



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 09:21 PM UTC

PDB ID : 9LZK / pdb_00009lzk
EMDB ID : EMD-63528
Title : The PSI1-IsiA13 complex with double-layered IsiA proteins bound to the monomeric PSI core
Authors : Si, L.; Cao, P.; Li, M.
Deposited on : 2025-02-21
Resolution : 3.50 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:

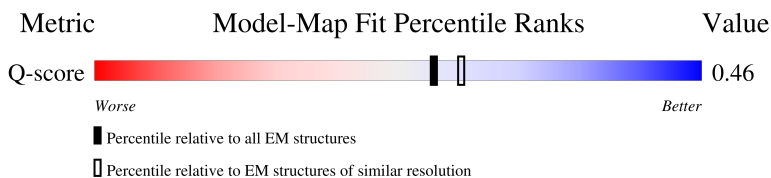
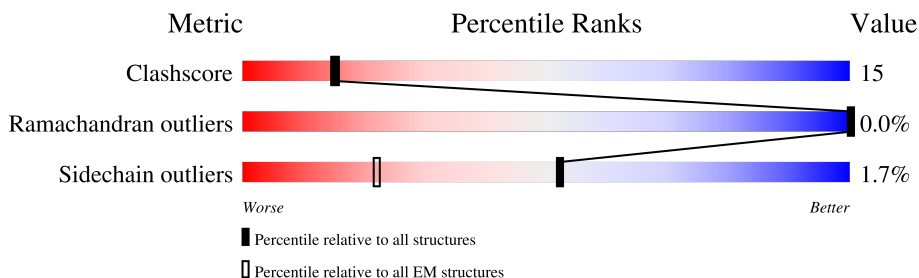
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.50 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	13950 (3.00 - 4.00)

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	1	358	51% 73% 22% 5%
1	2	358	9% 80% 14% • 5%
1	3	358	9% 76% 20% •
1	4	358	7% 73% 21% • •

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Mol	Chain	Length	Quality of chain
1	5	358	
1	6	358	
1	a	358	
1	b	358	
1	c	358	
1	d	358	
1	e	358	
1	f	358	
1	g	358	
2	A	755	
3	B	741	
4	C	81	
5	D	139	
6	E	76	
7	F	164	
8	I	38	
9	J	41	
10	K	83	
11	M	31	
12	X	39	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	1	501	X	-	-	-
13	CLA	1	502	X	-	-	-
13	CLA	1	503	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	3	512	X	-	-	-
13	CLA	3	513	X	-	-	-
13	CLA	3	516	X	-	-	-
13	CLA	3	517	X	-	-	-
13	CLA	3	518	X	-	-	-
13	CLA	3	519	X	-	-	-
13	CLA	4	501	X	-	-	-
13	CLA	4	503	X	-	-	-
13	CLA	4	504	X	-	-	-
13	CLA	4	505	X	-	-	-
13	CLA	4	506	X	-	-	-
13	CLA	4	507	X	-	-	-
13	CLA	4	508	X	-	-	-
13	CLA	4	509	X	-	-	-
13	CLA	4	510	X	-	-	-
13	CLA	4	512	X	-	-	-
13	CLA	4	513	X	-	-	-
13	CLA	4	516	X	-	-	-
13	CLA	4	517	X	-	-	-
13	CLA	4	518	X	-	-	-
13	CLA	4	519	X	-	-	-
13	CLA	5	501	X	-	-	-
13	CLA	5	502	X	-	-	-
13	CLA	5	503	X	-	-	-
13	CLA	5	504	X	-	-	-
13	CLA	5	505	X	-	-	-
13	CLA	5	506	X	-	-	-
13	CLA	5	507	X	-	-	-
13	CLA	5	508	X	-	-	-
13	CLA	5	509	X	-	-	-
13	CLA	5	510	X	-	-	-
13	CLA	5	511	X	-	-	-
13	CLA	5	512	X	-	-	-
13	CLA	5	513	X	-	-	-
13	CLA	5	516	X	-	-	-
13	CLA	5	517	X	-	-	-
13	CLA	5	518	X	-	-	-
13	CLA	5	519	X	-	-	-
13	CLA	6	501	X	-	-	-
13	CLA	6	502	X	-	-	-
13	CLA	6	503	X	-	-	-
13	CLA	6	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	6	505	X	-	-	-
13	CLA	6	506	X	-	-	-
13	CLA	6	507	X	-	-	-
13	CLA	6	508	X	-	-	-
13	CLA	6	509	X	-	-	-
13	CLA	6	510	X	-	-	-
13	CLA	6	511	X	-	-	-
13	CLA	6	512	X	-	-	-
13	CLA	6	513	X	-	-	-
13	CLA	6	516	X	-	-	-
13	CLA	6	517	X	-	-	-
13	CLA	6	518	X	-	-	-
13	CLA	6	519	X	-	-	-
13	CLA	A	1011	X	-	-	-
13	CLA	A	1013	X	-	-	-
13	CLA	A	1022	X	-	-	-
13	CLA	A	1101	X	-	-	-
13	CLA	A	1102	X	-	-	-
13	CLA	A	1103	X	-	-	-
13	CLA	A	1104	X	-	-	-
13	CLA	A	1105	X	-	-	-
13	CLA	A	1106	X	-	-	-
13	CLA	A	1107	X	-	-	-
13	CLA	A	1108	X	-	-	-
13	CLA	A	1109	X	-	-	-
13	CLA	A	1110	X	-	-	-
13	CLA	A	1111	X	-	-	-
13	CLA	A	1112	X	-	-	-
13	CLA	A	1113	X	-	-	-
13	CLA	A	1114	X	-	-	-
13	CLA	A	1115	X	-	-	-
13	CLA	A	1116	X	-	-	-
13	CLA	A	1117	X	-	-	-
13	CLA	A	1118	X	-	-	-
13	CLA	A	1119	X	-	-	-
13	CLA	A	1120	X	-	-	-
13	CLA	A	1121	X	-	-	-
13	CLA	A	1122	X	-	-	-
13	CLA	A	1123	X	-	-	-
13	CLA	A	1125	X	-	-	-
13	CLA	A	1126	X	-	-	-
13	CLA	A	1127	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	1128	X	-	-	-
13	CLA	A	1129	X	-	-	-
13	CLA	A	1130	X	-	-	-
13	CLA	A	1131	X	-	-	-
13	CLA	A	1132	X	-	-	-
13	CLA	A	1133	X	-	-	-
13	CLA	A	1134	X	-	-	-
13	CLA	A	1135	X	-	-	-
13	CLA	A	1136	X	-	-	-
13	CLA	A	1137	X	-	-	-
13	CLA	A	1138	X	-	-	-
13	CLA	A	1139	X	-	-	-
13	CLA	A	1140	X	-	-	-
13	CLA	A	1237	X	-	-	-
13	CLA	A	1801	X	-	-	-
13	CLA	B	1012	X	-	-	-
13	CLA	B	1021	X	-	-	-
13	CLA	B	1023	X	-	-	-
13	CLA	B	1201	X	-	-	-
13	CLA	B	1202	X	-	-	-
13	CLA	B	1203	X	-	-	-
13	CLA	B	1204	X	-	-	-
13	CLA	B	1205	X	-	-	-
13	CLA	B	1206	X	-	-	-
13	CLA	B	1208	X	-	-	-
13	CLA	B	1209	X	-	-	-
13	CLA	B	1210	X	-	-	-
13	CLA	B	1211	X	-	-	-
13	CLA	B	1212	X	-	-	-
13	CLA	B	1213	X	-	-	-
13	CLA	B	1214	X	-	-	-
13	CLA	B	1215	X	-	-	-
13	CLA	B	1216	X	-	-	-
13	CLA	B	1217	X	-	-	-
13	CLA	B	1218	X	-	-	-
13	CLA	B	1219	X	-	-	-
13	CLA	B	1220	X	-	-	-
13	CLA	B	1221	X	-	-	-
13	CLA	B	1222	X	-	-	-
13	CLA	B	1223	X	-	-	-
13	CLA	B	1224	X	-	-	-
13	CLA	B	1225	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	1226	X	-	-	-
13	CLA	B	1227	X	-	-	-
13	CLA	B	1228	X	-	-	-
13	CLA	B	1229	X	-	-	-
13	CLA	B	1230	X	-	-	-
13	CLA	B	1231	X	-	-	-
13	CLA	B	1232	X	-	-	-
13	CLA	B	1233	X	-	-	-
13	CLA	B	1234	X	-	-	-
13	CLA	B	1236	X	-	-	-
13	CLA	B	1238	X	-	-	-
13	CLA	F	1301	X	-	-	-
13	CLA	J	1302	X	-	-	-
13	CLA	K	1103	X	-	-	-
13	CLA	K	1401	X	-	-	-
13	CLA	X	1401	X	-	-	-
13	CLA	a	501	X	-	-	-
13	CLA	a	502	X	-	-	-
13	CLA	a	503	X	-	-	-
13	CLA	a	504	X	-	-	-
13	CLA	a	505	X	-	-	-
13	CLA	a	506	X	-	-	-
13	CLA	a	507	X	-	-	-
13	CLA	a	508	X	-	-	-
13	CLA	a	509	X	-	-	-
13	CLA	a	510	X	-	-	-
13	CLA	a	511	X	-	-	-
13	CLA	a	512	X	-	-	-
13	CLA	a	516	X	-	-	-
13	CLA	a	517	X	-	-	-
13	CLA	a	518	X	-	-	-
13	CLA	a	519	X	-	-	-
13	CLA	b	501	X	-	-	-
13	CLA	b	502	X	-	-	-
13	CLA	b	503	X	-	-	-
13	CLA	b	504	X	-	-	-
13	CLA	b	505	X	-	-	-
13	CLA	b	507	X	-	-	-
13	CLA	b	508	X	-	-	-
13	CLA	b	509	X	-	-	-
13	CLA	b	510	X	-	-	-
13	CLA	b	511	X	-	-	-

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	g	512	X	-	-	-
13	CLA	g	513	X	-	-	-
13	CLA	g	516	X	-	-	-
13	CLA	g	517	X	-	-	-
13	CLA	g	518	X	-	-	-
13	CLA	g	519	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 72827 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 Iron stress-induced chlorophyll-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
1	4	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
1	5	334	Total	C	N	O	S	0	0
			2613	1745	431	433	4		
1	6	339	Total	C	N	O	S	0	0
			2657	1774	437	442	4		
1	2	339	Total	C	N	O	S	0	0
			2657	1774	437	442	4		
1	1	340	Total	C	N	O	S	0	0
			2665	1780	438	443	4		
1	c	343	Total	C	N	O	S	0	0
			2685	1792	442	447	4		
1	d	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
1	e	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
1	f	341	Total	C	N	O	S	0	0
			2673	1784	440	445	4		
1	g	341	Total	C	N	O	S	0	0
			2673	1784	440	445	4		
1	b	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
1	a	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	745	Total	C	N	O	S	0	0
			5819	3818	994	981	26		

- Molecule 3 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	739	Total	C	N	O	S	0	0
			5889	3876	987	1005	21		

- Molecule 4 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	69	Total	C	N	O	S	0	0
			539	342	93	104			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	38	Total	C	N	O	S	0	0
			301	208	40	48	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	60	Total	C	N	O	S	0	0
			437	290	68	78	1		

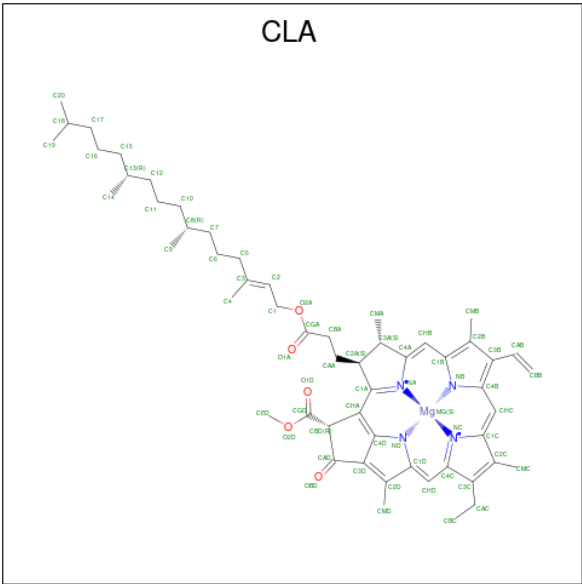
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	29	Total	C	N	O	0	0
			232	163	34	35		

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	4	1	Total 64	C 54	Mg 1	N 4	O 5	0
13	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	4	1	Total 55	C 45	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
13	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	6	1	Total 64	C 54	Mg 1	N 4	O 5	0
13	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	6	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	2	1	Total 64	C 54	Mg 1	N 4	O 5	0
13	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	2	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	1	1	Total 63	C 53	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
13	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 57	C 47	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	J	1	Total	C	Mg	N	O	0
			44	35	1	3	5	
13	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
13	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	c	1	Total 63	C 53	Mg 1	N 4	O 5	0
13	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	d	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	d	1	Total 63	C 53	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	d	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	d	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	d	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	d	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	e	1	Total 63	C 53	Mg 1	N 4	O 5	0
13	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	e	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	e	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	f	1	Total 63	C 53	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	f	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	g	1	Total 63	C 53	Mg 1	N 4	O 5	0
13	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	g	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	g	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	g	1	Total 45	C 35	Mg 1	N 4	O 5	0

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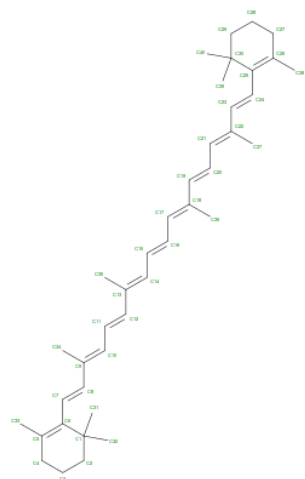
Mol	Chain	Residues	Atoms					AltConf
13	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	b	1	Total 63	C 53	Mg 1	N 4	O 5	0
13	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 14 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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Mol	Chain	Residues	Atoms	AltConf
14	6	1	Total C 40 40	0
14	6	1	Total C 40 40	0
14	2	1	Total C 40 40	0
14	2	1	Total C 40 40	0
14	2	1	Total C 40 40	0
14	2	1	Total C 40 40	0
14	1	1	Total C 40 40	0
14	1	1	Total C 40 40	0
14	1	1	Total C 40 40	0
14	1	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0

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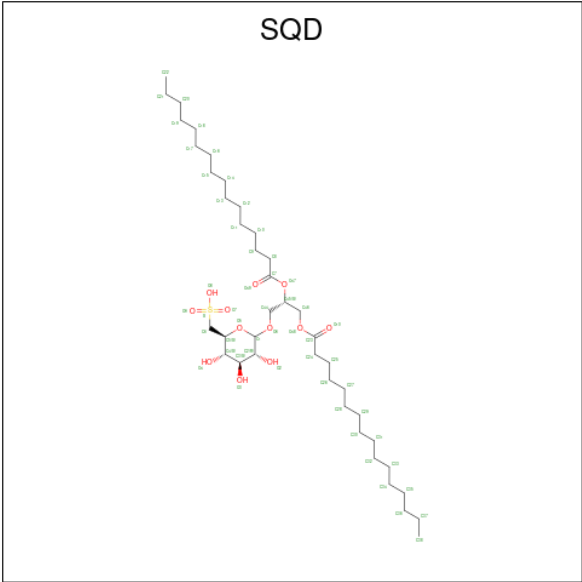
Mol	Chain	Residues	Atoms	AltConf
14	F	1	Total C 40 40	0
14	F	1	Total C 40 40	0
14	F	1	Total C 40 40	0
14	I	1	Total C 40 40	0
14	I	1	Total C 40 40	0
14	I	1	Total C 40 40	0
14	J	1	Total C 40 40	0
14	J	1	Total C 40 40	0
14	K	1	Total C 40 40	0
14	M	1	Total C 40 40	0
14	c	1	Total C 40 40	0
14	c	1	Total C 40 40	0
14	c	1	Total C 40 40	0
14	c	1	Total C 40 40	0
14	d	1	Total C 40 40	0
14	d	1	Total C 40 40	0
14	d	1	Total C 40 40	0
14	d	1	Total C 40 40	0
14	e	1	Total C 40 40	0
14	e	1	Total C 40 40	0
14	e	1	Total C 40 40	0

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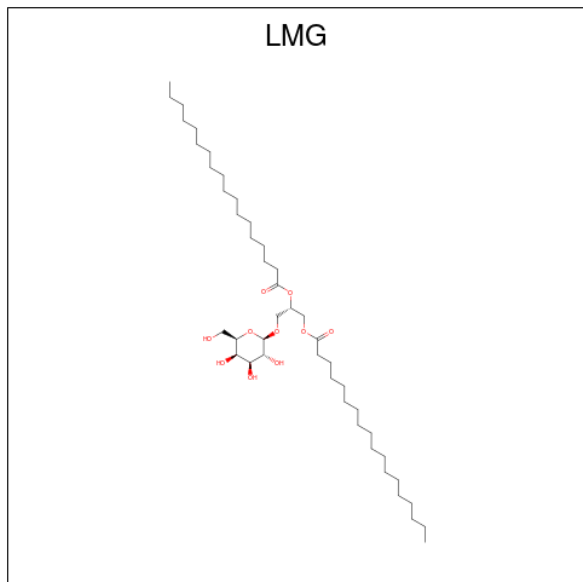
Mol	Chain	Residues	Atoms	AltConf
14	e	1	Total C 40 40	0
14	f	1	Total C 40 40	0
14	f	1	Total C 40 40	0
14	f	1	Total C 40 40	0
14	f	1	Total C 40 40	0
14	g	1	Total C 40 40	0
14	g	1	Total C 40 40	0
14	g	1	Total C 40 40	0
14	g	1	Total C 40 40	0
14	b	1	Total C 40 40	0
14	b	1	Total C 40 40	0
14	b	1	Total C 40 40	0
14	b	1	Total C 40 40	0
14	a	1	Total C 40 40	0
14	a	1	Total C 40 40	0
14	a	1	Total C 40 40	0
14	a	1	Total C 40 40	0

- Molecule 15 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



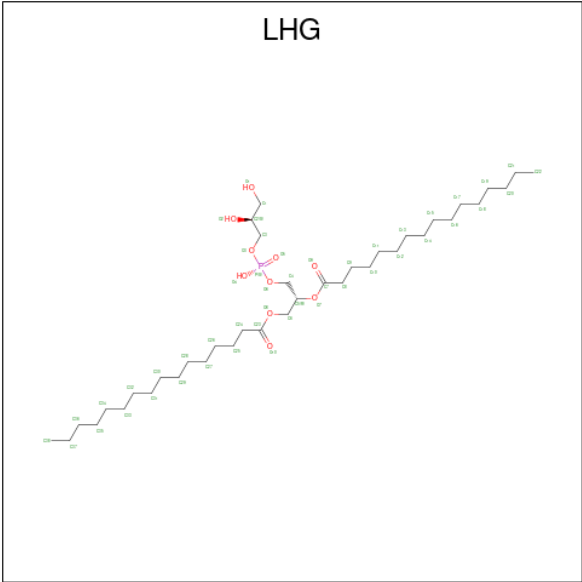
Mol	Chain	Residues	Atoms				AltConf
15	3	1	Total	C	O	S	0
			31	18	12	1	
15	4	1	Total	C	O	S	0
			31	18	12	1	
15	5	1	Total	C	O	S	0
			31	18	12	1	
15	6	1	Total	C	O	S	0
			31	18	12	1	
15	2	1	Total	C	O	S	0
			31	18	12	1	
15	1	1	Total	C	O	S	0
			31	18	12	1	
15	B	1	Total	C	O	S	0
			43	30	12	1	
15	c	1	Total	C	O	S	0
			31	18	12	1	
15	d	1	Total	C	O	S	0
			31	18	12	1	
15	e	1	Total	C	O	S	0
			31	18	12	1	
15	f	1	Total	C	O	S	0
			31	18	12	1	
15	g	1	Total	C	O	S	0
			31	18	12	1	
15	b	1	Total	C	O	S	0
			31	18	12	1	
15	a	1	Total	C	O	S	0
			31	18	12	1	

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



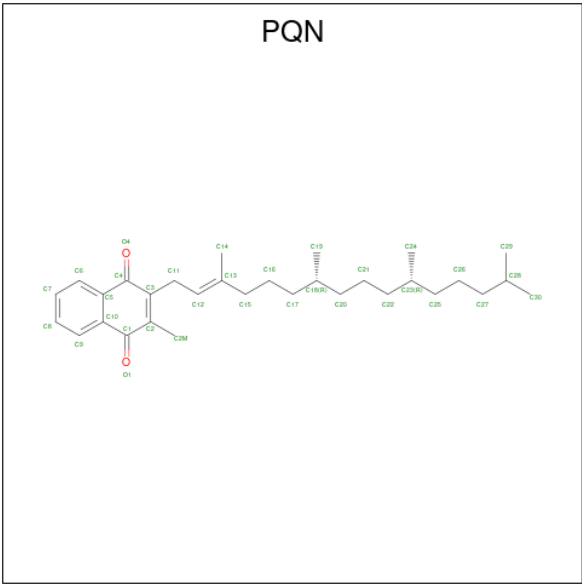
Mol	Chain	Residues	Atoms			AltConf
16	6	1	Total	C	O	0
			38	28	10	
16	2	1	Total	C	O	0
			40	30	10	
16	1	1	Total	C	O	0
			40	30	10	
16	B	1	Total	C	O	0
			55	45	10	
16	J	1	Total	C	O	0
			31	21	10	
16	g	1	Total	C	O	0
			40	30	10	

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



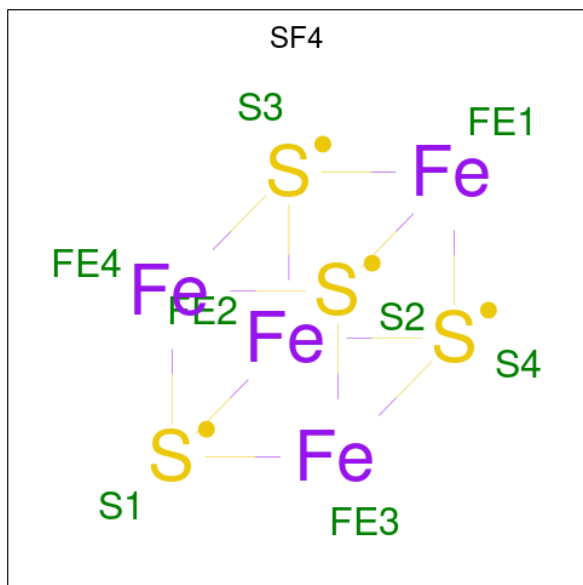
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			45	34	10	1	
17	A	1	Total	C	O	P	0
			35	24	10	1	
17	A	1	Total	C	O	P	0
			49	38	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	

- Molecule 18 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



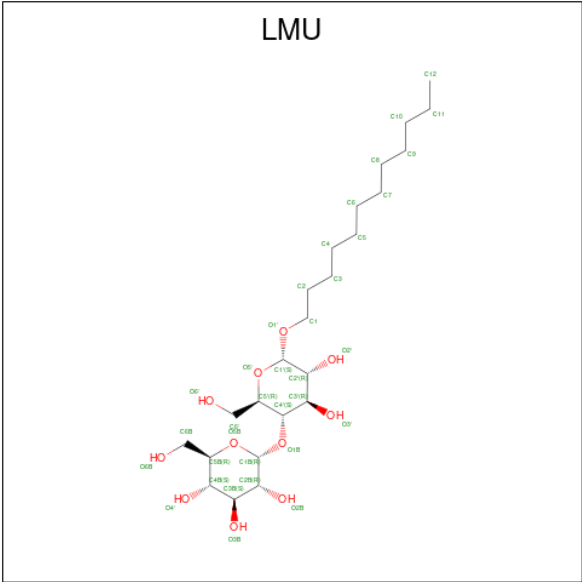
Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			33	31	2	
18	B	1	Total	C	O	0
			33	31	2	

- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	Fe	S	0
			8	4	4	
19	C	1	Total	Fe	S	0
			8	4	4	
19	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 20 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$) (labeled as "Ligand of Interest" by depositor).

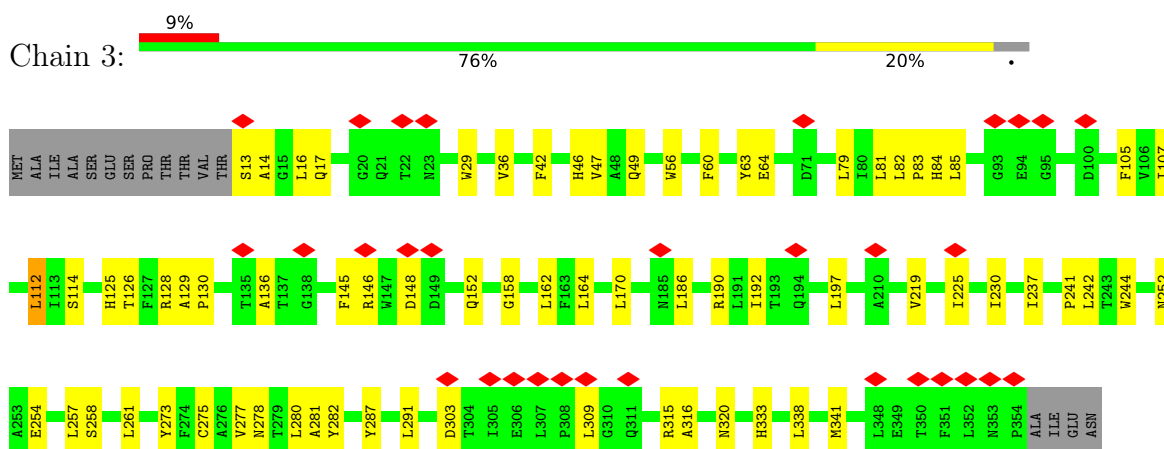


Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			24	18	6	
20	A	1	Total	C	O	0
			23	17	6	
20	B	1	Total	C	O	0
			35	24	11	
20	J	1	Total	C	O	0
			22	16	6	

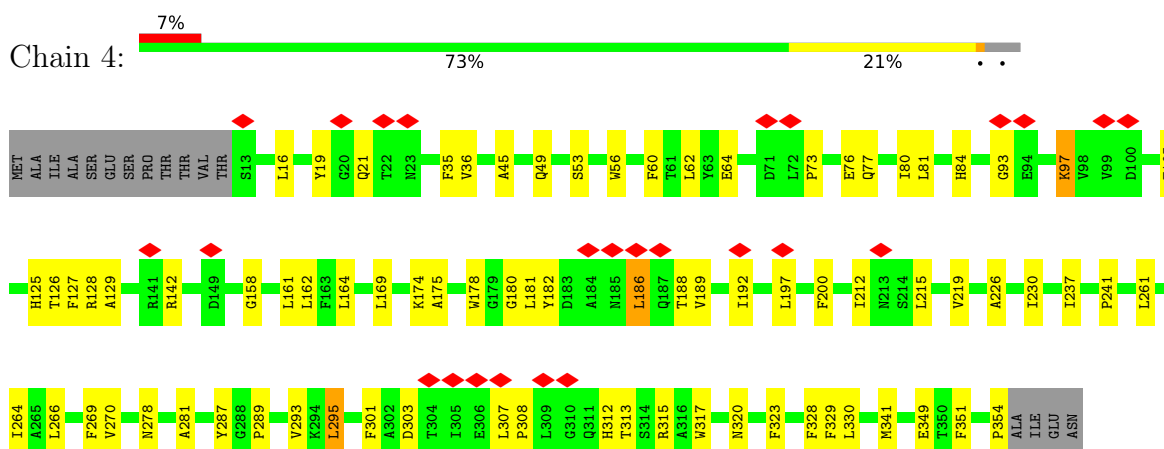
3 Residue-property plots

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.

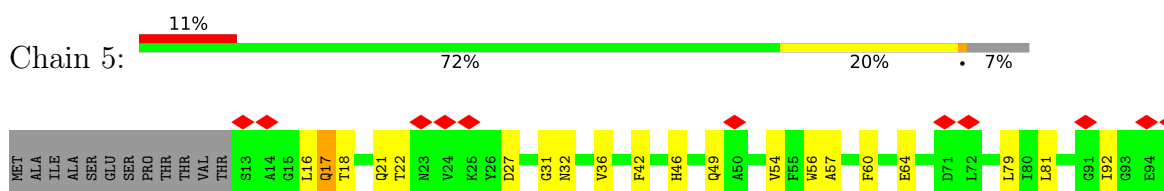
- Molecule 1: Iron stress-induced chlorophyll-binding protein

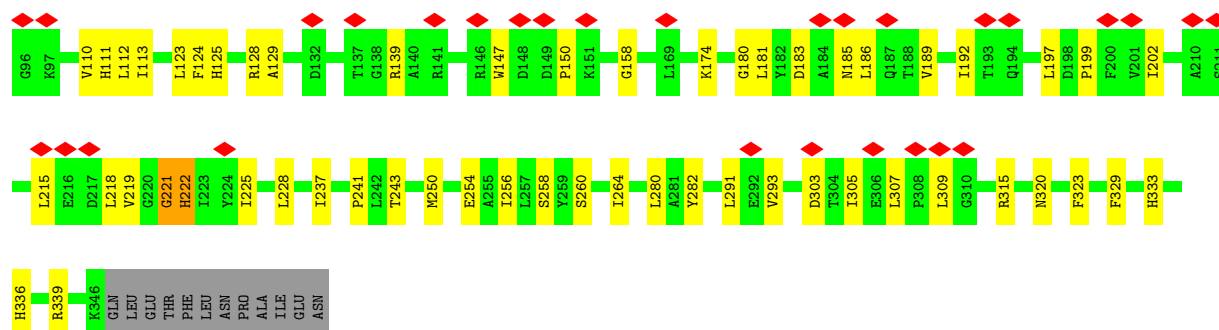


- Molecule 1: Iron stress-induced chlorophyll-binding protein

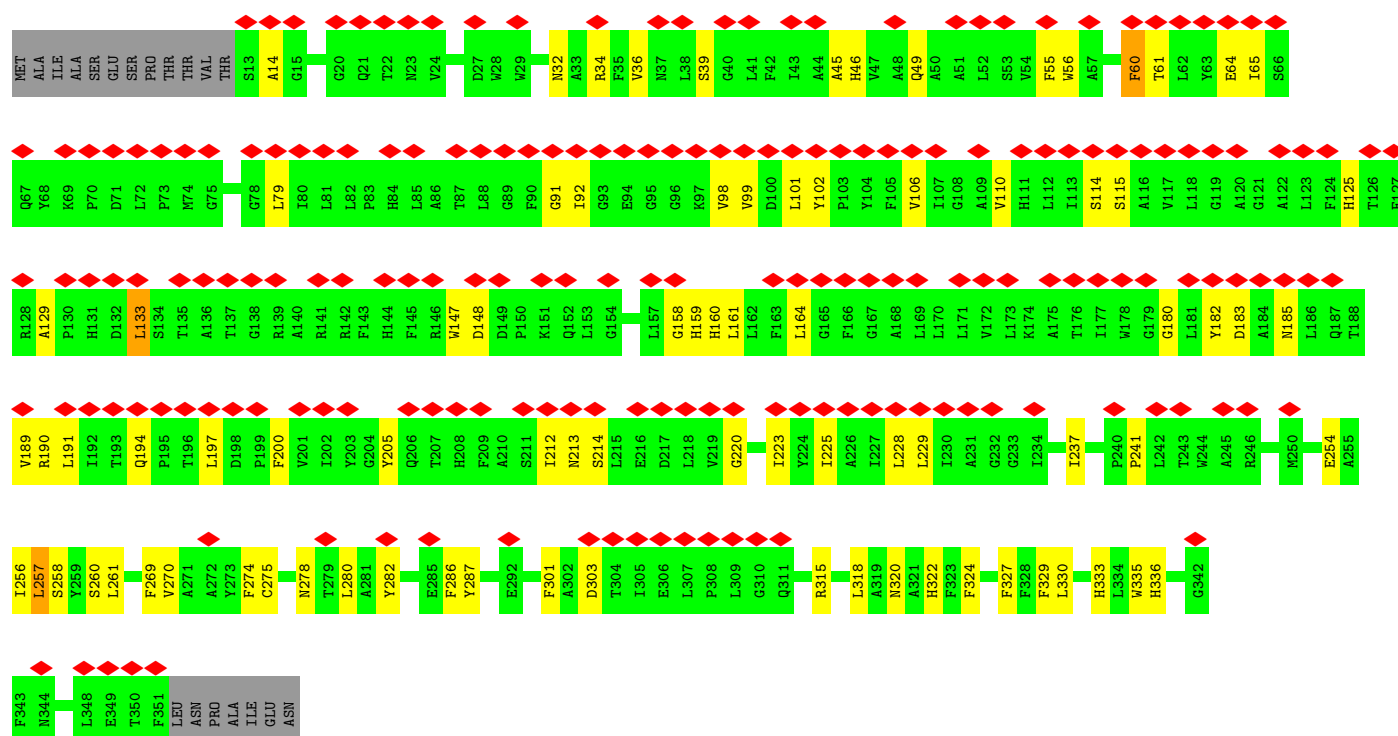


- Molecule 1: Iron stress-induced chlorophyll-binding protein

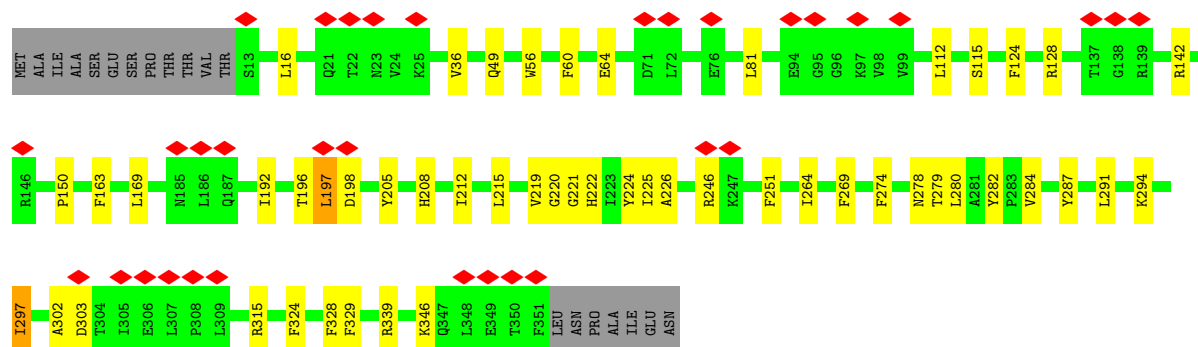
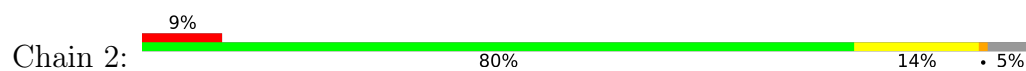




- Molecule 1: Iron stress-induced chlorophyll-binding protein



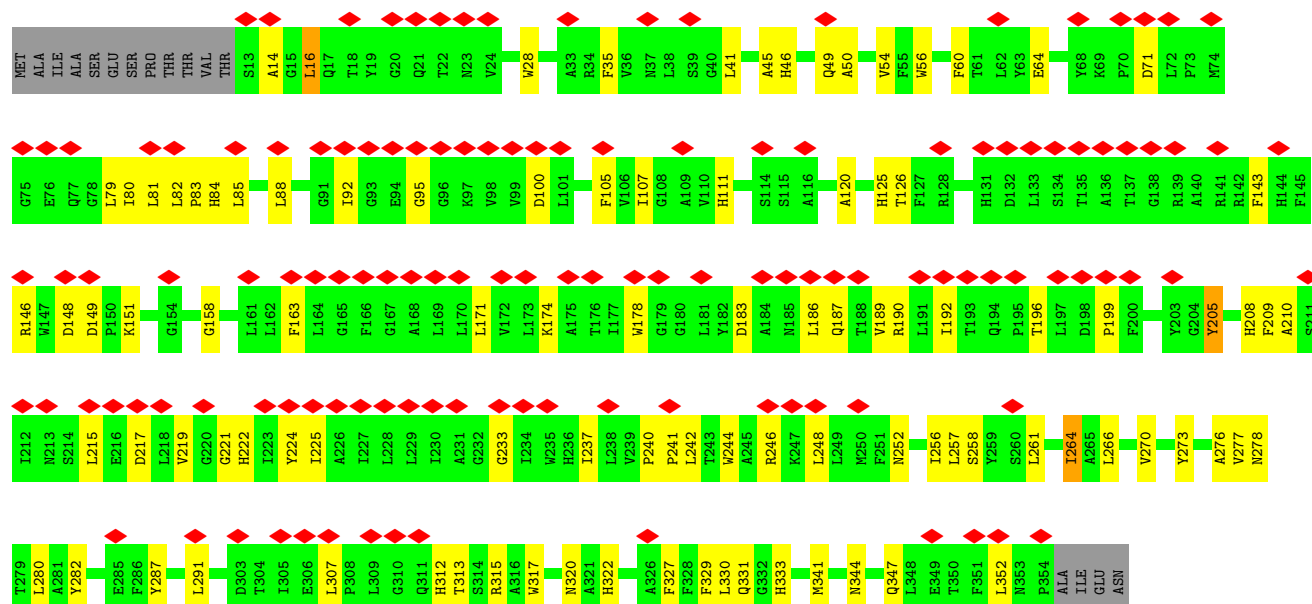
- Molecule 1: Iron stress-induced chlorophyll-binding protein



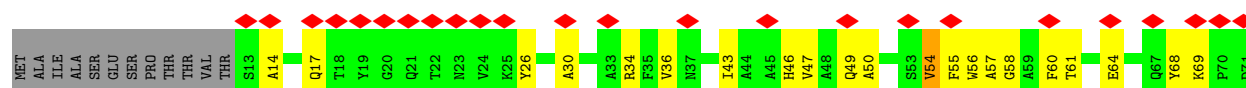


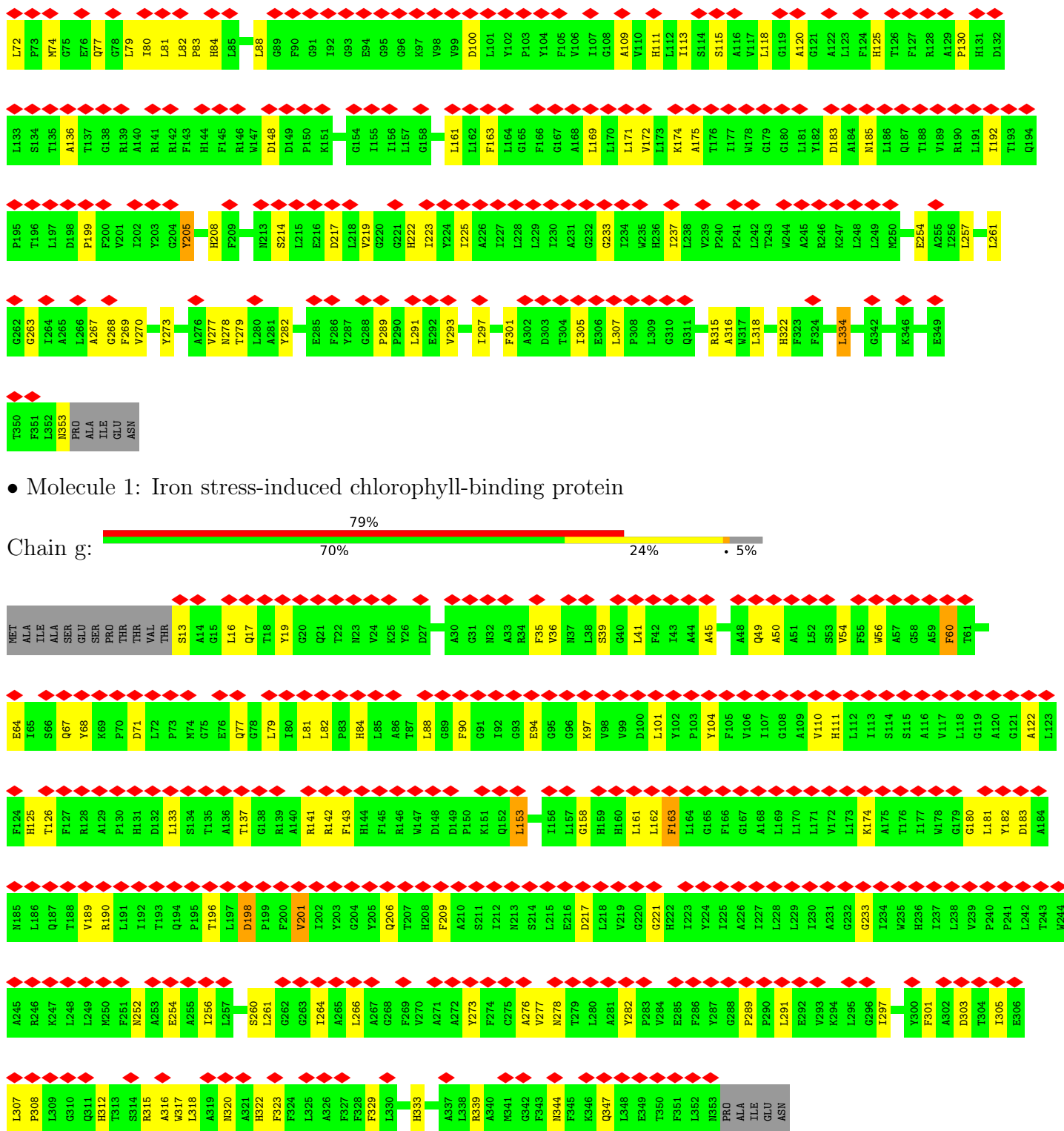


• Molecule 1: Iron stress-induced chlorophyll-binding protein

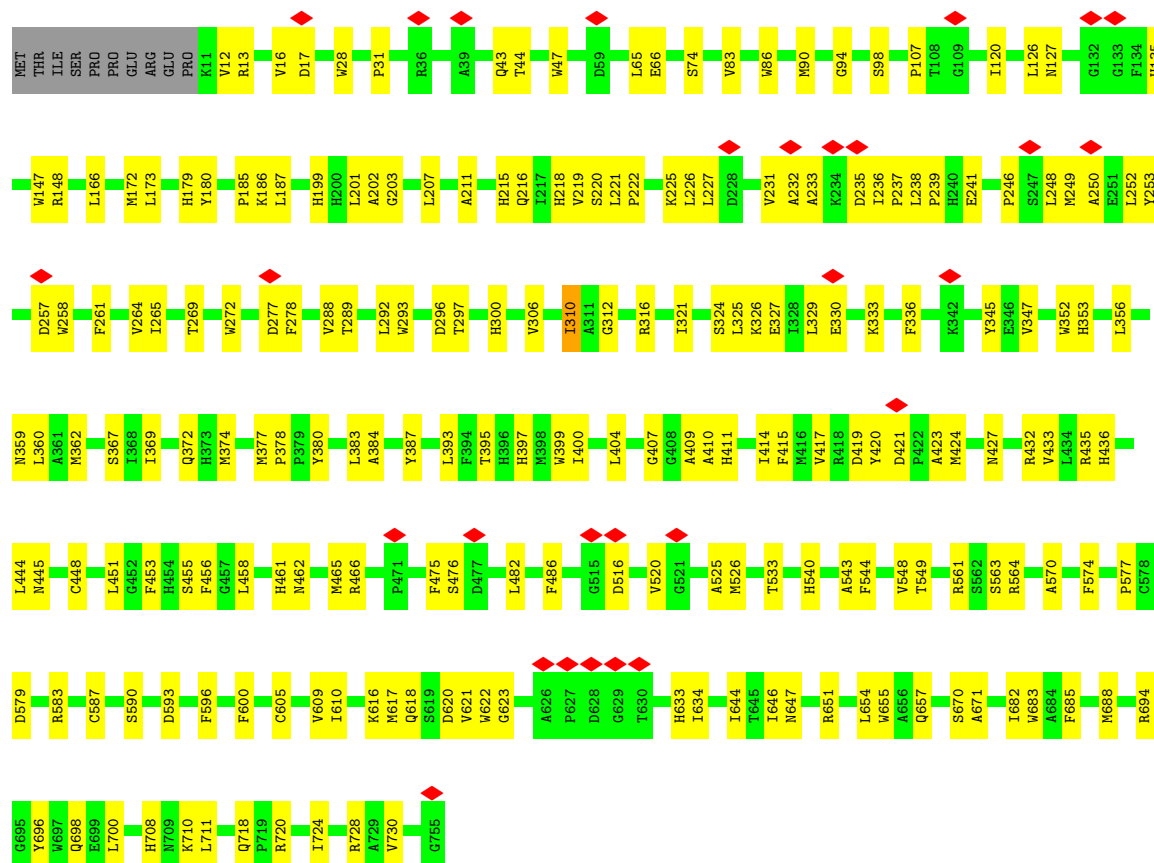


• Molecule 1: Iron stress-induced chlorophyll-binding protein

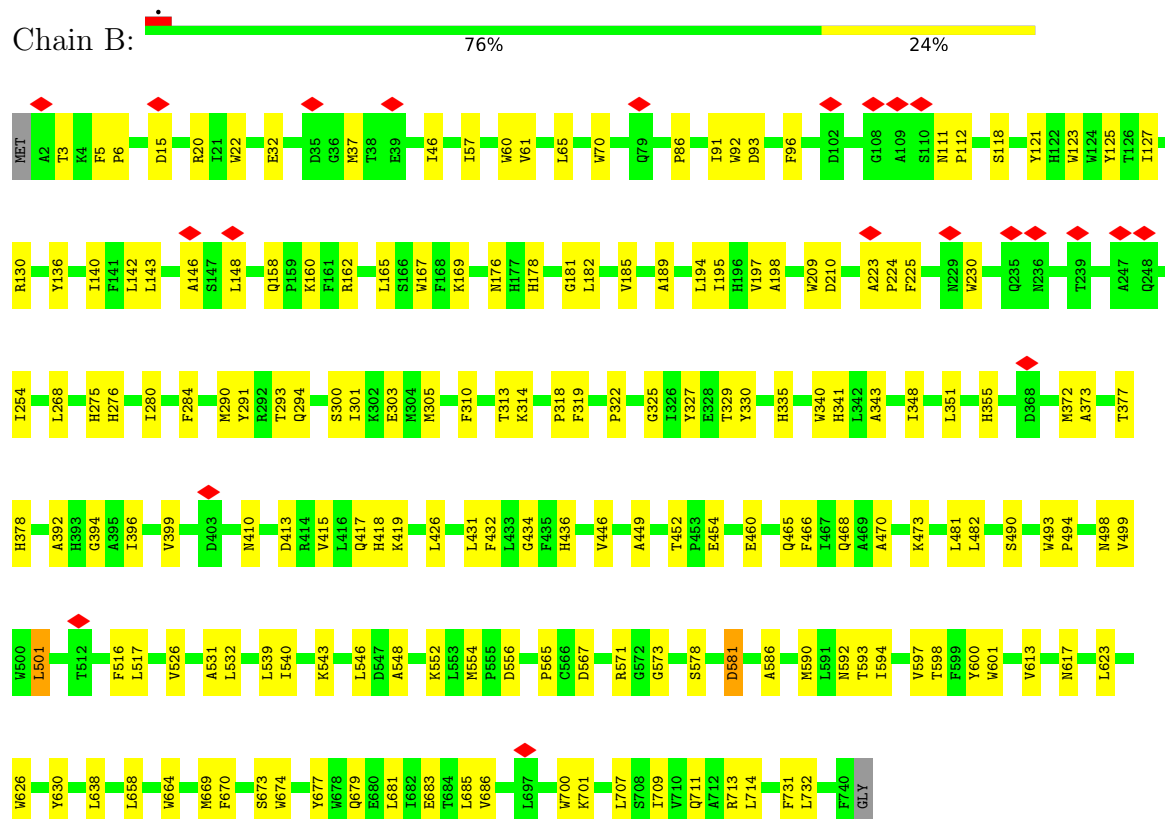




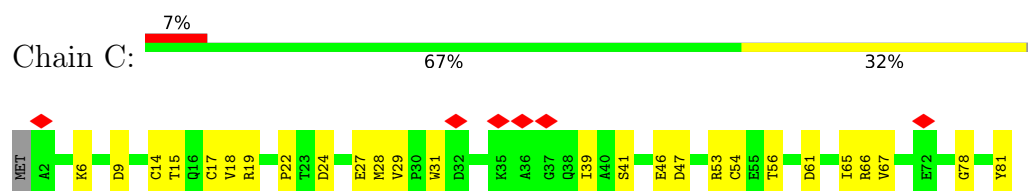
• Molecule 1: Iron stress-induced chlorophyll-binding protein



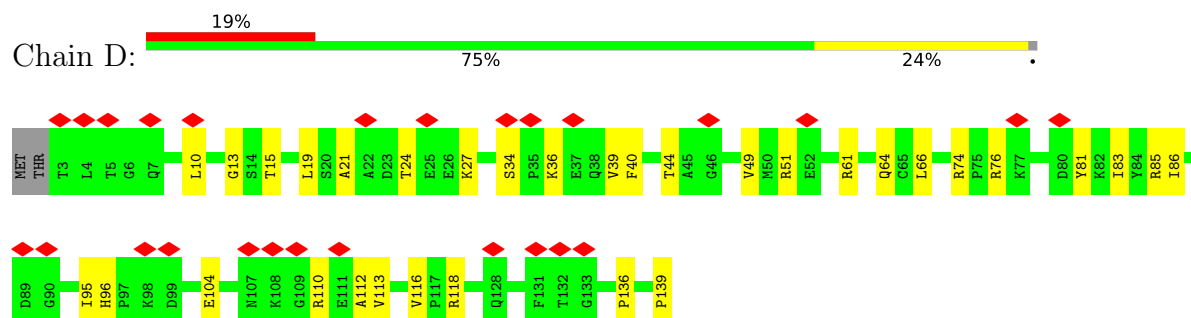
• Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2



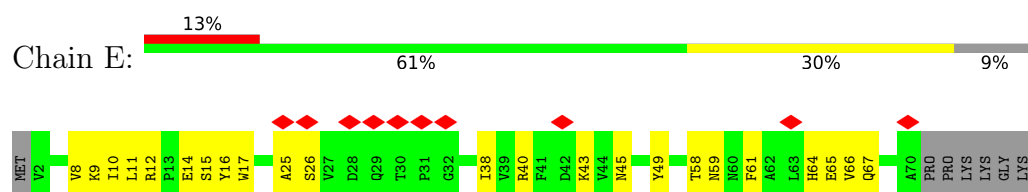
- Molecule 4: Photosystem I iron-sulfur center



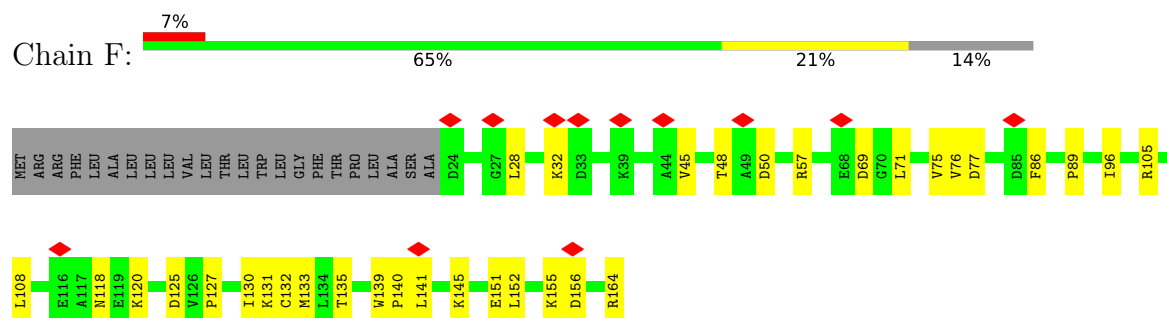
- Molecule 5: Photosystem I reaction center subunit II



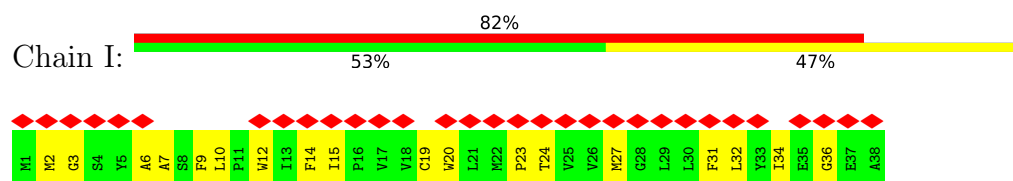
- Molecule 6: Photosystem I reaction center subunit IV



- Molecule 7: Photosystem I reaction center subunit III



- Molecule 8: Photosystem I reaction center subunit VIII

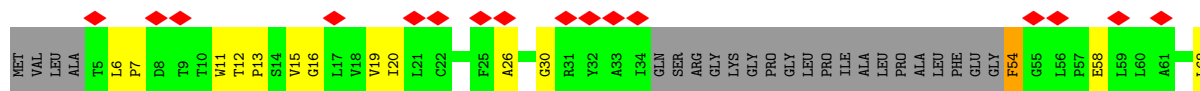


- Molecule 9: Photosystem I reaction center subunit IX

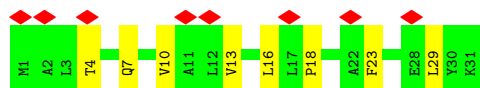
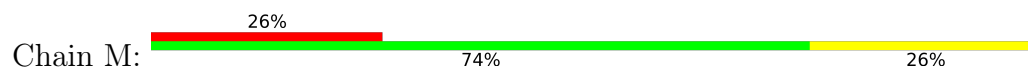




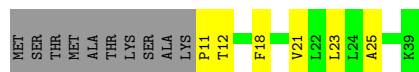
- Molecule 10: Photosystem I reaction center subunit PsaK



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 12: Photosystem I 4.8K protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55670	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	350.0, 350.0, 350.0	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.18	0/2754	0.31	1/3760 (0.0%)
1	2	0.15	0/2746	0.28	1/3749 (0.0%)
1	3	0.14	0/2770	0.26	0/3783
1	4	0.14	0/2770	0.26	0/3783
1	5	0.14	0/2701	0.53	3/3688 (0.1%)
1	6	0.13	0/2746	0.27	0/3749
1	a	0.14	0/2770	0.31	0/3783
1	b	0.17	0/2770	0.31	0/3783
1	c	0.15	0/2775	0.31	0/3790
1	d	0.23	1/2770 (0.0%)	0.32	2/3783 (0.1%)
1	e	0.16	0/2770	0.31	0/3783
1	f	0.21	1/2762 (0.0%)	0.31	1/3771 (0.0%)
1	g	0.16	0/2762	0.30	0/3771
2	A	0.25	0/6019	0.30	0/8209
3	B	0.23	0/6107	0.28	0/8345
4	C	0.22	0/608	0.34	0/824
5	D	0.24	0/1094	0.39	1/1482 (0.1%)
6	E	0.18	0/551	0.23	0/750
7	F	0.19	0/1087	0.30	0/1476
8	I	0.21	0/312	0.54	0/425
9	J	0.23	0/350	0.30	0/477
10	K	0.24	0/446	0.38	0/610
11	M	0.45	0/244	0.89	2/332 (0.6%)
12	X	0.22	0/241	0.30	0/330
All	All	0.19	2/52925 (0.0%)	0.32	11/72236 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	199	PRO	N-CD	-9.69	1.34	1.47
1	f	199	PRO	N-CD	-8.07	1.36	1.47

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	222	HIS	N-CA-CB	18.73	142.14	110.49
1	5	221	GLY	N-CA-C	-18.32	79.75	112.54
11	M	18	PRO	CA-N-CD	-11.80	95.48	112.00
11	M	18	PRO	N-CD-CG	-6.88	92.88	103.20
1	5	222	HIS	N-CA-C	-6.43	97.10	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2665	0	2652	69	0
1	2	2657	0	2641	46	0
1	3	2680	0	2665	67	0
1	4	2680	0	2665	65	0
1	5	2613	0	2600	57	0
1	6	2657	0	2641	64	0
1	a	2680	0	2665	91	0
1	b	2680	0	2665	86	0
1	c	2685	0	2670	81	0
1	d	2680	0	2665	79	0
1	e	2680	0	2665	80	0
1	f	2673	0	2658	81	0
1	g	2673	0	2658	83	0
2	A	5819	0	5684	190	0
3	B	5889	0	5646	162	0
4	C	598	0	578	26	0
5	D	1068	0	1067	28	0
6	E	539	0	525	16	0
7	F	1065	0	1074	40	0
8	I	301	0	306	19	0
9	J	338	0	347	10	0
10	K	437	0	451	12	0
11	M	241	0	264	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	X	232	0	220	4	0
13	1	945	0	881	48	0
13	2	936	0	867	46	0
13	3	945	0	881	47	0
13	4	924	0	848	42	0
13	5	956	0	900	50	0
13	6	914	0	832	59	0
13	A	2681	0	2703	185	0
13	B	2443	0	2455	161	0
13	F	45	0	33	1	0
13	J	89	0	66	1	0
13	K	96	0	78	4	0
13	X	45	0	33	2	0
13	a	925	0	849	64	0
13	b	945	0	881	51	0
13	c	933	0	861	70	0
13	d	945	0	880	48	0
13	e	935	0	865	53	0
13	f	938	0	871	68	0
13	g	942	0	875	54	0
14	1	160	0	224	22	0
14	2	160	0	224	17	0
14	3	160	0	224	20	0
14	4	160	0	224	14	0
14	5	160	0	224	22	0
14	6	160	0	224	18	0
14	A	200	0	280	31	0
14	B	240	0	336	25	0
14	F	120	0	168	14	0
14	I	120	0	167	16	0
14	J	80	0	112	8	0
14	K	40	0	56	6	0
14	M	40	0	56	3	0
14	a	160	0	224	27	0
14	b	160	0	224	22	0
14	c	160	0	224	26	0
14	d	160	0	224	18	0
14	e	160	0	224	20	0
14	f	160	0	224	22	0
14	g	160	0	223	24	0
15	1	31	0	26	0	0
15	2	31	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	3	31	0	26	0	0
15	4	31	0	26	7	0
15	5	31	0	26	2	0
15	6	31	0	26	2	0
15	B	43	0	50	2	0
15	a	31	0	26	0	0
15	b	31	0	26	0	0
15	c	31	0	26	0	0
15	d	31	0	26	0	0
15	e	31	0	26	0	0
15	f	31	0	26	0	0
15	g	31	0	26	1	0
16	1	40	0	50	0	0
16	2	40	0	50	1	0
16	6	38	0	46	2	0
16	B	55	0	86	5	0
16	J	31	0	32	0	0
16	g	40	0	50	1	0
17	A	211	0	281	21	0
18	A	33	0	46	2	0
18	B	33	0	46	4	0
19	A	8	0	0	1	0
19	C	16	0	0	2	0
20	A	47	0	65	3	0
20	B	35	0	46	1	0
20	J	22	0	28	10	0
All	All	72827	0	72631	2153	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 15.

The worst 5 of 2153 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)
1:1:309:LEU:HD21	2:A:250:ALA:CB	1.62	1.29
1:1:309:LEU:HD21	2:A:250:ALA:HB2	1.22	1.12
1:3:29:TRP:CE2	20:J:5105:LMU:H31	1.88	1.08
1:d:197:LEU:O	1:d:198:ASP:OD1	1.83	0.96
1:1:309:LEU:CD2	2:A:250:ALA:HB2	1.94	0.96

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	1	338/358 (94%)	334 (99%)	4 (1%)	0	100	100
1	2	337/358 (94%)	334 (99%)	3 (1%)	0	100	100
1	3	340/358 (95%)	336 (99%)	4 (1%)	0	100	100
1	4	340/358 (95%)	333 (98%)	7 (2%)	0	100	100
1	5	332/358 (93%)	325 (98%)	6 (2%)	1 (0%)	36	67
1	6	337/358 (94%)	332 (98%)	5 (2%)	0	100	100
1	a	340/358 (95%)	335 (98%)	5 (2%)	0	100	100
1	b	340/358 (95%)	336 (99%)	4 (1%)	0	100	100
1	c	341/358 (95%)	332 (97%)	9 (3%)	0	100	100
1	d	340/358 (95%)	334 (98%)	6 (2%)	0	100	100
1	e	340/358 (95%)	336 (99%)	4 (1%)	0	100	100
1	f	339/358 (95%)	333 (98%)	6 (2%)	0	100	100
1	g	339/358 (95%)	336 (99%)	3 (1%)	0	100	100
2	A	724/755 (96%)	694 (96%)	30 (4%)	0	100	100
3	B	687/741 (93%)	666 (97%)	21 (3%)	0	100	100
4	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
5	D	135/139 (97%)	129 (96%)	6 (4%)	0	100	100
6	E	67/76 (88%)	65 (97%)	2 (3%)	0	100	100
7	F	139/164 (85%)	135 (97%)	4 (3%)	0	100	100
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	39/41 (95%)	39 (100%)	0	0	100	100
10	K	56/83 (68%)	56 (100%)	0	0	100	100
11	M	29/31 (94%)	26 (90%)	3 (10%)	0	100	100
12	X	27/39 (69%)	27 (100%)	0	0	100	100
All	All	6420/6842 (94%)	6284 (98%)	135 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	5	222	HIS

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	1	264/279 (95%)	259 (98%)	5 (2%)	50	68
1	2	263/279 (94%)	260 (99%)	3 (1%)	65	74
1	3	266/279 (95%)	262 (98%)	4 (2%)	57	71
1	4	266/279 (95%)	261 (98%)	5 (2%)	50	68
1	5	258/279 (92%)	250 (97%)	8 (3%)	35	59
1	6	263/279 (94%)	258 (98%)	5 (2%)	50	68
1	a	266/279 (95%)	256 (96%)	10 (4%)	29	55
1	b	266/279 (95%)	259 (97%)	7 (3%)	40	62
1	c	266/279 (95%)	256 (96%)	10 (4%)	29	55
1	d	266/279 (95%)	261 (98%)	5 (2%)	50	68
1	e	266/279 (95%)	260 (98%)	6 (2%)	44	64
1	f	265/279 (95%)	262 (99%)	3 (1%)	65	74
1	g	265/279 (95%)	258 (97%)	7 (3%)	40	62
2	A	593/603 (98%)	592 (100%)	1 (0%)	87	85
3	B	597/598 (100%)	594 (100%)	3 (0%)	81	80
4	C	67/68 (98%)	66 (98%)	1 (2%)	57	71
5	D	114/116 (98%)	114 (100%)	0	100	100
6	E	59/65 (91%)	58 (98%)	1 (2%)	53	70
7	F	109/128 (85%)	109 (100%)	0	100	100
8	I	32/32 (100%)	31 (97%)	1 (3%)	35	59
9	J	36/36 (100%)	36 (100%)	0	100	100
10	K	45/61 (74%)	43 (96%)	2 (4%)	25	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	M	26/26 (100%)	26 (100%)	0	100	100
12	X	20/31 (64%)	20 (100%)	0	100	100
All	All	5138/5391 (95%)	5051 (98%)	87 (2%)	52	70

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	e	225	ILE
1	b	49	GLN
1	e	352	LEU
1	g	153	LEU
1	b	223	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	e	353	ASN
1	g	312	HIS
1	f	49	GLN
1	f	336	HIS
1	b	144	HIS

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](#)

420 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
13	CLA	1	504	-	59,63,73	1.27	8 (13%)	70,101,113	1.16	4 (5%)
14	BCR	f	523	-	41,41,41	0.72	0	56,56,56	1.89	12 (21%)
13	CLA	5	511	1	59,63,73	1.27	7 (11%)	70,101,113	1.25	7 (10%)
13	CLA	a	509	1	69,73,73	1.19	6 (8%)	82,113,113	1.19	4 (4%)
13	CLA	6	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.19	5 (6%)
13	CLA	5	501	1	69,73,73	1.17	7 (10%)	82,113,113	1.09	3 (3%)
18	PQN	B	2002	-	34,34,34	0.48	0	43,45,45	0.75	1 (2%)
13	CLA	3	505	1	69,73,73	1.15	6 (8%)	82,113,113	1.16	8 (9%)
13	CLA	B	1239	3	69,73,73	1.16	7 (10%)	82,113,113	1.18	6 (7%)
13	CLA	A	1105	2	55,59,73	1.29	7 (12%)	64,96,113	1.29	6 (9%)
13	CLA	4	508	1	59,63,73	1.25	7 (11%)	70,101,113	1.19	4 (5%)
13	CLA	c	506	1	49,53,73	1.39	5 (10%)	58,89,113	1.29	4 (6%)
13	CLA	2	501	1	69,73,73	1.17	8 (11%)	82,113,113	1.11	5 (6%)
14	BCR	I	4020	-	41,41,41	0.75	1 (2%)	56,56,56	2.13	19 (33%)
13	CLA	B	1201	3	61,65,73	1.22	7 (11%)	72,103,113	1.17	7 (9%)
13	CLA	g	503	1	67,71,73	1.20	6 (8%)	79,110,113	1.16	6 (7%)
13	CLA	B	1204	-	64,68,73	1.21	7 (10%)	76,107,113	1.19	3 (3%)
13	CLA	a	503	1	67,71,73	1.20	7 (10%)	79,110,113	1.16	5 (6%)
17	LHG	A	5005	-	44,44,48	0.97	2 (4%)	47,50,54	1.07	3 (6%)
13	CLA	K	1401	-	59,63,73	1.27	8 (13%)	70,101,113	1.20	6 (8%)
14	BCR	a	524	-	41,41,41	0.71	0	56,56,56	2.08	18 (32%)
13	CLA	d	511	1	59,63,73	1.28	7 (11%)	70,101,113	1.18	5 (7%)
13	CLA	A	1129	2	54,58,73	1.28	8 (14%)	64,95,113	1.21	6 (9%)
13	CLA	A	1113	2	53,57,73	1.28	7 (13%)	61,93,113	1.30	6 (9%)
13	CLA	6	504	-	49,53,73	1.39	6 (12%)	58,89,113	1.24	5 (8%)
13	CLA	e	508	1	59,63,73	1.25	8 (13%)	70,101,113	1.20	5 (7%)
13	CLA	f	502	1	64,68,73	1.21	8 (12%)	76,107,113	1.27	6 (7%)
14	BCR	e	524	-	41,41,41	0.70	0	56,56,56	2.21	17 (30%)
13	CLA	d	517	-	49,53,73	1.39	7 (14%)	58,89,113	1.15	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	d	504	-	59,63,73	1.25	7 (11%)	70,101,113	1.18	5 (7%)
13	CLA	f	504	-	59,63,73	1.27	6 (10%)	70,101,113	1.13	3 (4%)
13	CLA	f	518	1	59,63,73	1.27	7 (11%)	70,101,113	1.20	5 (7%)
13	CLA	c	503	1	67,71,73	1.19	6 (8%)	79,110,113	1.12	4 (5%)
13	CLA	e	518	1	59,63,73	1.26	7 (11%)	70,101,113	1.24	5 (7%)
14	BCR	c	524	-	41,41,41	0.70	0	56,56,56	2.18	18 (32%)
14	BCR	g	523	-	41,41,41	0.69	0	56,56,56	2.13	16 (28%)
17	LHG	A	5002	-	40,40,48	0.99	2 (5%)	43,46,54	1.14	4 (9%)
13	CLA	c	508	1	59,63,73	1.24	8 (13%)	70,101,113	1.15	5 (7%)
13	CLA	1	507	-	64,68,73	1.21	6 (9%)	76,107,113	1.14	4 (5%)
14	BCR	d	521	-	41,41,41	0.68	0	56,56,56	2.07	15 (26%)
13	CLA	1	519	-	49,53,73	1.40	5 (10%)	58,89,113	1.12	2 (3%)
13	CLA	1	503	1	67,71,73	1.18	6 (8%)	79,110,113	1.10	4 (5%)
13	CLA	2	512	1	56,60,73	1.29	7 (12%)	65,97,113	1.44	9 (13%)
13	CLA	1	508	1	59,63,73	1.26	7 (11%)	70,101,113	1.13	4 (5%)
13	CLA	4	507	-	64,68,73	1.21	6 (9%)	76,107,113	1.17	5 (6%)
13	CLA	b	516	1	49,53,73	1.38	6 (12%)	58,89,113	1.22	4 (6%)
13	CLA	A	1136	2	69,73,73	1.15	8 (11%)	82,113,113	1.11	6 (7%)
13	CLA	c	517	-	49,53,73	1.39	7 (14%)	58,89,113	1.14	5 (8%)
13	CLA	a	516	1	49,53,73	1.38	5 (10%)	58,89,113	1.25	4 (6%)
13	CLA	a	512	1	56,60,73	1.31	7 (12%)	65,97,113	1.20	5 (7%)
13	CLA	5	512	1	56,60,73	1.30	7 (12%)	65,97,113	1.23	6 (9%)
13	CLA	A	1115	-	64,68,73	1.21	7 (10%)	76,107,113	1.13	4 (5%)
13	CLA	A	1123	-	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)
13	CLA	B	1228	3	59,63,73	1.23	8 (13%)	70,101,113	1.22	7 (10%)
15	SQD	b	822	-	29,31,54	1.49	3 (10%)	39,42,65	1.17	3 (7%)
13	CLA	1	513	1	54,58,73	1.33	8 (14%)	64,95,113	1.26	6 (9%)
13	CLA	e	516	1	49,53,73	1.39	6 (12%)	58,89,113	1.20	4 (6%)
13	CLA	A	1125	2	69,73,73	1.15	8 (11%)	82,113,113	1.23	6 (7%)
13	CLA	a	510	1	69,73,73	1.17	6 (8%)	82,113,113	1.17	7 (8%)
13	CLA	B	1231	3	59,63,73	1.26	8 (13%)	70,101,113	1.18	6 (8%)
13	CLA	B	1220	3	54,58,73	1.29	8 (14%)	64,95,113	1.28	6 (9%)
13	CLA	g	502	1	64,68,73	1.21	7 (10%)	76,107,113	1.19	5 (6%)
13	CLA	g	506	1	49,53,73	1.38	7 (14%)	58,89,113	1.24	5 (8%)
14	BCR	A	4007	-	41,41,41	0.72	1 (2%)	56,56,56	2.01	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	4	513	1	54,58,73	1.32	8 (14%)	64,95,113	1.25	6 (9%)
13	CLA	g	504	-	59,63,73	1.28	6 (10%)	70,101,113	1.19	6 (8%)
13	CLA	d	509	1	69,73,73	1.17	6 (8%)	82,113,113	1.20	6 (7%)
13	CLA	c	507	-	64,68,73	1.22	7 (10%)	76,107,113	1.14	5 (6%)
13	CLA	A	1118	2	64,68,73	1.20	7 (10%)	76,107,113	1.20	5 (6%)
13	CLA	2	505	1	69,73,73	1.16	6 (8%)	82,113,113	1.15	5 (6%)
13	CLA	f	507	-	64,68,73	1.22	6 (9%)	76,107,113	1.22	5 (6%)
13	CLA	2	511	1	59,63,73	1.28	7 (11%)	70,101,113	1.19	6 (8%)
13	CLA	b	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.20	4 (5%)
14	BCR	1	521	-	41,41,41	0.65	0	56,56,56	2.06	15 (26%)
13	CLA	f	510	1	69,73,73	1.18	5 (7%)	82,113,113	1.15	5 (6%)
13	CLA	A	1128	2	69,73,73	1.14	7 (10%)	82,113,113	1.13	6 (7%)
13	CLA	4	510	1	69,73,73	1.17	8 (11%)	82,113,113	1.25	10 (12%)
13	CLA	e	503	1	67,71,73	1.20	7 (10%)	79,110,113	1.14	4 (5%)
13	CLA	A	1133	2	69,73,73	1.16	8 (11%)	82,113,113	1.15	8 (9%)
13	CLA	b	518	1	59,63,73	1.26	7 (11%)	70,101,113	1.15	4 (5%)
13	CLA	4	506	1	49,53,73	1.36	6 (12%)	58,89,113	1.26	4 (6%)
13	CLA	A	1112	2	51,55,73	1.32	8 (15%)	60,91,113	1.27	5 (8%)
13	CLA	1	505	1	69,73,73	1.17	7 (10%)	82,113,113	1.12	5 (6%)
14	BCR	4	521	-	41,41,41	0.66	0	56,56,56	2.05	14 (25%)
13	CLA	B	1202	3	69,73,73	1.14	8 (11%)	82,113,113	1.17	7 (8%)
13	CLA	B	1219	-	55,60,73	1.36	7 (12%)	57,93,113	1.35	7 (12%)
13	CLA	e	512	1	56,60,73	1.30	6 (10%)	65,97,113	1.27	5 (7%)
13	CLA	d	512	1	56,60,73	1.30	7 (12%)	65,97,113	1.30	5 (7%)
13	CLA	A	1121	2	55,59,73	1.29	6 (10%)	64,96,113	1.22	4 (6%)
13	CLA	B	1225	3	69,73,73	1.15	8 (11%)	82,113,113	1.15	6 (7%)
14	BCR	5	524	-	41,41,41	0.72	0	56,56,56	2.01	14 (25%)
15	SQD	B	1852	-	41,43,54	1.24	3 (7%)	51,54,65	1.12	4 (7%)
13	CLA	1	501	1	69,73,73	1.17	6 (8%)	82,113,113	1.09	5 (6%)
13	CLA	g	509	1	69,73,73	1.18	6 (8%)	82,113,113	1.15	5 (6%)
13	CLA	3	519	1	49,53,73	1.39	7 (14%)	58,89,113	1.29	4 (6%)
13	CLA	A	1022	-	69,73,73	1.15	8 (11%)	82,113,113	1.12	5 (6%)
13	CLA	e	511	1	49,53,73	1.39	7 (14%)	58,89,113	1.31	6 (10%)
13	CLA	A	1127	2	69,73,73	1.15	8 (11%)	82,113,113	1.18	7 (8%)
13	CLA	B	1218	3	64,68,73	1.20	9 (14%)	76,107,113	1.15	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	d	501	1	69,73,73	1.18	7 (10%)	82,113,113	1.13	5 (6%)
14	BCR	f	521	-	41,41,41	0.66	0	56,56,56	1.78	12 (21%)
13	CLA	A	1102	13,2	69,73,73	1.15	8 (11%)	82,113,113	1.17	6 (7%)
13	CLA	A	1011	2	69,73,73	1.16	6 (8%)	82,113,113	1.16	7 (8%)
13	CLA	f	513	1	54,58,73	1.32	6 (11%)	64,95,113	1.32	8 (12%)
16	LMG	2	5104	-	40,40,55	1.06	2 (5%)	48,48,63	1.08	4 (8%)
13	CLA	K	1103	10	45,49,73	1.41	6 (13%)	54,83,113	1.19	2 (3%)
13	CLA	6	519	1	49,53,73	1.39	7 (14%)	58,89,113	1.27	3 (5%)
13	CLA	f	508	1	59,63,73	1.27	8 (13%)	70,101,113	1.19	4 (5%)
13	CLA	B	1235	3	69,73,73	1.15	8 (11%)	82,113,113	1.17	6 (7%)
13	CLA	1	511	1	59,63,73	1.27	7 (11%)	70,101,113	1.17	5 (7%)
13	CLA	A	1013	-	69,73,73	1.15	7 (10%)	82,113,113	1.17	7 (8%)
13	CLA	B	1021	3	69,73,73	1.15	6 (8%)	82,113,113	1.13	7 (8%)
13	CLA	d	510	1	69,73,73	1.18	7 (10%)	82,113,113	1.16	6 (7%)
13	CLA	d	516	1	49,53,73	1.39	6 (12%)	58,89,113	1.21	4 (6%)
13	CLA	b	512	1	56,60,73	1.30	6 (10%)	65,97,113	1.22	3 (4%)
14	BCR	B	4005	-	41,41,41	0.74	0	56,56,56	2.01	15 (26%)
13	CLA	a	511	1	49,53,73	1.39	7 (14%)	58,89,113	1.25	4 (6%)
13	CLA	A	1106	2	69,73,73	1.13	7 (10%)	82,113,113	1.19	6 (7%)
13	CLA	g	517	-	49,53,73	1.40	6 (12%)	58,89,113	1.26	3 (5%)
13	CLA	e	509	1	69,73,73	1.18	6 (8%)	82,113,113	1.20	6 (7%)
13	CLA	5	506	1	49,53,73	1.38	6 (12%)	58,89,113	1.27	4 (6%)
13	CLA	a	504	-	59,63,73	1.27	8 (13%)	70,101,113	1.18	5 (7%)
13	CLA	5	517	-	49,53,73	1.39	6 (12%)	58,89,113	1.18	4 (6%)
13	CLA	B	1229	3	69,73,73	1.17	8 (11%)	82,113,113	1.17	7 (8%)
13	CLA	B	1215	3	64,68,73	1.19	8 (12%)	76,107,113	1.24	4 (5%)
13	CLA	B	1232	-	49,53,73	1.39	7 (14%)	58,89,113	1.27	5 (8%)
13	CLA	J	1302	9	49,53,73	1.35	7 (14%)	58,89,113	1.27	5 (8%)
14	BCR	5	523	-	41,41,41	0.96	2 (4%)	56,56,56	2.61	22 (39%)
13	CLA	a	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.25	5 (6%)
14	BCR	g	521	-	41,41,41	0.65	0	56,56,56	2.13	15 (26%)
14	BCR	3	522	-	41,41,41	0.72	1 (2%)	56,56,56	2.12	18 (32%)
13	CLA	a	518	1	49,53,73	1.39	6 (12%)	58,89,113	1.33	3 (5%)
13	CLA	3	501	1	69,73,73	1.16	6 (8%)	82,113,113	1.17	6 (7%)
13	CLA	A	1107	2	69,73,73	1.15	6 (8%)	82,113,113	1.16	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	6	503	1	68,72,73	1.18	6 (8%)	80,111,113	1.14	5 (6%)
13	CLA	F	1301	-	49,53,73	1.37	8 (16%)	58,89,113	1.32	6 (10%)
15	SQD	e	822	-	29,31,54	1.50	3 (10%)	39,42,65	1.18	2 (5%)
13	CLA	6	517	-	49,53,73	1.41	7 (14%)	58,89,113	1.18	5 (8%)
14	BCR	2	523	-	41,41,41	0.72	1 (2%)	56,56,56	1.91	17 (30%)
14	BCR	f	524	-	41,41,41	0.67	0	56,56,56	2.28	15 (26%)
13	CLA	b	501	1	69,73,73	1.18	8 (11%)	82,113,113	1.11	4 (4%)
13	CLA	1	516	1	49,53,73	1.40	6 (12%)	58,89,113	1.23	3 (5%)
13	CLA	c	509	1	69,73,73	1.16	7 (10%)	82,113,113	1.21	5 (6%)
13	CLA	4	511	1	49,53,73	1.44	8 (16%)	58,89,113	1.34	7 (12%)
13	CLA	A	1801	17	49,53,73	1.39	7 (14%)	58,89,113	1.26	3 (5%)
13	CLA	B	1221	3	64,68,73	1.17	7 (10%)	76,107,113	1.20	7 (9%)
13	CLA	c	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.23	6 (7%)
13	CLA	g	519	1	49,53,73	1.38	5 (10%)	58,89,113	1.24	4 (6%)
13	CLA	A	1139	-	64,68,73	1.20	8 (12%)	76,107,113	1.11	5 (6%)
14	BCR	b	524	-	41,41,41	0.73	1 (2%)	56,56,56	2.10	18 (32%)
13	CLA	b	511	1	59,63,73	1.27	7 (11%)	70,101,113	1.21	6 (8%)
14	BCR	2	524	-	41,41,41	0.69	0	56,56,56	2.01	16 (28%)
14	BCR	B	4017	-	41,41,41	0.74	0	56,56,56	2.18	17 (30%)
13	CLA	6	518	1	54,58,73	1.32	7 (12%)	64,95,113	1.21	5 (7%)
13	CLA	4	505	1	69,73,73	1.16	6 (8%)	82,113,113	1.15	5 (6%)
13	CLA	3	511	1	59,63,73	1.28	7 (11%)	70,101,113	1.27	7 (10%)
13	CLA	6	513	1	54,58,73	1.32	6 (11%)	64,95,113	1.23	5 (7%)
13	CLA	5	504	-	59,63,73	1.26	7 (11%)	70,101,113	1.18	4 (5%)
14	BCR	I	4018	-	41,41,41	0.79	2 (4%)	56,56,56	2.14	15 (26%)
13	CLA	B	1207	-	69,73,73	1.18	6 (8%)	82,113,113	1.20	5 (6%)
13	CLA	f	503	1	67,71,73	1.21	7 (10%)	79,110,113	1.09	4 (5%)
13	CLA	a	507	-	64,68,73	1.22	7 (10%)	76,107,113	1.13	4 (5%)
13	CLA	c	516	1	49,53,73	1.36	6 (12%)	58,89,113	1.22	4 (6%)
13	CLA	B	1234	3	64,68,73	1.19	9 (14%)	76,107,113	1.24	8 (10%)
13	CLA	B	1012	-	69,73,73	1.15	8 (11%)	82,113,113	1.23	8 (9%)
15	SQD	d	822	-	29,31,54	1.51	3 (10%)	39,42,65	1.24	4 (10%)
13	CLA	A	1134	2	59,63,73	1.23	6 (10%)	70,101,113	1.21	6 (8%)
13	CLA	f	511	1	59,63,73	1.28	7 (11%)	70,101,113	1.24	7 (10%)
19	SF4	C	3002	4	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	SQD	3	822	-	29,31,54	1.48	3 (10%)	39,42,65	1.14	3 (7%)
13	CLA	2	510	1	69,73,73	1.17	7 (10%)	82,113,113	1.17	4 (4%)
13	CLA	2	516	1	49,53,73	1.38	7 (14%)	58,89,113	1.21	4 (6%)
13	CLA	e	517	-	49,53,73	1.39	7 (14%)	58,89,113	1.12	3 (5%)
17	LHG	A	5003	13	40,40,48	1.01	2 (5%)	43,46,54	1.05	3 (6%)
14	BCR	B	4010	-	41,41,41	0.77	1 (2%)	56,56,56	2.12	18 (32%)
14	BCR	5	522	-	41,41,41	0.69	0	56,56,56	2.16	17 (30%)
13	CLA	g	511	1	59,63,73	1.27	7 (11%)	70,101,113	1.17	5 (7%)
13	CLA	c	510	1	69,73,73	1.16	6 (8%)	82,113,113	1.16	5 (6%)
13	CLA	g	501	1	69,73,73	1.18	7 (10%)	82,113,113	1.10	6 (7%)
13	CLA	b	504	-	59,63,73	1.27	7 (11%)	70,101,113	1.17	3 (4%)
13	CLA	4	512	1	49,53,73	1.40	8 (16%)	58,89,113	1.28	4 (6%)
13	CLA	6	512	1	49,53,73	1.39	7 (14%)	58,89,113	1.28	4 (6%)
13	CLA	2	518	1	59,63,73	1.27	7 (11%)	70,101,113	1.19	6 (8%)
14	BCR	3	524	-	41,41,41	0.66	0	56,56,56	2.03	16 (28%)
13	CLA	6	510	1	69,73,73	1.18	6 (8%)	82,113,113	1.19	6 (7%)
14	BCR	2	522	-	41,41,41	0.71	0	56,56,56	2.04	19 (33%)
16	LMG	J	5104	-	31,31,55	1.17	2 (6%)	39,39,63	1.16	4 (10%)
13	CLA	A	1116	2	64,68,73	1.21	8 (12%)	76,107,113	1.22	6 (7%)
13	CLA	5	502	1	64,68,73	1.21	7 (10%)	76,107,113	1.23	6 (7%)
14	BCR	c	523	-	41,41,41	0.69	0	56,56,56	1.88	19 (33%)
13	CLA	A	1140	2	69,73,73	1.15	7 (10%)	82,113,113	1.19	8 (9%)
13	CLA	d	518	1	59,63,73	1.26	7 (11%)	70,101,113	1.12	4 (5%)
17	LHG	A	5004	-	34,34,48	1.09	2 (5%)	37,40,54	1.15	5 (13%)
14	BCR	d	522	-	41,41,41	0.67	0	56,56,56	2.20	19 (33%)
14	BCR	e	521	-	41,41,41	0.64	0	56,56,56	2.04	13 (23%)
13	CLA	3	513	1	54,58,73	1.31	8 (14%)	64,95,113	1.24	5 (7%)
15	SQD	2	822	-	29,31,54	1.45	3 (10%)	39,42,65	1.30	5 (12%)
13	CLA	B	1213	3	69,73,73	1.14	8 (11%)	82,113,113	1.14	6 (7%)
13	CLA	d	508	1	59,63,73	1.25	8 (13%)	70,101,113	1.15	5 (7%)
13	CLA	4	509	1	69,73,73	1.16	7 (10%)	82,113,113	1.20	5 (6%)
13	CLA	6	509	1	69,73,73	1.17	8 (11%)	82,113,113	1.09	5 (6%)
13	CLA	1	517	-	49,53,73	1.40	6 (12%)	58,89,113	1.25	3 (5%)
13	CLA	B	1205	3	69,73,73	1.14	7 (10%)	82,113,113	1.16	7 (8%)
14	BCR	b	523	-	41,41,41	0.68	0	56,56,56	2.03	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	f	509	1	69,73,73	1.18	7 (10%)	82,113,113	1.16	5 (6%)
20	LMU	J	5105	-	22,22,36	1.10	1 (4%)	27,27,47	0.83	1 (3%)
13	CLA	B	1227	3	56,60,73	1.28	7 (12%)	65,97,113	1.21	6 (9%)
13	CLA	e	519	1	49,53,73	1.39	7 (14%)	58,89,113	1.24	3 (5%)
13	CLA	6	501	1	69,73,73	1.16	8 (11%)	82,113,113	1.13	5 (6%)
14	BCR	1	522	-	41,41,41	0.67	0	56,56,56	1.98	18 (32%)
13	CLA	c	518	1	59,63,73	1.26	6 (10%)	70,101,113	1.29	7 (10%)
13	CLA	B	1208	3	59,63,73	1.23	6 (10%)	70,101,113	1.19	6 (8%)
13	CLA	A	1138	2	69,73,73	1.14	7 (10%)	82,113,113	1.16	6 (7%)
16	LMG	1	5104	-	40,40,55	1.05	2 (5%)	48,48,63	1.03	2 (4%)
13	CLA	g	505	1	69,73,73	1.18	6 (8%)	82,113,113	1.15	5 (6%)
13	CLA	J	1303	9	41,50,73	2.04	10 (24%)	44,79,113	1.39	7 (15%)
13	CLA	a	506	1	49,53,73	1.37	7 (14%)	58,89,113	1.27	5 (8%)
13	CLA	d	507	-	64,68,73	1.23	6 (9%)	76,107,113	1.16	4 (5%)
13	CLA	2	504	-	49,53,73	1.39	7 (14%)	58,89,113	1.25	3 (5%)
14	BCR	a	523	-	41,41,41	0.71	1 (2%)	56,56,56	2.20	20 (35%)
13	CLA	1	510	1	69,73,73	1.19	7 (10%)	82,113,113	1.15	5 (6%)
15	SQD	g	822	-	29,31,54	1.47	3 (10%)	39,42,65	1.22	2 (5%)
13	CLA	B	1209	3	56,60,73	1.28	7 (12%)	65,97,113	1.27	7 (10%)
14	BCR	e	523	-	41,41,41	0.67	0	56,56,56	2.02	19 (33%)
13	CLA	B	1224	3	64,68,73	1.18	7 (10%)	76,107,113	1.25	7 (9%)
13	CLA	6	505	1	69,73,73	1.16	7 (10%)	82,113,113	1.12	5 (6%)
13	CLA	6	506	1	49,53,73	1.38	7 (14%)	58,89,113	1.28	4 (6%)
13	CLA	B	1223	3	69,73,73	1.14	7 (10%)	82,113,113	1.21	5 (6%)
13	CLA	b	508	1	59,63,73	1.27	8 (13%)	70,101,113	1.15	3 (4%)
13	CLA	4	517	-	49,53,73	1.38	5 (10%)	58,89,113	1.18	3 (5%)
13	CLA	5	516	1	49,53,73	1.39	7 (14%)	58,89,113	1.18	4 (6%)
13	CLA	A	1111	2	64,68,73	1.20	7 (10%)	76,107,113	1.26	7 (9%)
17	LHG	A	5001	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	4 (7%)
14	BCR	F	4014	-	41,41,41	0.76	1 (2%)	56,56,56	2.20	15 (26%)
13	CLA	f	517	-	49,53,73	1.38	7 (14%)	58,89,113	1.17	4 (6%)
15	SQD	c	822	-	29,31,54	1.49	3 (10%)	39,42,65	1.16	3 (7%)
13	CLA	3	516	1	49,53,73	1.38	6 (12%)	58,89,113	1.22	3 (5%)
13	CLA	A	1110	2	58,62,73	1.27	8 (13%)	68,99,113	1.19	4 (5%)
19	SF4	C	3003	4	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	SQD	4	822	-	29,31,54	1.46	3 (10%)	39,42,65	1.15	3 (7%)
15	SQD	6	822	-	29,31,54	1.50	3 (10%)	39,42,65	1.29	3 (7%)
13	CLA	e	501	1	69,73,73	1.18	7 (10%)	82,113,113	1.12	6 (7%)
13	CLA	e	513	1	54,58,73	1.31	7 (12%)	64,95,113	1.22	7 (10%)
14	BCR	3	523	-	41,41,41	0.71	0	56,56,56	1.91	15 (26%)
13	CLA	a	513	1	54,58,73	1.35	8 (14%)	64,95,113	1.26	5 (7%)
13	CLA	A	1237	-	69,73,73	1.17	8 (11%)	82,113,113	1.16	6 (7%)
13	CLA	A	1119	-	69,73,73	1.14	7 (10%)	82,113,113	1.16	7 (8%)
13	CLA	f	506	1	49,53,73	1.39	7 (14%)	58,89,113	1.30	5 (8%)
13	CLA	B	1226	3	69,73,73	1.15	7 (10%)	82,113,113	1.20	5 (6%)
13	CLA	2	513	1	49,53,73	1.38	8 (16%)	58,89,113	1.26	4 (6%)
14	BCR	a	521	-	41,41,41	0.66	0	56,56,56	2.11	14 (25%)
13	CLA	5	518	1	59,63,73	1.26	6 (10%)	70,101,113	1.19	4 (5%)
13	CLA	d	503	1	67,71,73	1.19	7 (10%)	79,110,113	1.17	6 (7%)
13	CLA	A	1126	2	69,73,73	1.15	7 (10%)	82,113,113	1.28	7 (8%)
13	CLA	d	519	1	49,53,73	1.39	7 (14%)	58,89,113	1.28	3 (5%)
13	CLA	B	1210	3	69,73,73	1.15	7 (10%)	82,113,113	1.22	6 (7%)
13	CLA	5	505	1	69,73,73	1.16	5 (7%)	82,113,113	1.15	7 (8%)
13	CLA	b	507	-	64,68,73	1.21	7 (10%)	76,107,113	1.19	4 (5%)
13	CLA	3	510	1	69,73,73	1.17	8 (11%)	82,113,113	1.21	7 (8%)
13	CLA	a	508	1	59,63,73	1.26	7 (11%)	70,101,113	1.18	4 (5%)
13	CLA	e	505	1	69,73,73	1.18	6 (8%)	82,113,113	1.13	6 (7%)
13	CLA	a	505	1	69,73,73	1.18	6 (8%)	82,113,113	1.13	4 (4%)
14	BCR	M	4021	-	41,41,41	0.66	0	56,56,56	2.09	17 (30%)
16	LMG	g	5104	-	40,40,55	1.06	2 (5%)	48,48,63	1.05	3 (6%)
13	CLA	4	501	1	69,73,73	1.17	8 (11%)	82,113,113	1.12	6 (7%)
14	BCR	4	523	-	41,41,41	0.68	0	56,56,56	1.99	16 (28%)
13	CLA	X	1401	12	49,53,73	1.38	8 (16%)	58,89,113	1.29	5 (8%)
13	CLA	6	508	1	59,63,73	1.25	7 (11%)	70,101,113	1.16	3 (4%)
13	CLA	A	1124	-	64,68,73	1.19	7 (10%)	76,107,113	1.19	7 (9%)
15	SQD	f	822	-	29,31,54	1.50	3 (10%)	39,42,65	1.13	3 (7%)
13	CLA	c	519	1	49,53,73	1.39	8 (16%)	58,89,113	1.23	4 (6%)
14	BCR	1	524	-	41,41,41	0.70	0	56,56,56	2.23	16 (28%)
18	PQN	A	2001	-	34,34,34	0.42	0	43,45,45	0.64	1 (2%)
13	CLA	3	504	-	59,63,73	1.26	8 (13%)	70,101,113	1.15	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	1	506	1	49,53,73	1.37	6 (12%)	58,89,113	1.26	4 (6%)
14	BCR	J	4013	-	41,41,41	0.75	1 (2%)	56,56,56	2.21	16 (28%)
13	CLA	b	510	1	69,73,73	1.17	6 (8%)	82,113,113	1.22	9 (10%)
13	CLA	A	1131	2	69,73,73	1.15	6 (8%)	82,113,113	1.18	6 (7%)
13	CLA	c	504	-	54,58,73	1.31	6 (11%)	64,95,113	1.24	5 (7%)
13	CLA	B	1023	-	69,73,73	1.15	7 (10%)	82,113,113	1.18	8 (9%)
14	BCR	b	521	-	41,41,41	0.67	0	56,56,56	2.05	16 (28%)
13	CLA	g	516	1	49,53,73	1.39	5 (10%)	58,89,113	1.19	5 (8%)
13	CLA	4	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.21	5 (6%)
13	CLA	B	1206	3	69,73,73	1.15	8 (11%)	82,113,113	1.23	5 (6%)
13	CLA	B	1212	3	49,53,73	1.35	7 (14%)	58,89,113	1.26	4 (6%)
19	SF4	A	3001	3,2	0,12,12	-	-	-	-	-
13	CLA	4	504	-	49,53,73	1.38	7 (14%)	58,89,113	1.22	3 (5%)
13	CLA	A	1104	2	69,73,73	1.14	8 (11%)	82,113,113	1.21	7 (8%)
13	CLA	4	518	1	59,63,73	1.26	7 (11%)	70,101,113	1.16	6 (8%)
13	CLA	B	1236	3	54,58,73	1.28	7 (12%)	64,95,113	1.33	7 (10%)
13	CLA	6	516	1	49,53,73	1.38	6 (12%)	58,89,113	1.21	3 (5%)
13	CLA	3	506	1	49,53,73	1.37	7 (14%)	58,89,113	1.30	7 (12%)
13	CLA	A	1108	2	49,53,73	1.34	6 (12%)	58,89,113	1.26	3 (5%)
13	CLA	b	517	-	49,53,73	1.42	7 (14%)	58,89,113	1.11	3 (5%)
13	CLA	f	501	1	69,73,73	1.19	7 (10%)	82,113,113	1.11	6 (7%)
14	BCR	d	523	-	41,41,41	0.70	0	56,56,56	1.96	12 (21%)
13	CLA	3	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.20	6 (7%)
13	CLA	4	516	1	49,53,73	1.38	7 (14%)	58,89,113	1.24	4 (6%)
13	CLA	2	508	1	59,63,73	1.26	8 (13%)	70,101,113	1.16	5 (7%)
13	CLA	3	507	-	64,68,73	1.21	8 (12%)	76,107,113	1.20	4 (5%)
13	CLA	2	503	1	68,72,73	1.18	8 (11%)	80,111,113	1.17	5 (6%)
13	CLA	3	512	1	56,60,73	1.30	7 (12%)	65,97,113	1.24	6 (9%)
13	CLA	b	519	1	49,53,73	1.38	7 (14%)	58,89,113	1.28	5 (8%)
13	CLA	g	510	1	69,73,73	1.17	6 (8%)	82,113,113	1.13	3 (3%)
14	BCR	f	522	-	41,41,41	0.73	0	56,56,56	2.20	15 (26%)
13	CLA	5	509	1	69,73,73	1.17	8 (11%)	82,113,113	1.20	4 (4%)
14	BCR	4	522	-	41,41,41	0.68	0	56,56,56	2.05	18 (32%)
13	CLA	a	519	-	49,53,73	1.39	6 (12%)	58,89,113	1.26	3 (5%)
13	CLA	f	505	1	69,73,73	1.16	8 (11%)	82,113,113	1.22	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	1132	2	69,73,73	1.16	5 (7%)	82,113,113	1.16	5 (6%)
13	CLA	3	509	1	69,73,73	1.17	7 (10%)	82,113,113	1.23	6 (7%)
13	CLA	B	1222	-	64,68,73	1.19	8 (12%)	76,107,113	1.21	8 (10%)
13	CLA	d	513	1	54,58,73	1.31	8 (14%)	64,95,113	1.24	5 (7%)
20	LMU	A	1848	-	24,24,36	1.05	1 (4%)	29,29,47	0.78	0
13	CLA	B	1203	3	69,73,73	1.15	9 (13%)	82,113,113	1.19	4 (4%)
13	CLA	1	512	1	56,60,73	1.28	6 (10%)	65,97,113	1.42	6 (9%)
13	CLA	6	507	-	64,68,73	1.22	6 (9%)	76,107,113	1.17	5 (6%)
13	CLA	2	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.22	6 (7%)
14	BCR	1	523	-	41,41,41	0.72	1 (2%)	56,56,56	1.93	16 (28%)
13	CLA	A	1135	2	55,59,73	1.28	7 (12%)	64,96,113	1.27	6 (9%)
13	CLA	A	1114	-	49,53,73	1.37	6 (12%)	58,89,113	1.36	3 (5%)
14	BCR	J	4012	-	41,41,41	0.75	0	56,56,56	2.14	18 (32%)
13	CLA	A	1122	2	64,68,73	1.19	8 (12%)	76,107,113	1.18	6 (7%)
20	LMU	B	1843	-	36,36,36	1.16	2 (5%)	47,47,47	0.96	1 (2%)
13	CLA	B	1238	-	69,73,73	1.14	7 (10%)	82,113,113	1.11	4 (4%)
14	BCR	B	4004	-	41,41,41	0.68	0	56,56,56	2.07	17 (30%)
14	BCR	3	521	-	41,41,41	0.68	0	56,56,56	1.96	11 (19%)
13	CLA	c	513	1	54,58,73	1.32	7 (12%)	64,95,113	1.22	6 (9%)
13	CLA	d	505	1	69,73,73	1.16	6 (8%)	82,113,113	1.14	6 (7%)
20	LMU	A	1849	-	23,23,36	1.08	1 (4%)	28,28,47	0.80	0
13	CLA	B	1214	3	69,73,73	1.15	8 (11%)	82,113,113	1.18	6 (7%)
13	CLA	A	1117	2	69,73,73	1.17	7 (10%)	82,113,113	1.19	7 (8%)
14	BCR	g	522	-	41,41,41	0.68	0	56,56,56	2.16	15 (26%)
13	CLA	1	502	1	64,68,73	1.21	7 (10%)	76,107,113	1.15	5 (6%)
13	CLA	1	518	1	59,63,73	1.28	7 (11%)	70,101,113	1.14	4 (5%)
13	CLA	A	1137	2	59,63,73	1.23	7 (11%)	70,101,113	1.24	7 (10%)
13	CLA	A	1120	2	57,61,73	1.28	8 (14%)	67,98,113	1.20	4 (5%)
13	CLA	2	506	1	49,53,73	1.39	8 (16%)	58,89,113	1.27	4 (6%)
13	CLA	3	503	1	67,71,73	1.18	7 (10%)	79,110,113	1.21	7 (8%)
13	CLA	f	512	1	49,53,73	1.39	6 (12%)	58,89,113	1.29	3 (5%)
13	CLA	3	517	-	49,53,73	1.39	8 (16%)	58,89,113	1.30	4 (6%)
14	BCR	6	521	-	41,41,41	0.67	0	56,56,56	2.14	16 (28%)
14	BCR	I	4019	-	41,41,41	0.71	0	56,56,56	1.84	10 (17%)
14	BCR	c	521	-	41,41,41	0.65	0	56,56,56	1.98	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	b	522	-	41,41,41	0.70	0	56,56,56	2.03	17 (30%)
14	BCR	B	4009	-	41,41,41	0.73	0	56,56,56	2.14	20 (35%)
13	CLA	5	510	1	69,73,73	1.17	7 (10%)	82,113,113	1.18	6 (7%)
13	CLA	c	505	1	69,73,73	1.18	7 (10%)	82,113,113	1.18	6 (7%)
13	CLA	4	519	1	54,58,73	1.30	7 (12%)	64,95,113	1.26	7 (10%)
13	CLA	b	513	1	54,58,73	1.31	7 (12%)	64,95,113	1.26	6 (9%)
13	CLA	d	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.17	5 (6%)
13	CLA	f	519	1	49,53,73	1.39	7 (14%)	58,89,113	1.24	5 (8%)
14	BCR	A	4002	-	41,41,41	0.77	1 (2%)	56,56,56	2.13	14 (25%)
15	SQD	a	822	-	29,31,54	1.50	3 (10%)	39,42,65	1.12	2 (5%)
13	CLA	2	507	-	64,68,73	1.21	7 (10%)	76,107,113	1.18	6 (7%)
14	BCR	F	4016	-	41,41,41	0.71	0	56,56,56	1.98	13 (23%)
13	CLA	c	501	1	69,73,73	1.17	7 (10%)	82,113,113	1.11	5 (6%)
13	CLA	3	508	1	59,63,73	1.26	8 (13%)	70,101,113	1.15	5 (7%)
13	CLA	5	507	-	64,68,73	1.22	6 (9%)	76,107,113	1.15	5 (6%)
13	CLA	1	509	1	69,73,73	1.17	7 (10%)	82,113,113	1.18	5 (6%)
13	CLA	a	517	-	49,53,73	1.41	6 (12%)	58,89,113	1.19	3 (5%)
15	SQD	1	822	-	29,31,54	1.51	3 (10%)	39,42,65	1.12	4 (10%)
13	CLA	B	1217	3	59,63,73	1.26	7 (11%)	70,101,113	1.22	4 (5%)
13	CLA	A	1101	2	64,68,73	1.20	8 (12%)	76,107,113	1.23	6 (7%)
13	CLA	a	501	1	69,73,73	1.17	6 (8%)	82,113,113	1.16	6 (7%)
13	CLA	2	509	1	69,73,73	1.16	7 (10%)	82,113,113	1.22	6 (7%)
14	BCR	6	523	-	41,41,41	0.67	0	56,56,56	2.05	15 (26%)
14	BCR	A	4008	-	41,41,41	0.78	1 (2%)	56,56,56	2.16	17 (30%)
13	CLA	b	505	1	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
14	BCR	A	4011	-	41,41,41	0.76	1 (2%)	56,56,56	2.19	16 (28%)
13	CLA	5	513	1	59,63,73	1.27	6 (10%)	70,101,113	1.17	5 (7%)
14	BCR	B	4006	-	41,41,41	0.73	0	56,56,56	2.15	15 (26%)
13	CLA	A	1130	2	59,63,73	1.24	7 (11%)	70,101,113	1.26	8 (11%)
14	BCR	4	524	-	41,41,41	0.69	0	56,56,56	2.20	16 (28%)
14	BCR	6	524	-	41,41,41	0.67	0	56,56,56	2.10	16 (28%)
13	CLA	c	511	1	59,63,73	1.27	7 (11%)	70,101,113	1.28	7 (10%)
13	CLA	3	518	1	59,63,73	1.26	7 (11%)	70,101,113	1.20	5 (7%)
13	CLA	g	507	-	64,68,73	1.23	7 (10%)	76,107,113	1.14	5 (6%)
13	CLA	f	516	1	49,53,73	1.38	6 (12%)	58,89,113	1.23	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	2	521	-	41,41,41	0.67	0	56,56,56	2.07	17 (30%)
13	CLA	g	512	1	56,60,73	1.30	6 (10%)	65,97,113	1.22	4 (6%)
13	CLA	d	506	1	49,53,73	1.38	6 (12%)	58,89,113	1.27	4 (6%)
14	BCR	d	524	-	41,41,41	0.69	0	56,56,56	2.18	19 (33%)
13	CLA	B	1216	-	64,68,73	1.21	8 (12%)	76,107,113	1.17	6 (7%)
13	CLA	g	508	1	56,60,73	1.30	7 (12%)	65,97,113	1.20	3 (4%)
14	BCR	g	524	-	41,41,41	0.70	0	56,56,56	2.06	15 (26%)
13	CLA	5	519	1	54,58,73	1.32	7 (12%)	64,95,113	1.29	5 (7%)
13	CLA	5	503	1	68,72,73	1.18	6 (8%)	80,111,113	1.17	5 (6%)
14	BCR	a	522	-	41,41,41	0.71	1 (2%)	56,56,56	2.26	18 (32%)
13	CLA	e	510	1	69,73,73	1.18	6 (8%)	82,113,113	1.17	5 (6%)
14	BCR	5	521	-	41,41,41	0.69	0	56,56,56	2.01	14 (25%)
13	CLA	e	502	1	64,68,73	1.23	7 (10%)	76,107,113	1.28	4 (5%)
13	CLA	5	508	1	59,63,73	1.26	8 (13%)	70,101,113	1.16	5 (7%)
13	CLA	e	506	1	49,53,73	1.39	7 (14%)	58,89,113	1.29	5 (8%)
13	CLA	e	504	-	59,63,73	1.27	7 (11%)	70,101,113	1.21	5 (7%)
14	BCR	A	4003	-	41,41,41	0.75	1 (2%)	56,56,56	2.11	15 (26%)
14	BCR	e	522	-	41,41,41	0.70	0	56,56,56	2.06	16 (28%)
13	CLA	2	519	1	54,58,73	1.32	6 (11%)	64,95,113	1.24	4 (6%)
13	CLA	g	513	1	54,58,73	1.34	6 (11%)	64,95,113	1.26	6 (9%)
13	CLA	2	517	-	49,53,73	1.39	8 (16%)	58,89,113	1.18	4 (6%)
13	CLA	B	1230	3	62,66,73	1.21	7 (11%)	73,104,113	1.21	5 (6%)
13	CLA	B	1233	-	49,53,73	1.38	7 (14%)	58,89,113	1.30	3 (5%)
13	CLA	4	503	1	68,72,73	1.18	7 (10%)	80,111,113	1.21	6 (7%)
15	SQD	5	822	-	29,31,54	1.47	3 (10%)	39,42,65	1.18	3 (7%)
14	BCR	F	4015	-	41,41,41	0.75	1 (2%)	56,56,56	2.10	17 (30%)
13	CLA	g	518	1	59,63,73	1.27	7 (11%)	70,101,113	1.20	5 (7%)
13	CLA	b	503	1	67,71,73	1.19	7 (10%)	79,110,113	1.16	4 (5%)
13	CLA	b	509	1	69,73,73	1.21	7 (10%)	82,113,113	1.21	5 (6%)
13	CLA	A	1109	13,2	69,73,73	1.14	7 (10%)	82,113,113	1.13	5 (6%)
13	CLA	6	511	1	49,53,73	1.40	7 (14%)	58,89,113	1.26	5 (8%)
13	CLA	e	507	-	64,68,73	1.21	7 (10%)	76,107,113	1.22	3 (3%)
14	BCR	c	522	-	41,41,41	0.71	0	56,56,56	2.31	18 (32%)
14	BCR	K	4001	-	41,41,41	0.72	0	56,56,56	1.93	16 (28%)
13	CLA	A	1103	2	69,73,73	1.15	7 (10%)	82,113,113	1.27	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	6	522	-	41,41,41	0.70	0	56,56,56	2.22	16 (28%)
13	CLA	B	1211	3	69,73,73	1.17	8 (11%)	82,113,113	1.16	7 (8%)
13	CLA	b	506	1	49,53,73	1.49	9 (18%)	58,89,113	1.74	12 (20%)
16	LMG	6	5104	-	38,38,55	1.07	2 (5%)	46,46,63	1.09	3 (6%)
16	LMG	B	5002	-	55,55,55	0.88	2 (3%)	63,63,63	0.94	2 (3%)
13	CLA	c	512	1	49,53,73	1.40	7 (14%)	58,89,113	1.31	4 (6%)

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
13	CLA	1	504	-	1/1/13/20	15/27/103/115	-
14	BCR	f	523	-	-	3/29/63/63	0/2/2/2
13	CLA	5	511	1	1/1/13/20	10/27/103/115	-
13	CLA	a	509	1	1/1/15/20	11/39/115/115	-
13	CLA	6	502	1	1/1/14/20	12/33/109/115	-
13	CLA	5	501	1	1/1/15/20	11/39/115/115	-
18	PQN	B	2002	-	-	10/23/43/43	0/2/2/2
13	CLA	3	505	1	1/1/15/20	18/39/115/115	-
13	CLA	B	1239	3	-	13/39/115/115	-
13	CLA	A	1105	2	1/1/12/20	2/23/99/115	-
13	CLA	4	508	1	1/1/13/20	4/27/103/115	-
13	CLA	c	506	1	1/1/11/20	4/15/91/115	-
13	CLA	2	501	1	1/1/15/20	13/39/115/115	-
14	BCR	I	4020	-	-	5/29/63/63	0/2/2/2
13	CLA	B	1201	3	1/1/13/20	9/30/106/115	-
13	CLA	g	503	1	1/1/14/20	14/37/113/115	-
13	CLA	B	1204	-	1/1/14/20	4/33/109/115	-
13	CLA	a	503	1	1/1/14/20	10/37/113/115	-
17	LHG	A	5005	-	-	15/49/49/53	-
13	CLA	K	1401	-	1/1/13/20	8/27/103/115	-
14	BCR	a	524	-	-	3/29/63/63	0/2/2/2
13	CLA	d	511	1	1/1/13/20	12/27/103/115	-
13	CLA	A	1129	2	1/1/12/20	4/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1113	2	1/1/11/20	6/20/96/115	-
13	CLA	6	504	-	1/1/11/20	4/15/91/115	-
13	CLA	e	508	1	1/1/13/20	5/27/103/115	-
13	CLA	f	502	1	1/1/14/20	11/33/109/115	-
14	BCR	e	524	-	-	3/29/63/63	0/2/2/2
13	CLA	d	517	-	1/1/11/20	6/15/91/115	-
13	CLA	d	504	-	1/1/13/20	9/27/103/115	-
13	CLA	f	504	-	1/1/13/20	11/27/103/115	-
13	CLA	f	518	1	1/1/13/20	15/27/103/115	-
13	CLA	c	503	1	1/1/14/20	13/37/113/115	-
13	CLA	e	518	1	1/1/13/20	15/27/103/115	-
14	BCR	c	524	-	-	4/29/63/63	0/2/2/2
14	BCR	g	523	-	-	4/29/63/63	0/2/2/2
17	LHG	A	5002	-	-	17/45/45/53	-
13	CLA	c	508	1	1/1/13/20	8/27/103/115	-
13	CLA	1	507	-	1/1/14/20	9/33/109/115	-
14	BCR	d	521	-	-	6/29/63/63	0/2/2/2
13	CLA	1	519	-	1/1/11/20	7/15/91/115	-
13	CLA	1	503	1	1/1/14/20	16/37/113/115	-
13	CLA	2	512	1	1/1/12/20	10/24/100/115	-
13	CLA	1	508	1	1/1/13/20	3/27/103/115	-
13	CLA	4	507	-	1/1/14/20	7/33/109/115	-
13	CLA	b	516	1	1/1/11/20	7/15/91/115	-
13	CLA	A	1136	2	1/1/15/20	12/39/115/115	-
13	CLA	c	517	-	1/1/11/20	6/15/91/115	-
13	CLA	a	516	1	1/1/11/20	5/15/91/115	-
13	CLA	a	512	1	1/1/12/20	9/24/100/115	-
13	CLA	5	512	1	1/1/12/20	3/24/100/115	-
13	CLA	A	1115	-	1/1/14/20	18/33/109/115	-
13	CLA	A	1123	-	1/1/15/20	6/39/115/115	-
13	CLA	B	1228	3	1/1/13/20	6/27/103/115	-
15	SQD	b	822	-	-	6/26/46/69	0/1/1/1
13	CLA	1	513	1	1/1/12/20	8/21/97/115	-
13	CLA	e	516	1	1/1/11/20	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1125	2	1/1/15/20	15/39/115/115	-
13	CLA	a	510	1	1/1/15/20	14/39/115/115	-
13	CLA	B	1231	3	1/1/13/20	12/27/103/115	-
13	CLA	B	1220	3	1/1/12/20	0/21/97/115	-
13	CLA	g	502	1	1/1/14/20	15/33/109/115	-
13	CLA	g	506	1	1/1/11/20	7/15/91/115	-
14	BCR	A	4007	-	-	2/29/63/63	0/2/2/2
13	CLA	4	513	1	1/1/12/20	2/21/97/115	-
13	CLA	g	504	-	1/1/13/20	8/27/103/115	-
13	CLA	d	509	1	1/1/15/20	8/39/115/115	-
13	CLA	c	507	-	1/1/14/20	10/33/109/115	-
13	CLA	A	1118	2	1/1/14/20	16/33/109/115	-
13	CLA	2	505	1	1/1/15/20	16/39/115/115	-
13	CLA	f	507	-	1/1/14/20	13/33/109/115	-
13	CLA	2	511	1	1/1/13/20	4/27/103/115	-
13	CLA	b	502	1	1/1/14/20	12/33/109/115	-
14	BCR	1	521	-	-	7/29/63/63	0/2/2/2
13	CLA	f	510	1	1/1/15/20	13/39/115/115	-
13	CLA	A	1128	2	1/1/15/20	6/39/115/115	-
13	CLA	4	510	1	1/1/15/20	16/39/115/115	-
13	CLA	e	503	1	1/1/14/20	11/37/113/115	-
13	CLA	A	1133	2	1/1/15/20	9/39/115/115	-
13	CLA	b	518	1	1/1/13/20	11/27/103/115	-
13	CLA	4	506	1	1/1/11/20	7/15/91/115	-
13	CLA	A	1112	2	1/1/11/20	8/18/94/115	-
13	CLA	1	505	1	1/1/15/20	18/39/115/115	-
14	BCR	4	521	-	-	6/29/63/63	0/2/2/2
13	CLA	B	1202	3	1/1/15/20	21/39/115/115	-
13	CLA	B	1219	-	1/1/13/20	8/28/95/115	-
13	CLA	e	512	1	1/1/12/20	7/24/100/115	-
13	CLA	d	512	1	1/1/12/20	6/24/100/115	-
13	CLA	A	1121	2	1/1/12/20	7/23/99/115	-
13	CLA	B	1225	3	1/1/15/20	12/39/115/115	-
14	BCR	5	524	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SQD	B	1852	-	-	4/38/58/69	0/1/1/1
13	CLA	1	501	1	1/1/15/20	14/39/115/115	-
13	CLA	g	509	1	1/1/15/20	15/39/115/115	-
13	CLA	3	519	1	1/1/11/20	4/15/91/115	-
13	CLA	A	1022	-	1/1/15/20	11/39/115/115	-
13	CLA	e	511	1	1/1/11/20	5/15/91/115	-
13	CLA	A	1127	2	1/1/15/20	11/39/115/115	-
13	CLA	B	1218	3	1/1/14/20	14/33/109/115	-
13	CLA	d	501	1	1/1/15/20	13/39/115/115	-
14	BCR	f	521	-	-	6/29/63/63	0/2/2/2
13	CLA	A	1102	13,2	1/1/15/20	7/39/115/115	-
13	CLA	A	1011	2	1/1/15/20	12/39/115/115	-
13	CLA	f	513	1	1/1/12/20	3/21/97/115	-
16	LMG	2	5104	-	-	4/35/55/70	0/1/1/1
13	CLA	K	1103	10	1/1/9/20	6/9/81/115	-
13	CLA	6	519	1	1/1/11/20	5/15/91/115	-
13	CLA	f	508	1	1/1/13/20	3/27/103/115	-
13	CLA	B	1235	3	-	9/39/115/115	-
13	CLA	1	511	1	1/1/13/20	6/27/103/115	-
13	CLA	A	1013	-	1/1/15/20	13/39/115/115	-
13	CLA	B	1021	3	1/1/15/20	17/39/115/115	-
13	CLA	d	510	1	1/1/15/20	9/39/115/115	-
13	CLA	d	516	1	1/1/11/20	6/15/91/115	-
13	CLA	b	512	1	1/1/12/20	12/24/100/115	-
14	BCR	B	4005	-	-	2/29/63/63	0/2/2/2
13	CLA	a	511	1	1/1/11/20	9/15/91/115	-
13	CLA	A	1106	2	1/1/15/20	20/39/115/115	-
13	CLA	g	517	-	1/1/11/20	8/15/91/115	-
13	CLA	e	509	1	1/1/15/20	9/39/115/115	-
13	CLA	5	506	1	1/1/11/20	6/15/91/115	-
13	CLA	a	504	-	1/1/13/20	6/27/103/115	-
13	CLA	5	517	-	1/1/11/20	6/15/91/115	-
13	CLA	B	1229	3	1/1/15/20	13/39/115/115	-
13	CLA	B	1215	3	1/1/14/20	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1232	-	1/1/11/20	9/15/91/115	-
13	CLA	J	1302	9	1/1/11/20	6/15/91/115	-
14	BCR	5	523	-	-	12/29/63/63	0/2/2/2
13	CLA	a	502	1	1/1/14/20	9/33/109/115	-
14	BCR	g	521	-	-	4/29/63/63	0/2/2/2
14	BCR	3	522	-	-	2/29/63/63	0/2/2/2
13	CLA	a	518	1	1/1/11/20	4/15/91/115	-
13	CLA	3	501	1	1/1/15/20	10/39/115/115	-
13	CLA	A	1107	2	1/1/15/20	14/39/115/115	-
13	CLA	6	503	1	1/1/14/20	18/38/114/115	-
13	CLA	F	1301	-	1/1/11/20	6/15/91/115	-
15	SQD	e	822	-	-	4/26/46/69	0/1/1/1
13	CLA	6	517	-	1/1/11/20	8/15/91/115	-
14	BCR	2	523	-	-	2/29/63/63	0/2/2/2
14	BCR	f	524	-	-	4/29/63/63	0/2/2/2
13	CLA	b	501	1	1/1/15/20	9/39/115/115	-
13	CLA	1	516	1	1/1/11/20	6/15/91/115	-
13	CLA	c	509	1	1/1/15/20	10/39/115/115	-
13	CLA	4	511	1	-	3/15/91/115	-
13	CLA	A	1801	17	1/1/11/20	8/15/91/115	-
13	CLA	B	1221	3	1/1/14/20	12/33/109/115	-
13	CLA	c	502	1	1/1/14/20	15/33/109/115	-
13	CLA	g	519	1	1/1/11/20	7/15/91/115	-
13	CLA	A	1139	-	1/1/14/20	12/33/109/115	-
14	BCR	b	524	-	-	6/29/63/63	0/2/2/2
13	CLA	b	511	1	1/1/13/20	3/27/103/115	-
14	BCR	2	524	-	-	3/29/63/63	0/2/2/2
14	BCR	B	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	6	518	1	1/1/12/20	7/21/97/115	-
13	CLA	4	505	1	1/1/15/20	18/39/115/115	-
13	CLA	3	511	1	1/1/13/20	7/27/103/115	-
13	CLA	6	513	1	1/1/12/20	7/21/97/115	-
13	CLA	5	504	-	1/1/13/20	11/27/103/115	-
14	BCR	I	4018	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1207	-	-	12/39/115/115	-
13	CLA	f	503	1	1/1/14/20	15/37/113/115	-
13	CLA	a	507	-	1/1/14/20	6/33/109/115	-
13	CLA	c	516	1	1/1/11/20	6/15/91/115	-
13	CLA	B	1234	3	1/1/14/20	7/33/109/115	-
13	CLA	B	1012	-	1/1/15/20	16/39/115/115	-
15	SQD	d	822	-	-	7/26/46/69	0/1/1/1
13	CLA	A	1134	2	1/1/13/20	11/27/103/115	-
13	CLA	f	511	1	1/1/13/20	6/27/103/115	-
19	SF4	C	3002	4	-	-	0/6/5/5
15	SQD	3	822	-	-	4/26/46/69	0/1/1/1
13	CLA	2	510	1	1/1/15/20	20/39/115/115	-
13	CLA	2	516	1	1/1/11/20	6/15/91/115	-
13	CLA	e	517	-	1/1/11/20	7/15/91/115	-
17	LHG	A	5003	13	-	10/45/45/53	-
14	BCR	B	4010	-	-	2/29/63/63	0/2/2/2
14	BCR	5	522	-	-	5/29/63/63	0/2/2/2
13	CLA	g	511	1	1/1/13/20	11/27/103/115	-
13	CLA	c	510	1	1/1/15/20	8/39/115/115	-
13	CLA	g	501	1	1/1/15/20	14/39/115/115	-
13	CLA	b	504	-	1/1/13/20	15/27/103/115	-
13	CLA	4	512	1	1/1/11/20	3/15/91/115	-
13	CLA	6	512	1	1/1/11/20	9/15/91/115	-
13	CLA	2	518	1	1/1/13/20	10/27/103/115	-
14	BCR	3	524	-	-	2/29/63/63	0/2/2/2
13	CLA	6	510	1	1/1/15/20	15/39/115/115	-
14	BCR	2	522	-	-	6/29/63/63	0/2/2/2
16	LMG	J	5104	-	-	5/26/46/70	0/1/1/1
13	CLA	A	1116	2	1/1/14/20	16/33/109/115	-
13	CLA	5	502	1	1/1/14/20	11/33/109/115	-
14	BCR	c	523	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1140	2	1/1/15/20	10/39/115/115	-
13	CLA	d	518	1	1/1/13/20	9/27/103/115	-
17	LHG	A	5004	-	-	15/39/39/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	d	522	-	-	4/29/63/63	0/2/2/2
14	BCR	e	521	-	-	5/29/63/63	0/2/2/2
13	CLA	3	513	1	1/1/12/20	3/21/97/115	-
15	SQD	2	822	-	-	5/26/46/69	0/1/1/1
13	CLA	B	1213	3	1/1/15/20	15/39/115/115	-
13	CLA	d	508	1	1/1/13/20	5/27/103/115	-
13	CLA	4	509	1	1/1/15/20	7/39/115/115	-
13	CLA	6	509	1	1/1/15/20	15/39/115/115	-
13	CLA	1	517	-	1/1/11/20	8/15/91/115	-
13	CLA	B	1205	3	1/1/15/20	8/39/115/115	-
14	BCR	b	523	-	-	3/29/63/63	0/2/2/2
13	CLA	f	509	1	1/1/15/20	8/39/115/115	-
20	LMU	J	5105	-	-	8/13/33/61	0/1/1/2
13	CLA	B	1227	3	1/1/12/20	10/24/100/115	-
13	CLA	e	519	1	1/1/11/20	7/15/91/115	-
13	CLA	6	501	1	1/1/15/20	13/39/115/115	-
14	BCR	1	522	-	-	5/29/63/63	0/2/2/2
13	CLA	c	518	1	1/1/13/20	12/27/103/115	-
13	CLA	B	1208	3	1/1/13/20	0/27/103/115	-
13	CLA	A	1138	2	1/1/15/20	13/39/115/115	-
16	LMG	1	5104	-	-	4/35/55/70	0/1/1/1
13	CLA	g	505	1	1/1/15/20	10/39/115/115	-
13	CLA	a	506	1	1/1/11/20	5/15/91/115	-
13	CLA	J	1303	9	-	10/27/77/115	-
13	CLA	d	507	-	1/1/14/20	4/33/109/115	-
13	CLA	2	504	-	1/1/11/20	5/15/91/115	-
14	BCR	a	523	-	-	5/29/63/63	0/2/2/2
13	CLA	1	510	1	1/1/15/20	10/39/115/115	-
15	SQD	g	822	-	-	7/26/46/69	0/1/1/1
13	CLA	B	1209	3	1/1/12/20	10/24/100/115	-
14	BCR	e	523	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1224	3	1/1/14/20	14/33/109/115	-
13	CLA	6	505	1	1/1/15/20	18/39/115/115	-
13	CLA	6	506	1	1/1/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1223	3	1/1/15/20	9/39/115/115	-
13	CLA	b	508	1	1/1/13/20	7/27/103/115	-
13	CLA	4	517	-	1/1/11/20	6/15/91/115	-
13	CLA	5	516	1	1/1/11/20	11/15/91/115	-
13	CLA	A	1111	2	1/1/14/20	10/33/109/115	-
17	LHG	A	5001	-	-	8/53/53/53	-
14	BCR	F	4014	-	-	6/29/63/63	0/2/2/2
13	CLA	f	517	-	1/1/11/20	7/15/91/115	-
15	SQD	c	822	-	-	4/26/46/69	0/1/1/1
13	CLA	3	516	1	1/1/11/20	8/15/91/115	-
13	CLA	A	1110	2	1/1/12/20	7/26/102/115	-
19	SF4	C	3003	4	-	-	0/6/5/5
15	SQD	4	822	-	-	5/26/46/69	0/1/1/1
15	SQD	6	822	-	-	8/26/46/69	0/1/1/1
13	CLA	e	501	1	1/1/15/20	13/39/115/115	-
13	CLA	e	513	1	1/1/12/20	3/21/97/115	-
14	BCR	3	523	-	-	9/29/63/63	0/2/2/2
13	CLA	a	513	1	-	7/21/97/115	-
13	CLA	A	1237	-	1/1/15/20	12/39/115/115	-
13	CLA	A	1119	-	1/1/15/20	12/39/115/115	-
13	CLA	f	506	1	-	2/15/91/115	-
13	CLA	B	1226	3	1/1/15/20	12/39/115/115	-
13	CLA	2	513	1	1/1/11/20	6/15/91/115	-
14	BCR	a	521	-	-	6/29/63/63	0/2/2/2
13	CLA	5	518	1	1/1/13/20	6/27/103/115	-
13	CLA	d	503	1	1/1/14/20	17/37/113/115	-
13	CLA	A	1126	2	1/1/15/20	20/39/115/115	-
13	CLA	d	519	1	1/1/11/20	5/15/91/115	-
13	CLA	B	1210	3	1/1/15/20	16/39/115/115	-
13	CLA	5	505	1	1/1/15/20	11/39/115/115	-
13	CLA	b	507	-	1/1/14/20	6/33/109/115	-
13	CLA	3	510	1	1/1/15/20	16/39/115/115	-
13	CLA	a	508	1	1/1/13/20	6/27/103/115	-
13	CLA	e	505	1	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	a	505	1	1/1/15/20	15/39/115/115	-
14	BCR	M	4021	-	-	7/29/63/63	0/2/2/2
16	LMG	g	5104	-	-	3/35/55/70	0/1/1/1
13	CLA	4	501	1	1/1/15/20	14/39/115/115	-
14	BCR	4	523	-	-	4/29/63/63	0/2/2/2
13	CLA	X	1401	12	1/1/11/20	3/15/91/115	-
13	CLA	6	508	1	1/1/13/20	8/27/103/115	-
13	CLA	A	1124	-	-	3/33/109/115	-
15	SQD	f	822	-	-	9/26/46/69	0/1/1/1
13	CLA	c	519	1	1/1/11/20	4/15/91/115	-
14	BCR	1	524	-	-	0/29/63/63	0/2/2/2
18	PQN	A	2001	-	-	10/23/43/43	0/2/2/2
13	CLA	3	504	-	1/1/13/20	6/27/103/115	-
13	CLA	1	506	1	1/1/11/20	7/15/91/115	-
14	BCR	J	4013	-	-	5/29/63/63	0/2/2/2
13	CLA	b	510	1	1/1/15/20	14/39/115/115	-
13	CLA	A	1131	2	1/1/15/20	9/39/115/115	-
13	CLA	c	504	-	1/1/12/20	6/21/97/115	-
13	CLA	B	1023	-	1/1/15/20	8/39/115/115	-
14	BCR	b	521	-	-	7/29/63/63	0/2/2/2
13	CLA	g	516	1	1/1/11/20	11/15/91/115	-
13	CLA	4	502	1	-	8/33/109/115	-
13	CLA	B	1206	3	1/1/15/20	13/39/115/115	-
13	CLA	B	1212	3	1/1/11/20	3/15/91/115	-
19	SF4	A	3001	3,2	-	-	0/6/5/5
13	CLA	4	504	-	1/1/11/20	2/15/91/115	-
13	CLA	A	1104	2	1/1/15/20	8/39/115/115	-
13	CLA	4	518	1	1/1/13/20	11/27/103/115	-
13	CLA	B	1236	3	1/1/12/20	3/21/97/115	-
13	CLA	6	516	1	1/1/11/20	9/15/91/115	-
13	CLA	3	506	1	1/1/11/20	4/15/91/115	-
13	CLA	A	1108	2	1/1/11/20	4/15/91/115	-
13	CLA	b	517	-	1/1/11/20	6/15/91/115	-
13	CLA	f	501	1	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	d	523	-	-	4/29/63/63	0/2/2/2
13	CLA	3	502	1	1/1/14/20	11/33/109/115	-
13	CLA	4	516	1	1/1/11/20	3/15/91/115	-
13	CLA	2	508	1	1/1/13/20	2/27/103/115	-
13	CLA	3	507	-	1/1/14/20	8/33/109/115	-
13	CLA	2	503	1	1/1/14/20	14/38/114/115	-
13	CLA	3	512	1	1/1/12/20	4/24/100/115	-
13	CLA	b	519	1	1/1/11/20	5/15/91/115	-
13	CLA	g	510	1	1/1/15/20	9/39/115/115	-
14	BCR	f	522	-	-	4/29/63/63	0/2/2/2
13	CLA	5	509	1	1/1/15/20	13/39/115/115	-
14	BCR	4	522	-	-	2/29/63/63	0/2/2/2
13	CLA	a	519	-	1/1/11/20	4/15/91/115	-
13	CLA	f	505	1	1/1/15/20	11/39/115/115	-
13	CLA	A	1132	2	1/1/15/20	12/39/115/115	-
13	CLA	3	509	1	1/1/15/20	11/39/115/115	-
13	CLA	B	1222	-	1/1/14/20	6/33/109/115	-
13	CLA	d	513	1	1/1/12/20	2/21/97/115	-
20	LMU	A	1848	-	-	11/15/35/61	0/1/1/2
13	CLA	B	1203	3	1/1/15/20	20/39/115/115	-
13	CLA	1	512	1	1/1/12/20	7/24/100/115	-
13	CLA	6	507	-	1/1/14/20	4/33/109/115	-
13	CLA	2	502	1	1/1/14/20	14/33/109/115	-
14	BCR	1	523	-	-	0/29/63/63	0/2/2/2
13	CLA	A	1135	2	1/1/12/20	7/23/99/115	-
13	CLA	A	1114	-	1/1/11/20	4/15/91/115	-
14	BCR	J	4012	-	-	4/29/63/63	0/2/2/2
13	CLA	A	1122	2	1/1/14/20	8/33/109/115	-
20	LMU	B	1843	-	-	13/21/61/61	0/2/2/2
13	CLA	B	1238	-	1/1/15/20	12/39/115/115	-
14	BCR	B	4004	-	-	7/29/63/63	0/2/2/2
14	BCR	3	521	-	-	4/29/63/63	0/2/2/2
13	CLA	c	513	1	1/1/12/20	7/21/97/115	-
13	CLA	d	505	1	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMU	A	1849	-	-	11/14/34/61	0/1/1/2
13	CLA	B	1214	3	1/1/15/20	18/39/115/115	-
13	CLA	A	1117	2	1/1/15/20	12/39/115/115	-
14	BCR	g	522	-	-	4/29/63/63	0/2/2/2
13	CLA	1	502	1	1/1/14/20	12/33/109/115	-
13	CLA	1	518	1	1/1/13/20	15/27/103/115	-
13	CLA	A	1137	2	1/1/13/20	11/27/103/115	-
13	CLA	A	1120	2	1/1/12/20	7/25/101/115	-
13	CLA	2	506	1	1/1/11/20	6/15/91/115	-
13	CLA	3	503	1	1/1/14/20	10/37/113/115	-
13	CLA	f	512	1	1/1/11/20	10/15/91/115	-
13	CLA	3	517	-	1/1/11/20	5/15/91/115	-
14	BCR	6	521	-	-	4/29/63/63	0/2/2/2
14	BCR	I	4019	-	-	4/29/63/63	0/2/2/2
14	BCR	c	521	-	-	3/29/63/63	0/2/2/2
14	BCR	b	522	-	-	7/29/63/63	0/2/2/2
14	BCR	B	4009	-	-	6/29/63/63	0/2/2/2
13	CLA	5	510	1	1/1/15/20	13/39/115/115	-
13	CLA	c	505	1	1/1/15/20	10/39/115/115	-
13	CLA	4	519	1	1/1/12/20	7/21/97/115	-
13	CLA	b	513	1	1/1/12/20	6/21/97/115	-
13	CLA	d	502	1	1/1/14/20	13/33/109/115	-
13	CLA	f	519	1	1/1/11/20	8/15/91/115	-
14	BCR	A	4002	-	-	4/29/63/63	0/2/2/2
15	SQD	a	822	-	-	4/26/46/69	0/1/1/1
13	CLA	2	507	-	1/1/14/20	8/33/109/115	-
14	BCR	F	4016	-	-	2/29/63/63	0/2/2/2
13	CLA	c	501	1	1/1/15/20	11/39/115/115	-
13	CLA	3	508	1	1/1/13/20	5/27/103/115	-
13	CLA	5	507	-	1/1/14/20	11/33/109/115	-
13	CLA	1	509	1	1/1/15/20	10/39/115/115	-
13	CLA	a	517	-	1/1/11/20	8/15/91/115	-
15	SQD	1	822	-	-	5/26/46/69	0/1/1/1
13	CLA	B	1217	3	1/1/13/20	12/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1101	2	1/1/14/20	10/33/109/115	-
13	CLA	a	501	1	1/1/15/20	11/39/115/115	-
13	CLA	2	509	1	1/1/15/20	11/39/115/115	-
14	BCR	6	523	-	-	2/29/63/63	0/2/2/2
14	BCR	A	4008	-	-	2/29/63/63	0/2/2/2
13	CLA	b	505	1	1/1/15/20	13/39/115/115	-
14	BCR	A	4011	-	-	8/29/63/63	0/2/2/2
13	CLA	5	513	1	1/1/13/20	3/27/103/115	-
14	BCR	B	4006	-	-	8/29/63/63	0/2/2/2
13	CLA	A	1130	2	1/1/13/20	5/27/103/115	-
14	BCR	4	524	-	-	4/29/63/63	0/2/2/2
14	BCR	6	524	-	-	3/29/63/63	0/2/2/2
13	CLA	c	511	1	1/1/13/20	6/27/103/115	-
13	CLA	3	518	1	1/1/13/20	11/27/103/115	-
13	CLA	g	507	-	1/1/14/20	7/33/109/115	-
13	CLA	f	516	1	1/1/11/20	7/15/91/115	-
14	BCR	2	521	-	-	6/29/63/63	0/2/2/2
13	CLA	g	512	1	1/1/12/20	3/24/100/115	-
13	CLA	d	506	1	1/1/11/20	9/15/91/115	-
14	BCR	d	524	-	-	7/29/63/63	0/2/2/2
13	CLA	B	1216	-	1/1/14/20	12/33/109/115	-
13	CLA	g	508	1	1/1/12/20	1/24/100/115	-
14	BCR	g	524	-	-	0/29/63/63	0/2/2/2
13	CLA	5	519	1	1/1/12/20	6/21/97/115	-
13	CLA	5	503	1	1/1/14/20	18/38/114/115	-
14	BCR	a	522	-	-	5/29/63/63	0/2/2/2
13	CLA	e	510	1	1/1/15/20	10/39/115/115	-
14	BCR	5	521	-	-	6/29/63/63	0/2/2/2
13	CLA	e	502	1	1/1/14/20	15/33/109/115	-
13	CLA	5	508	1	1/1/13/20	5/27/103/115	-
13	CLA	e	506	1	1/1/11/20	9/15/91/115	-
13	CLA	e	504	-	1/1/13/20	14/27/103/115	-
14	BCR	A	4003	-	-	4/29/63/63	0/2/2/2
14	BCR	e	522	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	2	519	1	1/1/12/20	5/21/97/115	-
13	CLA	g	513	1	1/1/12/20	5/21/97/115	-
13	CLA	2	517	-	1/1/11/20	10/15/91/115	-
13	CLA	B	1230	3	1/1/13/20	13/31/107/115	-
13	CLA	B	1233	-	1/1/11/20	0/15/91/115	-
13	CLA	4	503	1	1/1/14/20	10/38/114/115	-
15	SQD	5	822	-	-	5/26/46/69	0/1/1/1
14	BCR	F	4015	-	-	2/29/63/63	0/2/2/2
13	CLA	g	518	1	1/1/13/20	12/27/103/115	-
13	CLA	b	503	1	1/1/14/20	12/37/113/115	-
13	CLA	b	509	1	1/1/15/20	12/39/115/115	-
13	CLA	A	1109	13,2	1/1/15/20	11/39/115/115	-
13	CLA	6	511	1	1/1/11/20	5/15/91/115	-
13	CLA	e	507	-	1/1/14/20	7/33/109/115	-
14	BCR	c	522	-	-	2/29/63/63	0/2/2/2
14	BCR	K	4001	-	-	0/29/63/63	0/2/2/2
13	CLA	A	1103	2	1/1/15/20	16/39/115/115	-
14	BCR	6	522	-	-	5/29/63/63	0/2/2/2
13	CLA	B	1211	3	1/1/15/20	12/39/115/115	-
13	CLA	b	506	1	-	6/15/91/115	-
16	LMG	6	5104	-	-	4/33/53/70	0/1/1/1
16	LMG	B	5002	-	-	11/50/70/70	0/1/1/1
13	CLA	c	512	1	1/1/11/20	5/15/91/115	-

The worst 5 of 2268 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	1303	CLA	CHD-C1D	6.88	1.38	1.33
13	J	1303	CLA	C4C-CHD	-6.22	1.40	1.50
15	d	822	SQD	O8-S	4.61	1.64	1.47
15	1	822	SQD	O8-S	4.47	1.64	1.47
15	6	822	SQD	O47-C7	4.46	1.46	1.34

The worst 5 of 2876 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	5	523	BCR	C30-C25-C26	-8.71	110.74	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	4014	BCR	C24-C23-C22	-7.36	115.35	126.23
14	B	4017	BCR	C24-C23-C22	-7.34	115.37	126.23
14	4	524	BCR	C16-C17-C18	-7.34	116.98	127.28
13	1	512	CLA	C4A-NA-C1A	7.20	109.96	106.68

5 of 303 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	3	501	CLA	ND
13	3	502	CLA	ND
13	3	503	CLA	ND
13	3	504	CLA	ND
13	3	505	CLA	ND

5 of 3447 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	3	501	CLA	CAD-CBD-CGD-O1D
13	3	501	CLA	CAD-CBD-CGD-O2D
13	3	502	CLA	C4B-C3B-CAB-CBB
13	3	505	CLA	C6-C7-C8-C9
13	3	507	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

382 monomers are involved in 1314 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	1	504	CLA	3	0
14	f	523	BCR	8	0
13	5	511	CLA	1	0
13	a	509	CLA	11	0
13	6	502	CLA	4	0
13	5	501	CLA	8	0
18	B	2002	PQN	4	0
13	3	505	CLA	8	0
13	B	1239	CLA	4	0
13	A	1105	CLA	6	0
13	4	508	CLA	3	0
13	c	506	CLA	4	0
13	2	501	CLA	5	0
14	I	4020	BCR	4	0
13	B	1201	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	g	503	CLA	8	0
13	B	1204	CLA	6	0
13	a	503	CLA	8	0
17	A	5005	LHG	14	0
13	K	1401	CLA	4	0
14	a	524	BCR	7	0
13	d	511	CLA	2	0
13	A	1129	CLA	4	0
13	A	1113	CLA	3	0
13	6	504	CLA	3	0
13	e	508	CLA	2	0
13	f	502	CLA	8	0
14	e	524	BCR	8	0
13	d	517	CLA	3	0
13	d	504	CLA	2	0
13	f	504	CLA	1	0
13	f	518	CLA	2	0
13	c	503	CLA	5	0
13	e	518	CLA	2	0
14	c	524	BCR	10	0
14	g	523	BCR	6	0
17	A	5002	LHG	2	0
13	c	508	CLA	5	0
13	1	507	CLA	4	0
14	d	521	BCR	5	0
13	1	519	CLA	6	0
13	1	503	CLA	5	0
13	2	512	CLA	2	0
13	1	508	CLA	5	0
13	4	507	CLA	4	0
13	A	1136	CLA	4	0
13	c	517	CLA	3	0
13	a	516	CLA	1	0
13	a	512	CLA	2	0
13	5	512	CLA	1	0
13	A	1115	CLA	4	0
13	A	1123	CLA	6	0
13	B	1228	CLA	5	0
13	1	513	CLA	2	0
13	A	1125	CLA	7	0
13	a	510	CLA	9	0
13	B	1231	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1220	CLA	2	0
13	g	502	CLA	9	0
13	g	506	CLA	1	0
14	A	4007	BCR	6	0
13	g	504	CLA	1	0
13	d	509	CLA	4	0
13	c	507	CLA	5	0
13	A	1118	CLA	3	0
13	2	505	CLA	6	0
13	f	507	CLA	9	0
13	2	511	CLA	2	0
13	b	502	CLA	3	0
14	1	521	BCR	5	0
13	f	510	CLA	2	0
13	A	1128	CLA	7	0
13	4	510	CLA	3	0
13	e	503	CLA	6	0
13	A	1133	CLA	2	0
13	b	518	CLA	3	0
13	4	506	CLA	2	0
13	A	1112	CLA	3	0
13	1	505	CLA	2	0
14	4	521	BCR	4	0
13	B	1202	CLA	4	0
13	B	1219	CLA	1	0
13	e	512	CLA	3	0
13	d	512	CLA	3	0
13	B	1225	CLA	9	0
14	5	524	BCR	4	0
15	B	1852	SQD	2	0
13	1	501	CLA	7	0
13	g	509	CLA	3	0
13	A	1022	CLA	8	0
13	e	511	CLA	4	0
13	A	1127	CLA	6	0
13	d	501	CLA	6	0
14	f	521	BCR	2	0
13	A	1102	CLA	6	0
13	A	1011	CLA	6	0
13	f	513	CLA	7	0
16	2	5104	LMG	1	0
13	6	519	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	f	508	CLA	2	0
13	B	1235	CLA	2	0
13	A	1013	CLA	9	0
13	B	1021	CLA	6	0
13	d	510	CLA	3	0
13	b	512	CLA	4	0
14	B	4005	BCR	2	0
13	a	511	CLA	2	0
13	A	1106	CLA	9	0
13	g	517	CLA	2	0
13	e	509	CLA	8	0
13	5	506	CLA	4	0
13	a	504	CLA	1	0
13	B	1229	CLA	7	0
13	B	1215	CLA	4	0
13	B	1232	CLA	2	0
13	J	1302	CLA	1	0
14	5	523	BCR	6	0
13	a	502	CLA	11	0
14	g	521	BCR	7	0
14	3	522	BCR	10	0
13	a	518	CLA	1	0
13	3	501	CLA	5	0
13	A	1107	CLA	8	0
13	6	503	CLA	6	0
13	F	1301	CLA	1	0
13	6	517	CLA	1	0
14	2	523	BCR	2	0
14	f	524	BCR	7	0
13	b	501	CLA	5	0
13	1	516	CLA	1	0
13	c	509	CLA	9	0
13	4	511	CLA	3	0
13	A	1801	CLA	1	0
13	B	1221	CLA	5	0
13	c	502	CLA	8	0
13	g	519	CLA	1	0
13	A	1139	CLA	9	0
14	b	524	BCR	5	0
13	b	511	CLA	5	0
14	2	524	BCR	5	0
14	B	4017	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	4	505	CLA	5	0
13	3	511	CLA	3	0
13	5	504	CLA	1	0
14	I	4018	BCR	9	0
13	B	1207	CLA	2	0
13	f	503	CLA	3	0
13	a	507	CLA	7	0
13	B	1234	CLA	4	0
13	B	1012	CLA	10	0
13	A	1134	CLA	4	0
13	f	511	CLA	3	0
19	C	3002	SF4	1	0
13	2	510	CLA	6	0
13	2	516	CLA	2	0
13	e	517	CLA	2	0
17	A	5003	LHG	3	0
14	B	4010	BCR	10	0
14	5	522	BCR	4	0
13	g	511	CLA	3	0
13	c	510	CLA	5	0
13	g	501	CLA	6	0
13	4	512	CLA	2	0
13	6	512	CLA	4	0
13	2	518	CLA	5	0
14	3	524	BCR	4	0
13	6	510	CLA	12	0
14	2	522	BCR	2	0
13	A	1116	CLA	5	0
13	5	502	CLA	4	0
14	c	523	BCR	3	0
13	A	1140	CLA	7	0
13	d	518	CLA	2	0
17	A	5004	LHG	2	0
14	d	522	BCR	4	0
14	e	521	BCR	2	0
13	3	513	CLA	2	0
15	2	822	SQD	3	0
13	B	1213	CLA	3	0
13	d	508	CLA	2	0
13	4	509	CLA	9	0
13	6	509	CLA	11	0
13	B	1205	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	523	BCR	7	0
13	f	509	CLA	11	0
20	J	5105	LMU	10	0
13	B	1227	CLA	2	0
13	e	519	CLA	2	0
13	6	501	CLA	4	0
14	1	522	BCR	5	0
13	c	518	CLA	4	0
13	B	1208	CLA	1	0
13	A	1138	CLA	9	0
13	g	505	CLA	6	0
13	a	506	CLA	3	0
13	d	507	CLA	3	0
14	a	523	BCR	7	0
13	1	510	CLA	4	0
15	g	822	SQD	1	0
13	B	1209	CLA	2	0
14	e	523	BCR	4	0
13	B	1224	CLA	7	0
13	6	505	CLA	5	0
13	6	506	CLA	4	0
13	B	1223	CLA	7	0
13	b	508	CLA	3	0
13	A	1111	CLA	2	0
17	A	5001	LHG	1	0
14	F	4014	BCR	6	0
13	f	517	CLA	3	0
13	A	1110	CLA	1	0
19	C	3003	SF4	1	0
15	4	822	SQD	7	0
15	6	822	SQD	2	0
13	e	501	CLA	7	0
13	e	513	CLA	5	0
14	3	523	BCR	3	0
13	a	513	CLA	4	0
13	A	1237	CLA	6	0
13	A	1119	CLA	10	0
13	f	506	CLA	2	0
13	B	1226	CLA	2	0
13	2	513	CLA	1	0
14	a	521	BCR	5	0
13	5	518	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	d	503	CLA	6	0
13	A	1126	CLA	4	0
13	d	519	CLA	1	0
13	B	1210	CLA	5	0
13	5	505	CLA	4	0
13	b	507	CLA	4	0
13	3	510	CLA	5	0
13	a	508	CLA	6	0
13	e	505	CLA	11	0
13	a	505	CLA	4	0
14	M	4021	BCR	3	0
16	g	5104	LMG	1	0
13	4	501	CLA	4	0
14	4	523	BCR	2	0
13	X	1401	CLA	2	0
13	6	508	CLA	9	0
13	A	1124	CLA	4	0
13	c	519	CLA	2	0
14	1	524	BCR	8	0
18	A	2001	PQN	2	0
13	3	504	CLA	1	0
13	1	506	CLA	3	0
14	J	4013	BCR	6	0
13	b	510	CLA	4	0
13	A	1131	CLA	2	0
13	c	504	CLA	1	0
13	B	1023	CLA	14	0
14	b	521	BCR	5	0
13	g	516	CLA	1	0
13	4	502	CLA	4	0
13	B	1206	CLA	6	0
13	B	1212	CLA	2	0
19	A	3001	SF4	1	0
13	A	1104	CLA	6	0
13	4	518	CLA	1	0
13	B	1236	CLA	3	0
13	6	516	CLA	1	0
13	3	506	CLA	3	0
13	A	1108	CLA	2	0
13	b	517	CLA	2	0
13	f	501	CLA	10	0
14	d	523	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	3	502	CLA	4	0
13	4	516	CLA	1	0
13	2	508	CLA	2	0
13	3	507	CLA	4	0
13	2	503	CLA	5	0
13	3	512	CLA	2	0
13	g	510	CLA	3	0
14	f	522	BCR	5	0
13	5	509	CLA	3	0
14	4	522	BCR	4	0
13	a	519	CLA	1	0
13	f	505	CLA	8	0
13	A	1132	CLA	3	0
13	3	509	CLA	6	0
13	B	1222	CLA	4	0
20	A	1848	LMU	2	0
13	B	1203	CLA	5	0
13	1	512	CLA	1	0
13	6	507	CLA	3	0
13	2	502	CLA	5	0
14	1	523	BCR	4	0
13	A	1135	CLA	1	0
14	J	4012	BCR	2	0
13	A	1122	CLA	7	0
20	B	1843	LMU	1	0
13	B	1238	CLA	7	0
14	B	4004	BCR	1	0
14	3	521	BCR	3	0
13	c	513	CLA	5	0
13	d	505	CLA	8	0
20	A	1849	LMU	1	0
13	B	1214	CLA	7	0
13	A	1117	CLA	4	0
14	g	522	BCR	4	0
13	1	502	CLA	8	0
13	1	518	CLA	2	0
13	A	1137	CLA	7	0
13	A	1120	CLA	2	0
13	2	506	CLA	1	0
13	3	503	CLA	6	0
13	f	512	CLA	5	0
14	6	521	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	I	4019	BCR	4	0
14	c	521	BCR	4	0
14	b	522	BCR	5	0
14	B	4009	BCR	5	0
13	5	510	CLA	9	0
13	c	505	CLA	10	0
13	4	519	CLA	2	0
13	b	513	CLA	2	0
13	d	502	CLA	3	0
13	f	519	CLA	2	0
14	A	4002	BCR	7	0
13	2	507	CLA	6	0
14	F	4016	BCR	2	0
13	c	501	CLA	7	0
13	3	508	CLA	6	0
13	5	507	CLA	7	0
13	1	509	CLA	4	0
13	a	517	CLA	3	0
13	B	1217	CLA	2	0
13	A	1101	CLA	7	0
13	a	501	CLA	8	0
13	2	509	CLA	4	0
14	6	523	BCR	5	0
14	A	4008	BCR	9	0
13	b	505	CLA	11	0
14	A	4011	BCR	3	0
13	5	513	CLA	4	0
14	B	4006	BCR	3	0
13	A	1130	CLA	1	0
14	4	524	BCR	4	0
14	6	524	BCR	6	0
13	c	511	CLA	5	0
13	3	518	CLA	3	0
13	g	507	CLA	6	0
14	2	521	BCR	8	0
13	g	512	CLA	3	0
13	d	506	CLA	6	0
14	d	524	BCR	6	0
13	B	1216	CLA	5	0
13	g	508	CLA	2	0
14	g	524	BCR	8	0
13	5	519	CLA	2	0

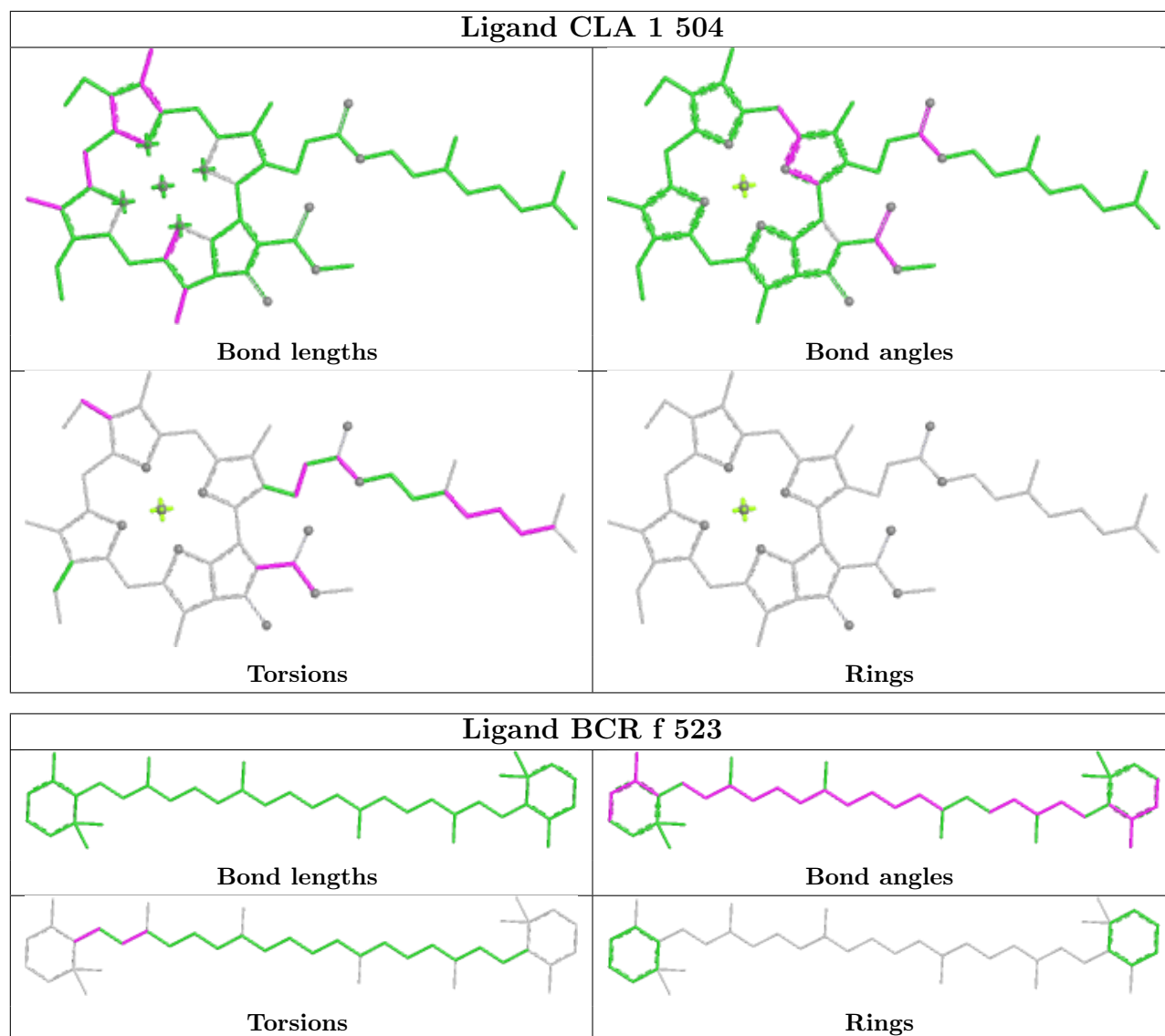
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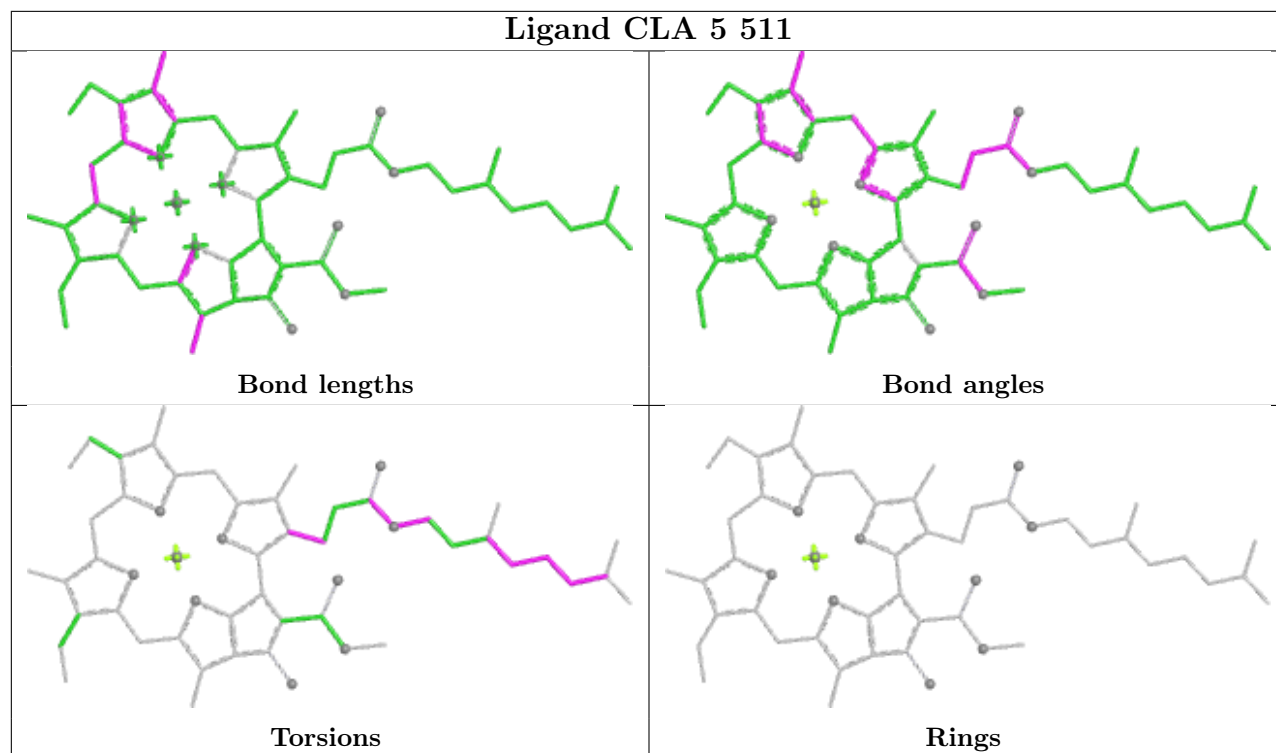
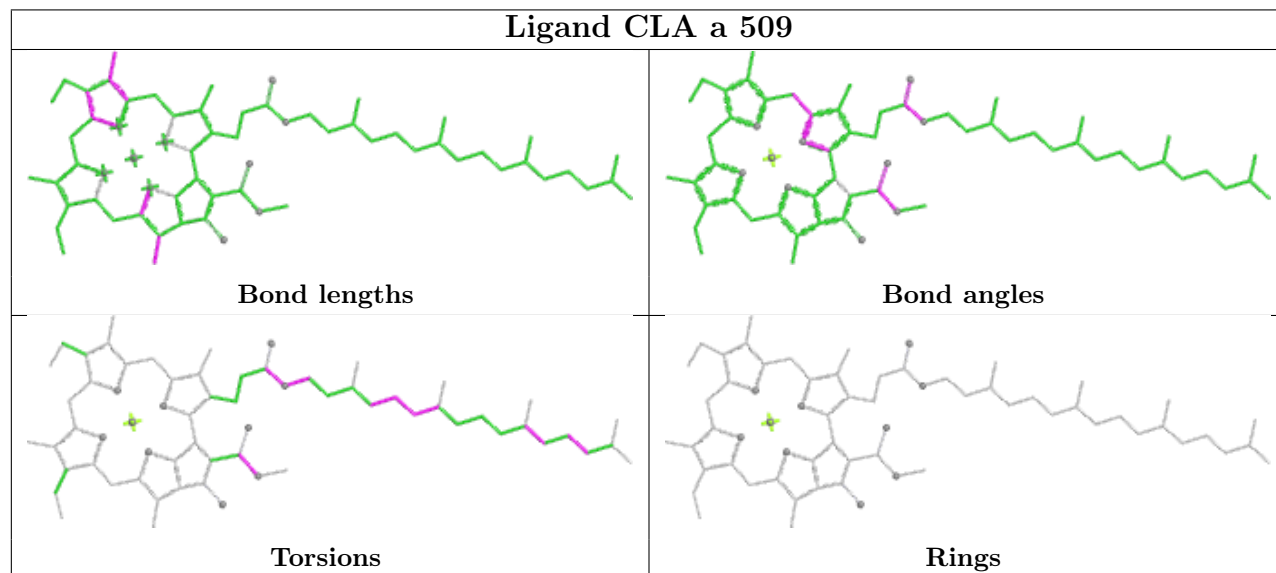
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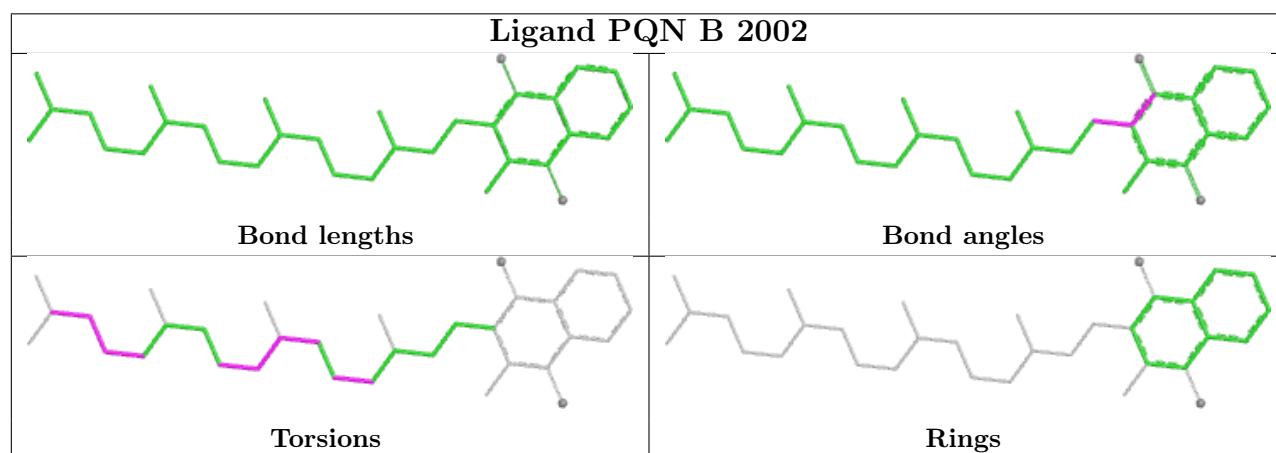
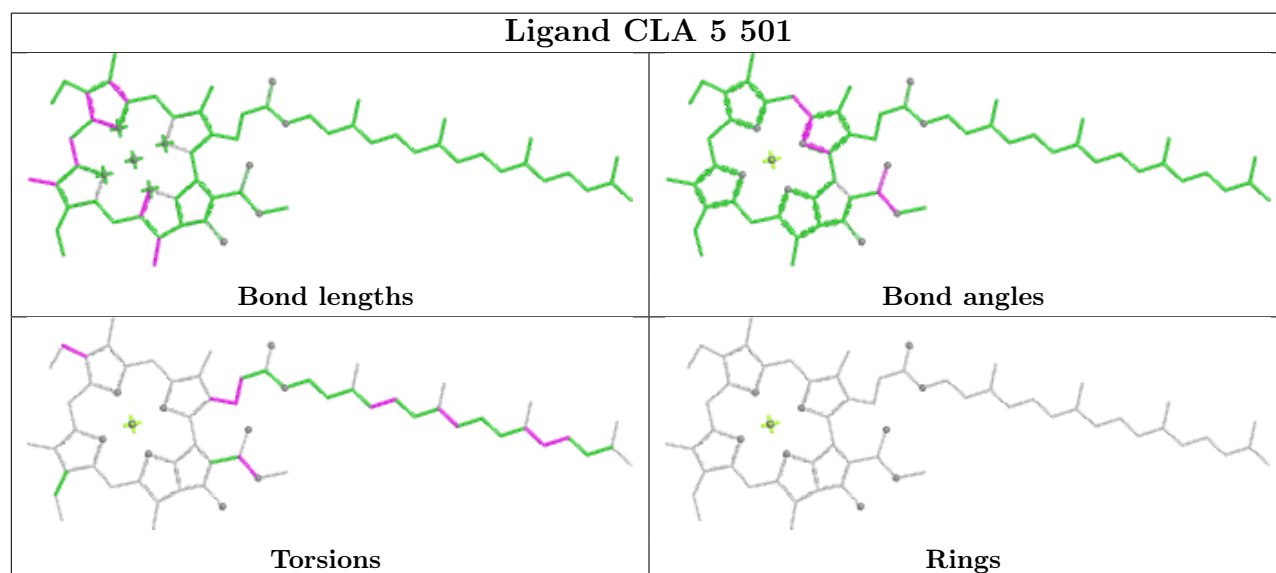
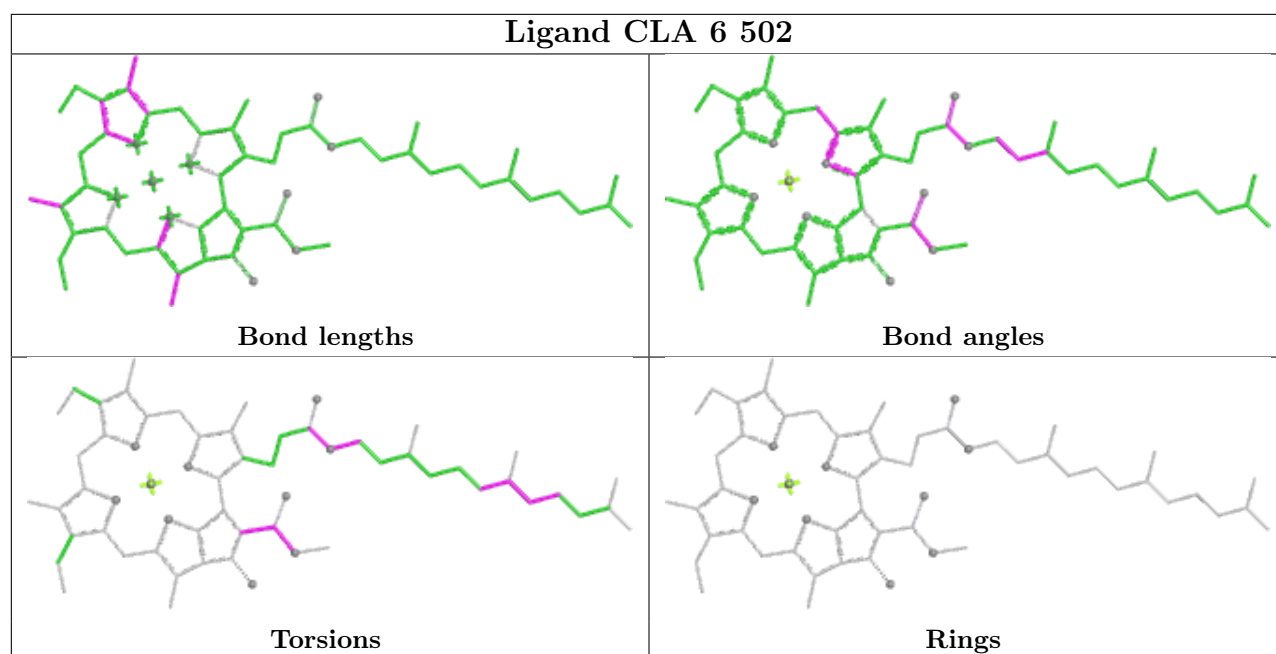
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	5	503	CLA	6	0
14	a	522	BCR	8	0
13	e	510	CLA	3	0
14	5	521	BCR	8	0
13	e	502	CLA	5	0
13	5	508	CLA	4	0
14	A	4003	BCR	7	0
14	e	522	BCR	6	0
13	2	519	CLA	2	0
13	g	513	CLA	5	0
13	2	517	CLA	1	0
13	B	1230	CLA	2	0
13	B	1233	CLA	2	0
13	4	503	CLA	5	0
15	5	822	SQD	2	0
14	F	4015	BCR	7	0
13	g	518	CLA	2	0
13	b	503	CLA	6	0
13	b	509	CLA	7	0
13	A	1109	CLA	3	0
13	6	511	CLA	5	0
13	e	507	CLA	1	0
14	c	522	BCR	9	0
14	K	4001	BCR	6	0
13	A	1103	CLA	8	0
14	6	522	BCR	2	0
13	B	1211	CLA	4	0
13	b	506	CLA	1	0
16	6	5104	LMG	2	0
16	B	5002	LMG	5	0
13	c	512	CLA	2	0

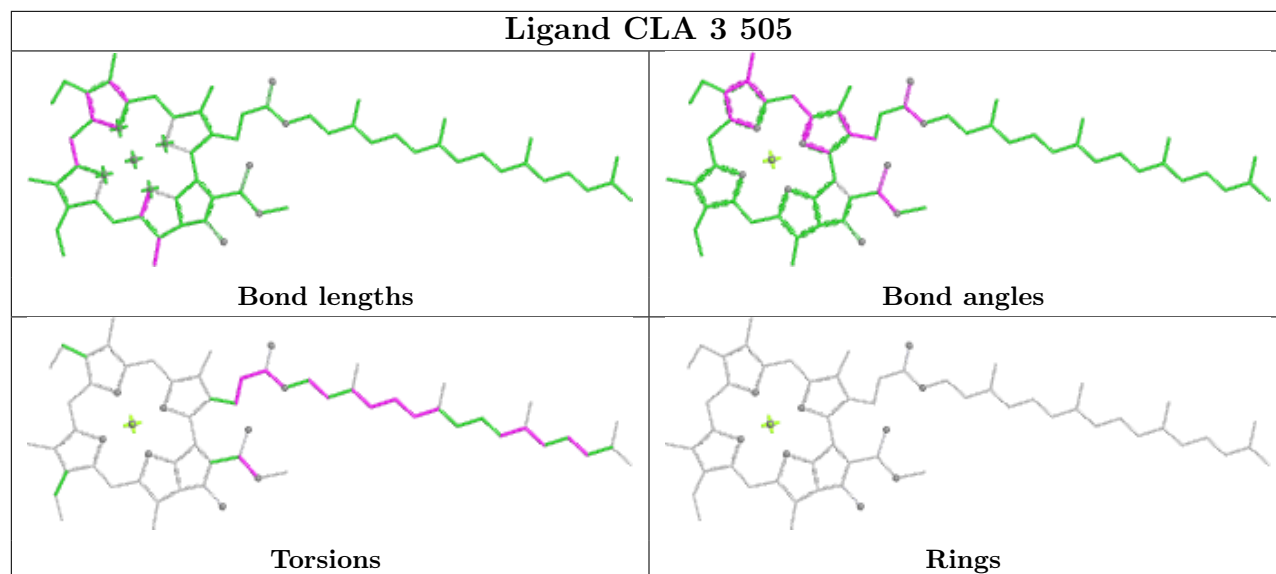
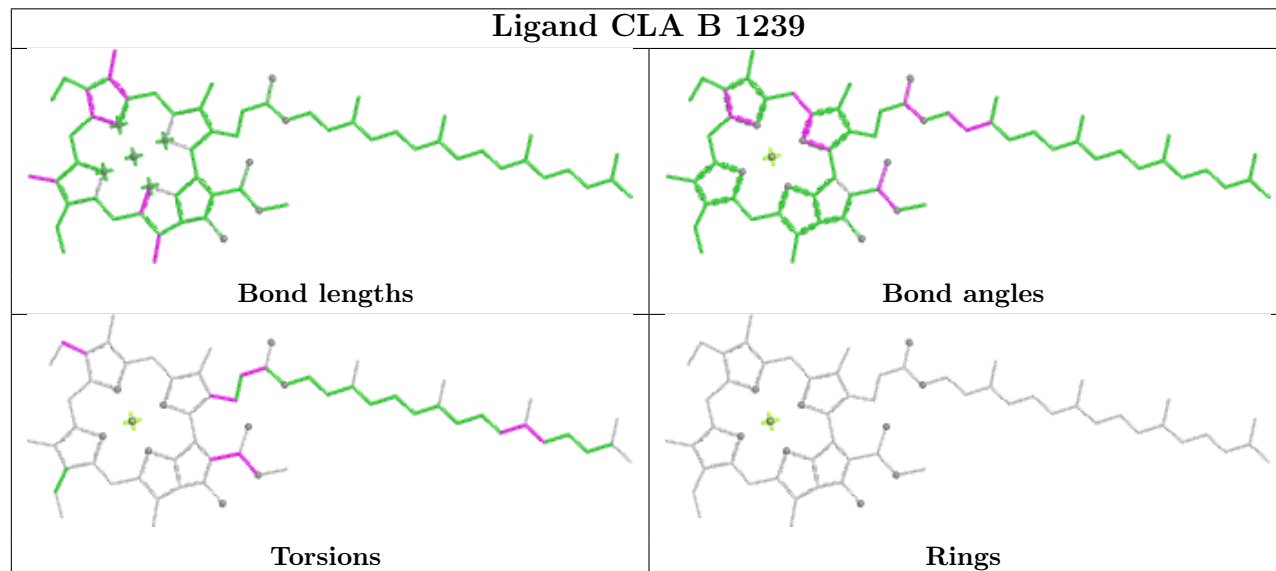
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

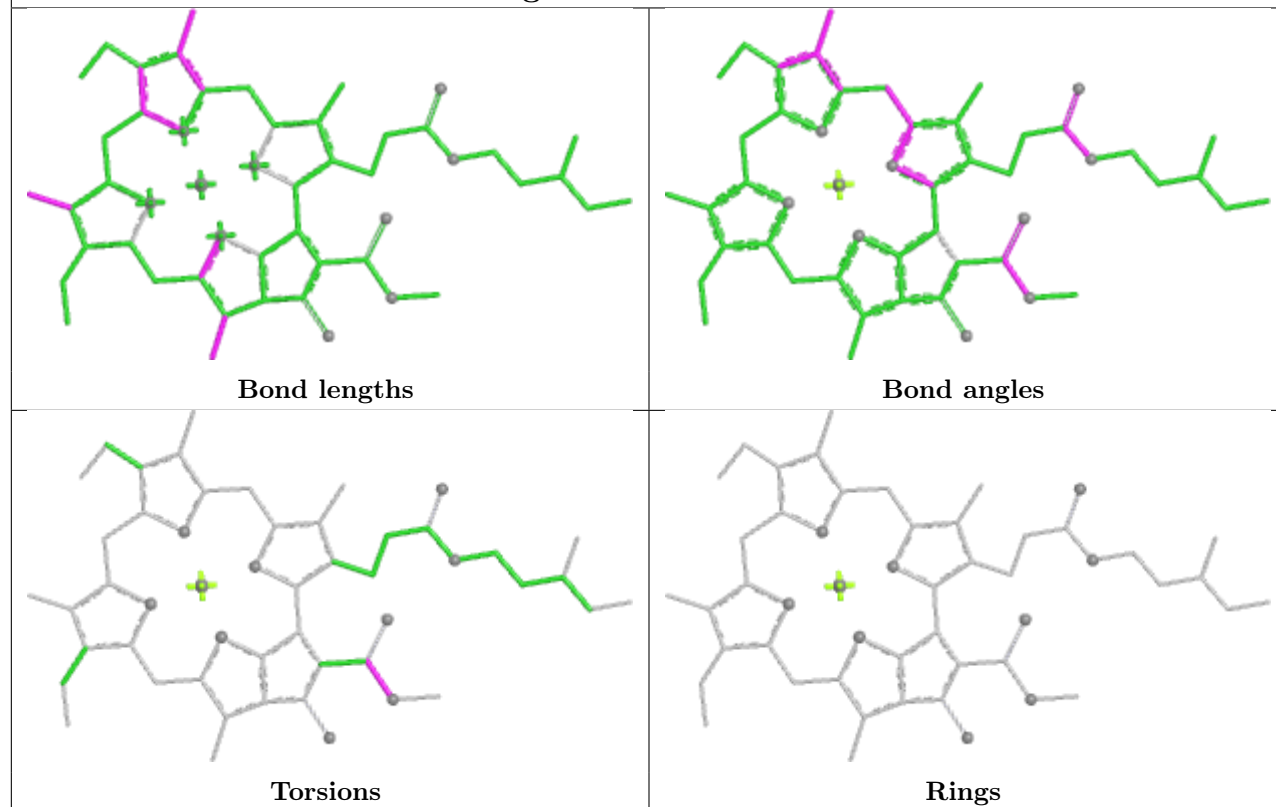


Ligand CLA 5 511**Ligand CLA a 509**

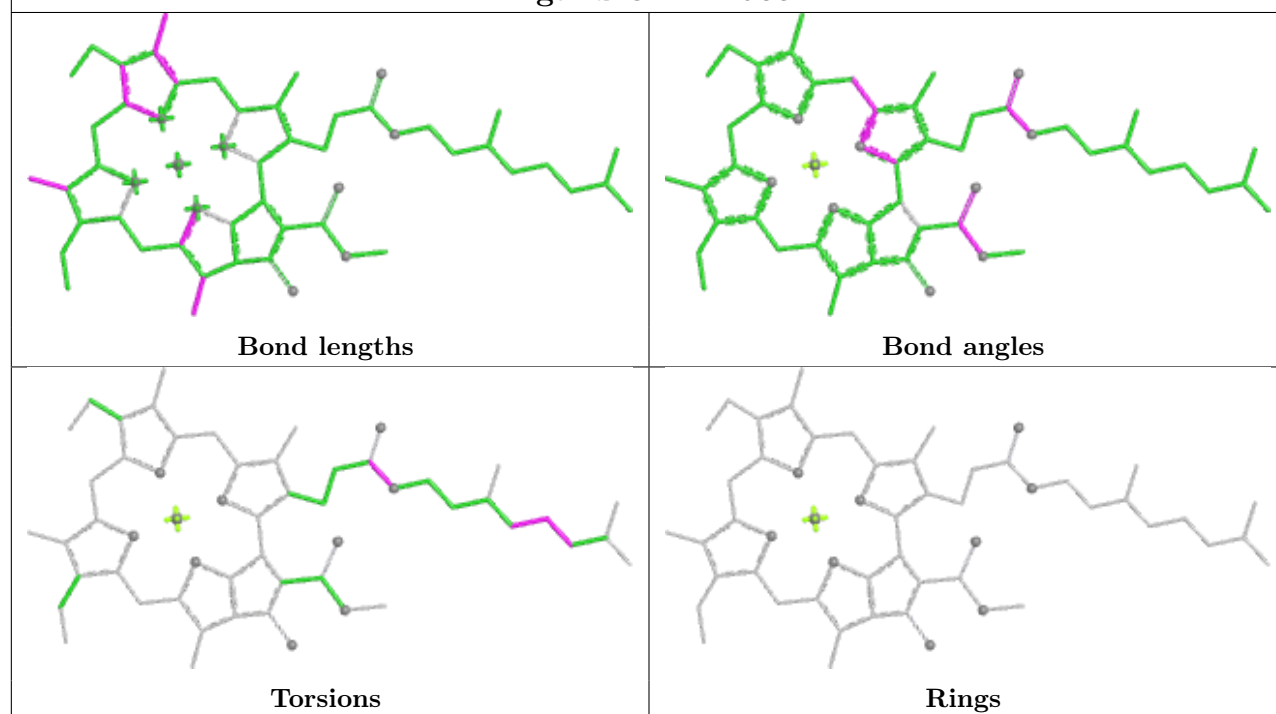


Ligand CLA 3 505**Ligand CLA B 1239**

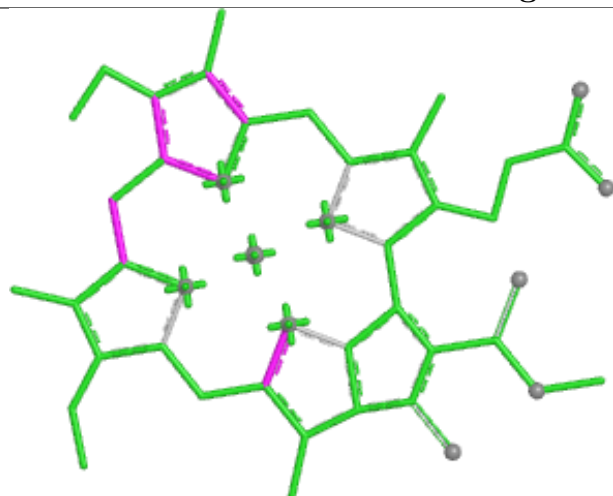
Ligand CLA A 1105



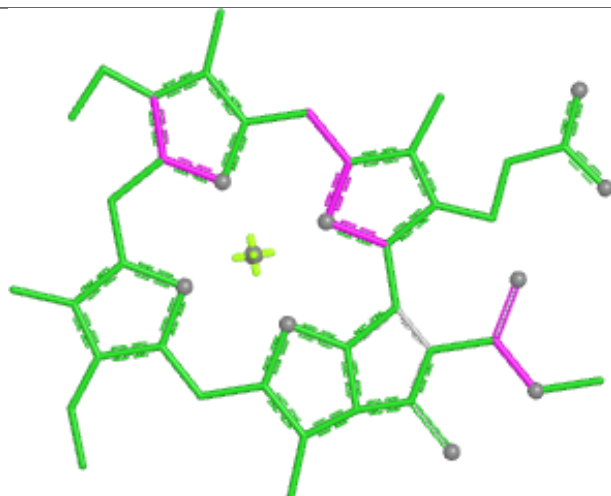
Ligand CLA 4 508



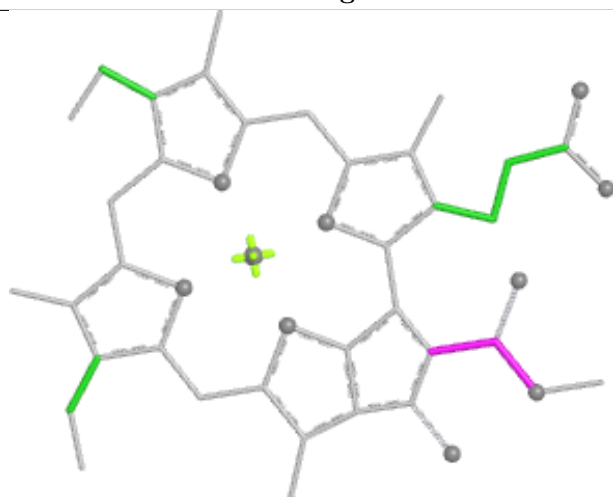
Ligand CLA c 506



Bond lengths



Bond angles

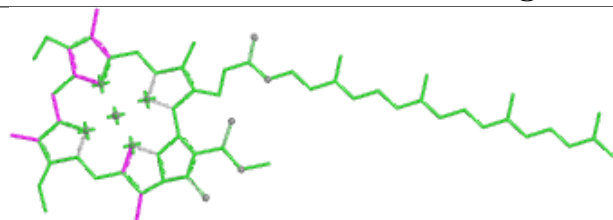


Torsions

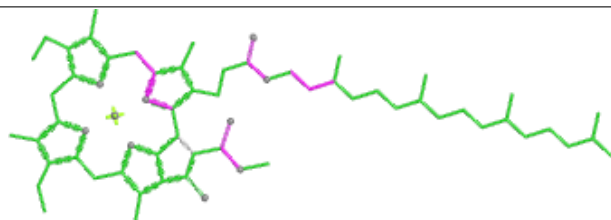


Rings

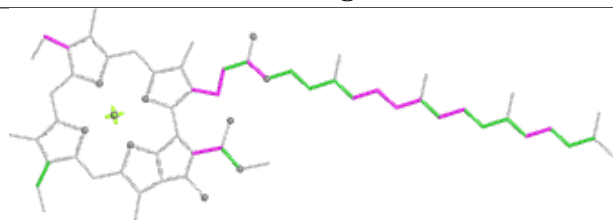
Ligand CLA 2 501



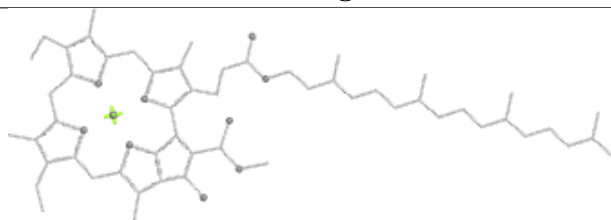
Bond lengths



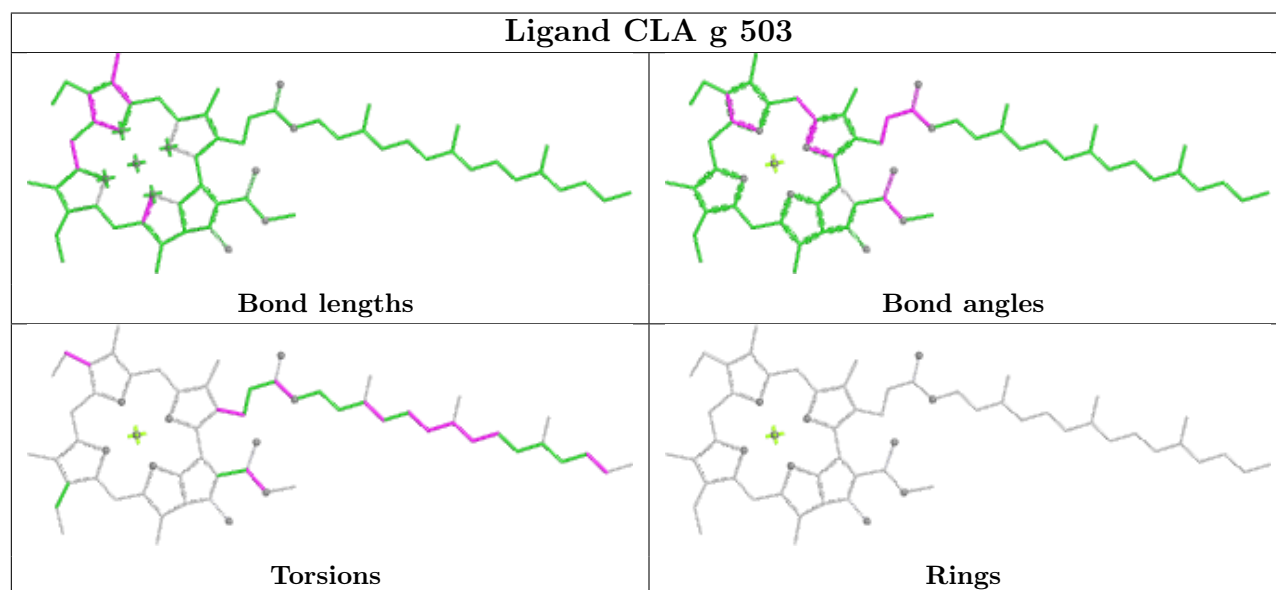
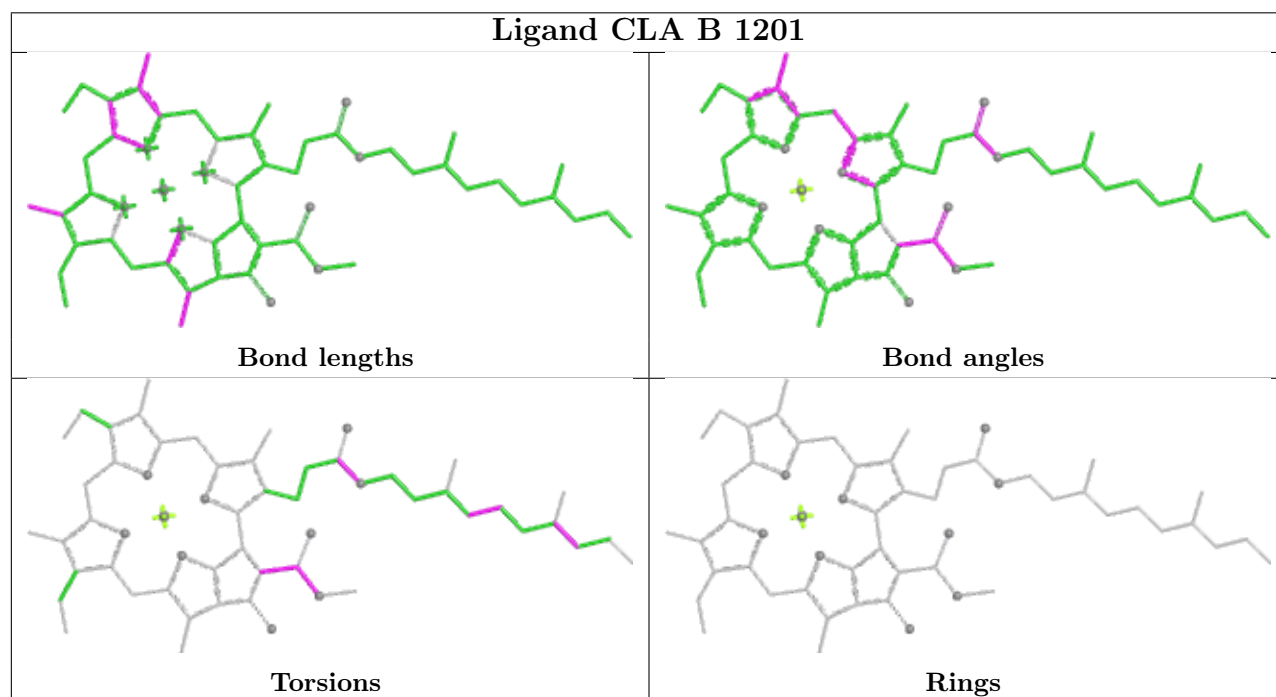
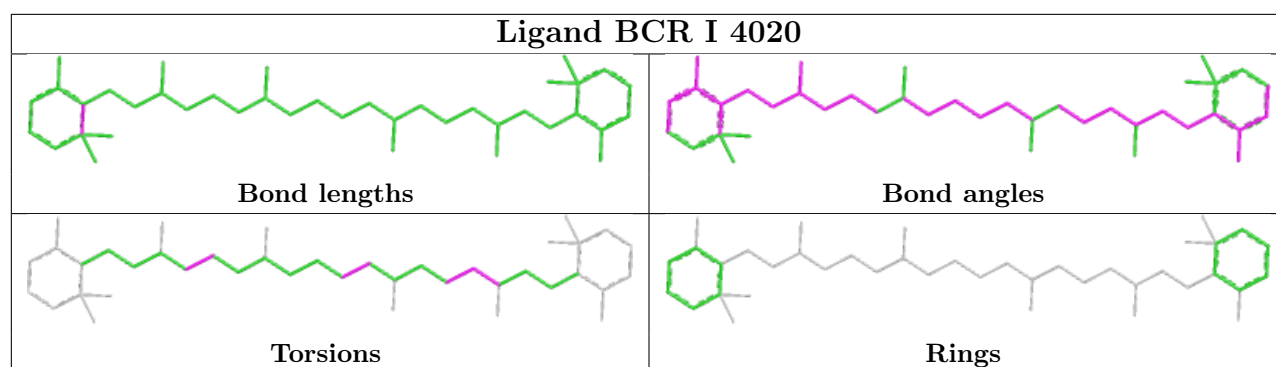
Bond angles

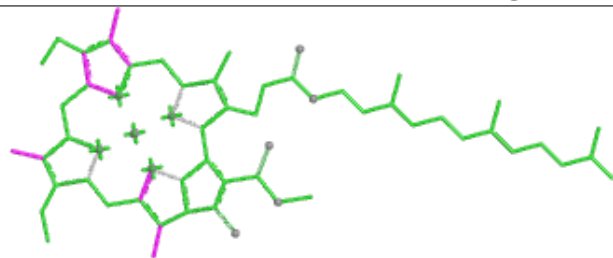
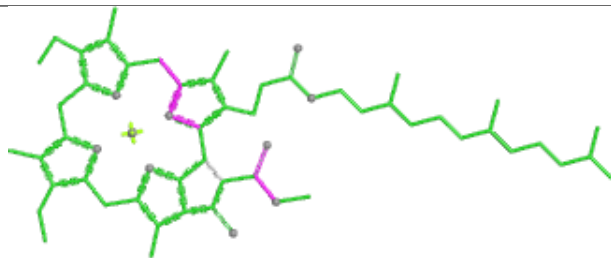
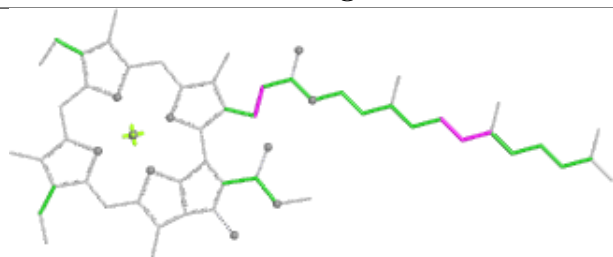
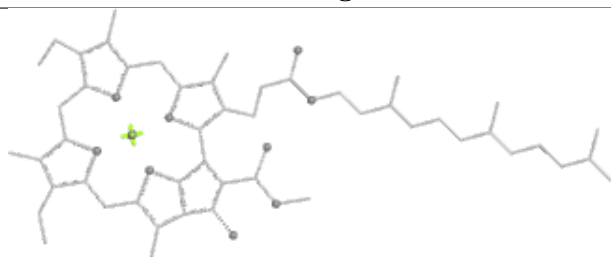
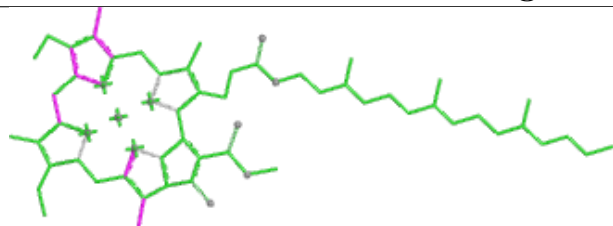
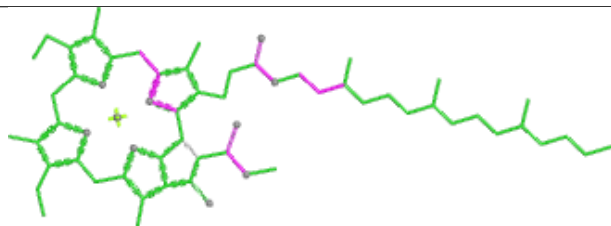
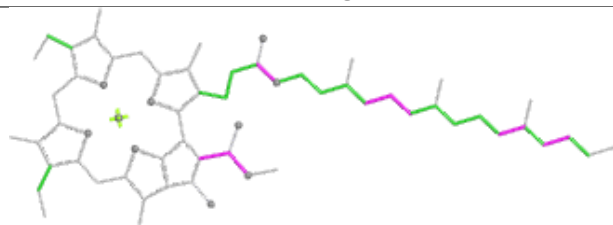
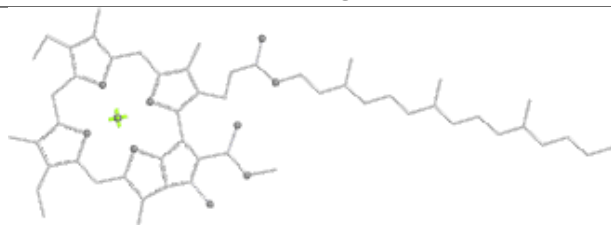


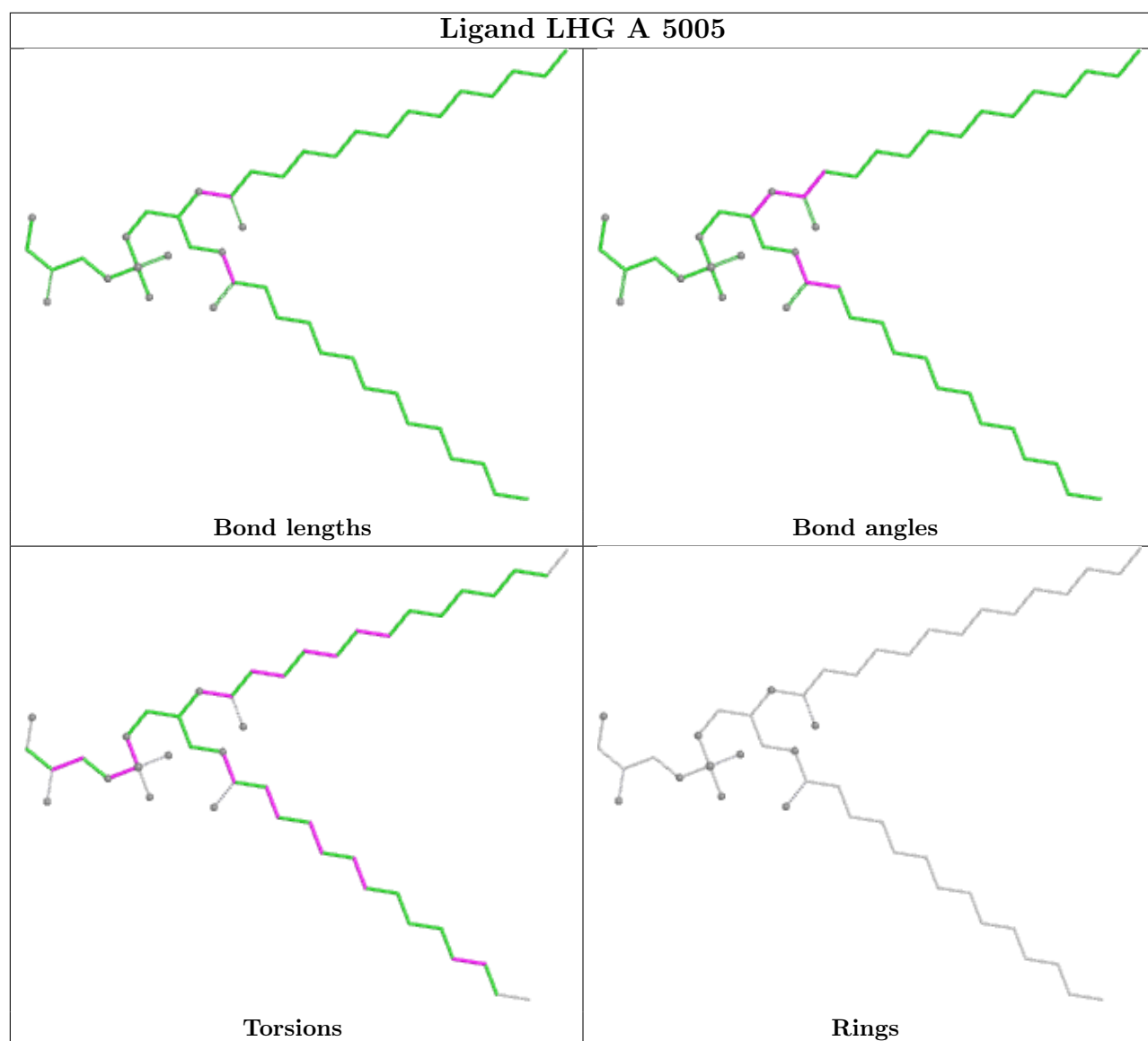
Torsions

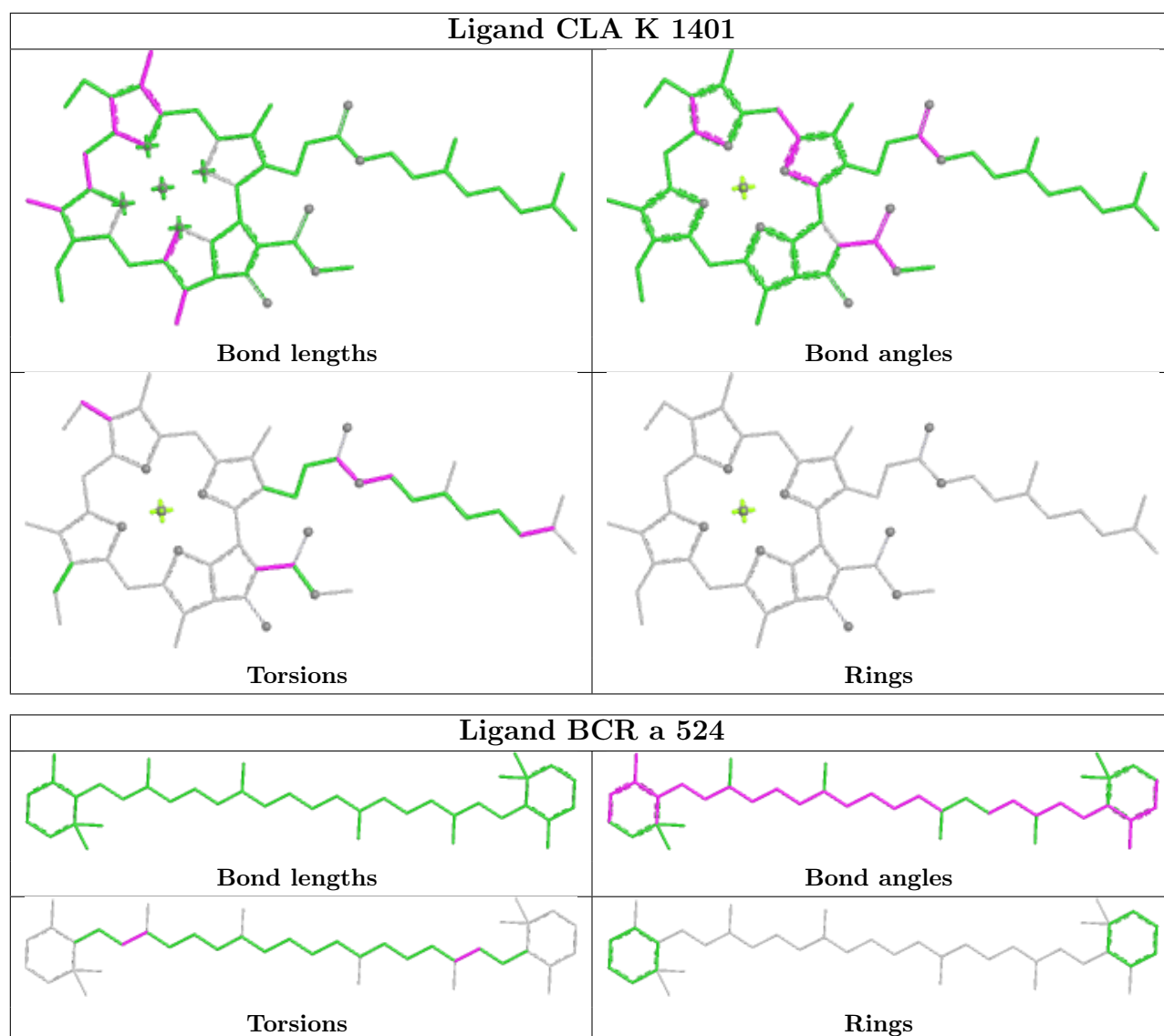


Rings

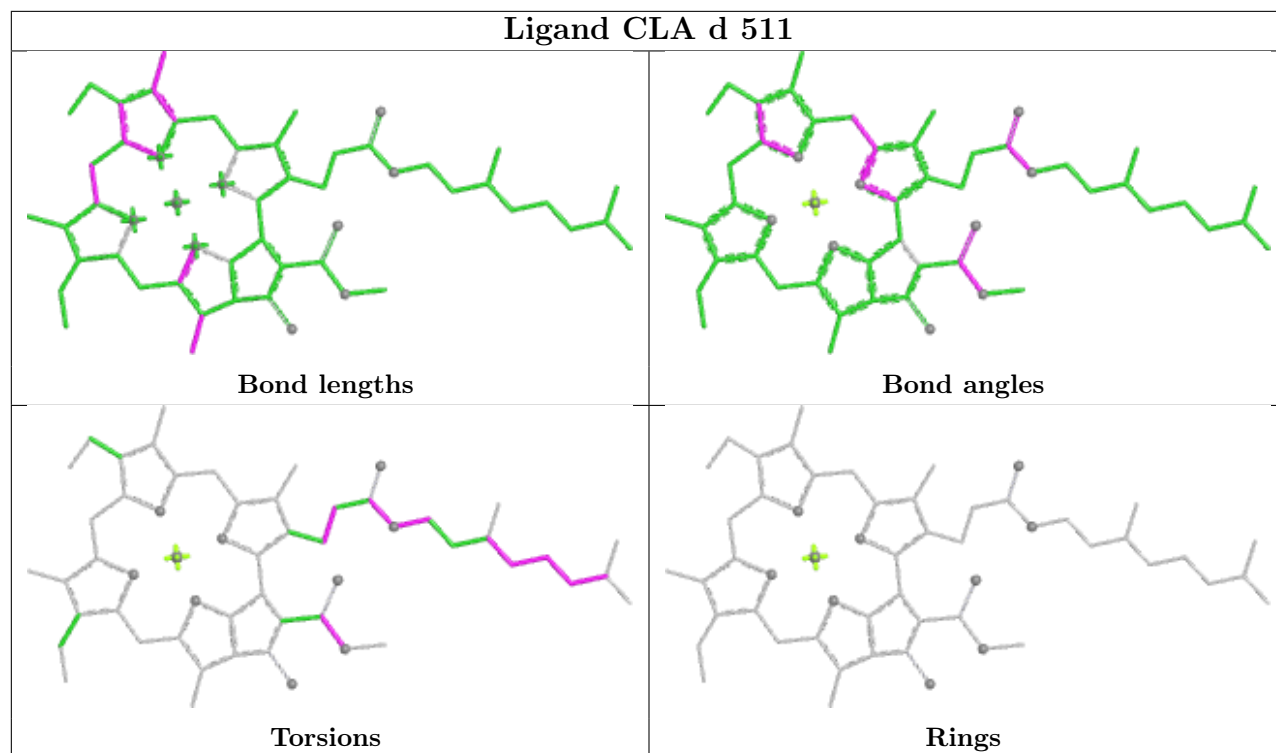


Ligand CLA B 1204**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA a 503****Bond lengths****Bond angles****Torsions****Rings**

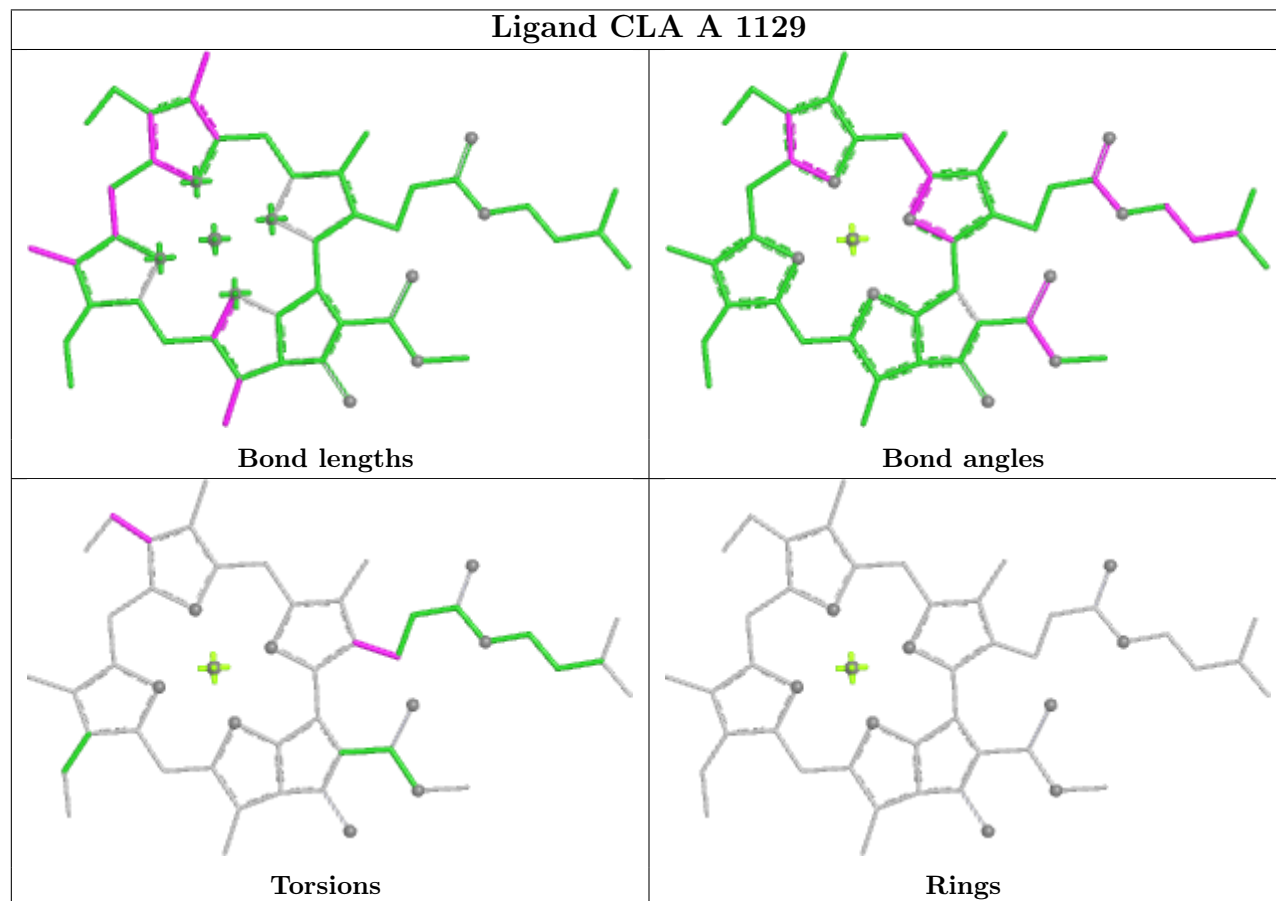


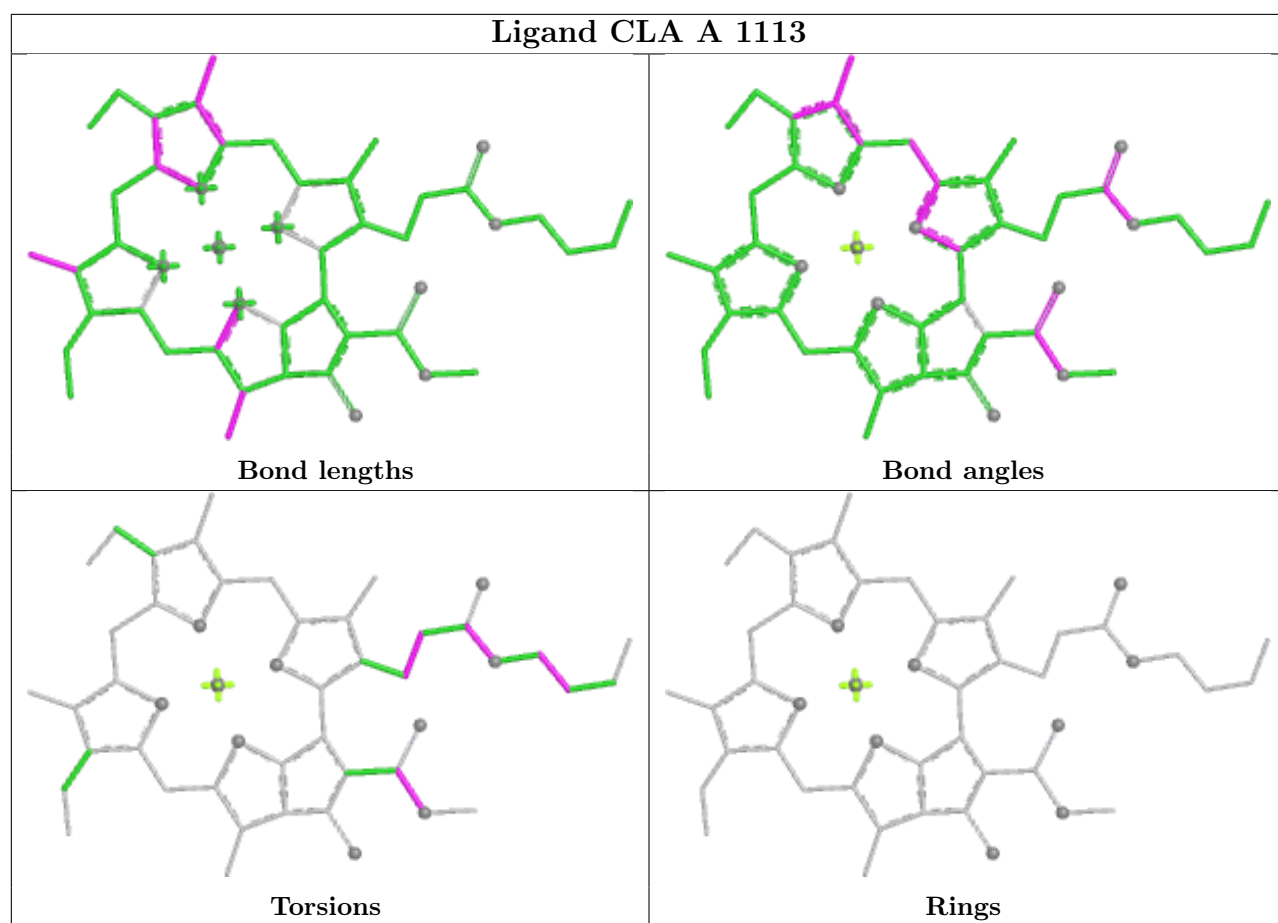


Ligand CLA d 511

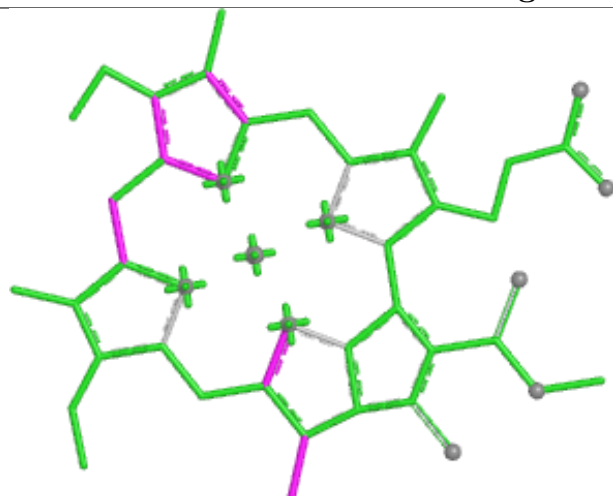


Ligand CLA A 1129

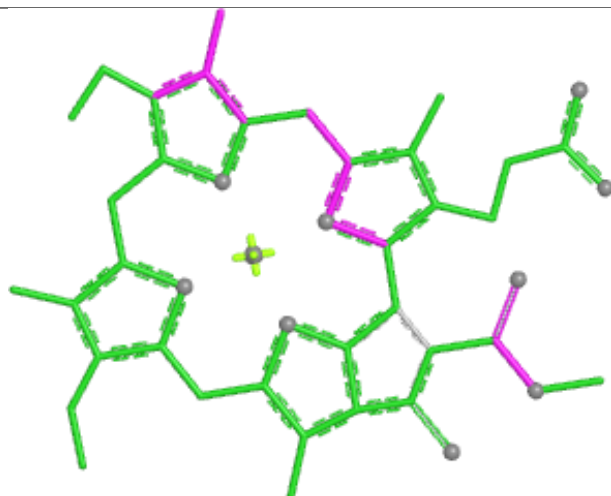




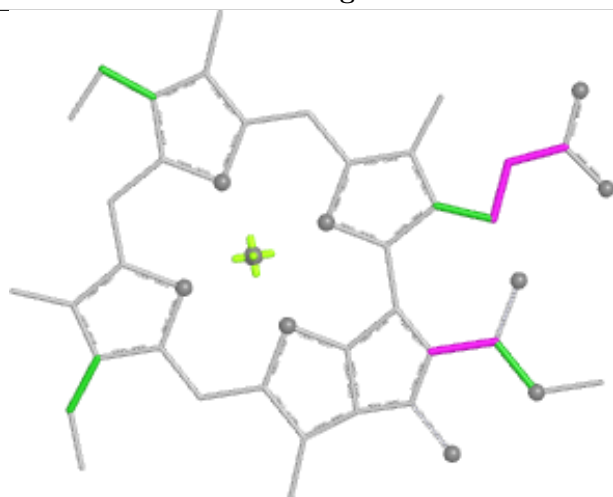
Ligand CLA 6 504



Bond lengths



Bond angles

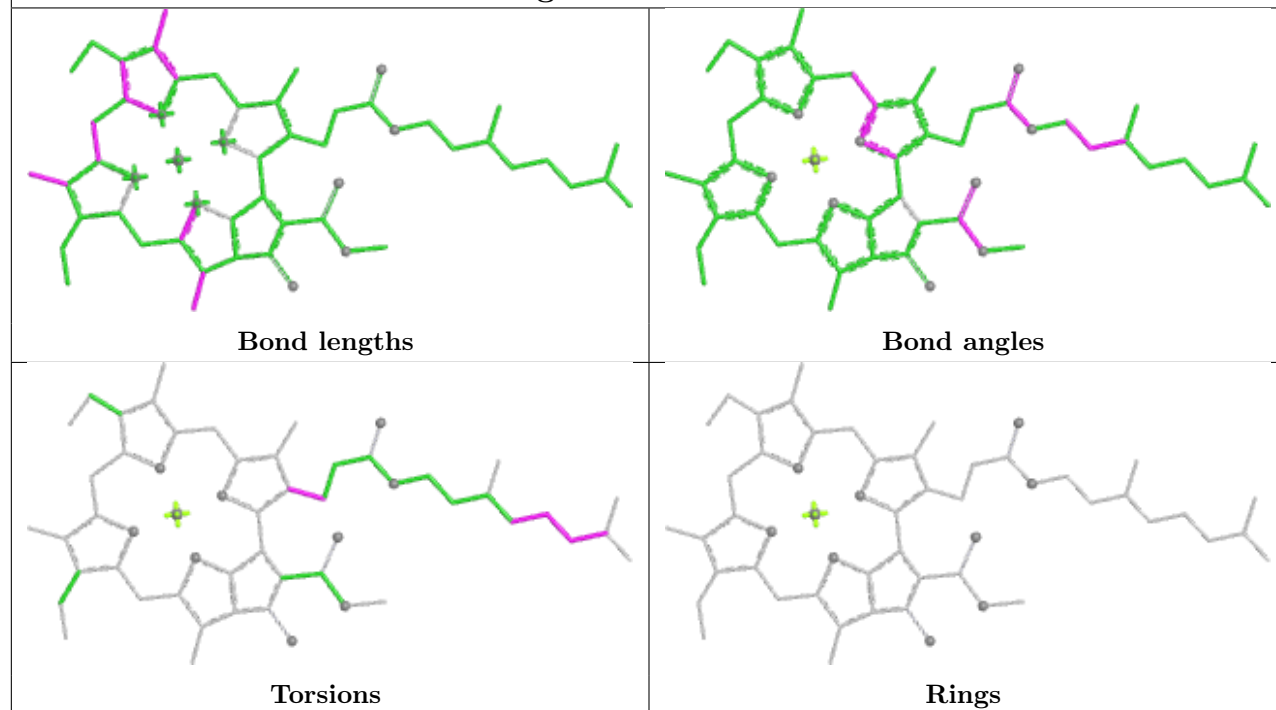


Torsions

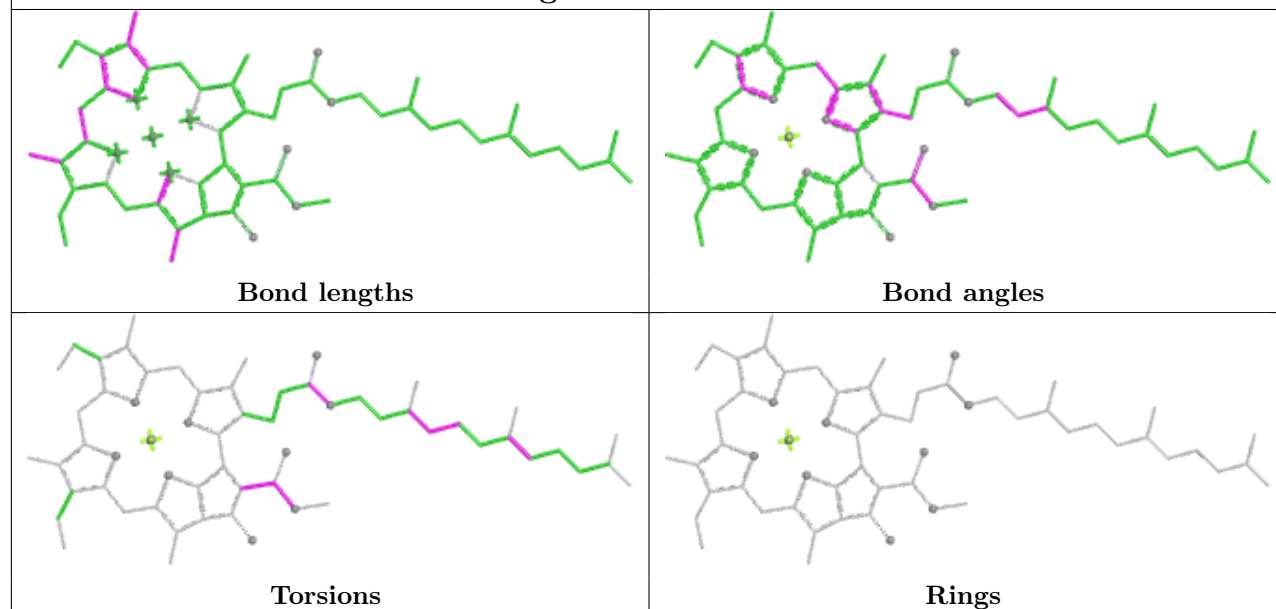


Rings

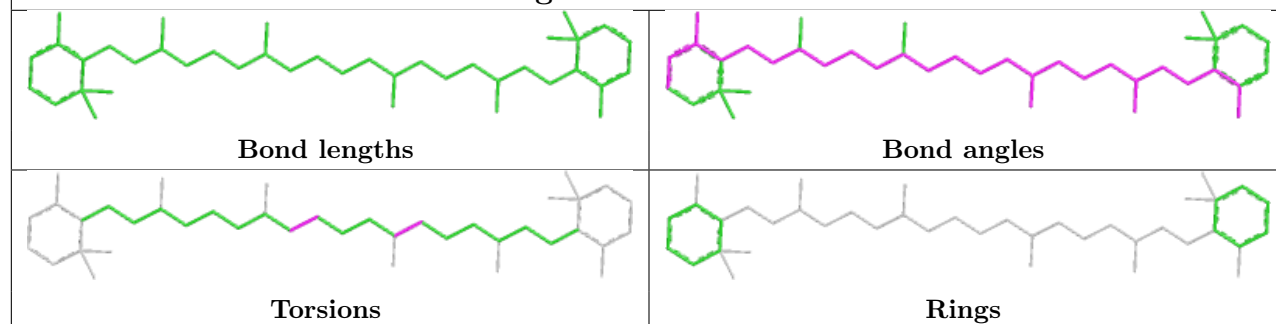
Ligand CLA e 508



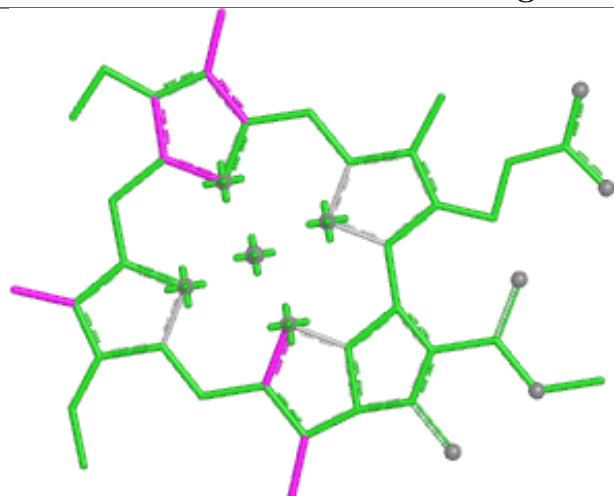
Ligand CLA f 502



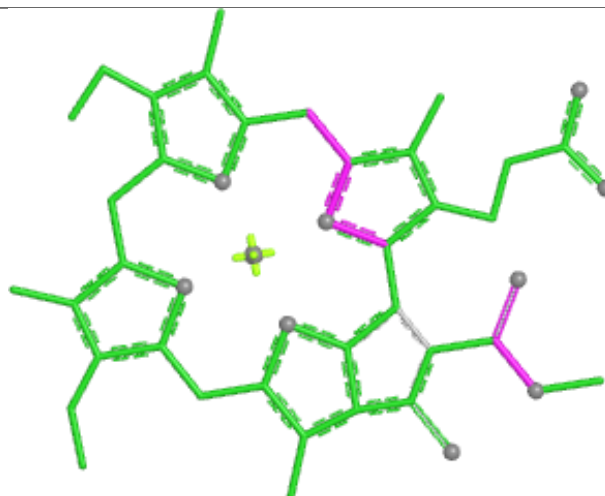
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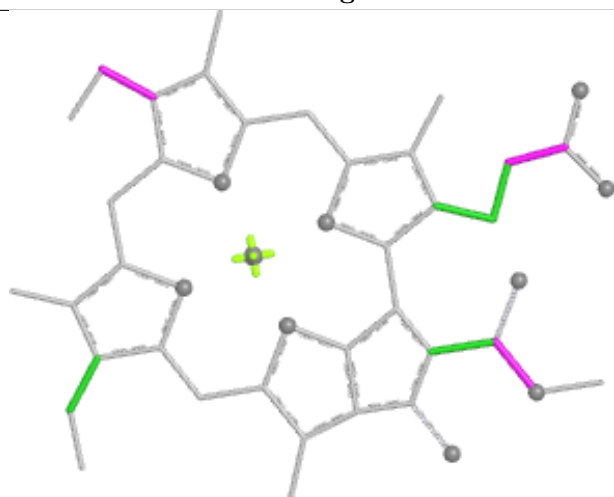
Ligand CLA d 517



Bond lengths



Bond angles

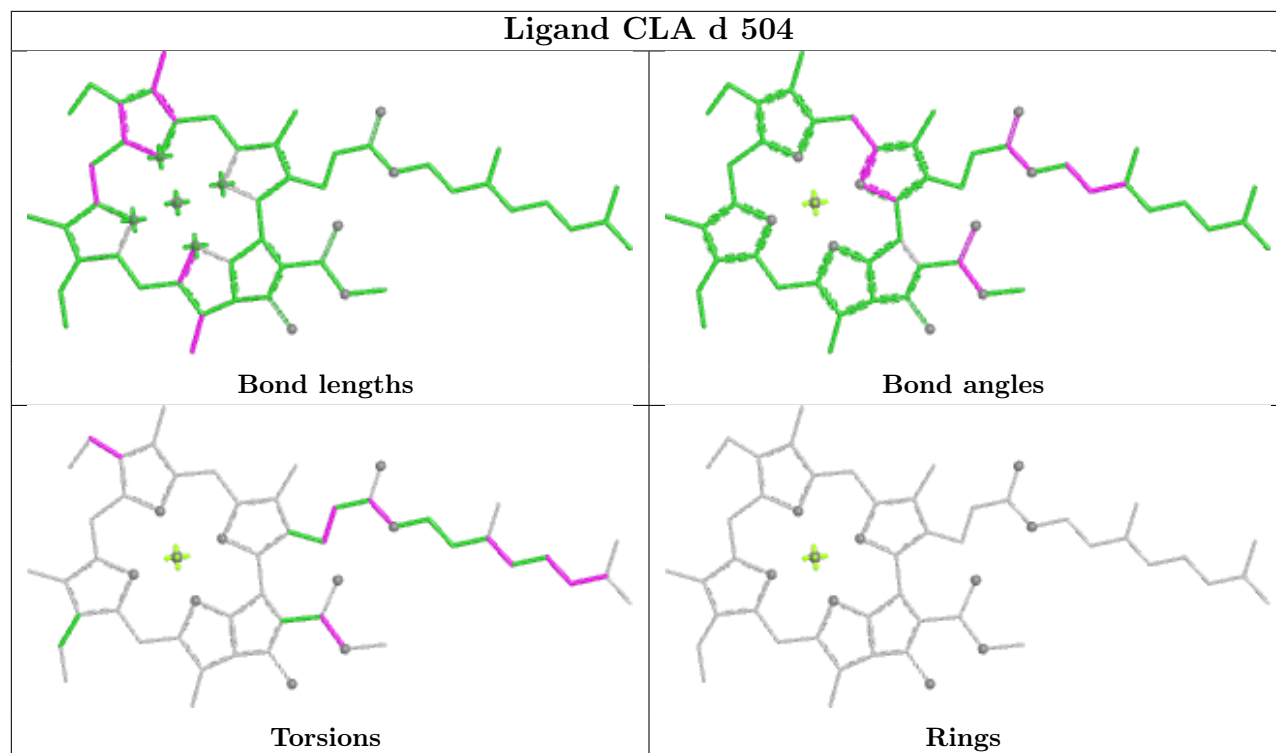


Torsions

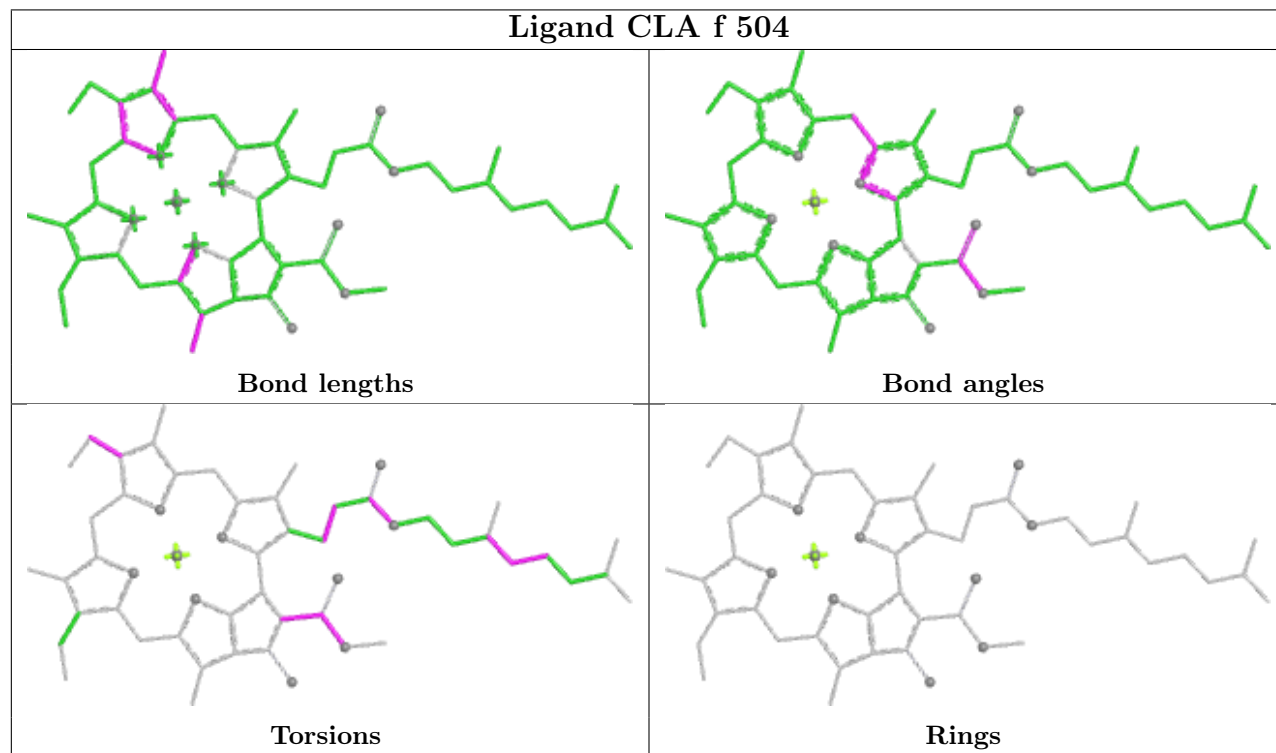


Rings

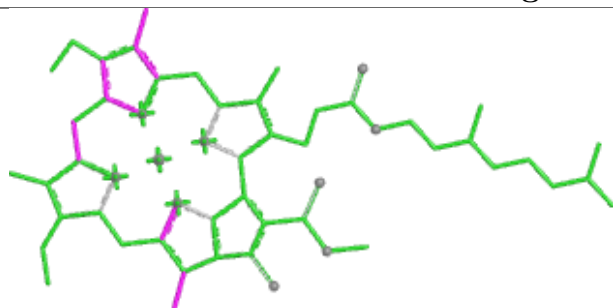
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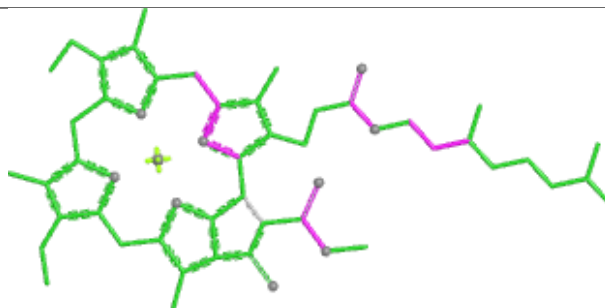
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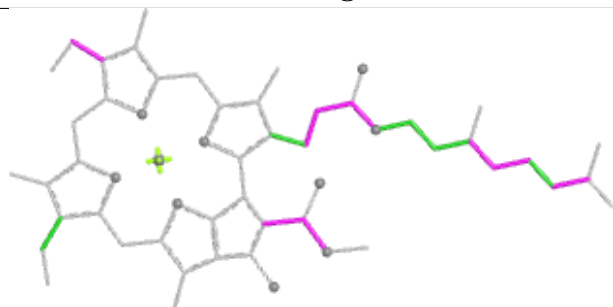
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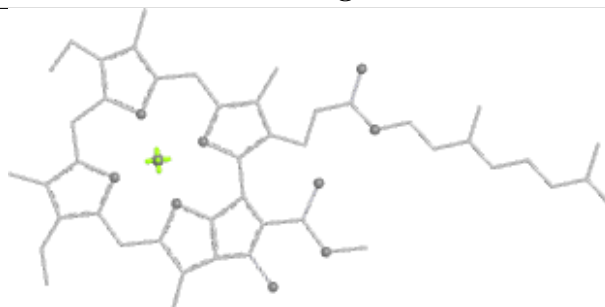
Bond lengths



Bond angles

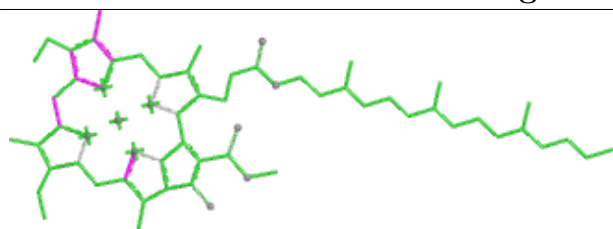


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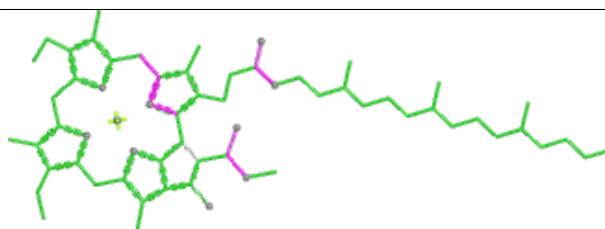


Rings

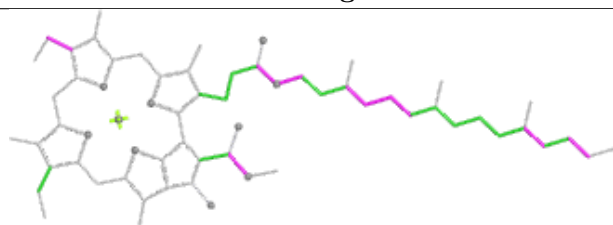
Ligand CLA c 503



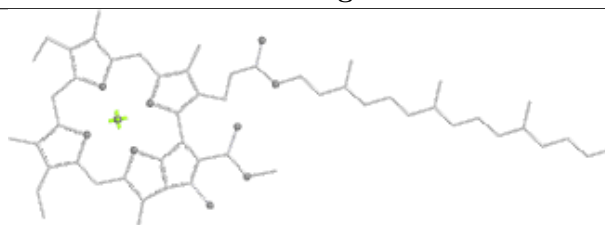
Bond lengths



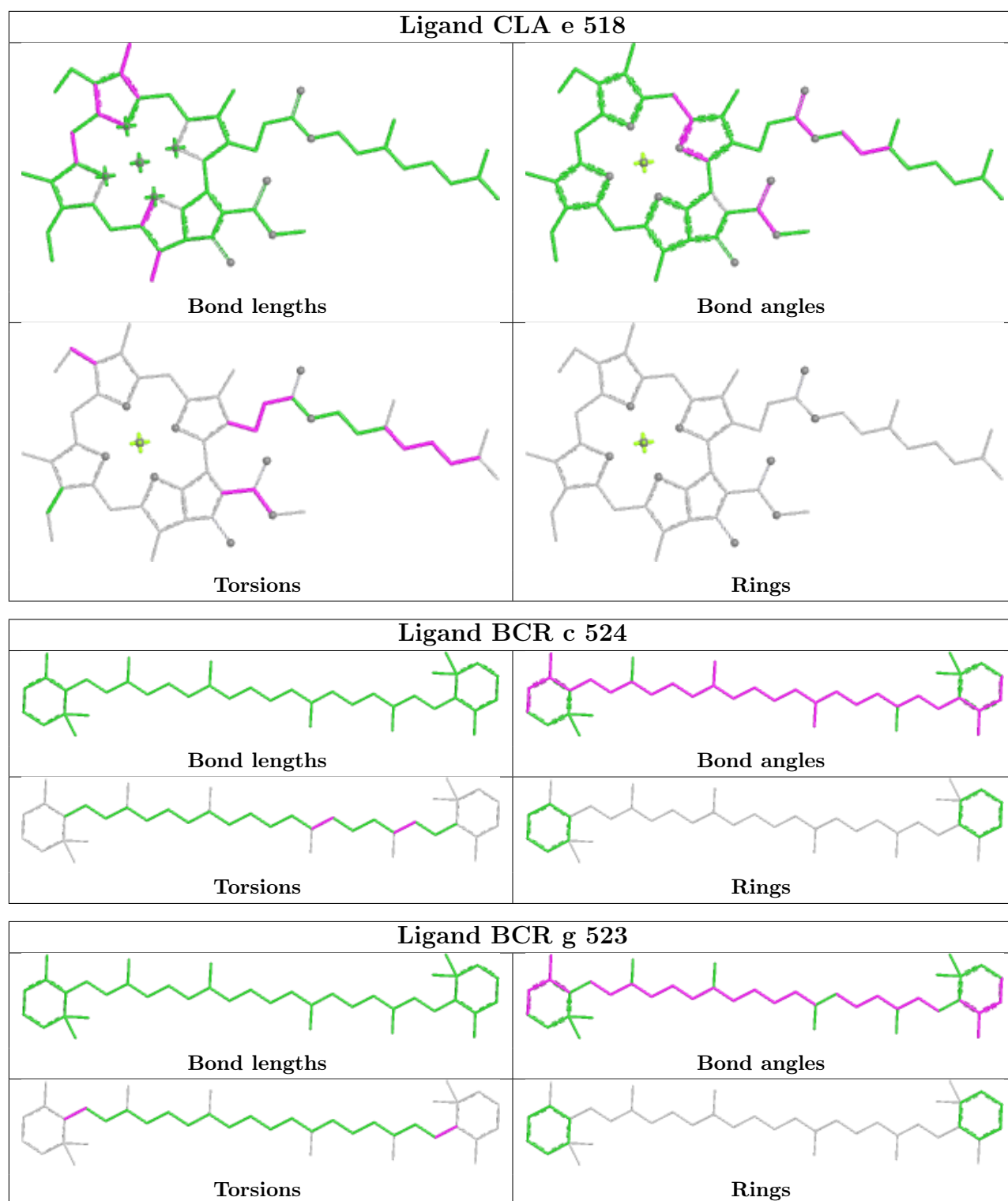
Bond angles

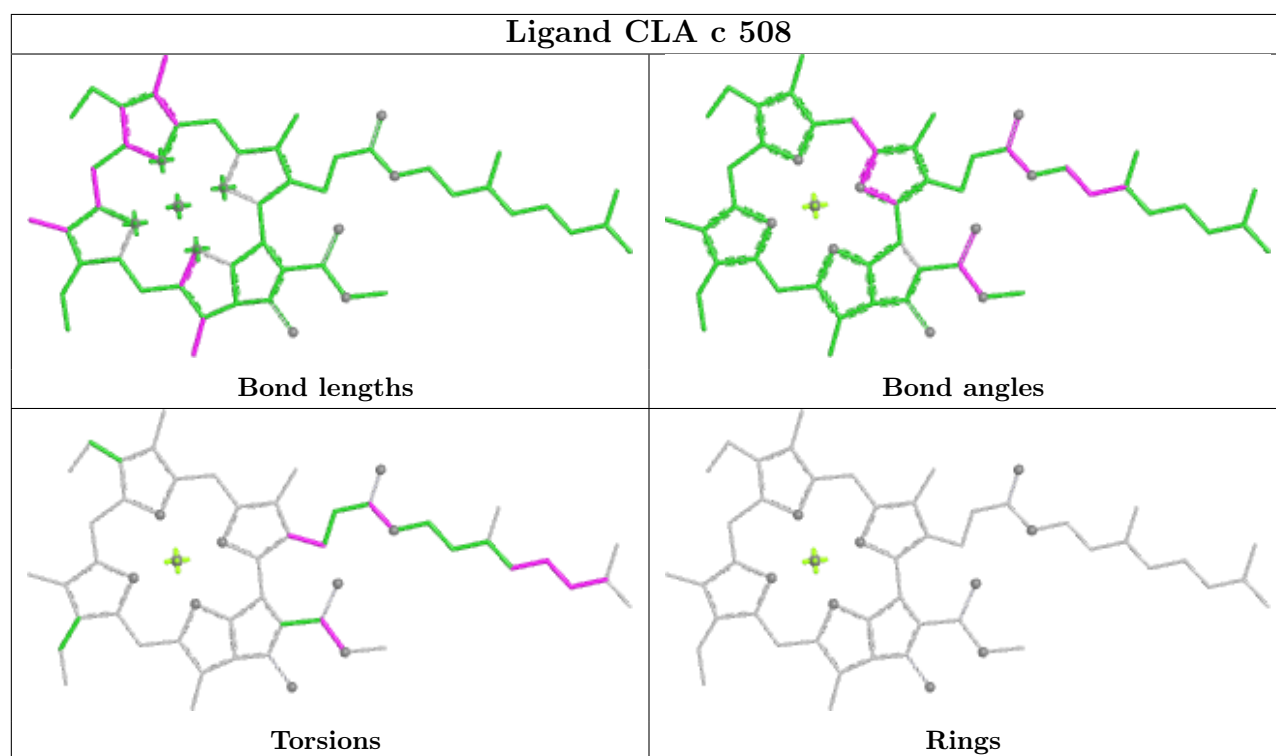
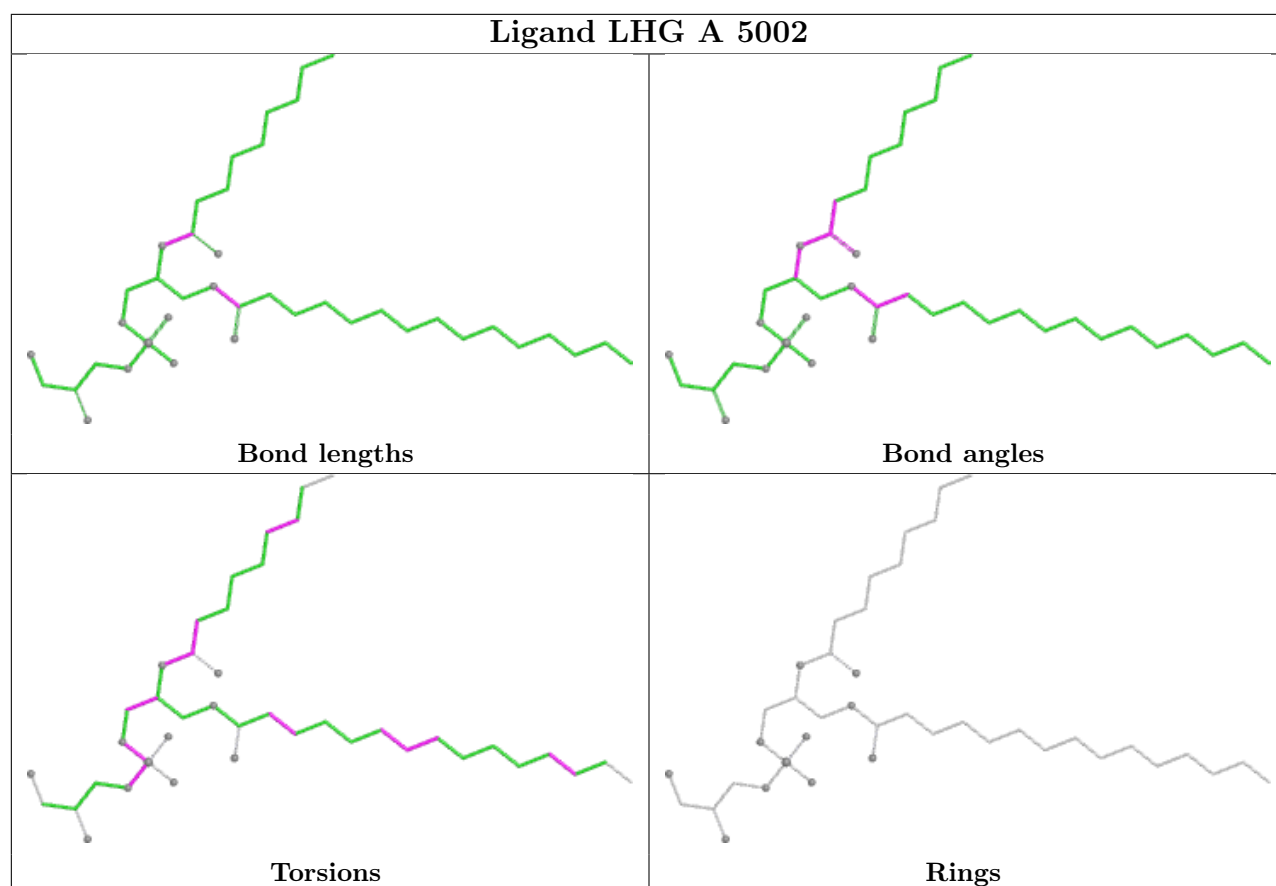


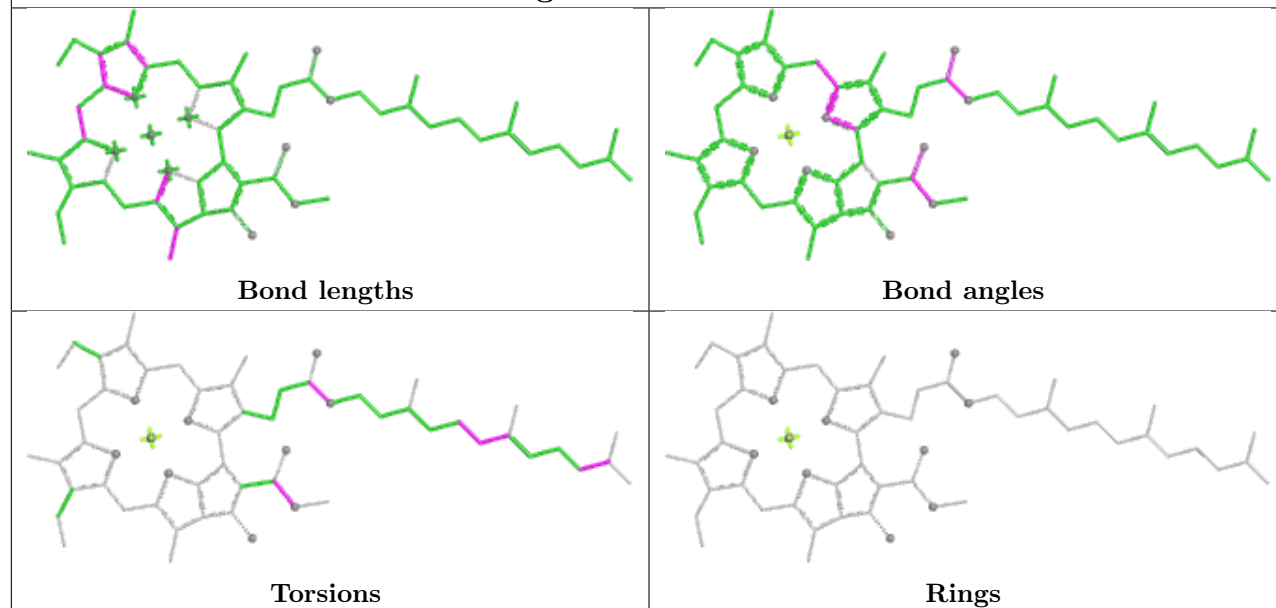
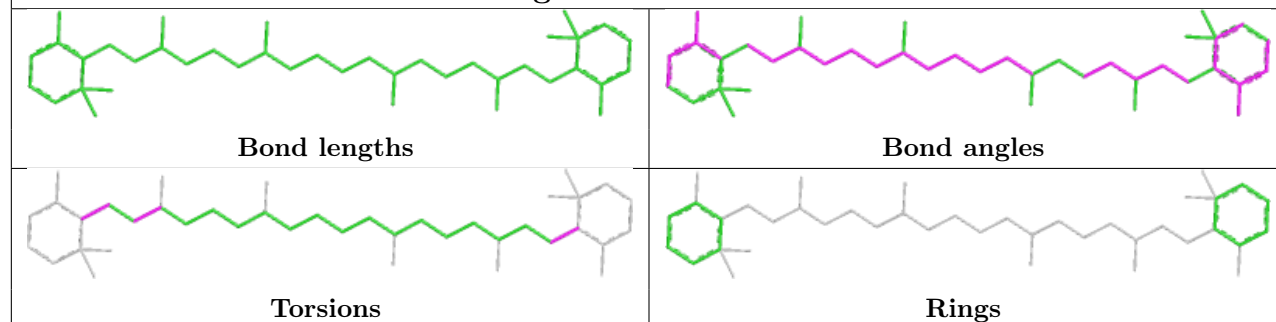
Torsions



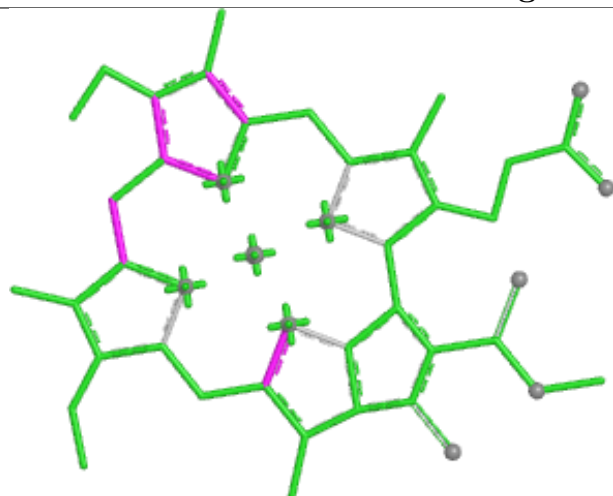
Rings



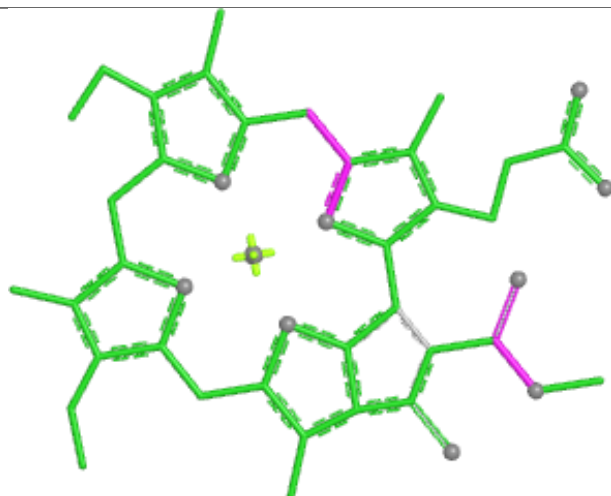


Ligand CLA 1 507**Ligand BCR d 521**

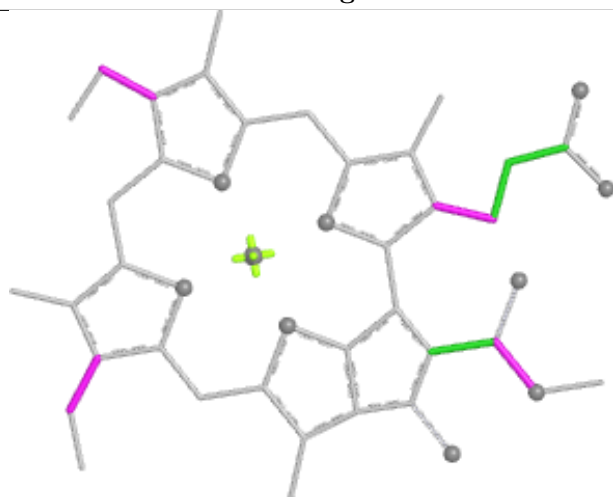
Ligand CLA 1 519



Bond lengths



Bond angles

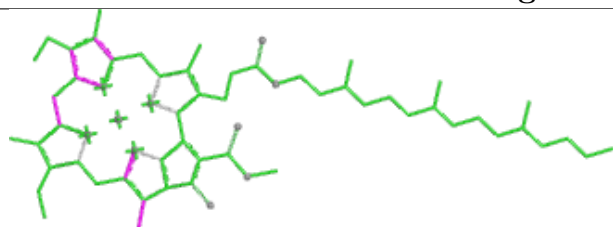


Torsions

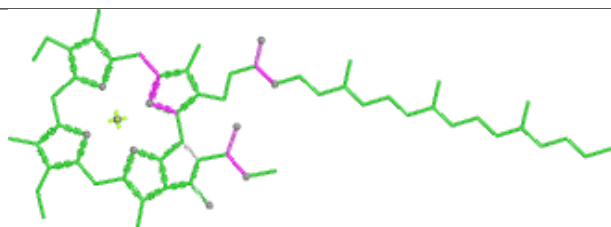


Rings

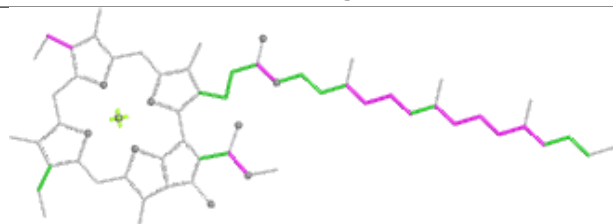
Ligand CLA 1 503



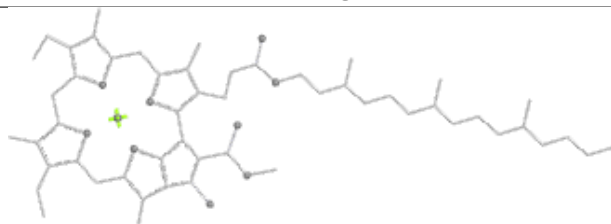
Bond lengths



Bond angles

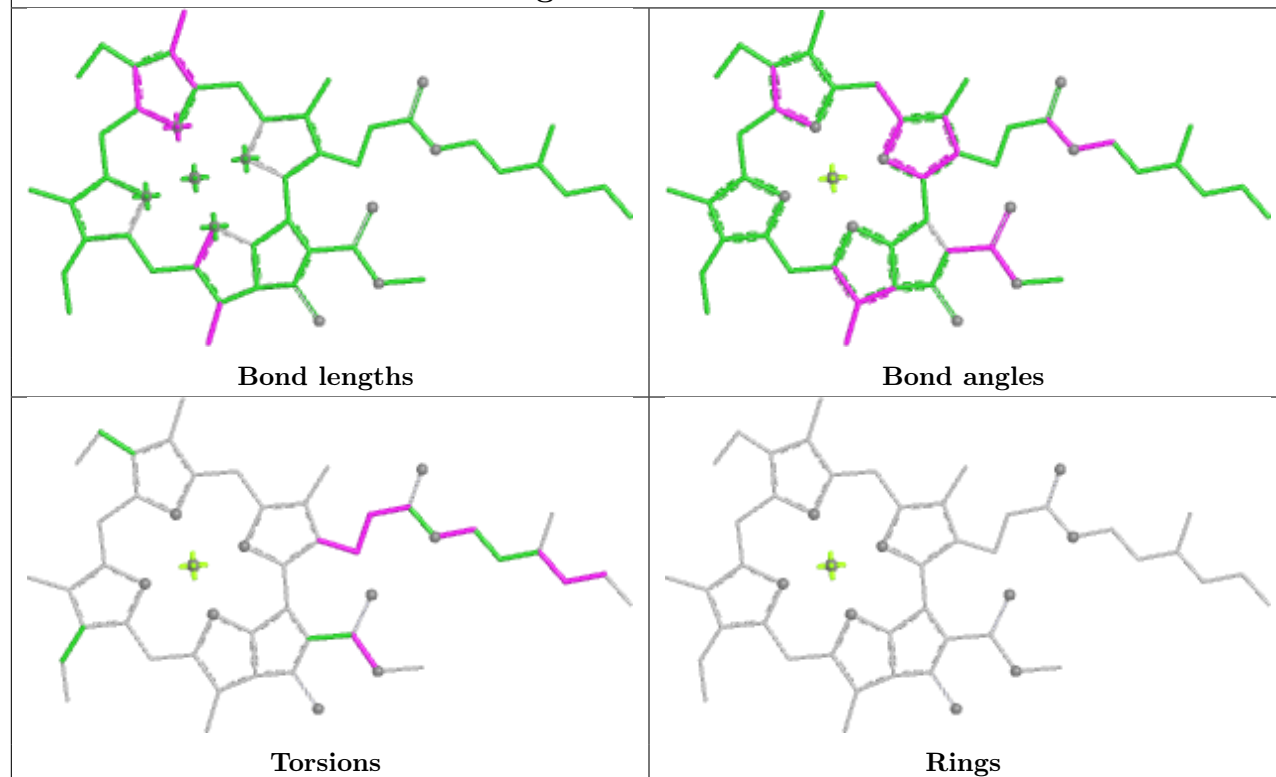


Torsions

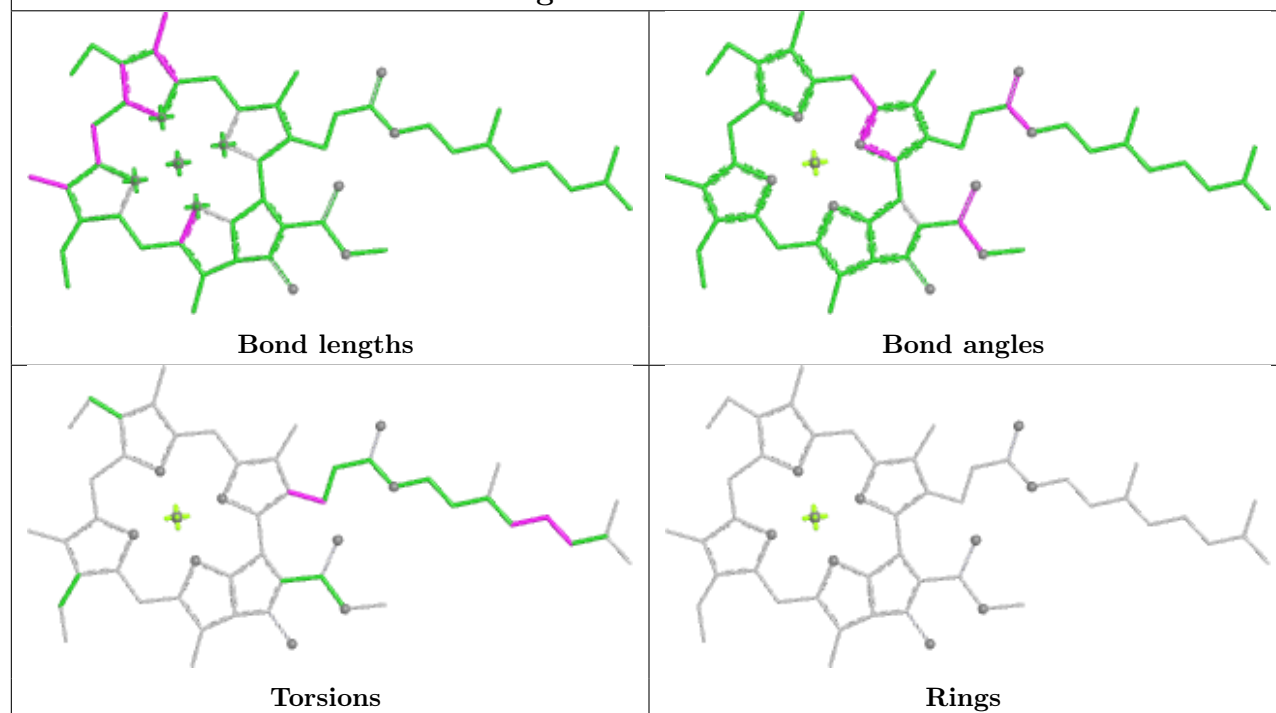


Rings

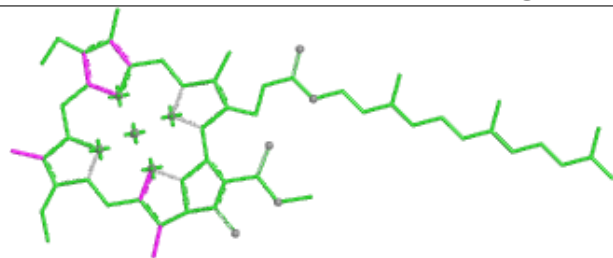
Ligand CLA 2 512



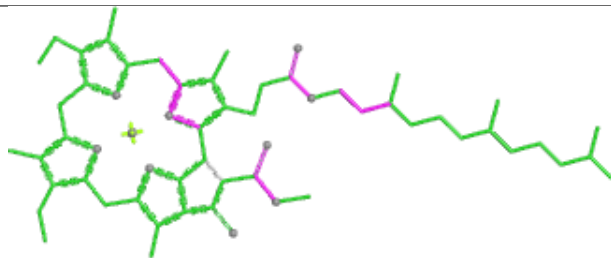
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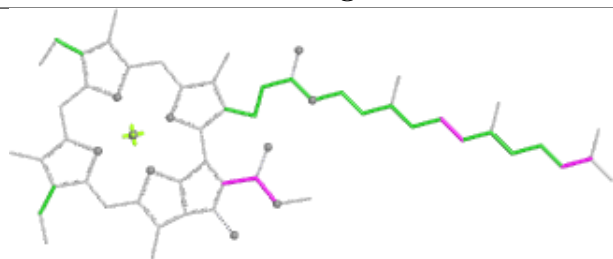
Ligand CLA 4 507



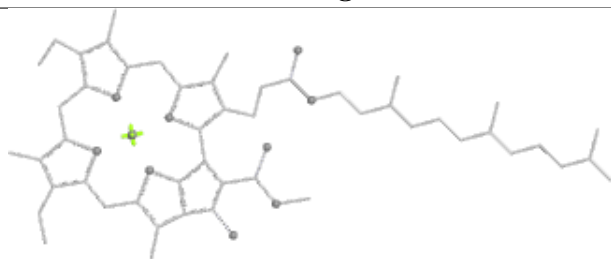
Bond lengths



Bond angles

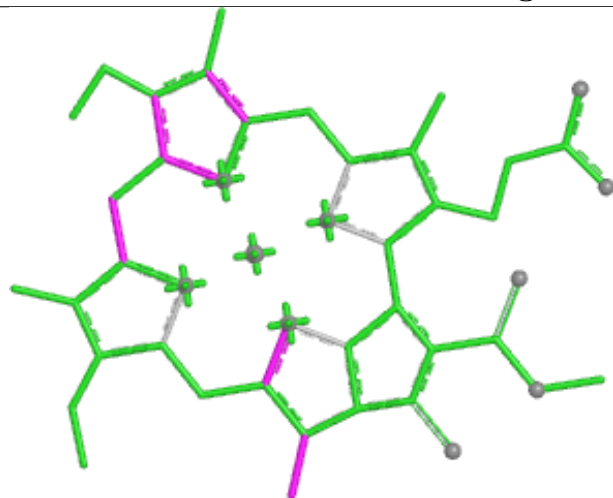


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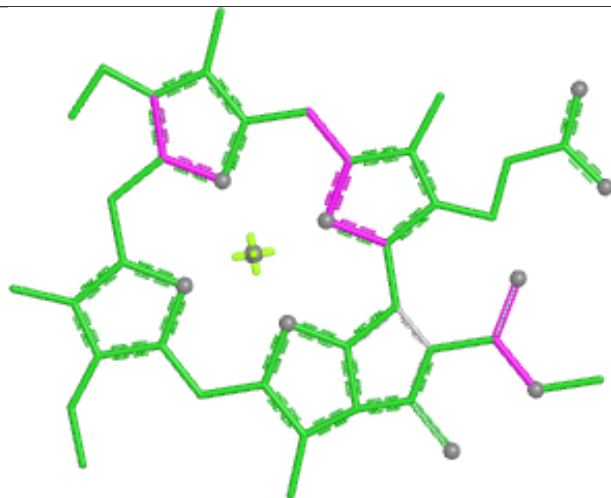


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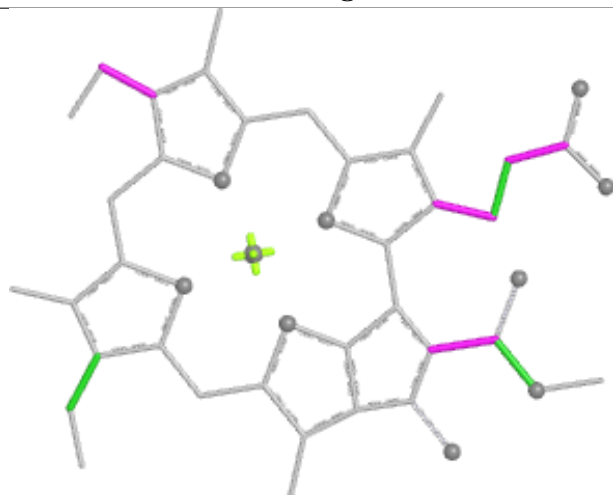
Ligand CLA b 516



Bond lengths



Bond angles

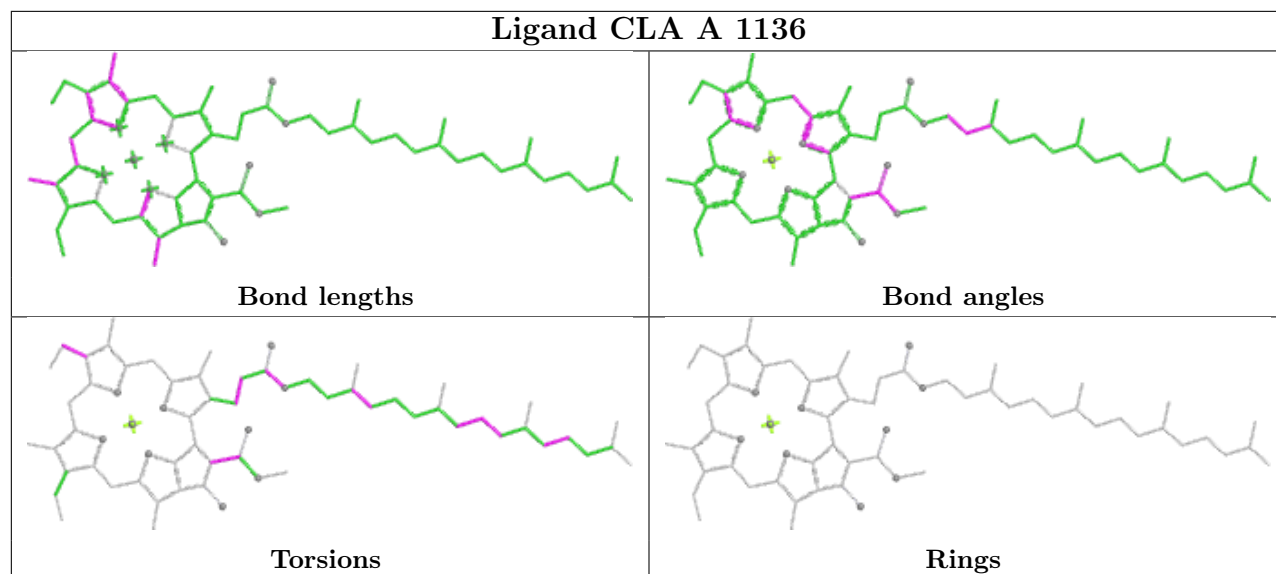


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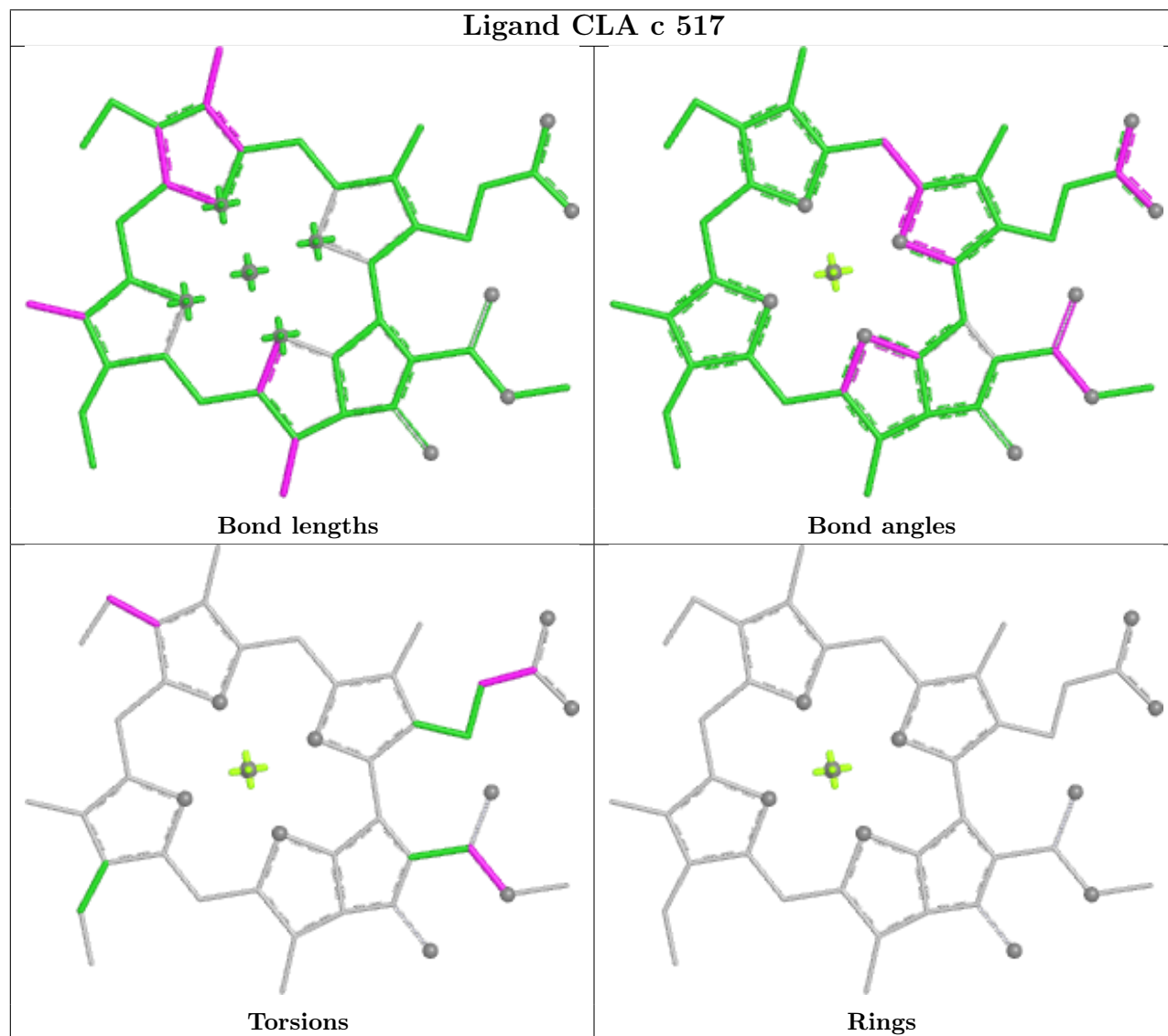


Rings

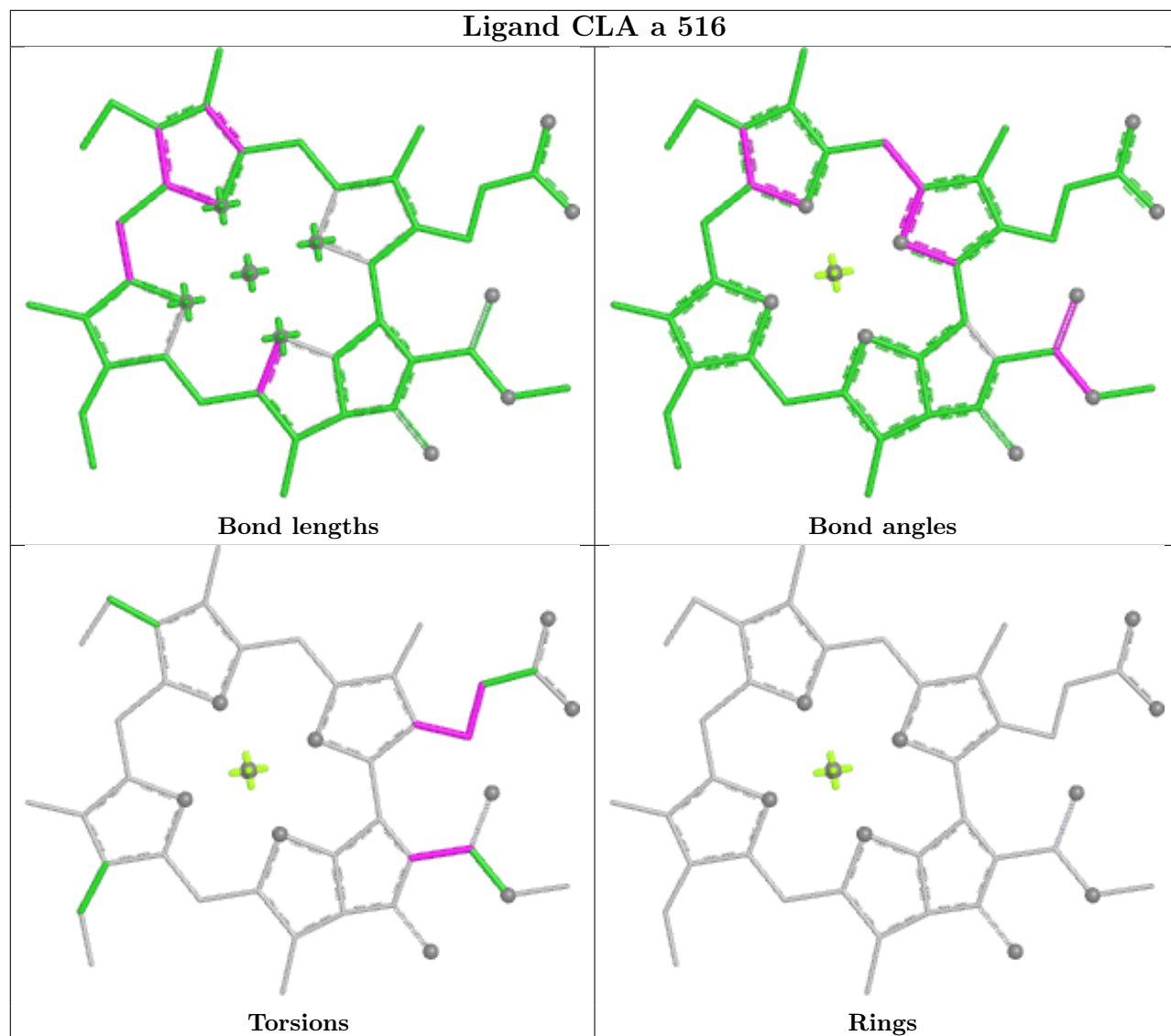
Ligand CLA A 1136



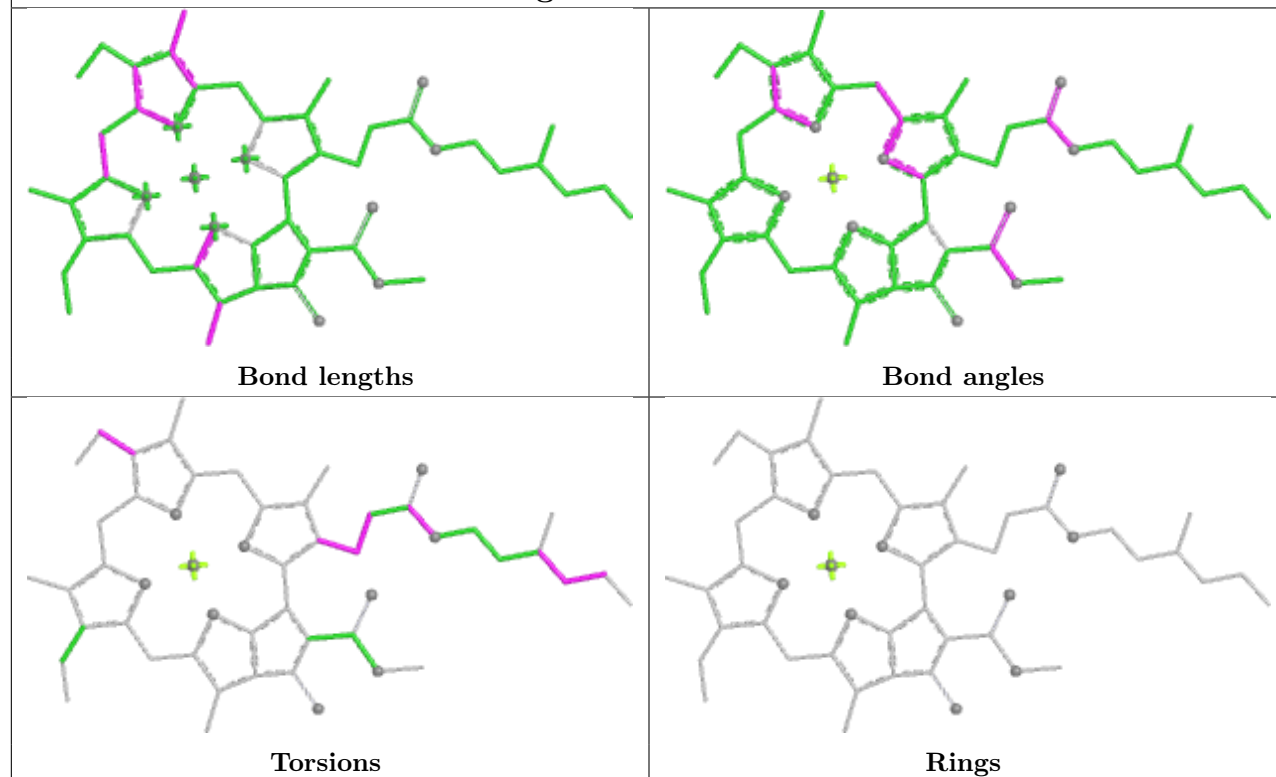
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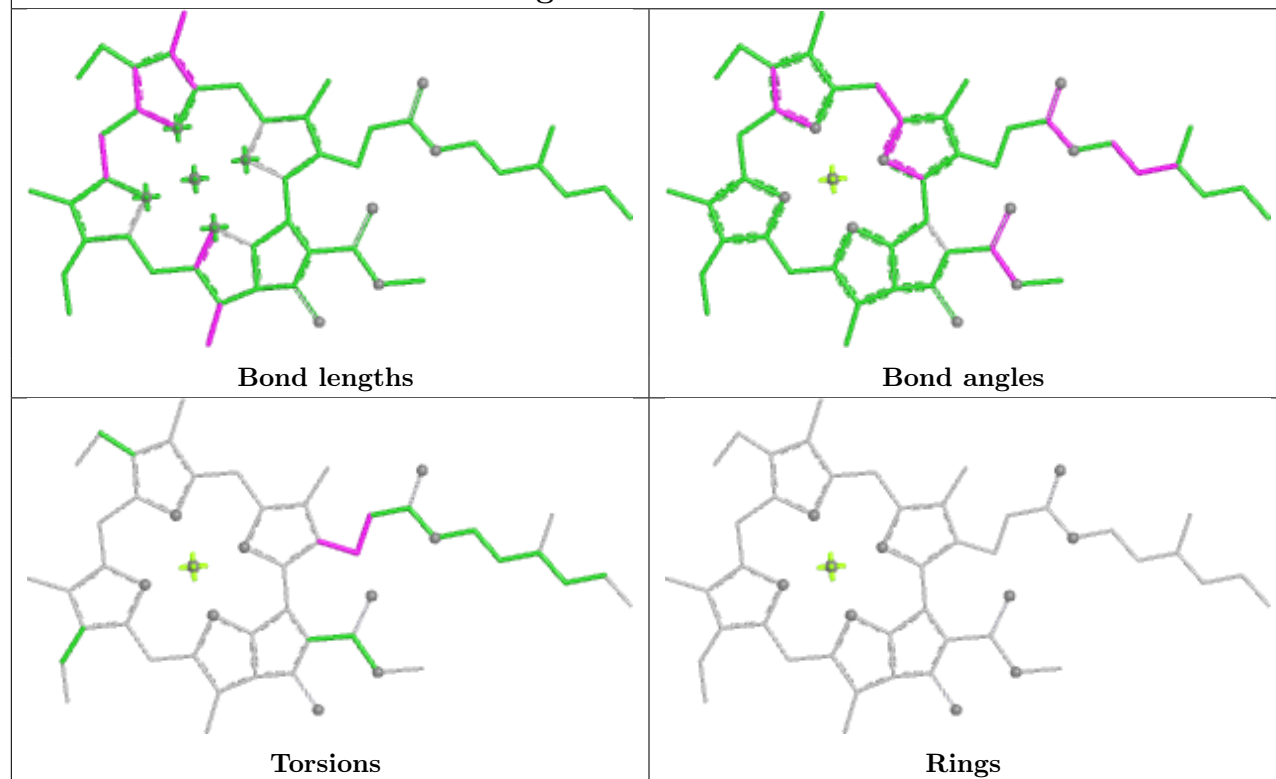
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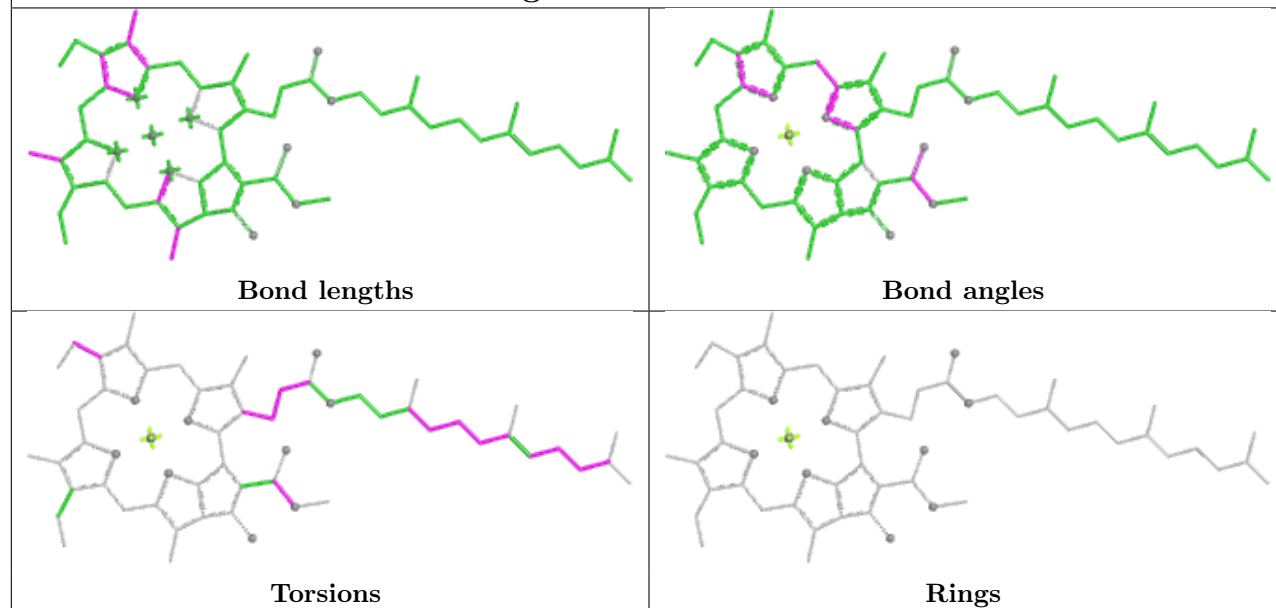
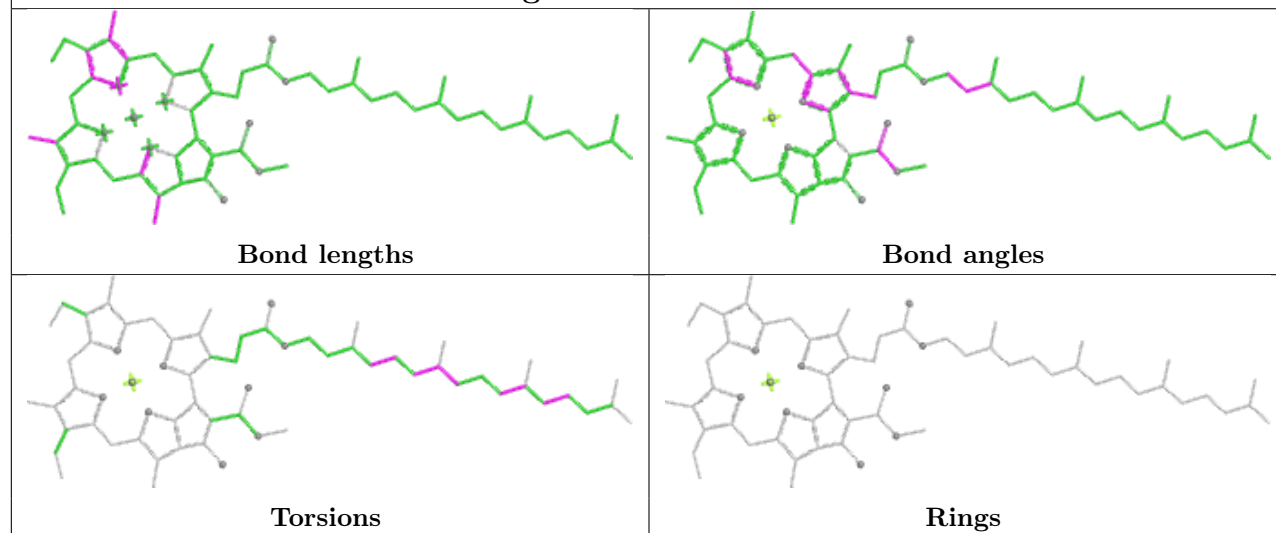


Ligand CLA a 512

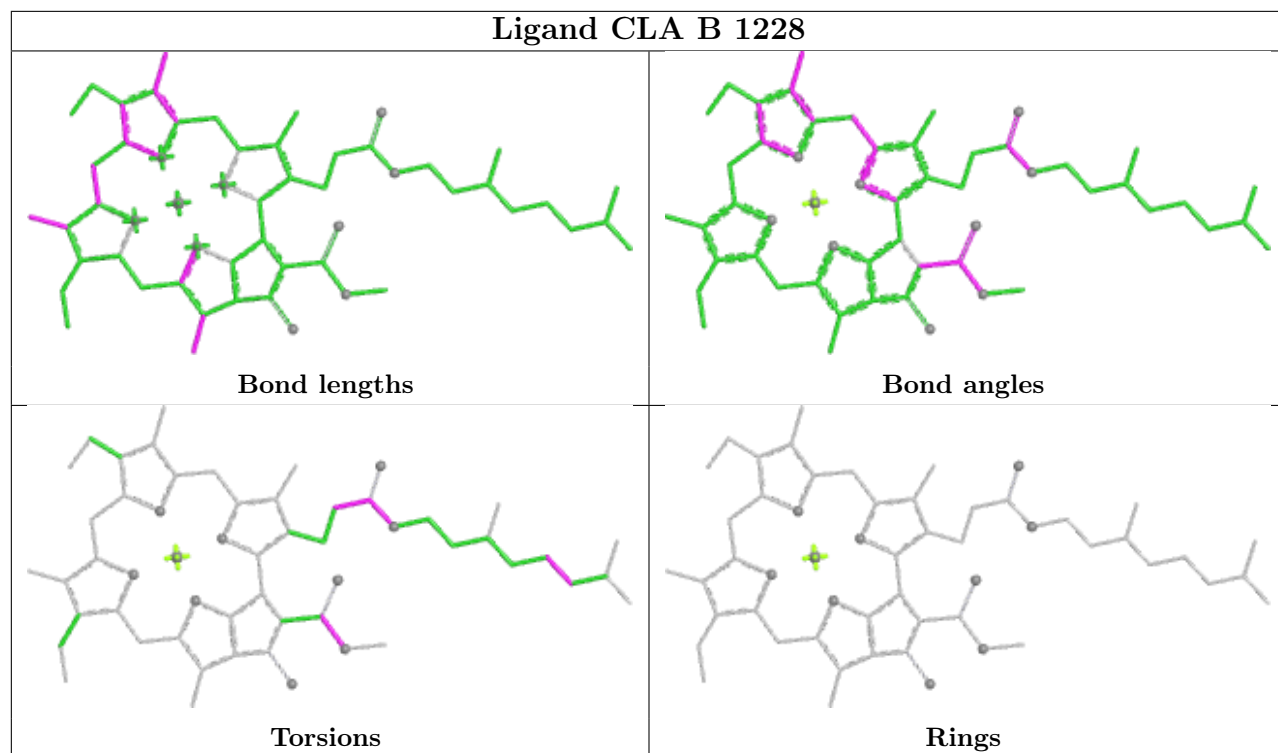


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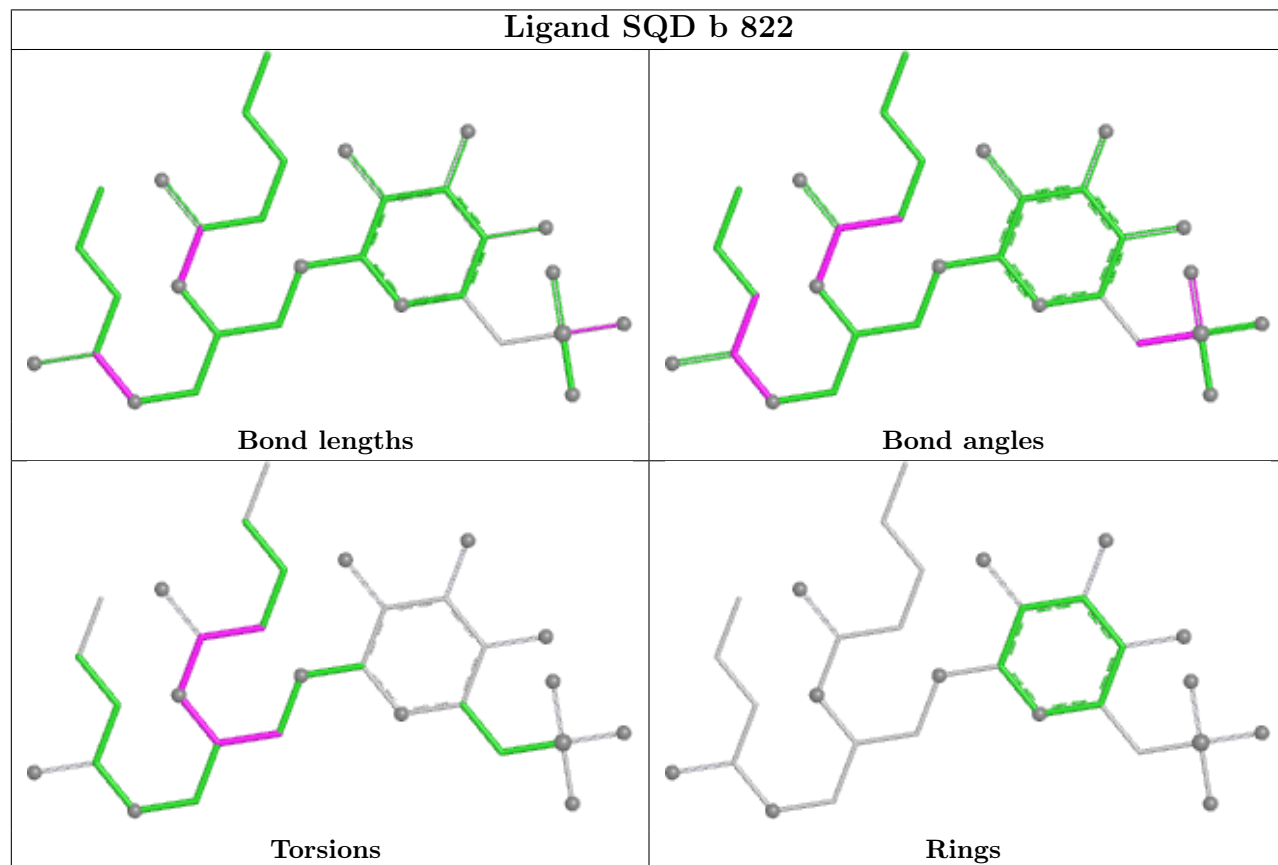


Ligand CLA A 1115**Ligand CLA A 1123**

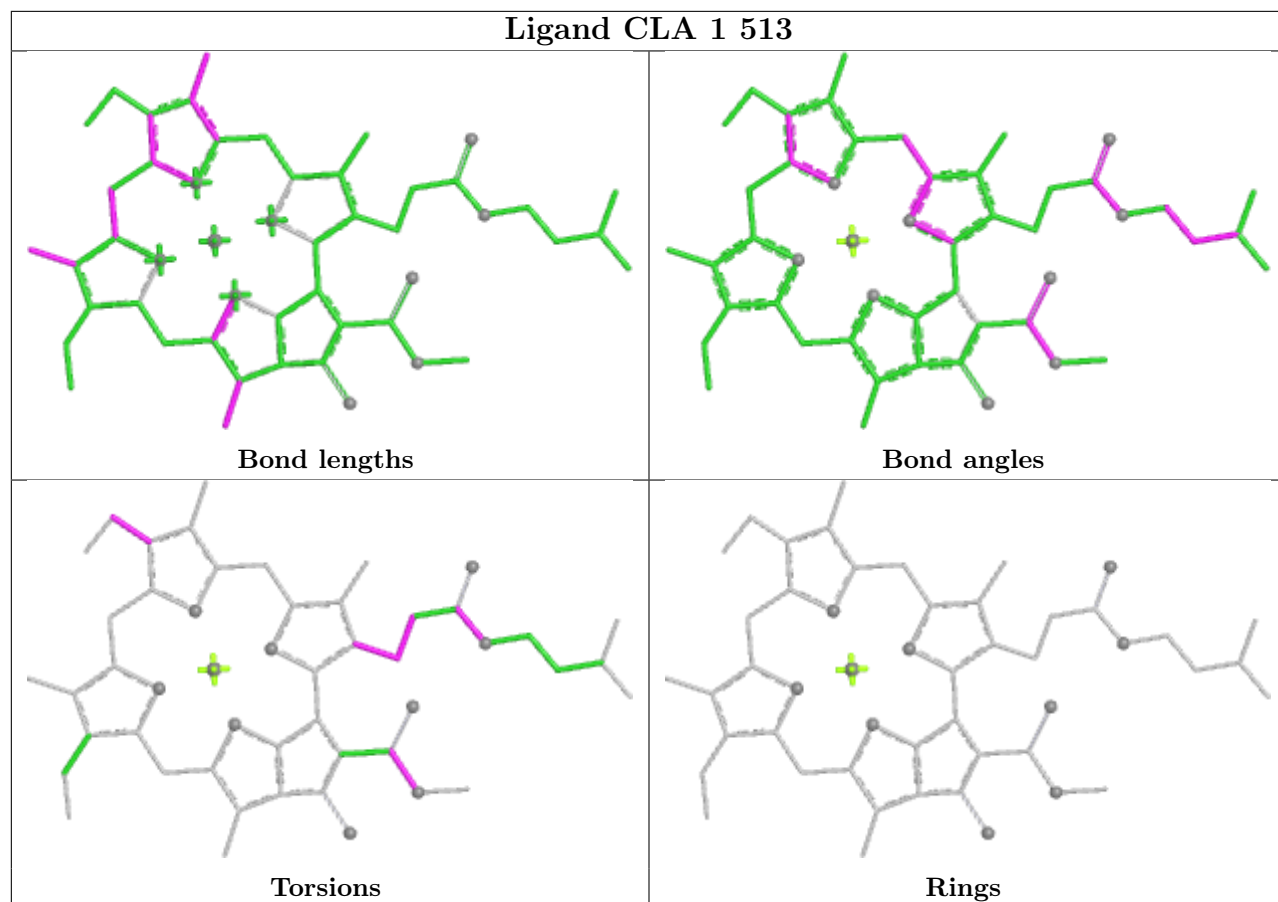
Ligand CLA B 1228



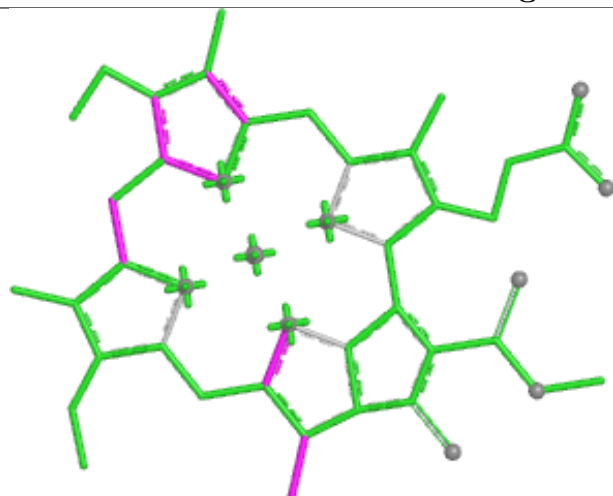
Ligand SQD b 822



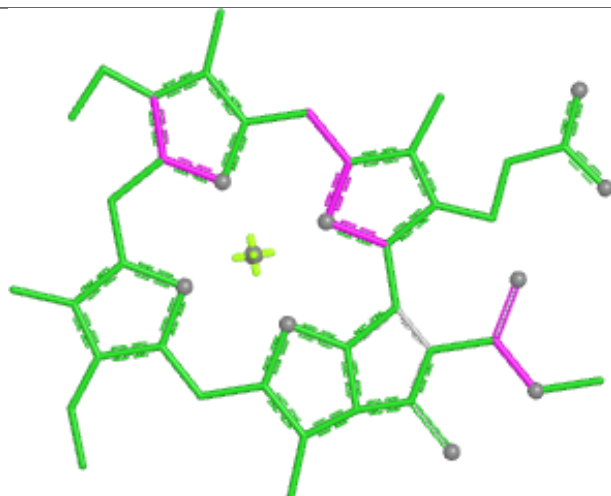
Ligand CLA 1 513



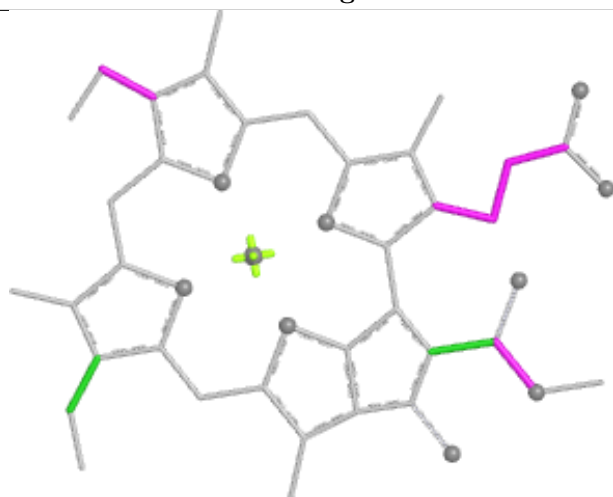
Ligand CLA e 516



Bond lengths



Bond angles

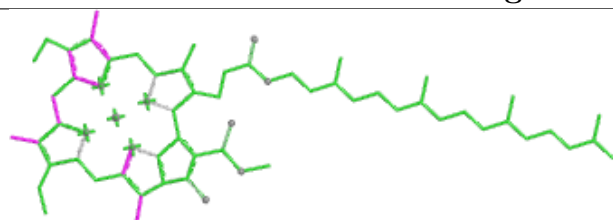


Torsions

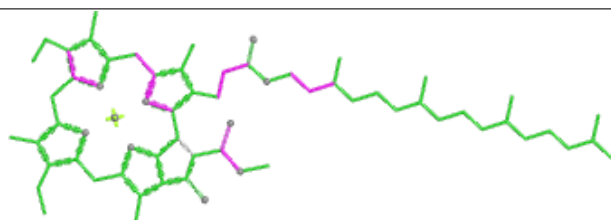


Rings

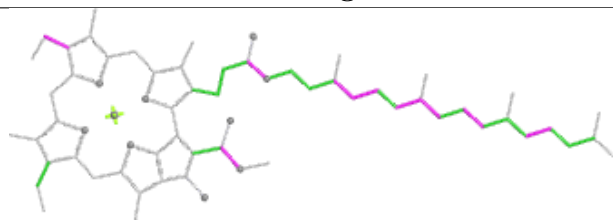
Ligand CLA A 1125



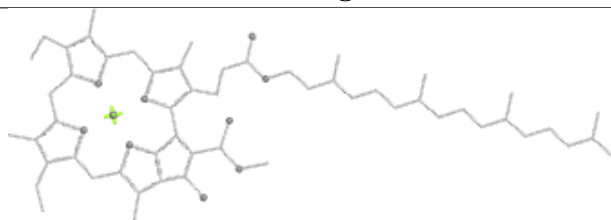
Bond lengths



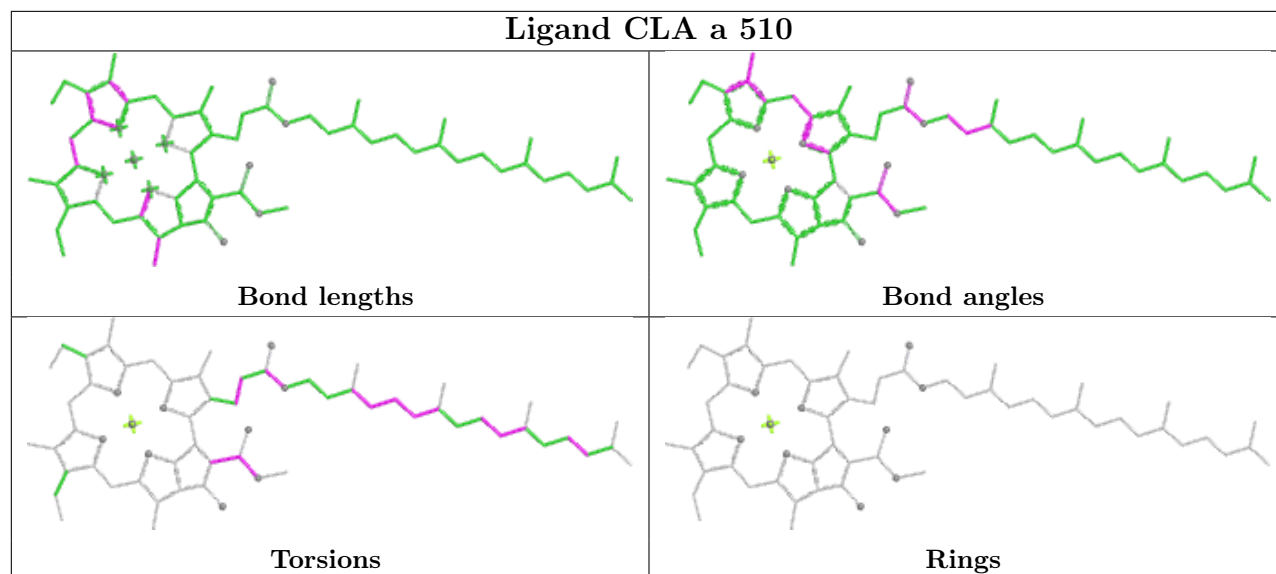
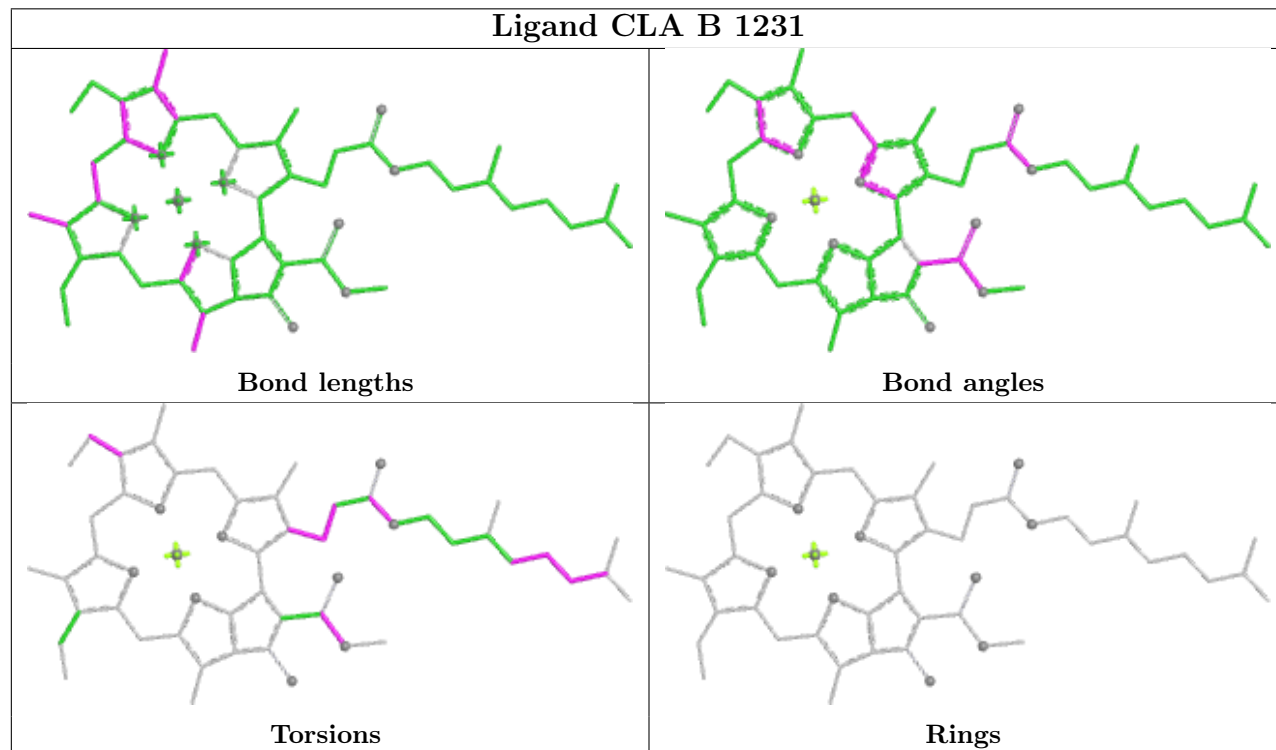
Bond angles



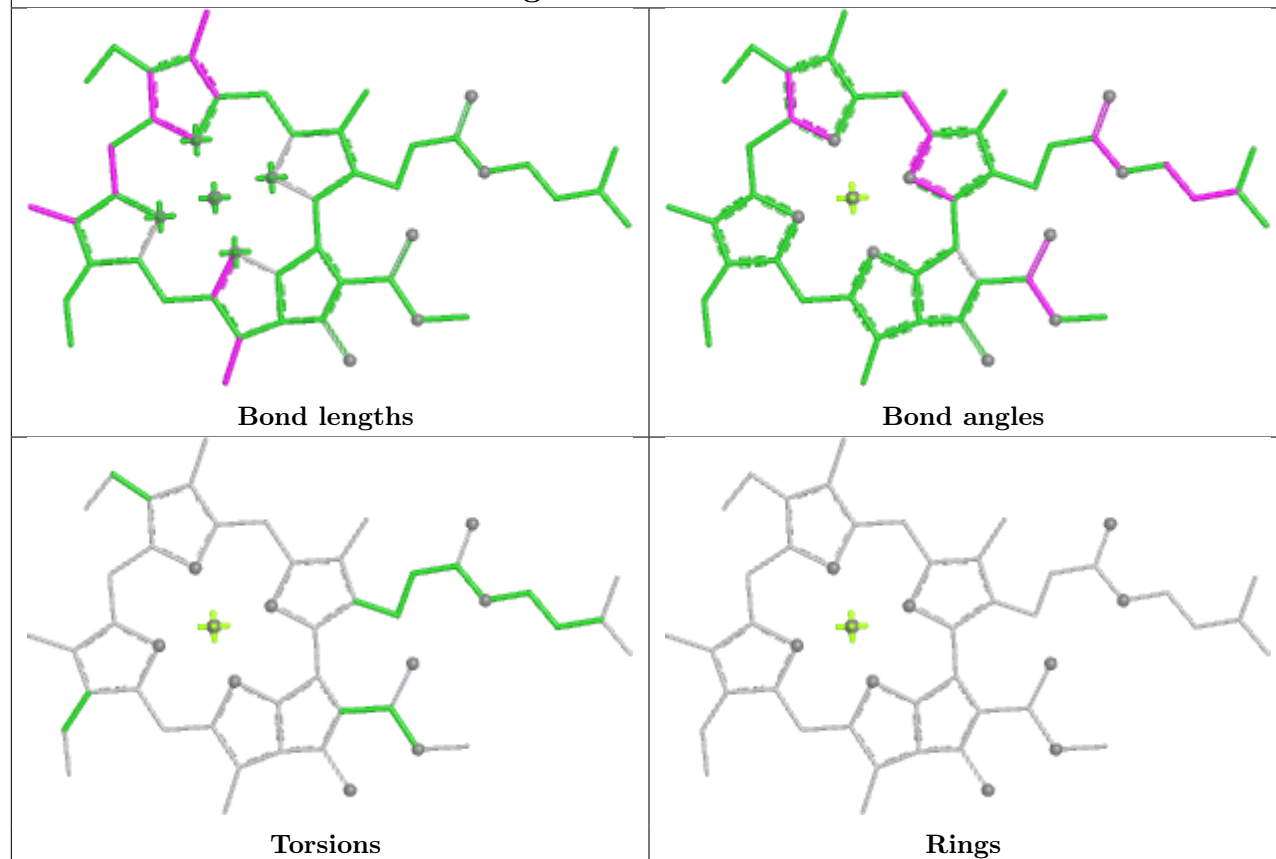
Torsions



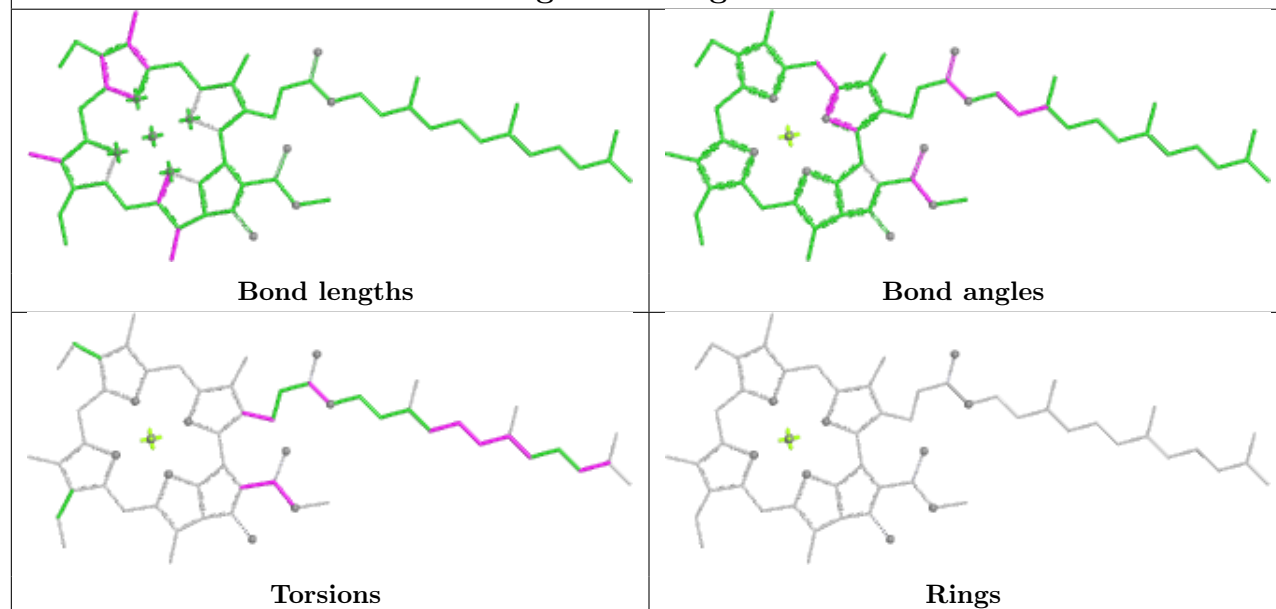
Rings

Ligand CLA a 510**Ligand CLA B 1231**

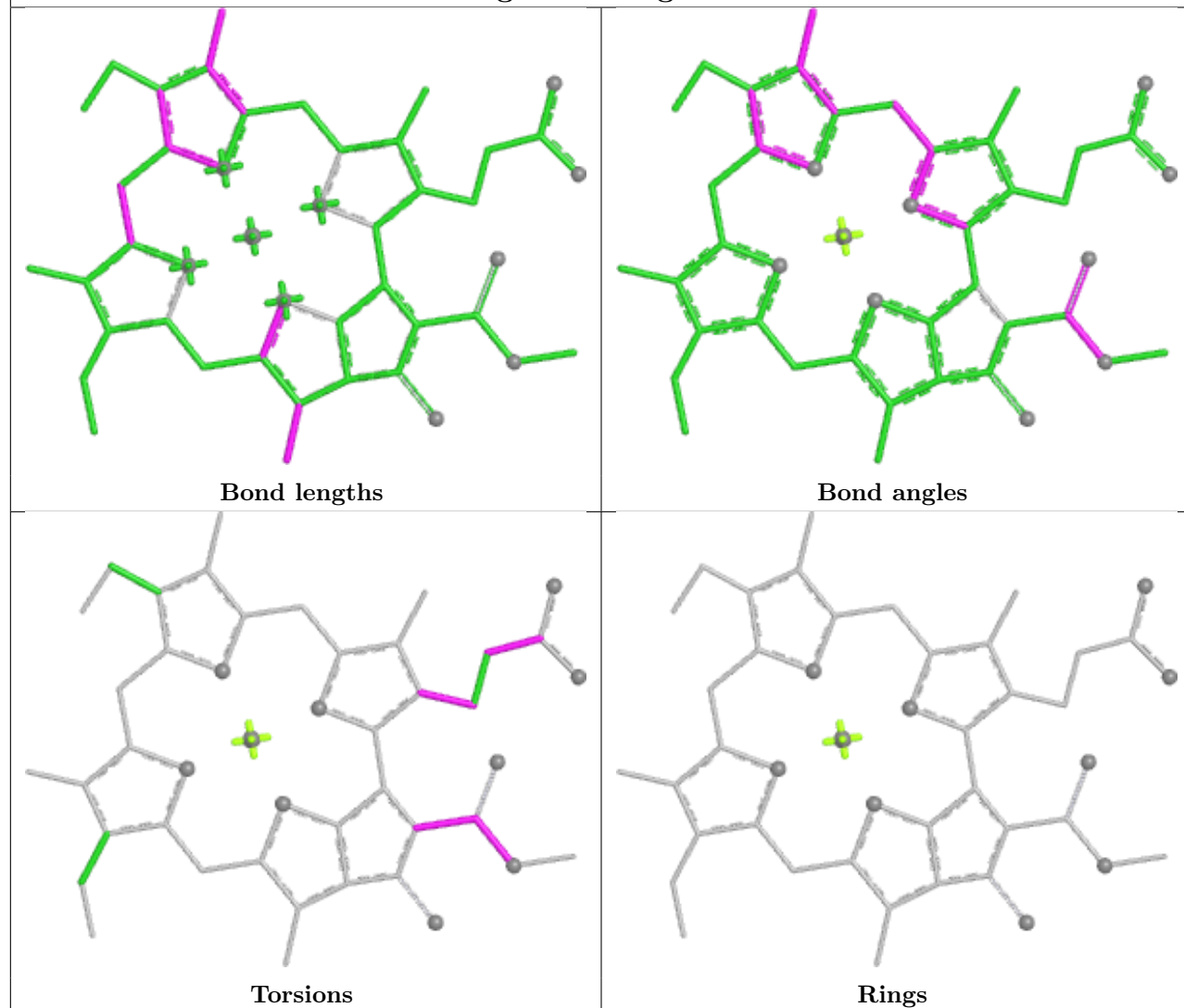
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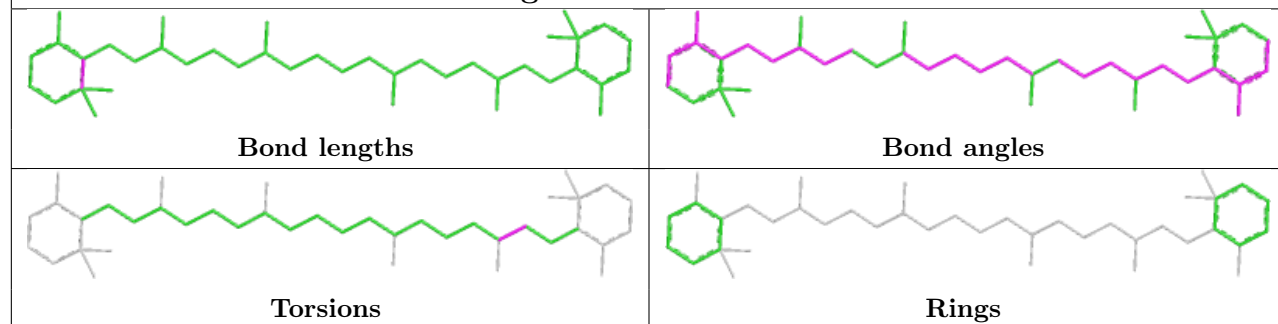
Ligand CLA g 502



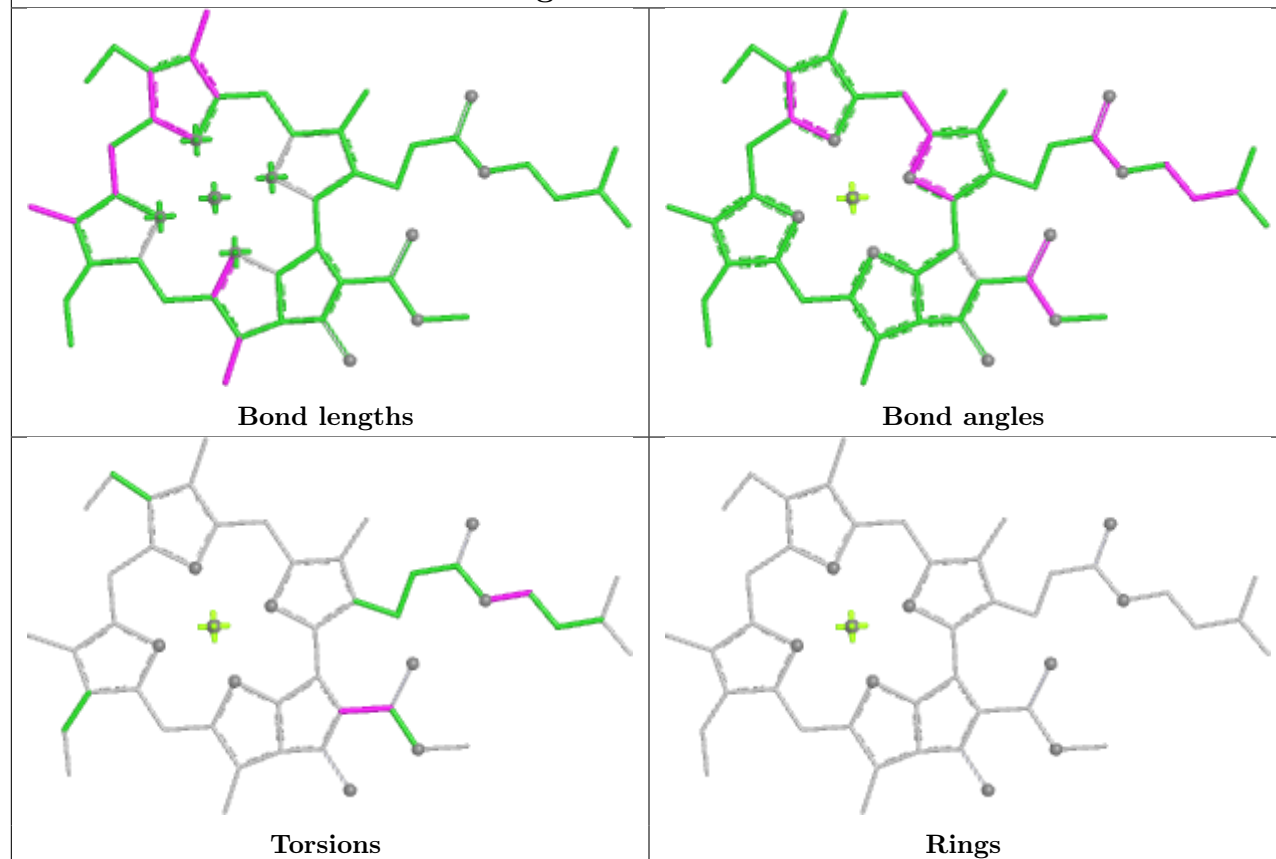
Ligand CLA g 506



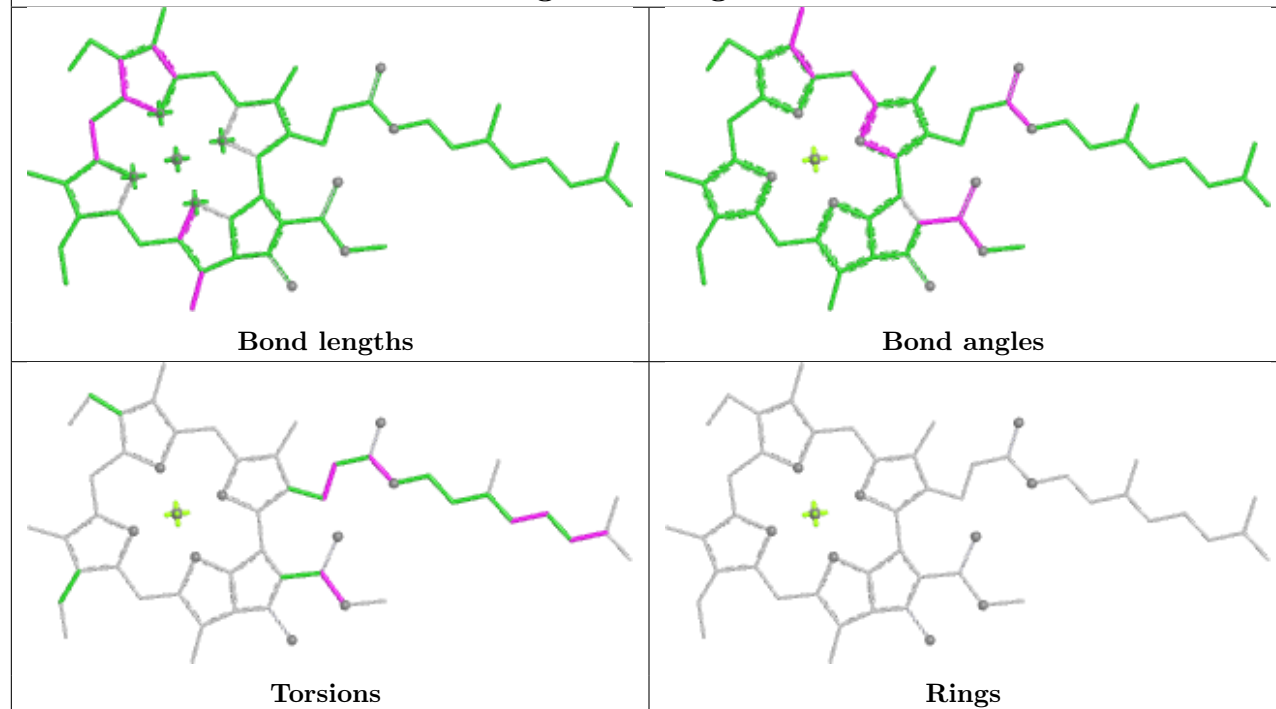
Ligand BCR A 4007

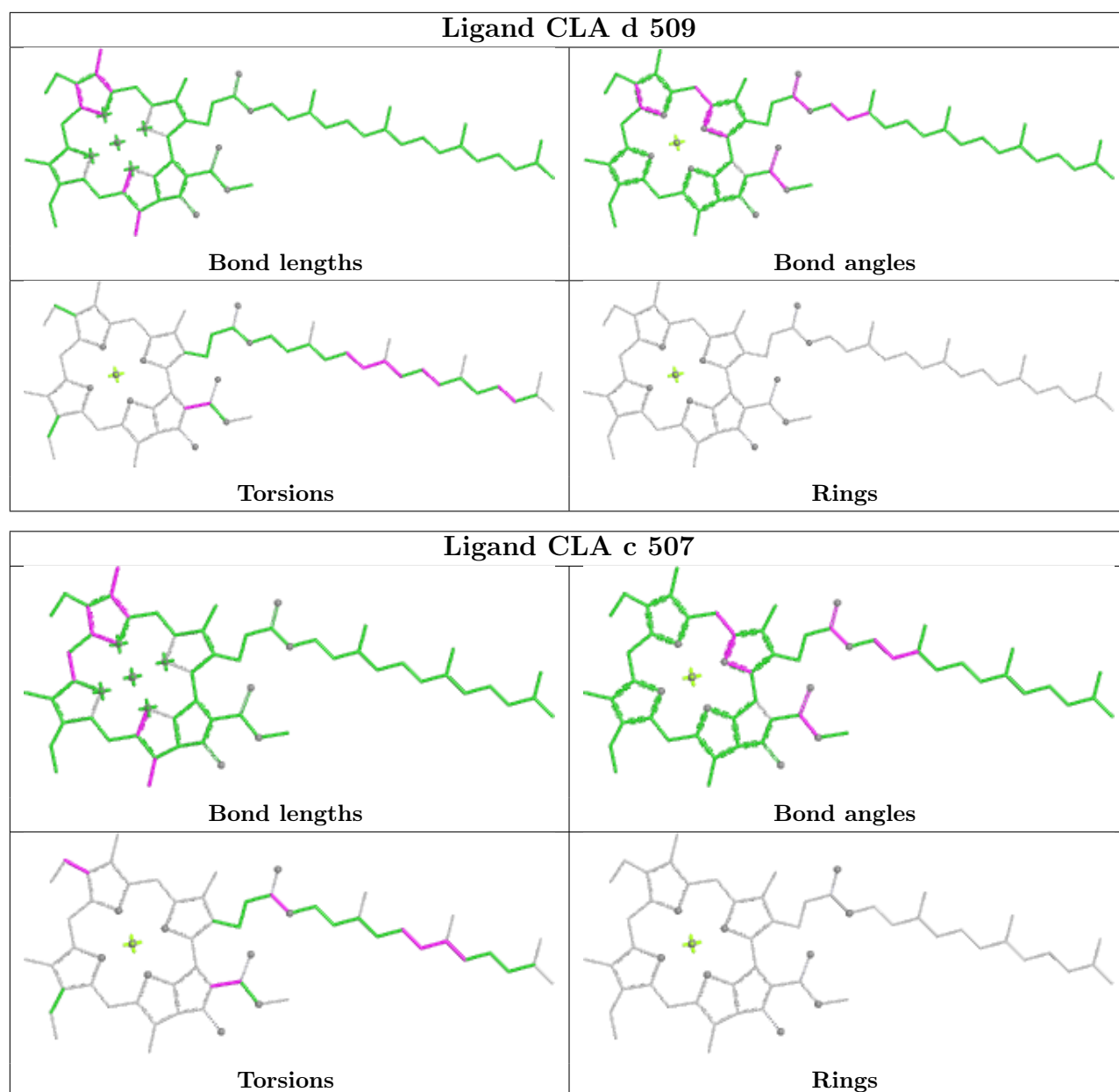


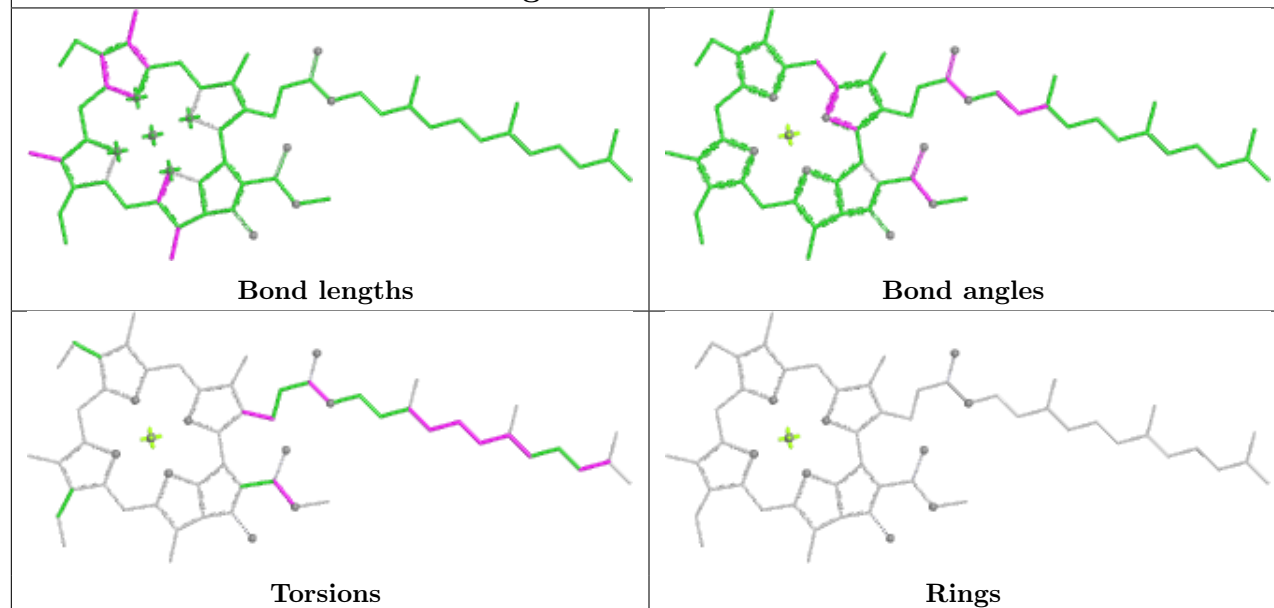
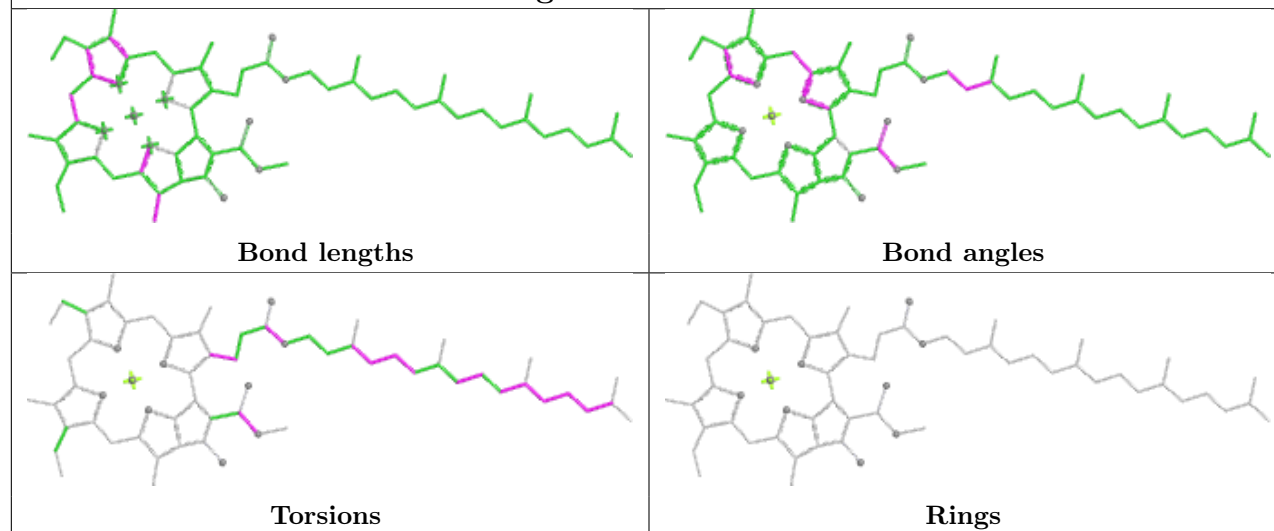
Ligand CLA 4 513



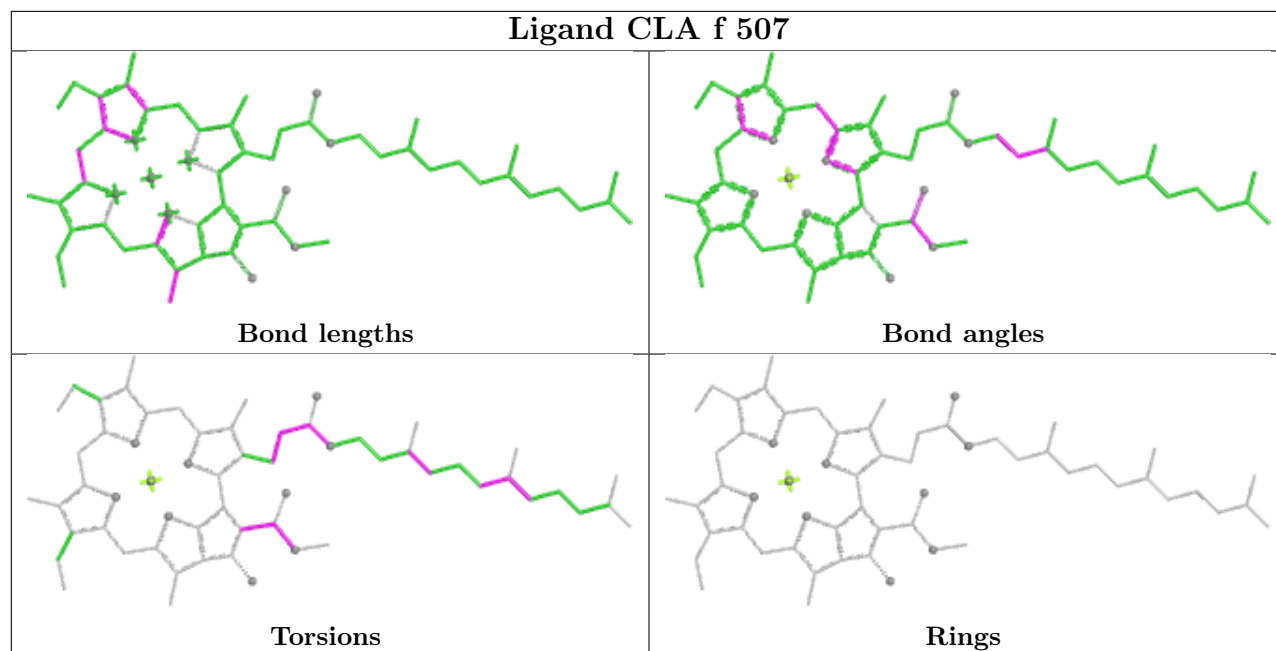
Ligand CLA g 504



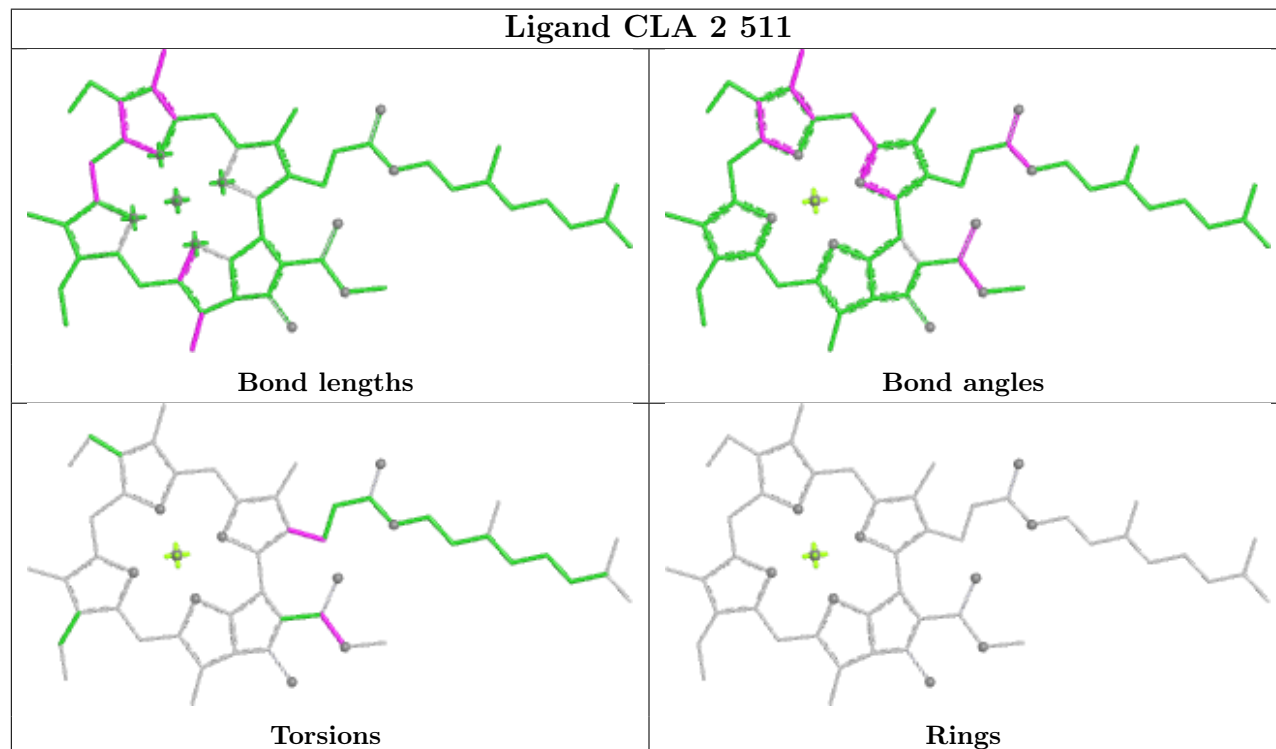


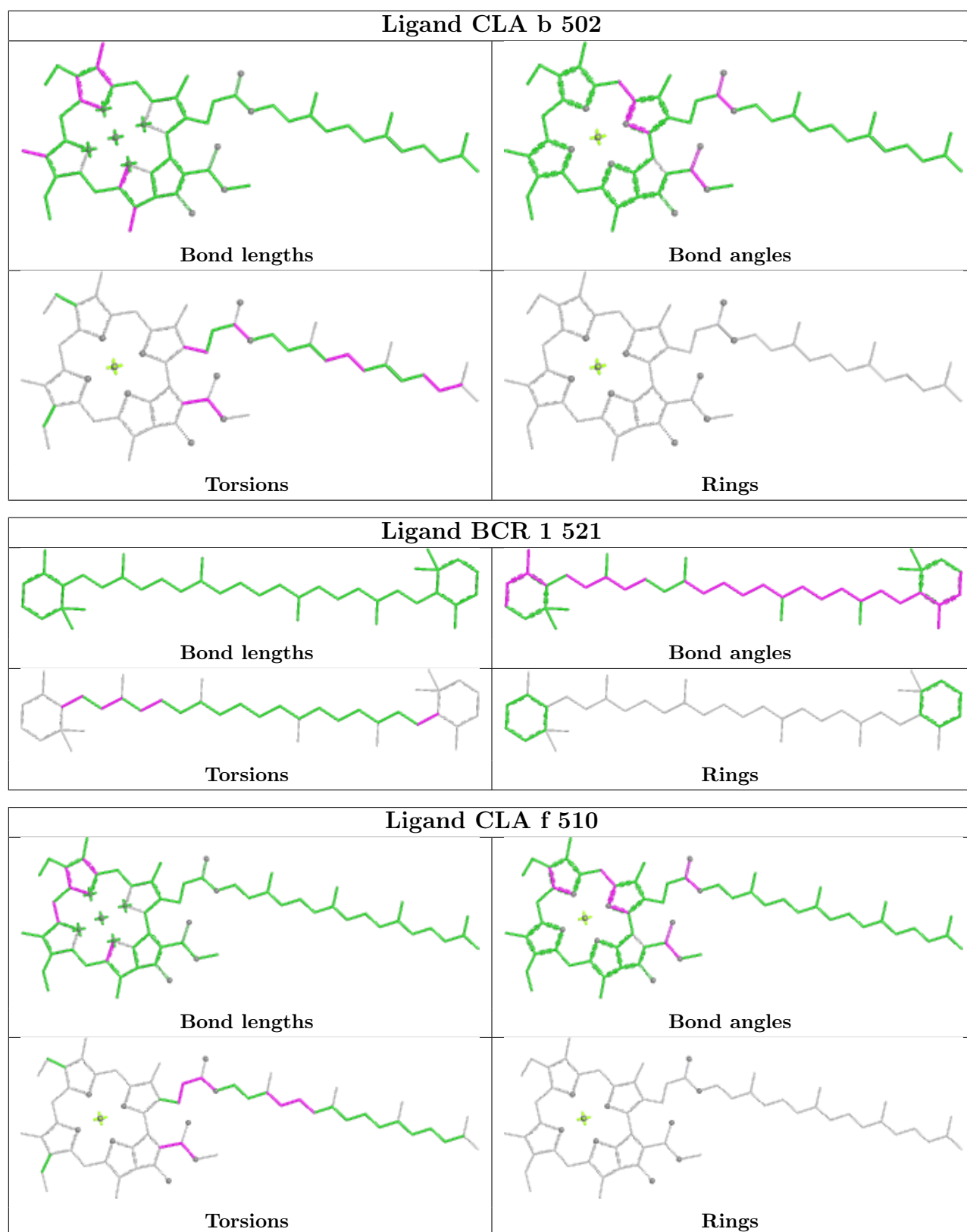
Ligand CLA A 1118**Ligand CLA 2 505**

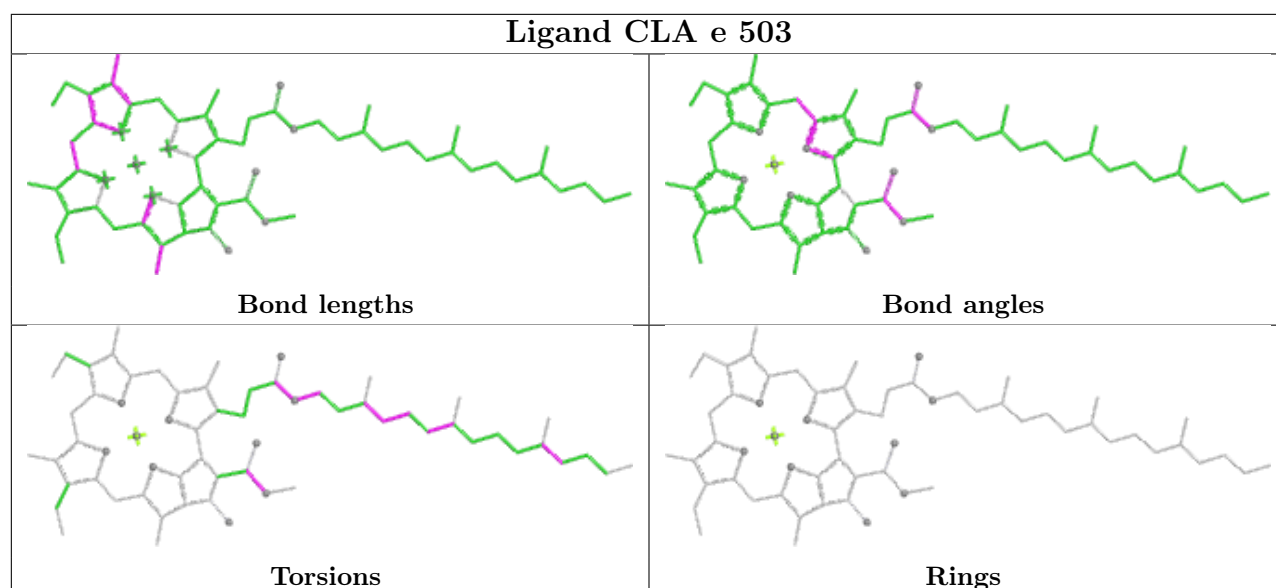
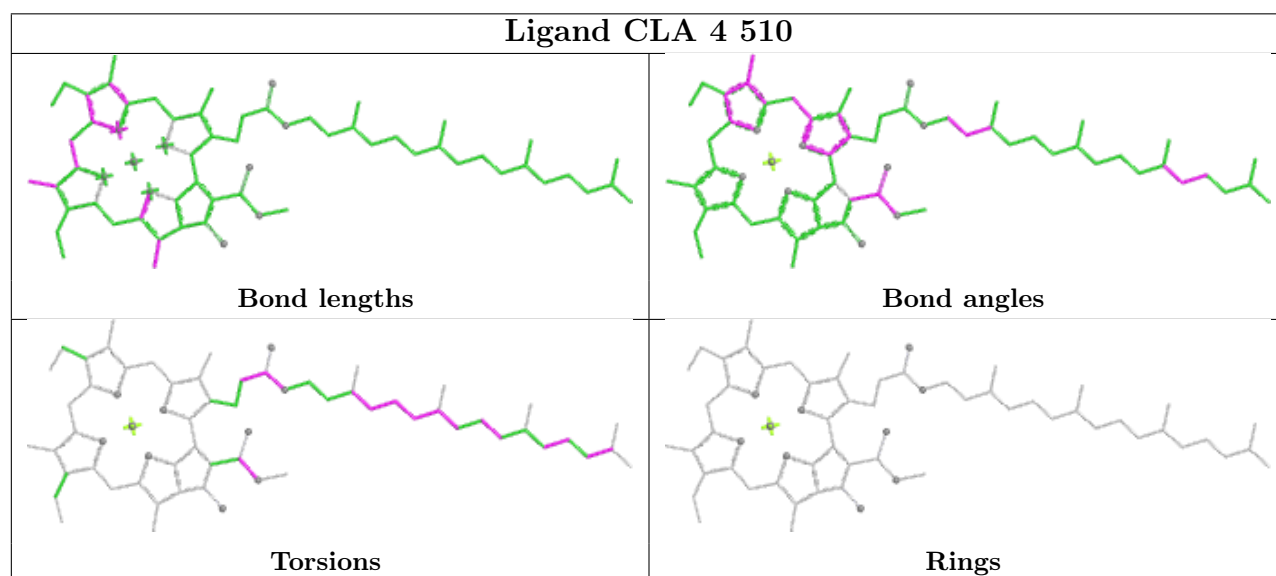
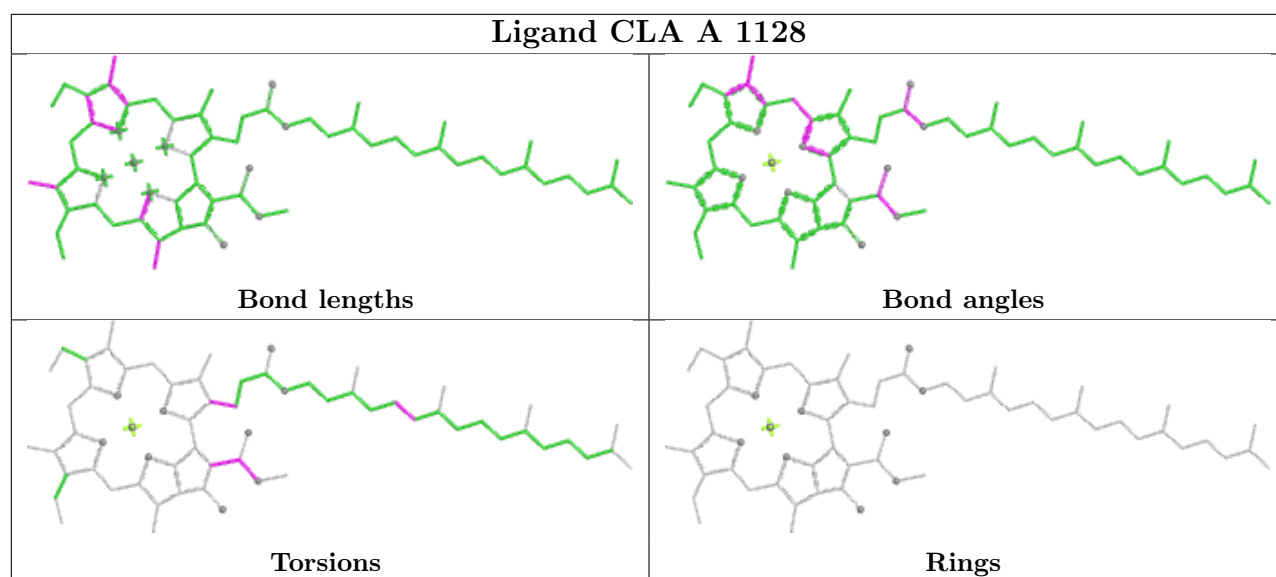
Ligand CLA f 507

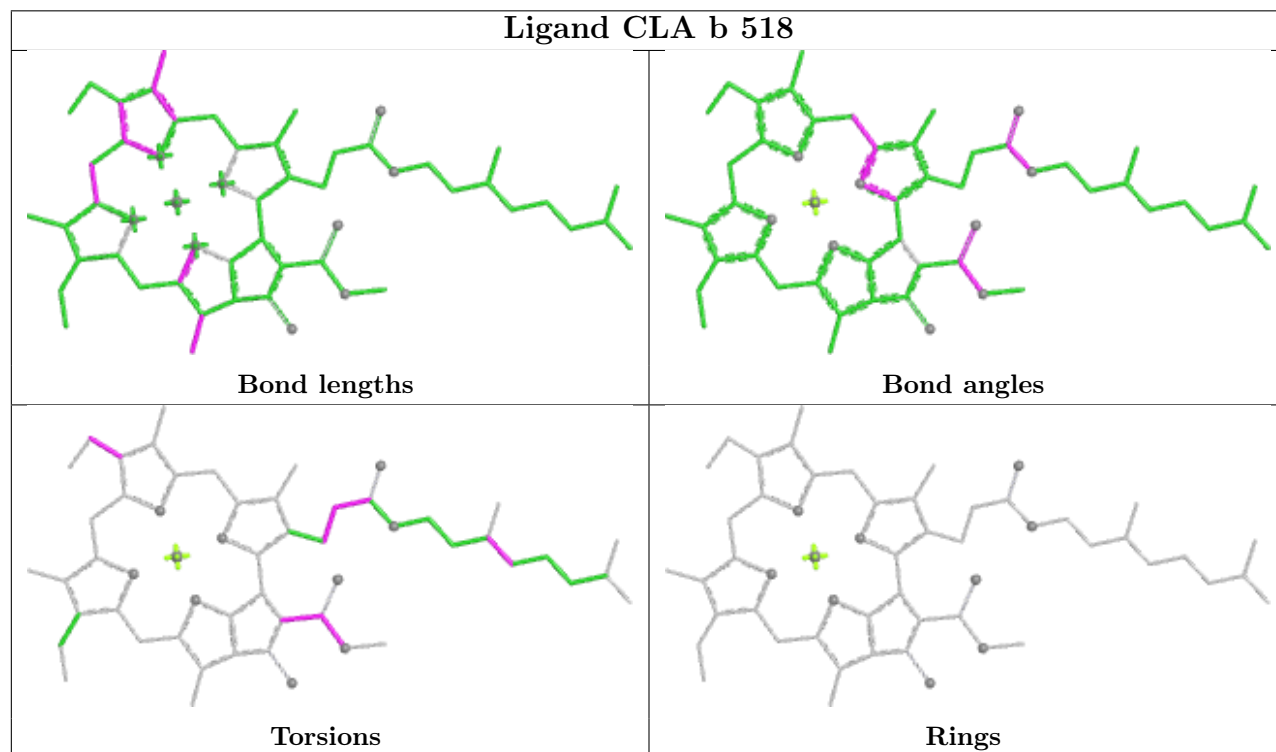
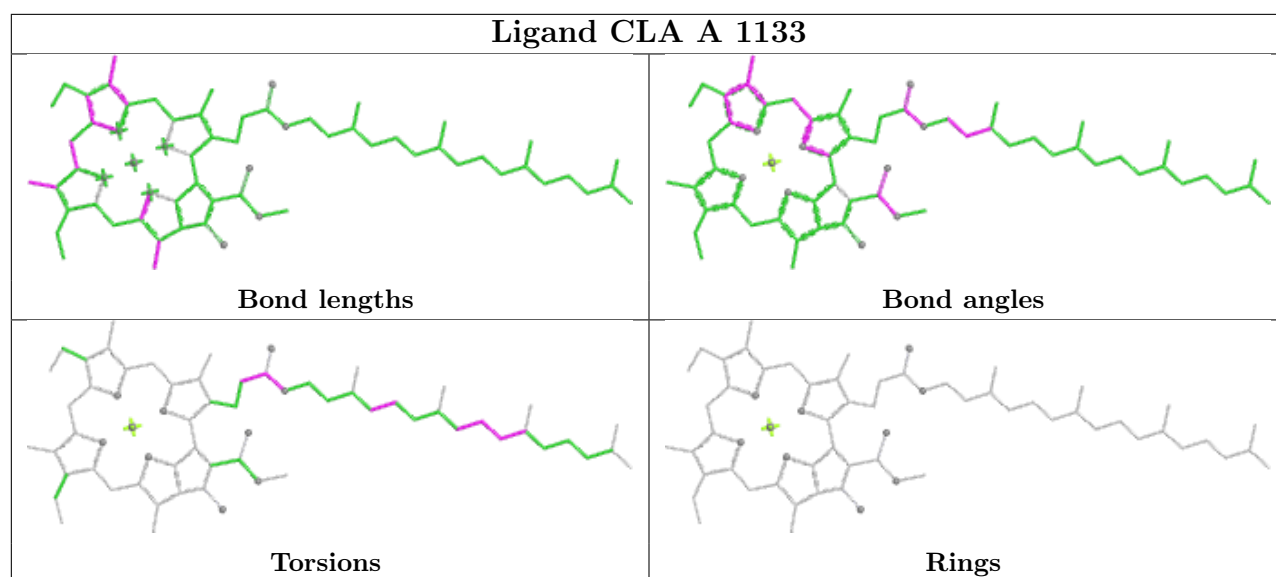


Ligand CLA 2 511

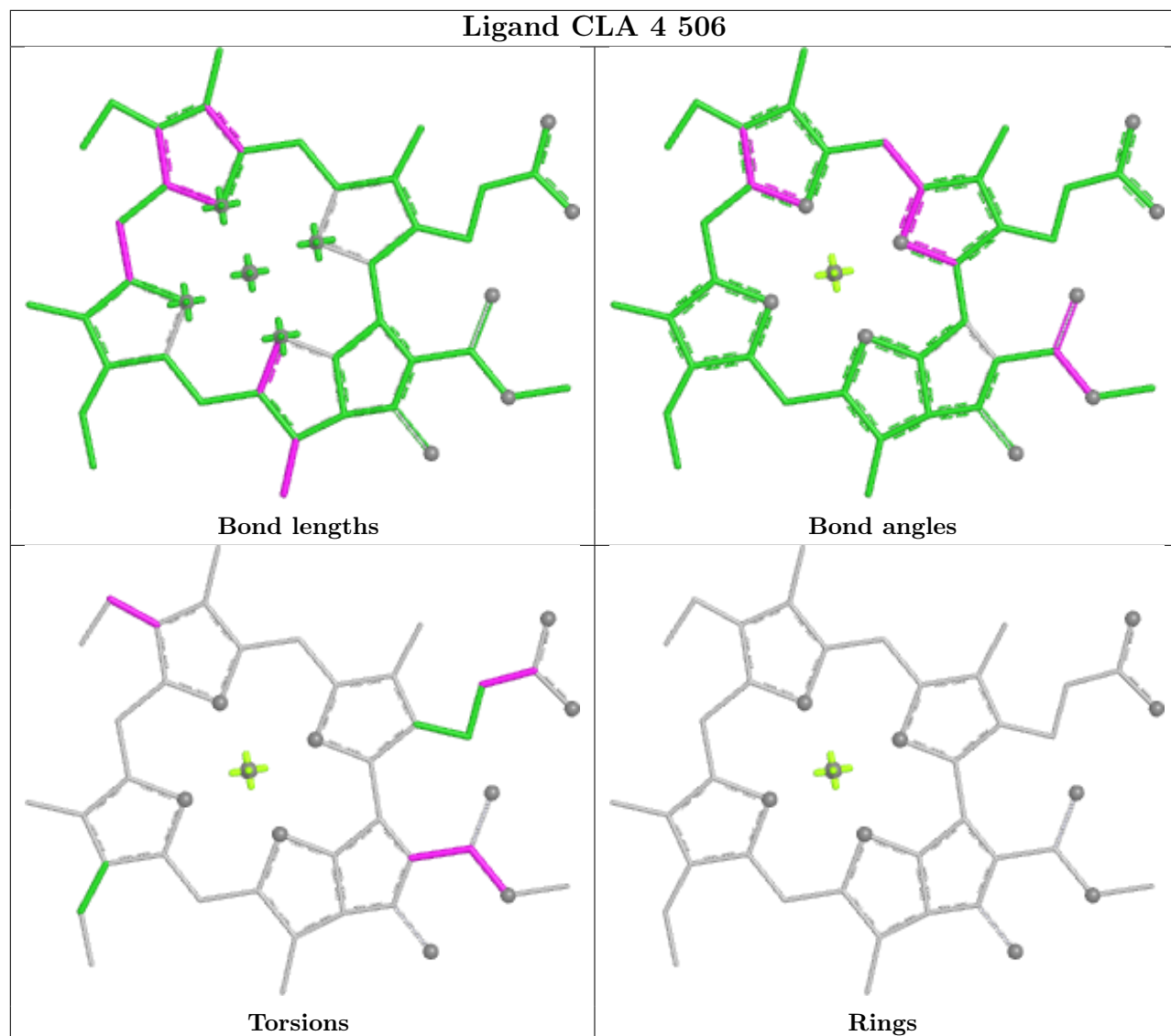




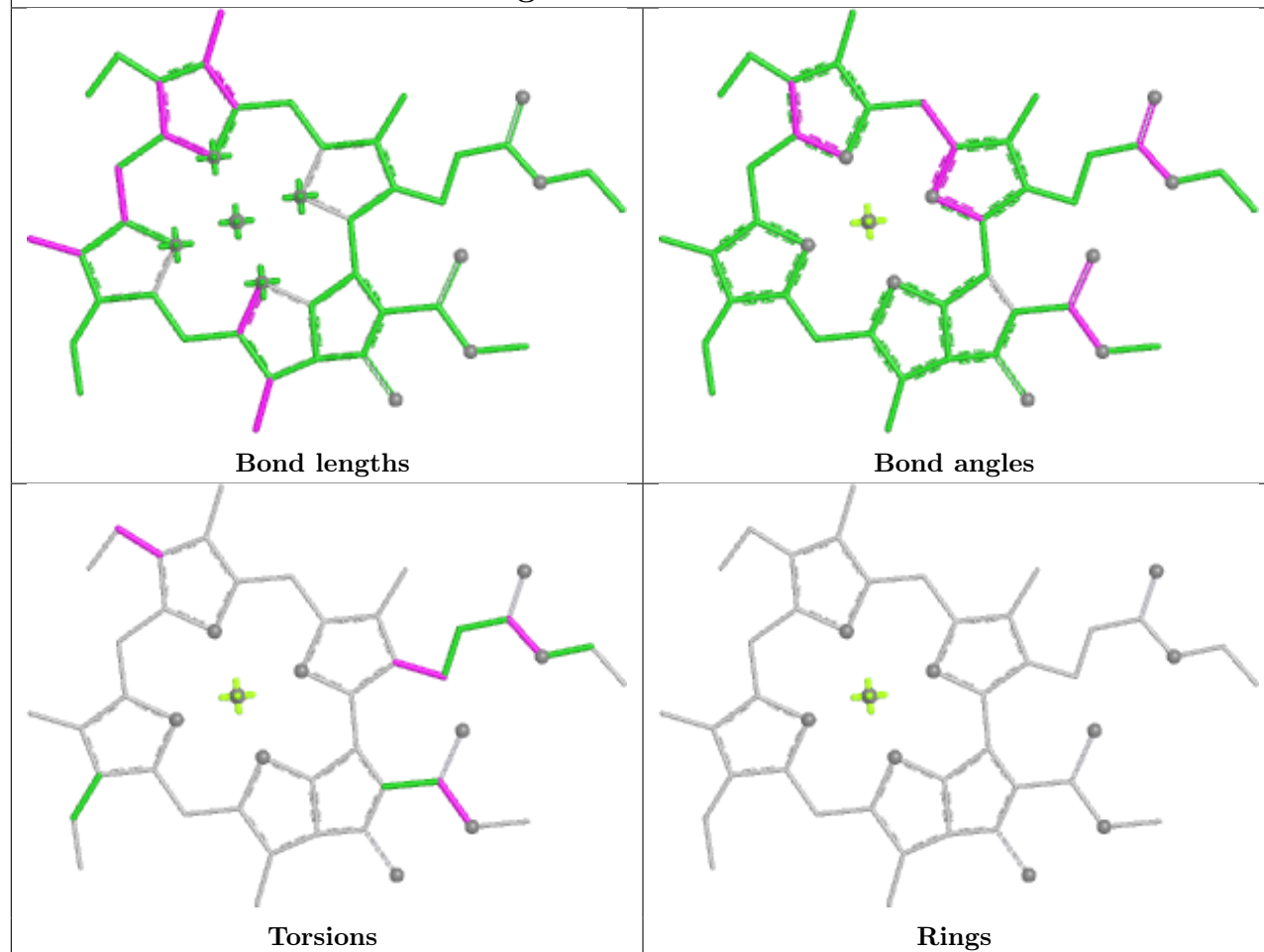




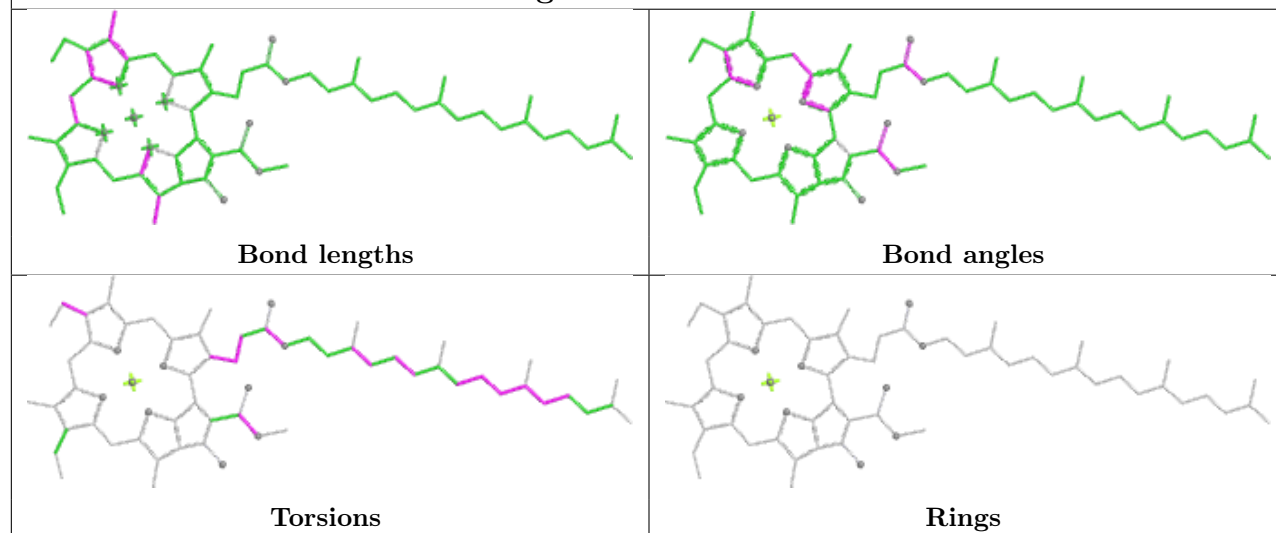
Ligand CLA 4 506

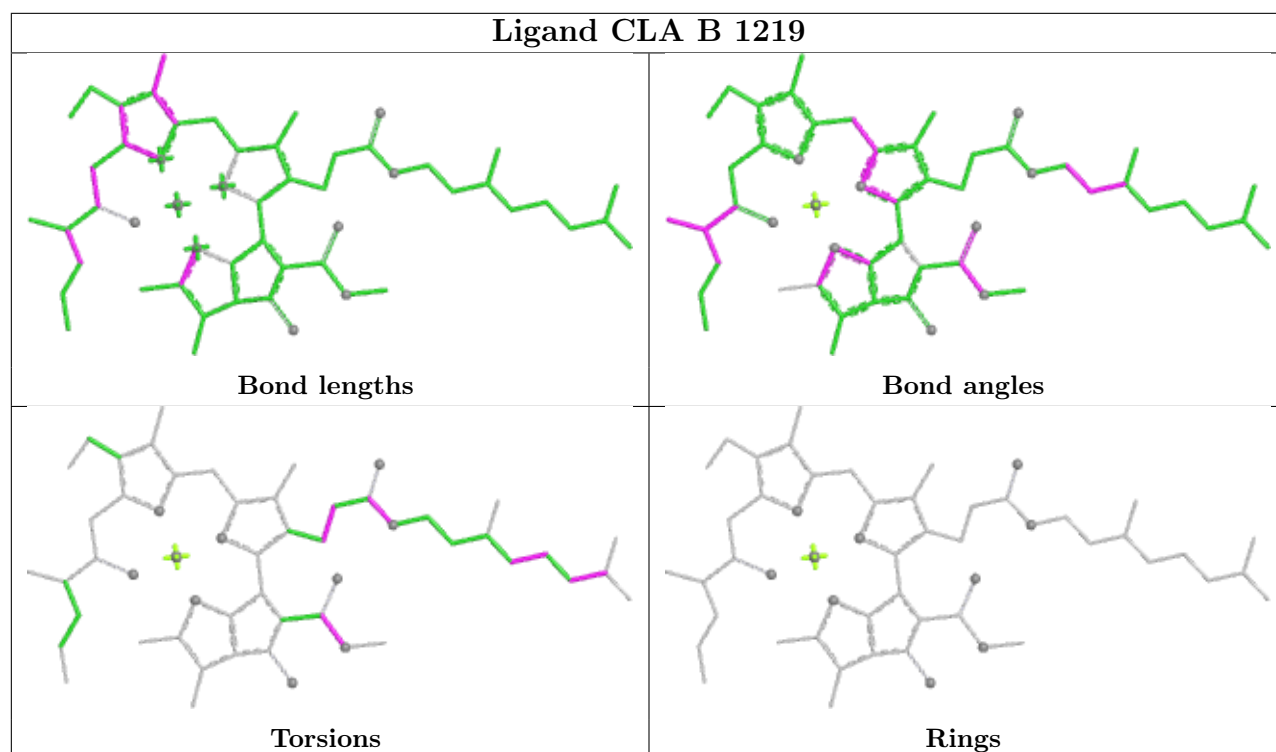
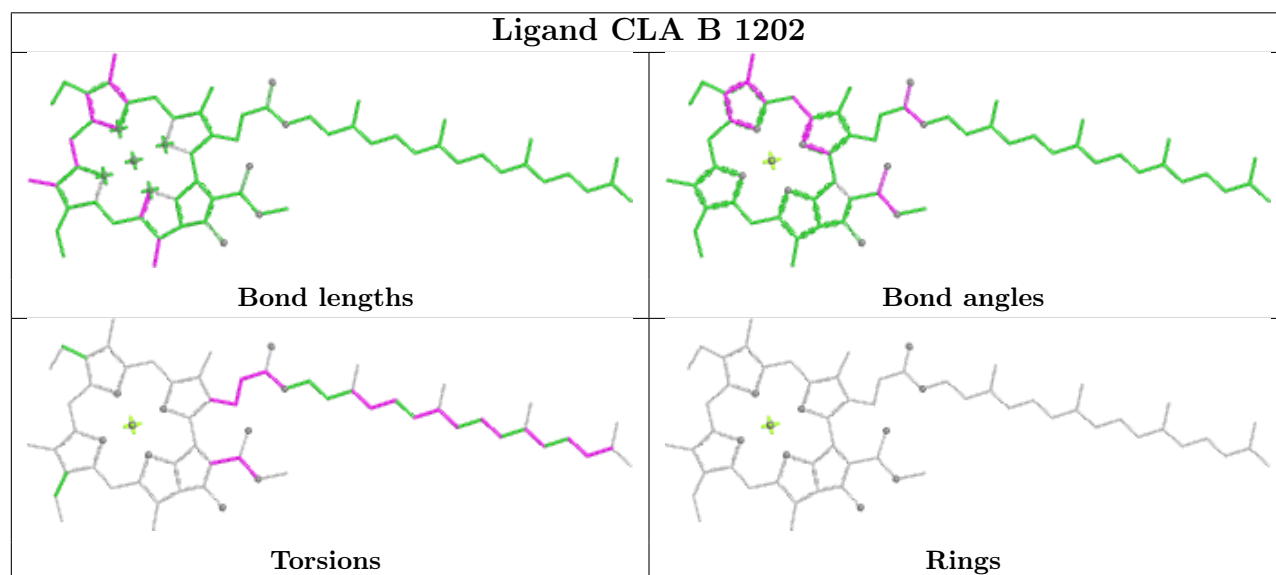
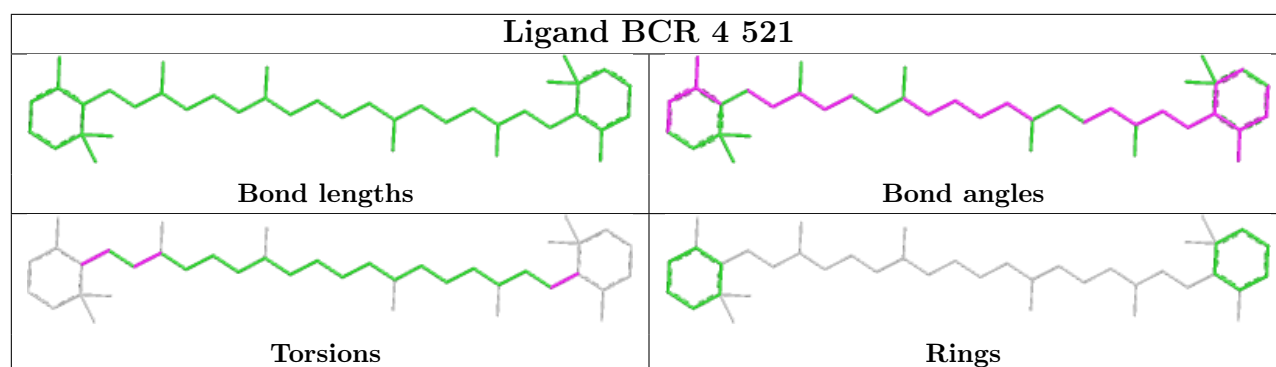


Ligand CLA A 1112

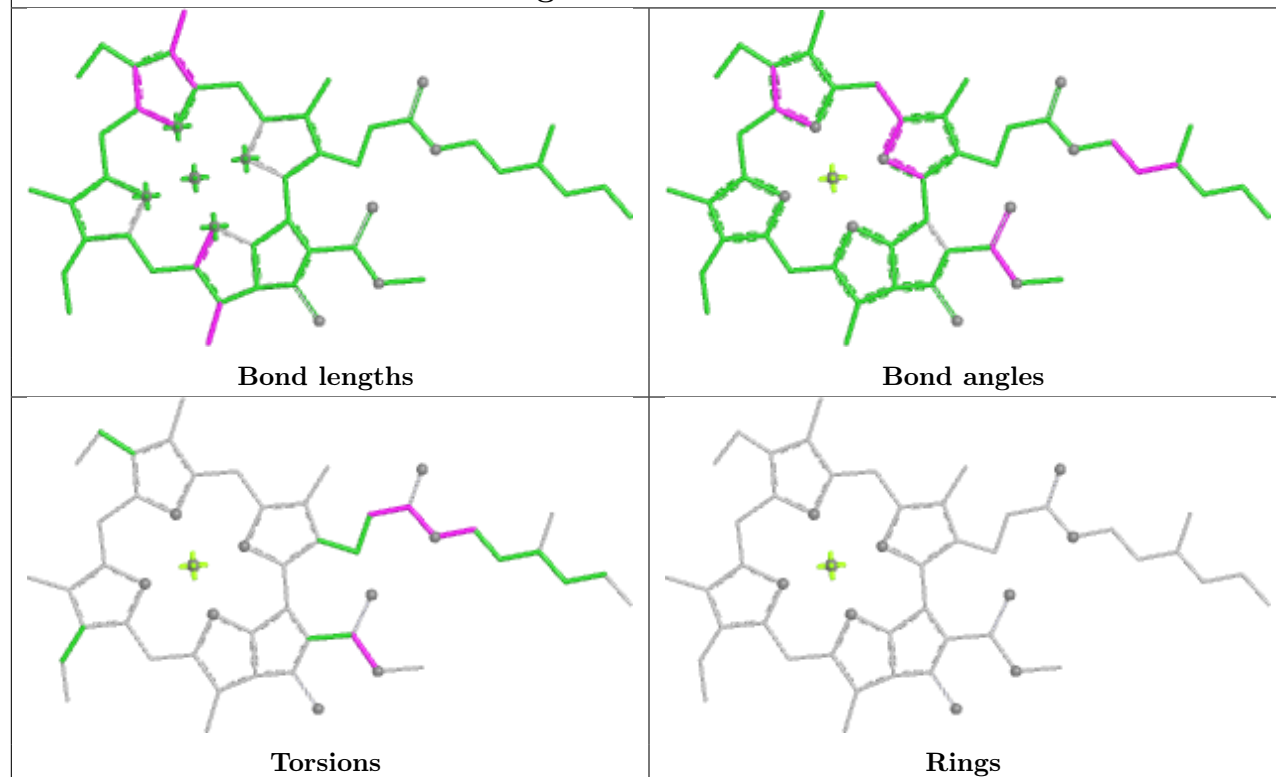


Ligand CLA 1 505

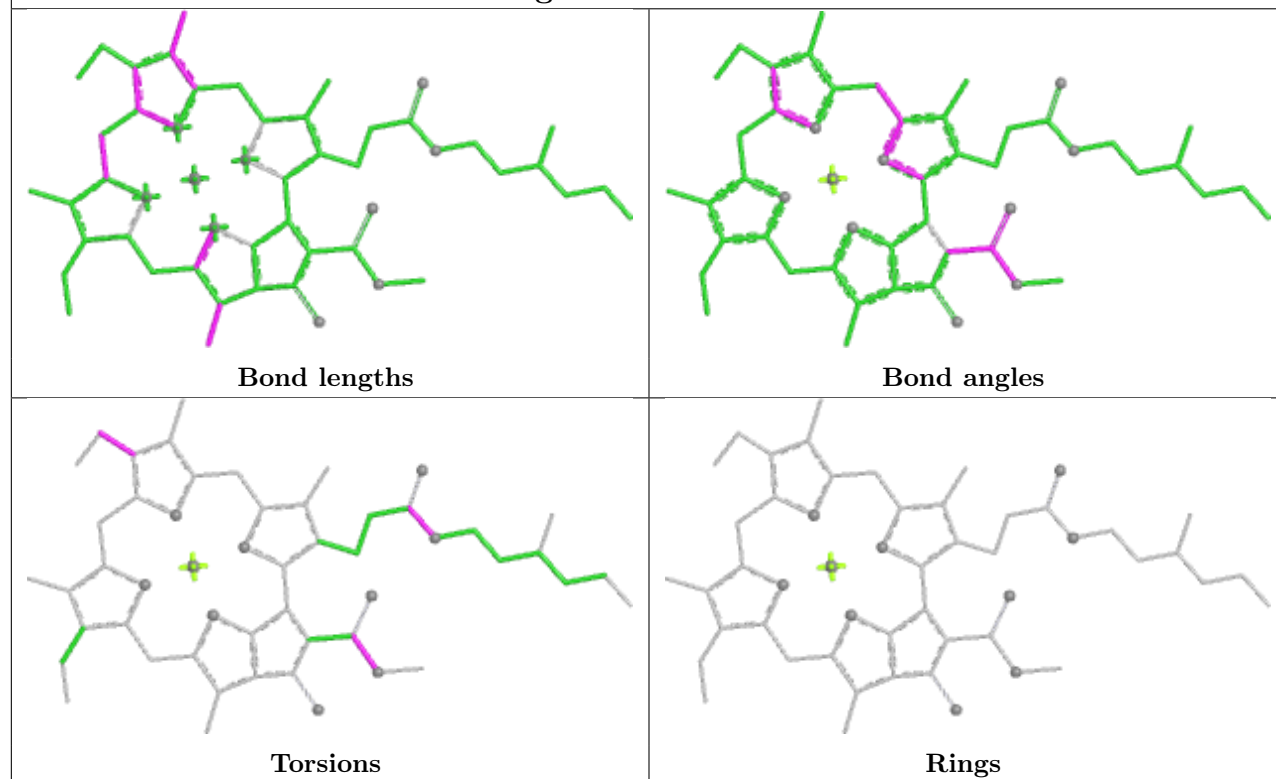




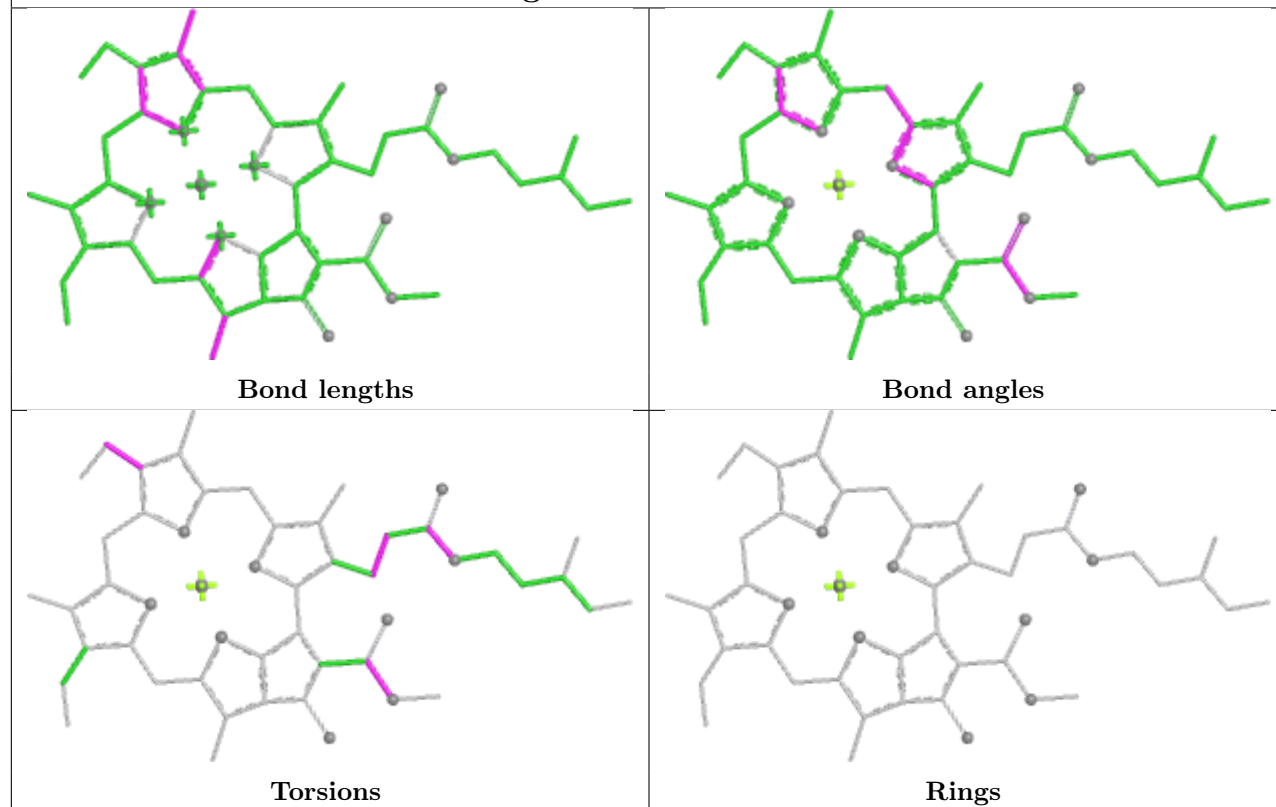
Ligand CLA e 512



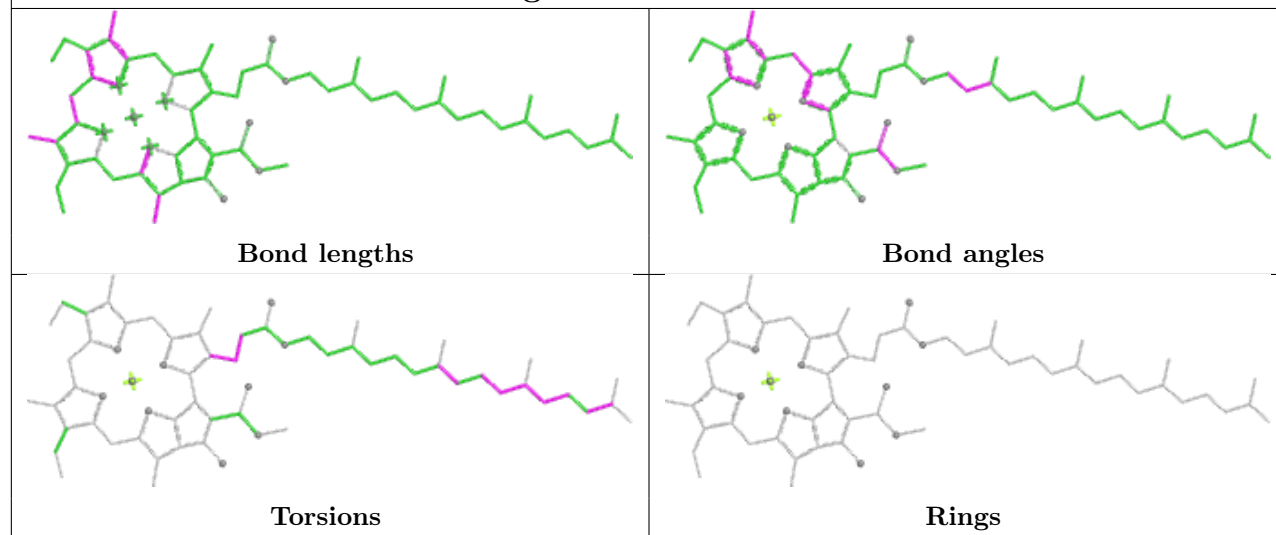
Ligand CLA d 512

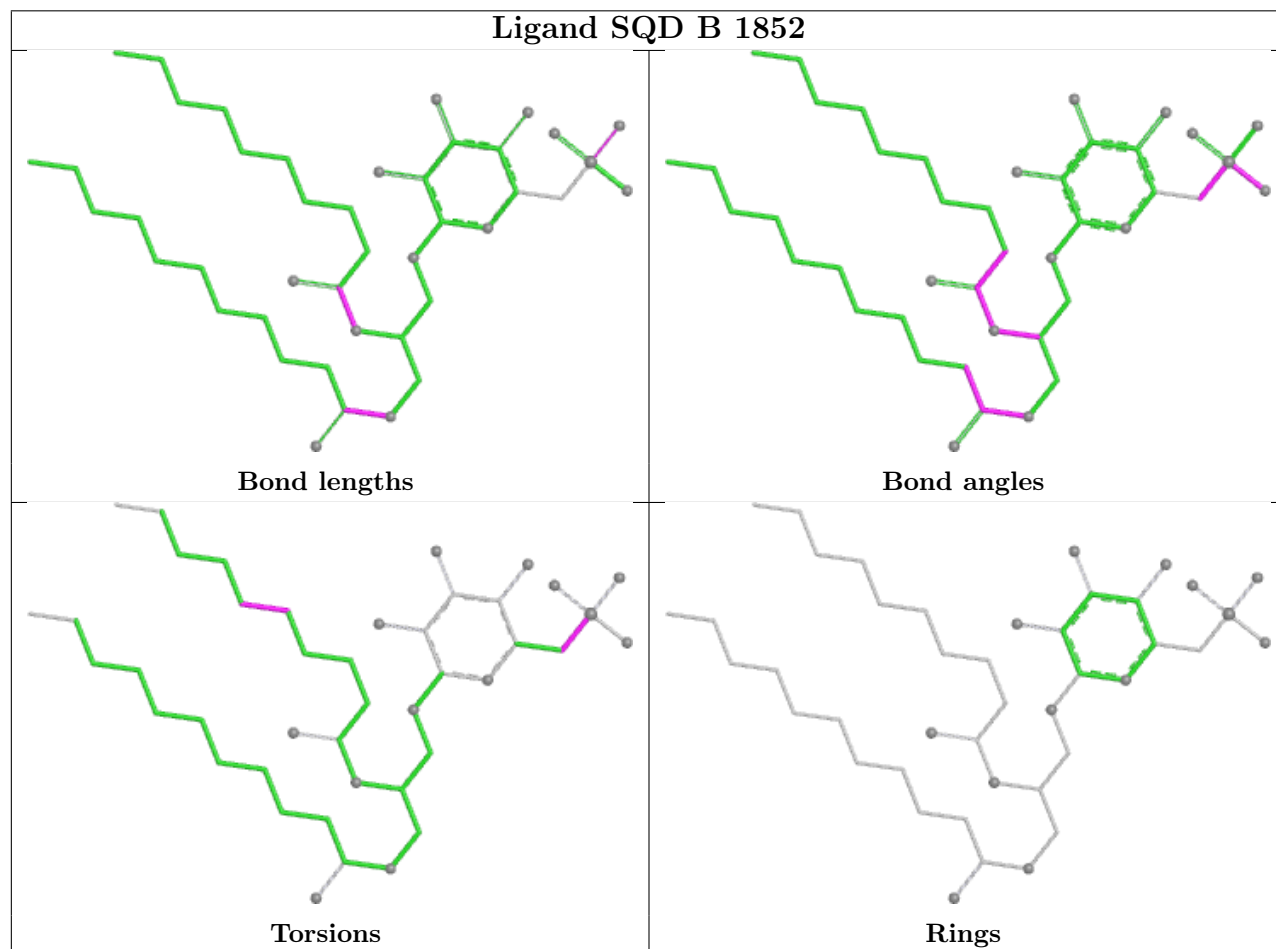
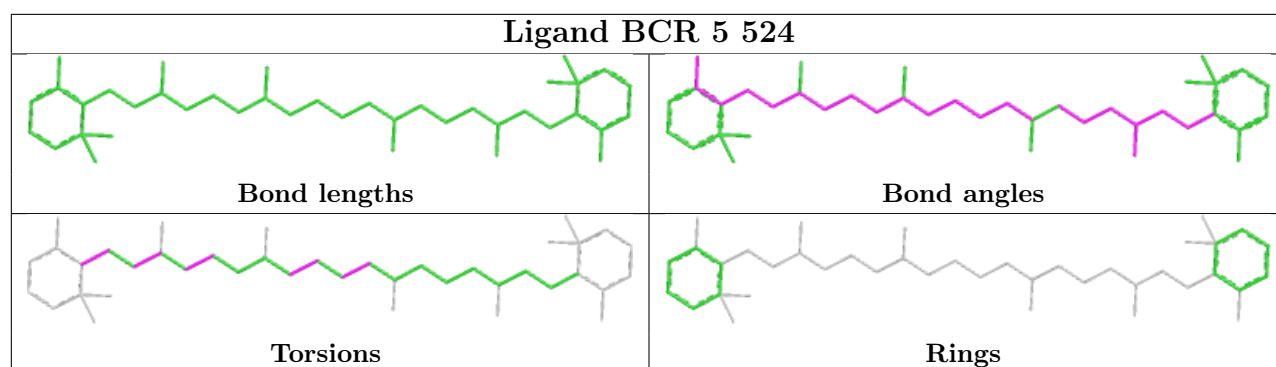


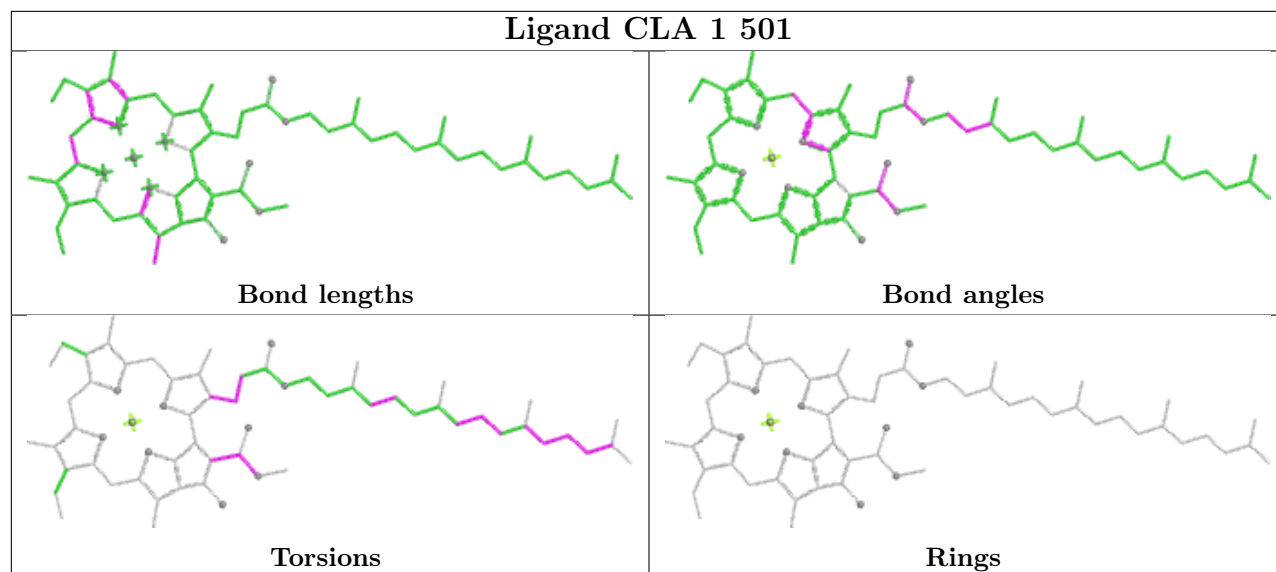
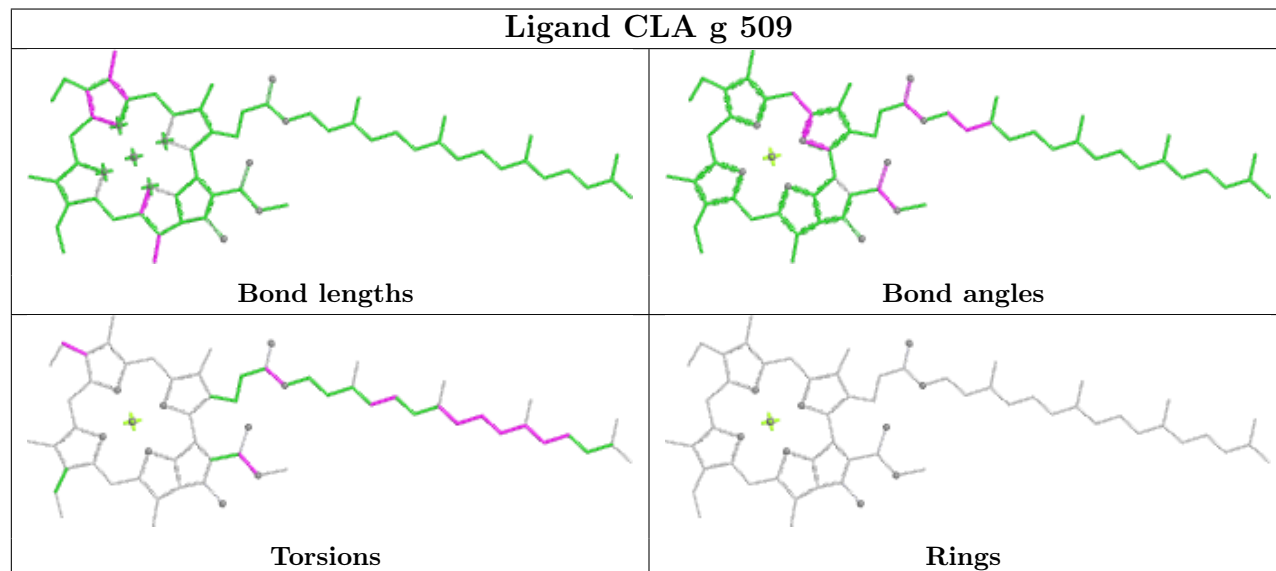
Ligand CLA A 1121



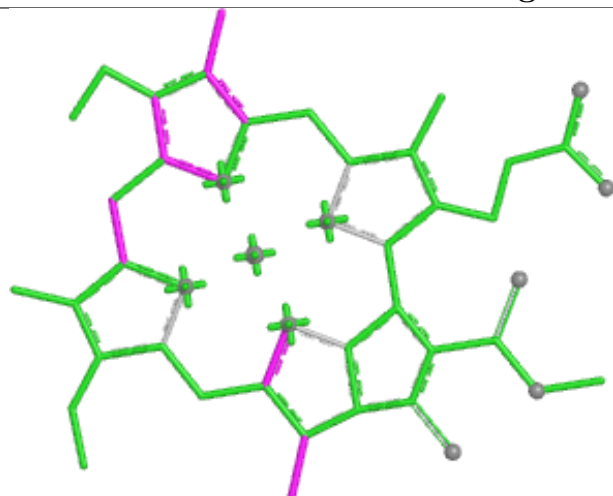
Ligand CLA B 1225



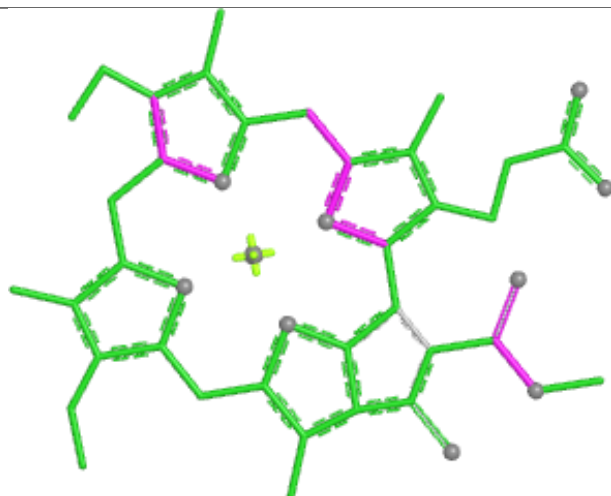


Ligand CLA 1 501**Ligand CLA g 509**

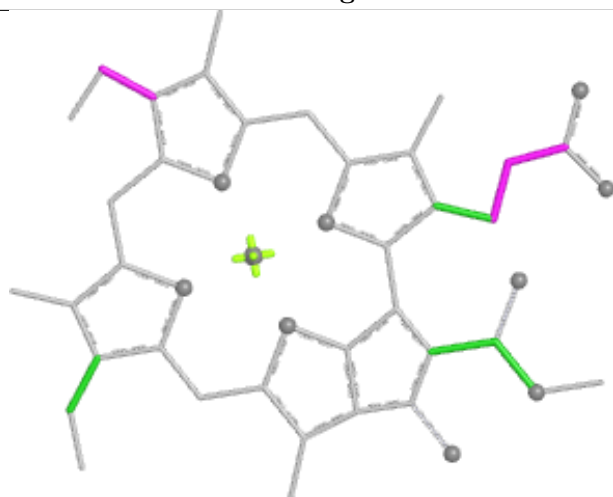
Ligand CLA 3 519



Bond lengths



Bond angles

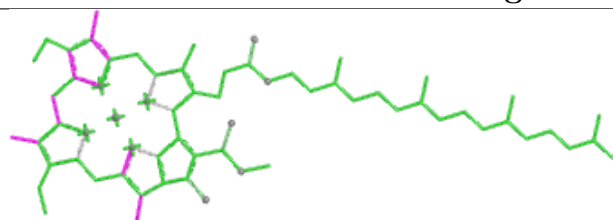


Torsions

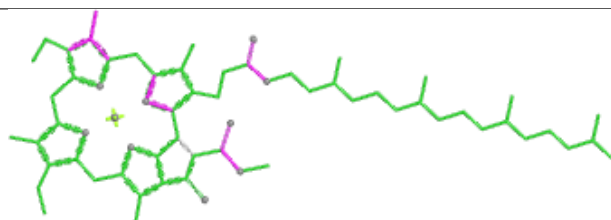


Rings

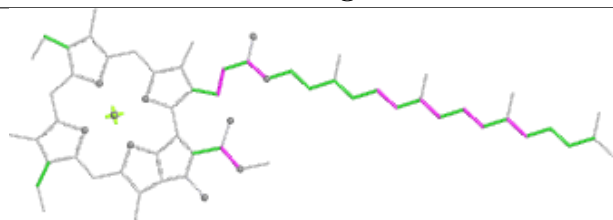
Ligand CLA A 1022



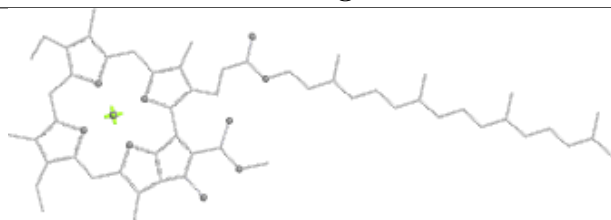
Bond lengths



Bond angles

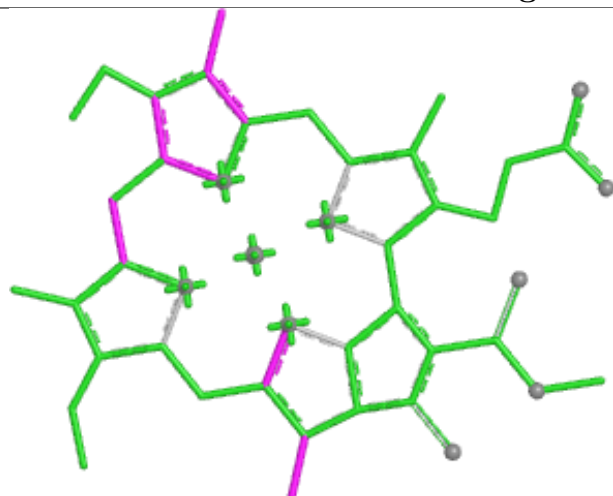


Torsions

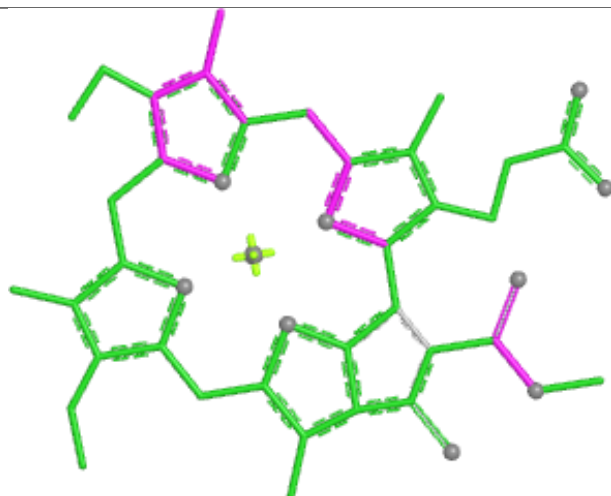


Rings

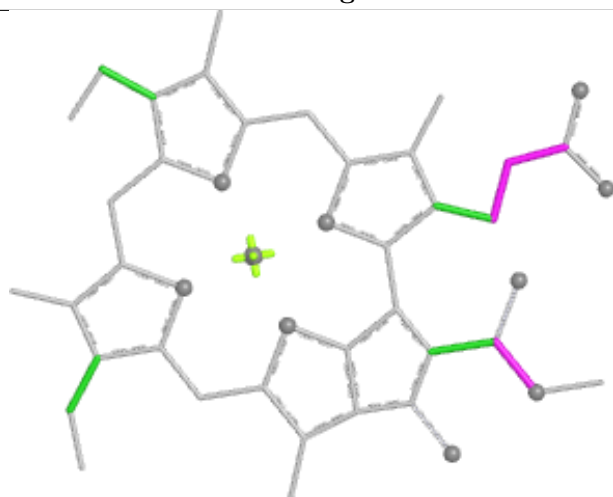
Ligand CLA e 511



Bond lengths



Bond angles

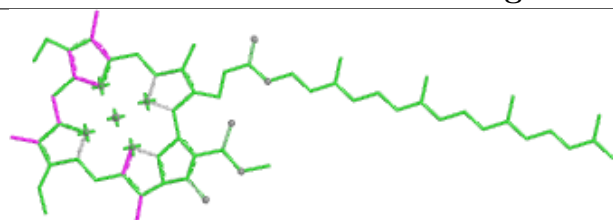


Torsions

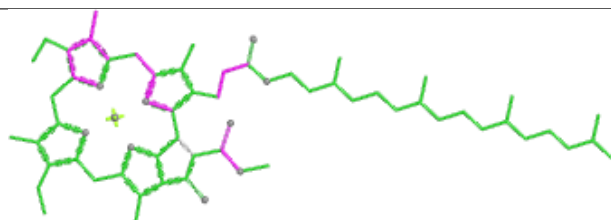


Rings

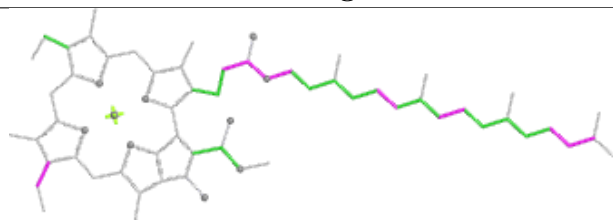
Ligand CLA A 1127



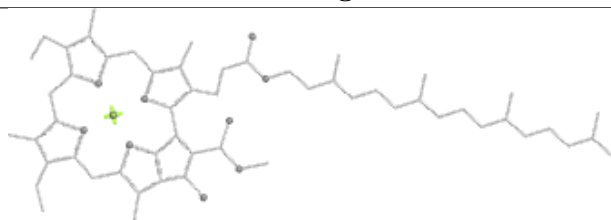
Bond lengths



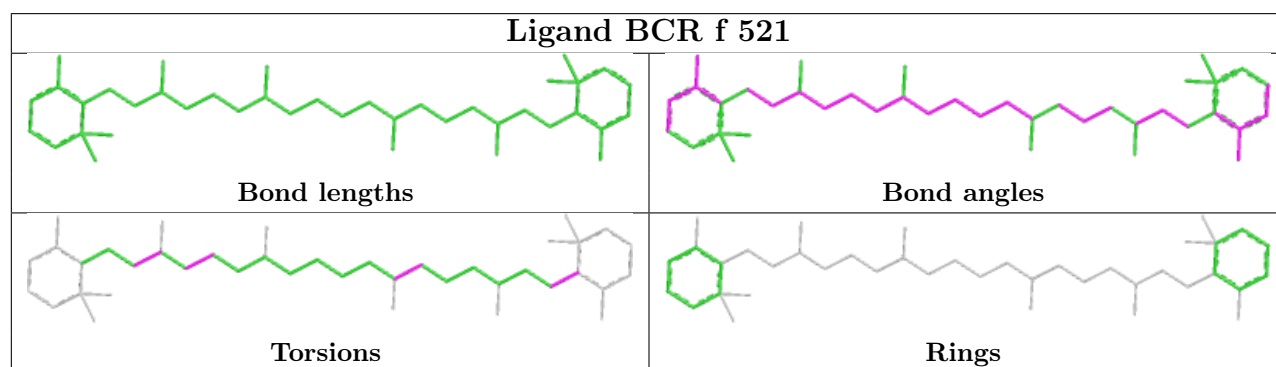
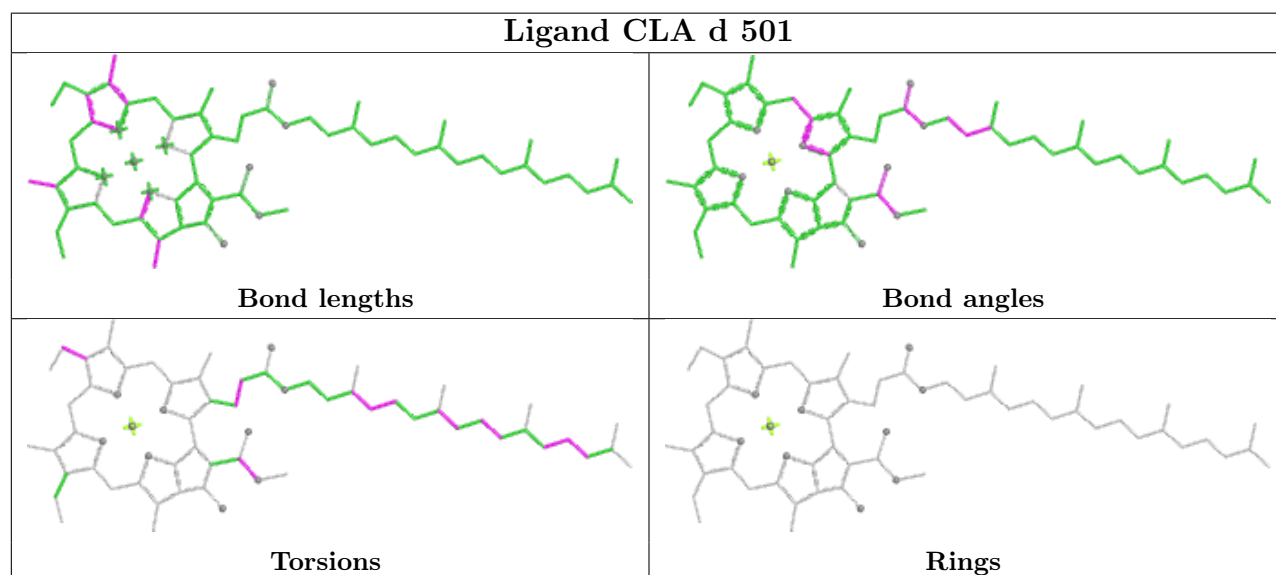
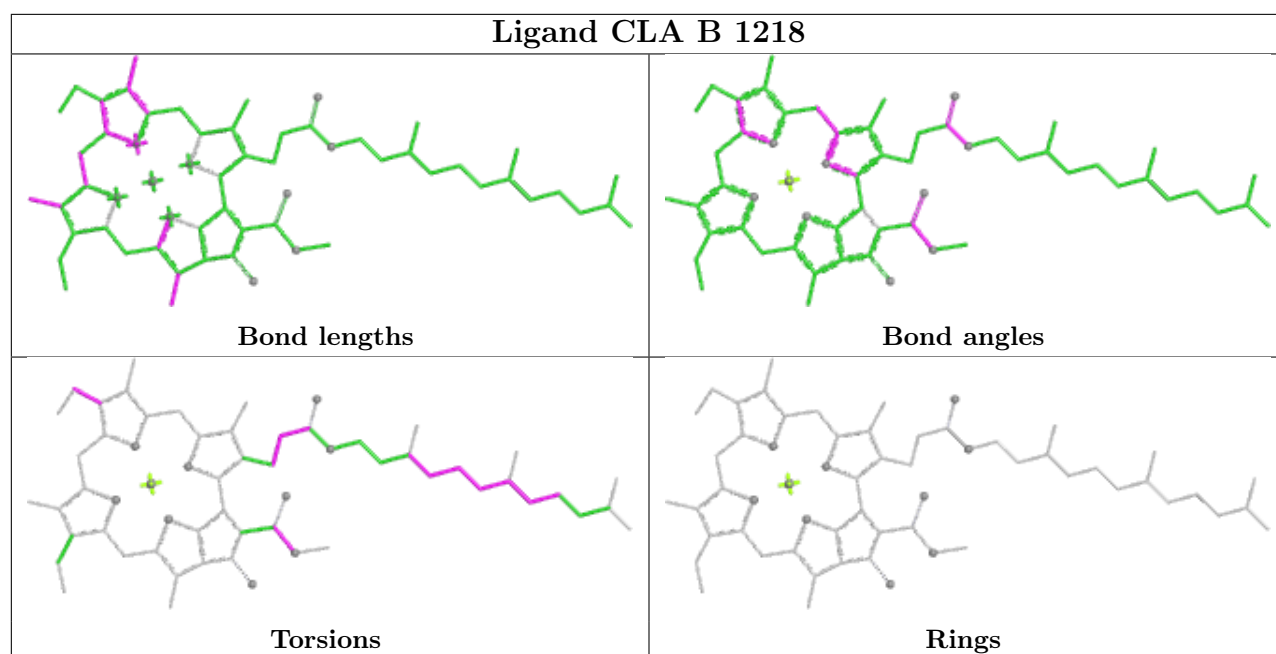
Bond angles

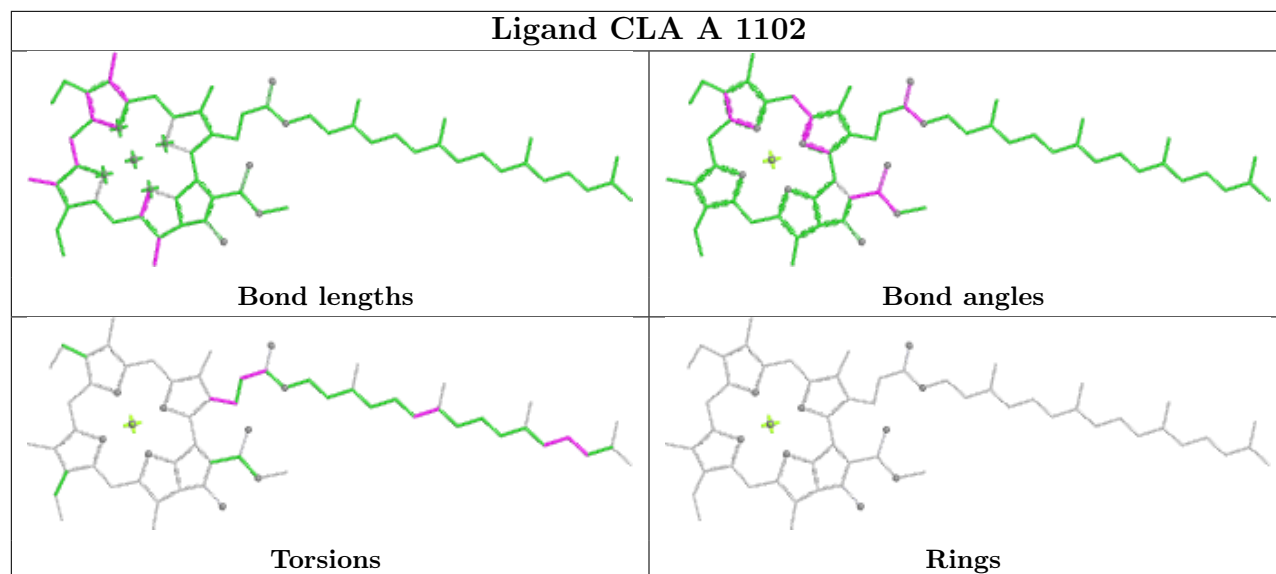
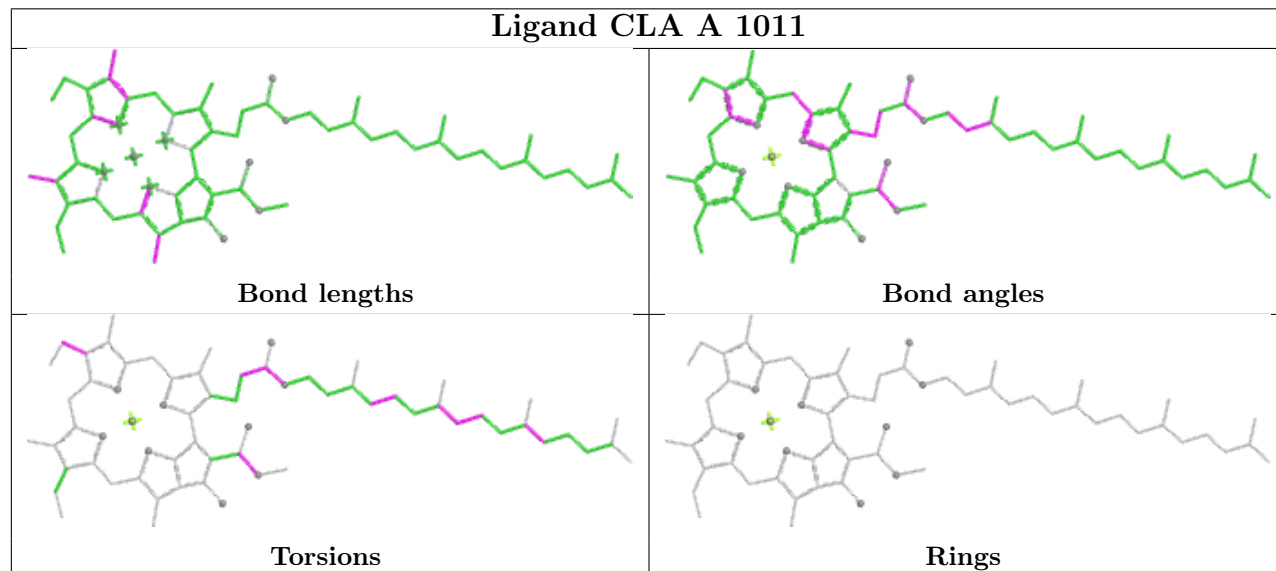


Torsions

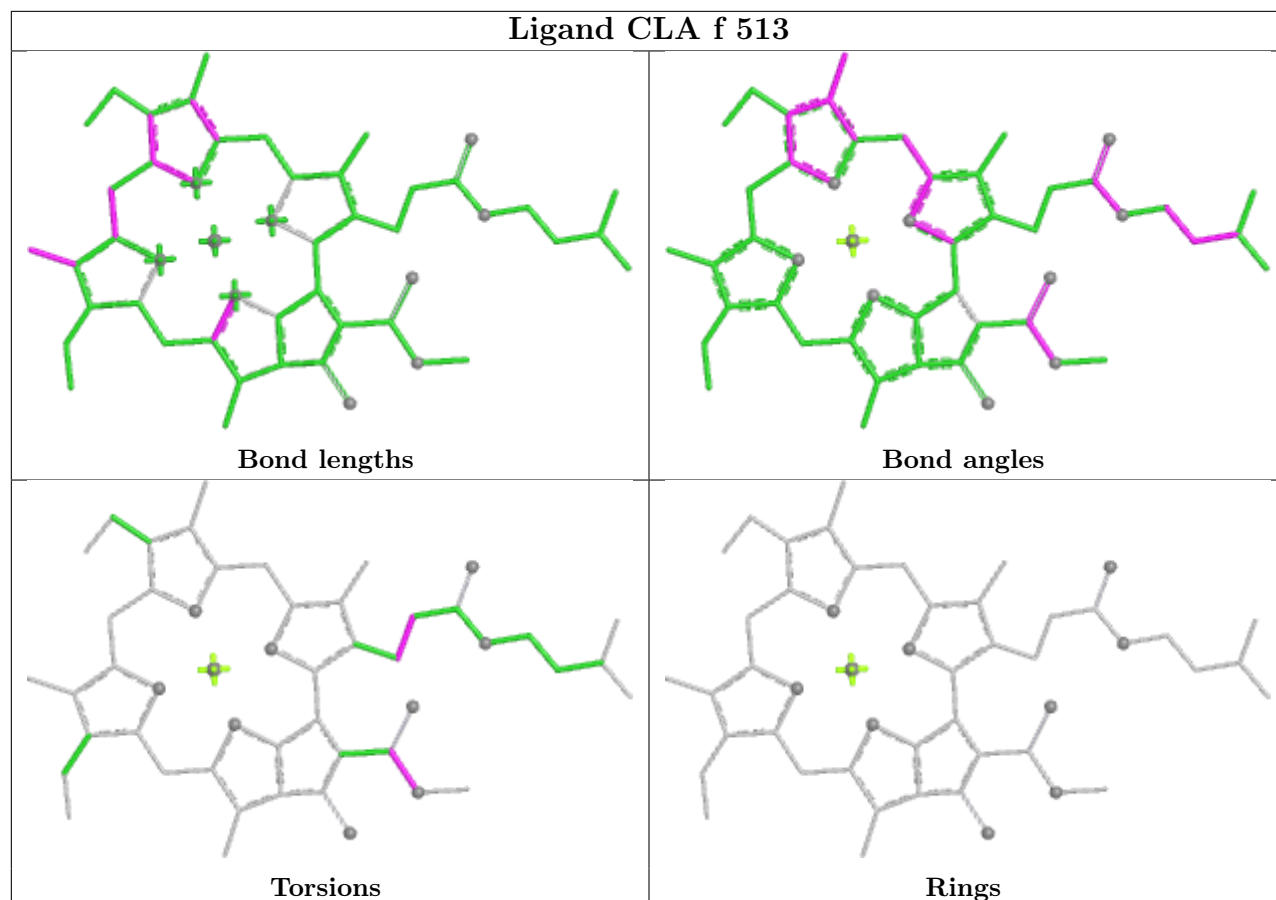


Rings

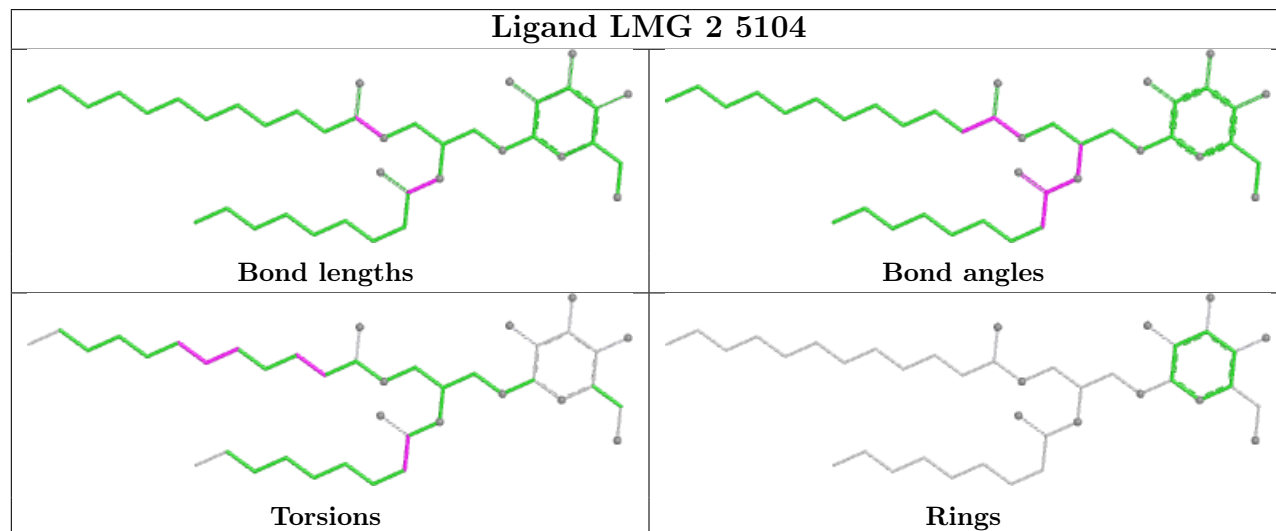


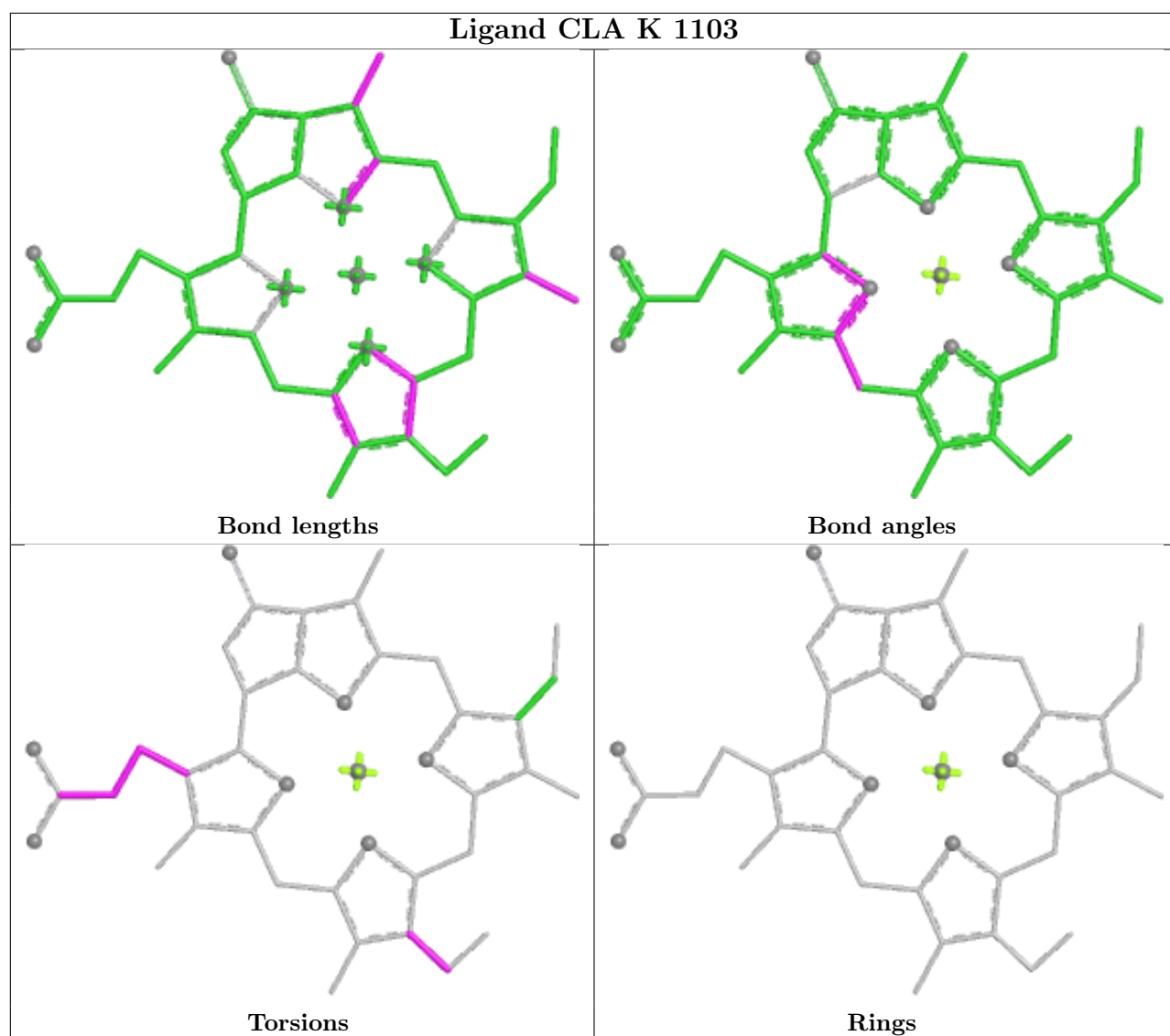
Ligand CLA A 1102**Ligand CLA A 1011**

Ligand CLA f 513

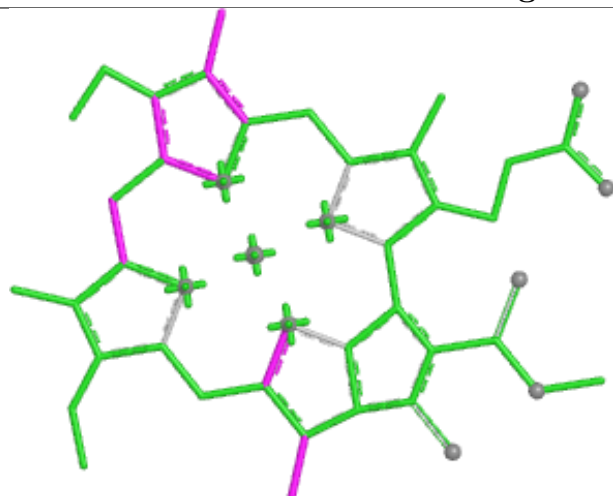


Ligand LMG 2 5104

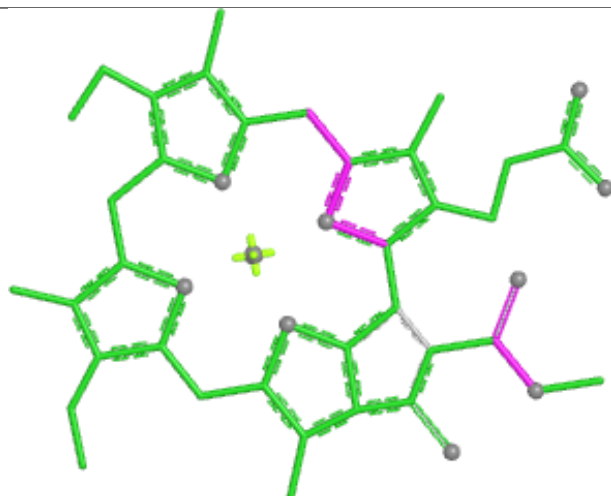




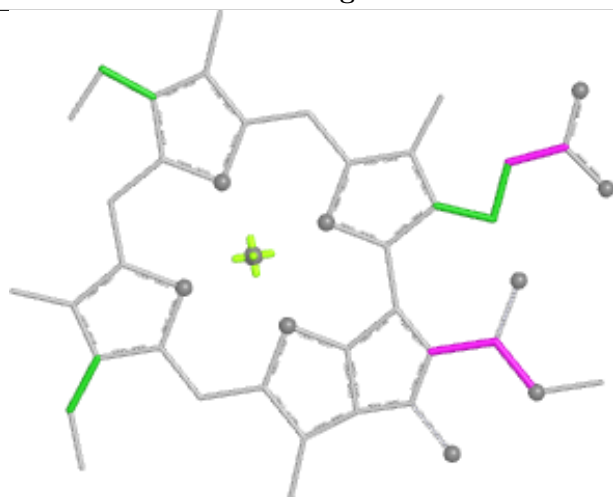
Ligand CLA 6 519



Bond lengths



Bond angles

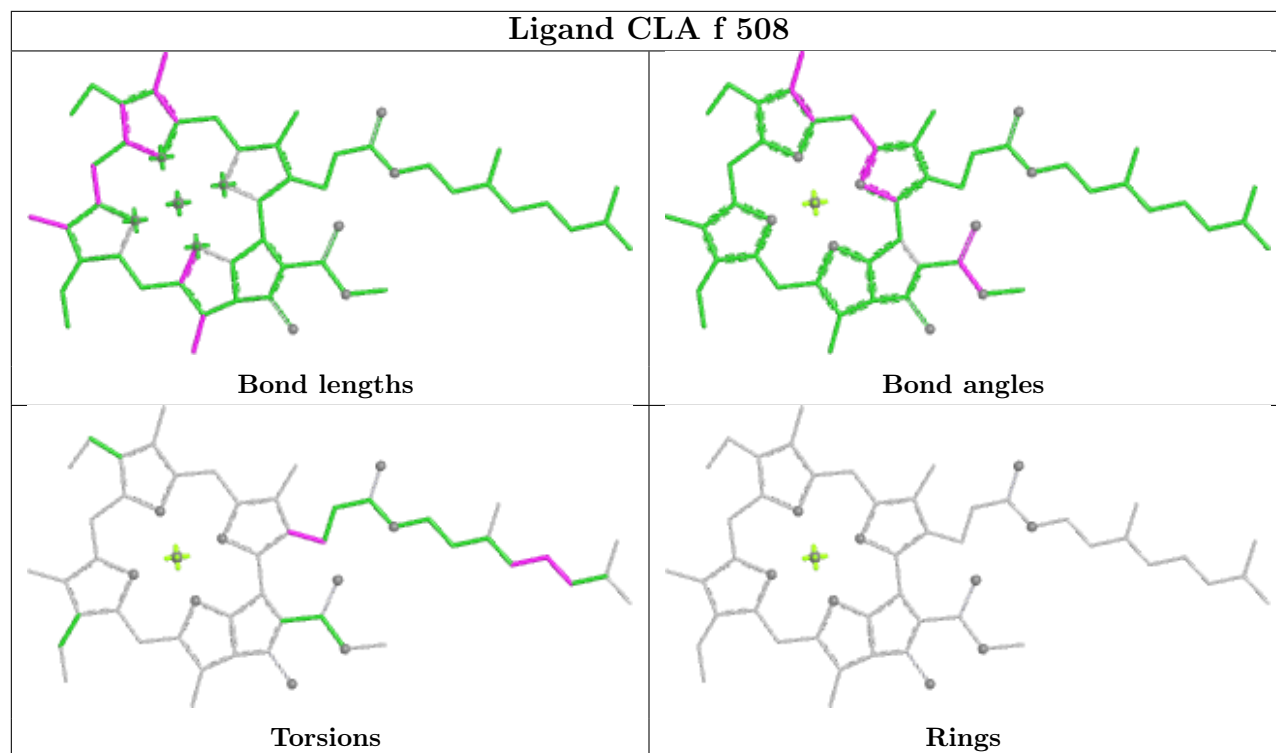


Torsions

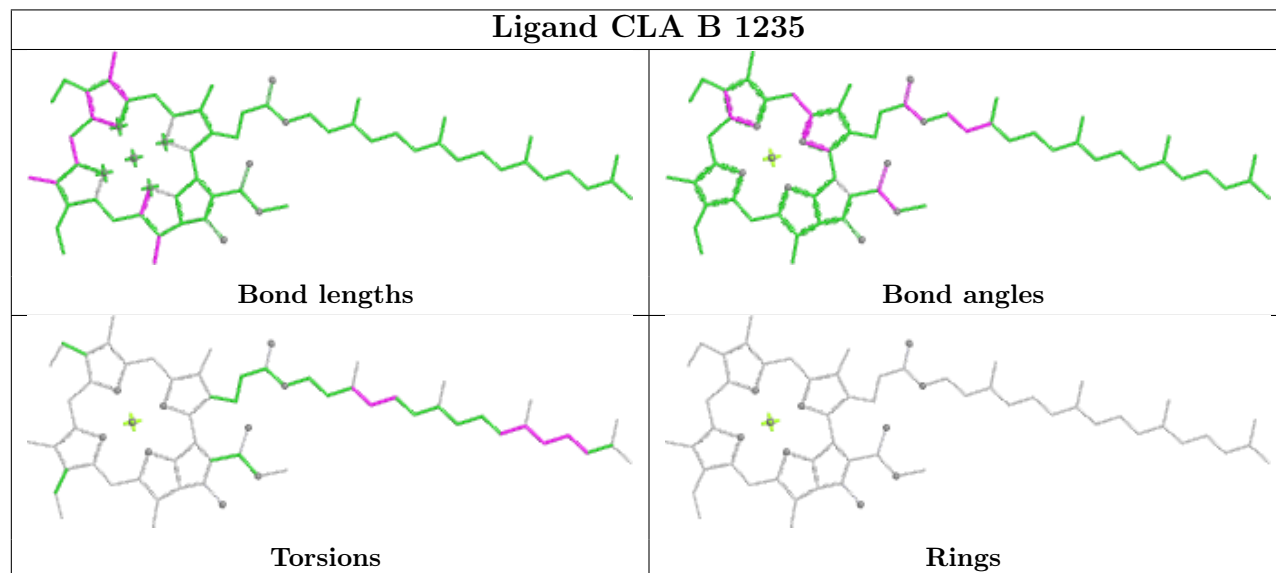


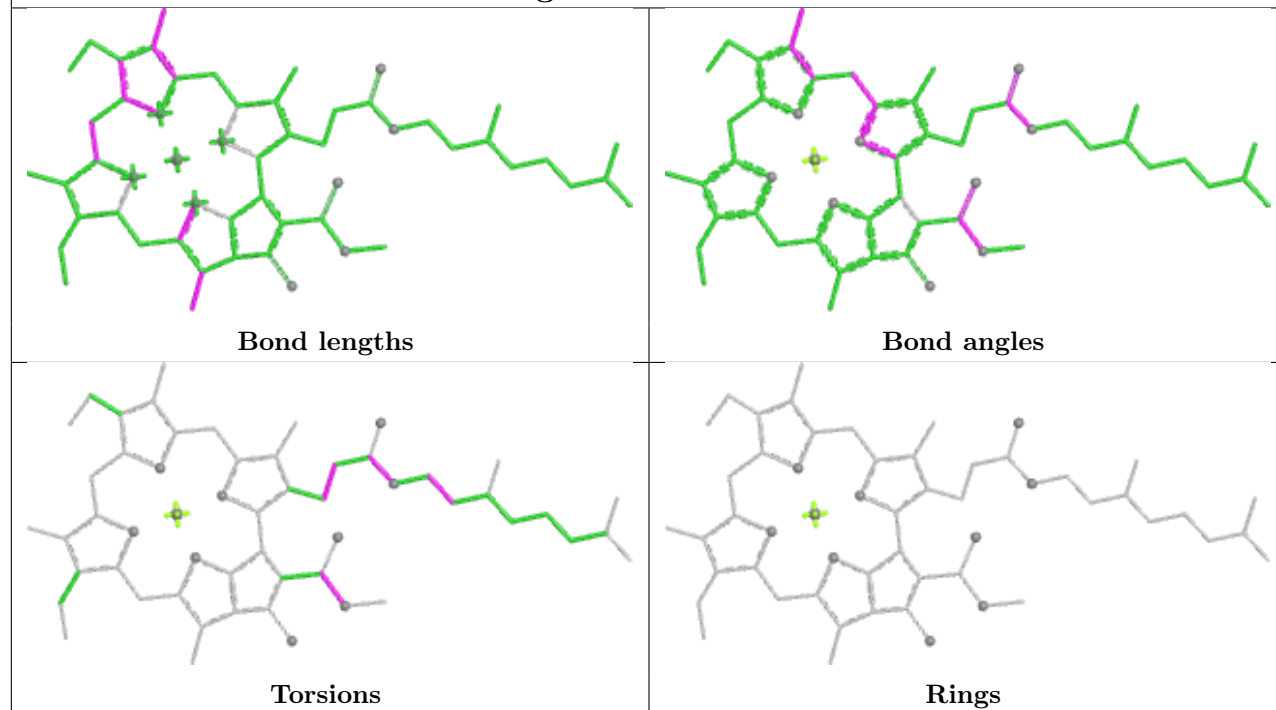
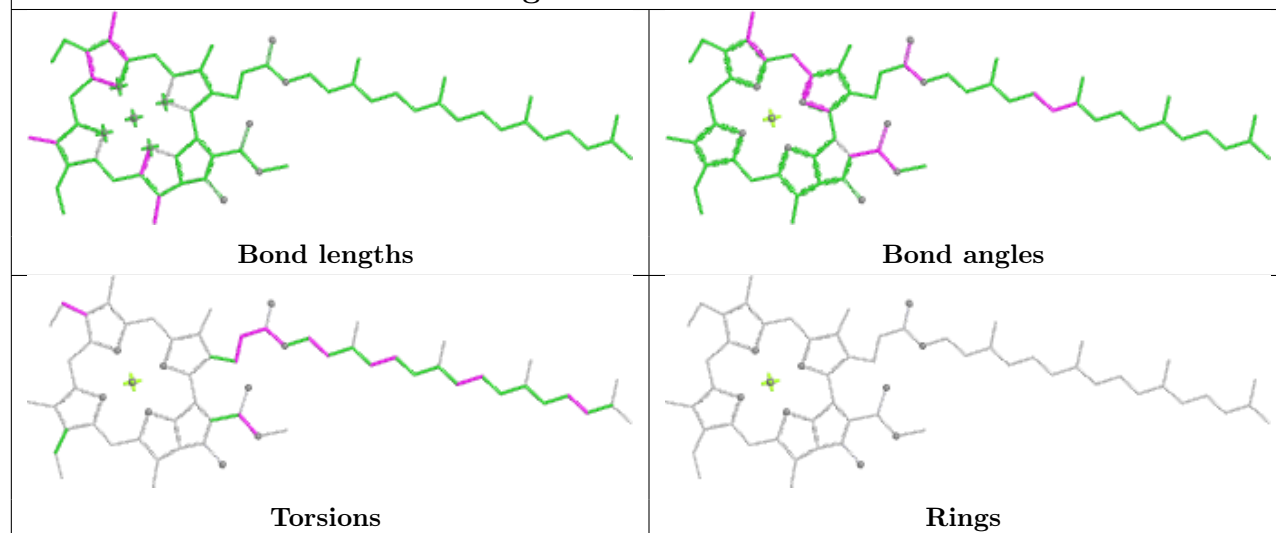
Rings

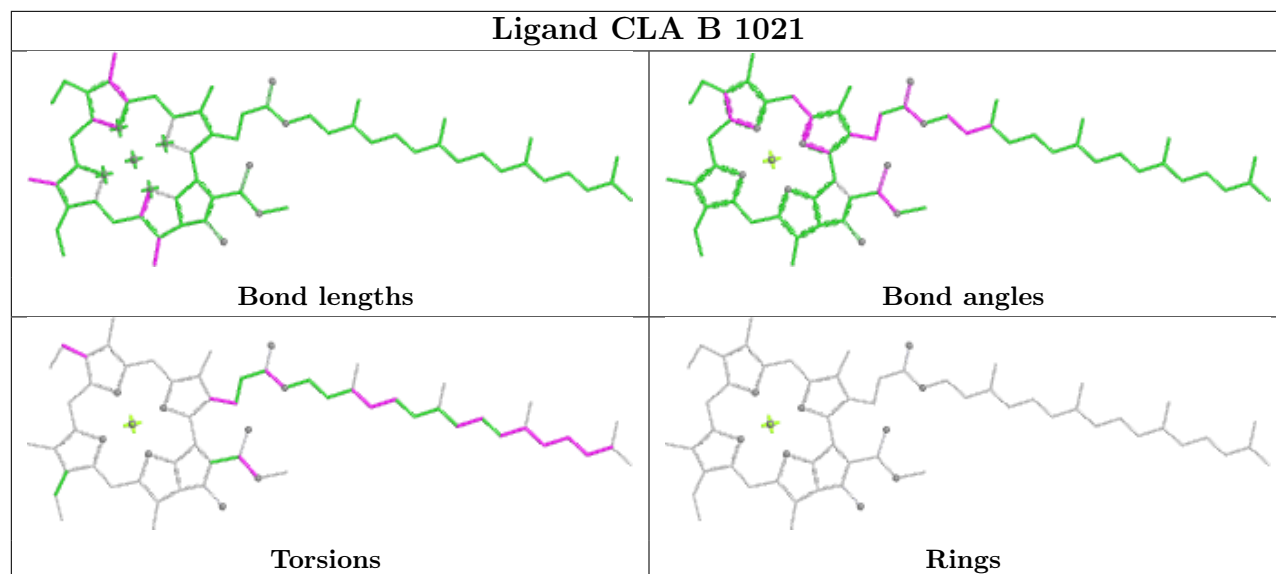
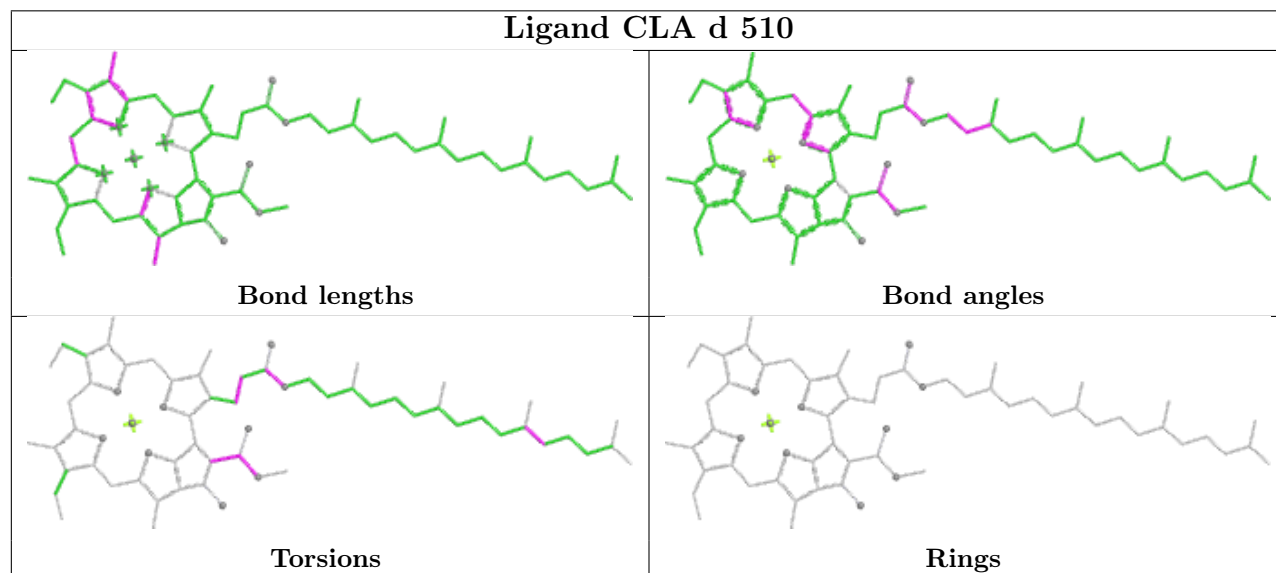
Ligand CLA f 508



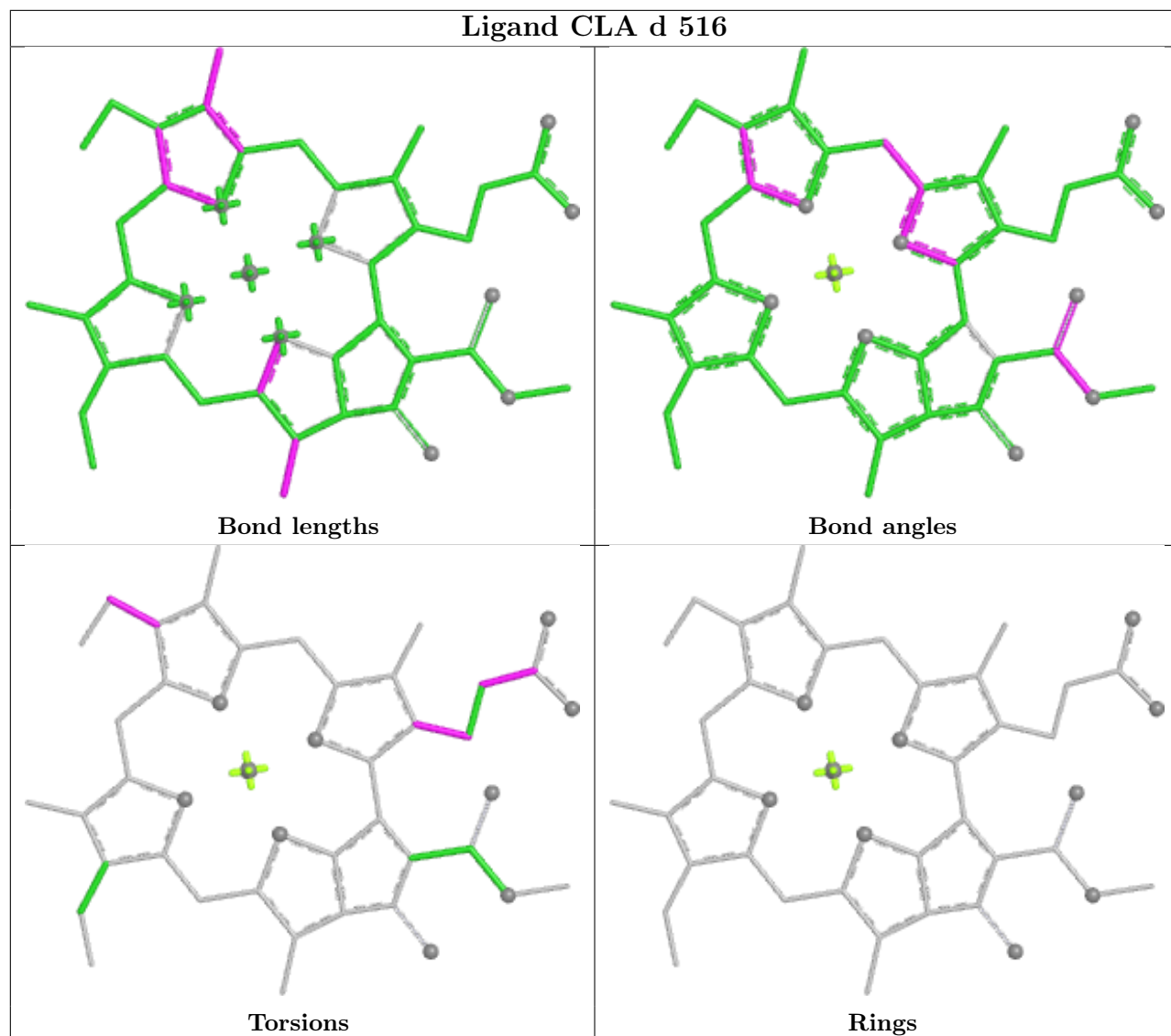
Ligand CLA B 1235



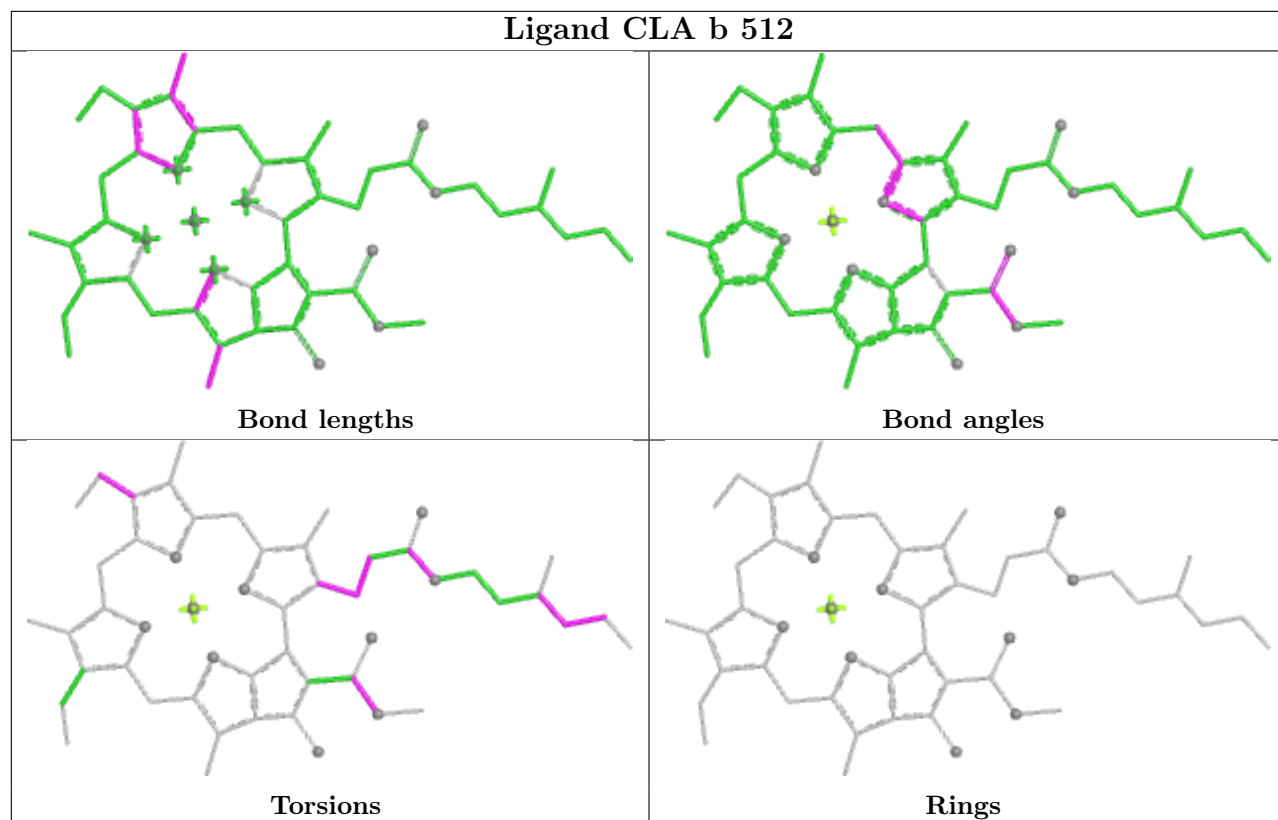
Ligand CLA 1 511**Ligand CLA A 1013**

Ligand CLA B 1021**Ligand CLA d 510**

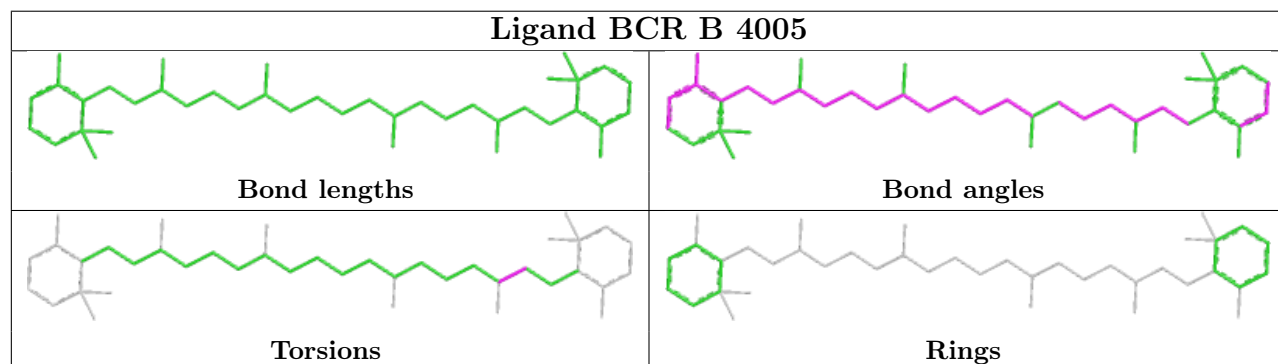
Ligand CLA d 516



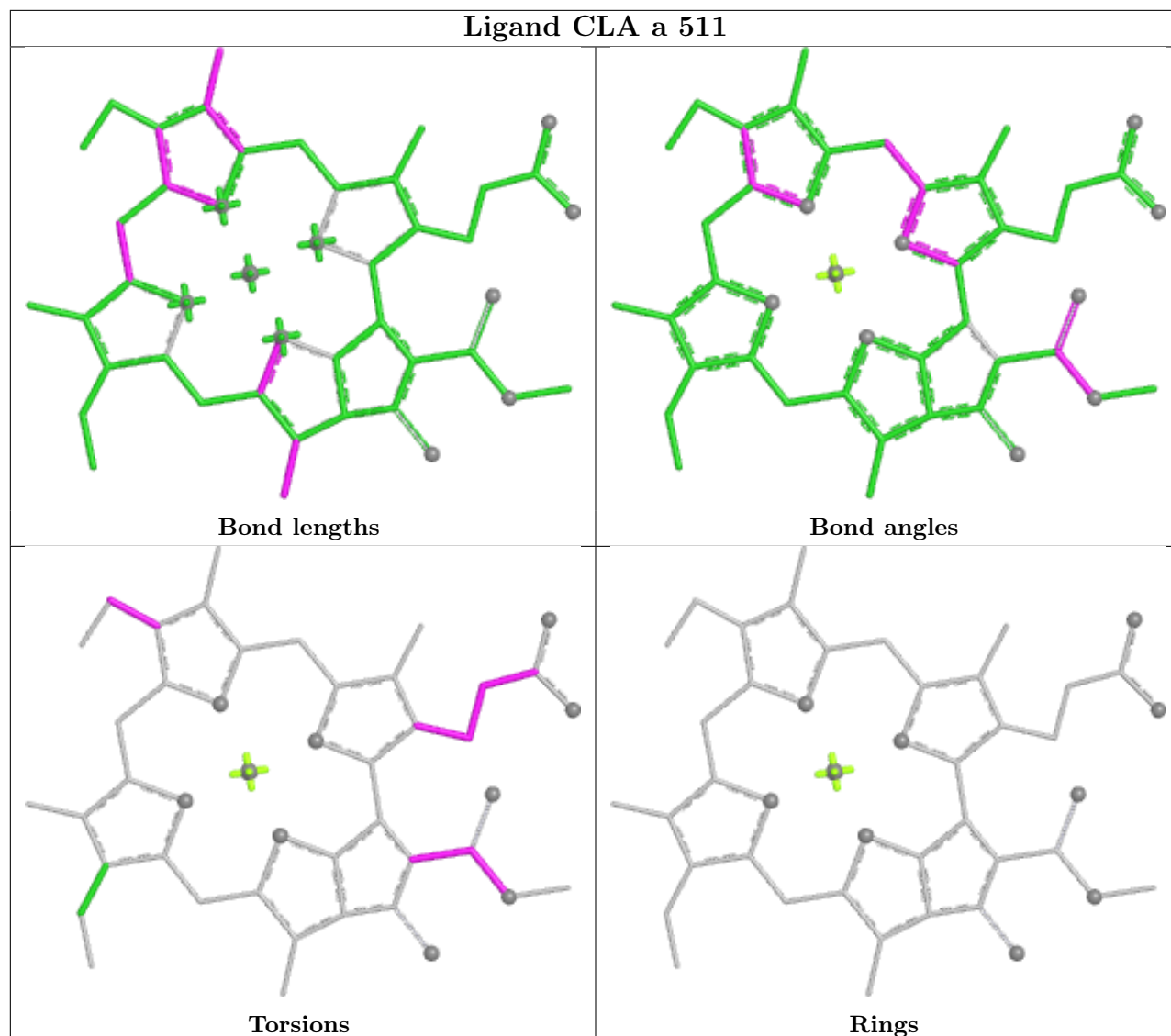
Ligand CLA b 512



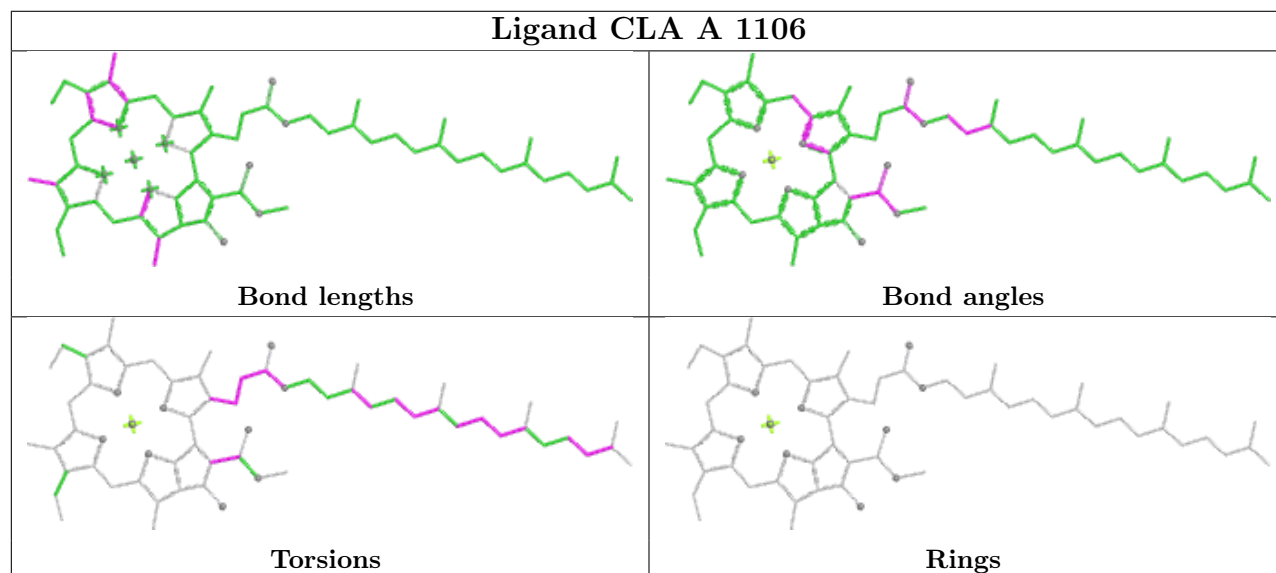
Ligand BCR B 4005



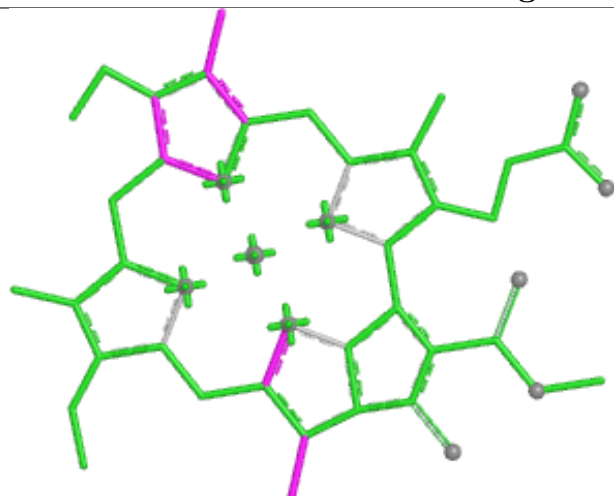
Ligand CLA a 511



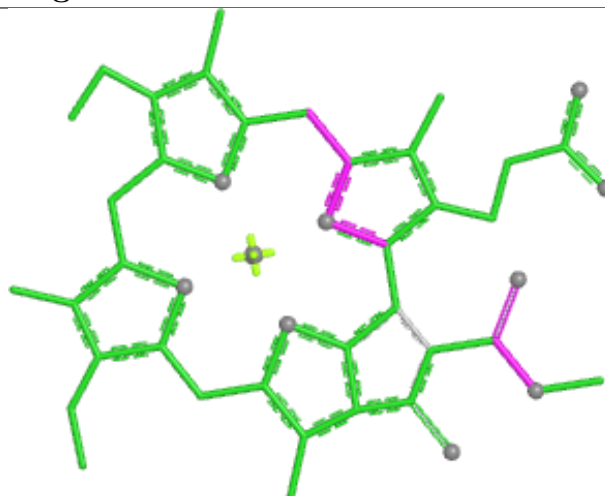
Ligand CLA A 1106



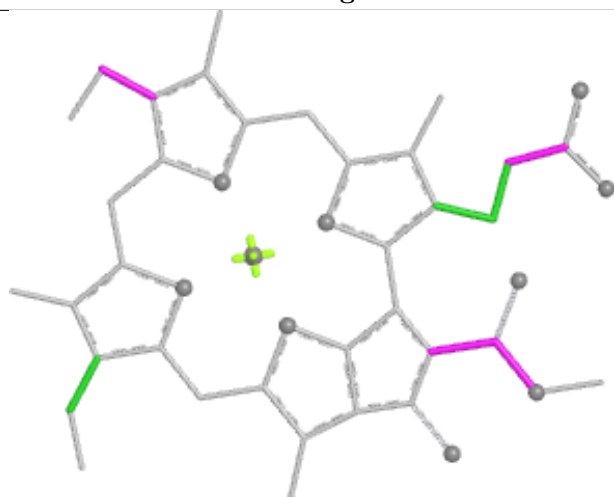
Ligand CLA g 517



Bond lengths



Bond angles

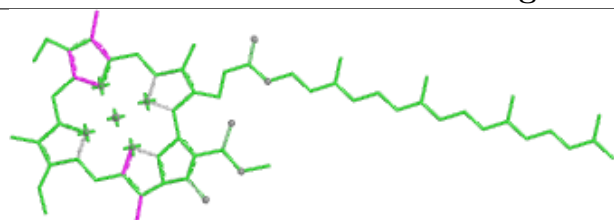


Torsions

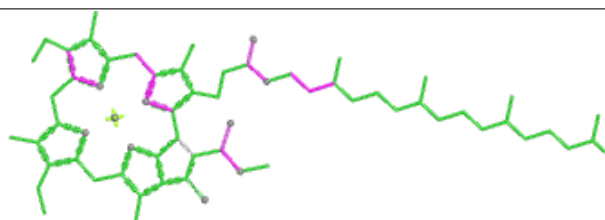


Rings

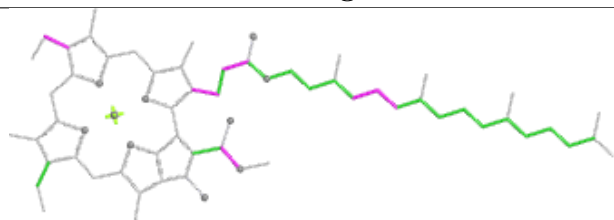
Ligand CLA e 509



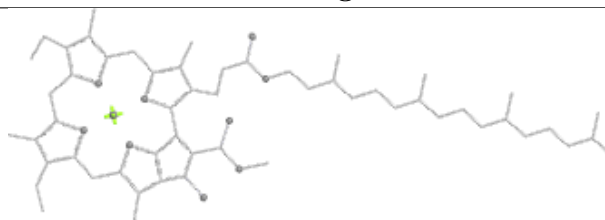
Bond lengths



Bond angles

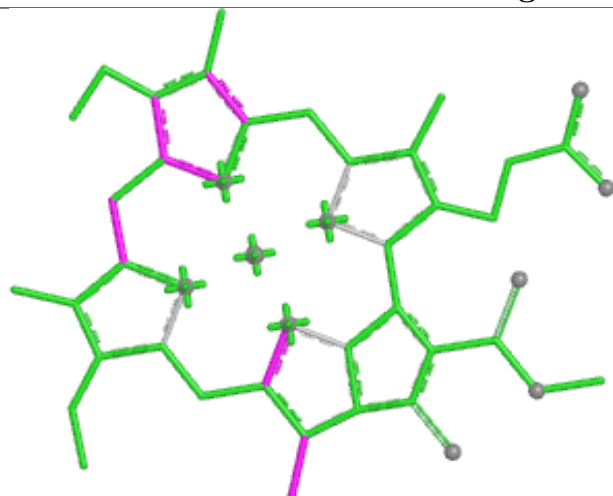


Torsions

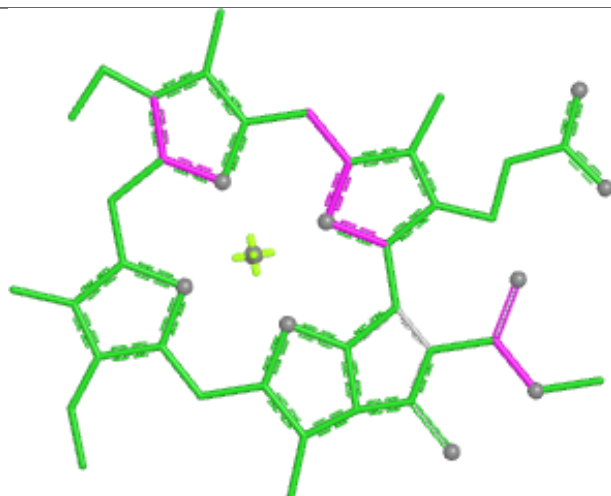


Rings

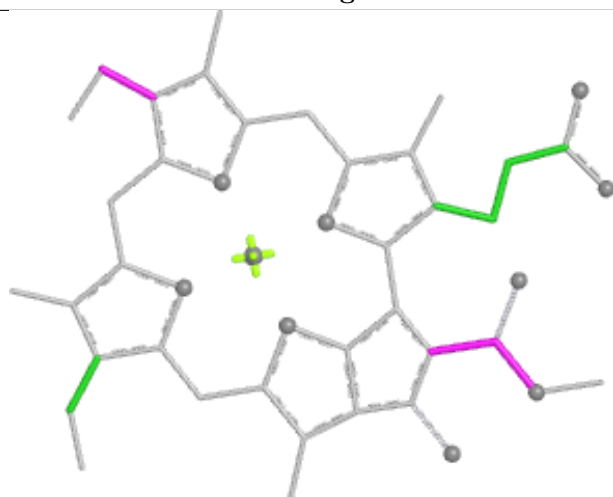
Ligand CLA 5 506



Bond lengths



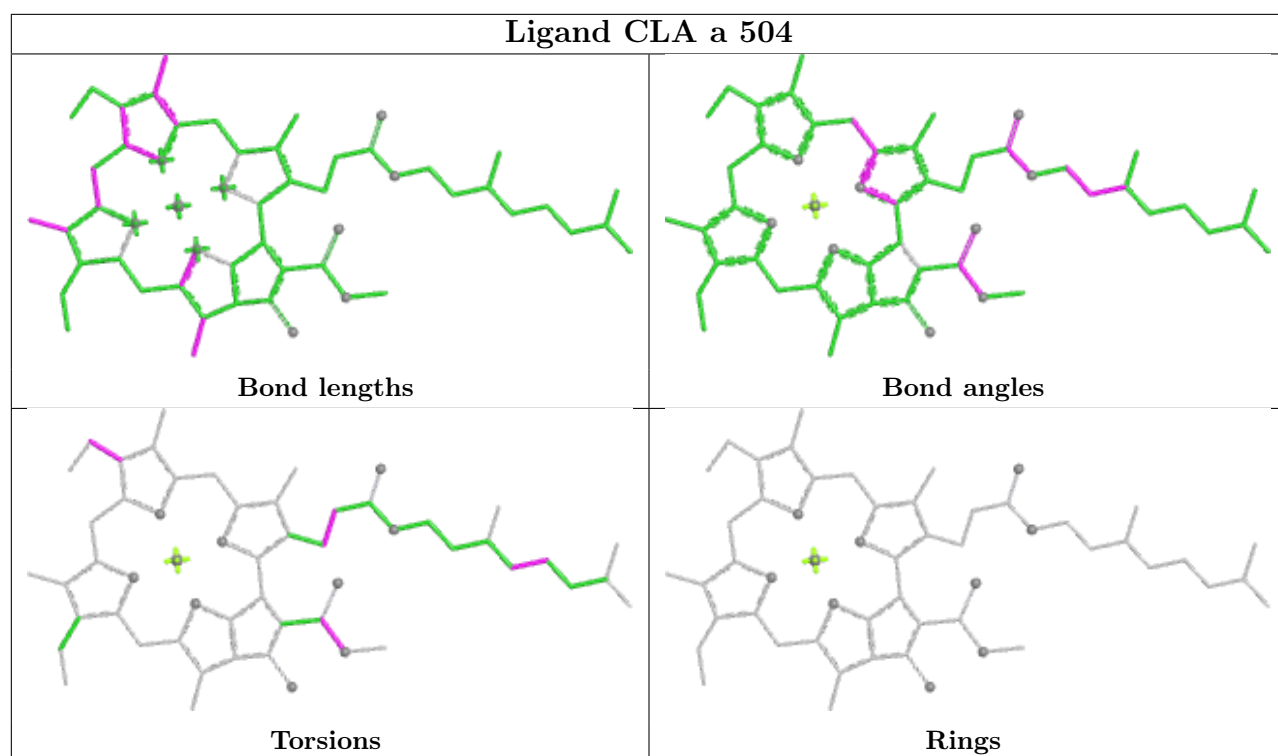
Bond angles



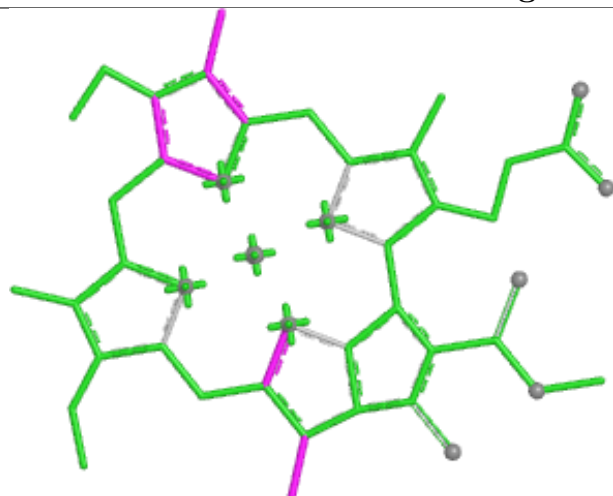
Torsions



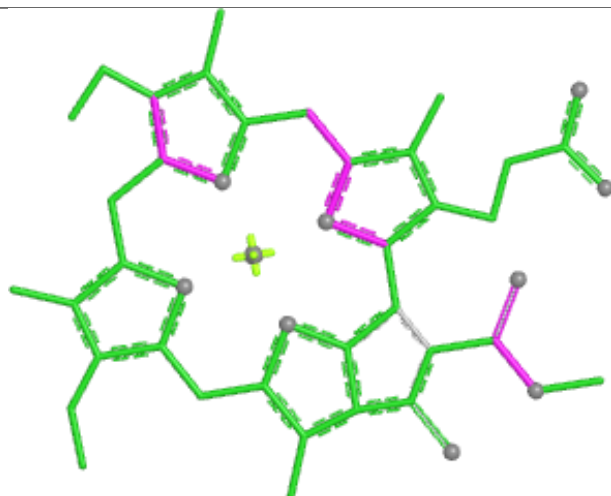
Rings



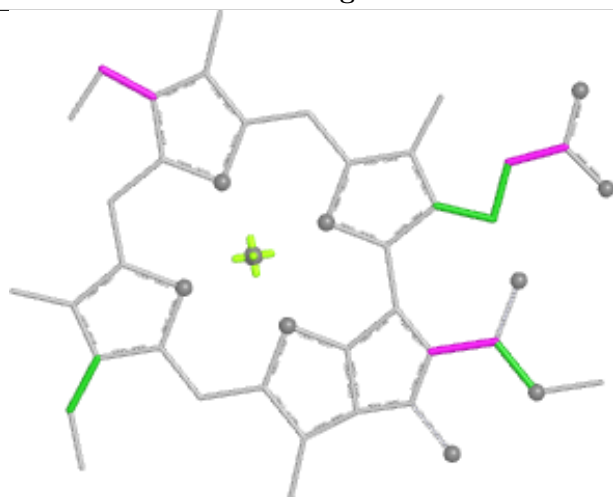
Ligand CLA 5 517



Bond lengths



Bond angles

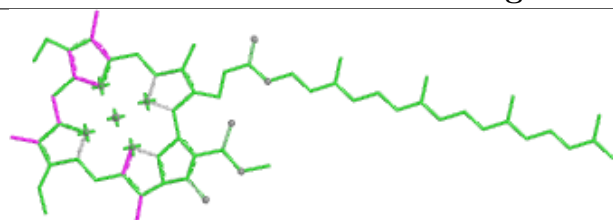


Torsions

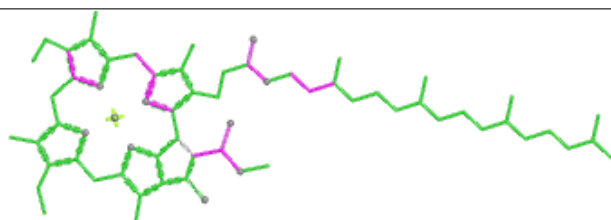


Rings

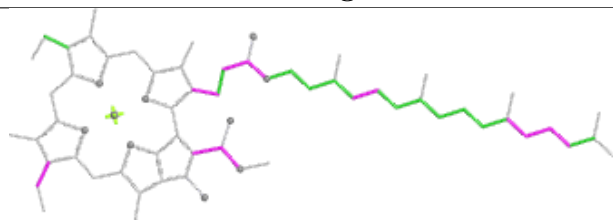
Ligand CLA B 1229



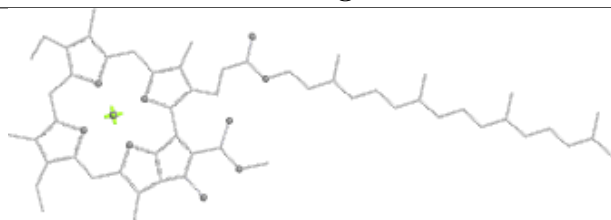
Bond lengths



Bond angles

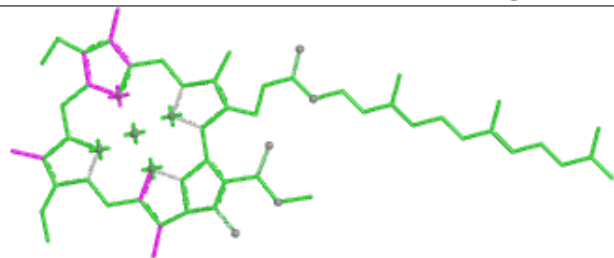


Torsions

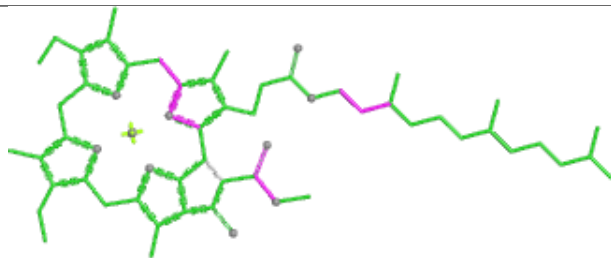


Rings

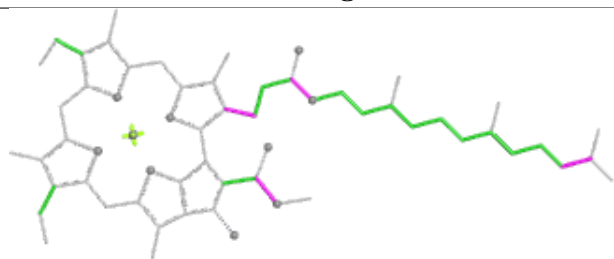
Ligand CLA B 1215



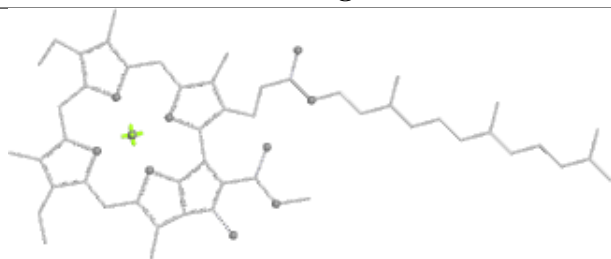
Bond lengths



Bond angles

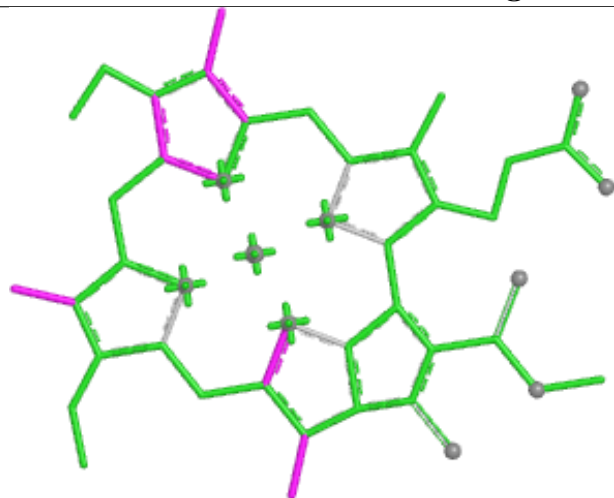


Torsions

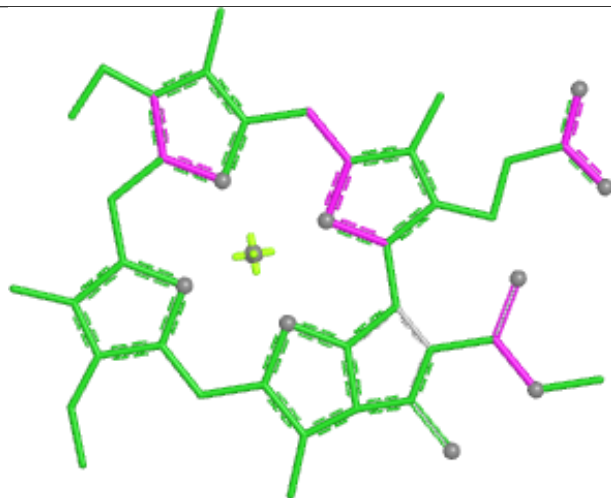


Rings

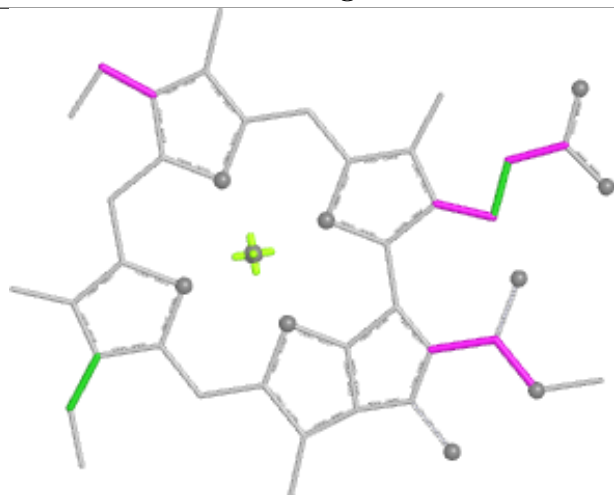
Ligand CLA B 1232



Bond lengths



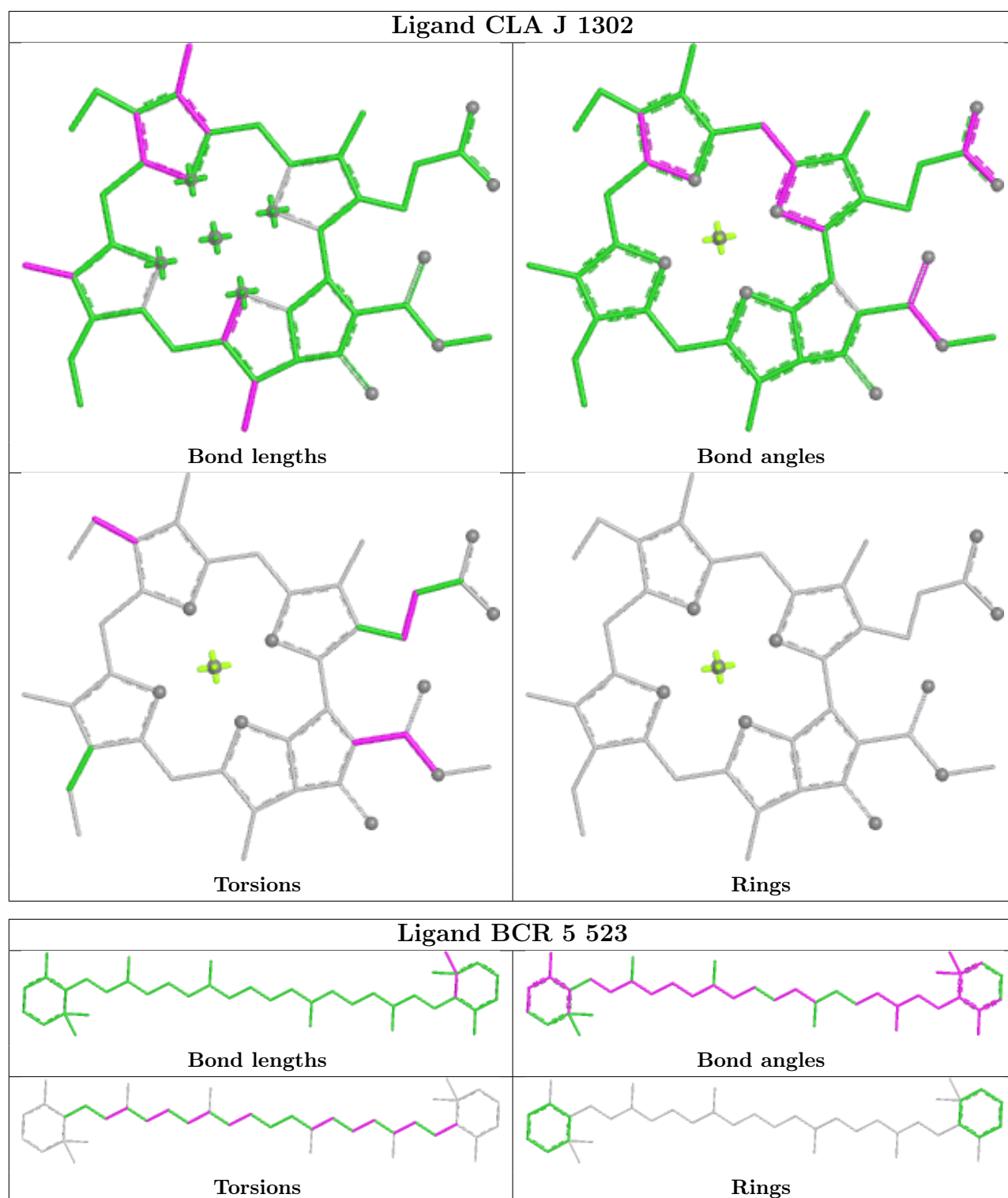
Bond angles

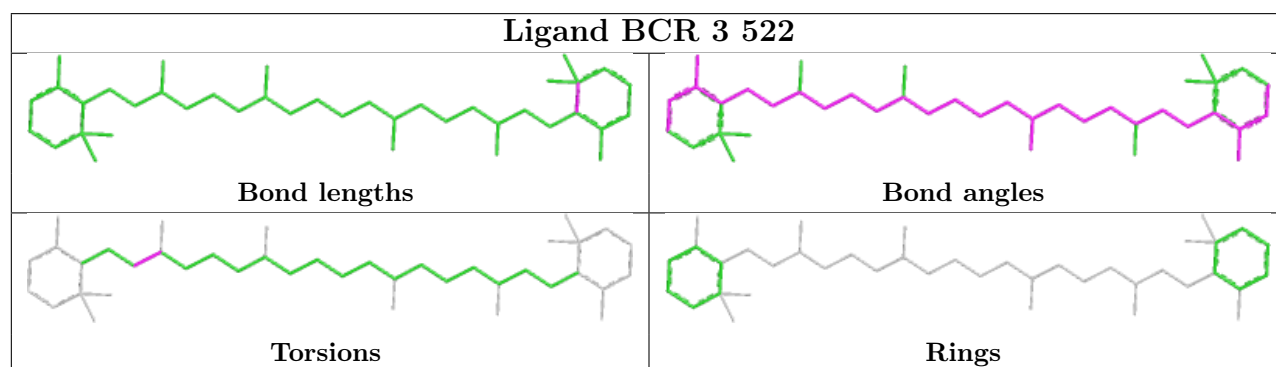
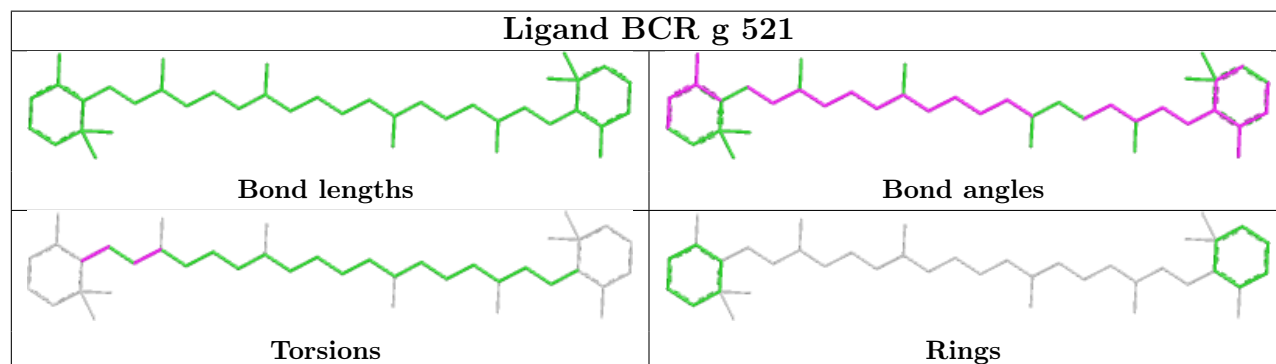
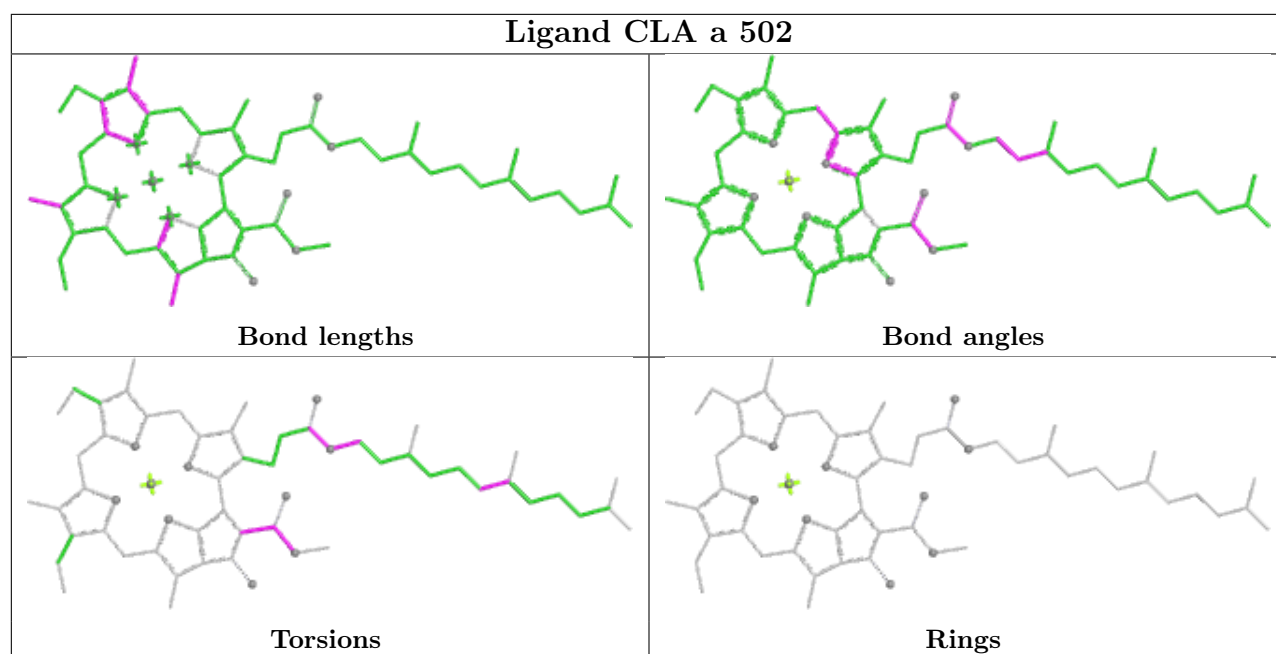


Torsions

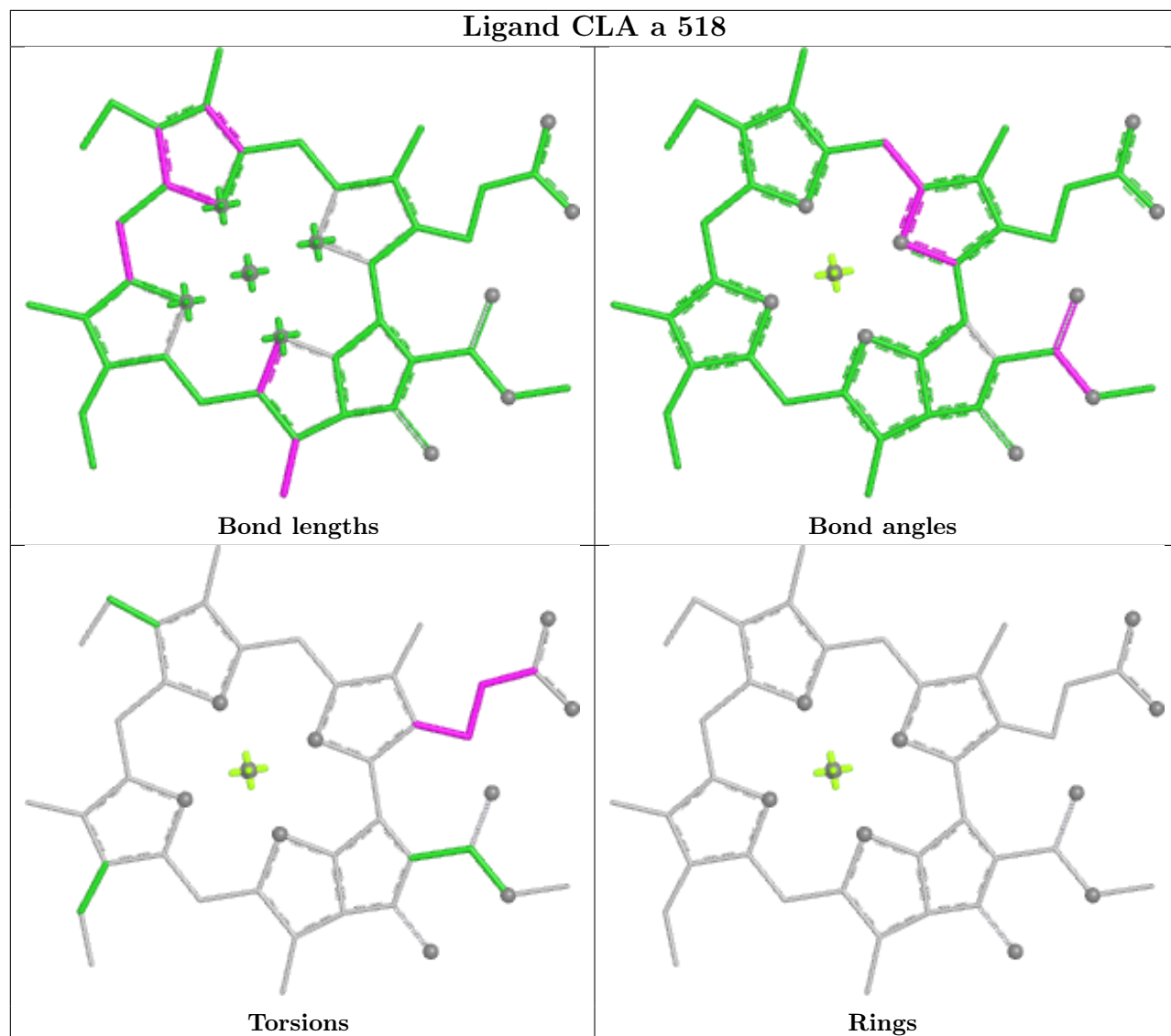


Rings

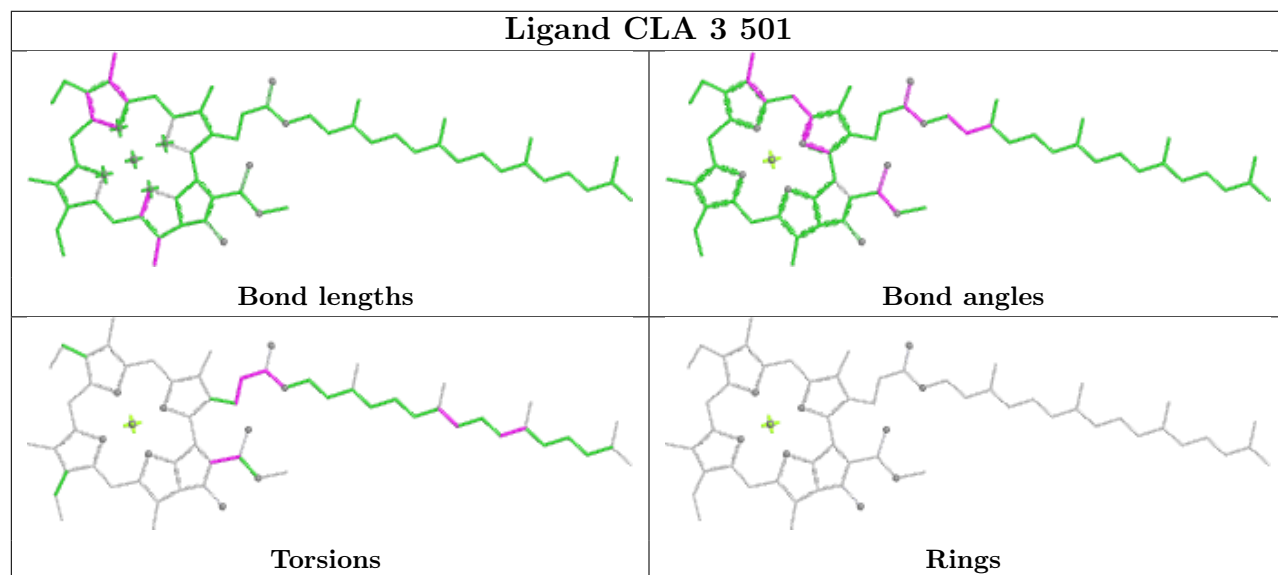


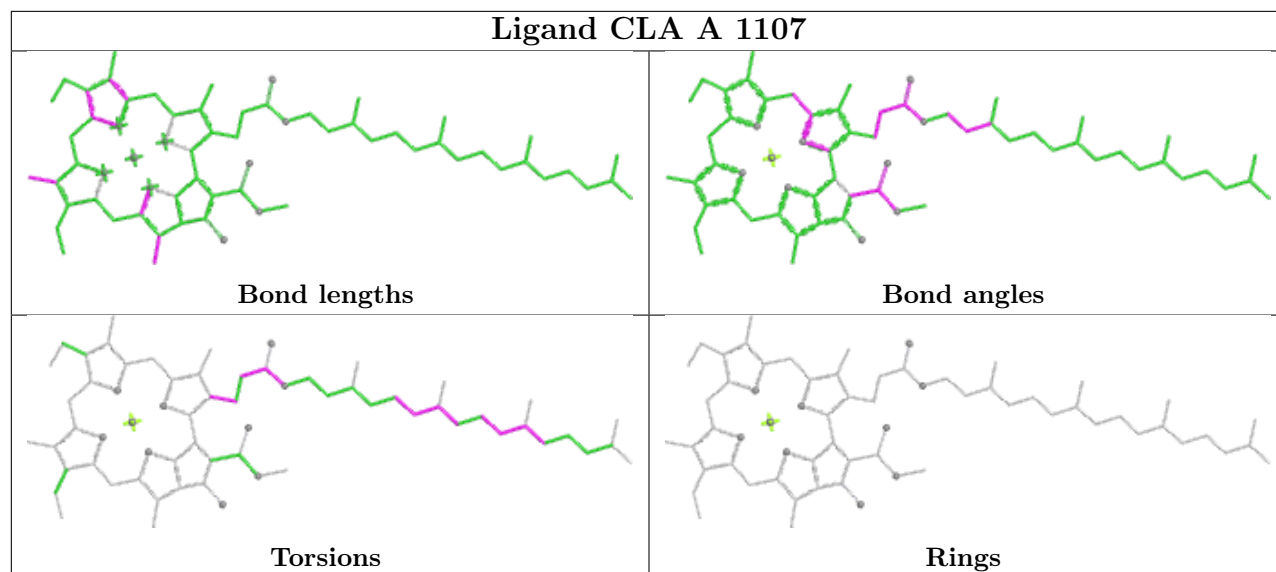
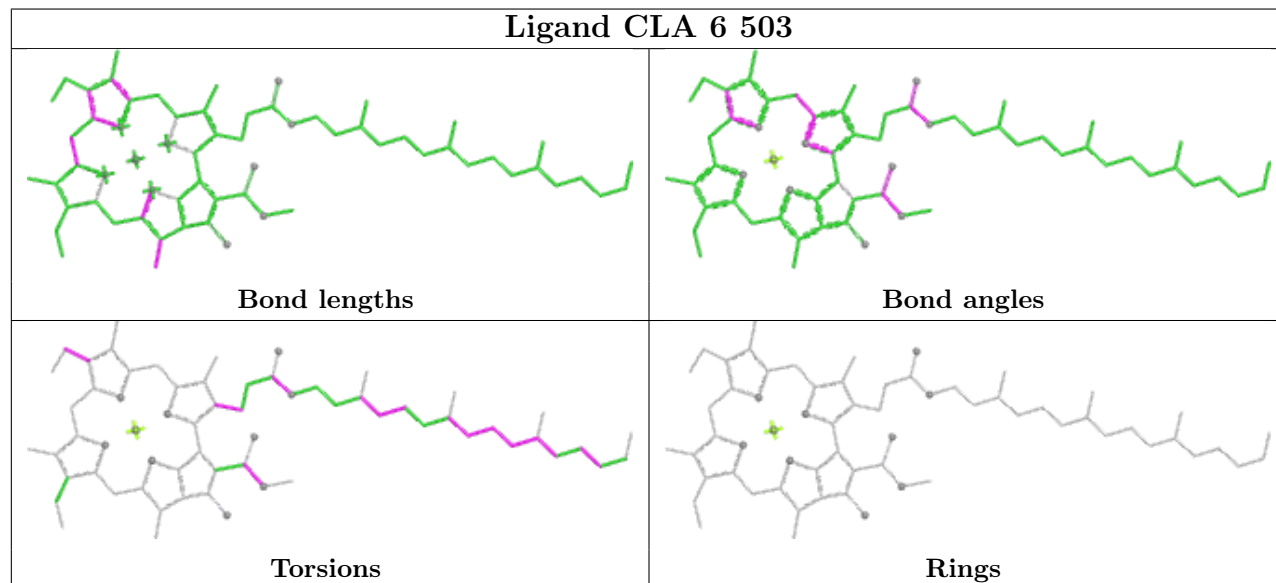


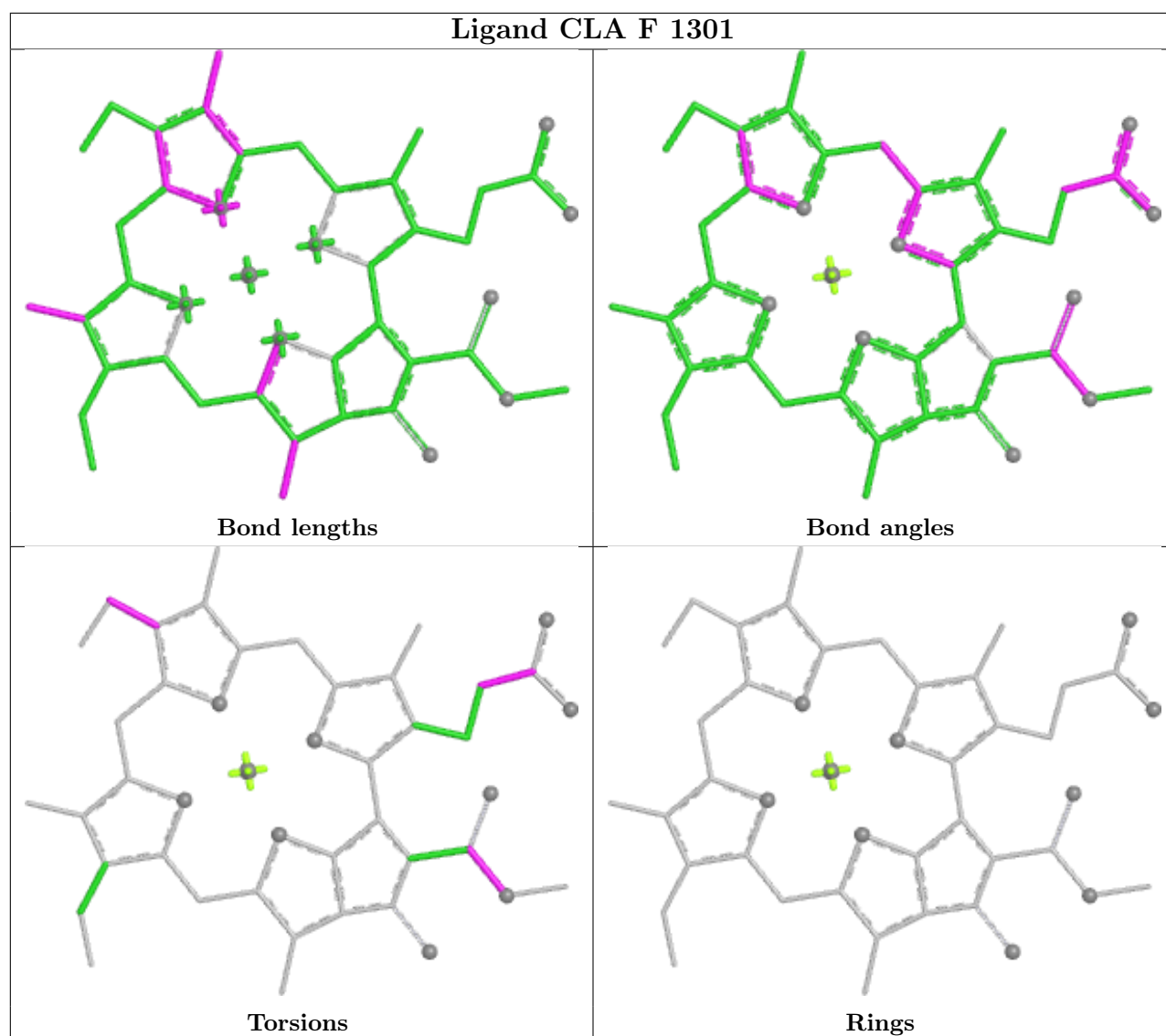
Ligand CLA a 518

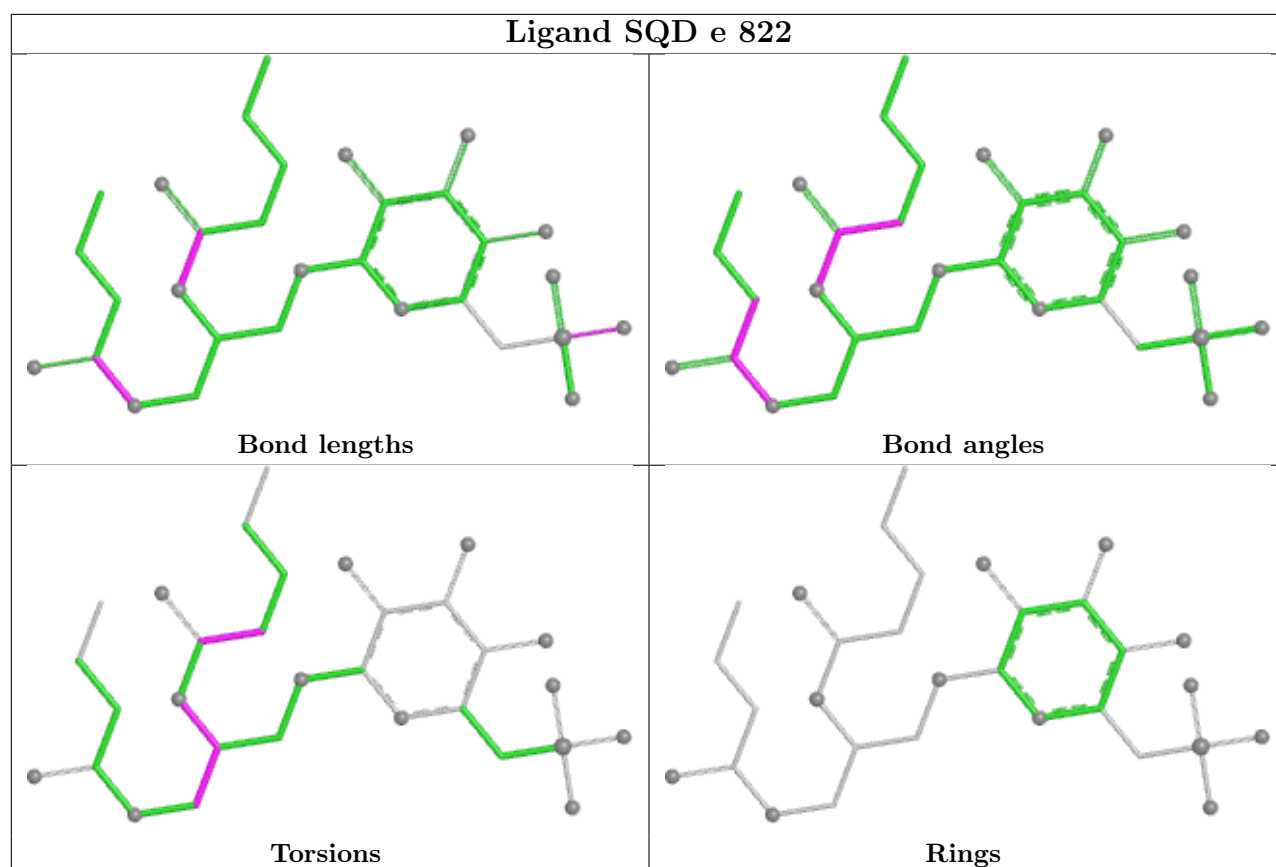


Ligand CLA 3 501

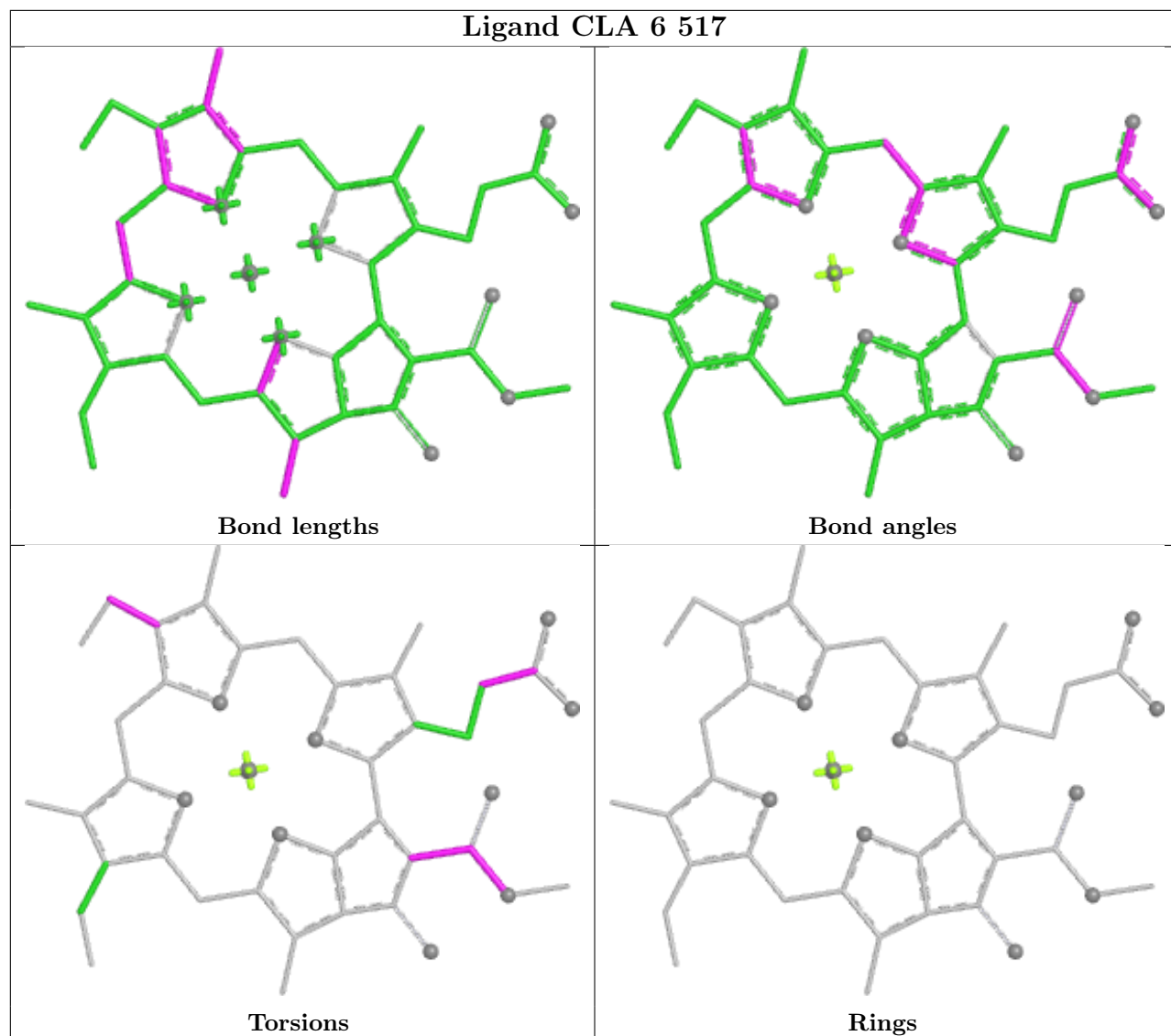


Ligand CLA A 1107**Ligand CLA 6 503**

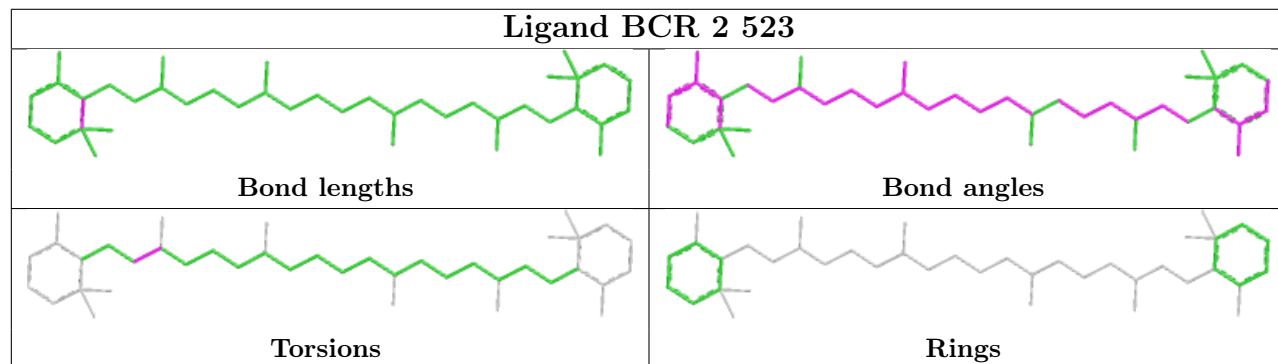


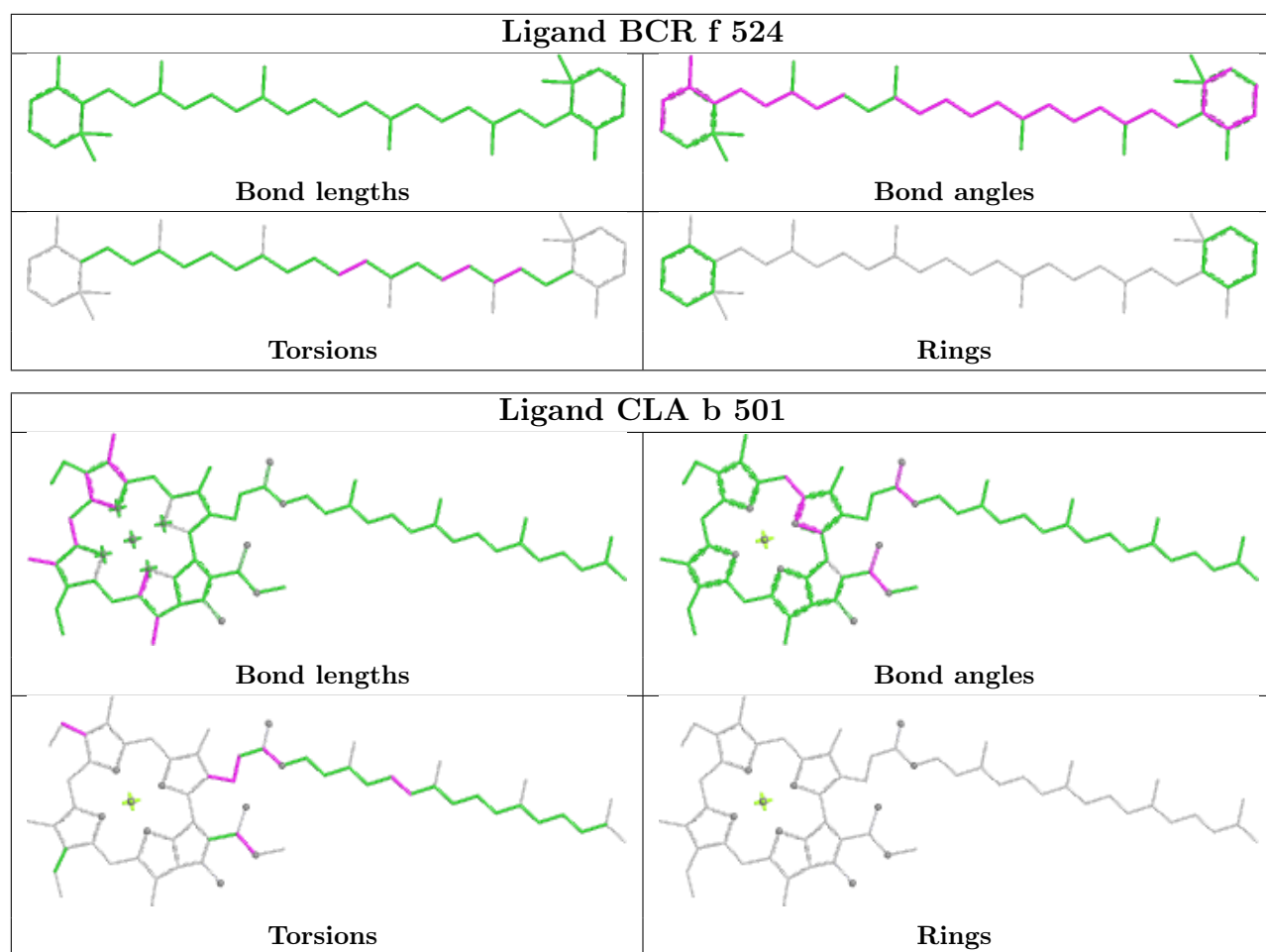


Ligand CLA 6 517

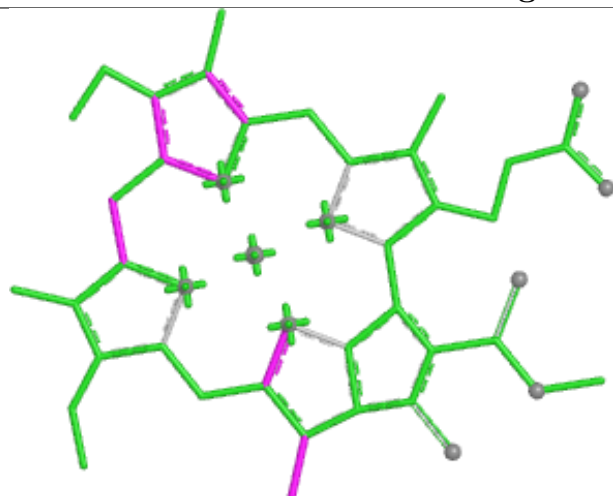


Ligand BCR 2 523

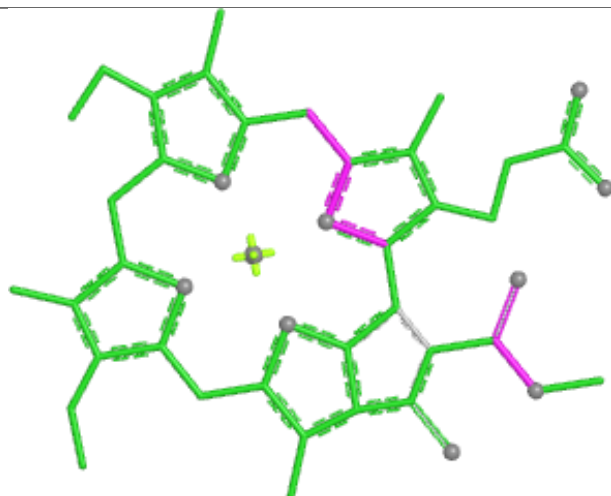




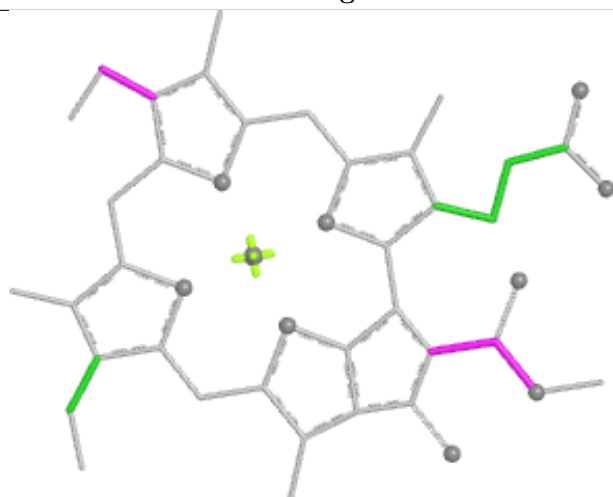
Ligand CLA 1 516



Bond lengths



Bond angles

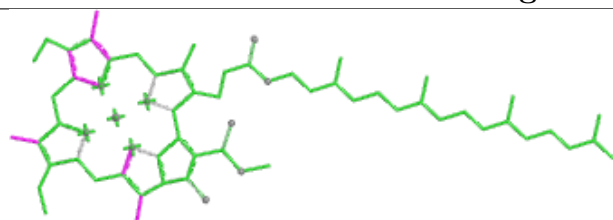


Torsions

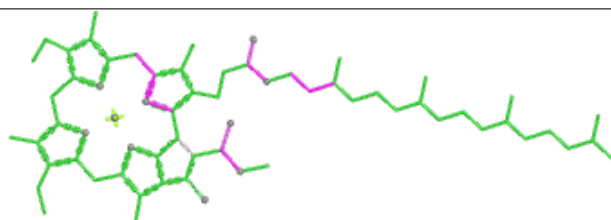


Rings

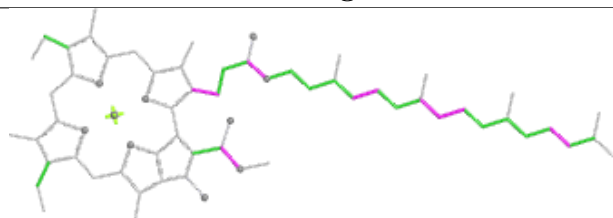
Ligand CLA c 509



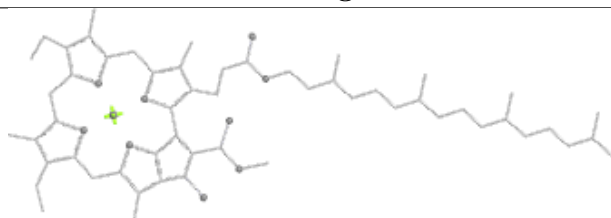
Bond lengths



Bond angles

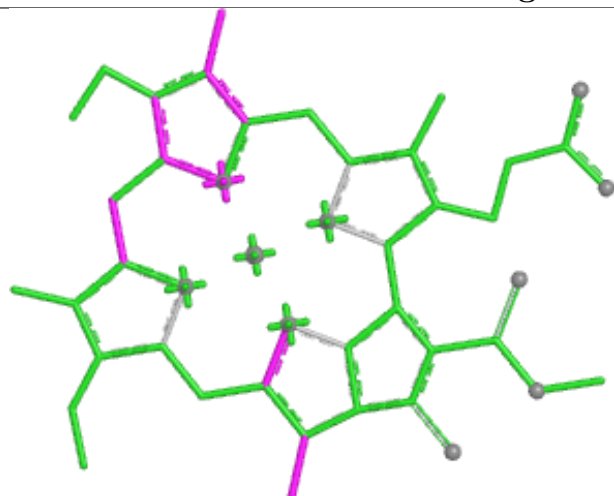


Torsions

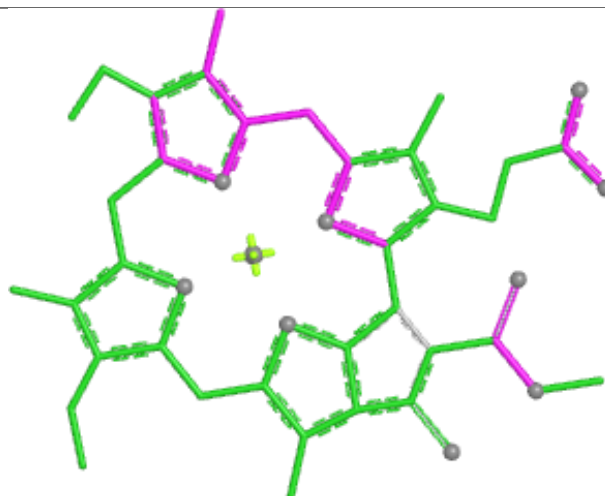


Rings

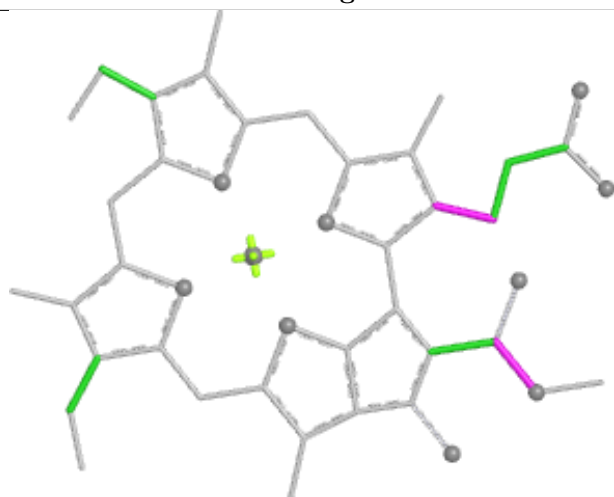
Ligand CLA 4 511



Bond lengths



Bond angles

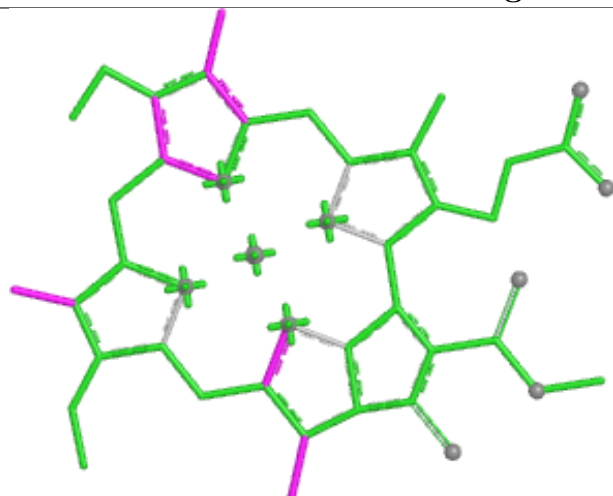


Torsions

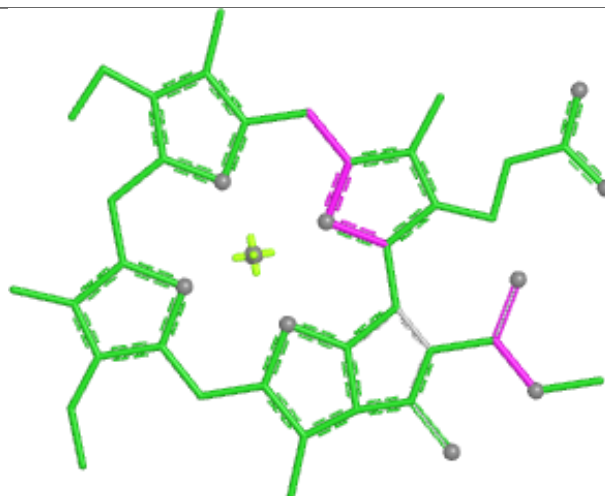


Rings

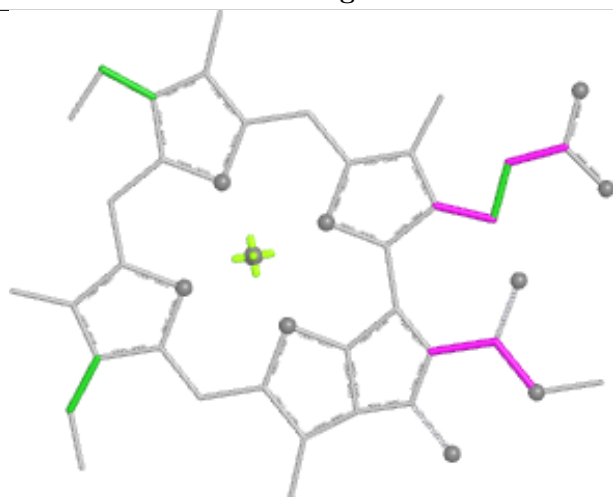
Ligand CLA A 1801



Bond lengths



Bond angles

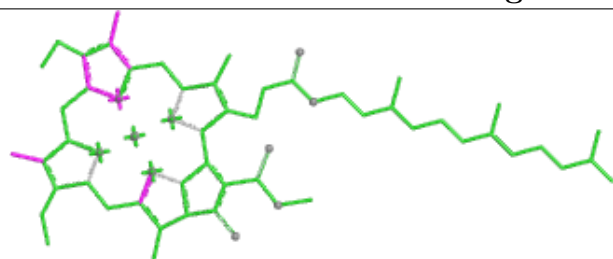


Torsions

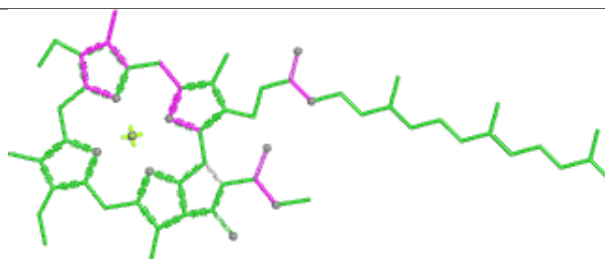


Rings

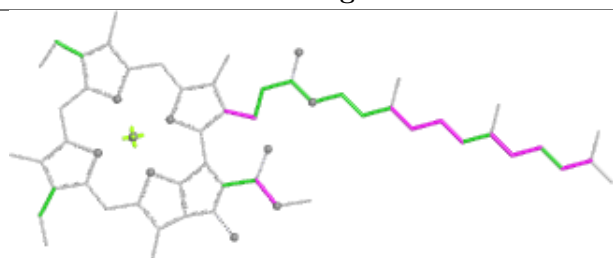
Ligand CLA B 1221



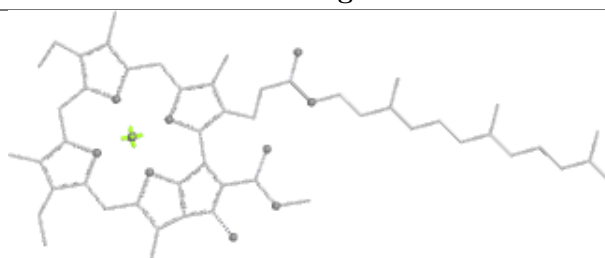
Bond lengths



Bond angles

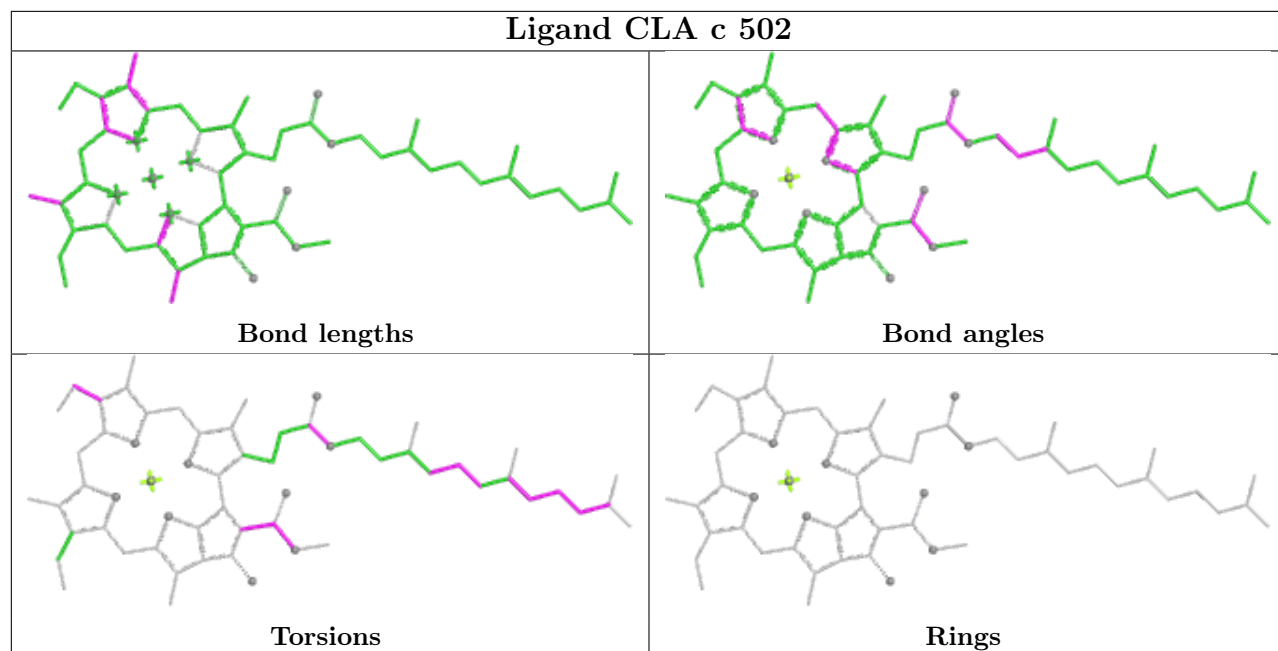


Torsions

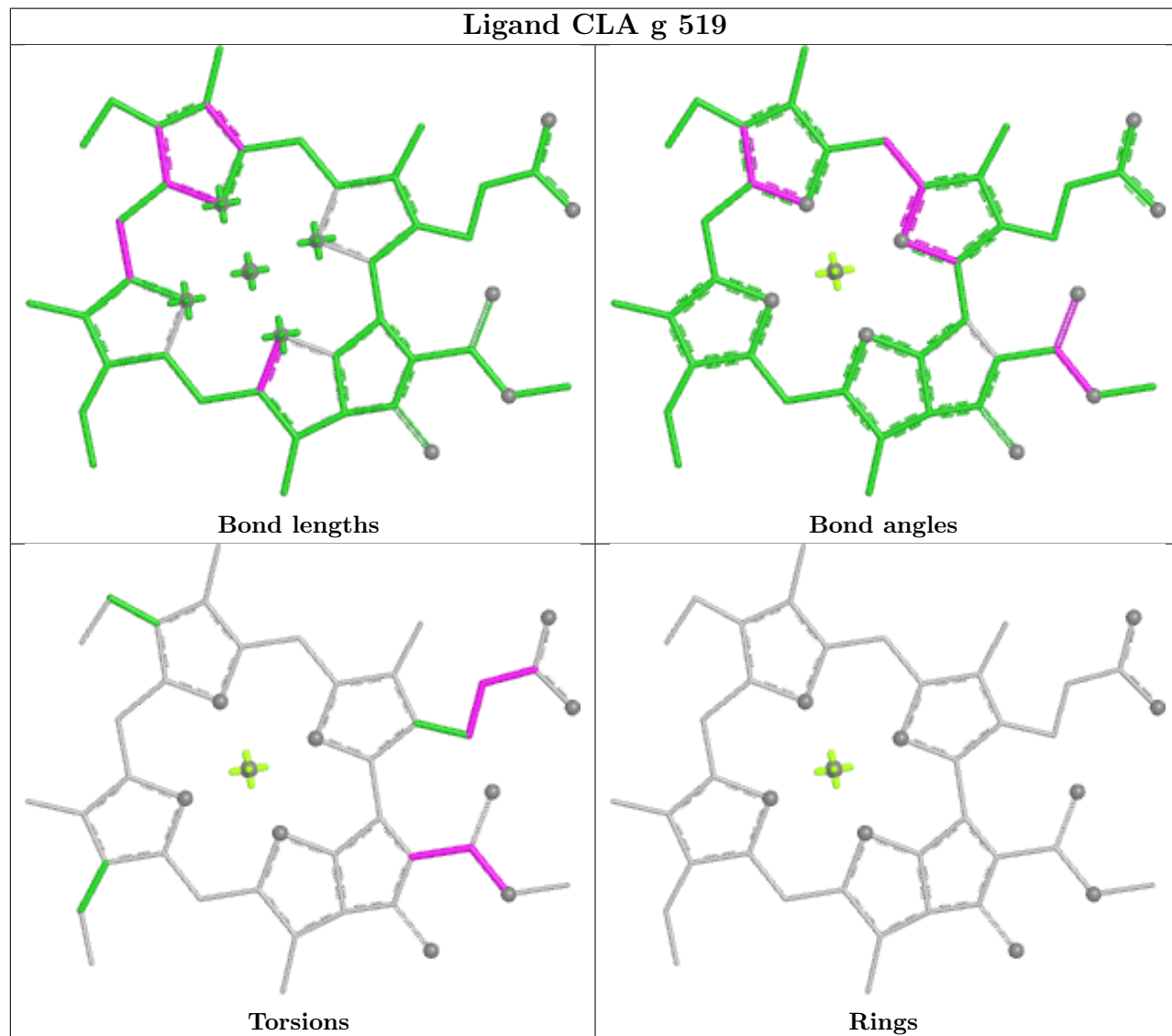


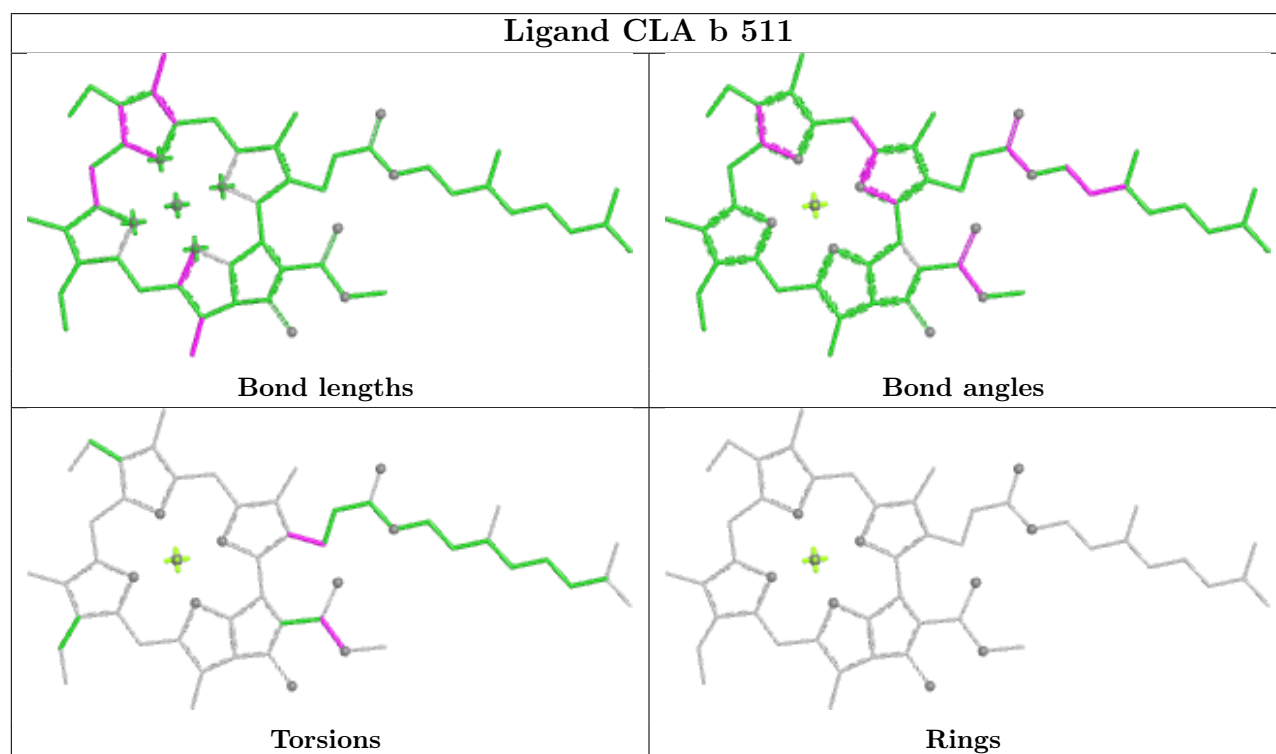
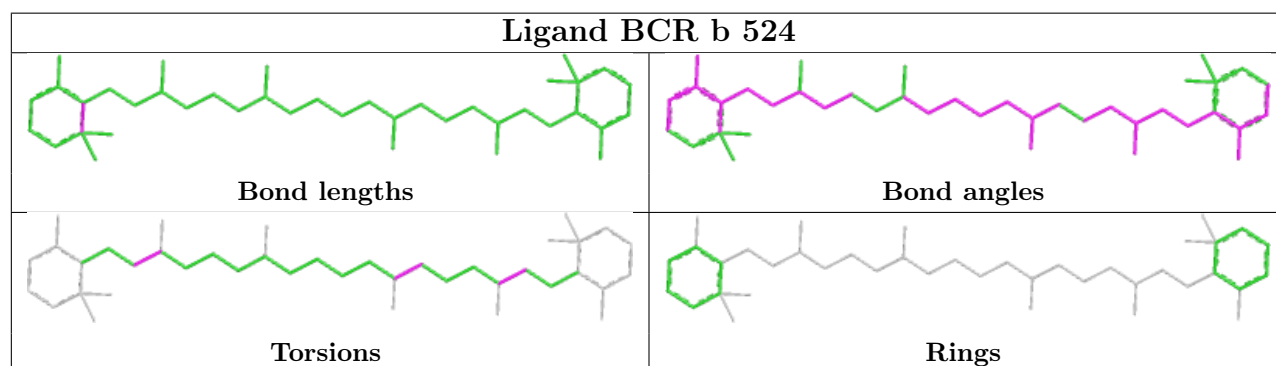
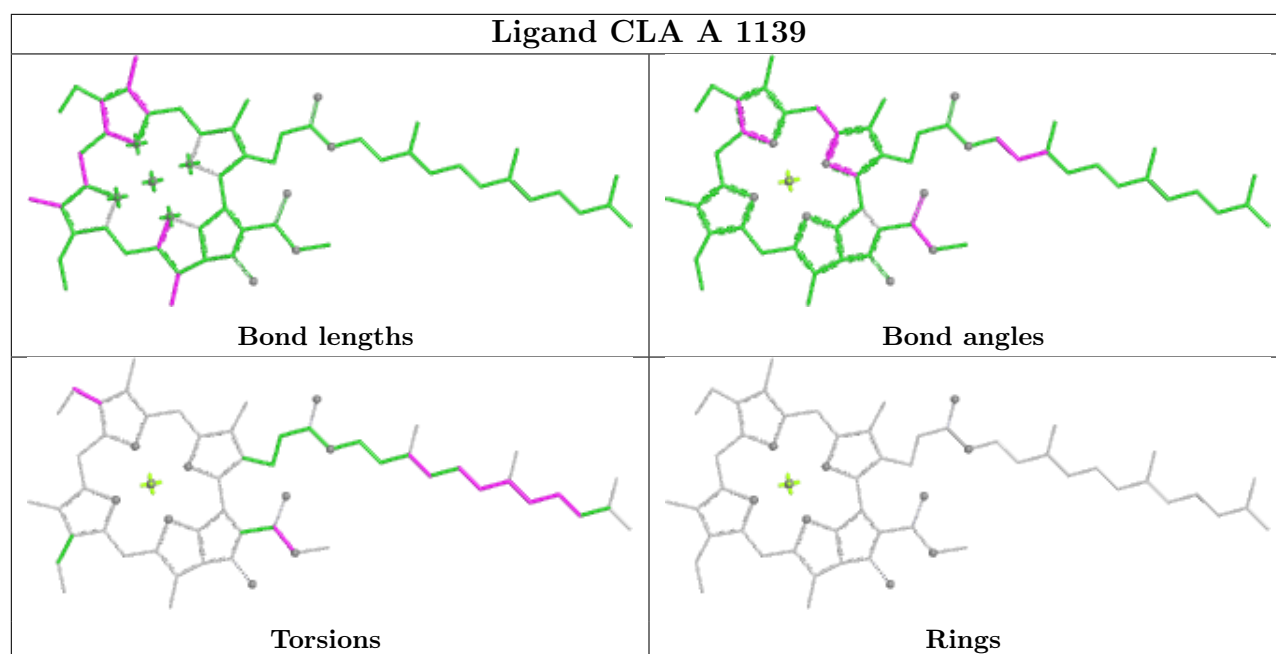
Rings

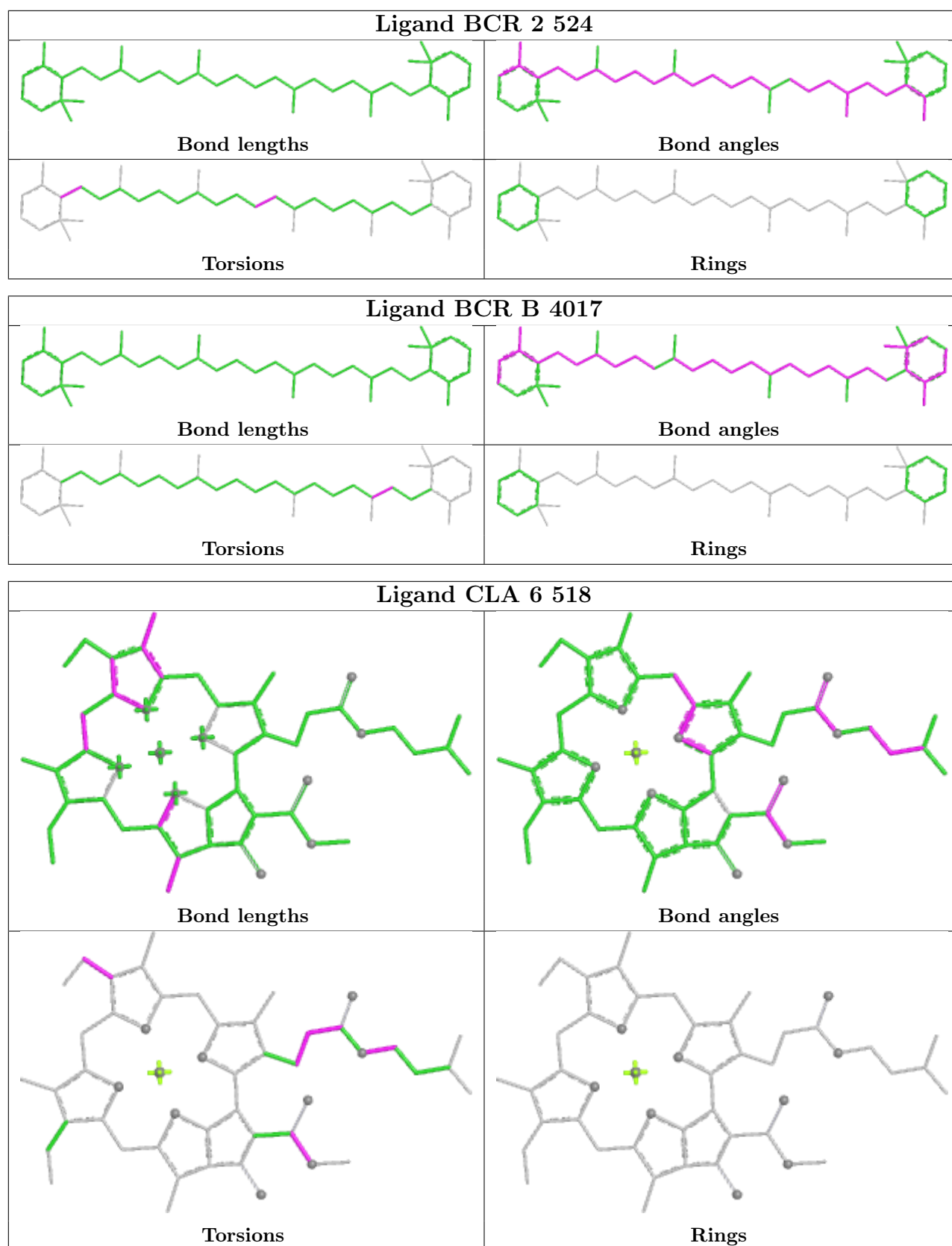
Ligand CLA c 502

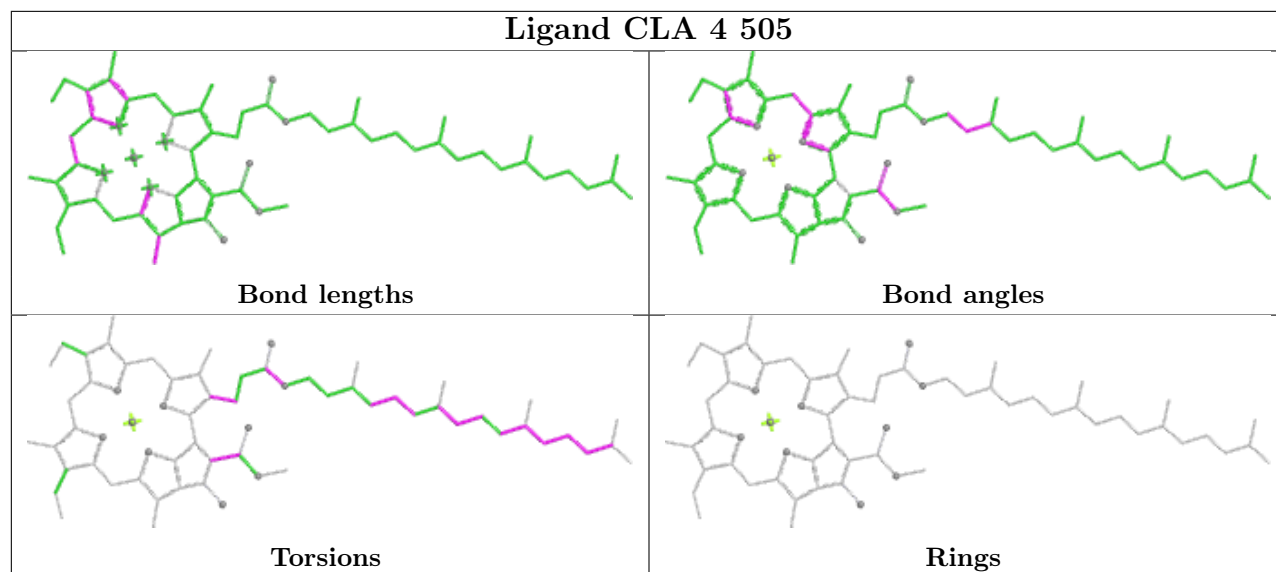
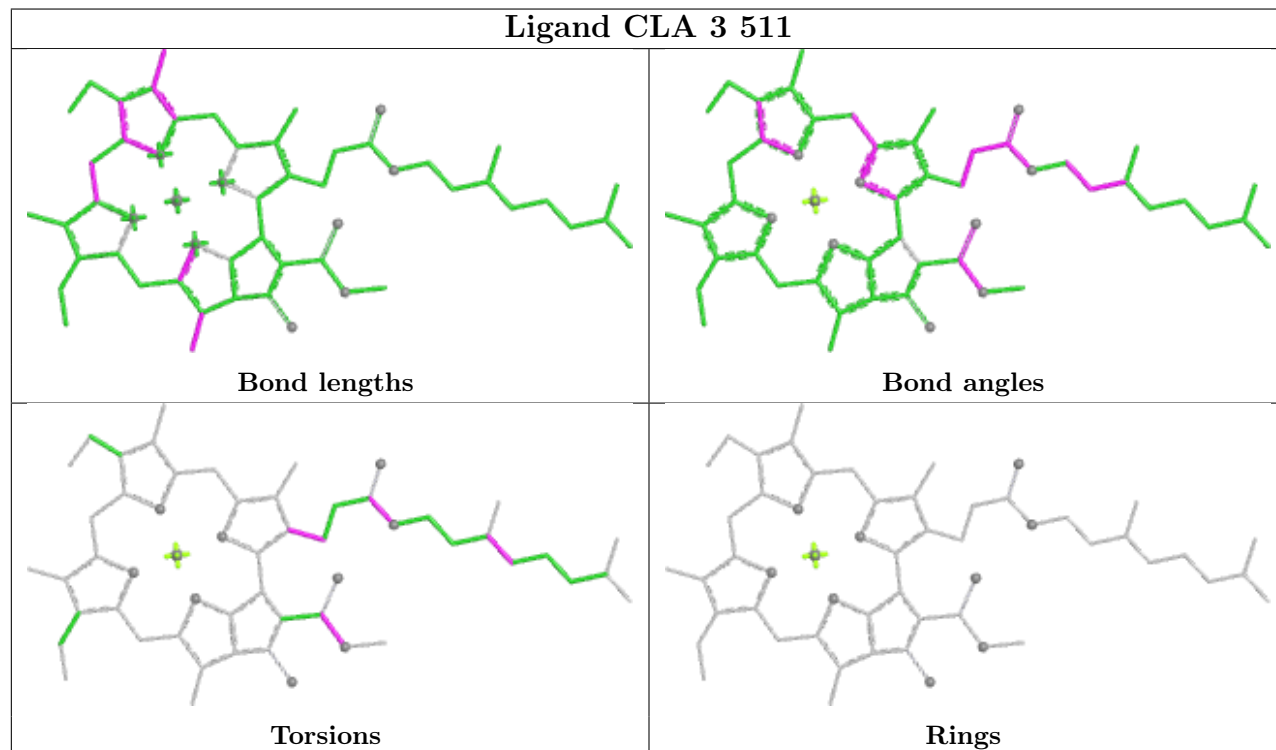


Ligand CLA g 519

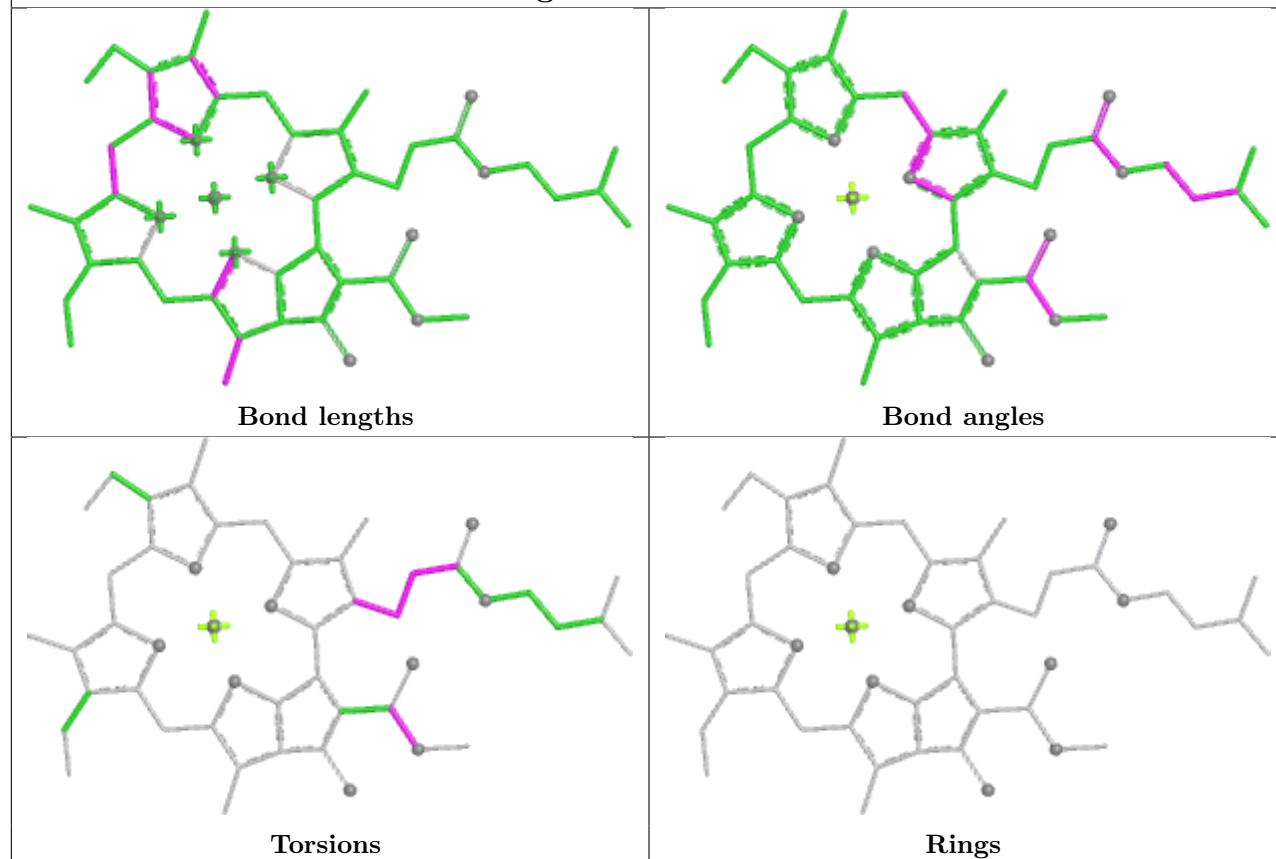




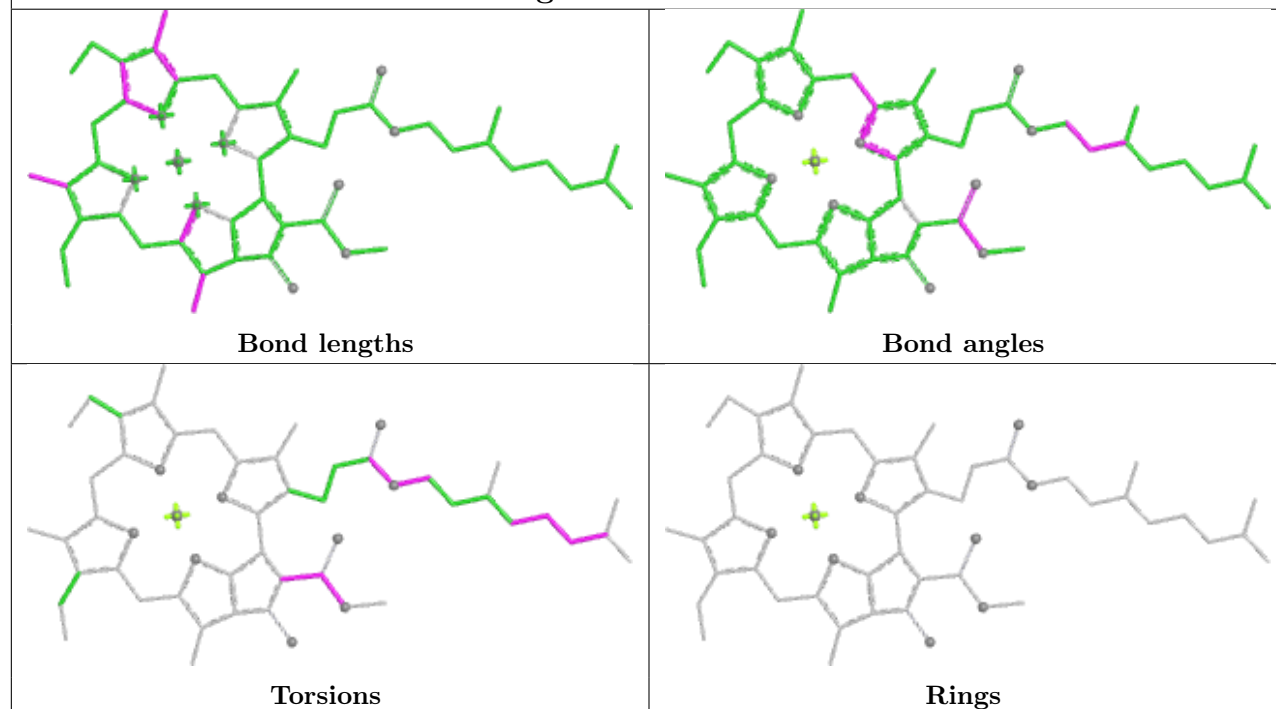


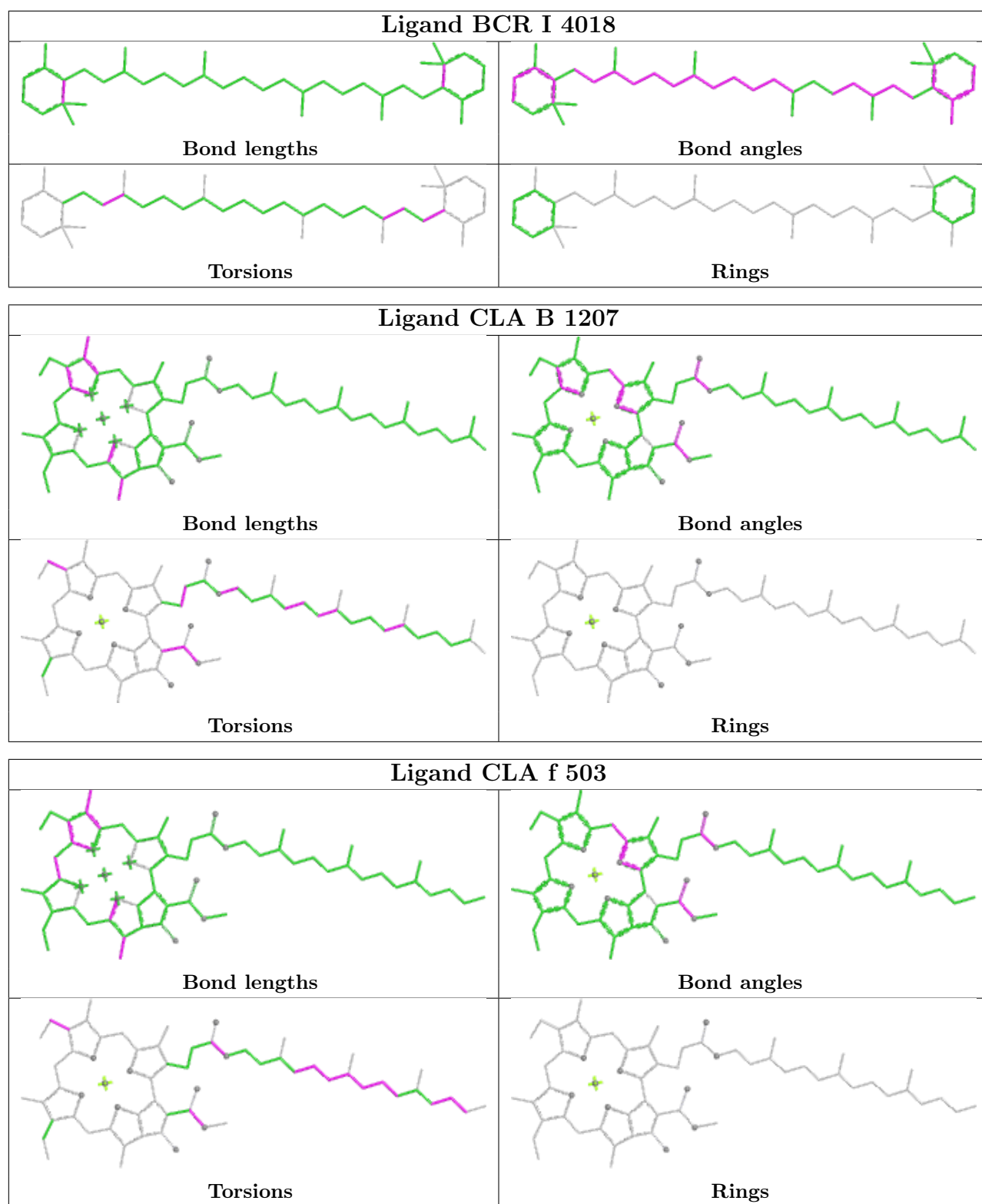
Ligand CLA 4 505**Ligand CLA 3 511**

Ligand CLA 6 513

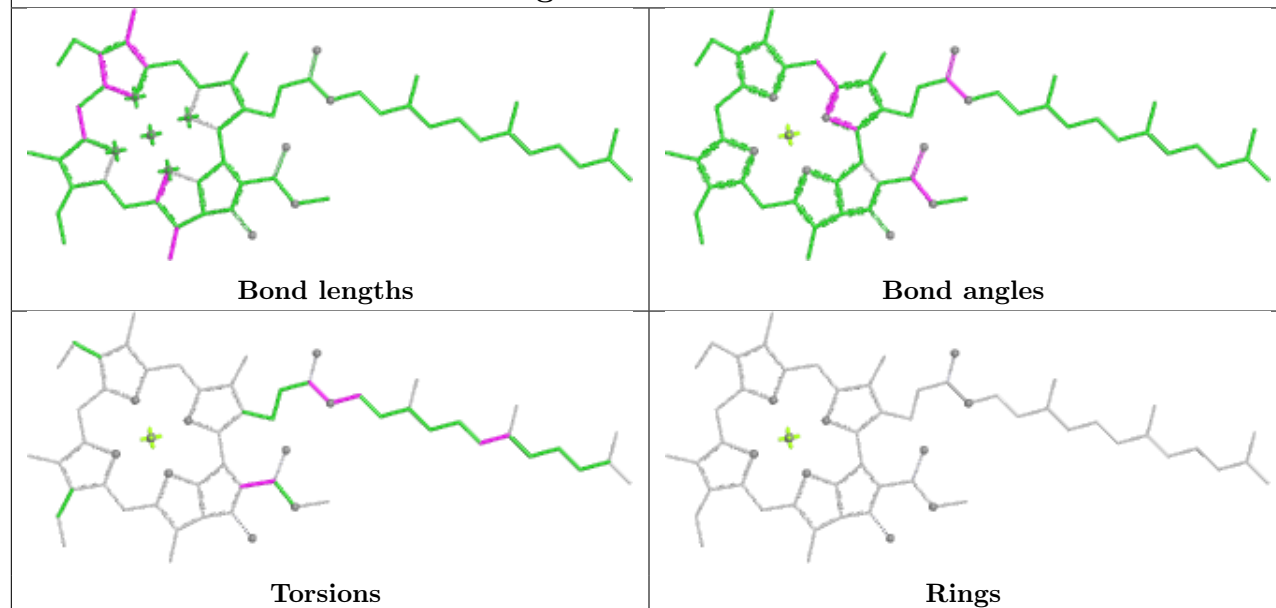


Ligand CLA 5 504

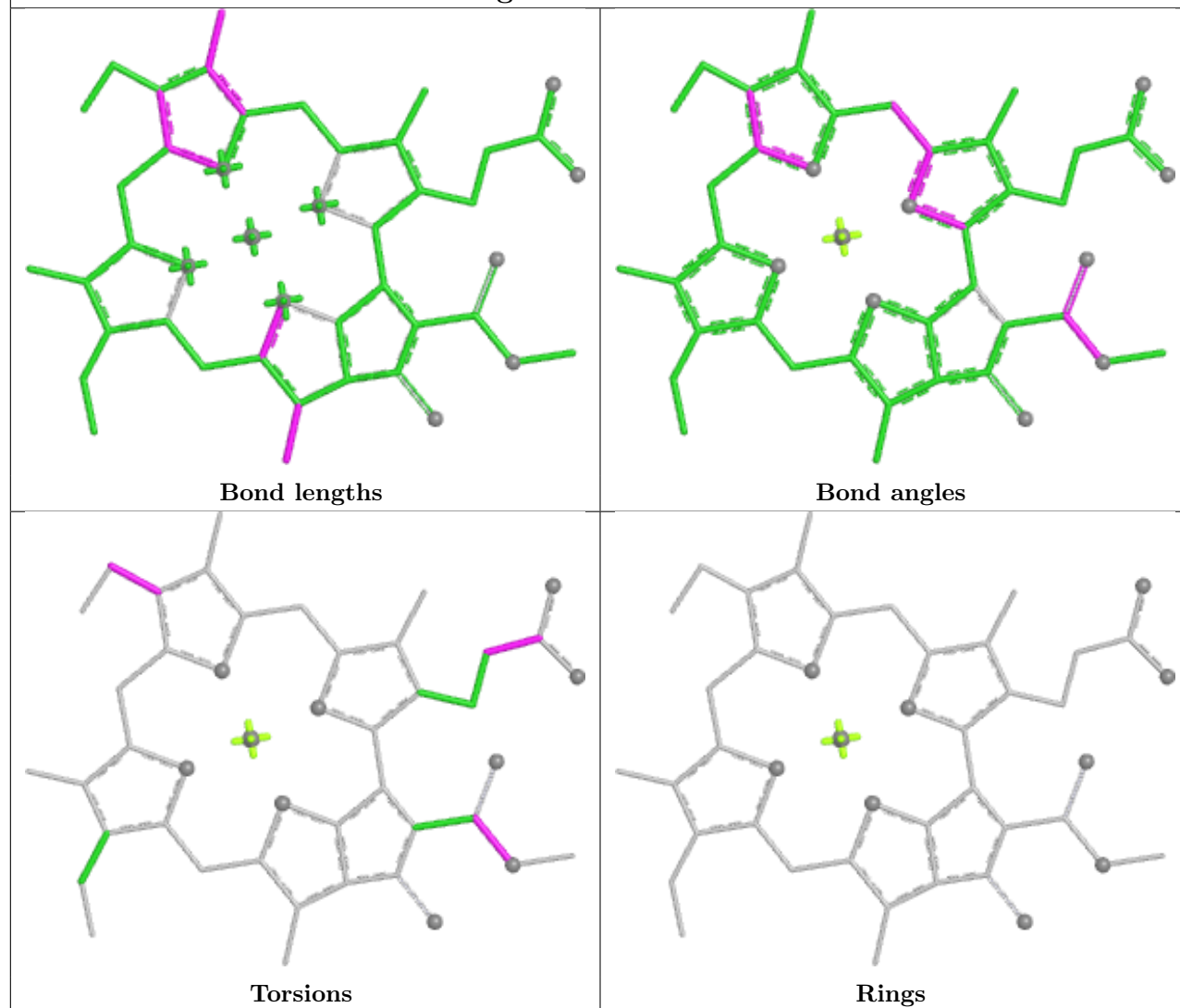


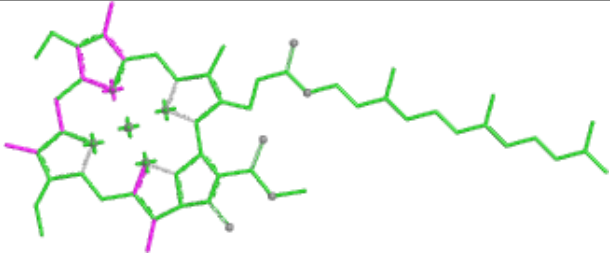
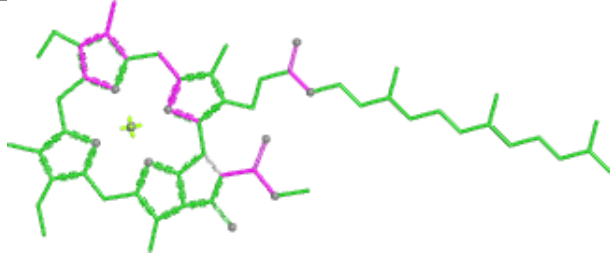
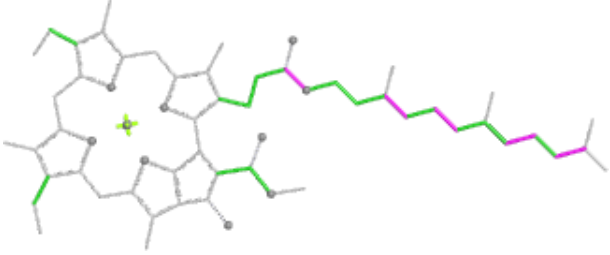
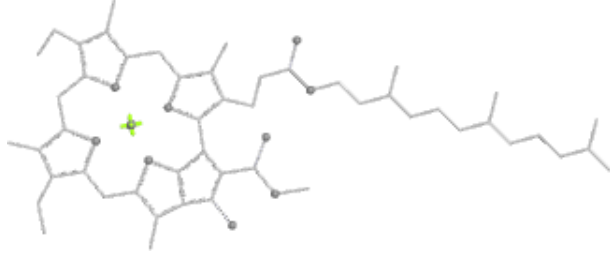
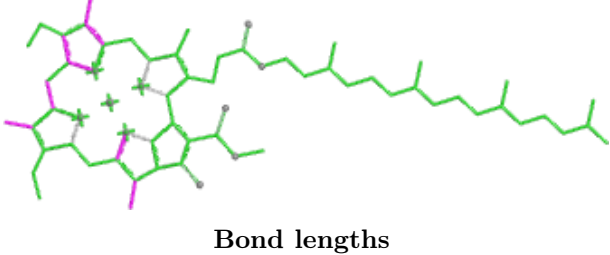
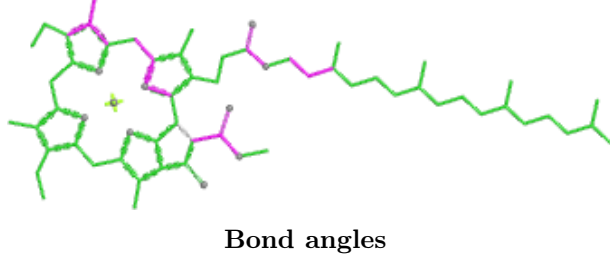
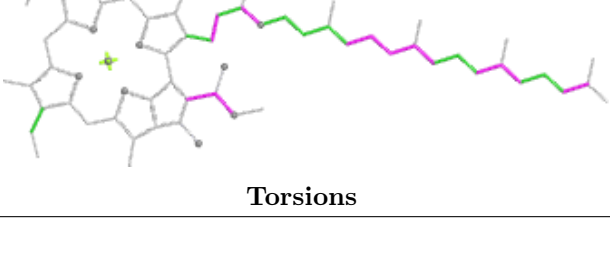
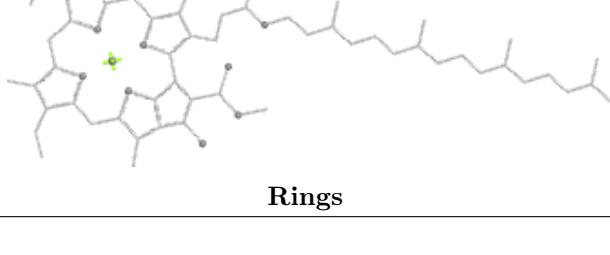


Ligand CLA a 507

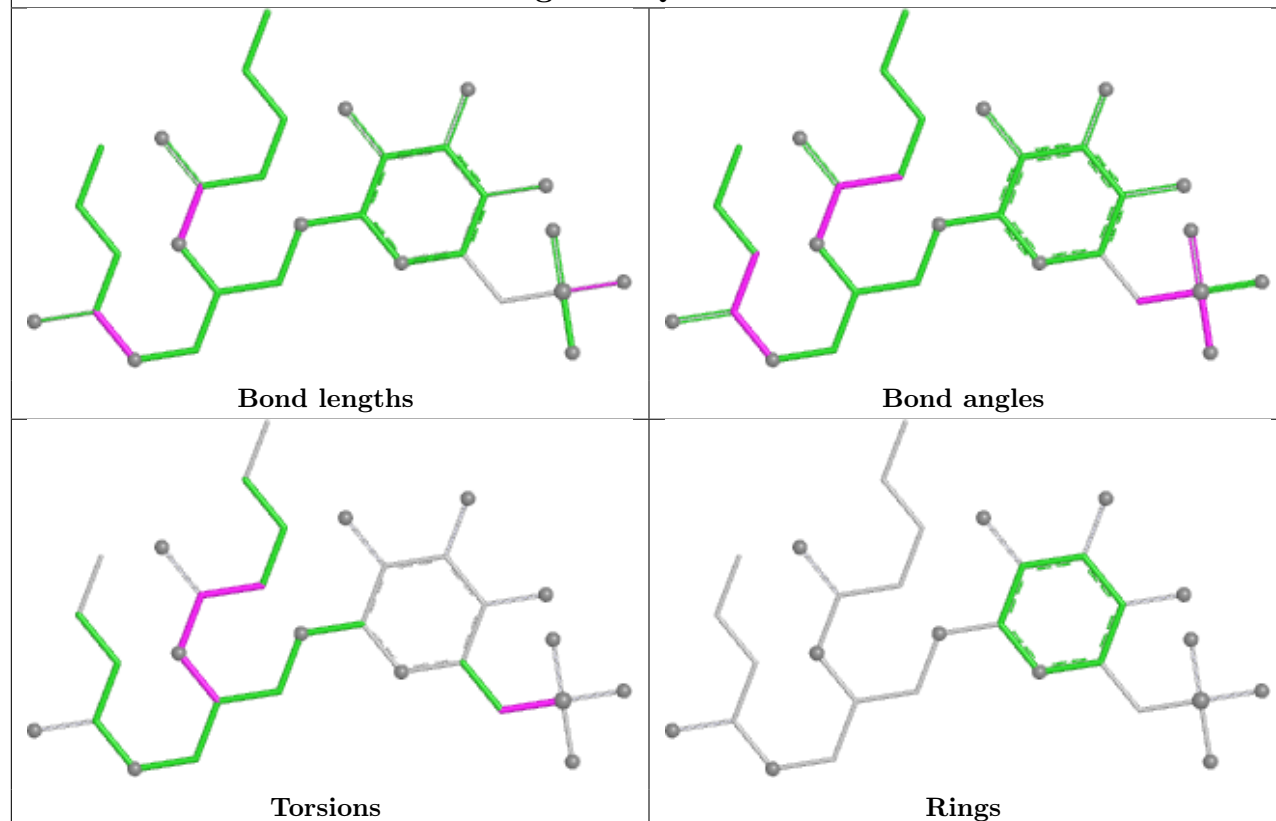


Ligand CLA c 516

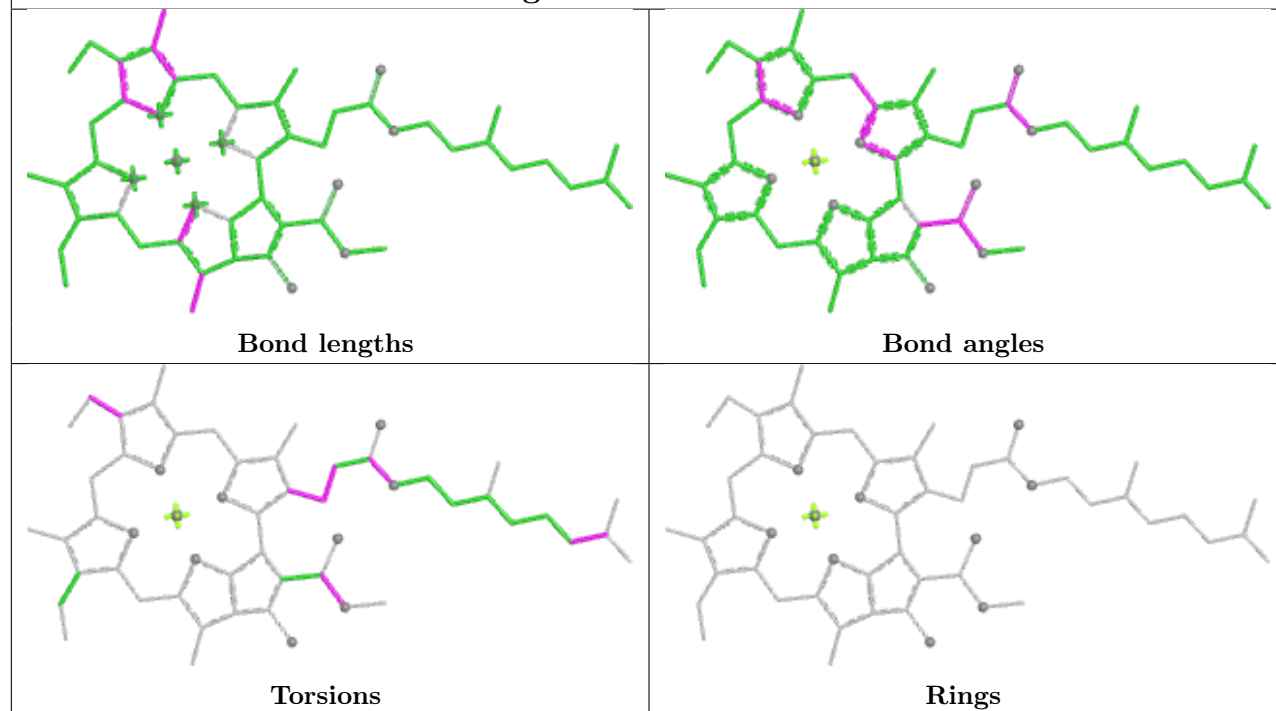


Ligand CLA B 1234	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 1012	
 Bond lengths	 Bond angles
 Torsions	 Rings

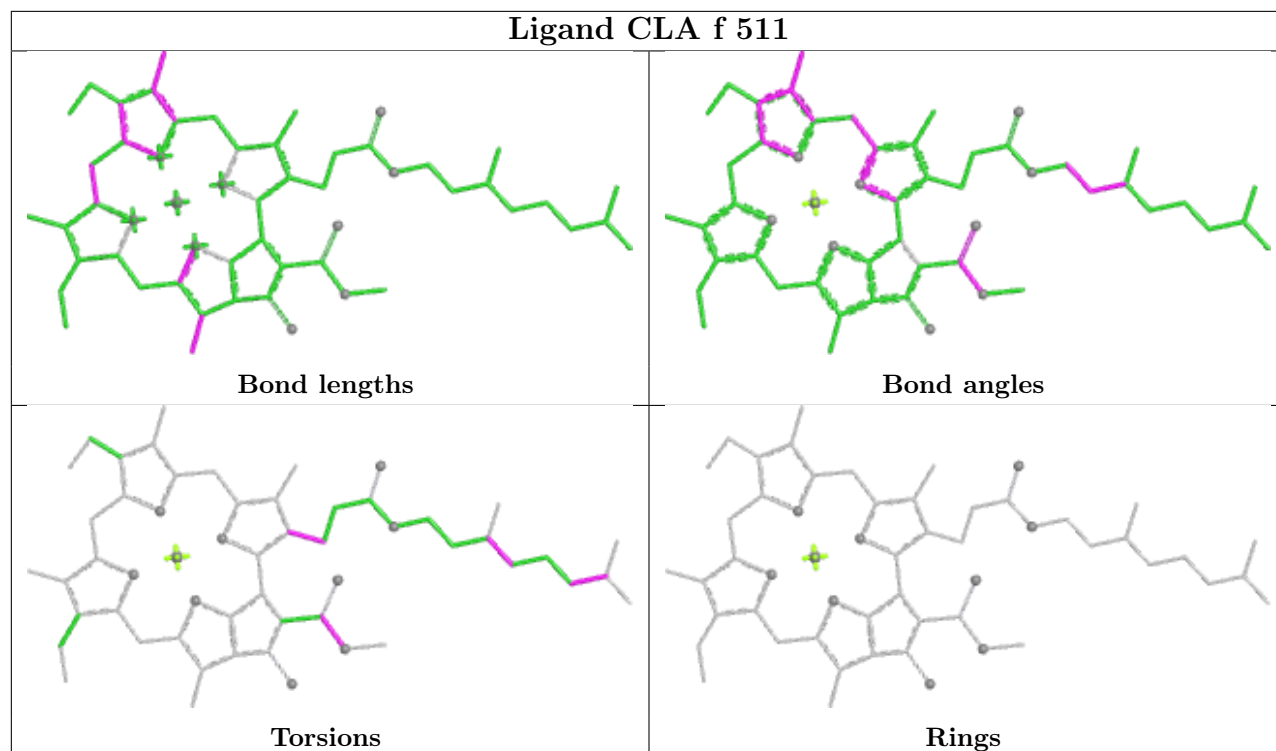
Ligand SQD d 822



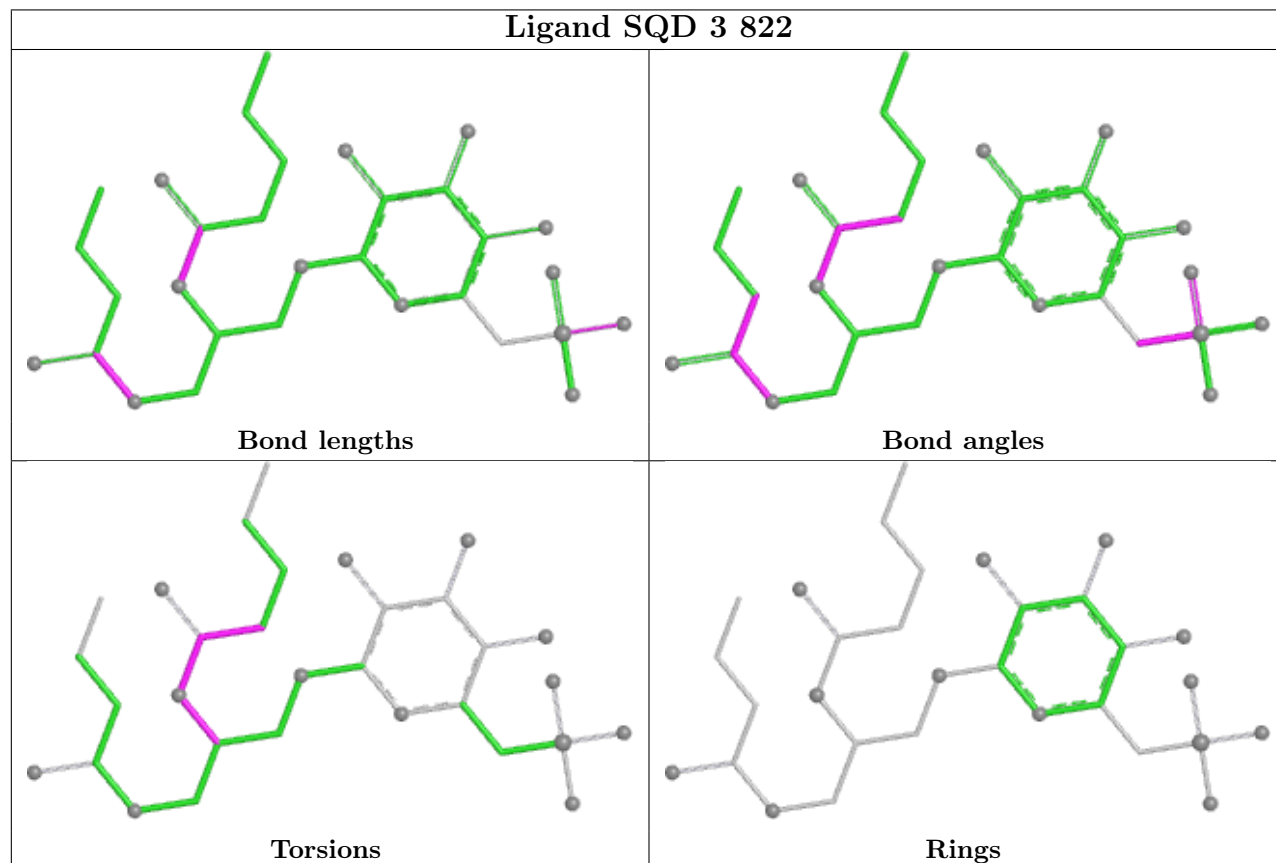
Ligand CLA A 1134



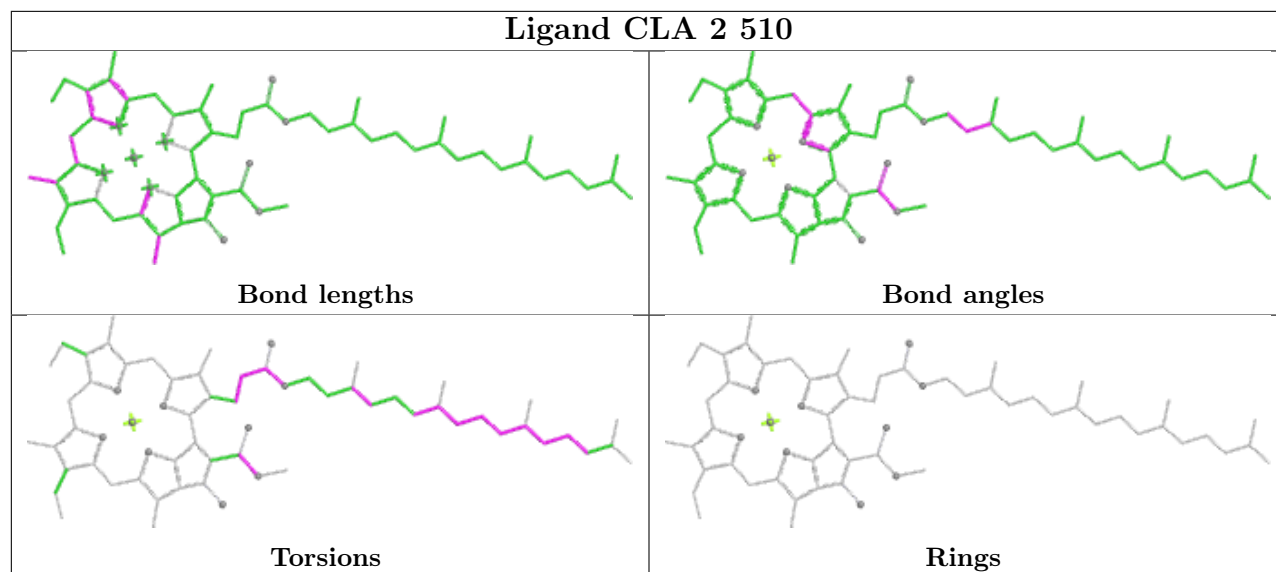
Ligand CLA f 511



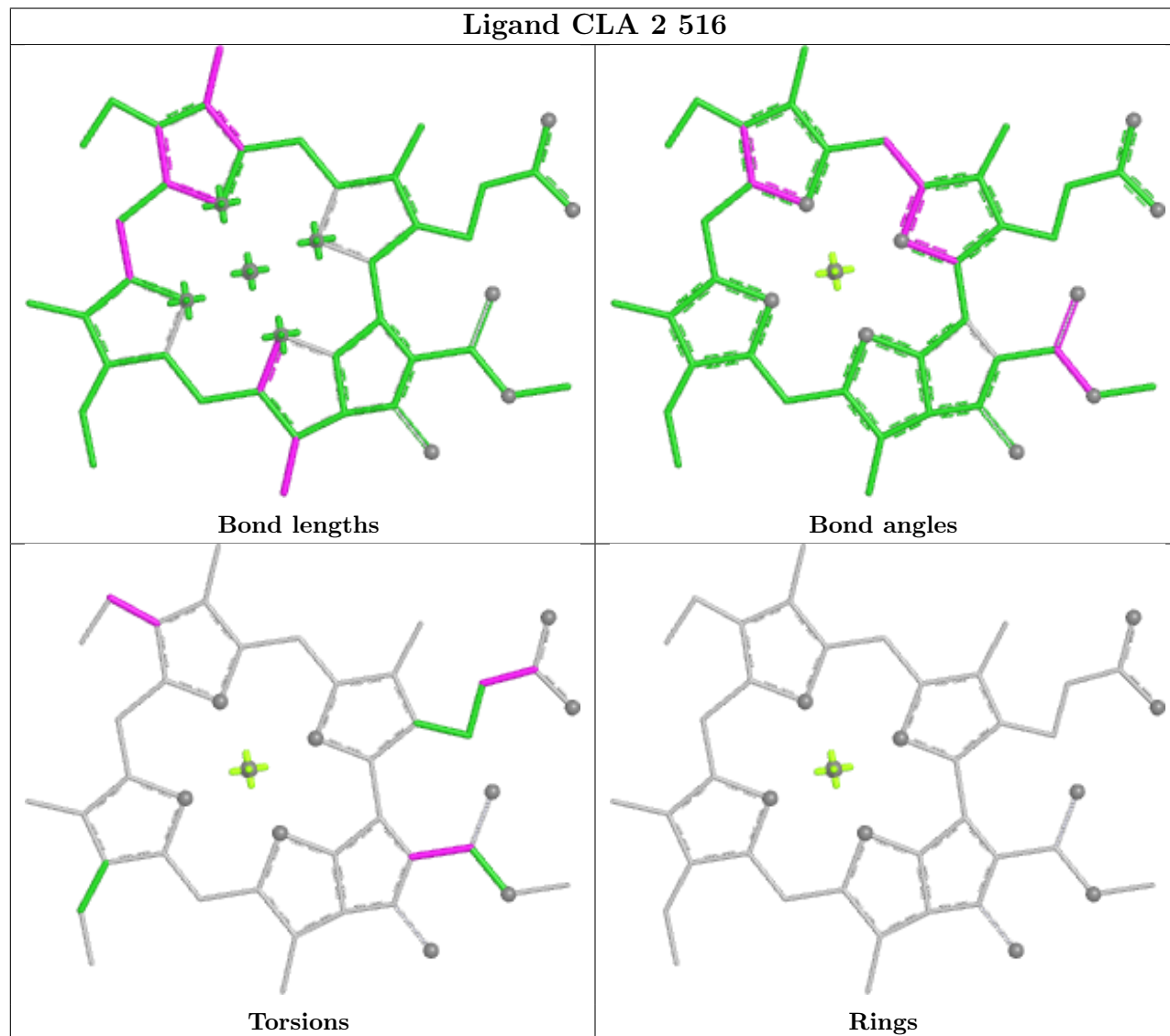
Ligand SQD 3 822



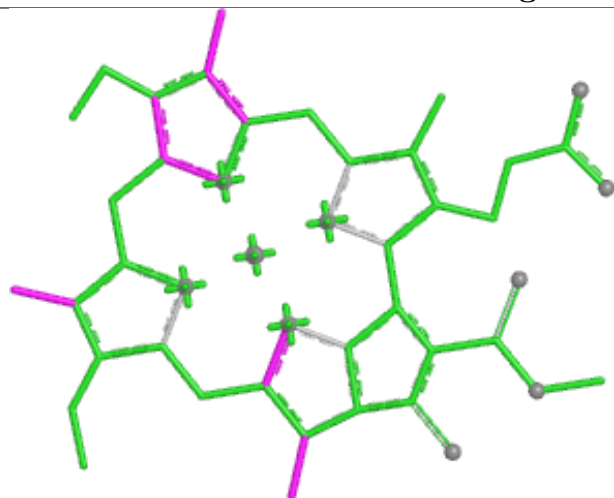
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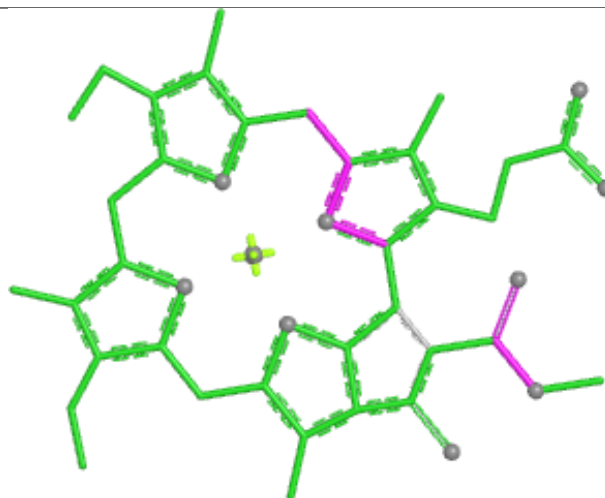
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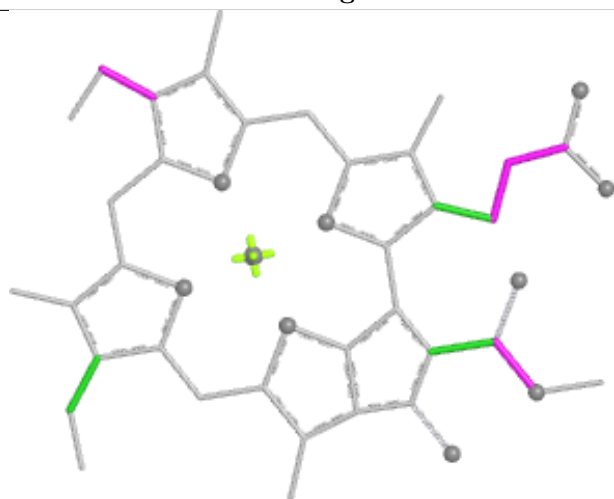
Ligand CLA e 517



Bond lengths



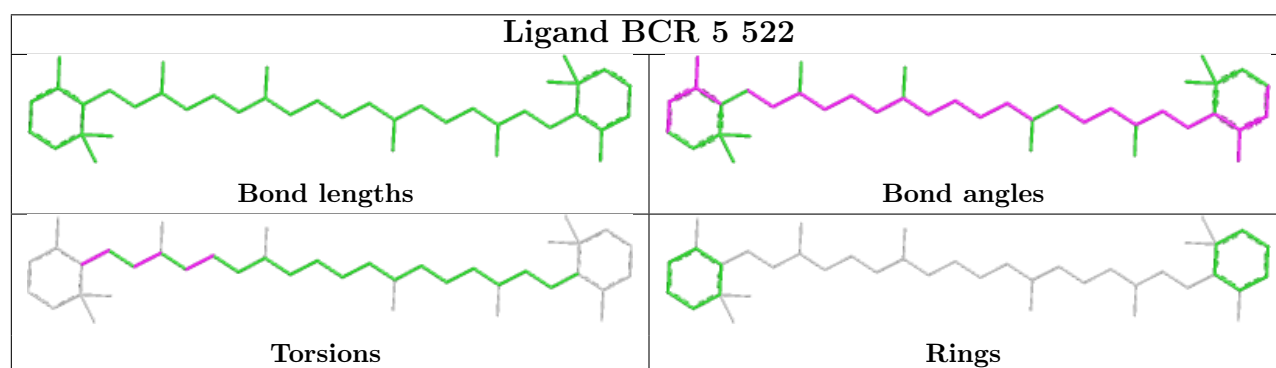
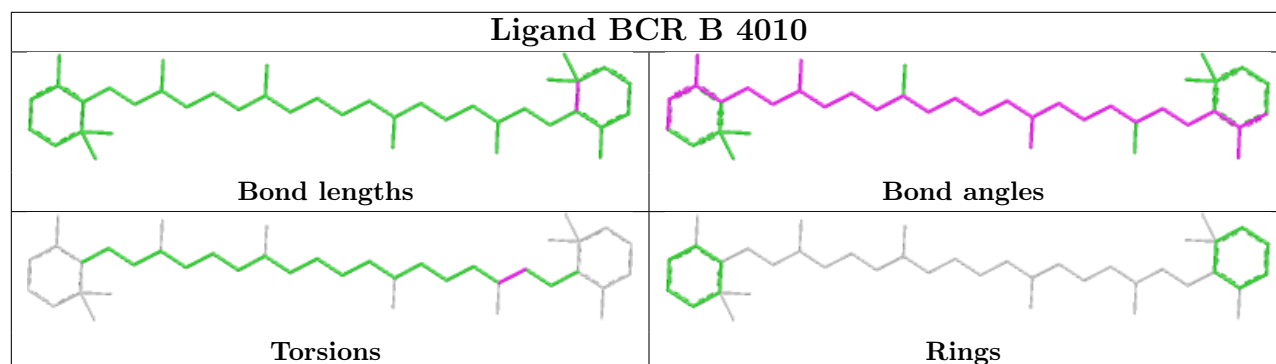
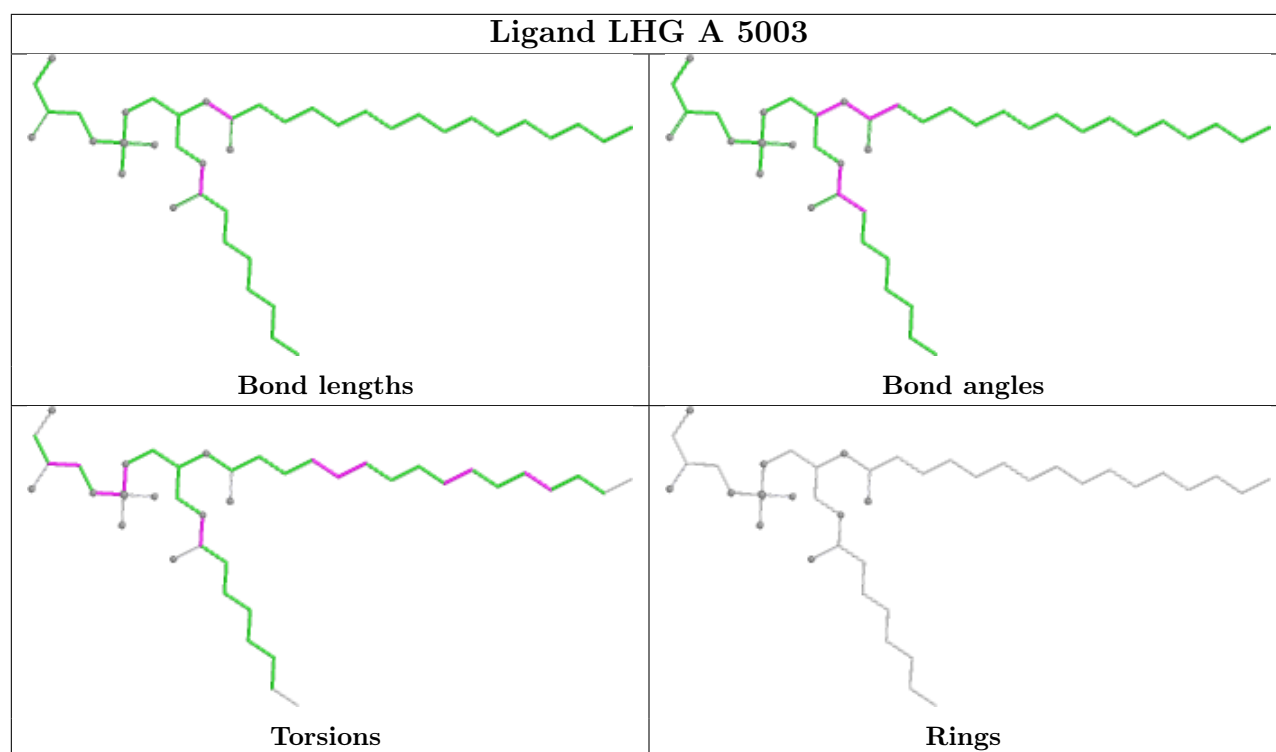
Bond angles

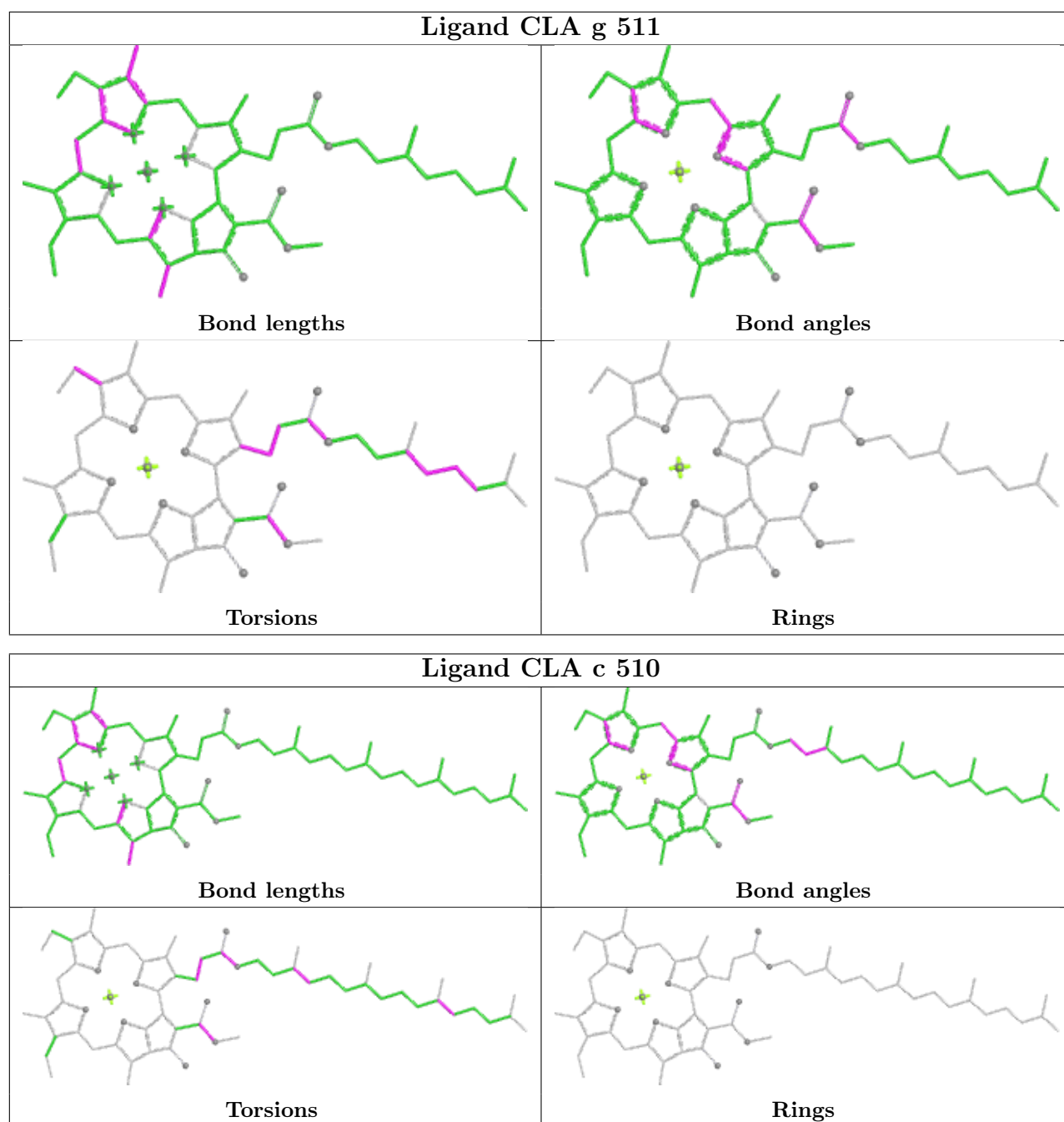


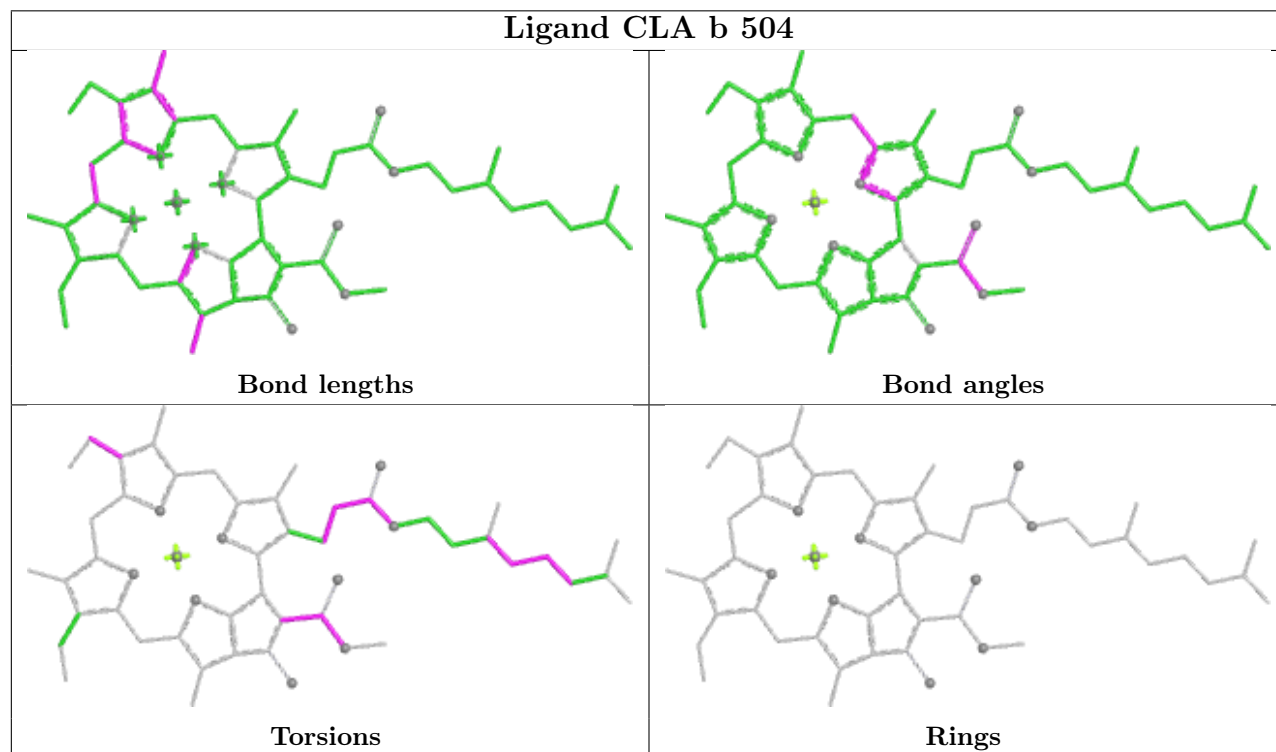
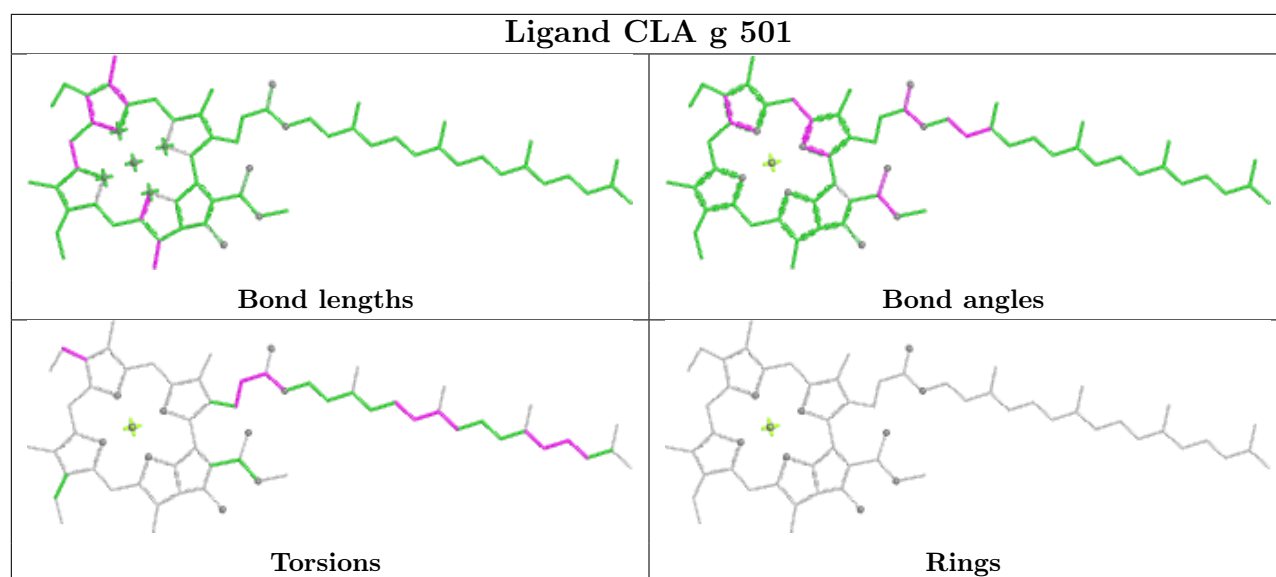
Torsions



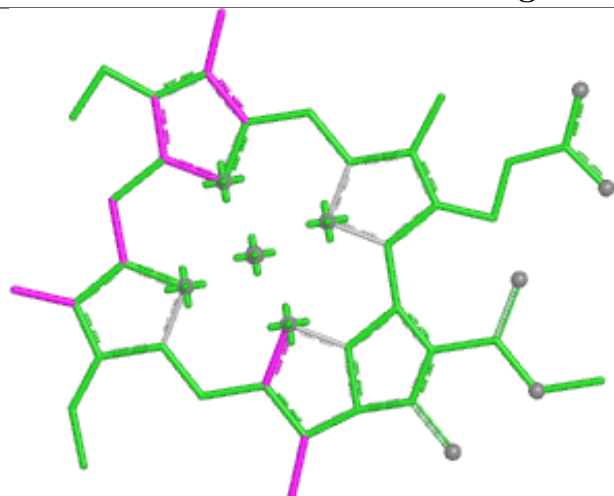
Rings



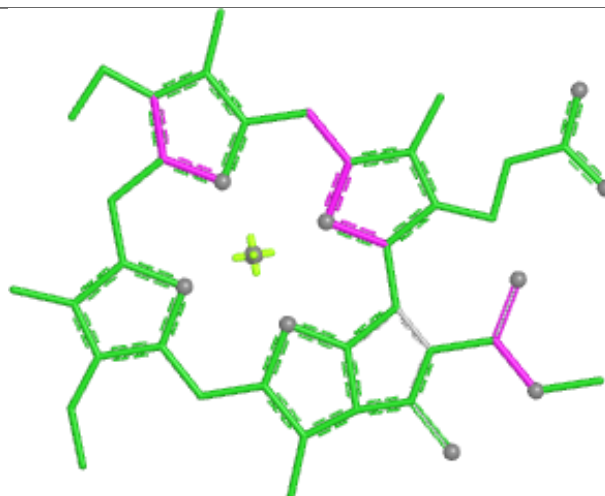




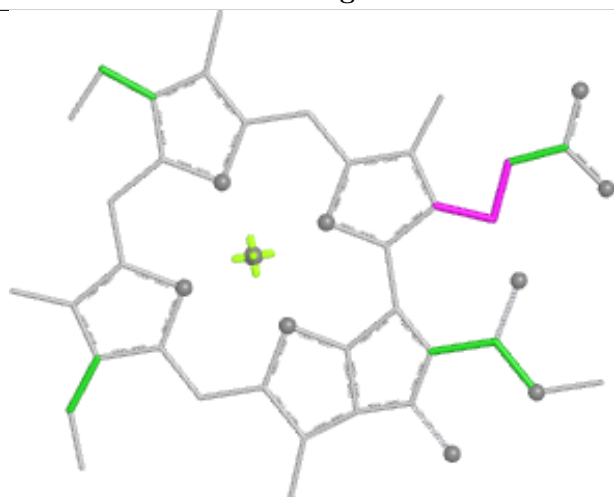
Ligand CLA 4 512



Bond lengths



Bond angles

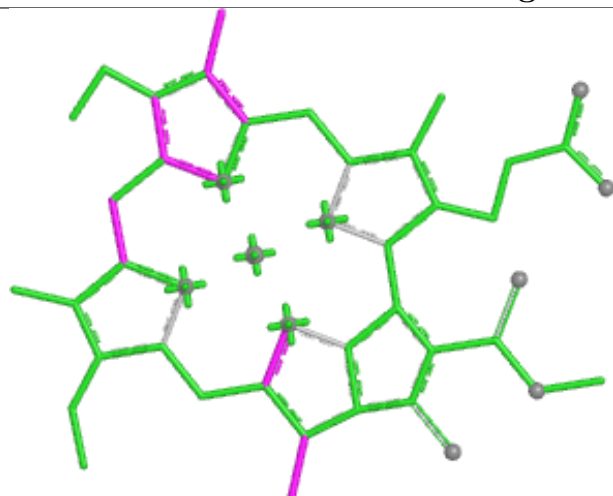


Torsions

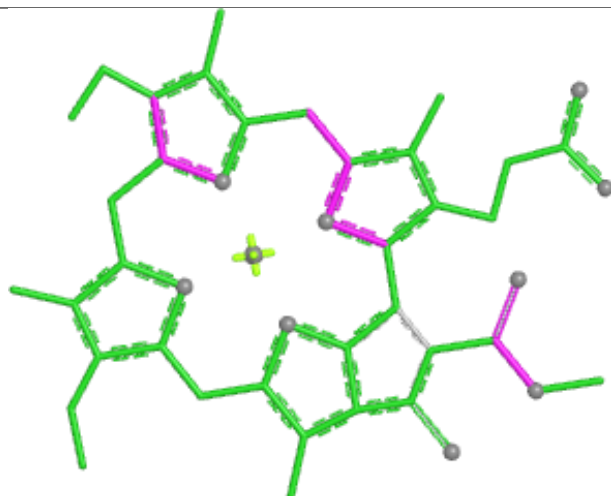


Rings

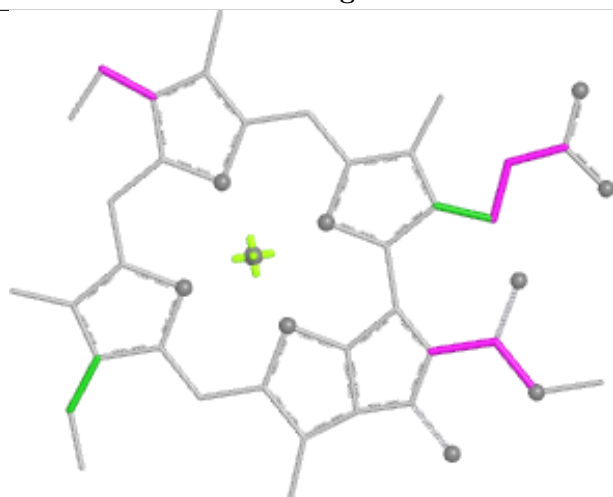
Ligand CLA 6 512



Bond lengths



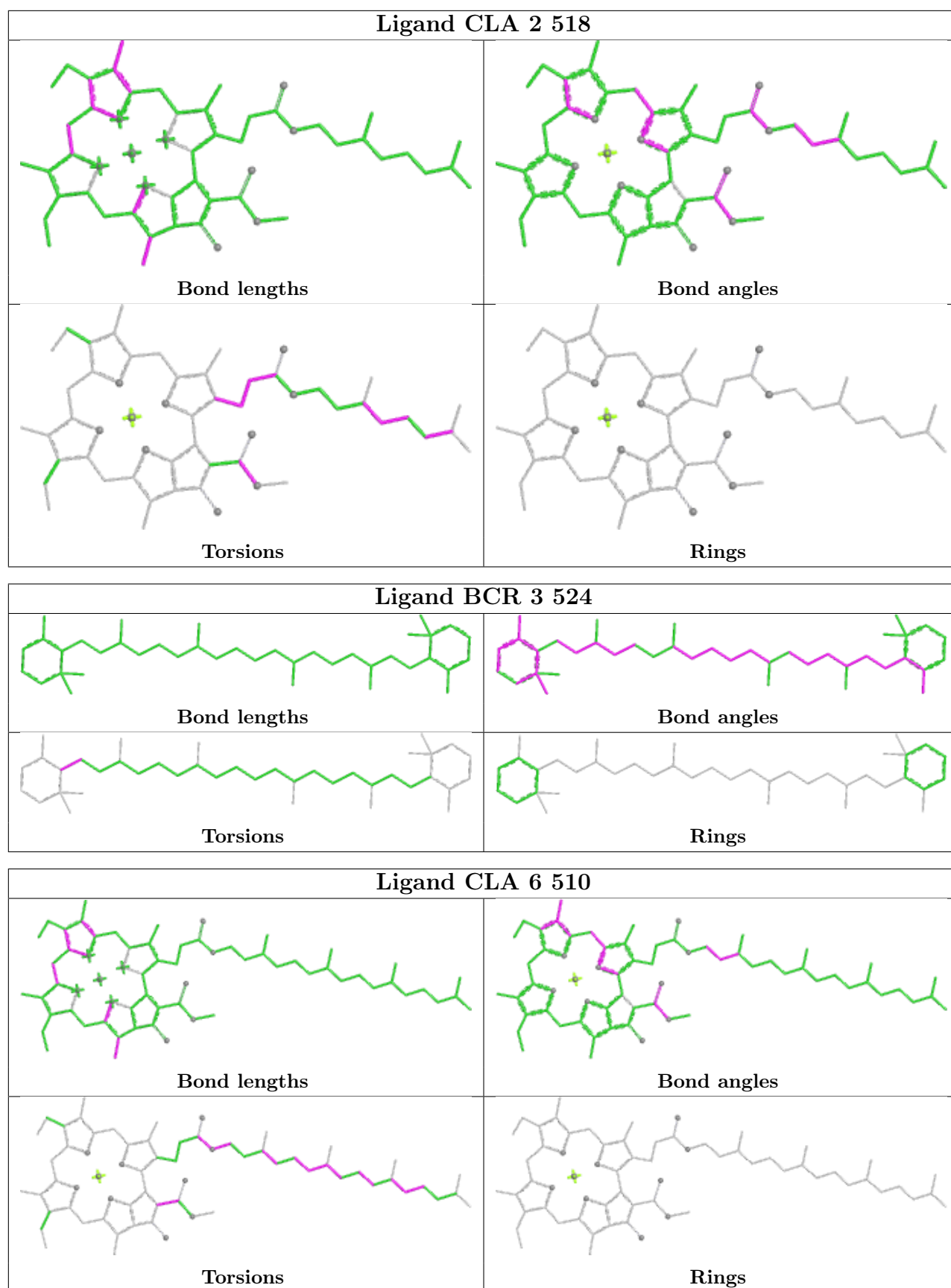
Bond angles

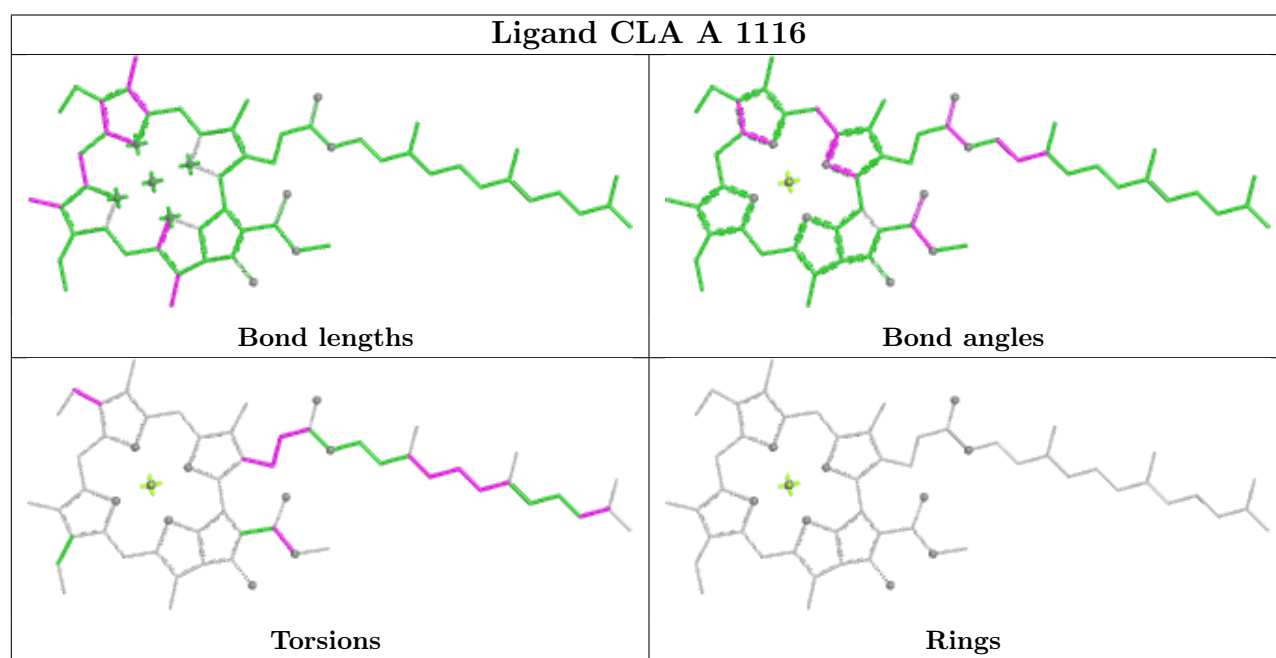
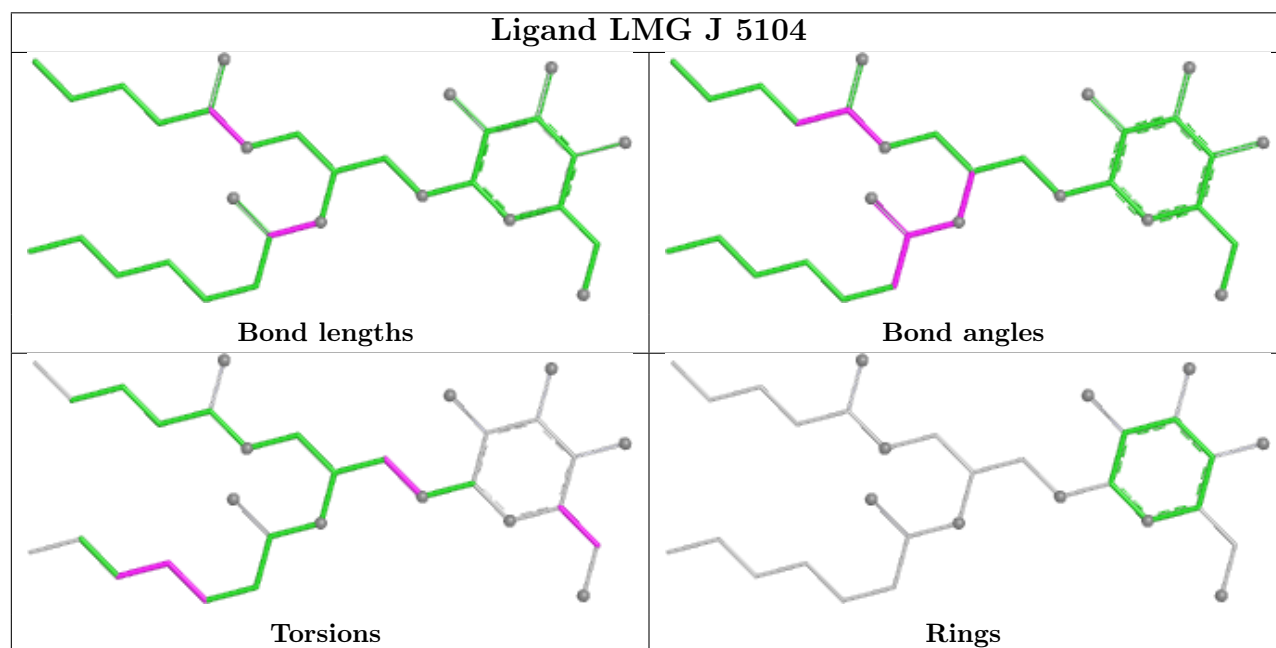
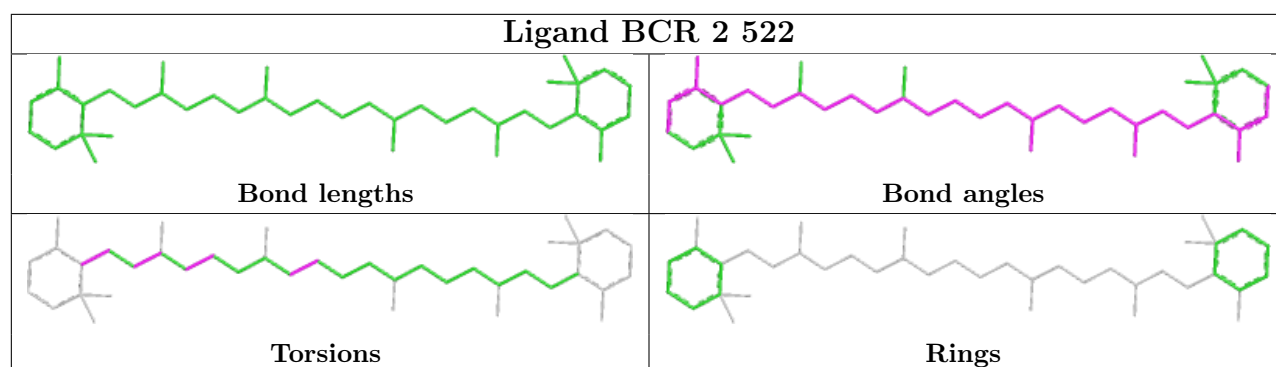


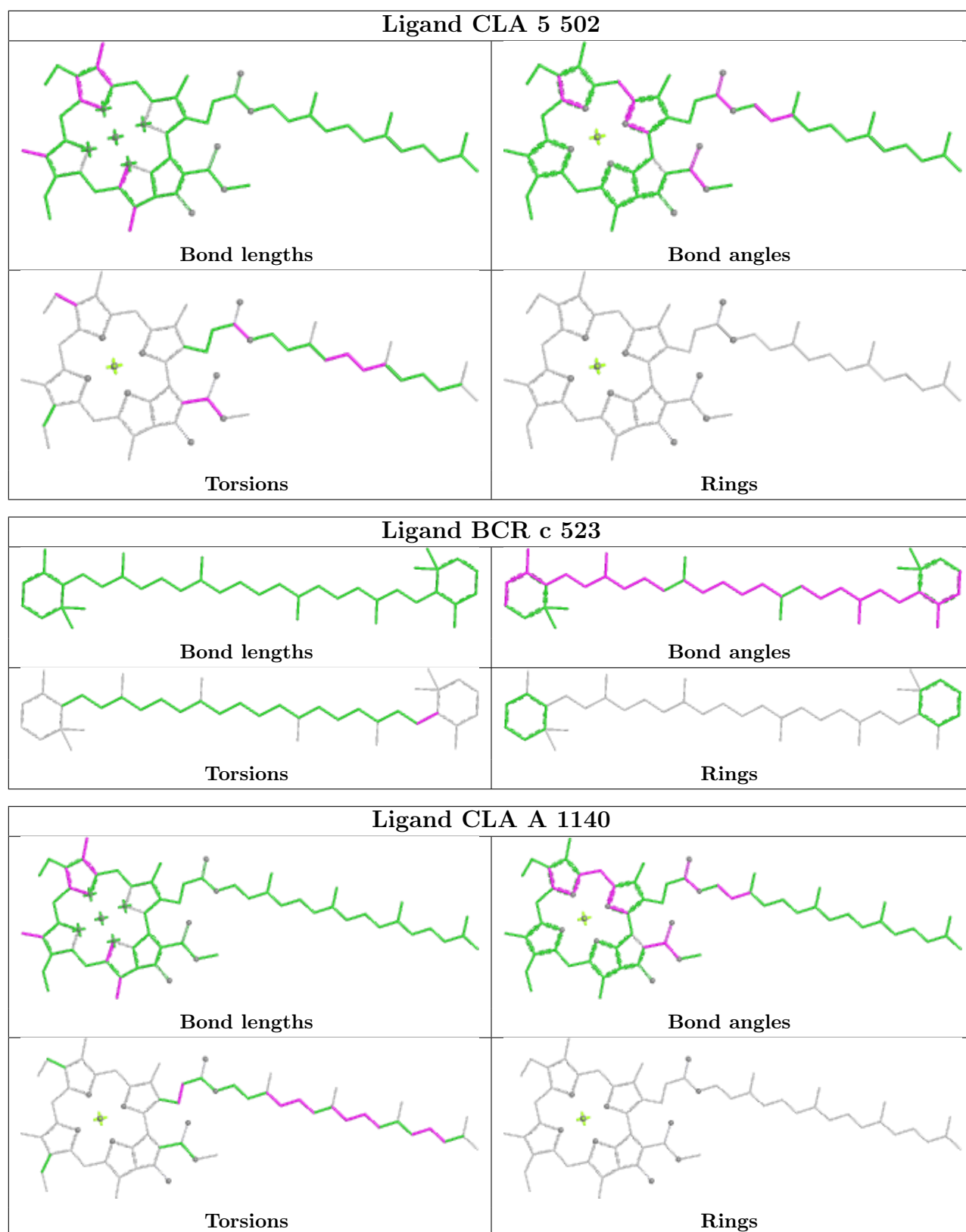
Torsions



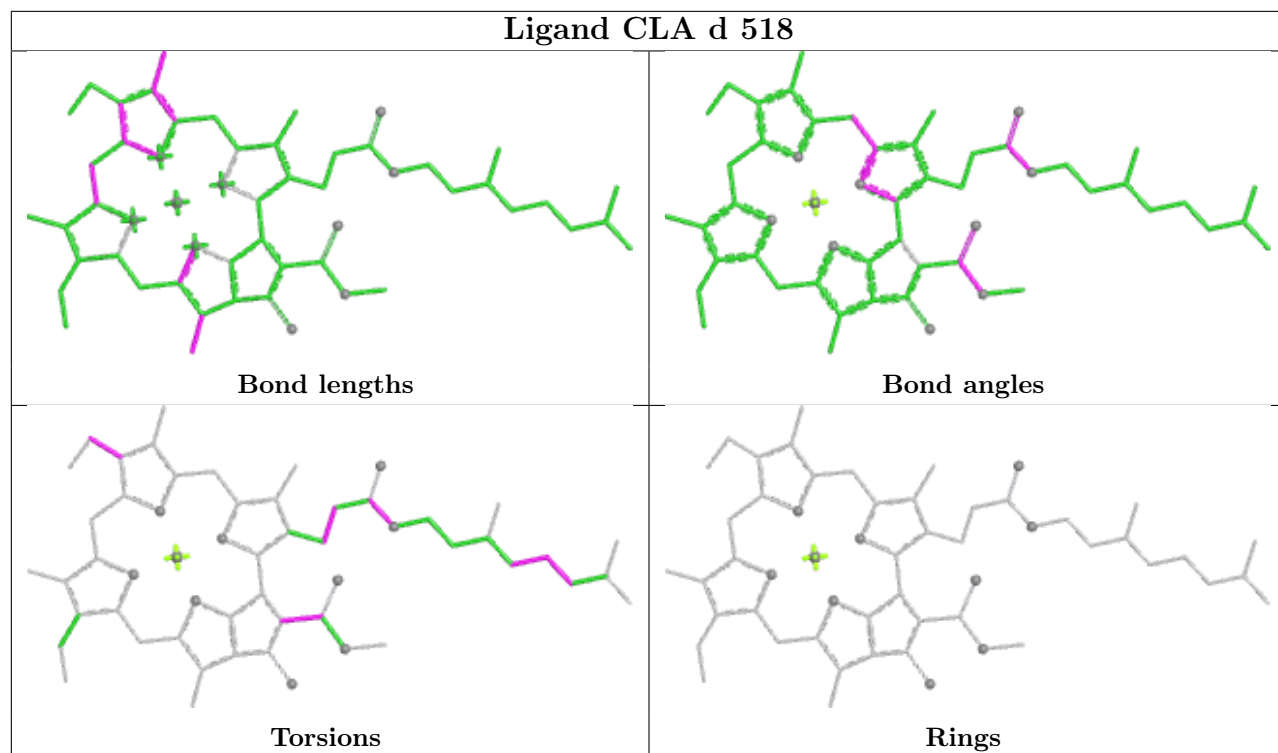
Rings



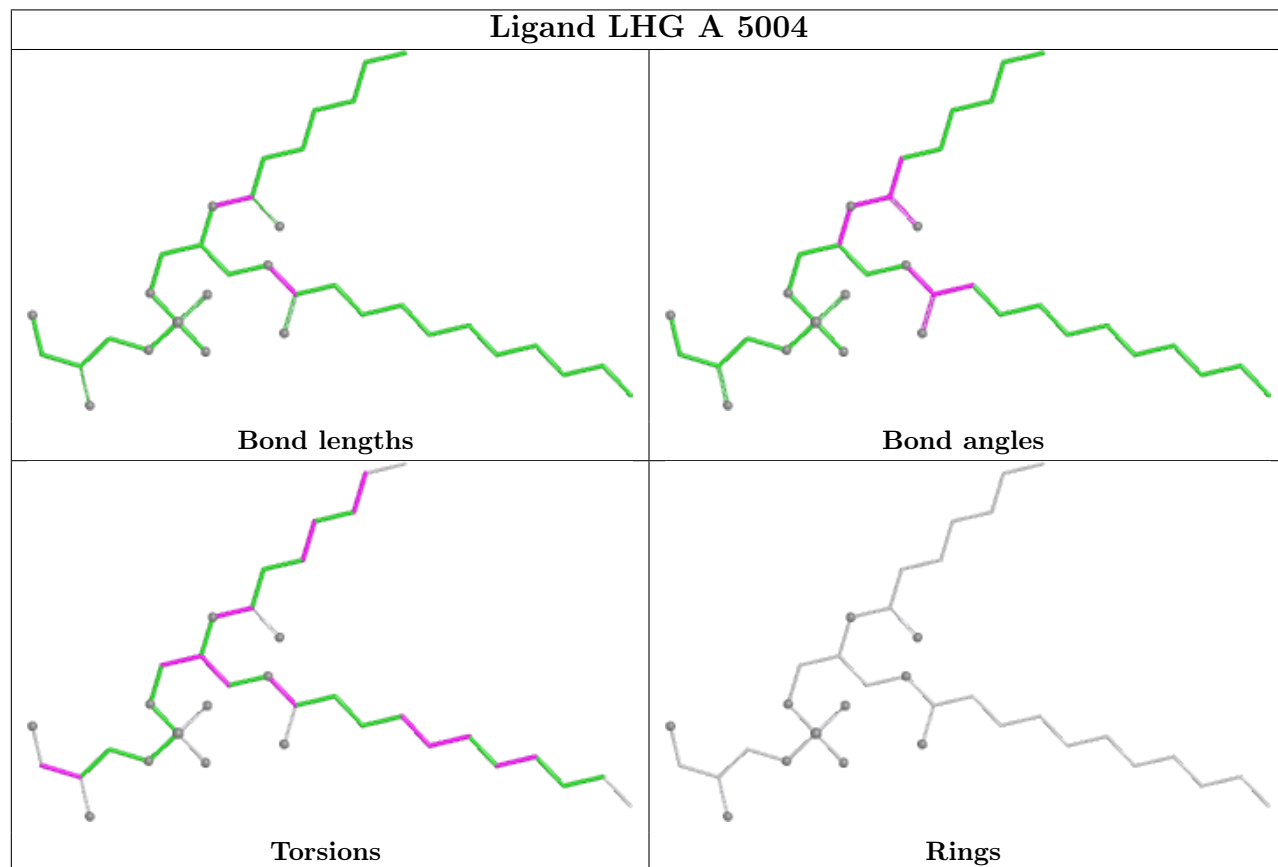


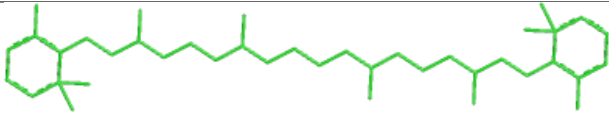
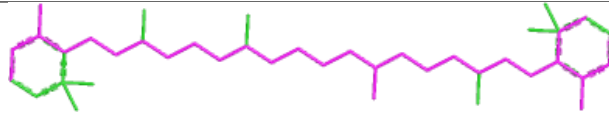
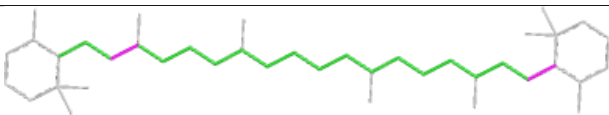
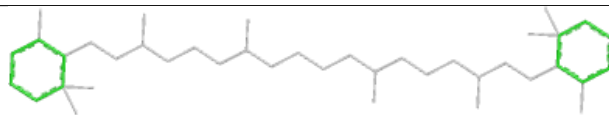


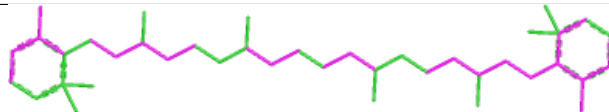
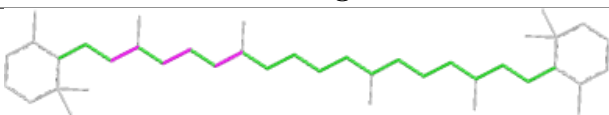
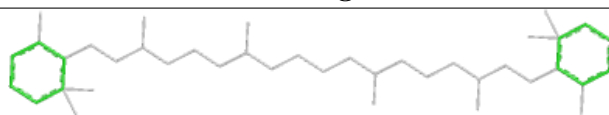
Ligand CLA d 518

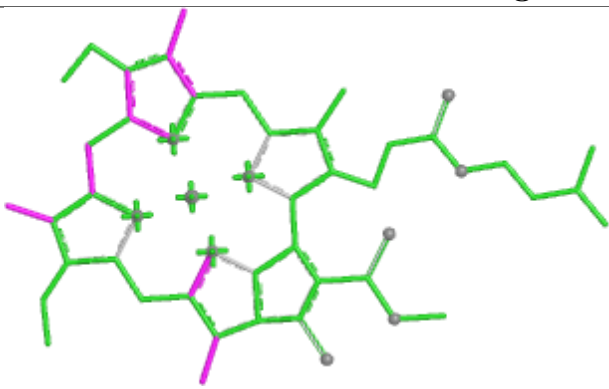
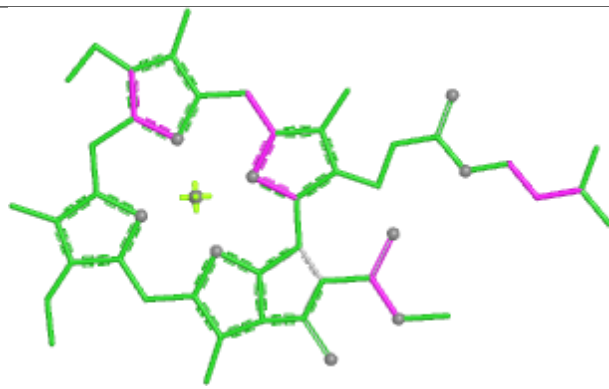
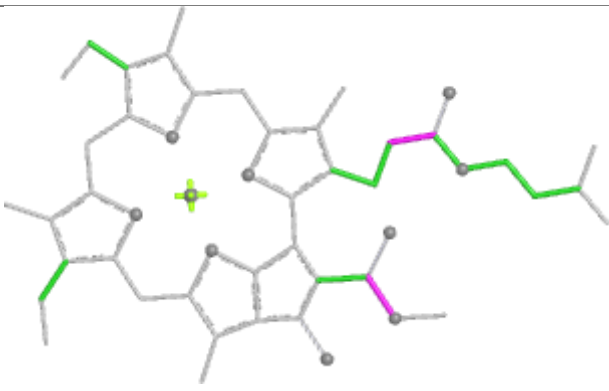
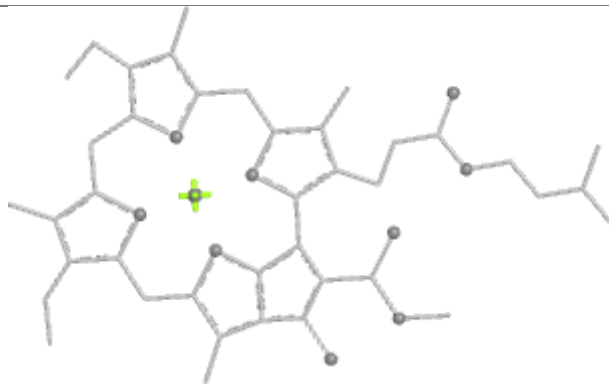


Ligand LHG A 5004

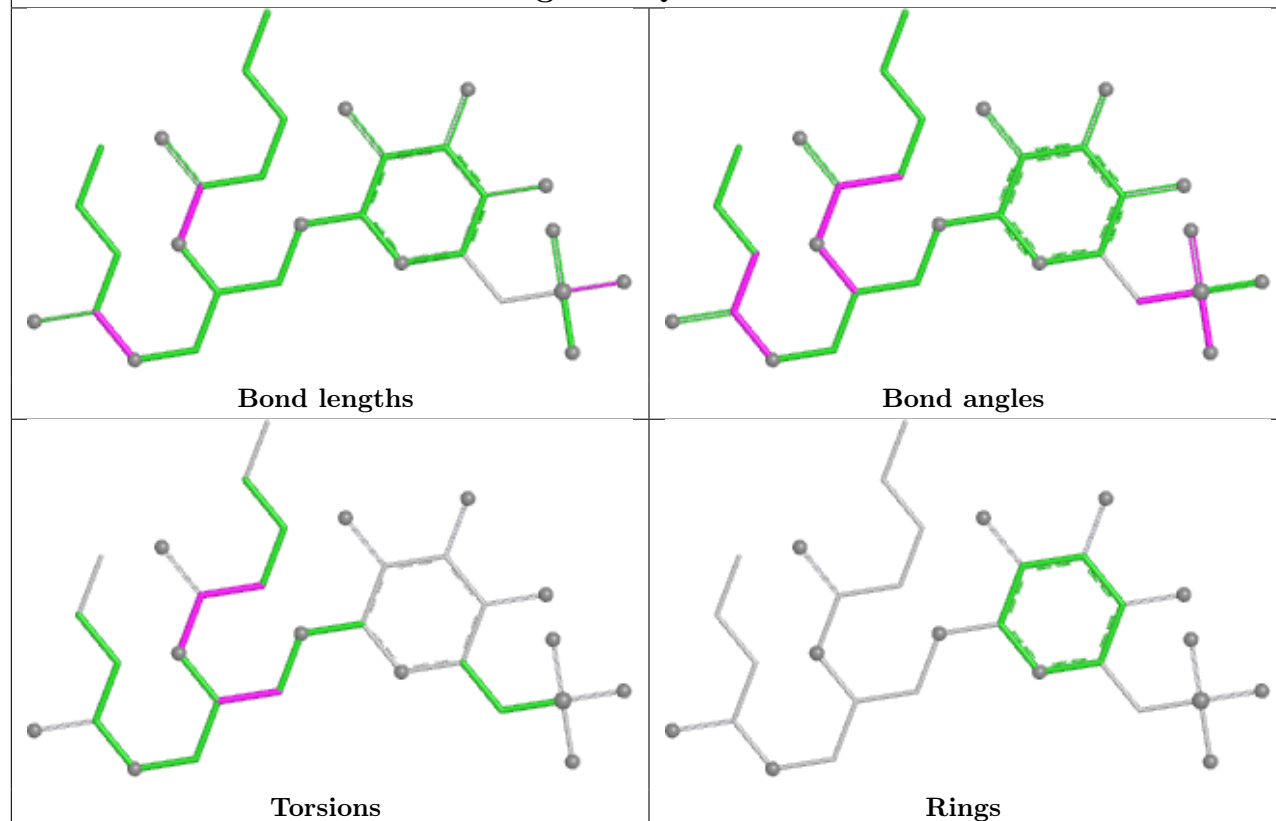


Ligand BCR d 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

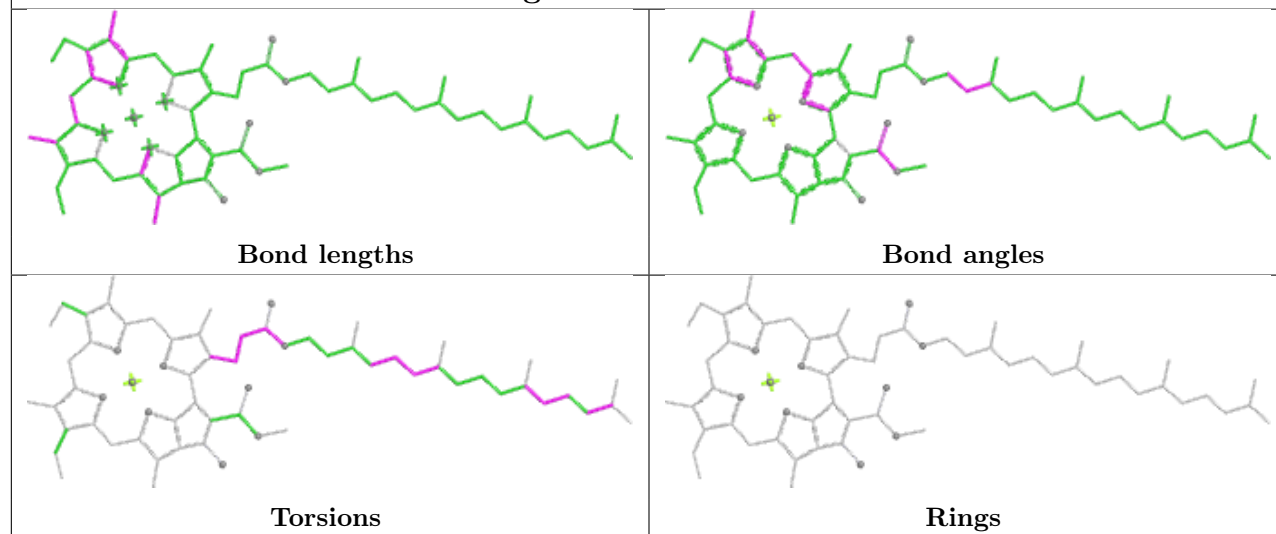
Ligand BCR e 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

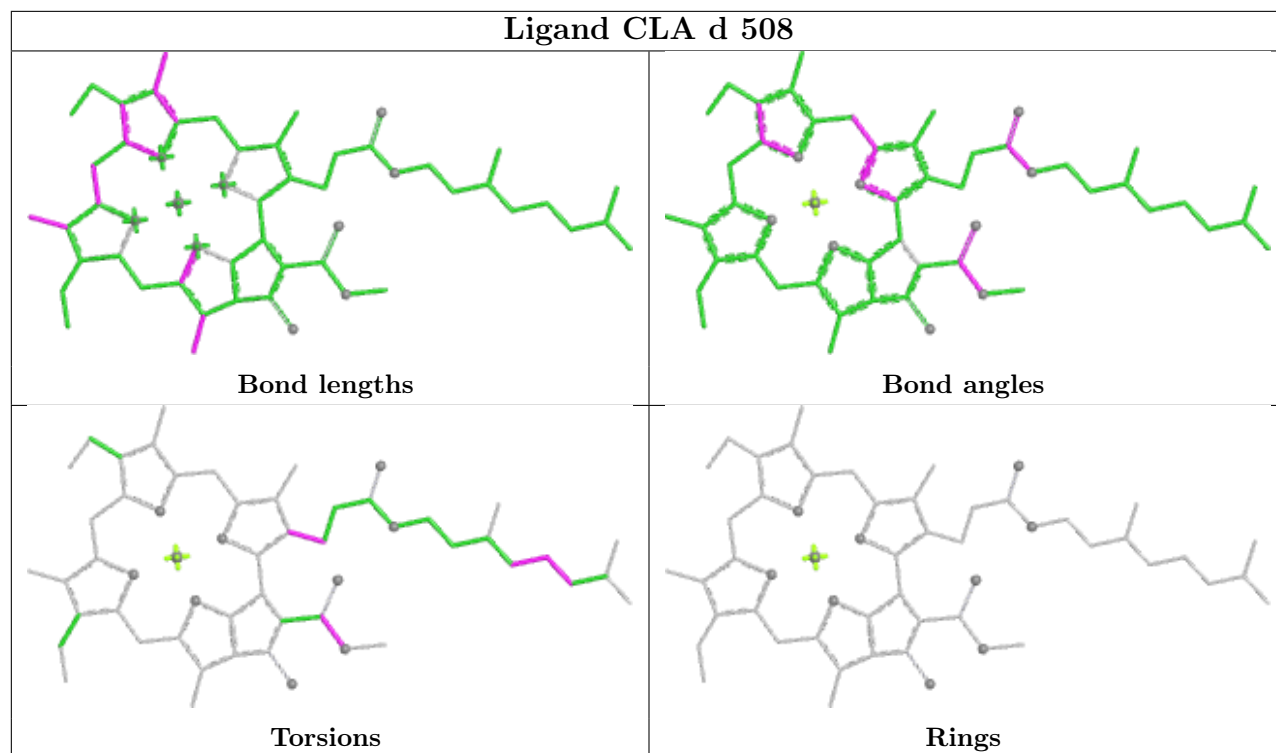
Ligand SQD 2 822



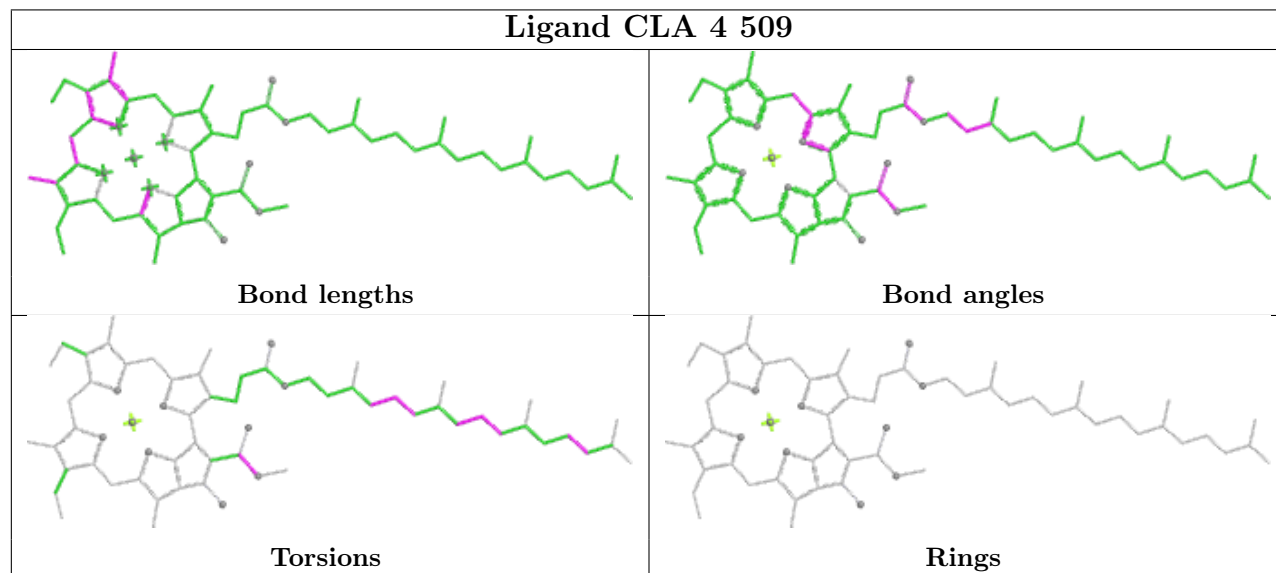
Ligand CLA B 1213



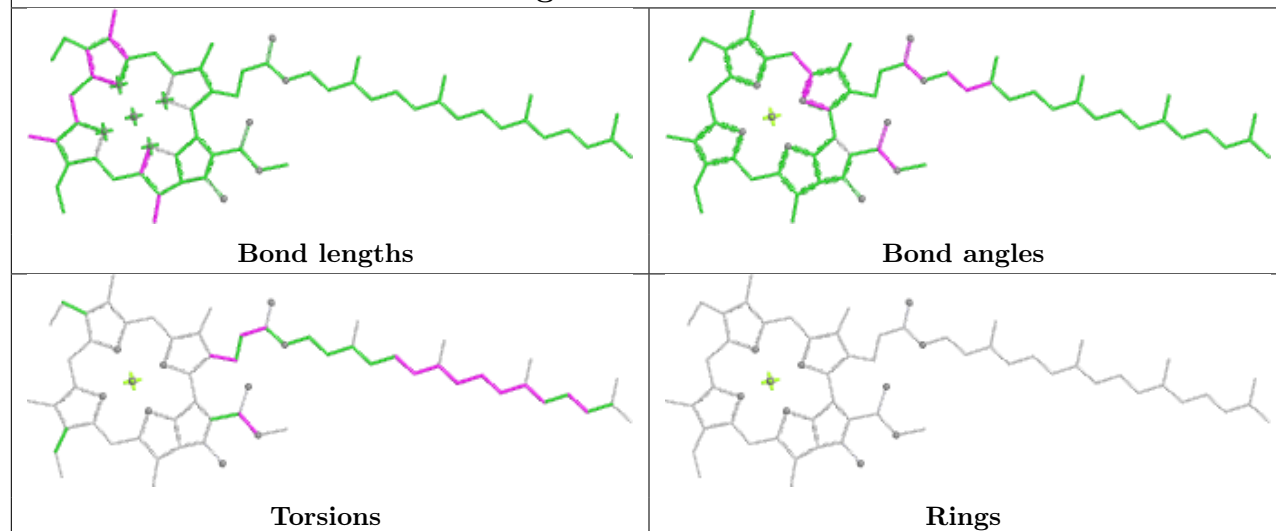
Ligand CLA d 508



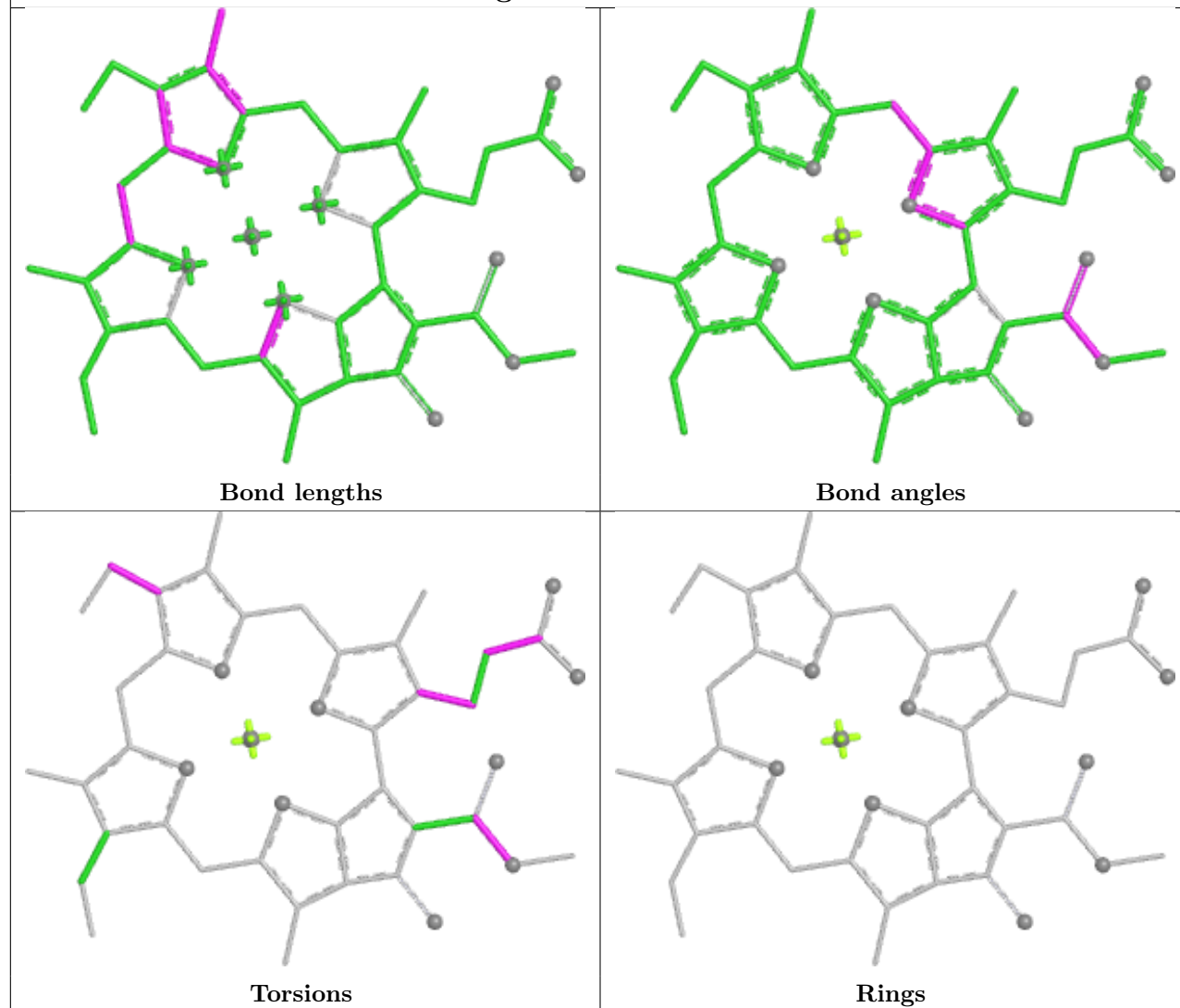
Ligand CLA 4 509

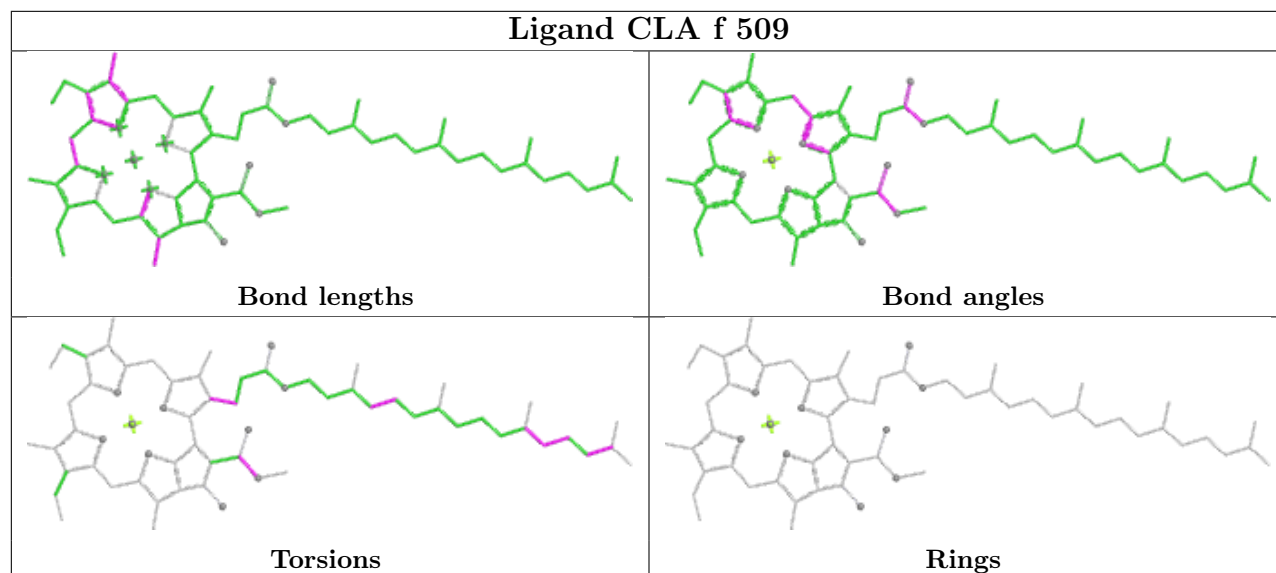
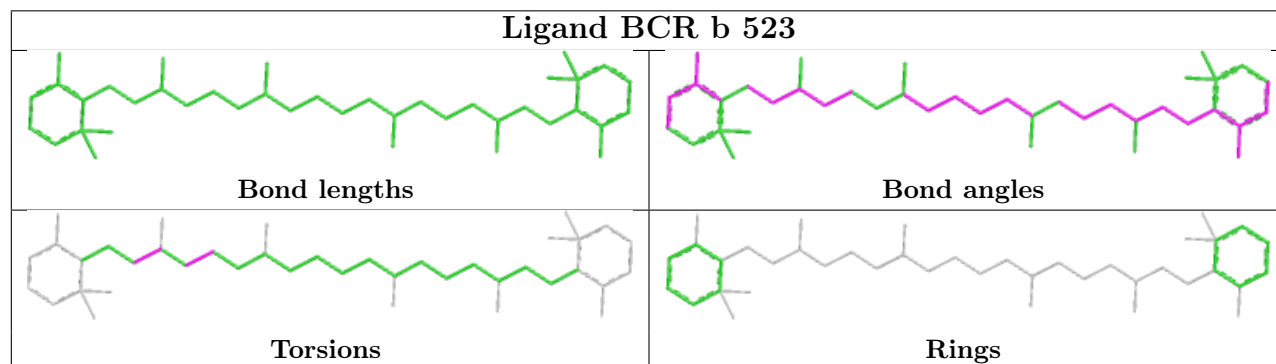
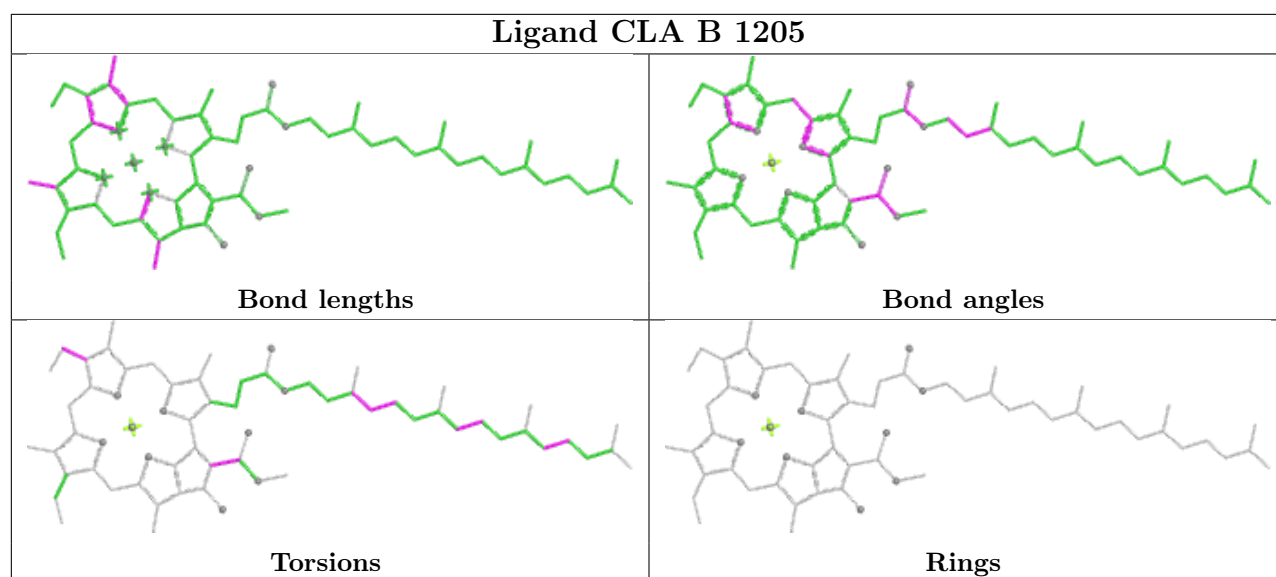


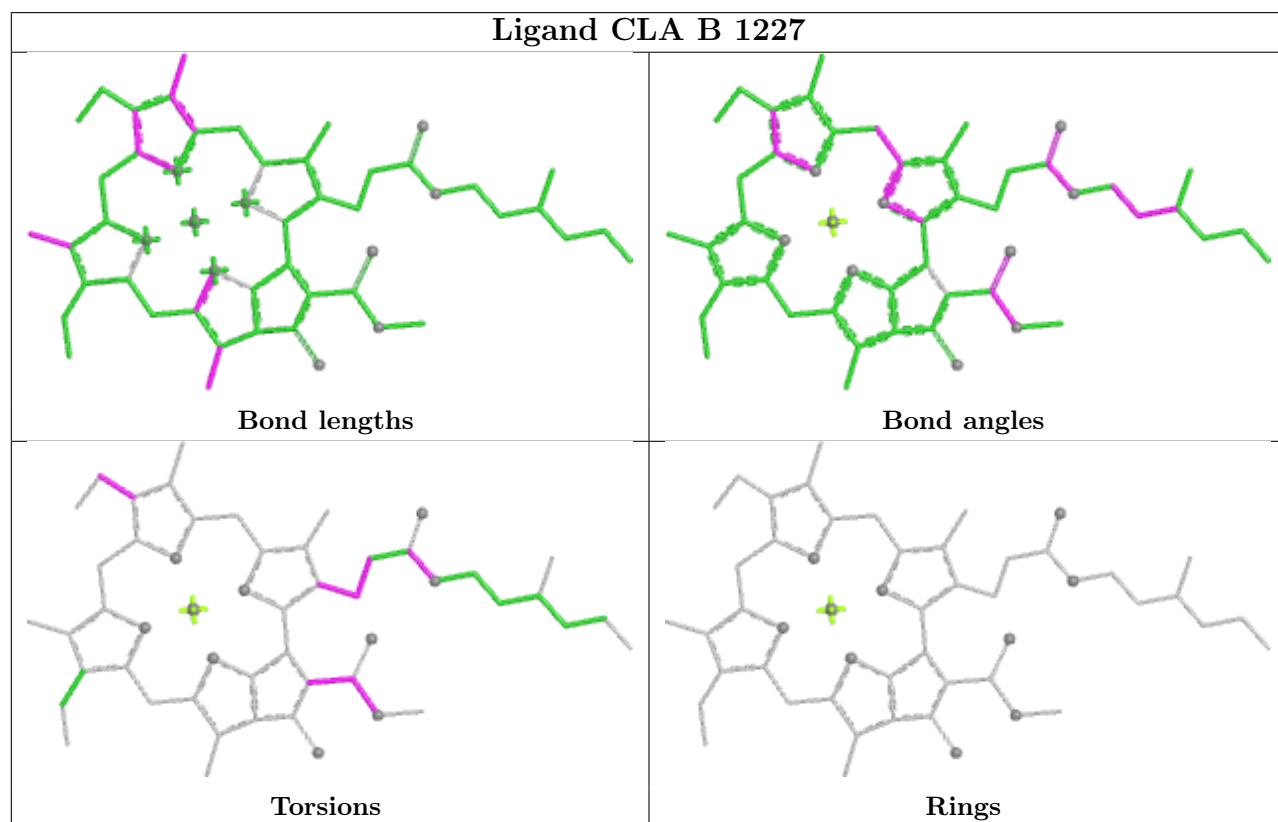
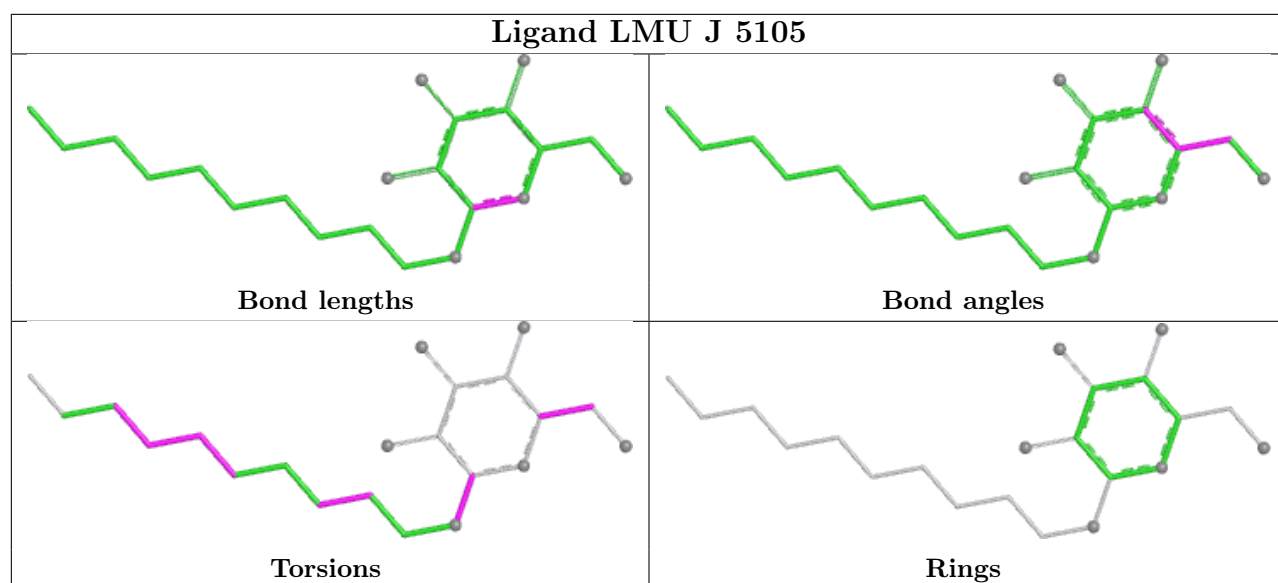
Ligand CLA 6 509



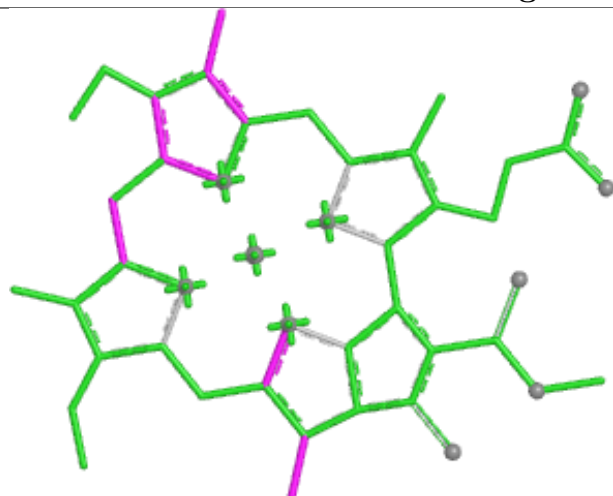
Ligand CLA 1 517



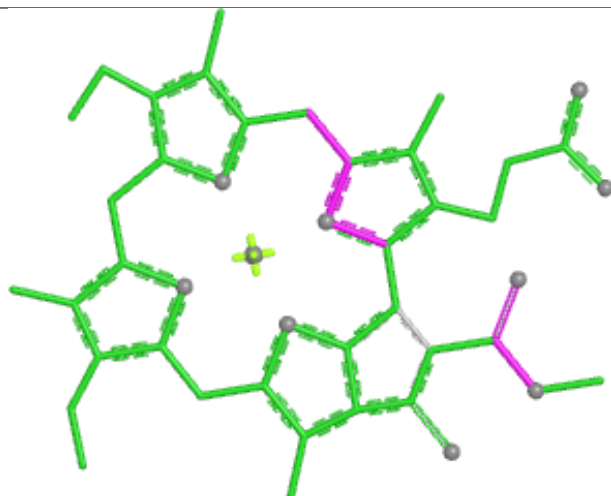




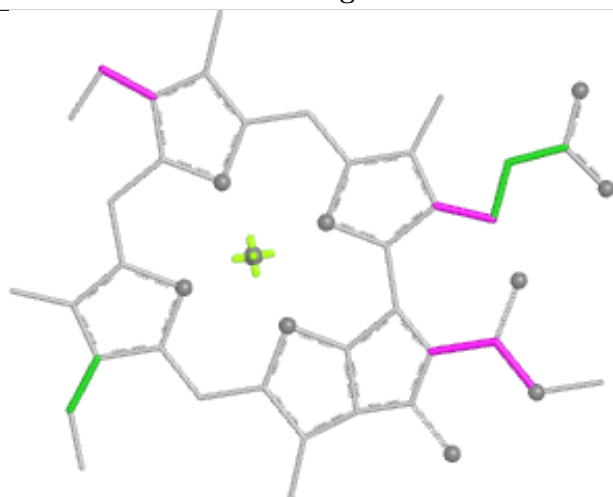
Ligand CLA e 519



Bond lengths



Bond angles

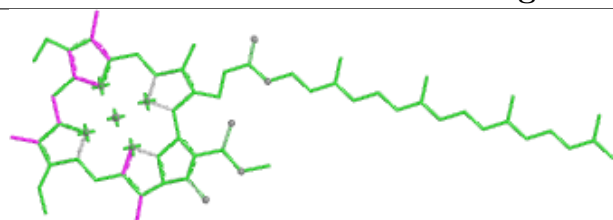


Torsions

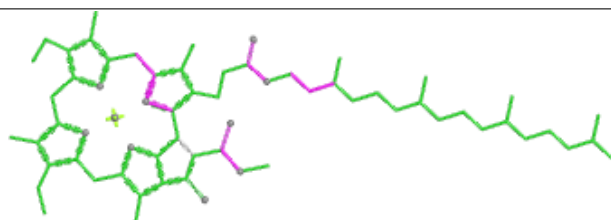


Rings

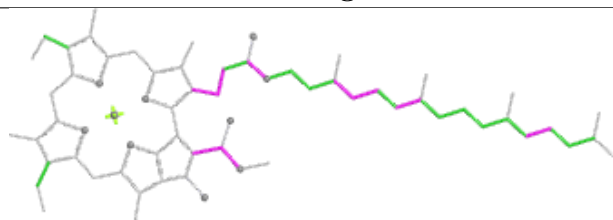
Ligand CLA 6 501



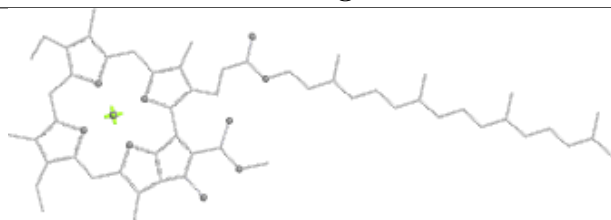
Bond lengths



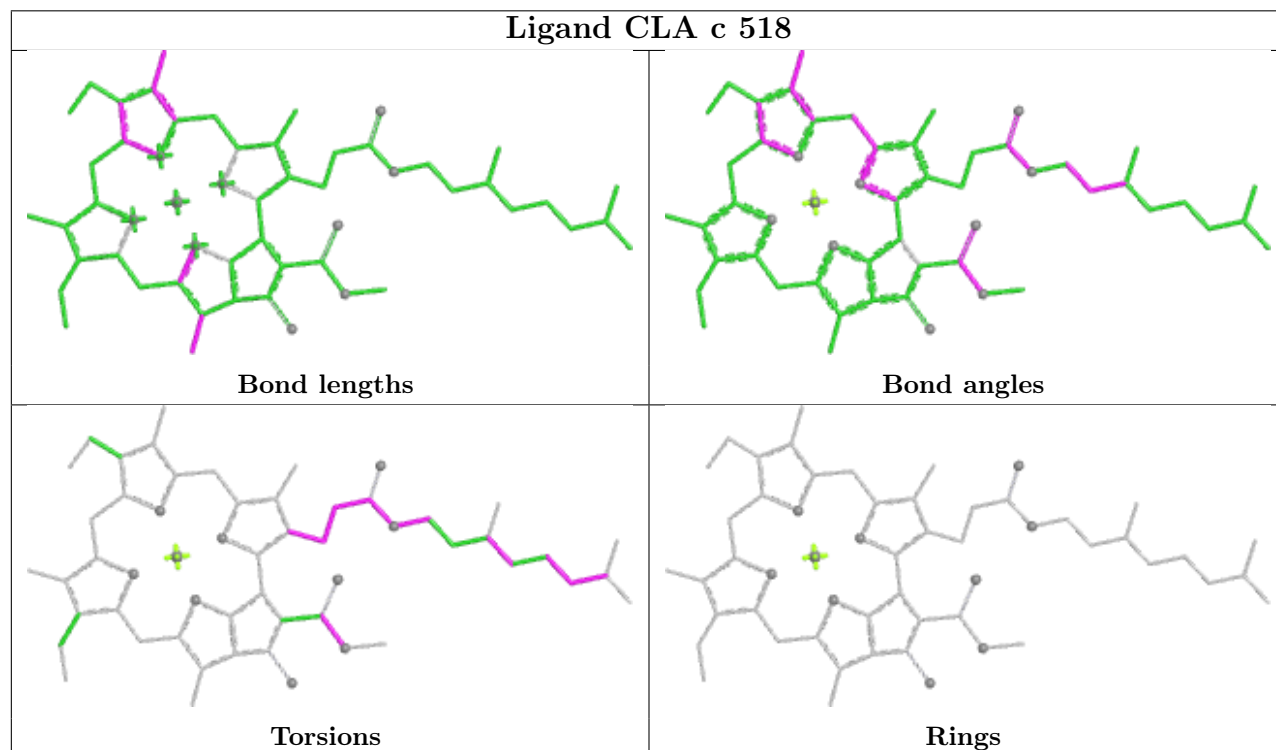
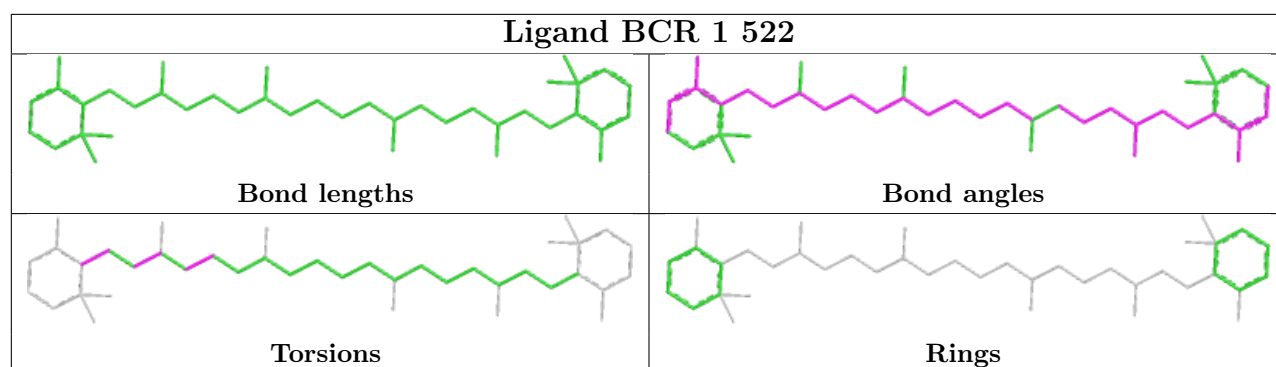
Bond angles



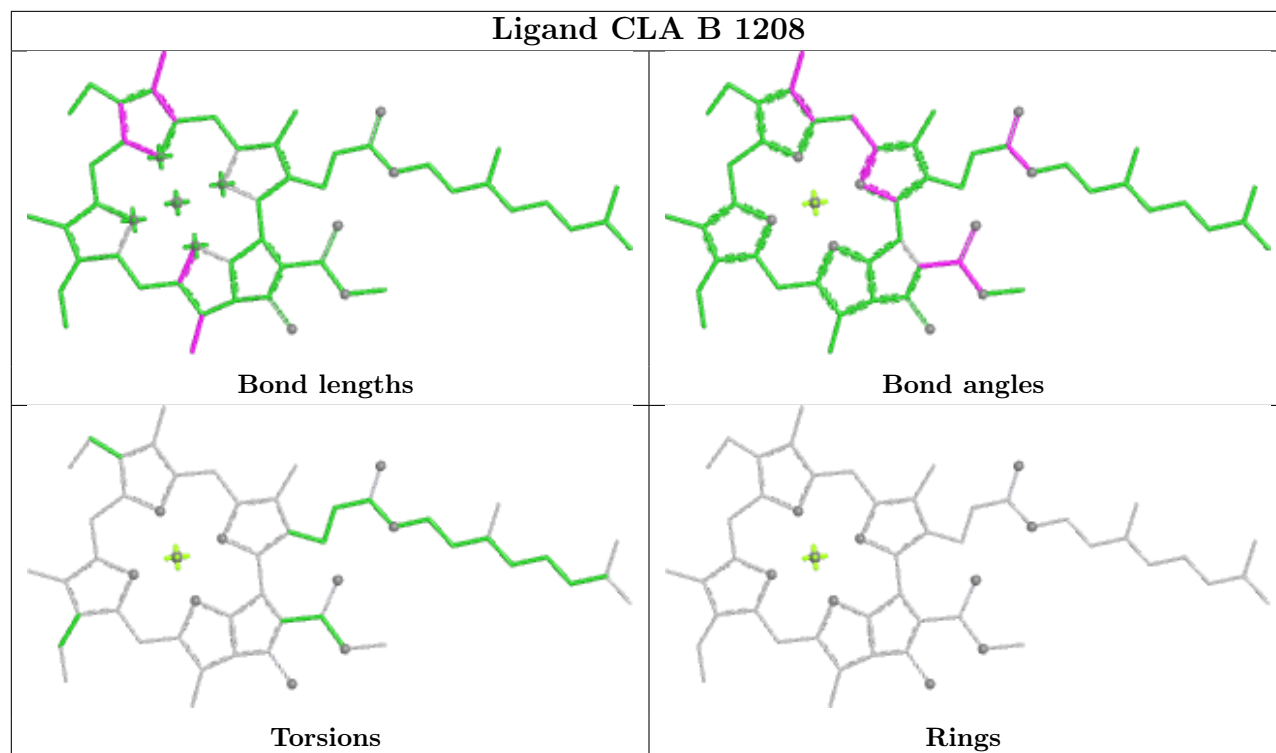
Torsions



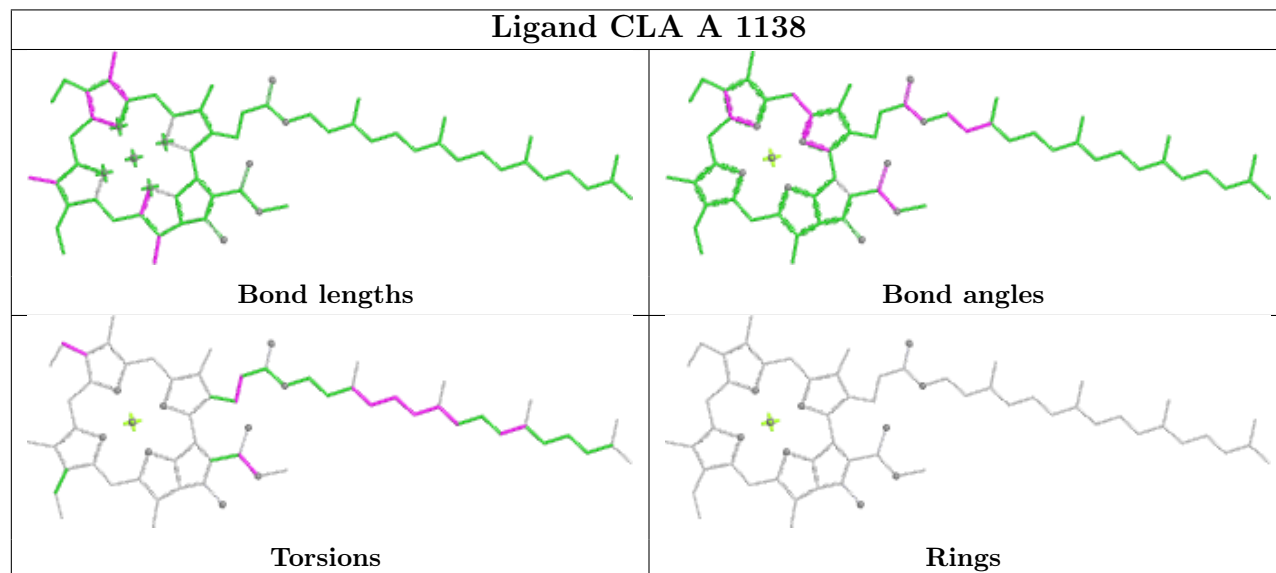
Rings

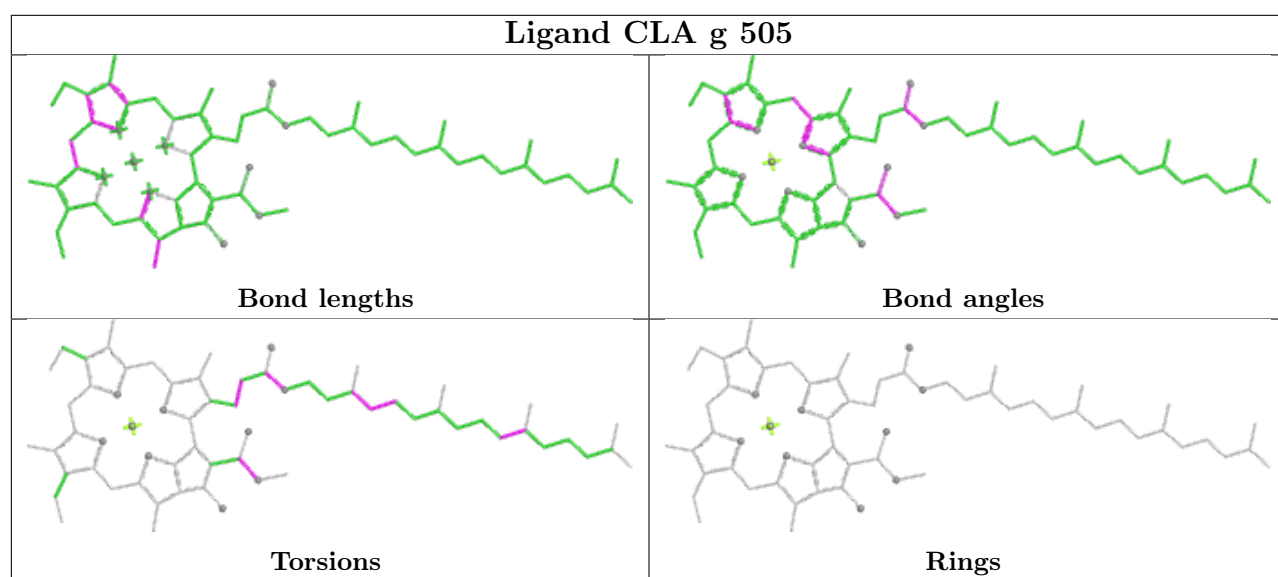
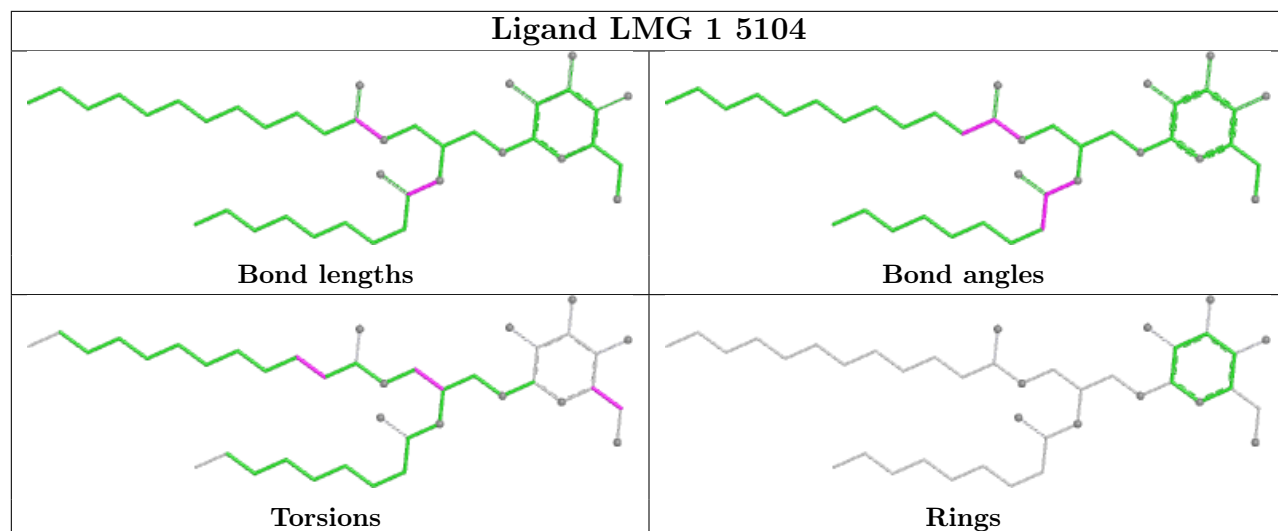


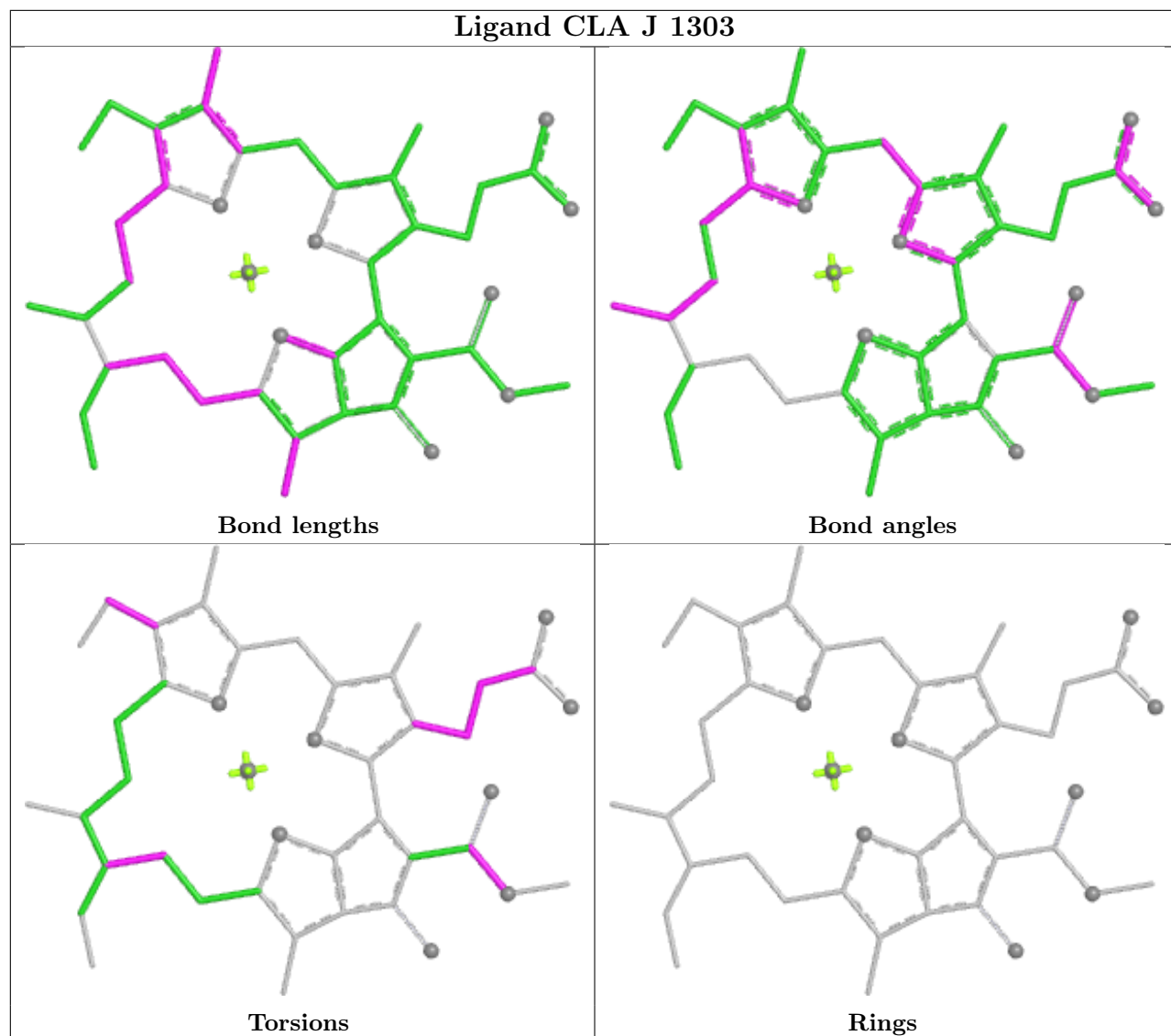
Ligand CLA B 1208



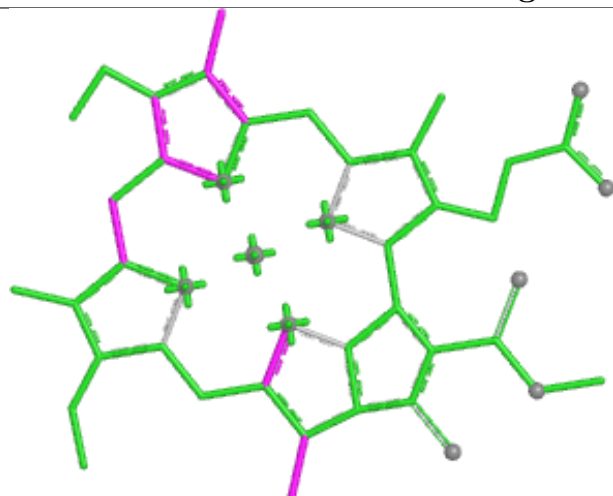
Ligand CLA A 1138



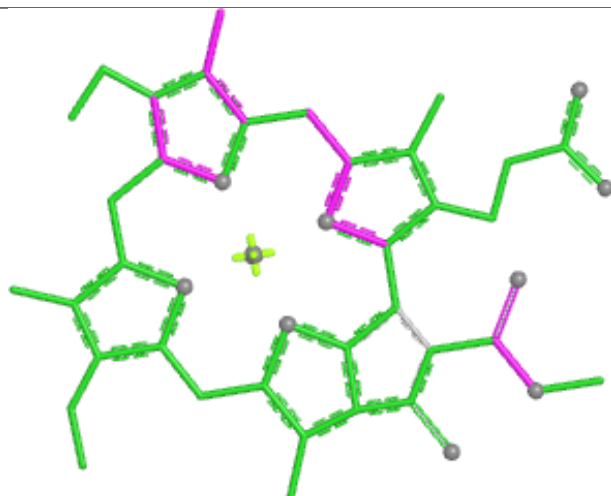




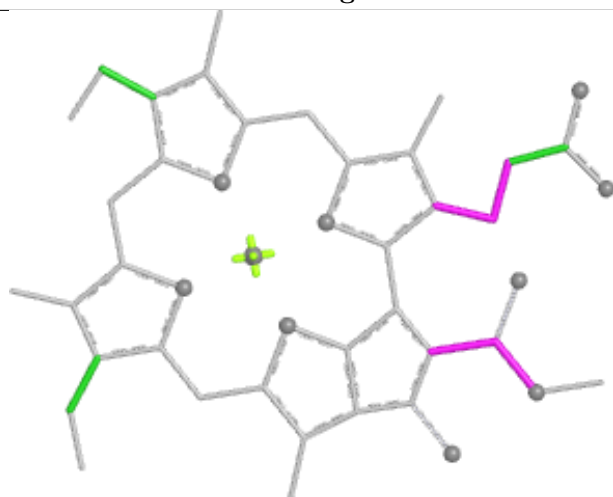
Ligand CLA a 506



Bond lengths



Bond angles

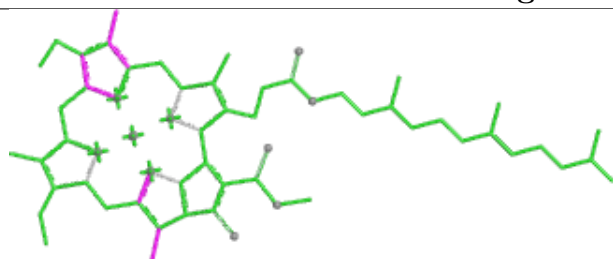


Torsions

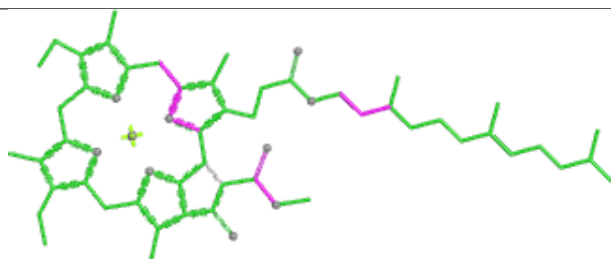


Rings

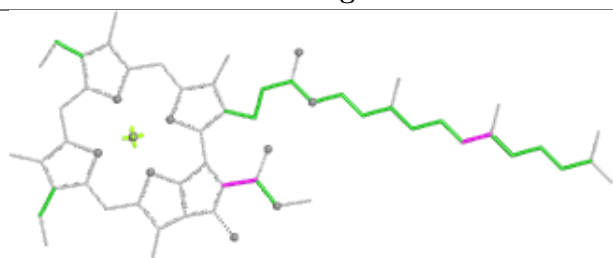
Ligand CLA d 507



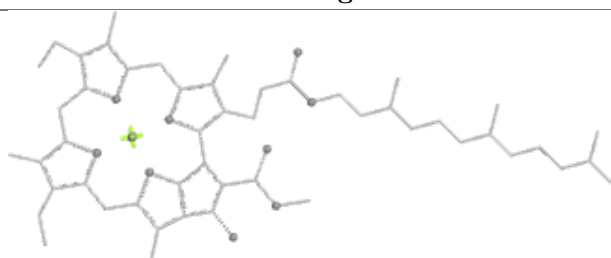
Bond lengths



Bond angles

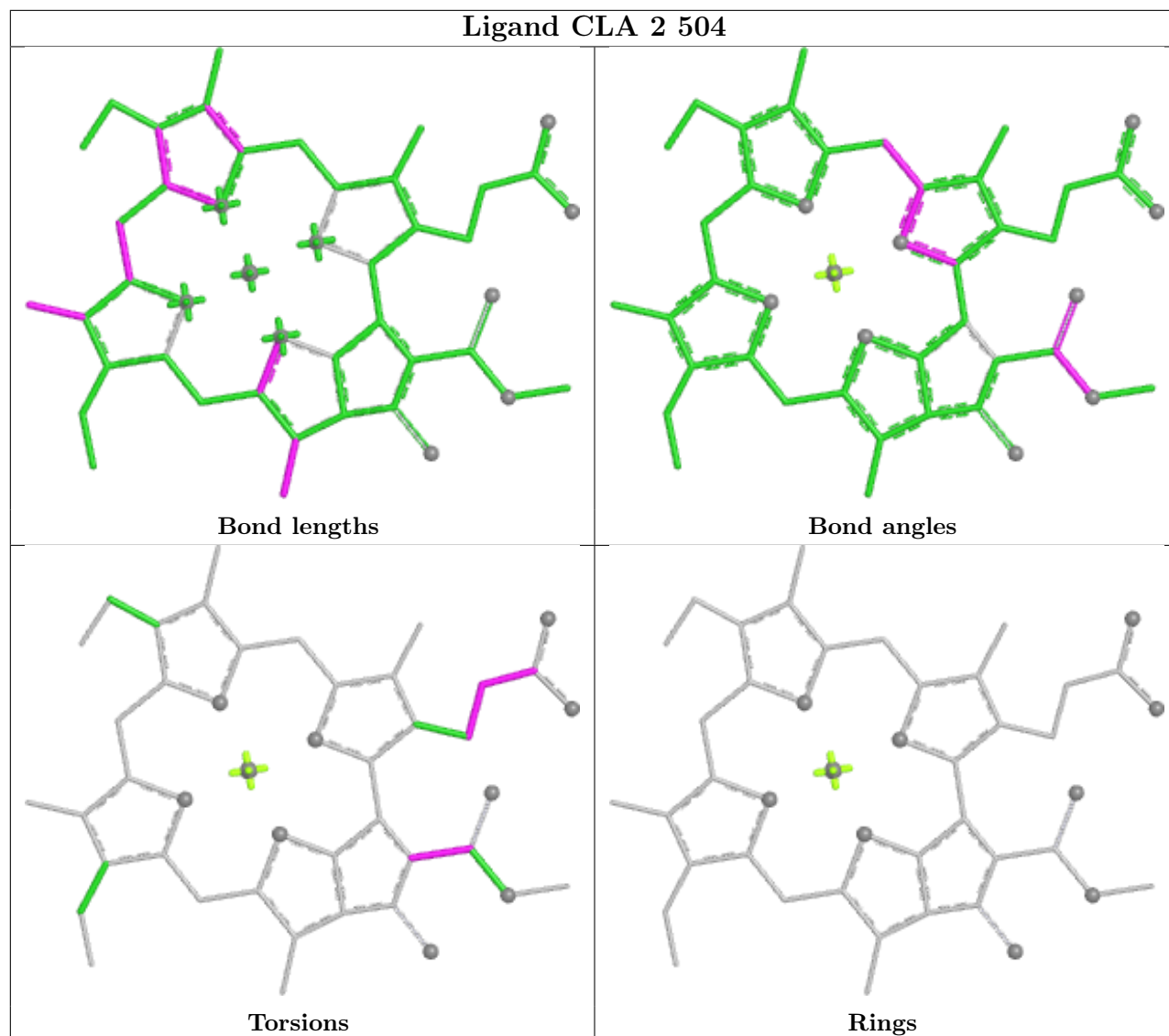


Torsions

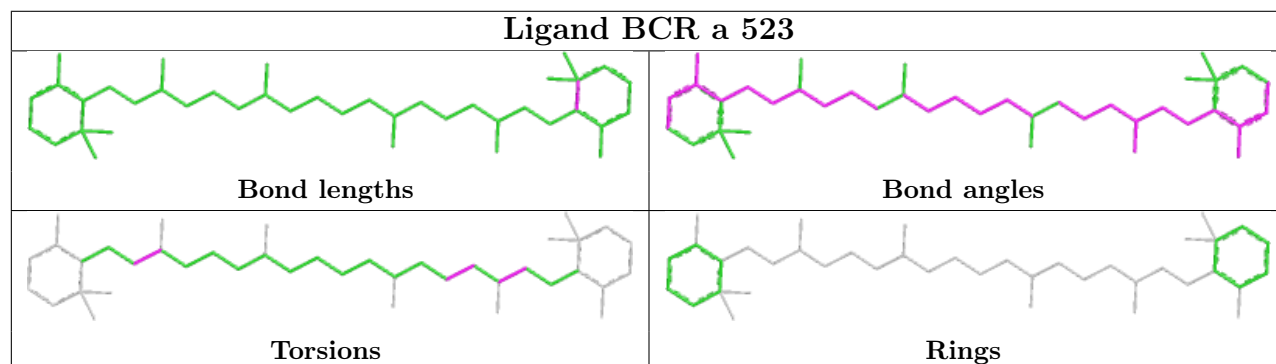


Rings

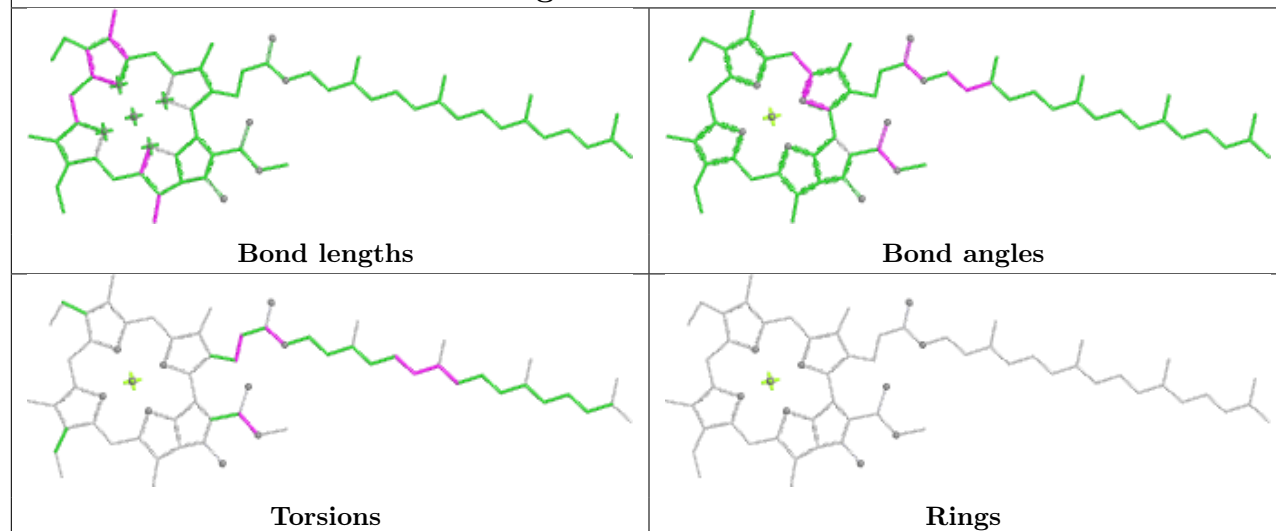
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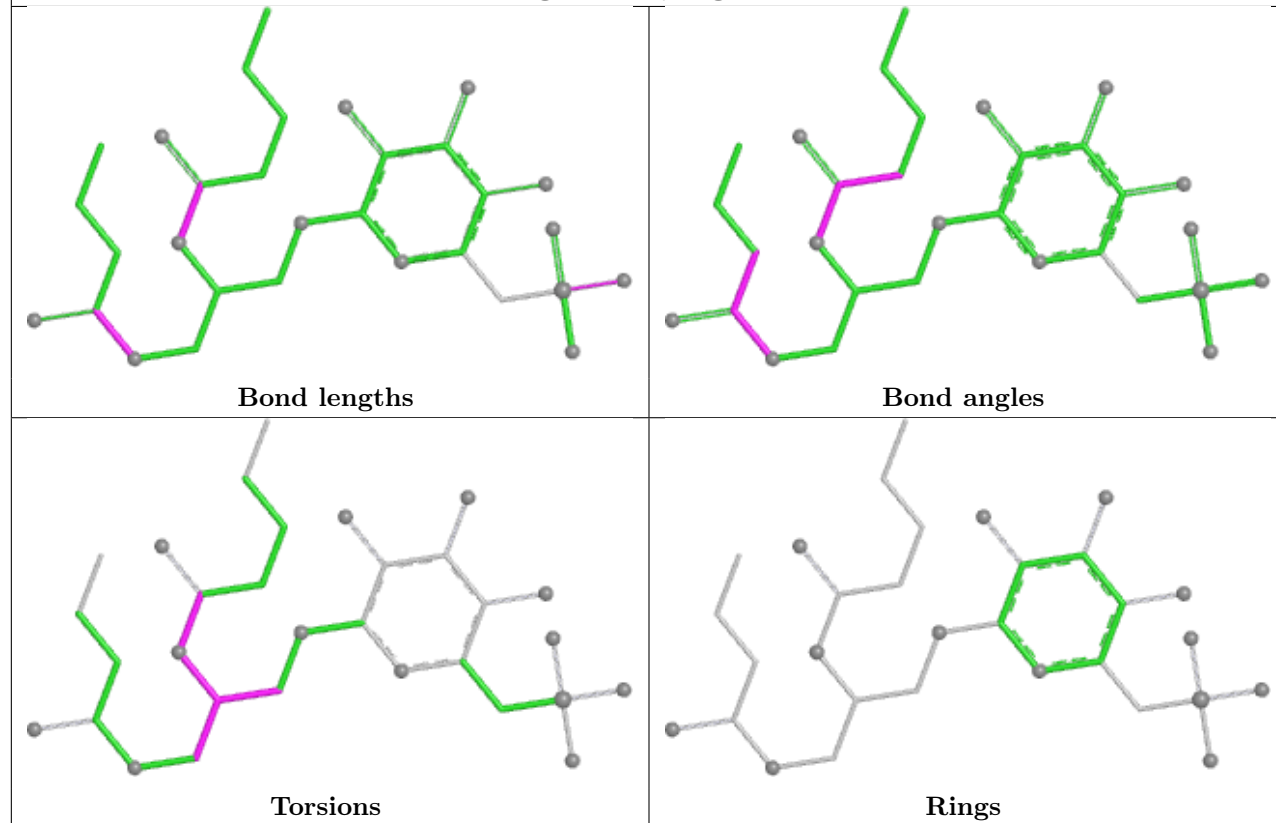
Ligand BCR a 523

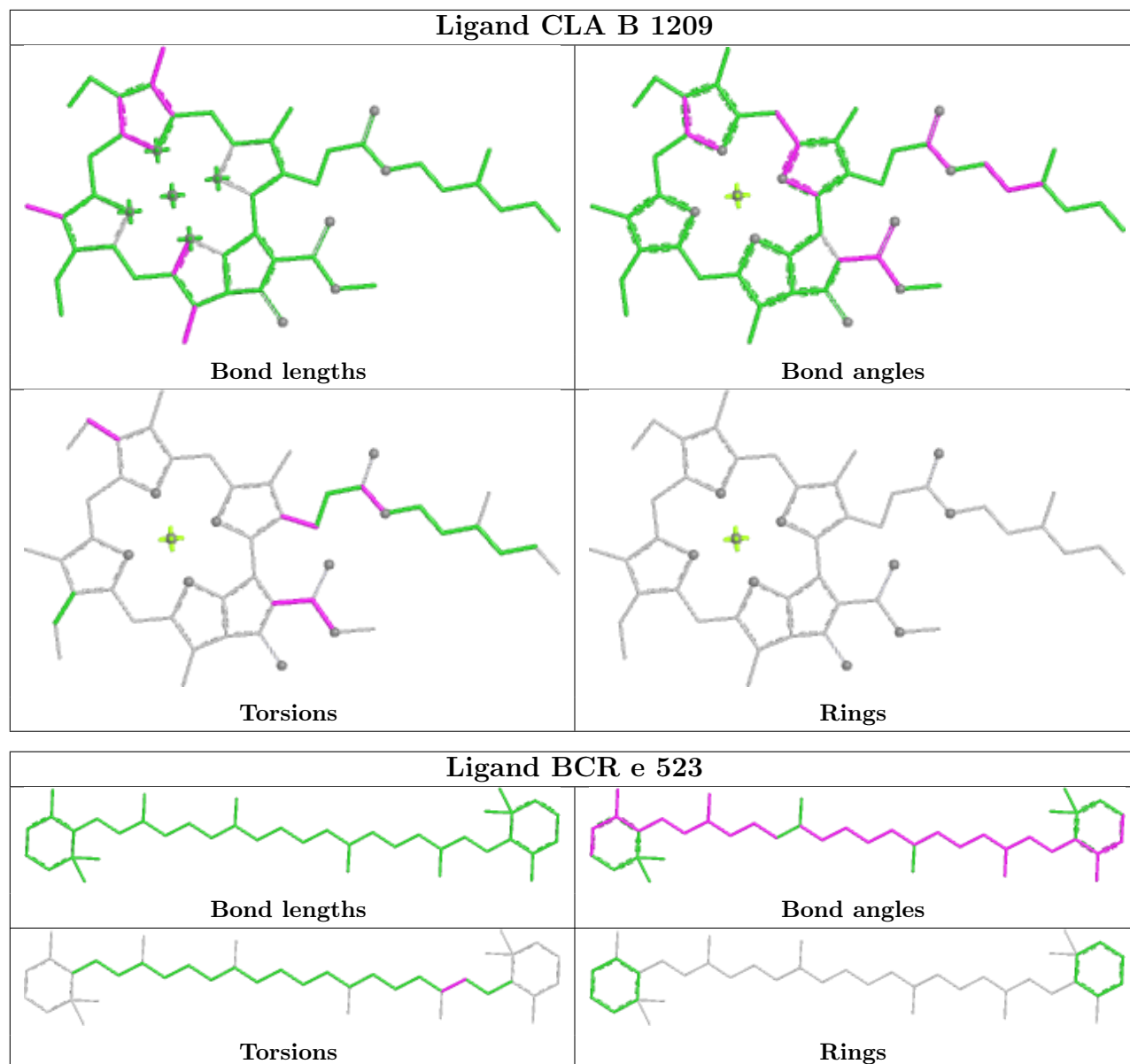


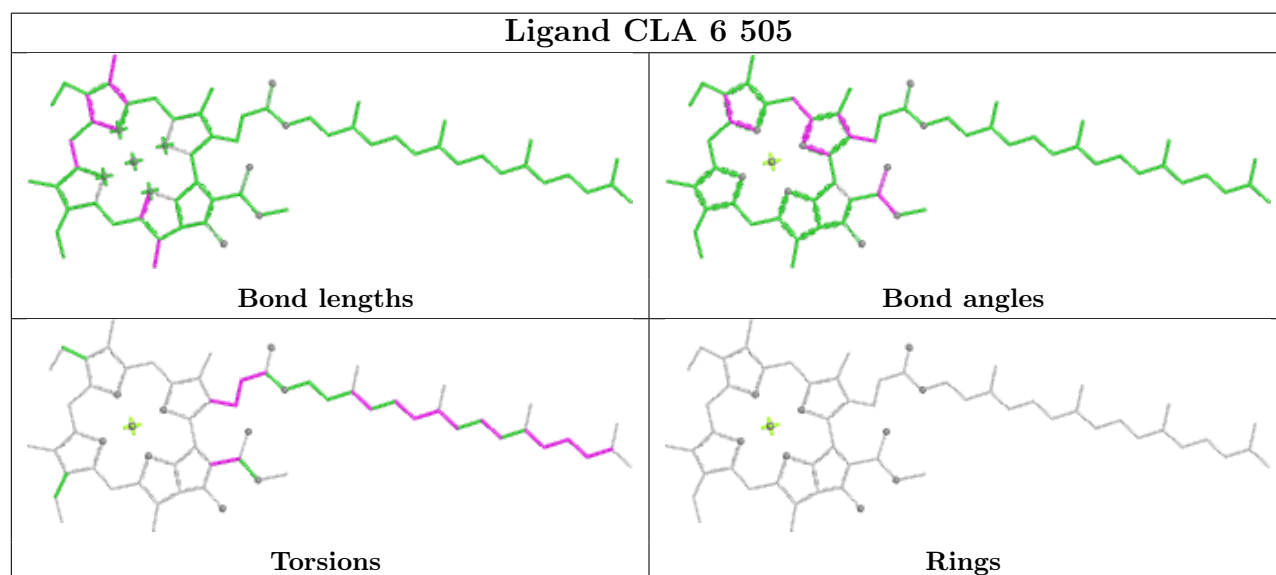
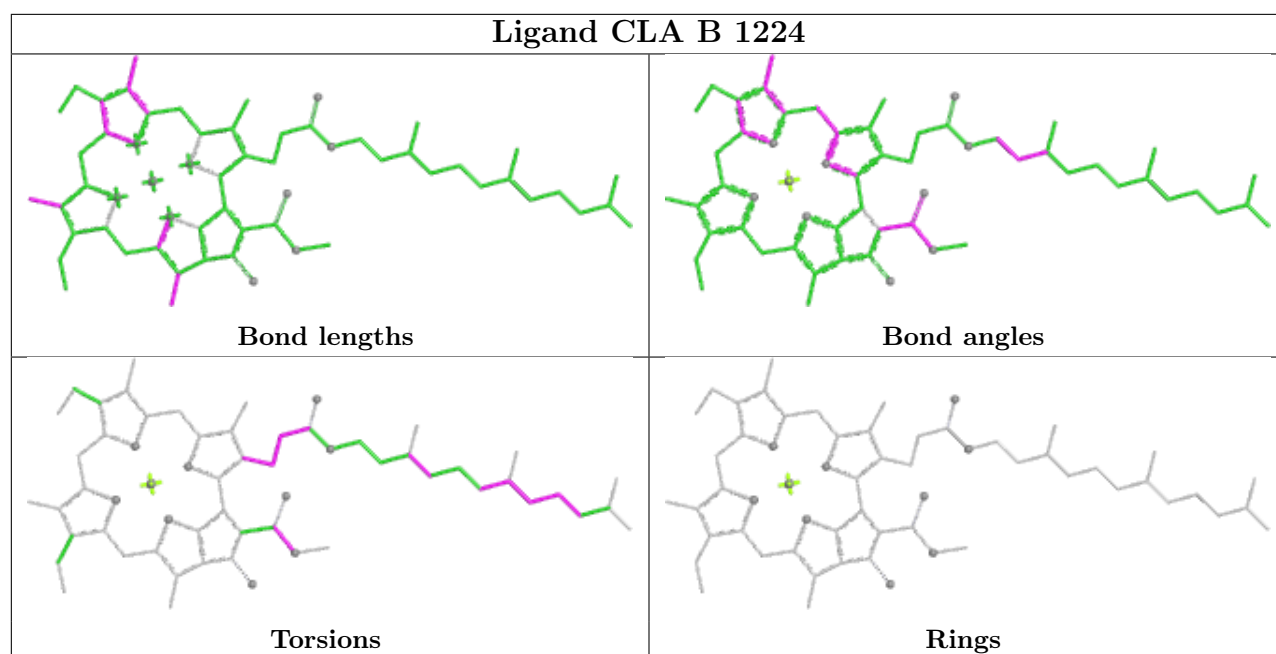
Ligand CLA 1 510



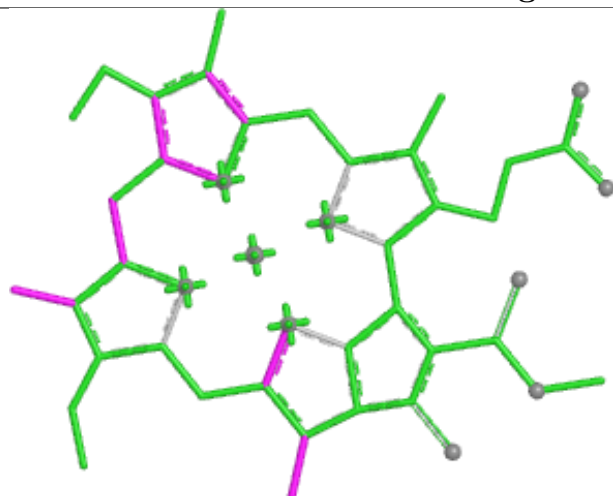
Ligand SQD g 822



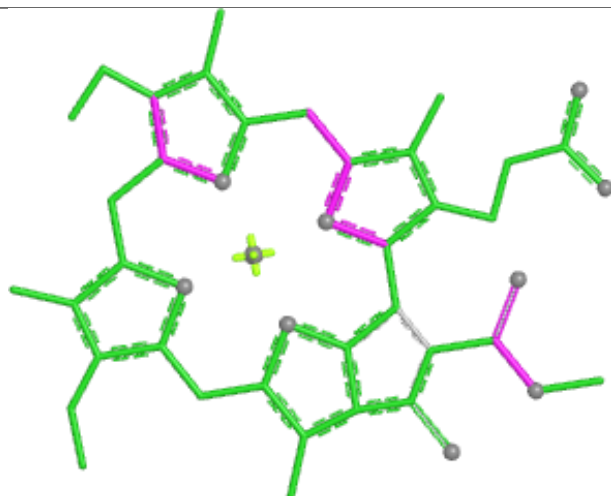




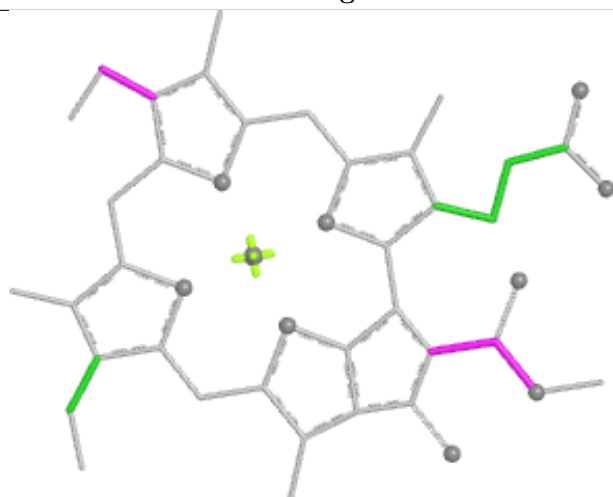
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Bond lengths



Bond angles

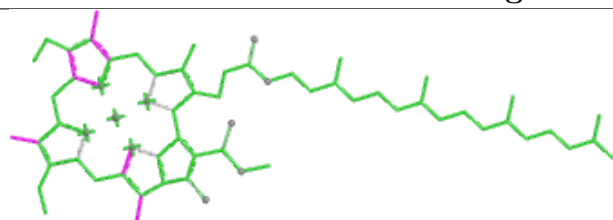


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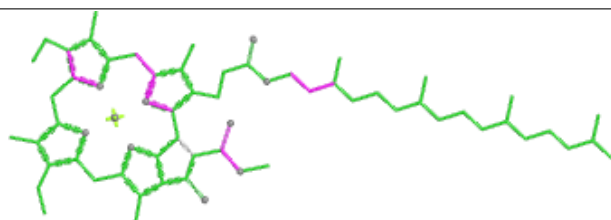


Rings

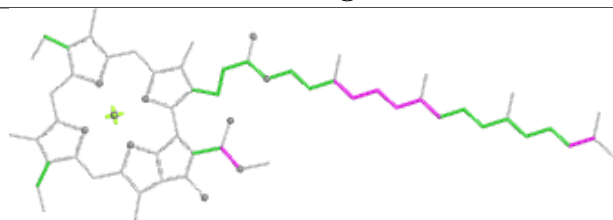
Ligand CLA B 1223



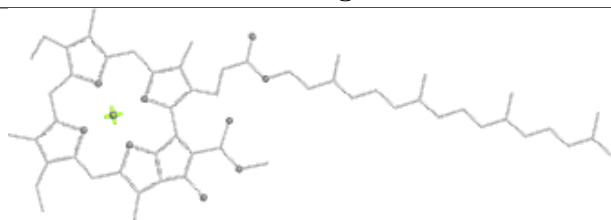
Bond lengths



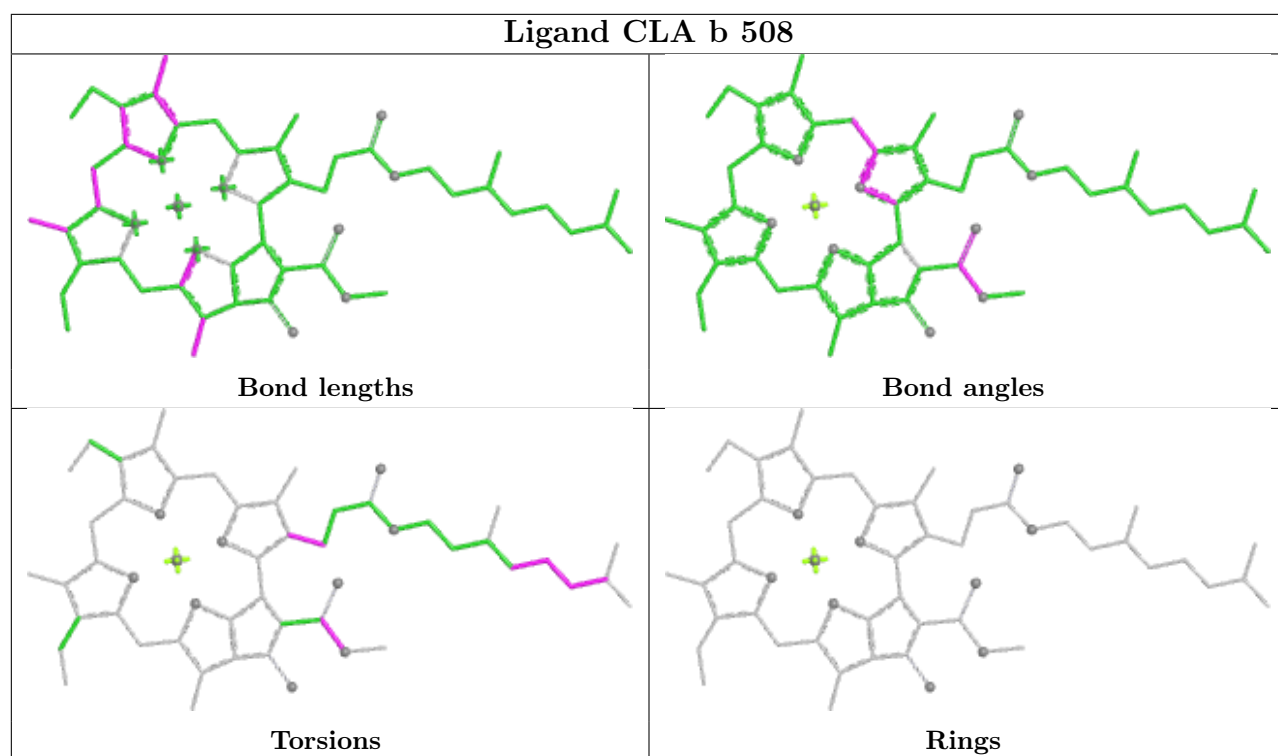
Bond angles



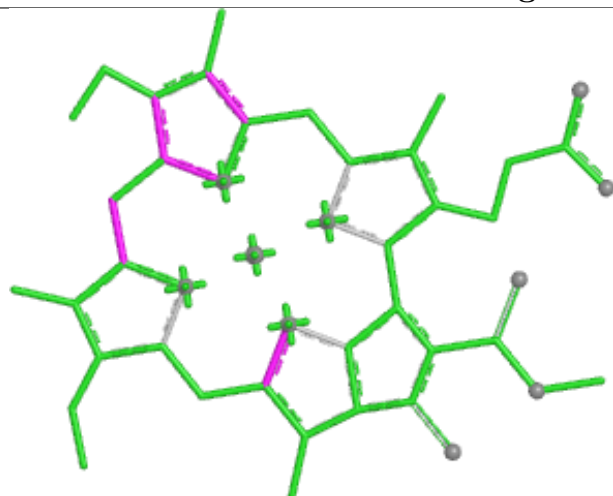
Torsions



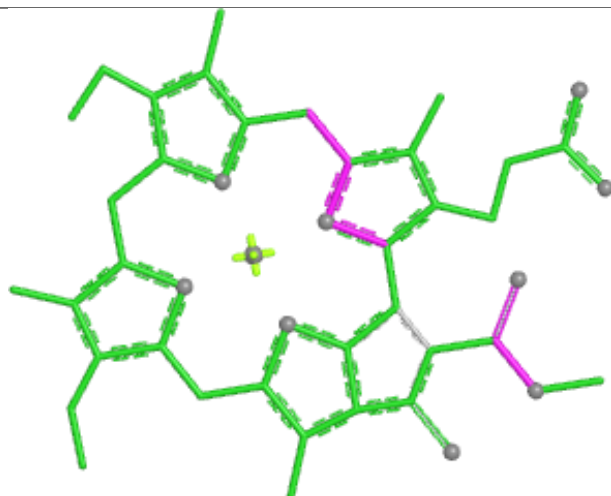
Rings



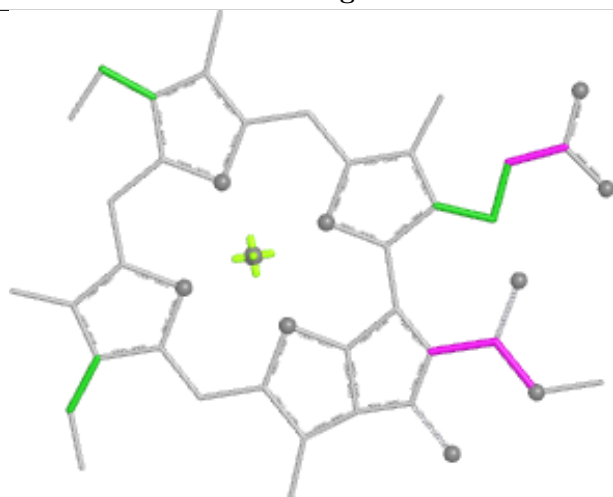
Ligand CLA 4 517



Bond lengths



Bond angles

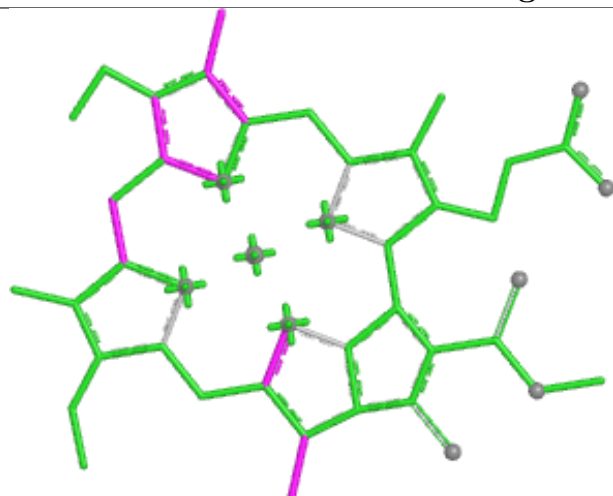


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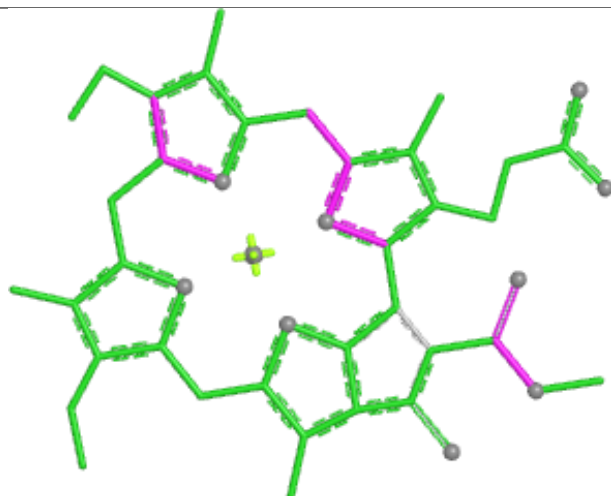


Rings

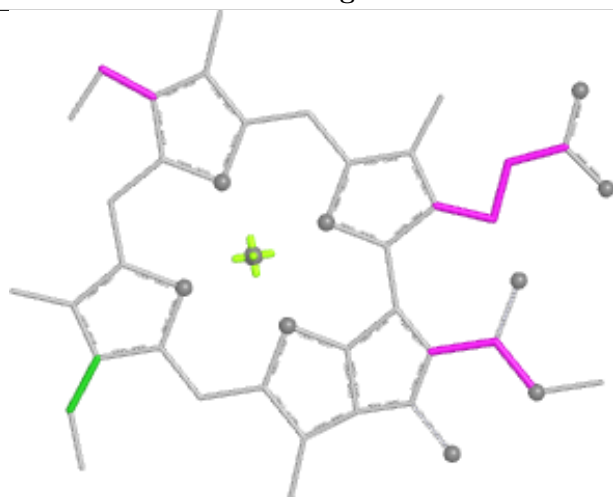
Ligand CLA 5 516



Bond lengths



Bond angles

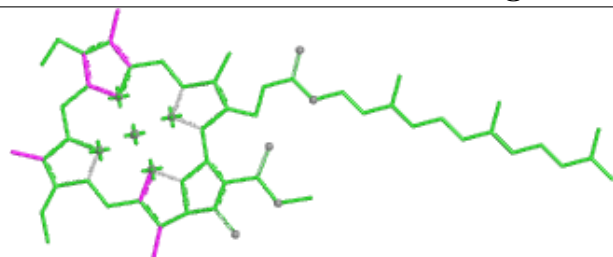


Torsions

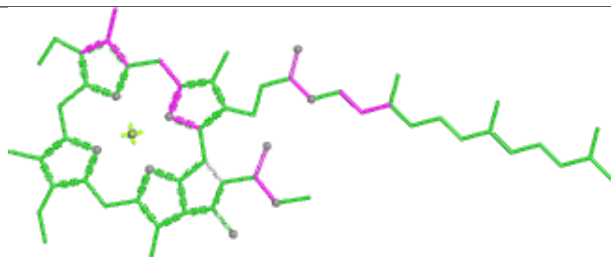


Rings

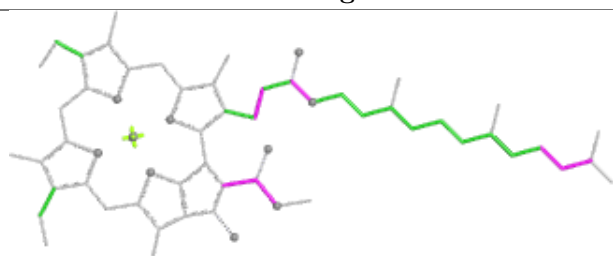
Ligand CLA A 1111



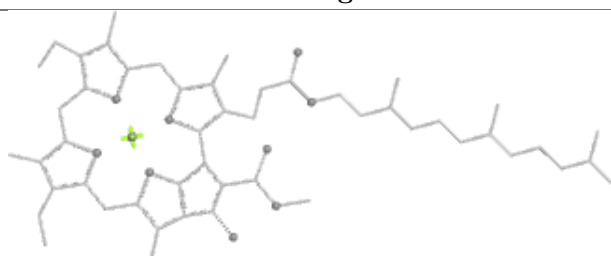
Bond lengths



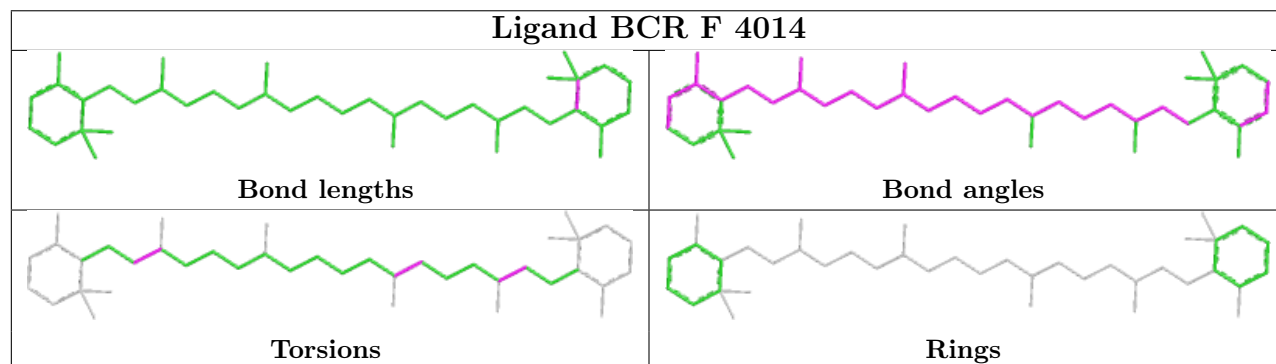
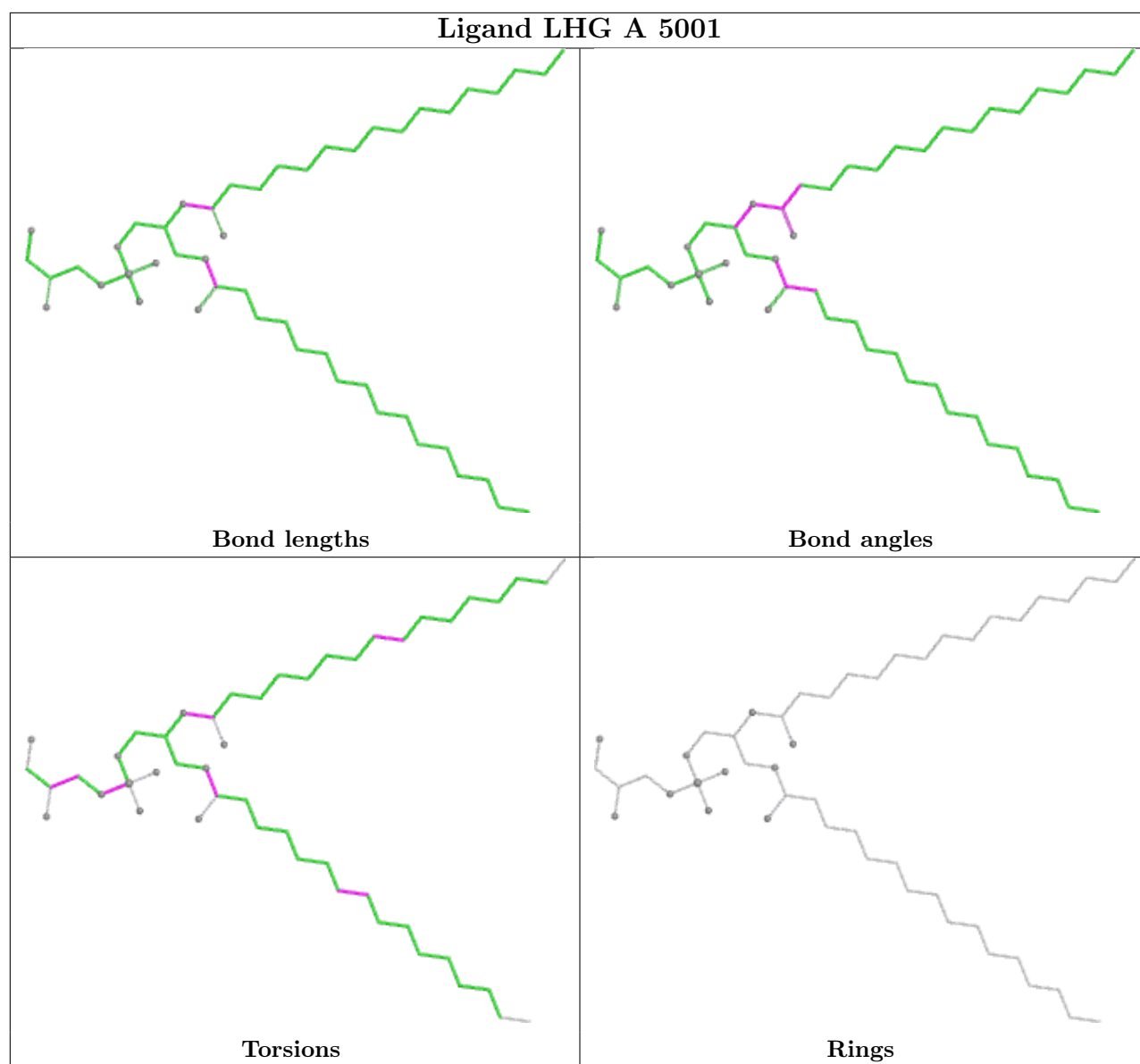
Bond angles



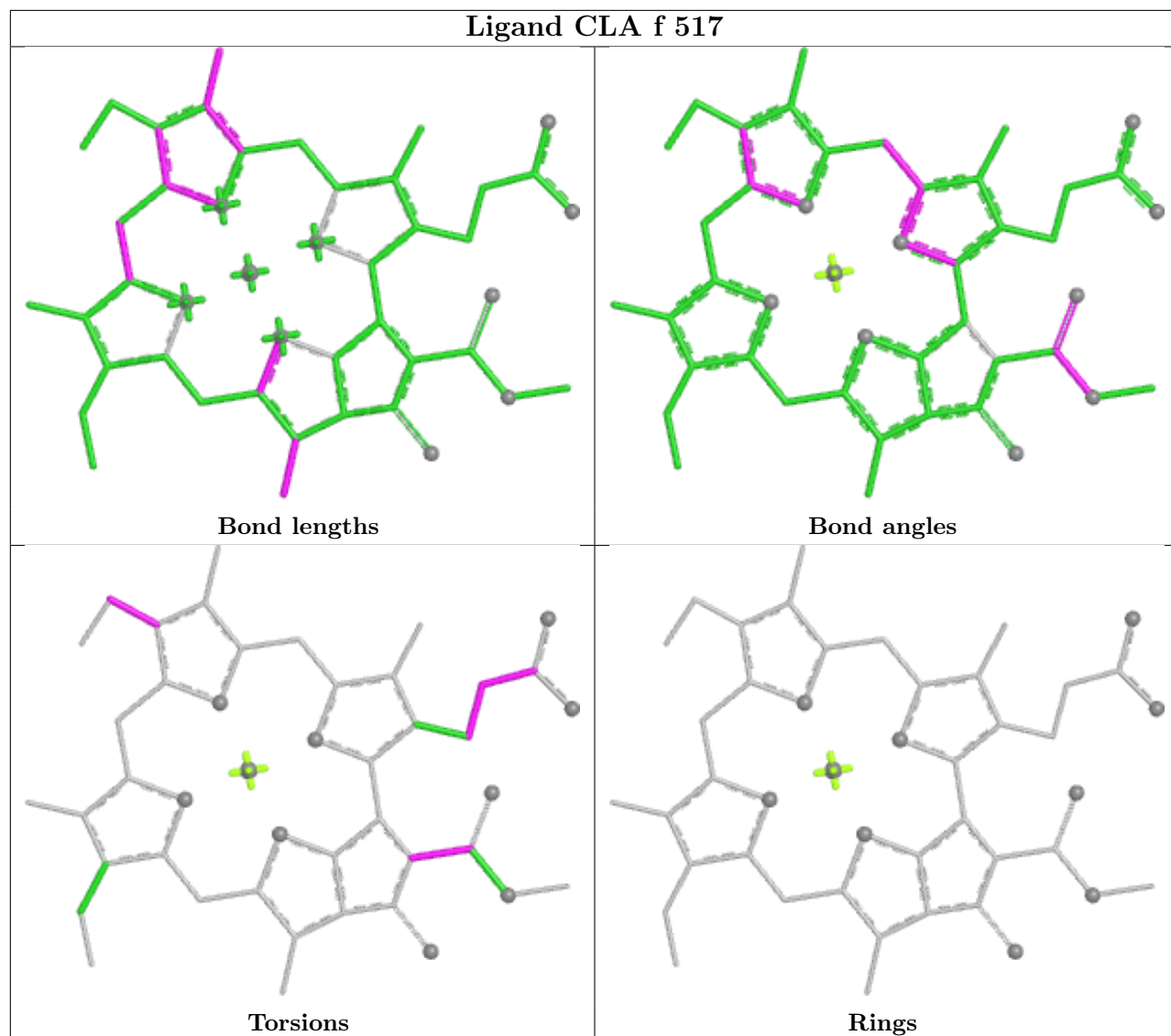
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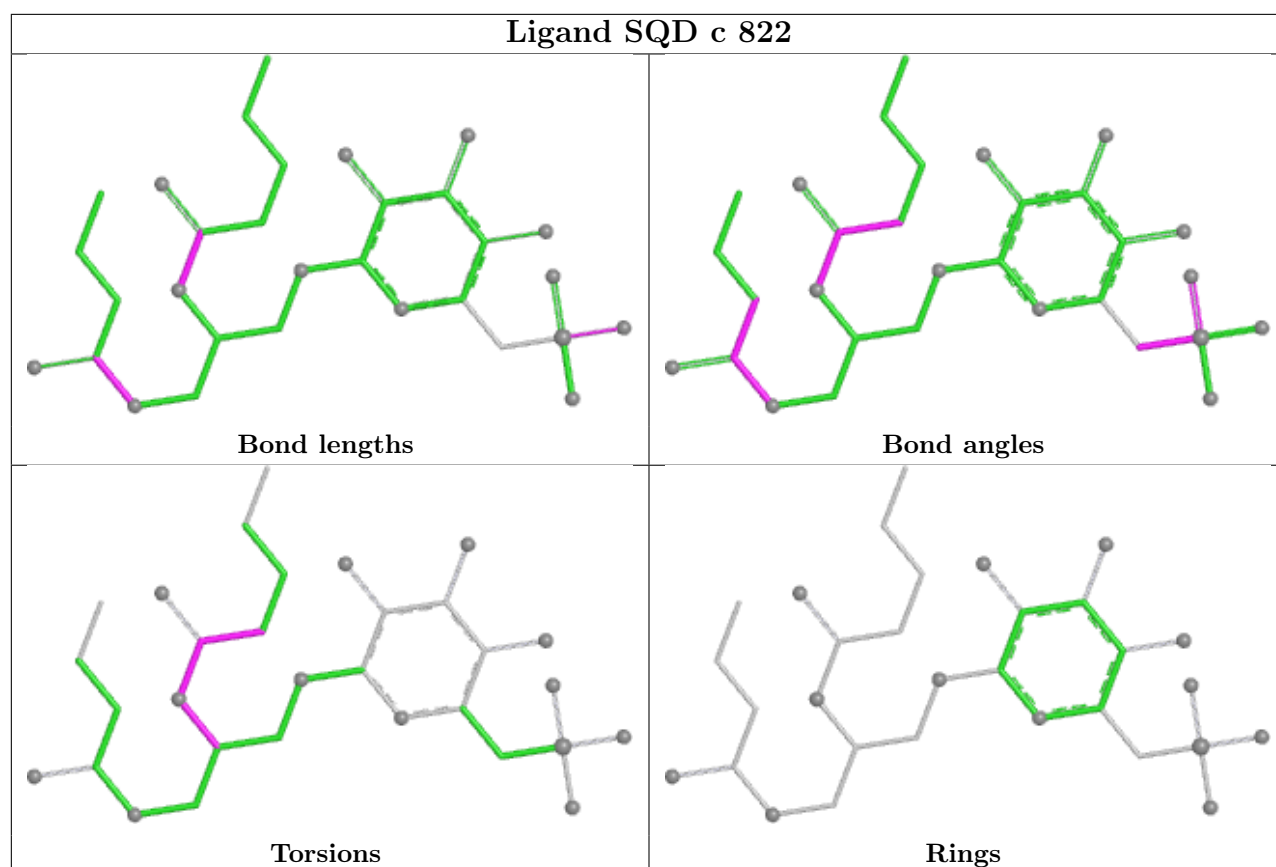


Rings

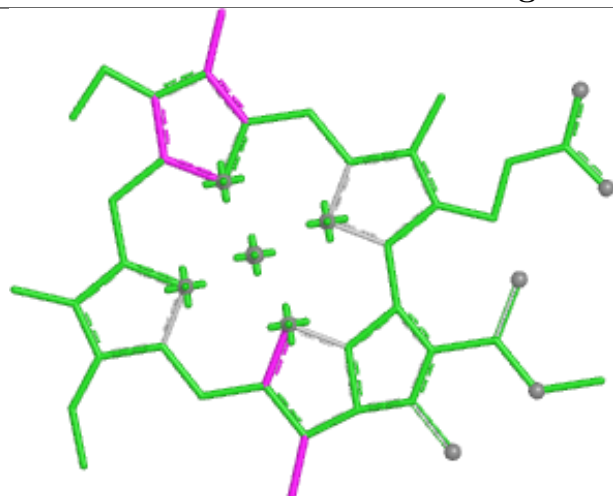


Ligand CLA f 517

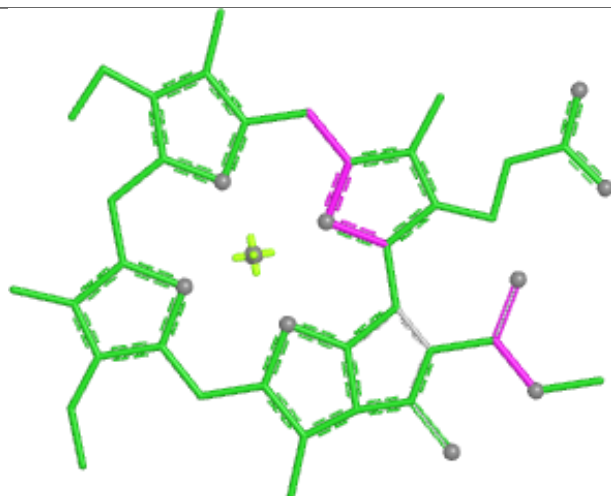




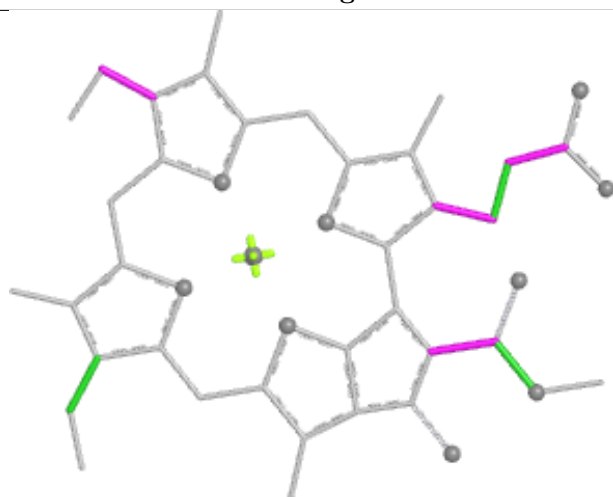
Ligand CLA 3 516



Bond lengths



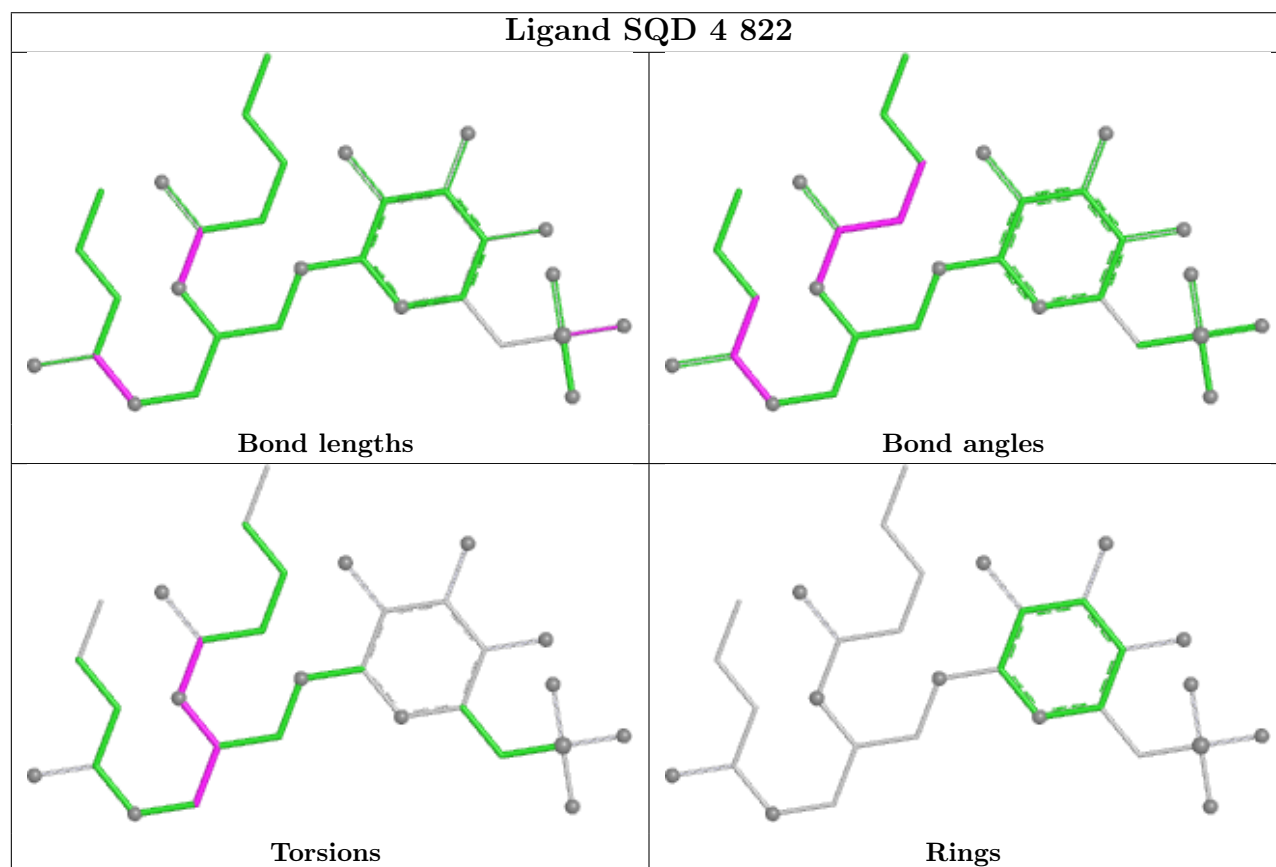
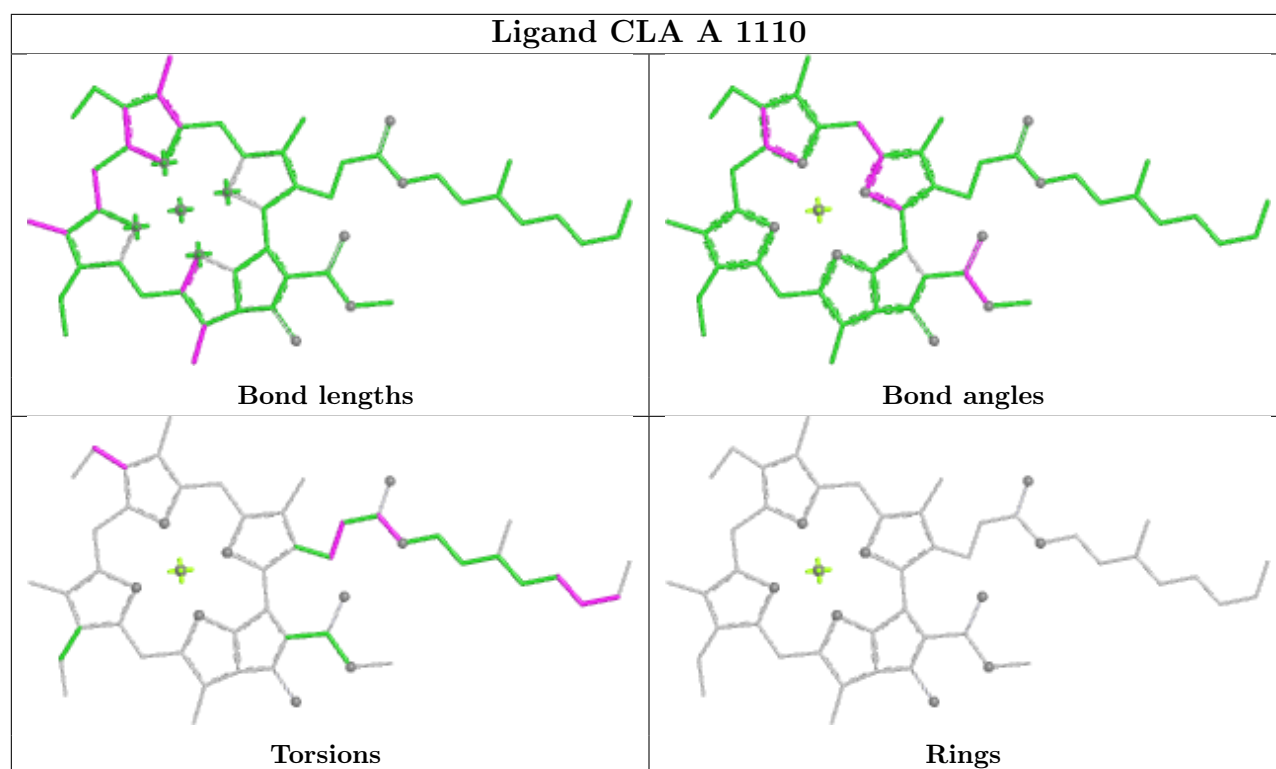
Bond angles



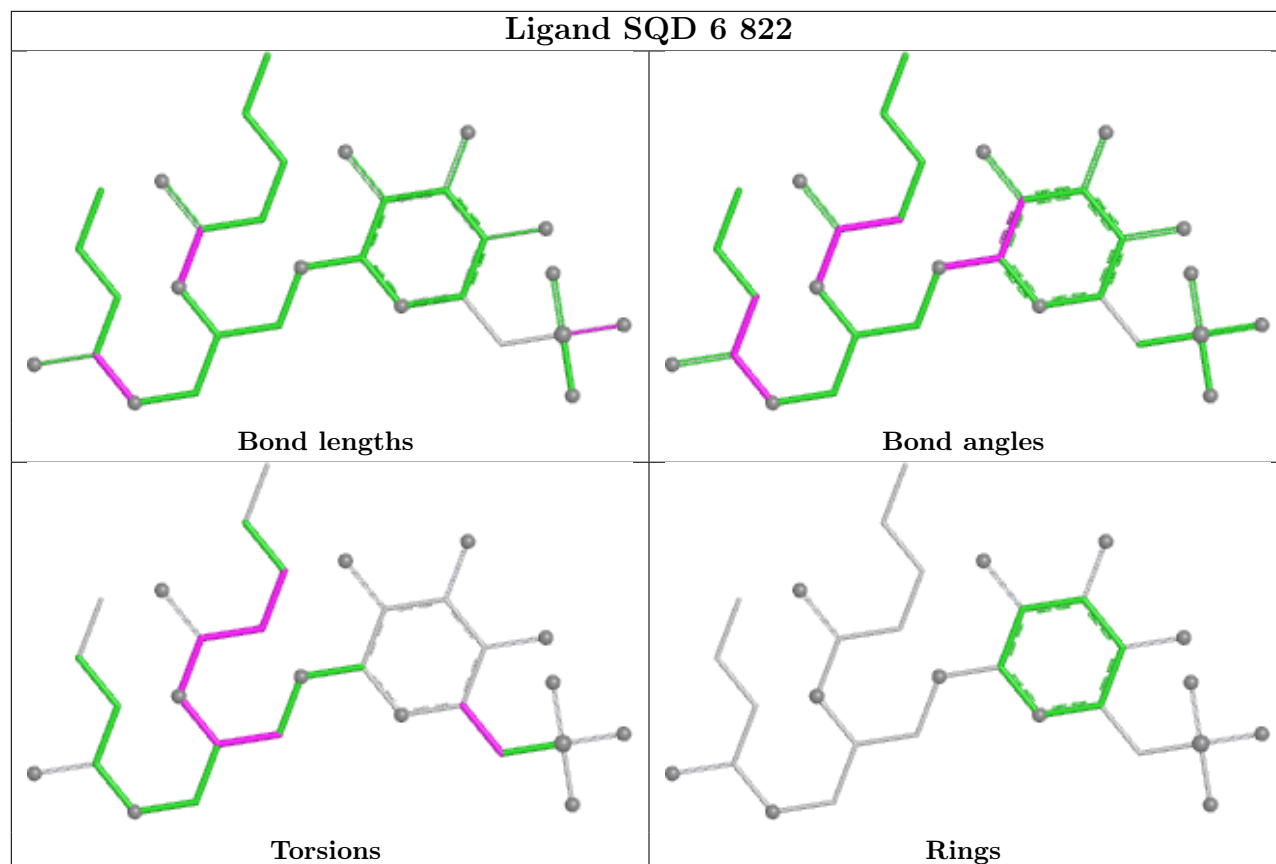
Torsions



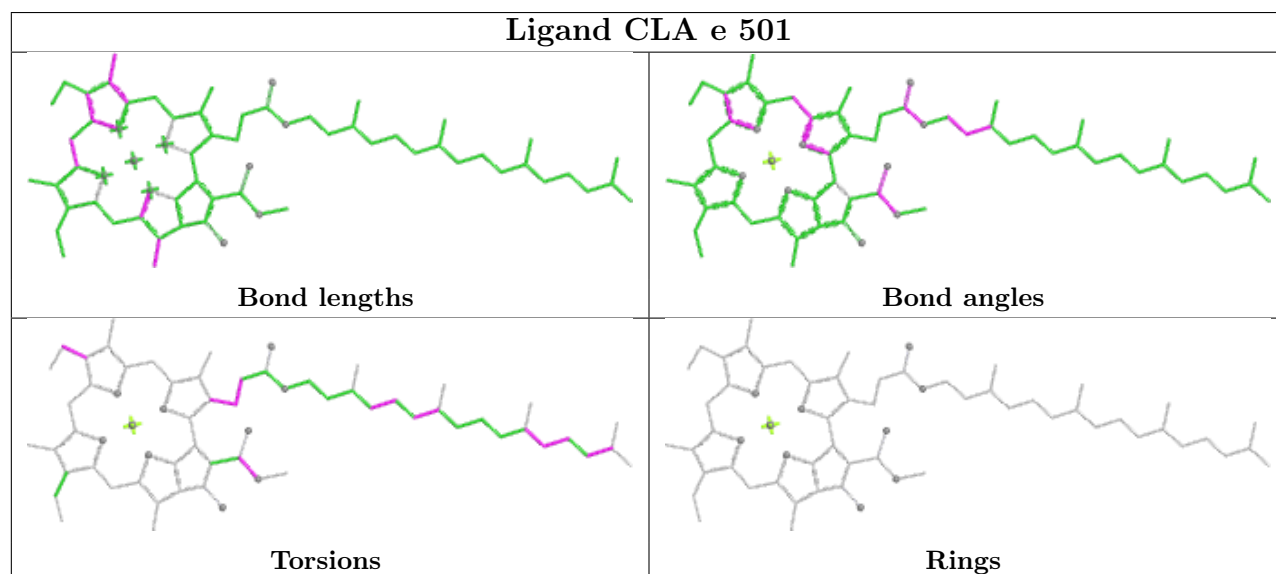
Rings



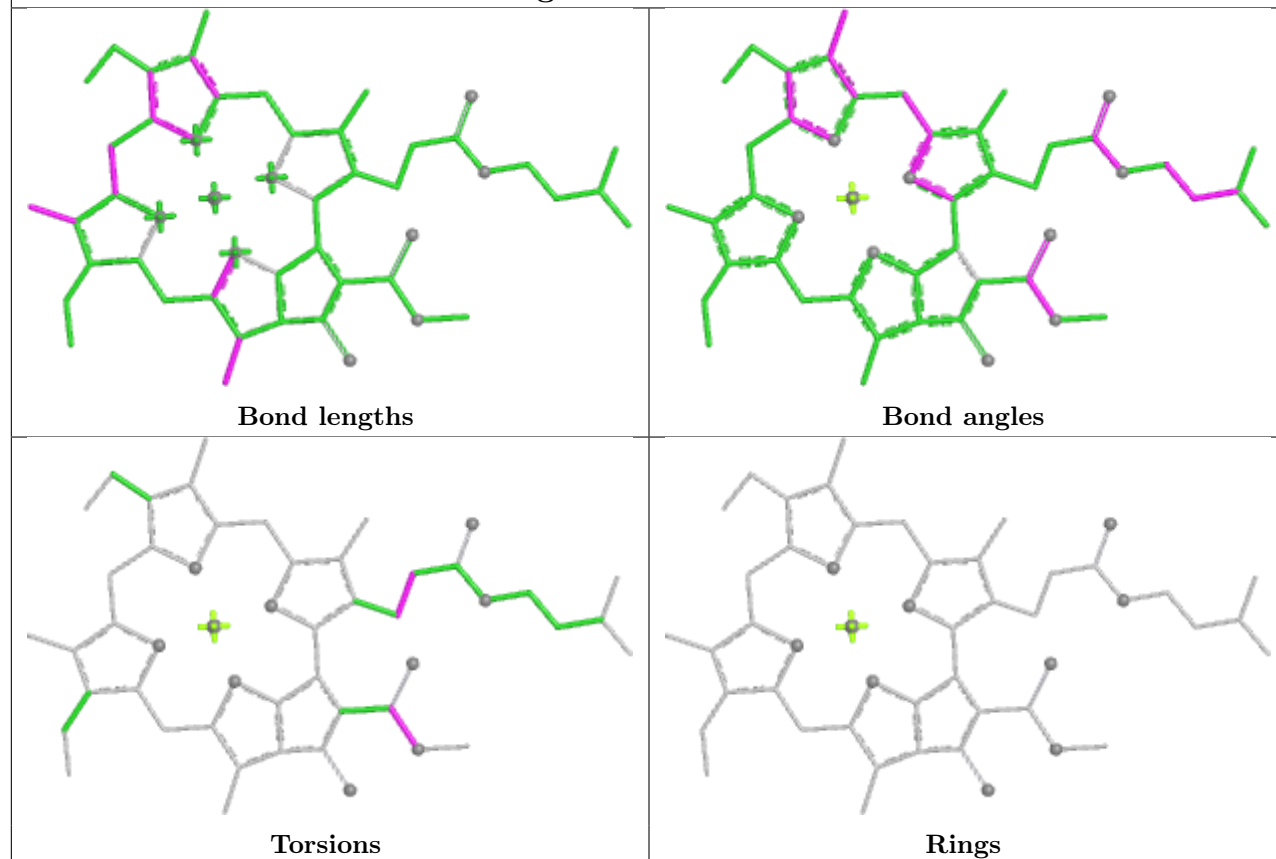
Ligand SQD 6 822



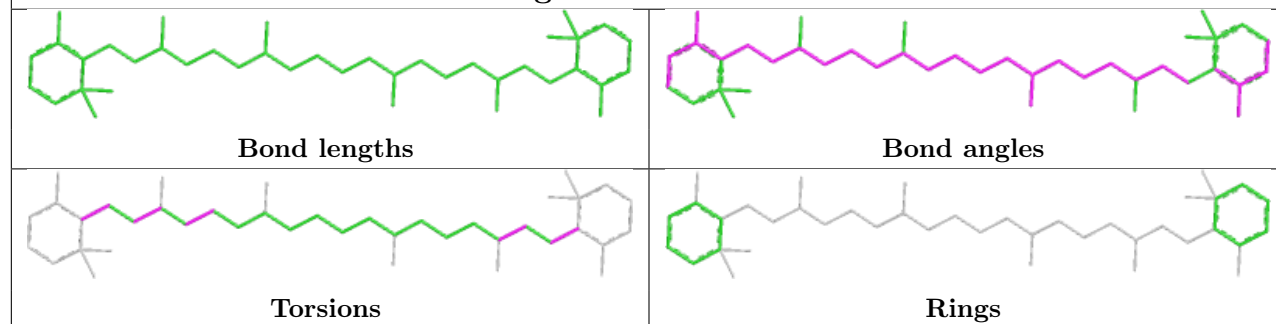
Ligand CLA e 501



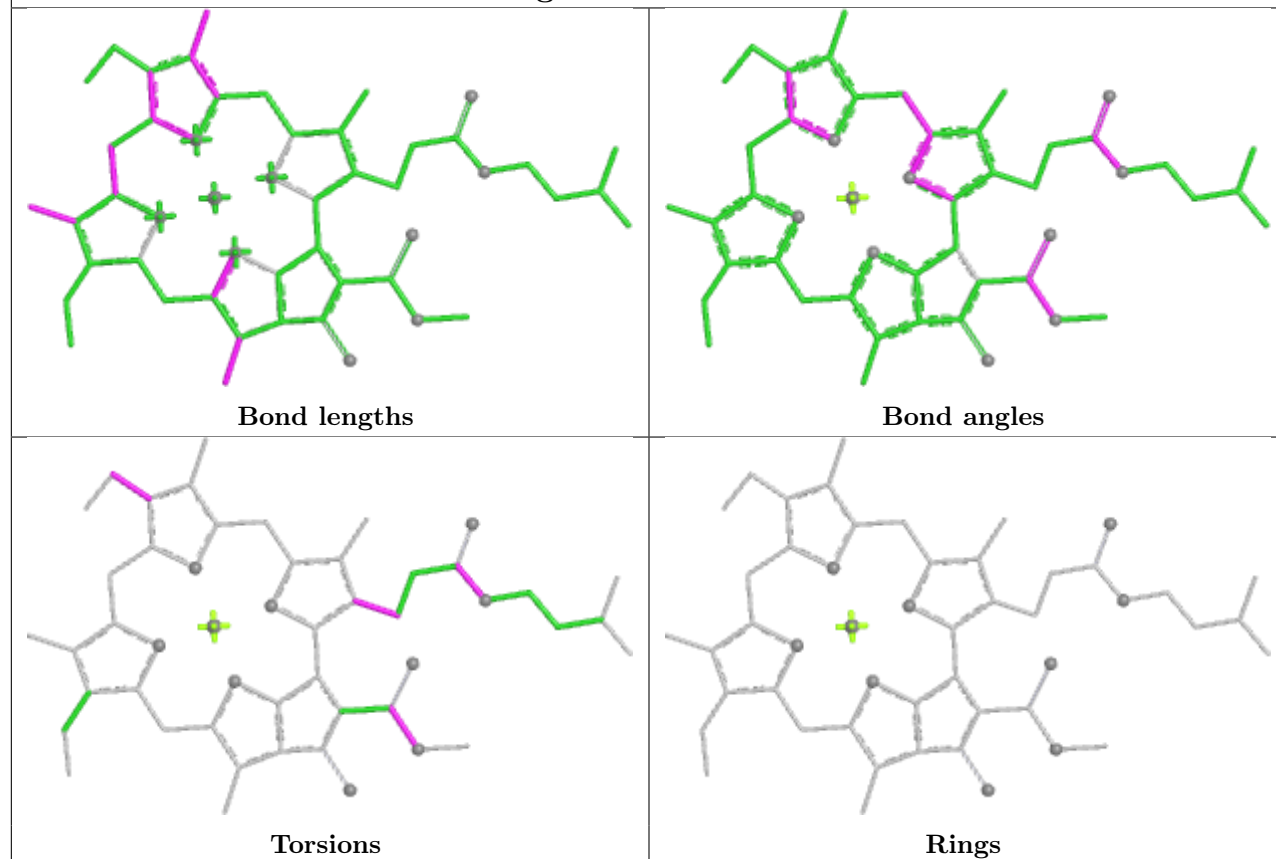
Ligand CLA e 513



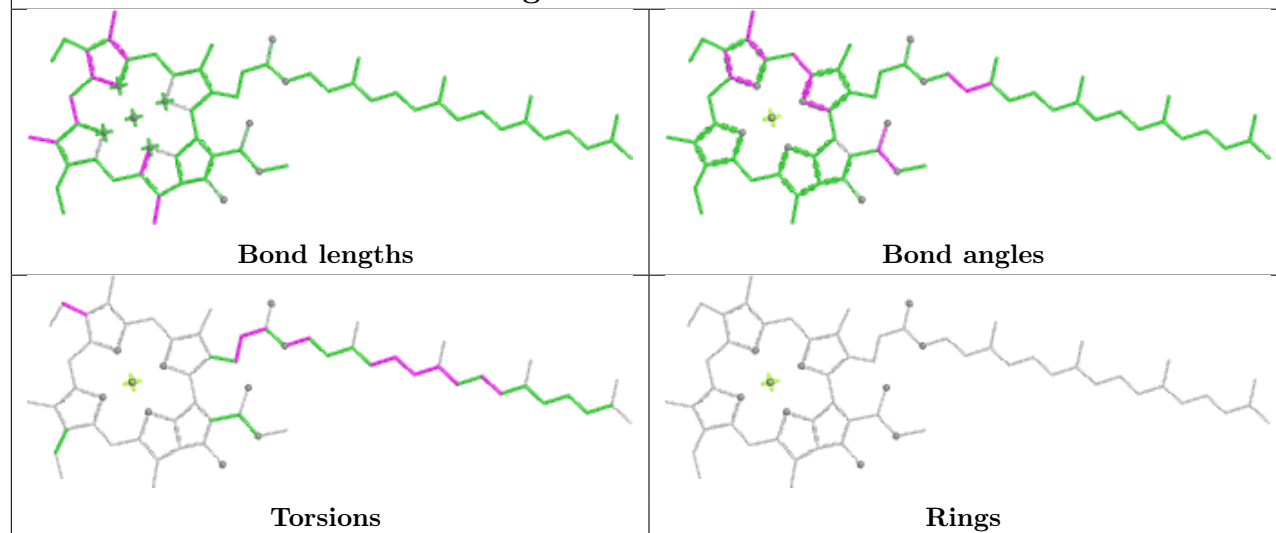
Ligand BCR 3 523



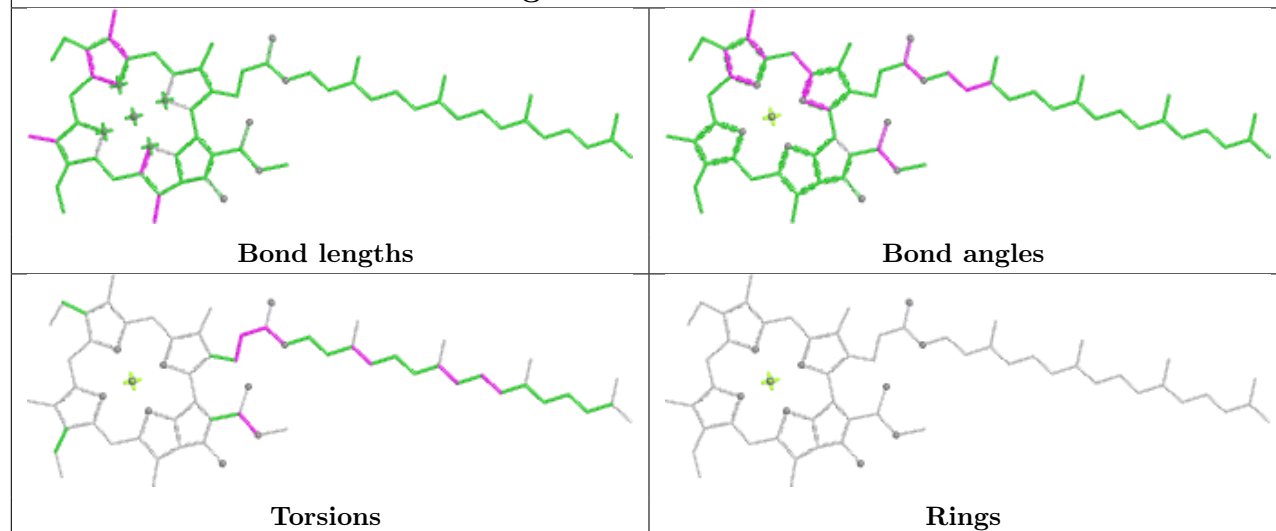
Ligand CLA a 513



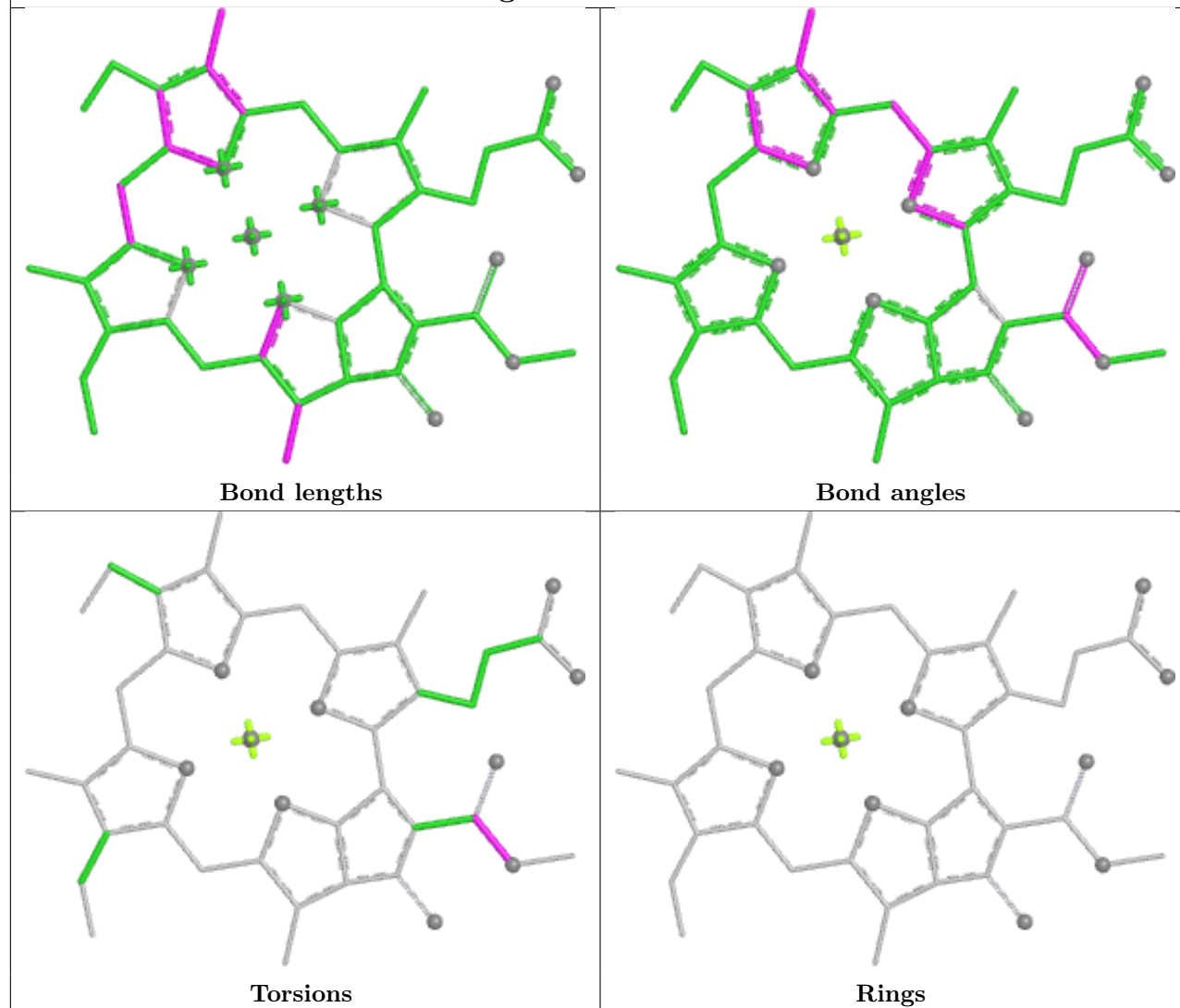
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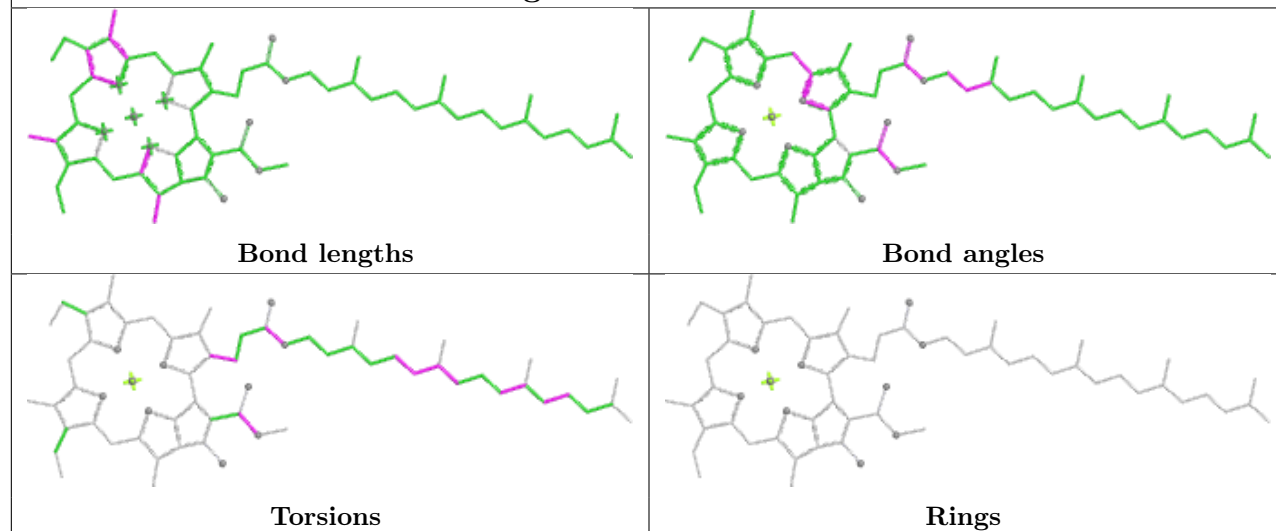
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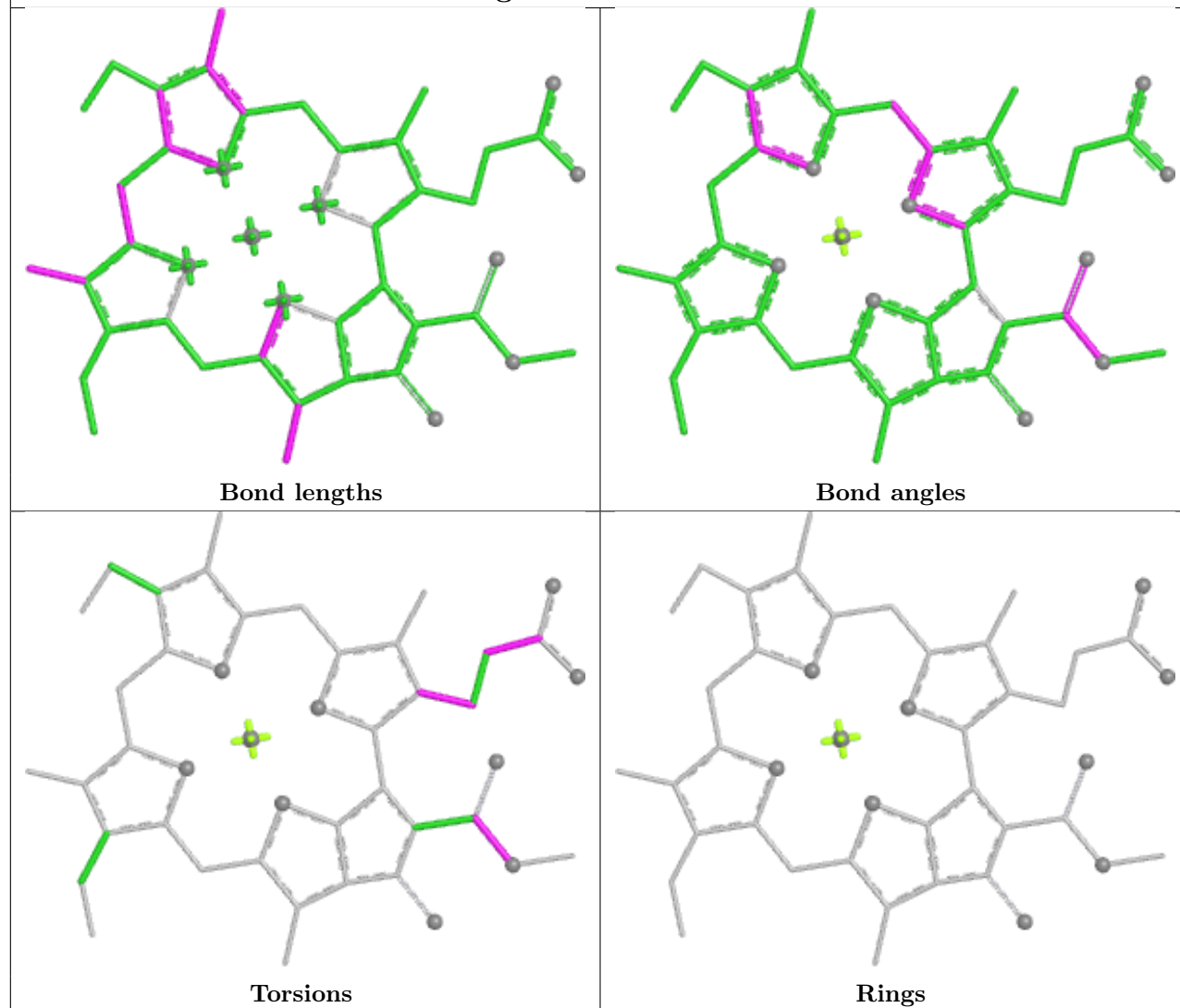
Ligand CLA f 506

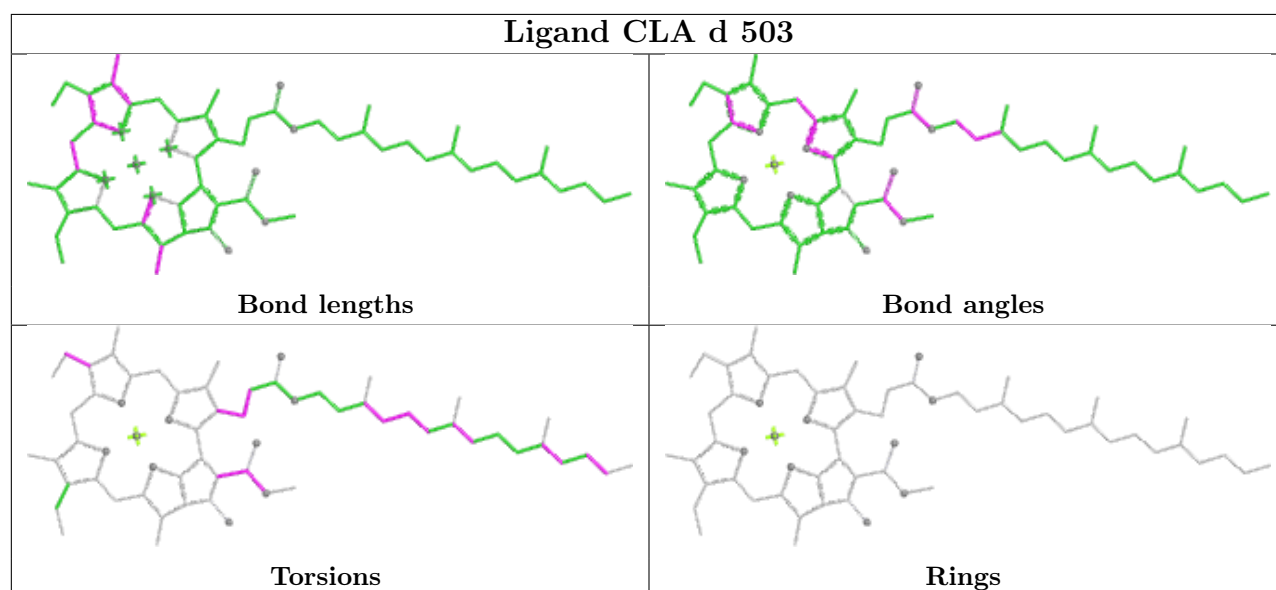
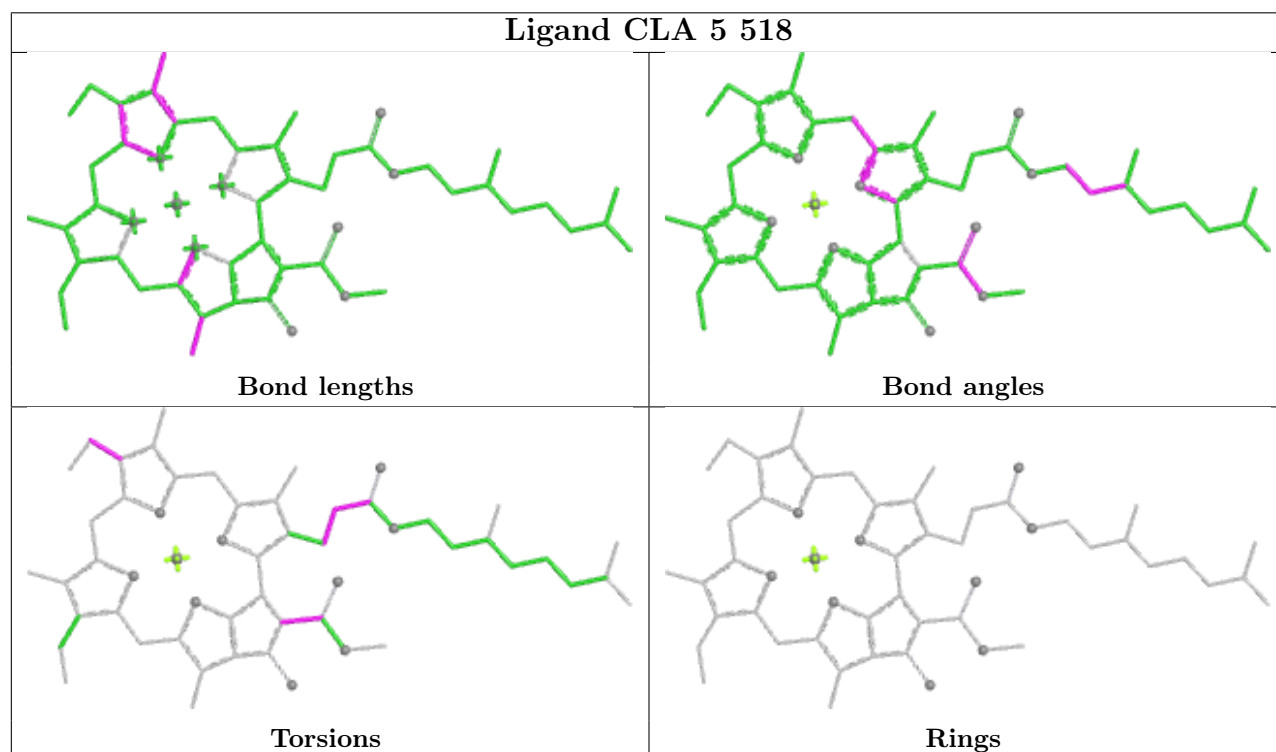
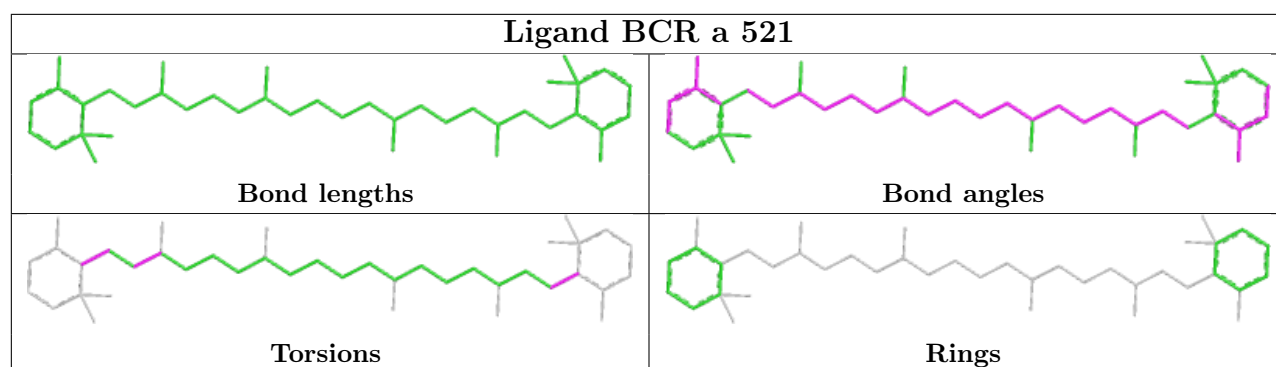


Ligand CLA B 1226

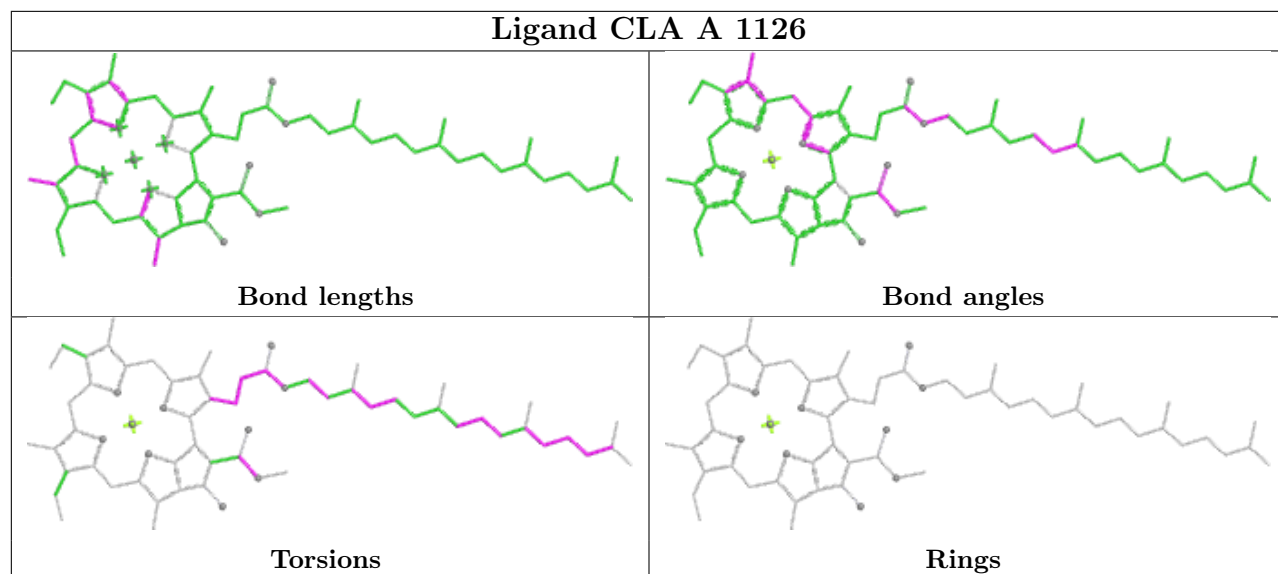


Ligand CLA 2 513

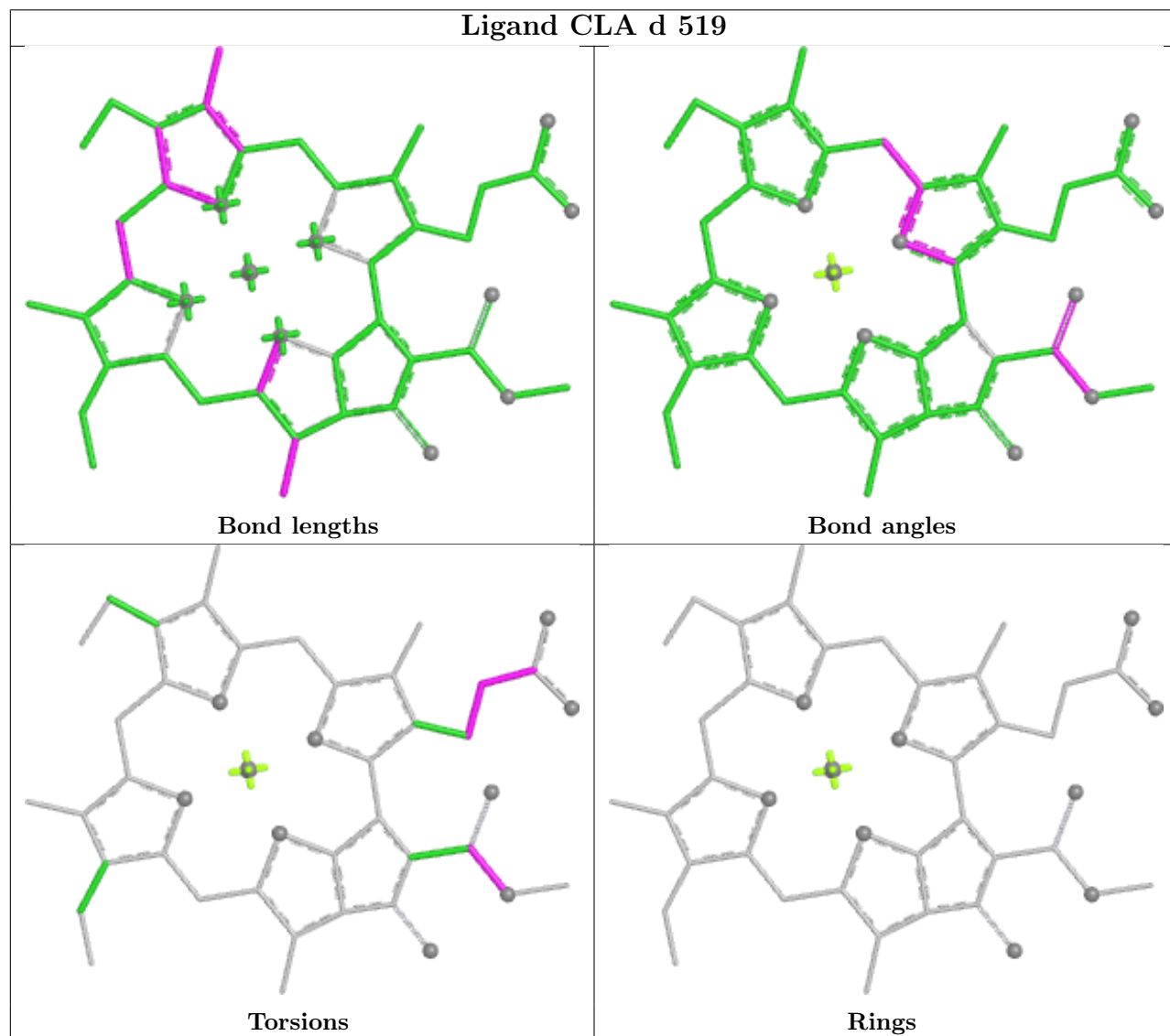


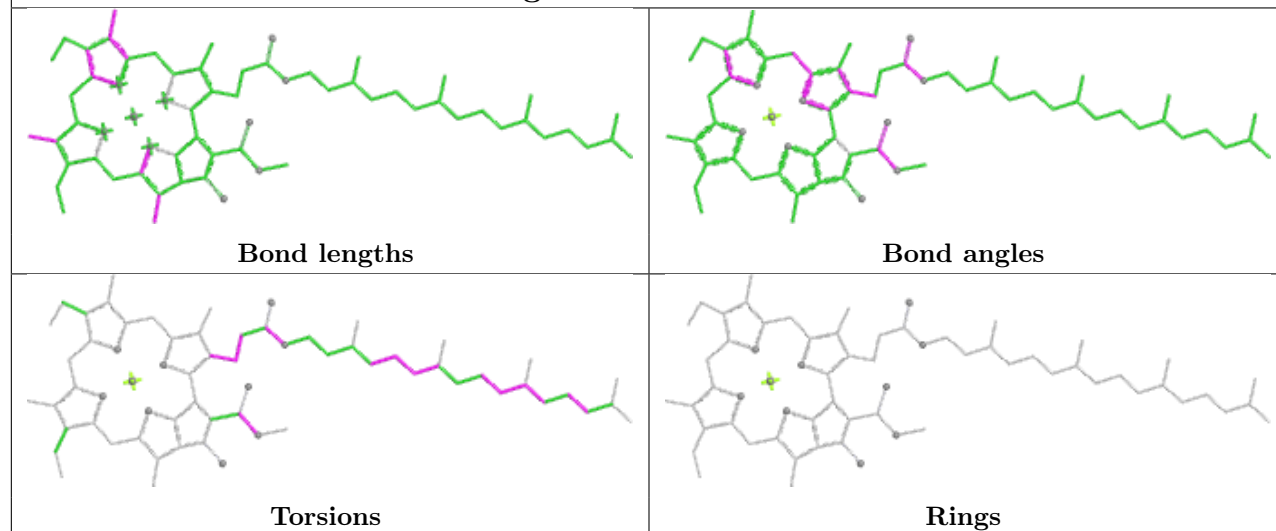
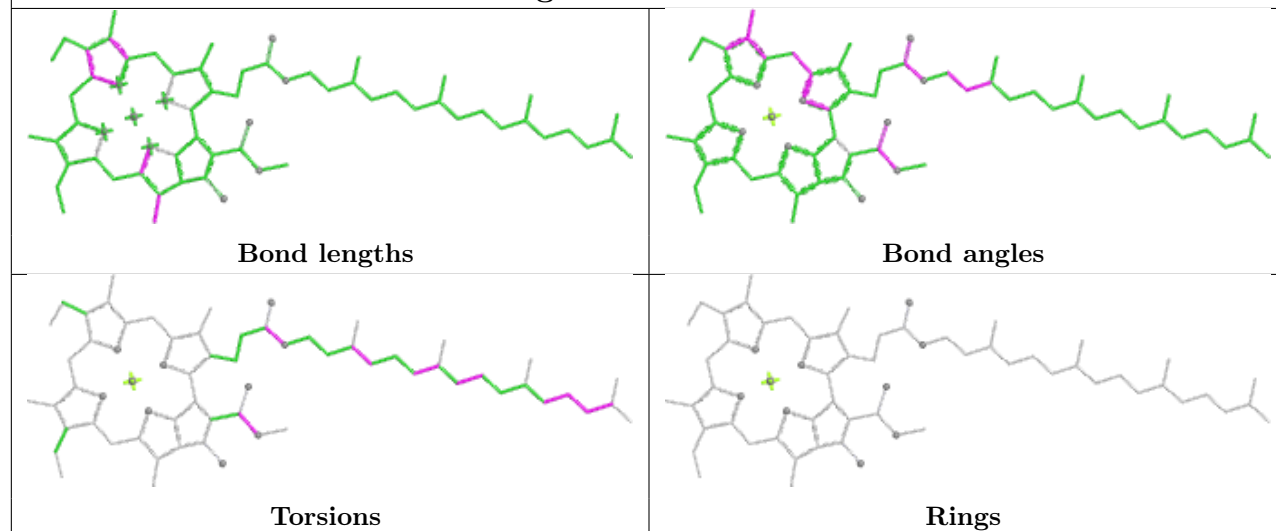


Ligand CLA A 1126

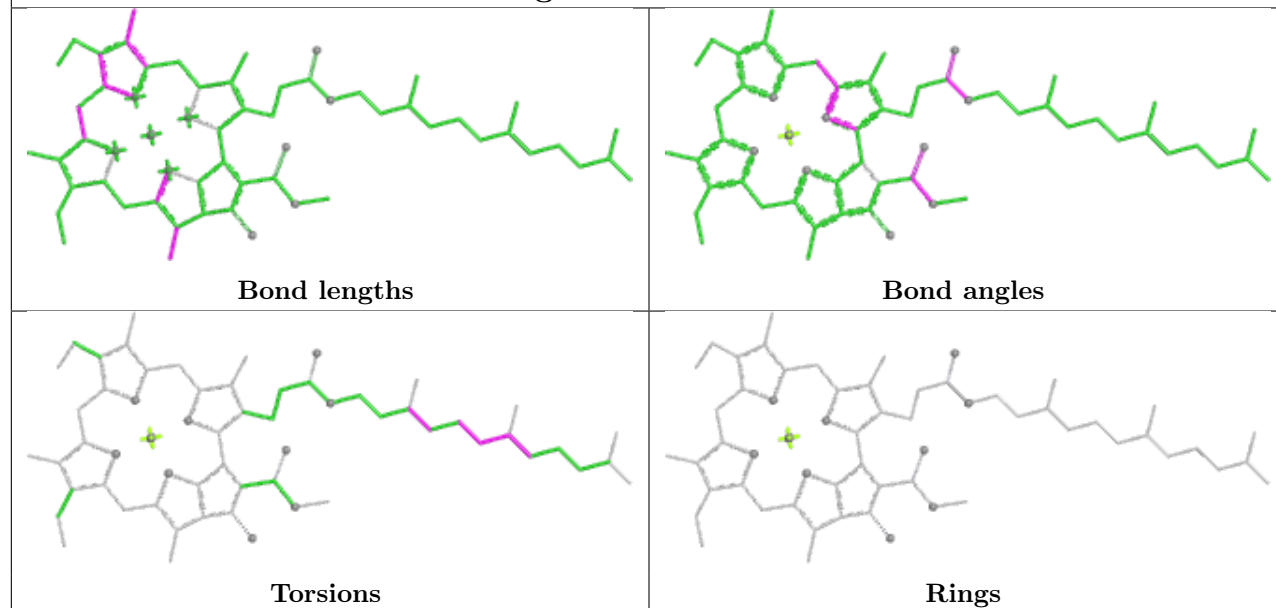


Ligand CLA d 519

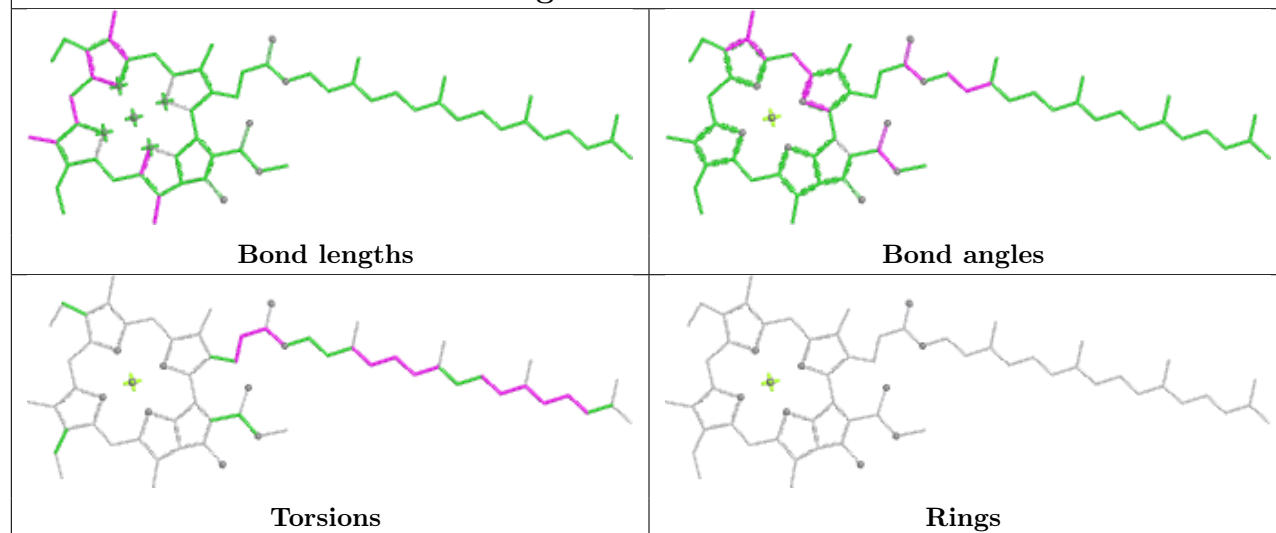


Ligand CLA B 1210**Ligand CLA 5 505**

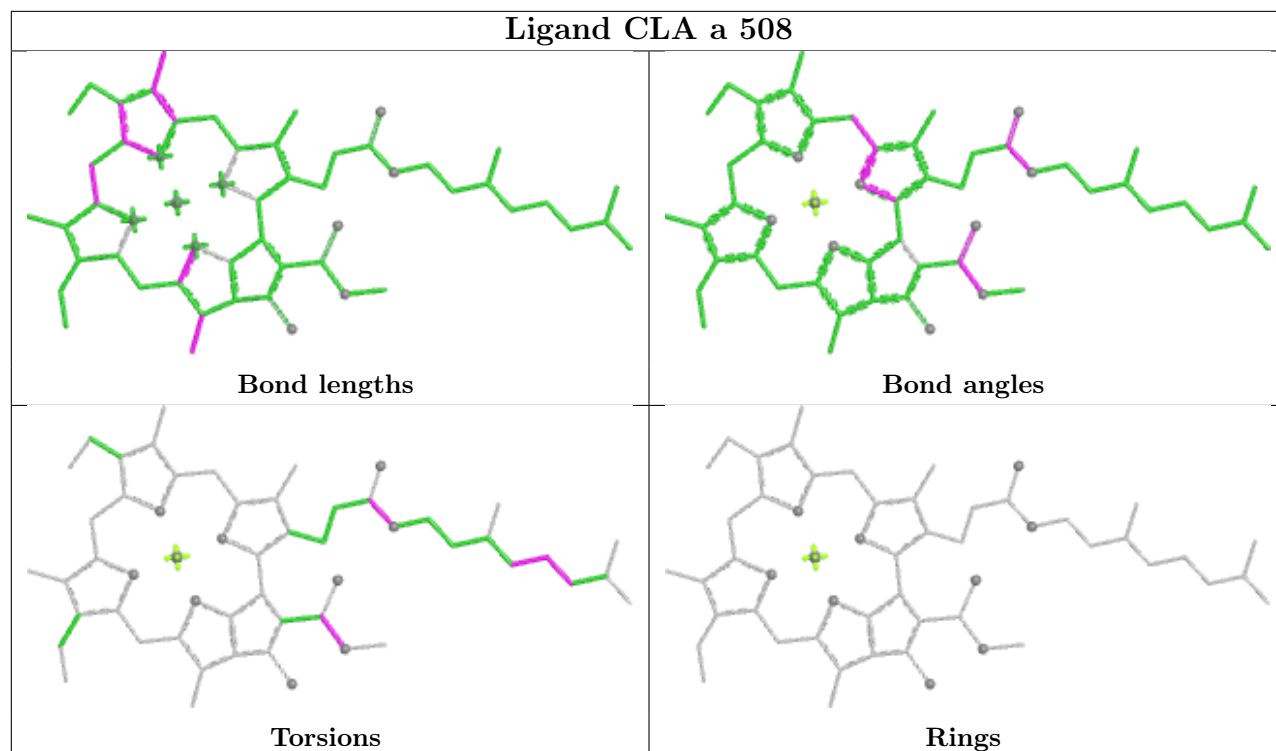
Ligand CLA b 507



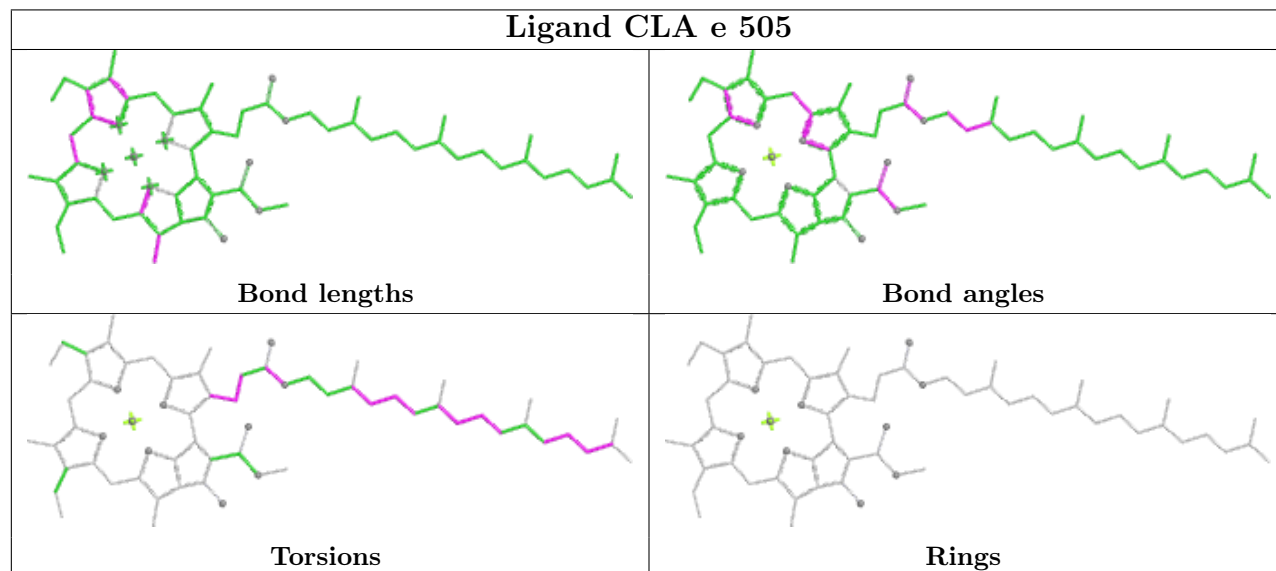
Ligand CLA 3 510

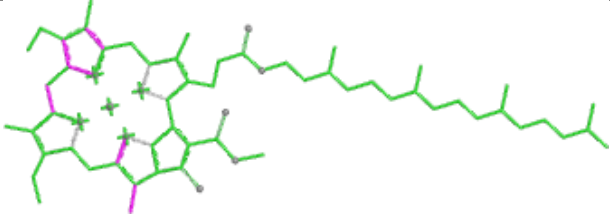
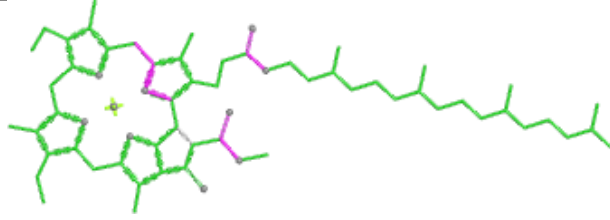
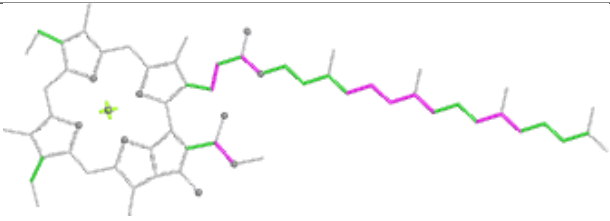
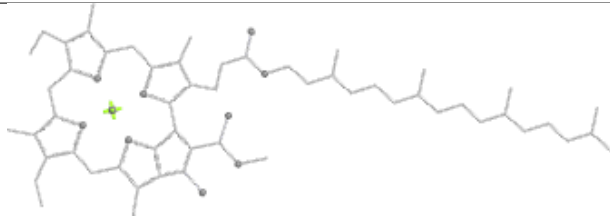
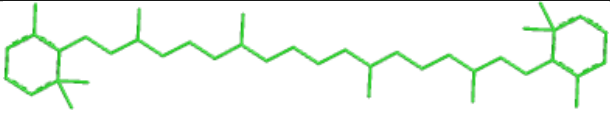
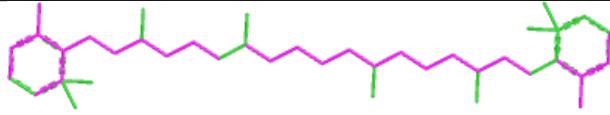
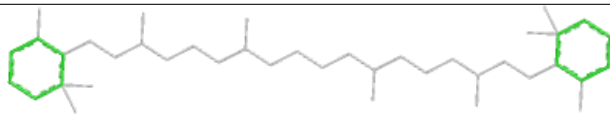
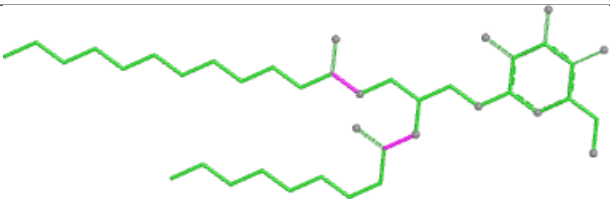
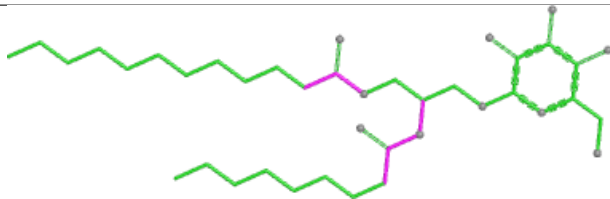
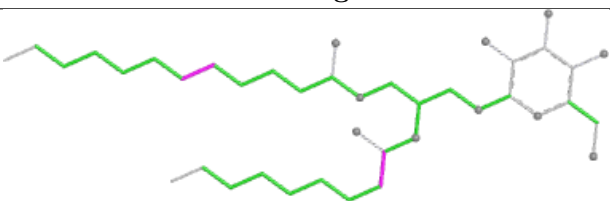
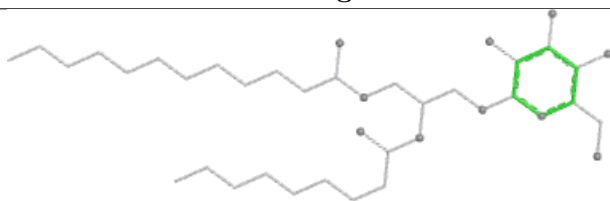


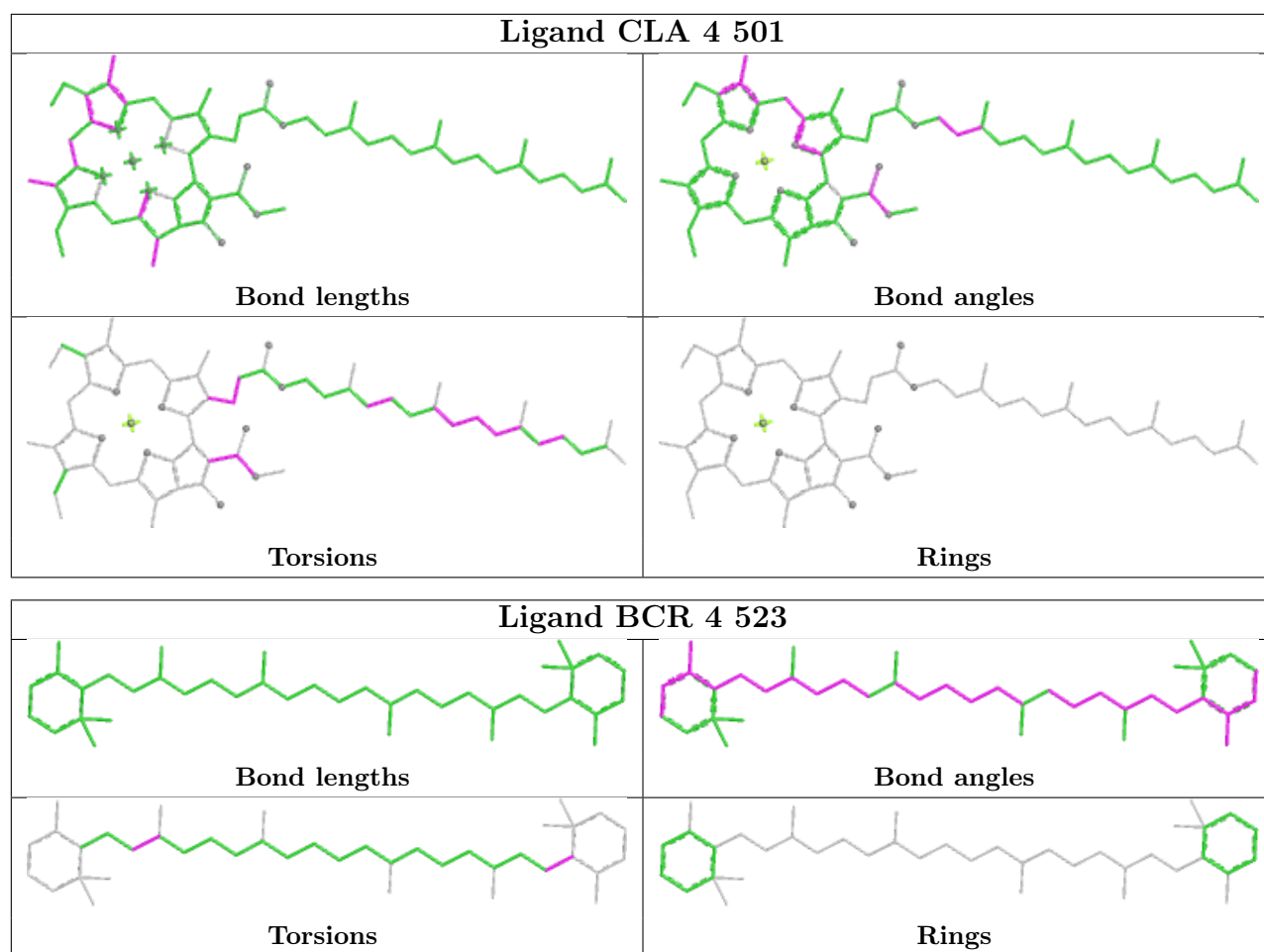
Ligand CLA a 508



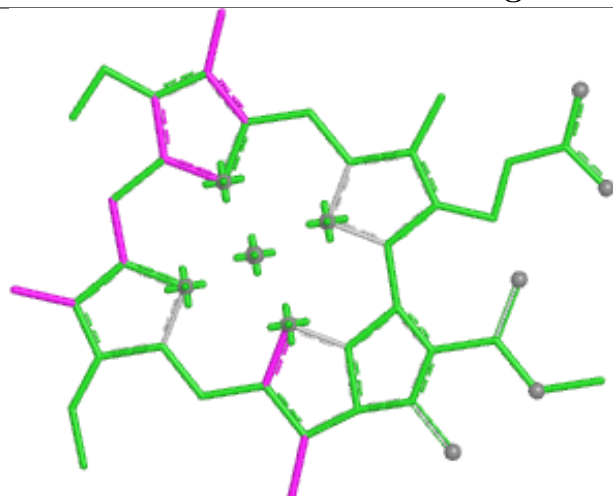
Ligand CLA e 505



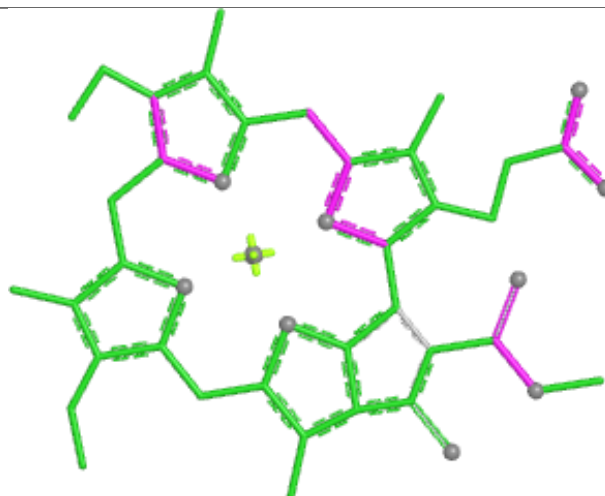
Ligand CLA a 505	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR M 4021	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG g 5104	
 Bond lengths	 Bond angles
 Torsions	 Rings



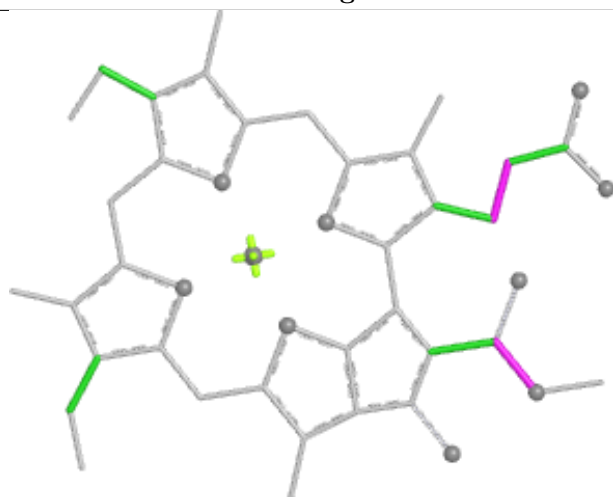
Ligand CLA X 1401



Bond lengths



Bond angles

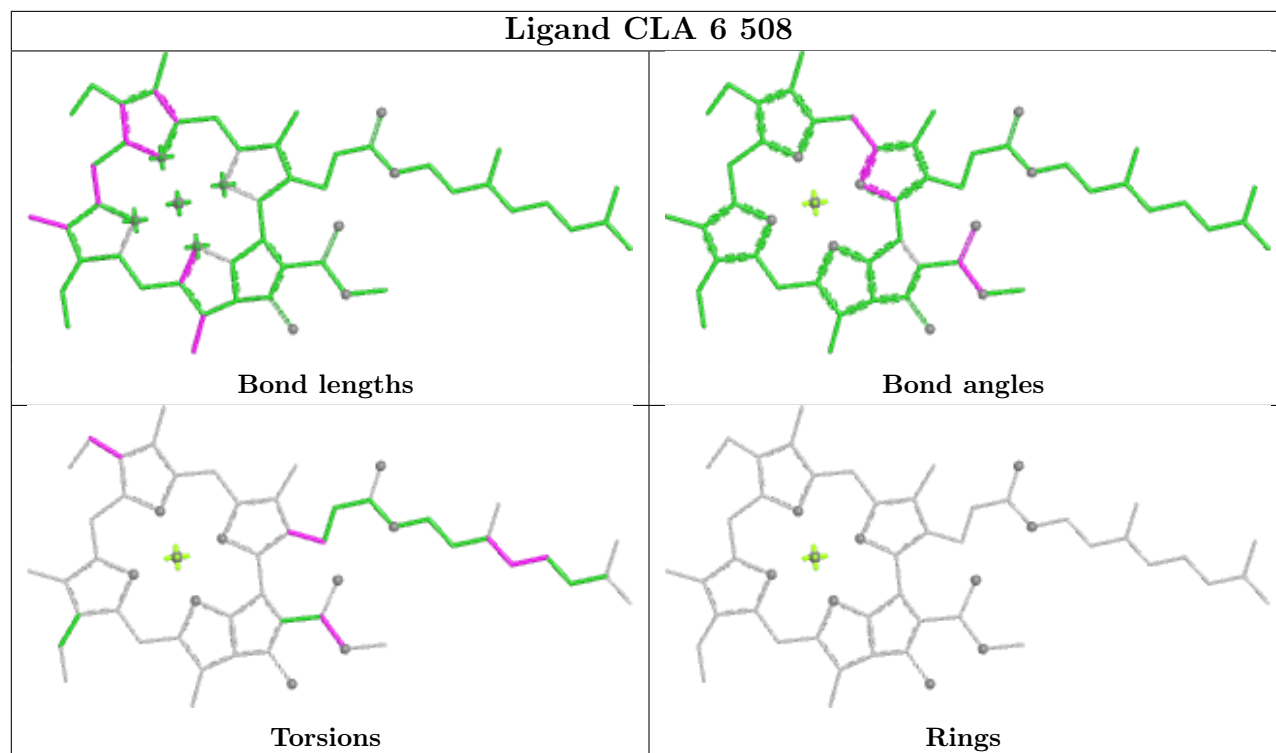


Torsions

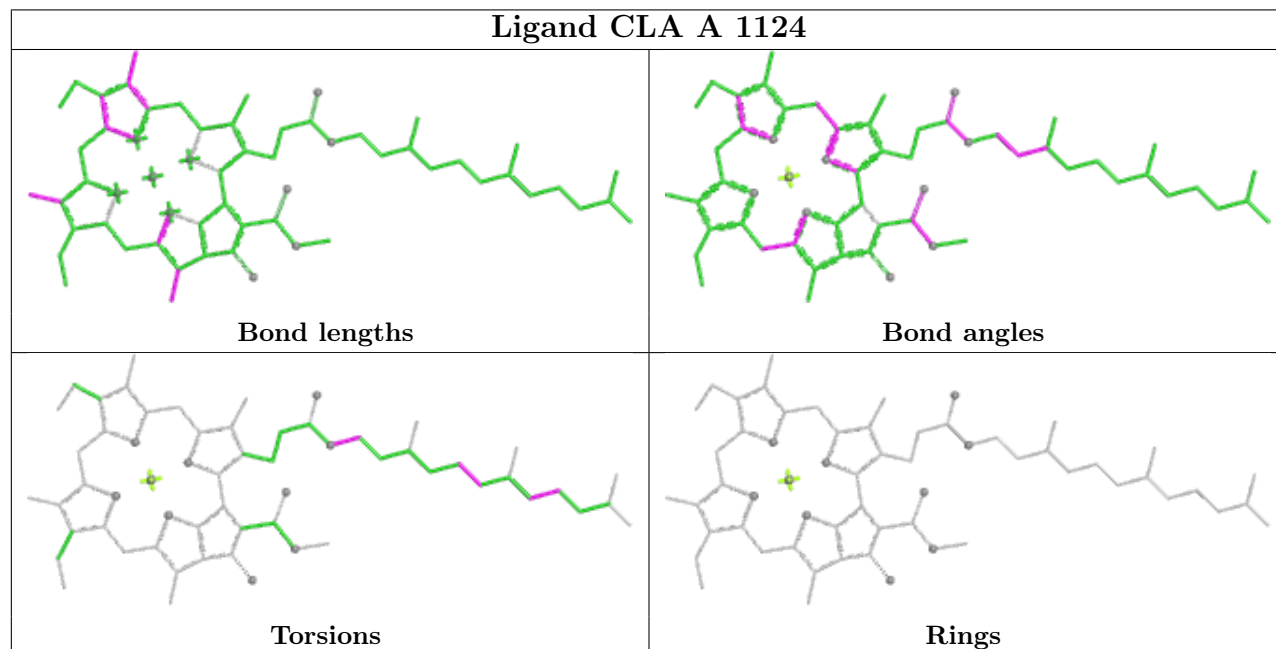


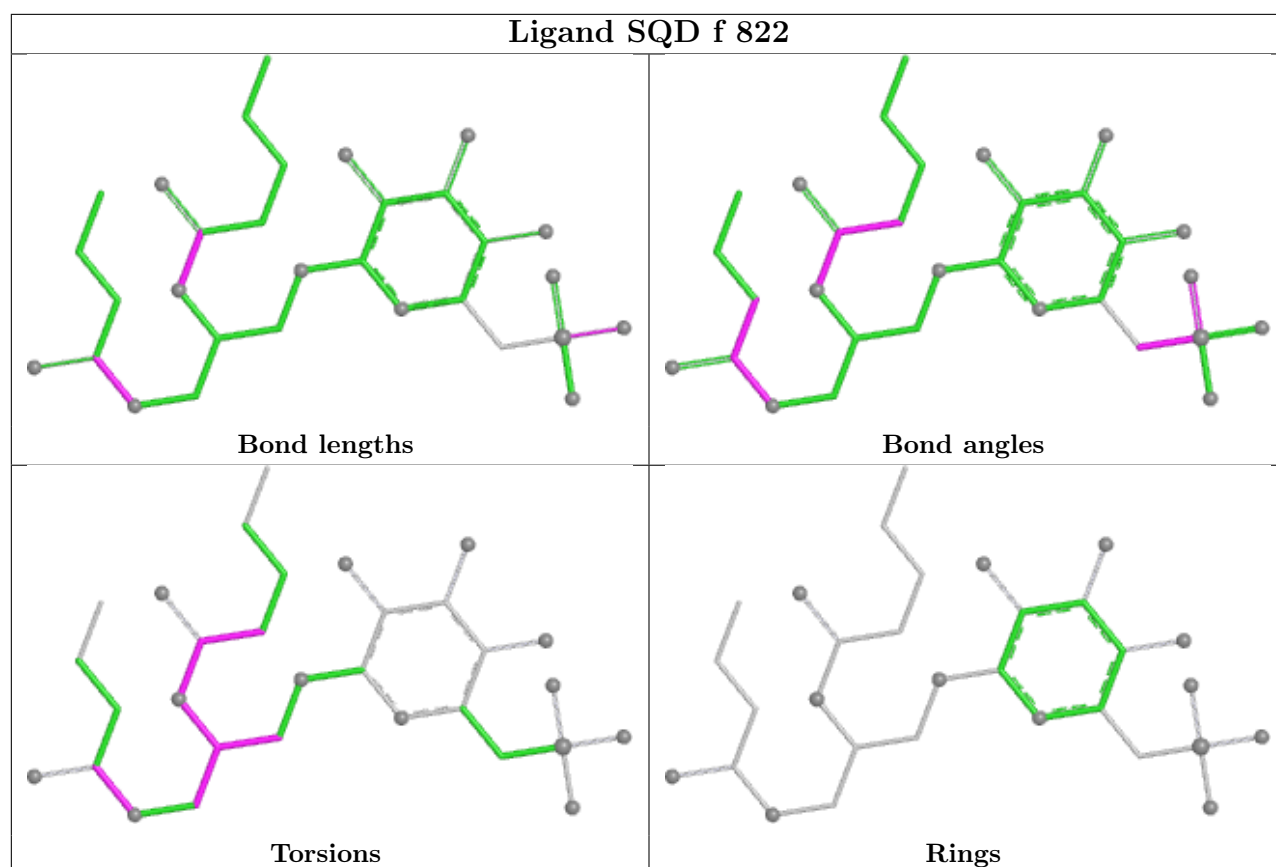
Rings

Ligand CLA 6 508

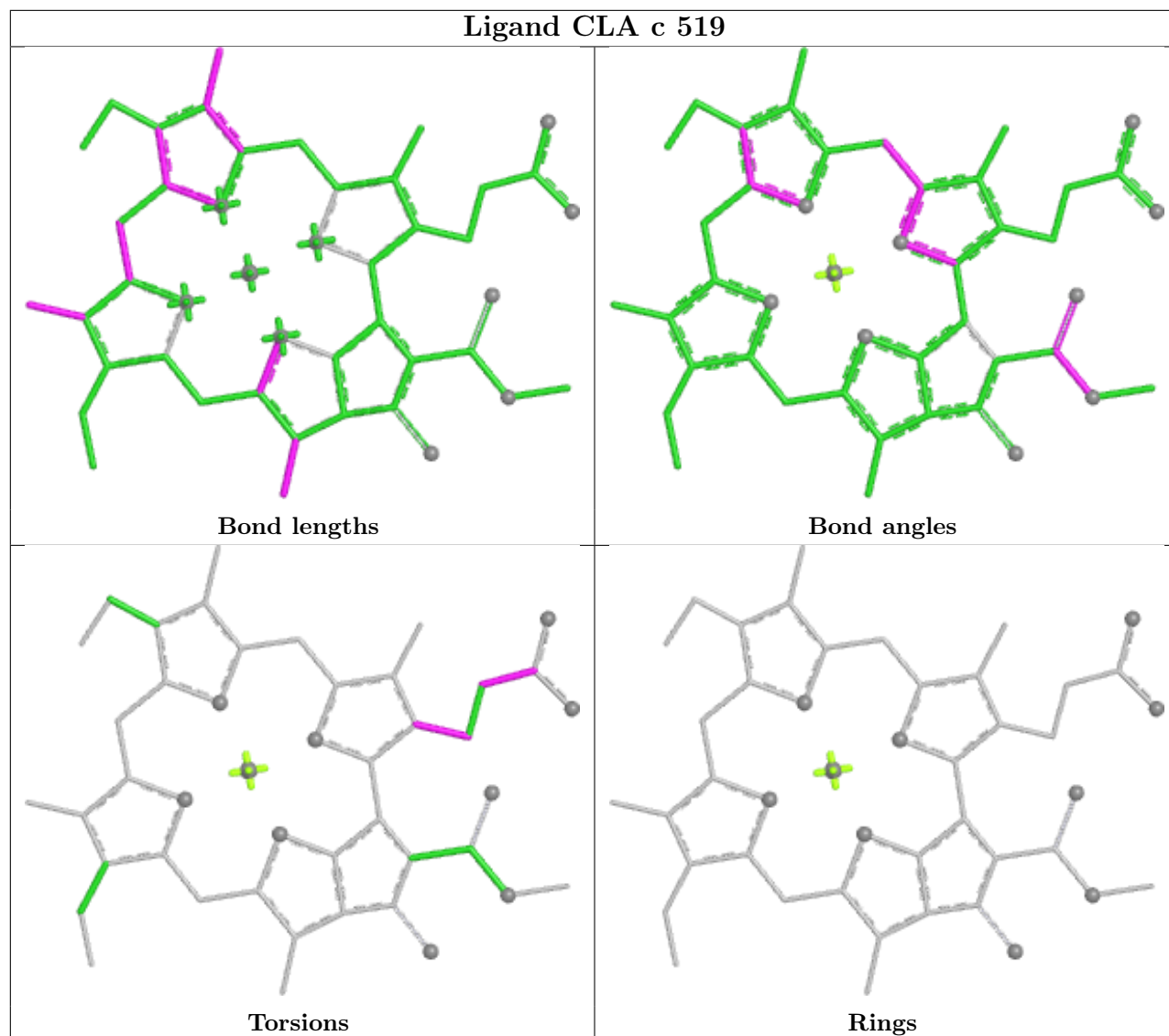


Ligand CLA A 1124

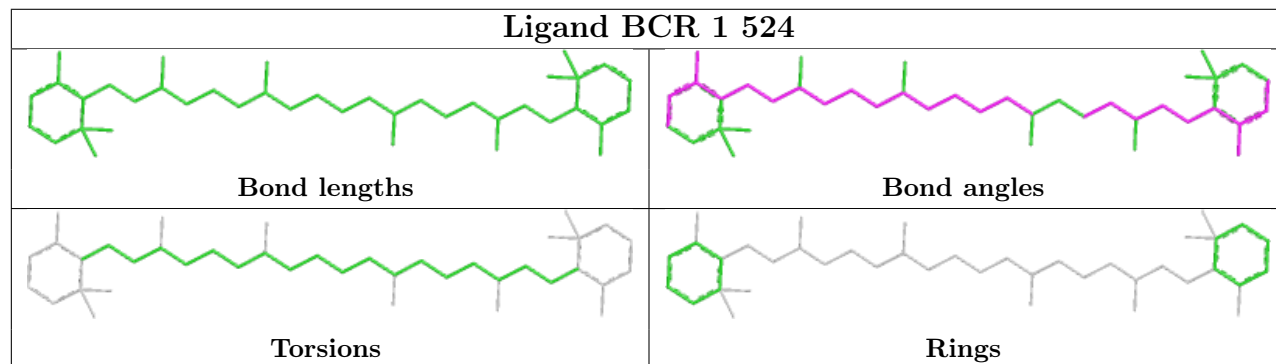


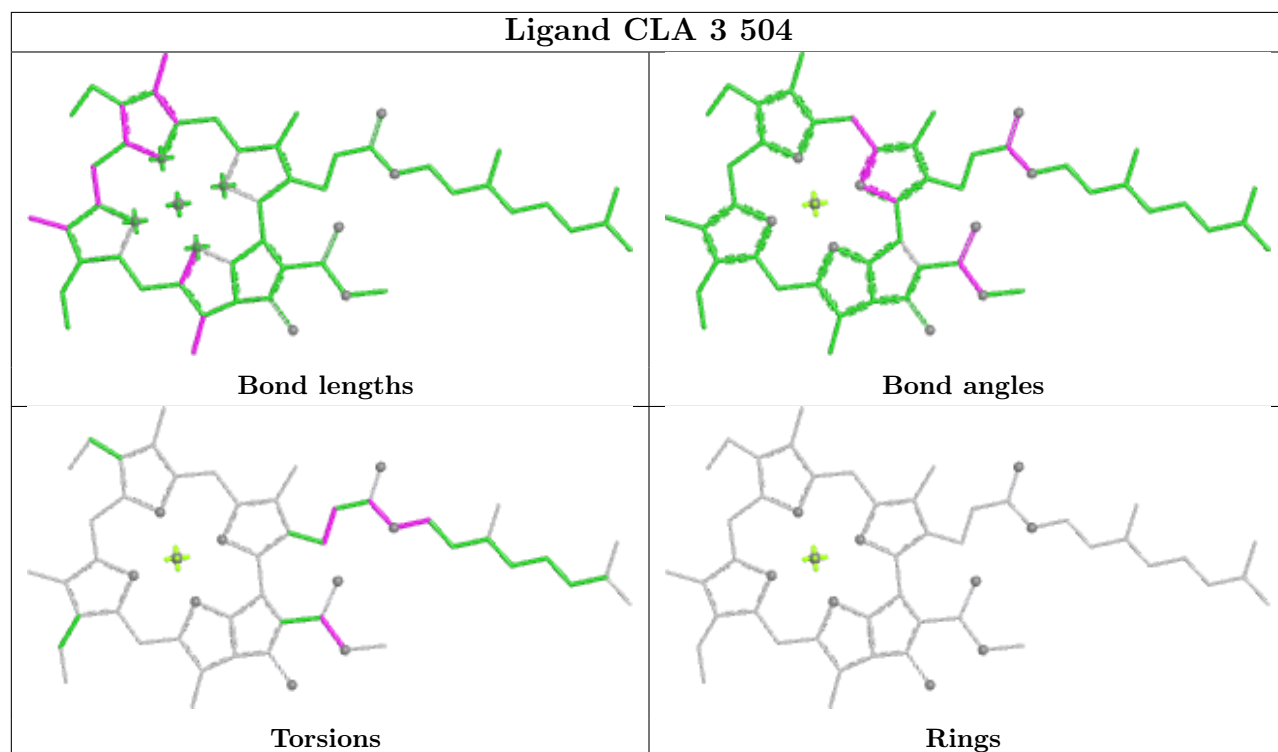
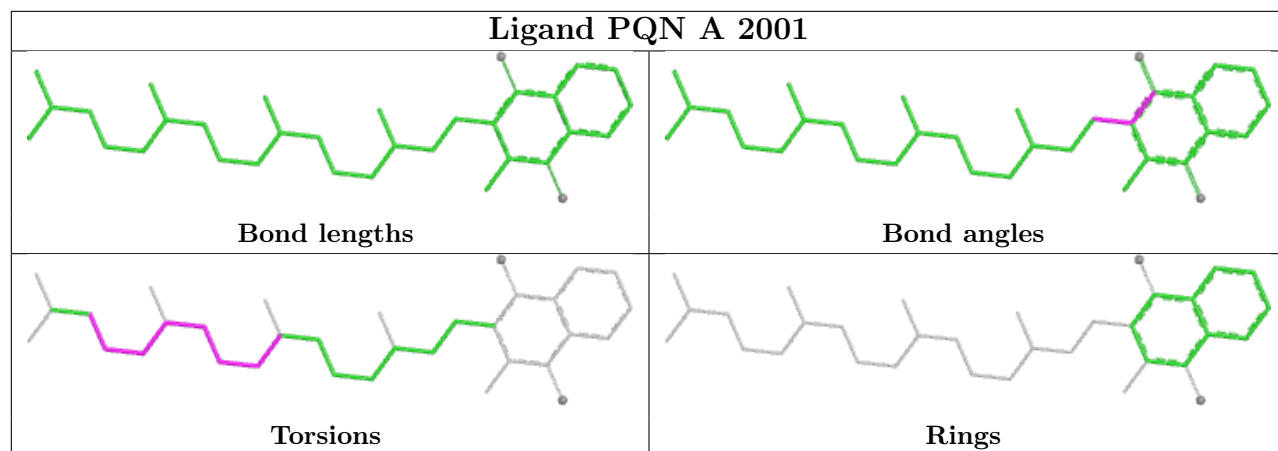


Ligand CLA c 519

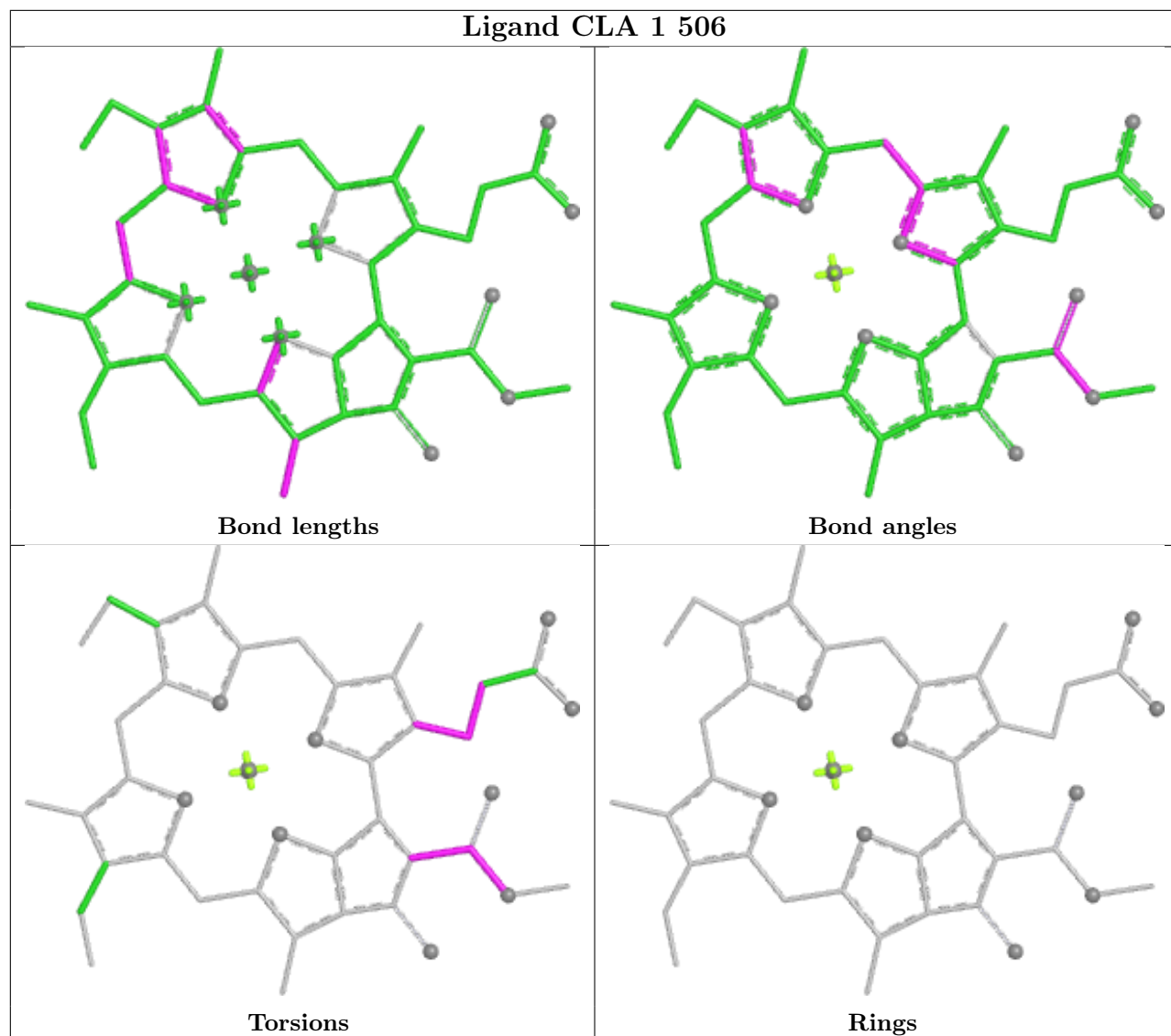


Ligand BCR 1 524

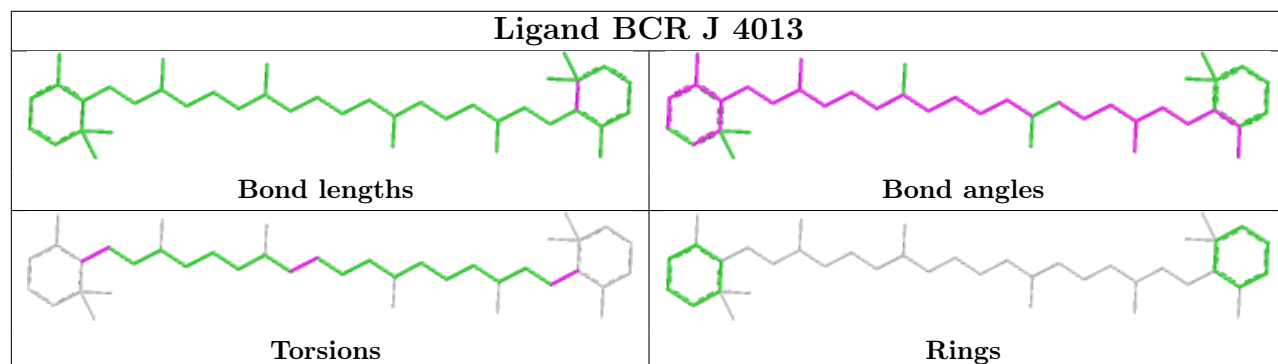


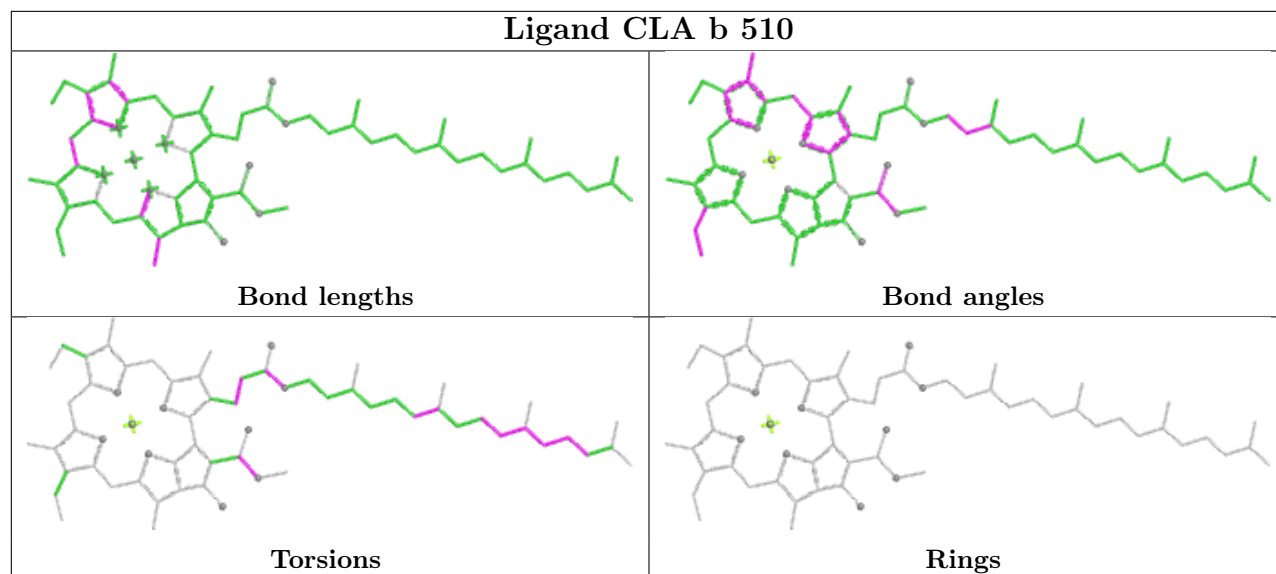
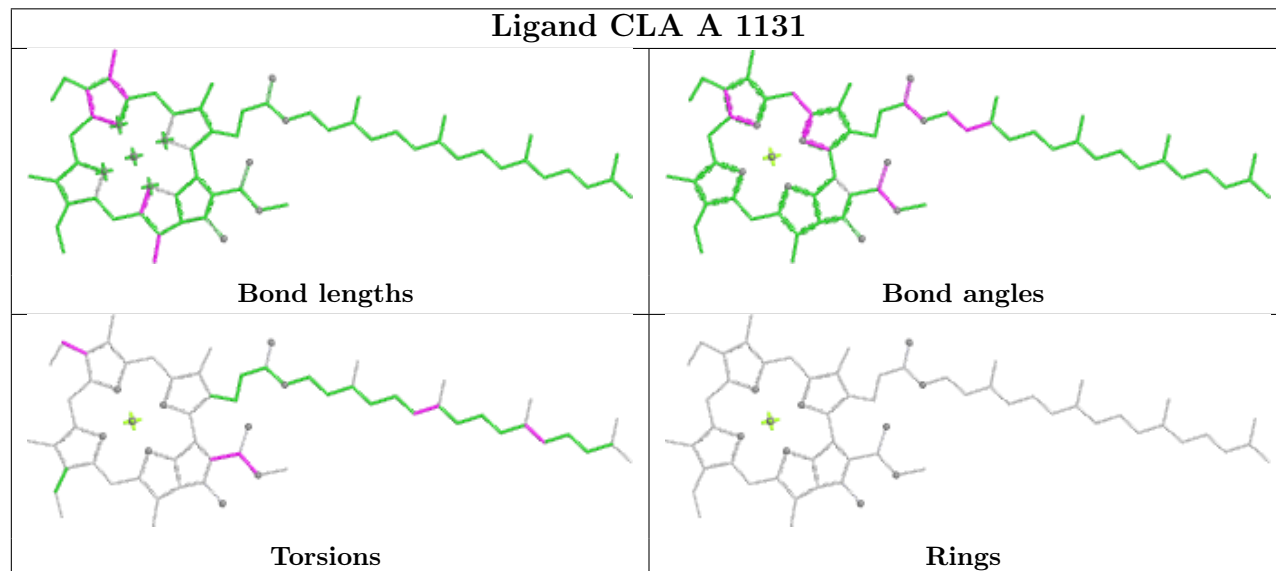


Ligand CLA 1 506

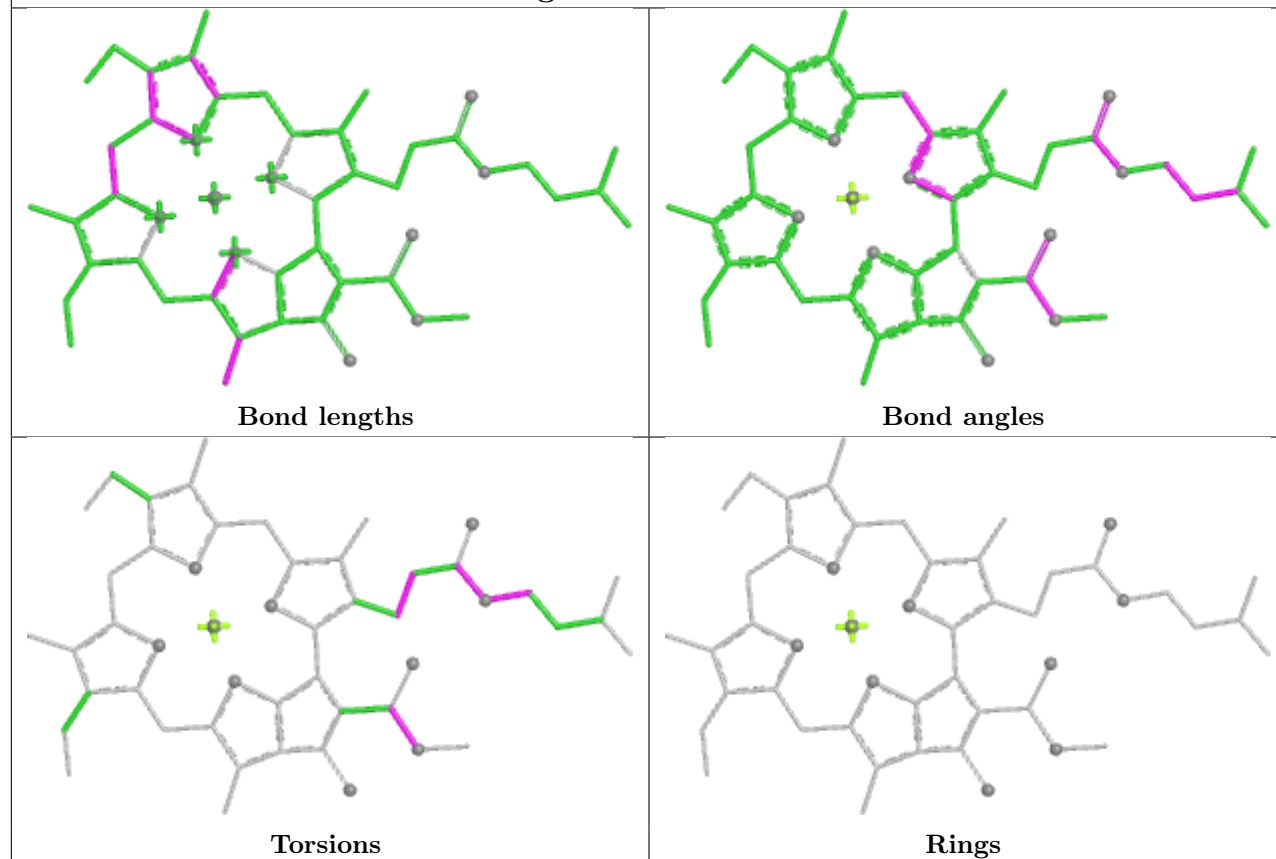


Ligand BCR J 4013

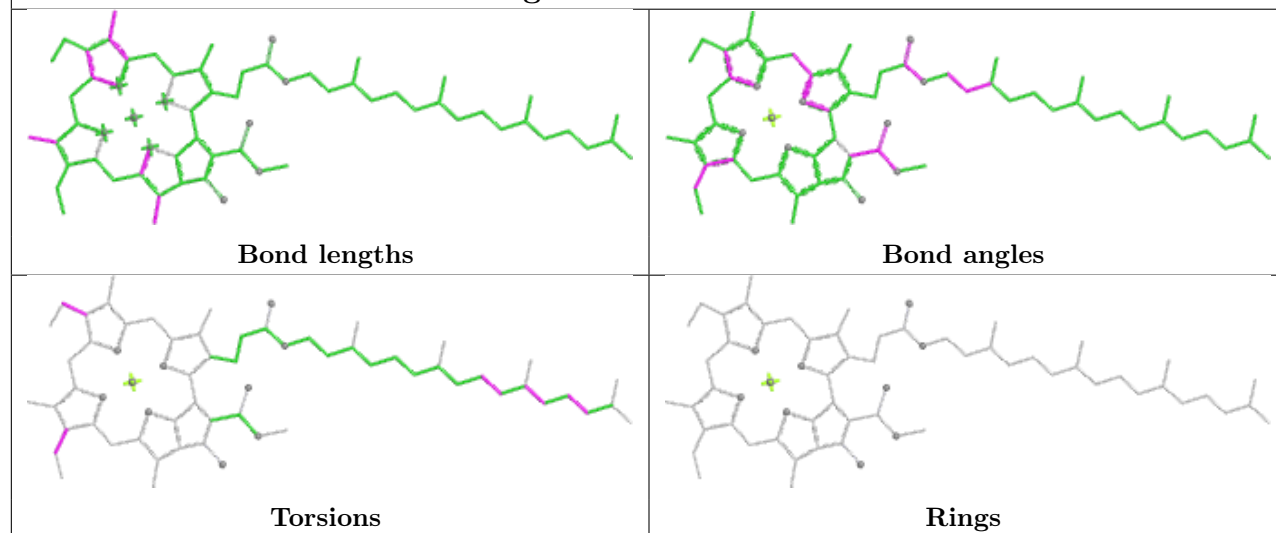


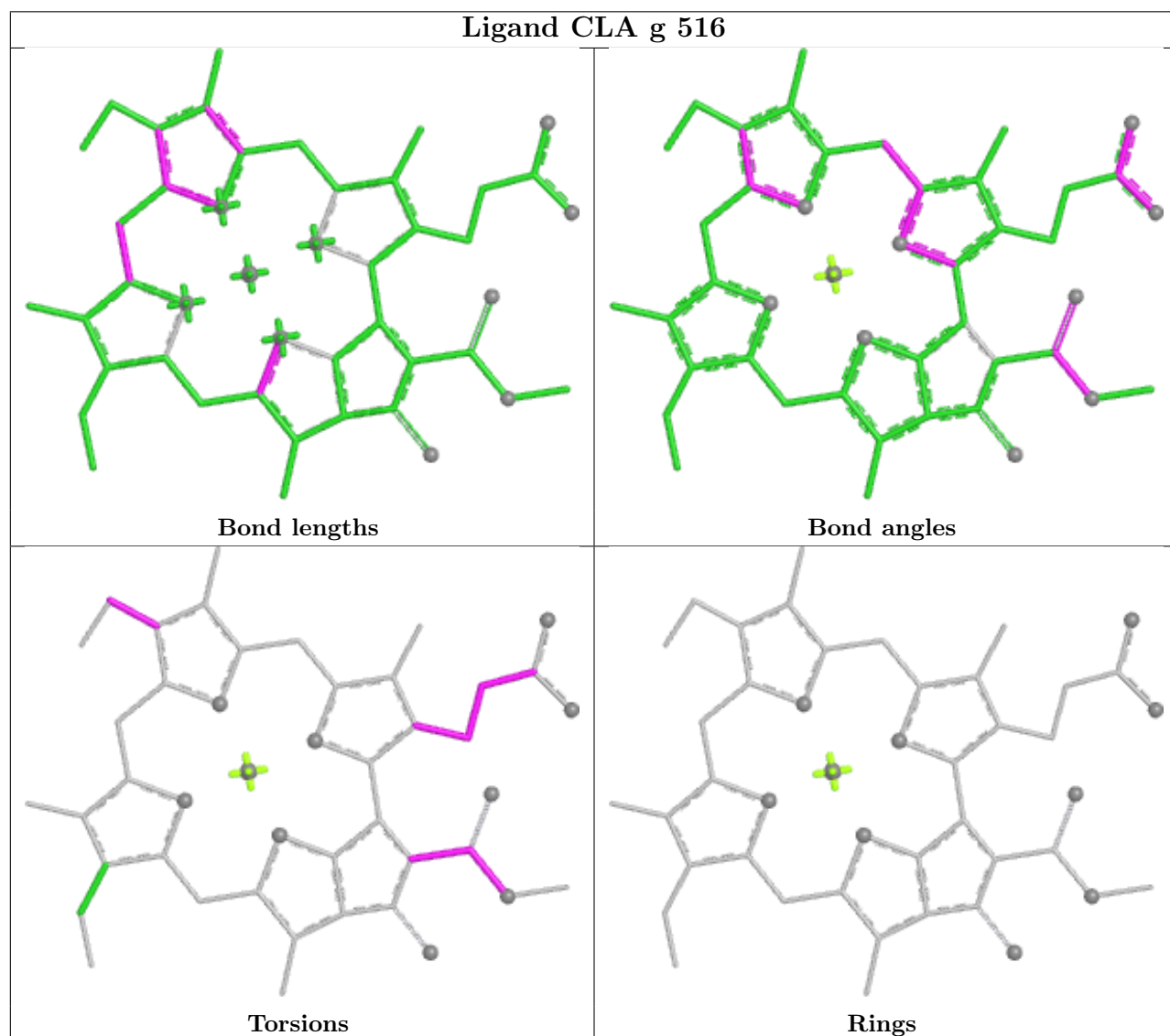
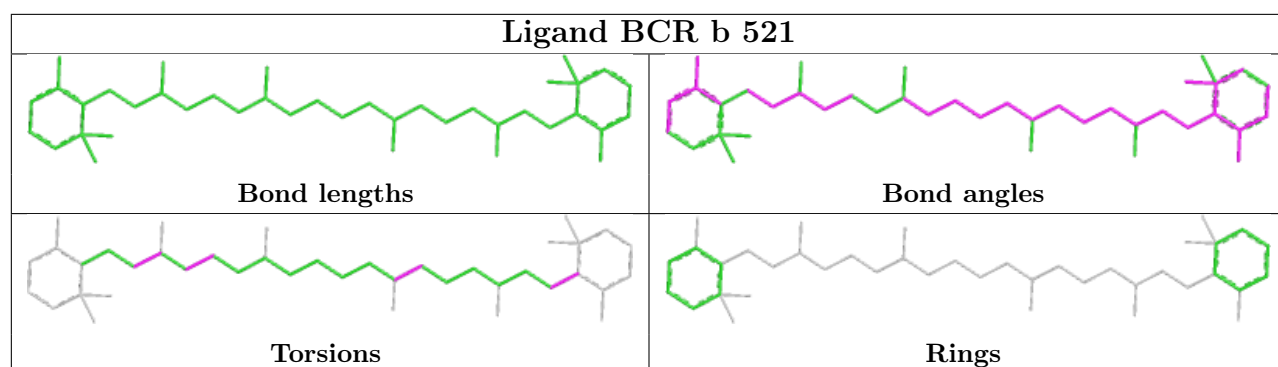
Ligand CLA b 510**Ligand CLA A 1131**

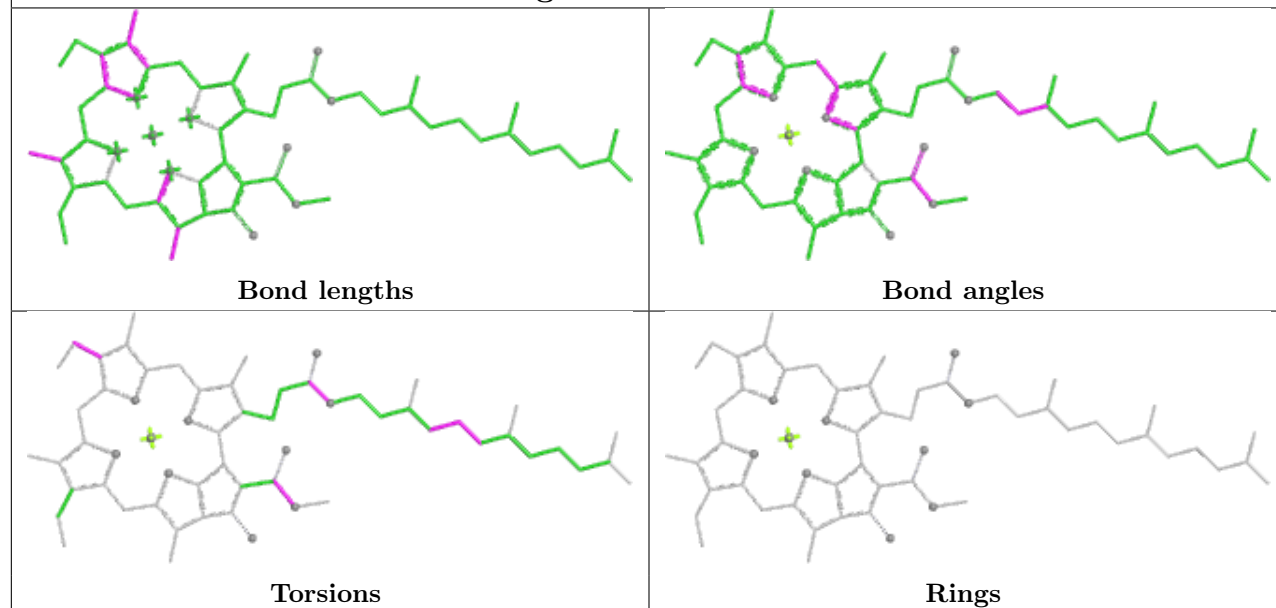
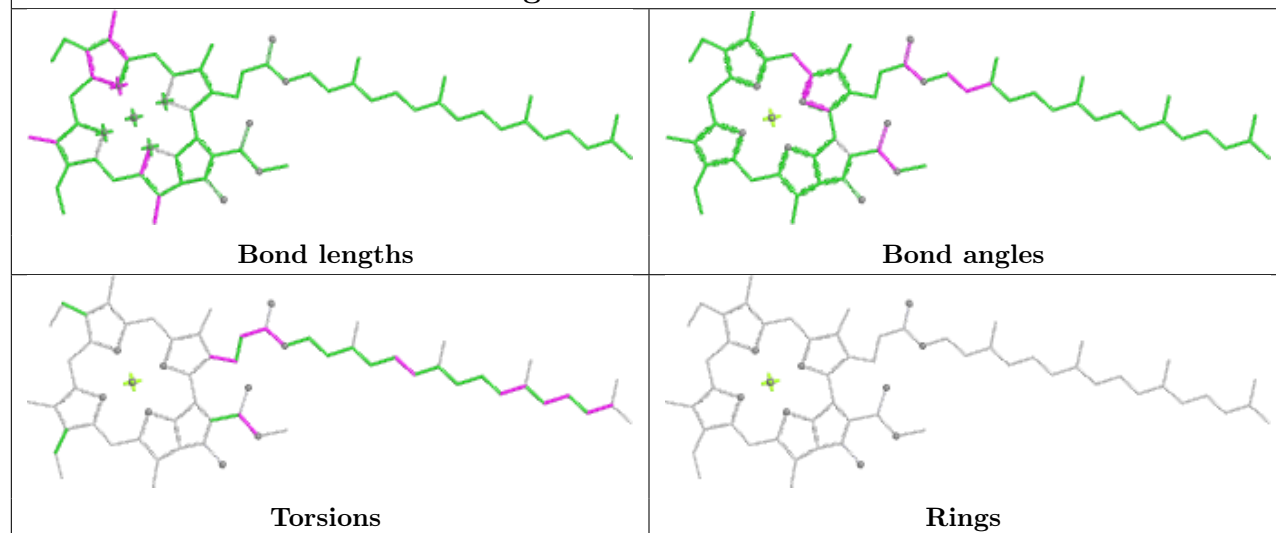
Ligand CLA c 504



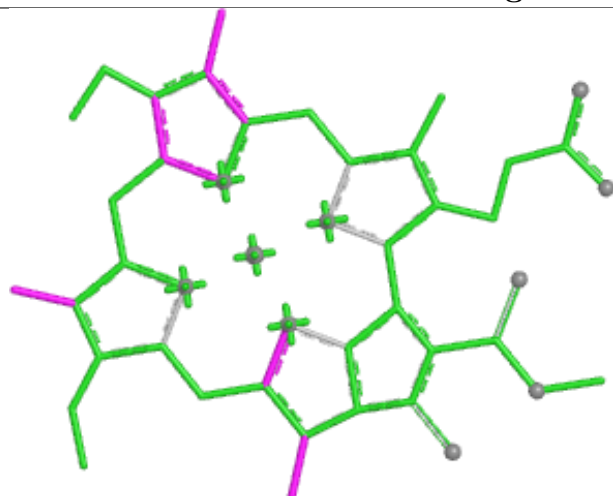
Ligand CLA B 1023



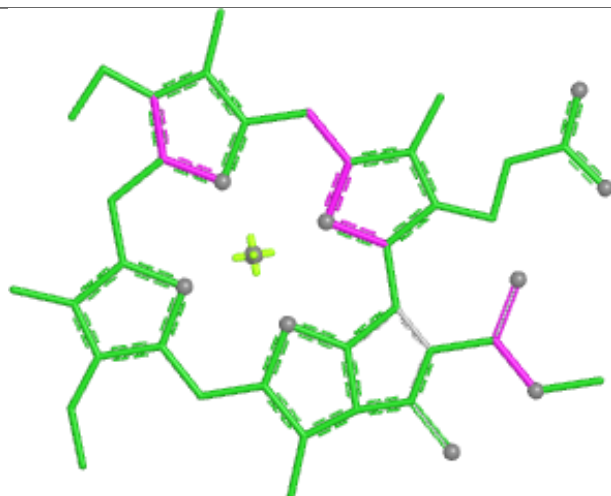


Ligand CLA 4 502**Ligand CLA B 1206**

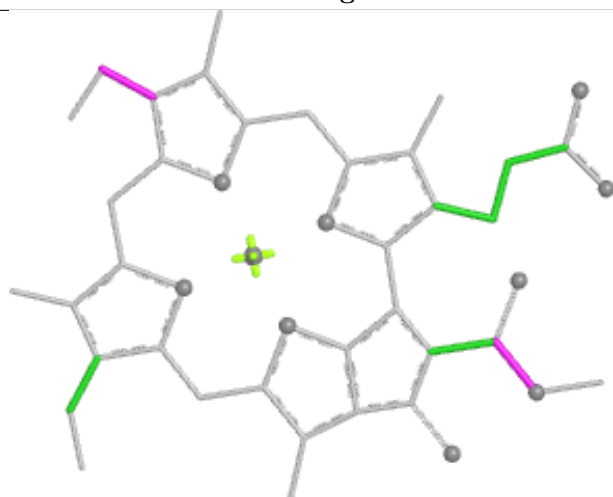
Ligand CLA B 1212



Bond lengths



Bond angles

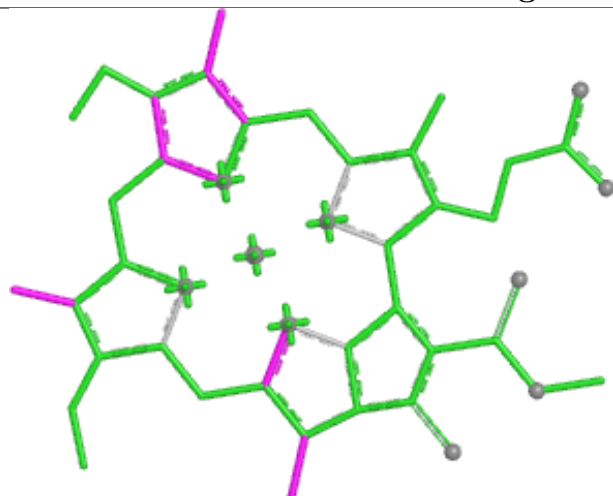


Torsions

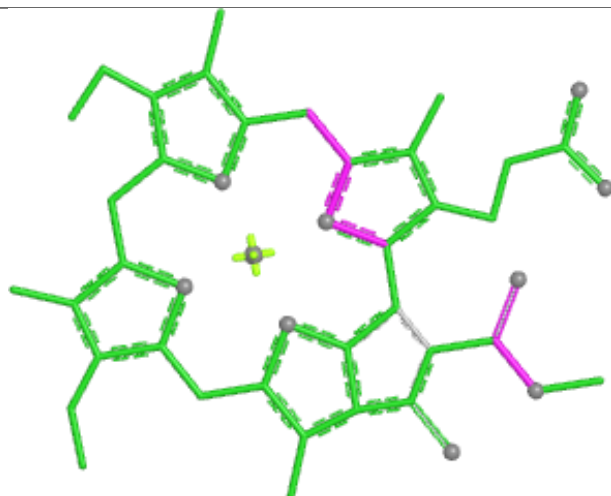


Rings

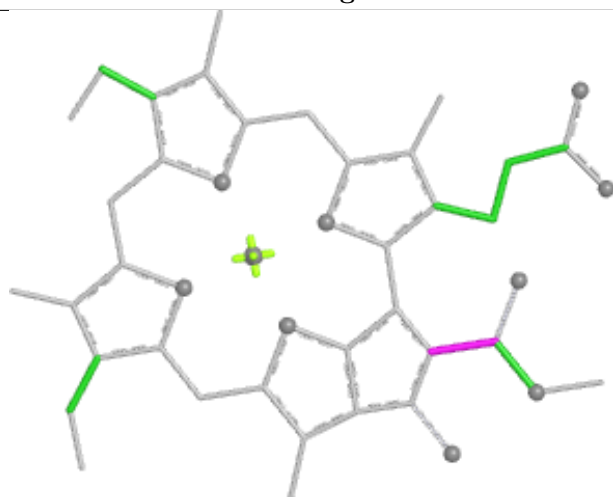
Ligand CLA 4 504



Bond lengths



Bond angles

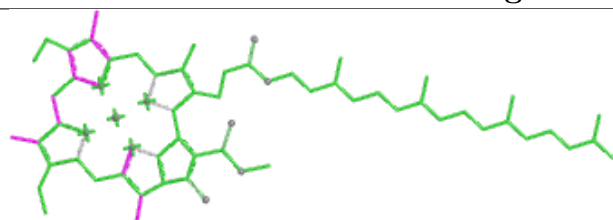


Torsions

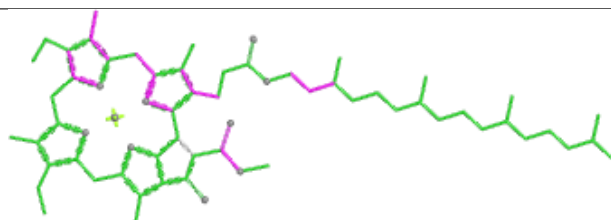


Rings

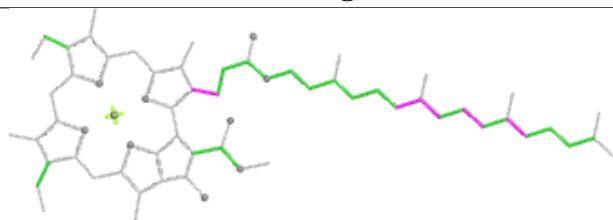
Ligand CLA A 1104



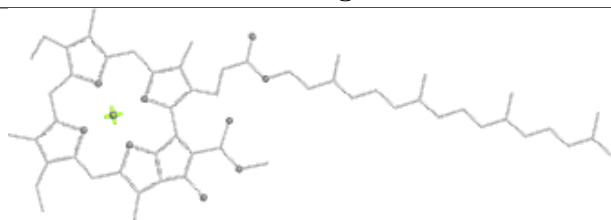
Bond lengths



Bond angles

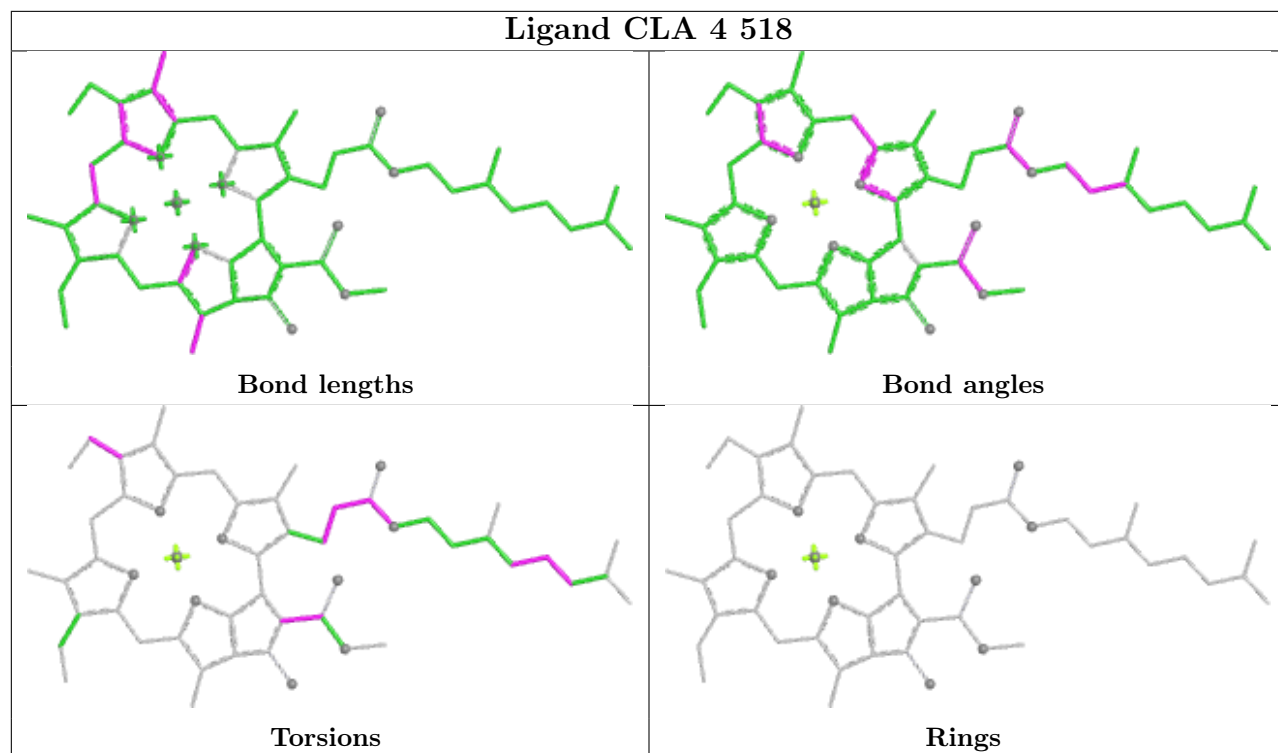


Torsions

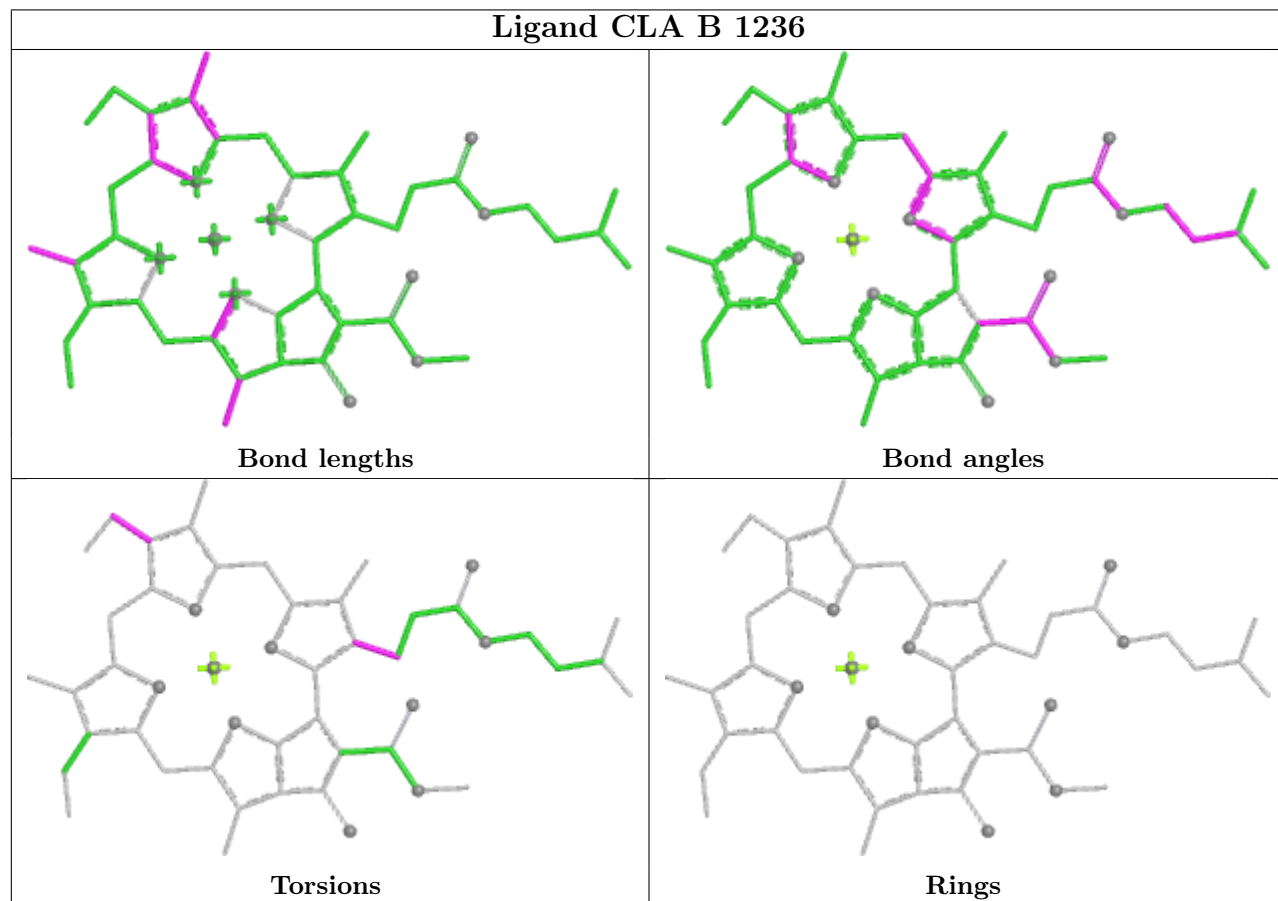


Rings

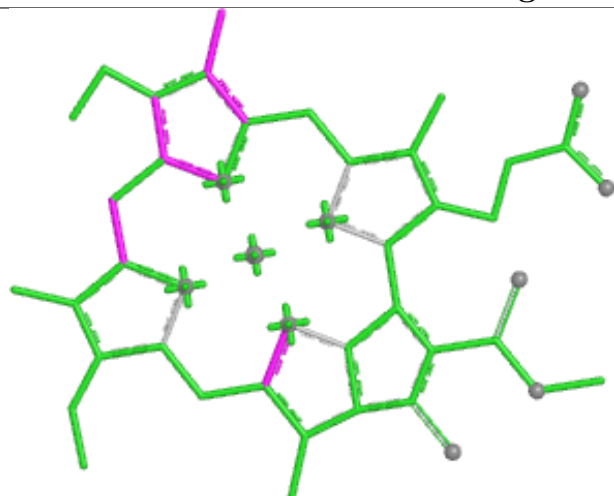
Ligand CLA 4 518



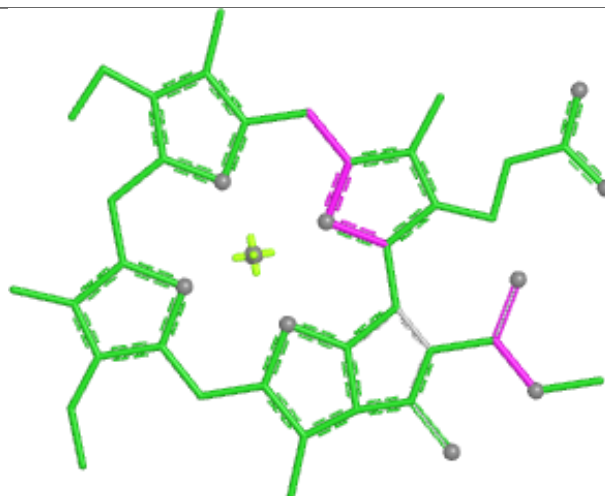
Ligand CLA B 1236



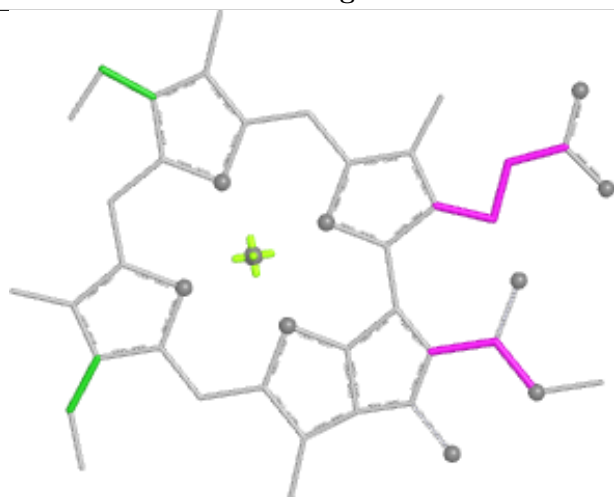
Ligand CLA 6 516



Bond lengths



Bond angles

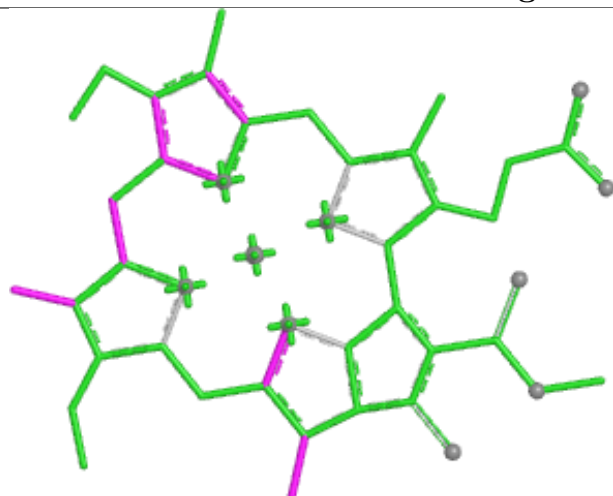


Torsions

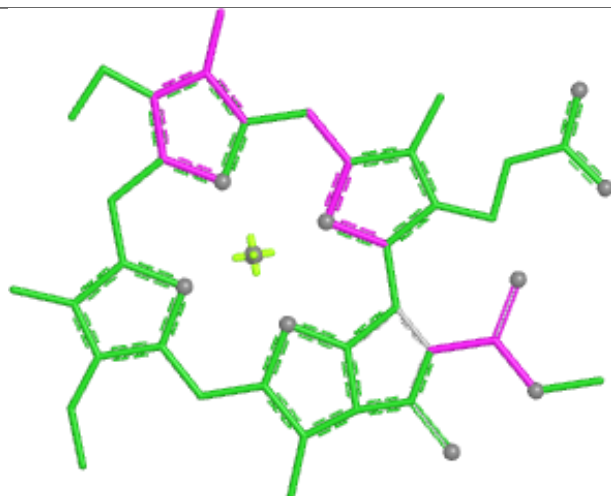


Rings

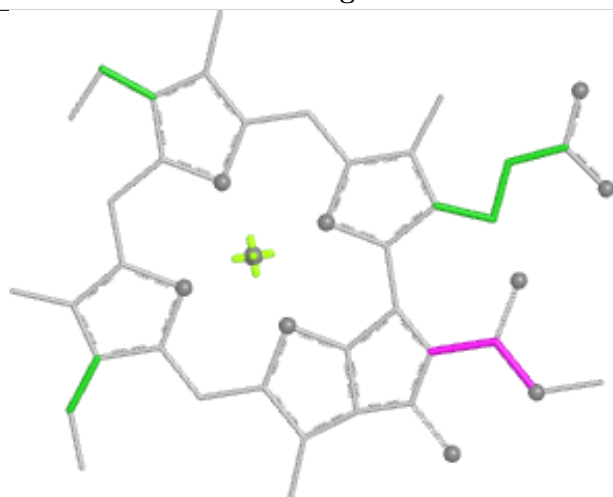
Ligand CLA 3 506



Bond lengths



Bond angles

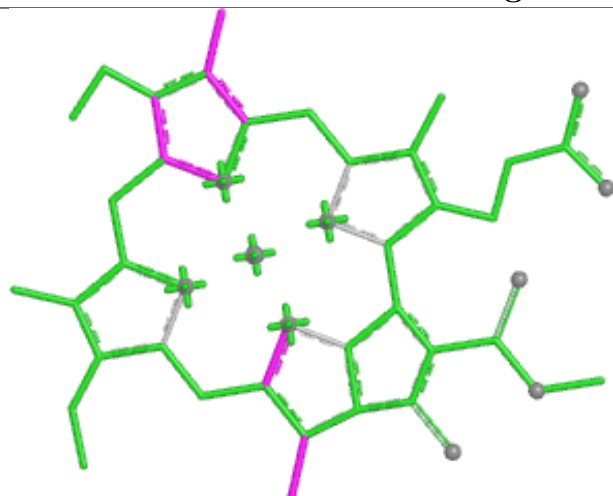


Torsions

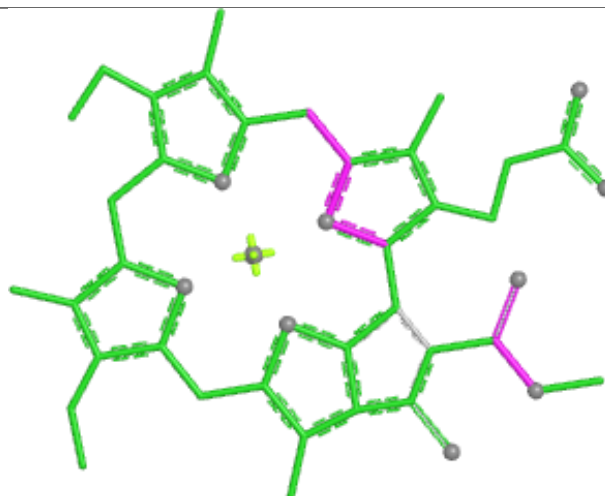


Rings

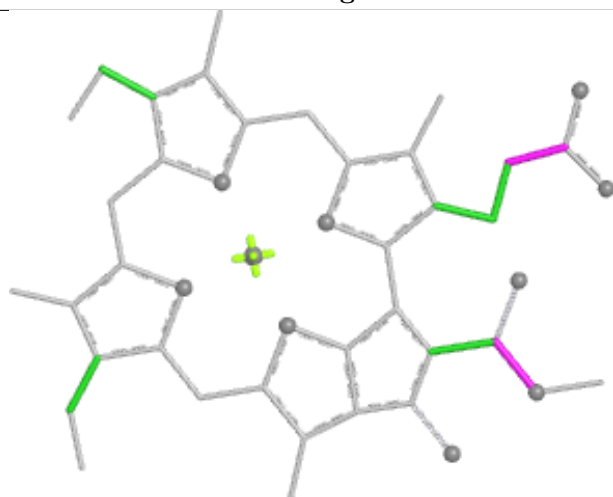
Ligand CLA A 1108



Bond lengths



Bond angles

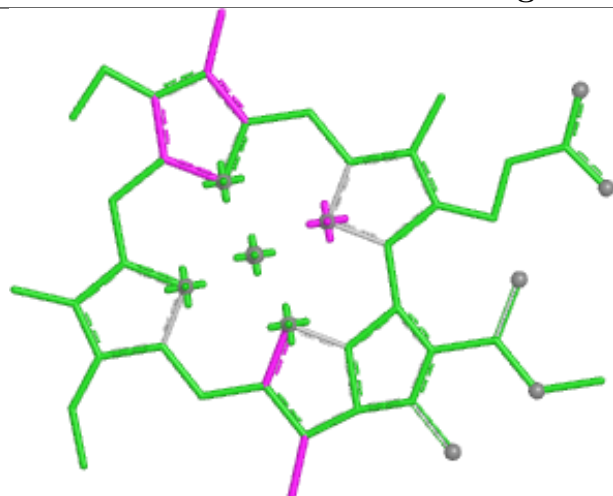


Torsions

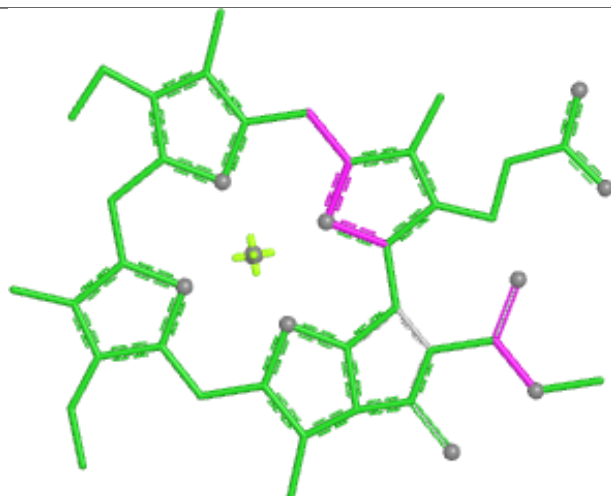


Rings

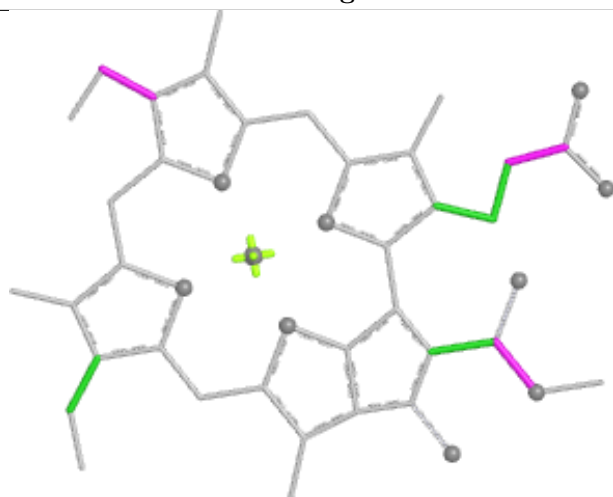
Ligand CLA b 517



Bond lengths



Bond angles

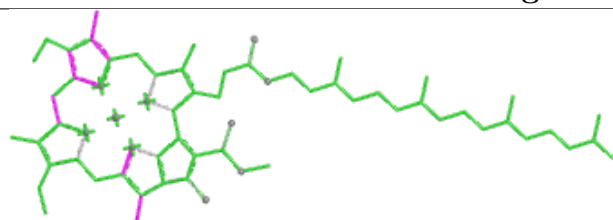


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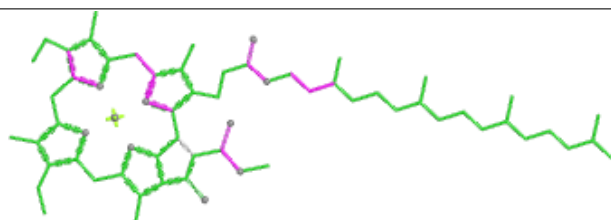


Rings

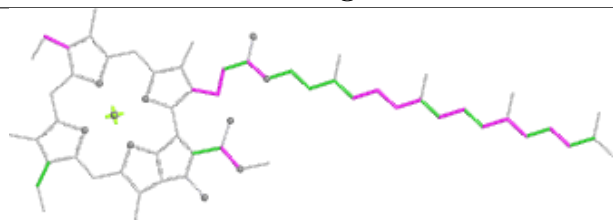
Ligand CLA f 501



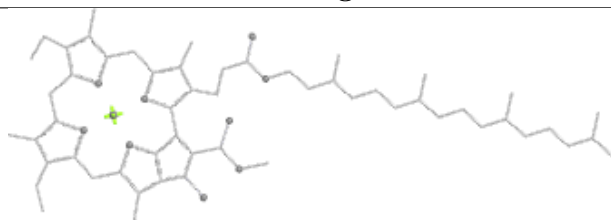
Bond lengths



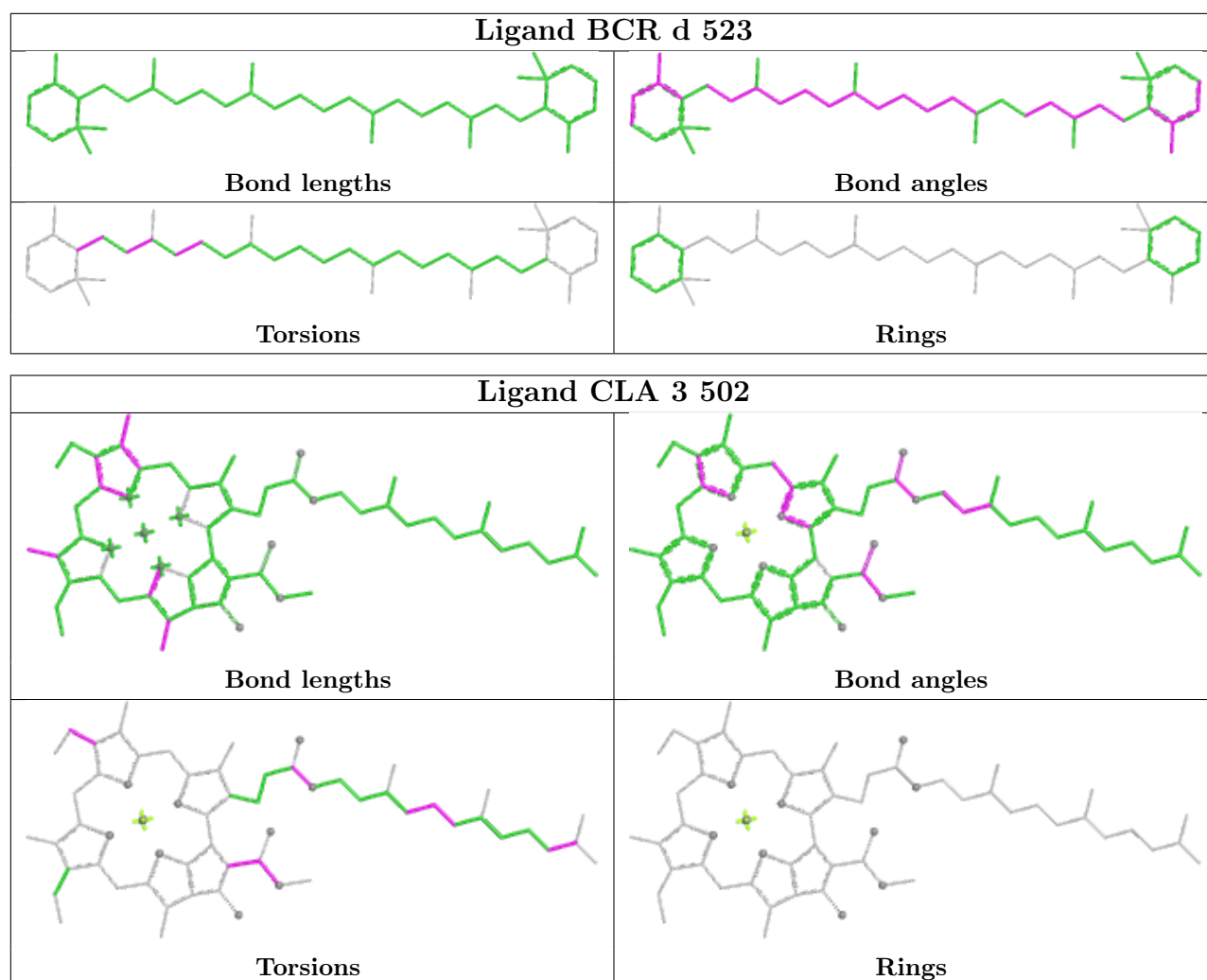
Bond angles



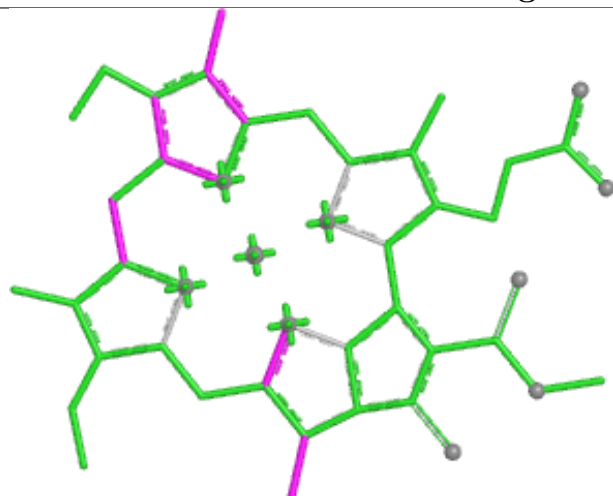
Torsions



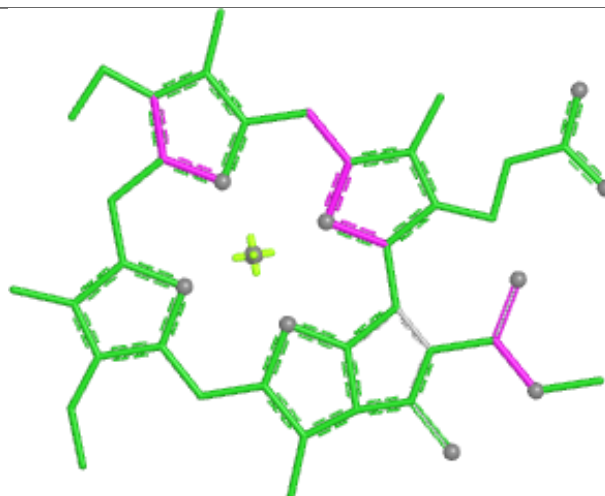
Rings



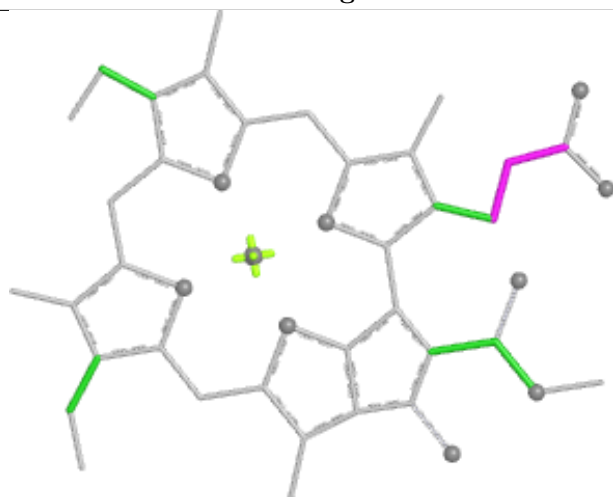
Ligand CLA 4 516



Bond lengths



Bond angles

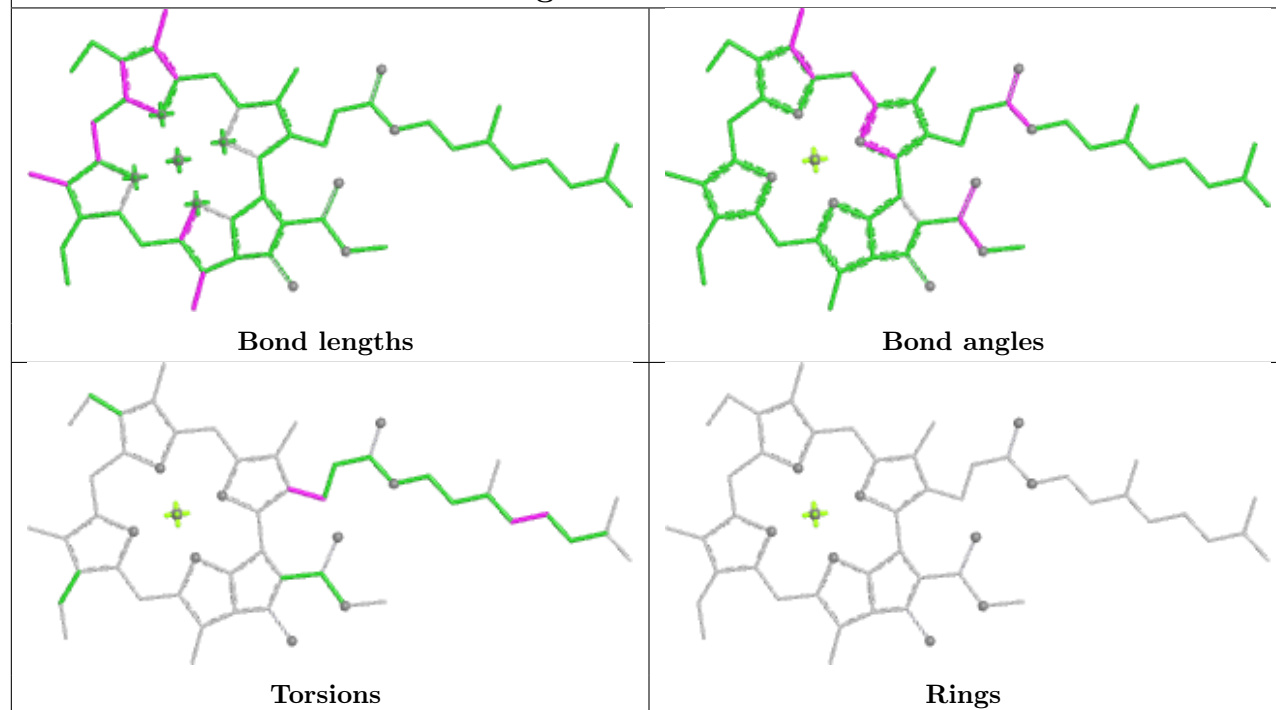


Torsions

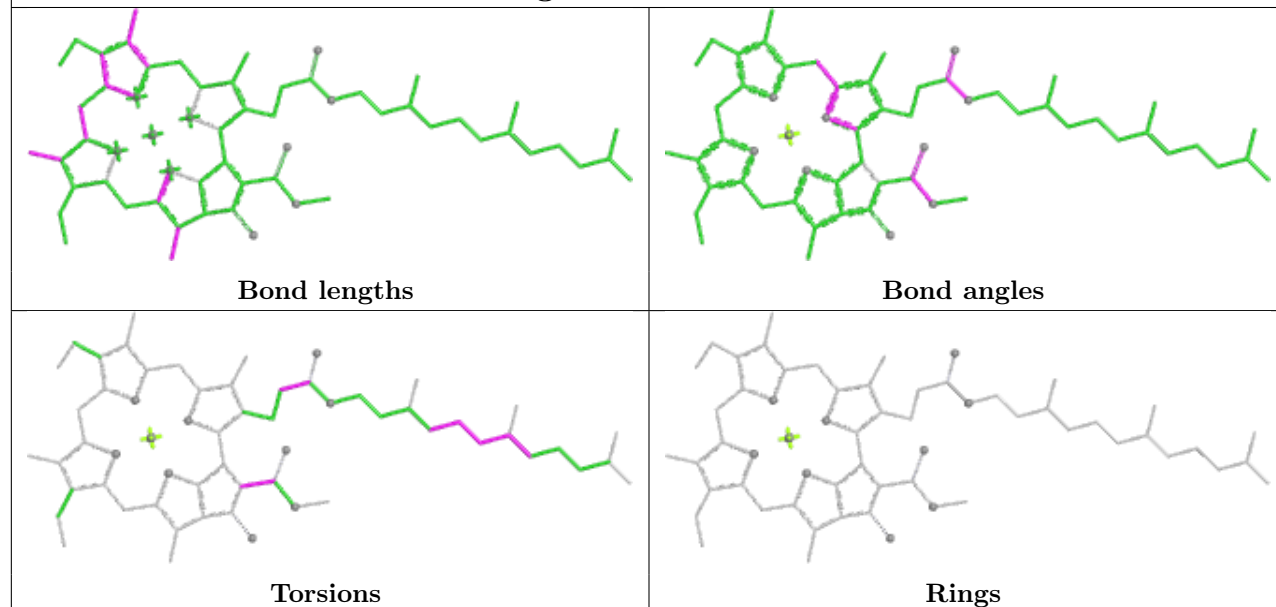


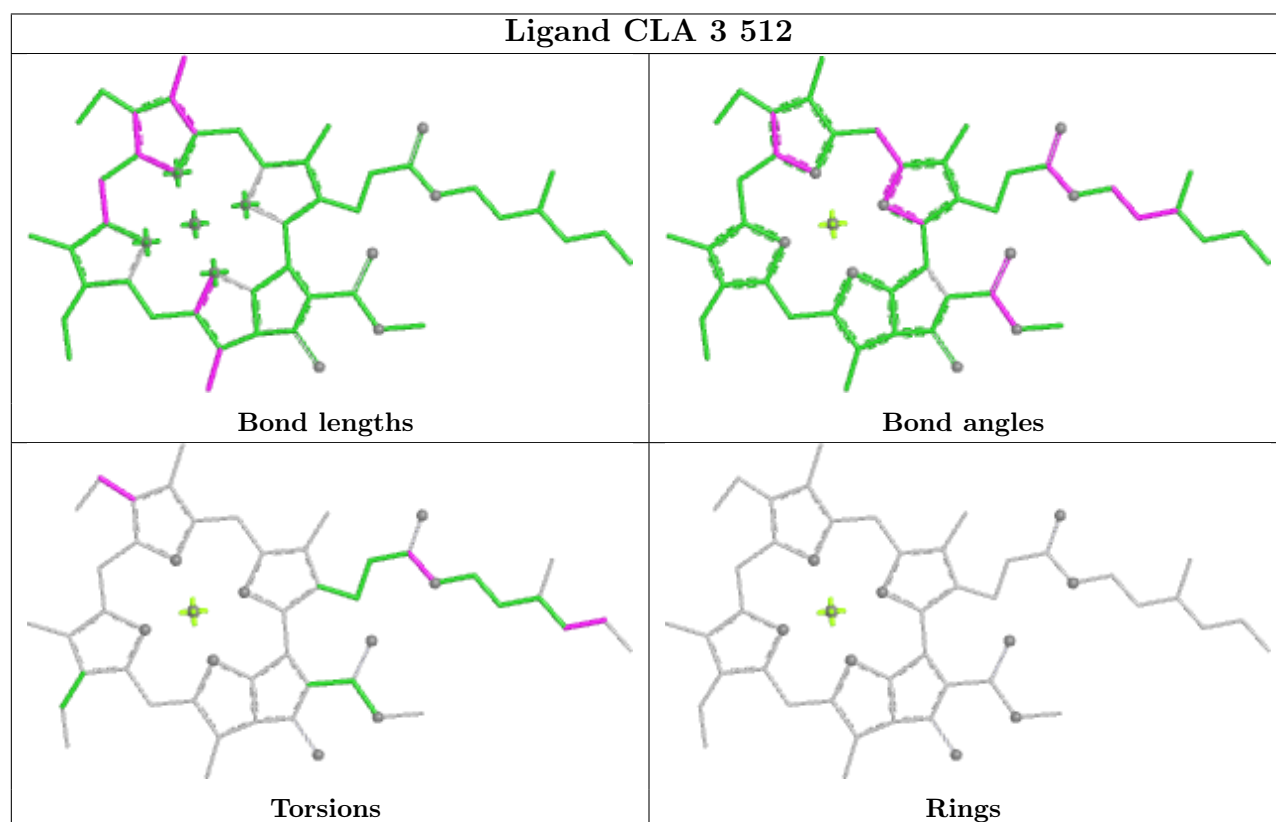
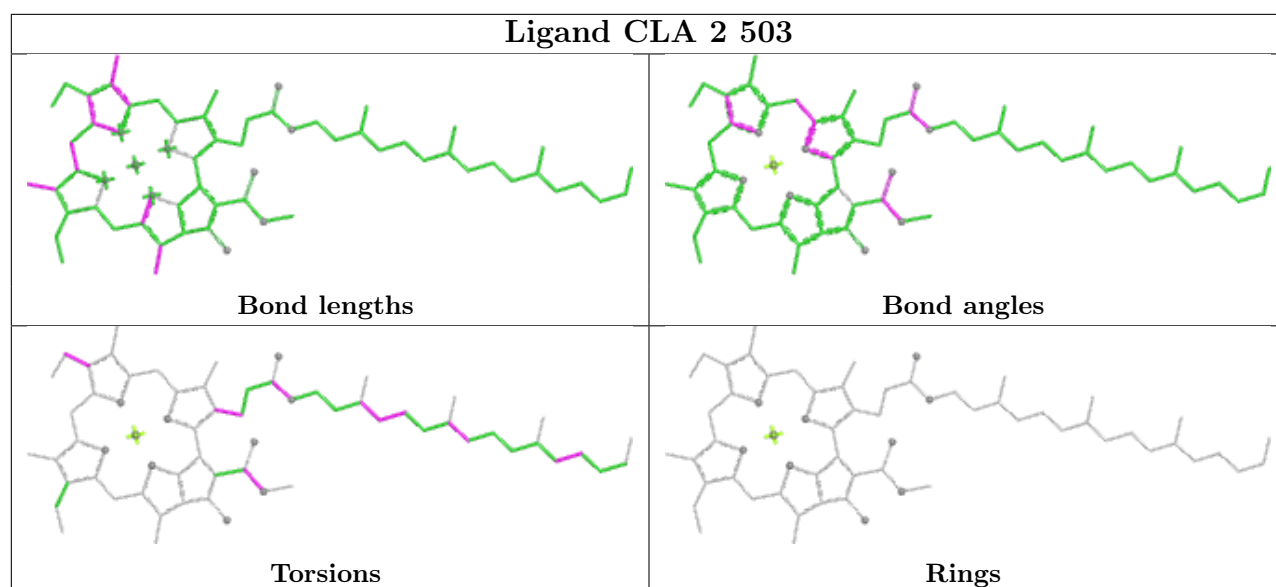
Rings

Ligand CLA 2 508

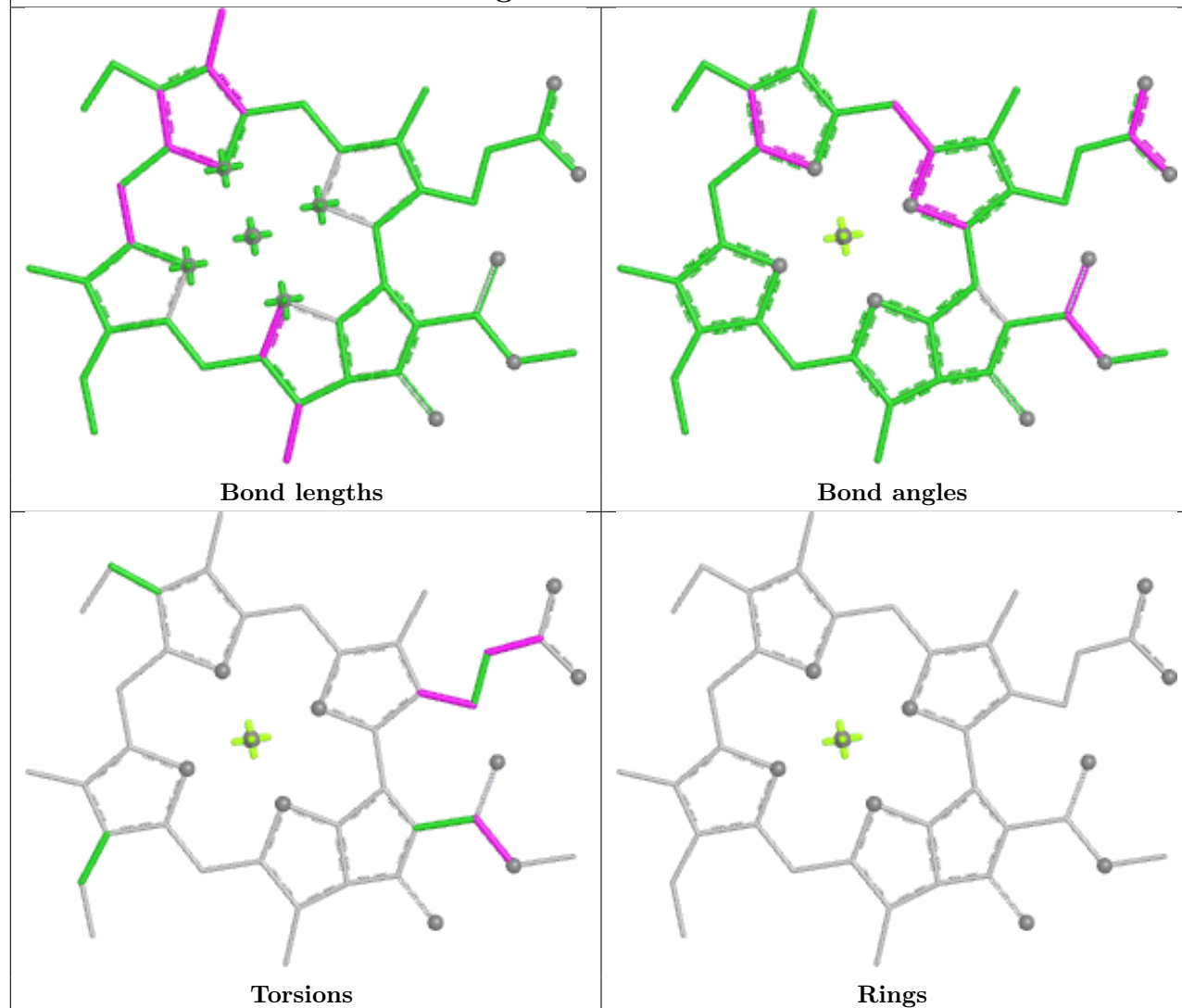


Ligand CLA 3 507

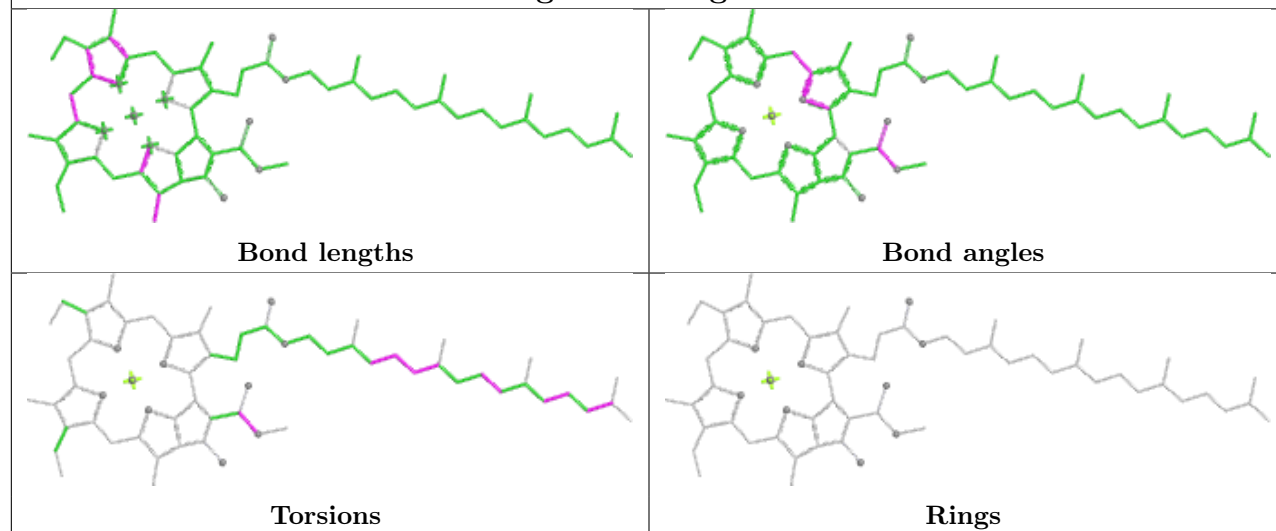


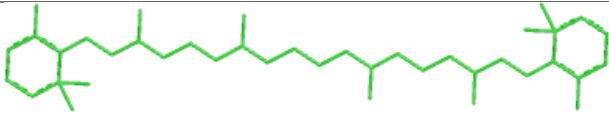
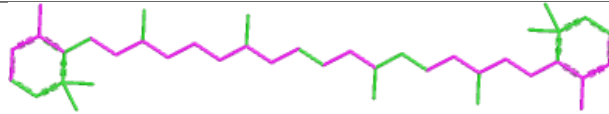
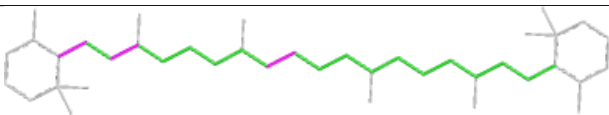
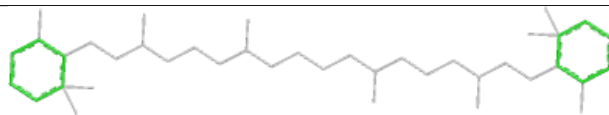


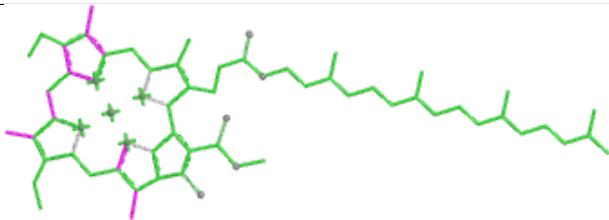
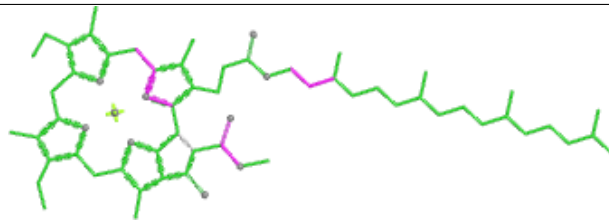
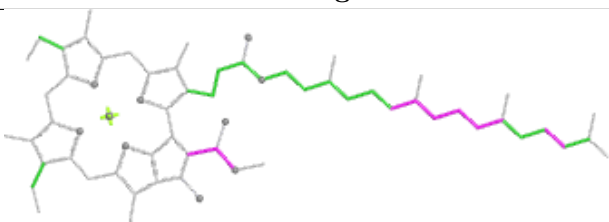
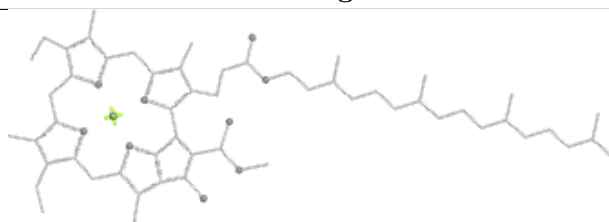
Ligand CLA b 519

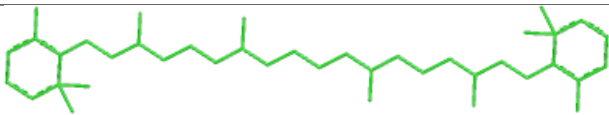
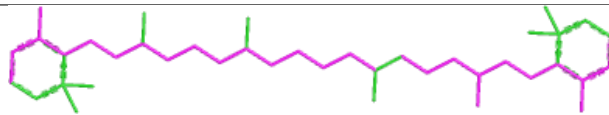
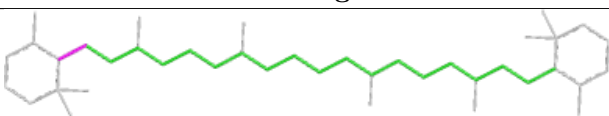
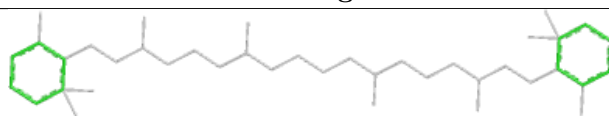


Ligand CLA g 510

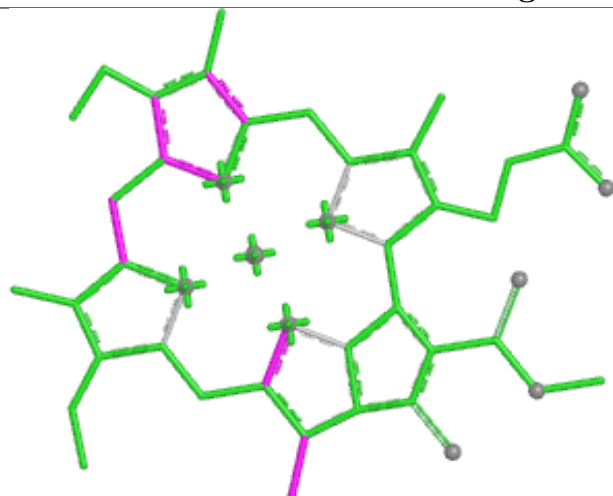


Ligand BCR f 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

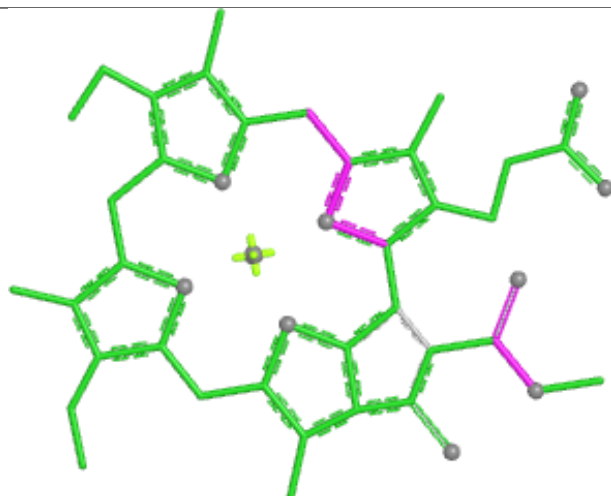
Ligand CLA 5 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 4 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

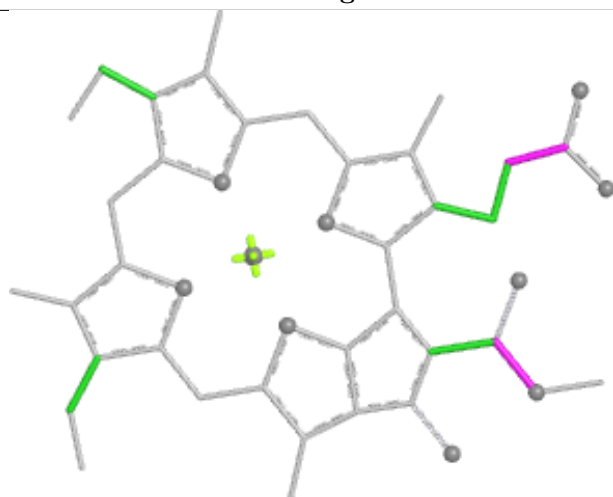
Ligand CLA a 519



Bond lengths



Bond angles

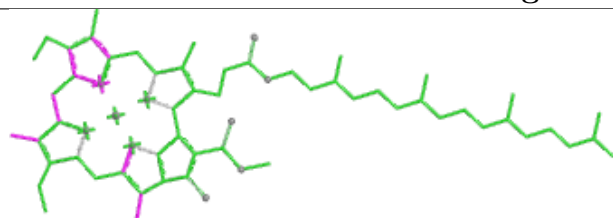


Torsions

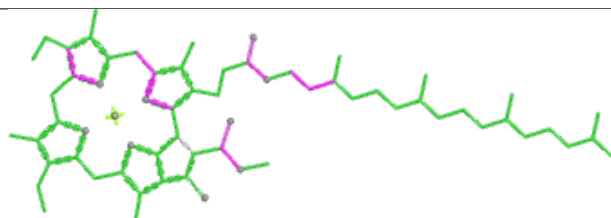


Rings

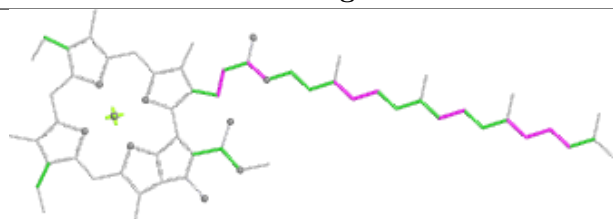
Ligand CLA f 505



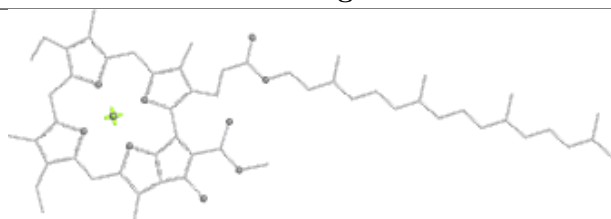
Bond lengths



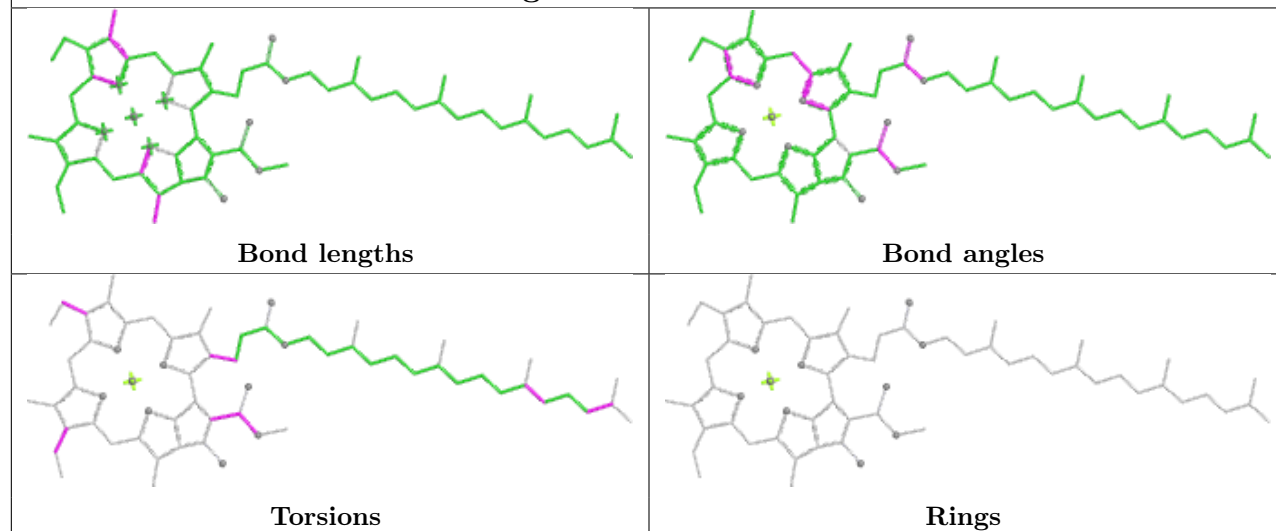
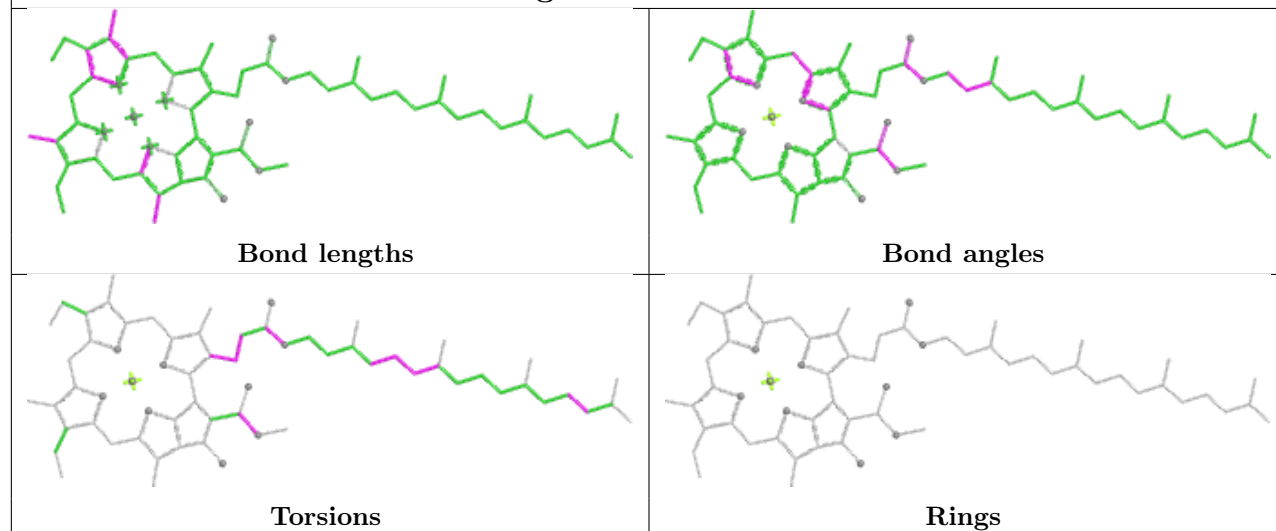
Bond angles



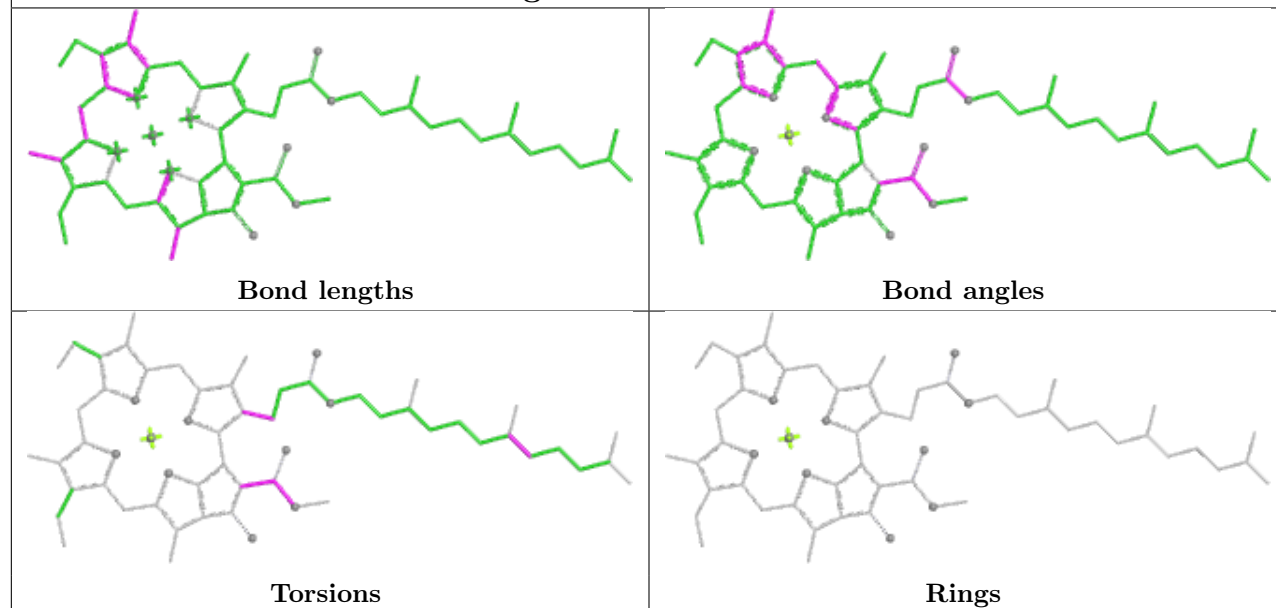
Torsions



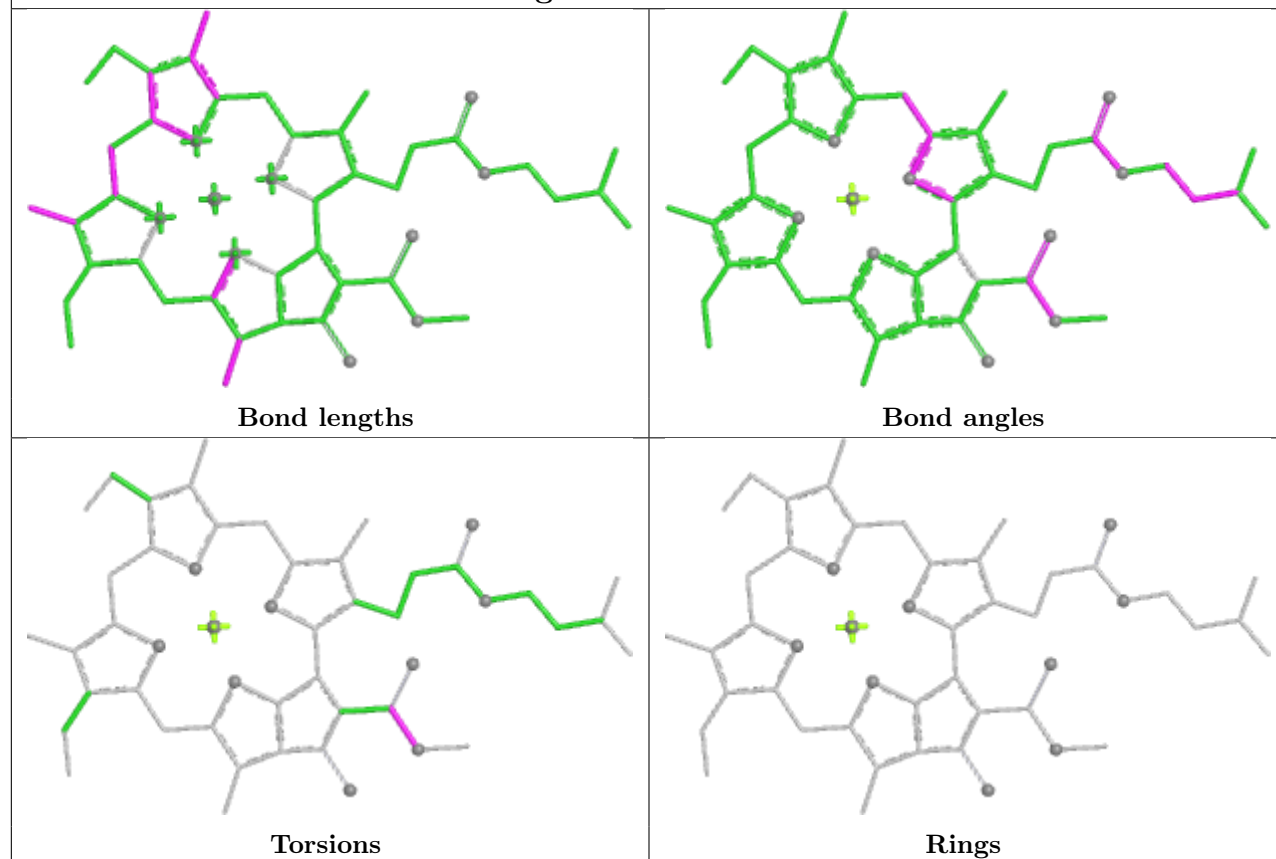
Rings

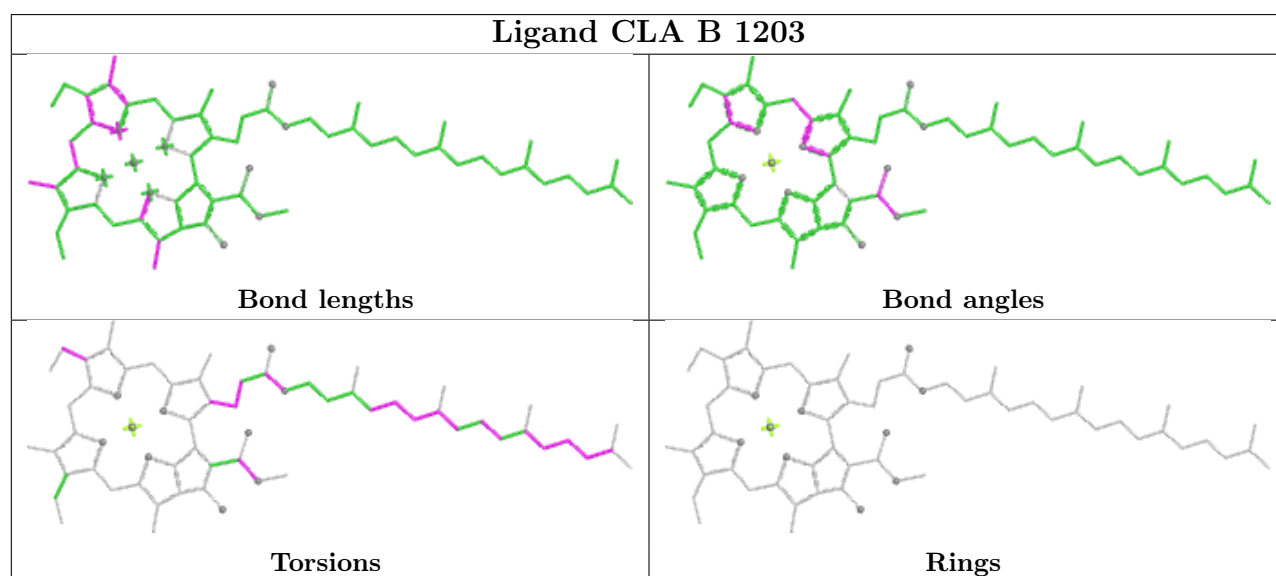
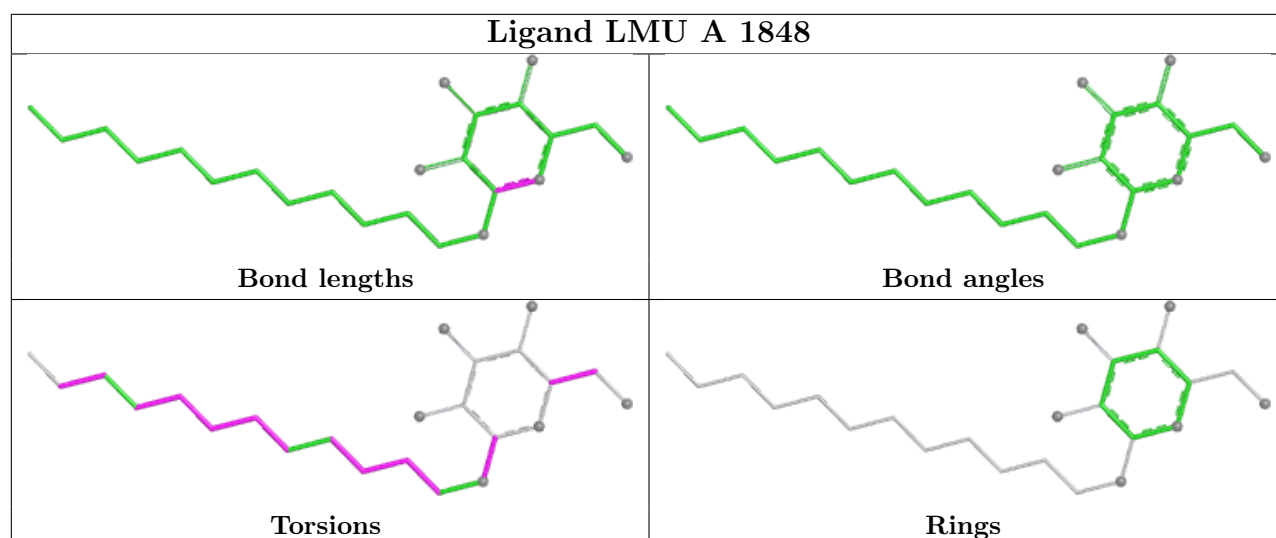
Ligand CLA A 1132**Ligand CLA 3 509**

Ligand CLA B 1222

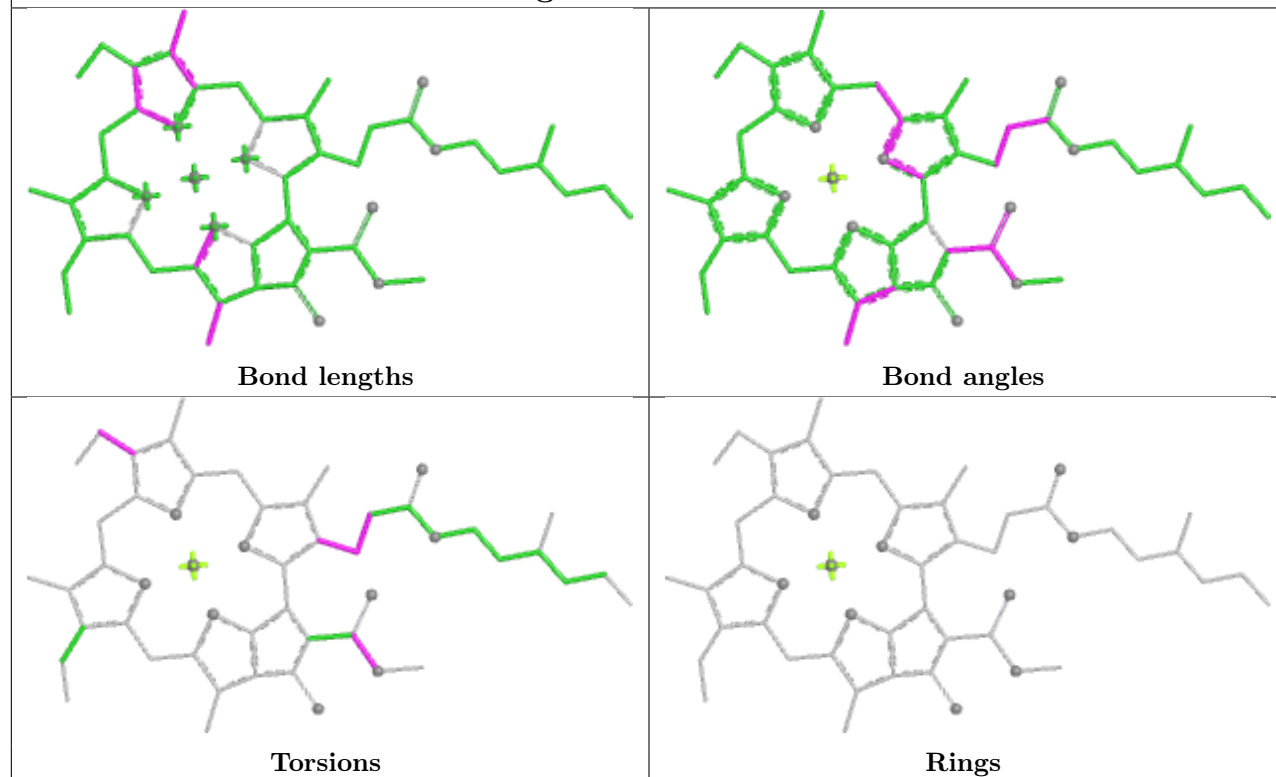


Ligand CLA d 513

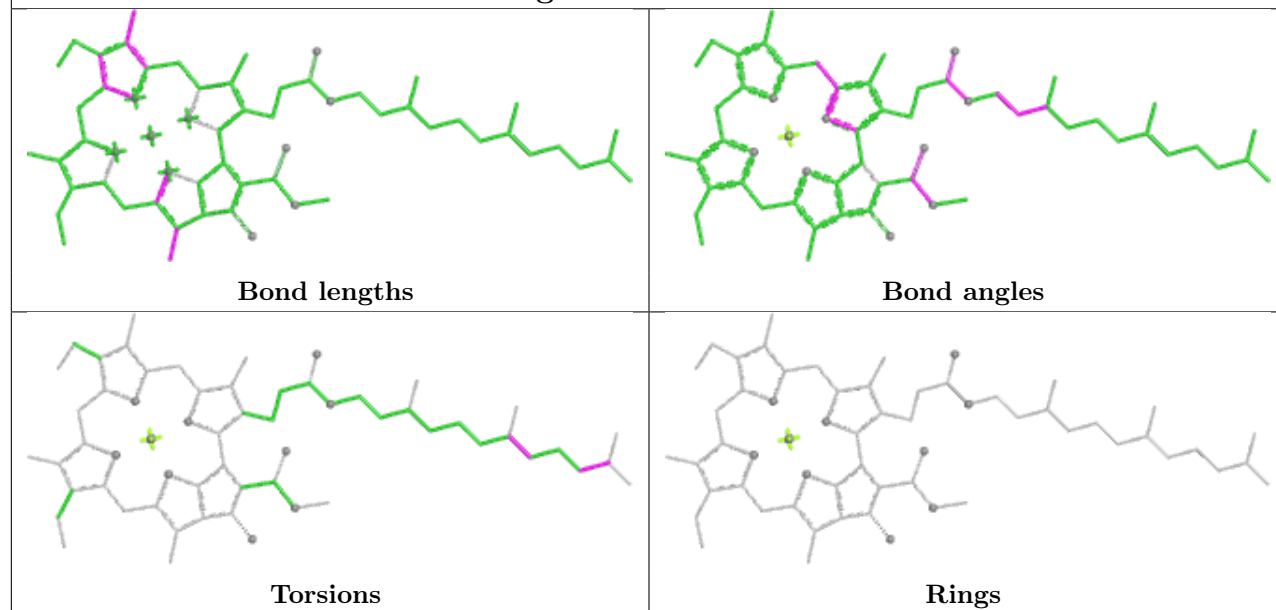


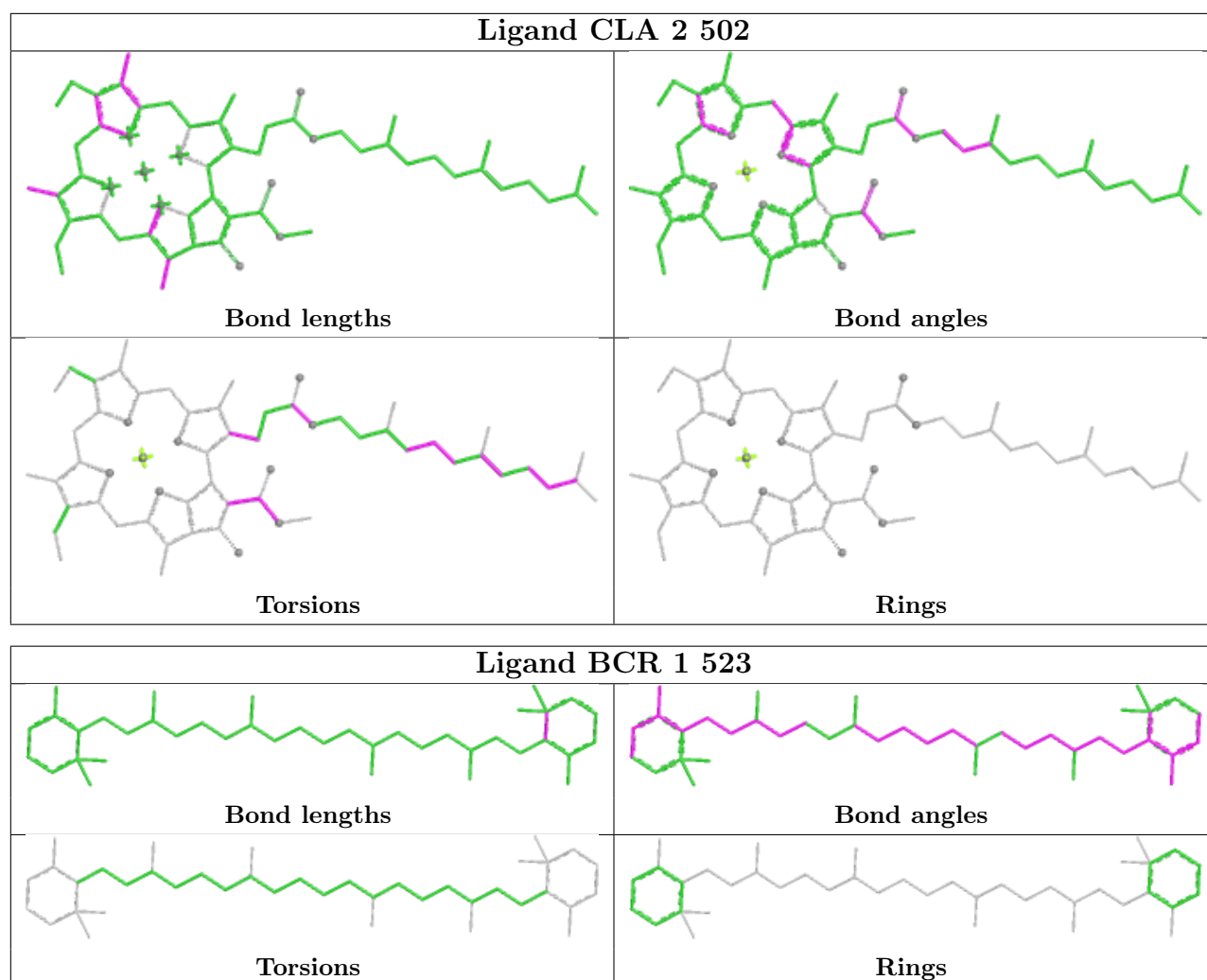


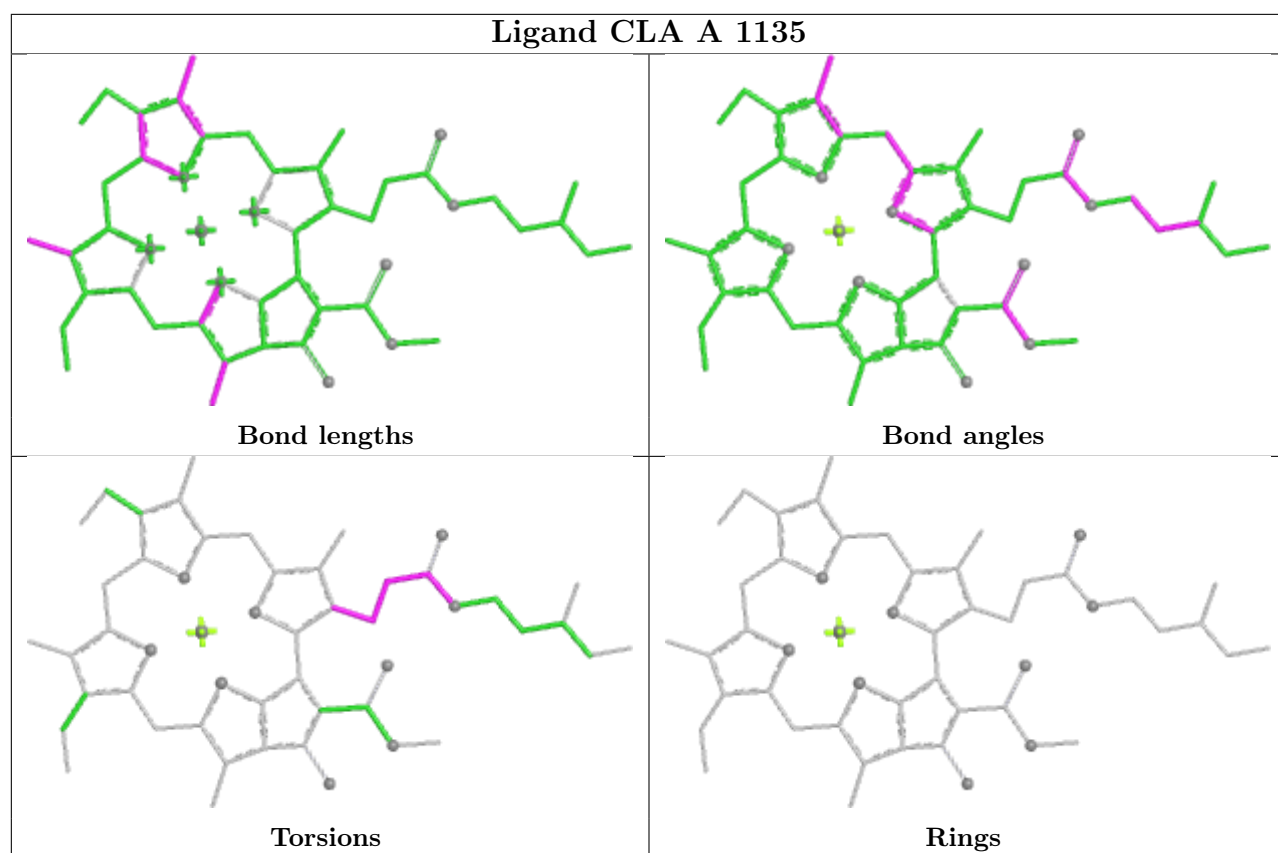
Ligand CLA 1 512



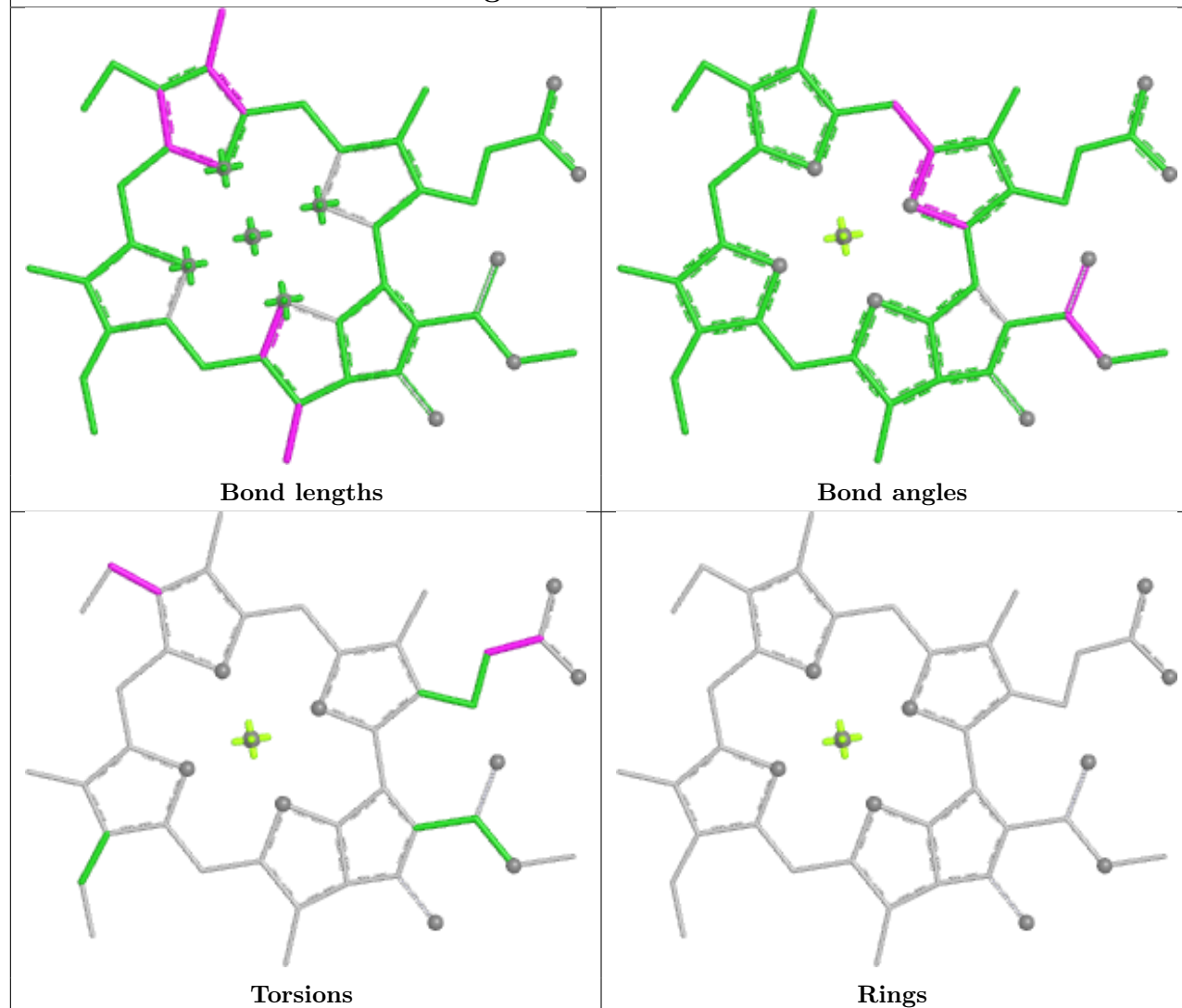
Ligand CLA 6 507



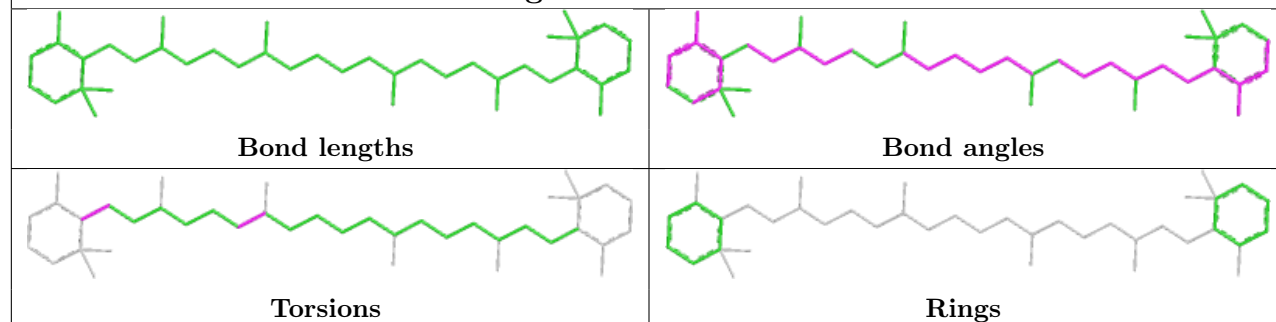


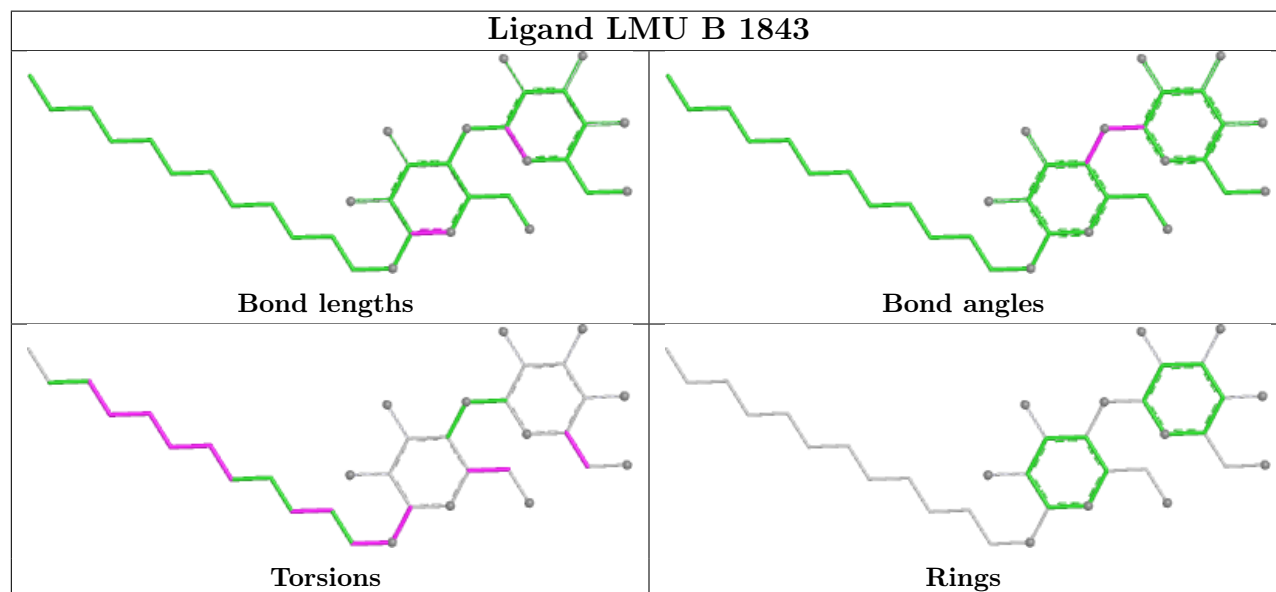
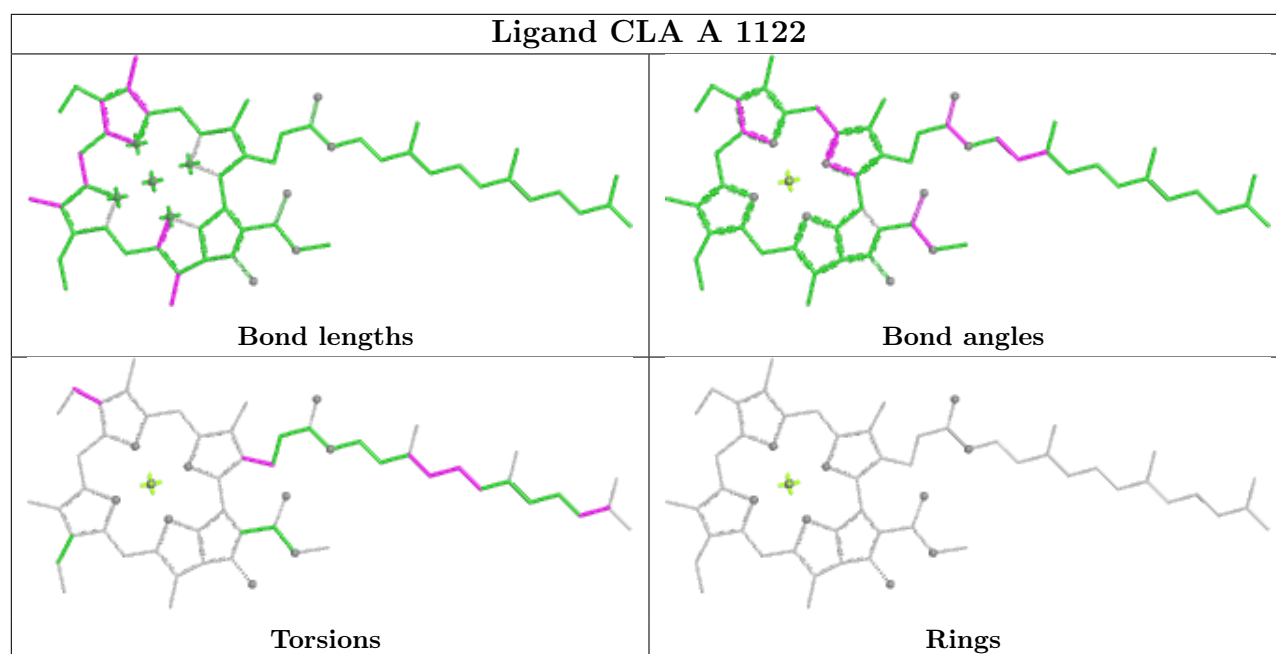


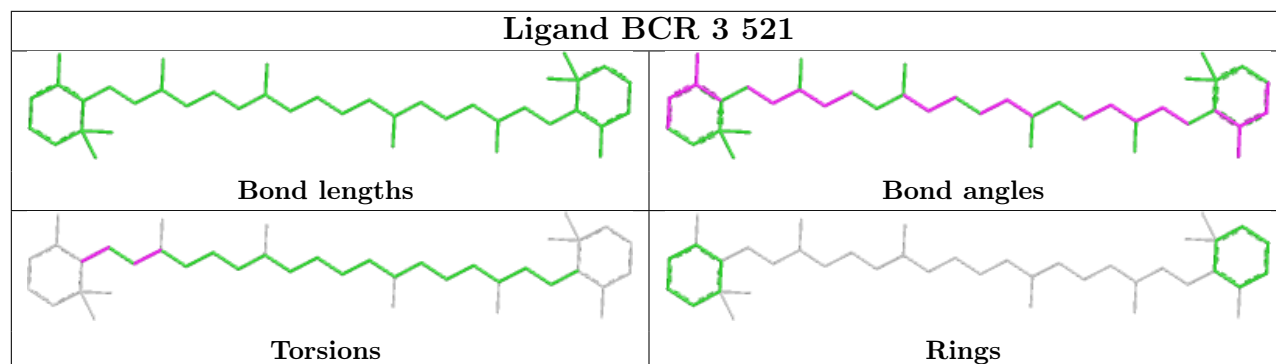
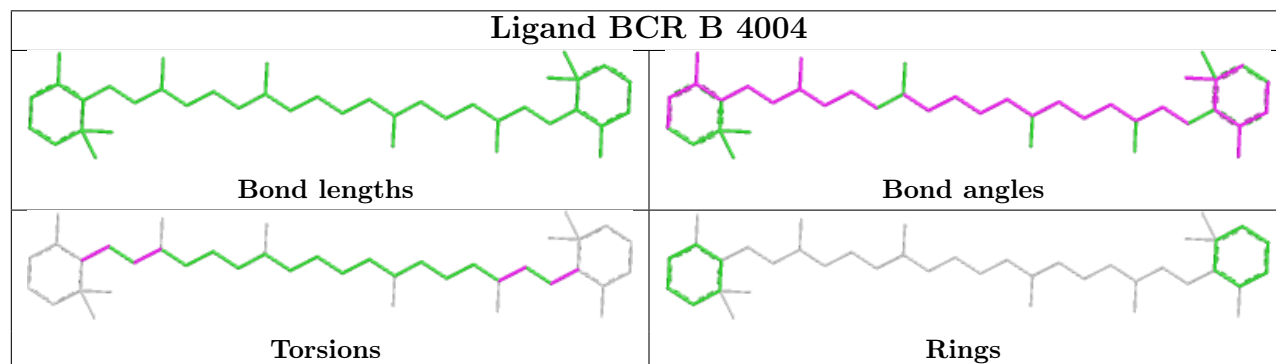
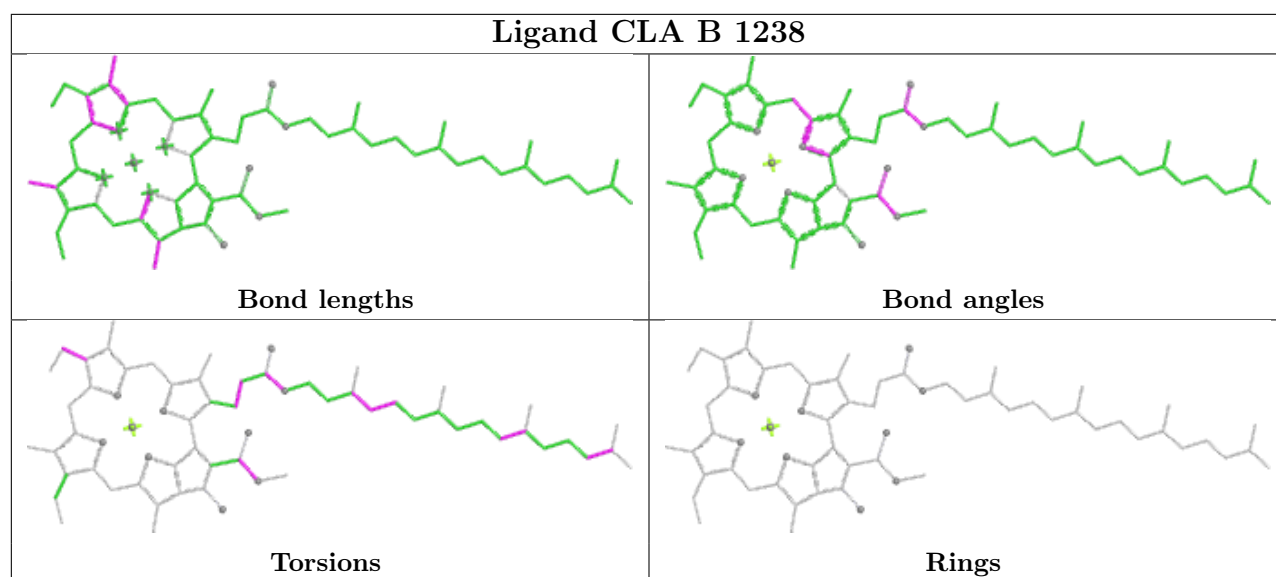
Ligand CLA A 1114



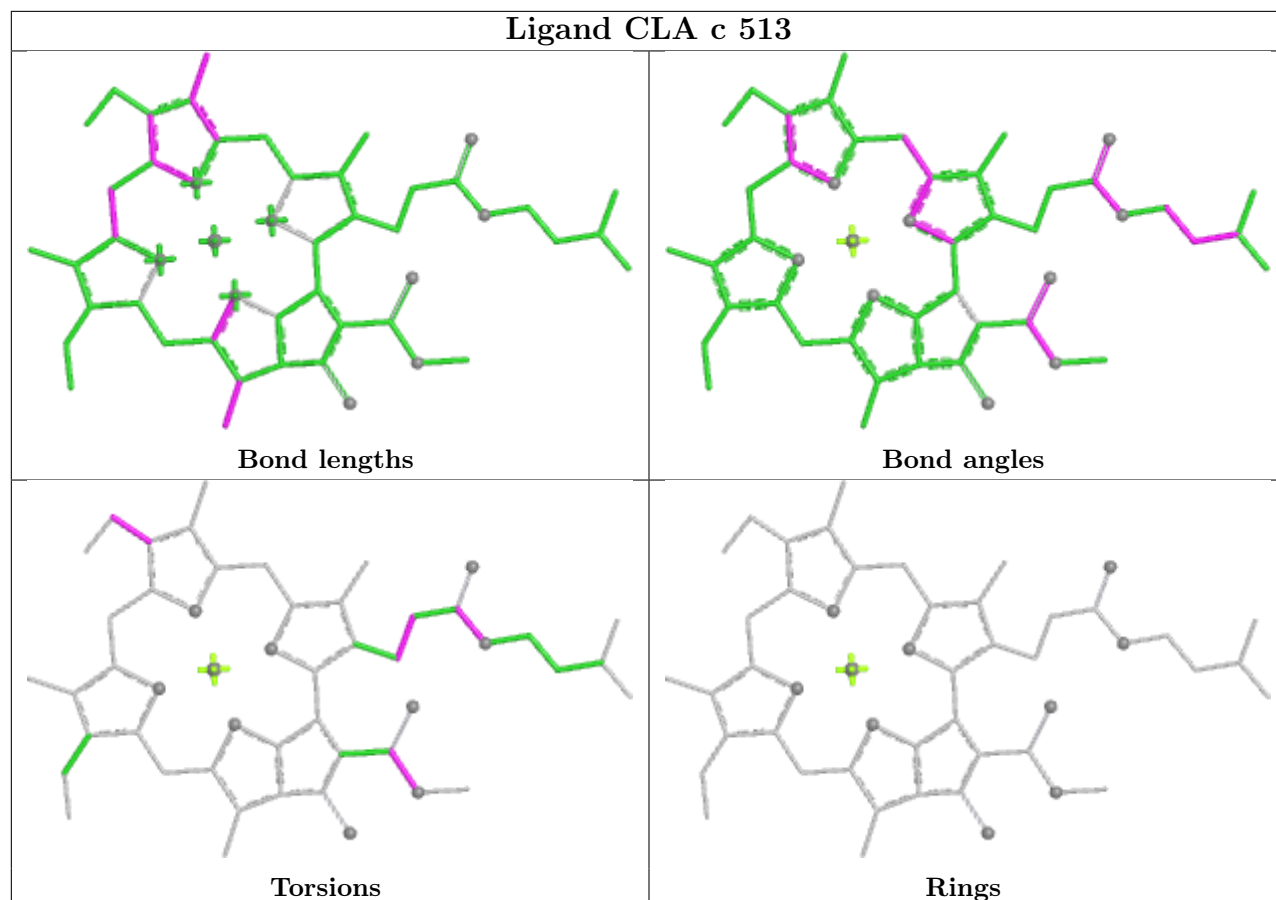
Ligand BCR J 4012



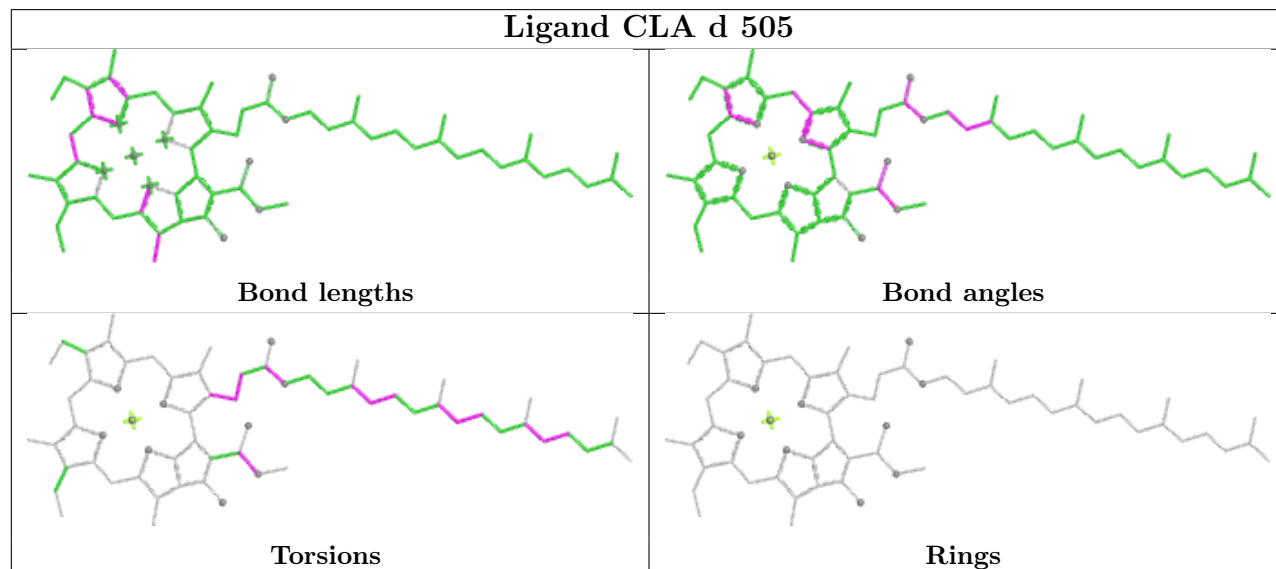


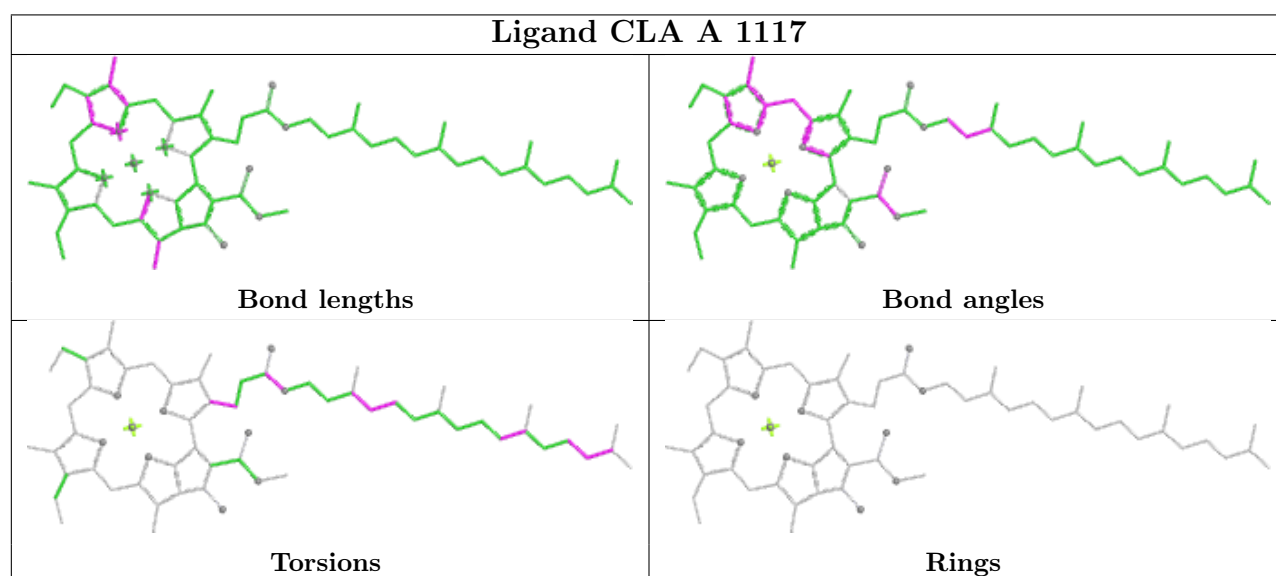
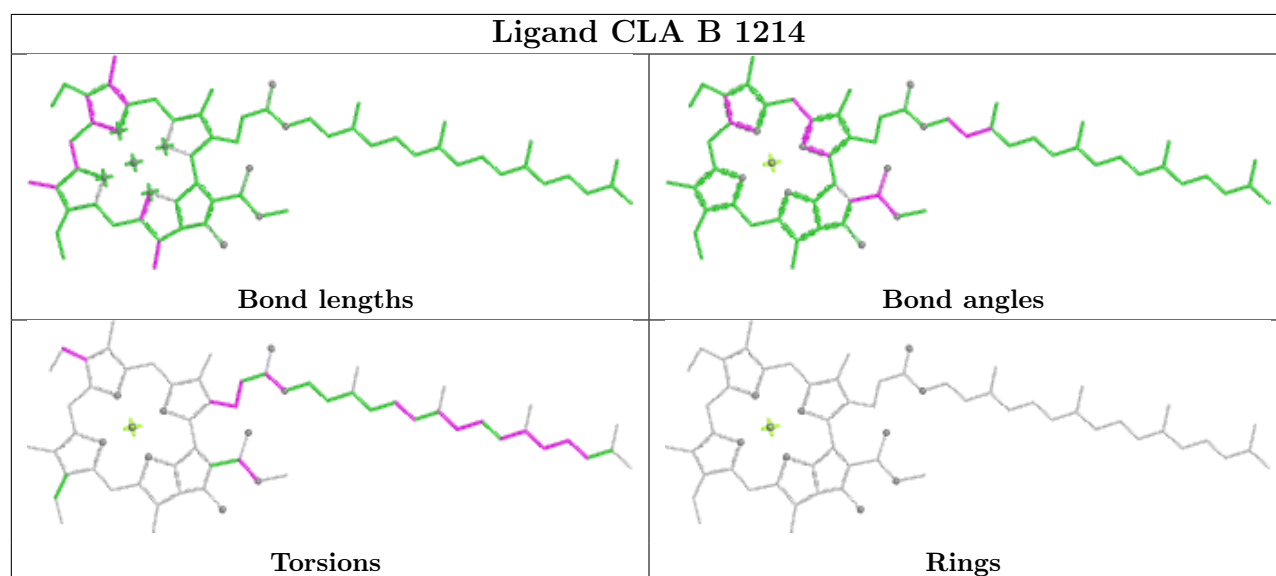
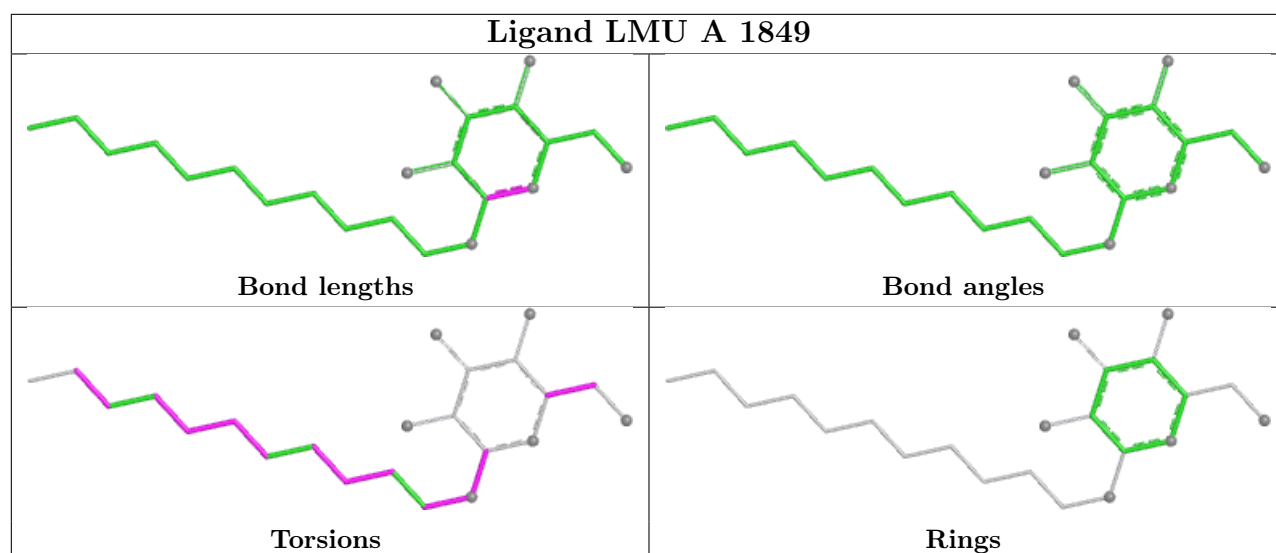


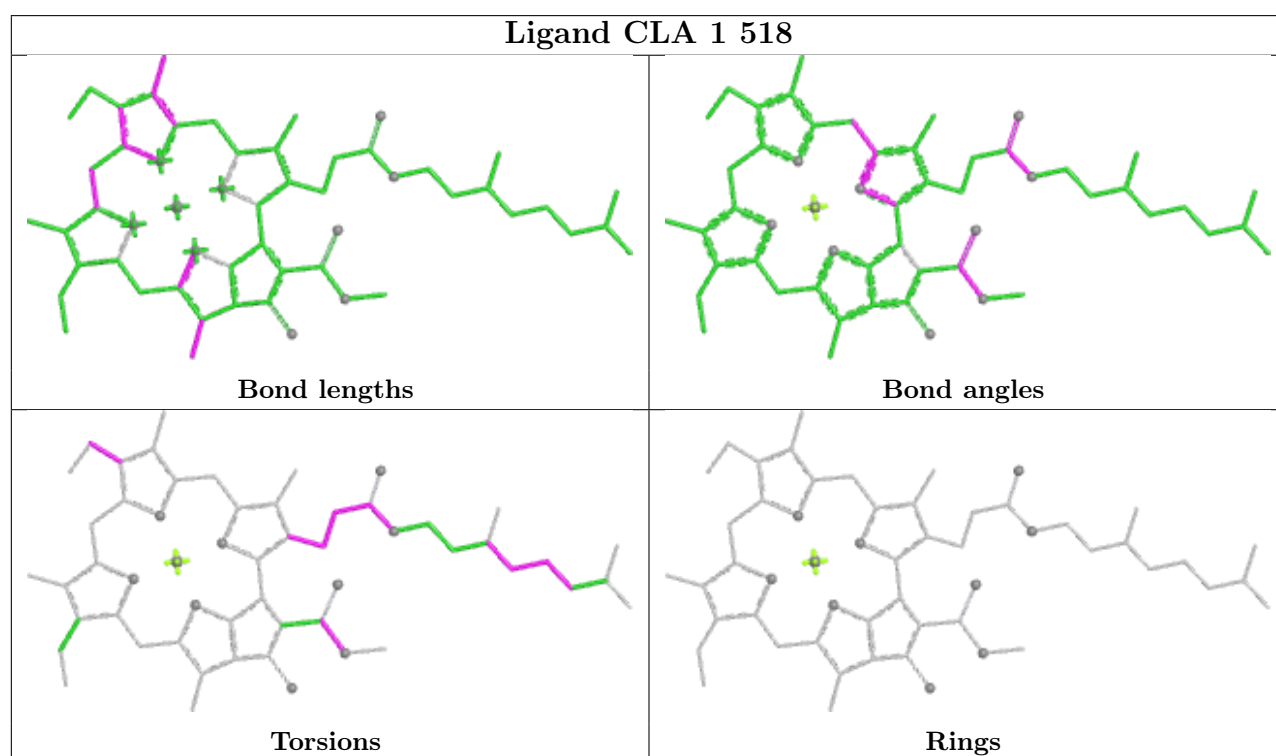
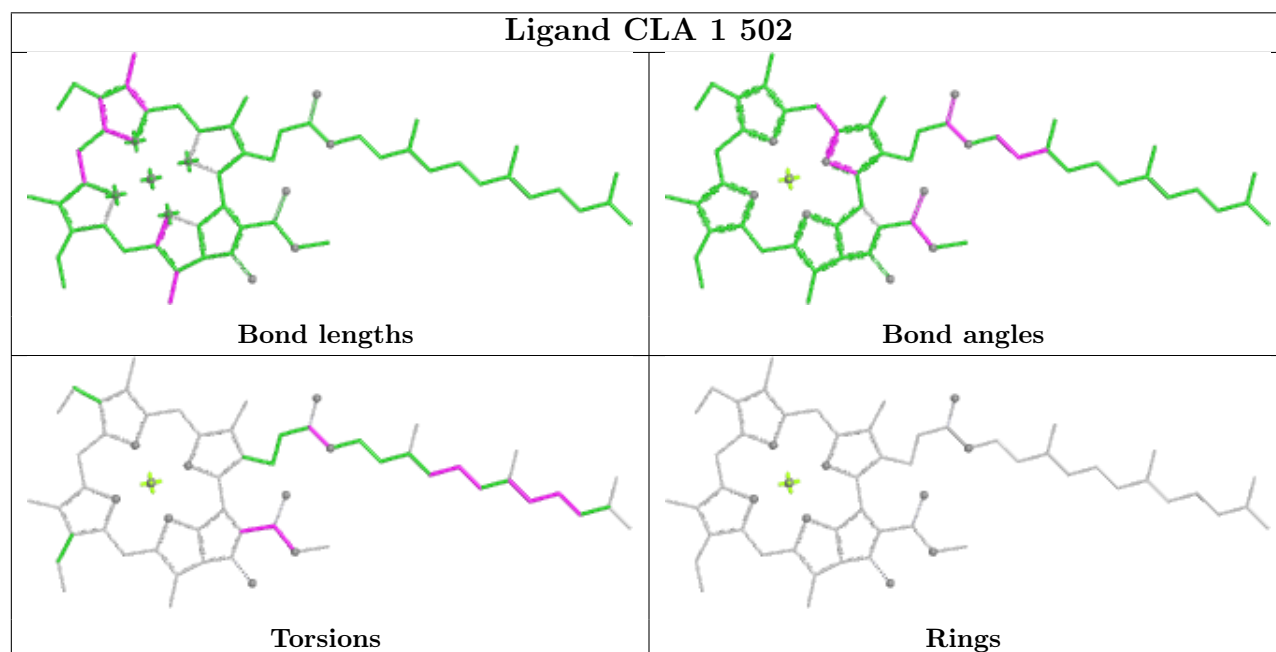
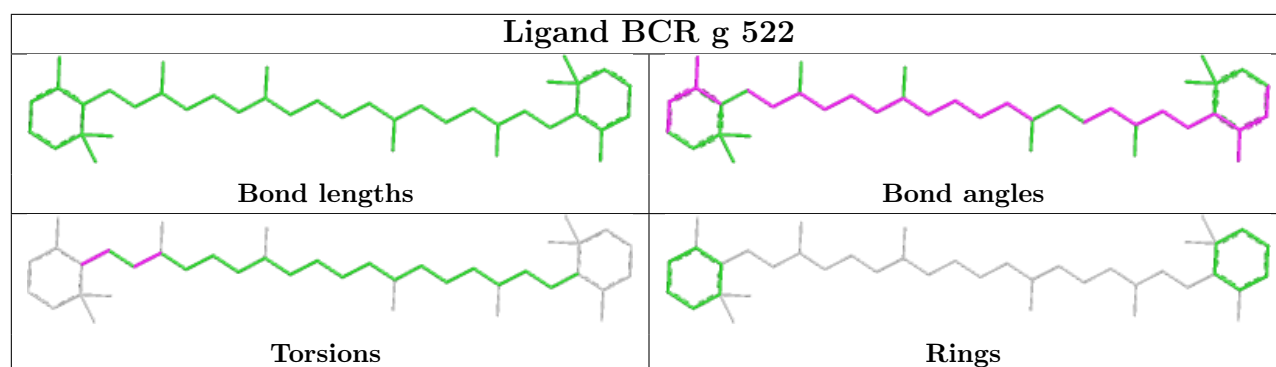
Ligand CLA c 513



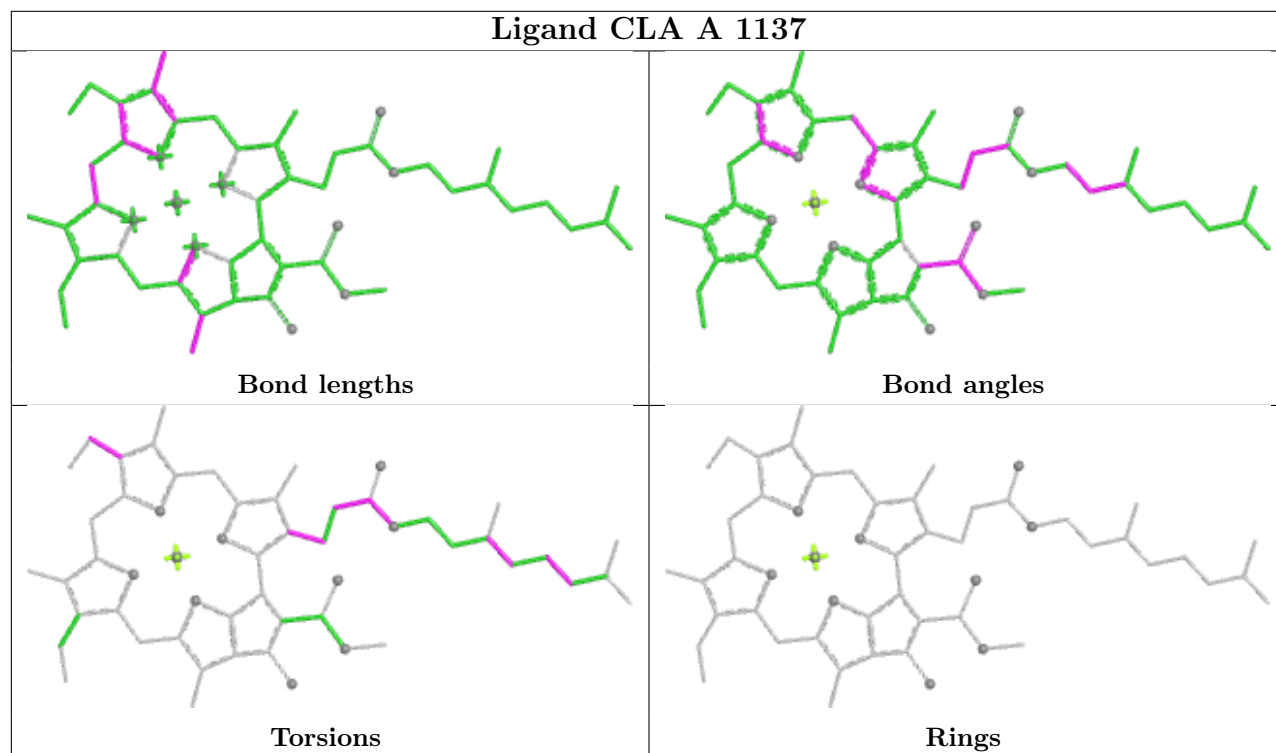
Ligand CLA d 505



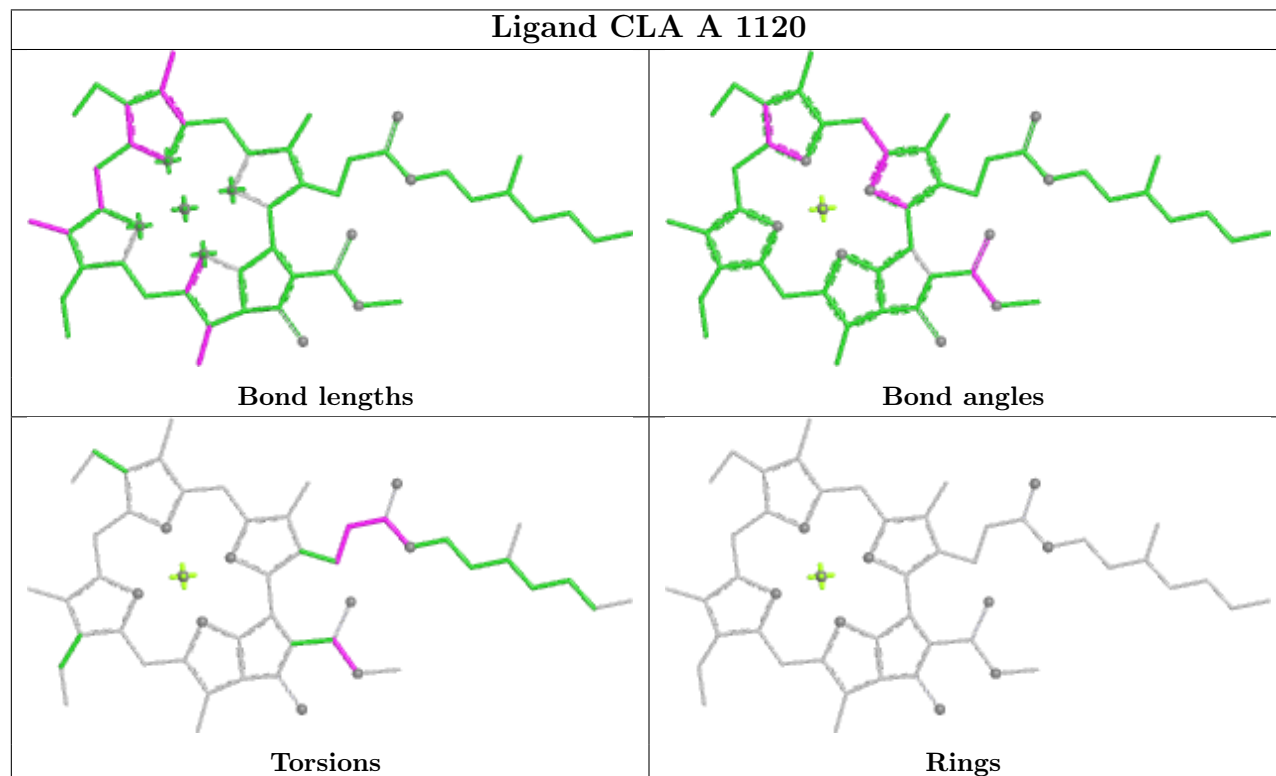




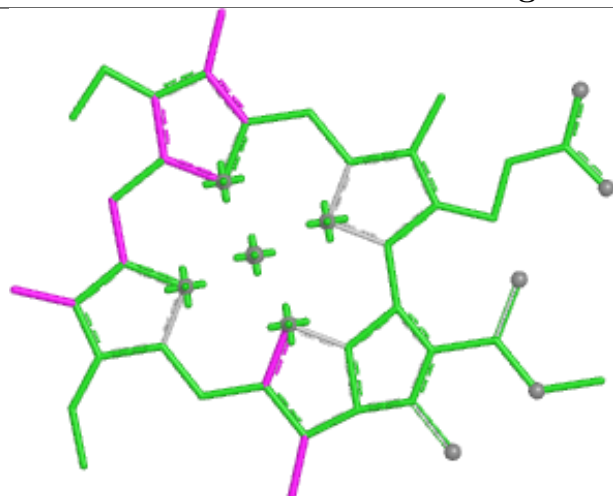
Ligand CLA A 1137



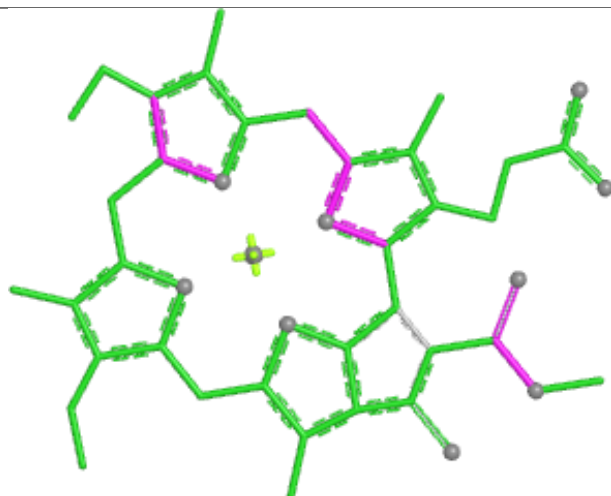
Ligand CLA A 1120



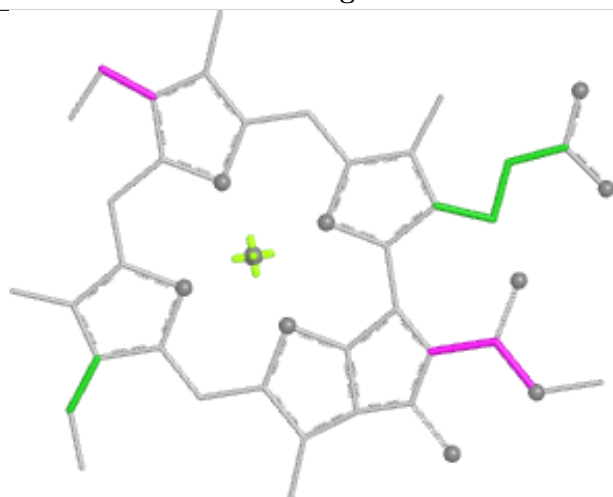
Ligand CLA 2 506



Bond lengths



Bond angles

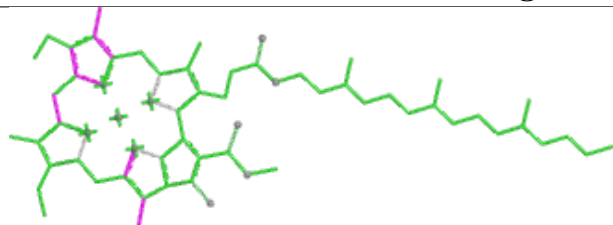


Torsions

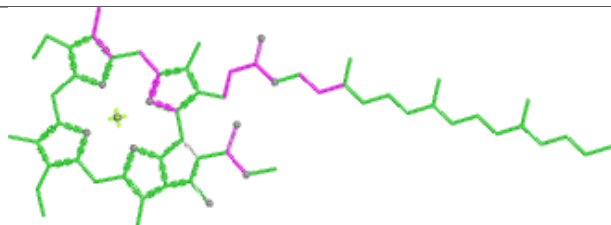


Rings

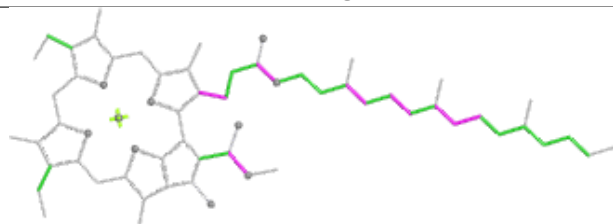
Ligand CLA 3 503



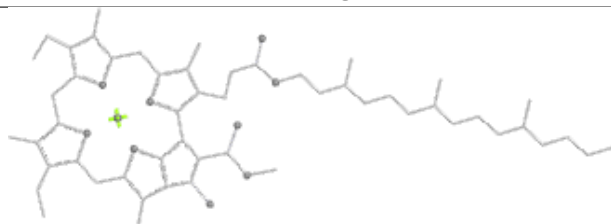
Bond lengths



Bond angles

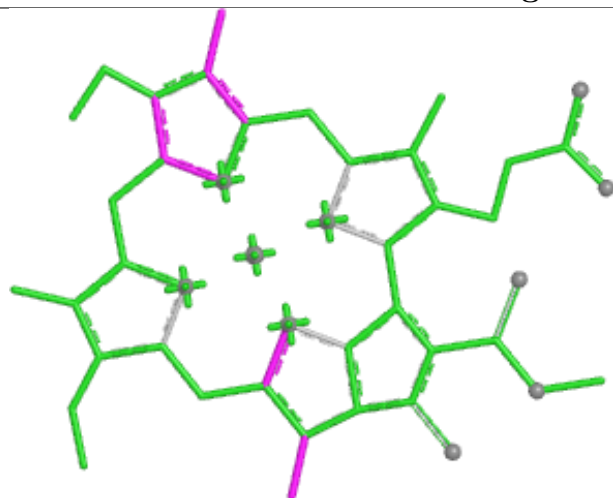


Torsions

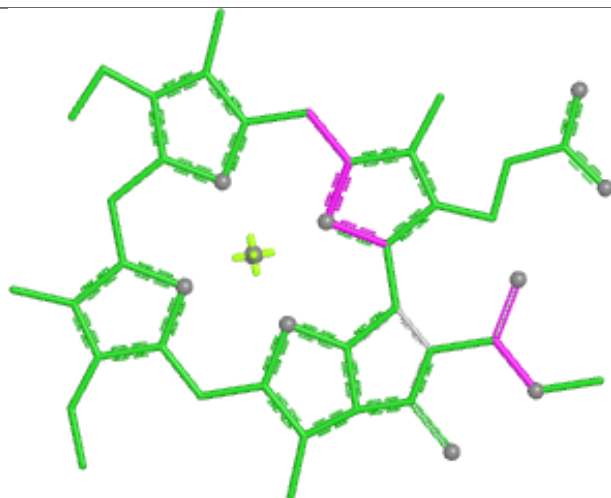


Rings

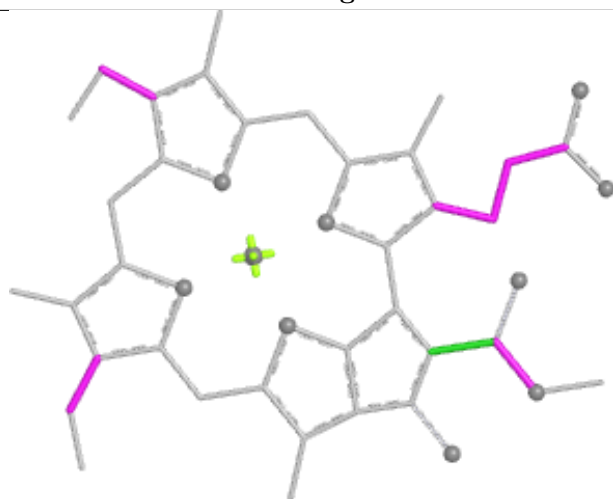
Ligand CLA f 512



Bond lengths



Bond angles

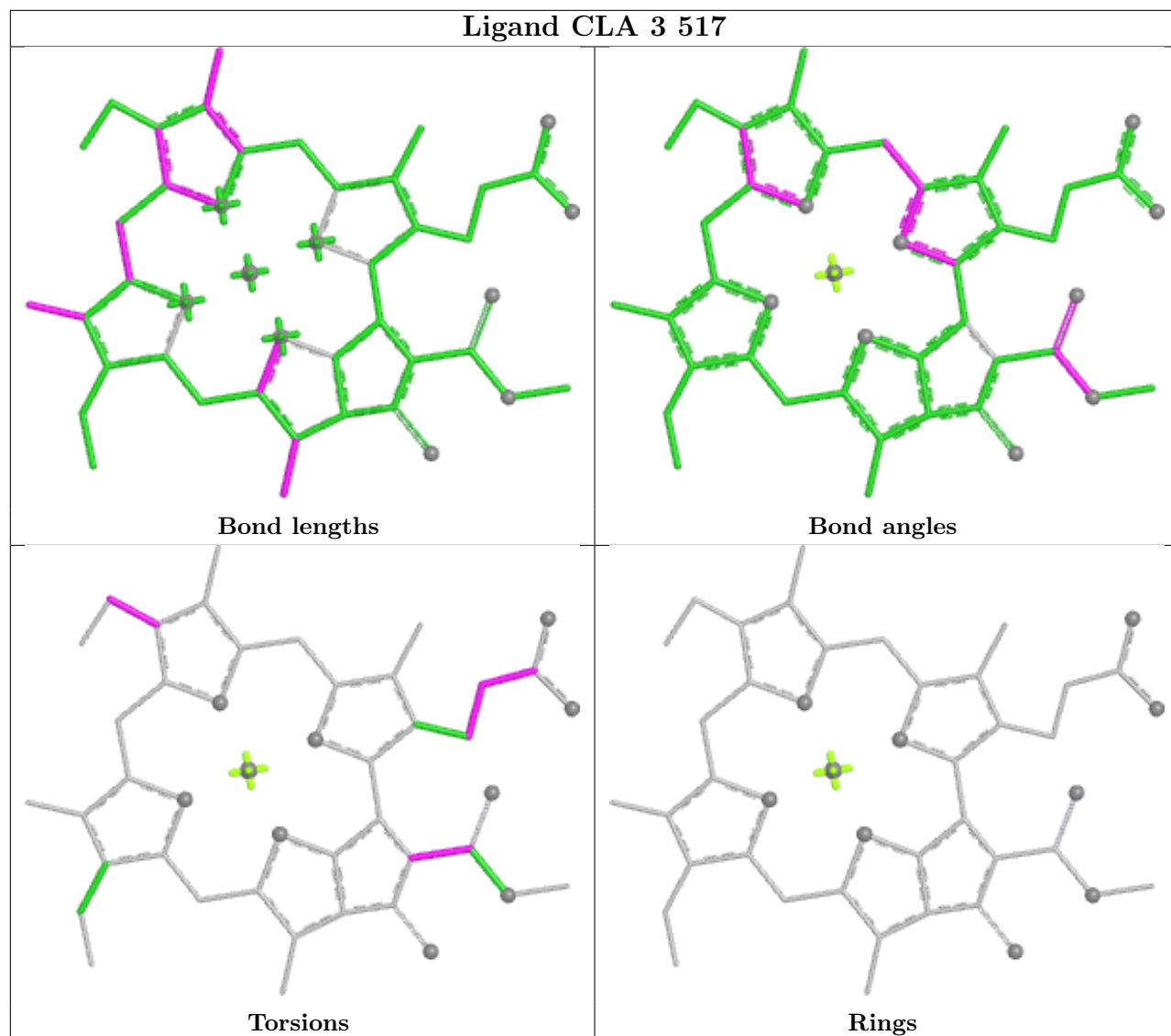


Torsions

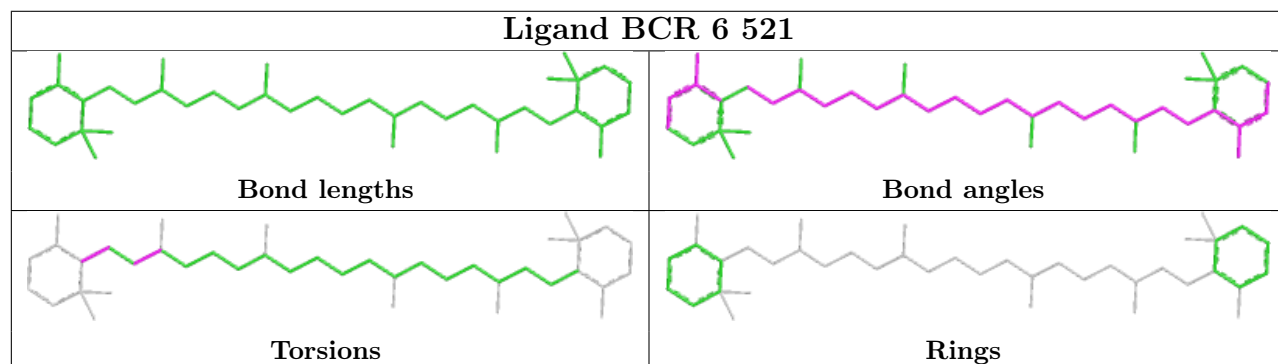


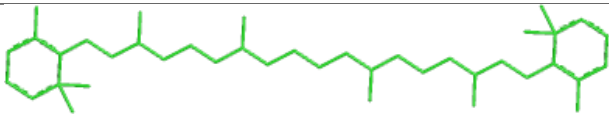
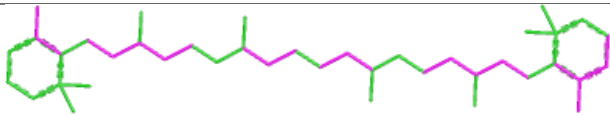
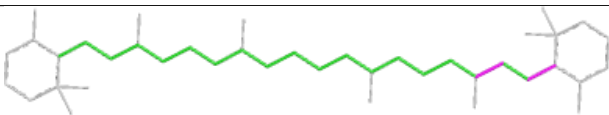
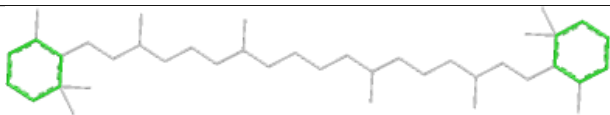
Rings

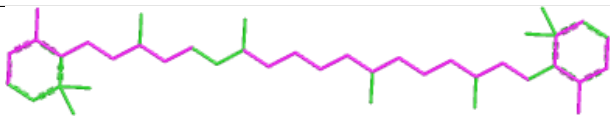
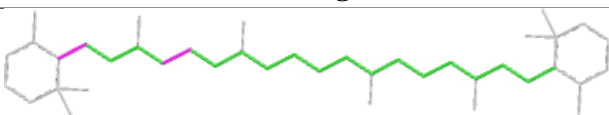
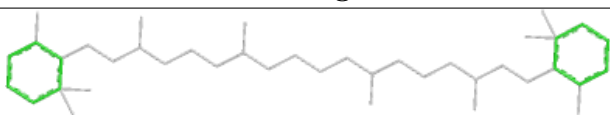
Ligand CLA 3 517

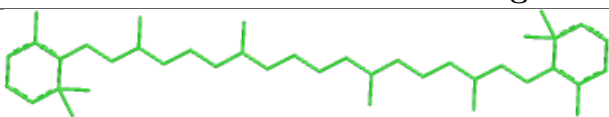
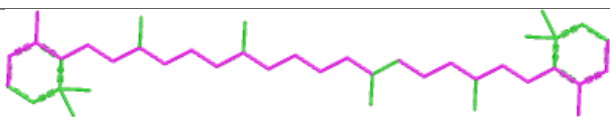
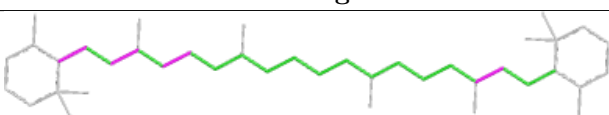
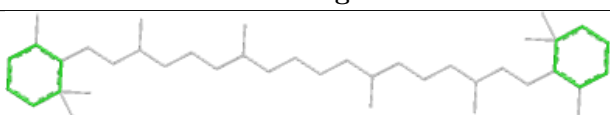


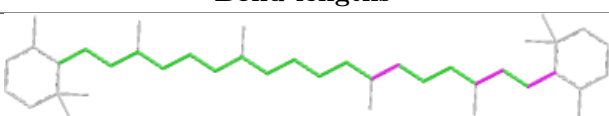
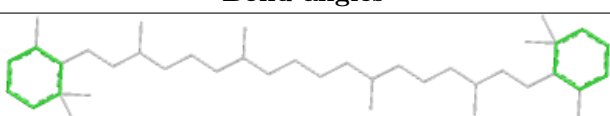
Ligand BCR 6 521

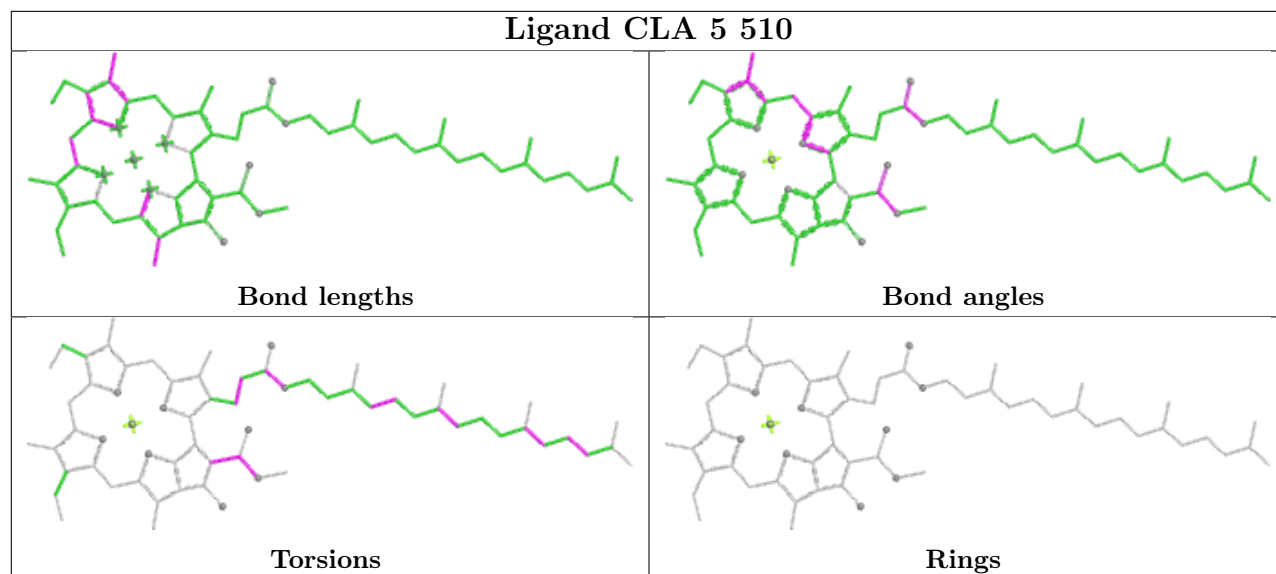
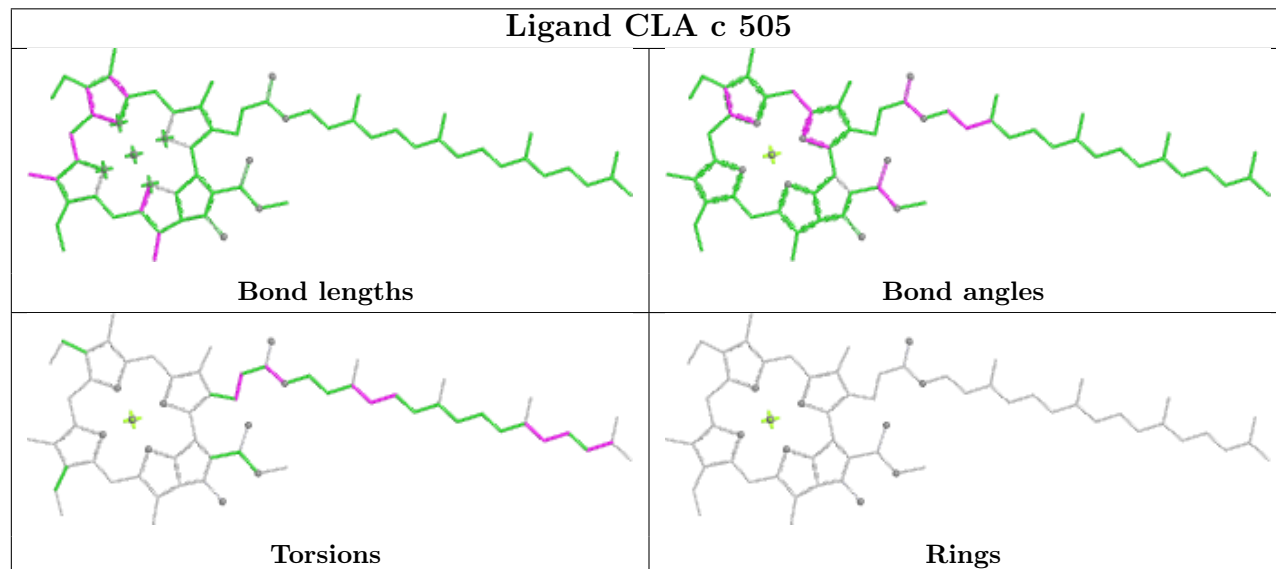


Ligand BCR I 4019	
 Bond lengths	 Bond angles
 Torsions	 Rings

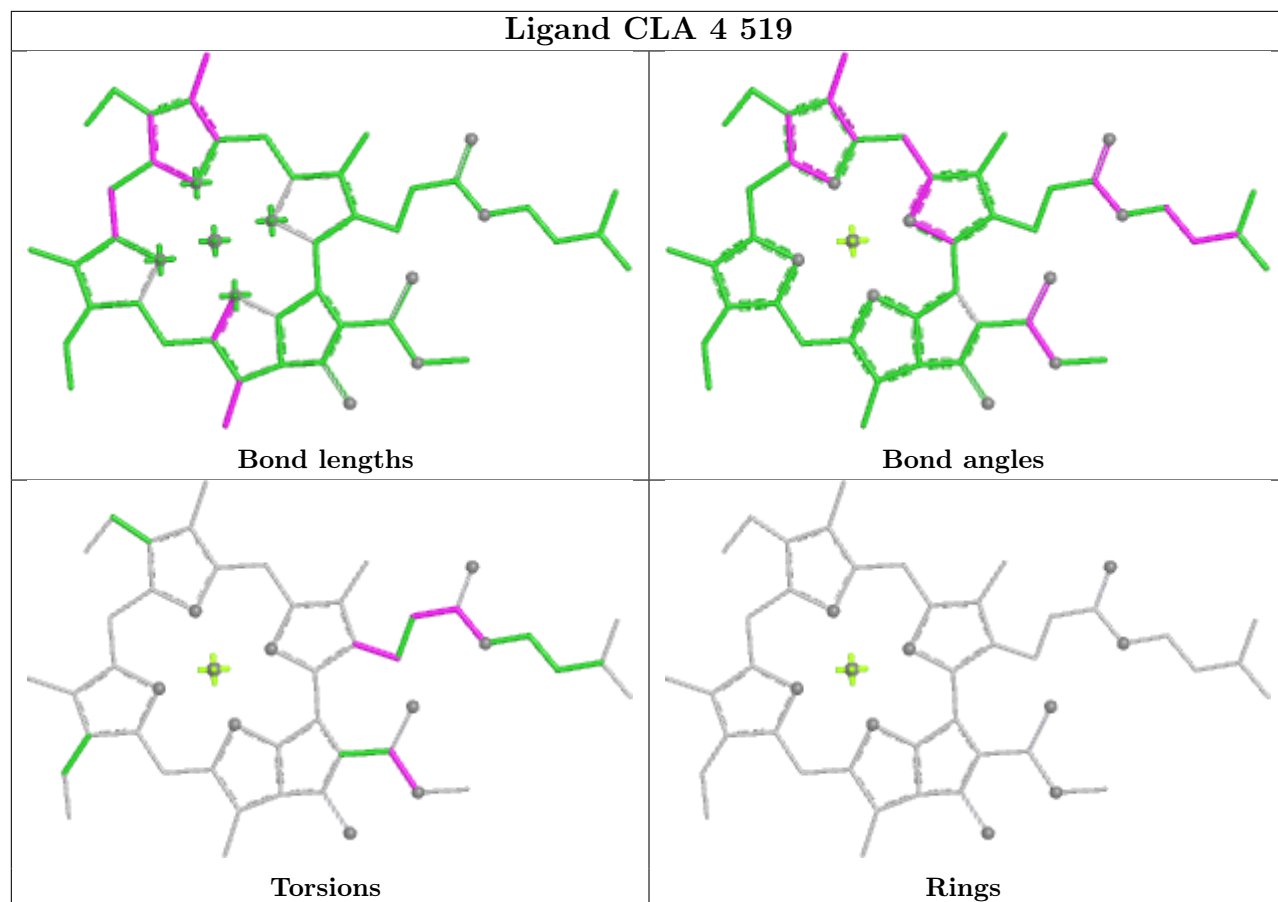
Ligand BCR c 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

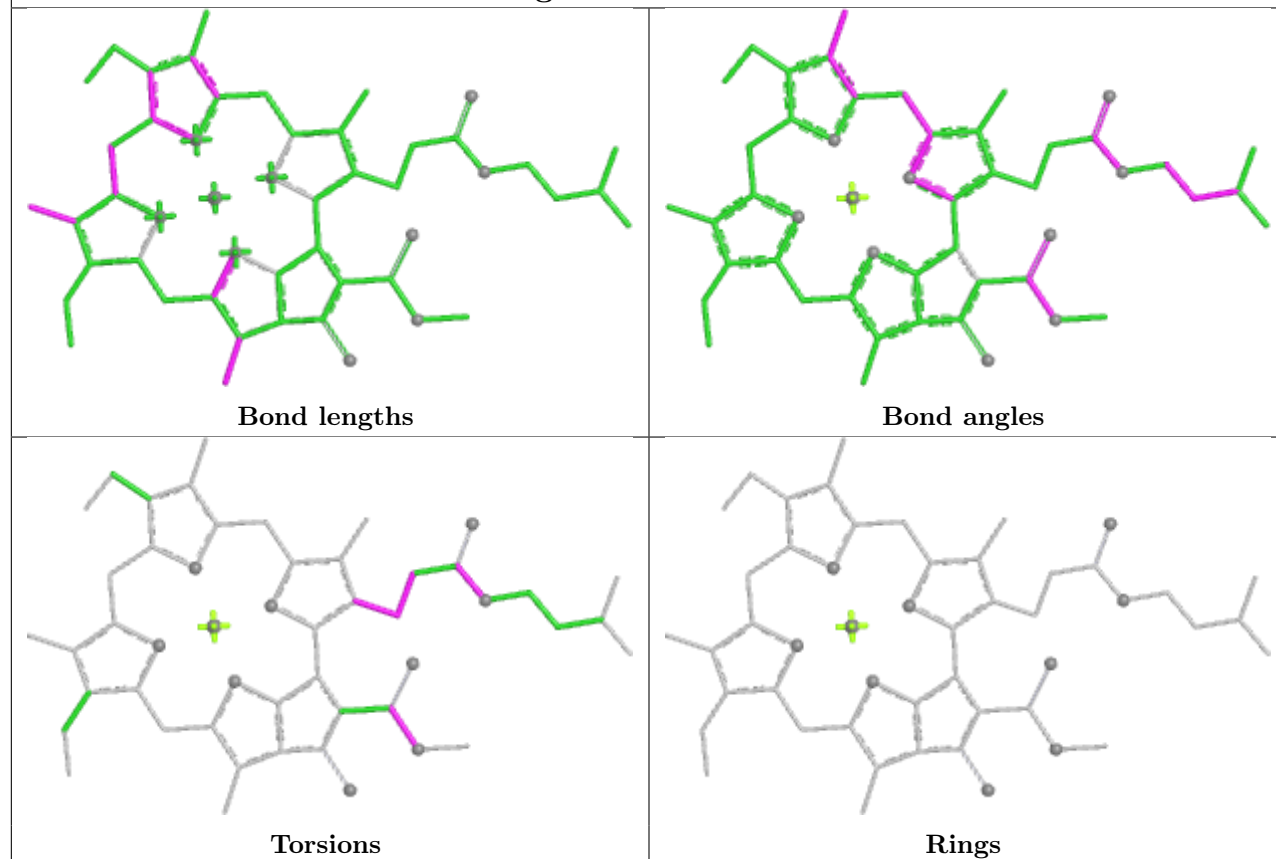
Ligand BCR B 4009	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 510**Ligand CLA c 505**

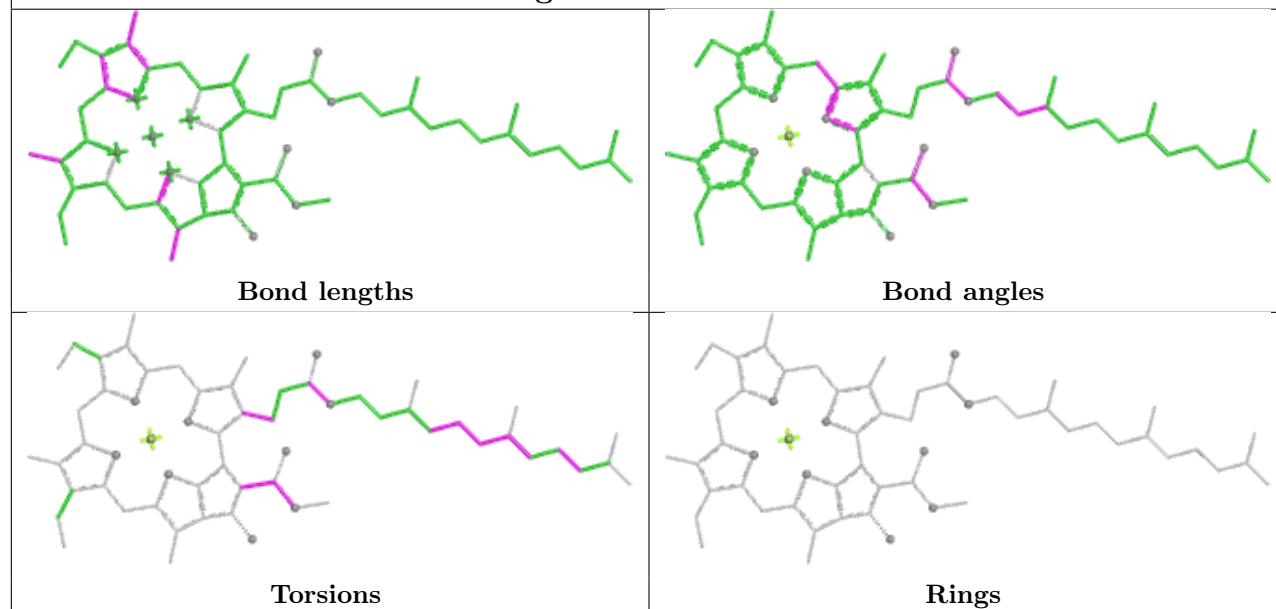
Ligand CLA 4 519



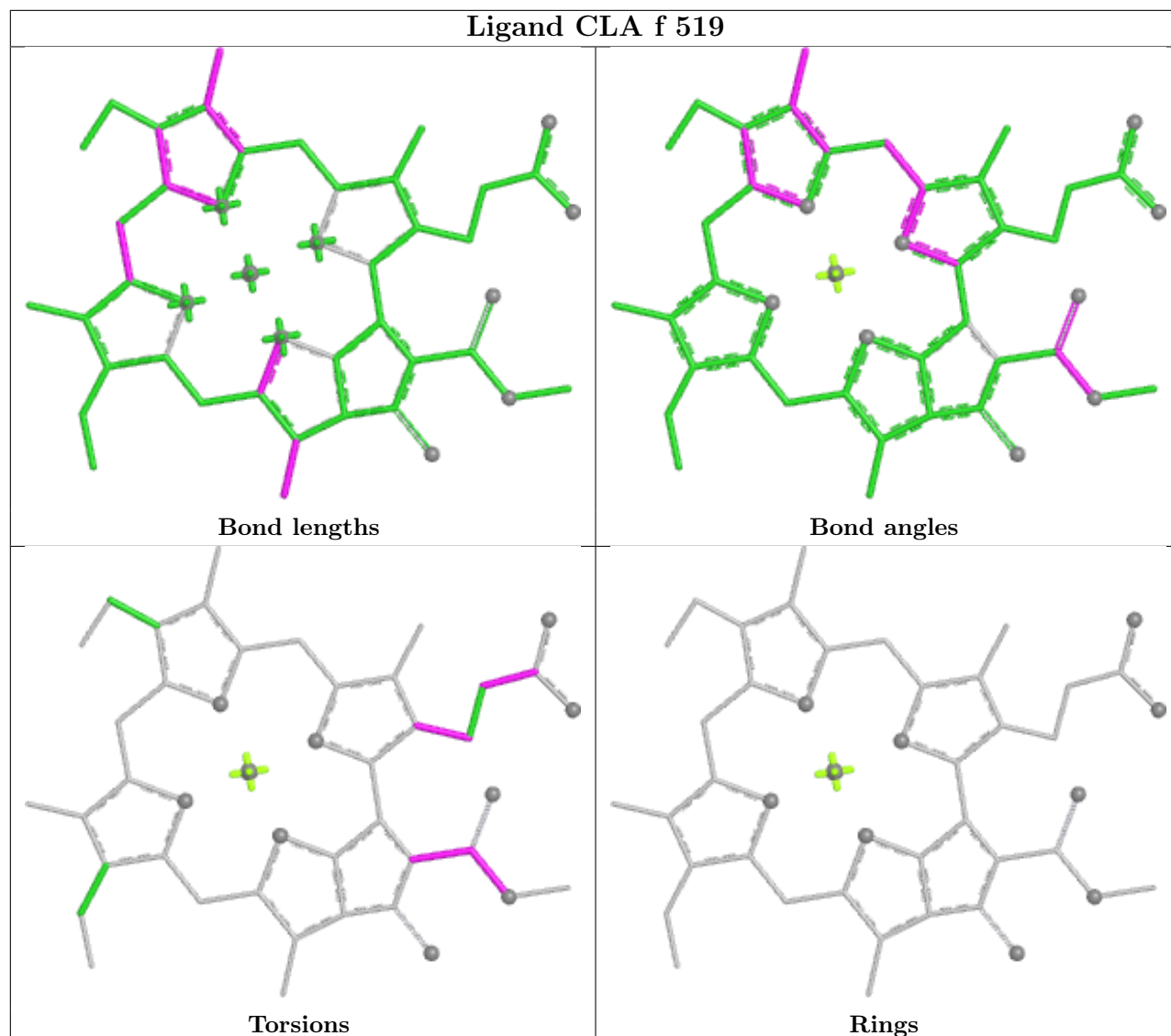
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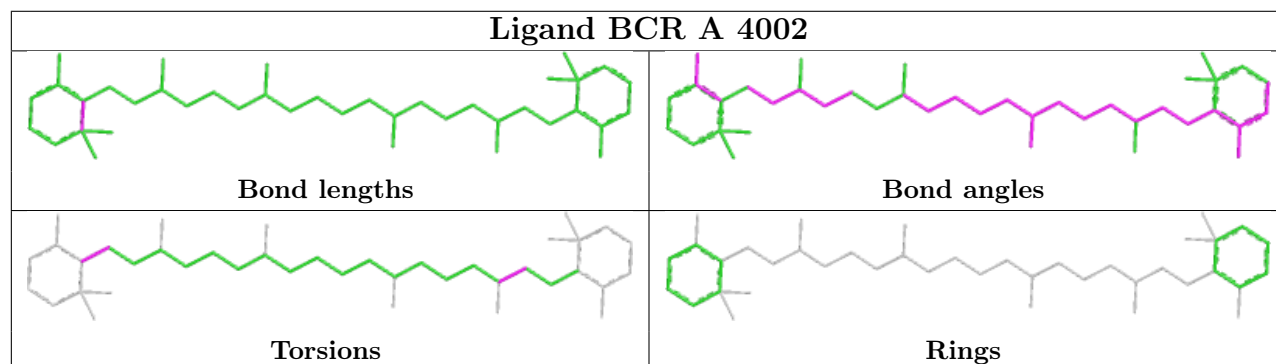
Ligand CLA d 502



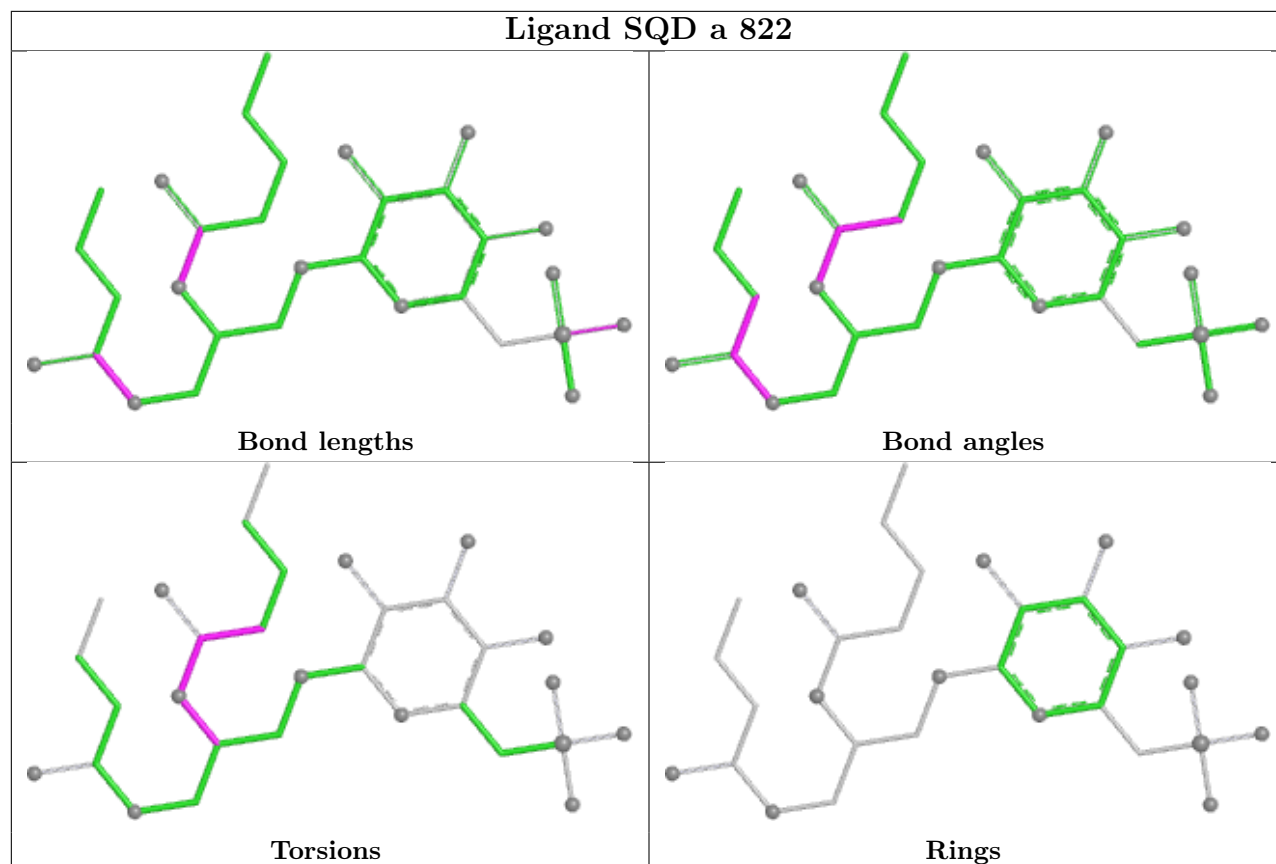
Ligand CLA f 519



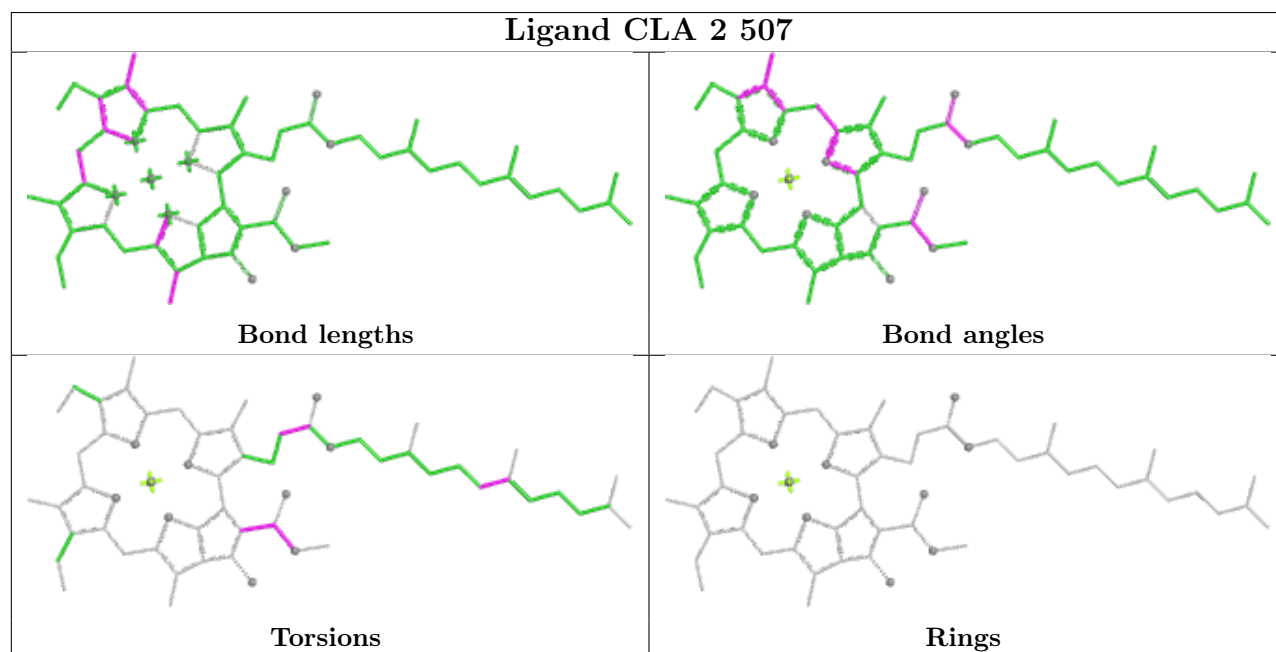
Ligand BCR A 4002

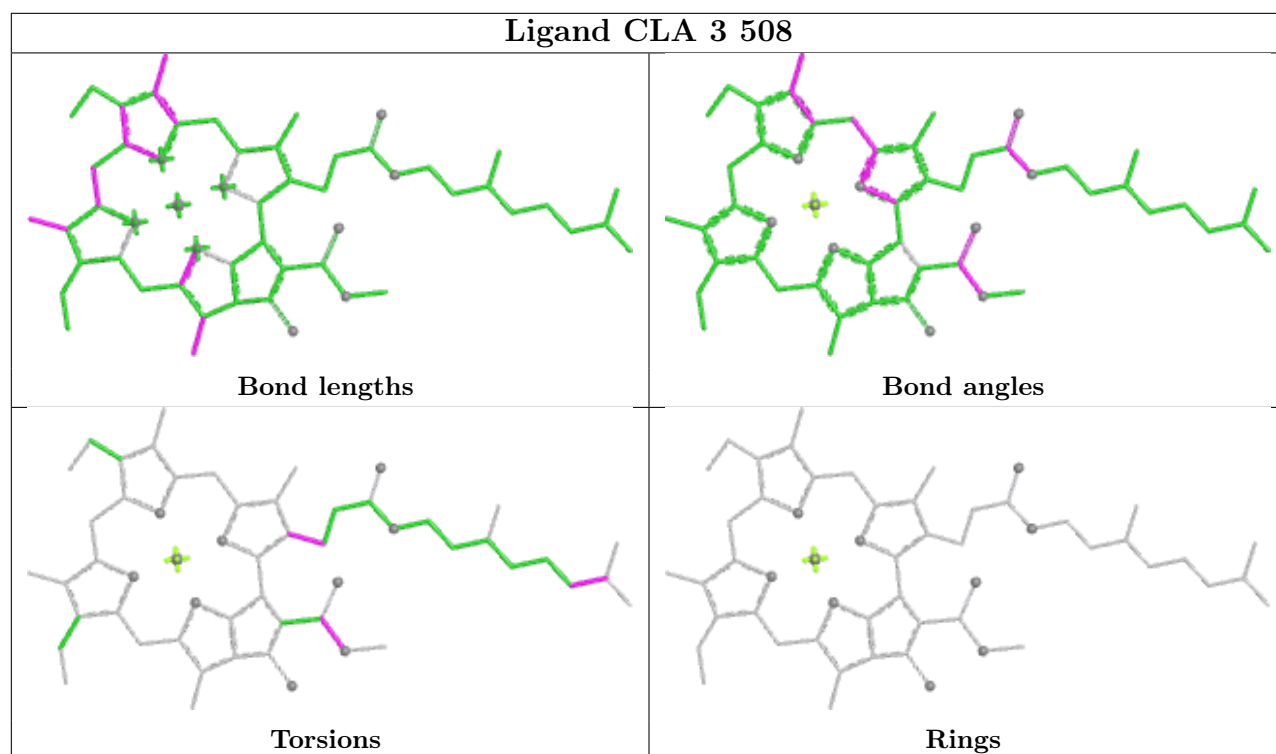
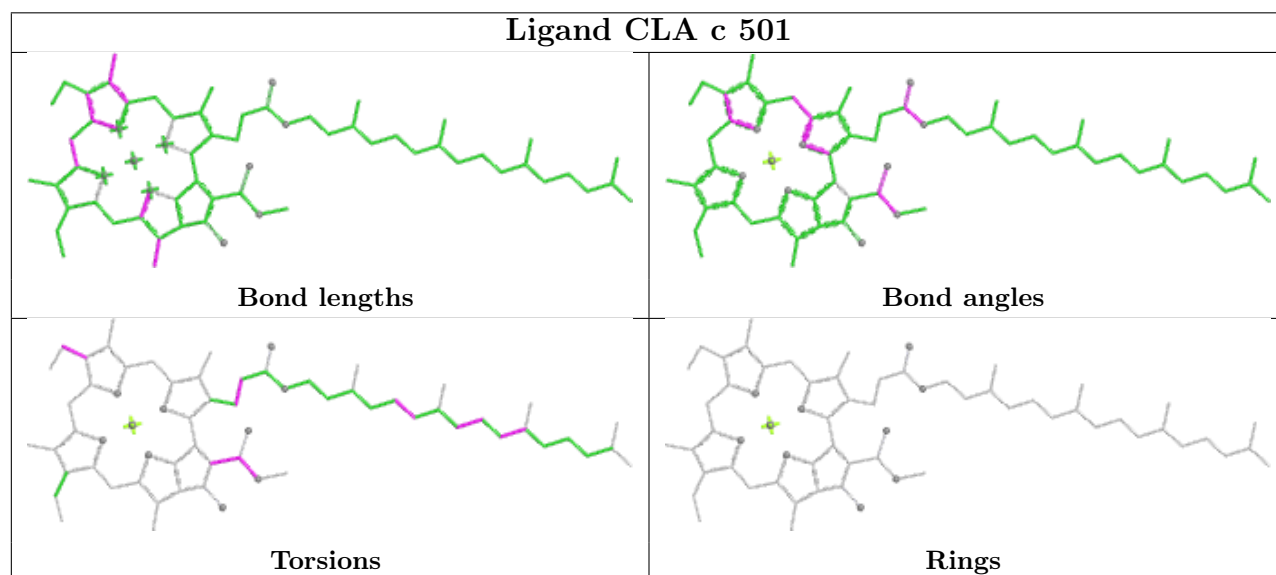
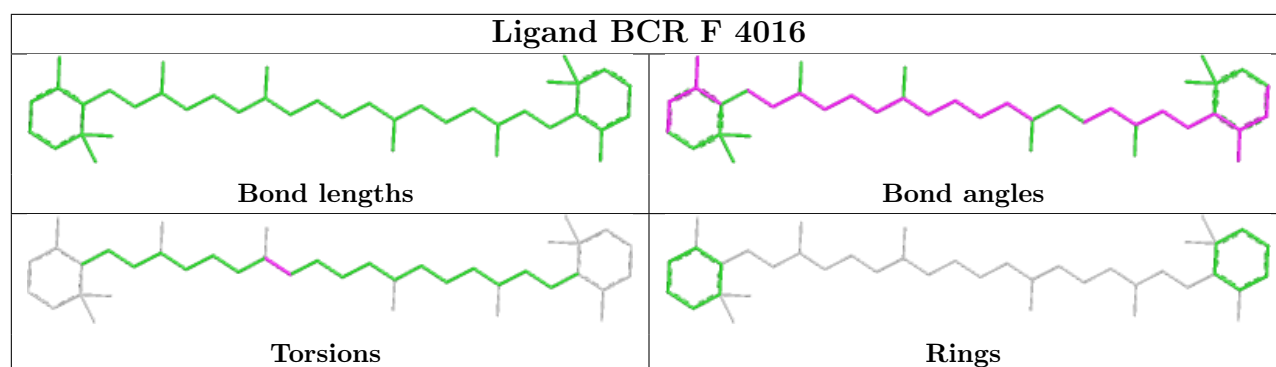


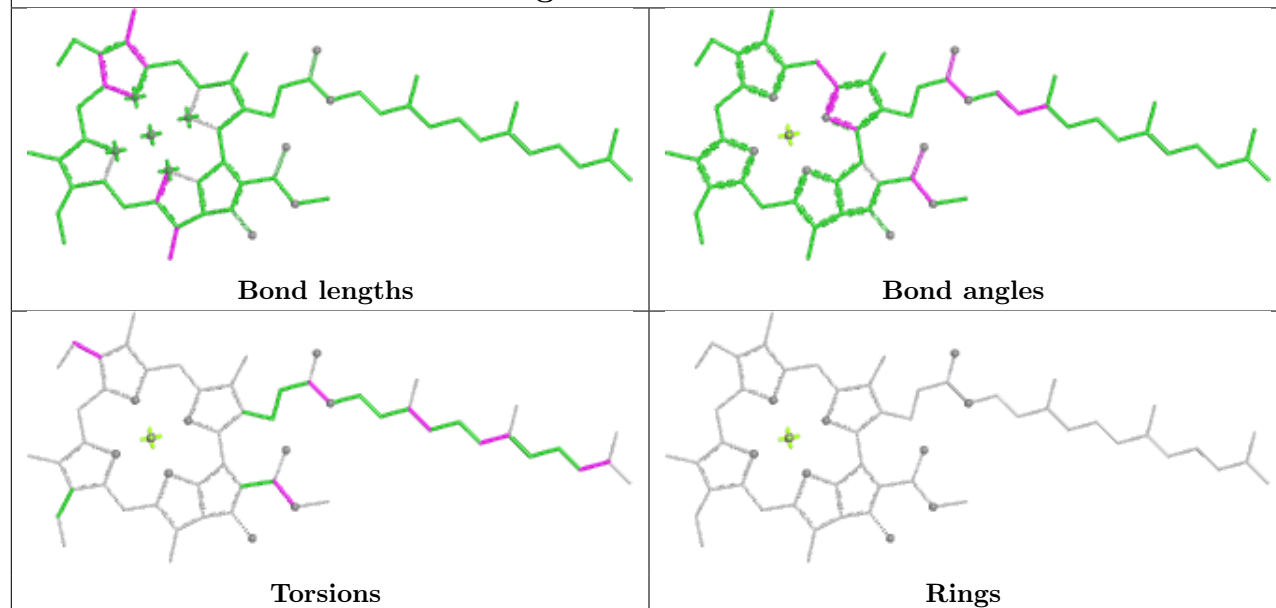
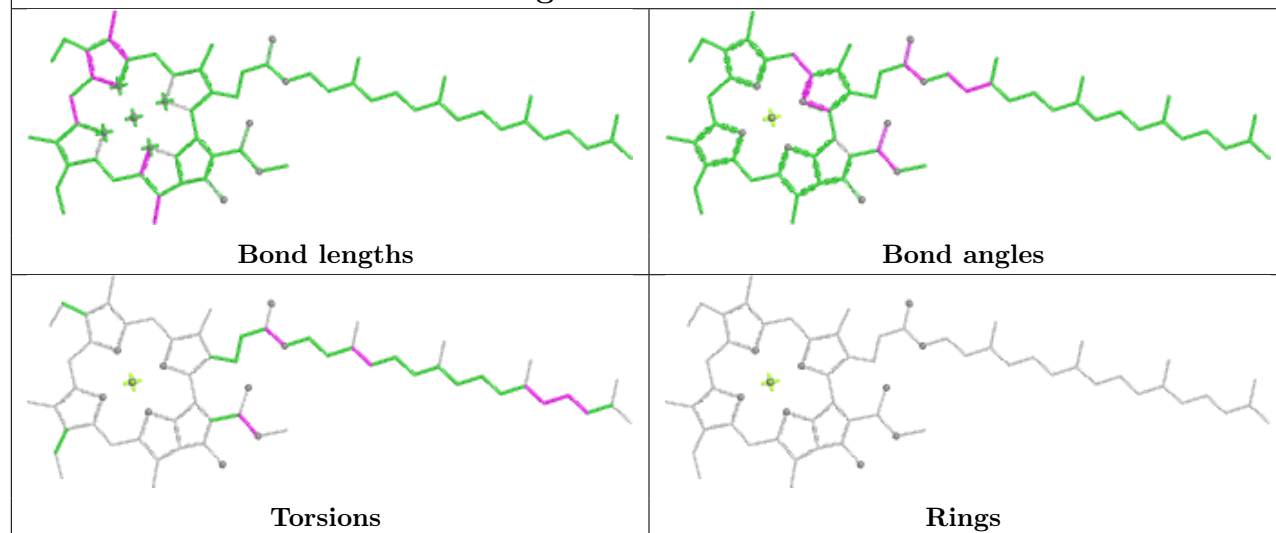
Ligand SQD a 822



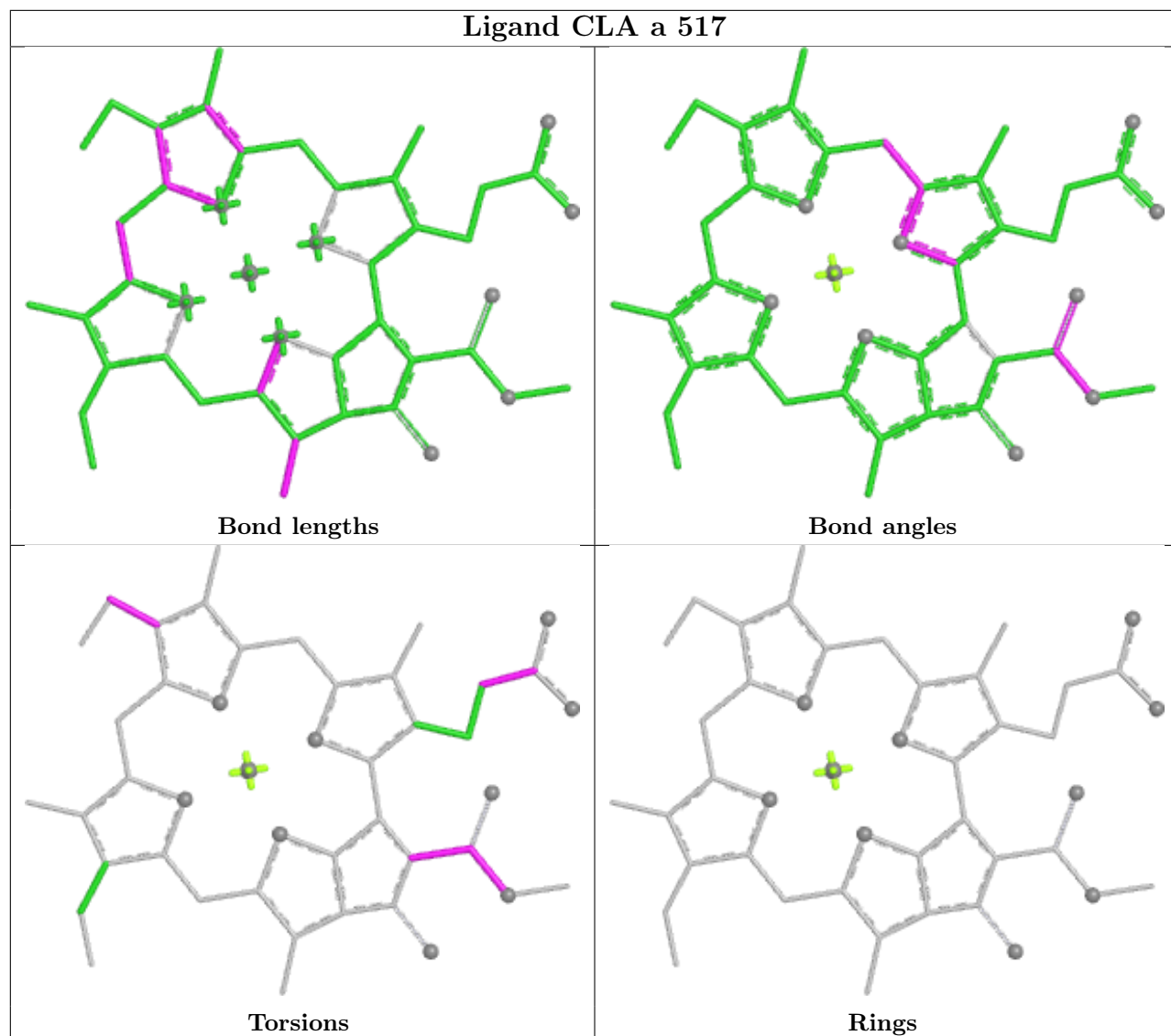
Ligand CLA 2 507



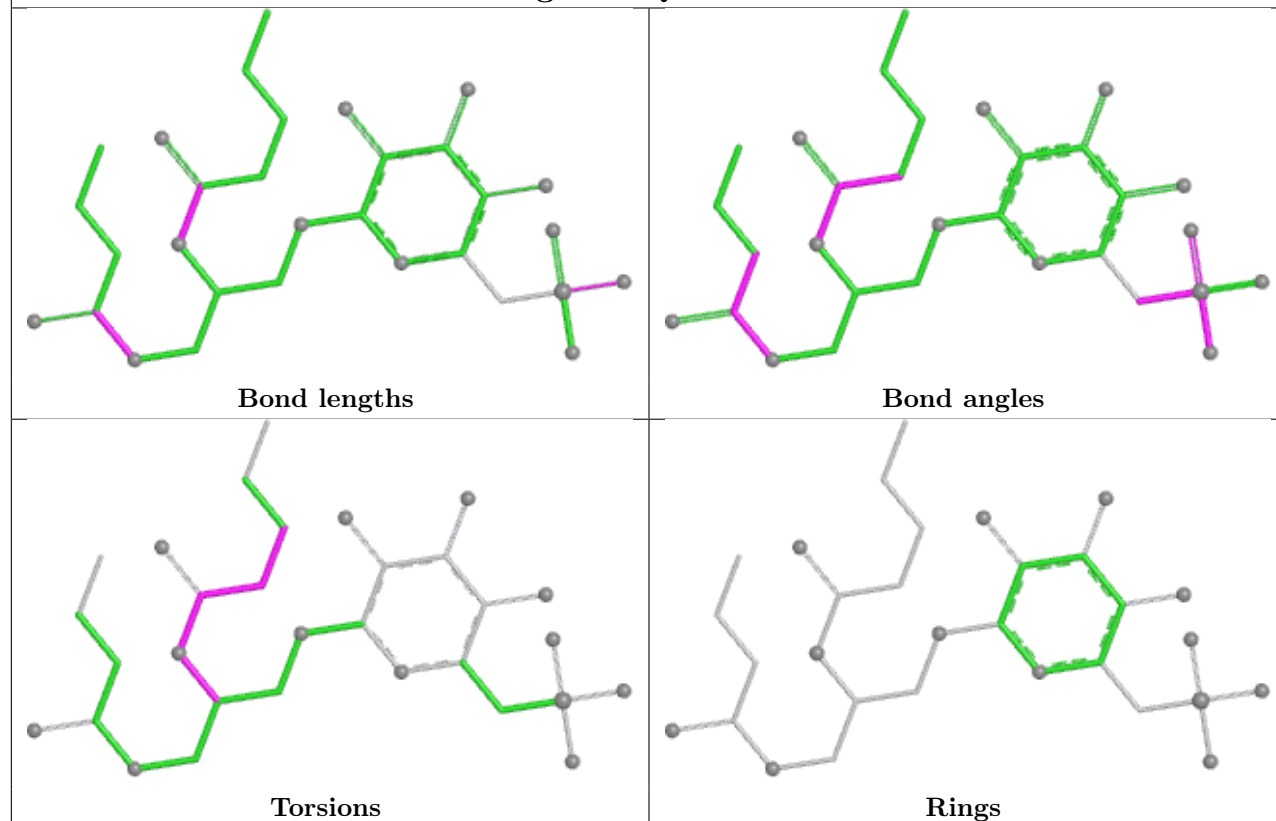


Ligand CLA 5 507**Ligand CLA 1 509**

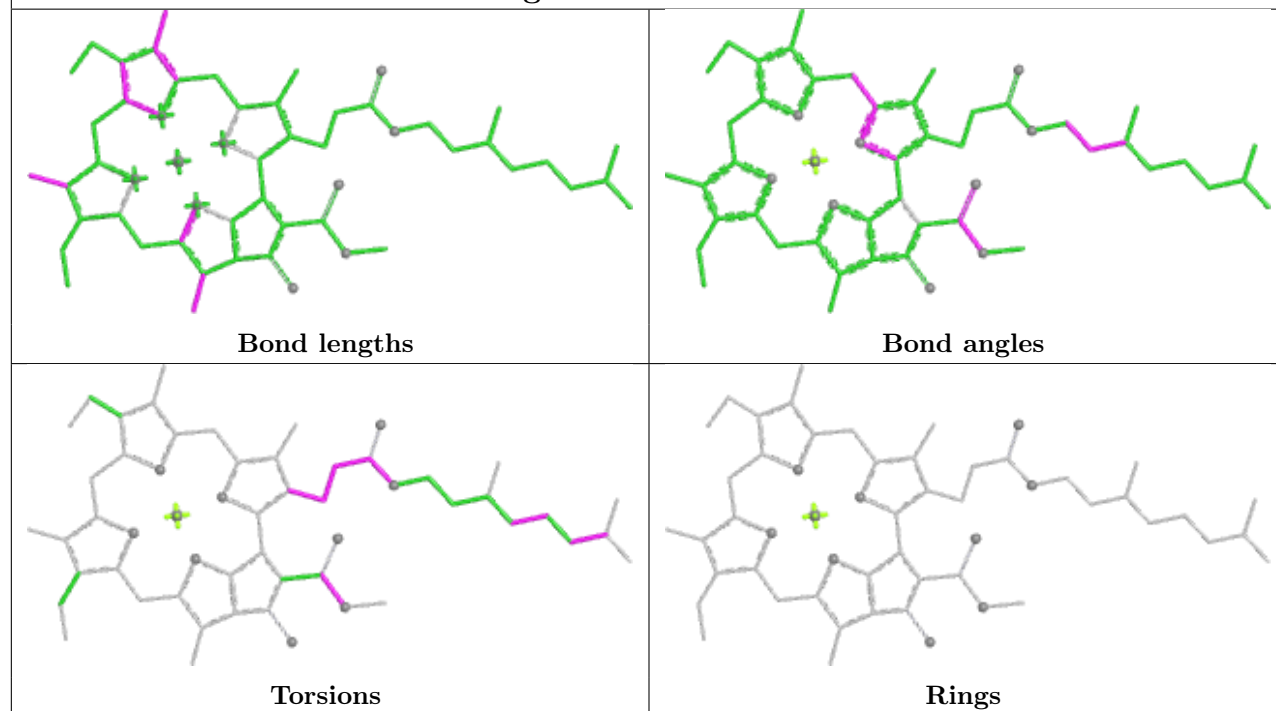
Ligand CLA a 517

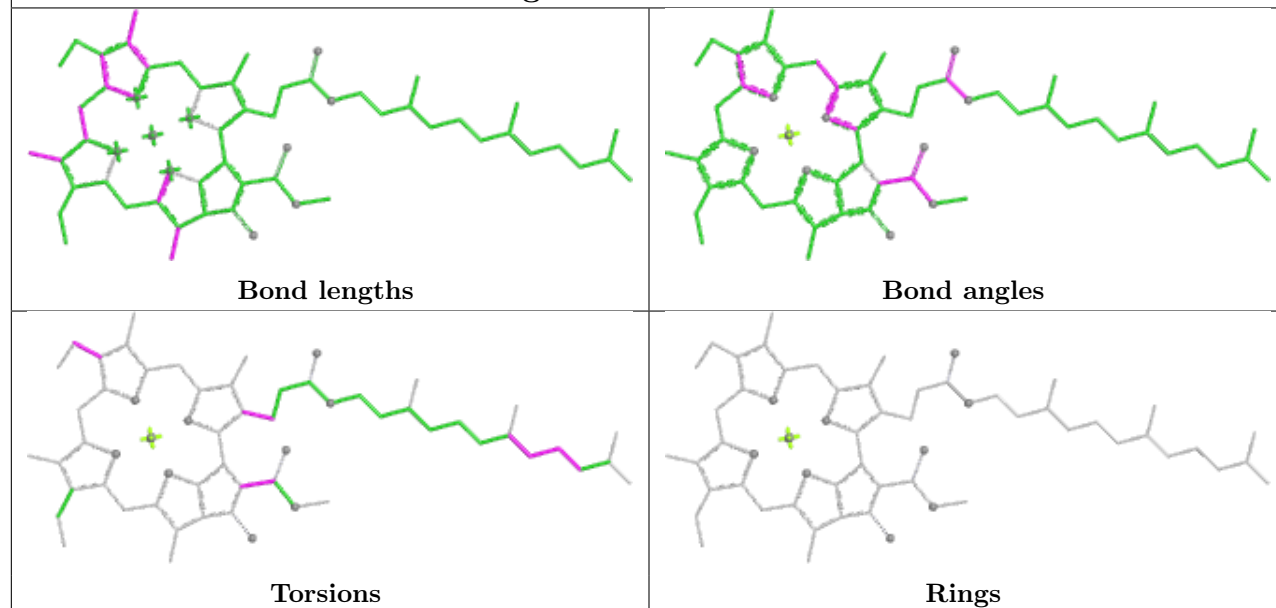
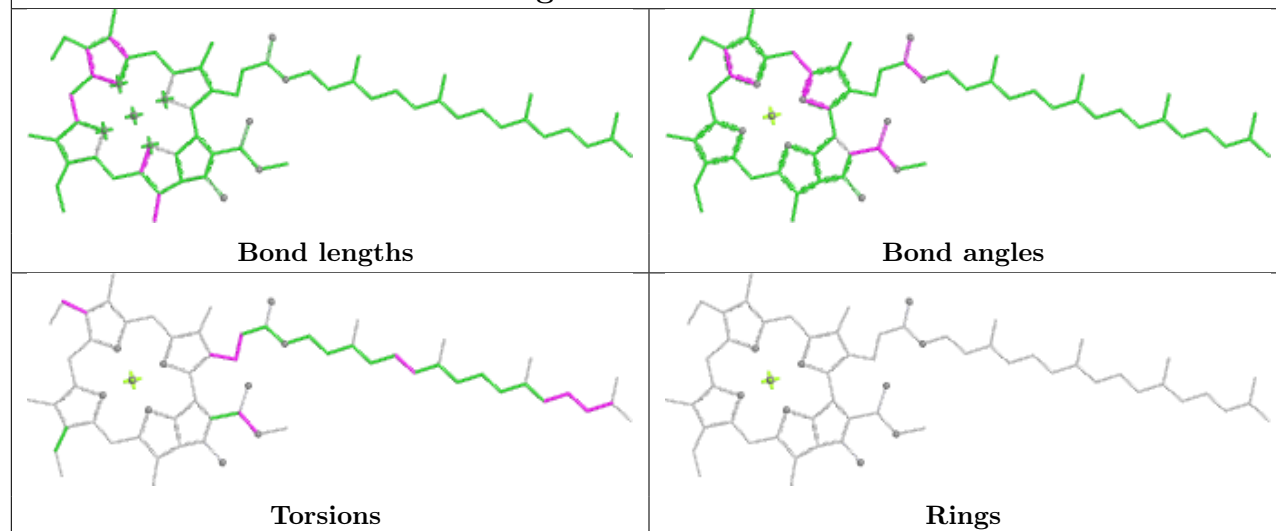


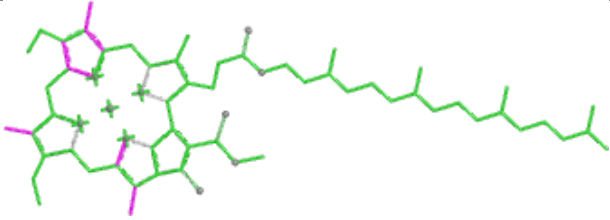
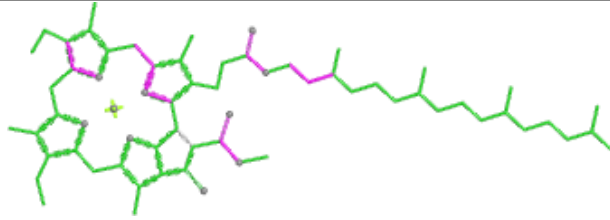
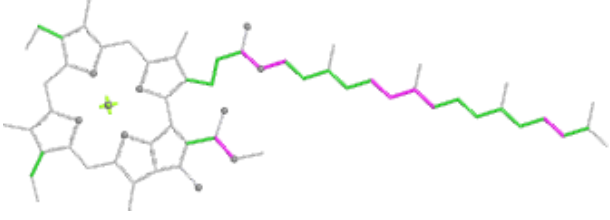
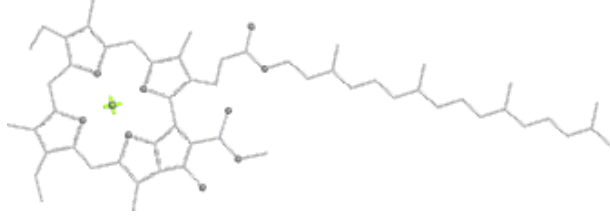
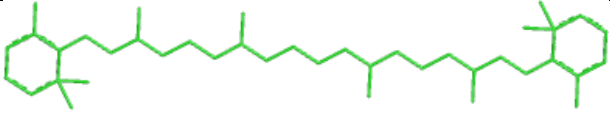
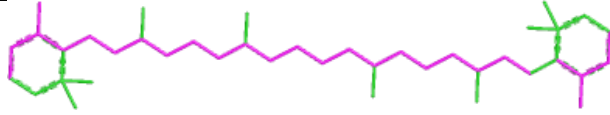
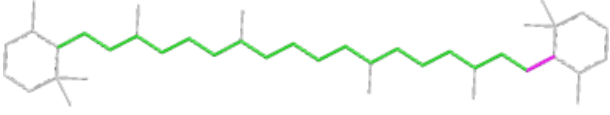
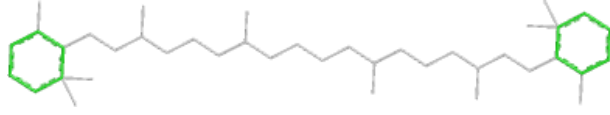
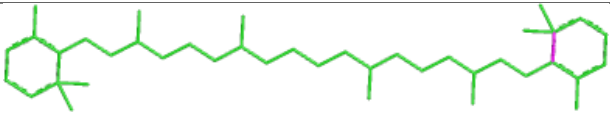
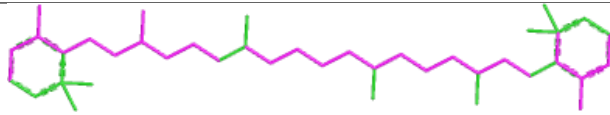
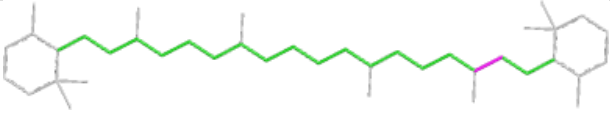
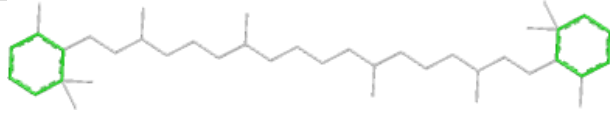
Ligand SQD 1 822

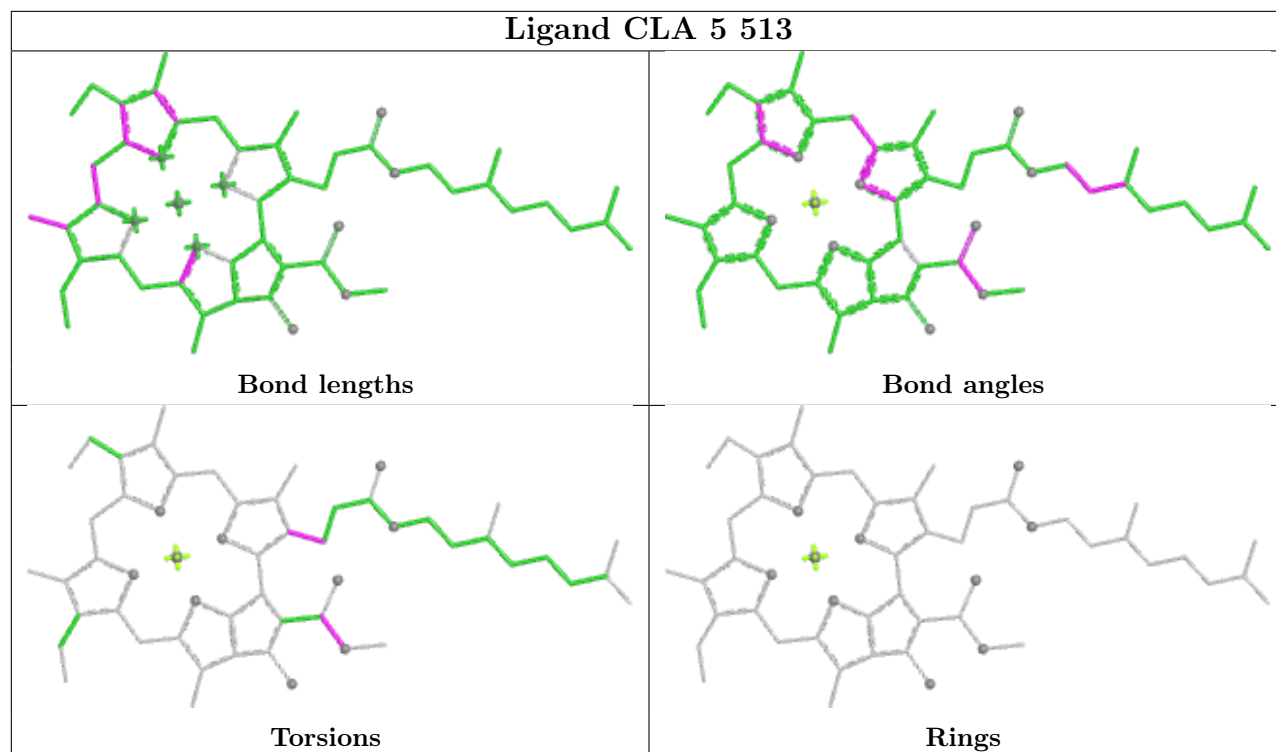
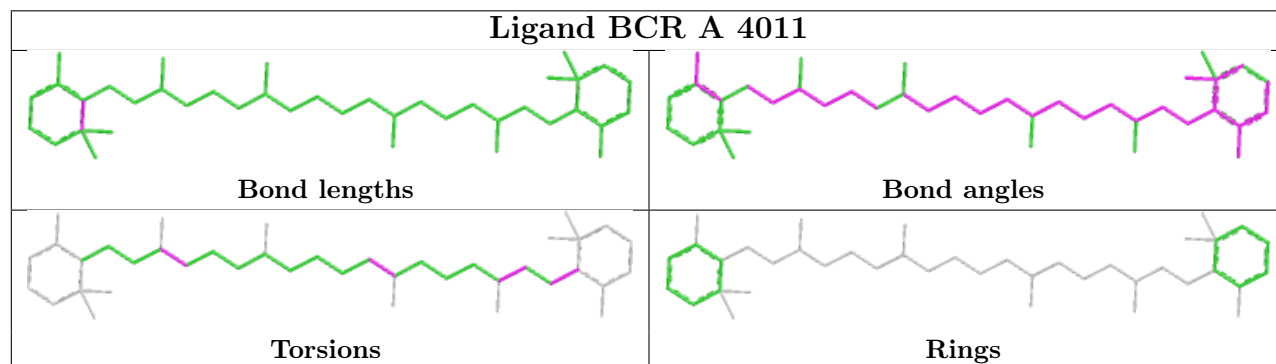
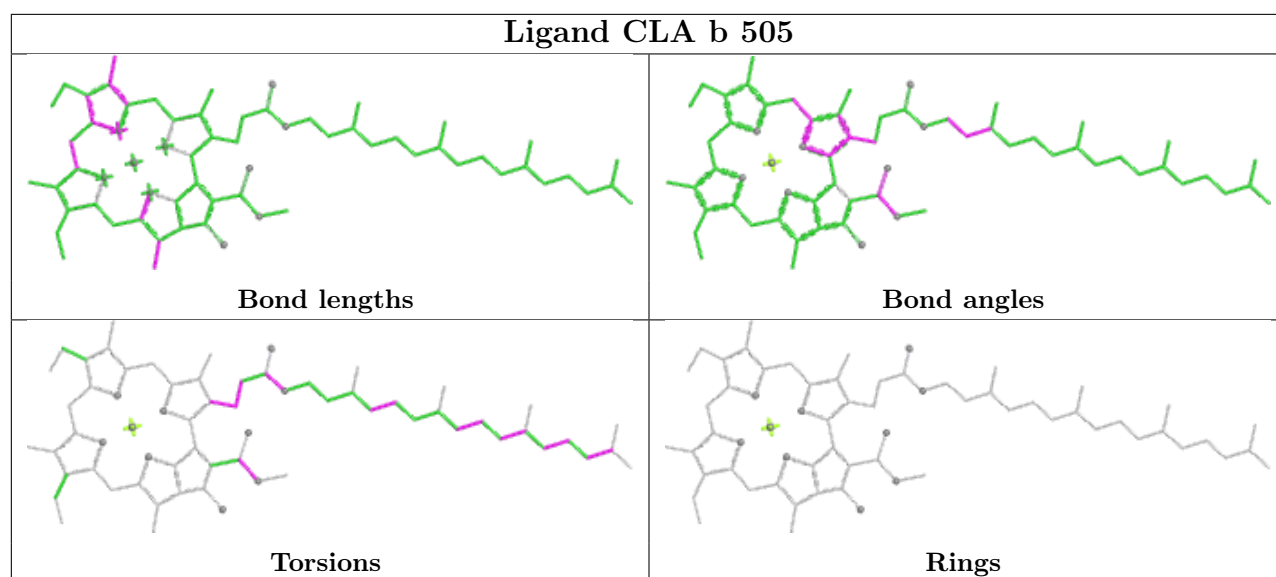


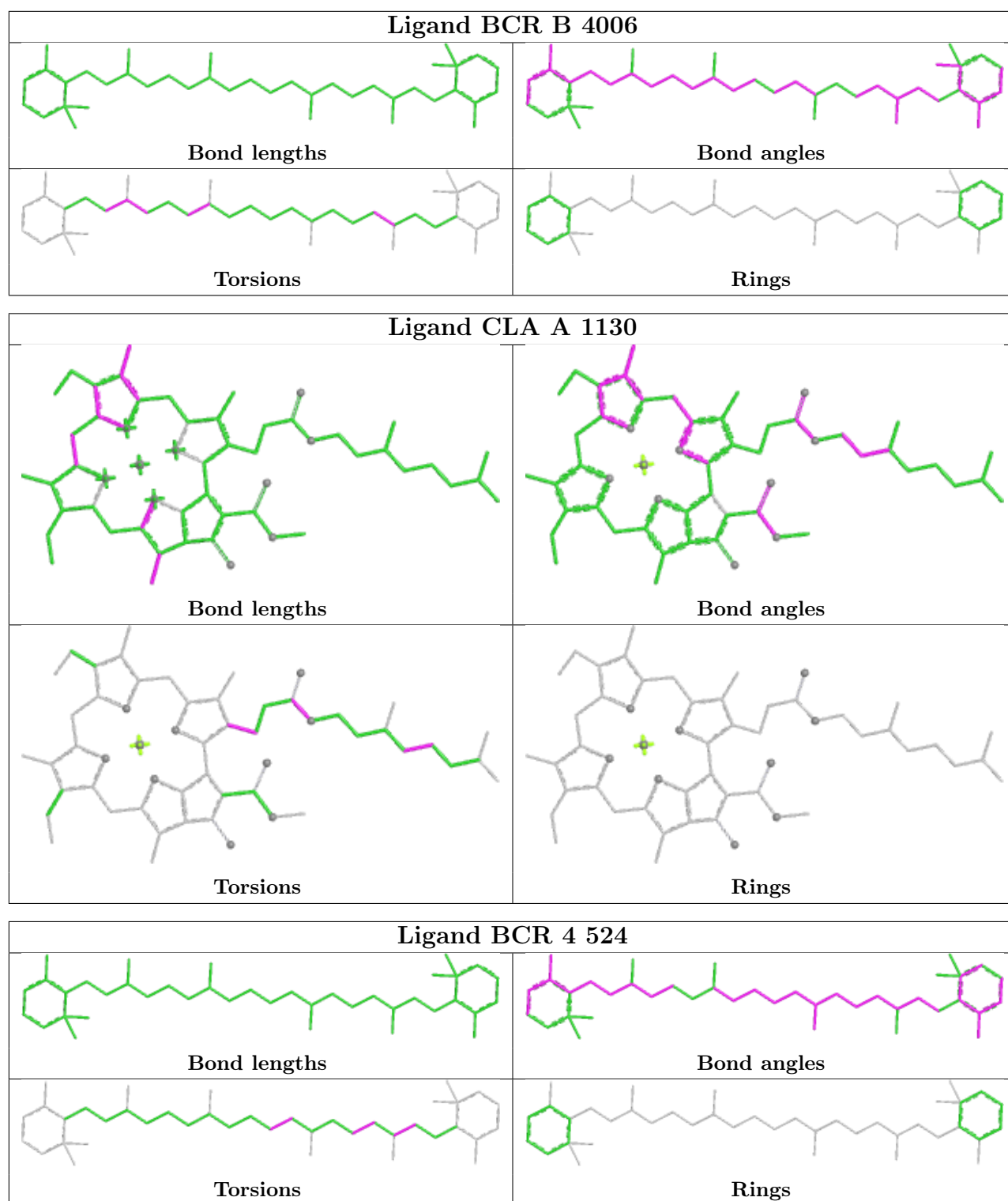
Ligand CLA B 1217

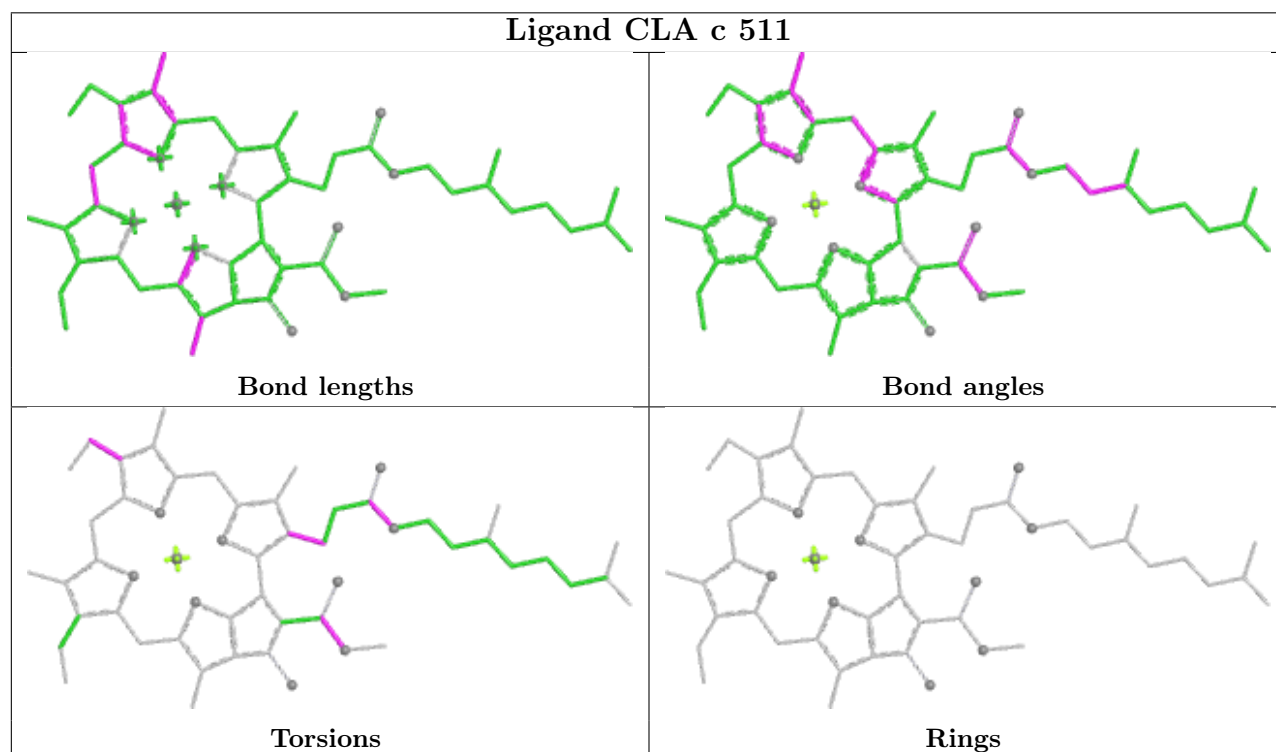
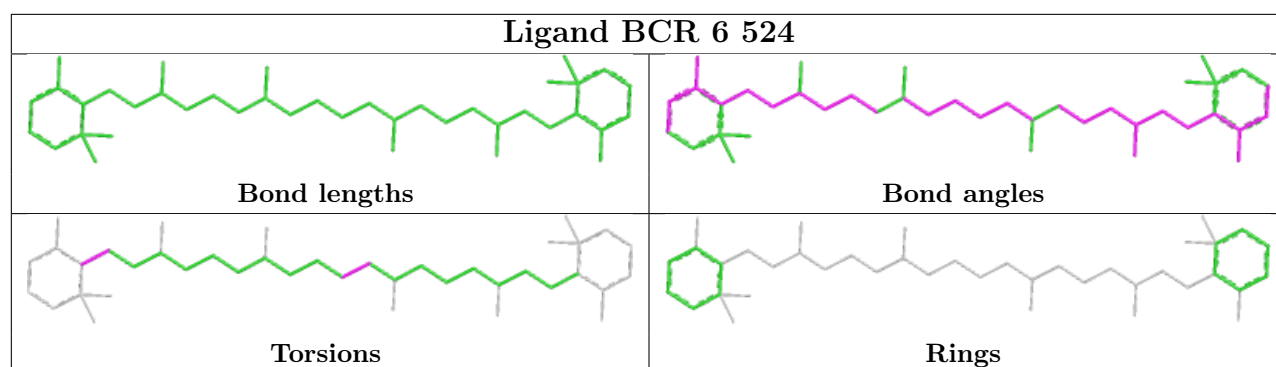


Ligand CLA A 1101**Ligand CLA a 501**

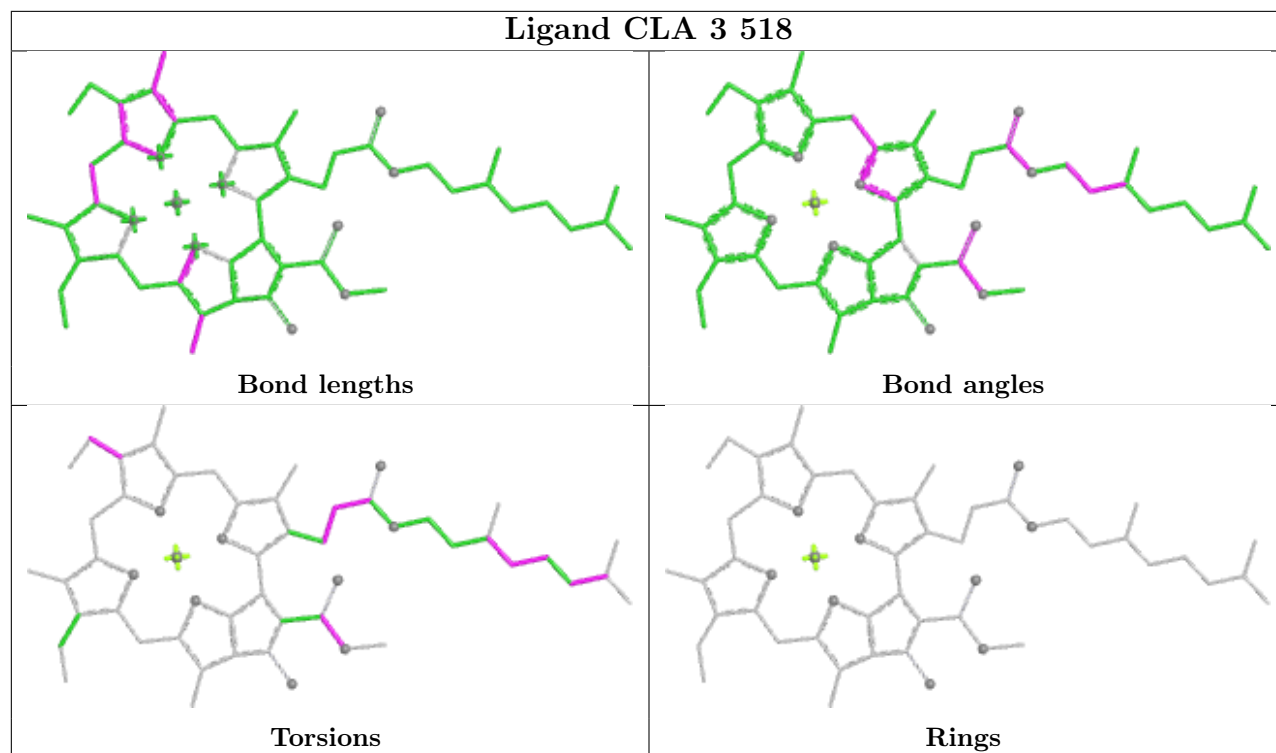
Ligand CLA 2 509	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 6 523	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 4008	
 Bond lengths	 Bond angles
 Torsions	 Rings



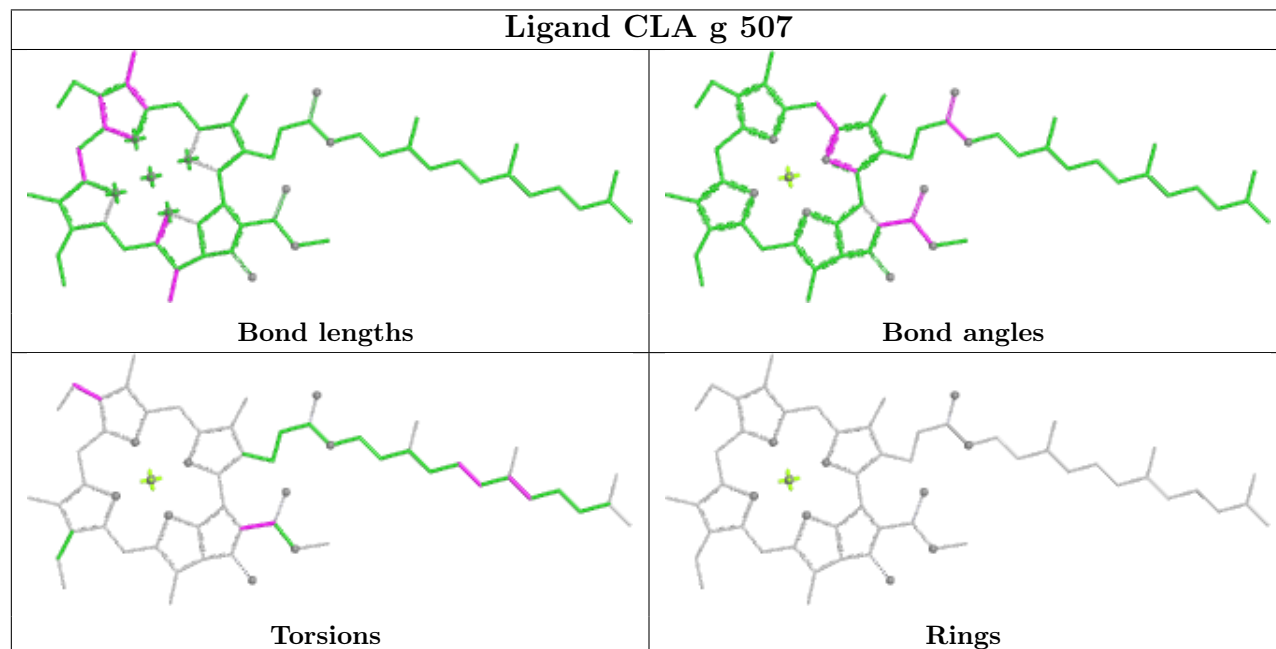




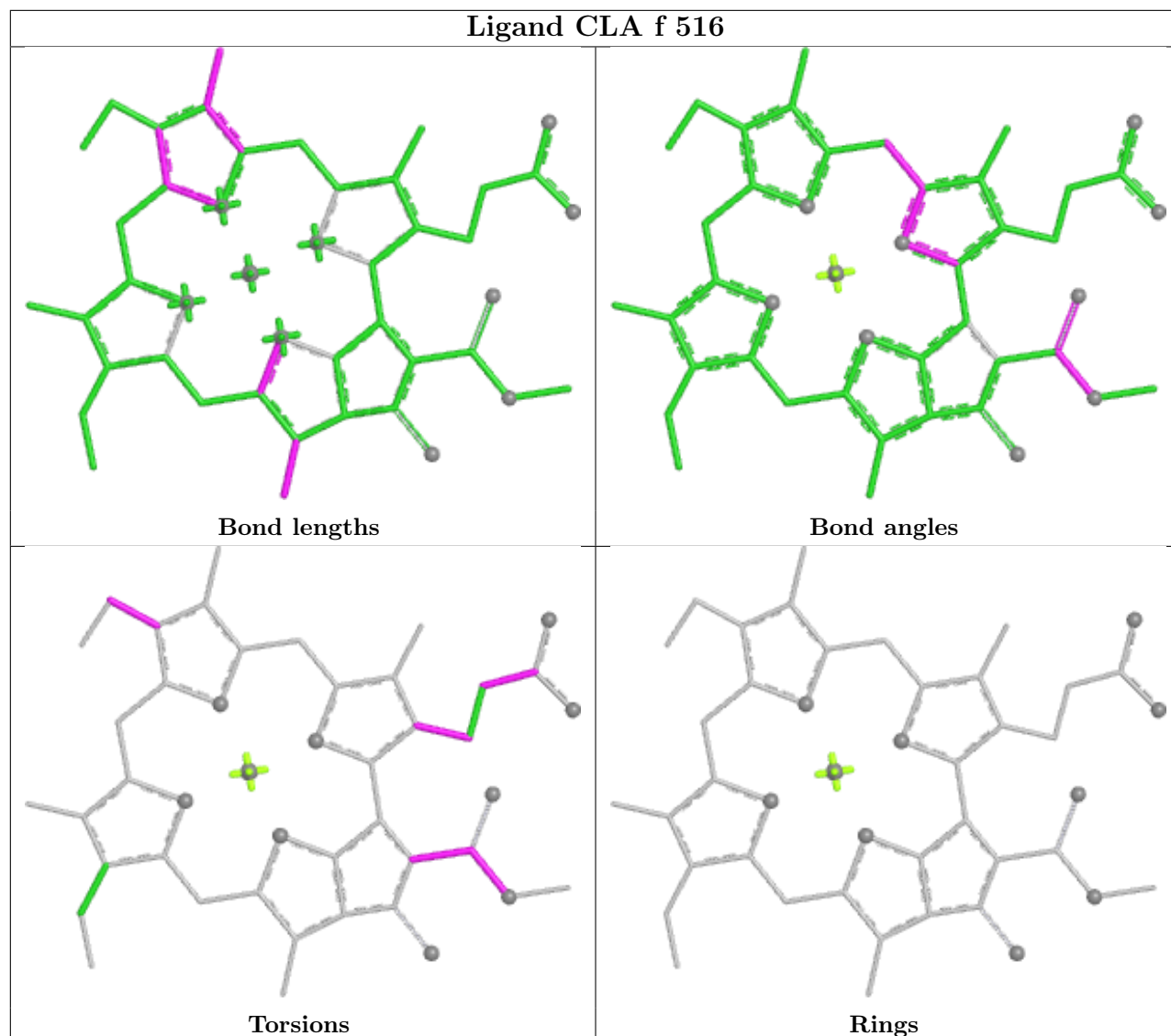
Ligand CLA 3 518



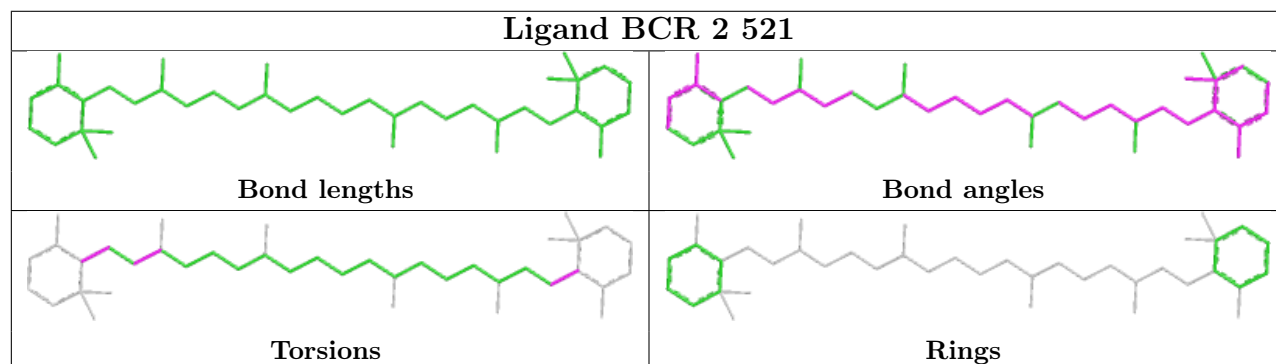
Ligand CLA g 507

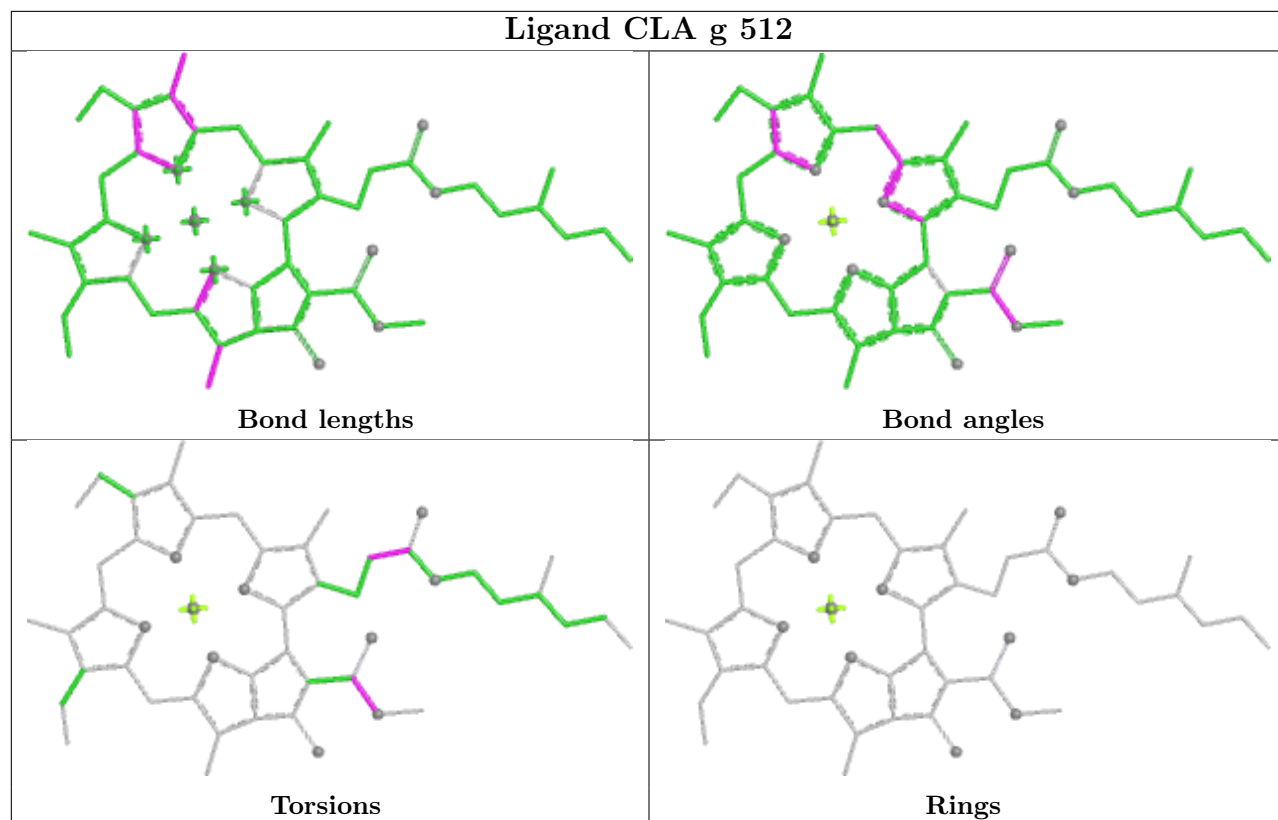


Ligand CLA f 516

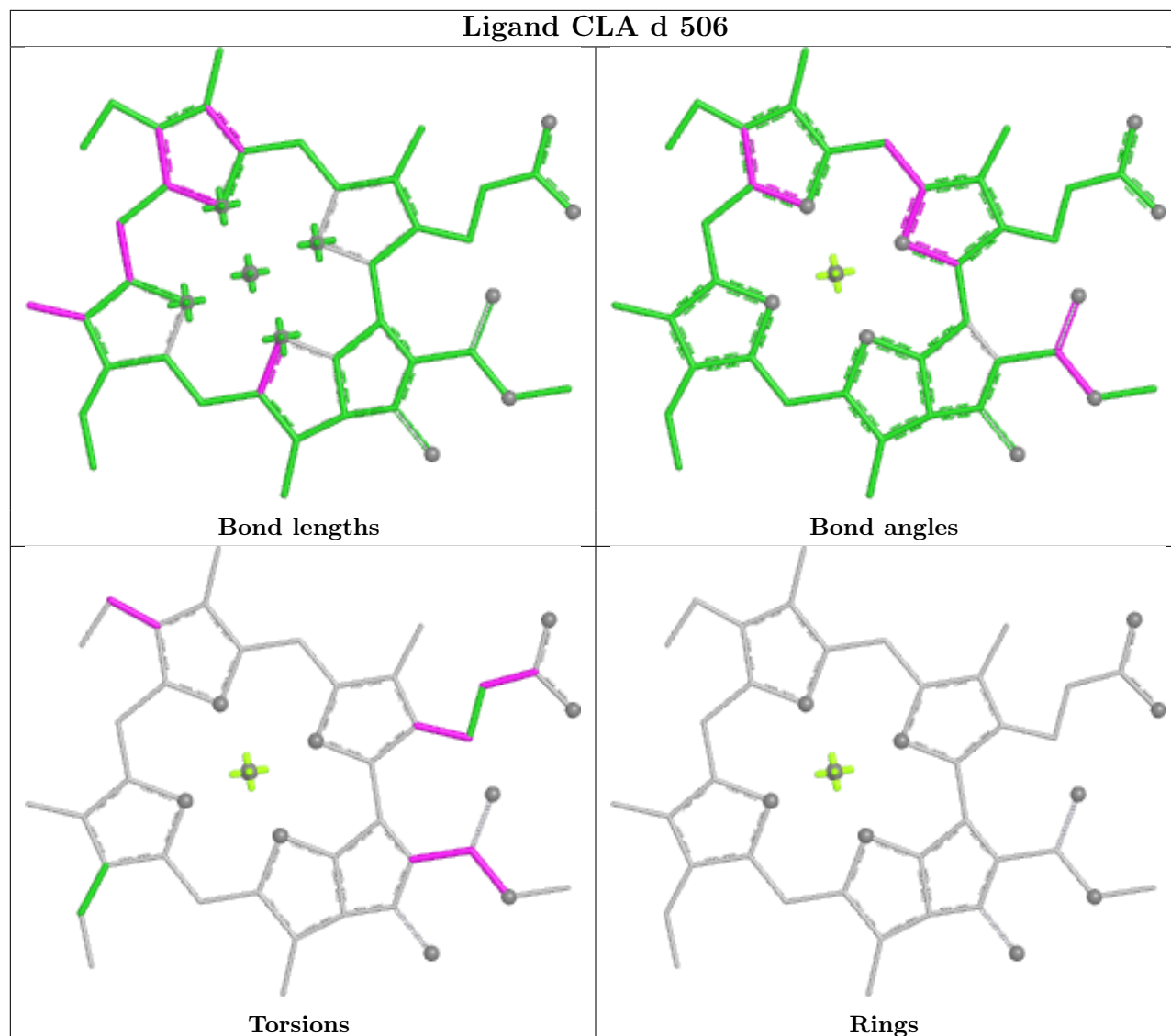


Ligand BCR 2 521

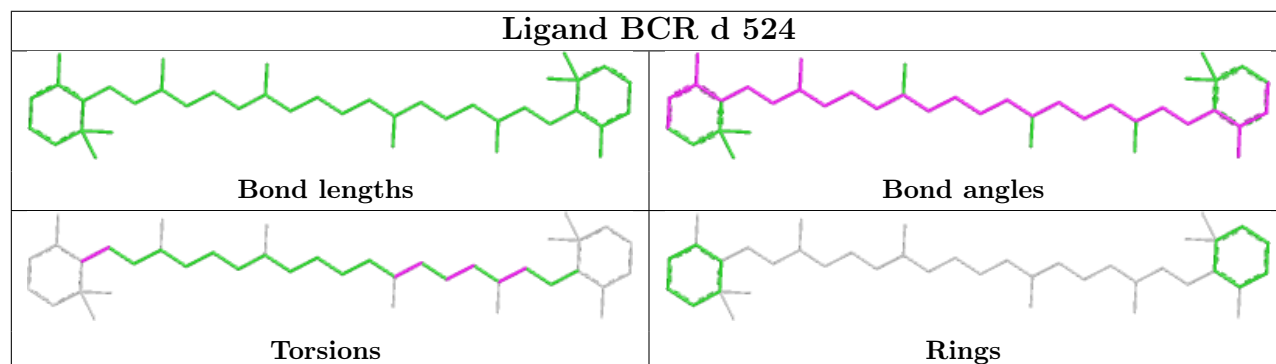




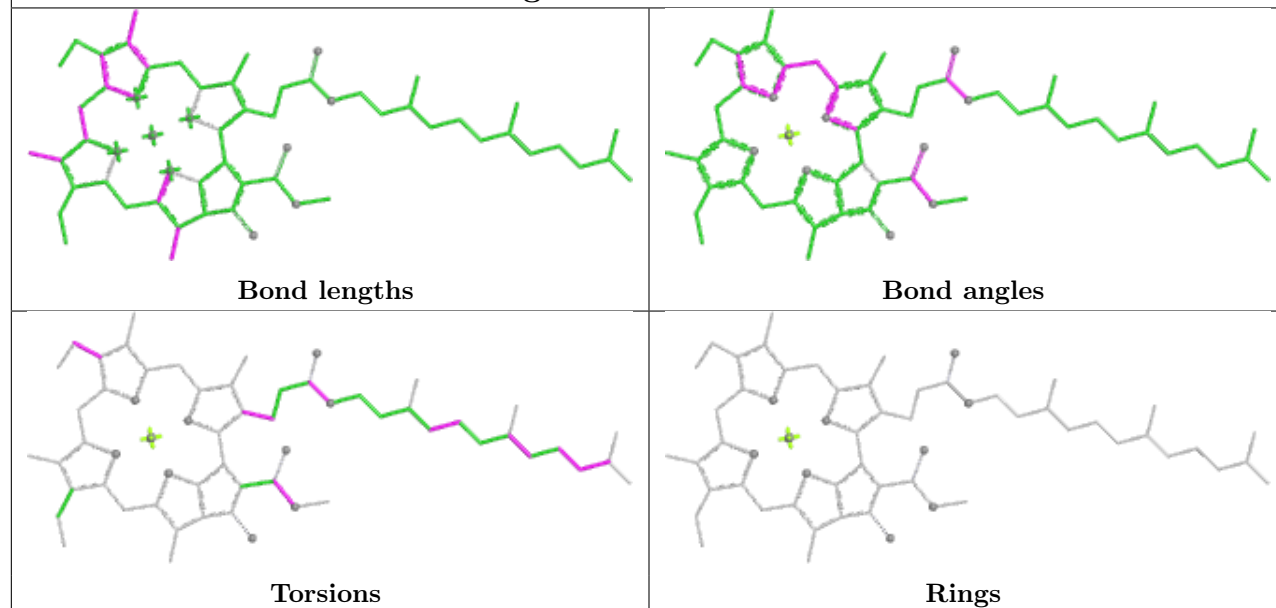
Ligand CLA d 506



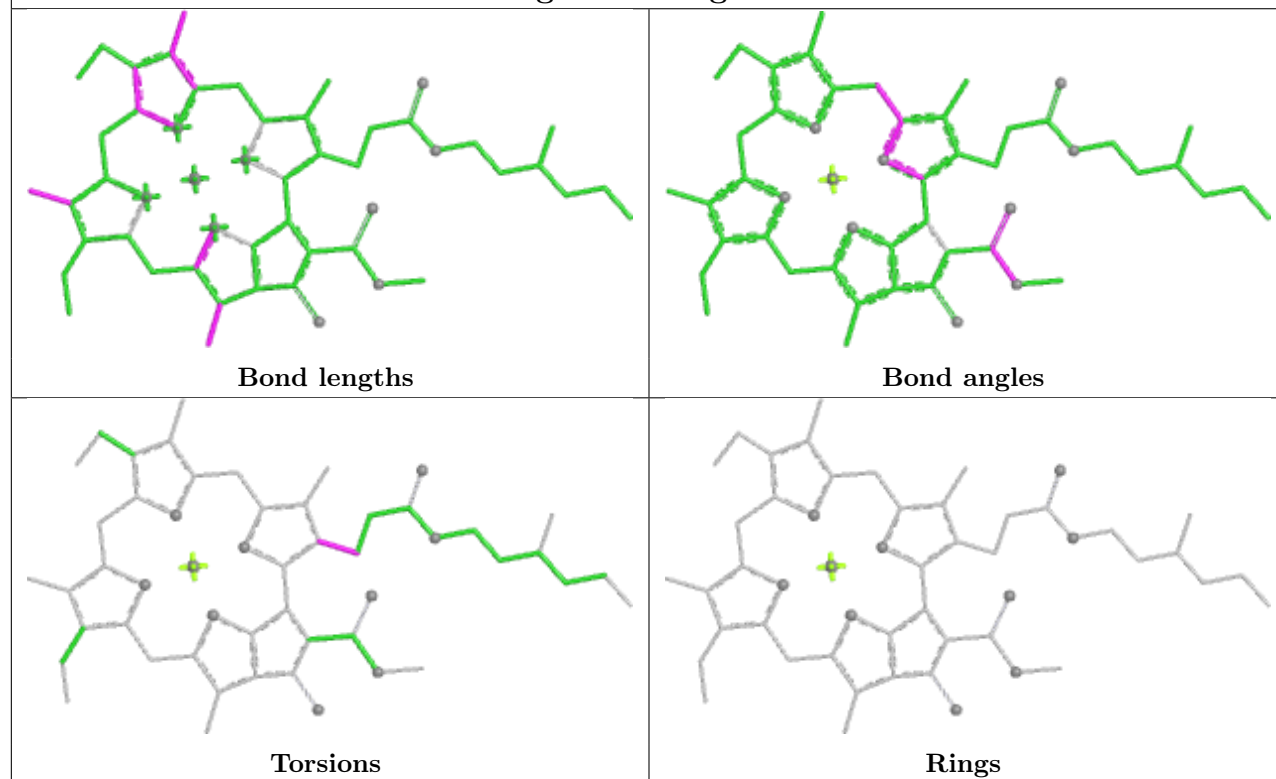
Ligand BCR d 524

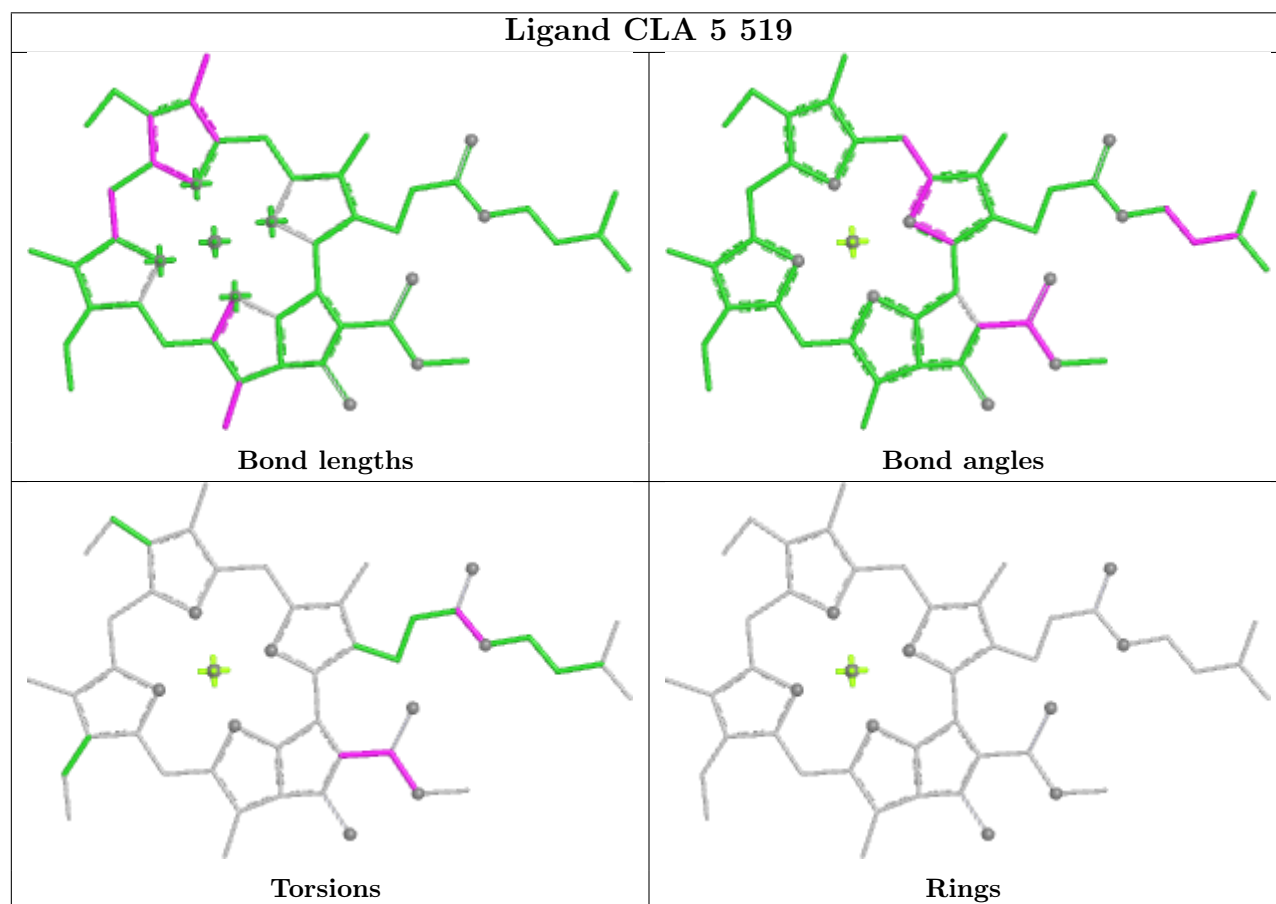
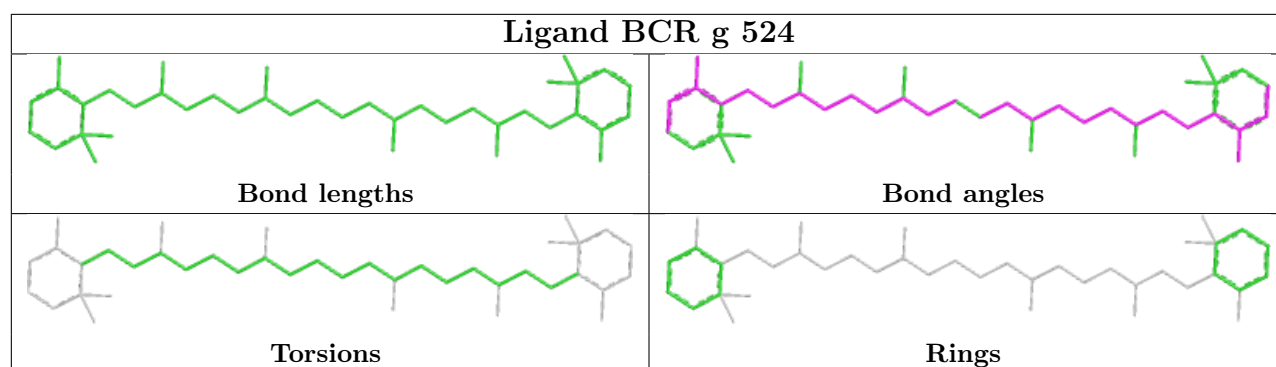


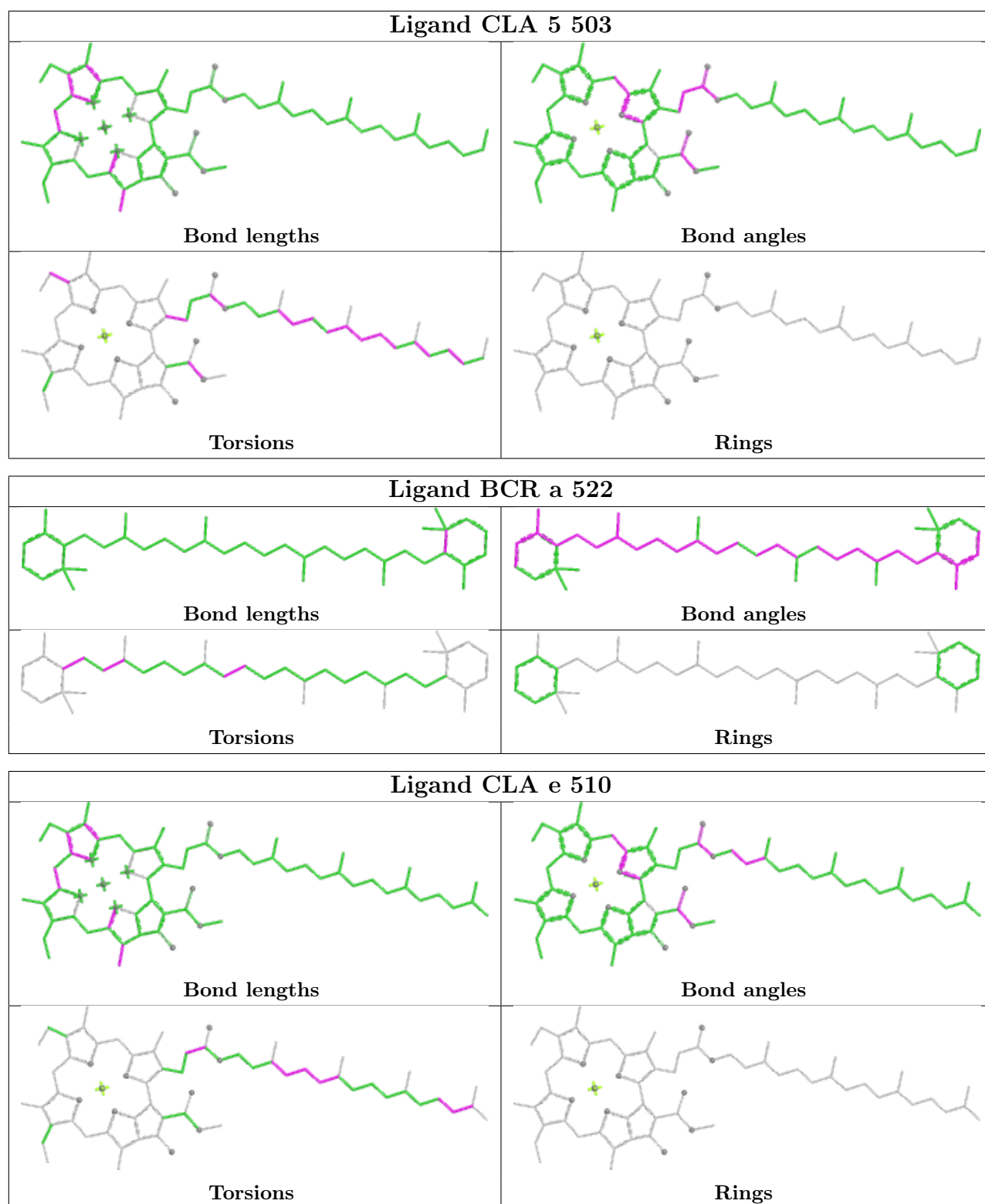
Ligand CLA B 1216

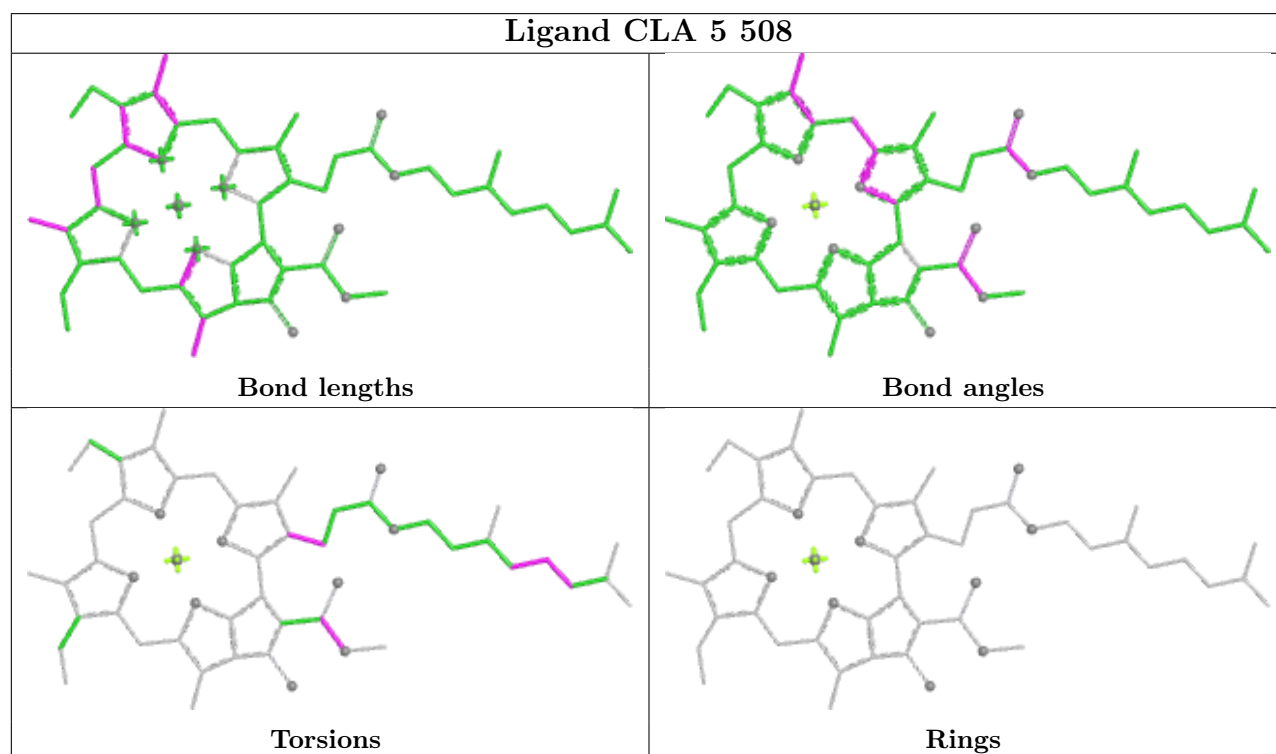
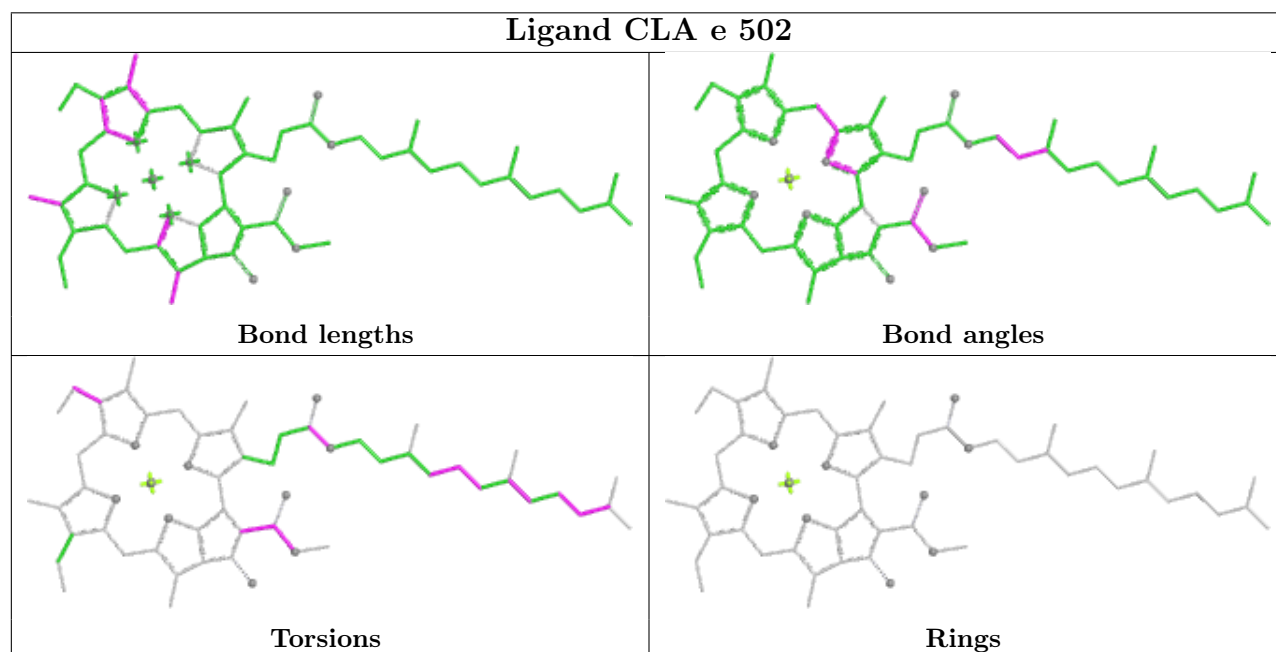
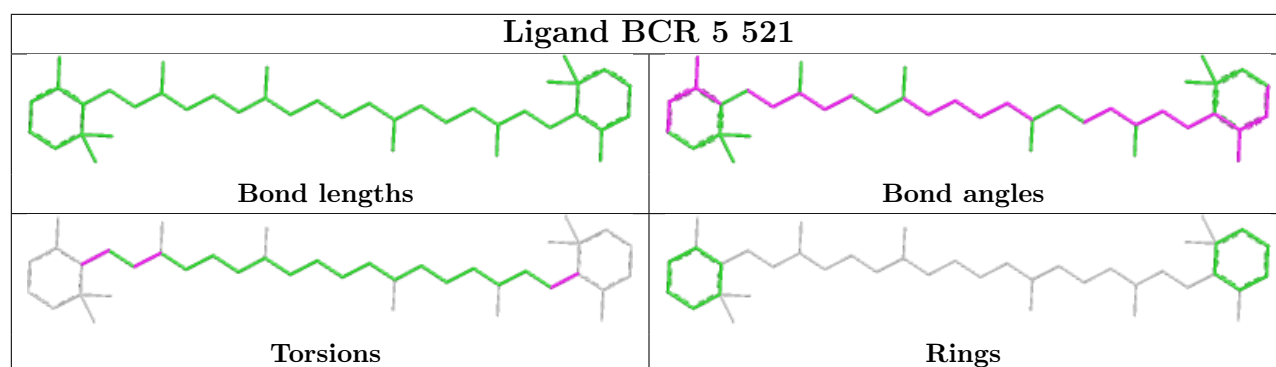


Ligand CLA g 508

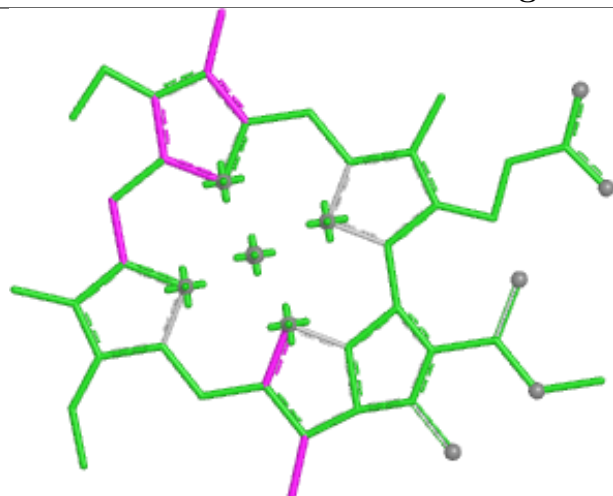




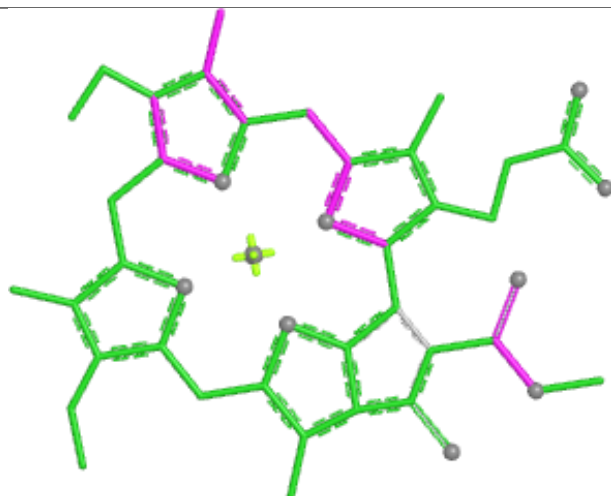




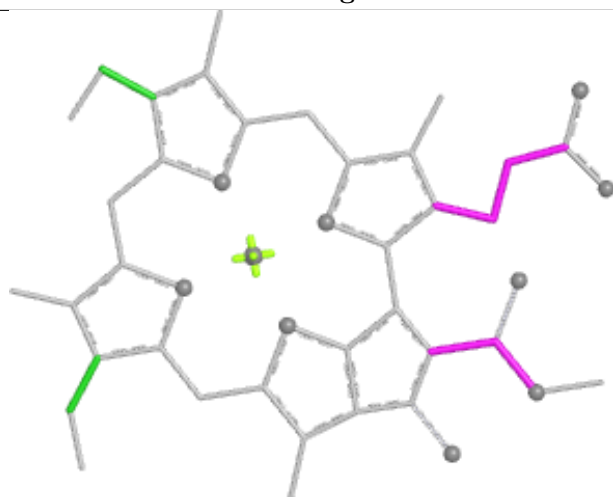
Ligand CLA e 506



Bond lengths



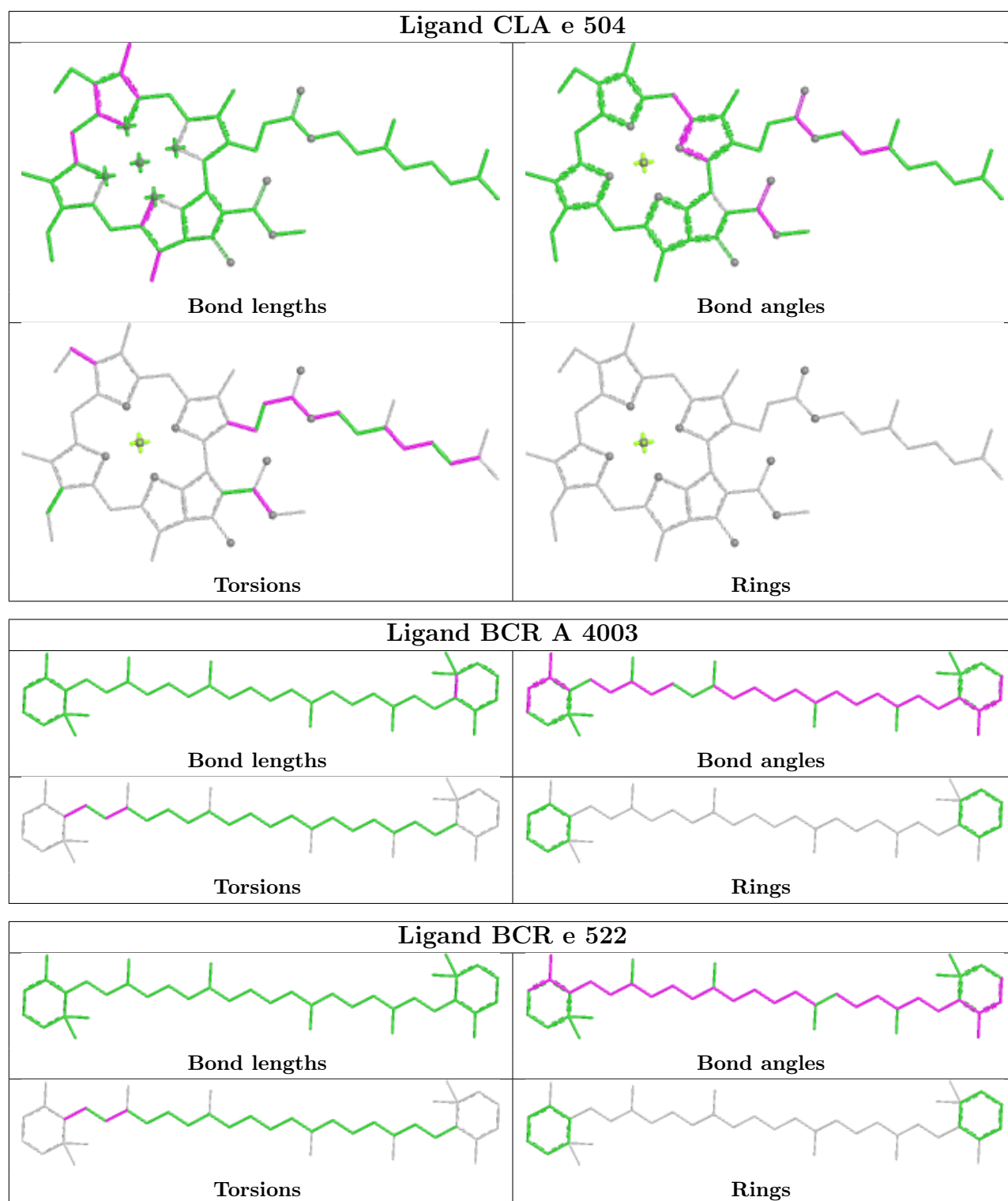
Bond angles



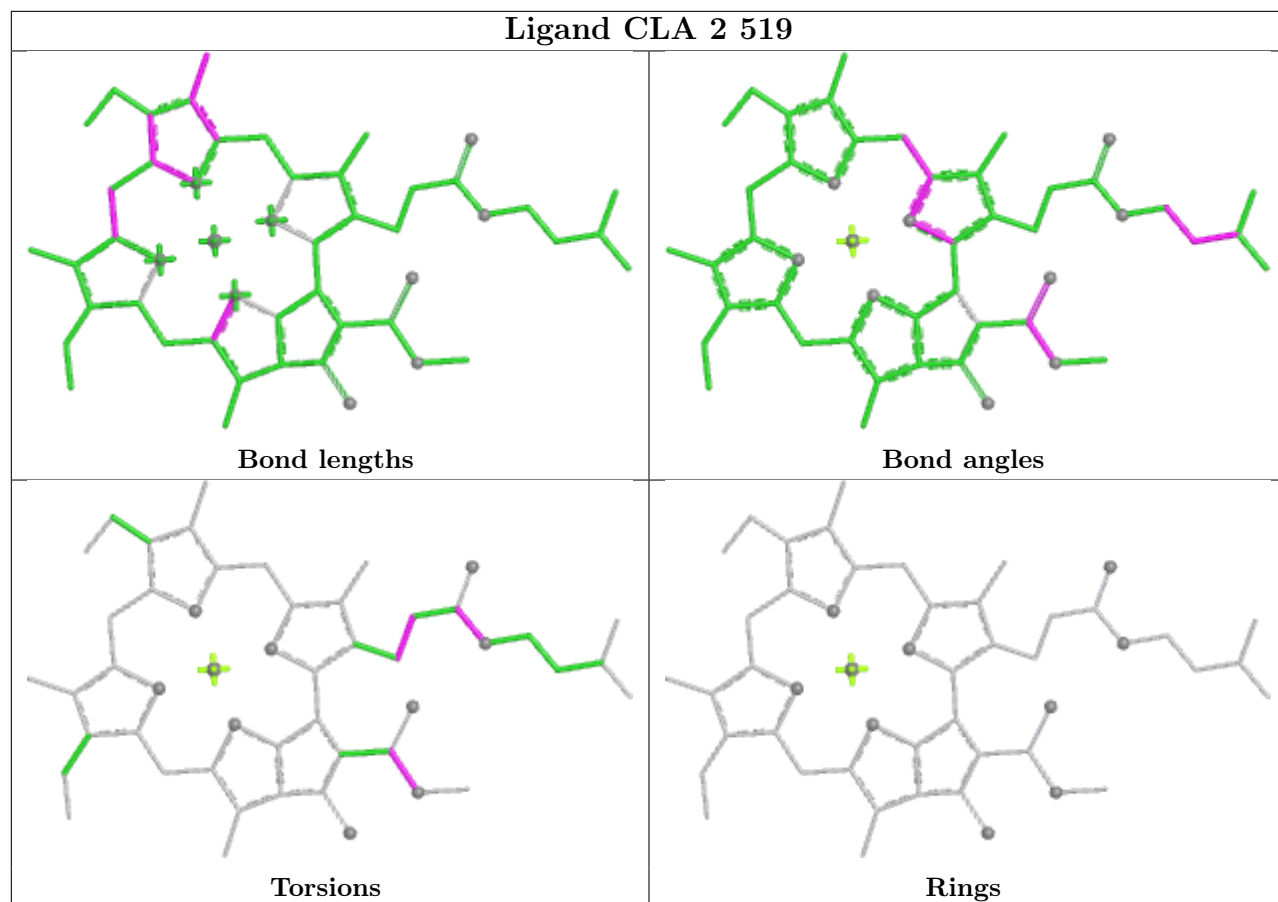
Torsions



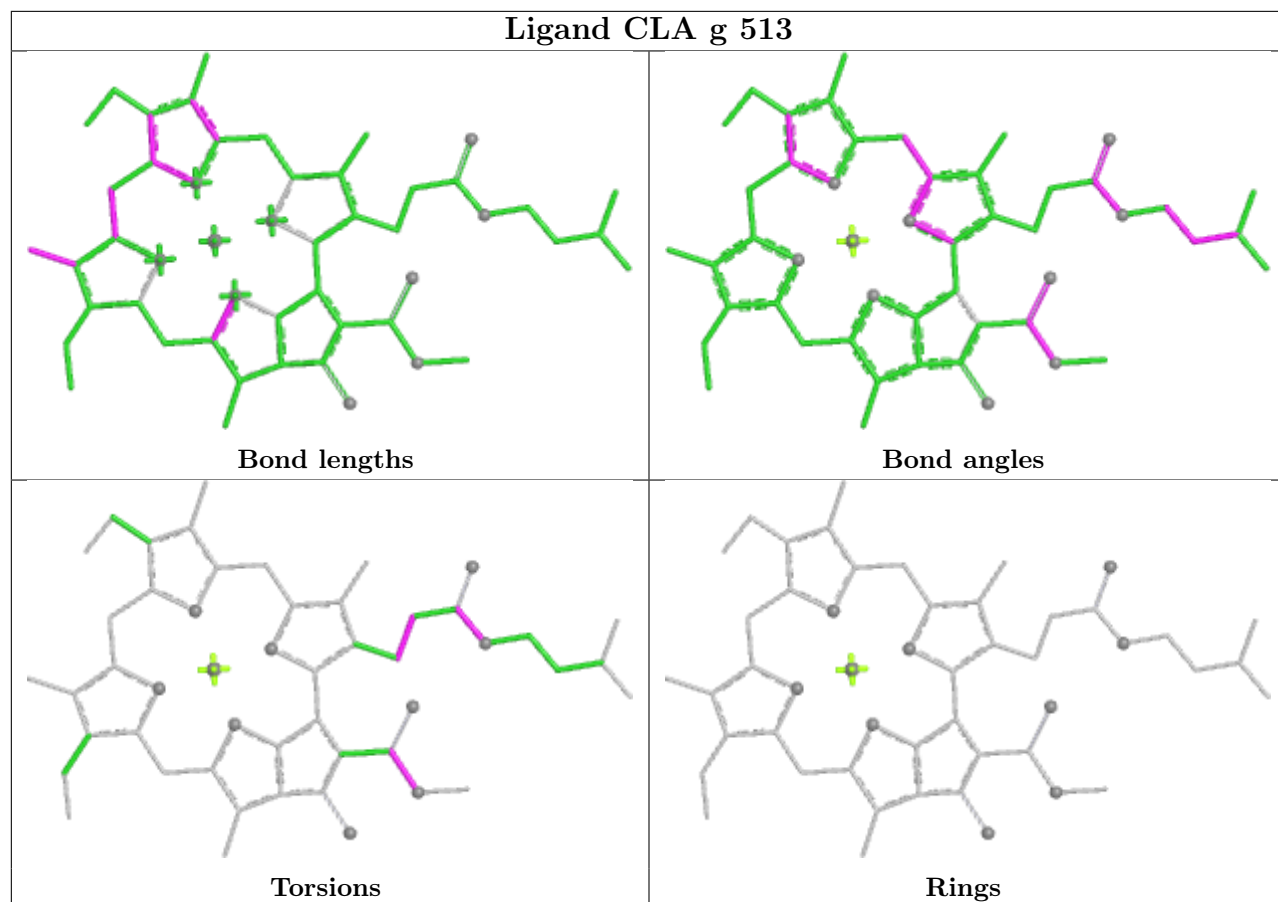
Rings



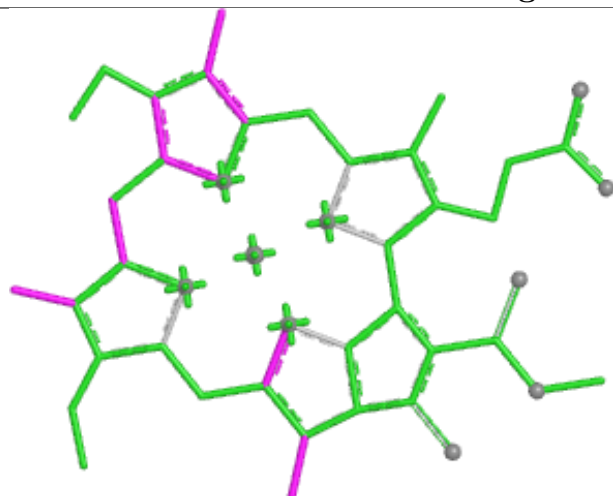
Ligand CLA 2 519



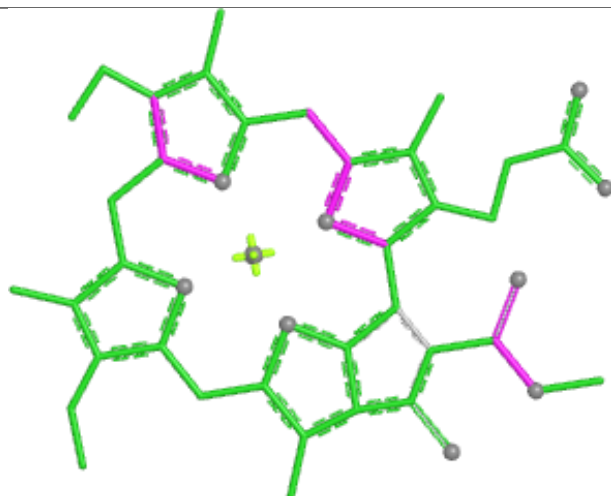
Ligand CLA g 513



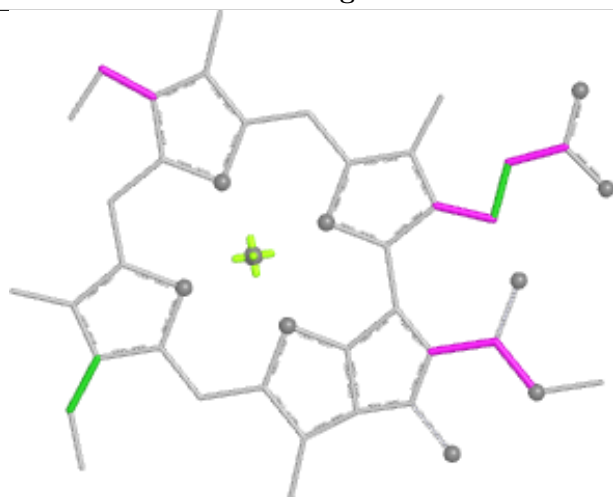
Ligand CLA 2 517



Bond lengths



Bond angles

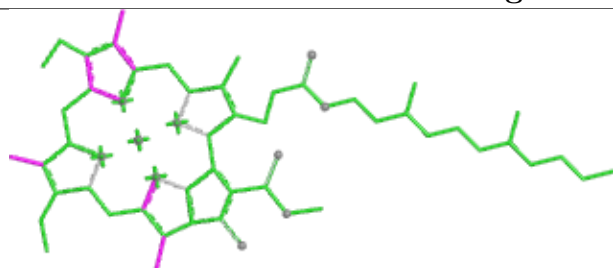


Torsions

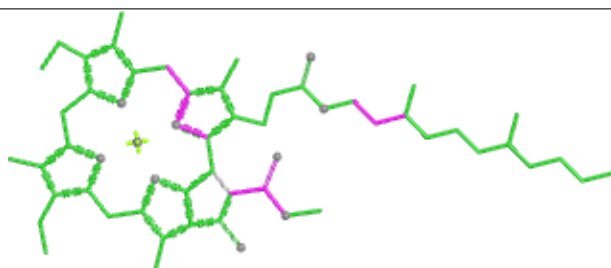


Rings

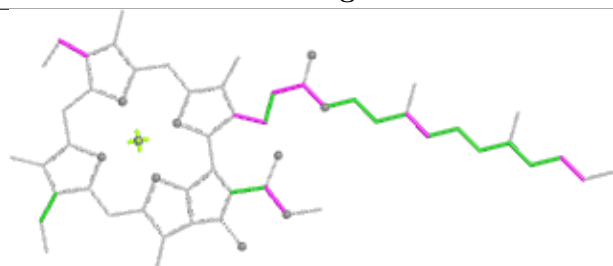
Ligand CLA B 1230



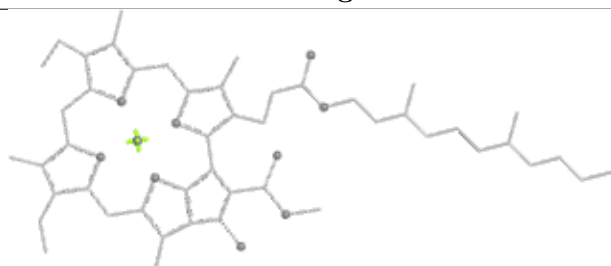
Bond lengths



Bond angles

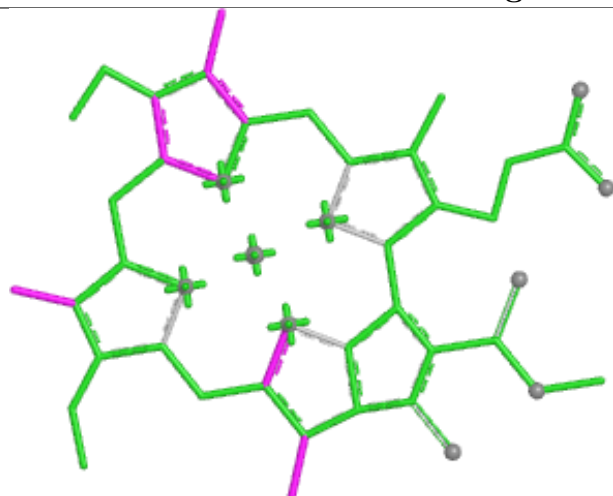


Torsions

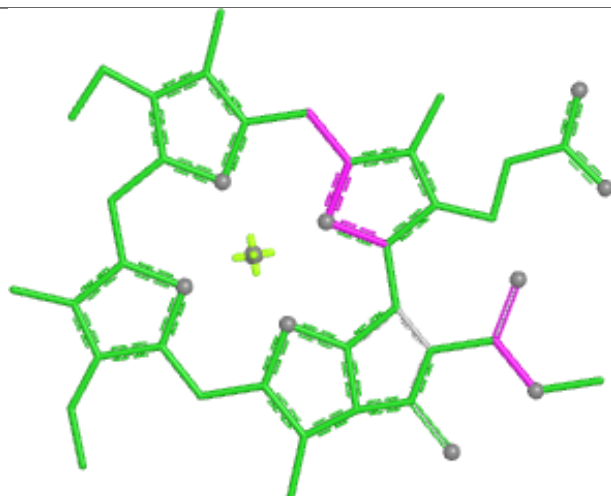


Rings

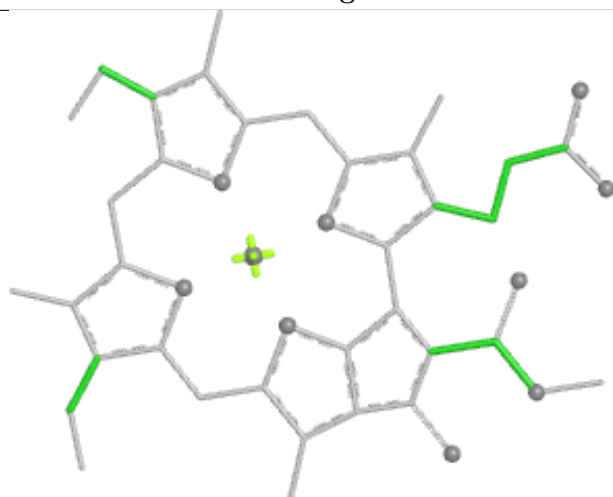
Ligand CLA B 1233



Bond lengths



Bond angles

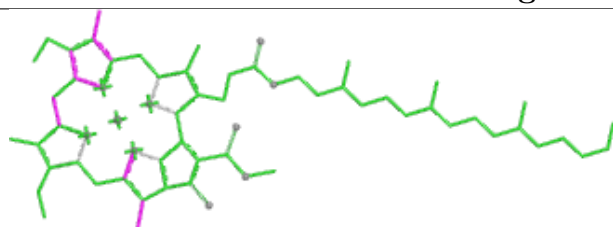


Torsions

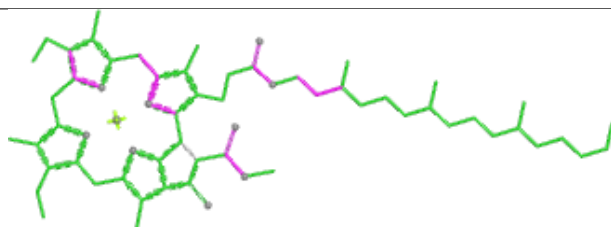


Rings

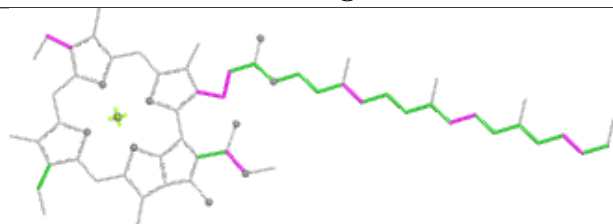
Ligand CLA 4 503



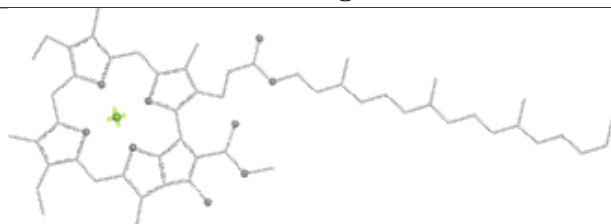
Bond lengths



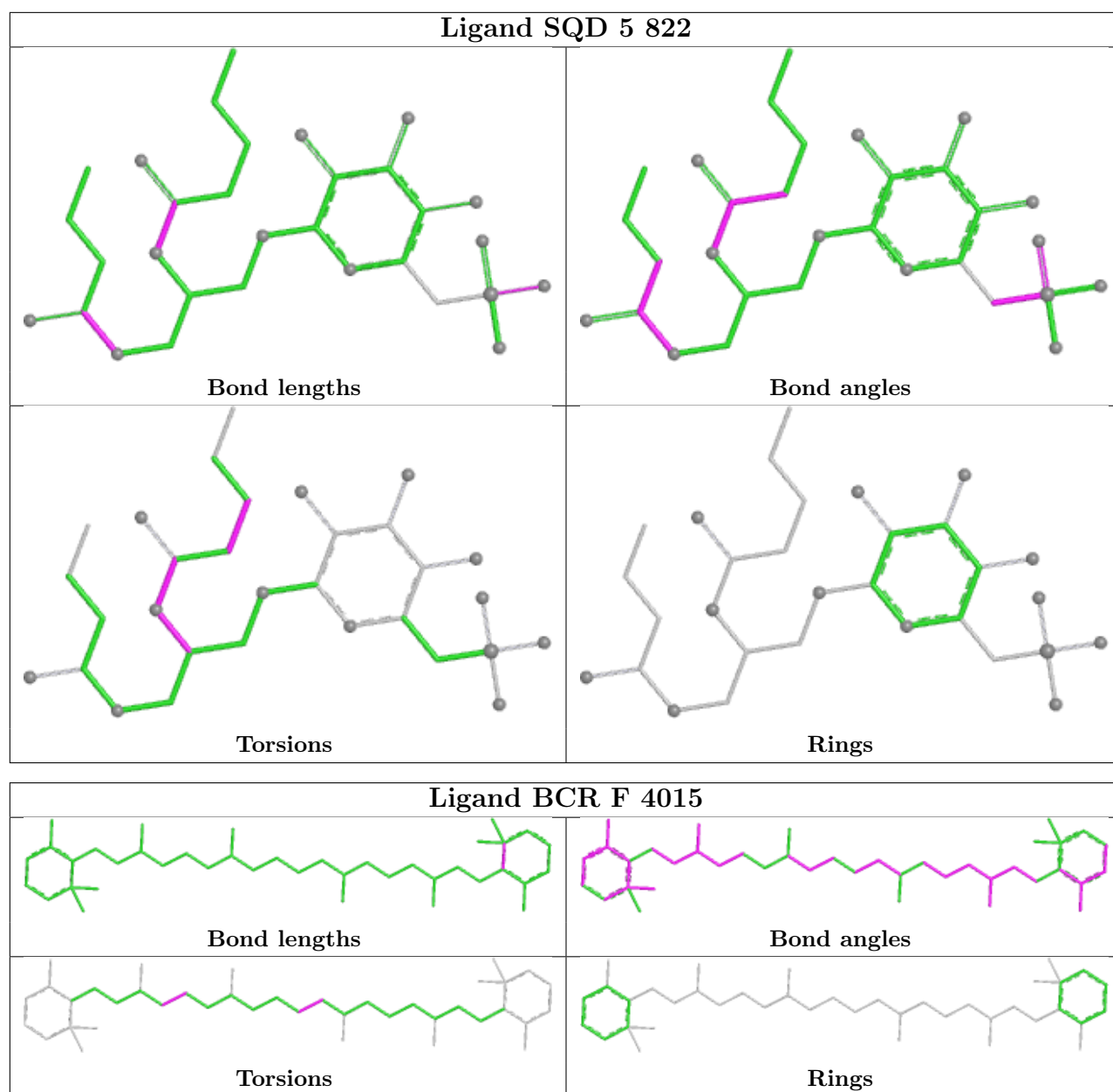
Bond angles



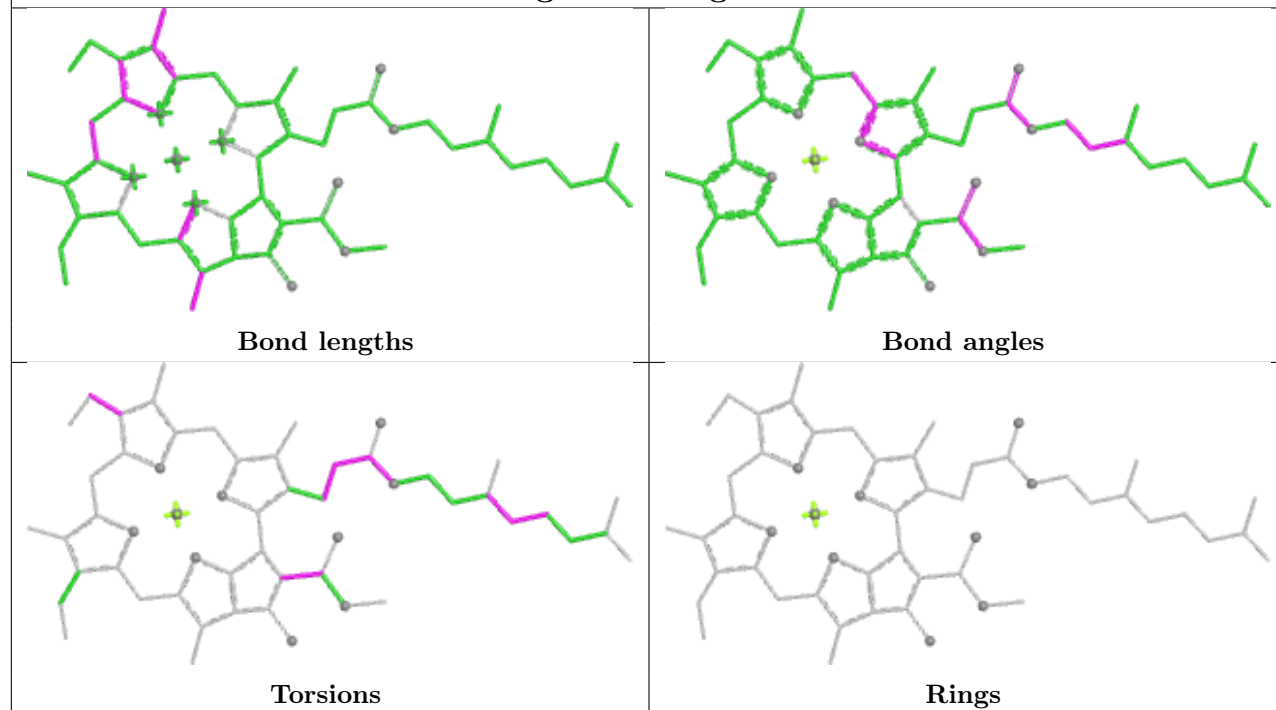
Torsions



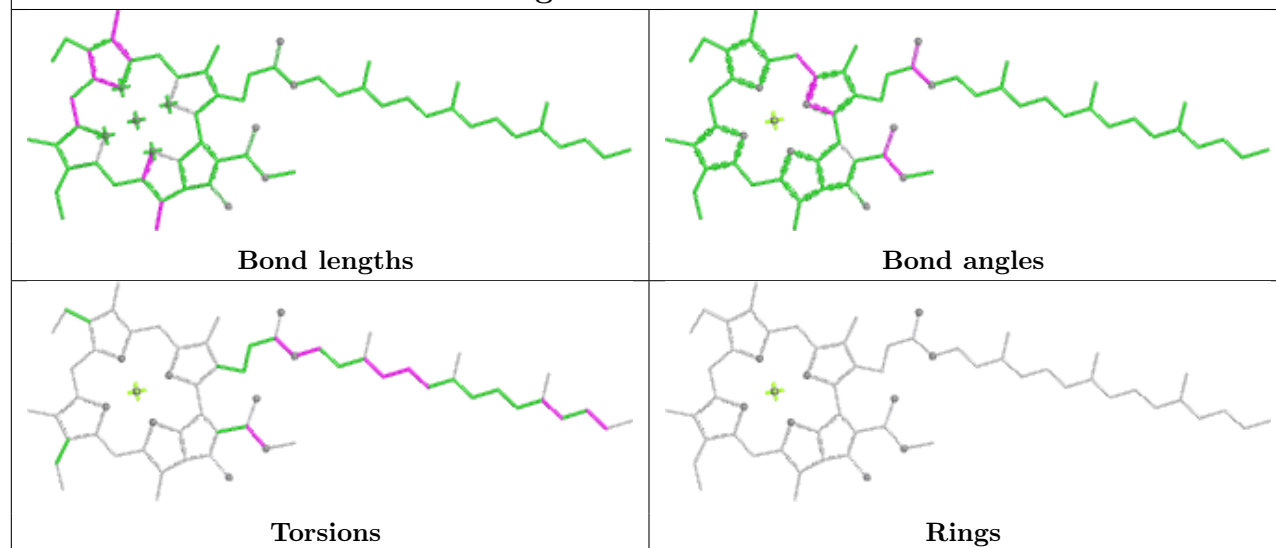
Rings

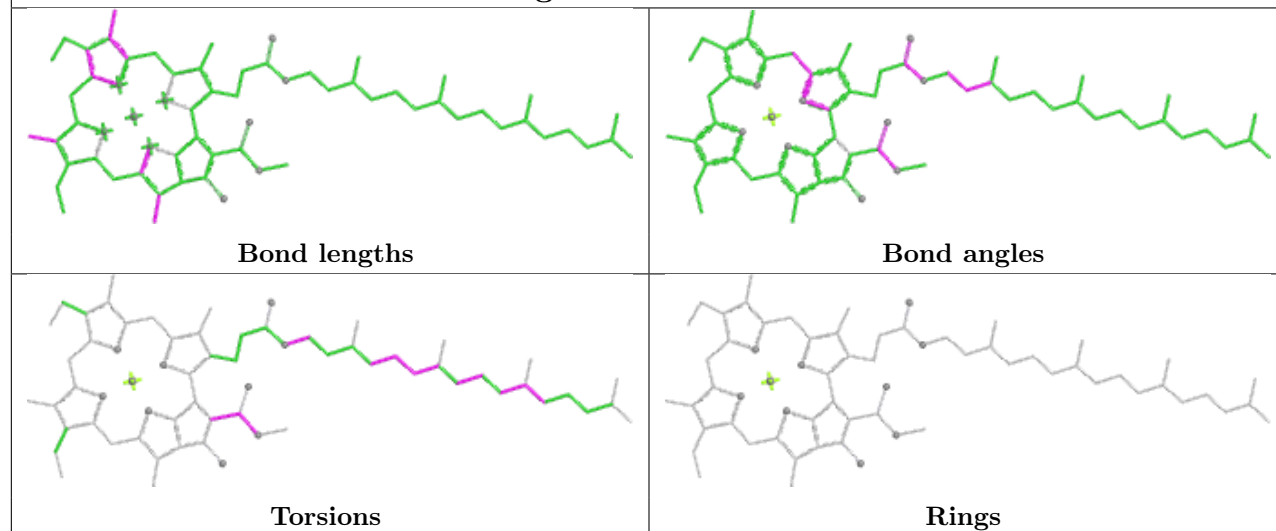
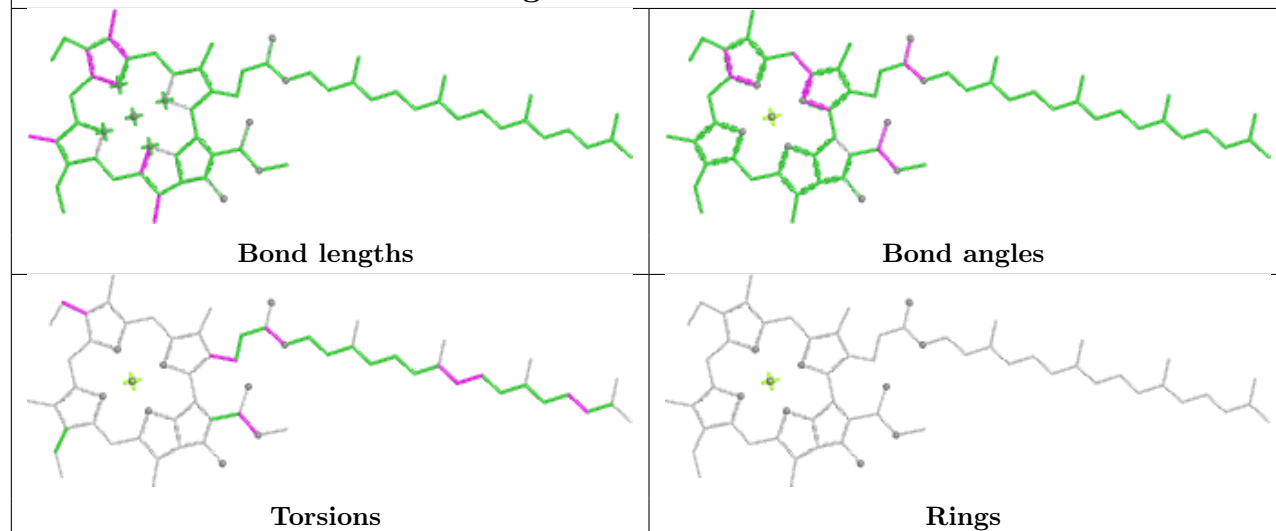


Ligand CLA g 518

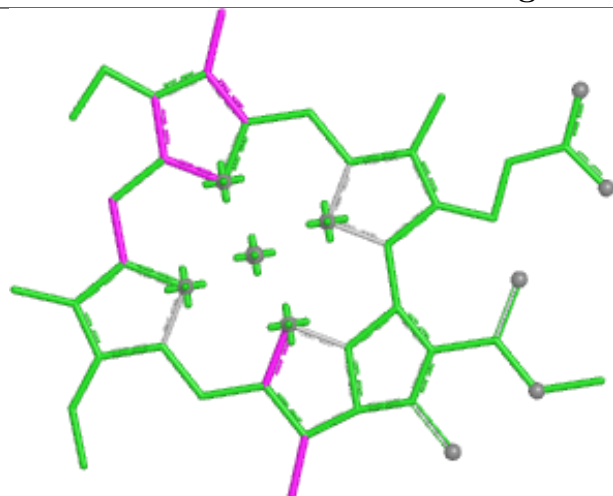


Ligand CLA b 503

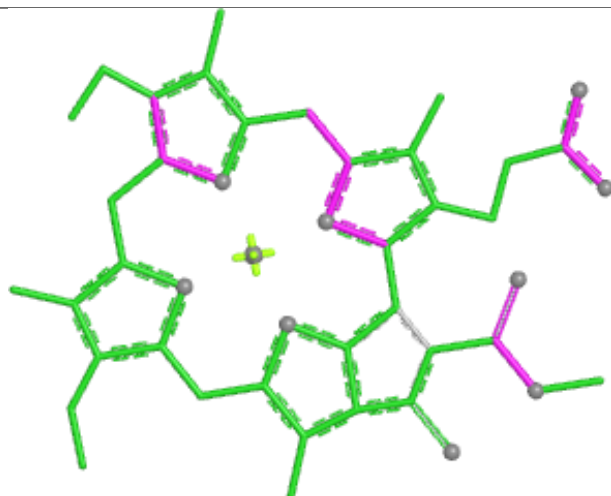


Ligand CLA b 509**Ligand CLA A 1109**

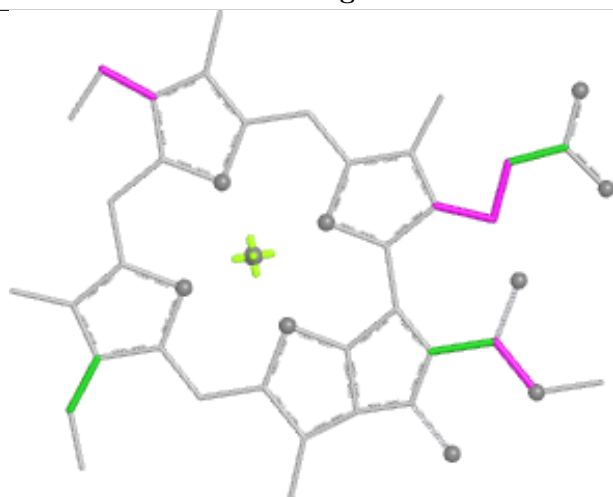
Ligand CLA 6 511



Bond lengths



Bond angles

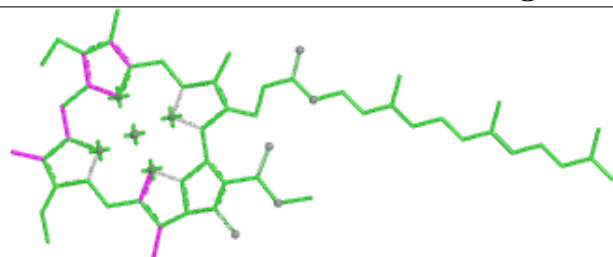


Torsions

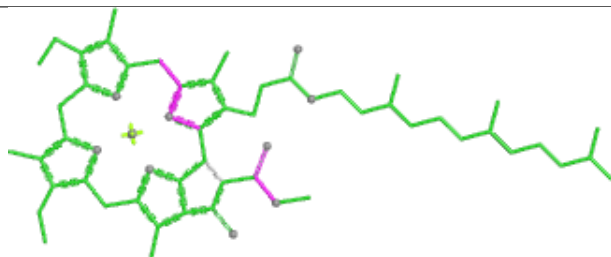


Rings

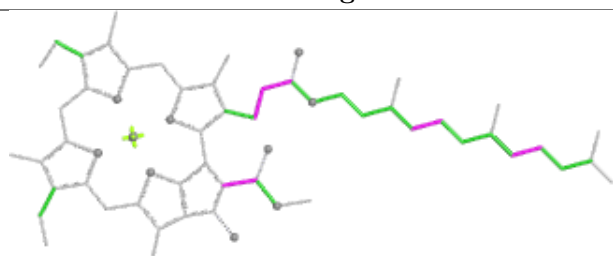
Ligand CLA e 507



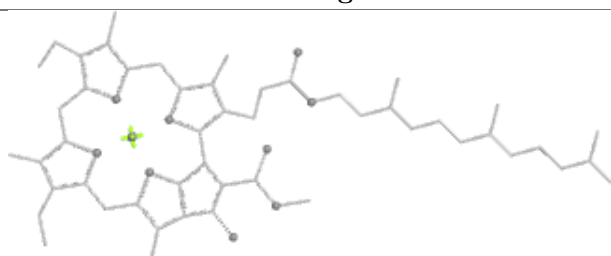
Bond lengths



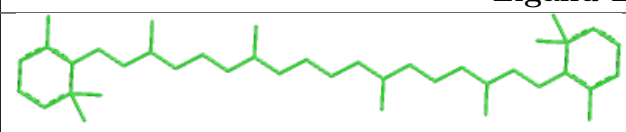
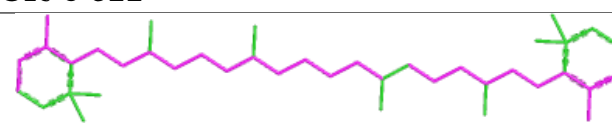
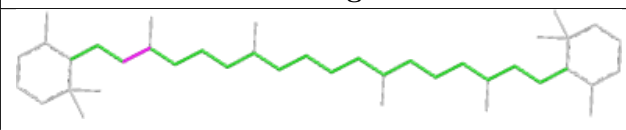
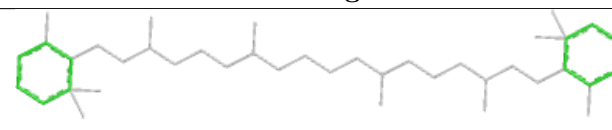
Bond angles

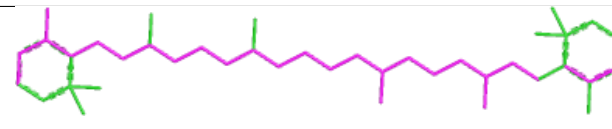
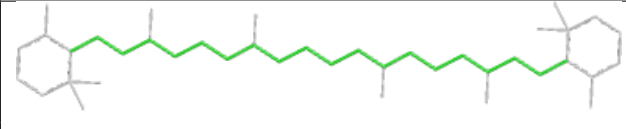
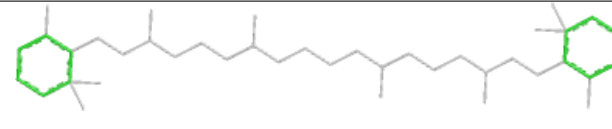


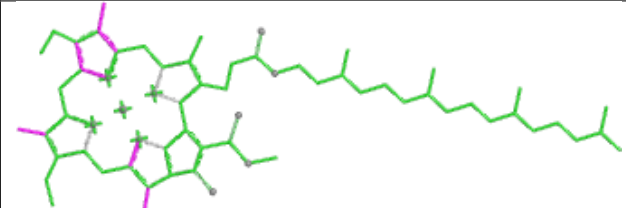
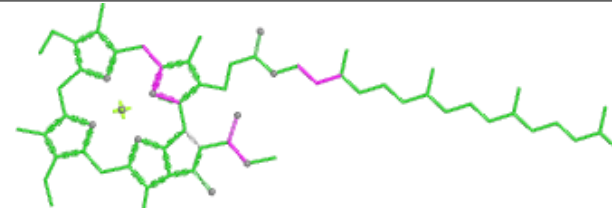
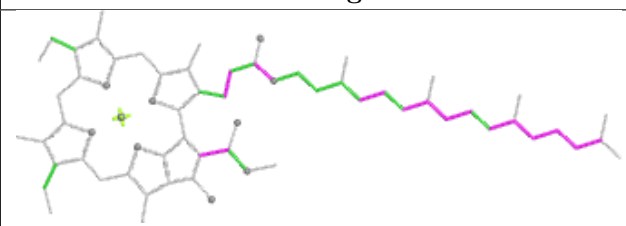
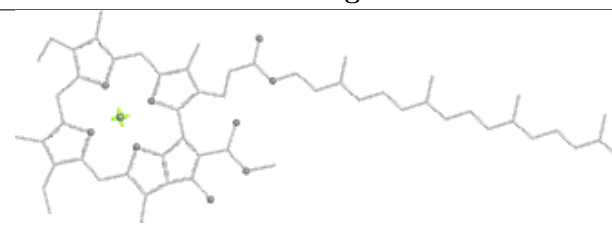
Torsions

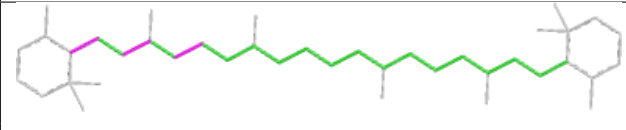
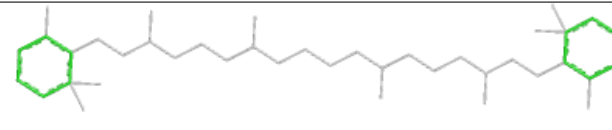


Rings

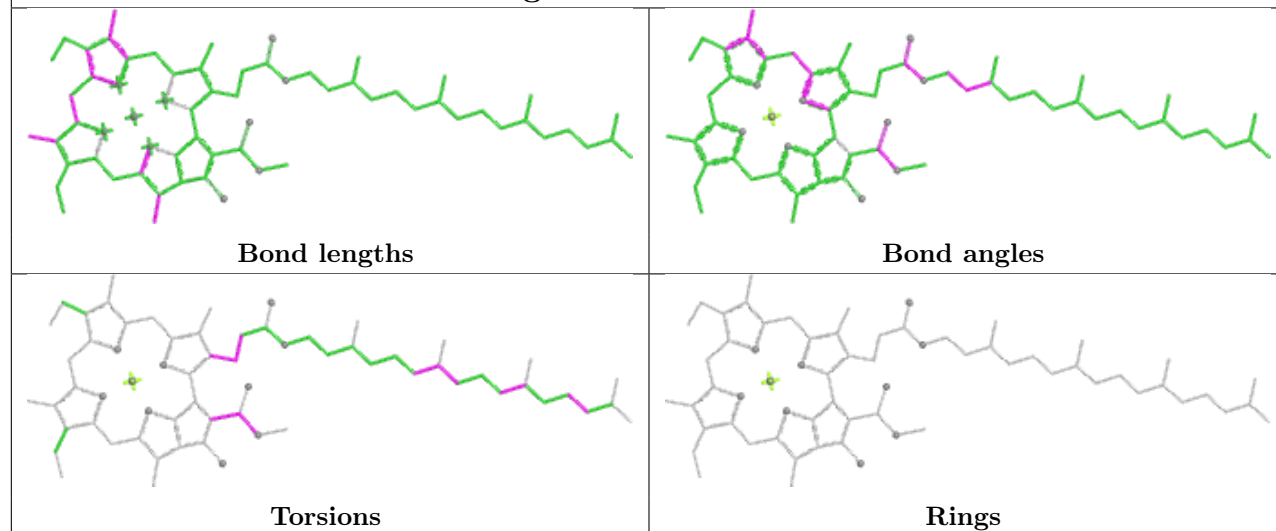
Ligand BCR c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR K 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

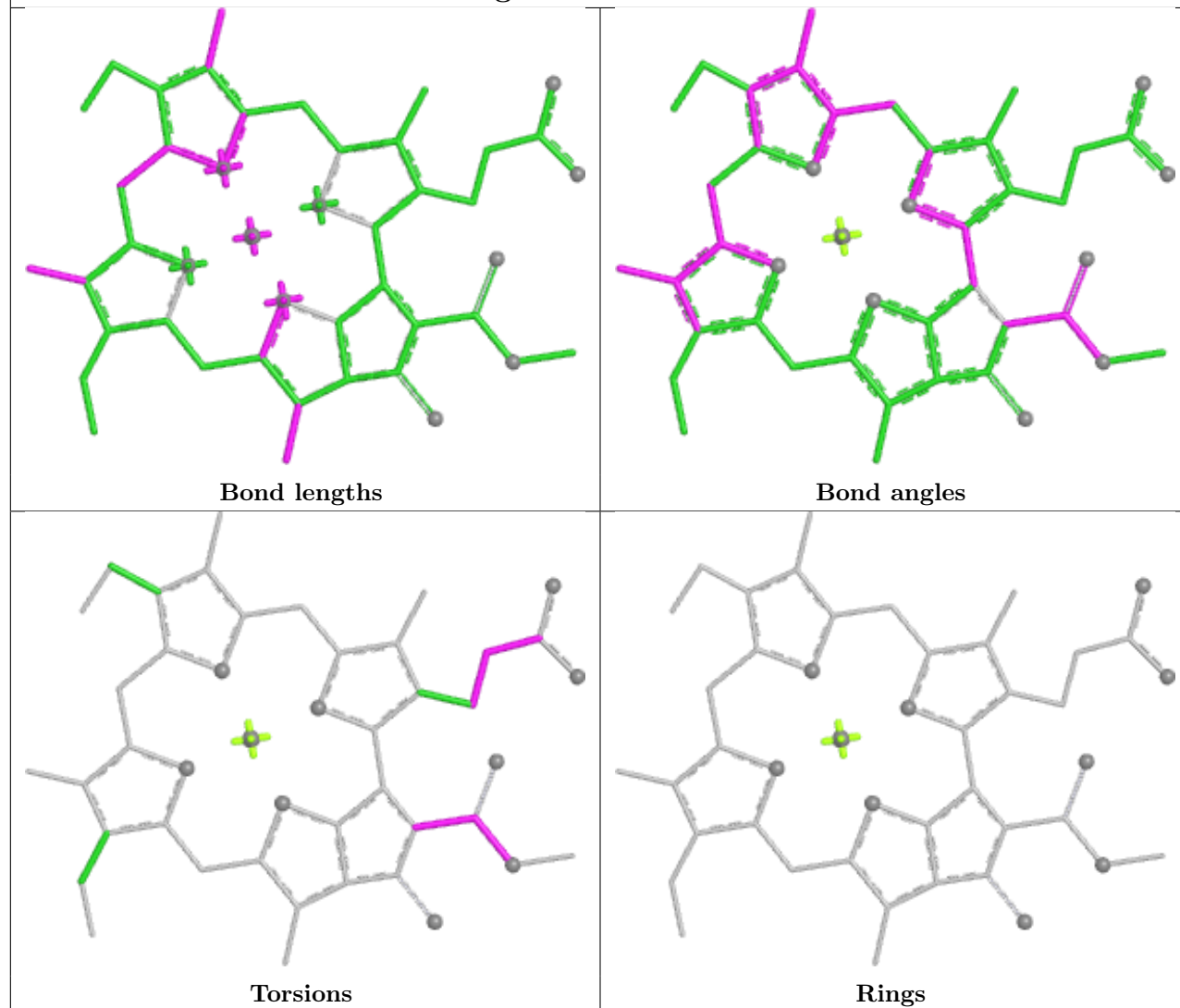
Ligand CLA A 1103	
	
Bond lengths	Bond angles
	
Torsions	Rings

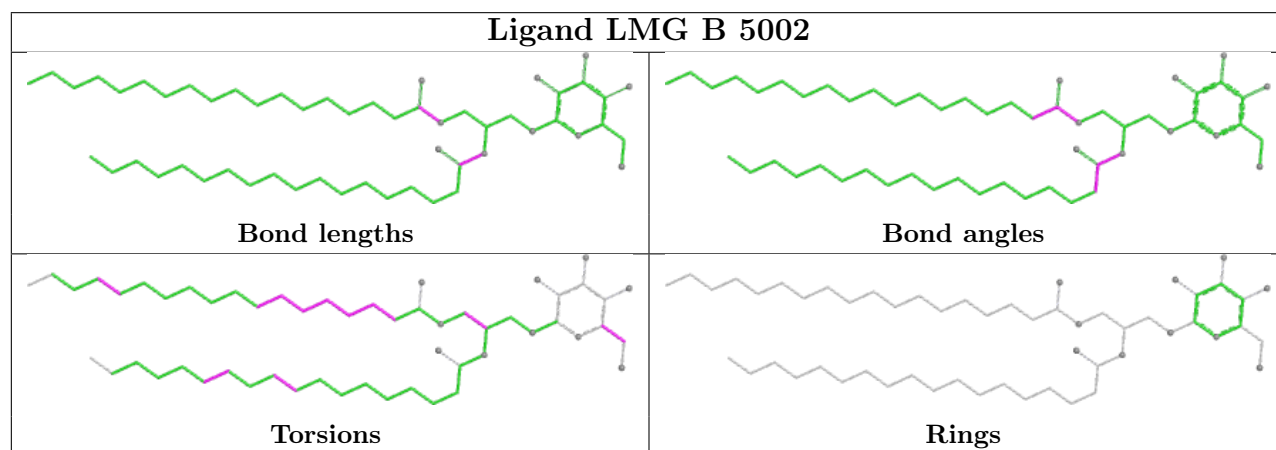
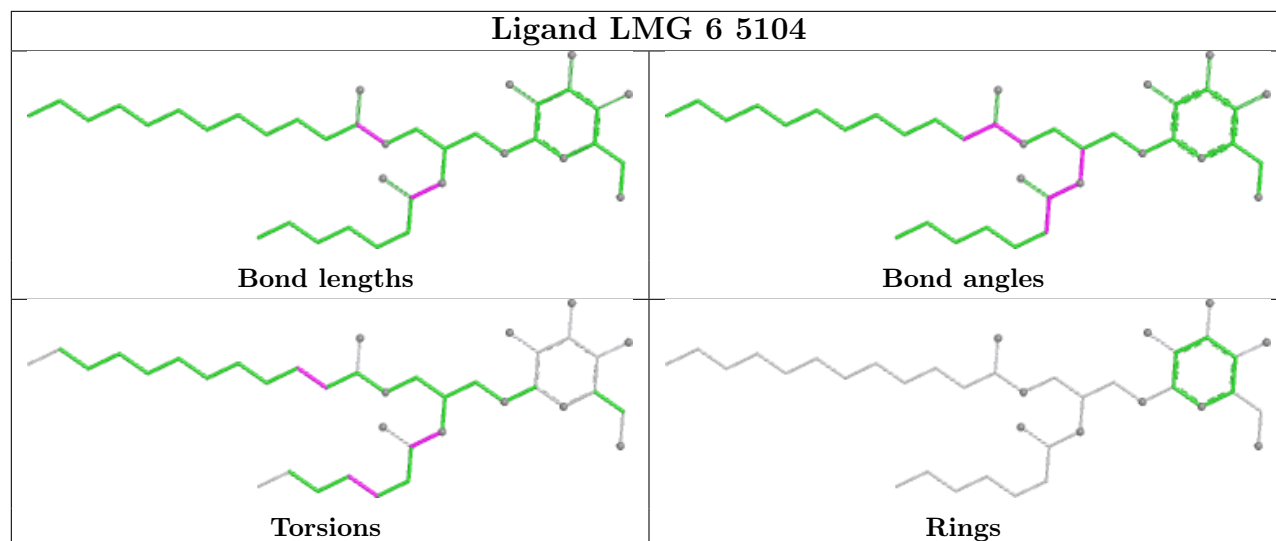
Ligand BCR 6 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

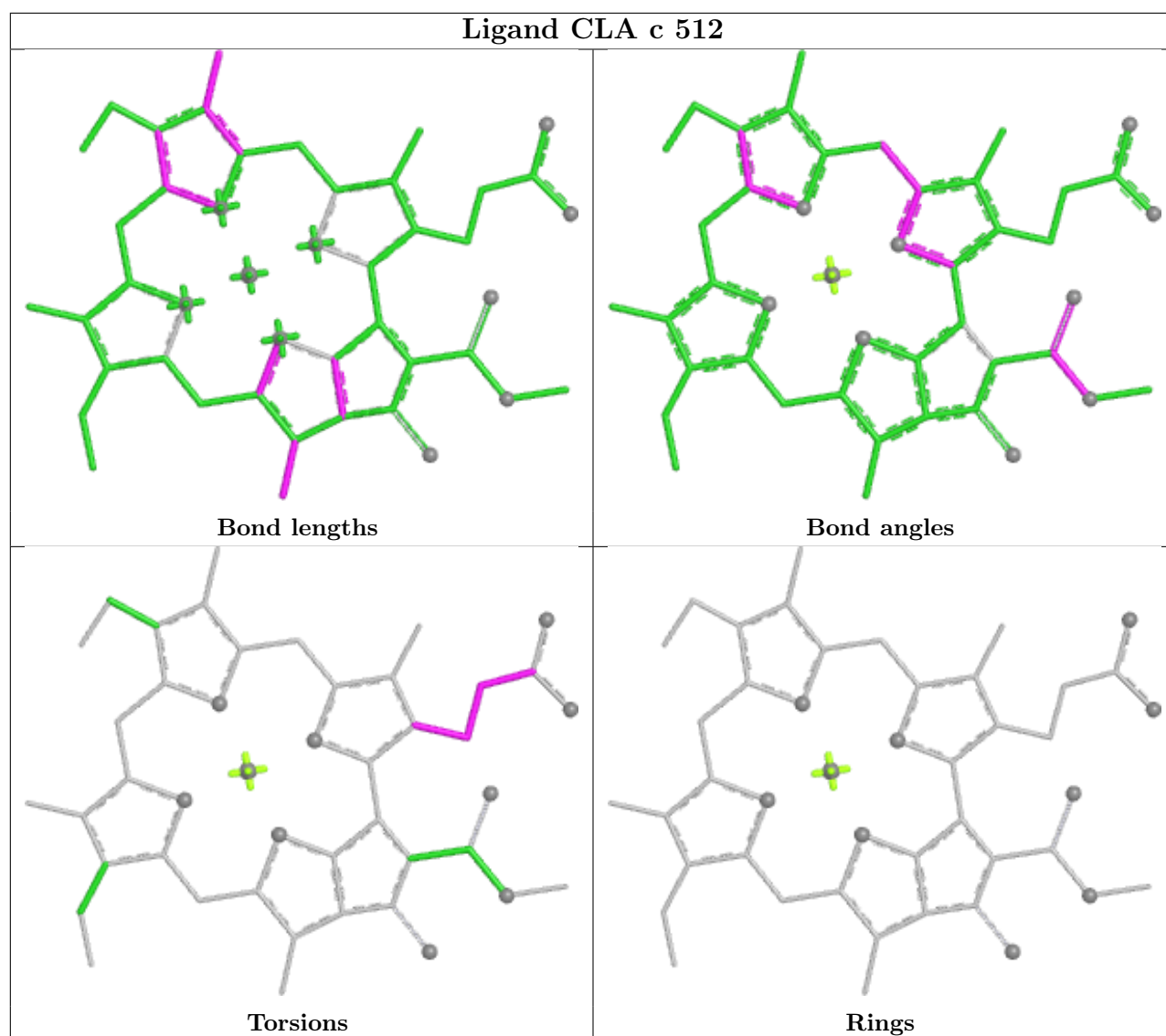
Ligand CLA B 1211



Ligand CLA b 506







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-63528. These allow visual inspection of the internal detail of the map and identification of artifacts.

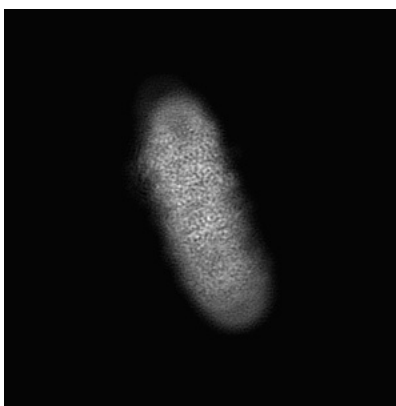
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

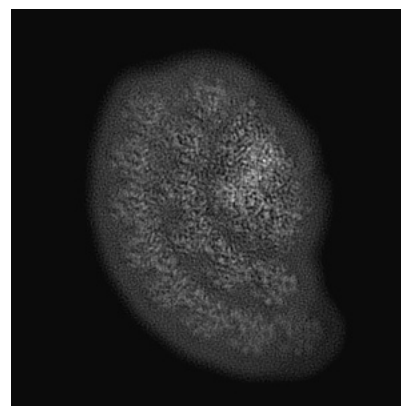
6.1.1 Primary map



X

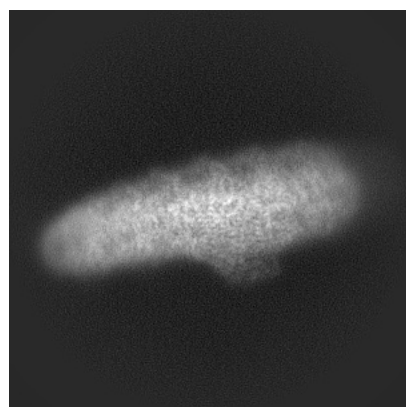


Y

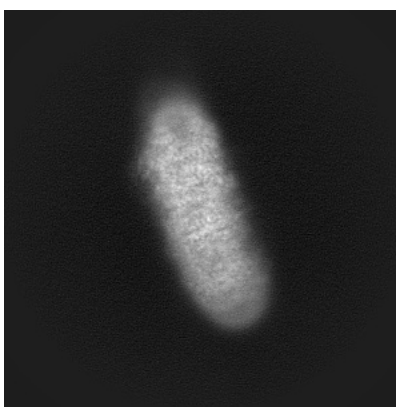


Z

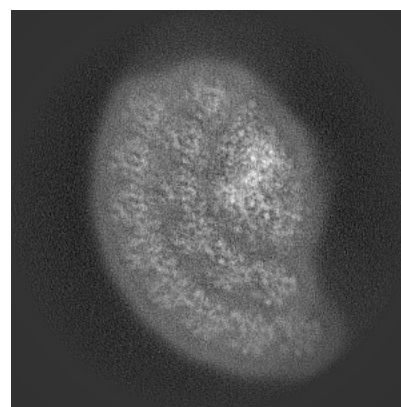
6.1.2 Raw map



X



Y

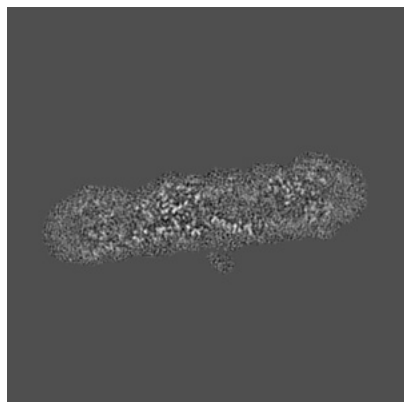


Z

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

6.2 Central slices [i](#)

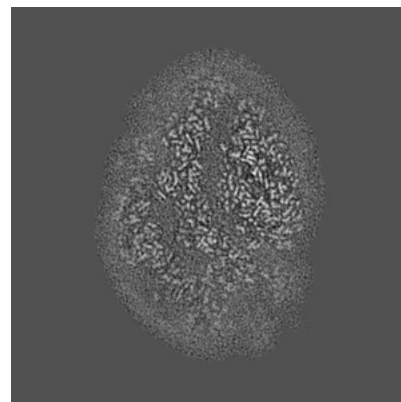
6.2.1 Primary map



X Index: 175

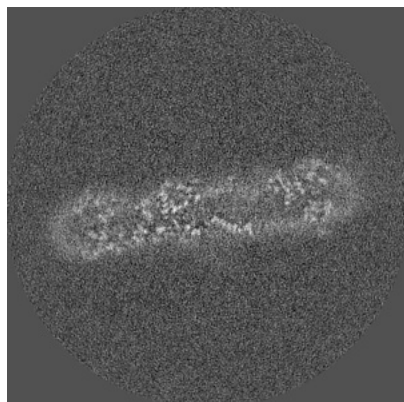


Y Index: 175

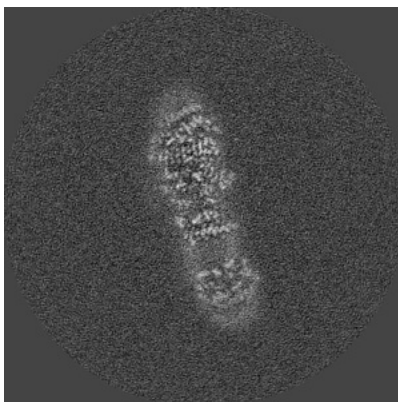


Z Index: 175

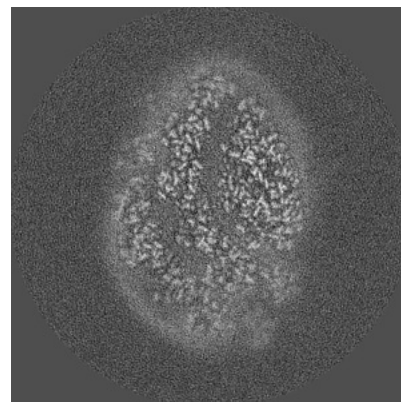
6.2.2 Raw map



X Index: 175



Y Index: 175

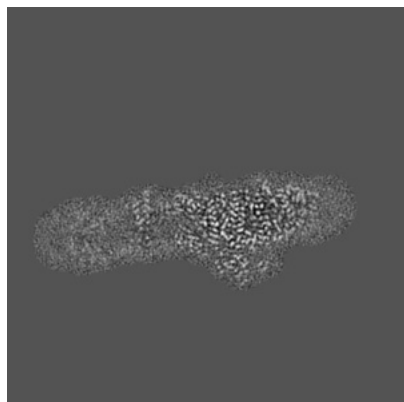


Z Index: 175

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

6.3 Largest variance slices [i](#)

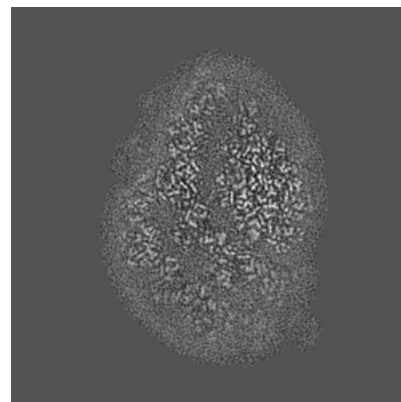
6.3.1 Primary map



X Index: 209

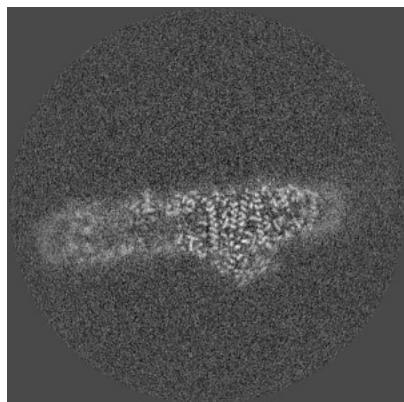


Y Index: 186

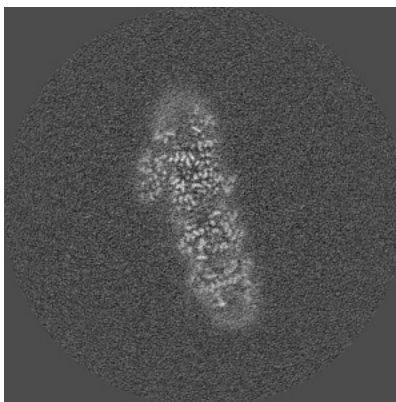


Z Index: 171

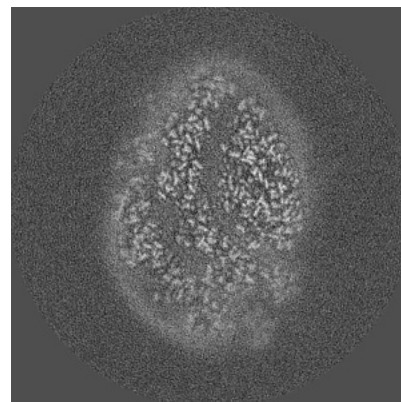
6.3.2 Raw map



X Index: 210



Y Index: 186

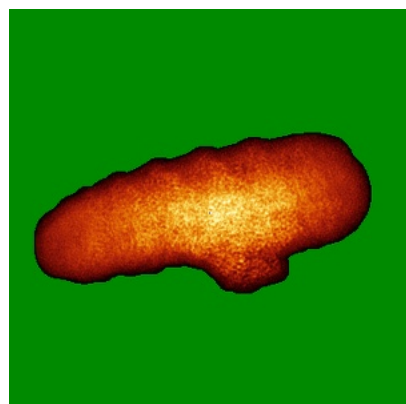


Z Index: 175

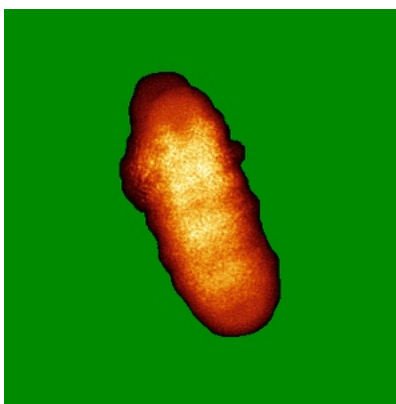
The images above show the largest variance slices of the map in three orthogonal directions.

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

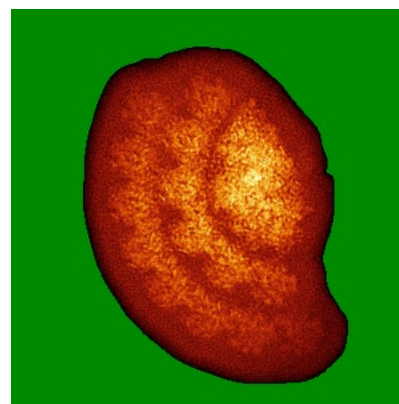
6.4.1 Primary map



X

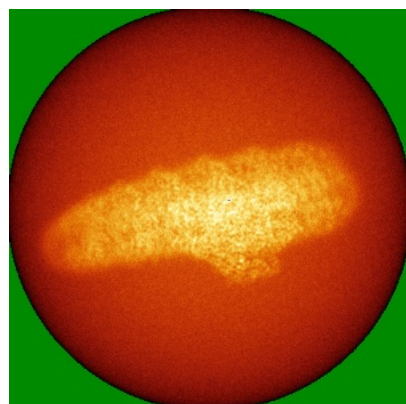


Y

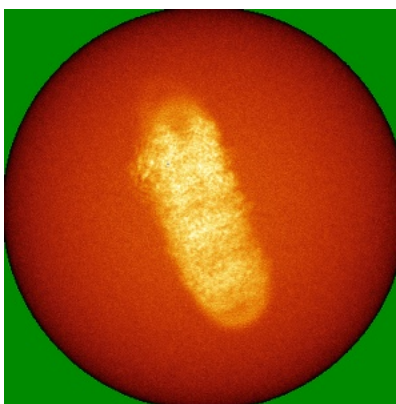


Z

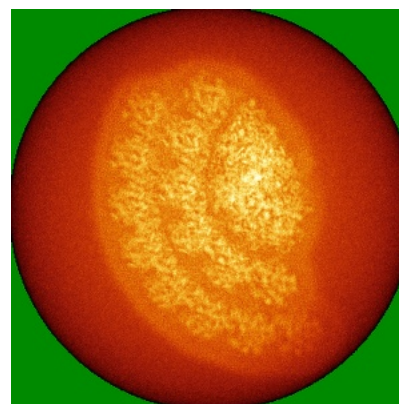
6.4.2 Raw map



X



Y

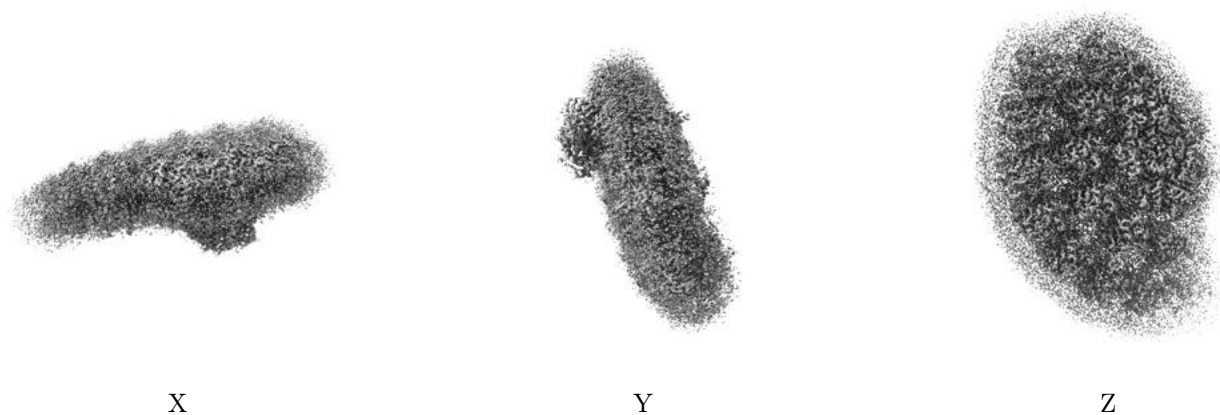


Z

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.

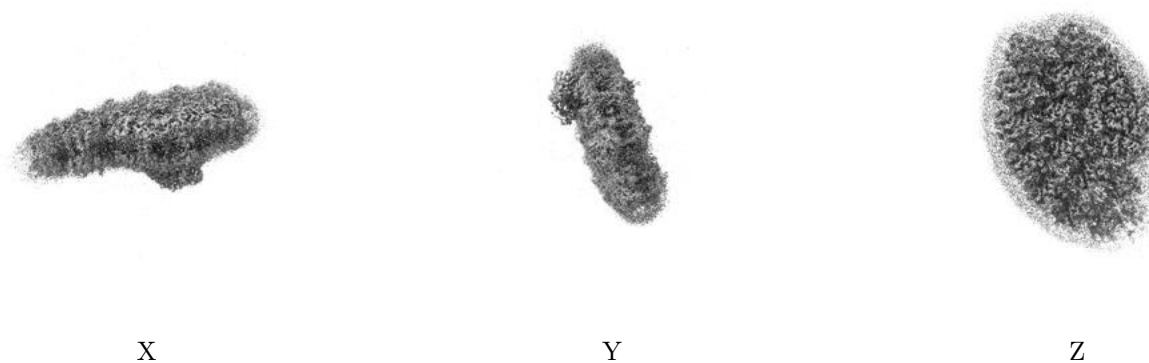
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.023. 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.

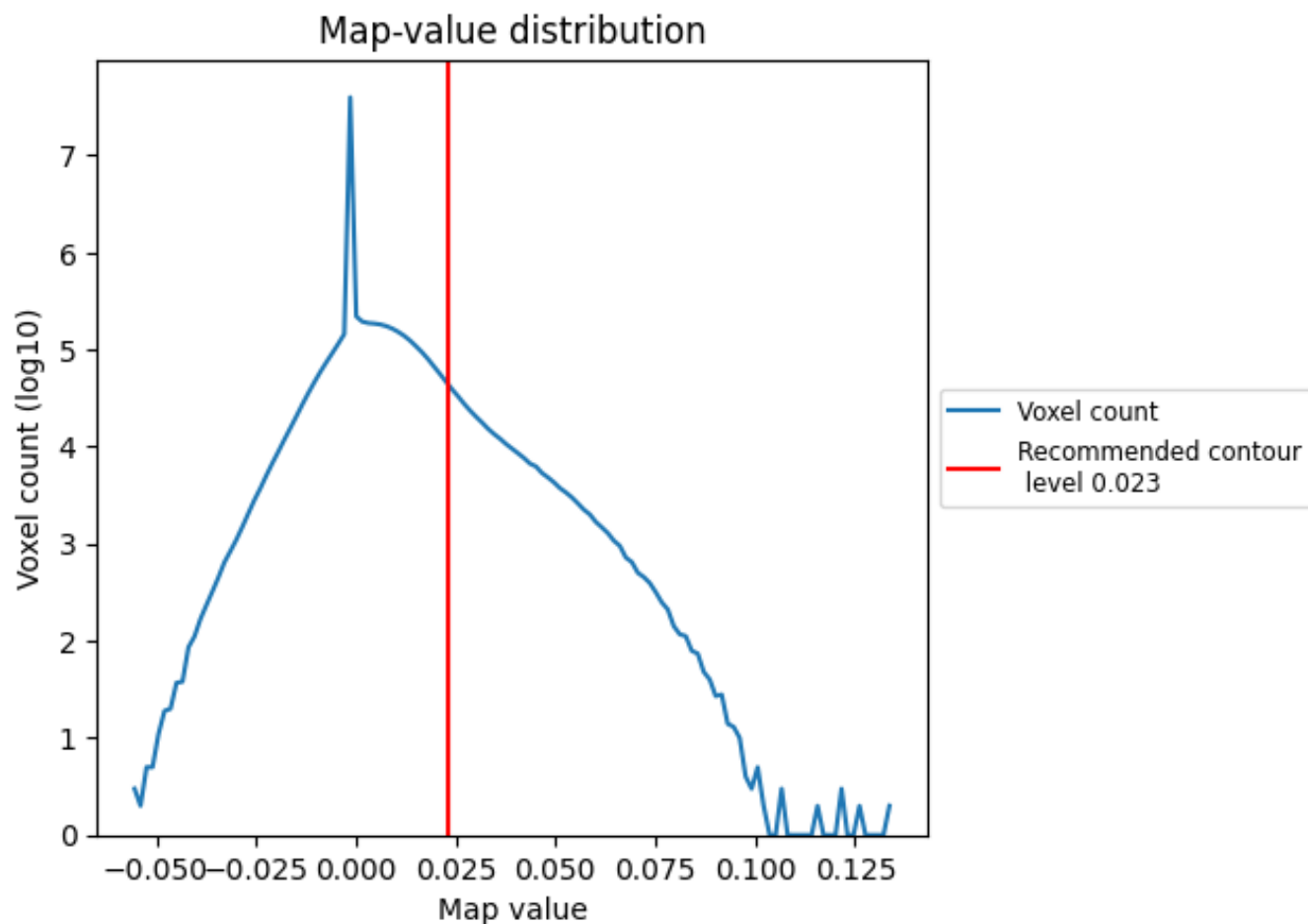
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

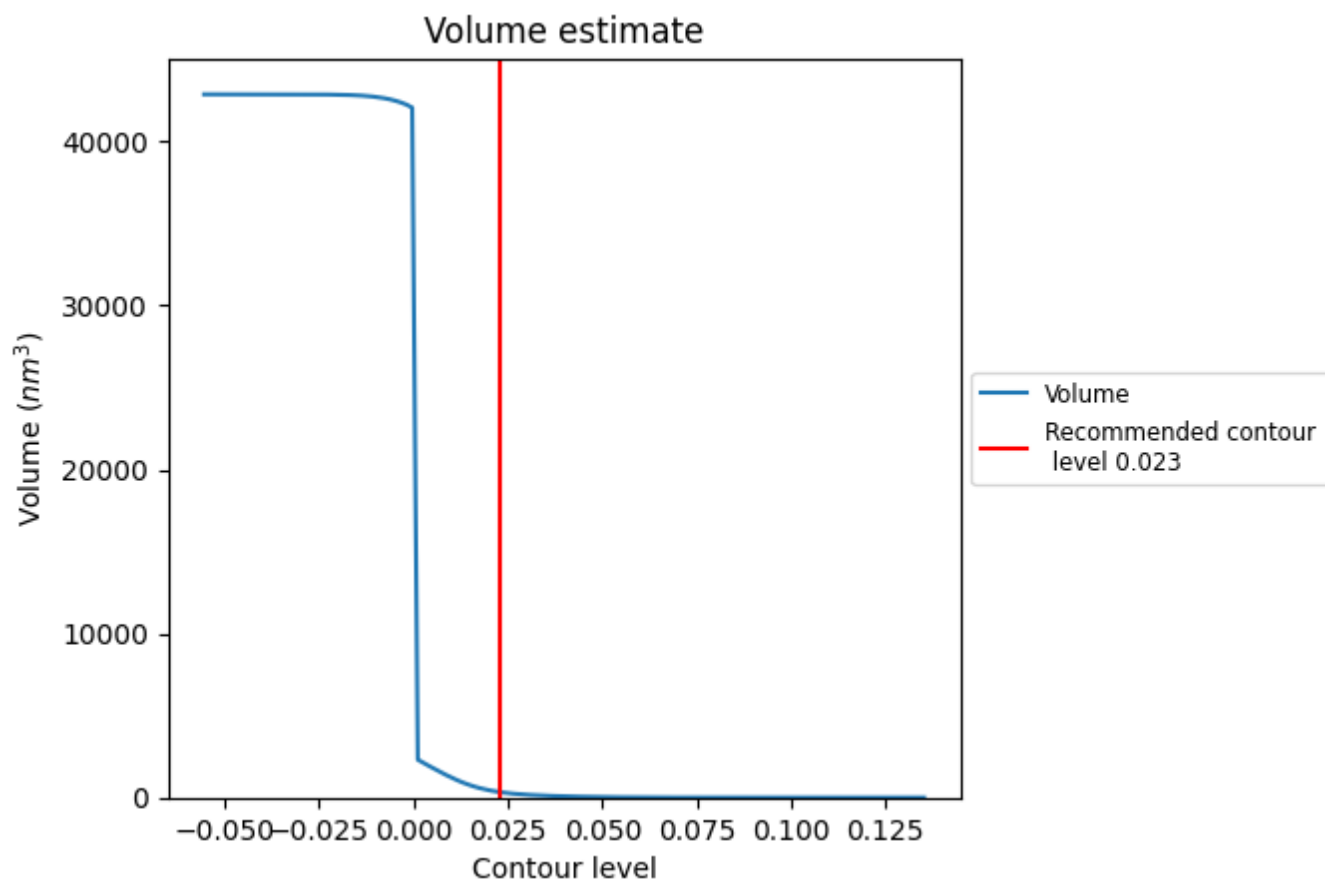
This section contains the results of statistical analysis of the map.

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.

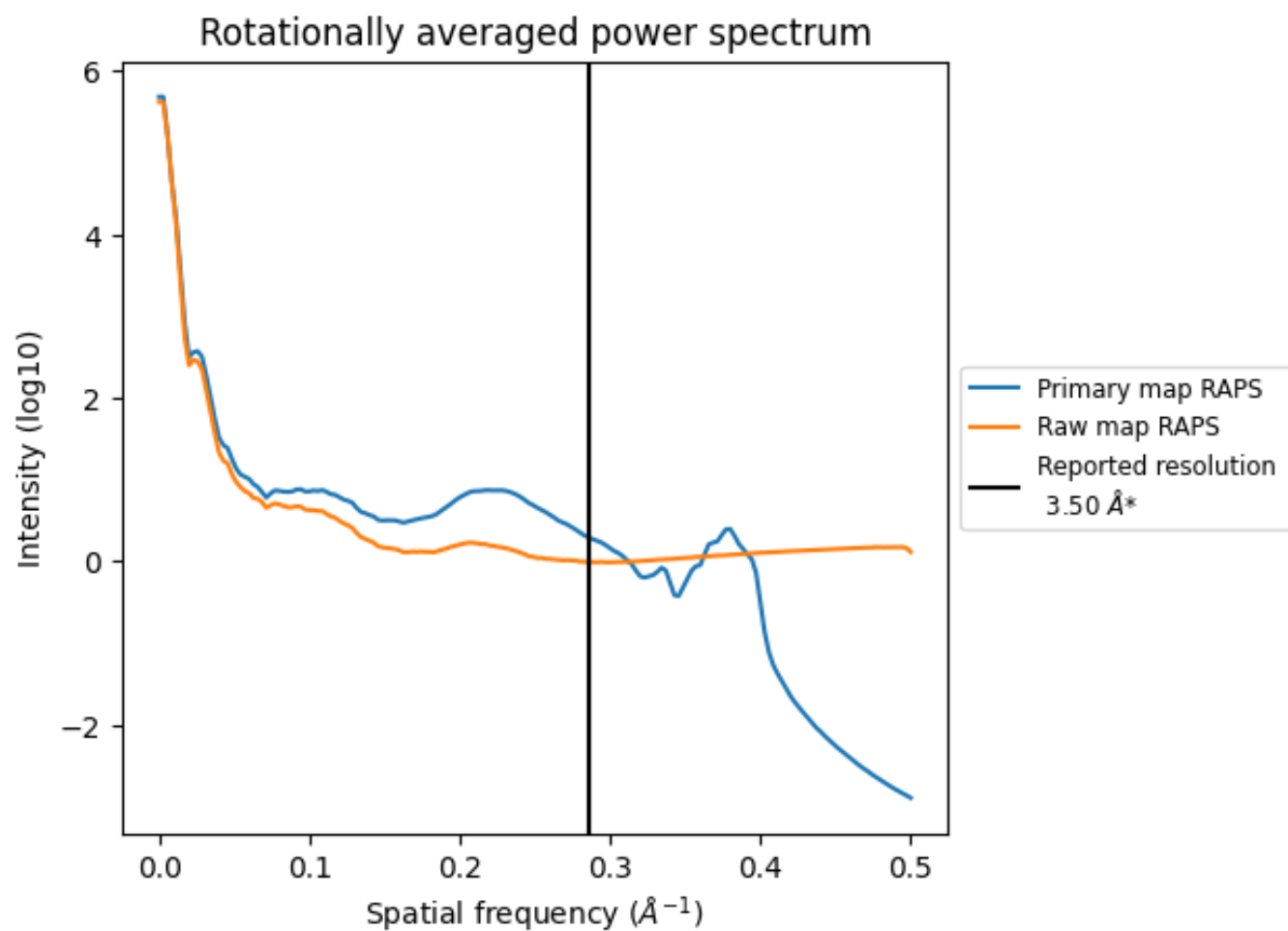
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 329 nm^3 ; this corresponds to an approximate mass of 297 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 ⓘ

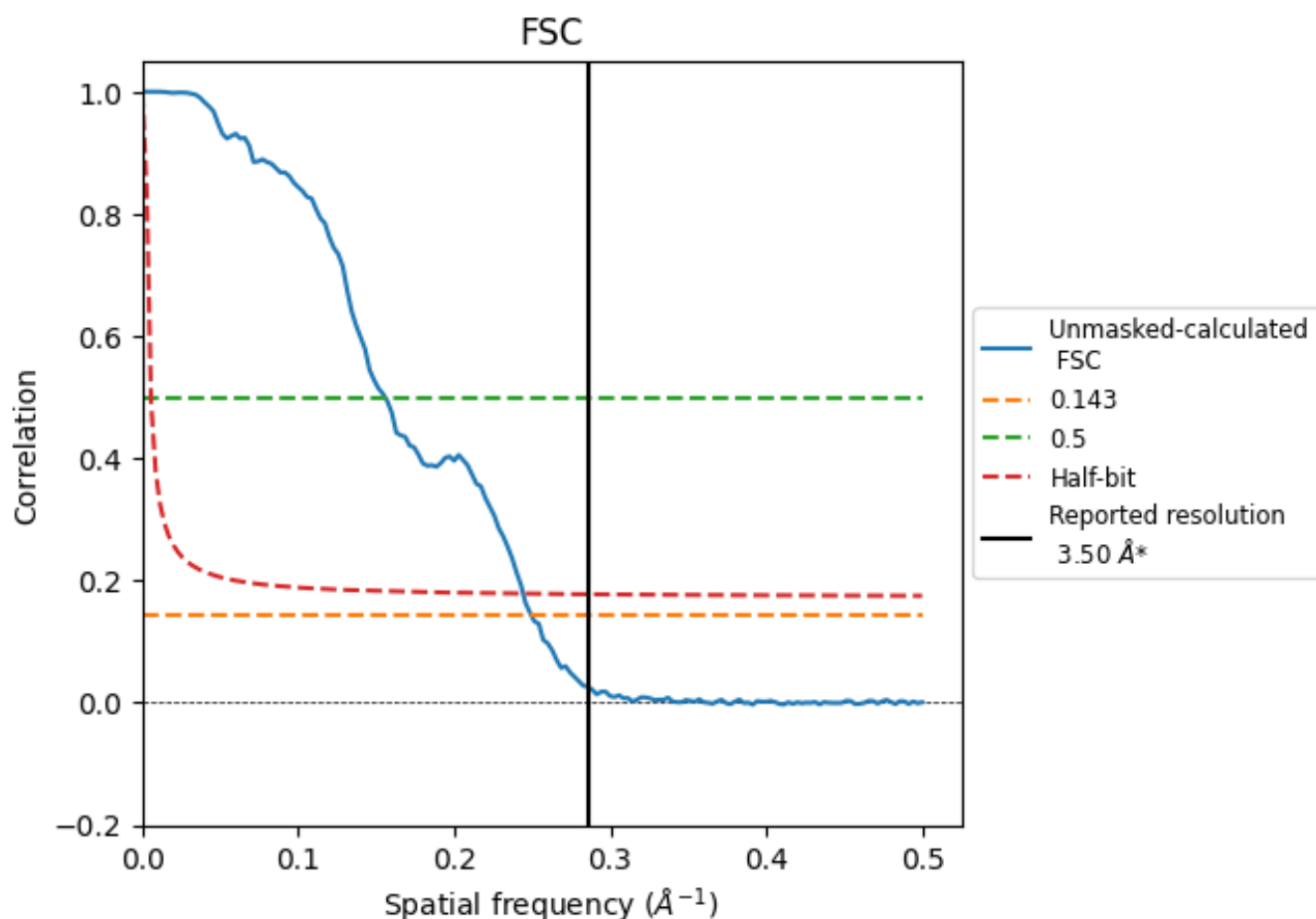


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	6.43	4.10

*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 4.01 differs from the reported value 3.5 by more than 10 %

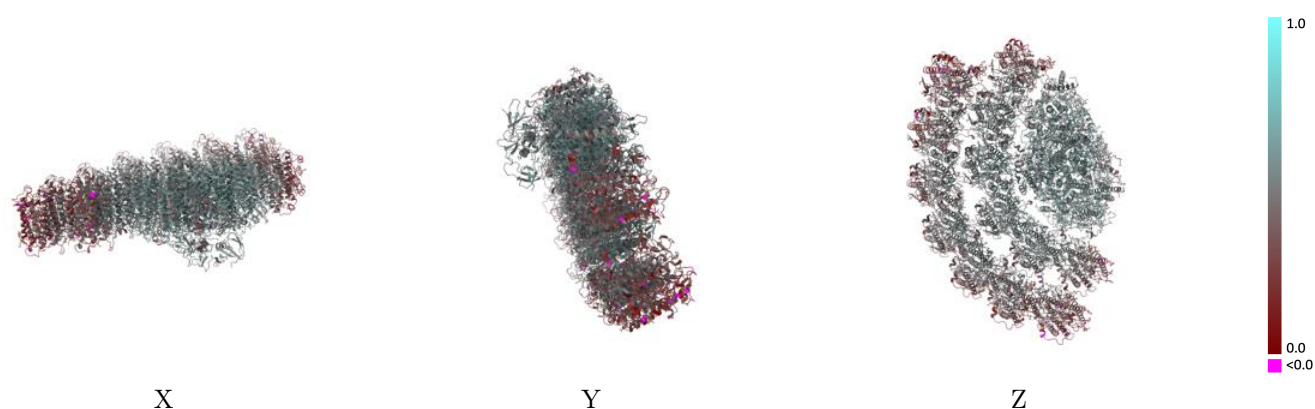
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63528 and PDB model 9LZK. Per-residue inclusion information can be found in section 3 on page 39.

9.1 Map-model overlay [i](#)

This section was not generated.

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

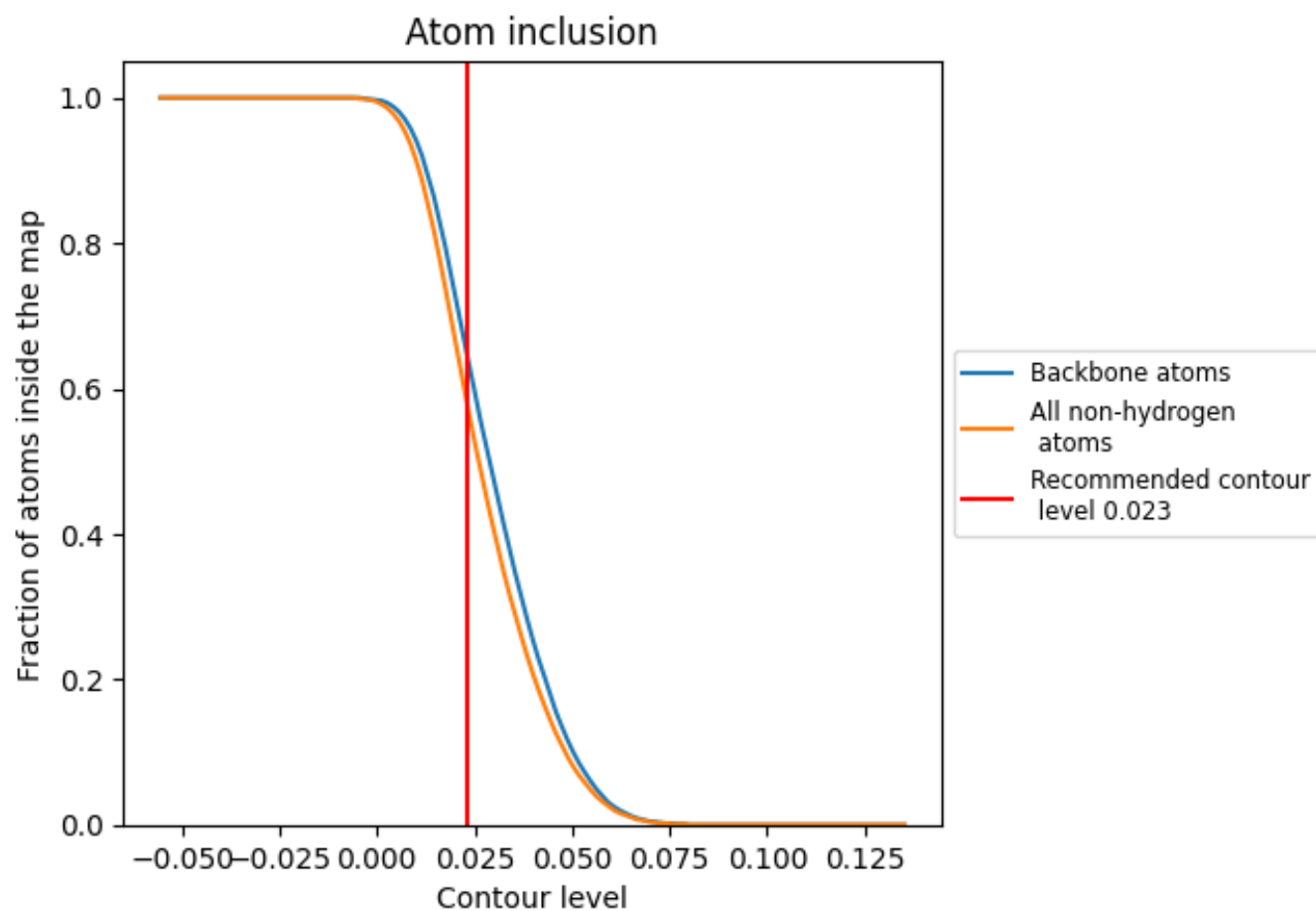


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 58% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5820	 0.4600
1	 0.4000	 0.3510
2	 0.6700	 0.4970
3	 0.7250	 0.5240
4	 0.7170	 0.5220
5	 0.6520	 0.4890
6	 0.4060	 0.3670
A	 0.7710	 0.5600
B	 0.7590	 0.5540
C	 0.7430	 0.5320
D	 0.5880	 0.4880
E	 0.6340	 0.5280
F	 0.7310	 0.5500
I	 0.2230	 0.3910
J	 0.7510	 0.5470
K	 0.5520	 0.4540
M	 0.4910	 0.4560
X	 0.8170	 0.5670
a	 0.3340	 0.3240
b	 0.4870	 0.4040
c	 0.5550	 0.4370
d	 0.5760	 0.4630
e	 0.5000	 0.4230
f	 0.3910	 0.3690
g	 0.2330	 0.2860

