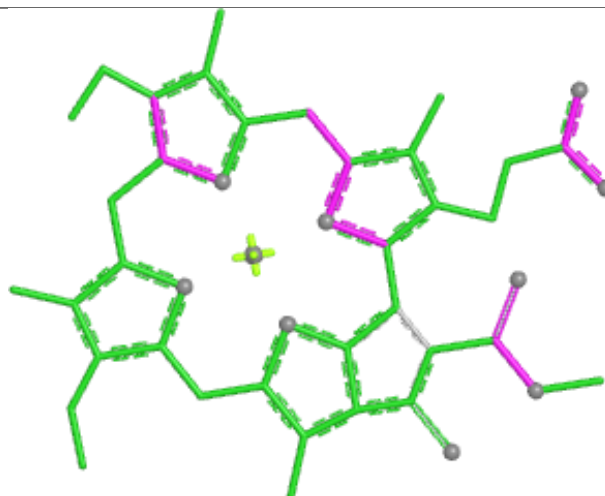


Rings

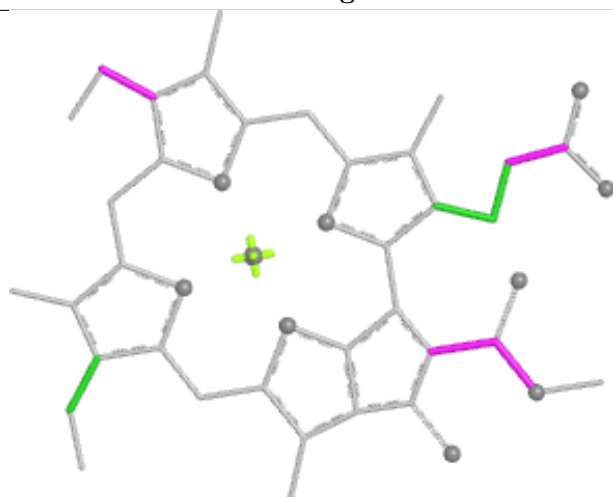
Ligand CLA i 516



Bond lengths



Bond angles

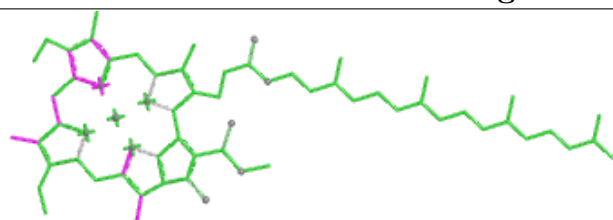


Torsions

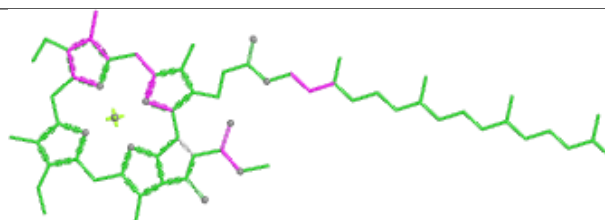


Rings

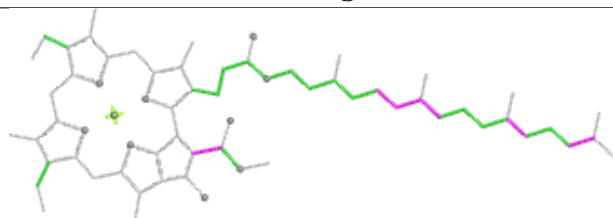
Ligand CLA cB 1223



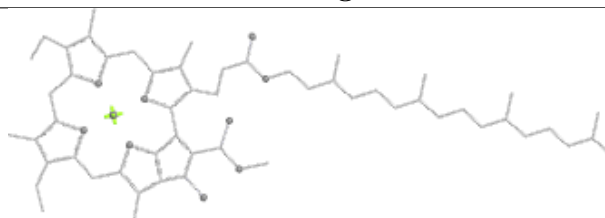
Bond lengths



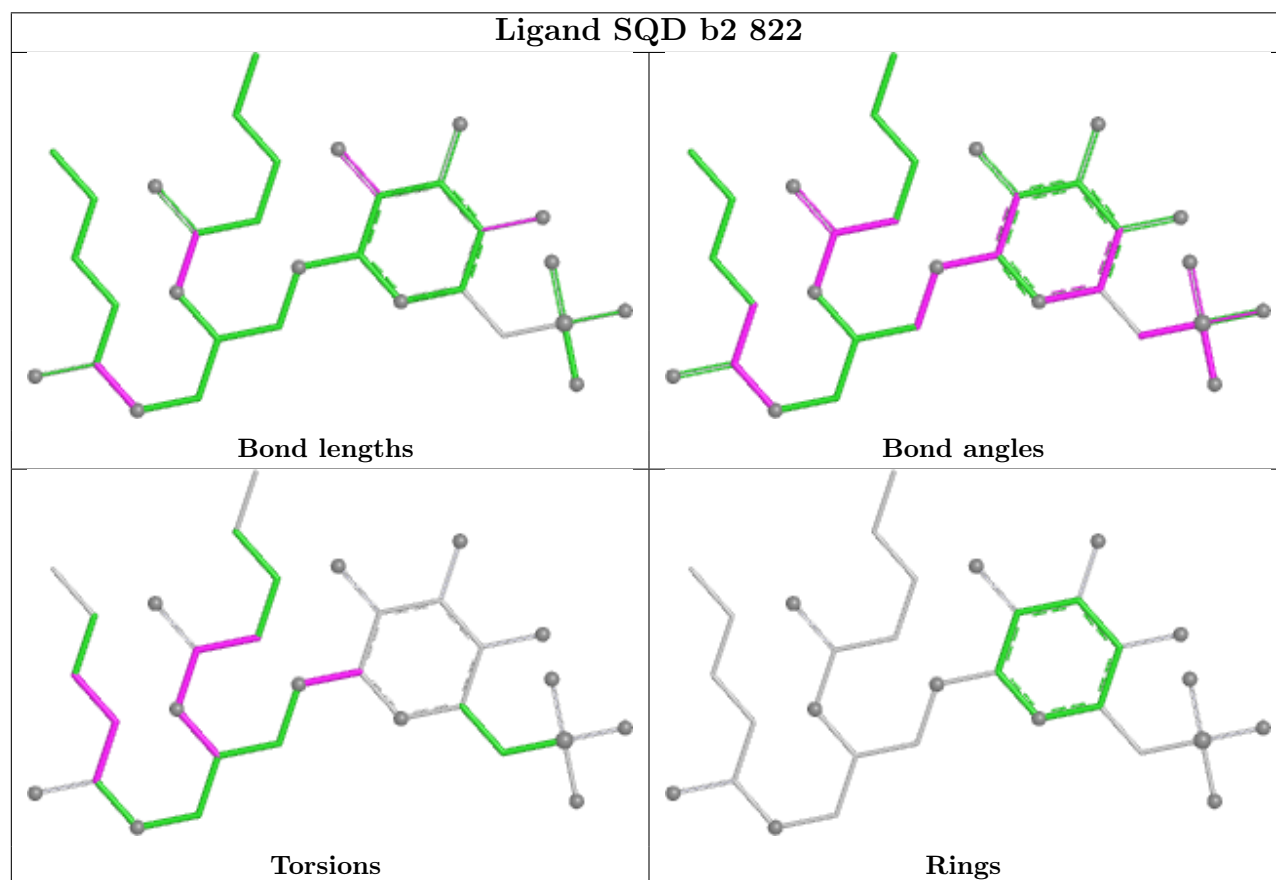
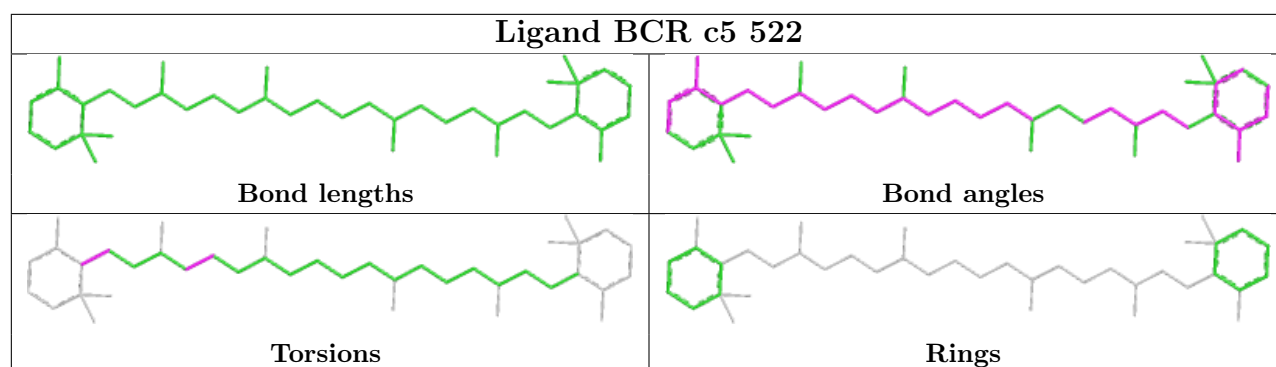
Bond angles

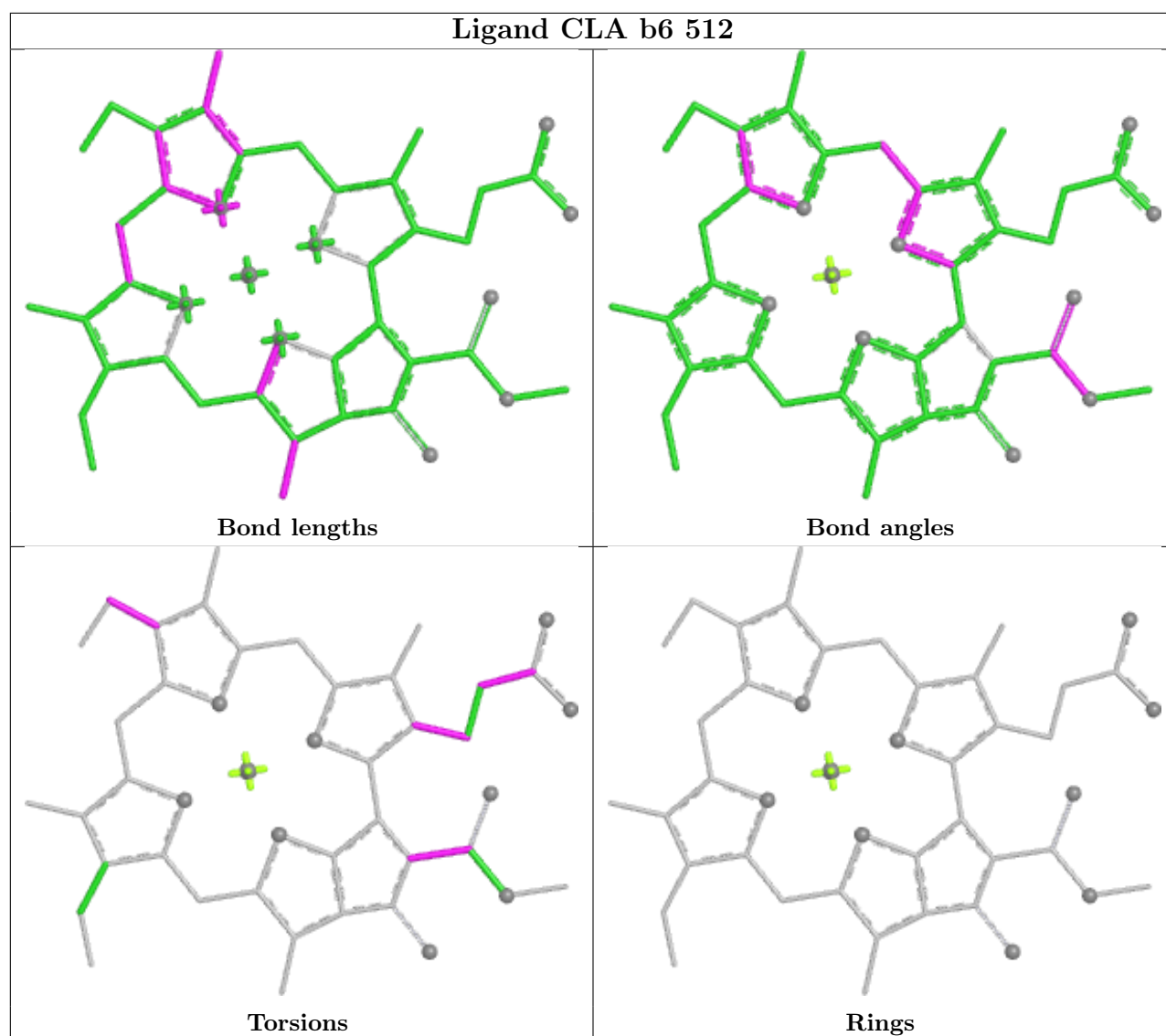


Torsions

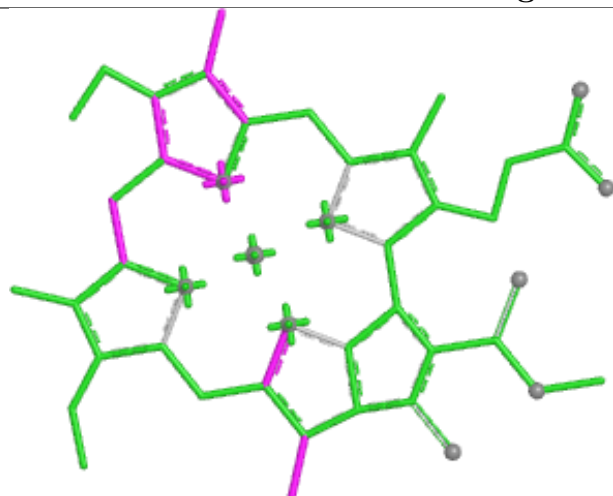


Rings

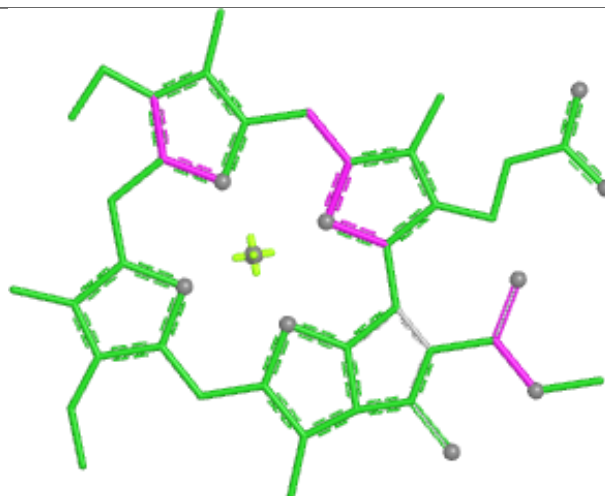




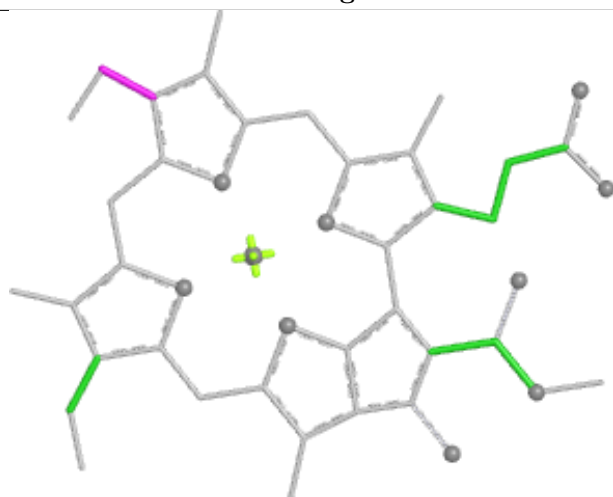
Ligand CLA d 504



Bond lengths



Bond angles

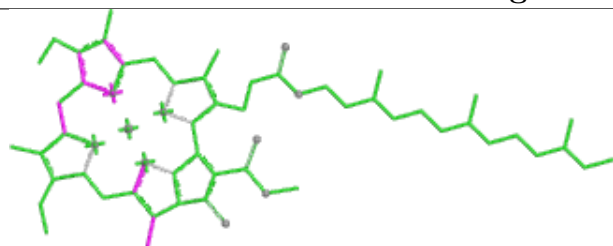


Torsions

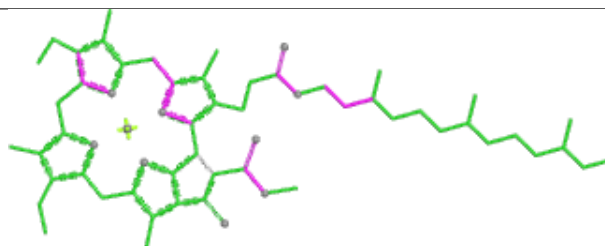


Rings

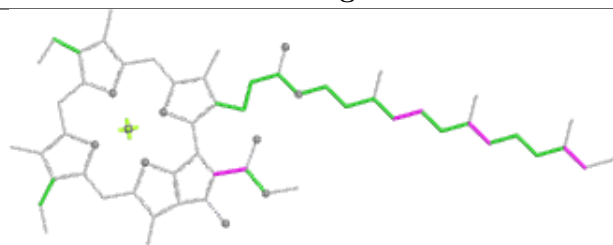
Ligand CLA a2 507



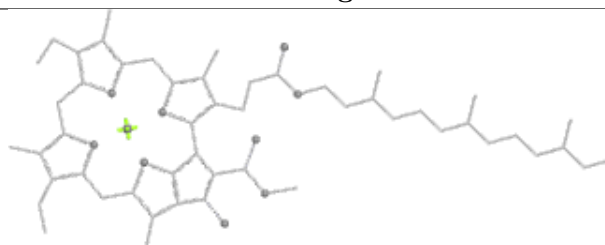
Bond lengths



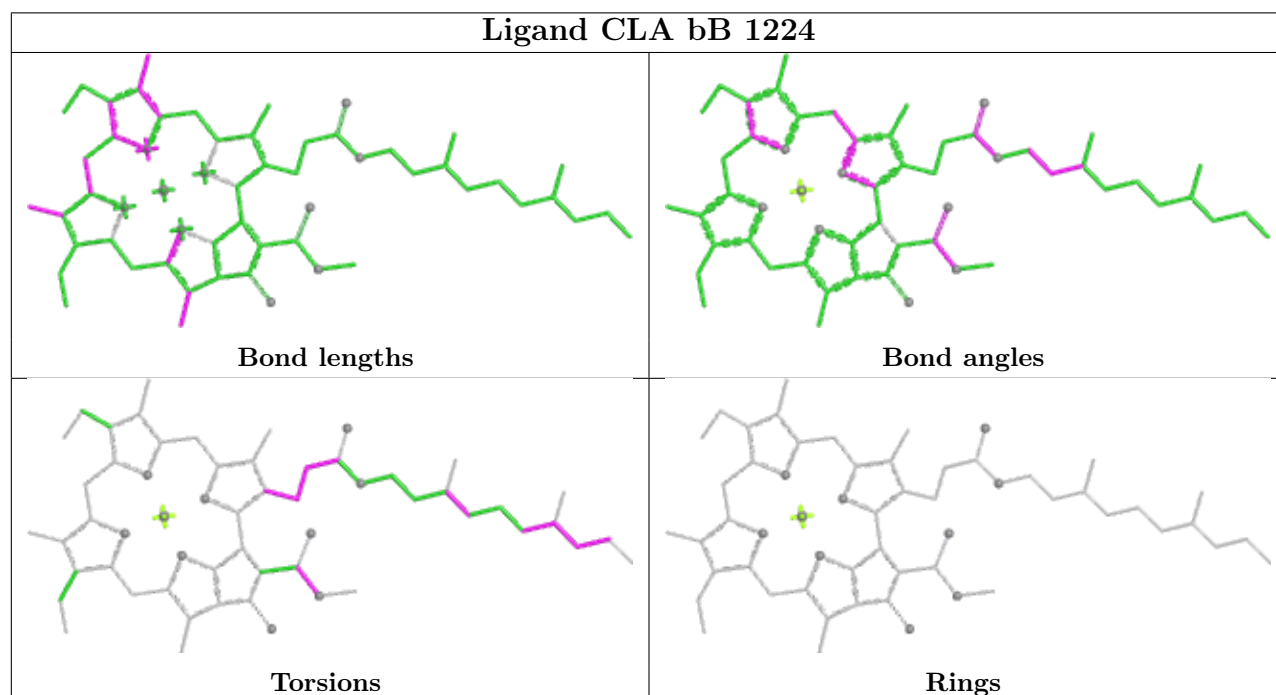
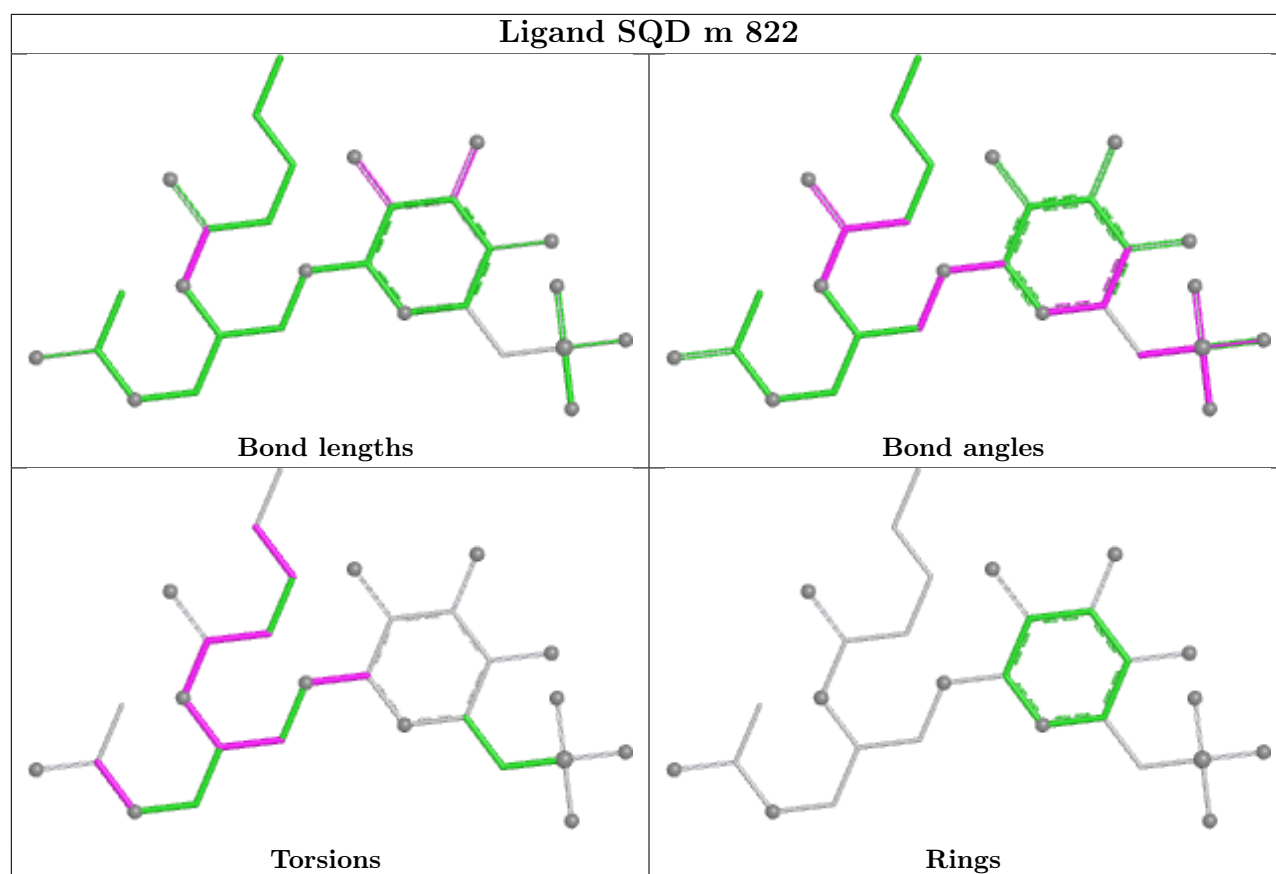
Bond angles

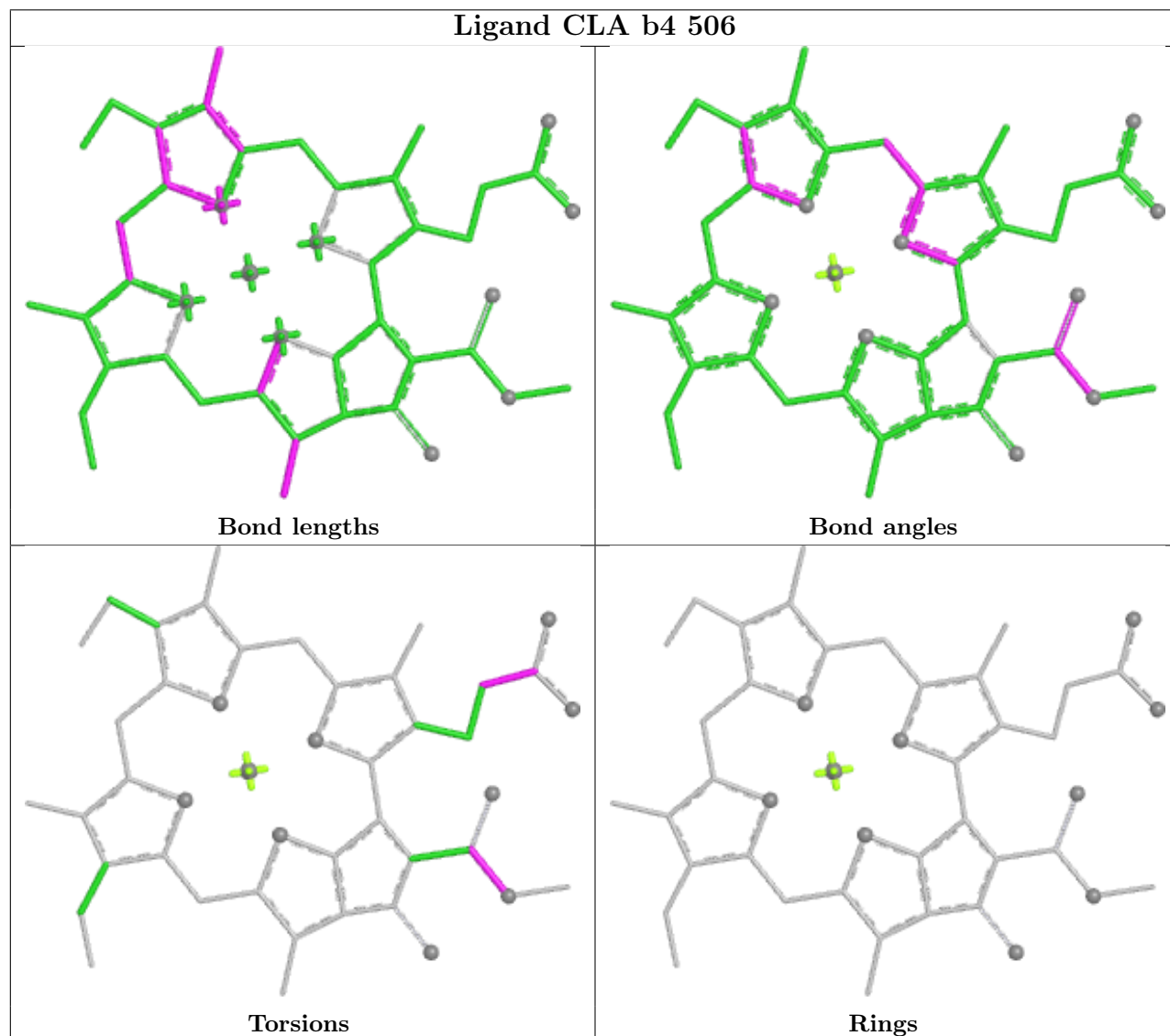
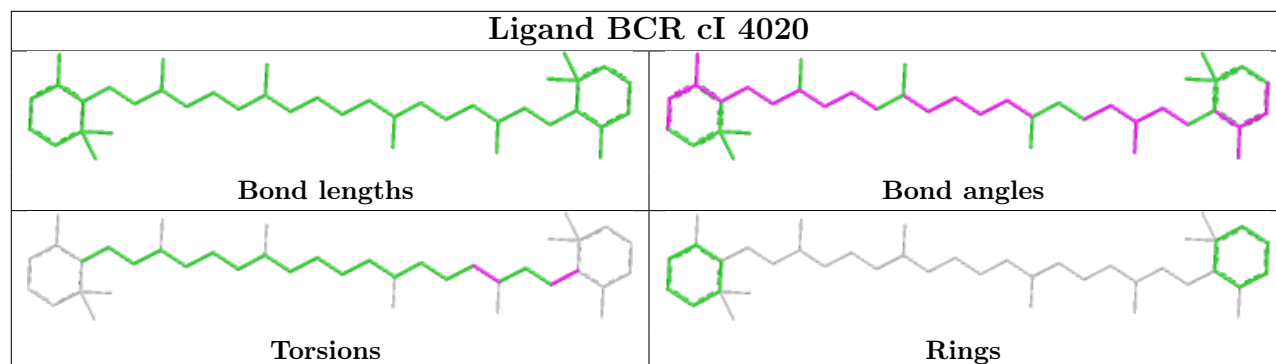


Torsions

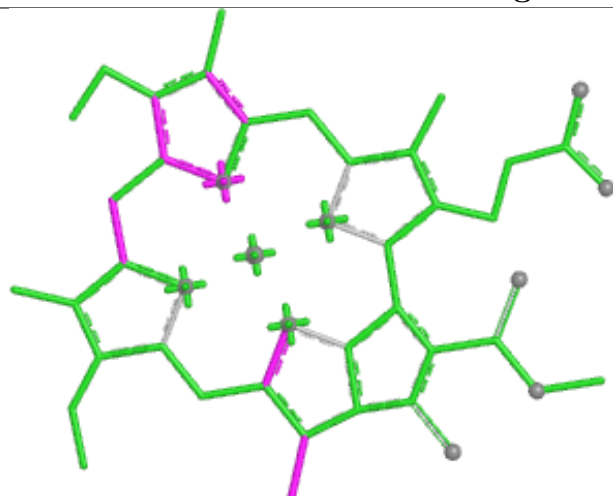


Rings

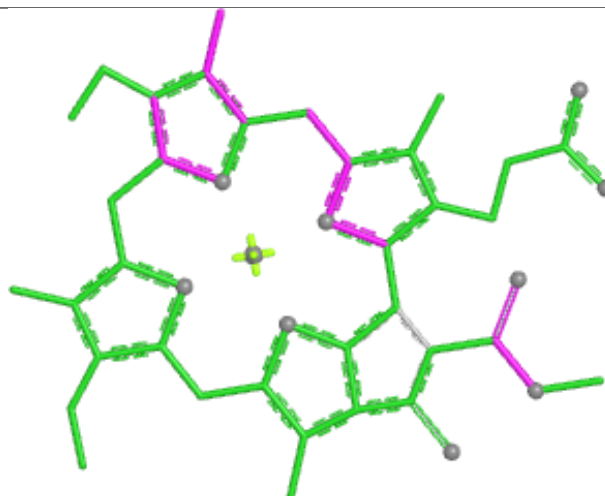




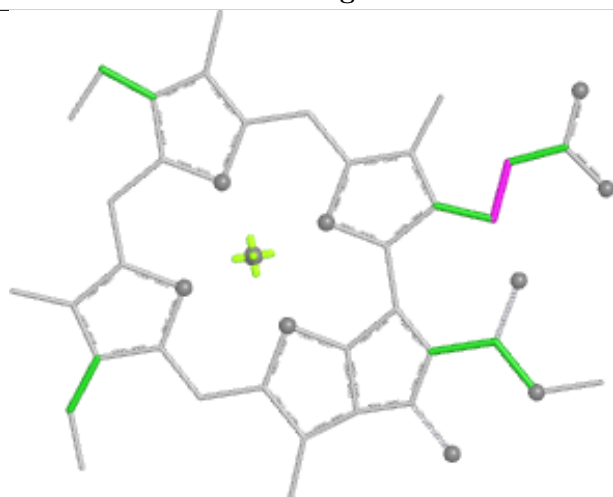
Ligand CLA Y 513



Bond lengths



Bond angles

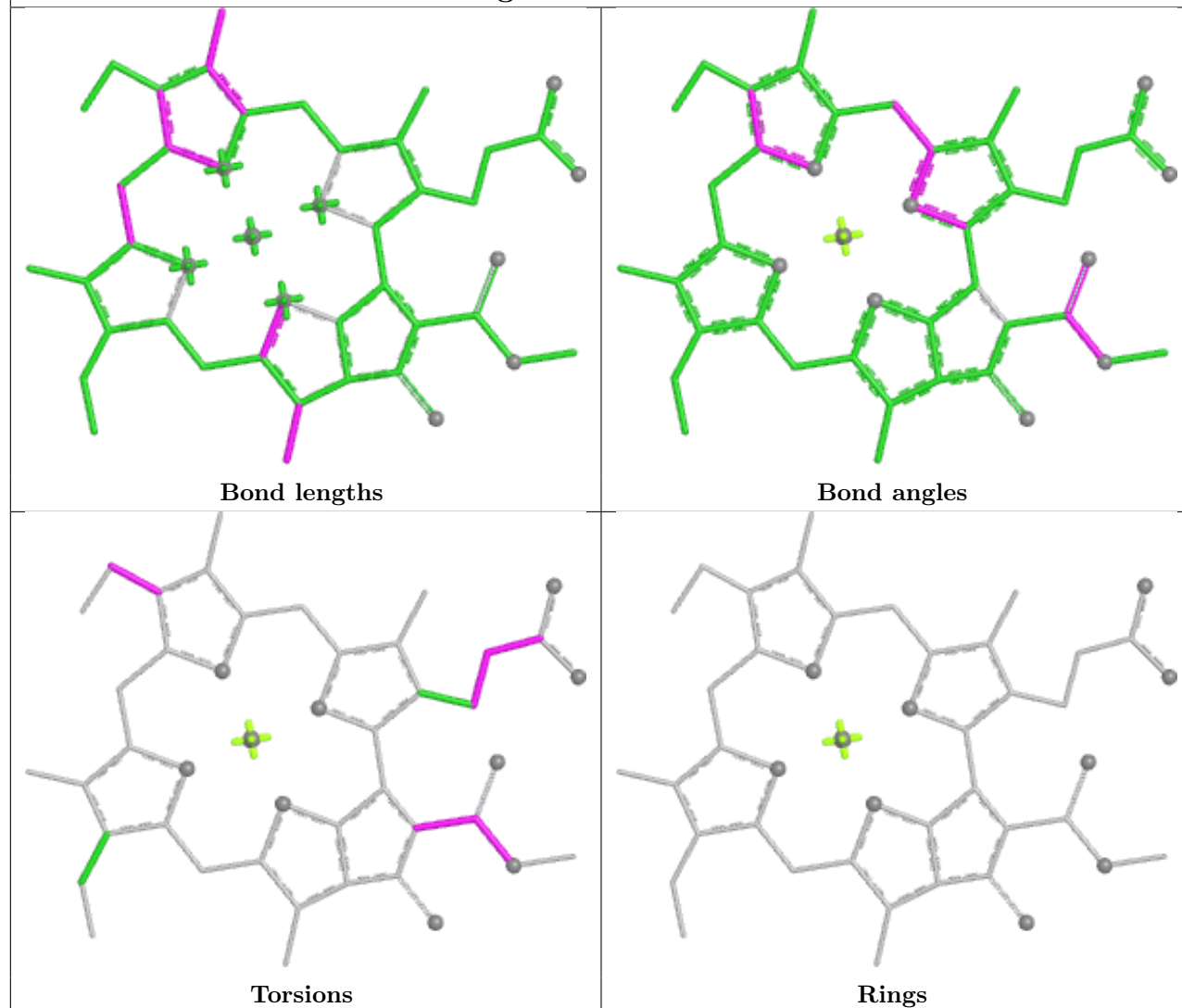


Torsions

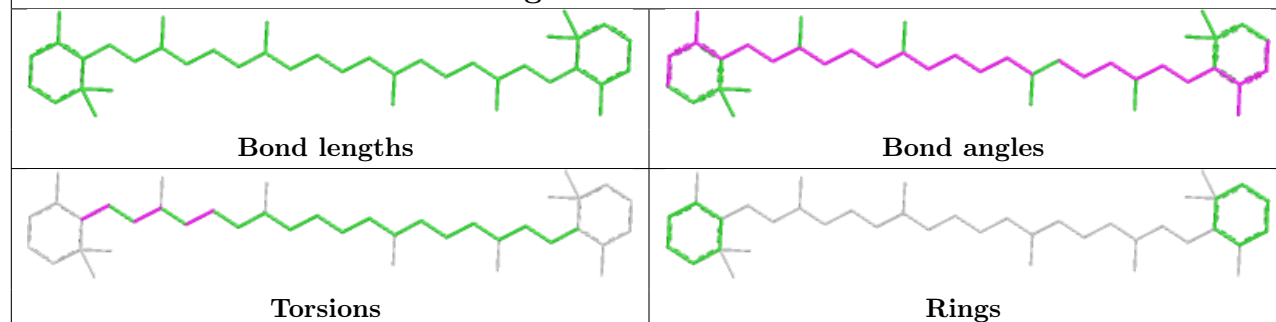


Rings

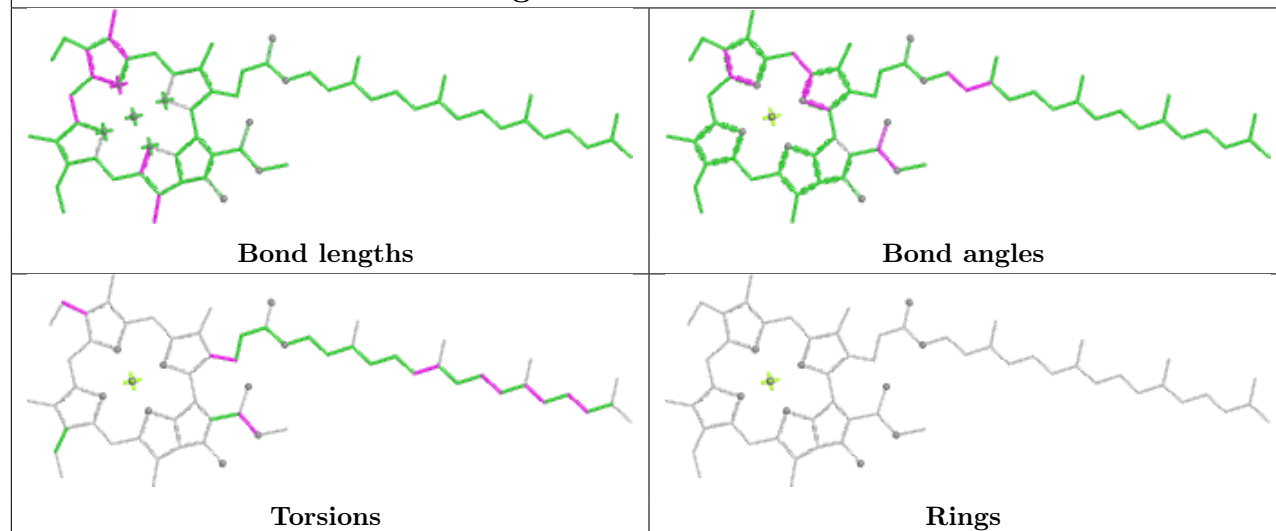
Ligand CLA e 512



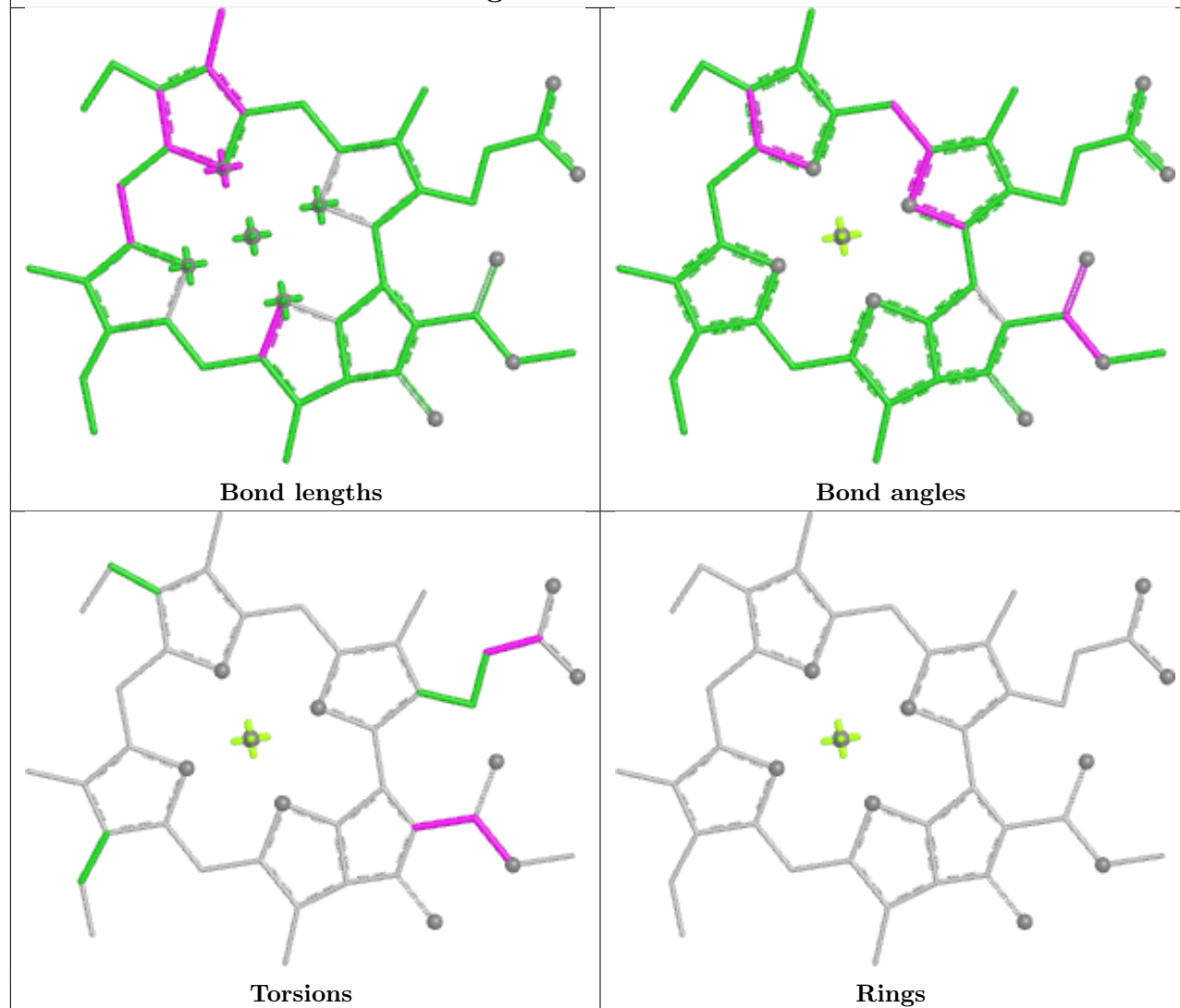
Ligand BCR b1 522

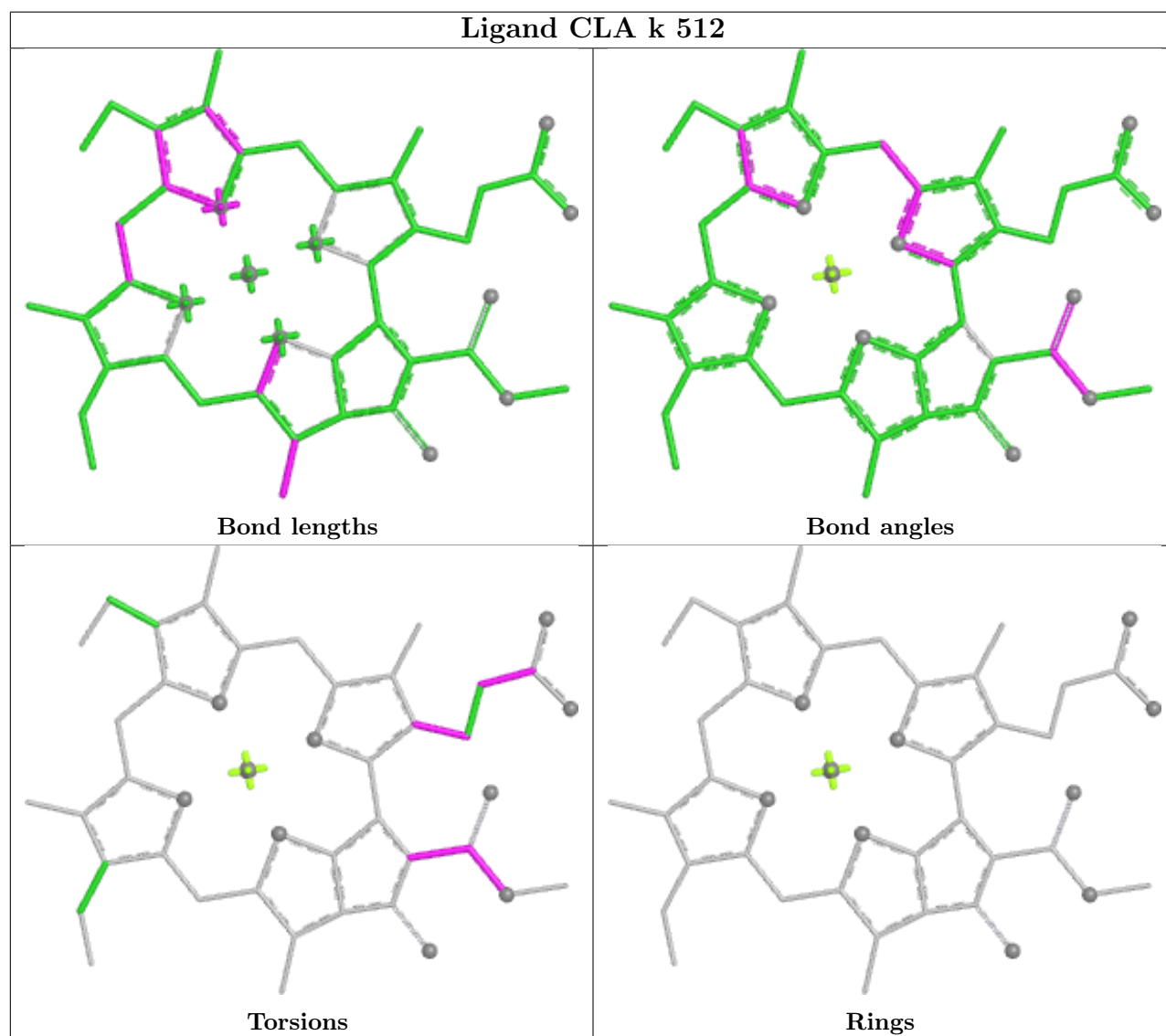
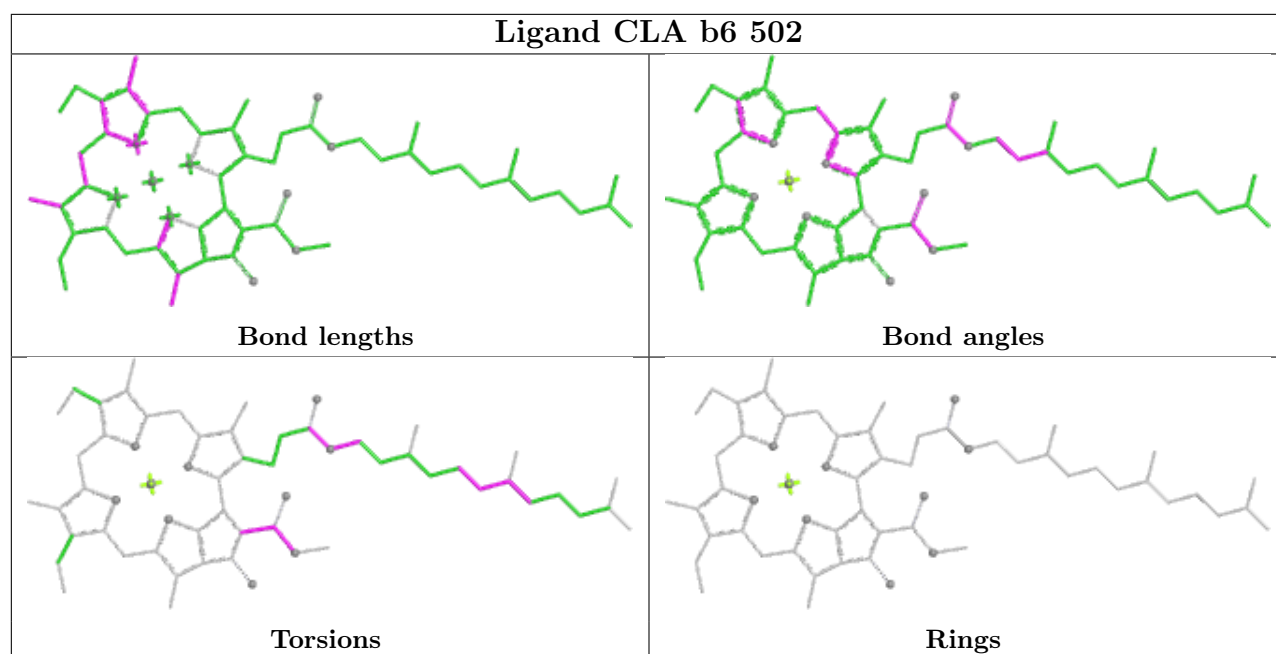


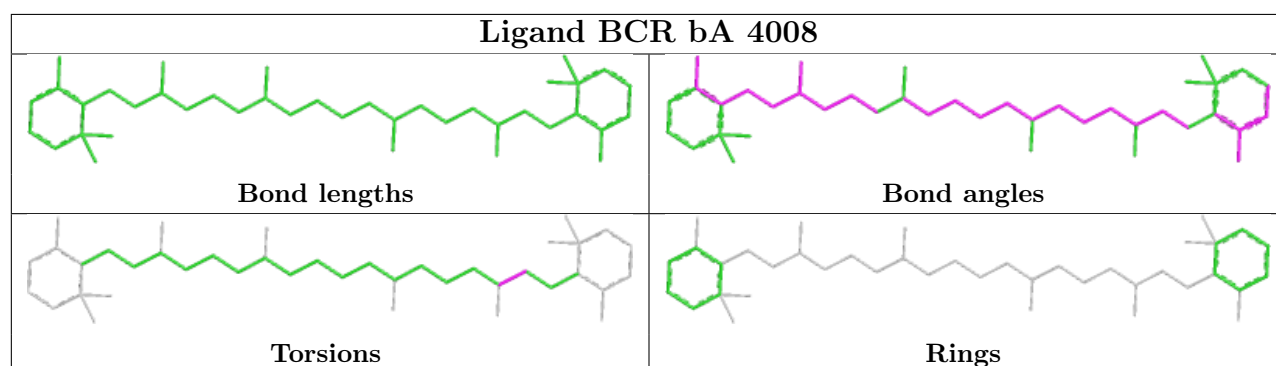
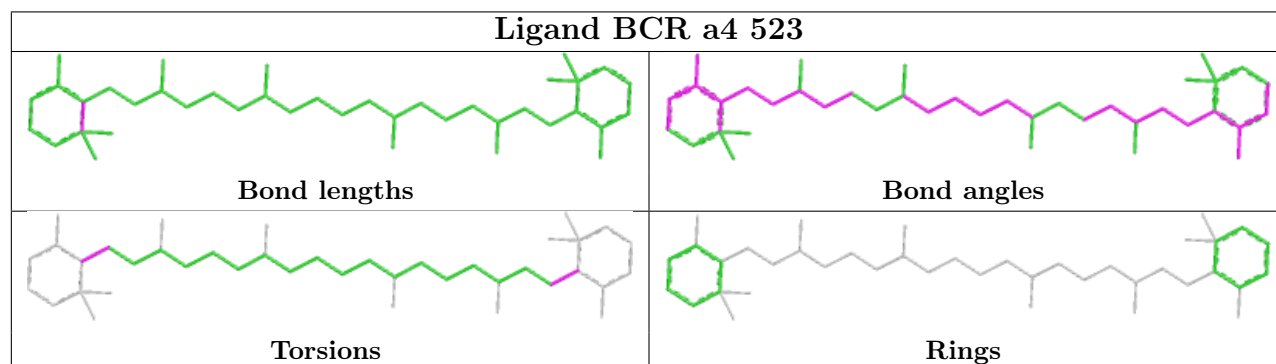
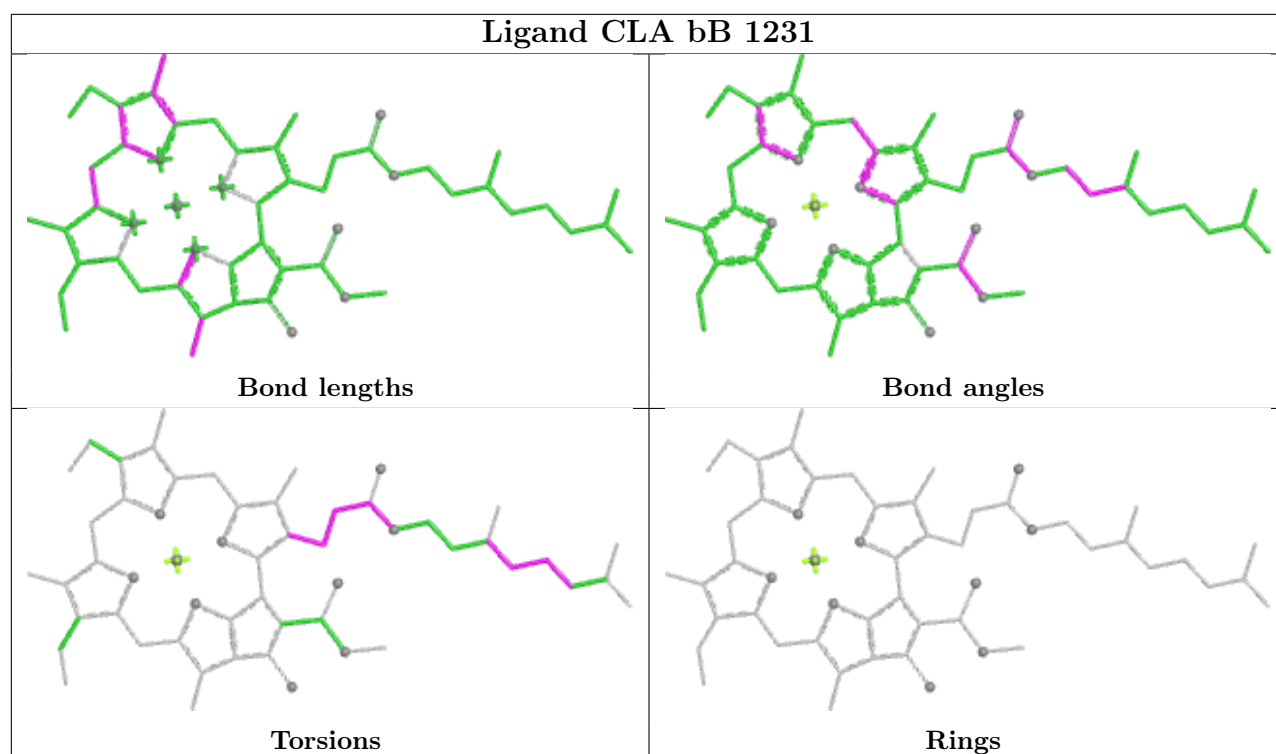
Ligand CLA bA 1104

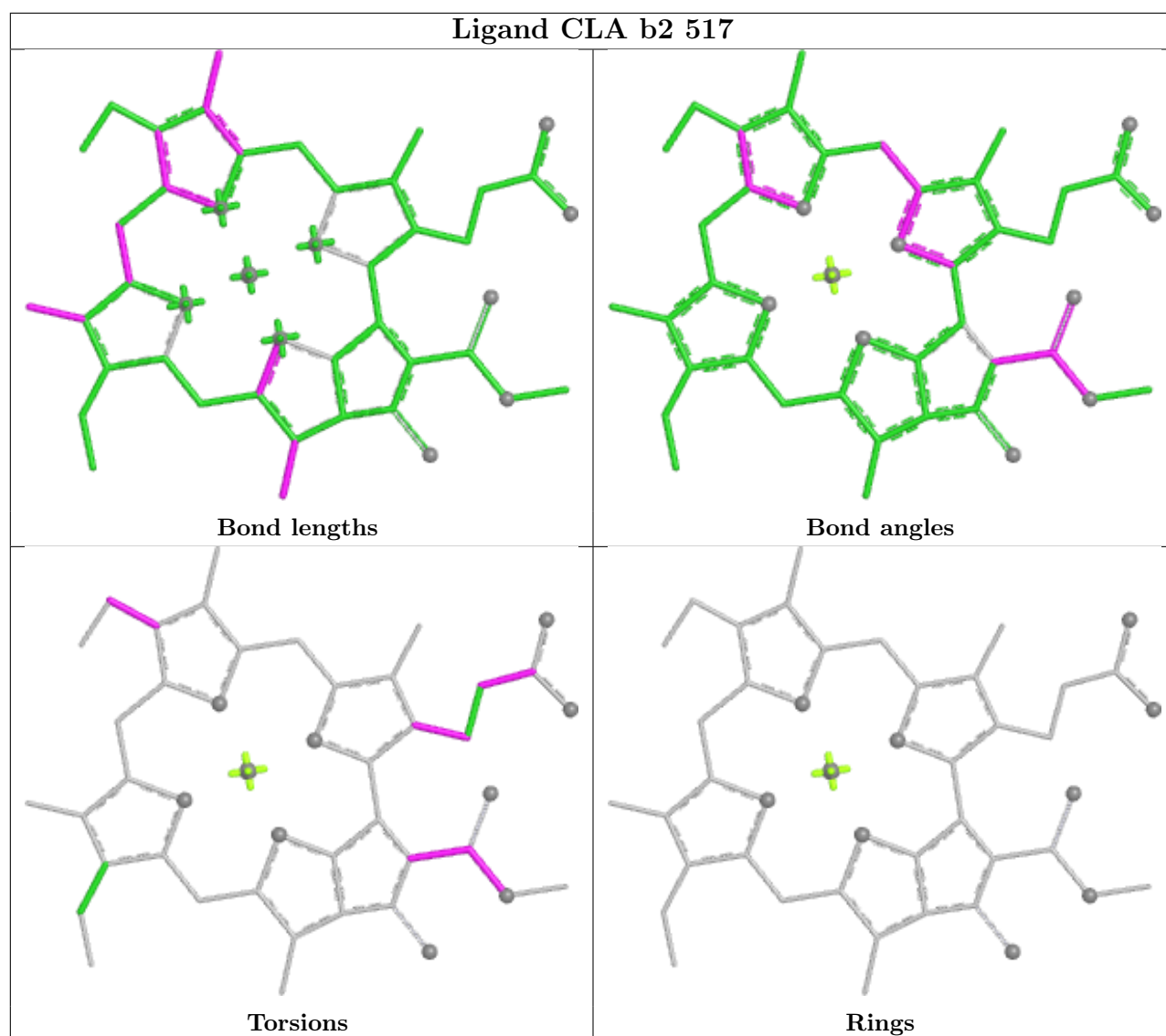


Ligand CLA b6 506

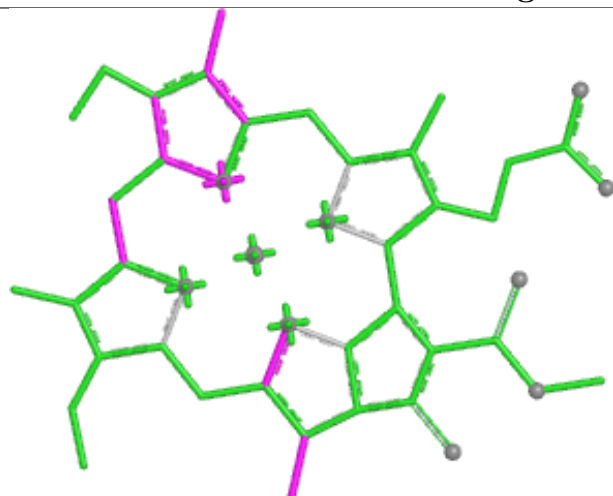




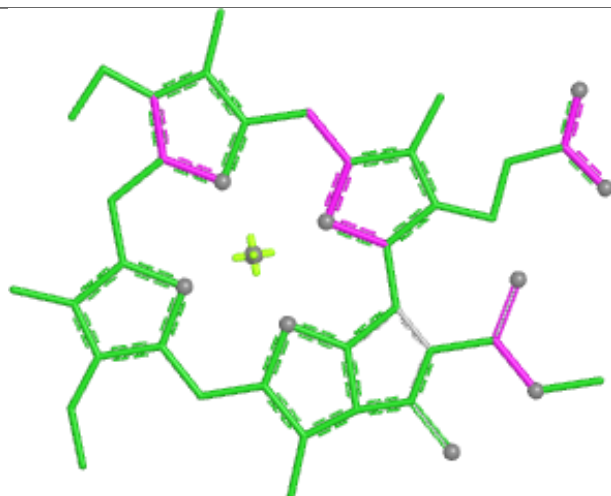




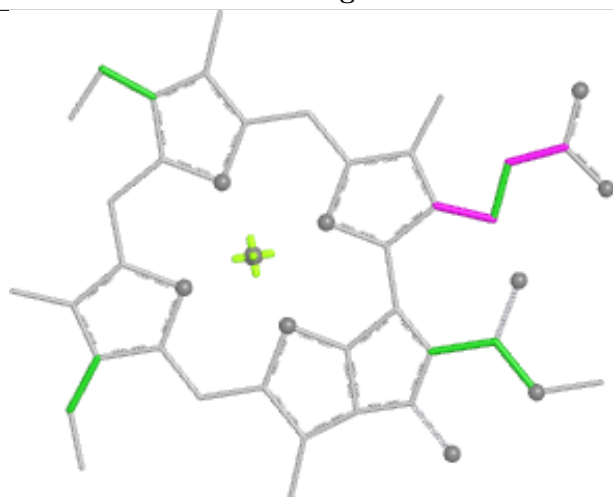
Ligand CLA h 504



Bond lengths



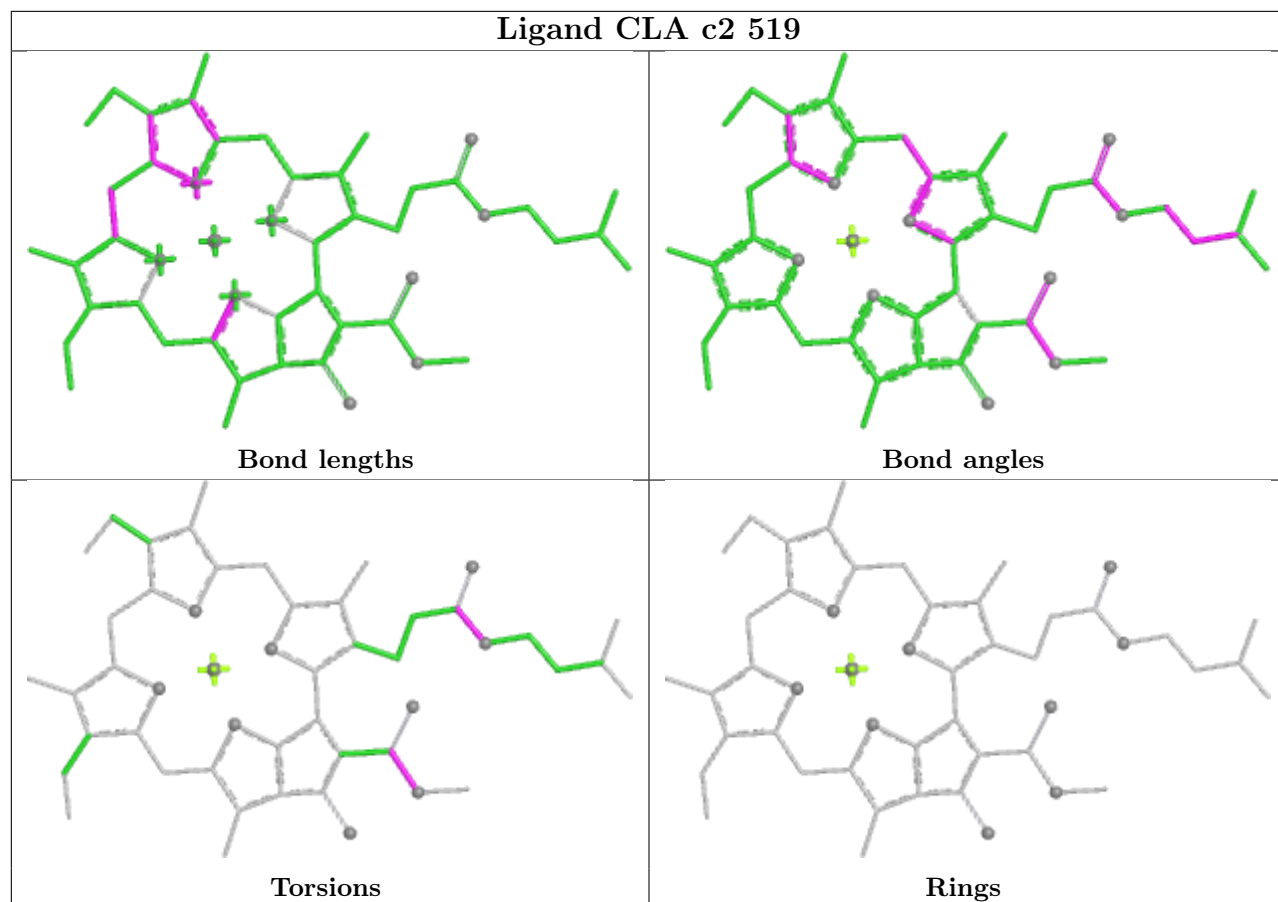
Bond angles

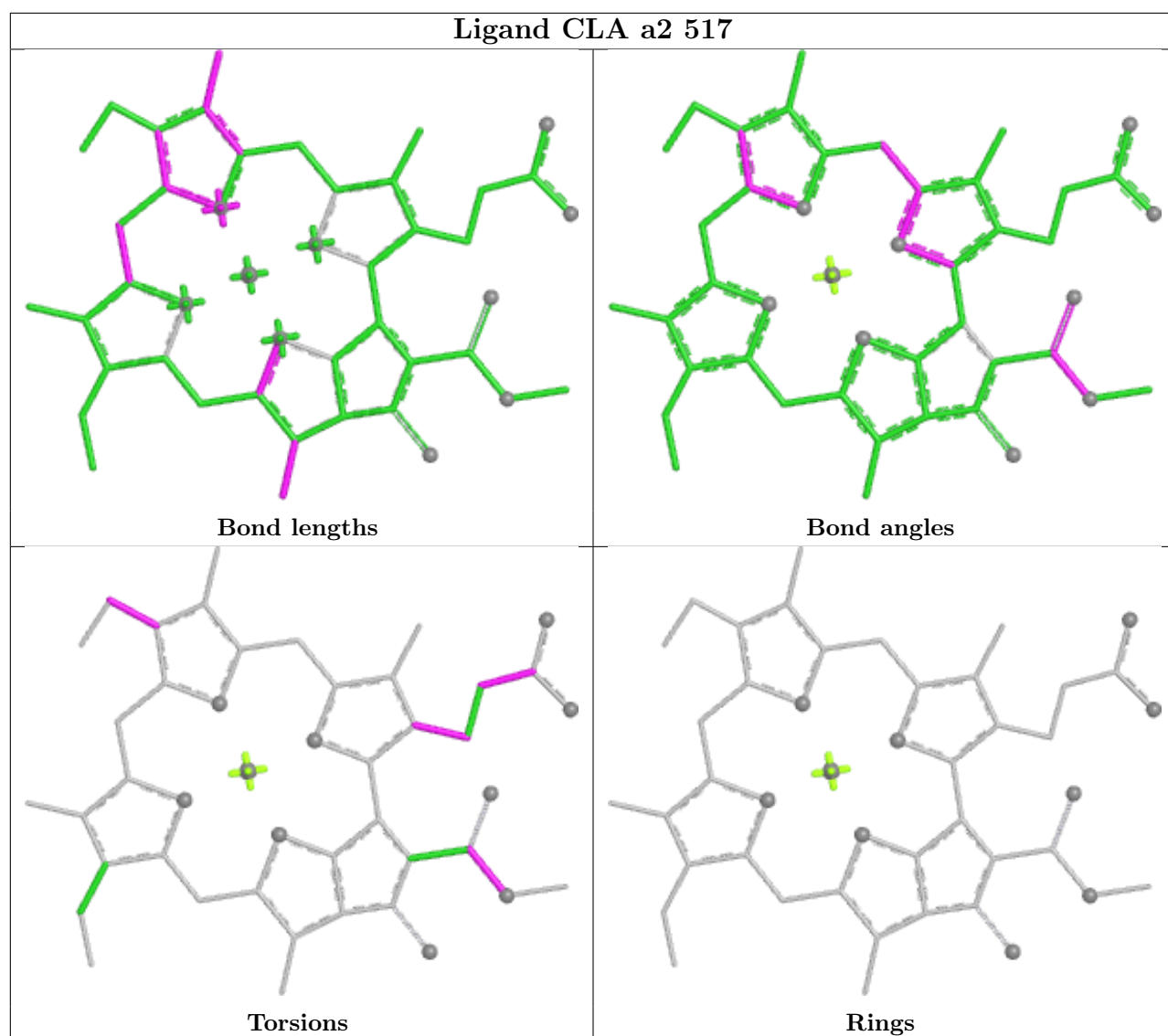


Torsions

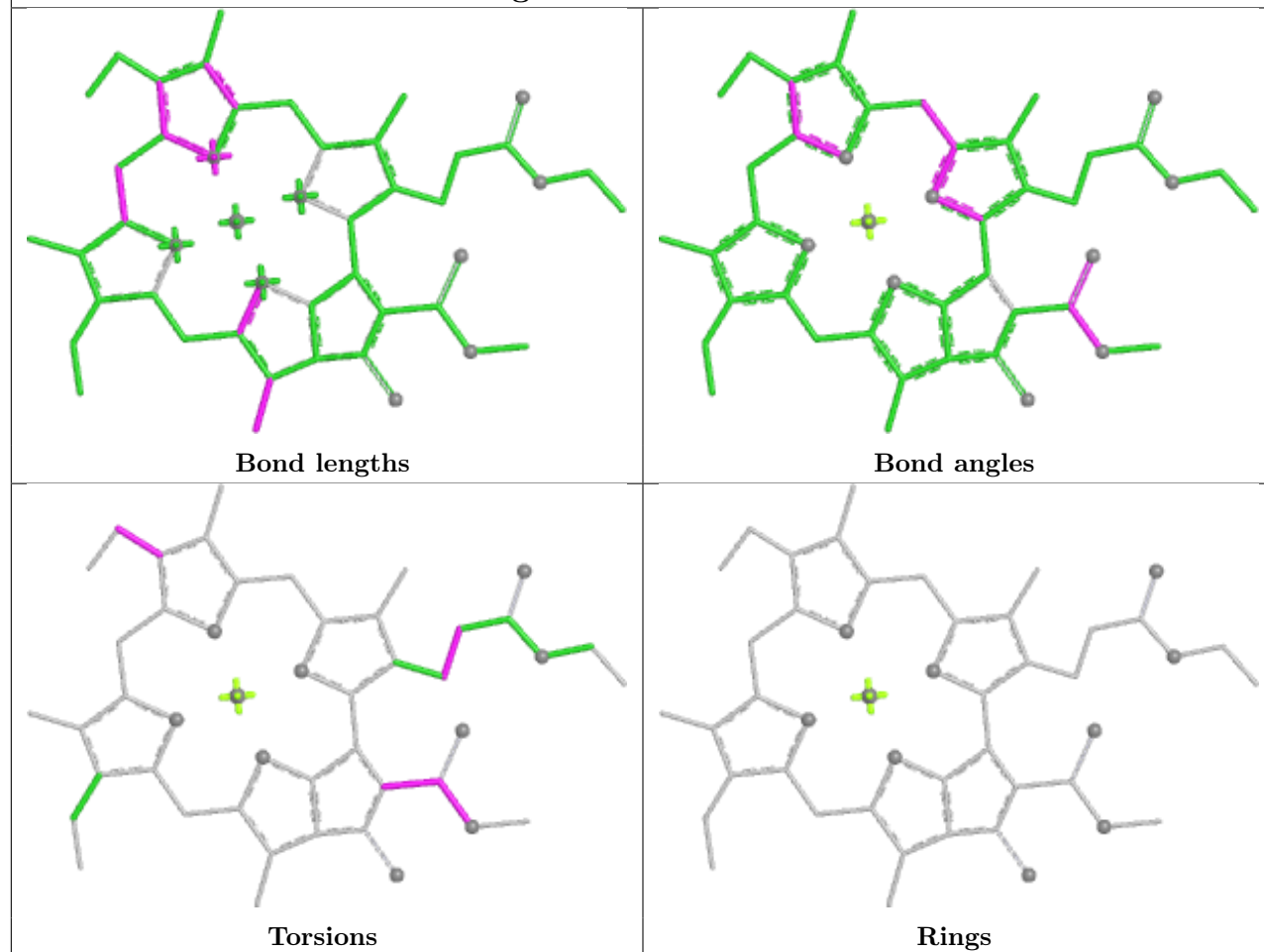


Rings

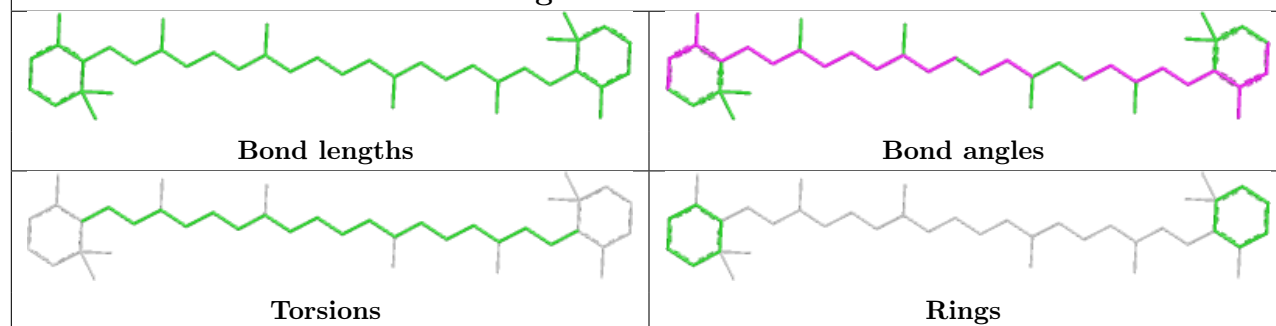




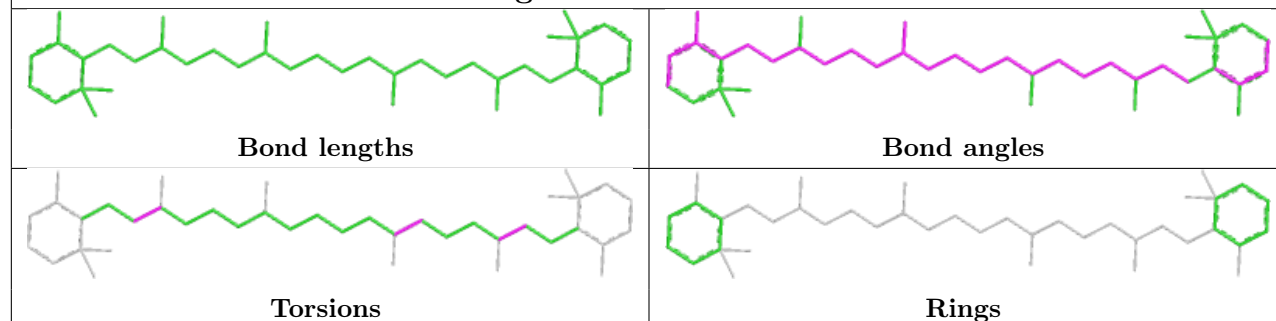
Ligand CLA bJ 1302

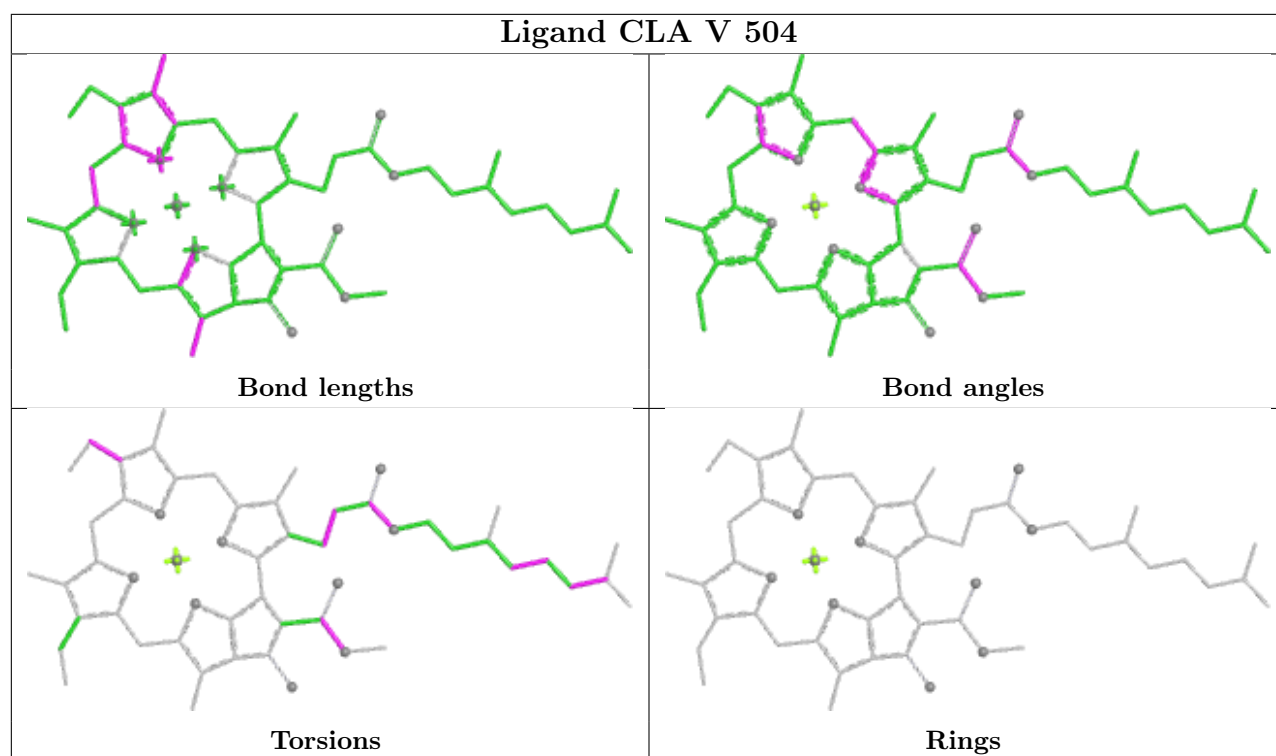


Ligand BCR c 524

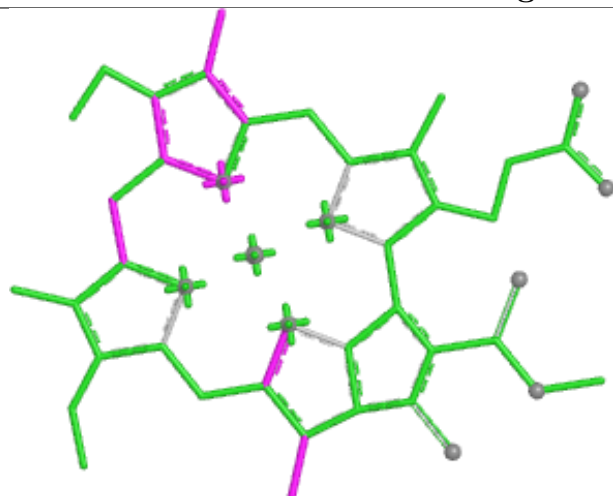


Ligand BCR cF 4014





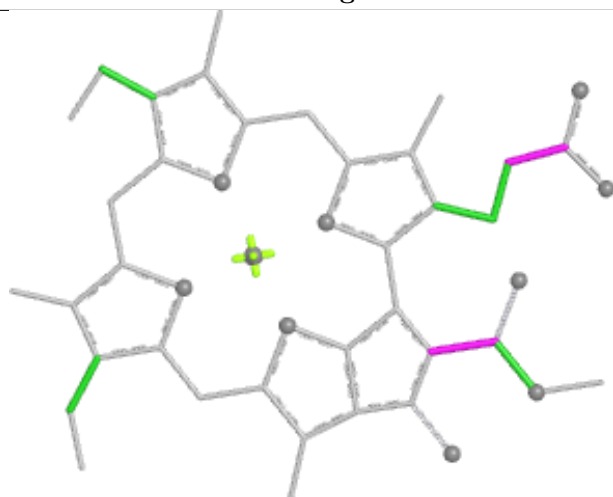
Ligand CLA d 512



Bond lengths



Bond angles

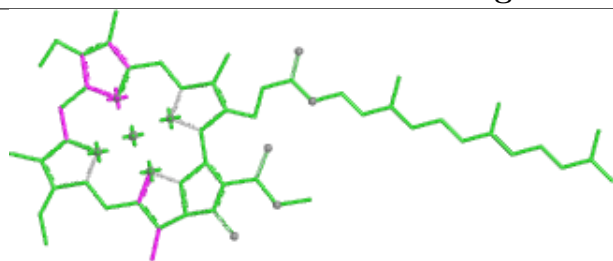


Torsions

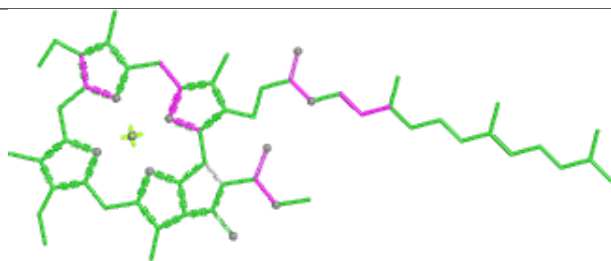


Rings

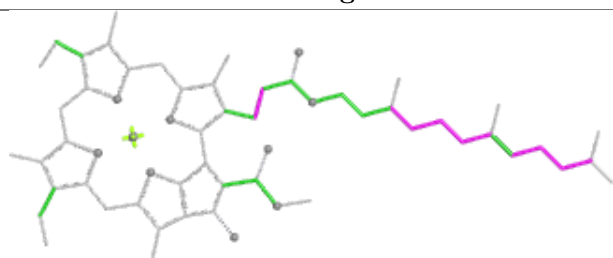
Ligand CLA bA 1115



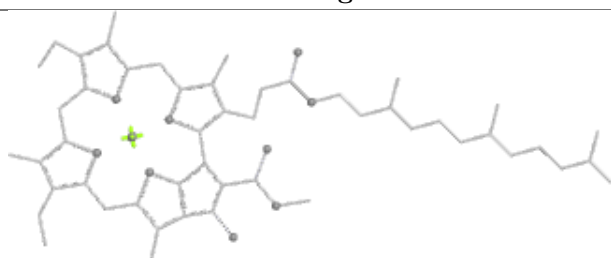
Bond lengths



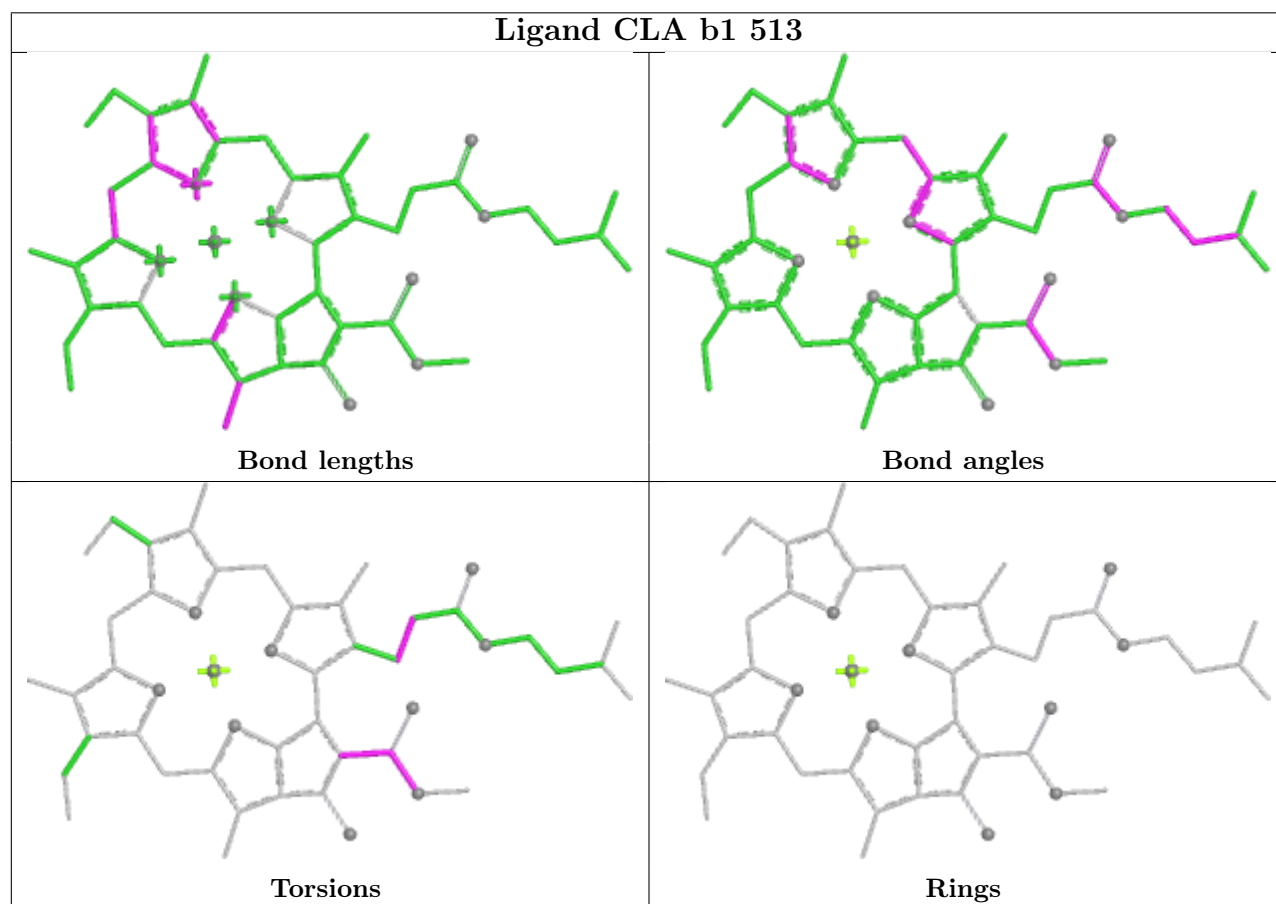
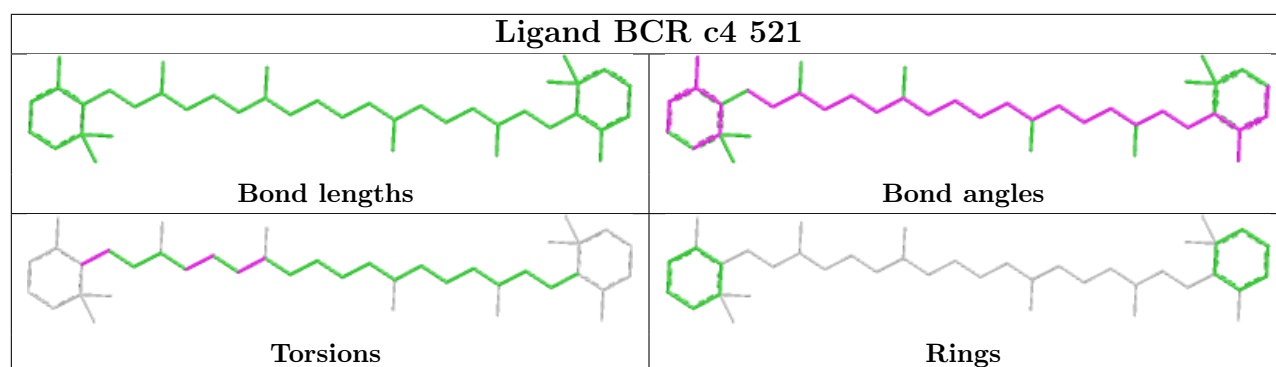
Bond angles



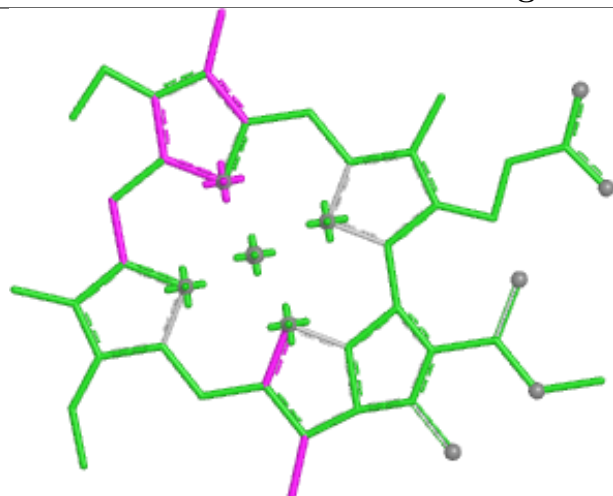
Torsions



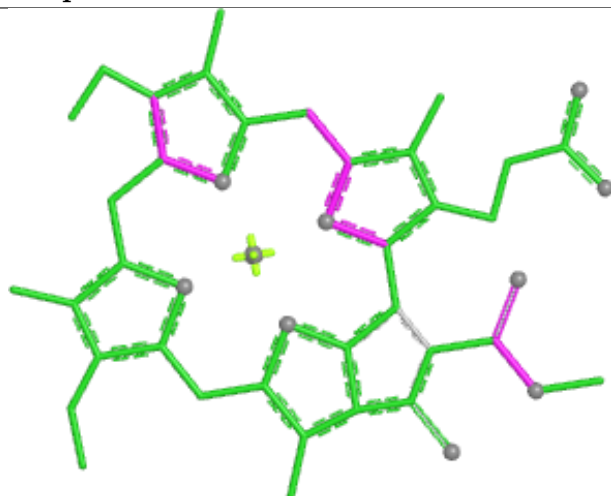
Rings



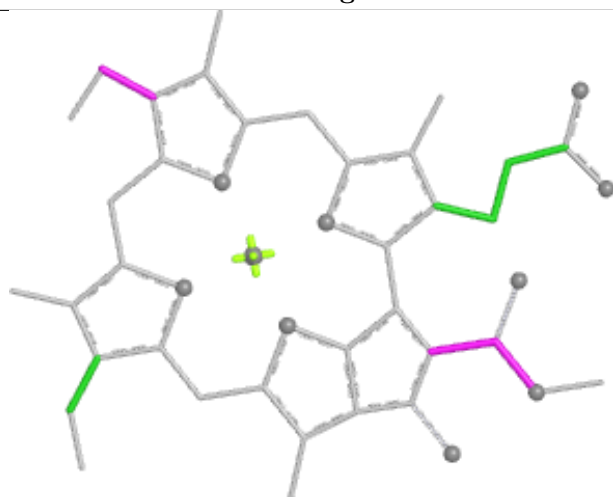
Ligand CLA q 502



Bond lengths



Bond angles

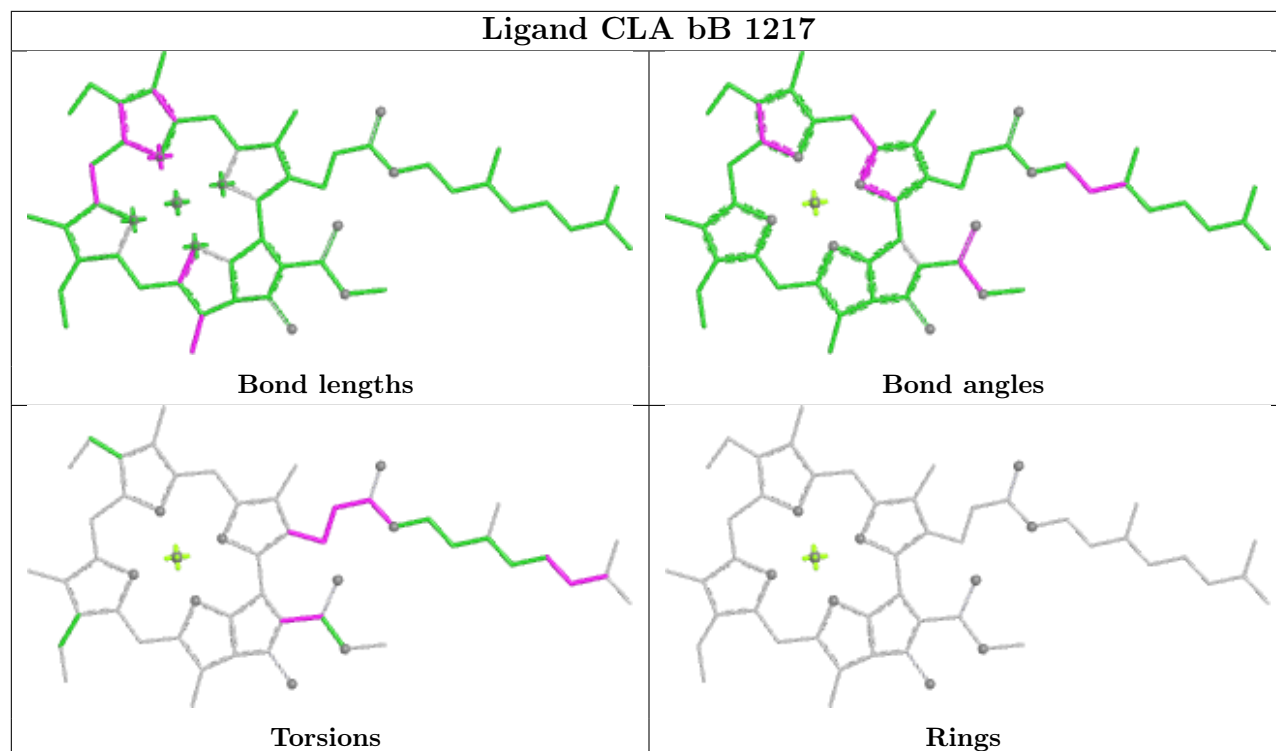


Torsions

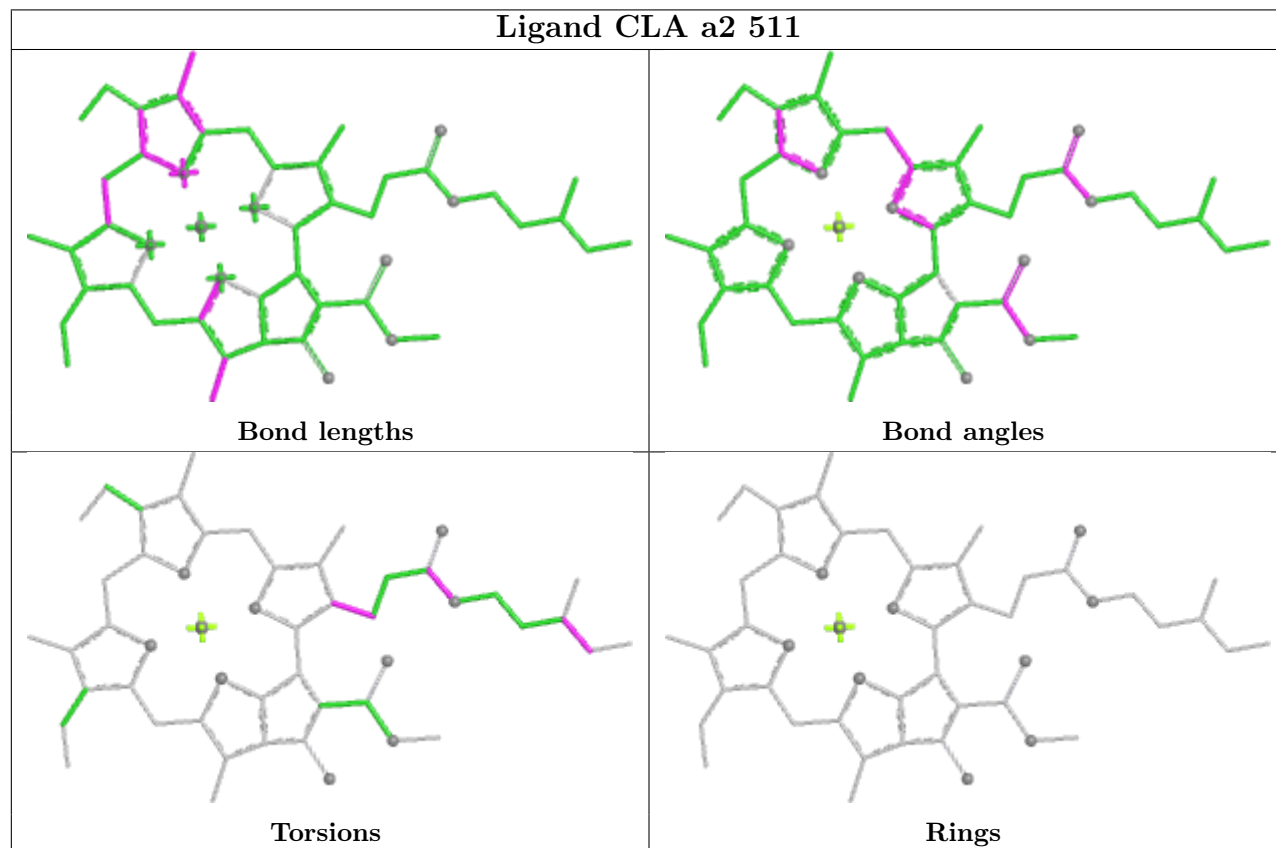


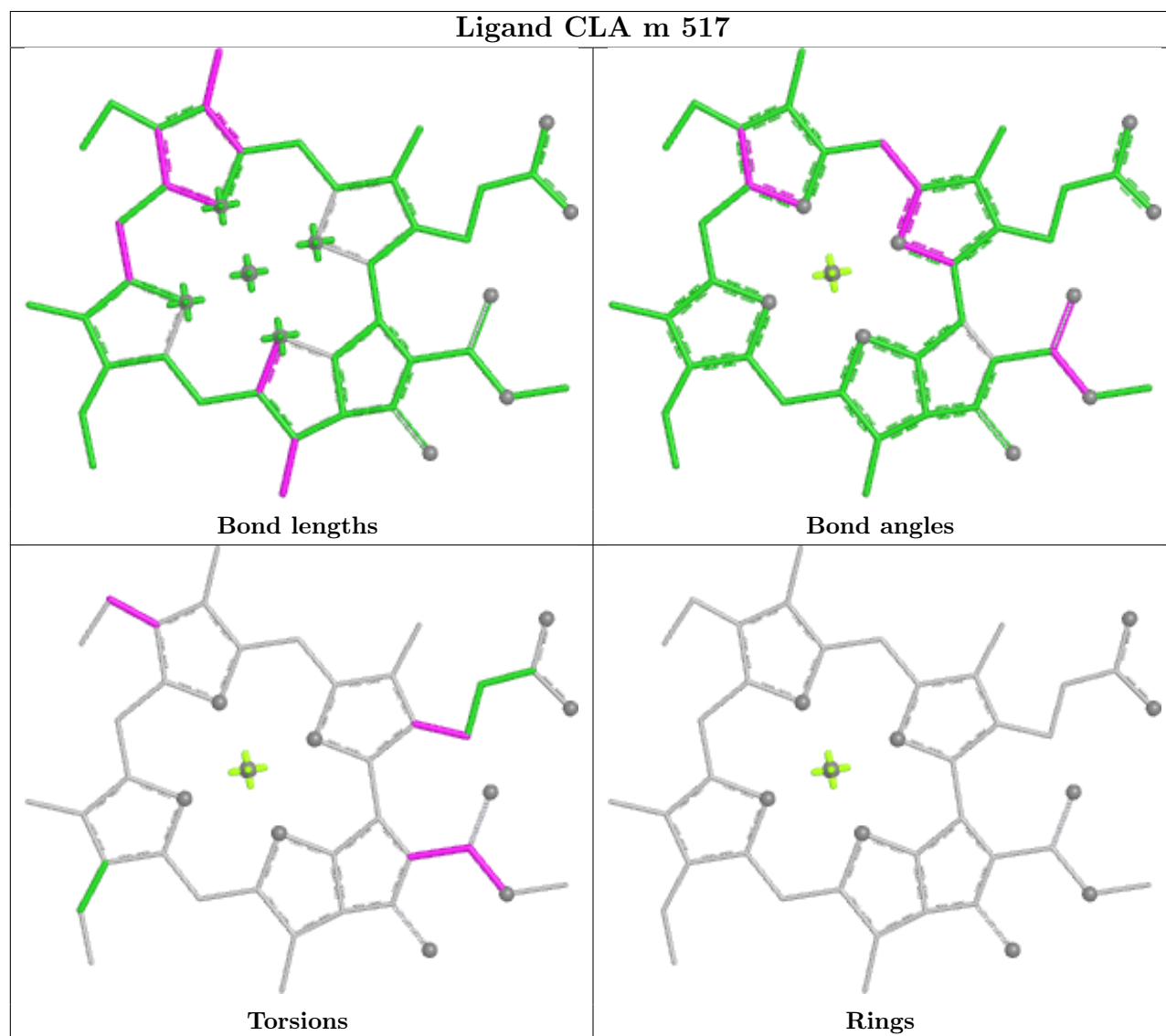
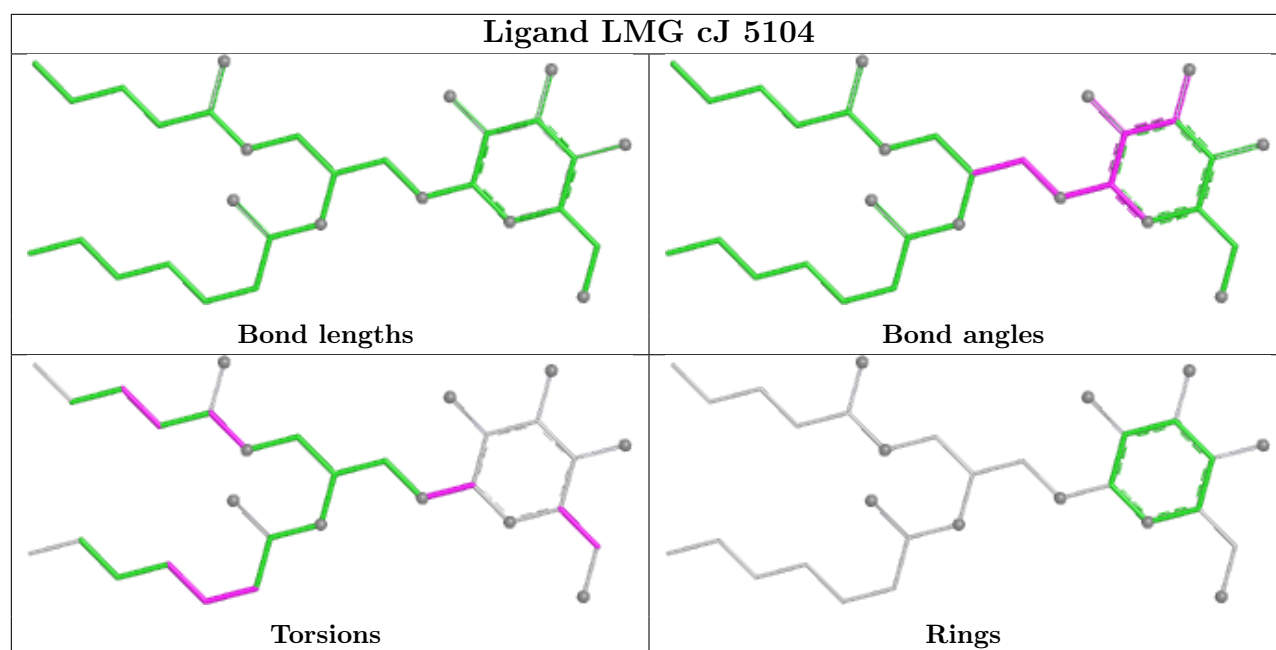
Rings

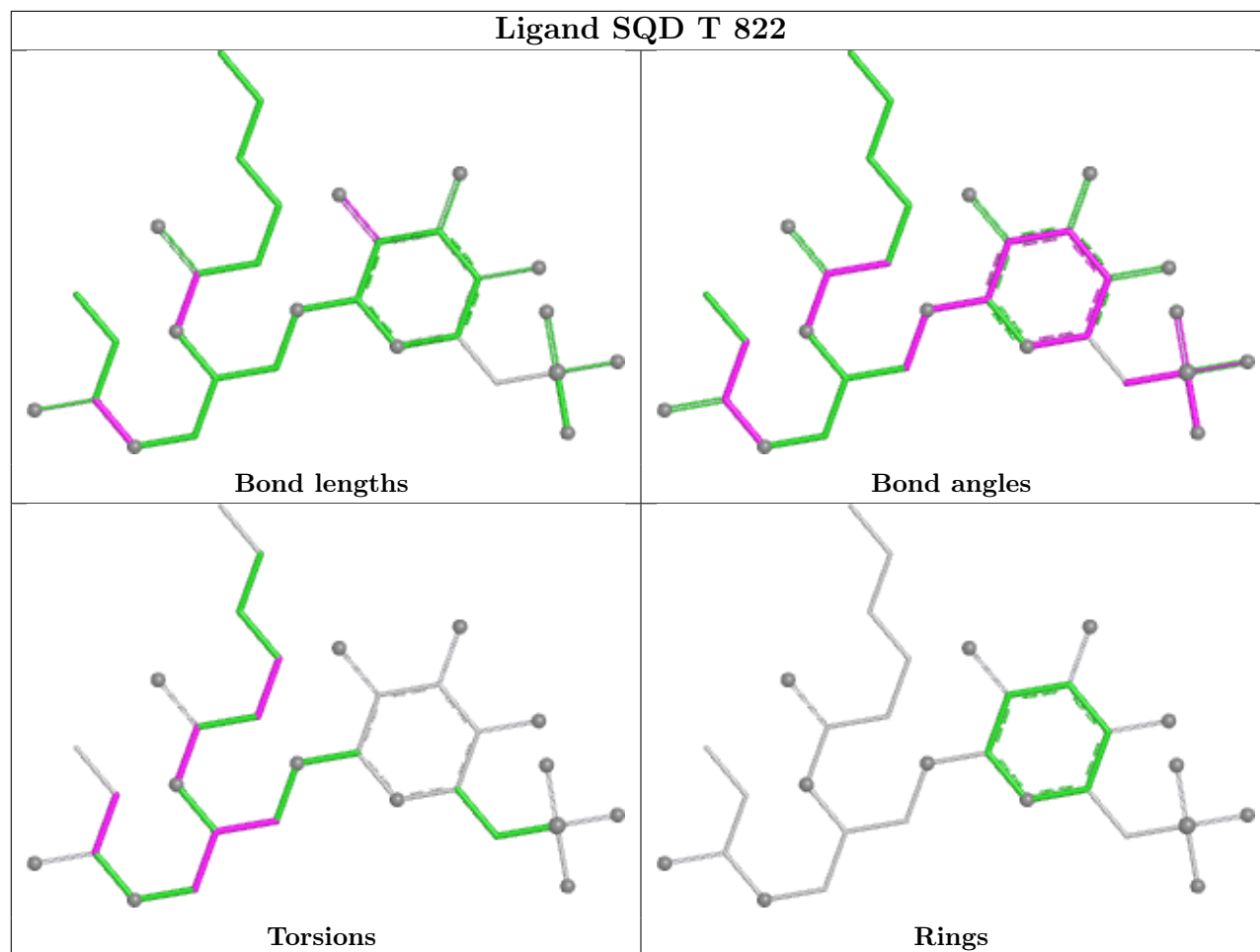
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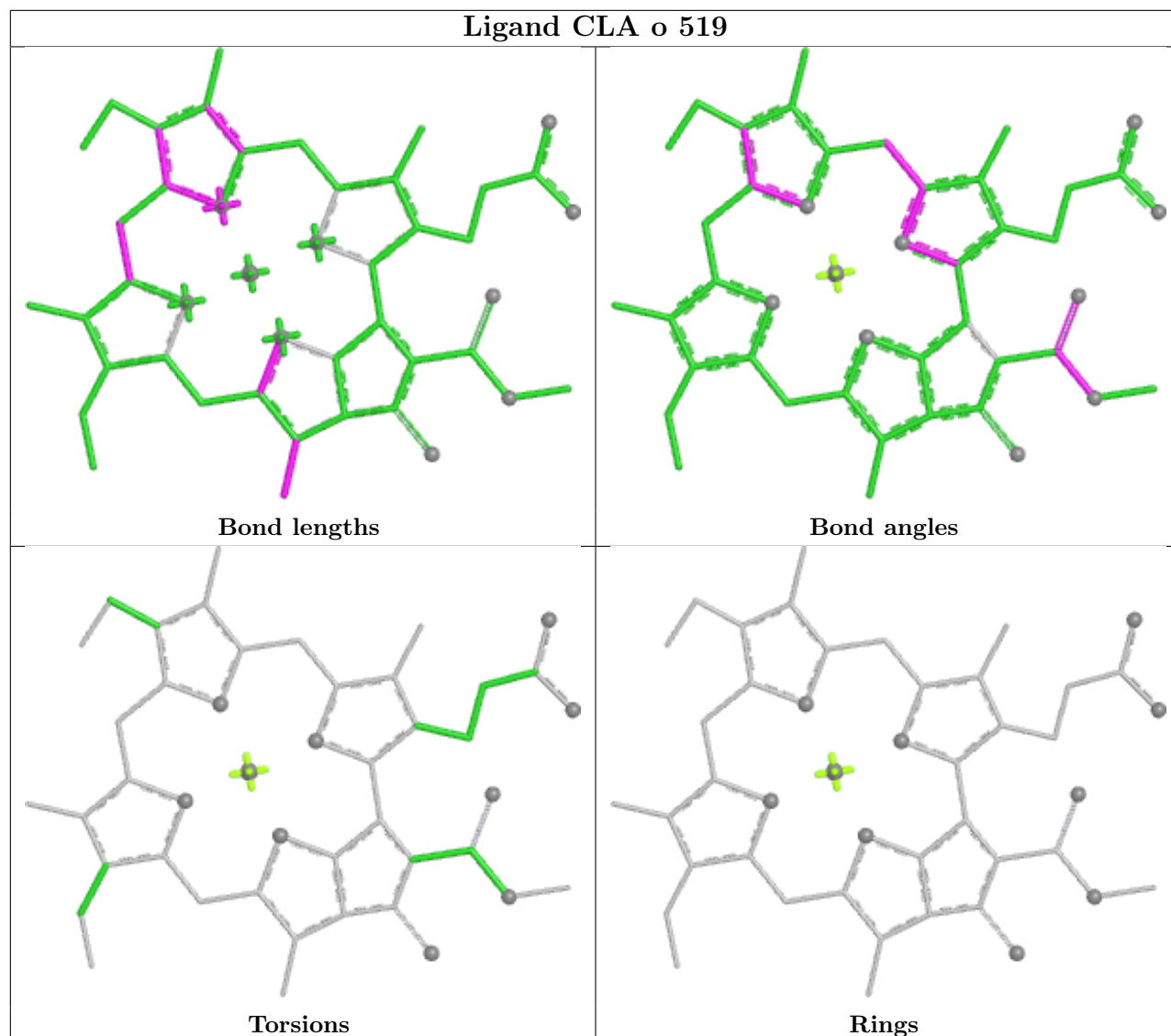
Ligand CLA a2 511



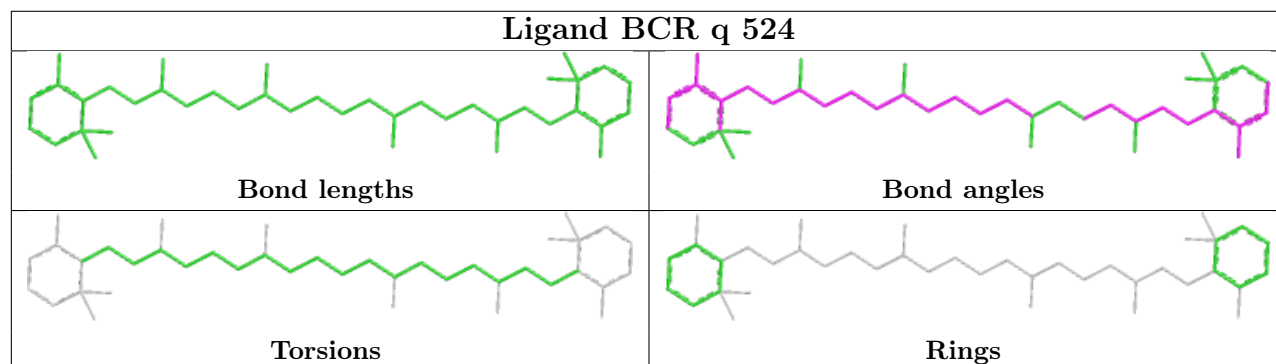


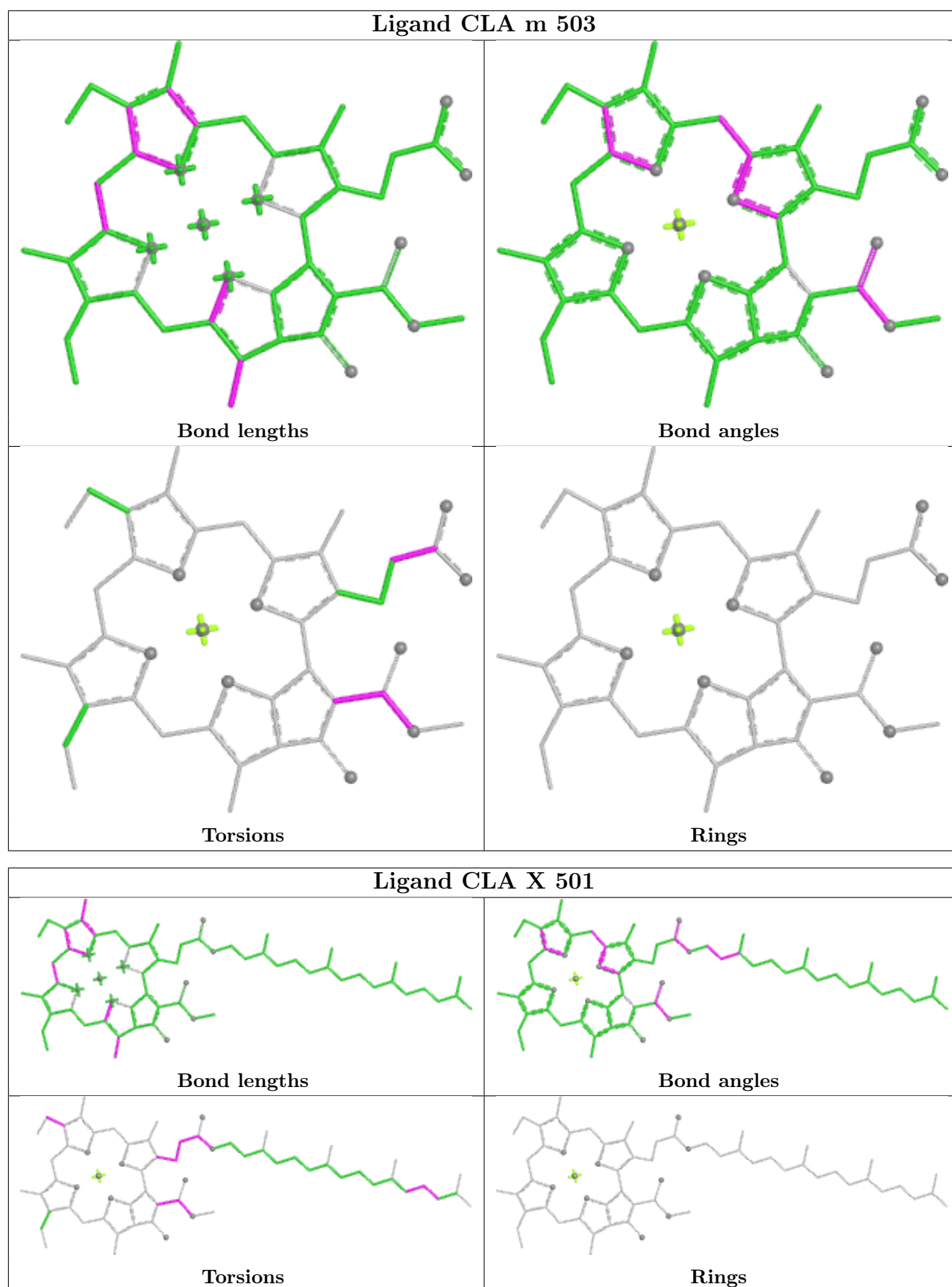


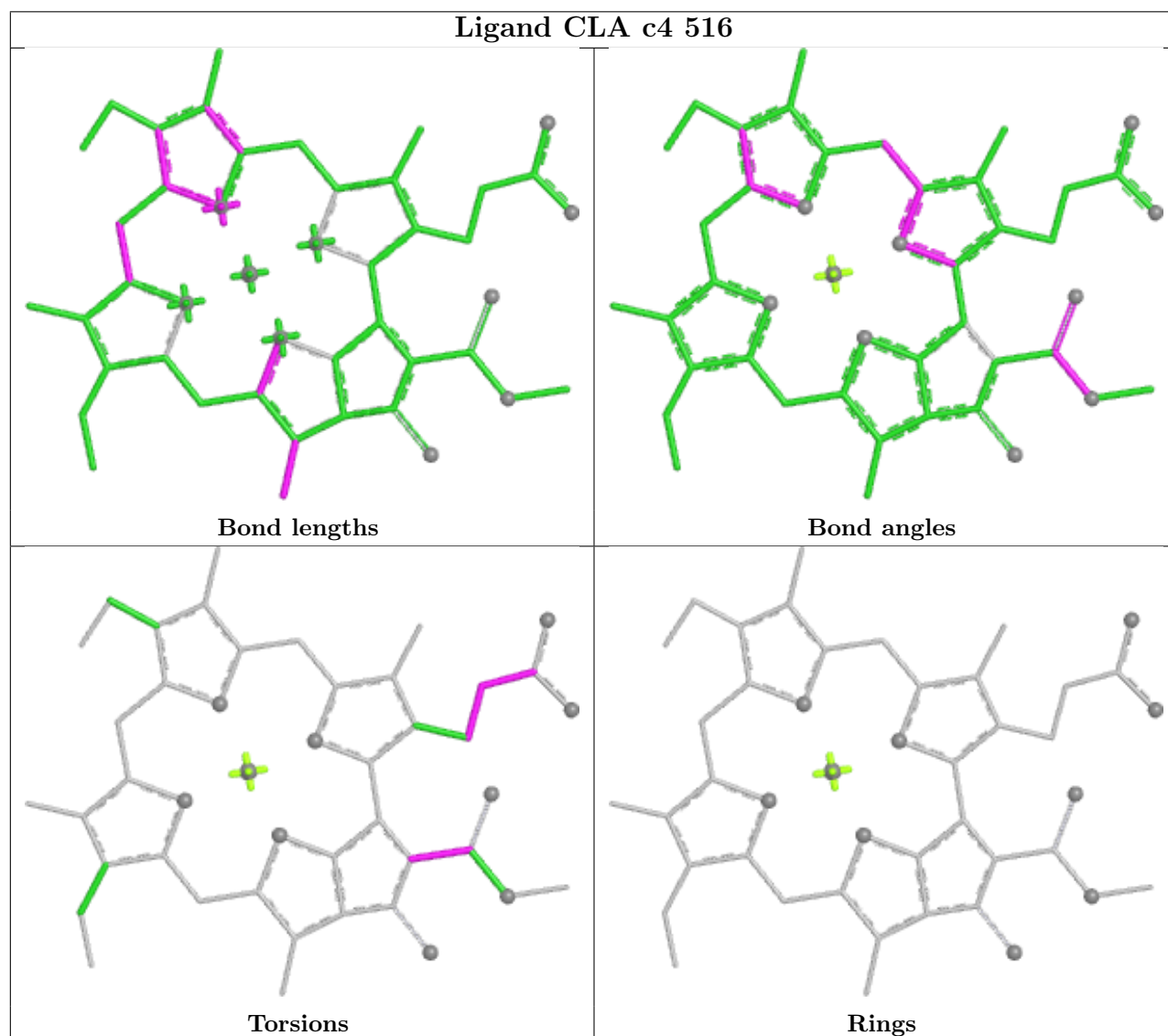
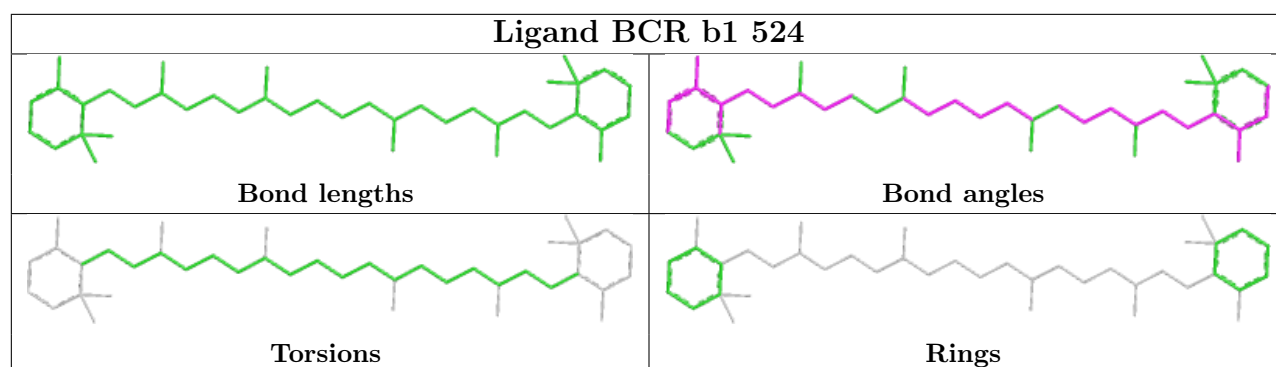
Ligand CLA o 519



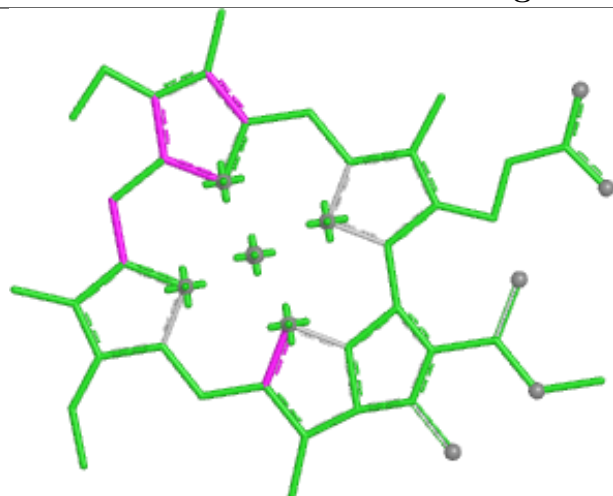
Ligand BCR q 524



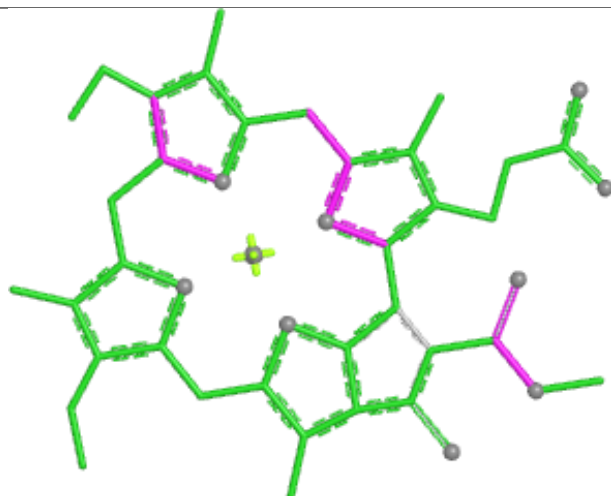




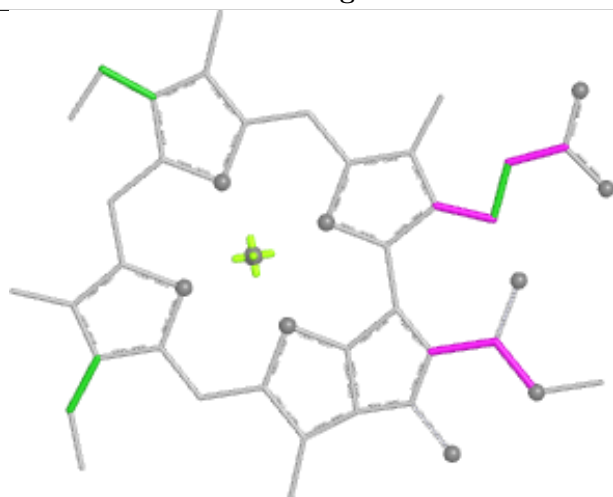
Ligand CLA Y 516



Bond lengths



Bond angles

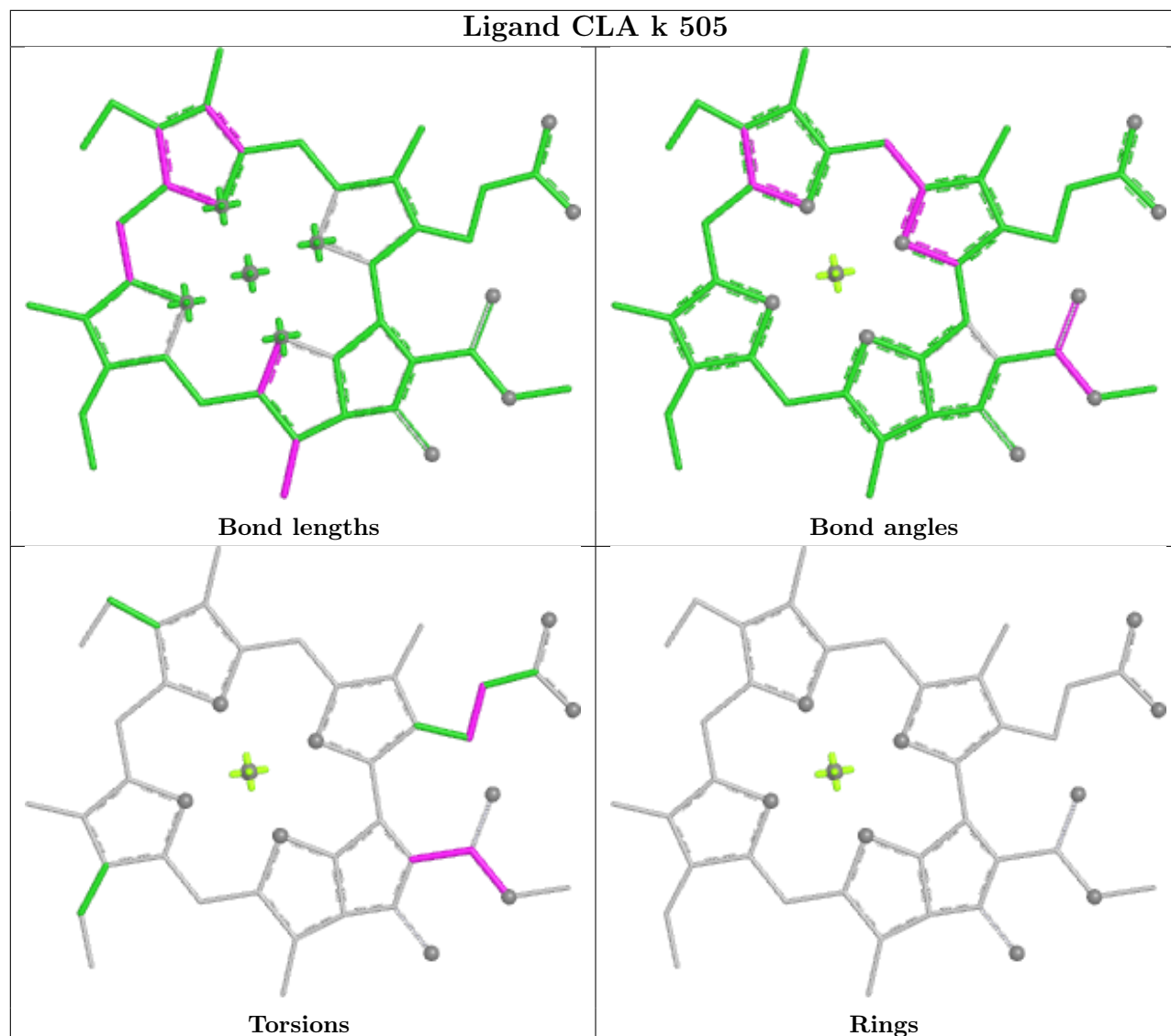


Torsions

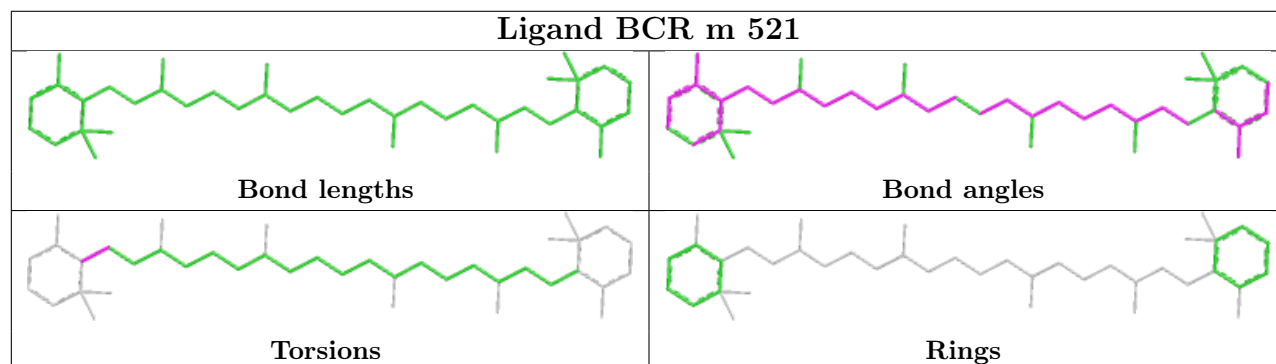


Rings

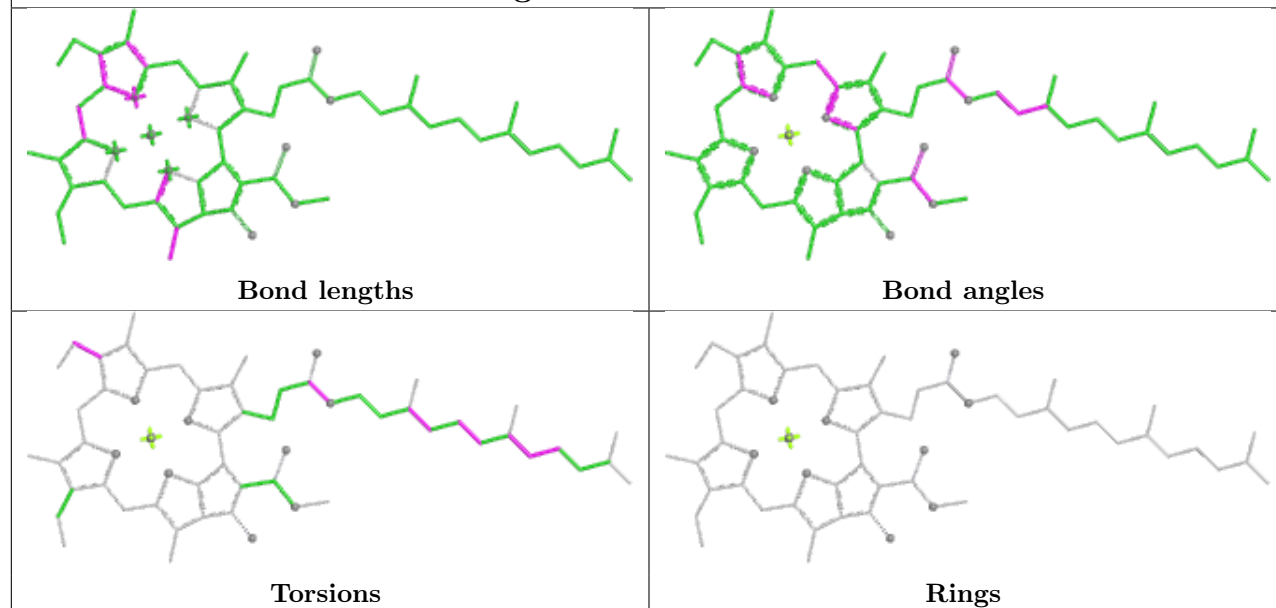
Ligand CLA k 505



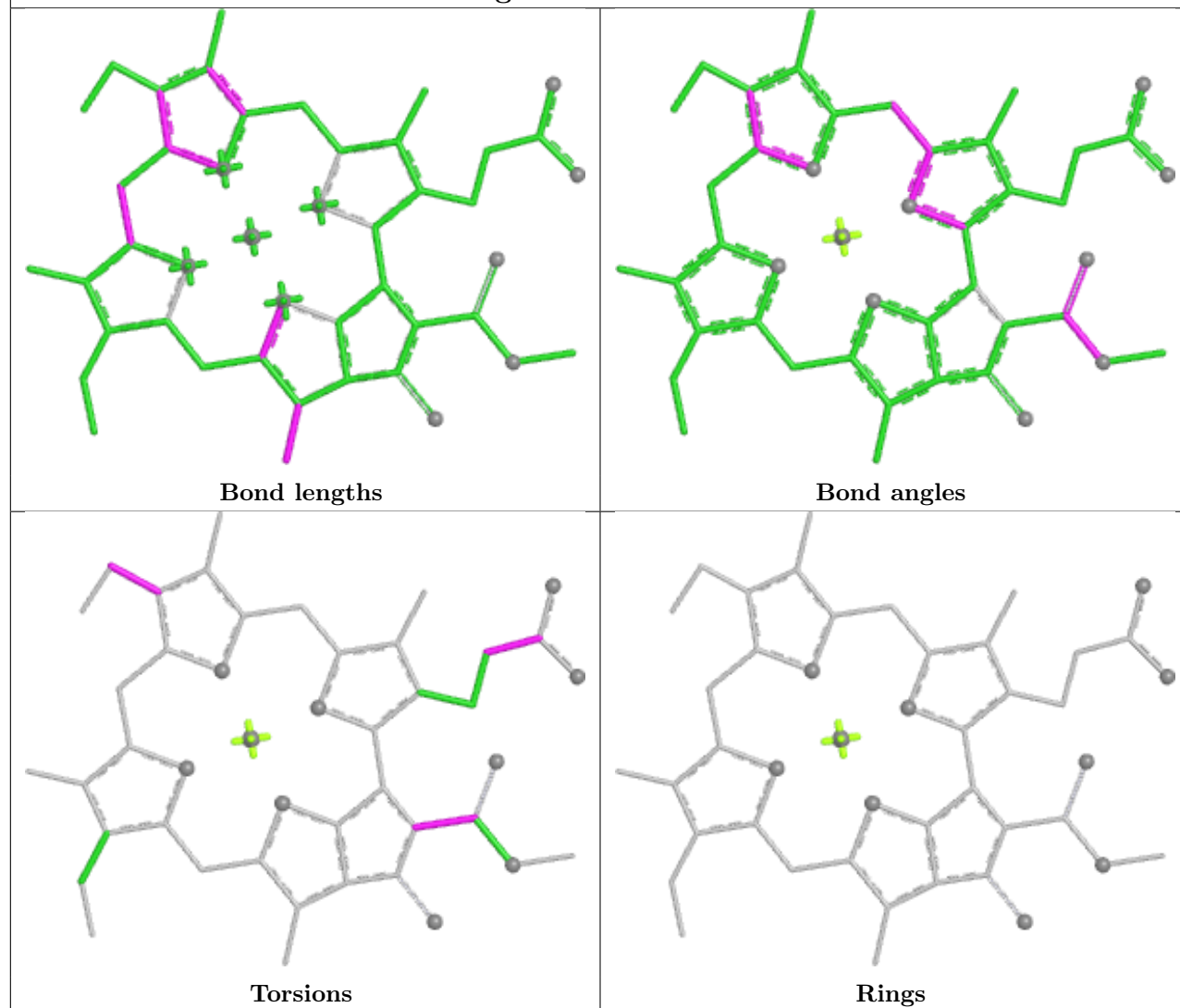
Ligand BCR m 521



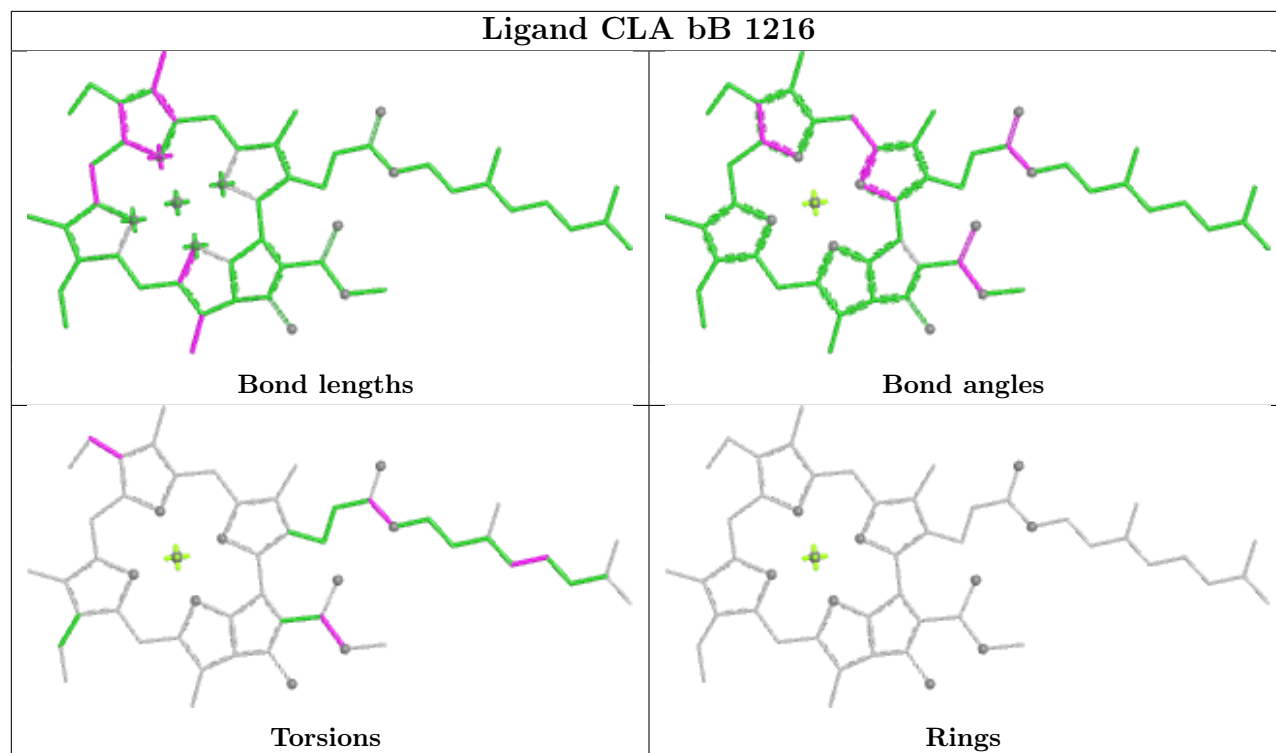
Ligand CLA aA 1122



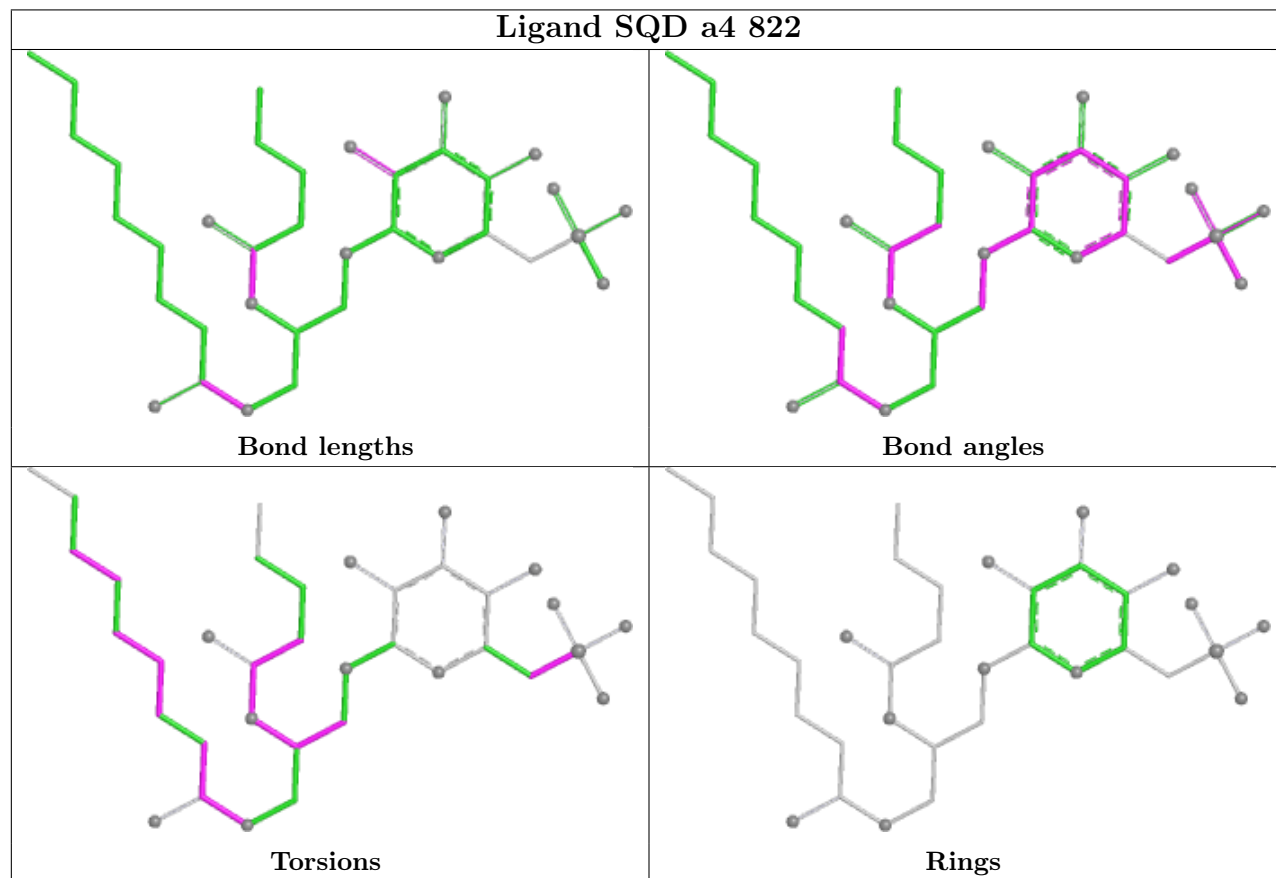
Ligand CLA k 504



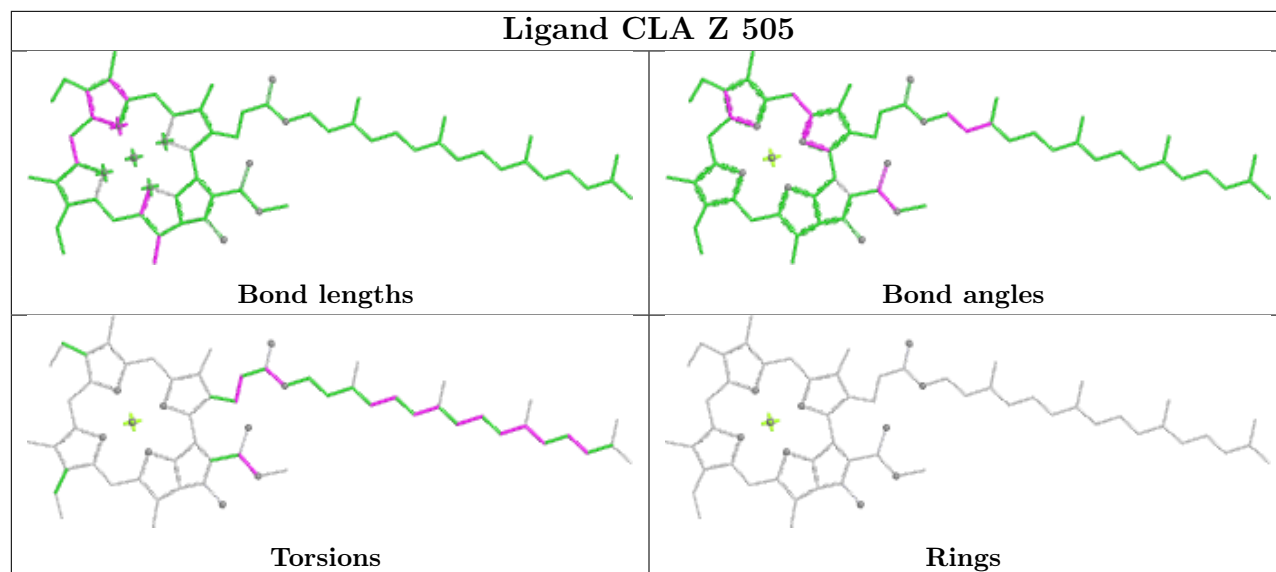
Ligand CLA bB 1216



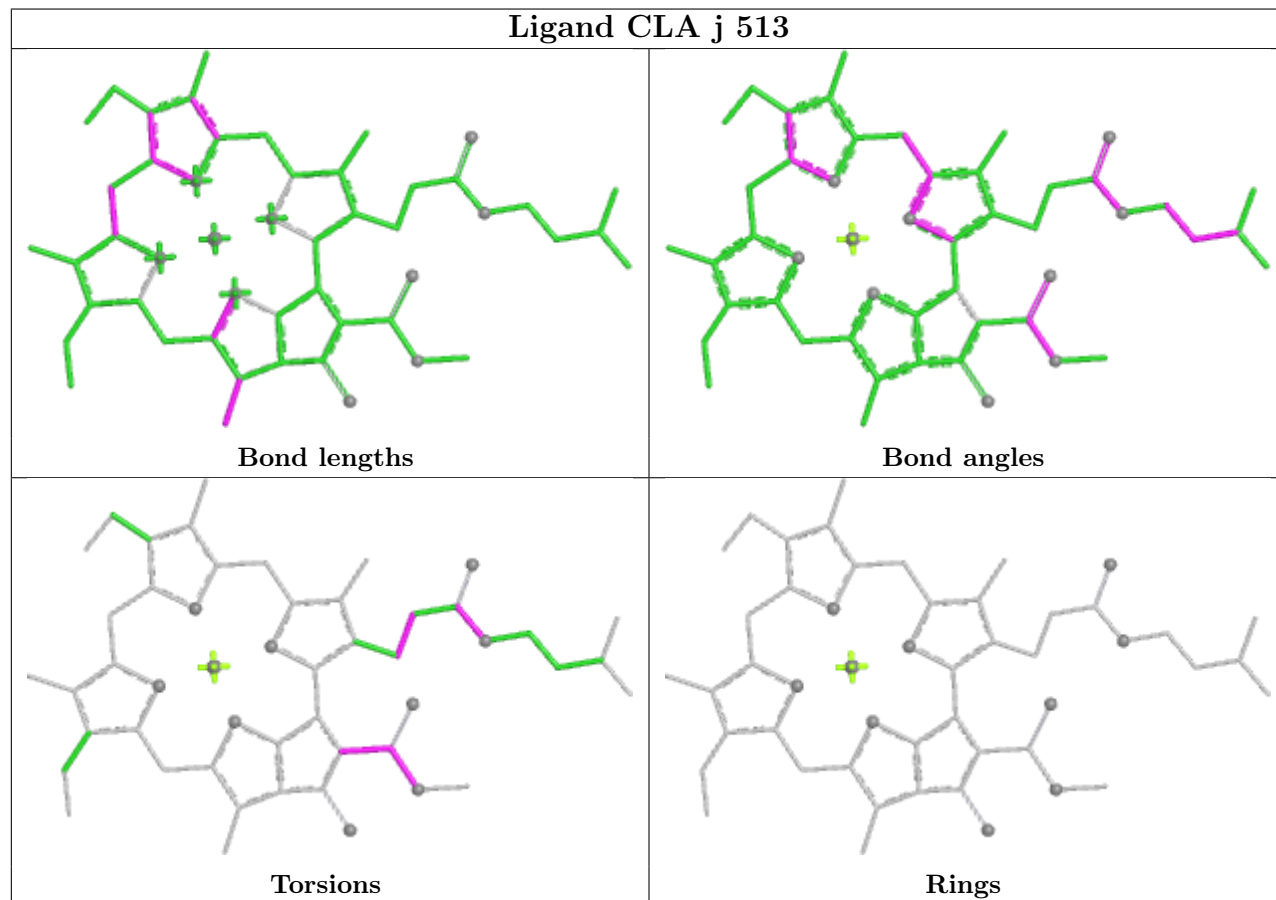
Ligand SQD a4 822

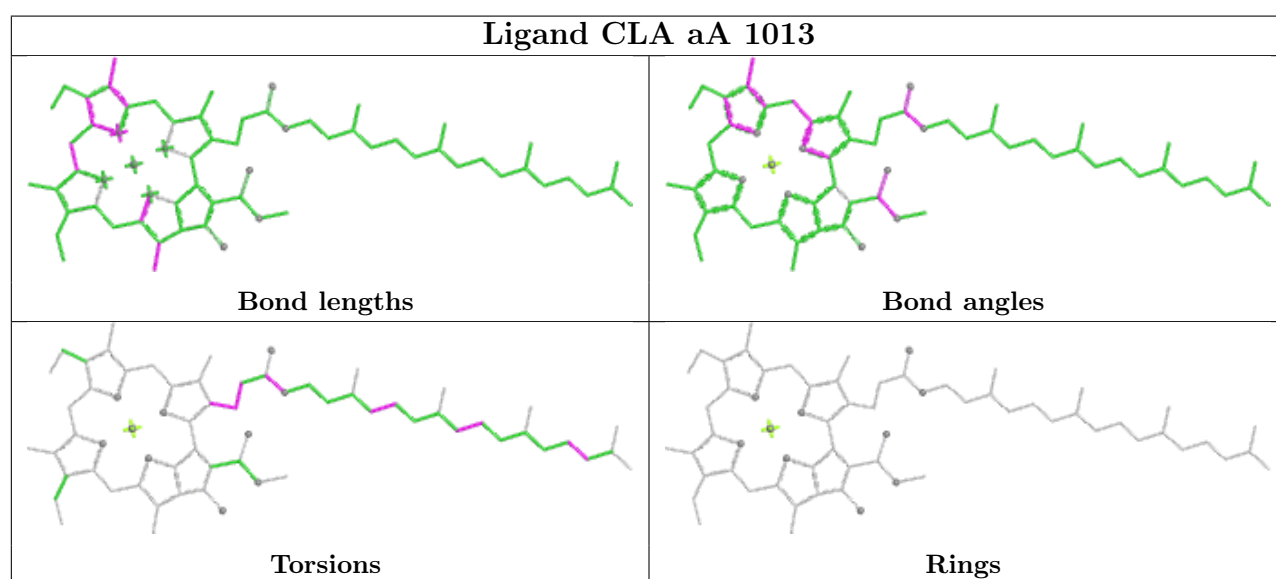
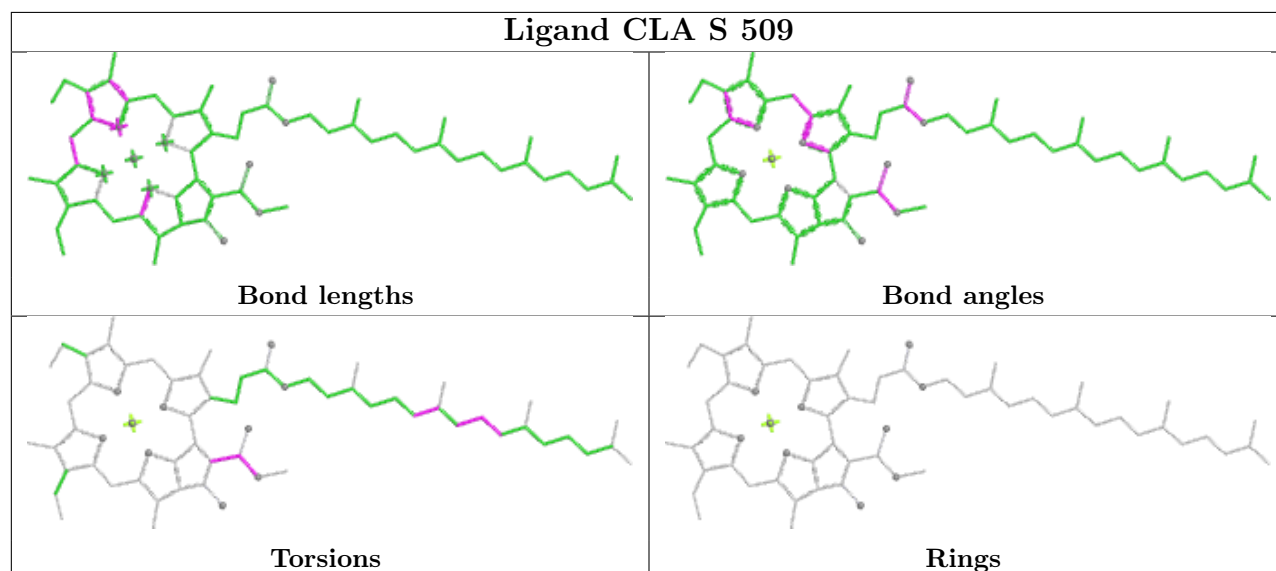
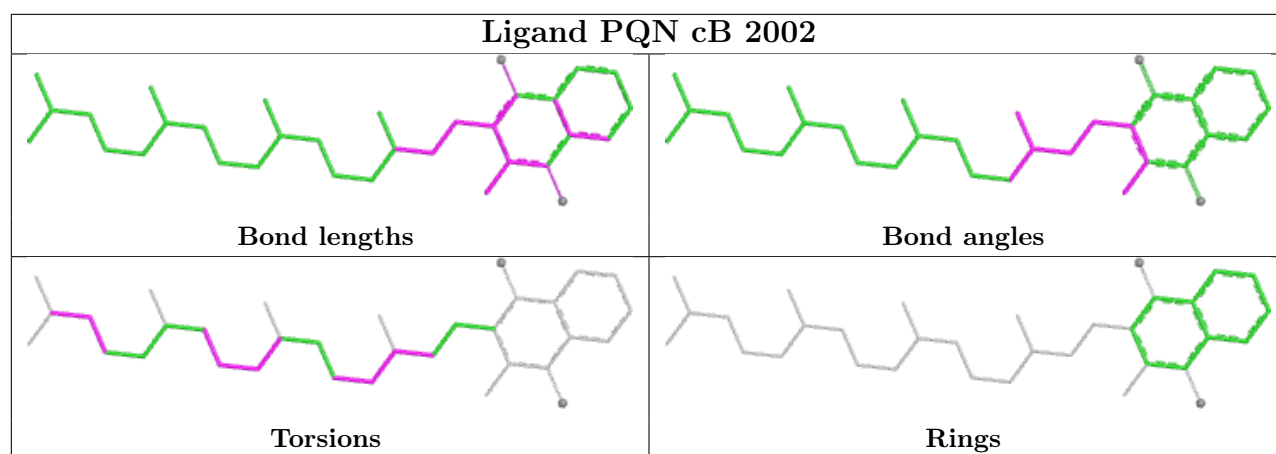


Ligand CLA Z 505

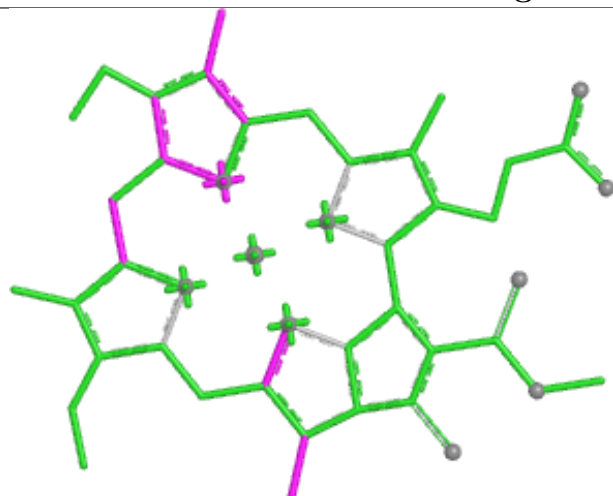


Ligand CLA j 513





Ligand CLA T 504



Bond lengths



Bond angles

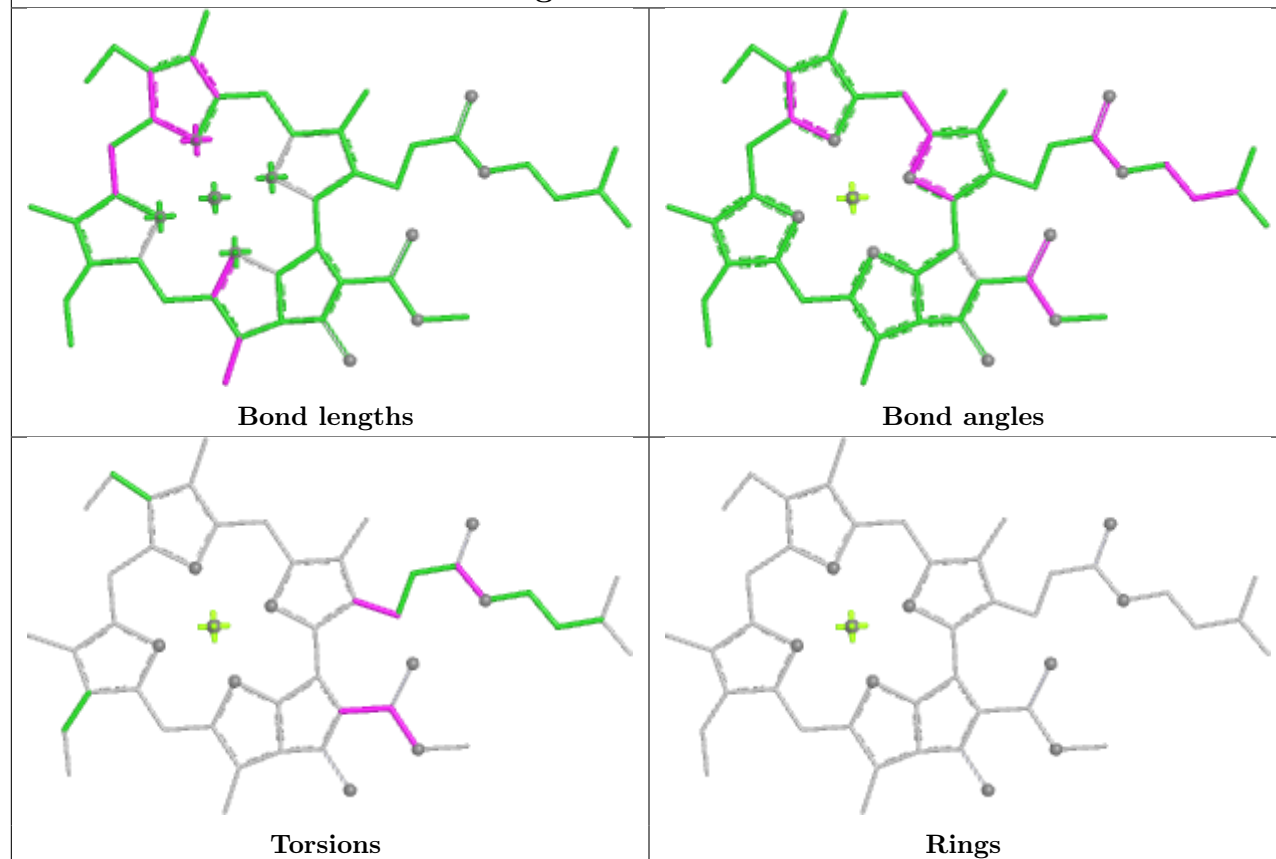


Torsions

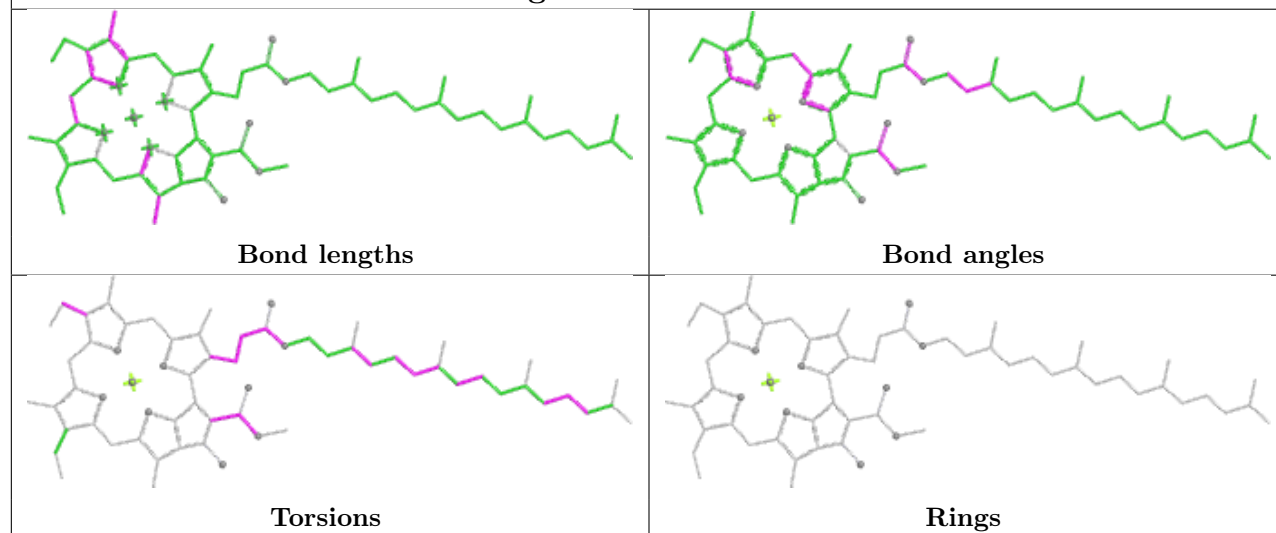


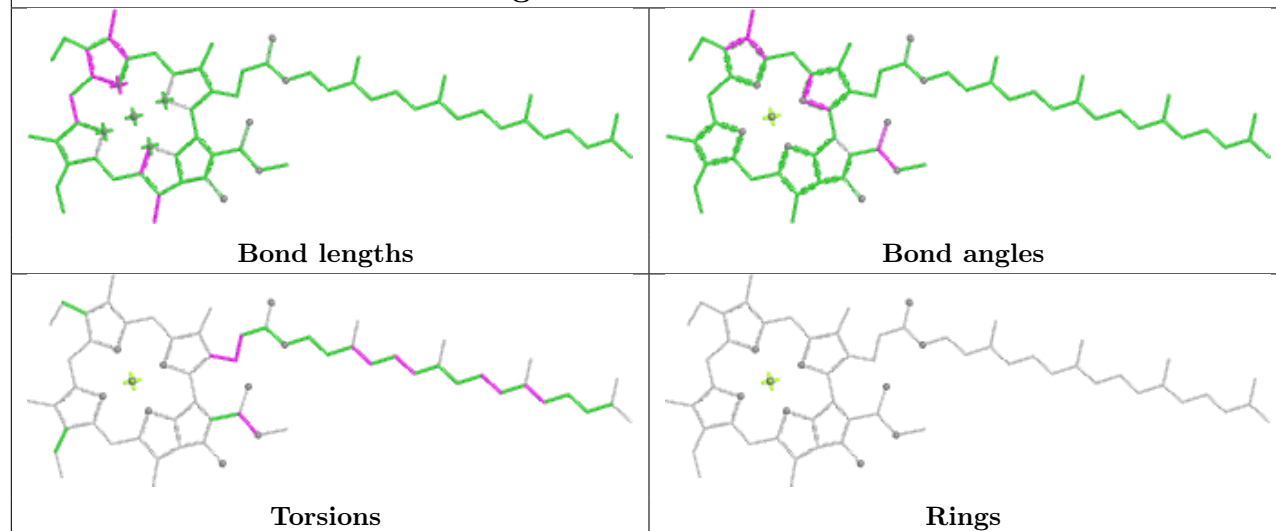
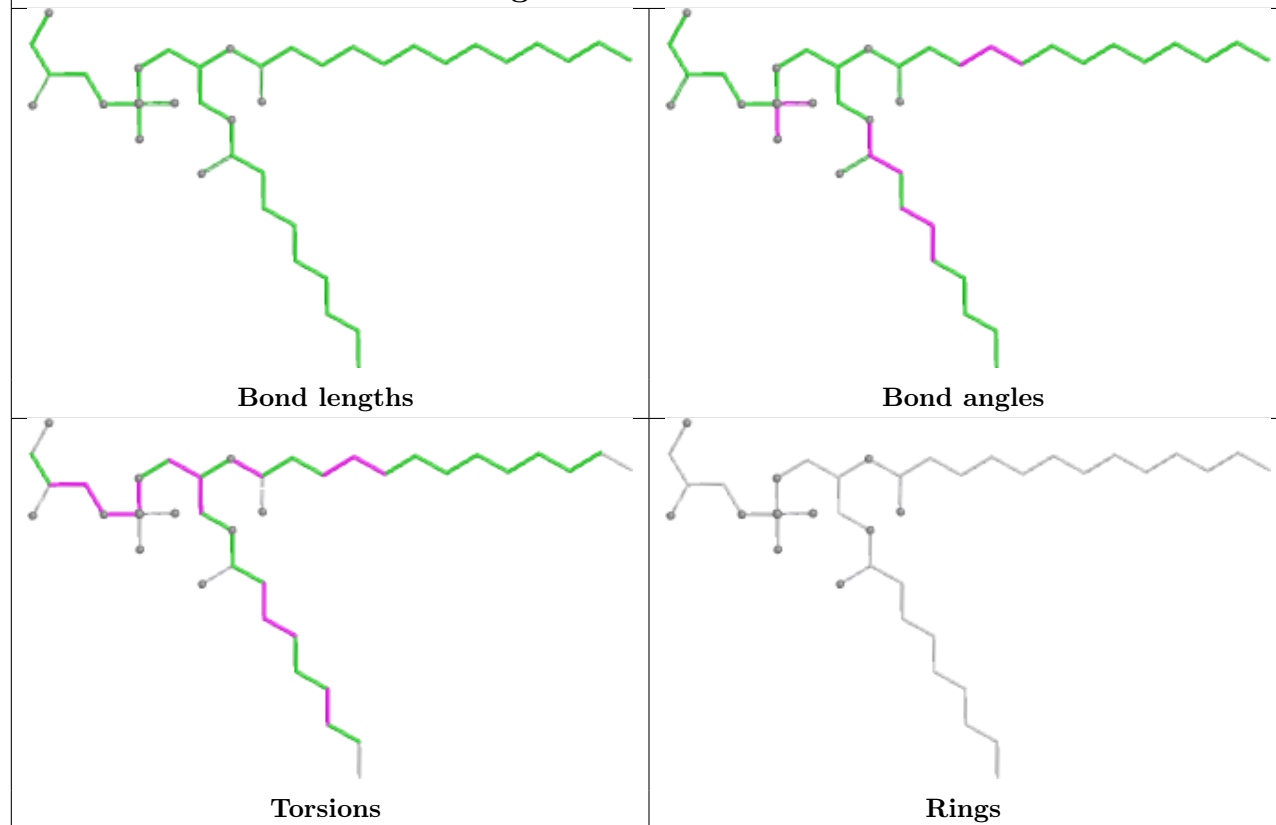
Rings

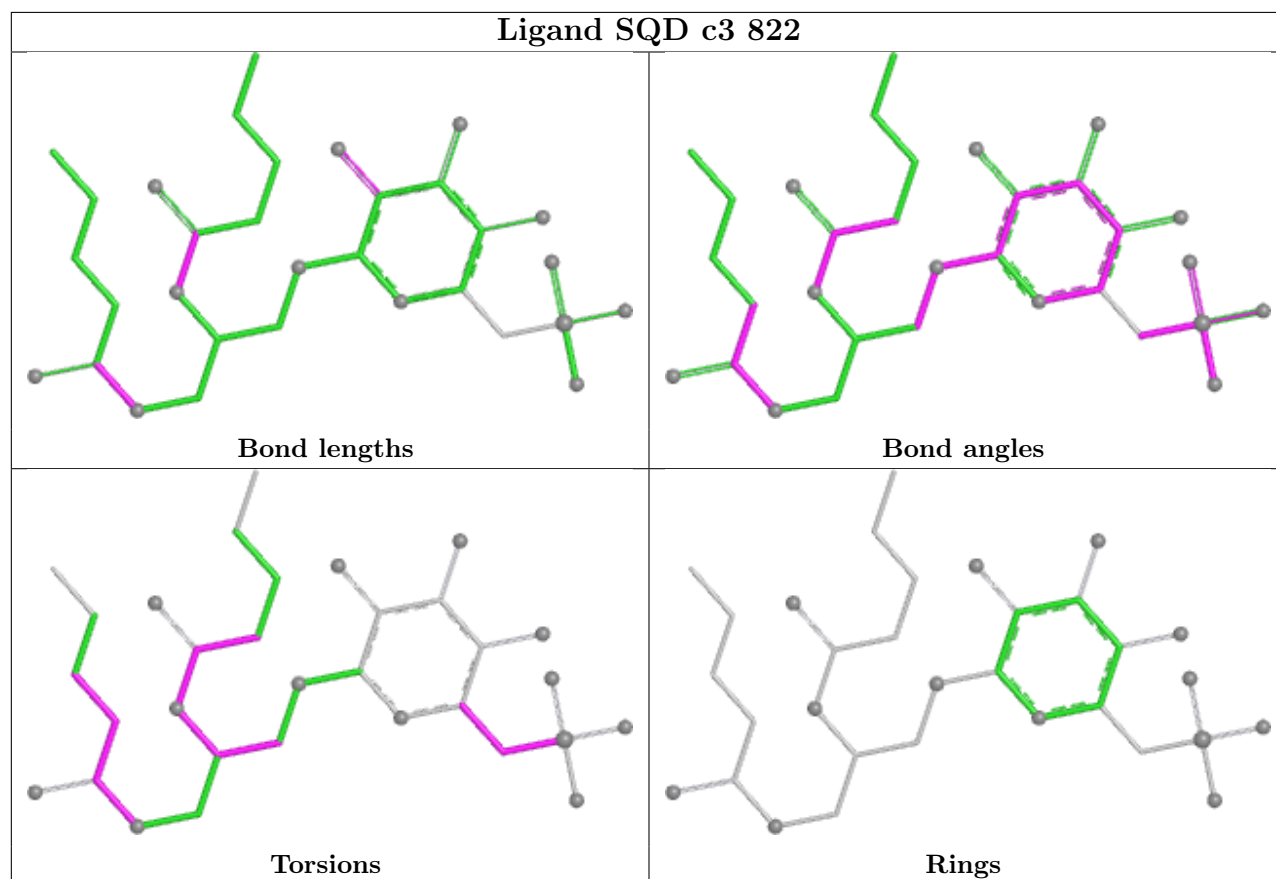
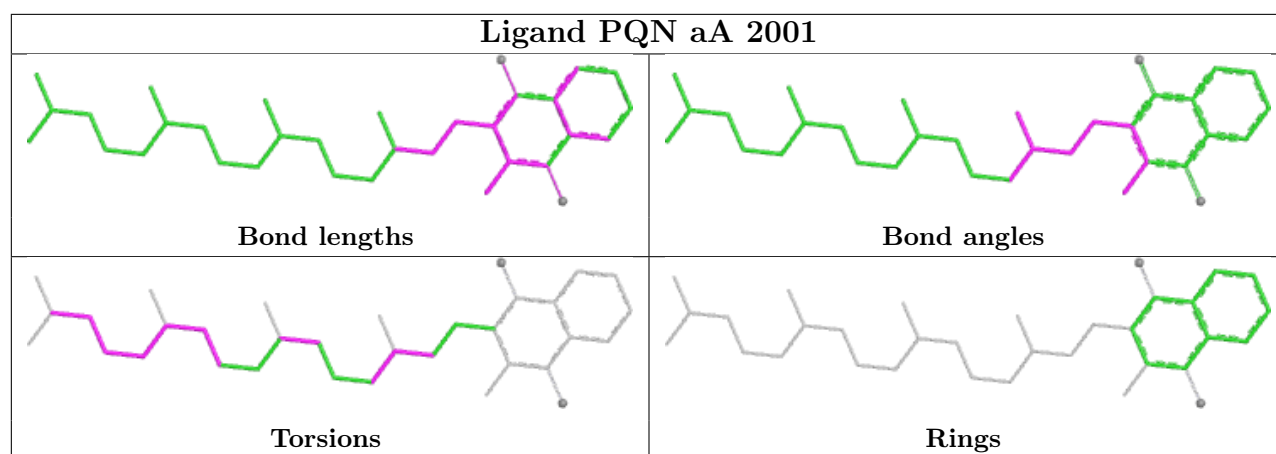
Ligand CLA S 511

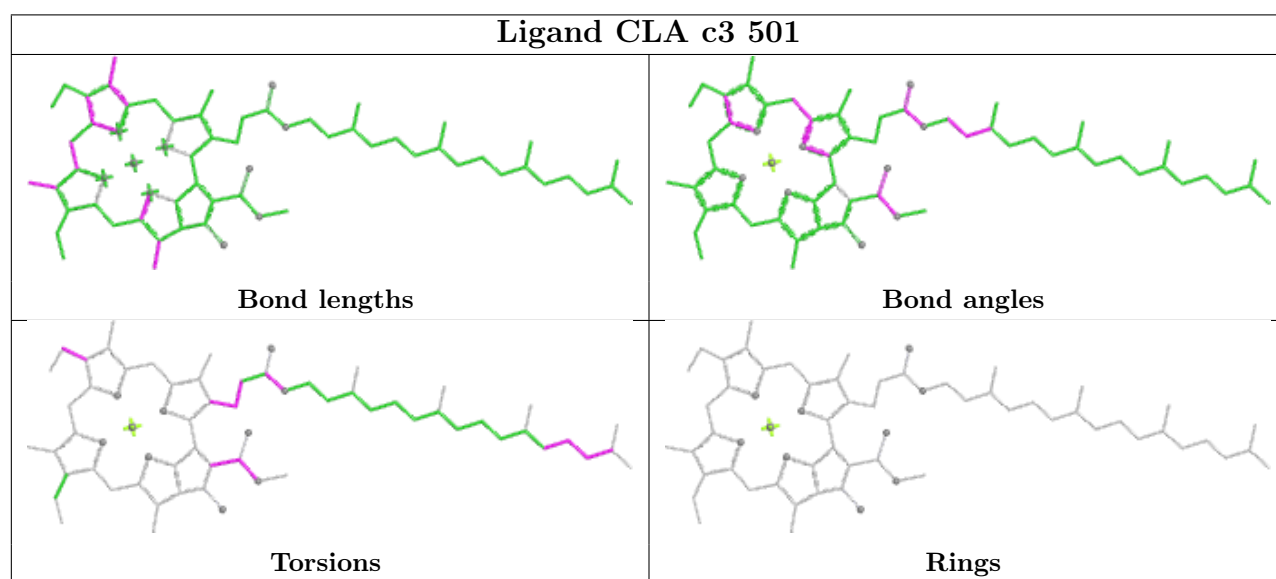
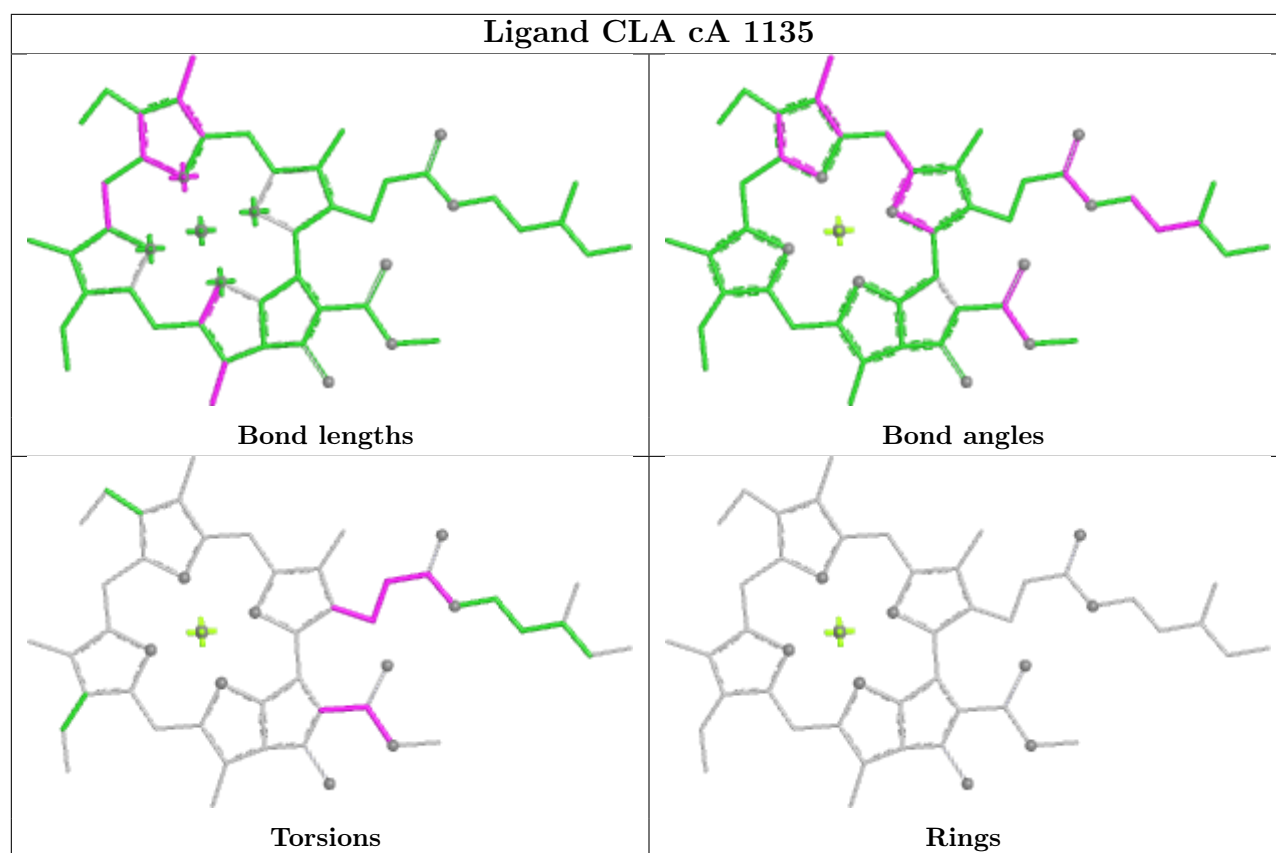


Ligand CLA c5 501

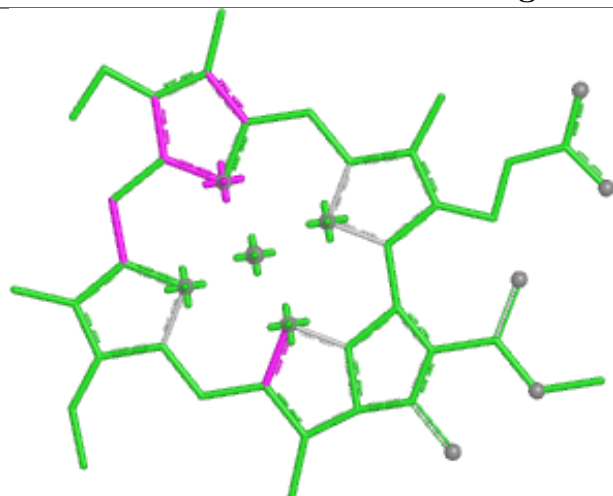


Ligand CLA bA 1022**Ligand LHG bA 5005**

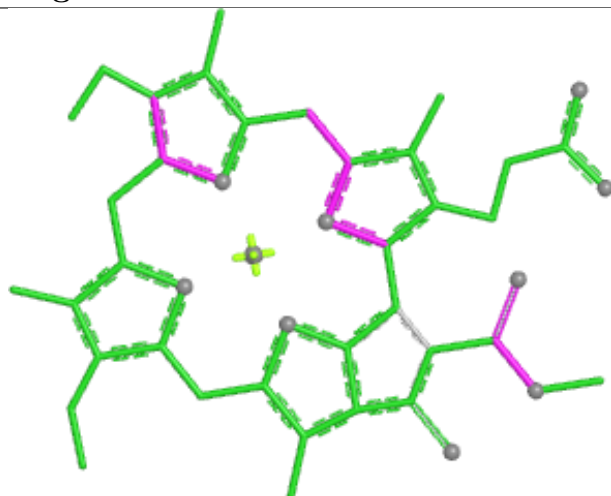




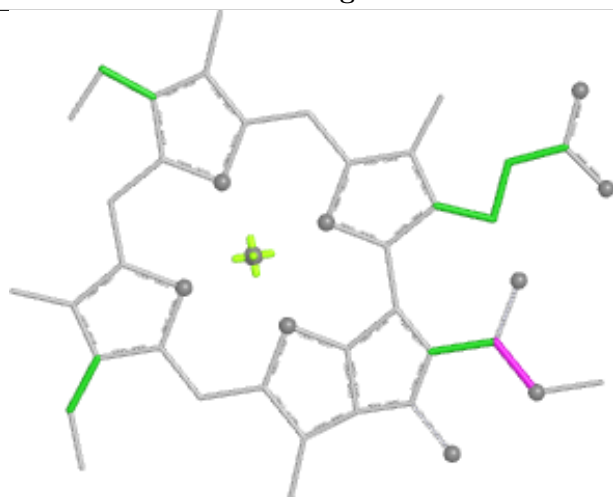
Ligand CLA g 503



Bond lengths



Bond angles

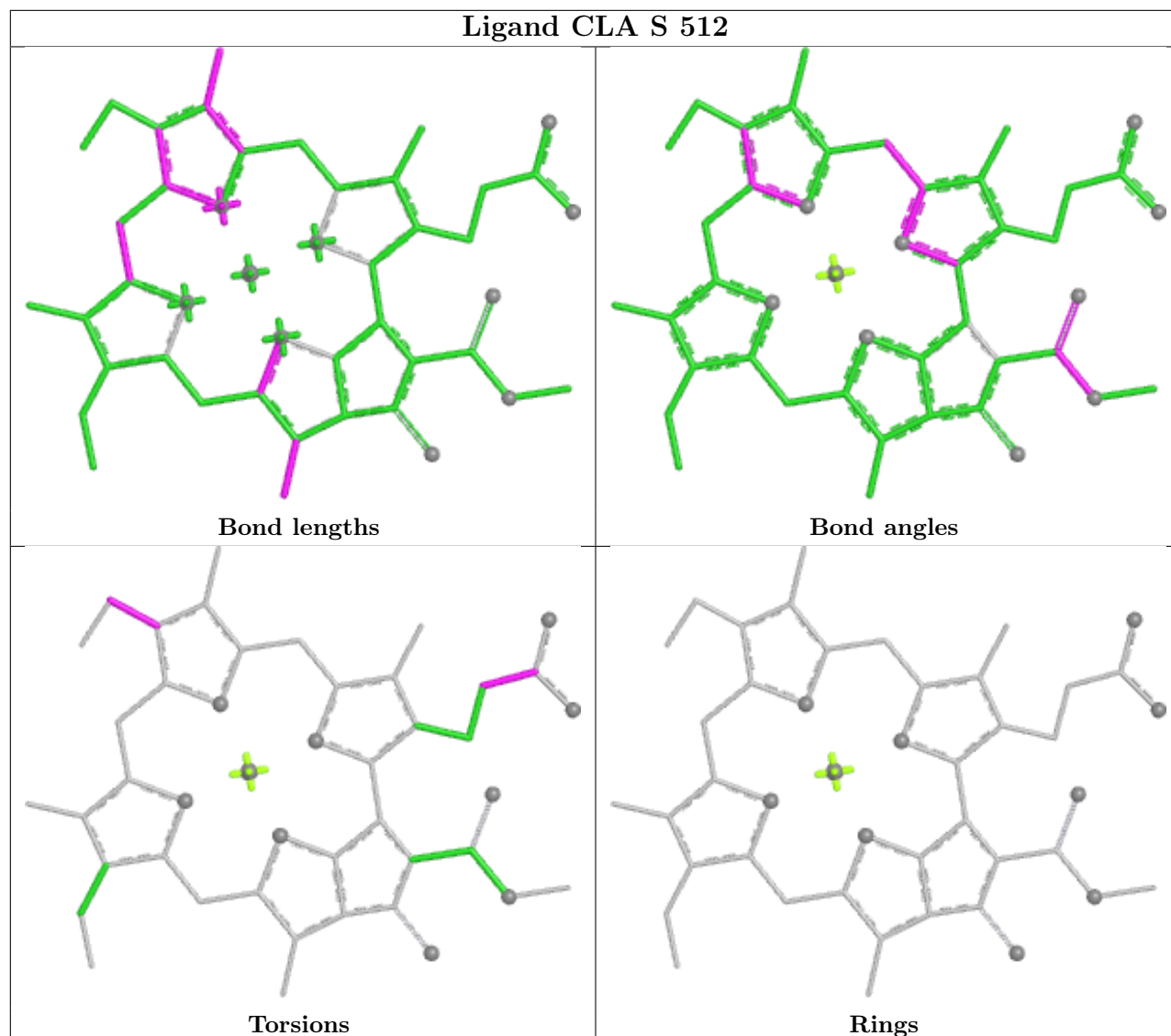


Torsions

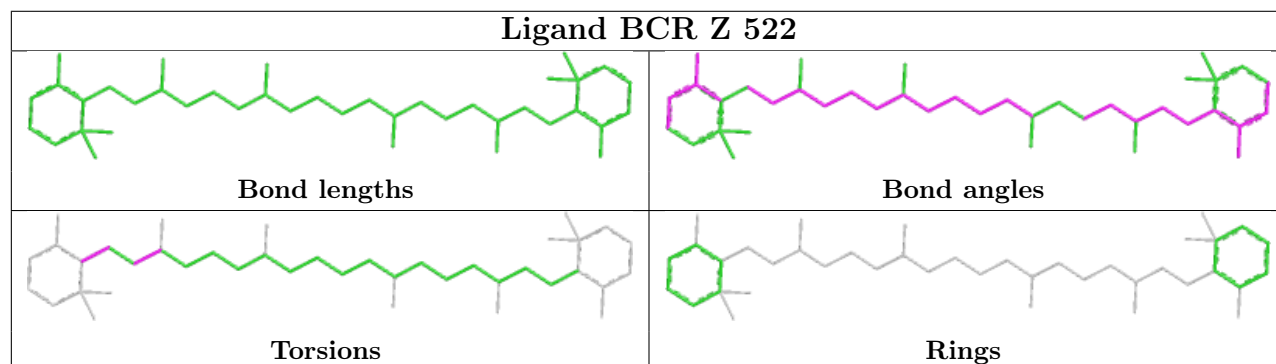


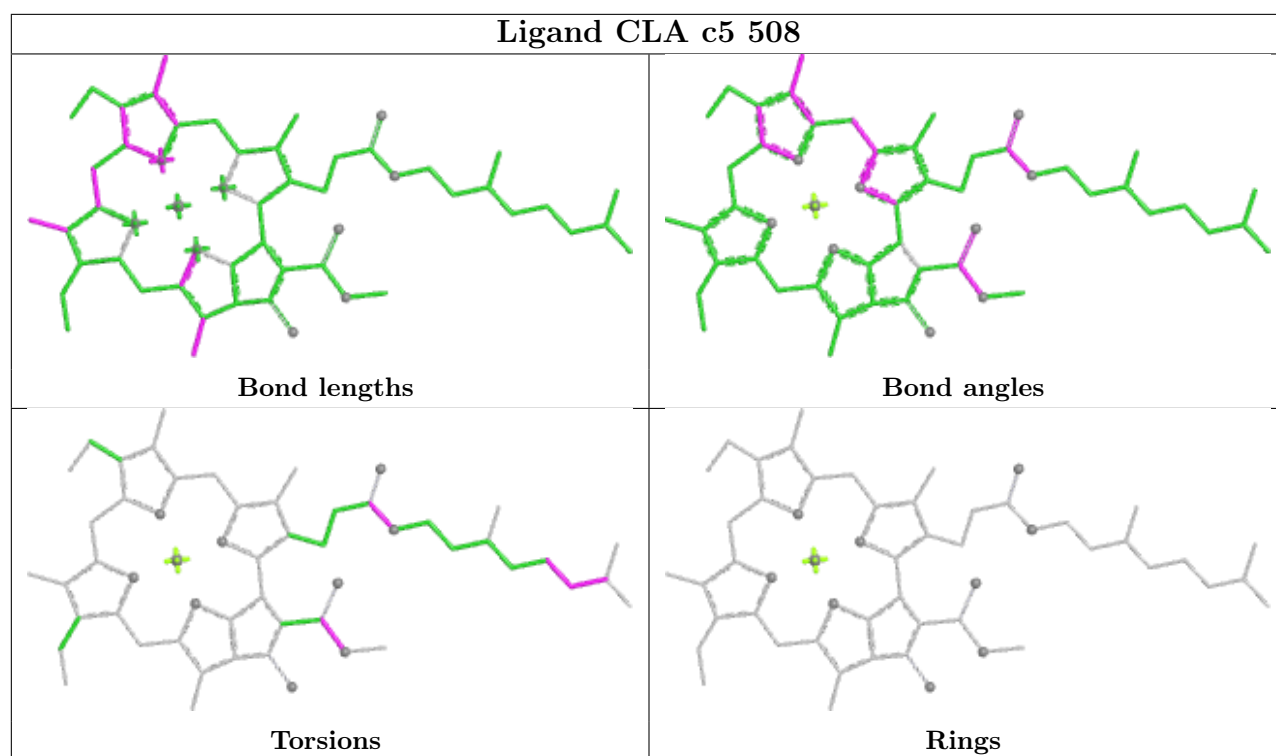
Rings

Ligand CLA S 512

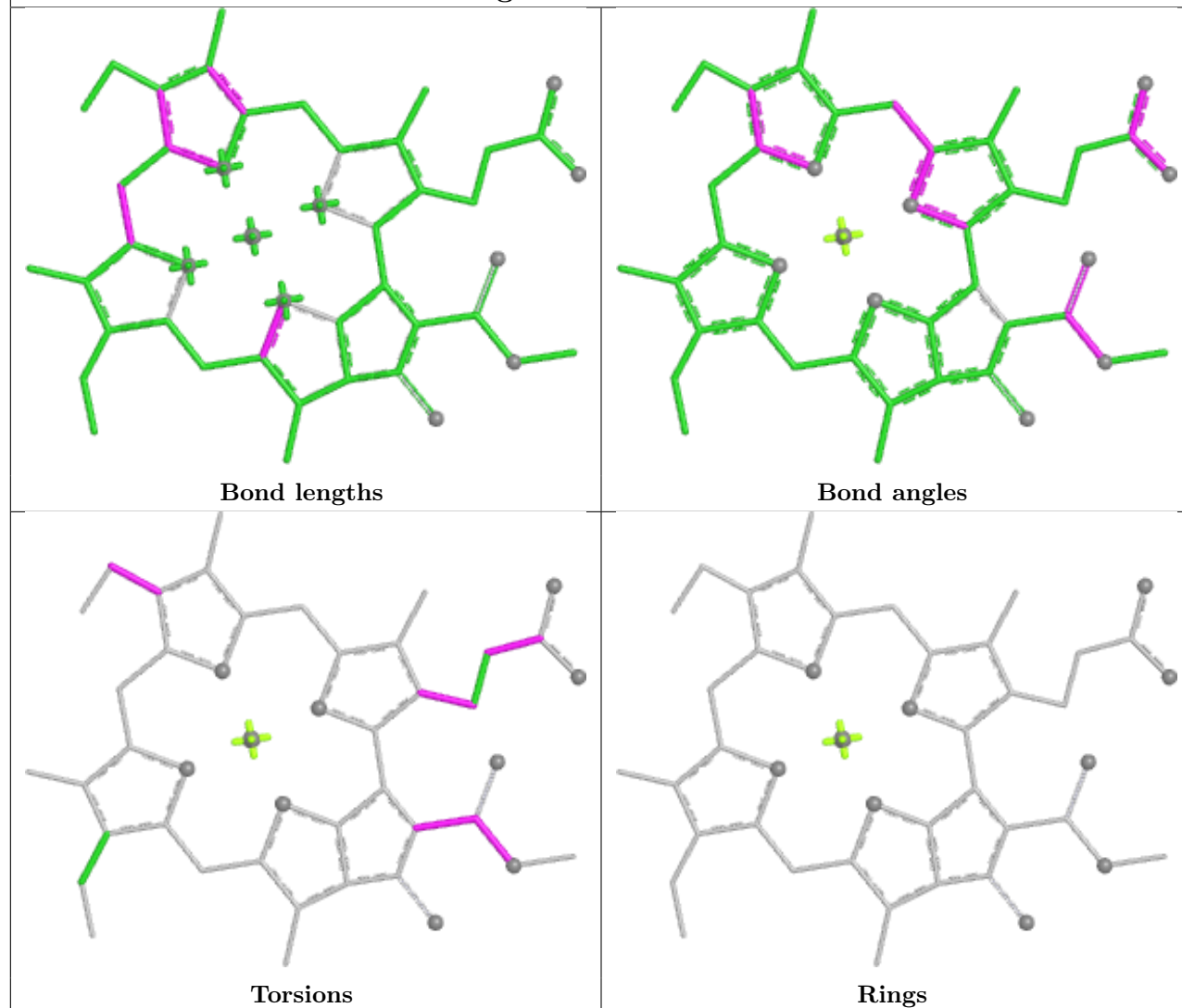


Ligand BCR Z 522

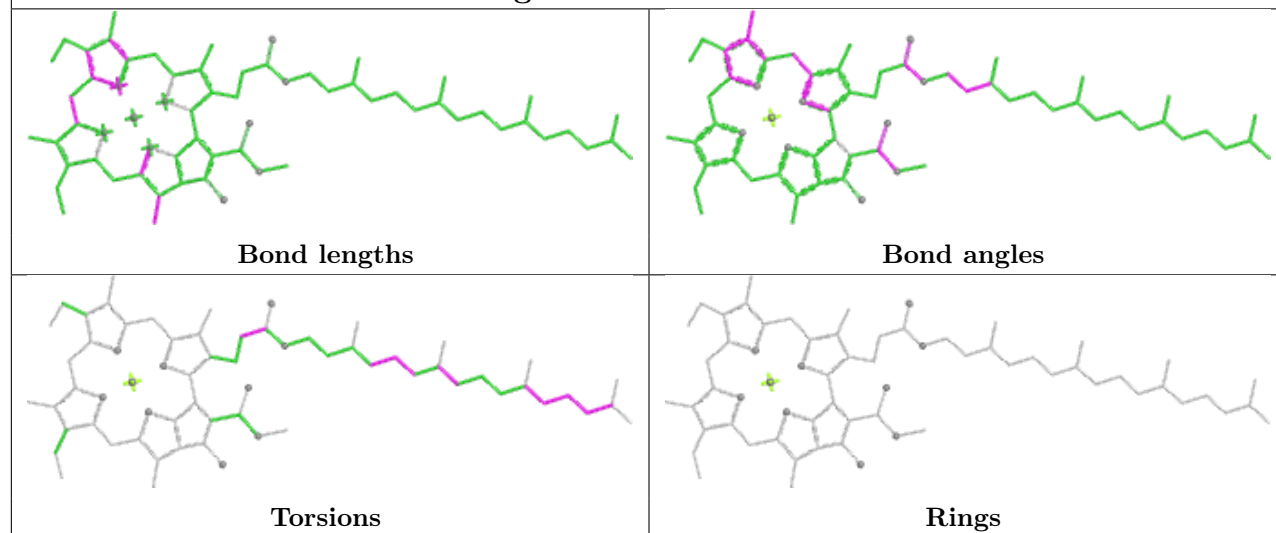


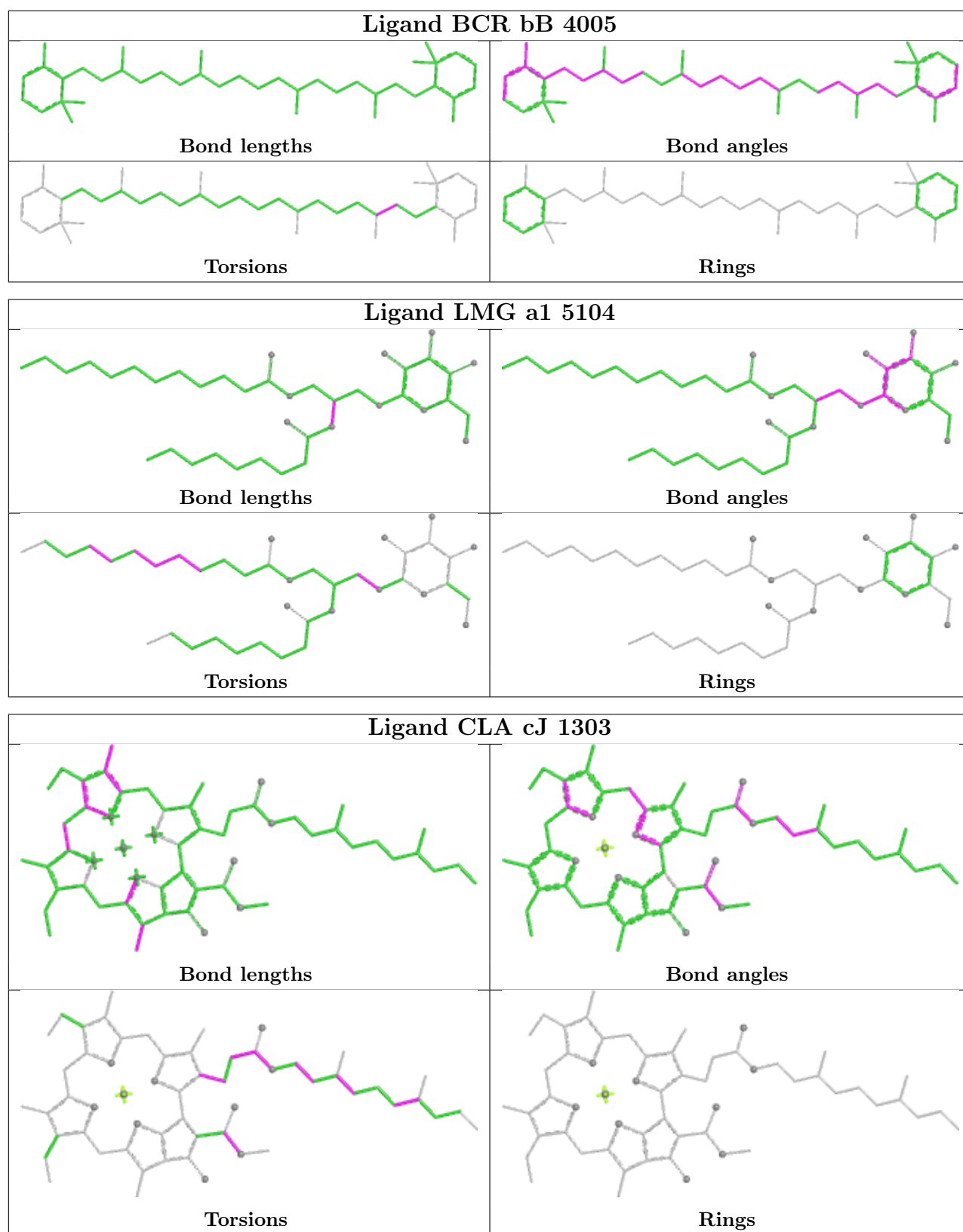


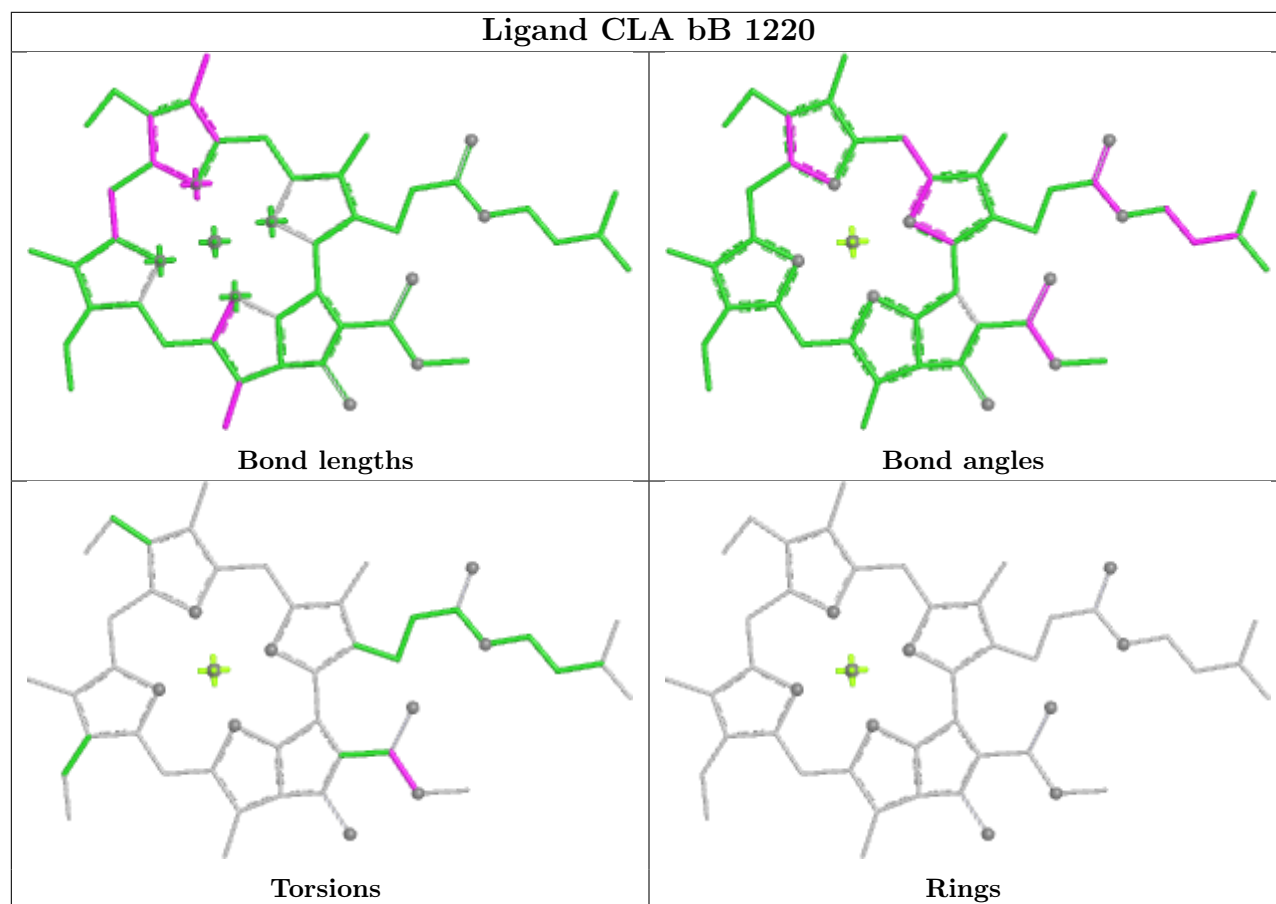
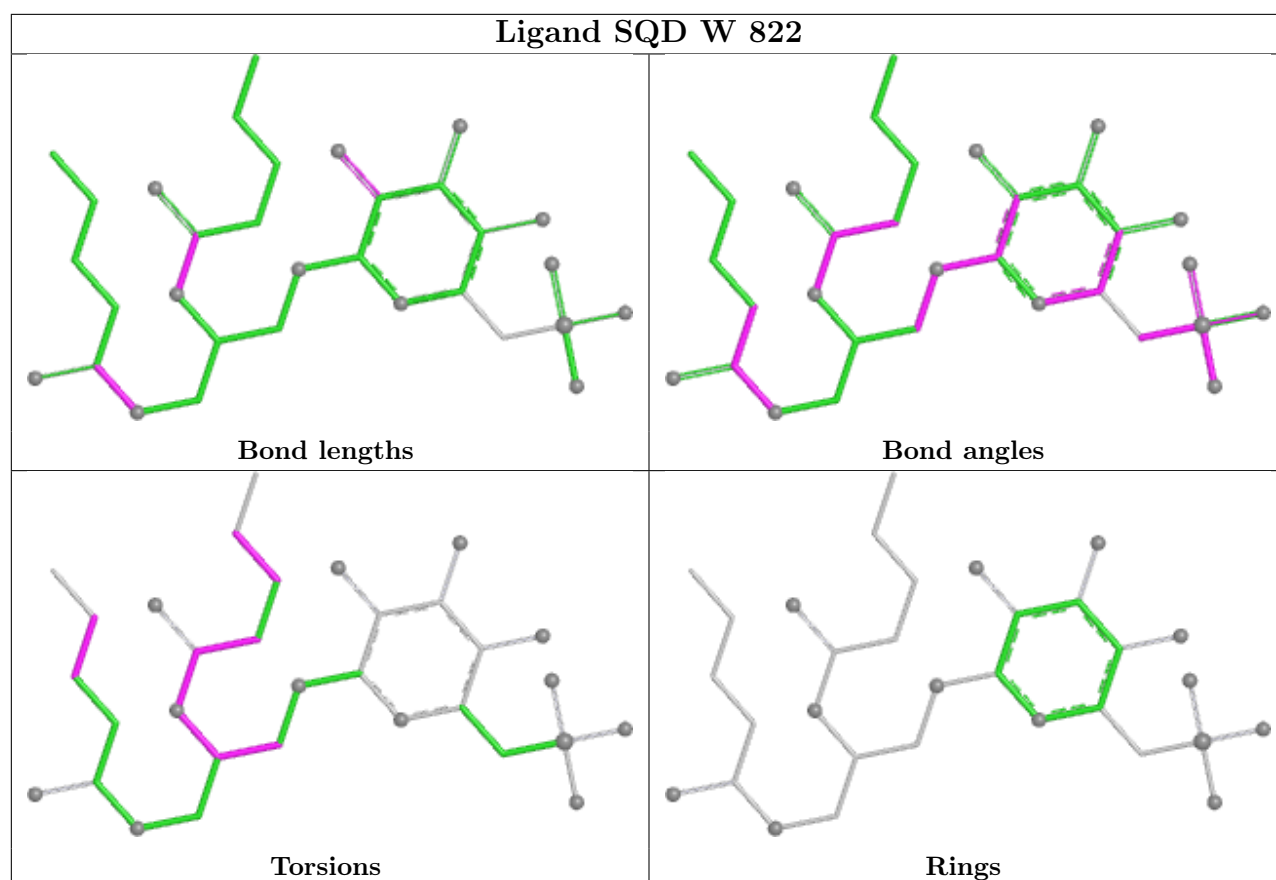
Ligand CLA o 516

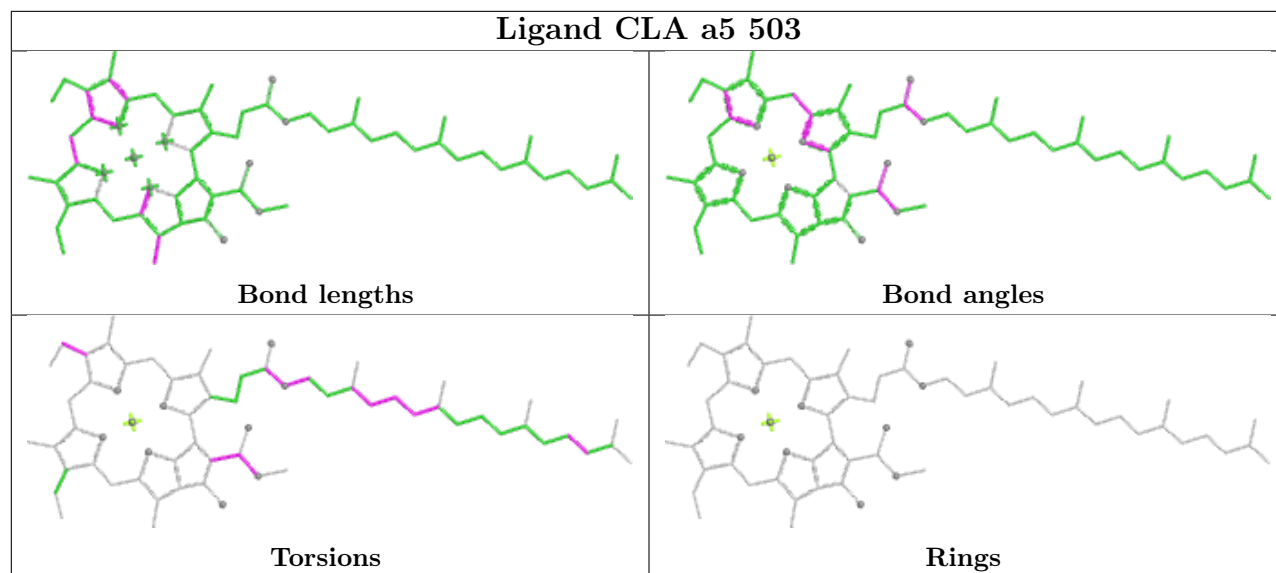
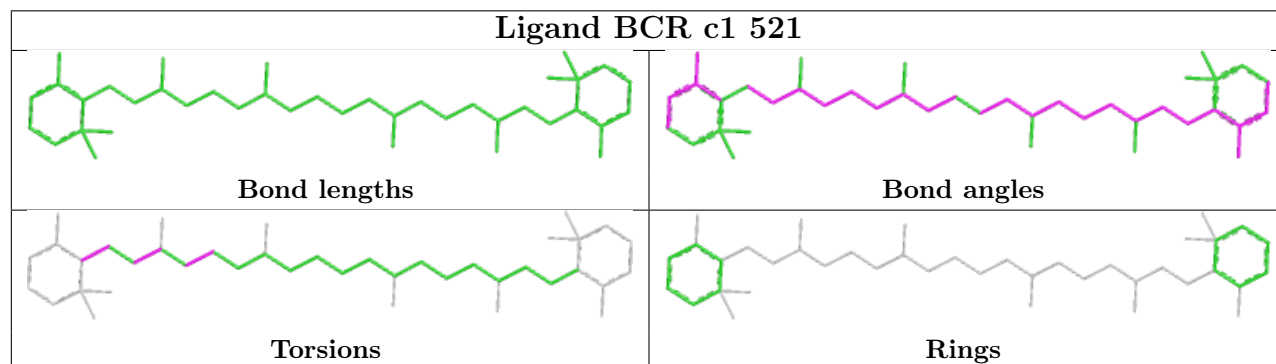
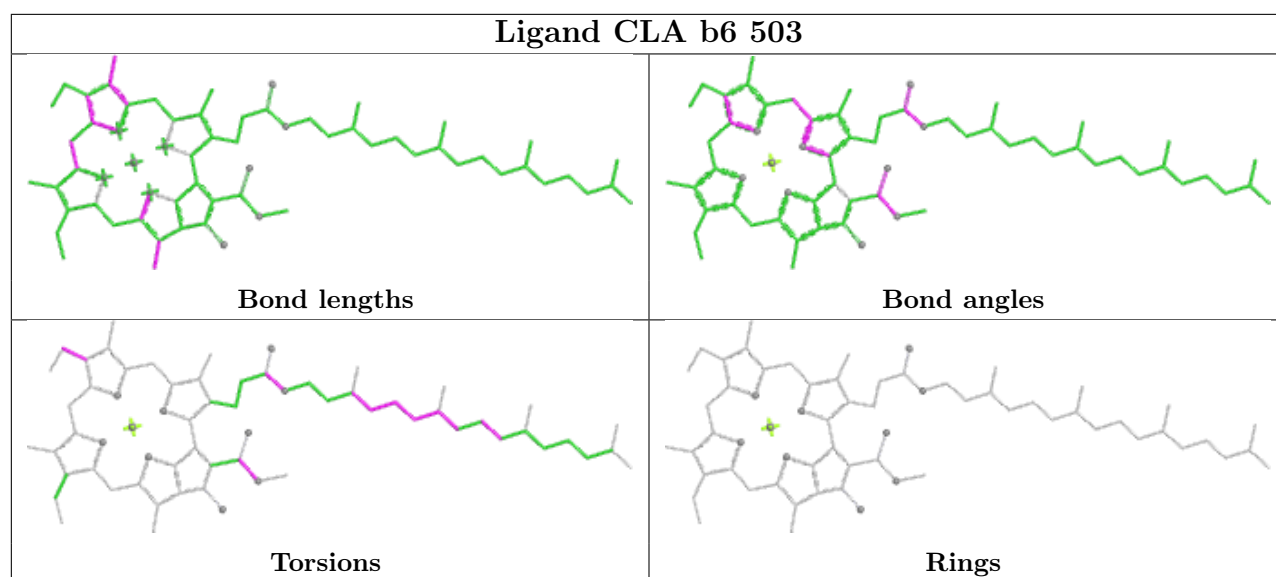


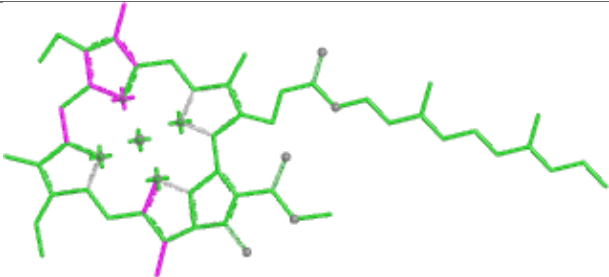
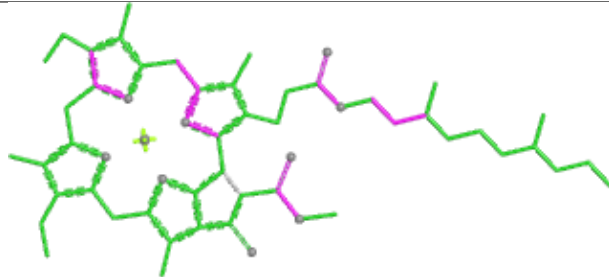
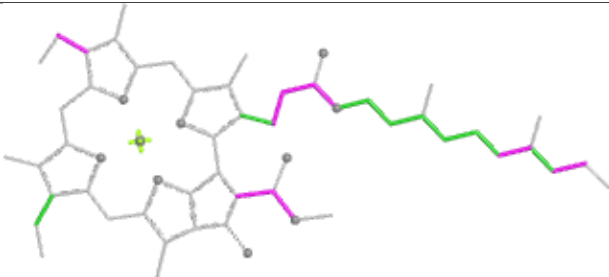
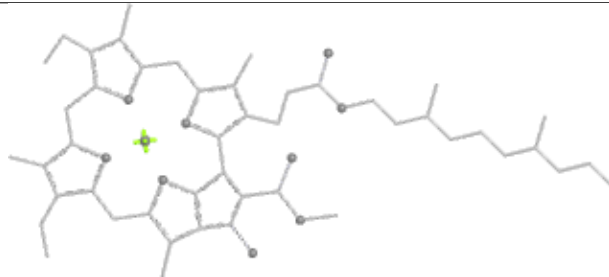
Ligand CLA aA 1123

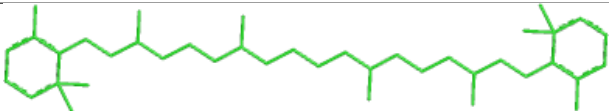
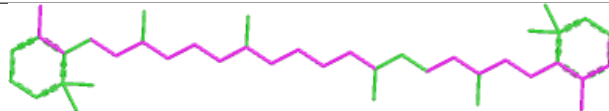
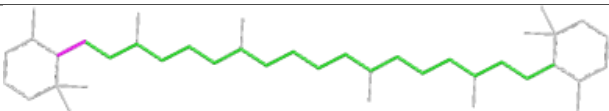
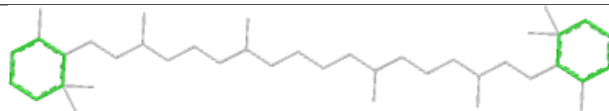


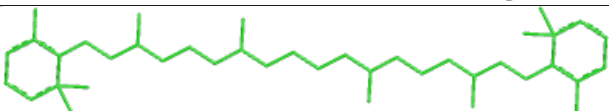
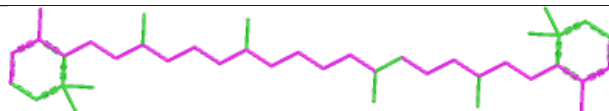

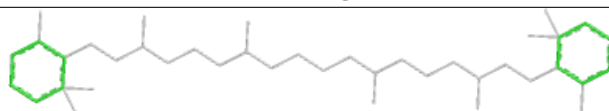




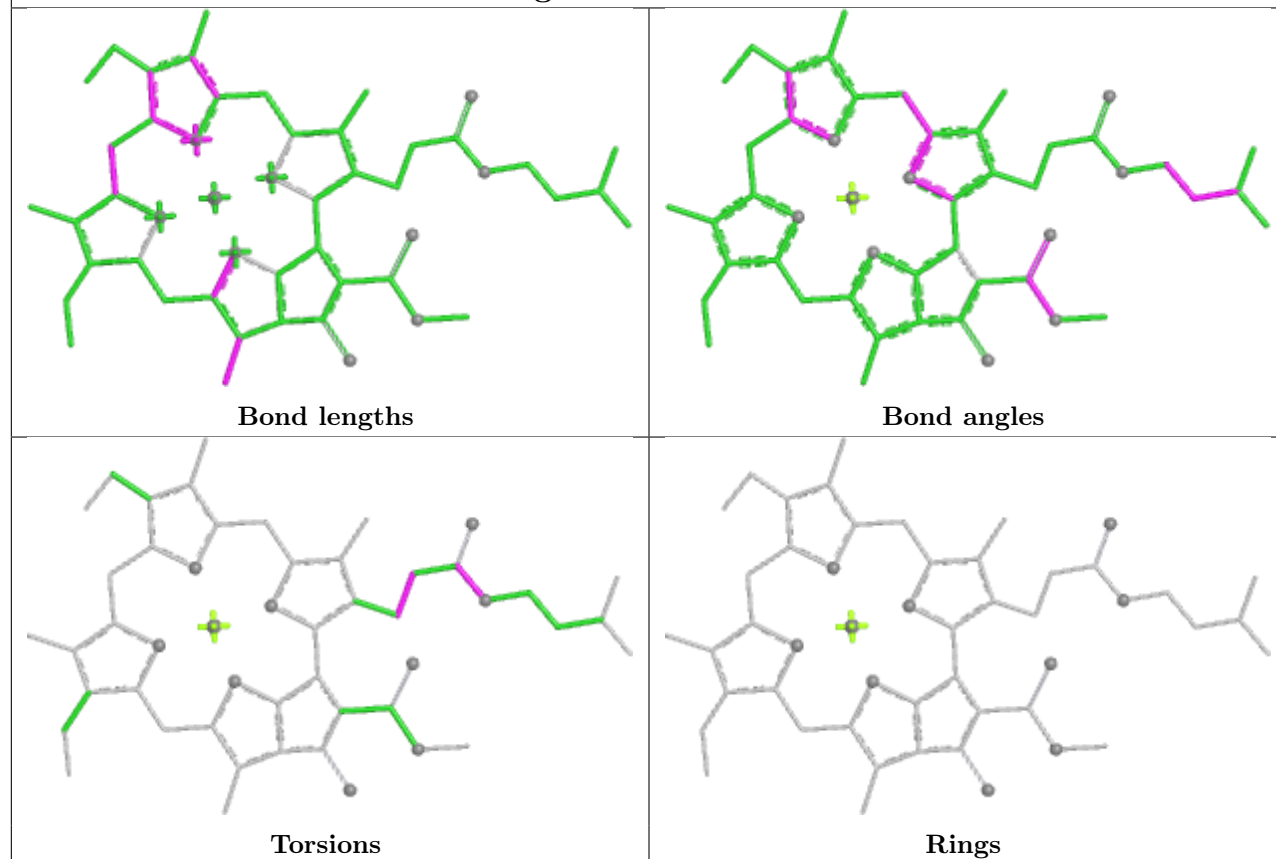


Ligand CLA q 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

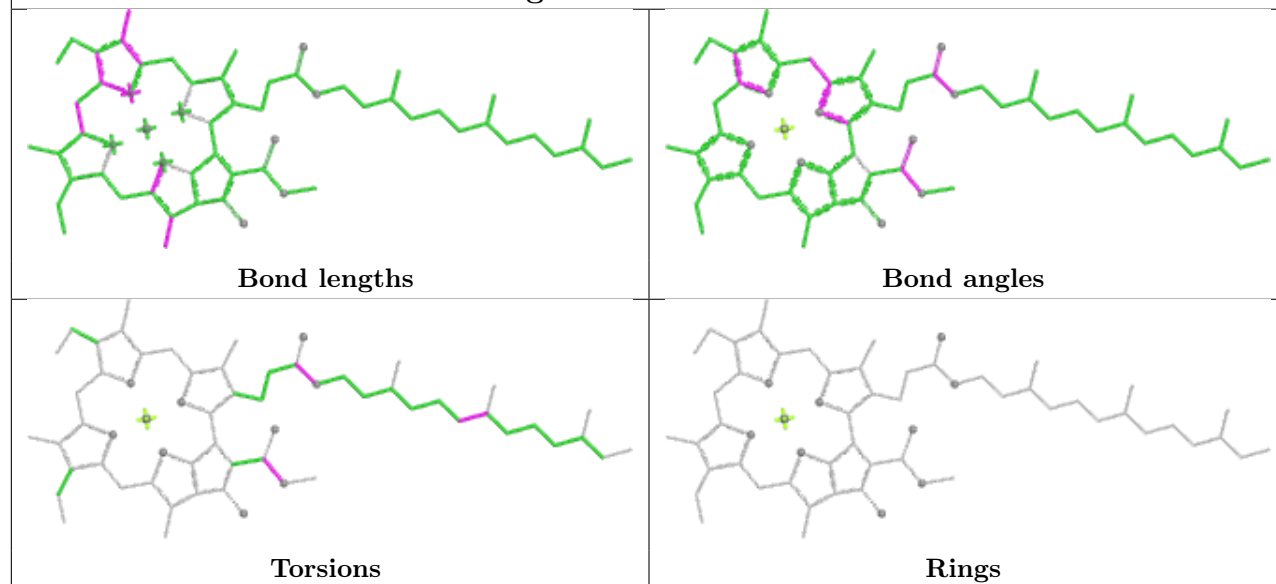
Ligand BCR b2 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

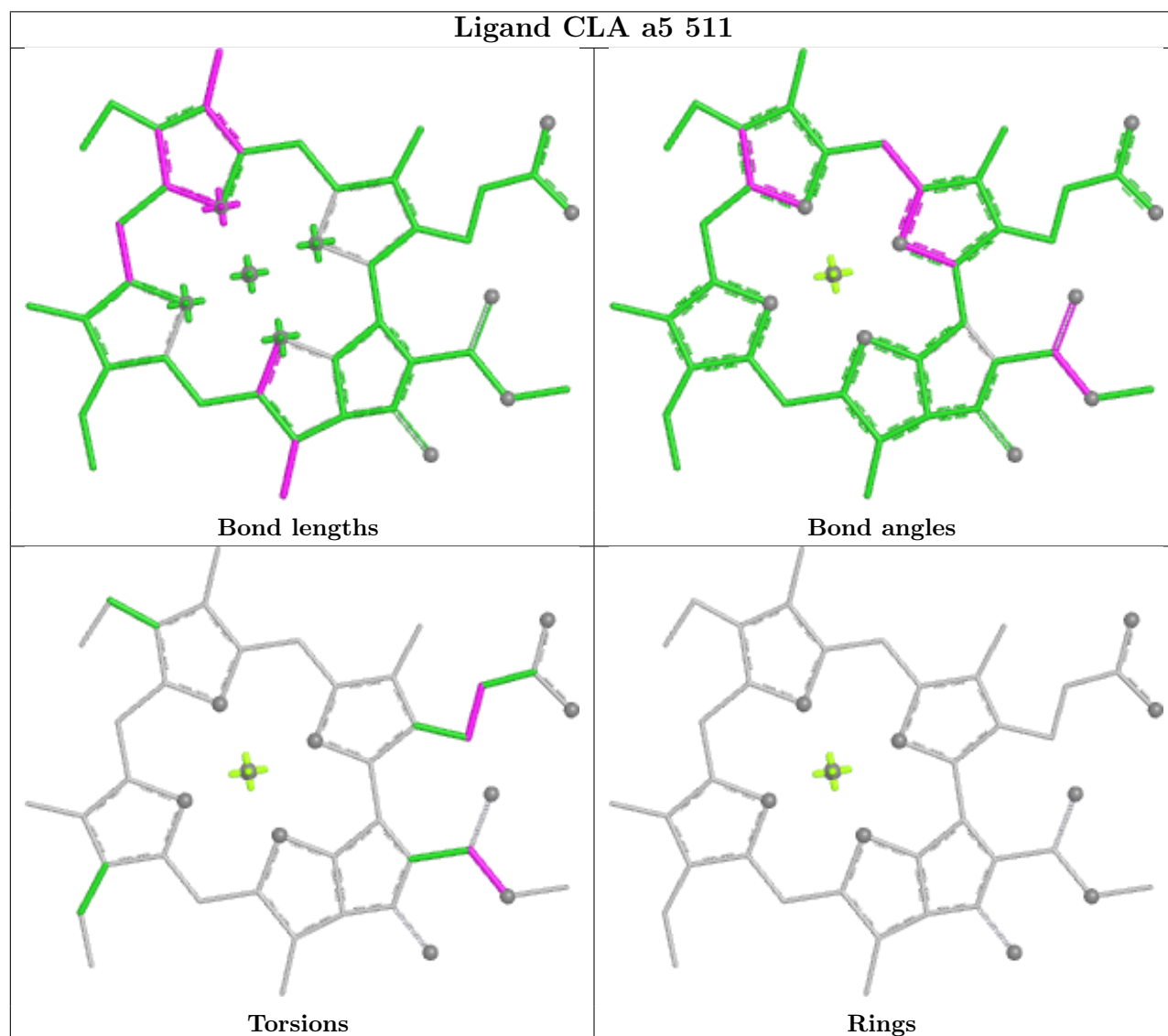
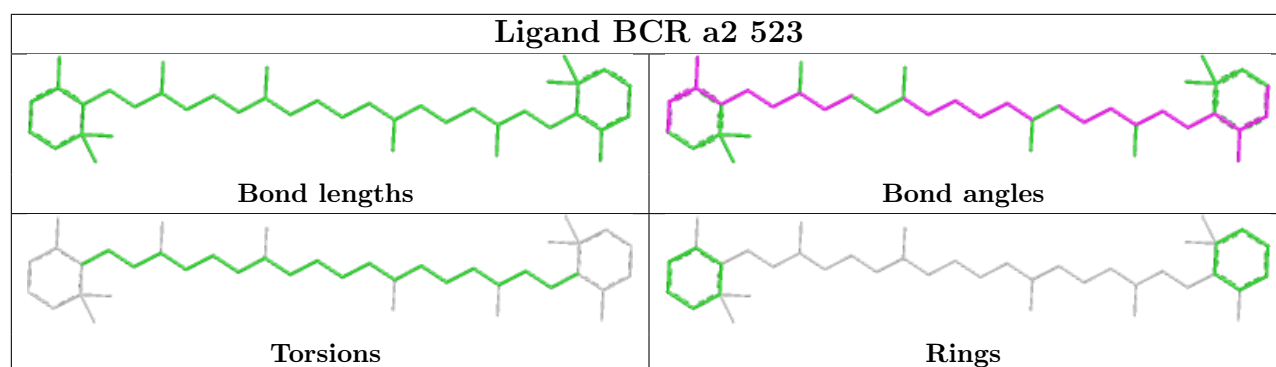
Ligand BCR b3 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Z 513

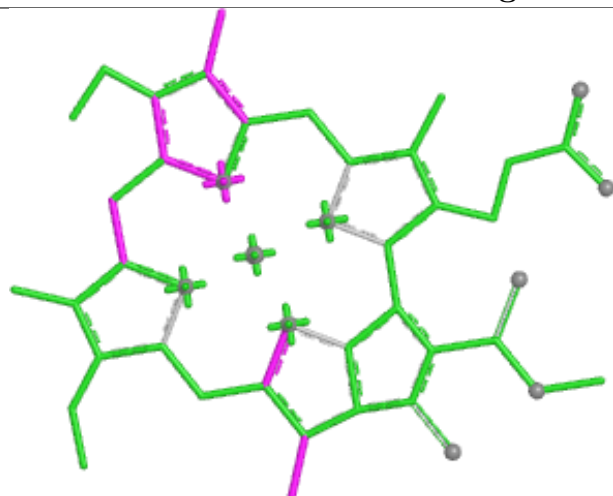


Ligand CLA b5 507

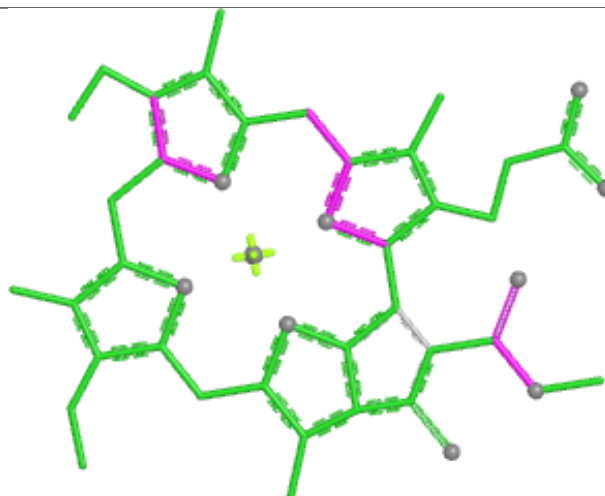




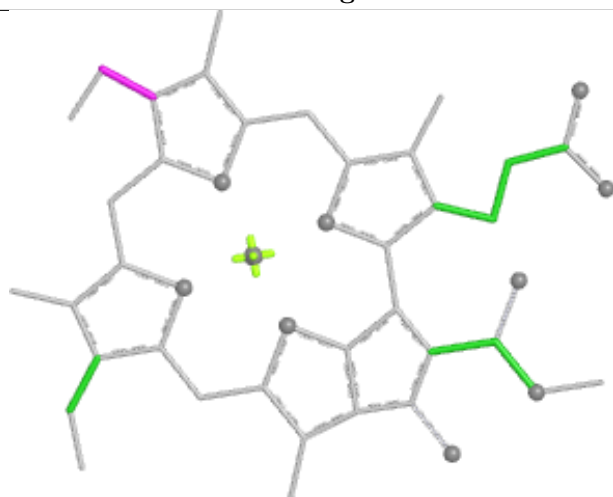
Ligand CLA cF 1301



Bond lengths



Bond angles

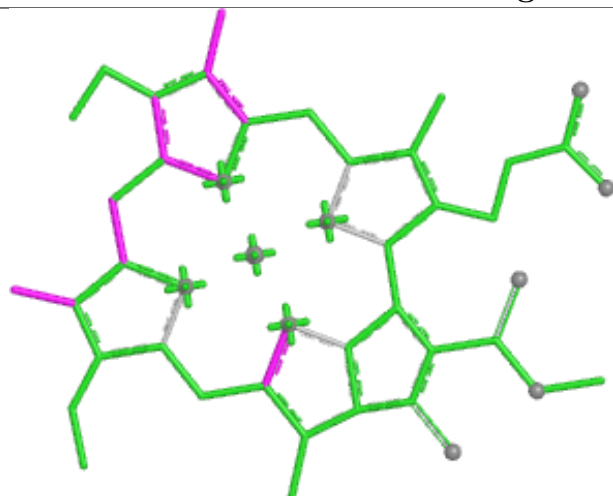


Torsions

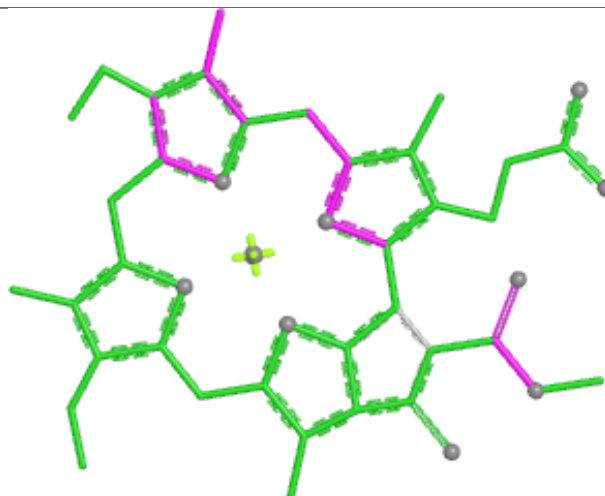


Rings

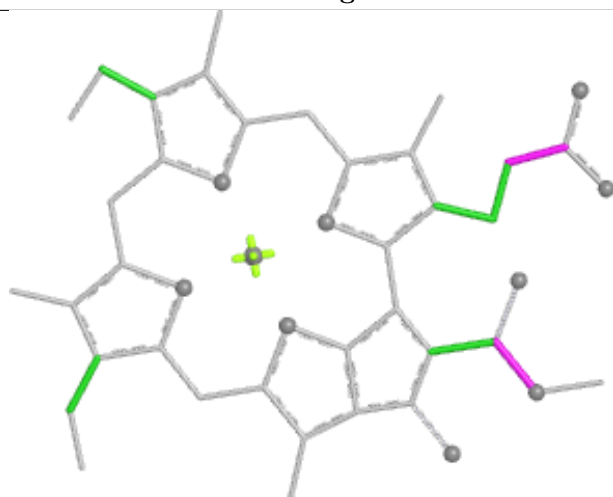
Ligand CLA b 508



Bond lengths



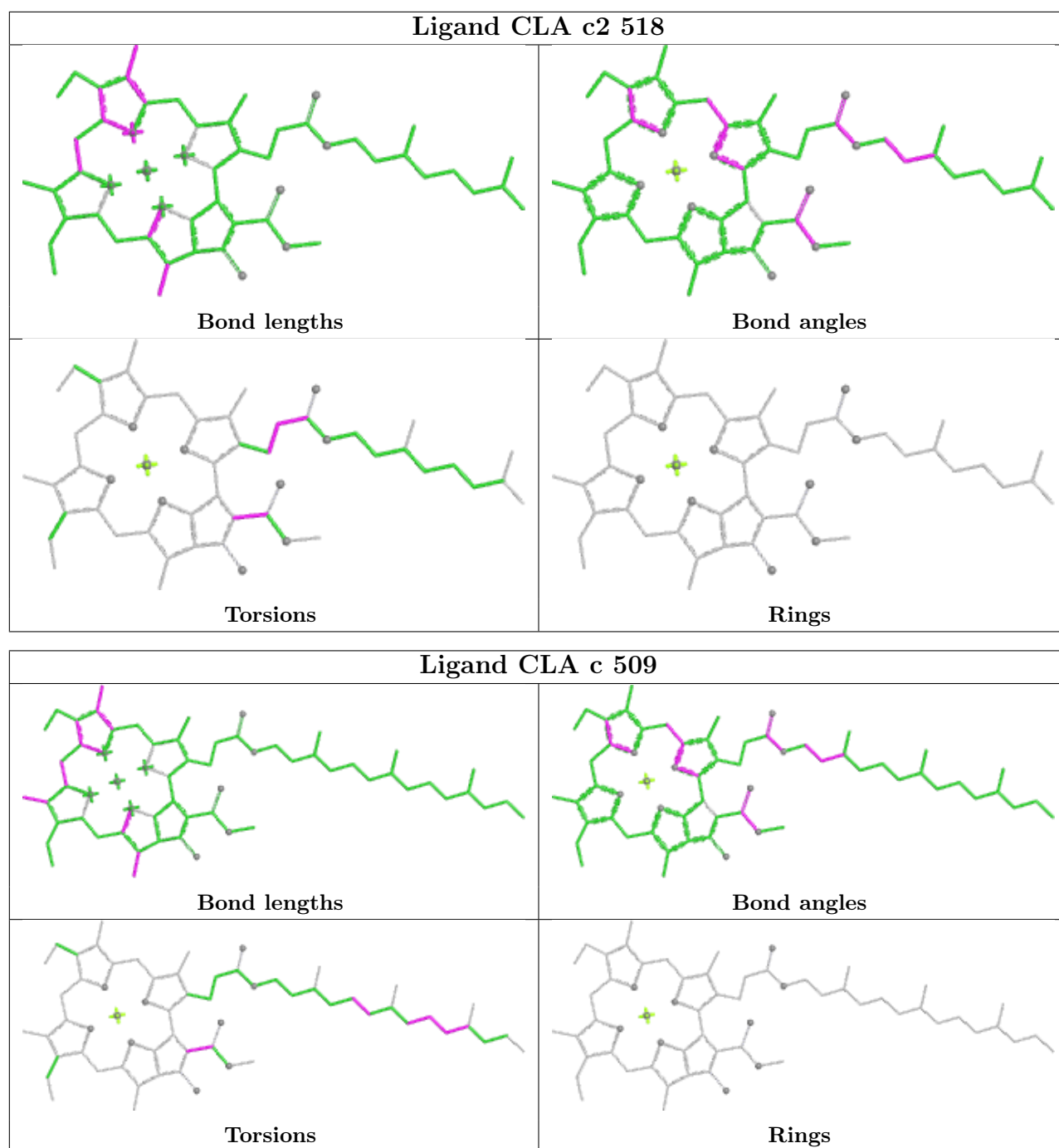
Bond angles



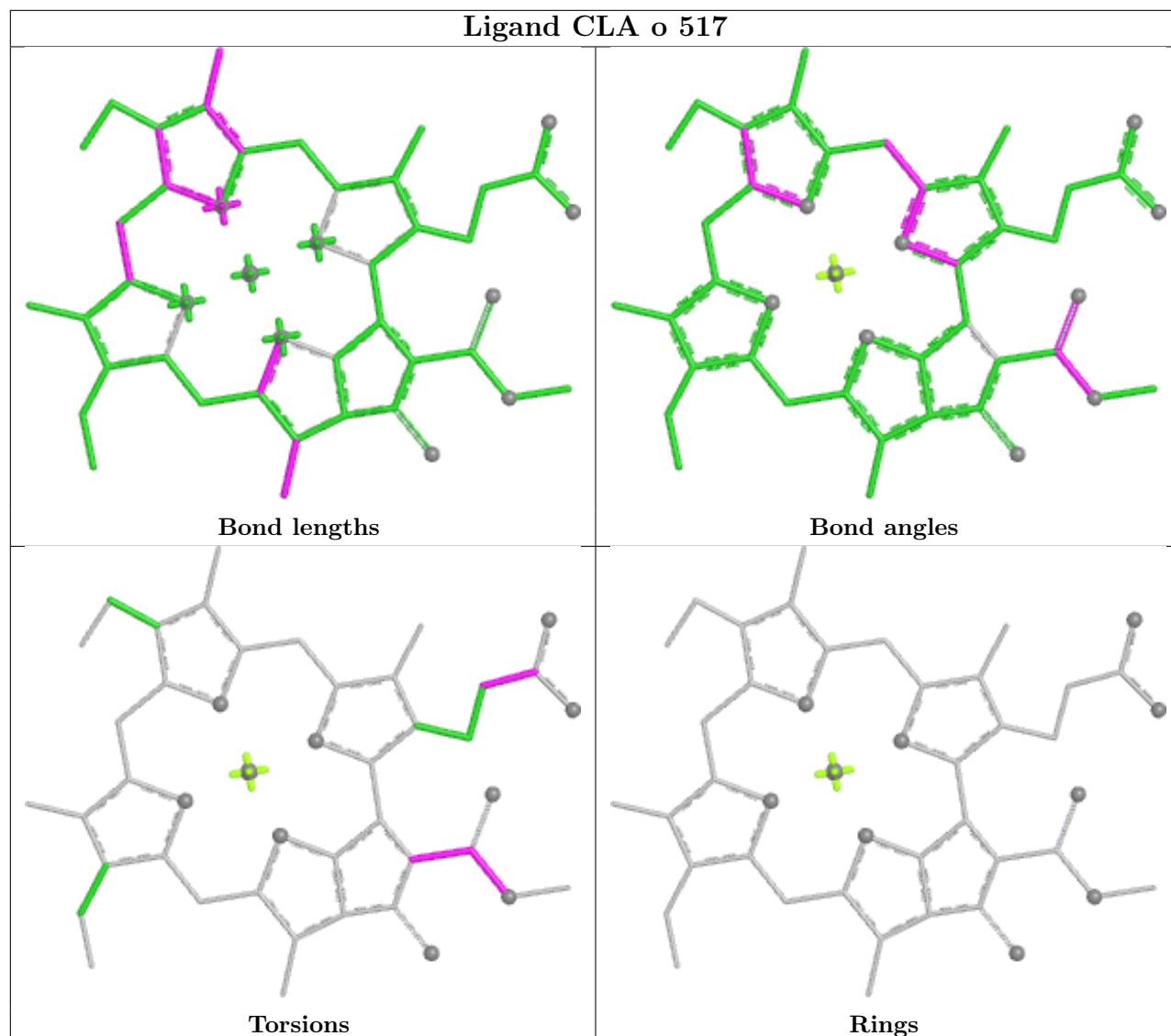
Torsions



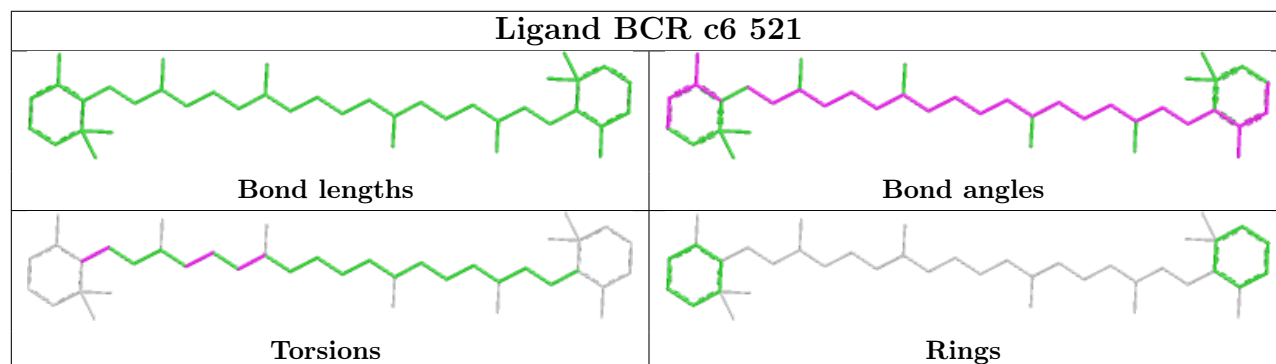
Rings

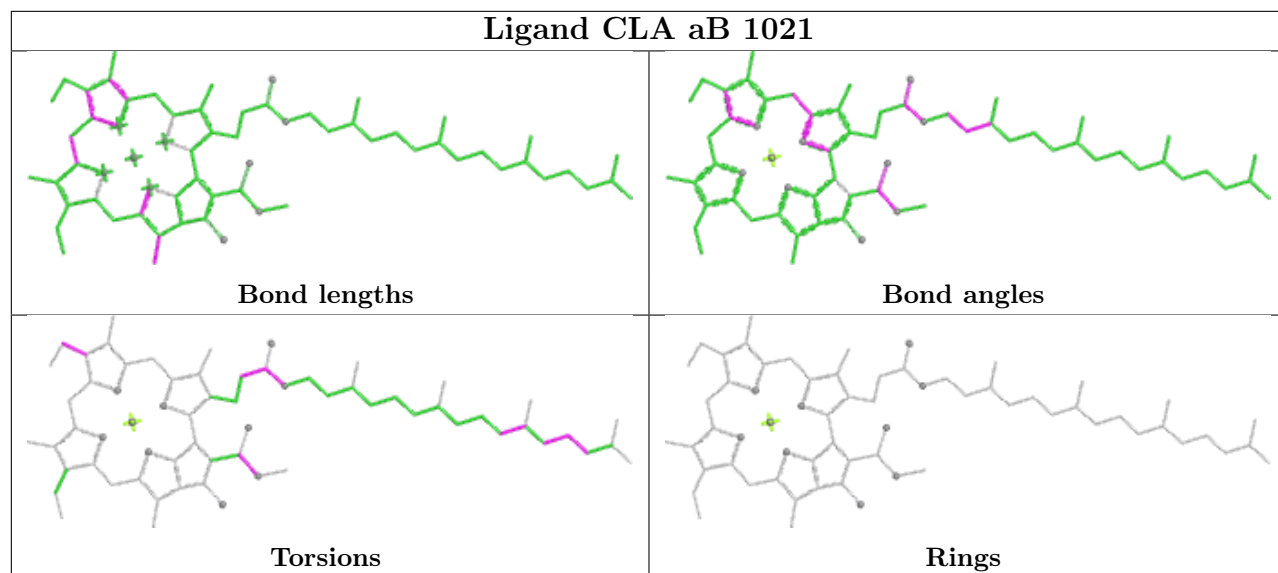
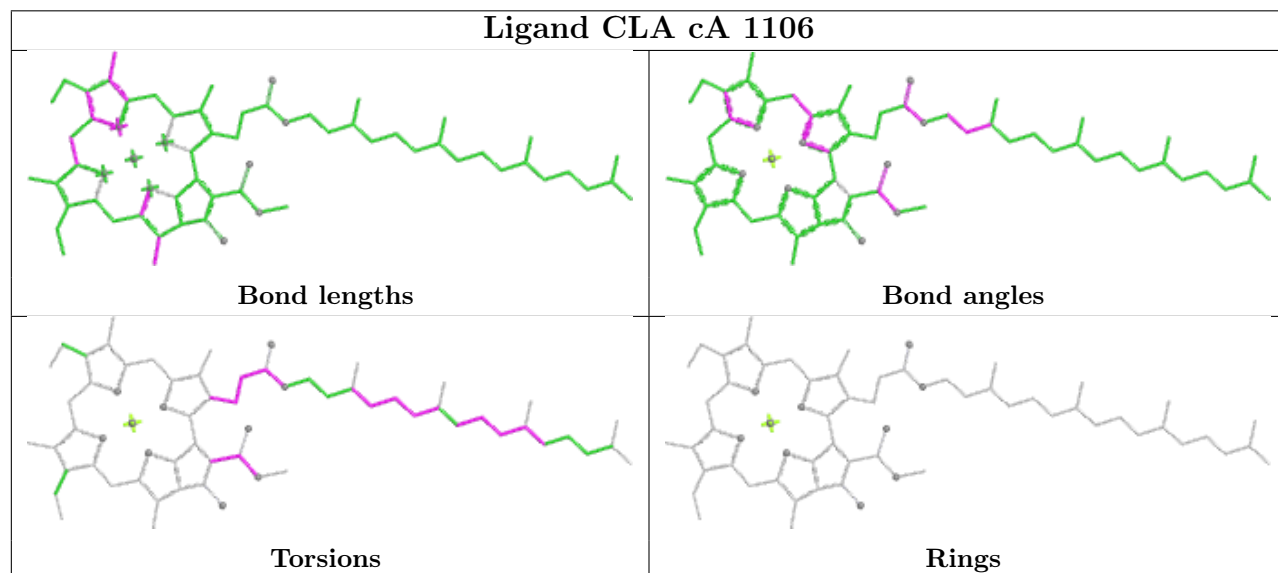
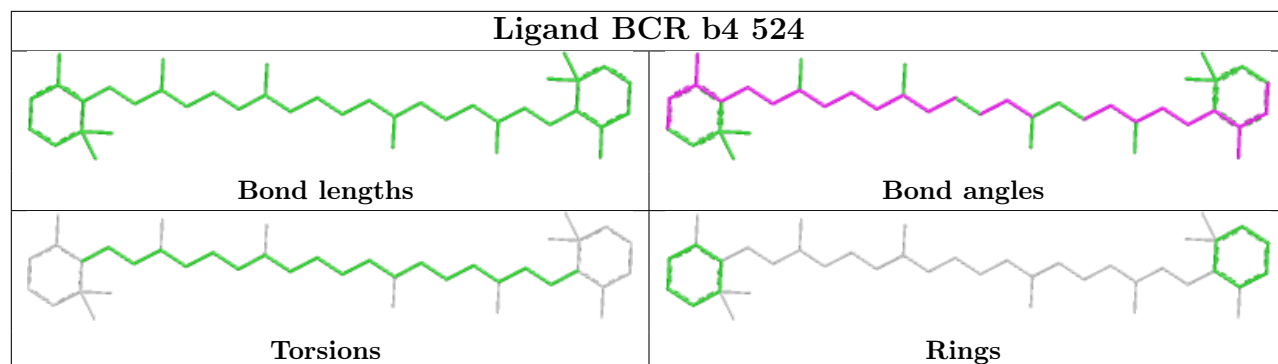


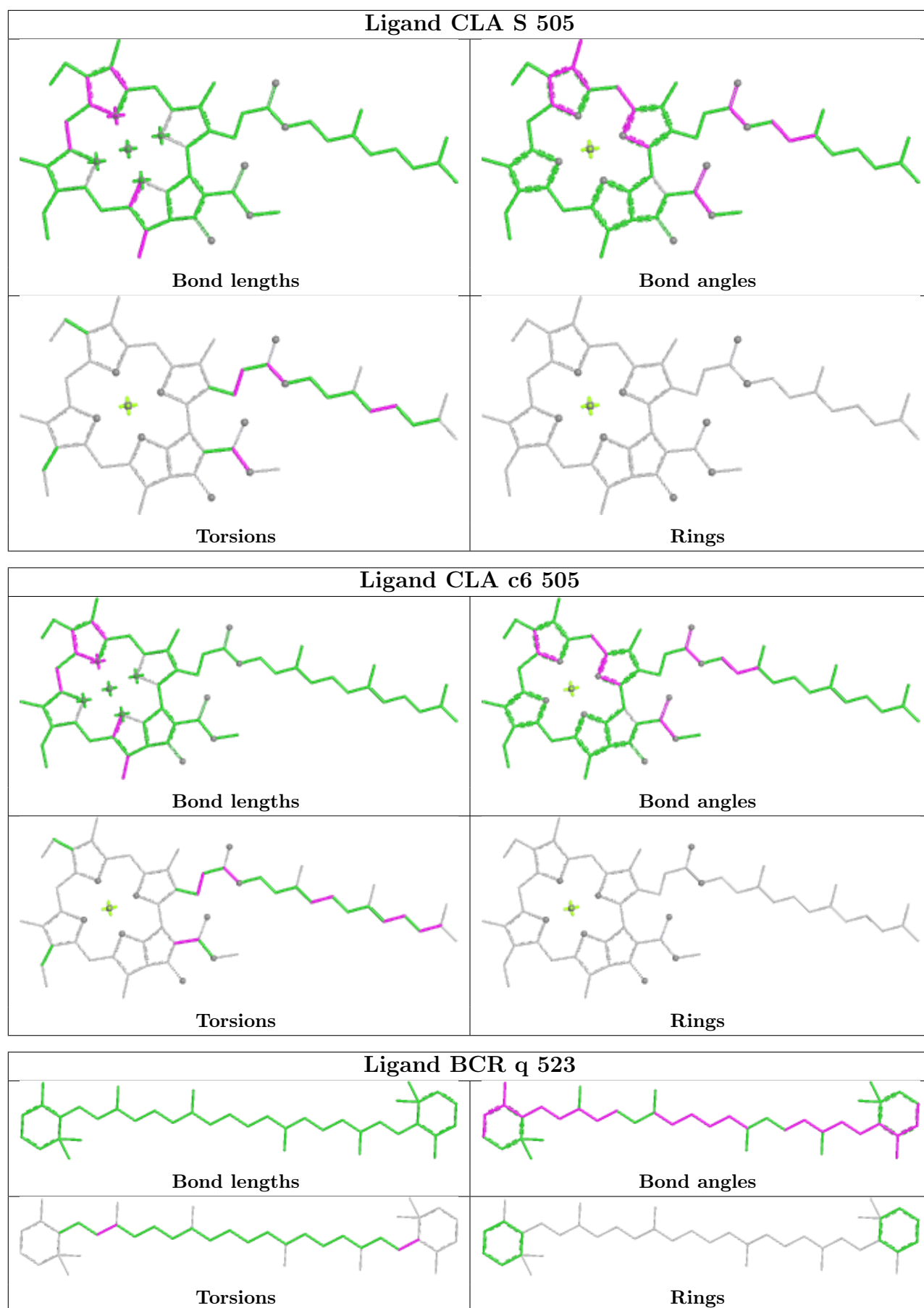
Ligand CLA o 517

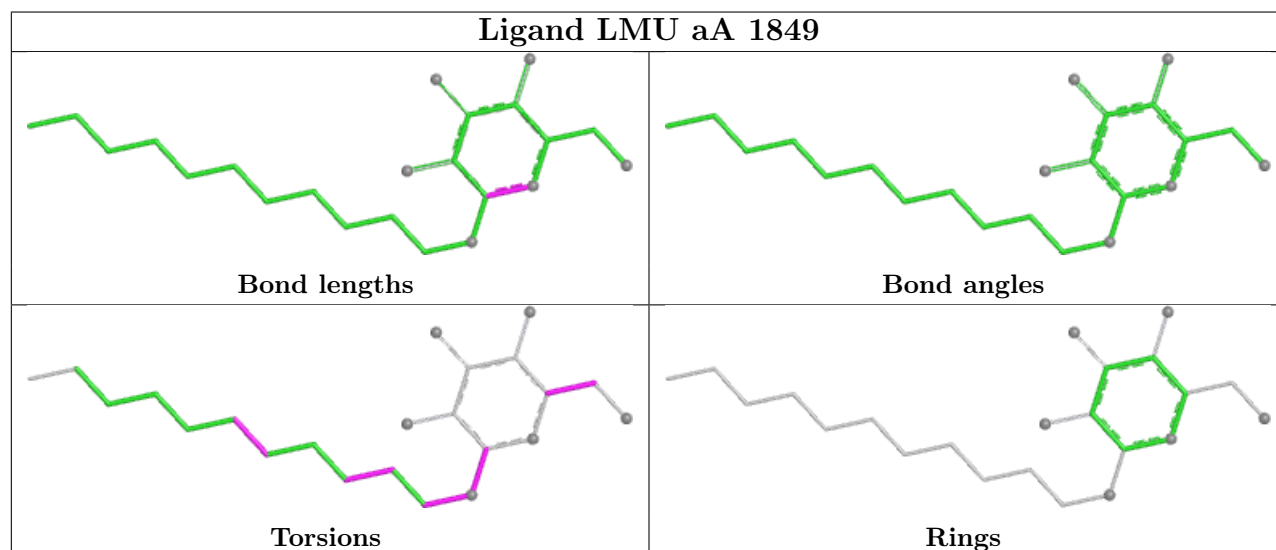
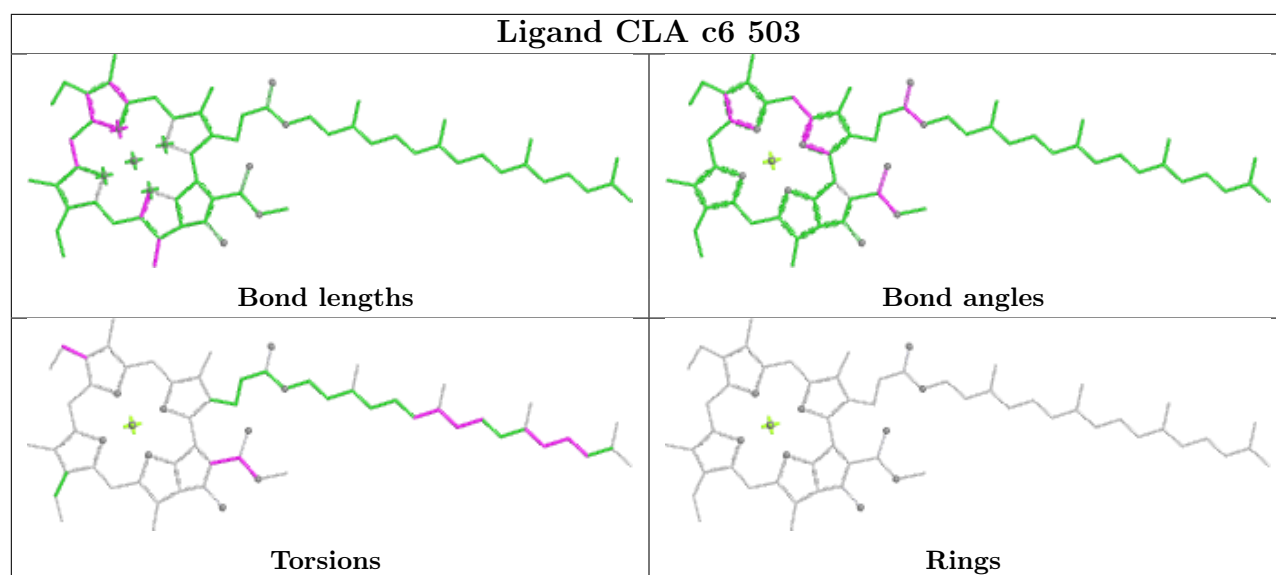


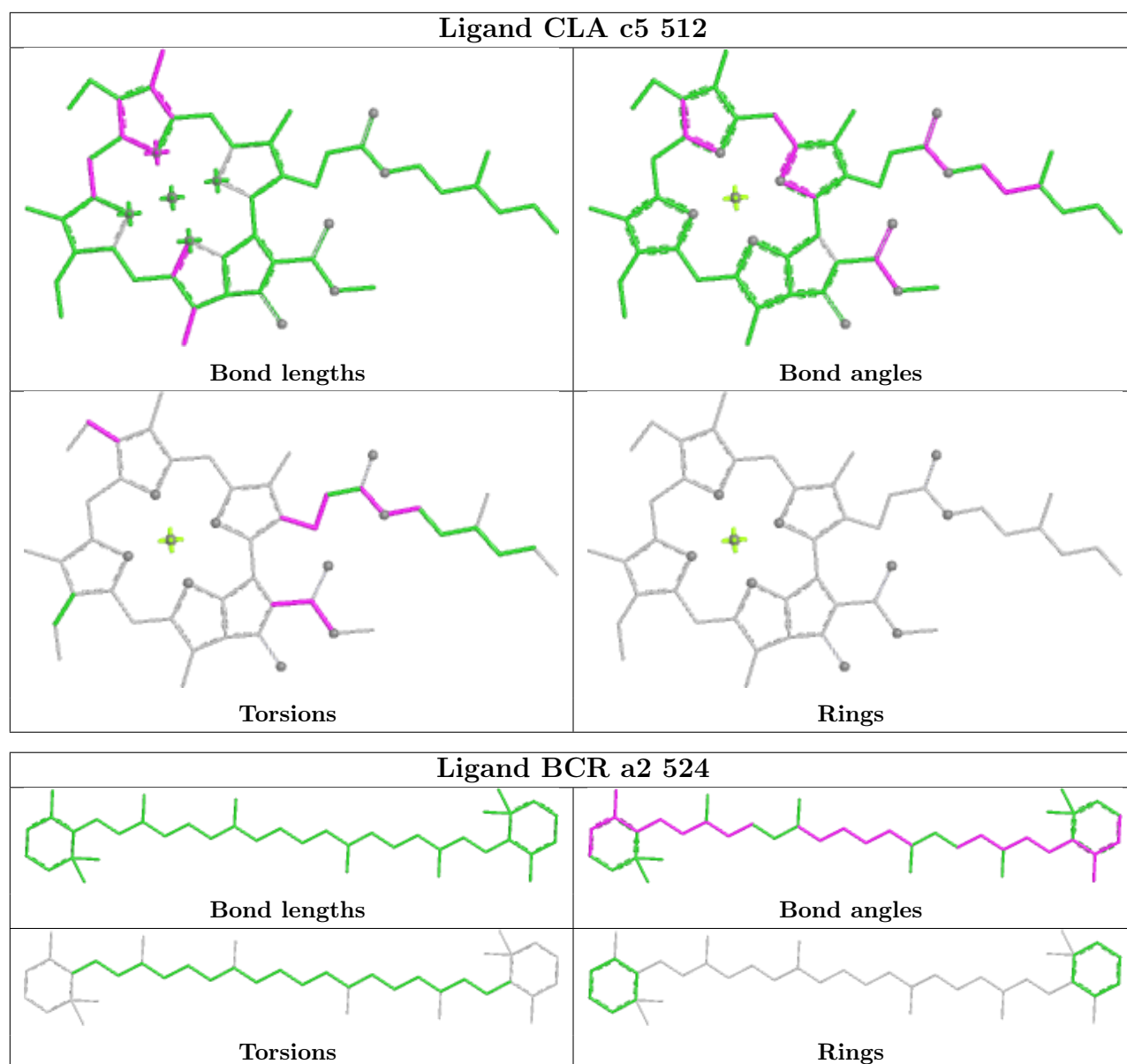
Ligand BCR c6 521



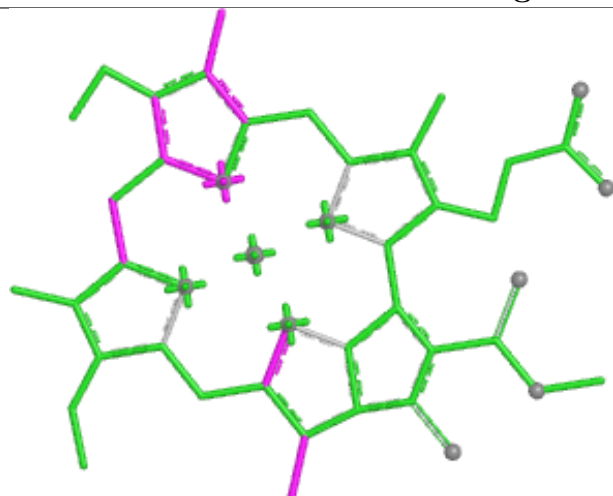




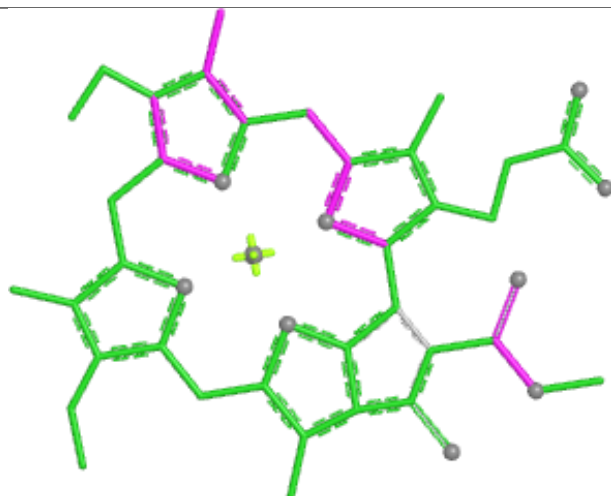




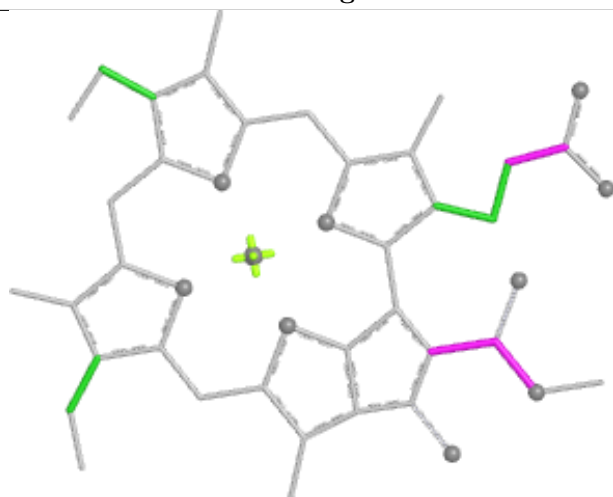
Ligand CLA Y 506



Bond lengths



Bond angles

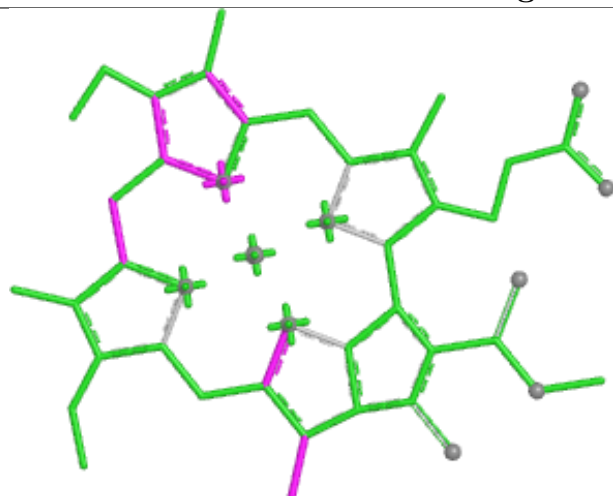


Torsions



Rings

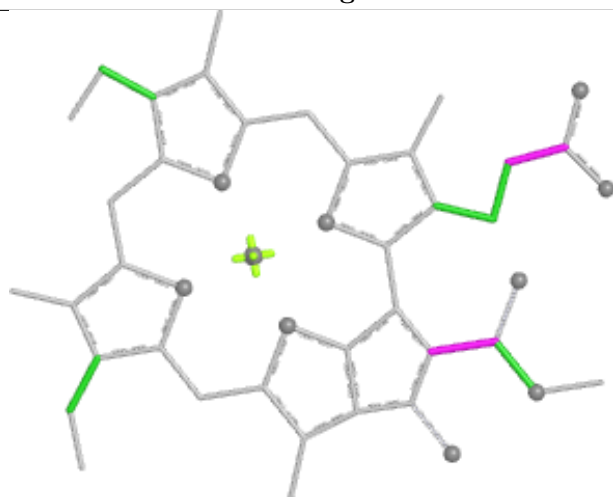
Ligand CLA d 519



Bond lengths



Bond angles

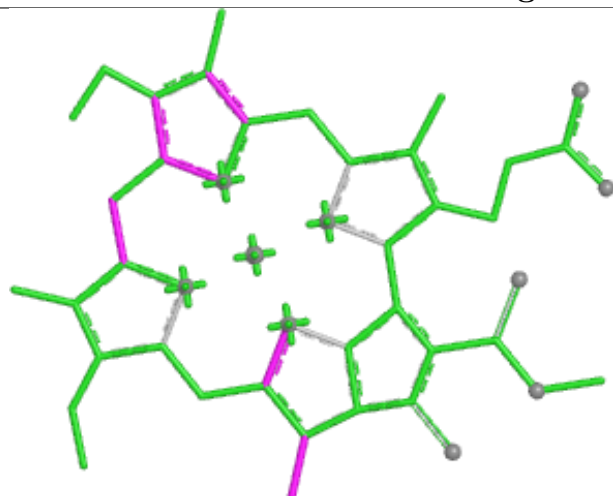


Torsions

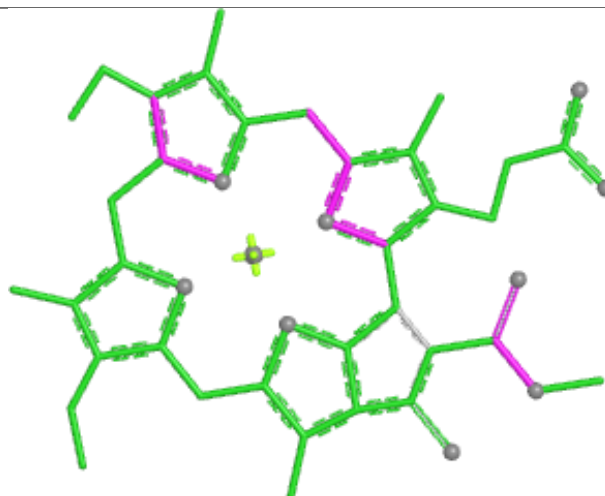


Rings

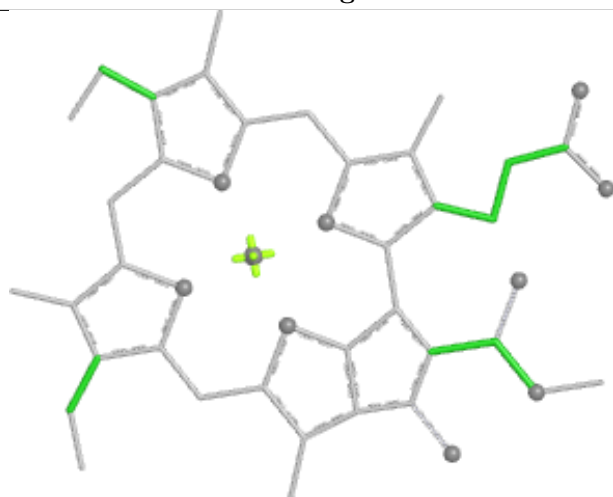
Ligand CLA k 503



Bond lengths



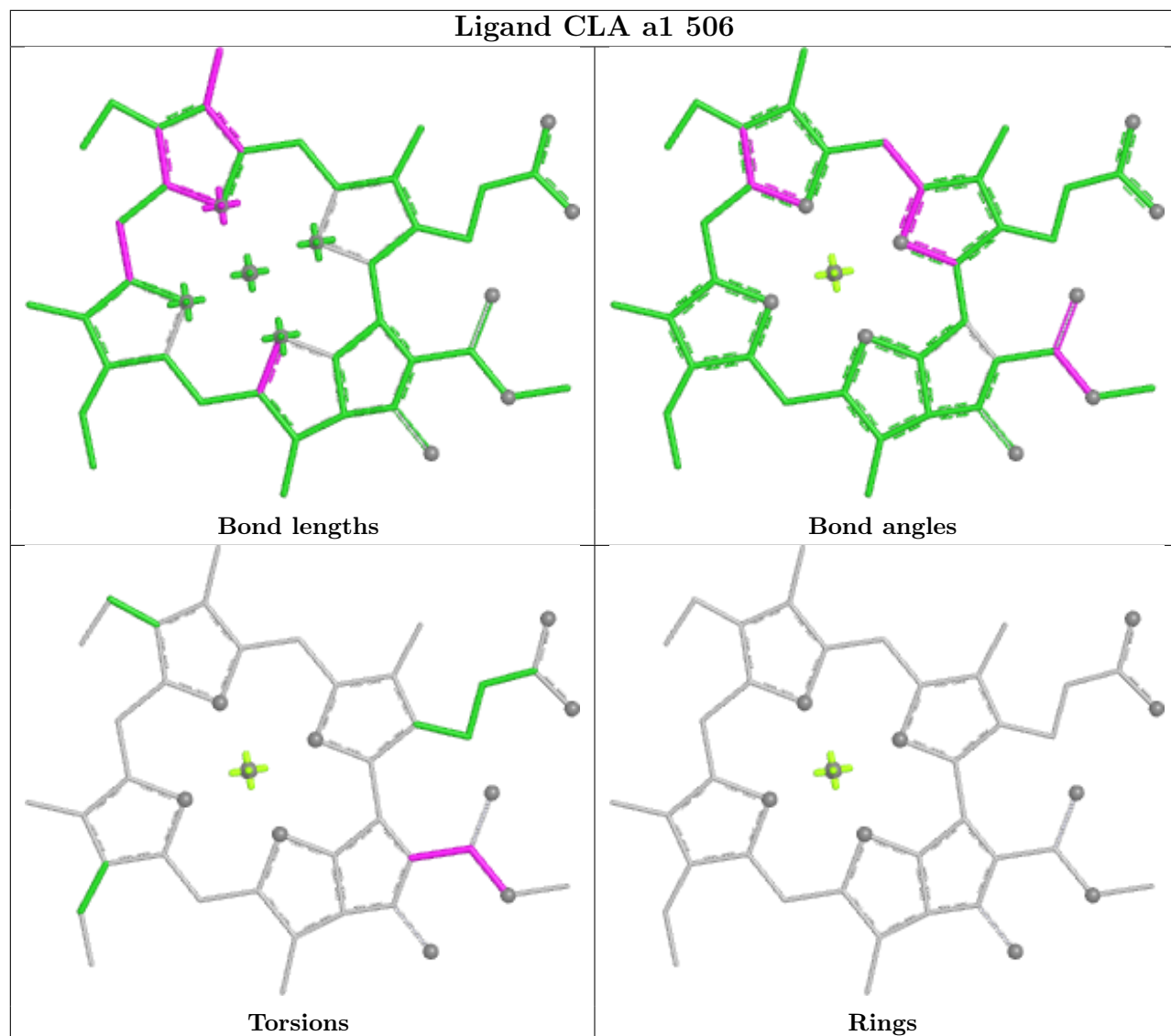
Bond angles



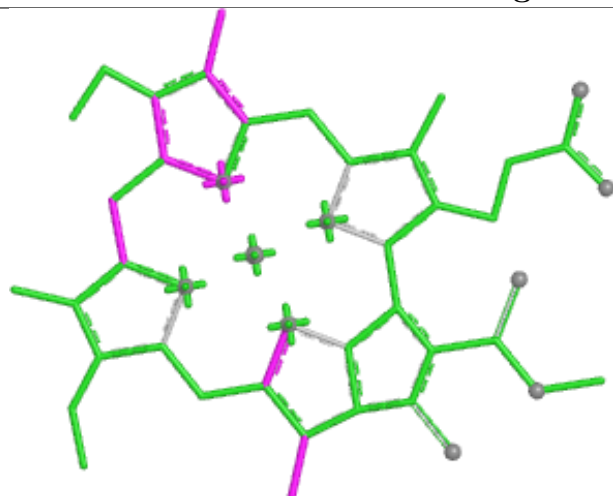
Torsions



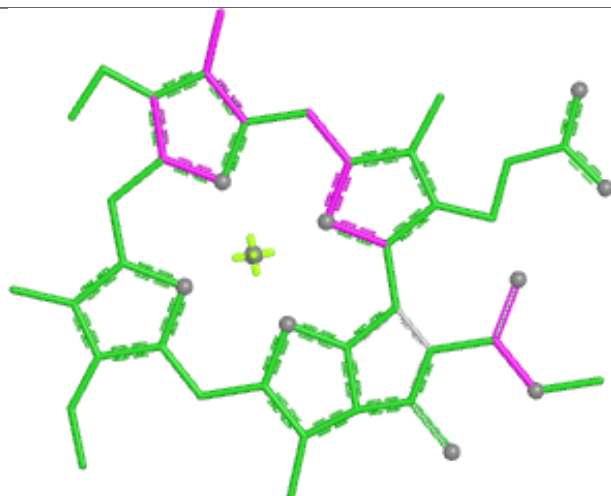
Rings



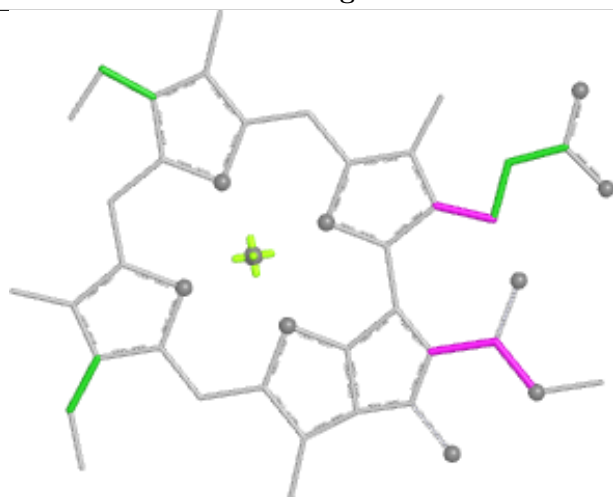
Ligand CLA U 512



Bond lengths



Bond angles

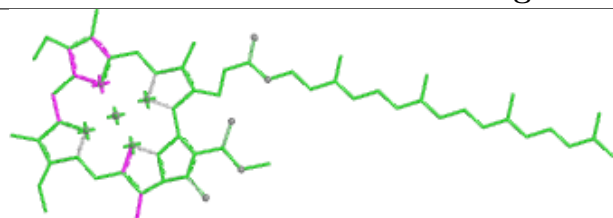


Torsions

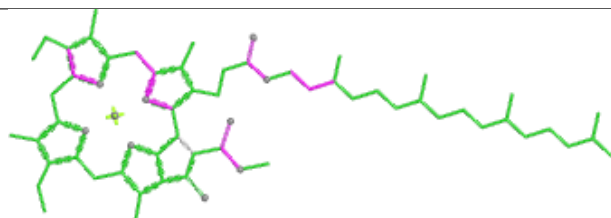


Rings

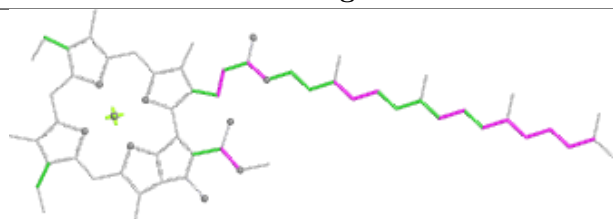
Ligand CLA Y 505



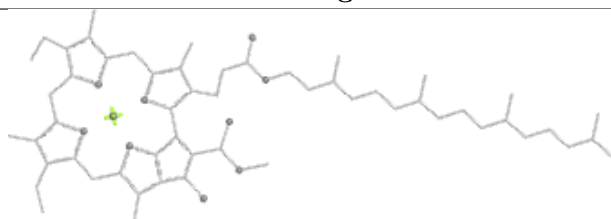
Bond lengths



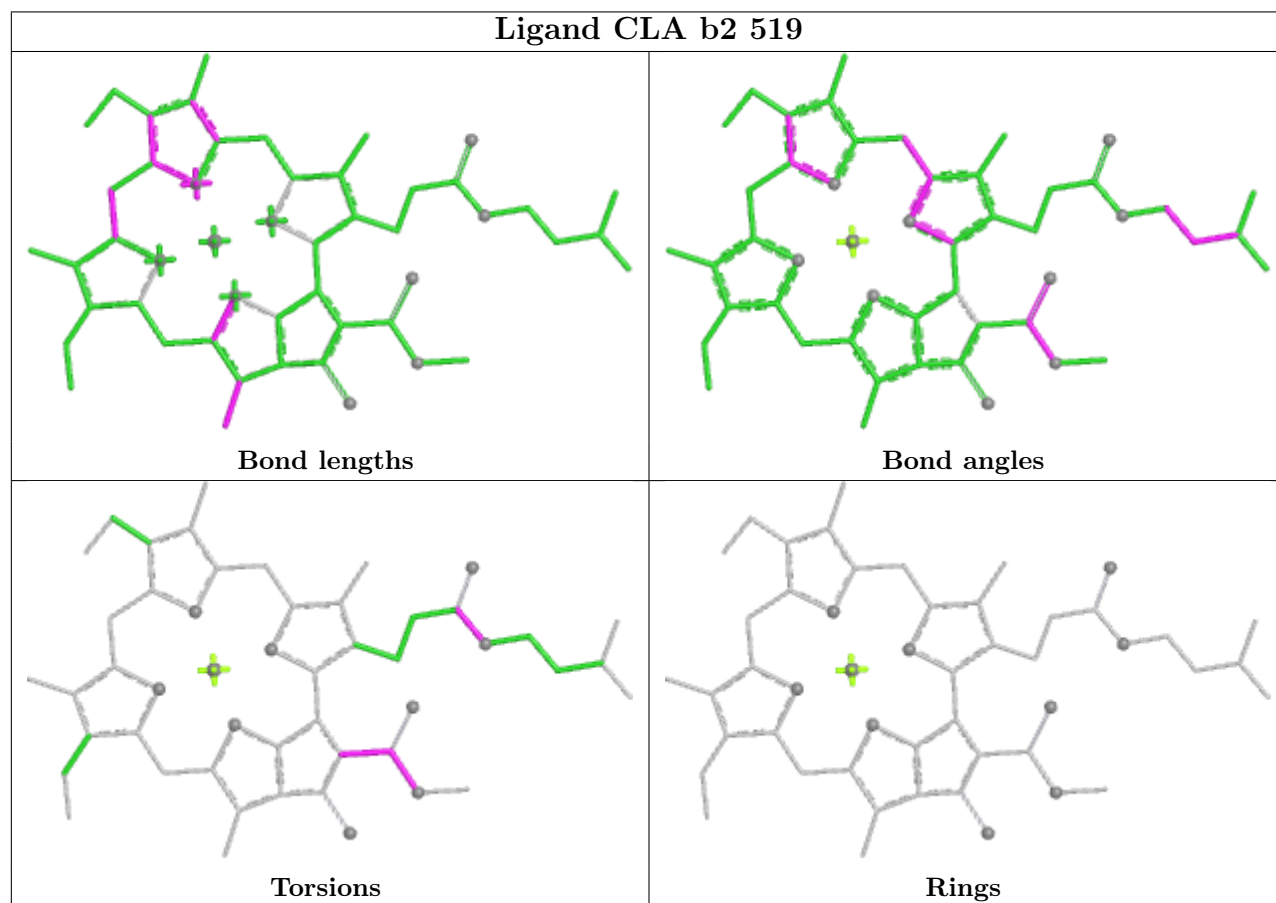
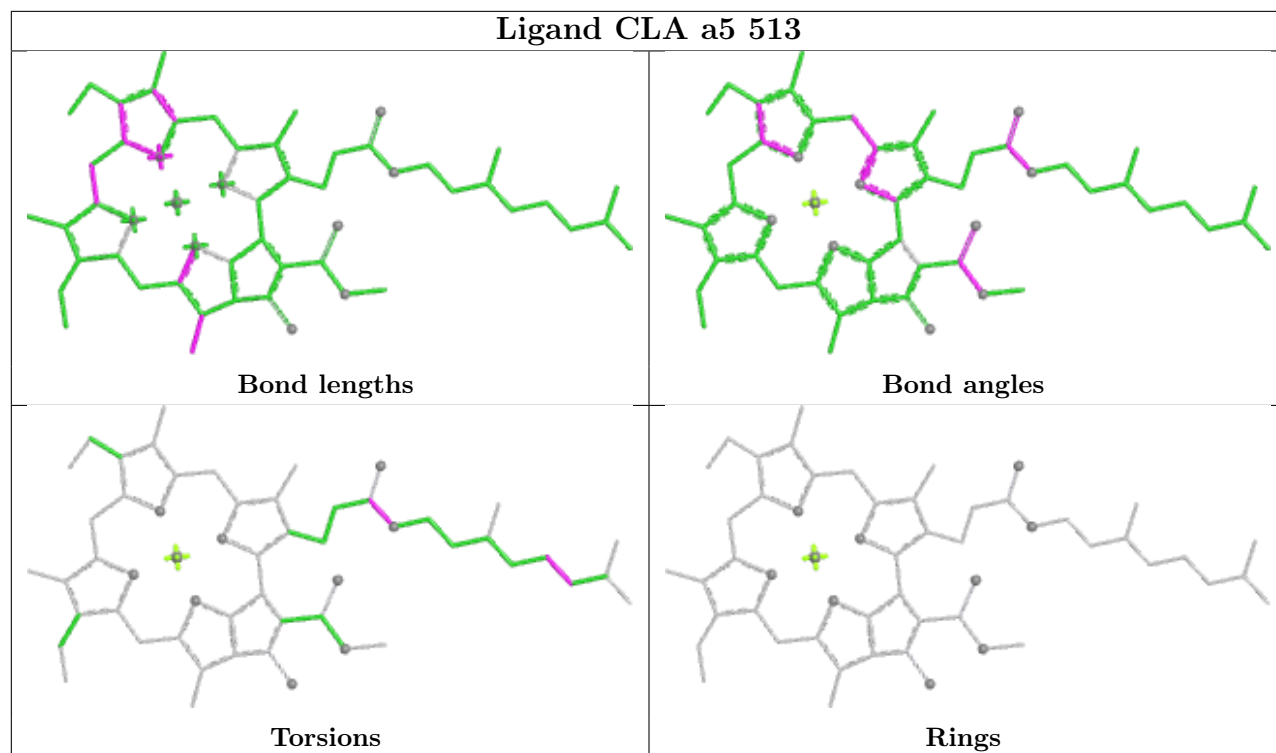
Bond angles

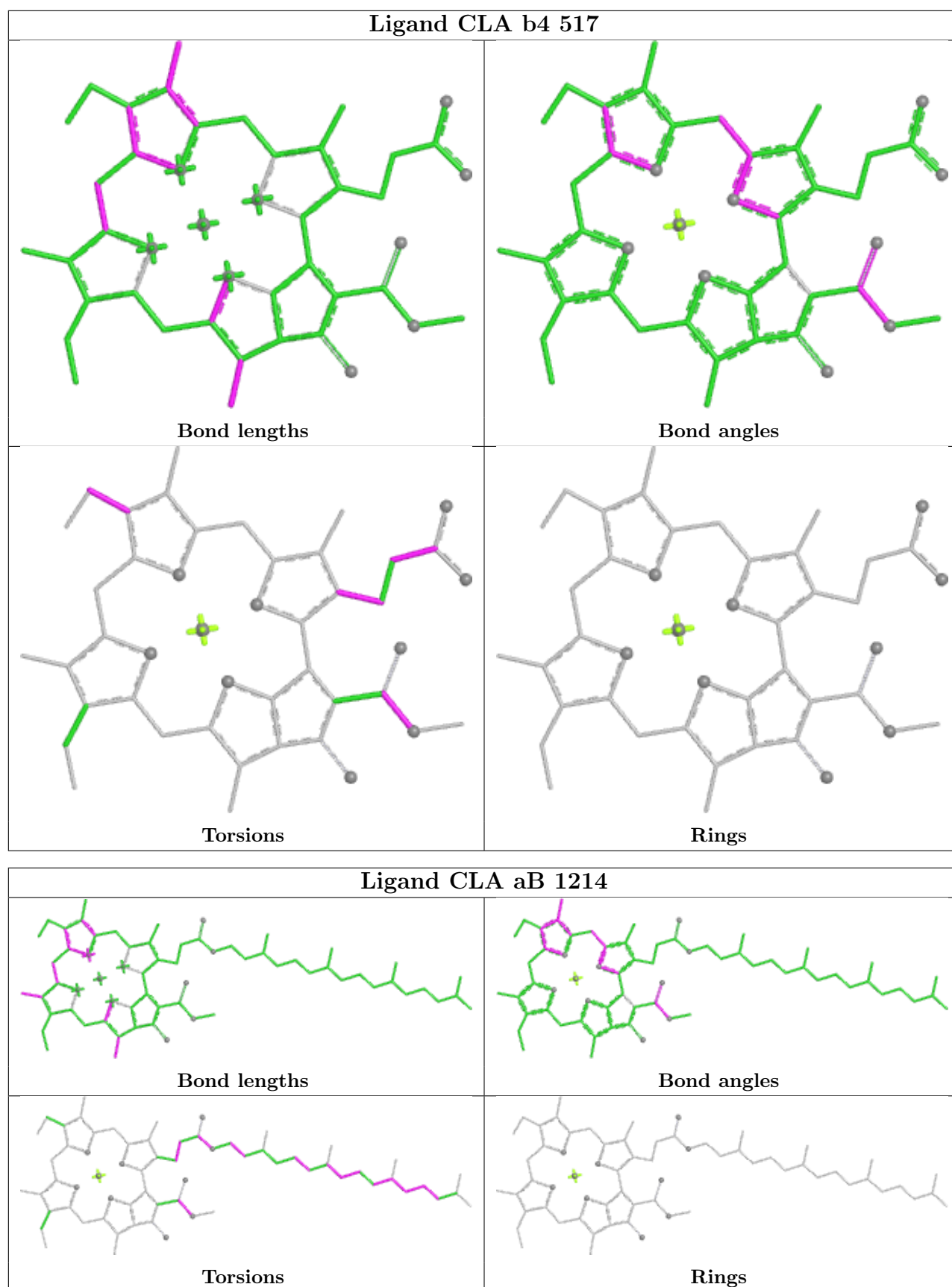


Torsions

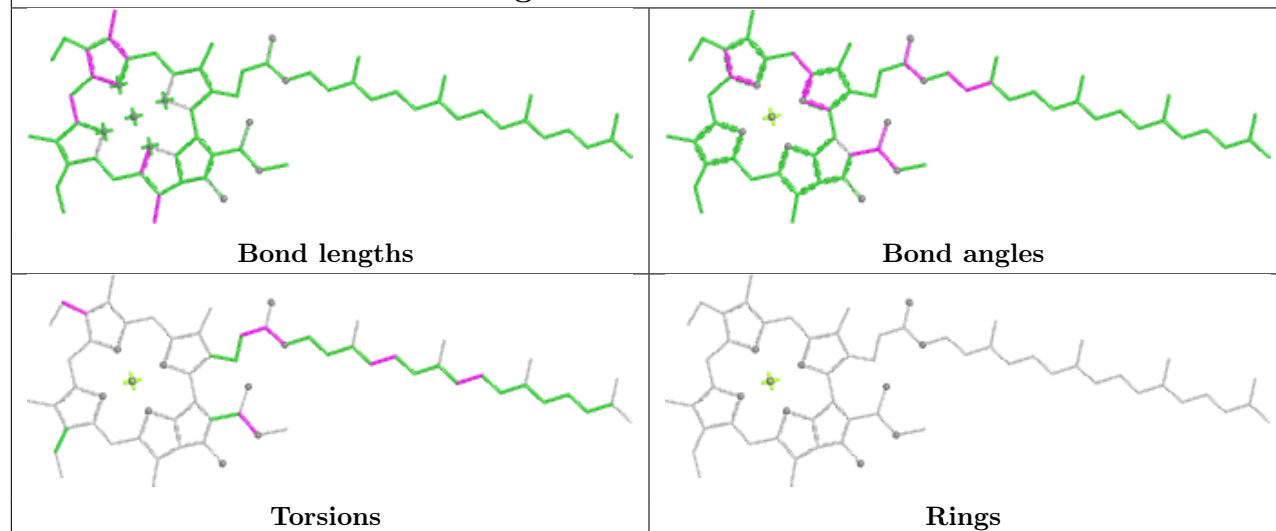


Rings

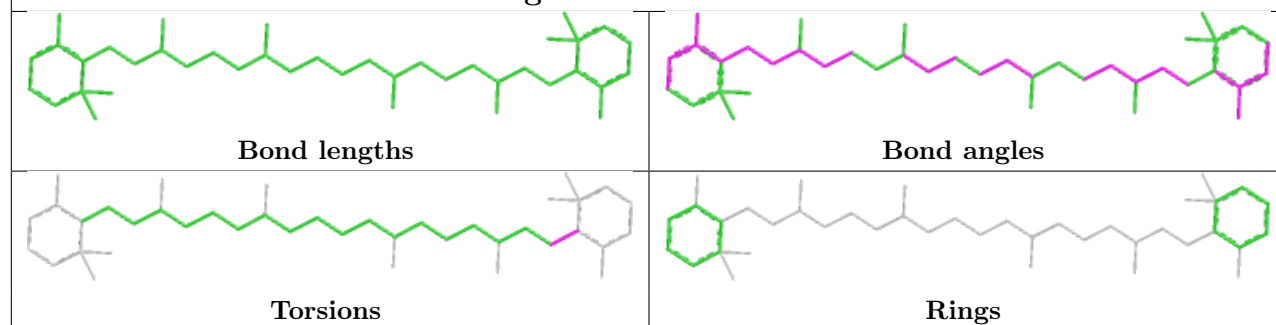




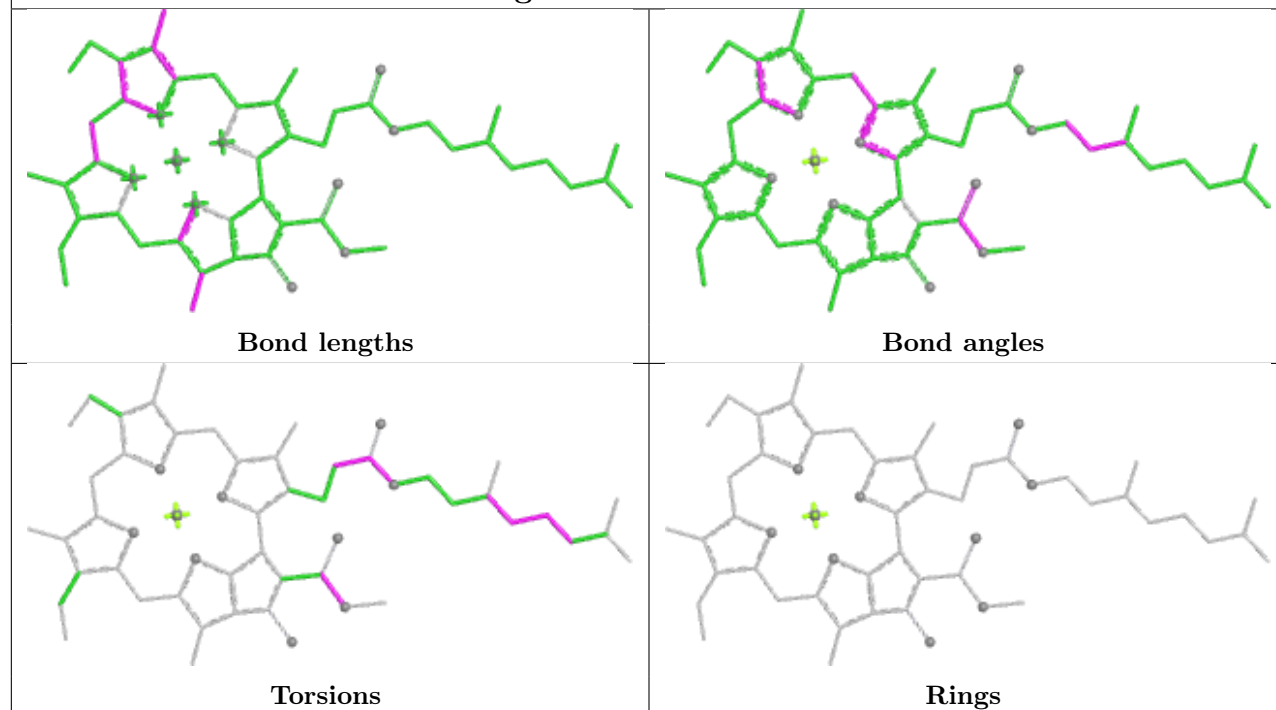
Ligand CLA cA 1011

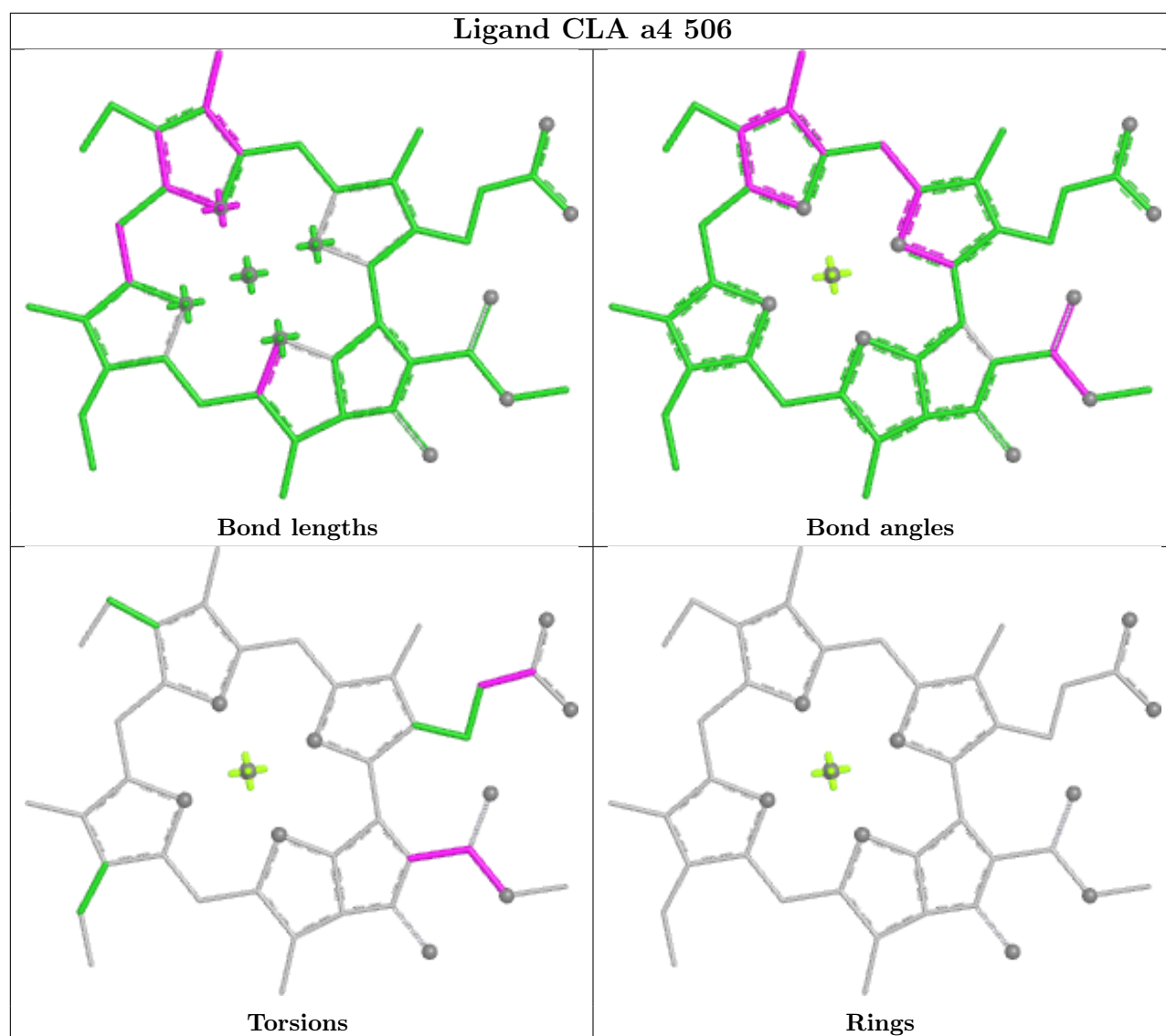


Ligand BCR b3 523

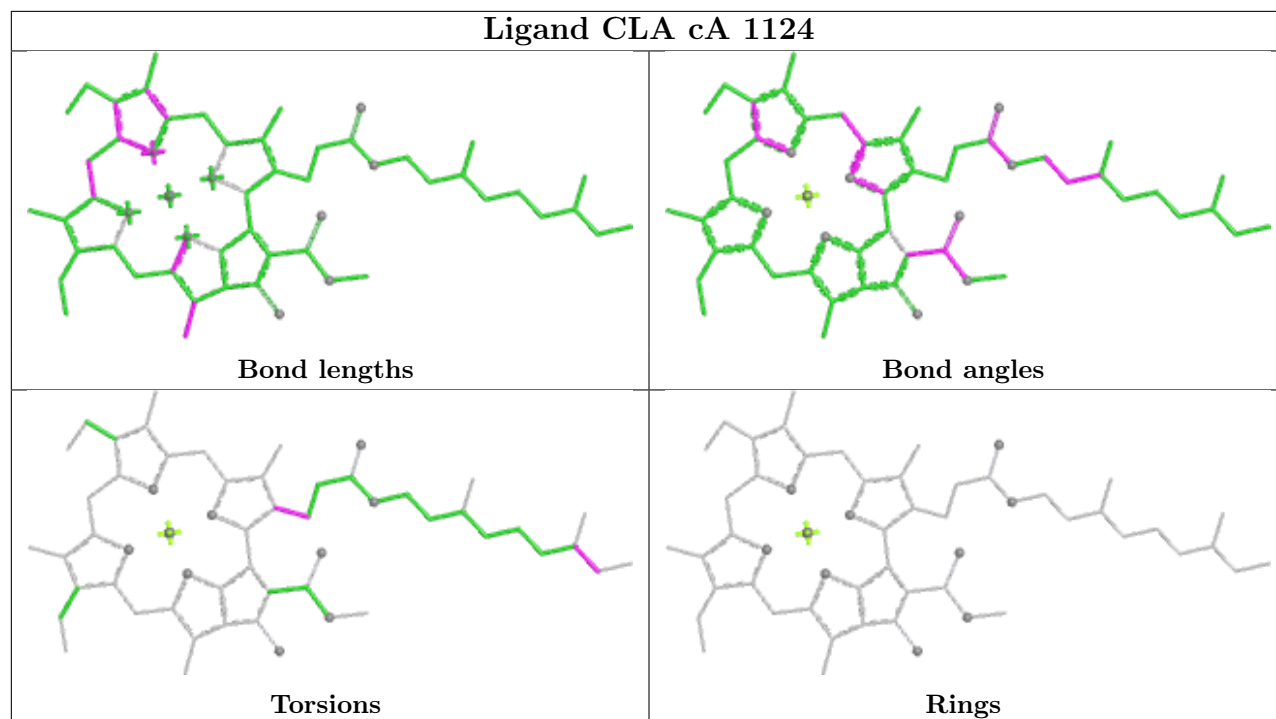


Ligand CLA cA 1137

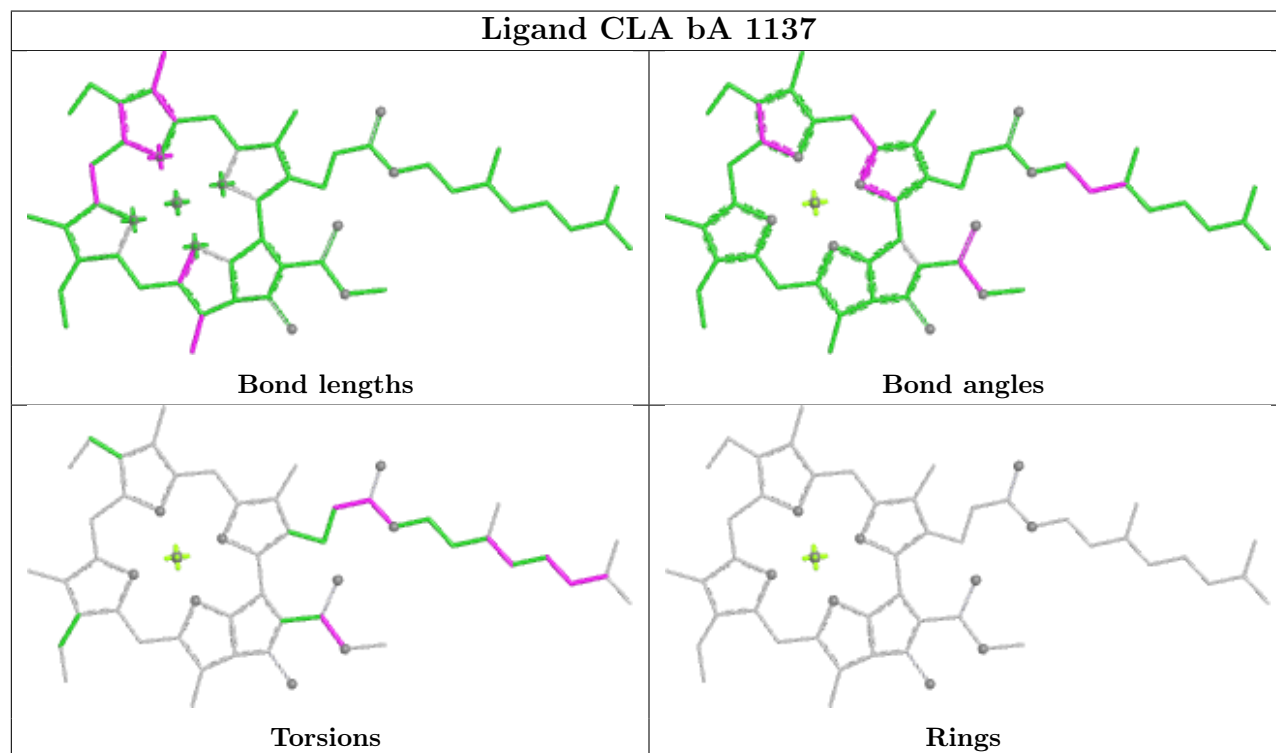


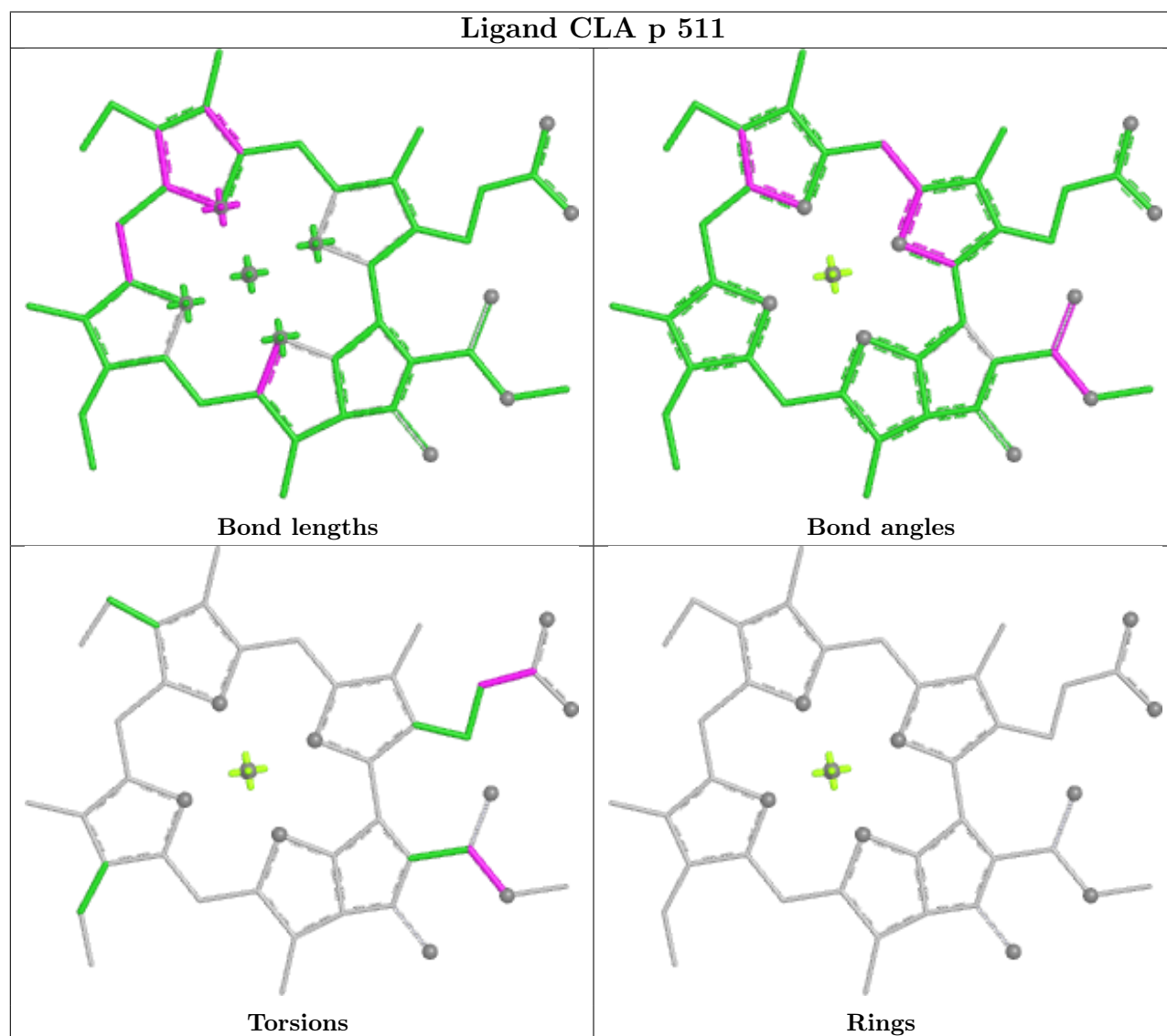
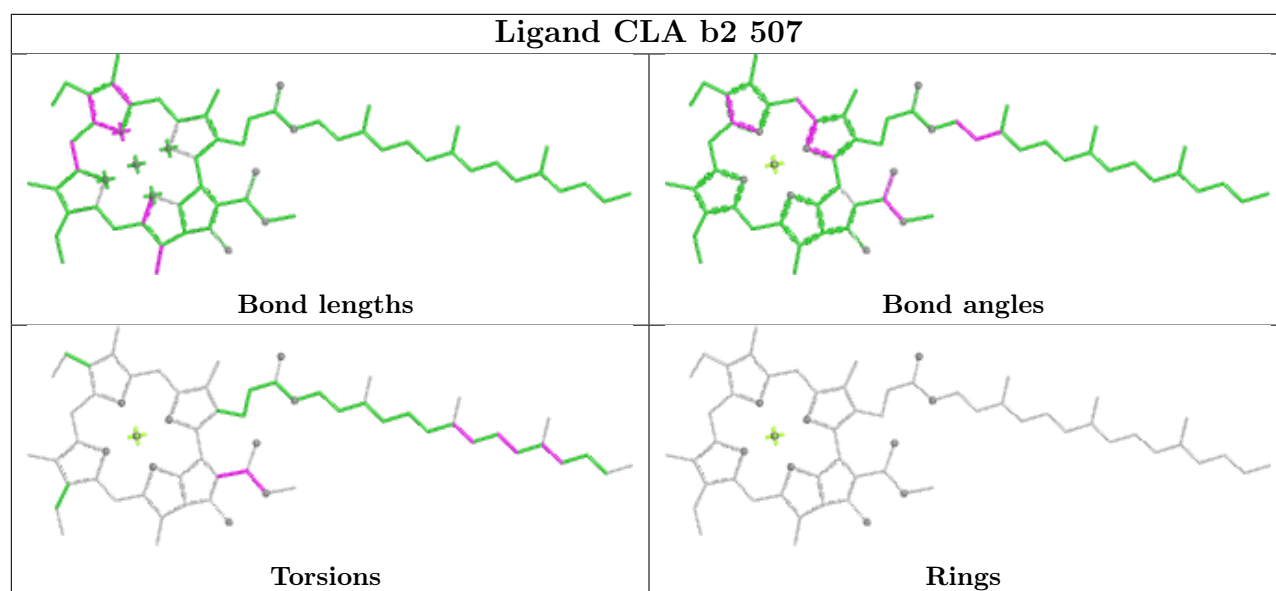


Ligand CLA cA 1124

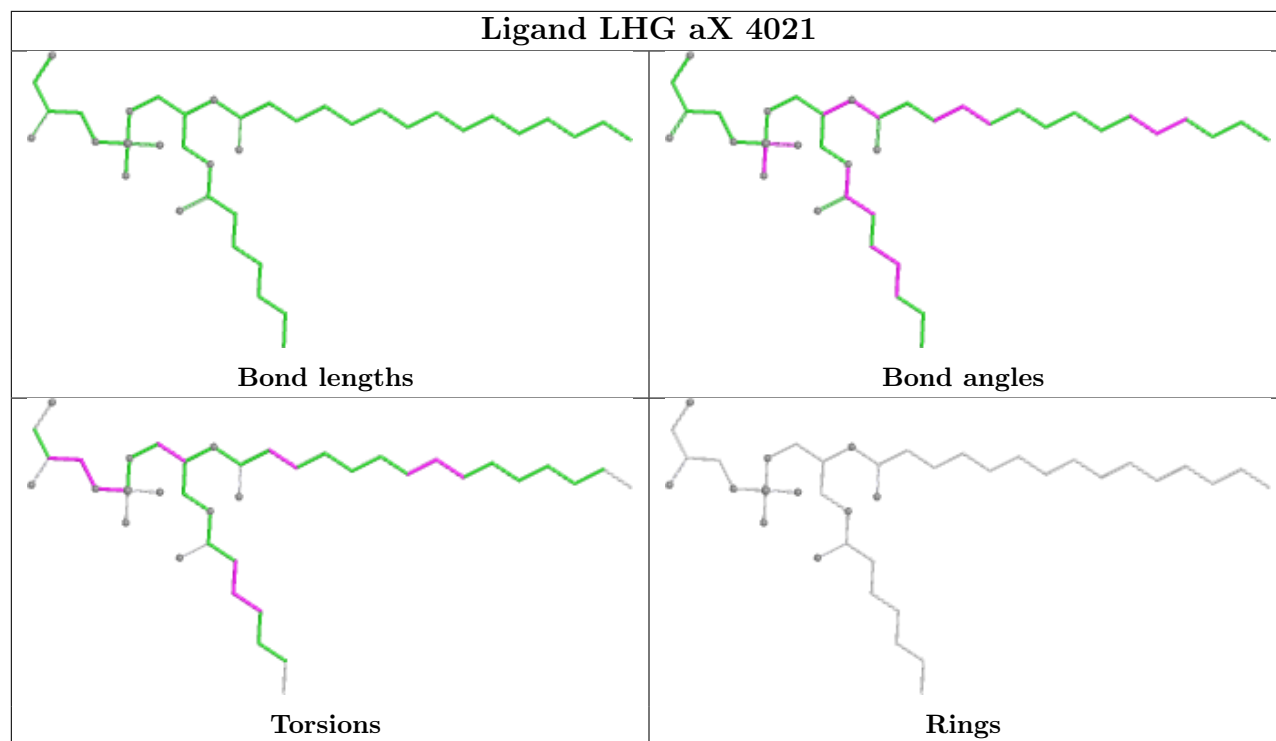


Ligand CLA bA 1137

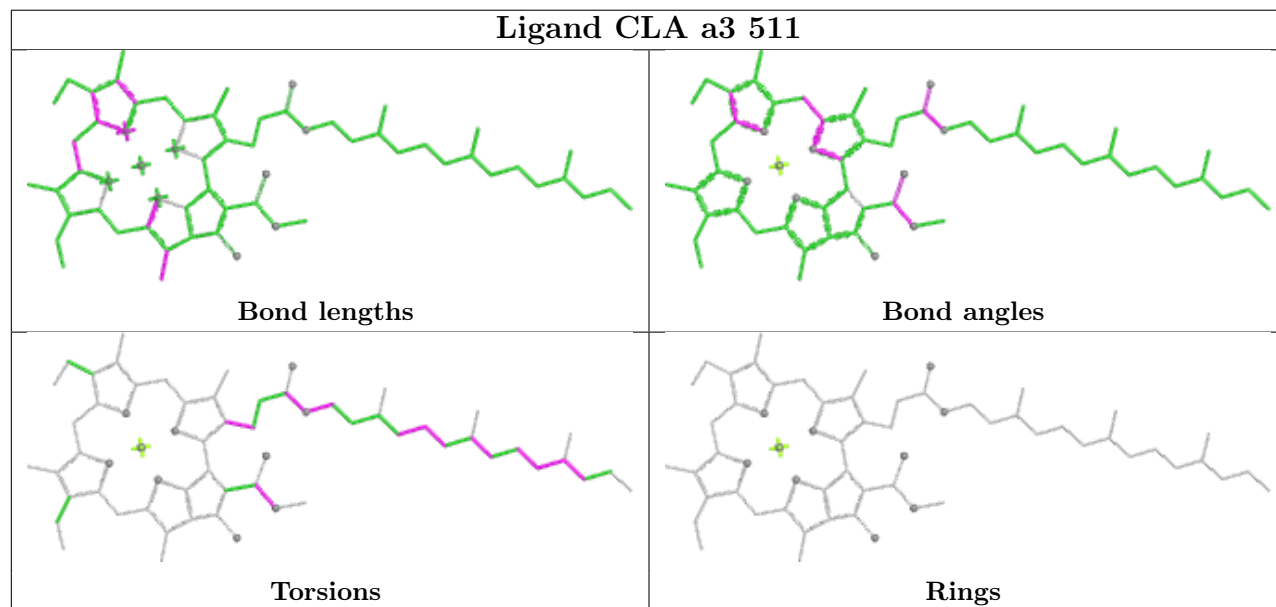




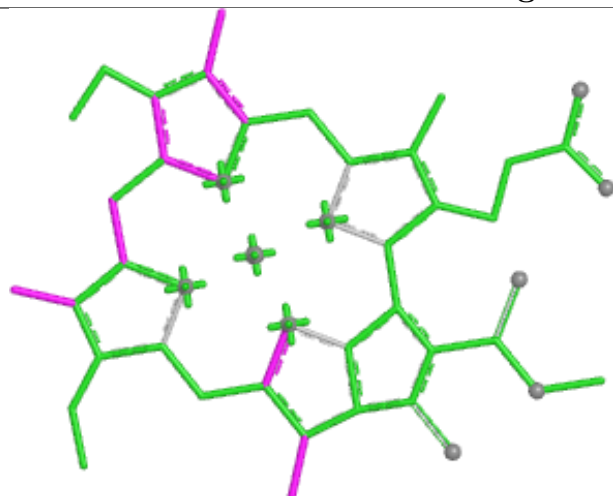
Ligand LHG aX 4021



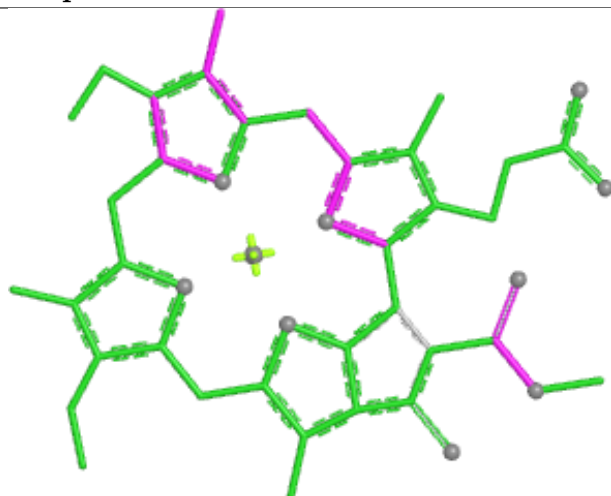
Ligand CLA a3 511



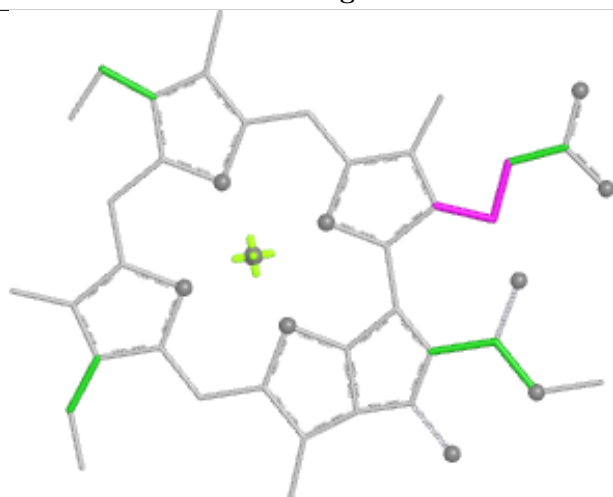
Ligand CLA q 508



Bond lengths



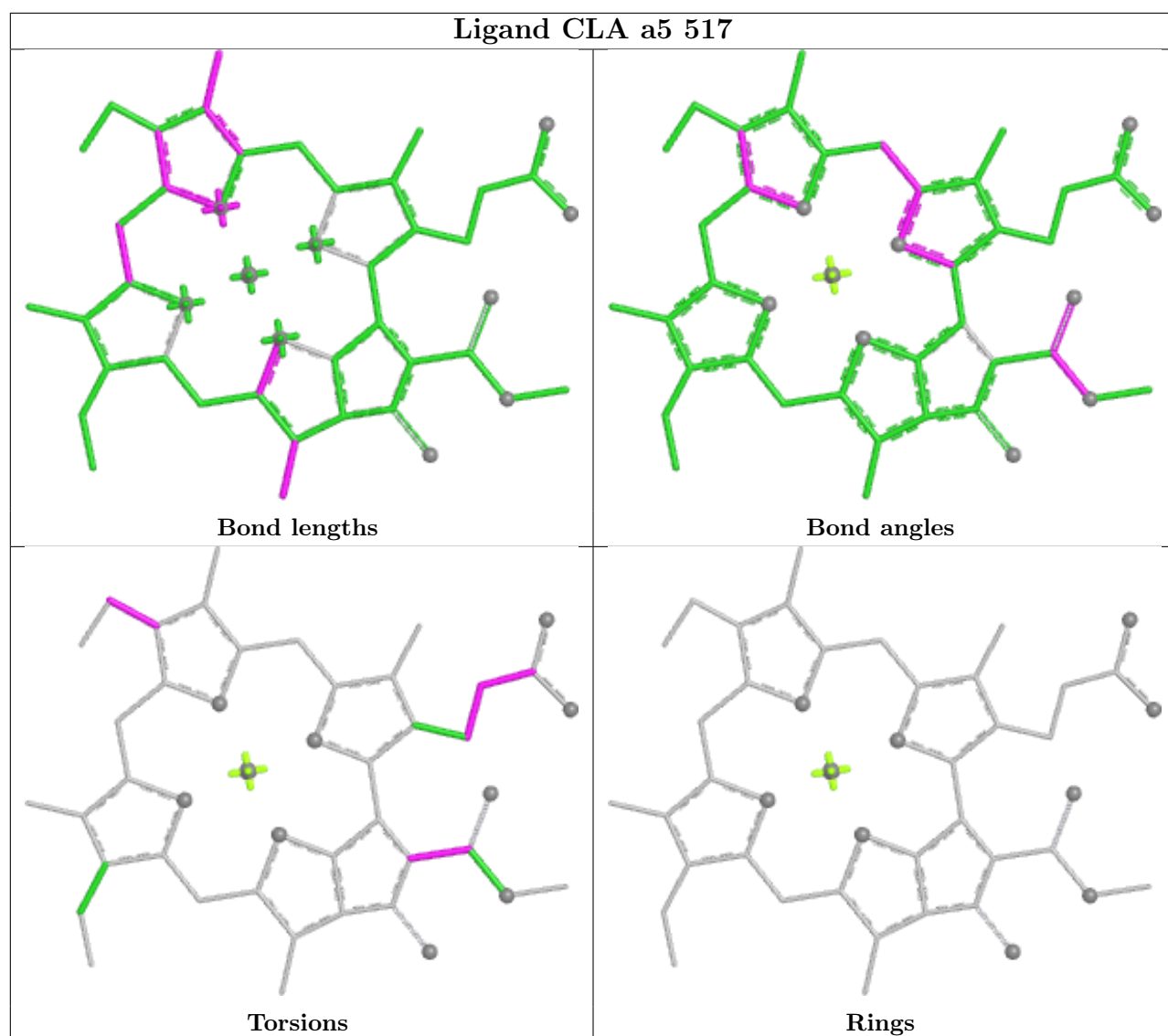
Bond angles



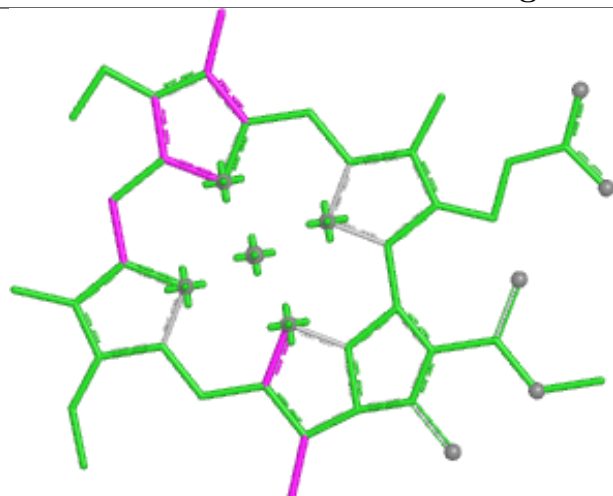
Torsions



Rings



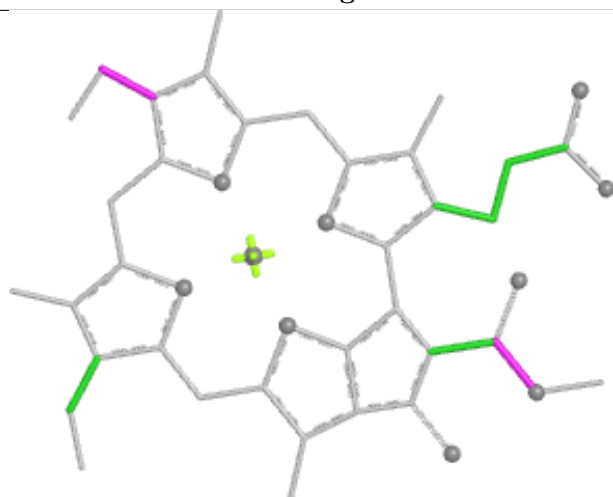
Ligand CLA c 504



Bond lengths



Bond angles

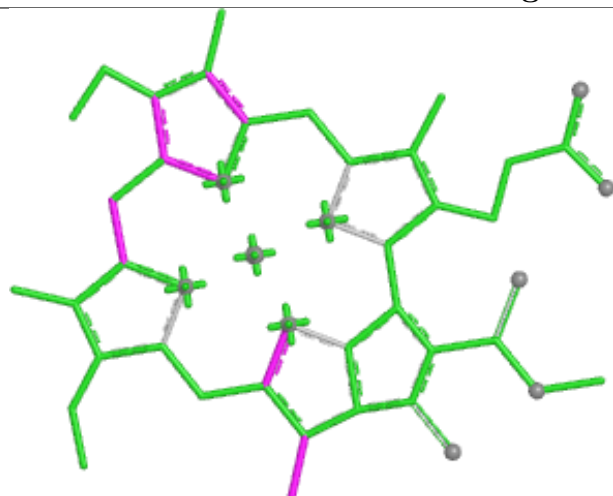


Torsions

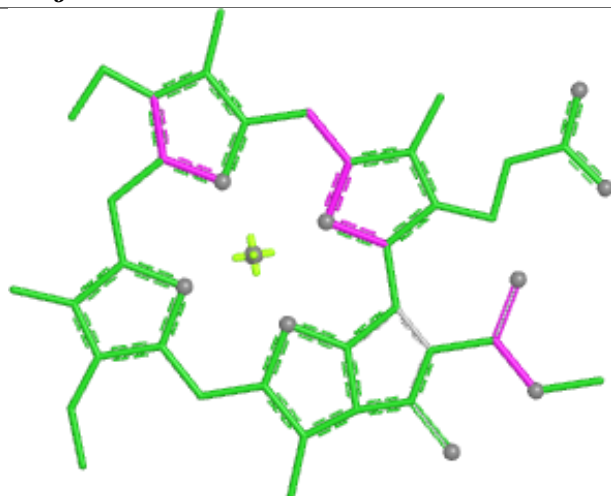


Rings

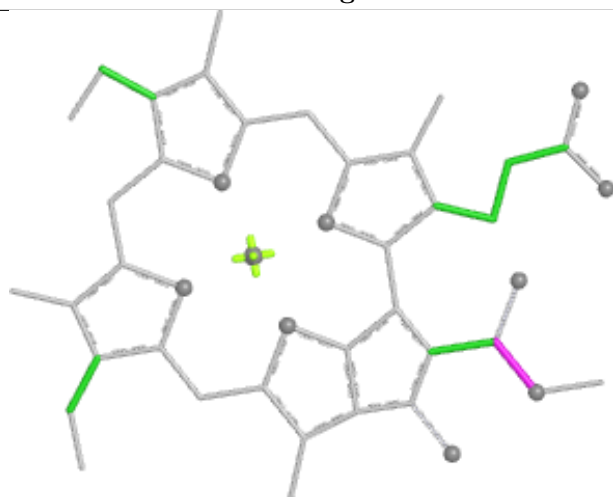
Ligand CLA j 503



Bond lengths



Bond angles

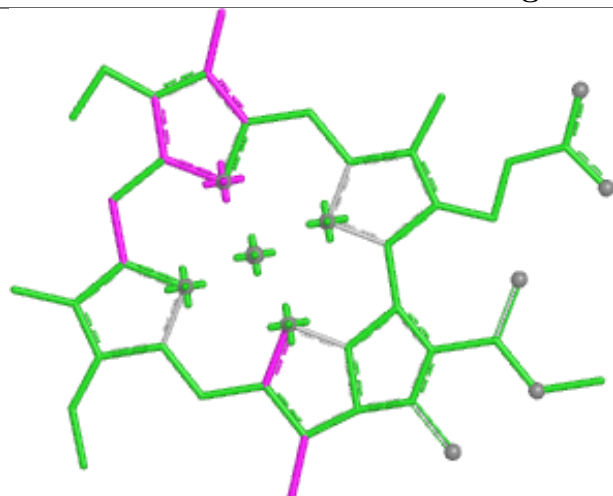


Torsions



Rings

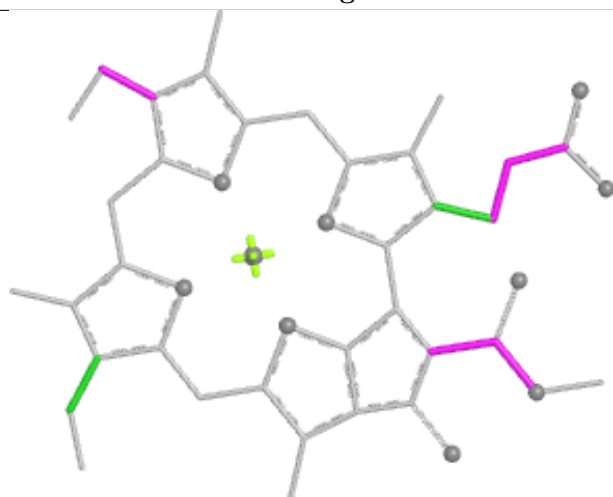
Ligand CLA f 518



Bond lengths



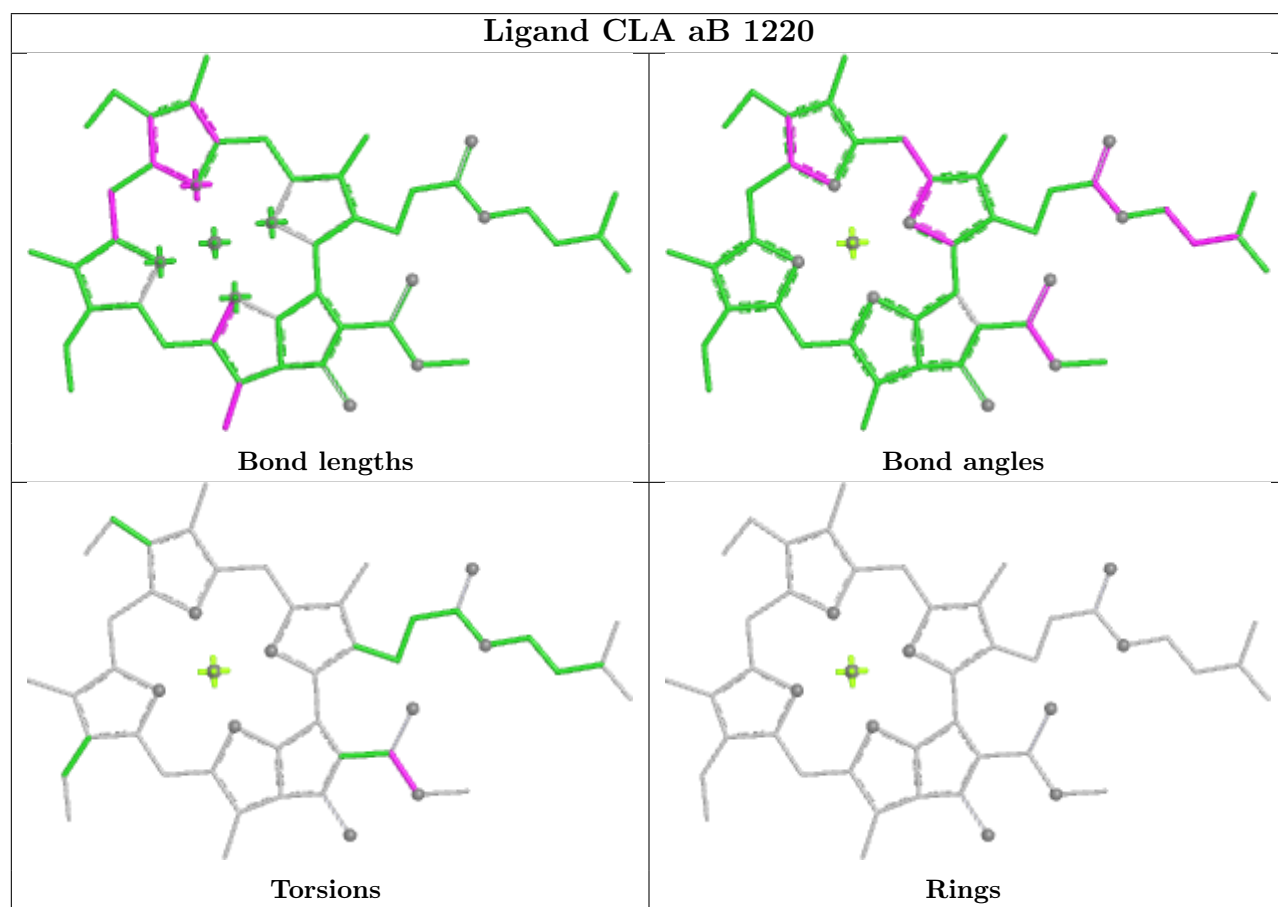
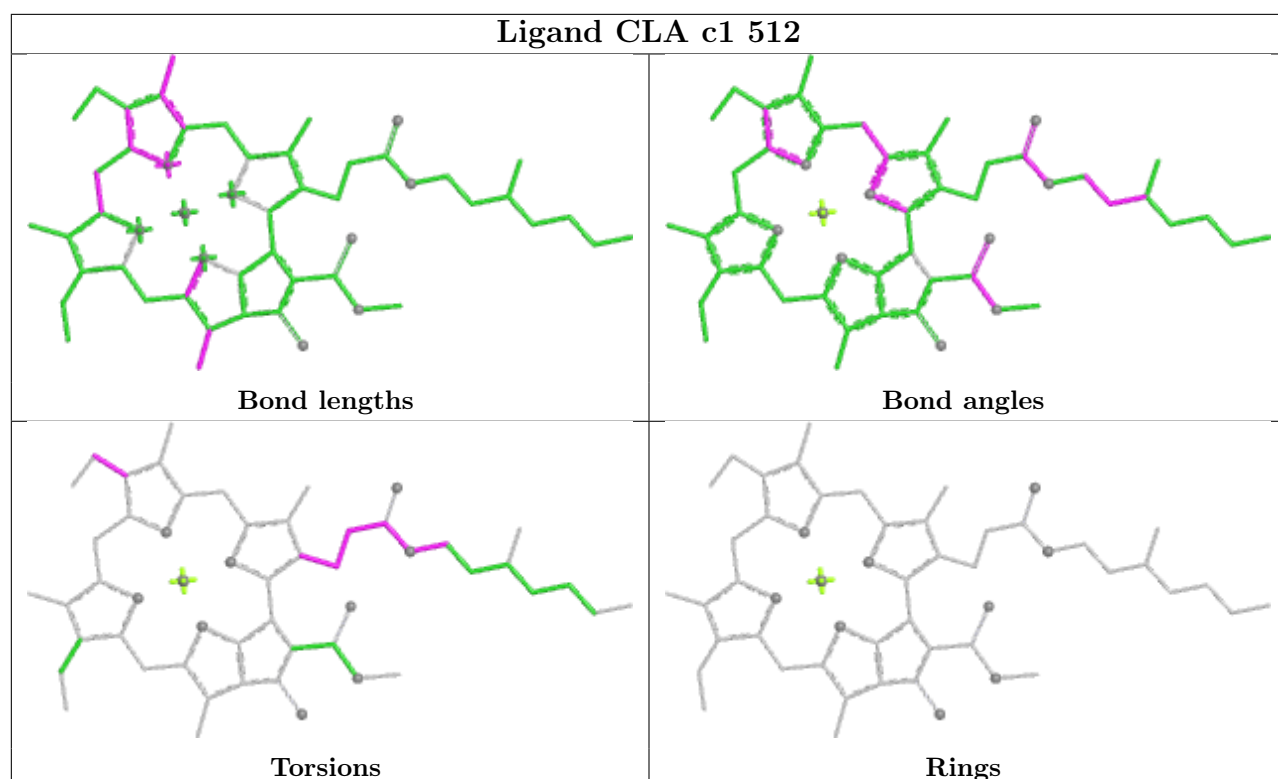
Bond angles

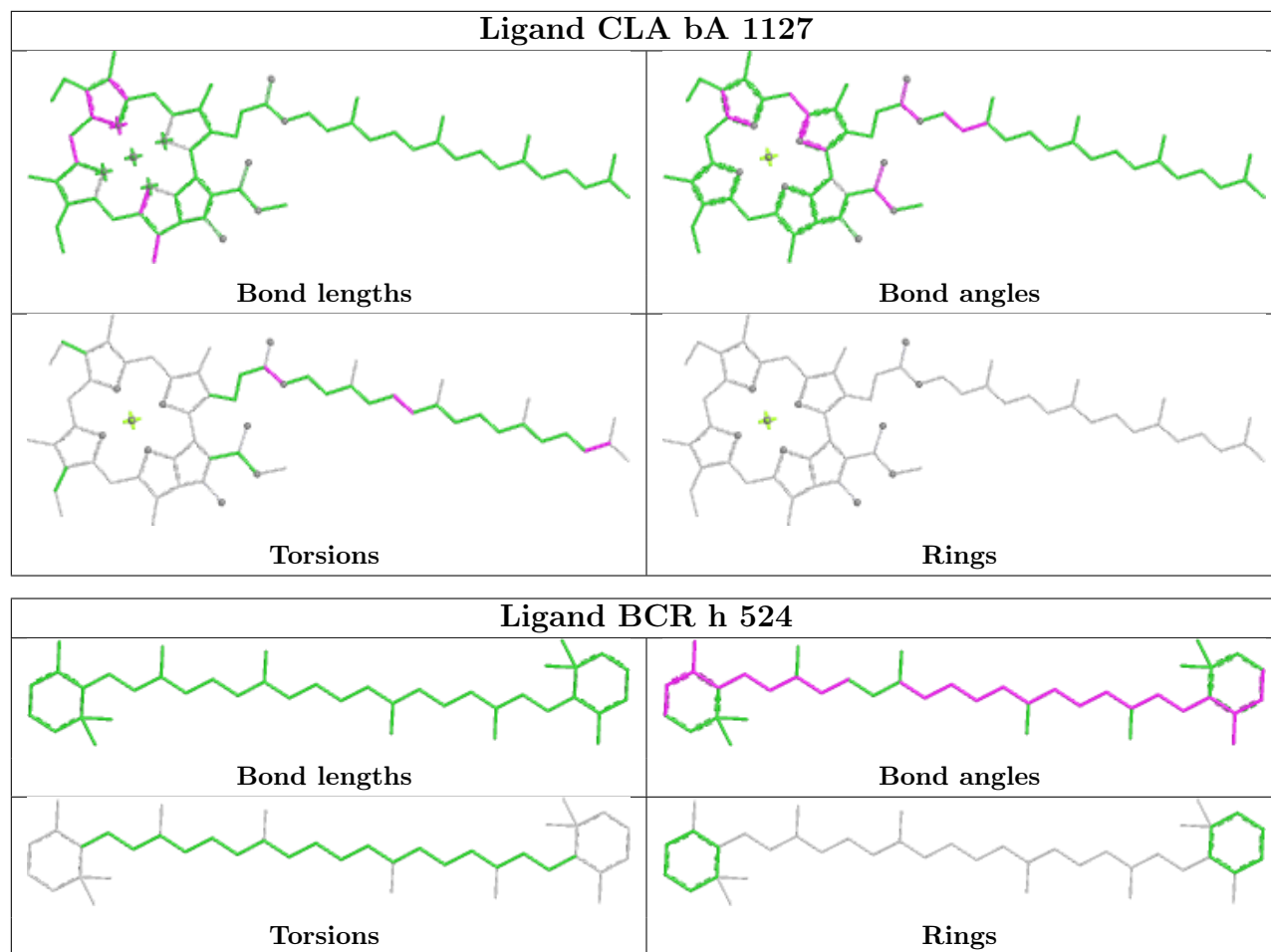


Torsions

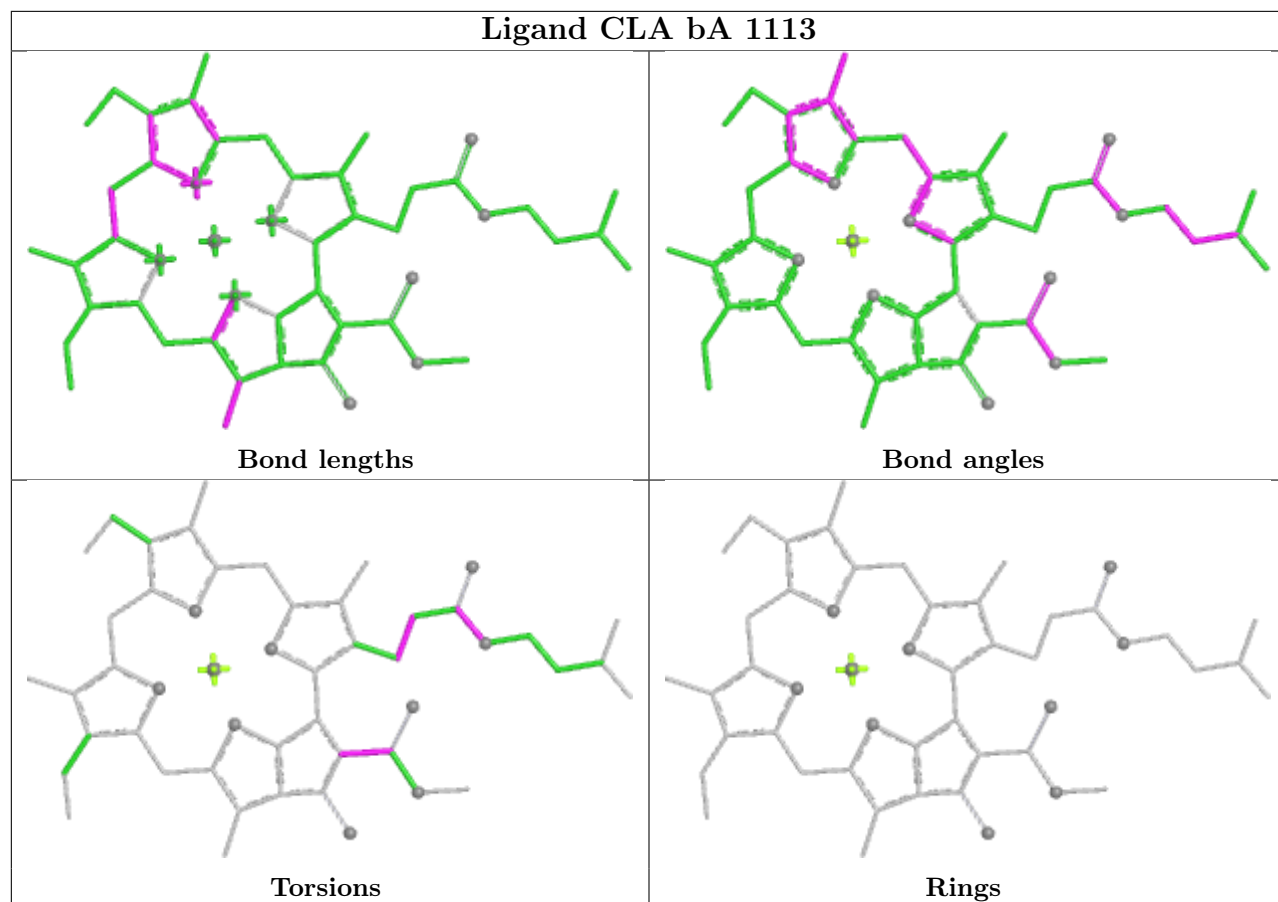


Rings

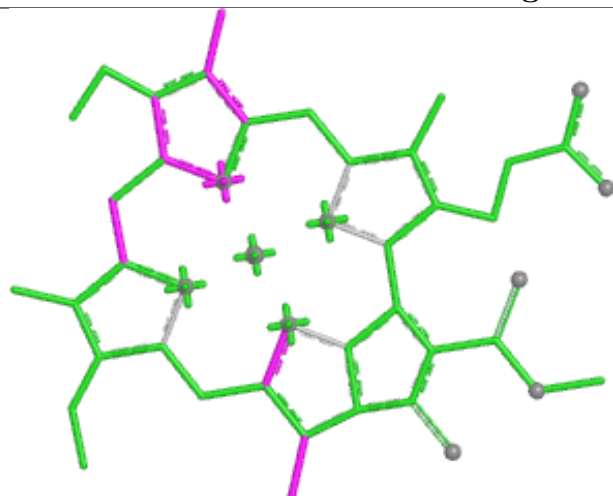




Ligand CLA bA 1113



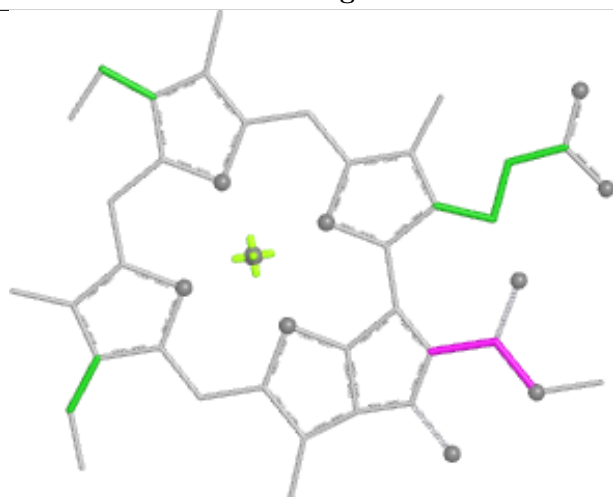
Ligand CLA f 506



Bond lengths



Bond angles

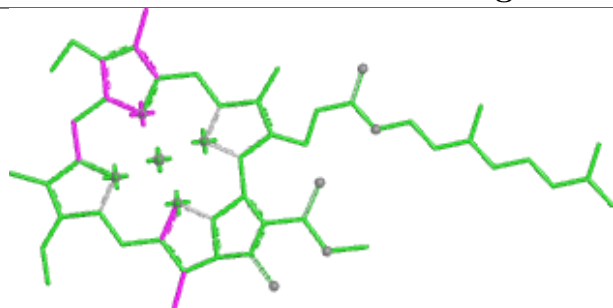


Torsions

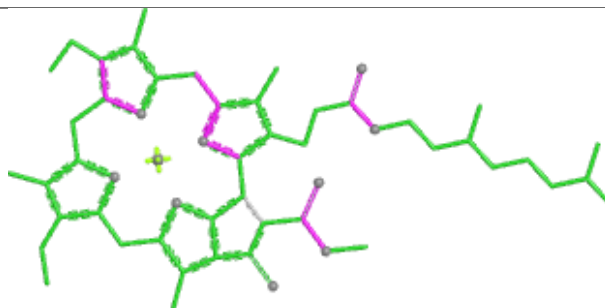


Rings

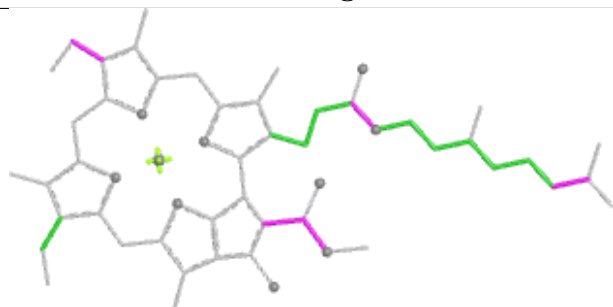
Ligand CLA aK 1401



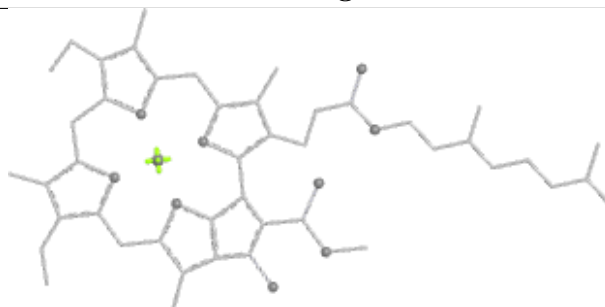
Bond lengths



Bond angles

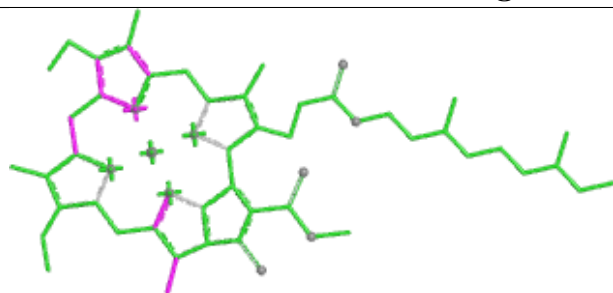


Torsions

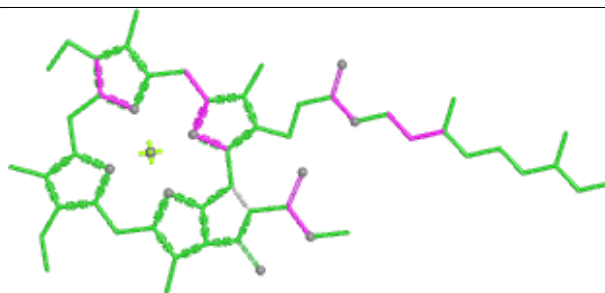


Rings

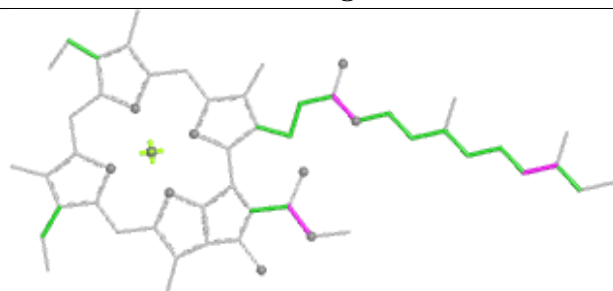
Ligand CLA bB 1228



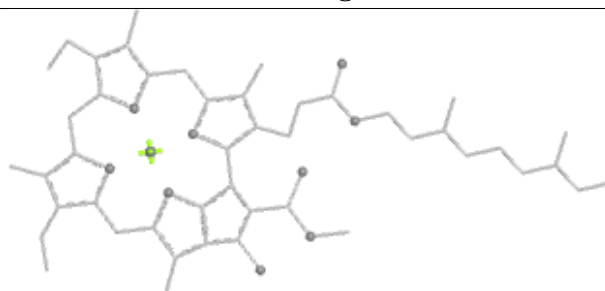
Bond lengths



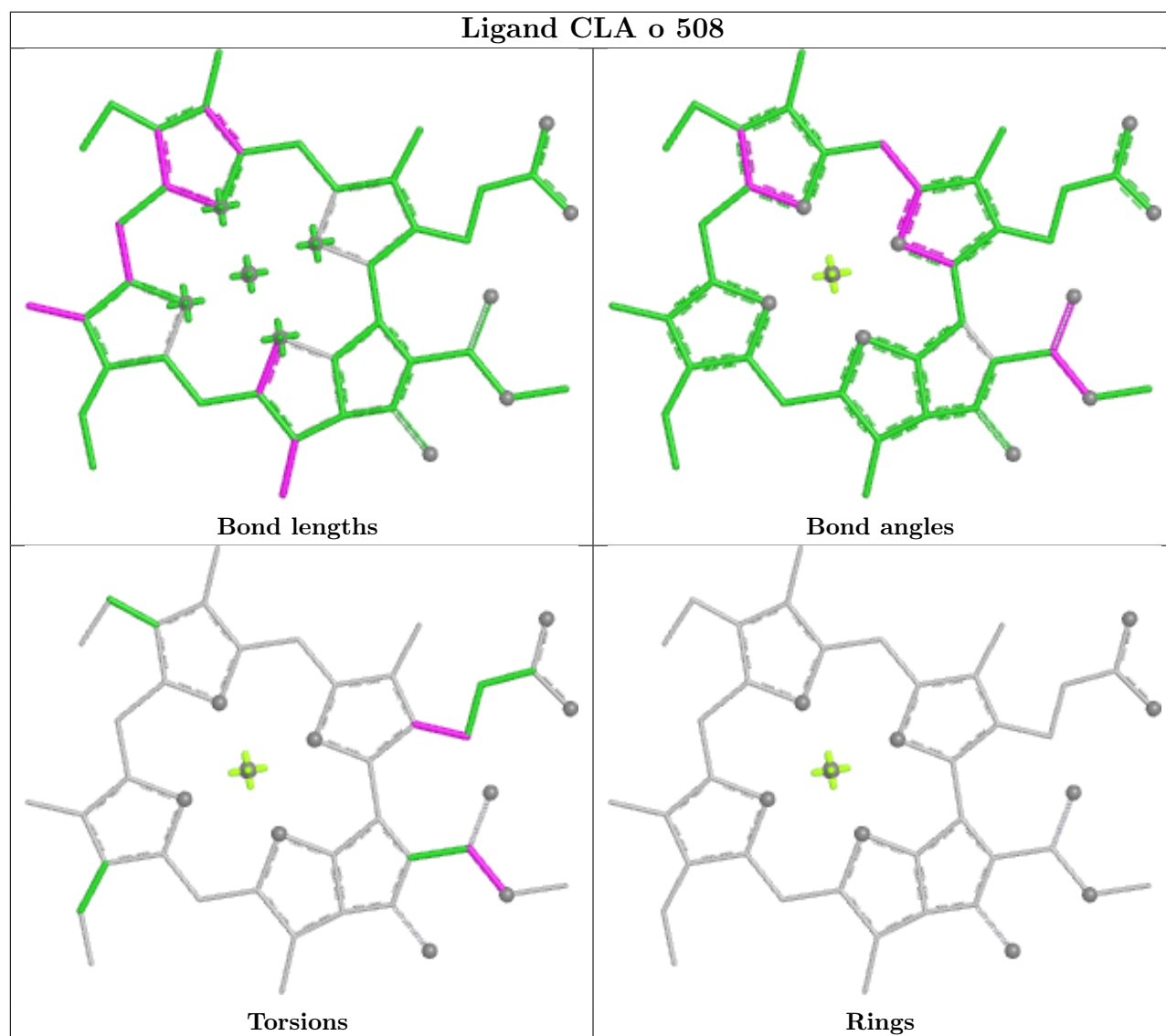
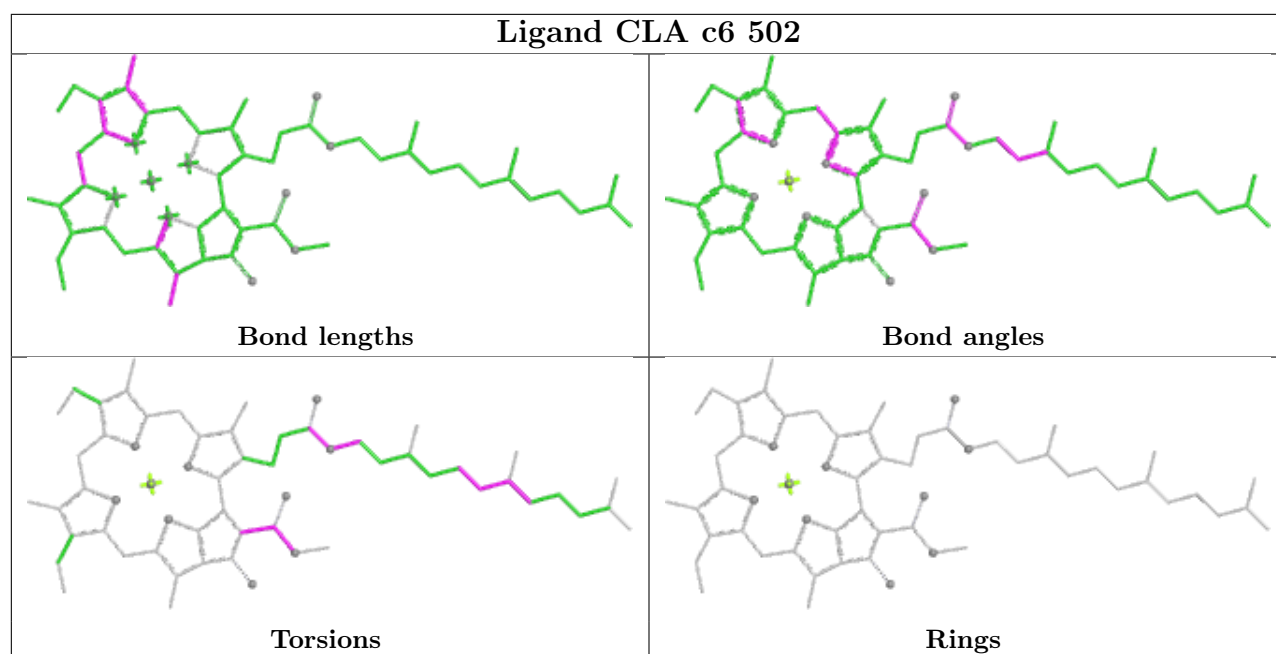
Bond angles



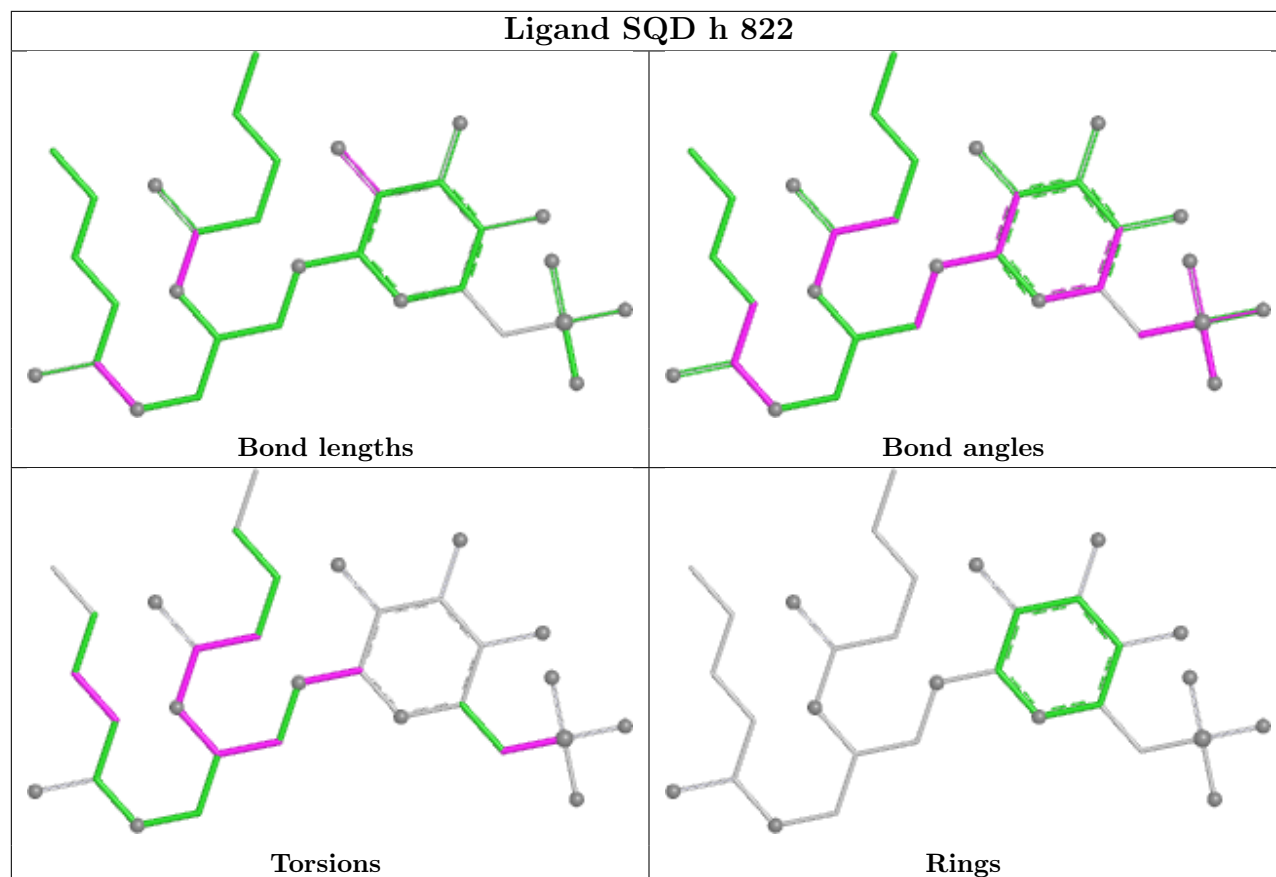
Torsions



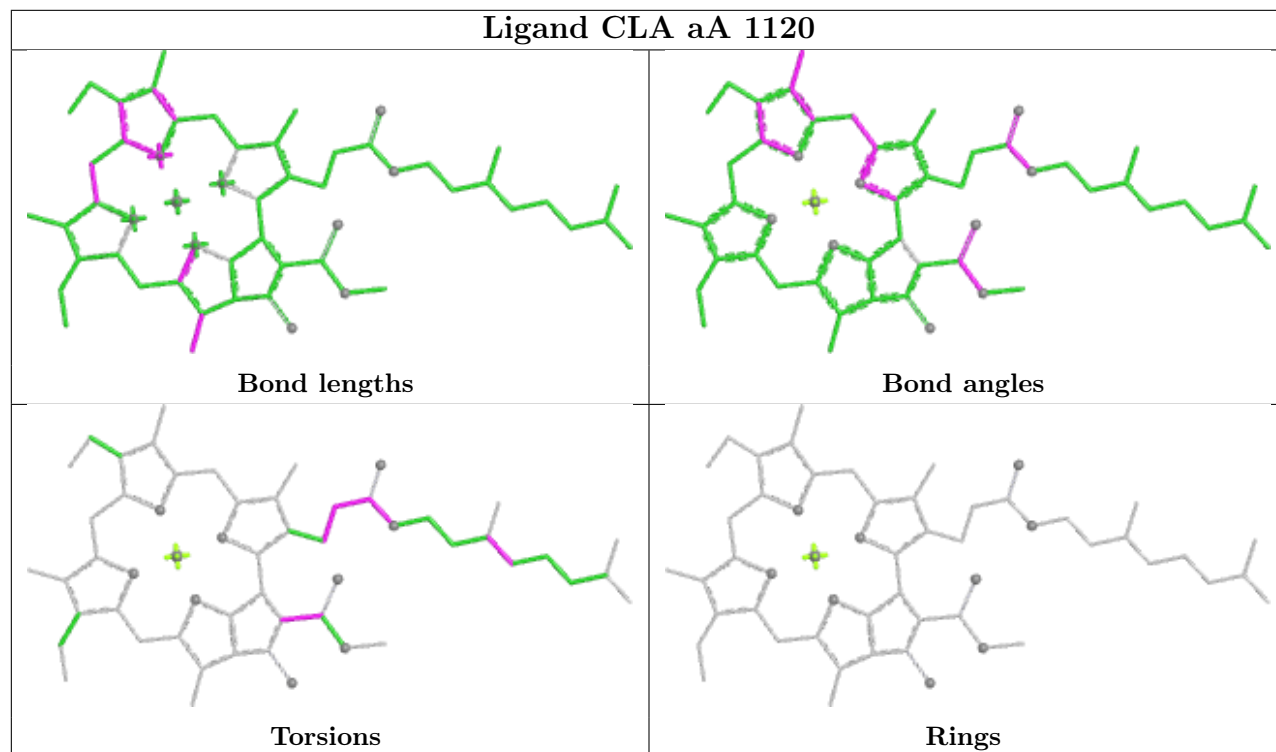
Rings



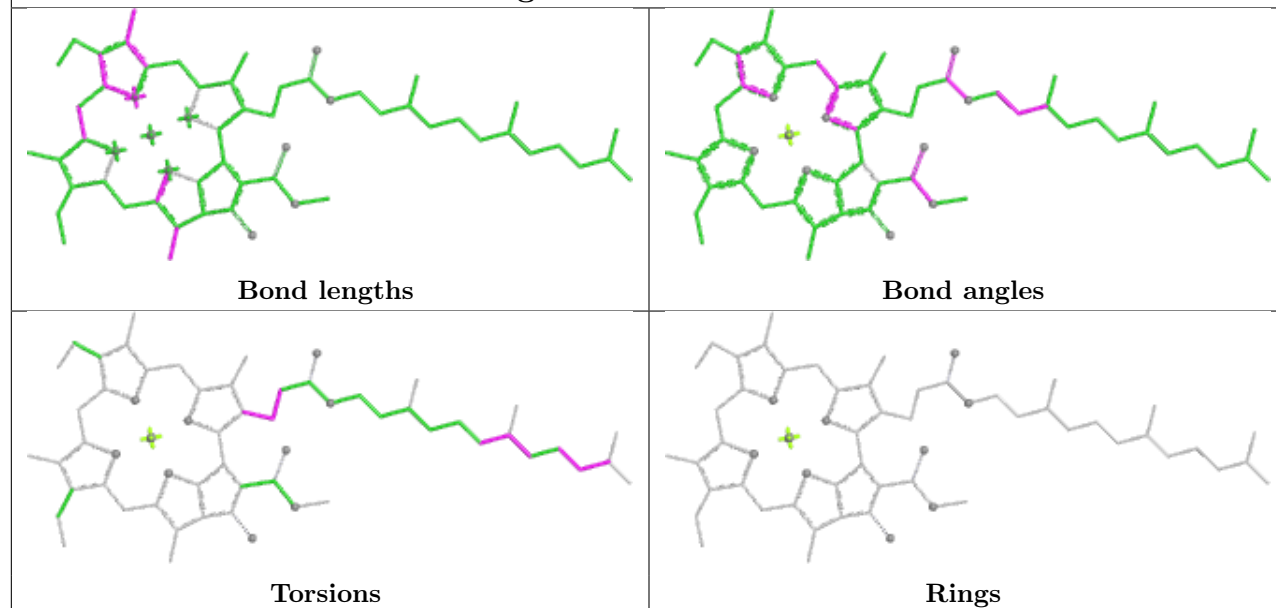
Ligand SQD h 822



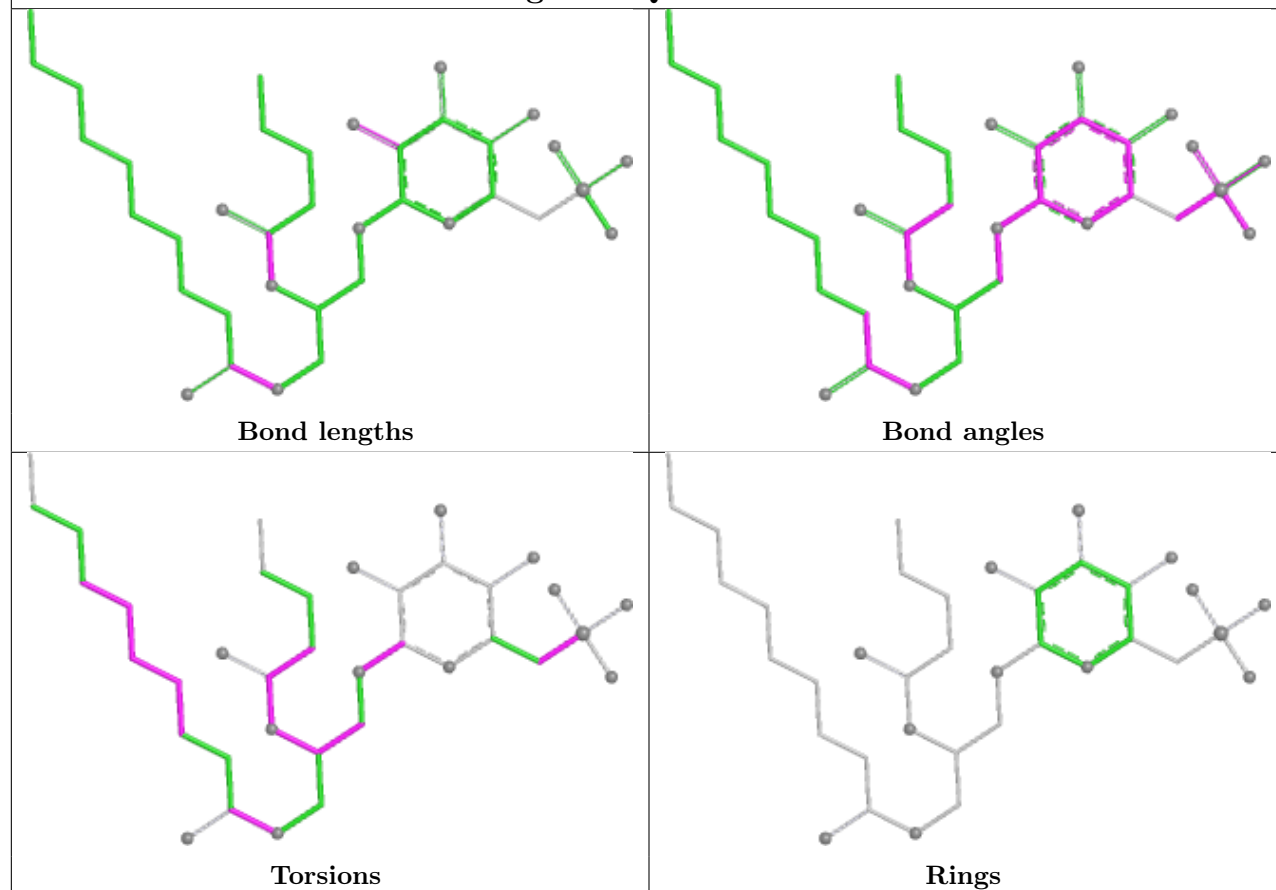
Ligand CLA aA 1120



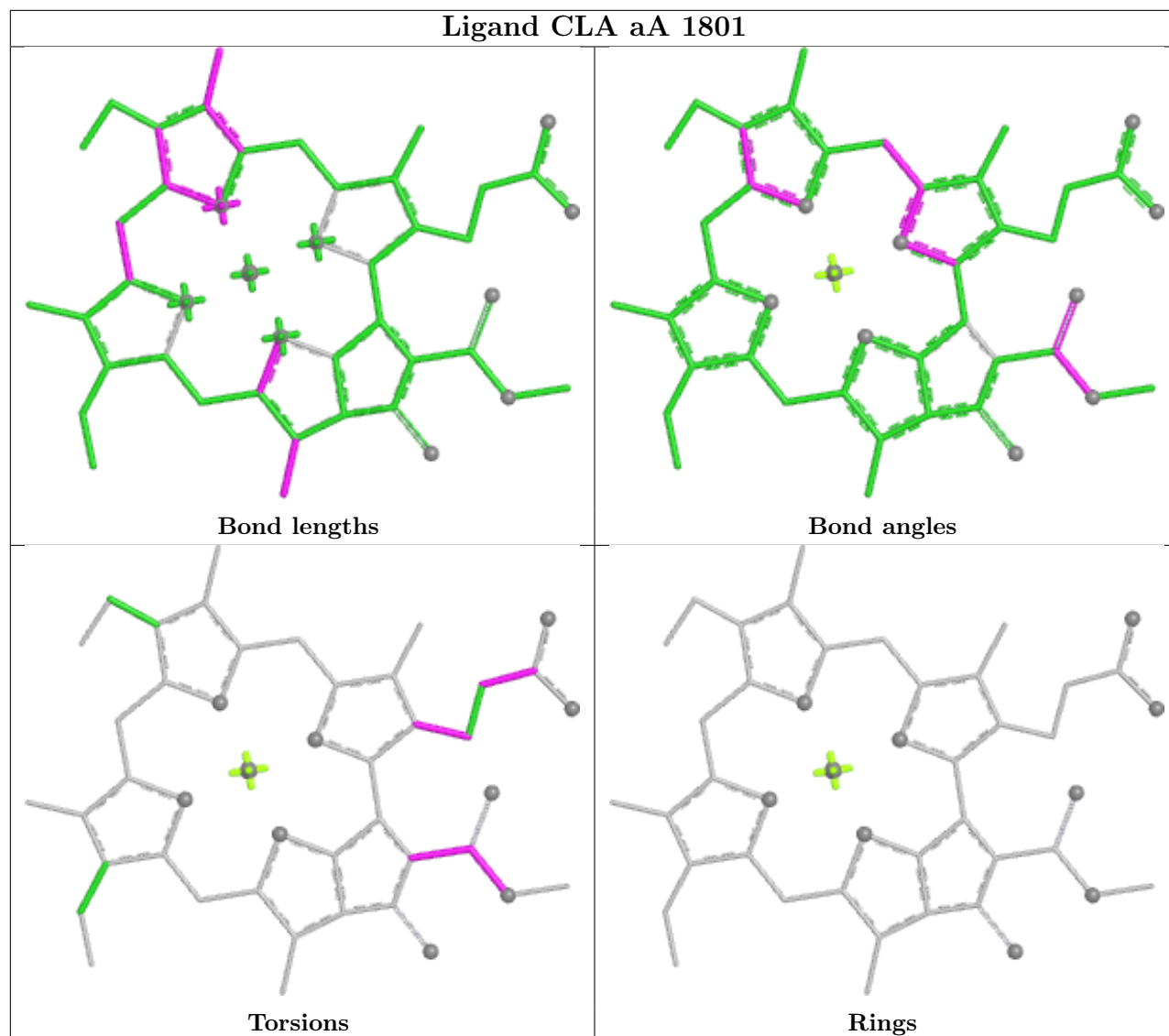
Ligand CLA cL 1502



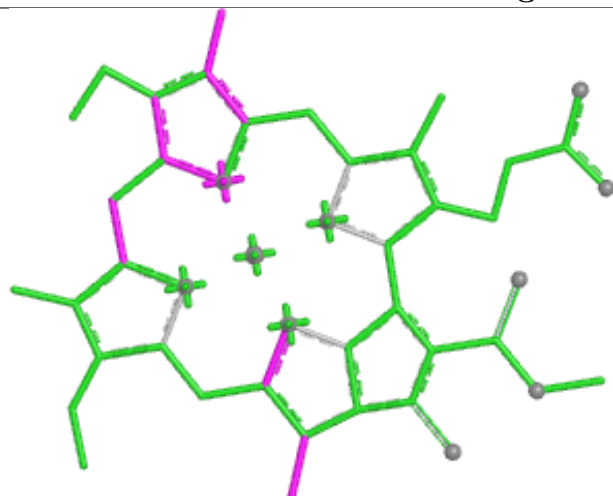
Ligand SQD b3 822



Ligand CLA aA 1801



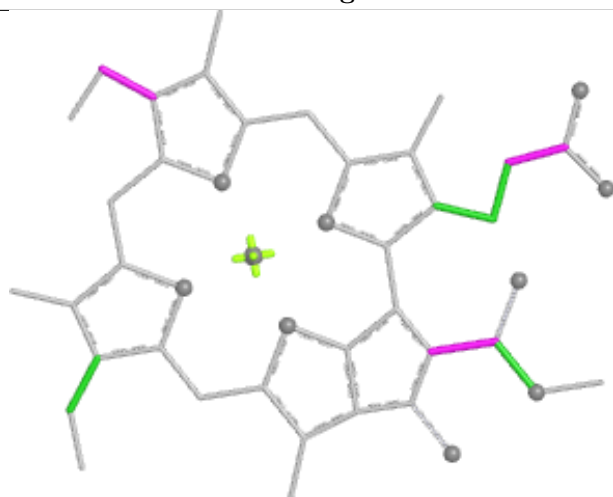
Ligand CLA k 509



Bond lengths



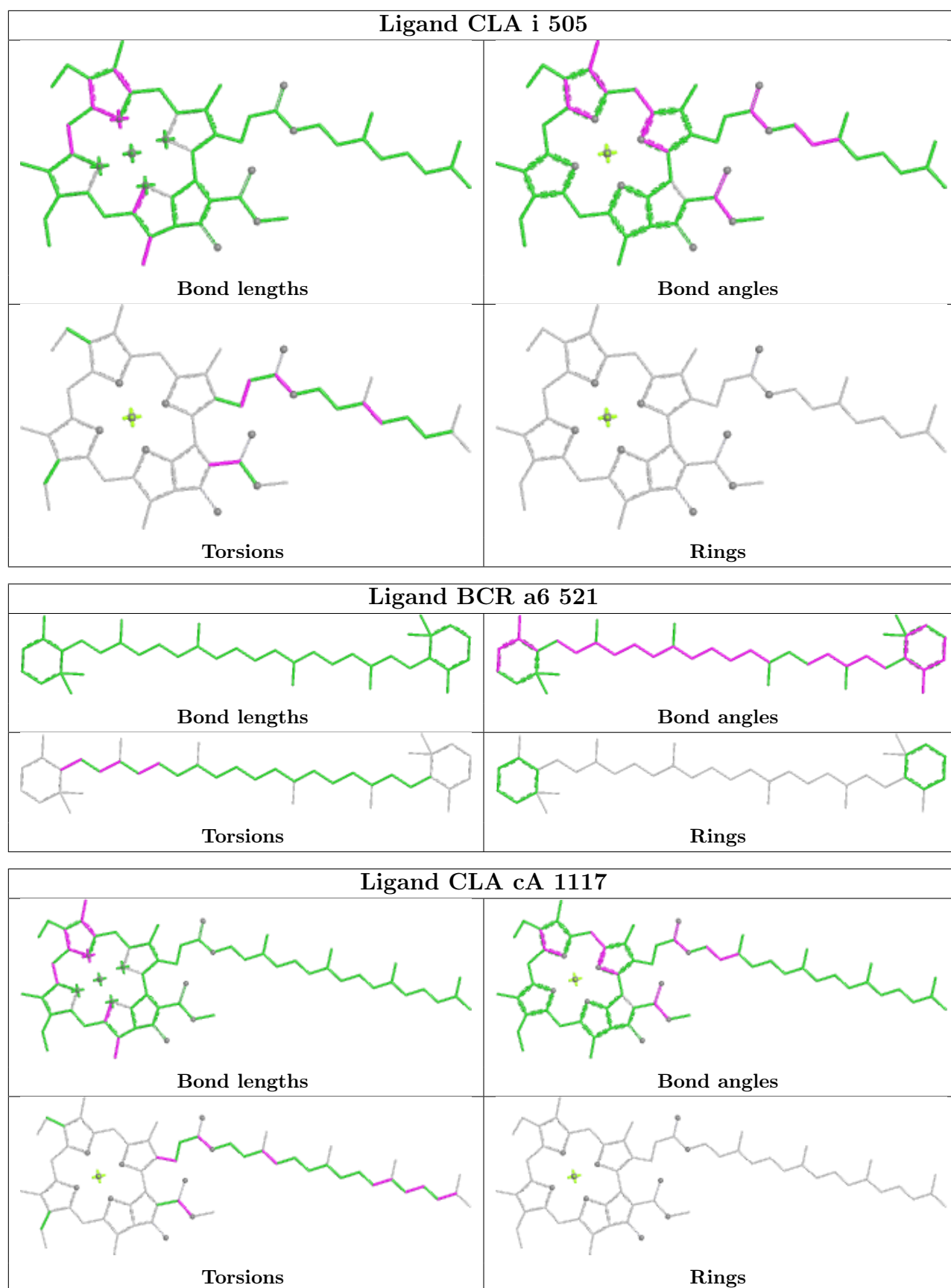
Bond angles

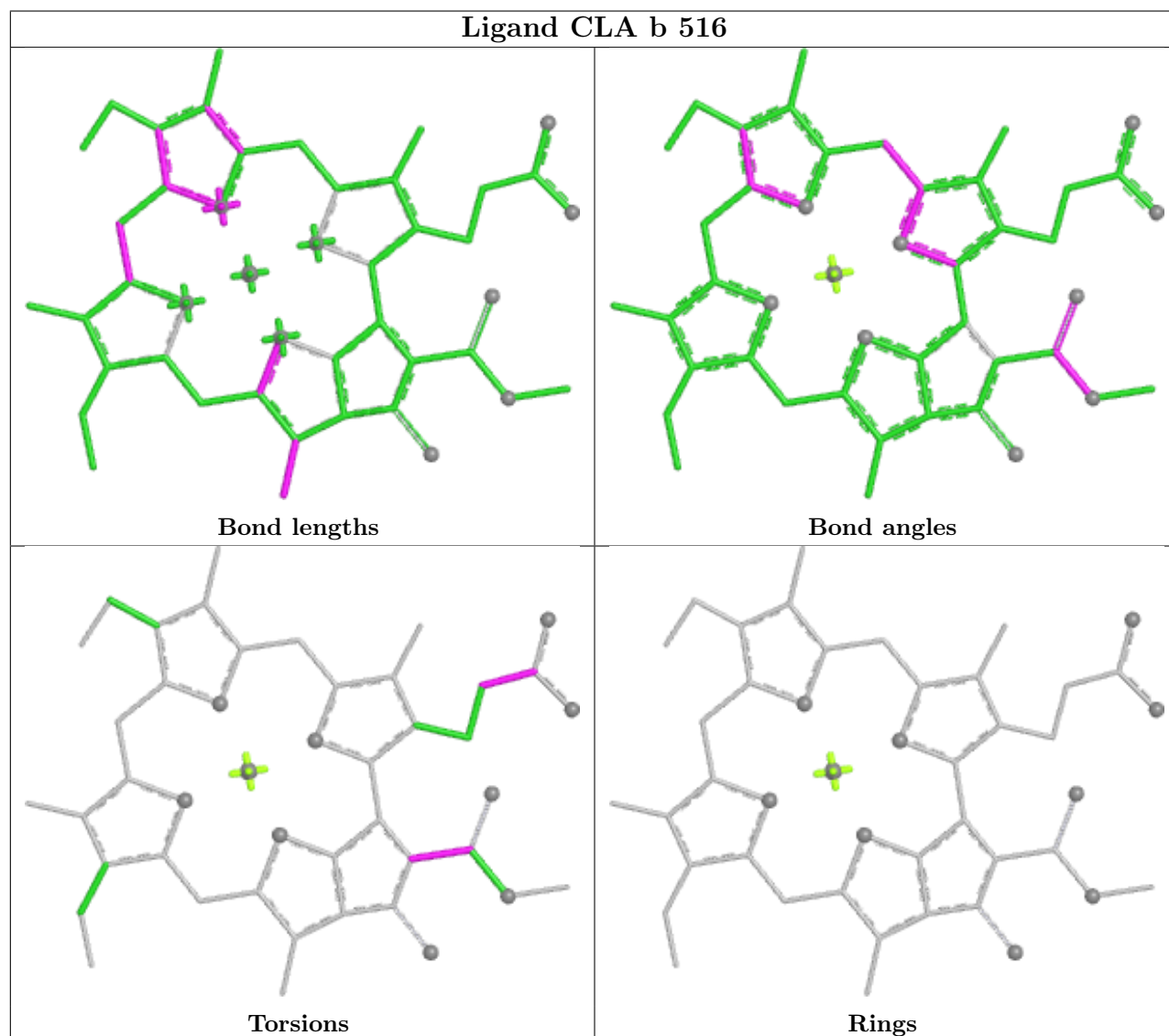
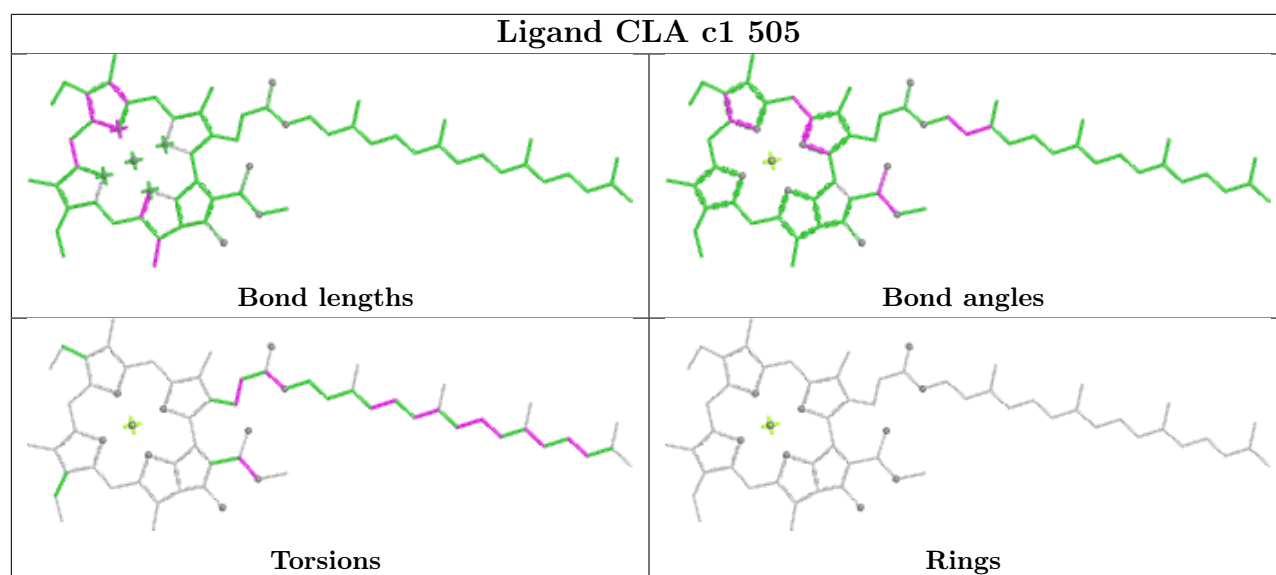


Torsions

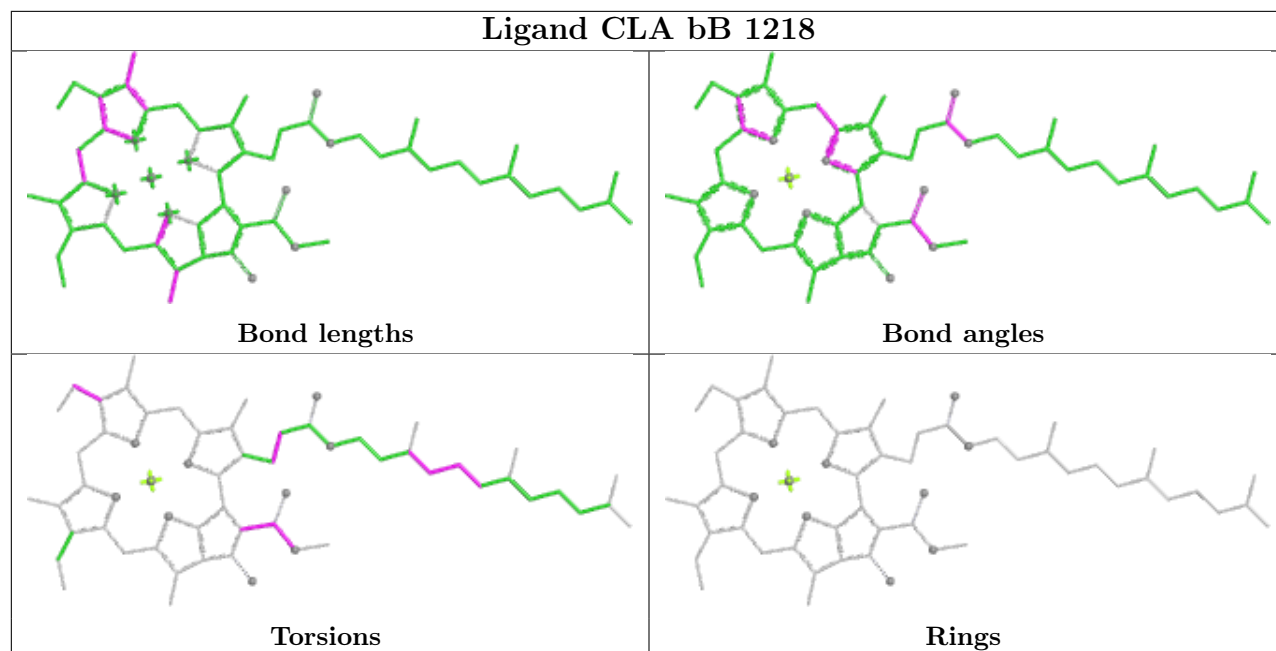


Rings

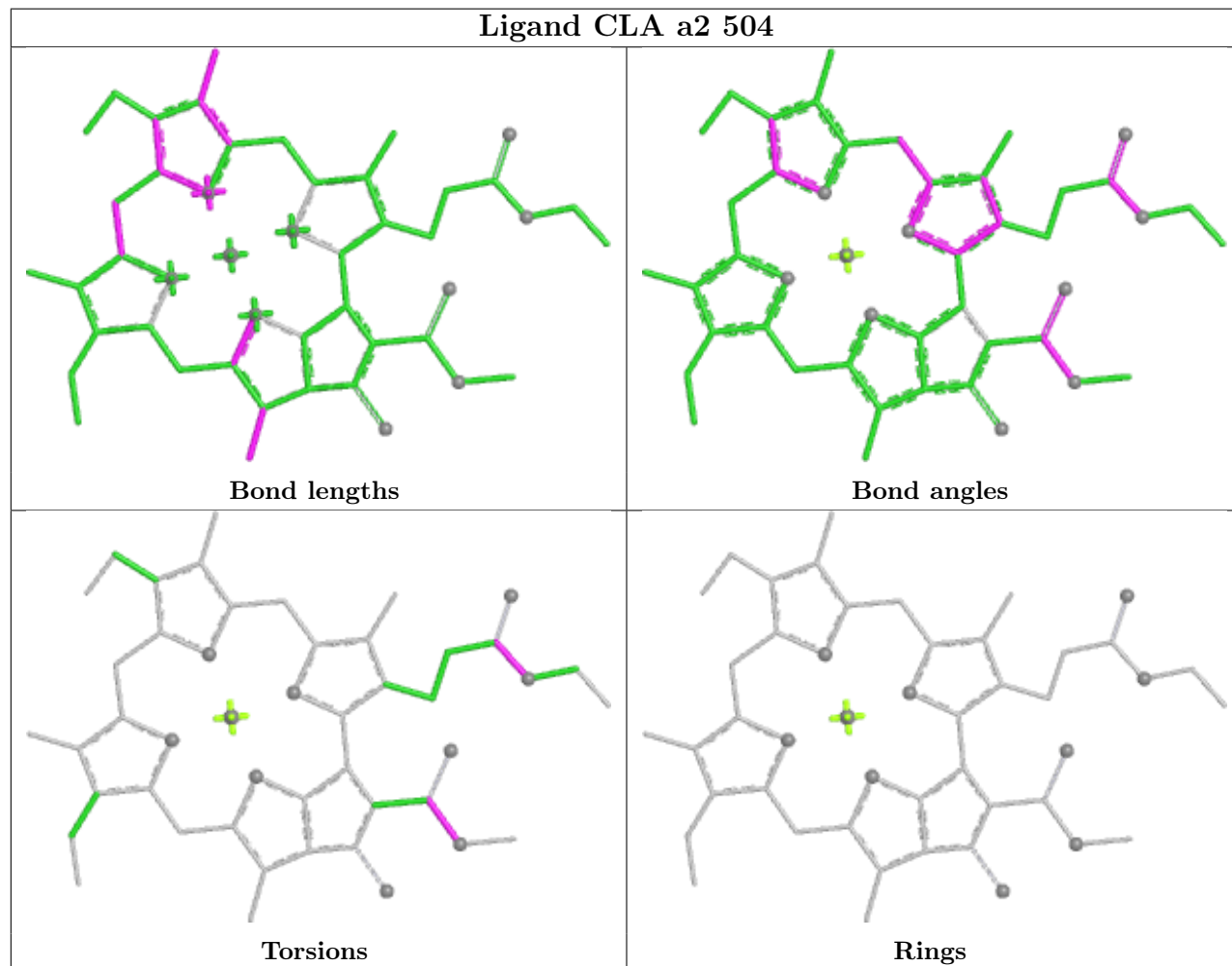




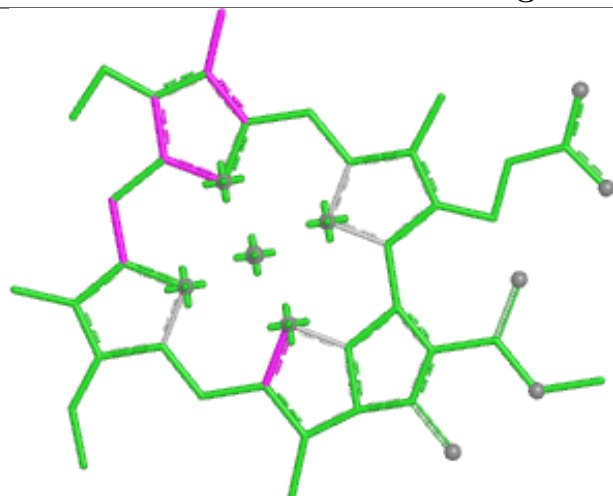
Ligand CLA bB 1218



Ligand CLA a2 504



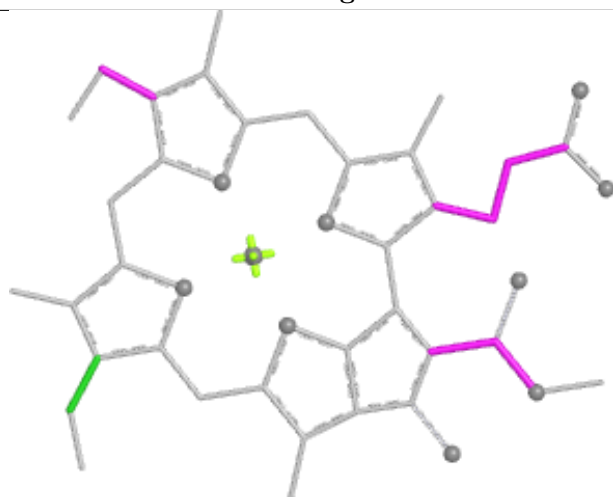
Ligand CLA d 501



Bond lengths



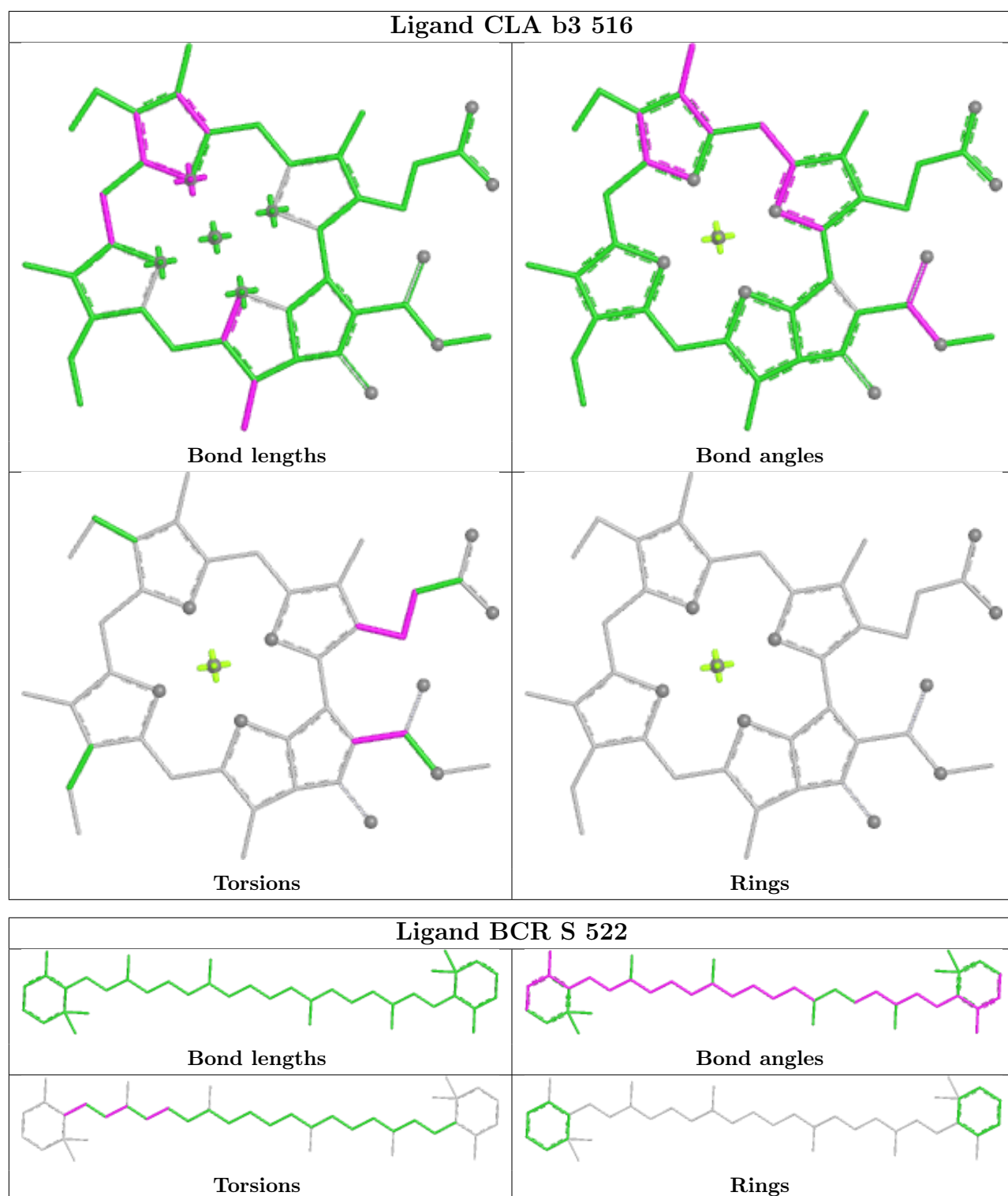
Bond angles



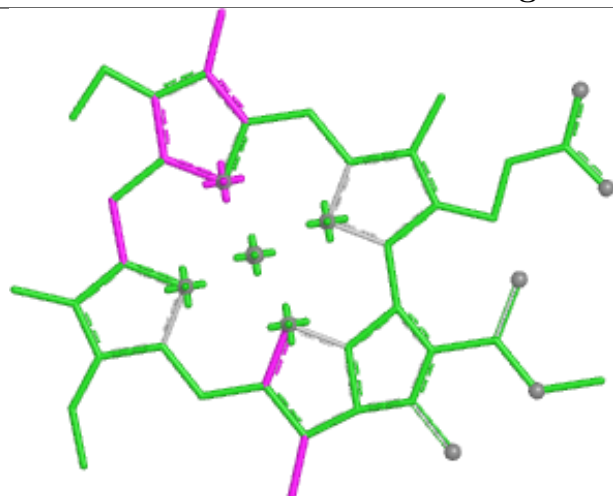
Torsions



Rings



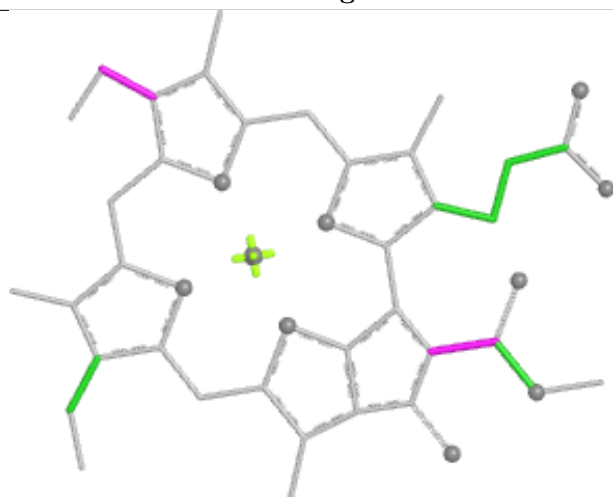
Ligand CLA e 502



Bond lengths



Bond angles

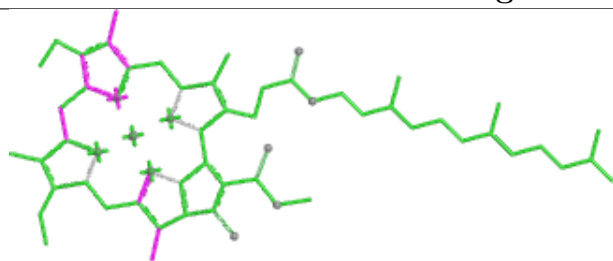


Torsions

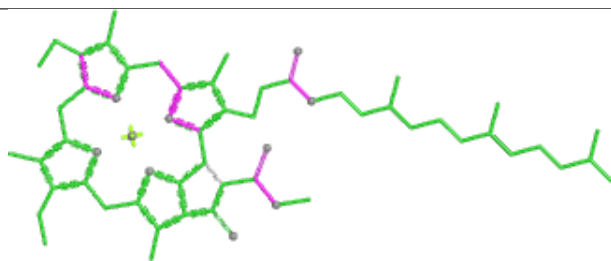


Rings

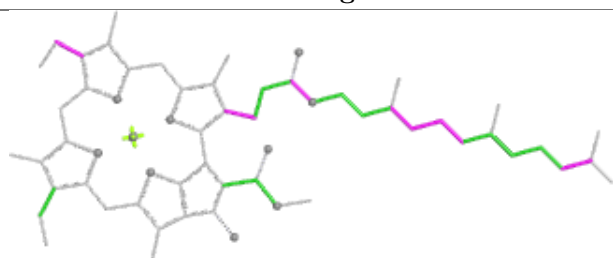
Ligand CLA aA 1118



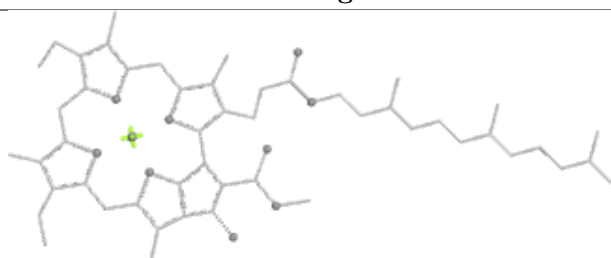
Bond lengths



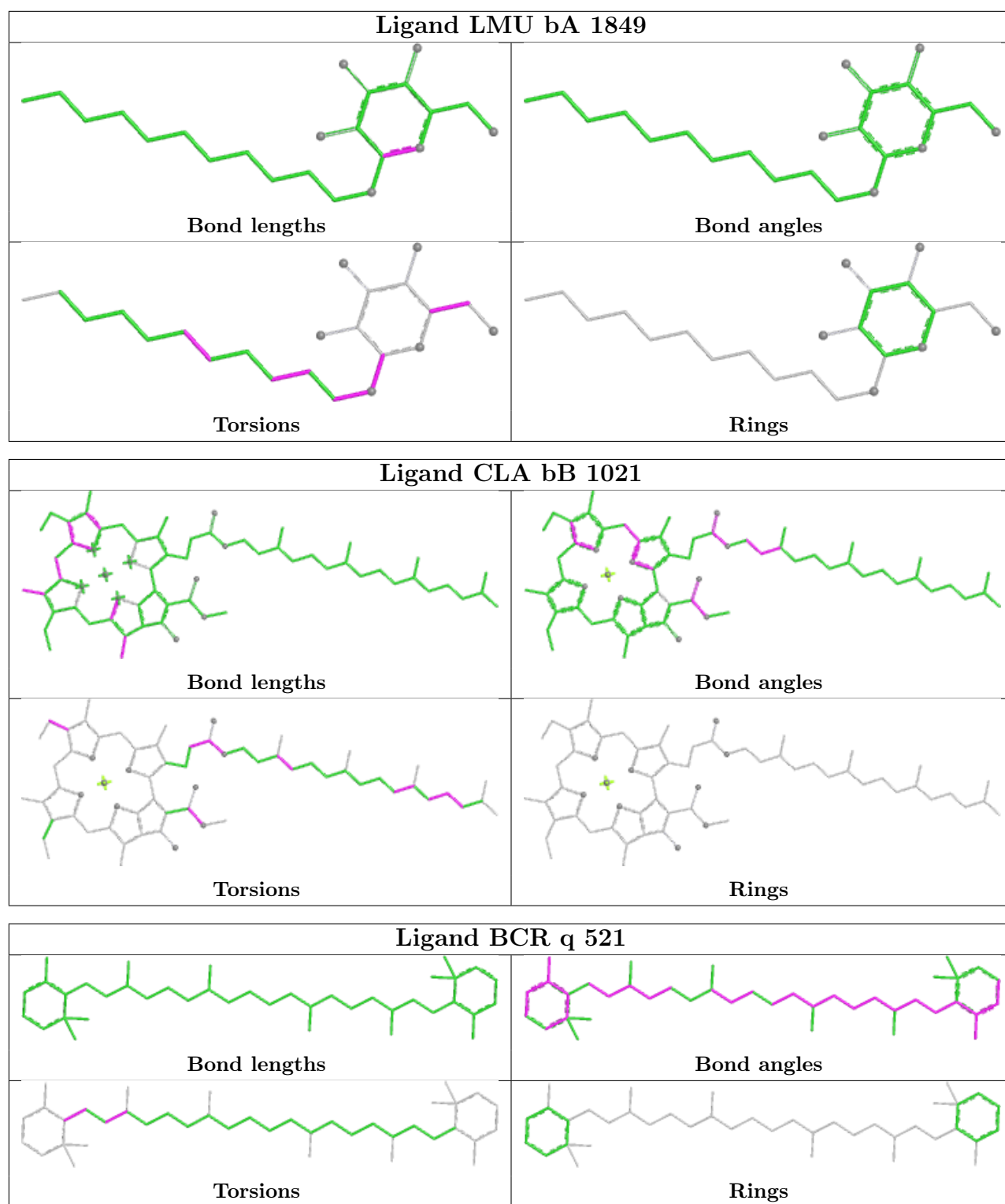
Bond angles

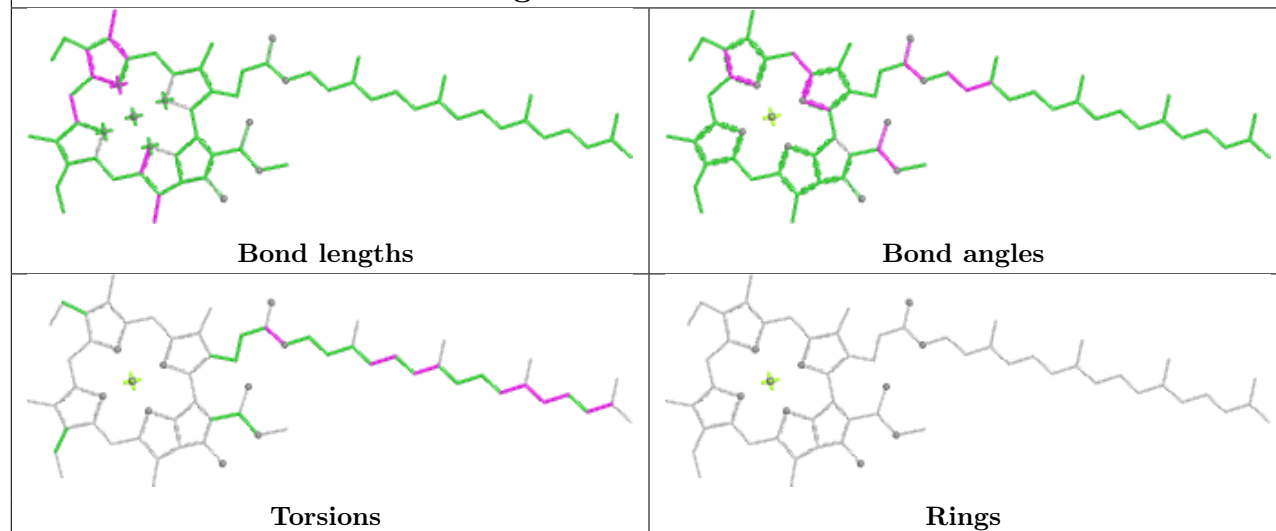
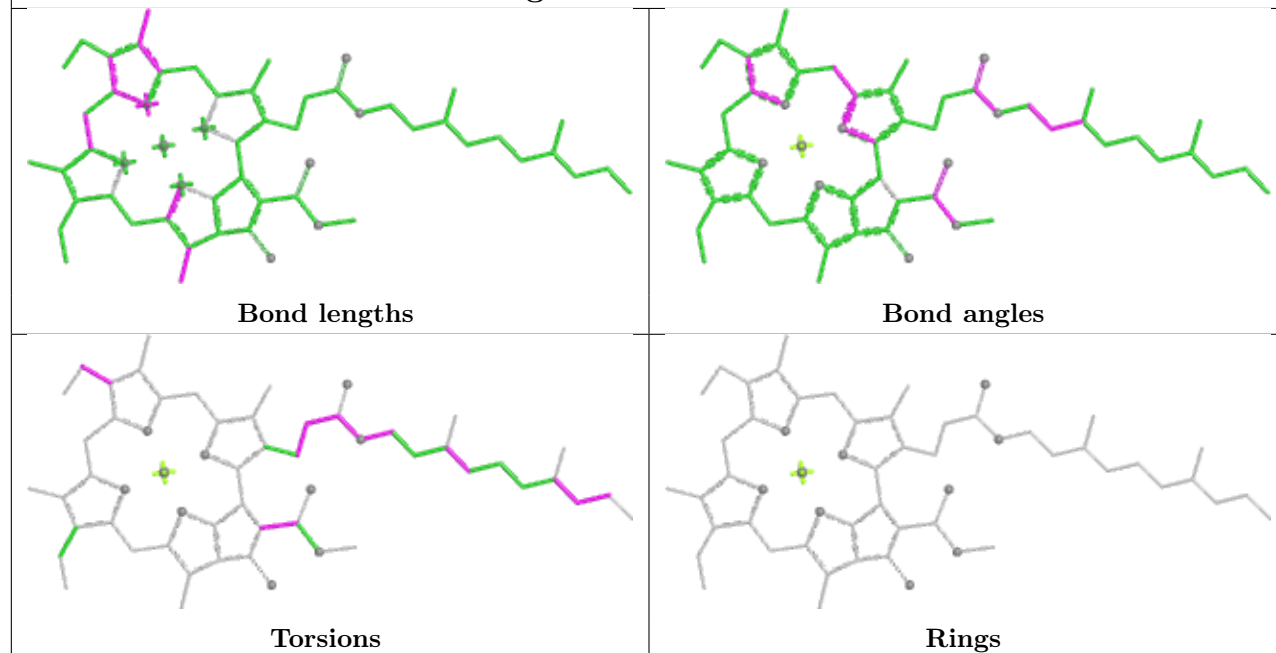


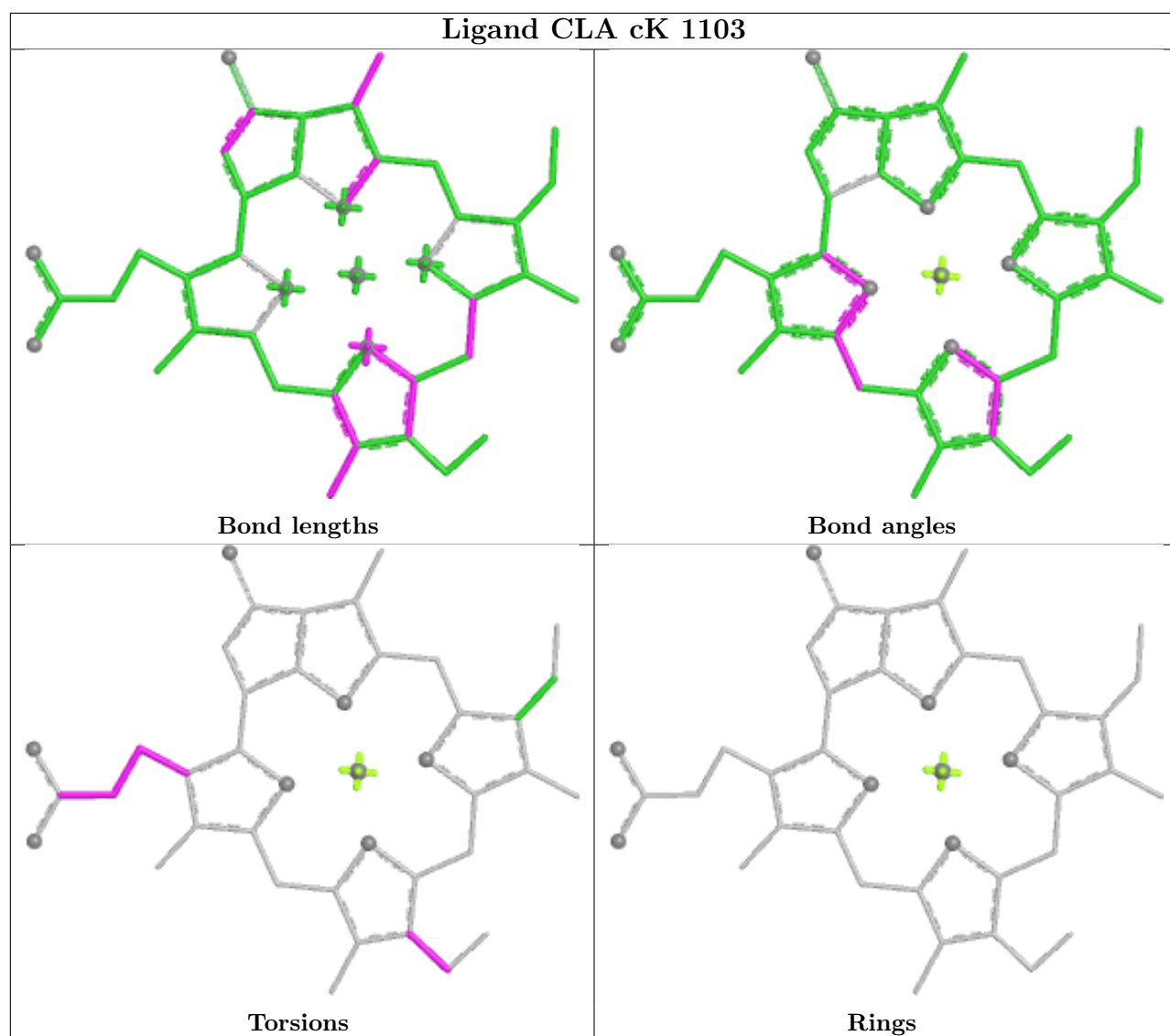
Torsions

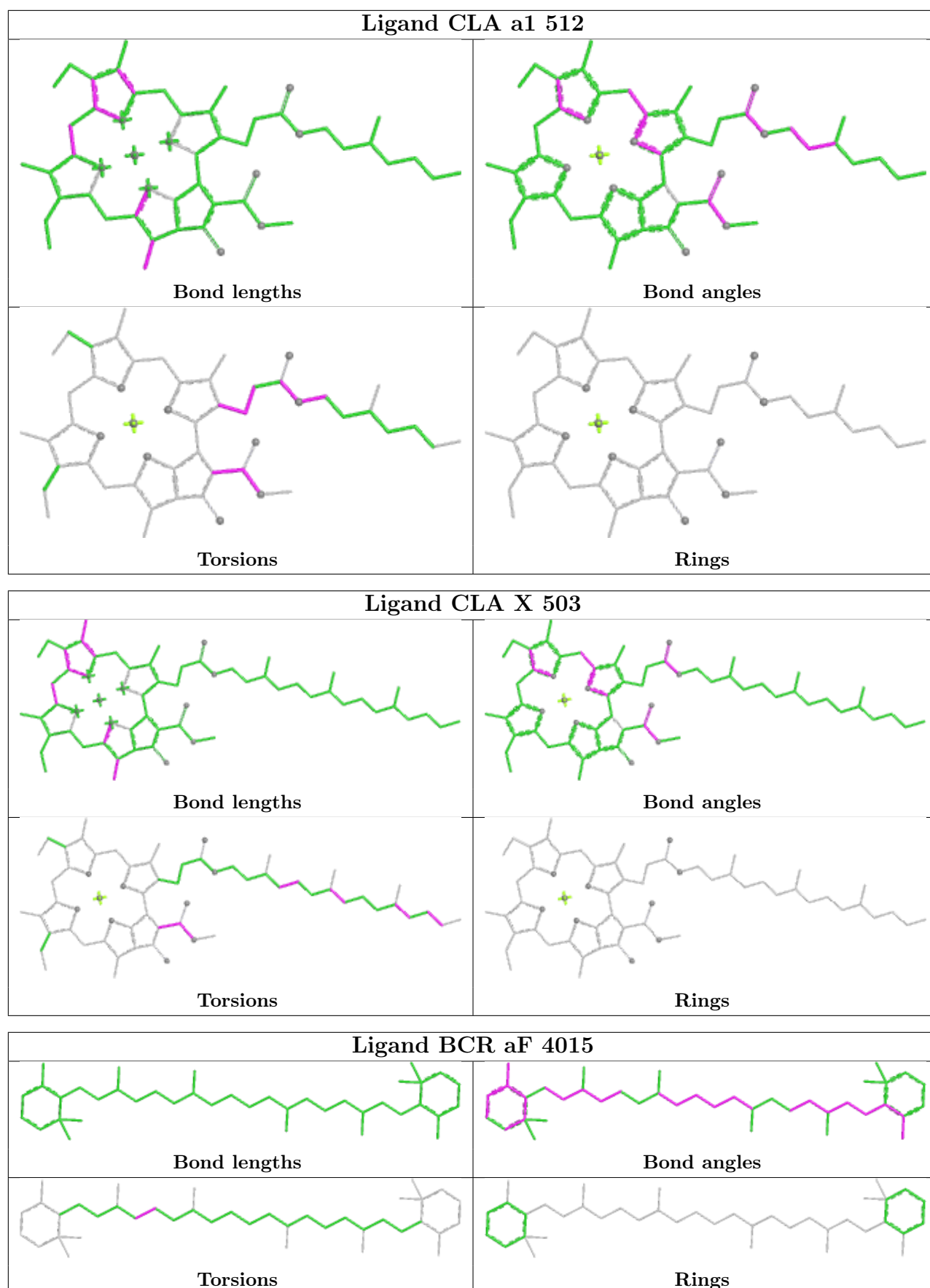


Rings

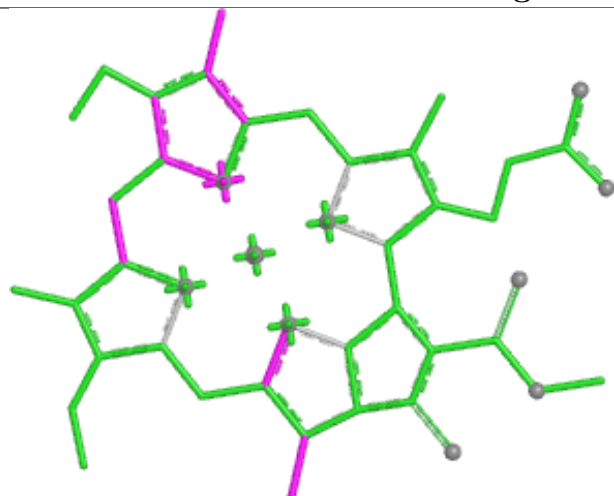


Ligand CLA bB 1235**Ligand CLA b3 504**

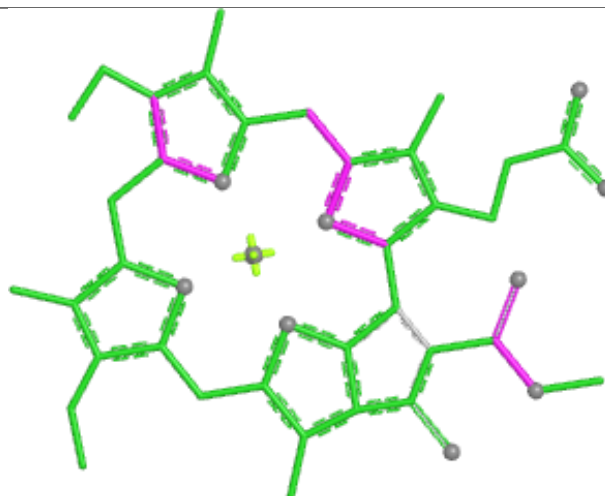




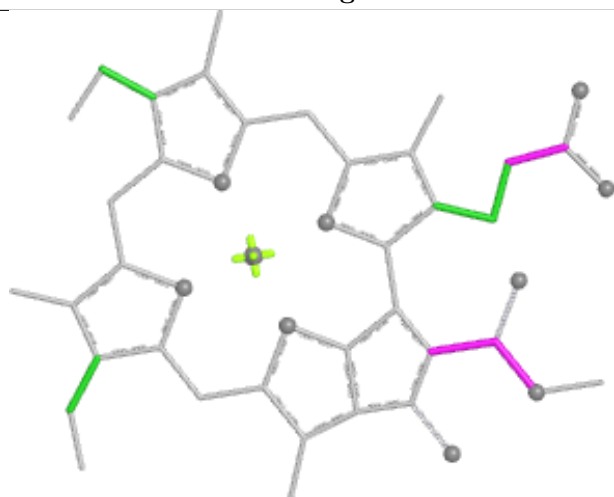
Ligand CLA U 506



Bond lengths



Bond angles

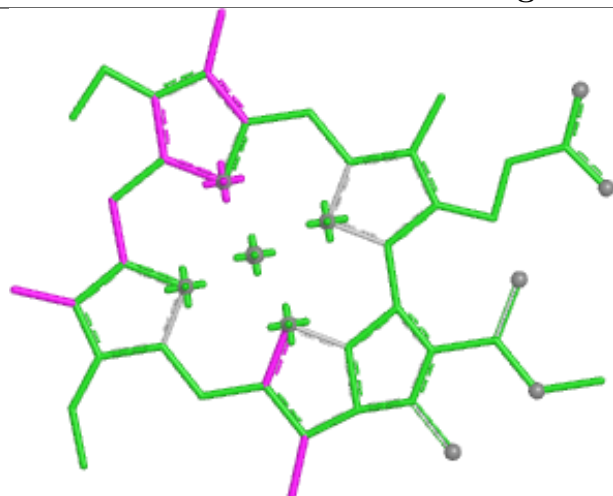


Torsions



Rings

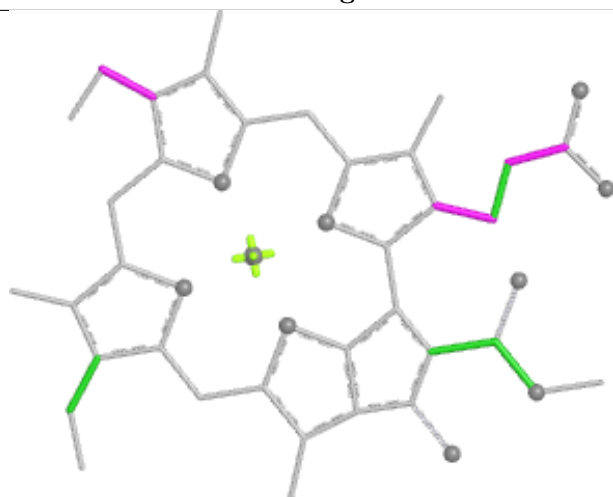
Ligand CLA S 501



Bond lengths



Bond angles

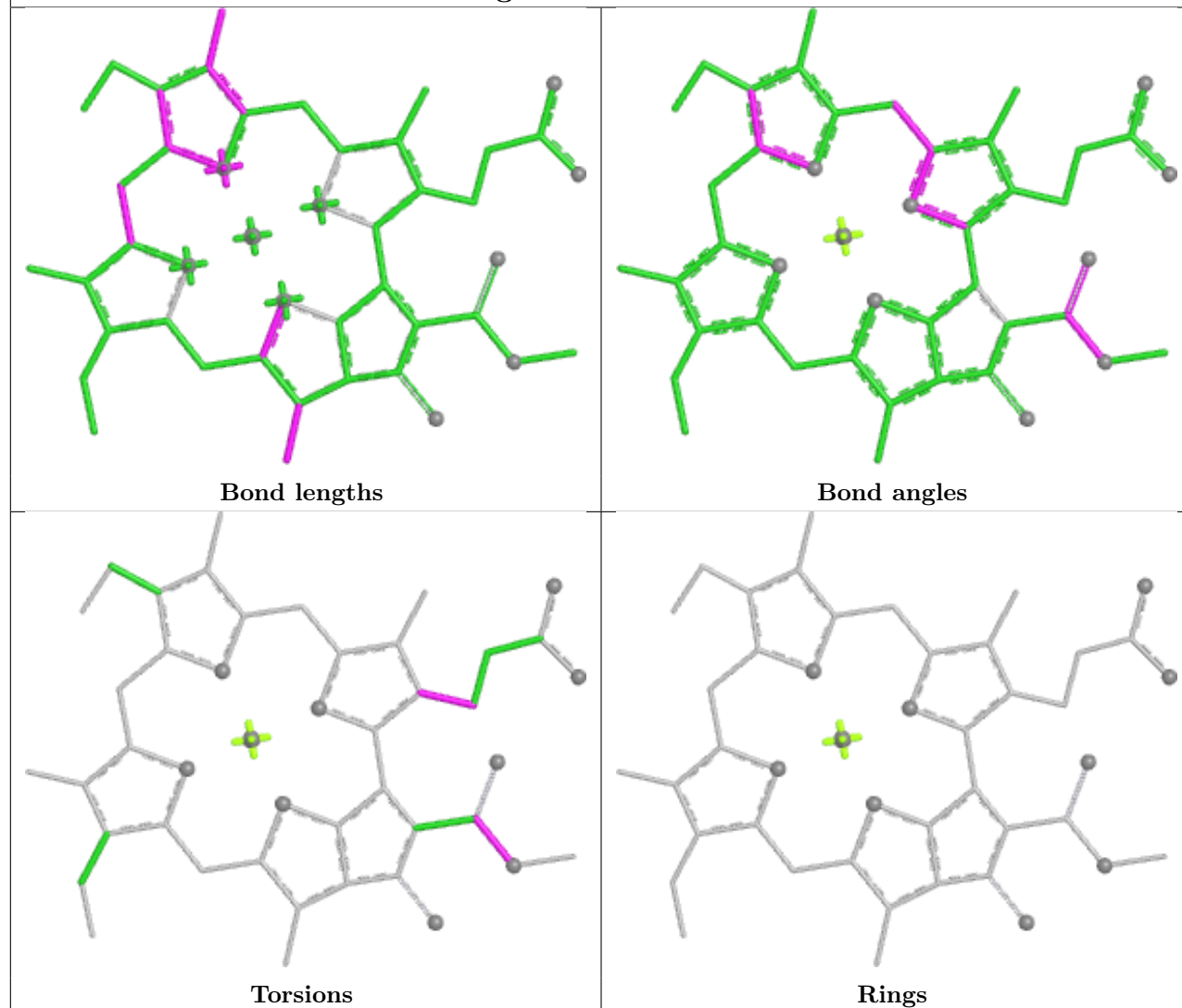


Torsions

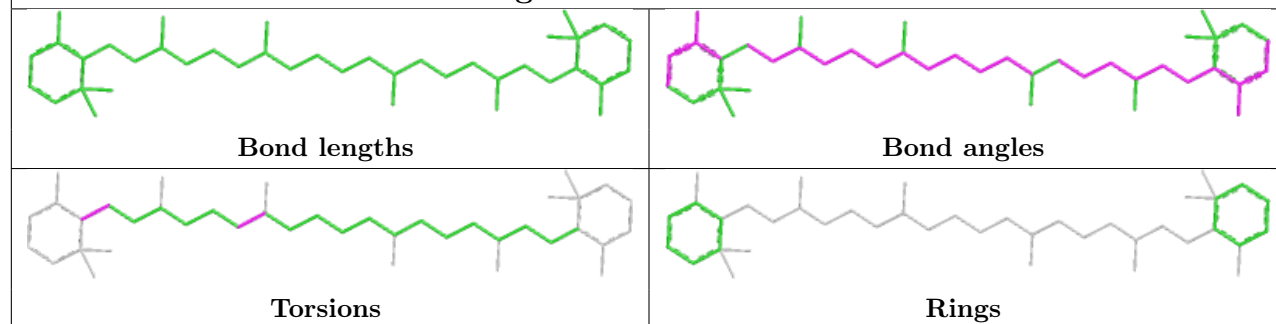


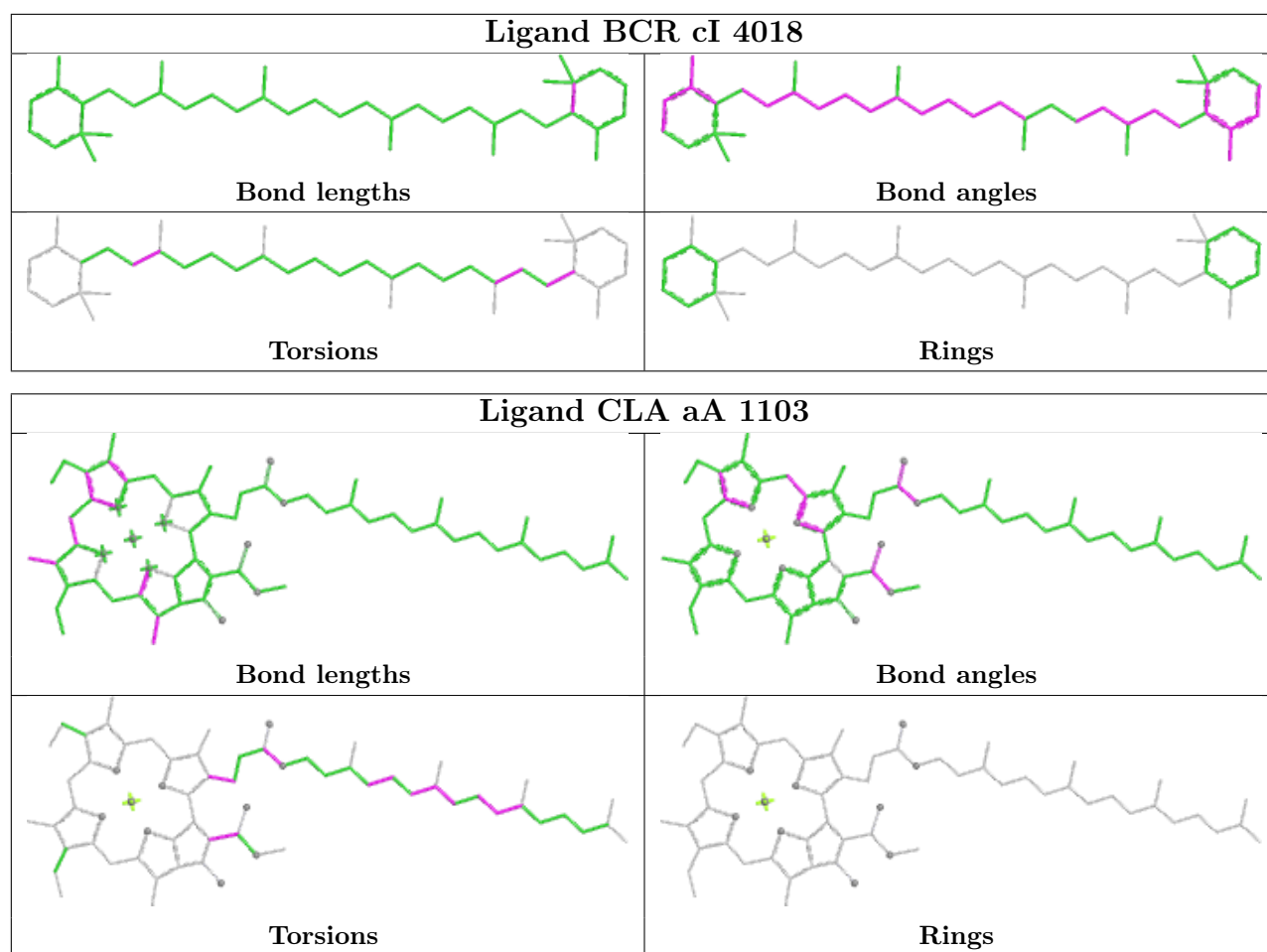
Rings

Ligand CLA k 508

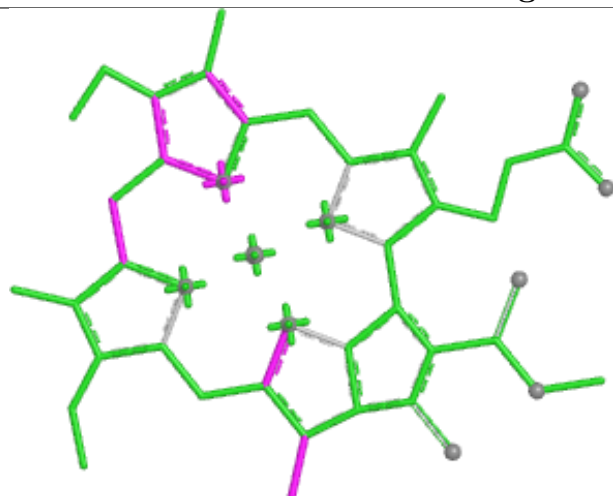


Ligand BCR bJ 4012

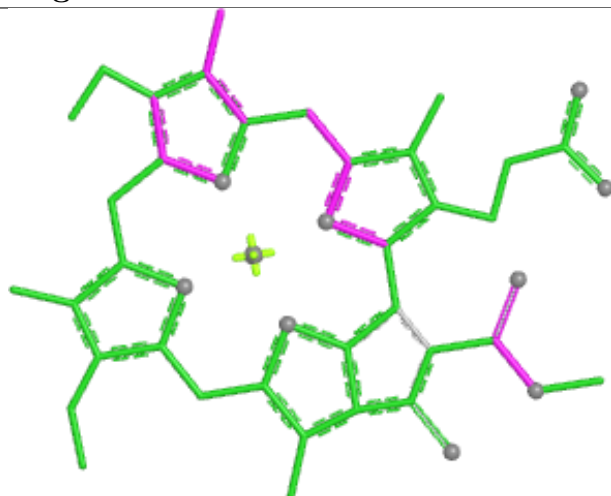




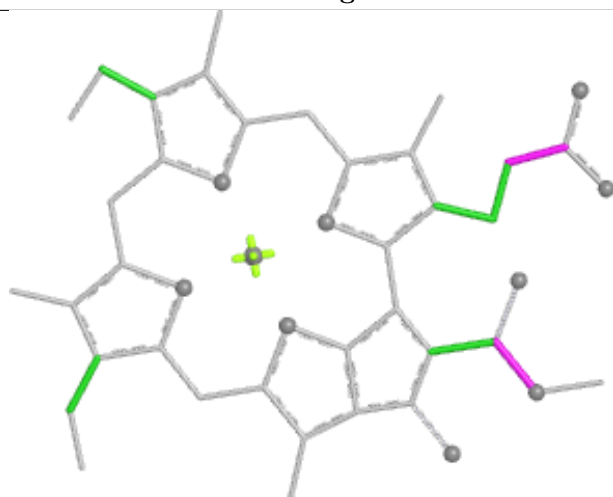
Ligand CLA g 513



Bond lengths



Bond angles

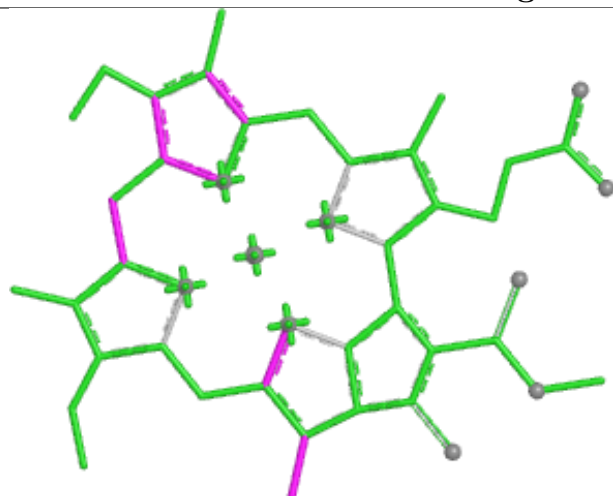


Torsions

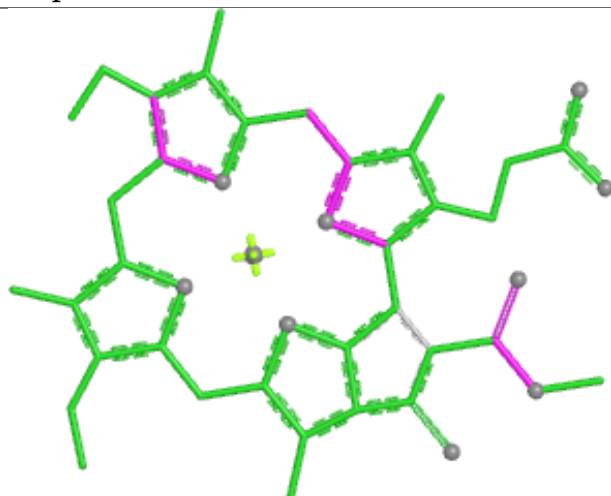


Rings

Ligand CLA p 501



Bond lengths



Bond angles

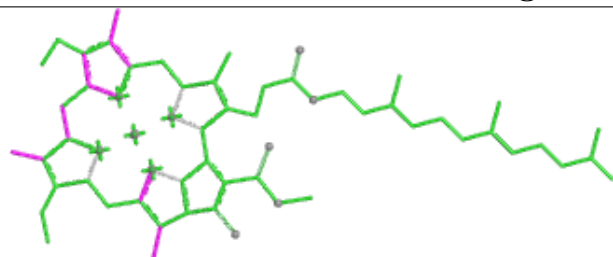


Torsions

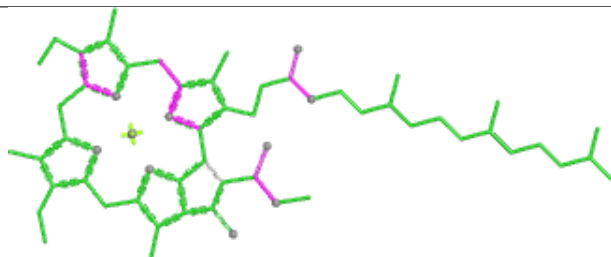


Rings

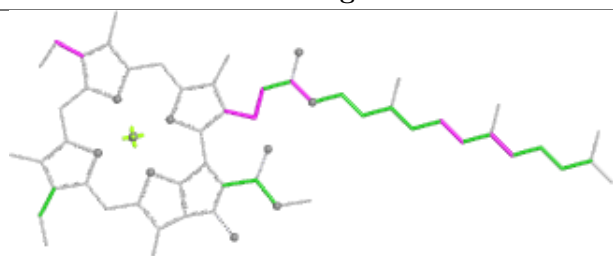
Ligand CLA a 501



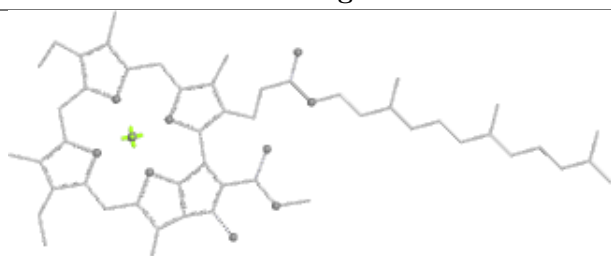
Bond lengths



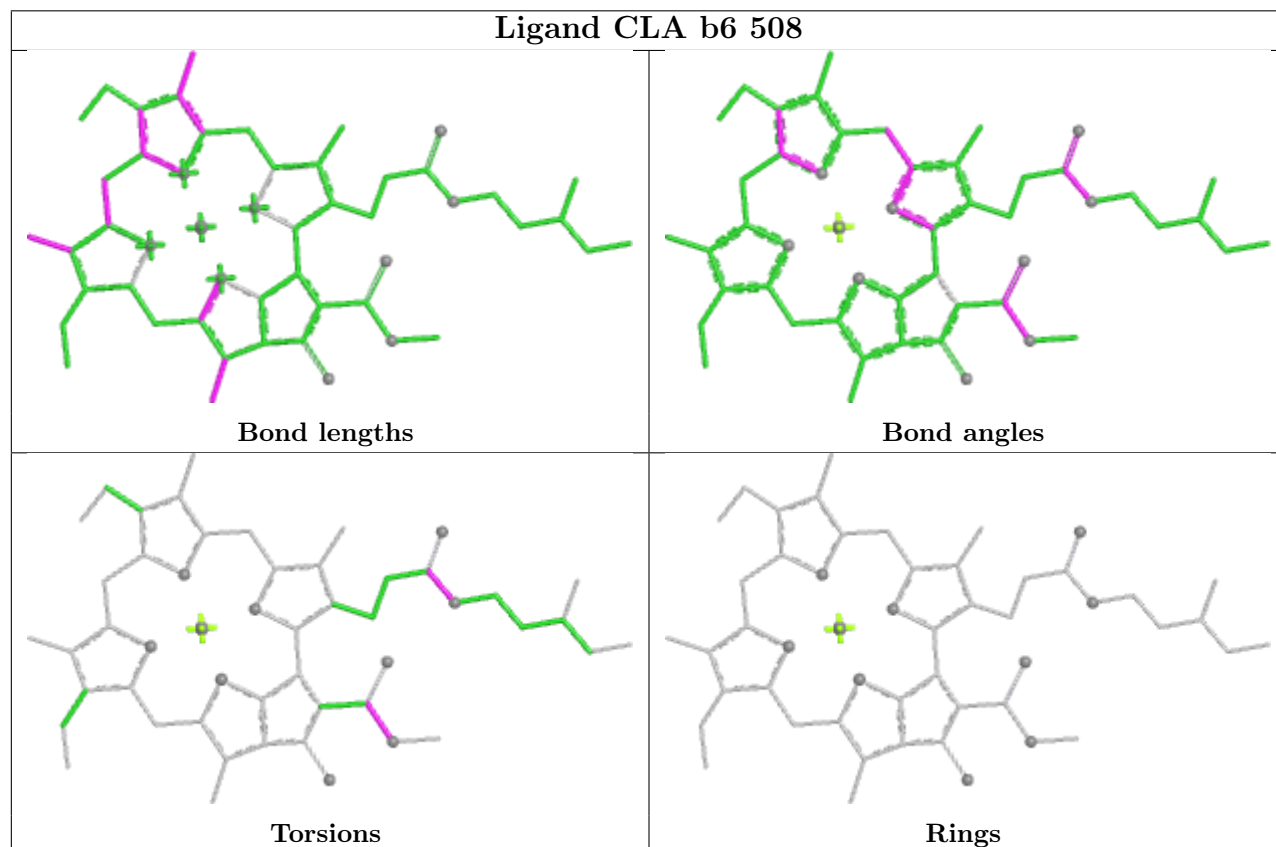
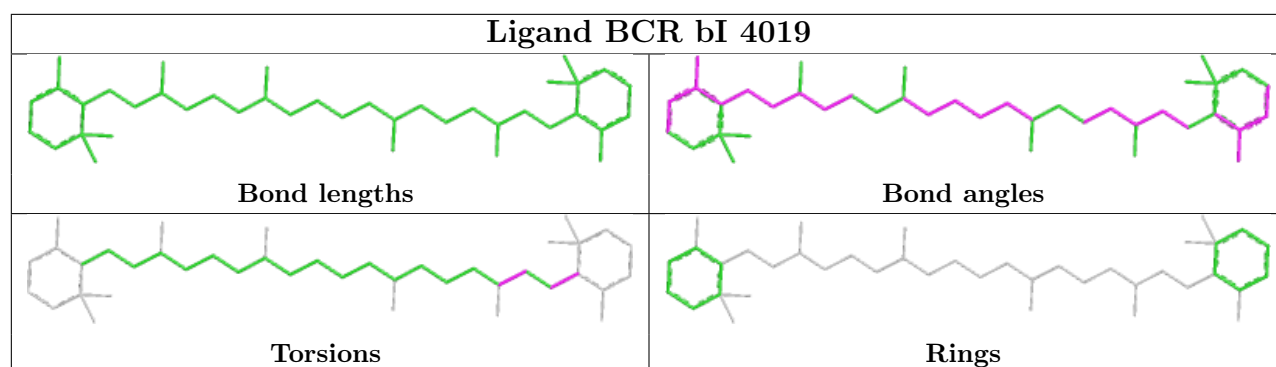
Bond angles

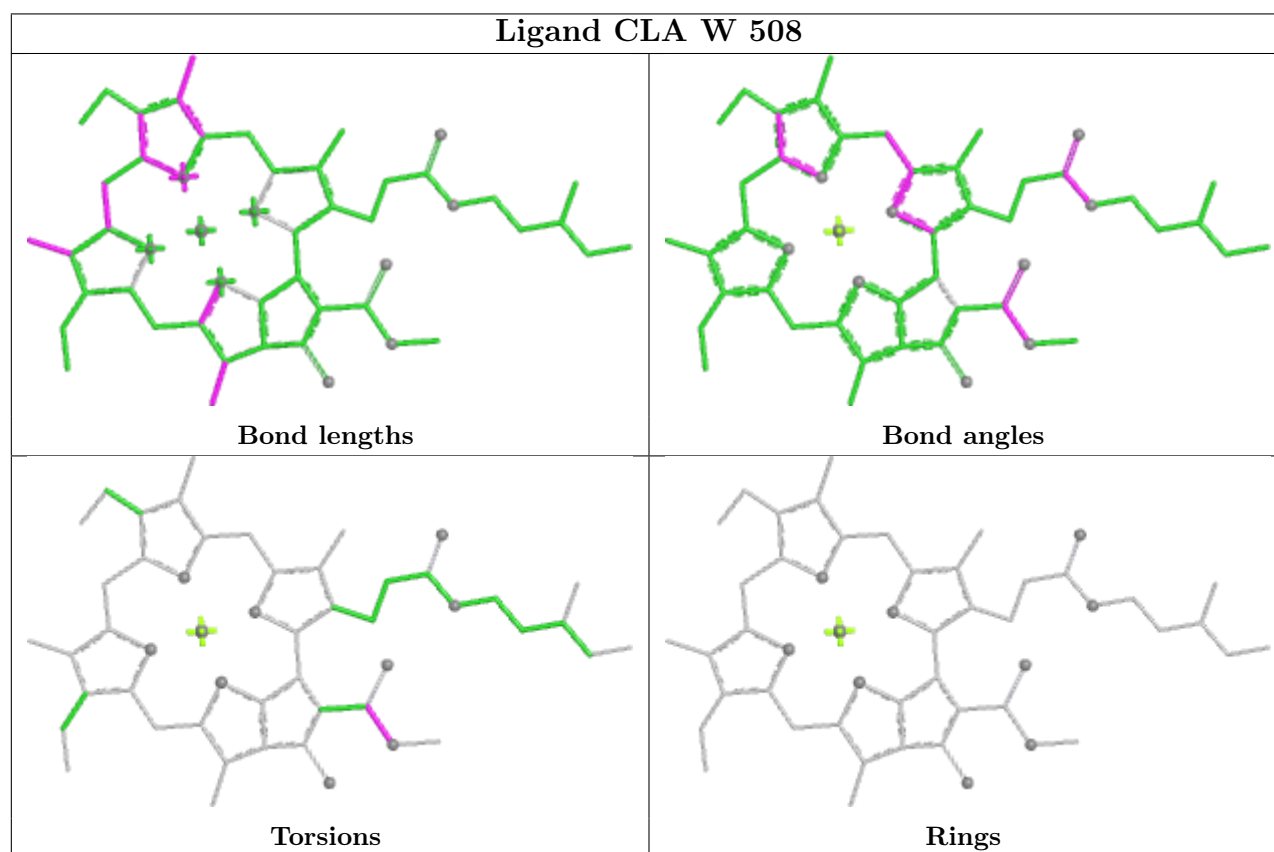
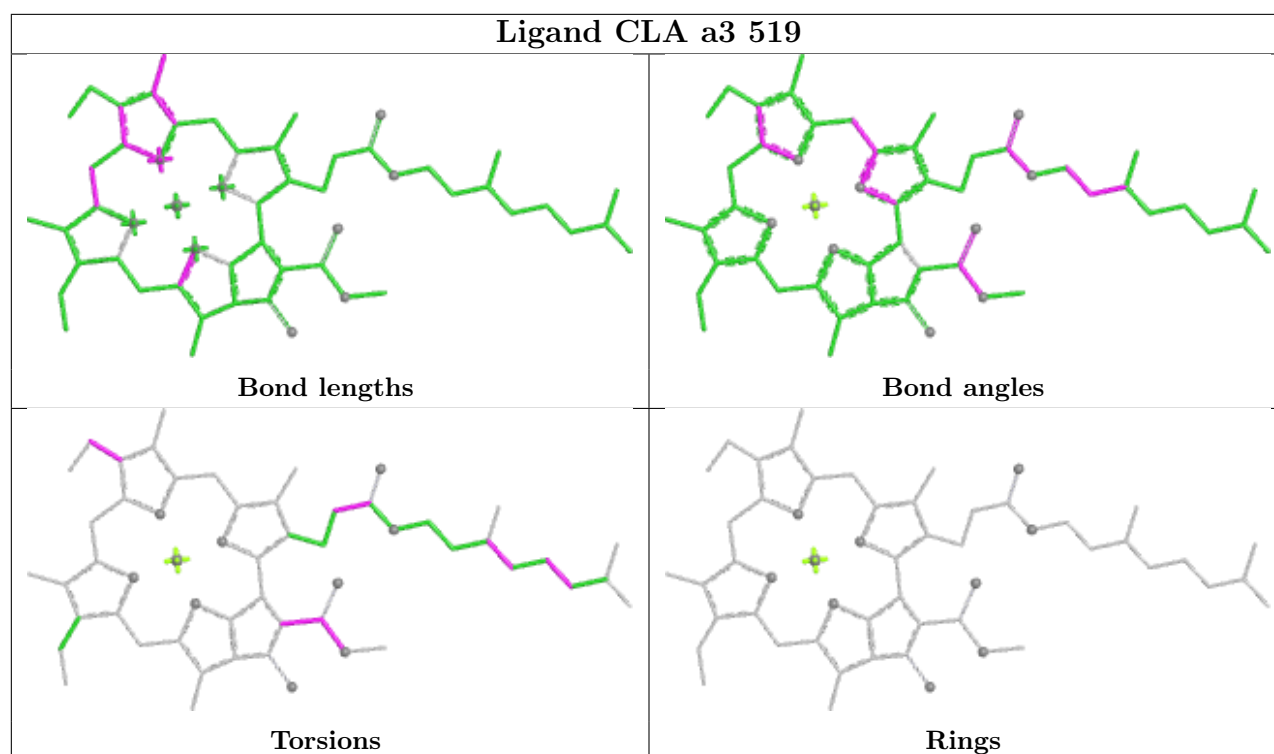


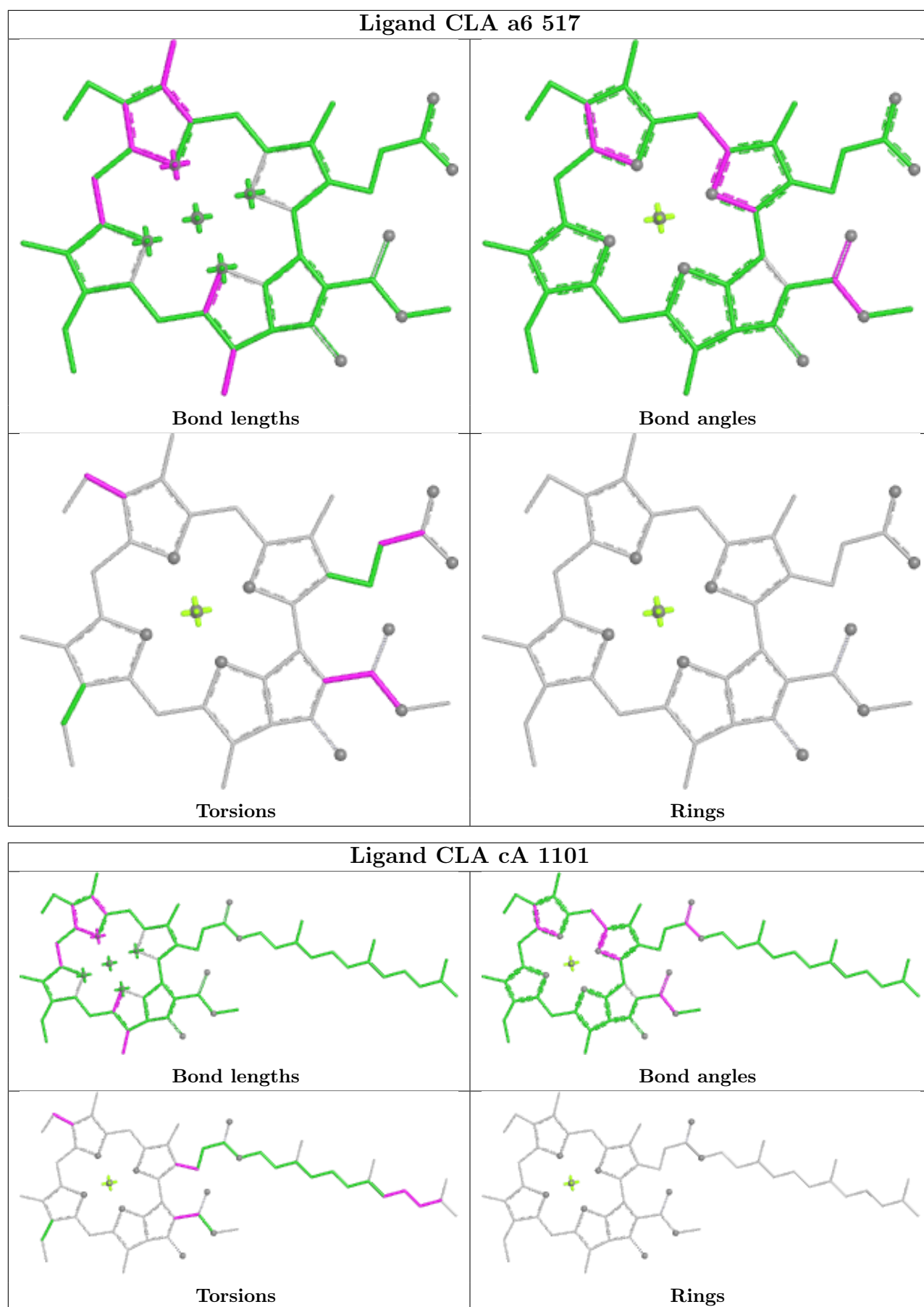
Torsions

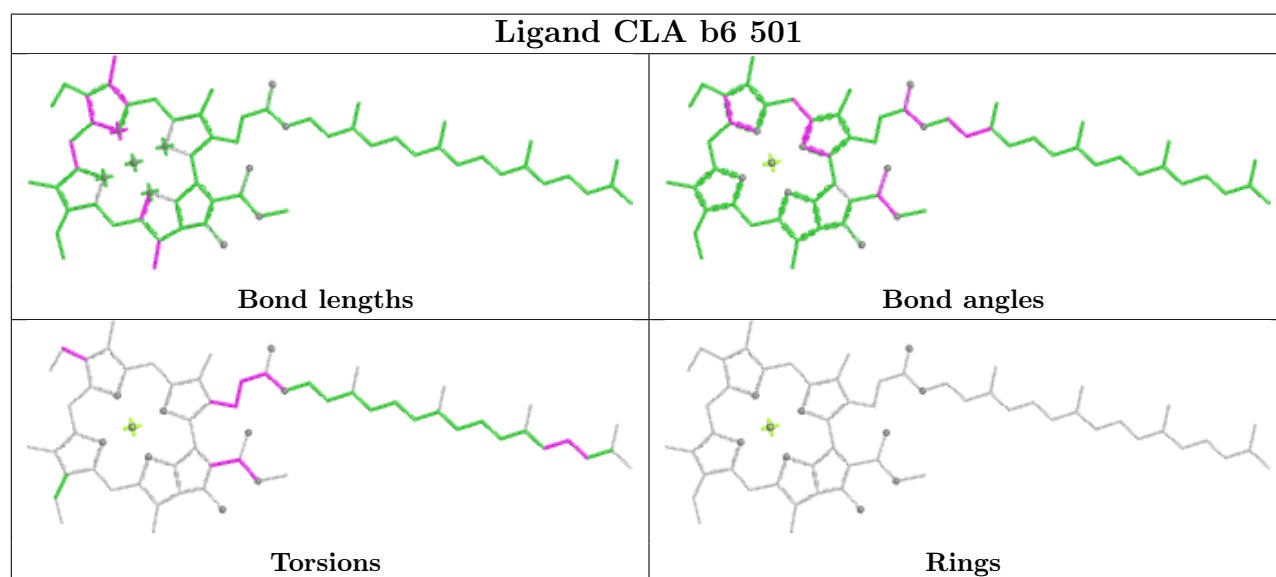
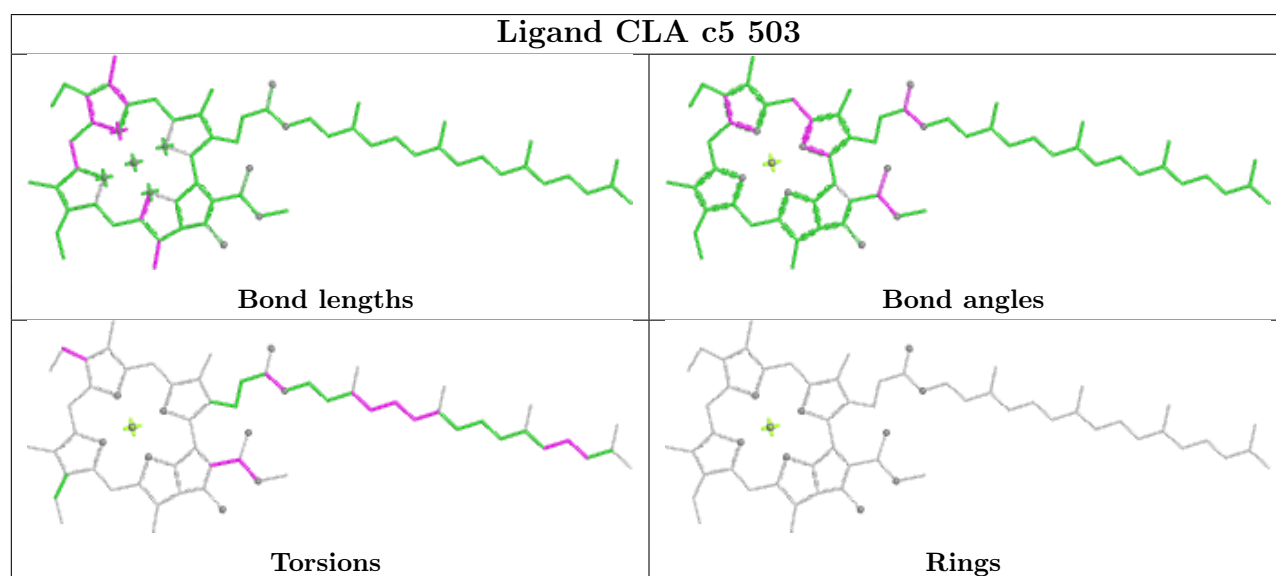
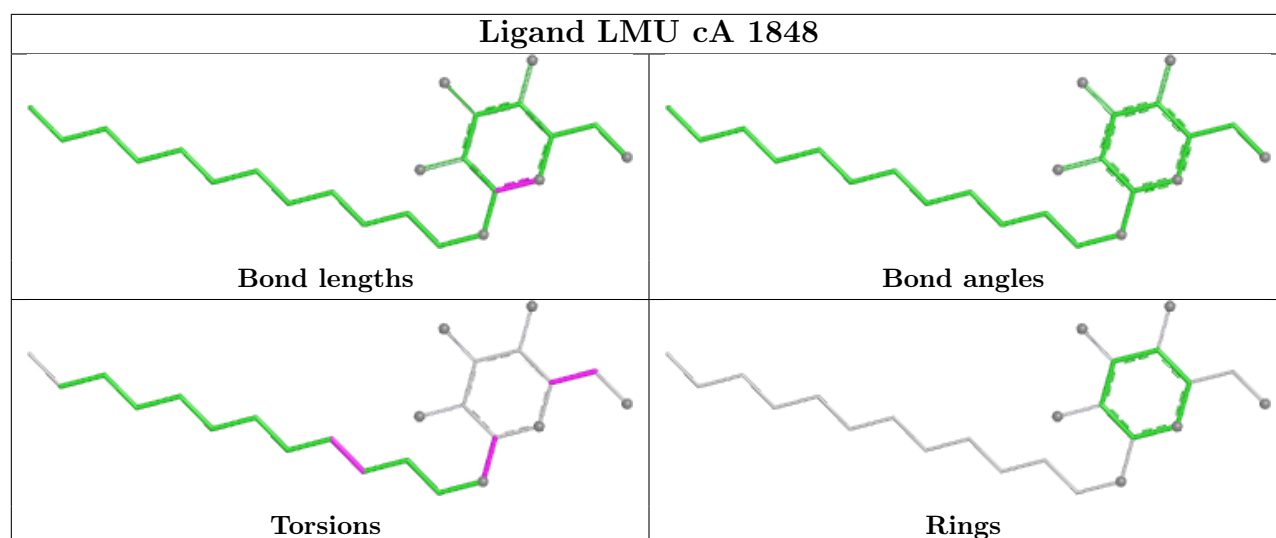


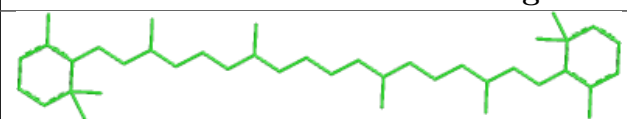
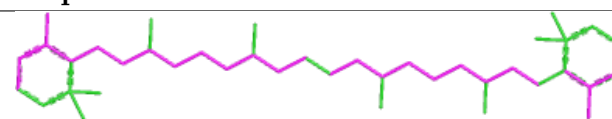
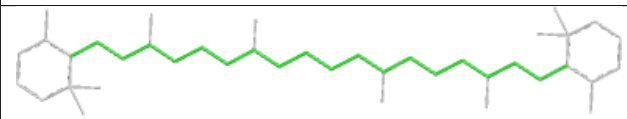
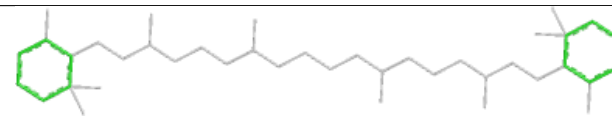
Rings

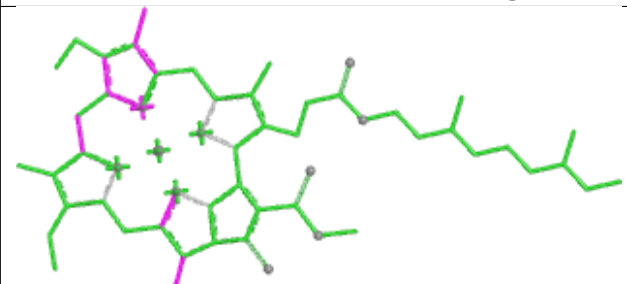
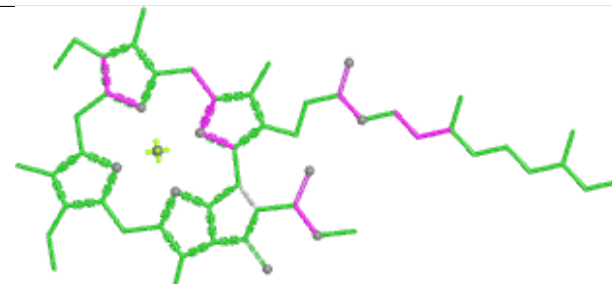
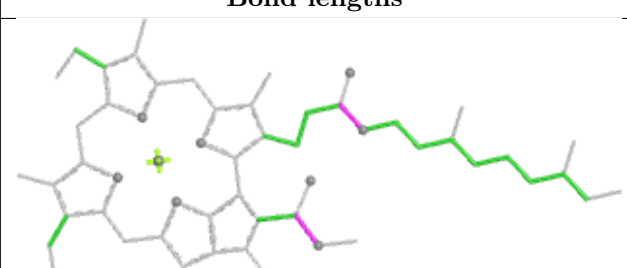
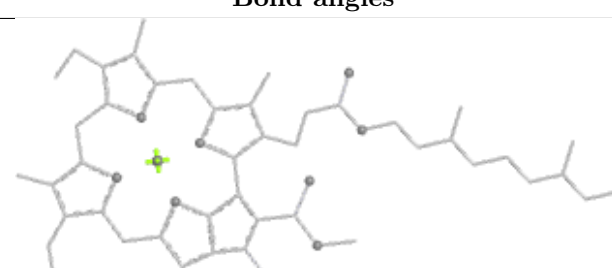



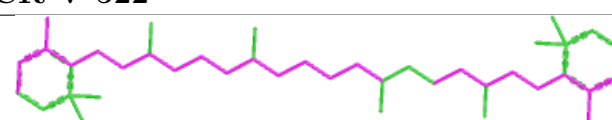
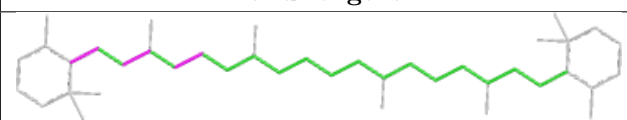
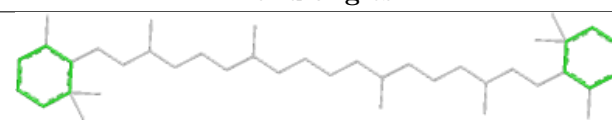




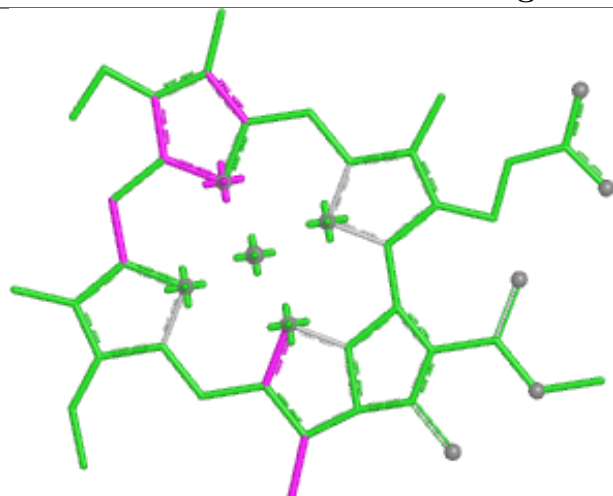


Ligand BCR p 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA aB 1228	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR V 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

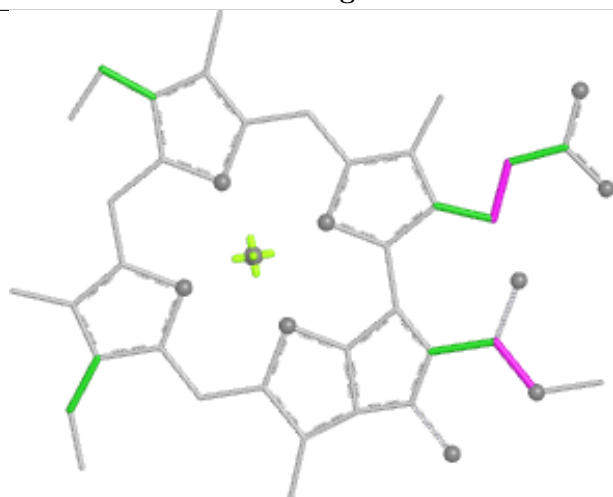
Ligand CLA h 505



Bond lengths



Bond angles

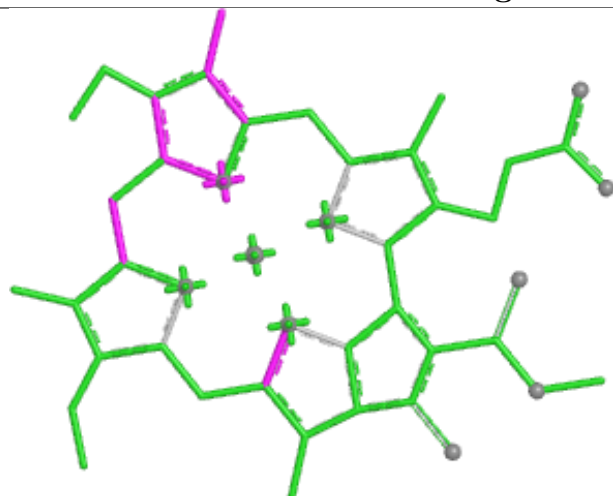


Torsions



Rings

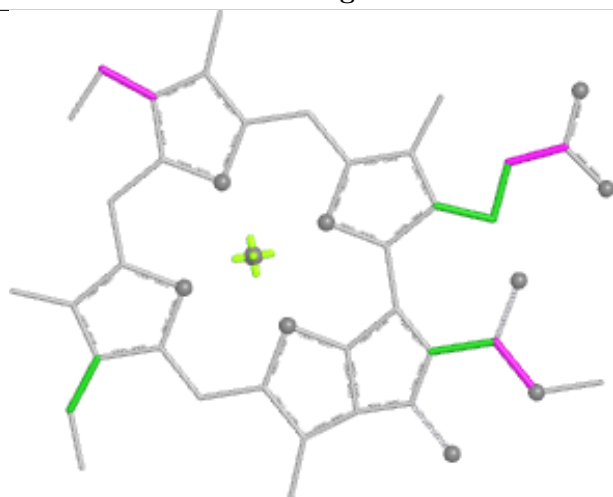
Ligand CLA bA 1114



Bond lengths



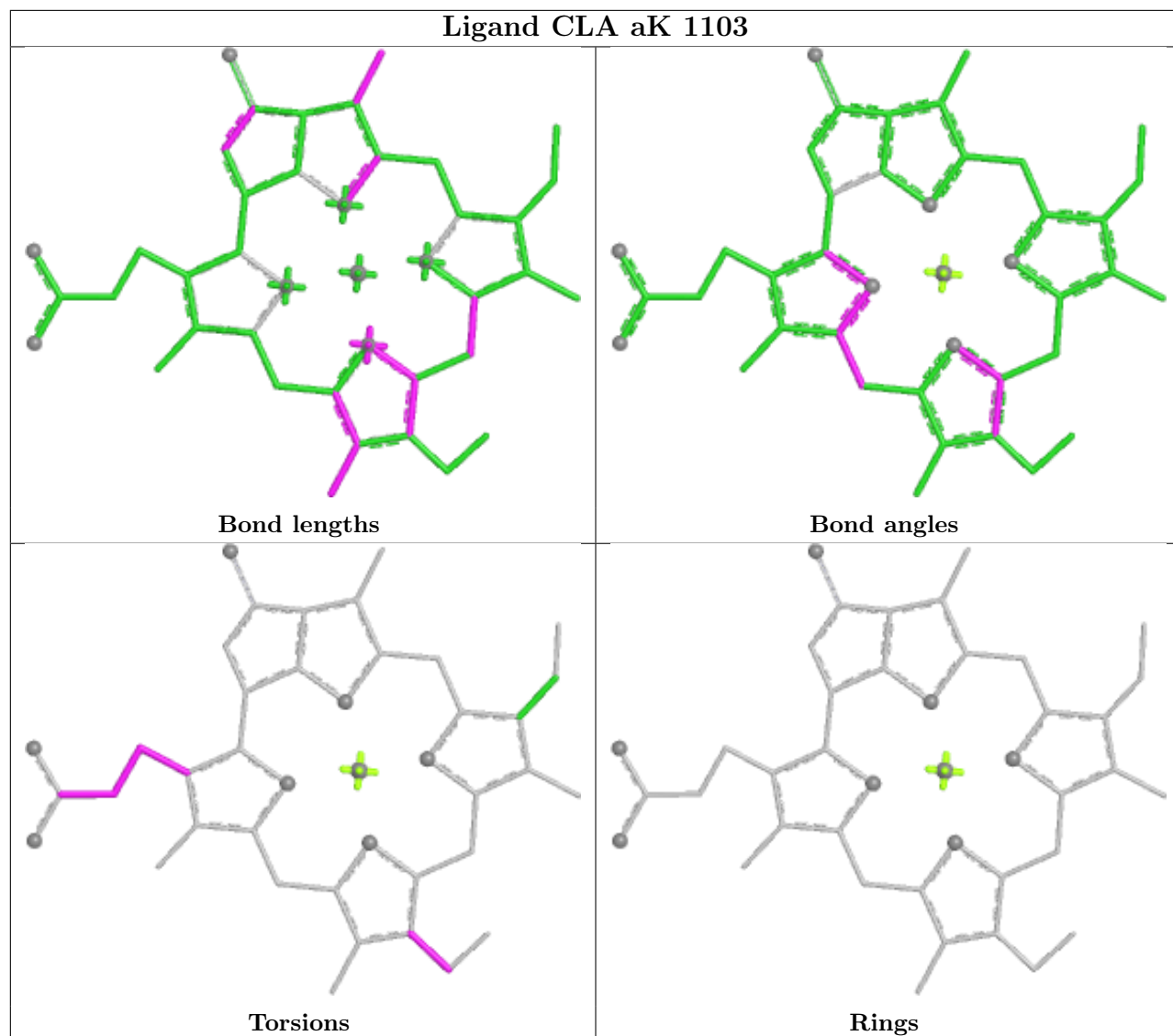
Bond angles



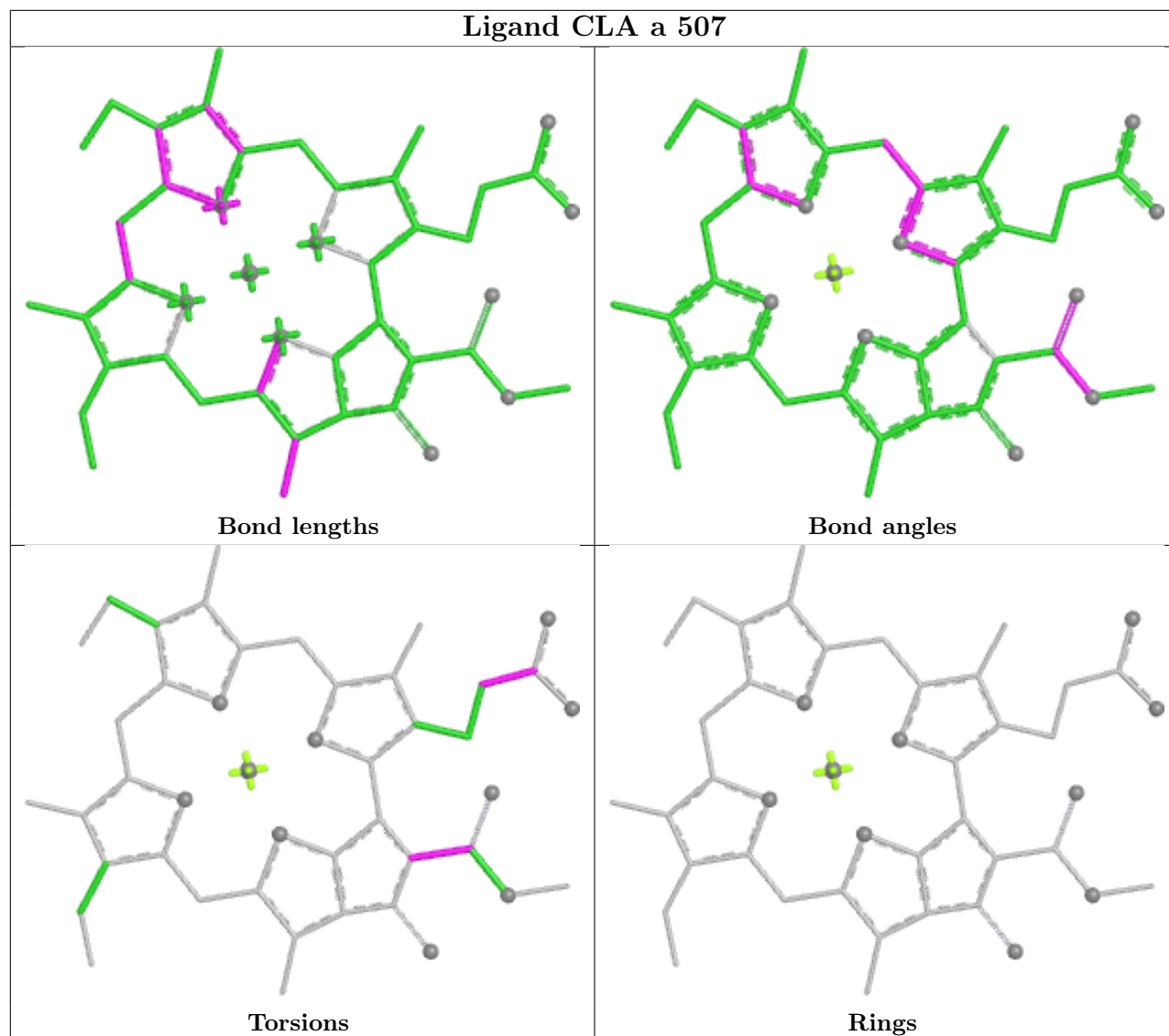
Torsions



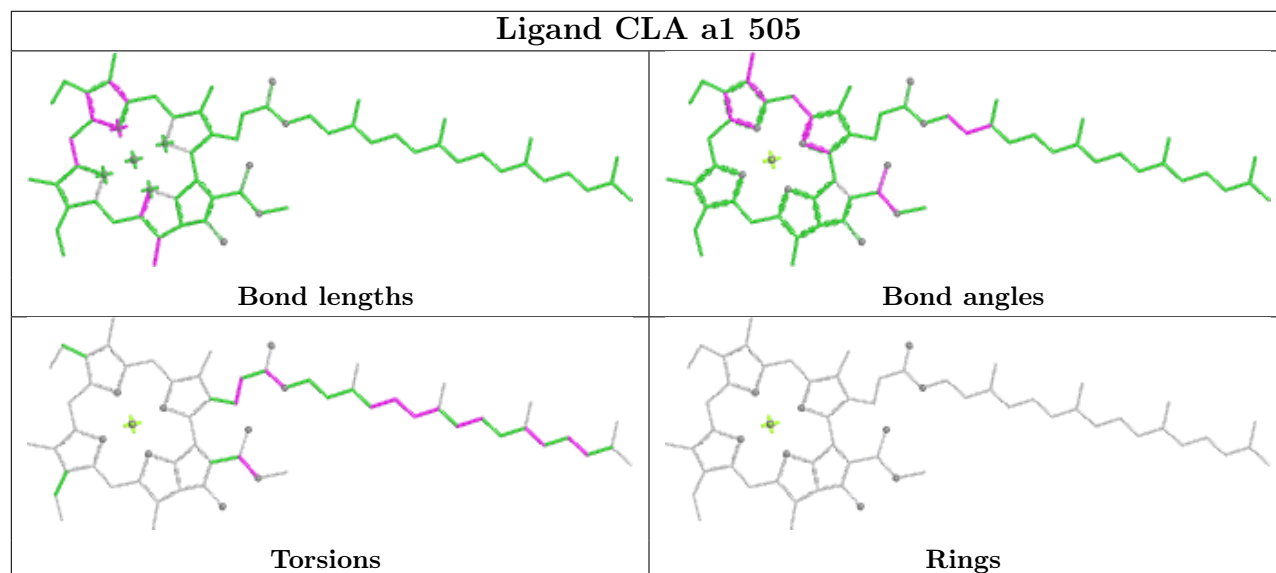
Rings

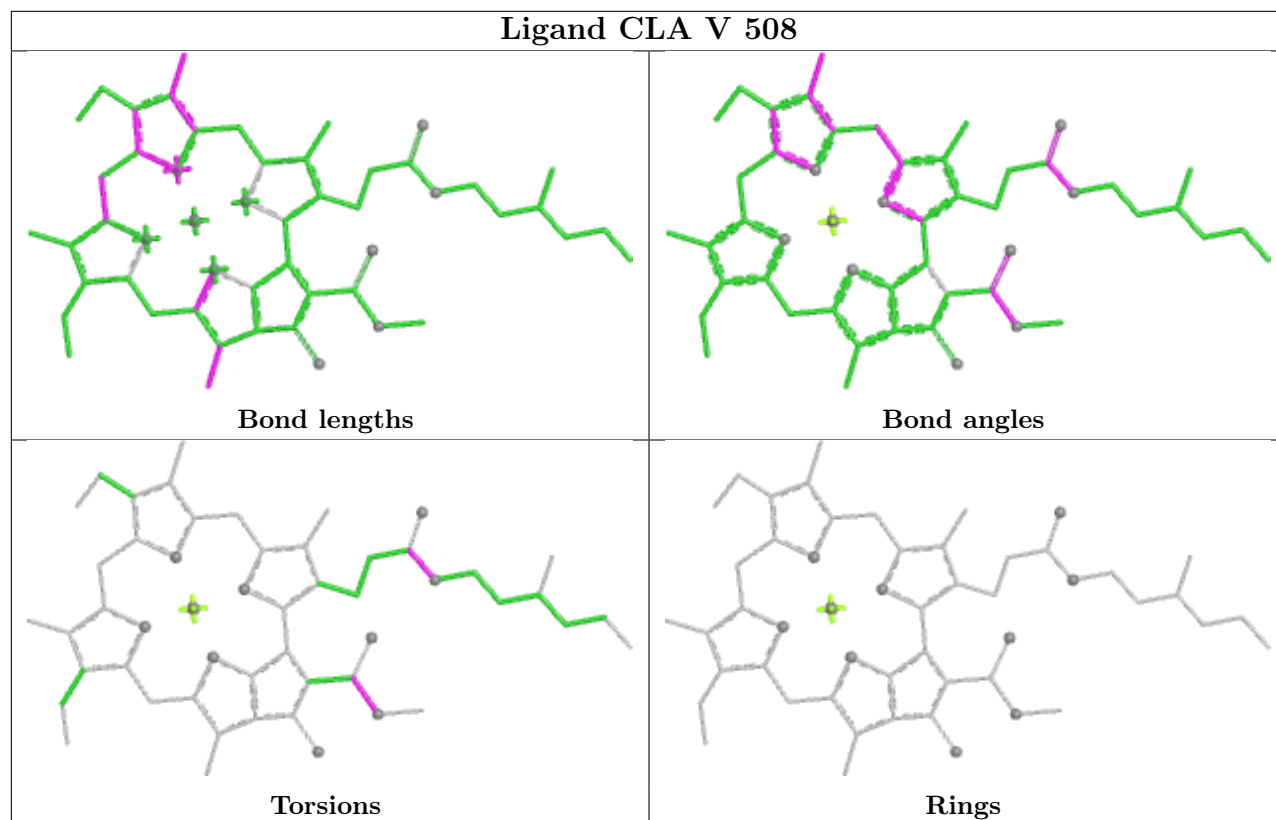
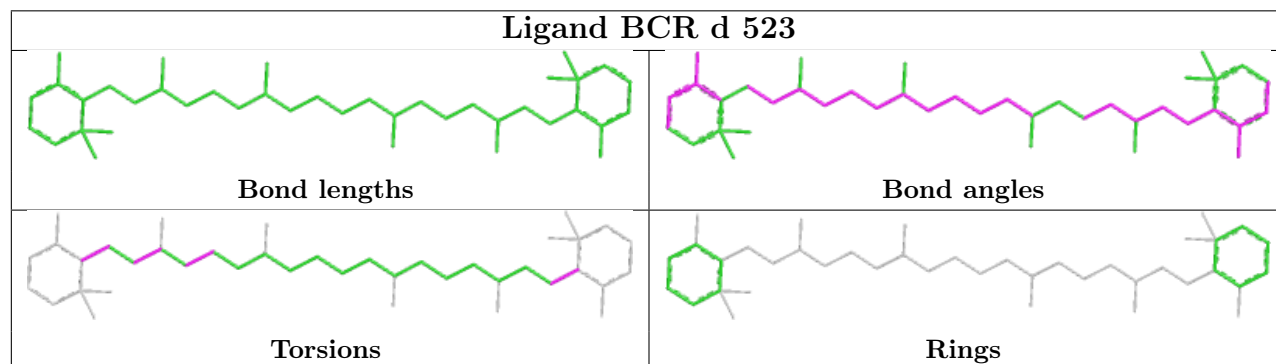
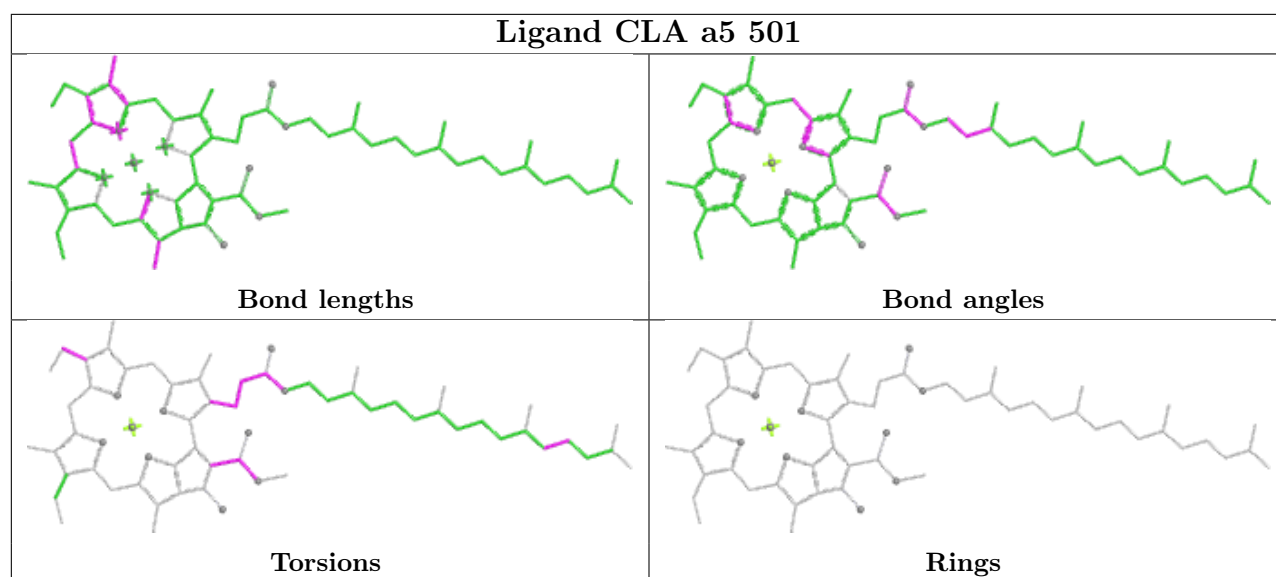


Ligand CLA a 507

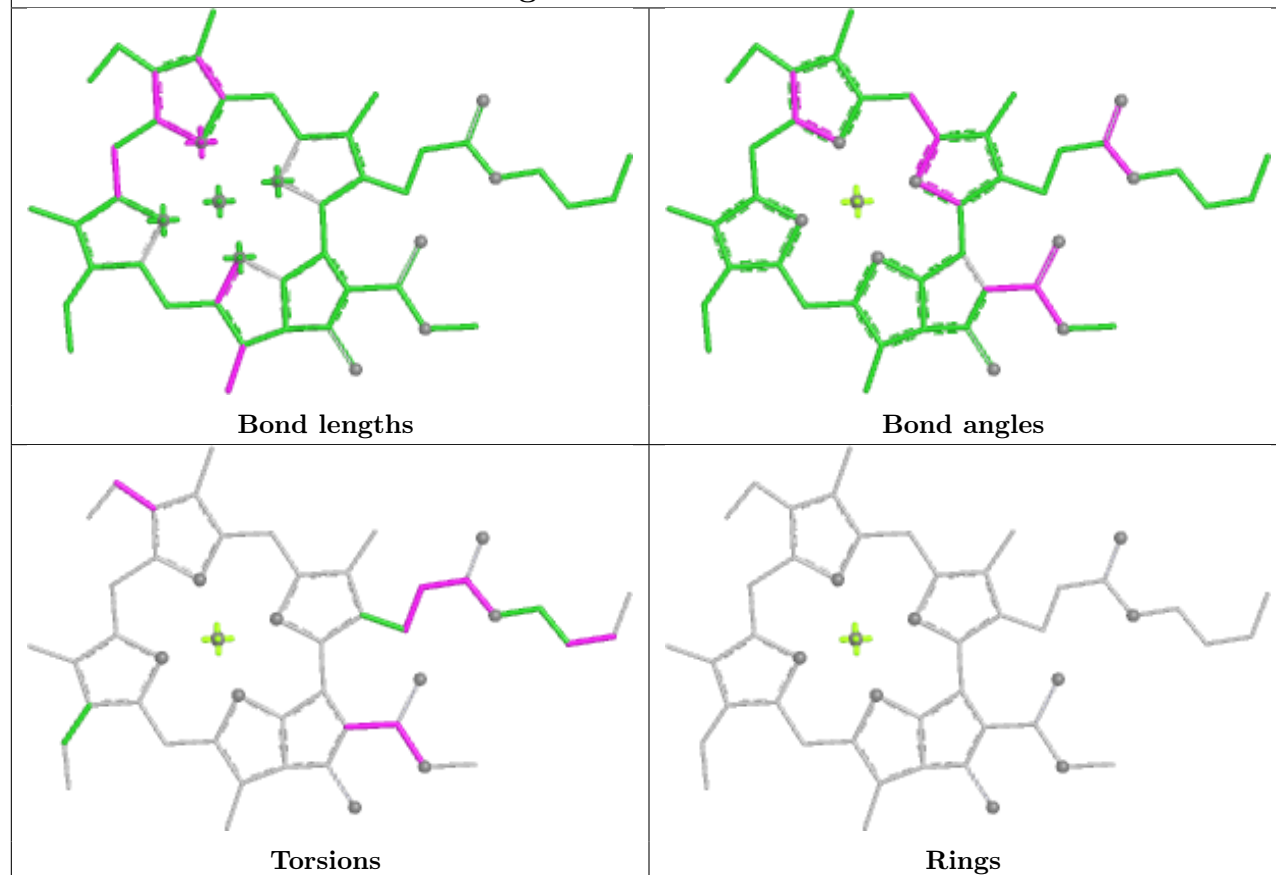


Ligand CLA a1 505

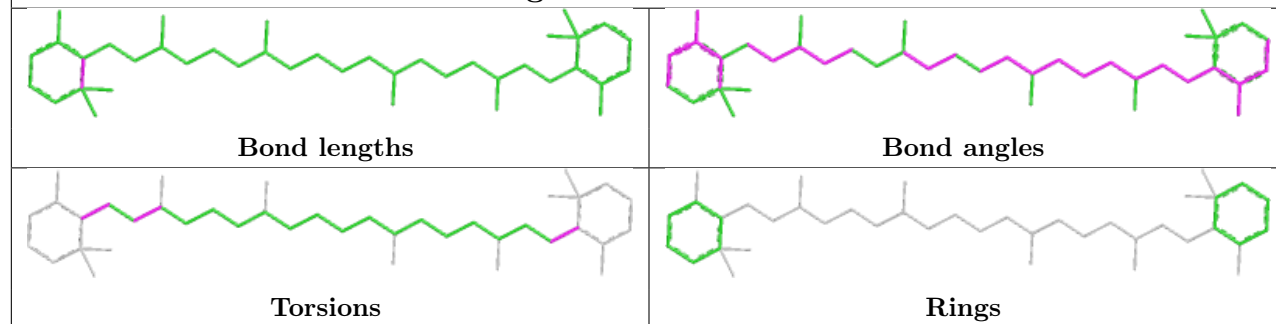


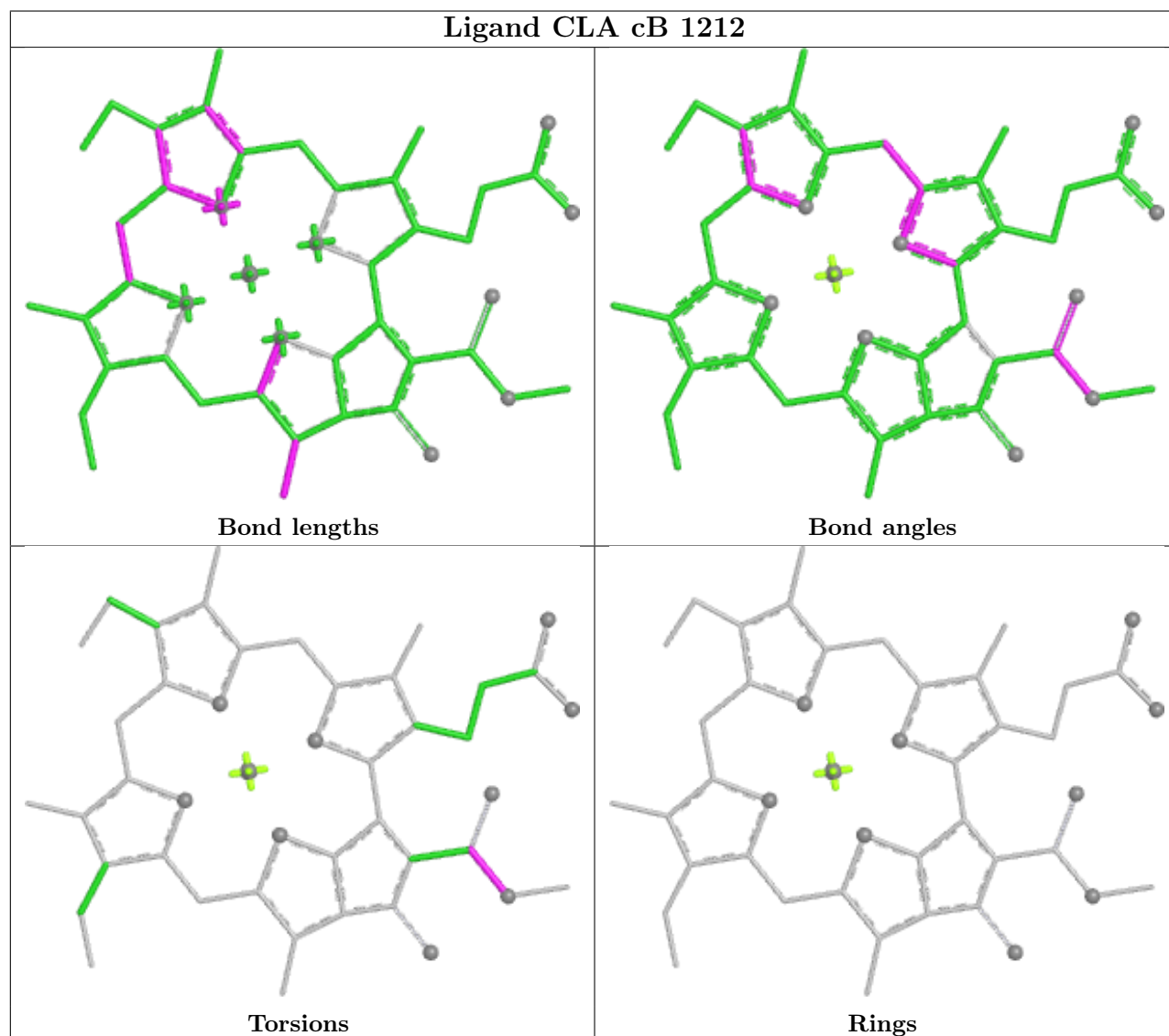
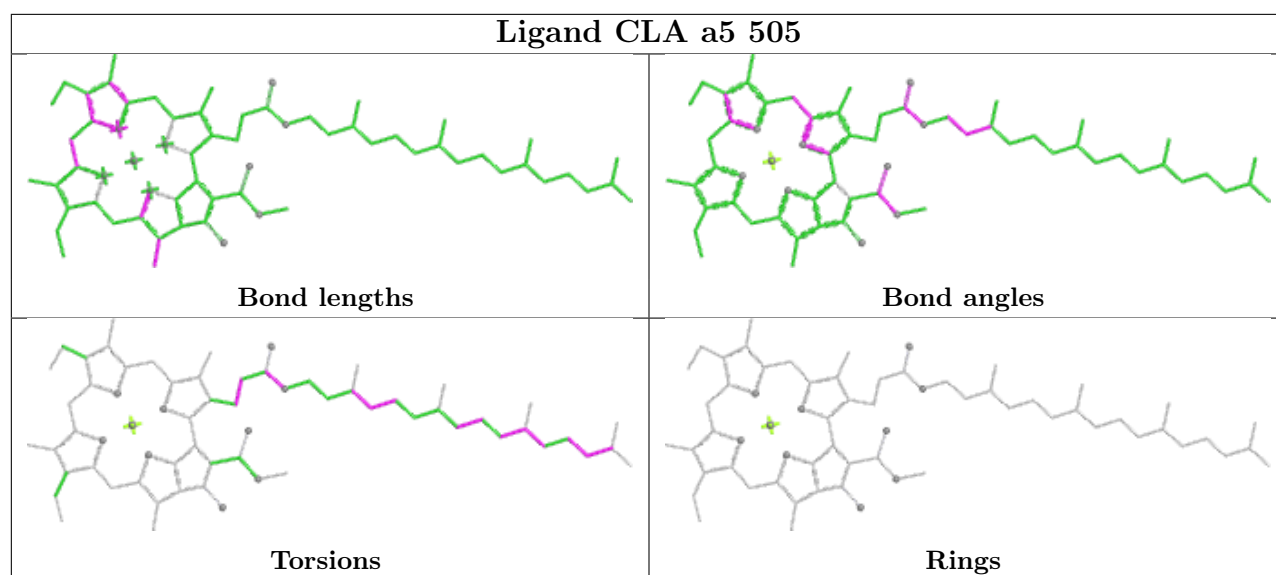


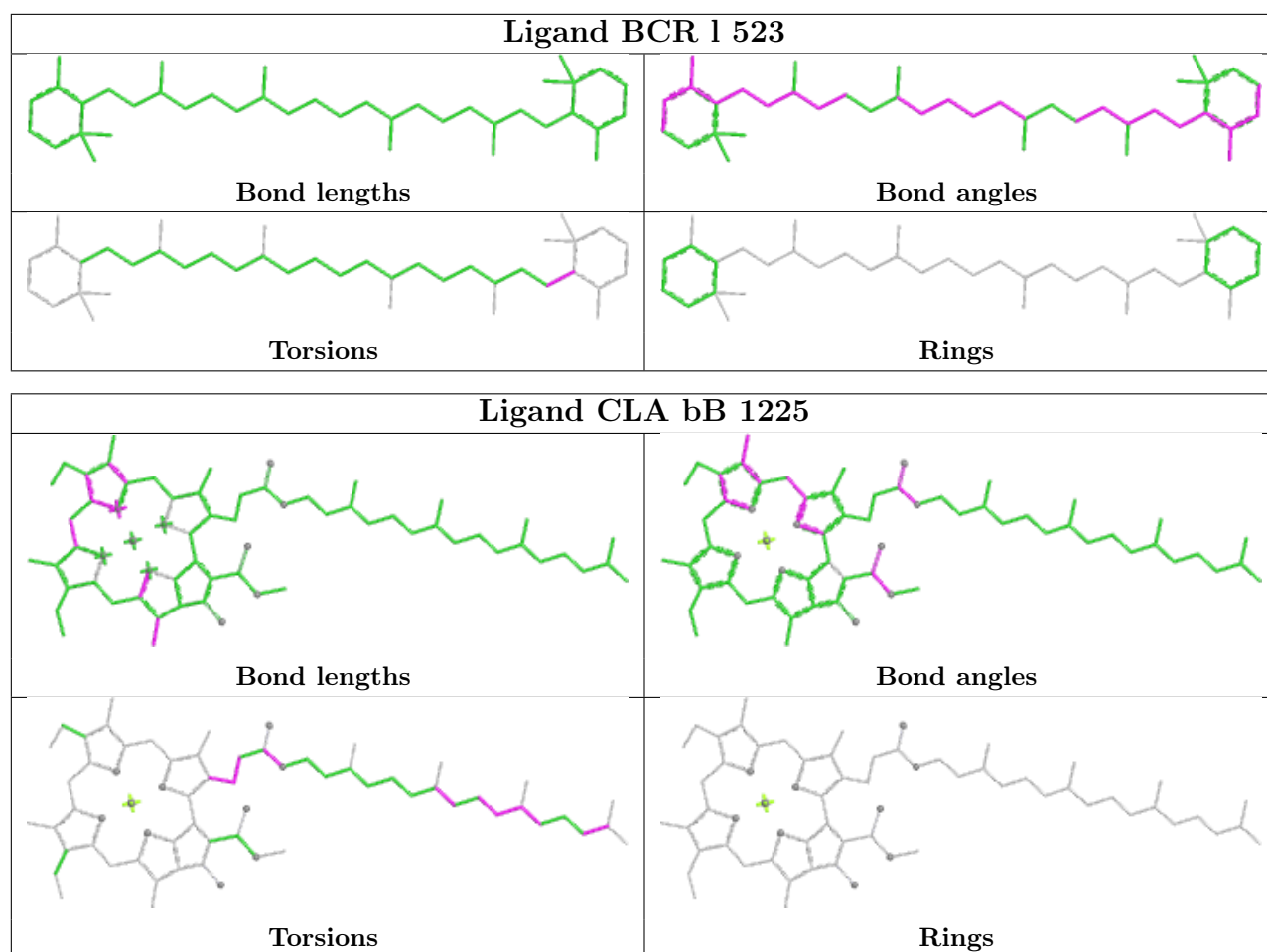
Ligand CLA cJ 1302

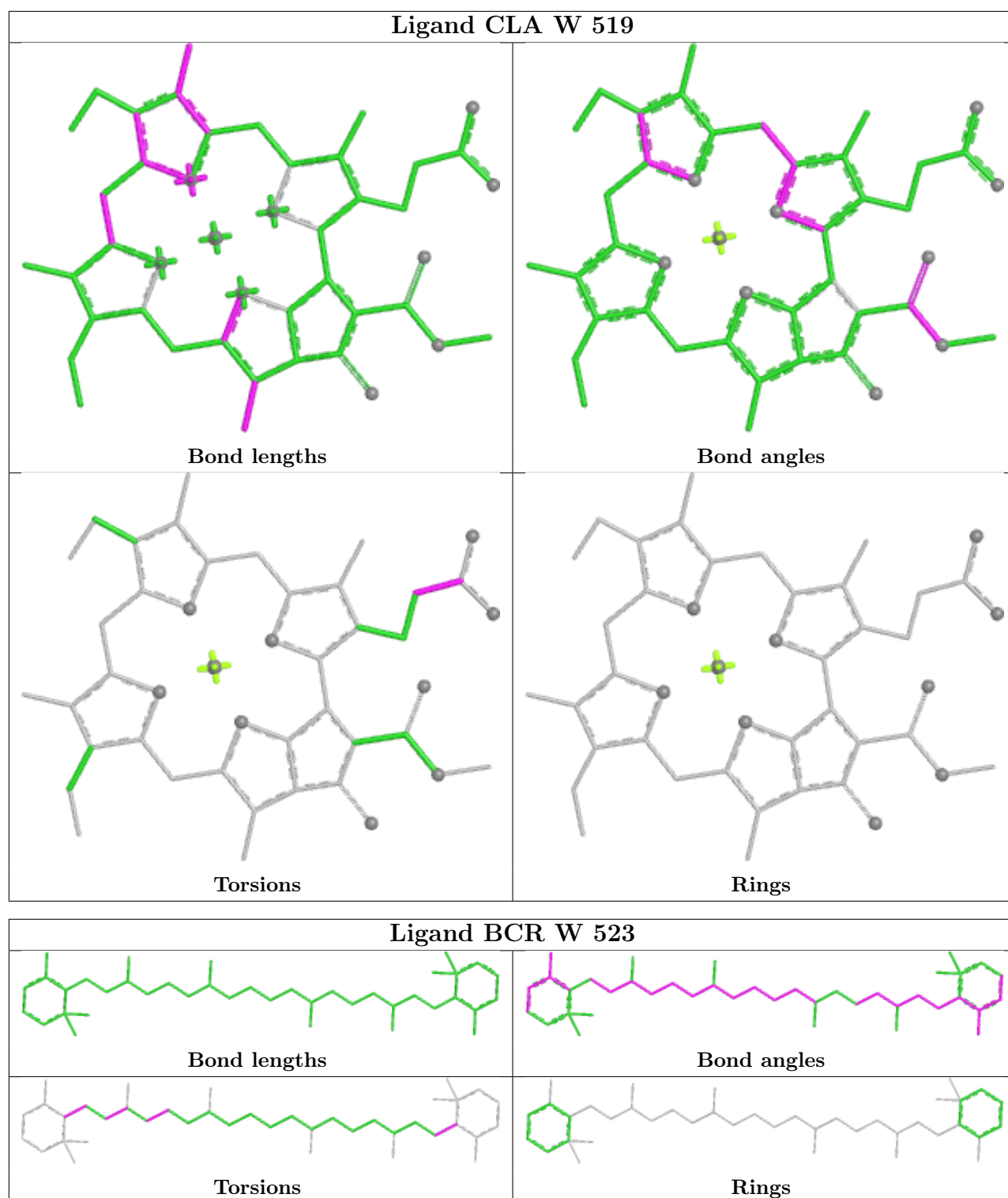


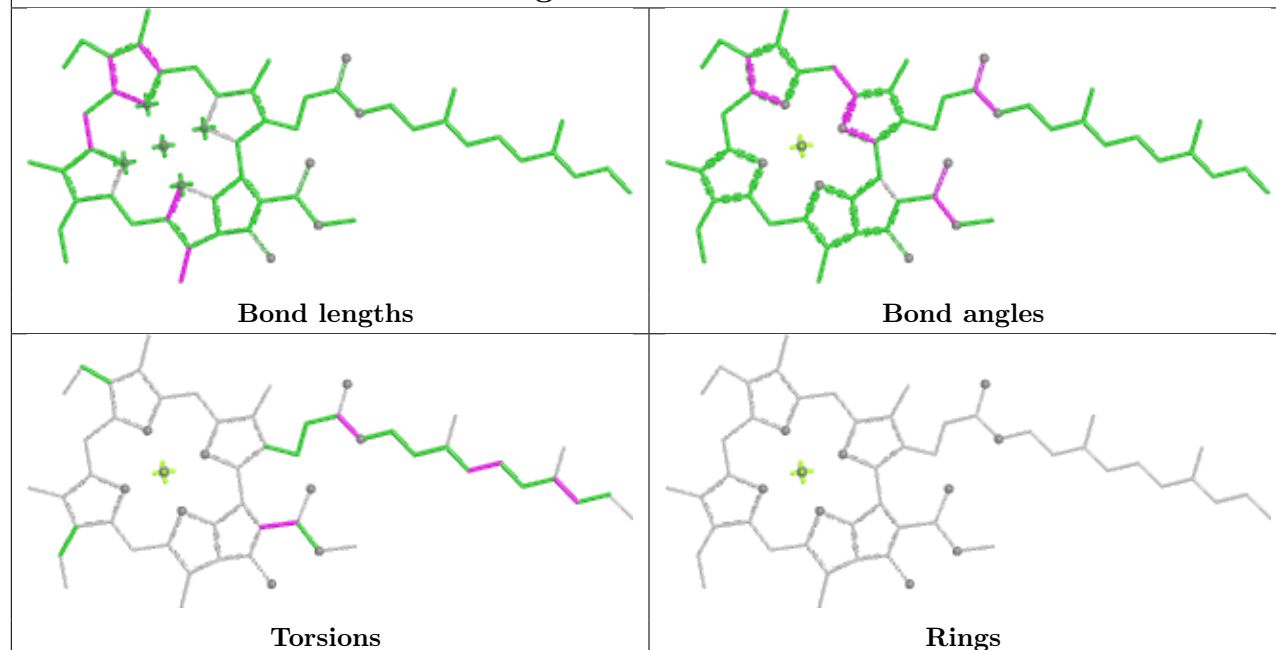
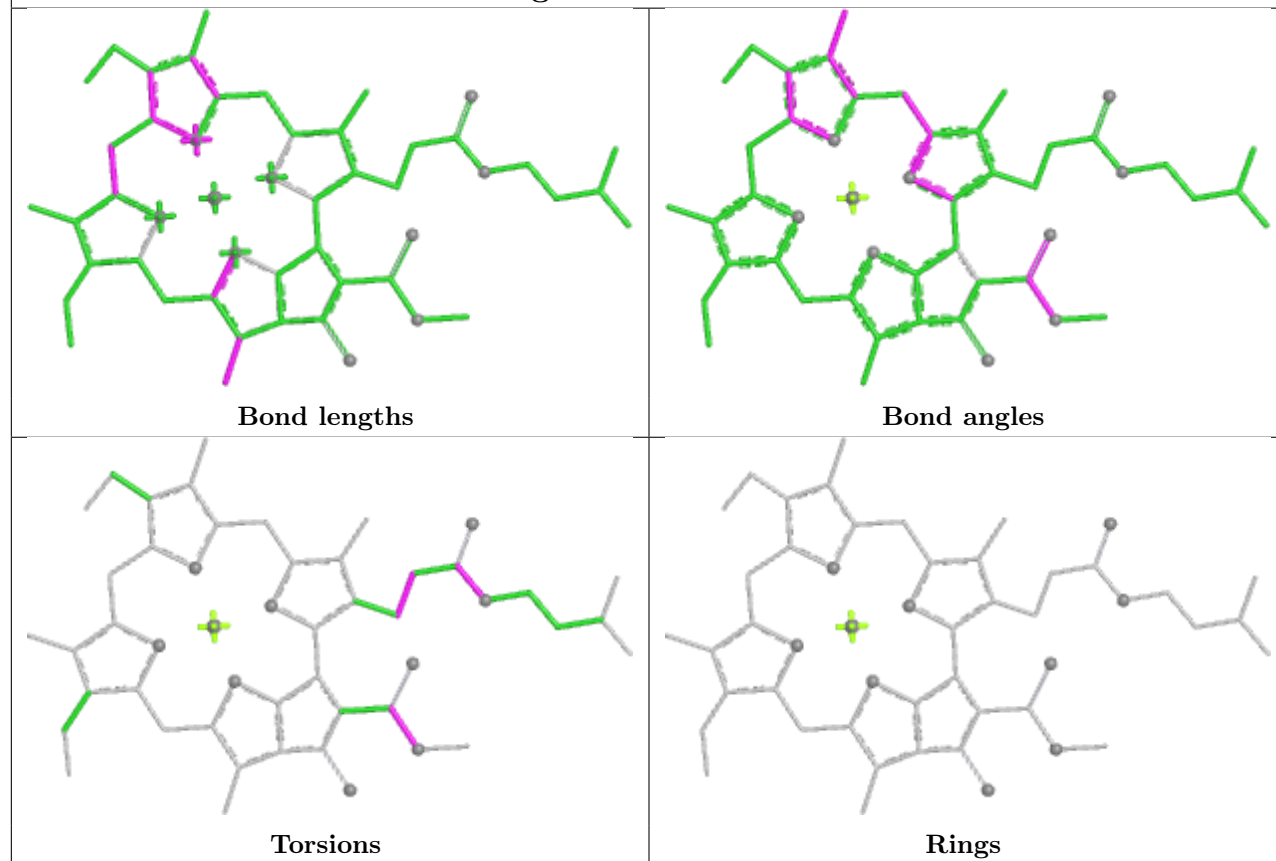
Ligand BCR c6 523

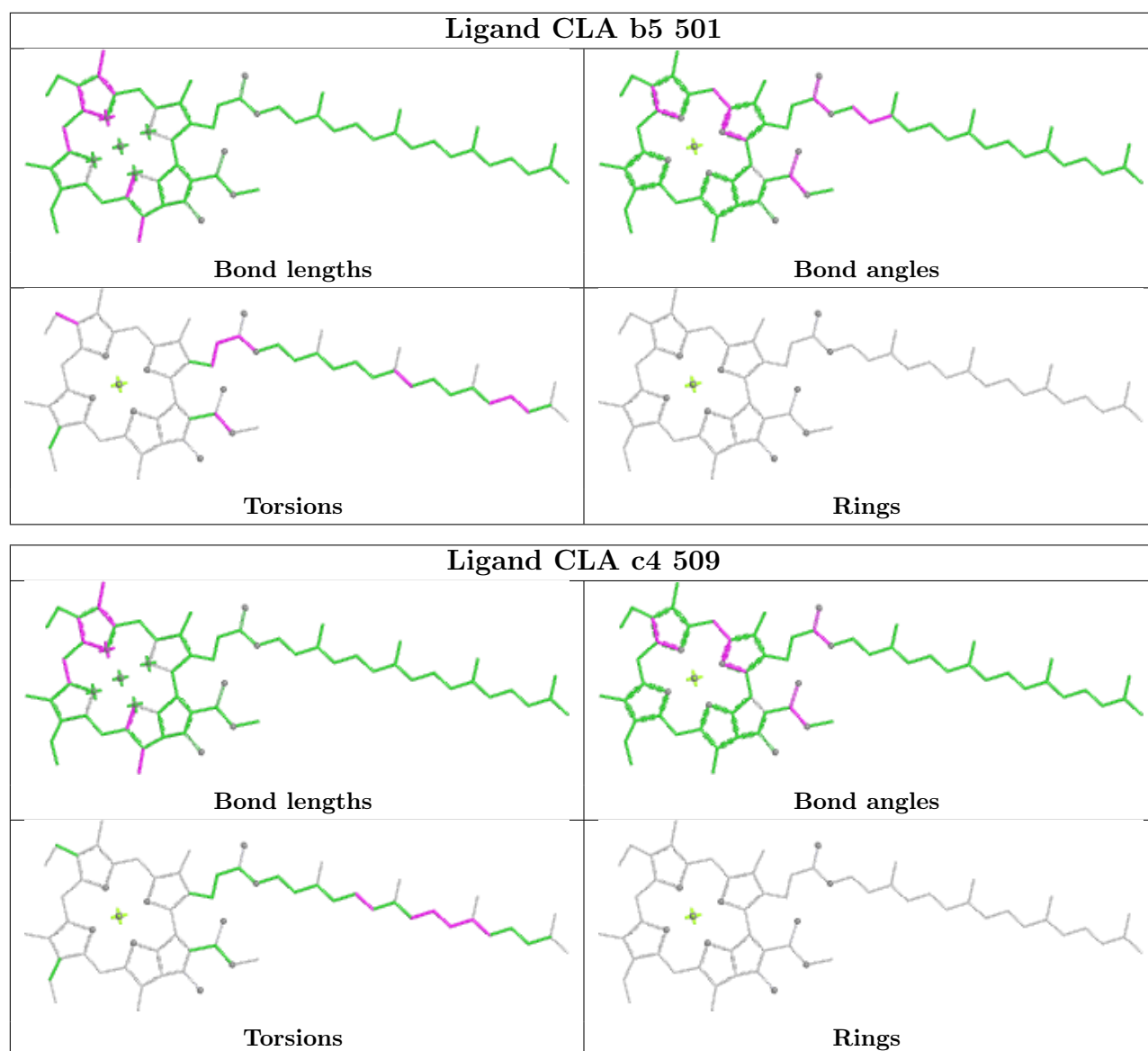


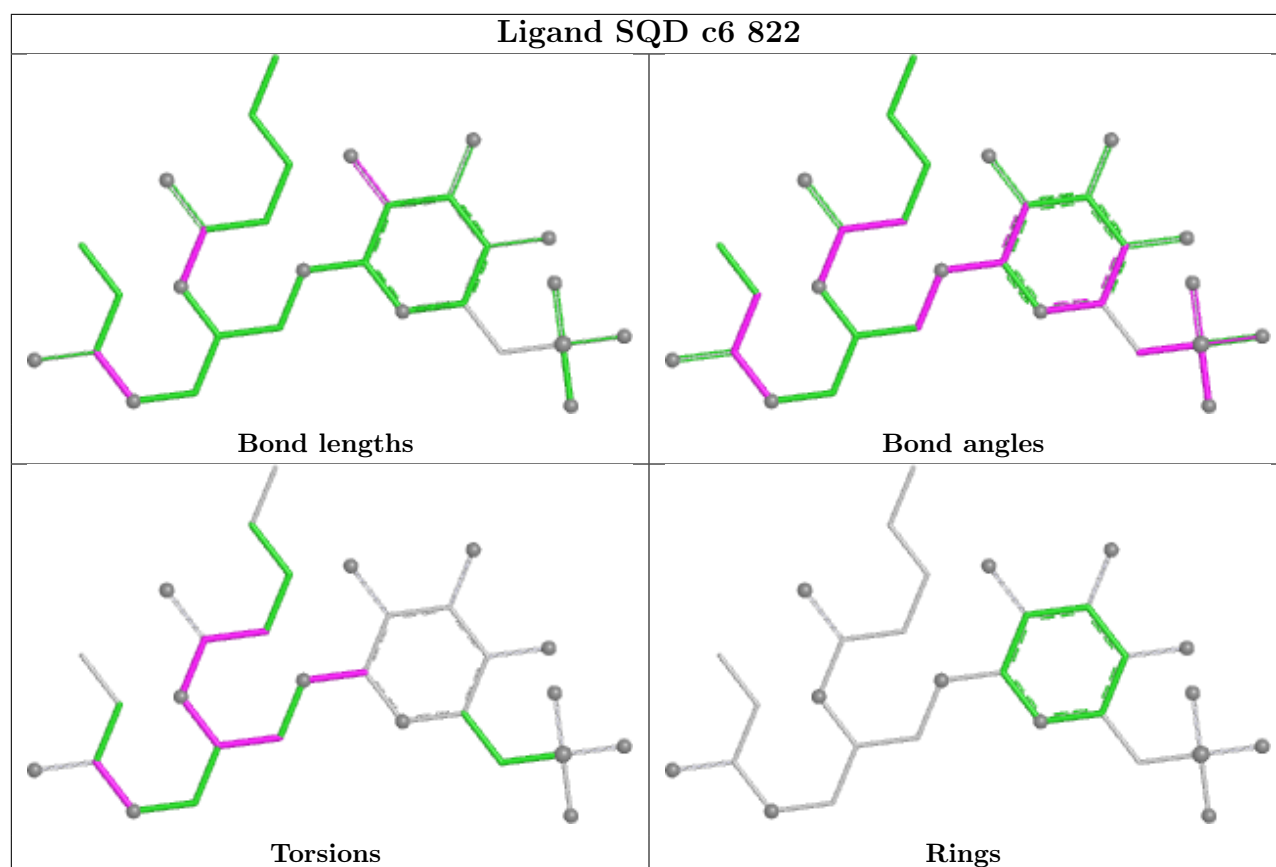


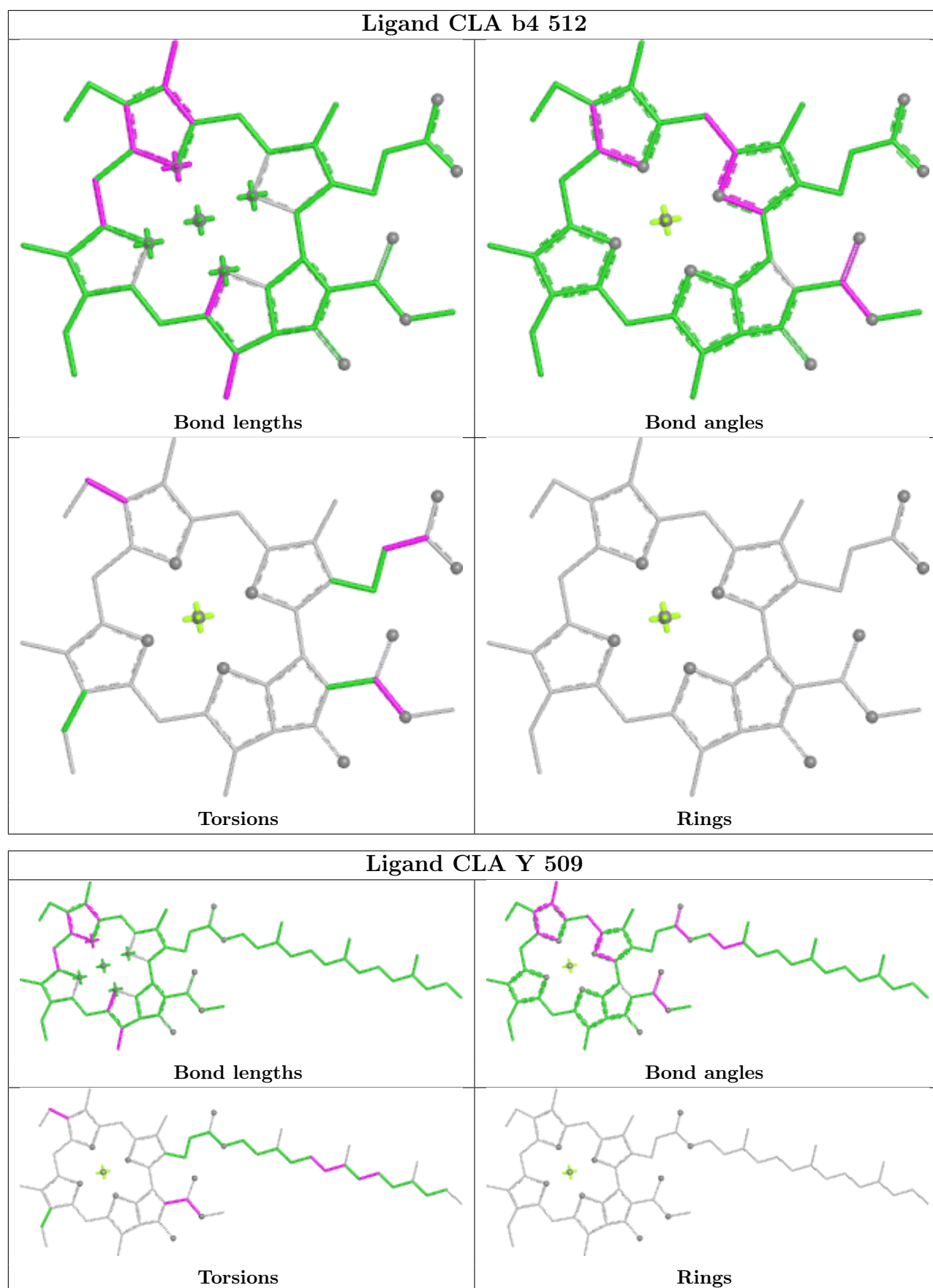




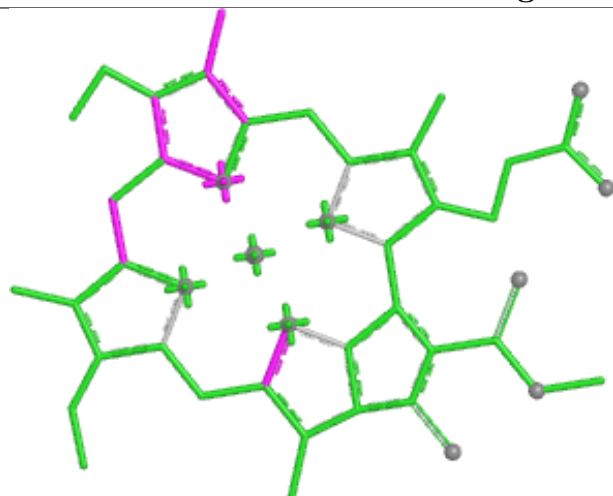
Ligand CLA b 503**Ligand CLA V 513**



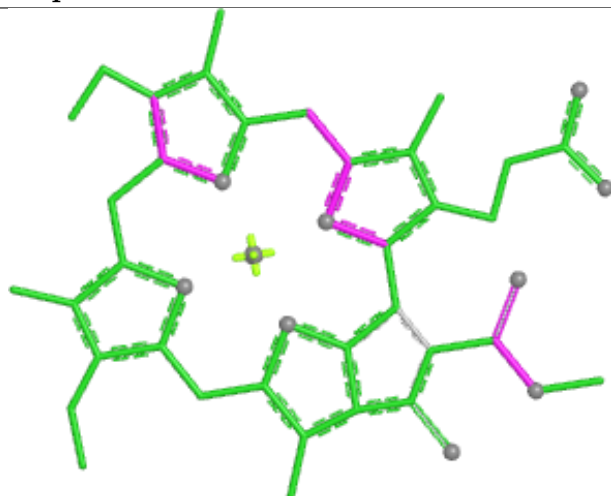




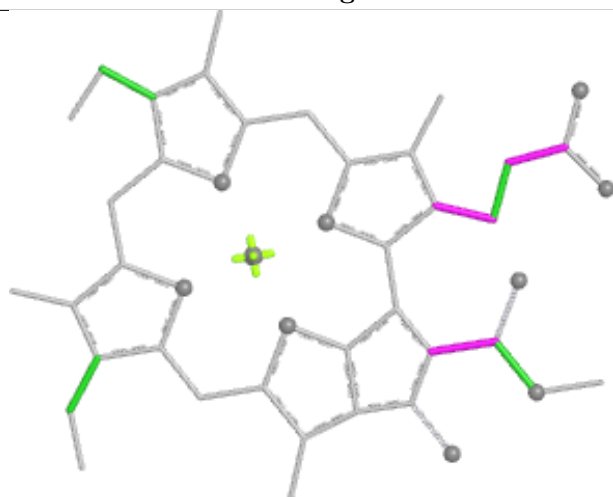
Ligand CLA p 517



Bond lengths



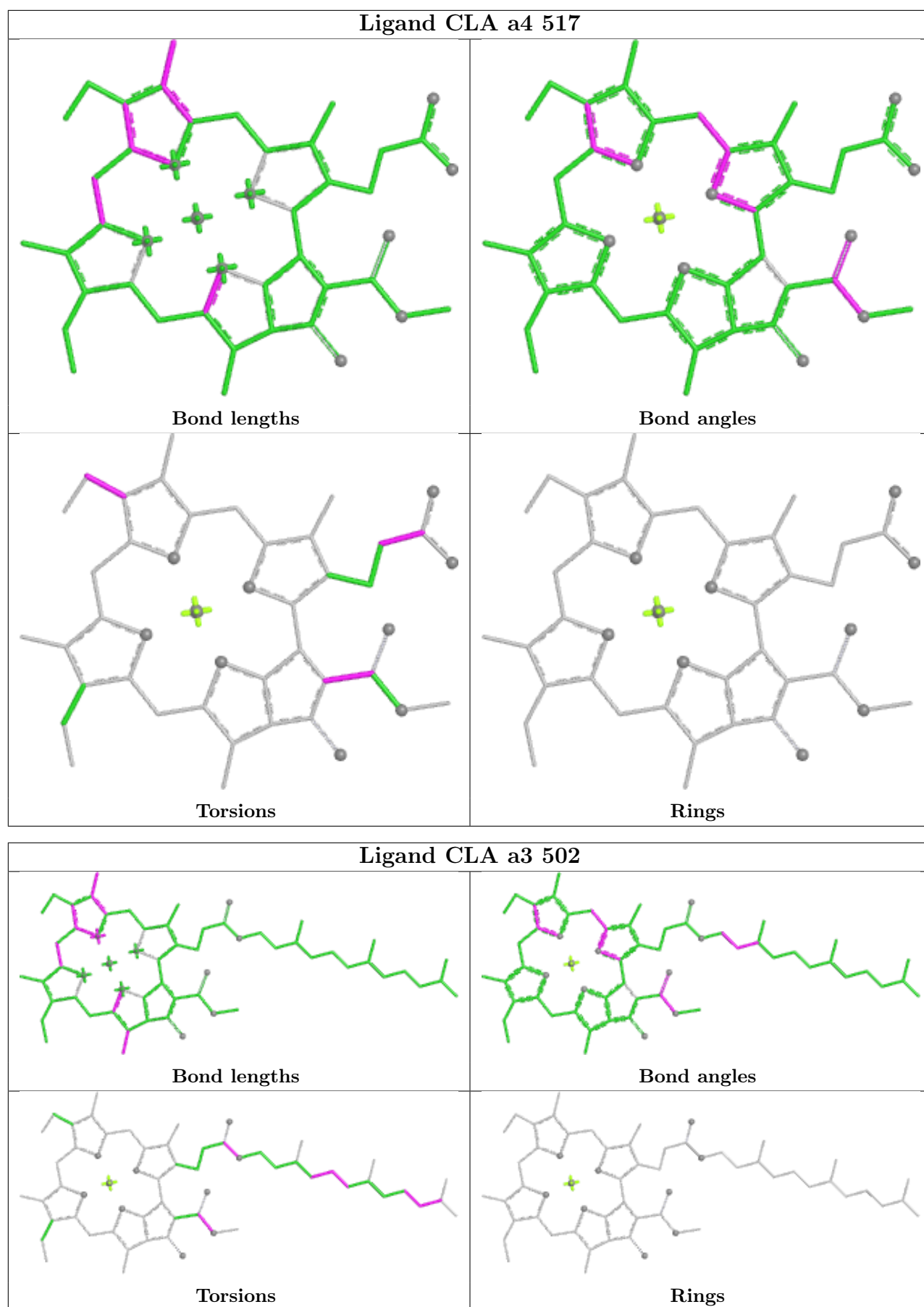
Bond angles

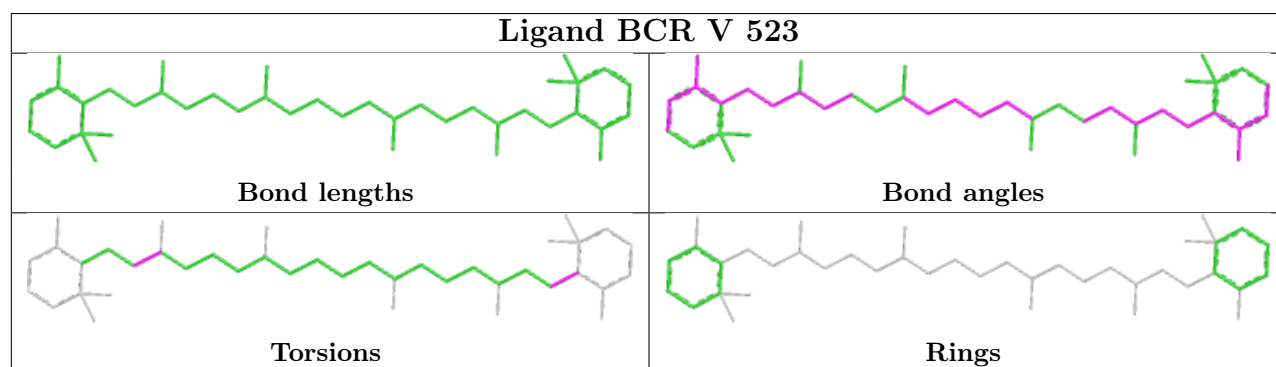
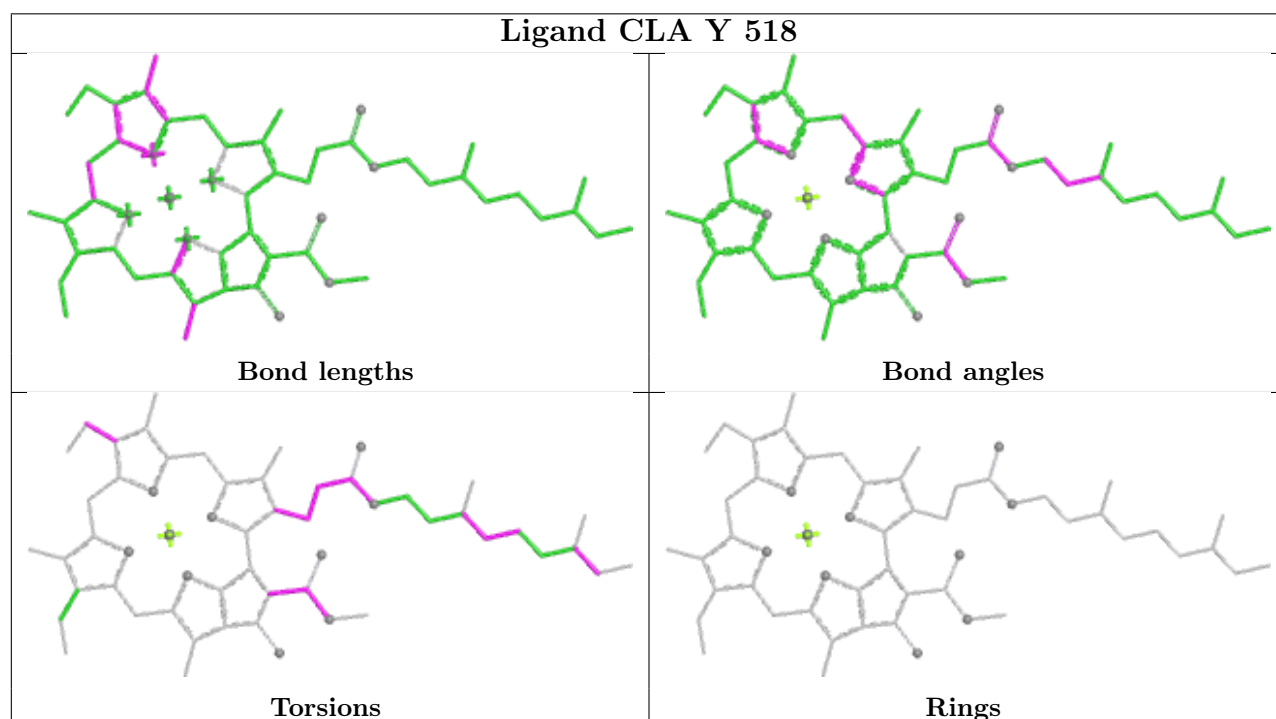
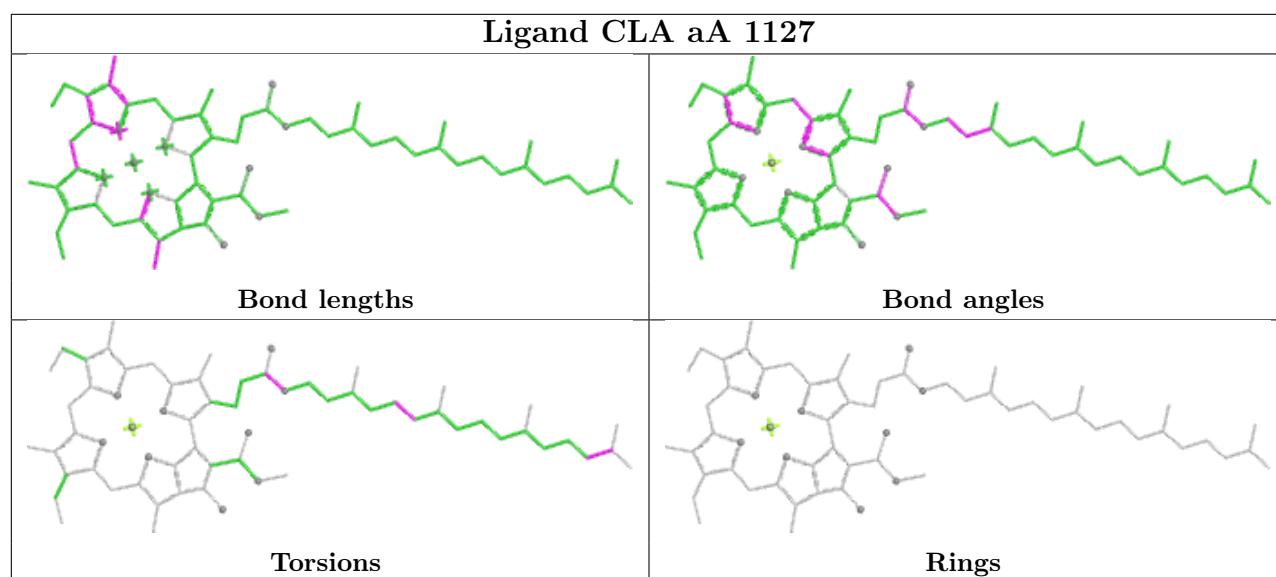


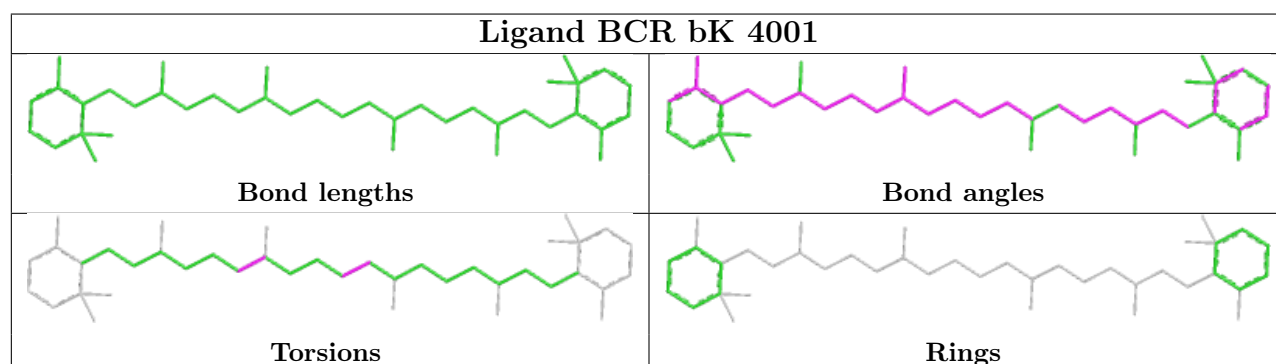
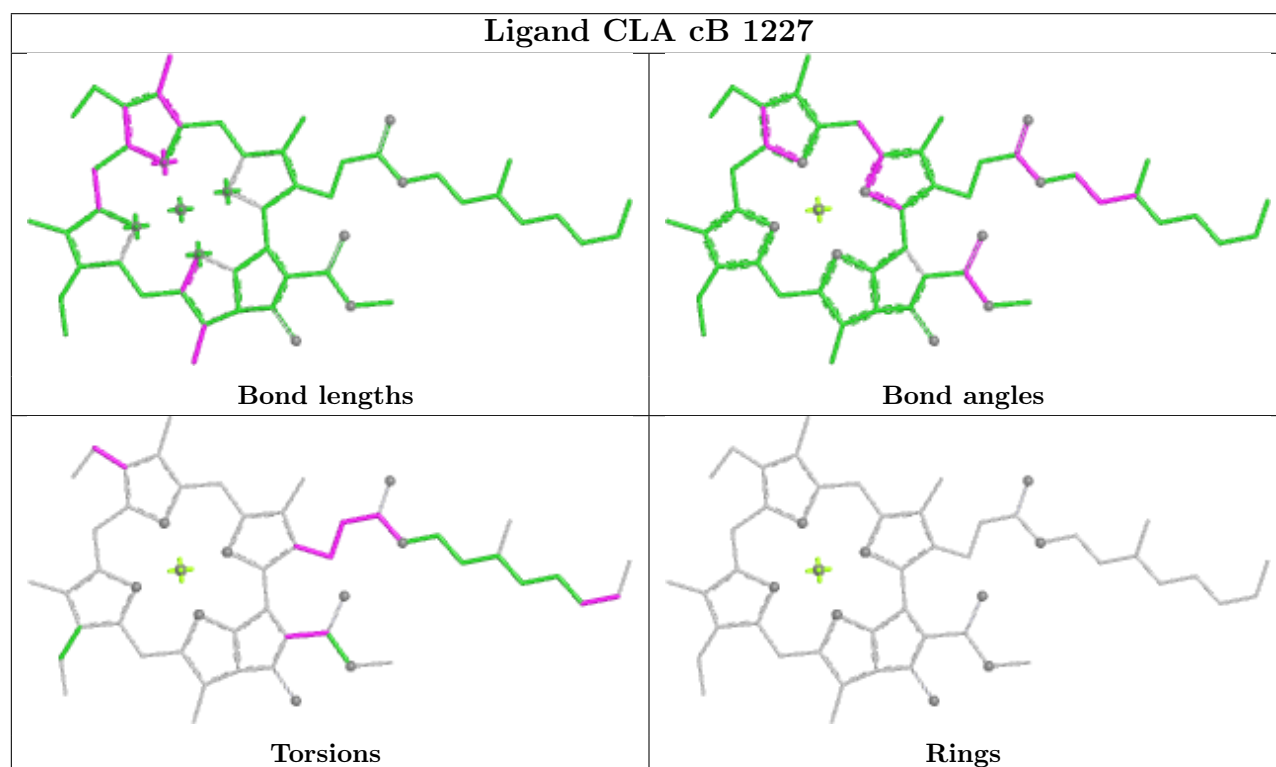
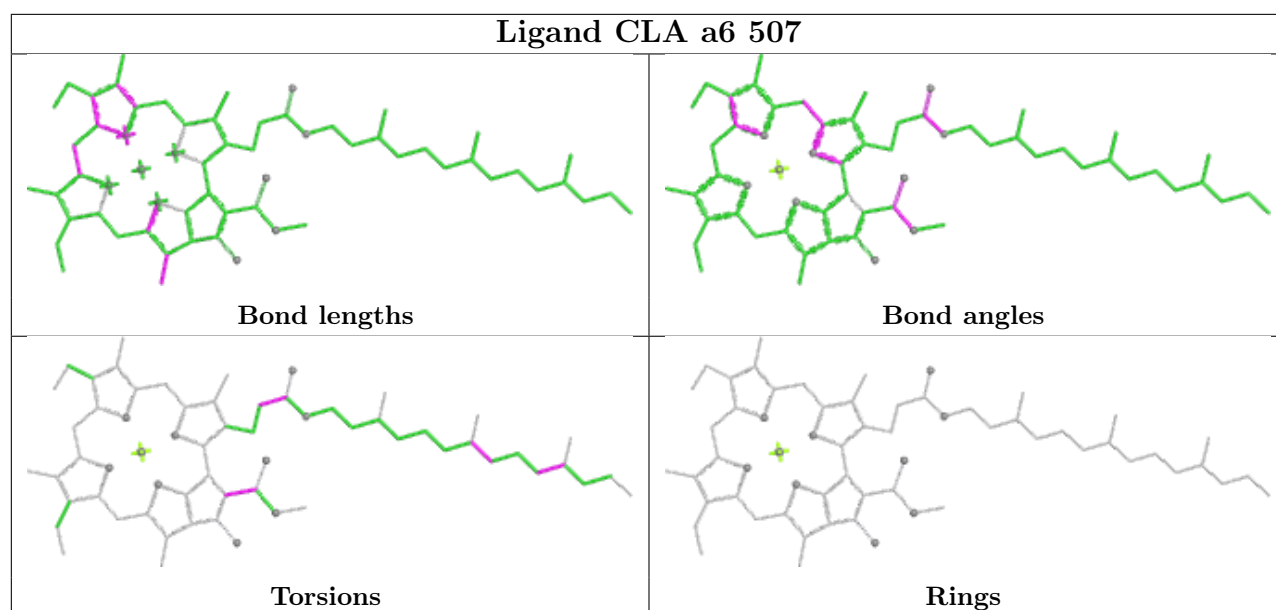
Torsions

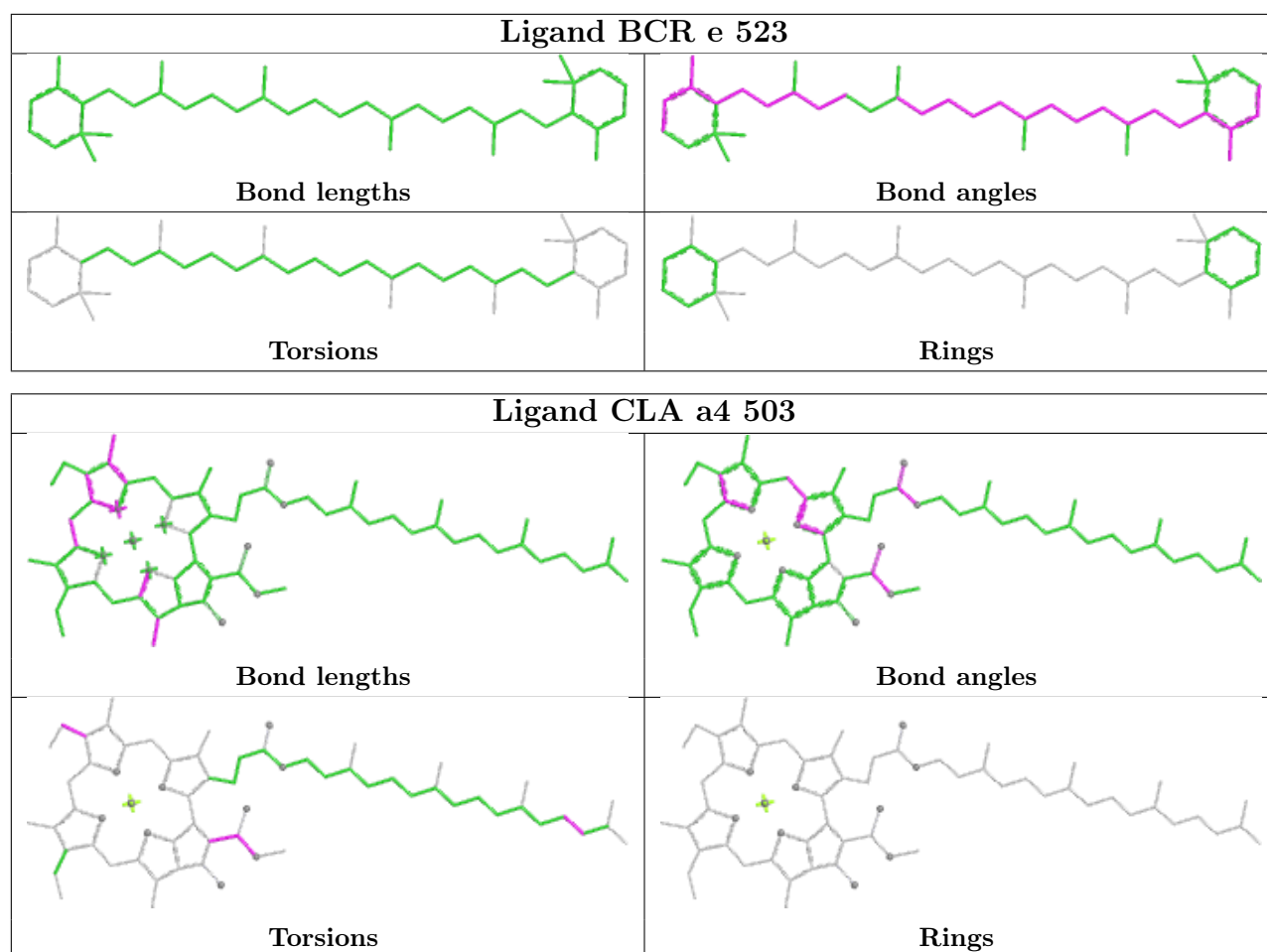


Rings

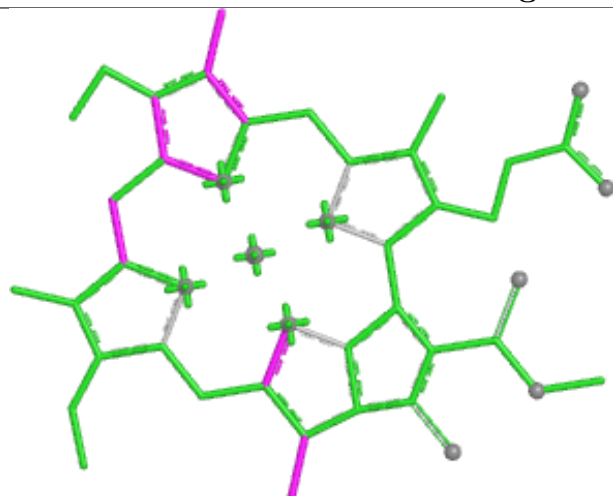








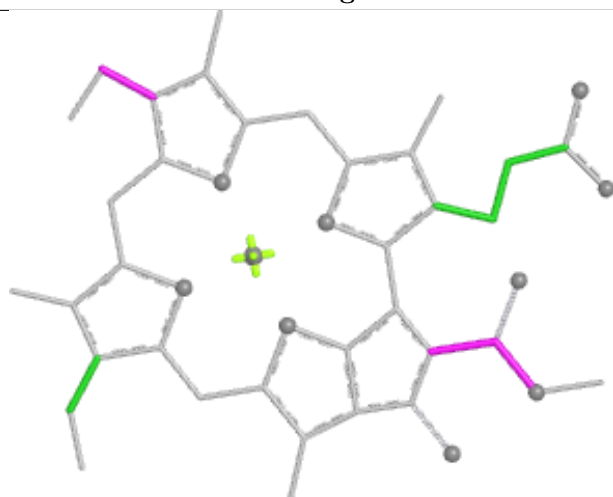
Ligand CLA e 503



Bond lengths



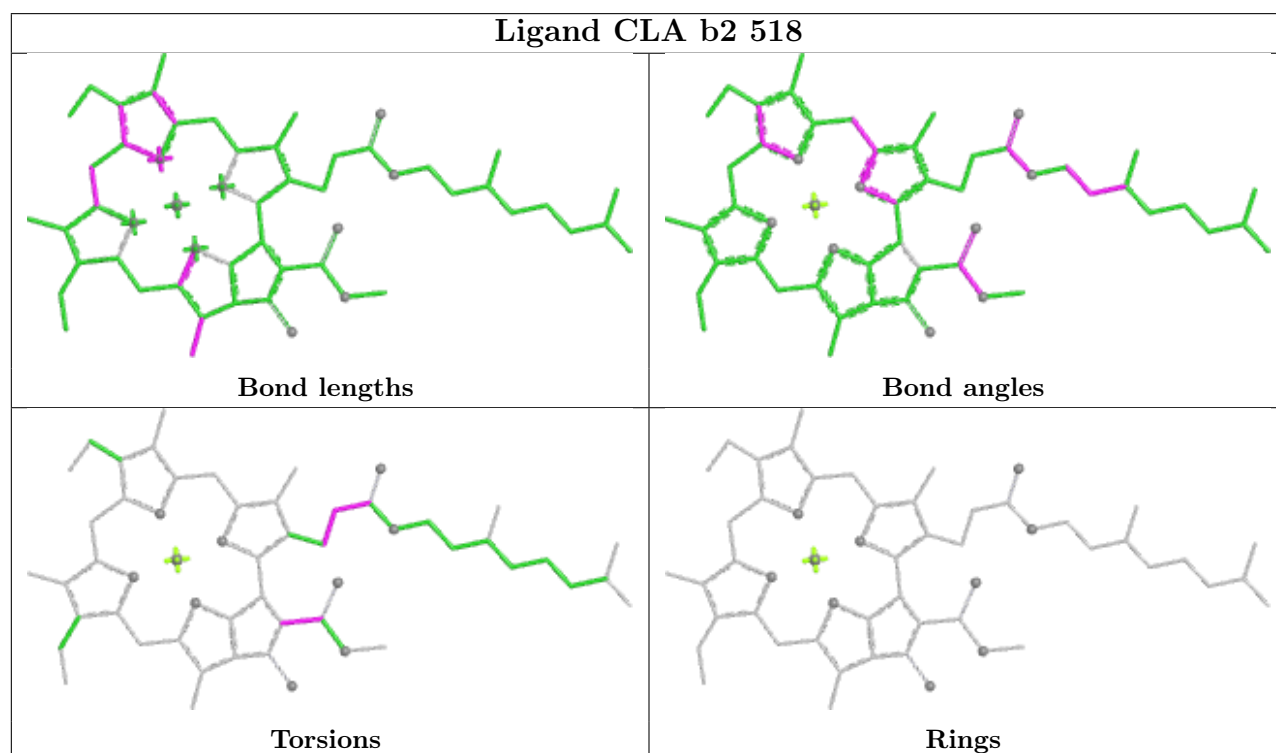
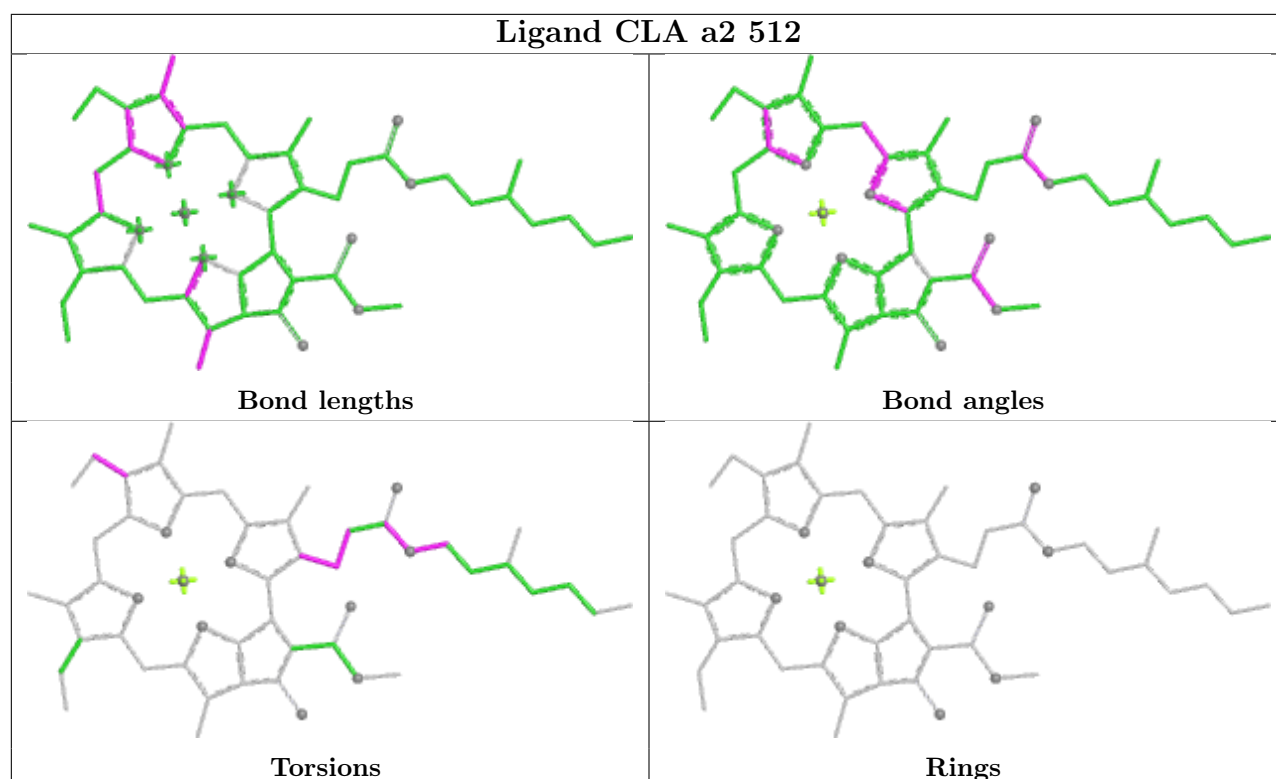
Bond angles



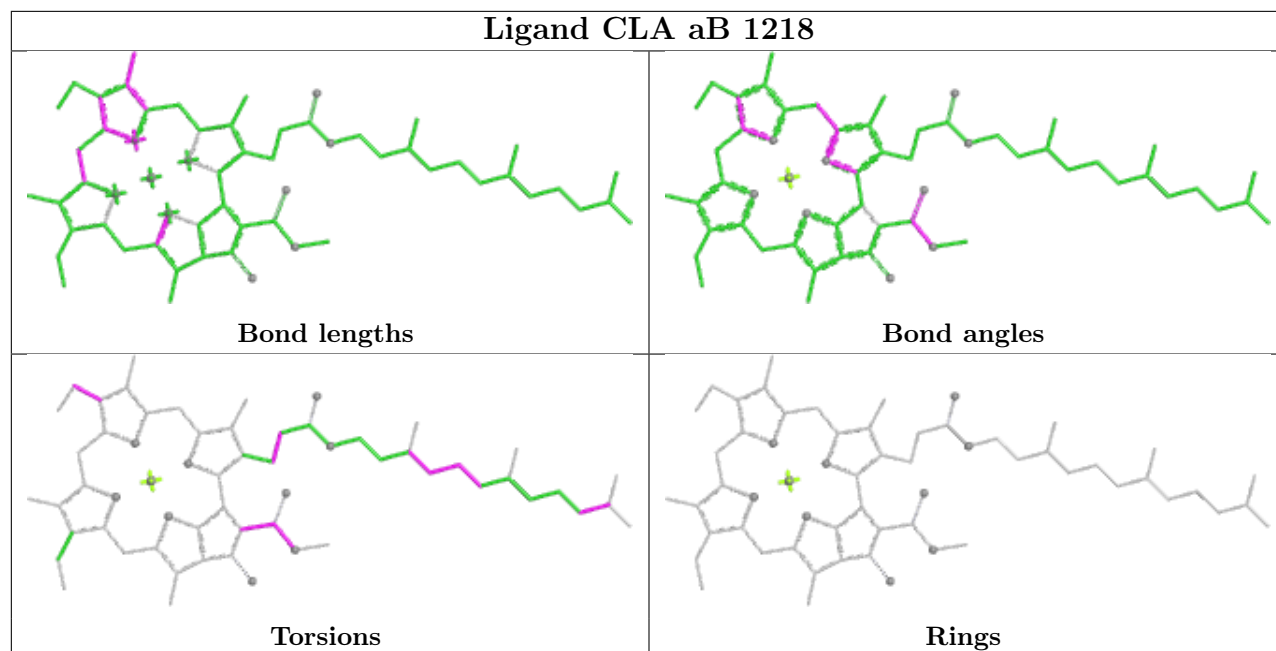
Torsions



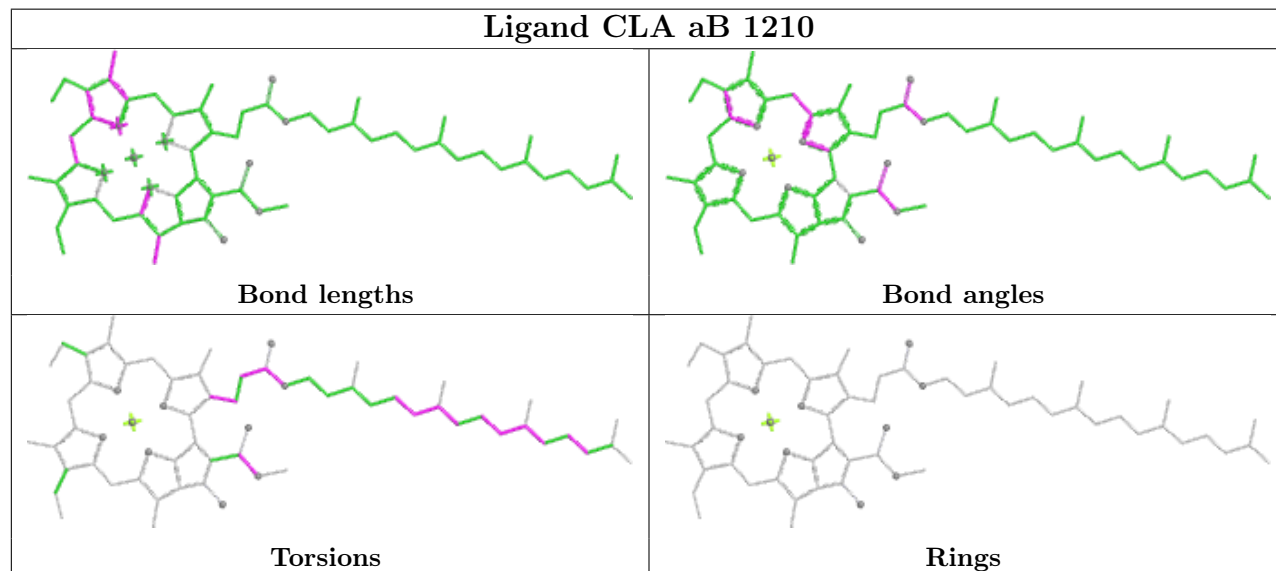
Rings

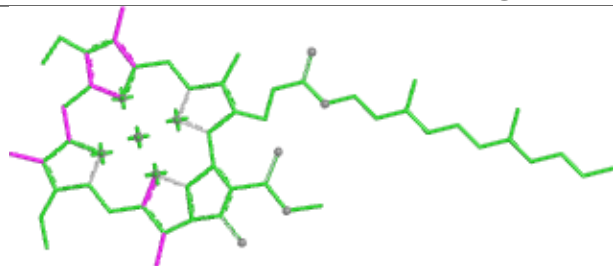
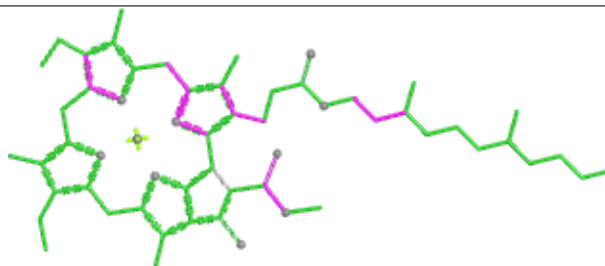
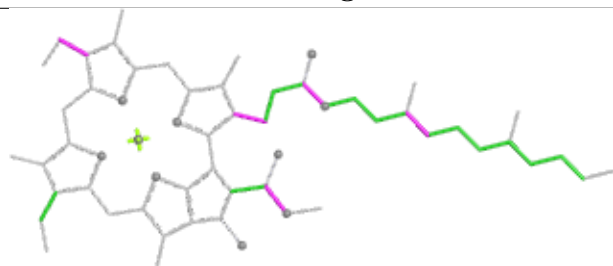
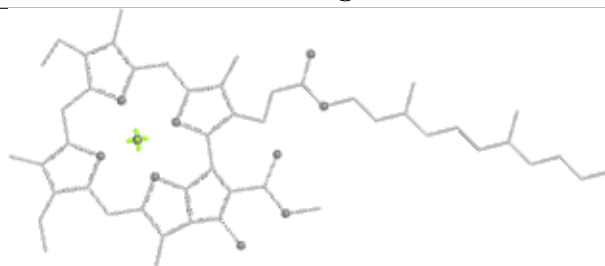
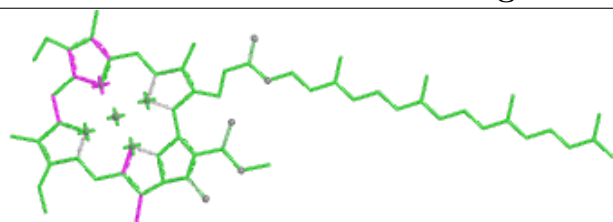
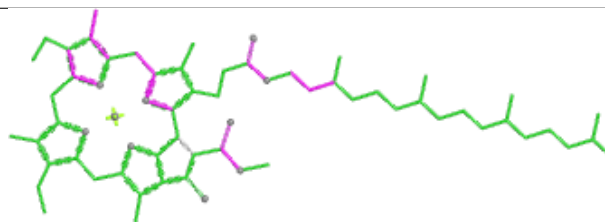
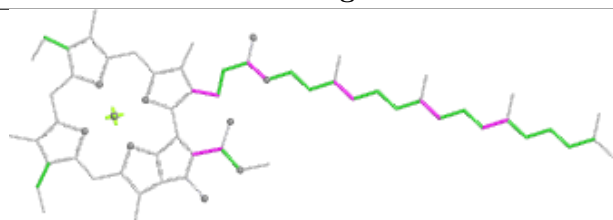
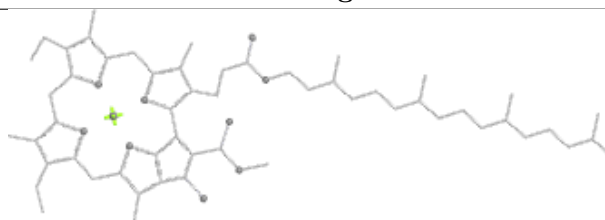


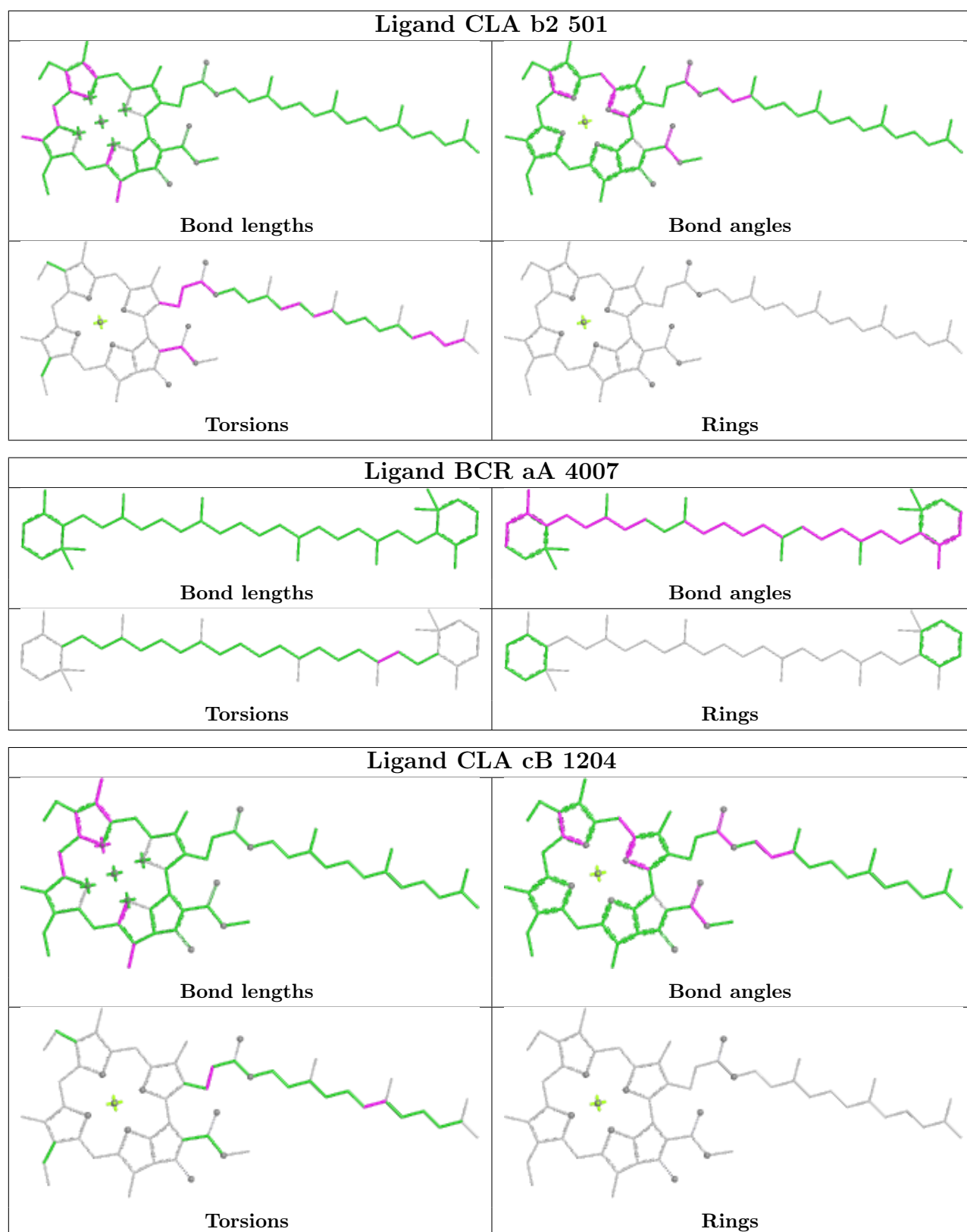
Ligand CLA aB 1218



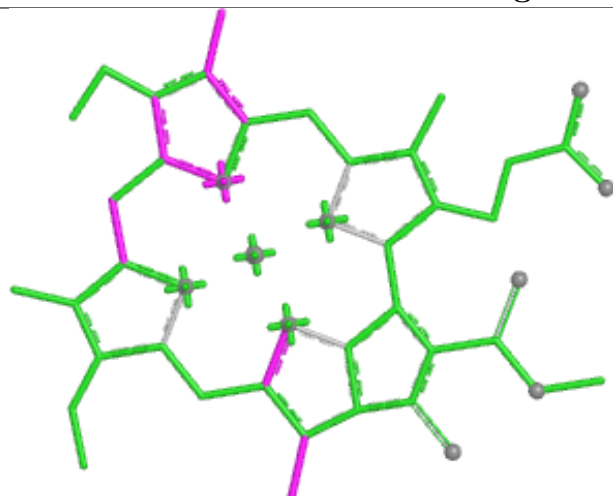
Ligand CLA aB 1210



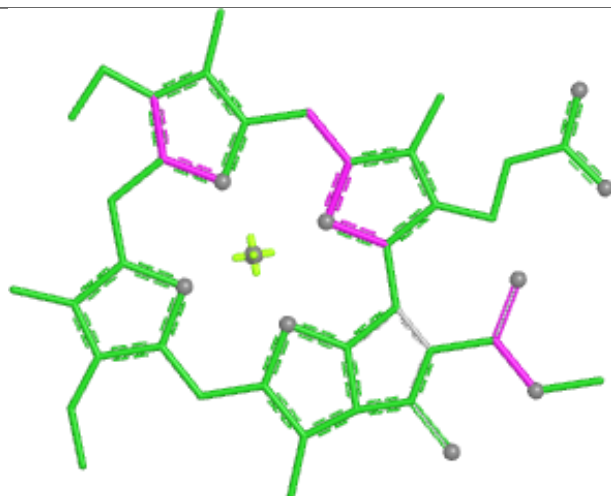
Ligand CLA bB 1230**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA bL 1501****Bond lengths****Bond angles****Torsions****Rings**



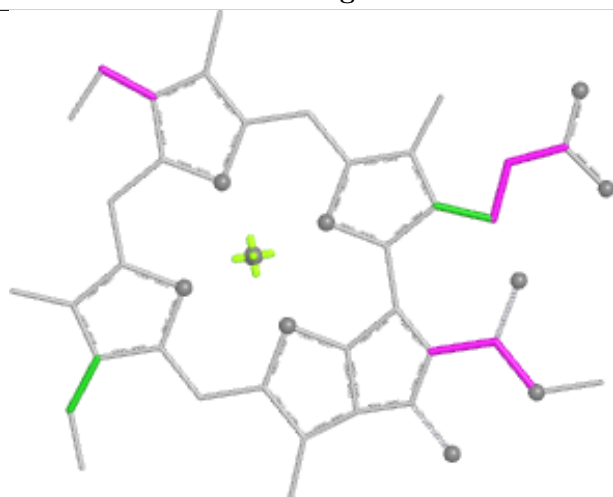
Ligand CLA V 512



Bond lengths



Bond angles

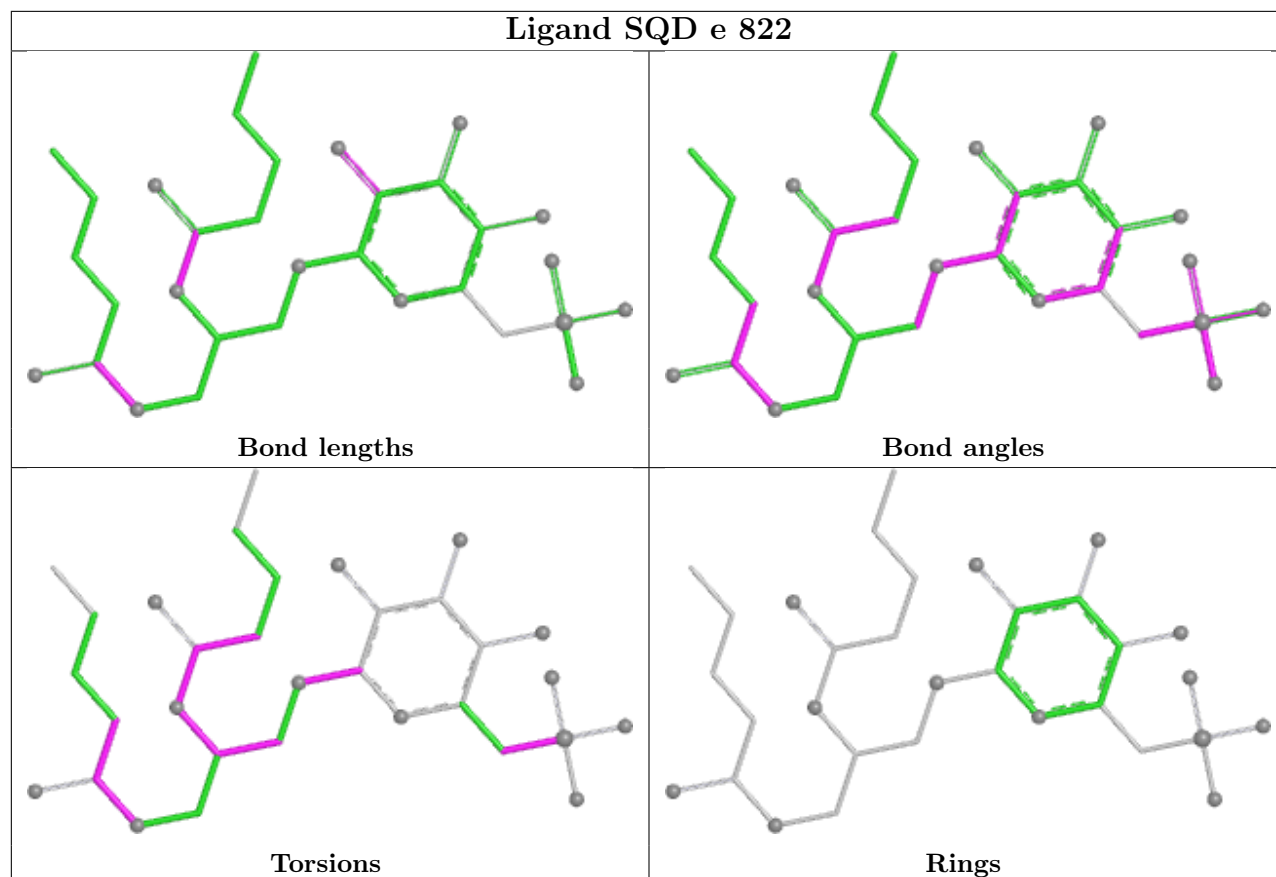


Torsions

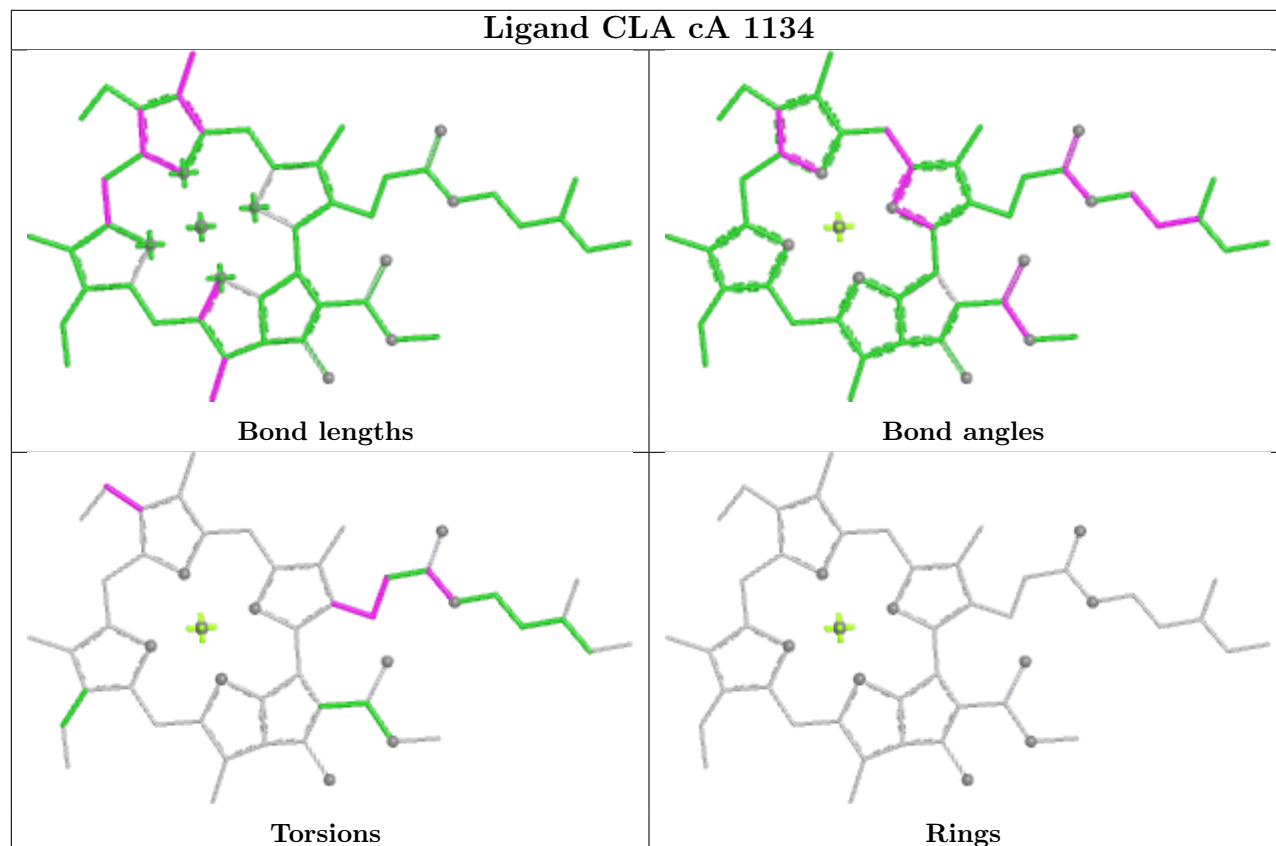


Rings

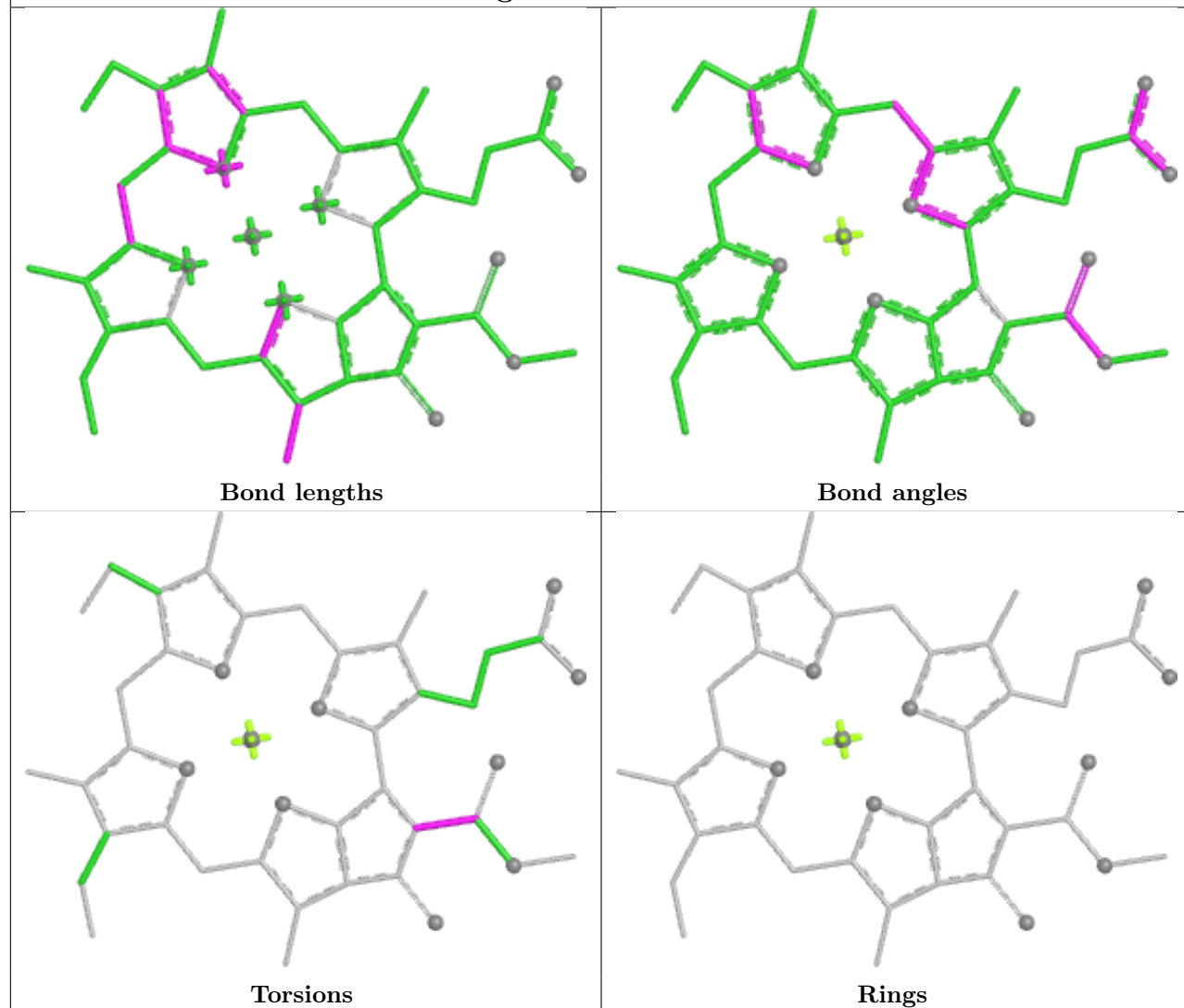
Ligand SQD e 822



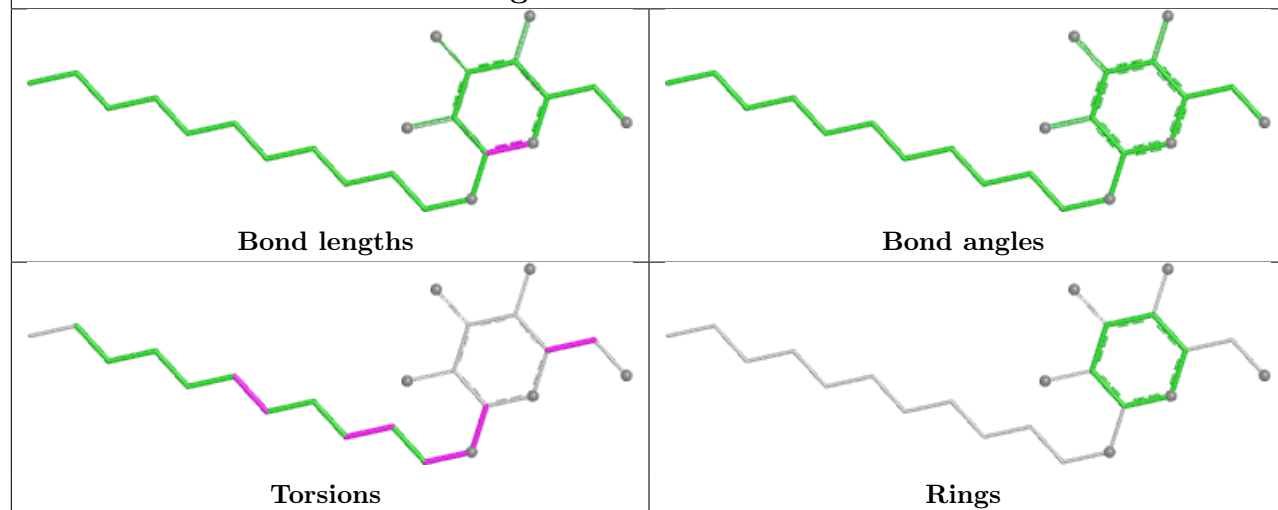
Ligand CLA cA 1134



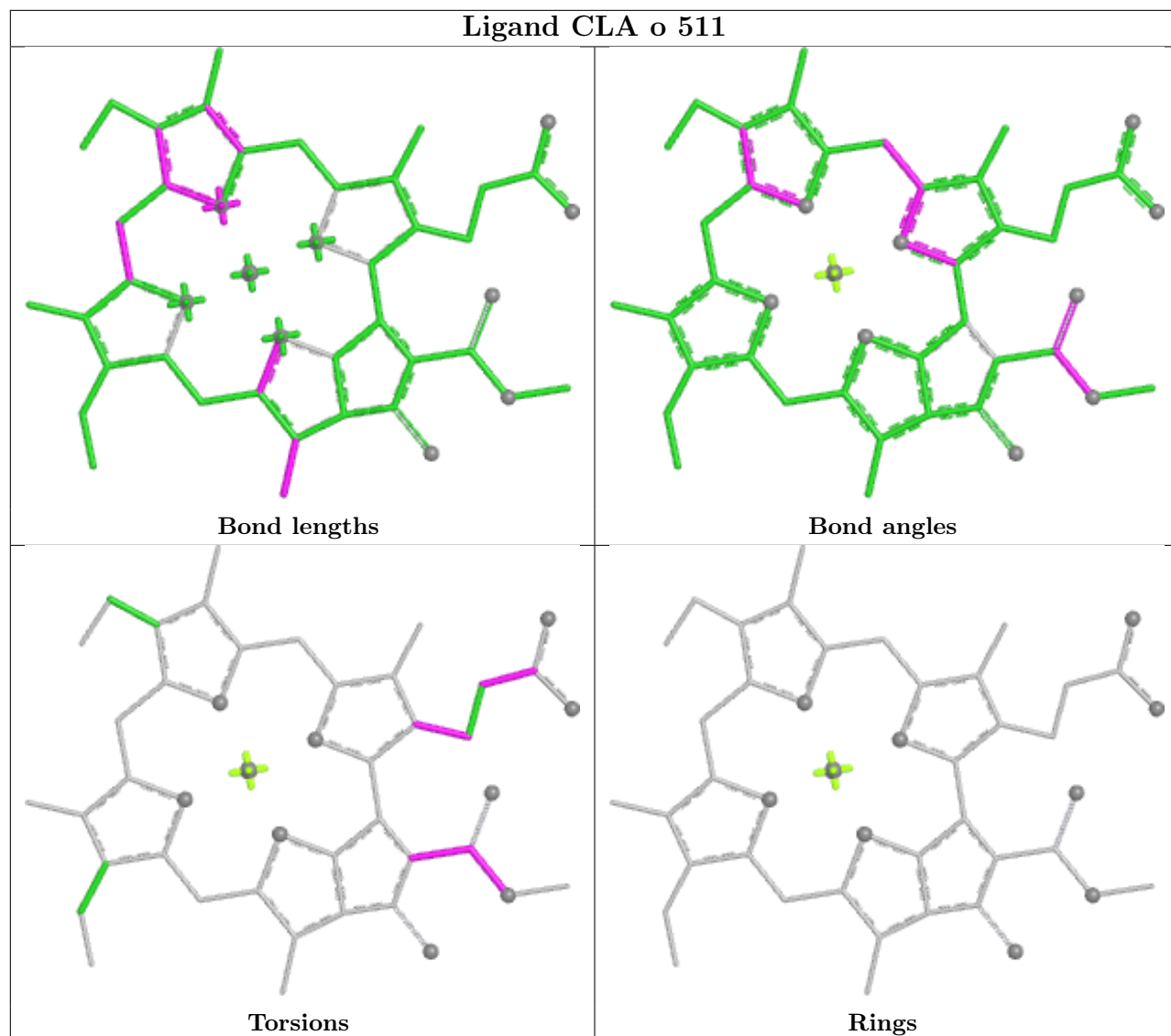
Ligand CLA o 509



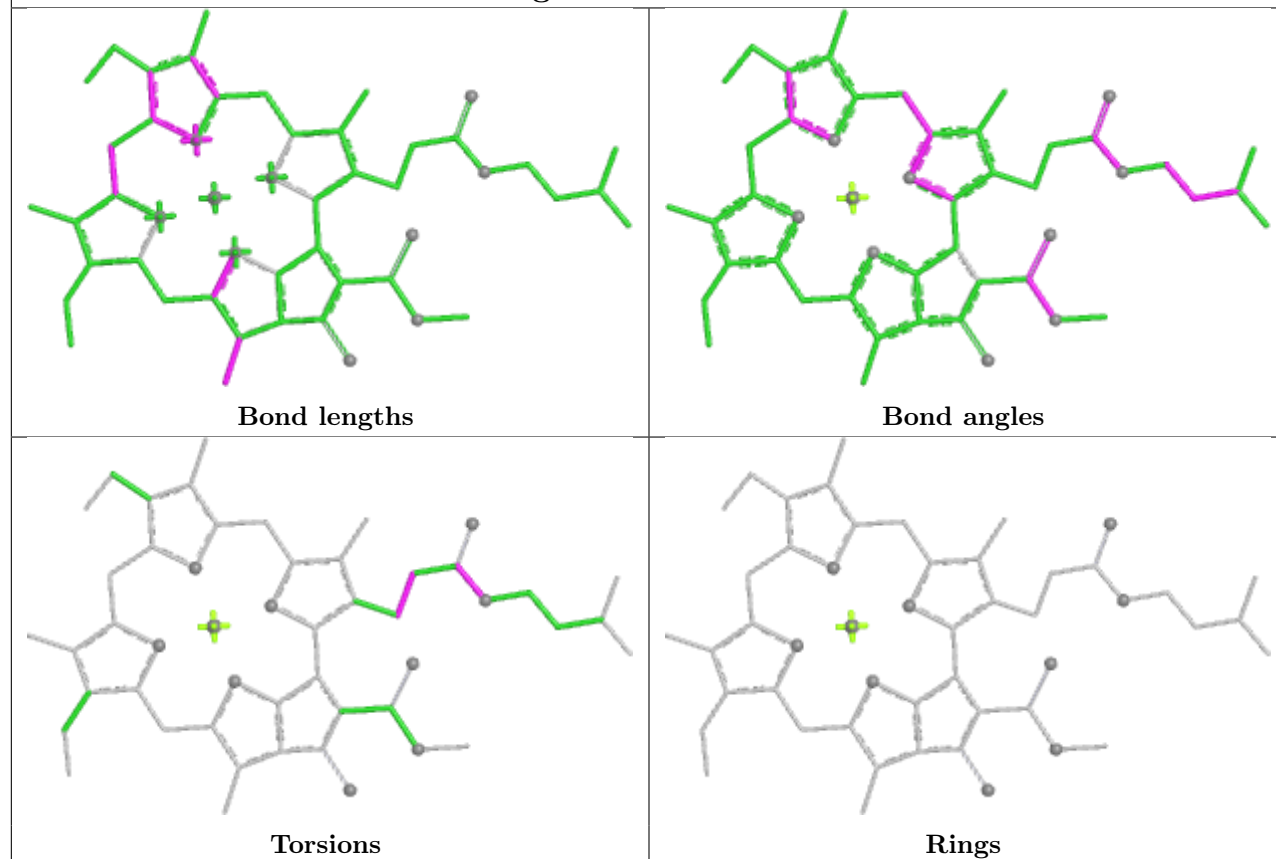
Ligand LMU cA 1849



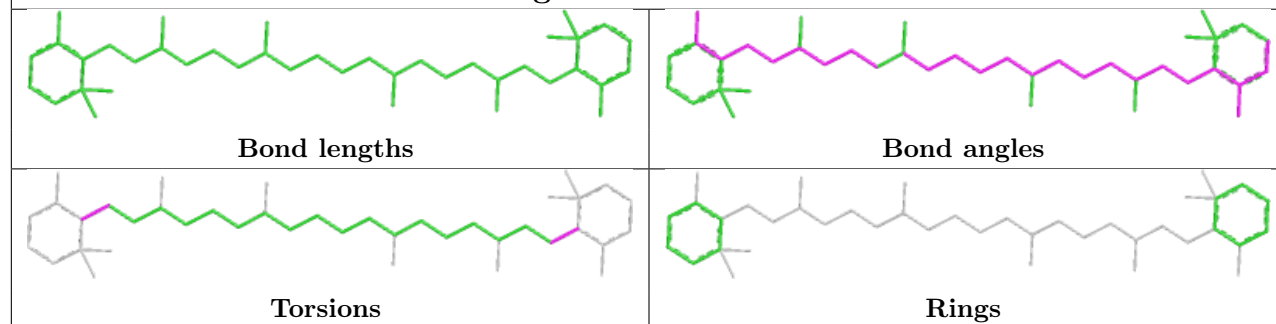
Ligand CLA o 511

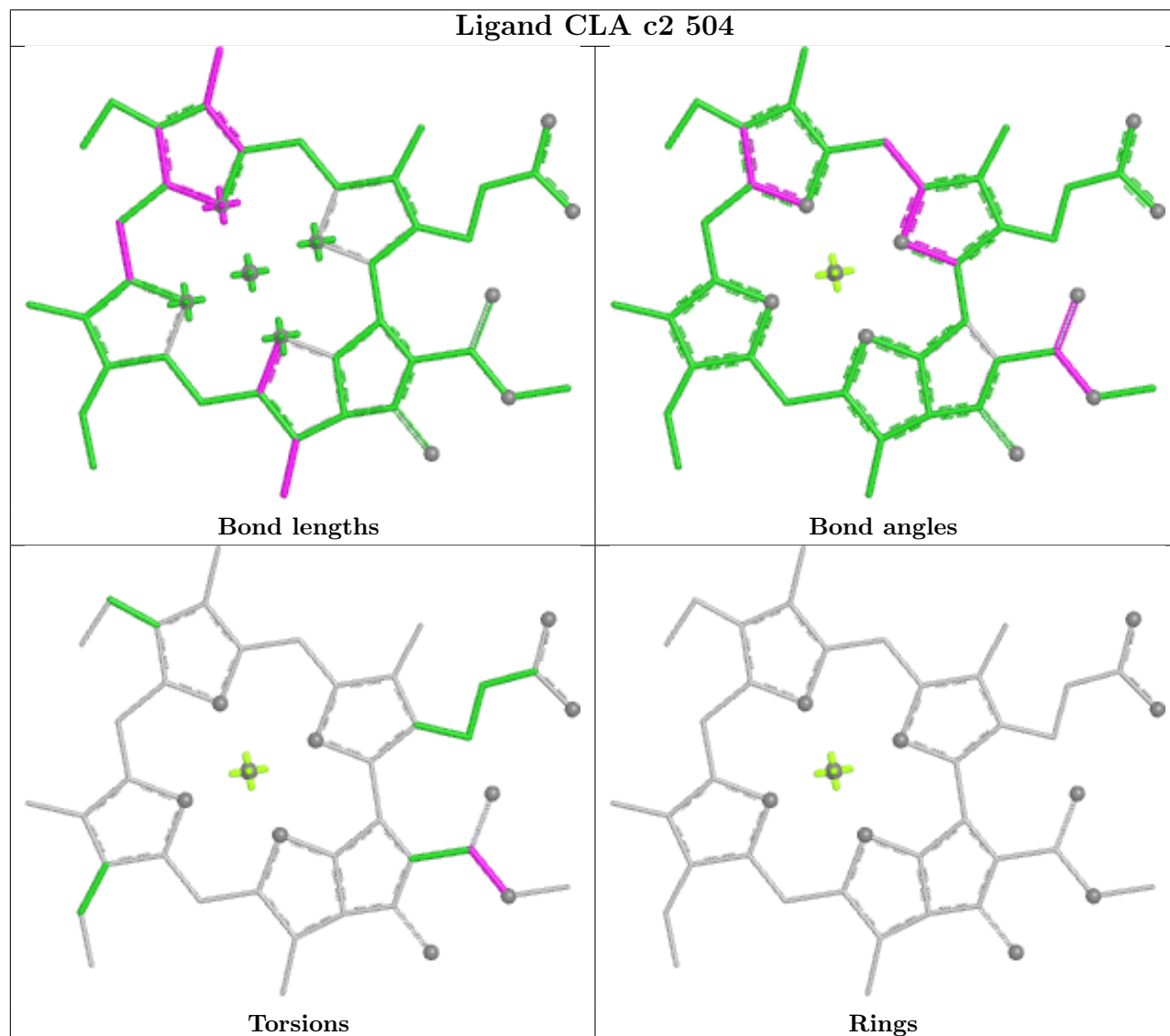
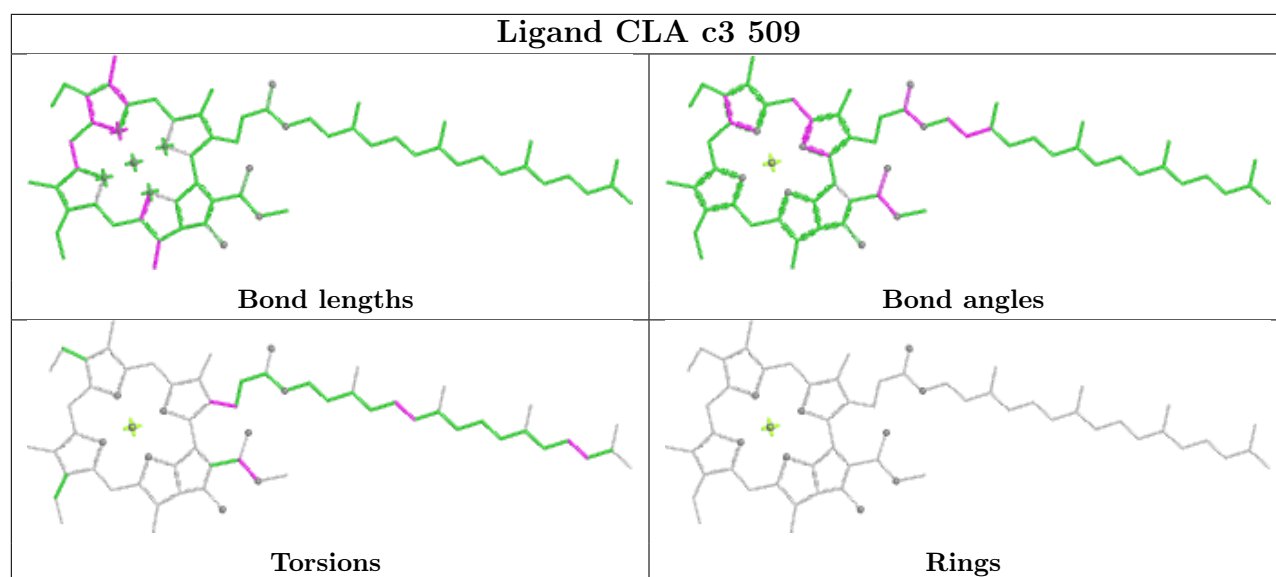


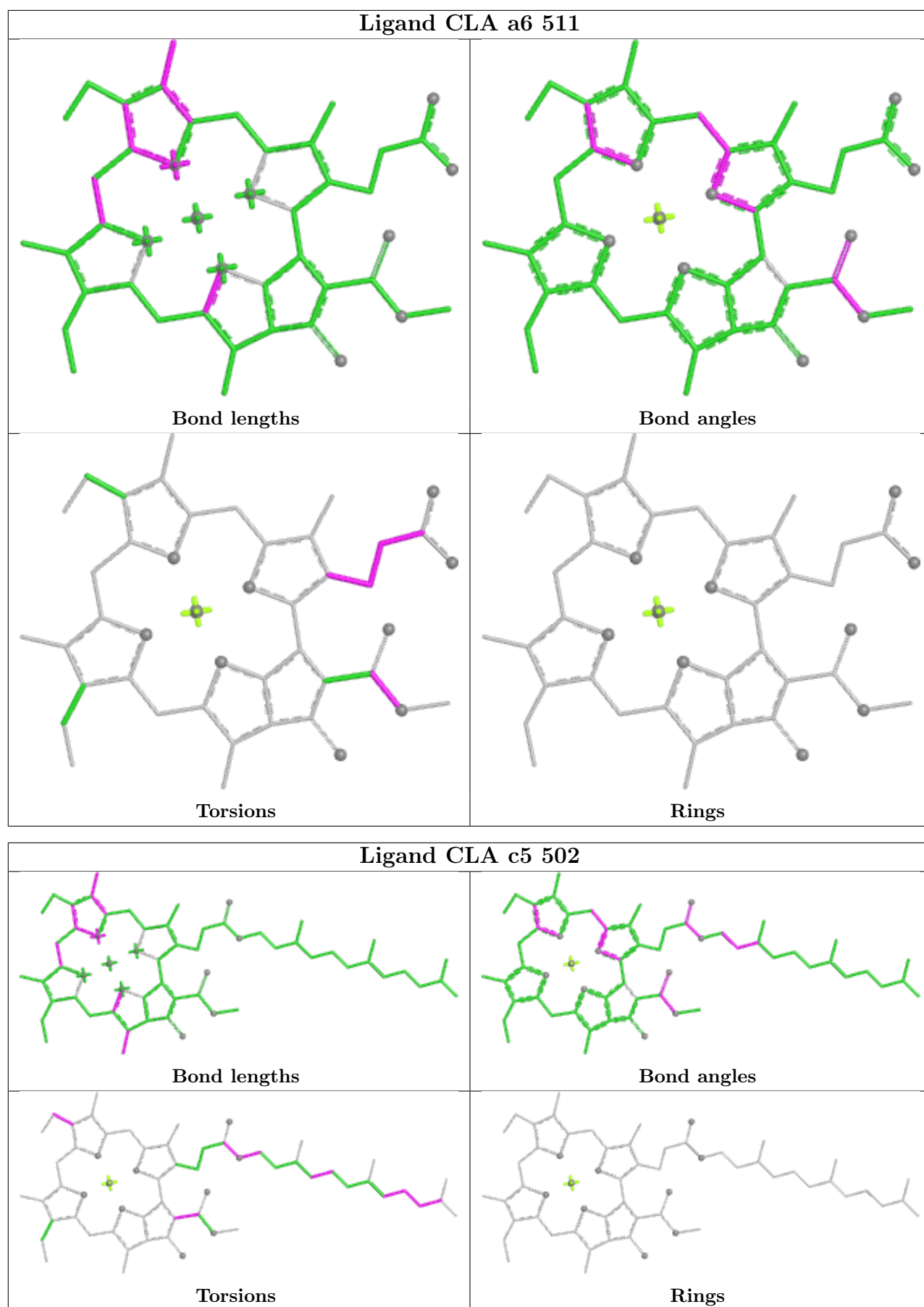
Ligand CLA T 513

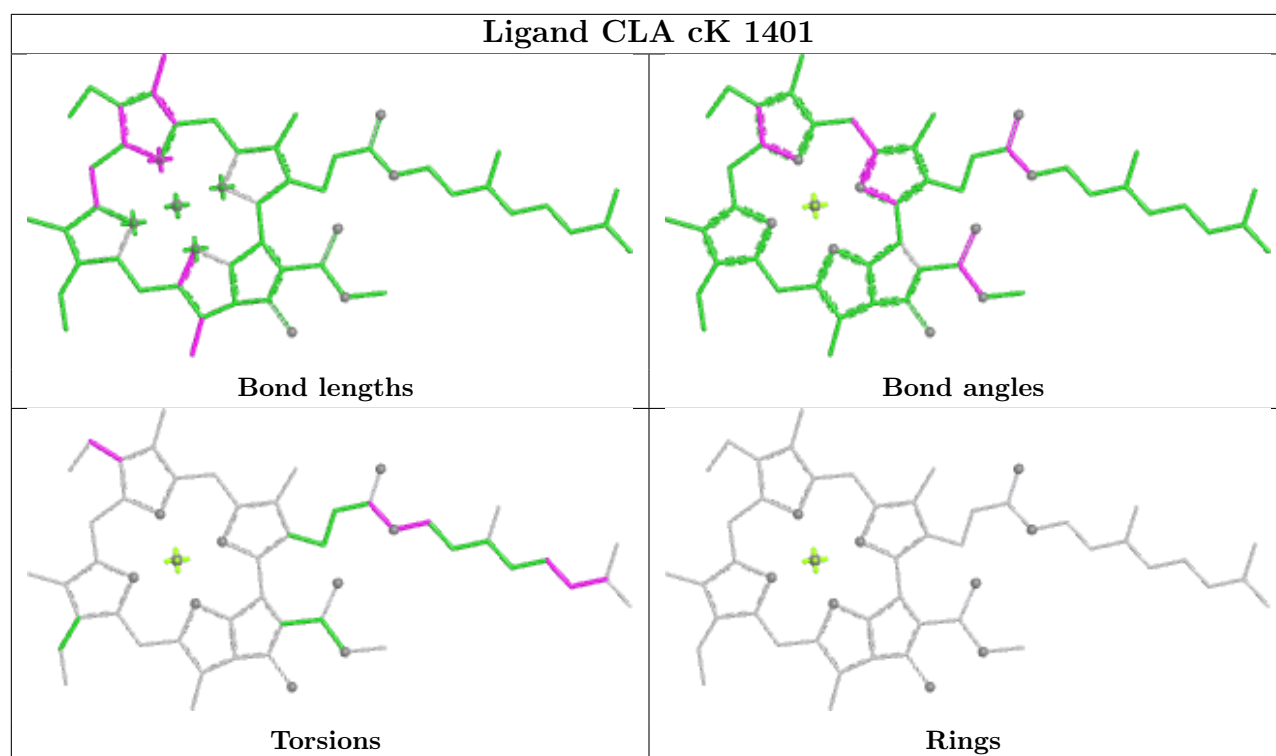


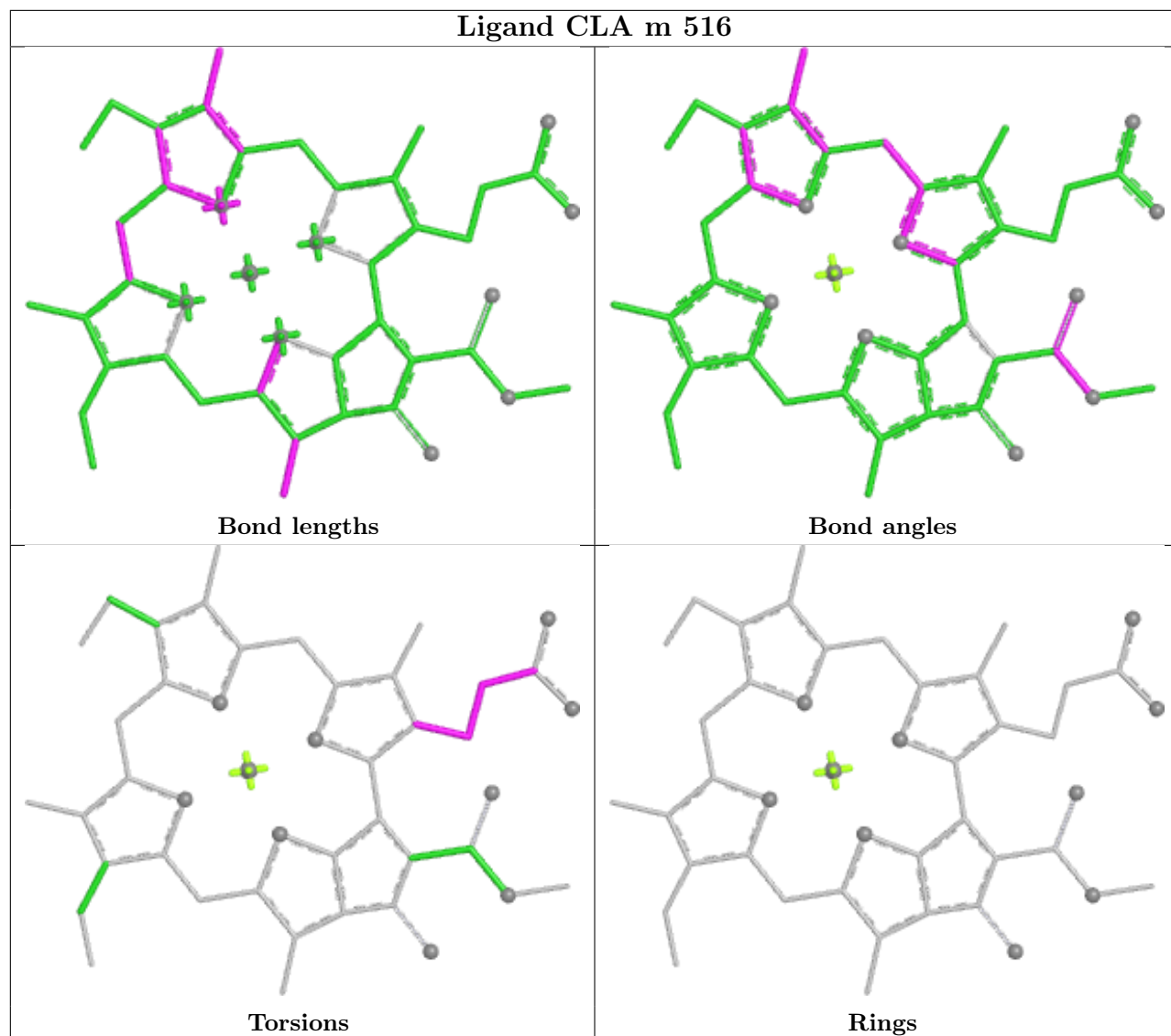
Ligand BCR S 523



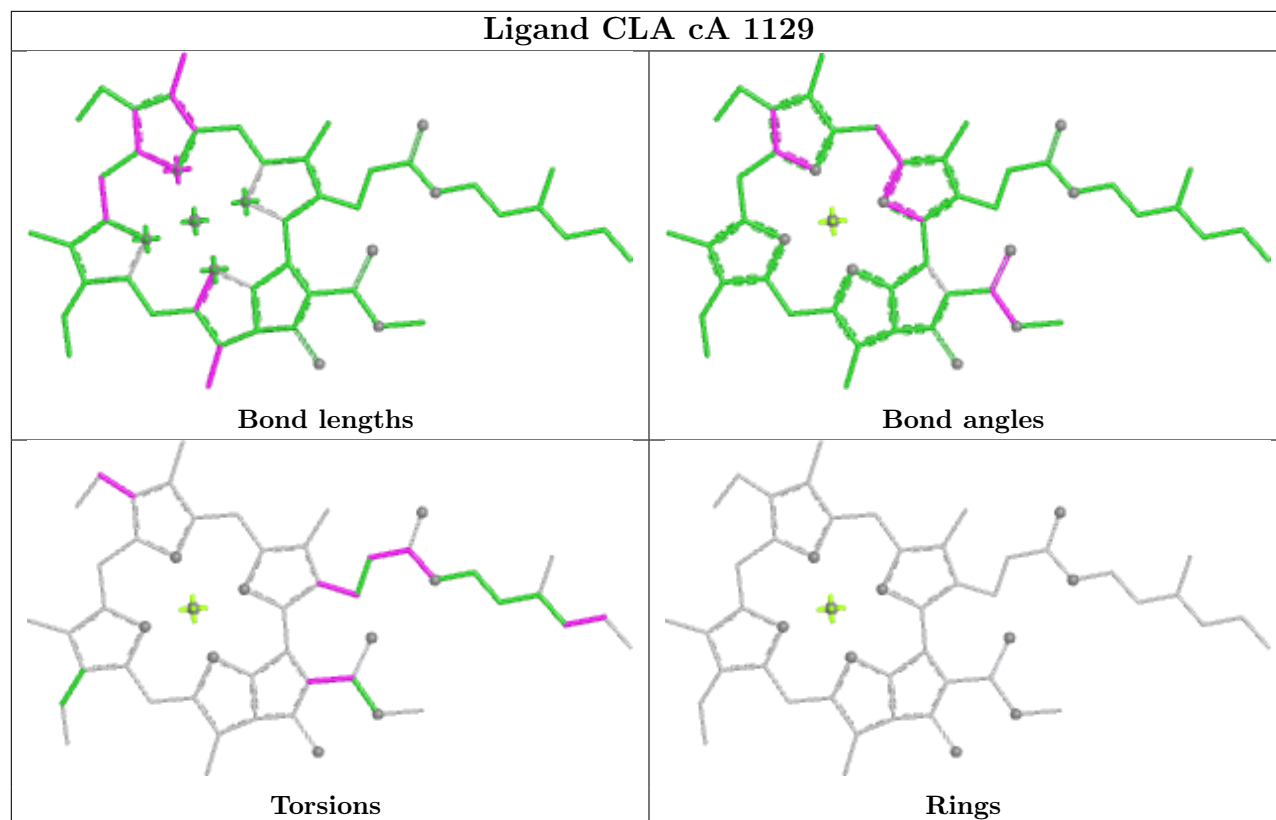




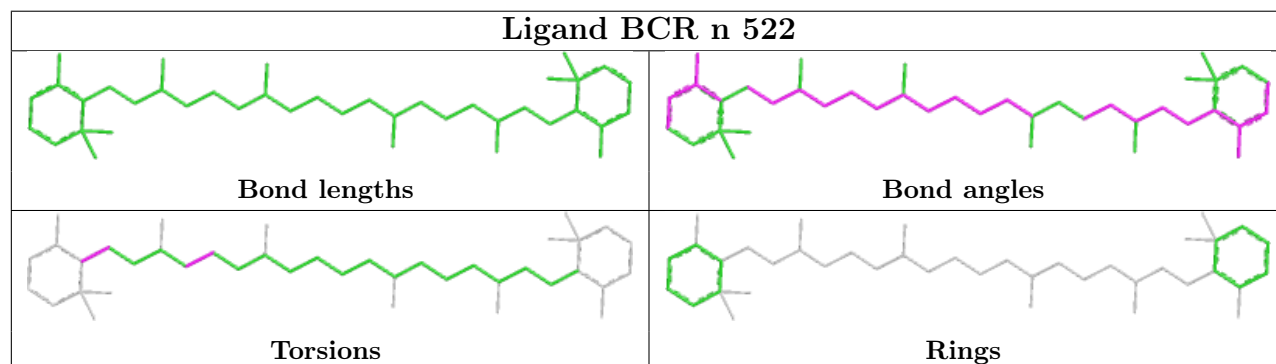




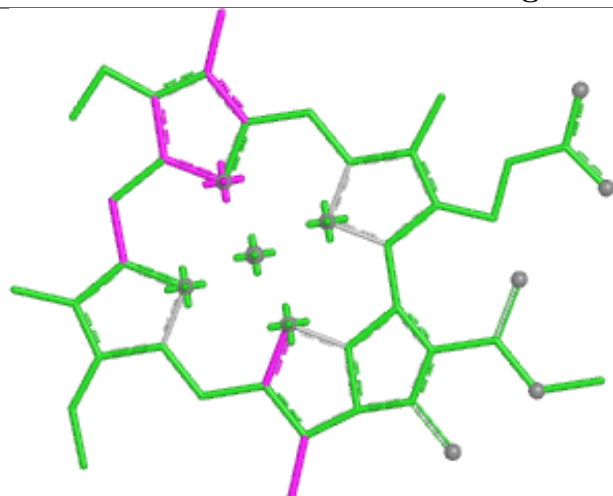
Ligand CLA cA 1129



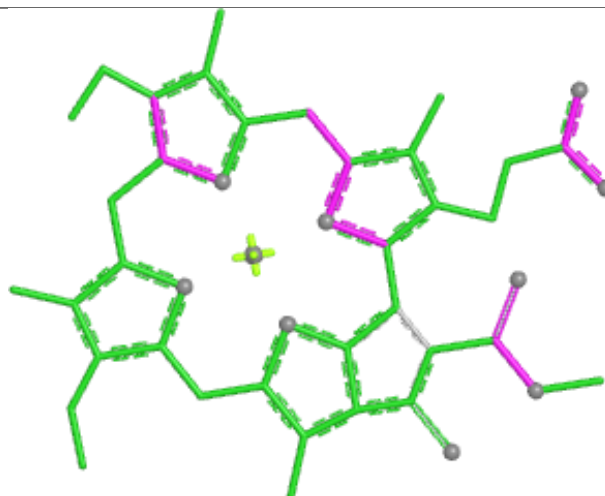
Ligand BCR n 522



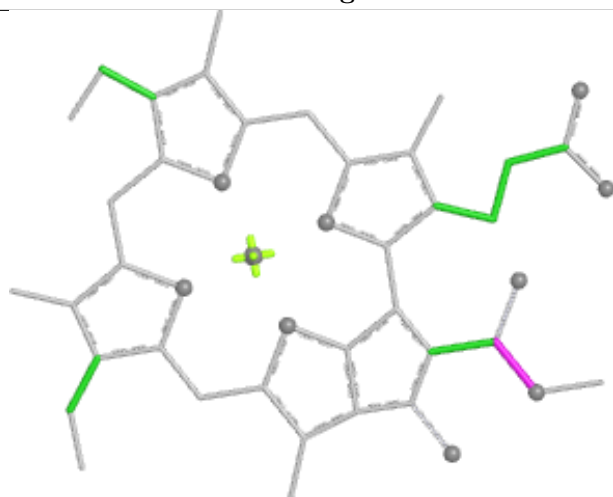
Ligand CLA f 509



Bond lengths



Bond angles

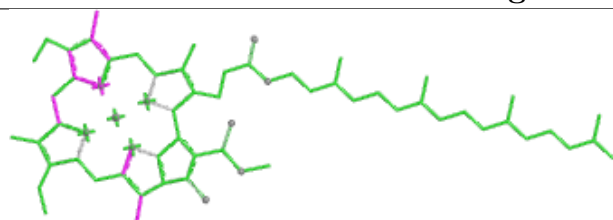


Torsions

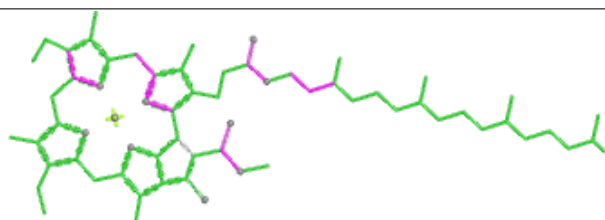


Rings

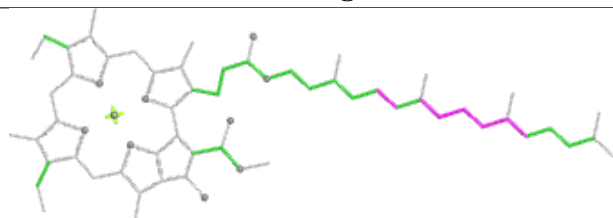
Ligand CLA b4 509



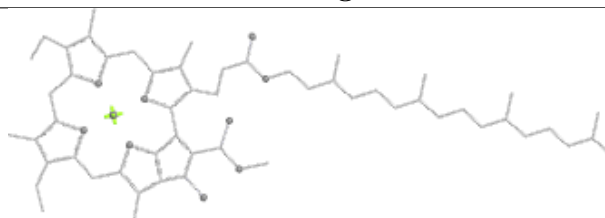
Bond lengths



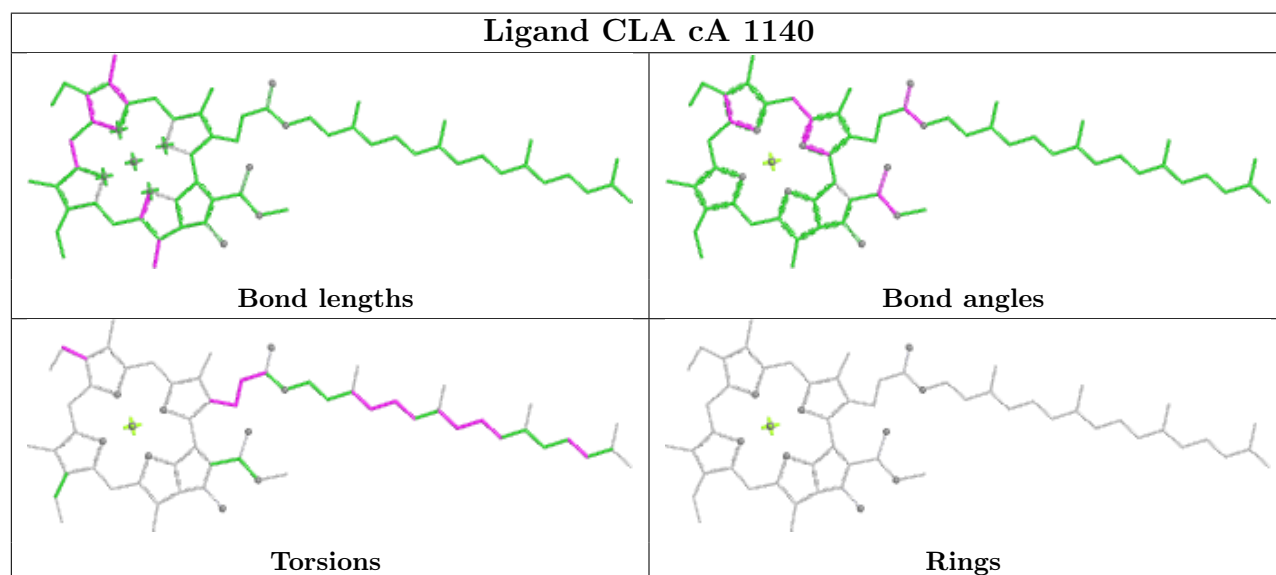
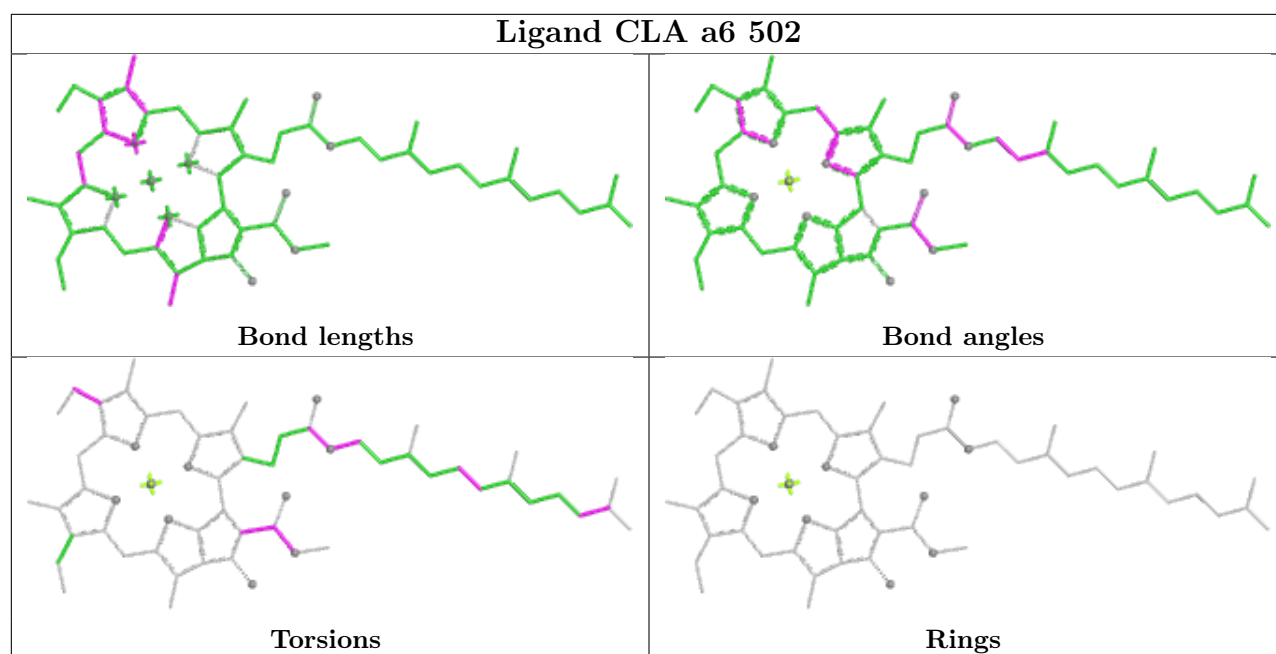
Bond angles



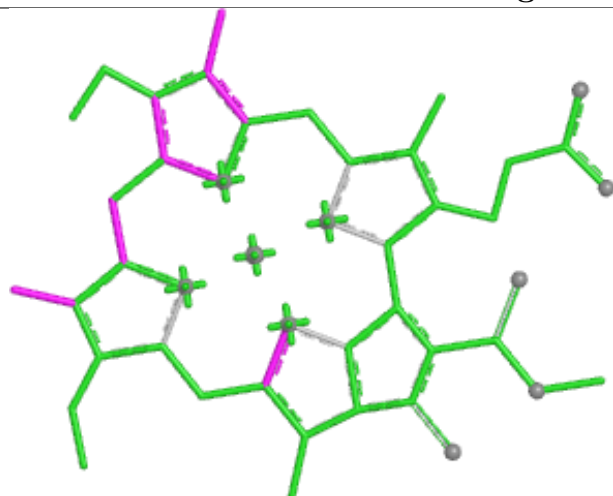
Torsions



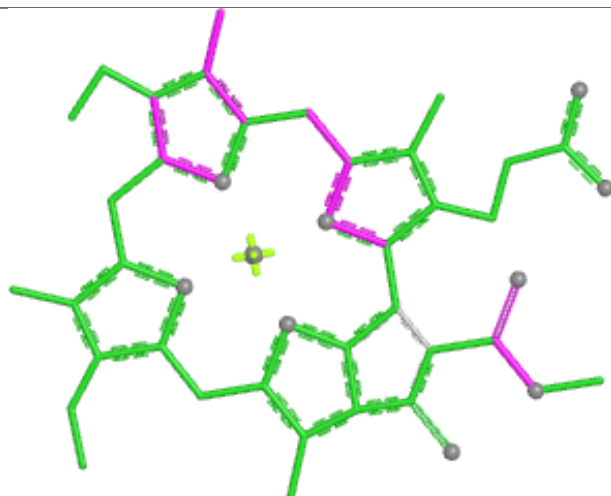
Rings



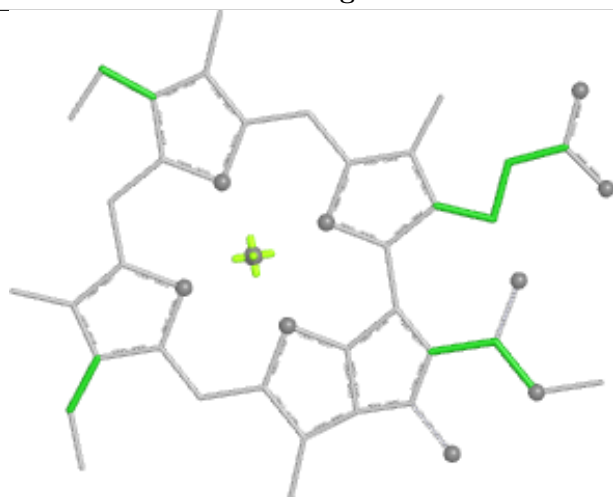
Ligand CLA n 508



Bond lengths



Bond angles

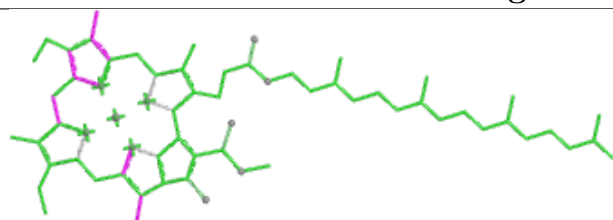


Torsions

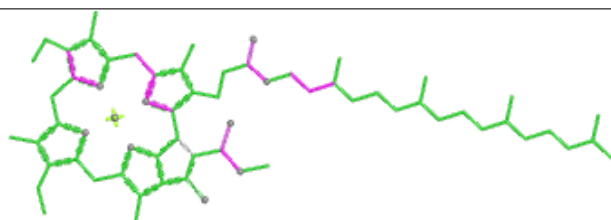


Rings

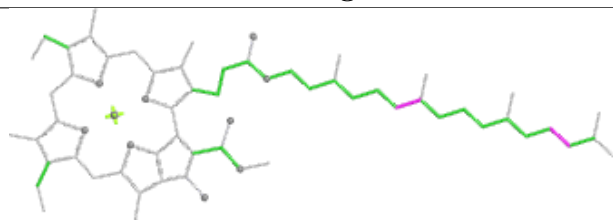
Ligand CLA b6 509



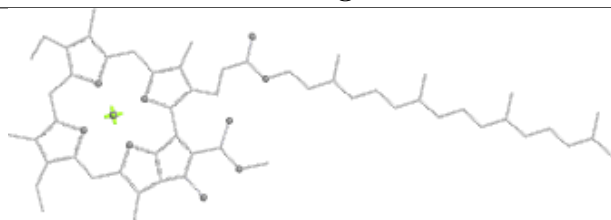
Bond lengths



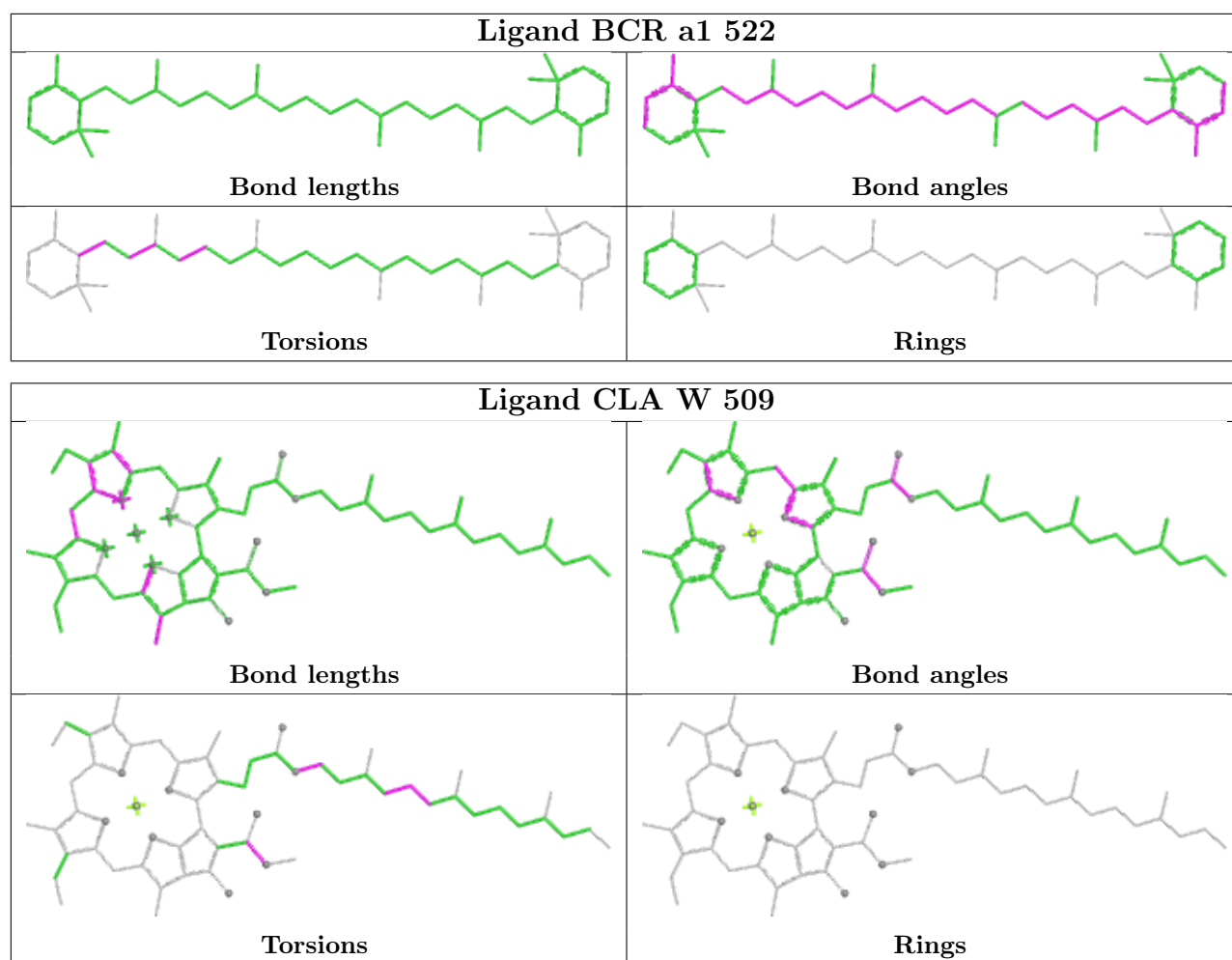
Bond angles

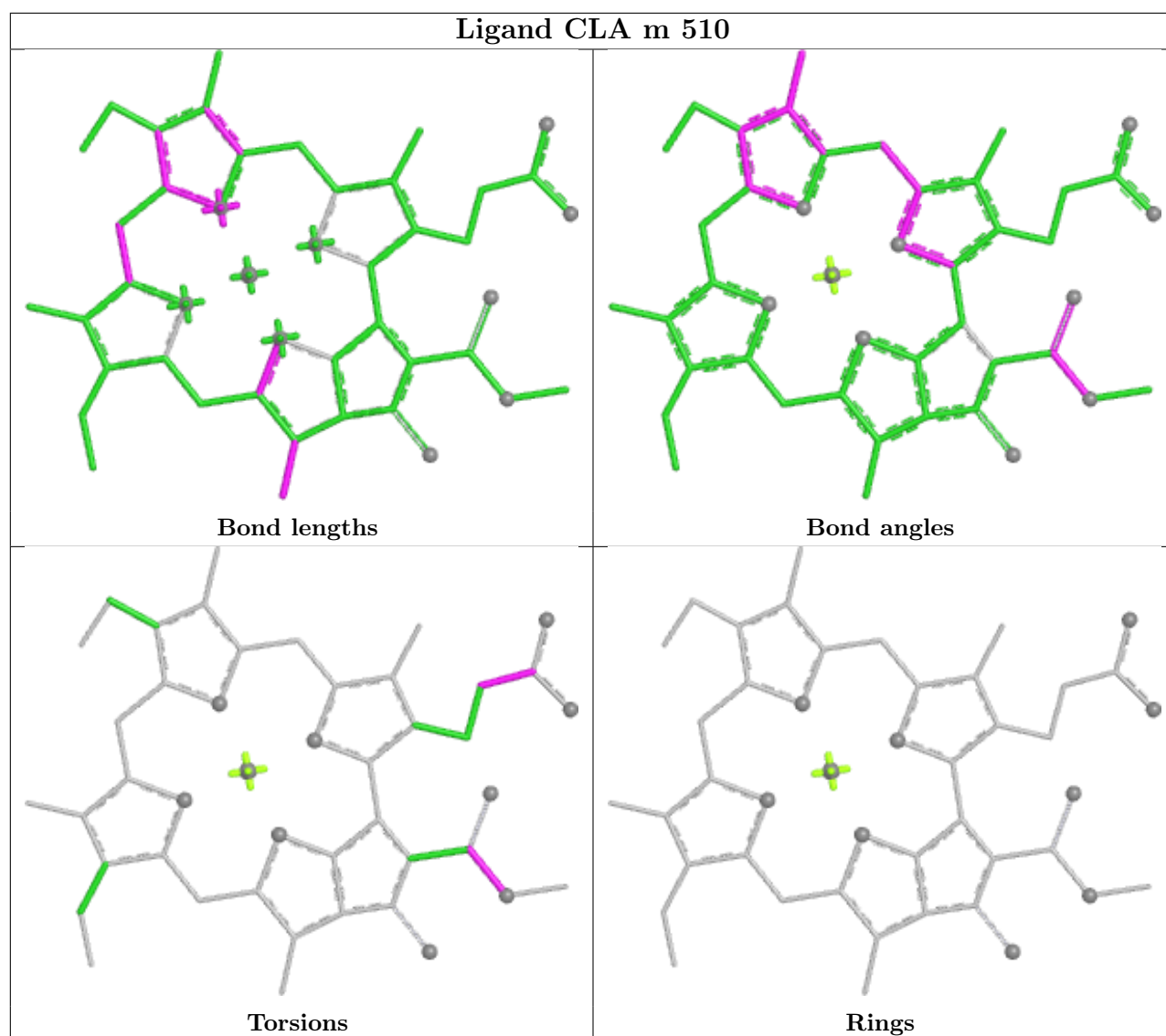


Torsions

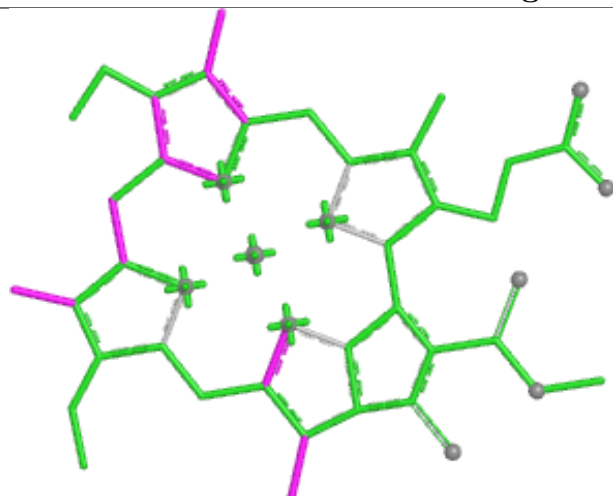


Rings

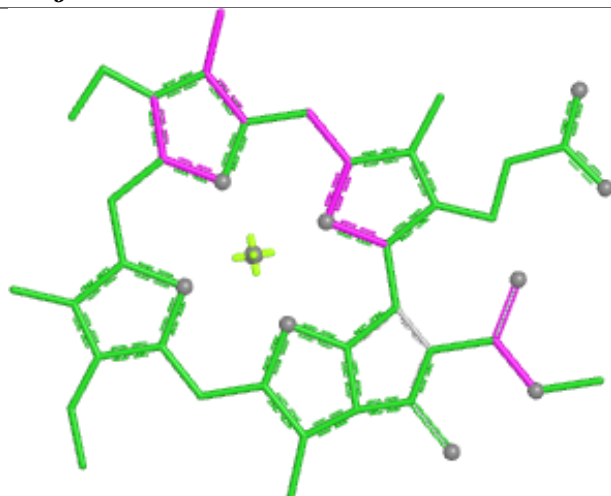




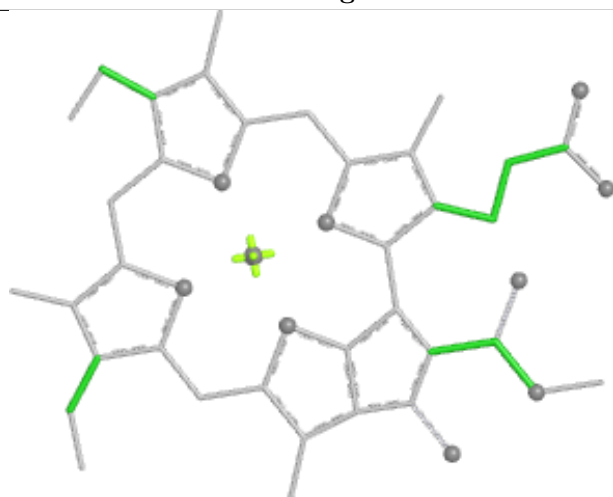
Ligand CLA j 508



Bond lengths



Bond angles

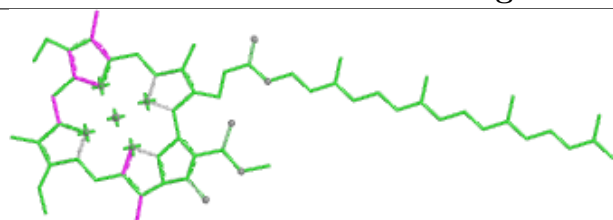


Torsions

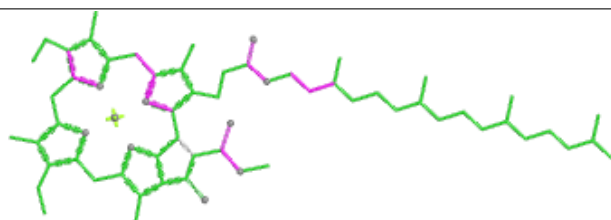


Rings

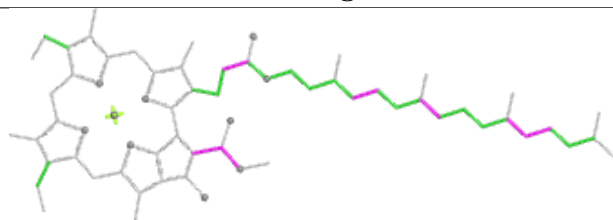
Ligand CLA bB 1229



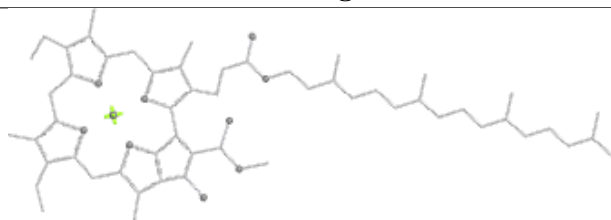
Bond lengths



Bond angles

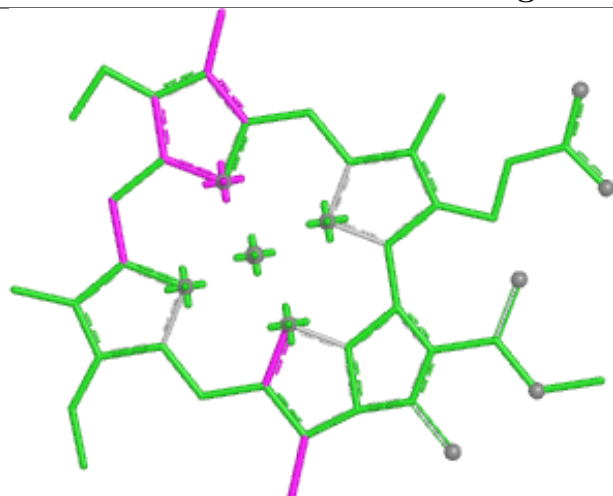


Torsions

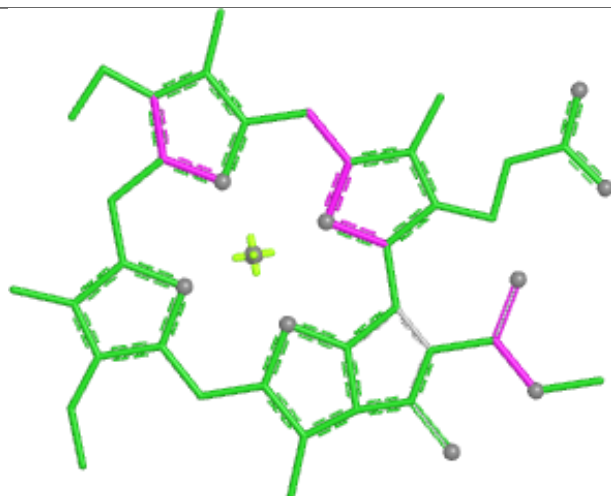


Rings

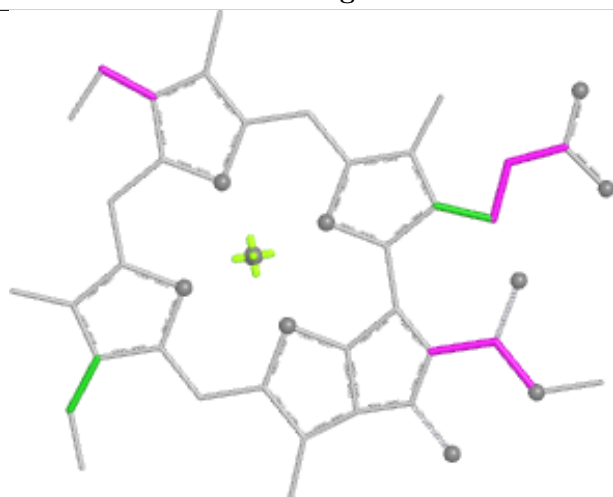
Ligand CLA b 501



Bond lengths



Bond angles

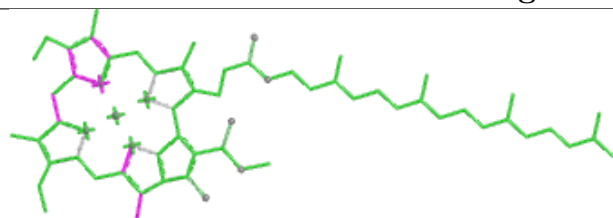


Torsions

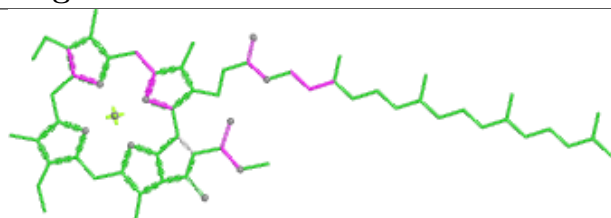


Rings

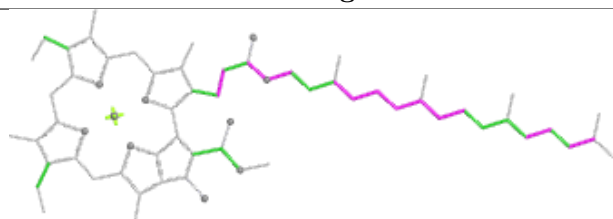
Ligand CLA g 505



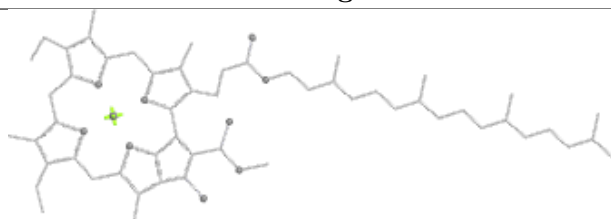
Bond lengths



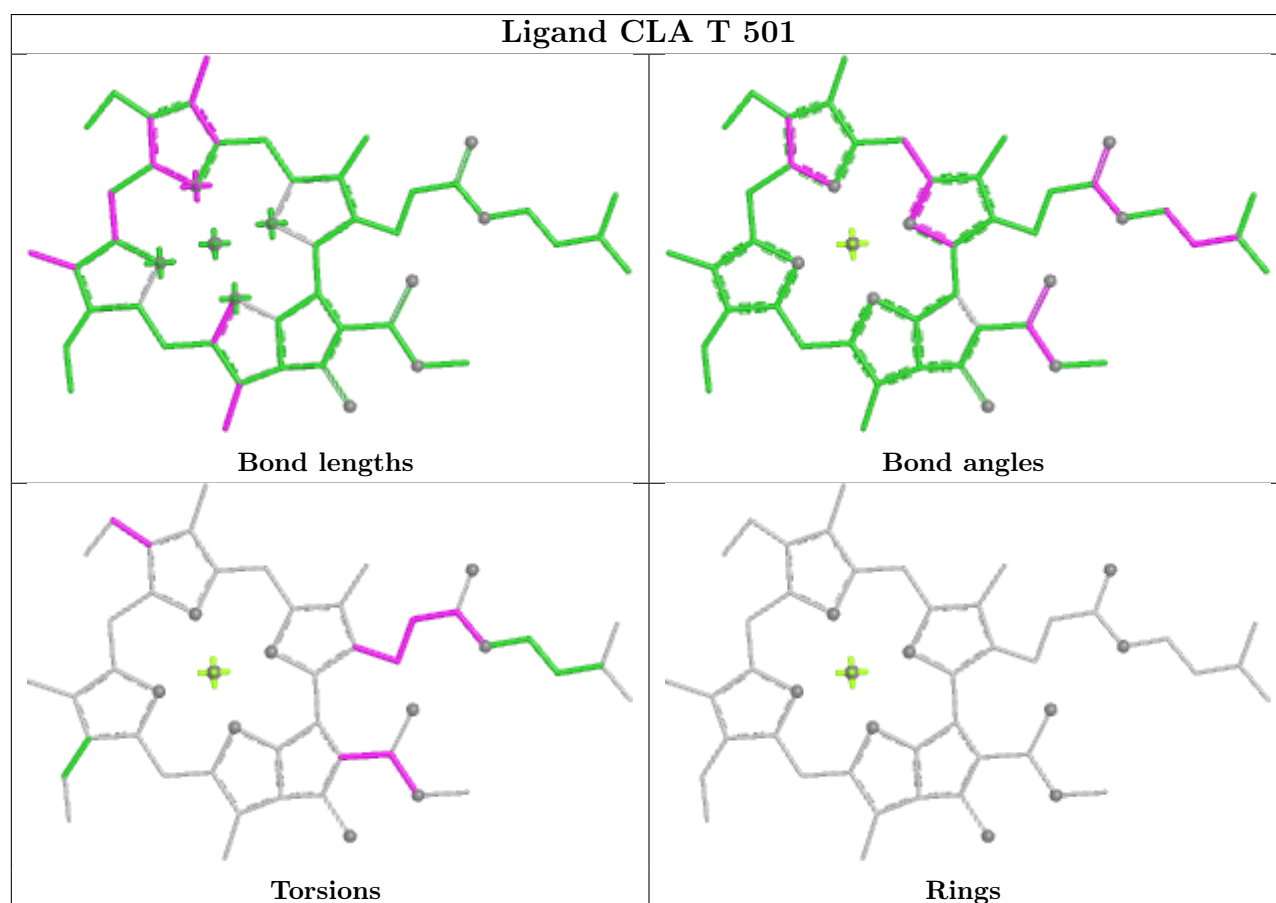
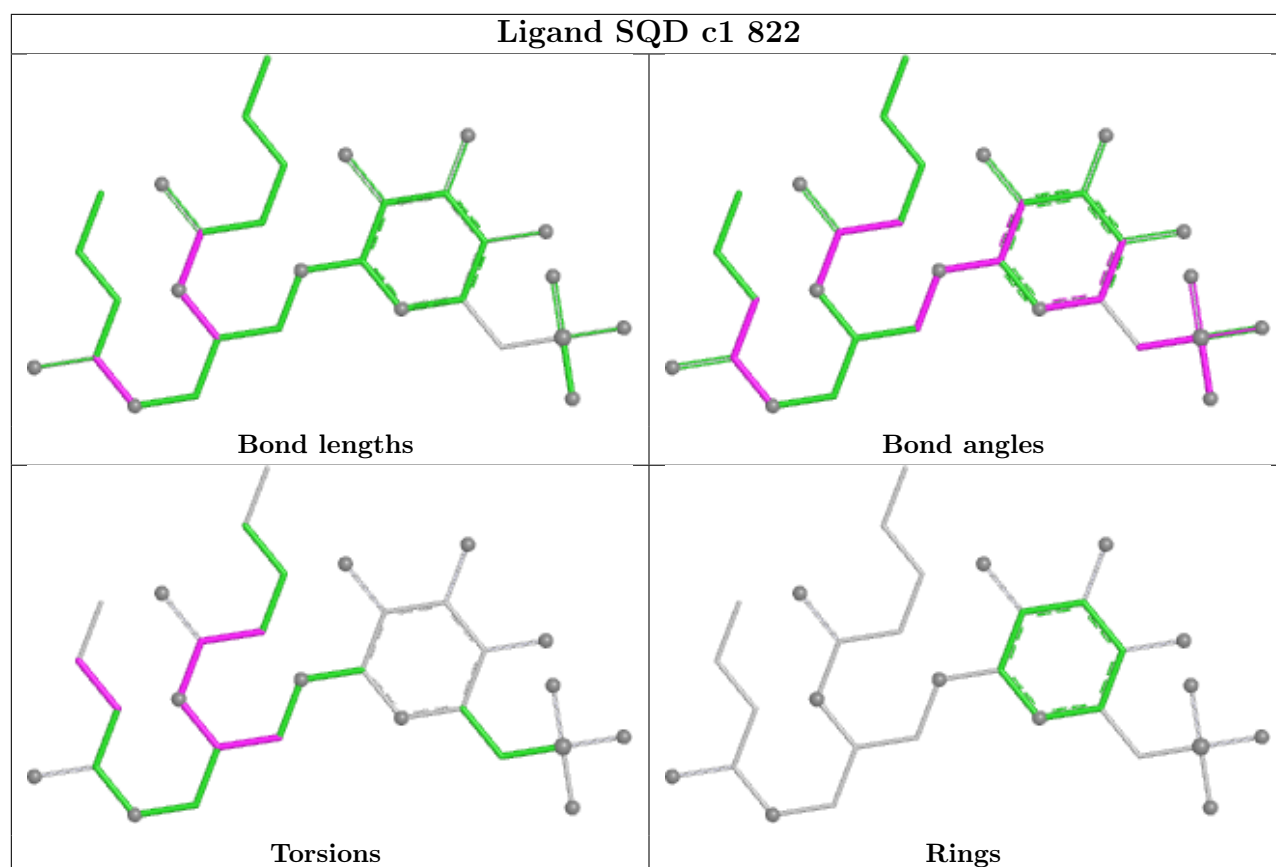
Bond angles

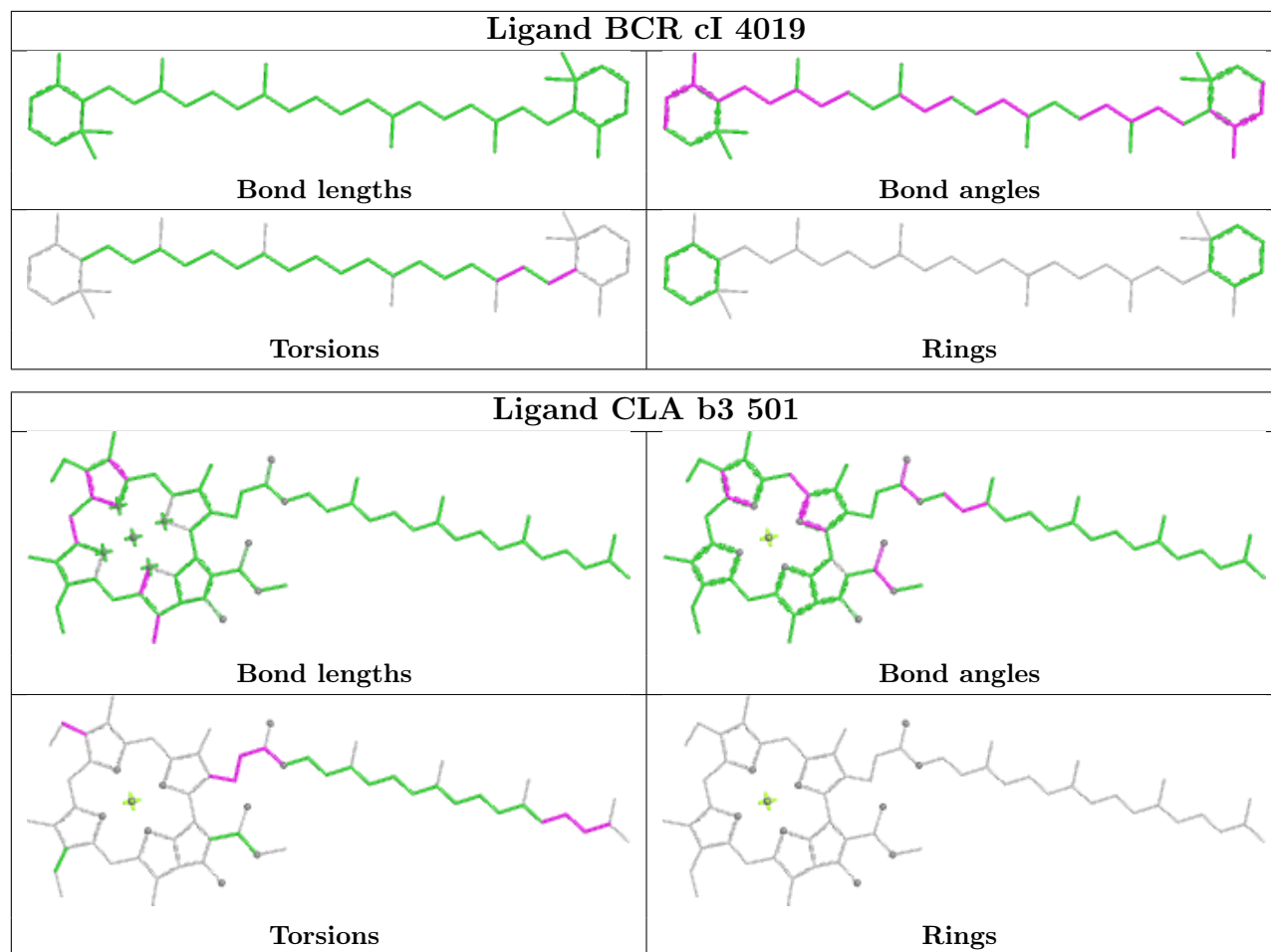


Torsions

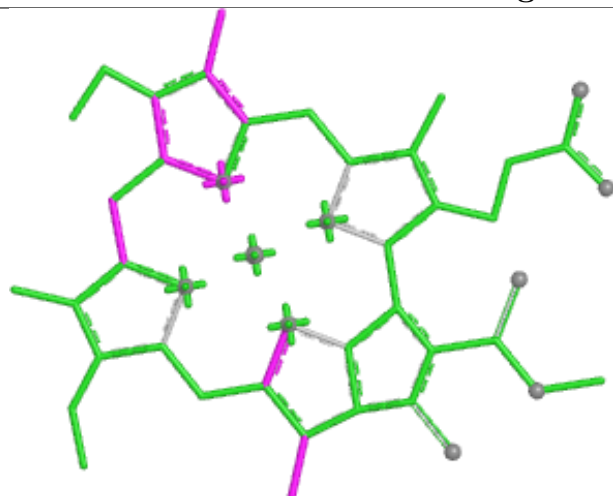


Rings





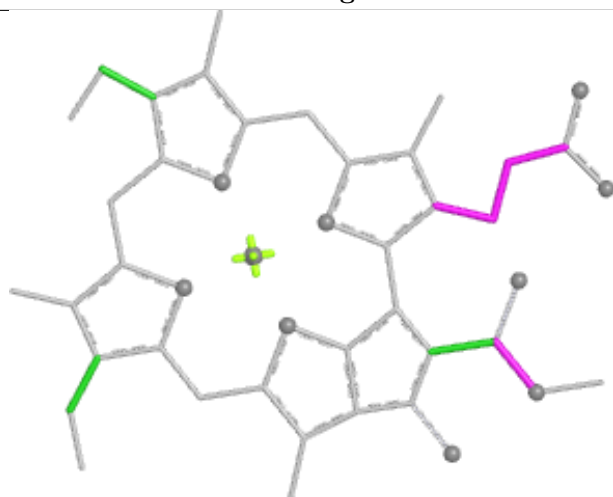
Ligand CLA d 506



Bond lengths



Bond angles

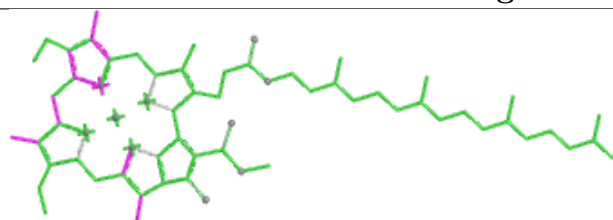


Torsions

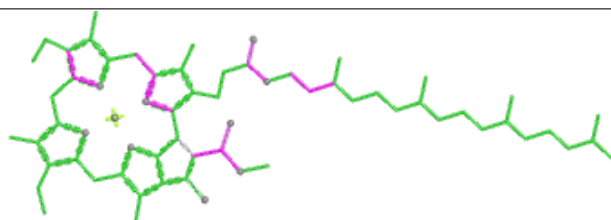


Rings

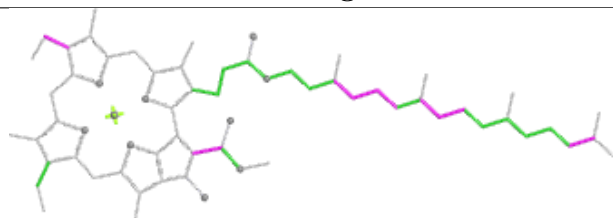
Ligand CLA aB 1205



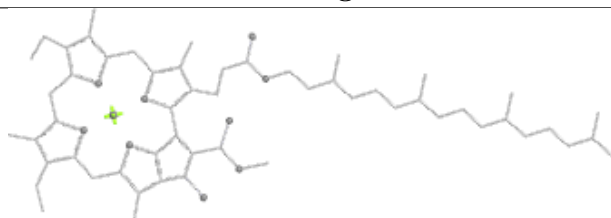
Bond lengths



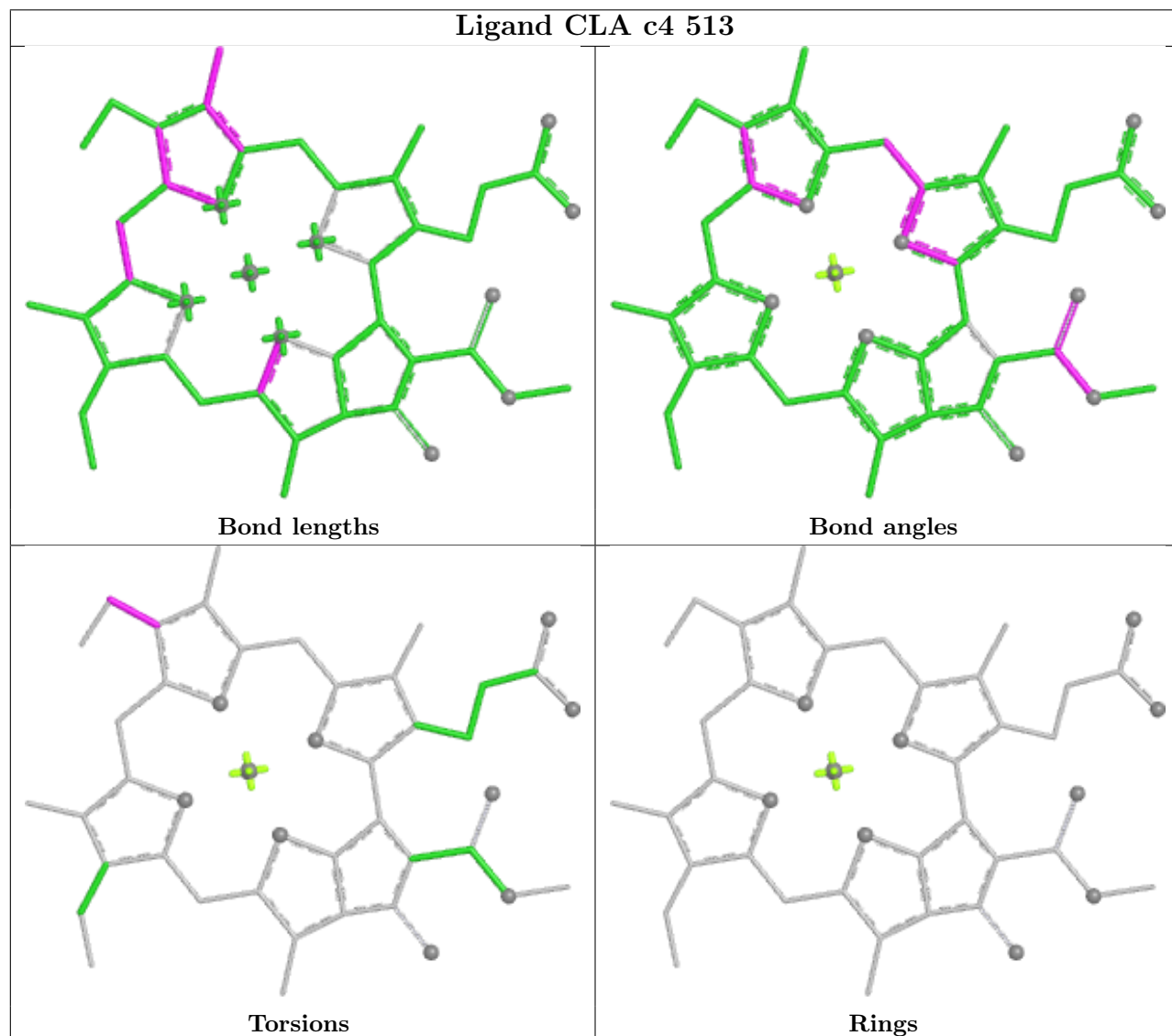
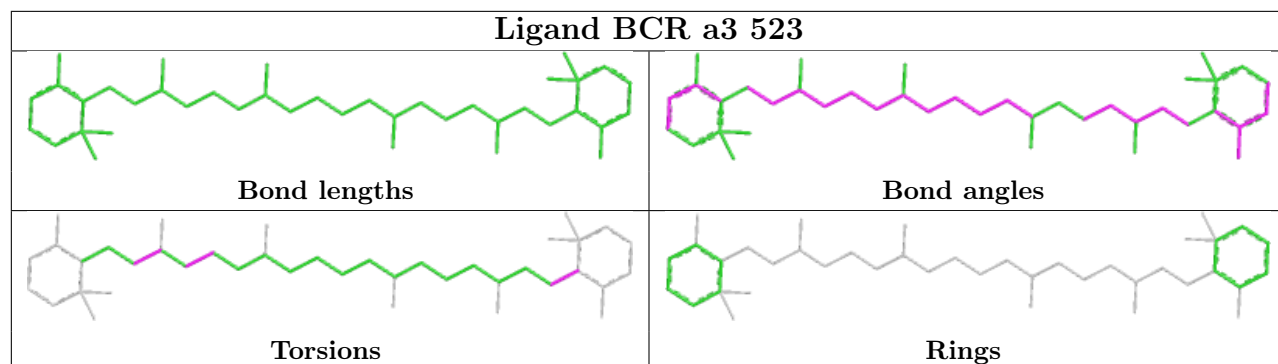
Bond angles

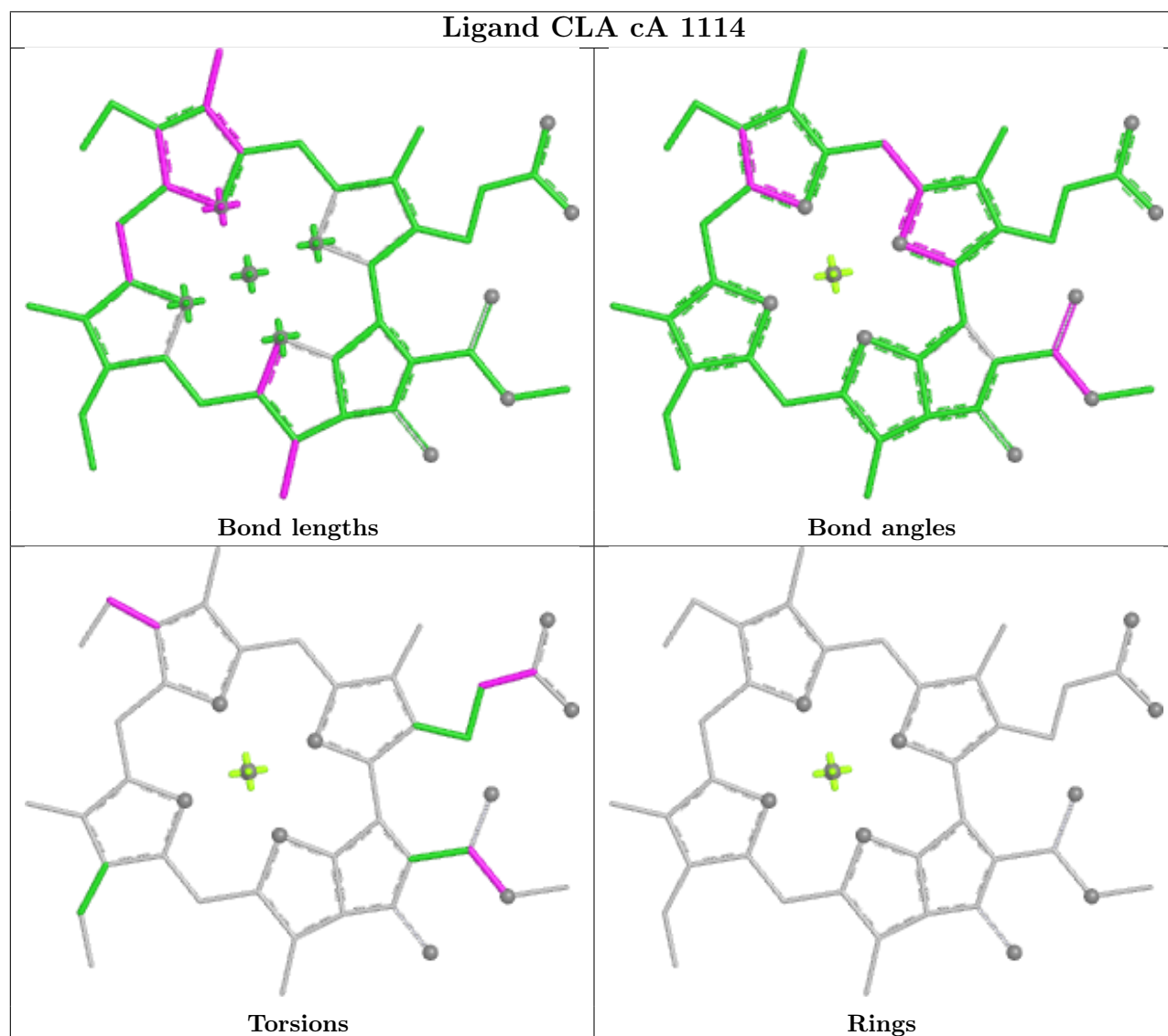
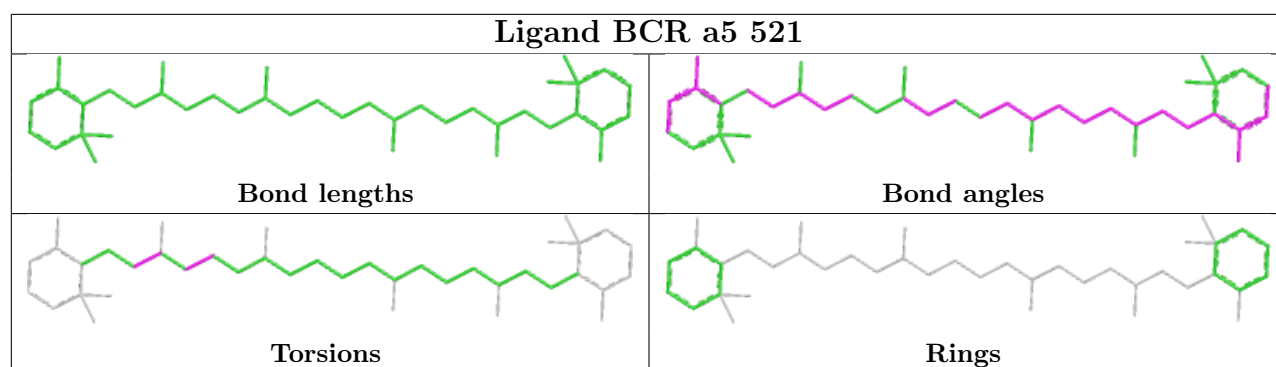


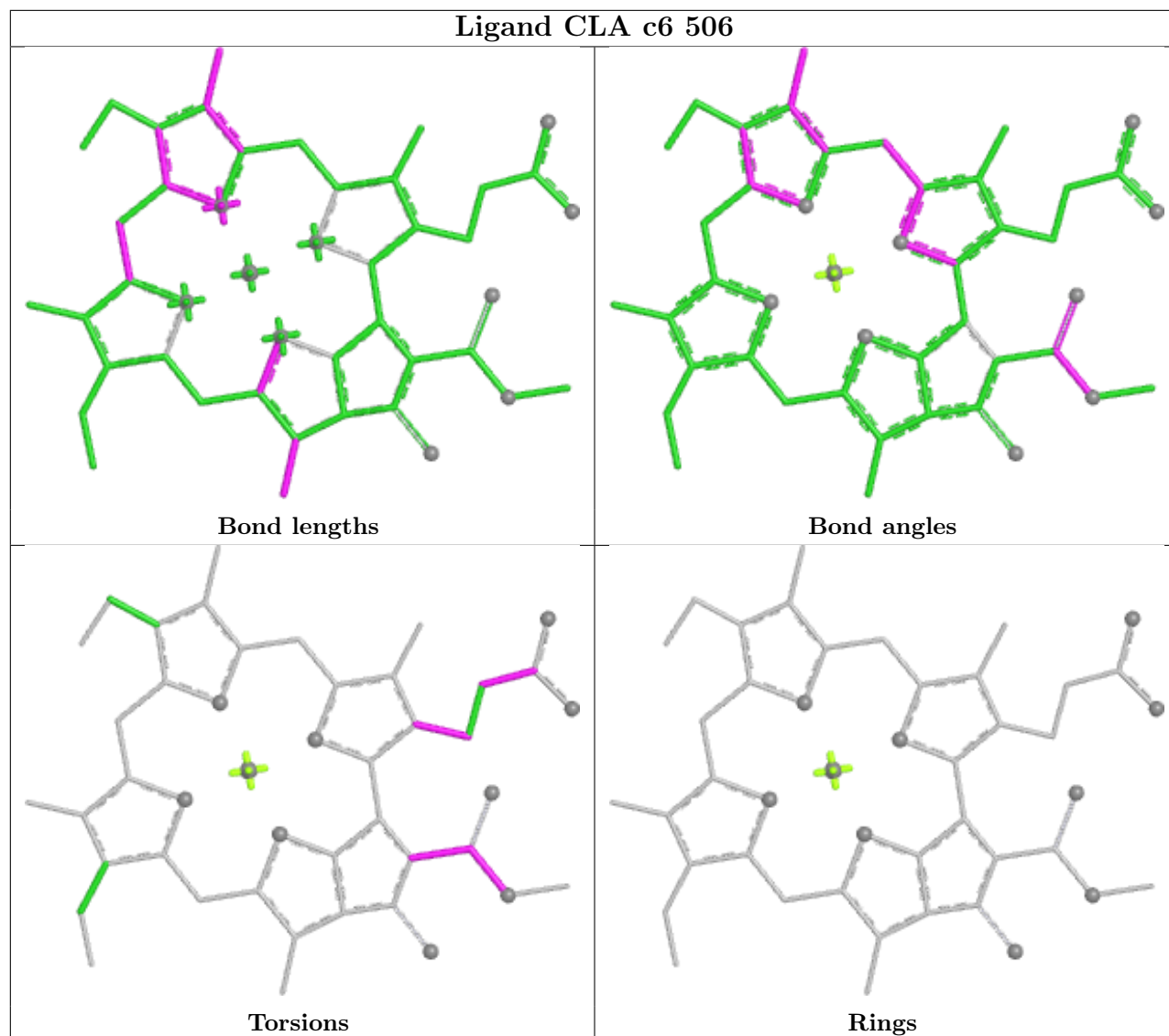
Torsions



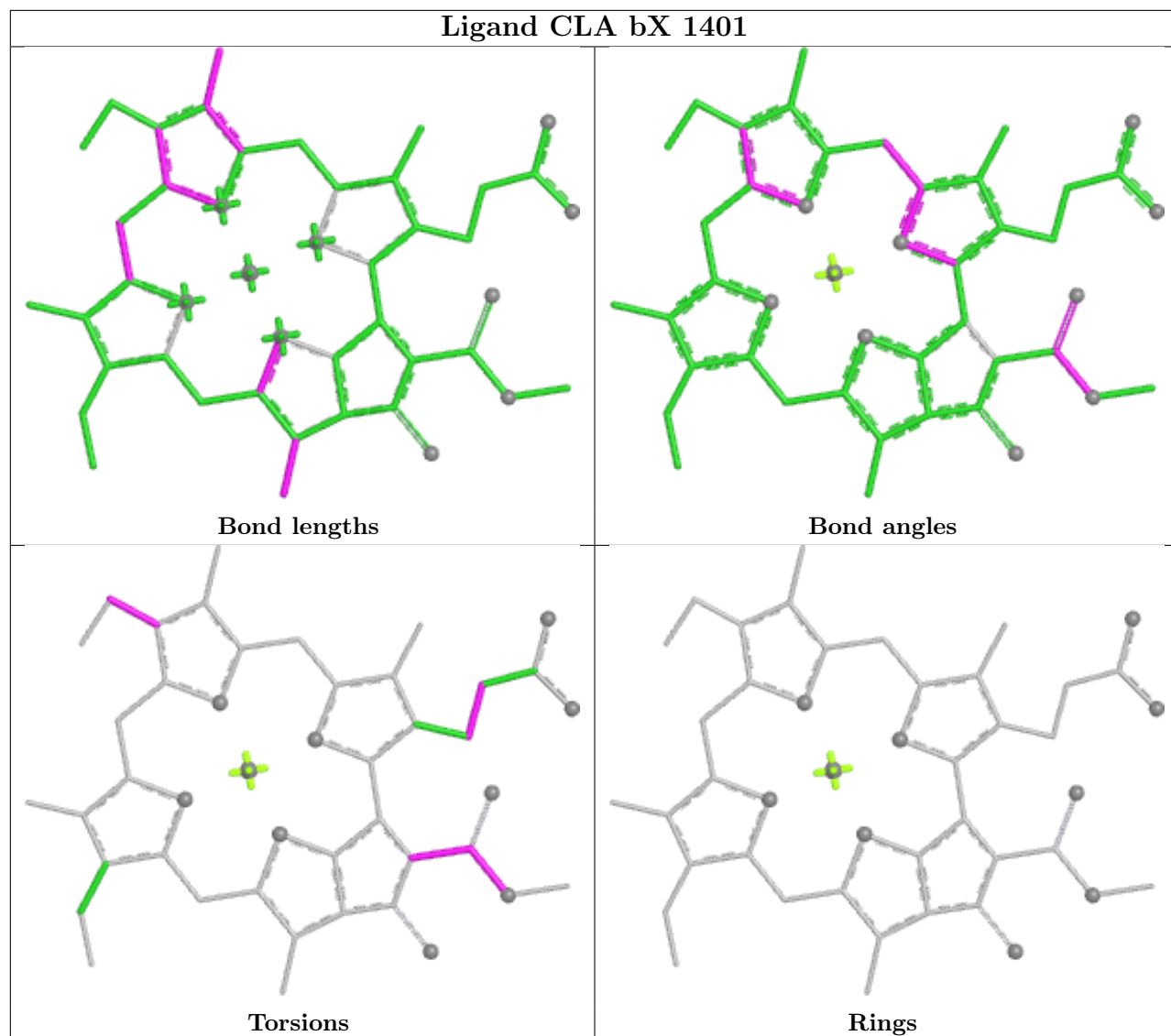
Rings

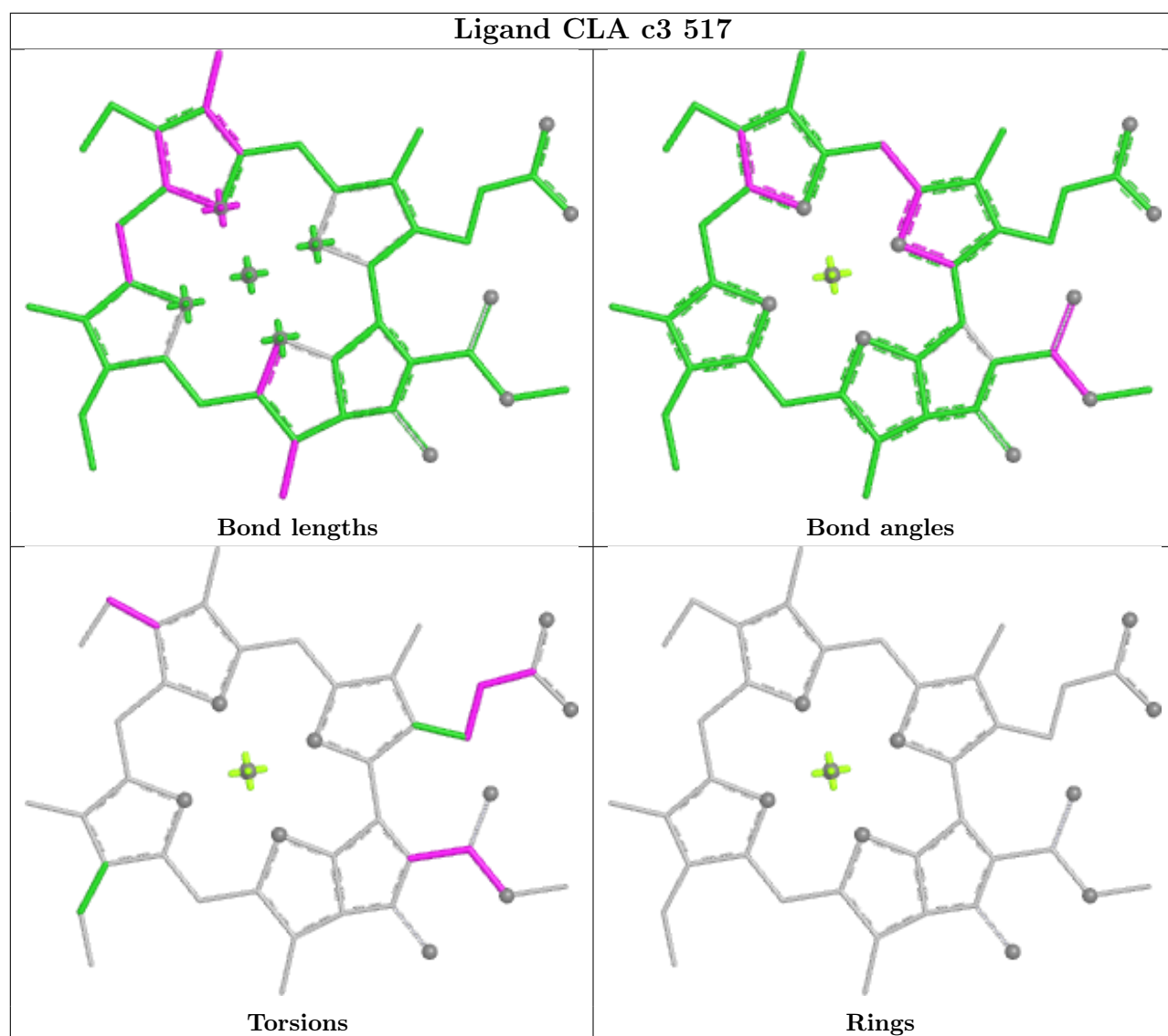




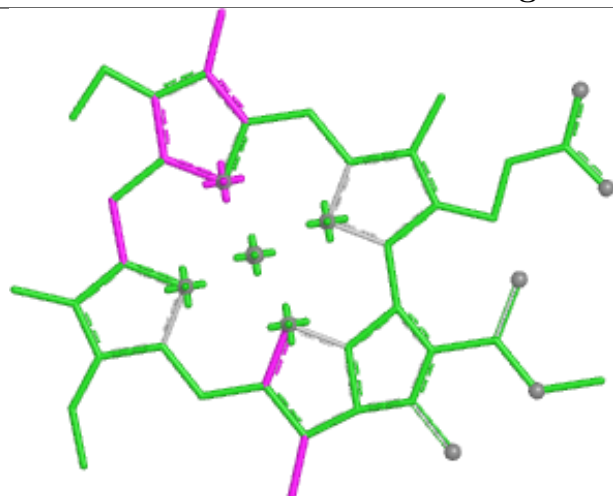


Ligand CLA bX 1401





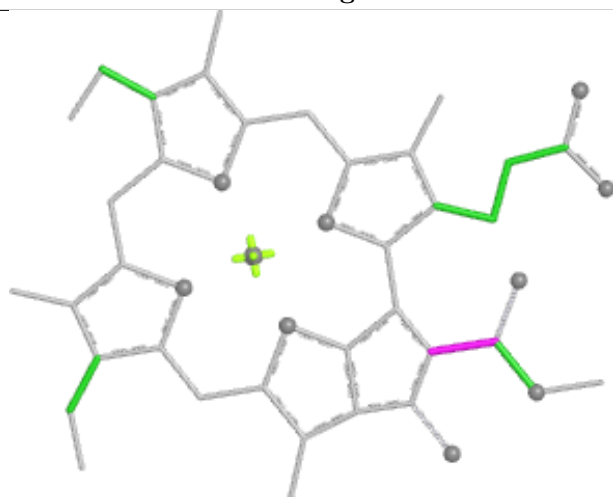
Ligand CLA e 509



Bond lengths



Bond angles

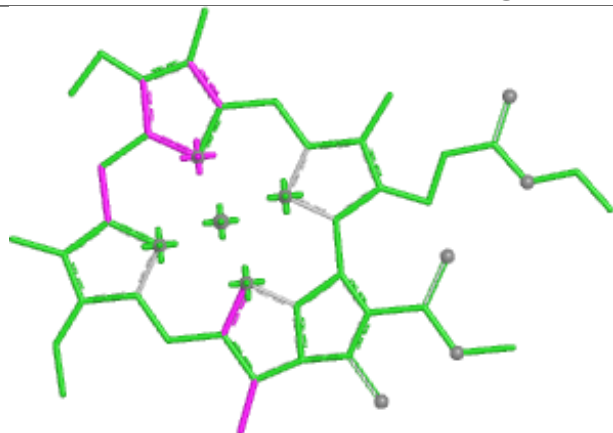


Torsions

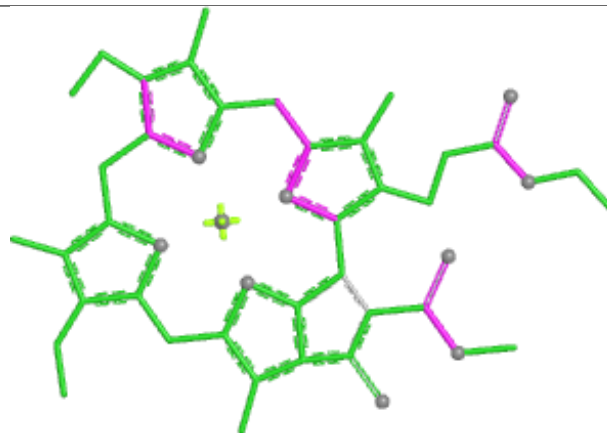


Rings

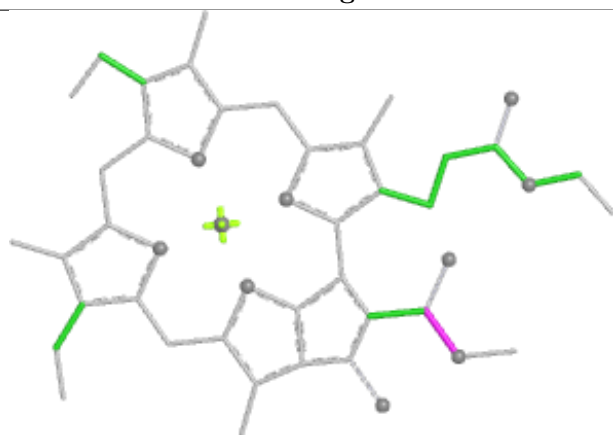
Ligand CLA cB 1220



Bond lengths



Bond angles

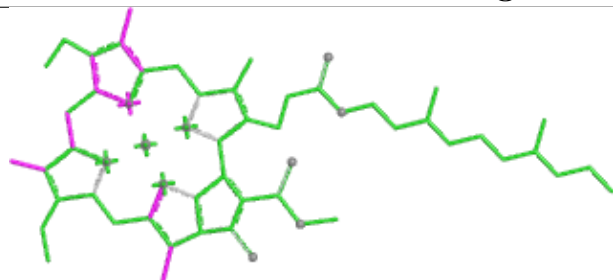


Torsions

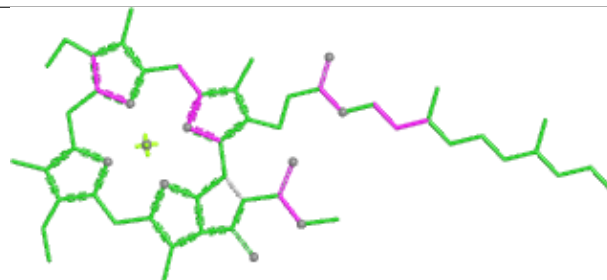


Rings

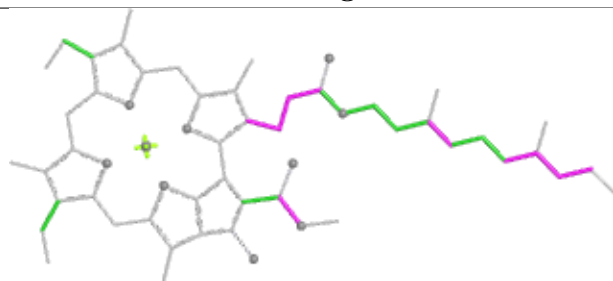
Ligand CLA aB 1224



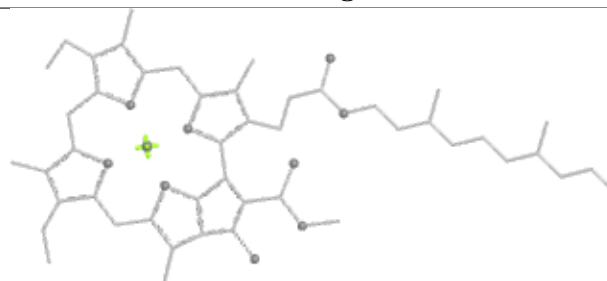
Bond lengths



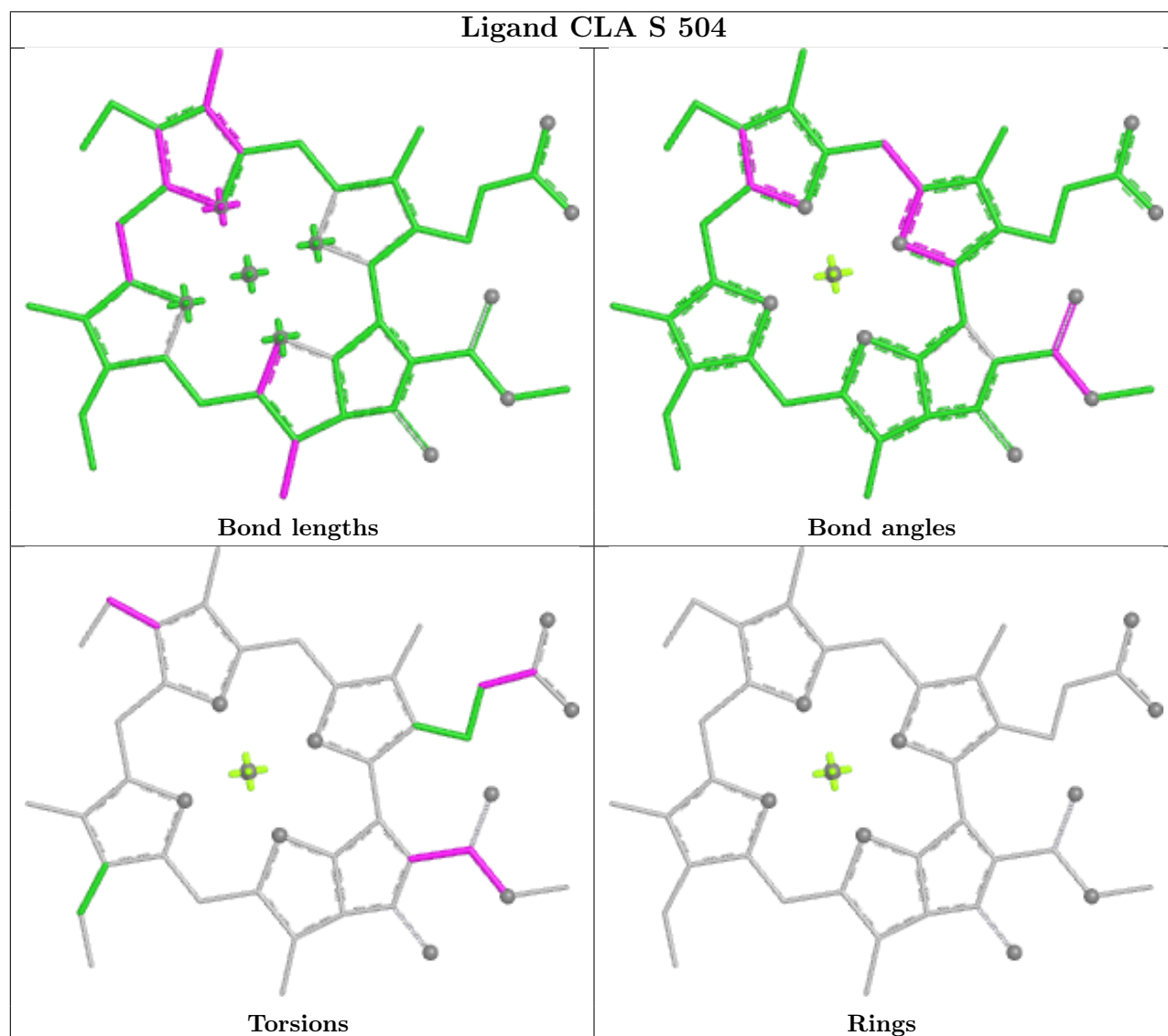
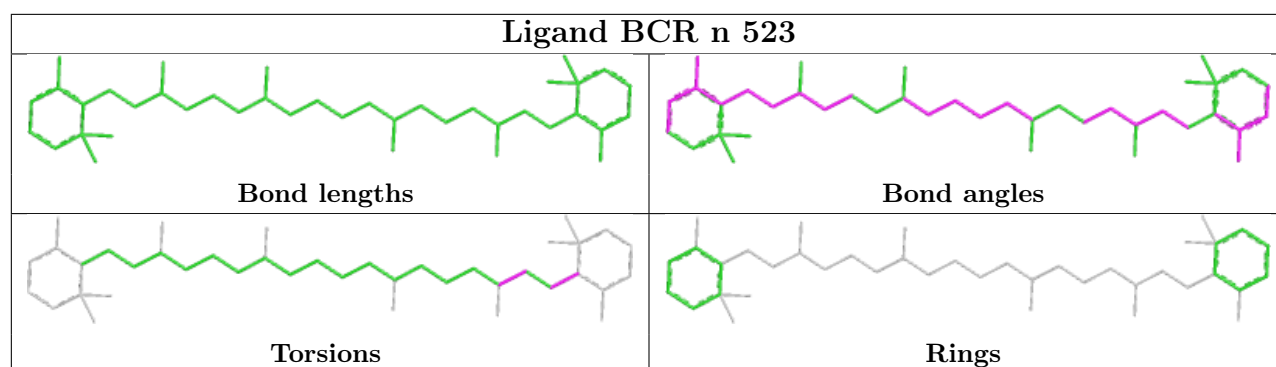
Bond angles



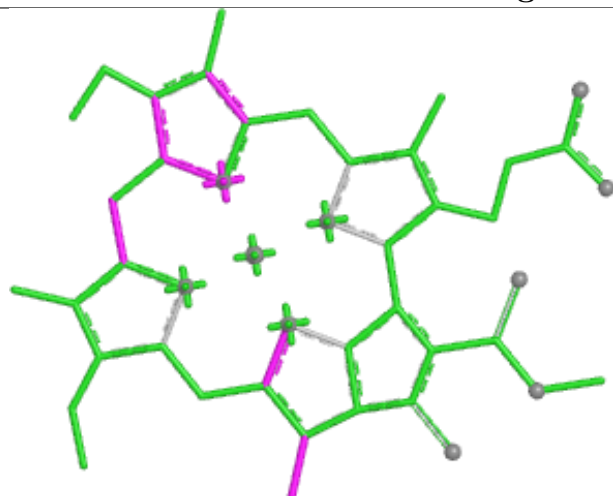
Torsions



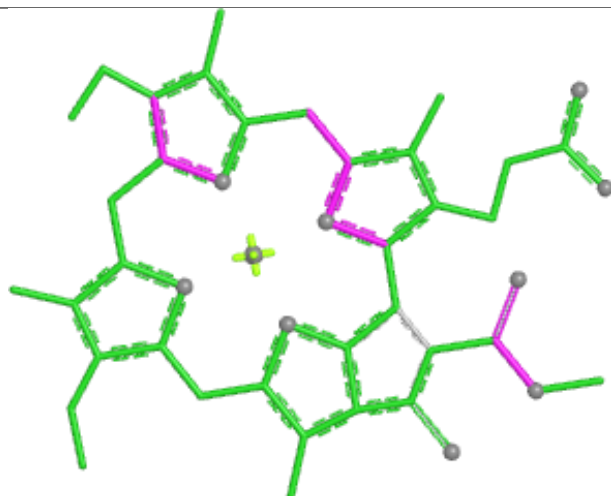
Rings



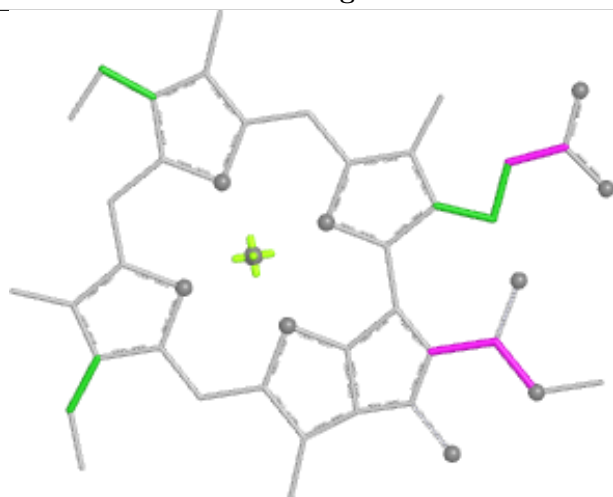
Ligand CLA b 507



Bond lengths



Bond angles

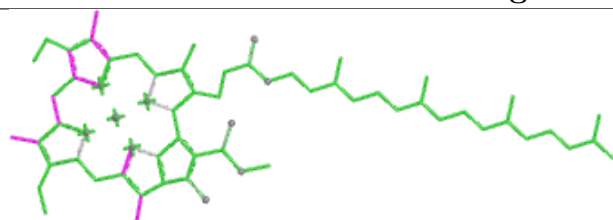


Torsions

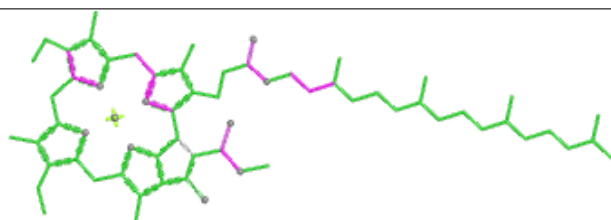


Rings

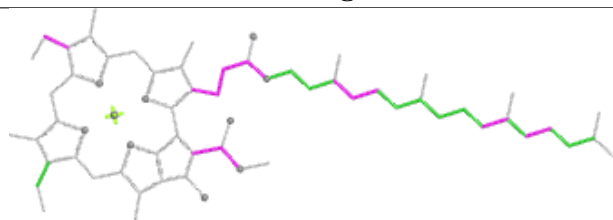
Ligand CLA a4 501



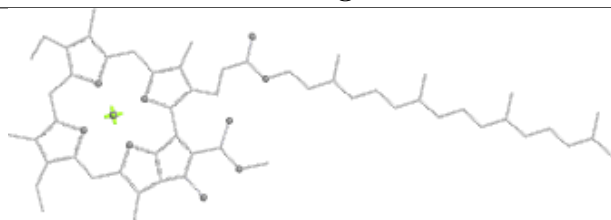
Bond lengths



Bond angles

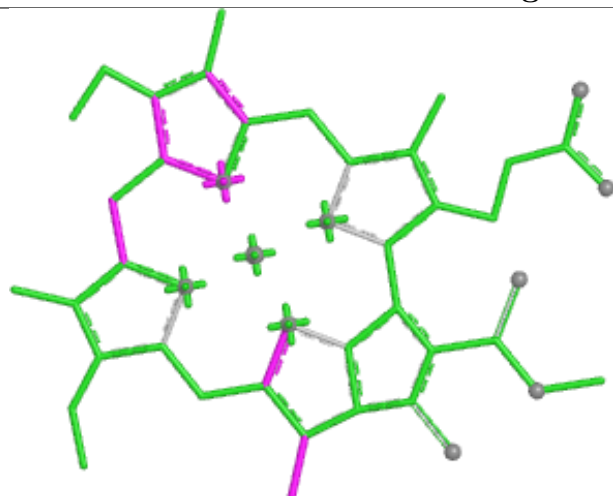


Torsions



Rings

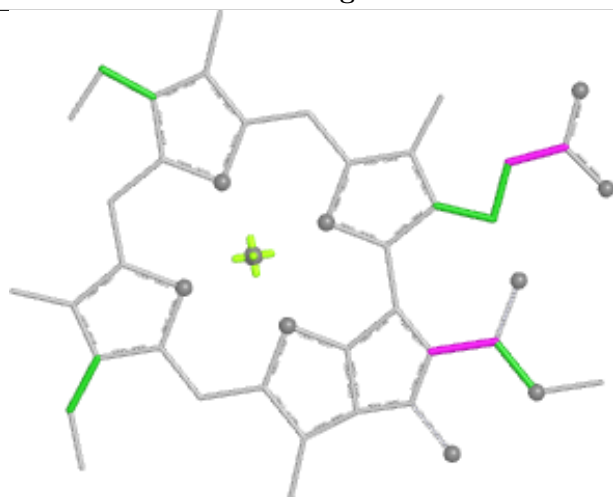
Ligand CLA f 507



Bond lengths



Bond angles

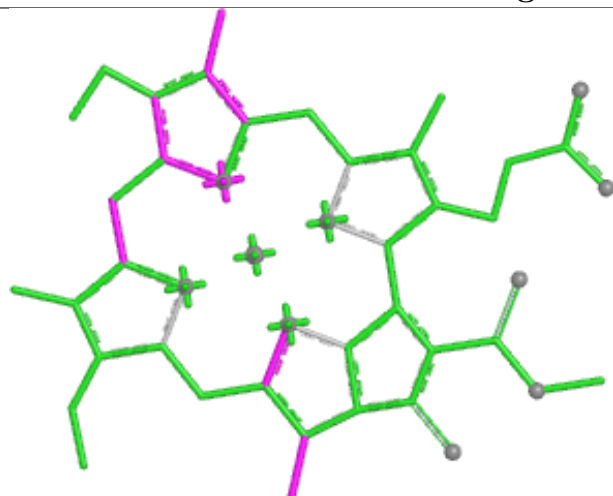


Torsions

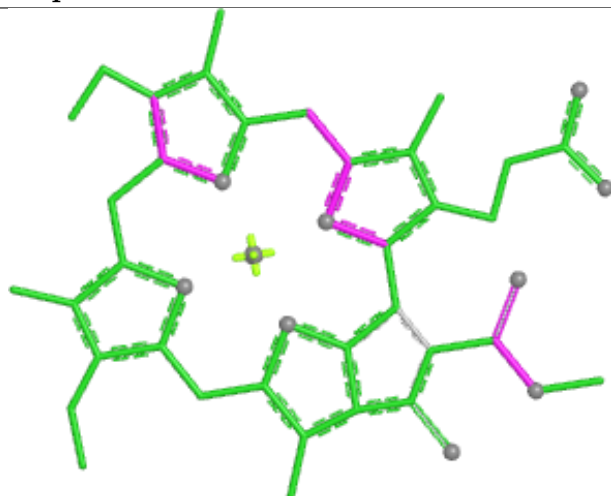


Rings

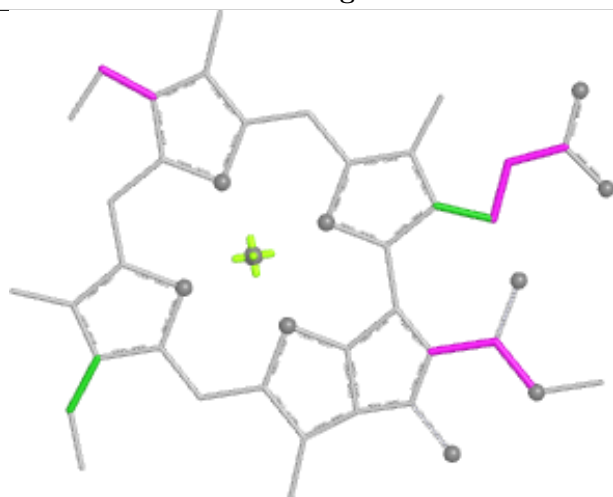
Ligand CLA p 504



Bond lengths



Bond angles

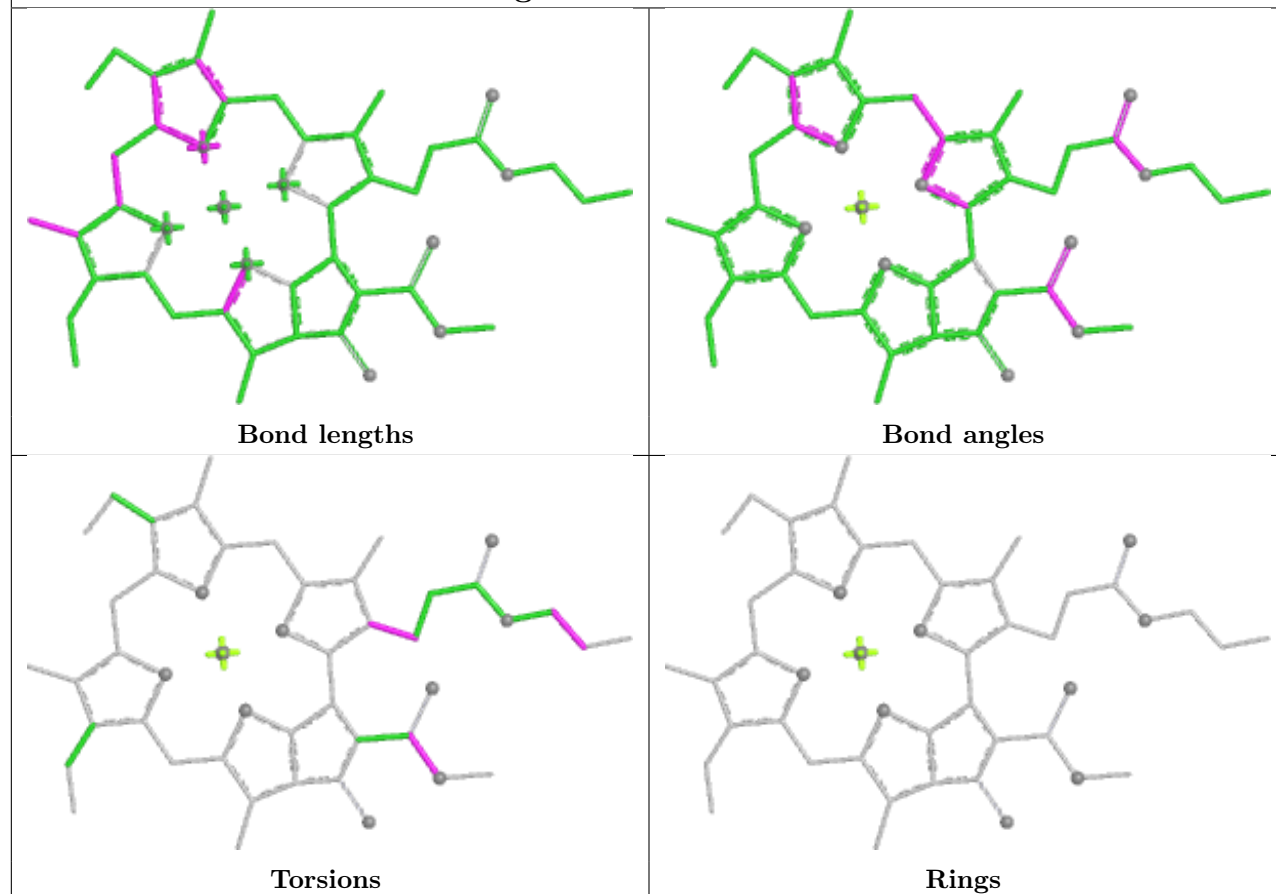


Torsions

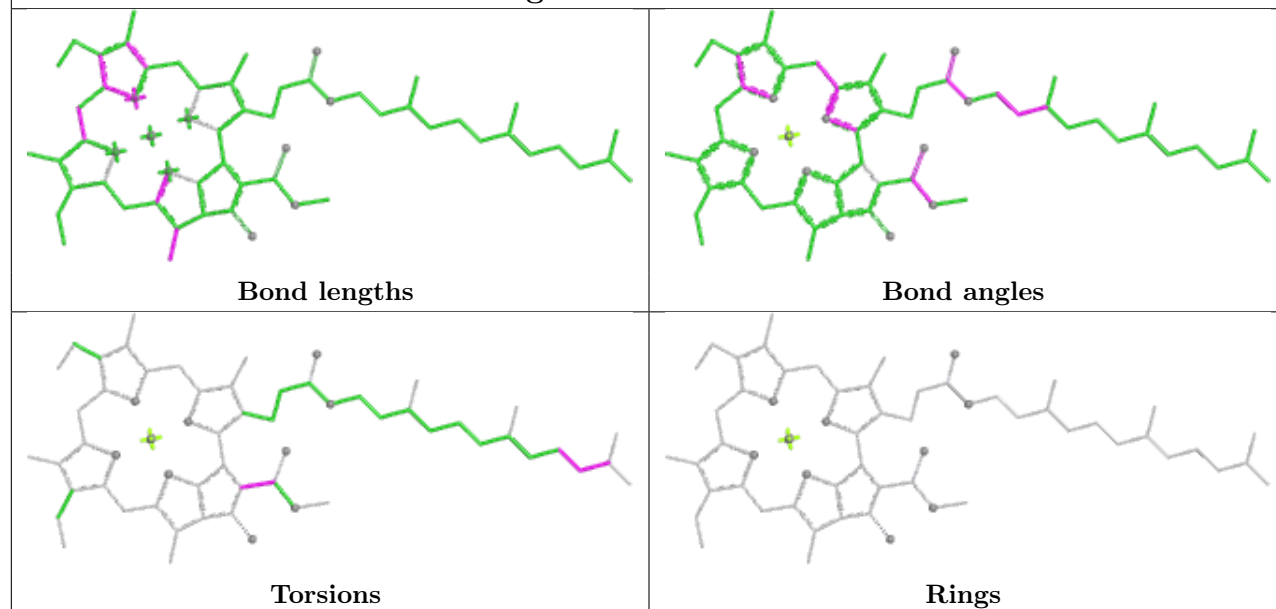


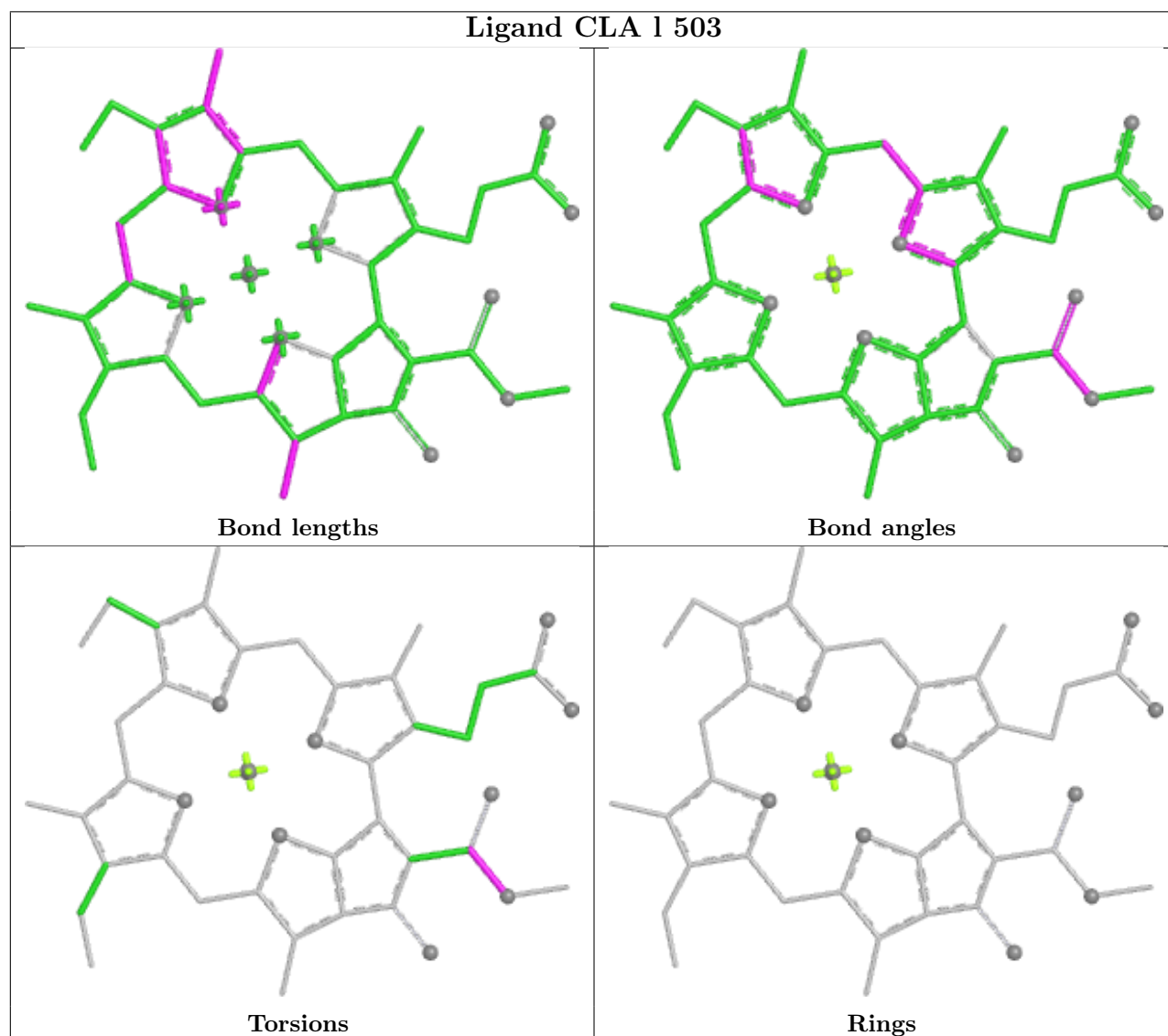
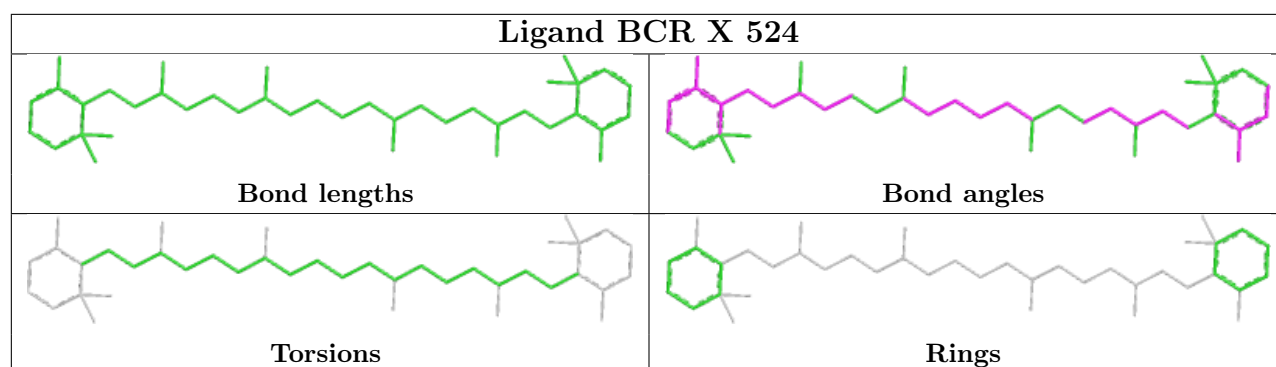
Rings

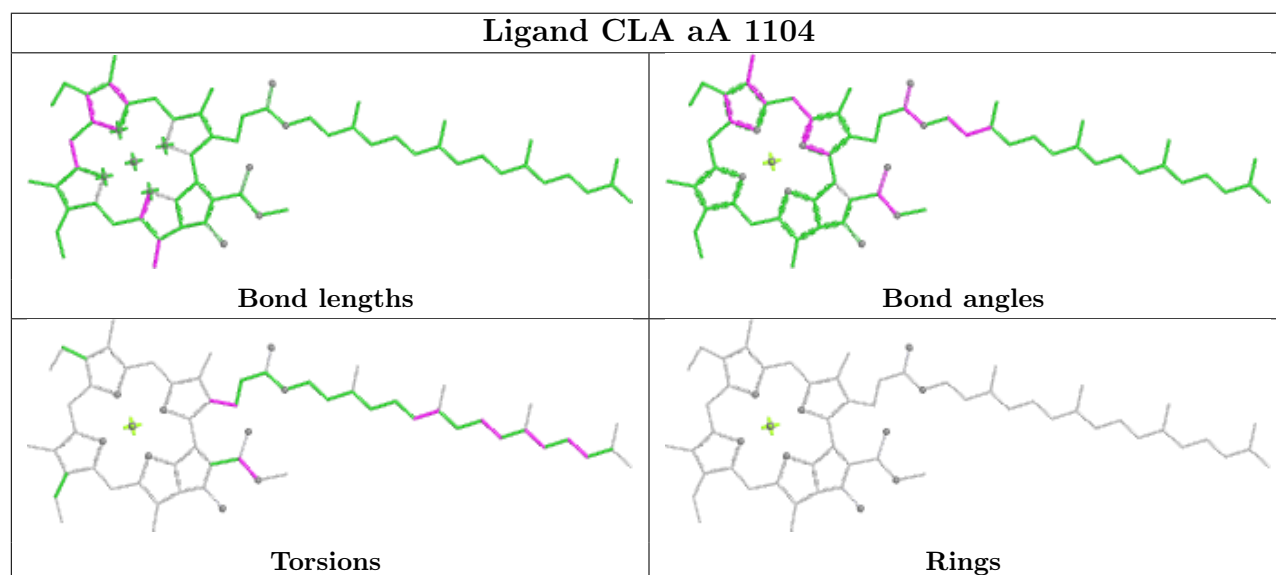
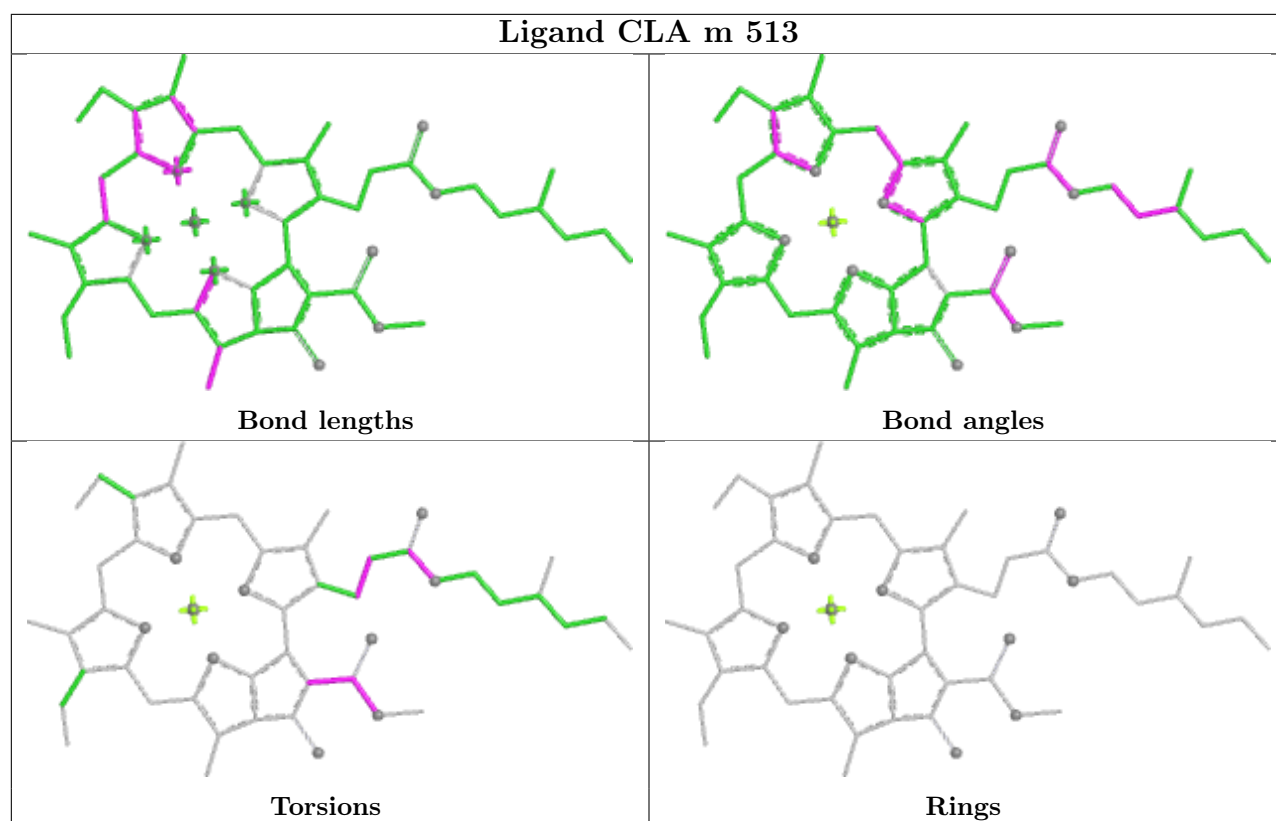
Ligand CLA cA 1112

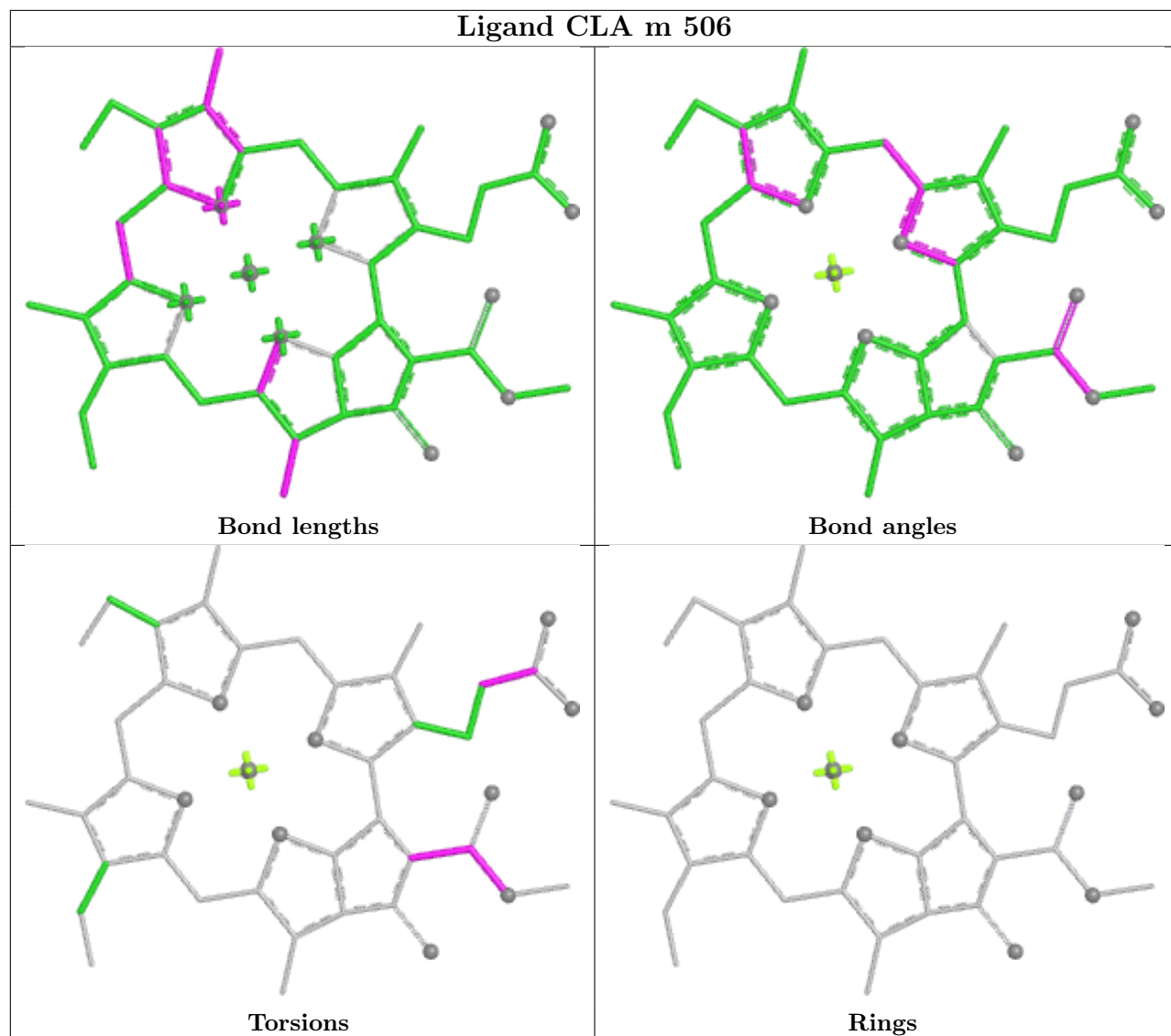


Ligand CLA b3 507

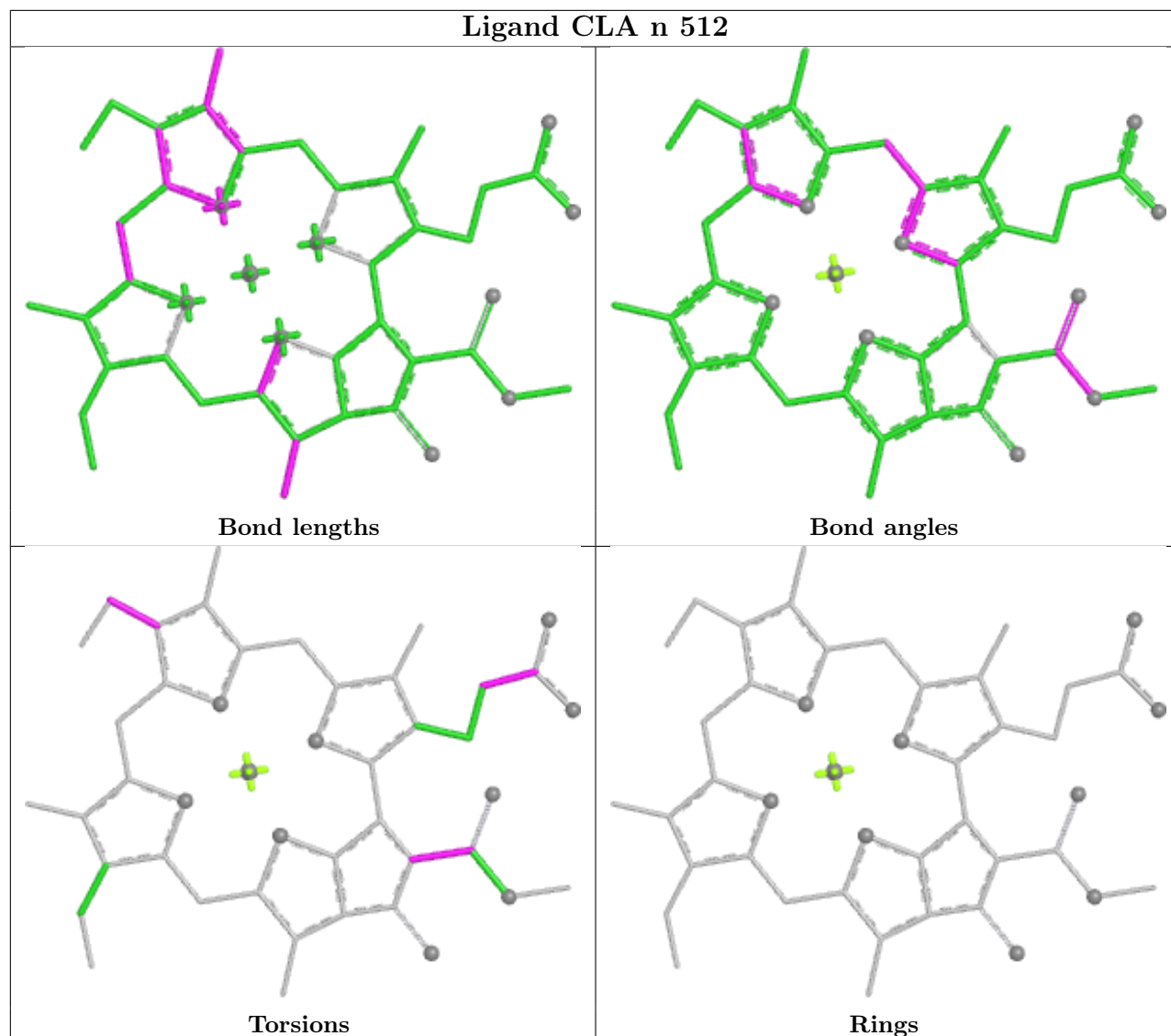




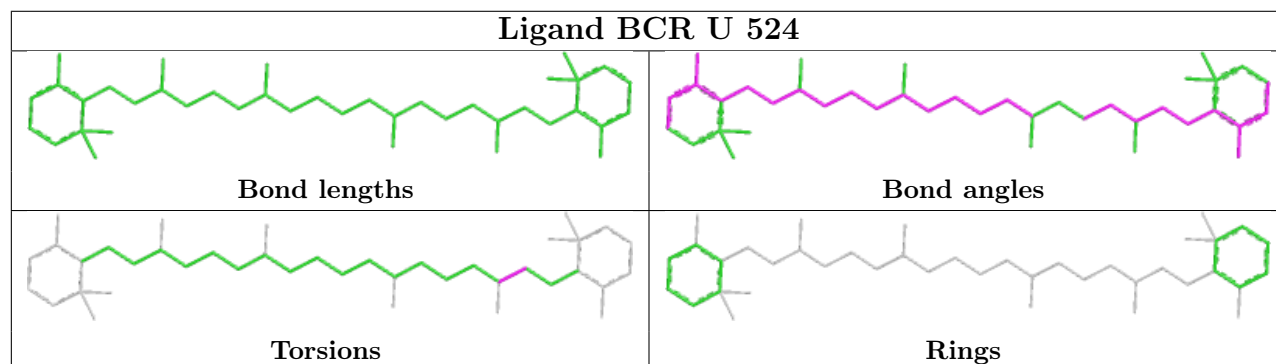


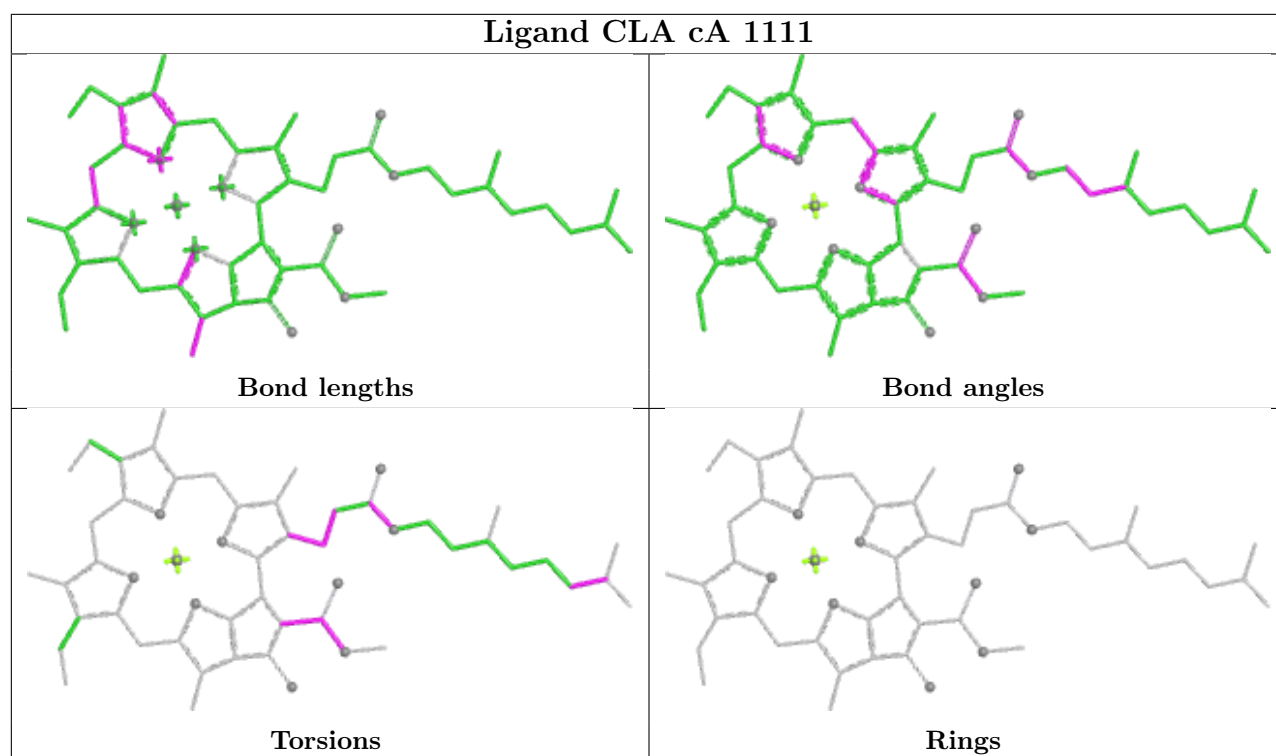


Ligand CLA n 512

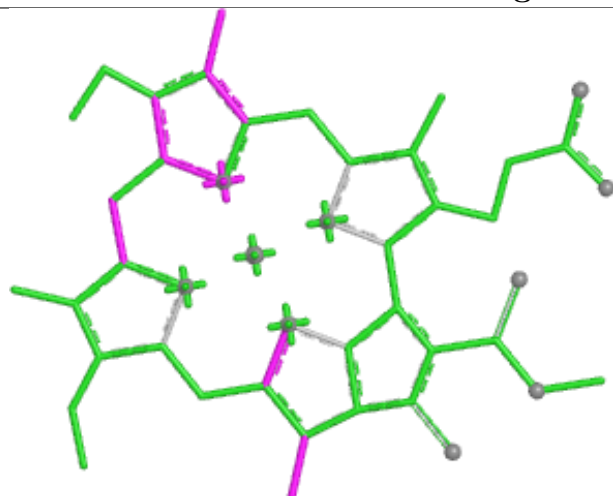


Ligand BCR U 524





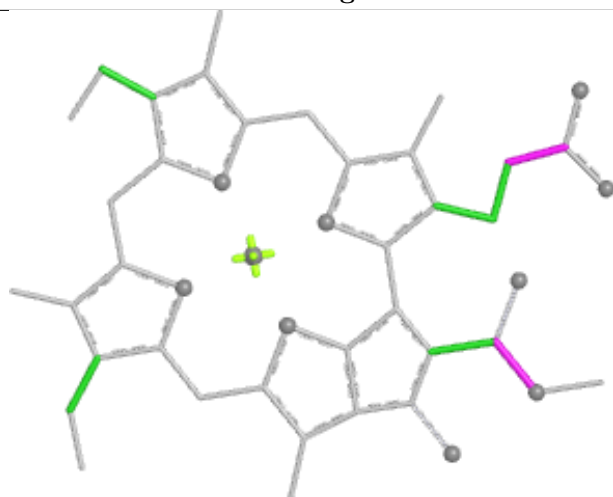
Ligand CLA V 506



Bond lengths



Bond angles

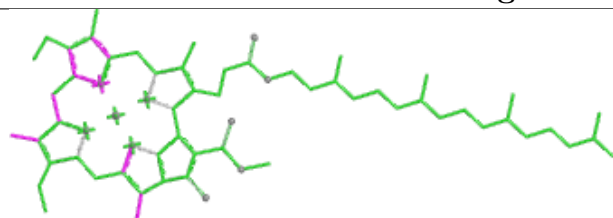


Torsions

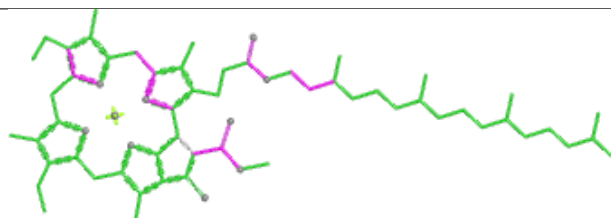


Rings

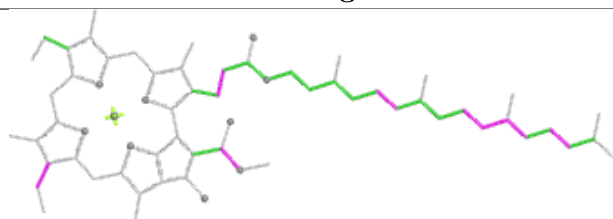
Ligand CLA cB 1023



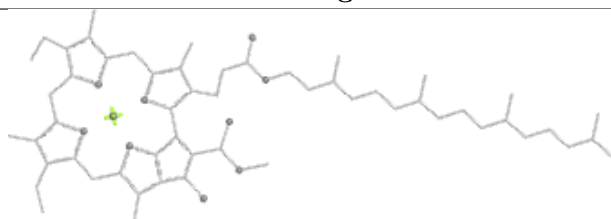
Bond lengths



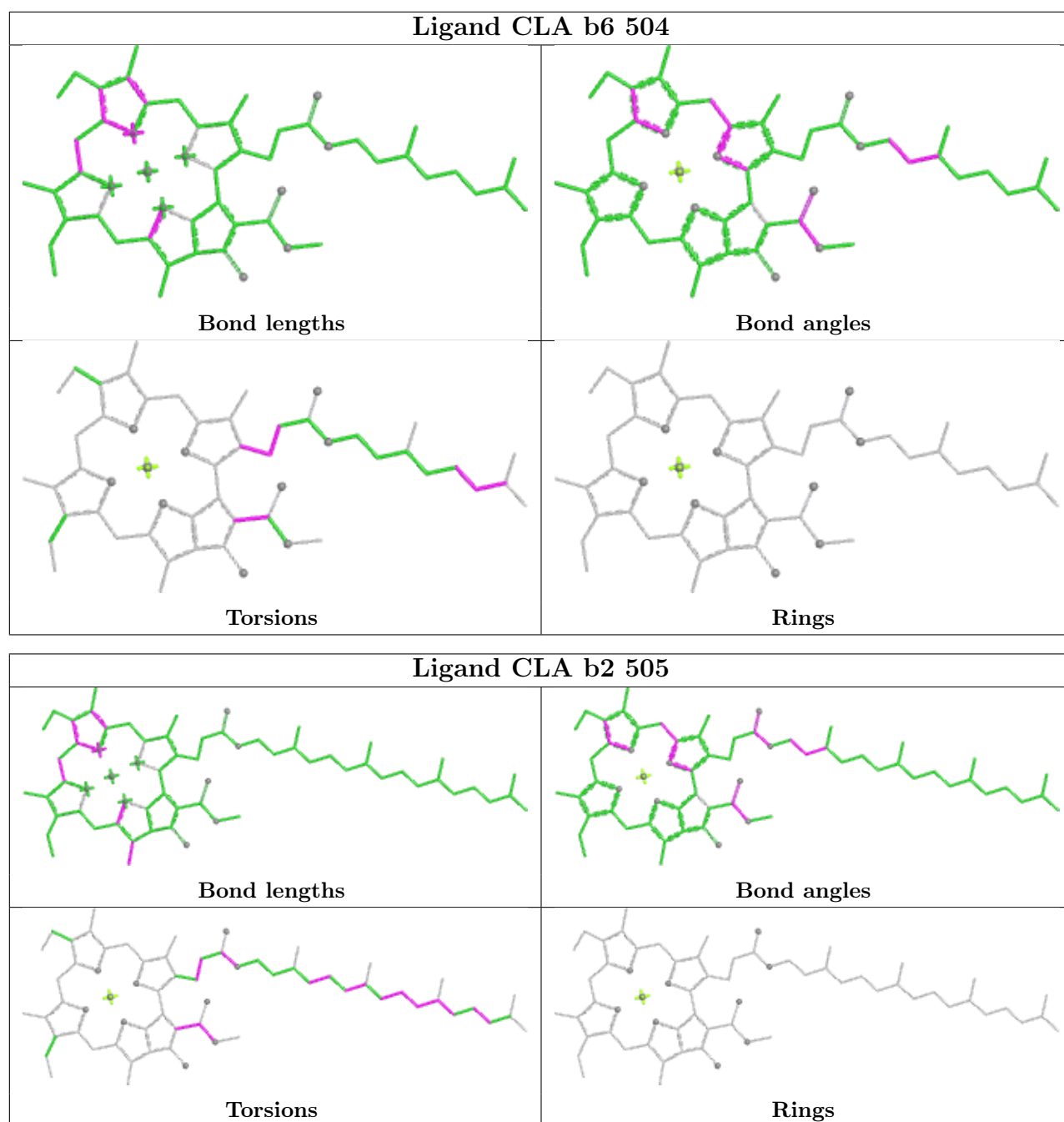
Bond angles



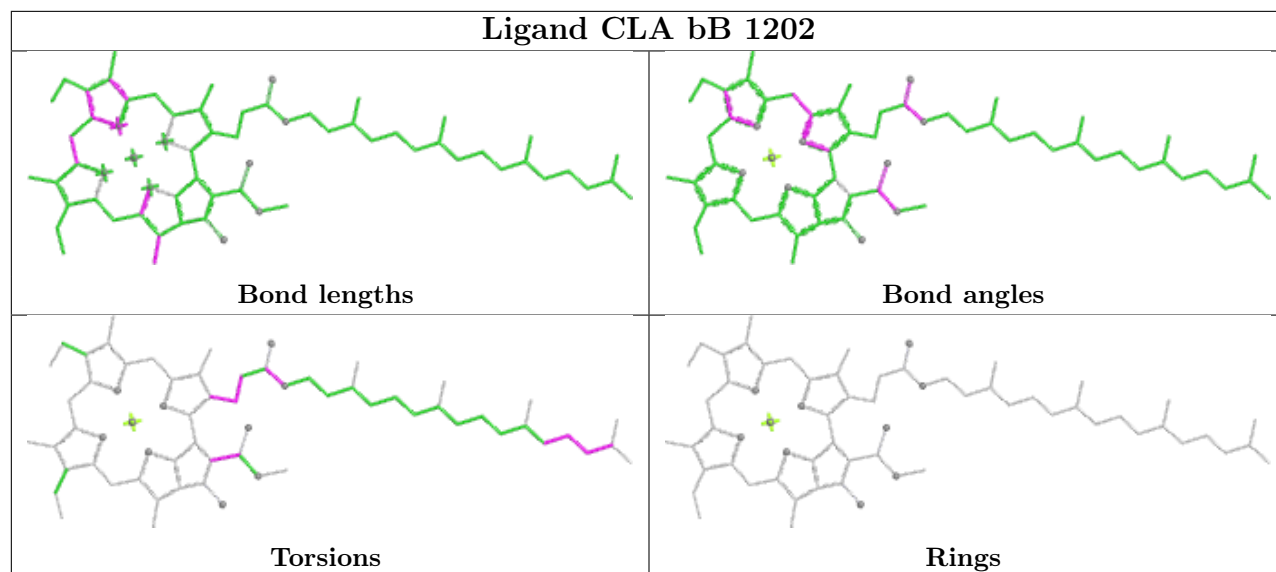
Torsions



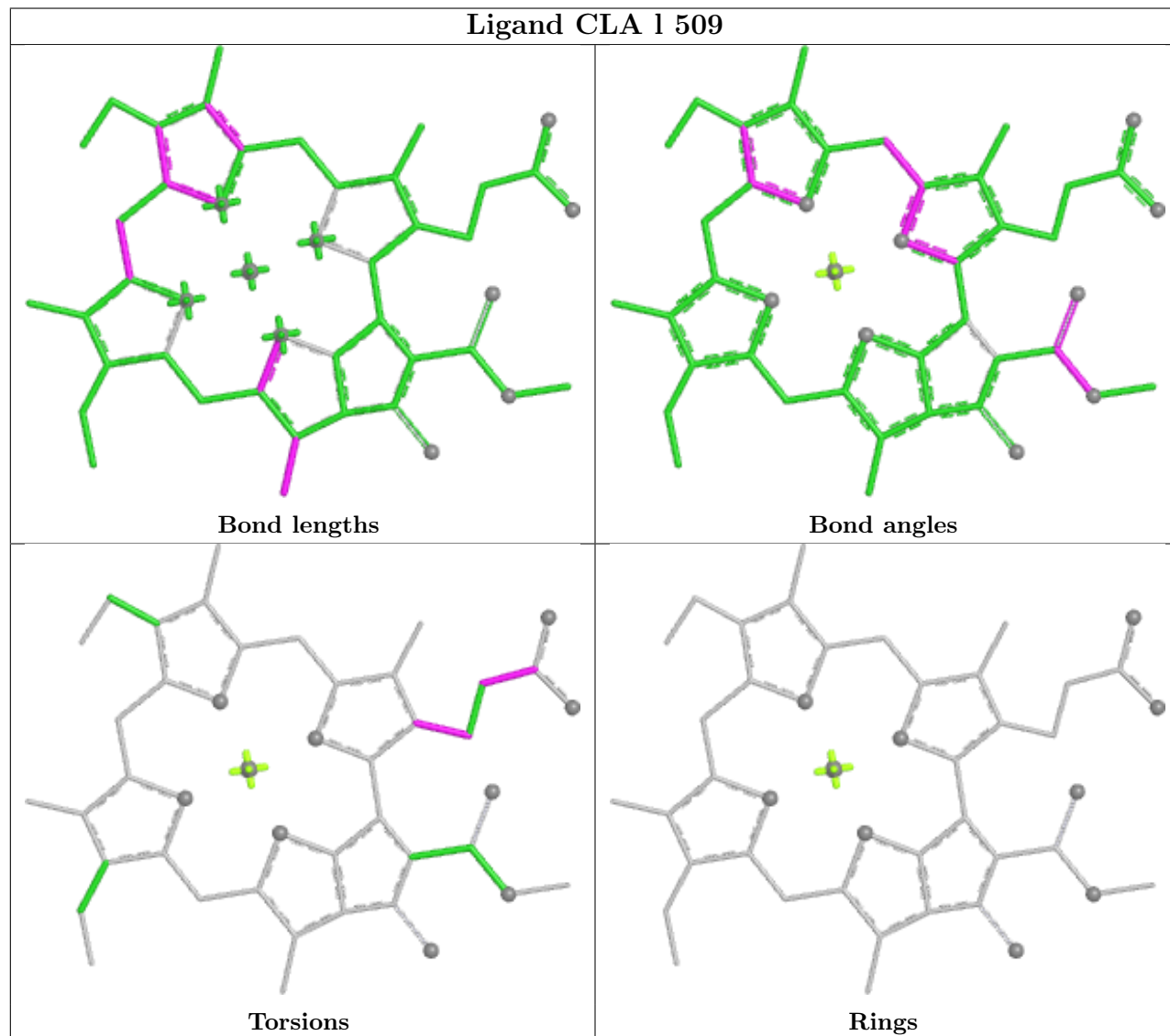
Rings

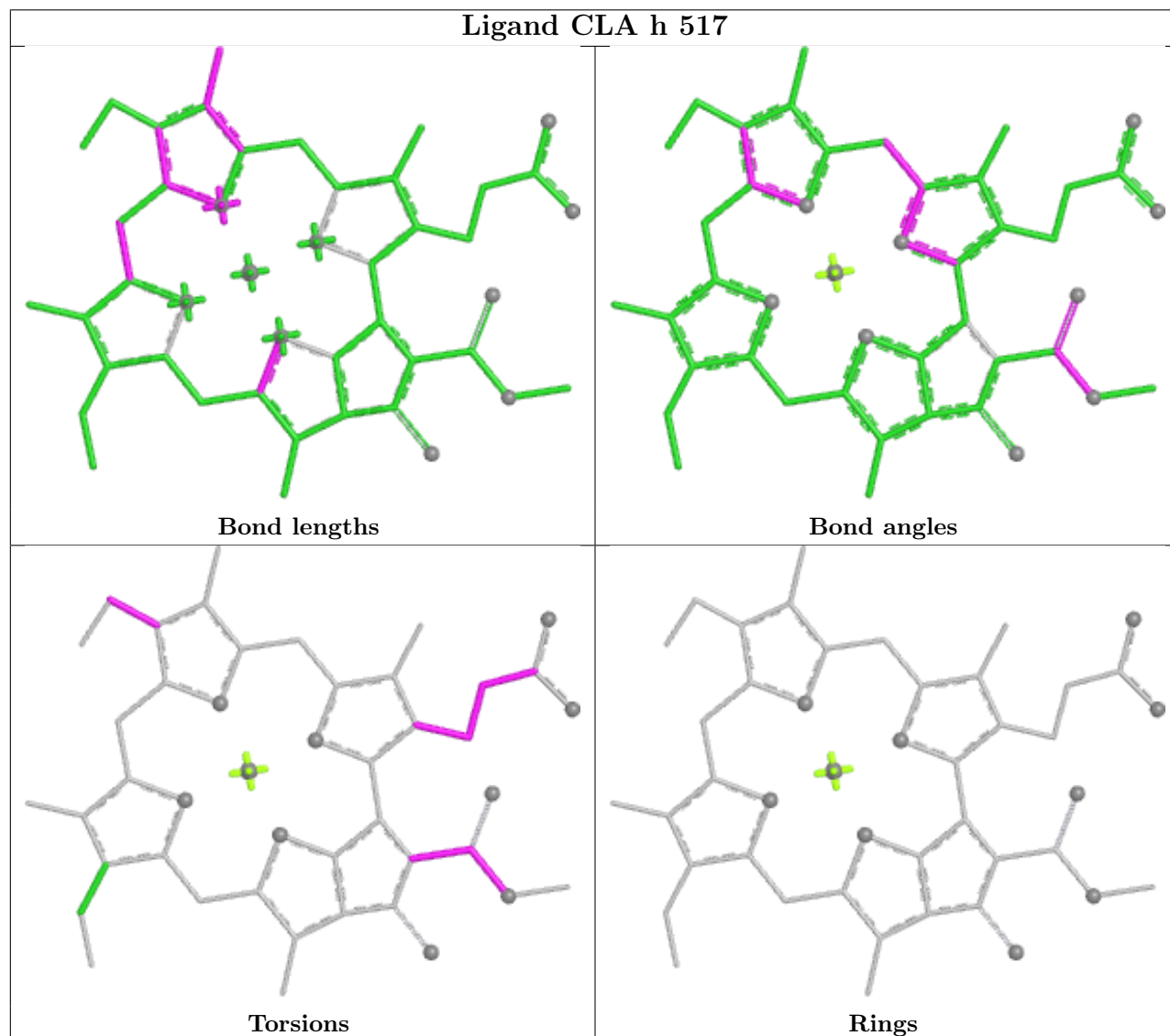
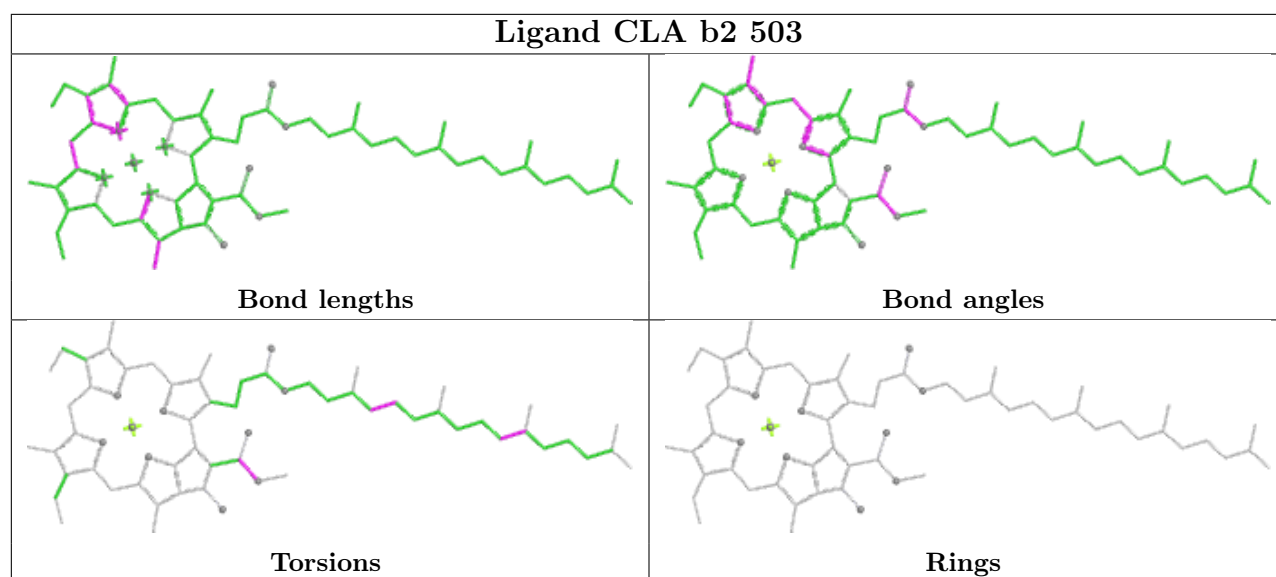


Ligand CLA bB 1202

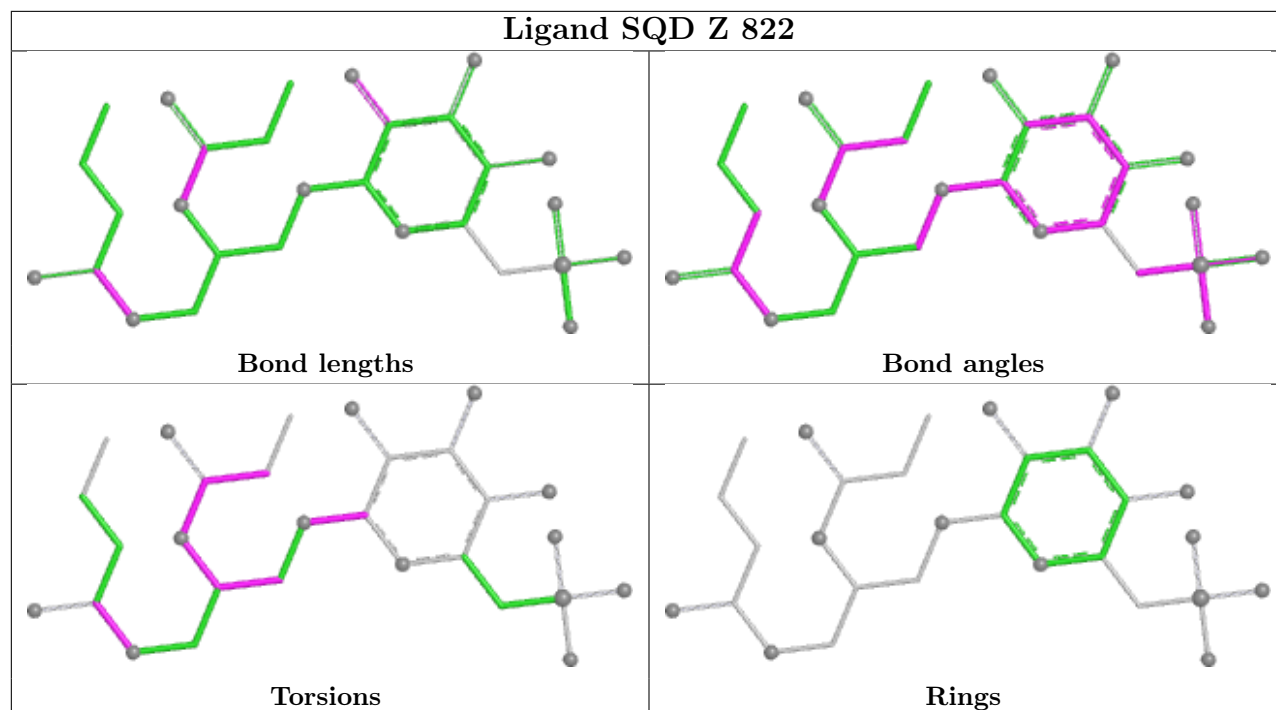


Ligand CLA l 509

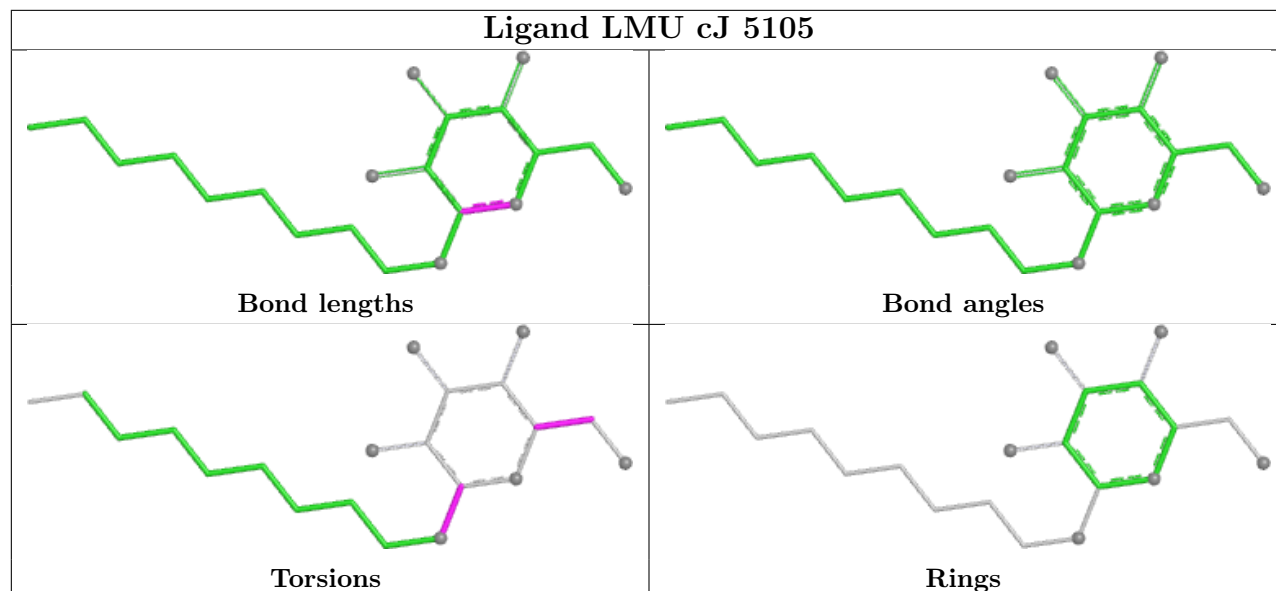




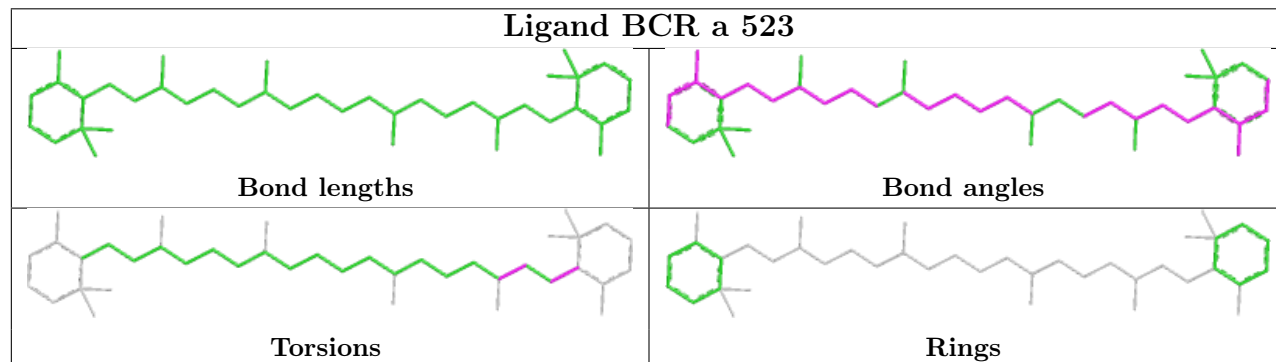
Ligand SQD Z 822

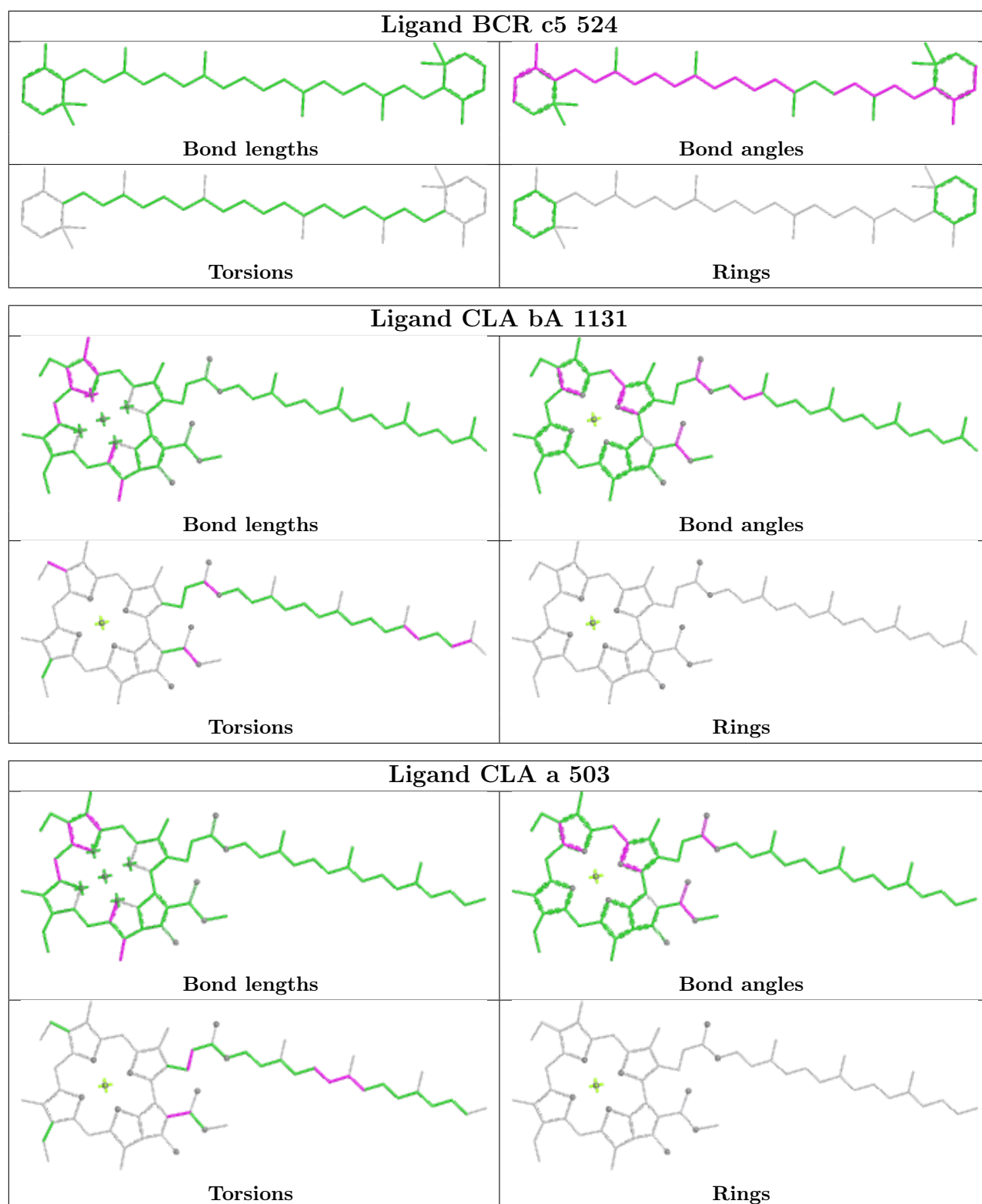


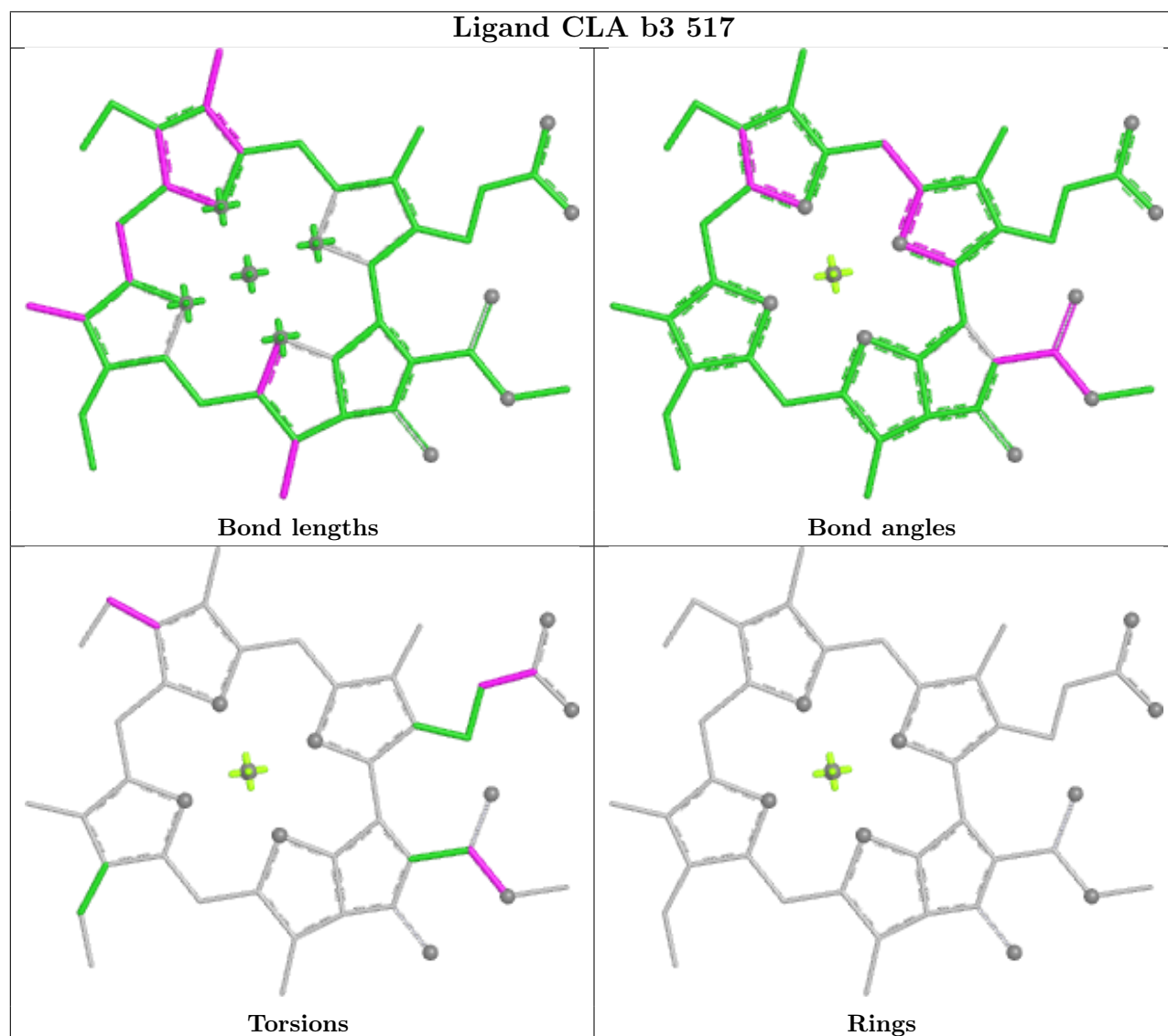
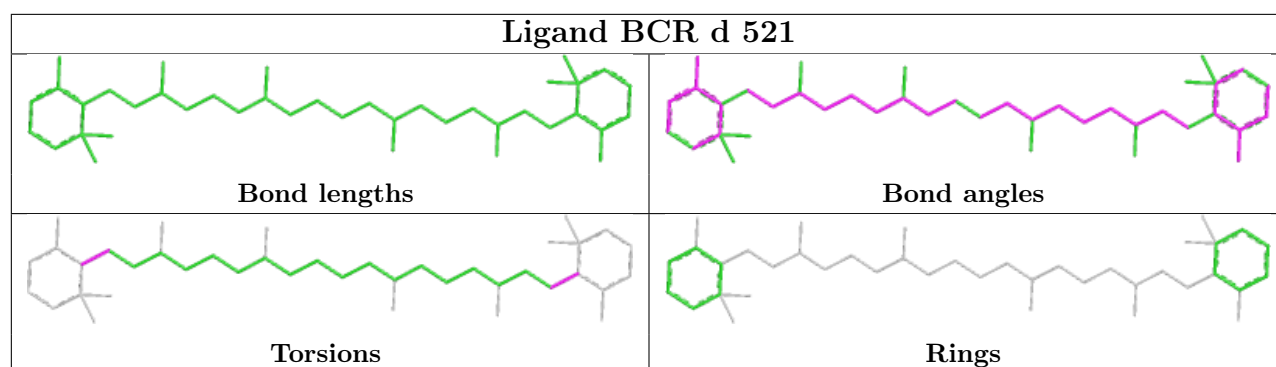
Ligand LMU cJ 5105



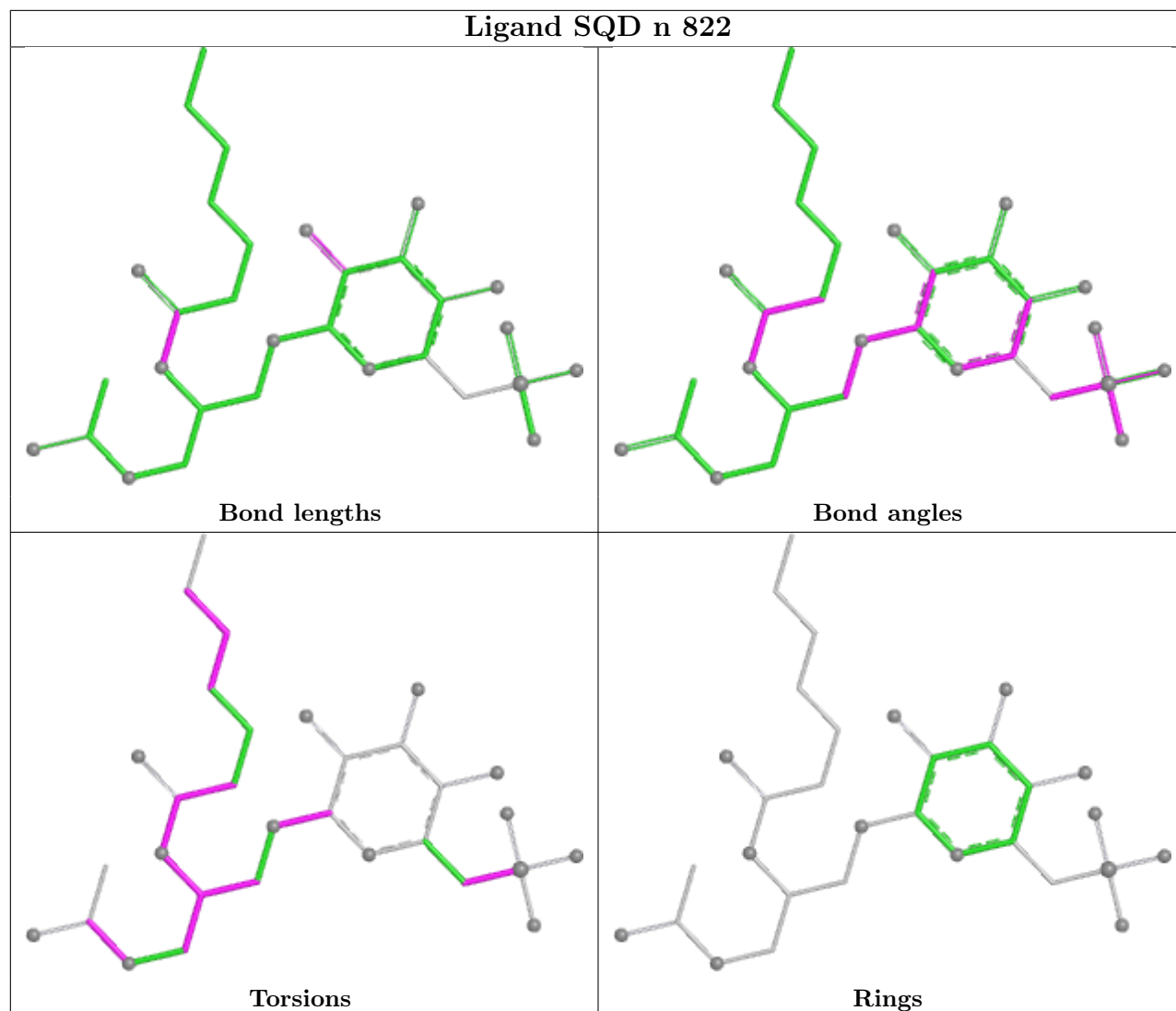
Ligand BCR a 523



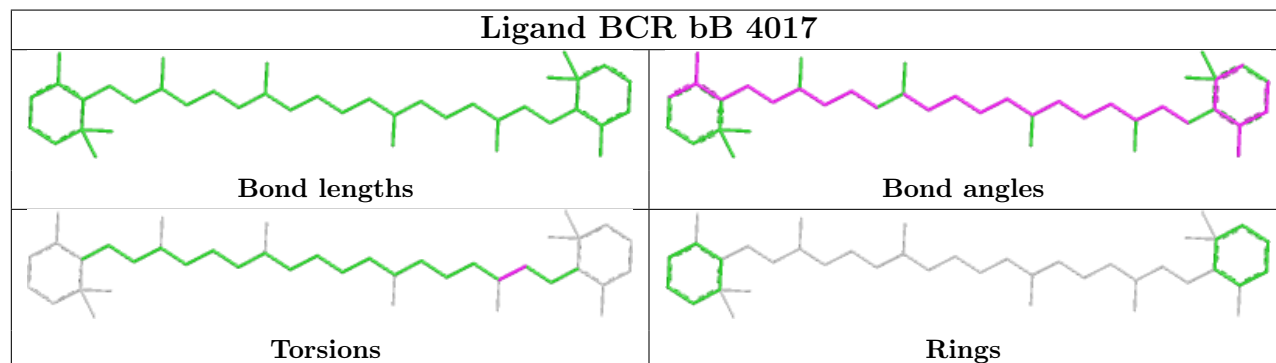


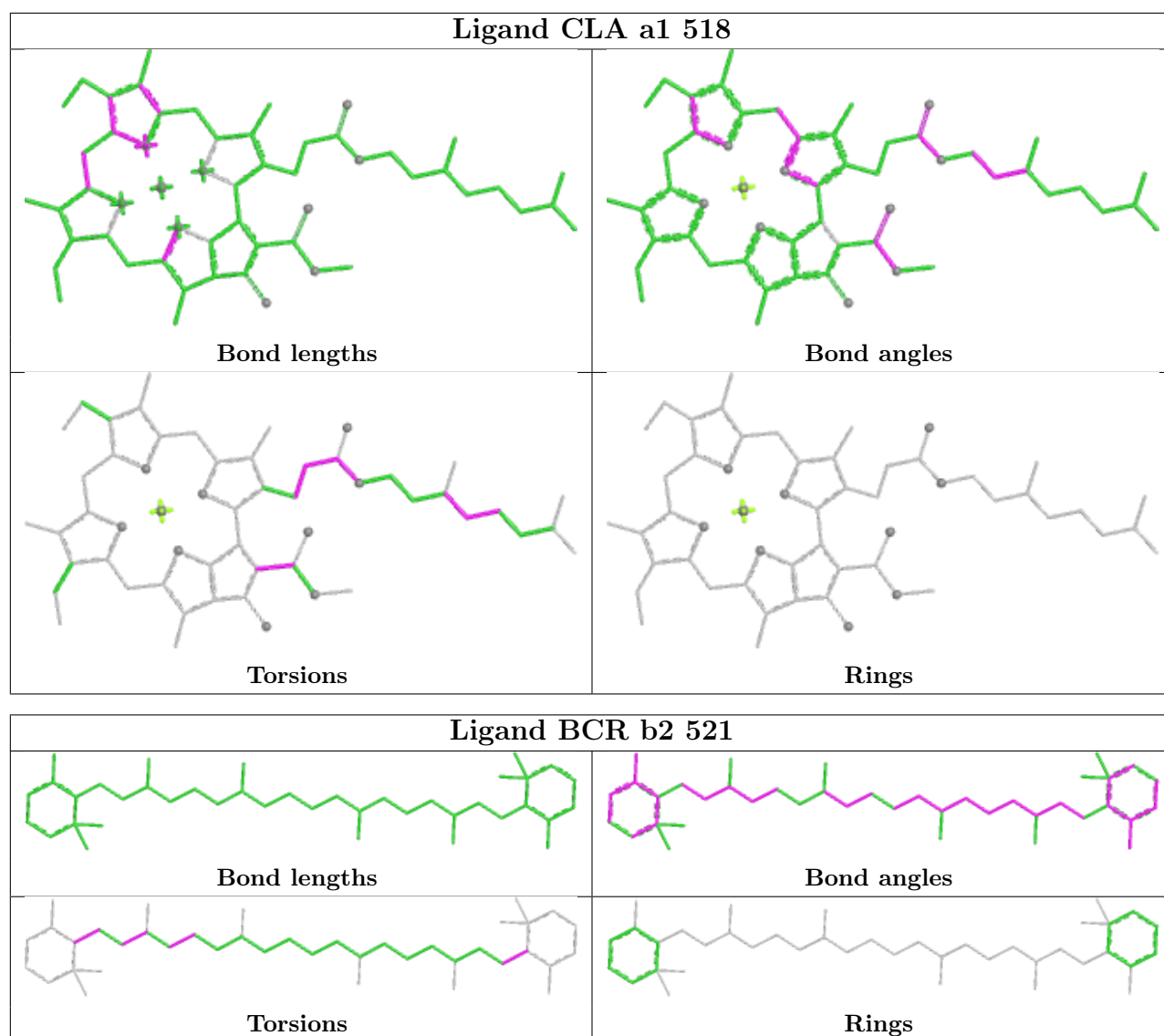


Ligand SQD n 822

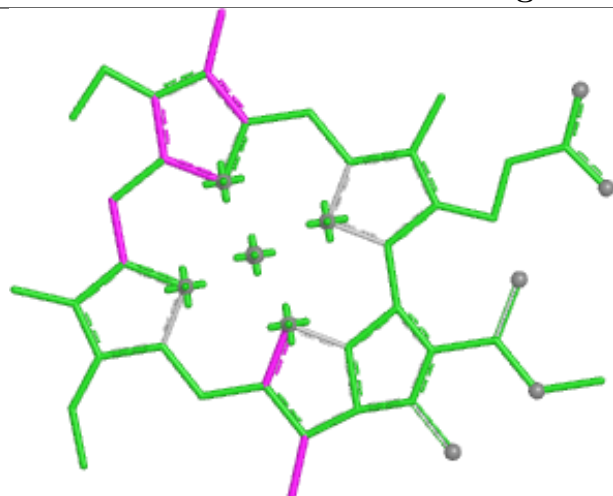


Ligand BCR bB 4017

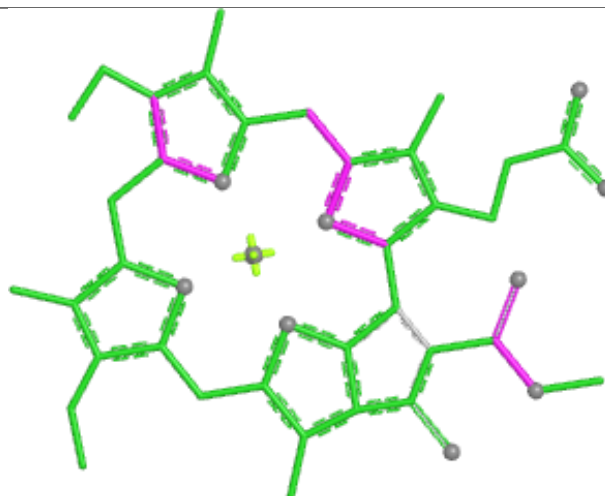




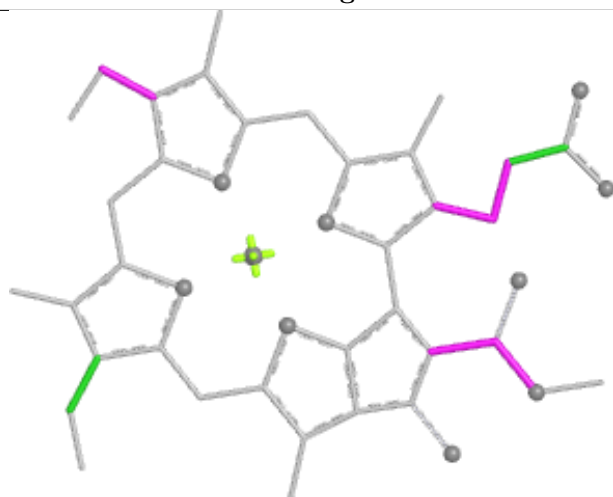
Ligand CLA Z 516



Bond lengths



Bond angles

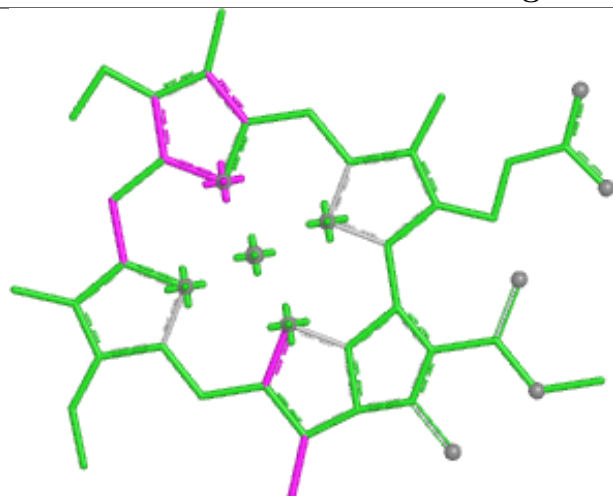


Torsions



Rings

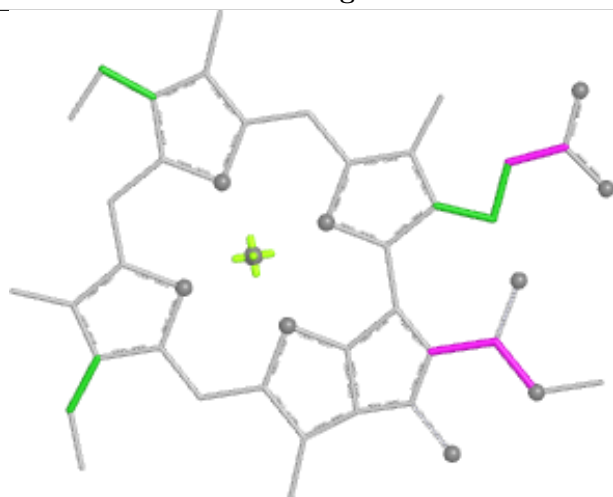
Ligand CLA 1 507



Bond lengths



Bond angles

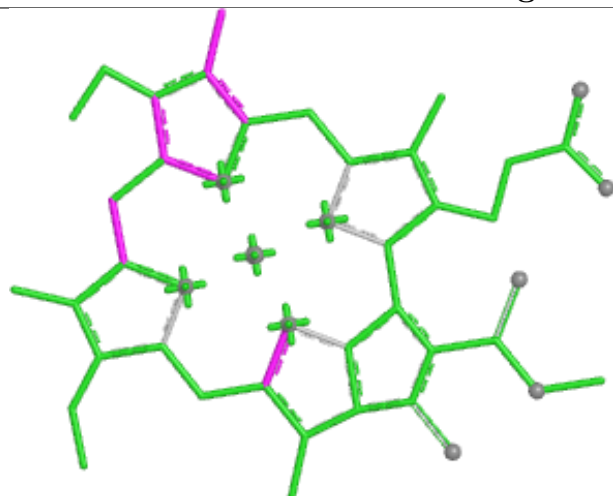


Torsions

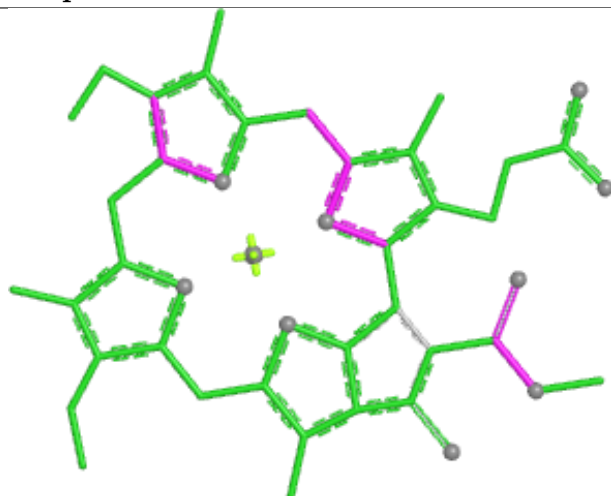


Rings

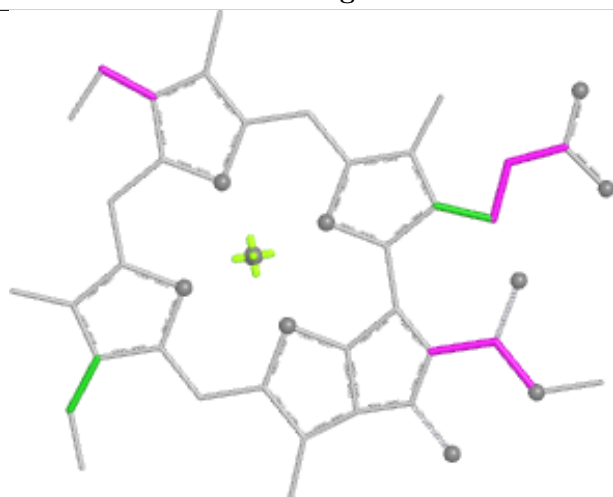
Ligand CLA q 504



Bond lengths



Bond angles

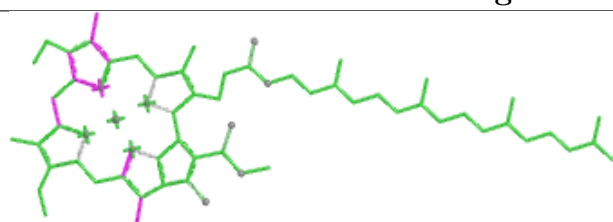


Torsions

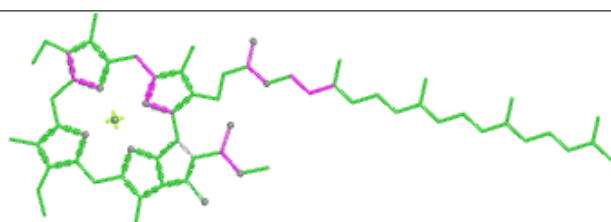


Rings

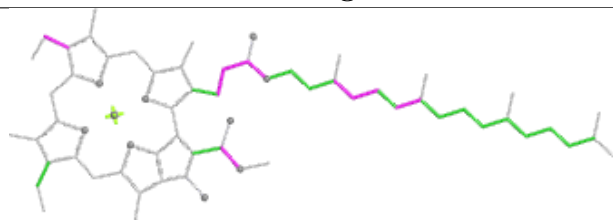
Ligand CLA bA 1237



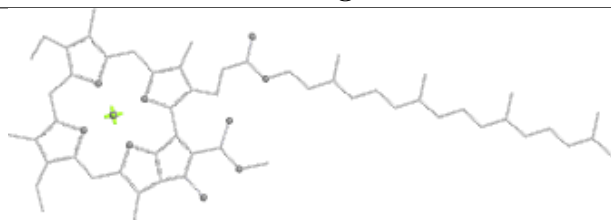
Bond lengths



Bond angles

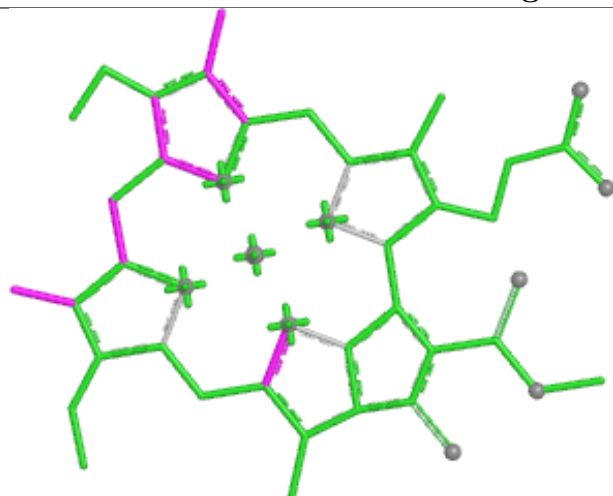


Torsions



Rings

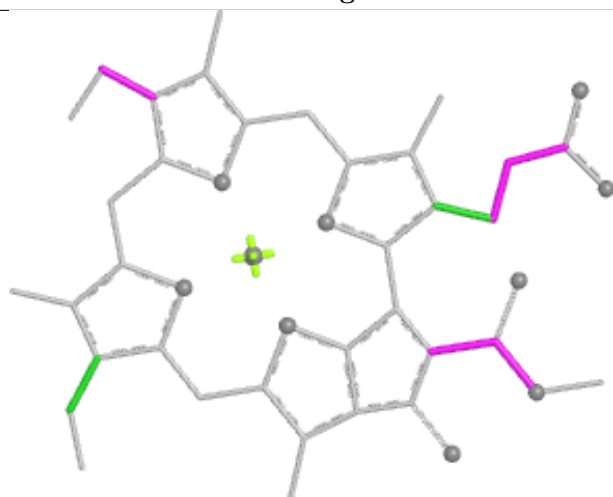
Ligand CLA f 504



Bond lengths



Bond angles

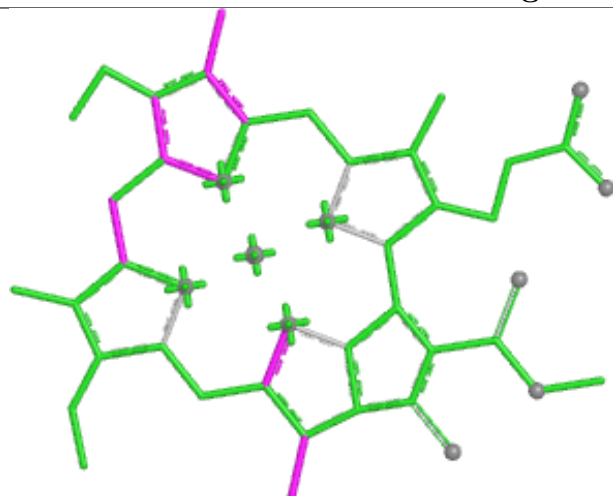


Torsions

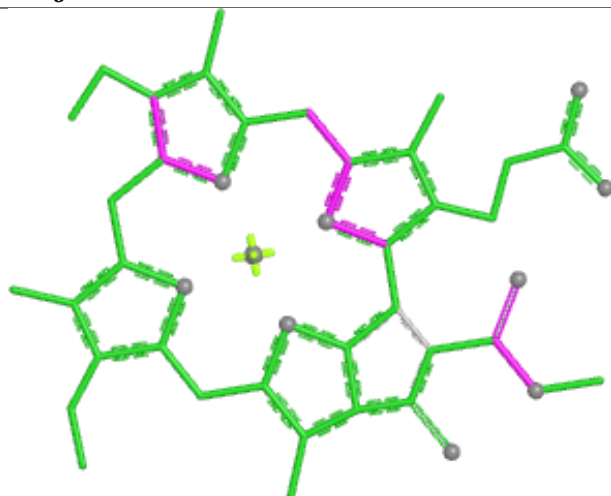


Rings

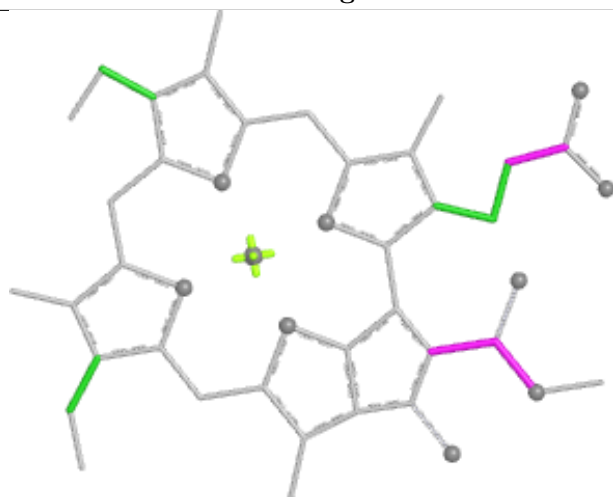
Ligand CLA j 512



Bond lengths



Bond angles

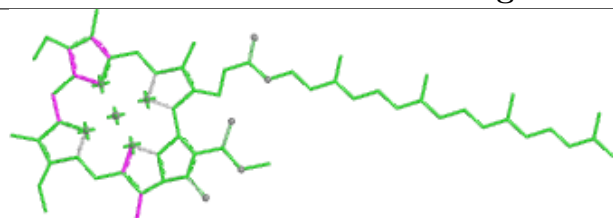


Torsions

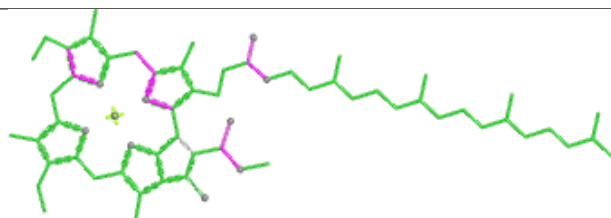


Rings

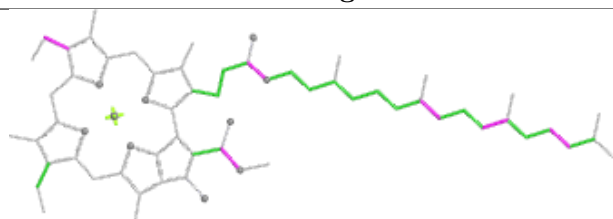
Ligand CLA cA 1109



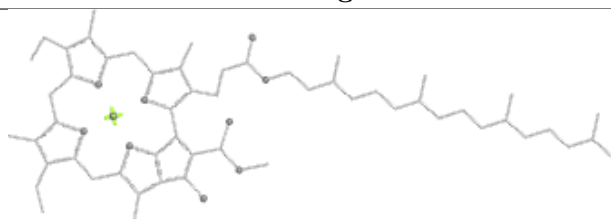
Bond lengths



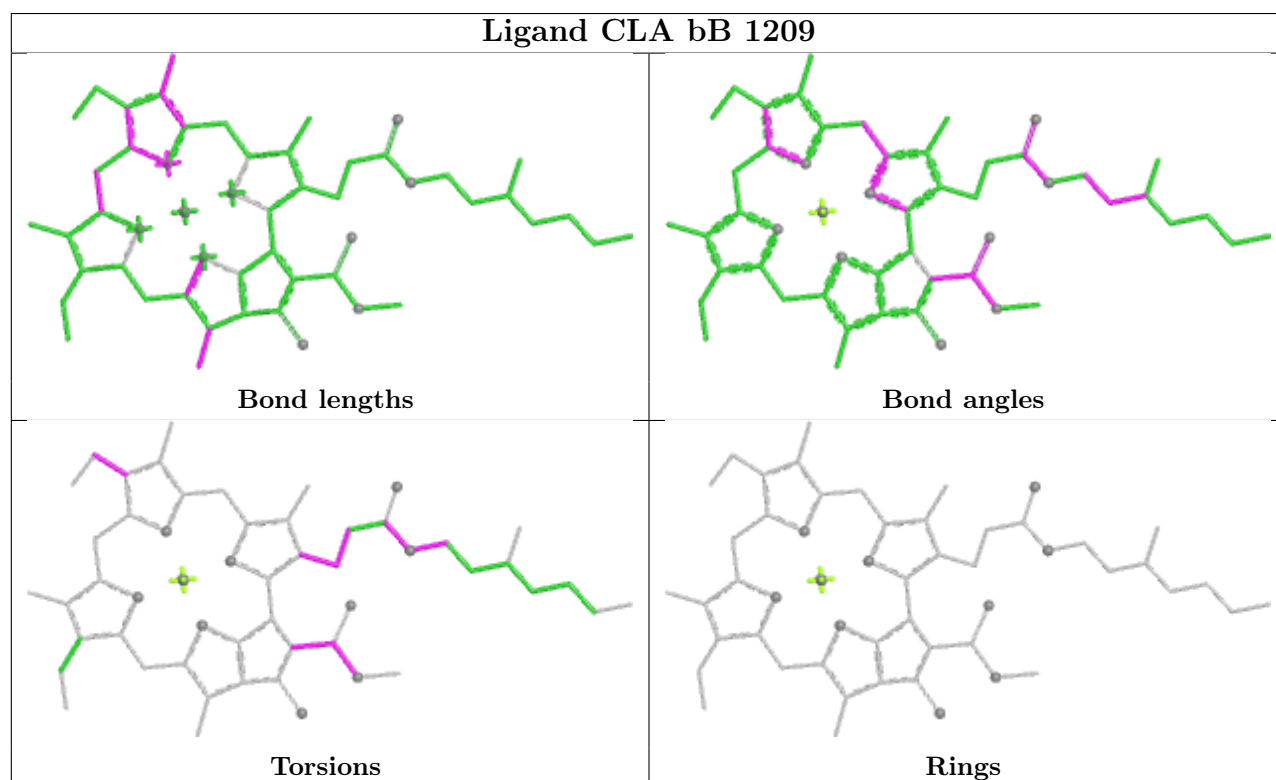
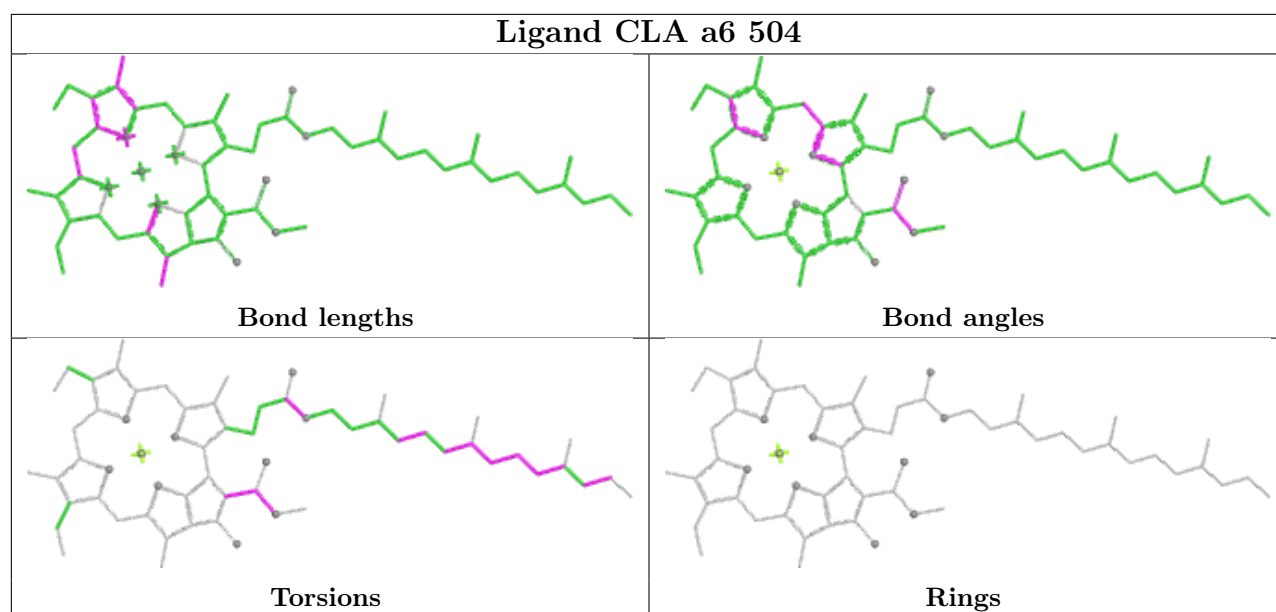
Bond angles



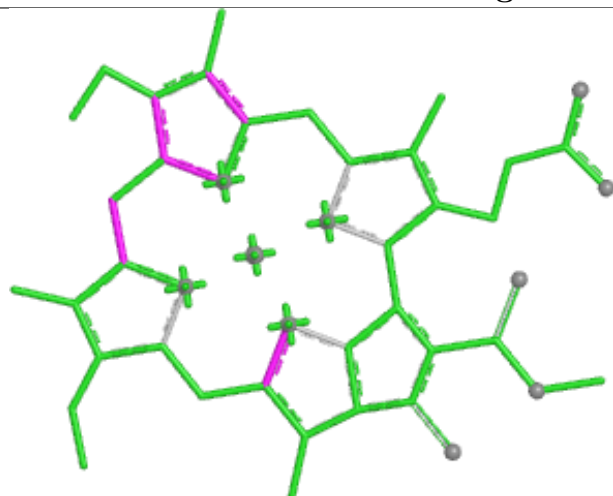
Torsions



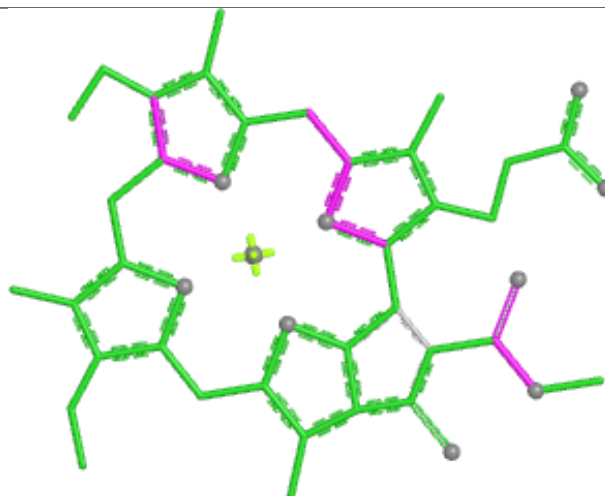
Rings



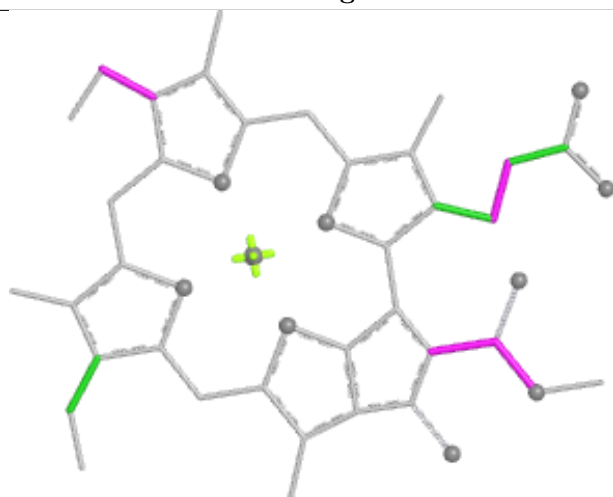
Ligand CLA aX 1401



Bond lengths



Bond angles

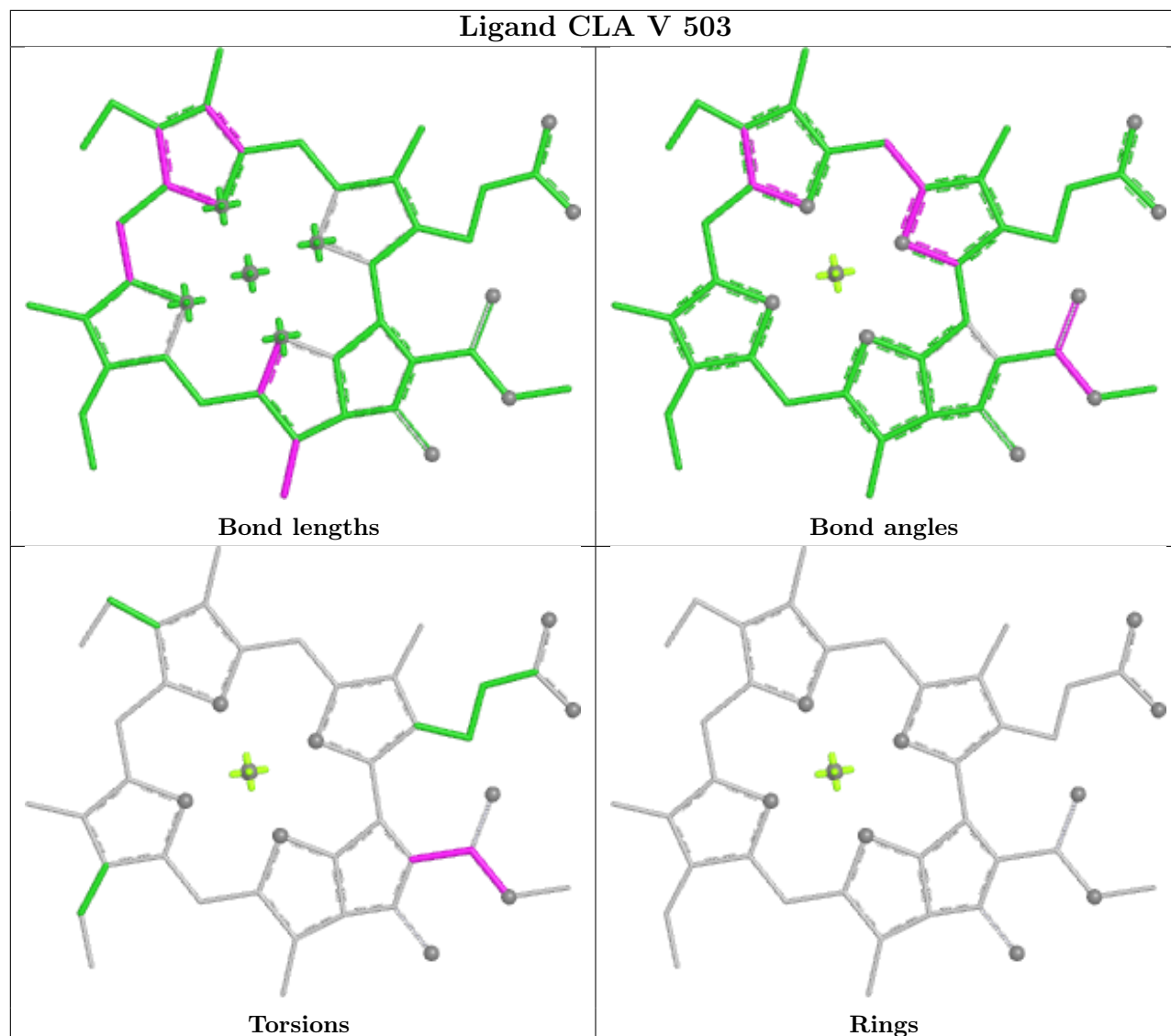


Torsions

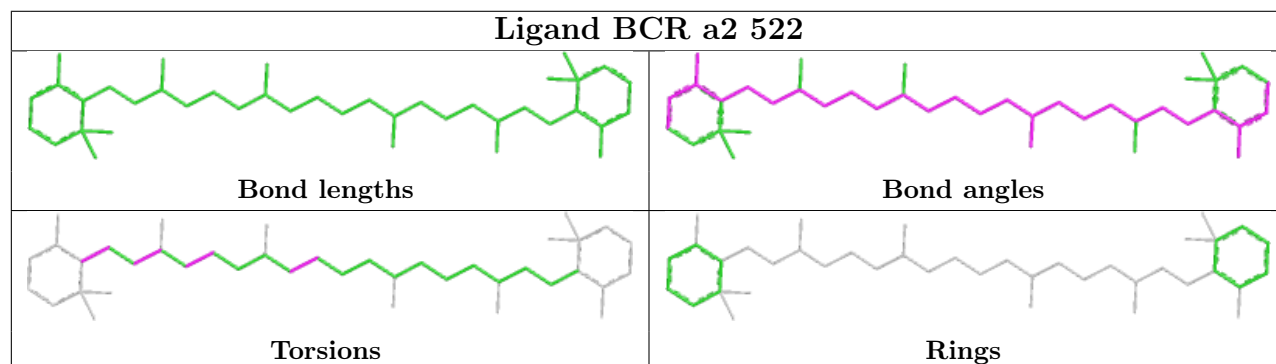


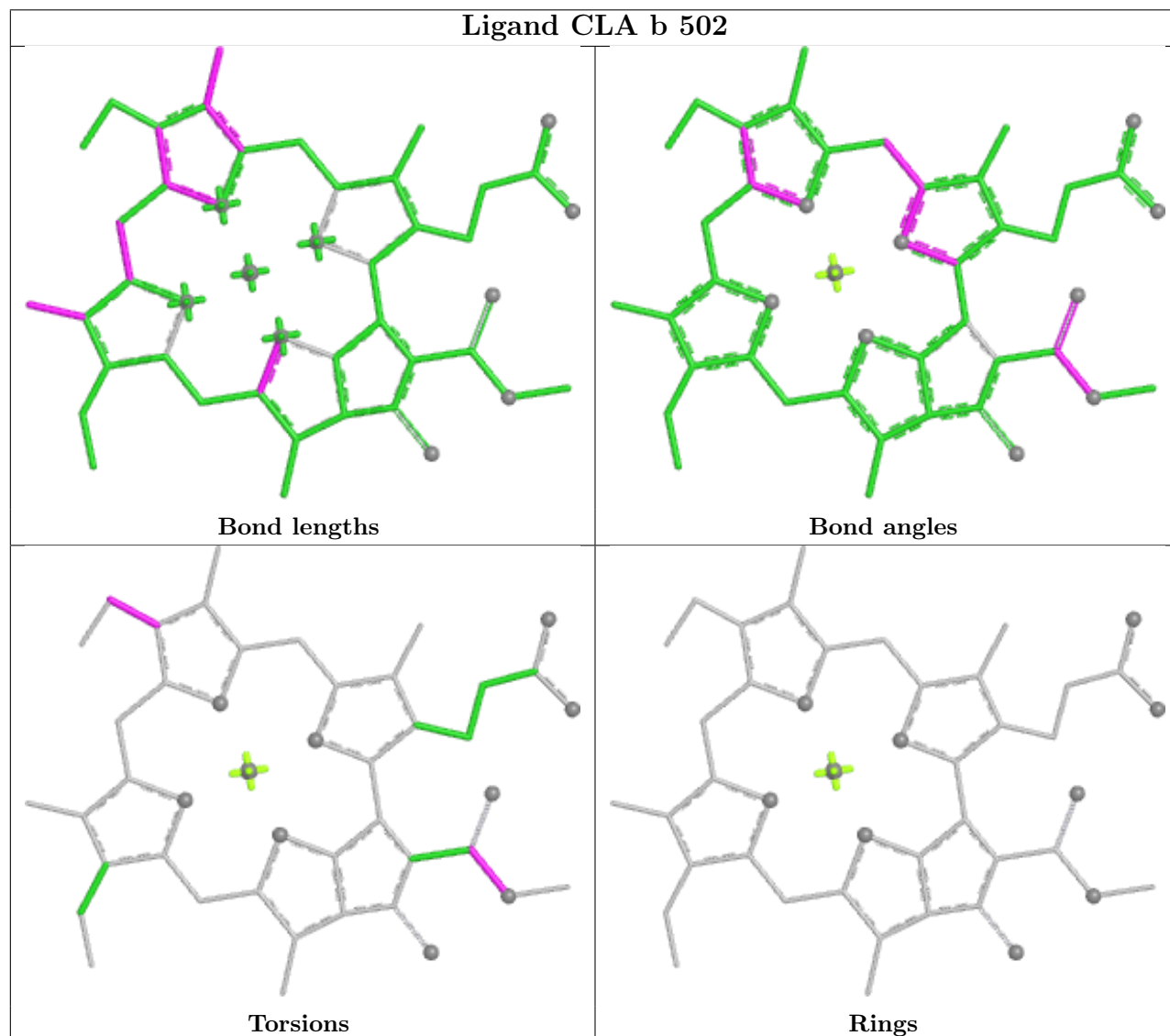
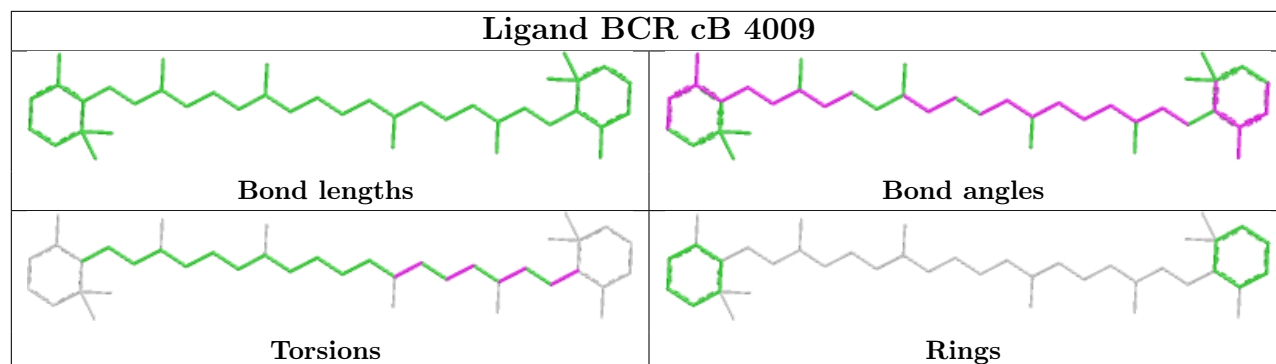
Rings

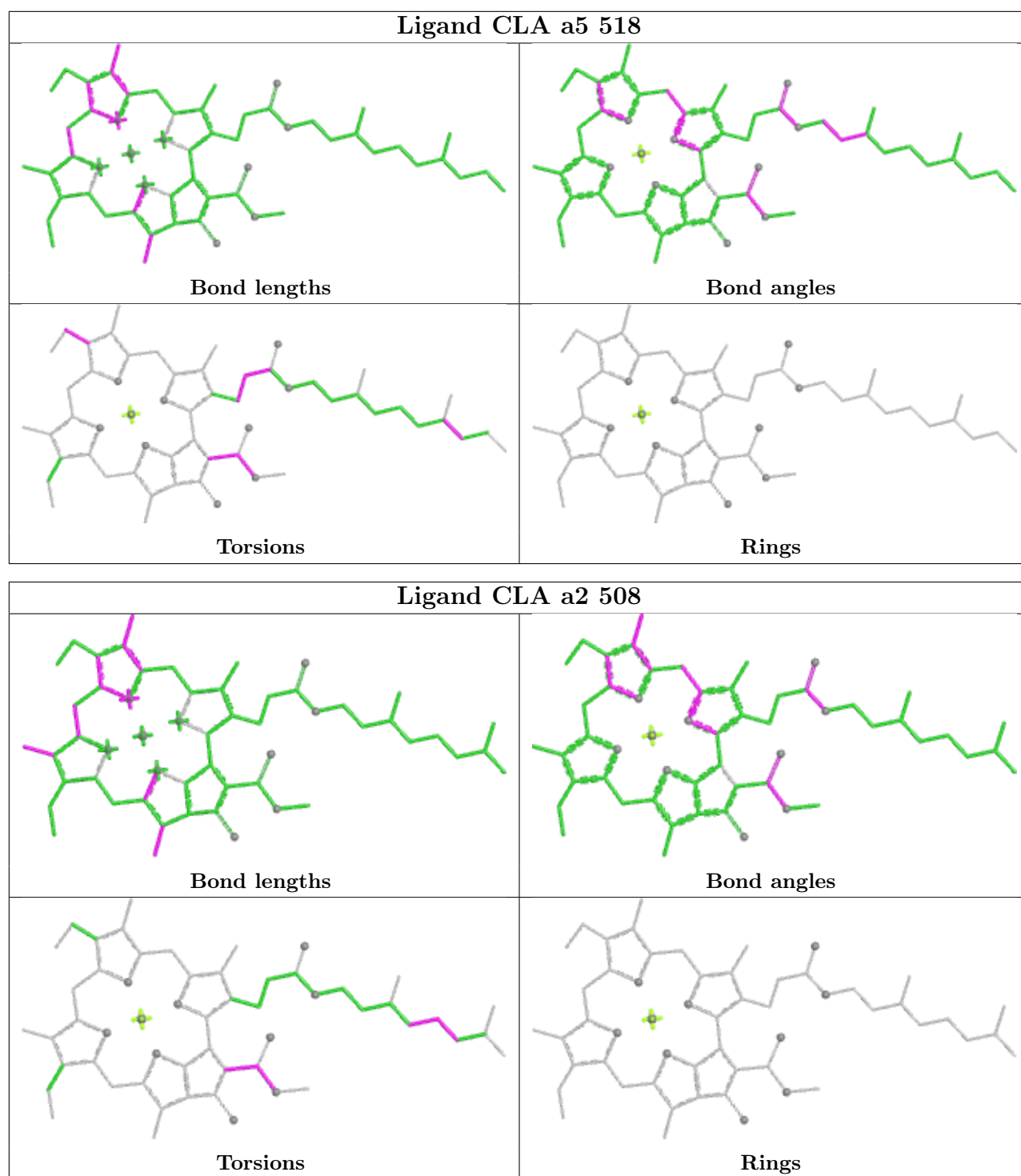
Ligand CLA V 503

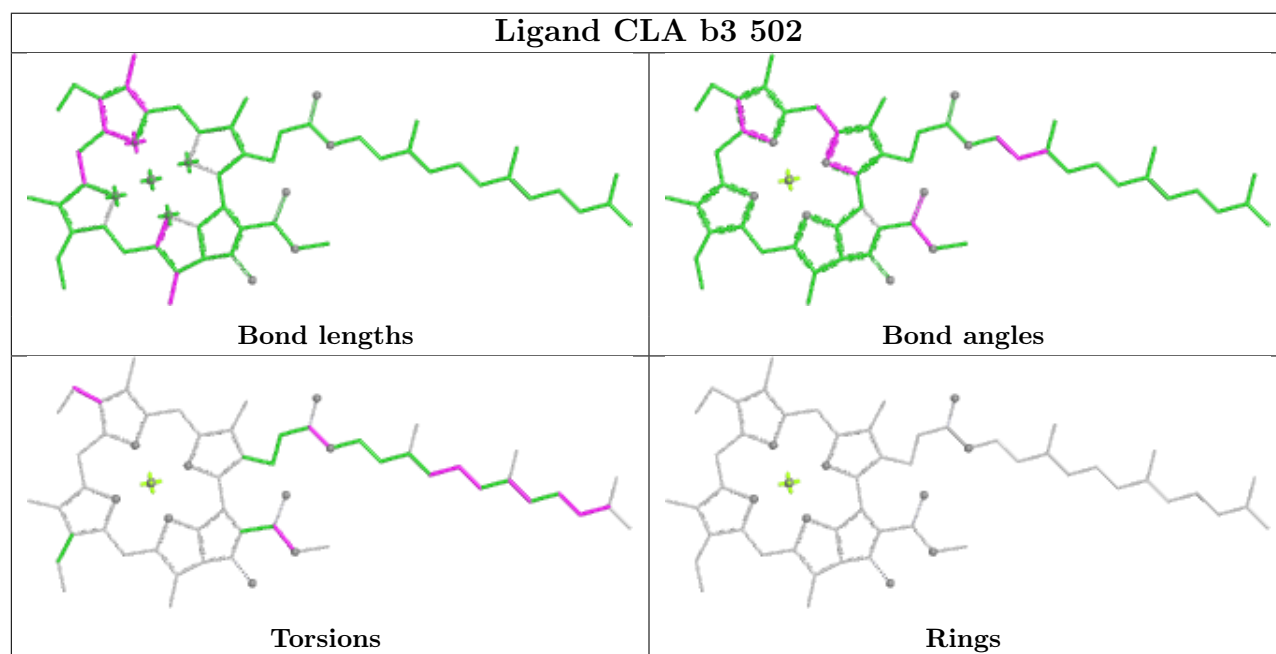
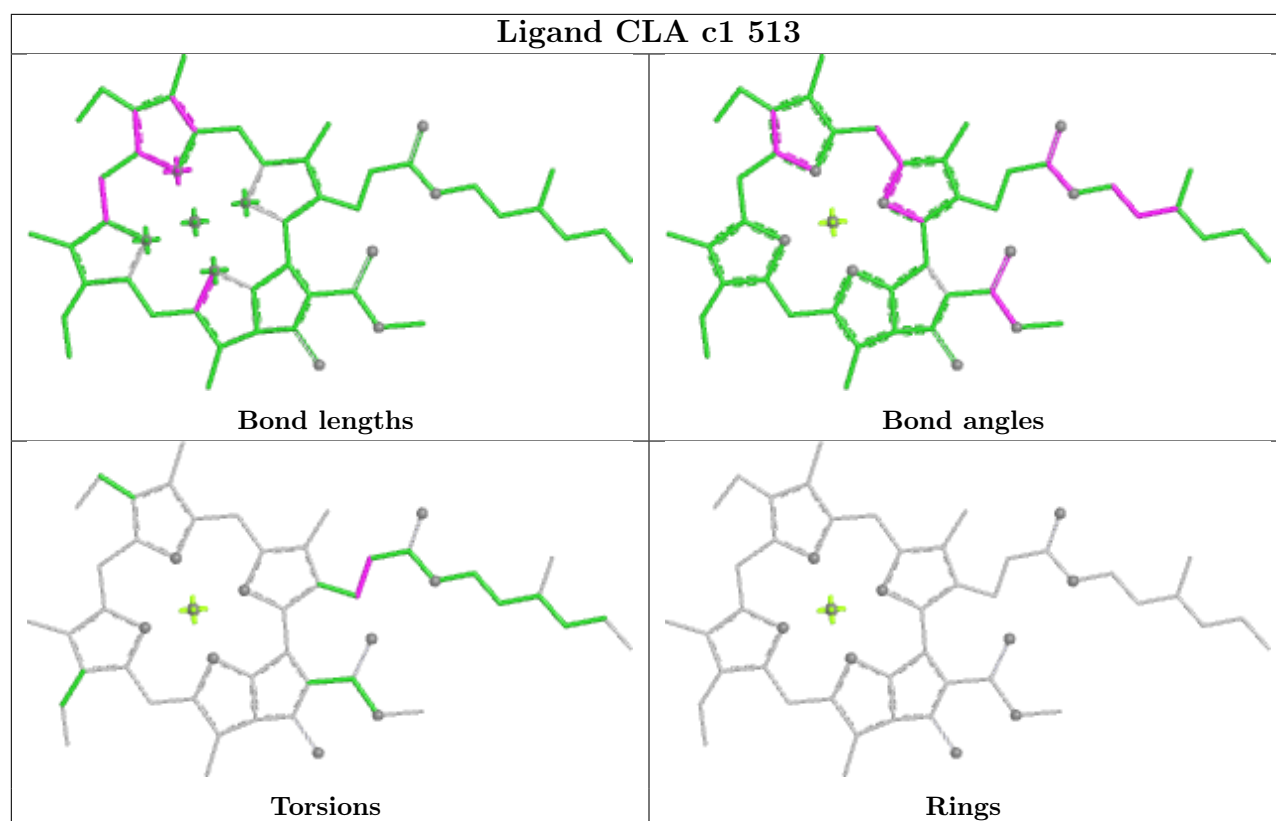


Ligand BCR a2 522

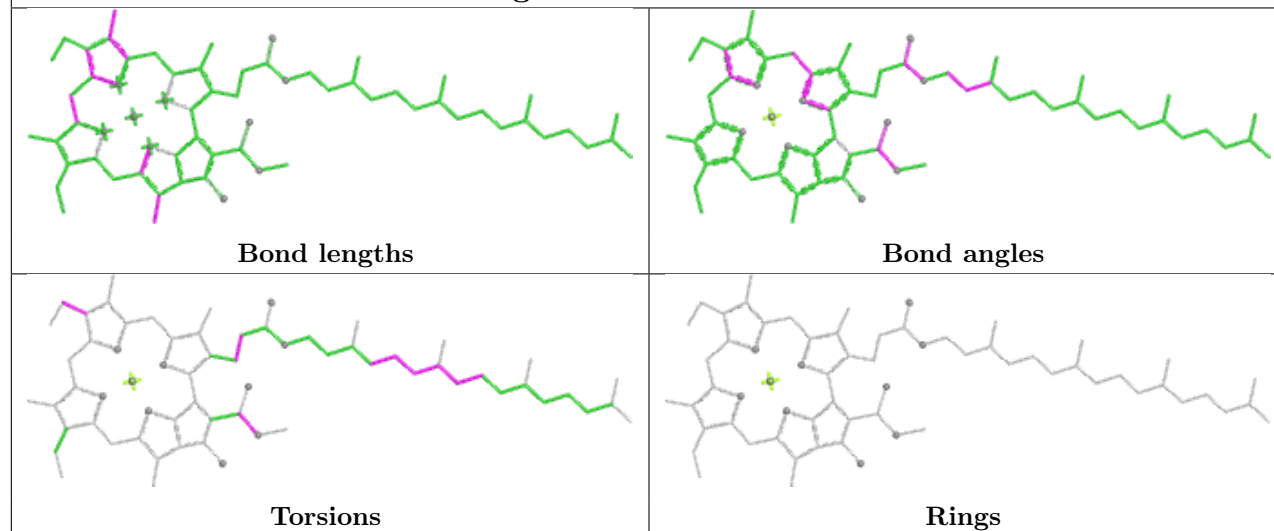




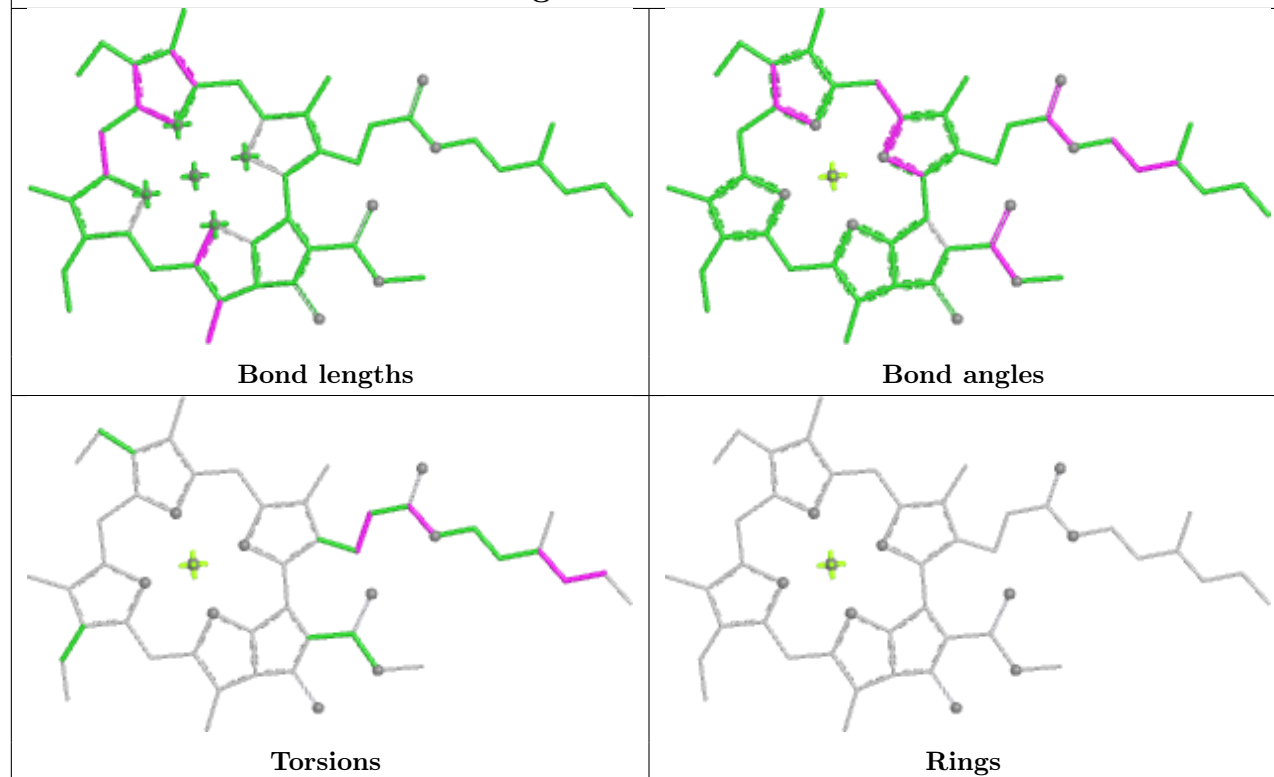


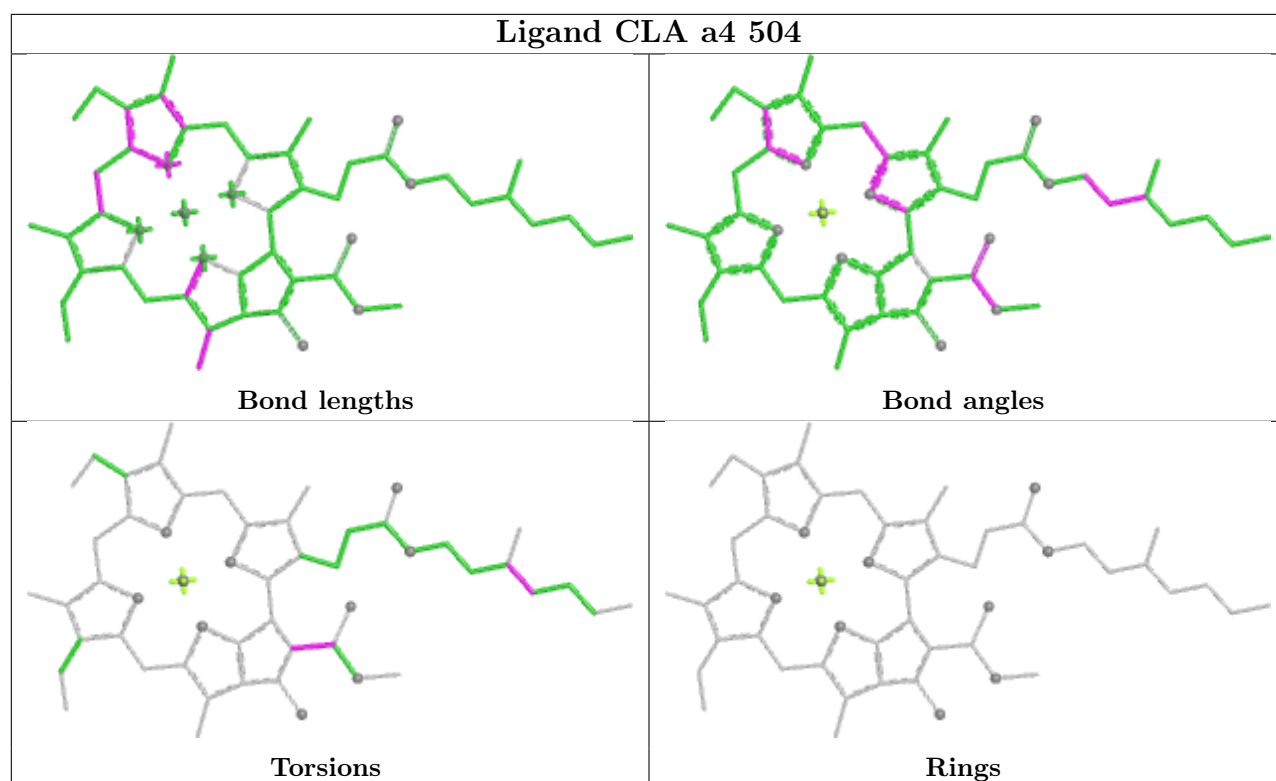


Ligand CLA bA 1138

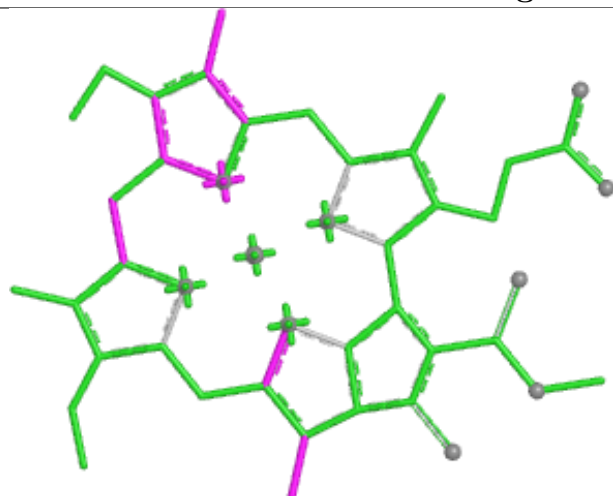


Ligand CLA T 505





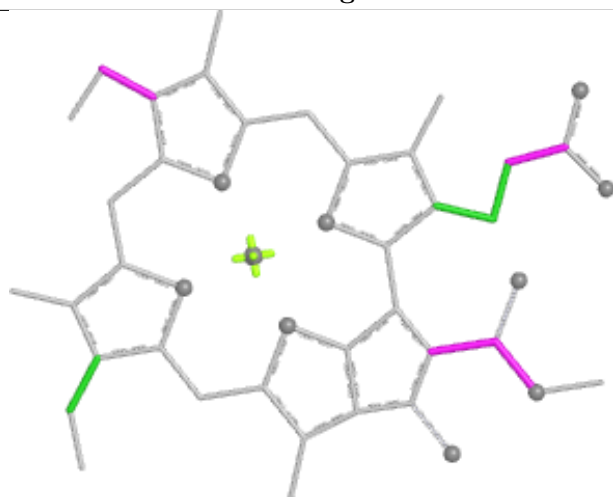
Ligand CLA Z 517



Bond lengths



Bond angles

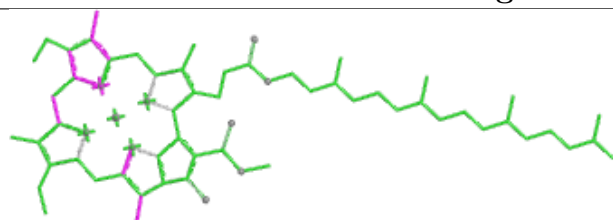


Torsions

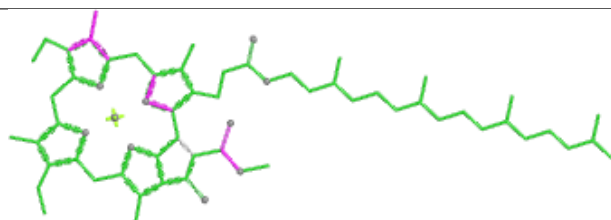


Rings

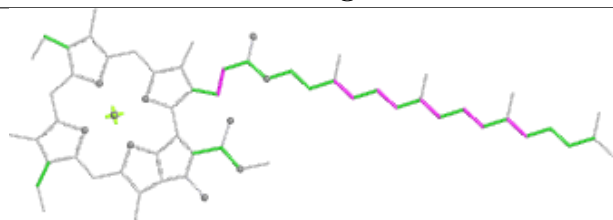
Ligand CLA aA 1022



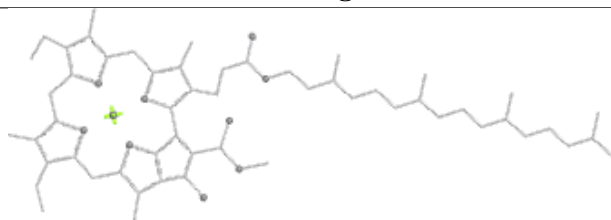
Bond lengths



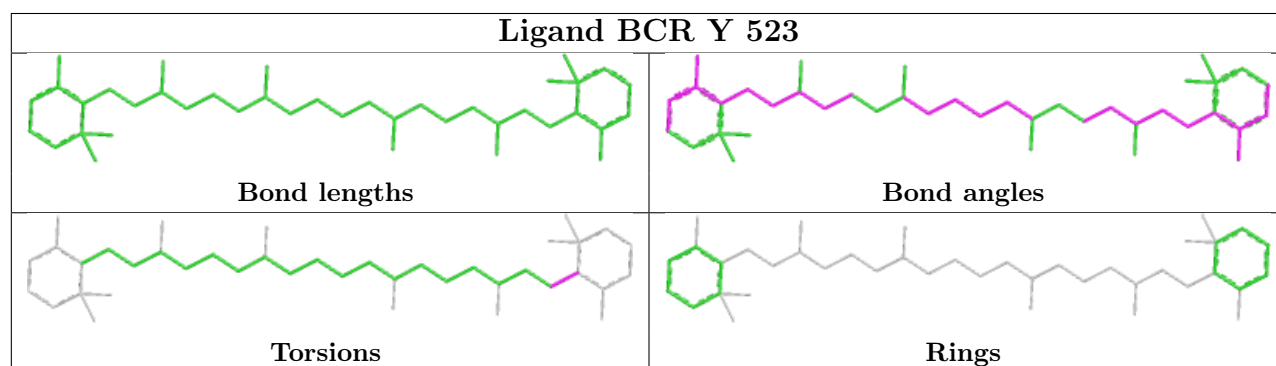
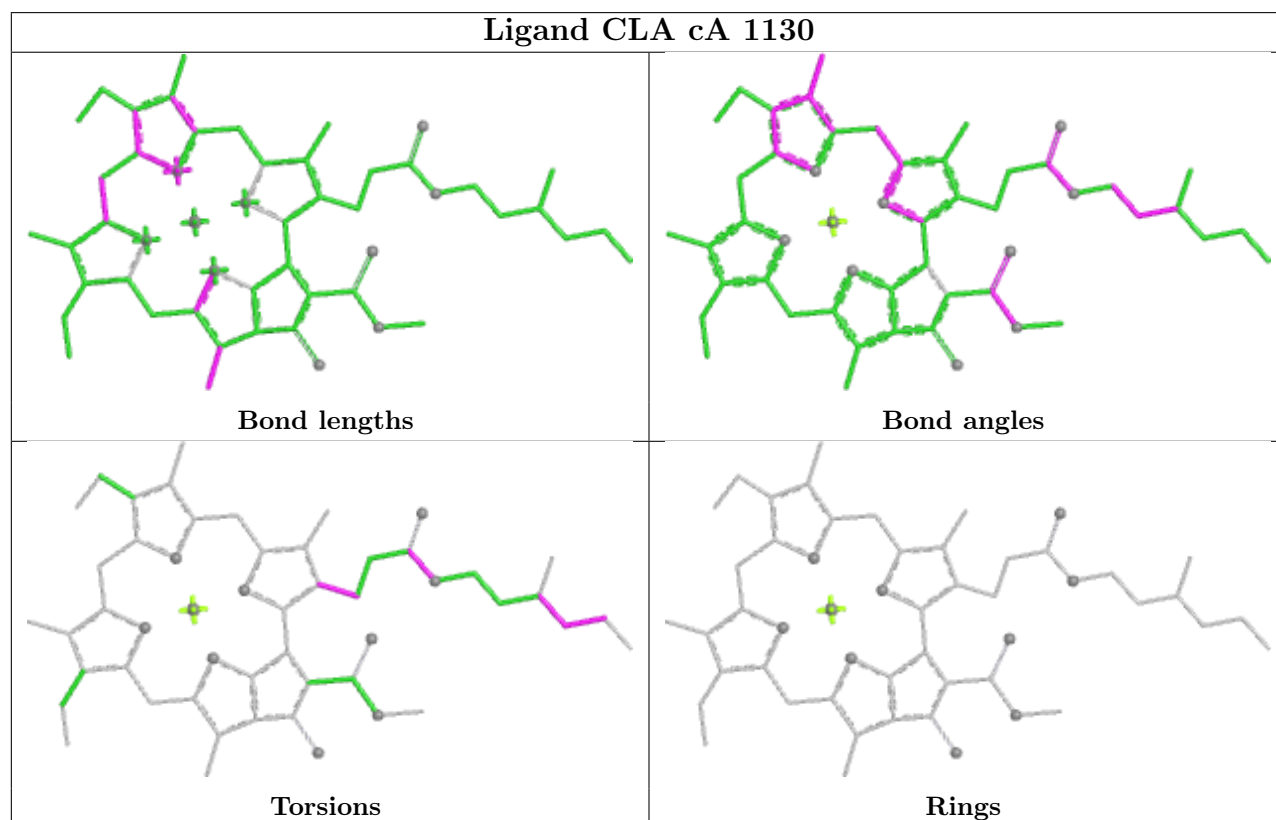
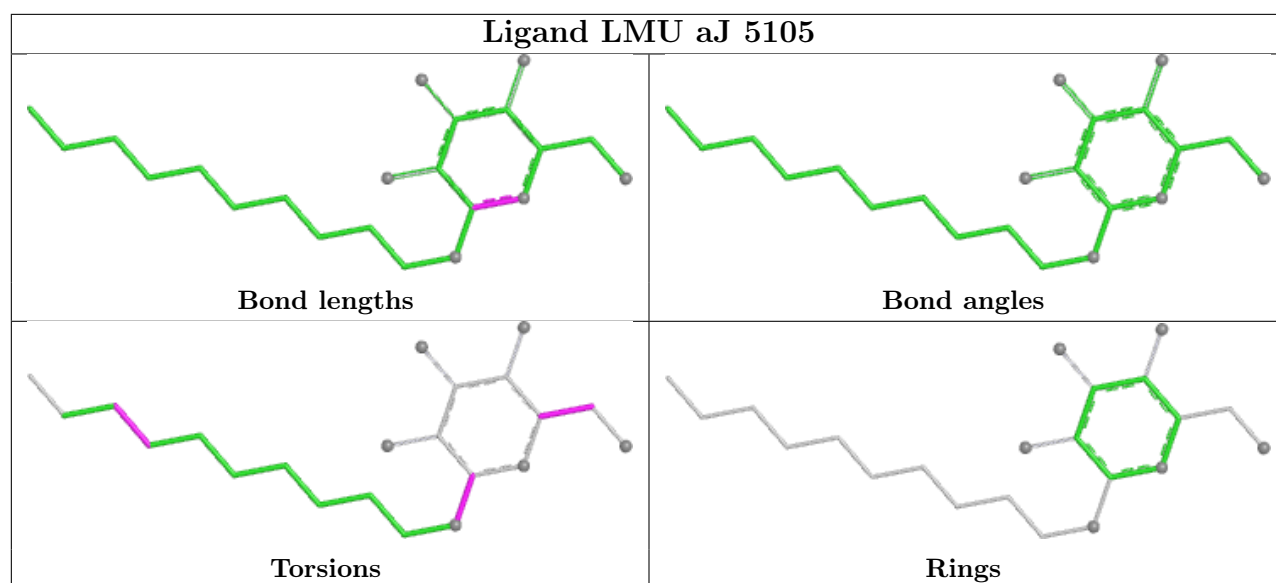
Bond angles

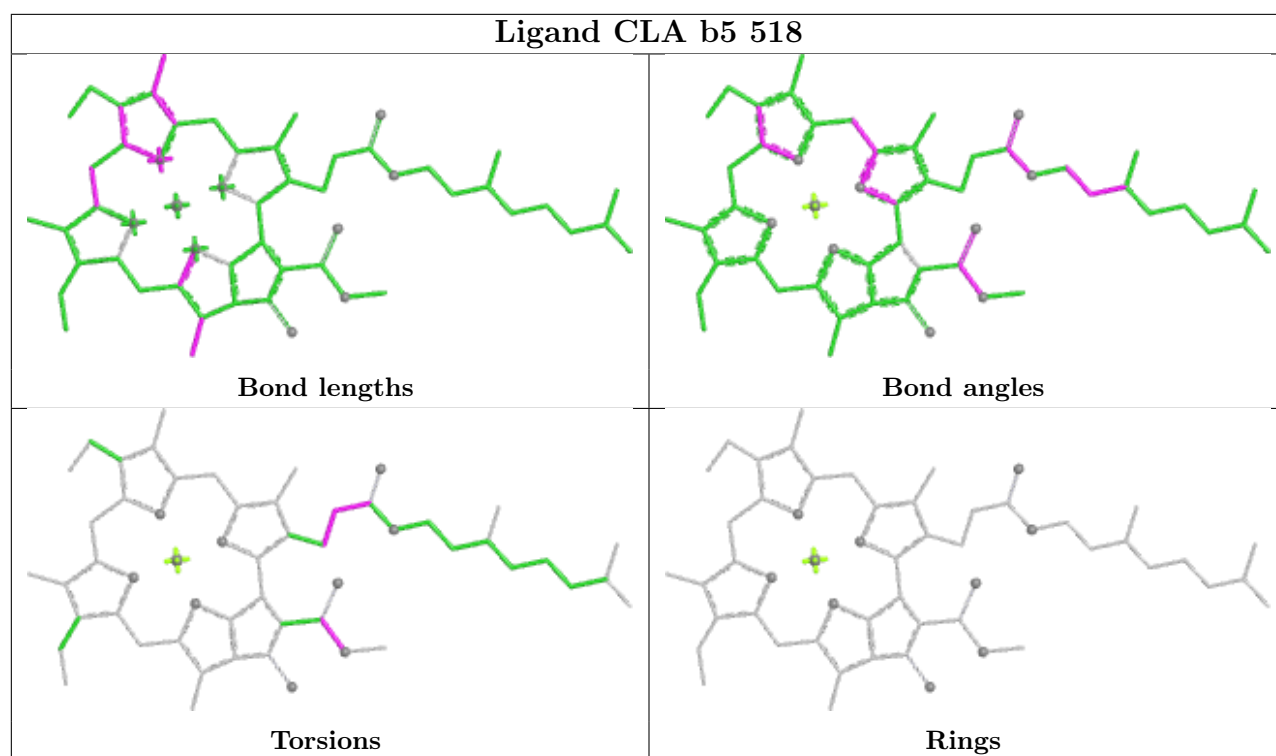


Torsions

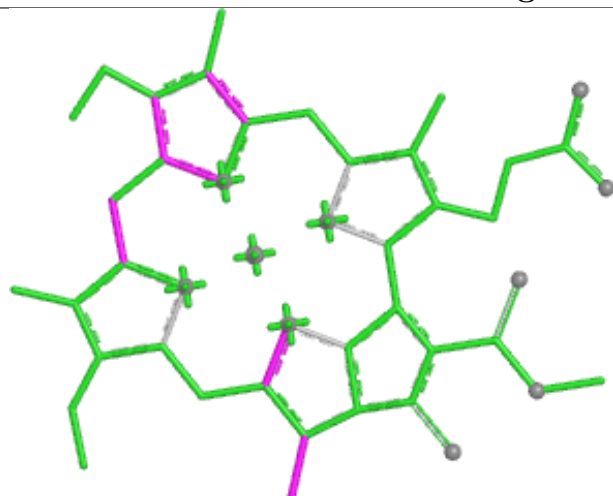


Rings

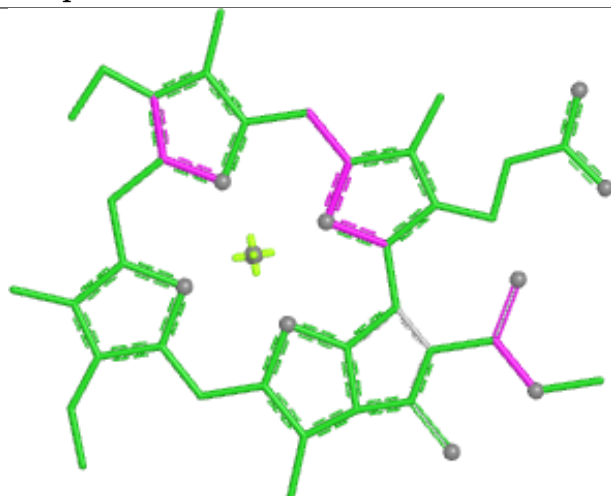




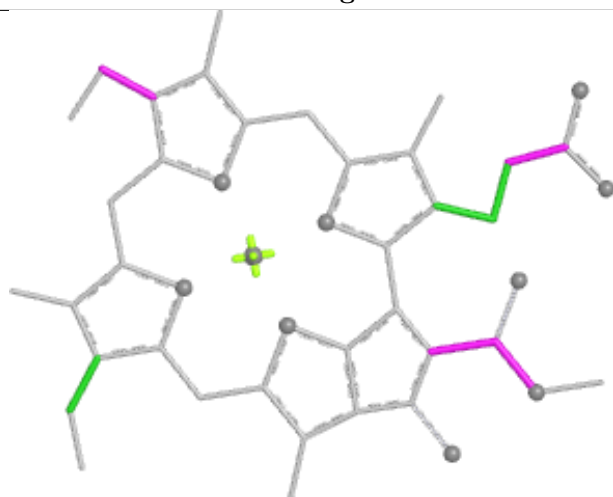
Ligand CLA q 517



Bond lengths



Bond angles

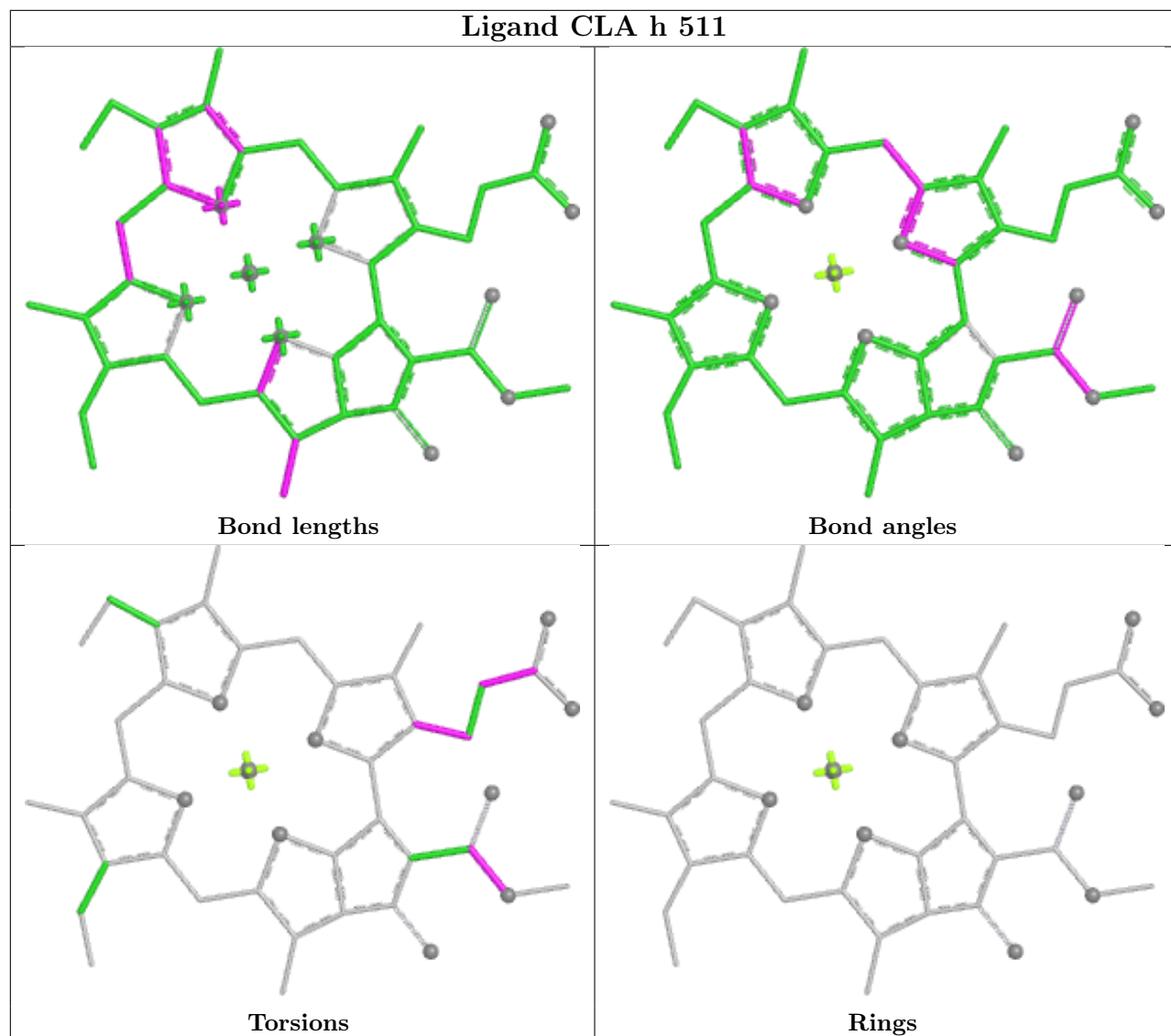


Torsions

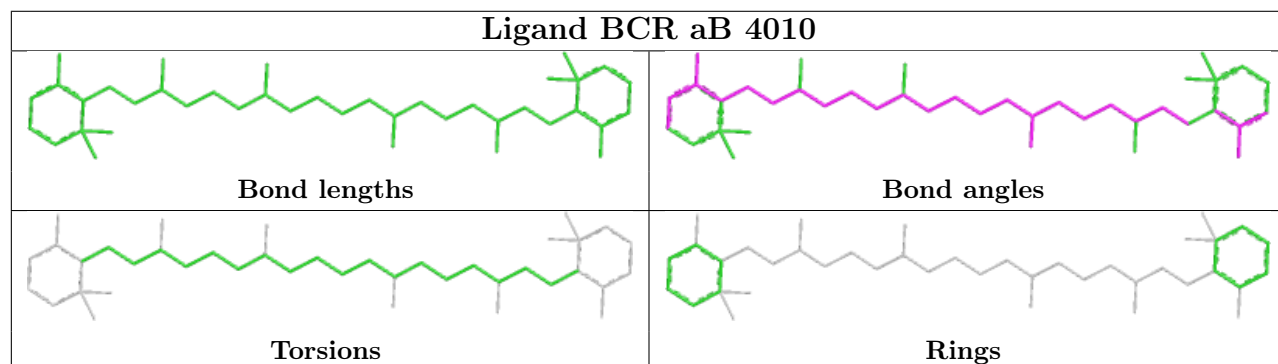


Rings

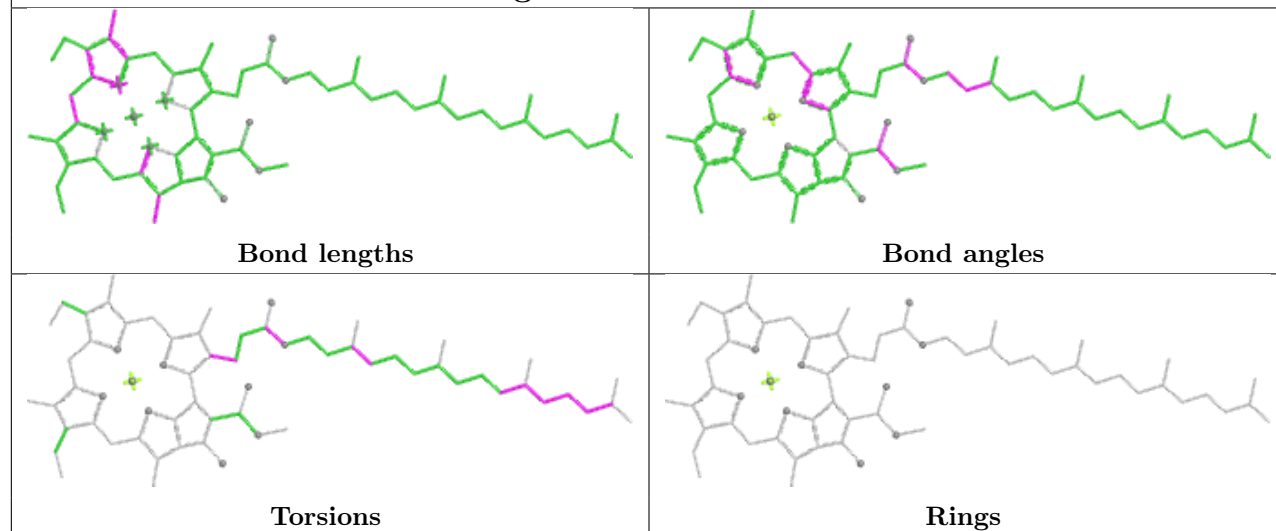
Ligand CLA h 511



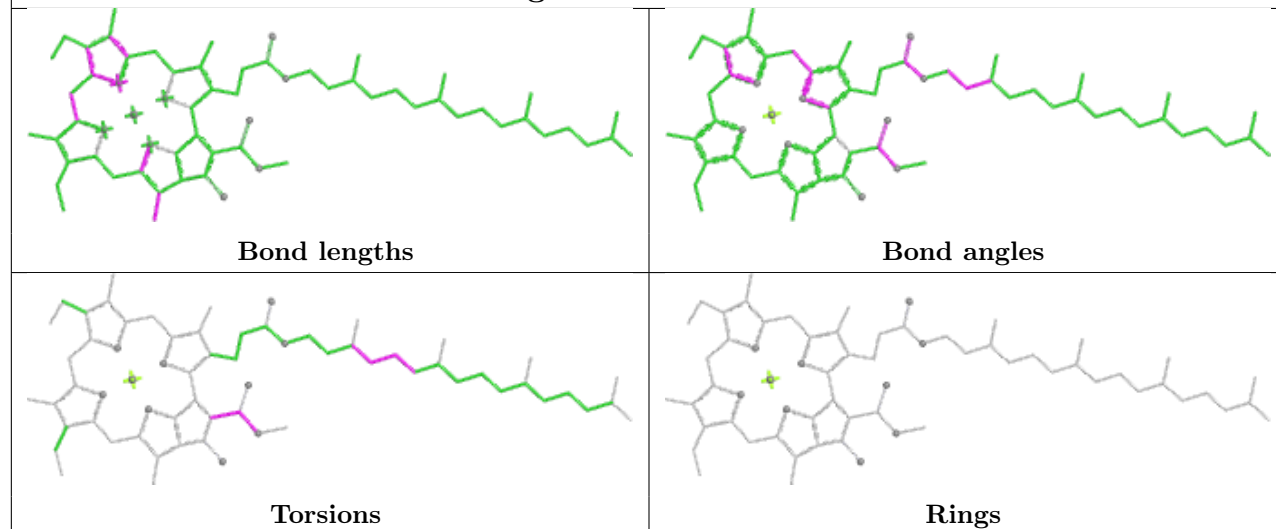
Ligand BCR aB 4010



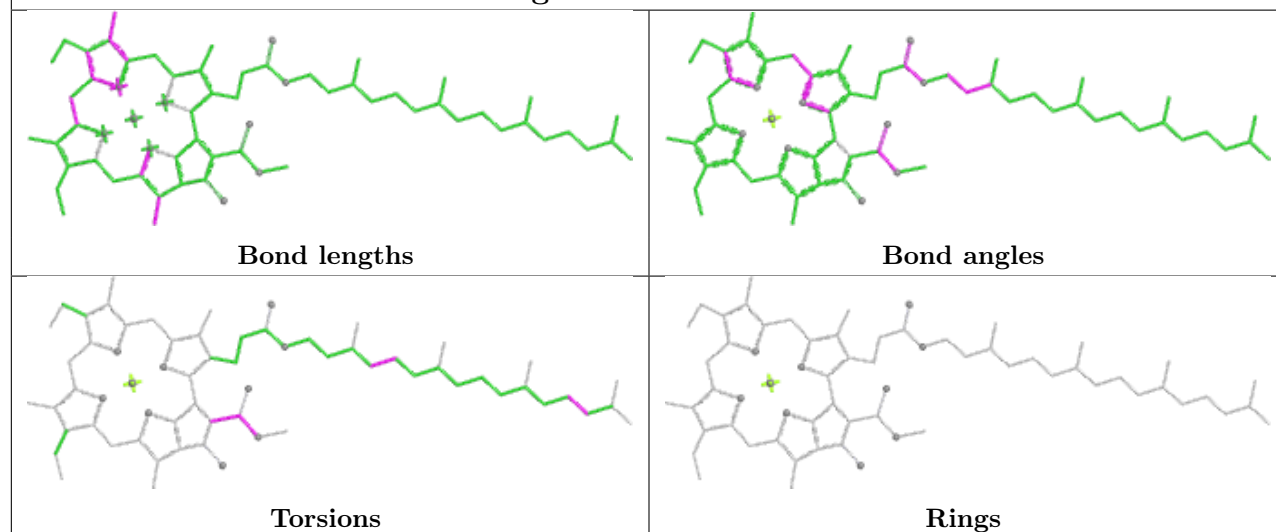
Ligand CLA aA 1117

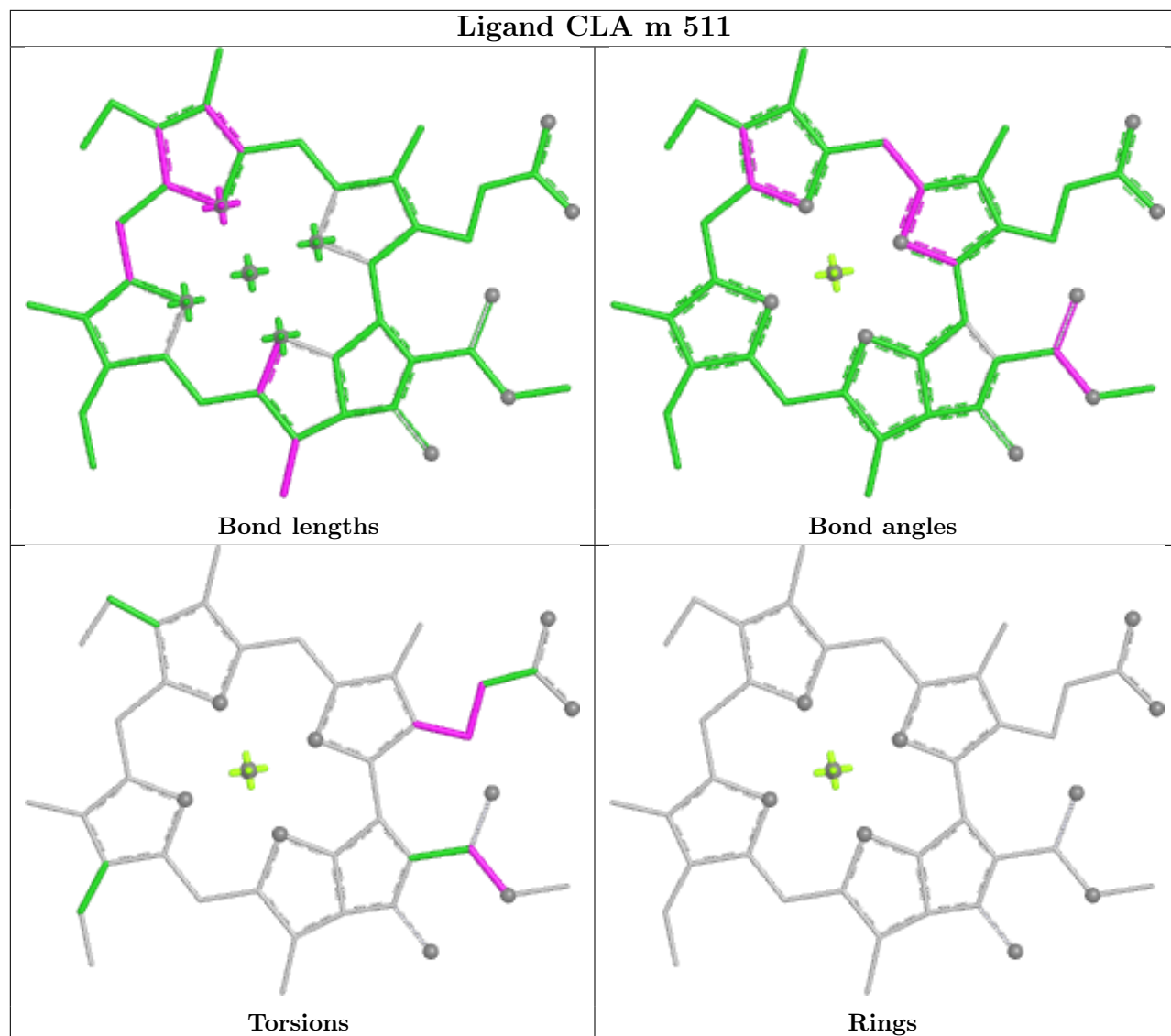


Ligand CLA aI 510

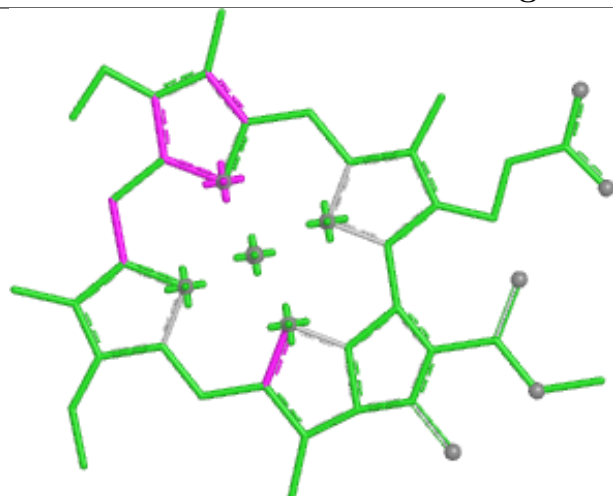


Ligand CLA X 509





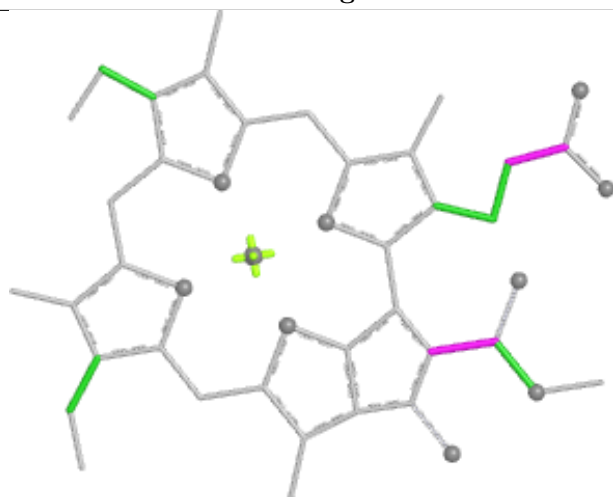
Ligand CLA c 507



Bond lengths



Bond angles

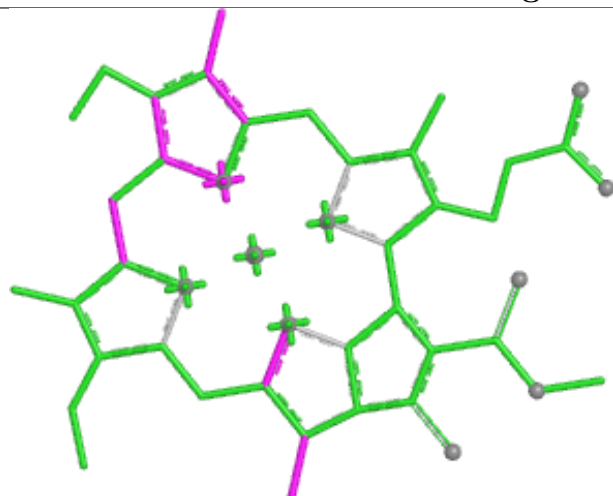


Torsions



Rings

Ligand CLA 1 501



Bond lengths



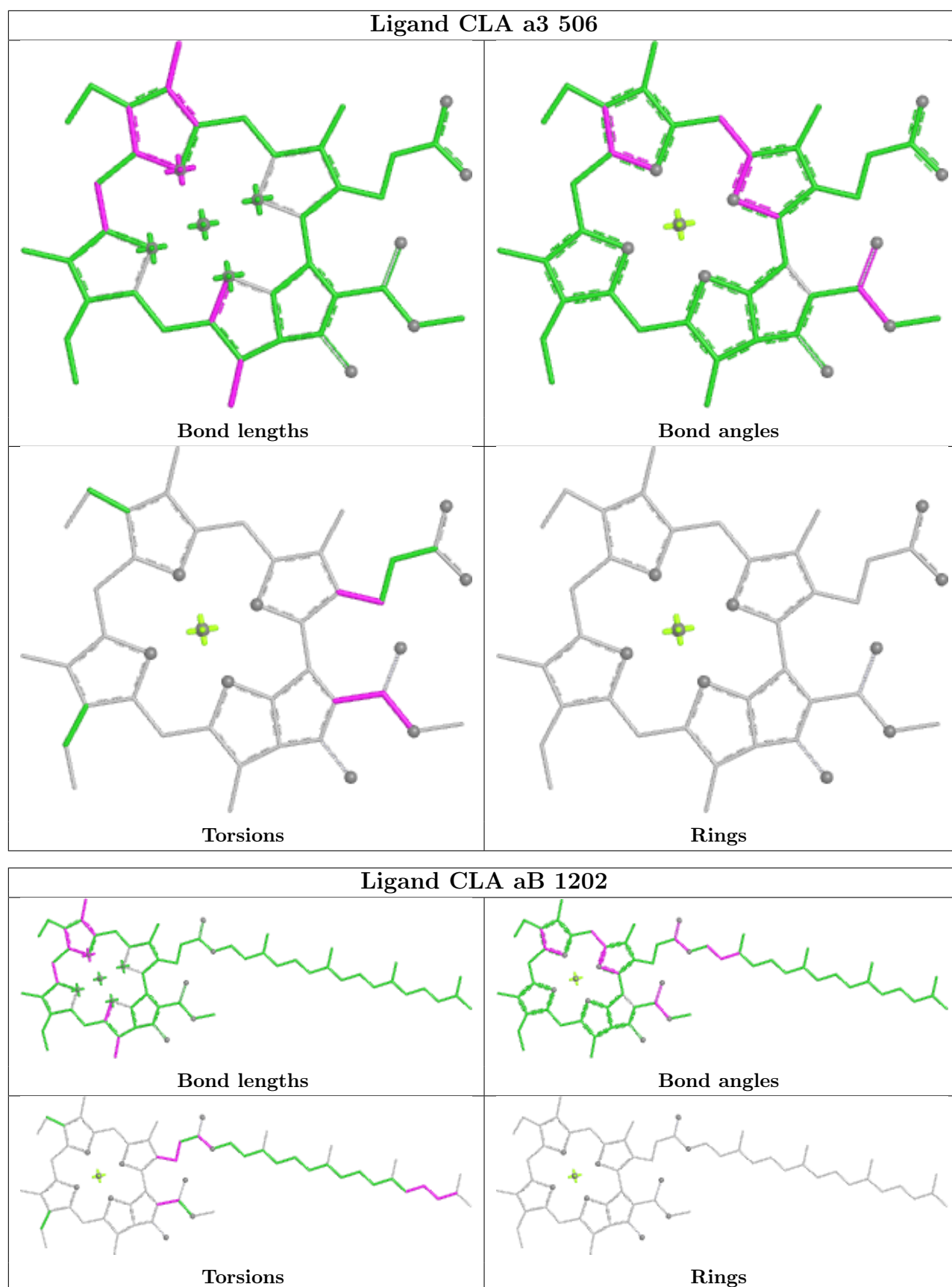
Bond angles



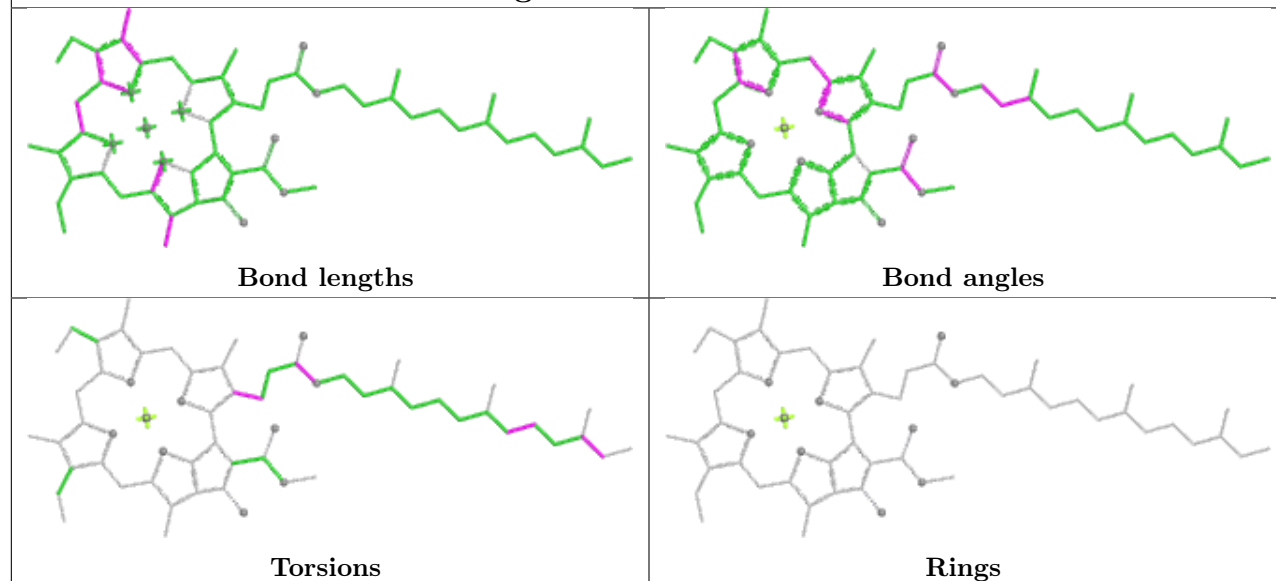
Torsions



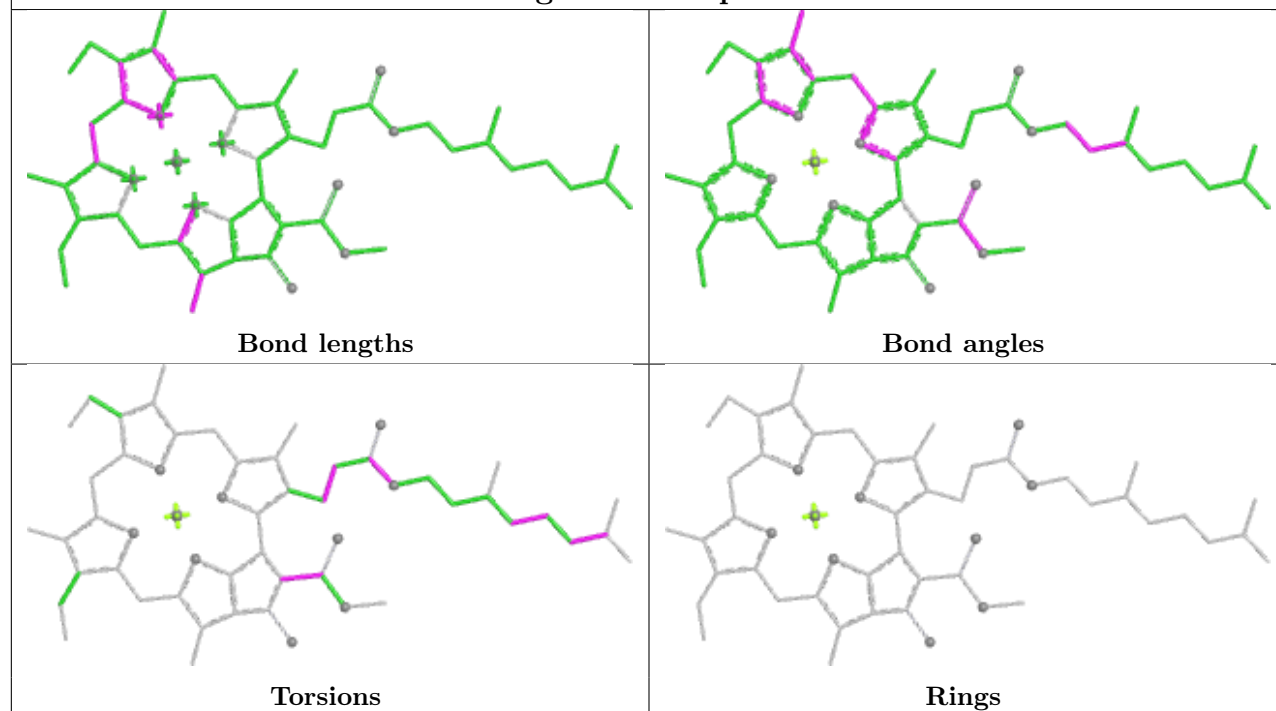
Rings



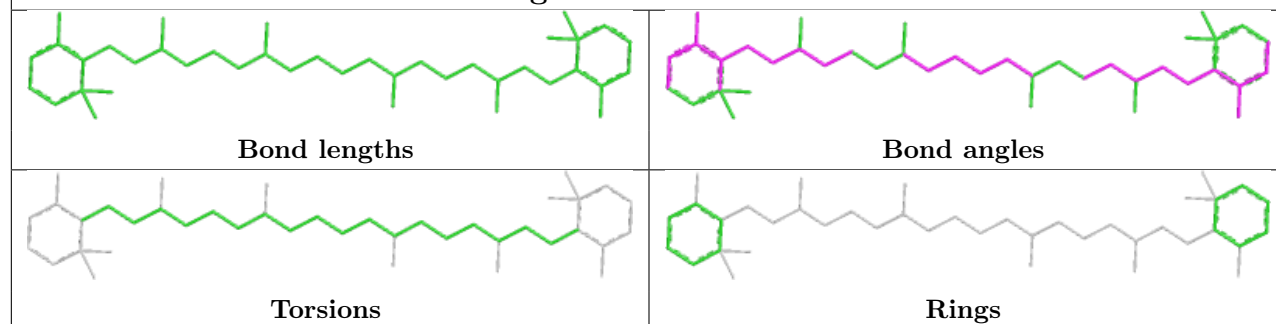
Ligand CLA aB 1215

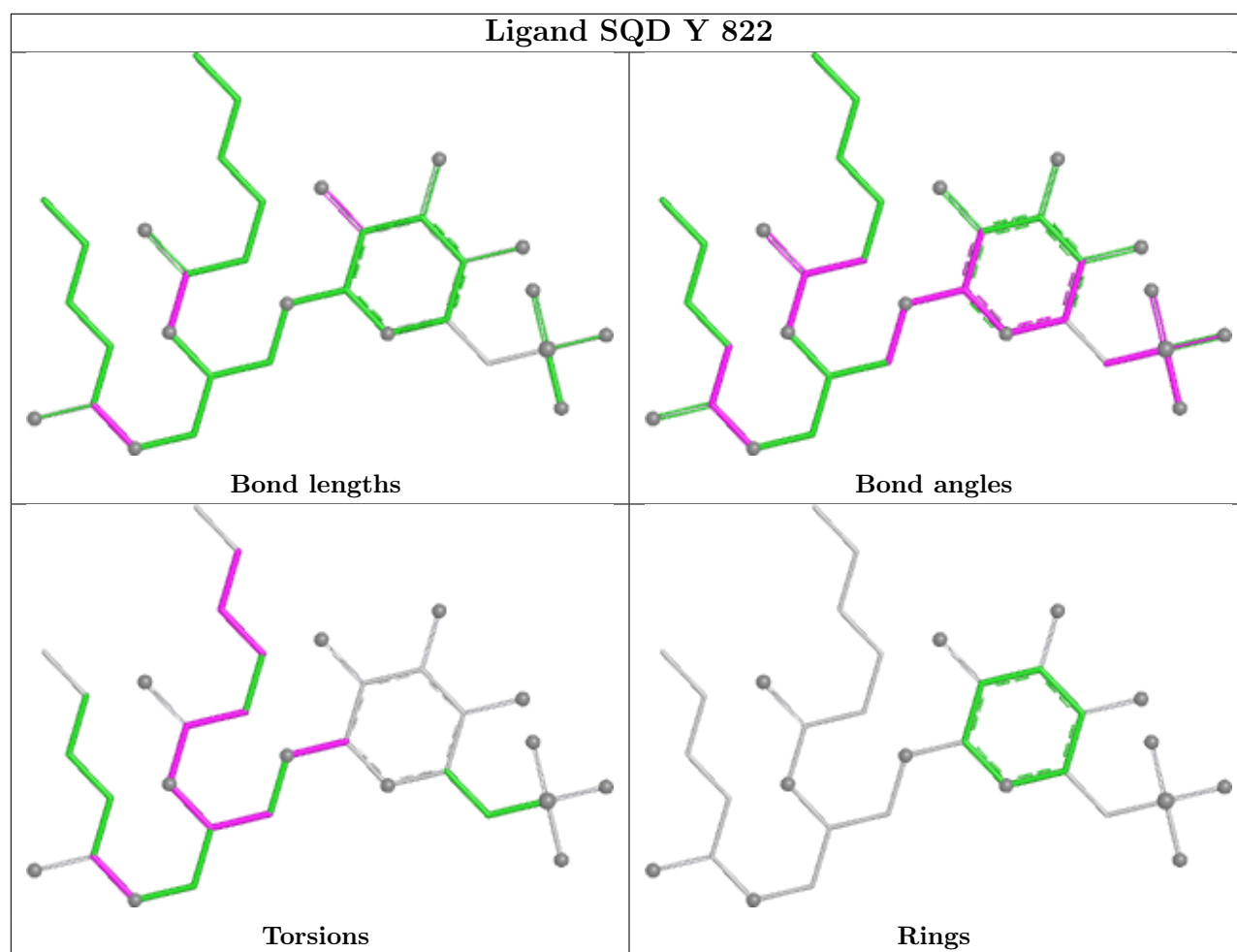


Ligand CLA q 505

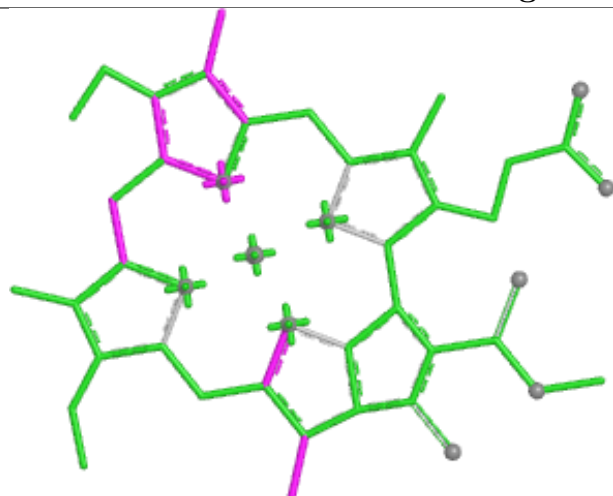


Ligand BCR Y 524





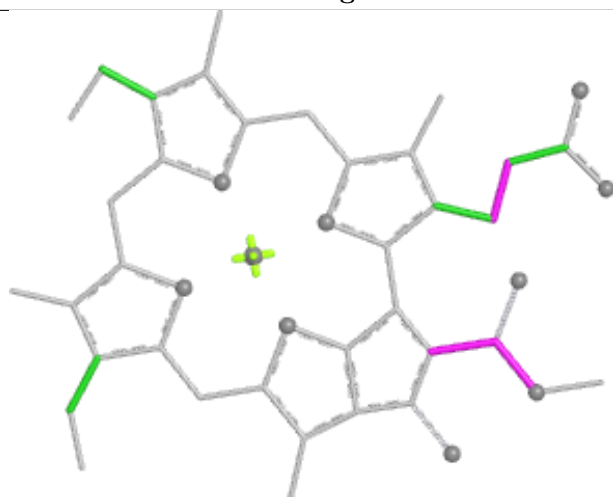
Ligand CLA e 518



Bond lengths



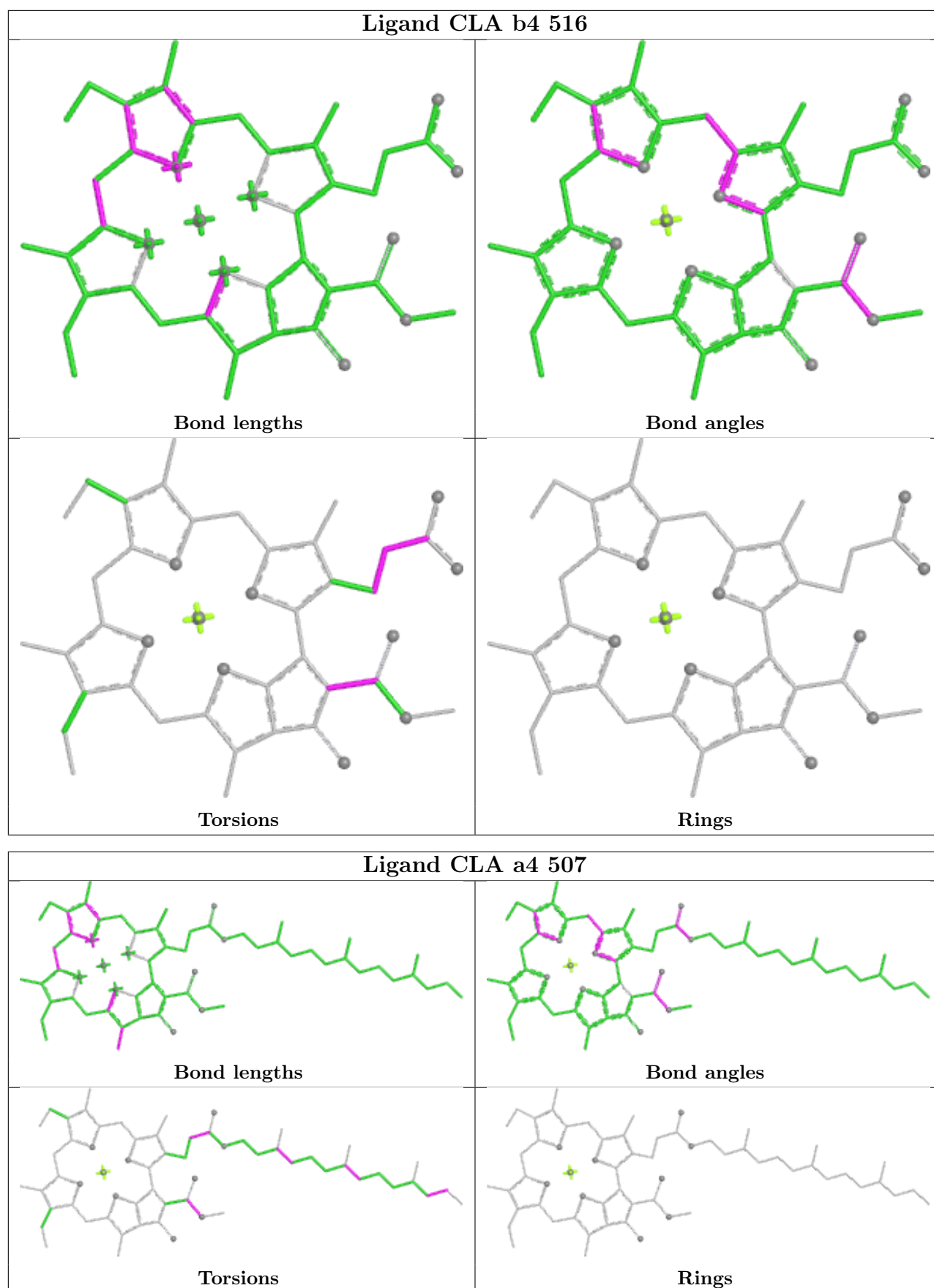
Bond angles

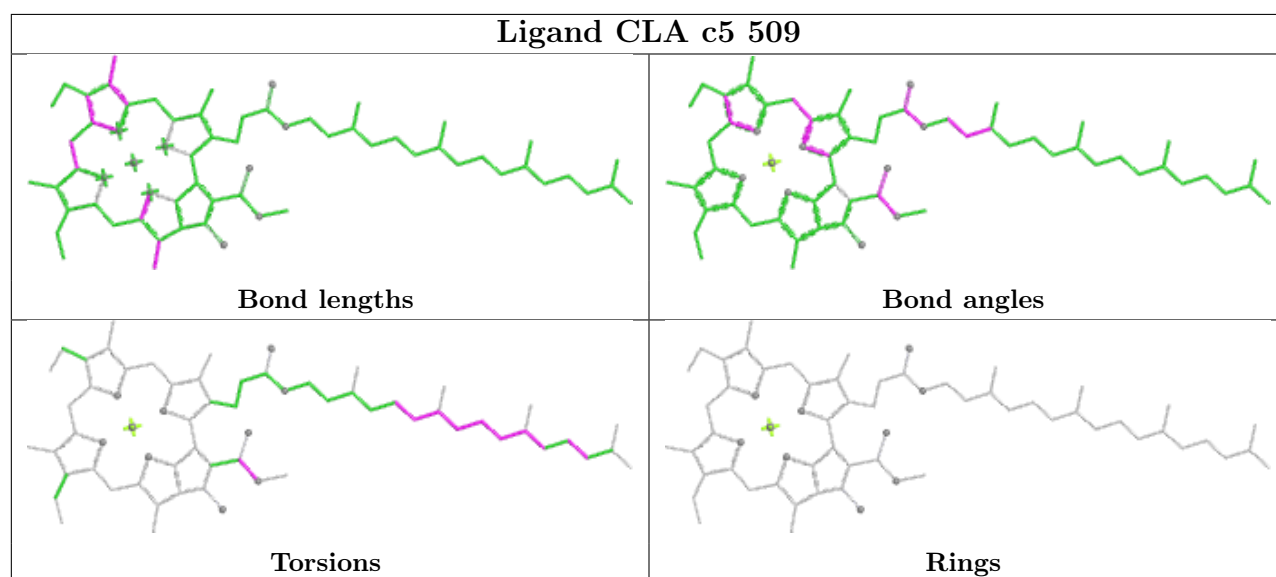
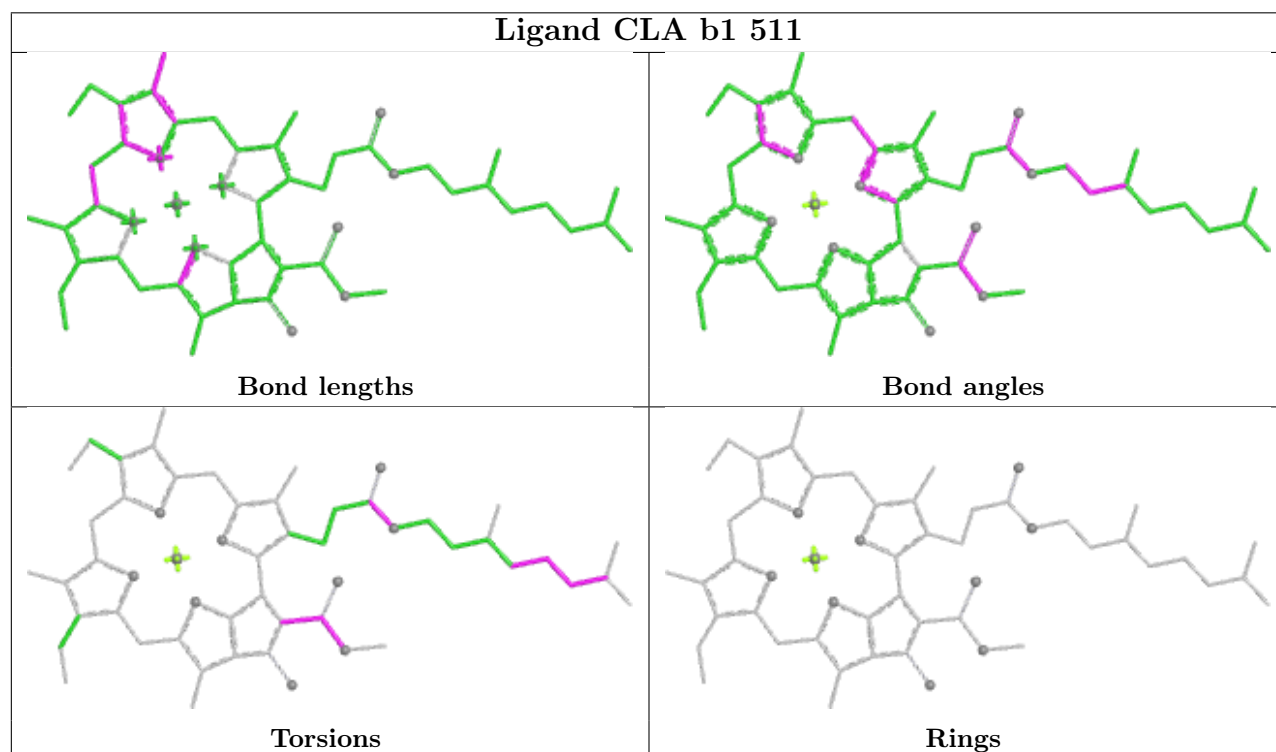
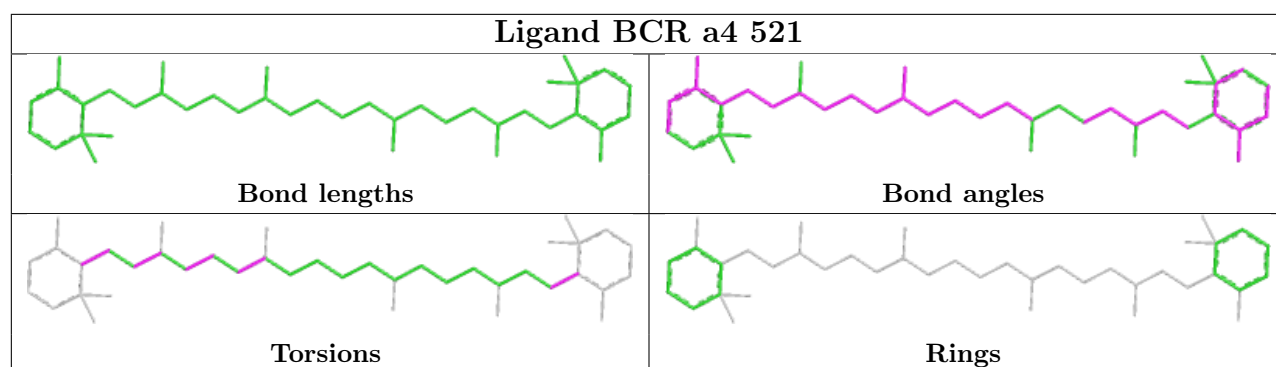


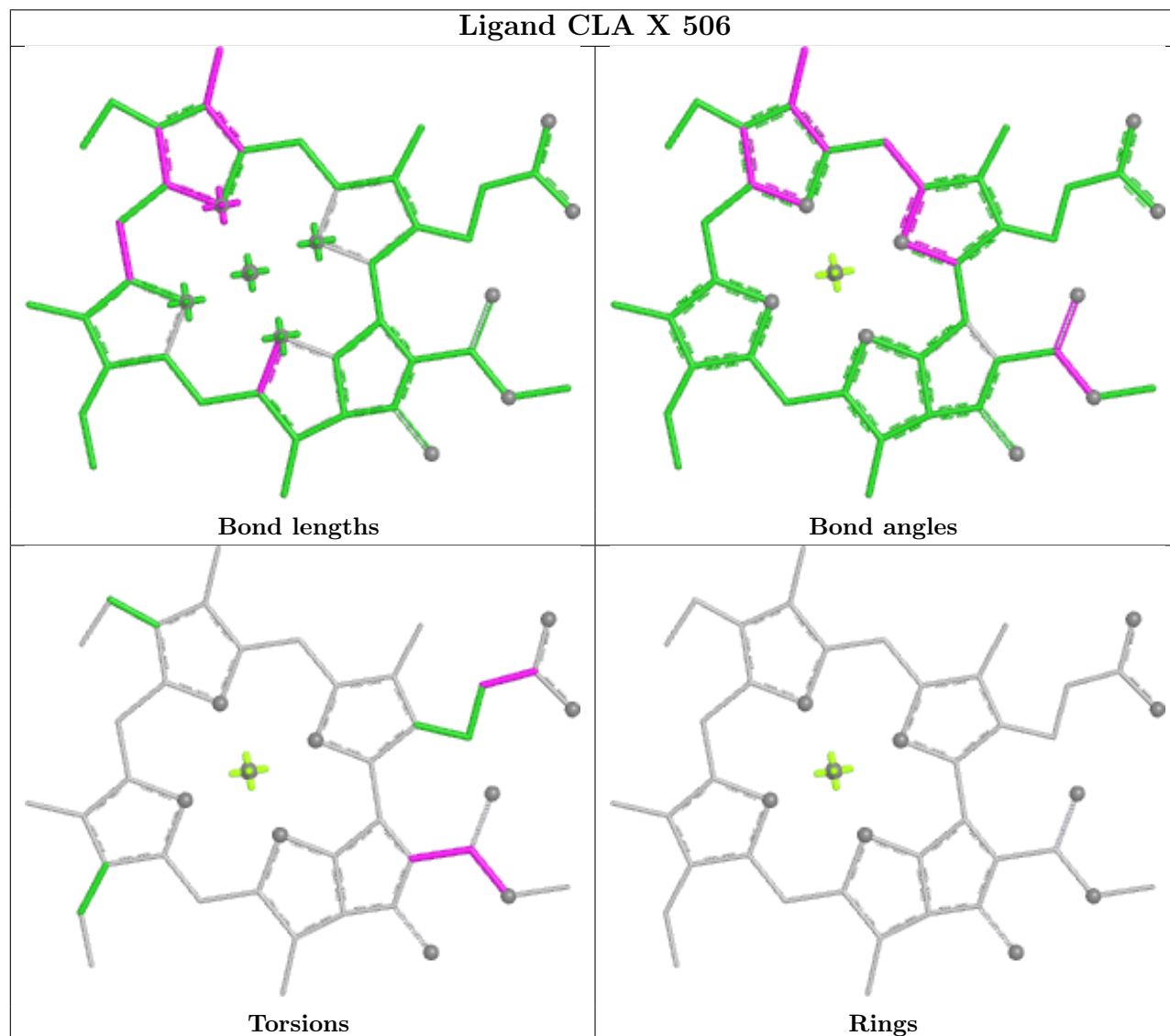
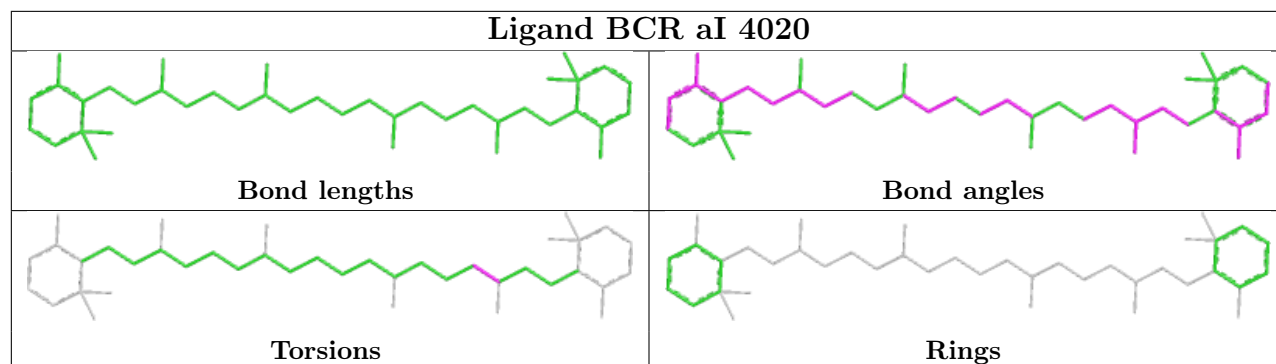
Torsions

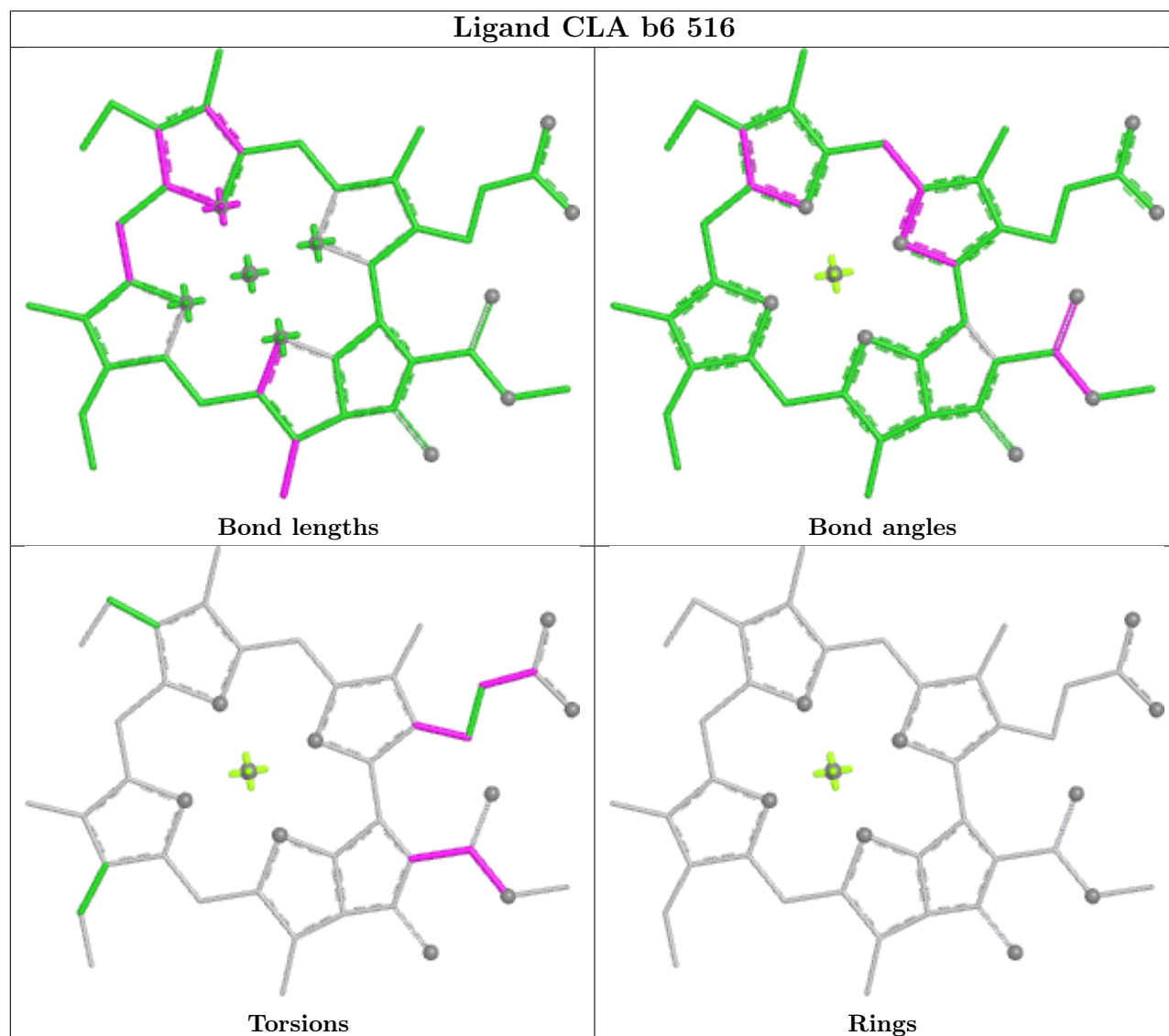
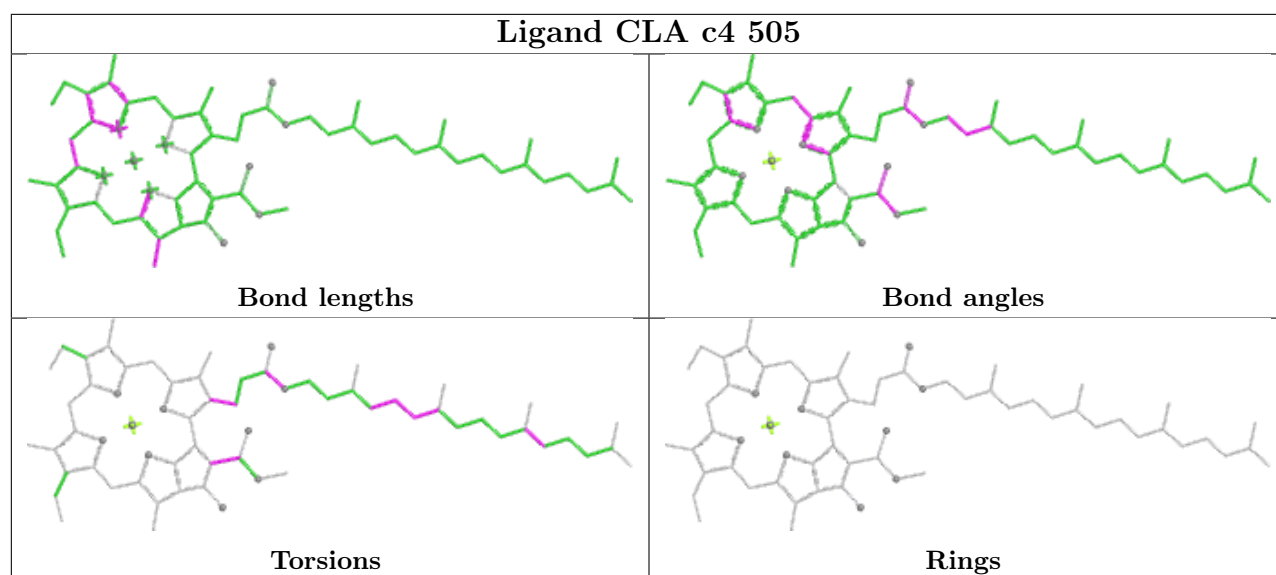


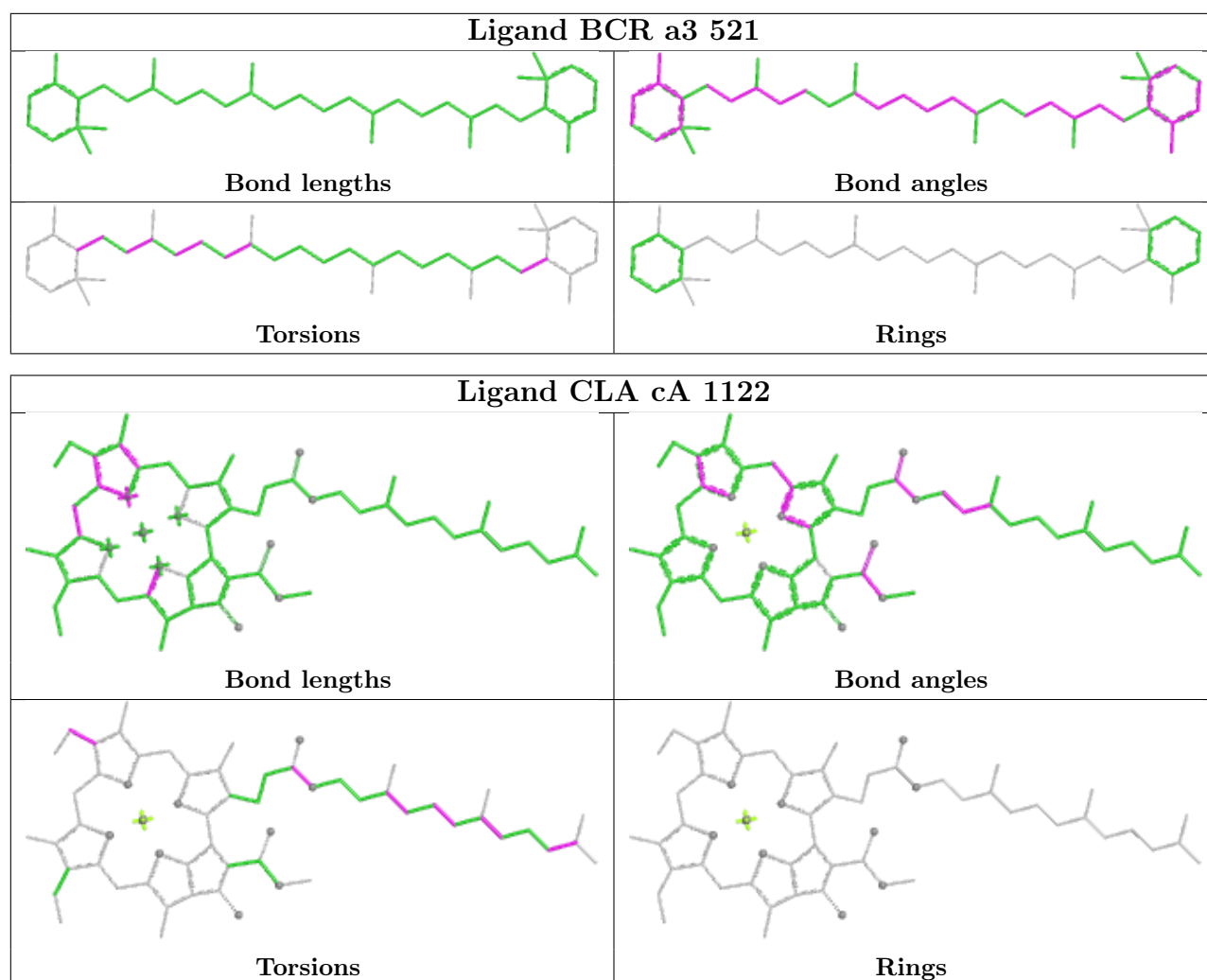
Rings

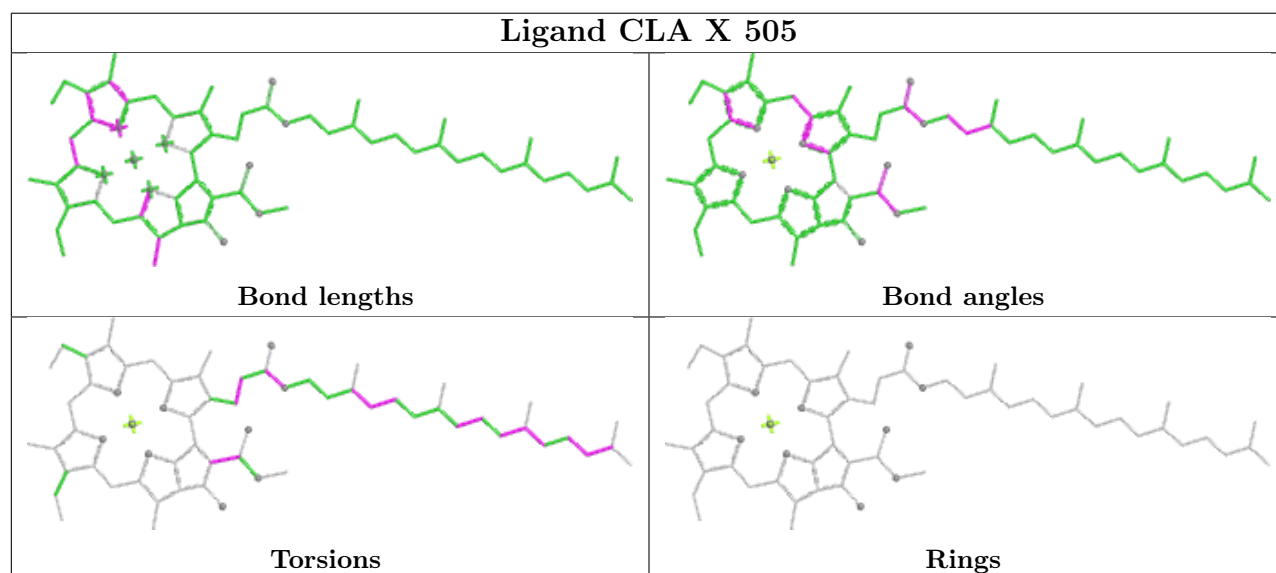
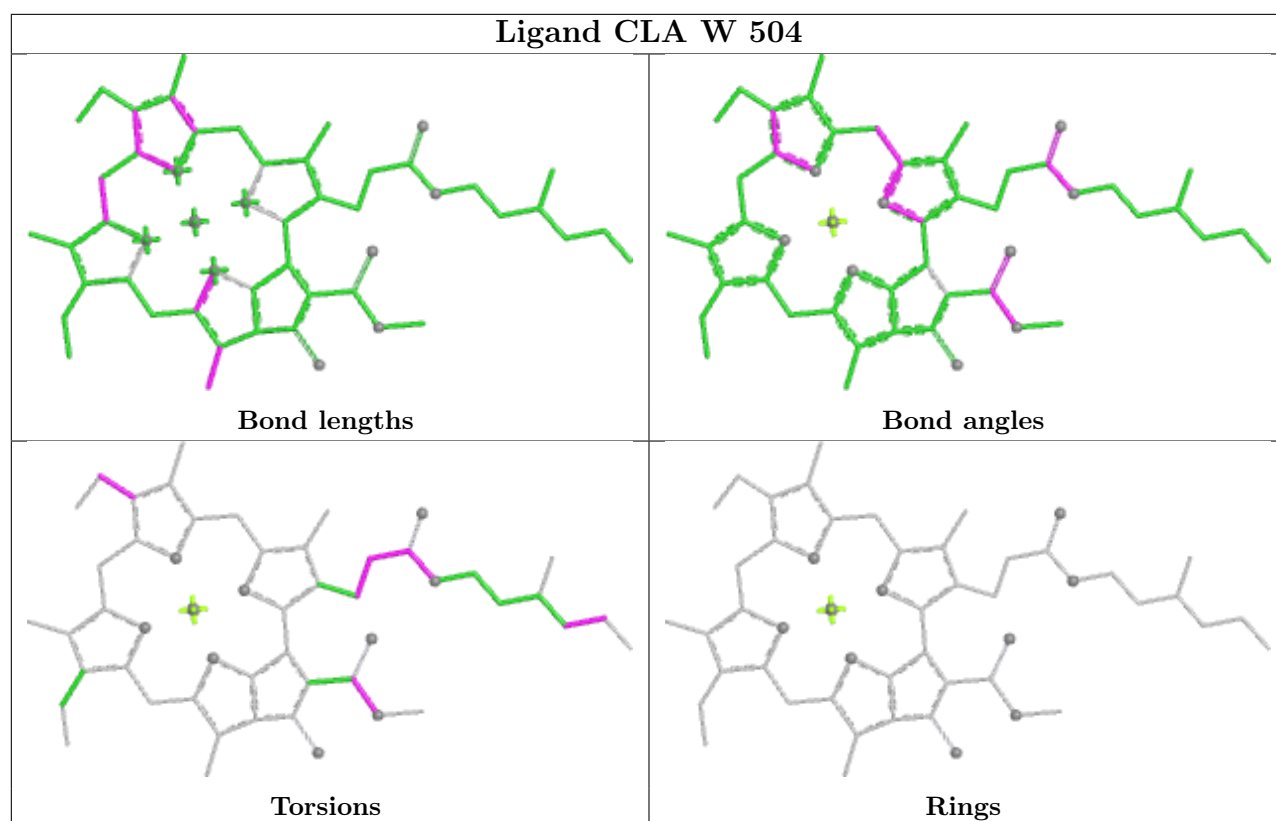




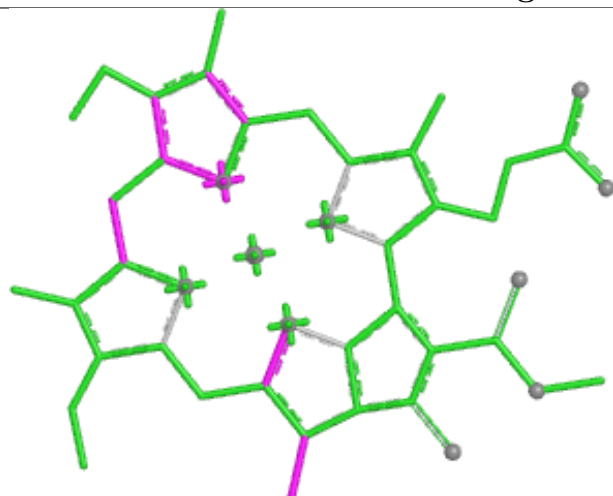




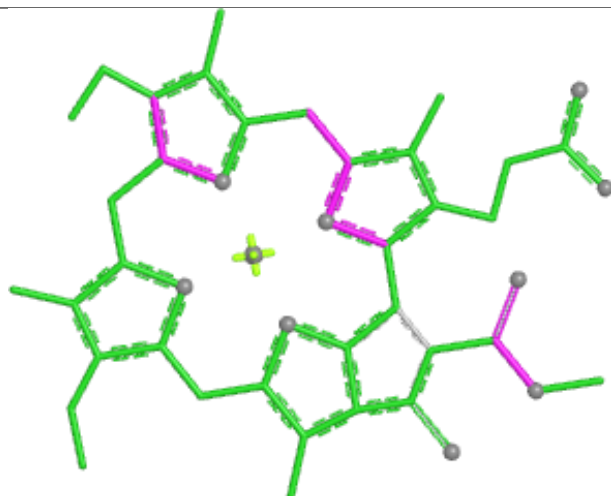




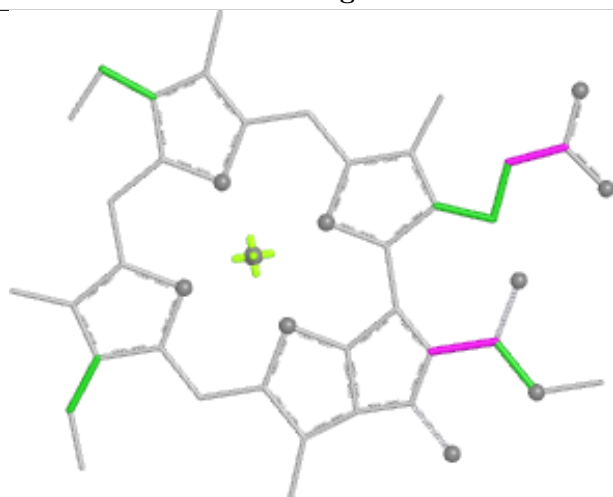
Ligand CLA d 507



Bond lengths



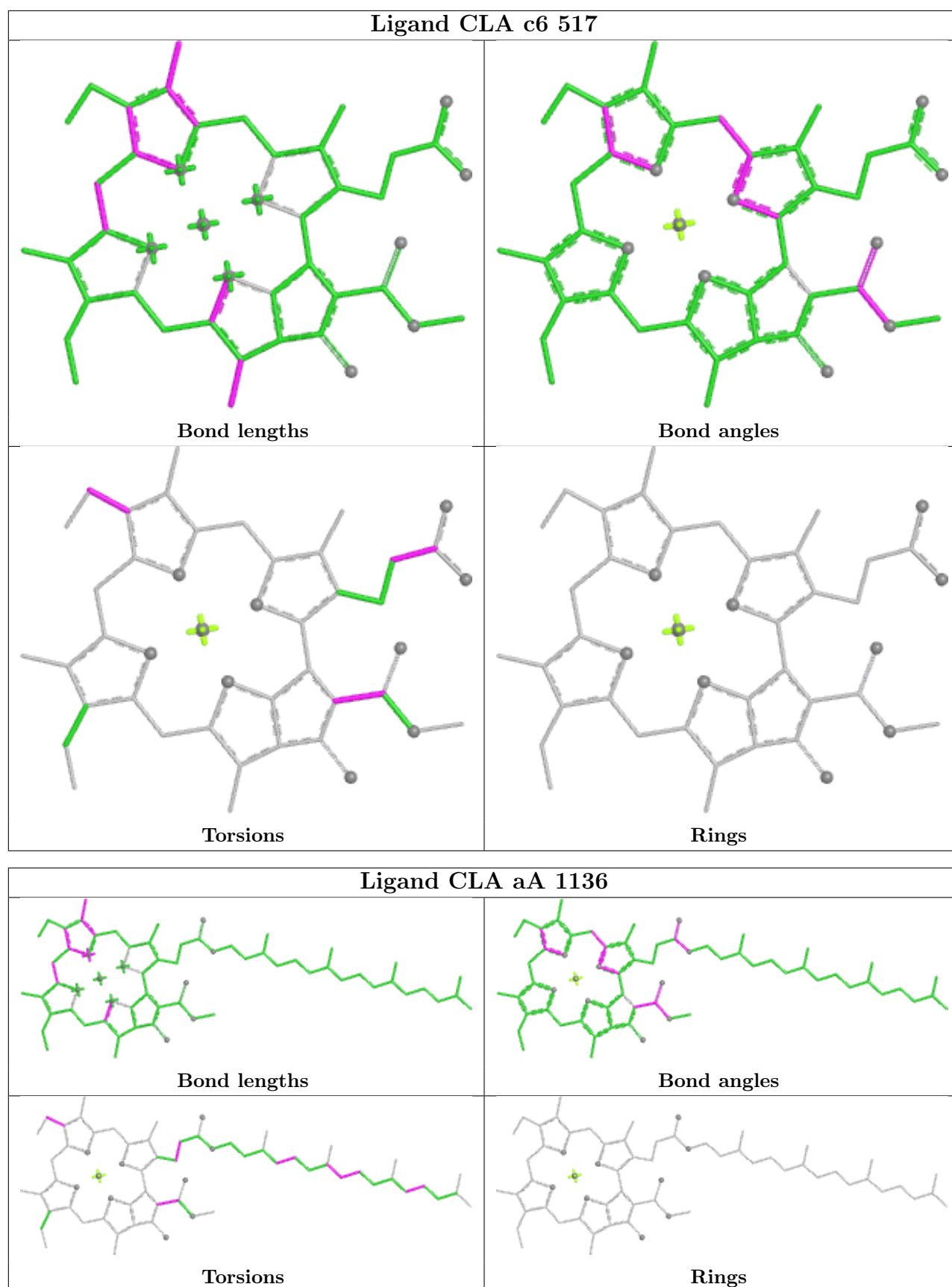
Bond angles



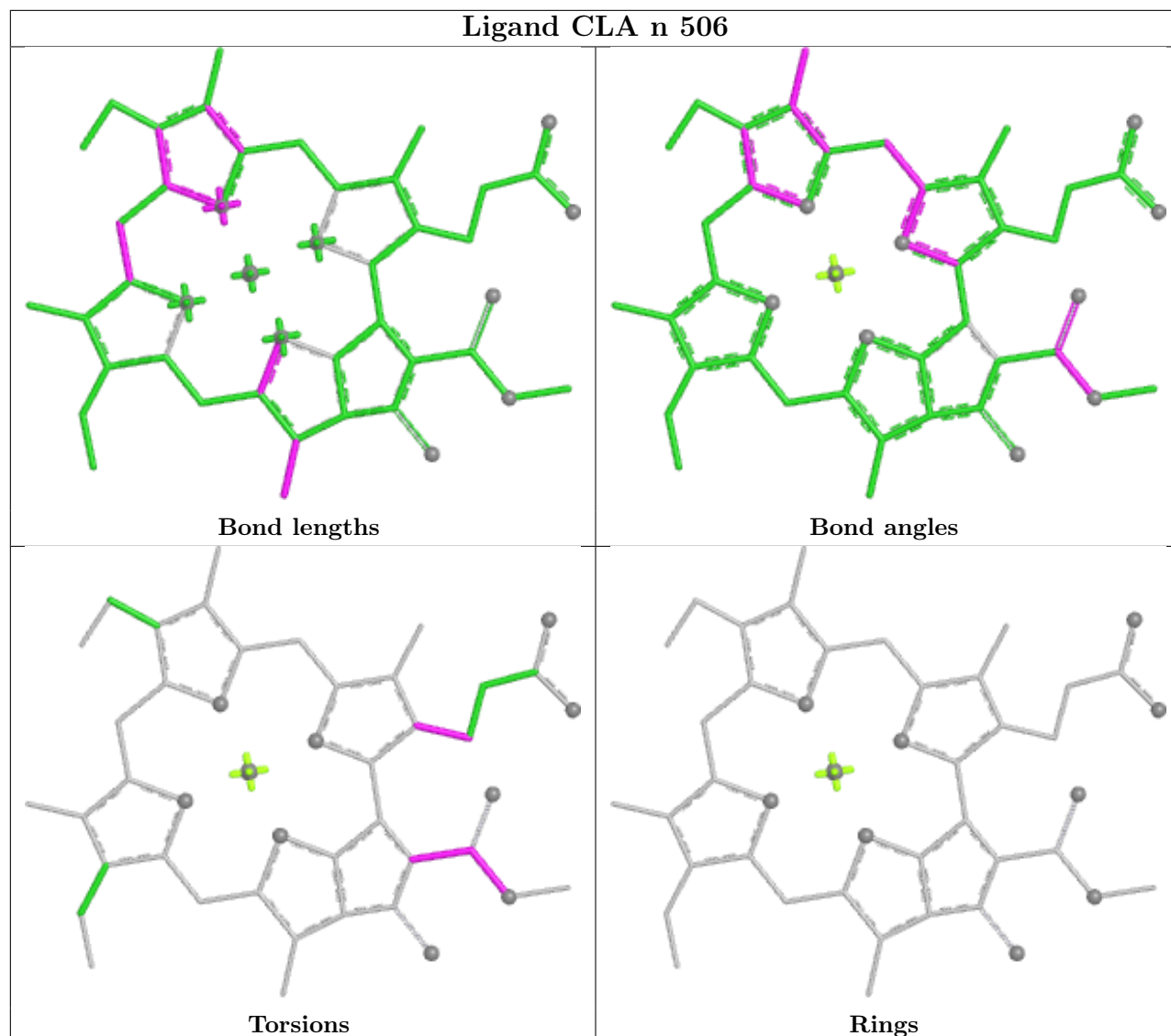
Torsions



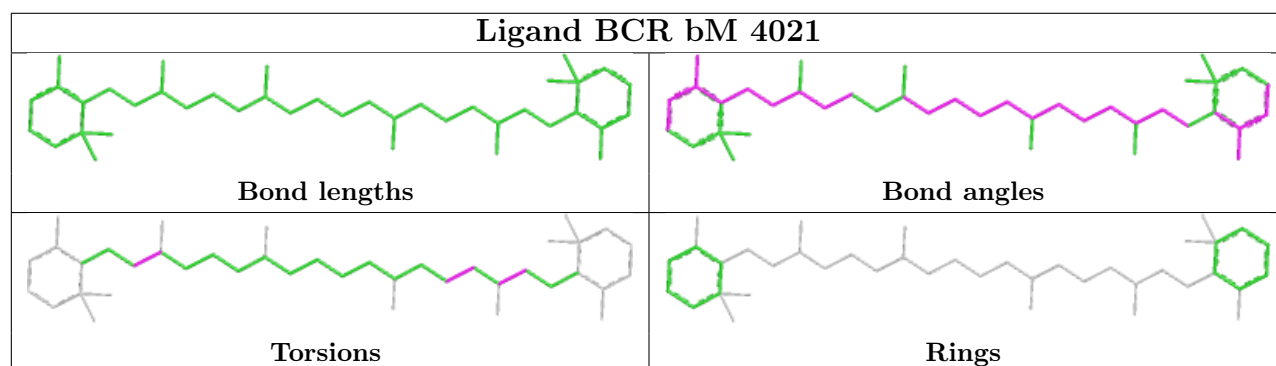
Rings



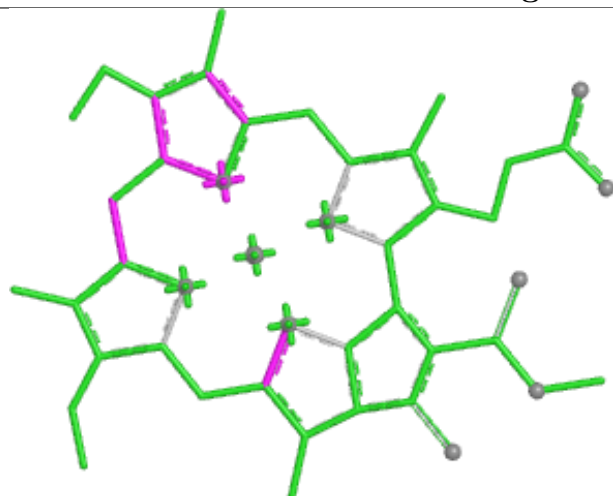
Ligand CLA n 506



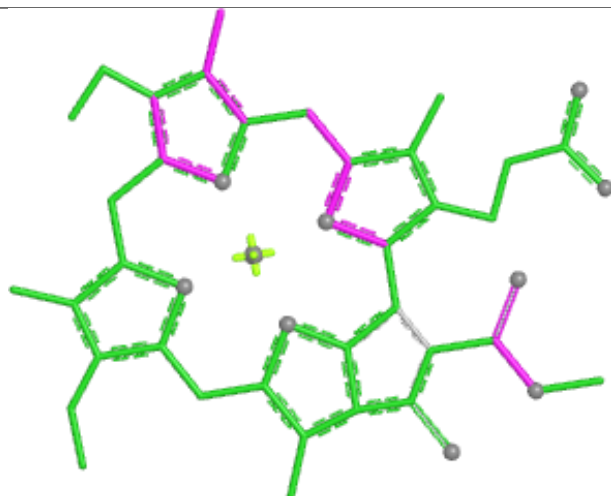
Ligand BCR bM 4021



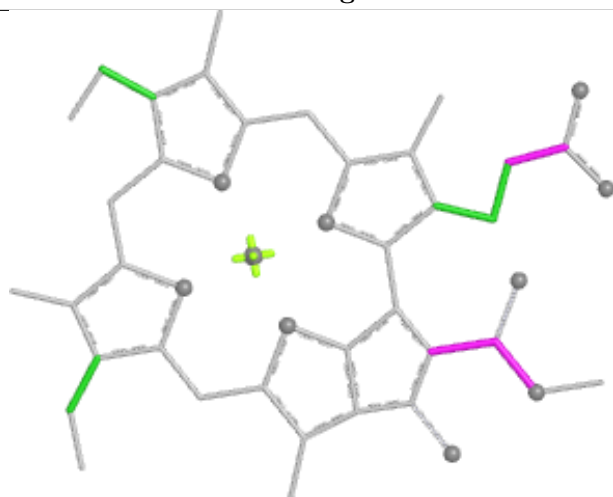
Ligand CLA f 510



Bond lengths



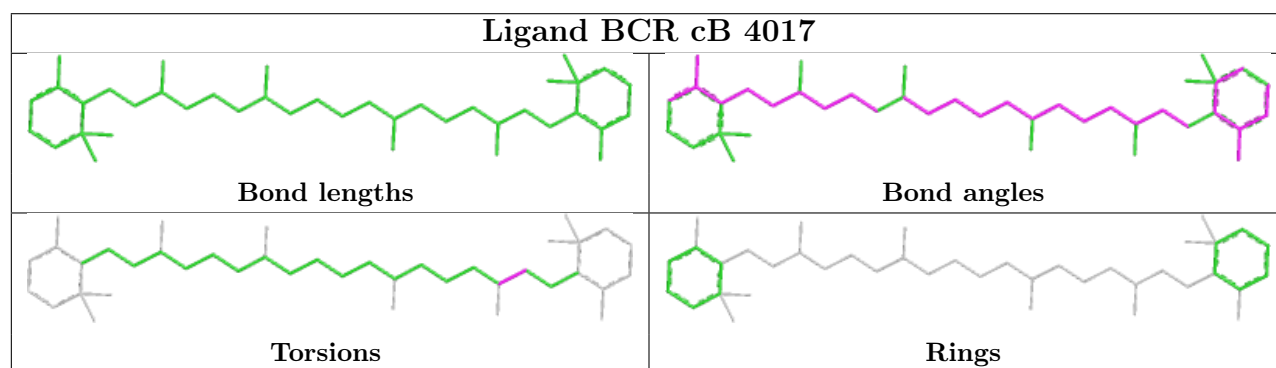
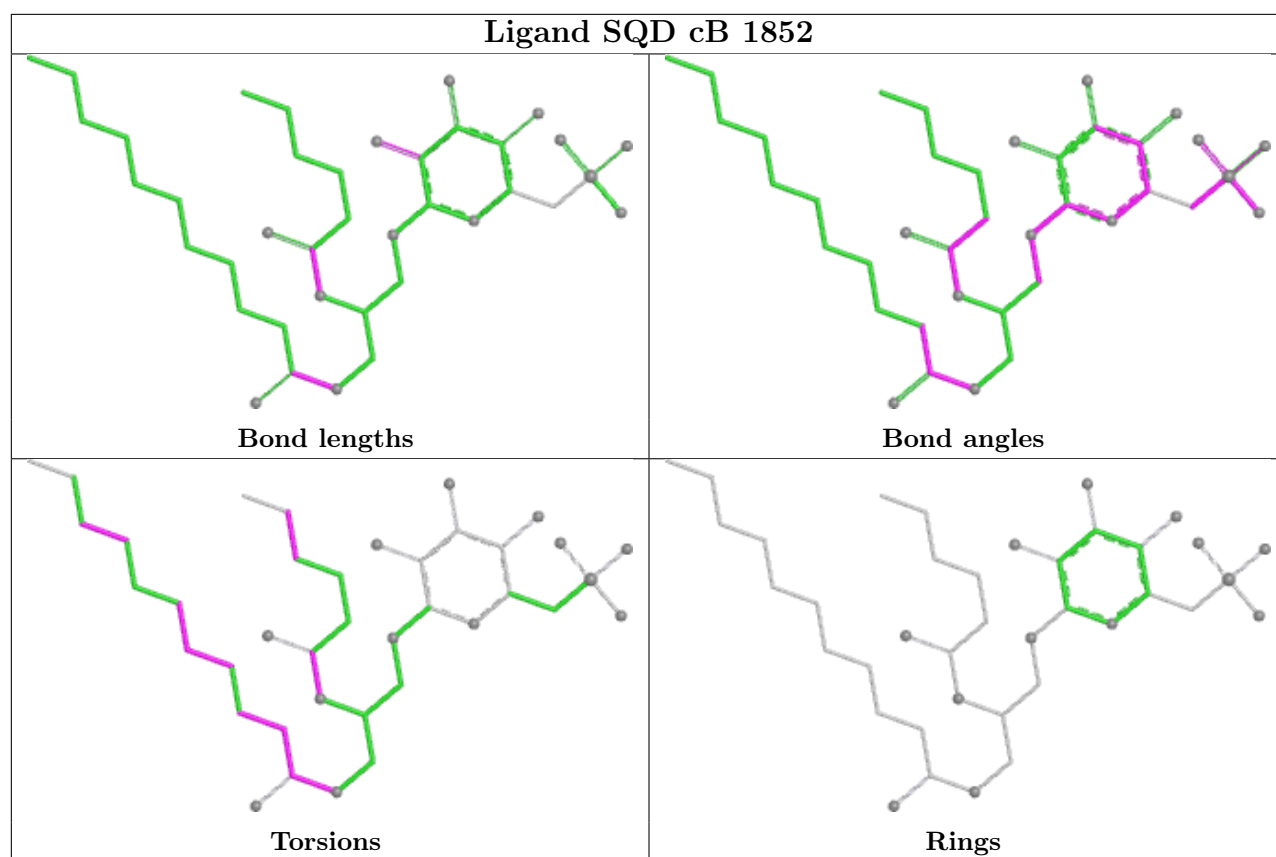
Bond angles



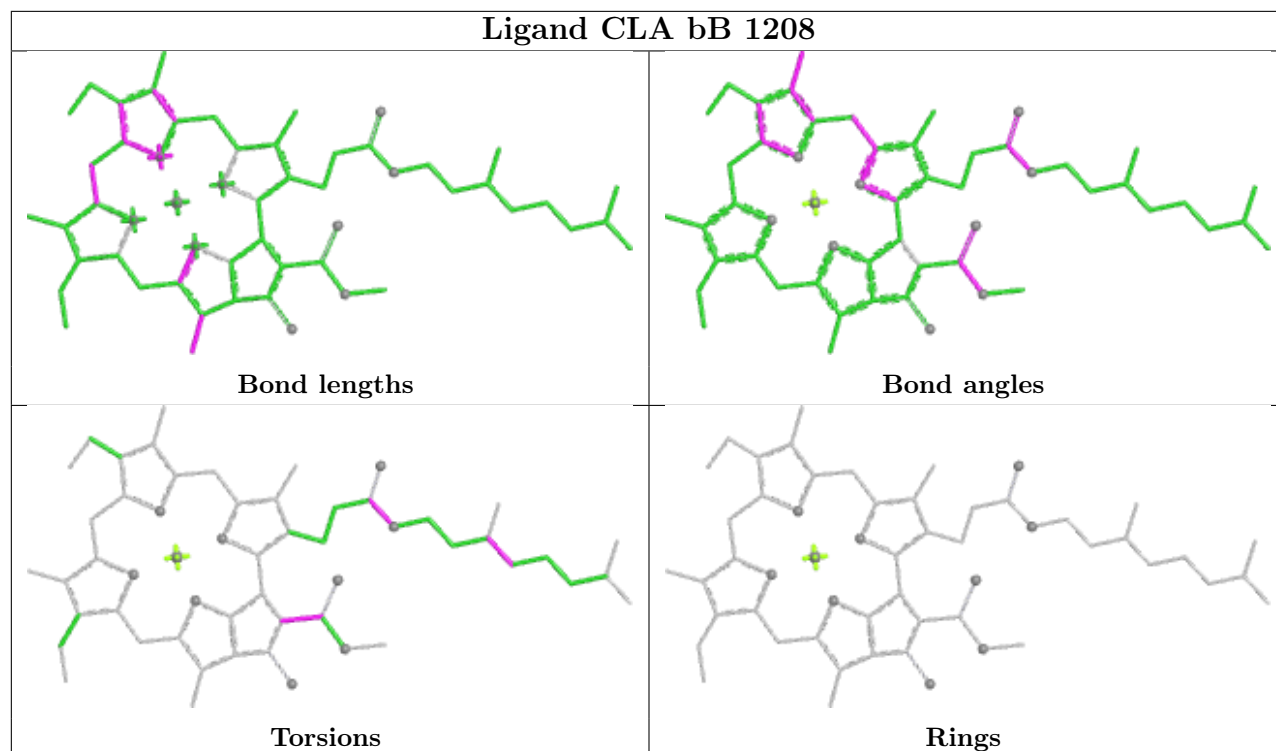
Torsions



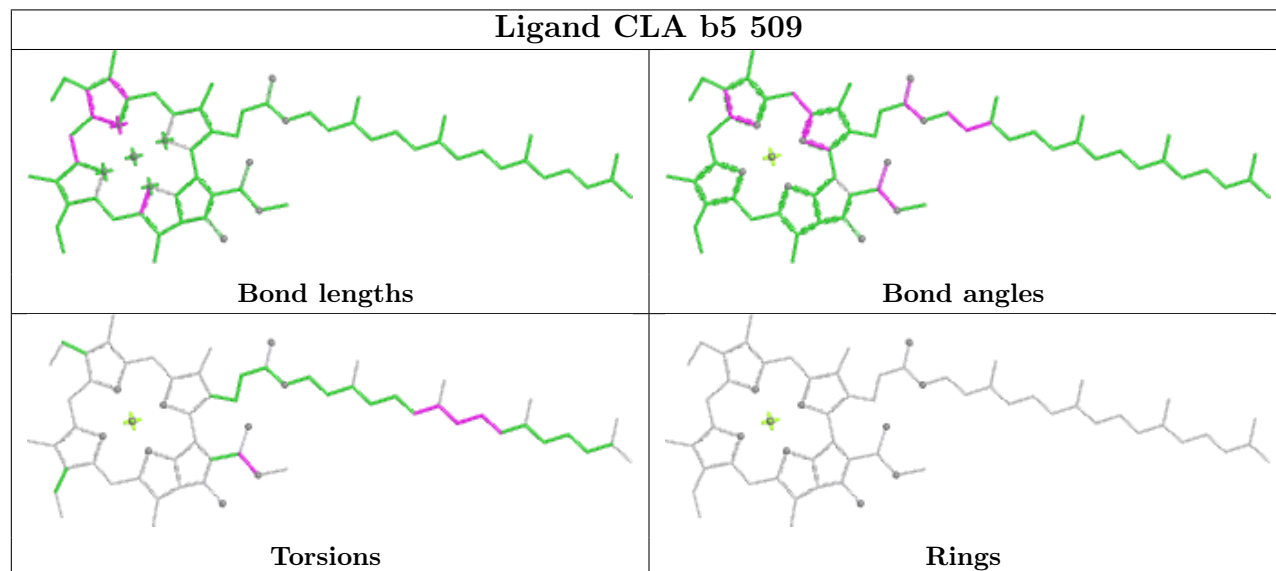
Rings

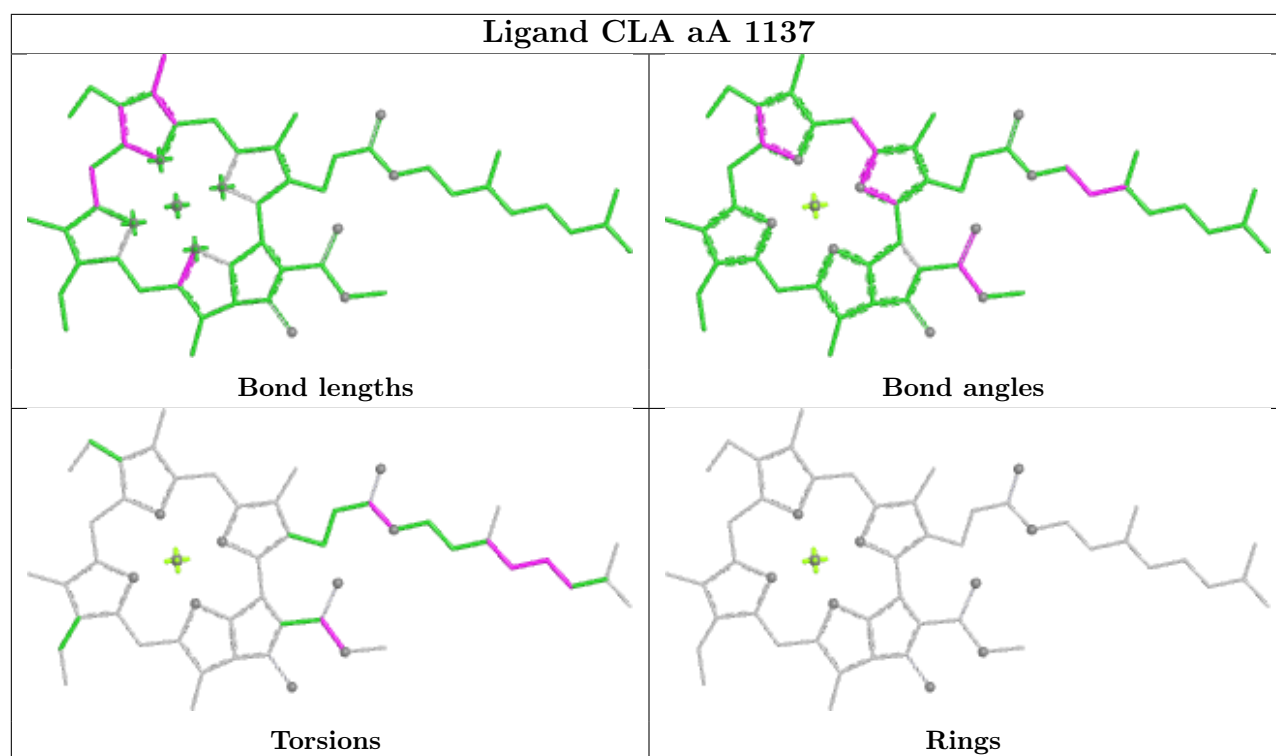


Ligand CLA bB 1208

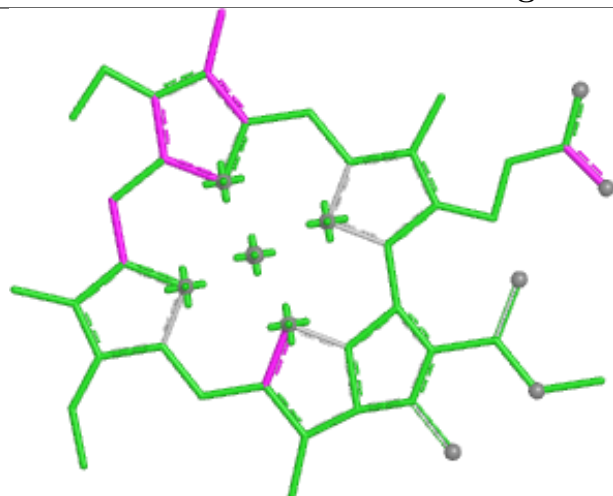


Ligand CLA b5 509

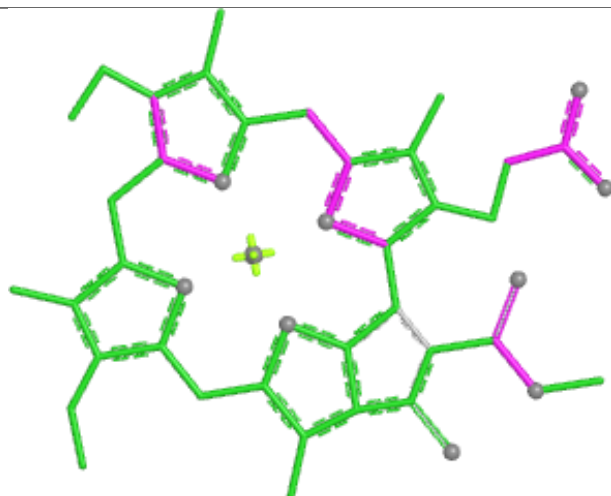




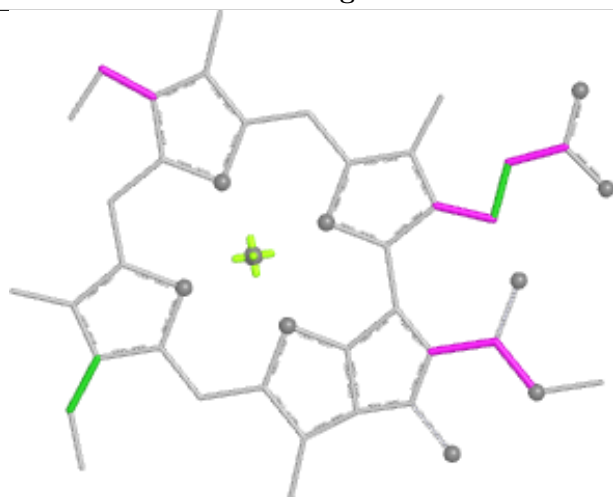
Ligand CLA k 517



Bond lengths



Bond angles

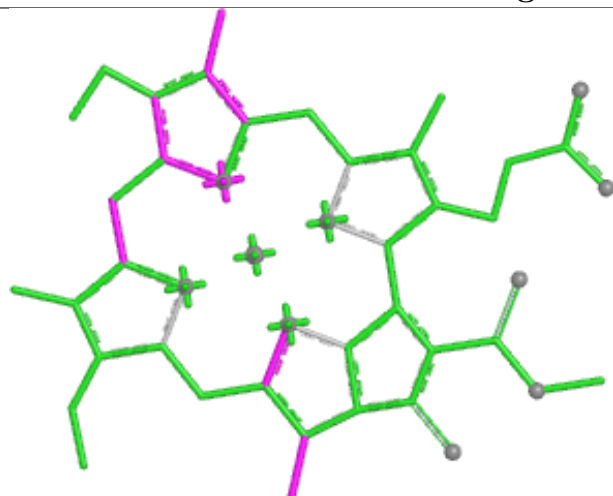


Torsions

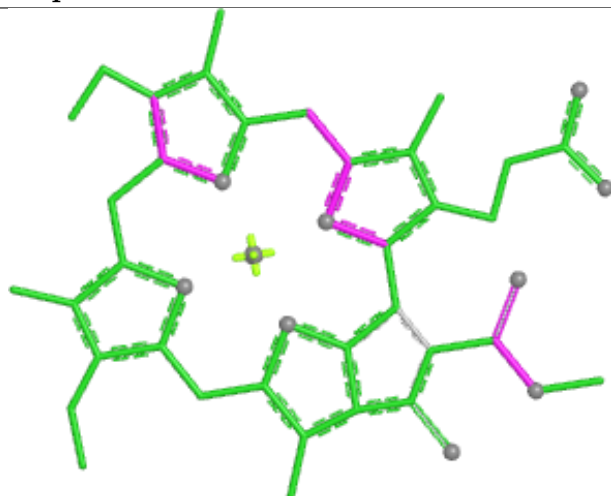


Rings

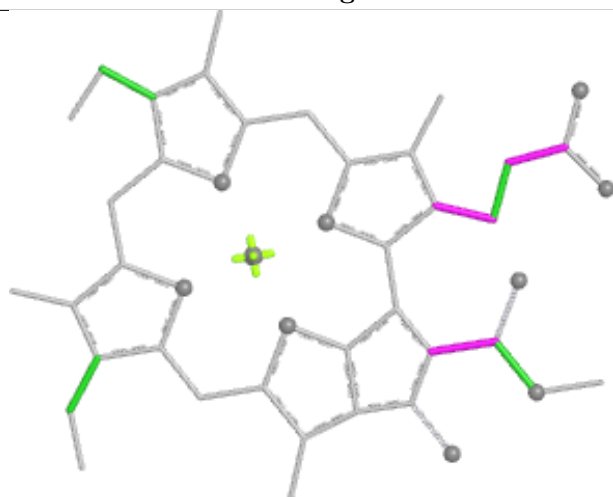
Ligand CLA p 519



Bond lengths



Bond angles

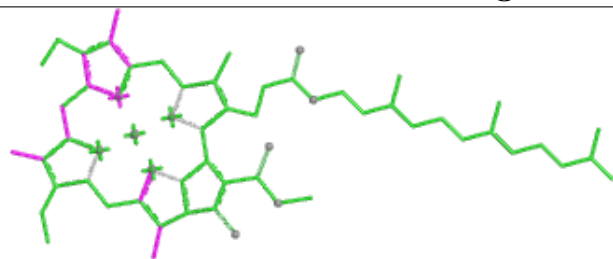


Torsions

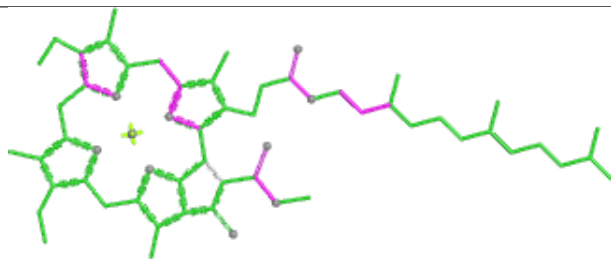


Rings

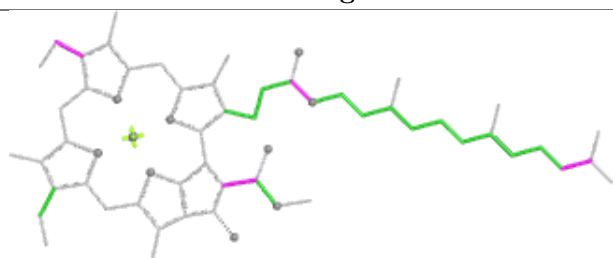
Ligand CLA bB 1234



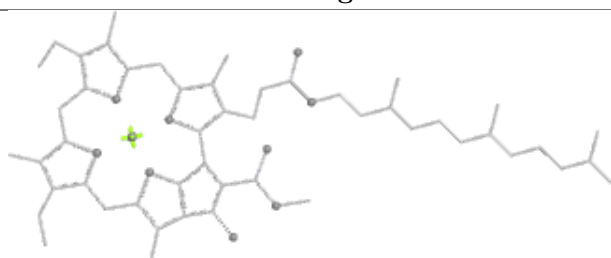
Bond lengths



Bond angles

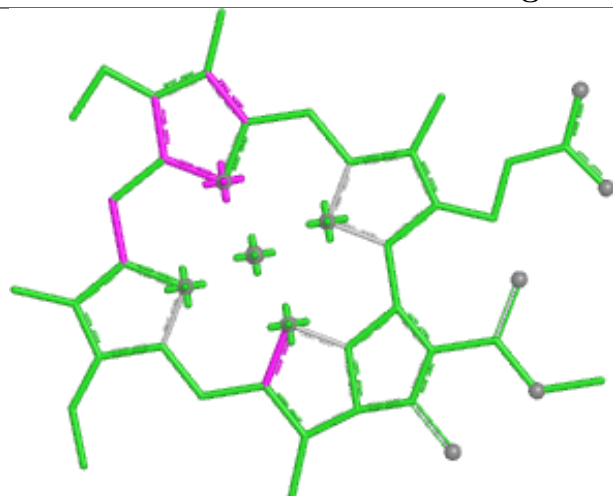


Torsions

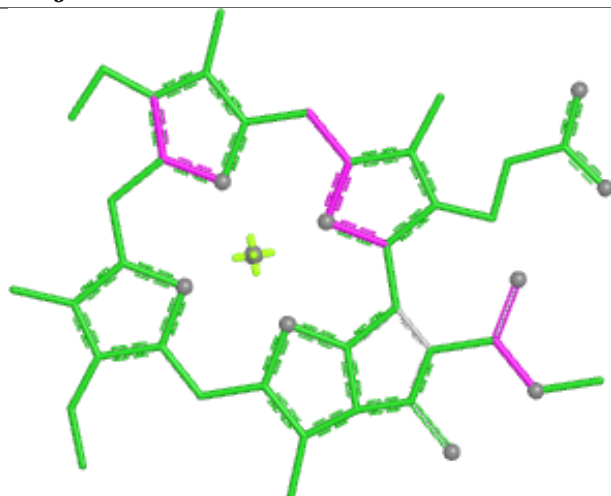


Rings

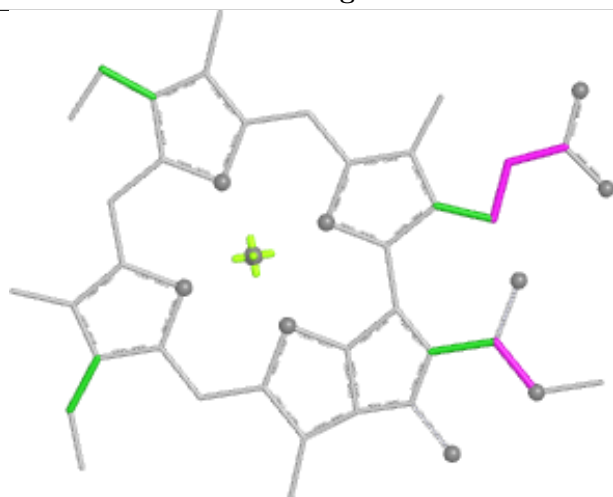
Ligand CLA j 511



Bond lengths



Bond angles

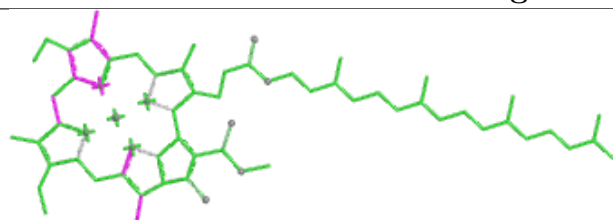


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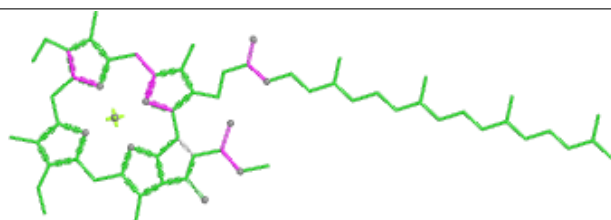


Rings

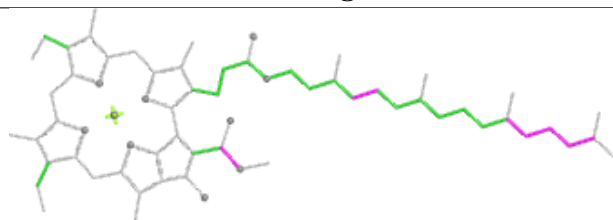
Ligand CLA c6 509



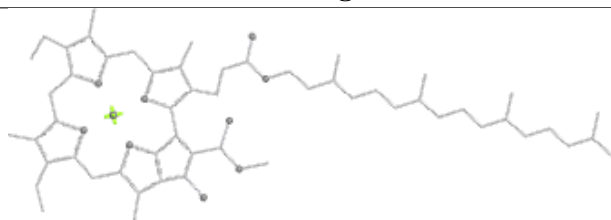
Bond lengths



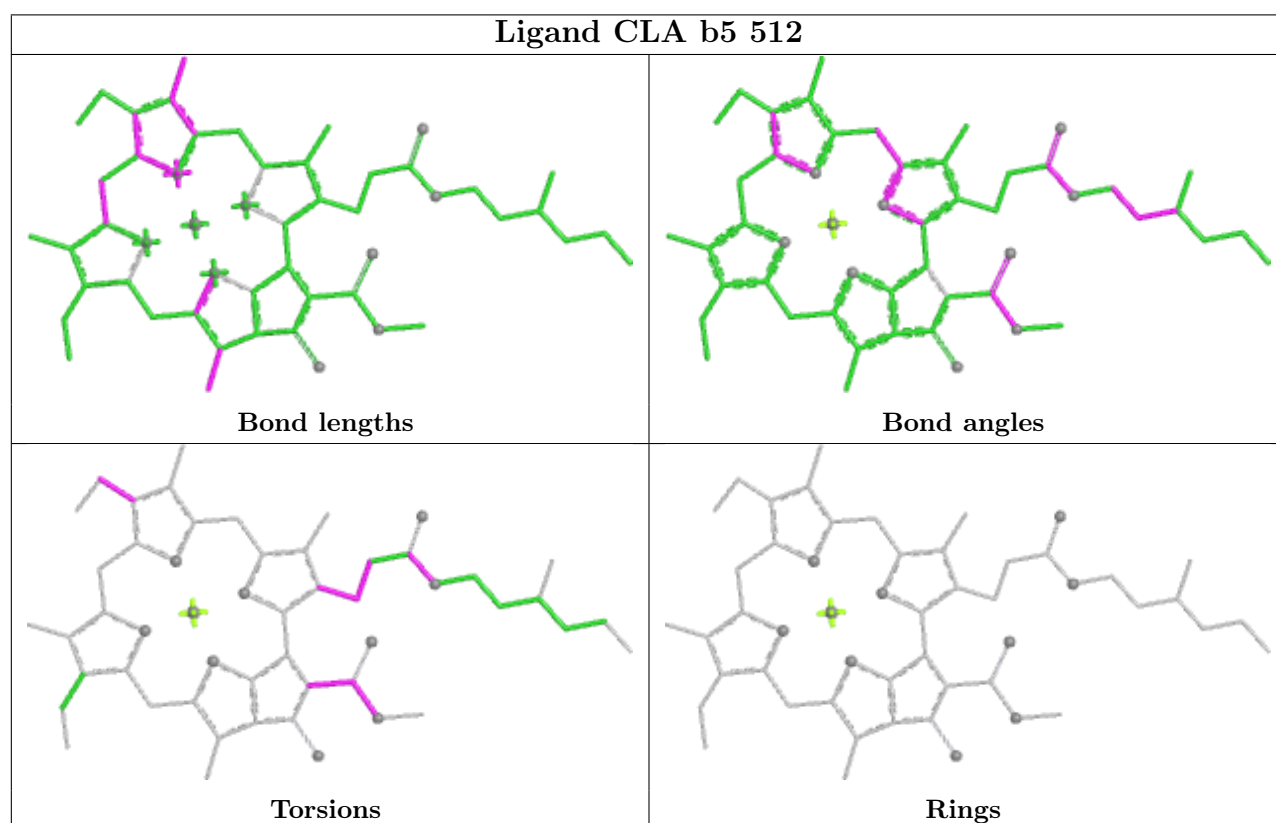
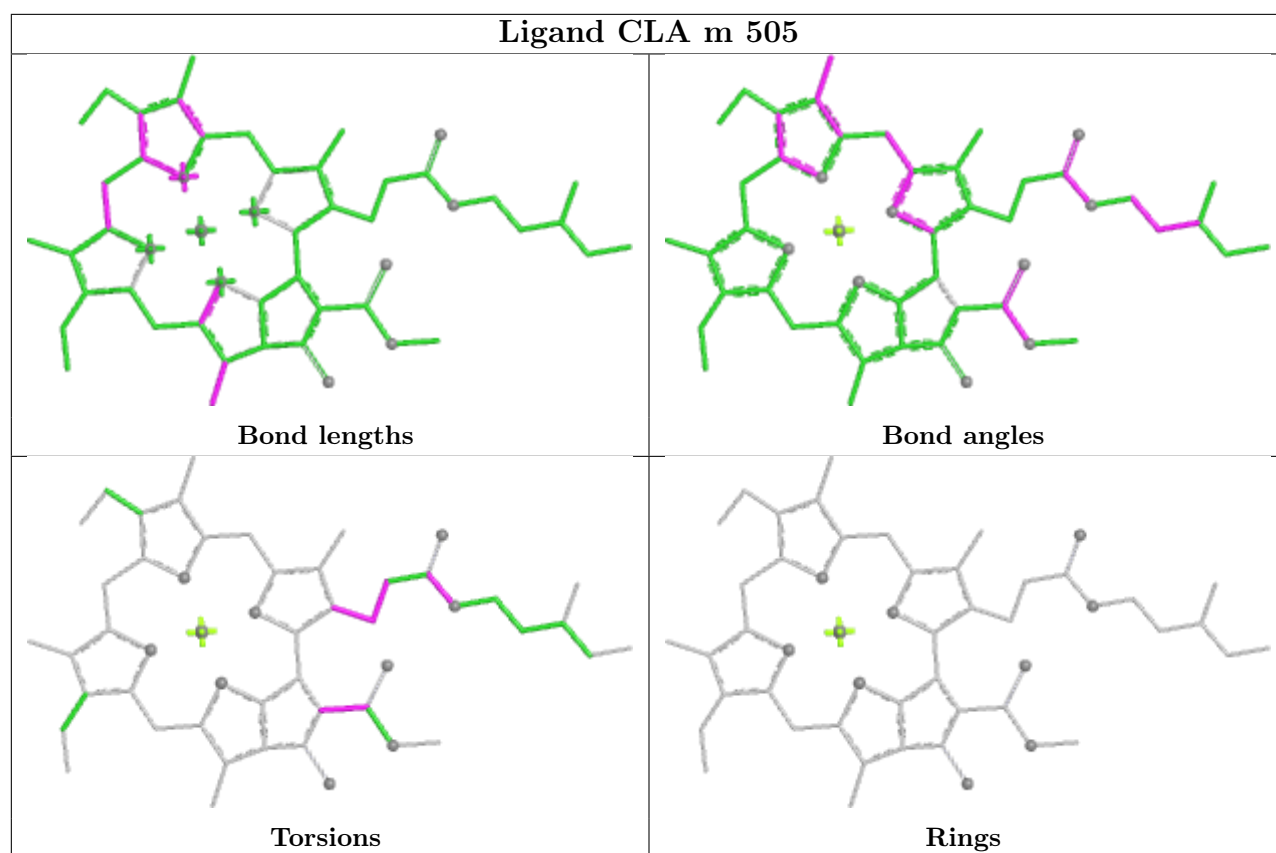
Bond angles



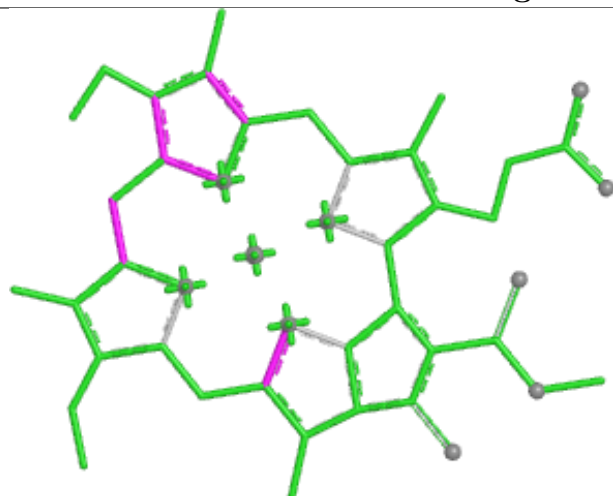
Torsions



Rings



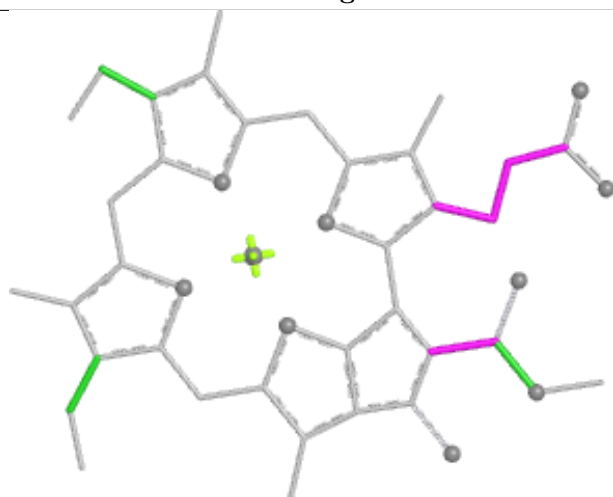
Ligand CLA V 516



Bond lengths



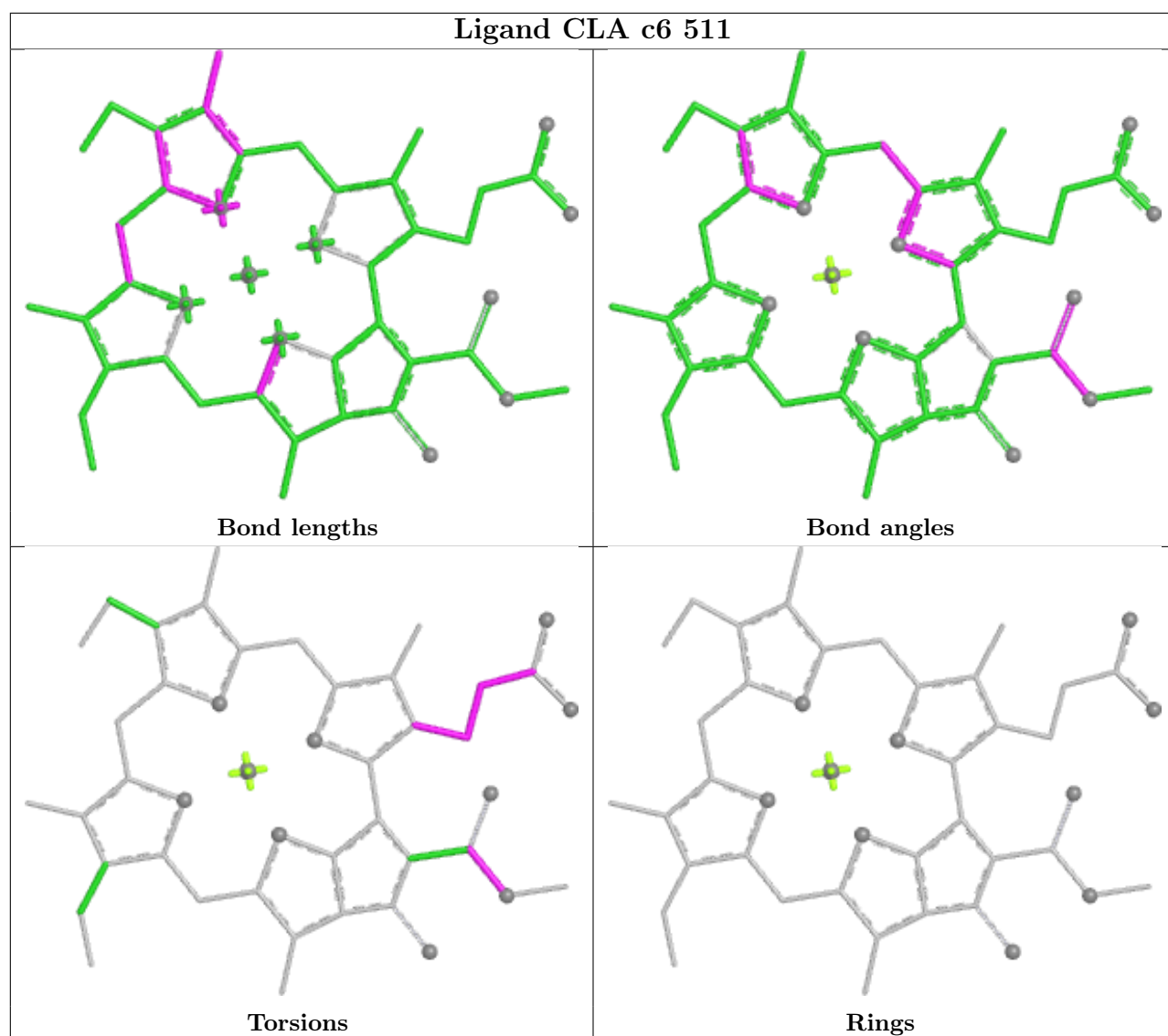
Bond angles



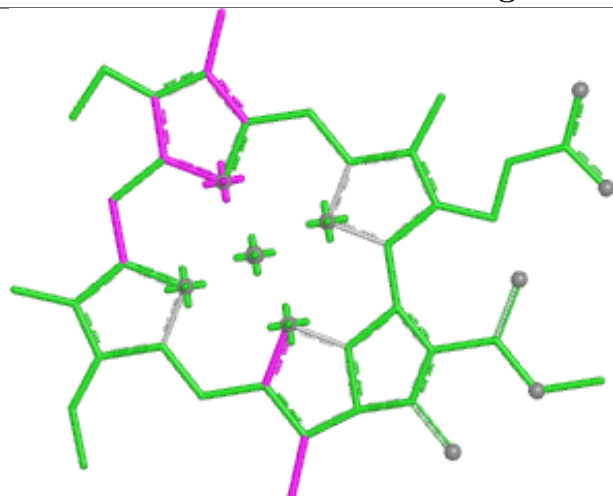
Torsions



Rings



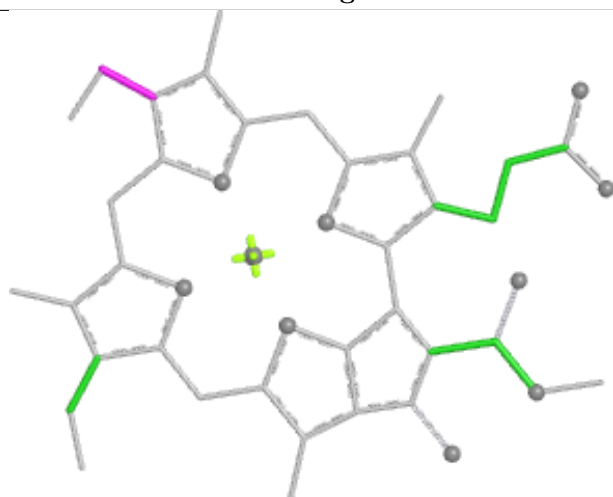
Ligand CLA aF 1301



Bond lengths



Bond angles

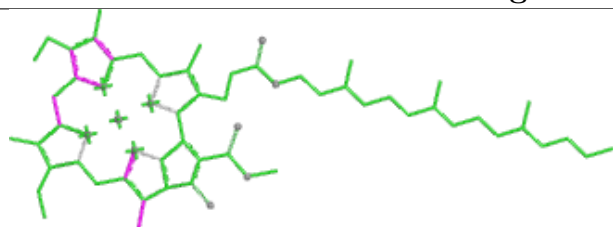


Torsions

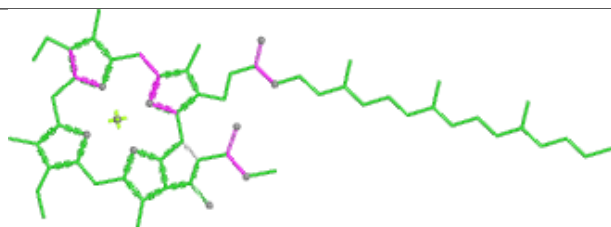


Rings

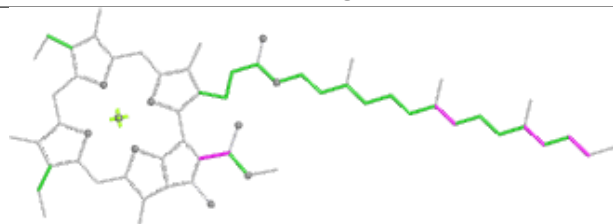
Ligand CLA a1 503



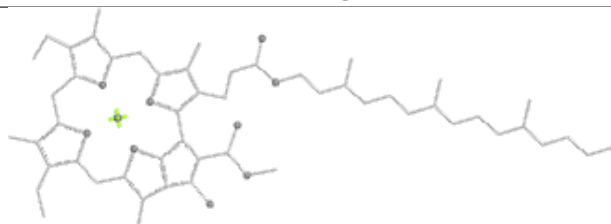
Bond lengths



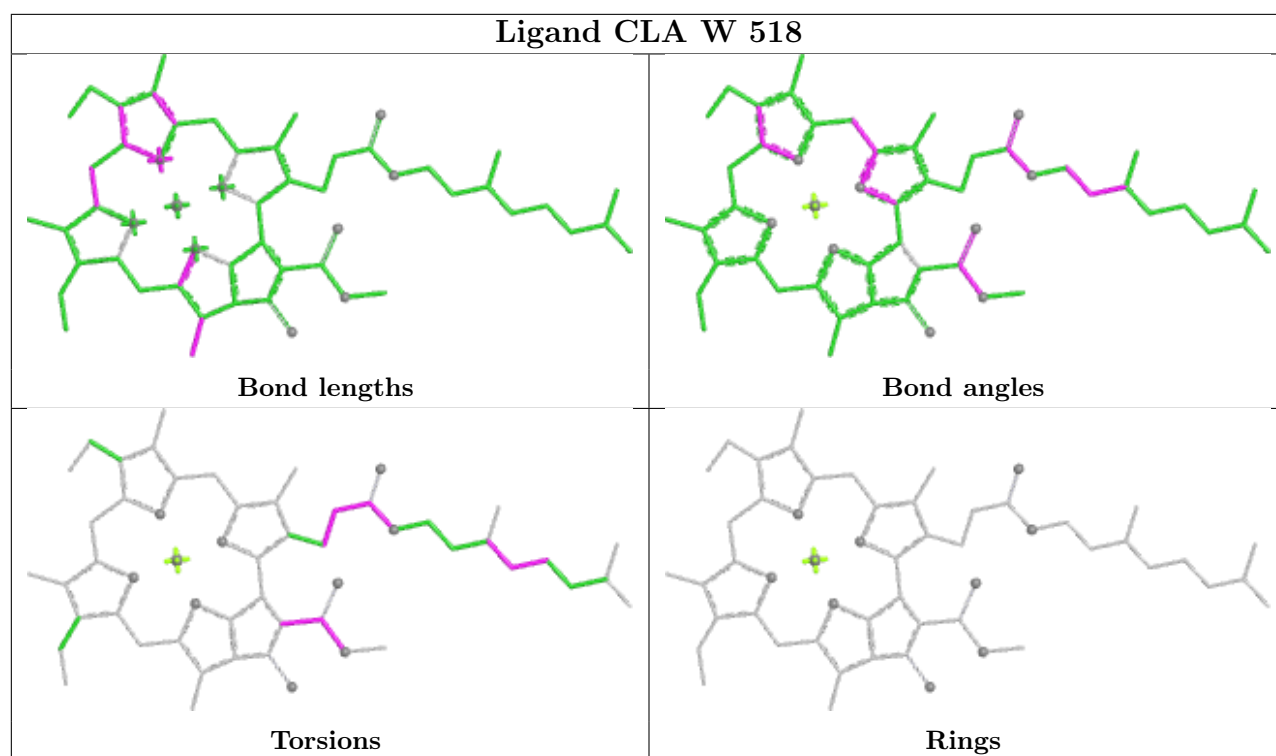
Bond angles



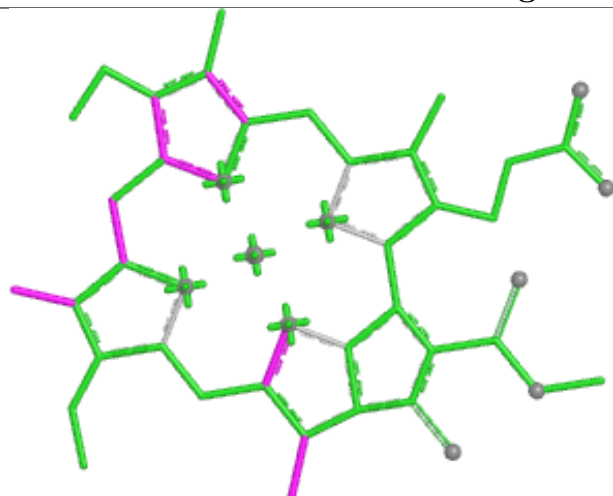
Torsions



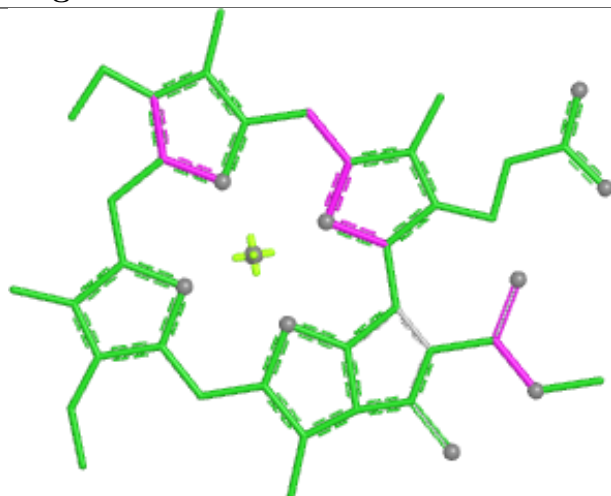
Rings



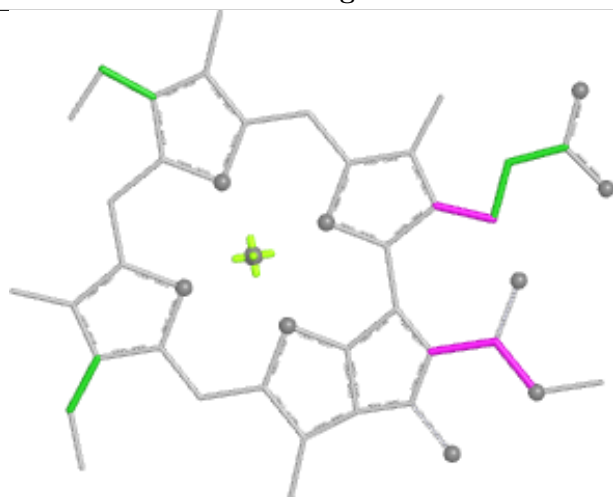
Ligand CLA g 508



Bond lengths



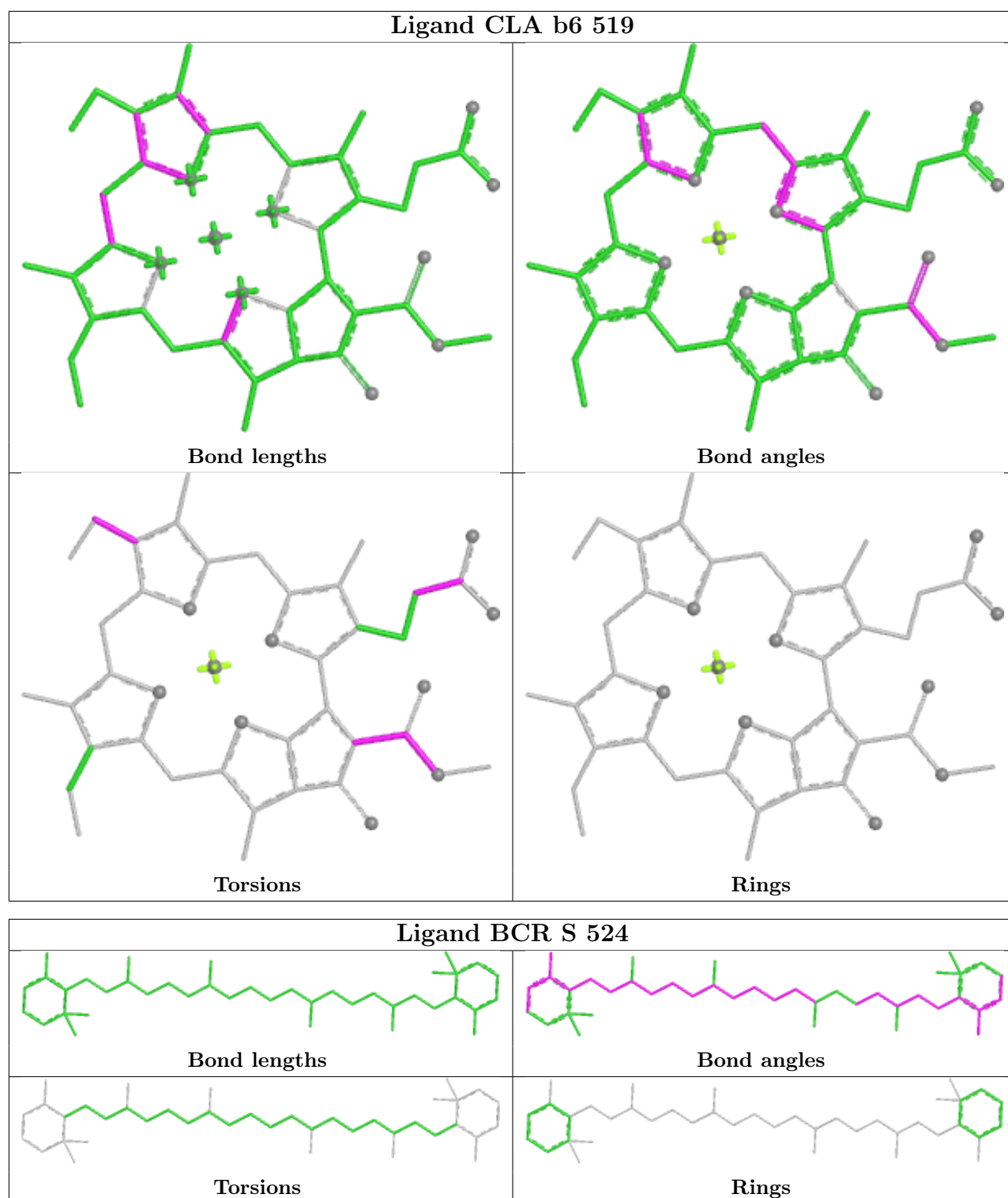
Bond angles

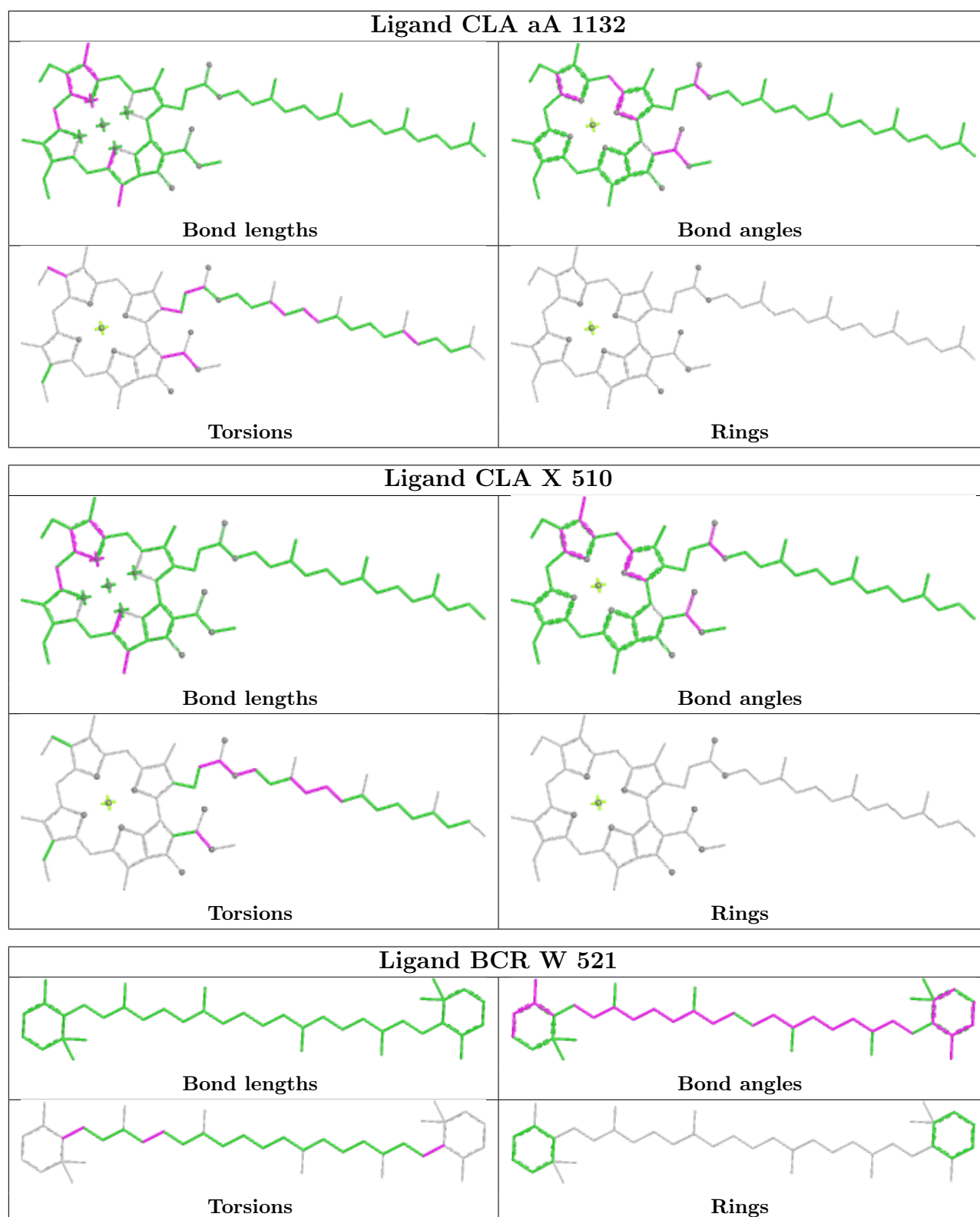


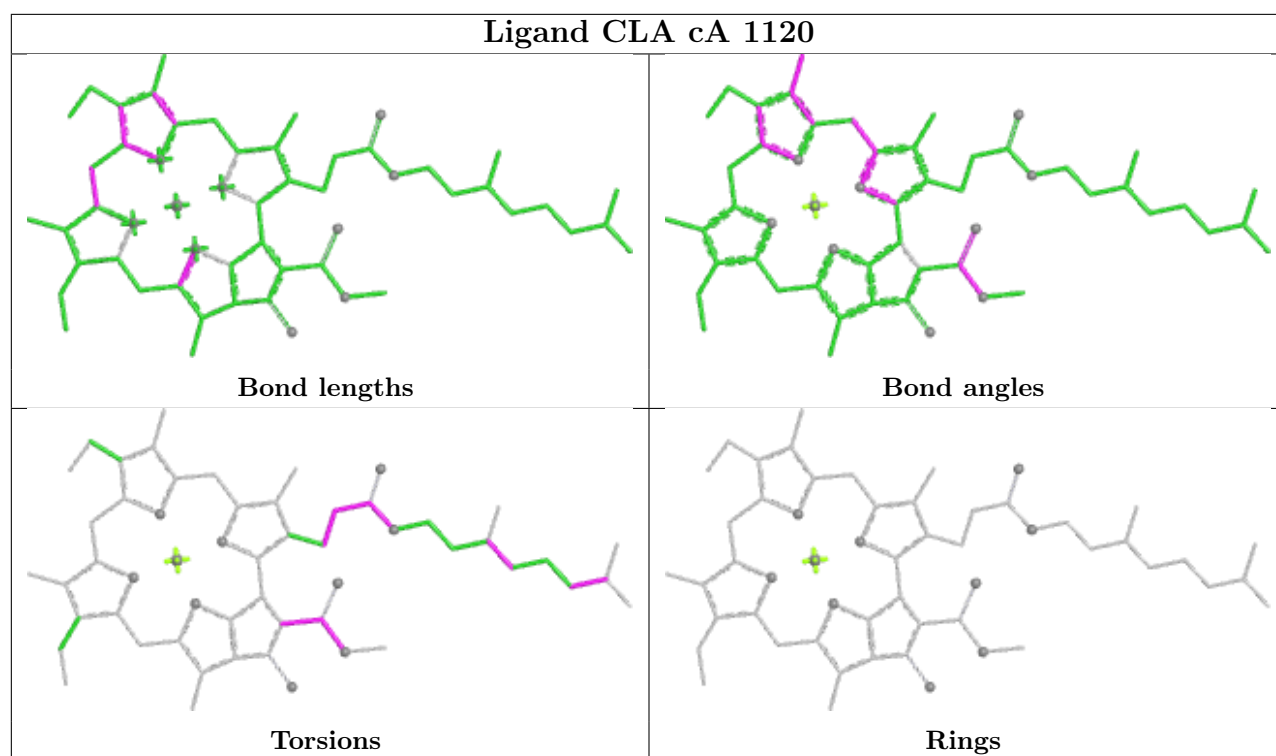
Torsions

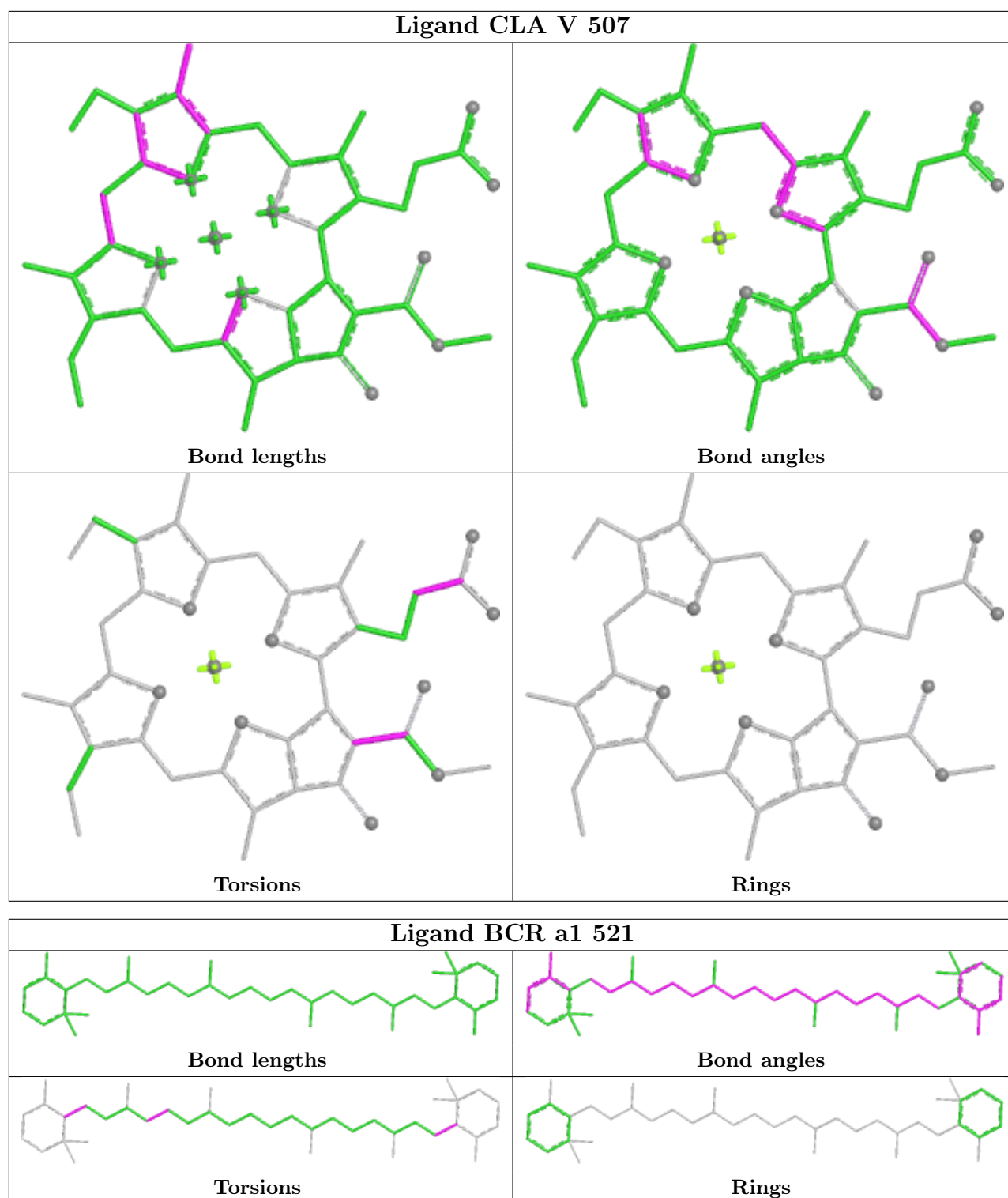


Rings

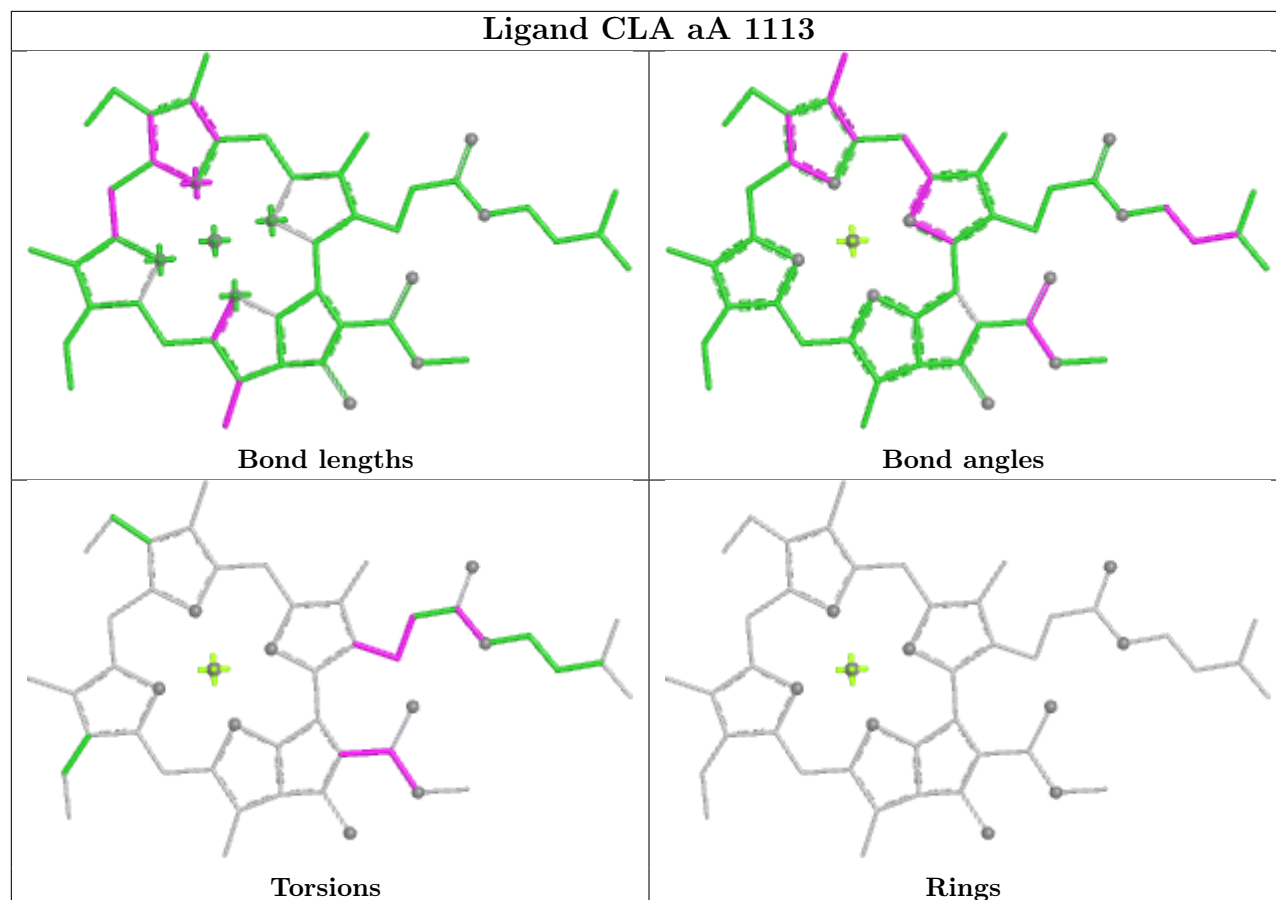




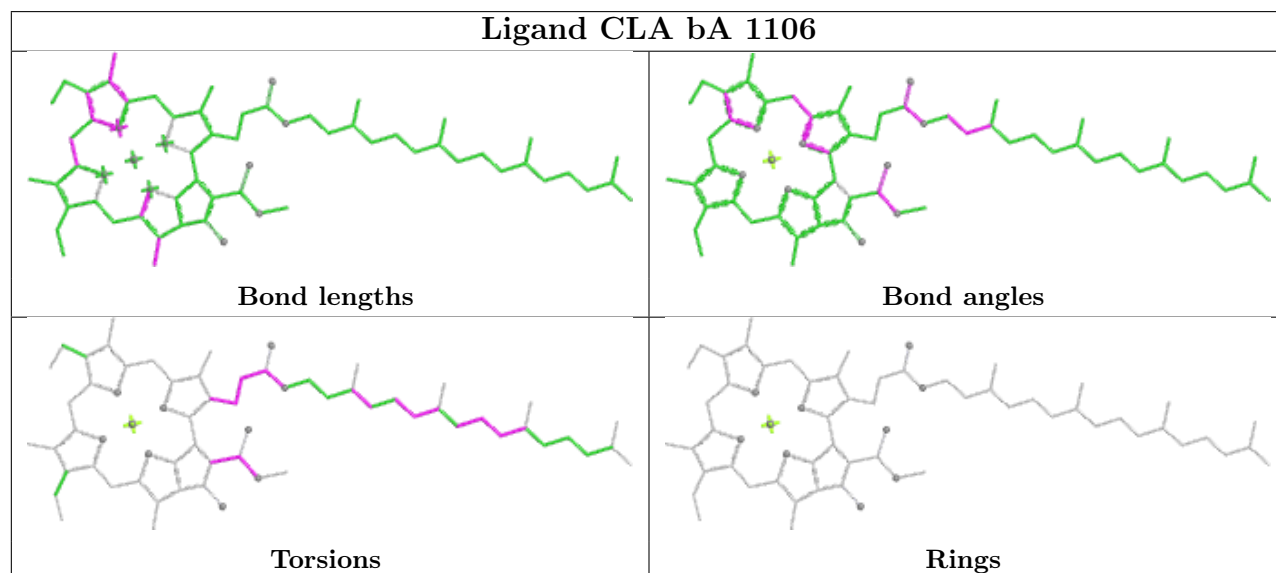


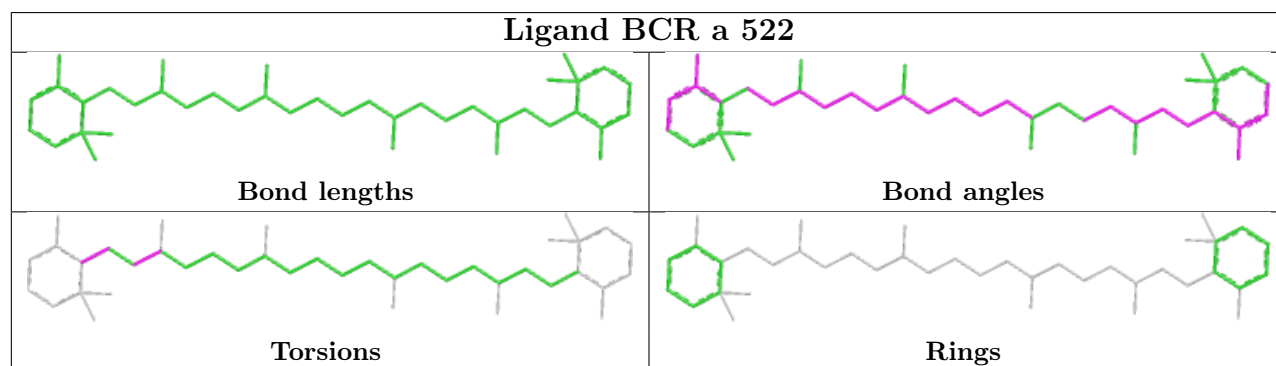
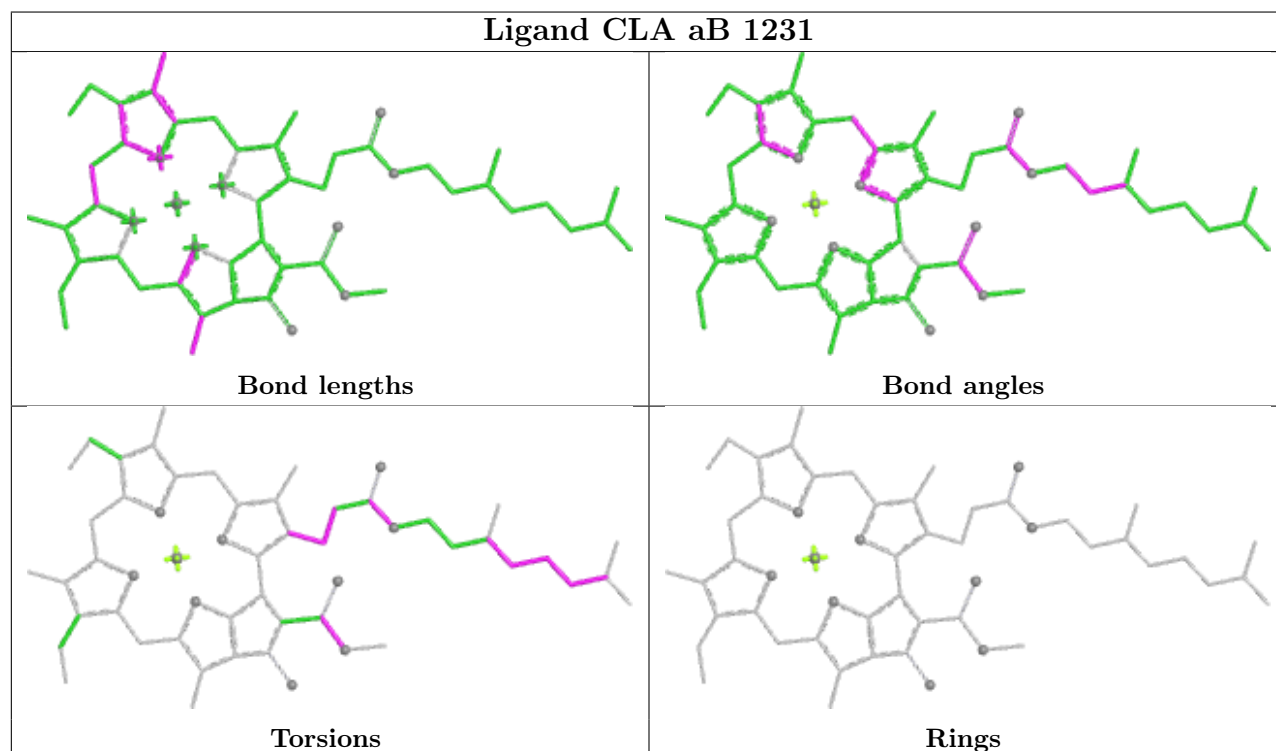
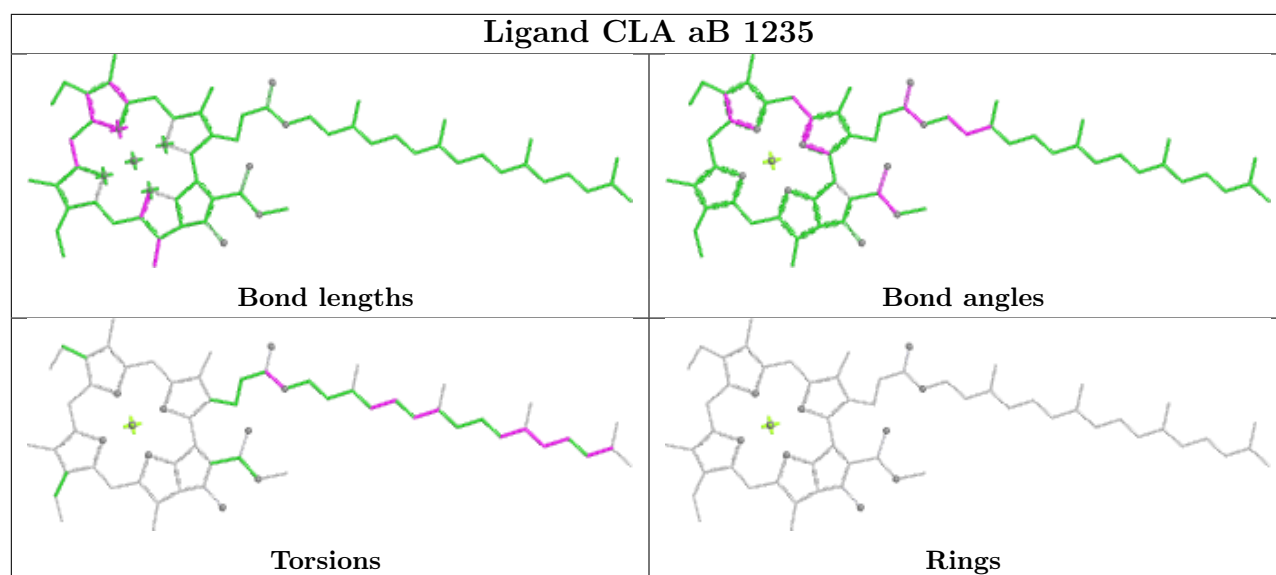


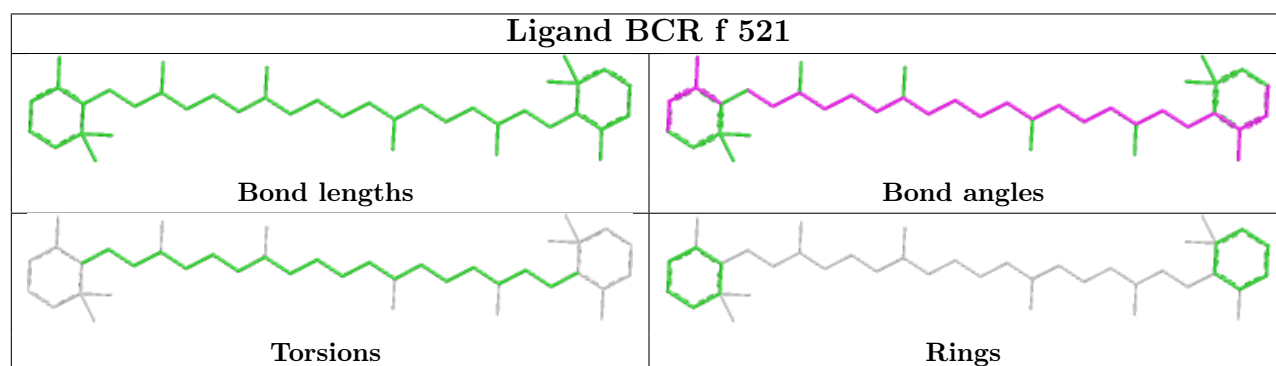
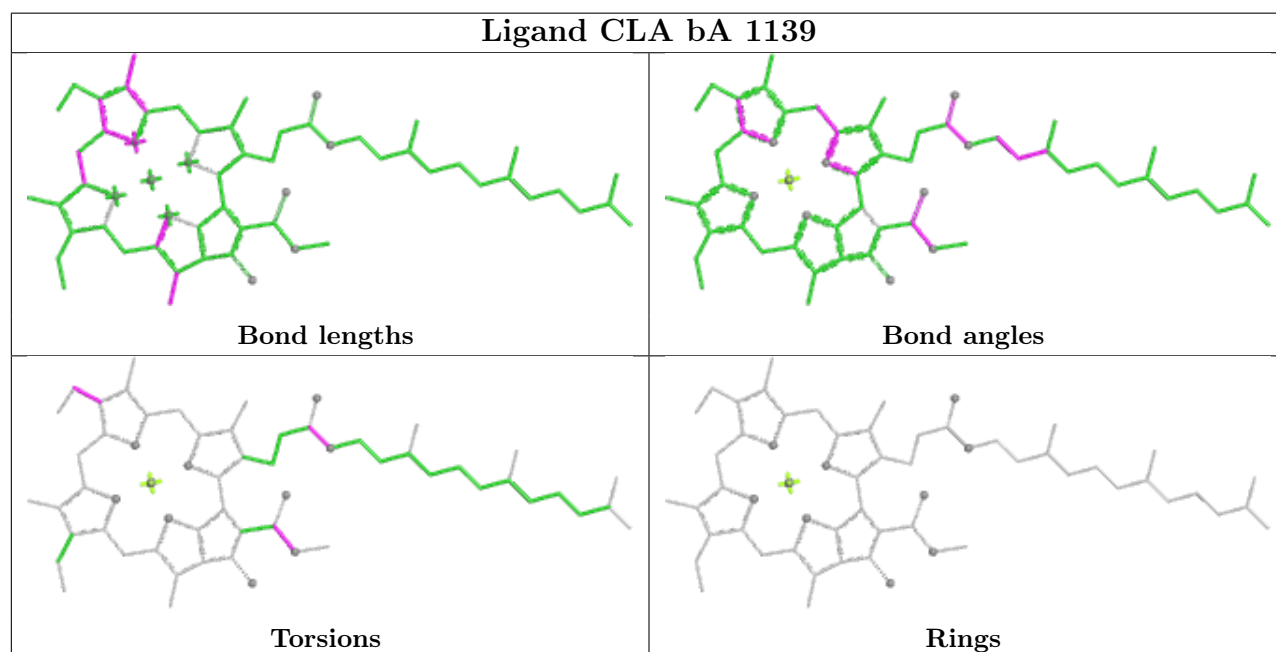
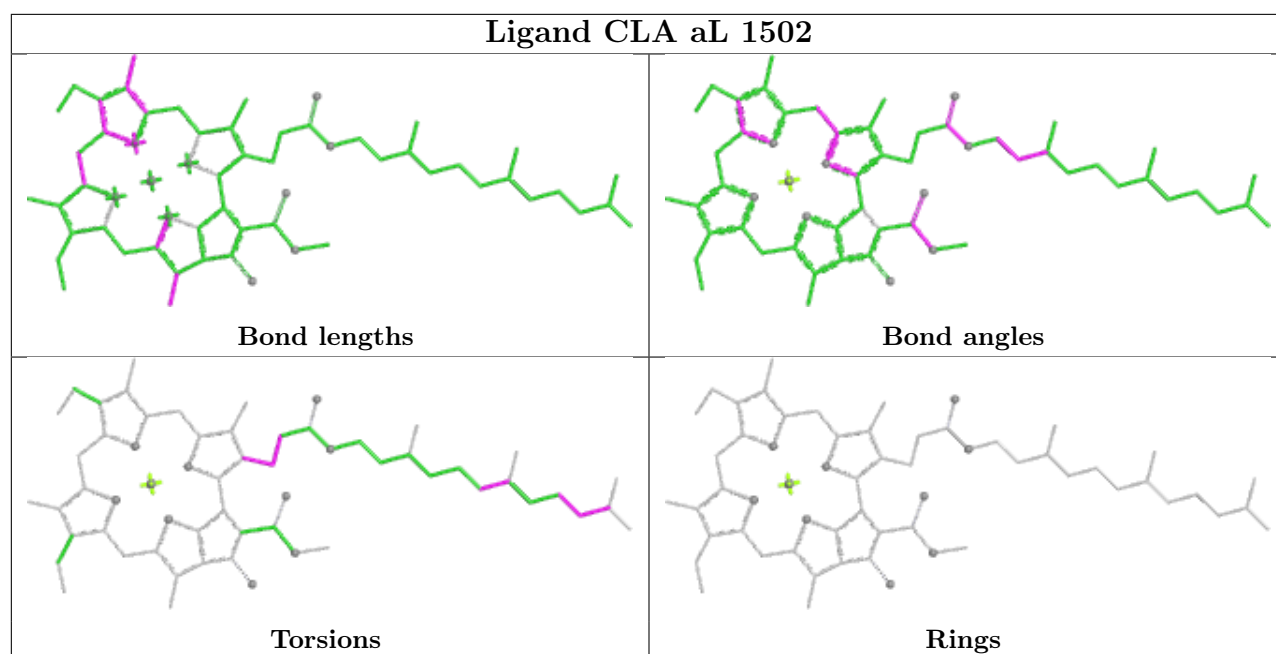
Ligand CLA aA 1113

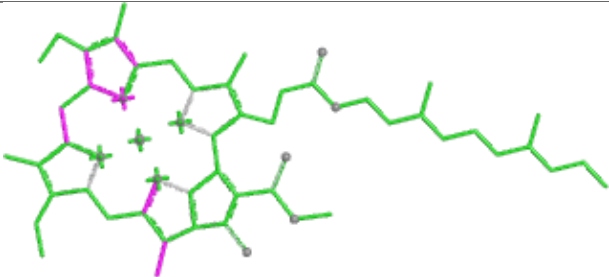
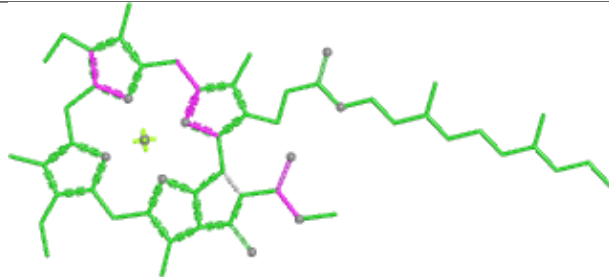
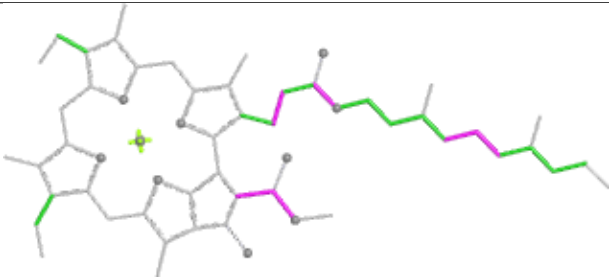
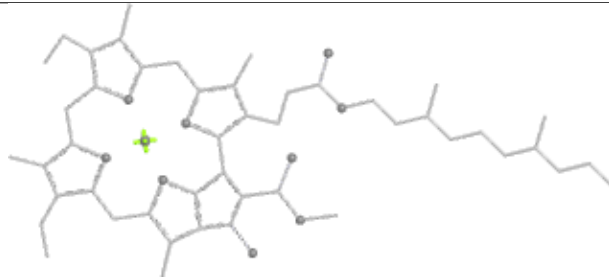
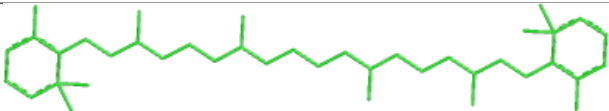
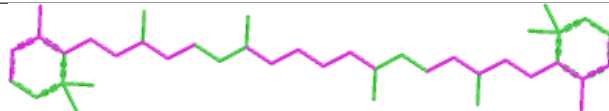
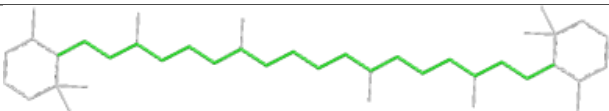
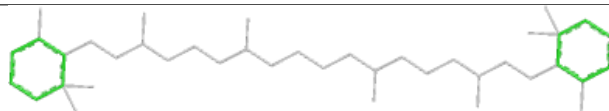
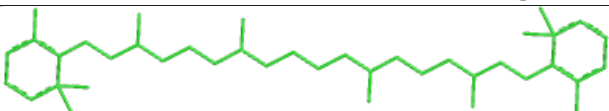
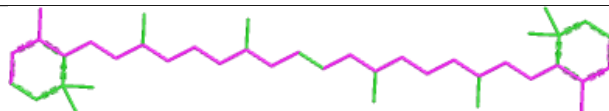

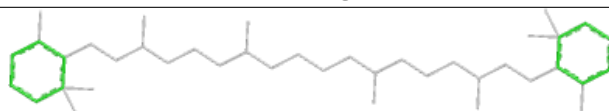


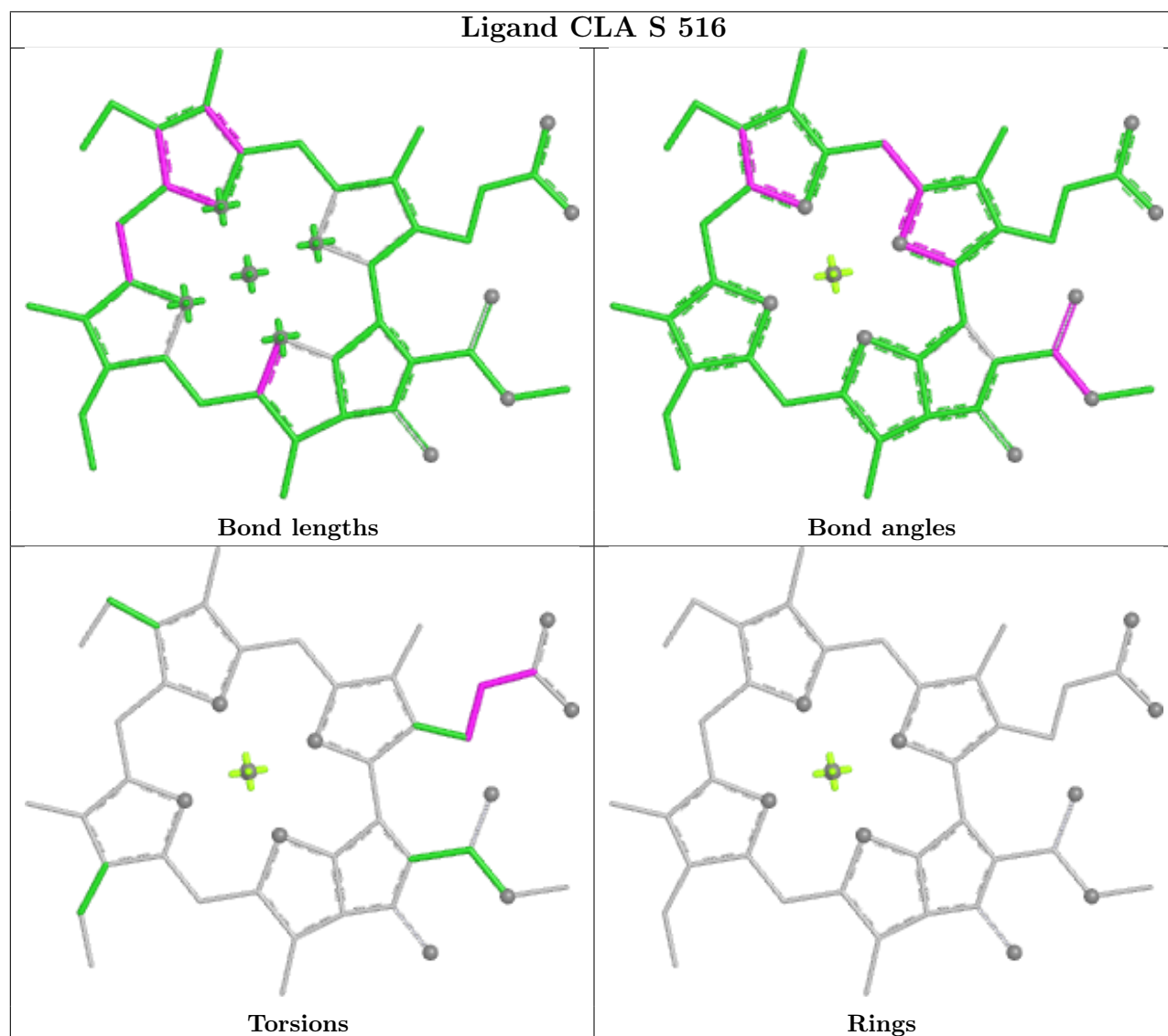
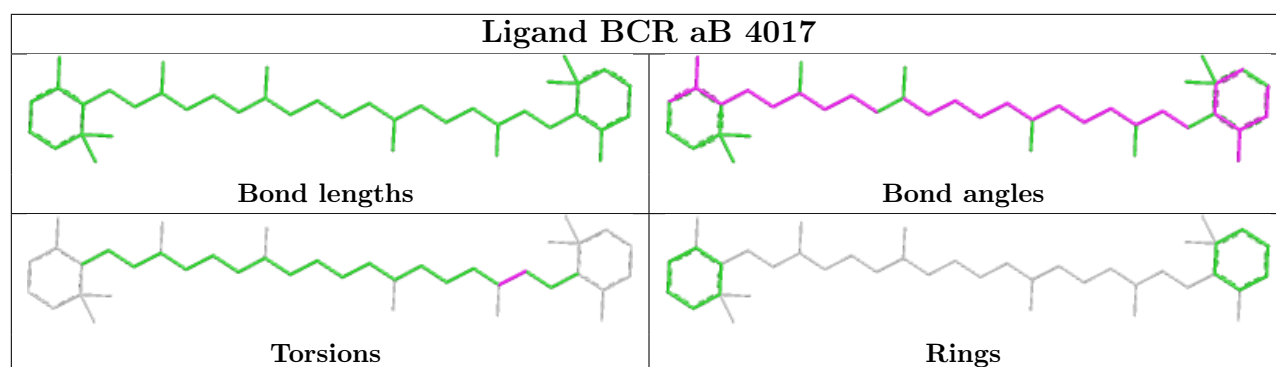
Ligand CLA bA 1106

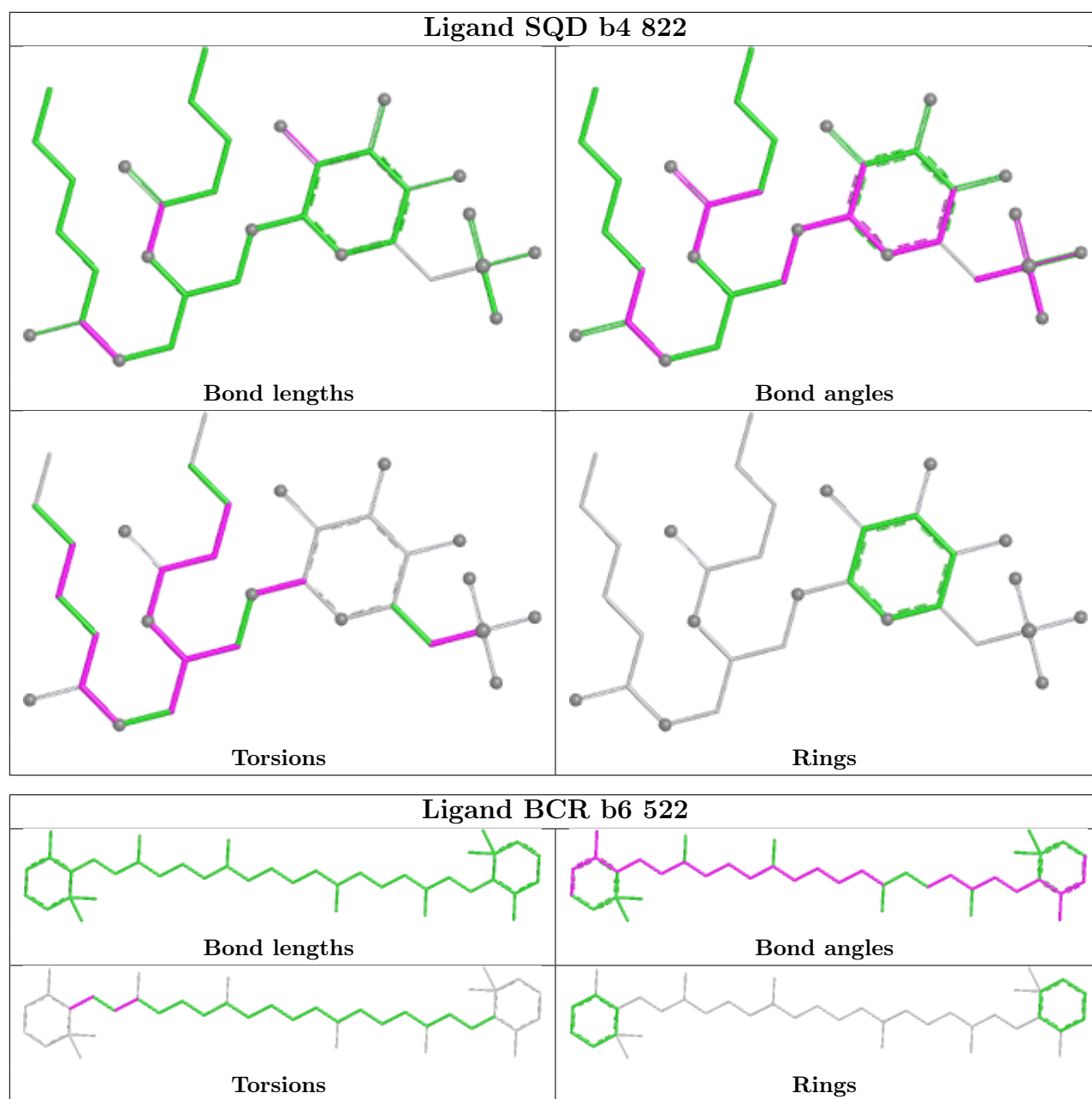




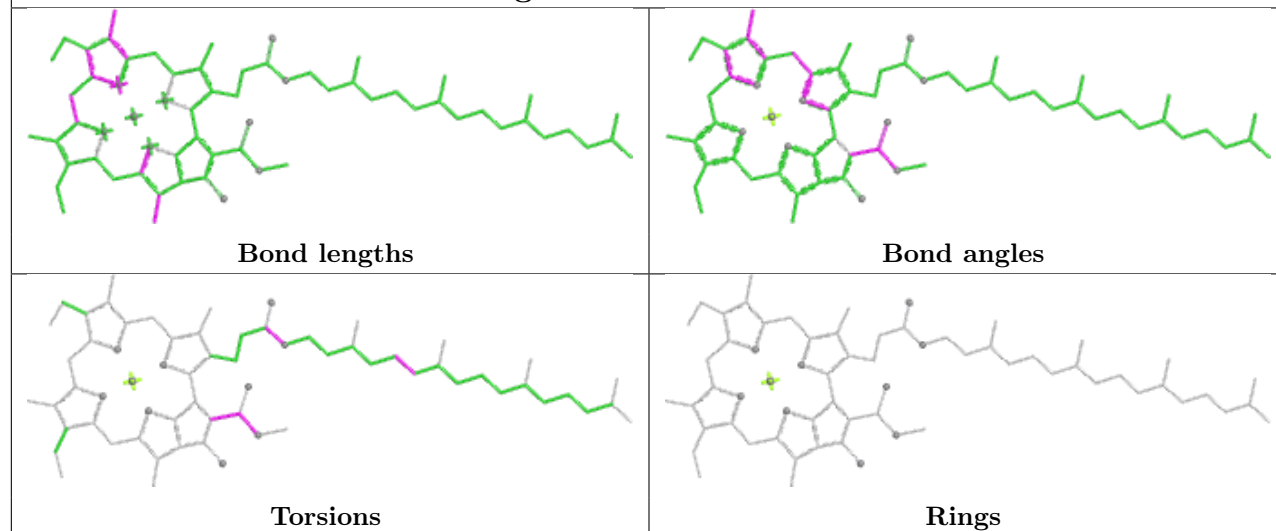


Ligand CLA c5 504	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR c4 524	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR i 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

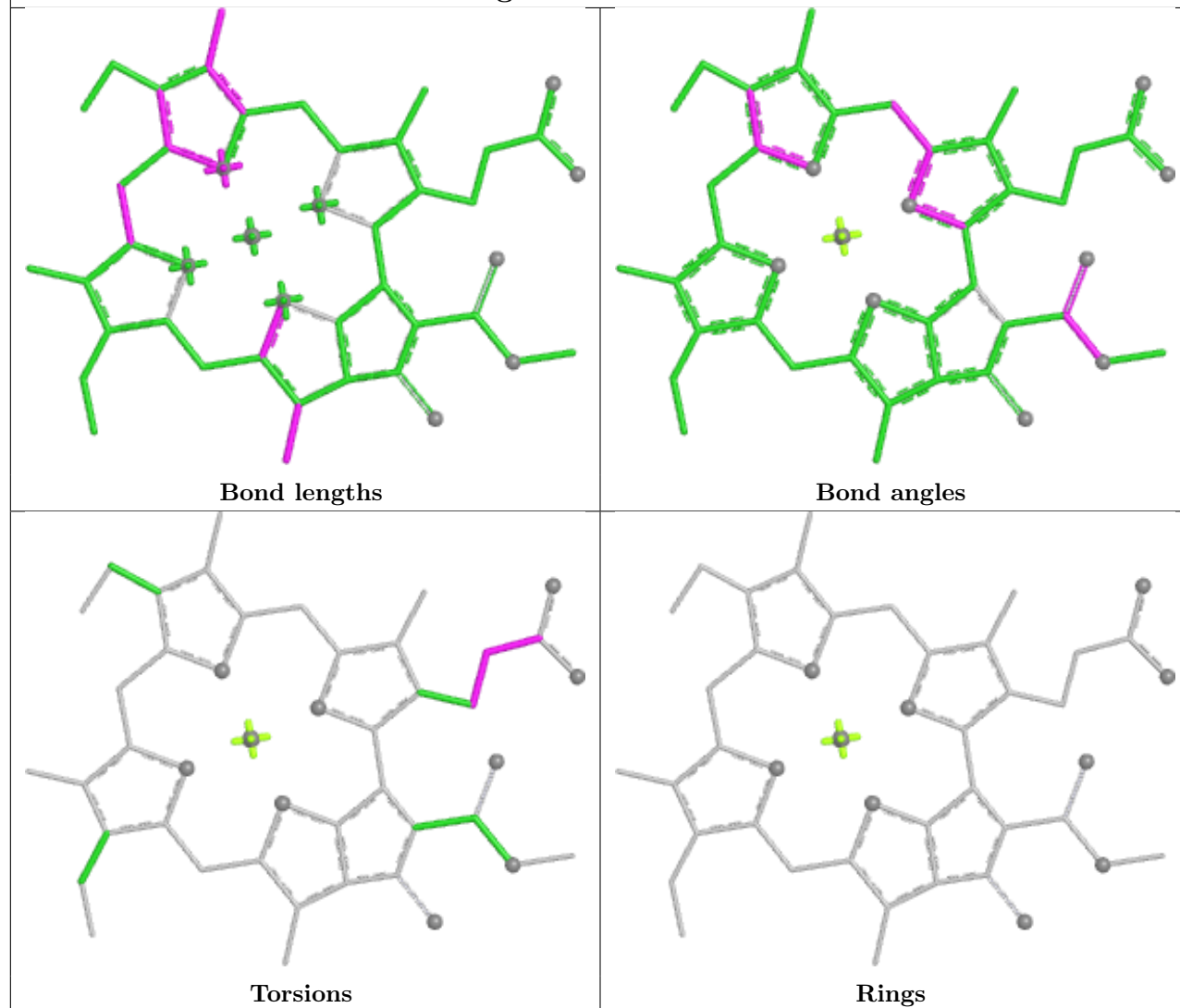




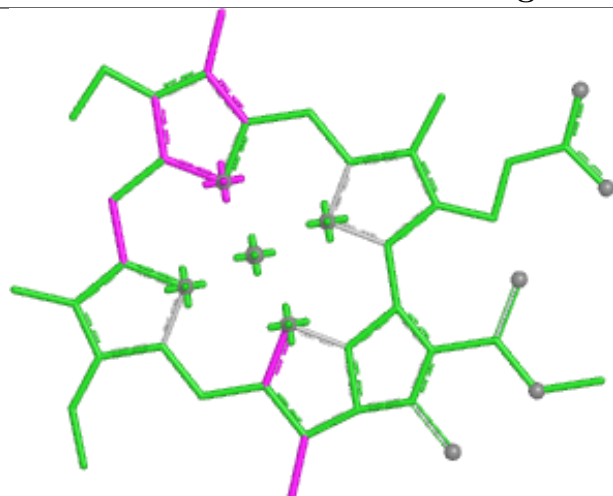
Ligand CLA cA 1128



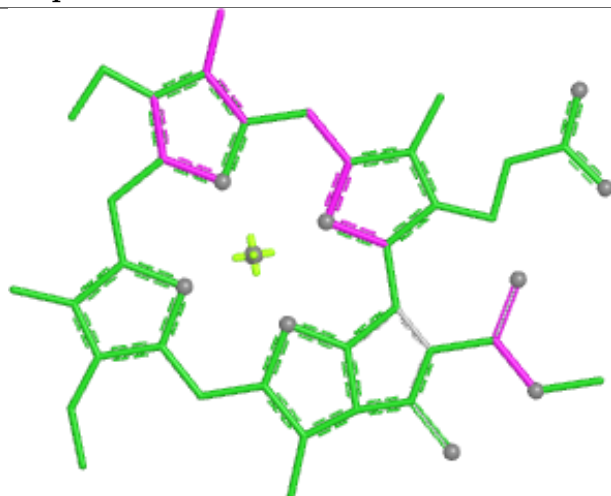
Ligand CLA e 511



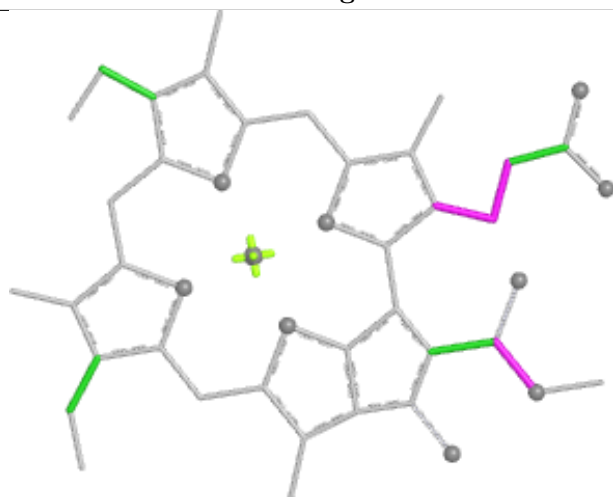
Ligand CLA p 508



Bond lengths



Bond angles

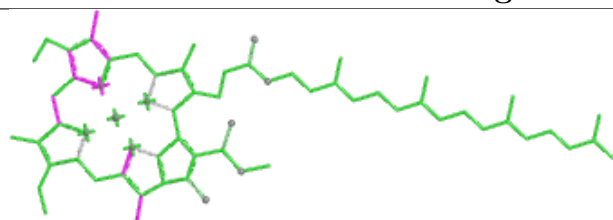


Torsions

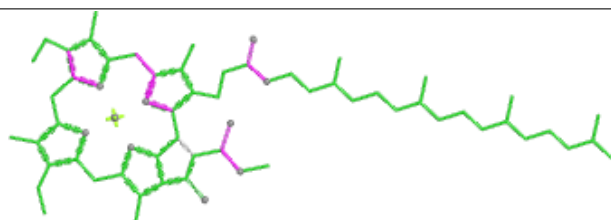


Rings

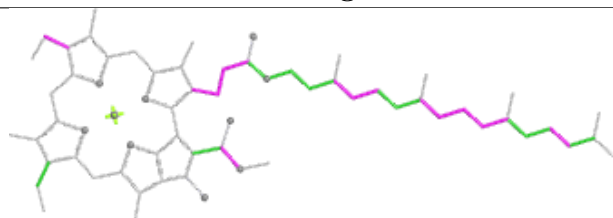
Ligand CLA bA 1140



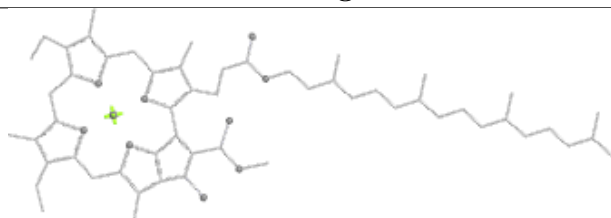
Bond lengths



Bond angles

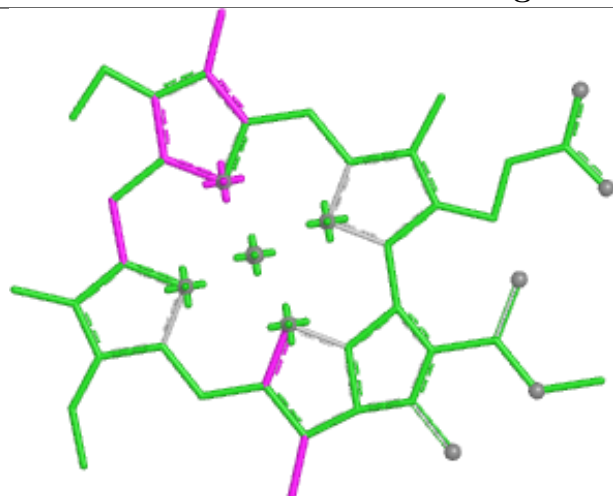


Torsions



Rings

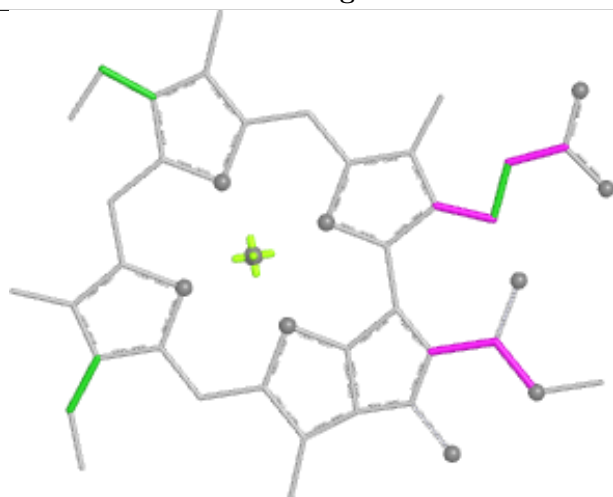
Ligand CLA X 512



Bond lengths



Bond angles

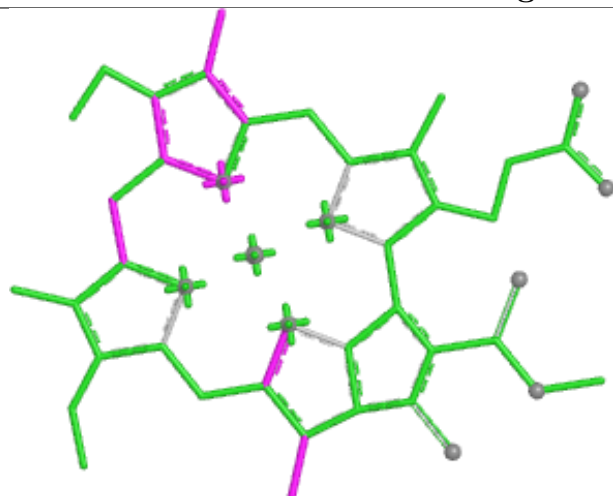


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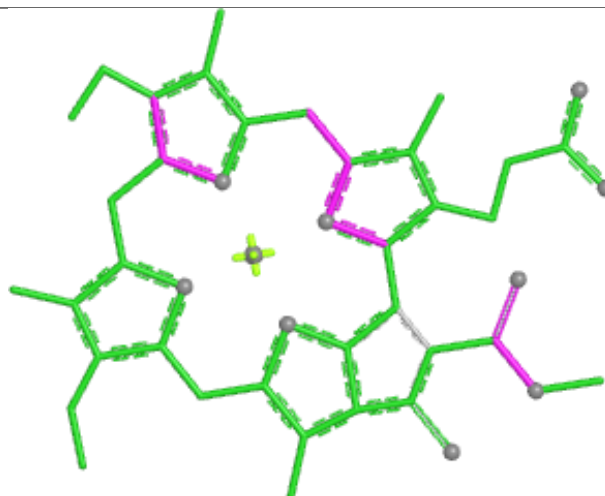


Rings

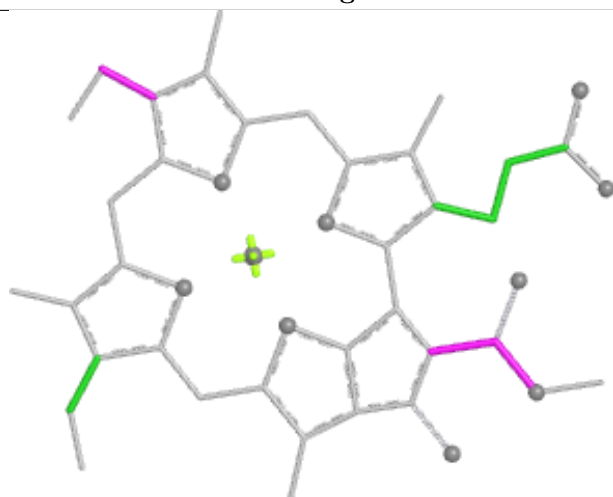
Ligand CLA d 502



Bond lengths



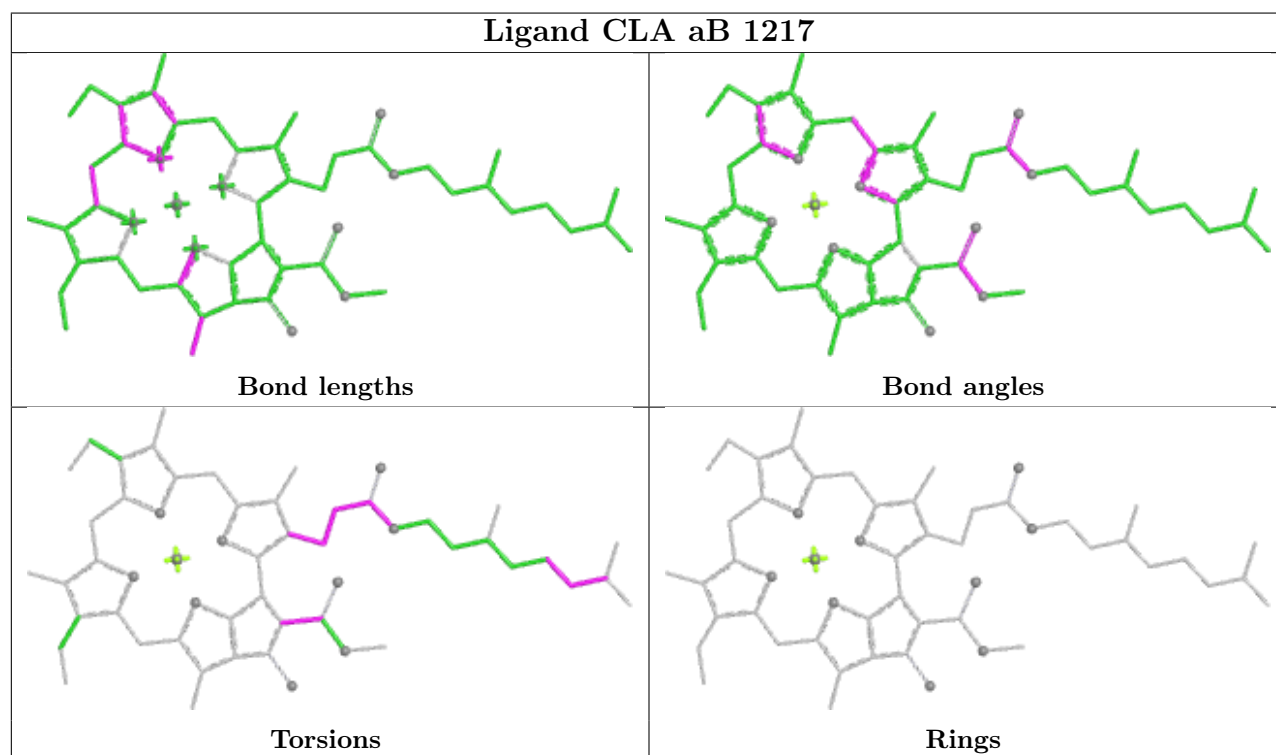
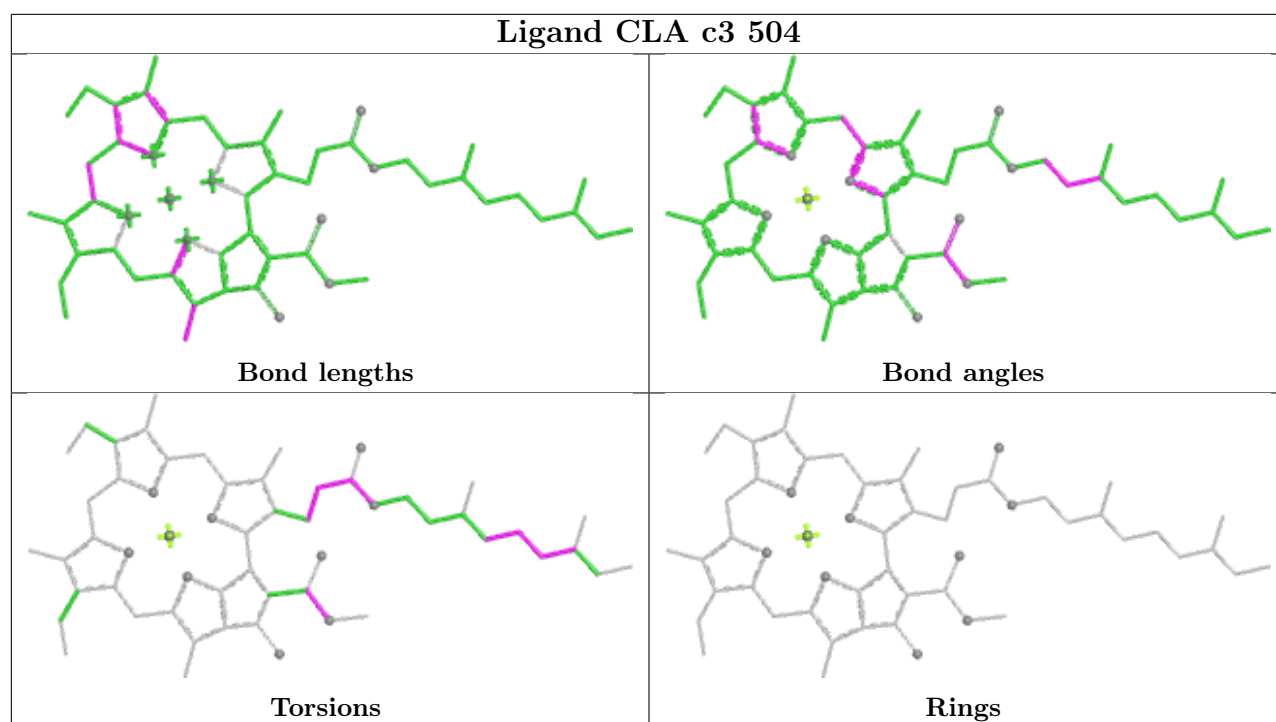
Bond angles

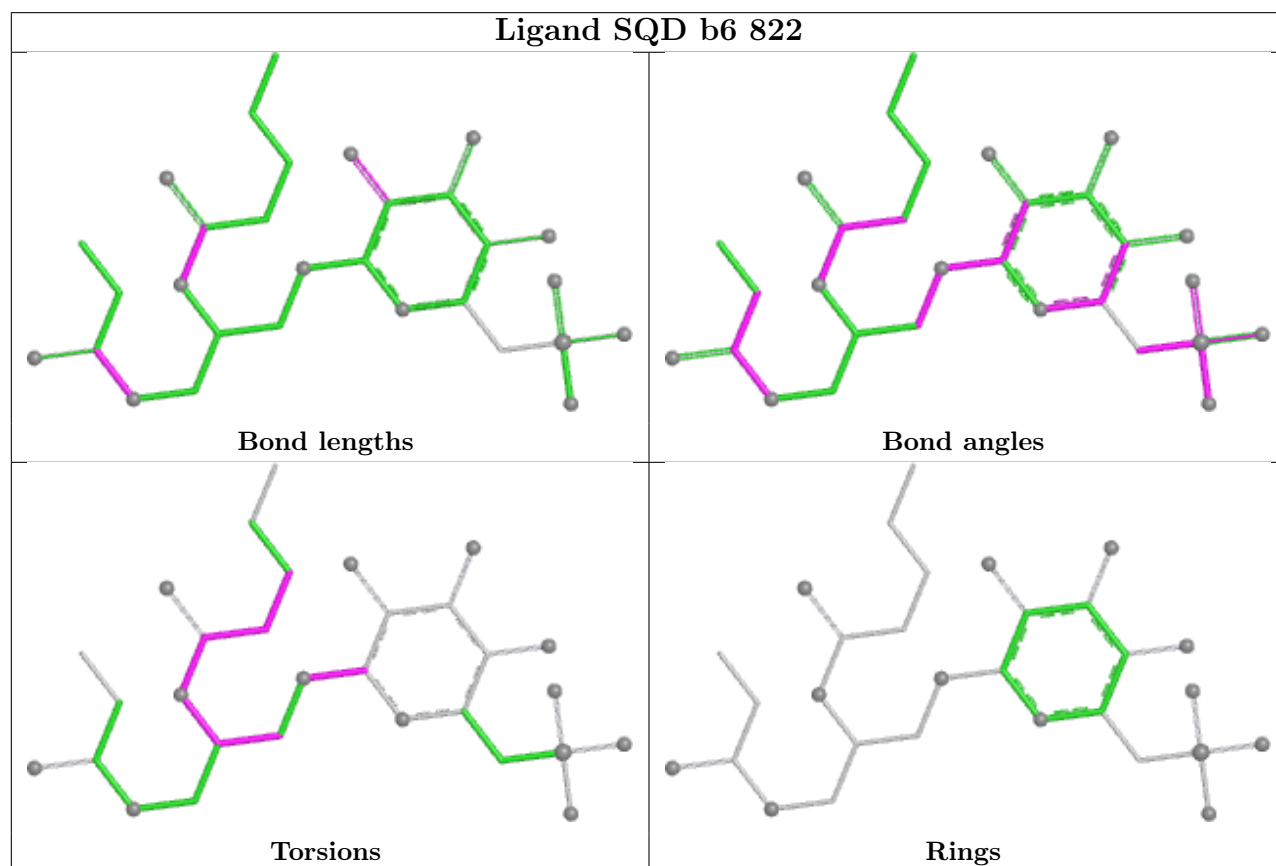
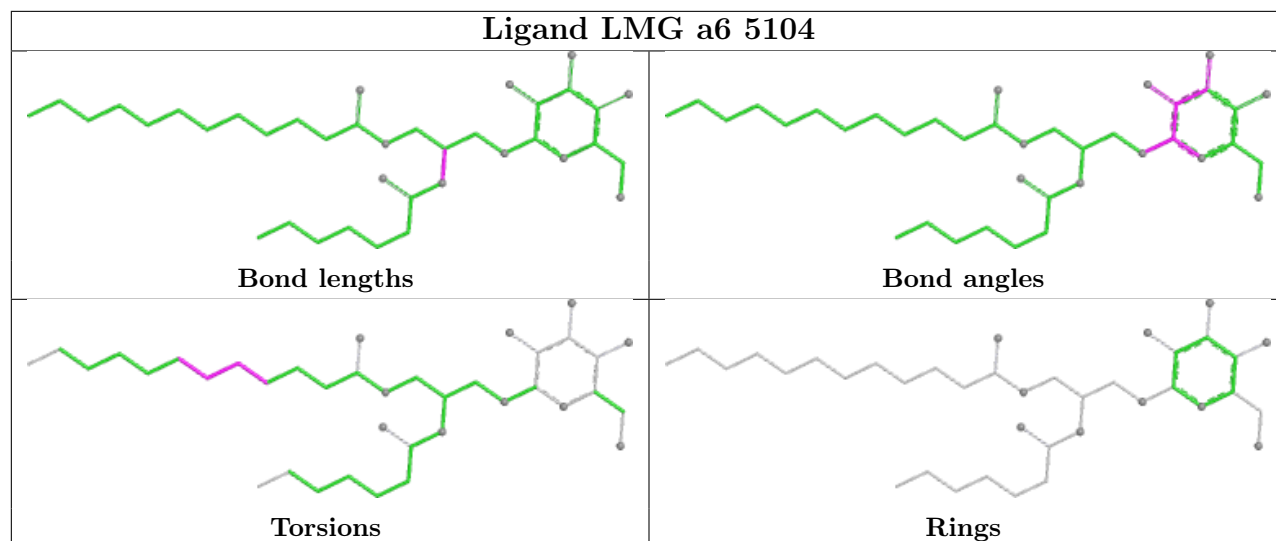


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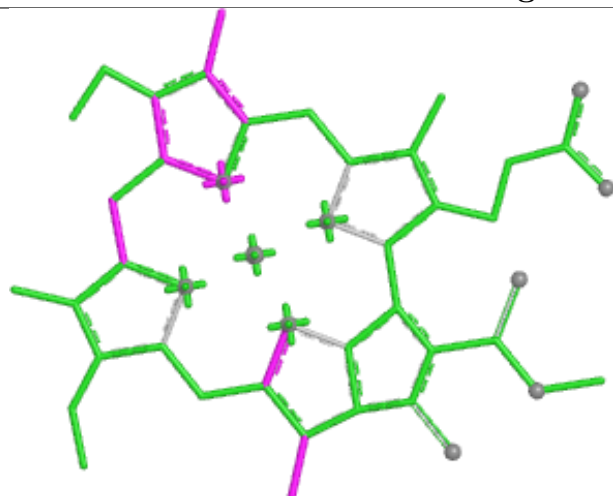


Rings

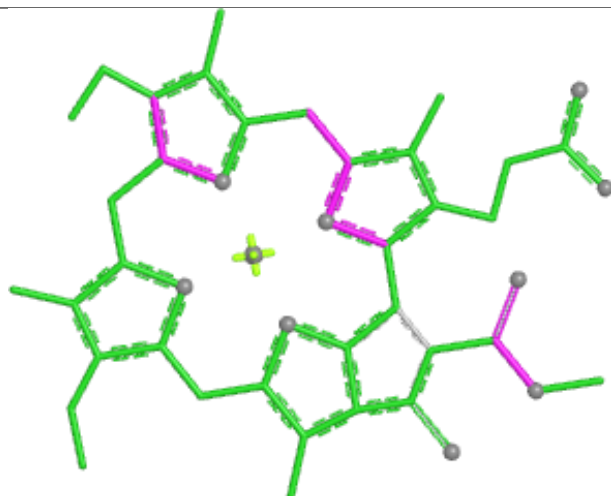




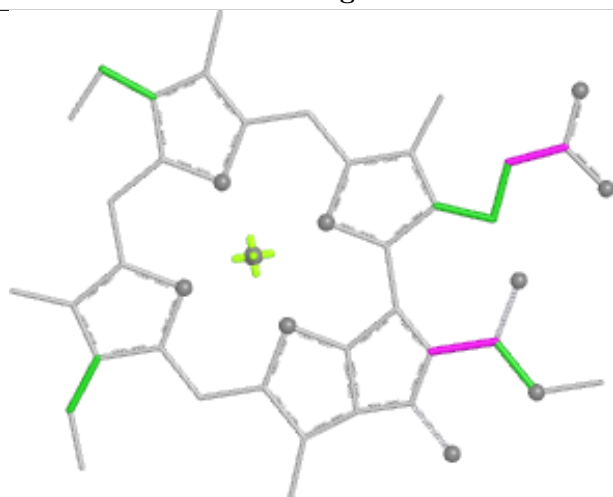
Ligand CLA k 507



Bond lengths



Bond angles

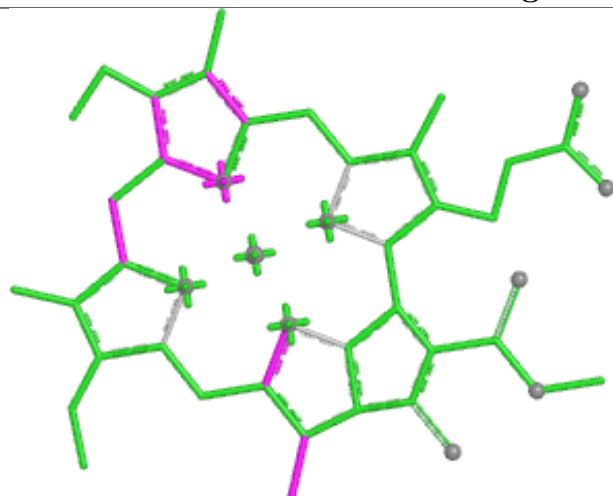


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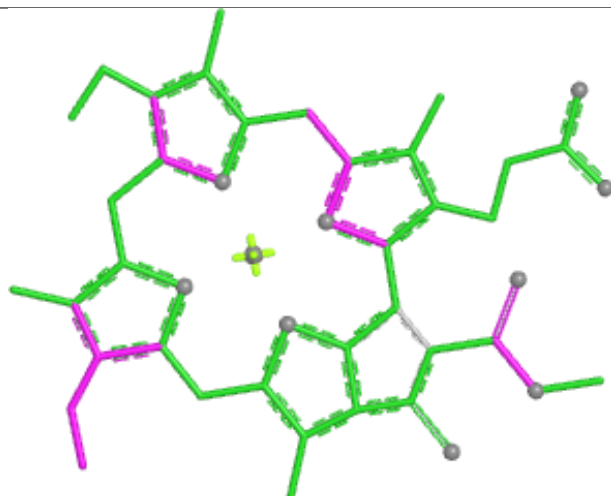


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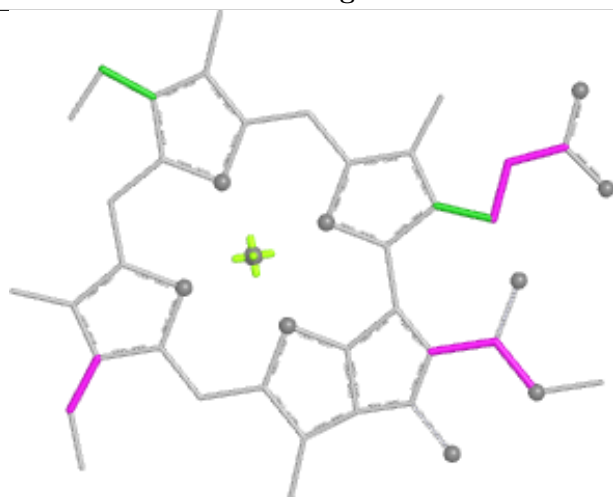
Ligand CLA f 516



Bond lengths



Bond angles

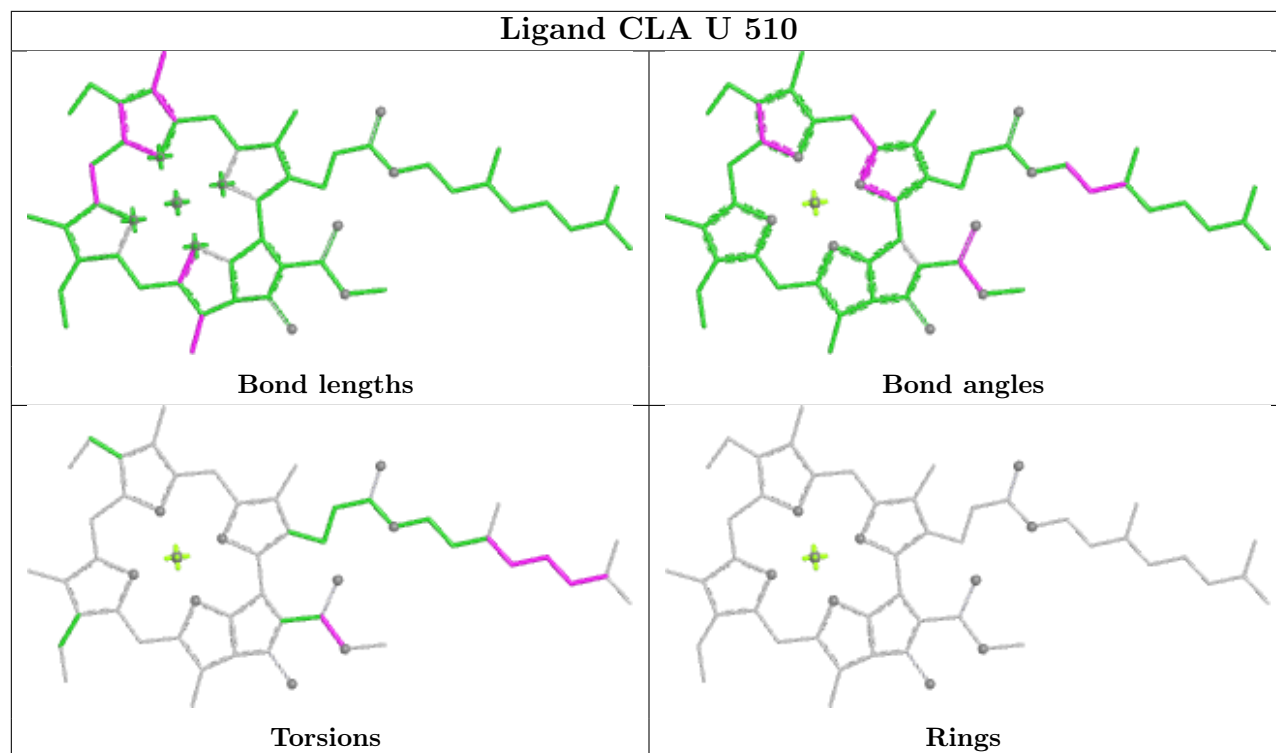


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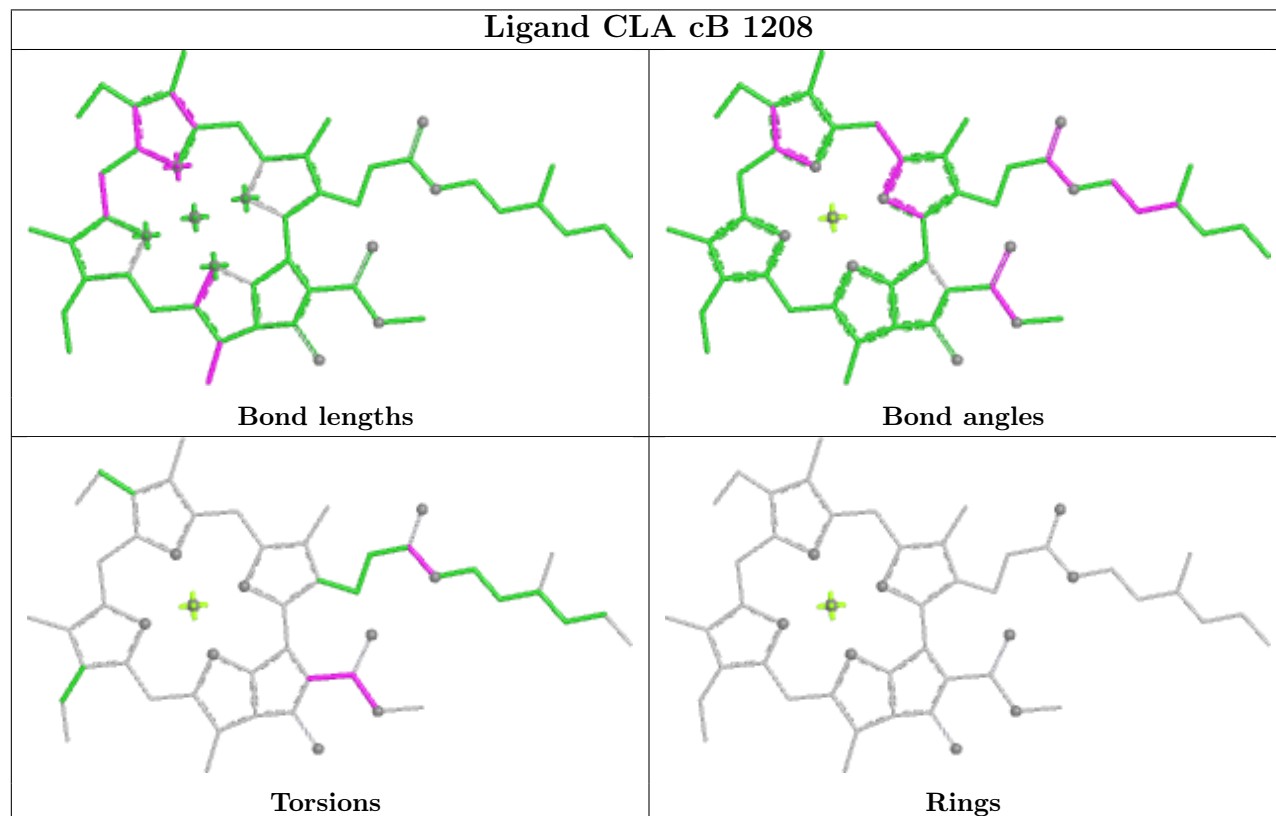


Rings

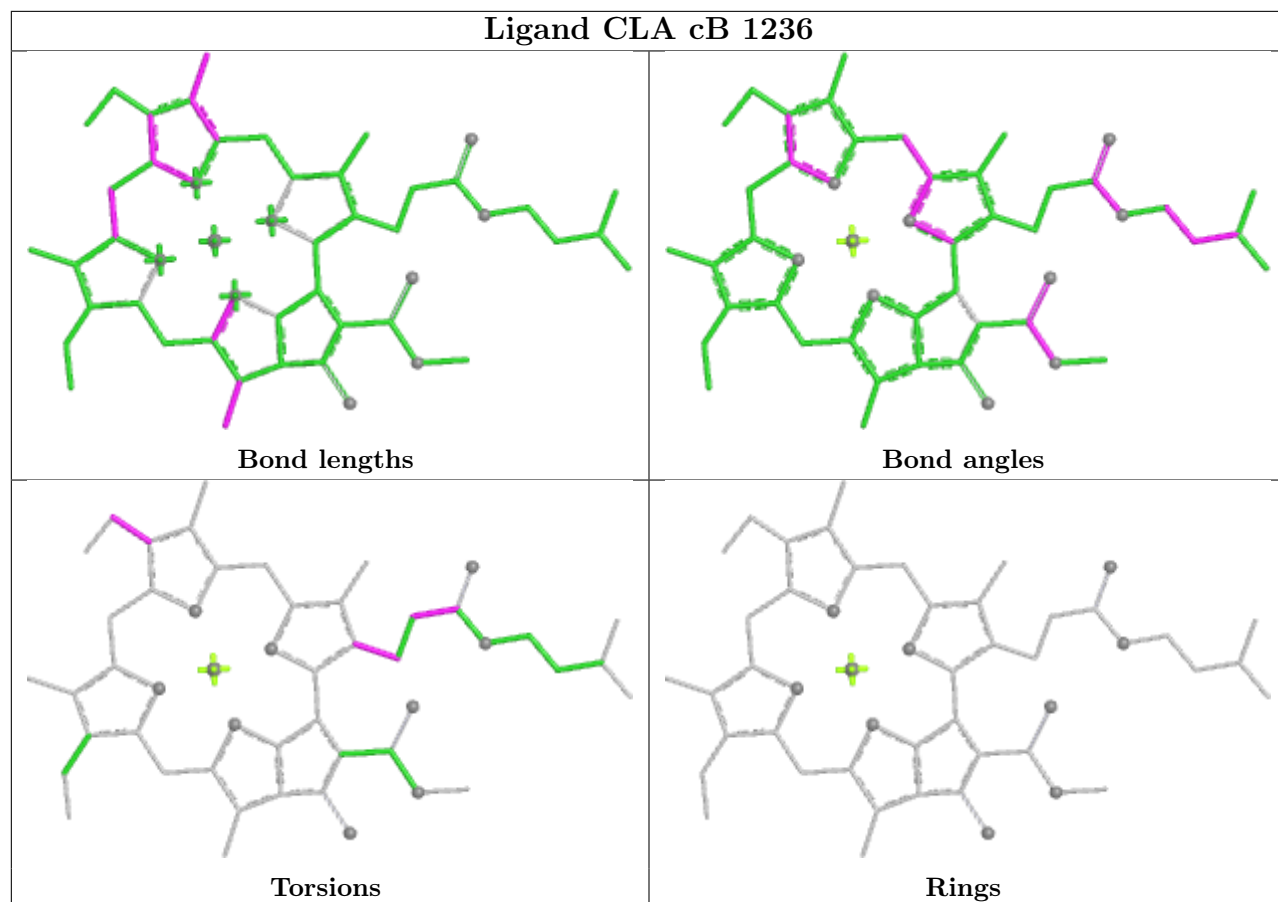
Ligand CLA U 510



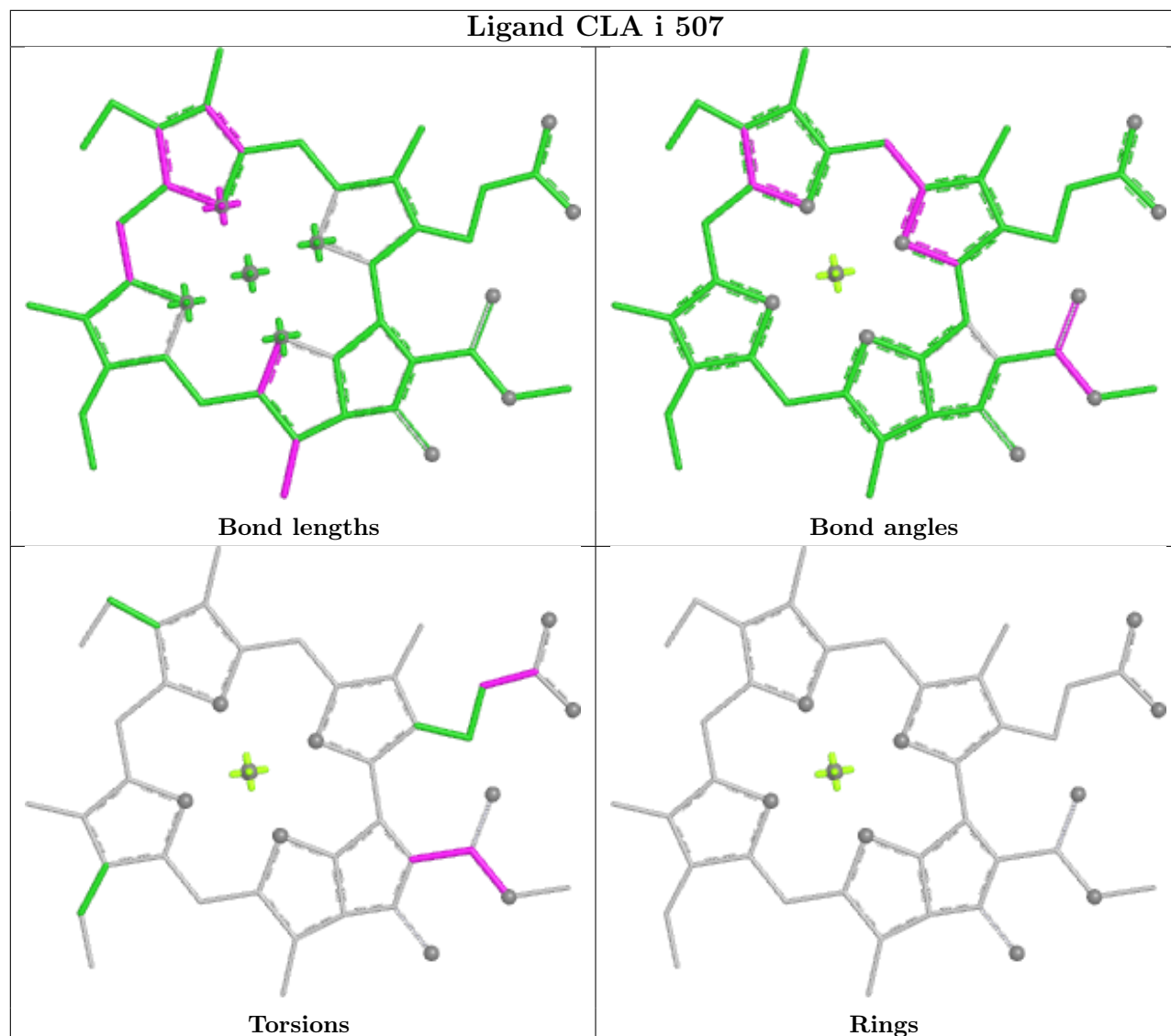
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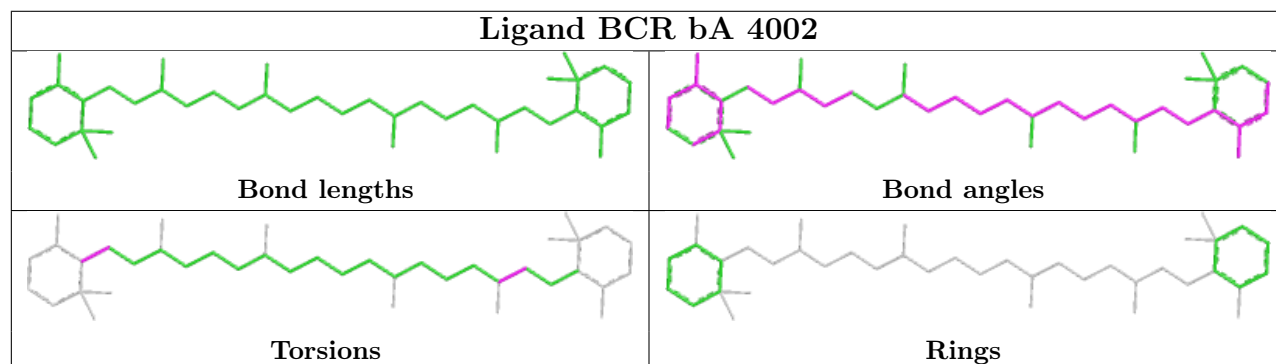
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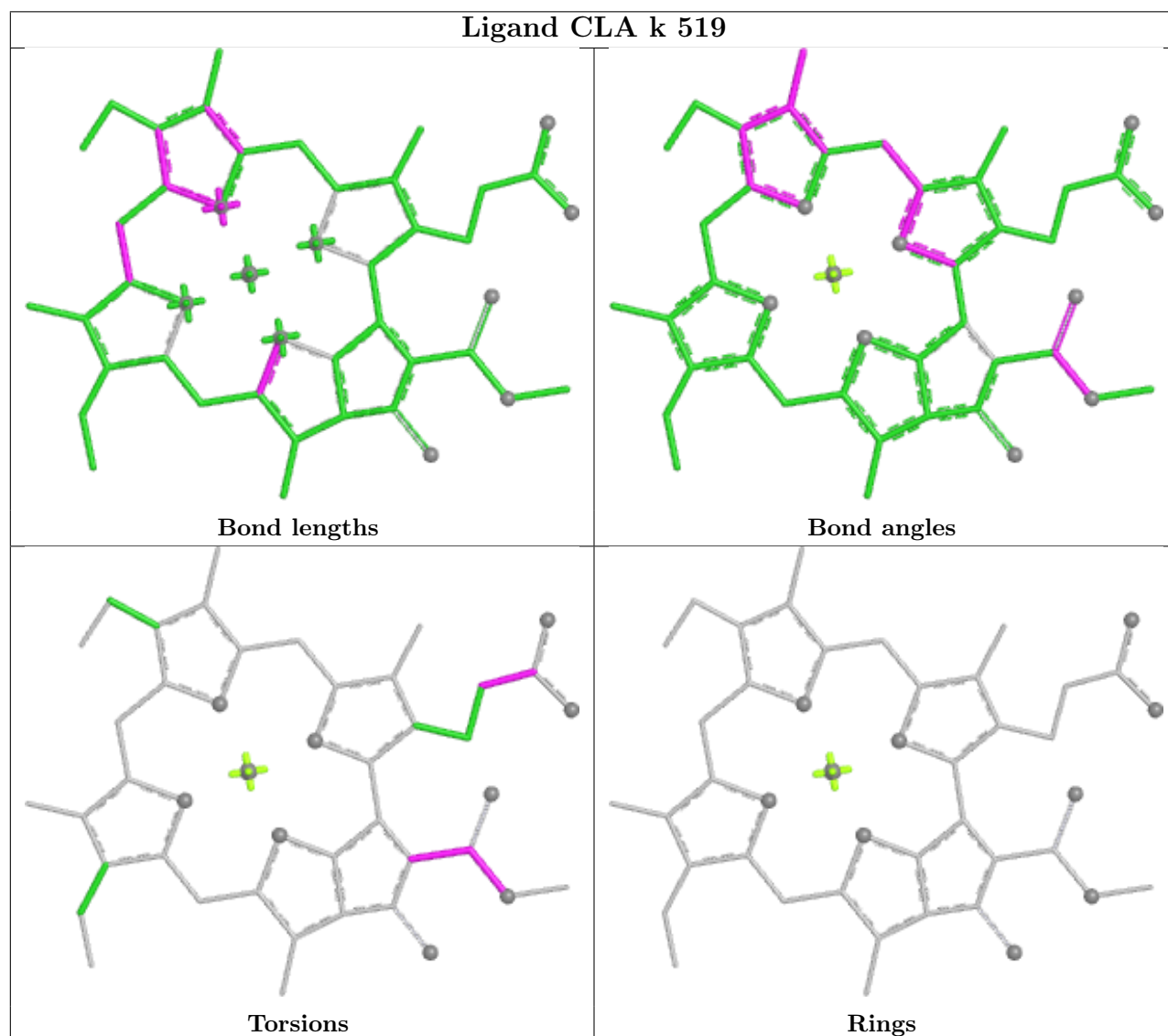
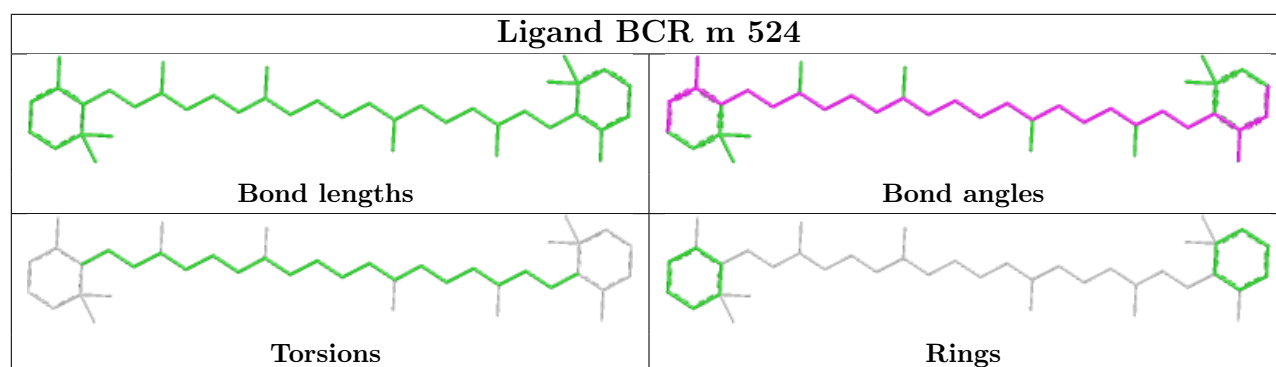


Ligand CLA i 507

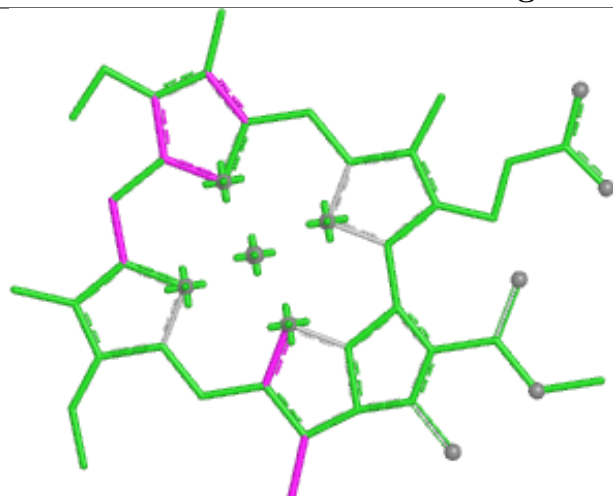


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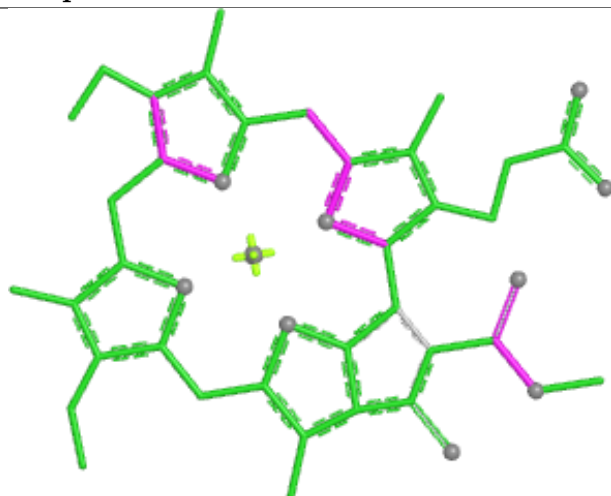




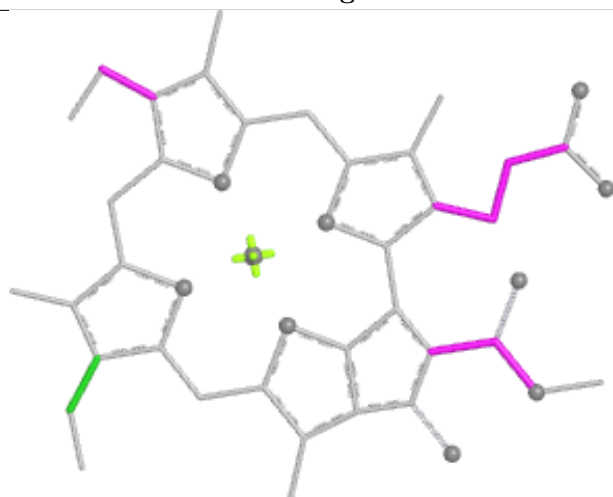
Ligand CLA q 519



Bond lengths



Bond angles

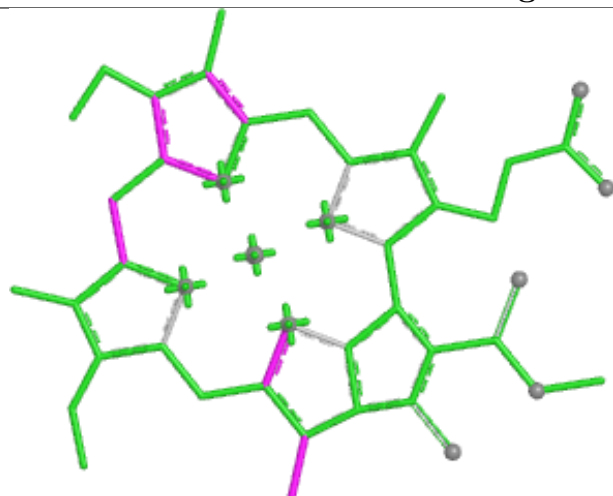


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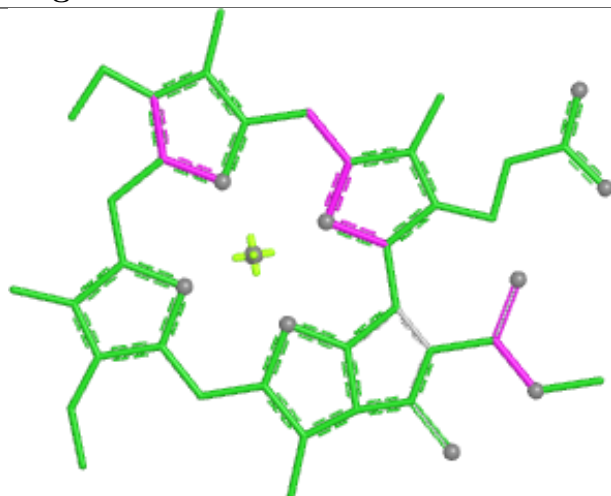


Rings

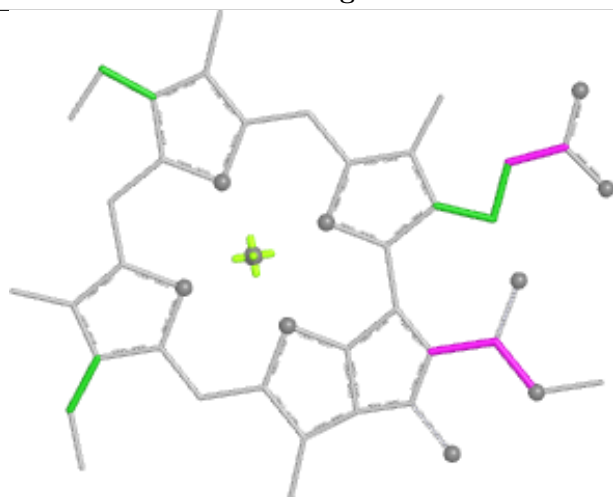
Ligand CLA g 510



Bond lengths



Bond angles

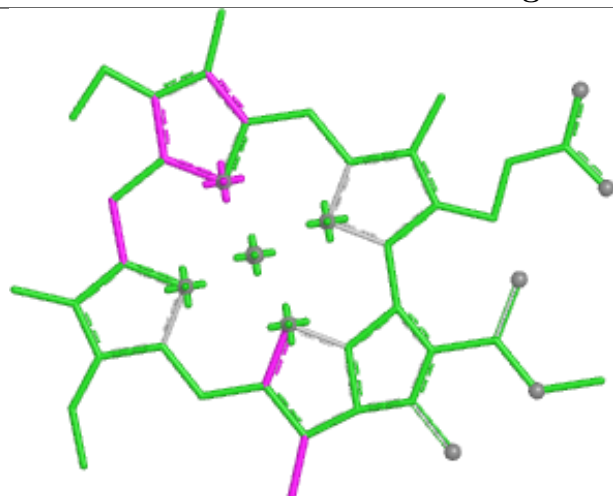


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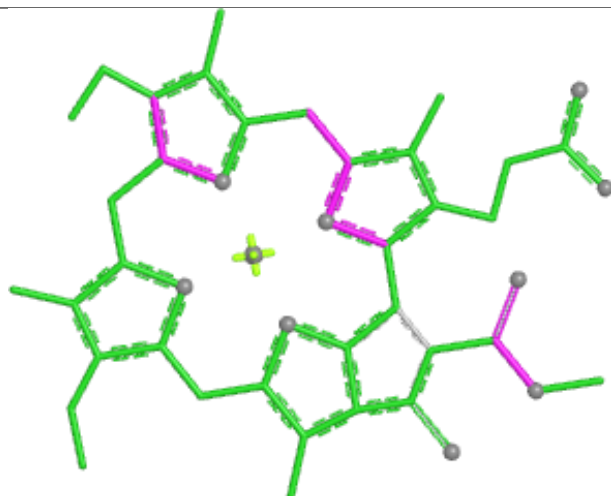


Rings

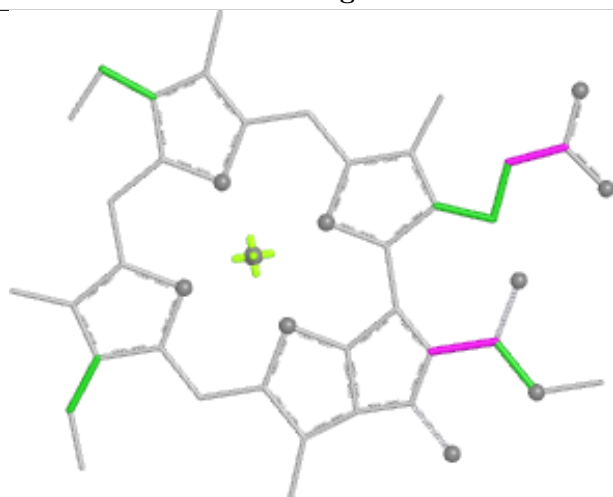
Ligand CLA i 519



Bond lengths



Bond angles

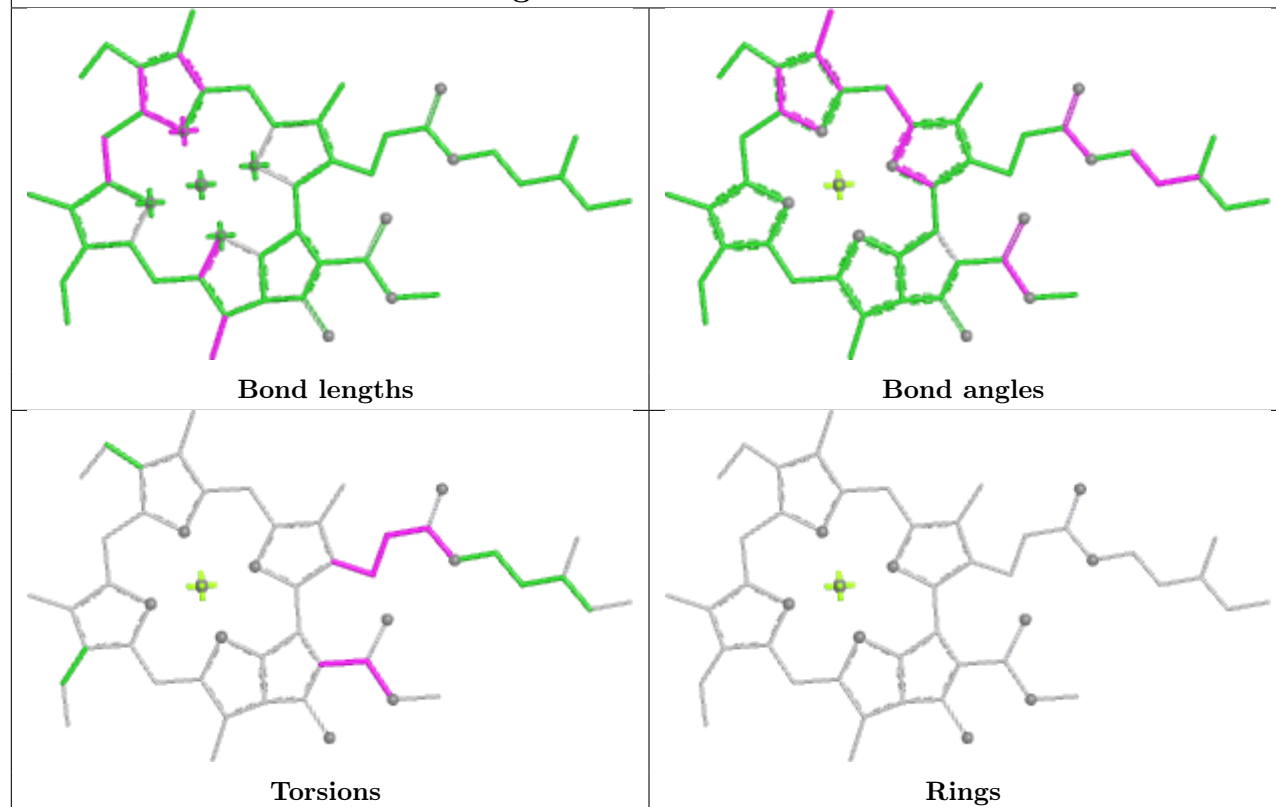


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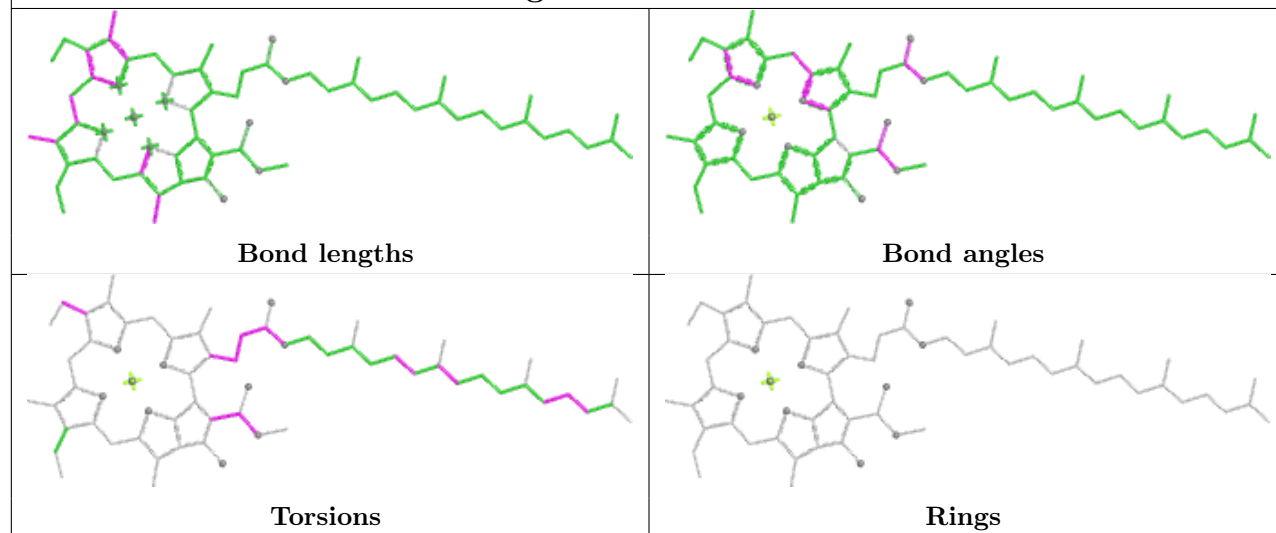


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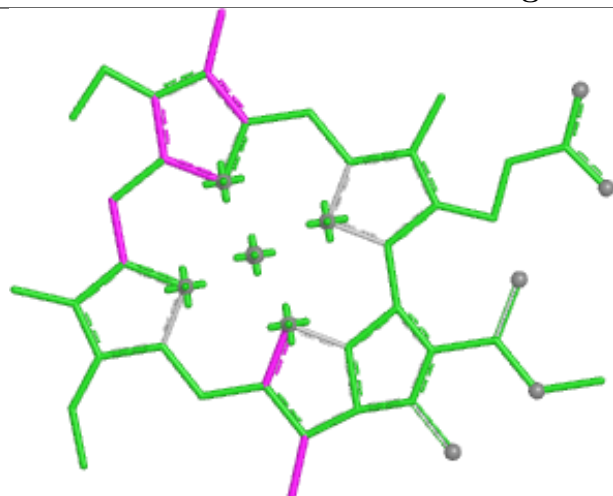
Ligand CLA bA 1135



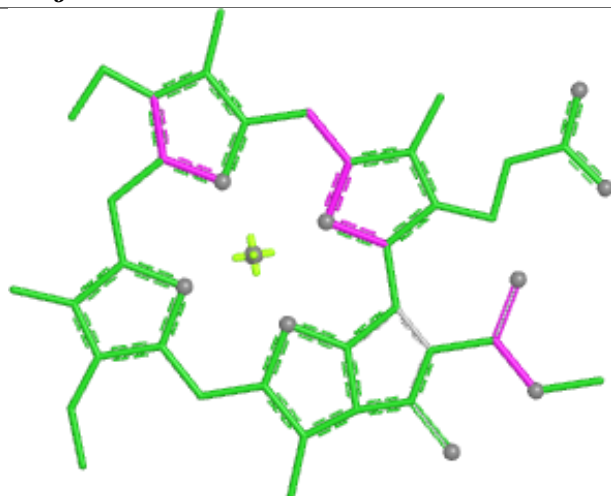
Ligand CLA b1 501



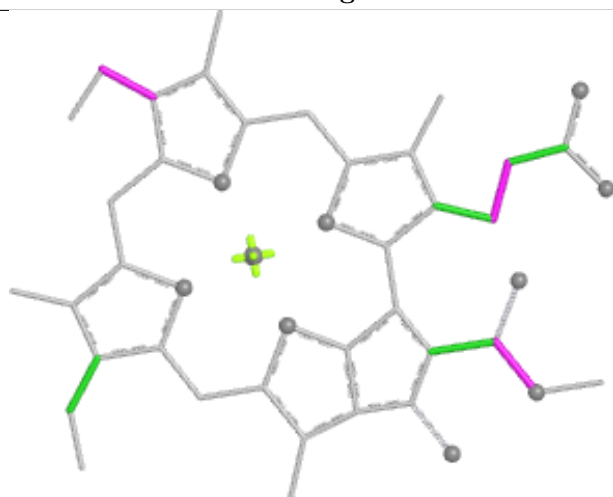
Ligand CLA j 519



Bond lengths



Bond angles

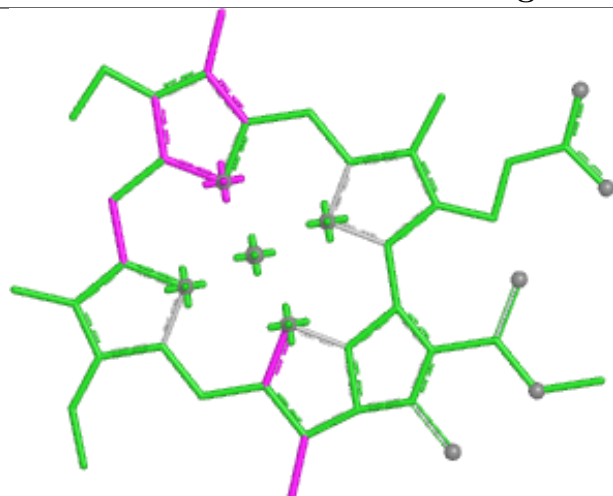


Torsions



Rings

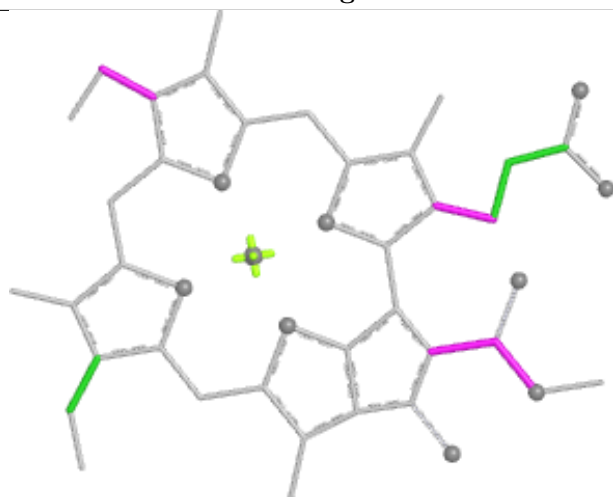
Ligand CLA S 517



Bond lengths



Bond angles

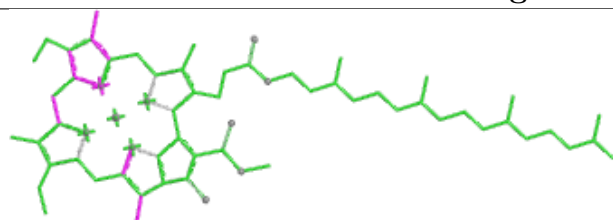


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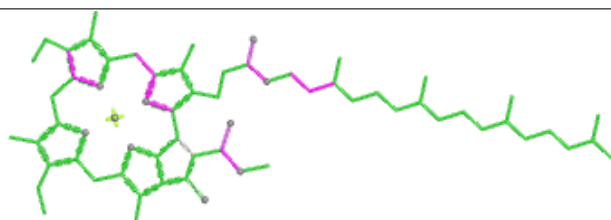


Rings

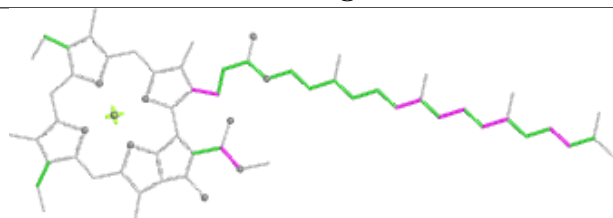
Ligand CLA a6 509



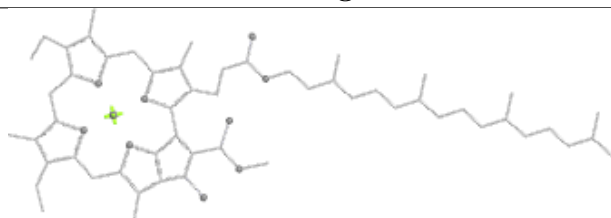
Bond lengths



Bond angles

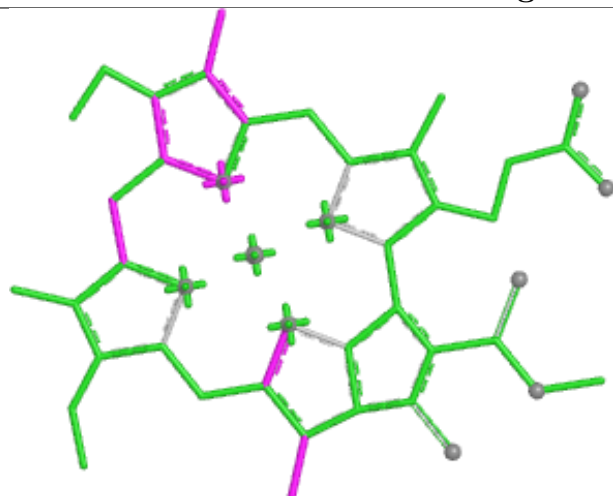


Torsions



Rings

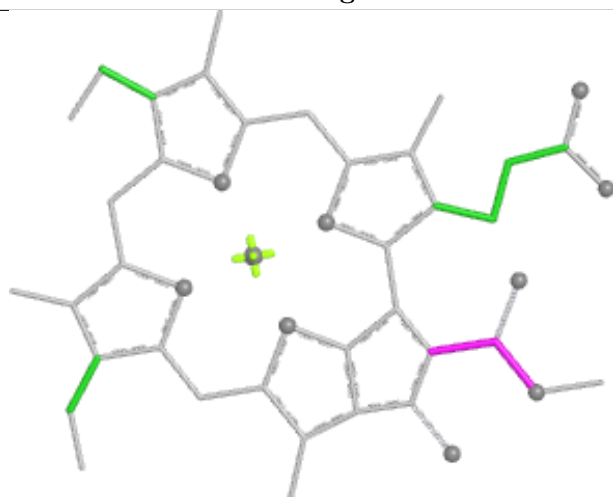
Ligand CLA h 502



Bond lengths



Bond angles

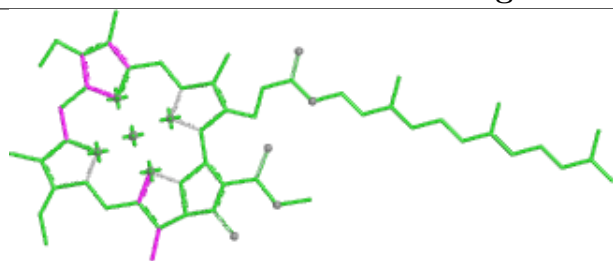


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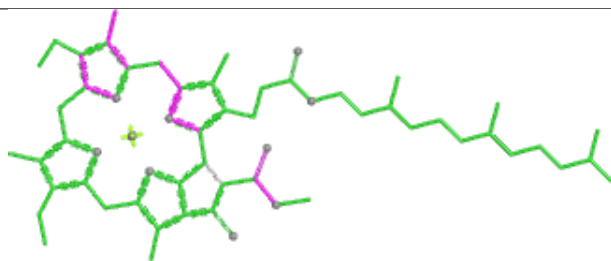


Rings

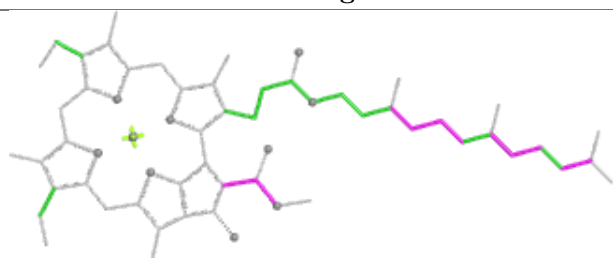
Ligand CLA bB 1221



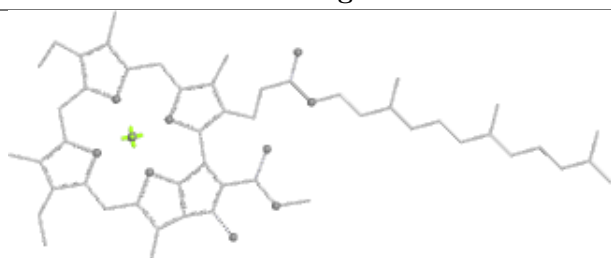
Bond lengths



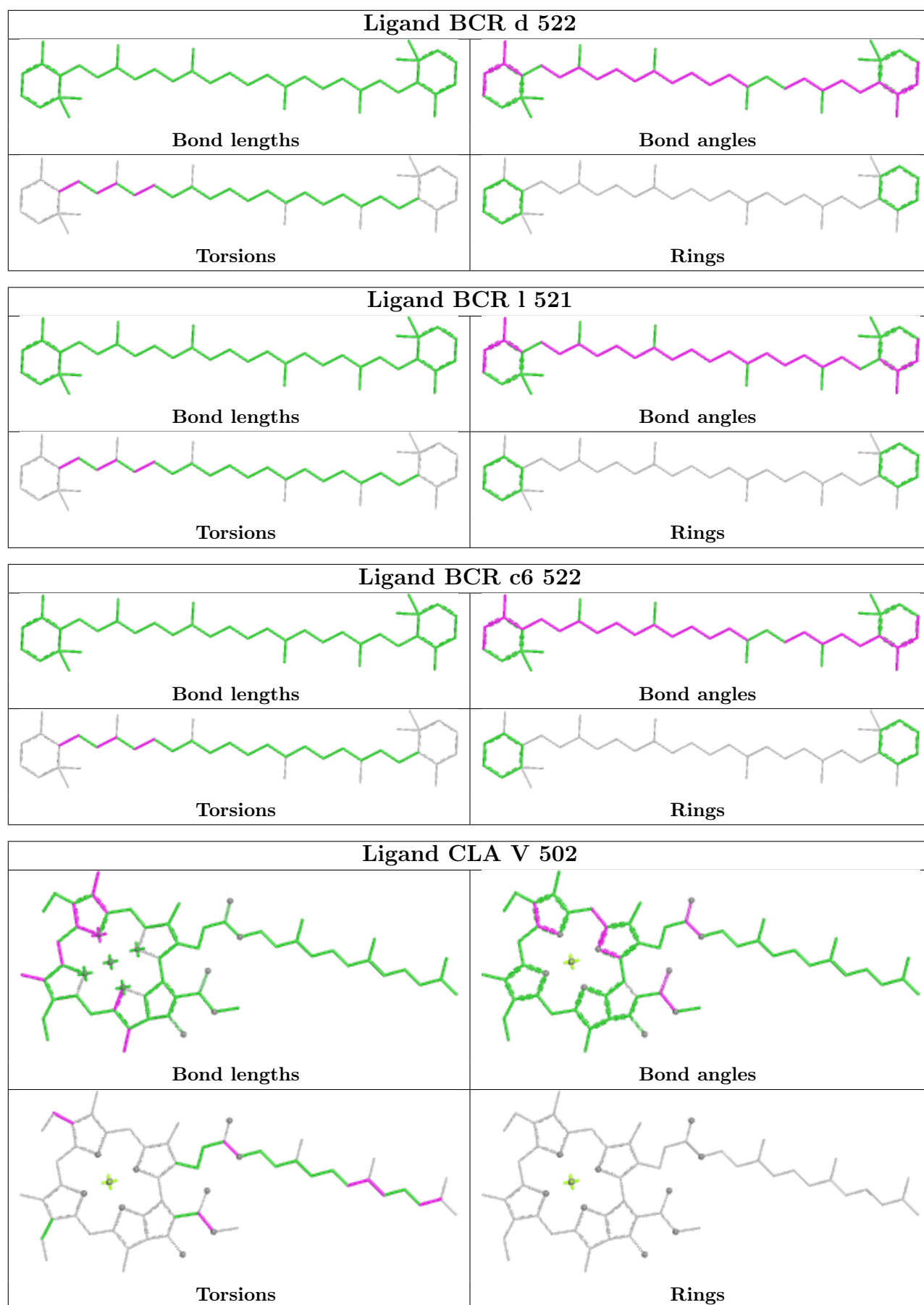
Bond angles

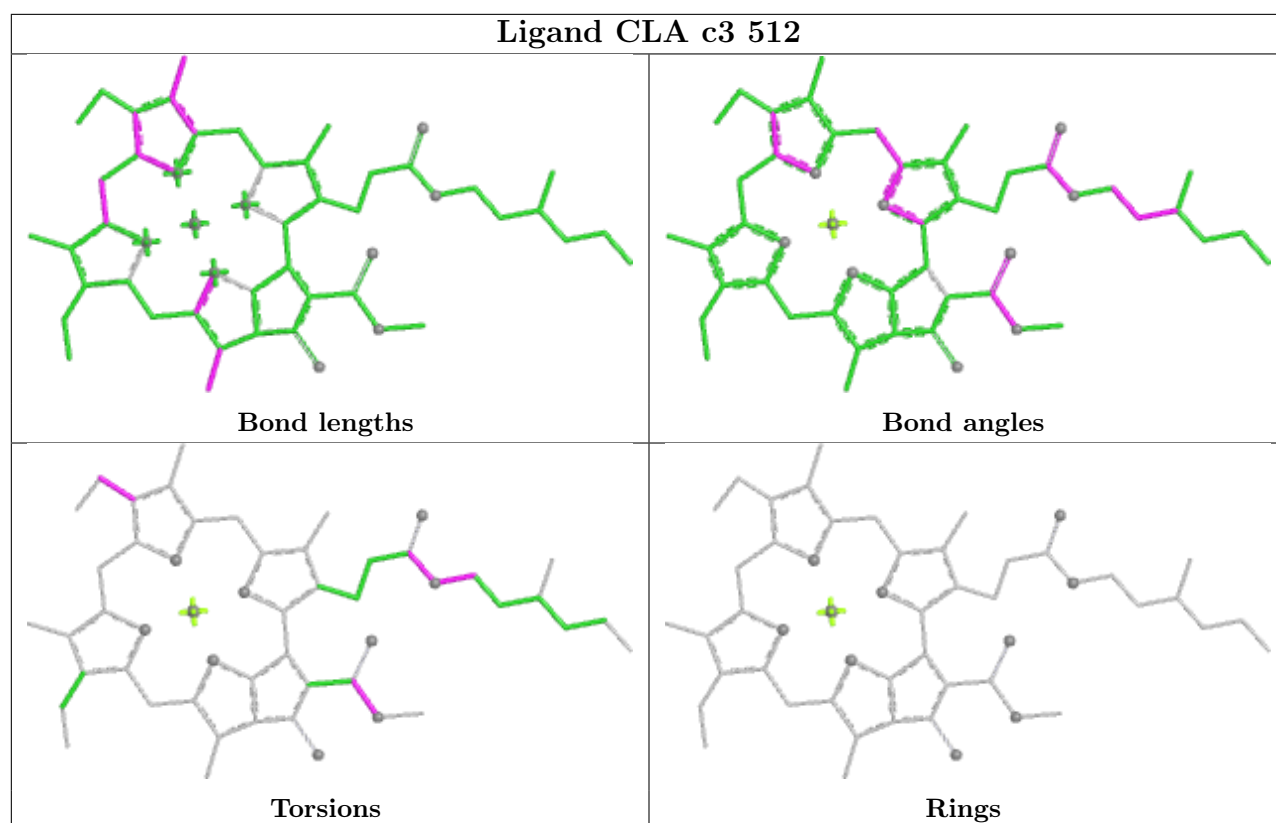


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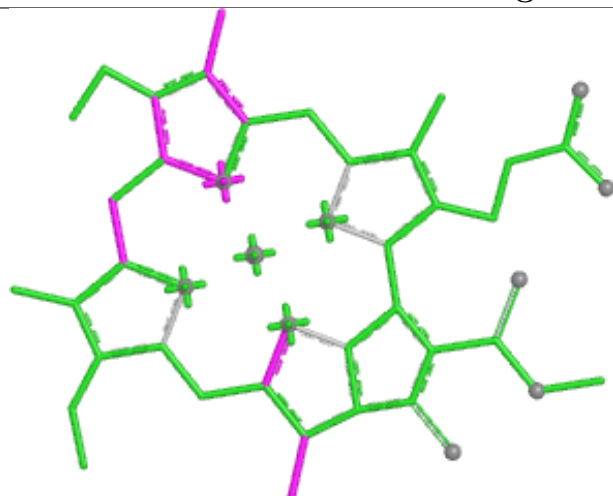


Rings





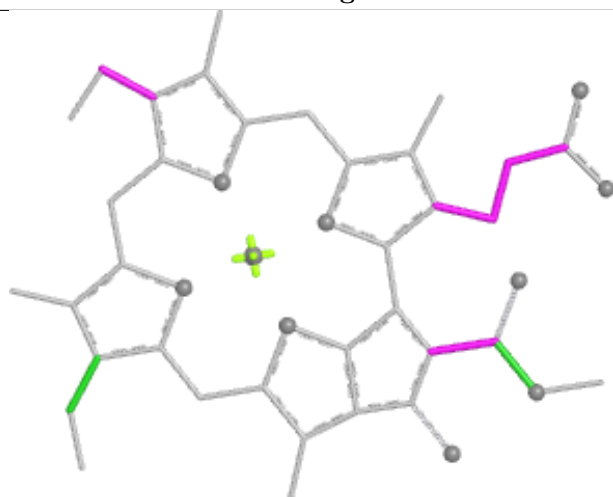
Ligand CLA Z 512



Bond lengths



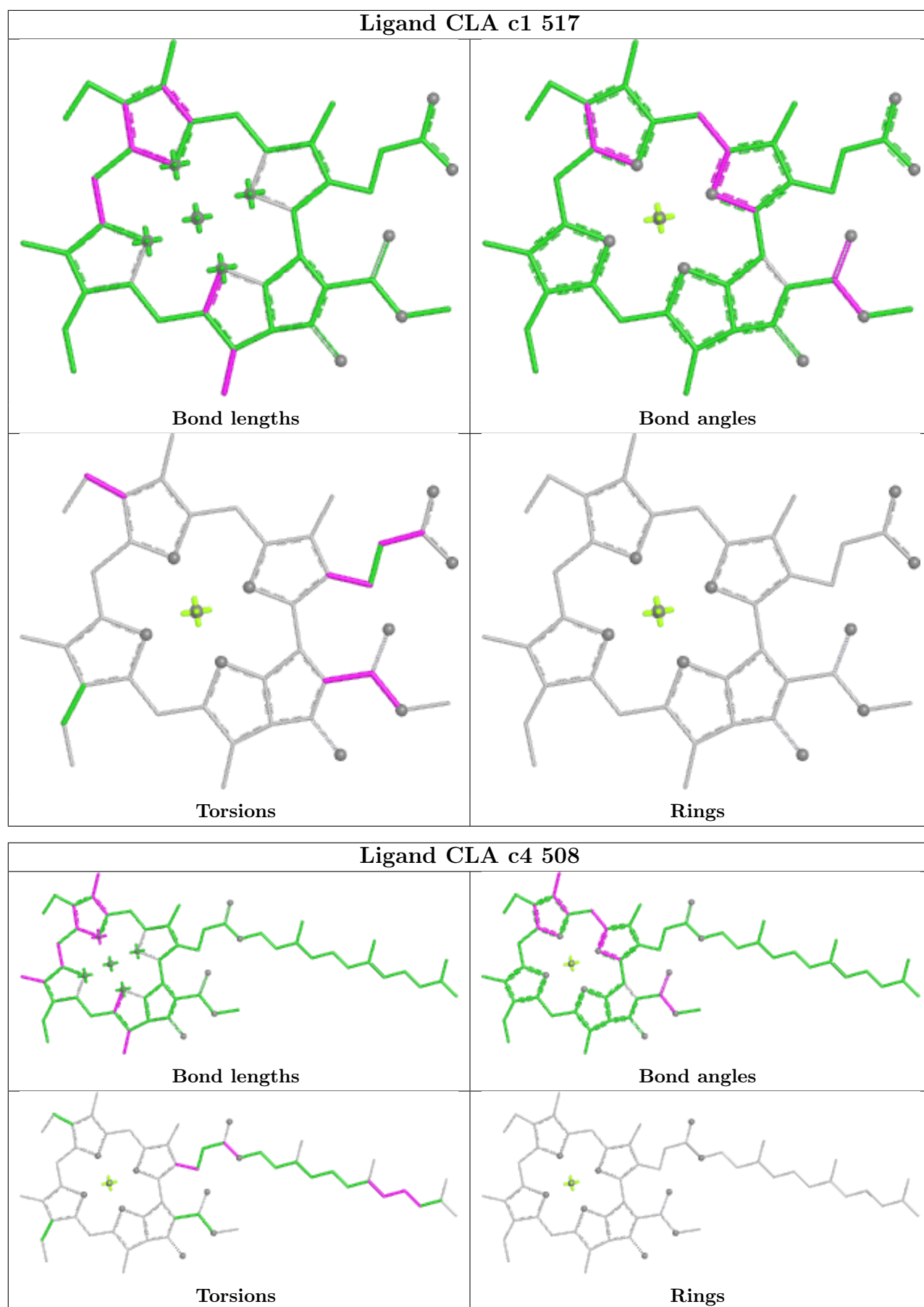
Bond angles



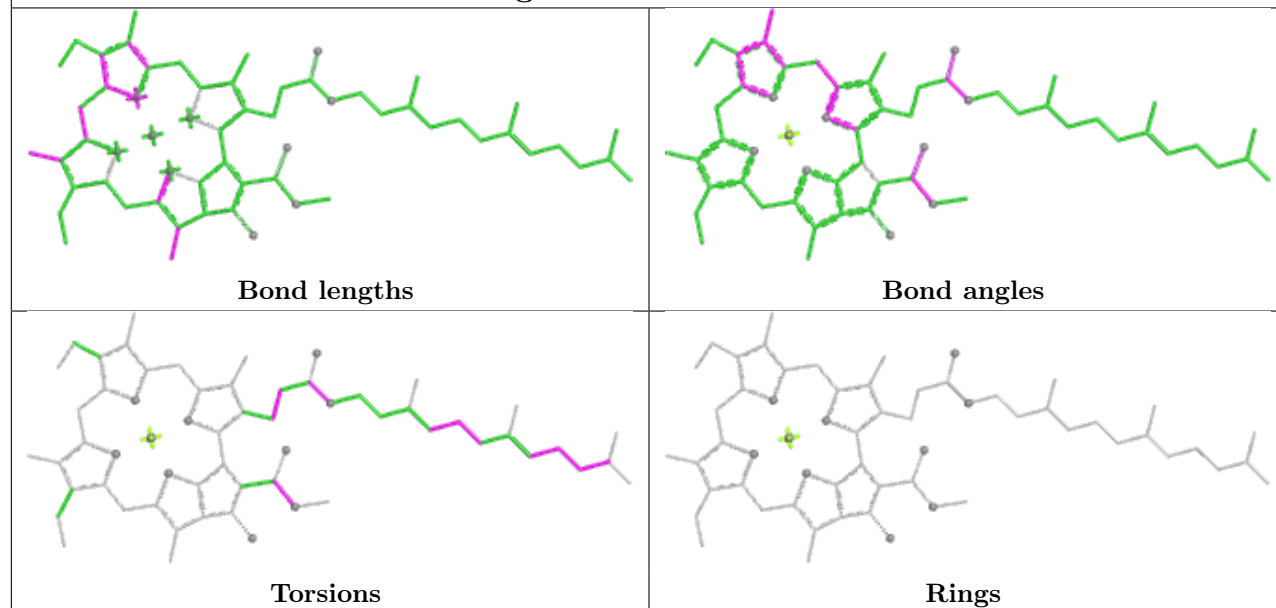
Torsions



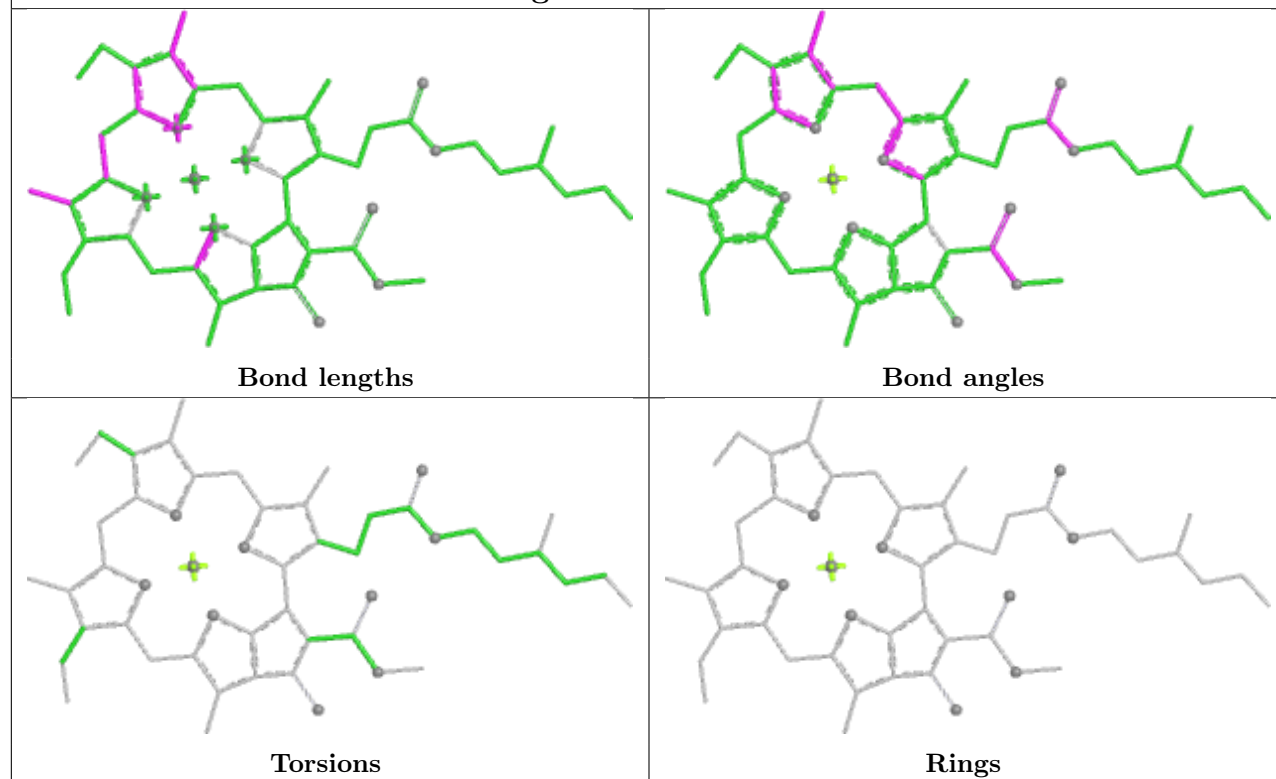
Rings



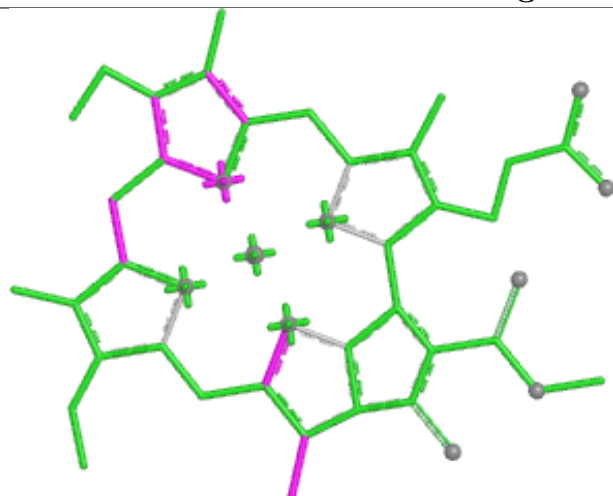
Ligand CLA cB 1214



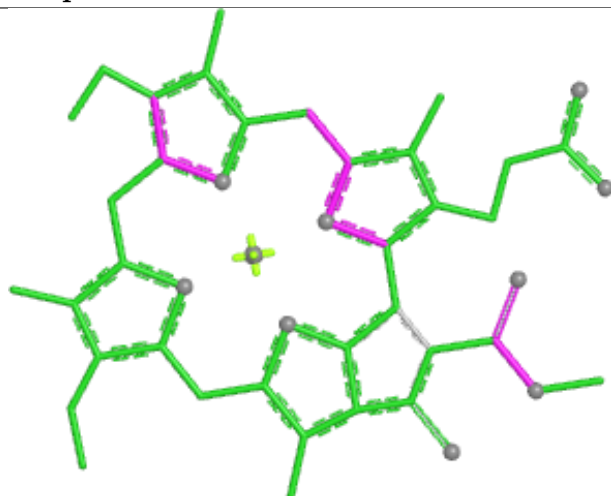
Ligand CLA Y 508



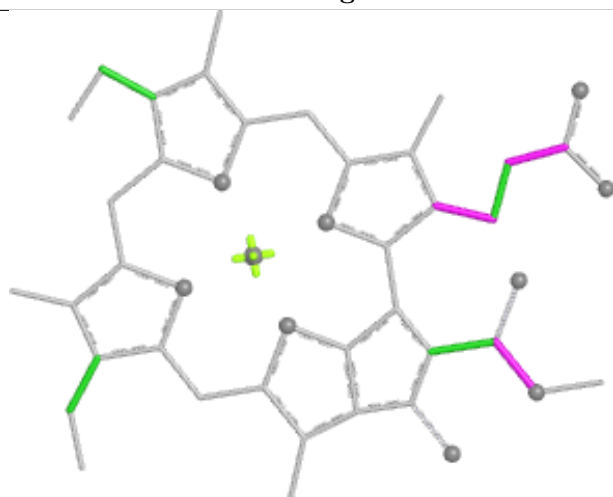
Ligand CLA q 507



Bond lengths



Bond angles

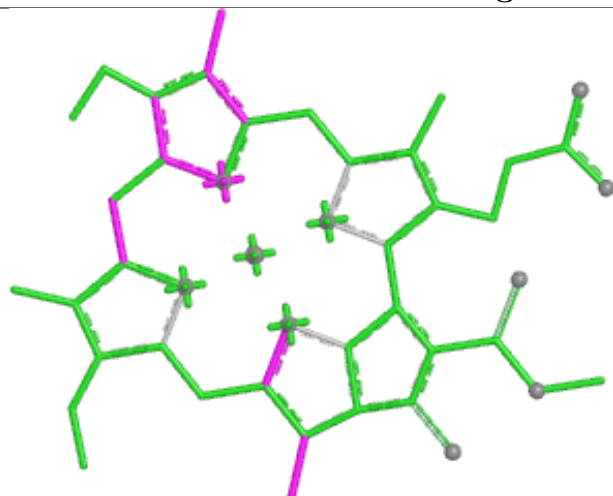


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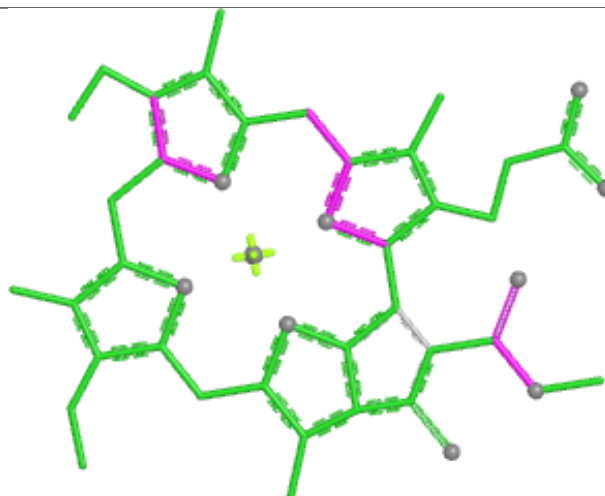


Rings

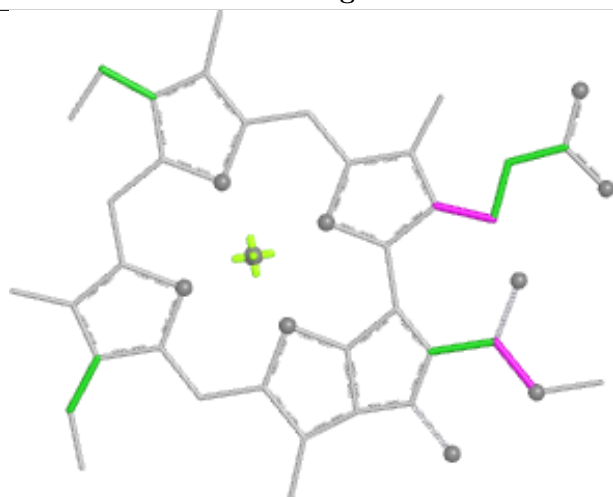
Ligand CLA aA 1108



Bond lengths



Bond angles

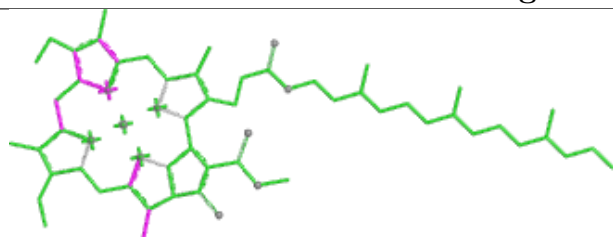


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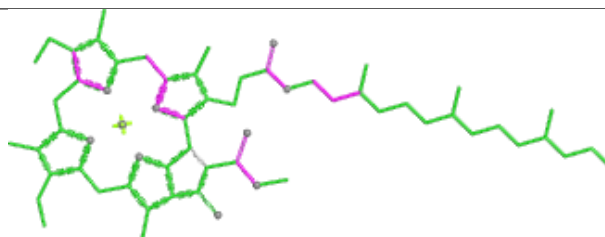


Rings

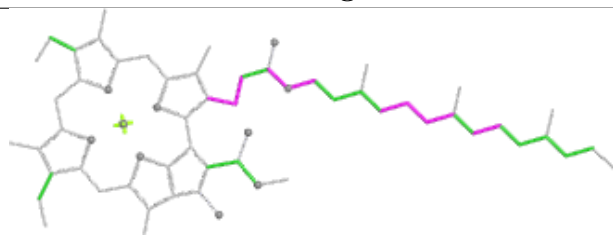
Ligand CLA e 505



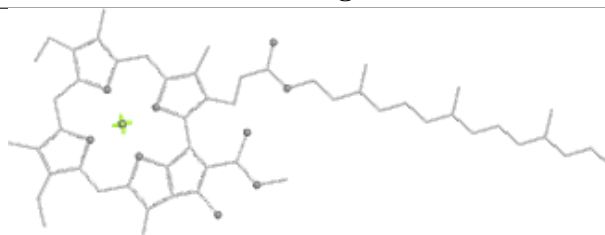
Bond lengths



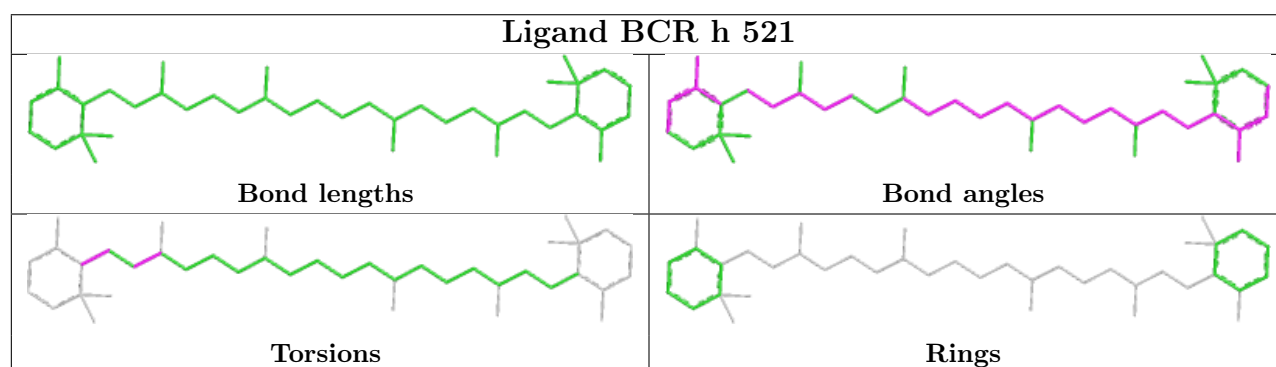
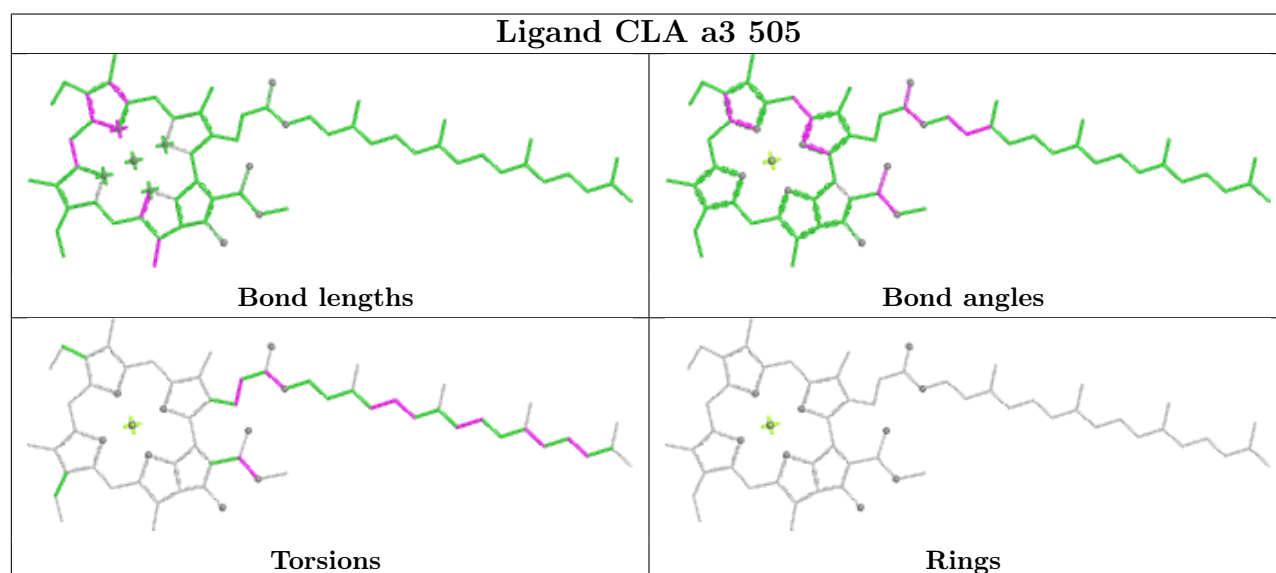
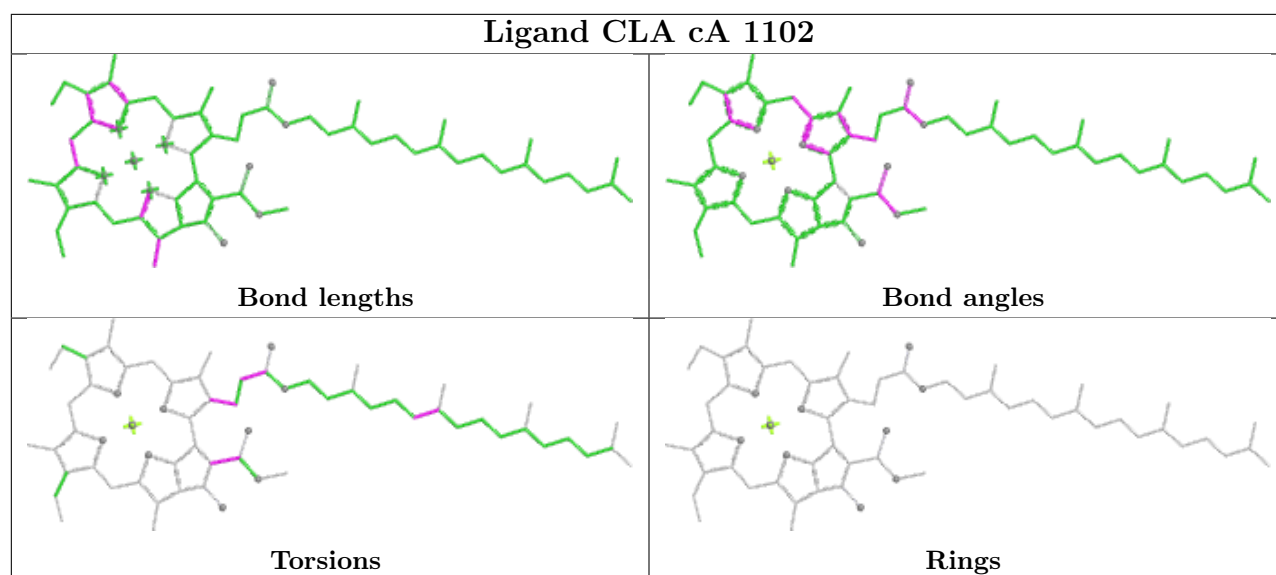
Bond angles

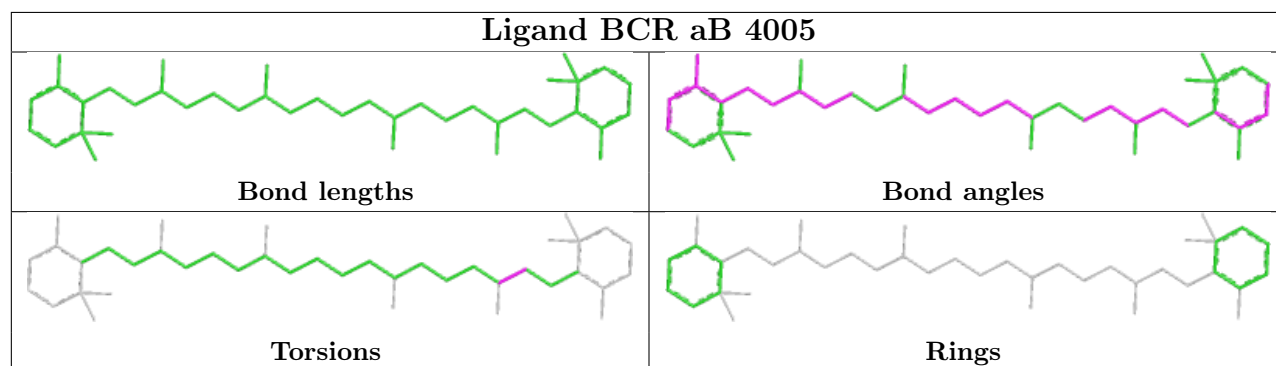
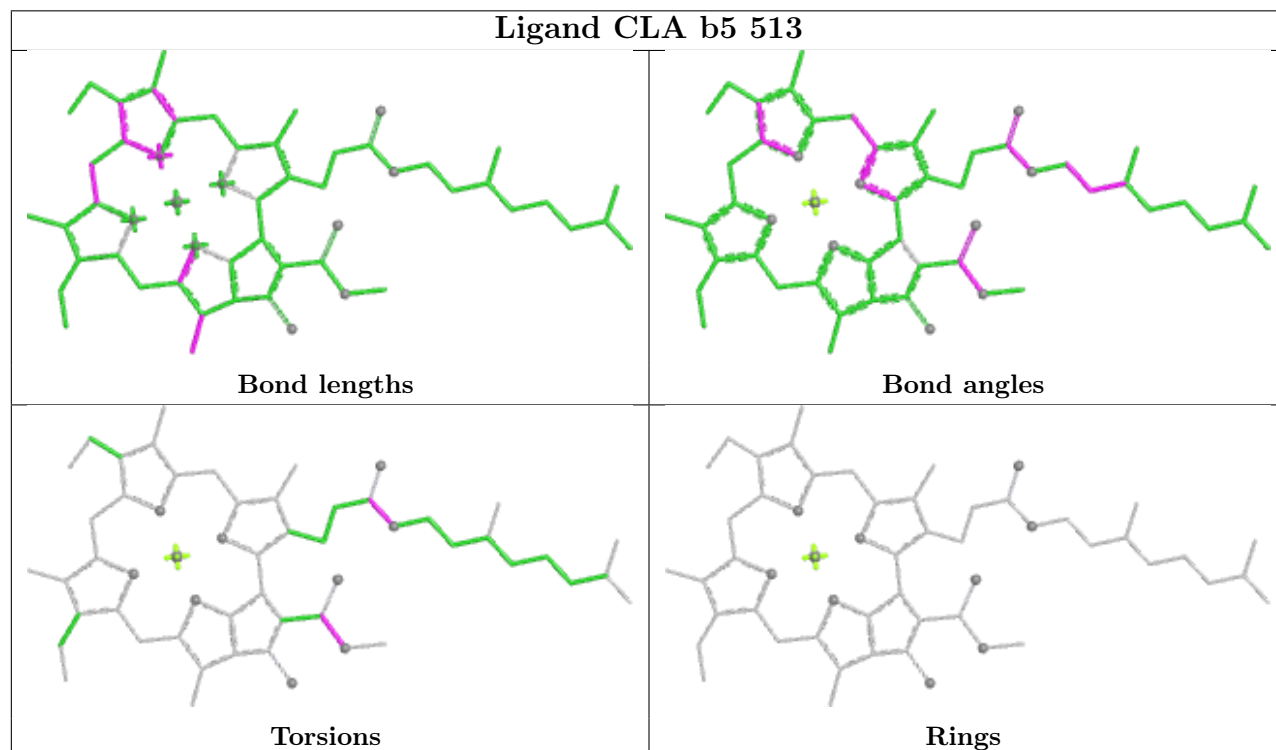
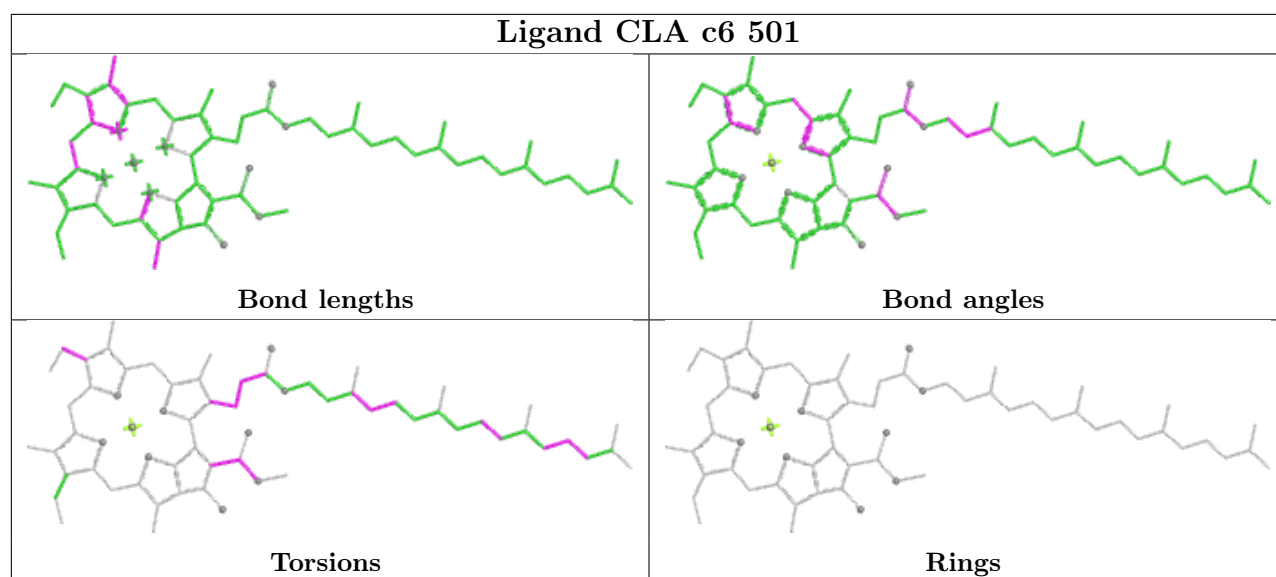


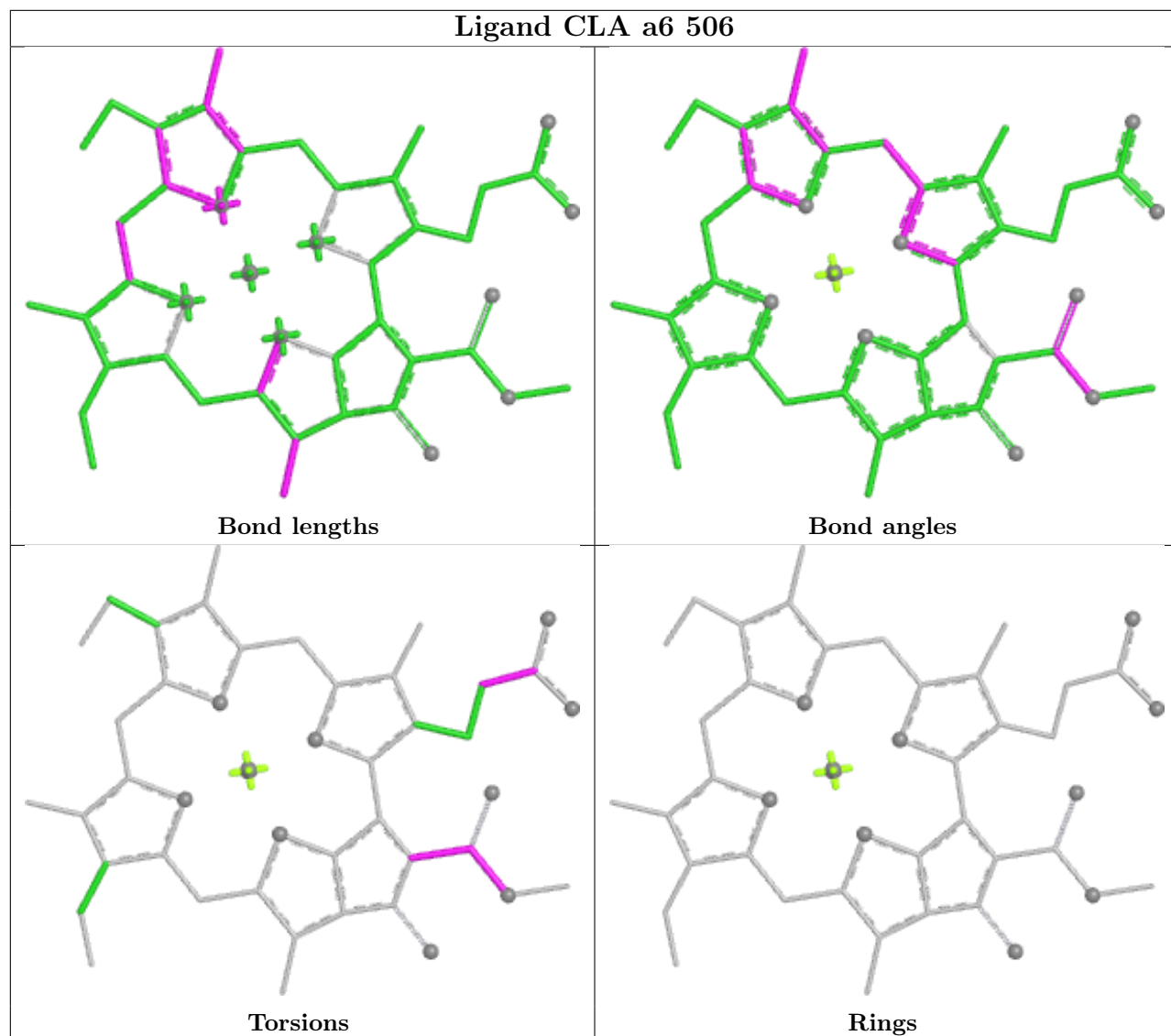
Torsions

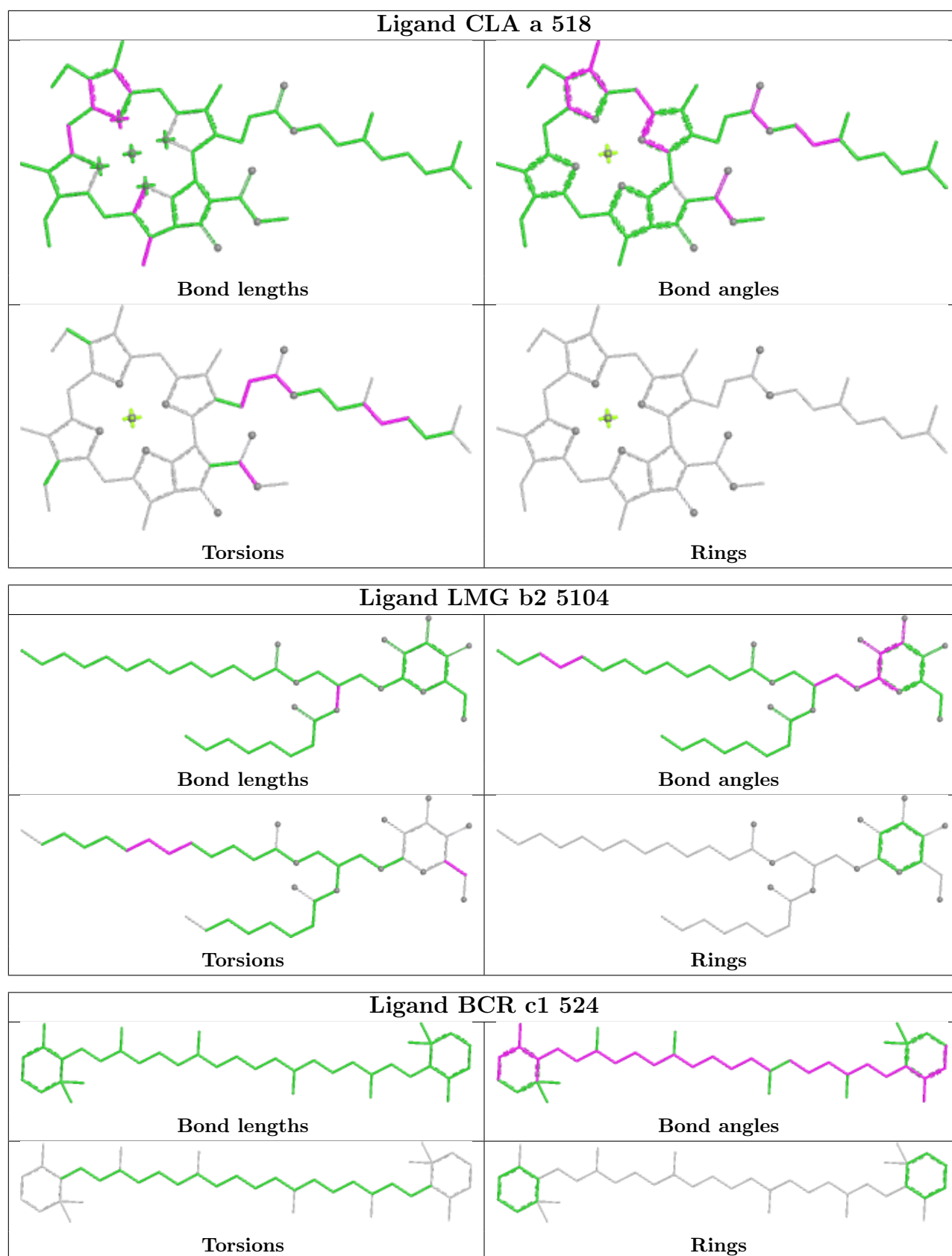


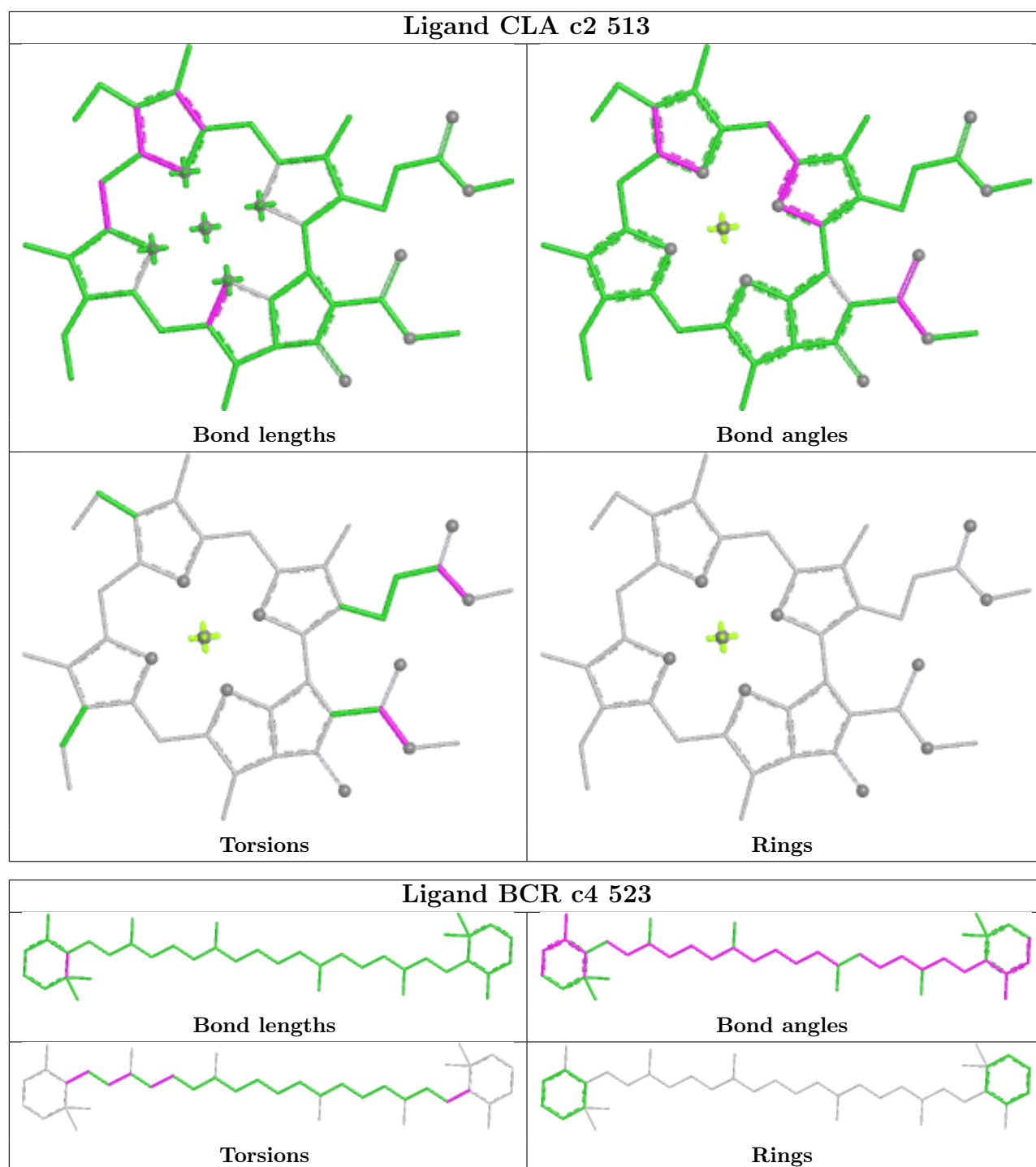
Rings

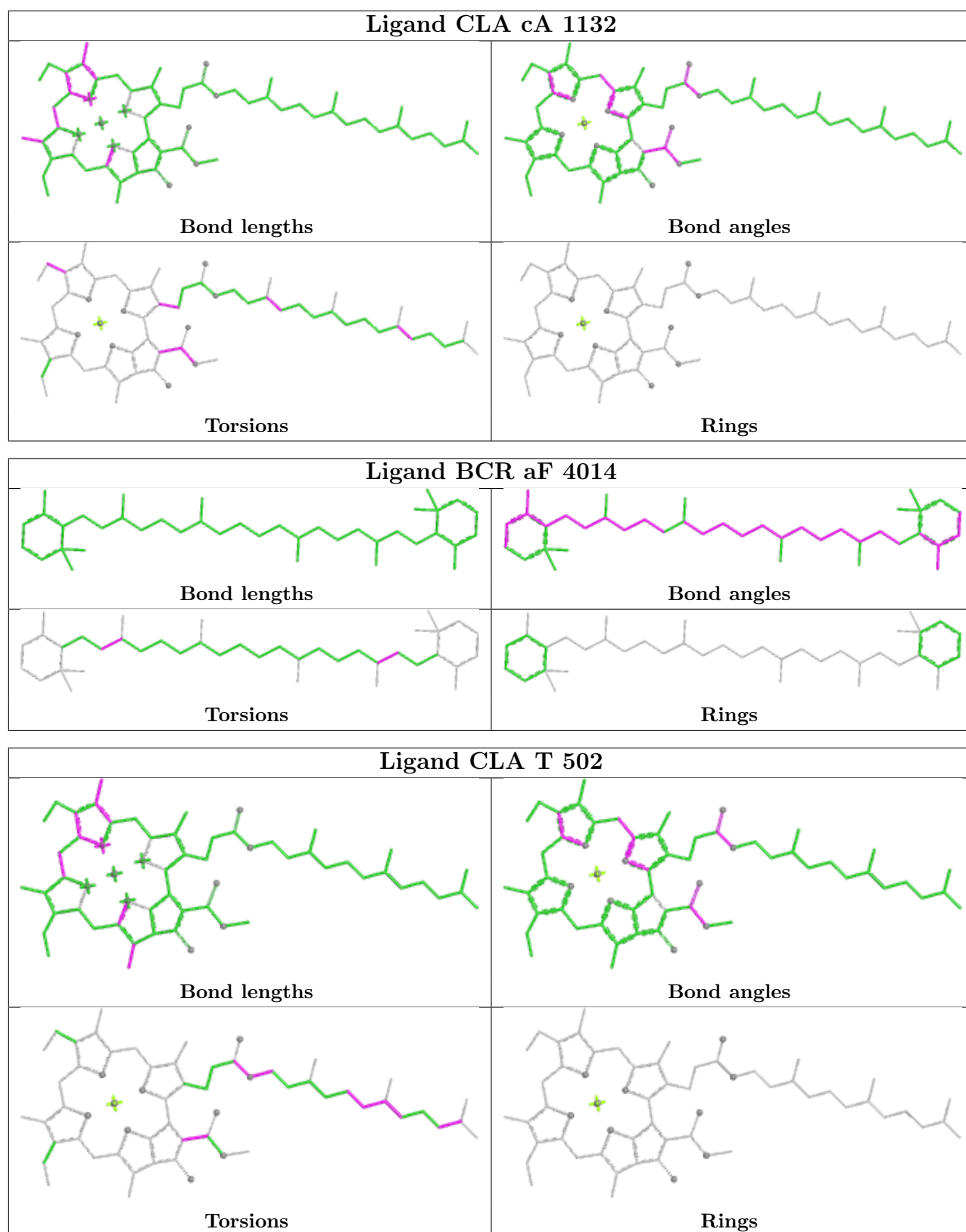




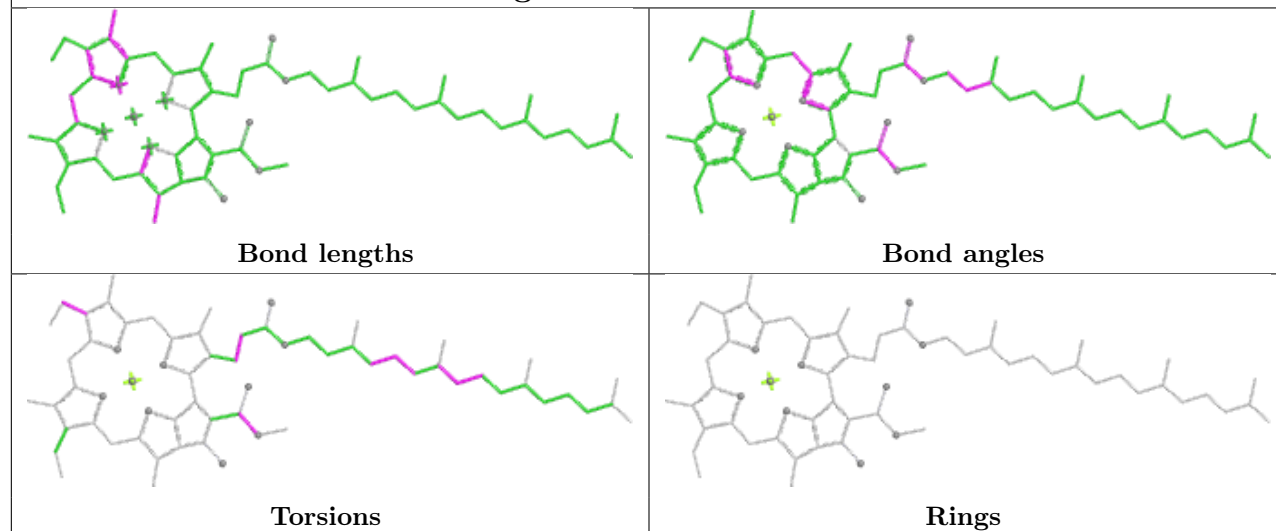




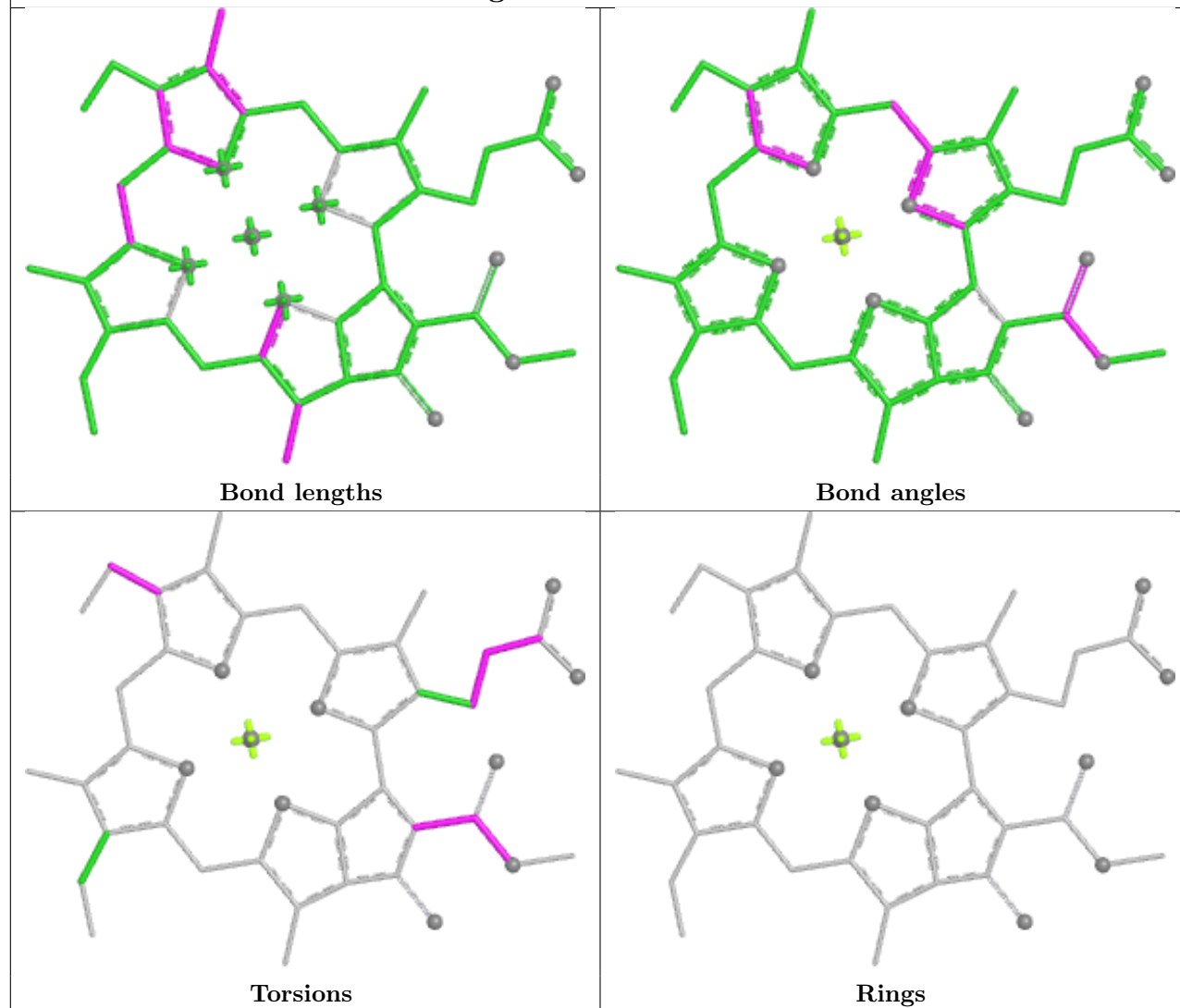




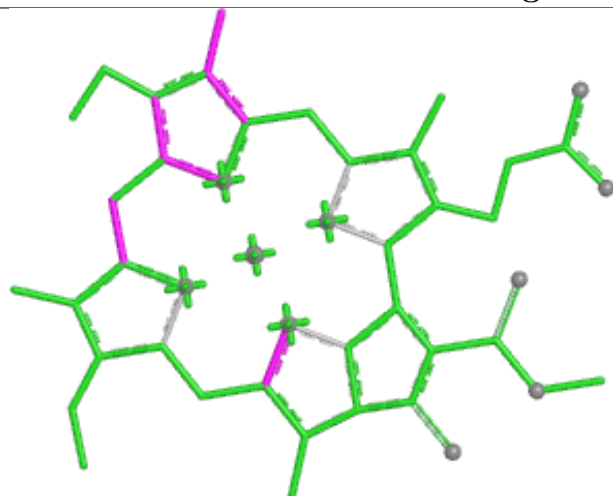
Ligand CLA aA 1138



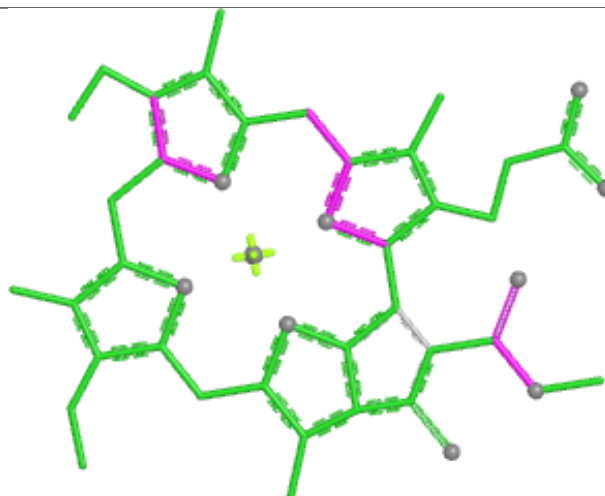
Ligand CLA c5 517



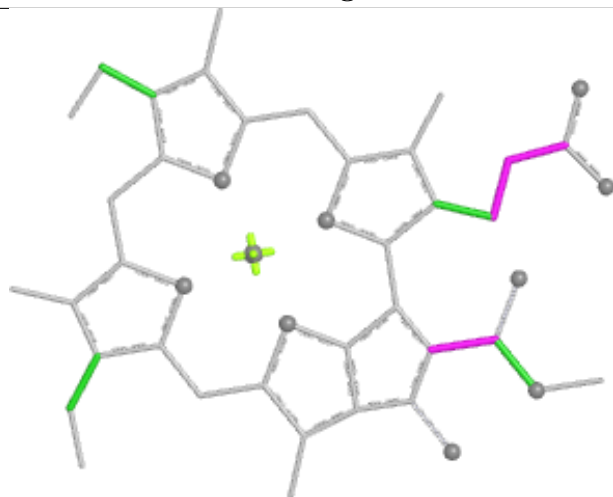
Ligand CLA 1 504



Bond lengths



Bond angles

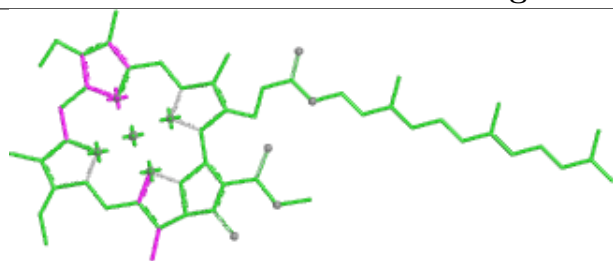


Torsions

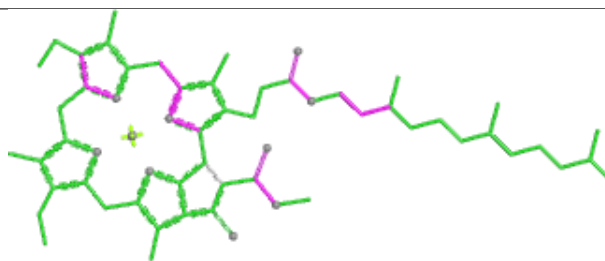


Rings

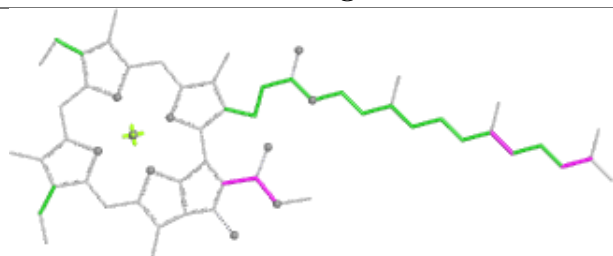
Ligand CLA a5 507



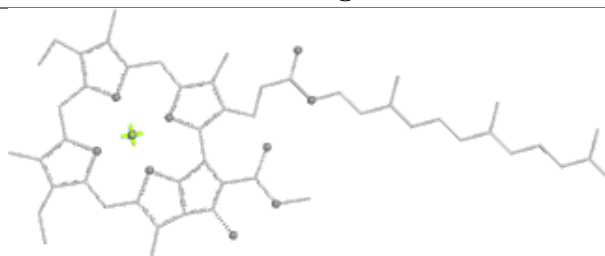
Bond lengths



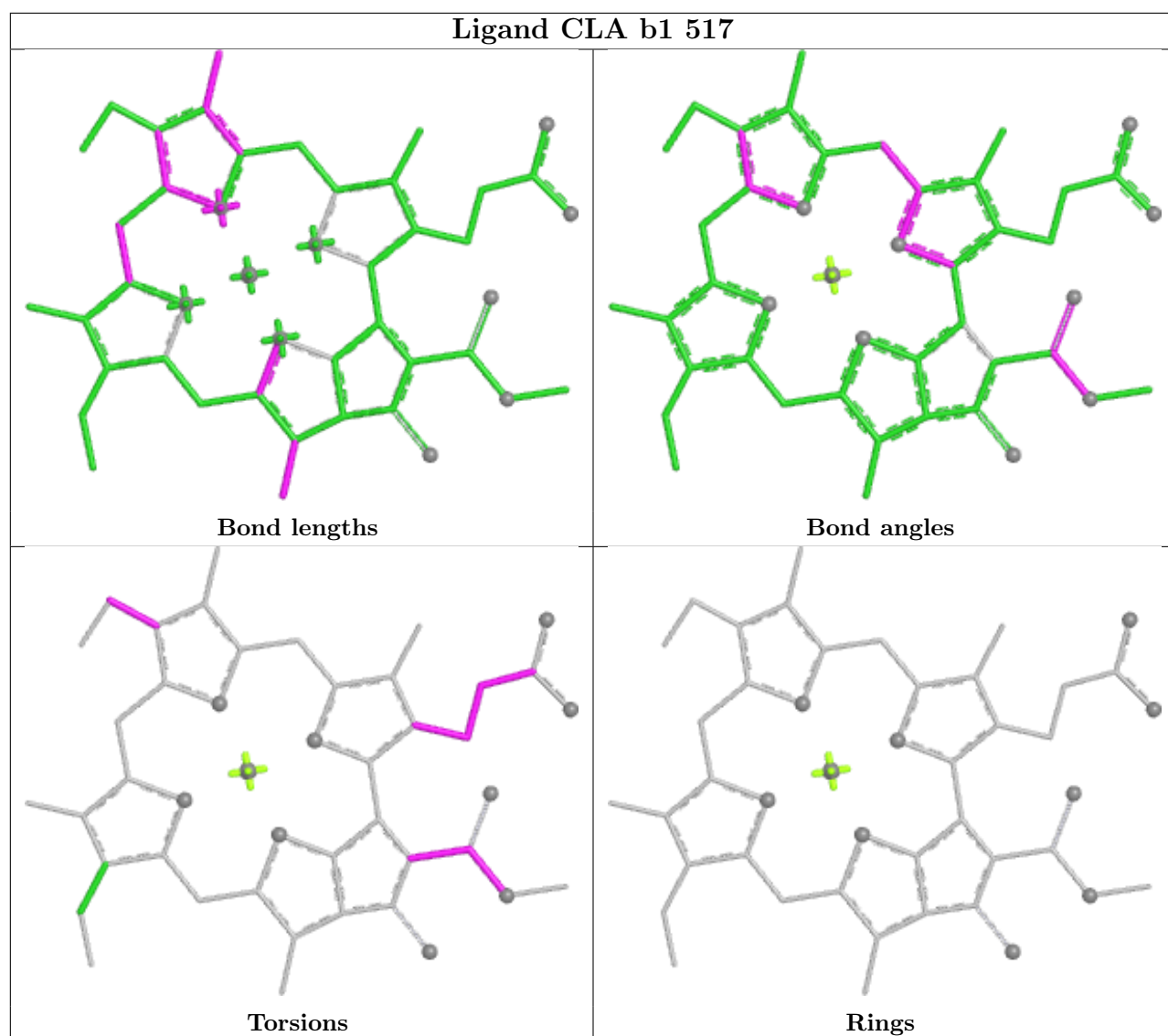
Bond angles

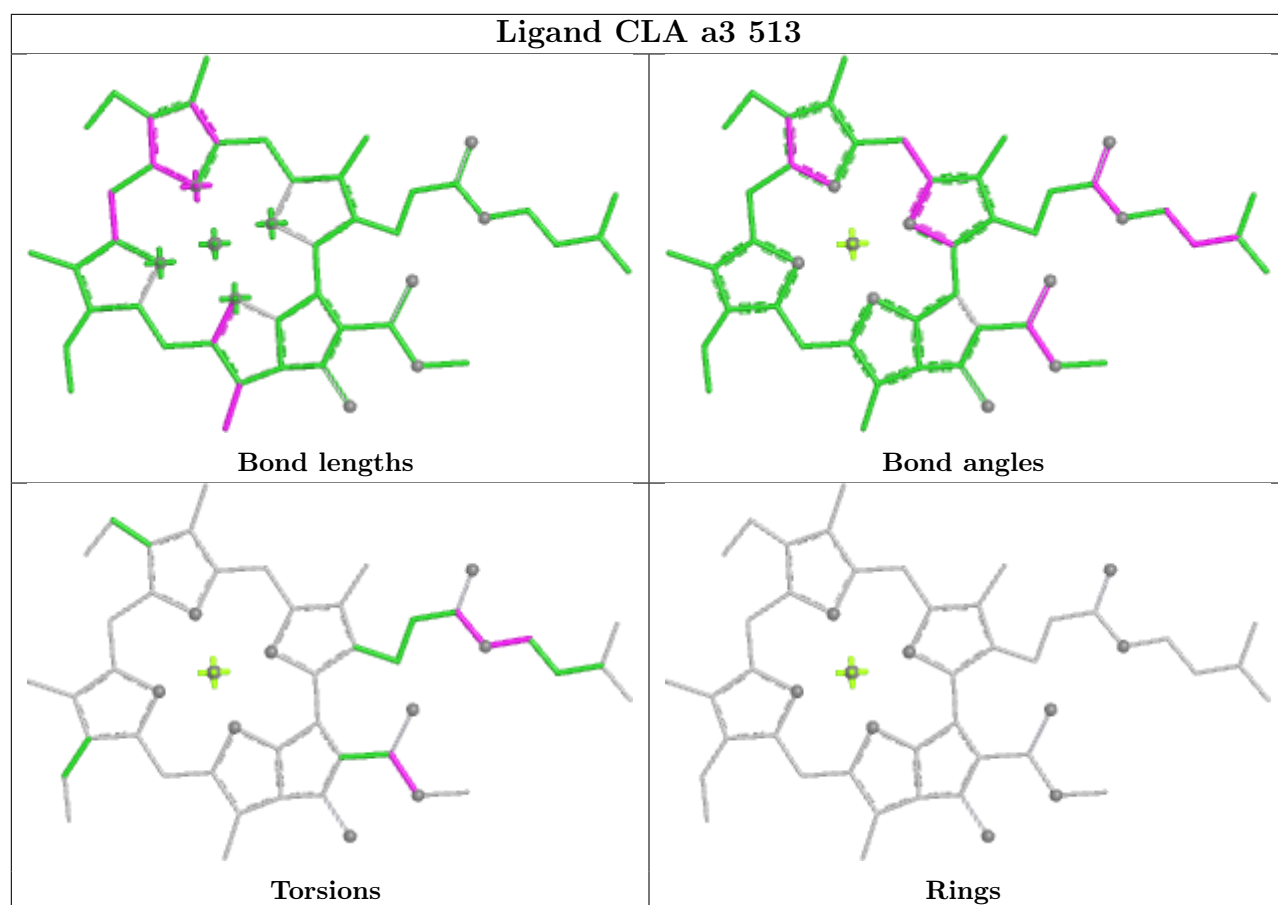


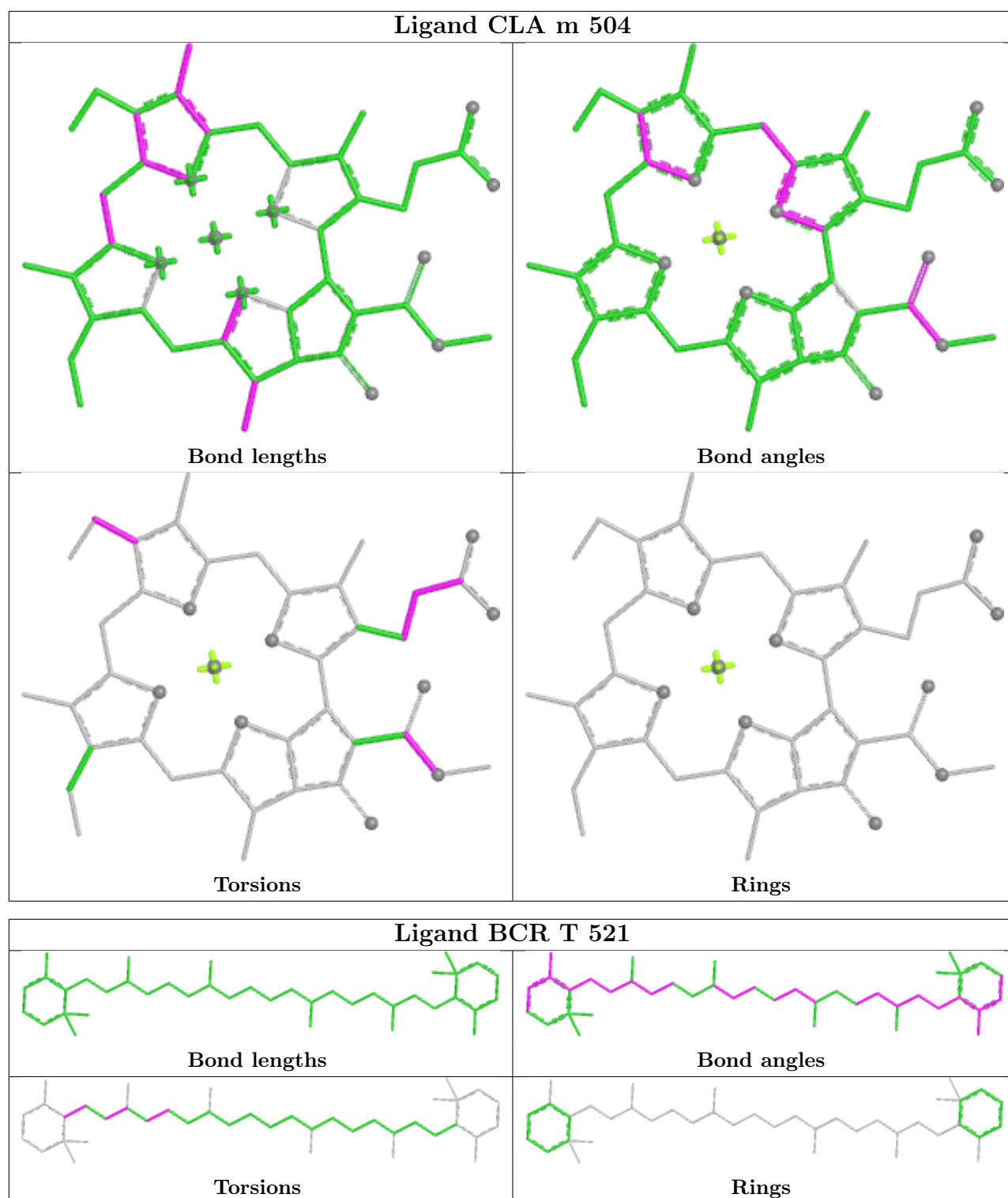
Torsions

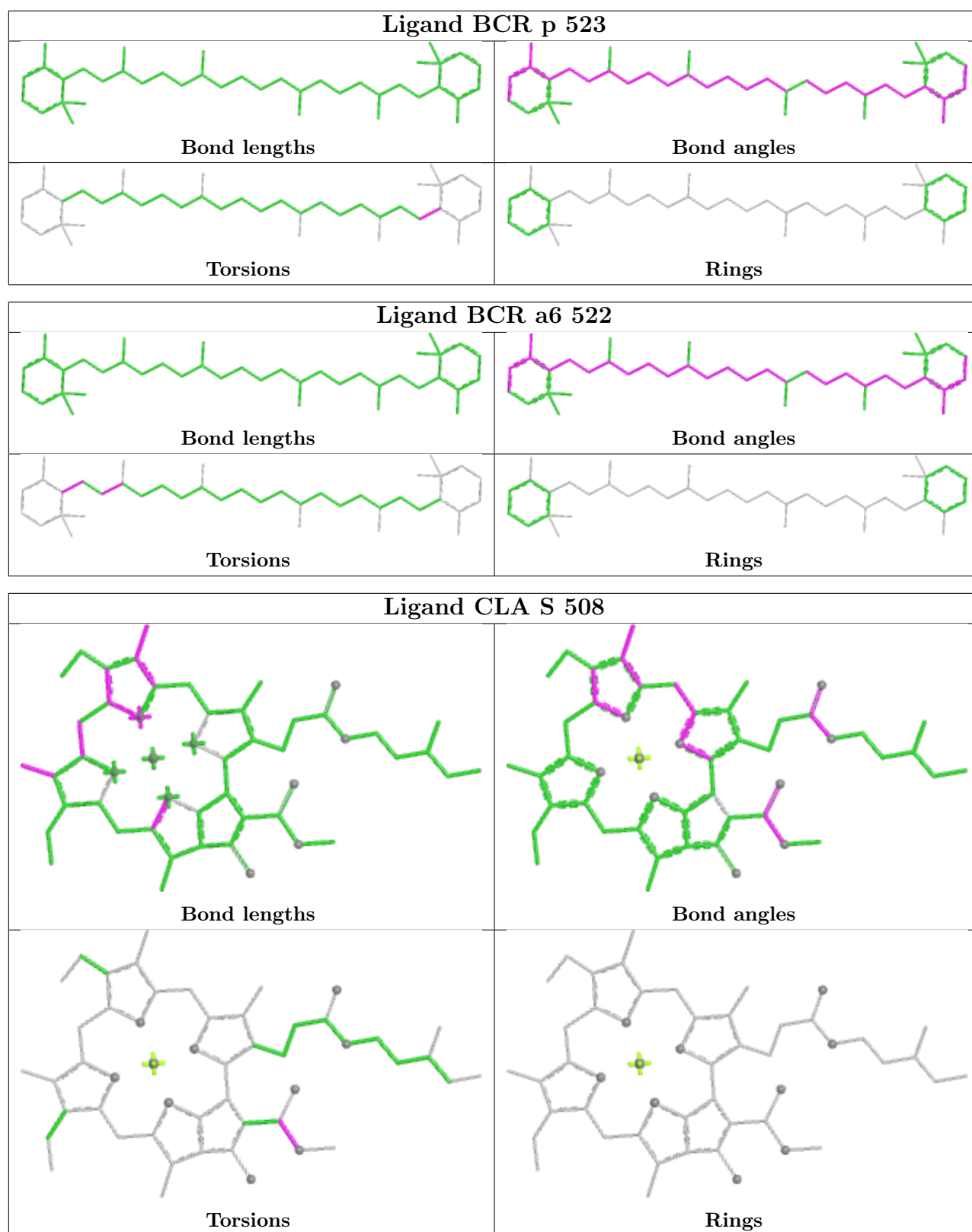


Rings

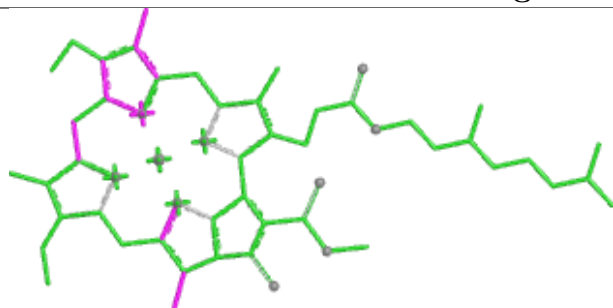




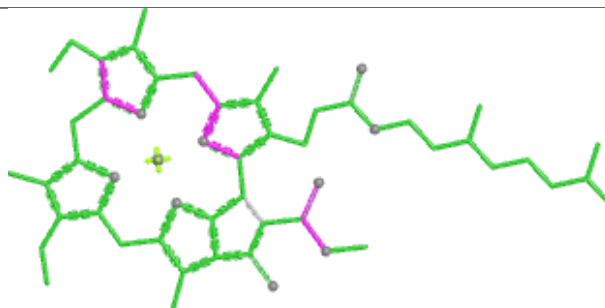




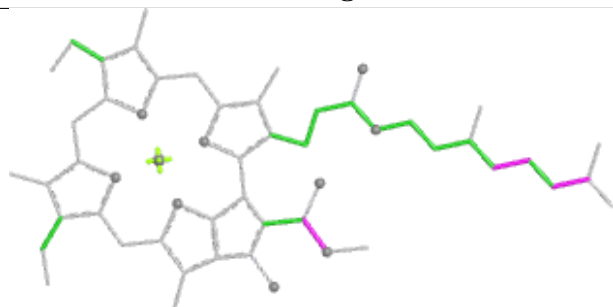
Ligand CLA X 511



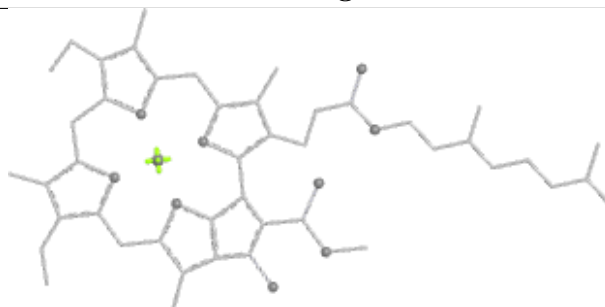
Bond lengths



Bond angles

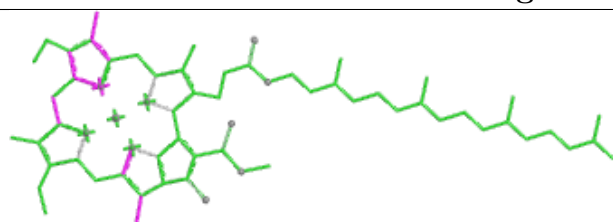


Torsions

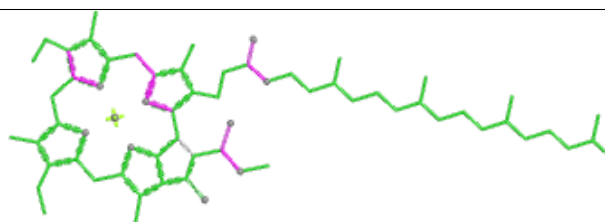


Rings

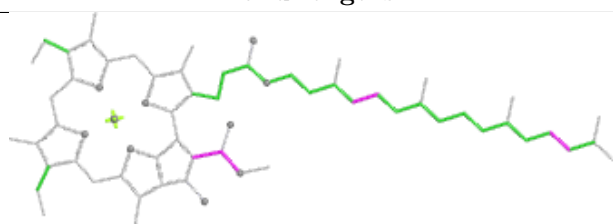
Ligand CLA Z 509



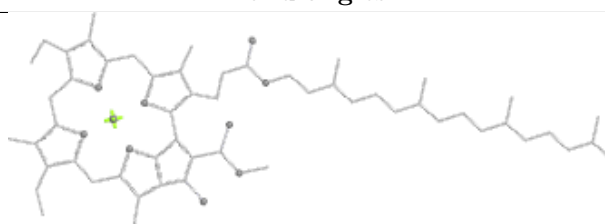
Bond lengths



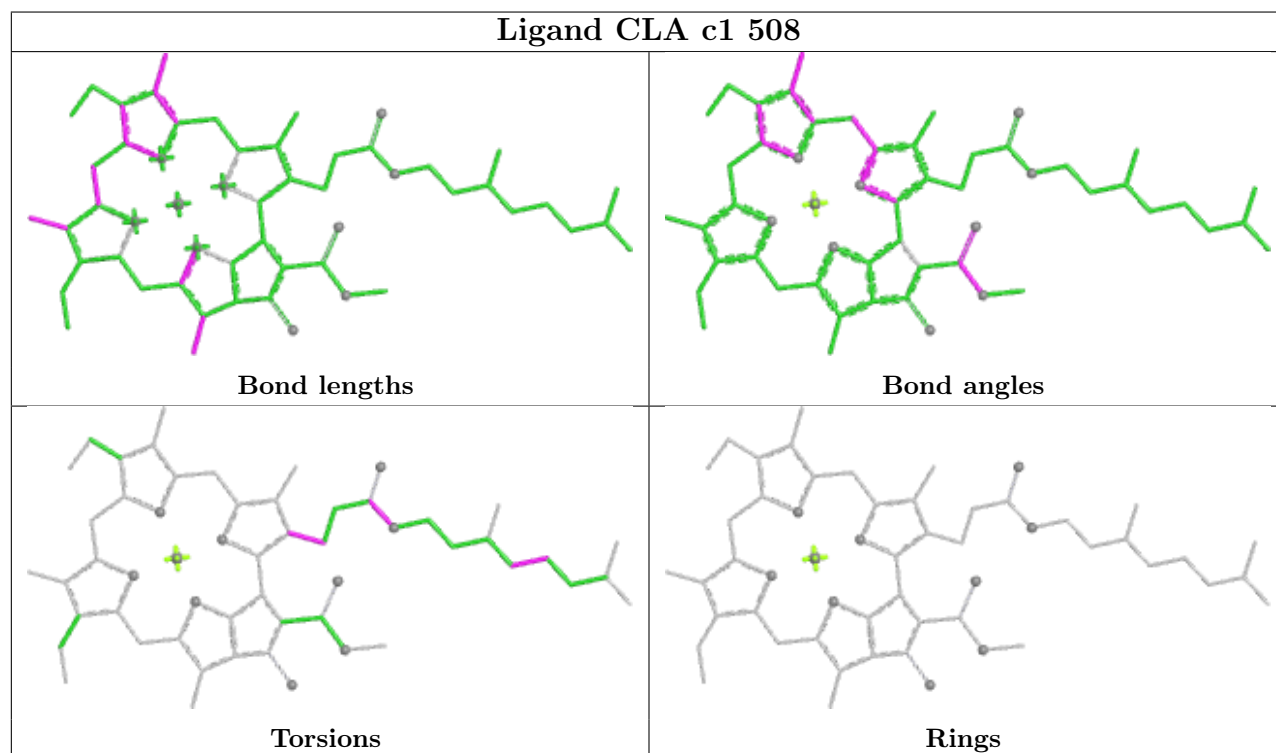
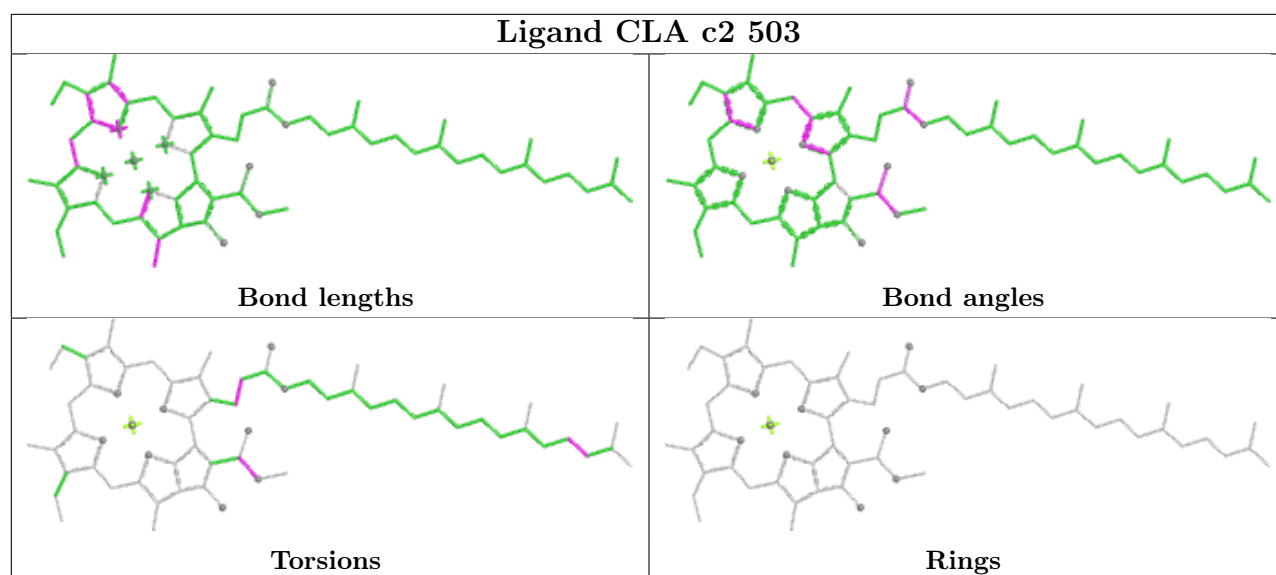
Bond angles

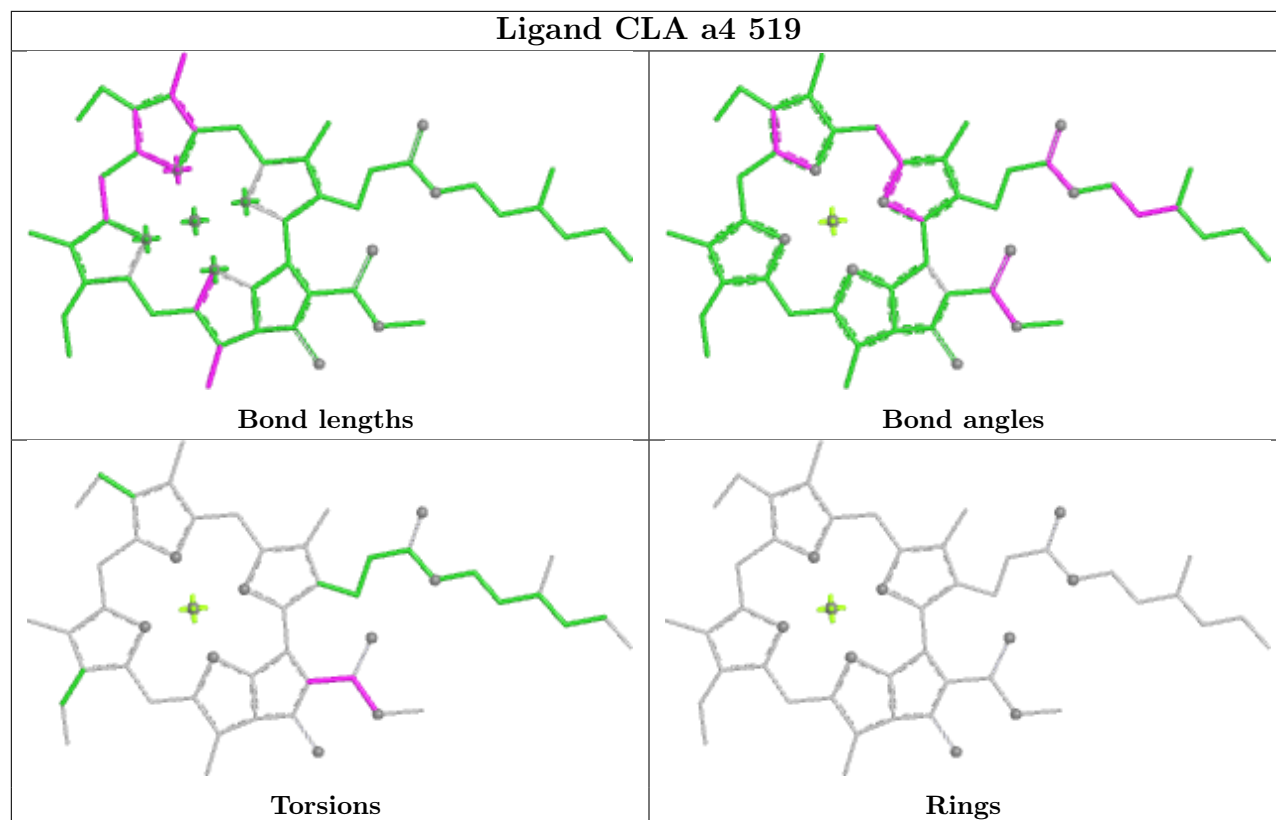


Torsions

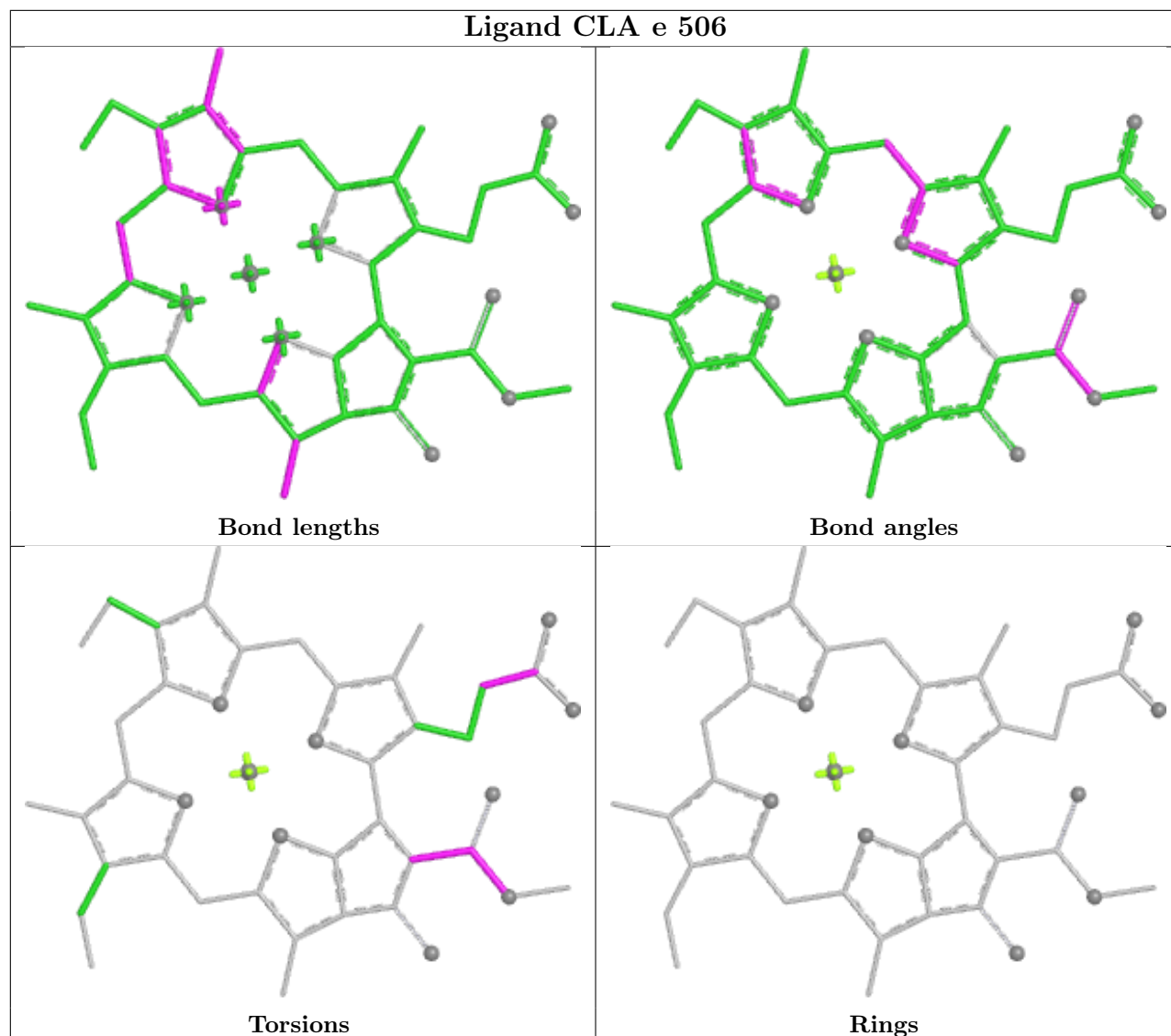


Rings

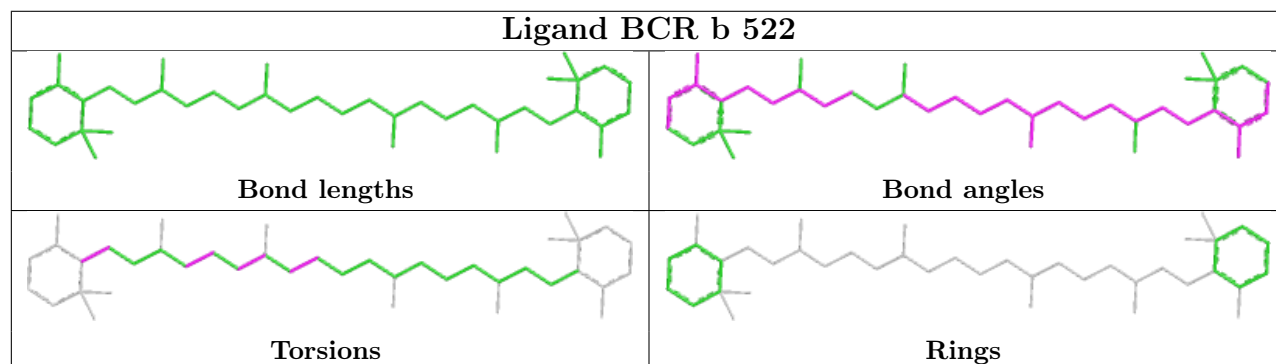


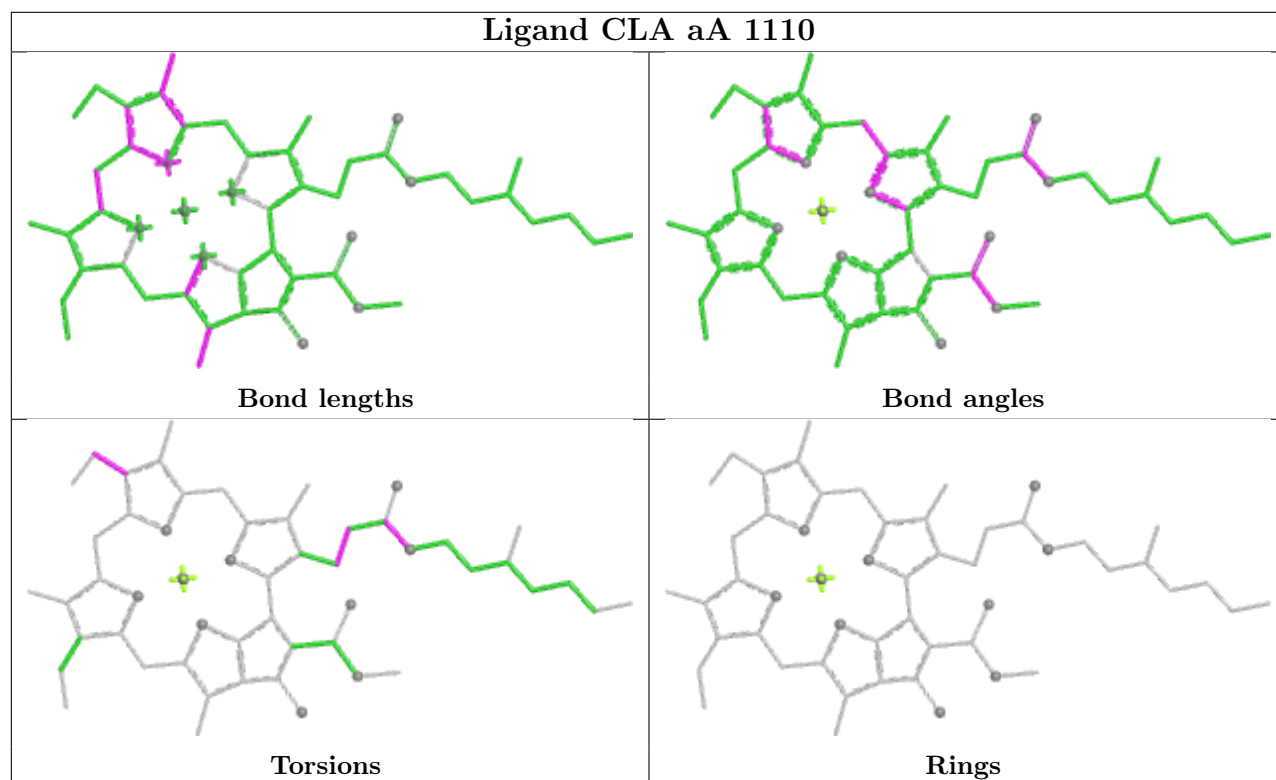
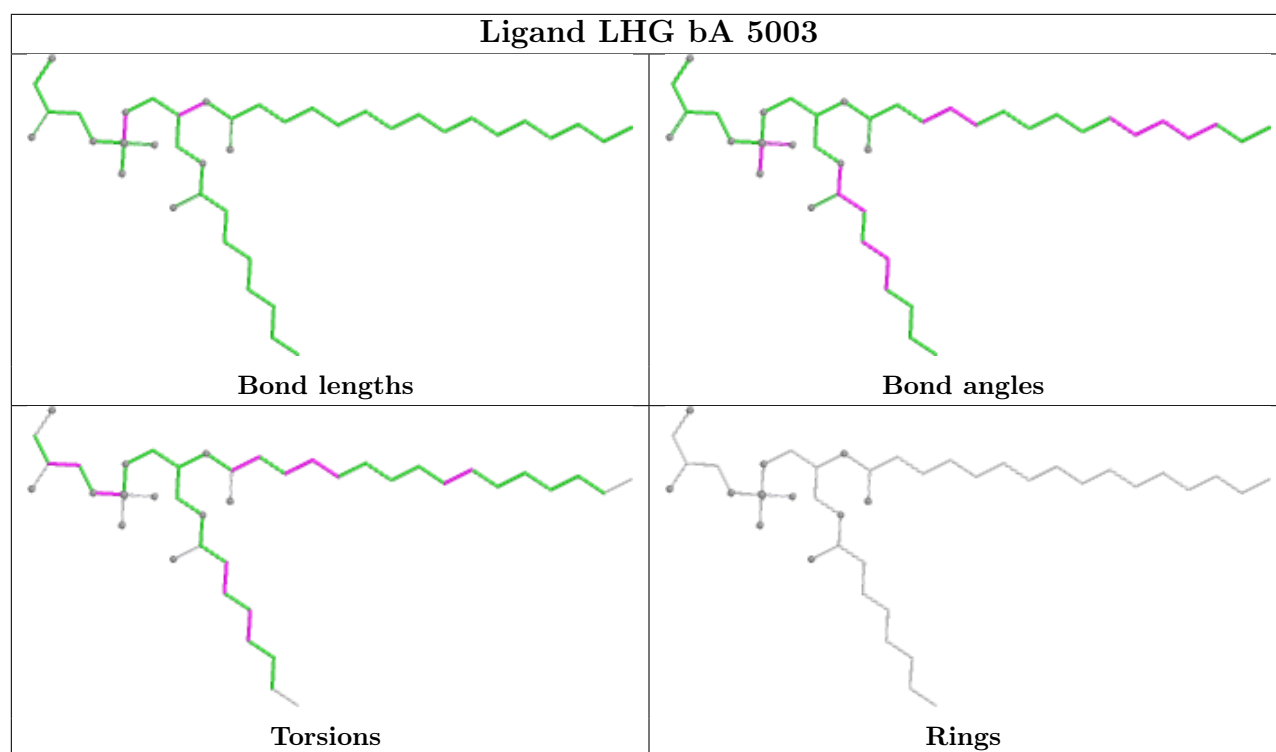


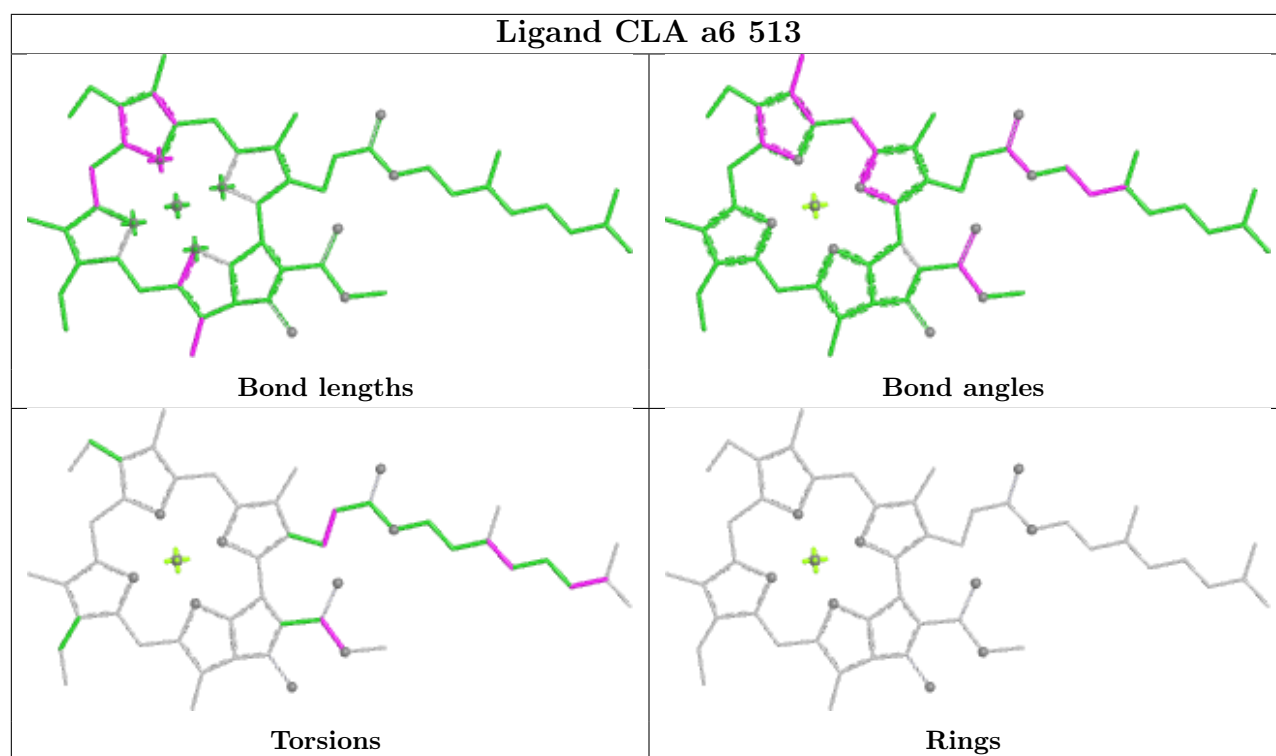
Ligand CLA e 506

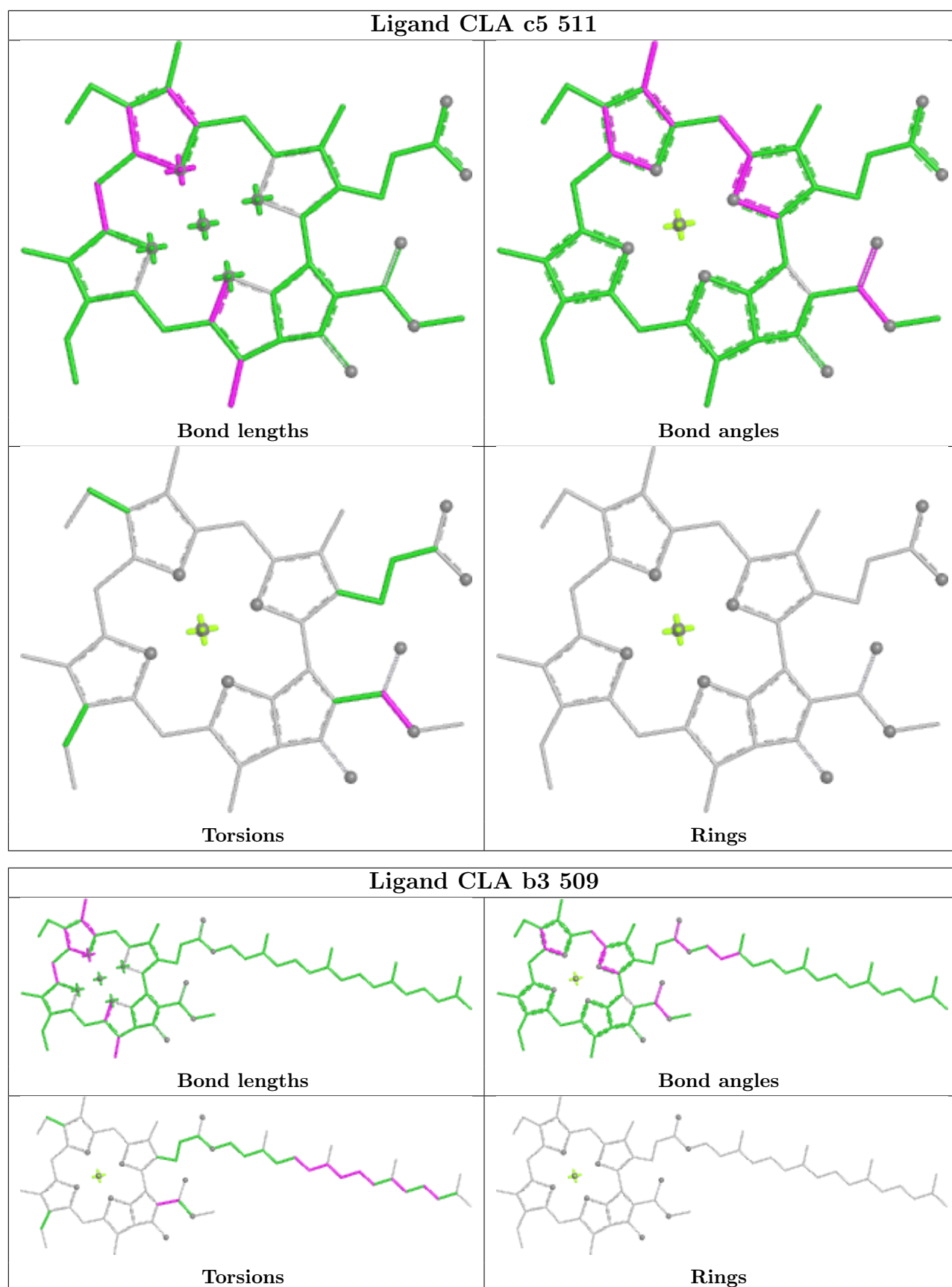


Ligand BCR b 522

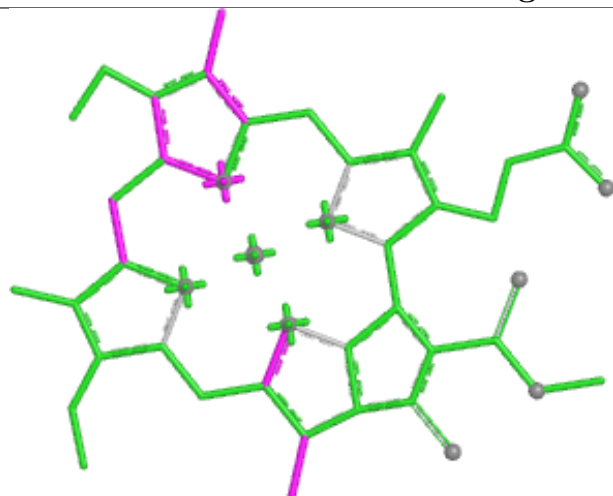








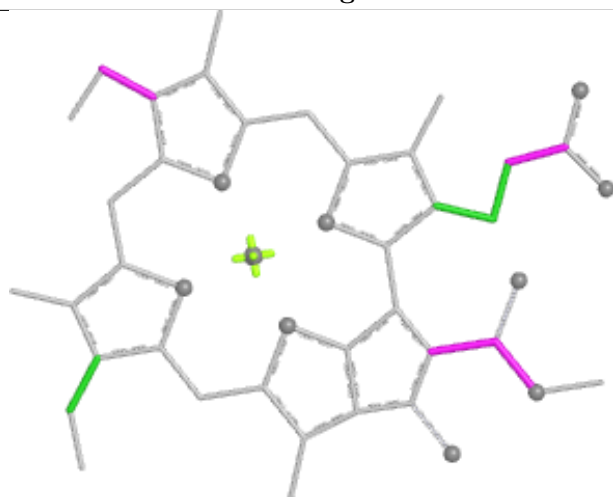
Ligand CLA a 512



Bond lengths



Bond angles

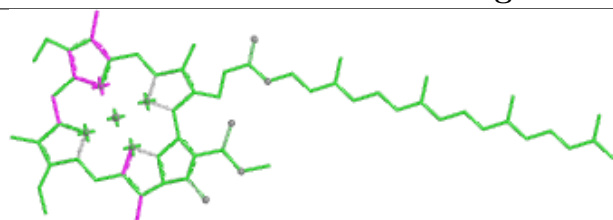


Torsions

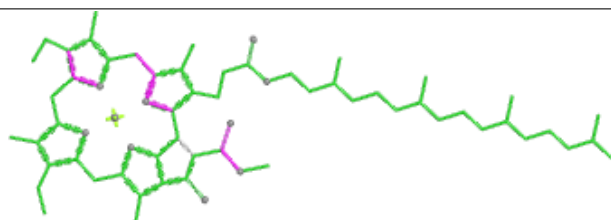


Rings

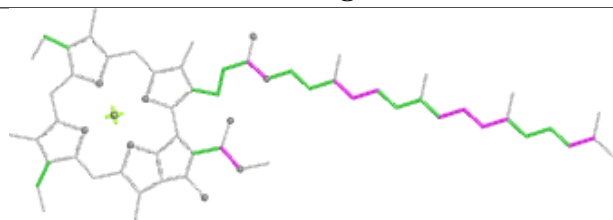
Ligand CLA bA 1133



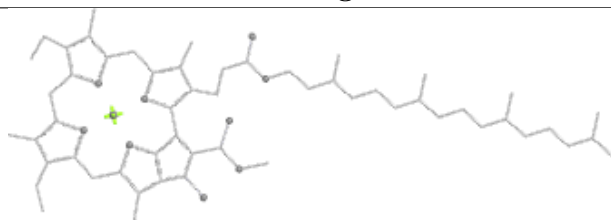
Bond lengths



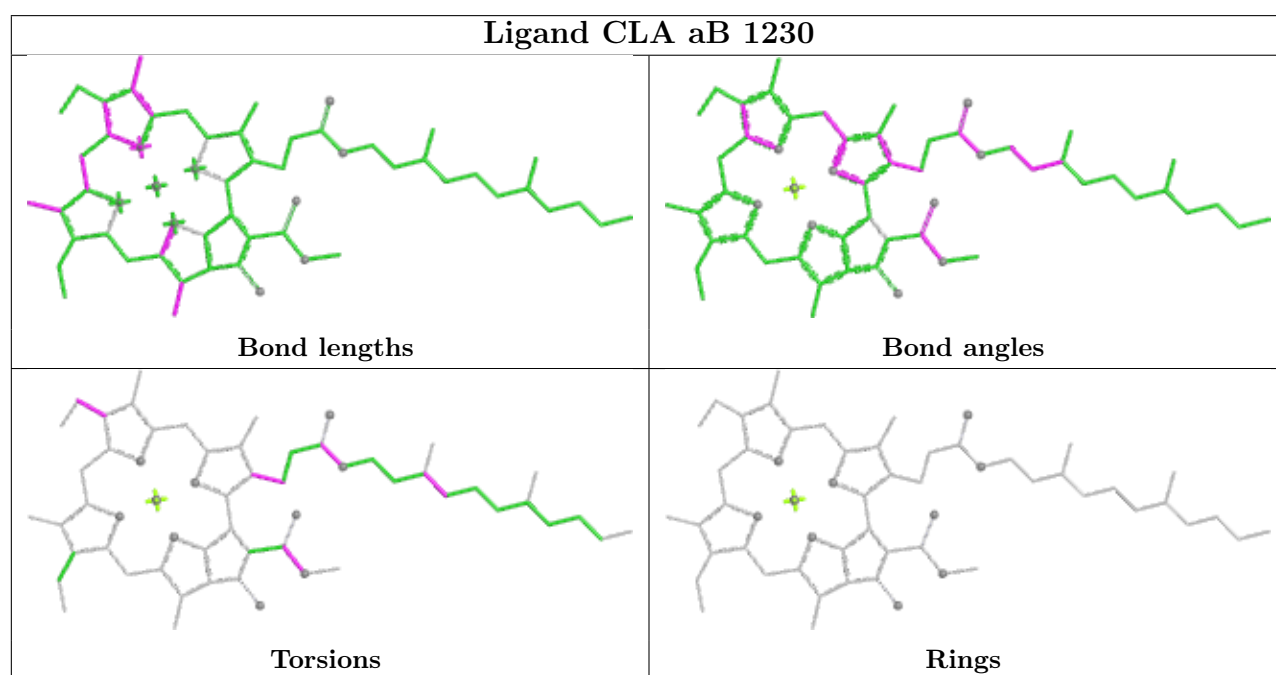
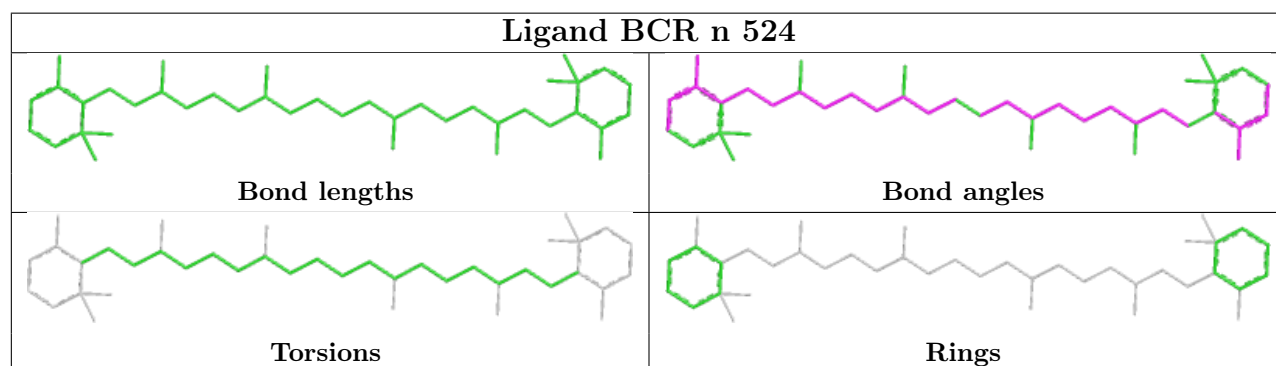
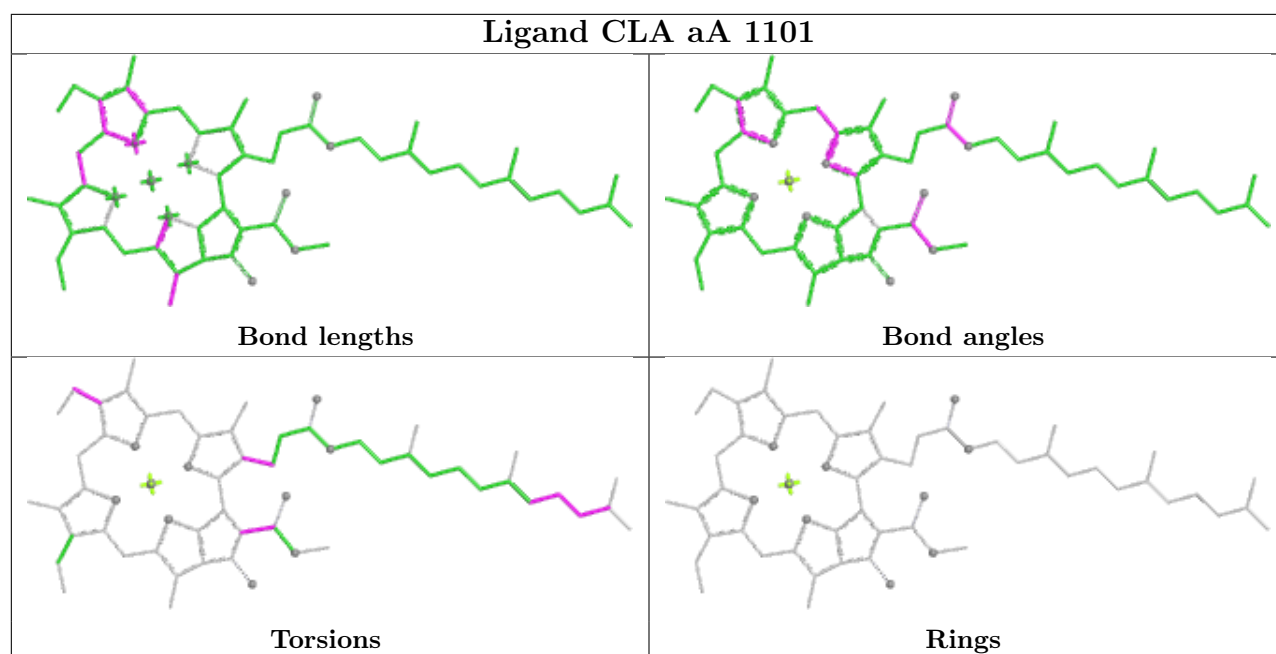
Bond angles



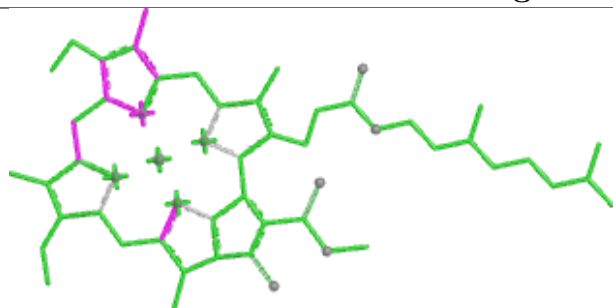
Torsions



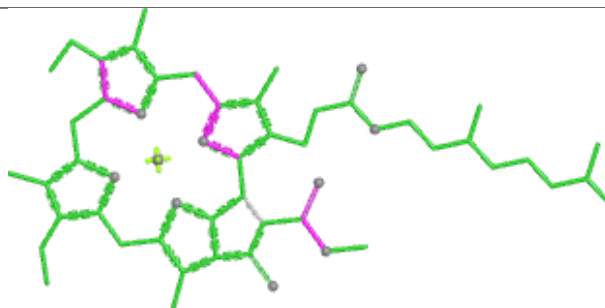
Rings



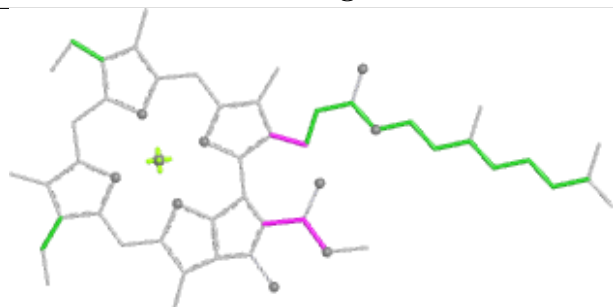
Ligand CLA U 511



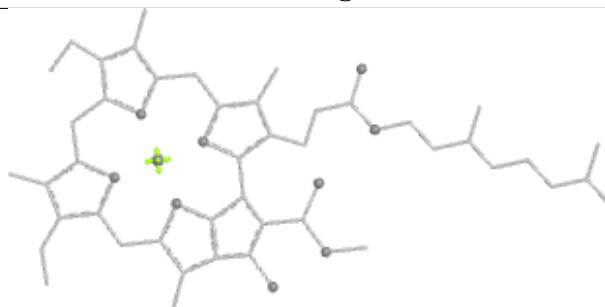
Bond lengths



Bond angles

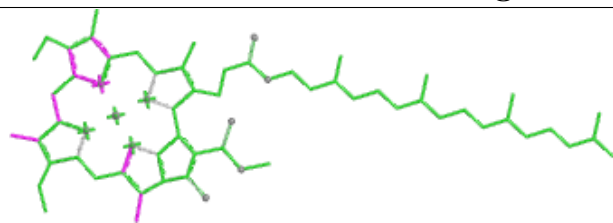


Torsions

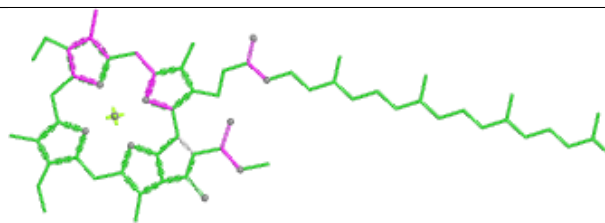


Rings

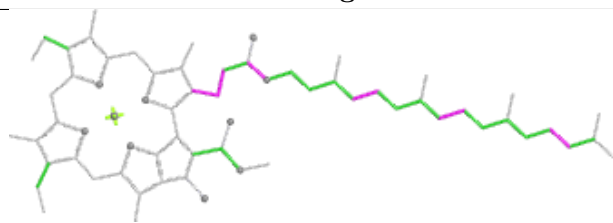
Ligand CLA bA 1013



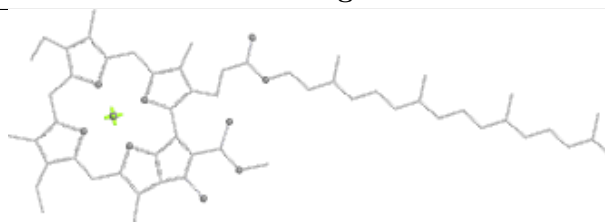
Bond lengths



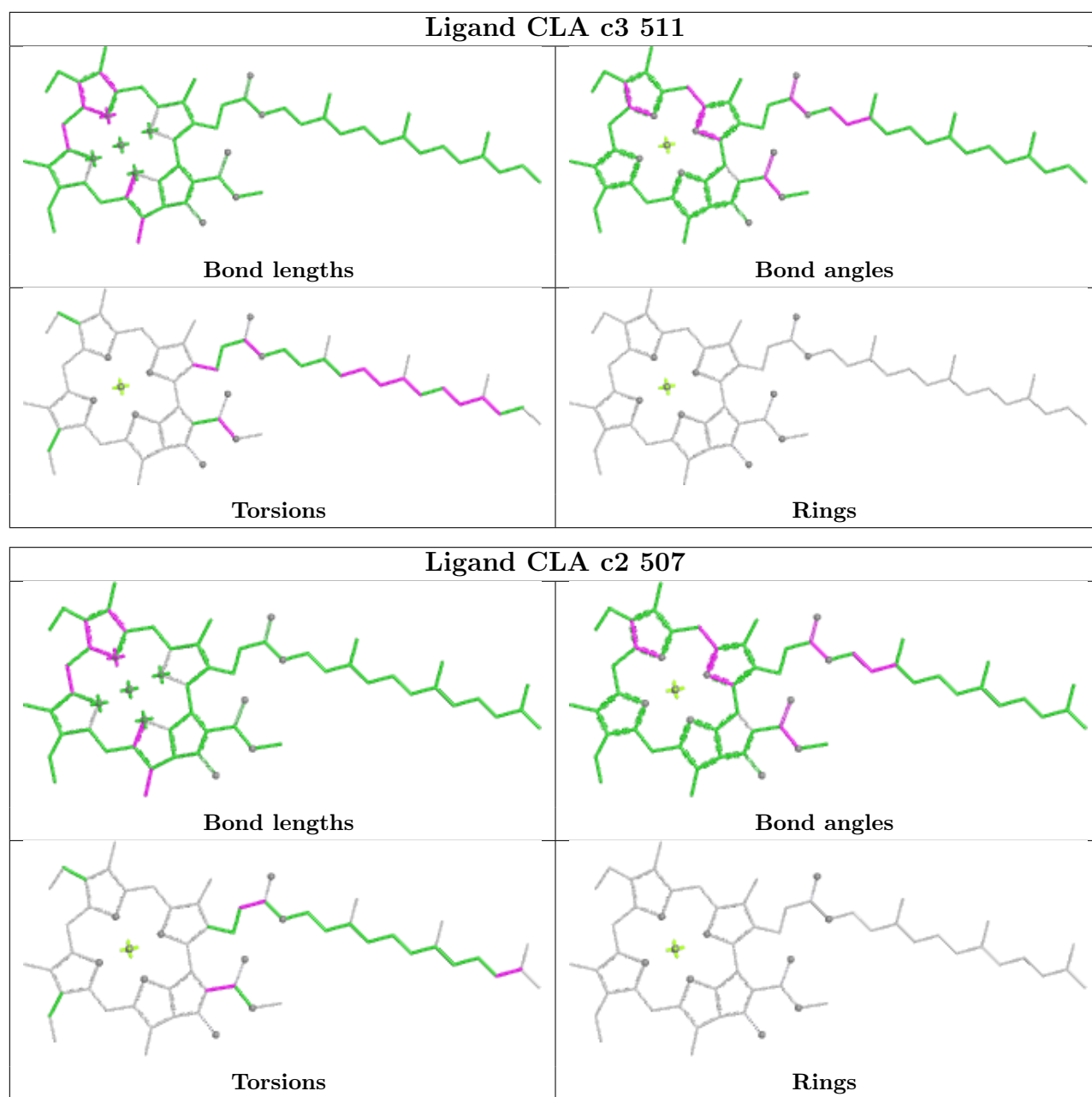
Bond angles



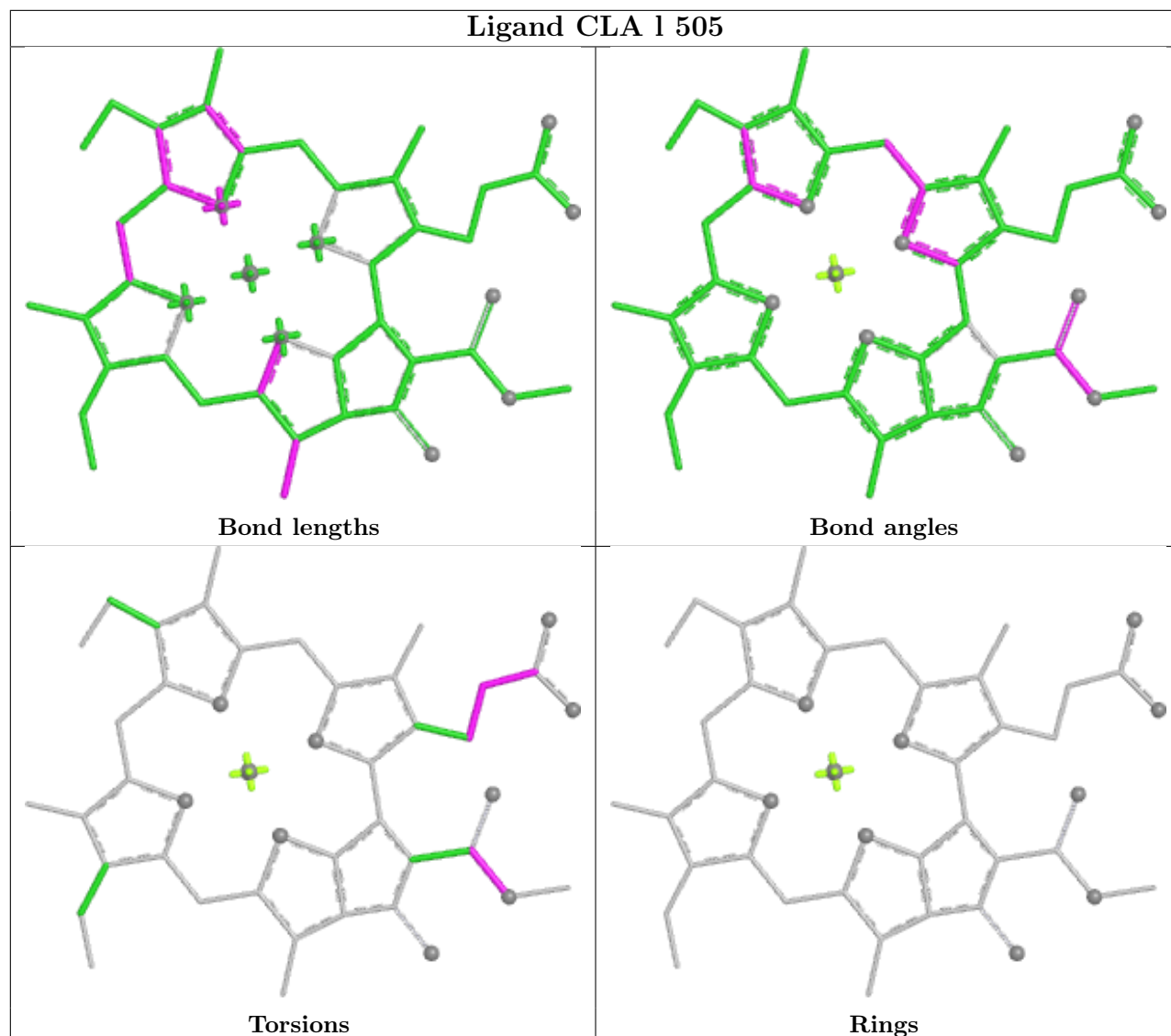
Torsions



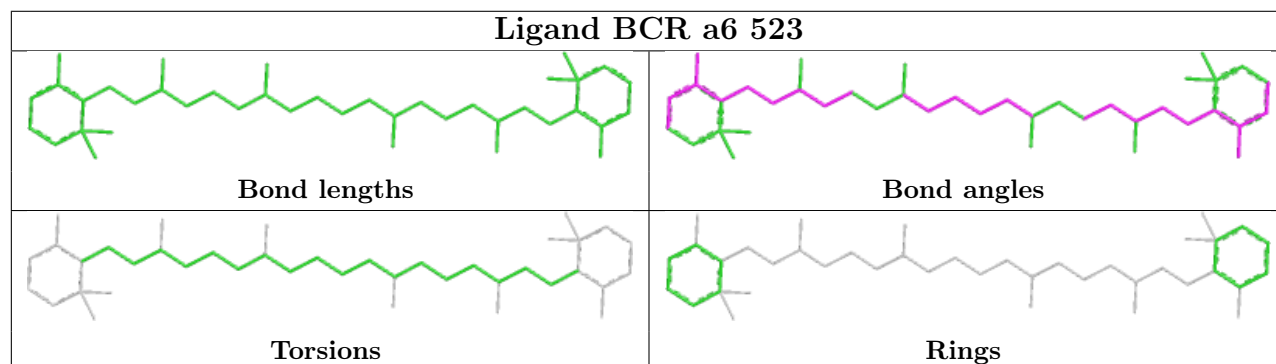
Rings



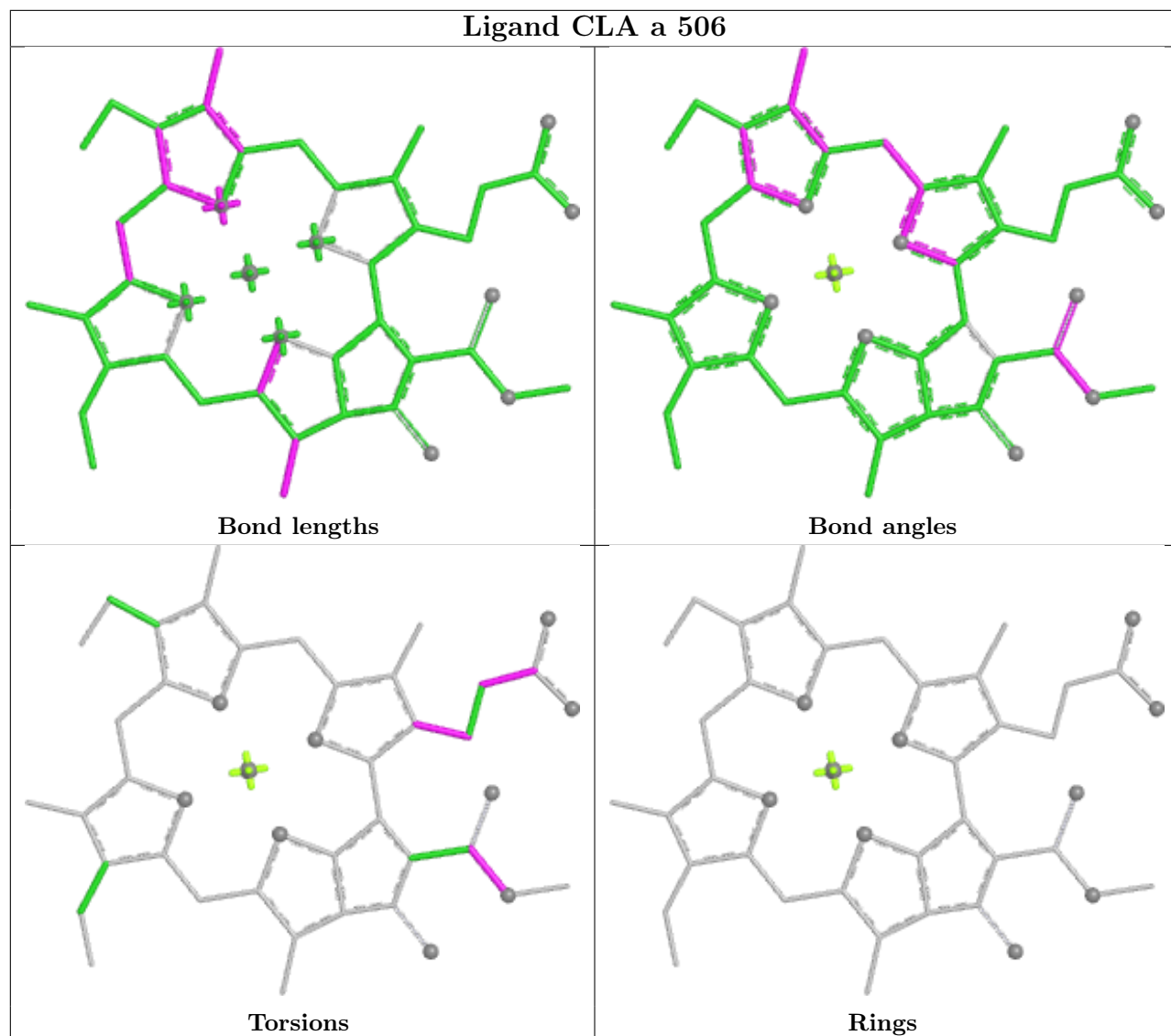
Ligand CLA 1 505



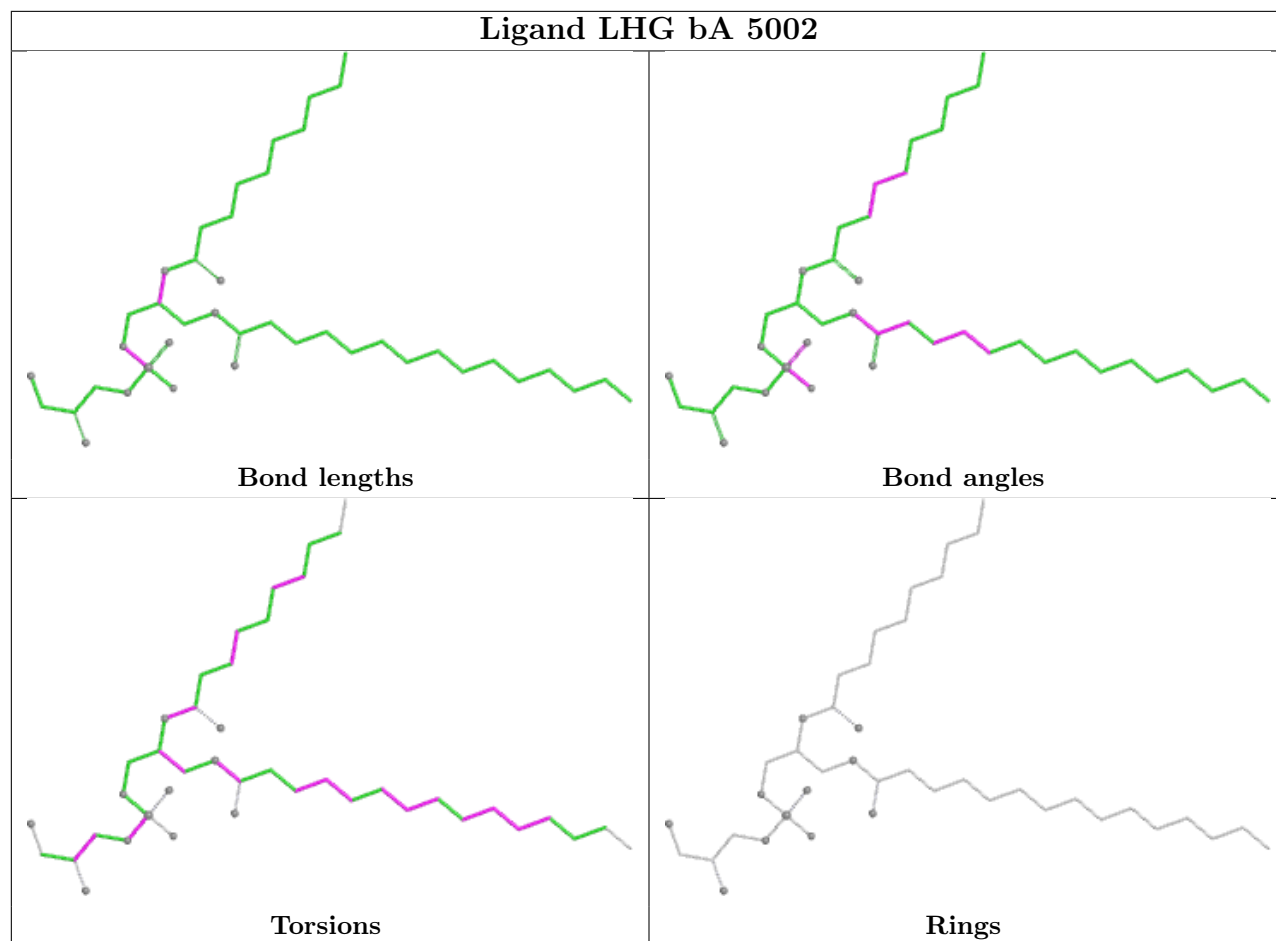
Ligand BCR a6 523



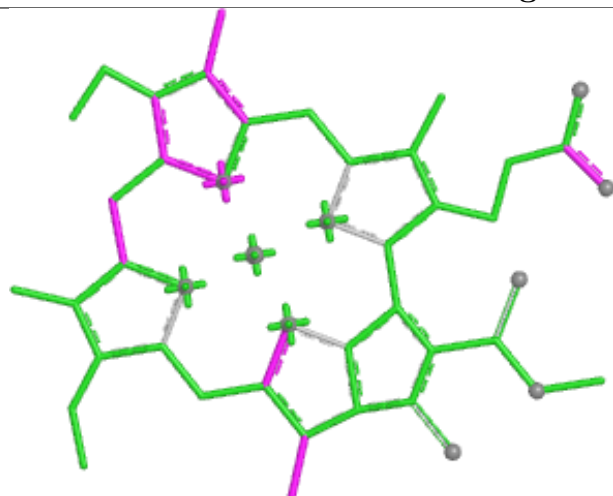
Ligand CLA a 506



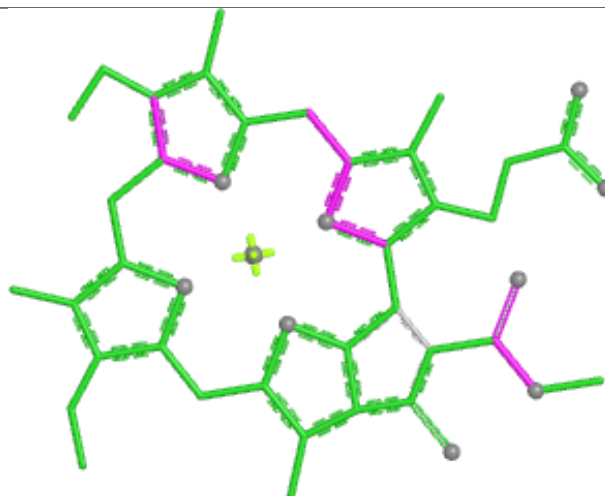
Ligand LHG bA 5002



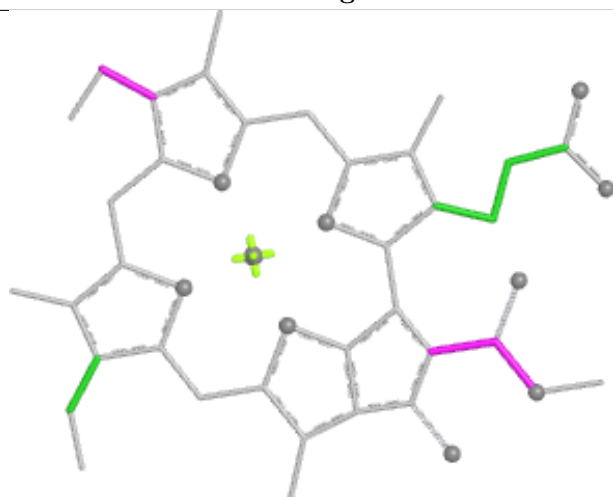
Ligand CLA c 517



Bond lengths



Bond angles

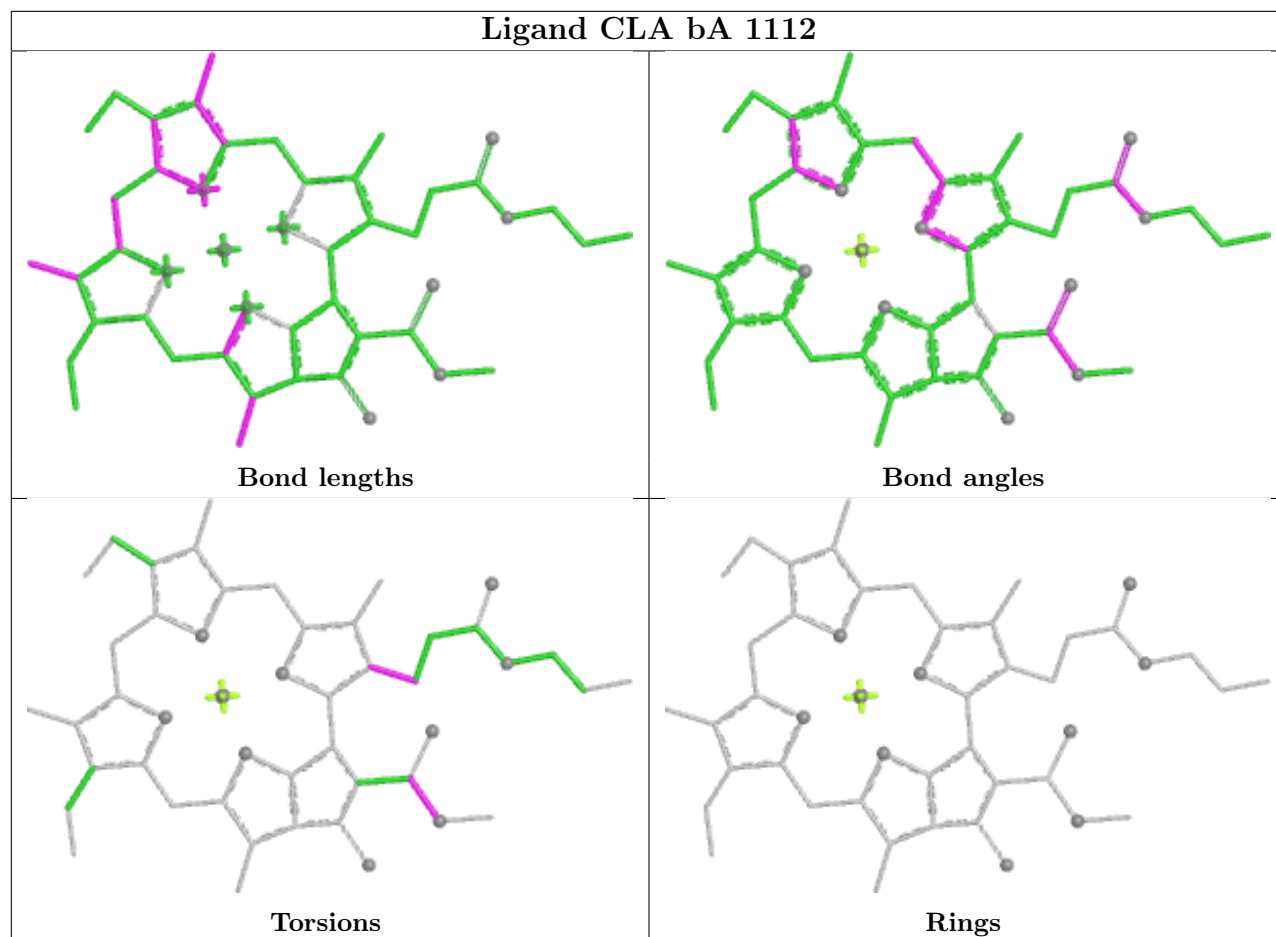


Torsions

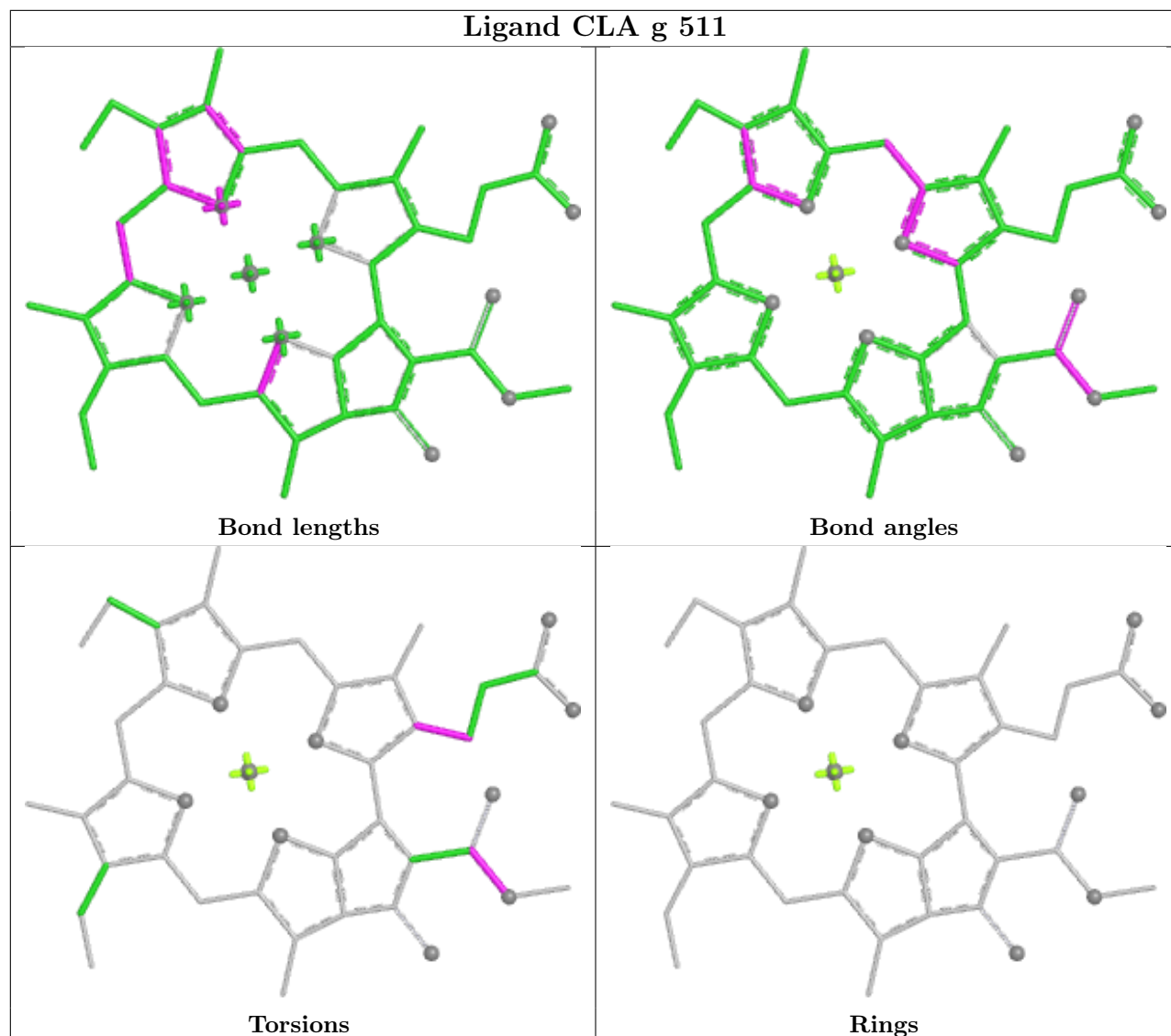


Rings

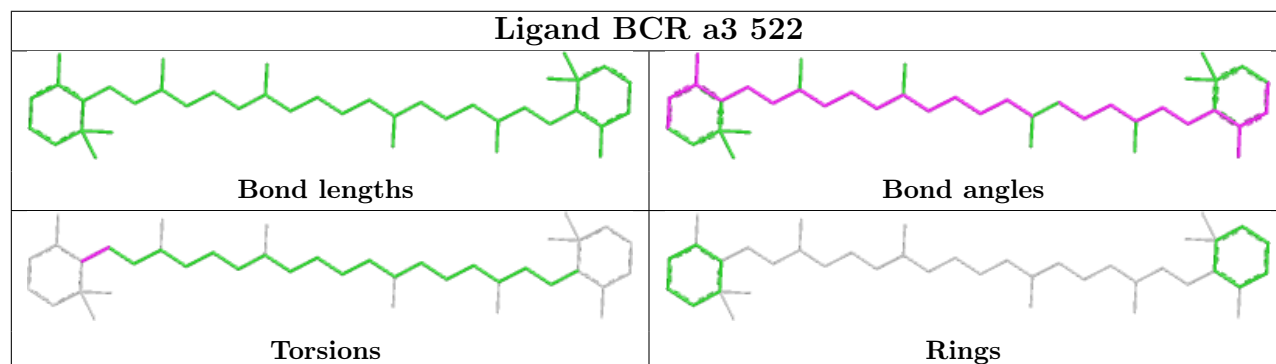
Ligand CLA bA 1112

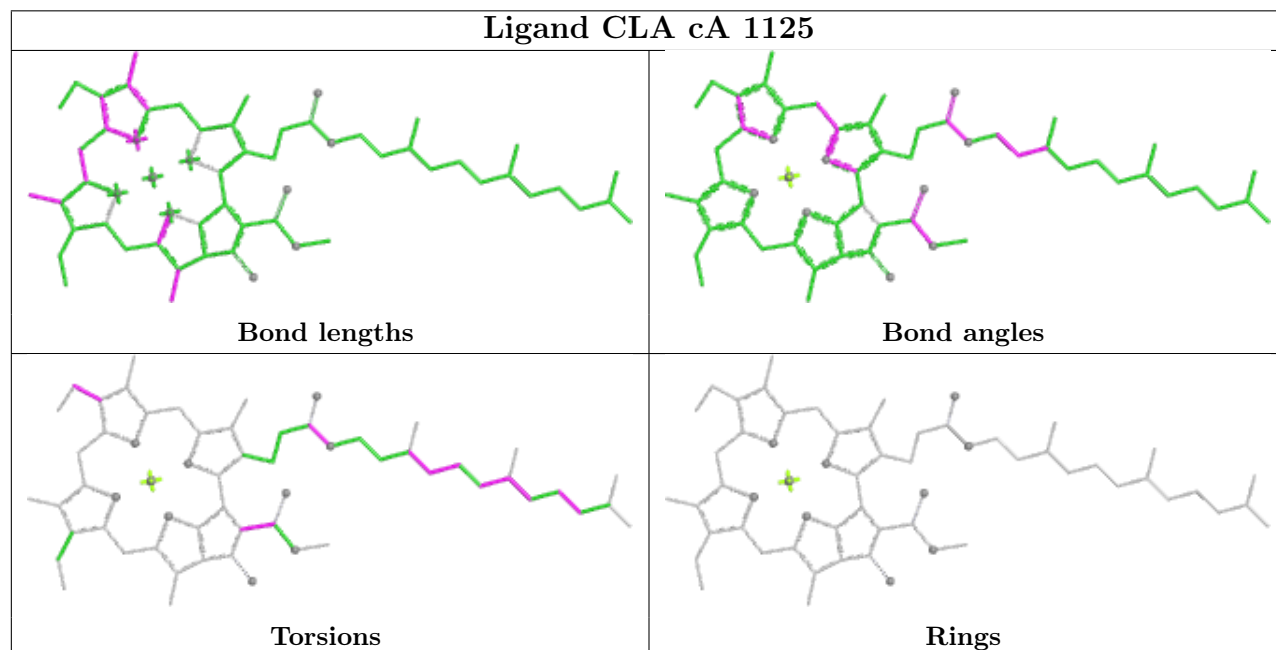
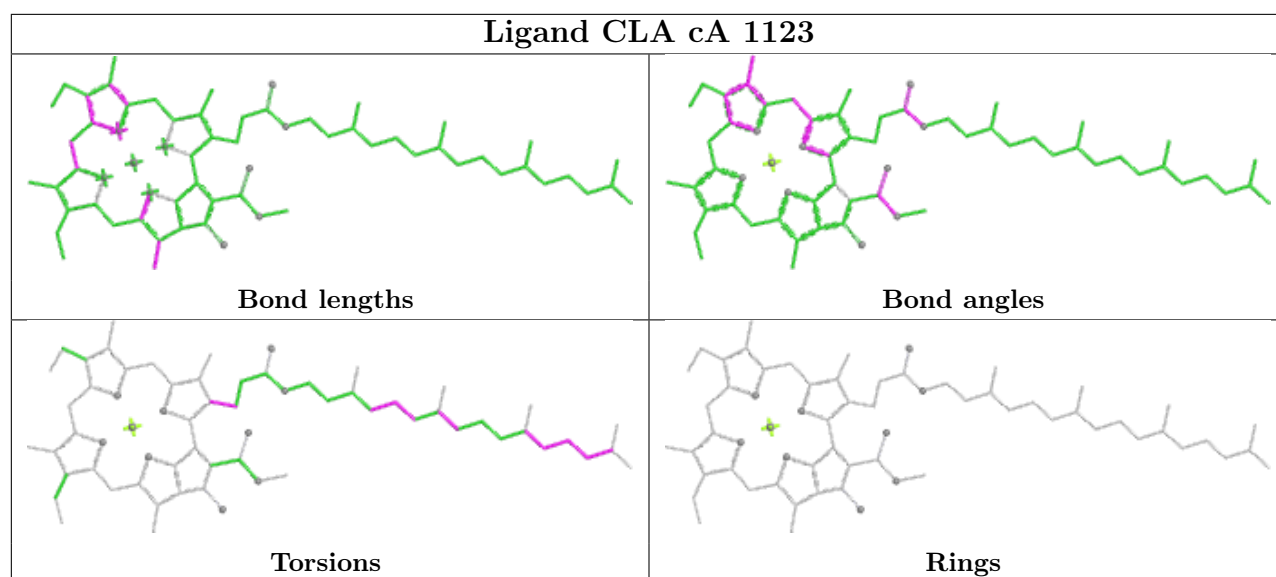


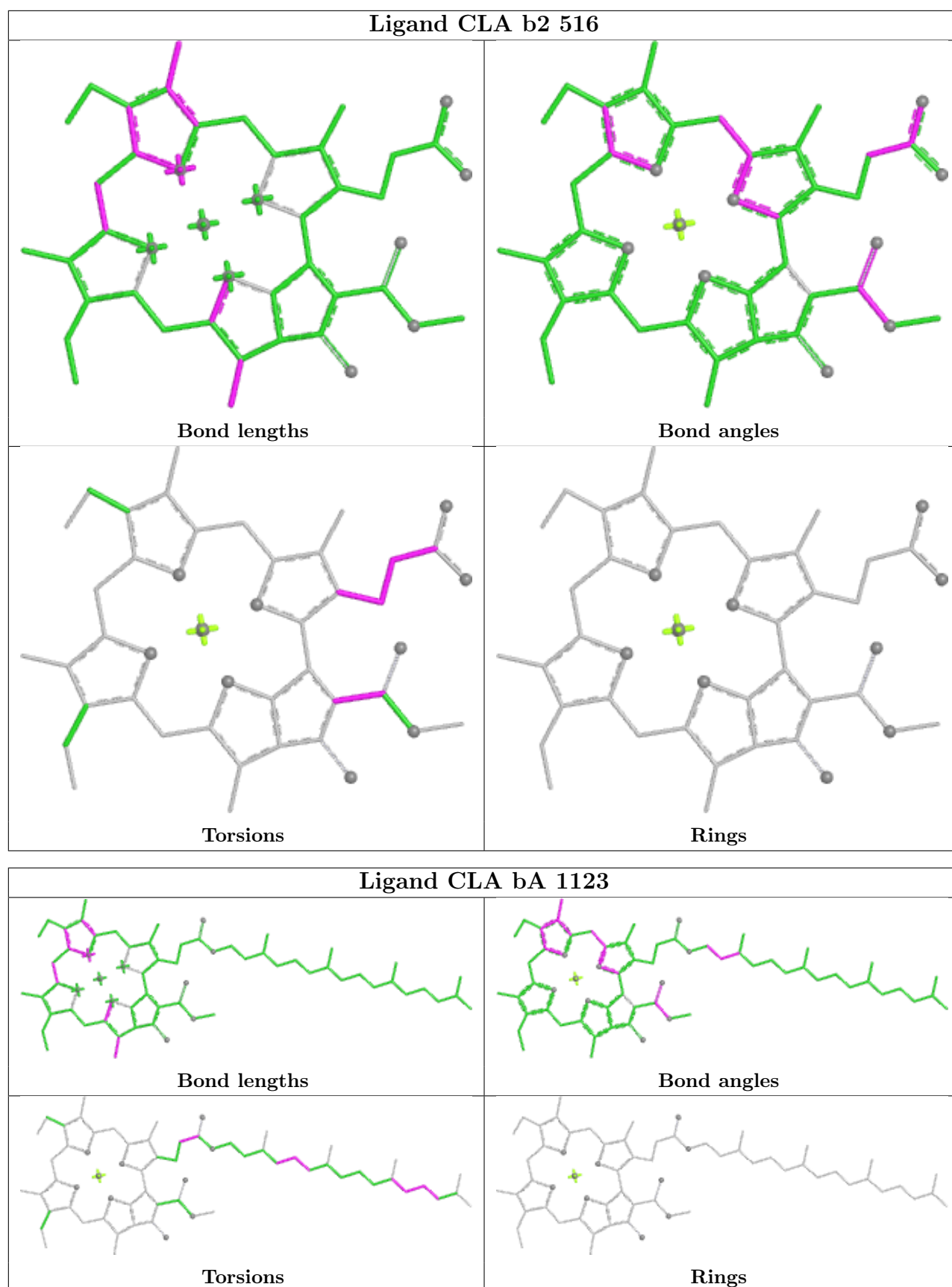
Ligand CLA g 511

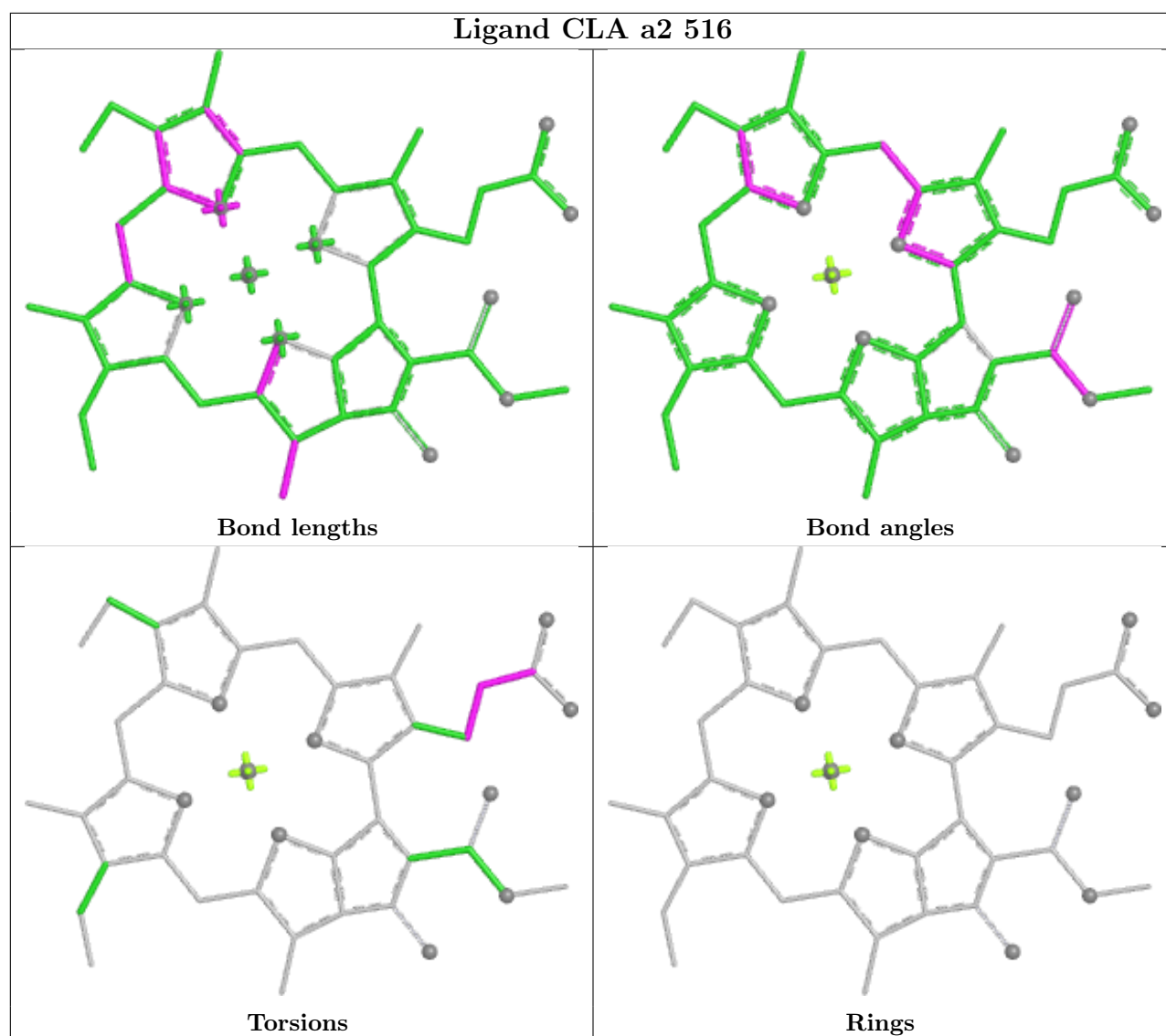


Ligand BCR a3 522

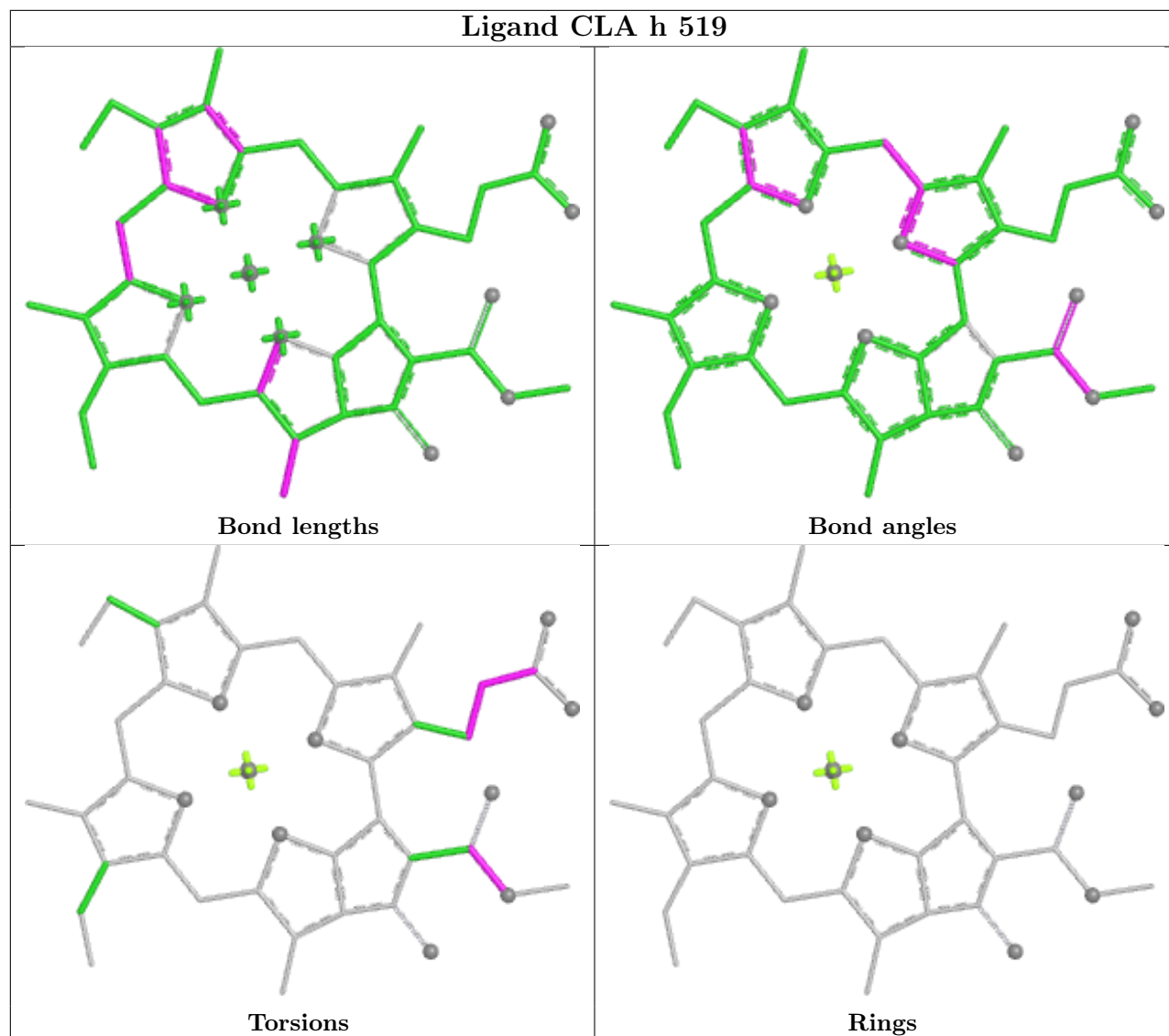




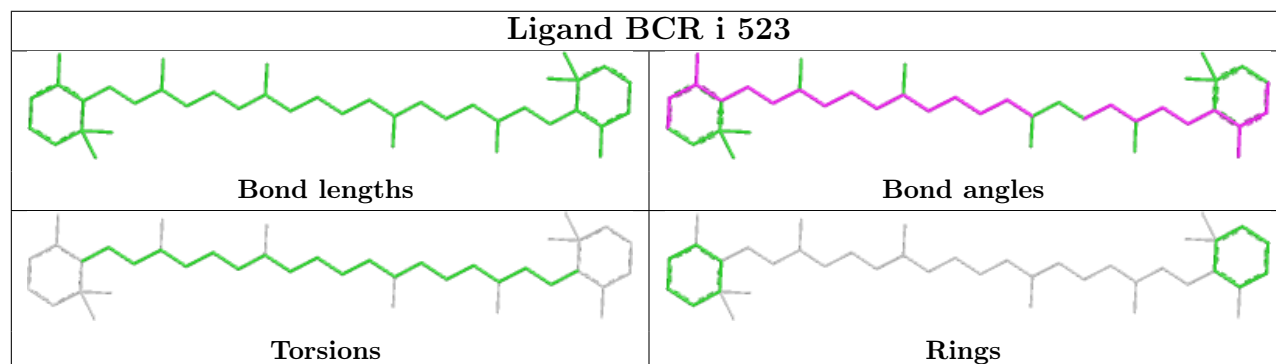


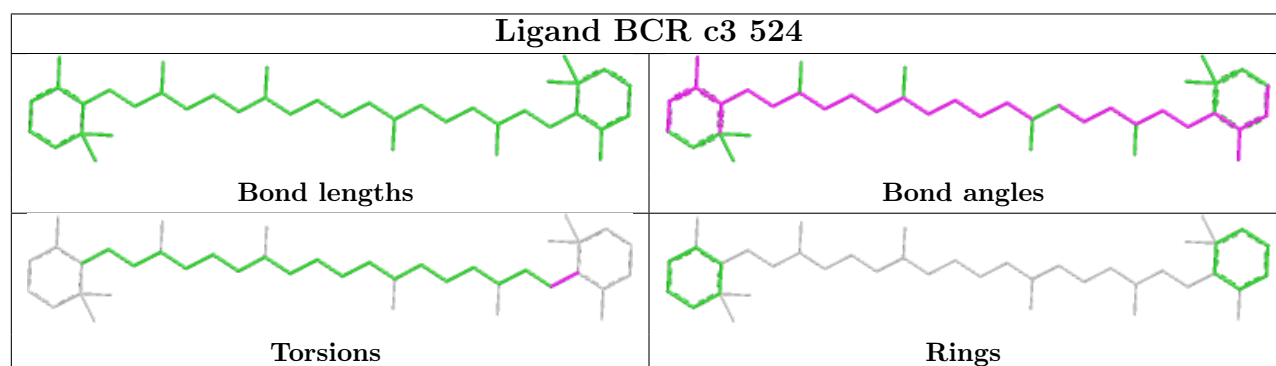
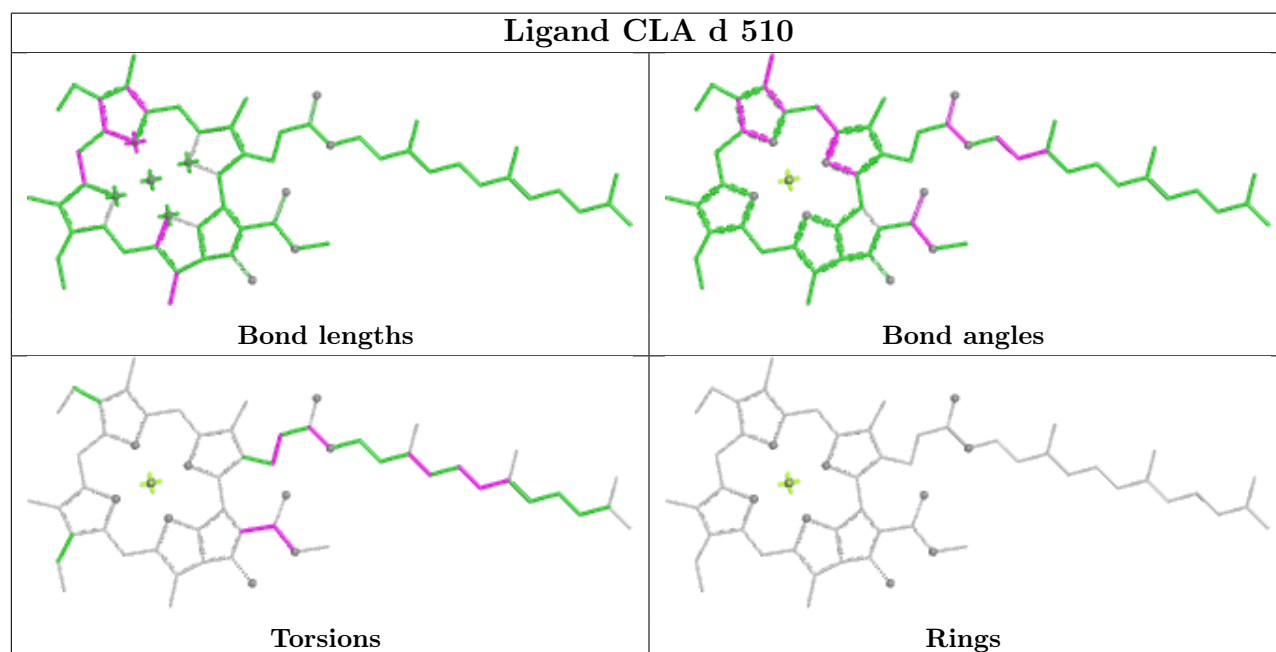
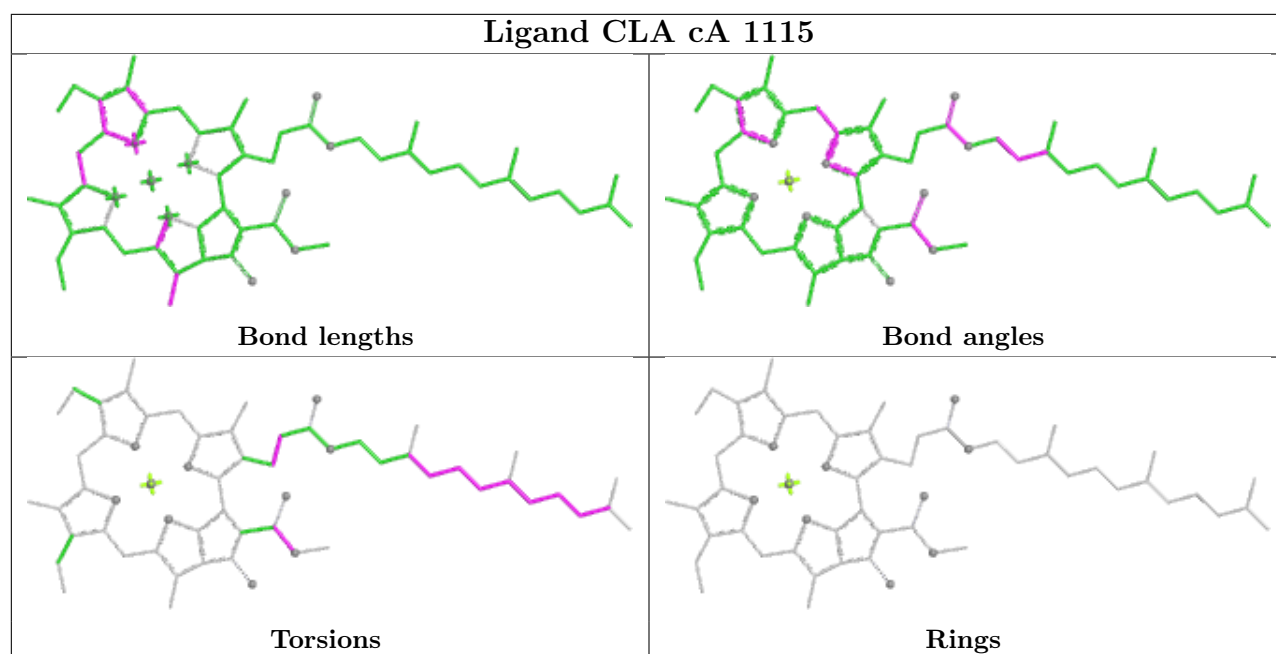


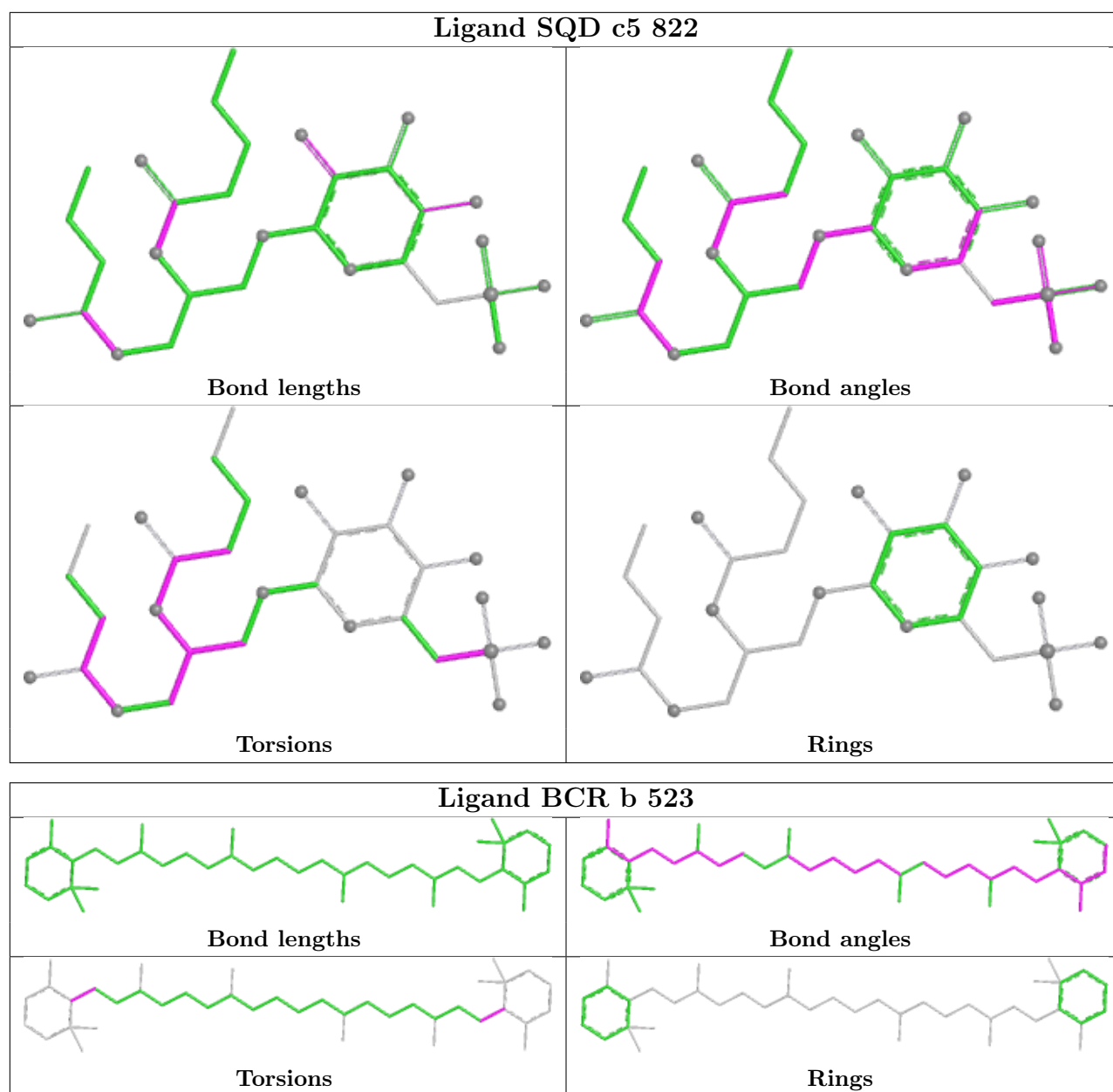
Ligand CLA h 519

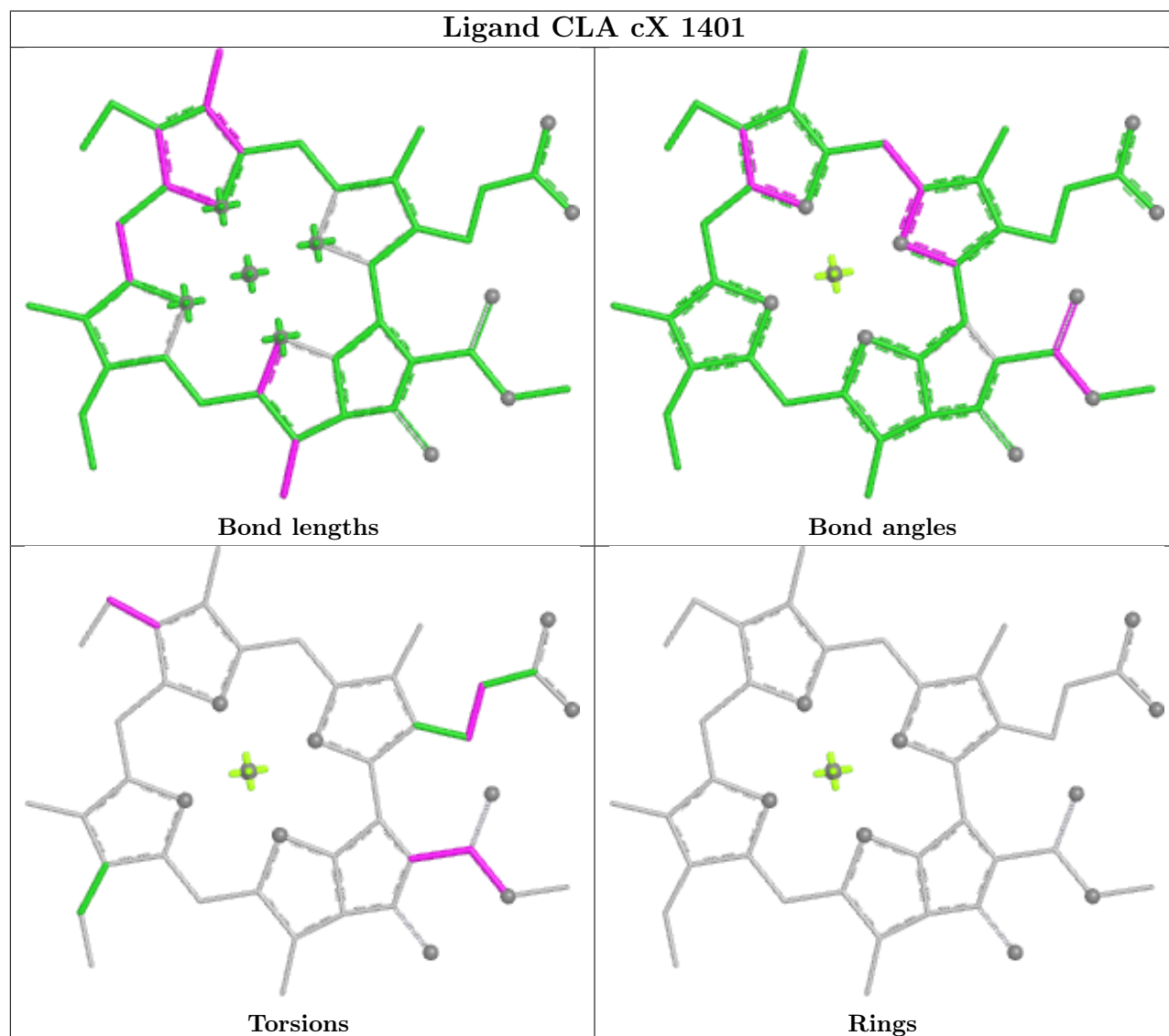
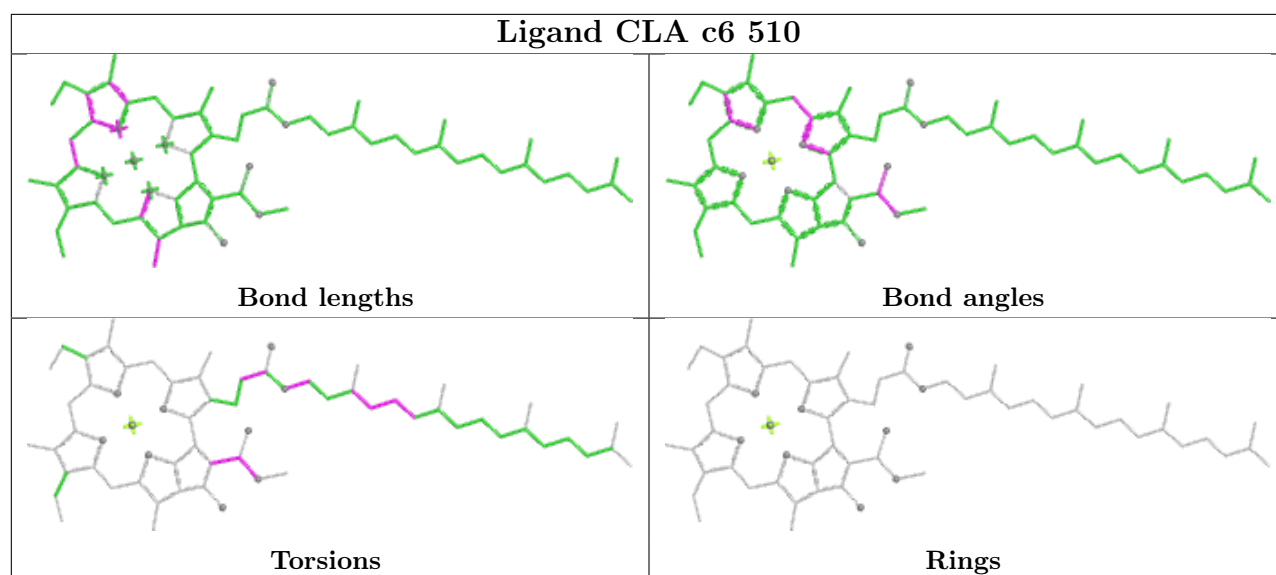


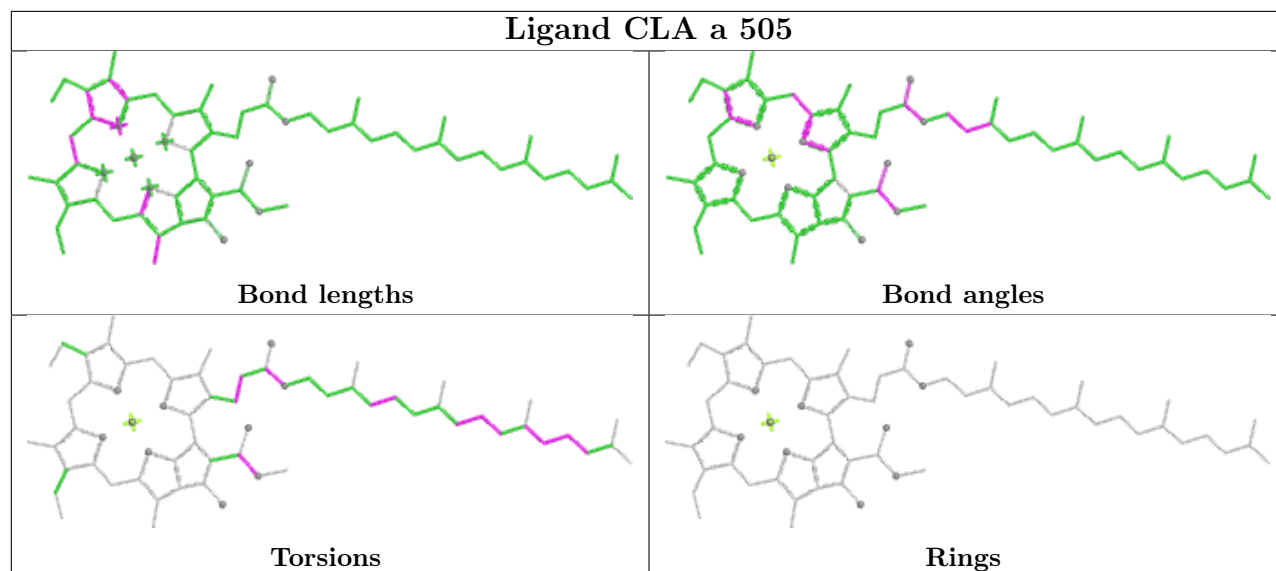
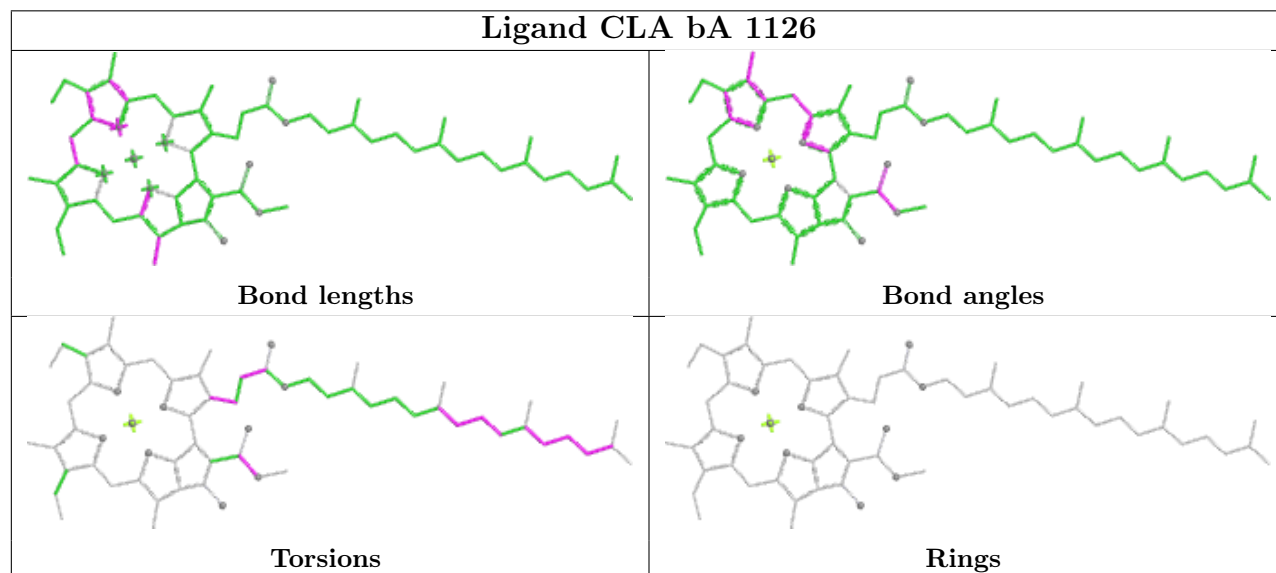
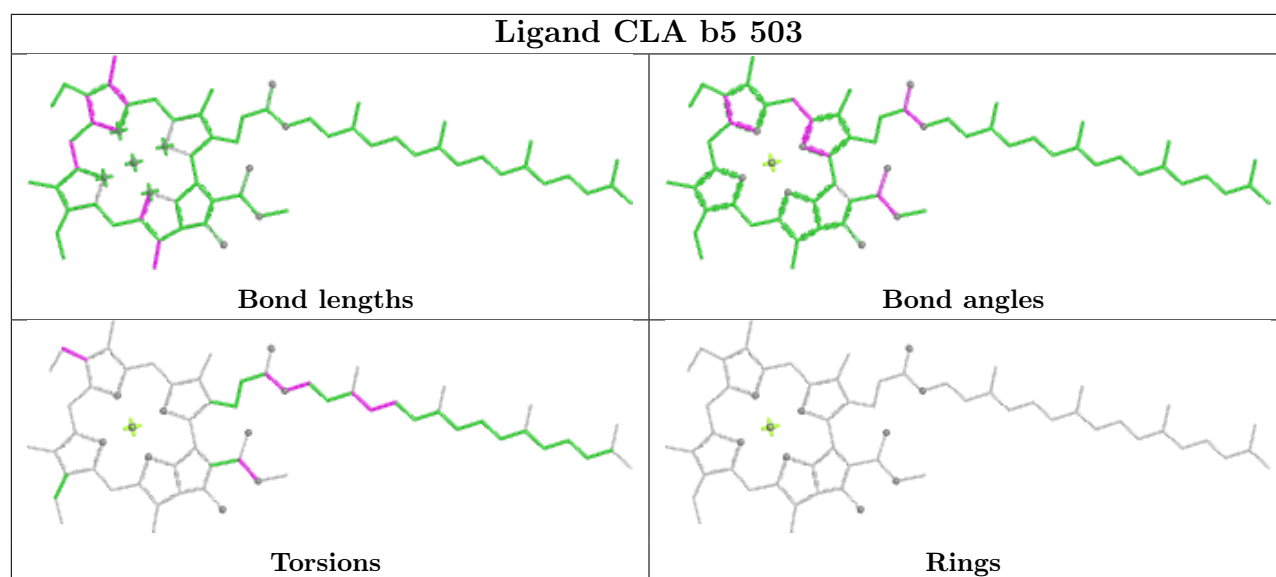
Ligand BCR i 523



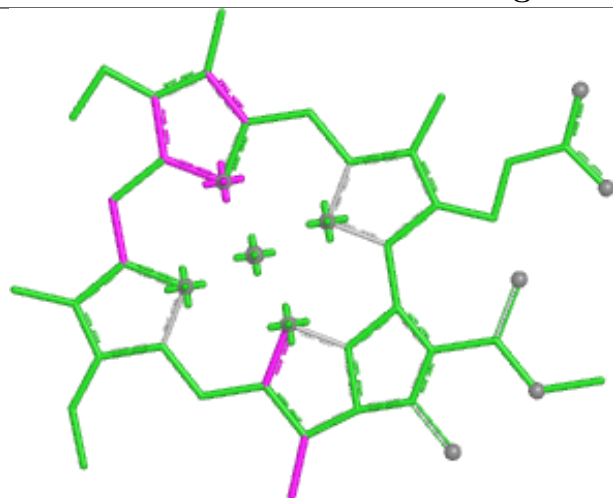




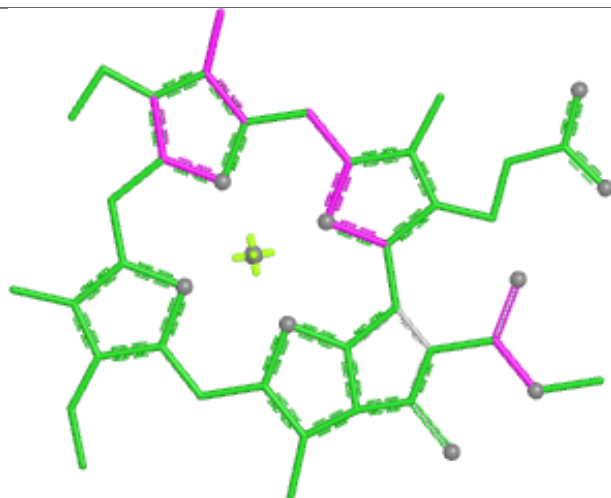




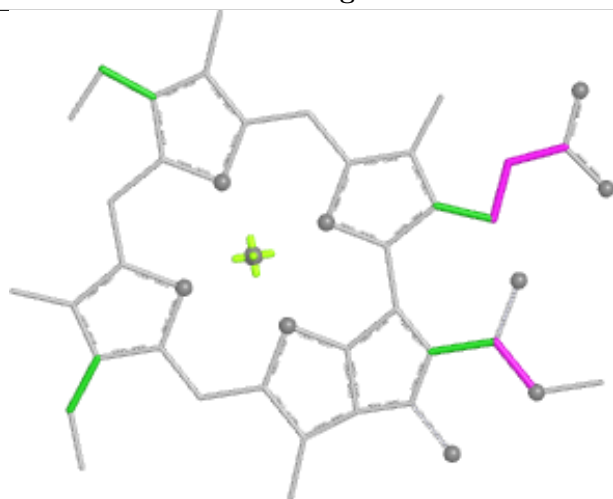
Ligand CLA U 513



Bond lengths



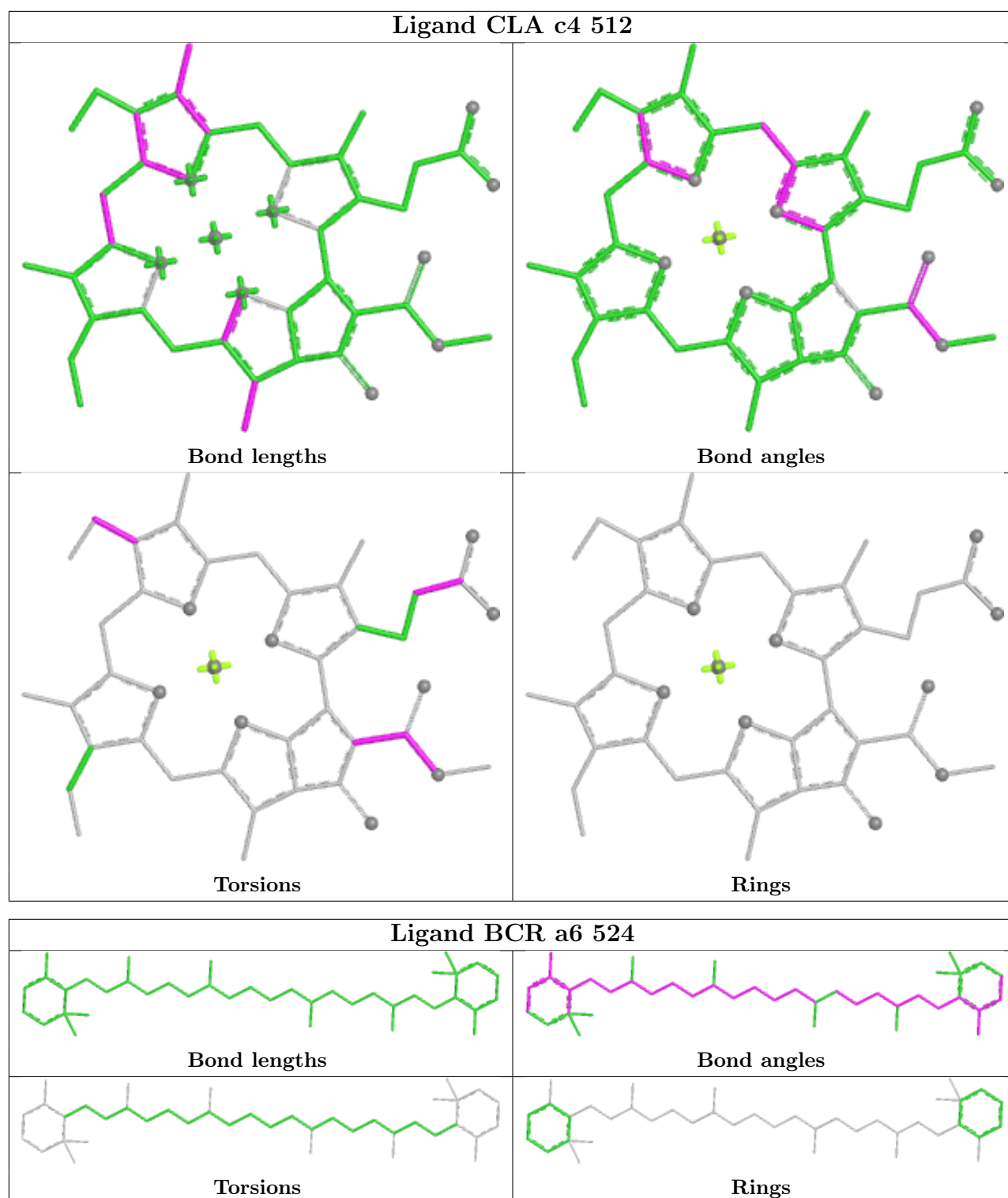
Bond angles

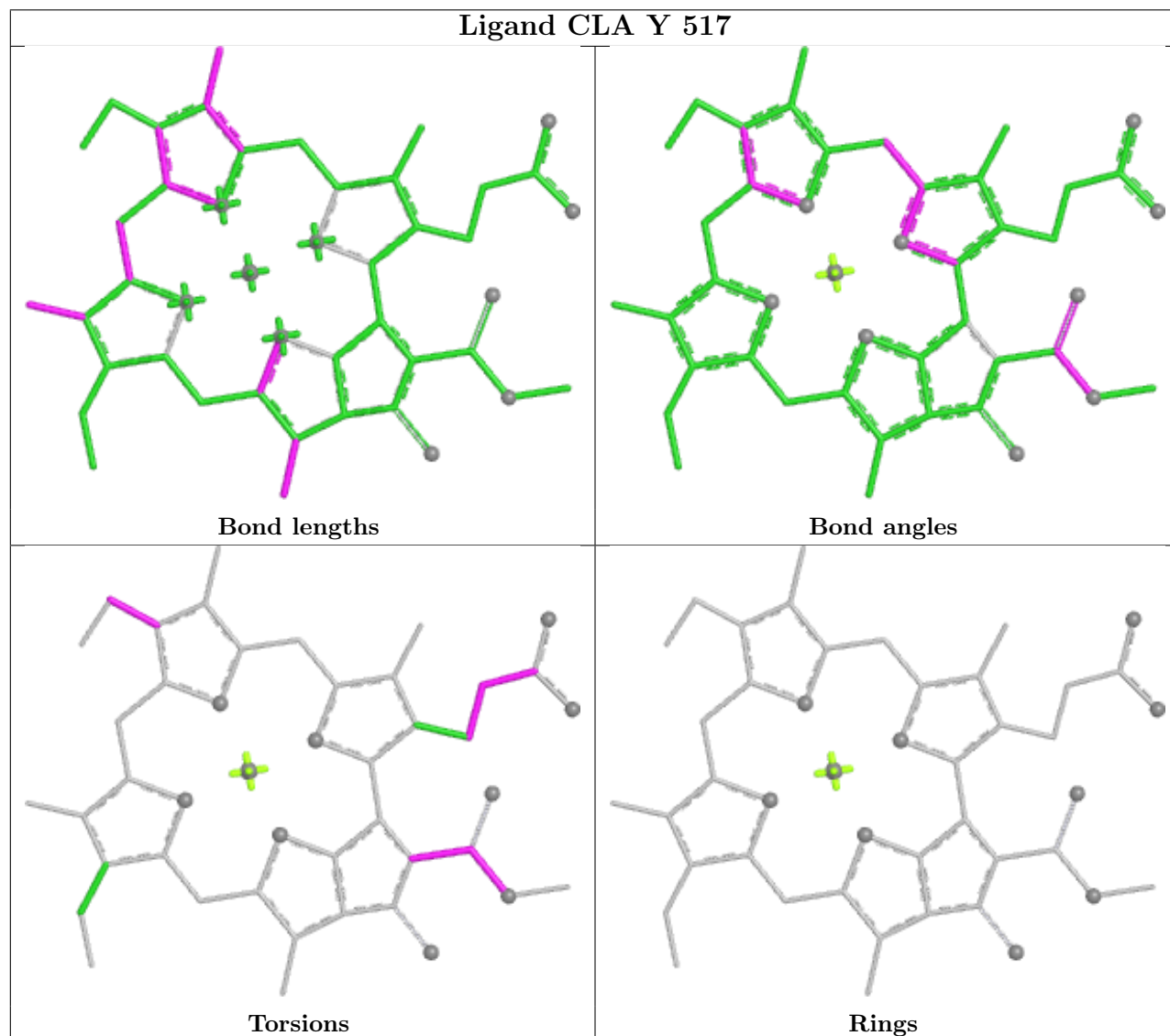
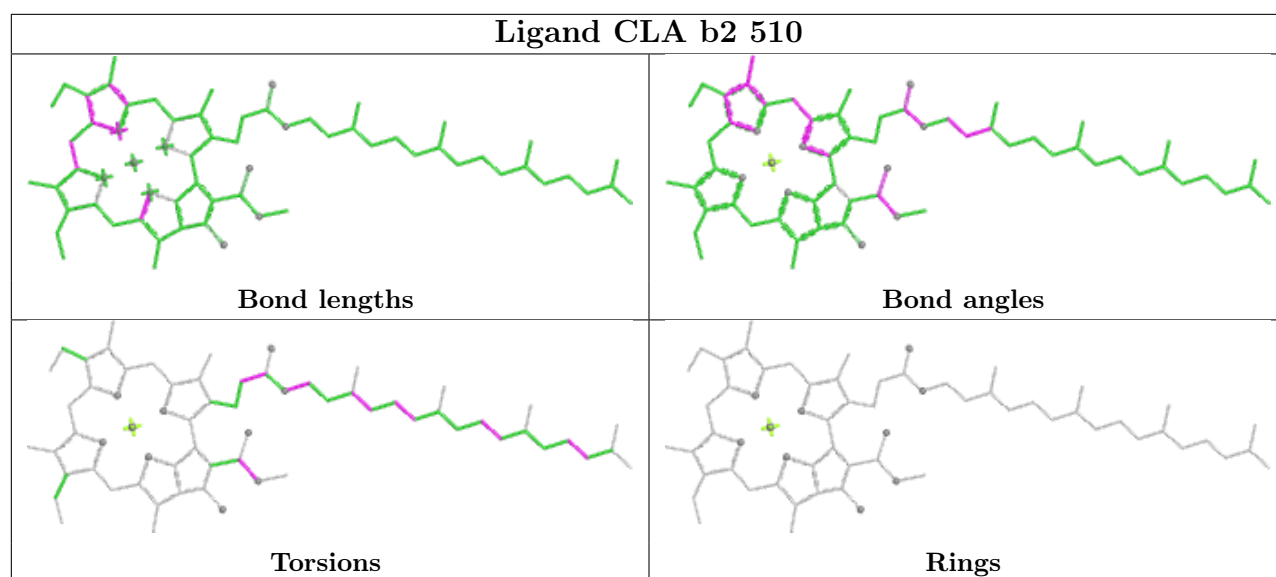


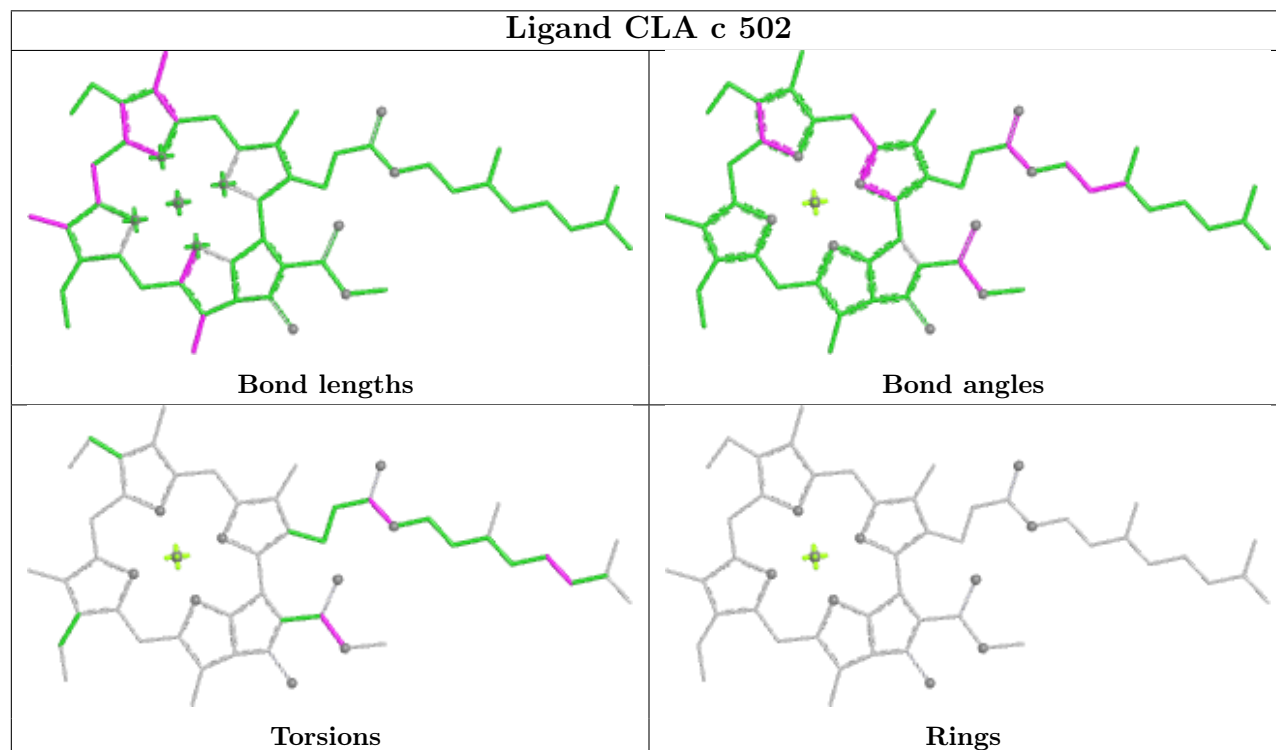
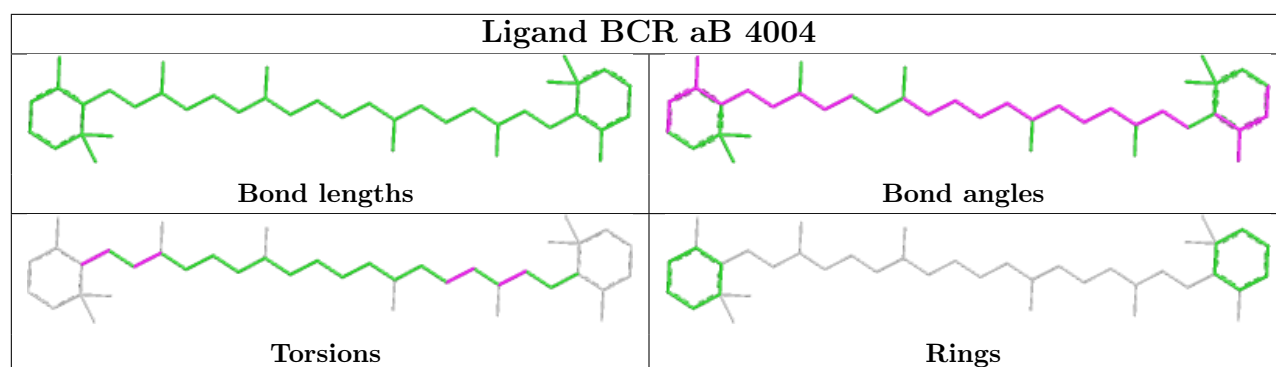
Torsions

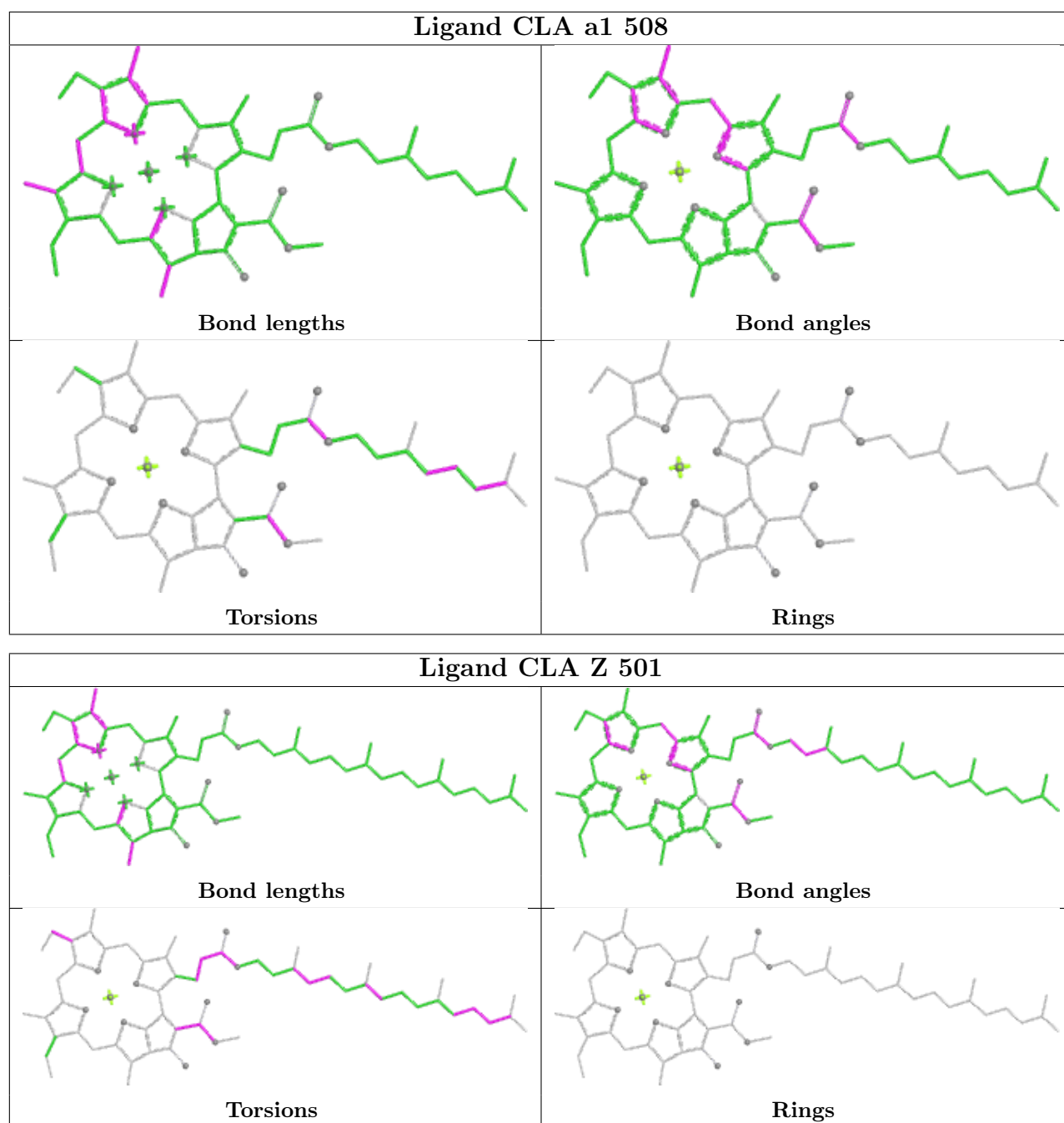


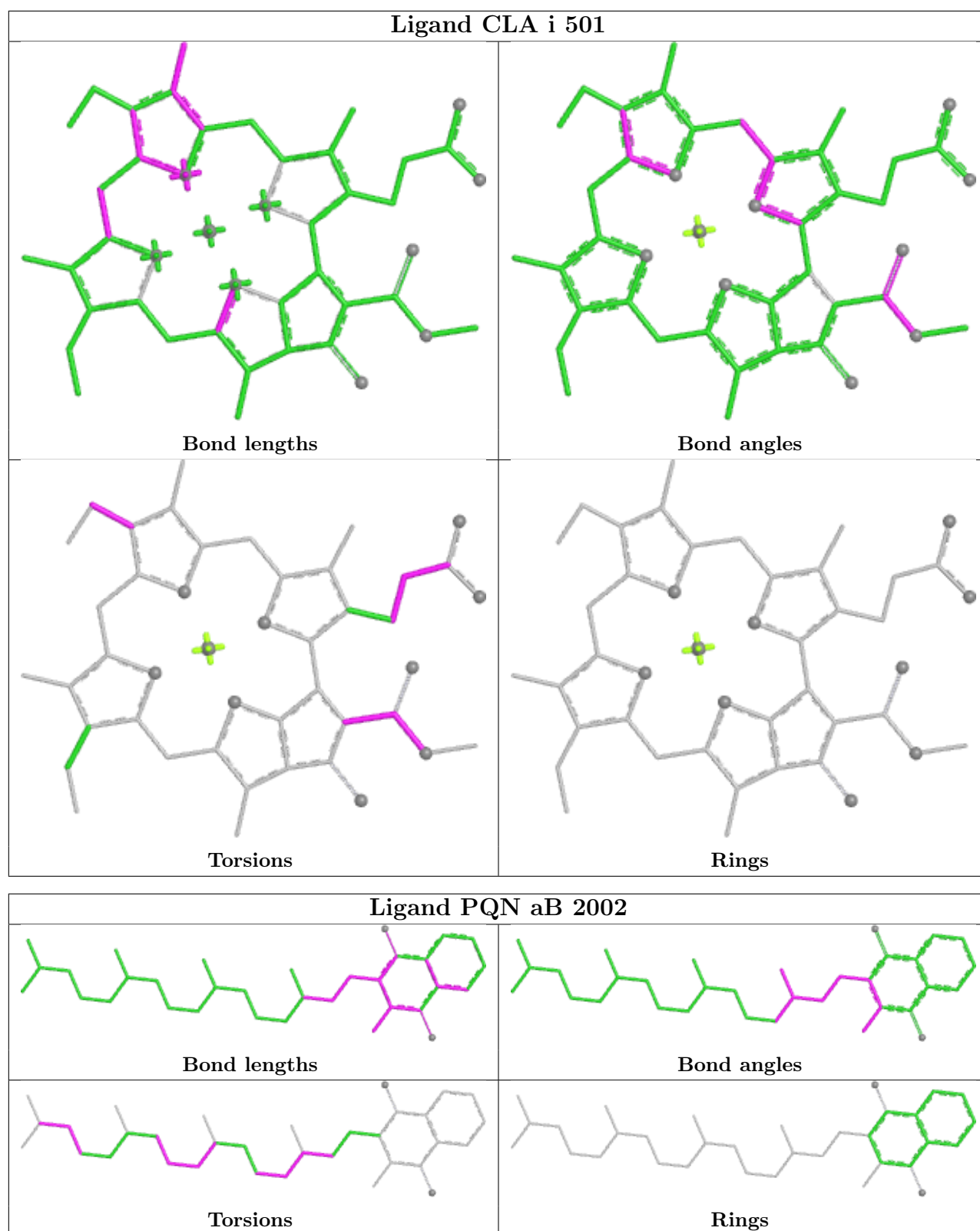
Rings

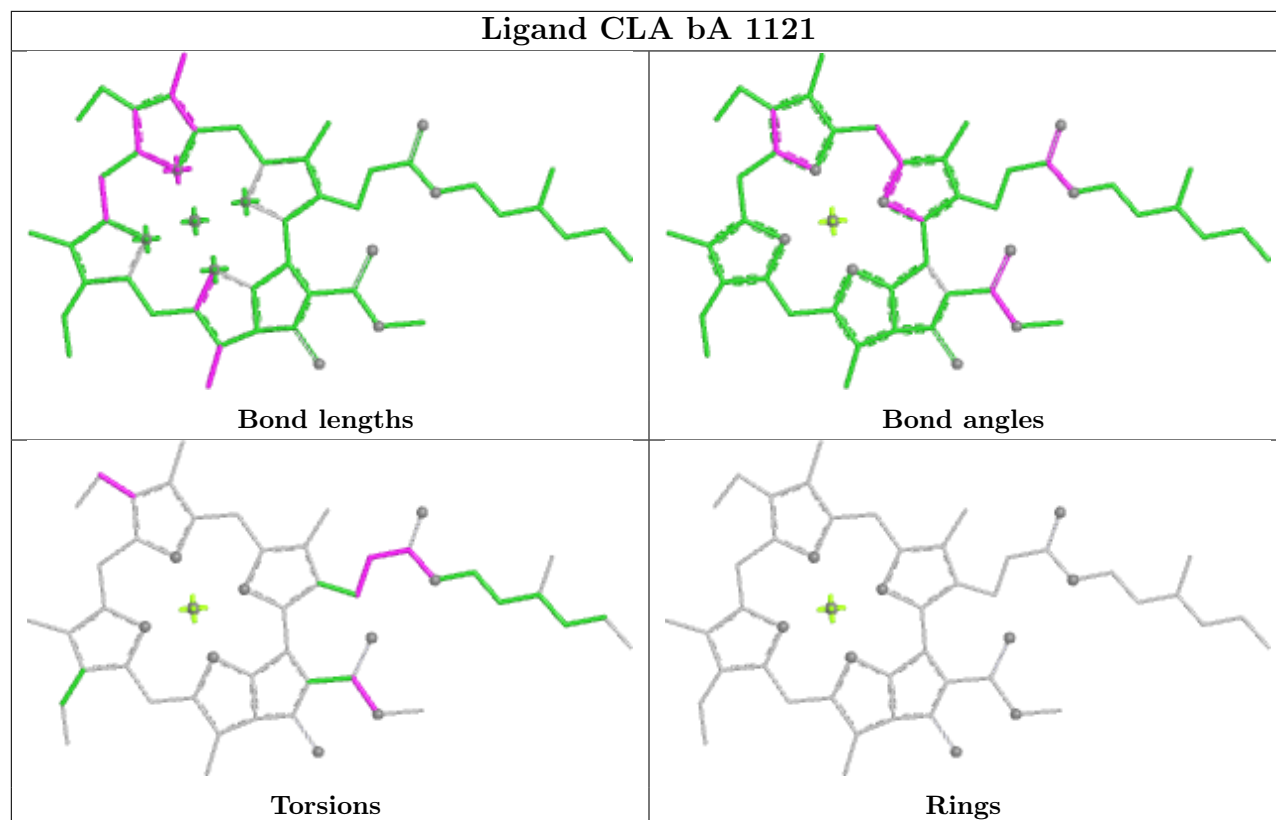




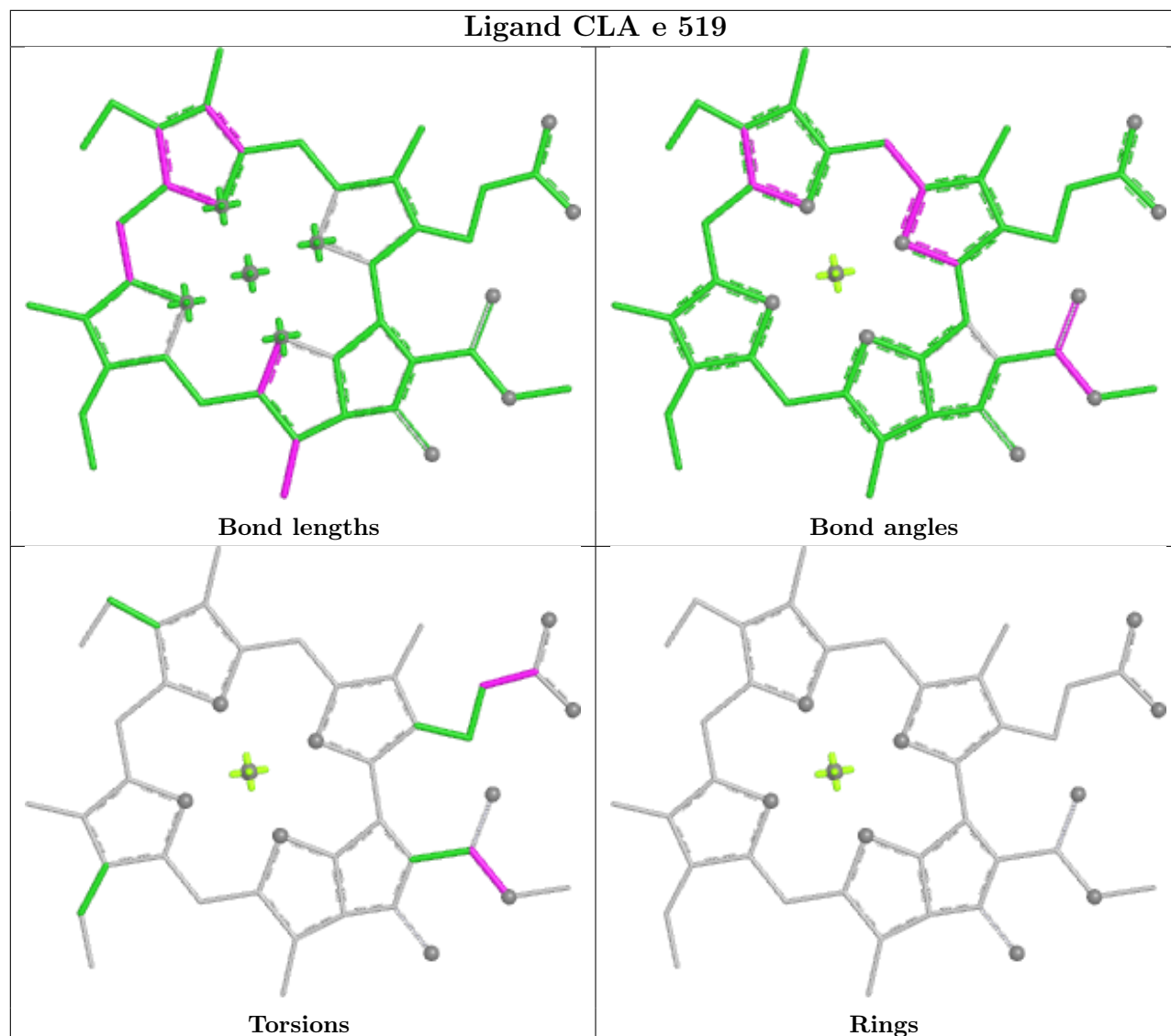




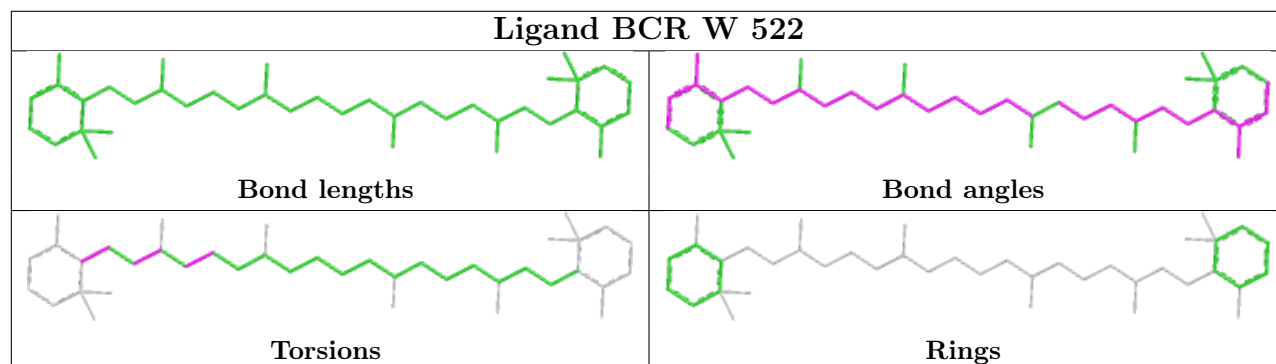


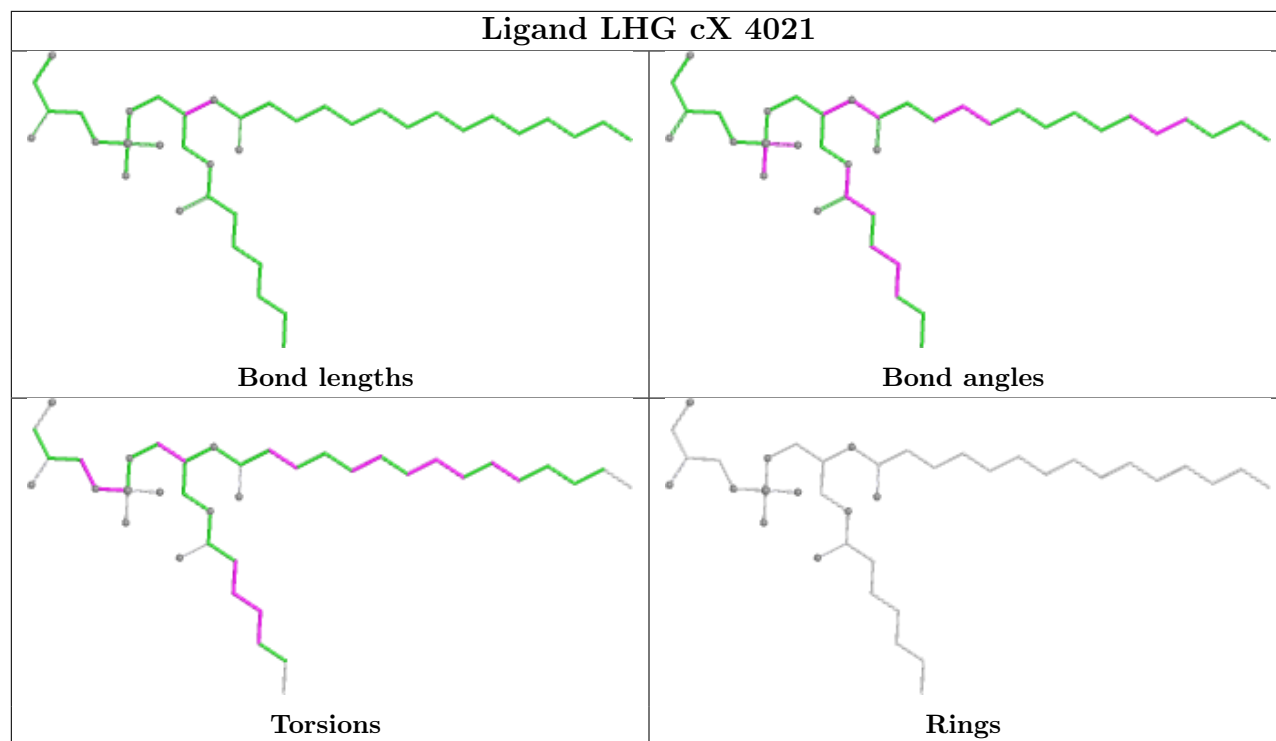


Ligand CLA e 519

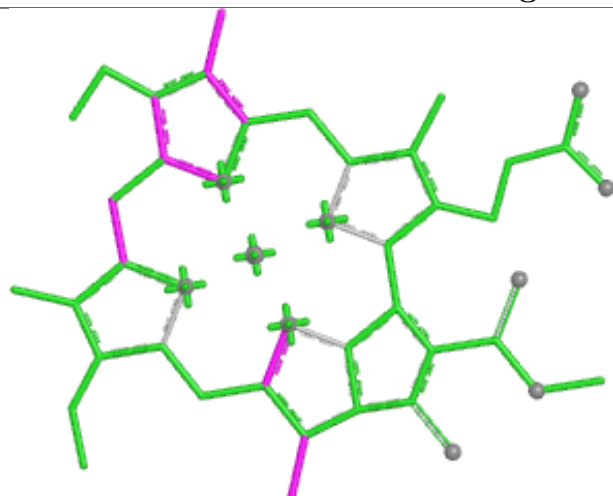


Ligand BCR W 522

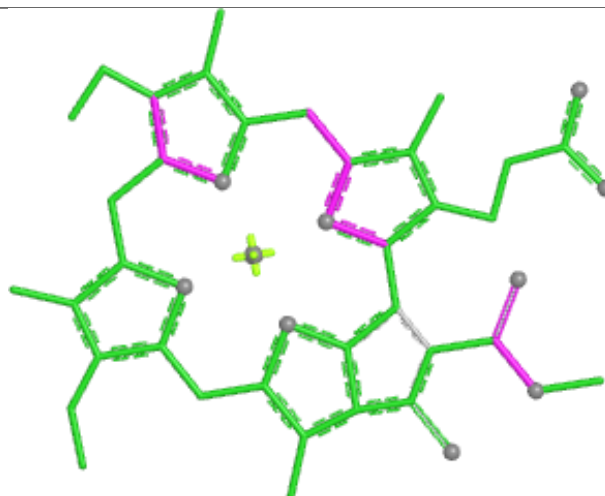




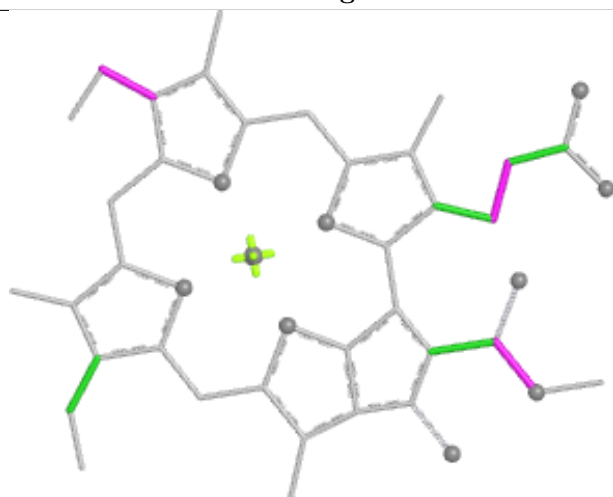
Ligand CLA c 503



Bond lengths



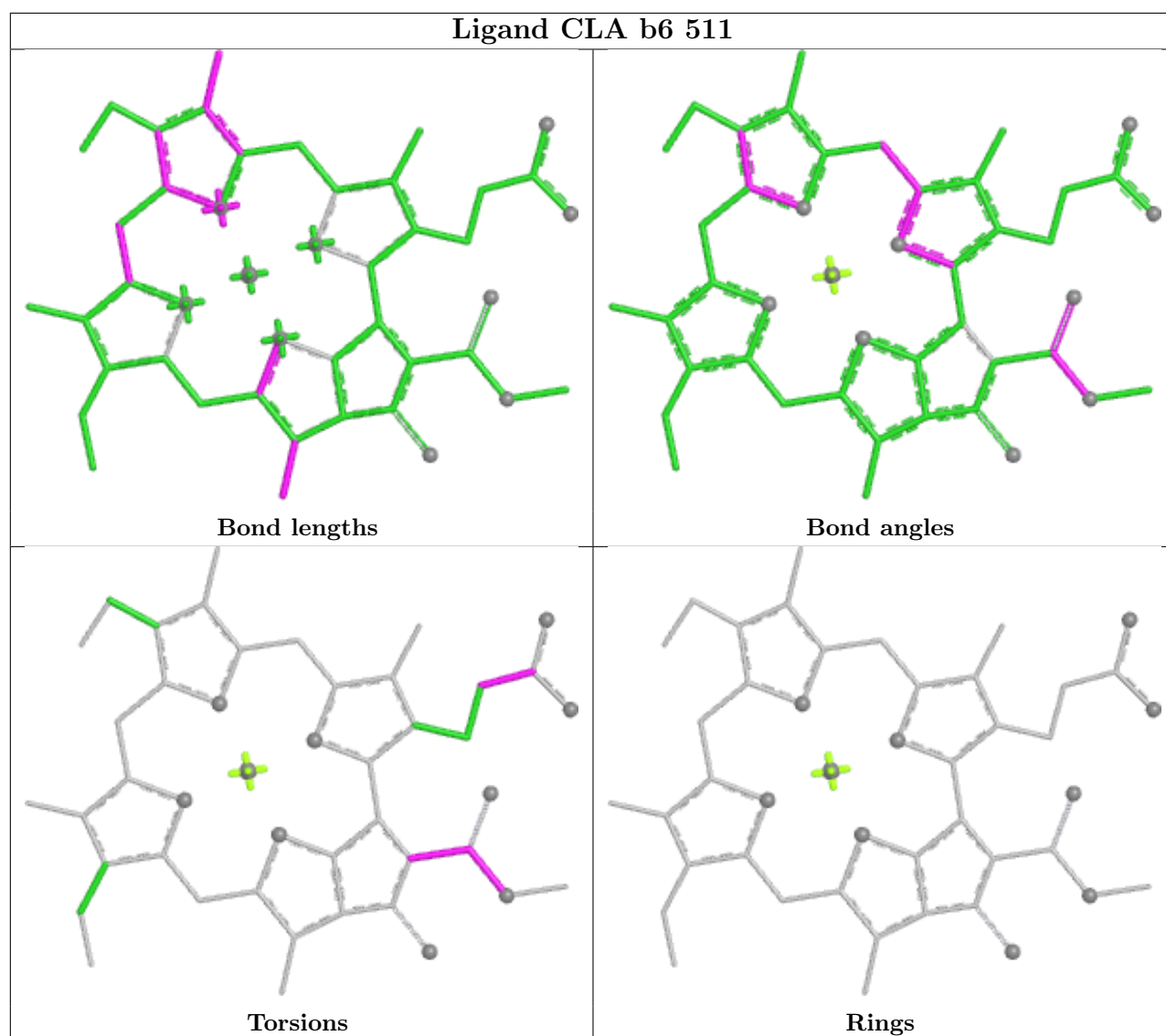
Bond angles

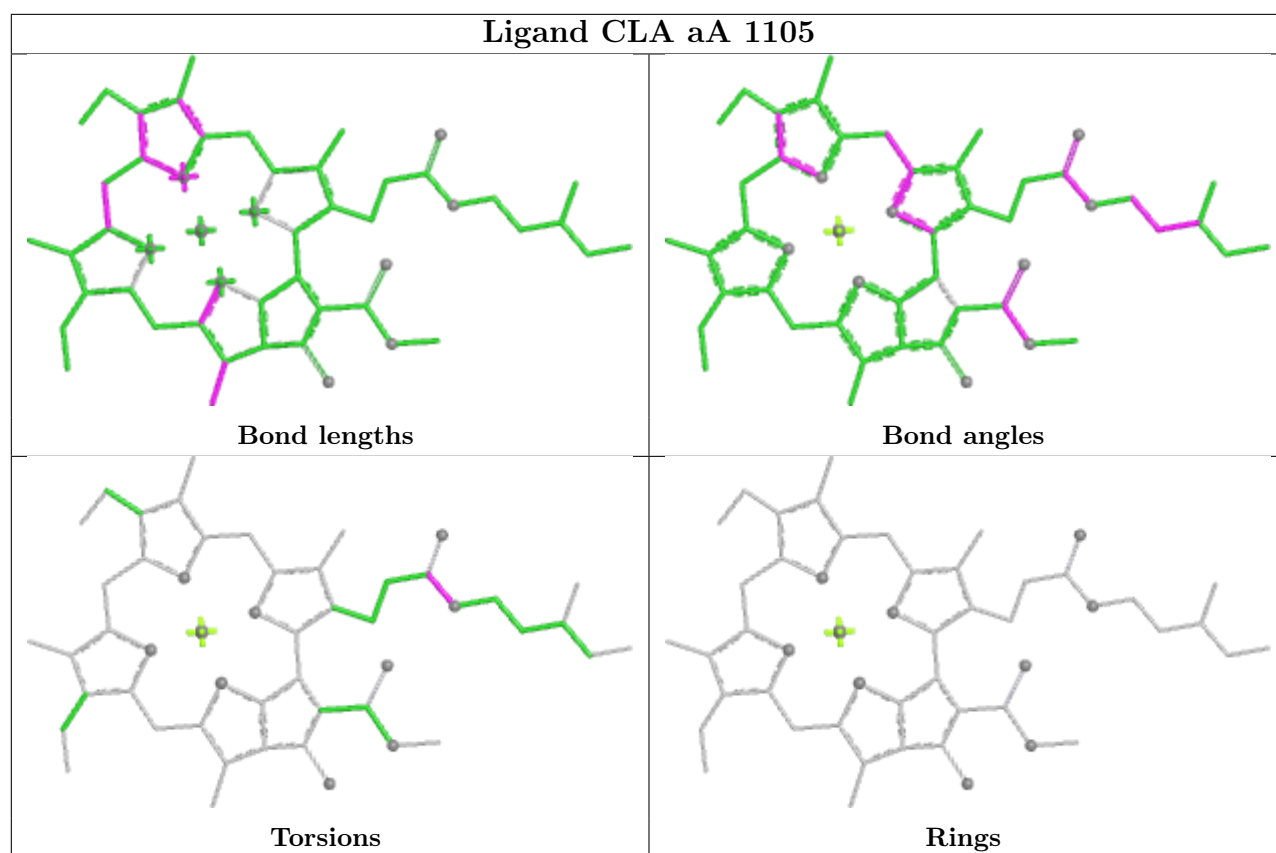


Torsions

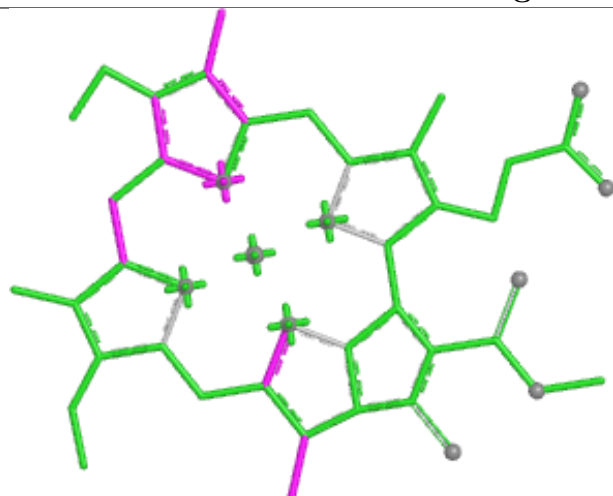


Rings





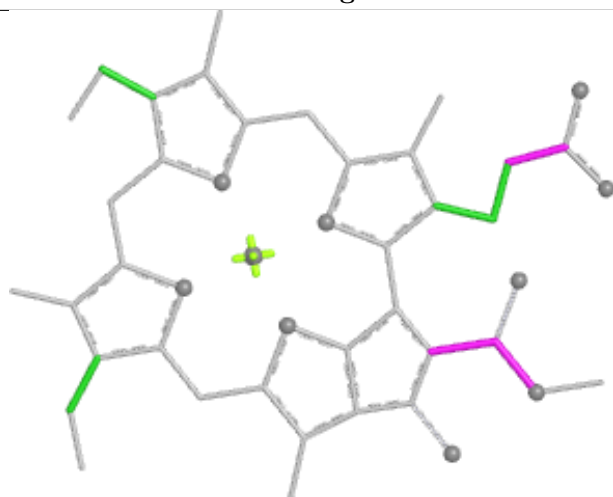
Ligand CLA Y 511



Bond lengths



Bond angles

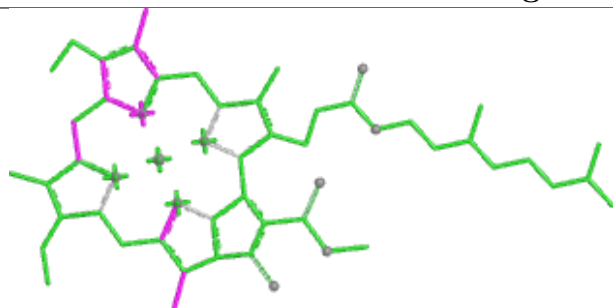


Torsions

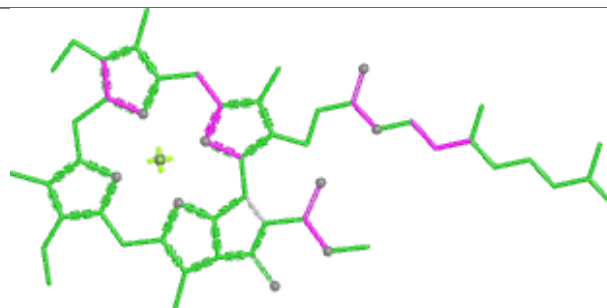


Rings

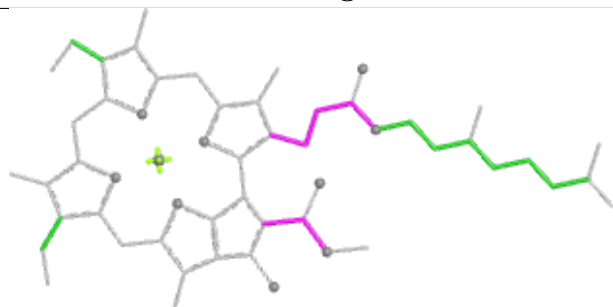
Ligand CLA i 518



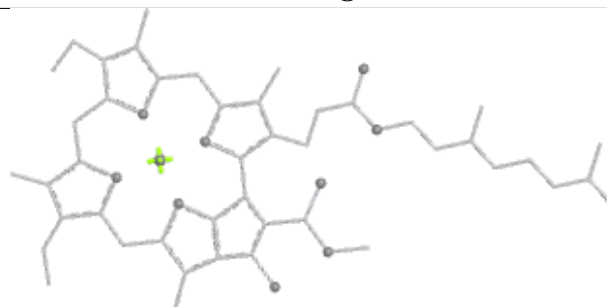
Bond lengths



Bond angles

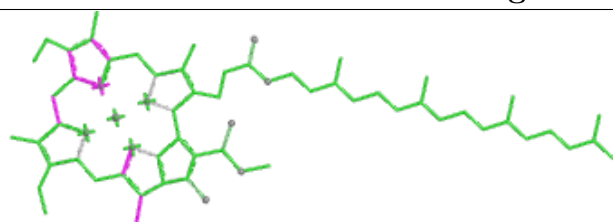


Torsions

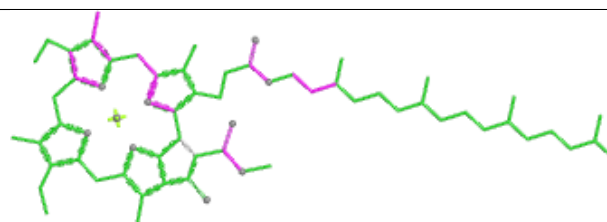


Rings

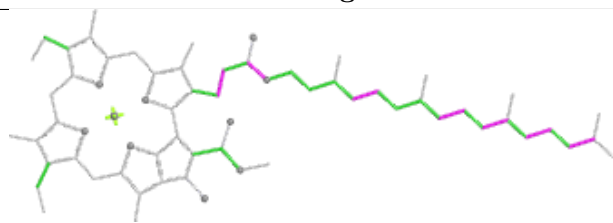
Ligand CLA b5 505



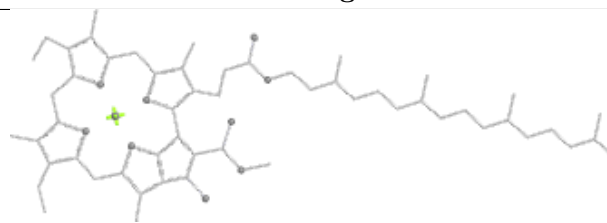
Bond lengths



Bond angles

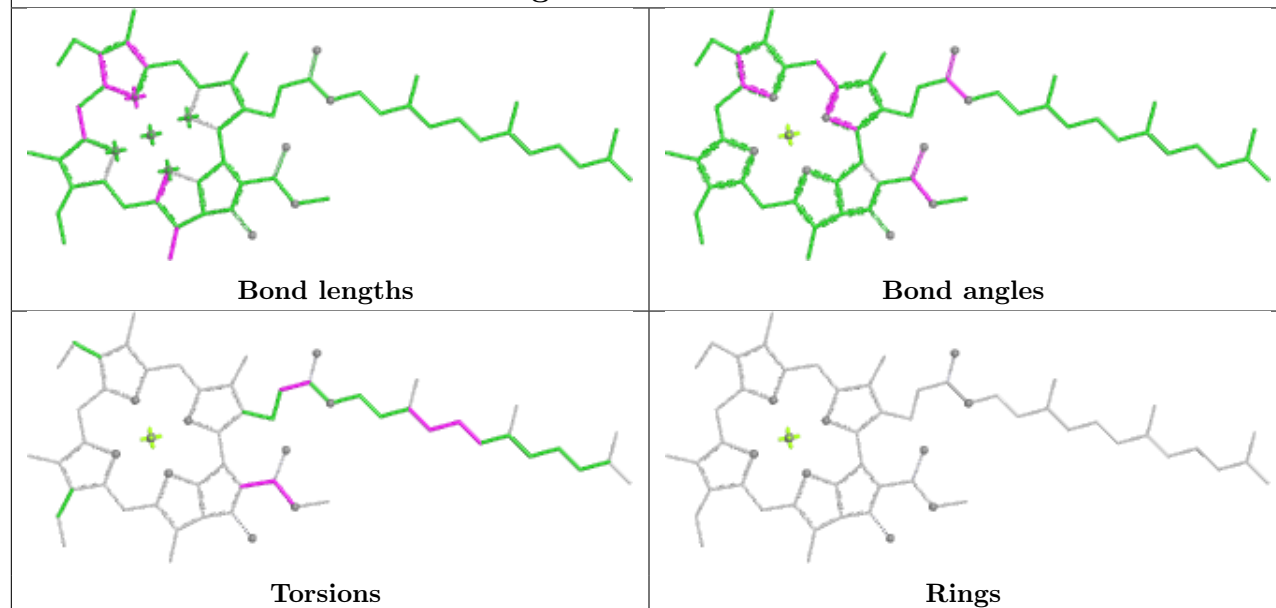


Torsions

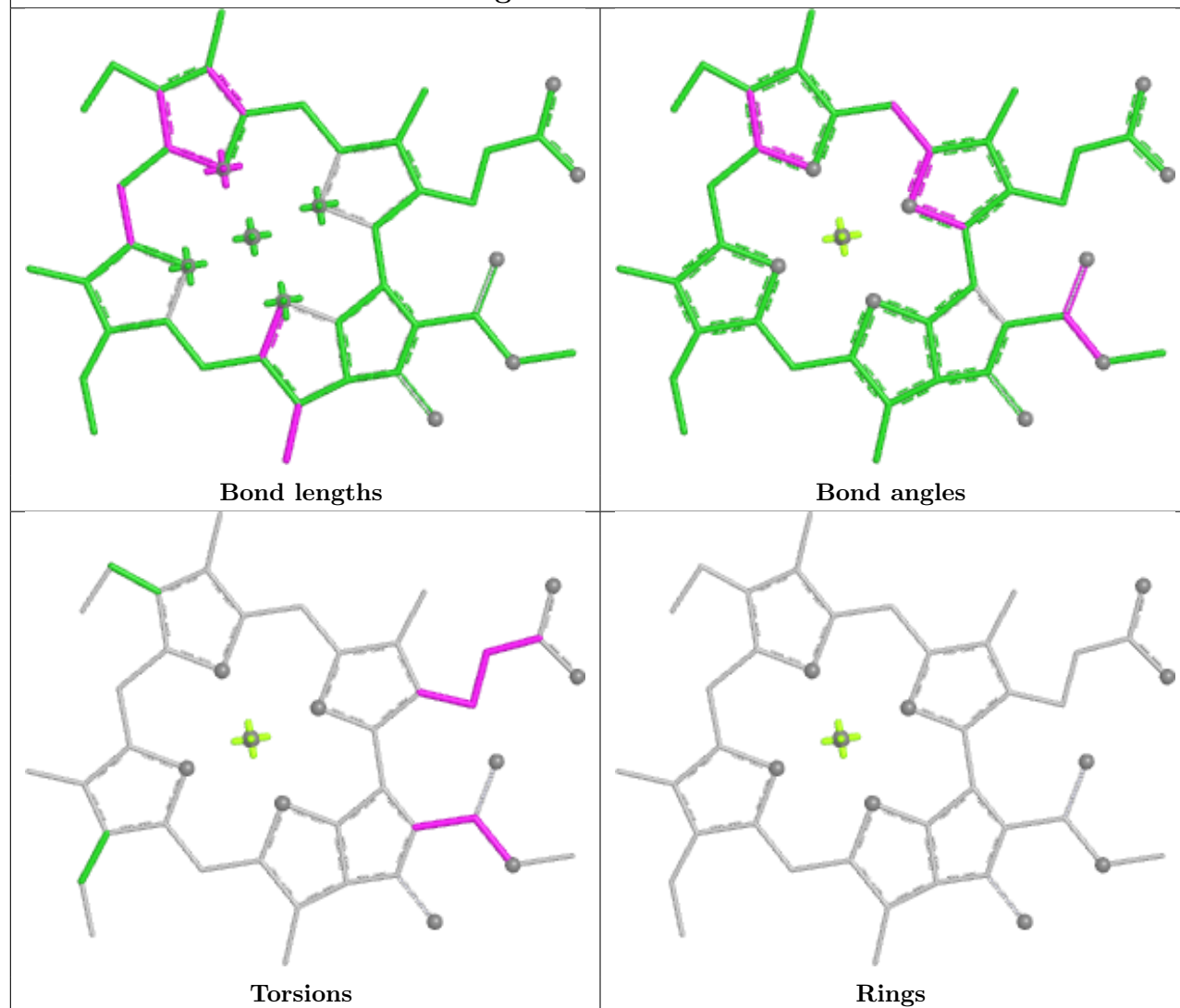


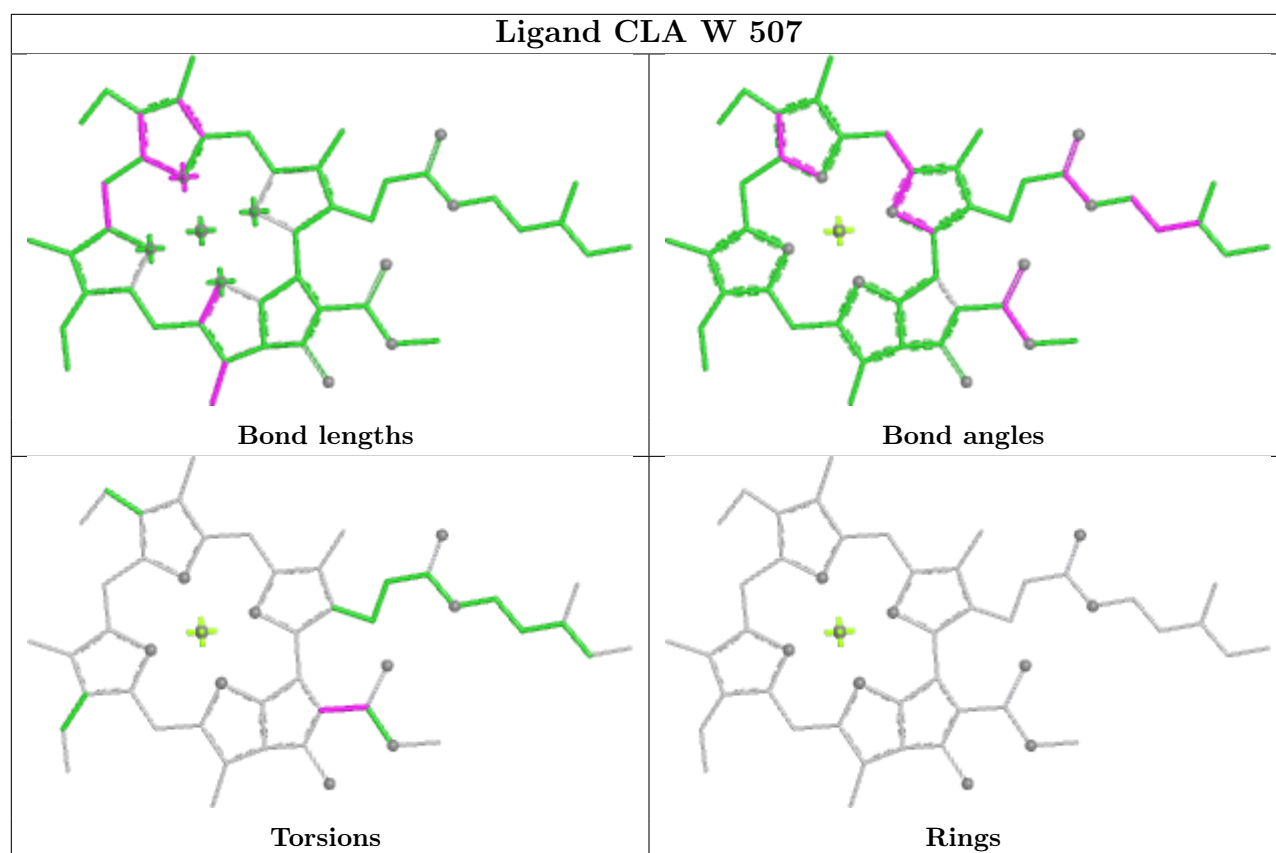
Rings

Ligand CLA V 510

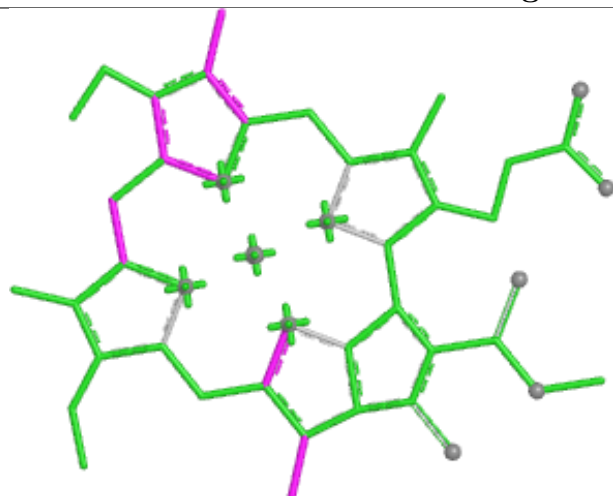


Ligand CLA n 501

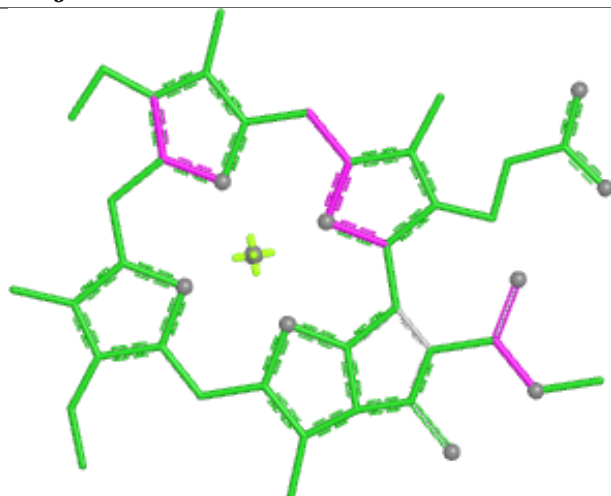




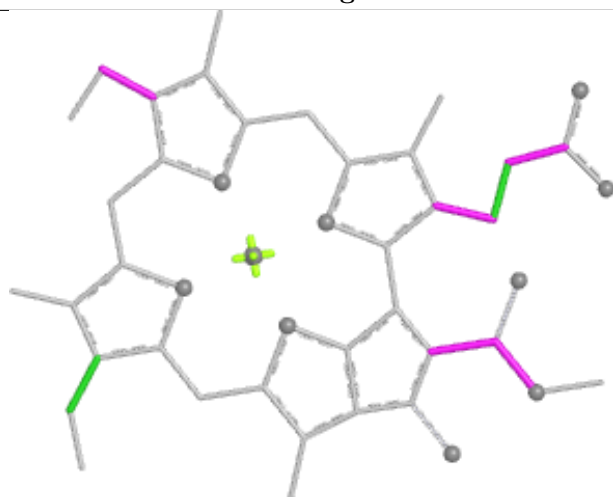
Ligand CLA j 501



Bond lengths



Bond angles

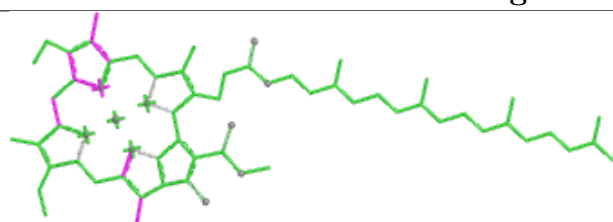


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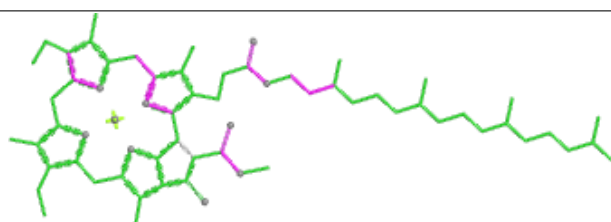


Rings

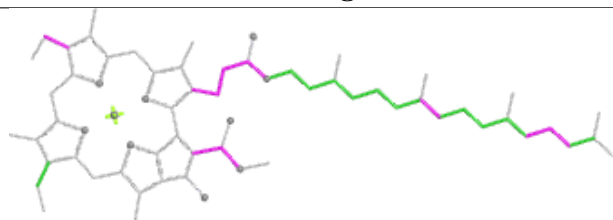
Ligand CLA a1 501



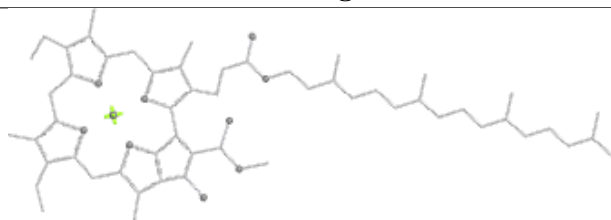
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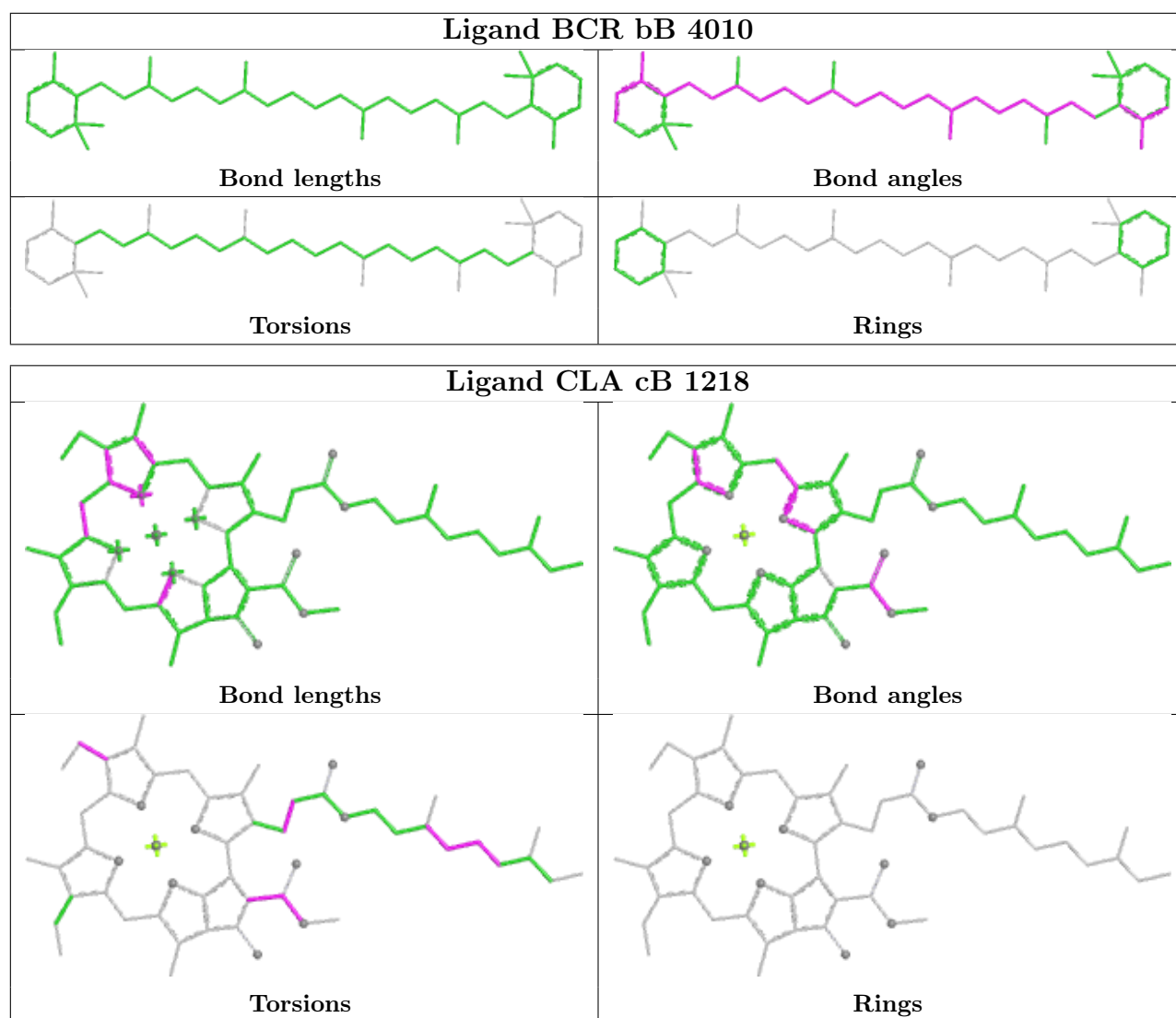
Bond angles

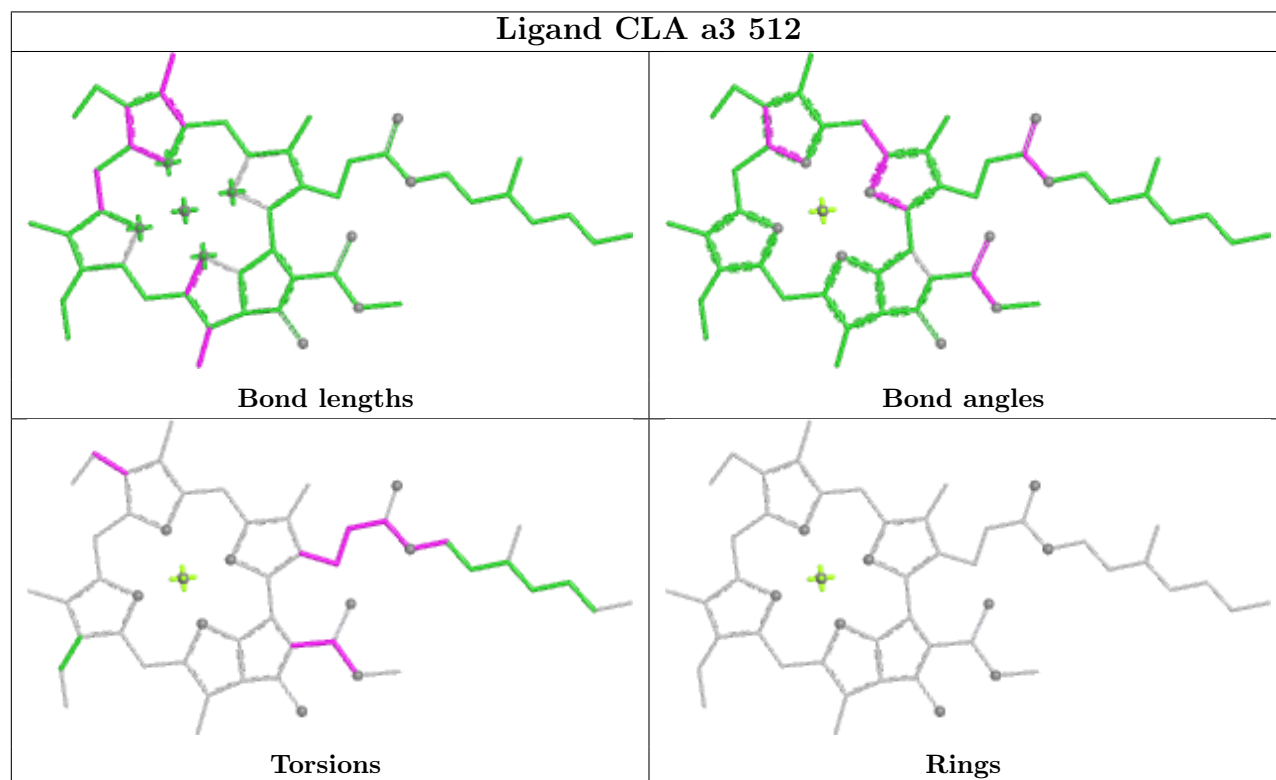
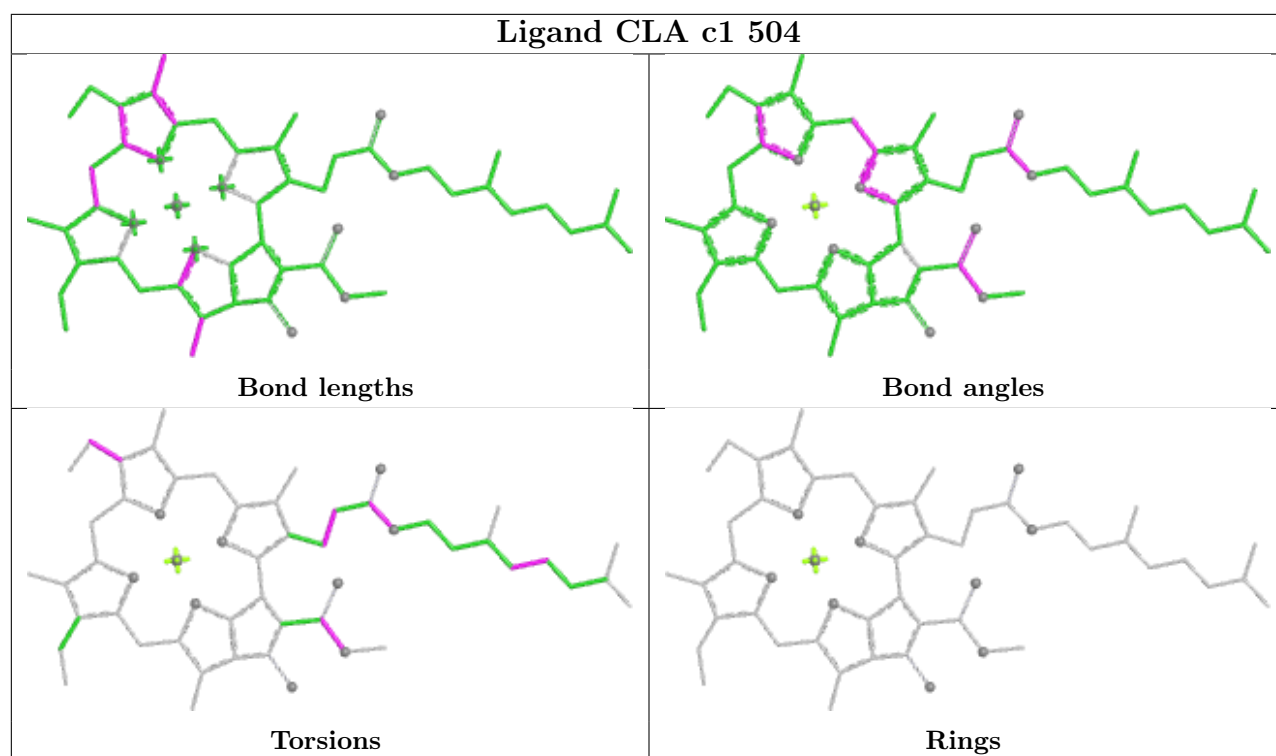


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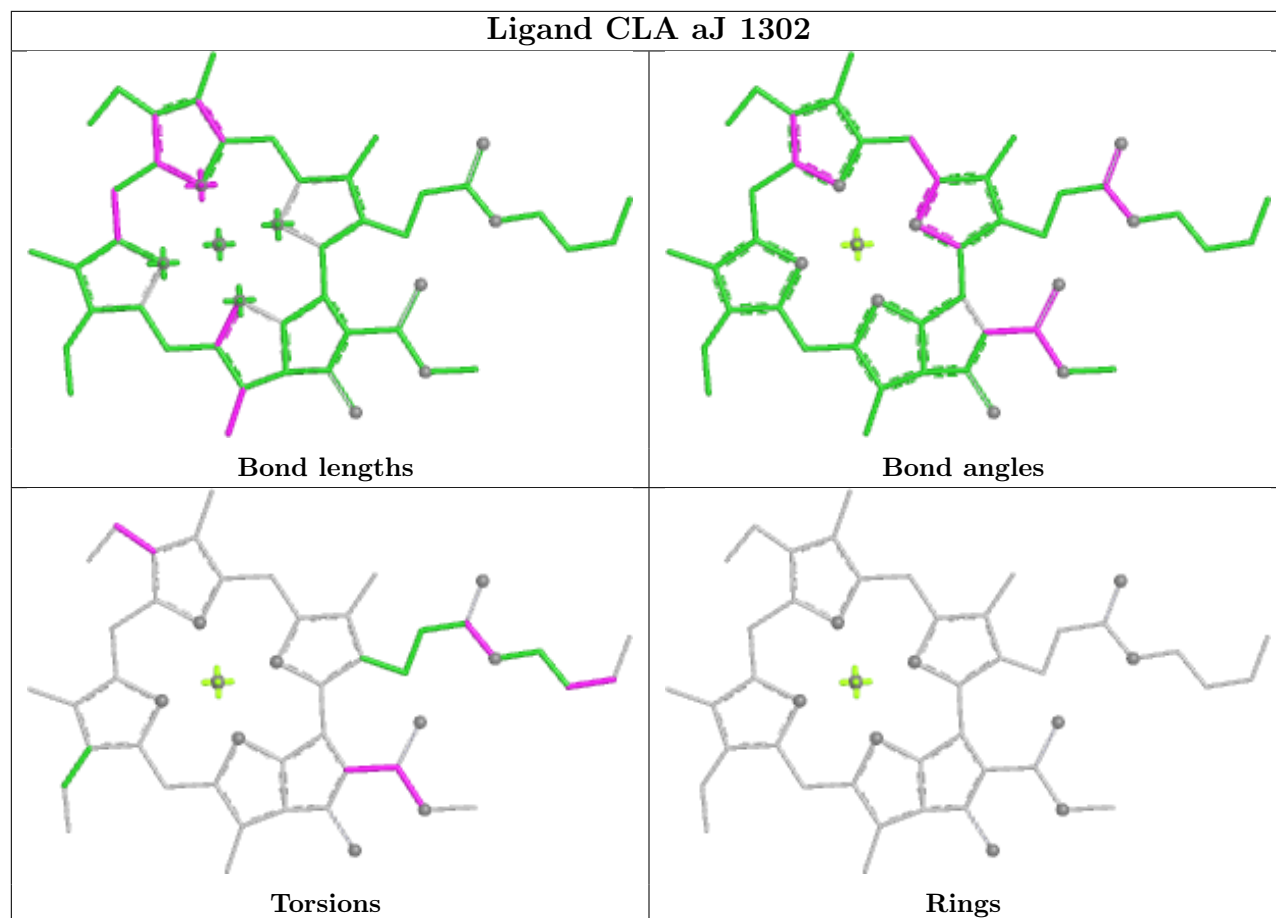


Rings

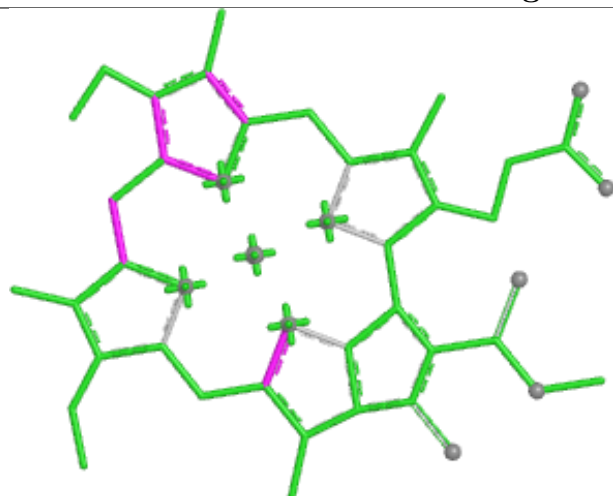




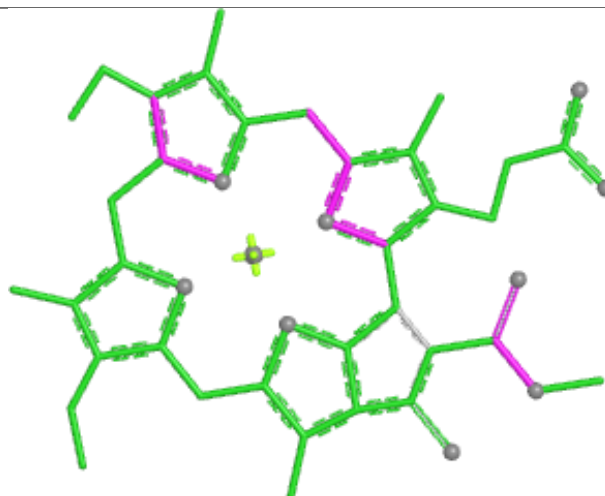
Ligand CLA aJ 1302



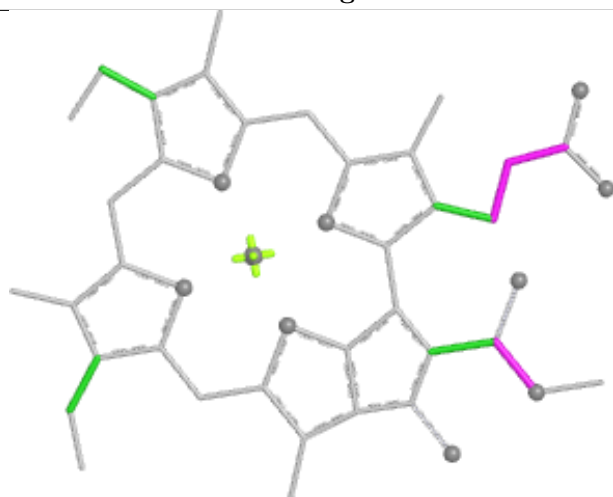
Ligand CLA 1 519



Bond lengths



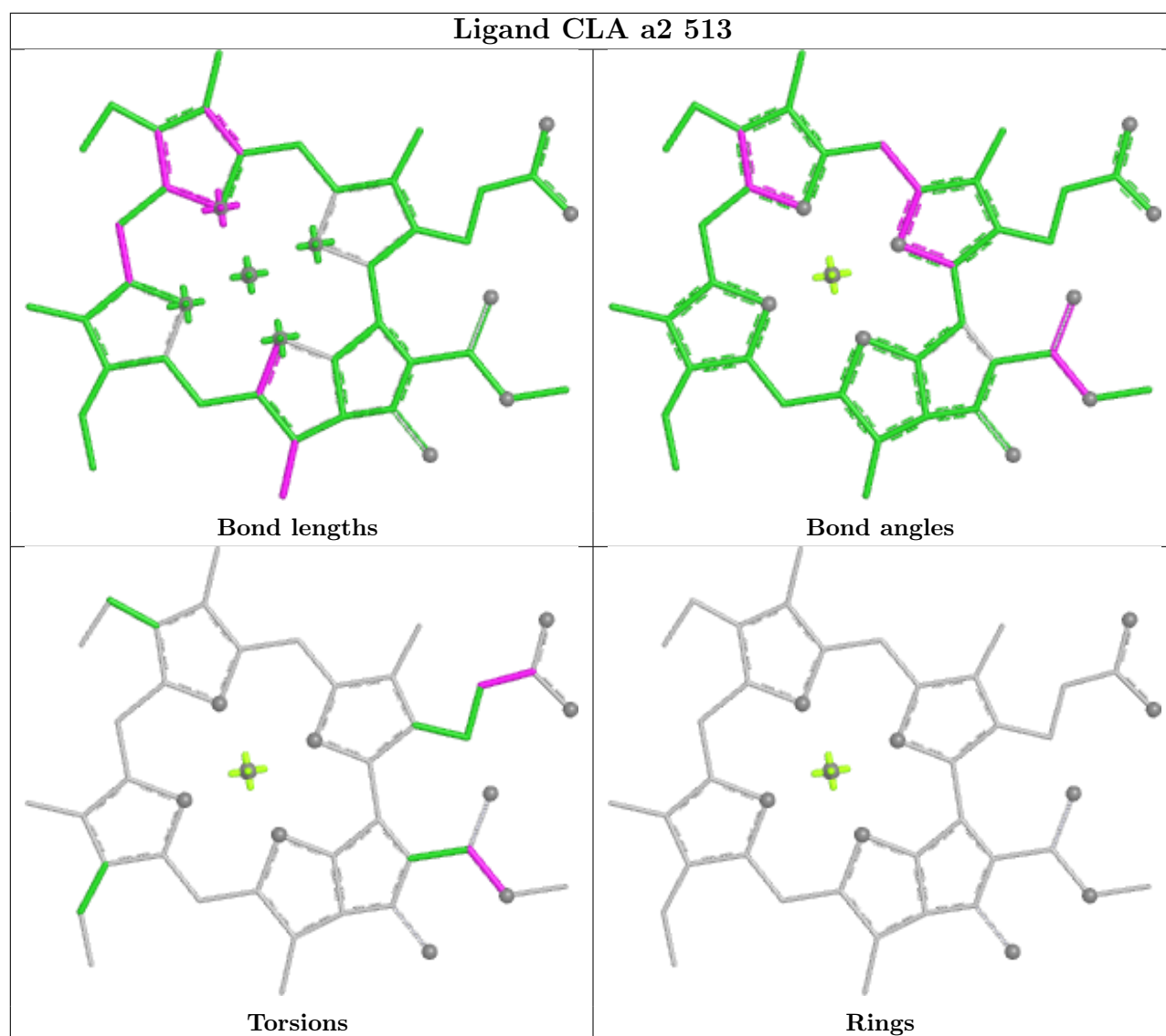
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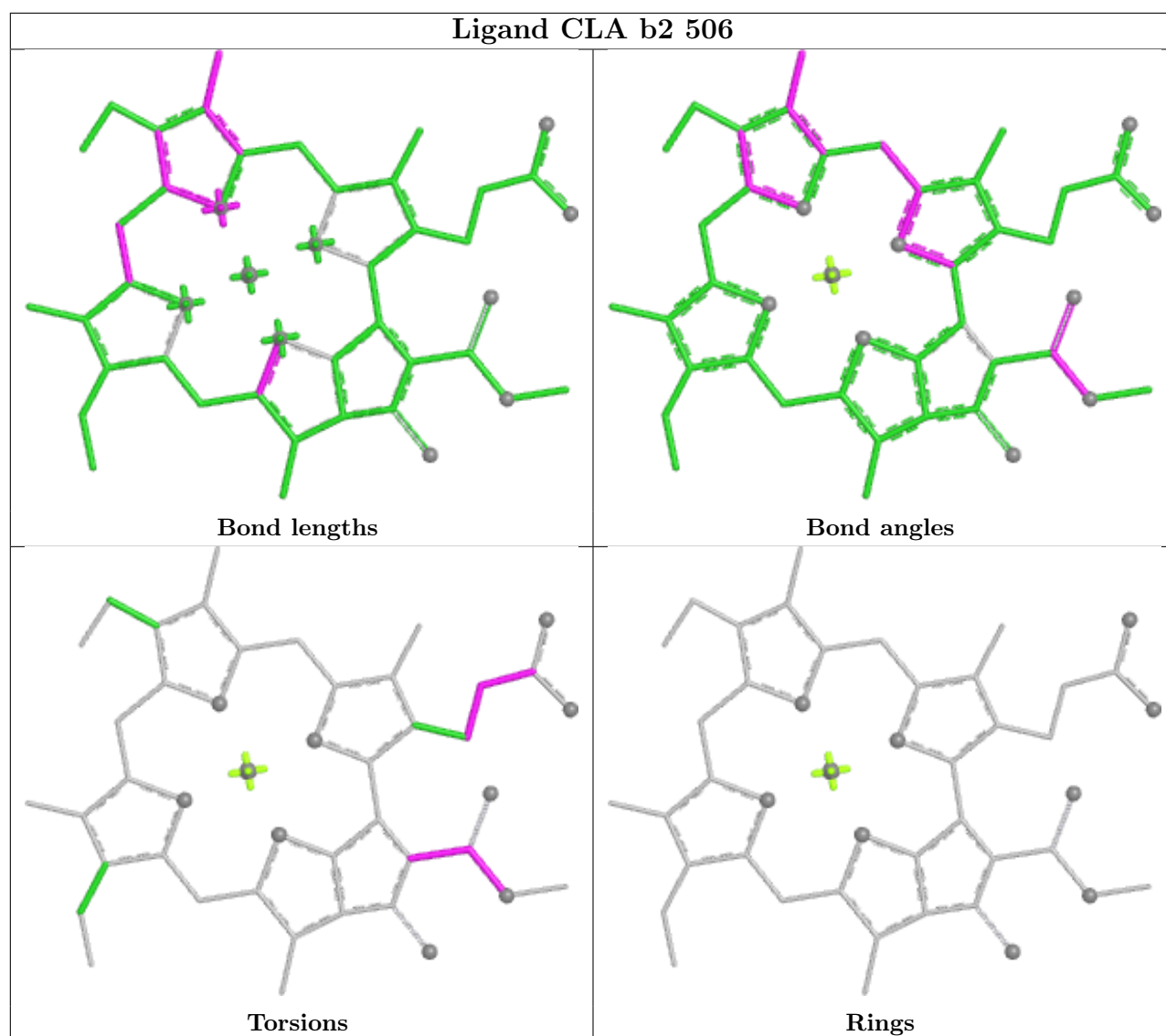


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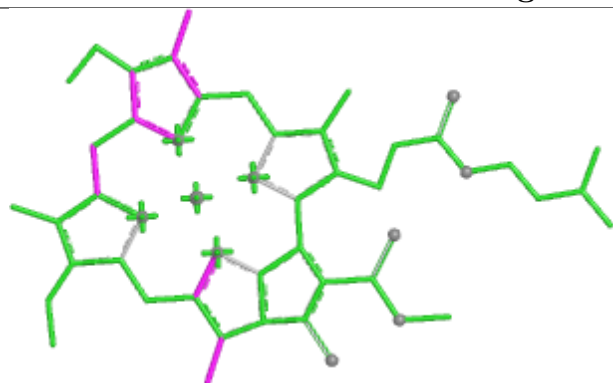


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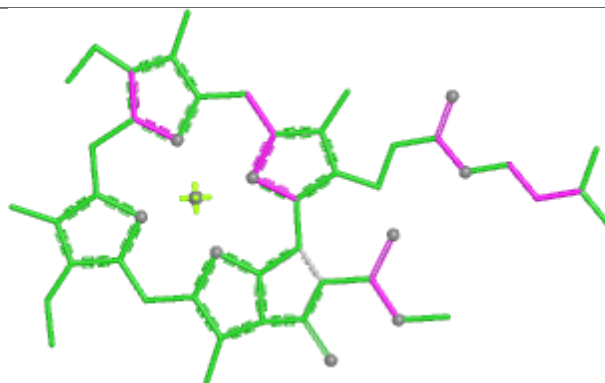




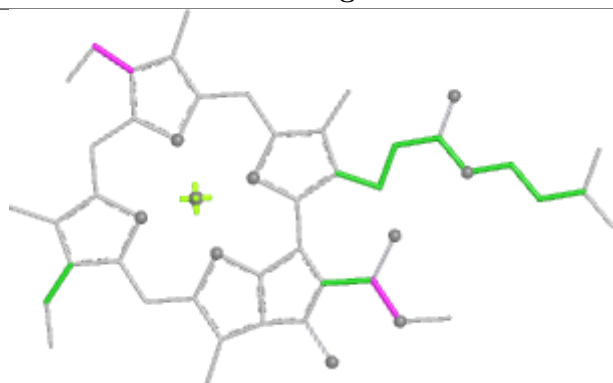
Ligand CLA d 503



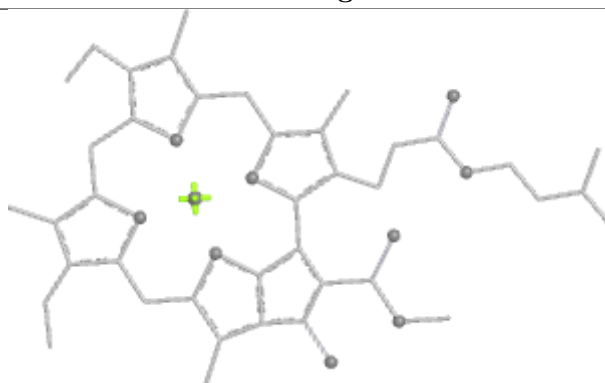
Bond lengths



Bond angles

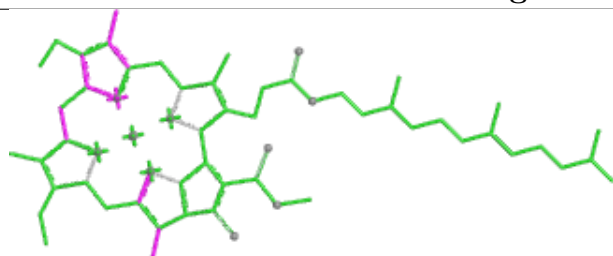


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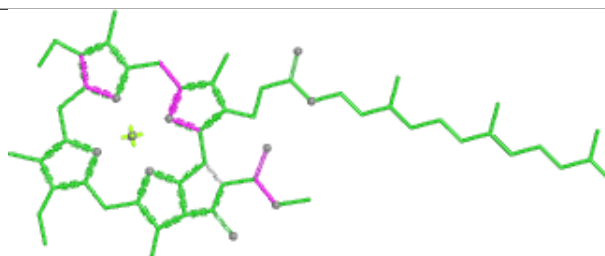


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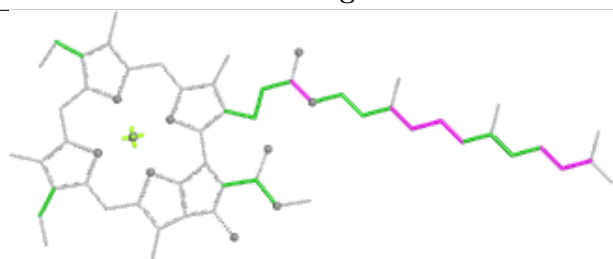
Ligand CLA a2 502



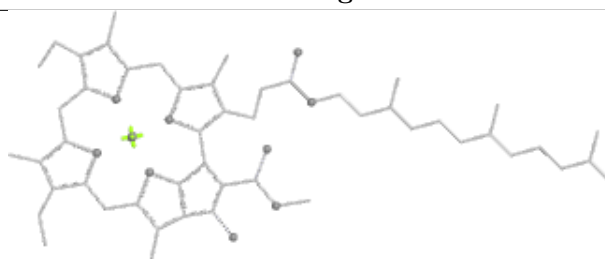
Bond lengths



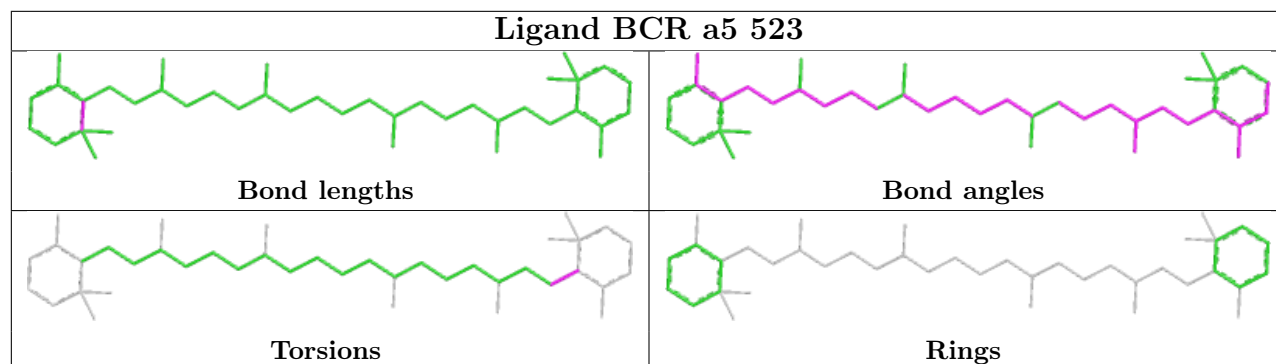
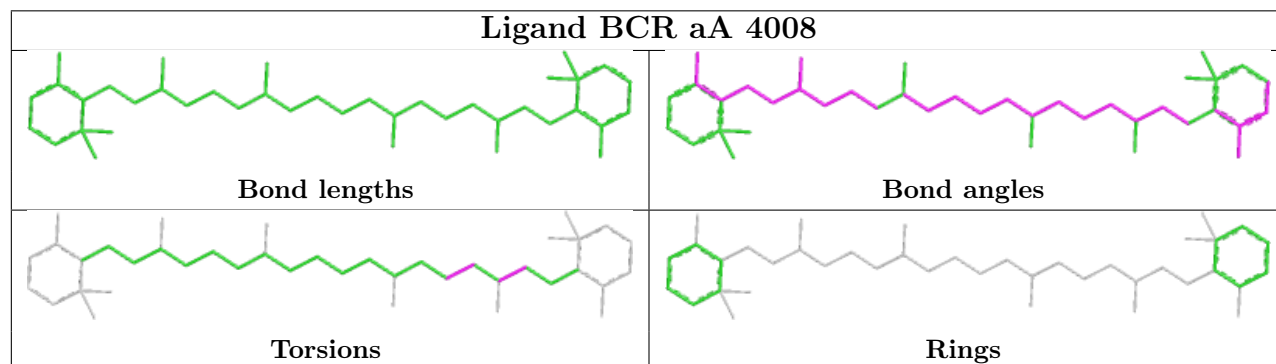
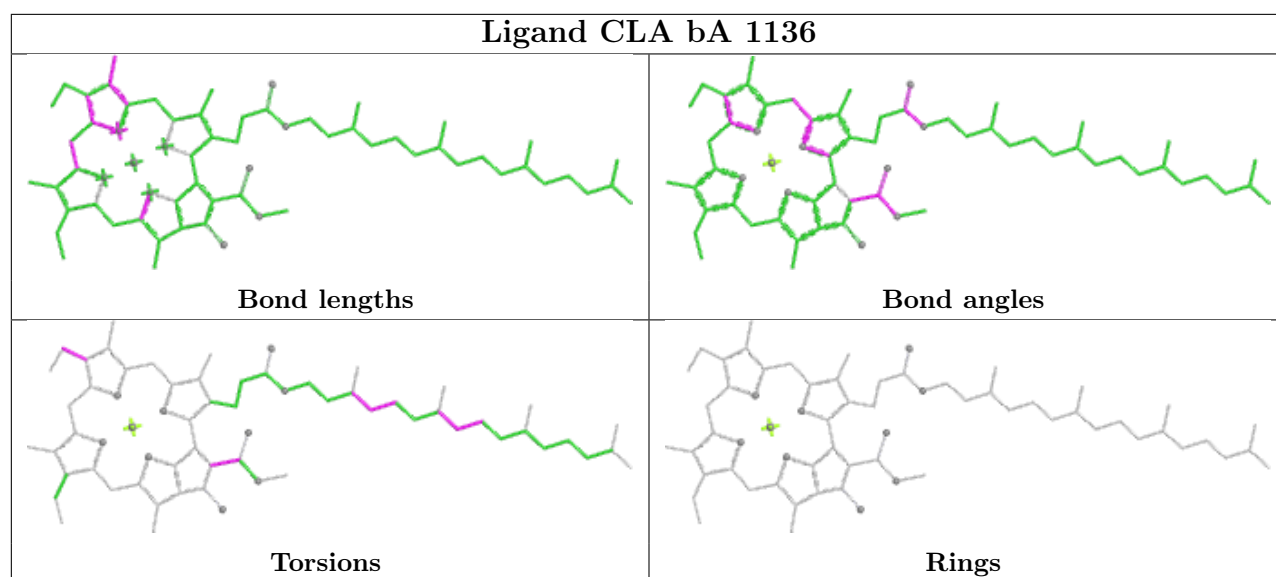
Bond angles

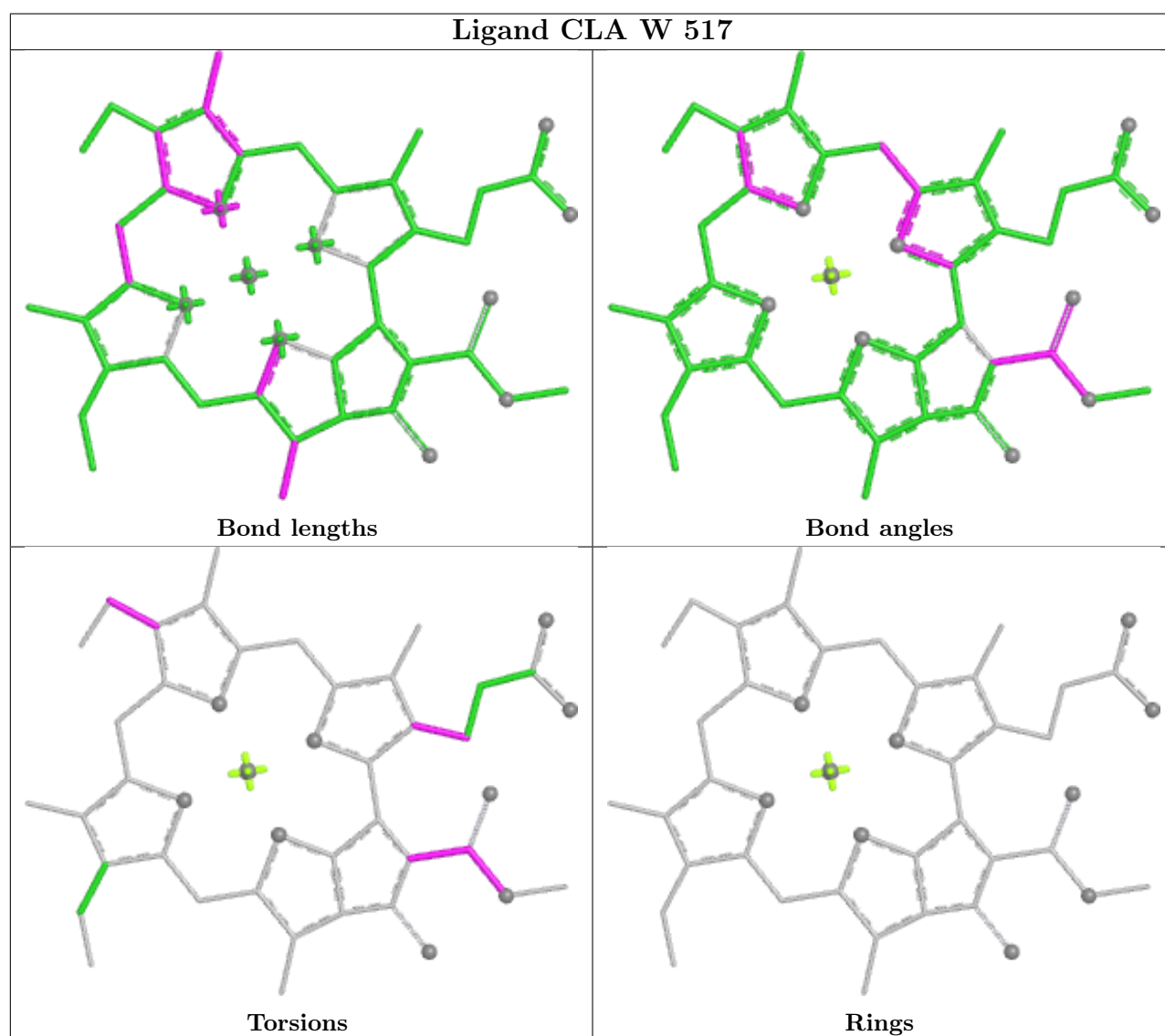
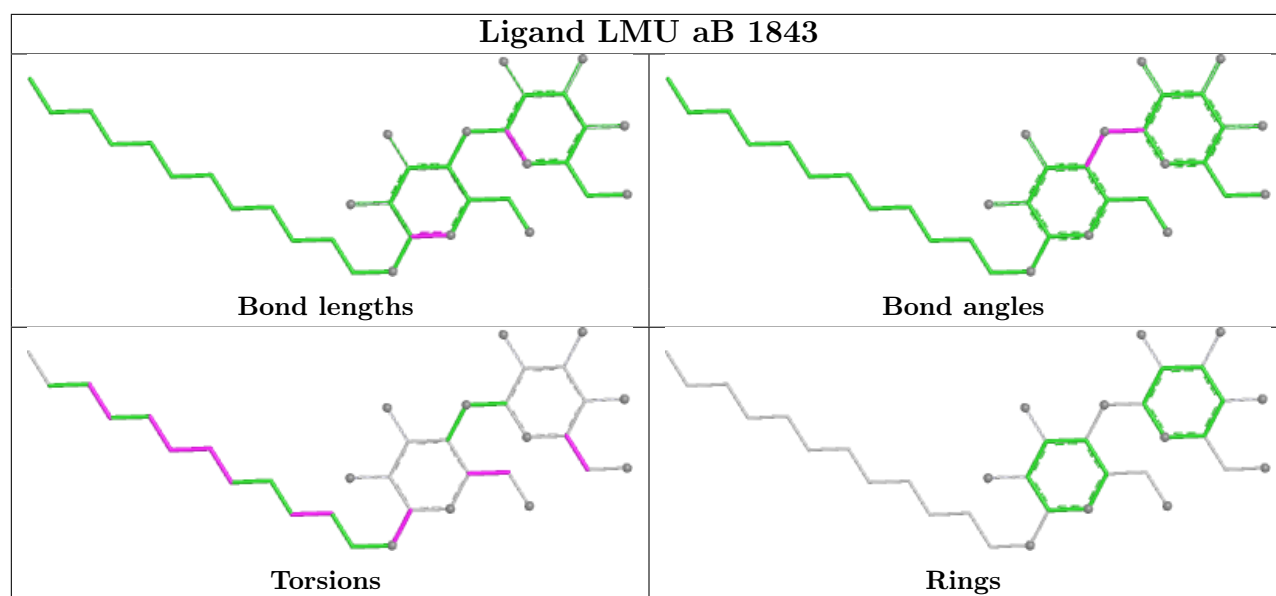


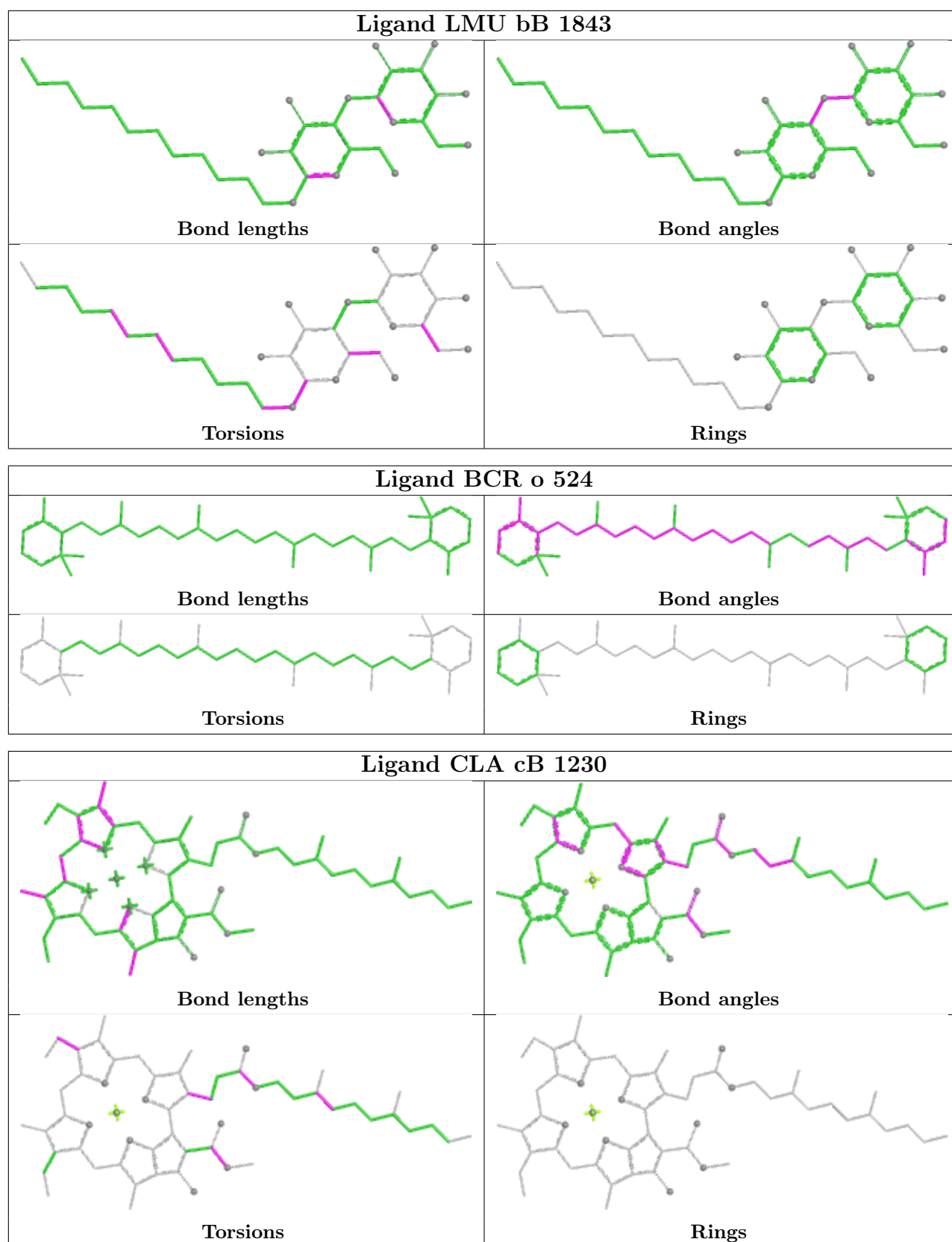
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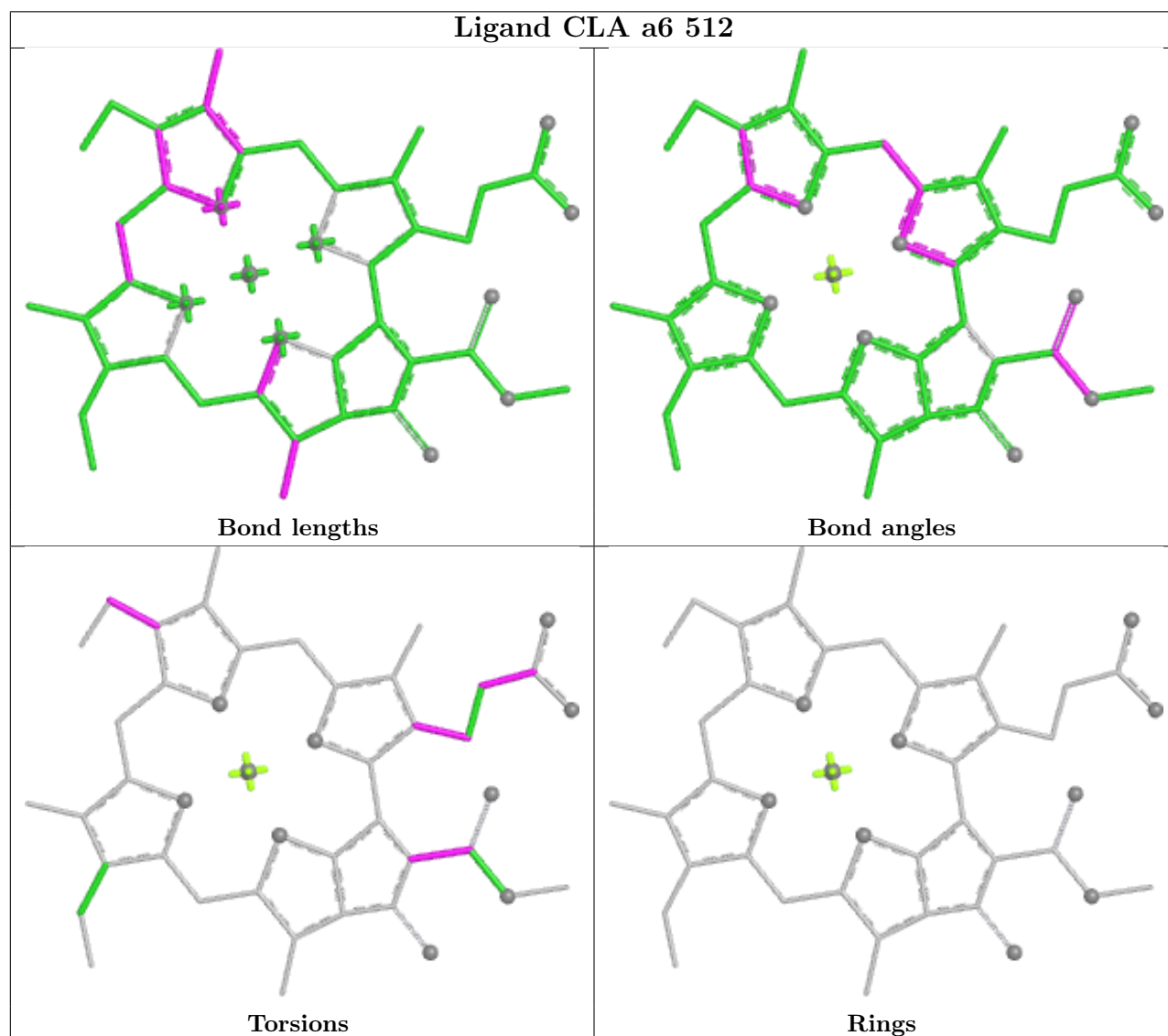
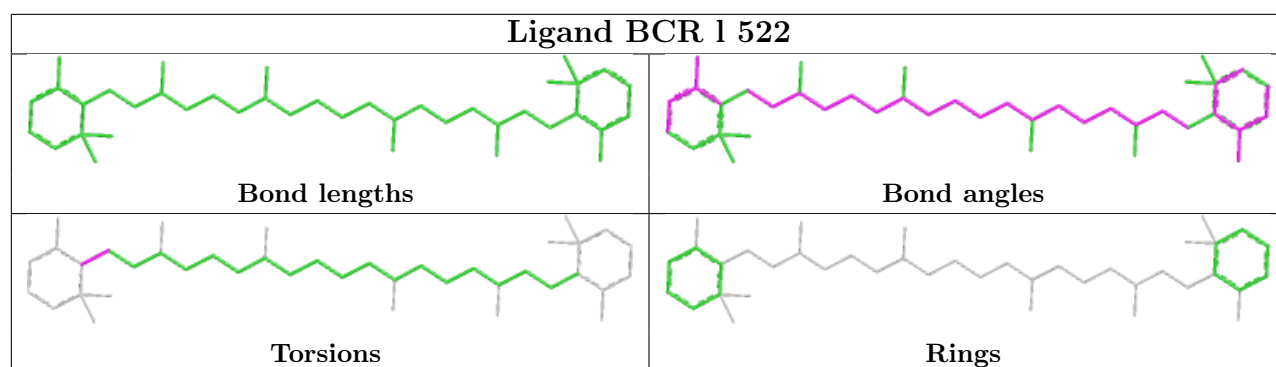


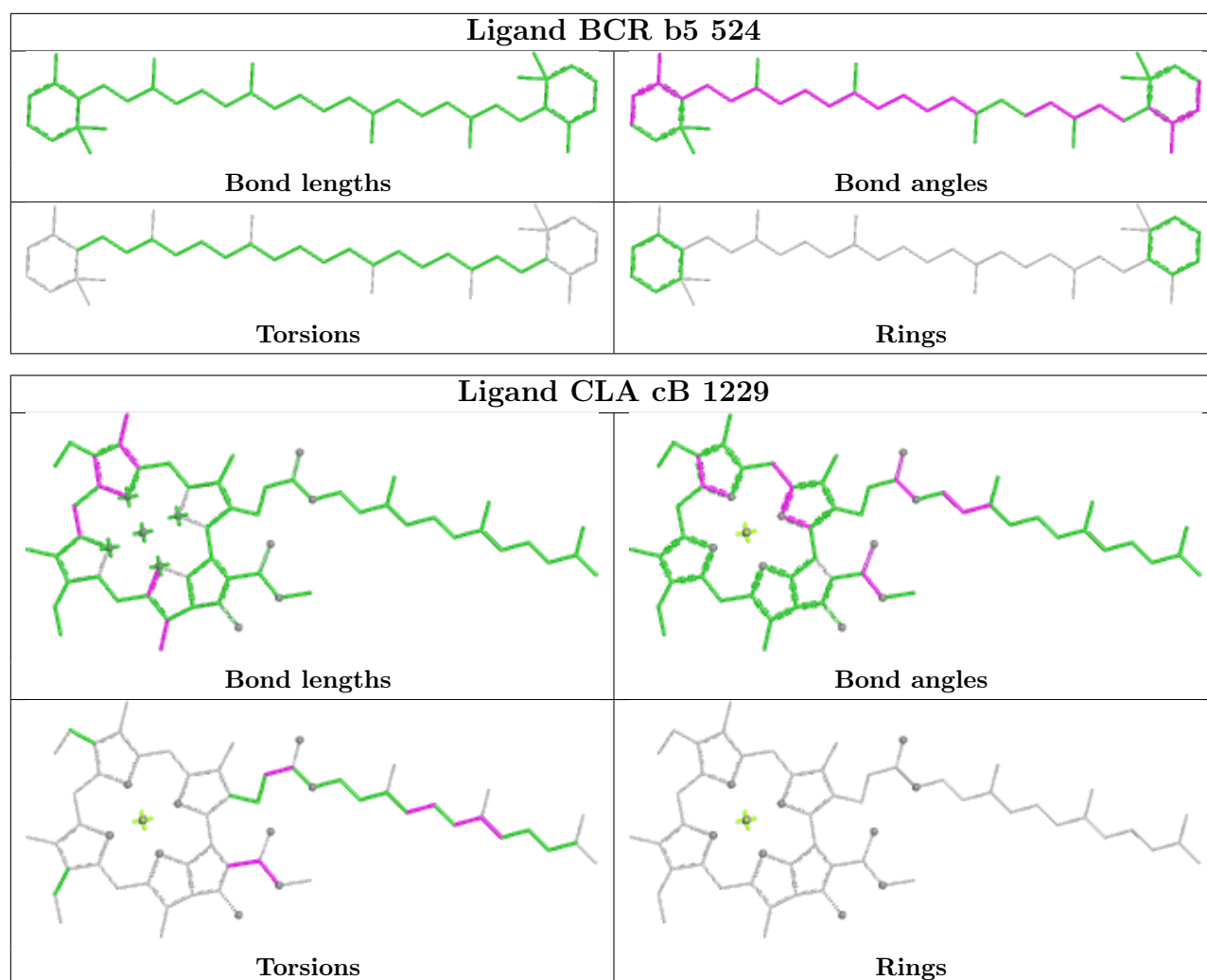
Rings



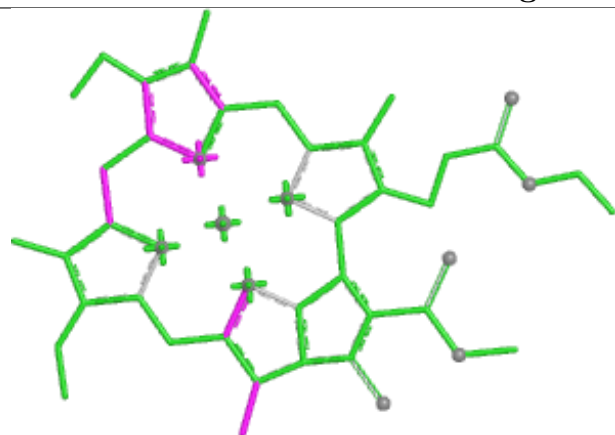




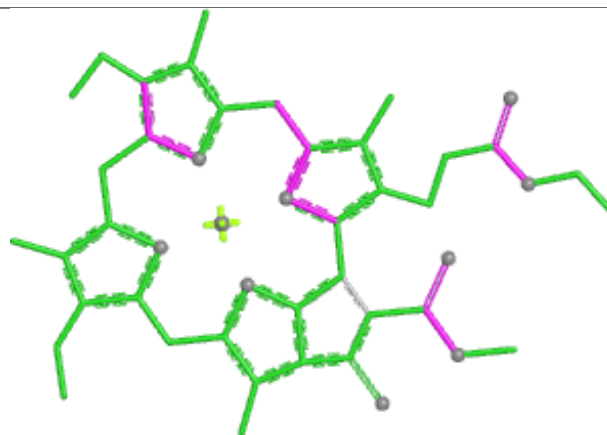




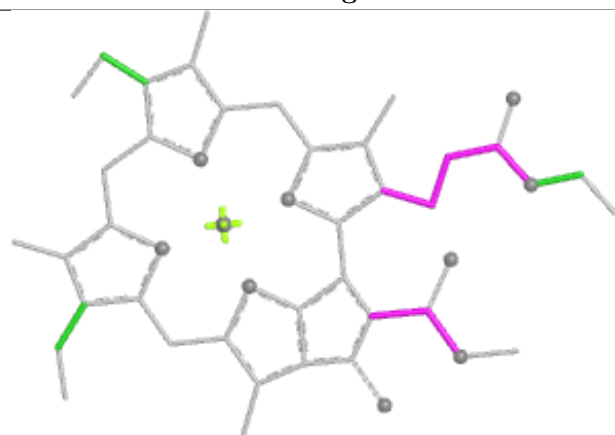
Ligand CLA h 518



Bond lengths



Bond angles

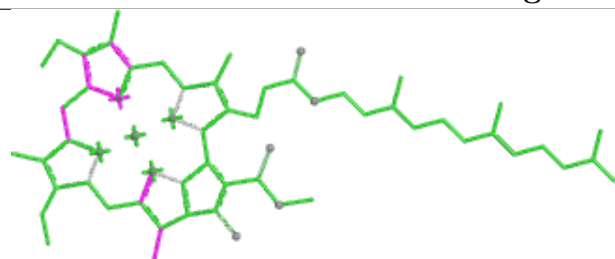


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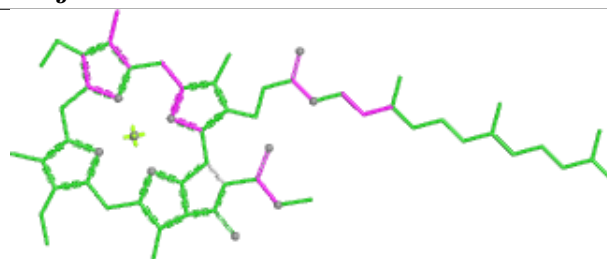


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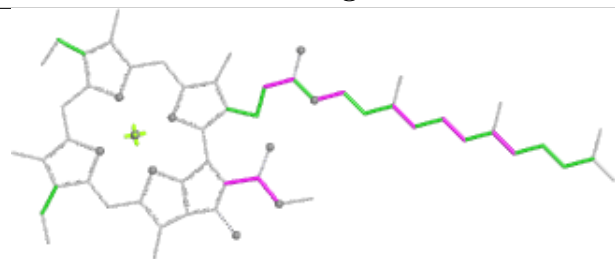
Ligand CLA j 510



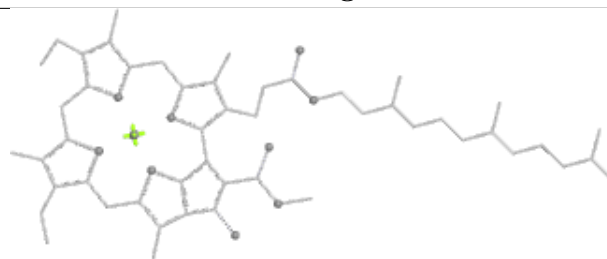
Bond lengths



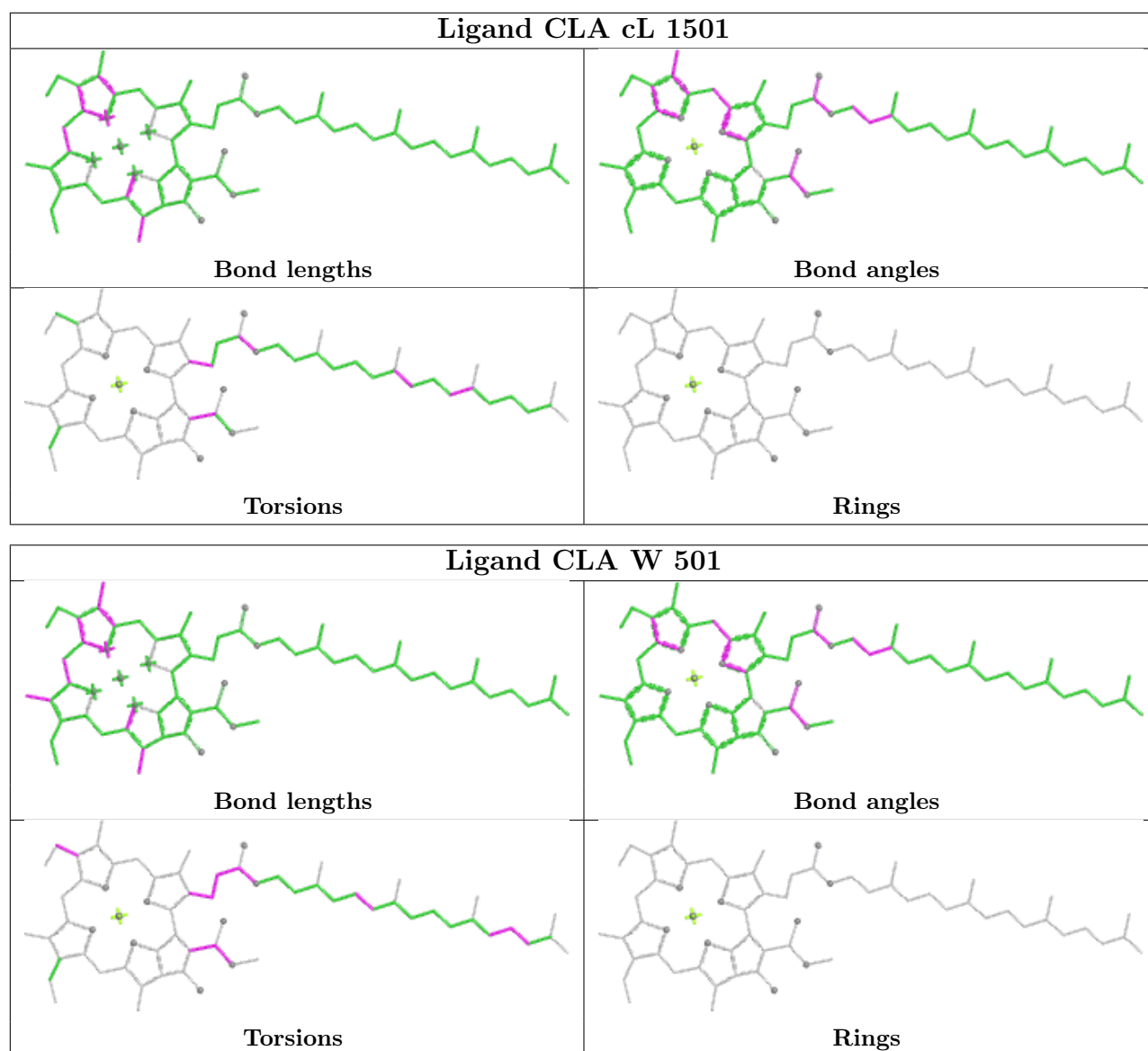
Bond angles



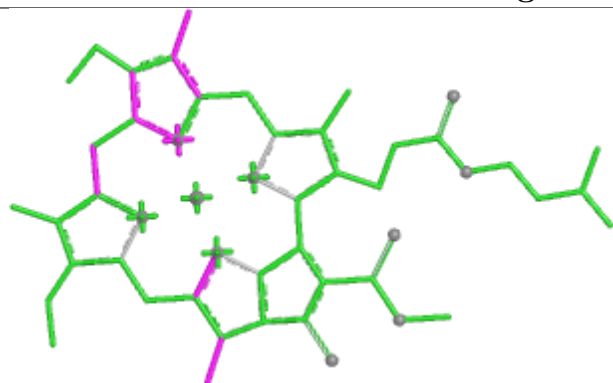
Torsions



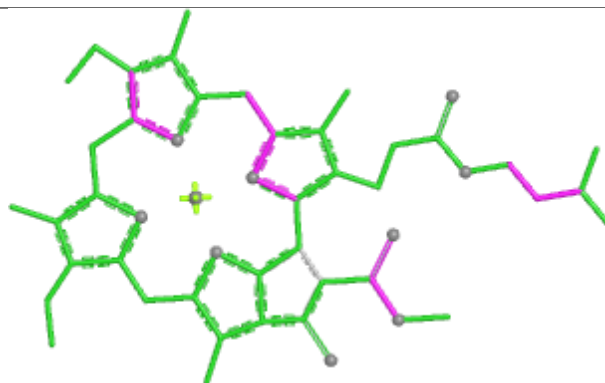
Rings



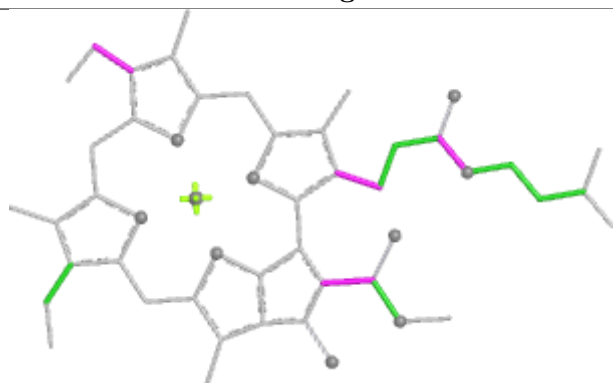
Ligand CLA b 512



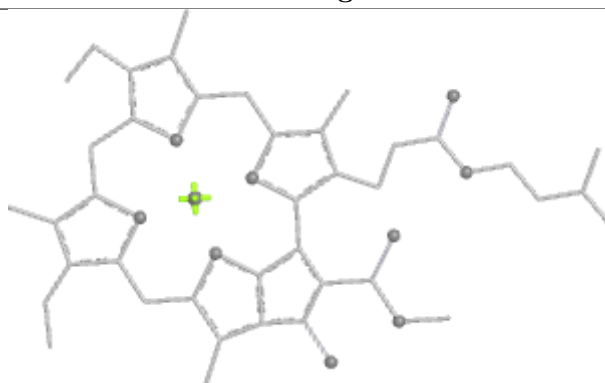
Bond lengths



Bond angles

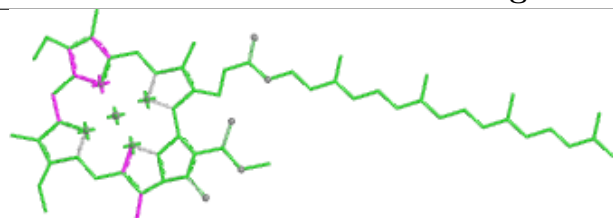


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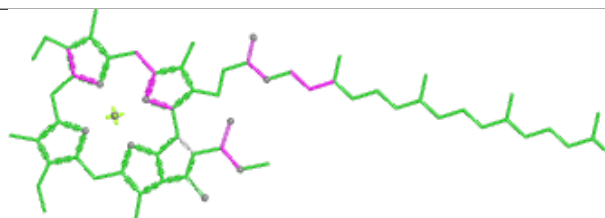


Rings

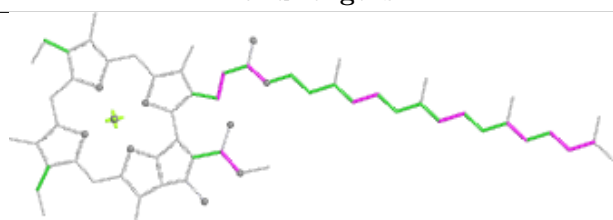
Ligand CLA a6 505



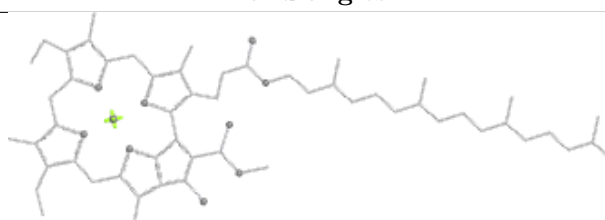
Bond lengths



Bond angles

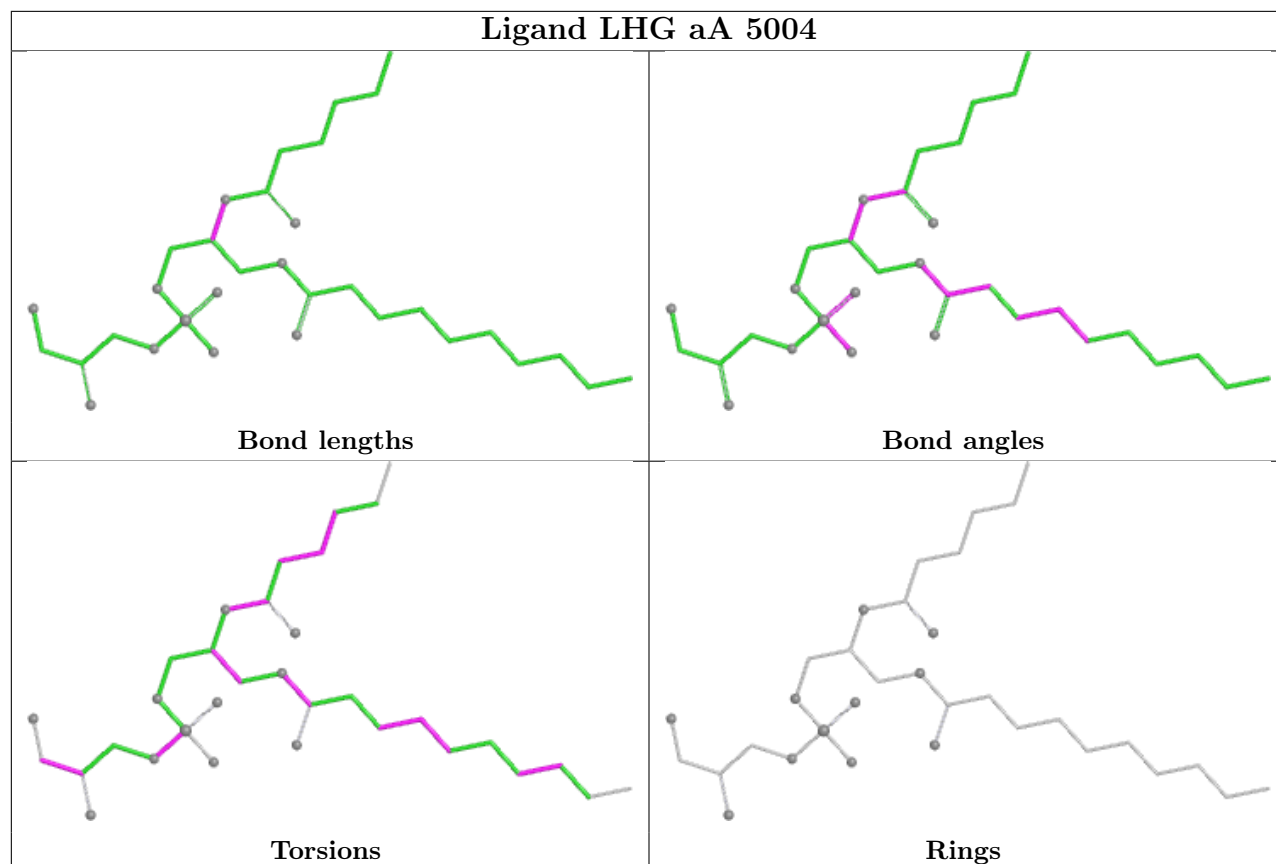


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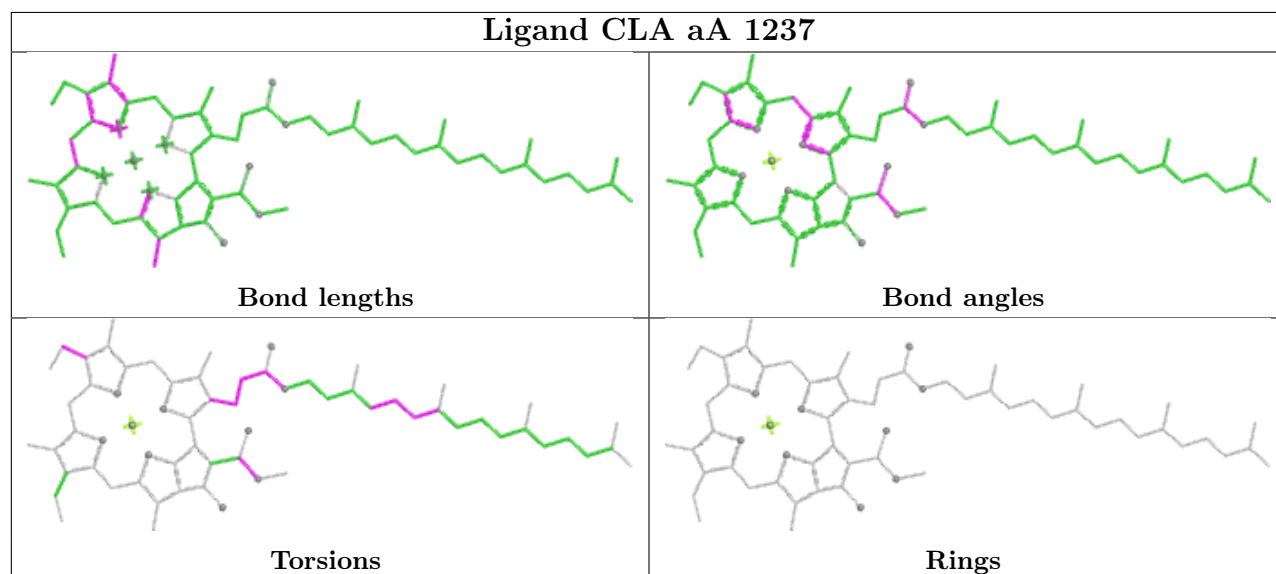


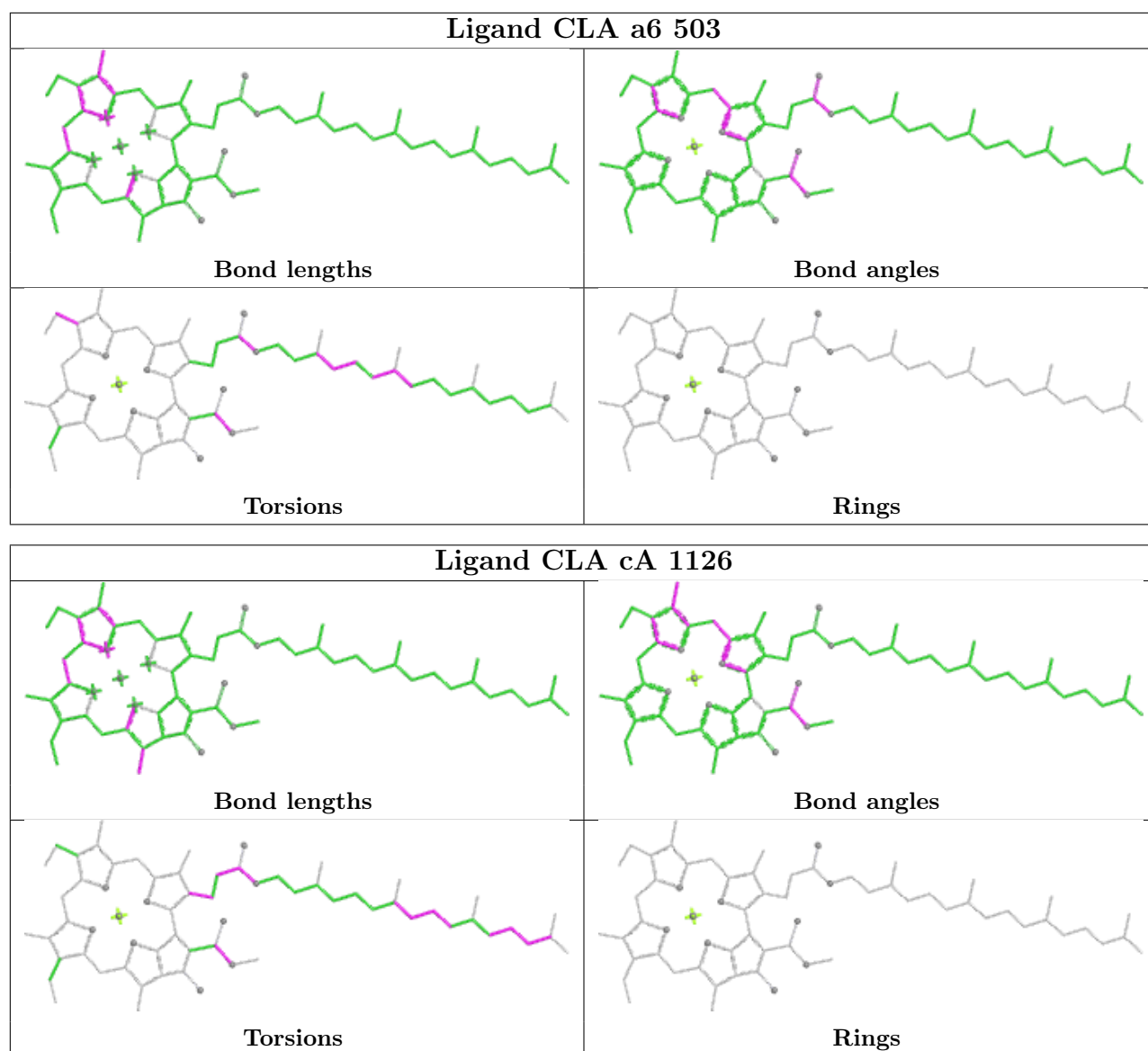
Rings

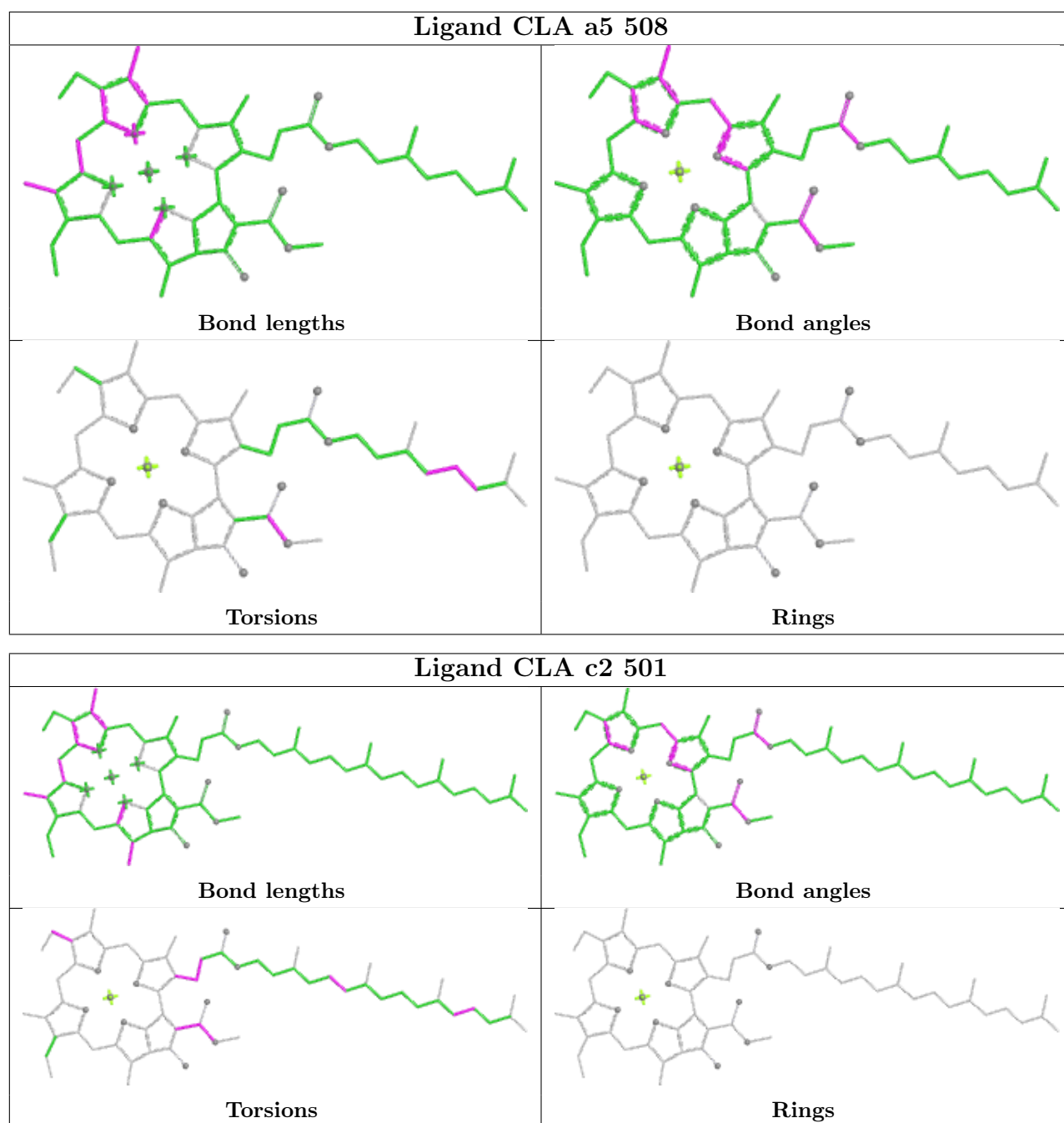
Ligand LHG aA 5004



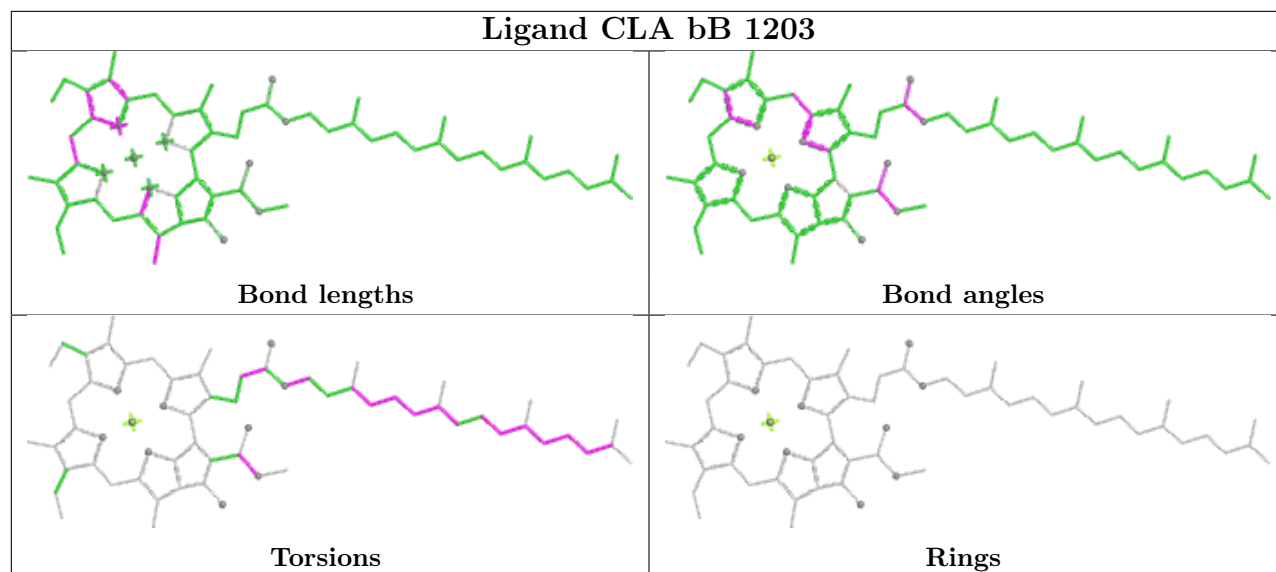
Ligand CLA aA 1237



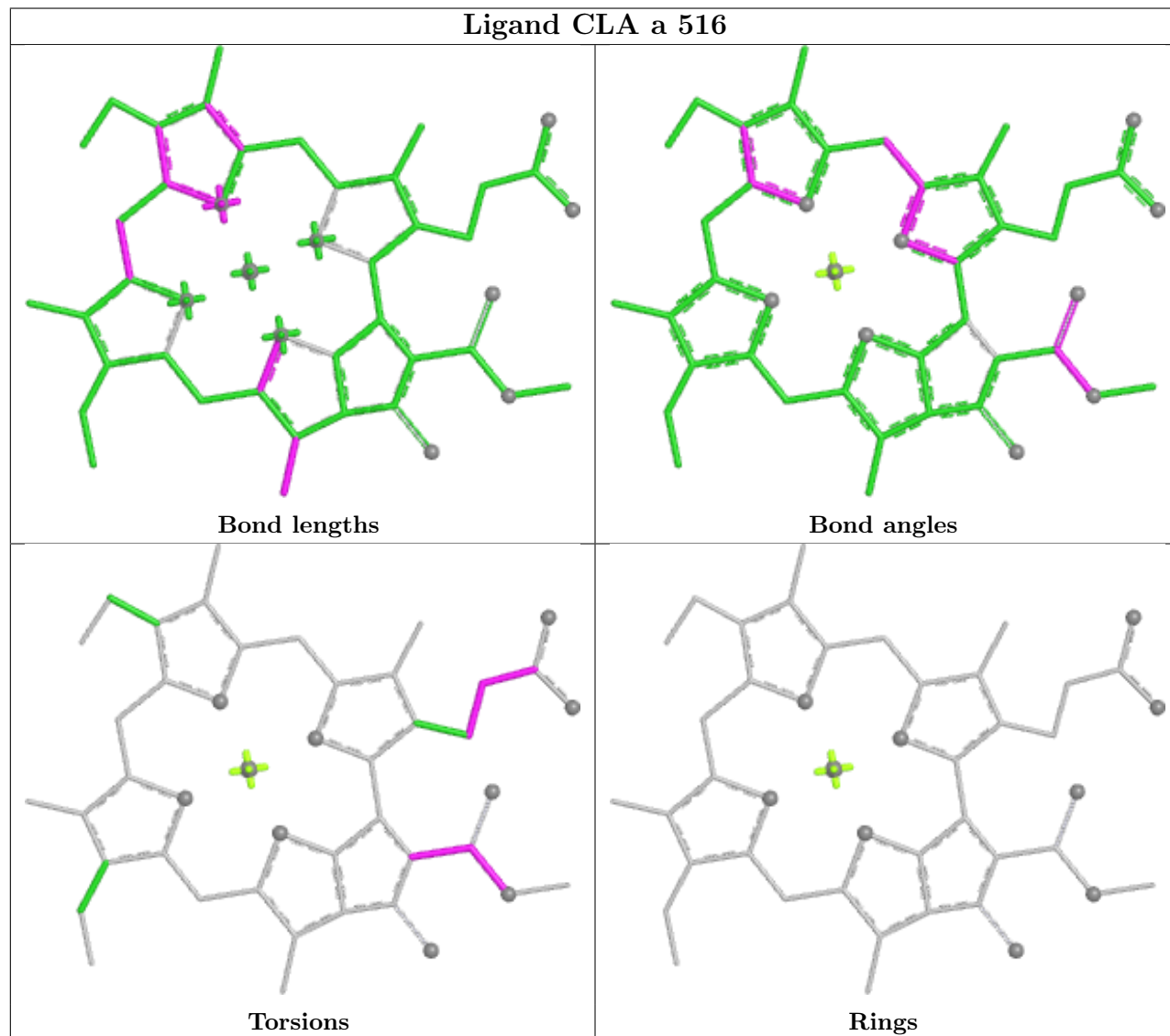


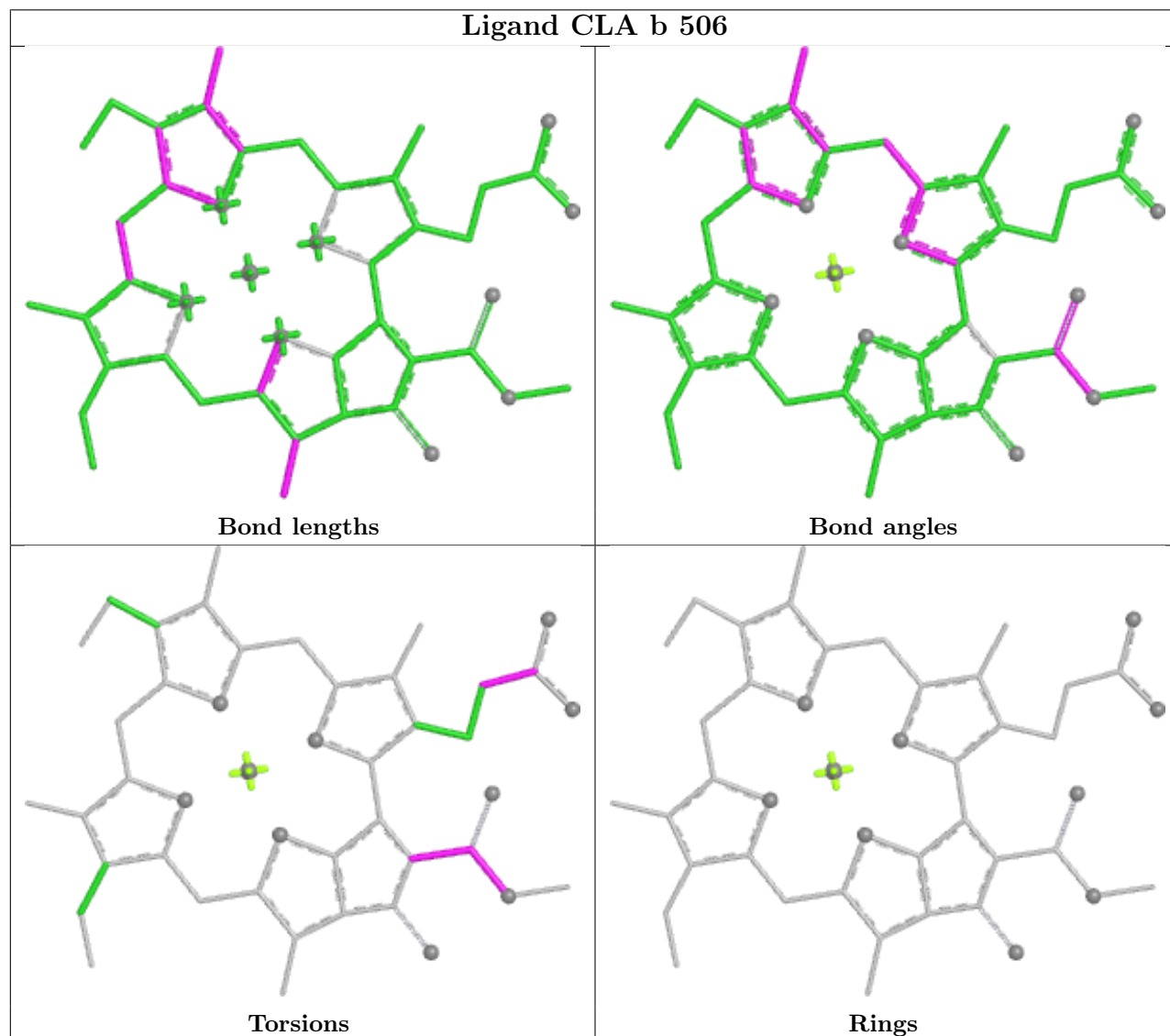
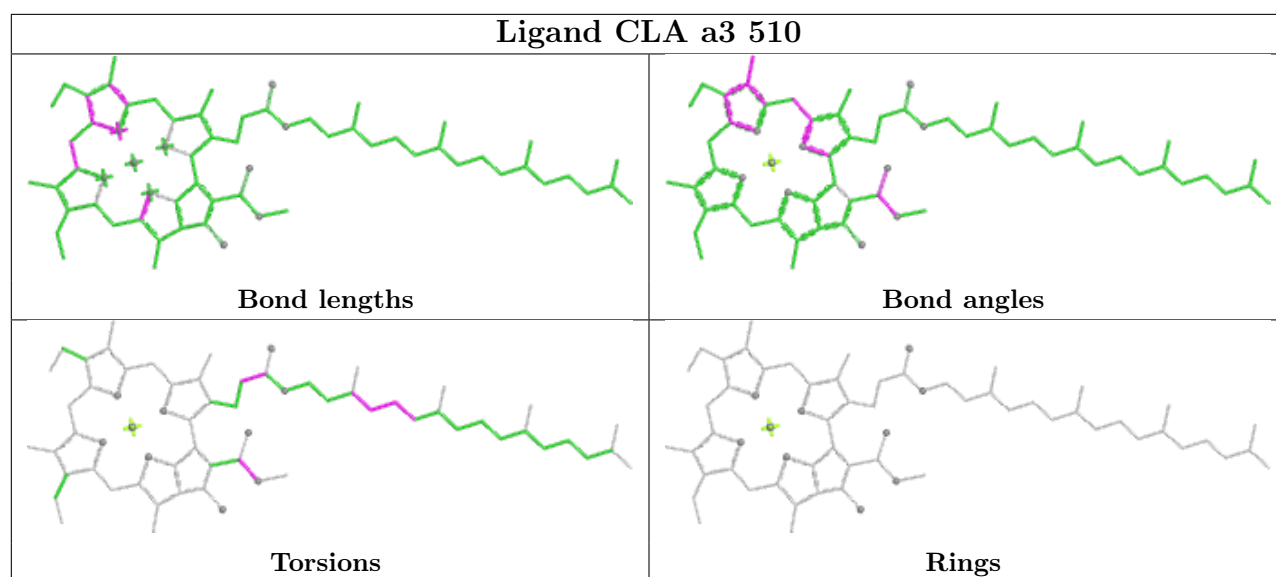


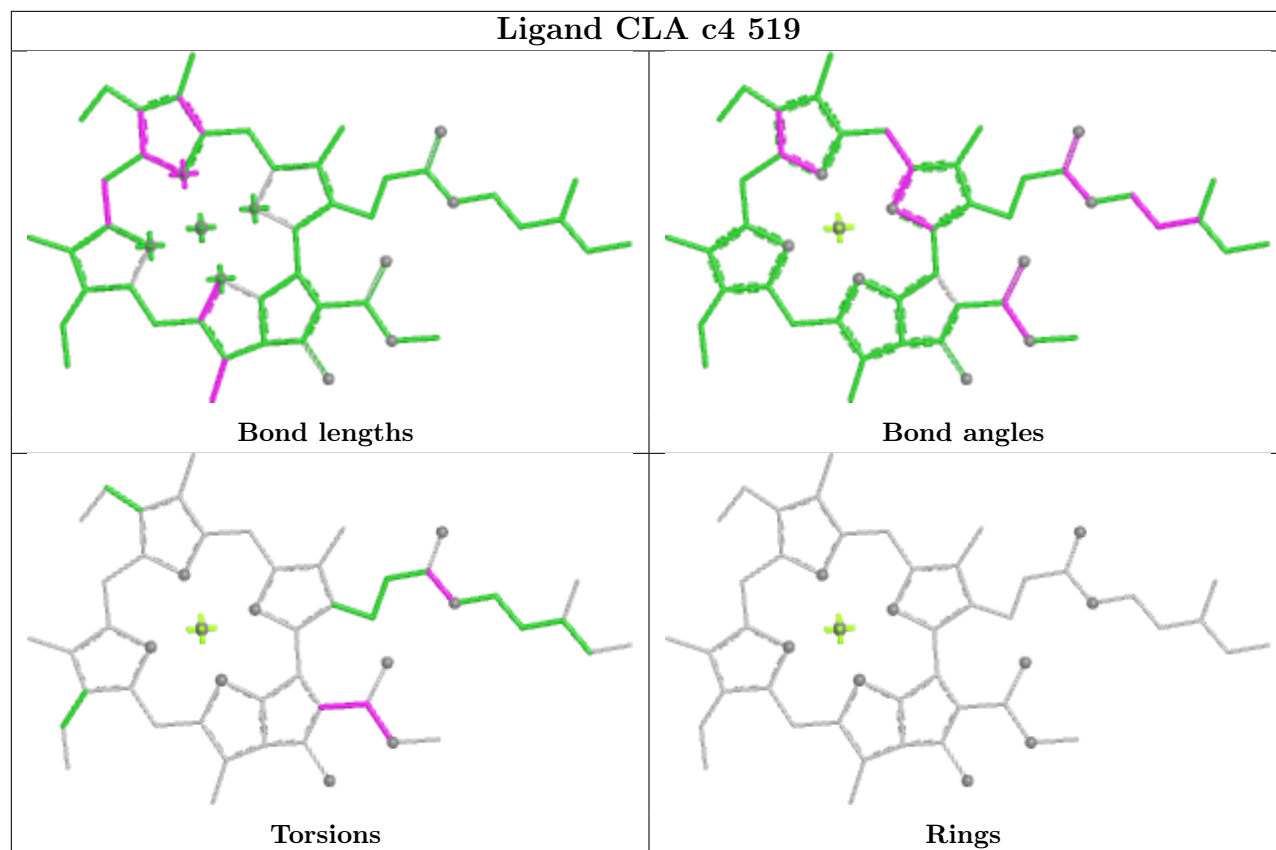
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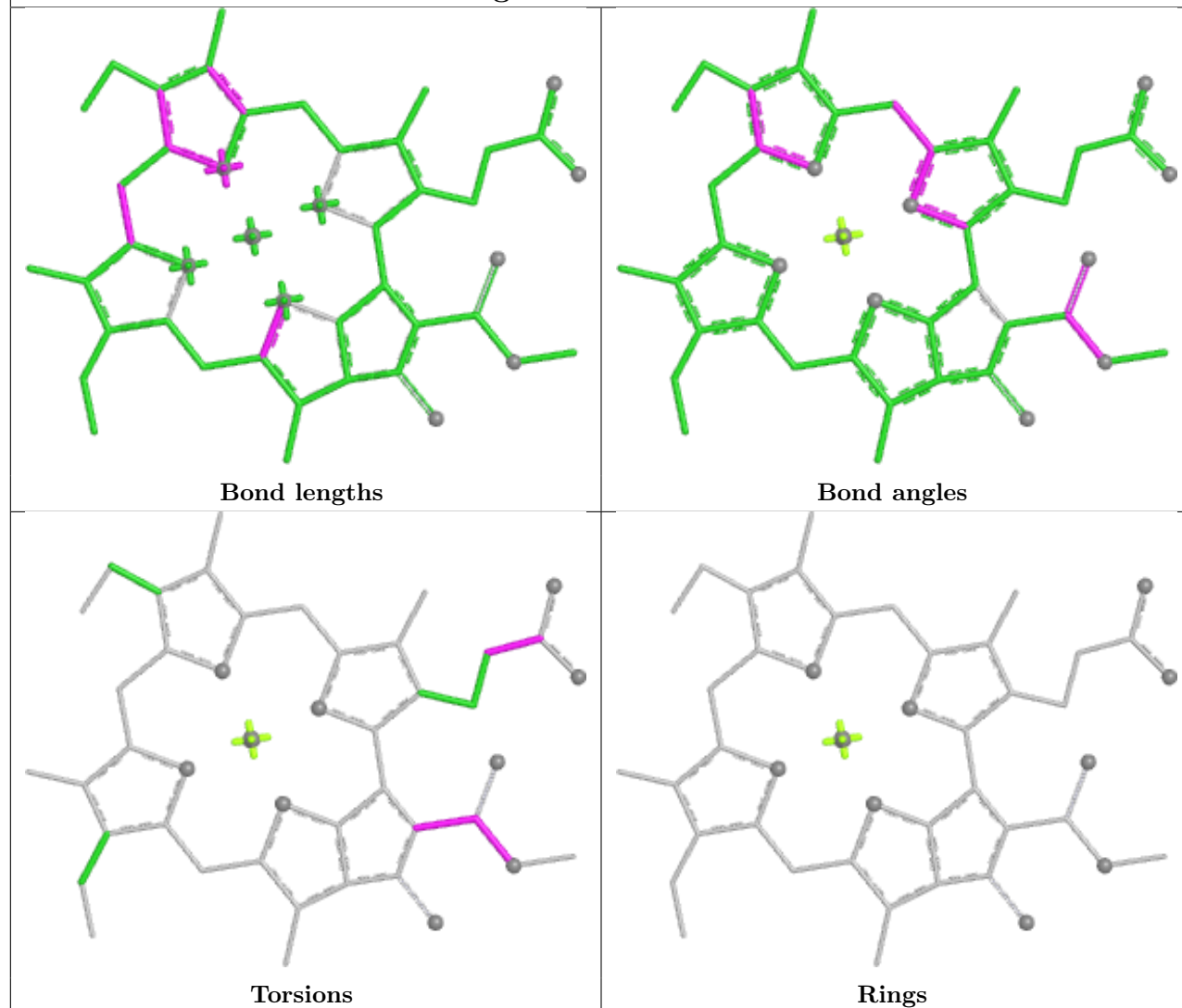
Ligand CLA a 516



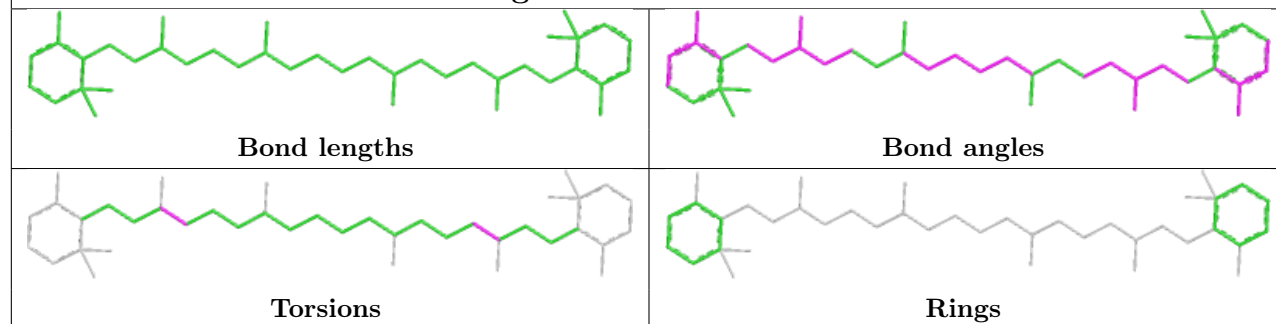




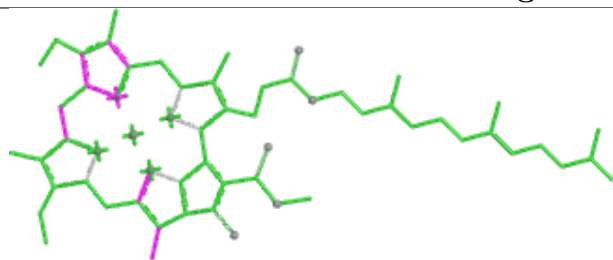
Ligand CLA T 519



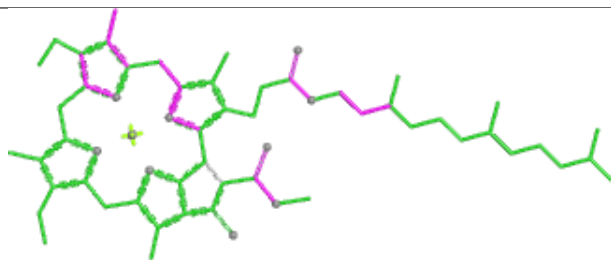
Ligand BCR bB 4006



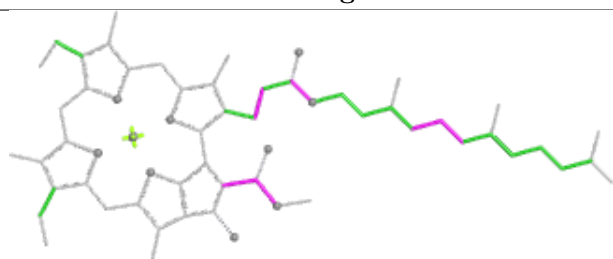
Ligand CLA b 505



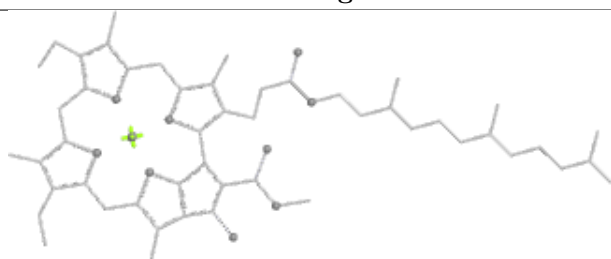
Bond lengths



Bond angles

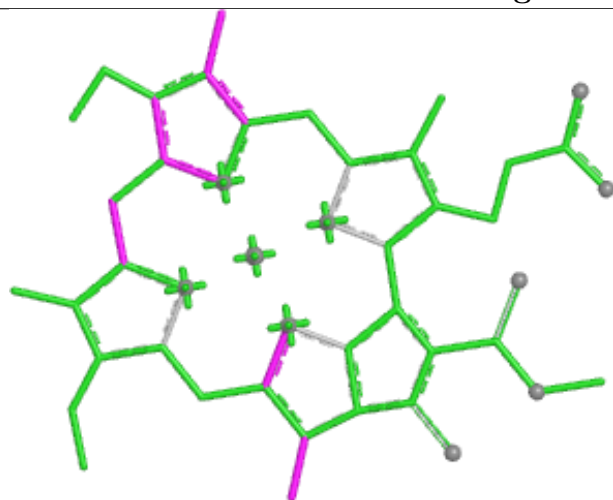


Torsions

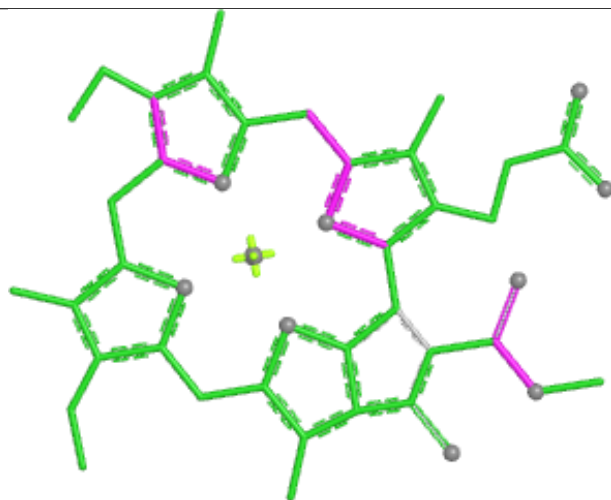


Rings

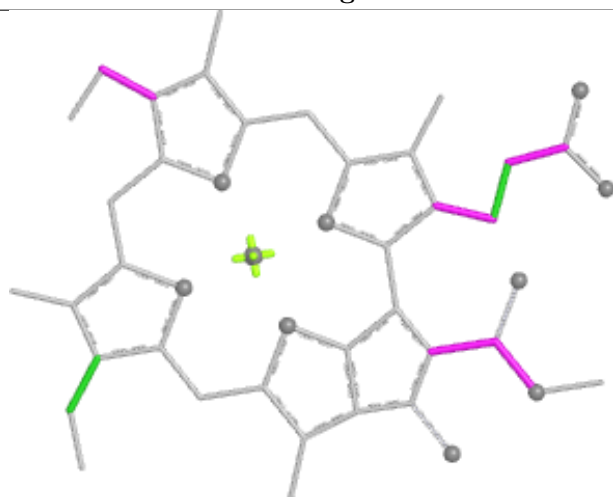
Ligand CLA X 519



Bond lengths



Bond angles

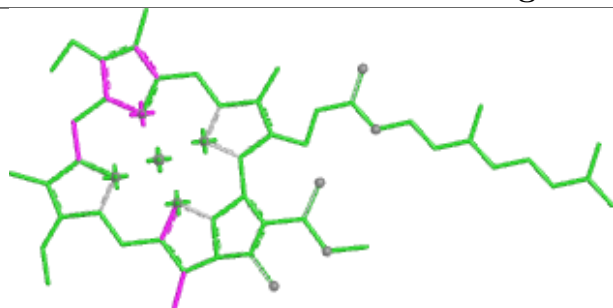


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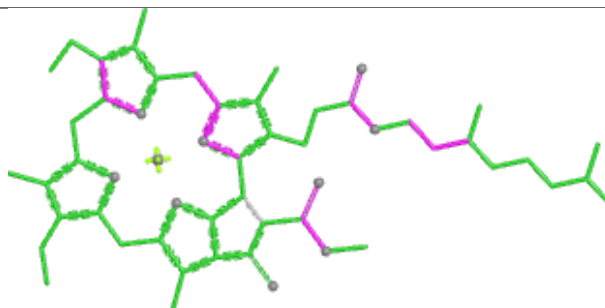


Rings

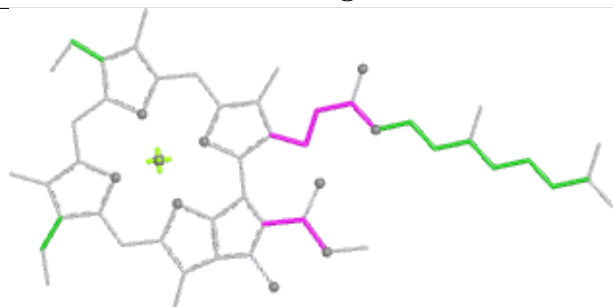
Ligand CLA o 518



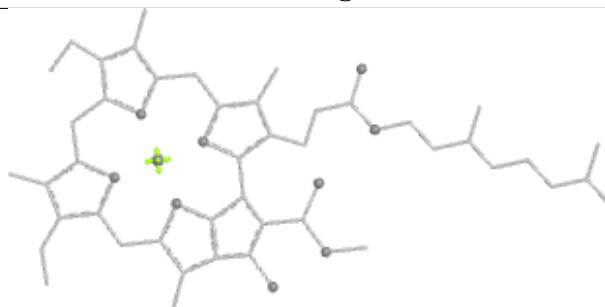
Bond lengths



Bond angles

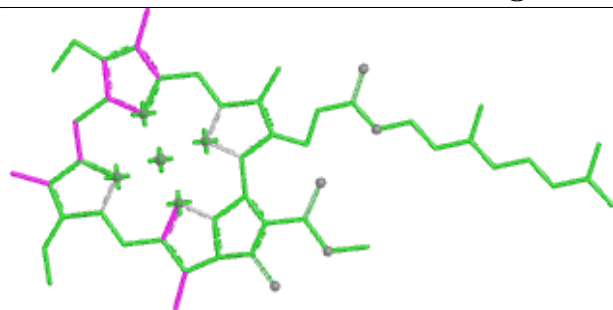


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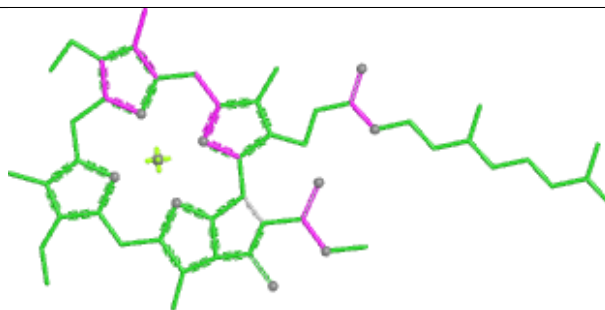


Rings

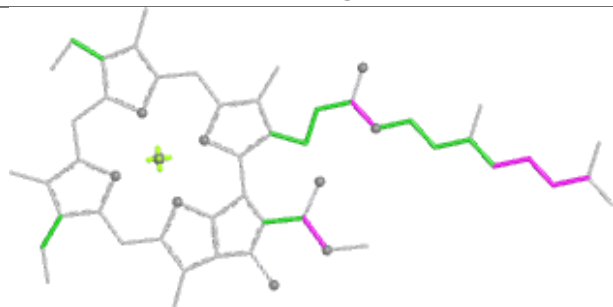
Ligand CLA b1 508



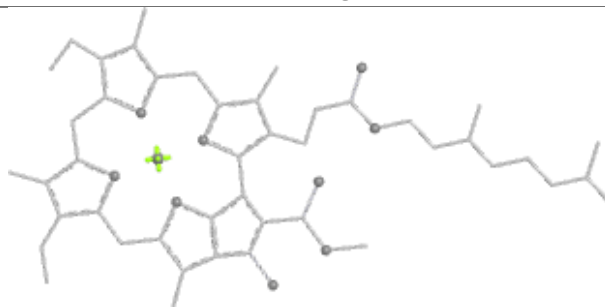
Bond lengths



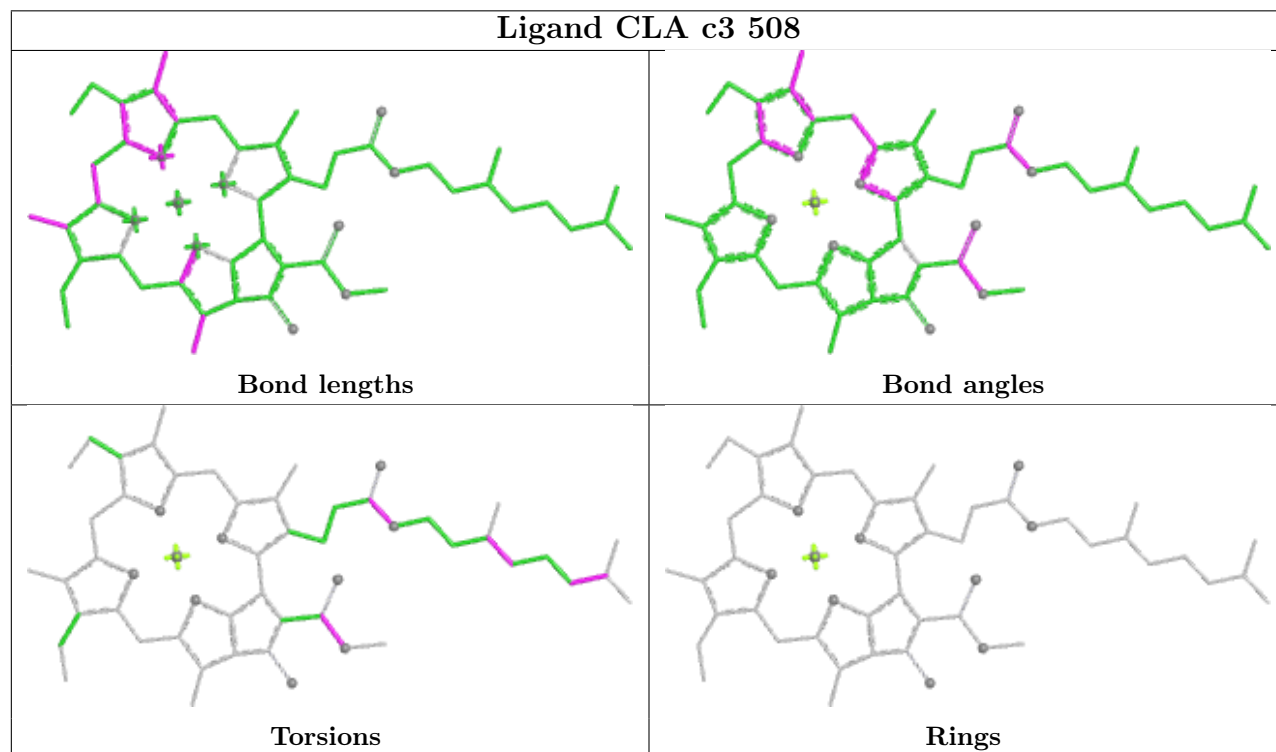
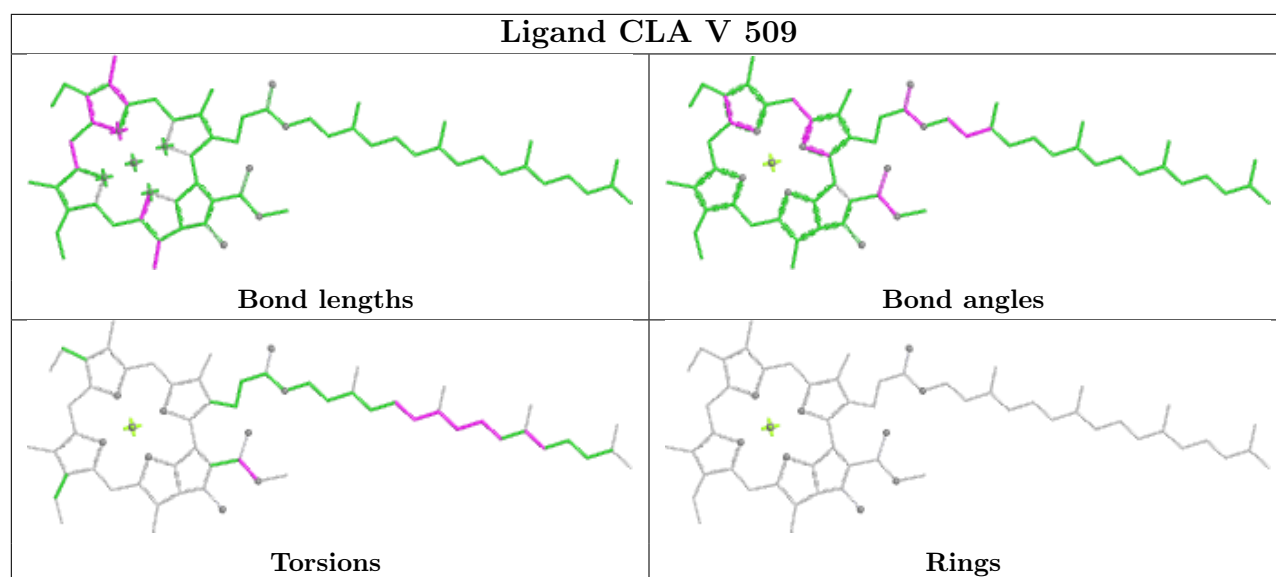
Bond angles

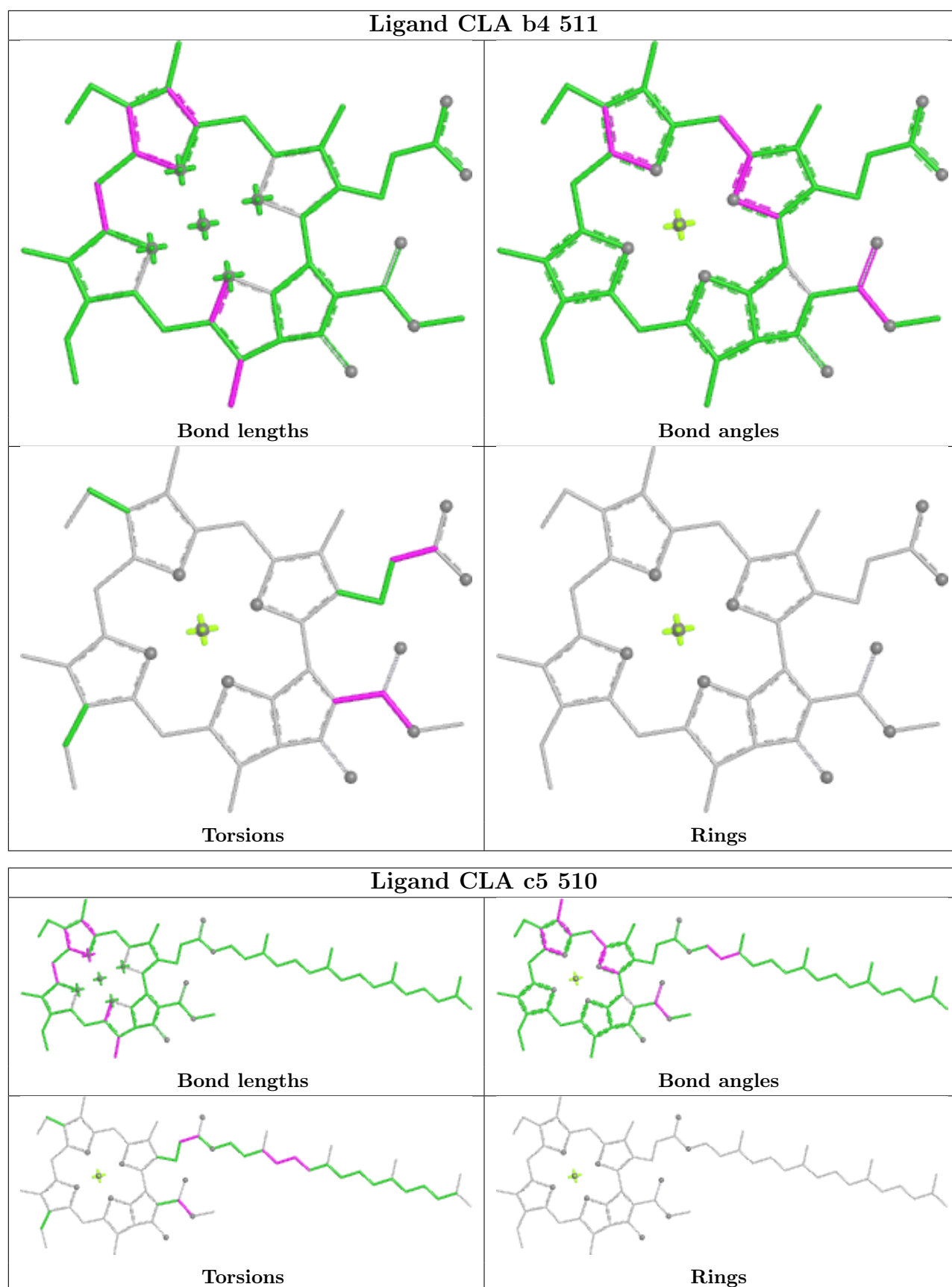


Torsions

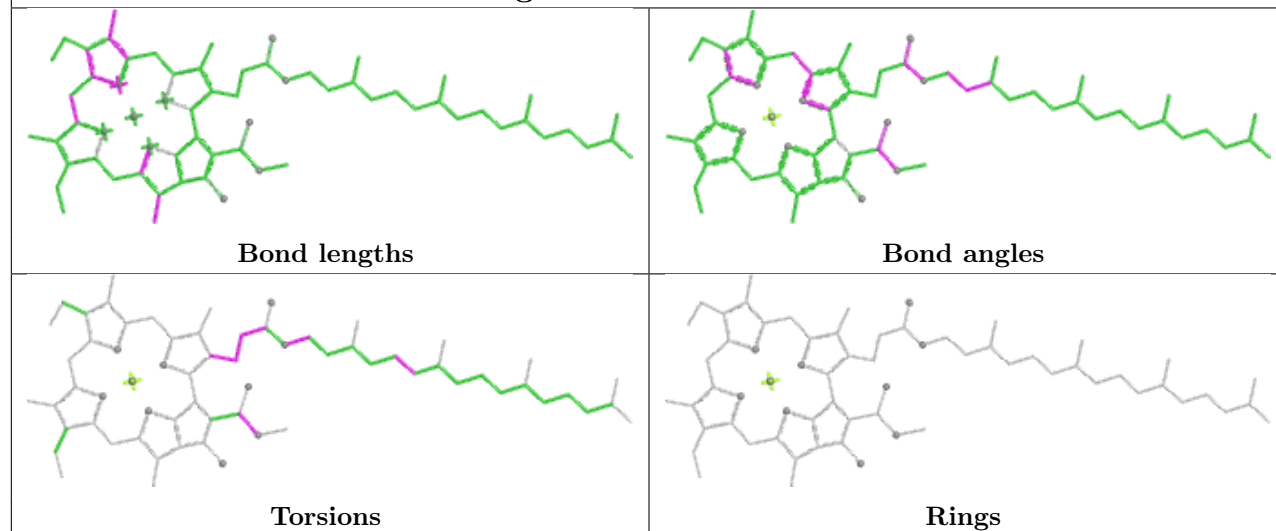


Rings

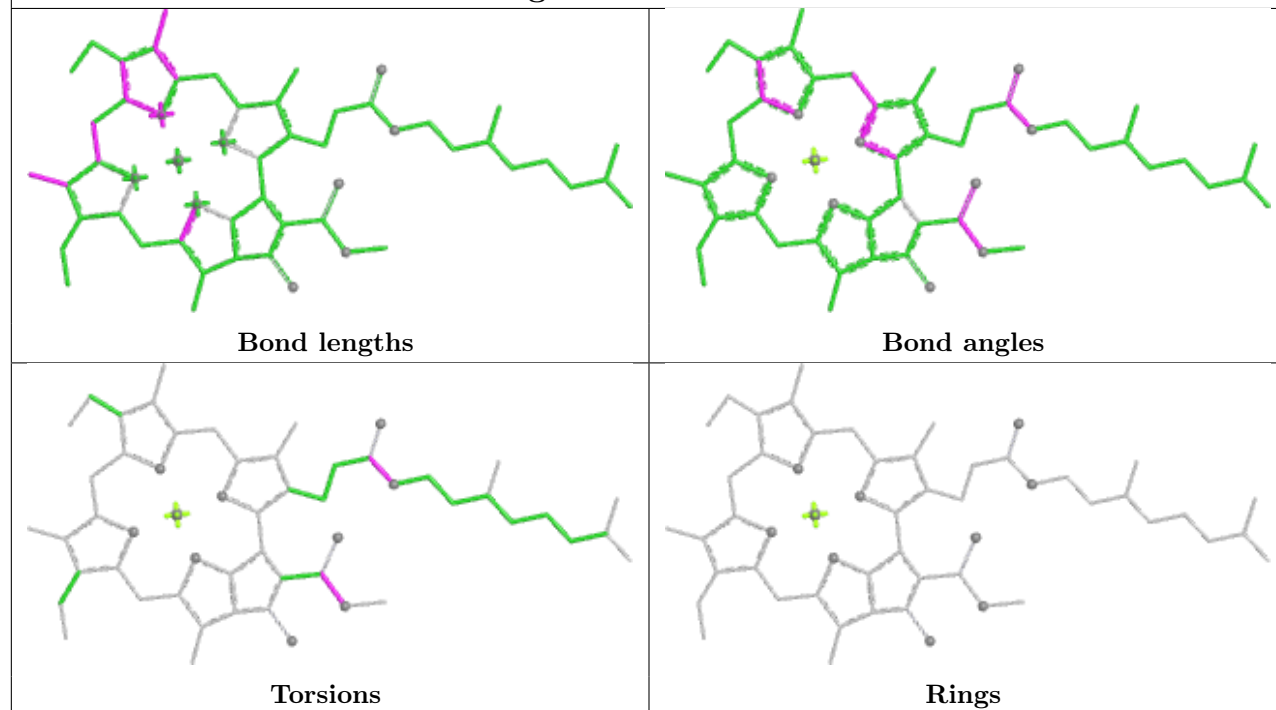


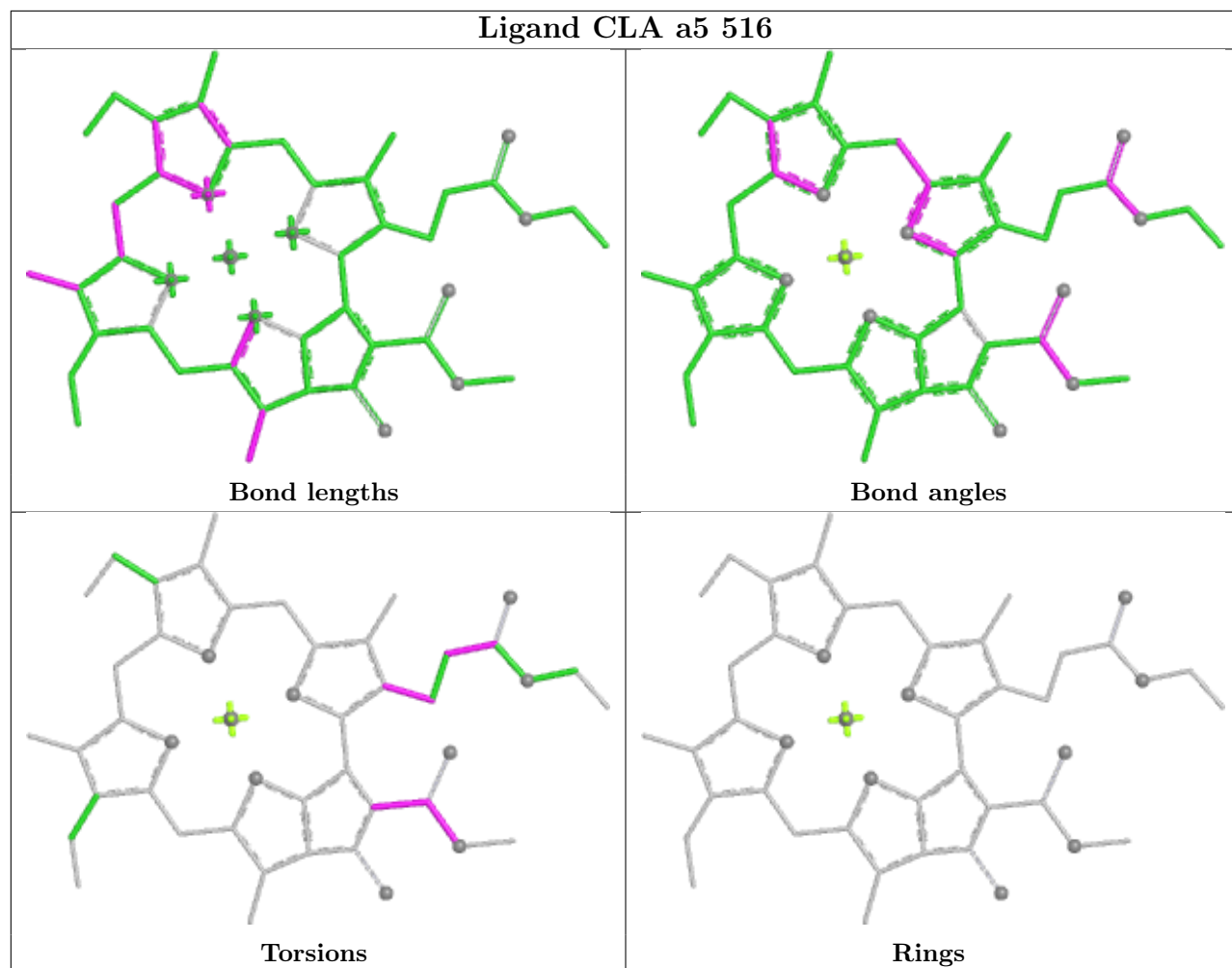


Ligand CLA cB 1206

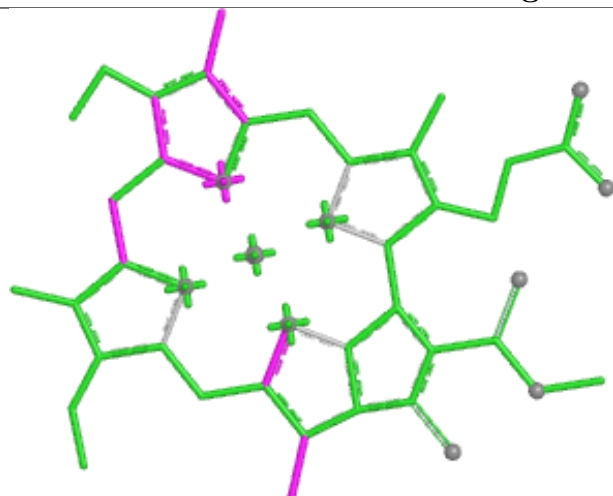


Ligand CLA c6 508

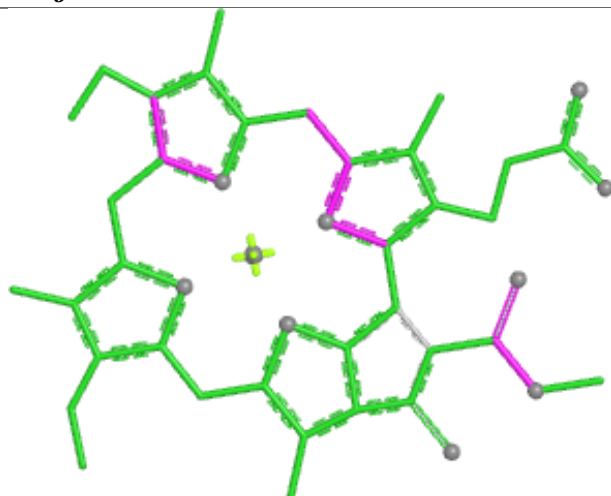




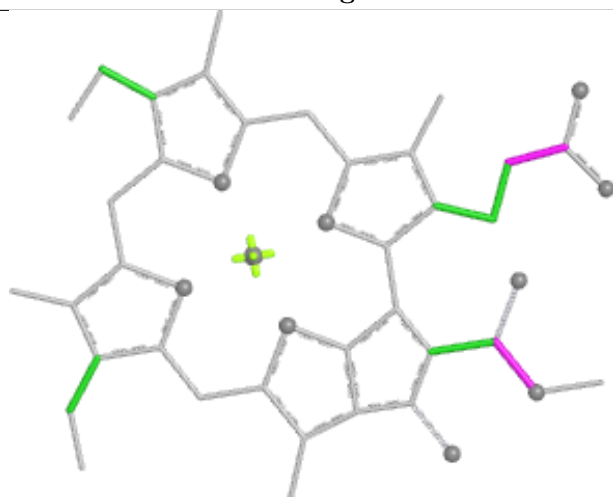
Ligand CLA j 506



Bond lengths



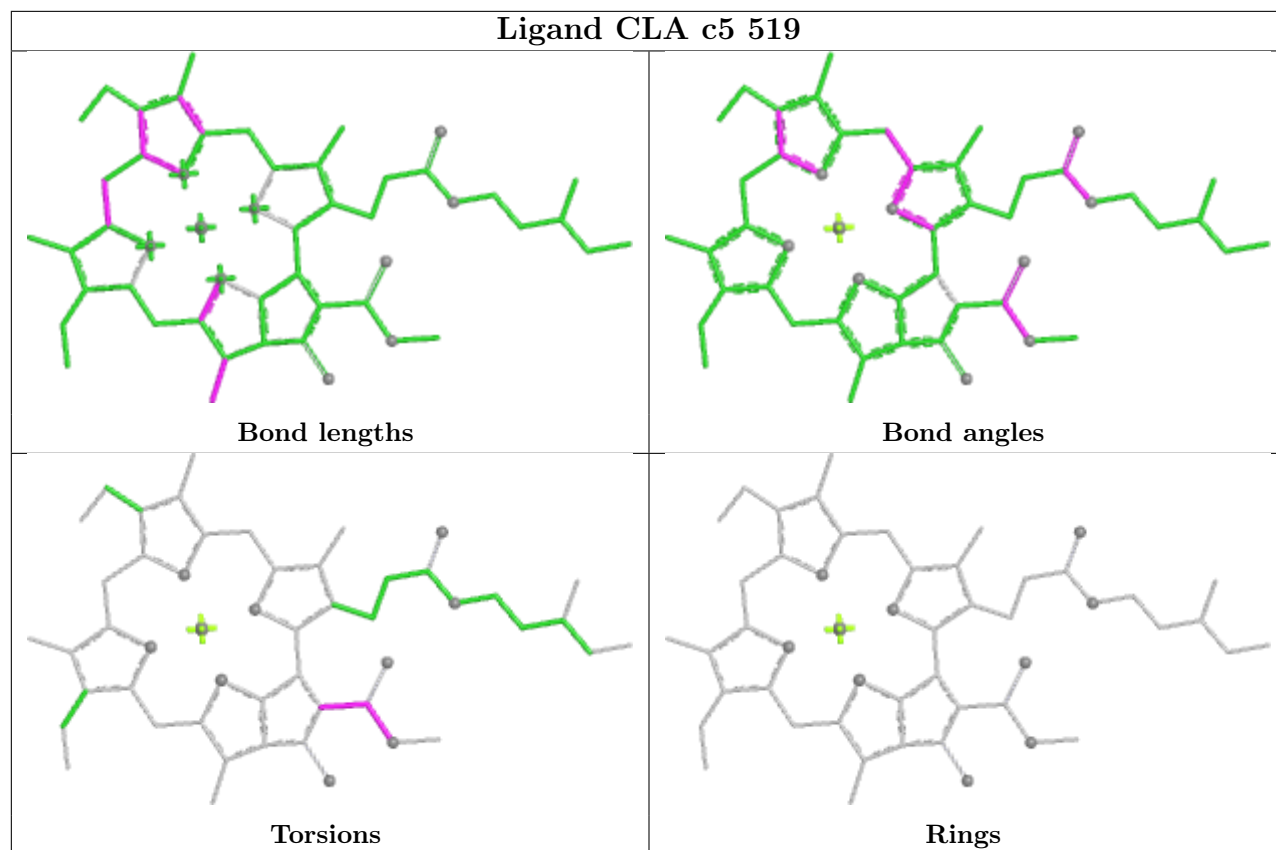
Bond angles

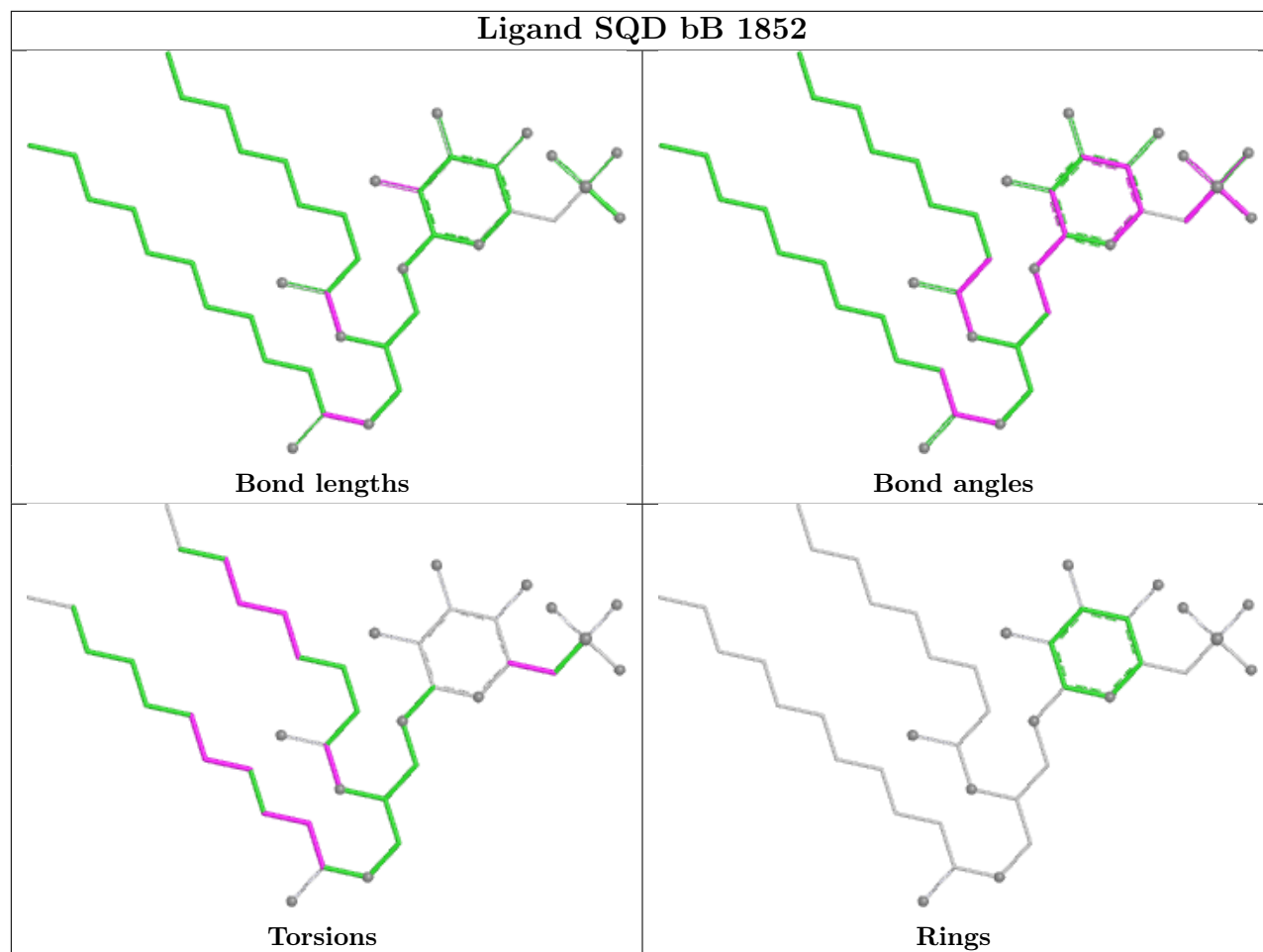


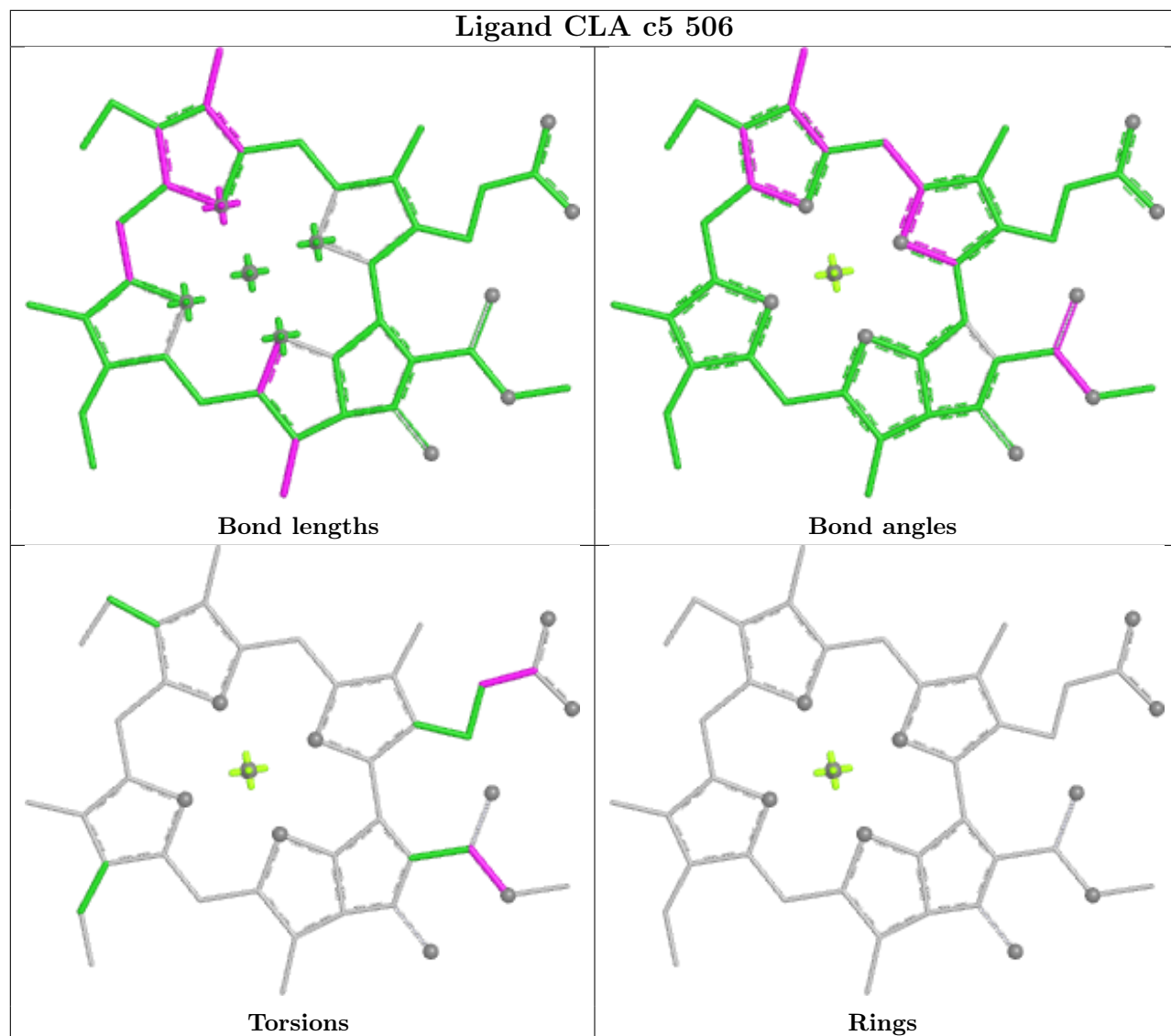
Torsions



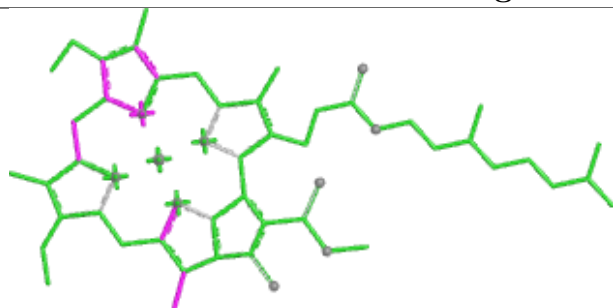
Rings



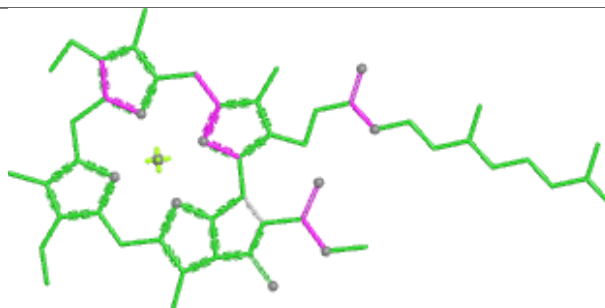




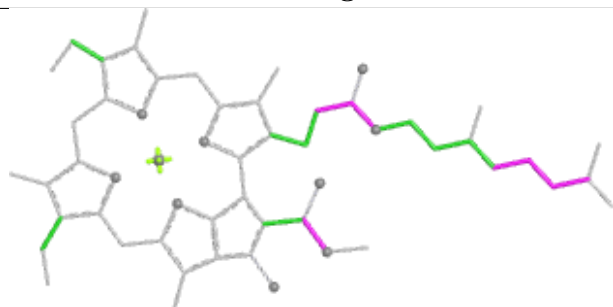
Ligand CLA bA 1107



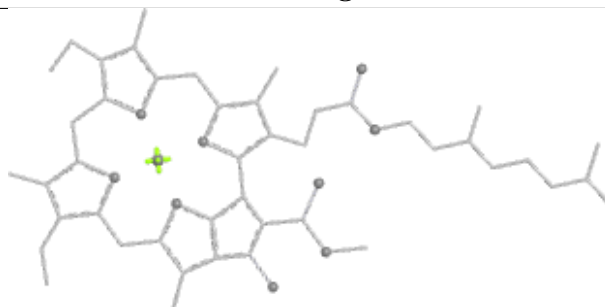
Bond lengths



Bond angles

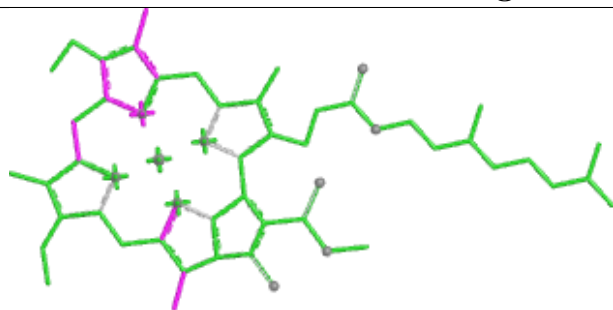


Torsions

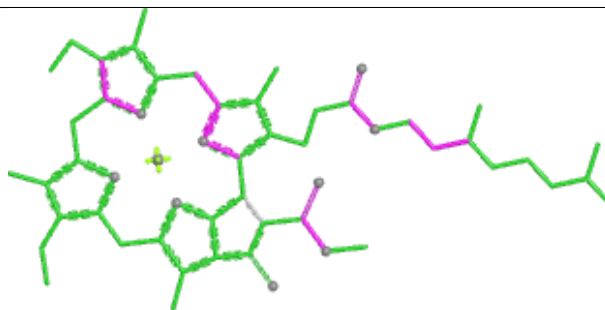


Rings

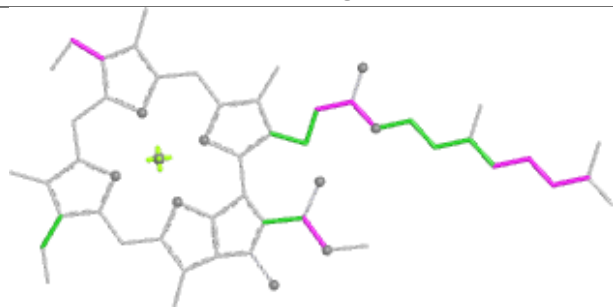
Ligand CLA aA 1107



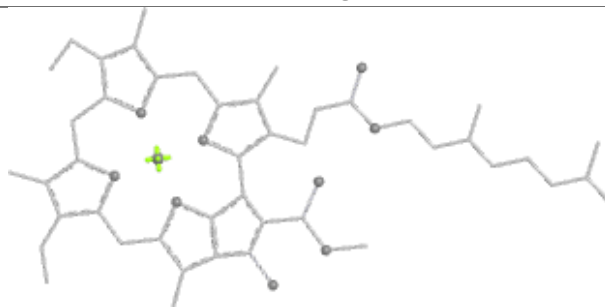
Bond lengths



Bond angles

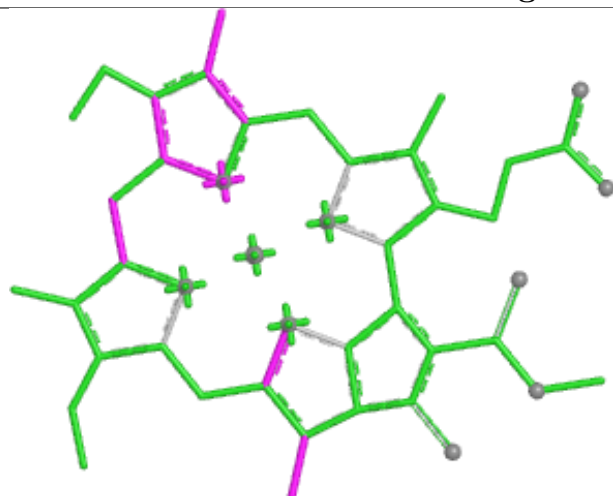


Torsions

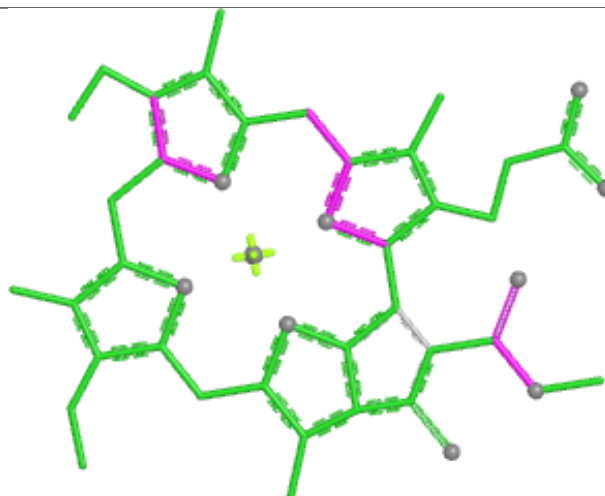


Rings

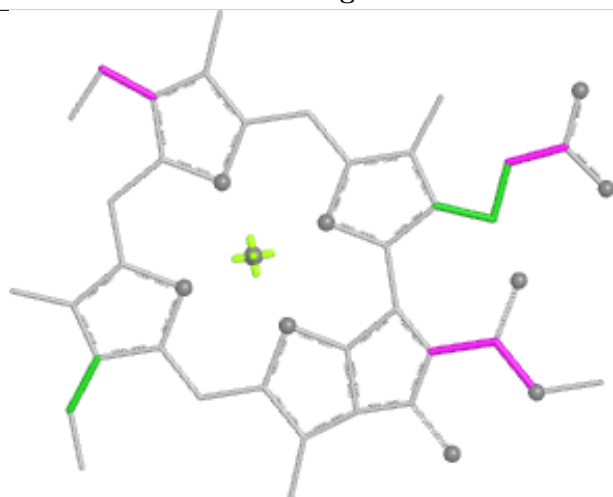
Ligand CLA a 517



Bond lengths



Bond angles

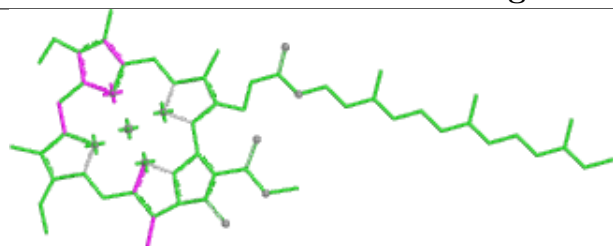


Torsions

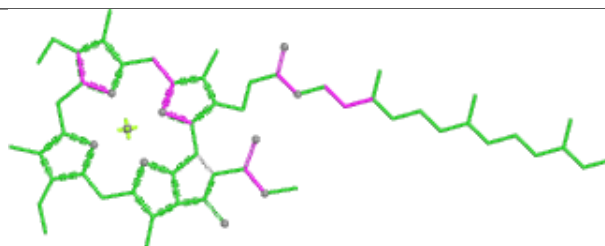


Rings

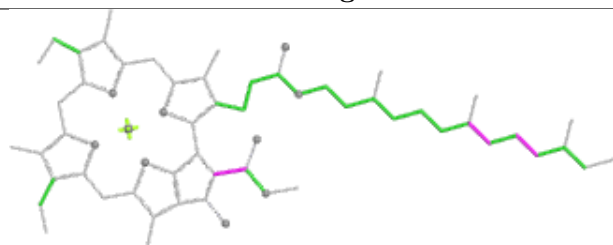
Ligand CLA b1 507



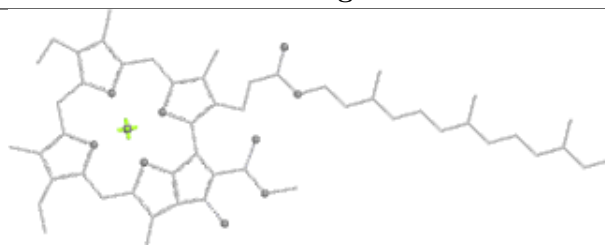
Bond lengths



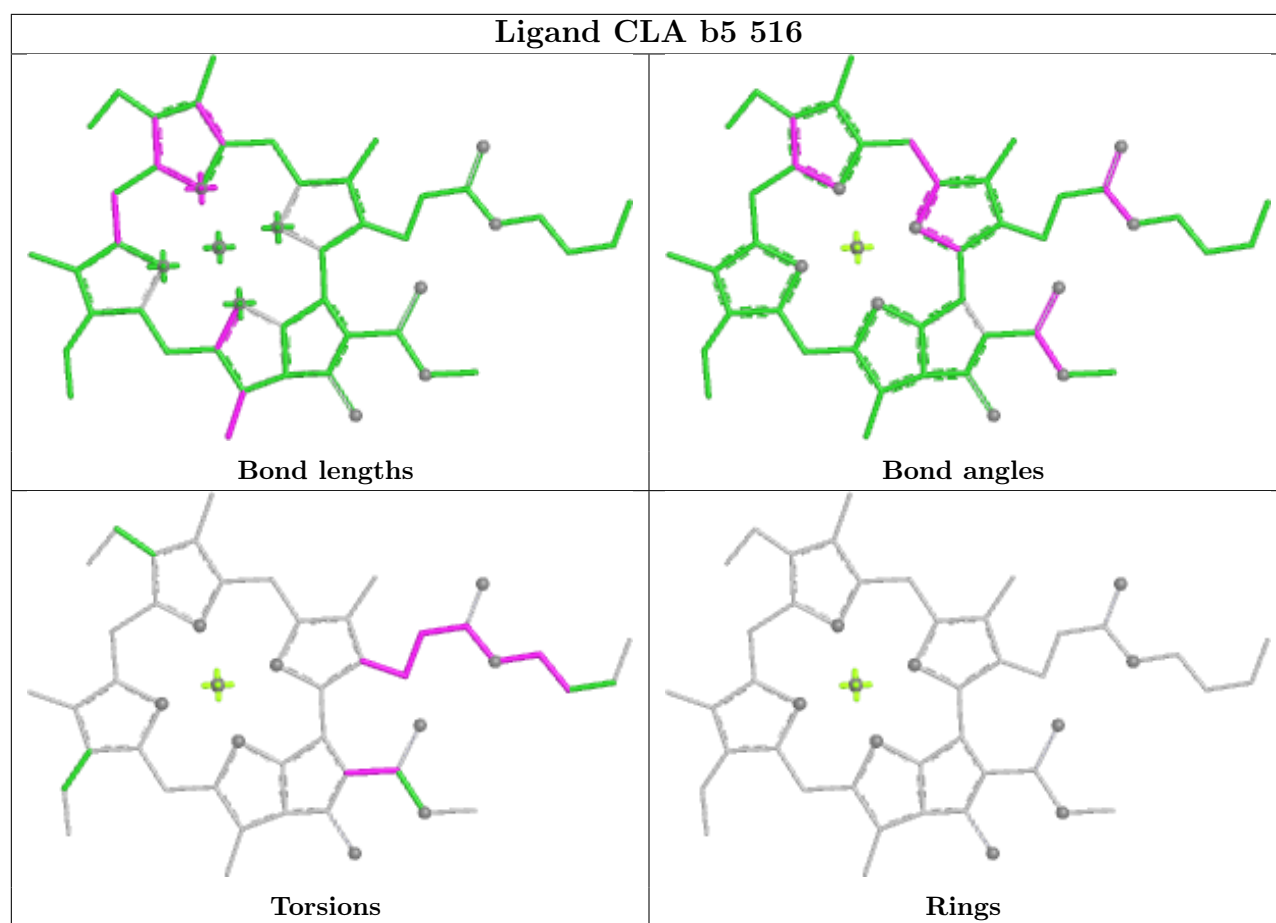
Bond angles



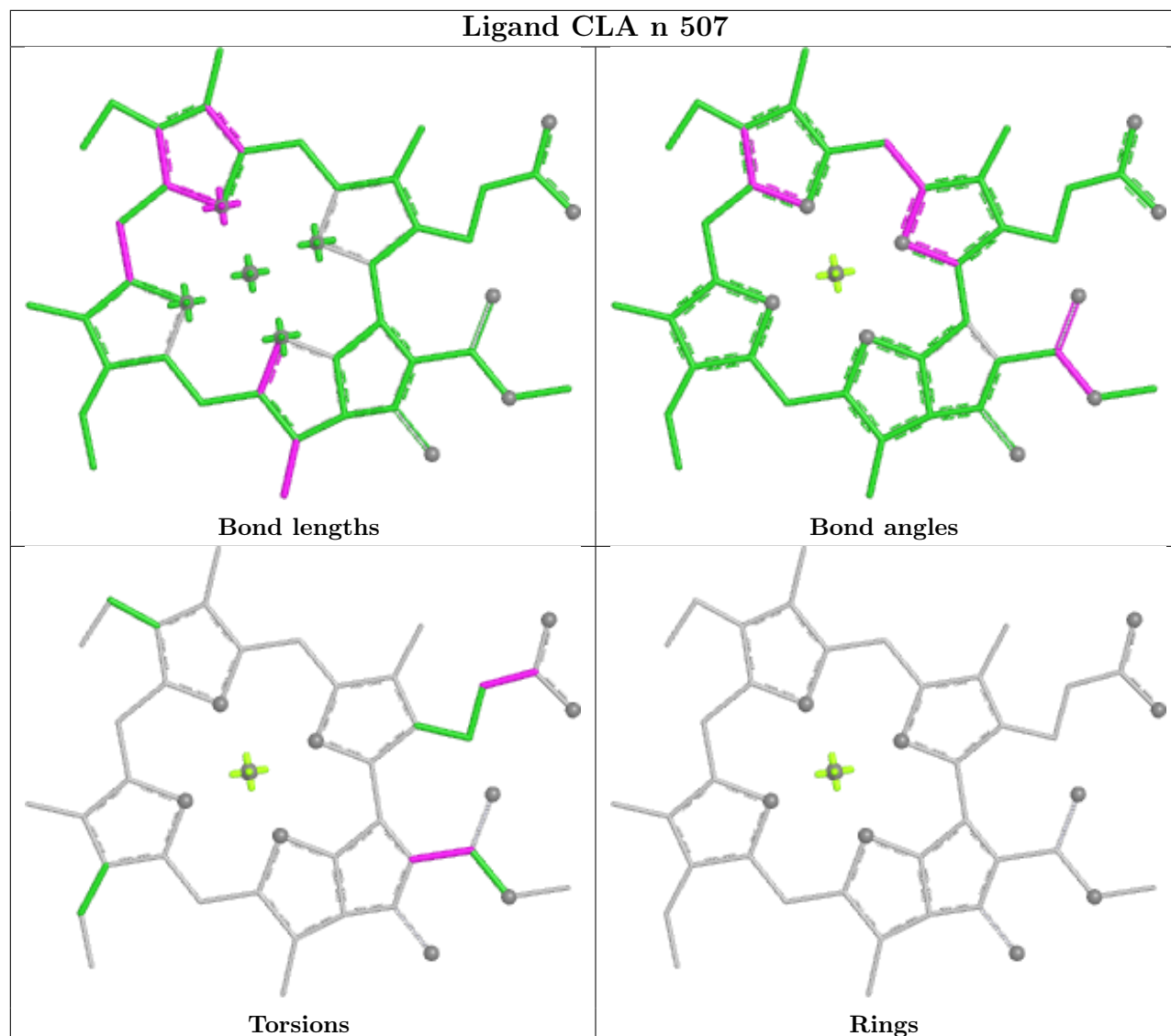
Torsions



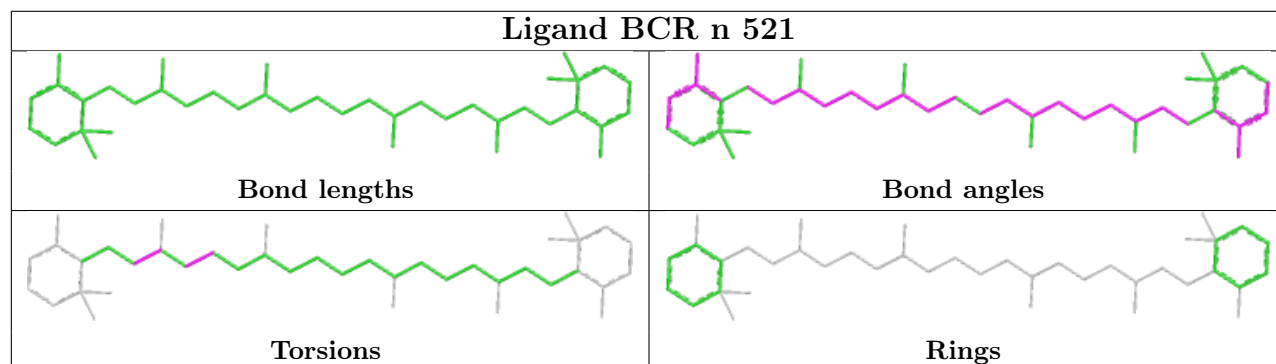
Rings



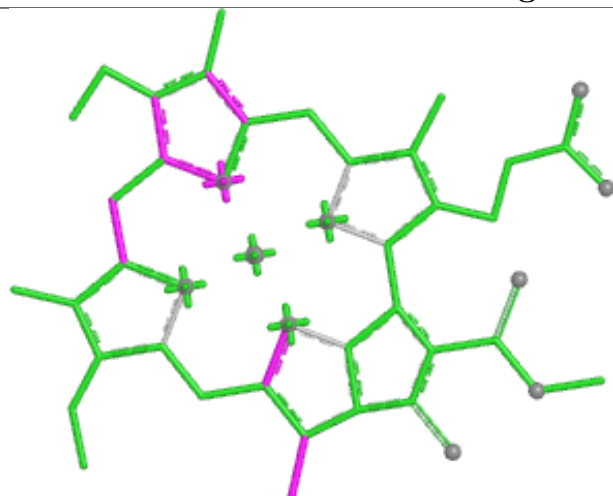
Ligand CLA n 507



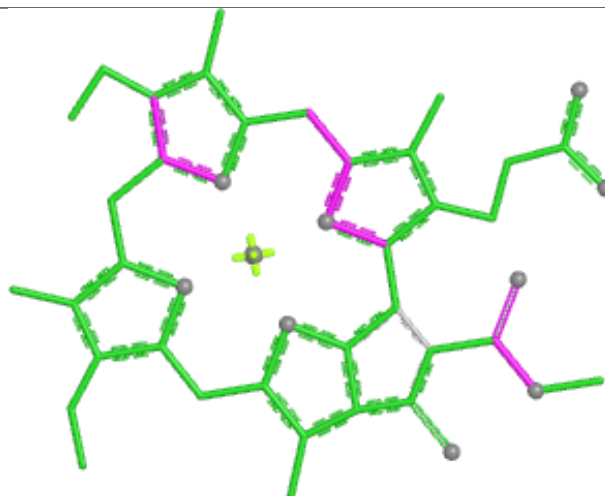
Ligand BCR n 521



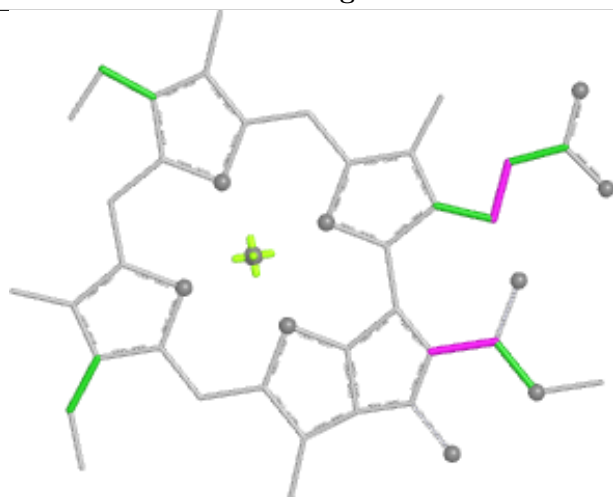
Ligand CLA o 505



Bond lengths



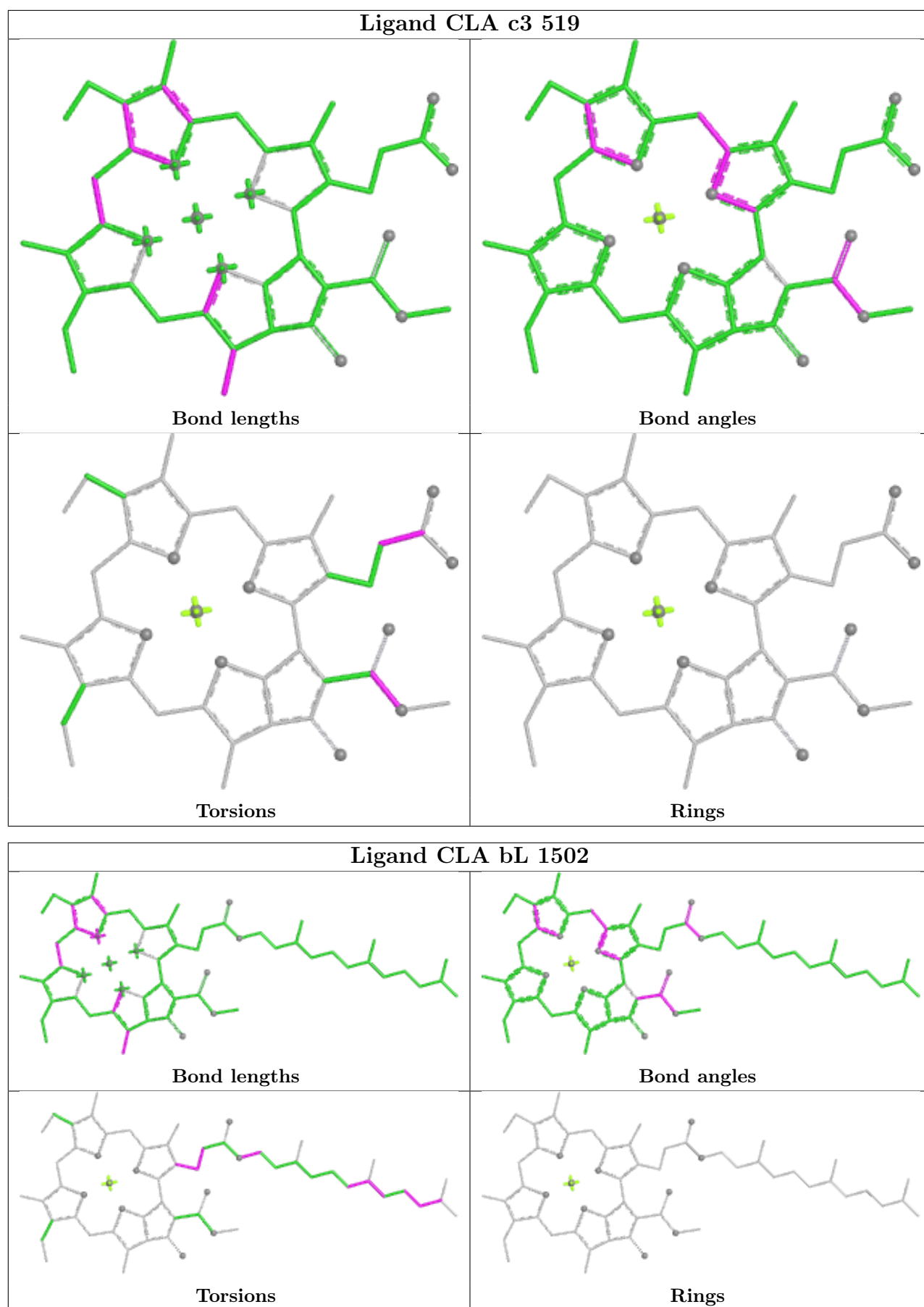
Bond angles

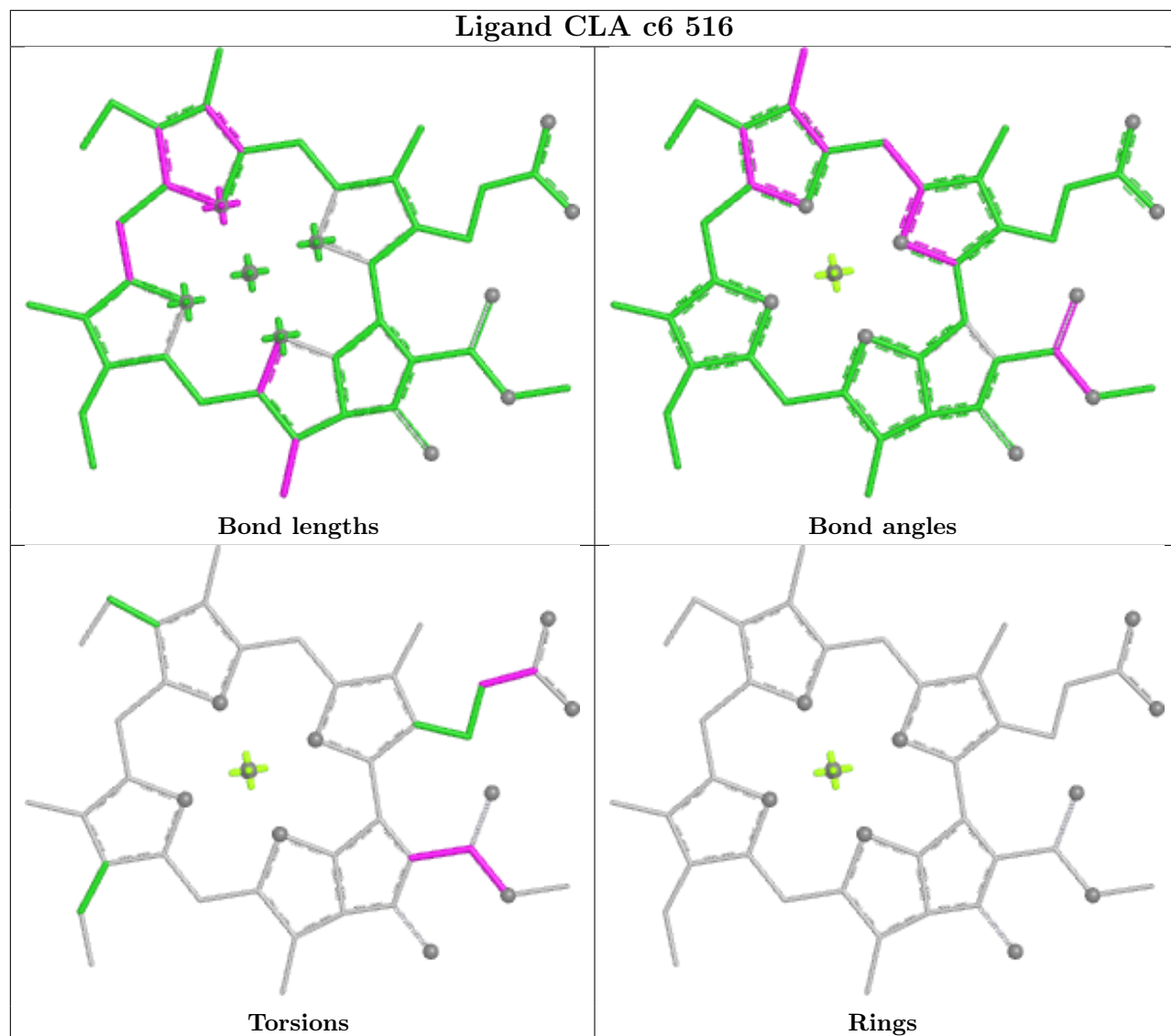


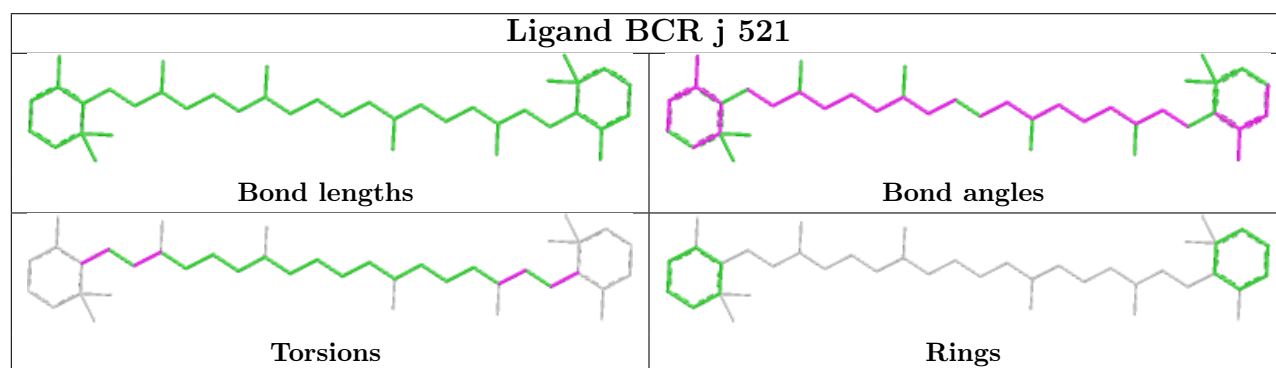
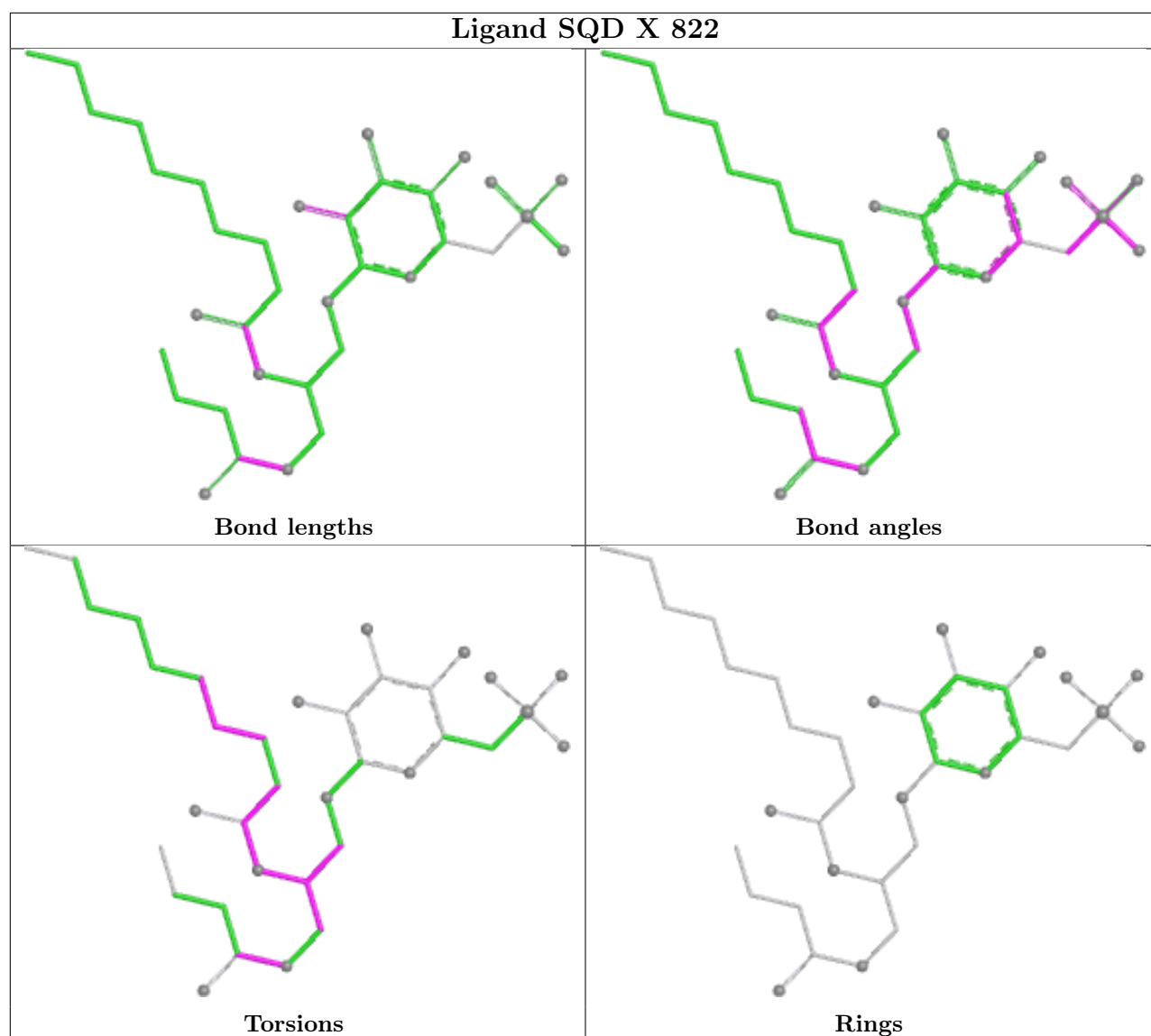
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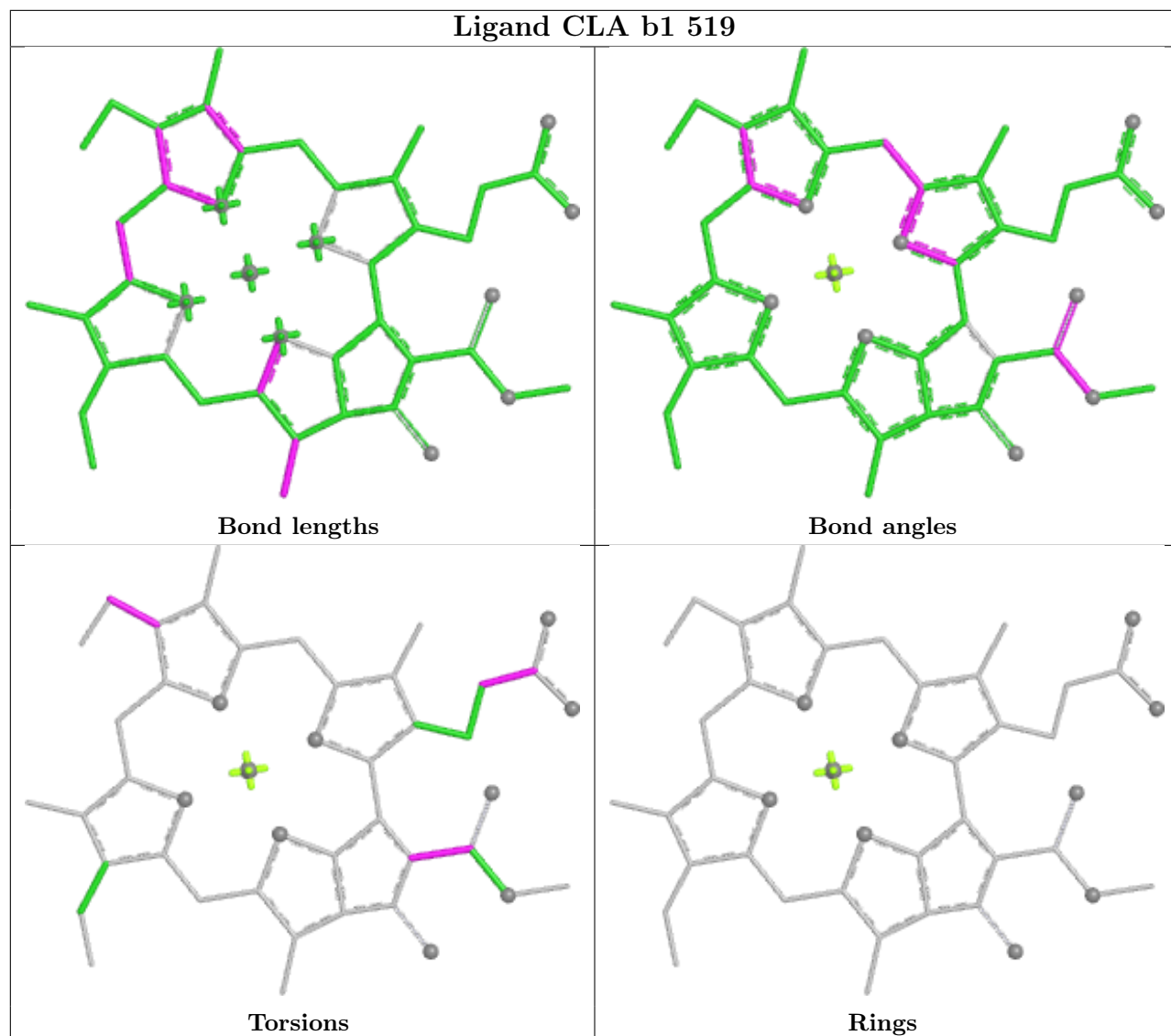


Rings

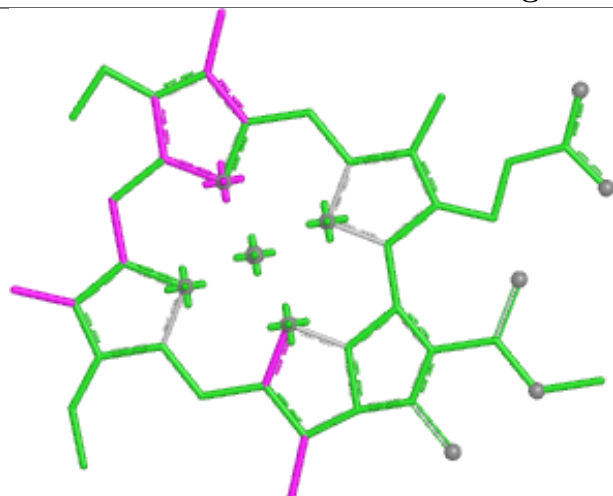








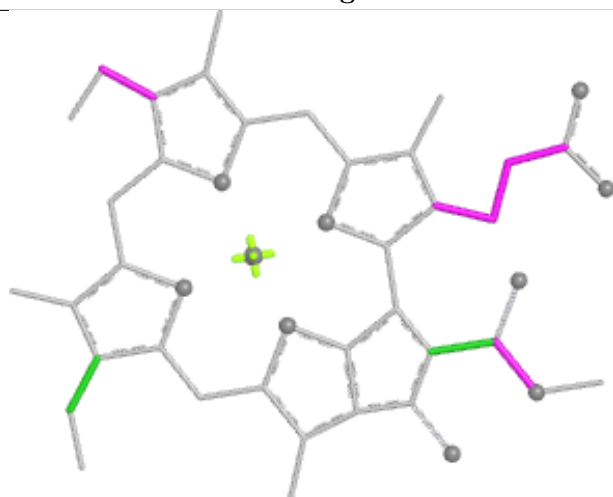
Ligand CLA f 501



Bond lengths



Bond angles

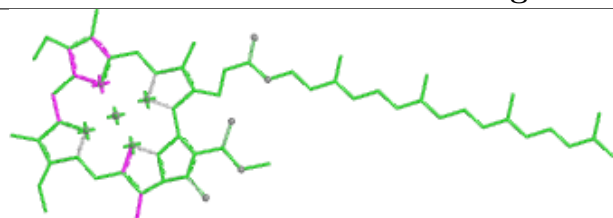


Torsions

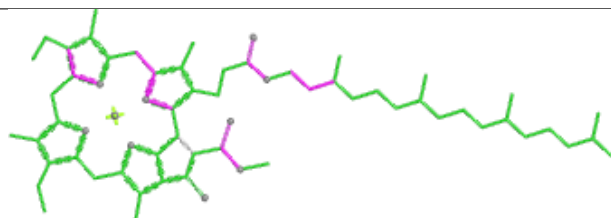


Rings

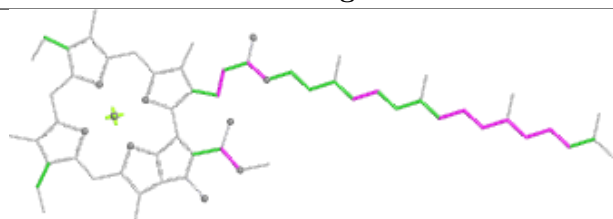
Ligand CLA c3 505



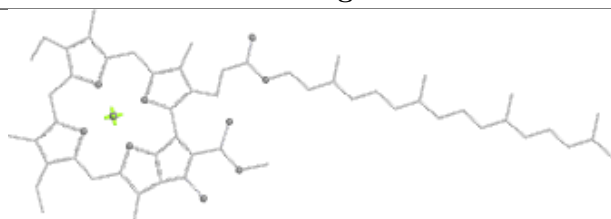
Bond lengths



Bond angles

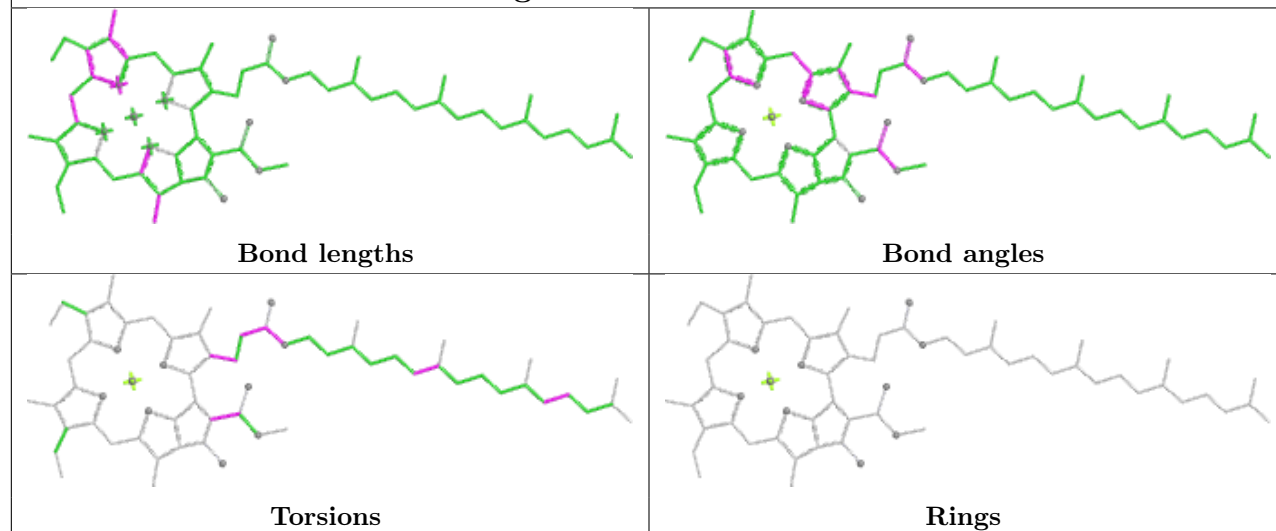


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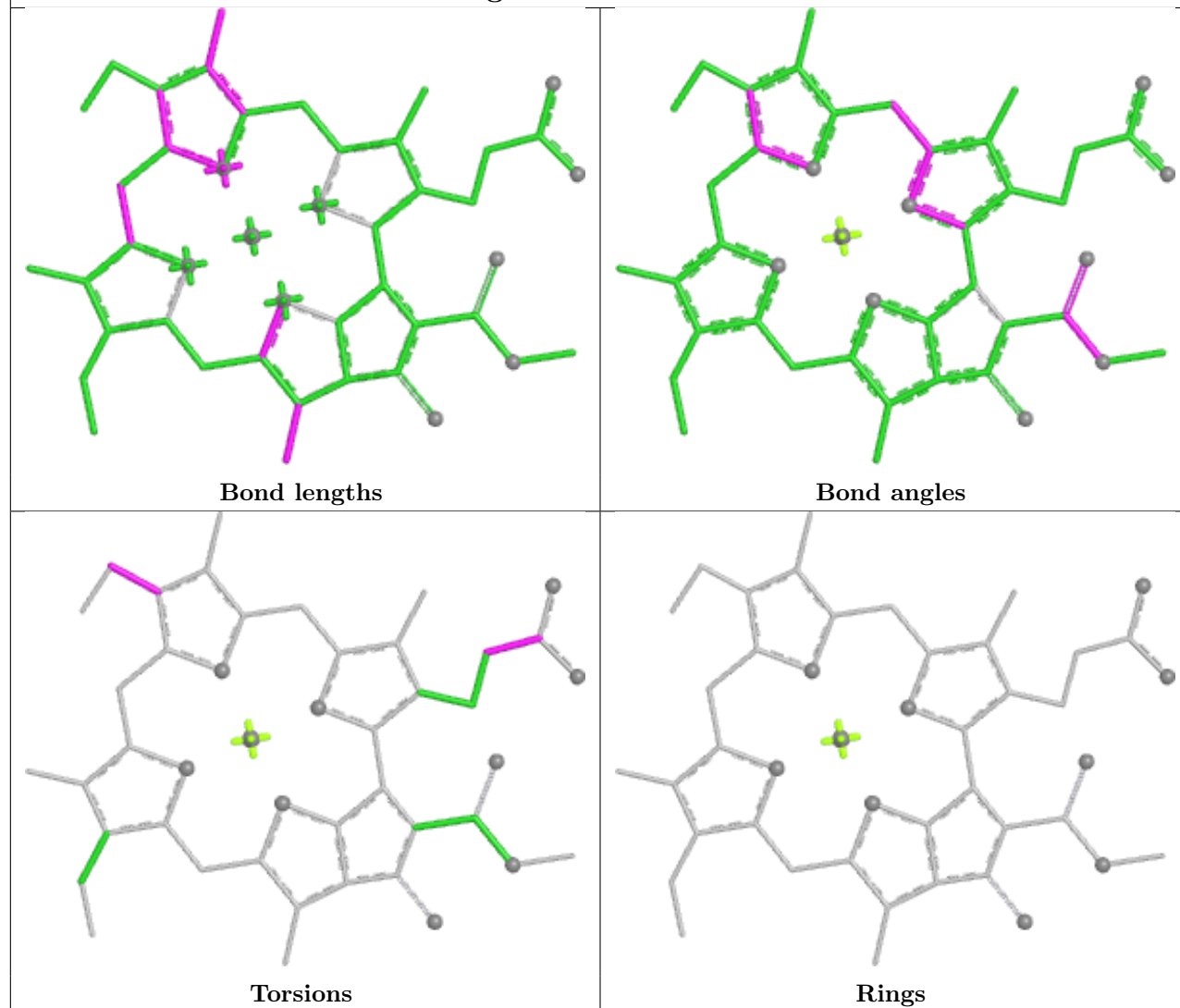


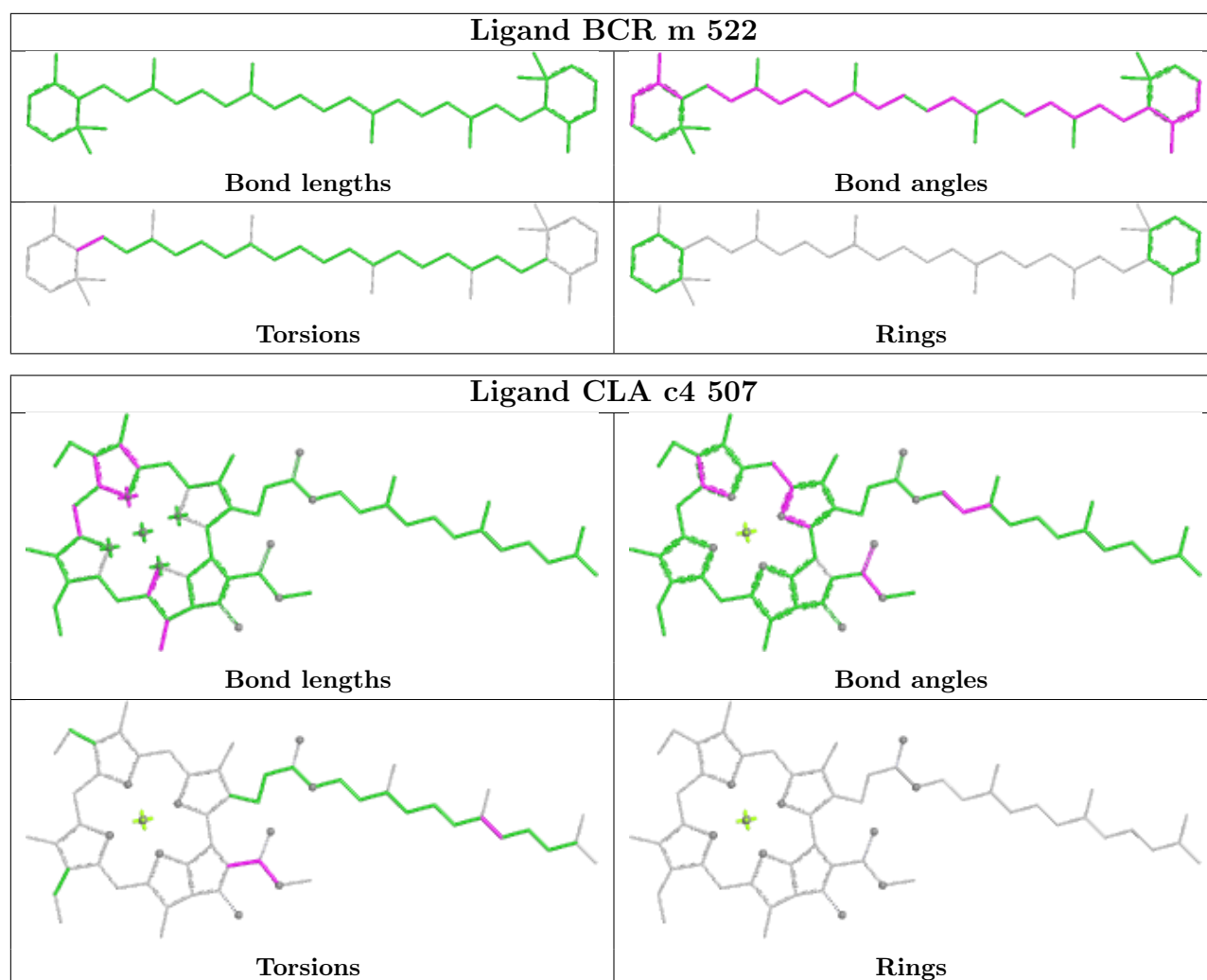
Rings

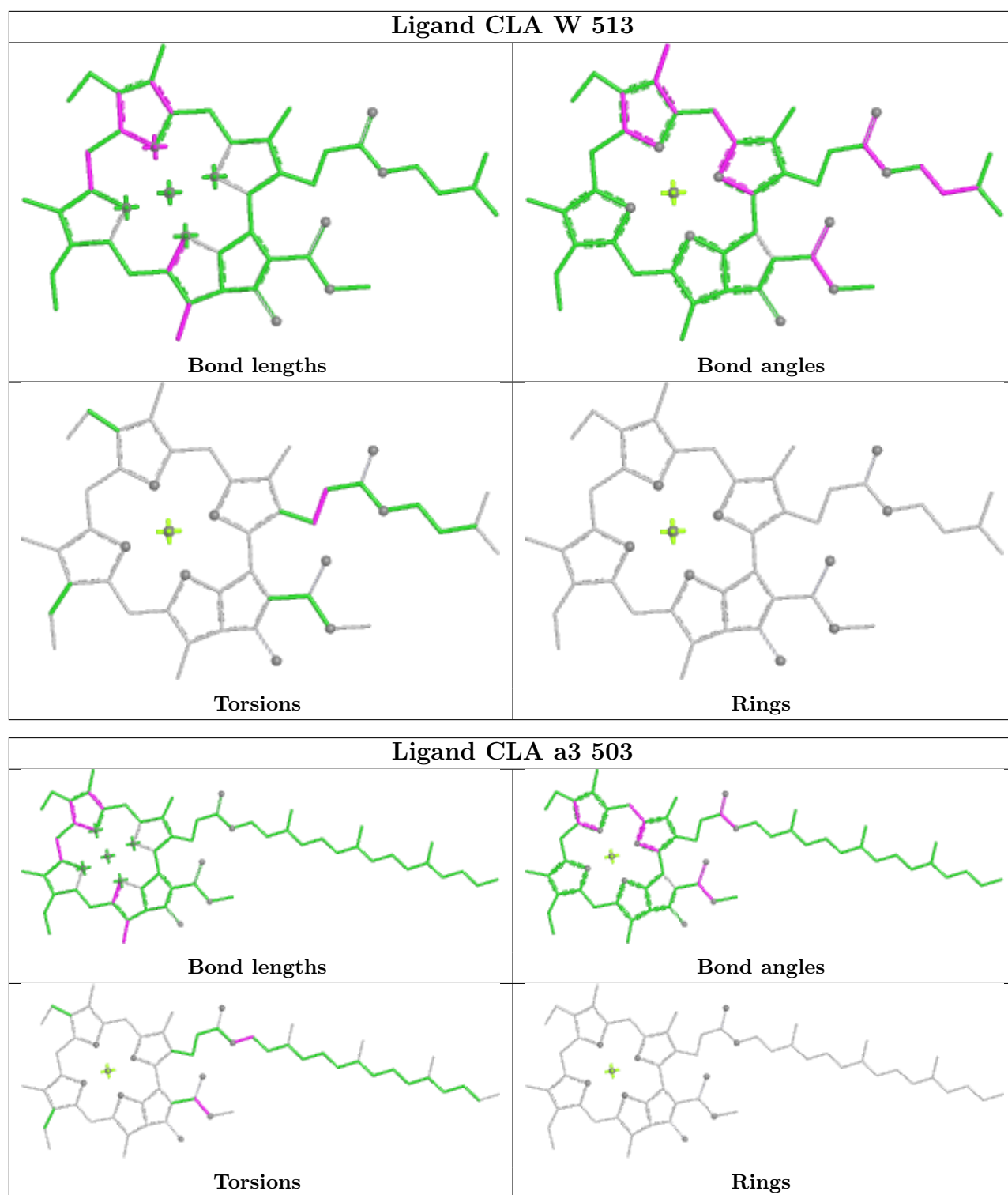
Ligand CLA aA 1102

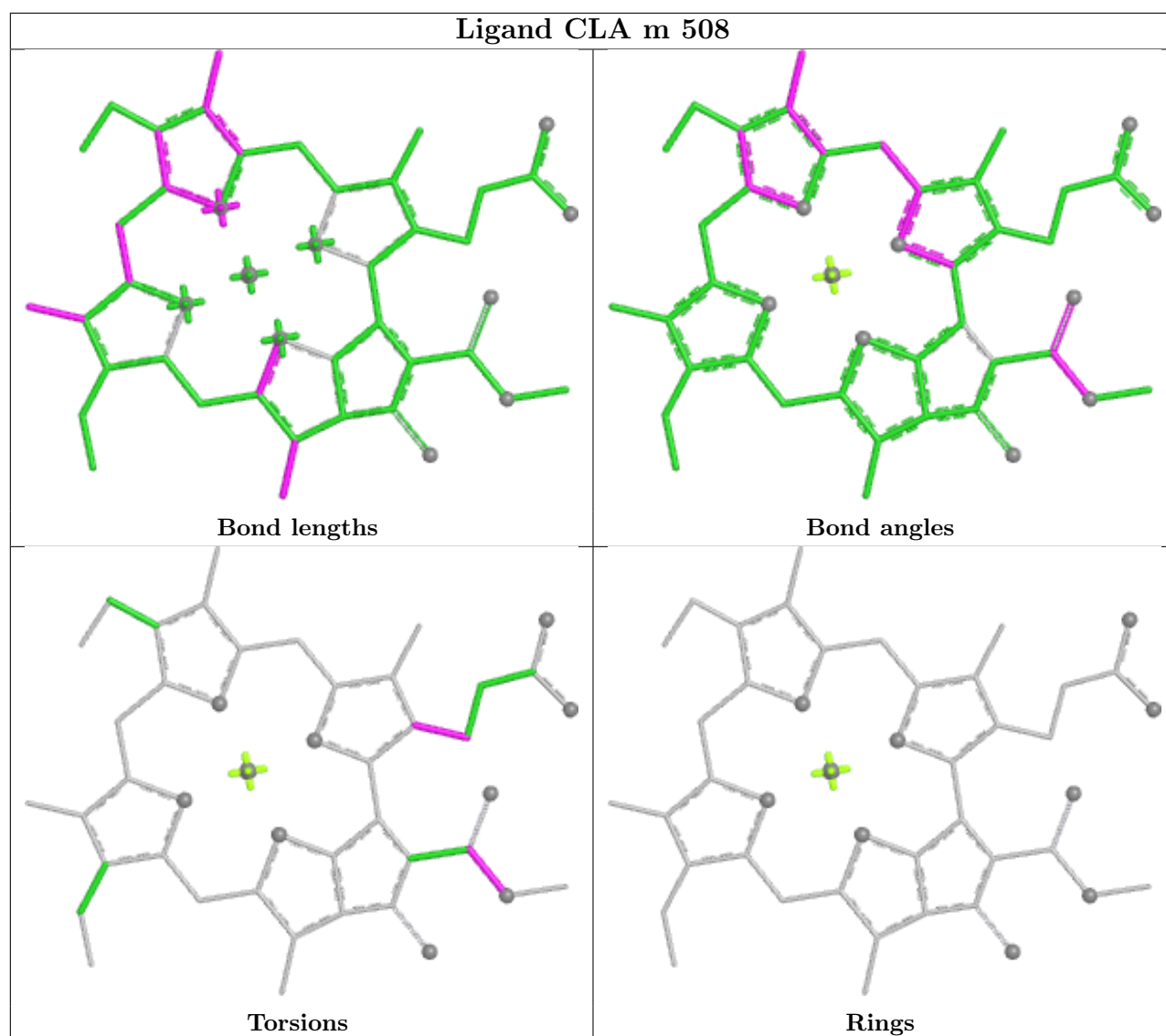


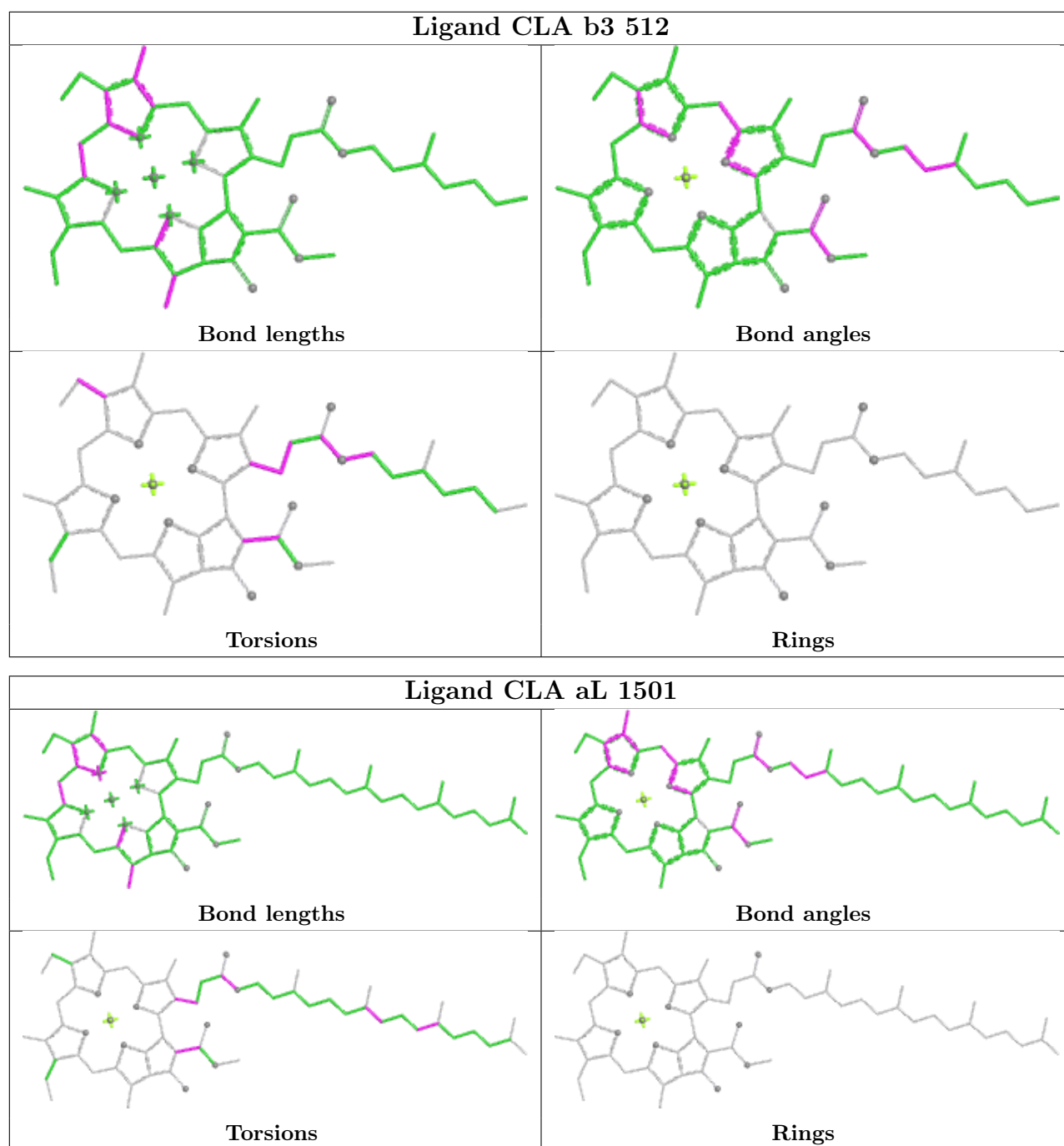
Ligand CLA b6 517



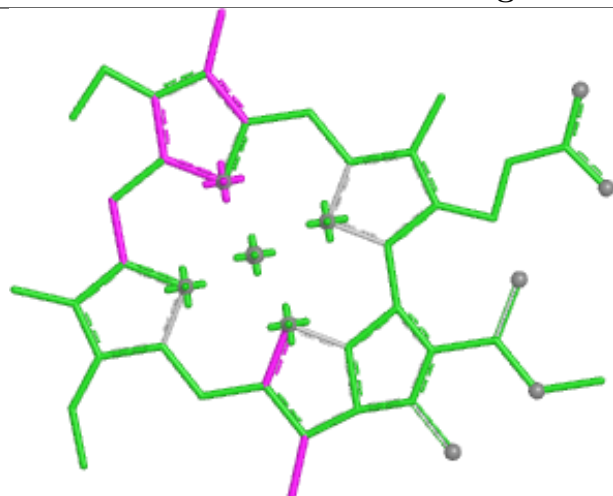




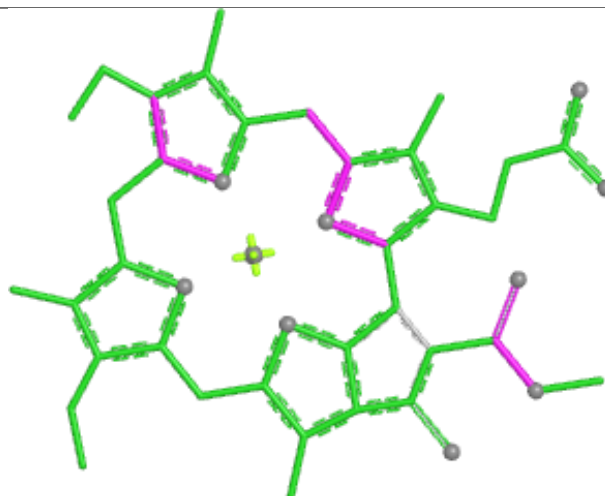




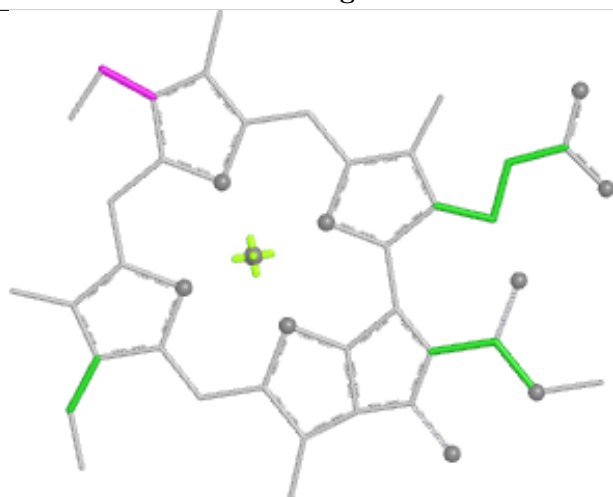
Ligand CLA bF 1301



Bond lengths



Bond angles

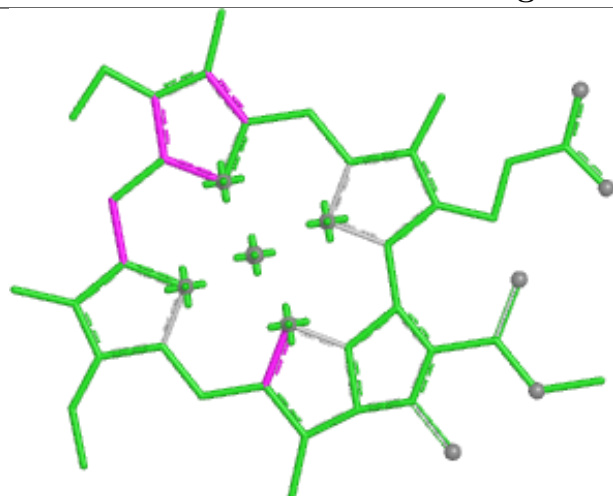


Torsions

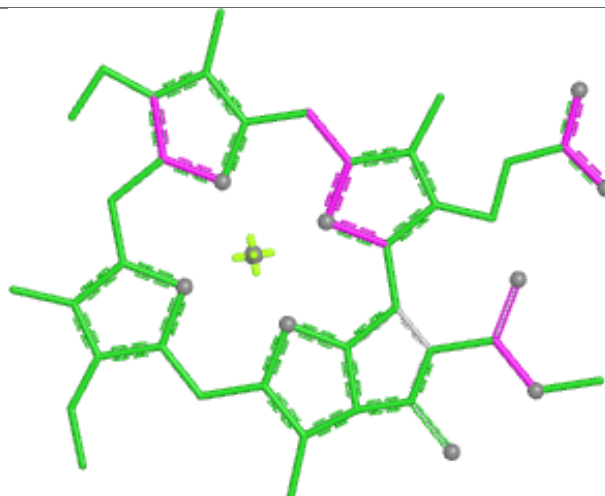


Rings

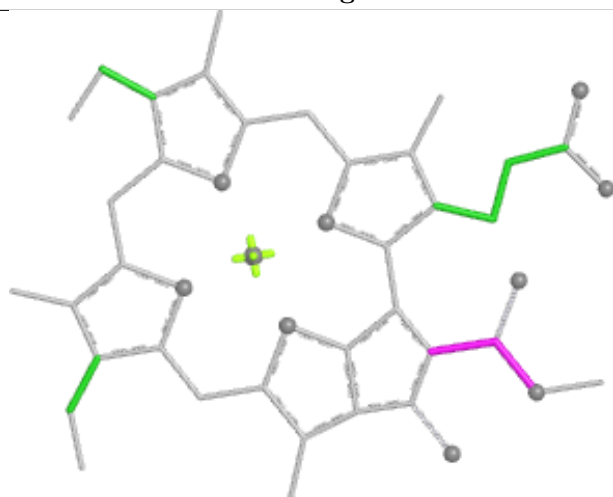
Ligand CLA h 516



Bond lengths



Bond angles

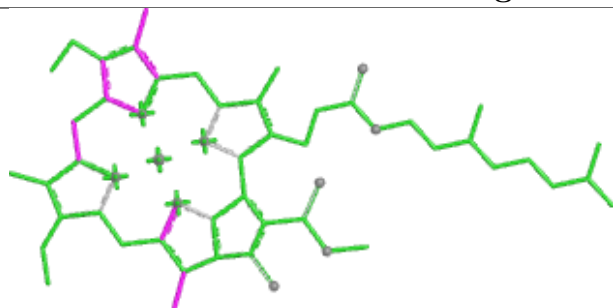


Torsions

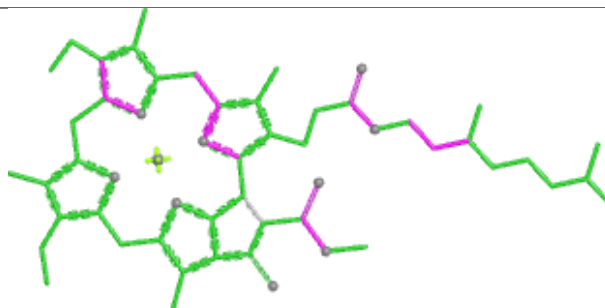


Rings

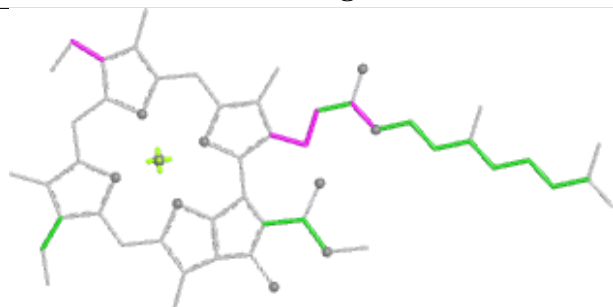
Ligand CLA bA 1134



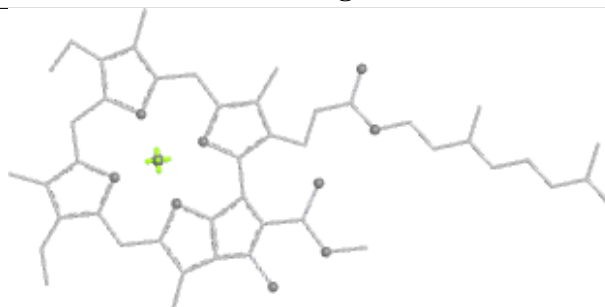
Bond lengths



Bond angles

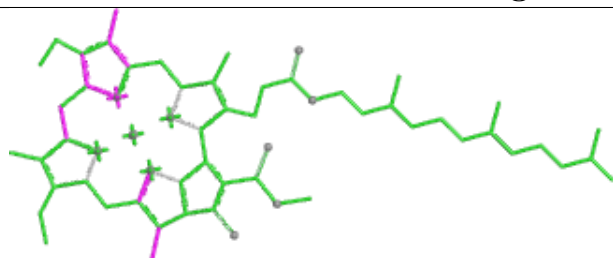


Torsions

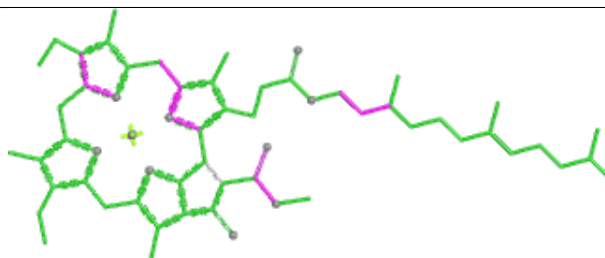


Rings

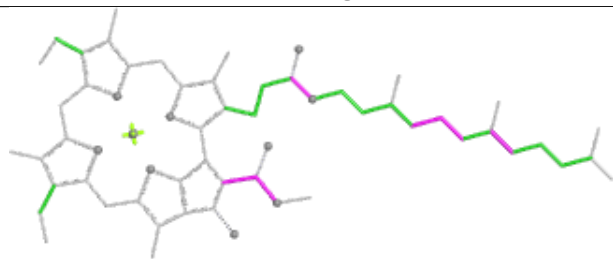
Ligand CLA c2 502



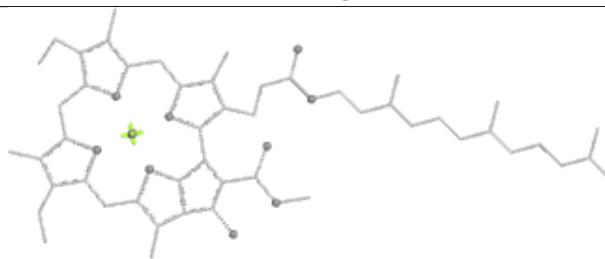
Bond lengths



Bond angles

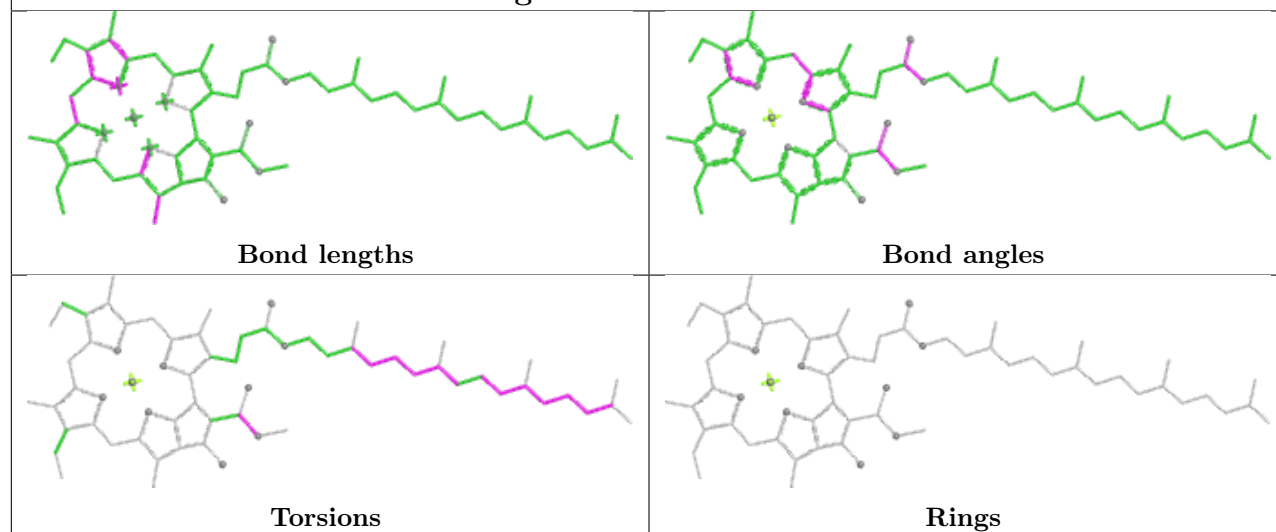


Torsions

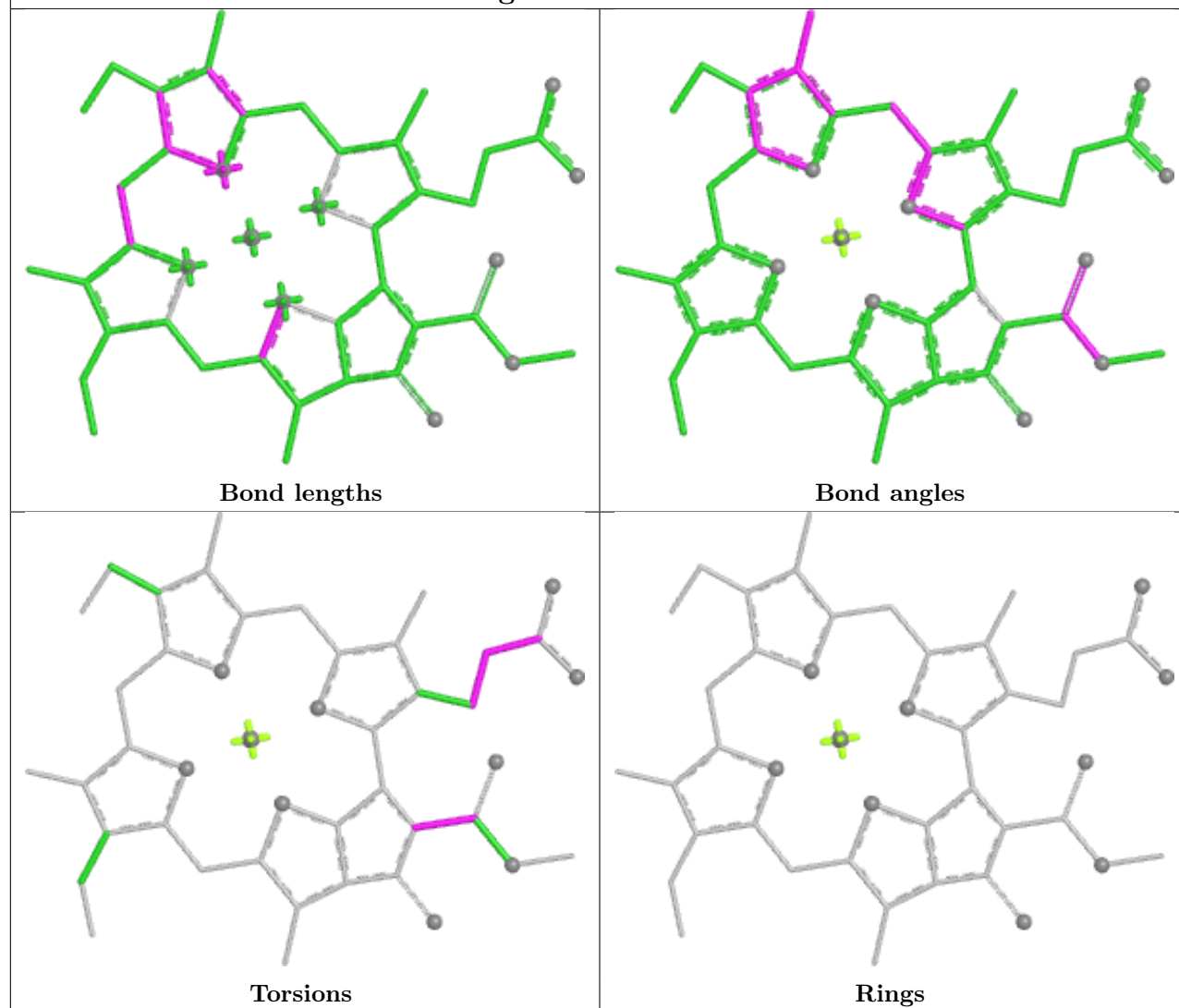


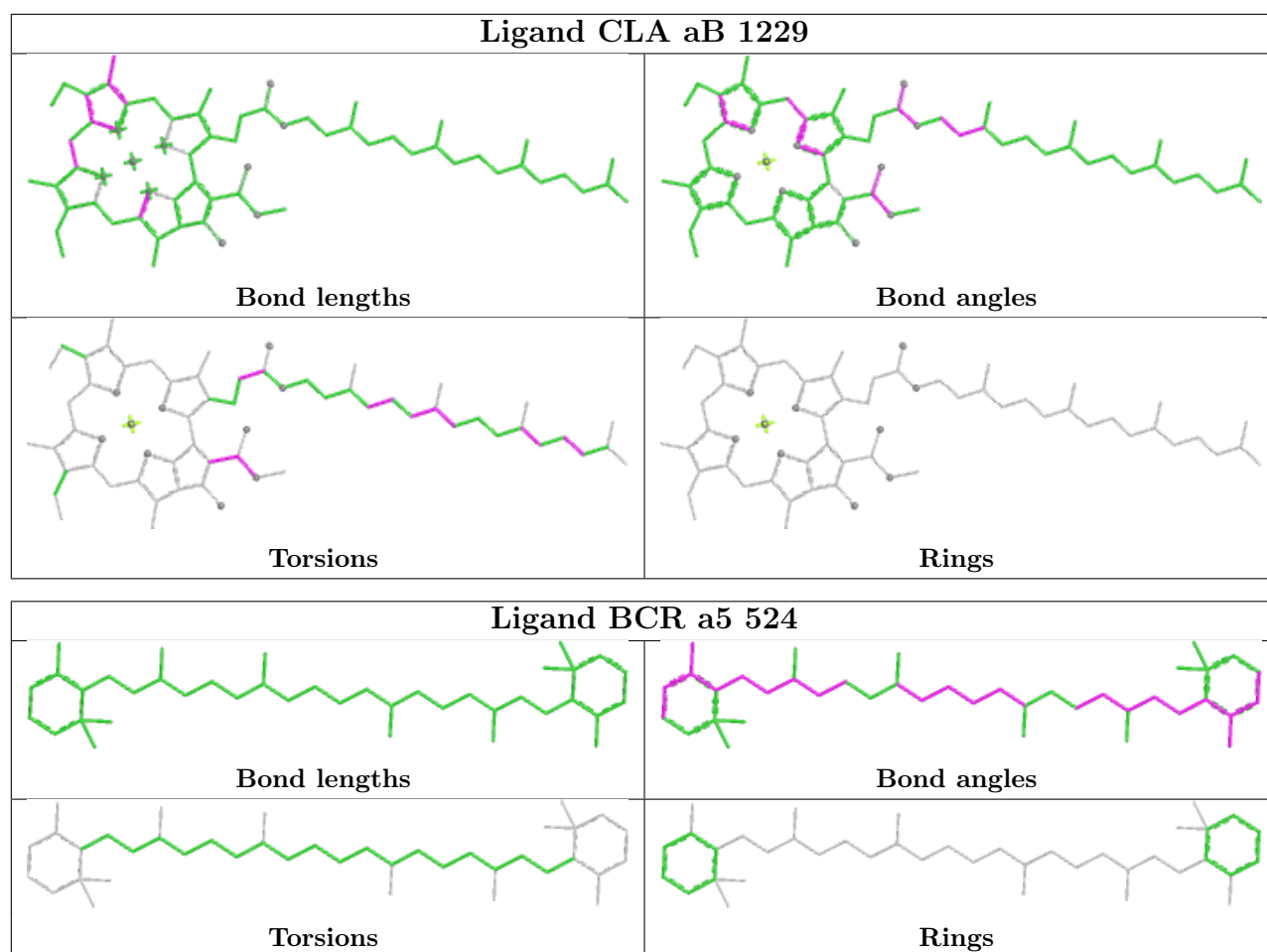
Rings

Ligand CLA aB 1203

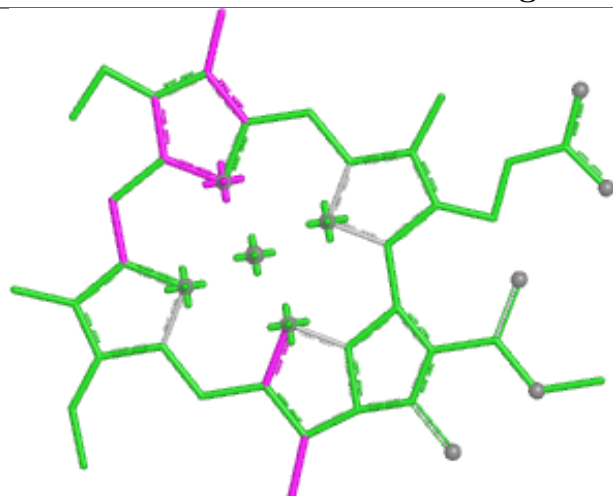


Ligand CLA f 513

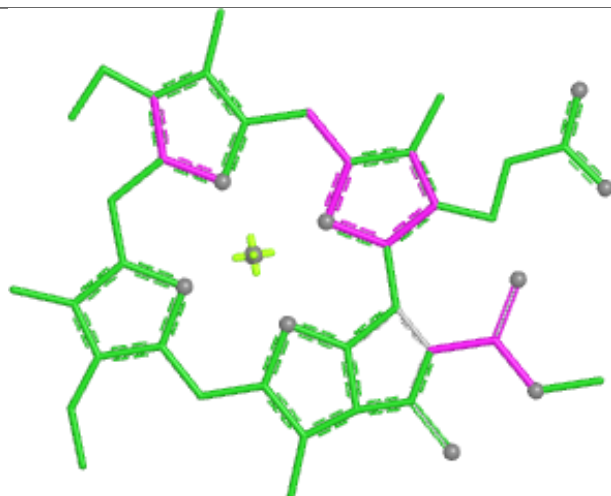




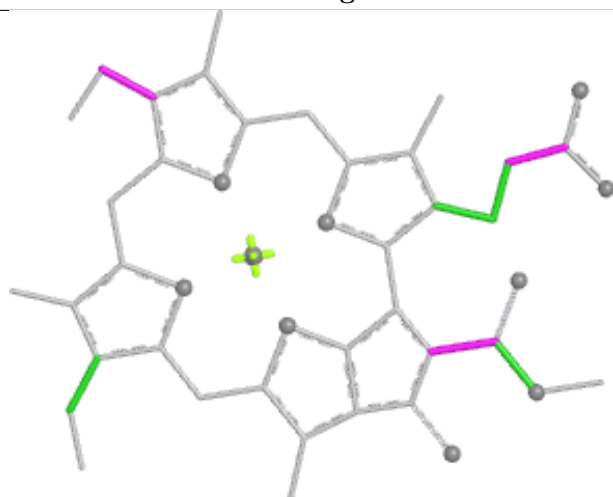
Ligand CLA e 516



Bond lengths



Bond angles

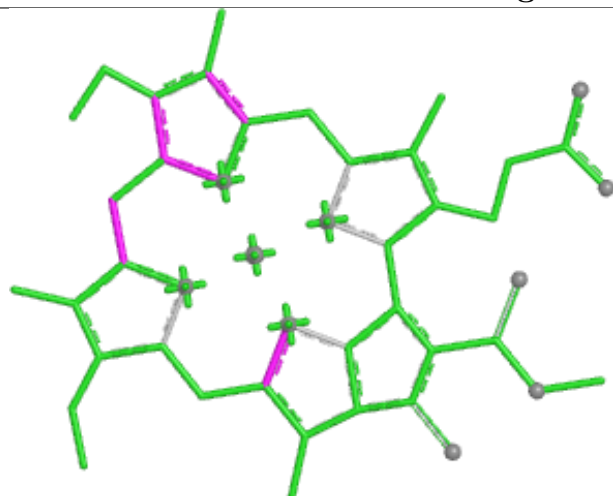


Torsions

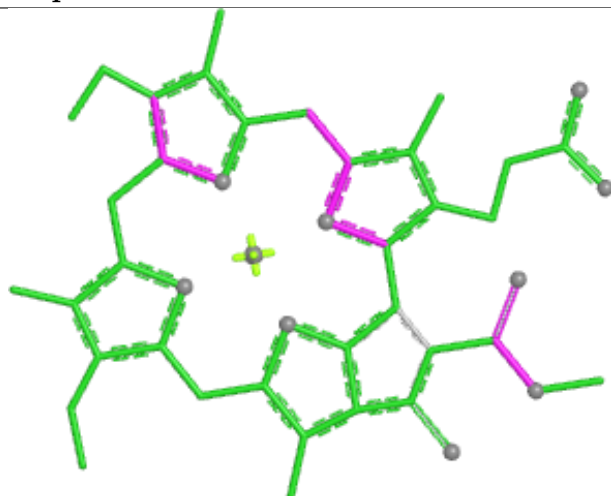


Rings

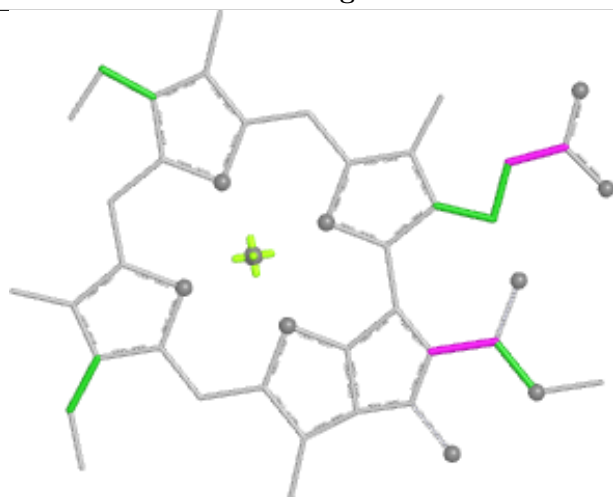
Ligand CLA p 507



Bond lengths



Bond angles

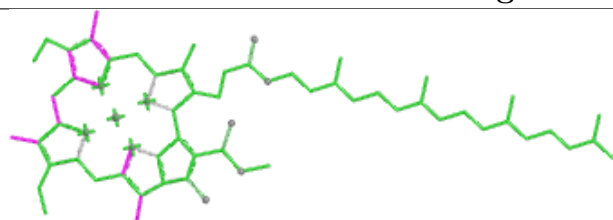


Torsions

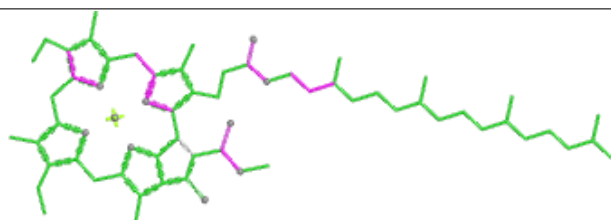


Rings

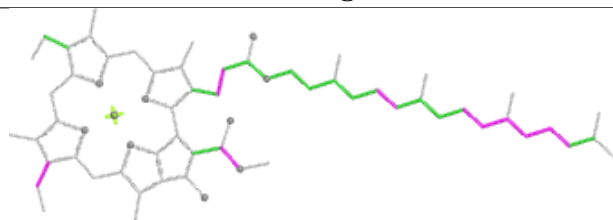
Ligand CLA aB 1023



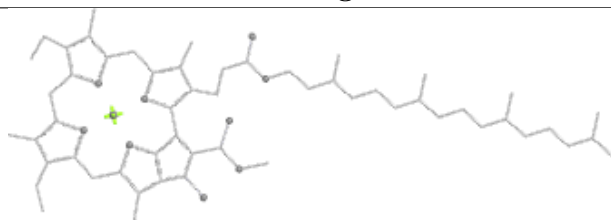
Bond lengths



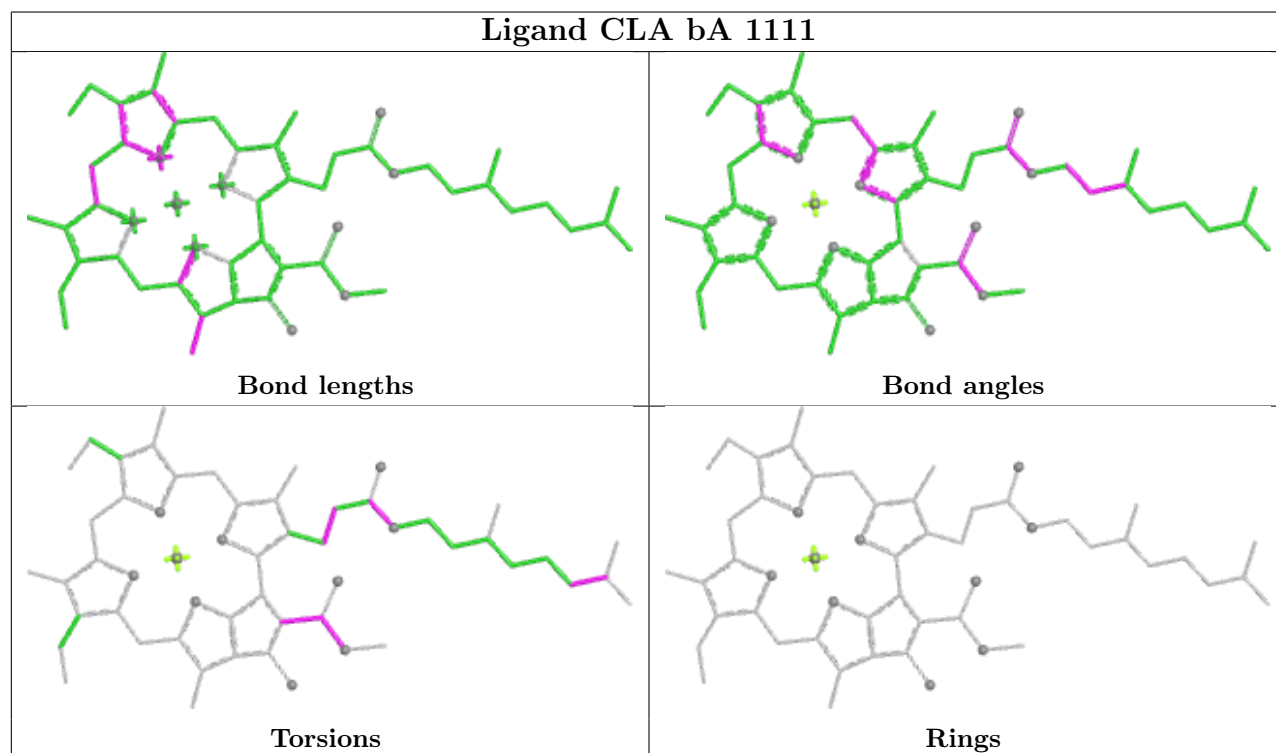
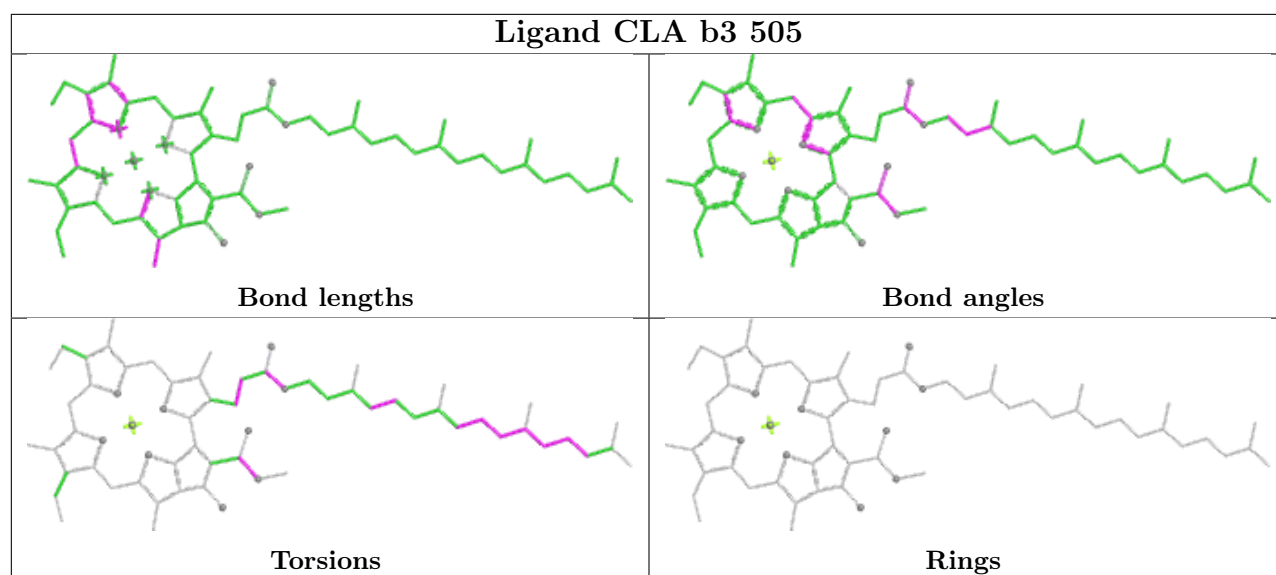
Bond angles

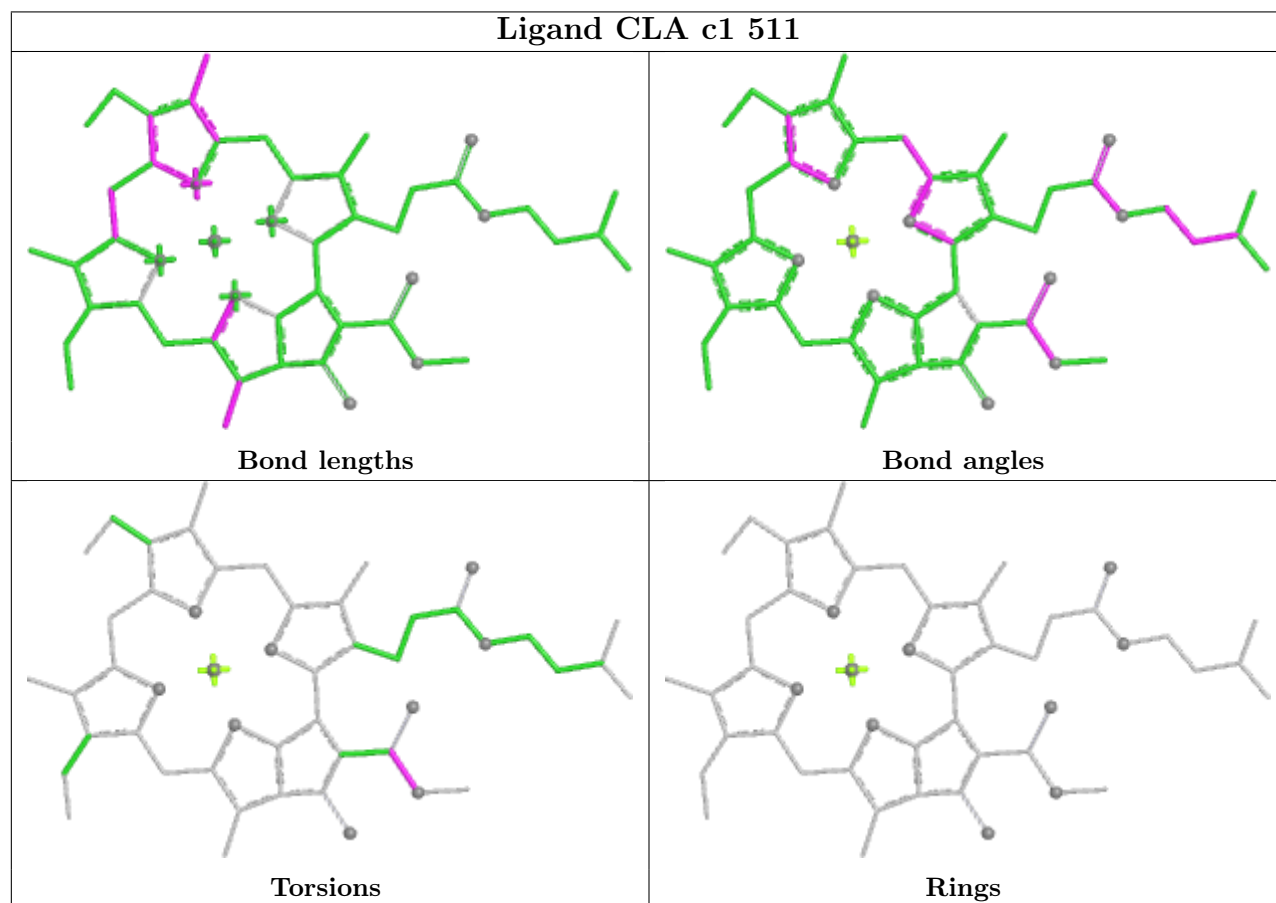
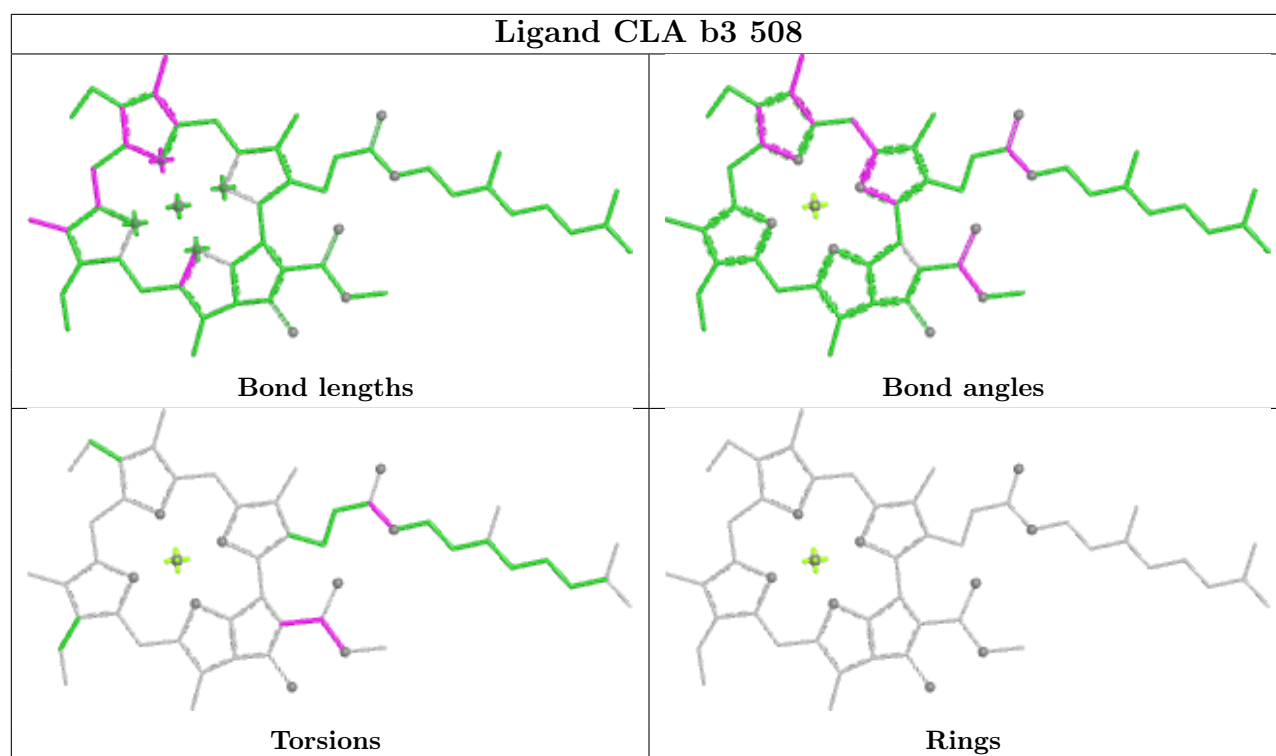


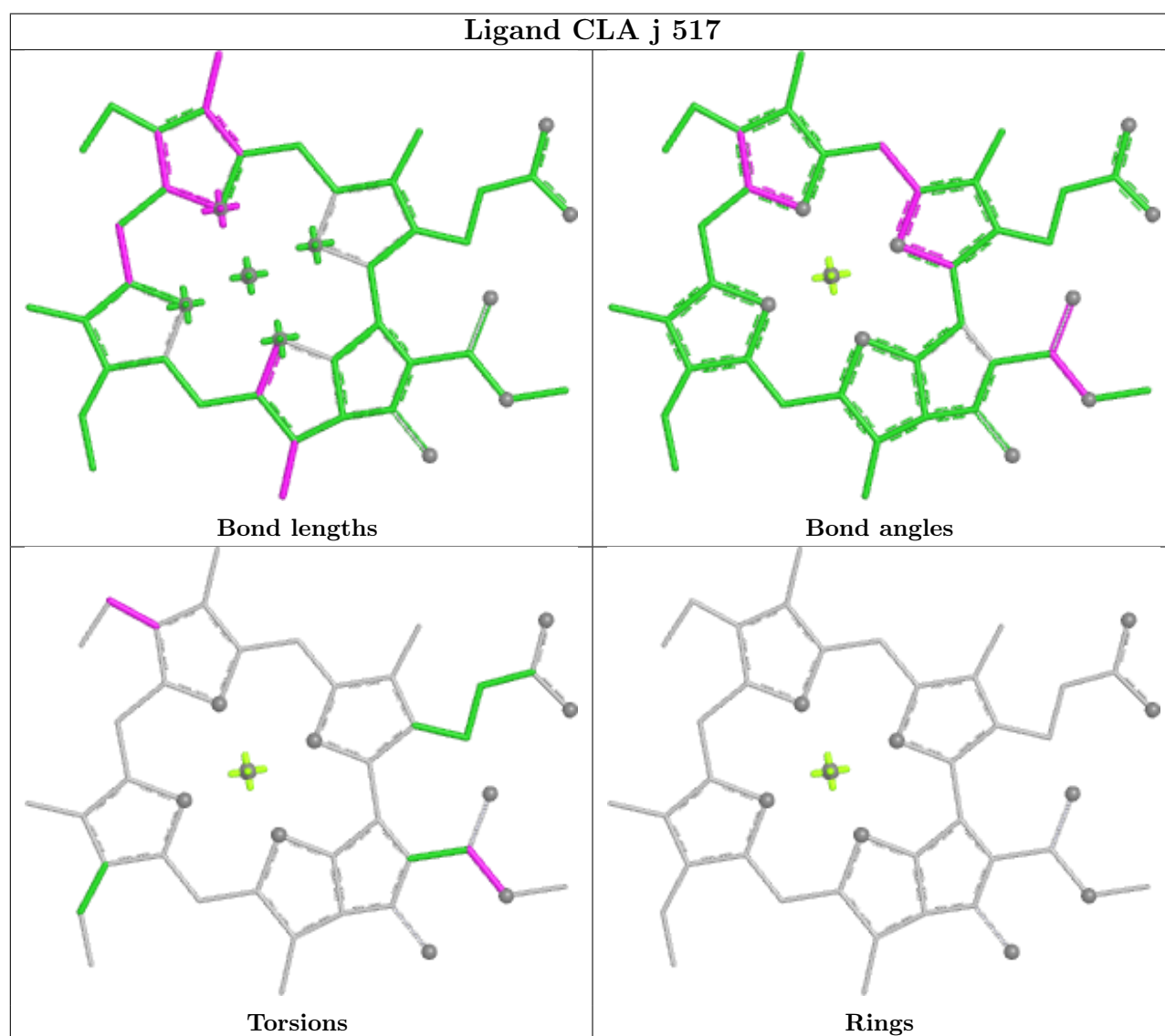
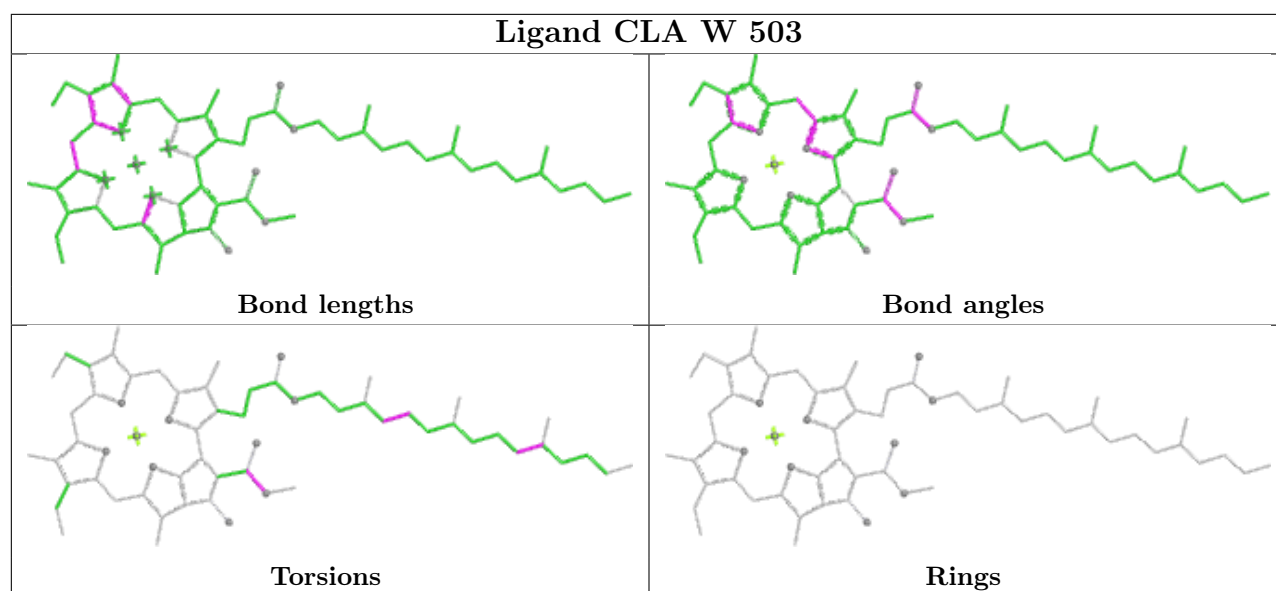
Torsions

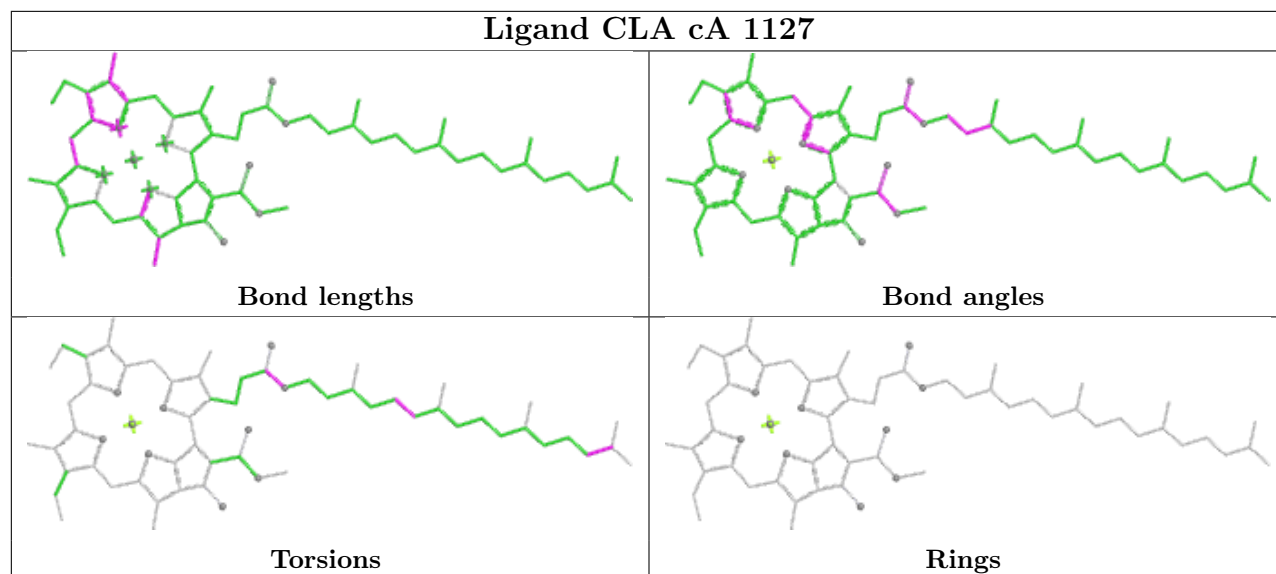
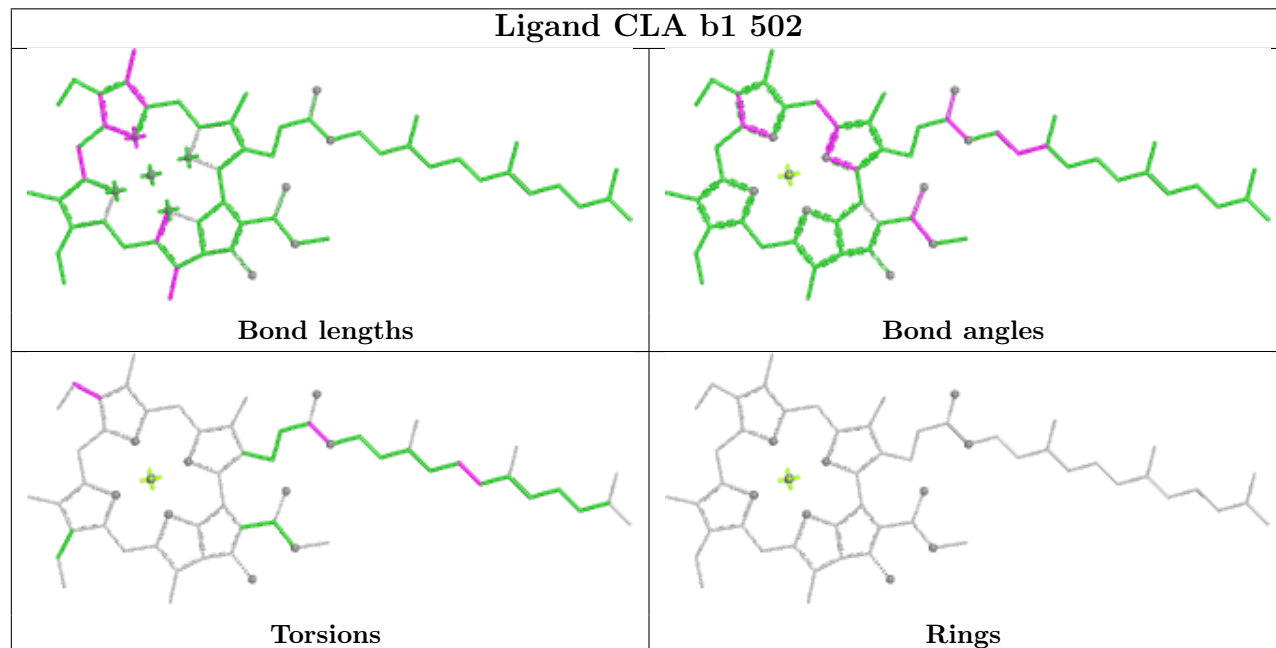


Rings

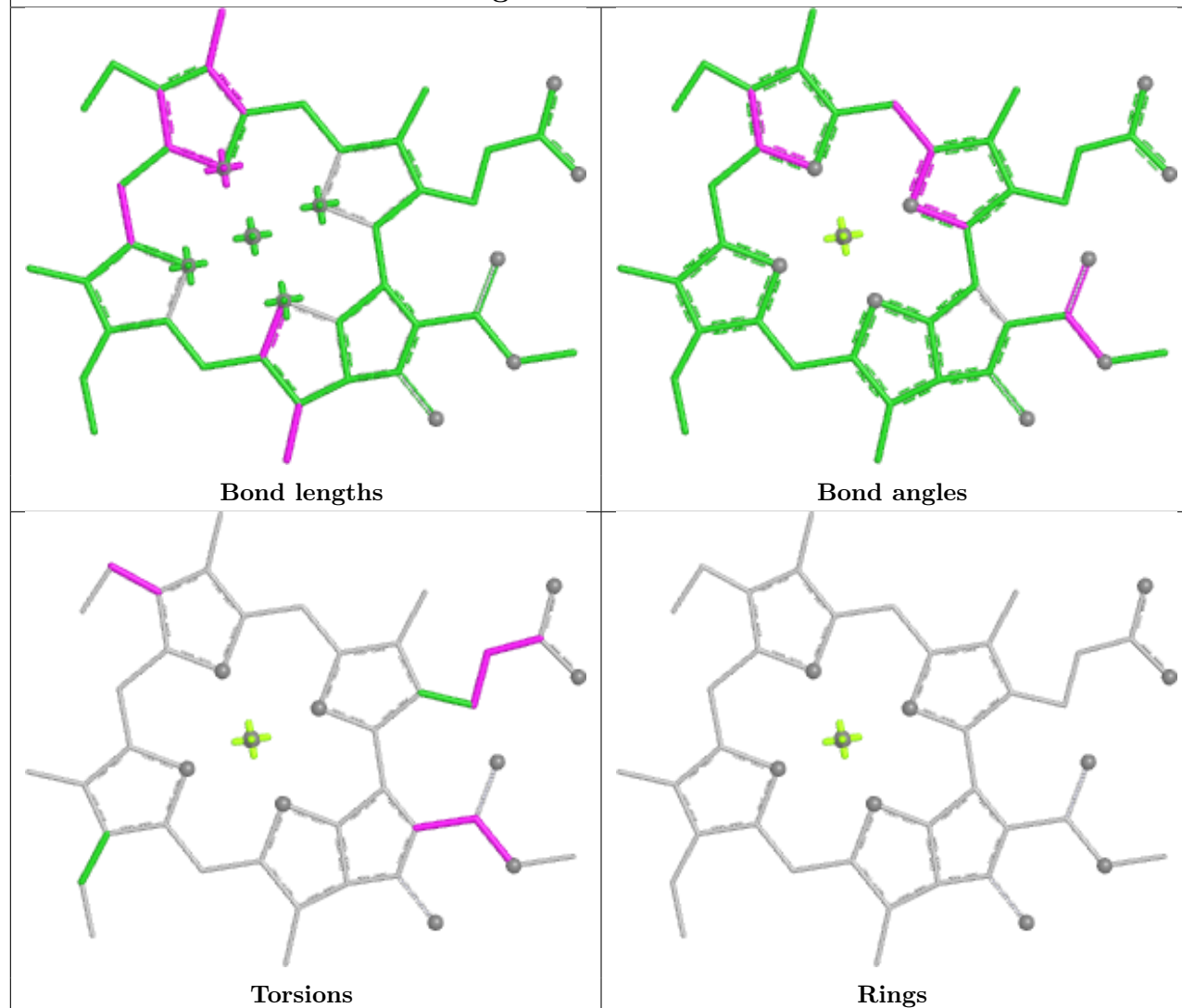




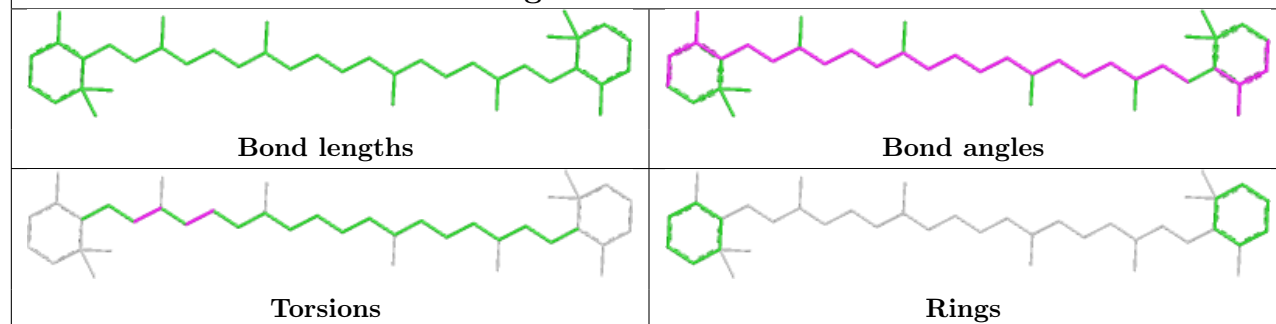


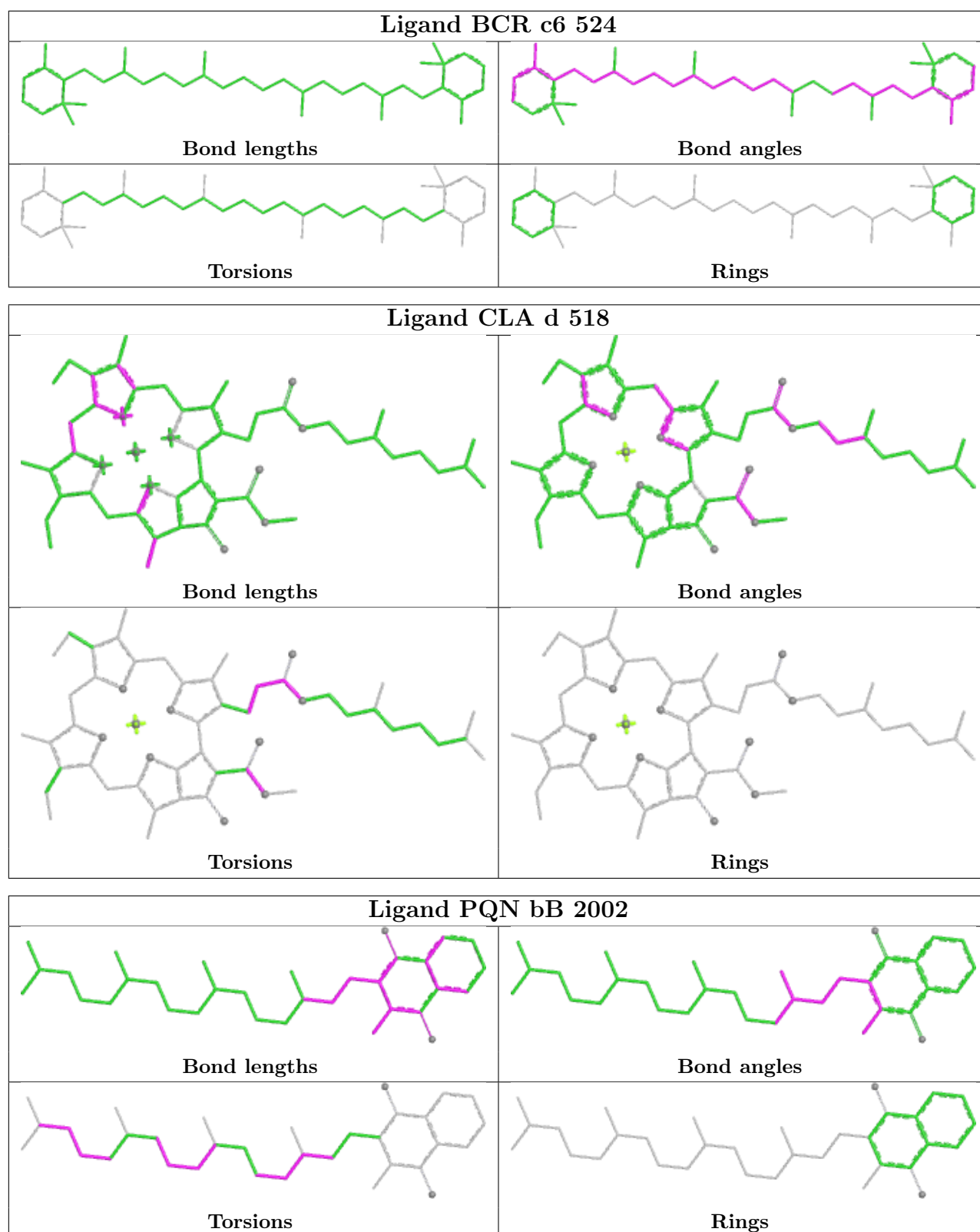
Ligand CLA cA 1127**Ligand CLA b1 502**

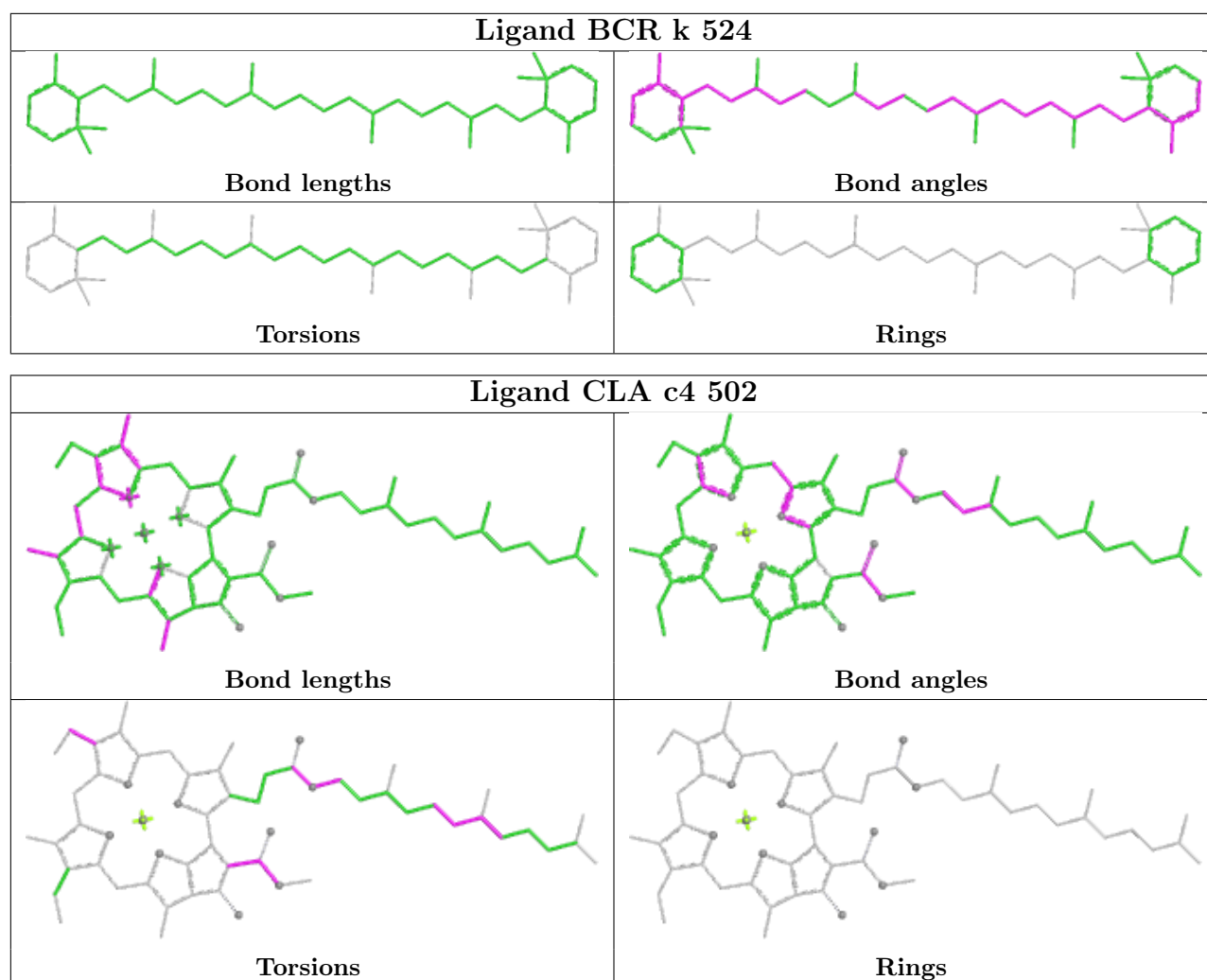
Ligand CLA Y 519



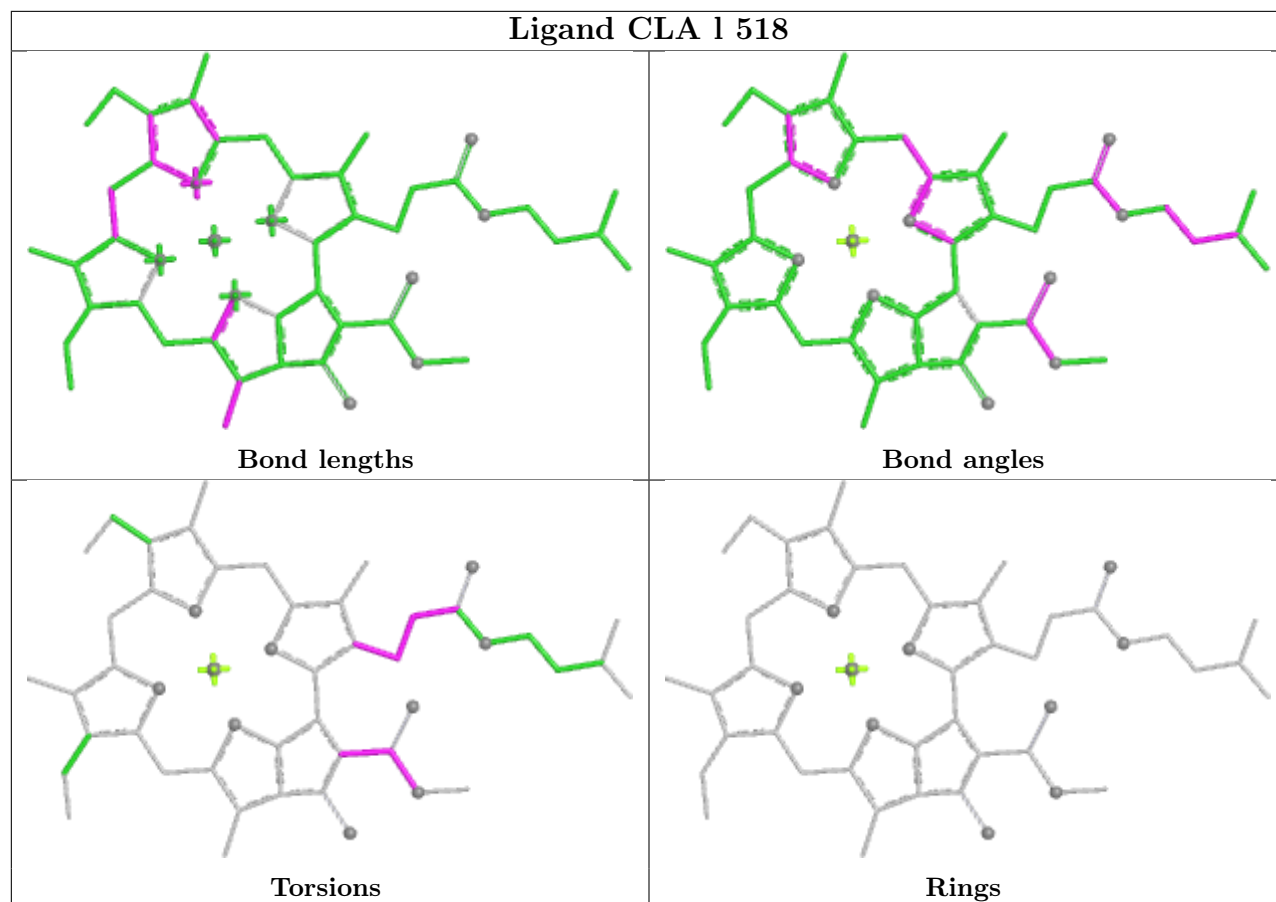
Ligand BCR b5 521



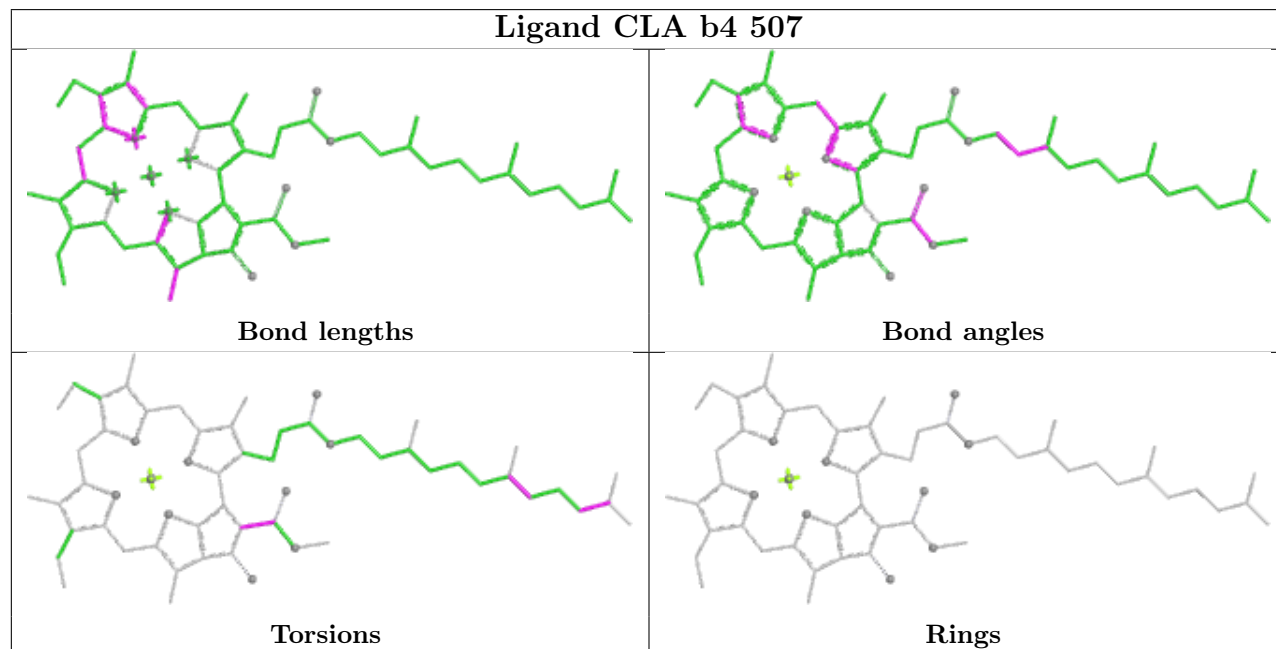


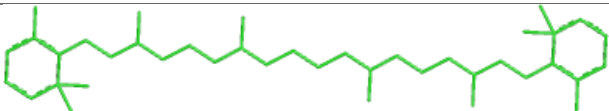
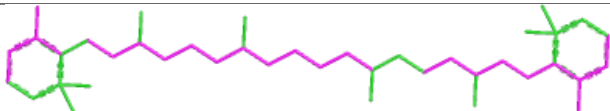
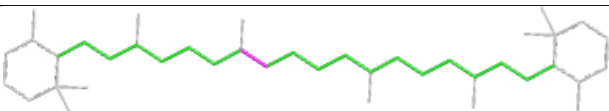
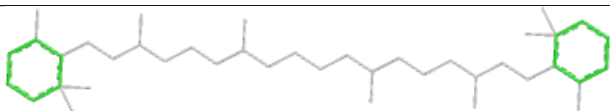




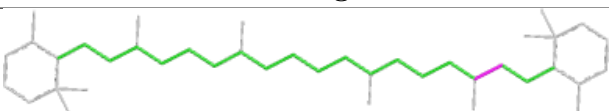
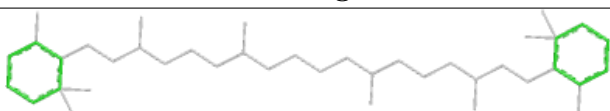
Ligand CLA l 518



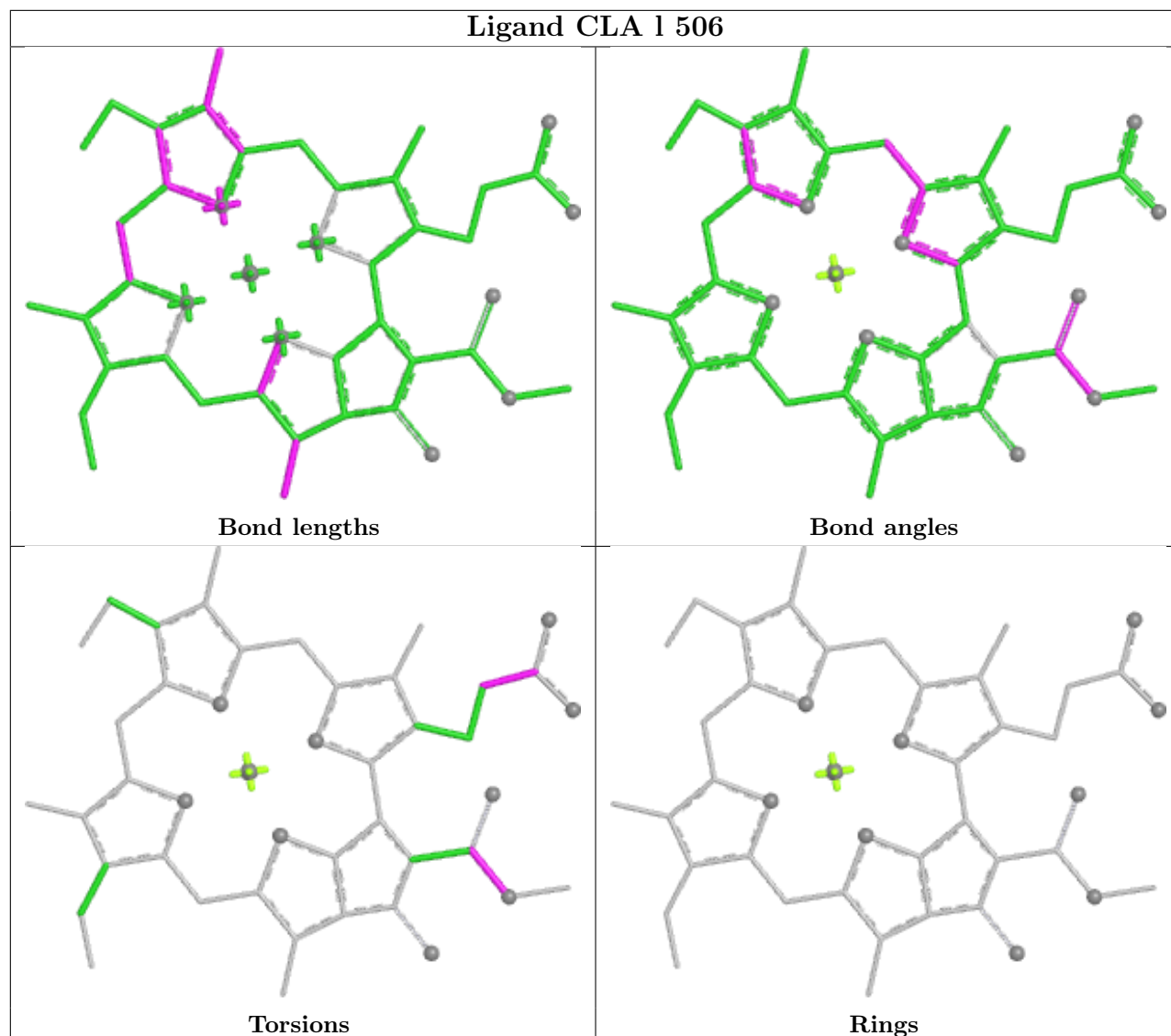
Ligand CLA b4 507



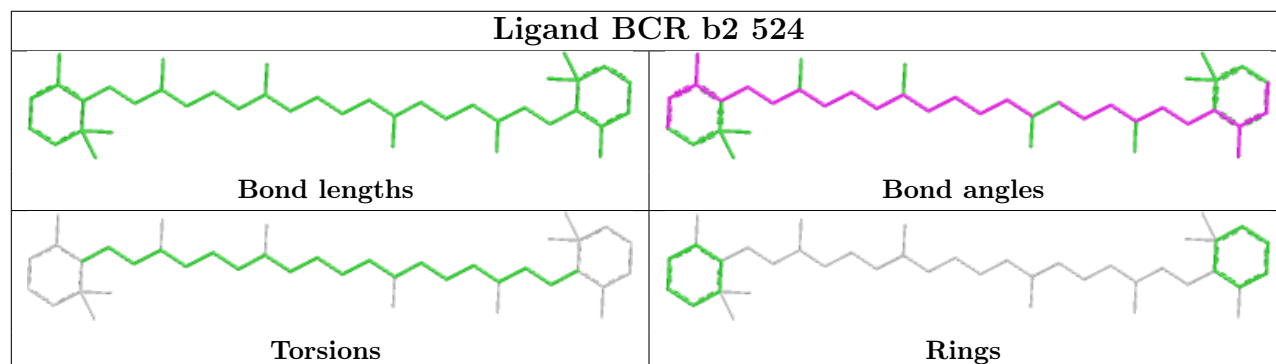
Ligand BCR aF 4016	
	
Bond lengths	Bond angles
	
Torsions	Rings

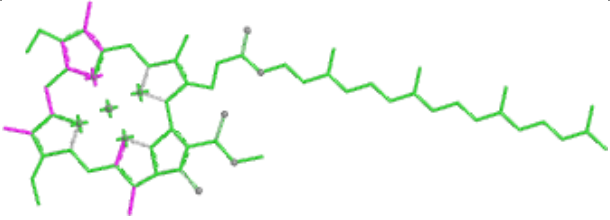
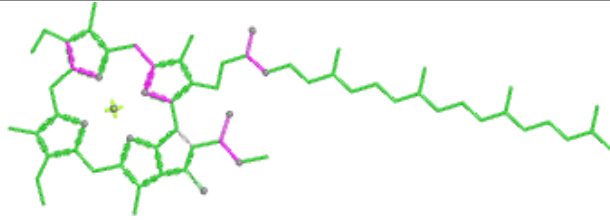
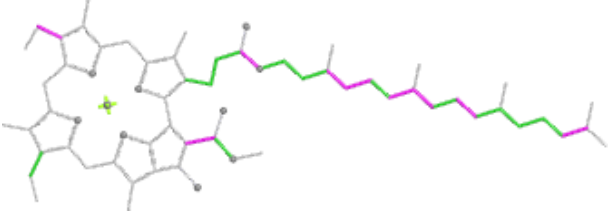
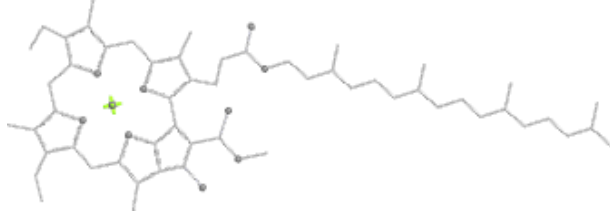
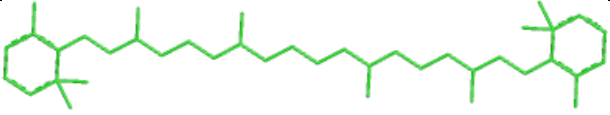
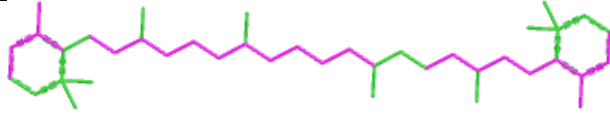
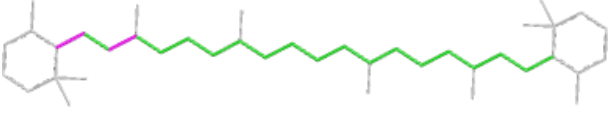
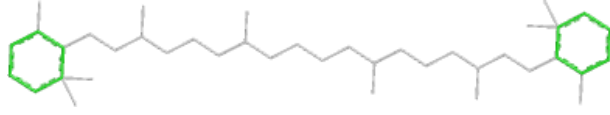
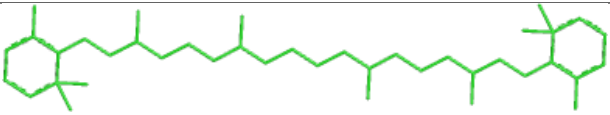
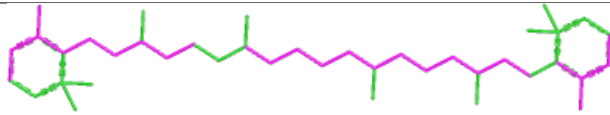
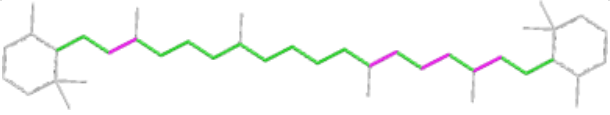
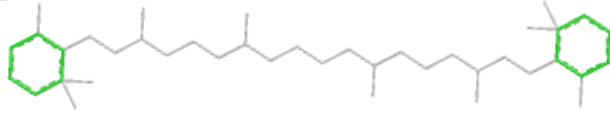
Ligand BCR cA 4007	
	
Bond lengths	Bond angles
	
Torsions	Rings

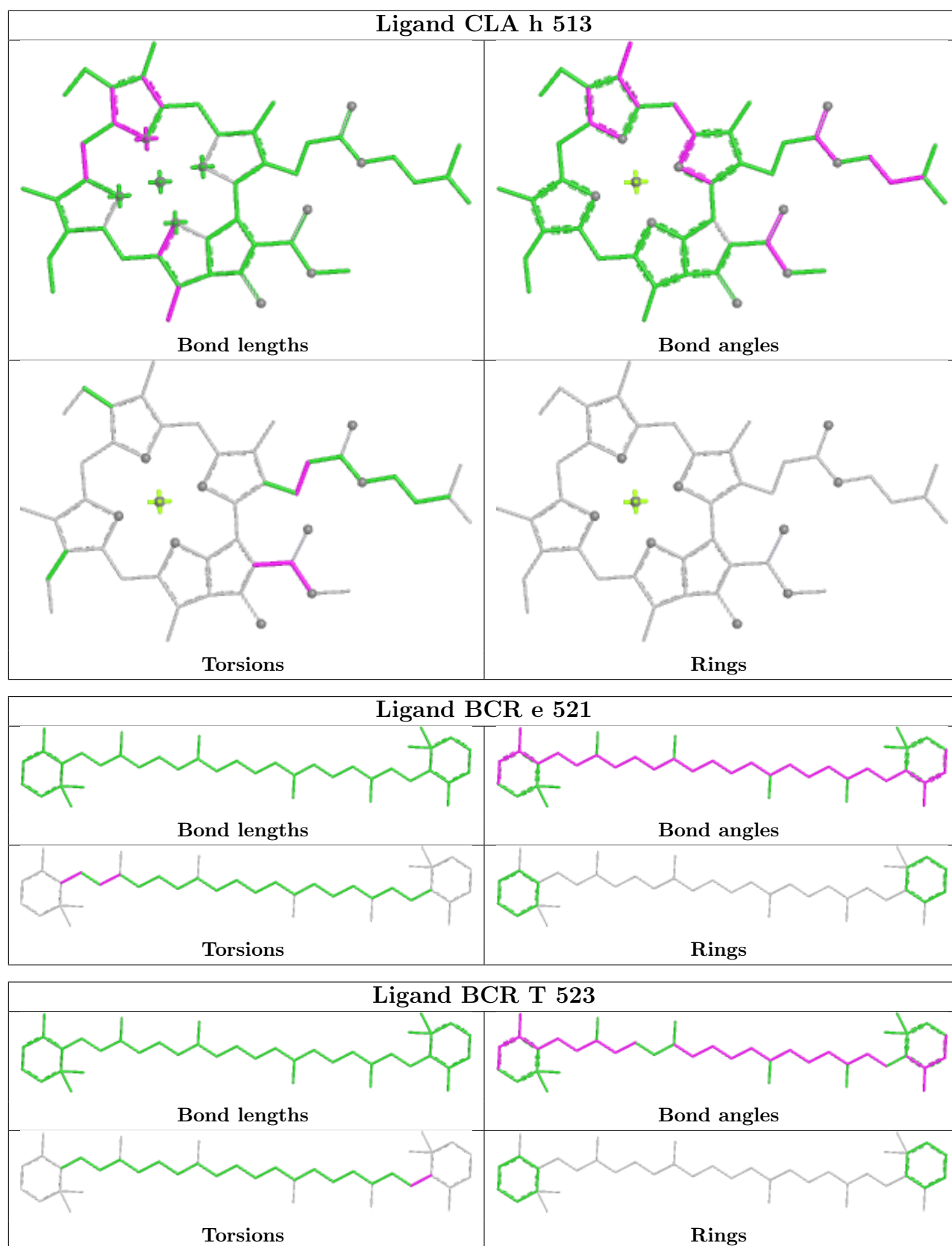
Ligand CLA 1 506

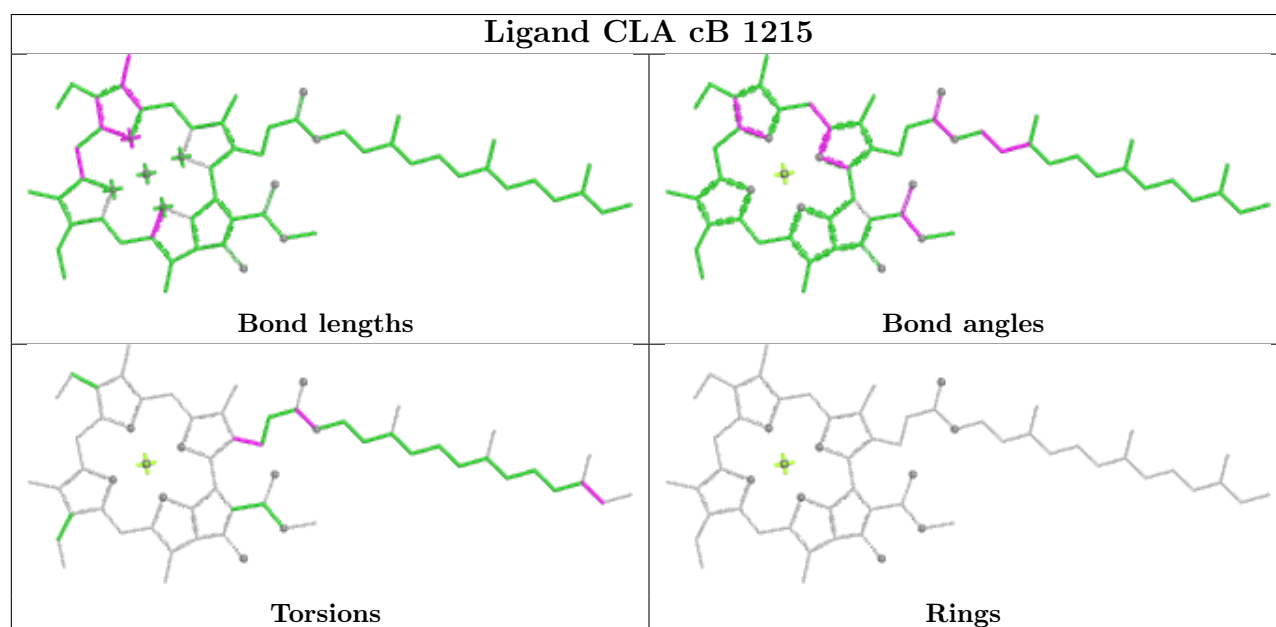
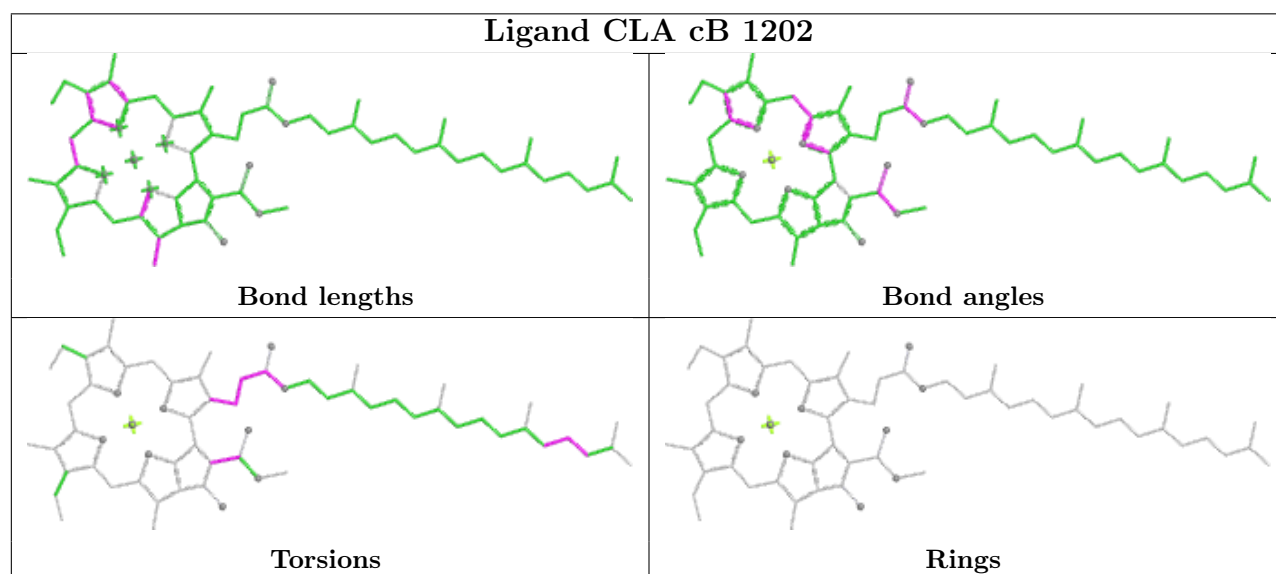
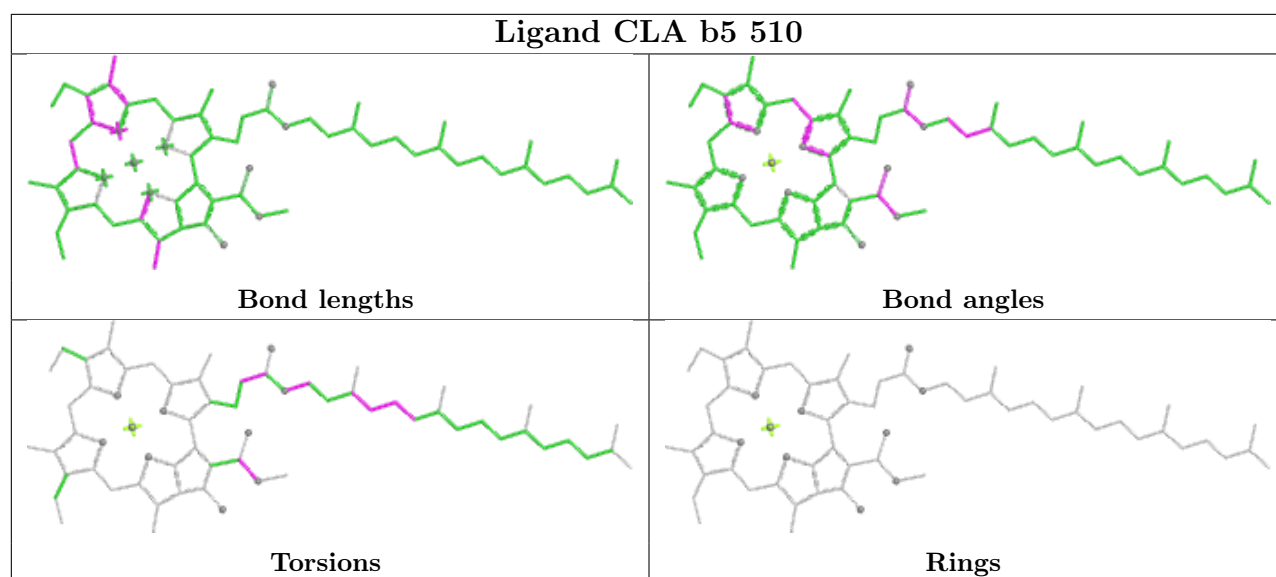


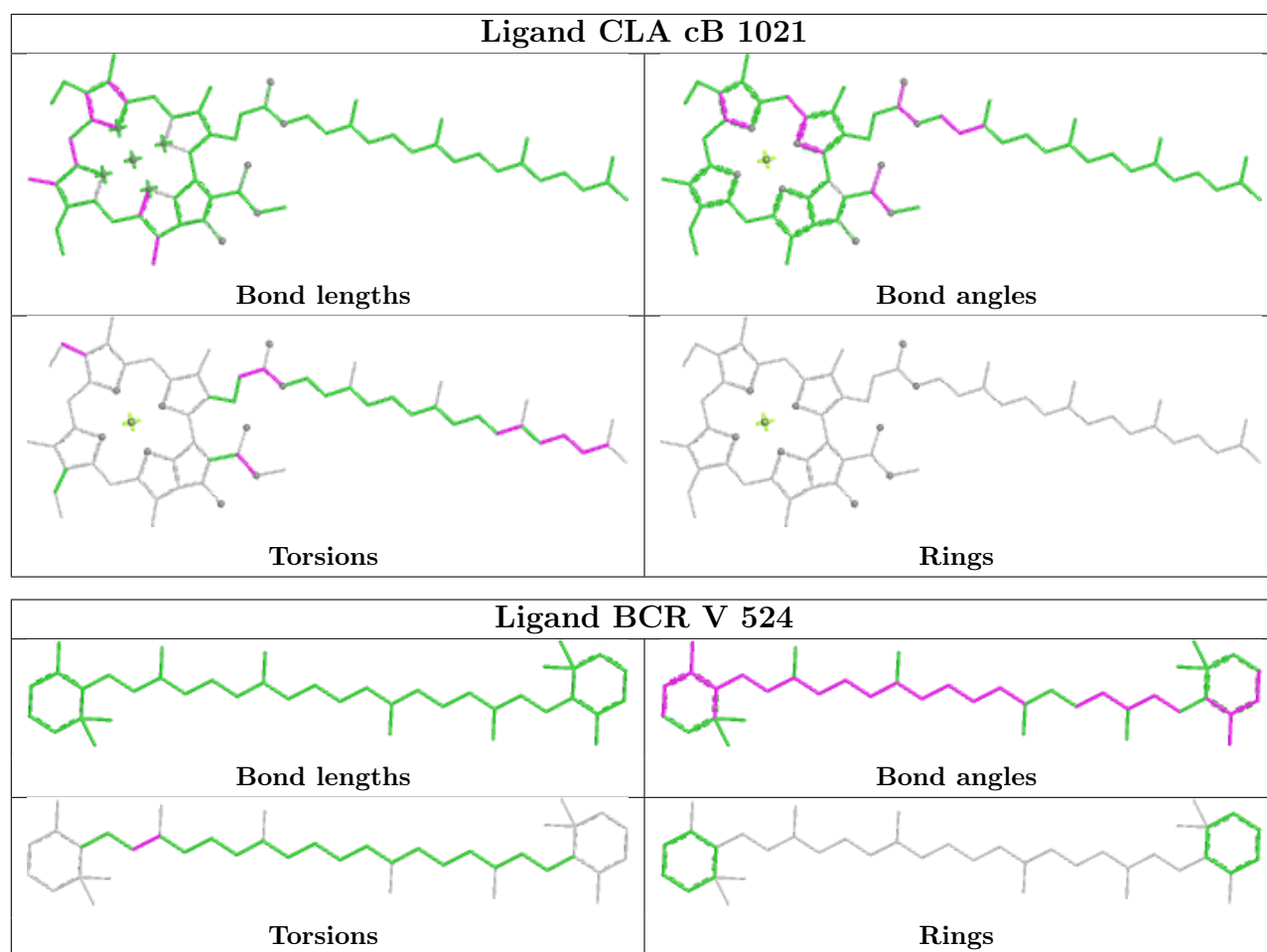
Ligand BCR b2 524



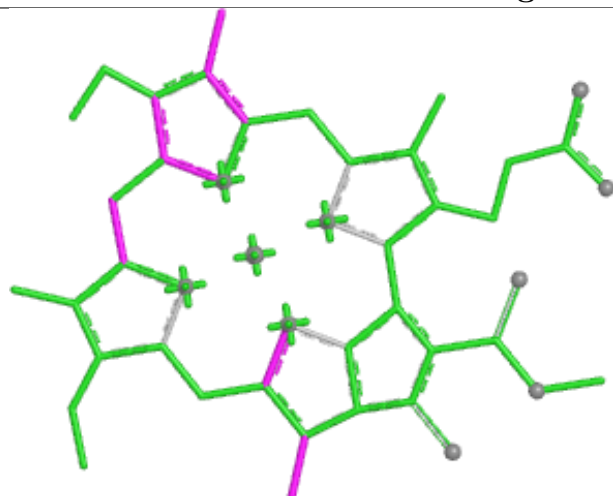
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 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR c 522	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR cM 4021	
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 <p>Torsions</p>	 <p>Rings</p>



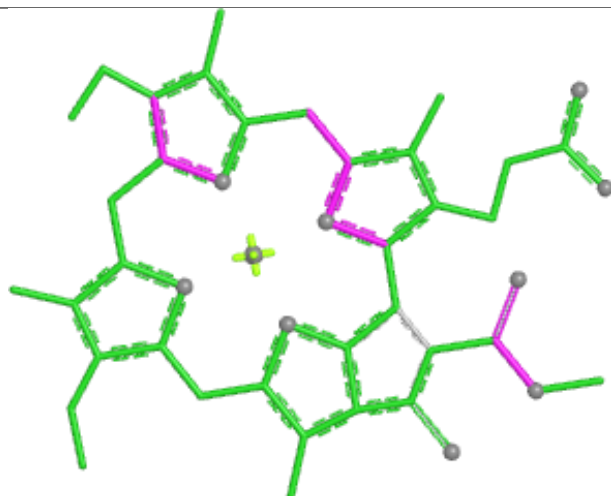




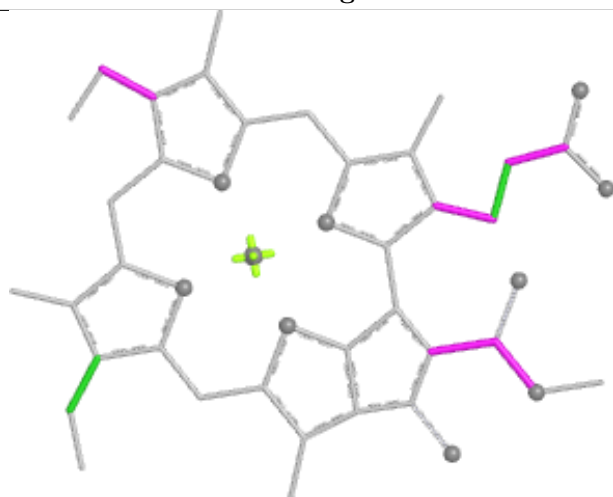
Ligand CLA d 517



Bond lengths



Bond angles

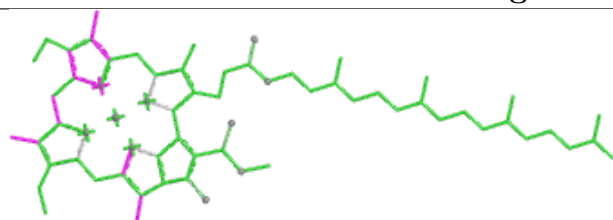


Torsions

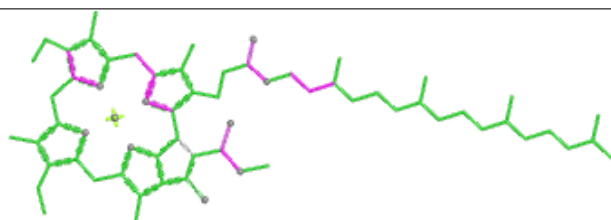


Rings

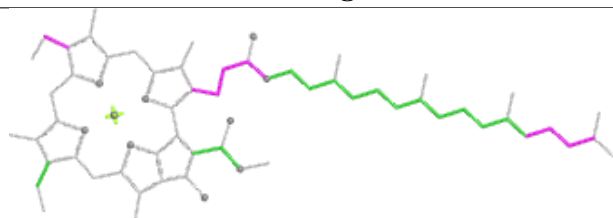
Ligand CLA a3 501



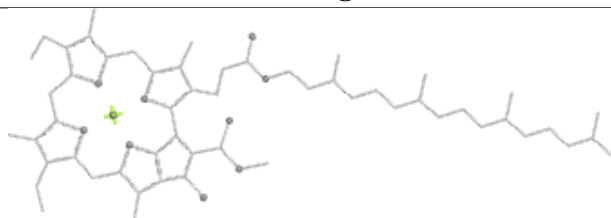
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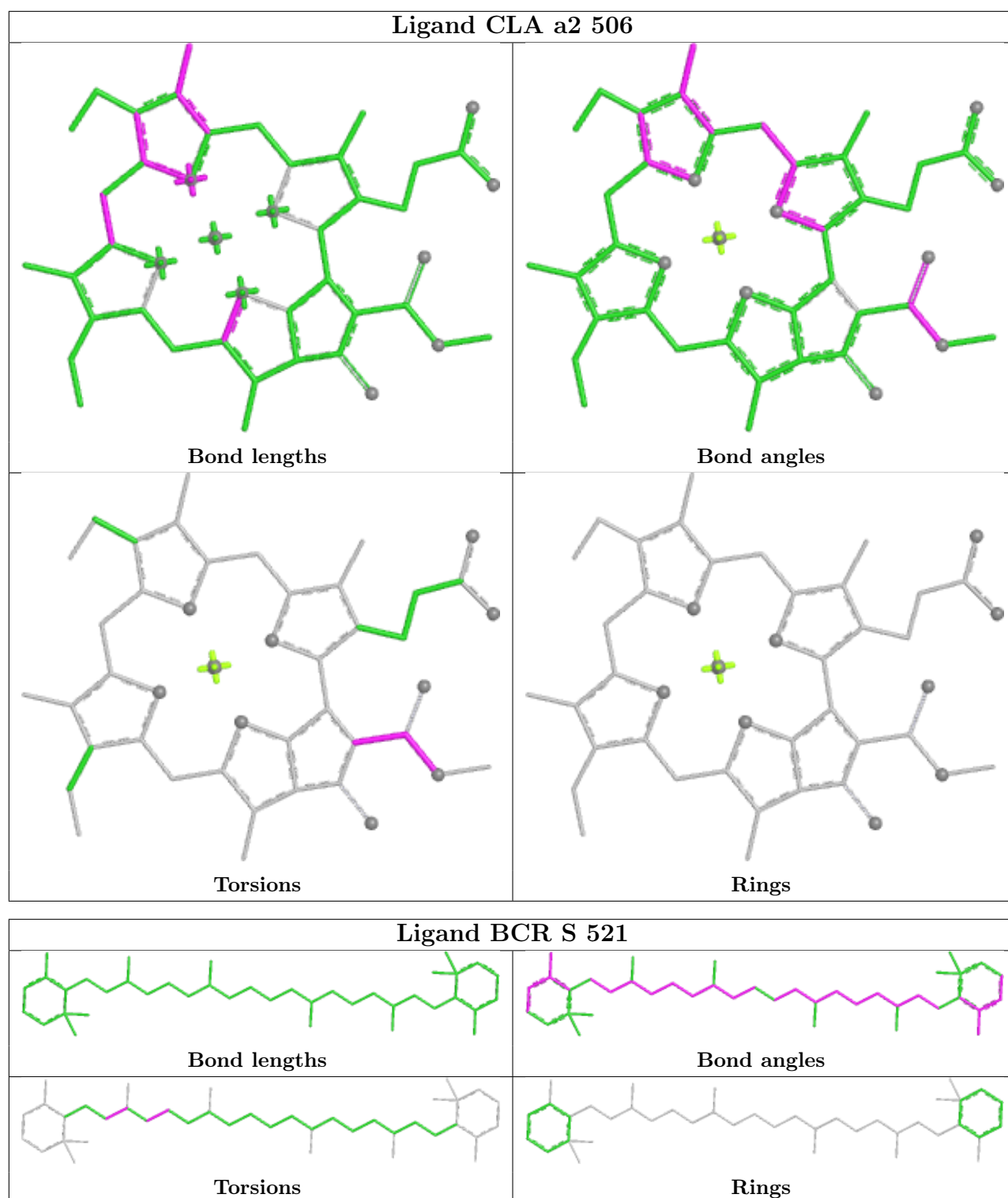
Bond angles



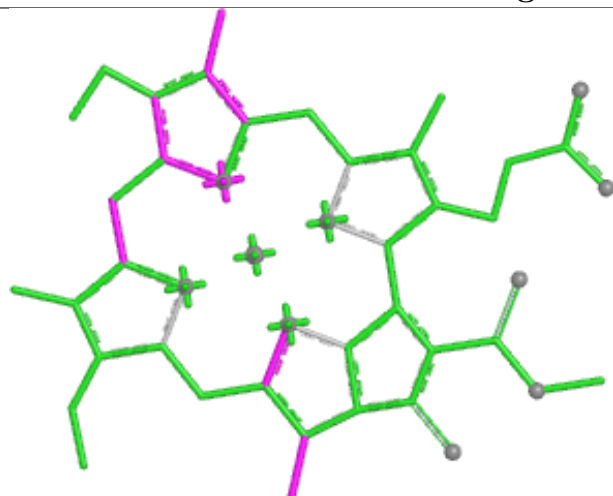
Torsions



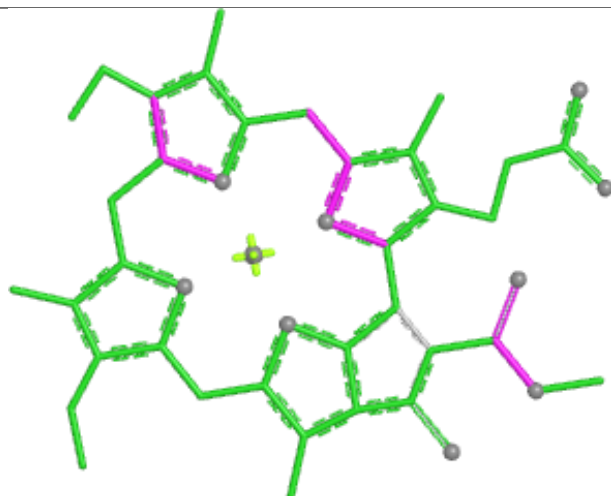
Rings



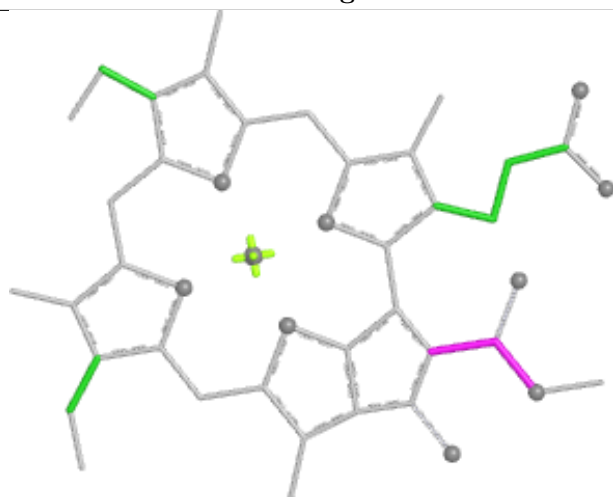
Ligand CLA h 506



Bond lengths



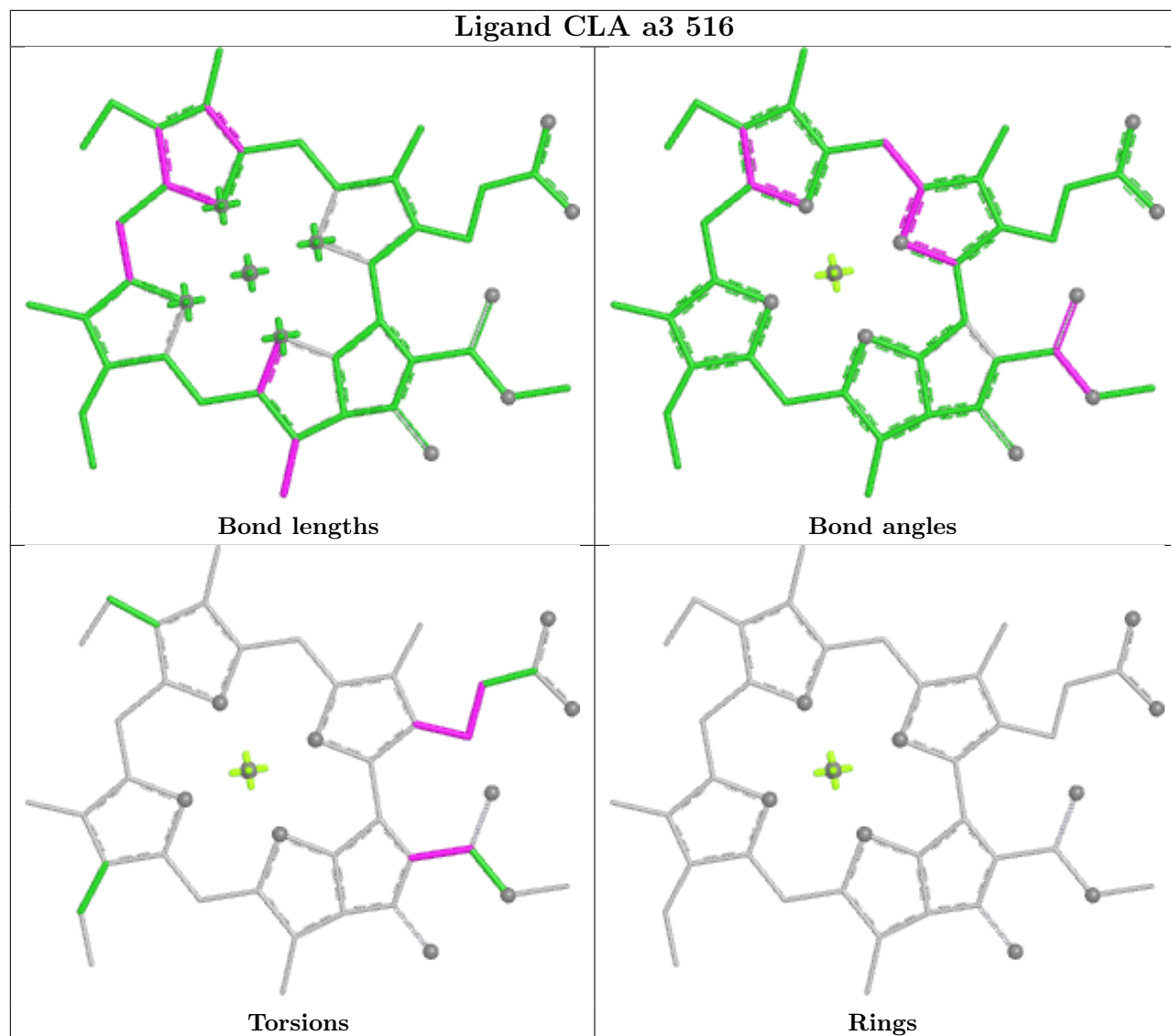
Bond angles



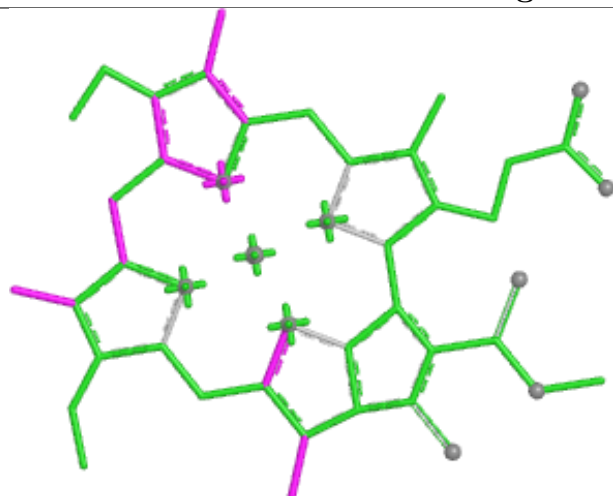
Torsions



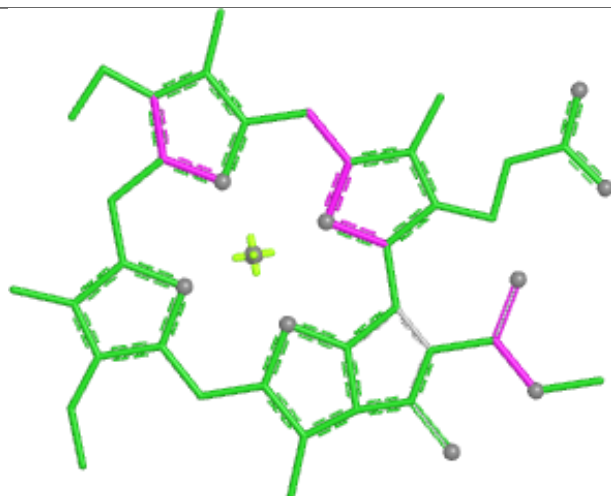
Rings



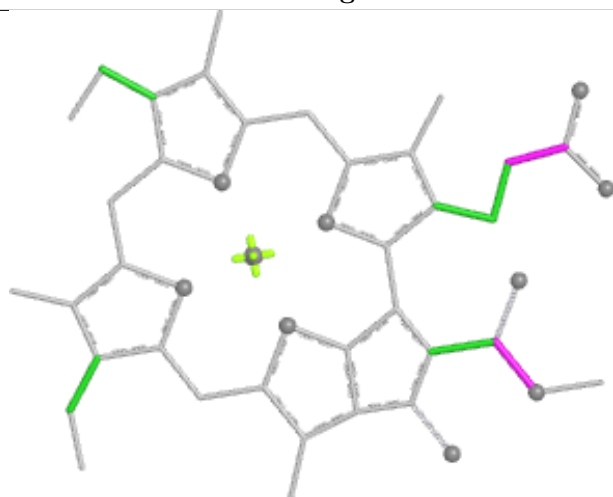
Ligand CLA Z 508



Bond lengths



Bond angles

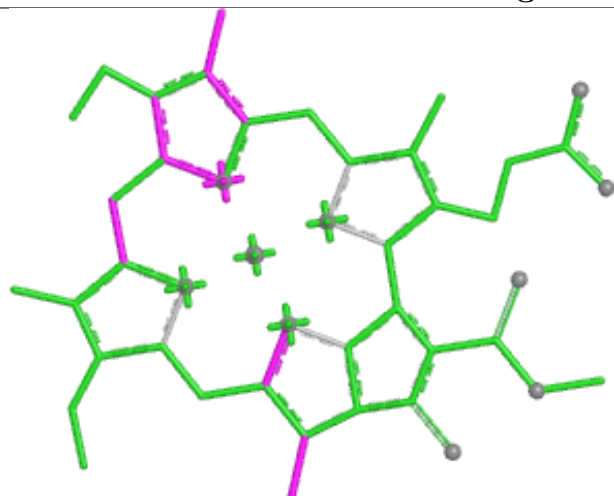


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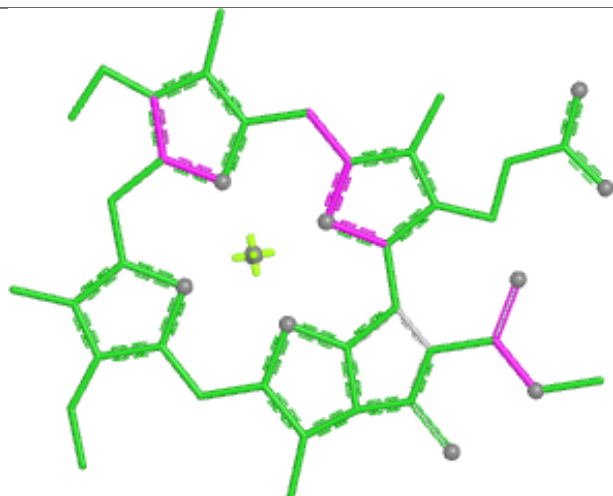


Rings

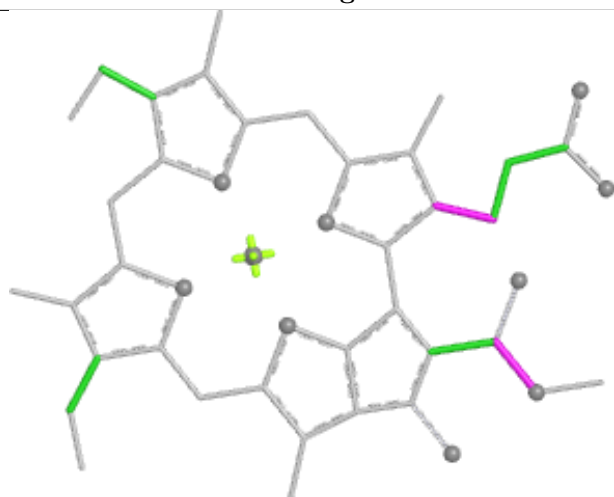
Ligand CLA b 511



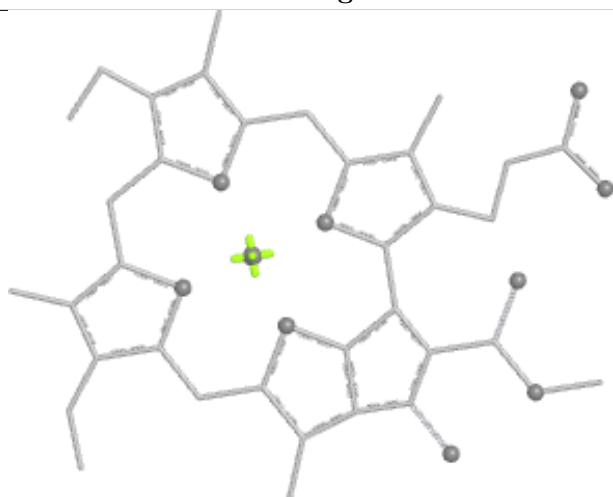
Bond lengths



Bond angles

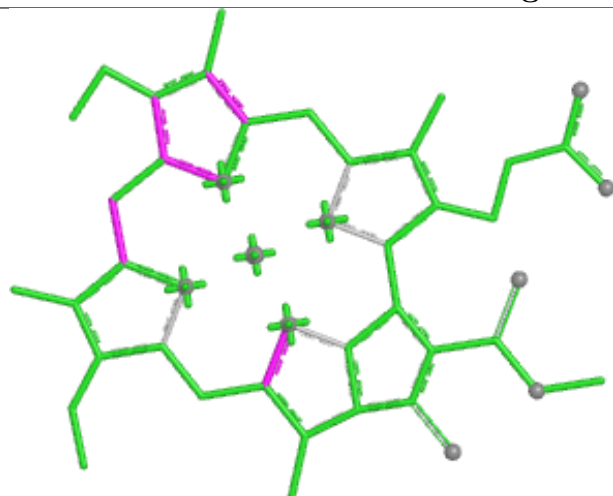


Torsions



Rings

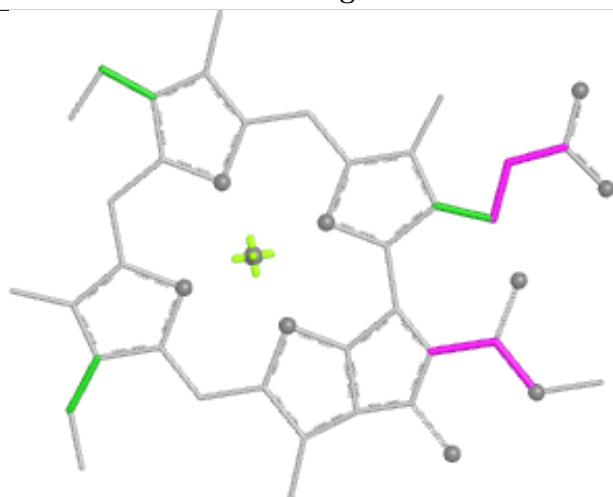
Ligand CLA f 511



Bond lengths



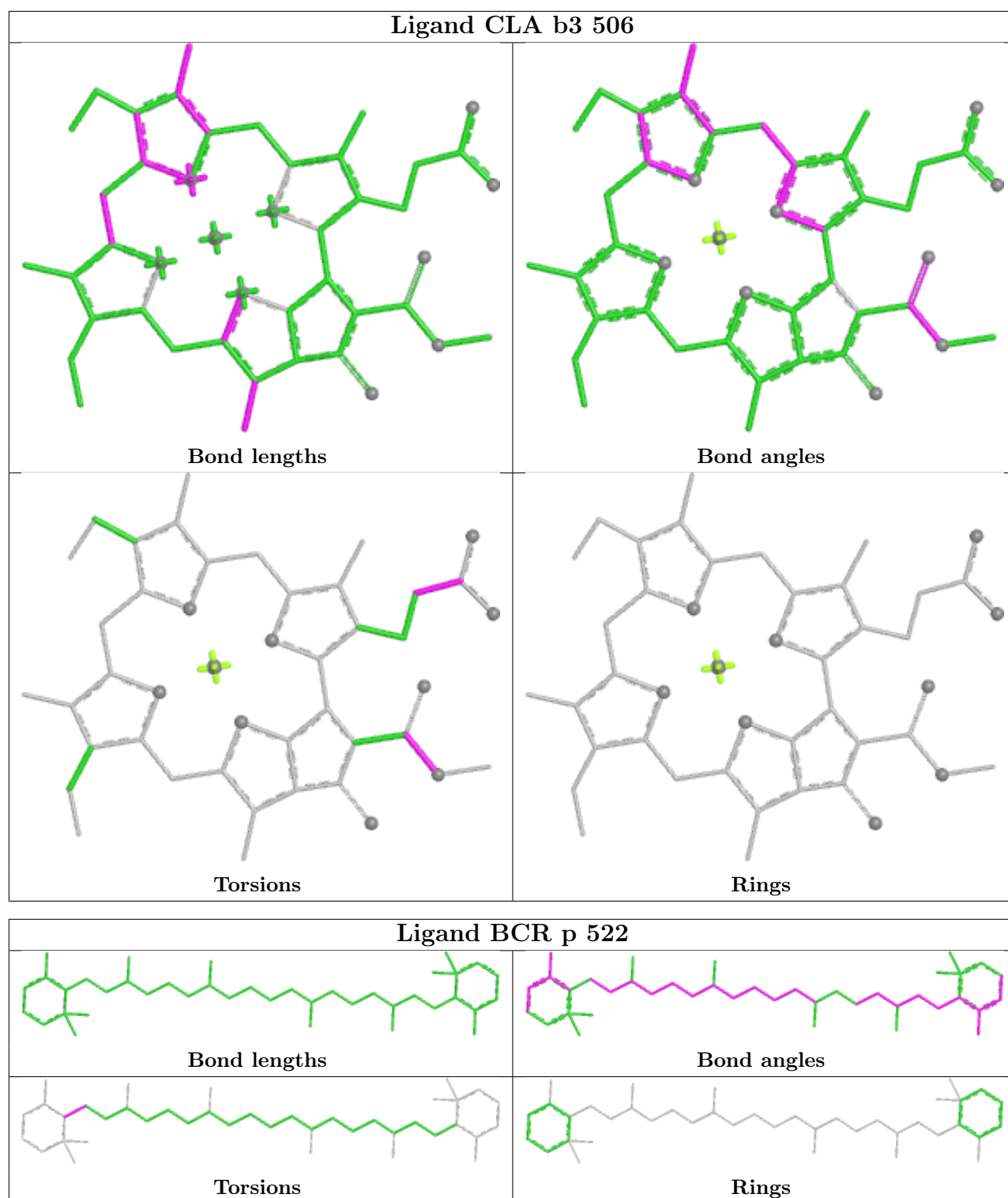
Bond angles



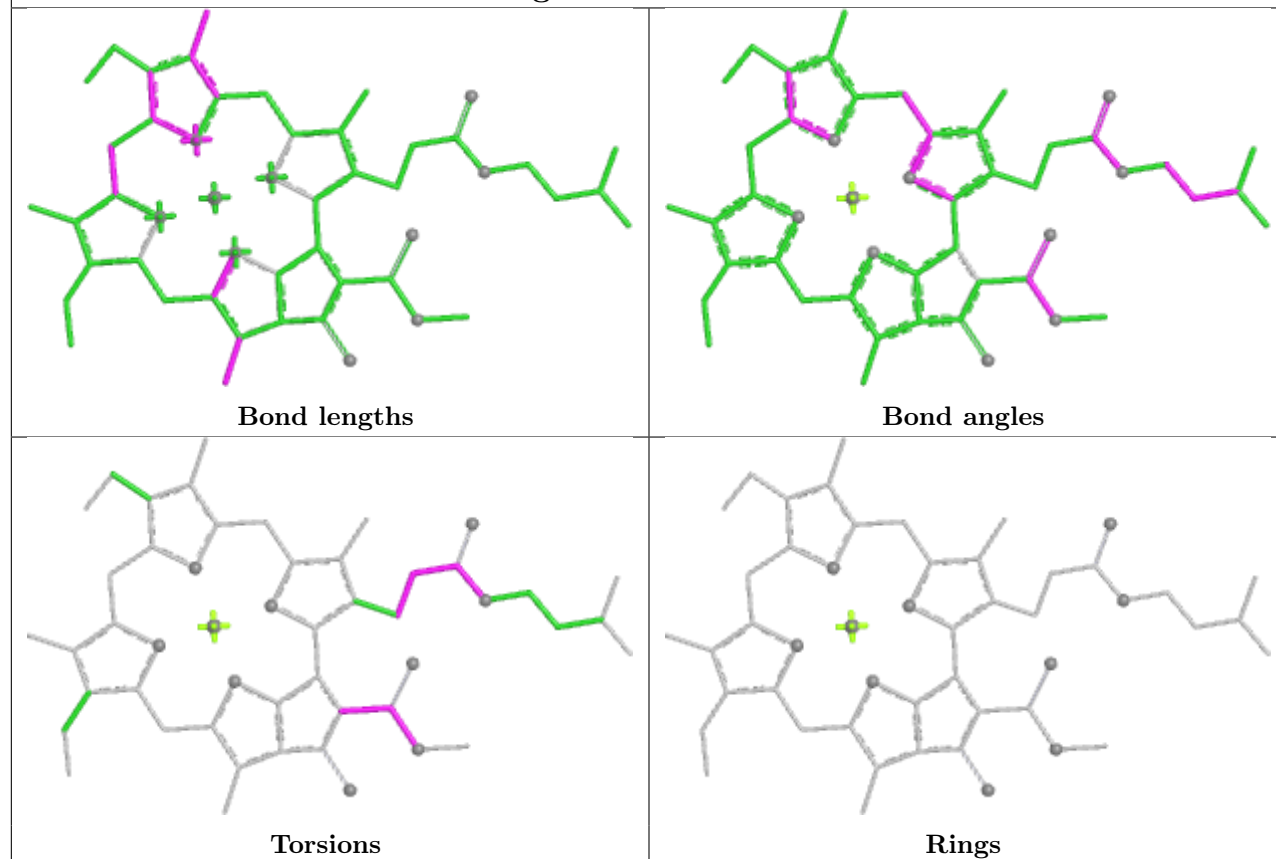
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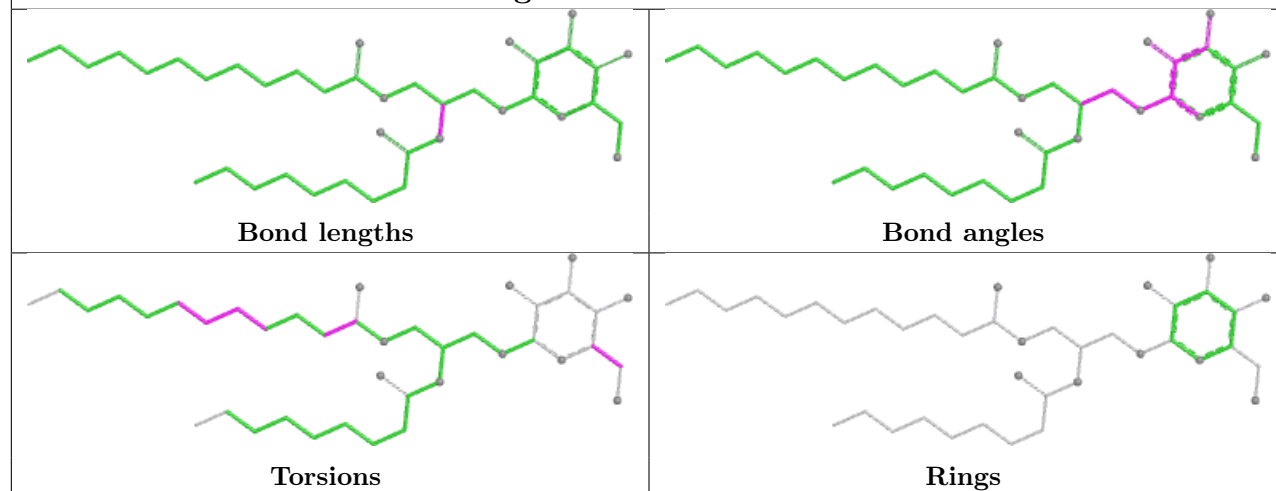
Rings



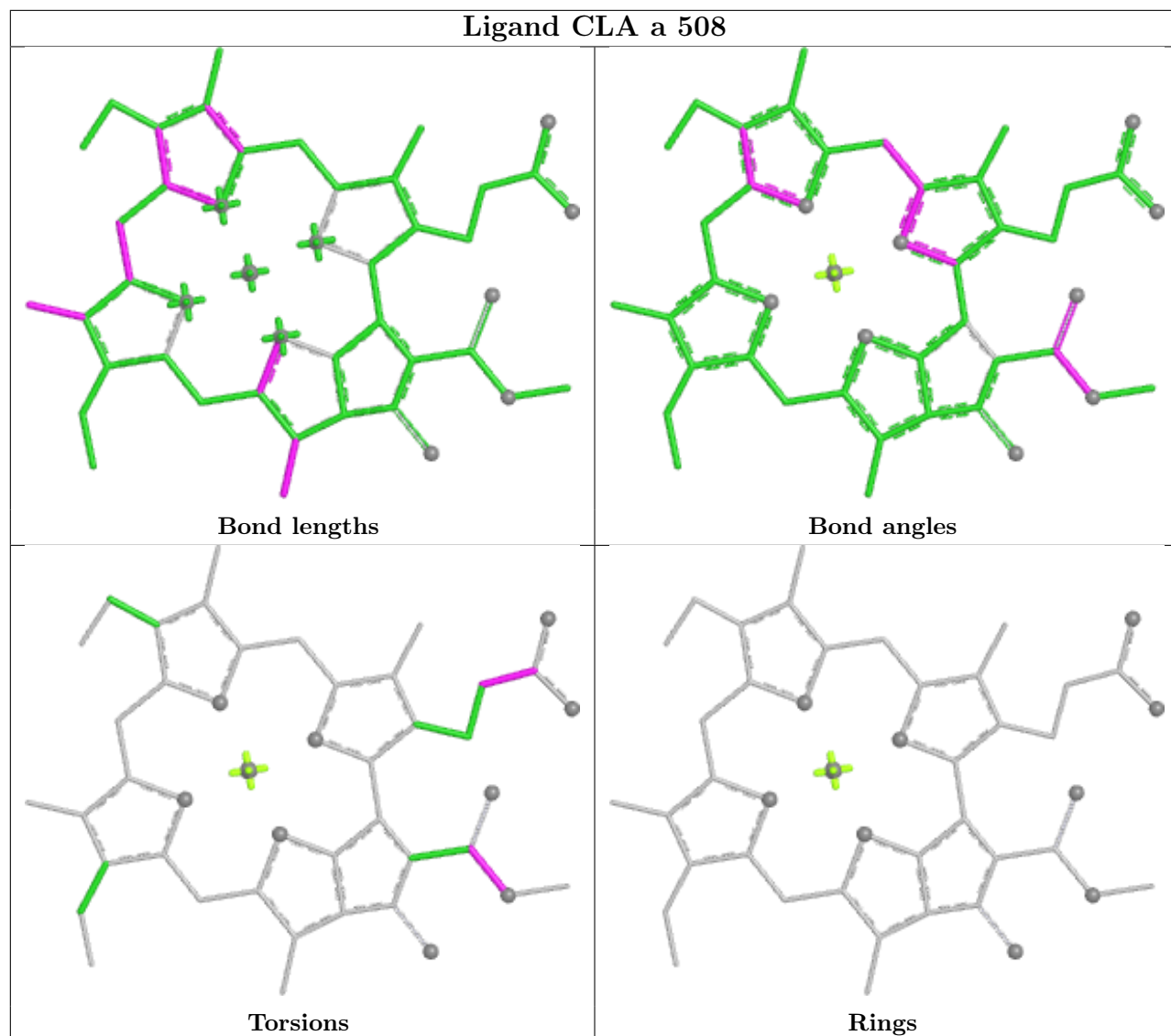
Ligand CLA T 518



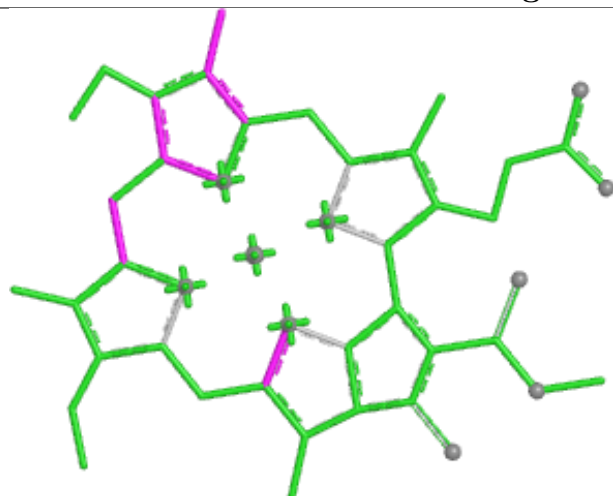
Ligand LMG a2 5104



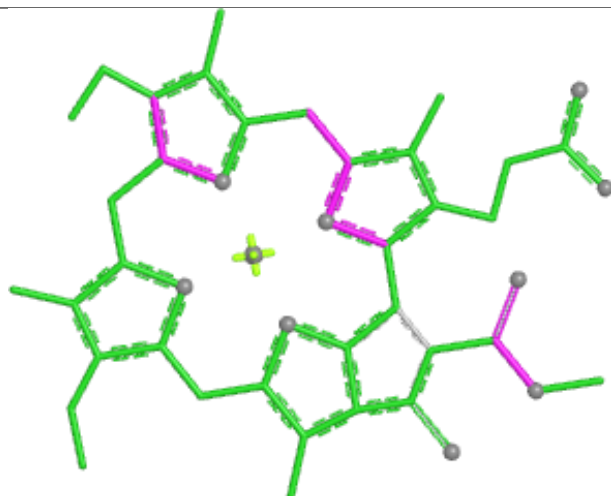
Ligand CLA a 508



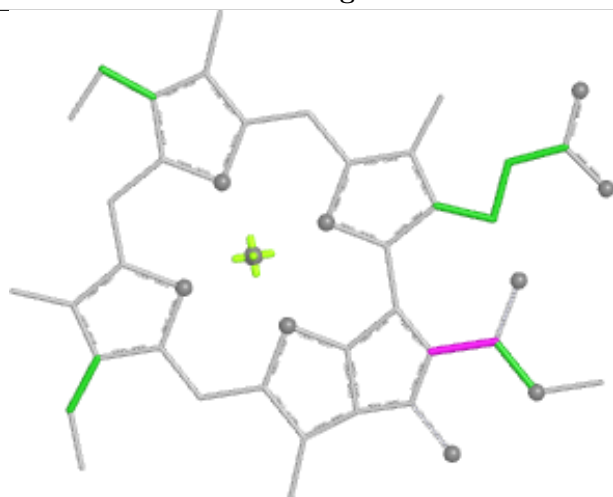
Ligand CLA i 502



Bond lengths



Bond angles

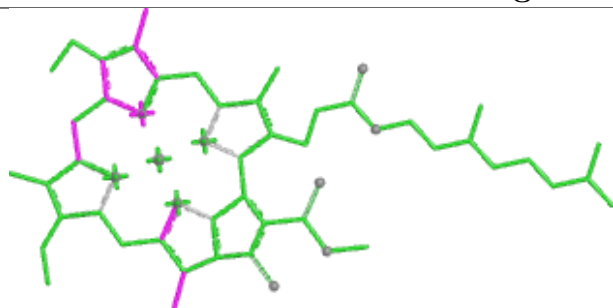


Torsions

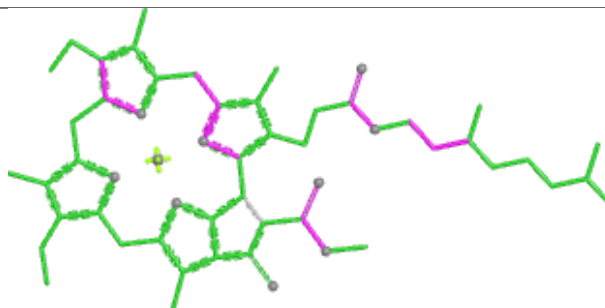


Rings

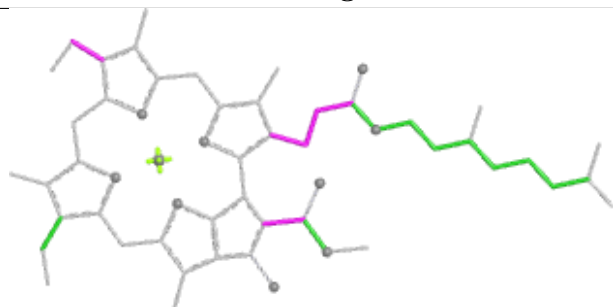
Ligand CLA X 518



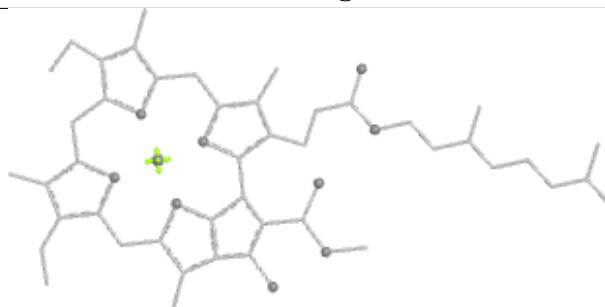
Bond lengths



Bond angles

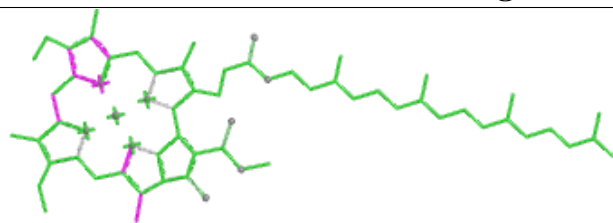


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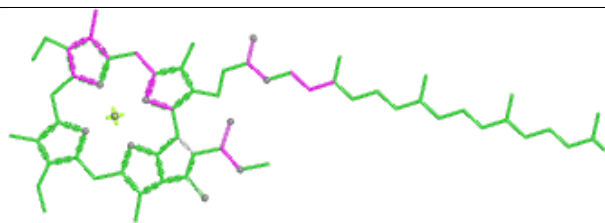


Rings

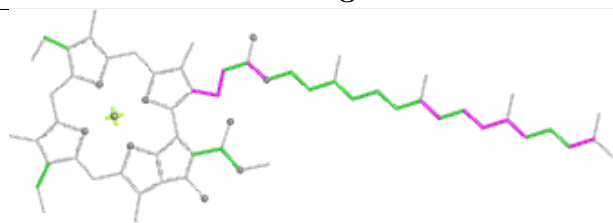
Ligand CLA aB 1225



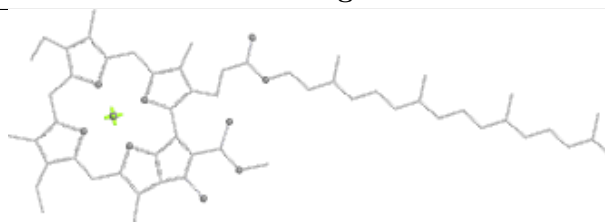
Bond lengths



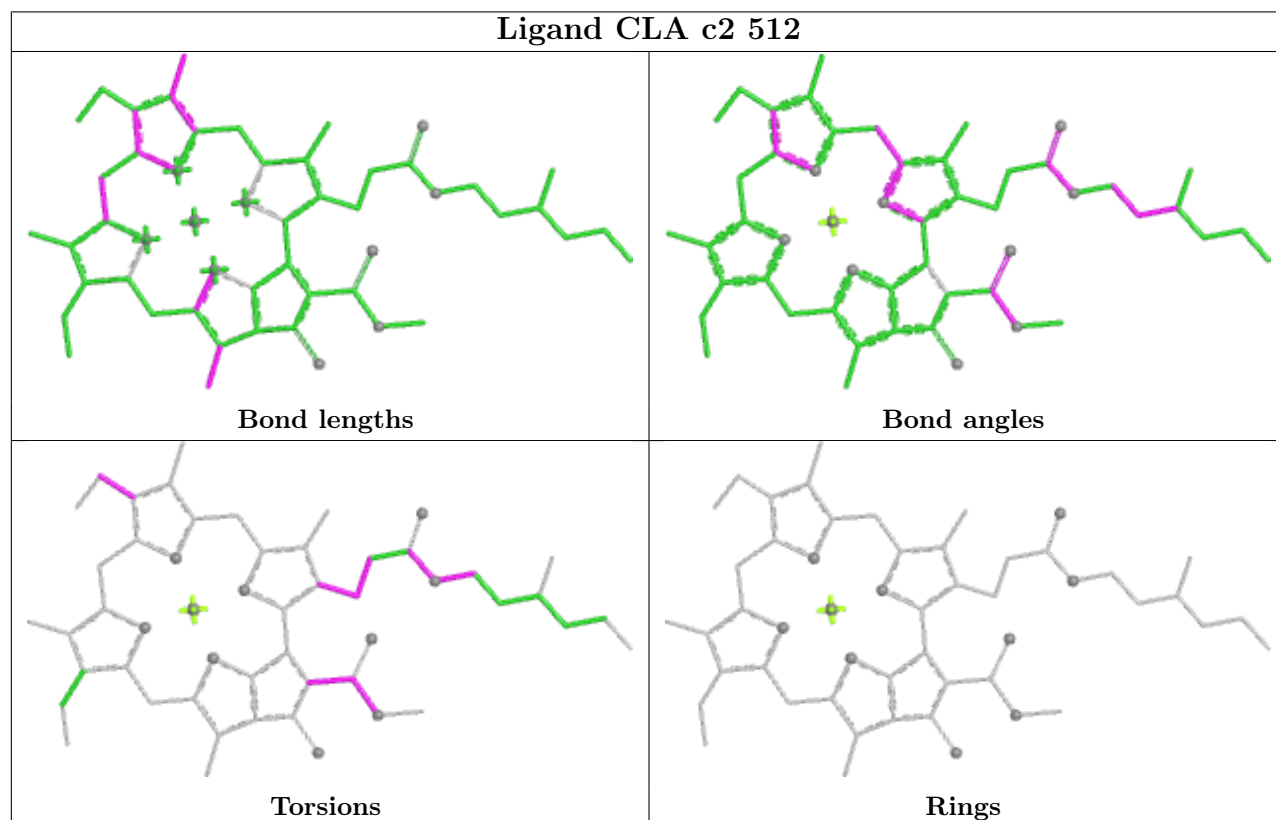
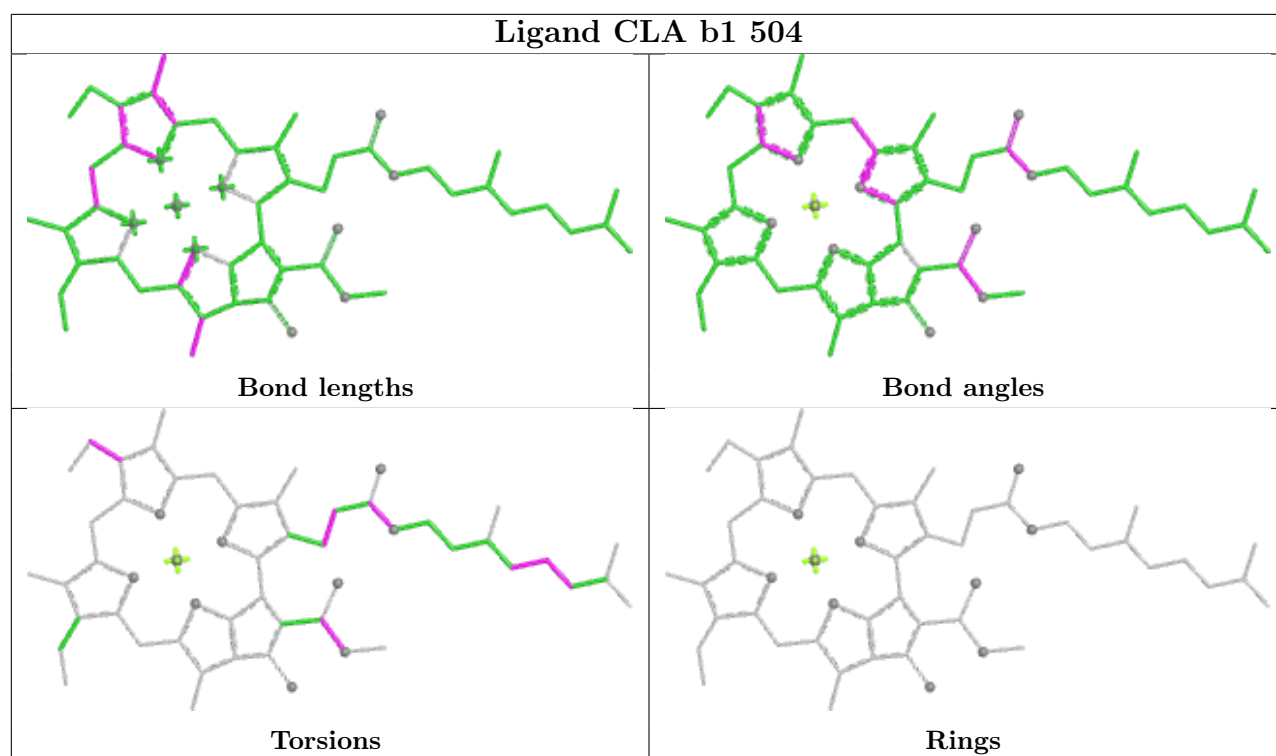
Bond angles

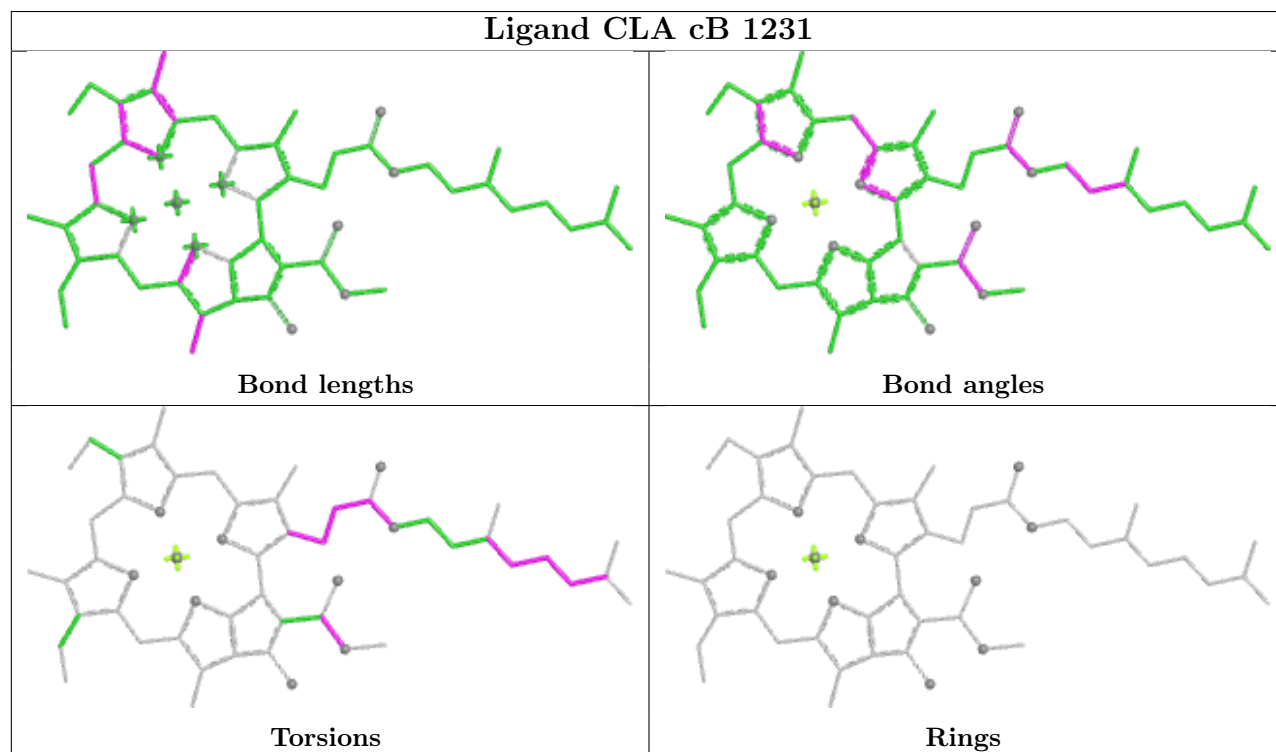
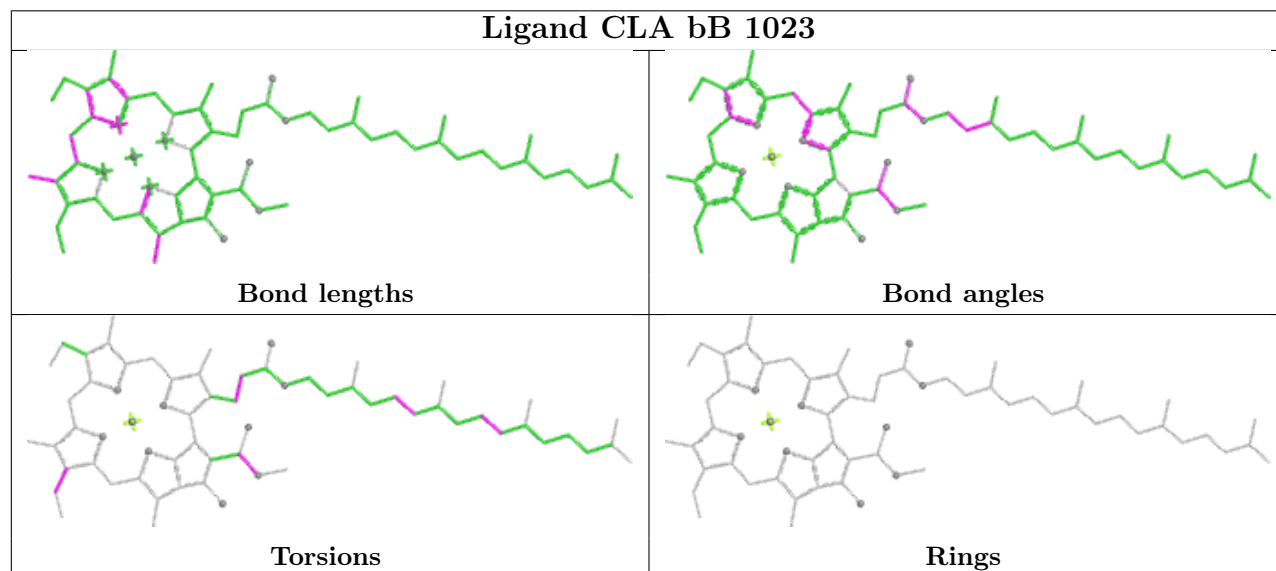
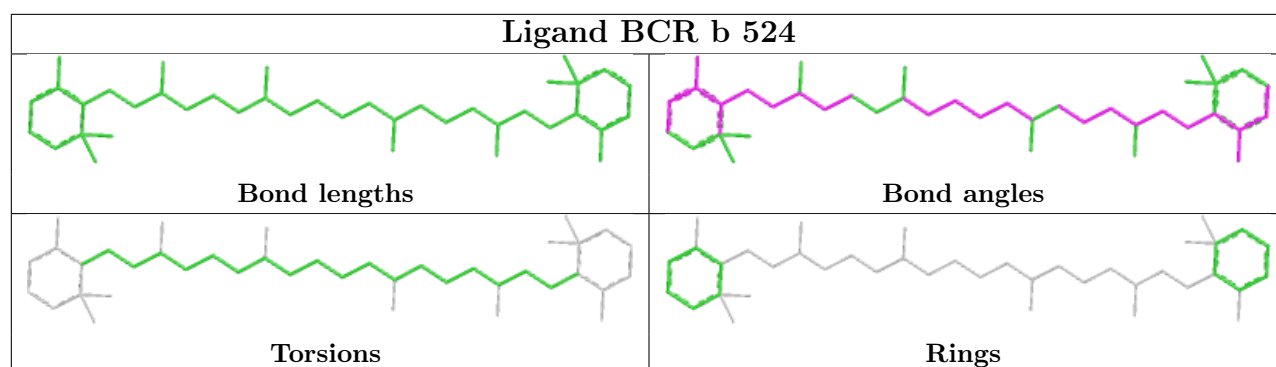


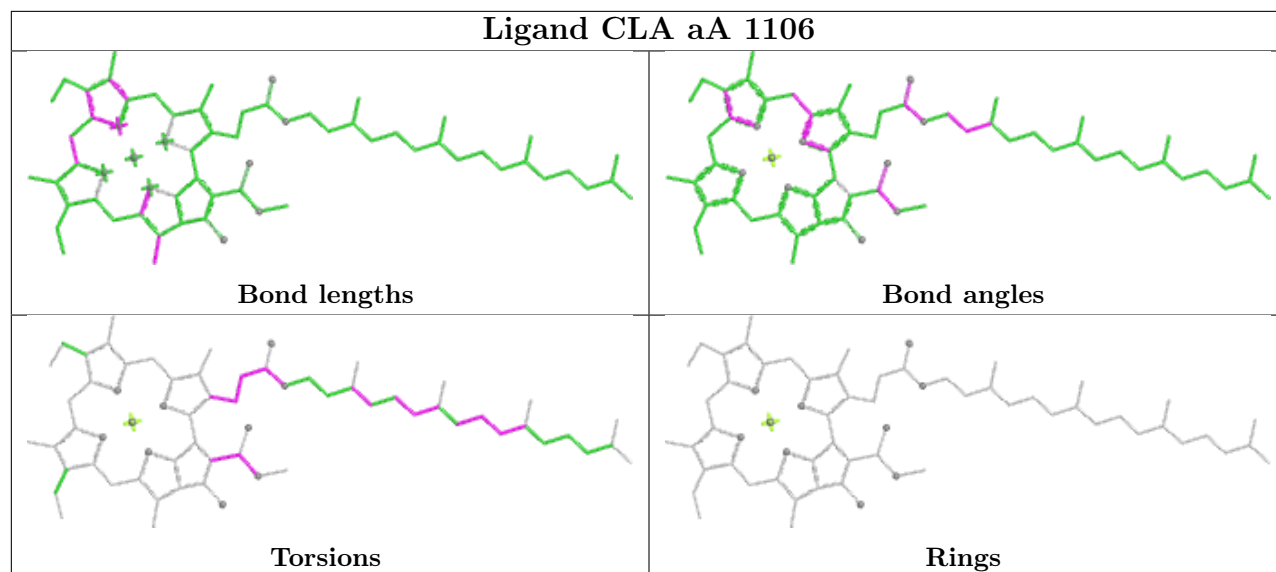
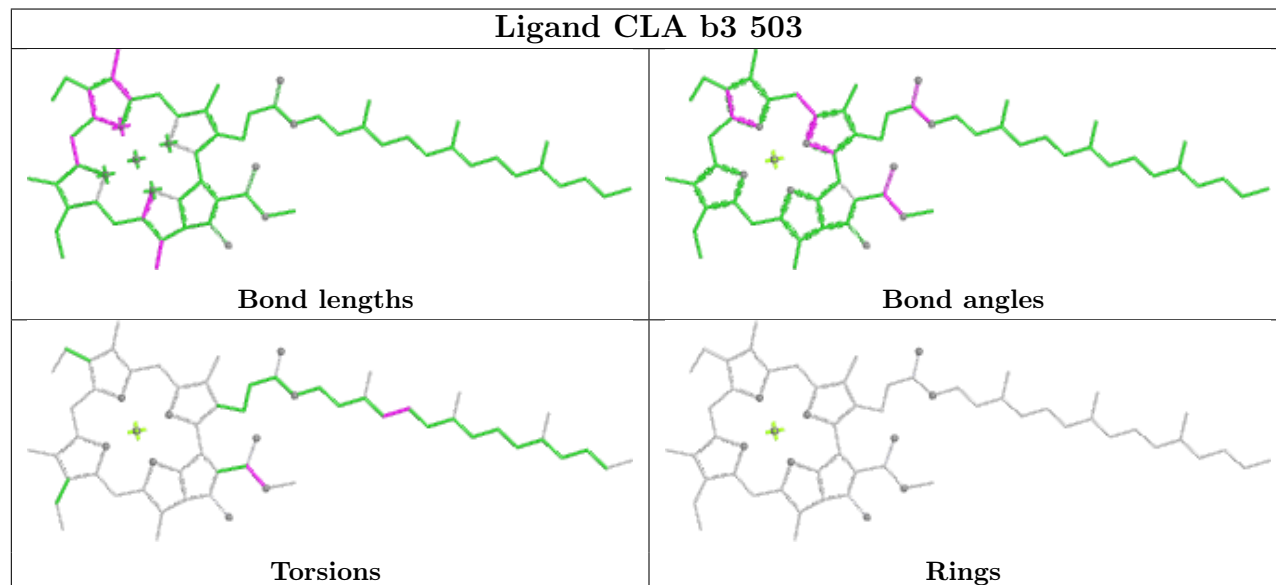
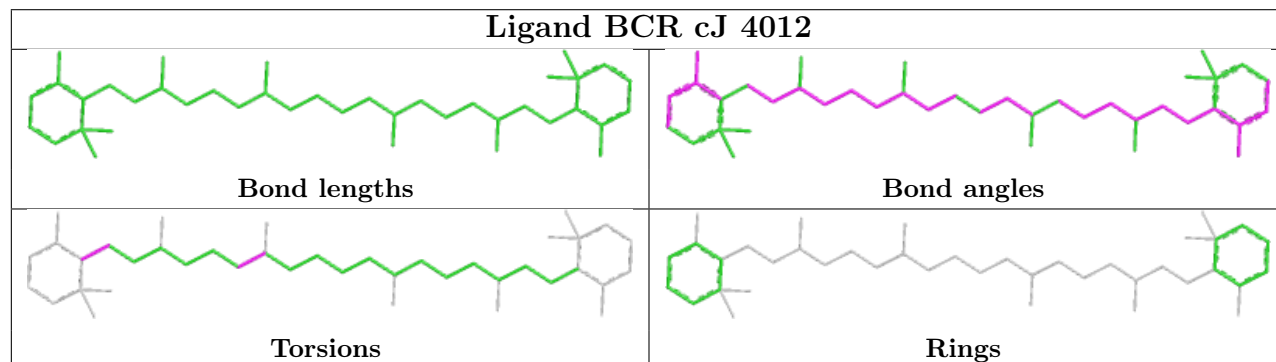
Torsions



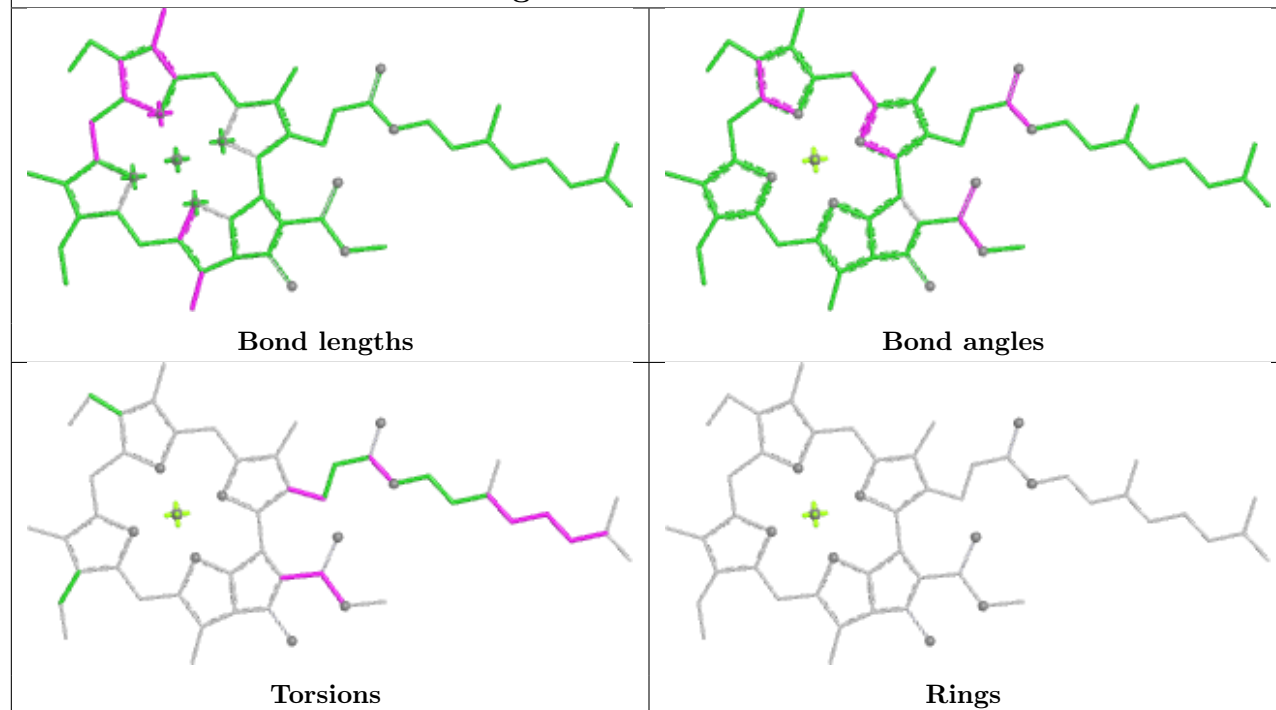
Rings



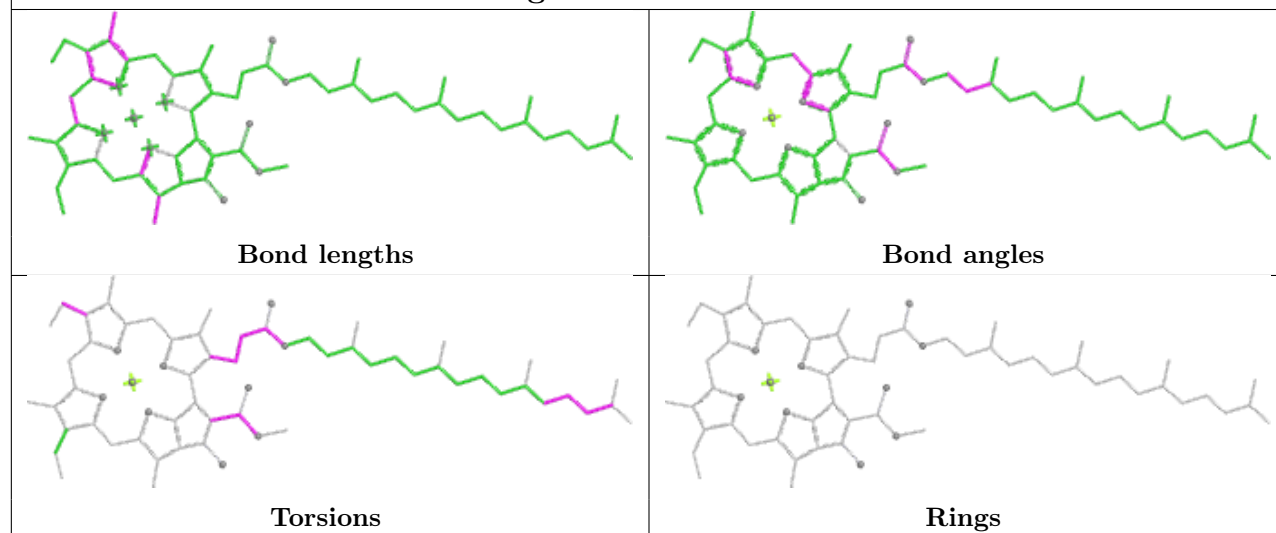


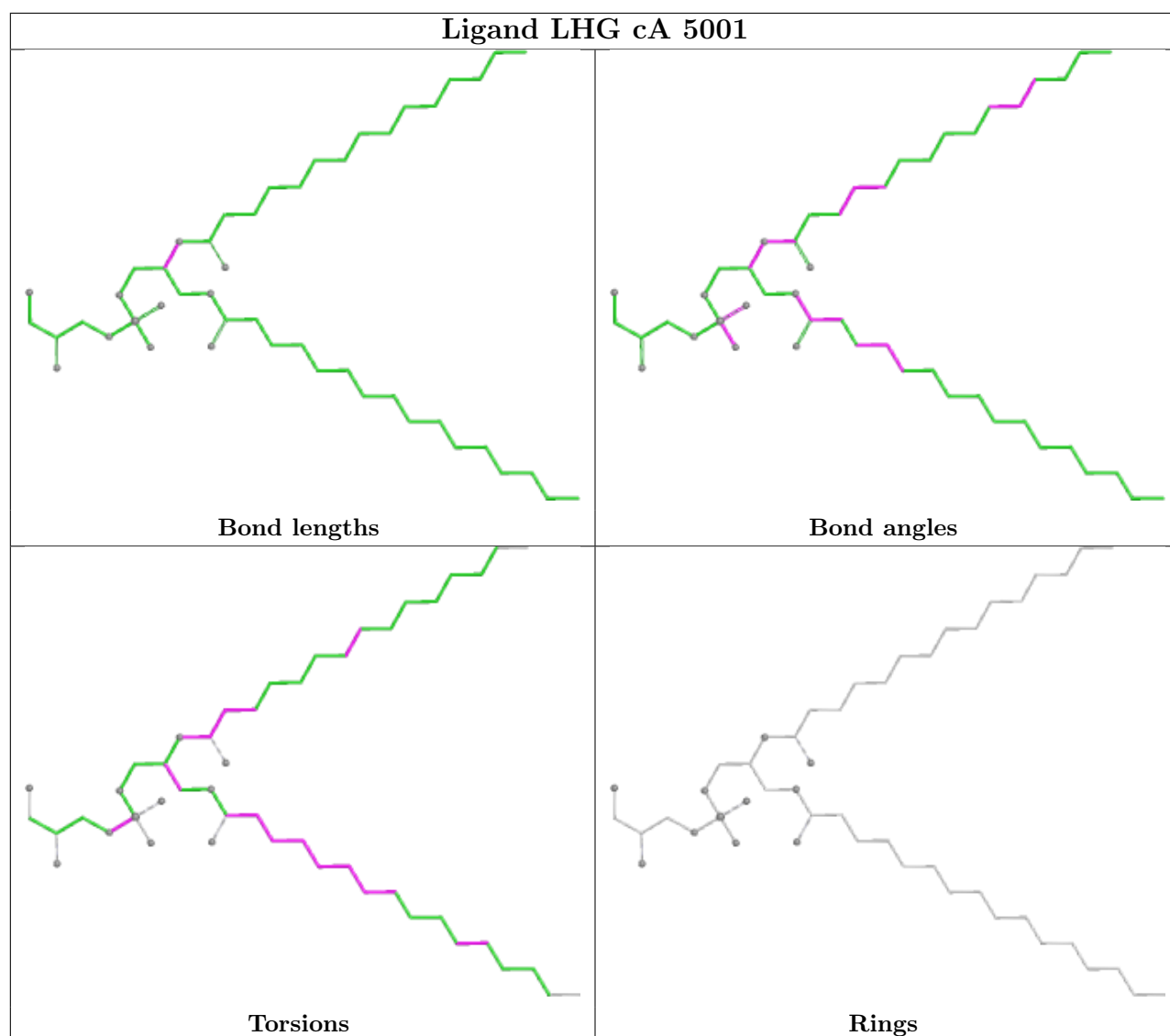
Ligand CLA aA 1106**Ligand CLA b3 503****Ligand BCR cJ 4012**

Ligand CLA bA 1129

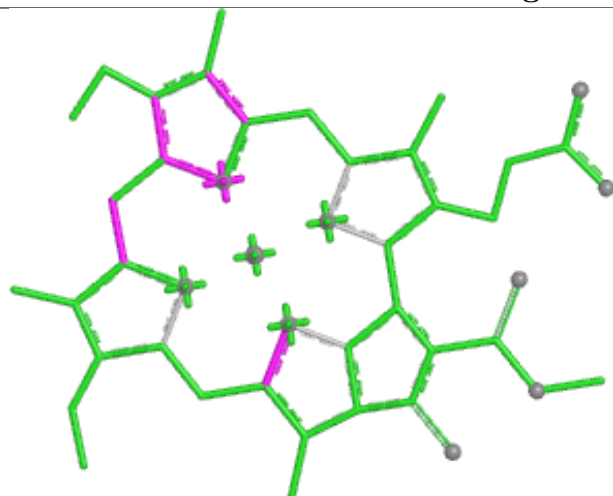


Ligand CLA a2 501

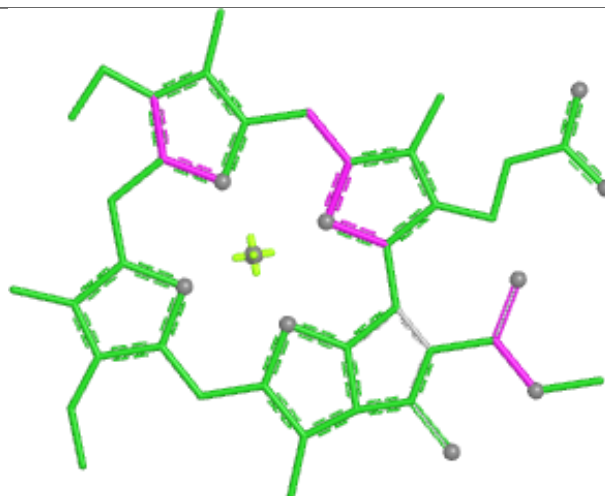




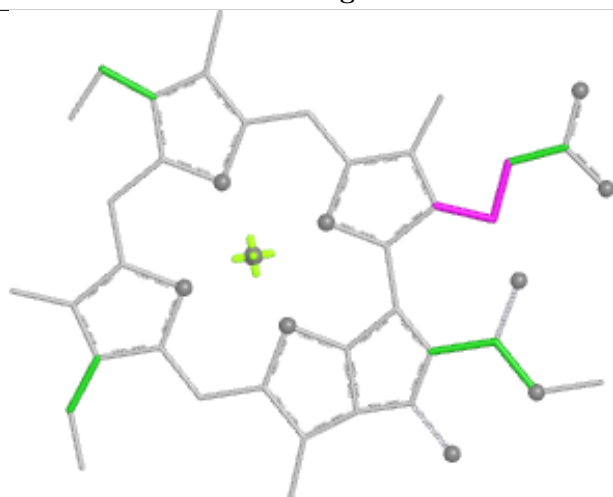
Ligand CLA l 513



Bond lengths



Bond angles

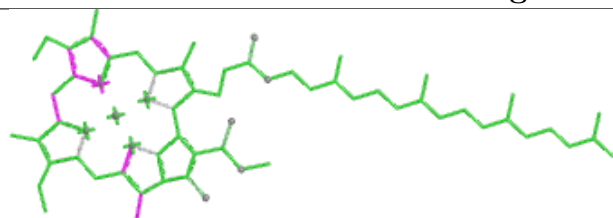


Torsions

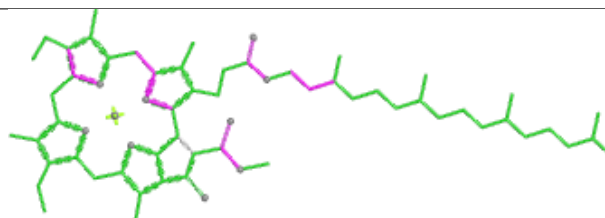


Rings

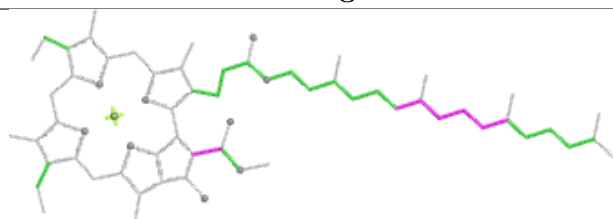
Ligand CLA a2 509



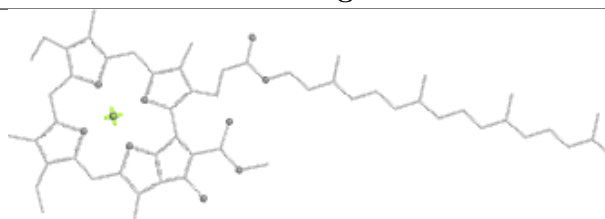
Bond lengths



Bond angles

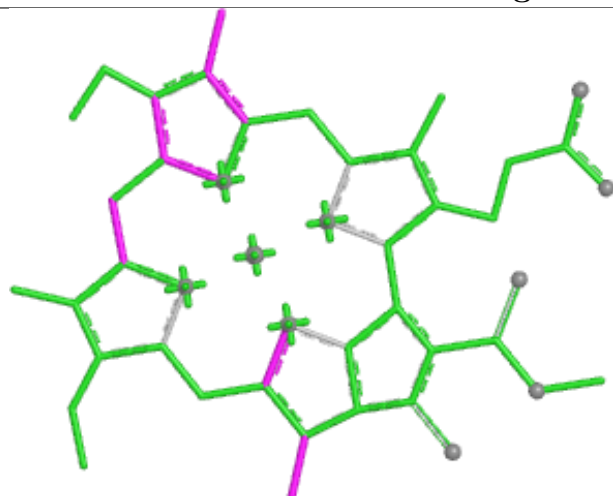


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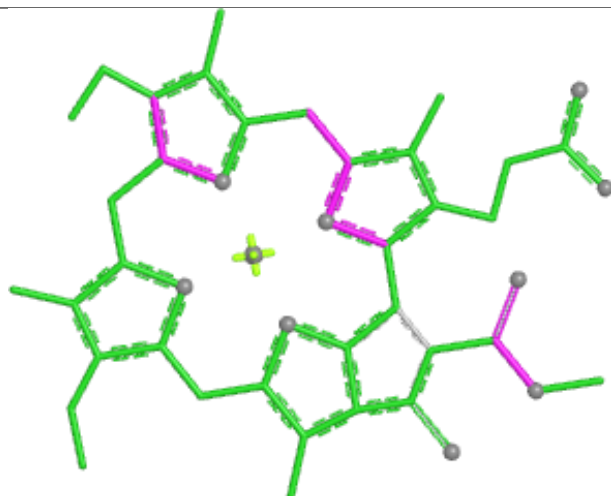


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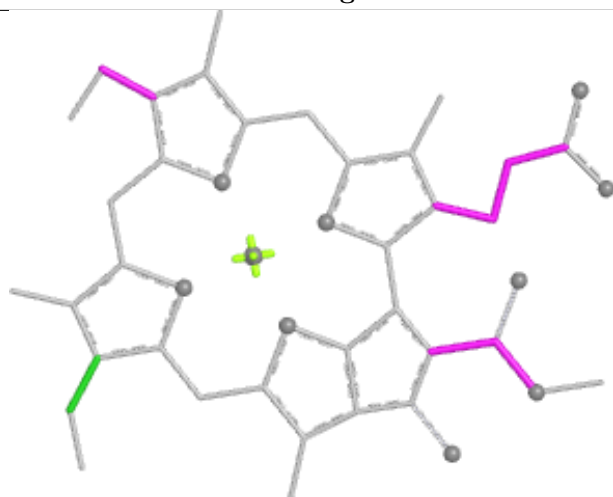
Ligand CLA U 517



Bond lengths



Bond angles

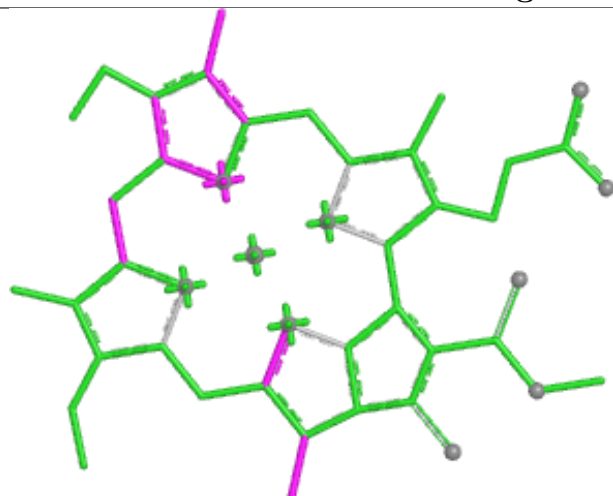


Torsions



Rings

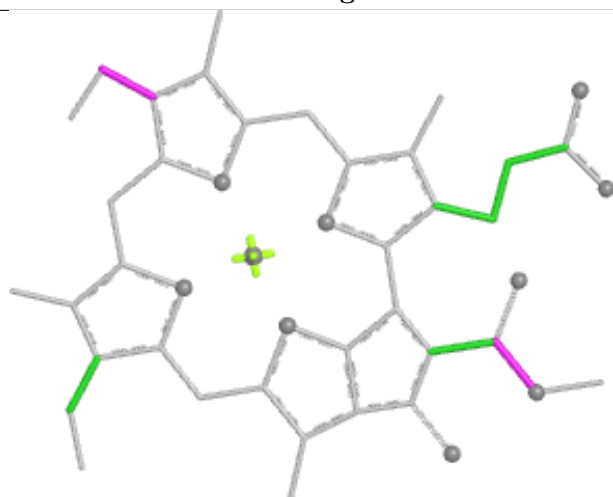
Ligand CLA Z 519



Bond lengths



Bond angles

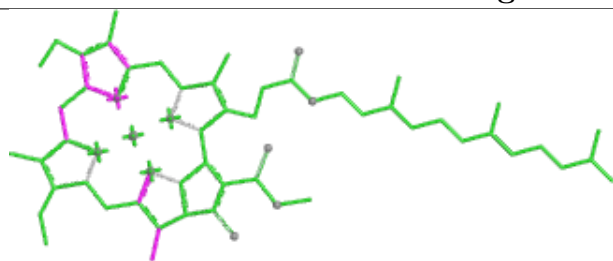


Torsions

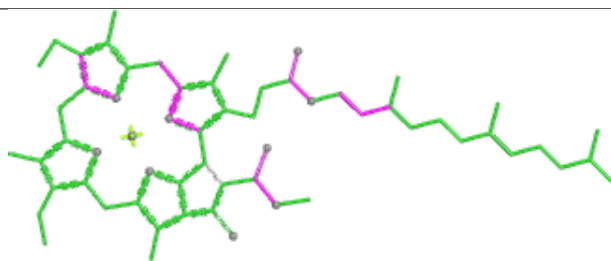


Rings

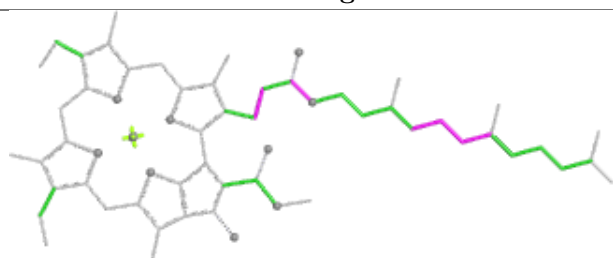
Ligand CLA cB 1213



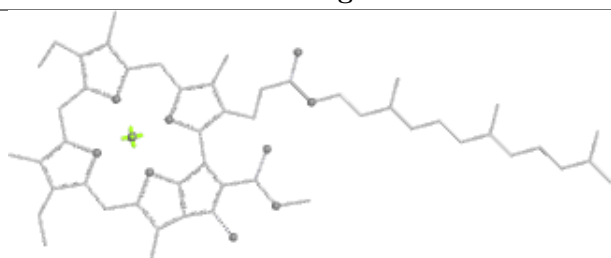
Bond lengths



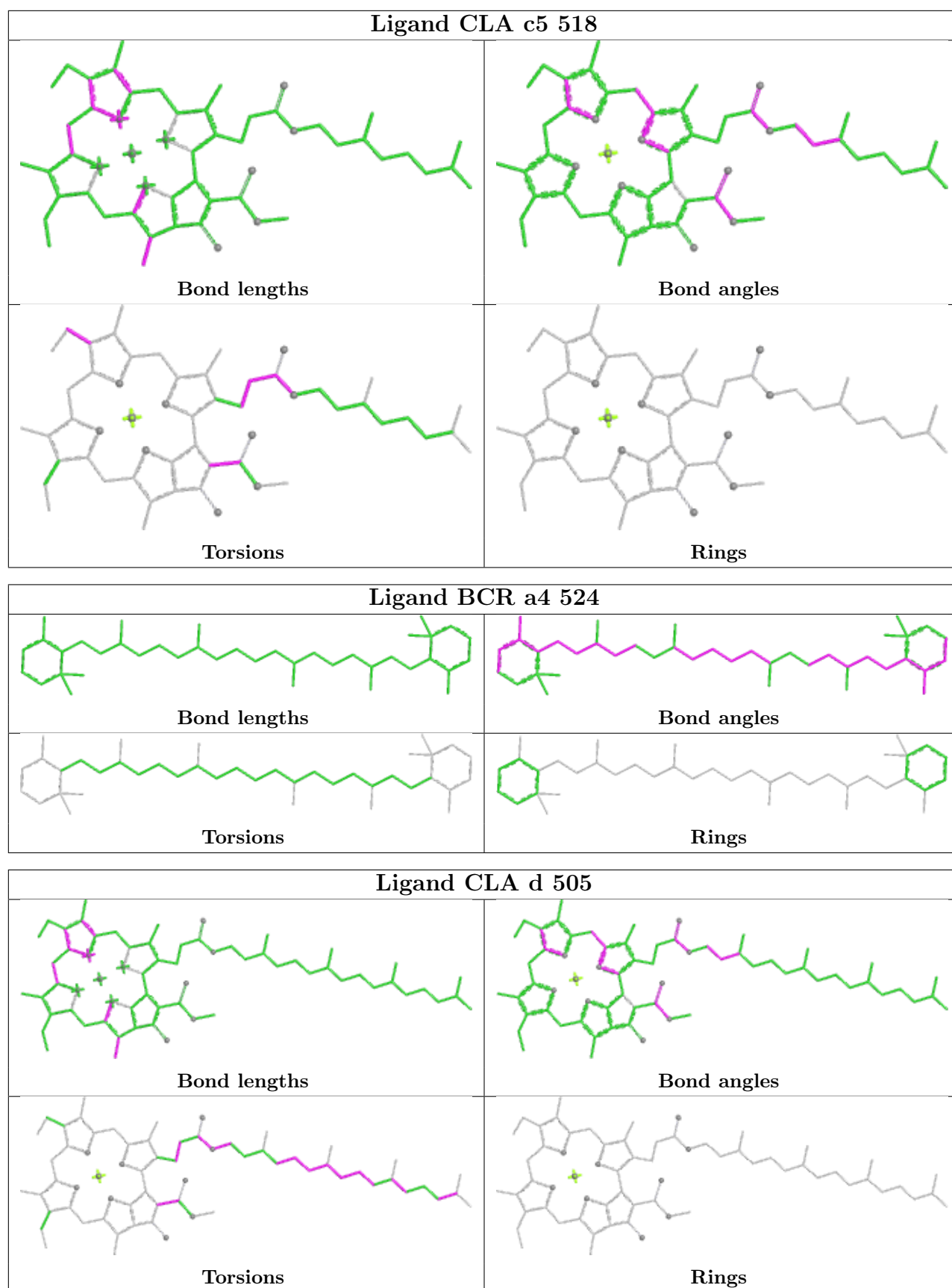
Bond angles



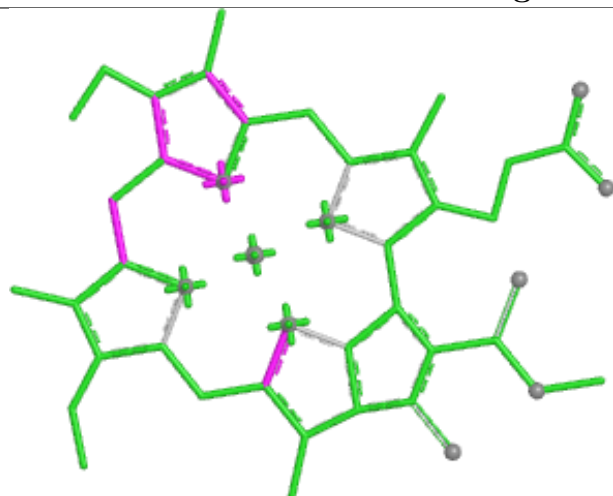
Torsions



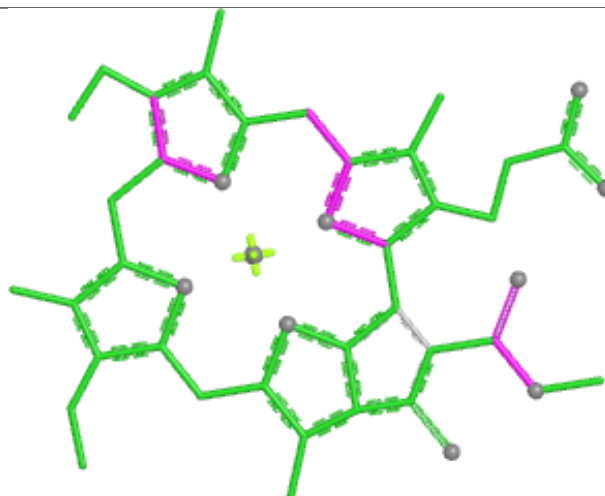
Rings



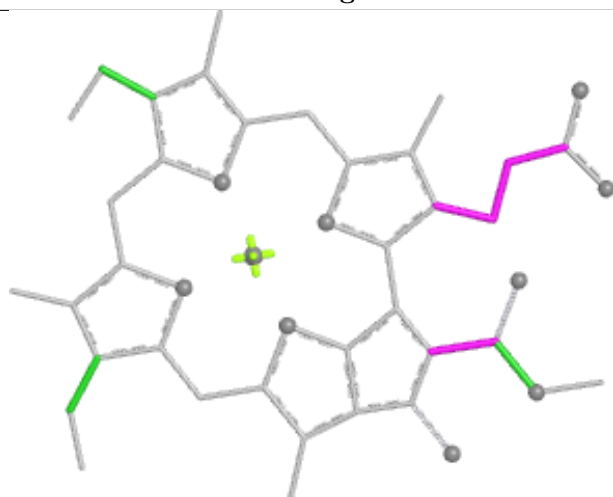
Ligand CLA U 518



Bond lengths



Bond angles

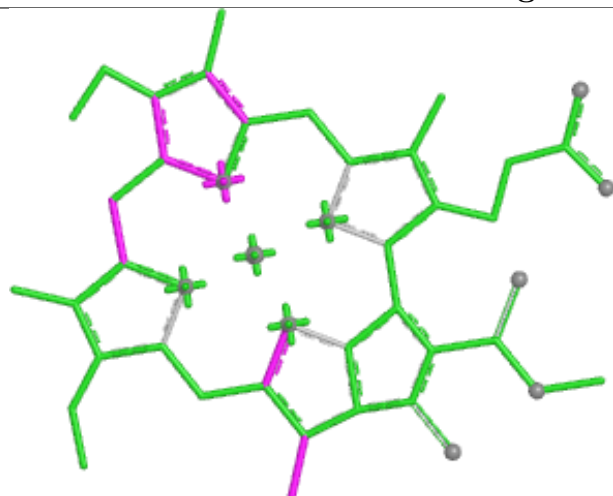


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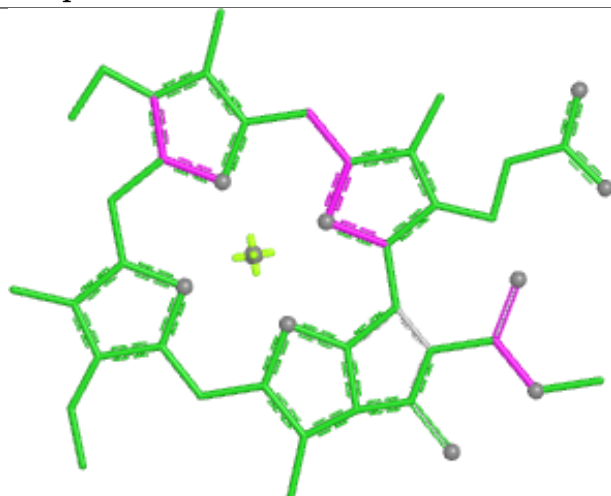


Rings

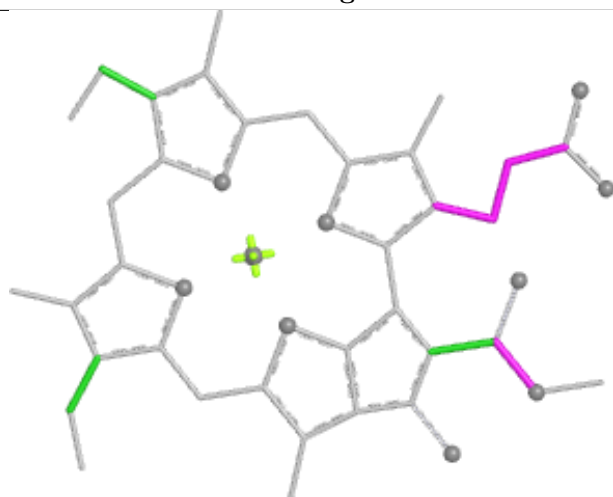
Ligand CLA q 518



Bond lengths



Bond angles

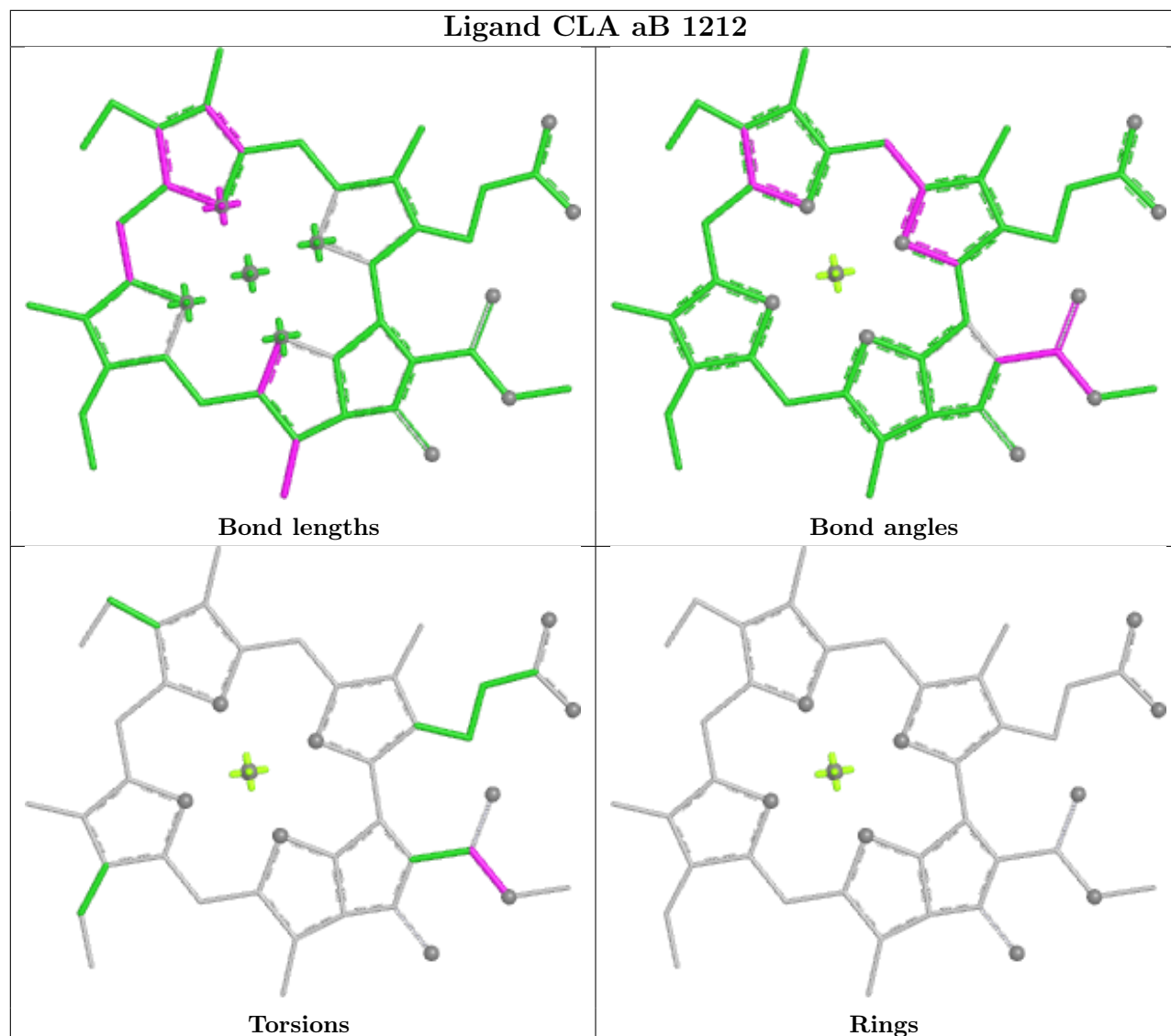


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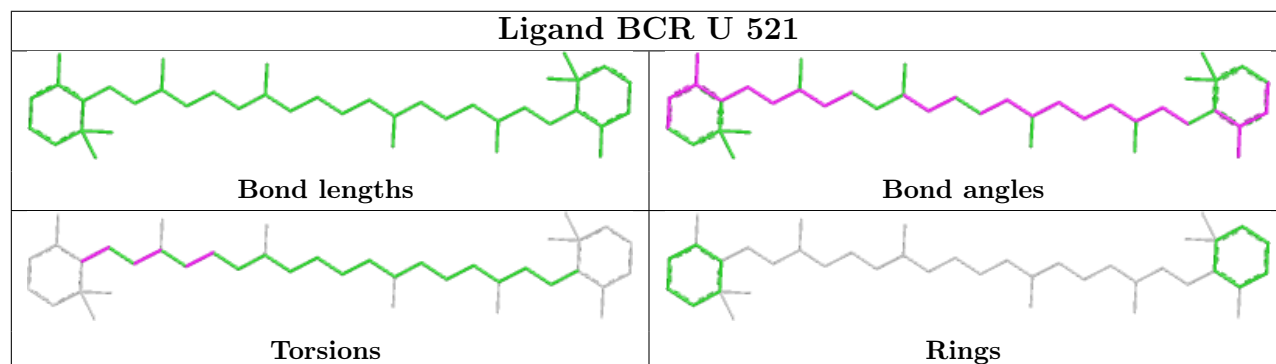


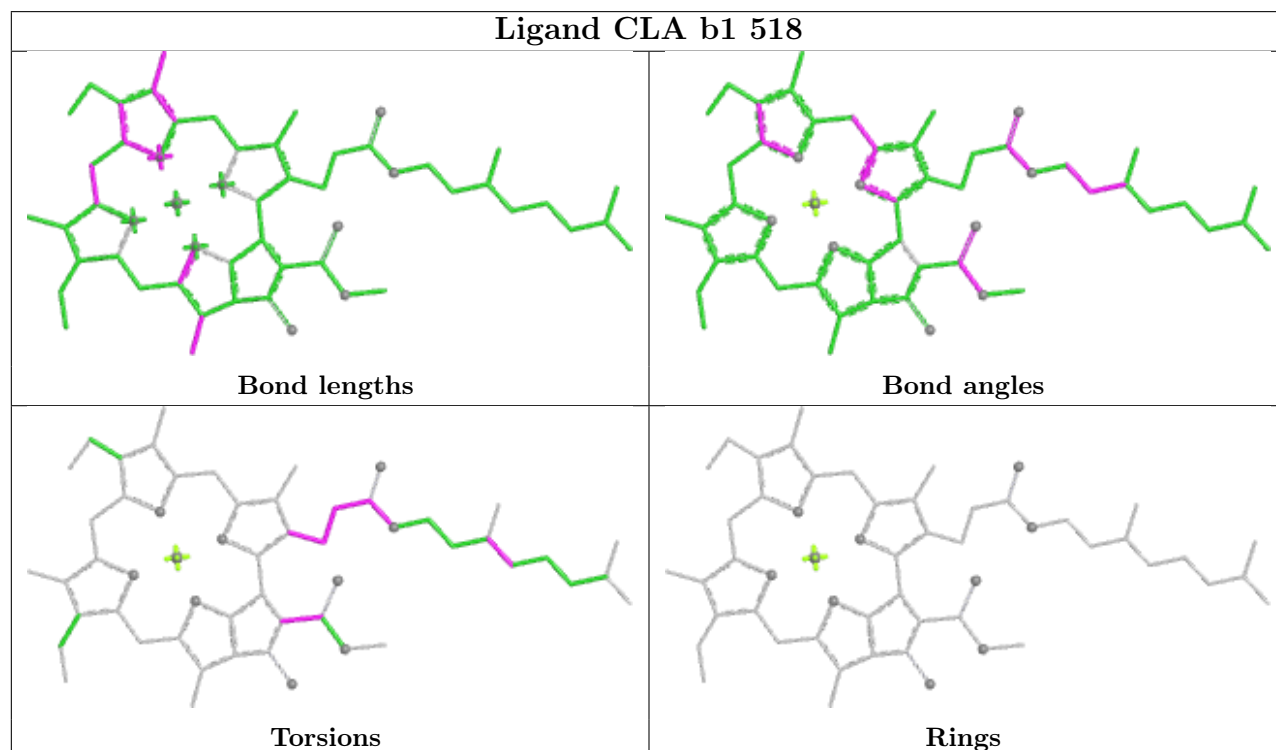
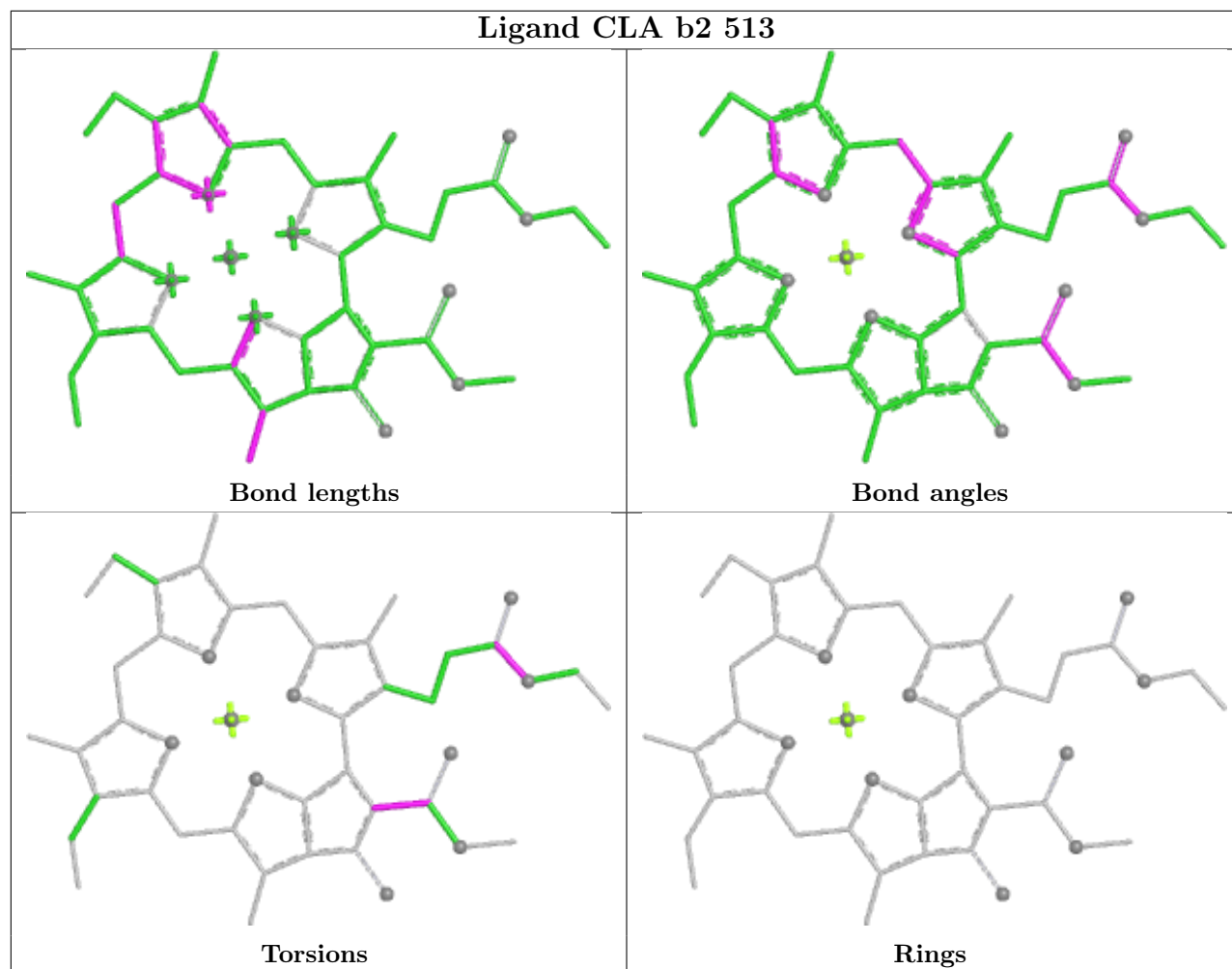
Rings

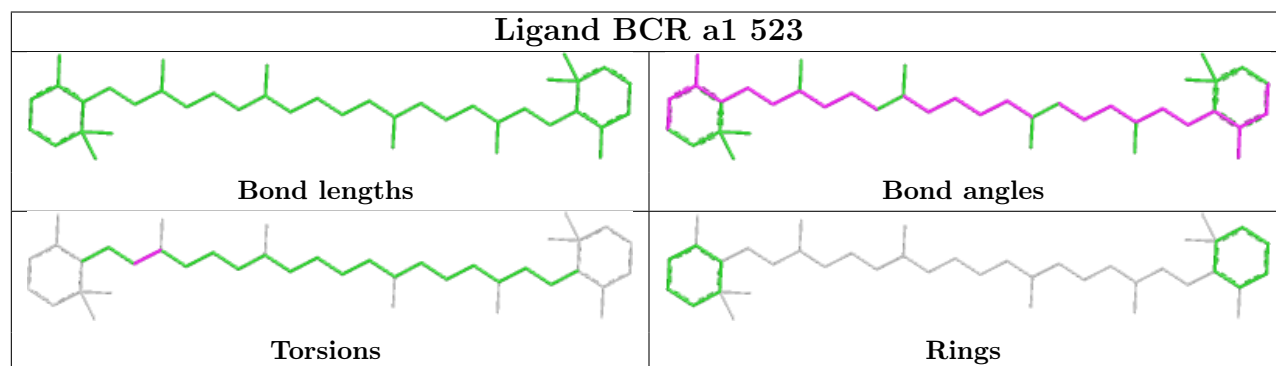
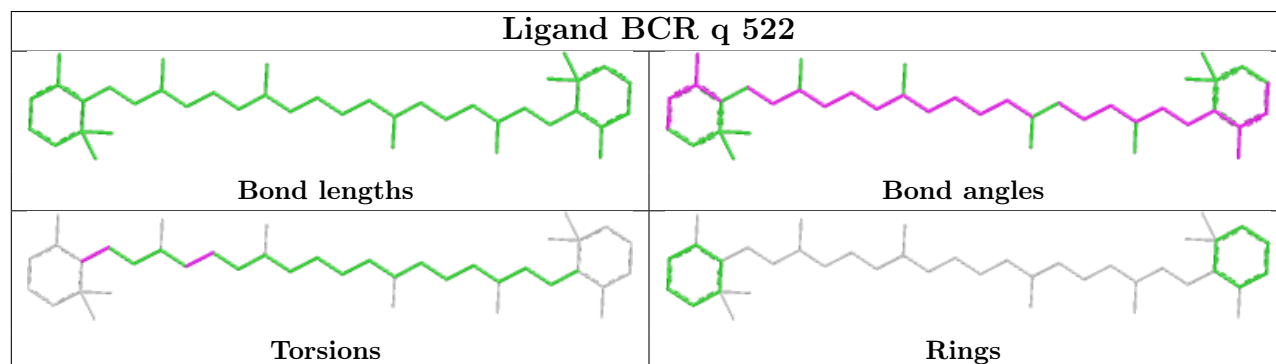
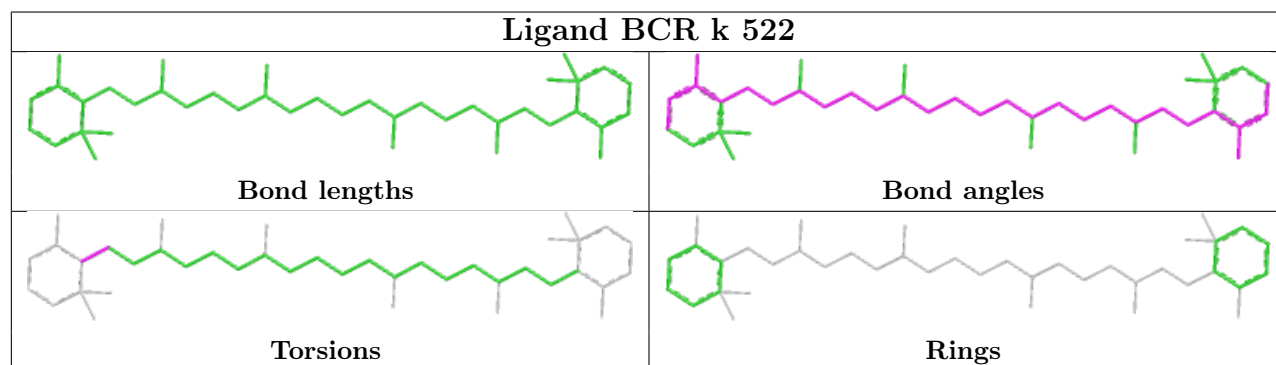
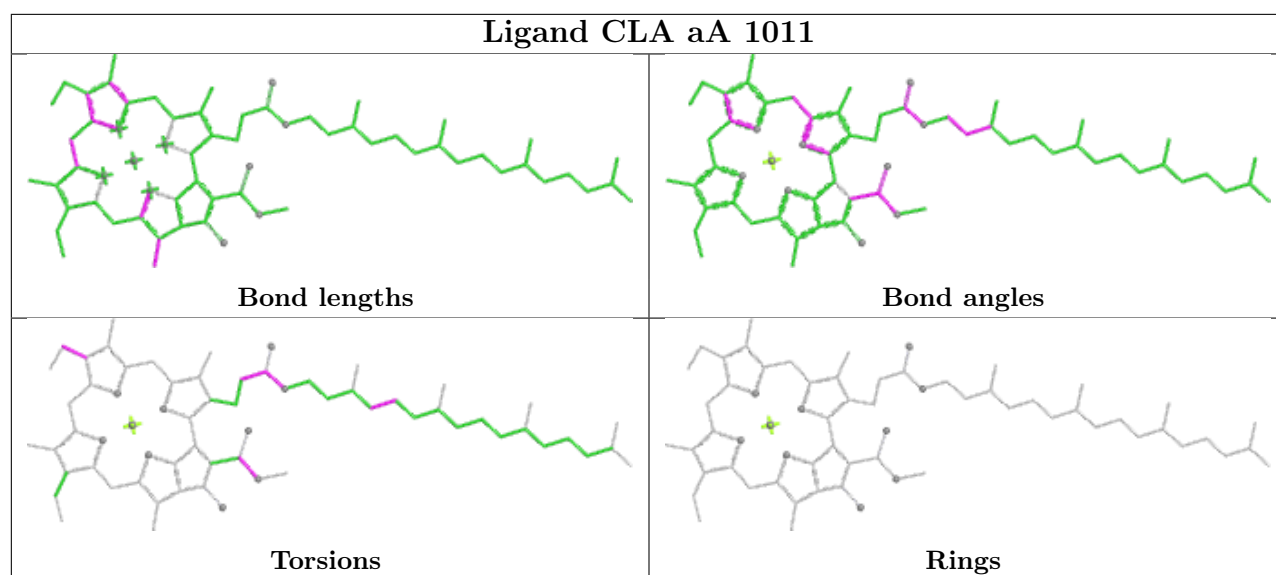
Ligand CLA aB 1212

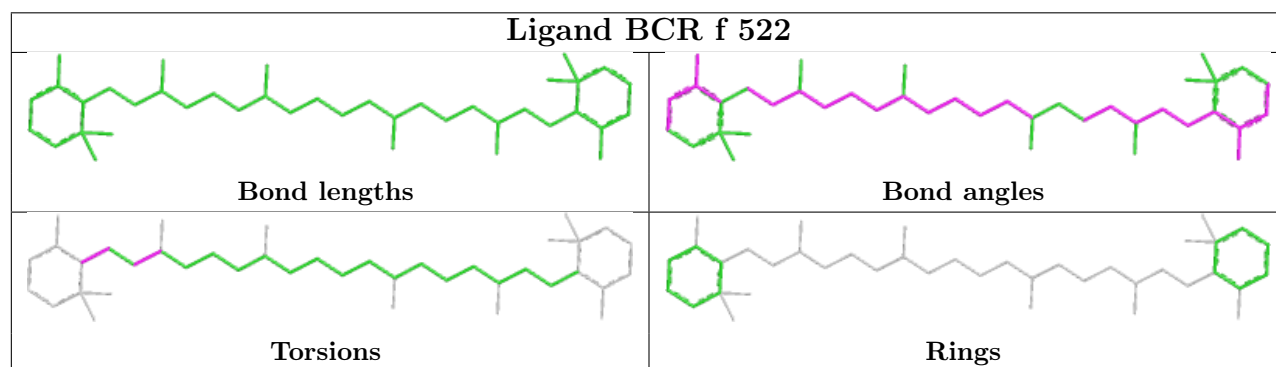
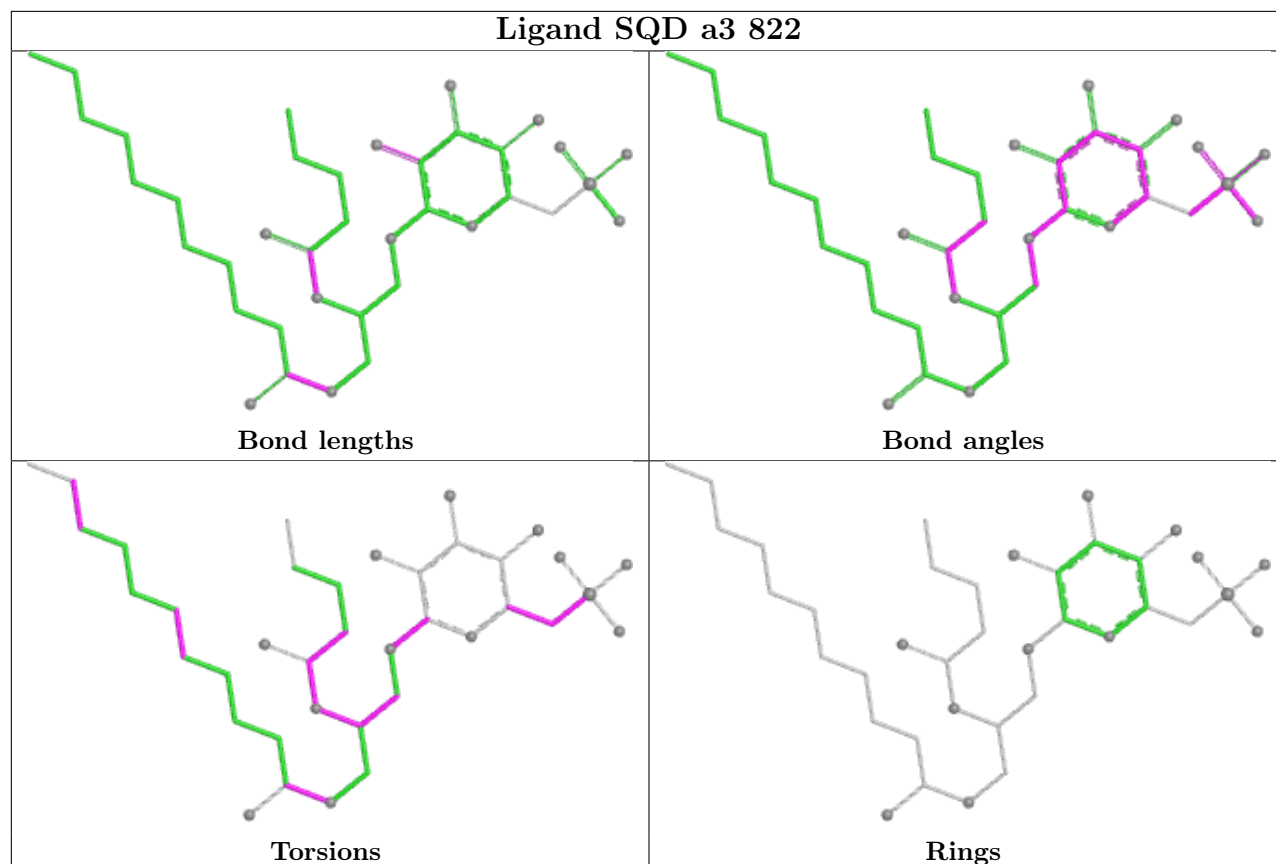


Ligand BCR U 521

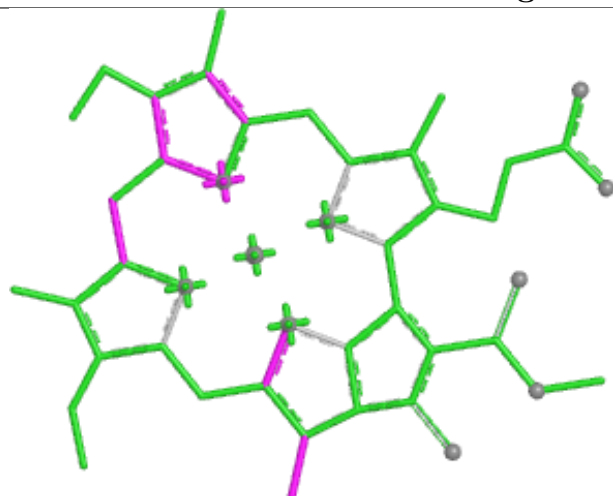




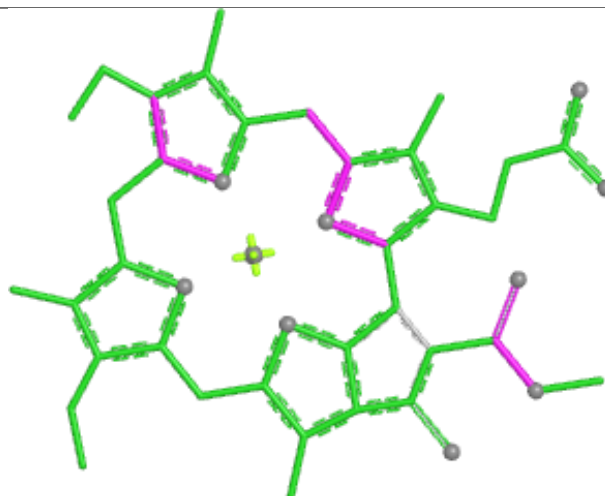




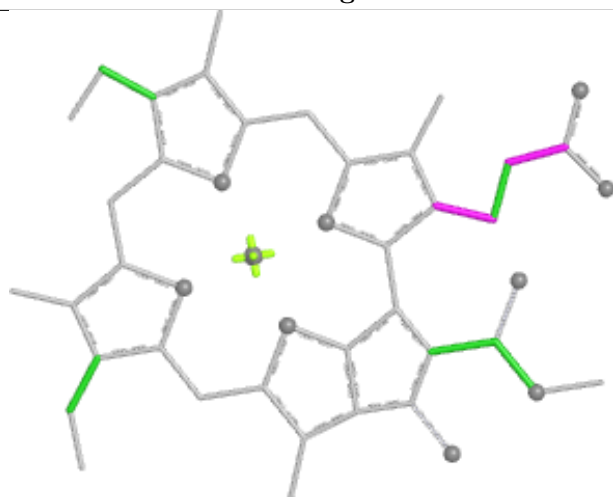
Ligand CLA n 519



Bond lengths



Bond angles

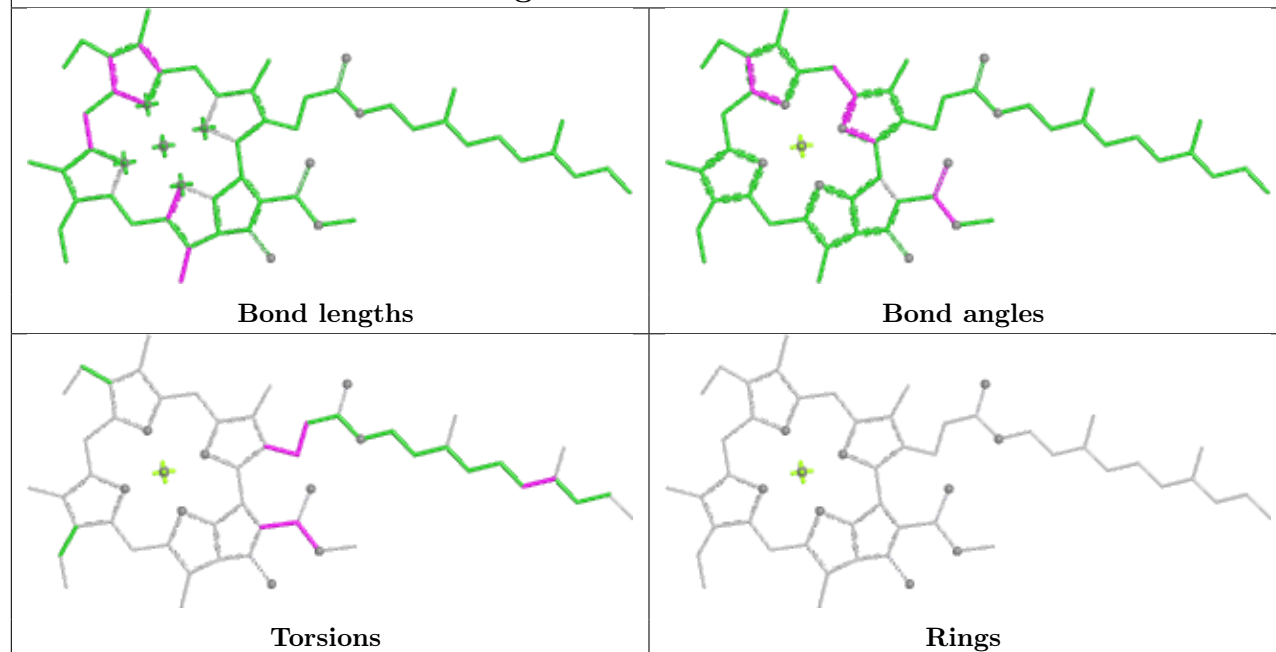


Torsions

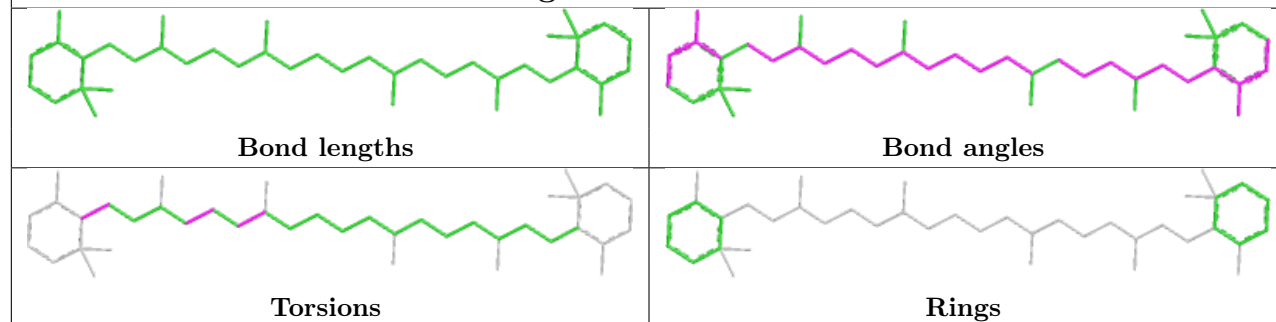


Rings

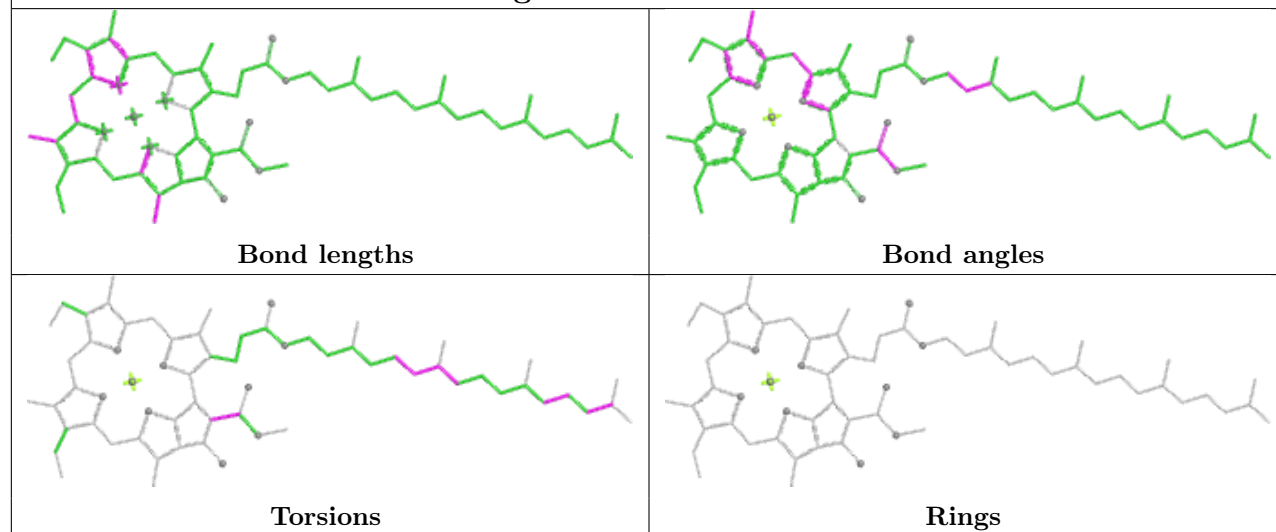
Ligand CLA aB 1201



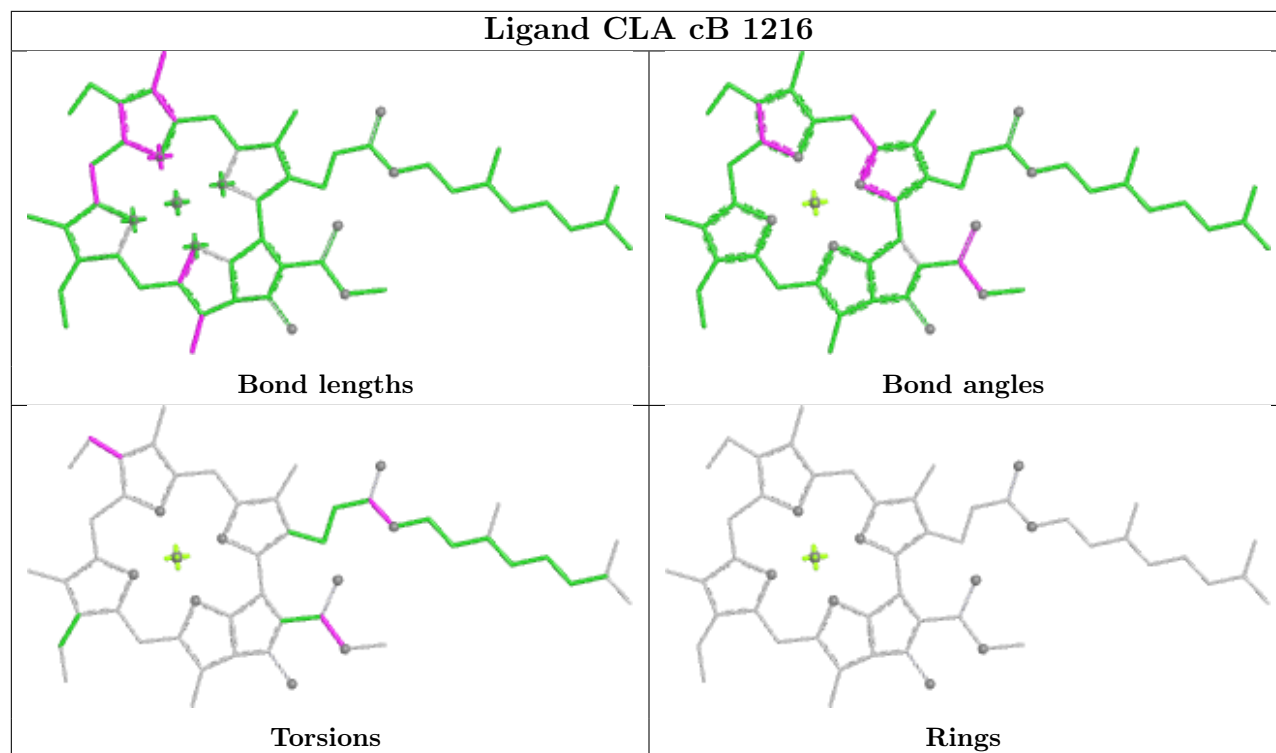
Ligand BCR i 522



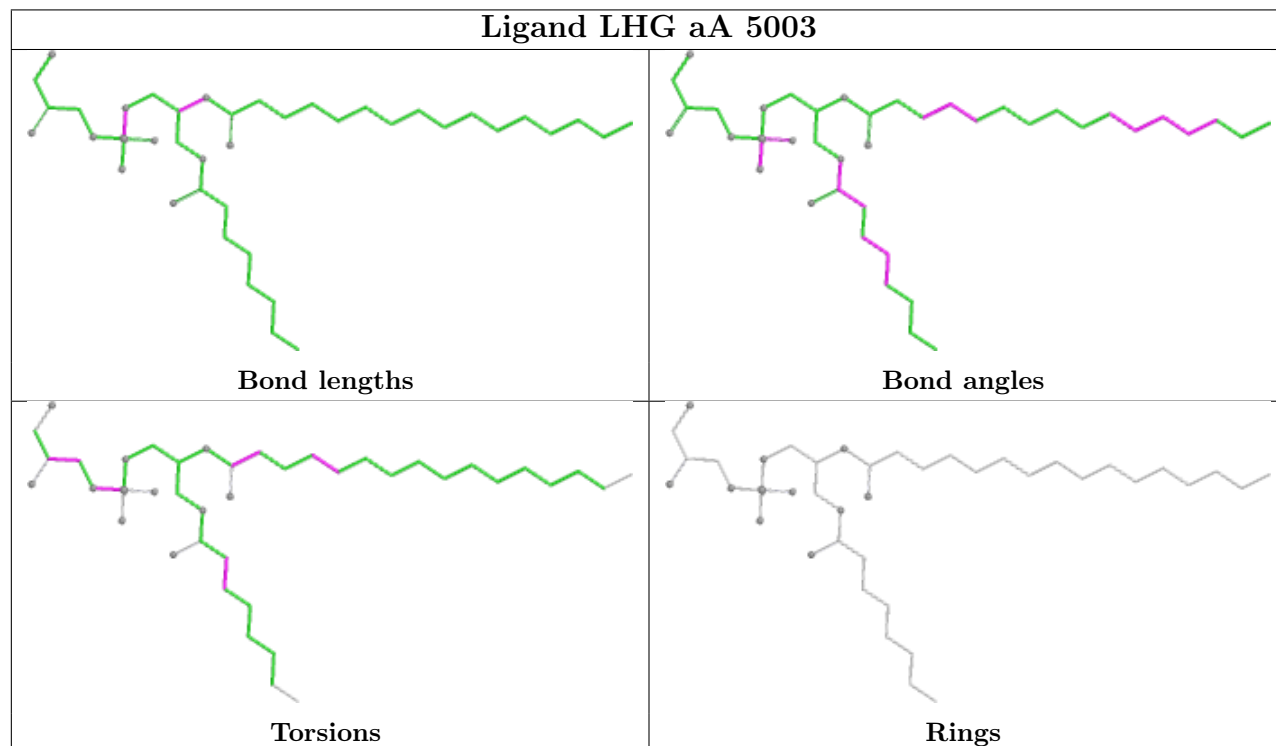
Ligand CLA bB 1223

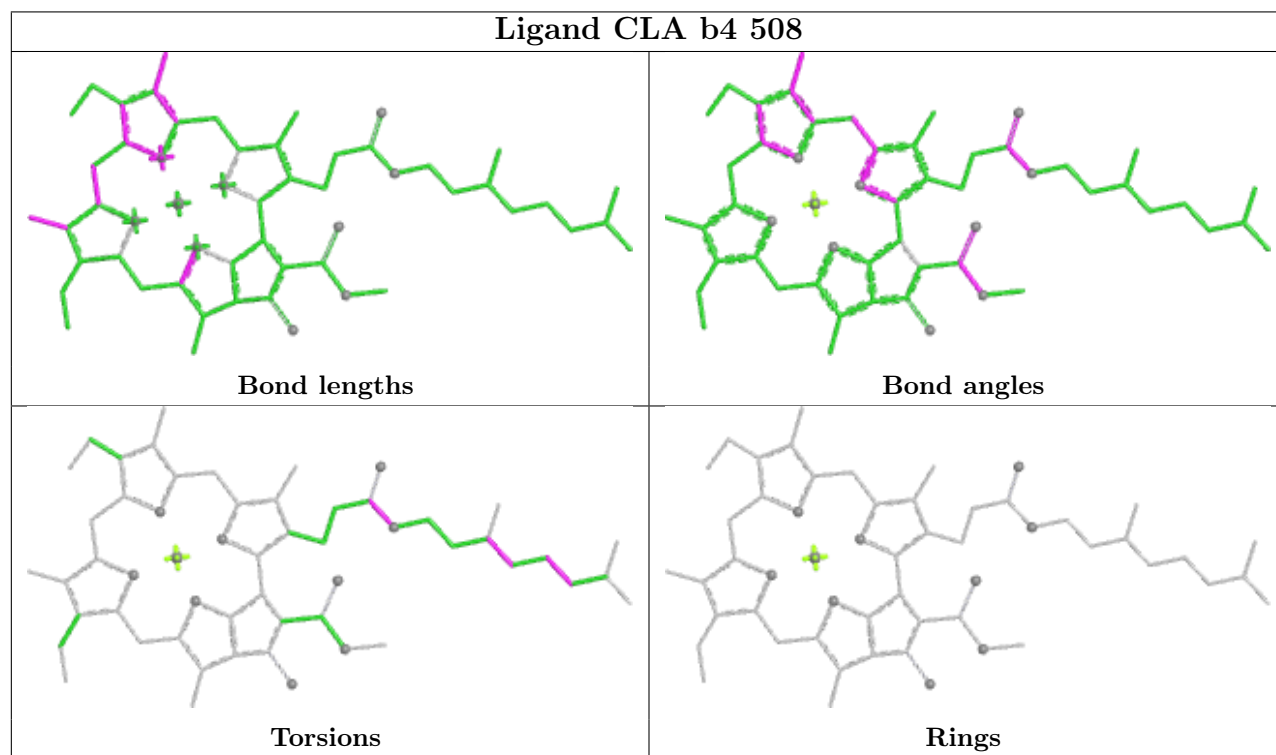
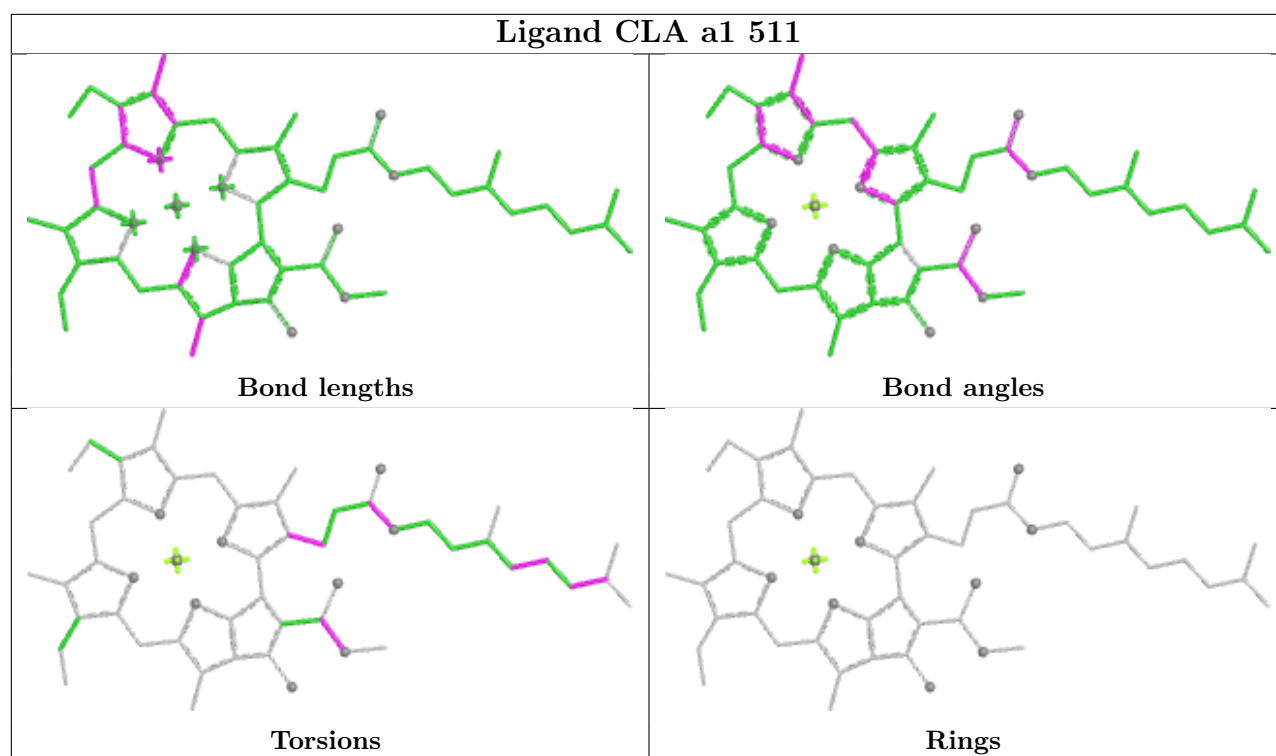


Ligand CLA cB 1216

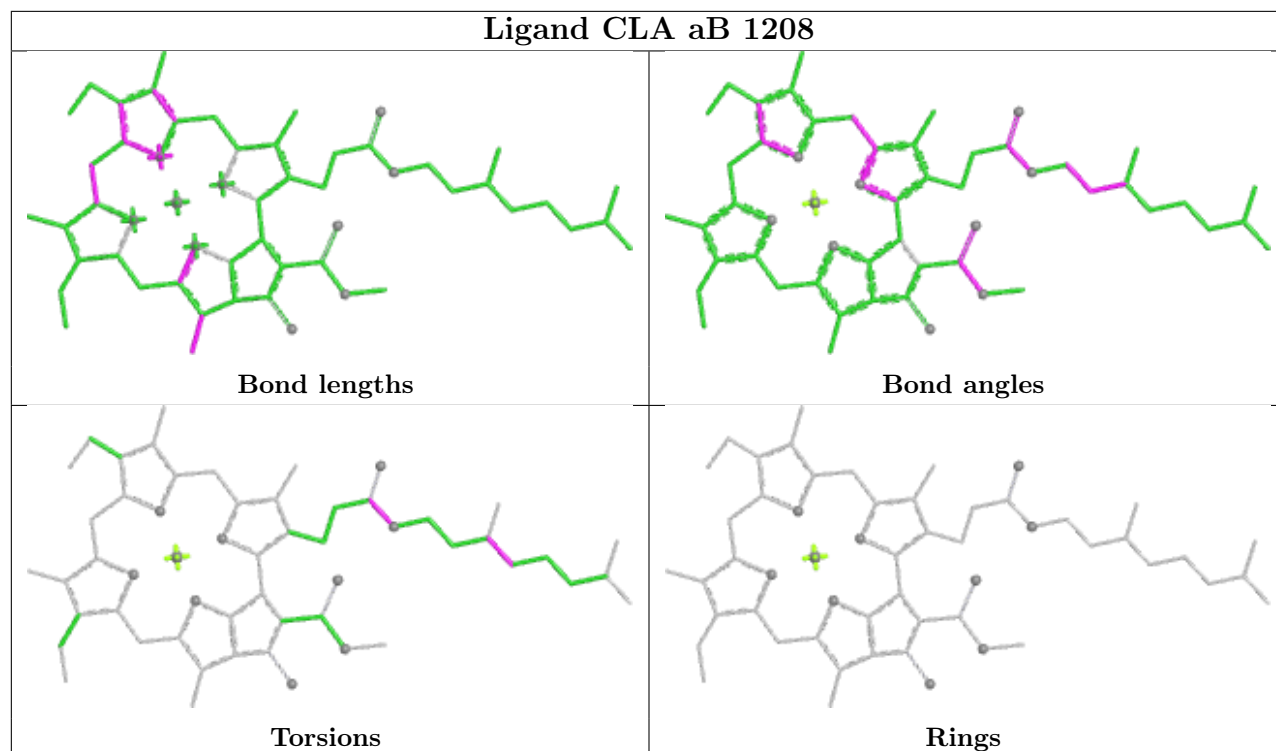


Ligand LHG aA 5003

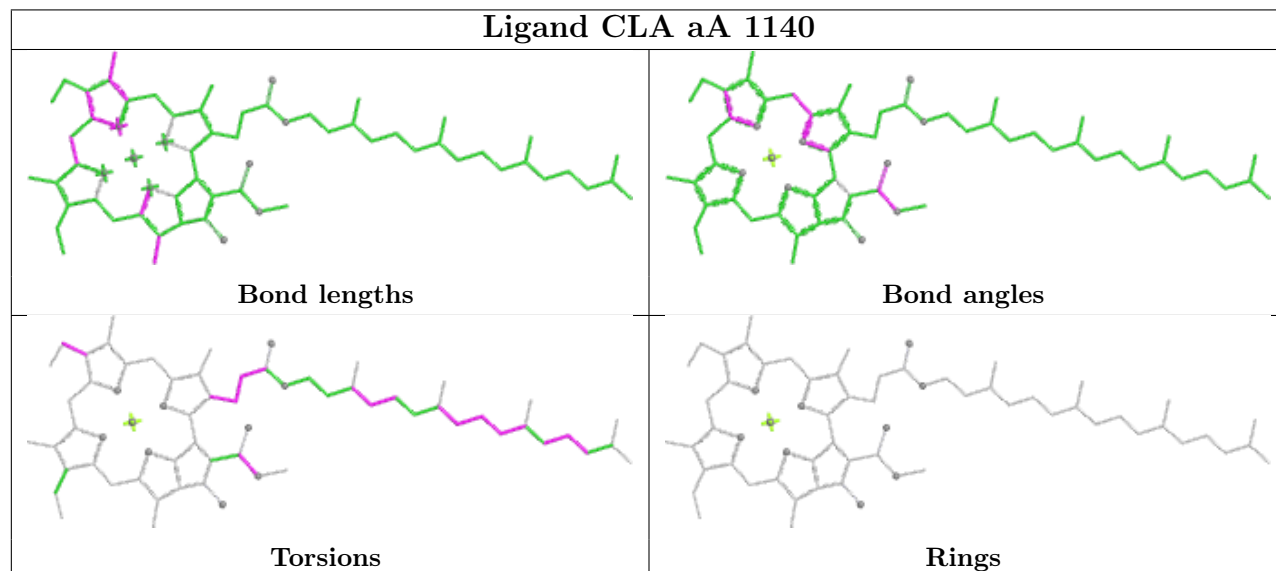




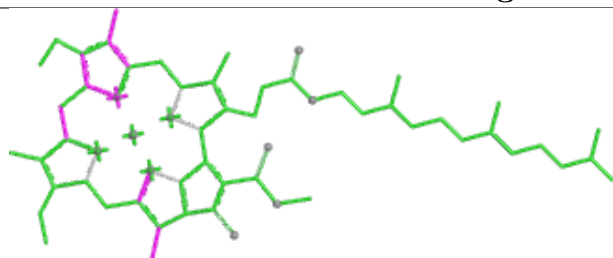
Ligand CLA aB 1208



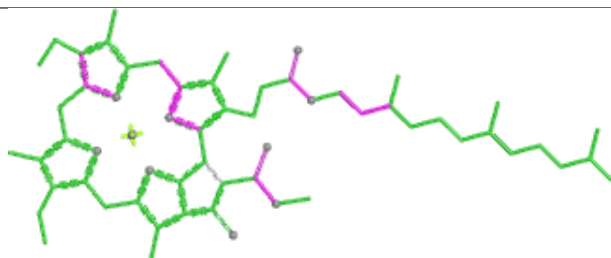
Ligand CLA aA 1140



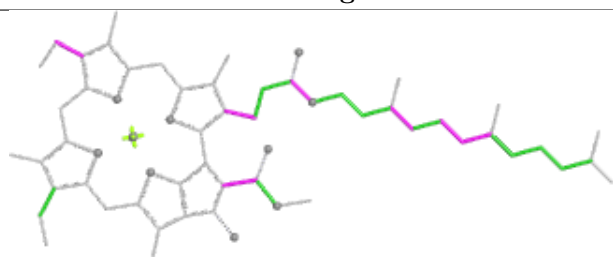
Ligand CLA aB 1234



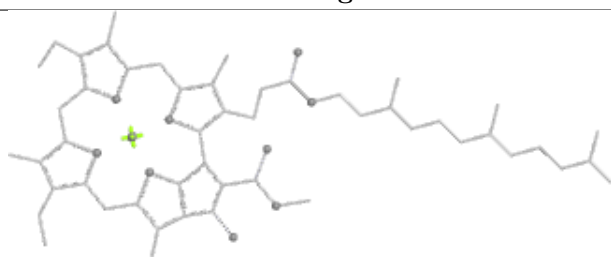
Bond lengths



Bond angles

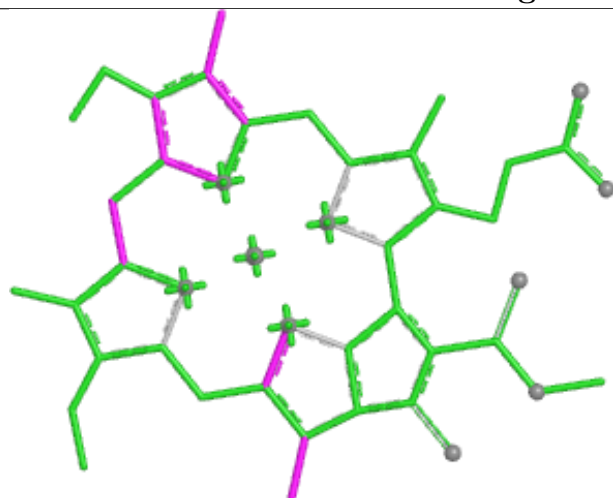


Torsions

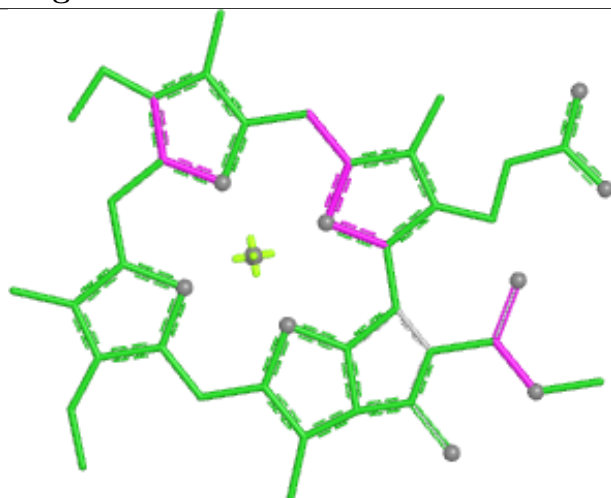


Rings

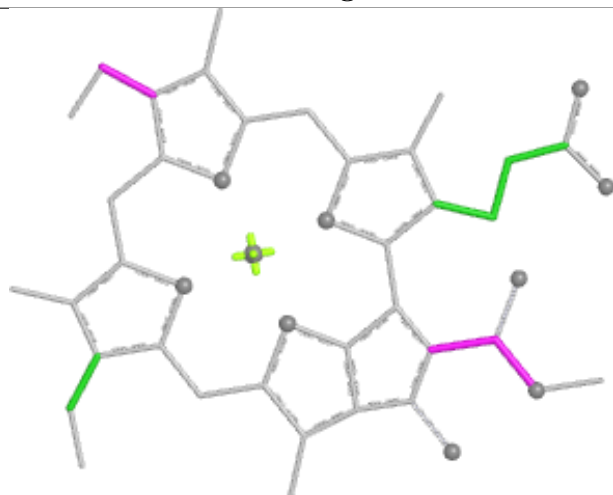
Ligand CLA g 502



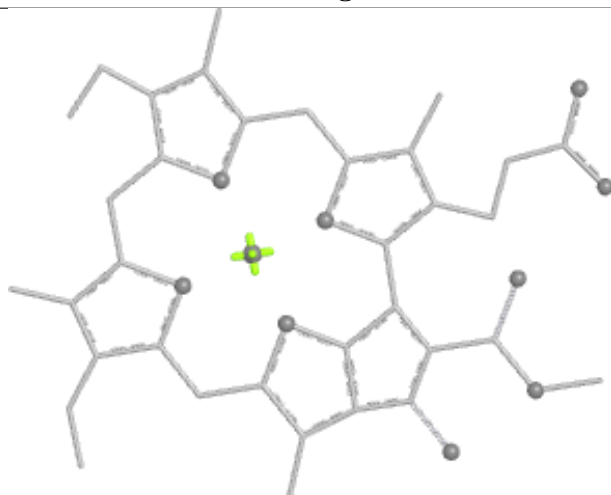
Bond lengths



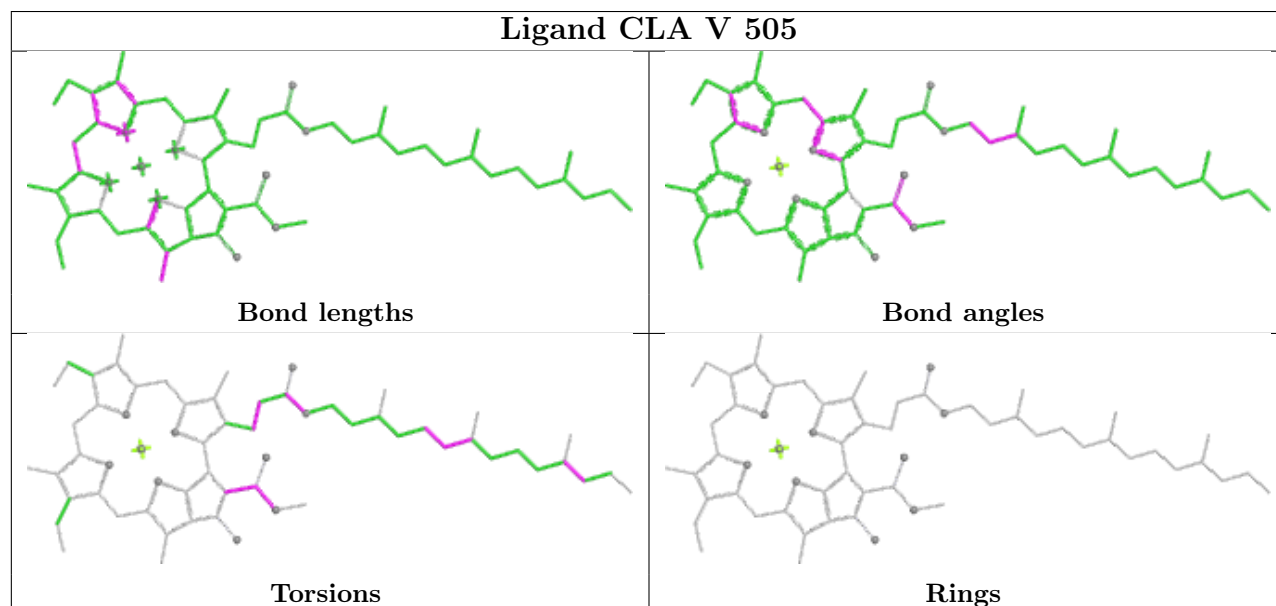
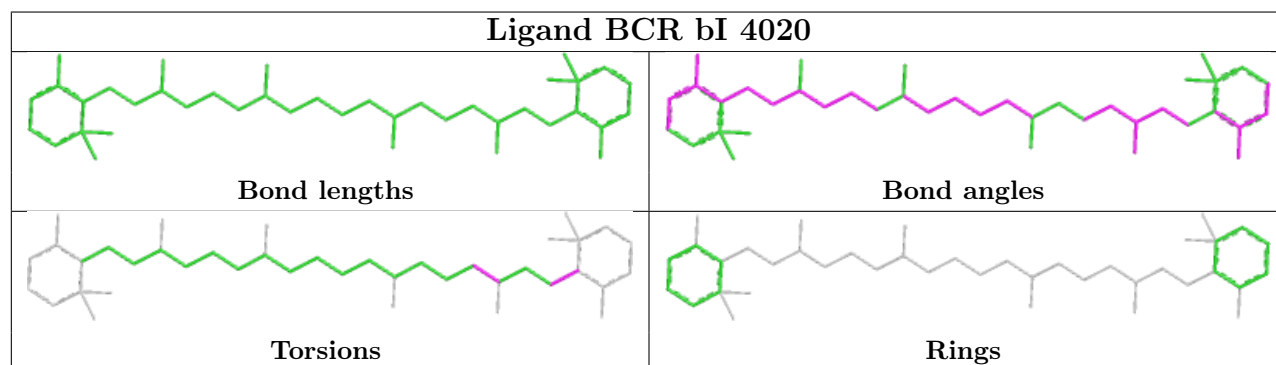
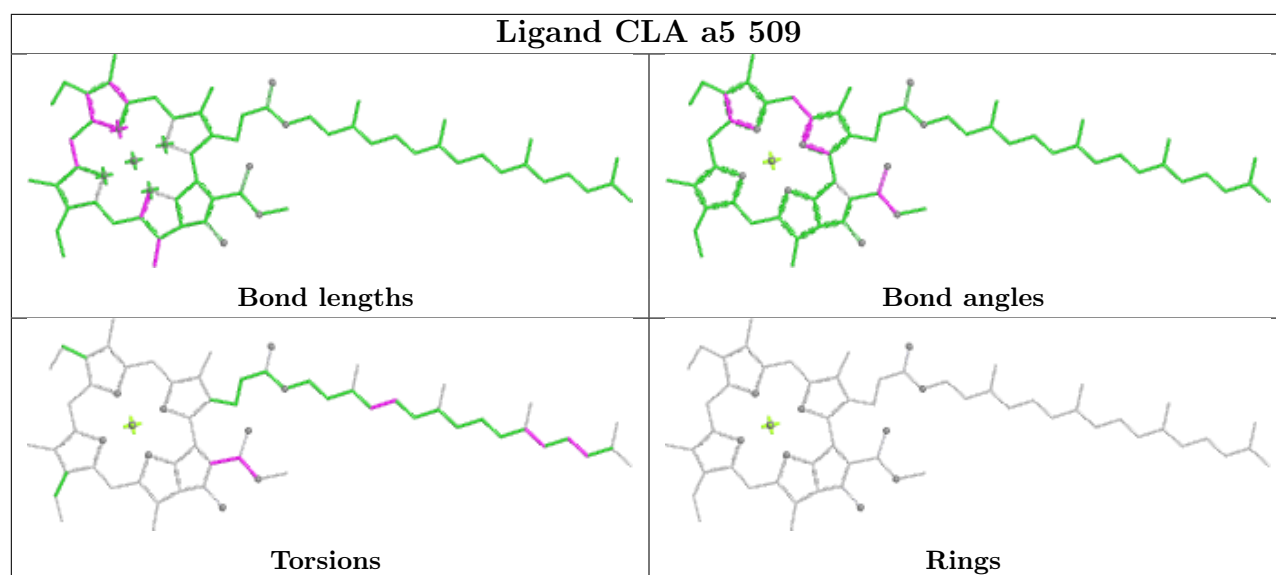
Bond angles



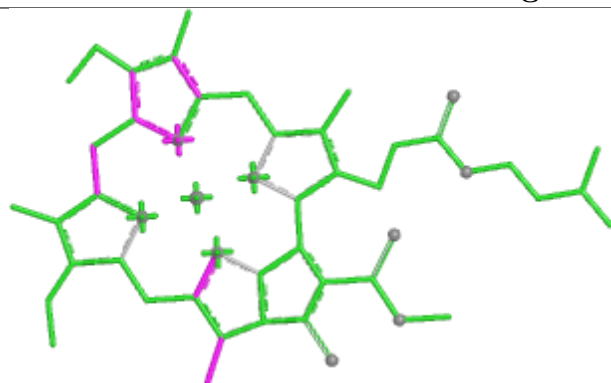
Torsions



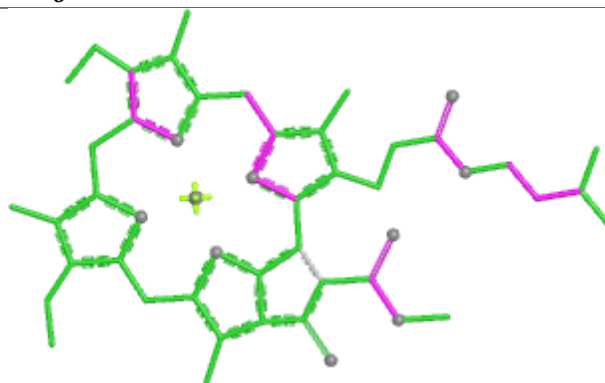
Rings



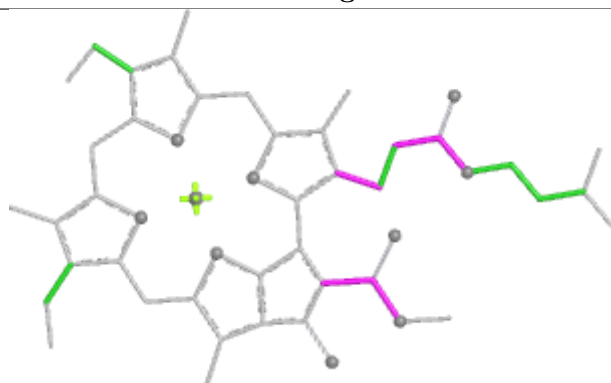
Ligand CLA j 518



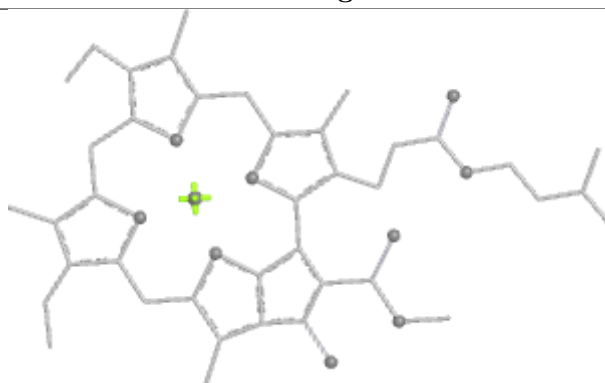
Bond lengths



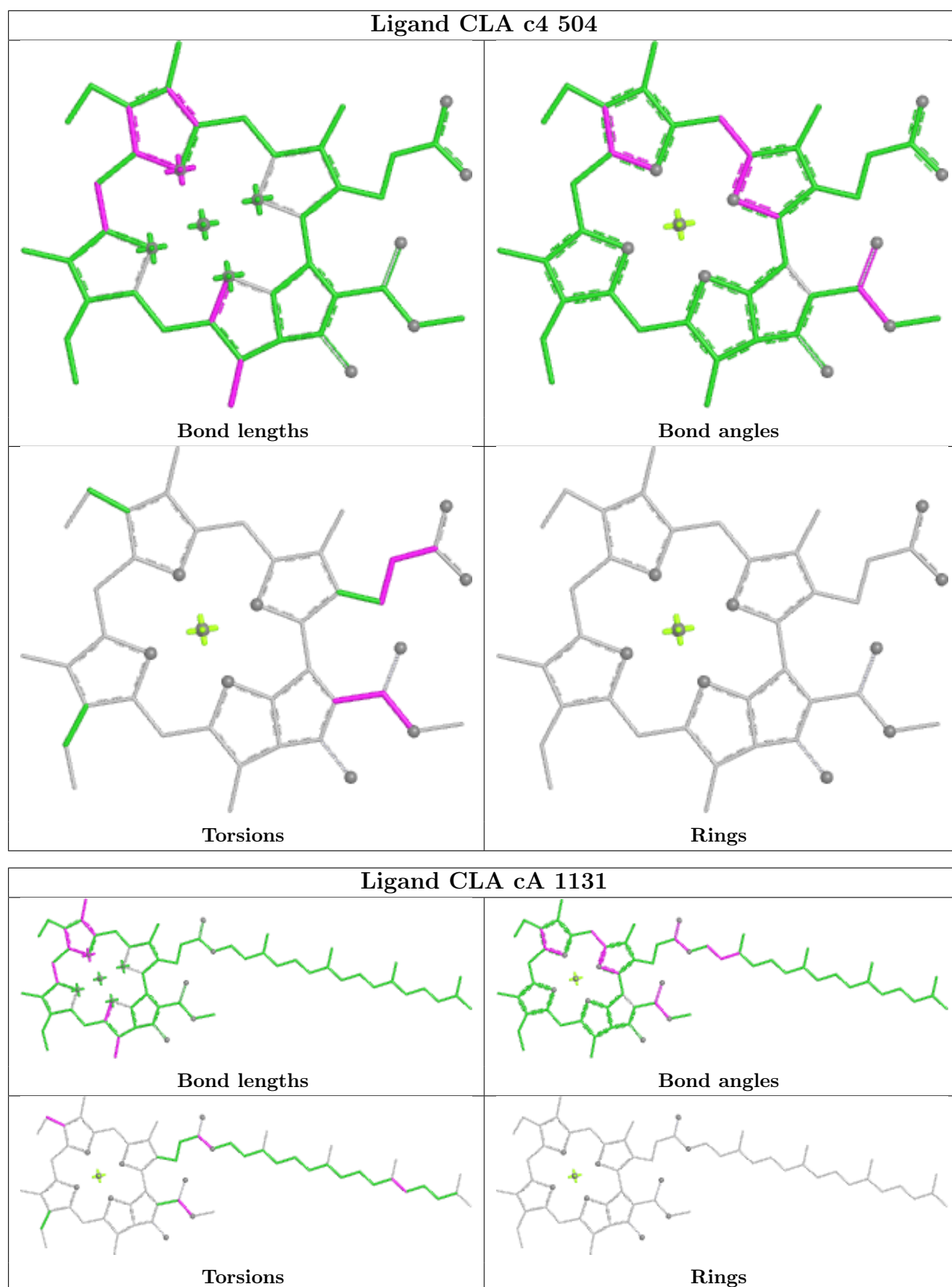
Bond angles



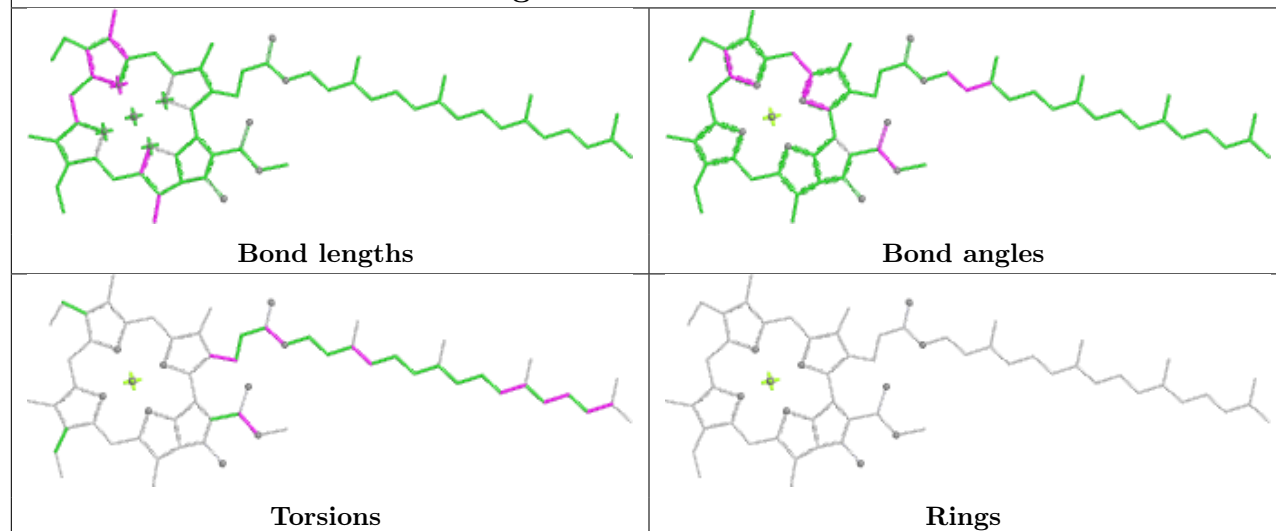
Torsions



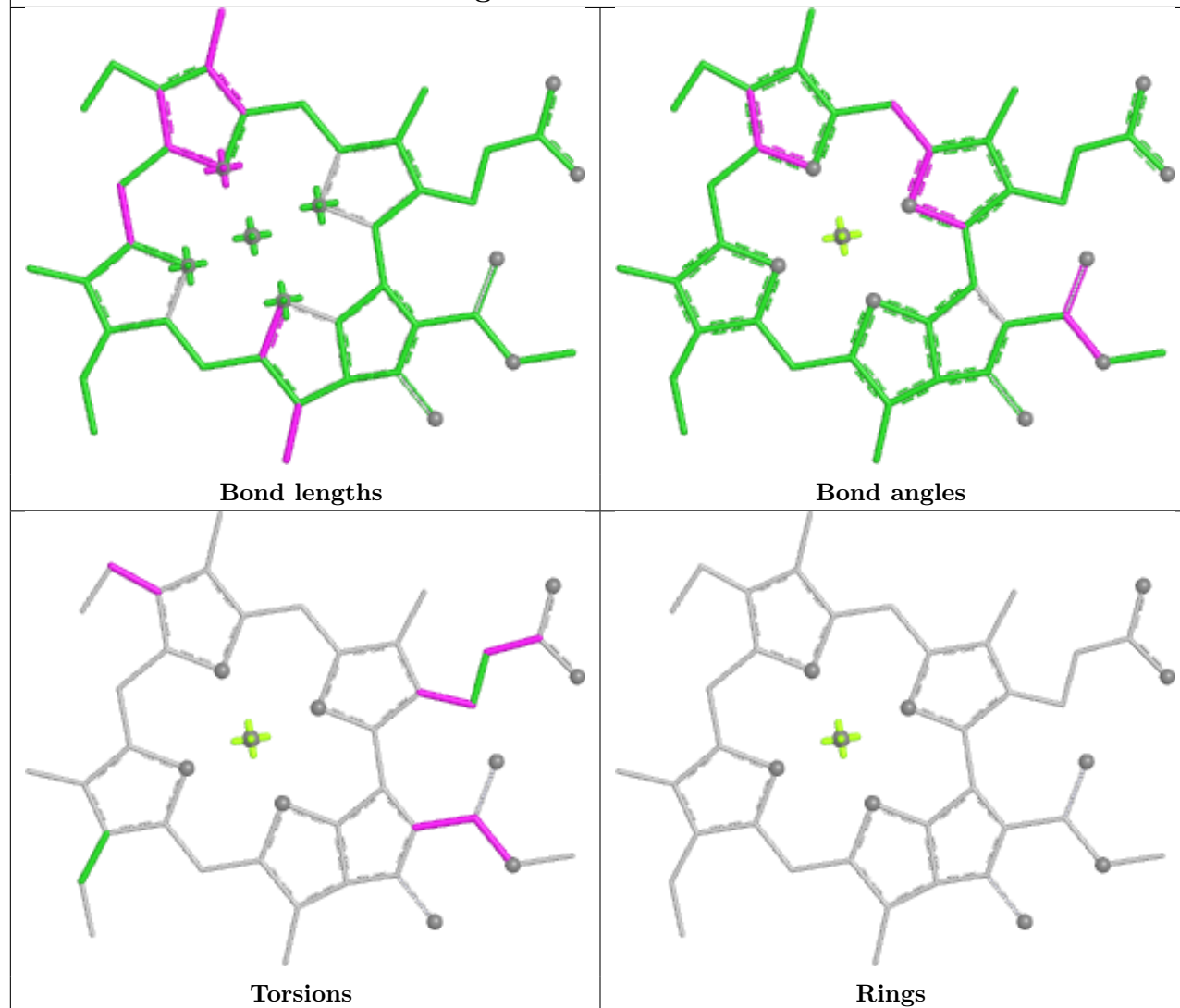
Rings

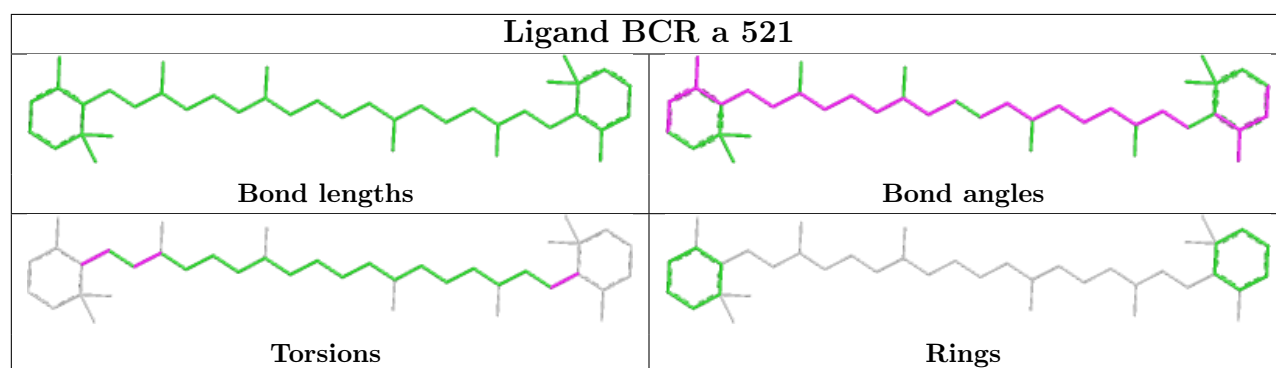
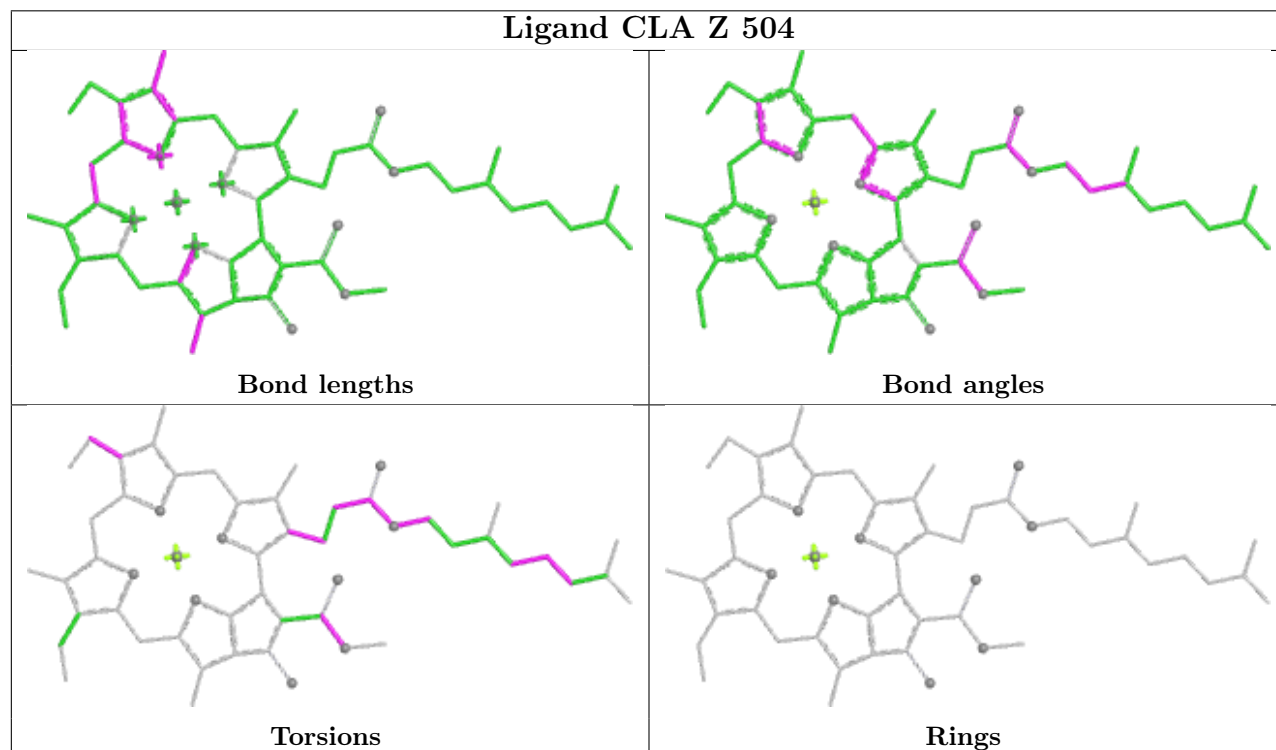
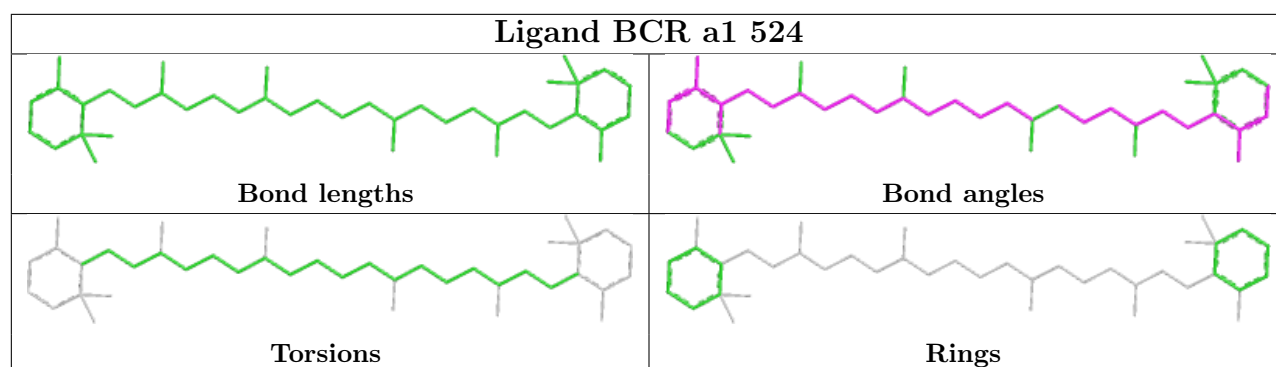


Ligand CLA bA 1117

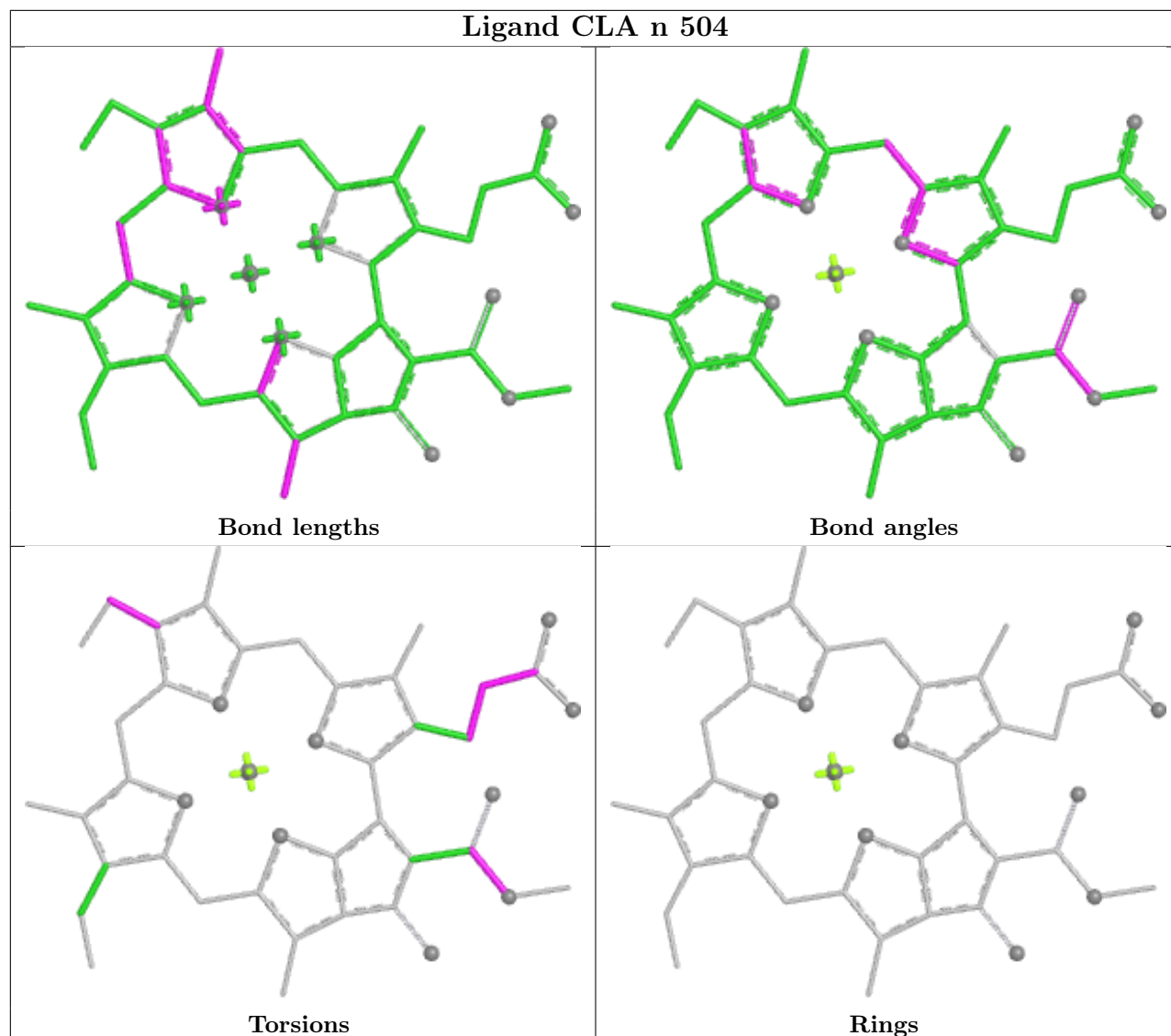


Ligand CLA bB 1232

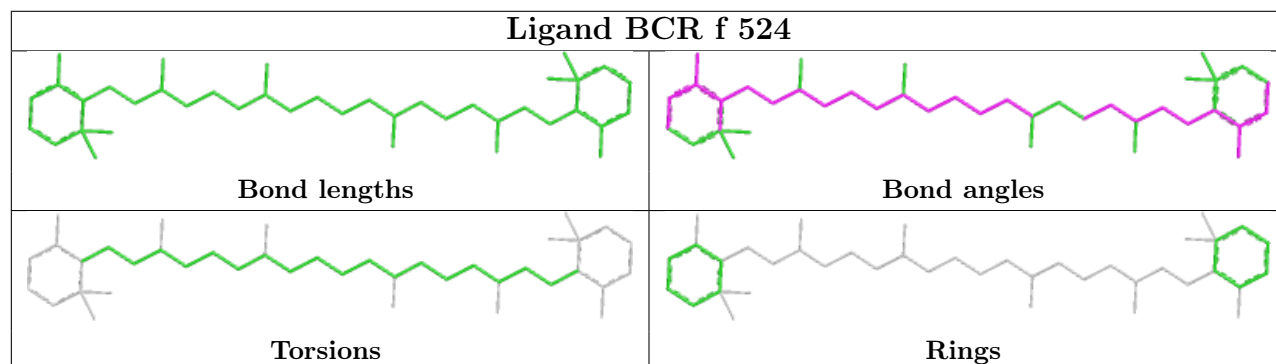




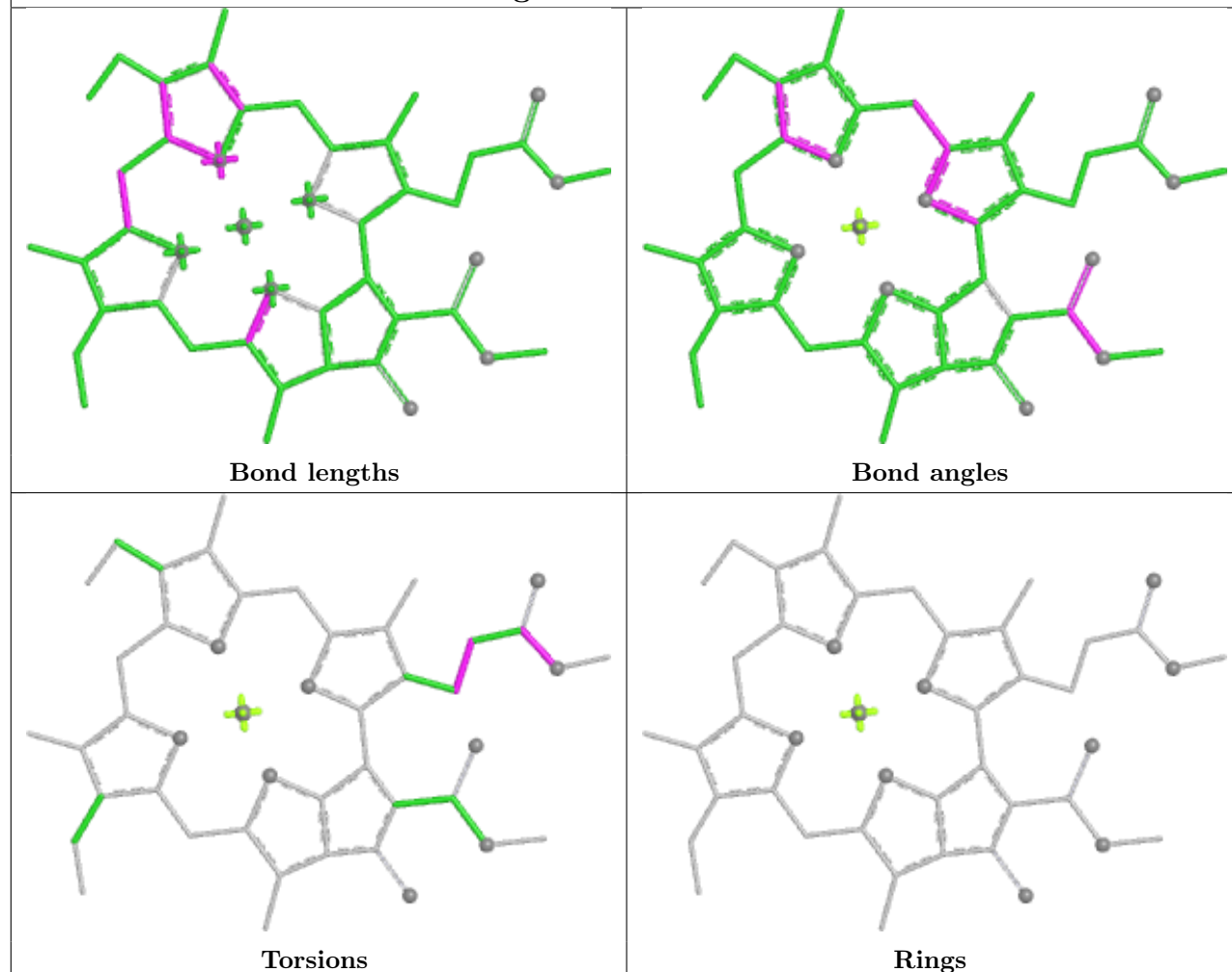
Ligand CLA n 504



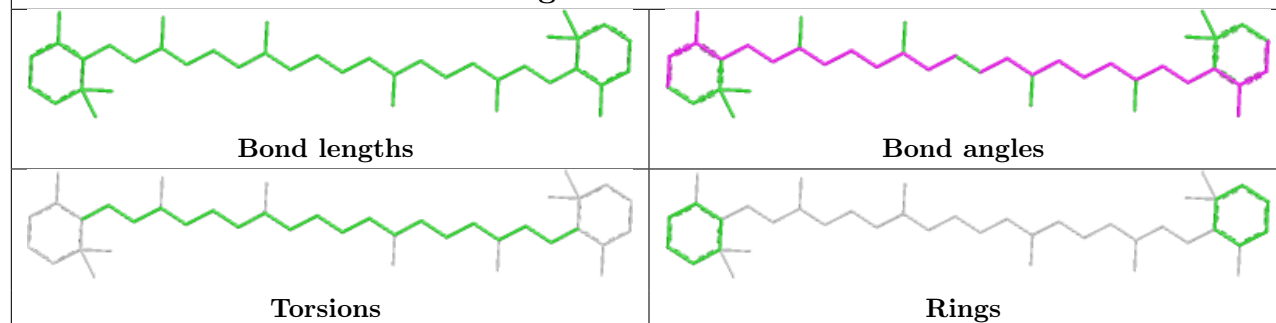
Ligand BCR f 524



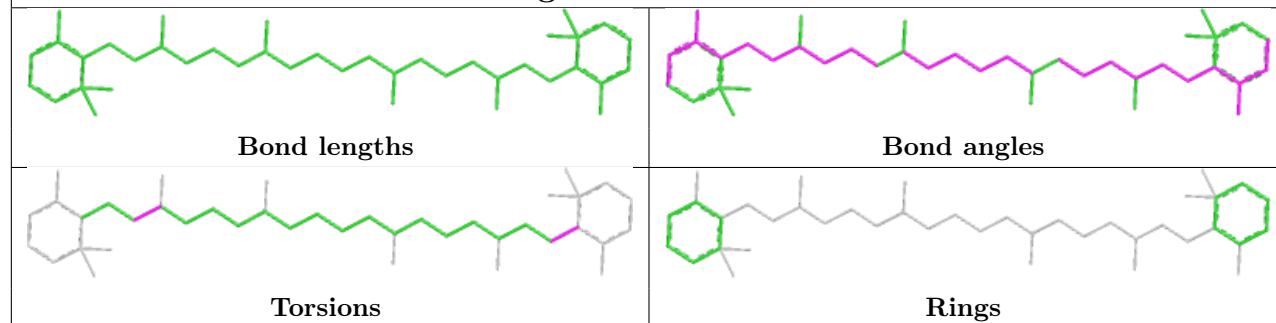
Ligand CLA X 513

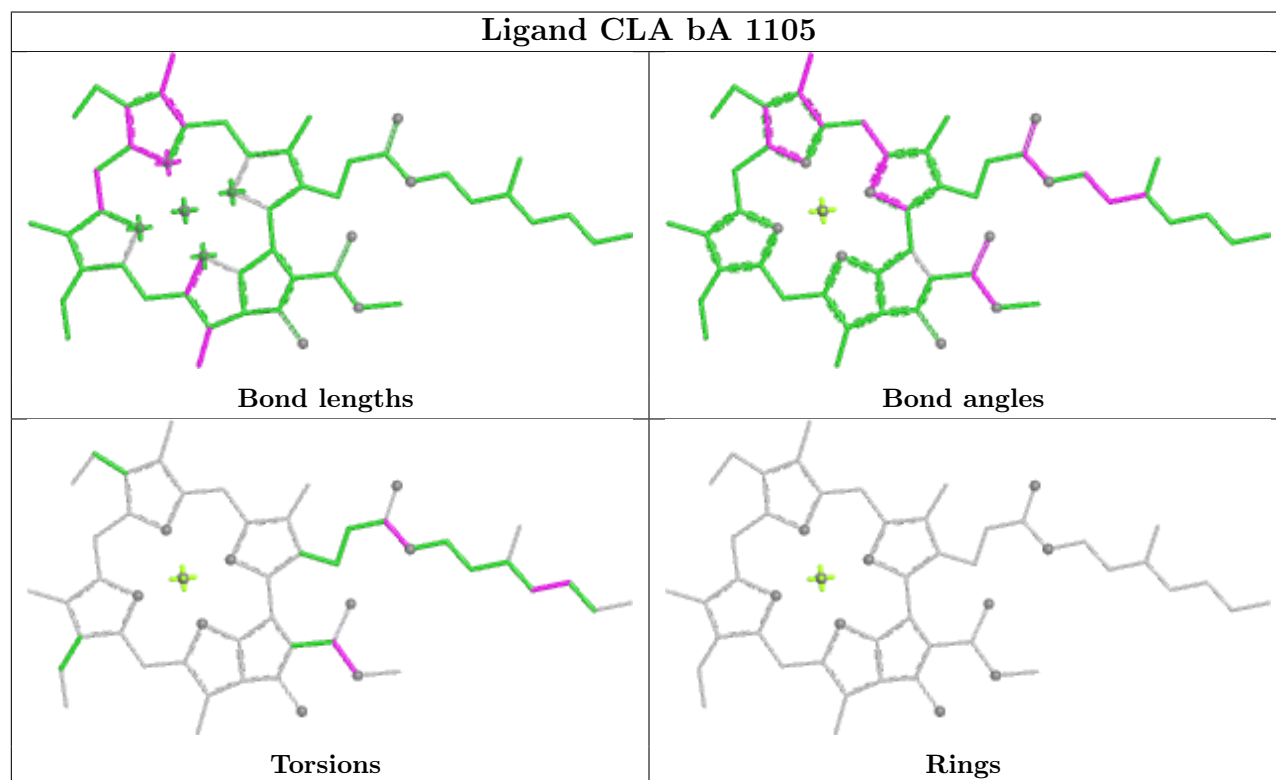
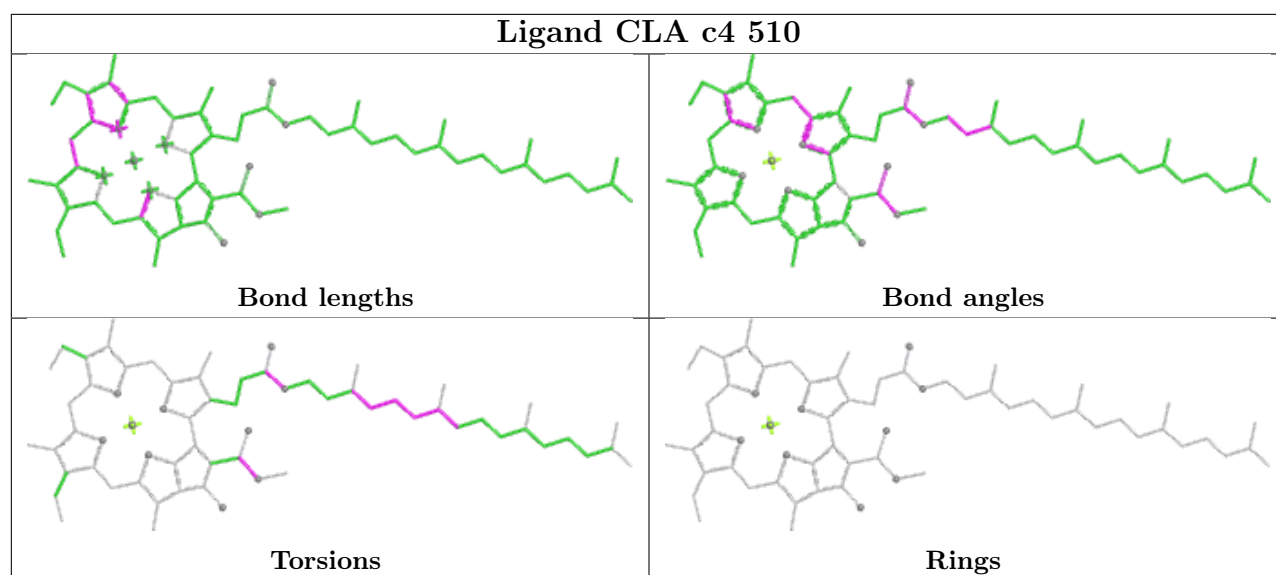


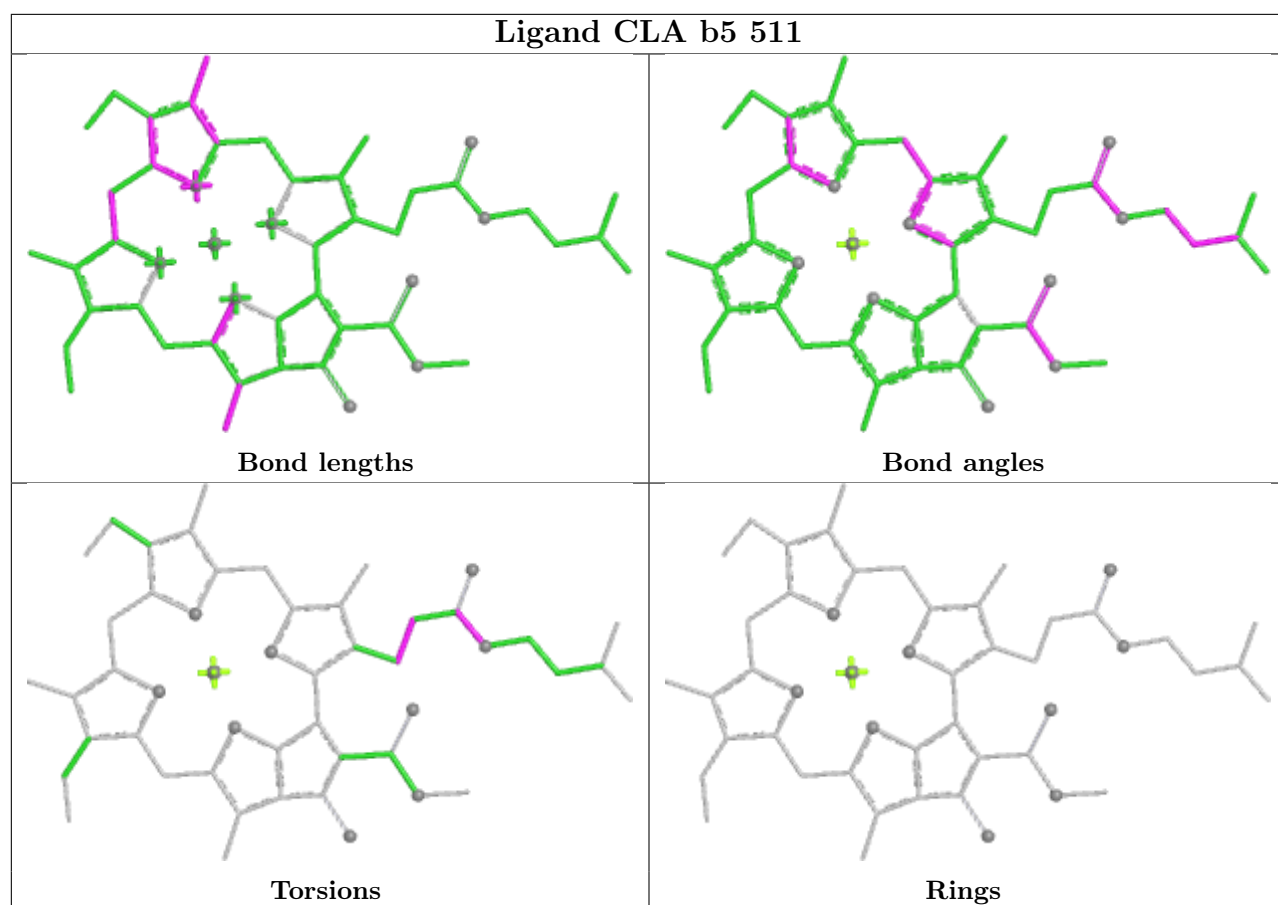
Ligand BCR i 524



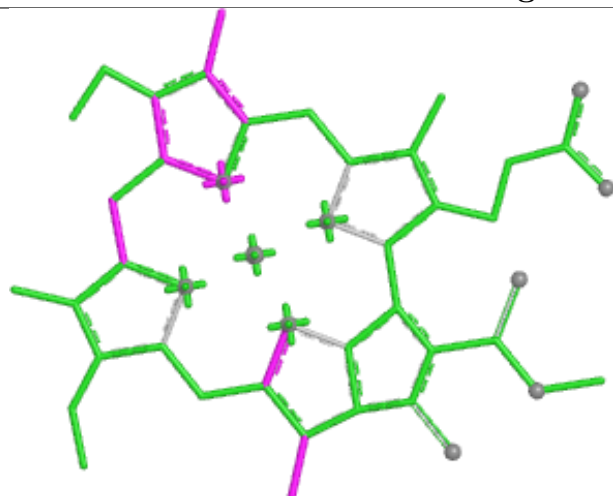
Ligand BCR f 523



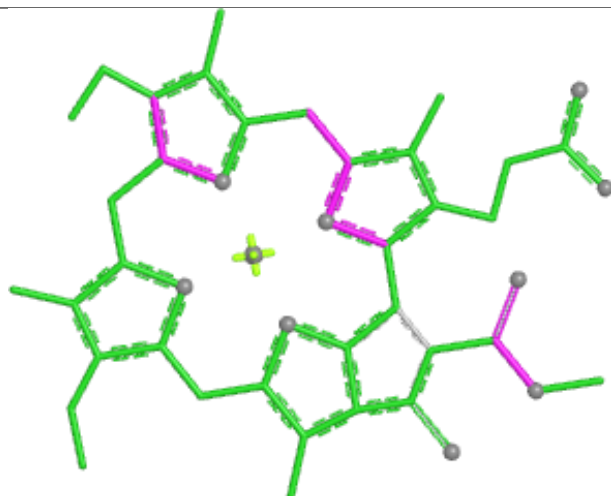




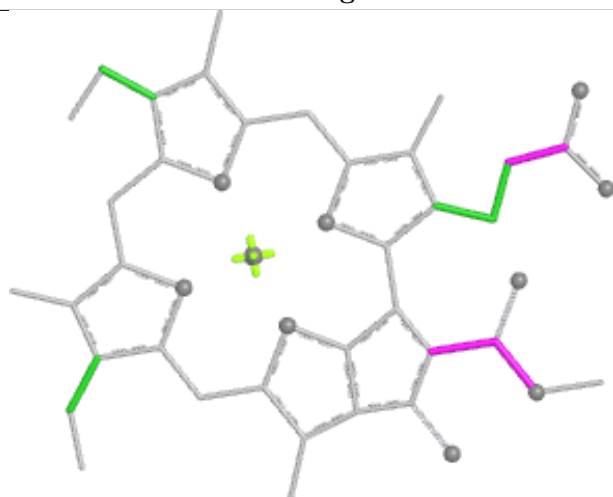
Ligand CLA k 506



Bond lengths



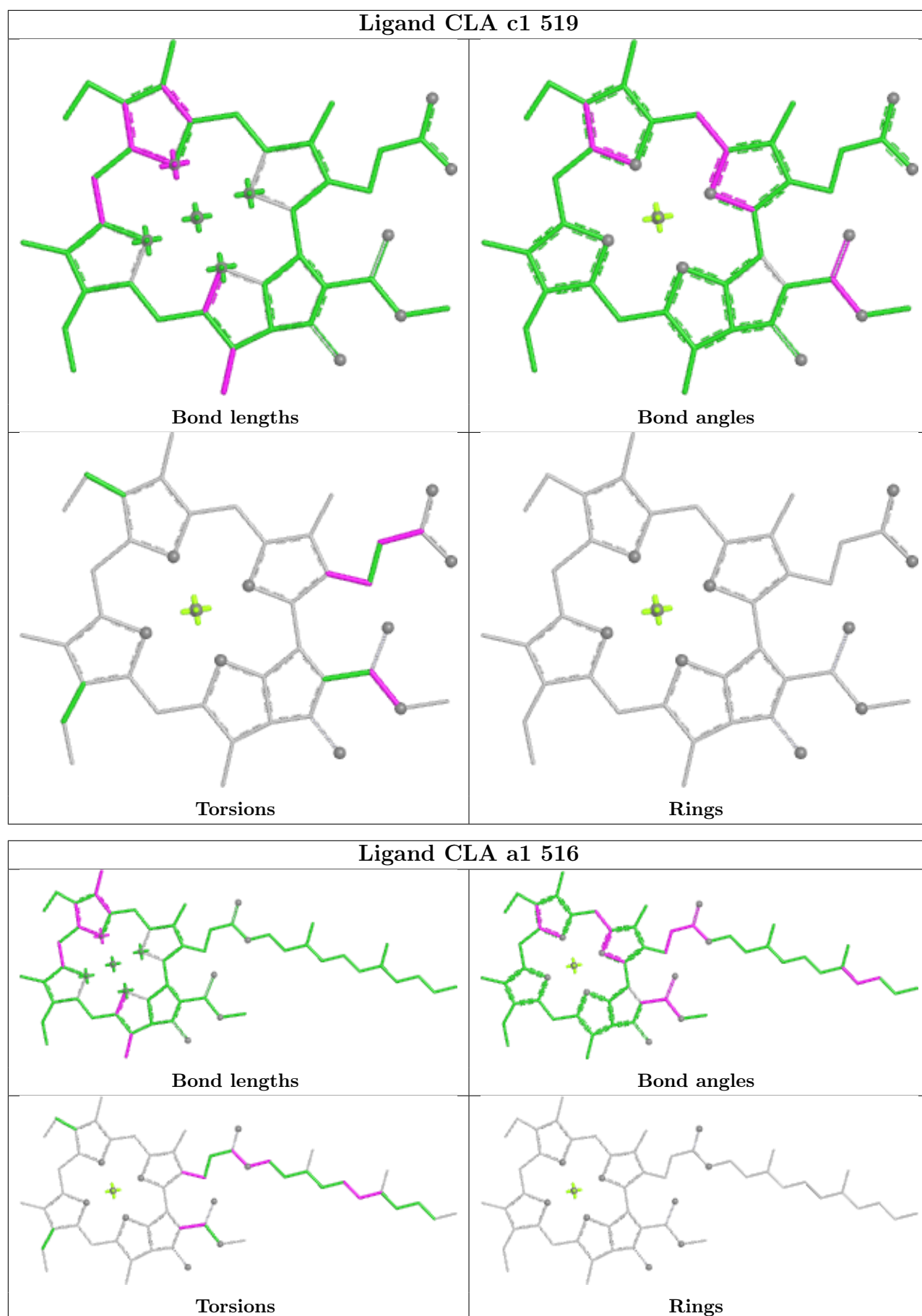
Bond angles

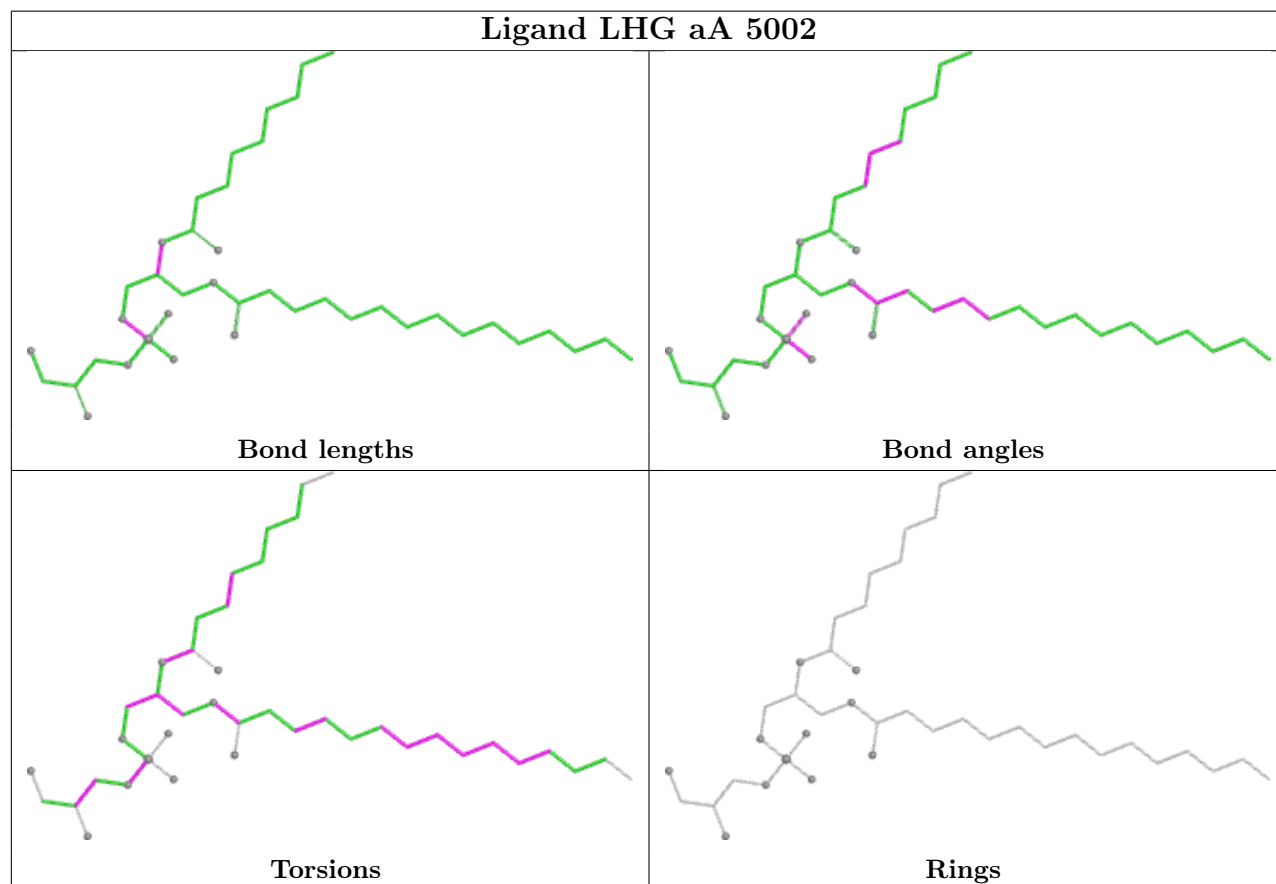
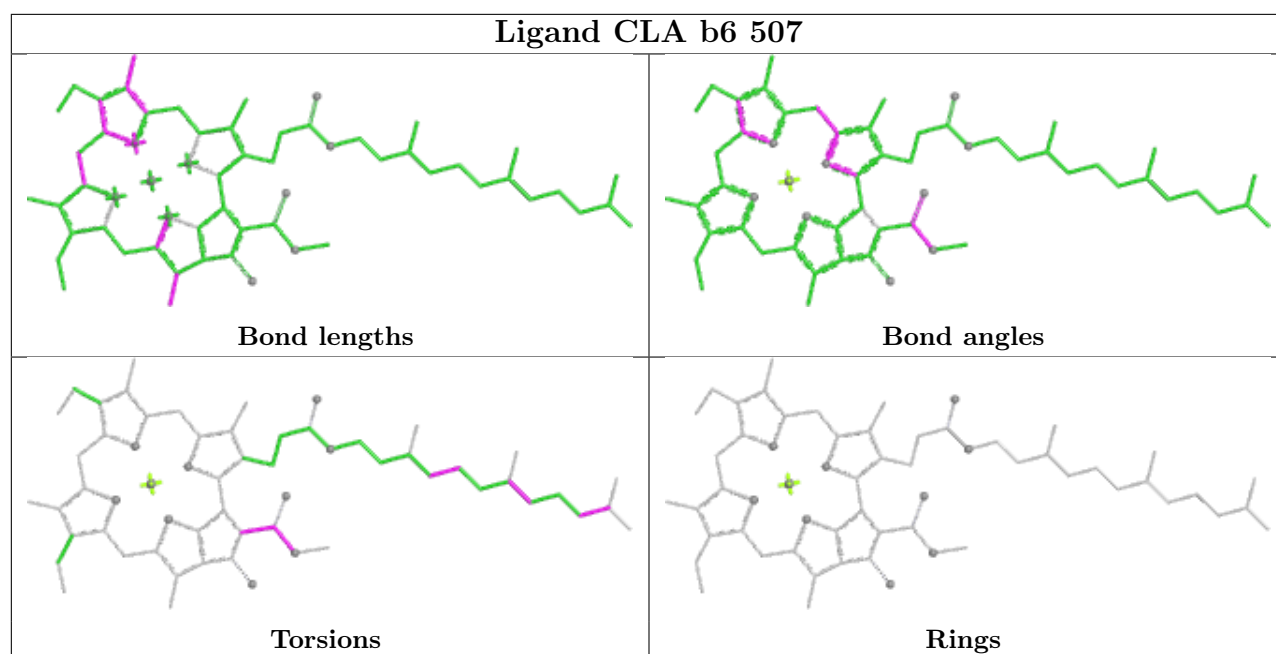


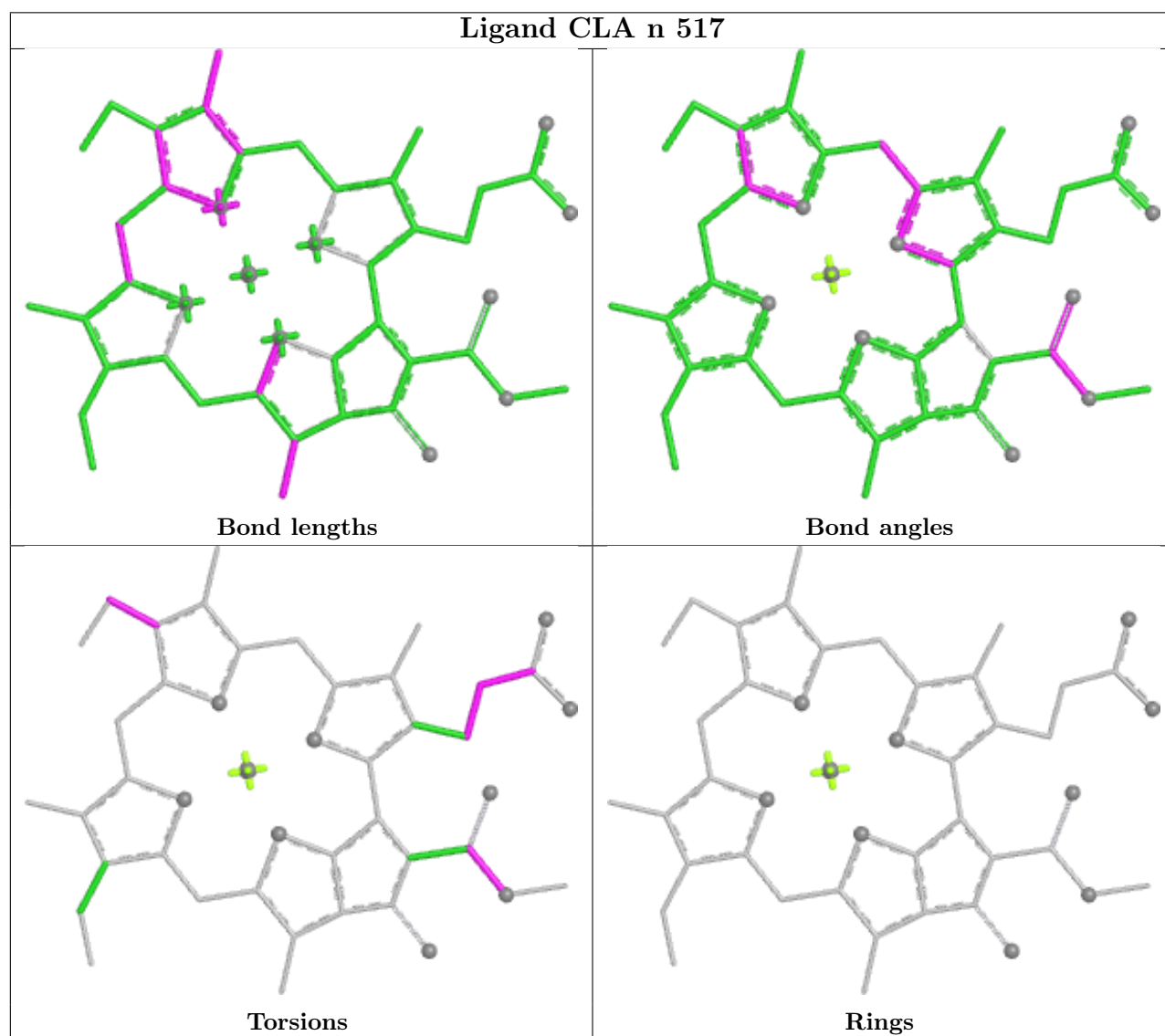
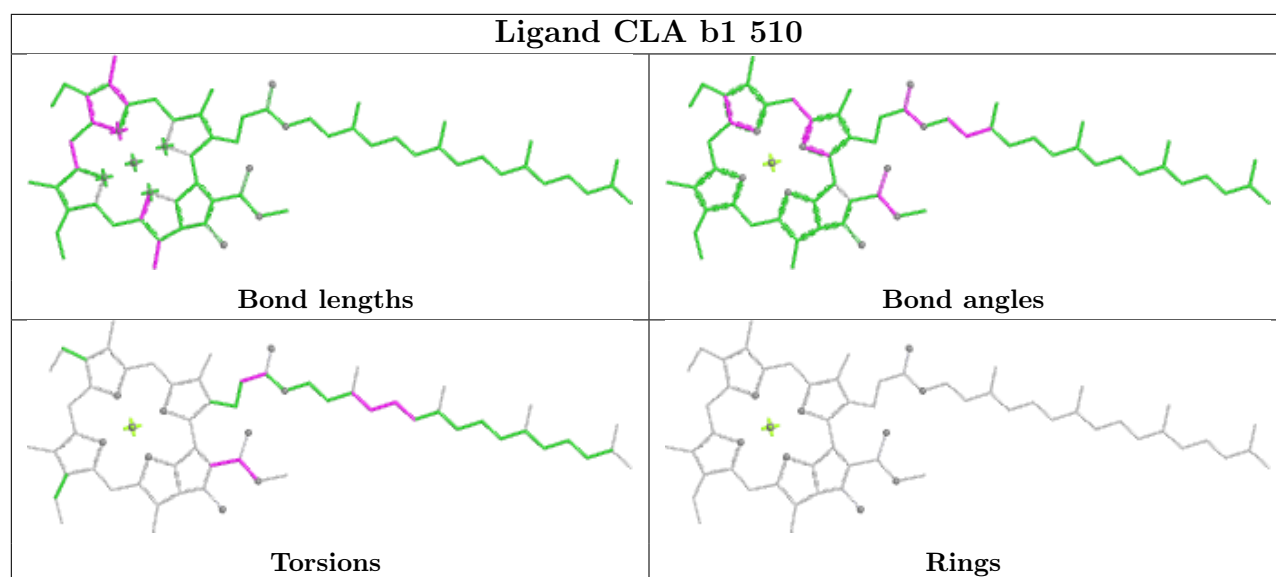
Torsions



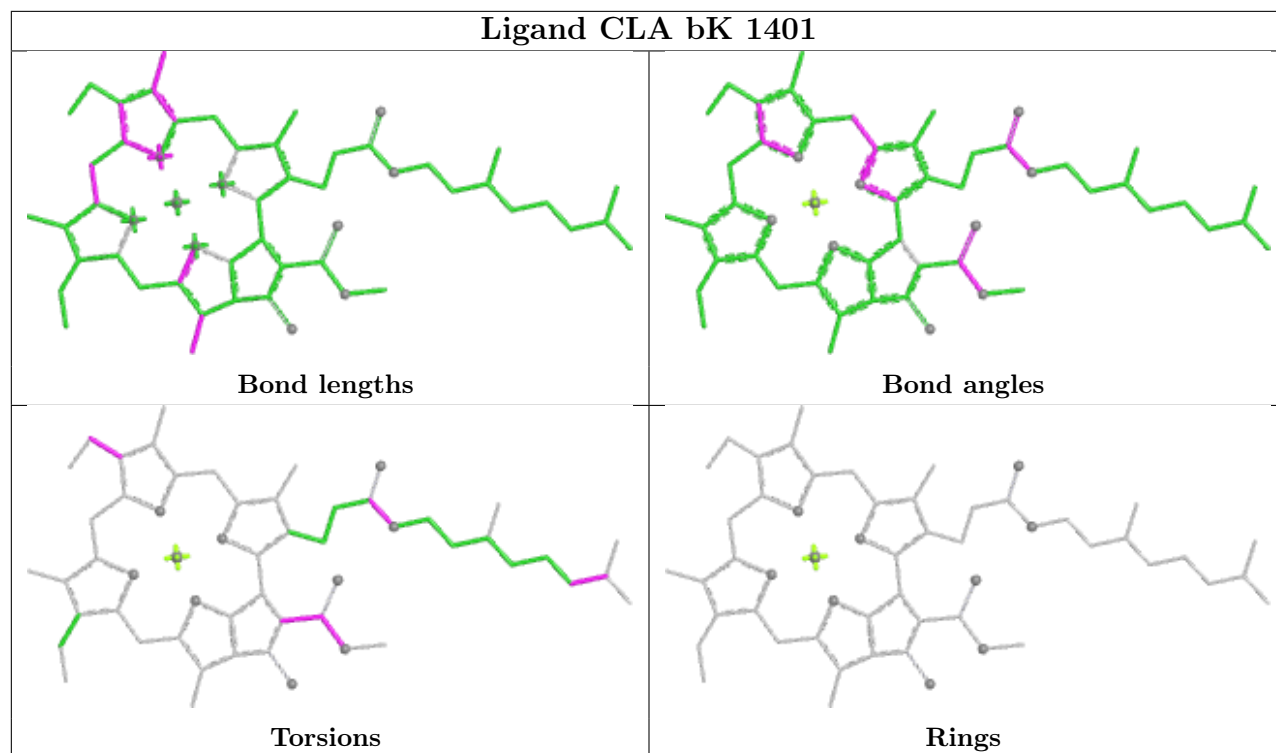
Rings



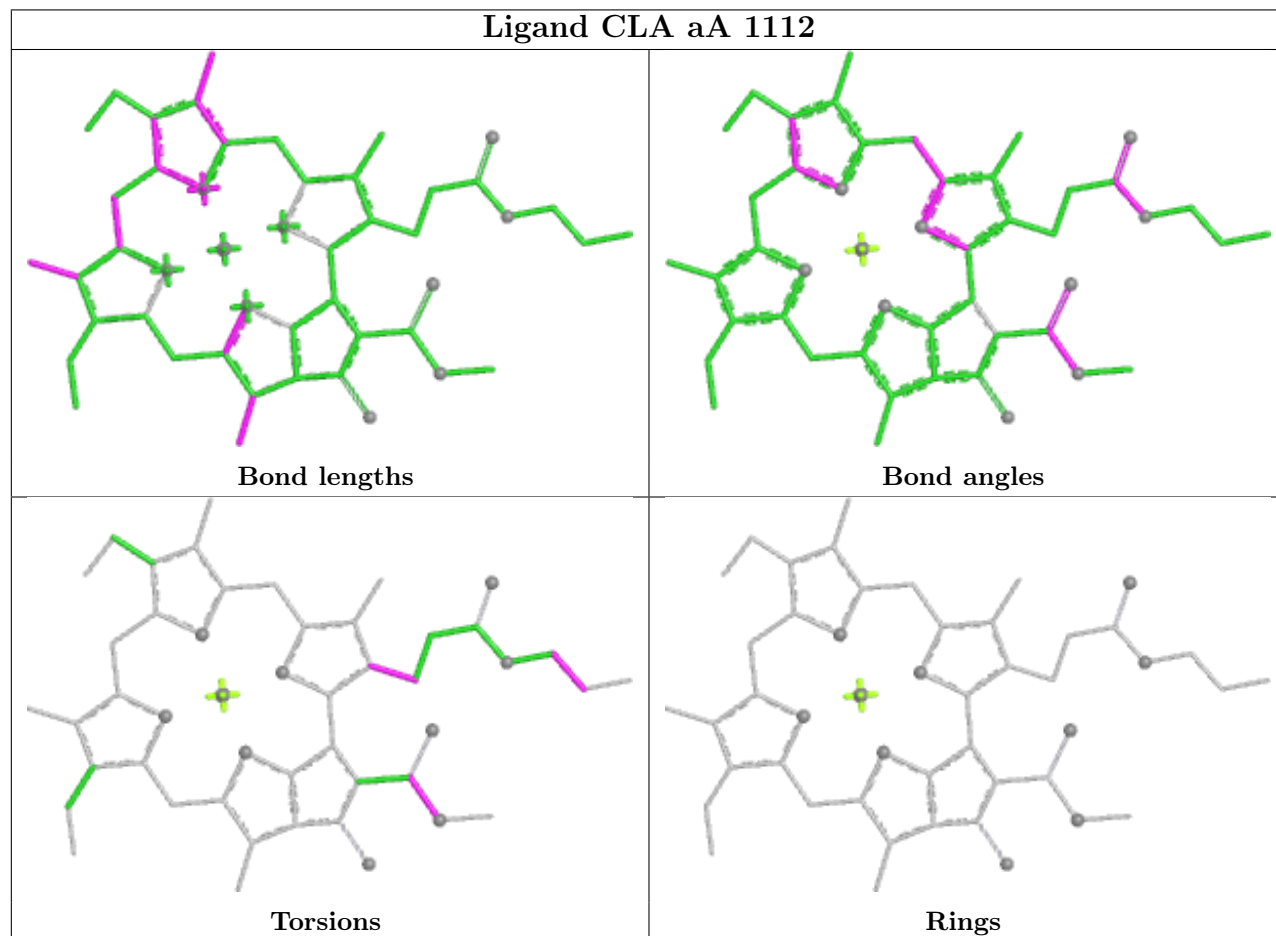


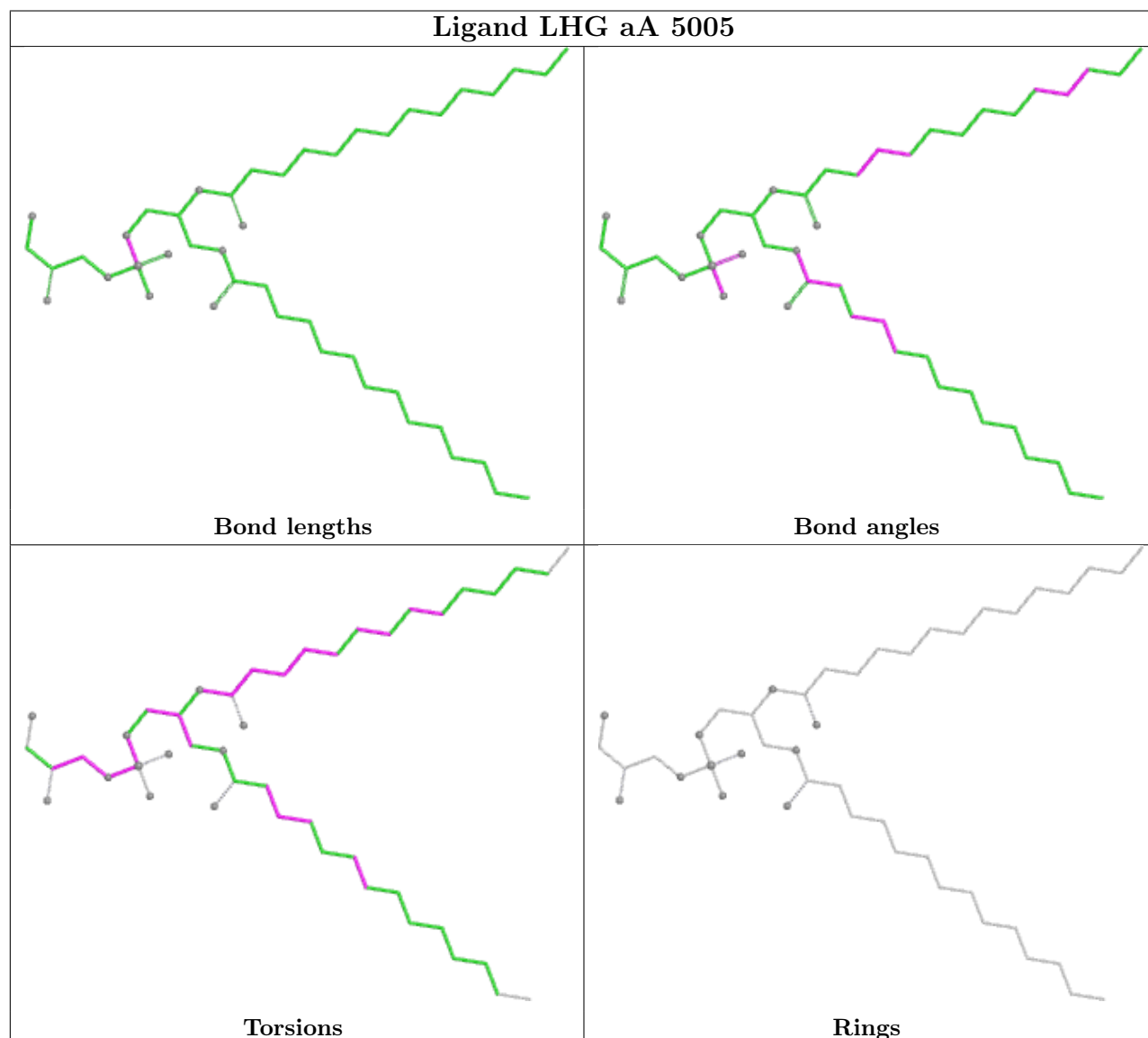
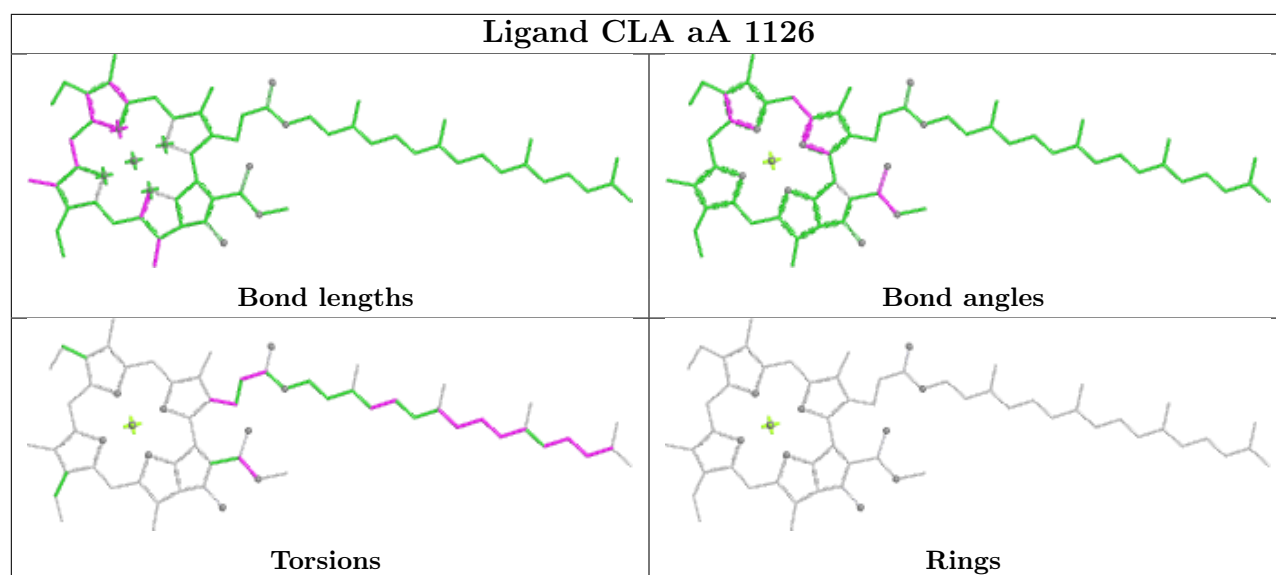


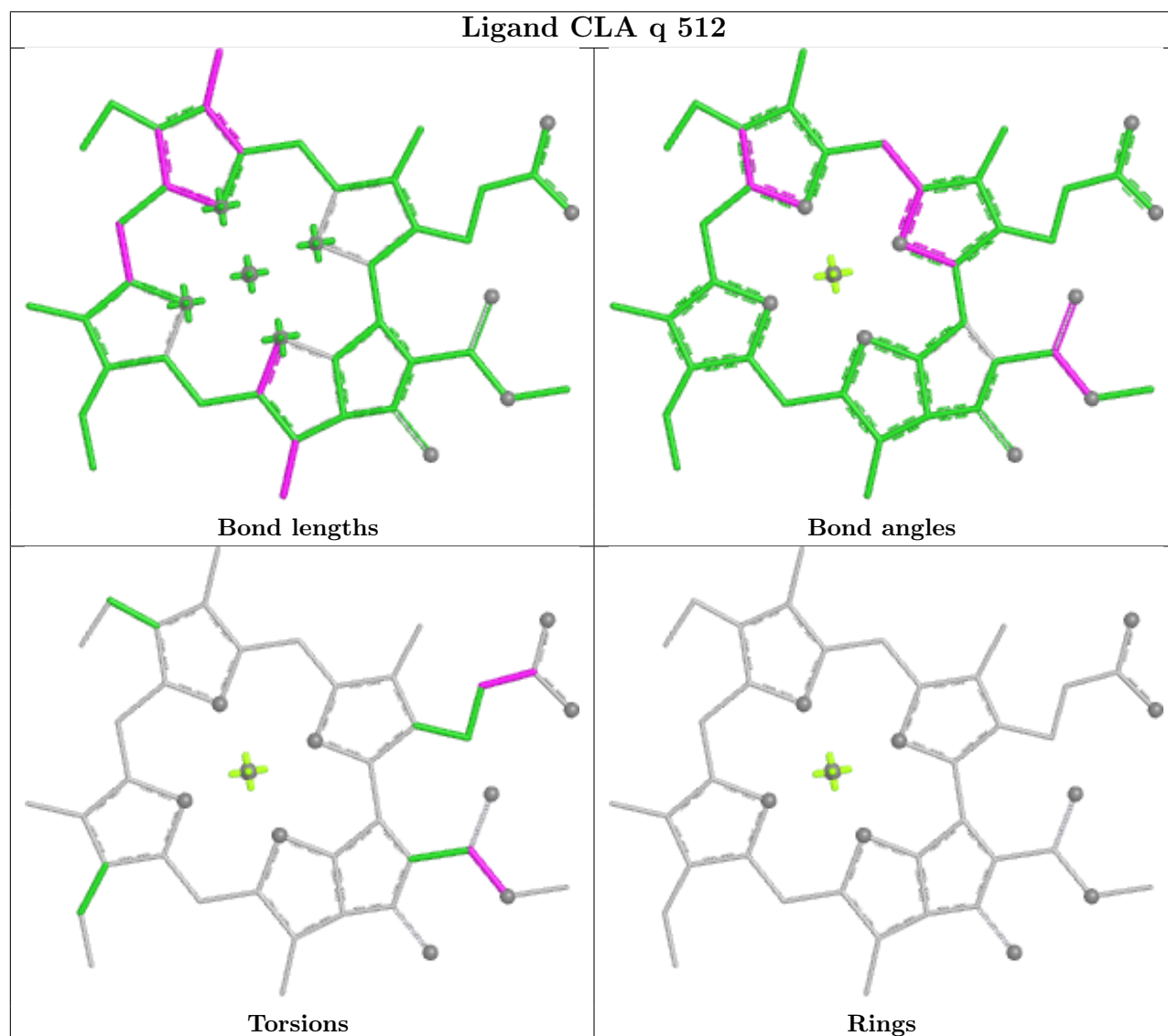
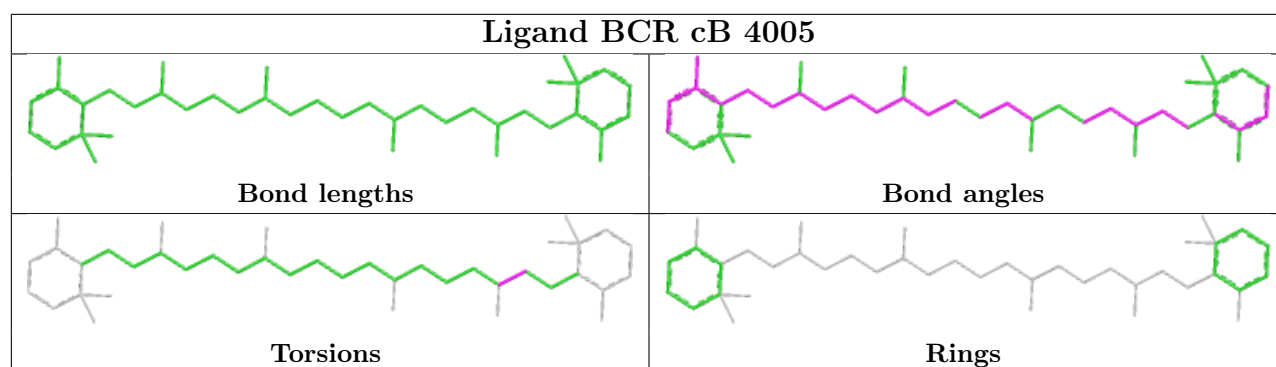
Ligand CLA bK 1401



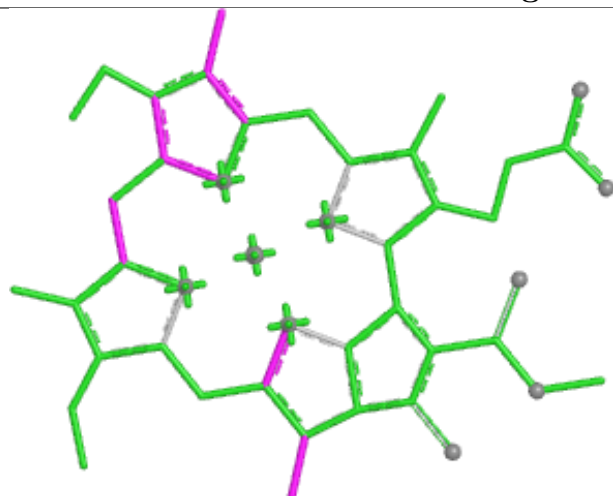
Ligand CLA aA 1112



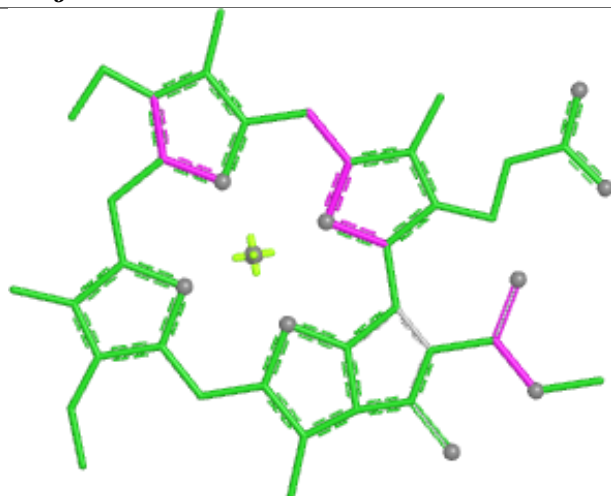




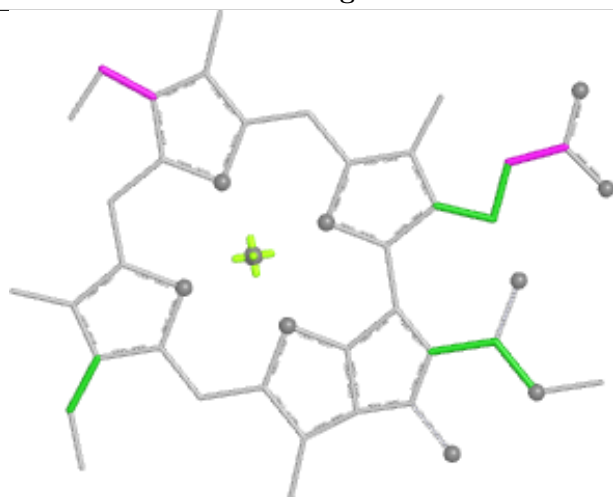
Ligand CLA j 504



Bond lengths



Bond angles

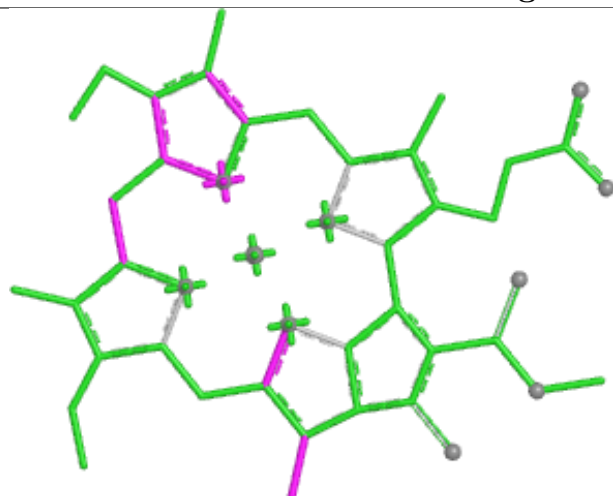


Torsions

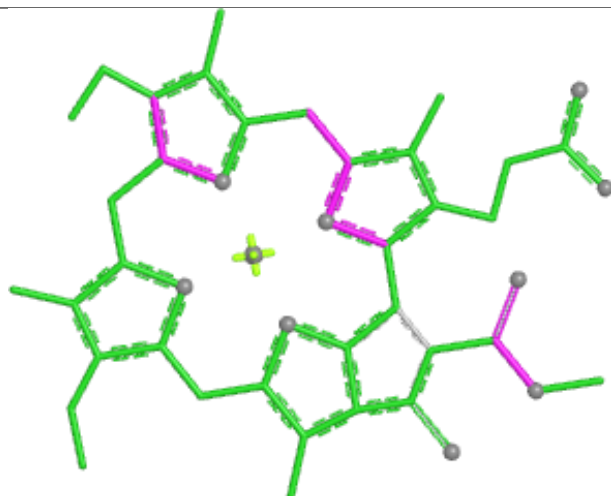


Rings

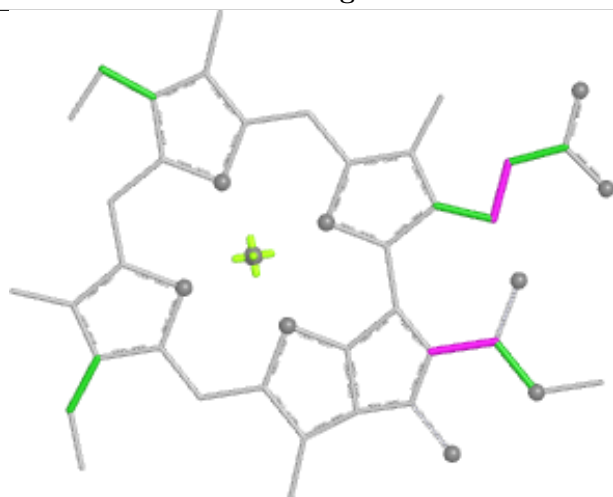
Ligand CLA o 513



Bond lengths



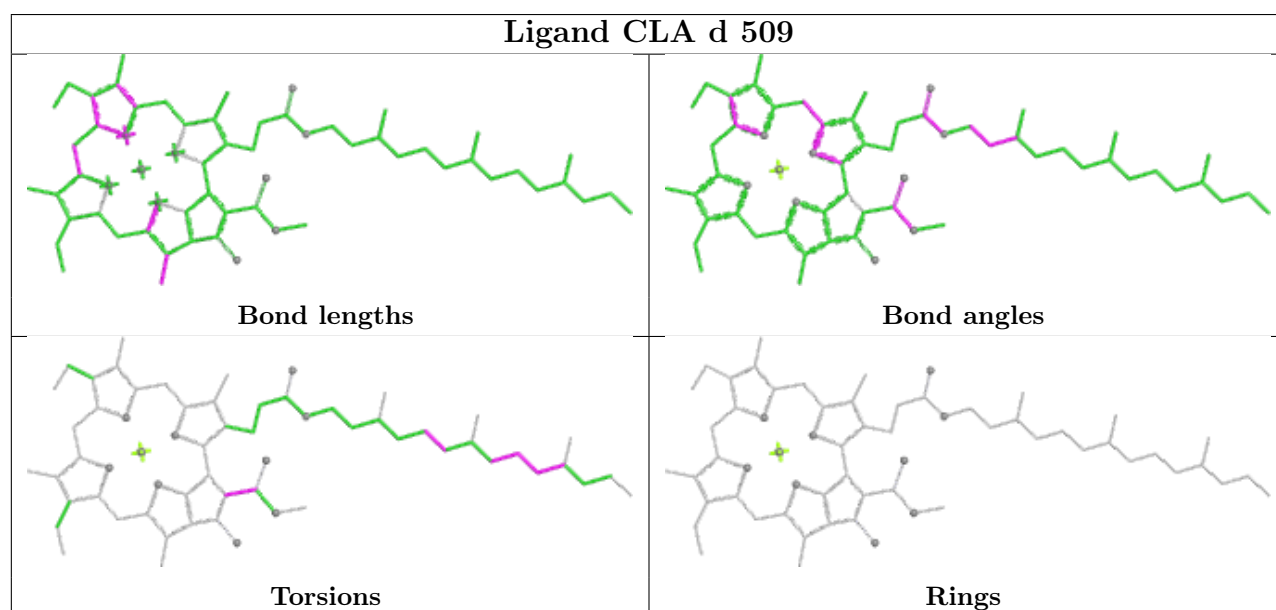
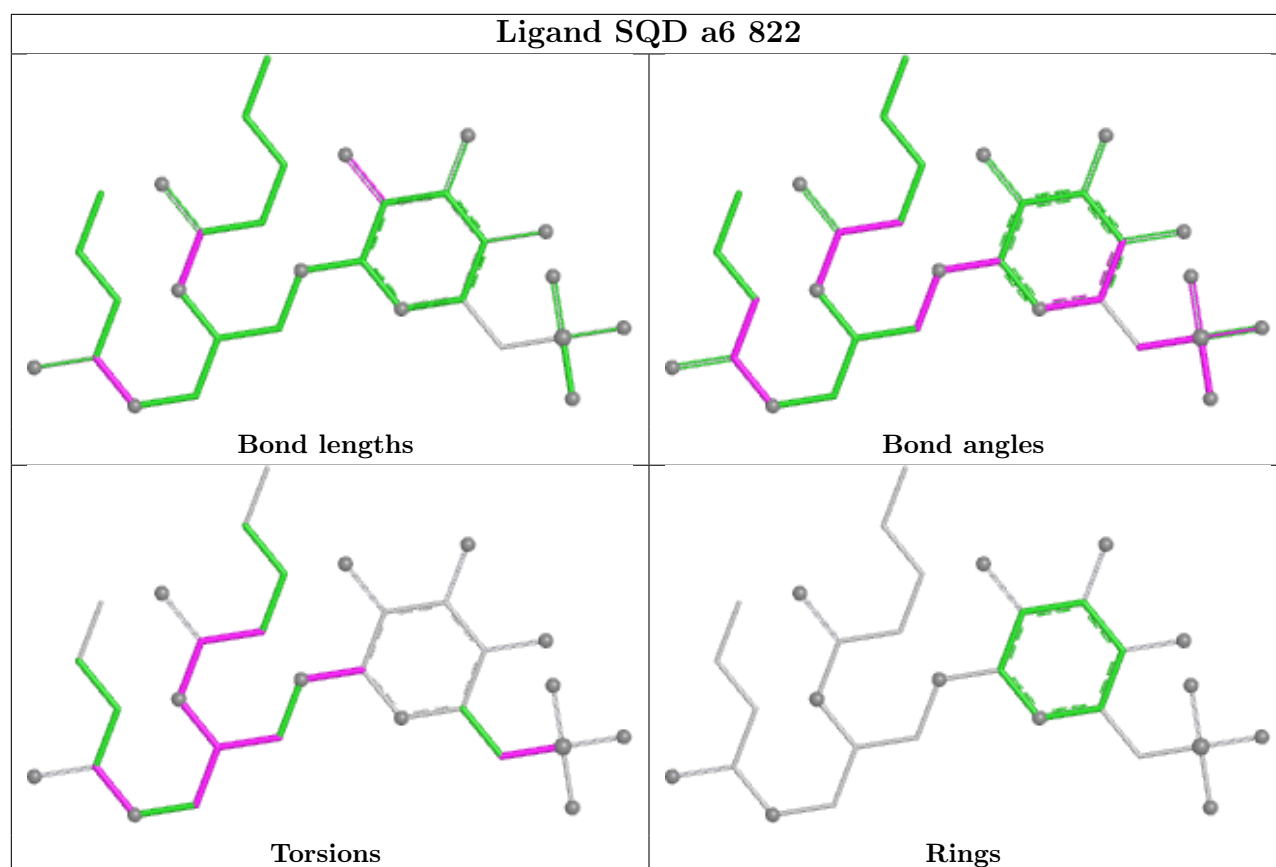
Bond angles

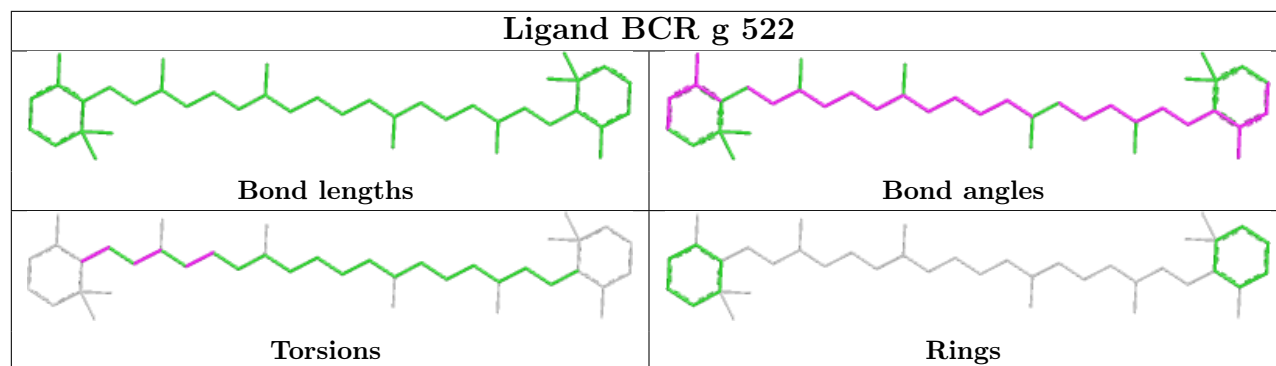


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

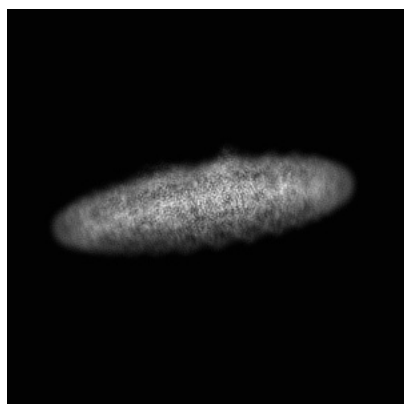
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63527. These allow visual inspection of the internal detail of the map and identification of artifacts.

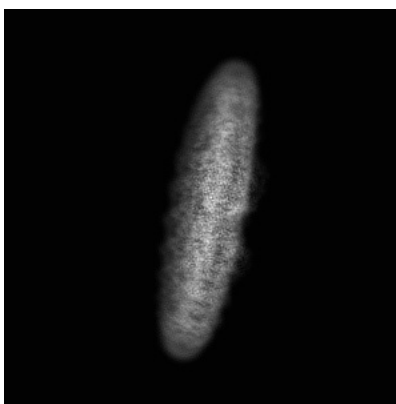
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

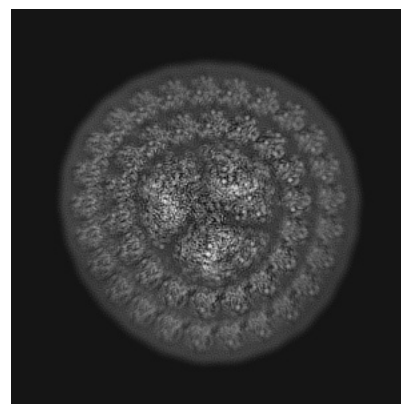
6.1.1 Primary map



X



Y

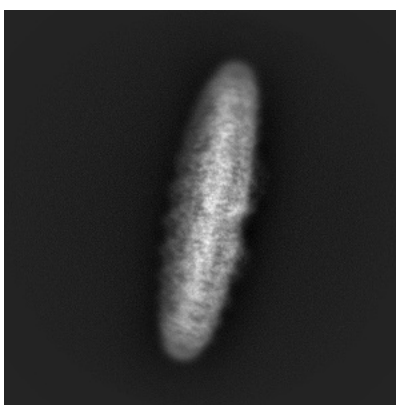


Z

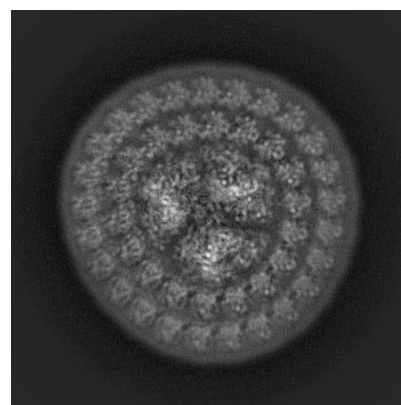
6.1.2 Raw map



X



Y

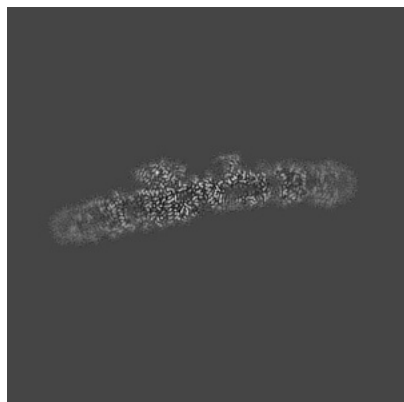


Z

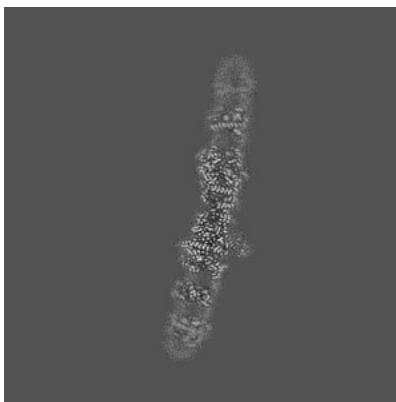
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

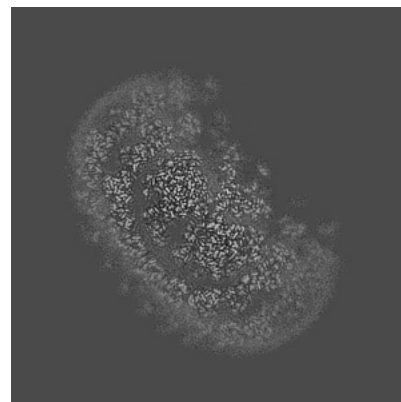
6.2.1 Primary map



X Index: 260

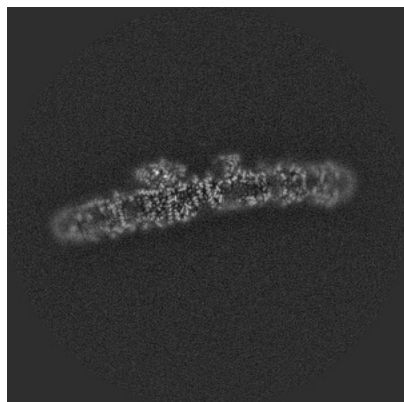


Y Index: 260

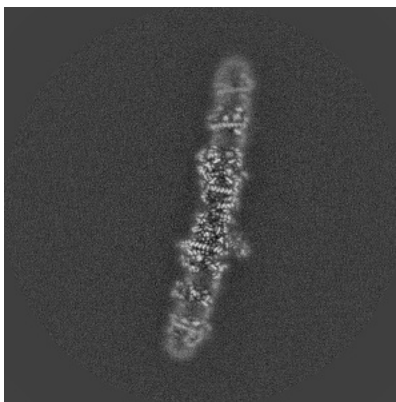


Z Index: 260

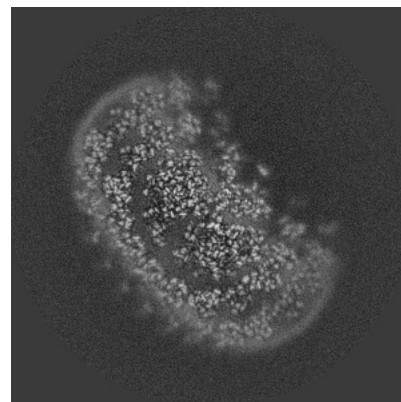
6.2.2 Raw map



X Index: 260



Y Index: 260

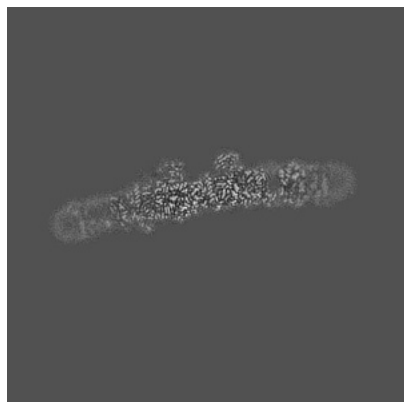


Z Index: 260

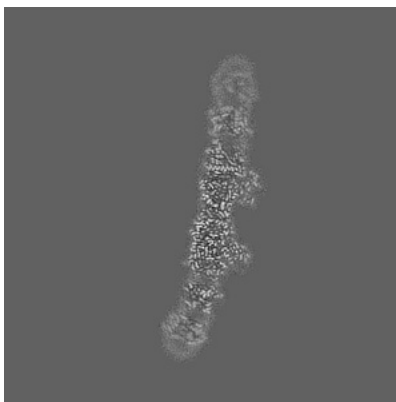
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

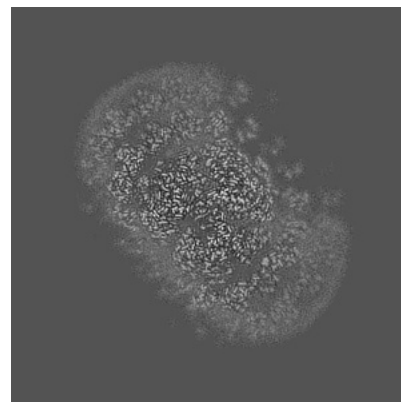
6.3.1 Primary map



X Index: 270

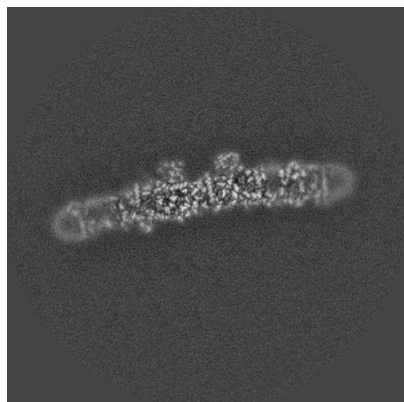


Y Index: 274

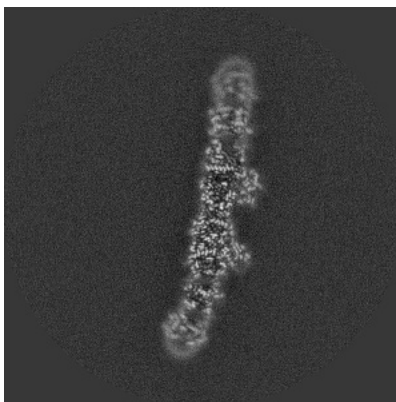


Z Index: 269

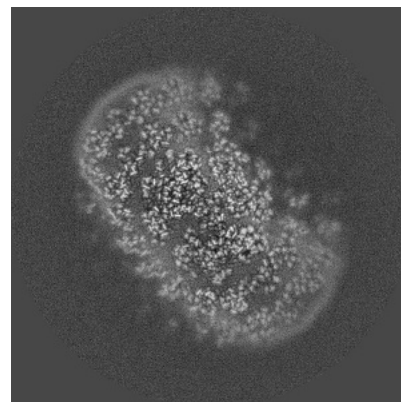
6.3.2 Raw map



X Index: 270



Y Index: 275

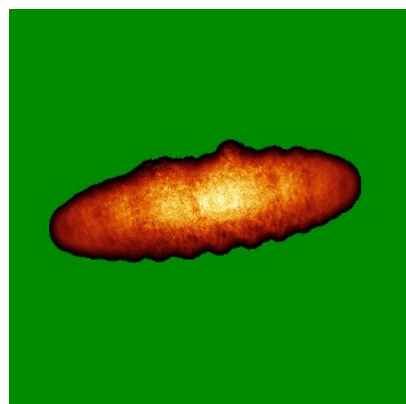


Z Index: 265

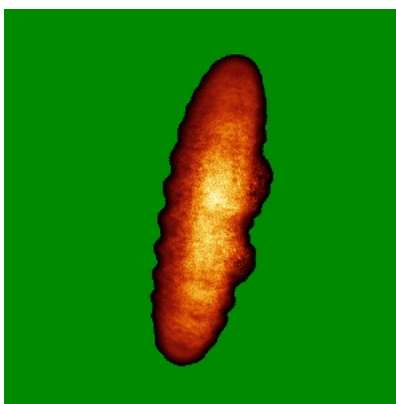
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

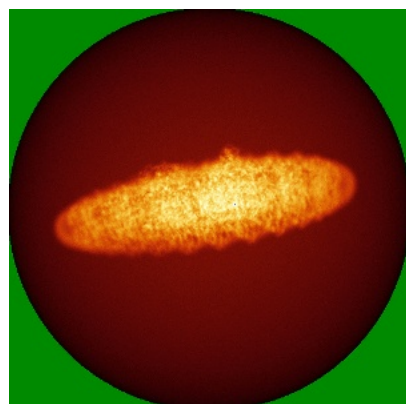


Y

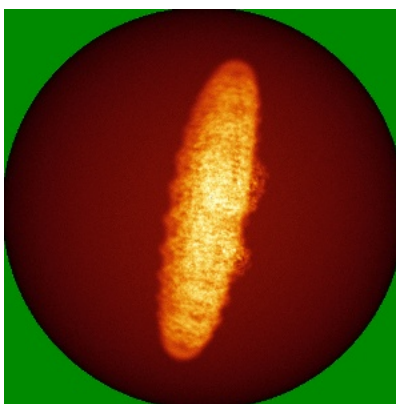


Z

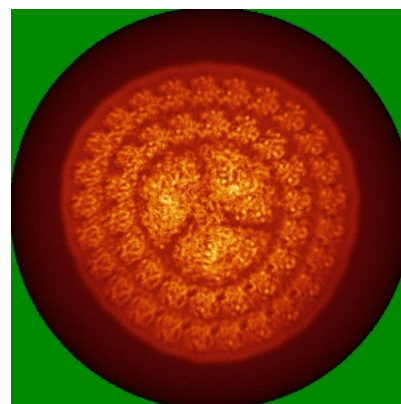
6.4.2 Raw map



X



Y

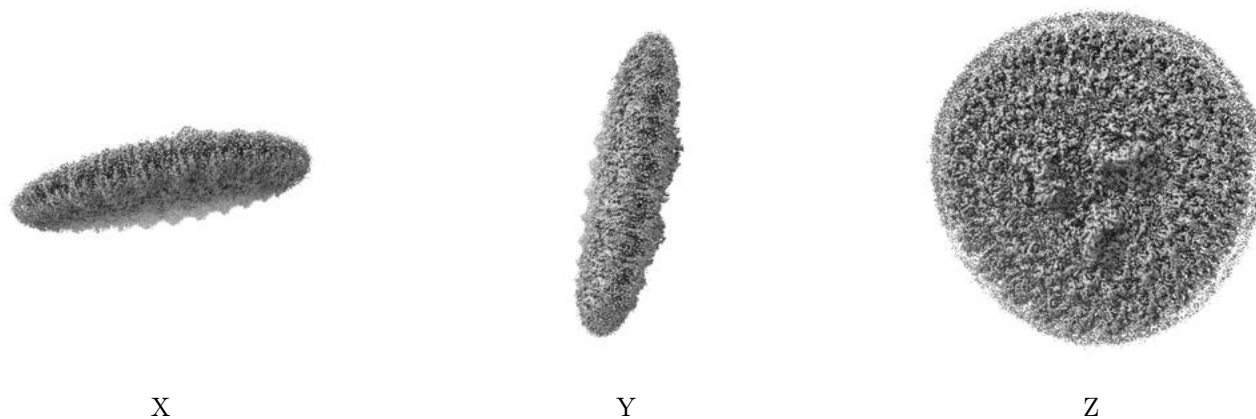


Z

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

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

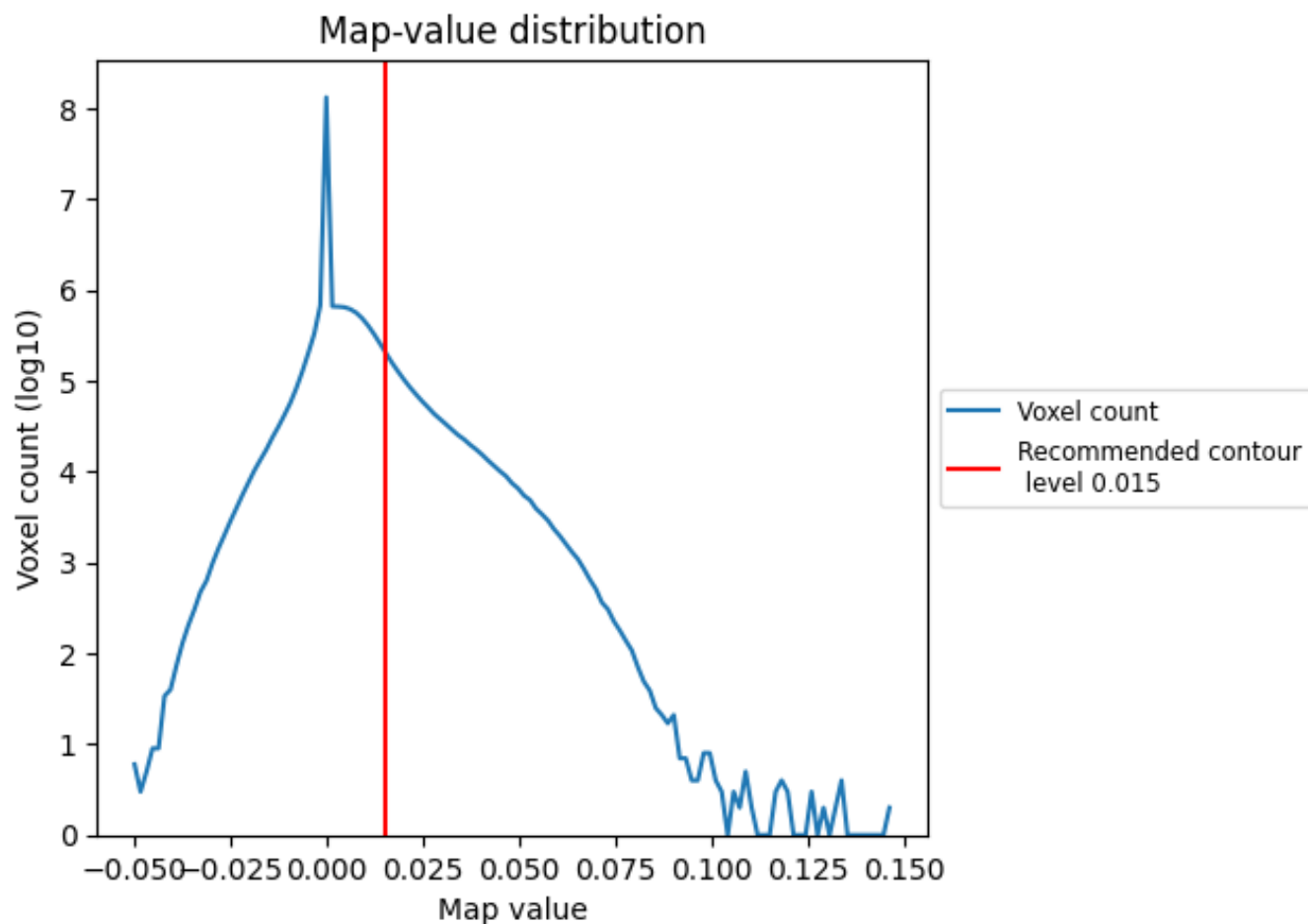
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

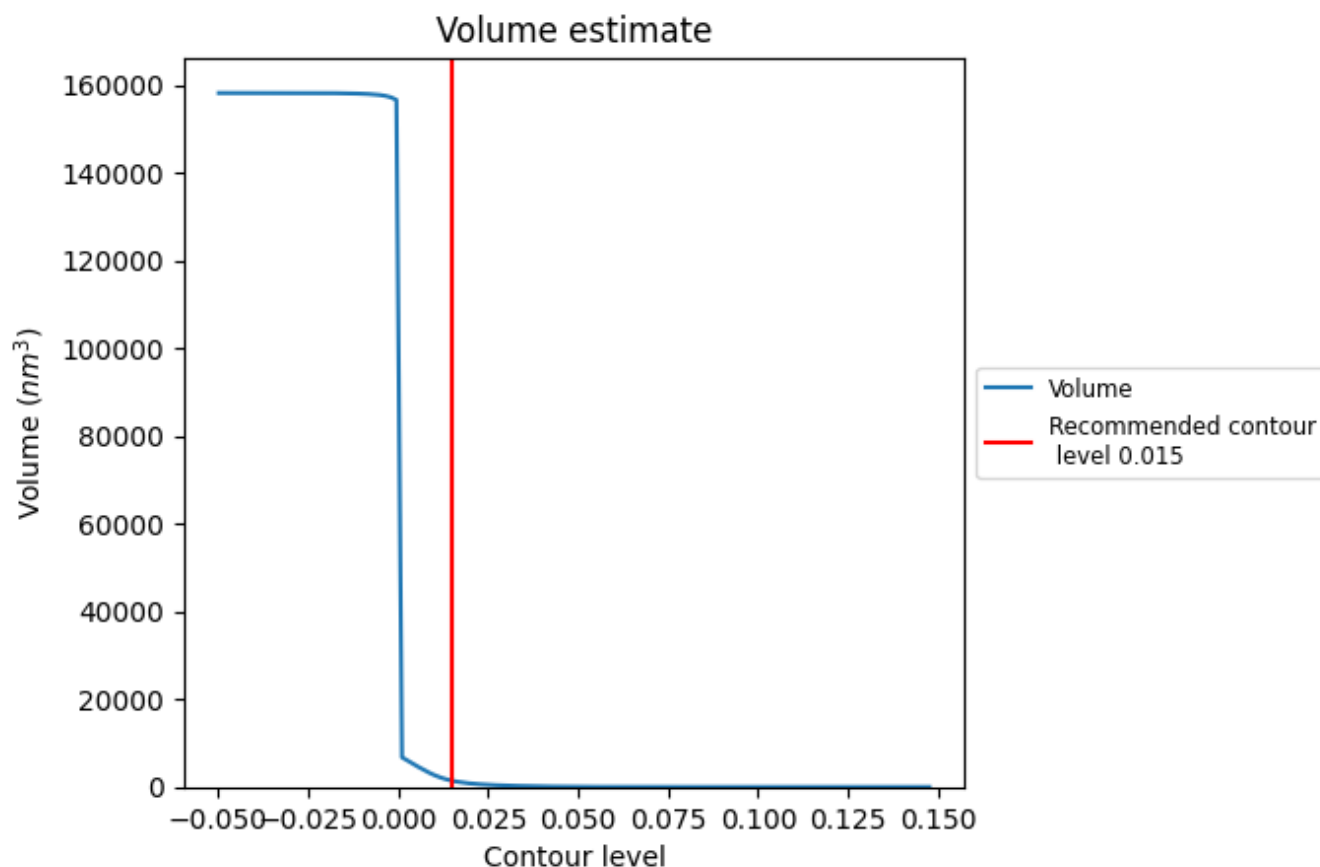
This section contains the results of statistical analysis of the map.

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.

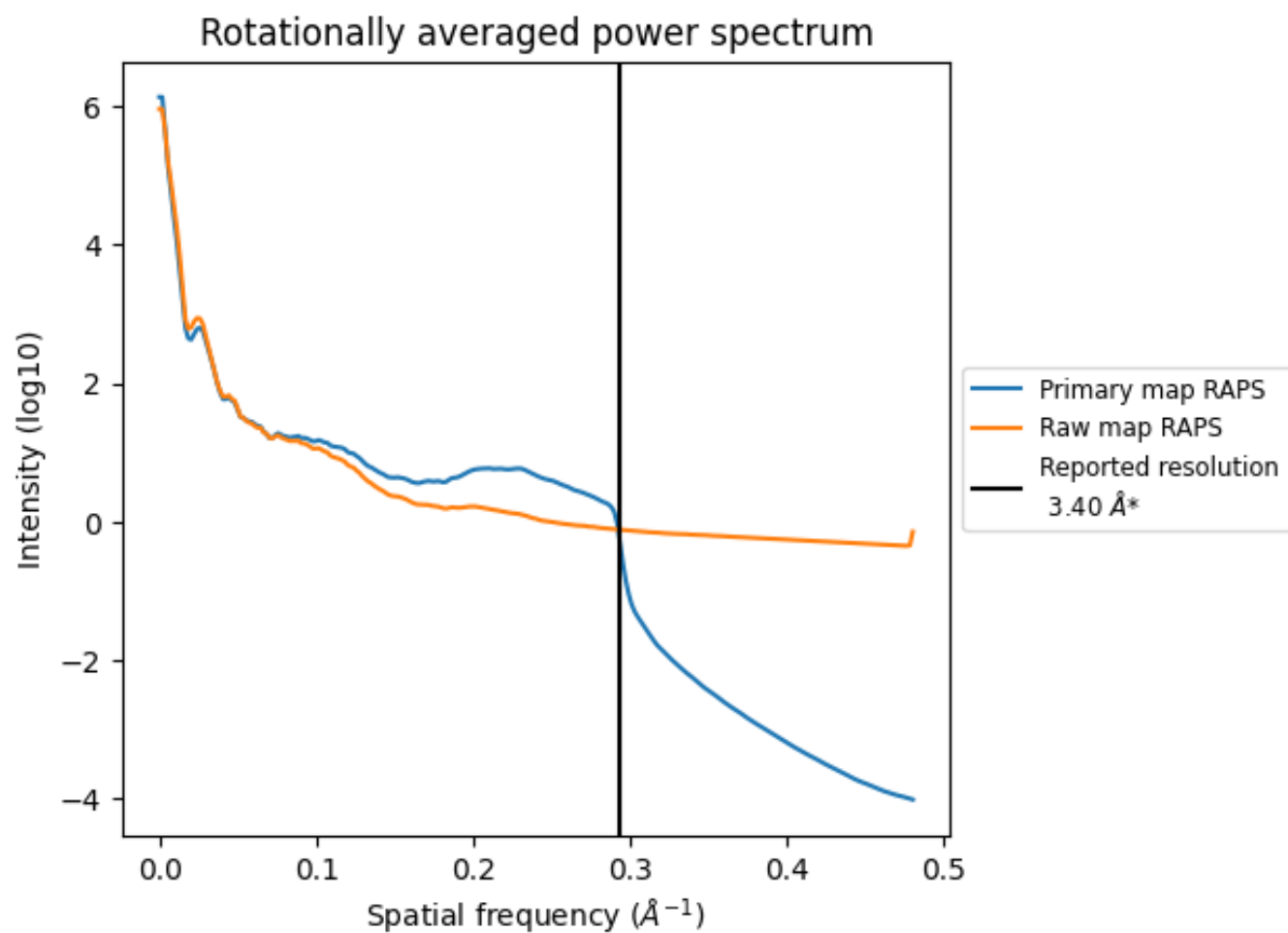
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1421 nm^3 ; this corresponds to an approximate mass of 1284 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 ⓘ

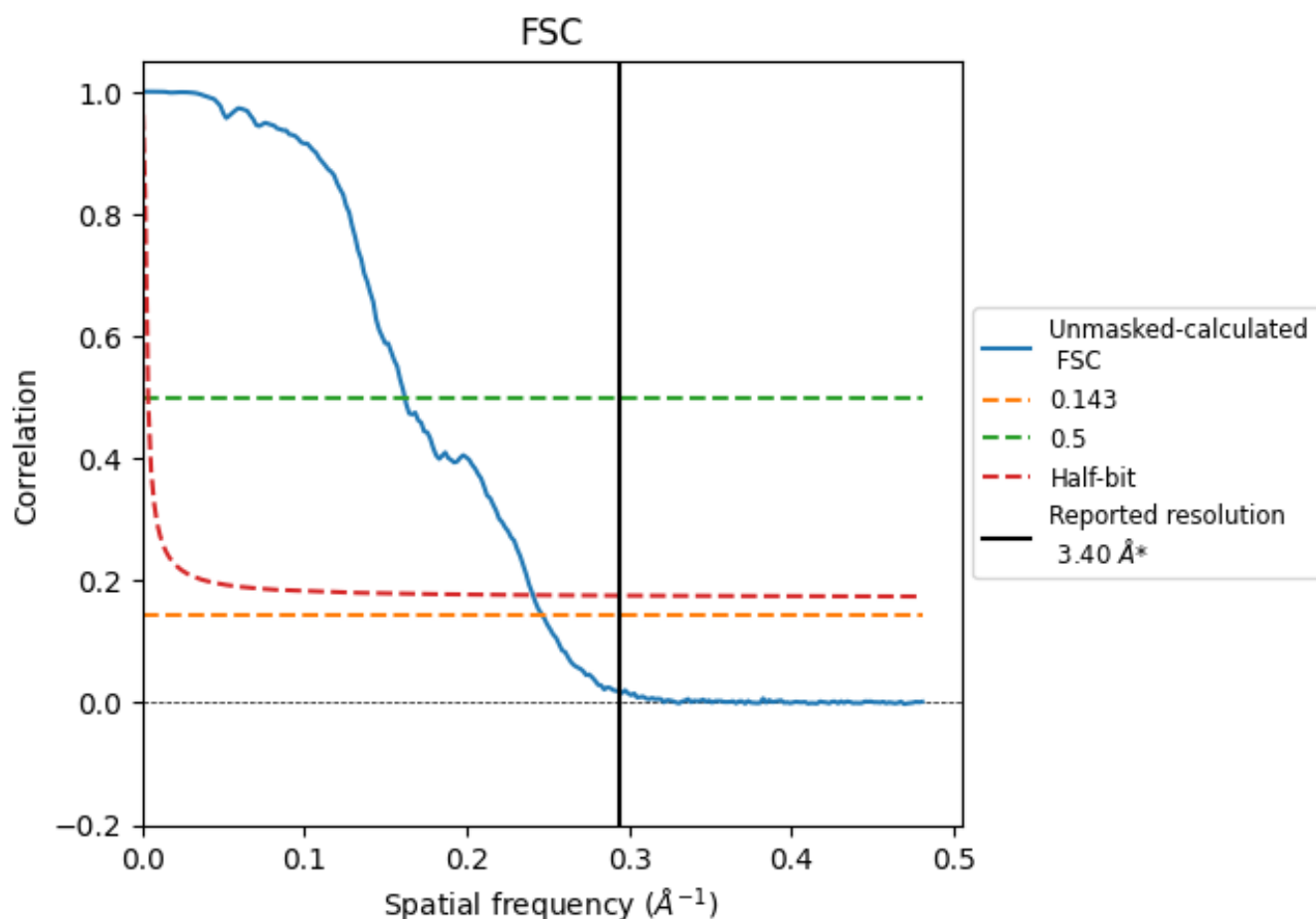


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

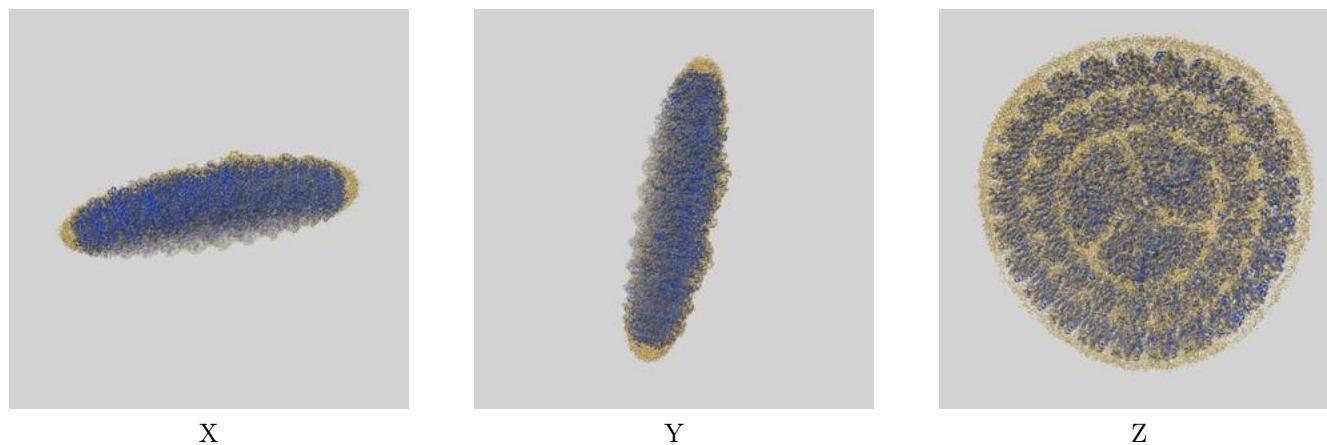
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.05	6.18	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

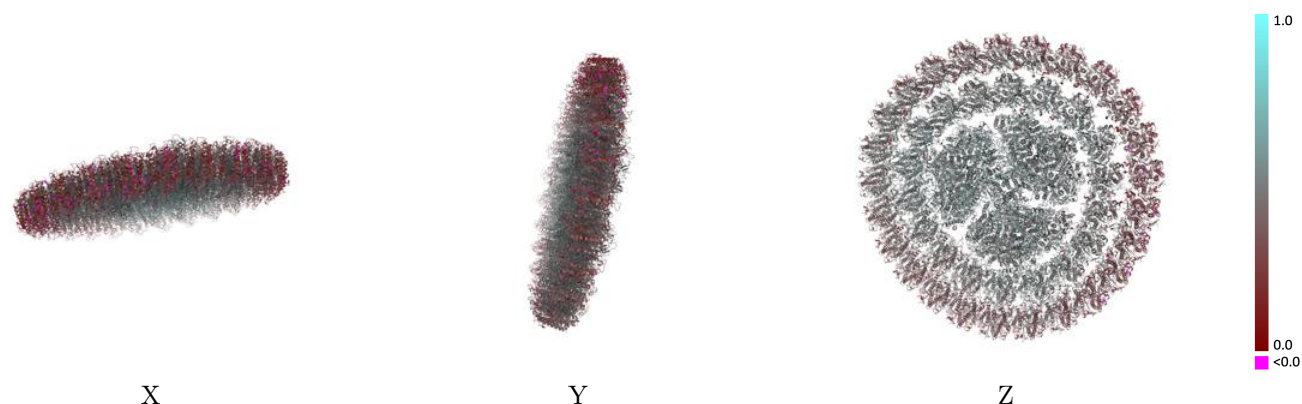
This section contains information regarding the fit between EMDB map EMD-63527 and PDB model 9LZJ. Per-residue inclusion information can be found in section [3](#) on page [106](#).

9.1 Map-model overlay [i](#)



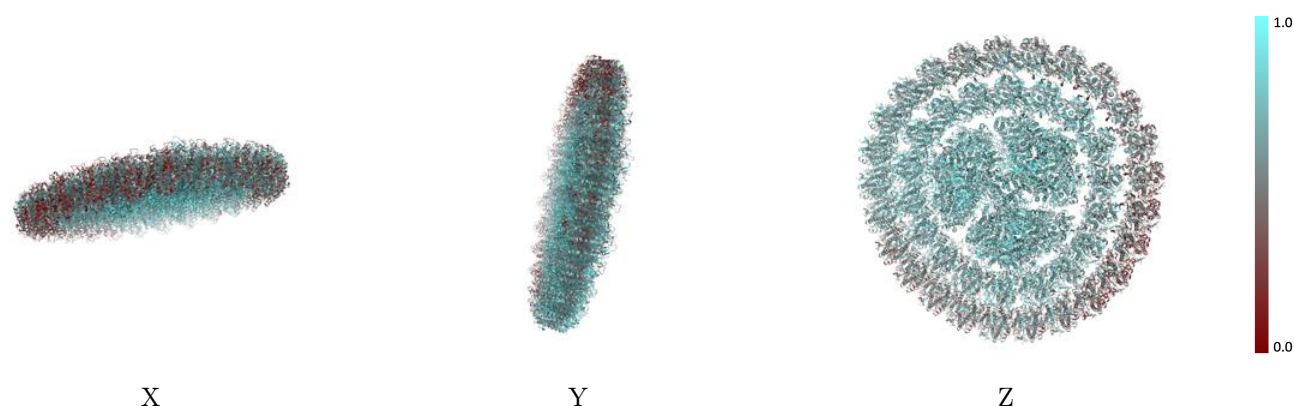
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



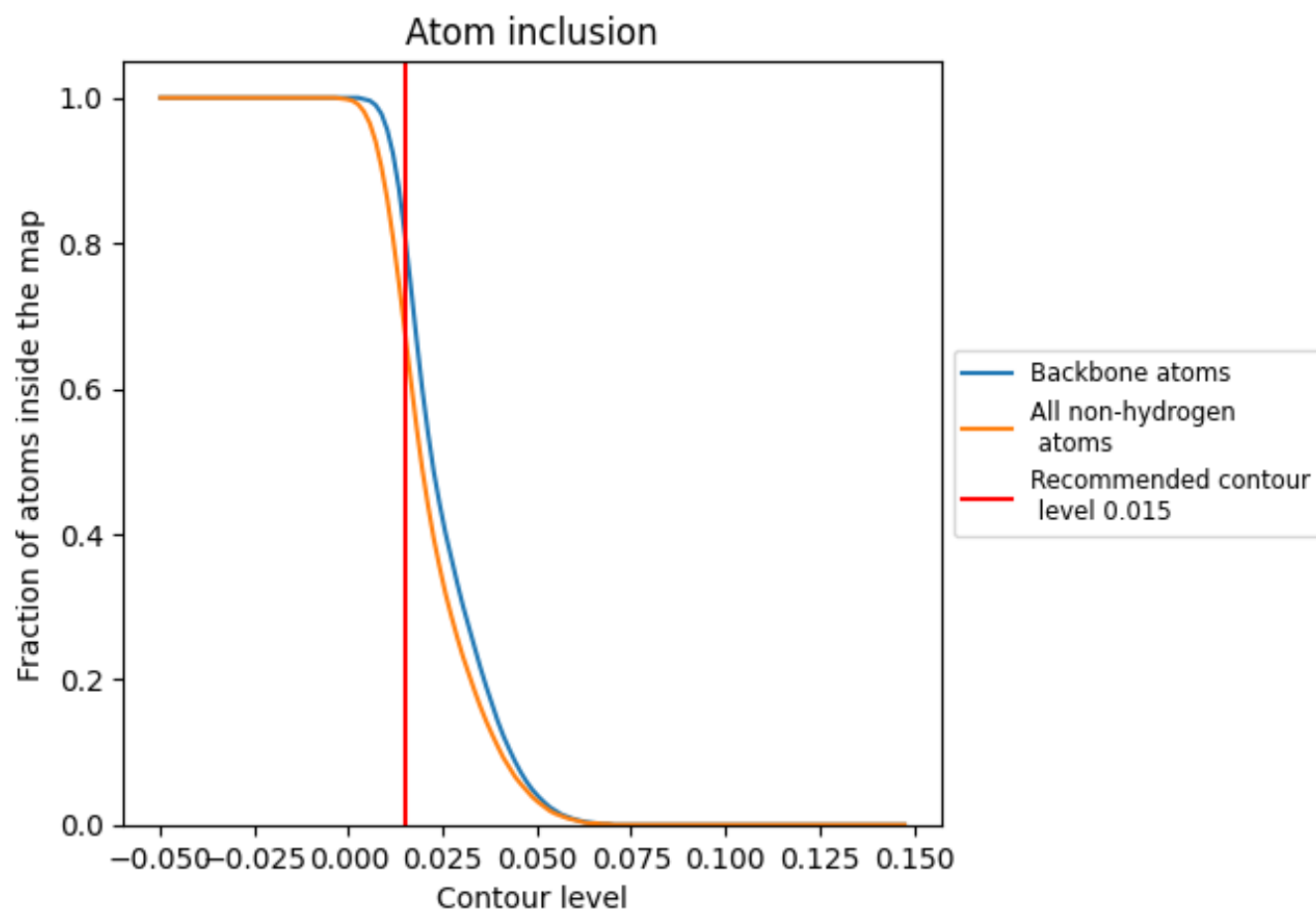
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 68% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6790	 0.4300
S	 0.4640	 0.3210
T	 0.4240	 0.3010
U	 0.4470	 0.2930
V	 0.6290	 0.3660
W	 0.6830	 0.4040
X	 0.7010	 0.4240
Y	 0.7010	 0.4290
Z	 0.6560	 0.3890
a	 0.5940	 0.3640
a1	 0.7640	 0.4770
a2	 0.8070	 0.5060
a3	 0.8360	 0.5220
a4	 0.8070	 0.5100
a5	 0.7810	 0.4880
a6	 0.7430	 0.4650
aA	 0.8520	 0.5450
aB	 0.8650	 0.5440
aC	 0.8600	 0.5040
aD	 0.8080	 0.5120
aE	 0.7610	 0.5030
aF	 0.8050	 0.5110
aI	 0.8730	 0.5510
aJ	 0.8080	 0.5250
aK	 0.7370	 0.4650
aL	 0.8540	 0.5350
aM	 0.8270	 0.5110
aX	 0.8110	 0.5100
b	 0.5220	 0.3430
b1	 0.7750	 0.4920
b2	 0.7750	 0.4920
b3	 0.7690	 0.4810
b4	 0.7500	 0.4730
b5	 0.7050	 0.4440
b6	 0.6570	 0.4090









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Chain	Atom inclusion	Q-score
bA	 0.8390	 0.5370
bB	 0.8350	 0.5250
bC	 0.8500	 0.5010
bD	 0.7950	 0.4990
bE	 0.7670	 0.4770
bF	 0.7820	 0.4820
bI	 0.8630	 0.5470
bJ	 0.8090	 0.5020
bK	 0.7290	 0.4560
bL	 0.8460	 0.5300
bM	 0.7760	 0.5010
bX	 0.7600	 0.4690
c	 0.5360	 0.3570
c1	 0.7160	 0.4550
c2	 0.7450	 0.4680
c3	 0.7600	 0.4880
c4	 0.7430	 0.4720
c5	 0.6950	 0.4380
c6	 0.6680	 0.4010
cA	 0.8240	 0.5270
cB	 0.8320	 0.5230
cC	 0.8580	 0.5060
cD	 0.7770	 0.4960
cE	 0.7530	 0.4570
cF	 0.7660	 0.4710
cI	 0.8630	 0.5500
cJ	 0.7410	 0.4980
cK	 0.6830	 0.4230
cL	 0.8430	 0.5320
cM	 0.7580	 0.4820
cX	 0.7630	 0.4670
d	 0.5450	 0.3380
e	 0.4470	 0.2800
f	 0.4910	 0.3040
g	 0.4950	 0.3110
h	 0.4850	 0.3200
i	 0.3610	 0.2790
j	 0.3390	 0.2800
k	 0.3420	 0.2760
l	 0.3350	 0.2420
m	 0.3760	 0.2540
n	 0.4510	 0.2780

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Chain	Atom inclusion	Q-score
o	 0.4860	 0.2960
p	 0.4980	 0.3060
q	 0.5280	 0.3290