



wwPDB EM Validation Summary Report ⓘ

Dec 29, 2024 – 09:18 AM EST

PDB ID : 7LX0
EMDB ID : EMD-23563
Title : Quantitative assessment of chlorophyll types in cryo-EM maps of photosystem I acclimated to far-red light
Authors : Gisriel, C.J.; Wang, J.
Deposited on : 2021-03-02
Resolution : 2.96 Å(reported)

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

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

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

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

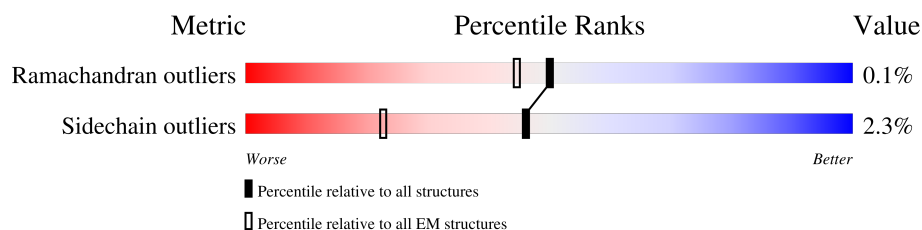
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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

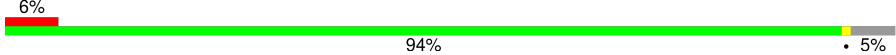
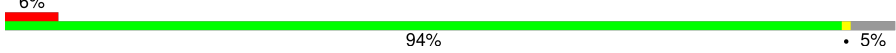
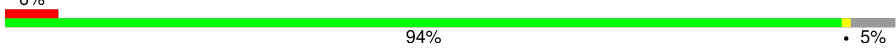
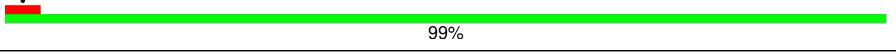
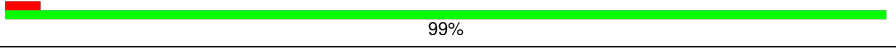
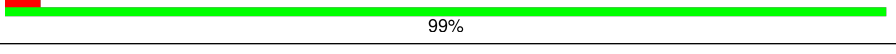
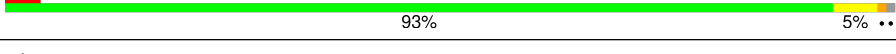
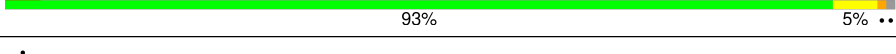
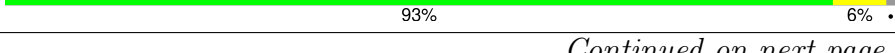
The reported resolution of this entry is 2.96 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	788	 6% 94% 5%
1	G	788	 6% 94% 5%
1	a	788	 6% 94% 5%
2	B	741	 1% 99%
2	H	741	 1% 99%
2	b	741	 1% 99%
3	C	81	 1% 93% 5% 1%
3	N	81	 1% 93% 5% 1%
3	c	81	 1% 93% 6%



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Mol	Chain	Length	Quality of chain
4	D	159	
4	O	159	
4	d	159	
5	E	72	
5	P	72	
5	e	72	
6	F	159	
6	Q	159	
6	f	159	
7	I	67	
7	R	67	
7	i	67	
8	J	48	
8	S	48	
8	j	48	
9	K	49	
9	T	49	
9	k	49	
10	L	174	
10	U	174	
10	l	174	
11	M	31	
11	V	31	
11	m	31	
12	W	101	

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Mol	Chain	Length	Quality of chain
12	X	101	
12	x	101	

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	CL0	A	1011	X	-	-	-
13	CL0	G	1011	X	-	-	-
13	CL0	a	1011	X	-	-	-
14	CLA	A	1012	X	-	-	-
14	CLA	A	1013	X	-	-	-
14	CLA	A	1101	X	-	-	-
14	CLA	A	1102	X	-	-	-
14	CLA	A	1103	X	-	-	-
14	CLA	A	1104	X	-	-	-
14	CLA	A	1105	X	-	-	-
14	CLA	A	1106	X	-	-	-
14	CLA	A	1107	X	-	-	-
14	CLA	A	1108	X	-	-	-
14	CLA	A	1109	X	-	-	-
14	CLA	A	1110	X	-	-	-
14	CLA	A	1111	X	-	-	-
14	CLA	A	1112	X	-	-	-
14	CLA	A	1113	X	-	-	-
14	CLA	A	1114	X	-	-	-
14	CLA	A	1115	X	-	-	-
14	CLA	A	1116	X	-	-	-
14	CLA	A	1117	X	-	-	-
14	CLA	A	1118	X	-	-	-
14	CLA	A	1119	X	-	-	-
14	CLA	A	1120	X	-	-	-
14	CLA	A	1122	X	-	-	-
14	CLA	A	1123	X	-	-	-
14	CLA	A	1124	X	-	-	-
14	CLA	A	1125	X	-	-	-
14	CLA	A	1126	X	-	-	-
14	CLA	A	1127	X	-	-	-
14	CLA	A	1128	X	-	-	-
14	CLA	A	1129	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	1130	X	-	-	-
14	CLA	A	1131	X	-	-	-
14	CLA	A	1132	X	-	-	-
14	CLA	A	1133	X	-	-	-
14	CLA	A	1134	X	-	-	-
14	CLA	A	1135	X	-	-	-
14	CLA	A	1136	X	-	-	-
14	CLA	A	1137	X	-	-	-
14	CLA	A	1138	X	-	-	-
14	CLA	A	1139	X	-	-	-
14	CLA	A	1140	X	-	-	-
14	CLA	B	1021	X	-	-	-
14	CLA	B	1022	X	-	-	-
14	CLA	B	1023	X	-	-	-
14	CLA	B	1201	X	-	-	-
14	CLA	B	1202	X	-	-	-
14	CLA	B	1203	X	-	-	-
14	CLA	B	1204	X	-	-	-
14	CLA	B	1205	X	-	-	-
14	CLA	B	1206	X	-	-	-
14	CLA	B	1208	X	-	-	-
14	CLA	B	1209	X	-	-	-
14	CLA	B	1210	X	-	-	-
14	CLA	B	1211	X	-	-	-
14	CLA	B	1212	X	-	-	-
14	CLA	B	1213	X	-	-	-
14	CLA	B	1214	X	-	-	-
14	CLA	B	1215	X	-	-	-
14	CLA	B	1216	X	-	-	-
14	CLA	B	1217	X	-	-	-
14	CLA	B	1218	X	-	-	-
14	CLA	B	1219	X	-	-	-
14	CLA	B	1220	X	-	-	-
14	CLA	B	1221	X	-	-	-
14	CLA	B	1222	X	-	-	-
14	CLA	B	1223	X	-	-	-
14	CLA	B	1224	X	-	-	-
14	CLA	B	1225	X	-	-	-
14	CLA	B	1226	X	-	-	-
14	CLA	B	1227	X	-	-	-
14	CLA	B	1228	X	-	-	-
14	CLA	B	1229	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	1231	X	-	-	-
14	CLA	B	1232	X	-	-	-
14	CLA	B	1233	X	-	-	-
14	CLA	B	1234	X	-	-	-
14	CLA	B	1235	X	-	-	-
14	CLA	B	1236	X	-	-	-
14	CLA	B	1239	X	-	-	-
14	CLA	G	1012	X	-	-	-
14	CLA	G	1013	X	-	-	-
14	CLA	G	1101	X	-	-	-
14	CLA	G	1102	X	-	-	-
14	CLA	G	1103	X	-	-	-
14	CLA	G	1104	X	-	-	-
14	CLA	G	1105	X	-	-	-
14	CLA	G	1106	X	-	-	-
14	CLA	G	1107	X	-	-	-
14	CLA	G	1108	X	-	-	-
14	CLA	G	1109	X	-	-	-
14	CLA	G	1110	X	-	-	-
14	CLA	G	1111	X	-	-	-
14	CLA	G	1112	X	-	-	-
14	CLA	G	1113	X	-	-	-
14	CLA	G	1114	X	-	-	-
14	CLA	G	1115	X	-	-	-
14	CLA	G	1116	X	-	-	-
14	CLA	G	1117	X	-	-	-
14	CLA	G	1118	X	-	-	-
14	CLA	G	1119	X	-	-	-
14	CLA	G	1120	X	-	-	-
14	CLA	G	1122	X	-	-	-
14	CLA	G	1123	X	-	-	-
14	CLA	G	1124	X	-	-	-
14	CLA	G	1125	X	-	-	-
14	CLA	G	1126	X	-	-	-
14	CLA	G	1127	X	-	-	-
14	CLA	G	1128	X	-	-	-
14	CLA	G	1129	X	-	-	-
14	CLA	G	1130	X	-	-	-
14	CLA	G	1131	X	-	-	-
14	CLA	G	1132	X	-	-	-
14	CLA	G	1133	X	-	-	-
14	CLA	G	1134	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	G	1135	X	-	-	-
14	CLA	G	1136	X	-	-	-
14	CLA	G	1137	X	-	-	-
14	CLA	G	1138	X	-	-	-
14	CLA	G	1139	X	-	-	-
14	CLA	G	1140	X	-	-	-
14	CLA	H	1021	X	-	-	-
14	CLA	H	1022	X	-	-	-
14	CLA	H	1023	X	-	-	-
14	CLA	H	1201	X	-	-	-
14	CLA	H	1202	X	-	-	-
14	CLA	H	1203	X	-	-	-
14	CLA	H	1204	X	-	-	-
14	CLA	H	1205	X	-	-	-
14	CLA	H	1206	X	-	-	-
14	CLA	H	1208	X	-	-	-
14	CLA	H	1209	X	-	-	-
14	CLA	H	1210	X	-	-	-
14	CLA	H	1211	X	-	-	-
14	CLA	H	1212	X	-	-	-
14	CLA	H	1213	X	-	-	-
14	CLA	H	1214	X	-	-	-
14	CLA	H	1215	X	-	-	-
14	CLA	H	1216	X	-	-	-
14	CLA	H	1217	X	-	-	-
14	CLA	H	1218	X	-	-	-
14	CLA	H	1219	X	-	-	-
14	CLA	H	1220	X	-	-	-
14	CLA	H	1221	X	-	-	-
14	CLA	H	1222	X	-	-	-
14	CLA	H	1223	X	-	-	-
14	CLA	H	1224	X	-	-	-
14	CLA	H	1225	X	-	-	-
14	CLA	H	1226	X	-	-	-
14	CLA	H	1227	X	-	-	-
14	CLA	H	1228	X	-	-	-
14	CLA	H	1229	X	-	-	-
14	CLA	H	1231	X	-	-	-
14	CLA	H	1232	X	-	-	-
14	CLA	H	1233	X	-	-	-
14	CLA	H	1234	X	-	-	-
14	CLA	H	1235	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	H	1236	X	-	-	-
14	CLA	H	1239	X	-	-	-
14	CLA	K	1401	X	-	-	-
14	CLA	L	1501	X	-	-	-
14	CLA	L	1502	X	-	-	-
14	CLA	L	1503	X	-	-	-
14	CLA	T	1401	X	-	-	-
14	CLA	U	1501	X	-	-	-
14	CLA	U	1502	X	-	-	-
14	CLA	U	1503	X	-	-	-
14	CLA	W	1701	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	a	1012	X	-	-	-
14	CLA	a	1013	X	-	-	-
14	CLA	a	1101	X	-	-	-
14	CLA	a	1102	X	-	-	-
14	CLA	a	1103	X	-	-	-
14	CLA	a	1104	X	-	-	-
14	CLA	a	1105	X	-	-	-
14	CLA	a	1106	X	-	-	-
14	CLA	a	1107	X	-	-	-
14	CLA	a	1108	X	-	-	-
14	CLA	a	1109	X	-	-	-
14	CLA	a	1110	X	-	-	-
14	CLA	a	1111	X	-	-	-
14	CLA	a	1112	X	-	-	-
14	CLA	a	1113	X	-	-	-
14	CLA	a	1114	X	-	-	-
14	CLA	a	1115	X	-	-	-
14	CLA	a	1116	X	-	-	-
14	CLA	a	1117	X	-	-	-
14	CLA	a	1118	X	-	-	-
14	CLA	a	1119	X	-	-	-
14	CLA	a	1120	X	-	-	-
14	CLA	a	1122	X	-	-	-
14	CLA	a	1123	X	-	-	-
14	CLA	a	1124	X	-	-	-
14	CLA	a	1125	X	-	-	-
14	CLA	a	1126	X	-	-	-
14	CLA	a	1127	X	-	-	-
14	CLA	a	1128	X	-	-	-
14	CLA	a	1129	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	1130	X	-	-	-
14	CLA	a	1131	X	-	-	-
14	CLA	a	1132	X	-	-	-
14	CLA	a	1133	X	-	-	-
14	CLA	a	1134	X	-	-	-
14	CLA	a	1135	X	-	-	-
14	CLA	a	1136	X	-	-	-
14	CLA	a	1137	X	-	-	-
14	CLA	a	1138	X	-	-	-
14	CLA	a	1139	X	-	-	-
14	CLA	a	1140	X	-	-	-
14	CLA	b	1021	X	-	-	-
14	CLA	b	1022	X	-	-	-
14	CLA	b	1023	X	-	-	-
14	CLA	b	1201	X	-	-	-
14	CLA	b	1202	X	-	-	-
14	CLA	b	1203	X	-	-	-
14	CLA	b	1204	X	-	-	-
14	CLA	b	1205	X	-	-	-
14	CLA	b	1206	X	-	-	-
14	CLA	b	1208	X	-	-	-
14	CLA	b	1209	X	-	-	-
14	CLA	b	1210	X	-	-	-
14	CLA	b	1211	X	-	-	-
14	CLA	b	1212	X	-	-	-
14	CLA	b	1213	X	-	-	-
14	CLA	b	1214	X	-	-	-
14	CLA	b	1215	X	-	-	-
14	CLA	b	1216	X	-	-	-
14	CLA	b	1217	X	-	-	-
14	CLA	b	1218	X	-	-	-
14	CLA	b	1219	X	-	-	-
14	CLA	b	1220	X	-	-	-
14	CLA	b	1221	X	-	-	-
14	CLA	b	1222	X	-	-	-
14	CLA	b	1223	X	-	-	-
14	CLA	b	1224	X	-	-	-
14	CLA	b	1225	X	-	-	-
14	CLA	b	1226	X	-	-	-
14	CLA	b	1227	X	-	-	-
14	CLA	b	1228	X	-	-	-
14	CLA	b	1229	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	1231	X	-	-	-
14	CLA	b	1232	X	-	-	-
14	CLA	b	1233	X	-	-	-
14	CLA	b	1234	X	-	-	-
14	CLA	b	1235	X	-	-	-
14	CLA	b	1236	X	-	-	-
14	CLA	b	1239	X	-	-	-
14	CLA	k	1401	X	-	-	-
14	CLA	l	1501	X	-	-	-
14	CLA	l	1502	X	-	-	-
14	CLA	l	1503	X	-	-	-
14	CLA	x	1701	X	-	-	-

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 72462 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	751	Total	C	N	O	S	0	0
			5931	3892	1013	993	33		
1	a	751	Total	C	N	O	S	0	0
			5931	3892	1013	993	33		
1	A	751	Total	C	N	O	S	0	0
			5931	3892	1013	993	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	739	Total	C	N	O	S	0	0
			5913	3896	997	1002	18		
2	b	739	Total	C	N	O	S	0	0
			5913	3896	997	1002	18		
2	B	739	Total	C	N	O	S	0	0
			5913	3896	997	1002	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	80	Total	C	N	O	S	0	0
			601	367	105	118	11		
3	c	80	Total	C	N	O	S	0	0
			601	367	105	118	11		
3	C	80	Total	C	N	O	S	0	0
			601	367	105	118	11		

- Molecule 4 is a protein called Photosystem I protein PsdA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	139	Total	C	N	O	S	0	0
			1092	694	192	203	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	139	Total	C	N	O	S	0	0
			1092	694	192	203	3		
4	D	139	Total	C	N	O	S	0	0
			1092	694	192	203	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	62	Total	C	N	O		0	0
			497	313	88	96			
5	e	62	Total	C	N	O		0	0
			497	313	88	96			
5	E	62	Total	C	N	O		0	0
			497	313	88	96			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	135	Total	C	N	O	S	0	0
			1060	694	167	192	7		
6	f	135	Total	C	N	O	S	0	0
			1060	694	167	192	7		
6	F	135	Total	C	N	O	S	0	0
			1060	694	167	192	7		

- Molecule 7 is a protein called photosystem I subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	42	Total	C	N	O	S	0	0
			350	246	48	54	2		
7	i	42	Total	C	N	O	S	0	0
			350	246	48	54	2		
7	I	42	Total	C	N	O	S	0	0
			350	246	48	54	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	-	initiating methionine	UNP A0A2N6MR25
i	1	MET	-	initiating methionine	UNP A0A2N6MR25
I	1	MET	-	initiating methionine	UNP A0A2N6MR25

- Molecule 8 is a protein called Photosystem I reaction centre subunit IX / PsaJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	S	43	Total	C	N	O	0	0
			344	238	51	55		
8	j	43	Total	C	N	O	0	0
			344	238	51	55		
8	J	43	Total	C	N	O	0	0
			344	238	51	55		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	44	Total	C	N	O	S	0	0
			253	161	46	45	1		
9	k	44	Total	C	N	O	S	0	0
			253	161	46	45	1		
9	K	44	Total	C	N	O	S	0	0
			253	161	46	45	1		

- Molecule 10 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	163	Total	C	N	O	S	0	0
			1227	792	207	223	5		
10	l	163	Total	C	N	O	S	0	0
			1227	792	207	223	5		
10	L	163	Total	C	N	O	S	0	0
			1227	792	207	223	5		

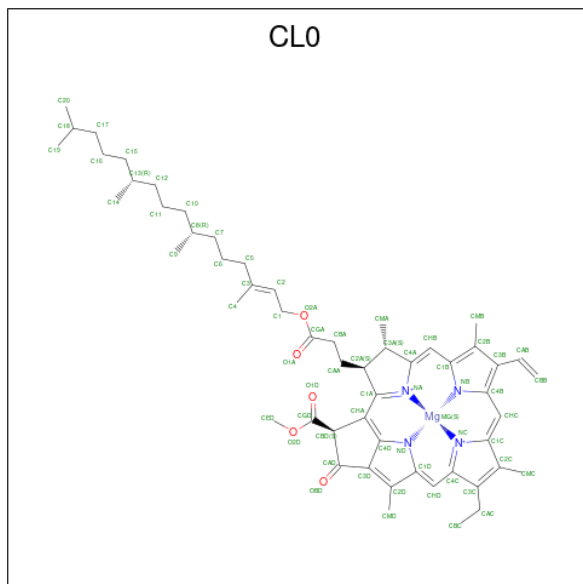
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	31	Total	C	N	O	S	0	0
			245	164	37	43	1		
11	m	31	Total	C	N	O	S	0	0
			245	164	37	43	1		
11	M	31	Total	C	N	O	S	0	0
			245	164	37	43	1		

- Molecule 12 is a protein called Photosystem one PsaX.

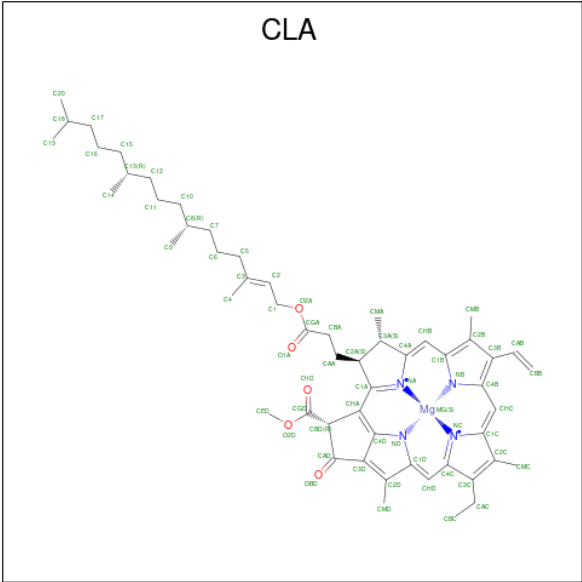
Mol	Chain	Residues	Atoms				AltConf	Trace
12	W	29	Total	C	N	O	0	0
			246	172	36	38		
12	x	29	Total	C	N	O	0	0
			246	172	36	38		
12	X	29	Total	C	N	O	0	0
			246	172	36	38		

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	U	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a	1	Total 55	C 45	Mg 1	N 4	O 5	0

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

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

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

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	l	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	x	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 55	C 45	Mg 1	N 4	O 5	0

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

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

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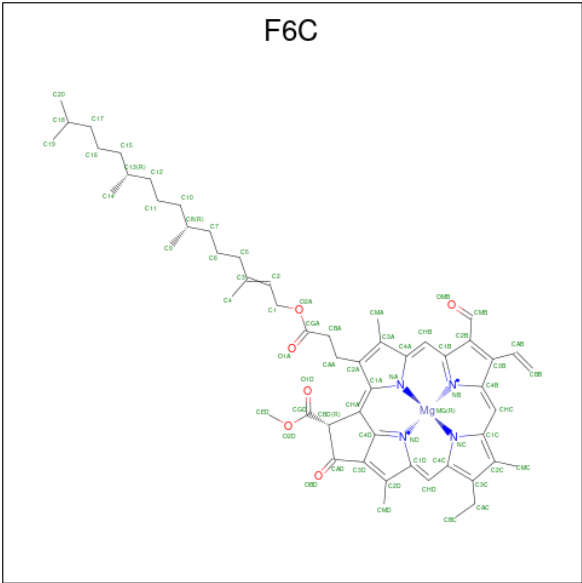
Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total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

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	X	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 15 is Chlorophyll F (three-letter code: F6C) (formula: C₅₅H₆₈MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



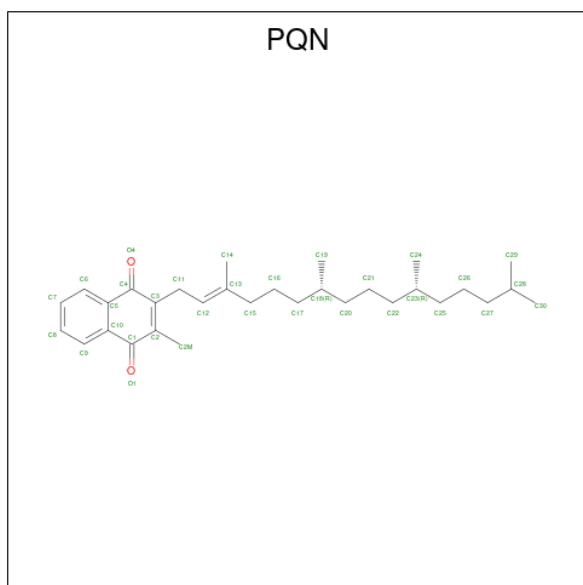
Mol	Chain	Residues	Atoms					AltConf
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			46	35	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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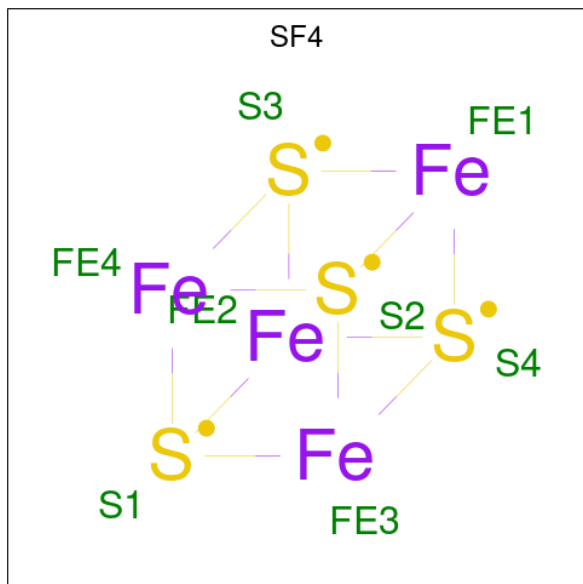
Mol	Chain	Residues	Atoms					AltConf
15	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 16 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



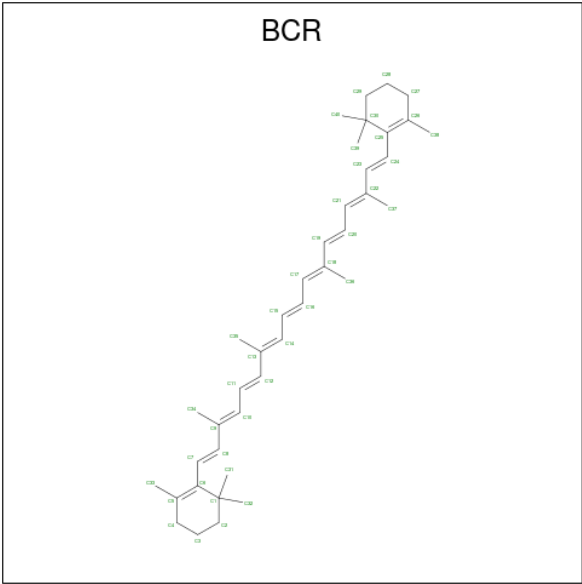
Mol	Chain	Residues	Atoms			AltConf
17	G	1	Total	Fe	S	0
			8	4	4	
17	N	1	Total	Fe	S	0
			8	4	4	
17	N	1	Total	Fe	S	0
			8	4	4	
17	a	1	Total	Fe	S	0
			8	4	4	
17	c	1	Total	Fe	S	0
			8	4	4	
17	c	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 18 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
18	G	1	Total	C	0
			40	40	
18	G	1	Total	C	0
			40	40	
18	G	1	Total	C	0
			40	40	
18	G	1	Total	C	0
			40	40	
18	G	1	Total	C	0
			40	40	
18	H	1	Total	C	0
			40	40	
18	H	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	R	1	Total C 40 40	0
18	R	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	V	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0

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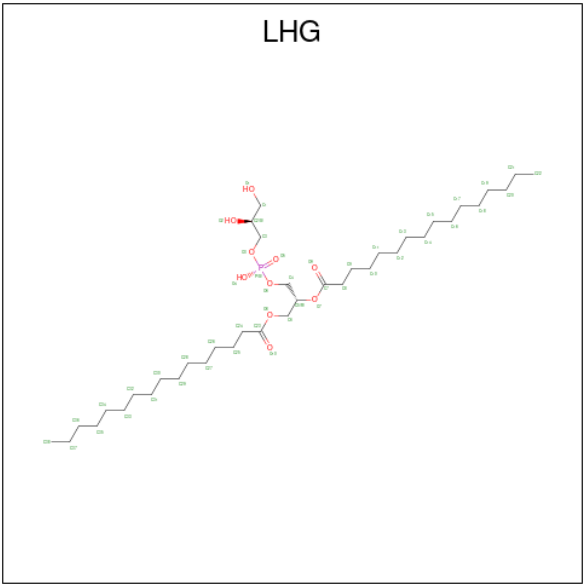
Mol	Chain	Residues	Atoms	AltConf
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	i	1	Total C 40 40	0
18	i	1	Total C 40 40	0
18	l	1	Total C 40 40	0
18	l	1	Total C 40 40	0
18	m	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	I	1	Total	C	0
			40	40	
18	I	1	Total	C	0
			40	40	
18	L	1	Total	C	0
			40	40	
18	L	1	Total	C	0
			40	40	
18	M	1	Total	C	0
			40	40	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



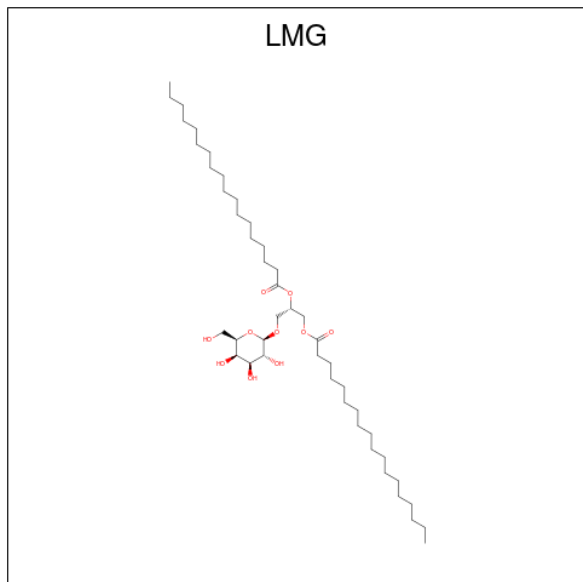
Mol	Chain	Residues	Atoms				AltConf
19	G	1	Total	C	O	P	0
			42	31	10	1	

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Mol	Chain	Residues	Atoms				AltConf
19	H	1	Total	C	O	P	0
			44	33	10	1	
19	a	1	Total	C	O	P	0
			42	31	10	1	
19	b	1	Total	C	O	P	0
			44	33	10	1	
19	A	1	Total	C	O	P	0
			42	31	10	1	
19	B	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



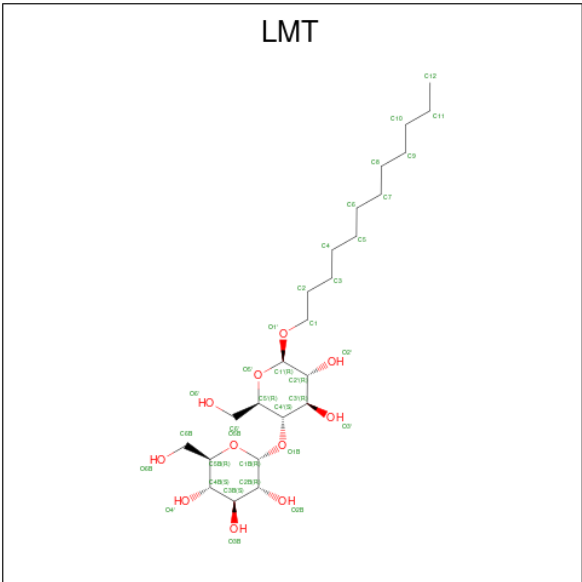
Mol	Chain	Residues	Atoms			AltConf
20	G	1	Total	C	O	0
			46	36	10	
20	H	1	Total	C	O	0
			46	36	10	
20	R	1	Total	C	O	0
			37	27	10	
20	U	1	Total	C	O	0
			50	40	10	
20	a	1	Total	C	O	0
			46	36	10	
20	b	1	Total	C	O	0
			46	36	10	

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Mol	Chain	Residues	Atoms			AltConf
20	i	1	Total	C	O	0
			37	27	10	
20	l	1	Total	C	O	0
			50	40	10	
20	A	1	Total	C	O	0
			46	36	10	
20	B	1	Total	C	O	0
			46	36	10	
20	I	1	Total	C	O	0
			37	27	10	
20	L	1	Total	C	O	0
			50	40	10	

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
21	G	1	Total	C	O	0
			31	20	11	
21	G	1	Total	C	O	0
			28	17	11	
21	a	1	Total	C	O	0
			31	20	11	
21	a	1	Total	C	O	0
			28	17	11	
21	A	1	Total	C	O	0
			31	20	11	

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Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			28	17	11	

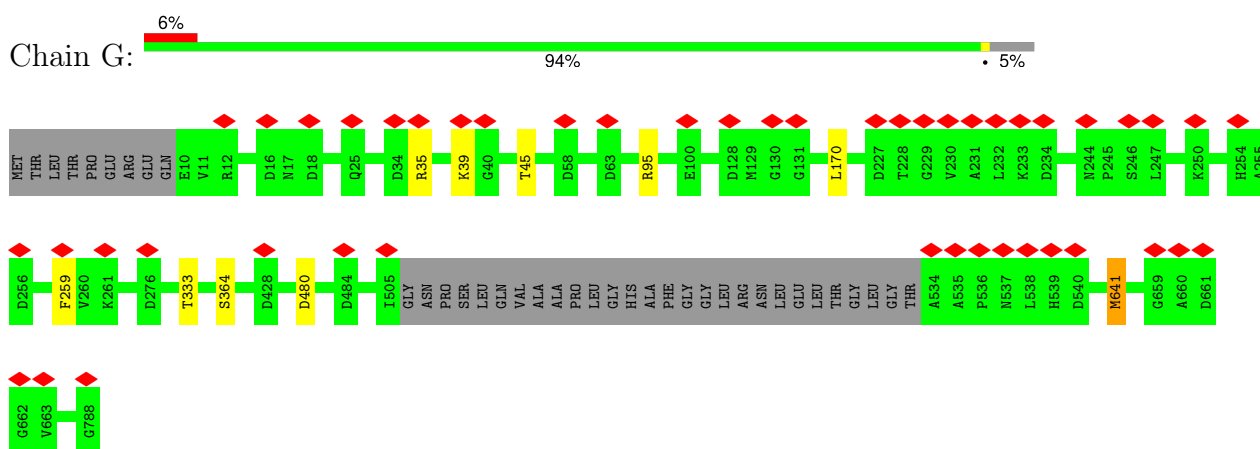
- Molecule 22 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

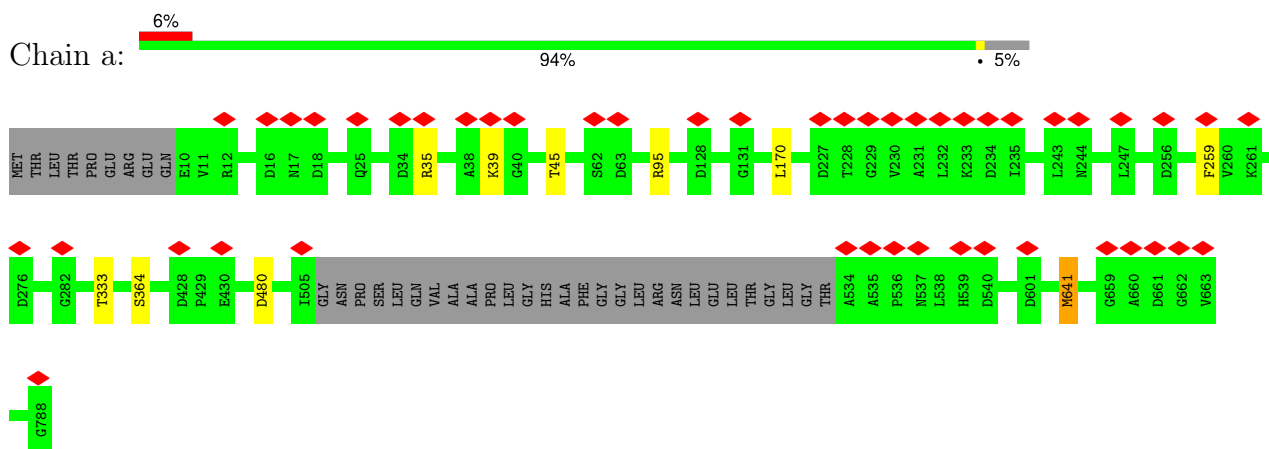
3 Residue-property plots [i](#)

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

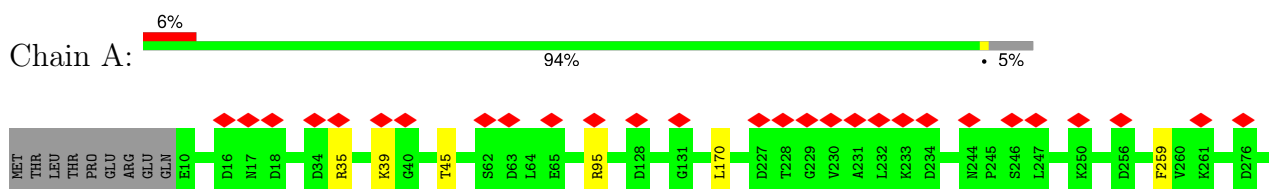
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

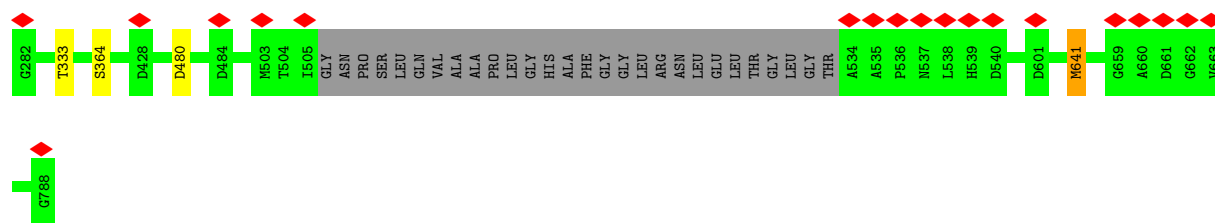


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



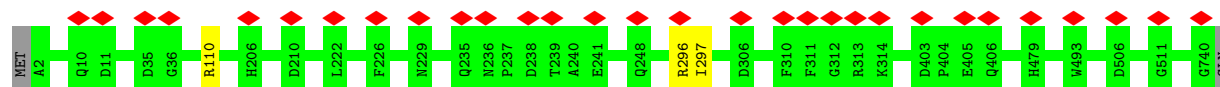
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





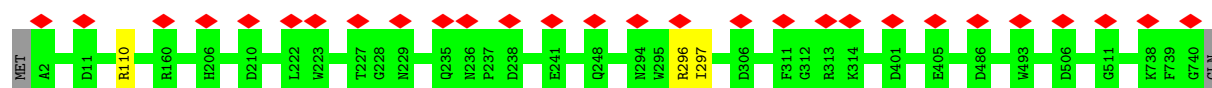
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain H: 99%



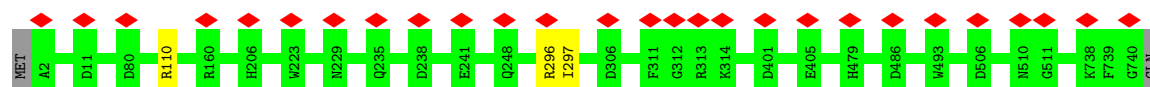
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 99%



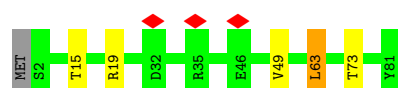
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 99%



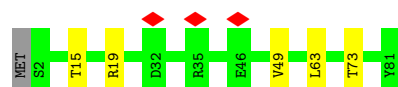
- Molecule 3: Photosystem I iron-sulfur center

Chain N: 93% 5% ..



- Molecule 3: Photosystem I iron-sulfur center

Chain c: 93% 6% .

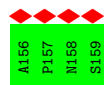
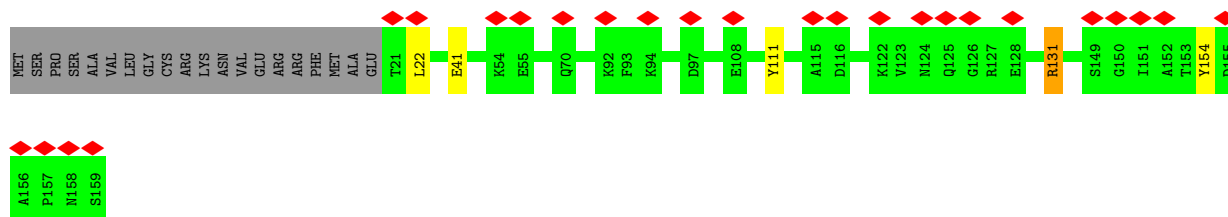
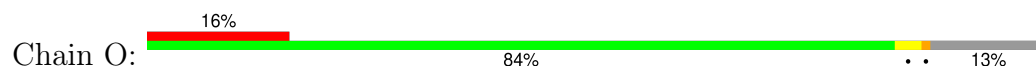


- Molecule 3: Photosystem I iron-sulfur center

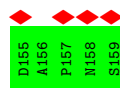
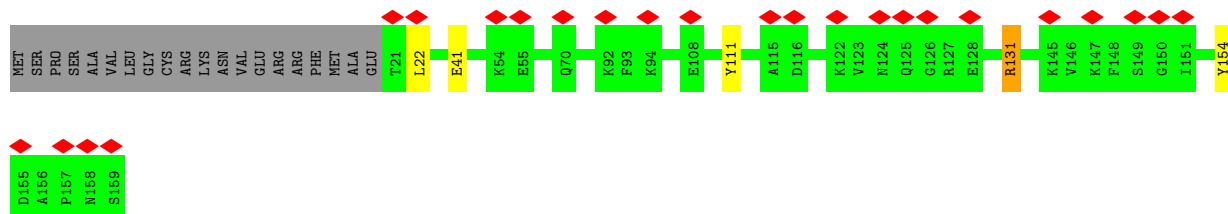
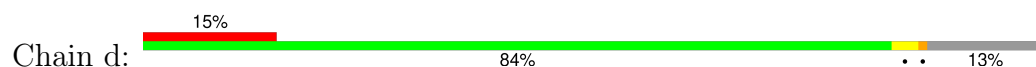
Chain C: 93% 5% ..



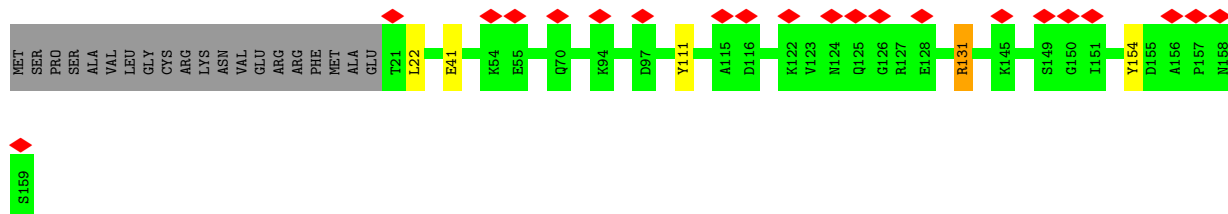
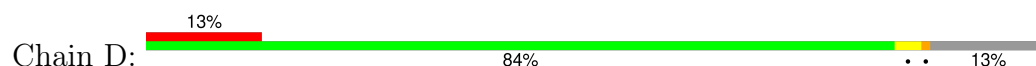
• Molecule 4: Photosystem I protein PsalD



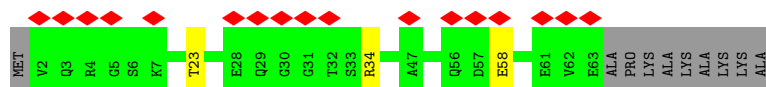
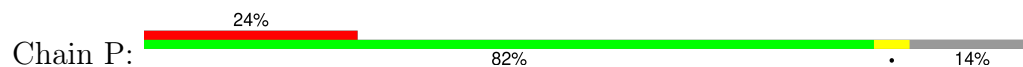
• Molecule 4: Photosystem I protein PsalD



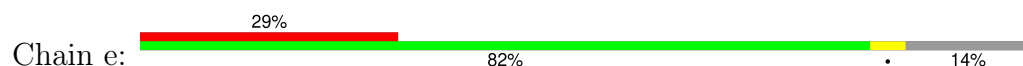
• Molecule 4: Photosystem I protein PsalD

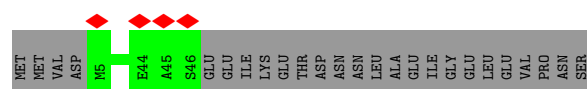


• Molecule 5: Photosystem I reaction center subunit IV

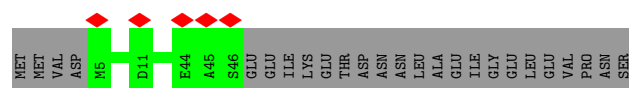


• Molecule 5: Photosystem I reaction center subunit IV

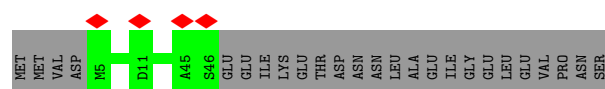




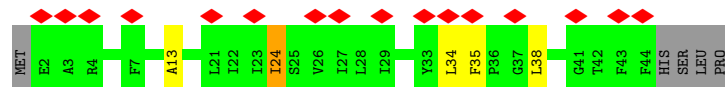
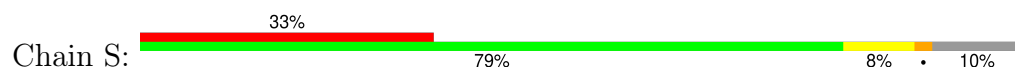
- Molecule 7: photosystem I subunit VIII



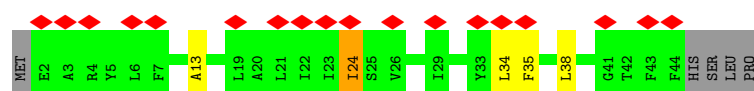
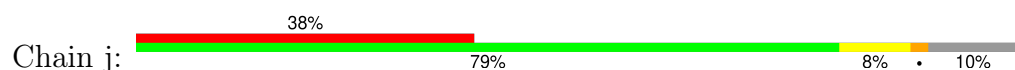
- Molecule 7: photosystem I subunit VIII



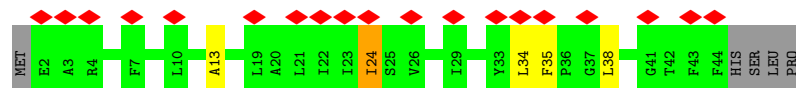
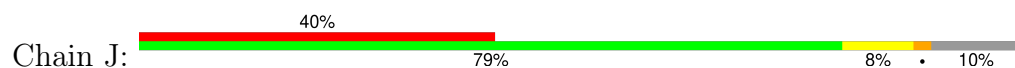
- Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



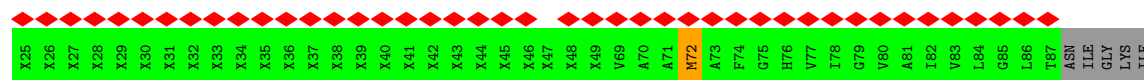
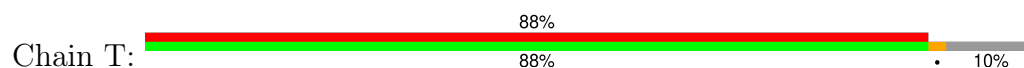
- Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



- Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



- Molecule 9: Photosystem I reaction center subunit PsaK



Chain m: 97%



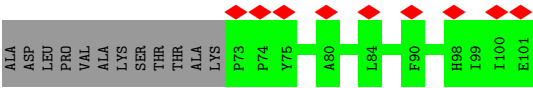
- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 12: Photosystem one Psax



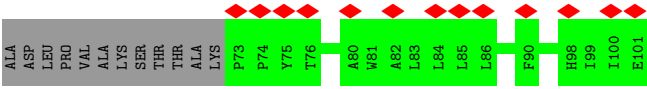
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- Molecule 12: Photosystem one Psax



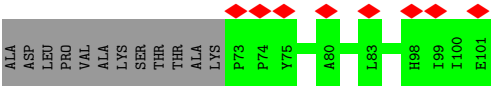
MET	PRO	GLY	GLY	LYS	VAL	SER	THR	ALA	PRO	ARG	LEU	HIS	THR	LEU	PRO	THR	SER	LEU	PRO	LEU	ALA	GLN	ASN	HIS	GLU	ASN	ILE	PHE	ASN	GLU	SER	GLY	GLY	LEU	GLY	HIS	LEU	PHE	GLY	ILE	SER	GLU	GLU	VAL	LEU	LYS	LEU	GLY	VAL	HIS	PHE	MET	ALA	LYS	ALA	ASP	THR	THR
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- Molecule 12: Photosystem one Psax



MET	PRO	GLY	GLY	LYS	VAL	SER	THR	ALA	PRO	ARG	LEU	HIS	THR	LEU	PRO	THR	SER	LEU	PRO	LEU	ALA	GLN	ASN	HIS	GLU	ASN	ILE	PHE	ASN	GLU	SER	GLY	GLY	LEU	GLY	HIS	LEU	PHE	GLY	ILE	SER	GLU	GLU	VAL	LEU	LYS	LEU	GLY	VAL	HIS	PHE	MET	ALA	LYS	ALA	ASP	THR	THR
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	201104	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.328	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.324	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	381.6013, 381.6013, 381.6013	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.49063, 1.49063, 1.49063	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, BCR, CL0, LMG, PQN, CLA, LHG, CA, LMT, F6C

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/6138	0.55	1/8362 (0.0%)
1	G	0.54	0/6138	0.55	1/8362 (0.0%)
1	a	0.54	0/6138	0.55	1/8362 (0.0%)
2	B	0.57	0/6135	0.54	0/8385
2	H	0.57	0/6135	0.54	0/8385
2	b	0.57	0/6135	0.54	0/8385
3	C	0.62	0/611	0.77	1/828 (0.1%)
3	N	0.62	0/611	0.77	1/828 (0.1%)
3	c	0.62	0/611	0.77	1/828 (0.1%)
4	D	0.49	0/1116	0.64	1/1505 (0.1%)
4	O	0.49	0/1116	0.64	1/1505 (0.1%)
4	d	0.49	0/1116	0.64	1/1505 (0.1%)
5	E	0.48	0/506	0.59	0/686
5	P	0.48	0/506	0.59	0/686
5	e	0.48	0/506	0.59	0/686
6	F	0.45	0/1084	0.74	2/1470 (0.1%)
6	Q	0.45	0/1084	0.74	2/1470 (0.1%)
6	f	0.45	0/1084	0.74	2/1470 (0.1%)
7	I	0.59	0/365	0.72	0/502
7	R	0.59	0/365	0.72	0/502
7	i	0.59	0/365	0.72	0/502
8	J	0.37	0/353	0.78	1/482 (0.2%)
8	S	0.36	0/353	0.78	1/482 (0.2%)
8	j	0.37	0/353	0.78	1/482 (0.2%)
9	K	0.31	0/129	1.21	3/175 (1.7%)
9	T	0.31	0/129	1.21	3/175 (1.7%)
9	k	0.31	0/129	1.21	3/175 (1.7%)
10	L	0.56	0/1255	0.84	5/1702 (0.3%)
10	U	0.56	0/1255	0.84	5/1702 (0.3%)
10	l	0.56	0/1255	0.84	5/1702 (0.3%)
11	M	0.45	0/250	0.64	0/340
11	V	0.45	0/250	0.64	0/340

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	m	0.45	0/250	0.64	0/340
12	W	0.40	0/256	0.47	0/350
12	X	0.40	0/256	0.47	0/350
12	x	0.39	0/256	0.47	0/350
All	All	0.54	0/54594	0.61	42/74361 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
1	a	0	1
6	F	0	2
6	Q	0	2
6	f	0	2
8	J	0	1
8	S	0	1
8	j	0	1
10	L	0	1
10	U	0	1
10	l	0	1
All	All	0	15

There are no bond length outliers.

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	132	ARG	CG-CD-NE	12.77	138.61	111.80
10	L	132	ARG	CG-CD-NE	12.75	138.57	111.80
10	l	132	ARG	CG-CD-NE	12.74	138.55	111.80
10	l	132	ARG	NE-CZ-NH2	-12.23	114.18	120.30
10	L	132	ARG	NE-CZ-NH2	-12.18	114.21	120.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	333	THR	Peptide

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Mol	Chain	Res	Type	Group
6	Q	47	SER	Peptide
6	Q	48	TYR	Peptide
8	S	35	PHE	Peptide
10	U	132	ARG	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	747/788 (95%)	707 (95%)	40 (5%)	0	100	100
1	G	747/788 (95%)	707 (95%)	40 (5%)	0	100	100
1	a	747/788 (95%)	707 (95%)	40 (5%)	0	100	100
2	B	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	H	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	b	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
3	C	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	10	27
3	N	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	10	27
3	c	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
4	D	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
4	O	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
4	d	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
5	E	60/72 (83%)	57 (95%)	3 (5%)	0	100	100
5	P	60/72 (83%)	57 (95%)	3 (5%)	0	100	100
5	e	60/72 (83%)	57 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	16	39
6	Q	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	16	39
6	f	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	16	39
7	I	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
7	R	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
7	i	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
8	J	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	5	13
8	S	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	5	13
8	j	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	5	13
9	K	17/49 (35%)	17 (100%)	0	0	100	100
9	T	17/49 (35%)	17 (100%)	0	0	100	100
9	k	17/49 (35%)	17 (100%)	0	0	100	100
10	L	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
10	U	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
10	l	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	V	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
12	W	27/101 (27%)	27 (100%)	0	0	100	100
12	X	27/101 (27%)	27 (100%)	0	0	100	100
12	x	27/101 (27%)	27 (100%)	0	0	100	100
All	All	6621/7410 (89%)	6240 (94%)	373 (6%)	8 (0%)	50	72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	Q	48	TYR
6	f	48	TYR
6	F	48	TYR
3	N	63	LEU
8	S	13	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	613/641 (96%)	604 (98%)	9 (2%)	60	78
1	G	613/641 (96%)	604 (98%)	9 (2%)	60	78
1	a	613/641 (96%)	604 (98%)	9 (2%)	60	78
2	B	595/597 (100%)	592 (100%)	3 (0%)	86	93
2	H	595/597 (100%)	592 (100%)	3 (0%)	86	93
2	b	595/597 (100%)	592 (100%)	3 (0%)	86	93
3	C	68/69 (99%)	64 (94%)	4 (6%)	16	37
3	N	68/69 (99%)	64 (94%)	4 (6%)	16	37
3	c	68/69 (99%)	64 (94%)	4 (6%)	16	37
4	D	115/132 (87%)	110 (96%)	5 (4%)	25	49
4	O	115/132 (87%)	110 (96%)	5 (4%)	25	49
4	d	115/132 (87%)	110 (96%)	5 (4%)	25	49
5	E	54/60 (90%)	51 (94%)	3 (6%)	17	40
5	P	54/60 (90%)	51 (94%)	3 (6%)	17	40
5	e	54/60 (90%)	51 (94%)	3 (6%)	17	40
6	F	115/134 (86%)	105 (91%)	10 (9%)	8	22
6	Q	115/134 (86%)	105 (91%)	10 (9%)	8	22
6	f	115/134 (86%)	105 (91%)	10 (9%)	8	22
7	I	37/60 (62%)	37 (100%)	0	100	100
7	R	37/60 (62%)	37 (100%)	0	100	100
7	i	37/60 (62%)	37 (100%)	0	100	100
8	J	36/42 (86%)	33 (92%)	3 (8%)	9	24
8	S	36/42 (86%)	33 (92%)	3 (8%)	9	24
8	j	36/42 (86%)	33 (92%)	3 (8%)	9	24
9	K	12/16 (75%)	11 (92%)	1 (8%)	9	24
9	T	12/16 (75%)	11 (92%)	1 (8%)	9	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	k	12/16 (75%)	11 (92%)	1 (8%)	9	24
10	L	128/138 (93%)	125 (98%)	3 (2%)	45	69
10	U	128/138 (93%)	125 (98%)	3 (2%)	45	69
10	l	128/138 (93%)	125 (98%)	3 (2%)	45	69
11	M	26/26 (100%)	25 (96%)	1 (4%)	28	53
11	V	26/26 (100%)	25 (96%)	1 (4%)	28	53
11	m	26/26 (100%)	25 (96%)	1 (4%)	28	53
12	W	24/84 (29%)	24 (100%)	0	100	100
12	X	24/84 (29%)	24 (100%)	0	100	100
12	x	24/84 (29%)	24 (100%)	0	100	100
All	All	5469/5997 (91%)	5343 (98%)	126 (2%)	46	69

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	73	THR
6	F	46	ASP
6	f	62	CYS
6	F	38	VAL
8	J	24	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	731	GLN
2	B	34	HIS
2	B	444	ASN
1	a	144	GLN
1	a	105	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 372 ligands modelled in this entry, 3 are monoatomic - leaving 369 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
18	BCR	H	4006	-	41,41,41	2.67	6 (14%)	56,56,56	6.76	21 (37%)
20	LMG	G	5005	-	46,46,55	1.37	5 (10%)	54,54,63	1.10	2 (3%)
19	LHG	G	5001	-	41,41,48	1.00	2 (4%)	44,47,54	1.11	3 (6%)
14	CLA	T	1401	-	43,53,73	2.63	19 (44%)	50,89,113	2.86	21 (42%)
18	BCR	b	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.65	25 (44%)
14	CLA	a	1112	-	53,63,73	2.44	18 (33%)	62,101,113	2.68	25 (40%)
14	CLA	B	1206	2	43,53,73	2.54	15 (34%)	50,89,113	2.69	20 (40%)
16	PQN	b	2002	-	34,34,34	1.51	2 (5%)	43,45,45	1.28	3 (6%)
14	CLA	H	1201	-	53,63,73	2.43	18 (33%)	62,101,113	2.79	23 (37%)
14	CLA	H	1226	-	63,73,73	2.25	18 (28%)	74,113,113	2.43	24 (32%)
18	BCR	H	4005	-	41,41,41	2.77	8 (19%)	56,56,56	6.74	24 (42%)
14	CLA	B	1221	-	63,73,73	2.22	18 (28%)	74,113,113	2.45	25 (33%)
14	CLA	a	1110	-	43,53,73	2.56	17 (39%)	50,89,113	2.77	20 (40%)
18	BCR	G	4011	-	41,41,41	2.80	7 (17%)	56,56,56	6.69	28 (50%)
14	CLA	a	1119	-	63,73,73	2.23	18 (28%)	74,113,113	2.51	24 (32%)
14	CLA	B	1202	-	58,68,73	2.24	18 (31%)	68,107,113	2.60	25 (36%)
14	CLA	H	1222	-	63,73,73	2.24	18 (28%)	74,113,113	2.55	27 (36%)
14	CLA	G	1137	-	48,58,73	2.55	18 (37%)	56,95,113	2.95	25 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	G	1109	-	63,73,73	2.23	18 (28%)	74,113,113	2.52	25 (33%)
14	CLA	G	1107	1	43,53,73	2.55	17 (39%)	50,89,113	2.74	21 (42%)
17	SF4	C	3002	3	0,12,12	-	-	-	-	-
18	BCR	H	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.65	25 (44%)
14	CLA	k	1401	-	43,53,73	2.63	19 (44%)	50,89,113	2.85	21 (42%)
14	CLA	a	1132	-	63,73,73	2.20	17 (26%)	74,113,113	2.60	24 (32%)
14	CLA	G	1131	-	58,68,73	2.33	17 (29%)	68,107,113	2.54	22 (32%)
14	CLA	A	1108	-	43,53,73	2.60	18 (41%)	50,89,113	2.78	21 (42%)
14	CLA	B	1232	-	43,53,73	2.59	17 (39%)	50,89,113	2.78	20 (40%)
20	LMG	a	5005	-	46,46,55	1.38	5 (10%)	54,54,63	1.10	2 (3%)
18	BCR	I	4018	-	41,41,41	2.84	7 (17%)	56,56,56	6.73	25 (44%)
18	BCR	G	4001	-	41,41,41	2.73	6 (14%)	56,56,56	6.76	23 (41%)
18	BCR	a	4002	-	41,41,41	2.74	6 (14%)	56,56,56	6.43	28 (50%)
14	CLA	B	1216	-	63,73,73	2.22	18 (28%)	74,113,113	2.40	25 (33%)
18	BCR	A	4007	-	41,41,41	2.87	8 (19%)	56,56,56	6.72	24 (42%)
14	CLA	a	1136	-	63,73,73	2.20	17 (26%)	74,113,113	2.49	24 (32%)
20	LMG	B	5002	-	46,46,55	1.34	5 (10%)	54,54,63	1.27	4 (7%)
20	LMG	L	5007	-	50,50,55	1.45	7 (14%)	58,58,63	1.10	2 (3%)
14	CLA	A	1117	-	63,73,73	2.20	17 (26%)	74,113,113	2.54	27 (36%)
14	CLA	B	1205	-	63,73,73	2.18	17 (26%)	74,113,113	2.52	23 (31%)
14	CLA	B	1204	-	63,73,73	2.23	17 (26%)	74,113,113	2.44	26 (35%)
18	BCR	a	4011	-	41,41,41	2.80	7 (17%)	56,56,56	6.69	28 (50%)
14	CLA	b	1220	-	53,63,73	2.44	17 (32%)	62,101,113	2.82	26 (41%)
18	BCR	b	4014	-	41,41,41	2.81	8 (19%)	56,56,56	6.59	25 (44%)
14	CLA	G	1102	-	58,68,73	2.34	17 (29%)	68,107,113	2.59	23 (33%)
21	LMT	G	6002	-	29,29,36	1.36	6 (20%)	40,40,47	1.18	4 (10%)
14	CLA	G	1119	-	63,73,73	2.22	18 (28%)	74,113,113	2.50	24 (32%)
14	CLA	H	1206	2	43,53,73	2.54	15 (34%)	50,89,113	2.70	20 (40%)
16	PQN	B	2002	-	34,34,34	1.50	2 (5%)	43,45,45	1.28	3 (6%)
15	F6C	b	1230	-	47,54,74	3.08	24 (51%)	48,90,114	3.96	25 (52%)
14	CLA	a	1133	-	58,68,73	2.34	19 (32%)	68,107,113	2.66	25 (36%)
14	CLA	A	1127	-	63,73,73	2.23	18 (28%)	74,113,113	2.50	22 (29%)
14	CLA	G	1128	-	58,68,73	2.33	18 (31%)	68,107,113	2.62	23 (33%)
20	LMG	R	5006	-	37,37,55	1.14	3 (8%)	45,45,63	1.21	4 (8%)
14	CLA	B	1227	-	43,53,73	2.62	18 (41%)	50,89,113	2.75	23 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	l	1503	-	63,73,73	2.24	18 (28%)	74,113,113	2.49	26 (35%)
14	CLA	a	1129	-	48,58,73	2.55	18 (37%)	56,95,113	2.80	23 (41%)
14	CLA	H	1231	2	53,63,73	2.43	18 (33%)	62,101,113	2.65	23 (37%)
18	BCR	b	4009	-	41,41,41	2.75	7 (17%)	56,56,56	6.58	20 (35%)
14	CLA	B	1226	-	63,73,73	2.24	18 (28%)	74,113,113	2.43	24 (32%)
14	CLA	H	1202	-	58,68,73	2.24	18 (31%)	68,107,113	2.60	25 (36%)
18	BCR	G	4002	-	41,41,41	2.74	6 (14%)	56,56,56	6.43	28 (50%)
14	CLA	b	1239	-	63,73,73	2.25	18 (28%)	74,113,113	2.62	32 (43%)
14	CLA	A	1012	-	63,73,73	2.20	16 (25%)	74,113,113	2.52	26 (35%)
14	CLA	U	1502	-	58,68,73	2.27	18 (31%)	68,107,113	2.61	22 (32%)
14	CLA	A	1138	-	58,68,73	2.35	17 (29%)	68,107,113	2.51	24 (35%)
14	CLA	b	1211	-	63,73,73	2.24	19 (30%)	74,113,113	2.51	23 (31%)
14	CLA	A	1129	-	48,58,73	2.54	18 (37%)	56,95,113	2.79	23 (41%)
18	BCR	l	4019	-	41,41,41	2.76	6 (14%)	56,56,56	7.19	28 (50%)
14	CLA	L	1503	-	63,73,73	2.24	18 (28%)	74,113,113	2.49	25 (33%)
14	CLA	A	1123	-	58,68,73	2.35	18 (31%)	68,107,113	2.55	25 (36%)
16	PQN	A	2001	-	34,34,34	1.47	2 (5%)	43,45,45	1.28	6 (13%)
14	CLA	l	1502	-	58,68,73	2.28	18 (31%)	68,107,113	2.61	22 (32%)
19	LHG	H	5004	-	43,43,48	0.96	2 (4%)	46,49,54	1.14	3 (6%)
15	F6C	A	1121	-	47,54,74	3.09	21 (44%)	48,90,114	3.94	28 (58%)
14	CLA	b	1216	-	63,73,73	2.22	18 (28%)	74,113,113	2.40	25 (33%)
14	CLA	H	1209	-	43,53,73	2.58	18 (41%)	50,89,113	2.90	21 (42%)
14	CLA	B	1235	-	58,68,73	2.34	18 (31%)	68,107,113	2.59	25 (36%)
14	CLA	H	1214	-	63,73,73	2.23	19 (30%)	74,113,113	2.47	27 (36%)
14	CLA	G	1114	-	43,53,73	2.60	19 (44%)	50,89,113	2.79	20 (40%)
14	CLA	H	1227	-	43,53,73	2.62	18 (41%)	50,89,113	2.75	22 (44%)
14	CLA	A	1126	-	58,68,73	2.33	17 (29%)	68,107,113	2.53	25 (36%)
13	CL0	A	1011	-	63,73,73	2.19	19 (30%)	74,113,113	2.52	24 (32%)
14	CLA	A	1140	-	63,73,73	2.22	18 (28%)	74,113,113	2.43	23 (31%)
14	CLA	G	1127	-	63,73,73	2.23	18 (28%)	74,113,113	2.50	22 (29%)
14	CLA	A	1134	-	43,53,73	2.69	19 (44%)	50,89,113	2.85	21 (42%)
14	CLA	a	1116	-	53,63,73	2.44	18 (33%)	62,101,113	2.69	27 (43%)
14	CLA	G	1133	-	58,68,73	2.34	18 (31%)	68,107,113	2.66	25 (36%)
14	CLA	H	1023	-	63,73,73	2.19	17 (26%)	74,113,113	2.64	26 (35%)
14	CLA	B	1215	-	58,68,73	2.27	17 (29%)	68,107,113	2.49	21 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMT	G	6001	-	32,32,36	1.25	5 (15%)	43,43,47	1.06	2 (4%)
18	BCR	G	4003	-	41,41,41	2.69	6 (14%)	56,56,56	6.71	22 (39%)
14	CLA	b	1229	-	58,68,73	2.34	18 (31%)	68,107,113	2.65	25 (36%)
14	CLA	a	1125	-	63,73,73	2.19	18 (28%)	74,113,113	2.58	24 (32%)
13	CL0	a	1011	-	63,73,73	2.19	19 (30%)	74,113,113	2.53	25 (33%)
14	CLA	H	1232	-	43,53,73	2.59	17 (39%)	50,89,113	2.78	21 (42%)
16	PQN	H	2002	-	34,34,34	1.51	2 (5%)	43,45,45	1.28	4 (9%)
14	CLA	a	1102	-	58,68,73	2.34	17 (29%)	68,107,113	2.59	23 (33%)
14	CLA	A	1107	1	43,53,73	2.55	17 (39%)	50,89,113	2.74	21 (42%)
14	CLA	b	1215	-	58,68,73	2.28	17 (29%)	68,107,113	2.49	21 (30%)
15	F6C	B	1207	-	67,74,74	2.65	22 (32%)	72,114,114	3.54	30 (41%)
18	BCR	B	4010	-	41,41,41	2.86	6 (14%)	56,56,56	6.84	20 (35%)
14	CLA	G	1136	-	63,73,73	2.20	17 (26%)	74,113,113	2.49	23 (31%)
14	CLA	L	1502	-	58,68,73	2.28	18 (31%)	68,107,113	2.61	22 (32%)
14	CLA	b	1233	-	43,53,73	2.60	19 (44%)	50,89,113	2.81	18 (36%)
17	SF4	C	3003	3	0,12,12	-	-	-	-	-
18	BCR	B	4013	-	41,41,41	2.62	6 (14%)	56,56,56	6.87	21 (37%)
14	CLA	B	1220	-	53,63,73	2.44	18 (33%)	62,101,113	2.81	26 (41%)
18	BCR	H	4014	-	41,41,41	2.81	8 (19%)	56,56,56	6.59	24 (42%)
18	BCR	b	4017	-	41,41,41	2.79	7 (17%)	56,56,56	6.89	20 (35%)
18	BCR	B	4014	-	41,41,41	2.81	8 (19%)	56,56,56	6.59	24 (42%)
21	LMT	A	6002	-	29,29,36	1.36	6 (20%)	40,40,47	1.18	4 (10%)
18	BCR	A	4003	-	41,41,41	2.69	7 (17%)	56,56,56	6.71	22 (39%)
14	CLA	B	1203	-	63,73,73	2.18	18 (28%)	74,113,113	2.54	22 (29%)
14	CLA	b	1210	-	63,73,73	2.25	20 (31%)	74,113,113	2.66	28 (37%)
14	CLA	A	1135	-	58,68,73	2.32	17 (29%)	68,107,113	2.60	25 (36%)
15	F6C	b	1207	-	67,74,74	2.65	22 (32%)	72,114,114	3.53	30 (41%)
19	LHG	b	5004	-	43,43,48	0.97	2 (4%)	46,49,54	1.14	3 (6%)
14	CLA	H	1224	-	63,73,73	2.22	17 (26%)	74,113,113	2.46	23 (31%)
14	CLA	H	1021	-	63,73,73	2.21	19 (30%)	74,113,113	2.47	25 (33%)
18	BCR	a	4003	-	41,41,41	2.69	6 (14%)	56,56,56	6.70	22 (39%)
14	CLA	A	1104	-	63,73,73	2.18	18 (28%)	74,113,113	2.65	24 (32%)
18	BCR	V	4021	-	41,41,41	2.77	7 (17%)	56,56,56	6.82	16 (28%)
18	BCR	B	4009	-	41,41,41	2.75	7 (17%)	56,56,56	6.58	20 (35%)
14	CLA	G	1139	-	43,53,73	2.56	17 (39%)	50,89,113	2.76	22 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	1213	-	63,73,73	2.24	18 (28%)	74,113,113	2.50	23 (31%)
15	F6C	G	1121	-	47,54,74	3.08	21 (44%)	48,90,114	3.95	28 (58%)
14	CLA	H	1219	-	43,53,73	2.59	19 (44%)	50,89,113	2.77	21 (42%)
14	CLA	A	1118	-	53,63,73	2.44	18 (33%)	62,101,113	2.69	28 (45%)
14	CLA	A	1130	-	53,63,73	2.44	17 (32%)	62,101,113	2.65	25 (40%)
14	CLA	G	1132	-	63,73,73	2.20	17 (26%)	74,113,113	2.60	24 (32%)
15	F6C	B	1238	-	67,74,74	2.63	20 (29%)	72,114,114	3.42	32 (44%)
14	CLA	G	1124	-	53,63,73	2.41	17 (32%)	62,101,113	2.75	25 (40%)
14	CLA	A	1013	-	58,68,73	2.29	17 (29%)	68,107,113	2.64	25 (36%)
14	CLA	G	1105	-	43,53,73	2.60	19 (44%)	50,89,113	2.85	21 (42%)
18	BCR	i	4018	-	41,41,41	2.84	7 (17%)	56,56,56	6.73	25 (44%)
14	CLA	a	1126	-	58,68,73	2.32	17 (29%)	68,107,113	2.52	25 (36%)
14	CLA	A	1122	-	53,63,73	2.41	18 (33%)	62,101,113	2.68	26 (41%)
18	BCR	a	4008	-	41,41,41	2.90	6 (14%)	56,56,56	6.61	20 (35%)
14	CLA	B	1239	-	63,73,73	2.25	18 (28%)	74,113,113	2.61	32 (43%)
14	CLA	B	1233	-	43,53,73	2.60	18 (41%)	50,89,113	2.81	19 (38%)
14	CLA	b	1219	-	43,53,73	2.58	18 (41%)	50,89,113	2.77	21 (42%)
14	CLA	a	1134	-	43,53,73	2.69	19 (44%)	50,89,113	2.84	22 (44%)
14	CLA	G	1129	-	48,58,73	2.55	18 (37%)	56,95,113	2.80	23 (41%)
18	BCR	U	4022	-	41,41,41	2.85	7 (17%)	56,56,56	6.64	22 (39%)
14	CLA	G	1108	-	43,53,73	2.60	18 (41%)	50,89,113	2.78	21 (42%)
14	CLA	A	1120	-	43,53,73	2.52	17 (39%)	50,89,113	2.87	20 (40%)
14	CLA	A	1116	-	53,63,73	2.44	18 (33%)	62,101,113	2.70	27 (43%)
17	SF4	a	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	H	1223	-	63,73,73	2.21	18 (28%)	74,113,113	2.57	27 (36%)
14	CLA	B	1231	2	53,63,73	2.43	18 (33%)	62,101,113	2.65	23 (37%)
14	CLA	H	1217	-	53,63,73	2.42	18 (33%)	62,101,113	2.70	22 (35%)
18	BCR	b	4016	-	41,41,41	2.74	6 (14%)	56,56,56	6.81	19 (33%)
14	CLA	b	1222	-	63,73,73	2.24	18 (28%)	74,113,113	2.55	27 (36%)
17	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	A	1128	-	58,68,73	2.33	18 (31%)	68,107,113	2.62	24 (35%)
14	CLA	b	1205	-	63,73,73	2.18	17 (26%)	74,113,113	2.52	23 (31%)
14	CLA	b	1203	-	63,73,73	2.18	18 (28%)	74,113,113	2.55	23 (31%)
14	CLA	A	1111	-	58,68,73	2.31	18 (31%)	68,107,113	4.62	27 (39%)
18	BCR	i	4020	-	41,41,41	2.94	8 (19%)	56,56,56	6.92	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	H	1205	-	63,73,73	2.18	17 (26%)	74,113,113	2.52	24 (32%)
14	CLA	b	1217	-	53,63,73	2.42	18 (33%)	62,101,113	2.71	22 (35%)
14	CLA	a	1105	-	43,53,73	2.60	19 (44%)	50,89,113	2.85	21 (42%)
15	F6C	H	1230	-	47,54,74	3.08	24 (51%)	48,90,114	3.96	25 (52%)
14	CLA	b	1206	2	43,53,73	2.54	15 (34%)	50,89,113	2.70	20 (40%)
18	BCR	H	4016	-	41,41,41	2.74	6 (14%)	56,56,56	6.81	19 (33%)
18	BCR	B	4005	-	41,41,41	2.77	7 (17%)	56,56,56	6.74	23 (41%)
14	CLA	b	1214	-	63,73,73	2.24	19 (30%)	74,113,113	2.47	27 (36%)
14	CLA	b	1223	-	63,73,73	2.21	18 (28%)	74,113,113	2.56	27 (36%)
14	CLA	G	1110	-	43,53,73	2.57	17 (39%)	50,89,113	2.78	20 (40%)
14	CLA	B	1211	-	63,73,73	2.24	19 (30%)	74,113,113	2.51	23 (31%)
14	CLA	G	1116	-	53,63,73	2.44	18 (33%)	62,101,113	2.68	27 (43%)
14	CLA	A	1139	-	43,53,73	2.56	17 (39%)	50,89,113	2.77	22 (44%)
14	CLA	a	1138	-	58,68,73	2.35	17 (29%)	68,107,113	2.50	22 (32%)
18	BCR	G	4007	-	41,41,41	2.87	8 (19%)	56,56,56	6.72	24 (42%)
14	CLA	A	1132	-	63,73,73	2.20	17 (26%)	74,113,113	2.60	24 (32%)
14	CLA	b	1236	-	43,53,73	2.52	17 (39%)	50,89,113	2.82	19 (38%)
14	CLA	A	1124	-	53,63,73	2.41	17 (32%)	62,101,113	2.74	25 (40%)
20	LMG	l	5007	-	50,50,55	1.45	7 (14%)	58,58,63	1.10	2 (3%)
17	SF4	G	3001	2,1	0,12,12	-	-	-	-	-
20	LMG	H	5002	-	46,46,55	1.34	5 (10%)	54,54,63	1.27	4 (7%)
21	LMT	A	6001	-	32,32,36	1.25	5 (15%)	43,43,47	1.06	2 (4%)
14	CLA	A	1101	-	43,53,73	2.51	17 (39%)	50,89,113	2.85	20 (40%)
19	LHG	B	5004	-	43,43,48	0.96	2 (4%)	46,49,54	1.14	3 (6%)
14	CLA	a	1013	-	58,68,73	2.29	17 (29%)	68,107,113	2.63	24 (35%)
14	CLA	a	1130	-	53,63,73	2.44	17 (32%)	62,101,113	2.65	25 (40%)
20	LMG	U	5007	-	50,50,55	1.45	7 (14%)	58,58,63	1.10	2 (3%)
14	CLA	B	1222	-	63,73,73	2.25	18 (28%)	74,113,113	2.56	27 (36%)
14	CLA	A	1113	-	43,53,73	2.55	17 (39%)	50,89,113	2.80	23 (46%)
18	BCR	B	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.65	25 (44%)
14	CLA	b	1213	-	63,73,73	2.24	18 (28%)	74,113,113	2.50	23 (31%)
14	CLA	A	1110	-	43,53,73	2.56	17 (39%)	50,89,113	2.77	20 (40%)
14	CLA	H	1022	-	63,73,73	2.19	17 (26%)	74,113,113	2.52	27 (36%)
14	CLA	B	1219	-	43,53,73	2.59	19 (44%)	50,89,113	2.77	21 (42%)
14	CLA	A	1125	-	63,73,73	2.19	17 (26%)	74,113,113	2.58	24 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	1117	-	63,73,73	2.20	17 (26%)	74,113,113	2.54	27 (36%)
14	CLA	B	1023	-	63,73,73	2.19	17 (26%)	74,113,113	2.64	26 (35%)
14	CLA	H	1228	-	53,63,73	2.44	20 (37%)	62,101,113	2.71	26 (41%)
14	CLA	G	1012	-	63,73,73	2.20	16 (25%)	74,113,113	2.52	26 (35%)
14	CLA	G	1138	-	58,68,73	2.35	17 (29%)	68,107,113	2.51	24 (35%)
14	CLA	B	1201	-	53,63,73	2.43	18 (33%)	62,101,113	2.78	23 (37%)
16	PQN	a	2001	-	34,34,34	1.46	2 (5%)	43,45,45	1.28	6 (13%)
14	CLA	a	1122	-	53,63,73	2.41	18 (33%)	62,101,113	2.67	26 (41%)
14	CLA	b	1234	-	63,73,73	2.19	18 (28%)	74,113,113	2.45	22 (29%)
14	CLA	G	1101	-	43,53,73	2.51	17 (39%)	50,89,113	2.85	20 (40%)
14	CLA	H	1218	-	43,53,73	2.64	17 (39%)	50,89,113	2.73	19 (38%)
14	CLA	H	1233	-	43,53,73	2.60	19 (44%)	50,89,113	2.81	19 (38%)
14	CLA	A	1112	-	53,63,73	2.43	18 (33%)	62,101,113	2.67	25 (40%)
18	BCR	B	4016	-	41,41,41	2.74	6 (14%)	56,56,56	6.81	18 (32%)
14	CLA	H	1212	-	43,53,73	2.55	17 (39%)	50,89,113	2.79	19 (38%)
14	CLA	A	1131	-	58,68,73	2.32	17 (29%)	68,107,113	2.54	22 (32%)
15	F6C	H	1237	-	67,74,74	2.60	19 (28%)	72,114,114	3.39	29 (40%)
14	CLA	b	1023	-	63,73,73	2.19	17 (26%)	74,113,113	2.64	26 (35%)
13	CL0	G	1011	-	63,73,73	2.20	19 (30%)	74,113,113	2.52	24 (32%)
14	CLA	G	1140	-	63,73,73	2.22	18 (28%)	74,113,113	2.43	24 (32%)
18	BCR	R	4020	-	41,41,41	2.94	8 (19%)	56,56,56	6.92	22 (39%)
15	F6C	H	1207	-	67,74,74	2.66	22 (32%)	72,114,114	3.53	30 (41%)
18	BCR	a	4007	-	41,41,41	2.87	8 (19%)	56,56,56	6.72	24 (42%)
14	CLA	a	1127	-	63,73,73	2.23	18 (28%)	74,113,113	2.50	22 (29%)
18	BCR	G	4008	-	41,41,41	2.90	7 (17%)	56,56,56	6.61	20 (35%)
14	CLA	b	1231	2	53,63,73	2.44	18 (33%)	62,101,113	2.66	23 (37%)
14	CLA	B	1210	-	63,73,73	2.24	19 (30%)	74,113,113	2.66	27 (36%)
14	CLA	a	1135	-	58,68,73	2.33	18 (31%)	68,107,113	2.60	25 (36%)
14	CLA	B	1223	-	63,73,73	2.21	18 (28%)	74,113,113	2.57	28 (37%)
14	CLA	a	1106	-	58,68,73	2.31	18 (31%)	68,107,113	2.68	25 (36%)
15	F6C	b	1238	-	67,74,74	2.62	20 (29%)	72,114,114	3.42	32 (44%)
14	CLA	G	1115	-	63,73,73	2.25	18 (28%)	74,113,113	2.62	26 (35%)
18	BCR	U	4019	-	41,41,41	2.75	6 (14%)	56,56,56	7.19	28 (50%)
18	BCR	l	4022	-	41,41,41	2.85	7 (17%)	56,56,56	6.65	22 (39%)
14	CLA	G	1130	-	53,63,73	2.43	17 (32%)	62,101,113	2.65	26 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMG	A	5005	-	46,46,55	1.38	5 (10%)	54,54,63	1.10	2 (3%)
18	BCR	B	4017	-	41,41,41	2.80	7 (17%)	56,56,56	6.90	20 (35%)
14	CLA	b	1021	-	63,73,73	2.20	19 (30%)	74,113,113	2.48	24 (32%)
18	BCR	H	4010	-	41,41,41	2.86	6 (14%)	56,56,56	6.84	20 (35%)
14	CLA	G	1134	-	43,53,73	2.68	19 (44%)	50,89,113	2.84	21 (42%)
17	SF4	N	3002	3	0,12,12	-	-	-	-	-
14	CLA	U	1501	10	63,73,73	2.22	18 (28%)	74,113,113	2.42	23 (31%)
20	LMG	I	5006	-	37,37,55	1.13	3 (8%)	45,45,63	1.21	4 (8%)
14	CLA	H	1204	-	63,73,73	2.23	16 (25%)	74,113,113	2.45	26 (35%)
14	CLA	a	1104	-	63,73,73	2.18	18 (28%)	74,113,113	2.64	24 (32%)
14	CLA	a	1114	-	43,53,73	2.60	19 (44%)	50,89,113	2.79	20 (40%)
14	CLA	a	1120	-	43,53,73	2.53	17 (39%)	50,89,113	2.88	20 (40%)
14	CLA	B	1021	-	63,73,73	2.21	19 (30%)	74,113,113	2.47	24 (32%)
18	BCR	b	4010	-	41,41,41	2.86	6 (14%)	56,56,56	6.84	20 (35%)
18	BCR	b	4006	-	41,41,41	2.67	6 (14%)	56,56,56	6.76	21 (37%)
14	CLA	a	1108	-	43,53,73	2.60	18 (41%)	50,89,113	2.78	21 (42%)
18	BCR	L	4022	-	41,41,41	2.85	6 (14%)	56,56,56	6.64	22 (39%)
14	CLA	A	1136	-	63,73,73	2.21	17 (26%)	74,113,113	2.50	23 (31%)
14	CLA	H	1229	-	58,68,73	2.34	19 (32%)	68,107,113	2.64	25 (36%)
14	CLA	a	1137	-	48,58,73	2.55	18 (37%)	56,95,113	2.95	25 (44%)
14	CLA	a	1109	-	63,73,73	2.23	18 (28%)	74,113,113	2.52	25 (33%)
14	CLA	b	1225	-	63,73,73	2.26	18 (28%)	74,113,113	2.38	21 (28%)
19	LHG	A	5001	-	41,41,48	0.99	2 (4%)	44,47,54	1.12	3 (6%)
14	CLA	G	1122	-	53,63,73	2.41	18 (33%)	62,101,113	2.68	26 (41%)
15	F6C	H	1238	-	67,74,74	2.62	20 (29%)	72,114,114	3.42	32 (44%)
18	BCR	A	4011	-	41,41,41	2.80	7 (17%)	56,56,56	6.69	28 (50%)
14	CLA	B	1228	-	53,63,73	2.44	20 (37%)	62,101,113	2.71	26 (41%)
14	CLA	b	1208	-	63,73,73	2.24	18 (28%)	74,113,113	2.46	25 (33%)
14	CLA	A	1137	-	48,58,73	2.55	18 (37%)	56,95,113	2.94	25 (44%)
14	CLA	B	1225	-	63,73,73	2.26	18 (28%)	74,113,113	2.39	21 (28%)
14	CLA	H	1215	-	58,68,73	2.28	17 (29%)	68,107,113	2.49	21 (30%)
14	CLA	G	1135	-	58,68,73	2.32	18 (31%)	68,107,113	2.60	25 (36%)
14	CLA	b	1226	-	63,73,73	2.26	18 (28%)	74,113,113	2.43	24 (32%)
14	CLA	l	1501	10	63,73,73	2.22	18 (28%)	74,113,113	2.43	23 (31%)
14	CLA	A	1115	-	63,73,73	2.25	18 (28%)	74,113,113	2.62	26 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	1123	-	58,68,73	2.35	18 (31%)	68,107,113	2.55	25 (36%)
14	CLA	B	1236	-	43,53,73	2.52	17 (39%)	50,89,113	2.83	19 (38%)
18	BCR	b	4013	-	41,41,41	2.62	6 (14%)	56,56,56	6.87	21 (37%)
17	SF4	N	3003	3	0,12,12	-	-	-	-	-
17	SF4	c	3002	3	0,12,12	-	-	-	-	-
20	LMG	i	5006	-	37,37,55	1.13	3 (8%)	45,45,63	1.21	4 (8%)
19	LHG	a	5001	-	41,41,48	0.99	2 (4%)	44,47,54	1.11	3 (6%)
14	CLA	a	1107	1	43,53,73	2.55	17 (39%)	50,89,113	2.73	21 (42%)
14	CLA	H	1221	-	63,73,73	2.22	18 (28%)	74,113,113	2.45	25 (33%)
14	CLA	H	1234	-	63,73,73	2.19	18 (28%)	74,113,113	2.45	22 (29%)
14	CLA	H	1235	-	58,68,73	2.33	18 (31%)	68,107,113	2.59	25 (36%)
14	CLA	a	1124	-	53,63,73	2.41	17 (32%)	62,101,113	2.74	25 (40%)
14	CLA	B	1217	-	53,63,73	2.42	18 (33%)	62,101,113	2.71	22 (35%)
14	CLA	a	1140	-	63,73,73	2.22	18 (28%)	74,113,113	2.43	23 (31%)
14	CLA	B	1022	-	63,73,73	2.19	18 (28%)	74,113,113	2.51	27 (36%)
14	CLA	a	1118	-	53,63,73	2.44	18 (33%)	62,101,113	2.69	28 (45%)
15	F6C	a	1121	-	47,54,74	3.08	21 (44%)	48,90,114	3.94	28 (58%)
14	CLA	a	1111	-	58,68,73	2.31	18 (31%)	68,107,113	4.62	27 (39%)
14	CLA	G	1104	-	63,73,73	2.18	18 (28%)	74,113,113	2.65	24 (32%)
14	CLA	A	1103	-	58,68,73	2.28	18 (31%)	68,107,113	2.63	24 (35%)
21	LMT	a	6002	-	29,29,36	1.36	6 (20%)	40,40,47	1.18	4 (10%)
18	BCR	H	4013	-	41,41,41	2.62	6 (14%)	56,56,56	6.87	21 (37%)
14	CLA	x	1701	-	53,63,73	2.46	18 (33%)	62,101,113	2.67	24 (38%)
14	CLA	G	1013	-	58,68,73	2.28	17 (29%)	68,107,113	2.63	24 (35%)
14	CLA	H	1220	-	53,63,73	2.44	18 (33%)	62,101,113	2.82	26 (41%)
14	CLA	A	1102	-	58,68,73	2.34	17 (29%)	68,107,113	2.59	23 (33%)
14	CLA	G	1118	-	53,63,73	2.44	18 (33%)	62,101,113	2.69	28 (45%)
14	CLA	b	1212	-	43,53,73	2.55	17 (39%)	50,89,113	2.79	19 (38%)
18	BCR	A	4002	-	41,41,41	2.74	6 (14%)	56,56,56	6.43	28 (50%)
14	CLA	B	1218	-	43,53,73	2.64	17 (39%)	50,89,113	2.73	19 (38%)
14	CLA	a	1103	-	58,68,73	2.28	18 (31%)	68,107,113	2.63	24 (35%)
14	CLA	a	1139	-	43,53,73	2.57	17 (39%)	50,89,113	2.77	22 (44%)
18	BCR	a	4001	-	41,41,41	2.73	6 (14%)	56,56,56	6.76	23 (41%)
14	CLA	H	1211	-	63,73,73	2.24	19 (30%)	74,113,113	2.52	23 (31%)
18	BCR	H	4009	-	41,41,41	2.75	7 (17%)	56,56,56	6.58	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	1224	-	63,73,73	2.22	18 (28%)	74,113,113	2.46	23 (31%)
14	CLA	X	1701	-	53,63,73	2.46	18 (33%)	62,101,113	2.68	24 (38%)
14	CLA	G	1103	-	58,68,73	2.29	18 (31%)	68,107,113	2.63	23 (33%)
21	LMT	a	6001	-	32,32,36	1.24	5 (15%)	43,43,47	1.06	2 (4%)
18	BCR	R	4018	-	41,41,41	2.83	7 (17%)	56,56,56	6.73	25 (44%)
14	CLA	G	1117	-	63,73,73	2.20	17 (26%)	74,113,113	2.54	27 (36%)
15	F6C	B	1230	-	47,54,74	3.08	24 (51%)	48,90,114	3.96	25 (52%)
14	CLA	H	1236	-	43,53,73	2.53	17 (39%)	50,89,113	2.83	19 (38%)
14	CLA	A	1133	-	58,68,73	2.34	18 (31%)	68,107,113	2.66	25 (36%)
14	CLA	b	1202	-	58,68,73	2.24	18 (31%)	68,107,113	2.61	25 (36%)
18	BCR	m	4021	-	41,41,41	2.76	7 (17%)	56,56,56	6.81	16 (28%)
14	CLA	A	1106	-	58,68,73	2.31	18 (31%)	68,107,113	2.69	25 (36%)
14	CLA	B	1234	-	63,73,73	2.18	18 (28%)	74,113,113	2.45	22 (29%)
14	CLA	a	1128	-	58,68,73	2.33	18 (31%)	68,107,113	2.62	23 (33%)
18	BCR	B	4006	-	41,41,41	2.66	6 (14%)	56,56,56	6.77	21 (37%)
14	CLA	B	1209	-	43,53,73	2.58	18 (41%)	50,89,113	2.90	21 (42%)
14	CLA	b	1232	-	43,53,73	2.59	17 (39%)	50,89,113	2.78	21 (42%)
14	CLA	A	1109	-	63,73,73	2.22	18 (28%)	74,113,113	2.52	25 (33%)
20	LMG	b	5002	-	46,46,55	1.34	5 (10%)	54,54,63	1.27	4 (7%)
14	CLA	H	1216	-	63,73,73	2.22	18 (28%)	74,113,113	2.40	25 (33%)
14	CLA	U	1503	-	63,73,73	2.24	18 (28%)	74,113,113	2.50	26 (35%)
14	CLA	a	1115	-	63,73,73	2.25	18 (28%)	74,113,113	2.62	26 (35%)
18	BCR	L	4019	-	41,41,41	2.75	6 (14%)	56,56,56	7.19	28 (50%)
14	CLA	H	1239	-	63,73,73	2.26	18 (28%)	74,113,113	2.62	31 (41%)
14	CLA	A	1119	-	63,73,73	2.23	18 (28%)	74,113,113	2.51	25 (33%)
18	BCR	M	4021	-	41,41,41	2.77	7 (17%)	56,56,56	6.82	16 (28%)
18	BCR	A	4001	-	41,41,41	2.73	6 (14%)	56,56,56	6.76	23 (41%)
18	BCR	A	4008	-	41,41,41	2.90	7 (17%)	56,56,56	6.61	20 (35%)
14	CLA	B	1214	-	63,73,73	2.23	19 (30%)	74,113,113	2.47	27 (36%)
14	CLA	b	1221	-	63,73,73	2.22	18 (28%)	74,113,113	2.44	25 (33%)
14	CLA	b	1201	-	53,63,73	2.44	17 (32%)	62,101,113	2.78	23 (37%)
14	CLA	H	1213	-	63,73,73	2.25	18 (28%)	74,113,113	2.51	23 (31%)
14	CLA	A	1114	-	43,53,73	2.59	18 (41%)	50,89,113	2.79	20 (40%)
14	CLA	L	1501	10	63,73,73	2.22	18 (28%)	74,113,113	2.43	23 (31%)
14	CLA	a	1131	-	58,68,73	2.32	17 (29%)	68,107,113	2.53	21 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	1235	-	58,68,73	2.34	18 (31%)	68,107,113	2.59	25 (36%)
14	CLA	G	1112	-	53,63,73	2.44	18 (33%)	62,101,113	2.68	25 (40%)
14	CLA	b	1209	-	43,53,73	2.58	18 (41%)	50,89,113	2.89	21 (42%)
18	BCR	b	4005	-	41,41,41	2.77	7 (17%)	56,56,56	6.74	24 (42%)
14	CLA	G	1106	-	58,68,73	2.31	18 (31%)	68,107,113	2.68	25 (36%)
14	CLA	b	1022	-	63,73,73	2.19	17 (26%)	74,113,113	2.51	27 (36%)
16	PQN	G	2001	-	34,34,34	1.47	2 (5%)	43,45,45	1.28	6 (13%)
14	CLA	G	1113	-	43,53,73	2.55	17 (39%)	50,89,113	2.81	23 (46%)
18	BCR	H	4017	-	41,41,41	2.80	7 (17%)	56,56,56	6.90	20 (35%)
14	CLA	B	1212	-	43,53,73	2.55	17 (39%)	50,89,113	2.78	19 (38%)
14	CLA	W	1701	-	53,63,73	2.45	18 (33%)	62,101,113	2.67	24 (38%)
14	CLA	b	1228	-	53,63,73	2.45	20 (37%)	62,101,113	2.70	26 (41%)
18	BCR	I	4020	-	41,41,41	2.94	8 (19%)	56,56,56	6.92	22 (39%)
14	CLA	a	1012	-	63,73,73	2.20	16 (25%)	74,113,113	2.53	26 (35%)
14	CLA	G	1125	-	63,73,73	2.19	18 (28%)	74,113,113	2.58	24 (32%)
14	CLA	G	1120	-	43,53,73	2.53	17 (39%)	50,89,113	2.88	20 (40%)
14	CLA	H	1225	-	63,73,73	2.25	18 (28%)	74,113,113	2.38	21 (28%)
14	CLA	G	1123	-	58,68,73	2.35	18 (31%)	68,107,113	2.56	25 (36%)
14	CLA	H	1210	-	63,73,73	2.25	20 (31%)	74,113,113	2.66	28 (37%)
14	CLA	G	1126	-	58,68,73	2.32	17 (29%)	68,107,113	2.53	25 (36%)
14	CLA	b	1204	-	63,73,73	2.23	17 (26%)	74,113,113	2.45	26 (35%)
14	CLA	b	1218	-	43,53,73	2.63	17 (39%)	50,89,113	2.72	19 (38%)
14	CLA	B	1208	-	63,73,73	2.24	18 (28%)	74,113,113	2.46	25 (33%)
15	F6C	b	1237	-	67,74,74	2.59	21 (31%)	72,114,114	3.37	29 (40%)
14	CLA	a	1101	-	43,53,73	2.51	17 (39%)	50,89,113	2.86	20 (40%)
14	CLA	G	1111	-	58,68,73	2.31	18 (31%)	68,107,113	4.62	27 (39%)
14	CLA	H	1208	-	63,73,73	2.25	18 (28%)	74,113,113	2.46	24 (32%)
14	CLA	b	1224	-	63,73,73	2.22	18 (28%)	74,113,113	2.46	23 (31%)
15	F6C	B	1237	-	67,74,74	2.60	19 (28%)	72,114,114	3.38	29 (40%)
14	CLA	B	1229	-	58,68,73	2.34	19 (32%)	68,107,113	2.65	25 (36%)
14	CLA	a	1113	-	43,53,73	2.55	17 (39%)	50,89,113	2.81	22 (44%)
14	CLA	K	1401	-	43,53,73	2.64	19 (44%)	50,89,113	2.86	21 (42%)
14	CLA	H	1203	-	63,73,73	2.18	18 (28%)	74,113,113	2.55	23 (31%)
14	CLA	b	1227	-	43,53,73	2.62	18 (41%)	50,89,113	2.75	22 (44%)
14	CLA	A	1105	-	43,53,73	2.60	18 (41%)	50,89,113	2.85	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	SF4	c	3003	3	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	H	4006	-	-	10/29/63/63	0/2/2/2
20	LMG	G	5005	-	-	19/41/61/70	0/1/1/1
19	LHG	G	5001	-	-	23/46/46/53	-
14	CLA	T	1401	-	1/1/11/20	7/13/91/115	-
18	BCR	b	4004	-	-	7/29/63/63	0/2/2/2
14	CLA	a	1112	-	1/1/13/20	14/25/103/115	-
14	CLA	B	1206	2	1/1/11/20	5/13/91/115	-
16	PQN	b	2002	-	-	12/23/43/43	0/2/2/2
14	CLA	H	1201	-	1/1/13/20	7/25/103/115	-
14	CLA	H	1226	-	1/1/15/20	11/37/115/115	-
18	BCR	H	4005	-	-	4/29/63/63	0/2/2/2
14	CLA	B	1221	-	1/1/15/20	10/37/115/115	-
14	CLA	a	1110	-	1/1/11/20	5/13/91/115	-
18	BCR	G	4011	-	-	17/29/63/63	0/2/2/2
14	CLA	a	1119	-	1/1/15/20	9/37/115/115	-
14	CLA	B	1202	-	1/1/14/20	13/31/109/115	-
14	CLA	H	1222	-	1/1/15/20	17/37/115/115	-
14	CLA	G	1137	-	1/1/12/20	5/19/97/115	-
14	CLA	G	1109	-	1/1/15/20	19/37/115/115	-
14	CLA	G	1107	1	1/1/11/20	3/13/91/115	-
18	BCR	H	4004	-	-	7/29/63/63	0/2/2/2
17	SF4	C	3002	3	-	-	0/6/5/5
14	CLA	k	1401	-	1/1/11/20	7/13/91/115	-
14	CLA	a	1132	-	1/1/15/20	12/37/115/115	-
14	CLA	G	1131	-	1/1/14/20	12/31/109/115	-
14	CLA	A	1108	-	1/1/11/20	4/13/91/115	-
14	CLA	B	1232	-	1/1/11/20	2/13/91/115	-
20	LMG	a	5005	-	-	19/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	I	4018	-	-	8/29/63/63	0/2/2/2
18	BCR	G	4001	-	-	14/29/63/63	0/2/2/2
18	BCR	a	4002	-	-	6/29/63/63	0/2/2/2
14	CLA	B	1216	-	1/1/15/20	19/37/115/115	-
18	BCR	A	4007	-	-	12/29/63/63	0/2/2/2
14	CLA	a	1136	-	1/1/15/20	17/37/115/115	-
20	LMG	B	5002	-	-	13/41/61/70	0/1/1/1
20	LMG	L	5007	-	-	15/45/65/70	0/1/1/1
14	CLA	A	1117	-	1/1/15/20	19/37/115/115	-
14	CLA	B	1205	-	1/1/15/20	10/37/115/115	-
14	CLA	B	1204	-	1/1/15/20	13/37/115/115	-
18	BCR	a	4011	-	-	17/29/63/63	0/2/2/2
14	CLA	b	1220	-	1/1/13/20	10/25/103/115	-
18	BCR	b	4014	-	-	7/29/63/63	0/2/2/2
14	CLA	G	1102	-	1/1/14/20	14/31/109/115	-
21	LMT	G	6002	-	-	7/14/54/61	0/2/2/2
14	CLA	G	1119	-	1/1/15/20	9/37/115/115	-
14	CLA	H	1206	2	1/1/11/20	5/13/91/115	-
16	PQN	B	2002	-	-	12/23/43/43	0/2/2/2
15	F6C	b	1230	-	-	8/17/73/97	-
14	CLA	a	1133	-	1/1/14/20	9/31/109/115	-
14	CLA	A	1127	-	1/1/15/20	13/37/115/115	-
14	CLA	G	1128	-	1/1/14/20	15/31/109/115	-
20	LMG	R	5006	-	-	10/32/52/70	0/1/1/1
14	CLA	B	1227	-	1/1/11/20	5/13/91/115	-
14	CLA	l	1503	-	1/1/15/20	15/37/115/115	-
14	CLA	a	1129	-	1/1/12/20	5/19/97/115	-
14	CLA	H	1231	2	1/1/13/20	5/25/103/115	-
18	BCR	b	4009	-	-	8/29/63/63	0/2/2/2
14	CLA	B	1226	-	1/1/15/20	11/37/115/115	-
14	CLA	H	1202	-	1/1/14/20	13/31/109/115	-
18	BCR	G	4002	-	-	6/29/63/63	0/2/2/2
14	CLA	b	1239	-	1/1/15/20	20/37/115/115	-
14	CLA	A	1012	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	U	1502	-	1/1/14/20	9/31/109/115	-
14	CLA	A	1138	-	1/1/14/20	15/31/109/115	-
14	CLA	b	1211	-	1/1/15/20	18/37/115/115	-
14	CLA	A	1129	-	1/1/12/20	5/19/97/115	-
18	BCR	l	4019	-	-	12/29/63/63	0/2/2/2
14	CLA	L	1503	-	1/1/15/20	15/37/115/115	-
14	CLA	A	1123	-	1/1/14/20	13/31/109/115	-
16	PQN	A	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	l	1502	-	1/1/14/20	9/31/109/115	-
19	LHG	H	5004	-	-	25/48/48/53	-
15	F6C	A	1121	-	-	9/17/73/97	-
14	CLA	b	1216	-	1/1/15/20	19/37/115/115	-
14	CLA	H	1209	-	1/1/11/20	3/13/91/115	-
14	CLA	B	1235	-	1/1/14/20	12/31/109/115	-
14	CLA	H	1214	-	1/1/15/20	15/37/115/115	-
14	CLA	G	1114	-	1/1/11/20	9/13/91/115	-
14	CLA	H	1227	-	1/1/11/20	5/13/91/115	-
14	CLA	A	1126	-	1/1/14/20	19/31/109/115	-
13	CL0	A	1011	-	3/3/20/25	11/37/135/135	-
14	CLA	A	1140	-	1/1/15/20	21/37/115/115	-
14	CLA	G	1127	-	1/1/15/20	13/37/115/115	-
14	CLA	A	1134	-	1/1/11/20	5/13/91/115	-
14	CLA	a	1116	-	1/1/13/20	10/25/103/115	-
14	CLA	G	1133	-	1/1/14/20	9/31/109/115	-
14	CLA	H	1023	-	1/1/15/20	13/37/115/115	-
14	CLA	B	1215	-	1/1/14/20	16/31/109/115	-
21	LMT	G	6001	-	-	7/17/57/61	0/2/2/2
18	BCR	G	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	b	1229	-	1/1/14/20	14/31/109/115	-
14	CLA	a	1125	-	1/1/15/20	18/37/115/115	-
13	CL0	a	1011	-	3/3/20/25	11/37/135/135	-
14	CLA	H	1232	-	1/1/11/20	2/13/91/115	-
16	PQN	H	2002	-	-	12/23/43/43	0/2/2/2
14	CLA	a	1102	-	1/1/14/20	14/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1107	1	1/1/11/20	3/13/91/115	-
14	CLA	b	1215	-	1/1/14/20	16/31/109/115	-
15	F6C	B	1207	-	-	20/41/97/97	-
18	BCR	B	4010	-	-	10/29/63/63	0/2/2/2
14	CLA	G	1136	-	1/1/15/20	17/37/115/115	-
14	CLA	L	1502	-	1/1/14/20	9/31/109/115	-
14	CLA	b	1233	-	1/1/11/20	5/13/91/115	-
17	SF4	C	3003	3	-	-	0/6/5/5
18	BCR	B	4013	-	-	11/29/63/63	0/2/2/2
14	CLA	B	1220	-	1/1/13/20	10/25/103/115	-
18	BCR	H	4014	-	-	7/29/63/63	0/2/2/2
18	BCR	b	4017	-	-	13/29/63/63	0/2/2/2
18	BCR	B	4014	-	-	7/29/63/63	0/2/2/2
21	LMT	A	6002	-	-	8/14/54/61	0/2/2/2
18	BCR	A	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	B	1203	-	1/1/15/20	17/37/115/115	-
14	CLA	b	1210	-	1/1/15/20	14/37/115/115	-
14	CLA	A	1135	-	1/1/14/20	14/31/109/115	-
15	F6C	b	1207	-	-	20/41/97/97	-
19	LHG	b	5004	-	-	25/48/48/53	-
14	CLA	H	1224	-	1/1/15/20	14/37/115/115	-
14	CLA	H	1021	-	1/1/15/20	20/37/115/115	-
18	BCR	a	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	A	1104	-	1/1/15/20	9/37/115/115	-
18	BCR	V	4021	-	-	18/29/63/63	0/2/2/2
18	BCR	B	4009	-	-	8/29/63/63	0/2/2/2
14	CLA	G	1139	-	1/1/11/20	3/13/91/115	-
14	CLA	B	1213	-	1/1/15/20	16/37/115/115	-
15	F6C	G	1121	-	-	9/17/73/97	-
14	CLA	H	1219	-	1/1/11/20	3/13/91/115	-
14	CLA	A	1118	-	1/1/13/20	10/25/103/115	-
14	CLA	A	1130	-	1/1/13/20	9/25/103/115	-
14	CLA	G	1132	-	1/1/15/20	12/37/115/115	-
15	F6C	B	1238	-	-	16/41/97/97	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1124	-	1/1/13/20	9/25/103/115	-
14	CLA	A	1013	-	1/1/14/20	12/31/109/115	-
14	CLA	G	1105	-	1/1/11/20	4/13/91/115	-
18	BCR	i	4018	-	-	8/29/63/63	0/2/2/2
14	CLA	a	1126	-	1/1/14/20	19/31/109/115	-
14	CLA	A	1122	-	1/1/13/20	13/25/103/115	-
18	BCR	a	4008	-	-	12/29/63/63	0/2/2/2
14	CLA	B	1239	-	1/1/15/20	20/37/115/115	-
14	CLA	B	1233	-	1/1/11/20	5/13/91/115	-
14	CLA	b	1219	-	1/1/11/20	3/13/91/115	-
14	CLA	a	1134	-	1/1/11/20	5/13/91/115	-
14	CLA	G	1129	-	1/1/12/20	5/19/97/115	-
18	BCR	U	4022	-	-	6/29/63/63	0/2/2/2
14	CLA	G	1108	-	1/1/11/20	4/13/91/115	-
14	CLA	A	1120	-	1/1/11/20	7/13/91/115	-
14	CLA	A	1116	-	1/1/13/20	10/25/103/115	-
17	SF4	a	3001	2,1	-	-	0/6/5/5
14	CLA	H	1223	-	1/1/15/20	17/37/115/115	-
14	CLA	B	1231	2	1/1/13/20	5/25/103/115	-
14	CLA	H	1217	-	1/1/13/20	11/25/103/115	-
18	BCR	b	4016	-	-	10/29/63/63	0/2/2/2
14	CLA	b	1222	-	1/1/15/20	17/37/115/115	-
17	SF4	A	3001	2,1	-	-	0/6/5/5
14	CLA	A	1128	-	1/1/14/20	15/31/109/115	-
14	CLA	b	1205	-	1/1/15/20	10/37/115/115	-
14	CLA	b	1203	-	1/1/15/20	17/37/115/115	-
14	CLA	A	1111	-	1/1/14/20	13/31/109/115	-
18	BCR	i	4020	-	-	12/29/63/63	0/2/2/2
14	CLA	H	1205	-	1/1/15/20	10/37/115/115	-
14	CLA	b	1217	-	1/1/13/20	11/25/103/115	-
14	CLA	a	1105	-	1/1/11/20	4/13/91/115	-
15	F6C	H	1230	-	-	8/17/73/97	-
14	CLA	b	1206	2	1/1/11/20	5/13/91/115	-
18	BCR	H	4016	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	B	4005	-	-	4/29/63/63	0/2/2/2
14	CLA	b	1214	-	1/1/15/20	15/37/115/115	-
14	CLA	b	1223	-	1/1/15/20	17/37/115/115	-
14	CLA	G	1110	-	1/1/11/20	5/13/91/115	-
14	CLA	B	1211	-	1/1/15/20	18/37/115/115	-
14	CLA	G	1116	-	1/1/13/20	10/25/103/115	-
14	CLA	A	1139	-	1/1/11/20	3/13/91/115	-
14	CLA	a	1138	-	1/1/14/20	15/31/109/115	-
18	BCR	G	4007	-	-	12/29/63/63	0/2/2/2
14	CLA	A	1132	-	1/1/15/20	12/37/115/115	-
14	CLA	b	1236	-	1/1/11/20	3/13/91/115	-
14	CLA	A	1124	-	1/1/13/20	9/25/103/115	-
20	LMG	l	5007	-	-	14/45/65/70	0/1/1/1
17	SF4	G	3001	2,1	-	-	0/6/5/5
20	LMG	H	5002	-	-	12/41/61/70	0/1/1/1
21	LMT	A	6001	-	-	6/17/57/61	0/2/2/2
14	CLA	A	1101	-	1/1/11/20	6/13/91/115	-
19	LHG	B	5004	-	-	25/48/48/53	-
14	CLA	a	1013	-	1/1/14/20	12/31/109/115	-
14	CLA	a	1130	-	1/1/13/20	9/25/103/115	-
20	LMG	U	5007	-	-	14/45/65/70	0/1/1/1
14	CLA	B	1222	-	1/1/15/20	17/37/115/115	-
14	CLA	A	1113	-	1/1/11/20	7/13/91/115	-
18	BCR	B	4004	-	-	7/29/63/63	0/2/2/2
14	CLA	b	1213	-	1/1/15/20	16/37/115/115	-
14	CLA	A	1110	-	1/1/11/20	5/13/91/115	-
14	CLA	H	1022	-	1/1/15/20	17/37/115/115	-
14	CLA	B	1219	-	1/1/11/20	3/13/91/115	-
14	CLA	A	1125	-	1/1/15/20	18/37/115/115	-
14	CLA	a	1117	-	1/1/15/20	19/37/115/115	-
14	CLA	B	1023	-	1/1/15/20	13/37/115/115	-
14	CLA	H	1228	-	1/1/13/20	14/25/103/115	-
14	CLA	G	1012	-	1/1/15/20	9/37/115/115	-
14	CLA	G	1138	-	1/1/14/20	15/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	1201	-	1/1/13/20	7/25/103/115	-
16	PQN	a	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	a	1122	-	1/1/13/20	13/25/103/115	-
14	CLA	b	1234	-	1/1/15/20	16/37/115/115	-
14	CLA	G	1101	-	1/1/11/20	6/13/91/115	-
14	CLA	H	1218	-	1/1/11/20	6/13/91/115	-
14	CLA	H	1233	-	1/1/11/20	5/13/91/115	-
14	CLA	A	1112	-	1/1/13/20	14/25/103/115	-
18	BCR	B	4016	-	-	10/29/63/63	0/2/2/2
14	CLA	H	1212	-	1/1/11/20	4/13/91/115	-
14	CLA	A	1131	-	1/1/14/20	12/31/109/115	-
15	F6C	H	1237	-	-	18/41/97/97	-
14	CLA	b	1023	-	1/1/15/20	13/37/115/115	-
13	CL0	G	1011	-	3/3/20/25	11/37/135/135	-
14	CLA	G	1140	-	1/1/15/20	21/37/115/115	-
18	BCR	R	4020	-	-	12/29/63/63	0/2/2/2
15	F6C	H	1207	-	-	20/41/97/97	-
18	BCR	a	4007	-	-	12/29/63/63	0/2/2/2
14	CLA	a	1127	-	1/1/15/20	13/37/115/115	-
18	BCR	G	4008	-	-	12/29/63/63	0/2/2/2
14	CLA	b	1231	2	1/1/13/20	5/25/103/115	-
14	CLA	B	1210	-	1/1/15/20	14/37/115/115	-
14	CLA	a	1135	-	1/1/14/20	14/31/109/115	-
14	CLA	B	1223	-	1/1/15/20	17/37/115/115	-
14	CLA	a	1106	-	1/1/14/20	13/31/109/115	-
15	F6C	b	1238	-	-	16/41/97/97	-
14	CLA	G	1115	-	1/1/15/20	20/37/115/115	-
18	BCR	U	4019	-	-	12/29/63/63	0/2/2/2
18	BCR	l	4022	-	-	6/29/63/63	0/2/2/2
14	CLA	G	1130	-	1/1/13/20	9/25/103/115	-
20	LMG	A	5005	-	-	19/41/61/70	0/1/1/1
18	BCR	B	4017	-	-	13/29/63/63	0/2/2/2
14	CLA	b	1021	-	1/1/15/20	20/37/115/115	-
18	BCR	H	4010	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1134	-	1/1/11/20	5/13/91/115	-
17	SF4	N	3002	3	-	-	0/6/5/5
14	CLA	U	1501	10	1/1/15/20	12/37/115/115	-
20	LMG	I	5006	-	-	10/32/52/70	0/1/1/1
14	CLA	H	1204	-	1/1/15/20	14/37/115/115	-
14	CLA	a	1104	-	1/1/15/20	9/37/115/115	-
14	CLA	a	1114	-	1/1/11/20	9/13/91/115	-
14	CLA	a	1120	-	1/1/11/20	7/13/91/115	-
14	CLA	B	1021	-	1/1/15/20	20/37/115/115	-
18	BCR	b	4010	-	-	10/29/63/63	0/2/2/2
18	BCR	b	4006	-	-	10/29/63/63	0/2/2/2
14	CLA	a	1108	-	1/1/11/20	4/13/91/115	-
18	BCR	L	4022	-	-	6/29/63/63	0/2/2/2
14	CLA	A	1136	-	1/1/15/20	17/37/115/115	-
14	CLA	H	1229	-	1/1/14/20	14/31/109/115	-
14	CLA	a	1137	-	1/1/12/20	5/19/97/115	-
14	CLA	a	1109	-	1/1/15/20	19/37/115/115	-
14	CLA	b	1225	-	1/1/15/20	14/37/115/115	-
19	LHG	A	5001	-	-	23/46/46/53	-
14	CLA	G	1122	-	1/1/13/20	12/25/103/115	-
15	F6C	H	1238	-	-	16/41/97/97	-
18	BCR	A	4011	-	-	17/29/63/63	0/2/2/2
14	CLA	B	1228	-	1/1/13/20	14/25/103/115	-
14	CLA	b	1208	-	1/1/15/20	16/37/115/115	-
14	CLA	A	1137	-	1/1/12/20	5/19/97/115	-
14	CLA	B	1225	-	1/1/15/20	14/37/115/115	-
14	CLA	H	1215	-	1/1/14/20	16/31/109/115	-
14	CLA	G	1135	-	1/1/14/20	14/31/109/115	-
14	CLA	b	1226	-	1/1/15/20	11/37/115/115	-
14	CLA	l	1501	10	1/1/15/20	12/37/115/115	-
14	CLA	A	1115	-	1/1/15/20	20/37/115/115	-
14	CLA	a	1123	-	1/1/14/20	13/31/109/115	-
14	CLA	B	1236	-	1/1/11/20	3/13/91/115	-
18	BCR	b	4013	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SF4	N	3003	3	-	-	0/6/5/5
17	SF4	c	3002	3	-	-	0/6/5/5
20	LMG	i	5006	-	-	10/32/52/70	0/1/1/1
19	LHG	a	5001	-	-	23/46/46/53	-
14	CLA	a	1107	1	1/1/11/20	3/13/91/115	-
14	CLA	H	1221	-	1/1/15/20	11/37/115/115	-
14	CLA	H	1234	-	1/1/15/20	16/37/115/115	-
14	CLA	H	1235	-	1/1/14/20	12/31/109/115	-
14	CLA	a	1124	-	1/1/13/20	9/25/103/115	-
14	CLA	B	1217	-	1/1/13/20	11/25/103/115	-
14	CLA	a	1140	-	1/1/15/20	21/37/115/115	-
14	CLA	B	1022	-	1/1/15/20	17/37/115/115	-
14	CLA	a	1118	-	1/1/13/20	10/25/103/115	-
15	F6C	a	1121	-	-	9/17/73/97	-
14	CLA	a	1111	-	1/1/14/20	13/31/109/115	-
14	CLA	G	1104	-	1/1/15/20	9/37/115/115	-
14	CLA	A	1103	-	1/1/14/20	13/31/109/115	-
21	LMT	a	6002	-	-	8/14/54/61	0/2/2/2
18	BCR	H	4013	-	-	11/29/63/63	0/2/2/2
14	CLA	x	1701	-	1/1/13/20	11/25/103/115	-
14	CLA	G	1013	-	1/1/14/20	12/31/109/115	-
14	CLA	H	1220	-	1/1/13/20	10/25/103/115	-
14	CLA	A	1102	-	1/1/14/20	14/31/109/115	-
14	CLA	G	1118	-	1/1/13/20	10/25/103/115	-
14	CLA	b	1212	-	1/1/11/20	4/13/91/115	-
18	BCR	A	4002	-	-	6/29/63/63	0/2/2/2
14	CLA	B	1218	-	1/1/11/20	6/13/91/115	-
14	CLA	a	1103	-	1/1/14/20	13/31/109/115	-
14	CLA	a	1139	-	1/1/11/20	3/13/91/115	-
18	BCR	a	4001	-	-	14/29/63/63	0/2/2/2
14	CLA	H	1211	-	1/1/15/20	18/37/115/115	-
18	BCR	H	4009	-	-	8/29/63/63	0/2/2/2
14	CLA	B	1224	-	1/1/15/20	14/37/115/115	-
14	CLA	X	1701	-	1/1/13/20	11/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1103	-	1/1/14/20	13/31/109/115	-
21	LMT	a	6001	-	-	7/17/57/61	0/2/2/2
18	BCR	R	4018	-	-	8/29/63/63	0/2/2/2
14	CLA	G	1117	-	1/1/15/20	19/37/115/115	-
15	F6C	B	1230	-	-	8/17/73/97	-
14	CLA	H	1236	-	1/1/11/20	3/13/91/115	-
14	CLA	A	1133	-	1/1/14/20	9/31/109/115	-
14	CLA	b	1202	-	1/1/14/20	13/31/109/115	-
18	BCR	m	4021	-	-	18/29/63/63	0/2/2/2
14	CLA	A	1106	-	1/1/14/20	13/31/109/115	-
14	CLA	B	1234	-	1/1/15/20	16/37/115/115	-
14	CLA	a	1128	-	1/1/14/20	15/31/109/115	-
18	BCR	B	4006	-	-	10/29/63/63	0/2/2/2
14	CLA	B	1209	-	1/1/11/20	3/13/91/115	-
14	CLA	b	1232	-	1/1/11/20	2/13/91/115	-
14	CLA	A	1109	-	1/1/15/20	19/37/115/115	-
20	LMG	b	5002	-	-	13/41/61/70	0/1/1/1
14	CLA	H	1216	-	1/1/15/20	19/37/115/115	-
14	CLA	U	1503	-	1/1/15/20	15/37/115/115	-
14	CLA	a	1115	-	1/1/15/20	20/37/115/115	-
18	BCR	L	4019	-	-	12/29/63/63	0/2/2/2
14	CLA	H	1239	-	1/1/15/20	20/37/115/115	-
14	CLA	A	1119	-	1/1/15/20	9/37/115/115	-
18	BCR	M	4021	-	-	18/29/63/63	0/2/2/2
18	BCR	A	4001	-	-	14/29/63/63	0/2/2/2
18	BCR	A	4008	-	-	12/29/63/63	0/2/2/2
14	CLA	B	1214	-	1/1/15/20	15/37/115/115	-
14	CLA	b	1221	-	1/1/15/20	10/37/115/115	-
14	CLA	b	1201	-	1/1/13/20	7/25/103/115	-
14	CLA	H	1213	-	1/1/15/20	16/37/115/115	-
14	CLA	A	1114	-	1/1/11/20	9/13/91/115	-
14	CLA	L	1501	10	1/1/15/20	12/37/115/115	-
14	CLA	a	1131	-	1/1/14/20	12/31/109/115	-
14	CLA	b	1235	-	1/1/14/20	12/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1112	-	1/1/13/20	14/25/103/115	-
14	CLA	b	1209	-	1/1/11/20	3/13/91/115	-
18	BCR	b	4005	-	-	4/29/63/63	0/2/2/2
14	CLA	G	1106	-	1/1/14/20	13/31/109/115	-
14	CLA	b	1022	-	1/1/15/20	17/37/115/115	-
16	PQN	G	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	G	1113	-	1/1/11/20	7/13/91/115	-
18	BCR	H	4017	-	-	13/29/63/63	0/2/2/2
14	CLA	B	1212	-	1/1/11/20	4/13/91/115	-
14	CLA	W	1701	-	1/1/13/20	11/25/103/115	-
14	CLA	b	1228	-	1/1/13/20	14/25/103/115	-
18	BCR	I	4020	-	-	12/29/63/63	0/2/2/2
14	CLA	a	1012	-	1/1/15/20	9/37/115/115	-
14	CLA	G	1125	-	1/1/15/20	18/37/115/115	-
14	CLA	G	1120	-	1/1/11/20	7/13/91/115	-
14	CLA	H	1225	-	1/1/15/20	14/37/115/115	-
14	CLA	G	1123	-	1/1/14/20	13/31/109/115	-
14	CLA	H	1210	-	1/1/15/20	14/37/115/115	-
14	CLA	G	1126	-	1/1/14/20	19/31/109/115	-
14	CLA	b	1204	-	1/1/15/20	14/37/115/115	-
14	CLA	b	1218	-	1/1/11/20	6/13/91/115	-
14	CLA	B	1208	-	1/1/15/20	16/37/115/115	-
15	F6C	b	1237	-	-	18/41/97/97	-
14	CLA	a	1101	-	1/1/11/20	6/13/91/115	-
14	CLA	G	1111	-	1/1/14/20	13/31/109/115	-
14	CLA	H	1208	-	1/1/15/20	16/37/115/115	-
14	CLA	b	1224	-	1/1/15/20	14/37/115/115	-
15	F6C	B	1237	-	-	18/41/97/97	-
14	CLA	B	1229	-	1/1/14/20	14/31/109/115	-
14	CLA	a	1113	-	1/1/11/20	7/13/91/115	-
14	CLA	K	1401	-	1/1/11/20	7/13/91/115	-
14	CLA	H	1203	-	1/1/15/20	17/37/115/115	-
14	CLA	b	1227	-	1/1/11/20	5/13/91/115	-
14	CLA	A	1105	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SF4	c	3003	3	-	-	0/6/5/5

The worst 5 of 5377 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	1230	F6C	C1A-CHA	9.56	1.50	1.35
15	B	1230	F6C	C1A-CHA	9.54	1.50	1.35
15	H	1230	F6C	C1A-CHA	9.53	1.50	1.35
15	b	1207	F6C	C1A-CHA	9.52	1.50	1.35
15	H	1207	F6C	C1A-CHA	9.51	1.50	1.35

The worst 5 of 7920 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	H	4010	BCR	C16-C17-C18	26.23	164.06	127.28
18	b	4010	BCR	C16-C17-C18	26.18	164.00	127.28
18	B	4010	BCR	C16-C17-C18	26.16	163.97	127.28
18	H	4017	BCR	C20-C21-C22	24.75	161.99	127.28
18	B	4017	BCR	C20-C21-C22	24.75	161.99	127.28

5 of 261 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	G	1011	CL0	NC
13	G	1011	CL0	NA
13	G	1011	CL0	ND
13	a	1011	CL0	NC
13	a	1011	CL0	NA

5 of 4164 torsion outliers are listed below:

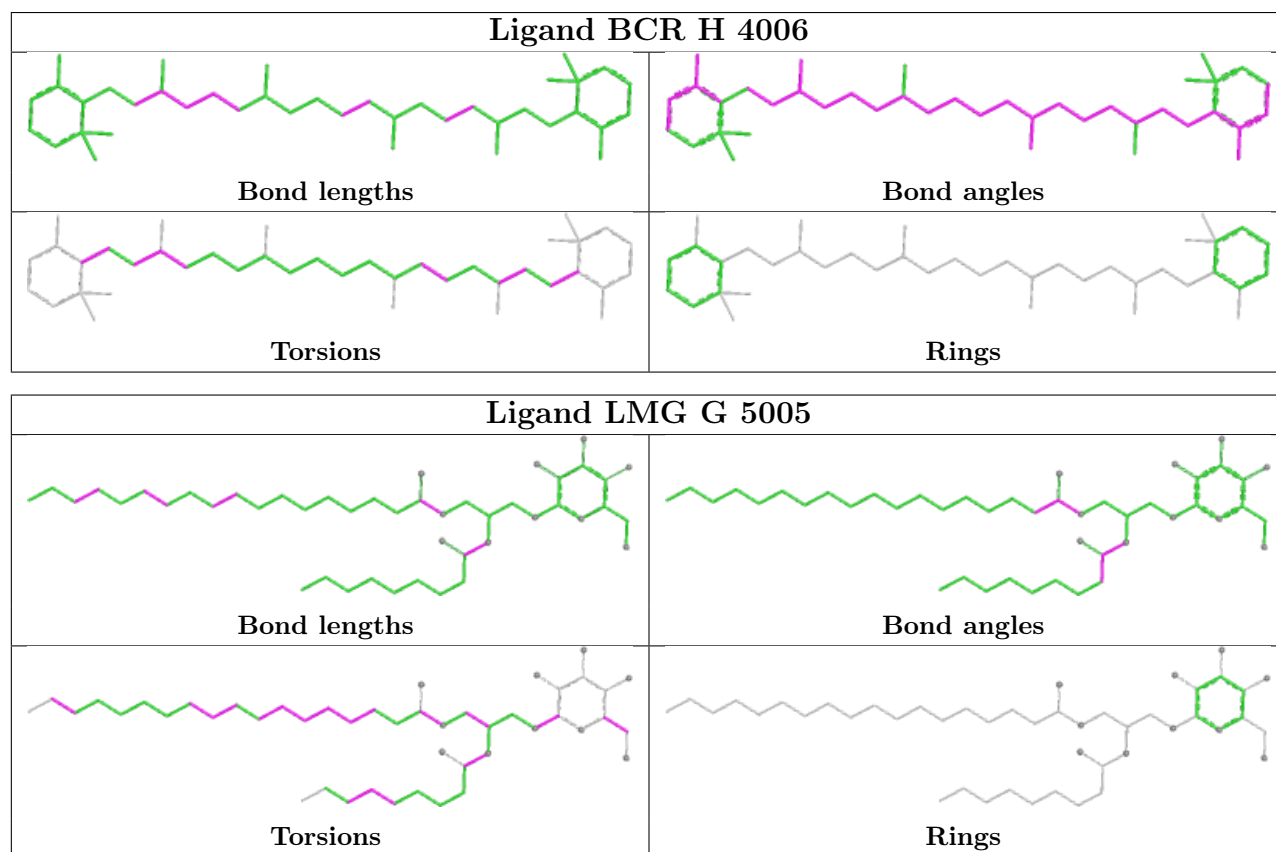
Mol	Chain	Res	Type	Atoms
14	G	1013	CLA	C1A-C2A-CAA-CBA
14	G	1013	CLA	C3A-C2A-CAA-CBA
14	G	1013	CLA	C11-C10-C8-C9
14	G	1101	CLA	CHA-CBD-CGD-O1D
14	G	1101	CLA	CHA-CBD-CGD-O2D

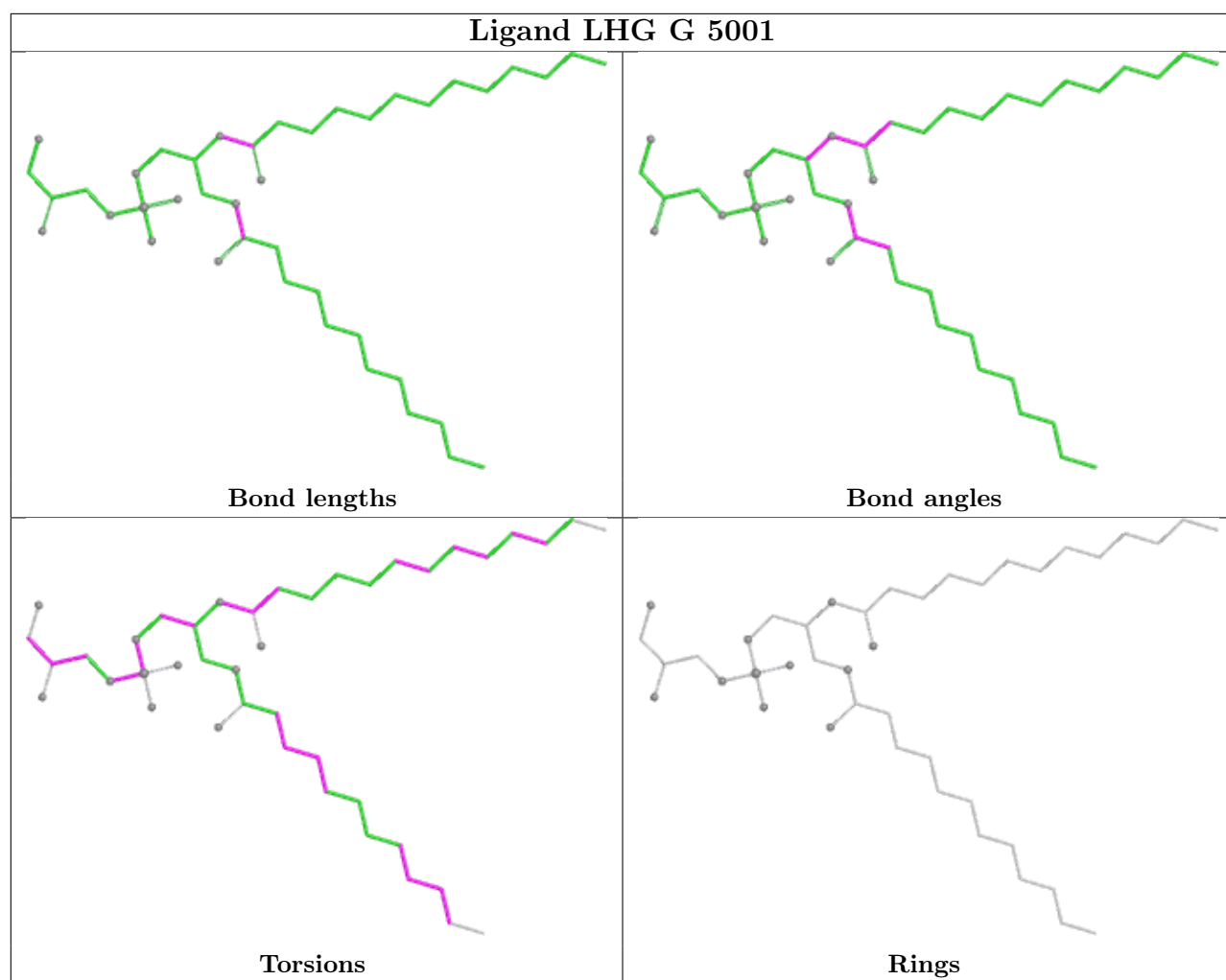
There are no ring outliers.

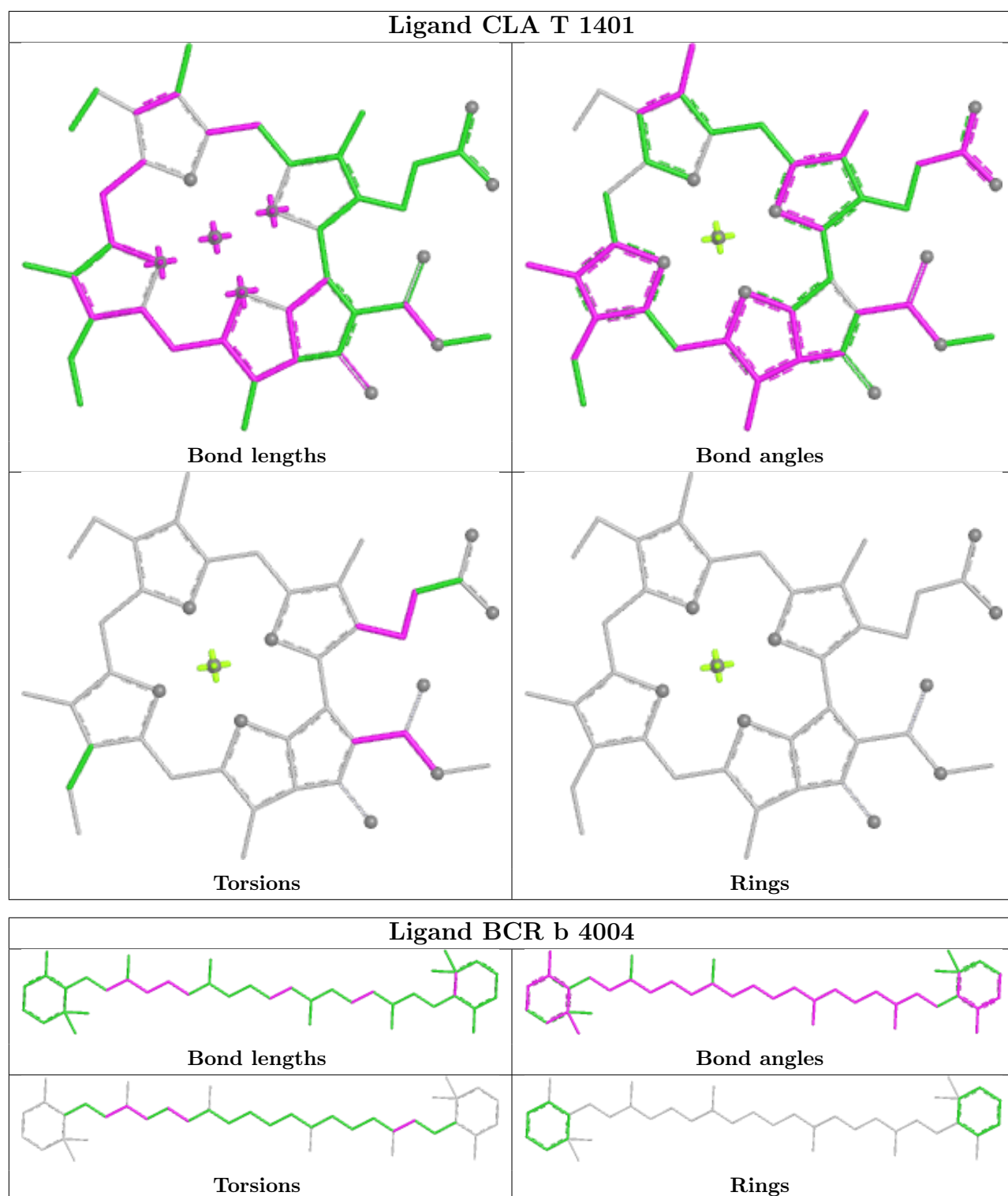
No monomer is involved in short contacts.

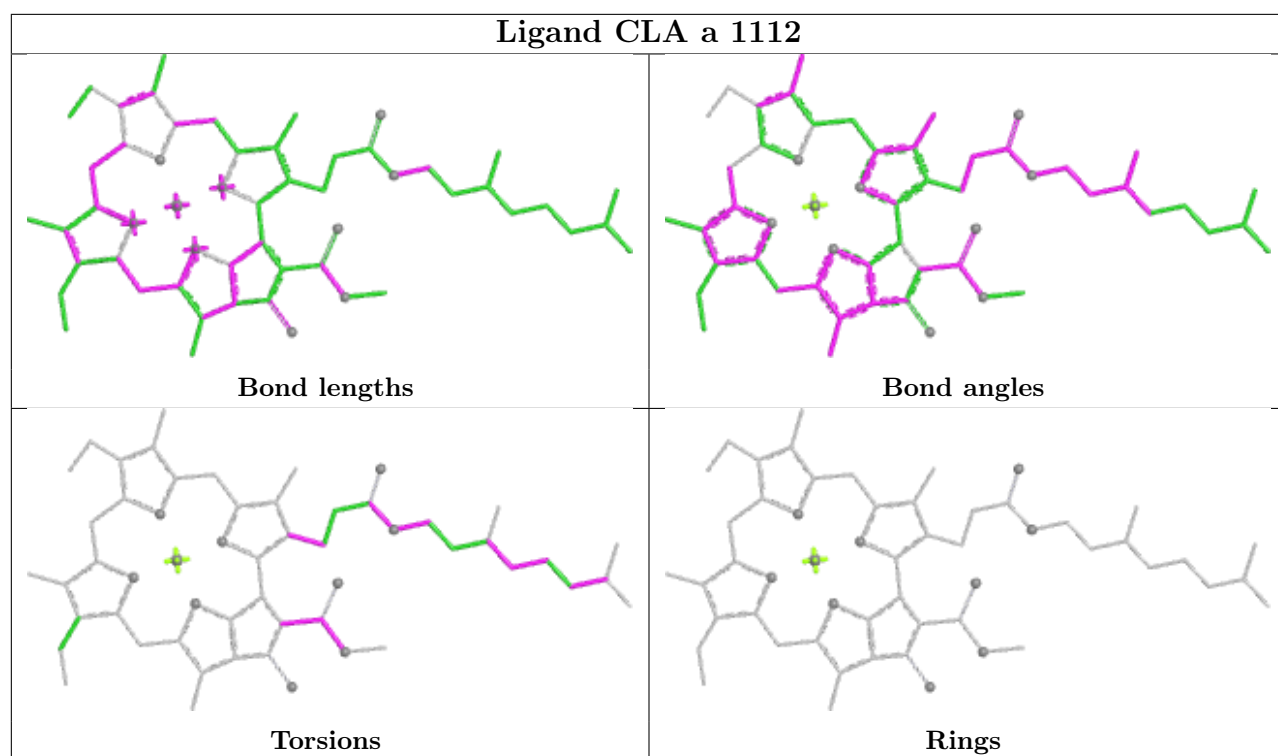
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

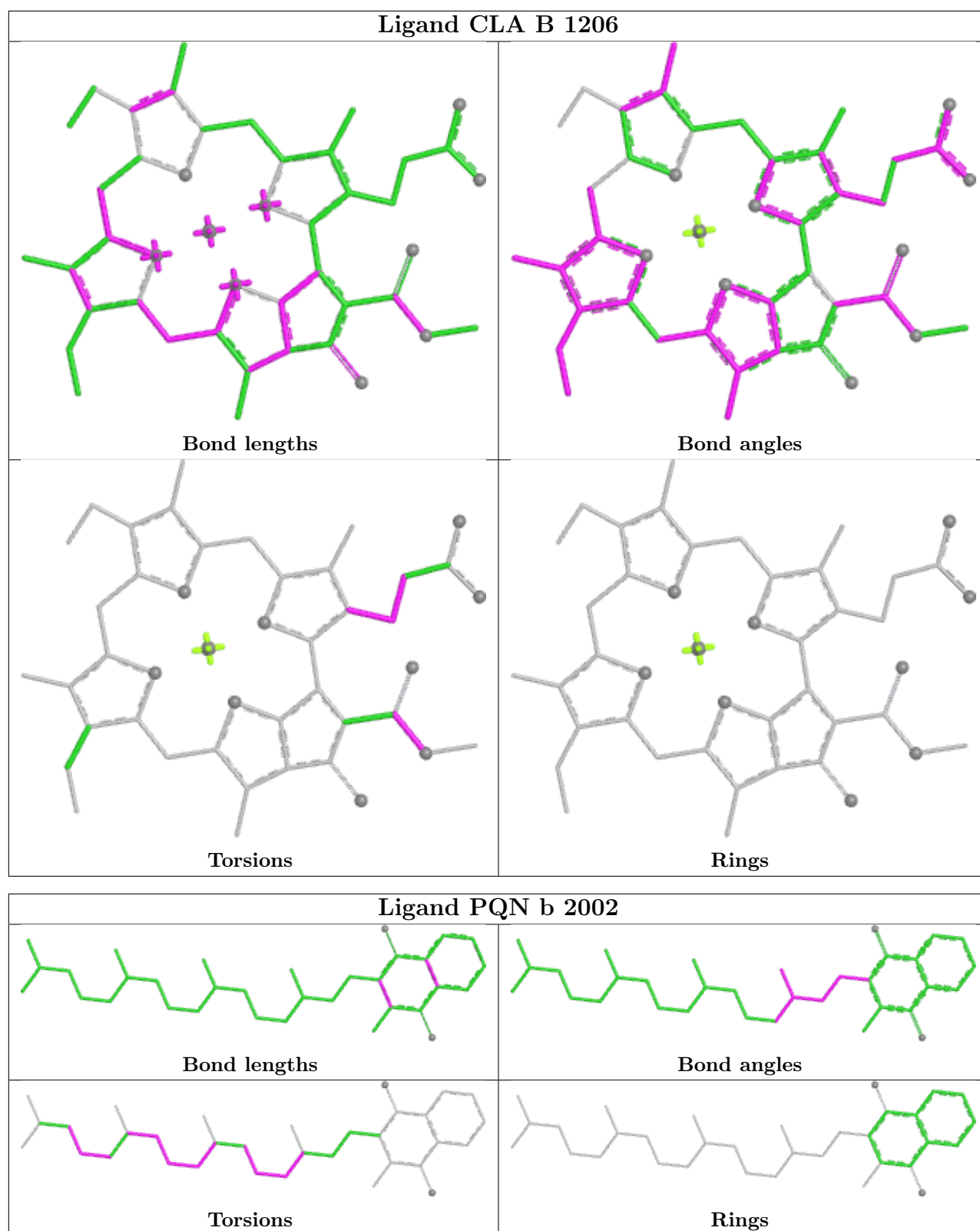
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

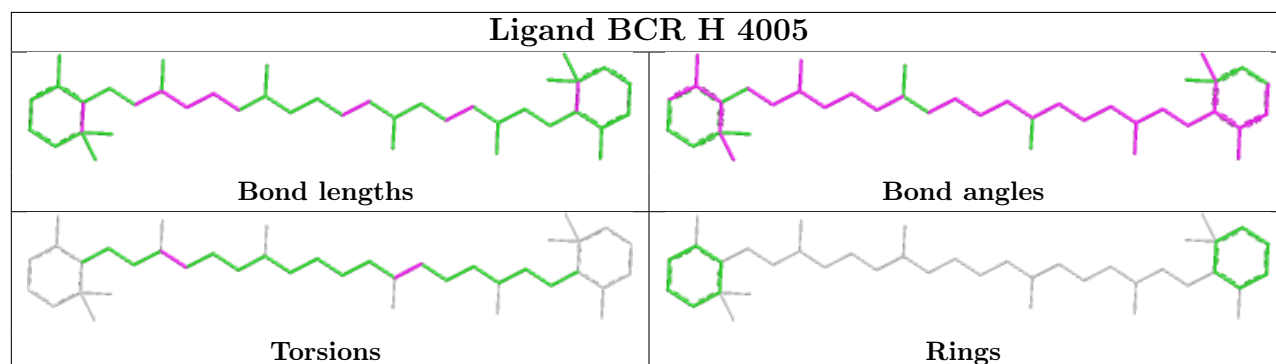
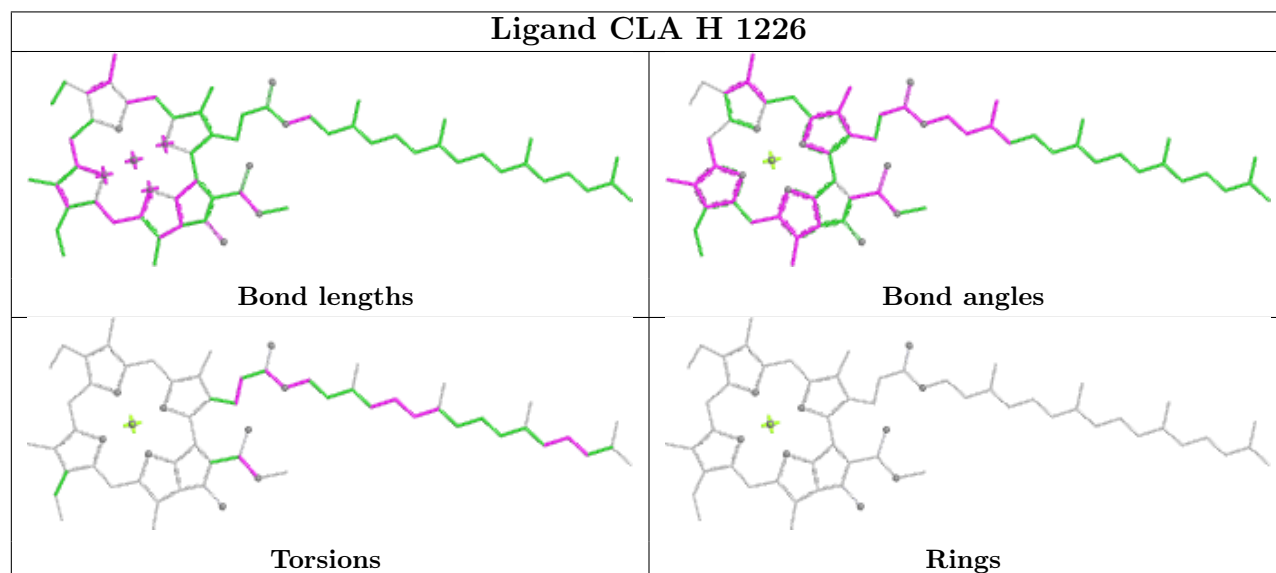
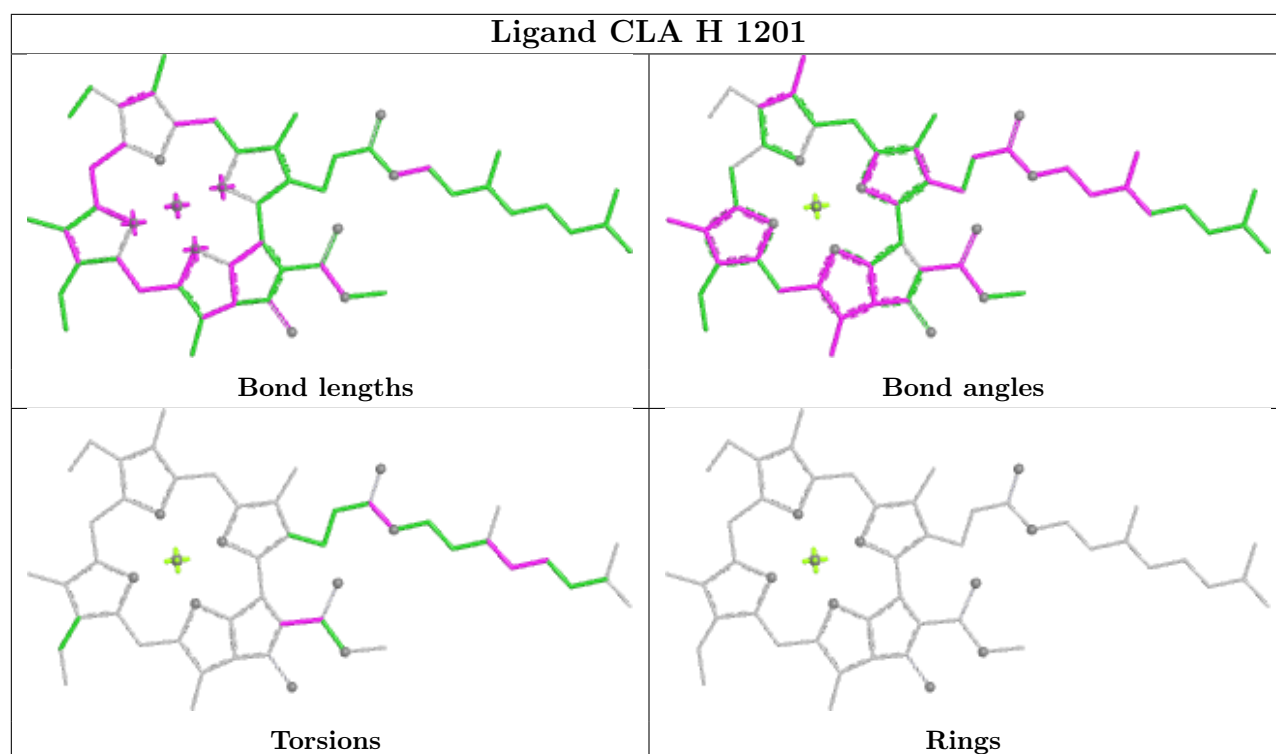


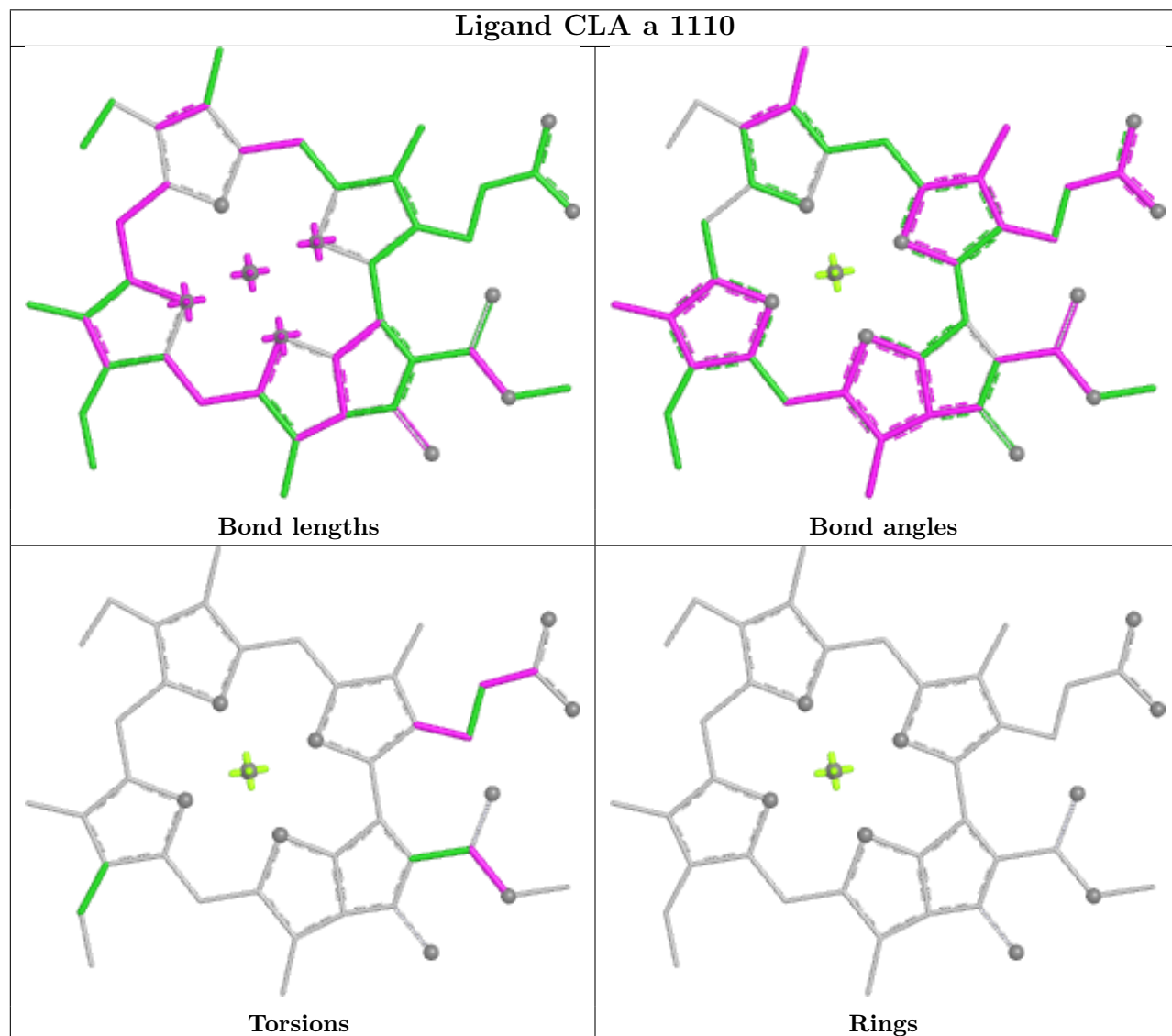
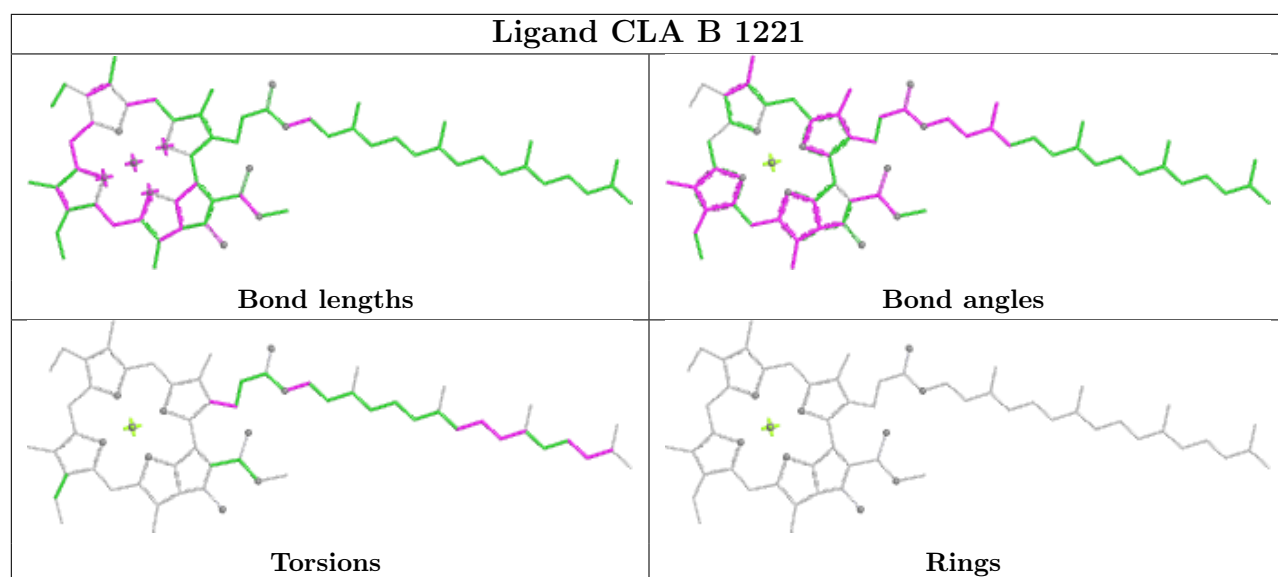


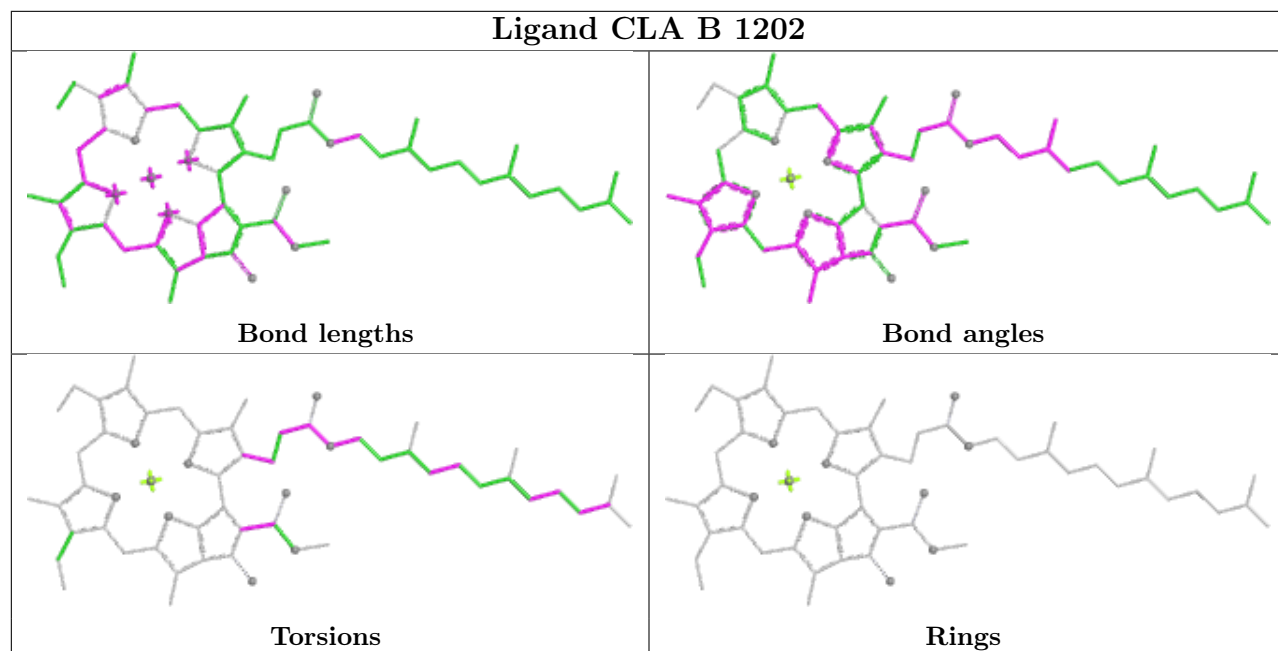
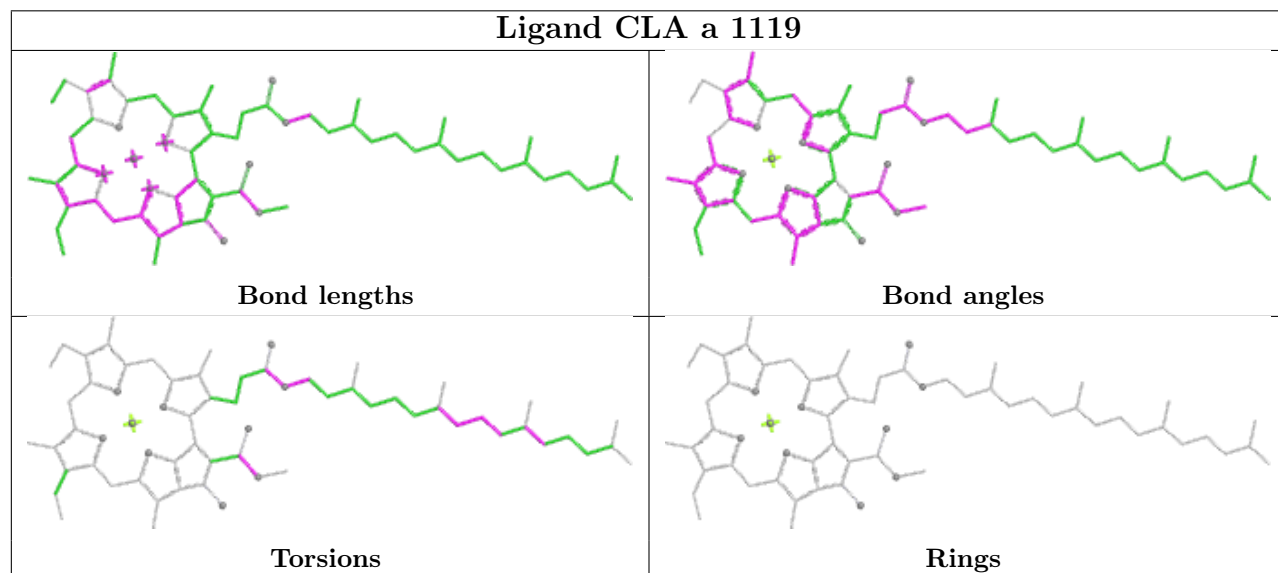
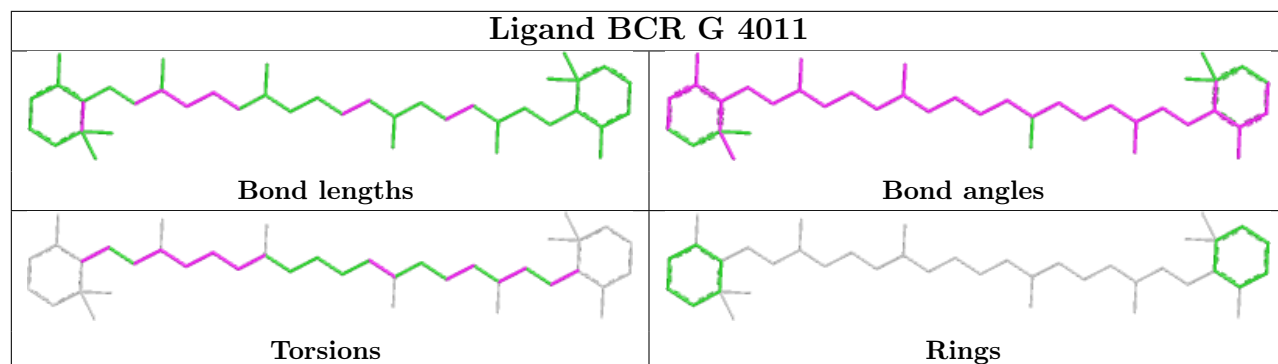




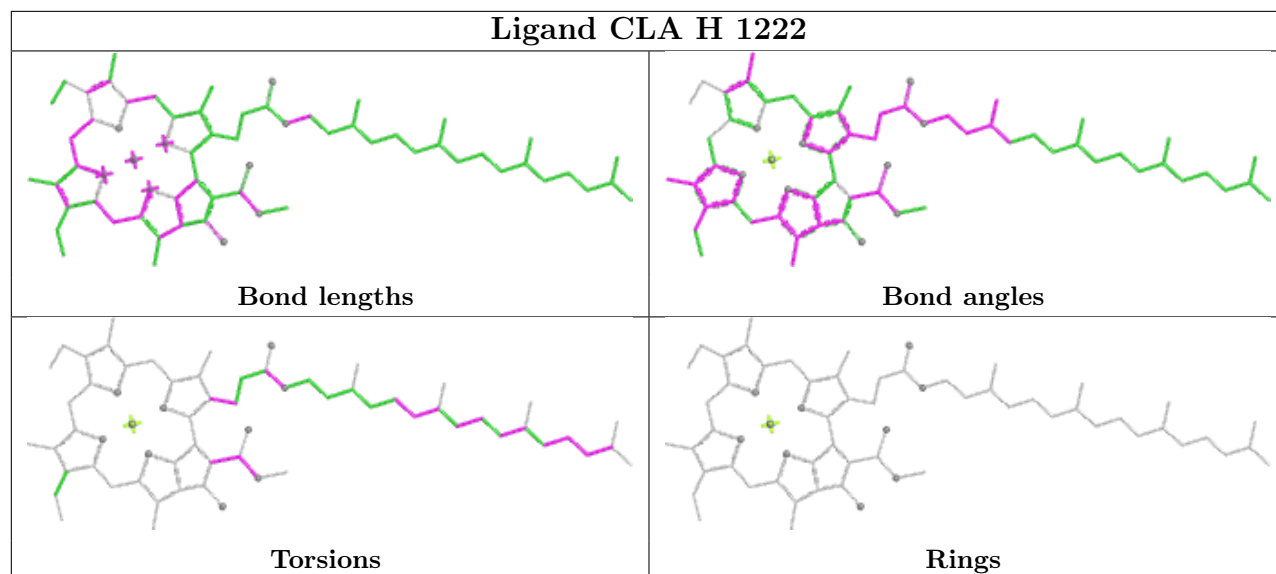




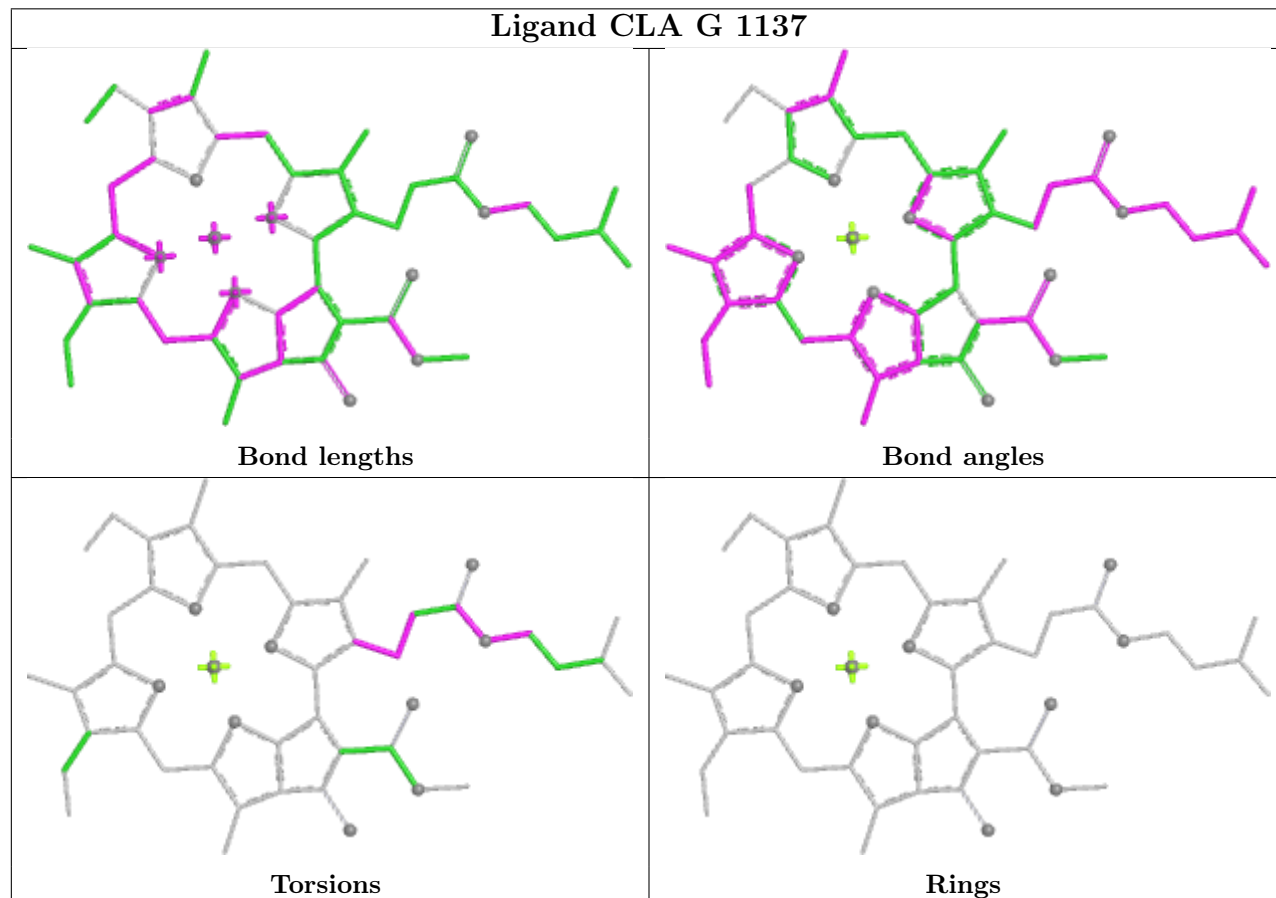


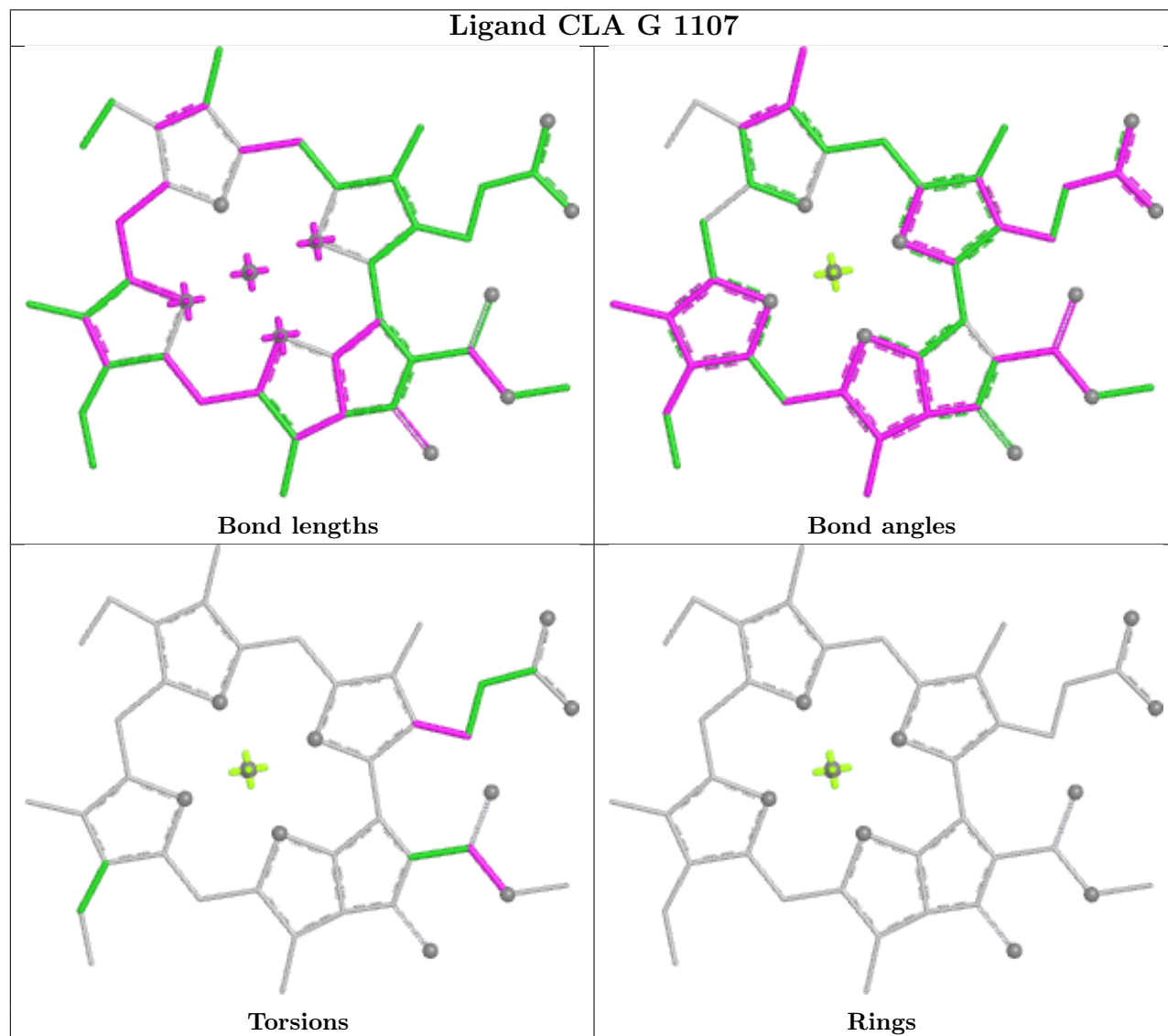
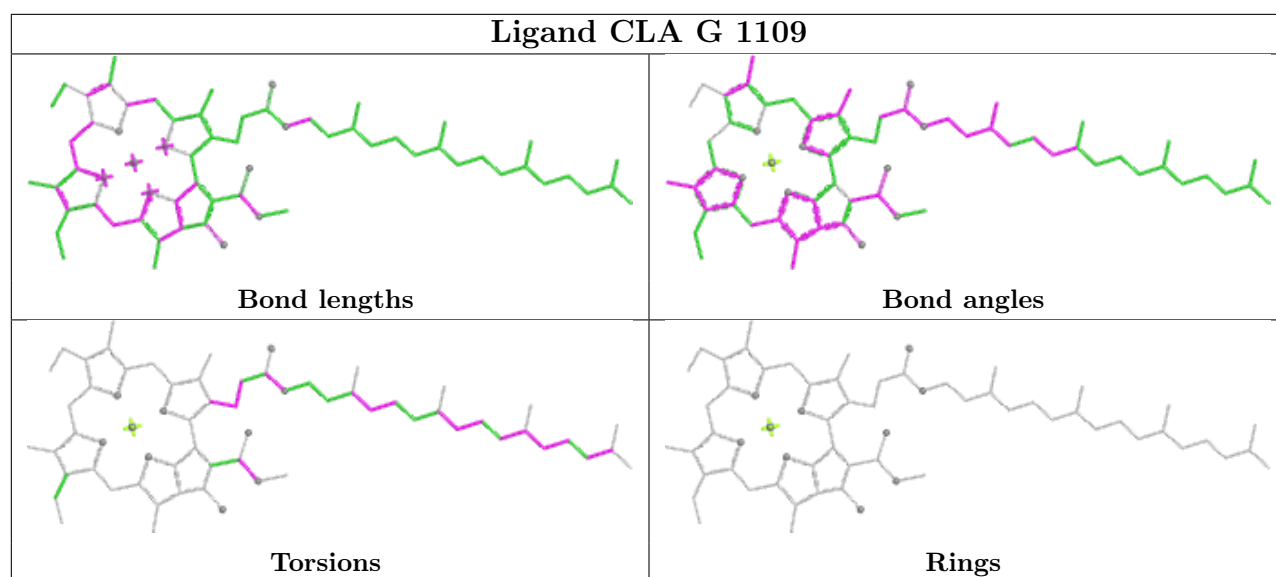


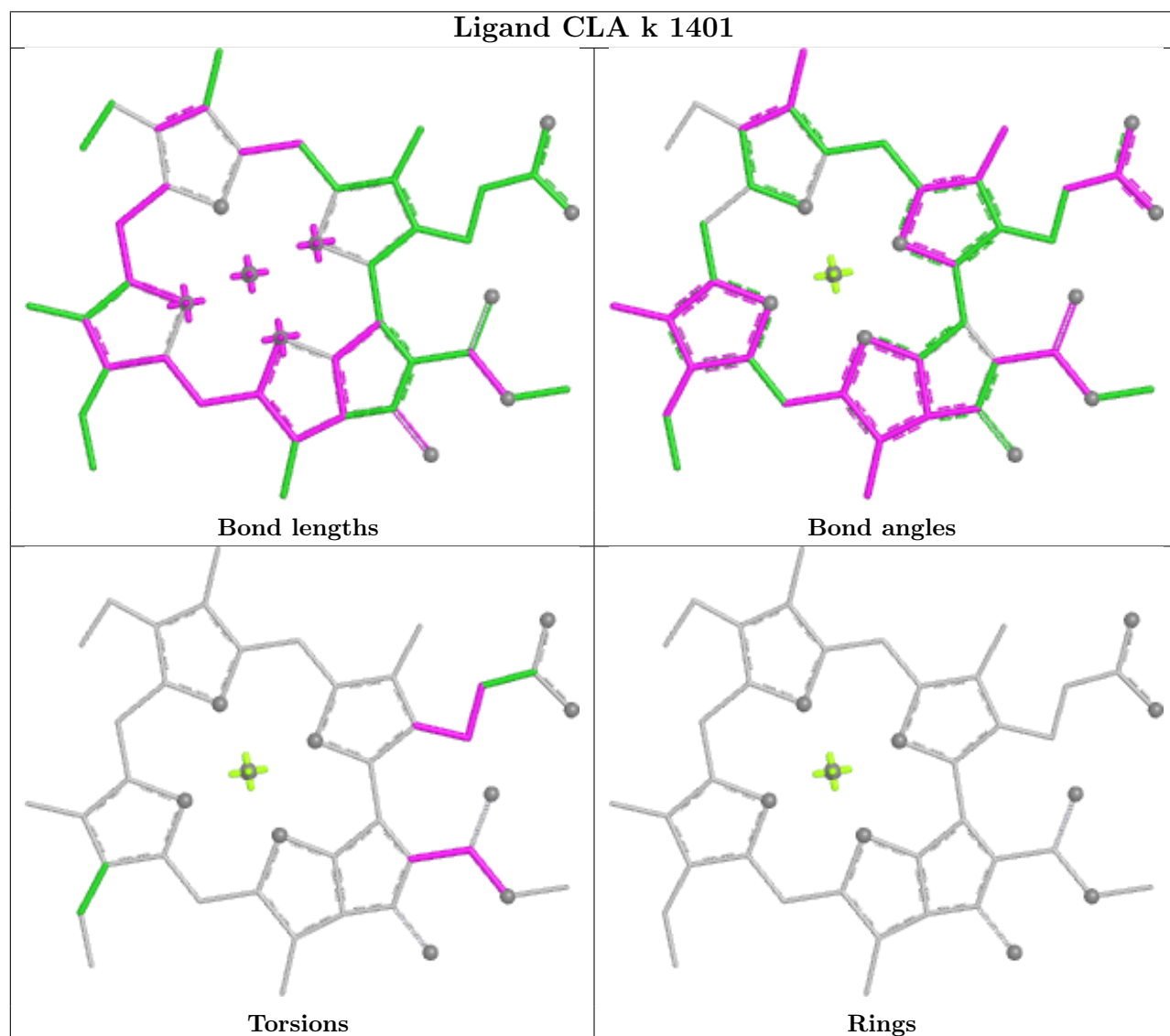
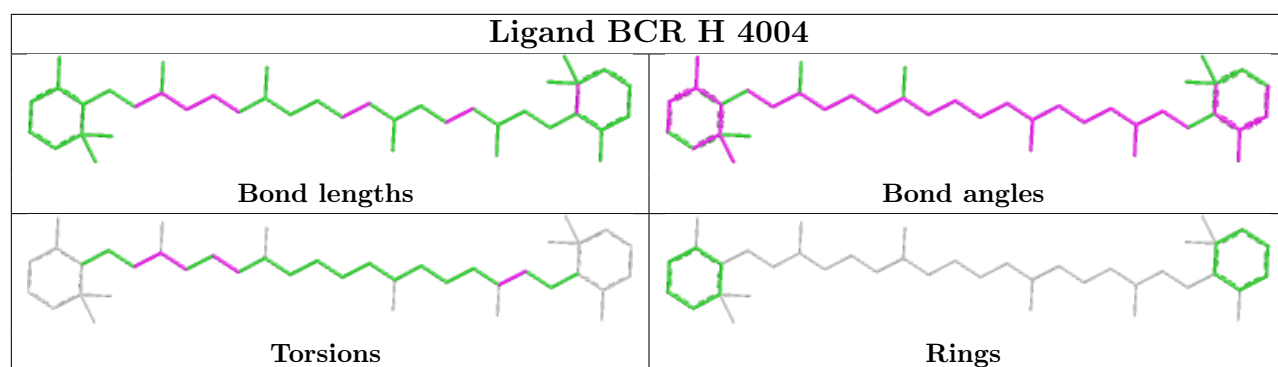
Ligand CLA H 1222

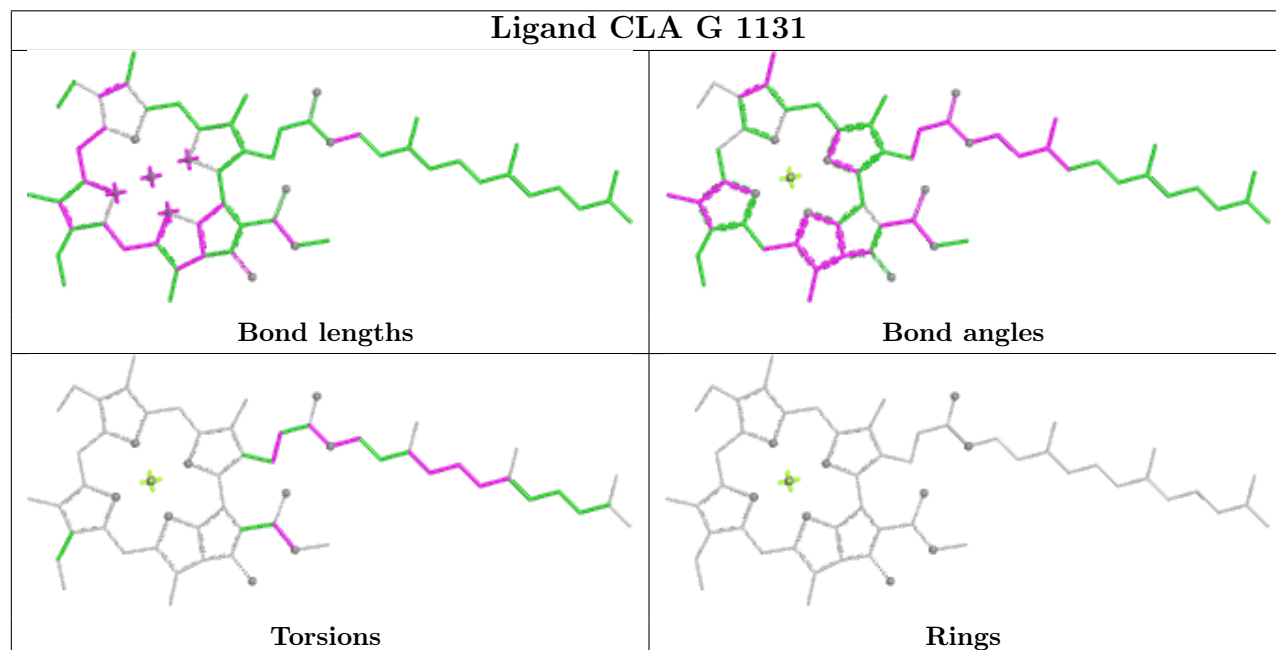
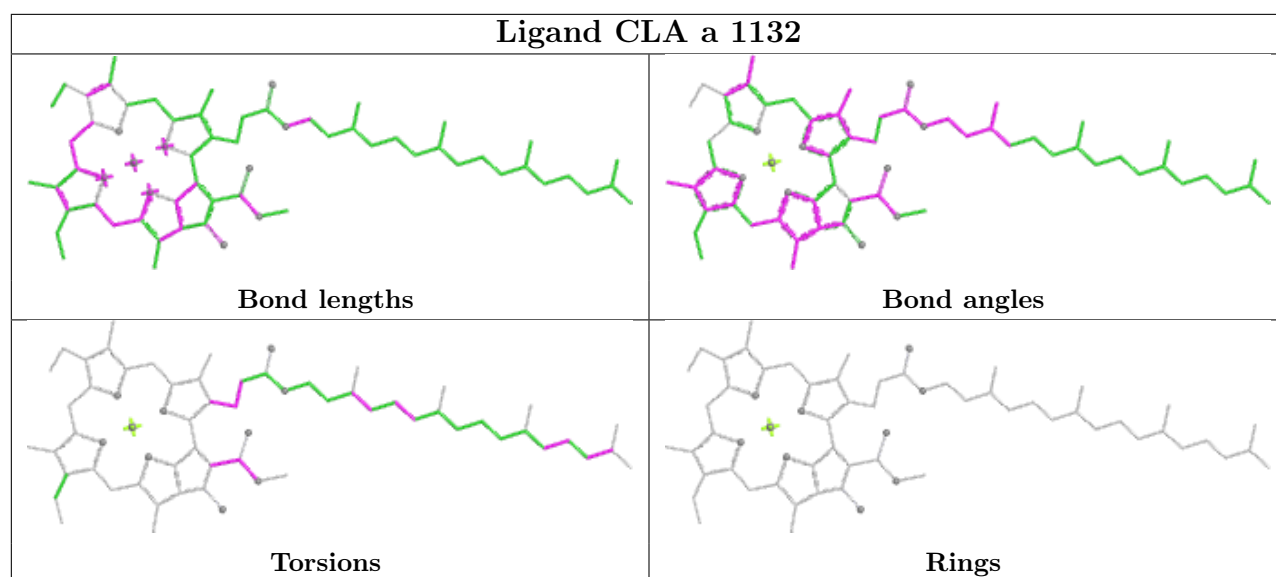


Ligand CLA G 1137

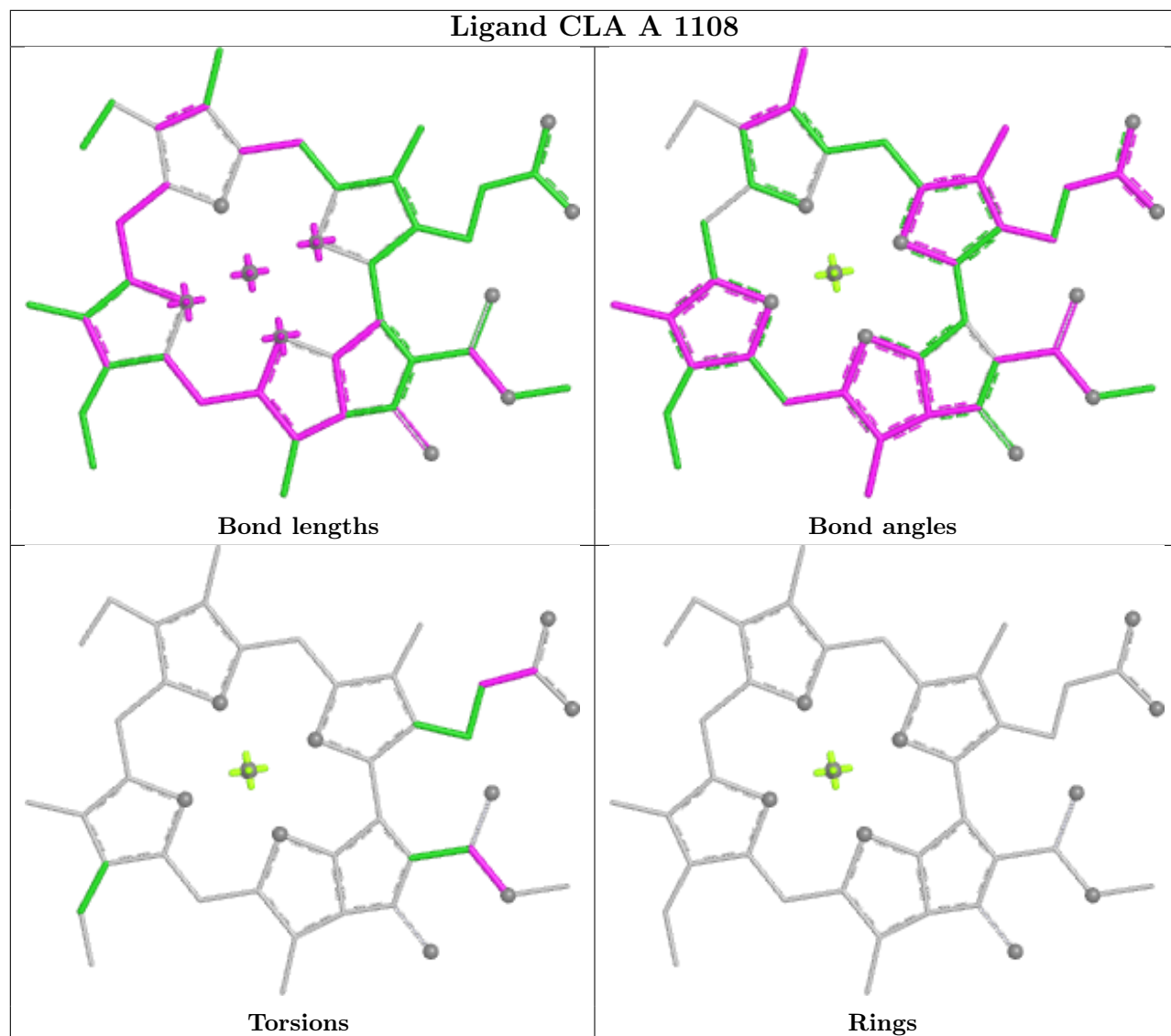


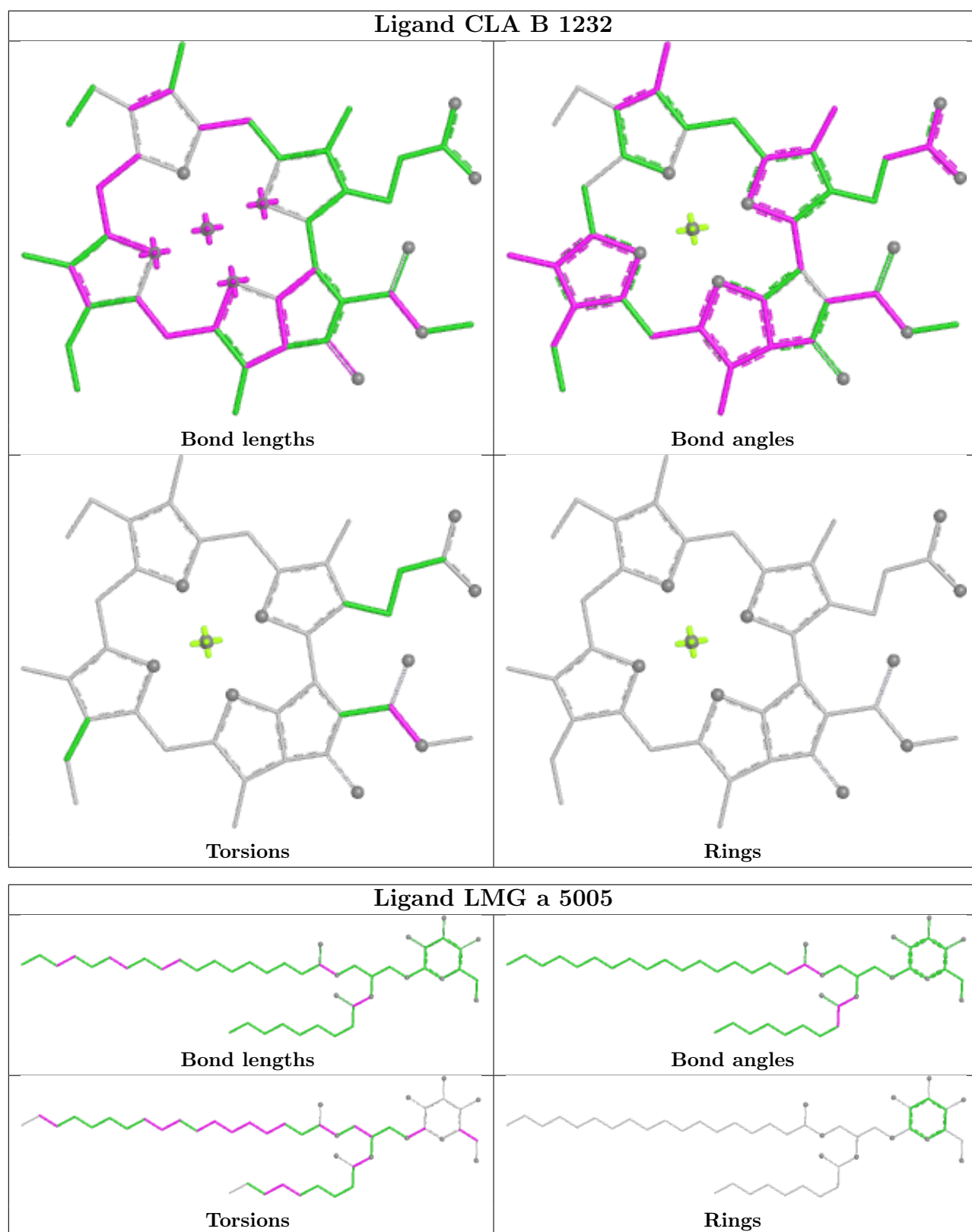


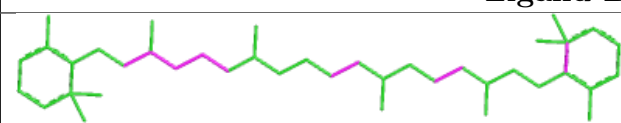
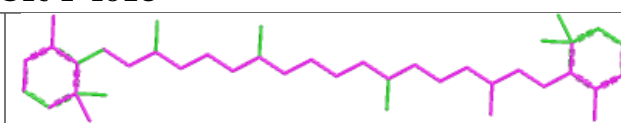
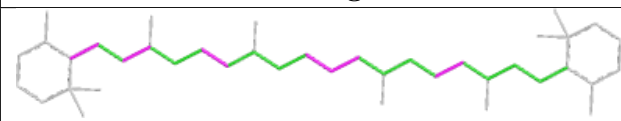
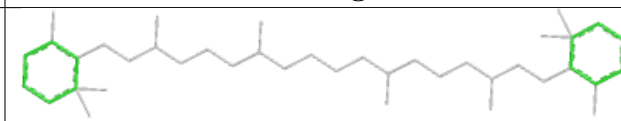


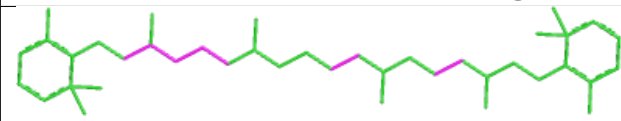
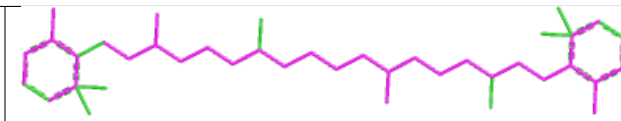
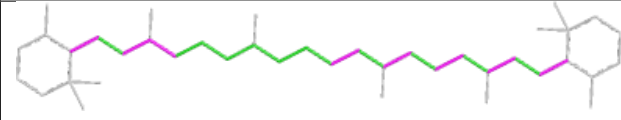
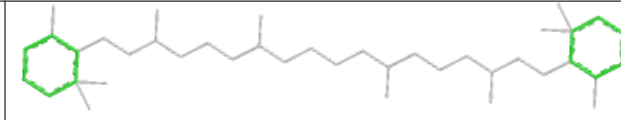


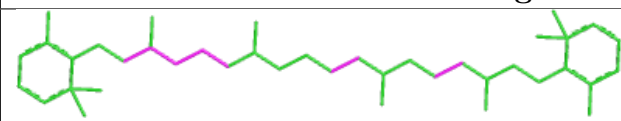
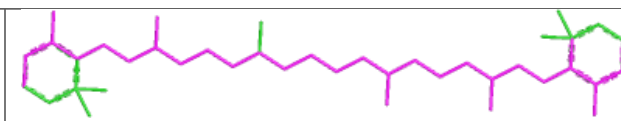
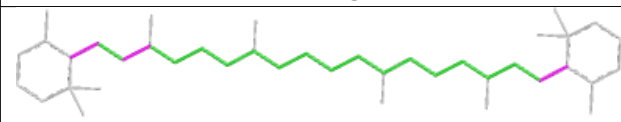
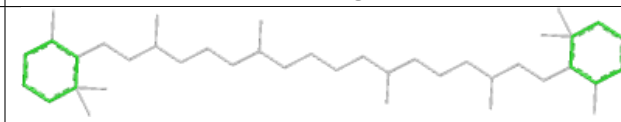
Ligand CLA A 1108

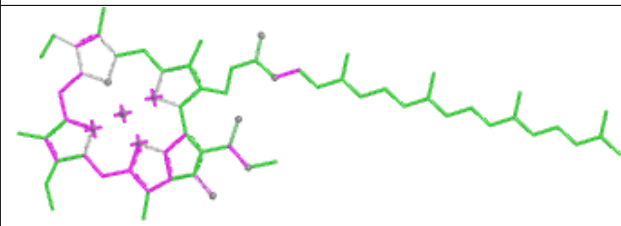
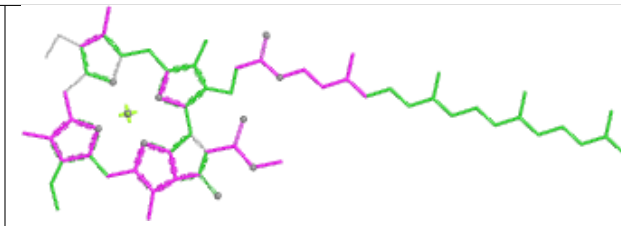
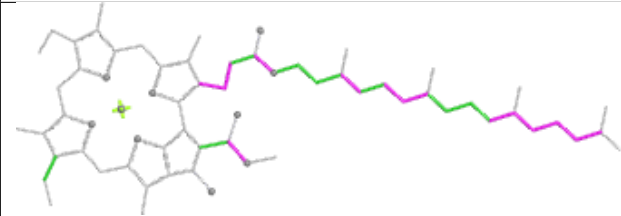
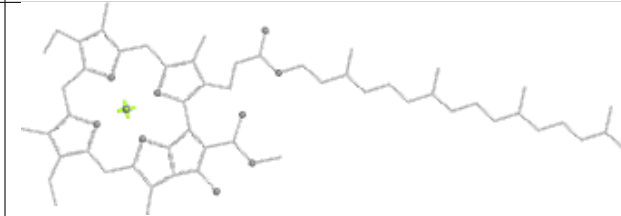


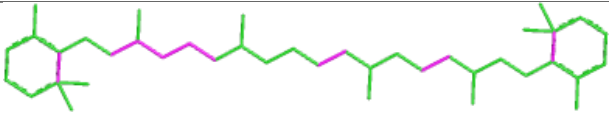
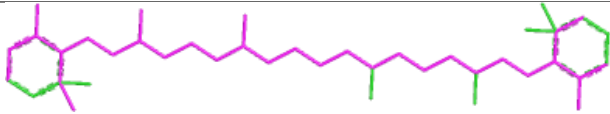
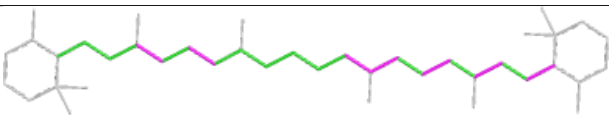
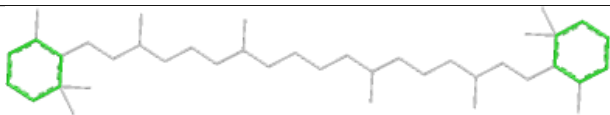


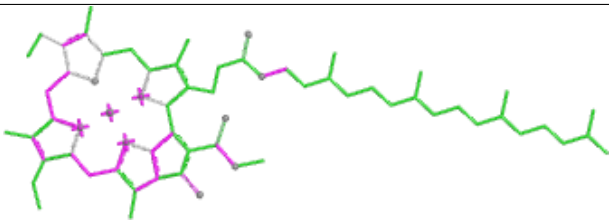
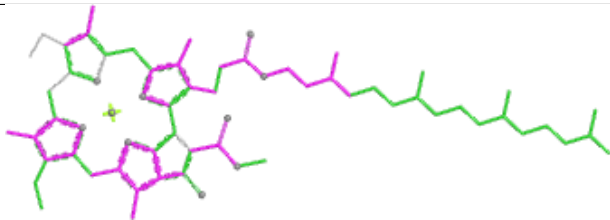
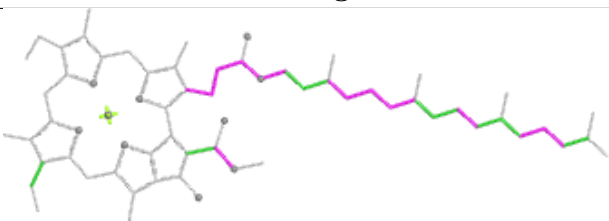
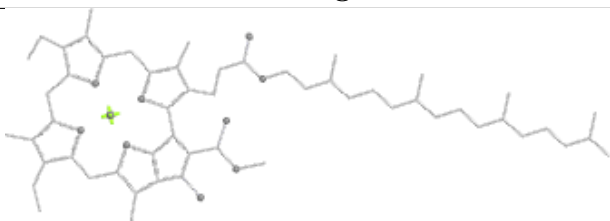
Ligand BCR I 4018	
	
Bond lengths	Bond angles
	
Torsions	Rings

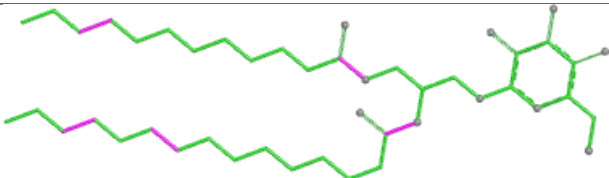
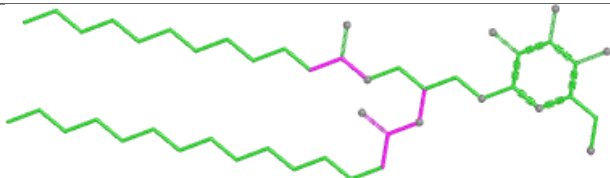
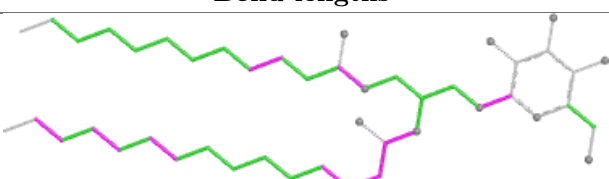
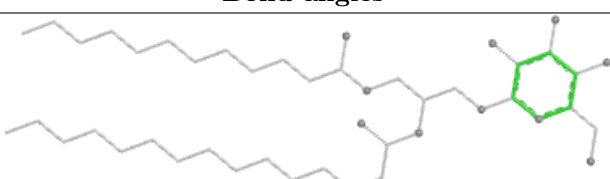
Ligand BCR G 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

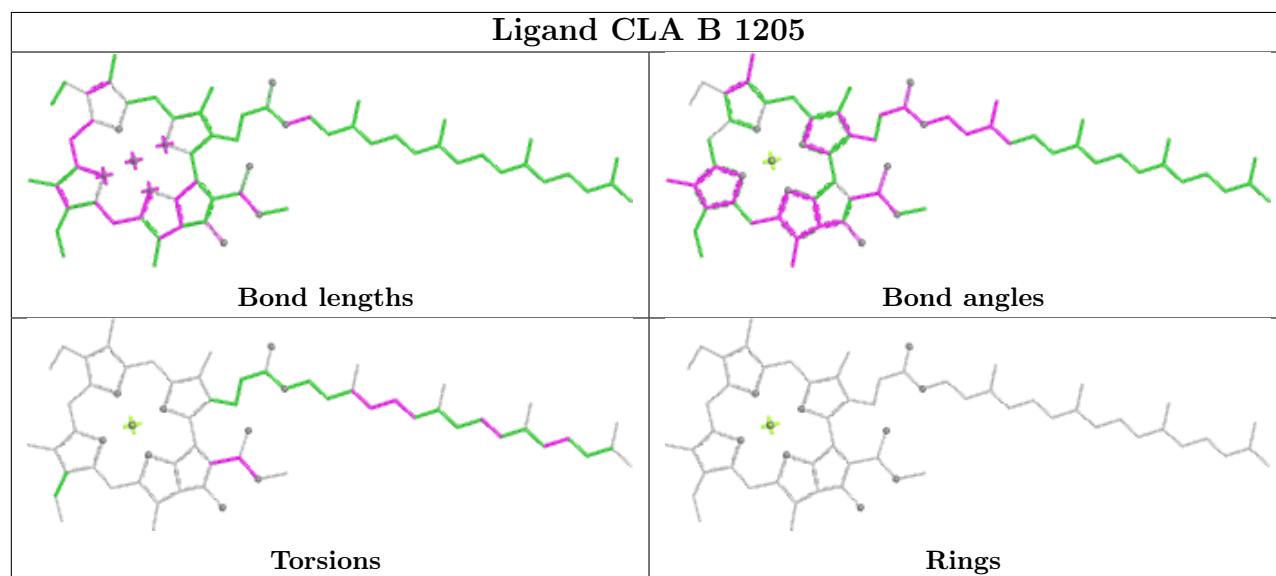
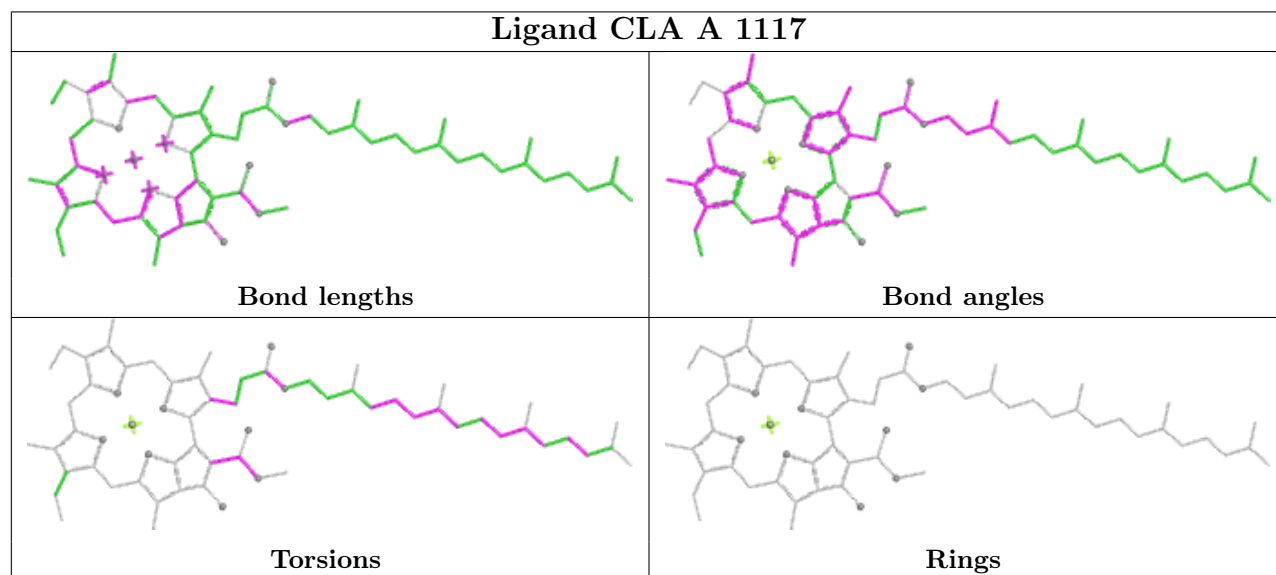
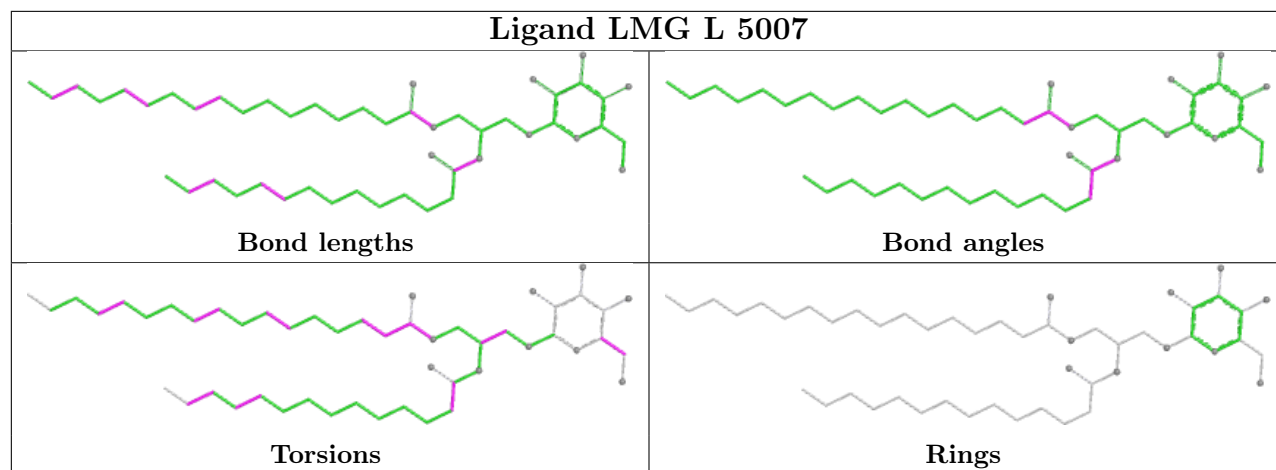
Ligand BCR a 4002	
	
Bond lengths	Bond angles
	
Torsions	Rings

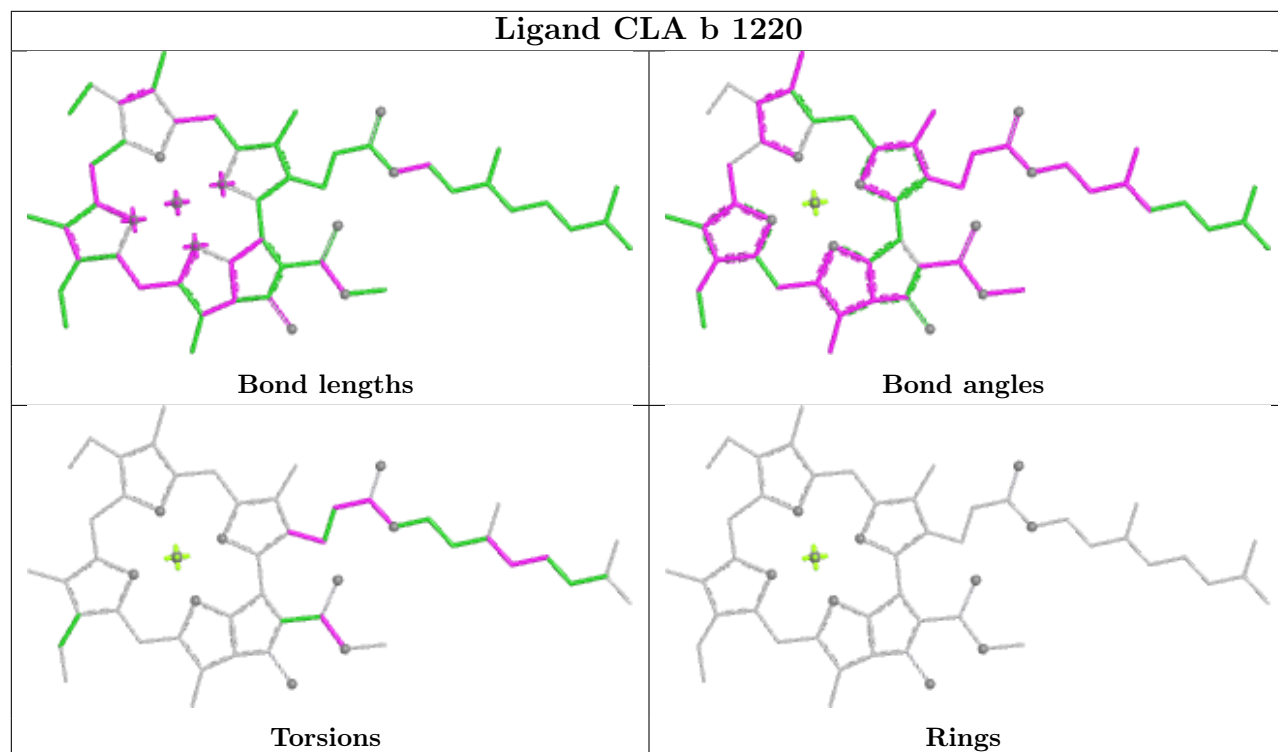
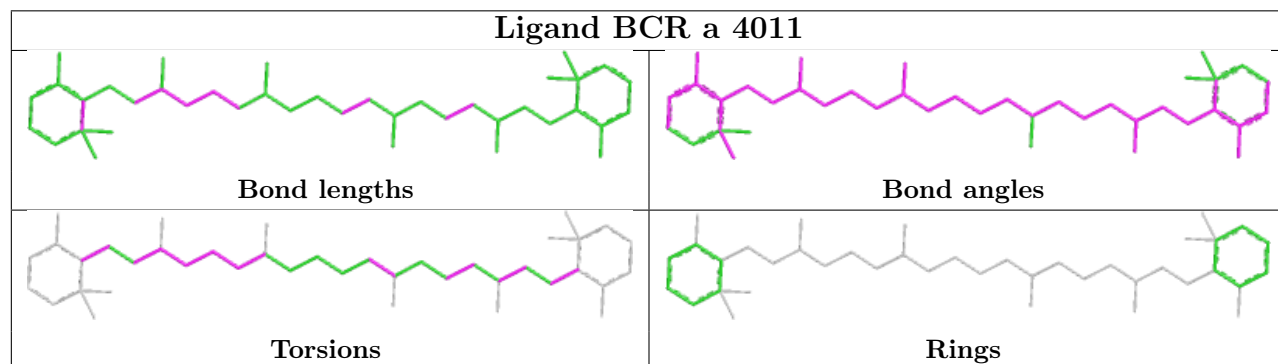
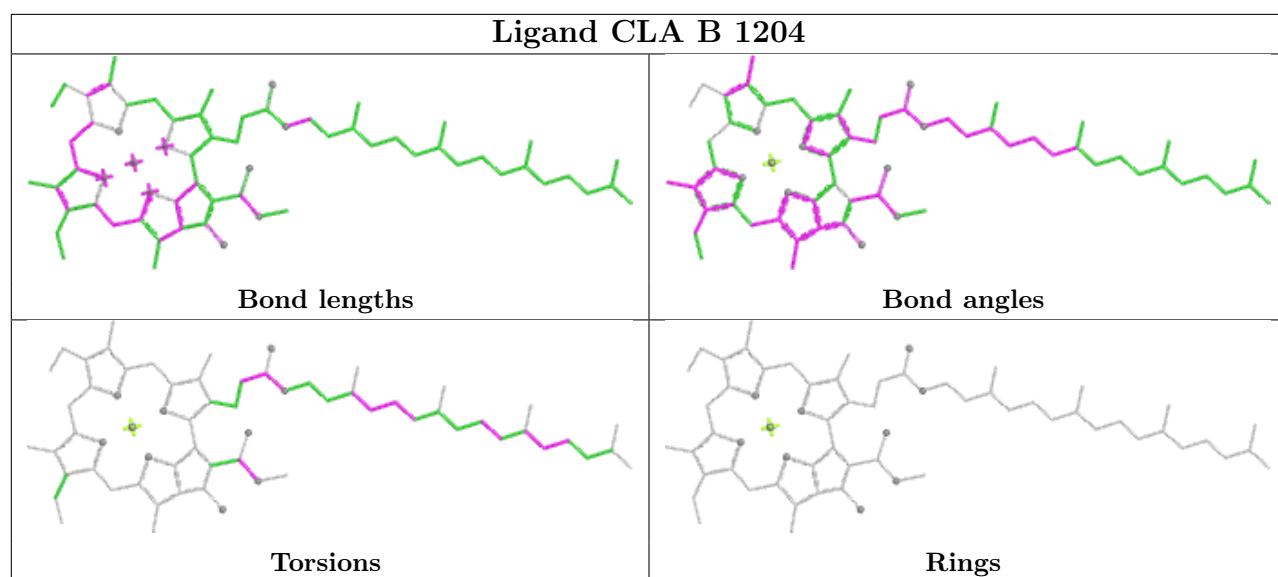
Ligand CLA B 1216	
	
Bond lengths	Bond angles
	
Torsions	Rings

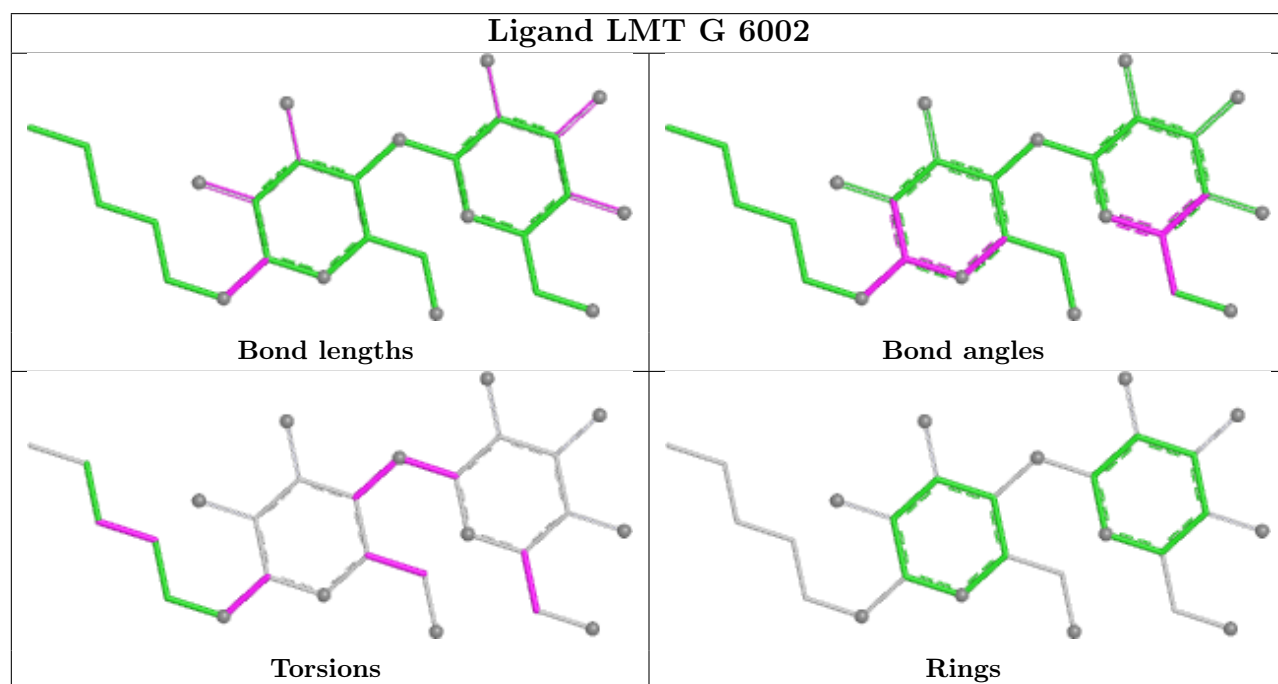
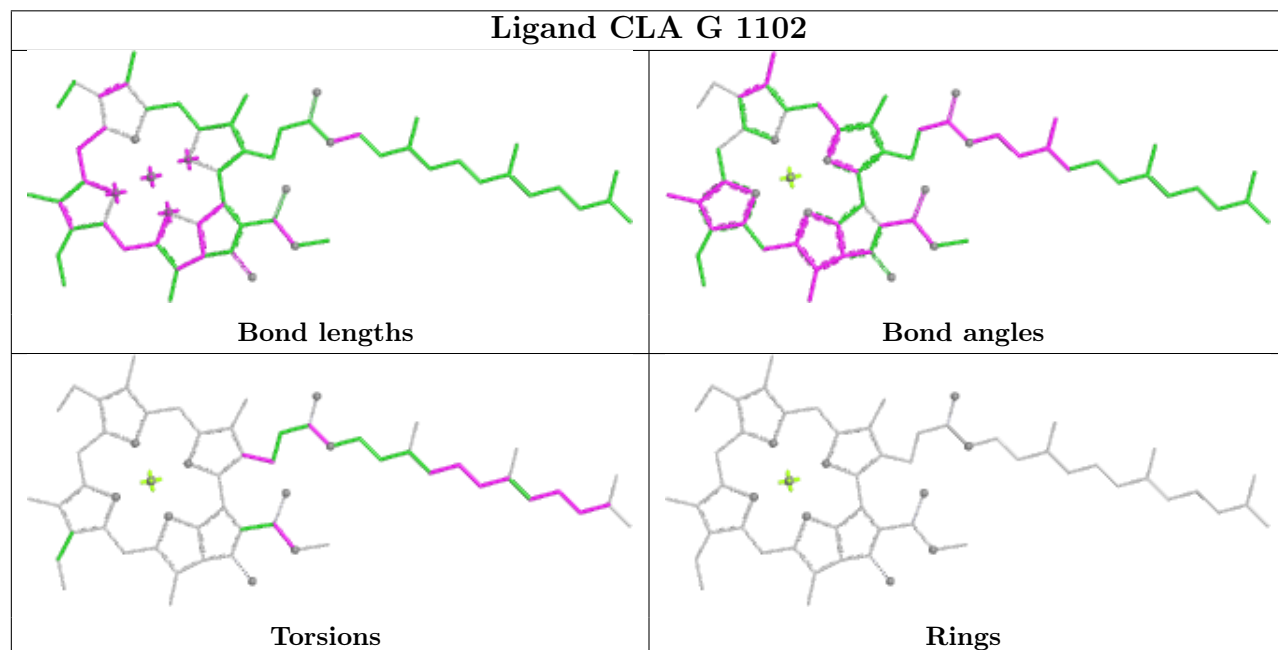
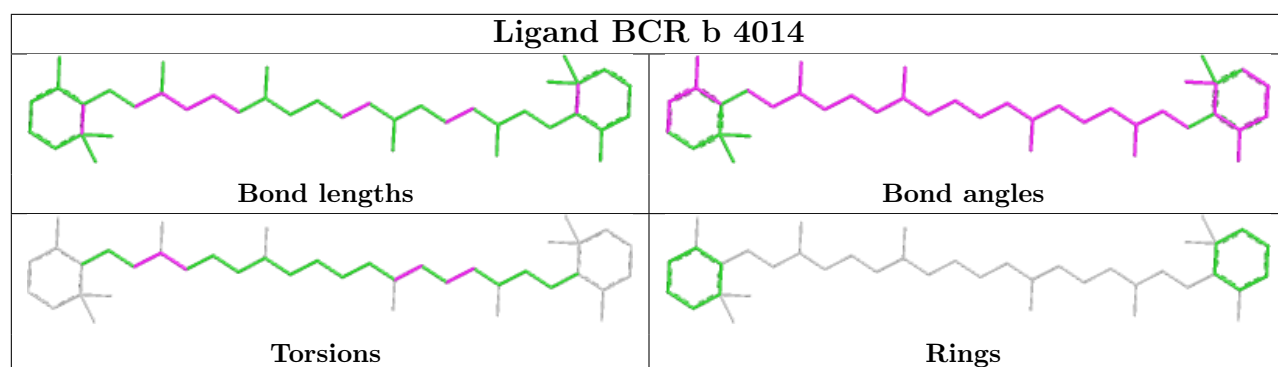
Ligand BCR A 4007	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 1136	
	
Bond lengths	Bond angles
	
Torsions	Rings

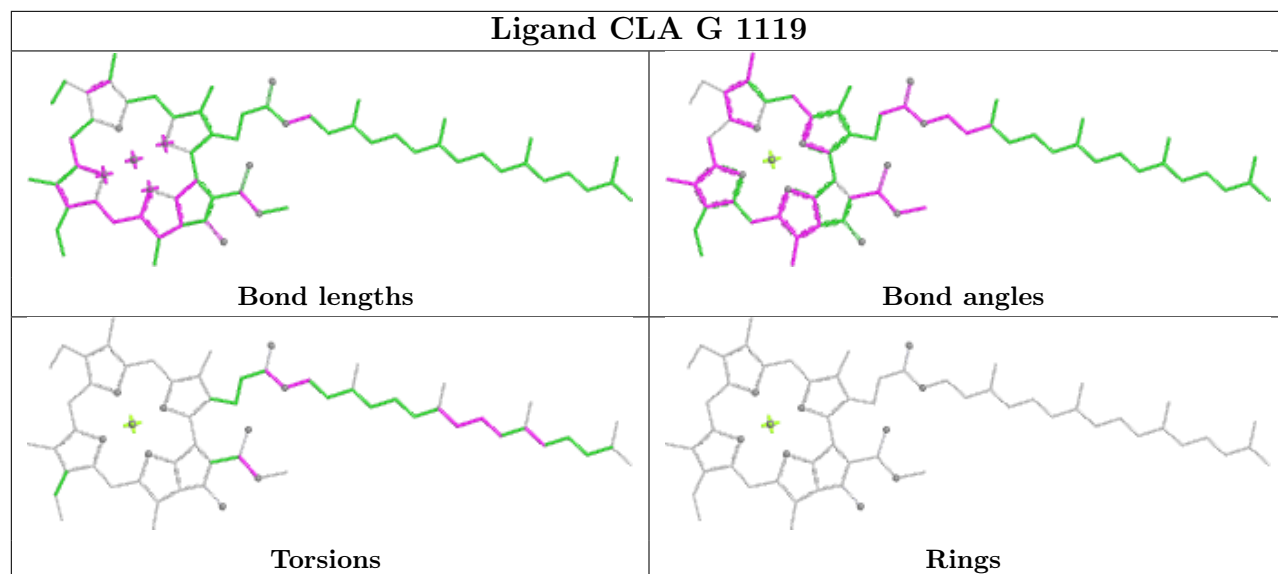
Ligand LMG B 5002	
	
Bond lengths	Bond angles
	
Torsions	Rings



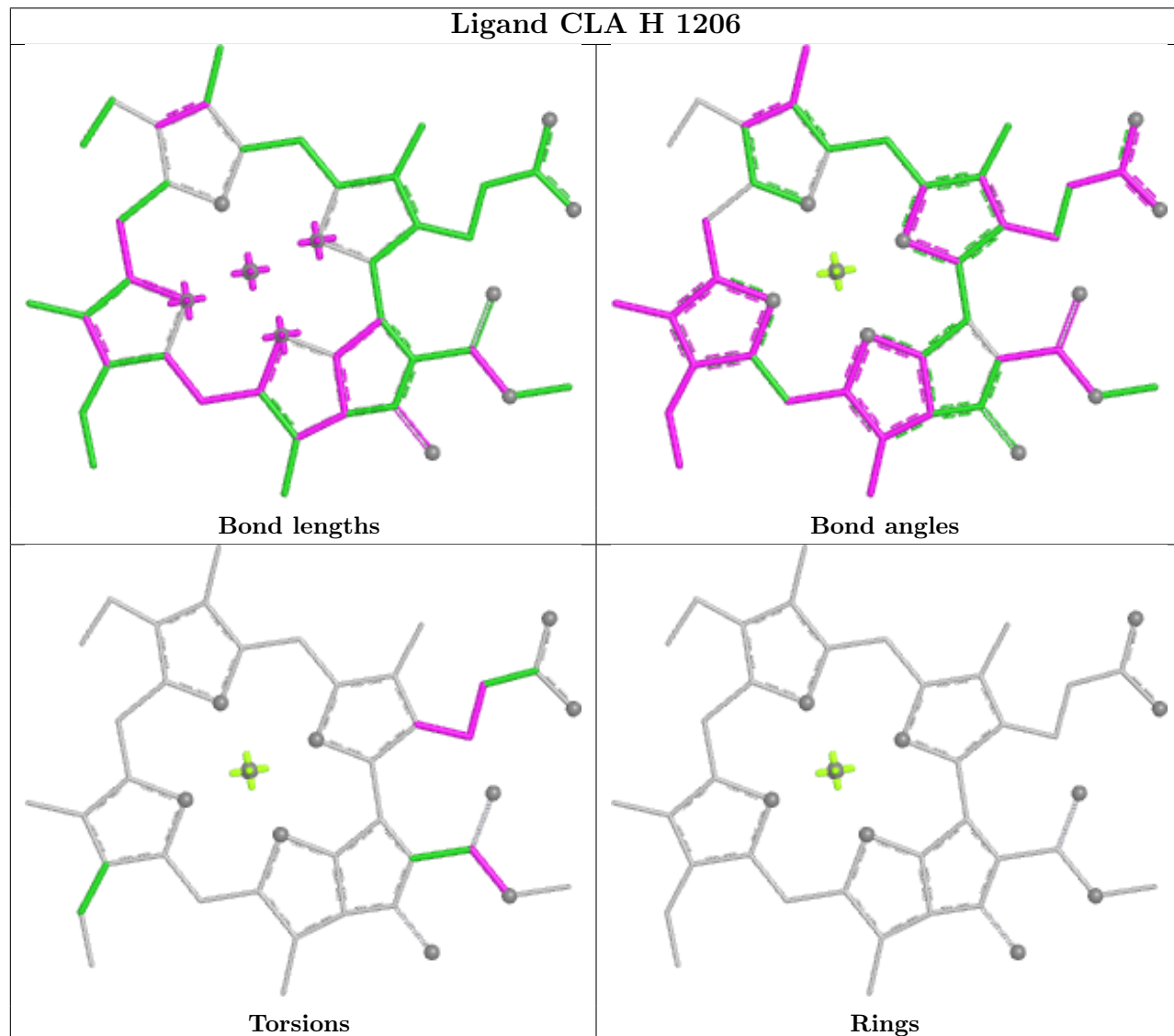


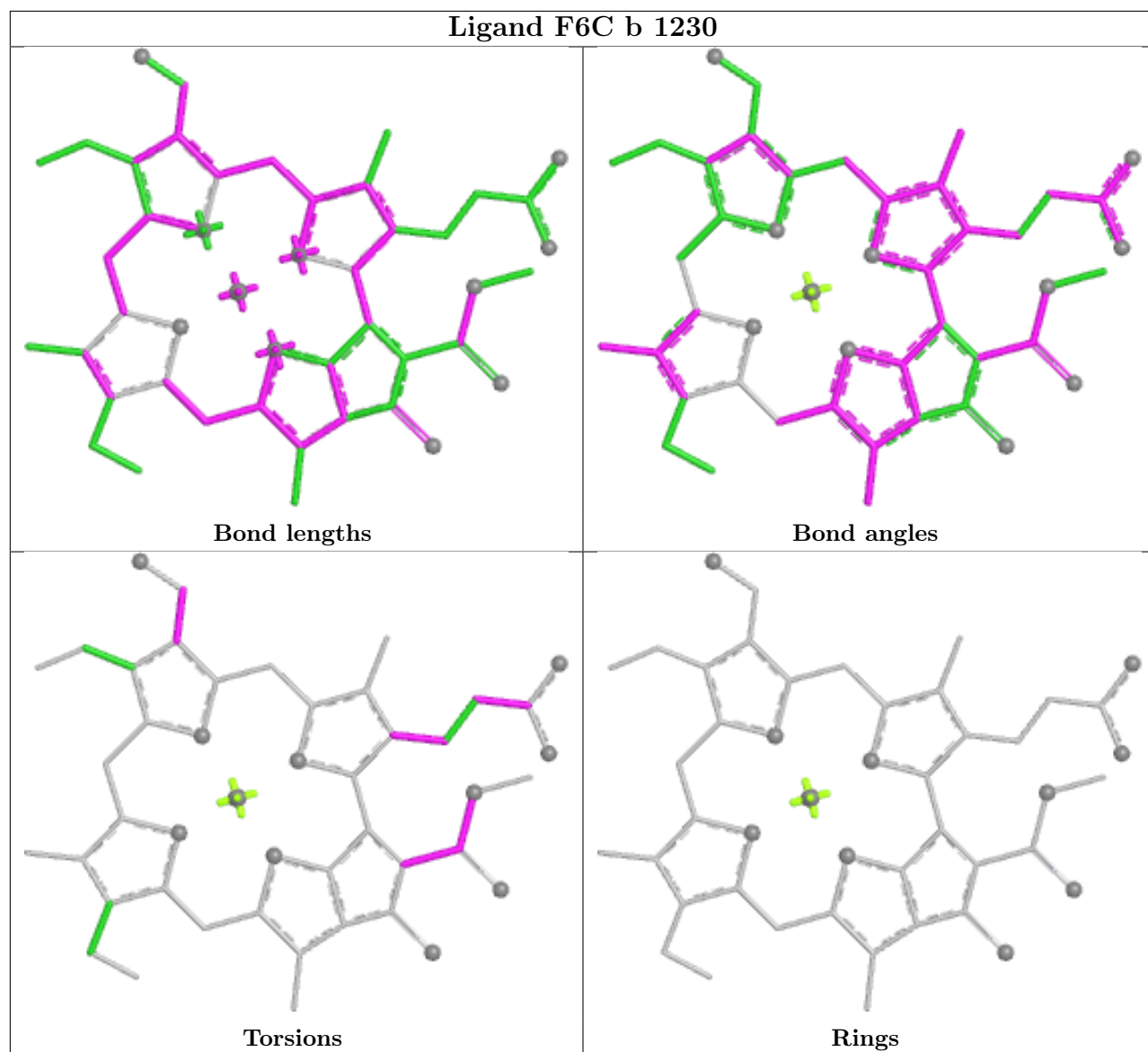
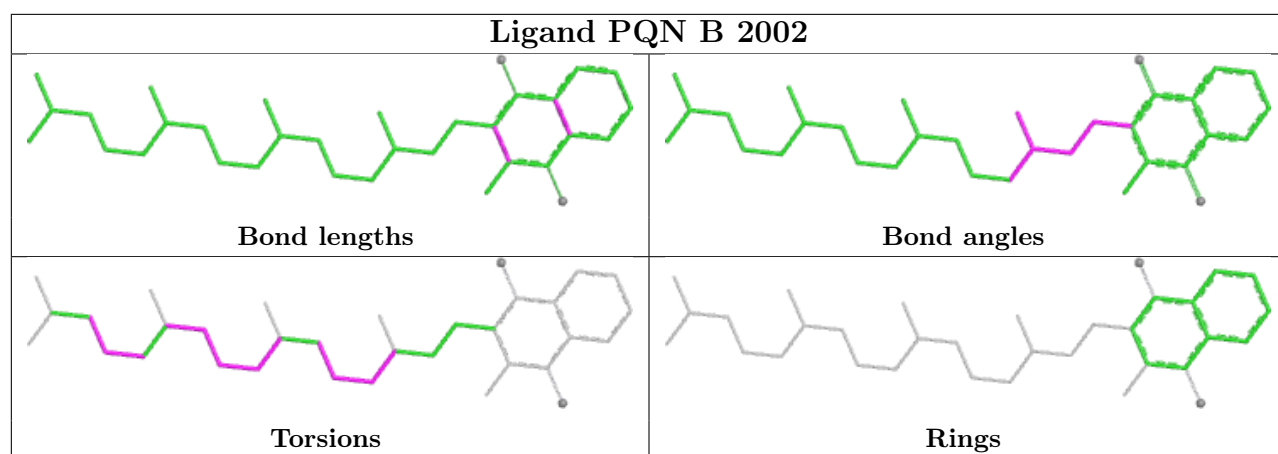


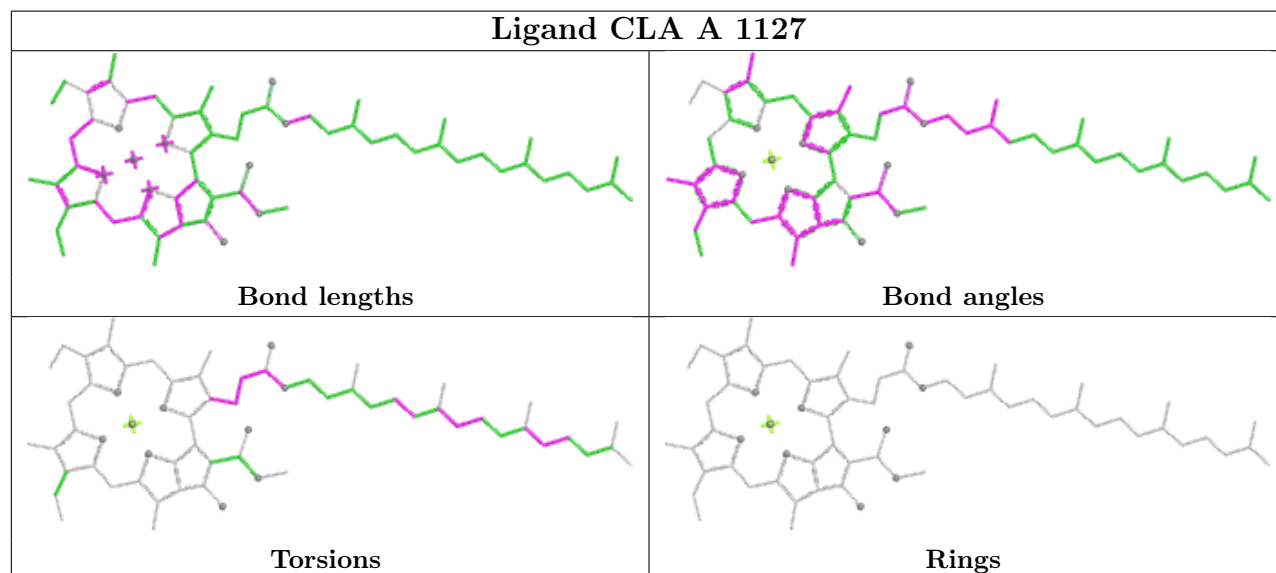
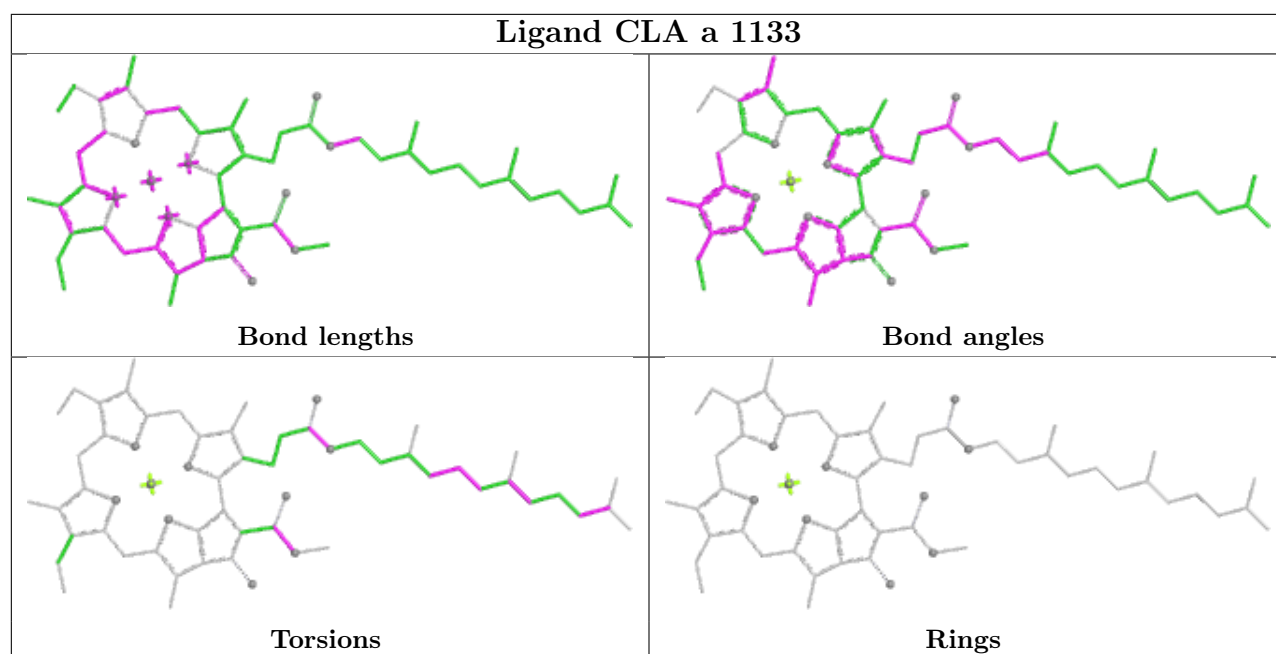
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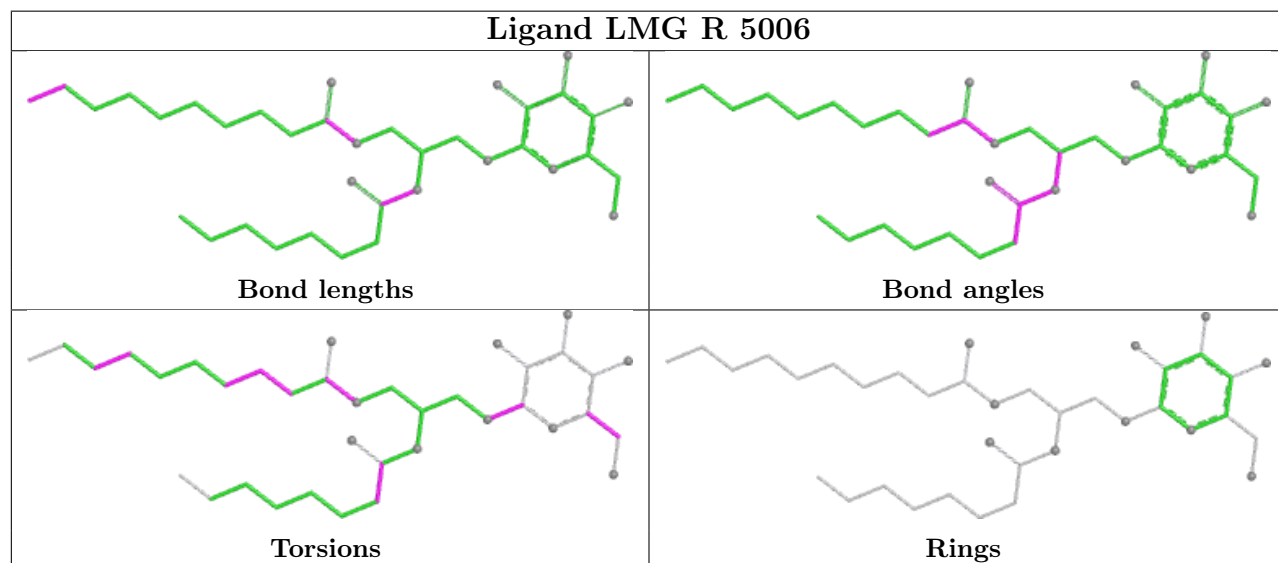
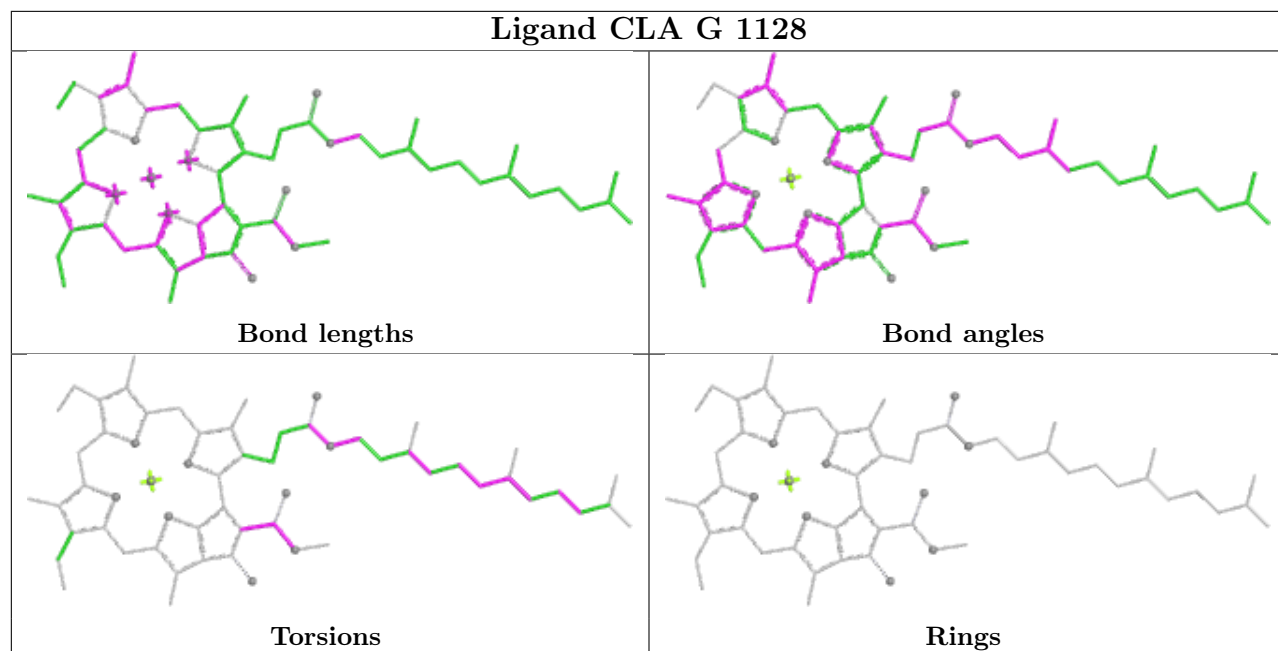


Ligand CLA H 1206

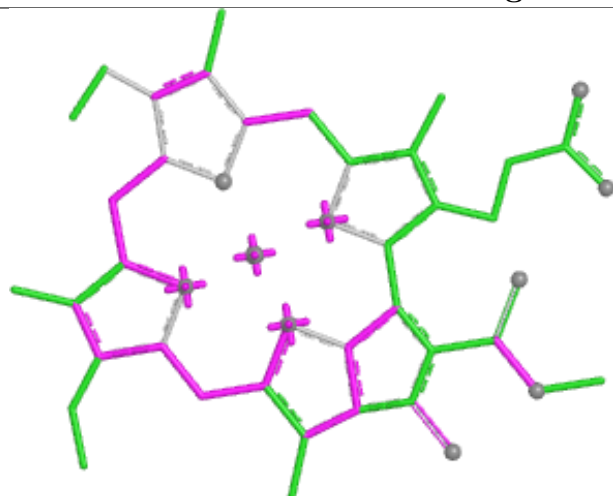




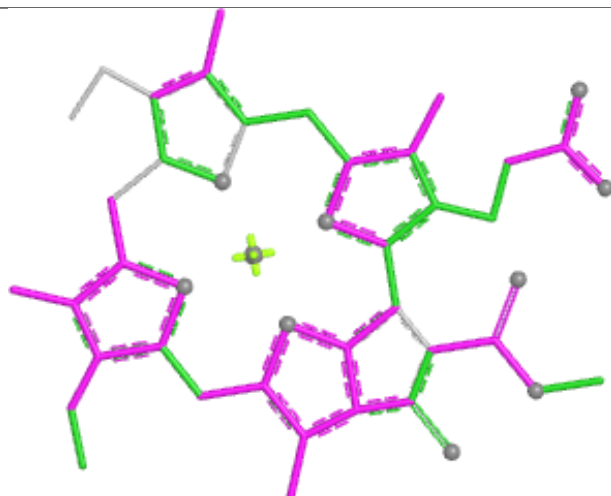




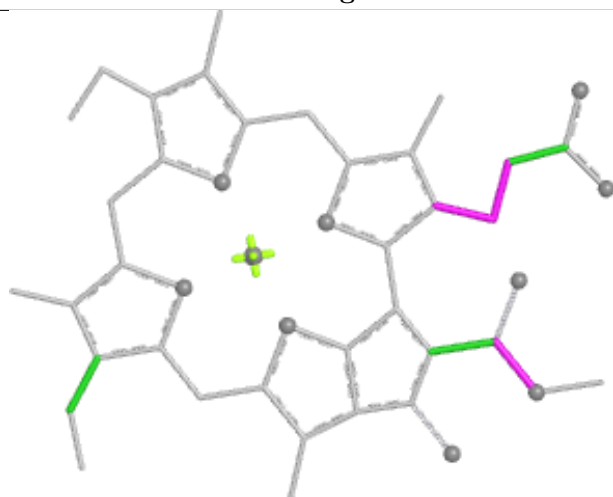
Ligand CLA B 1227



Bond lengths



Bond angles

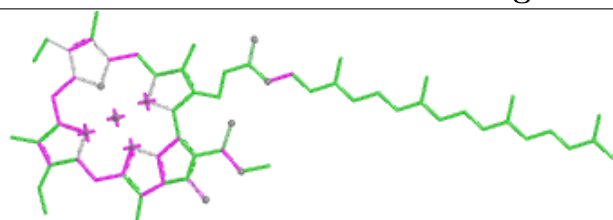


Torsions

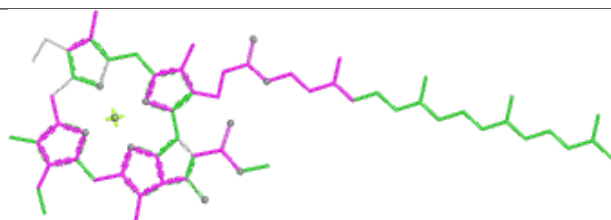


Rings

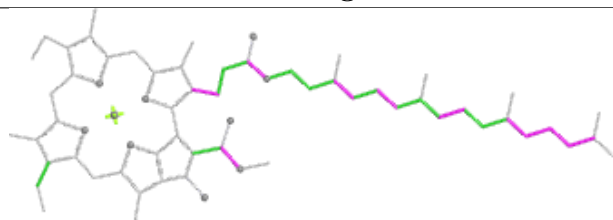
Ligand CLA I 1503



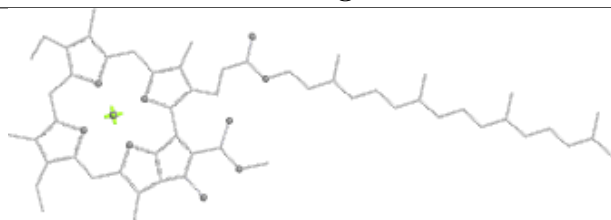
Bond lengths



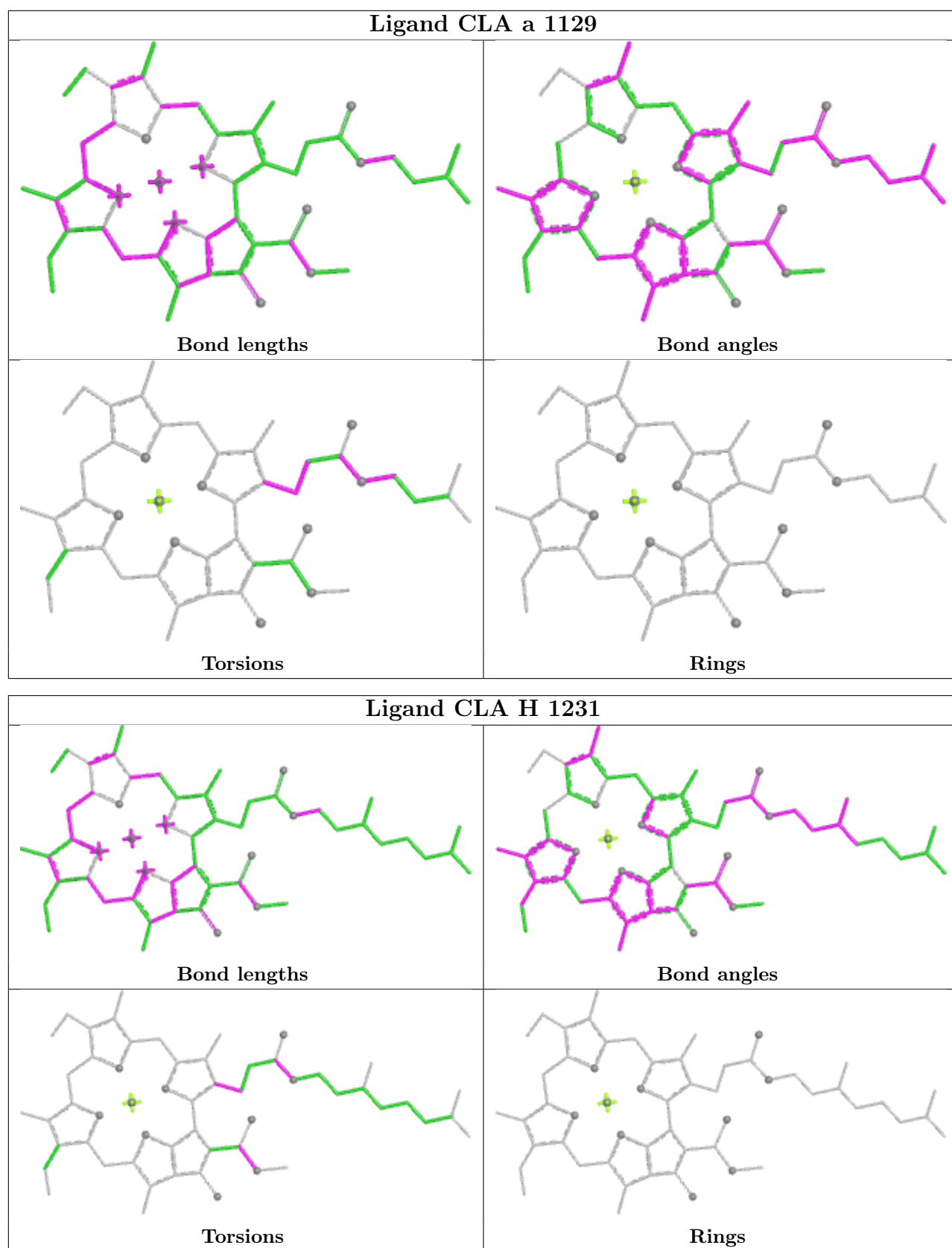
Bond angles

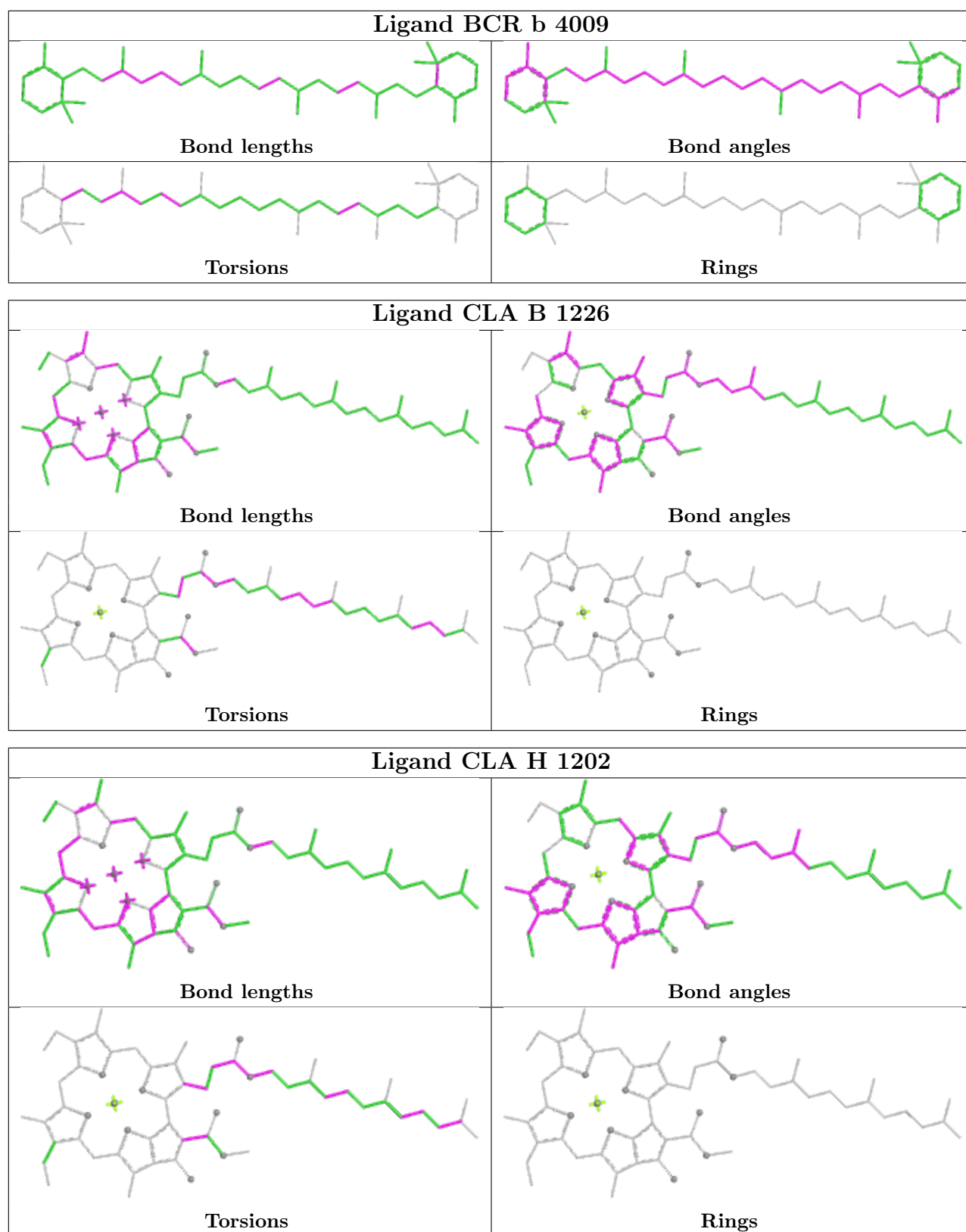


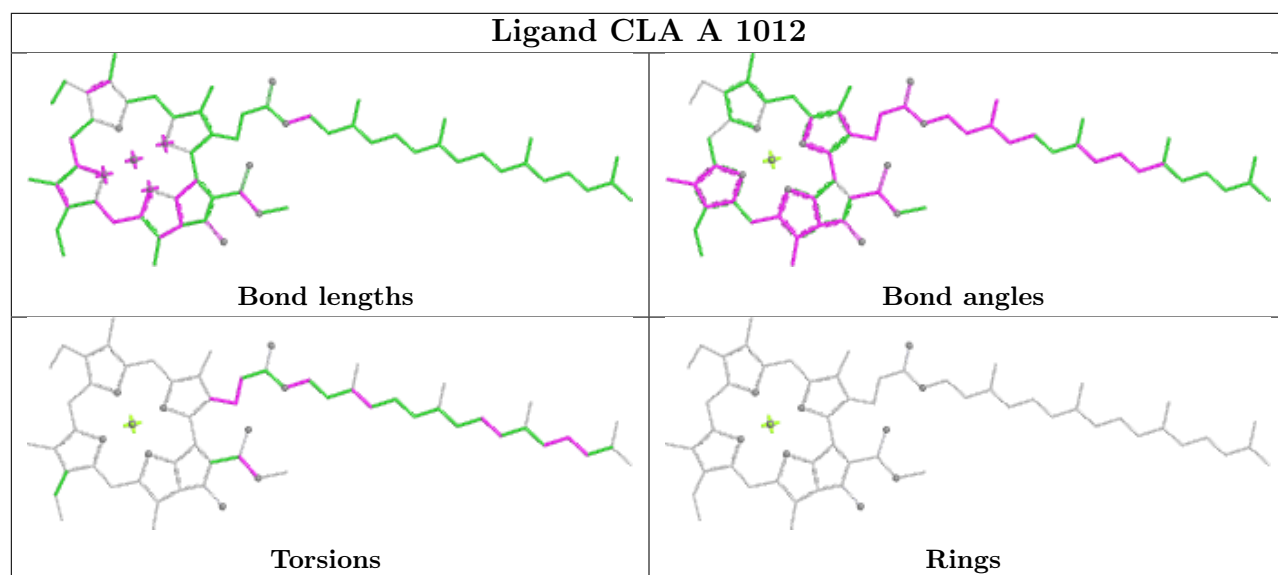
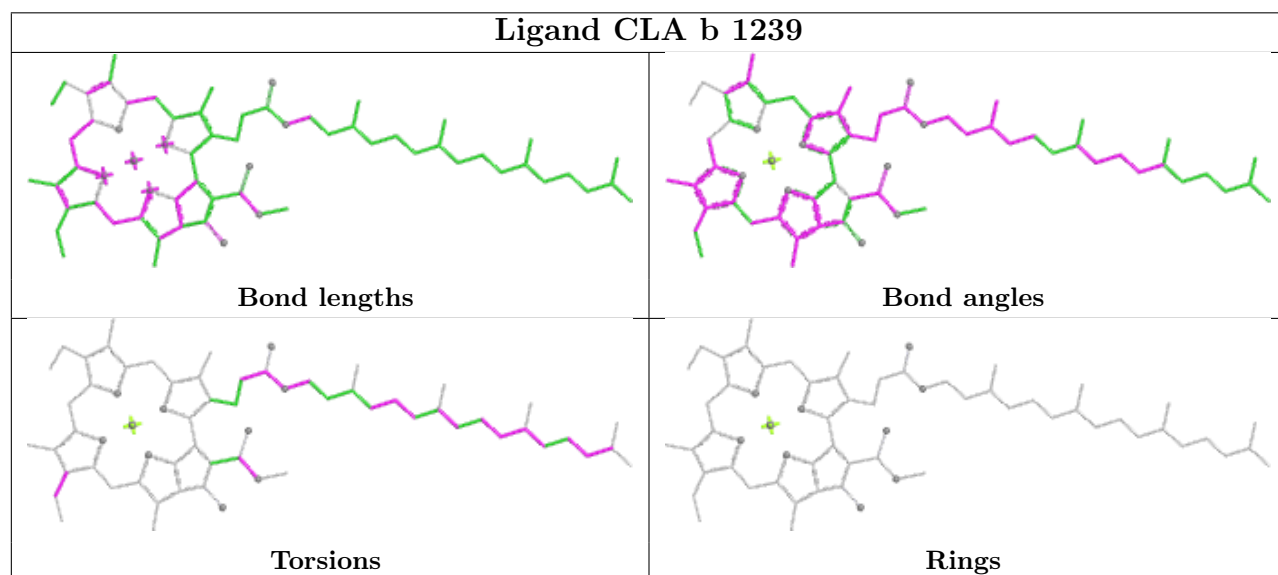
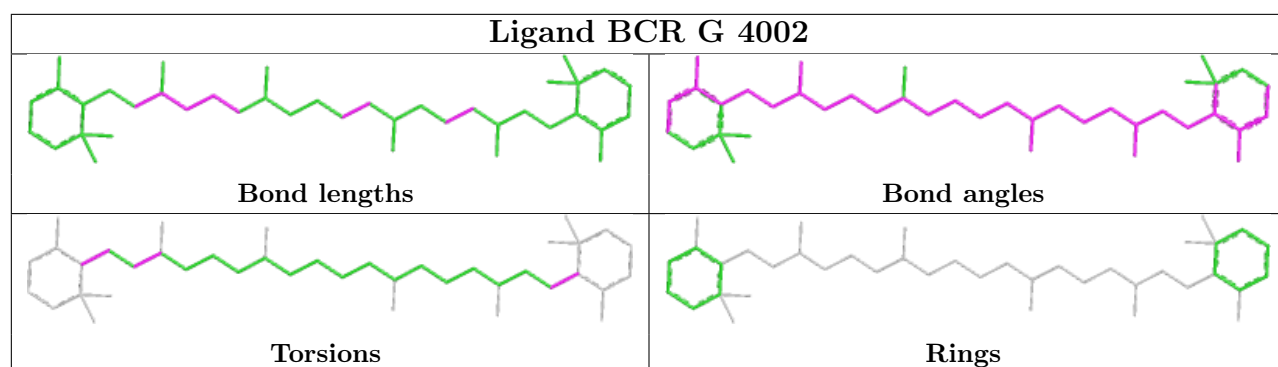
Torsions

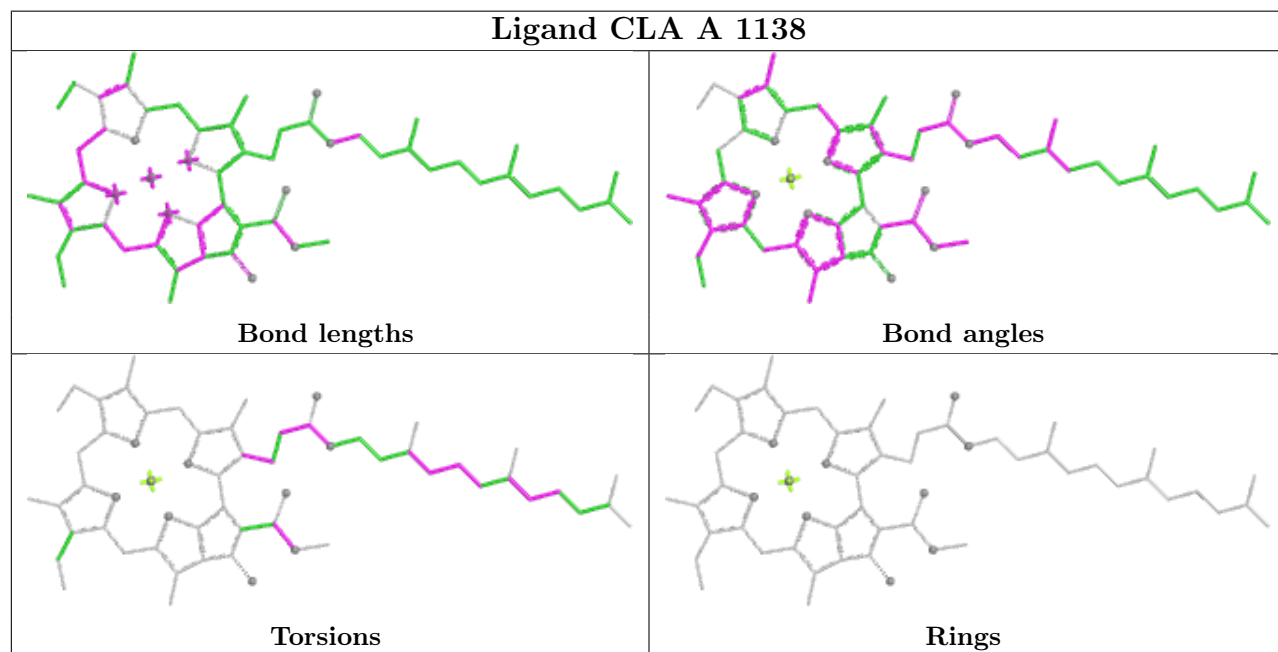
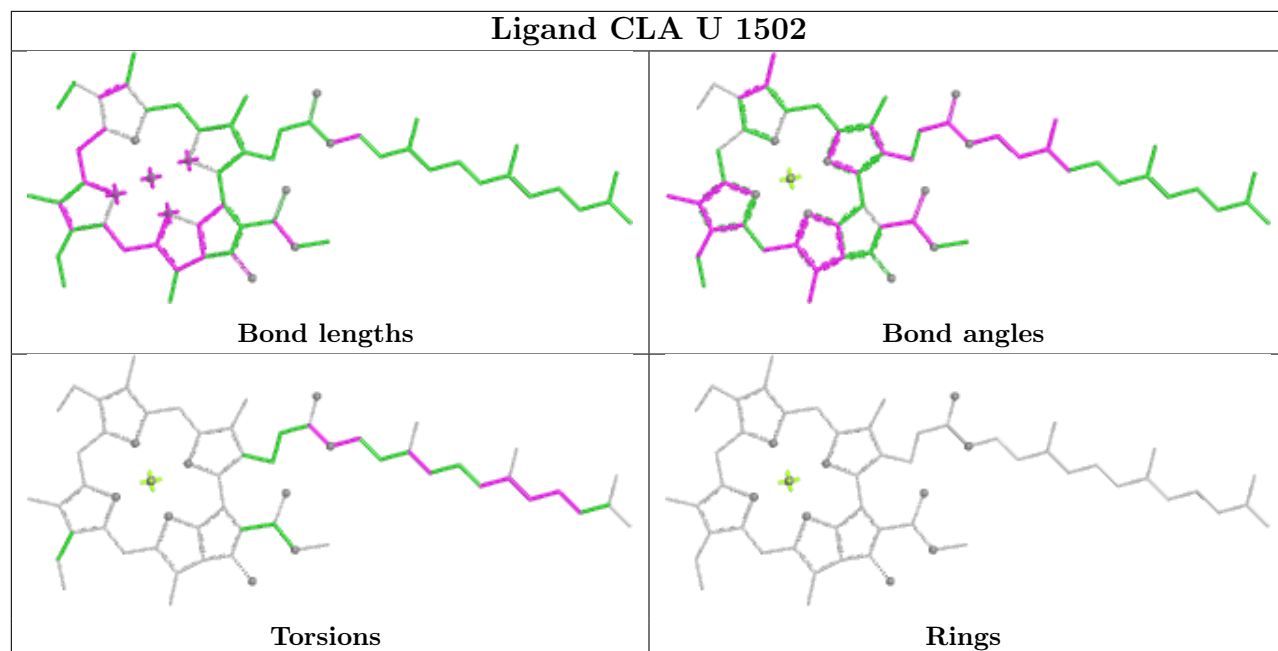


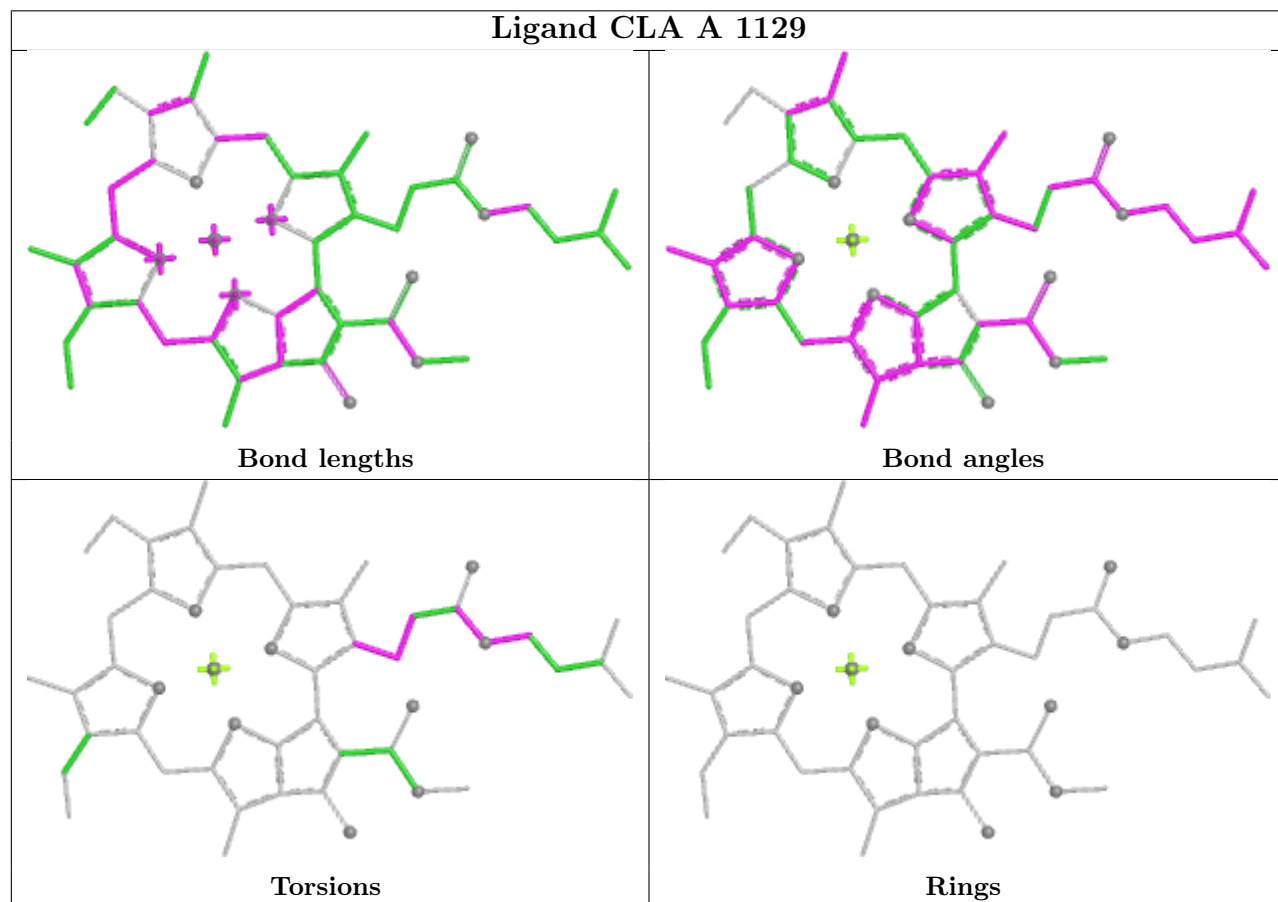
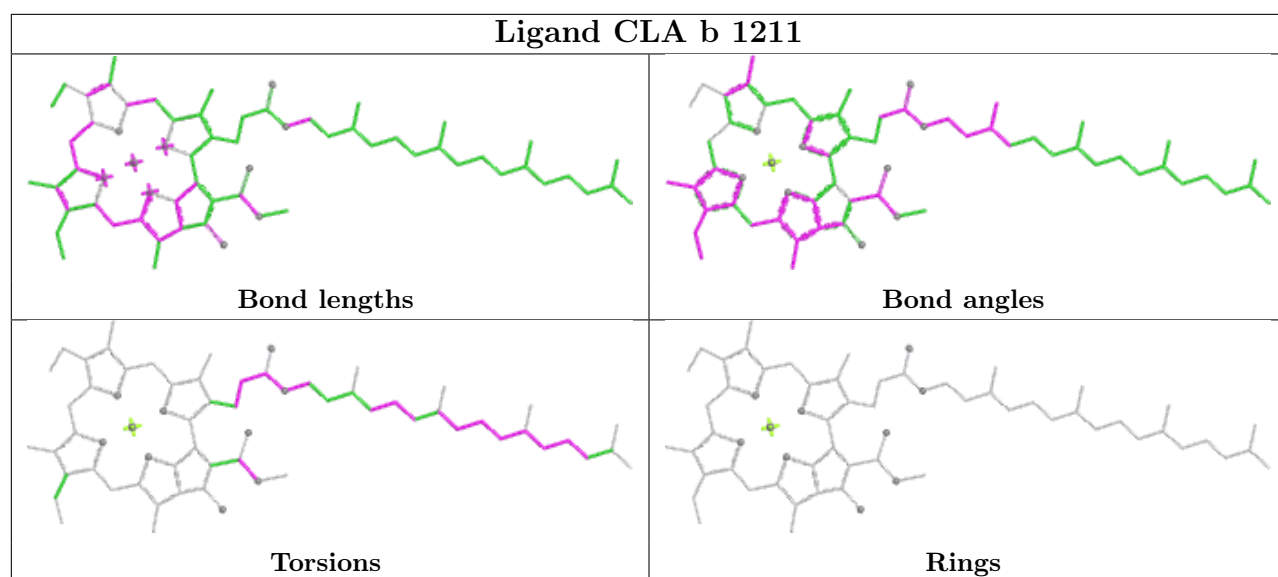
Rings

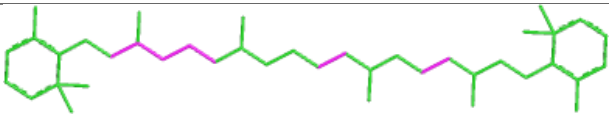
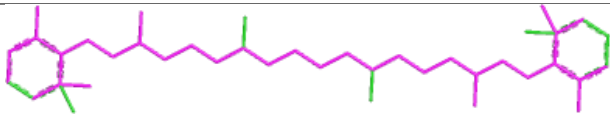
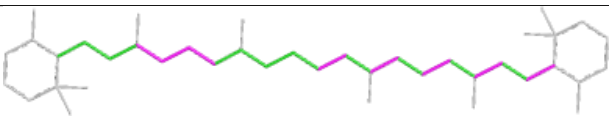
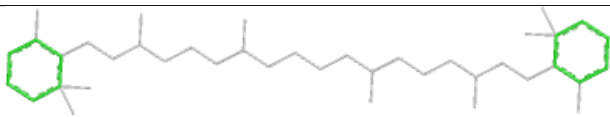


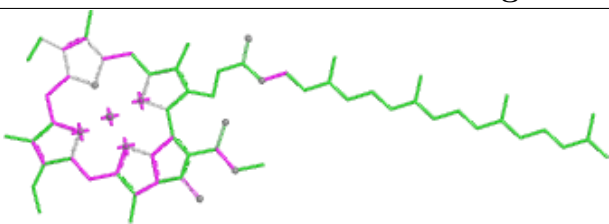
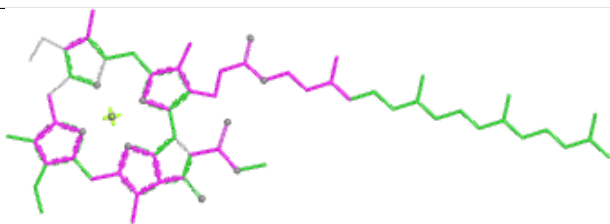
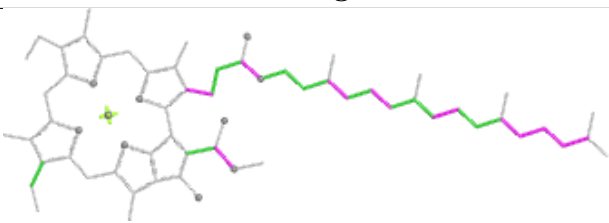
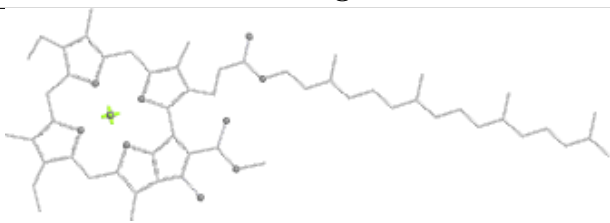


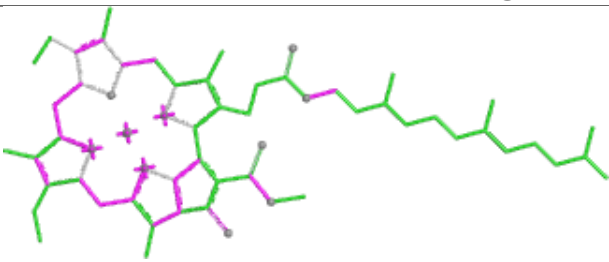
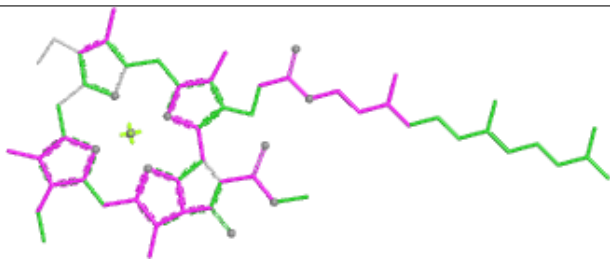
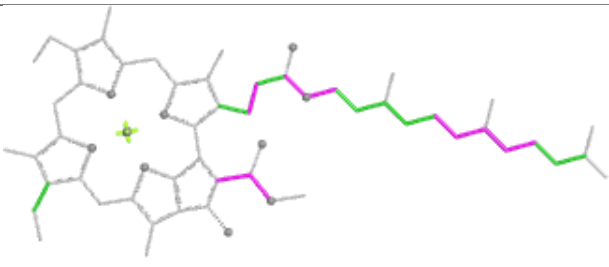
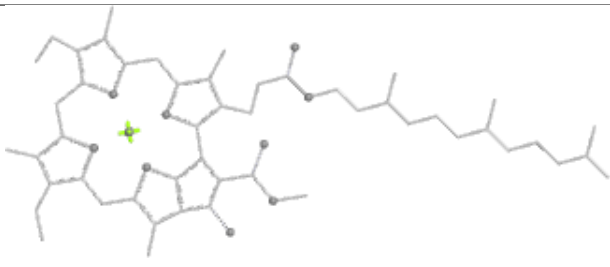


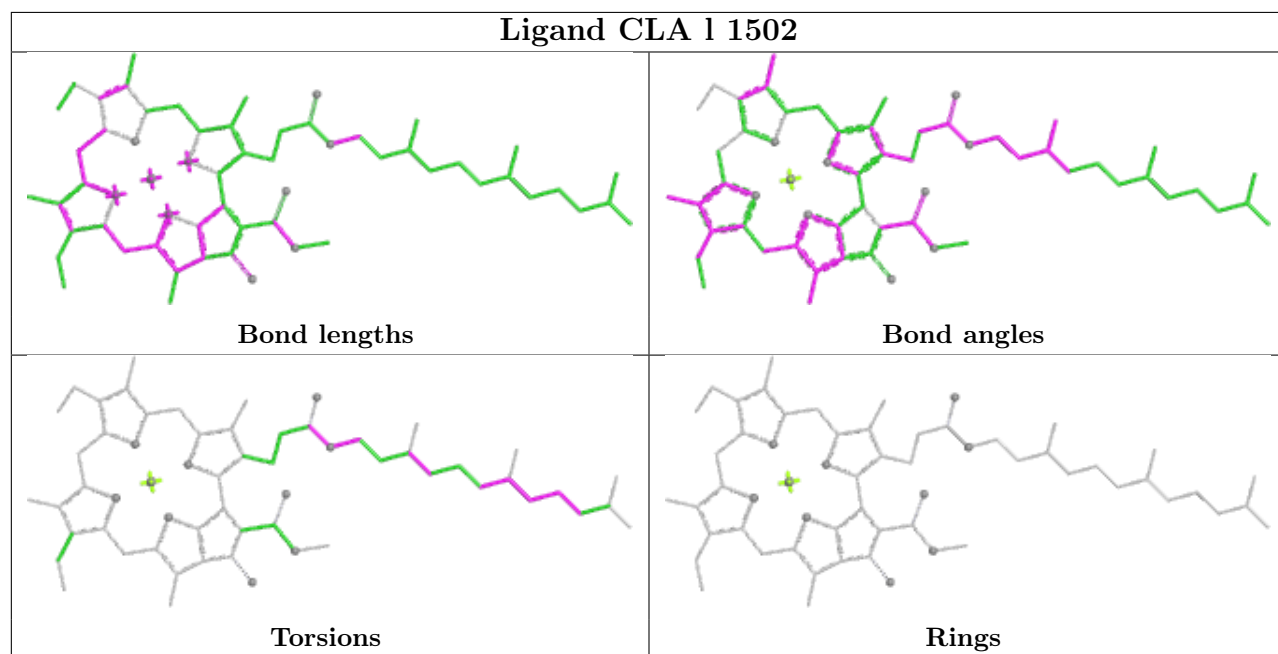
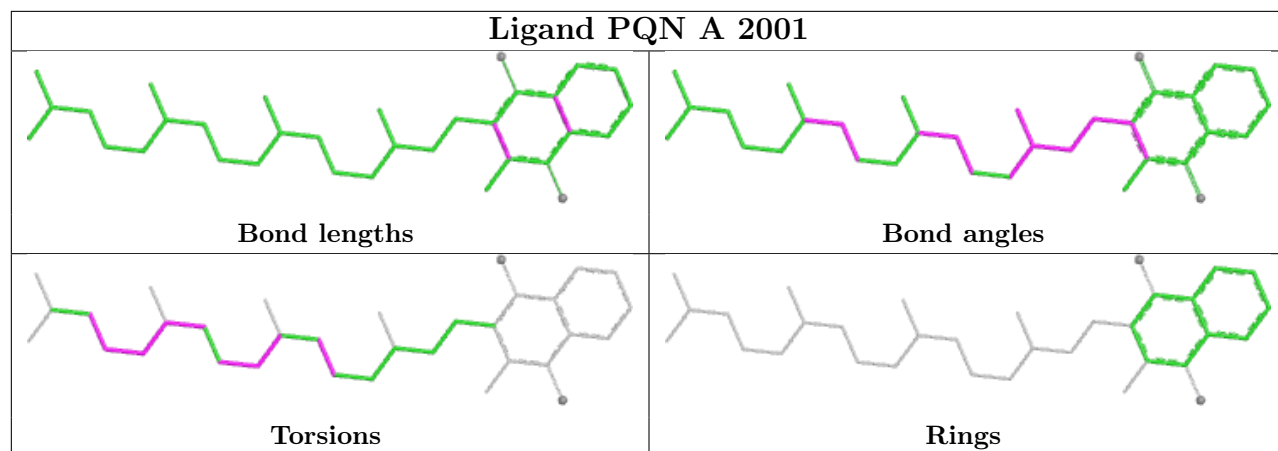


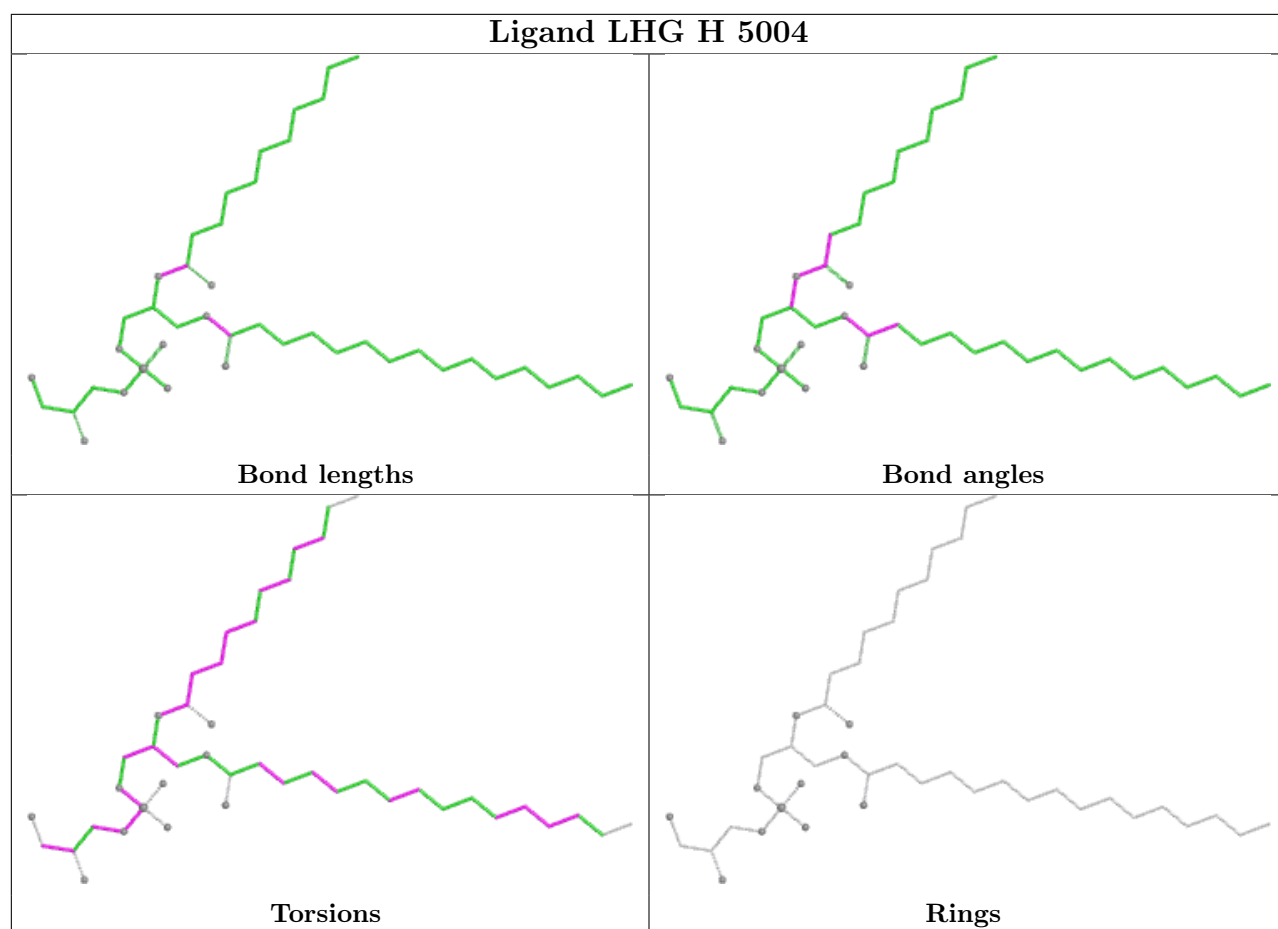


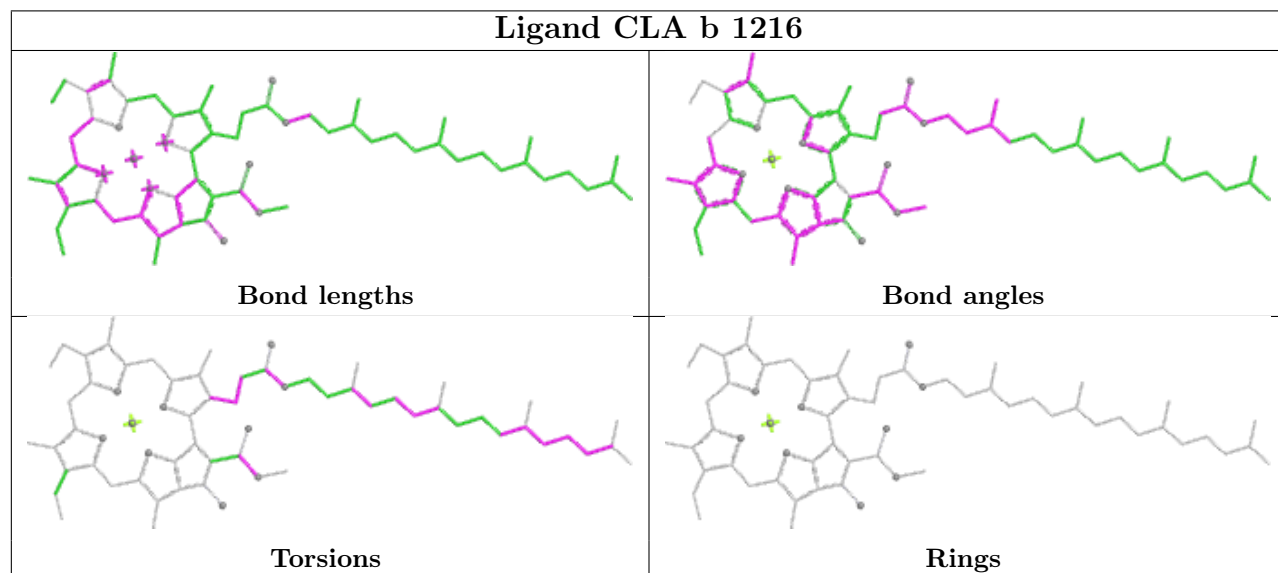
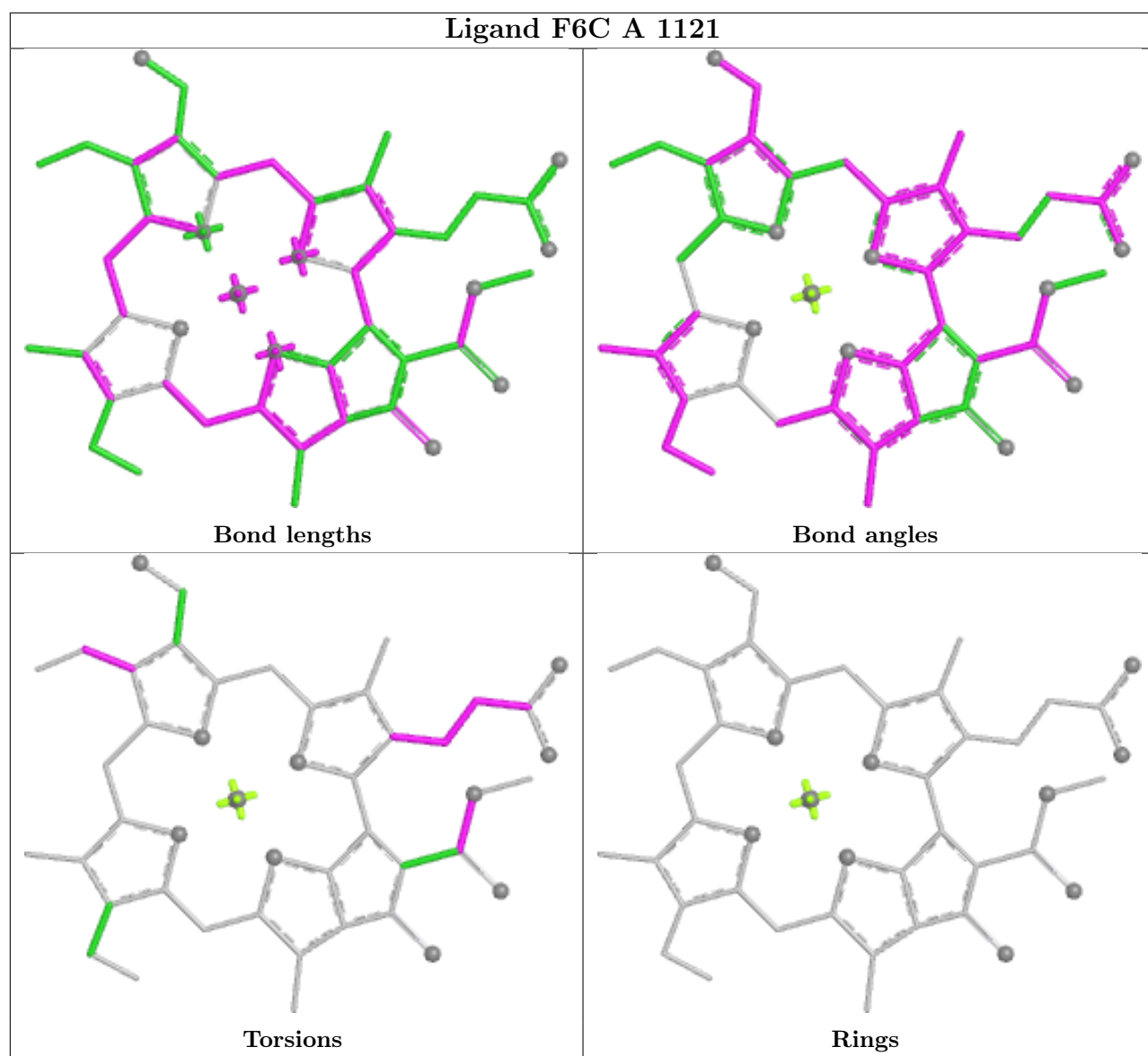
Ligand BCR I 4019	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA L 1503	
	
Bond lengths	Bond angles
	
Torsions	Rings

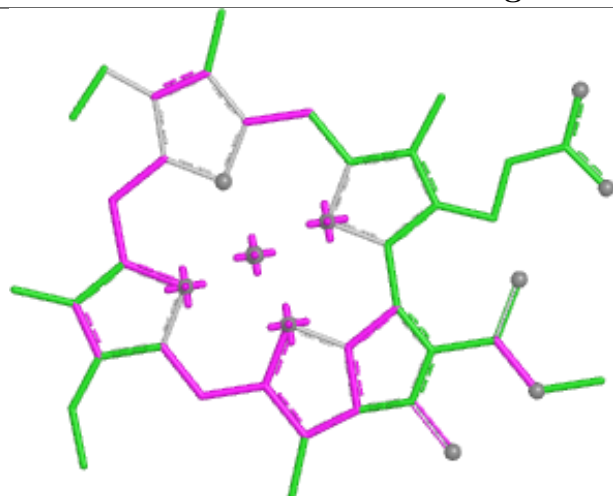
Ligand CLA A 1123	
	
Bond lengths	Bond angles
	
Torsions	Rings



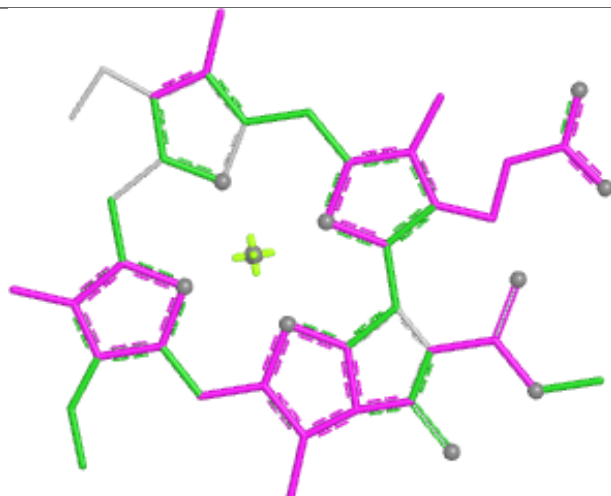




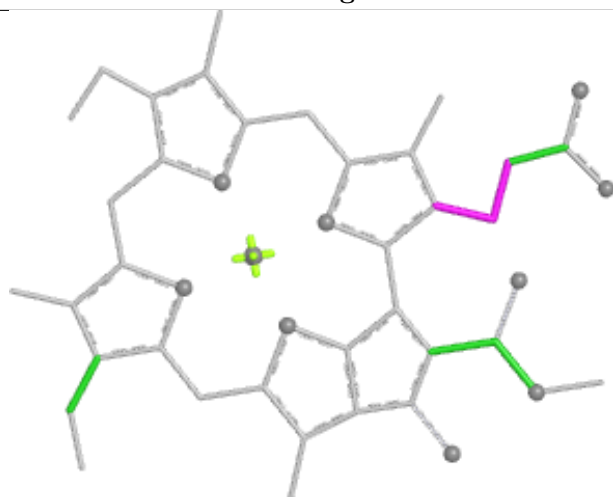
Ligand CLA H 1209



Bond lengths



Bond angles

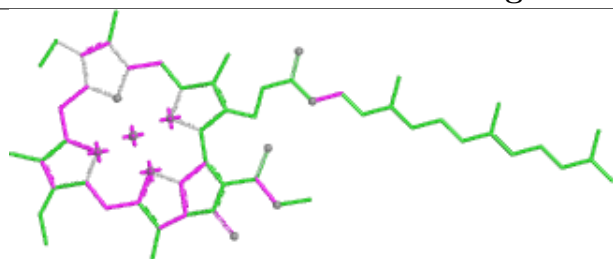


Torsions

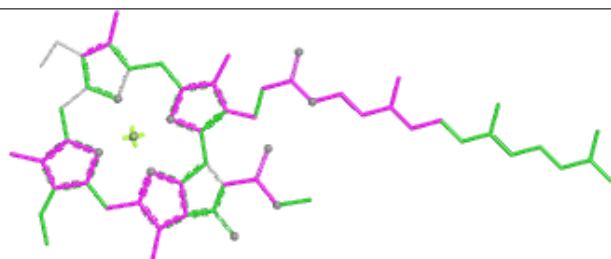


Rings

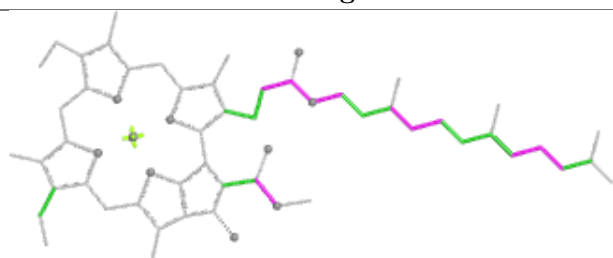
Ligand CLA B 1235



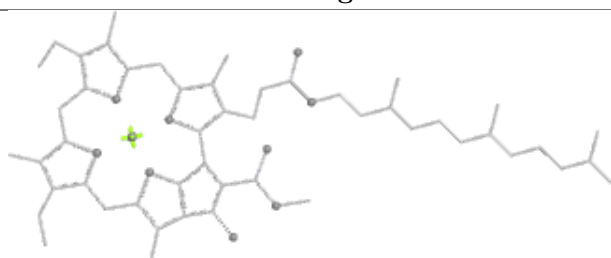
Bond lengths



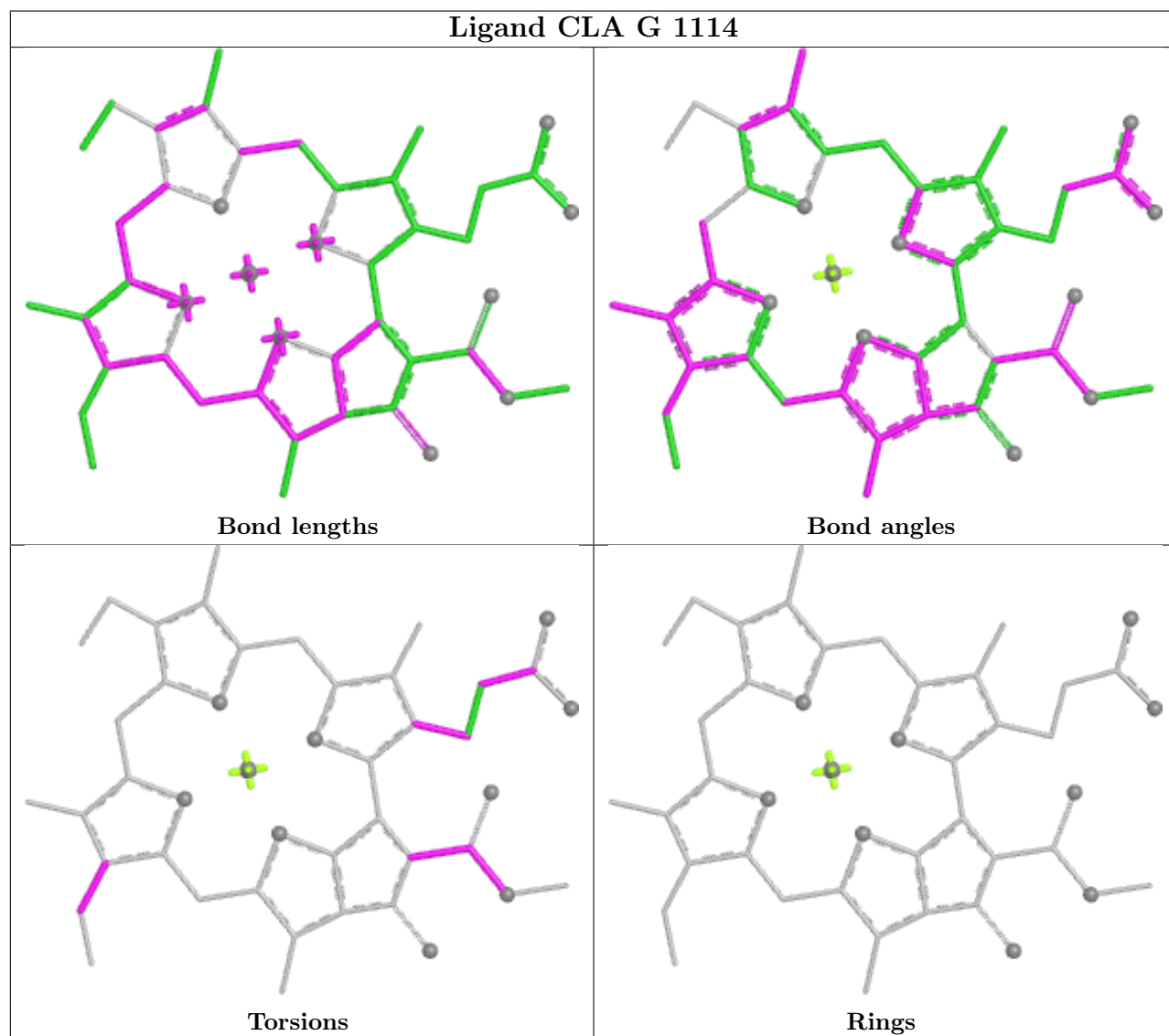
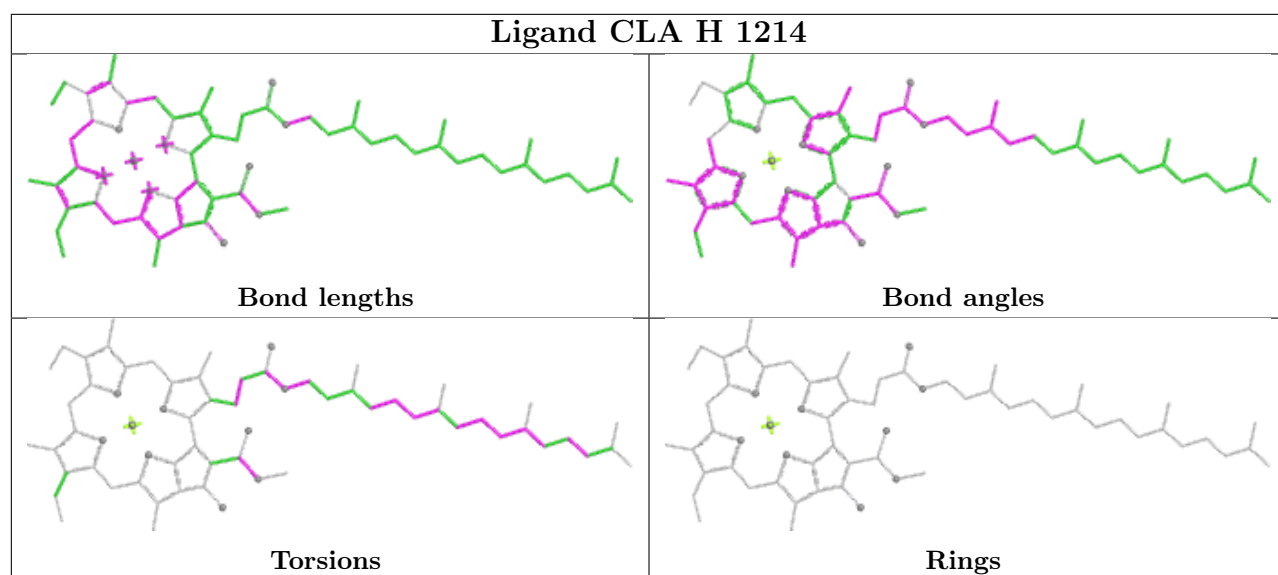
Bond angles



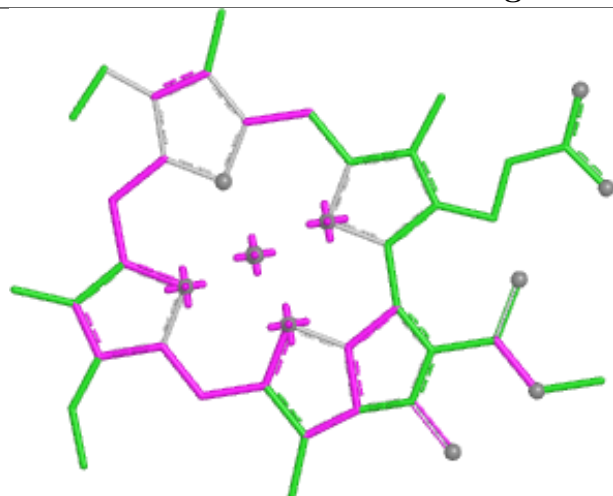
Torsions



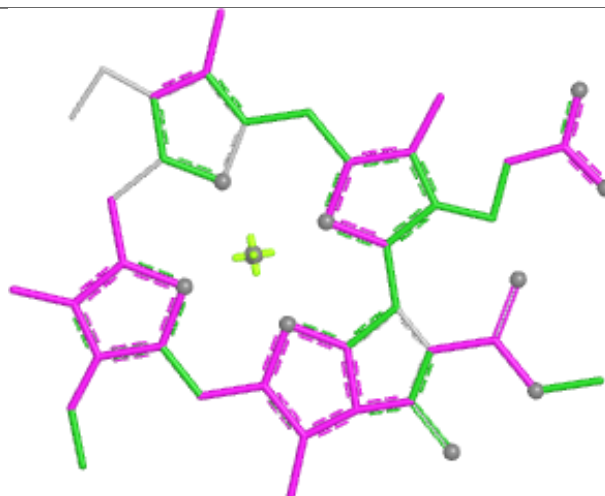
Rings



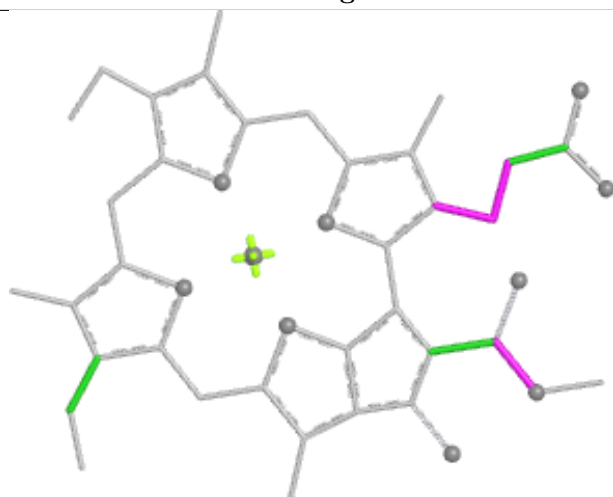
Ligand CLA H 1227



Bond lengths



Bond angles

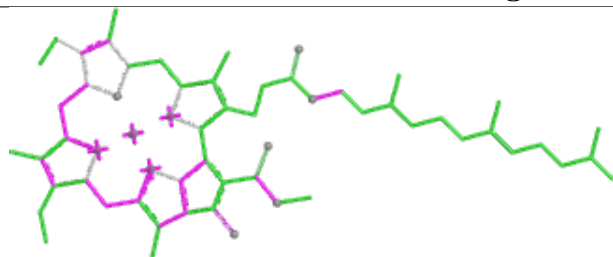


Torsions

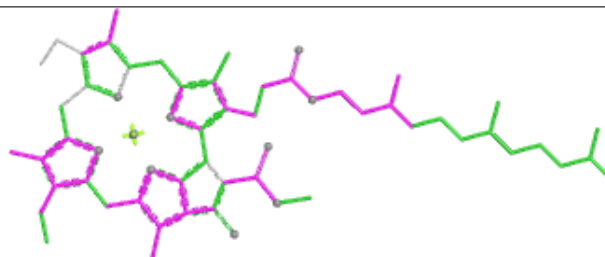


Rings

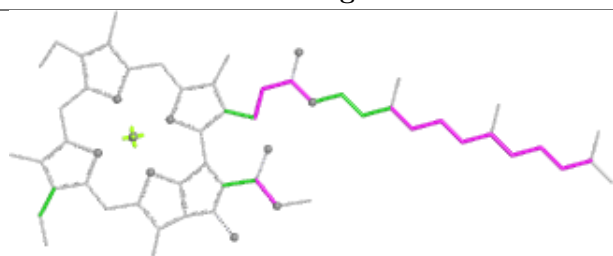
Ligand CLA A 1126



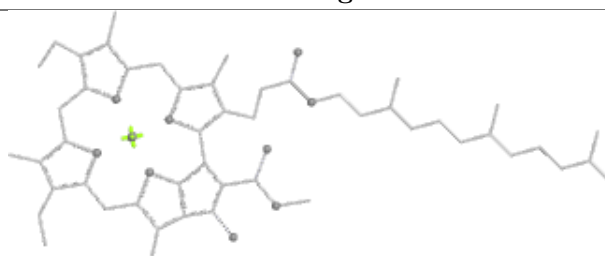
Bond lengths



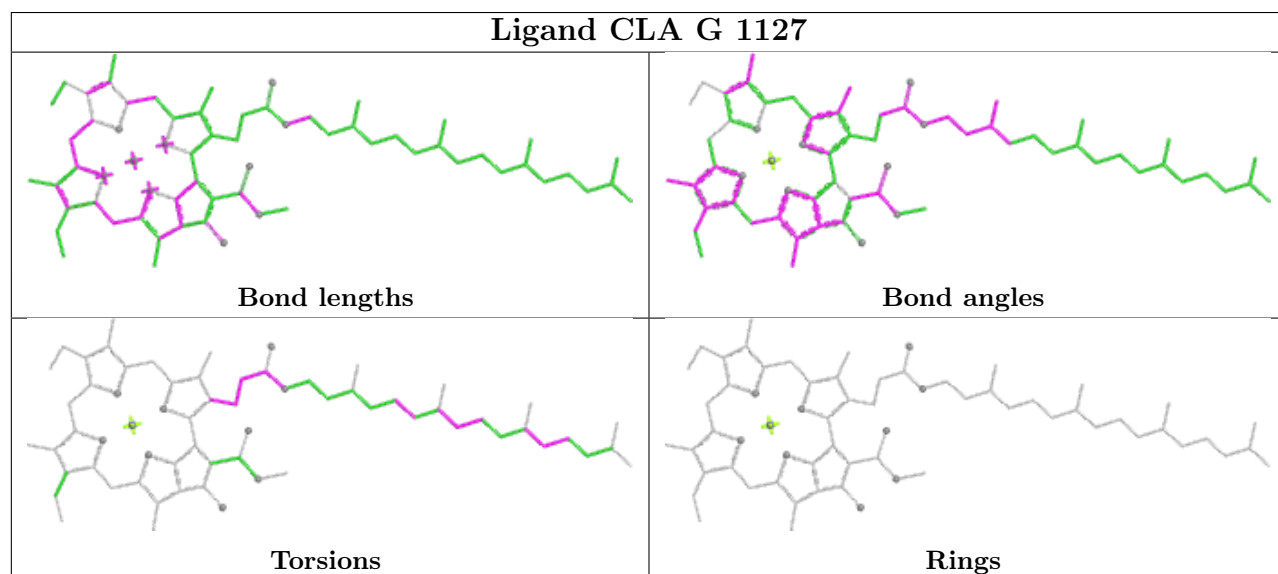
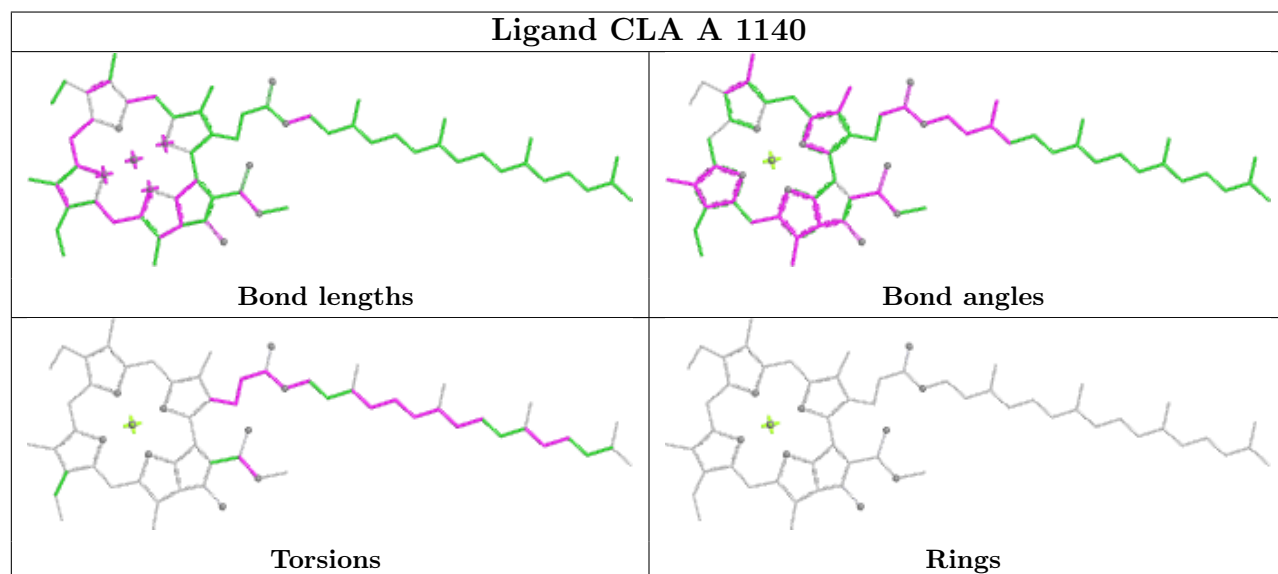
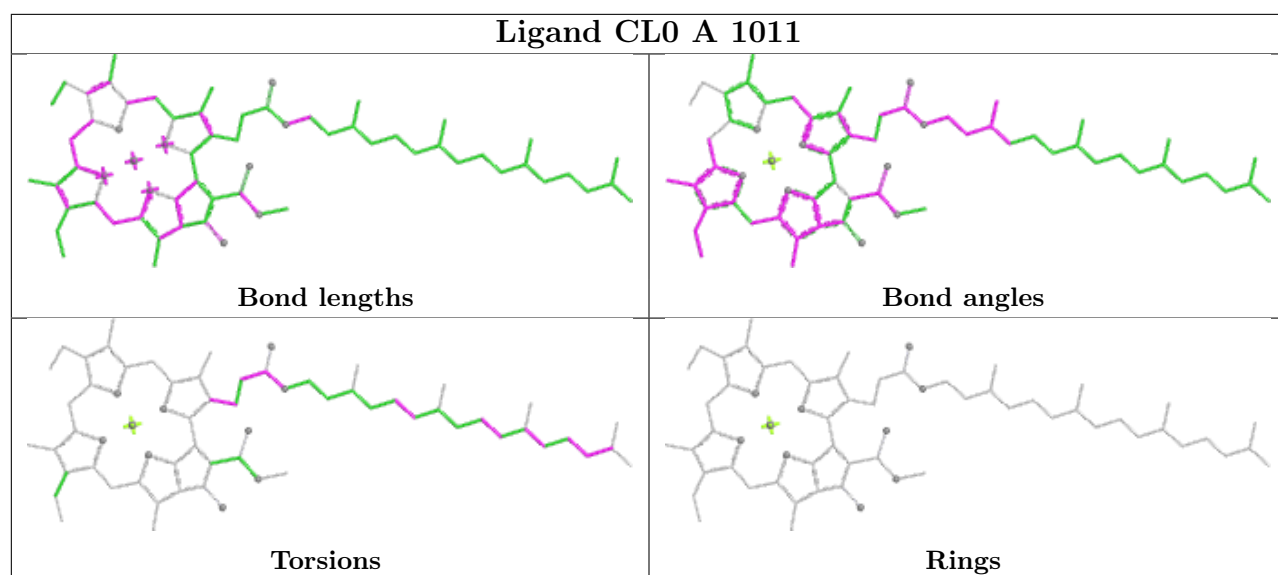
Bond angles



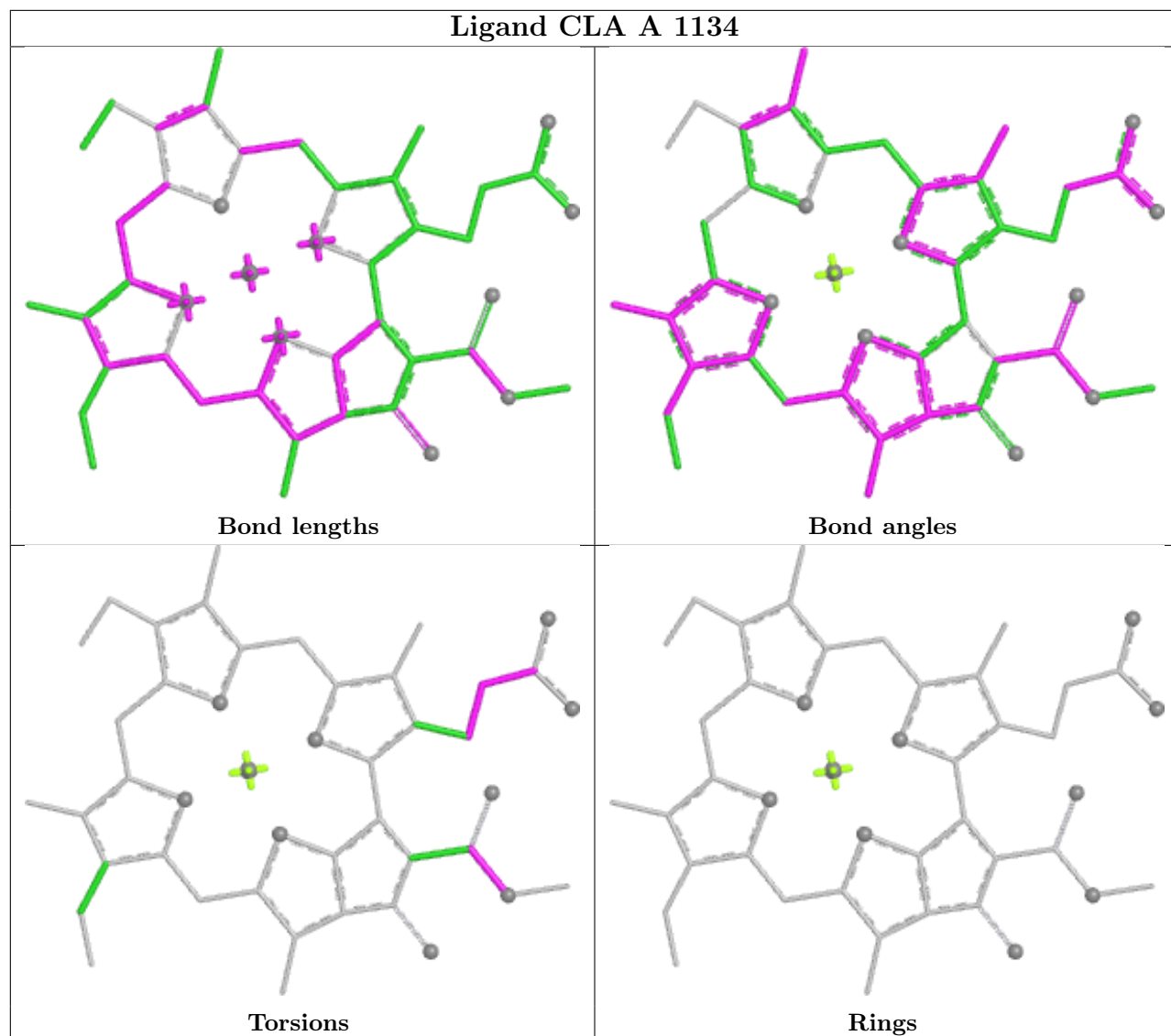
Torsions

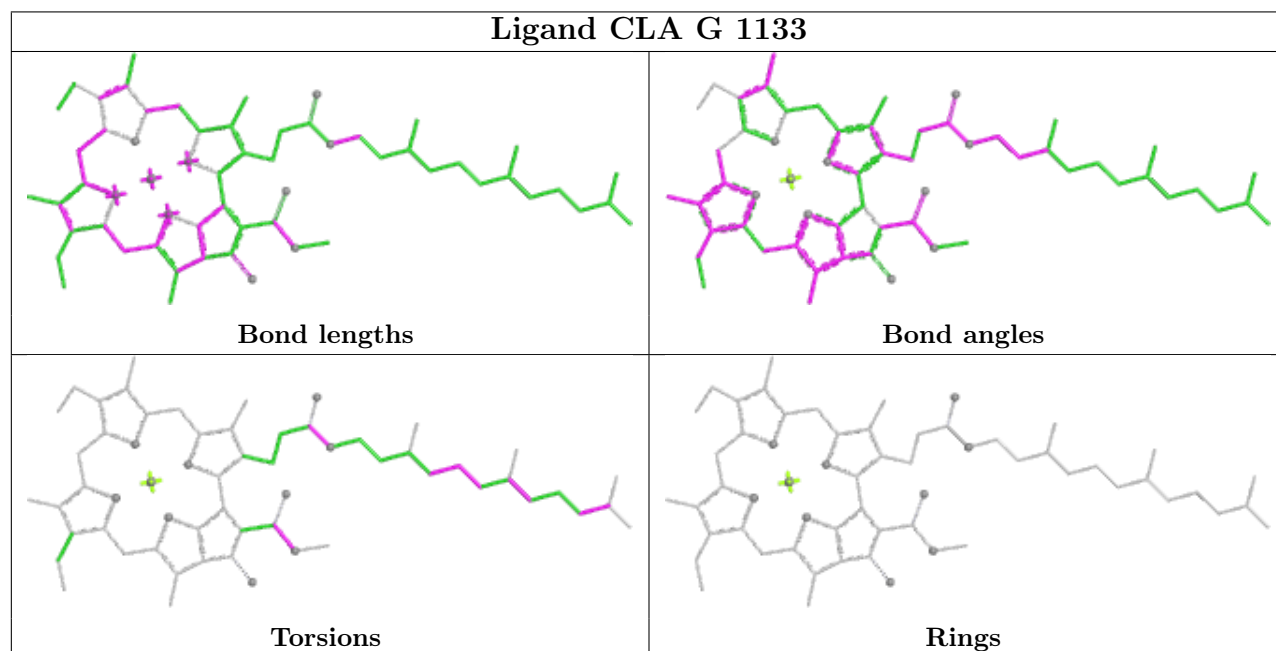
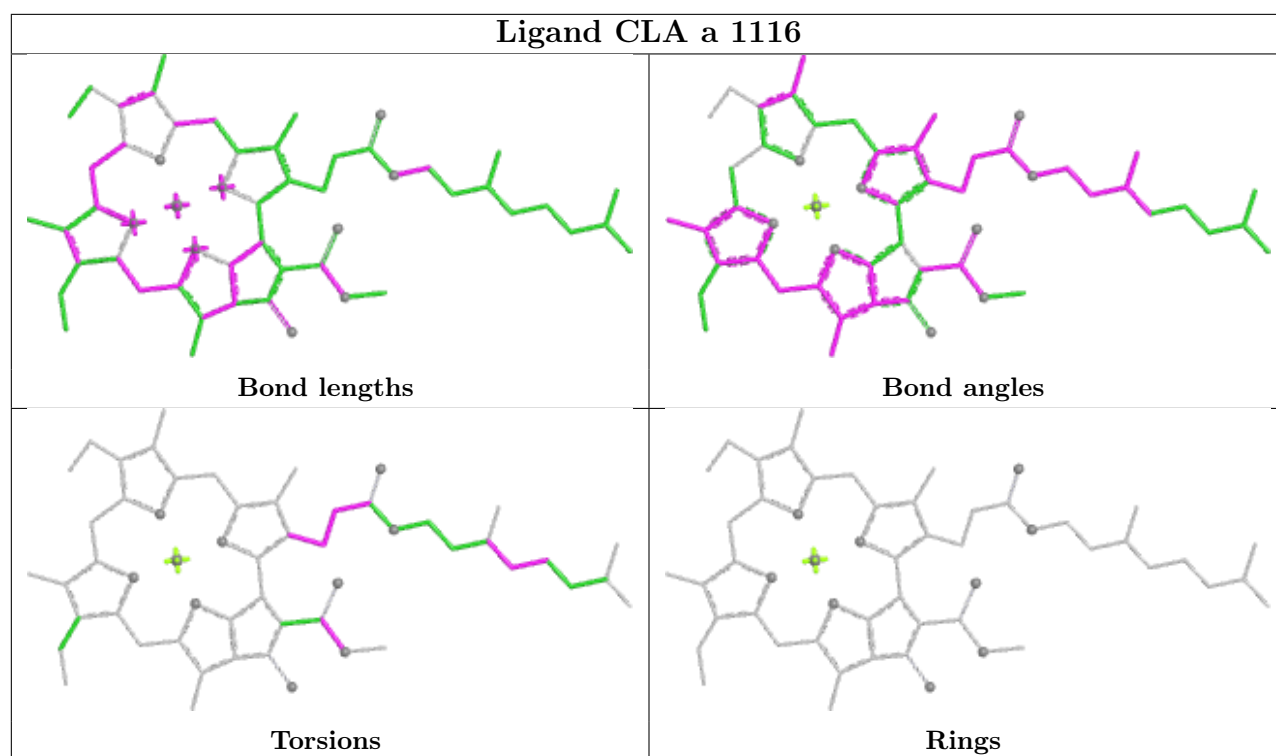


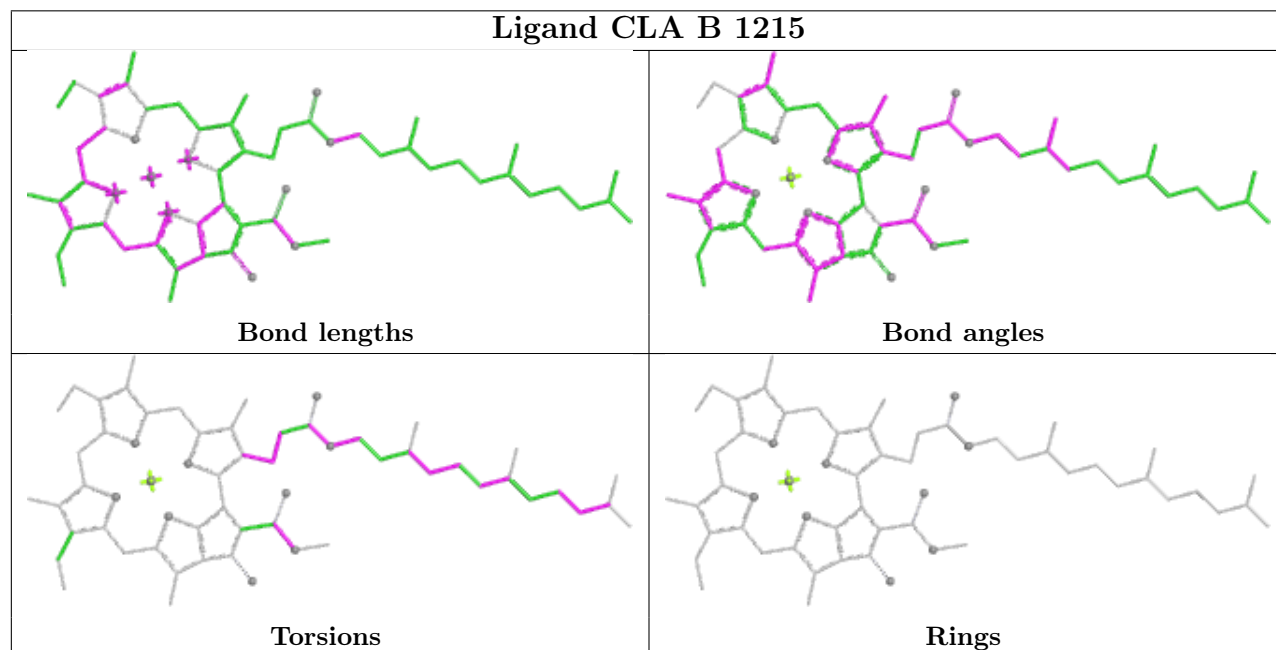
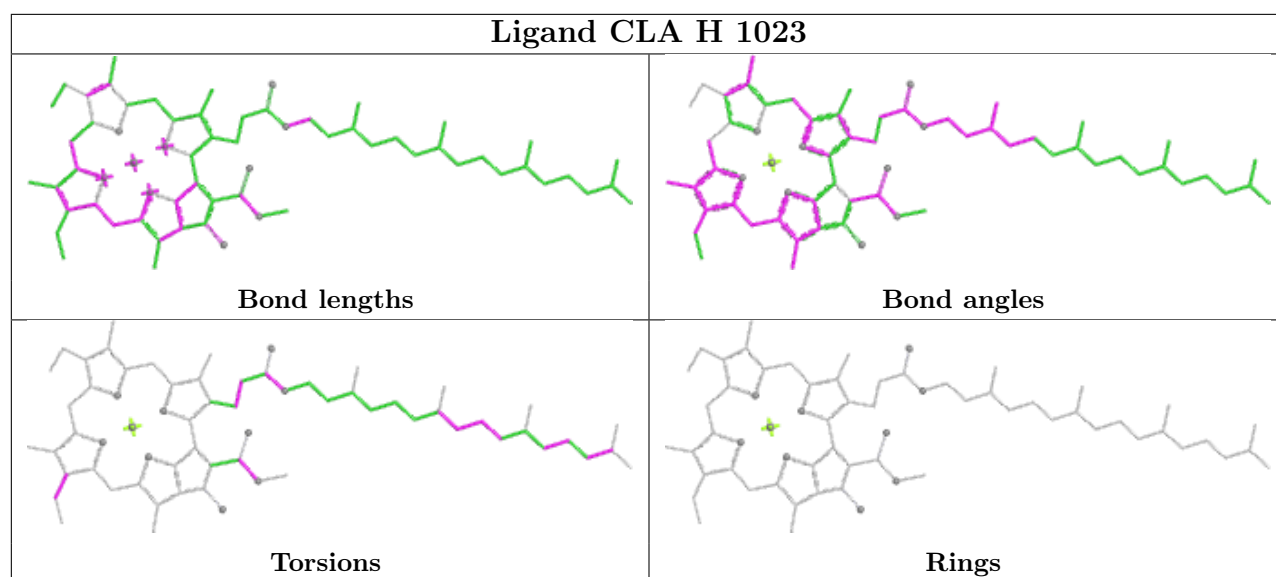
Rings

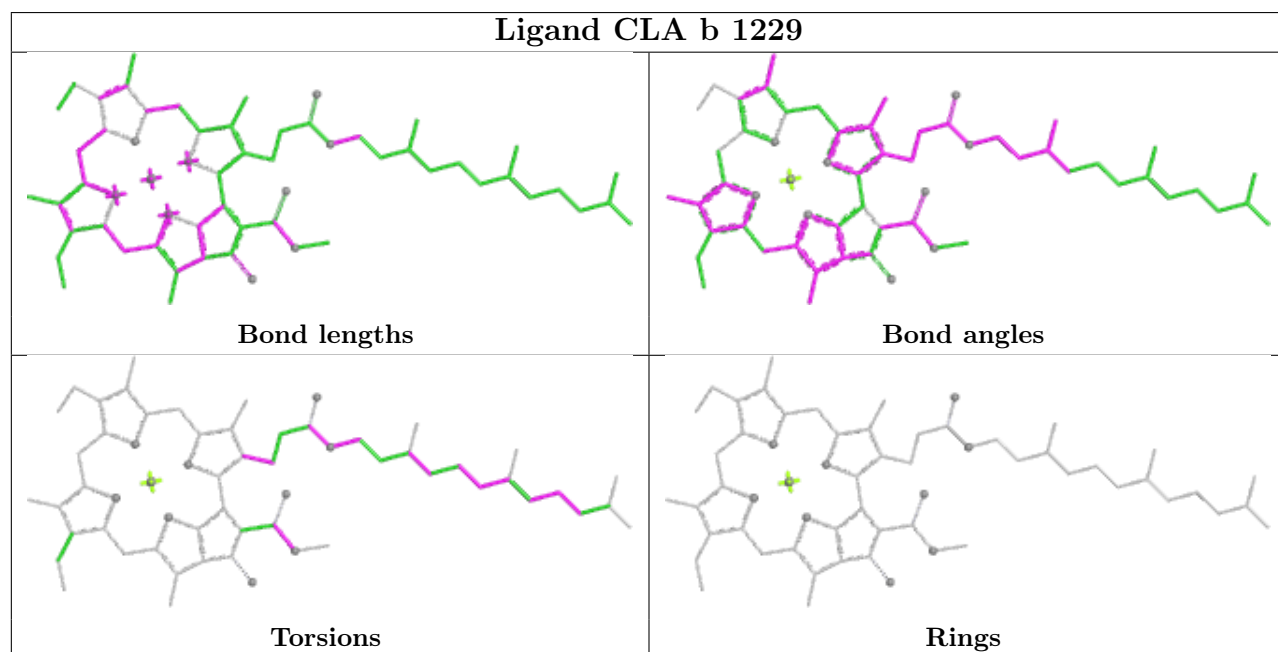
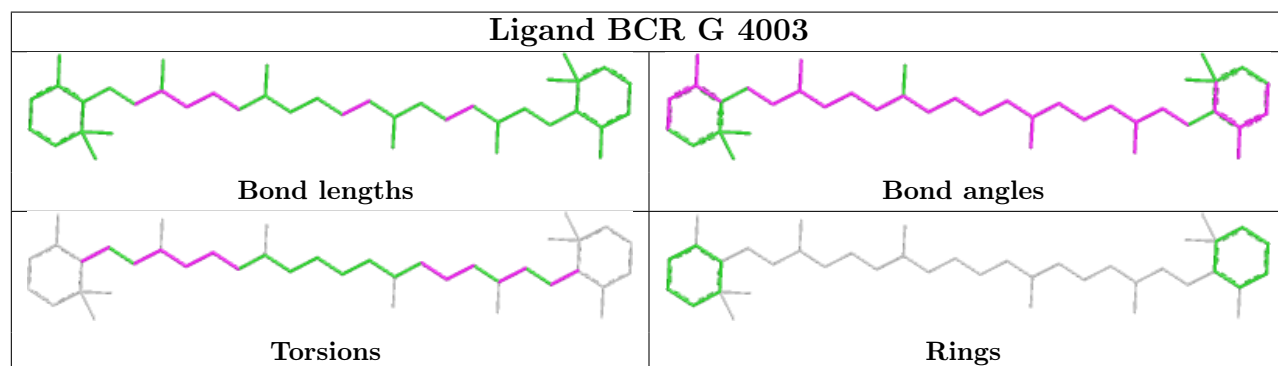
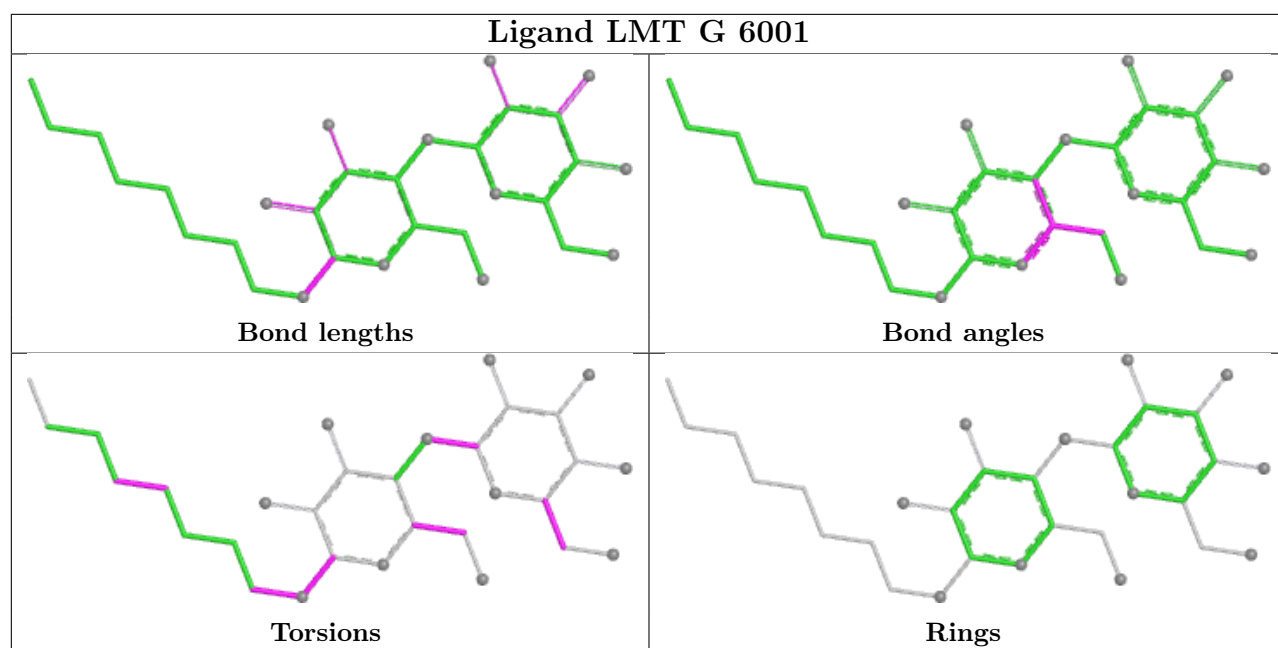


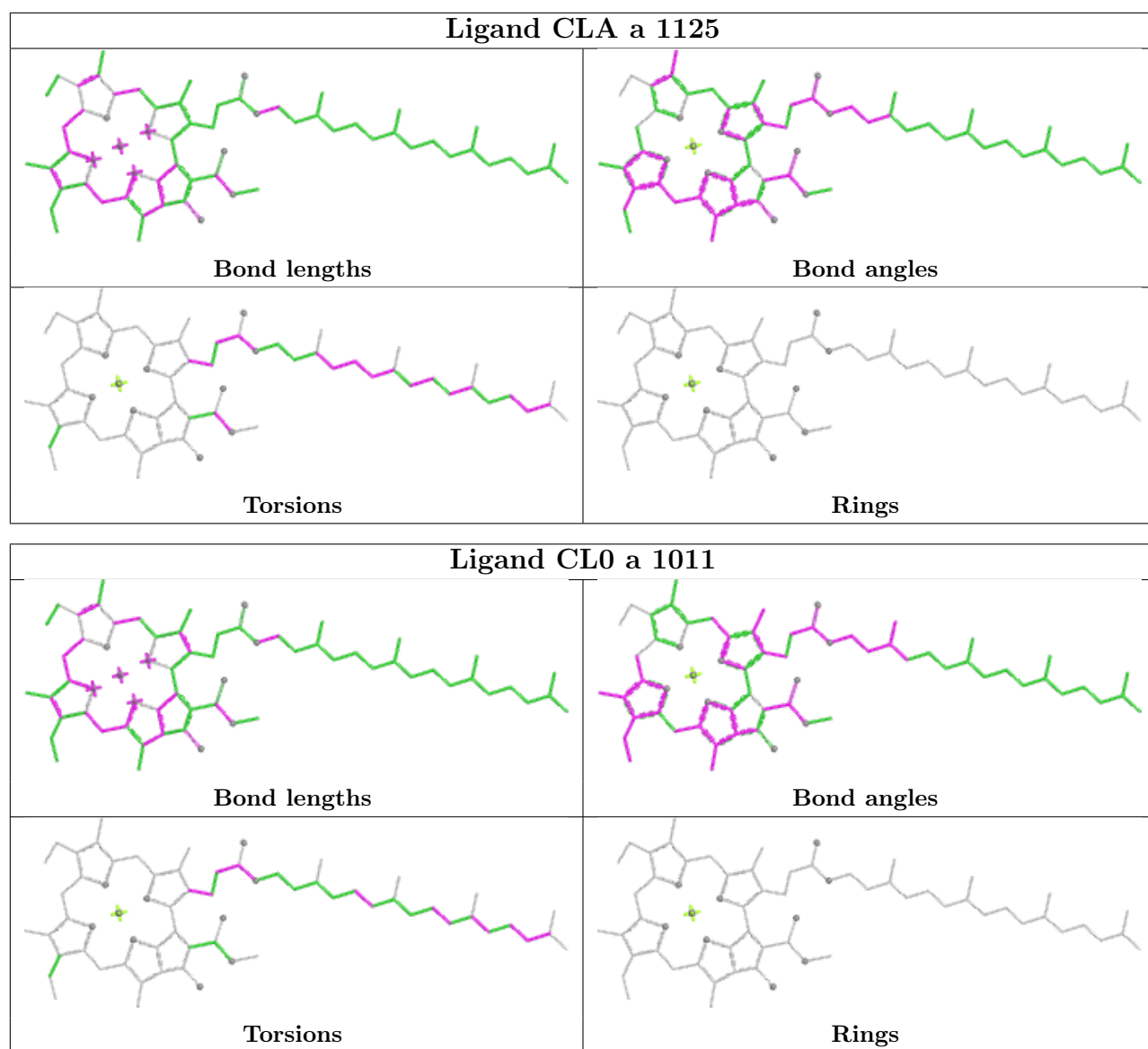
Ligand CLA A 1134



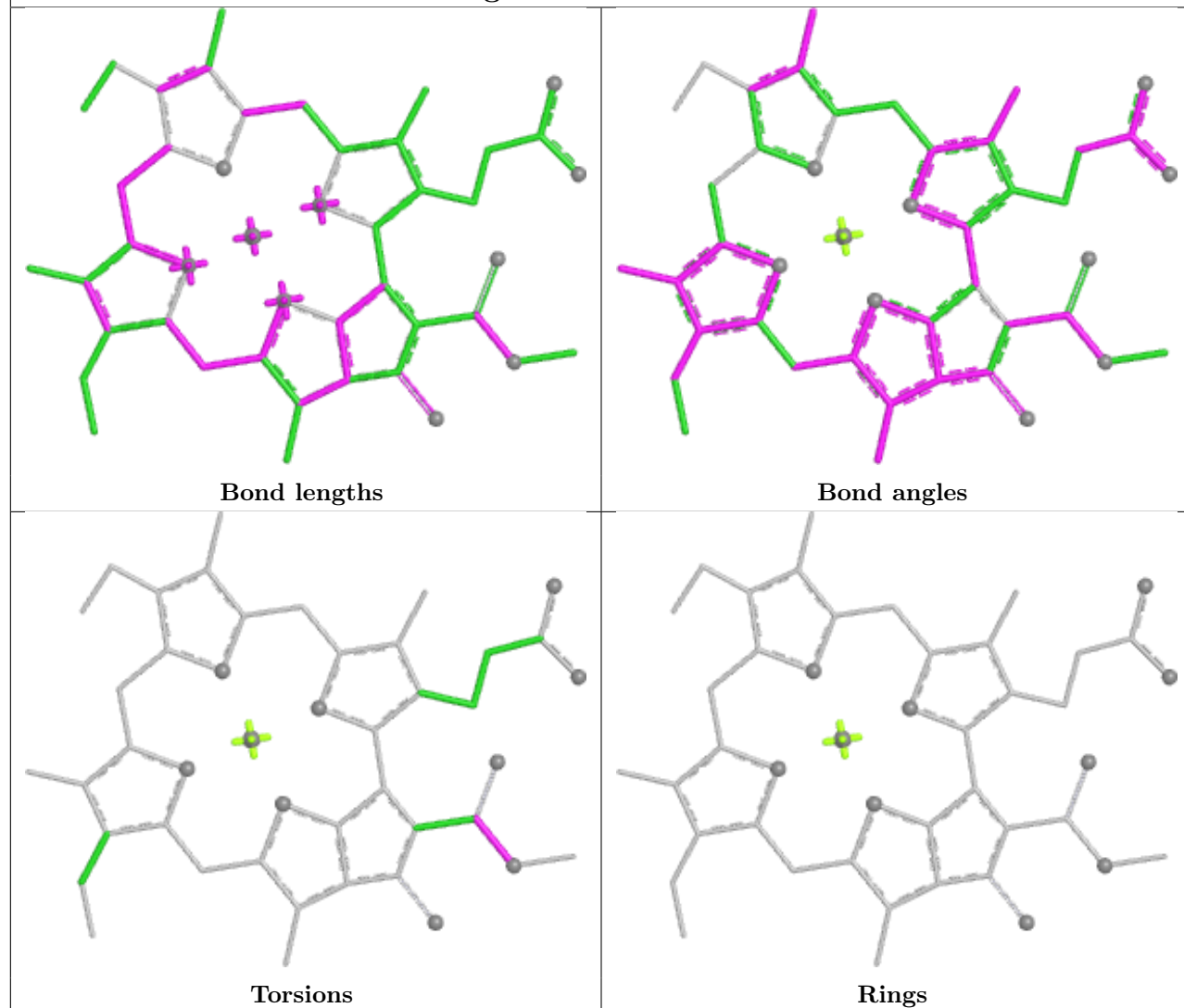




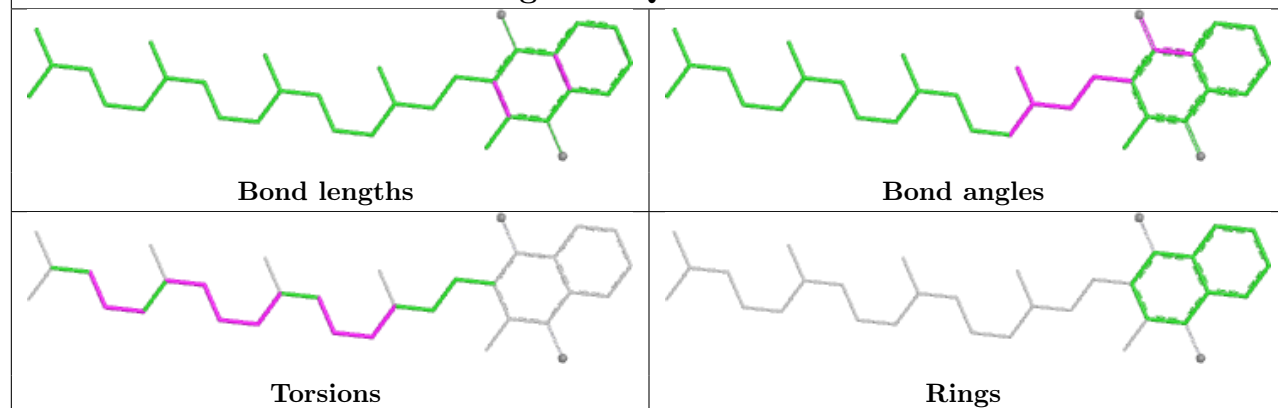


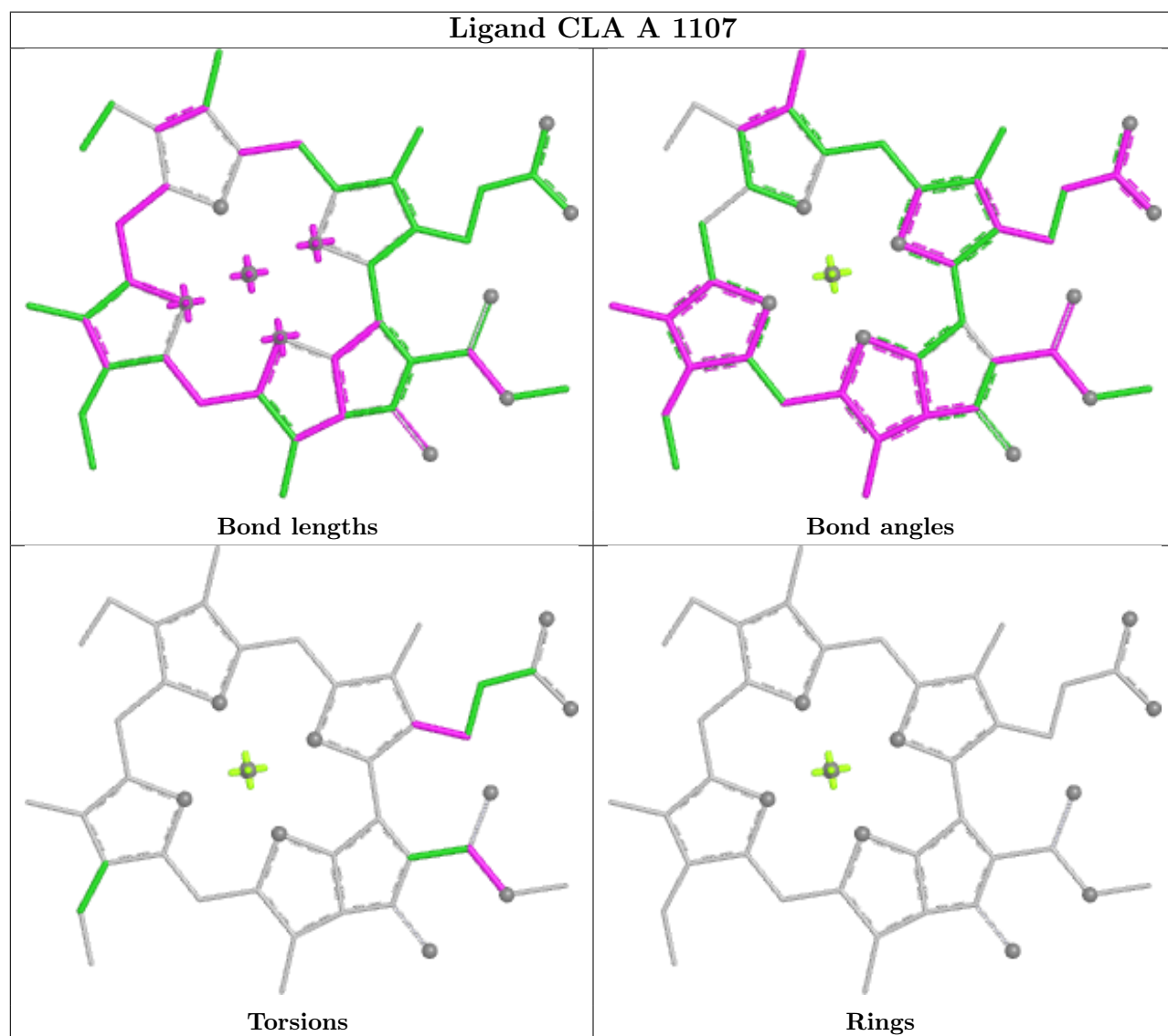
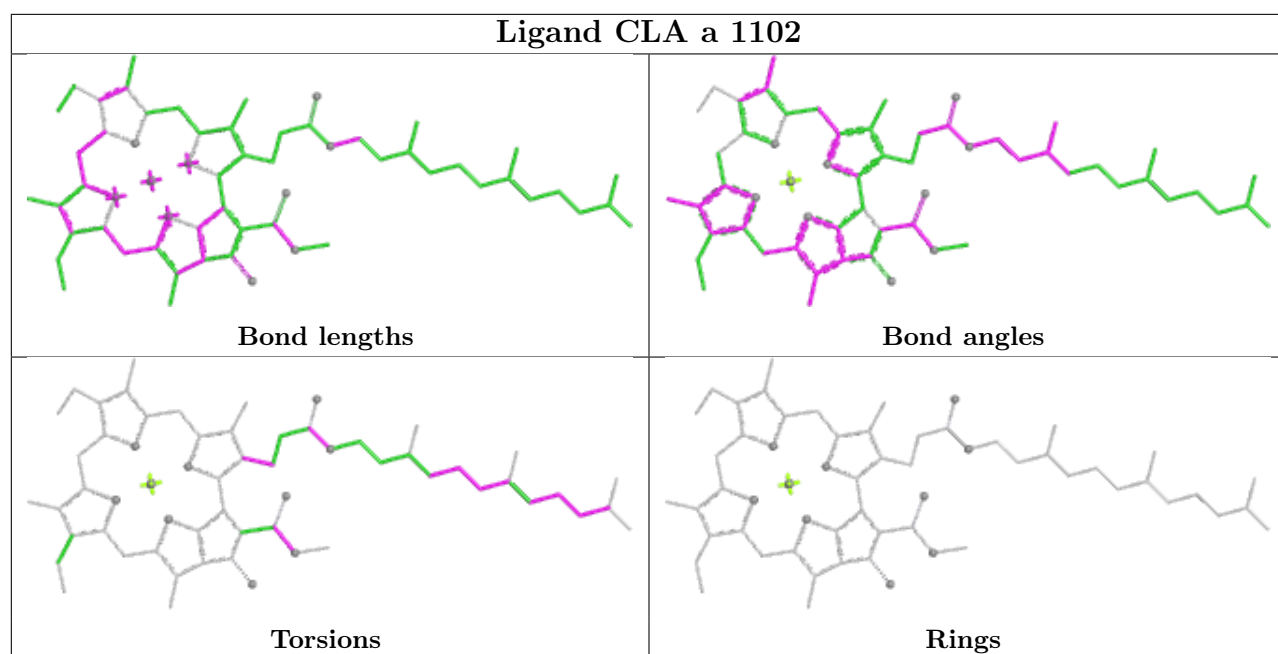


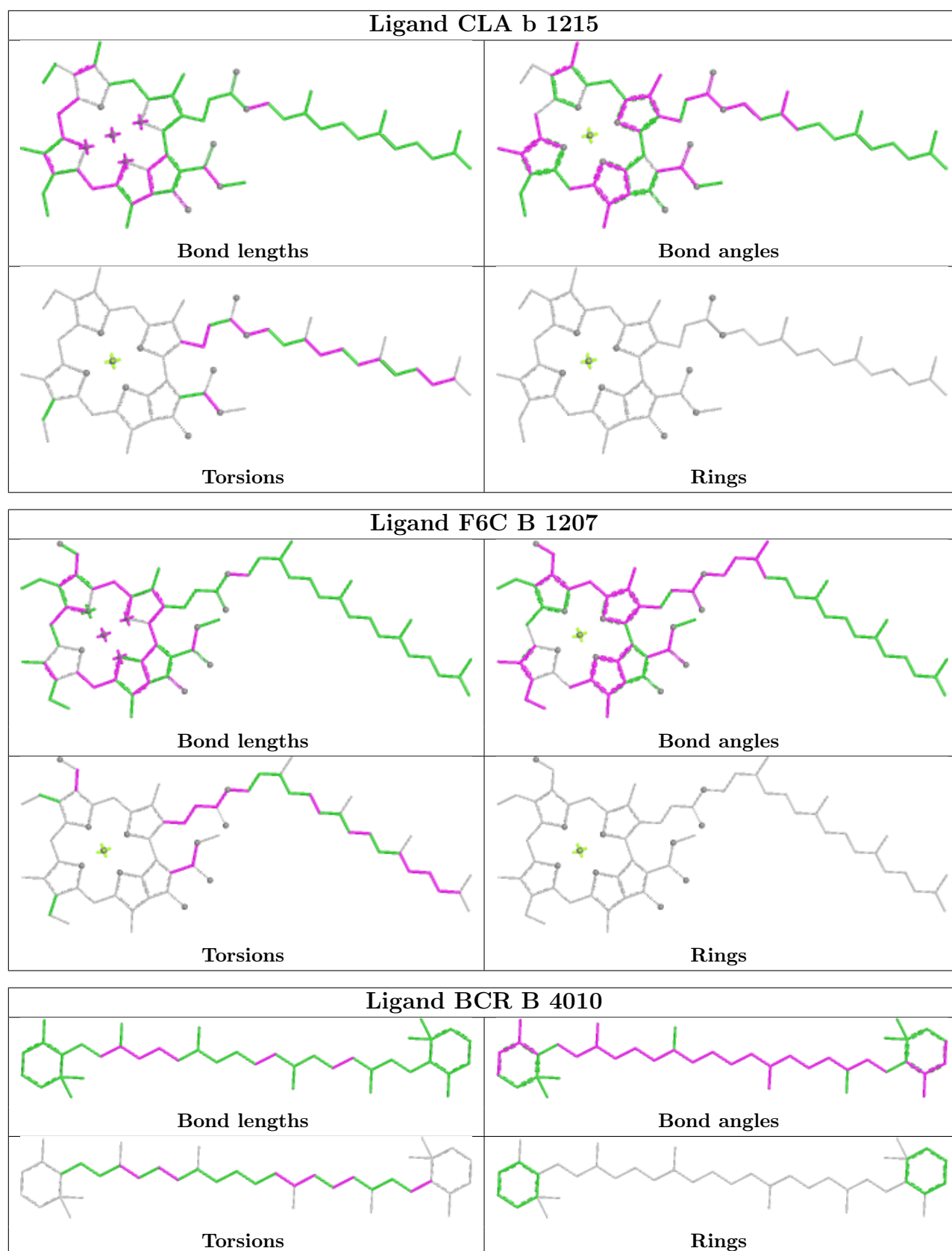
Ligand CLA H 1232

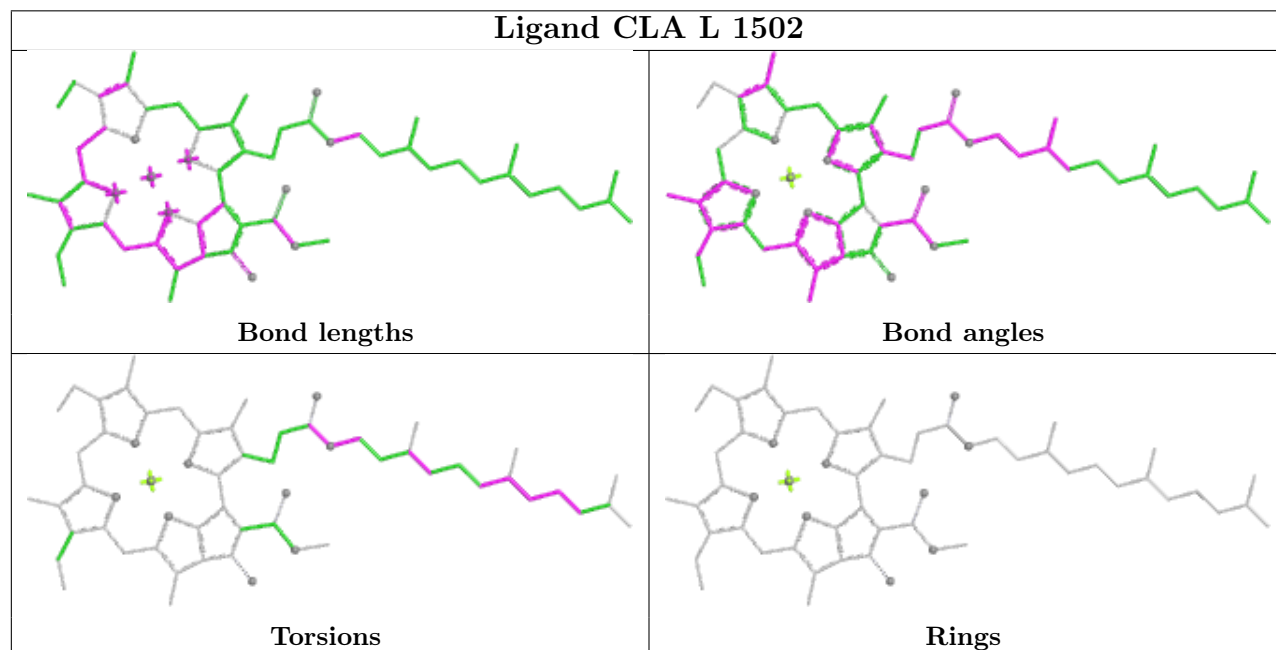
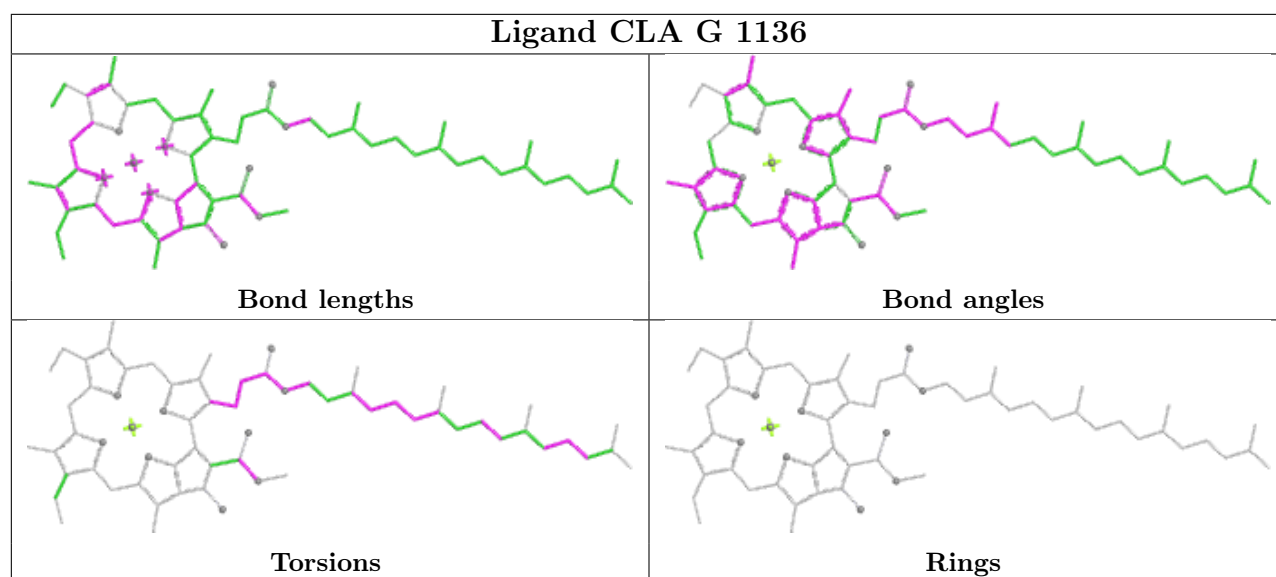


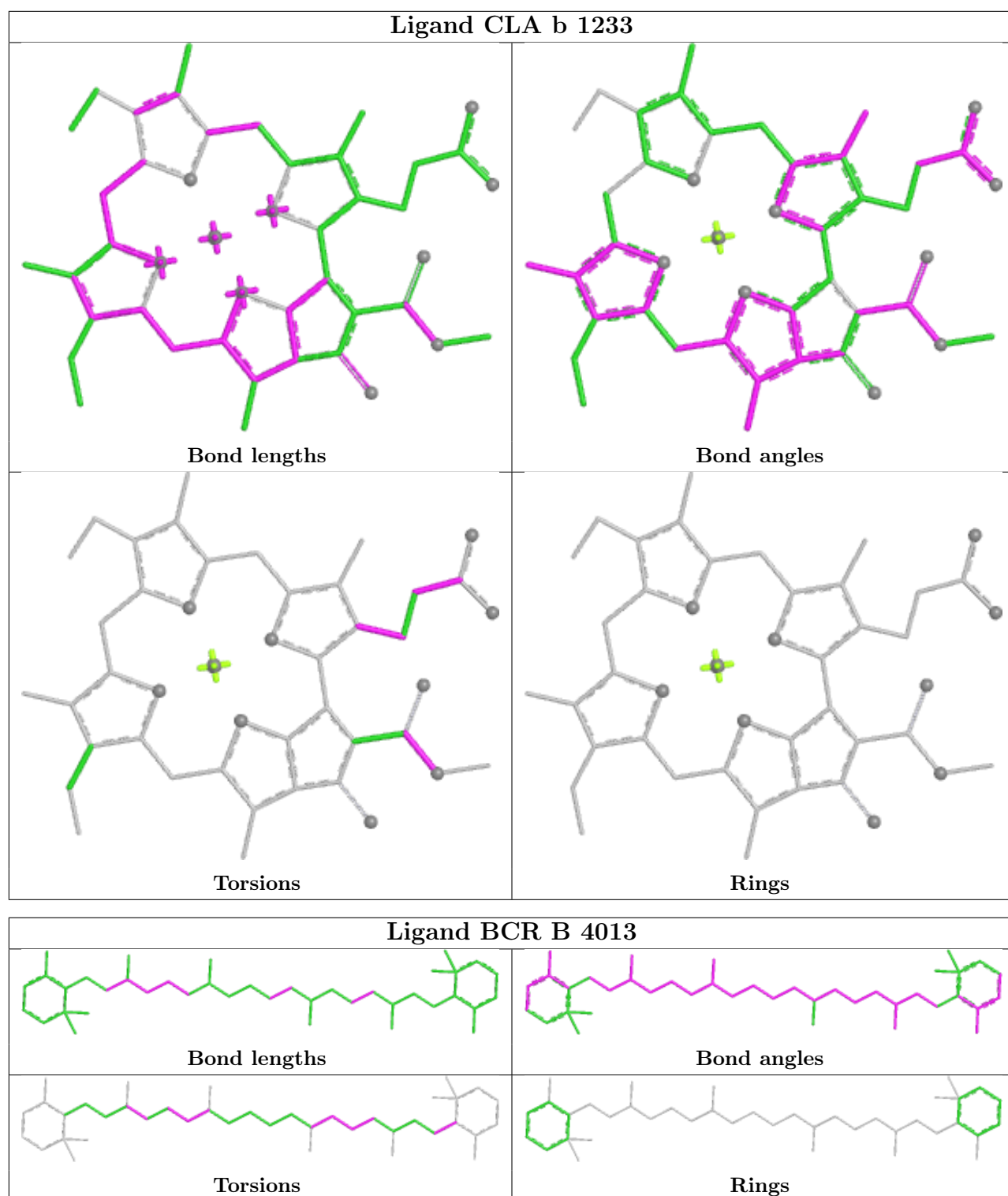
Ligand PQN H 2002

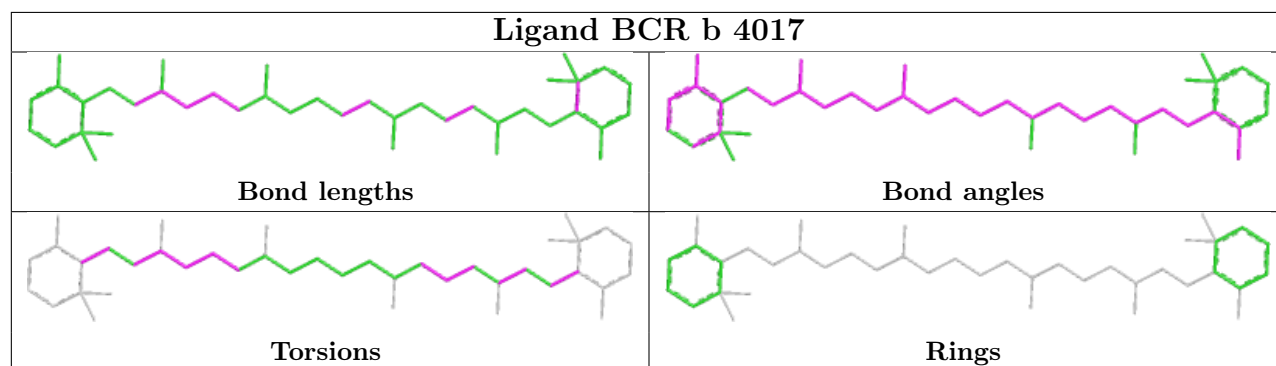
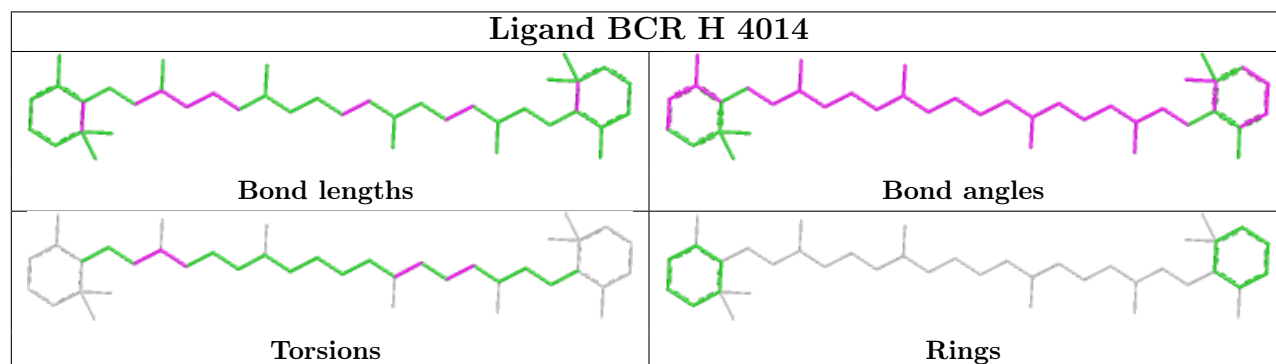
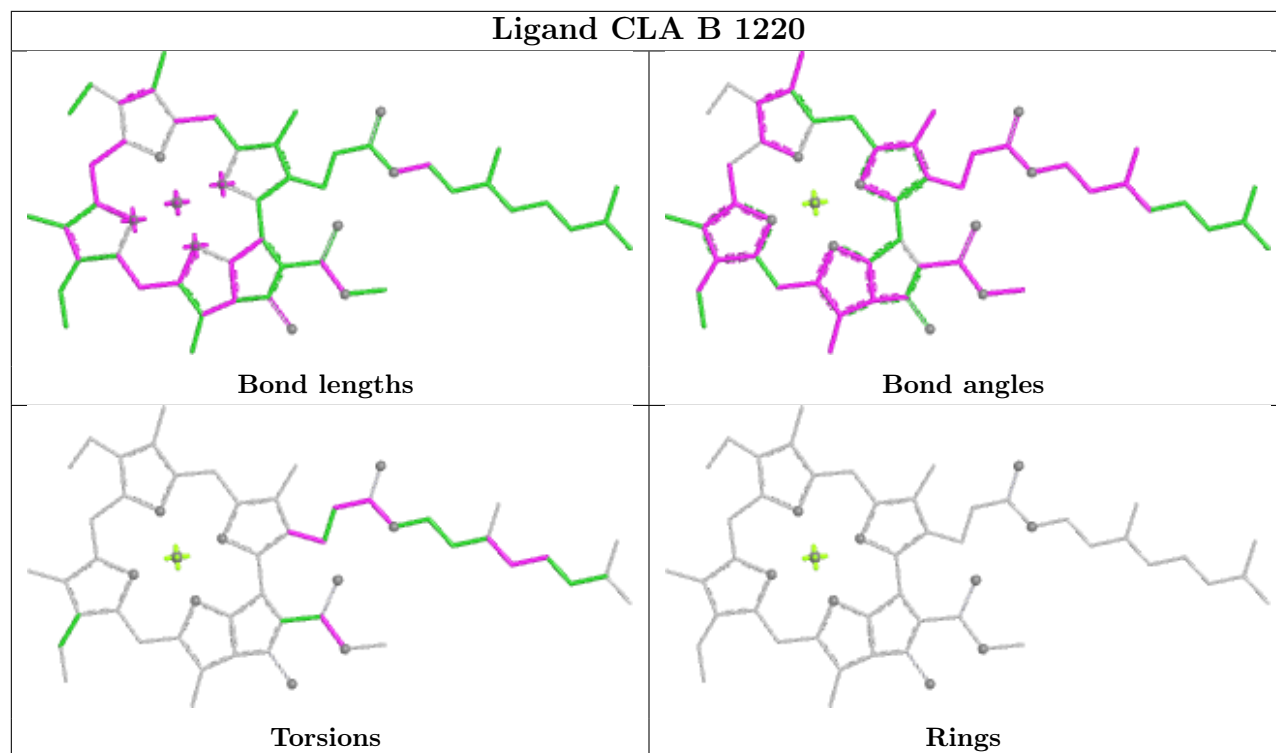


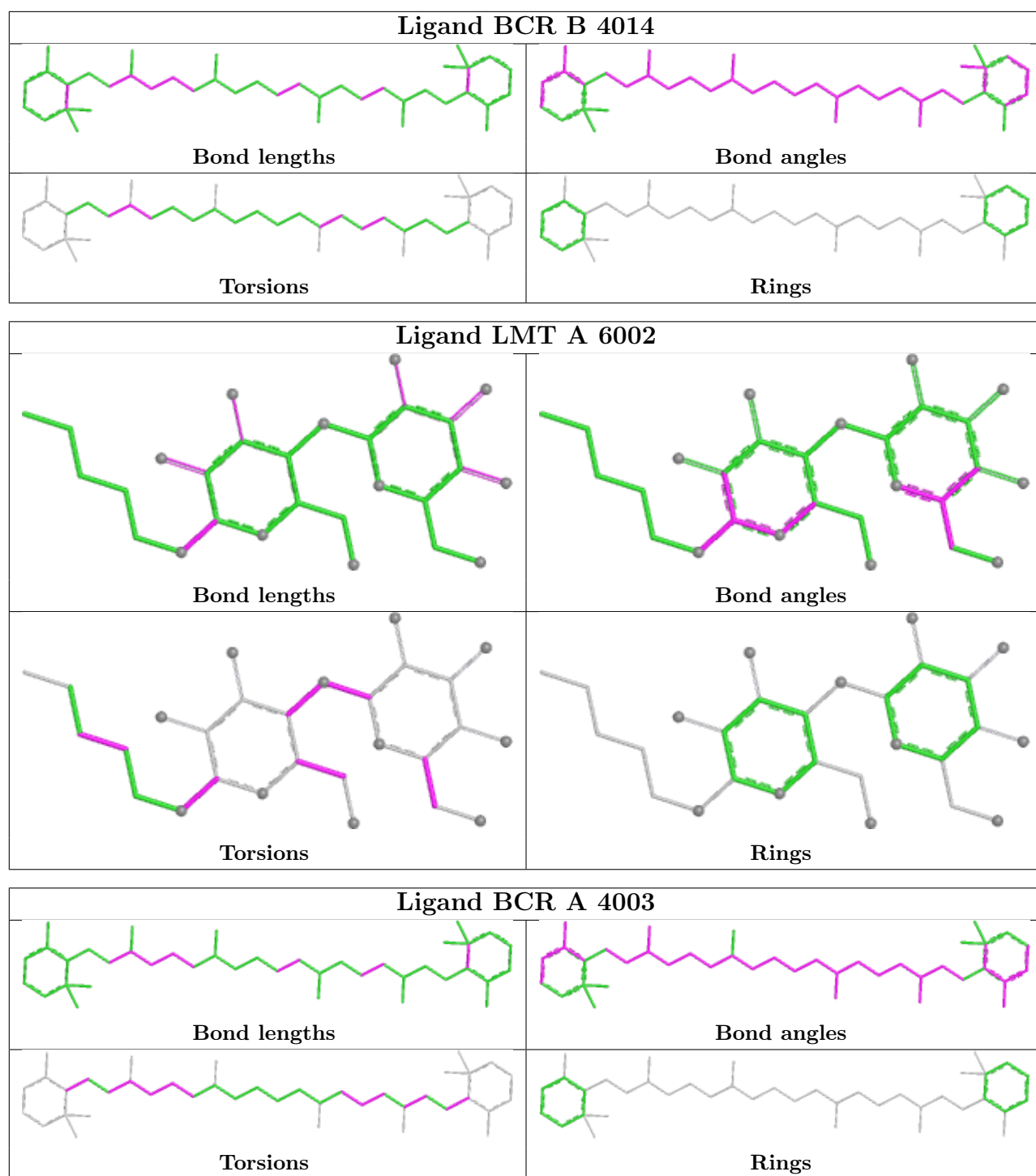


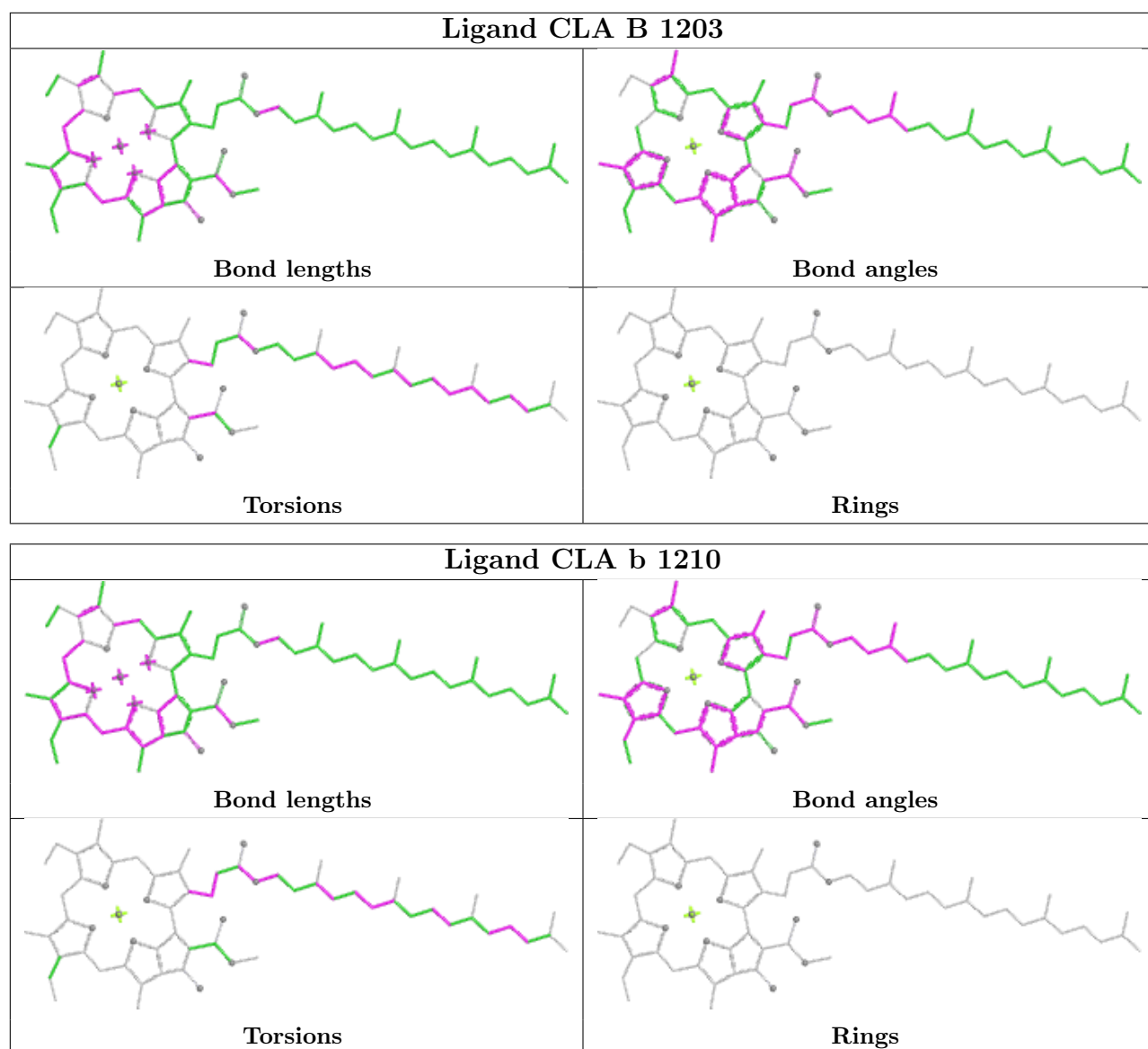


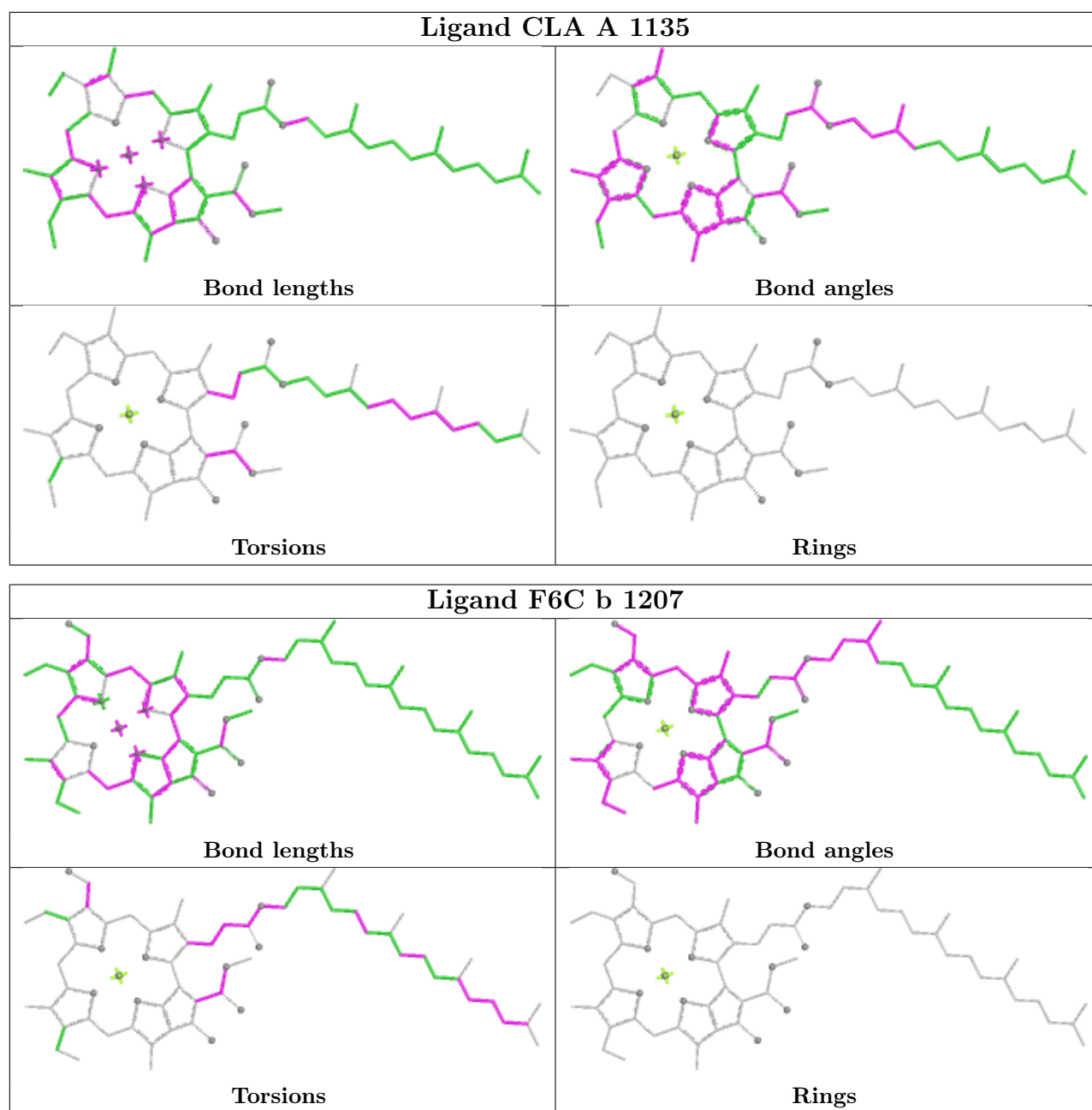


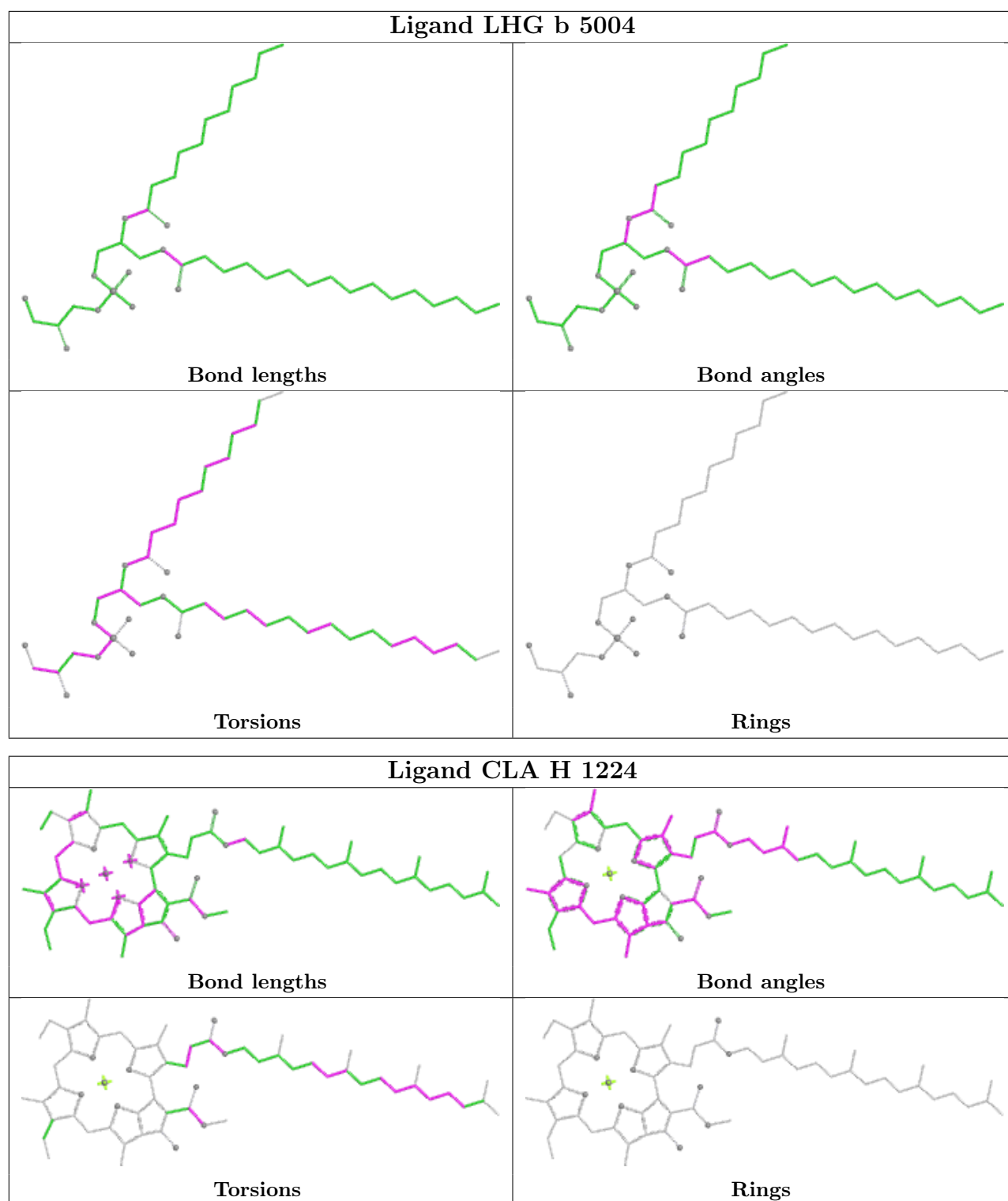


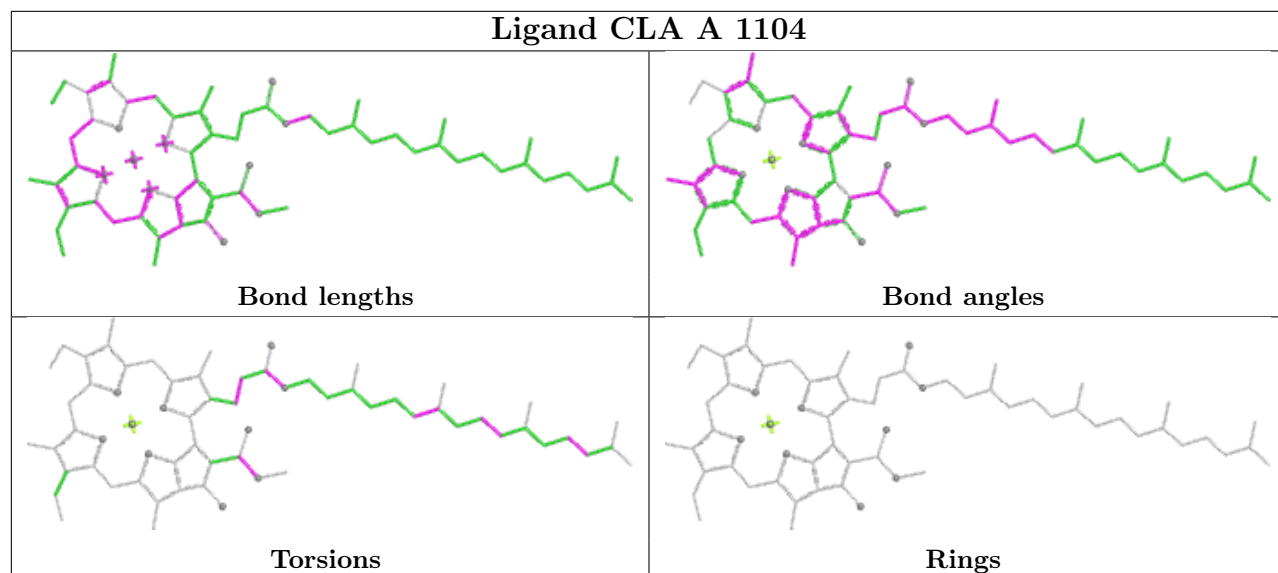
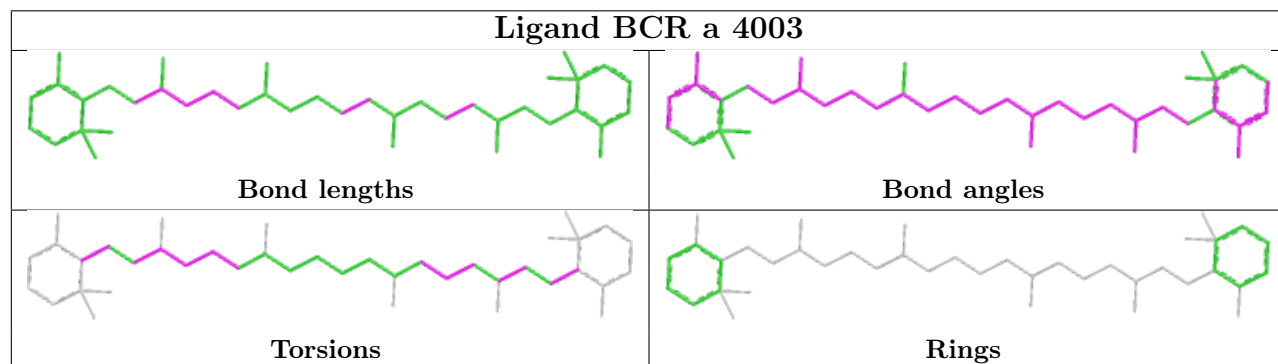
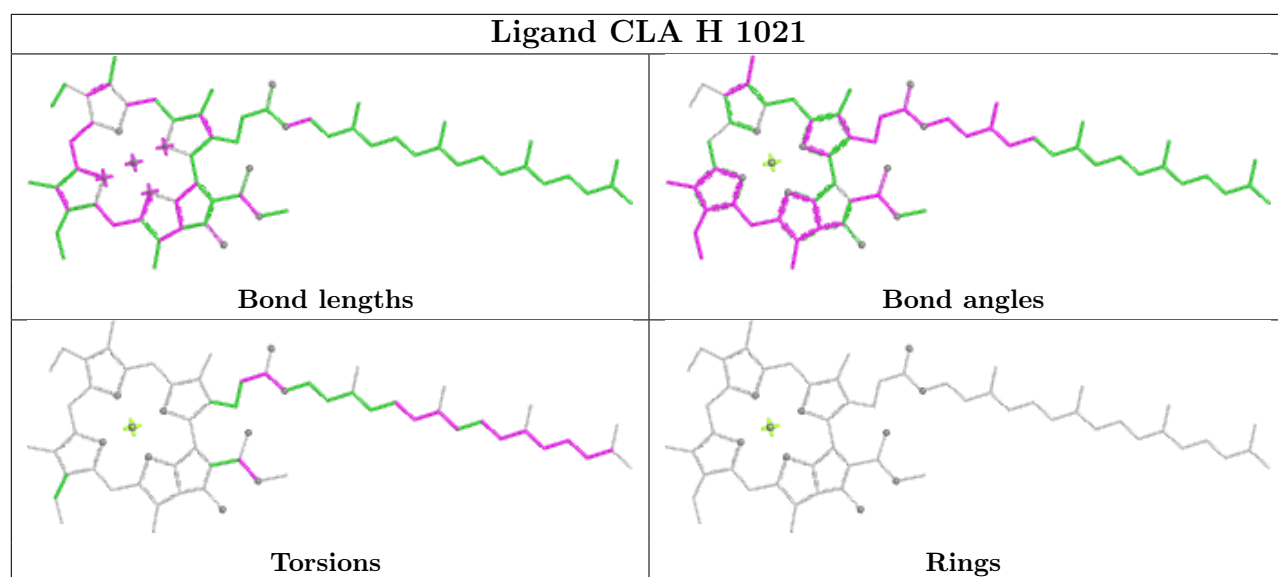


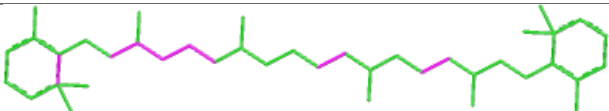
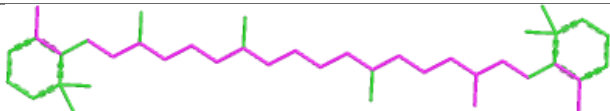
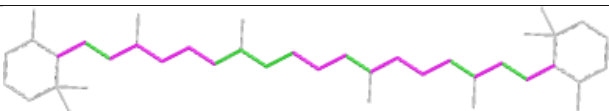
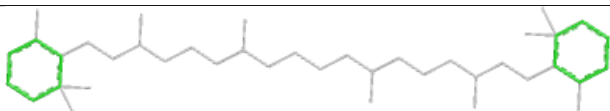




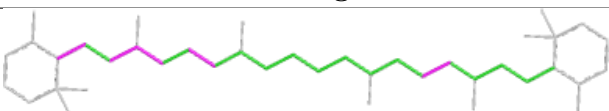
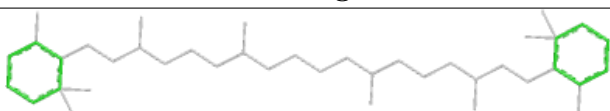




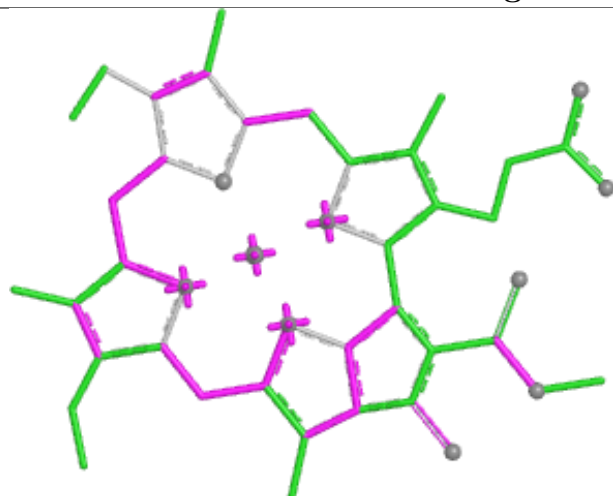




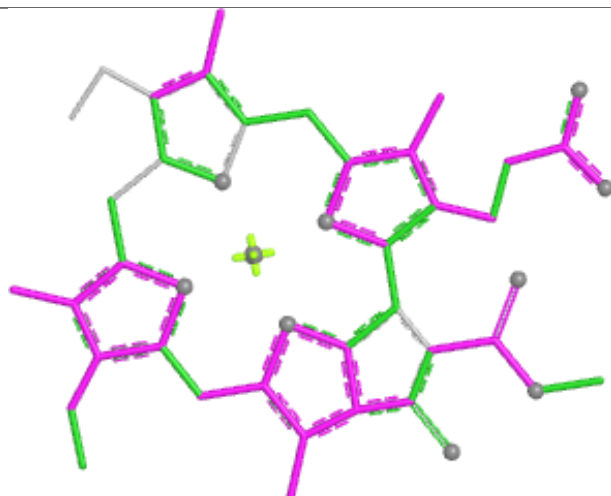
Ligand BCR V 4021	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 4009	
 Bond lengths	 Bond angles
 Torsions	 Rings

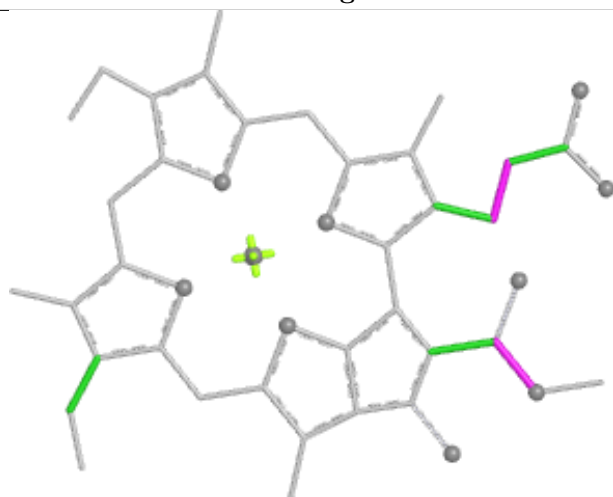
Ligand CLA G 1139



Bond lengths



Bond angles

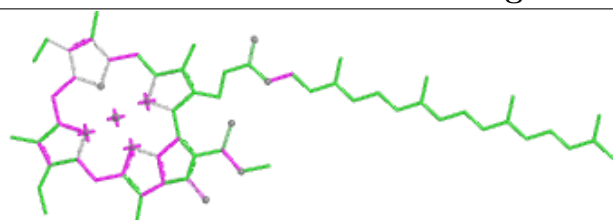


Torsions

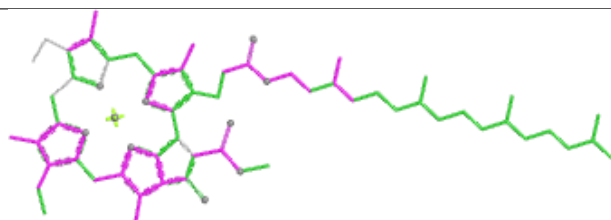


Rings

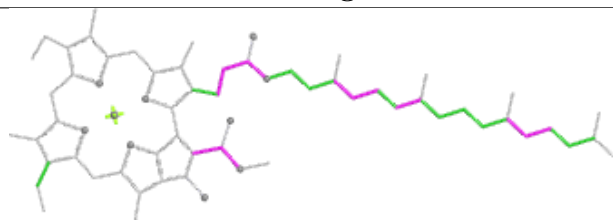
Ligand CLA B 1213



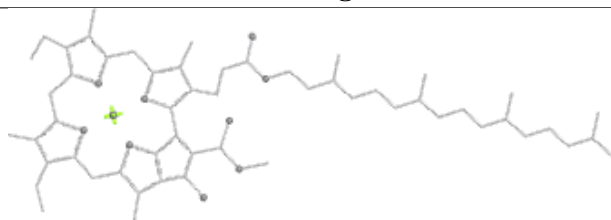
Bond lengths



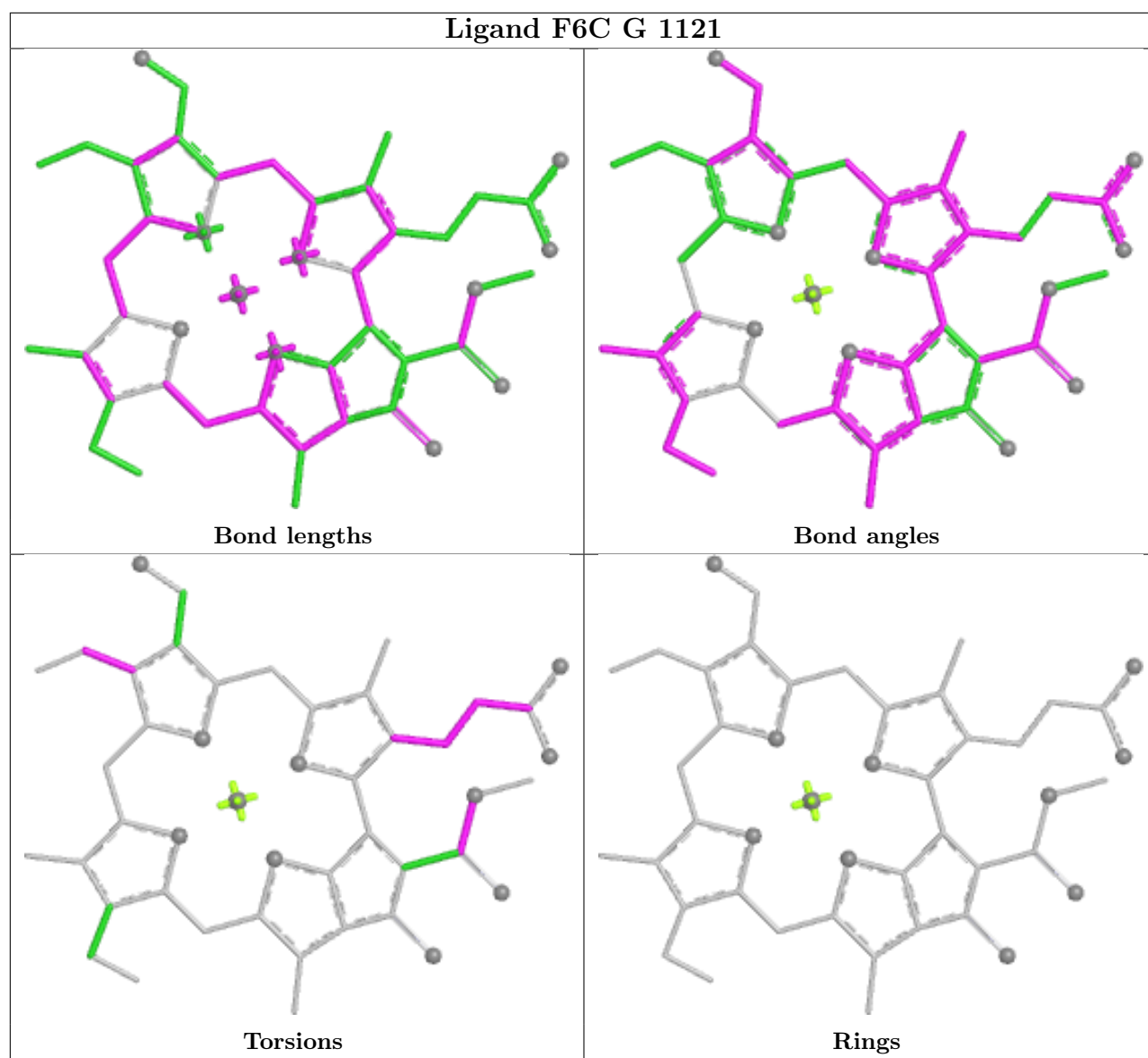
Bond angles



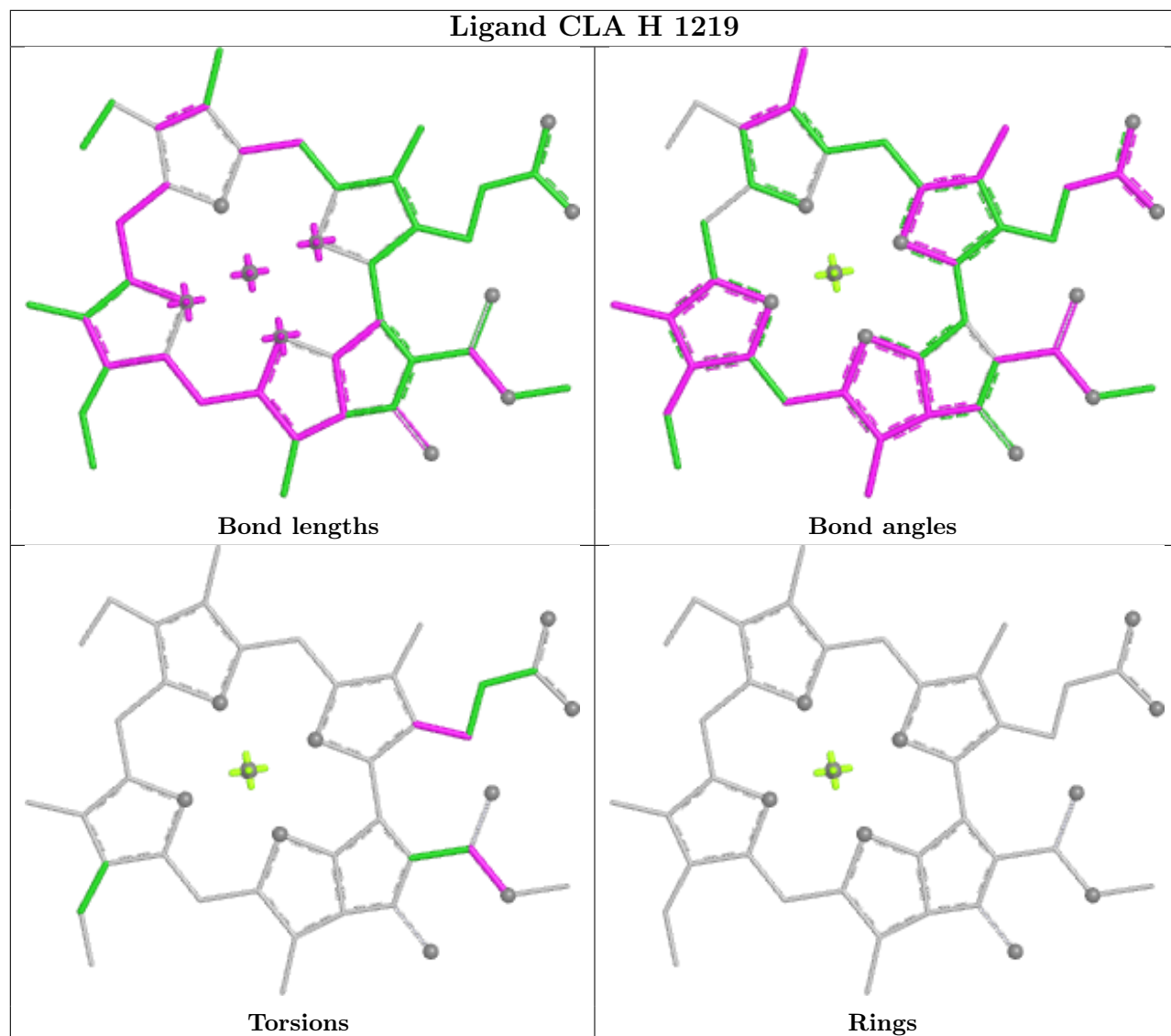
Torsions



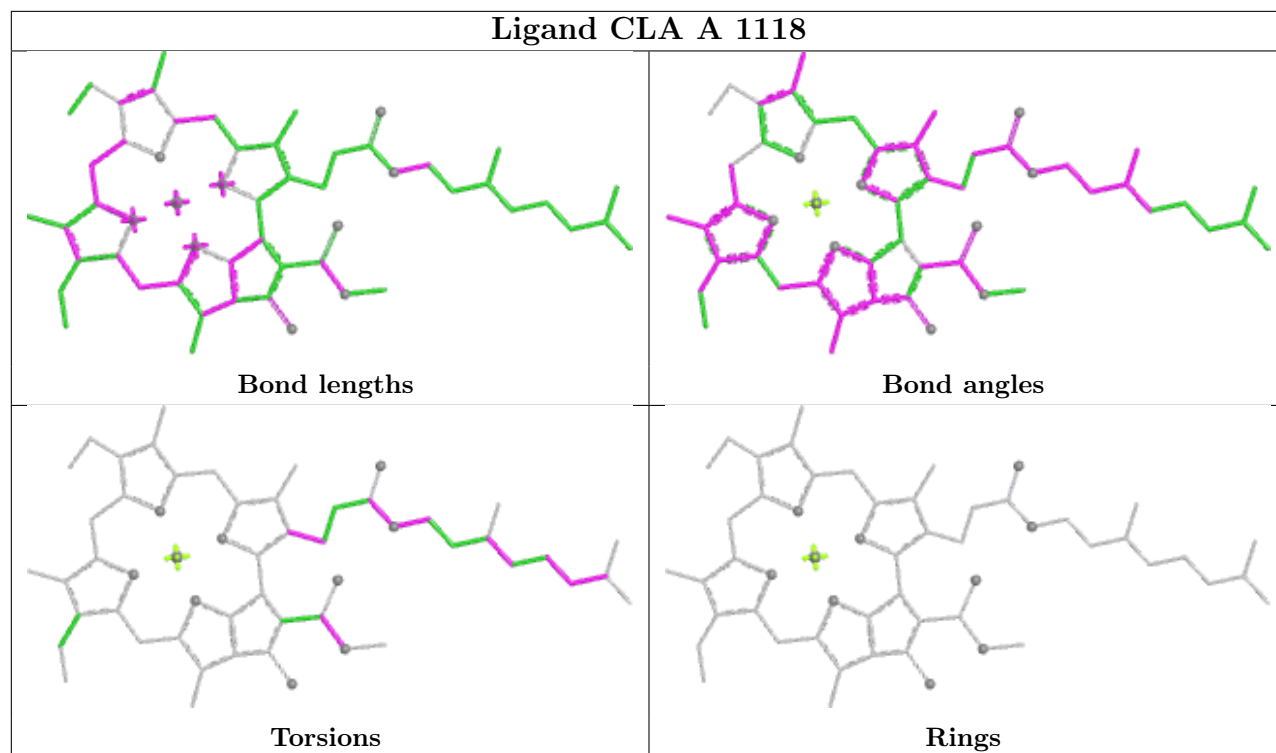
Rings



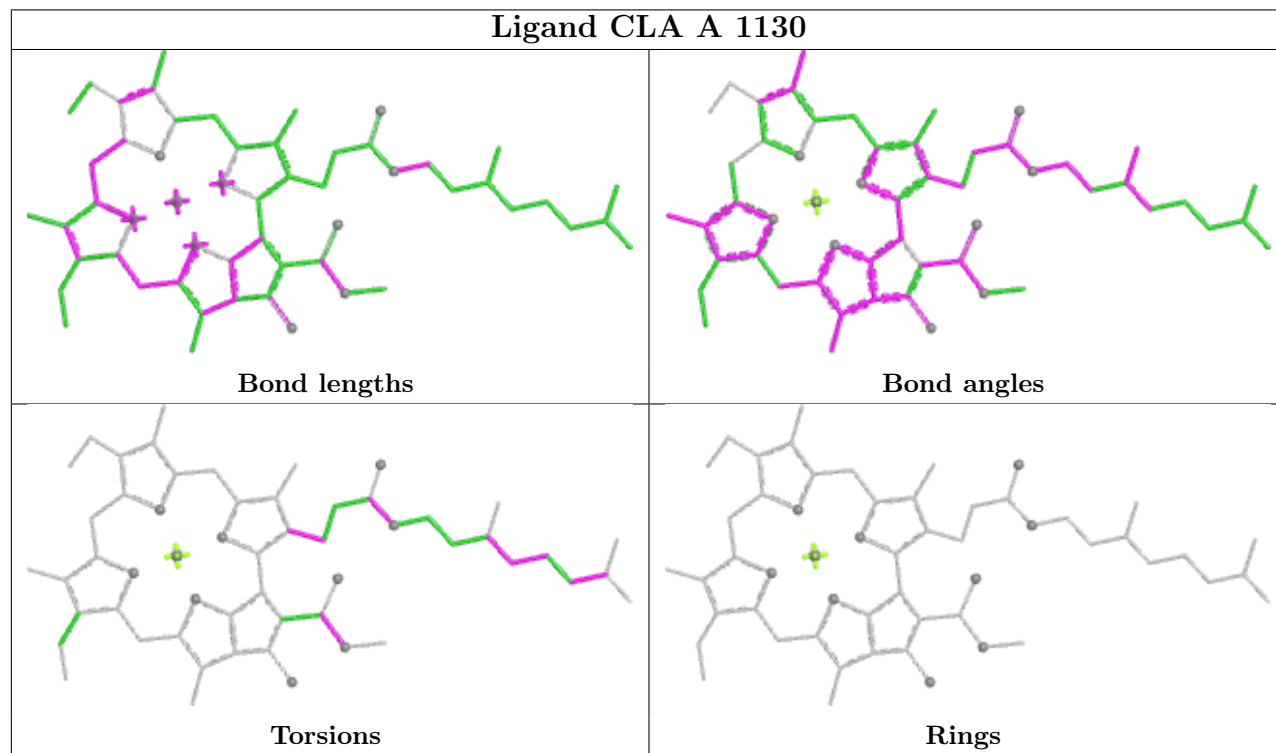
Ligand CLA H 1219

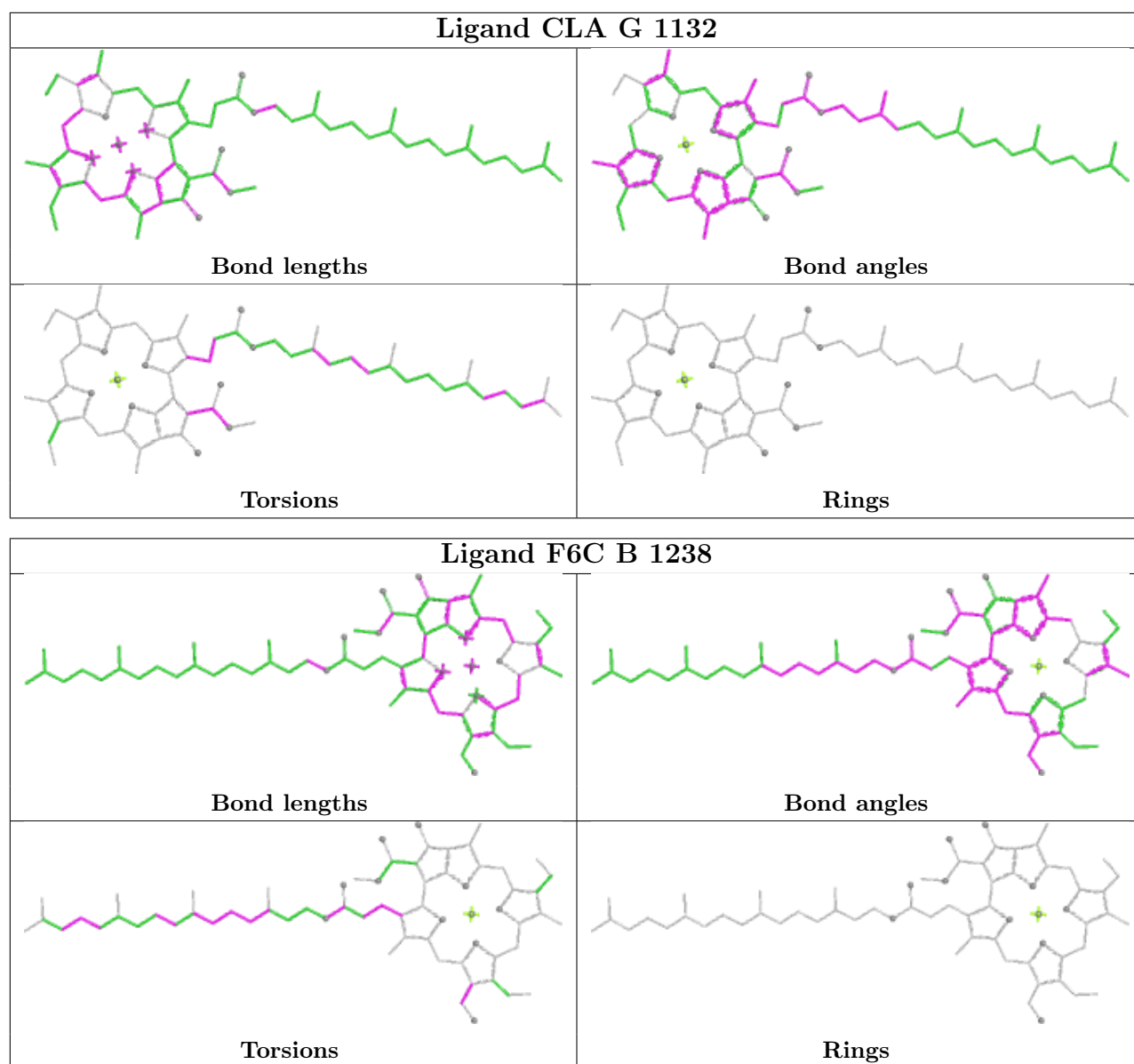


Ligand CLA A 1118

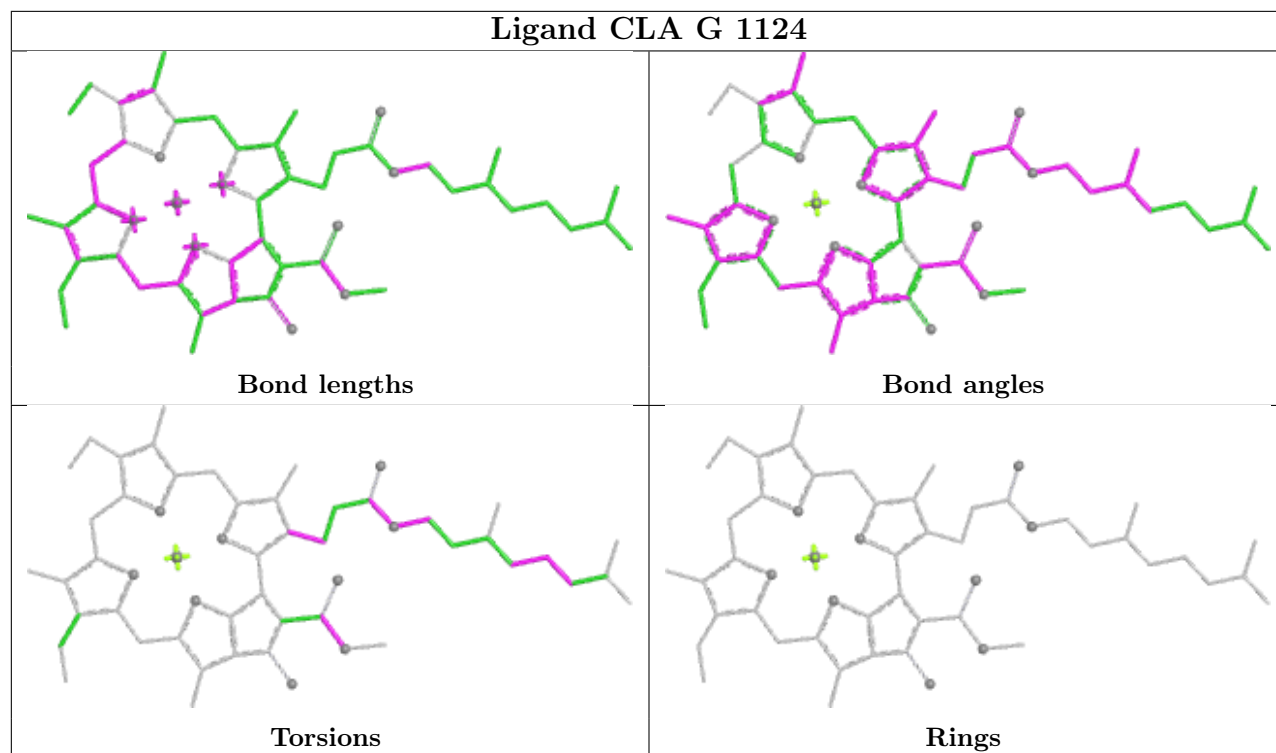


Ligand CLA A 1130

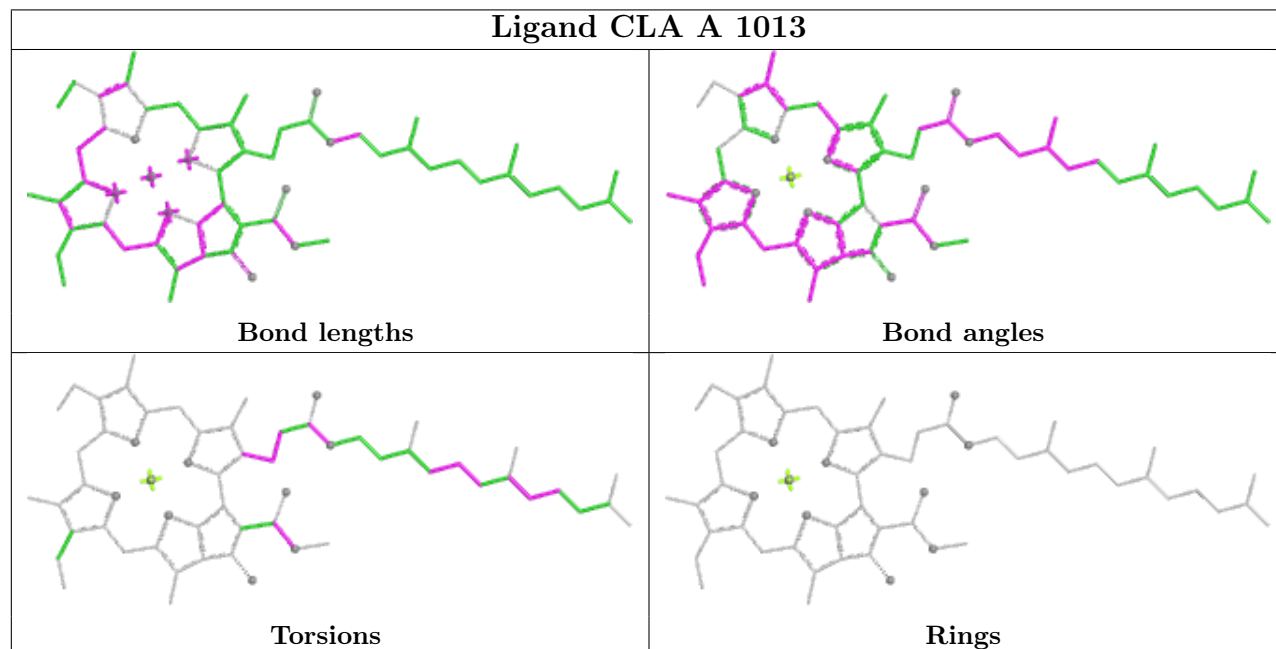


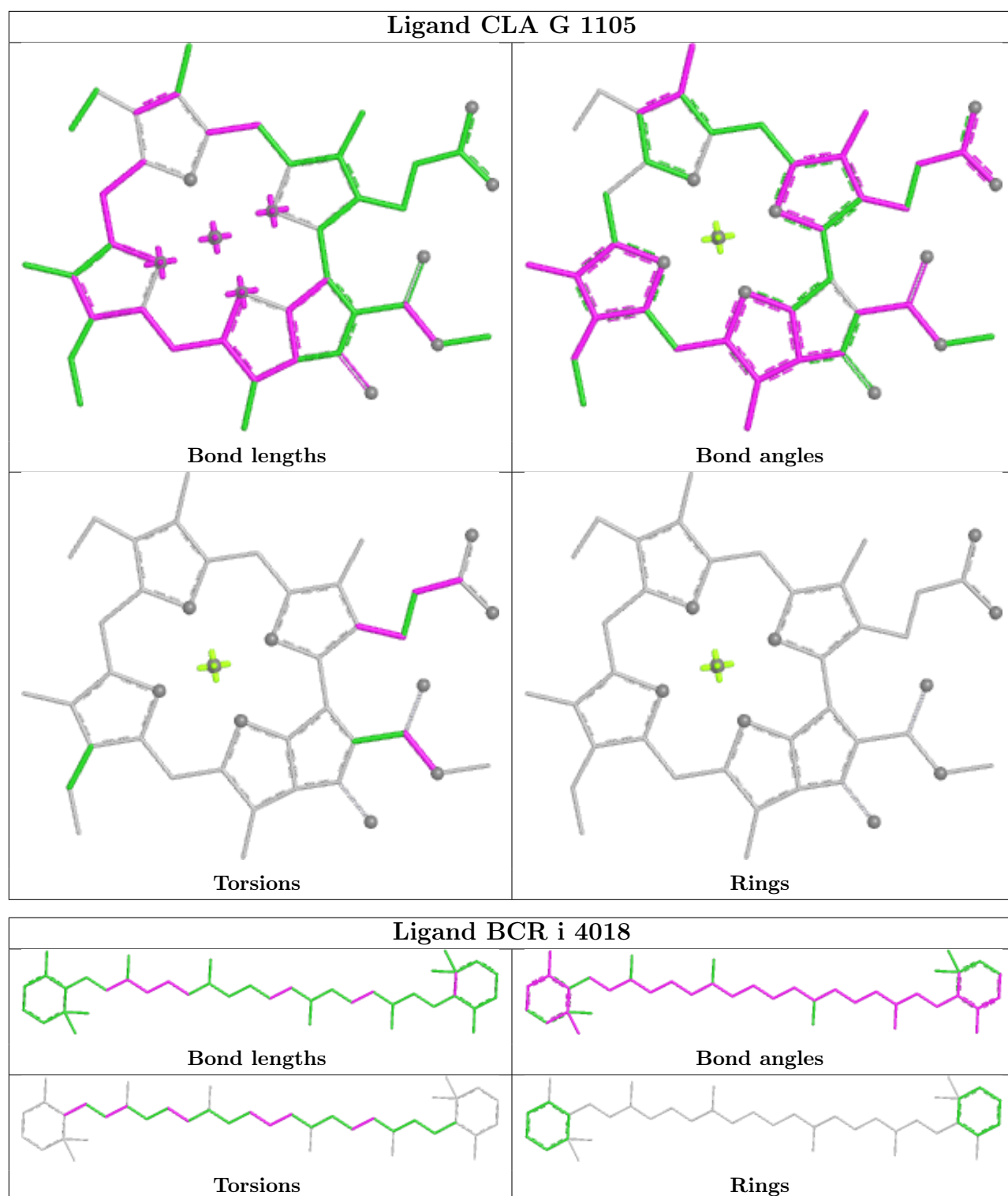


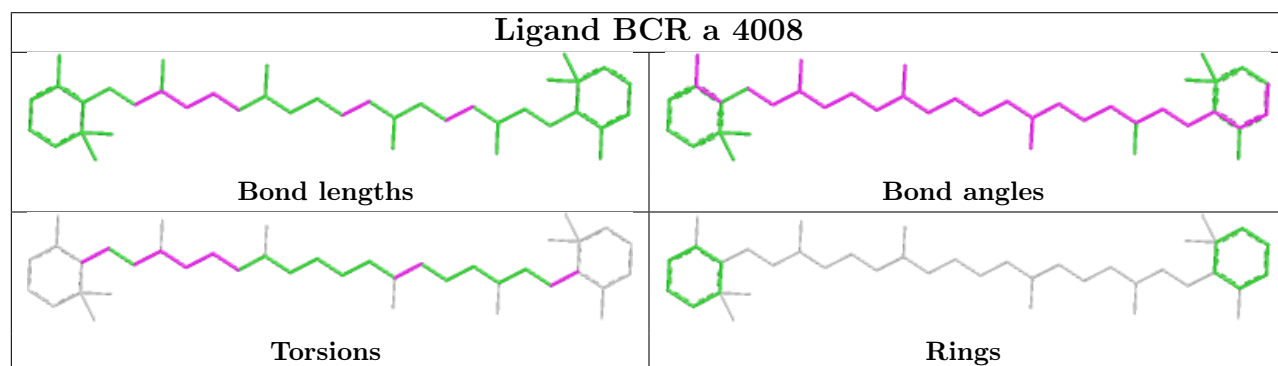
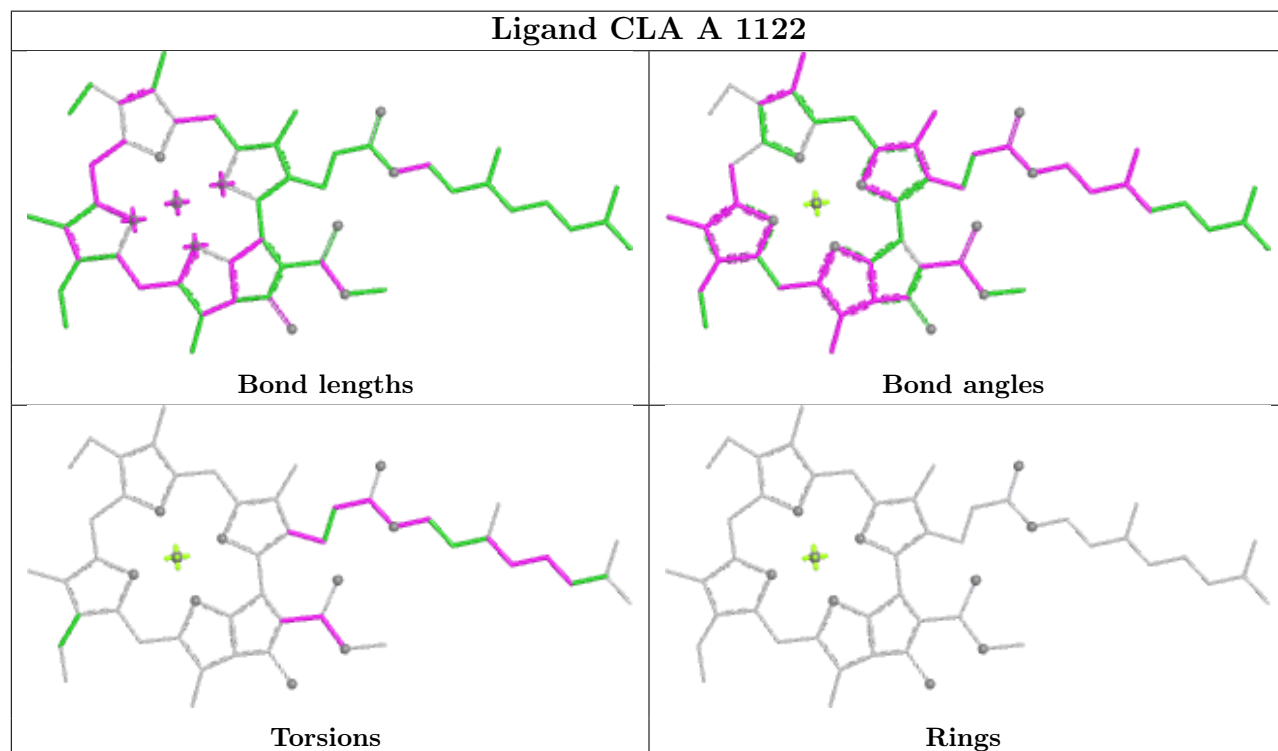
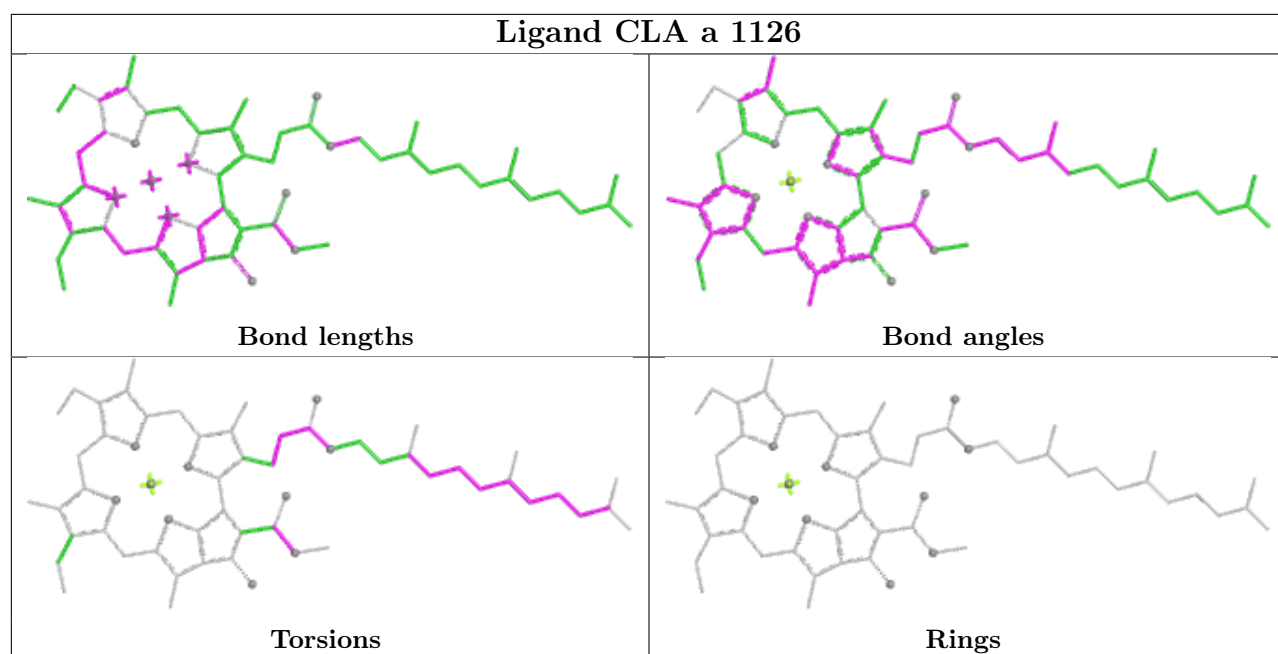
Ligand CLA G 1124

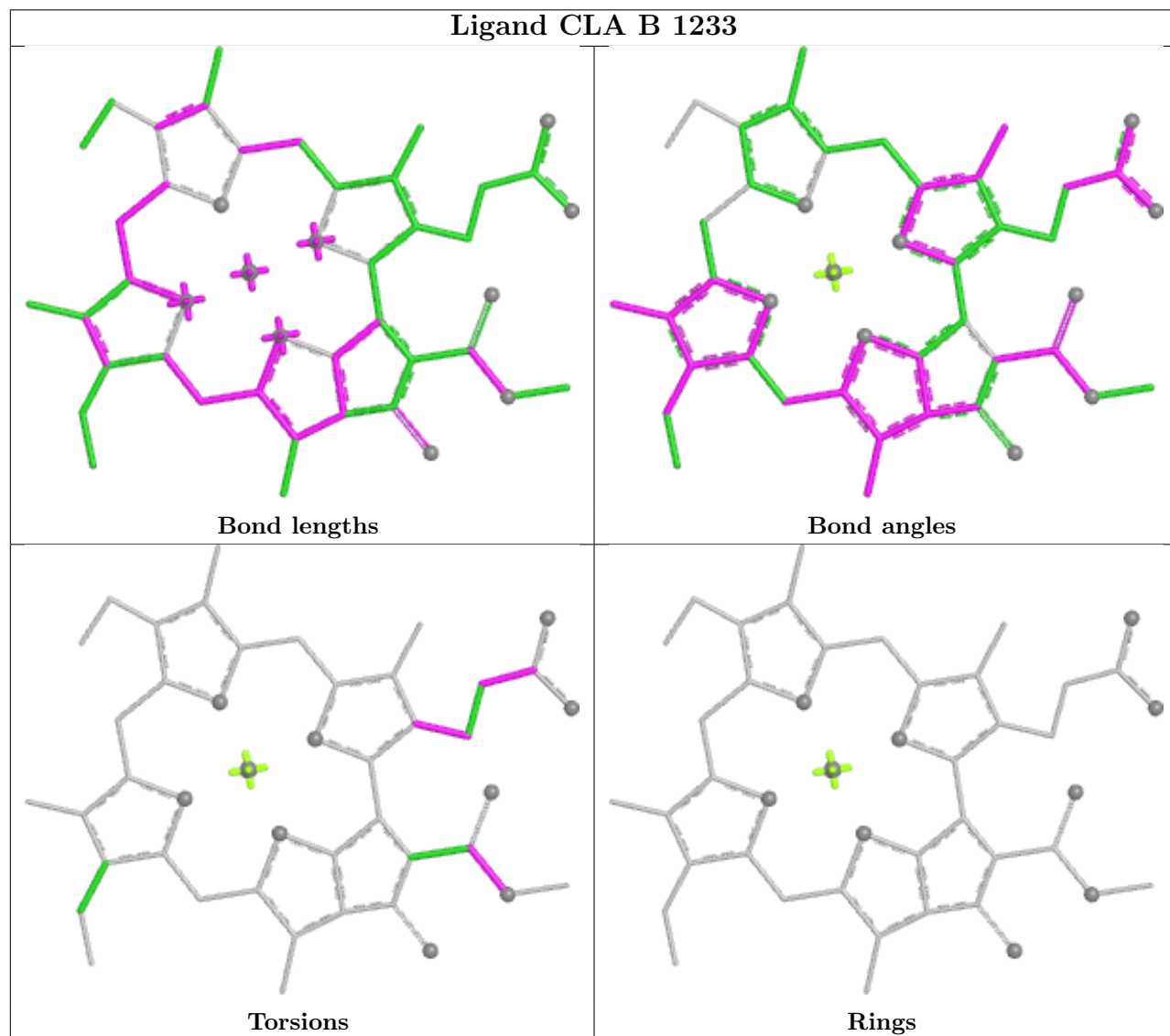
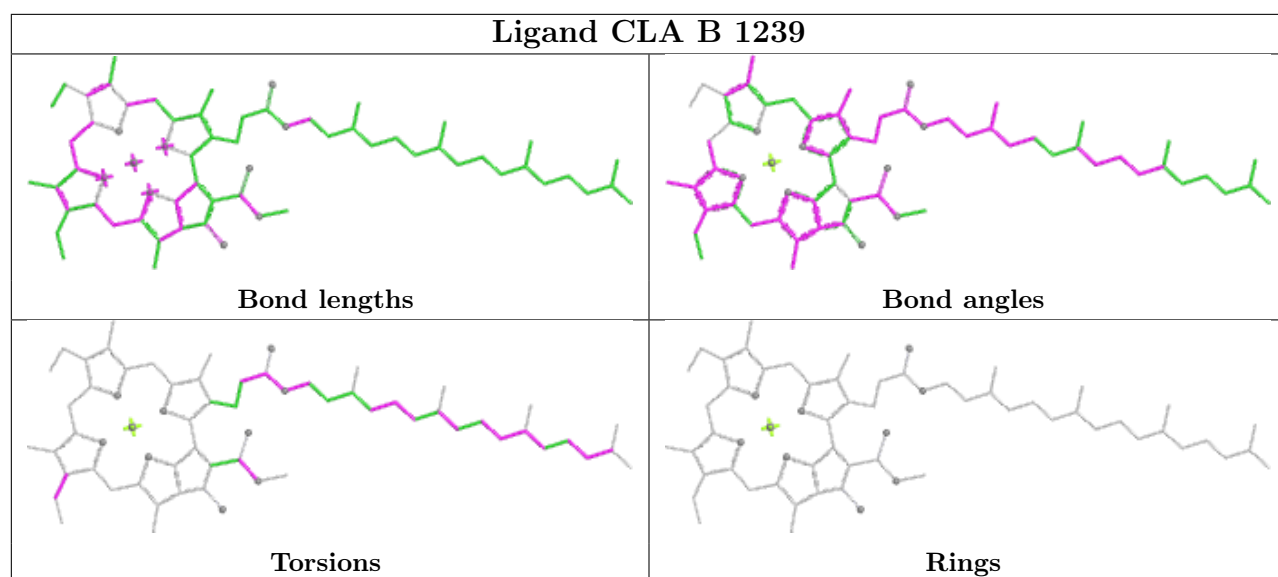


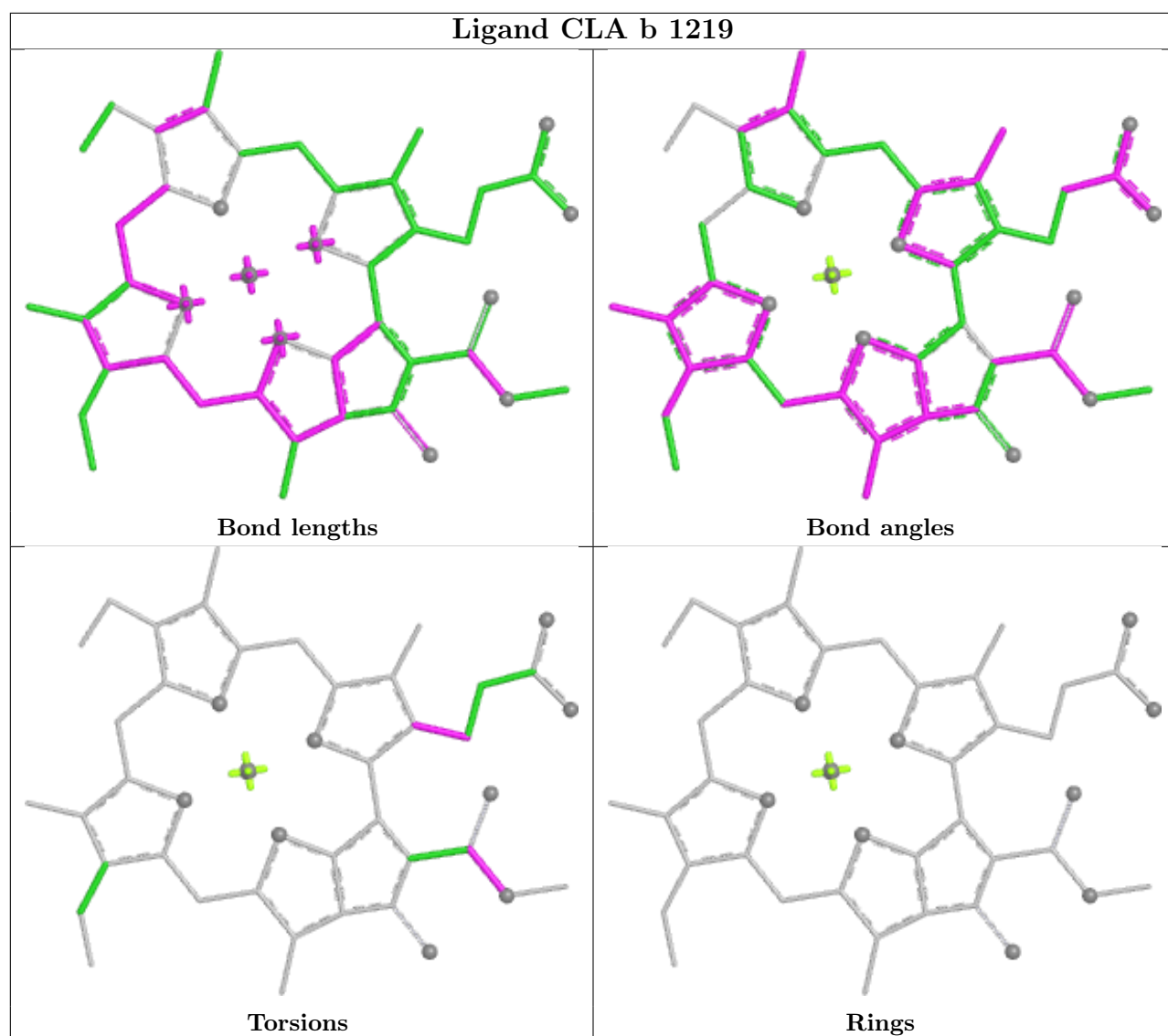
Ligand CLA A 1013

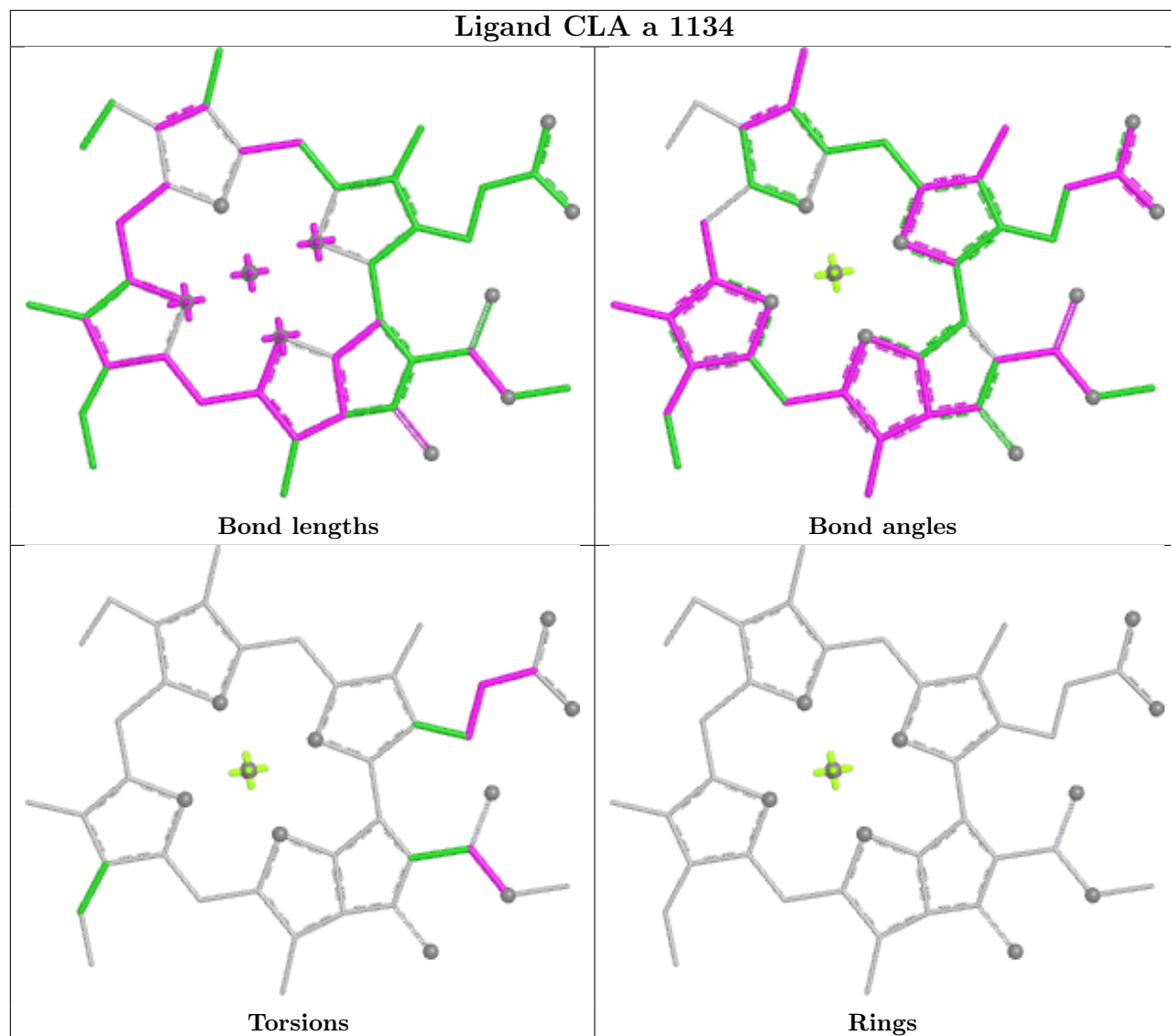


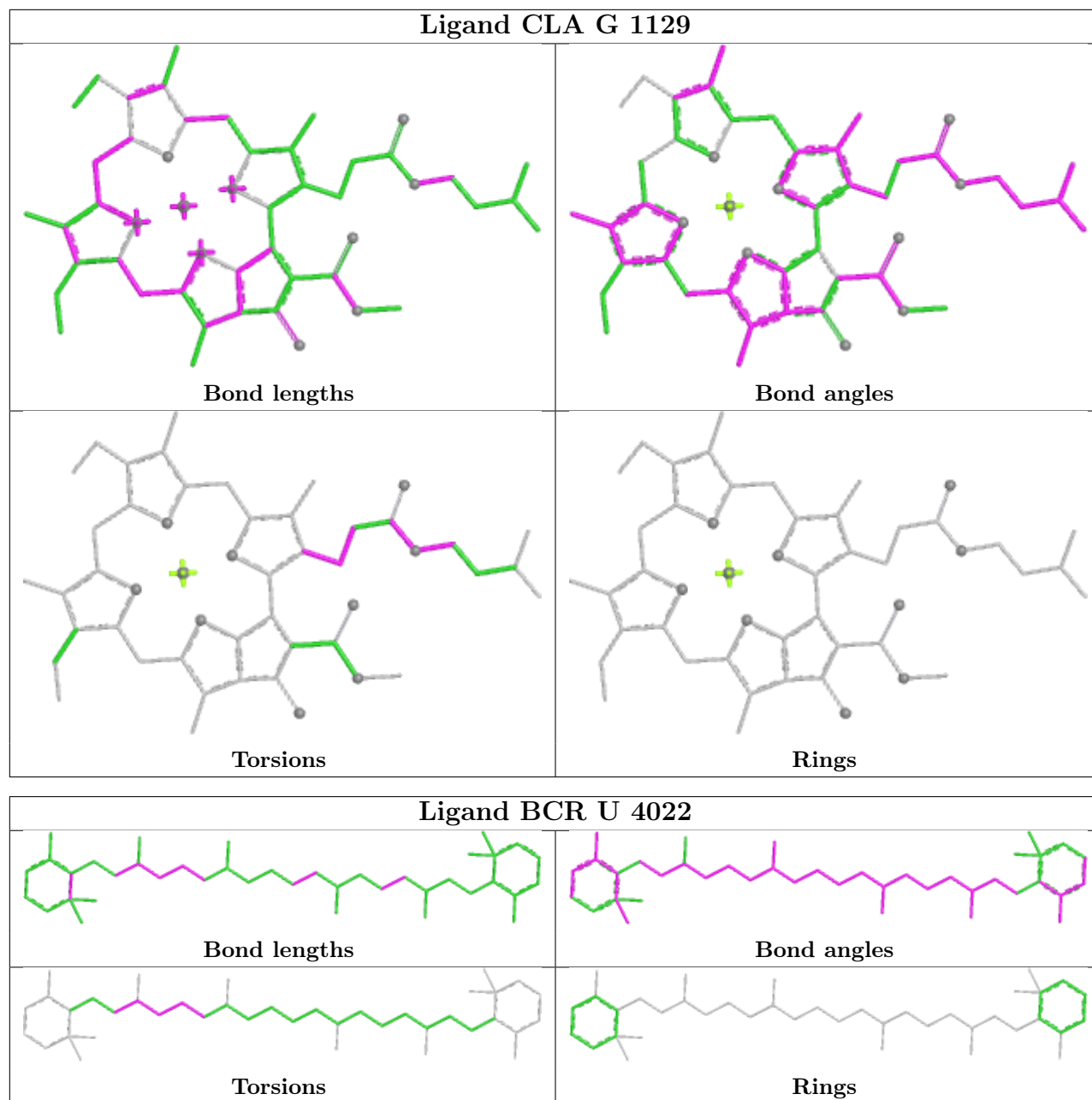




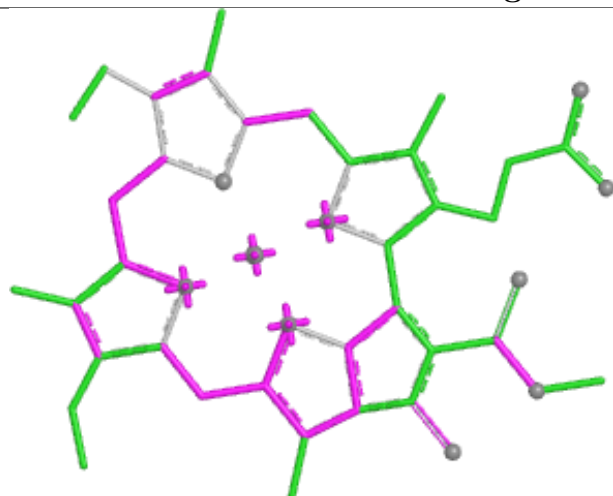




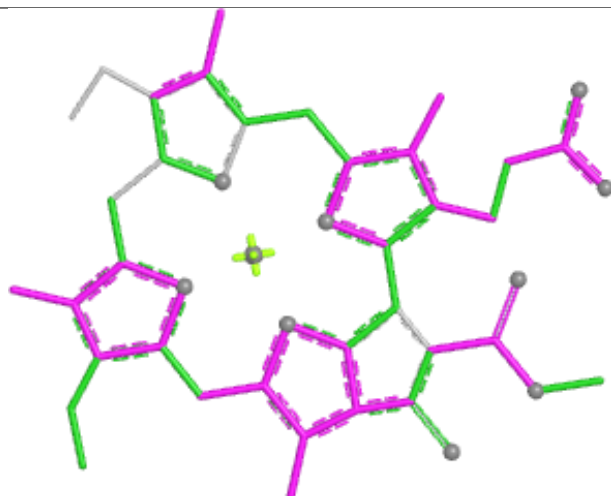




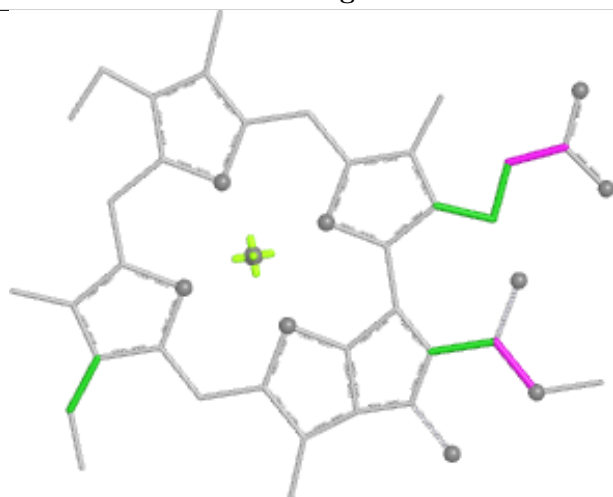
Ligand CLA G 1108



Bond lengths



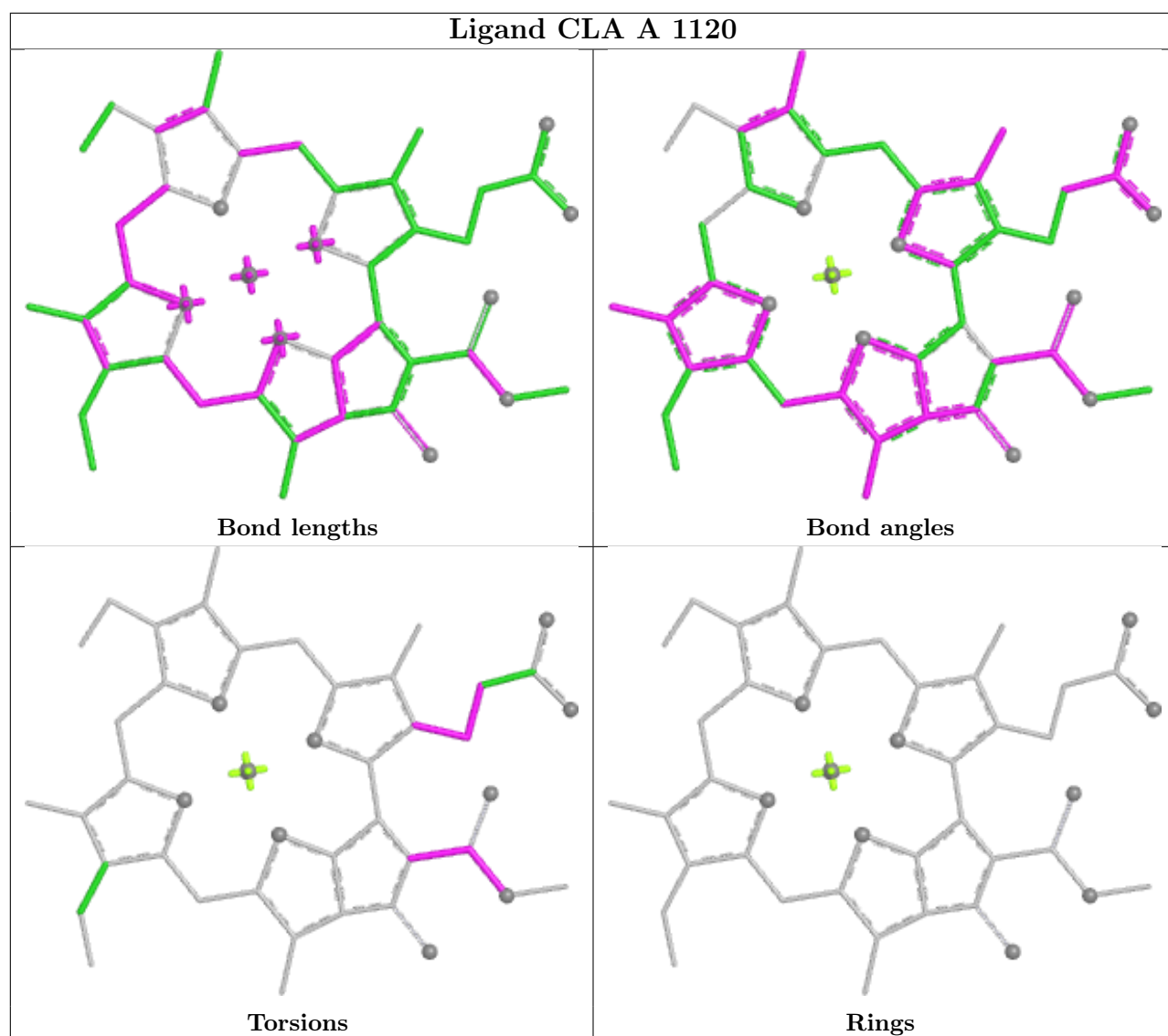
Bond angles



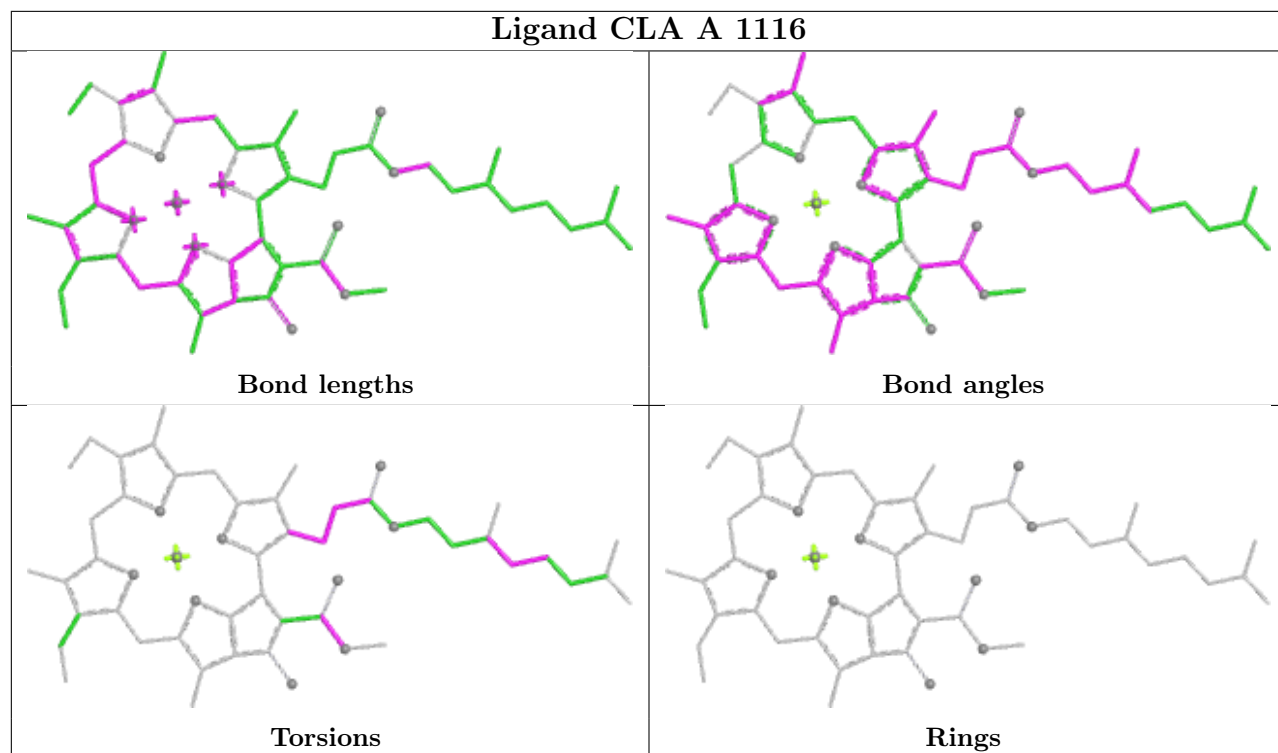
Torsions



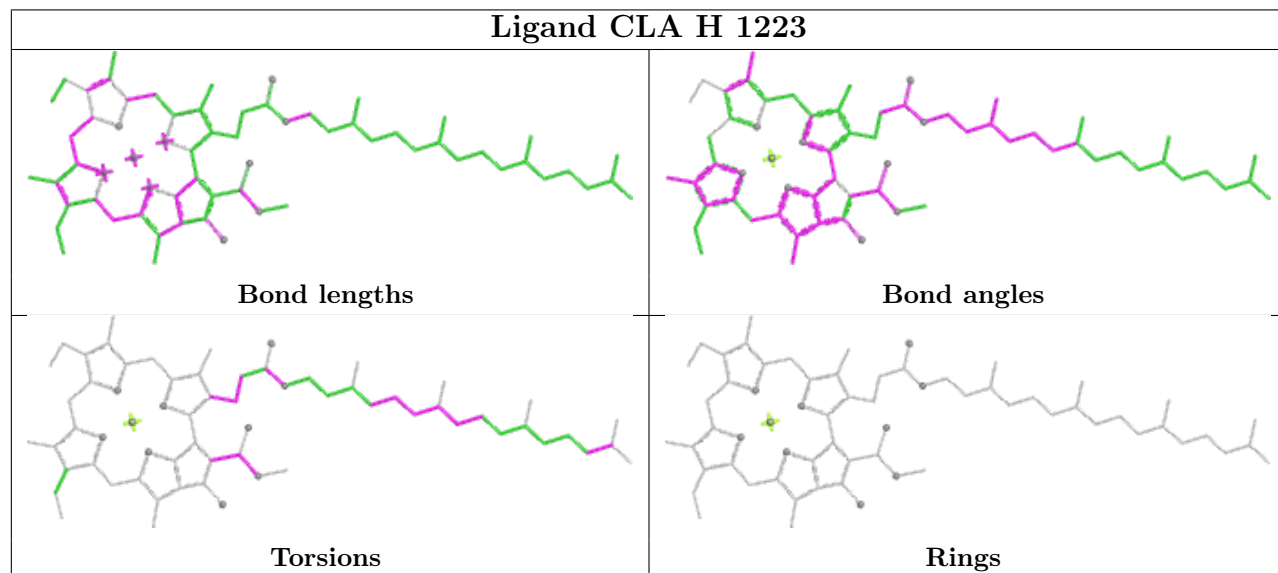
Rings

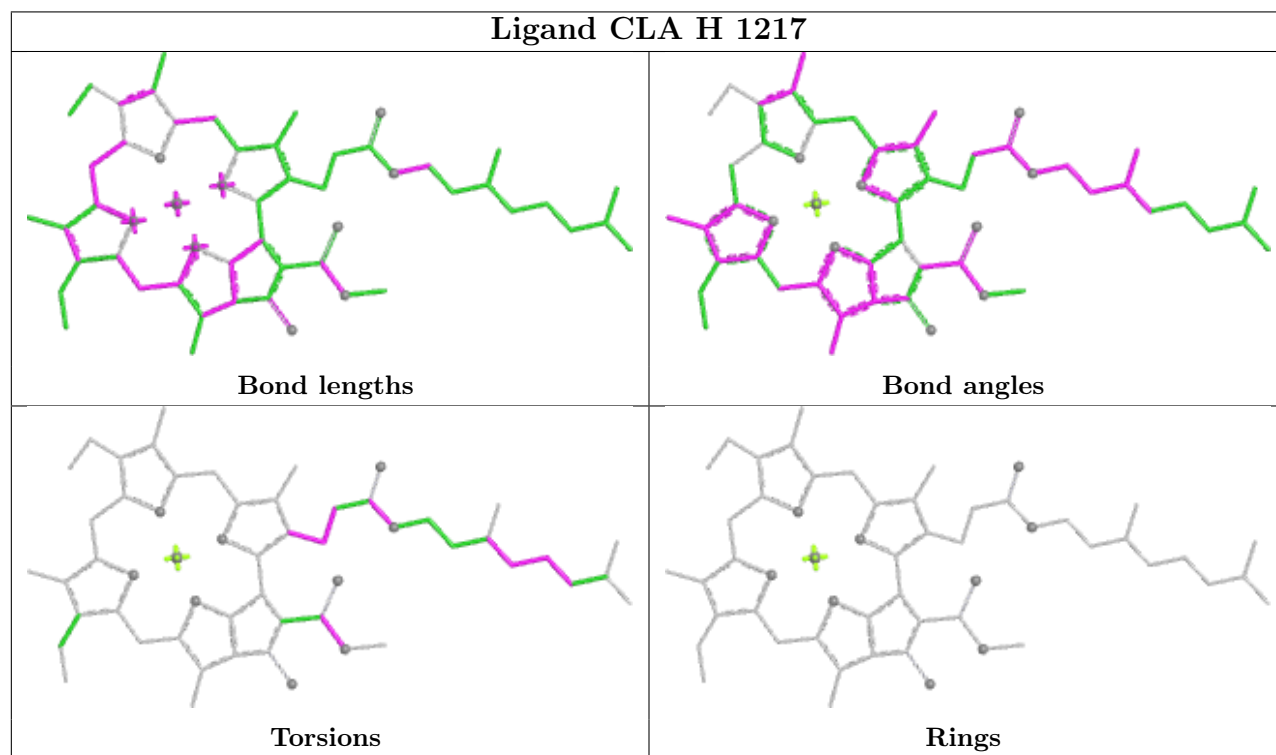
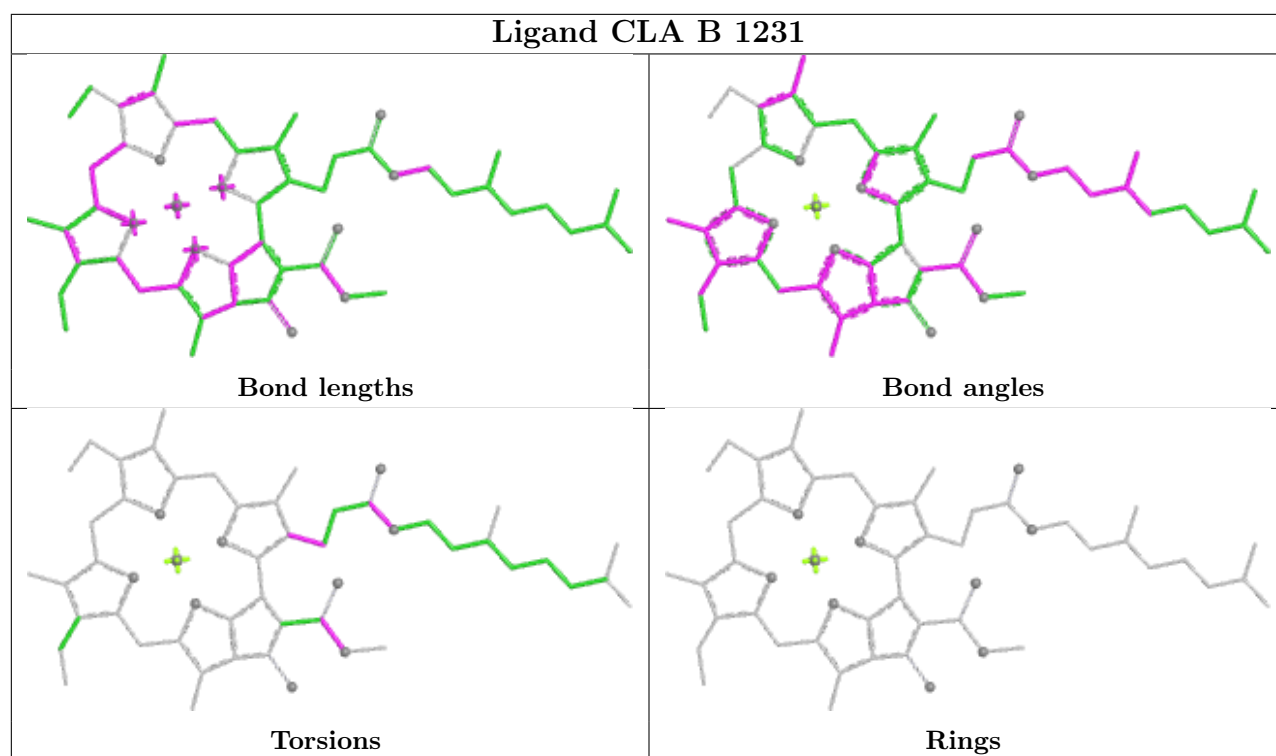


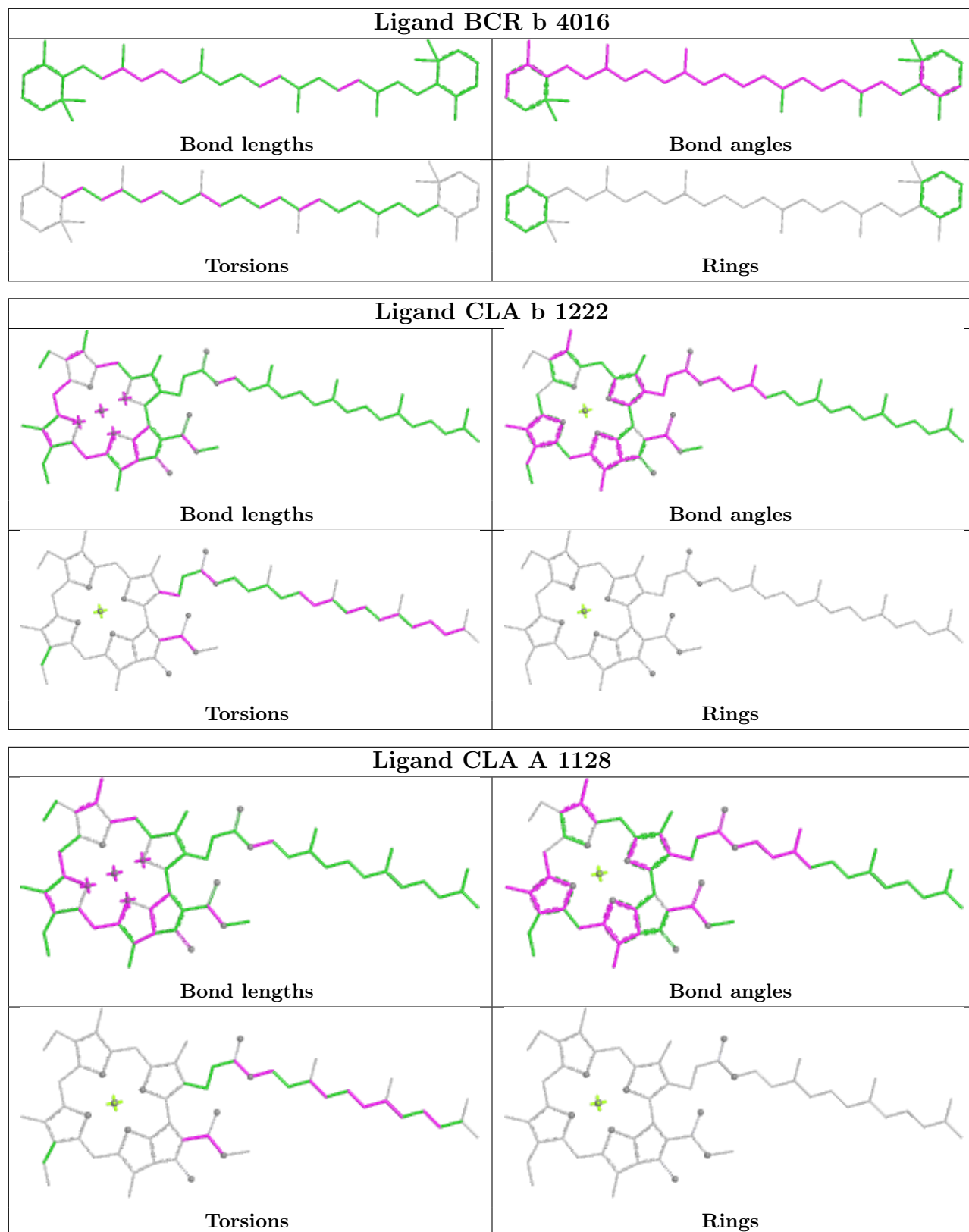
Ligand CLA A 1116

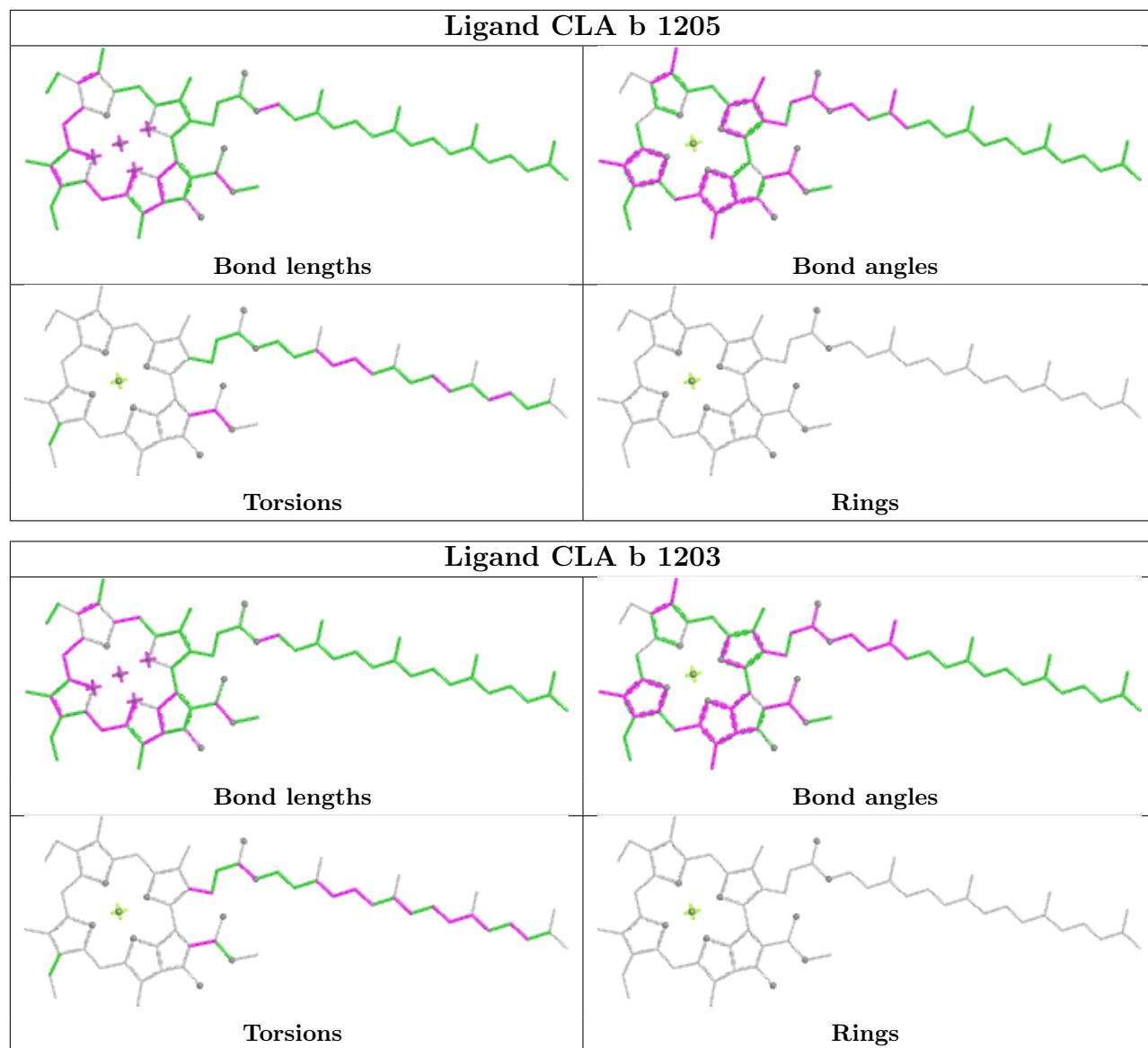


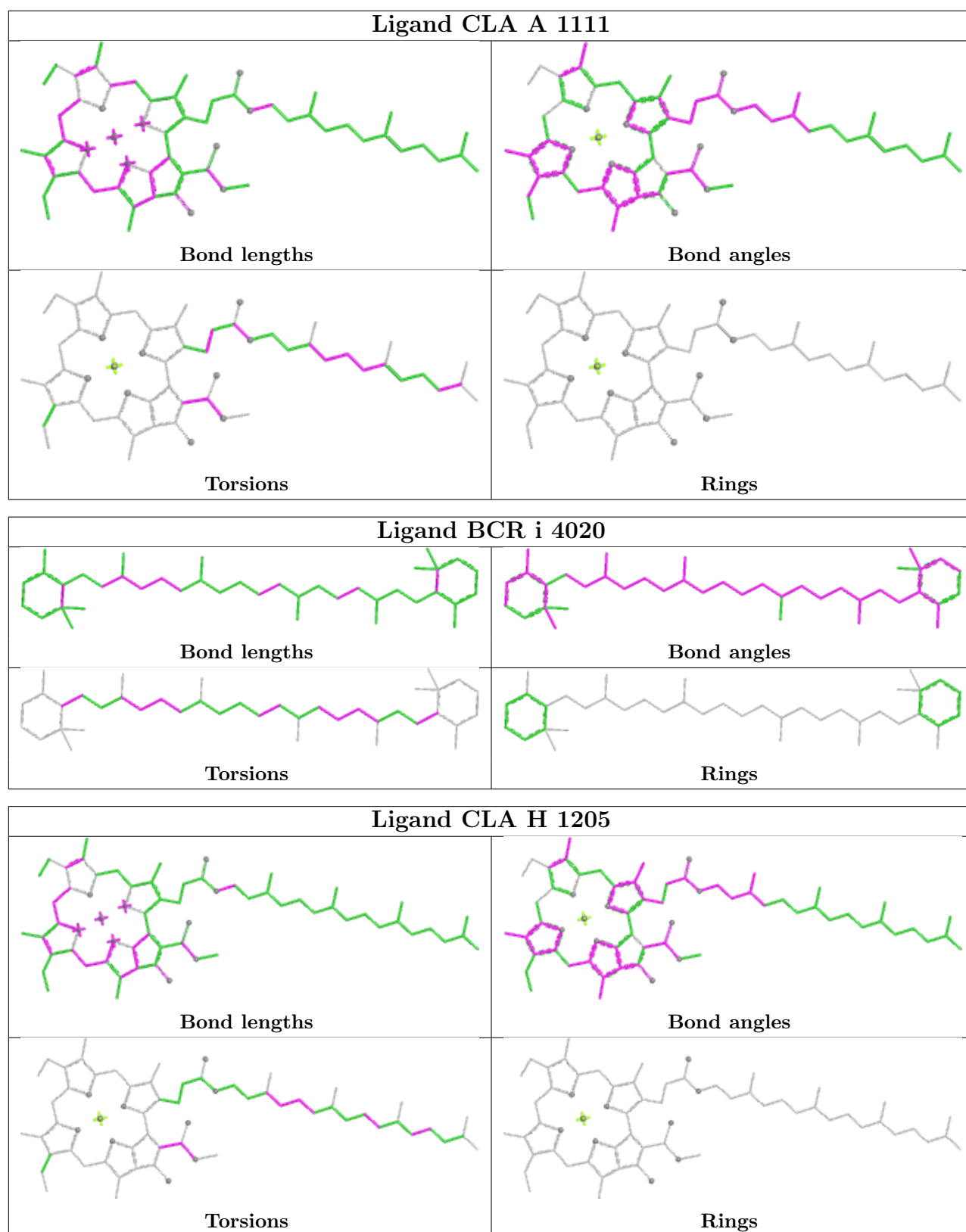
Ligand CLA H 1223

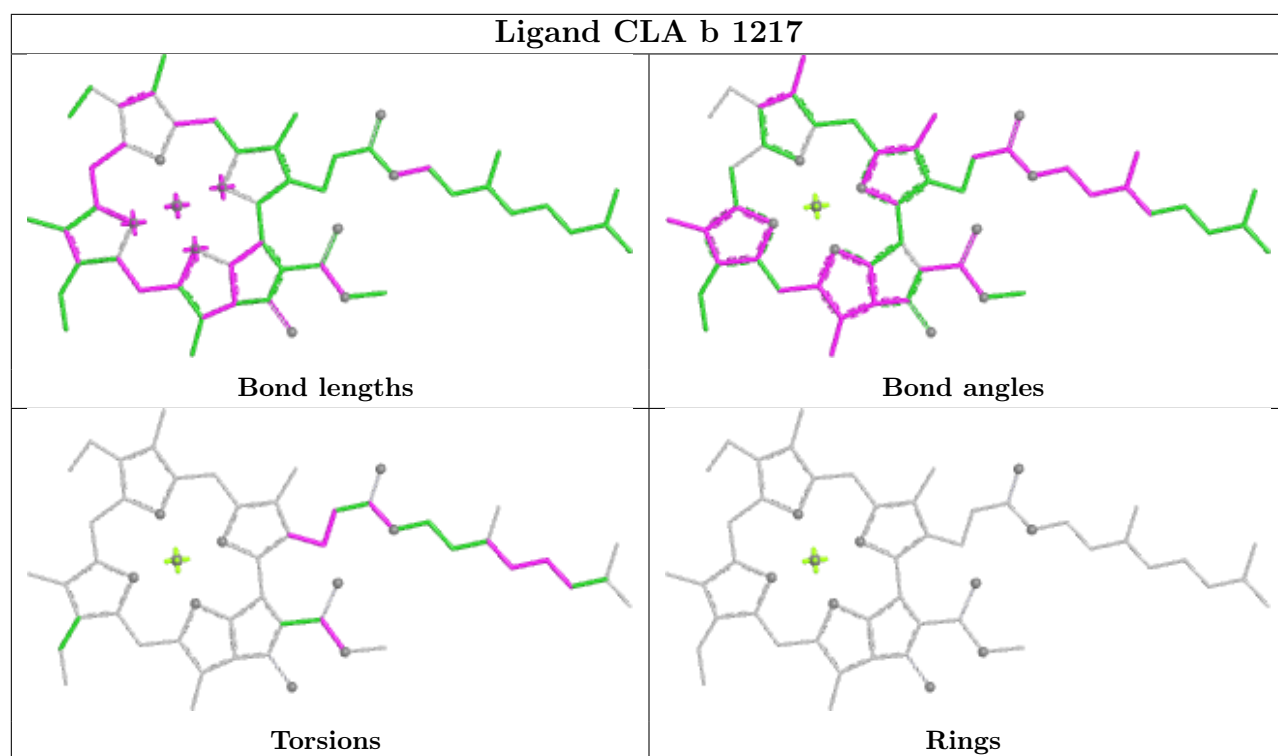


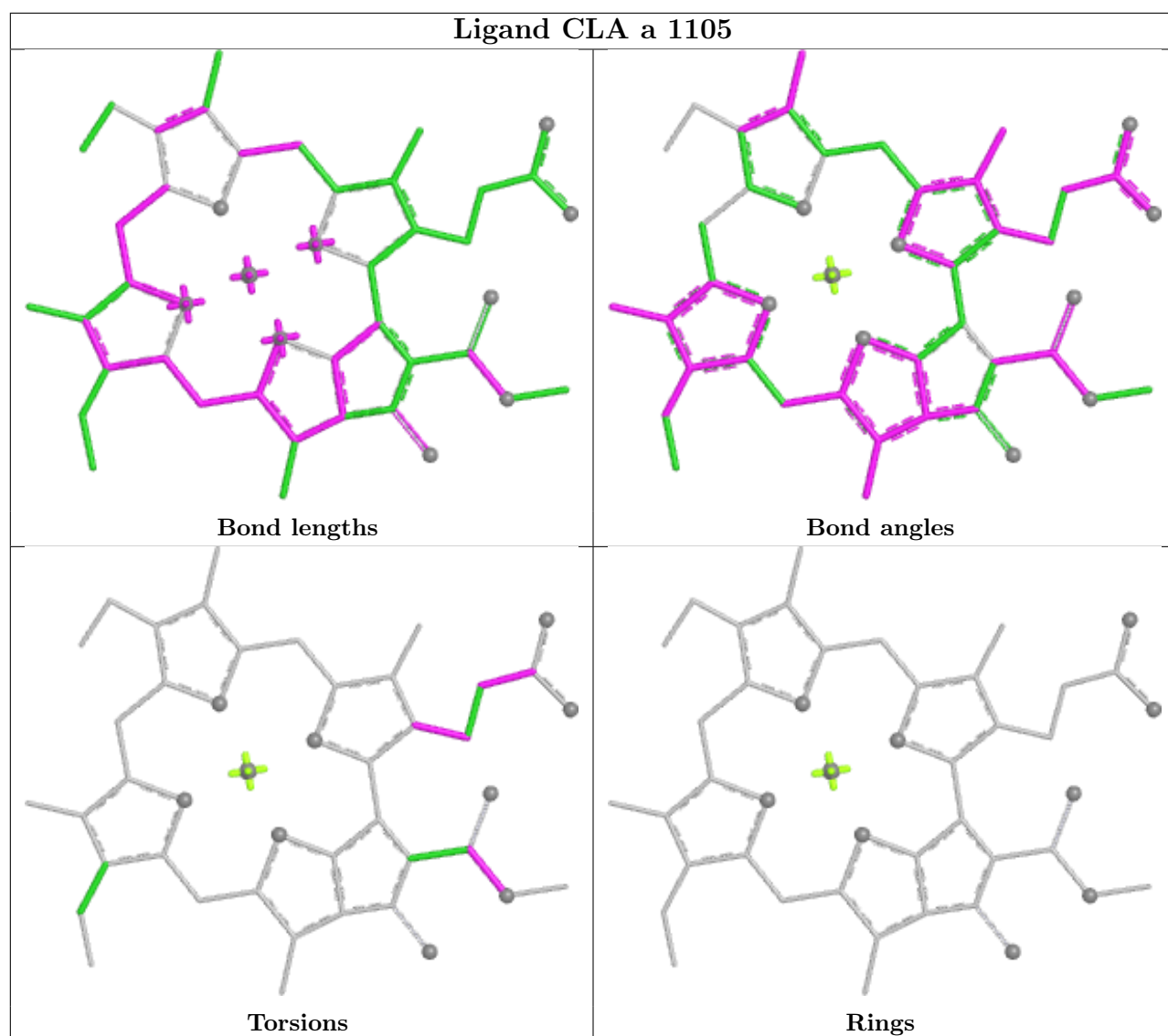


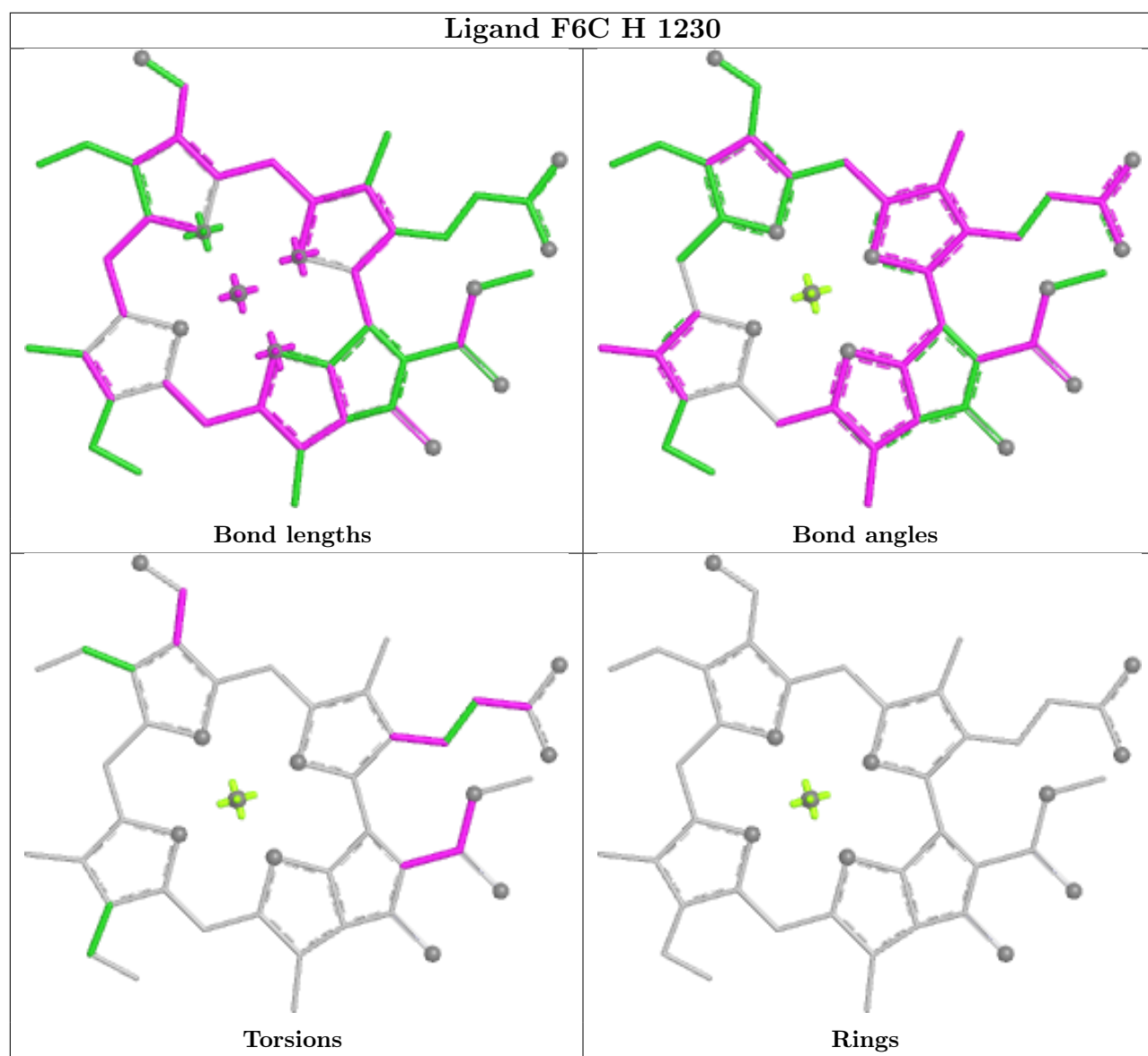


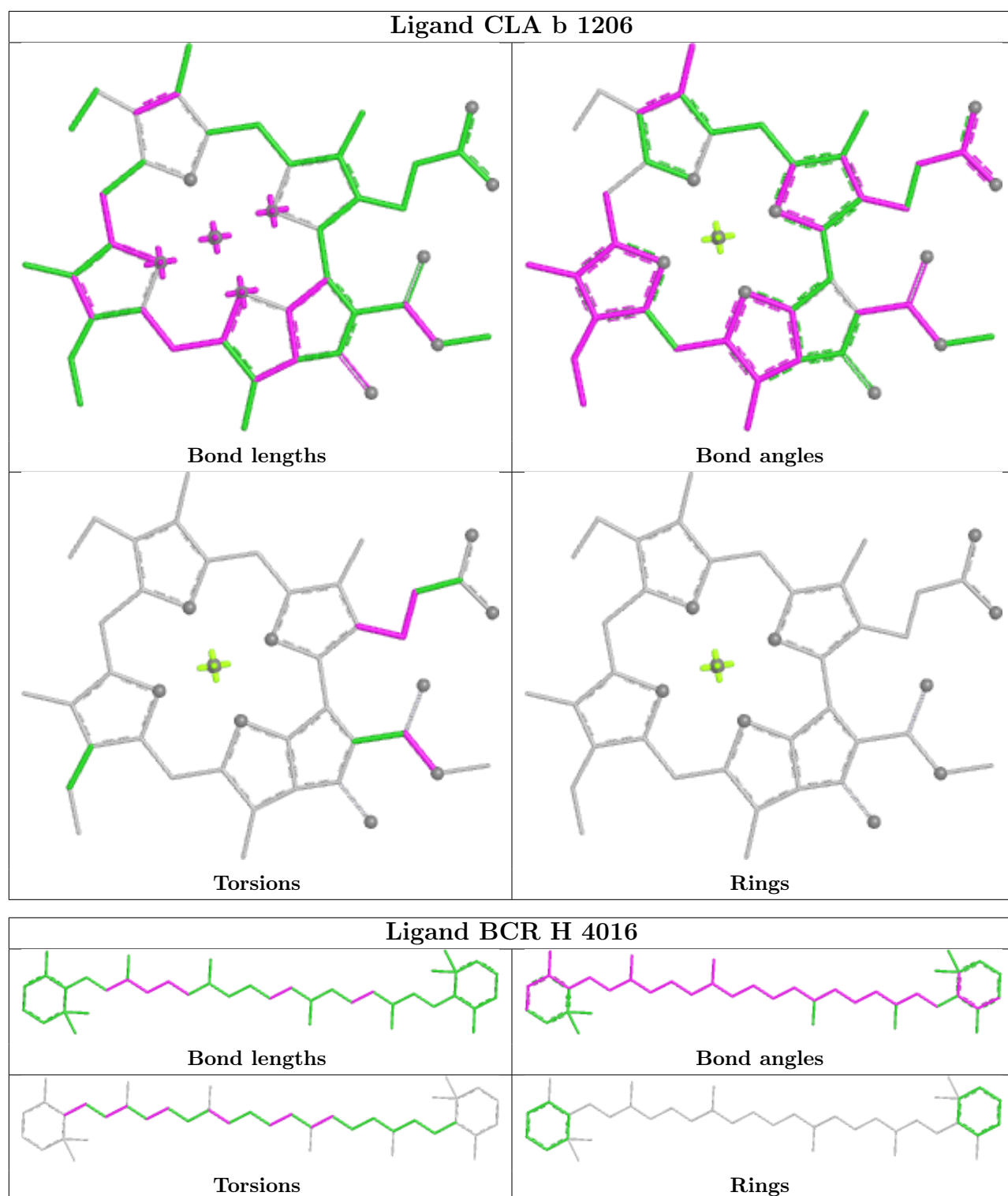


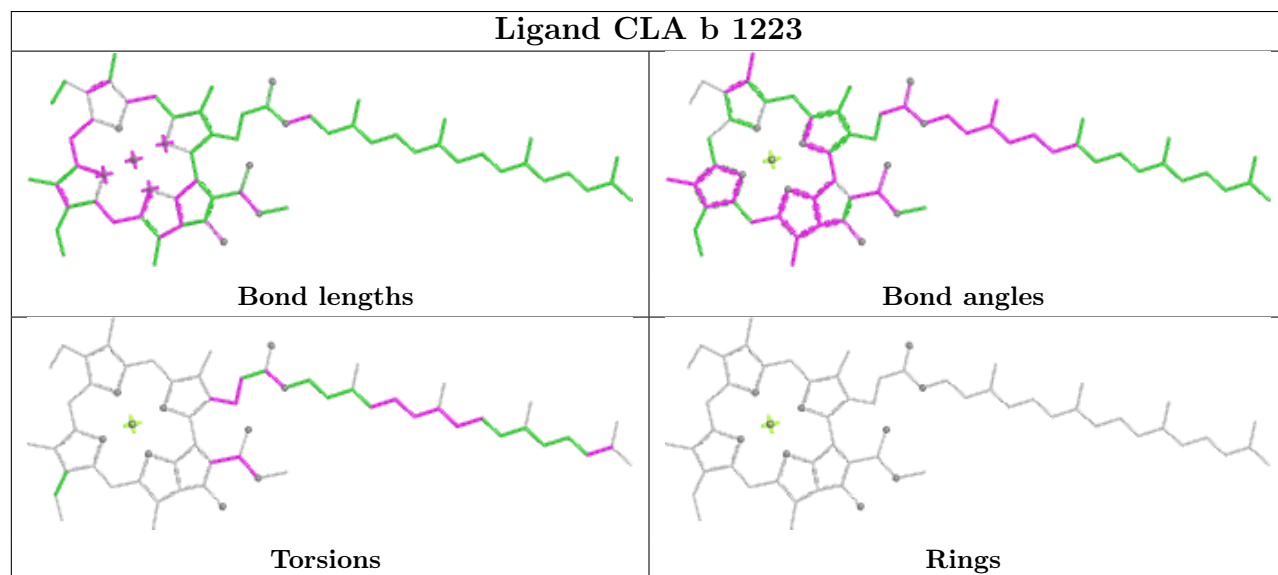
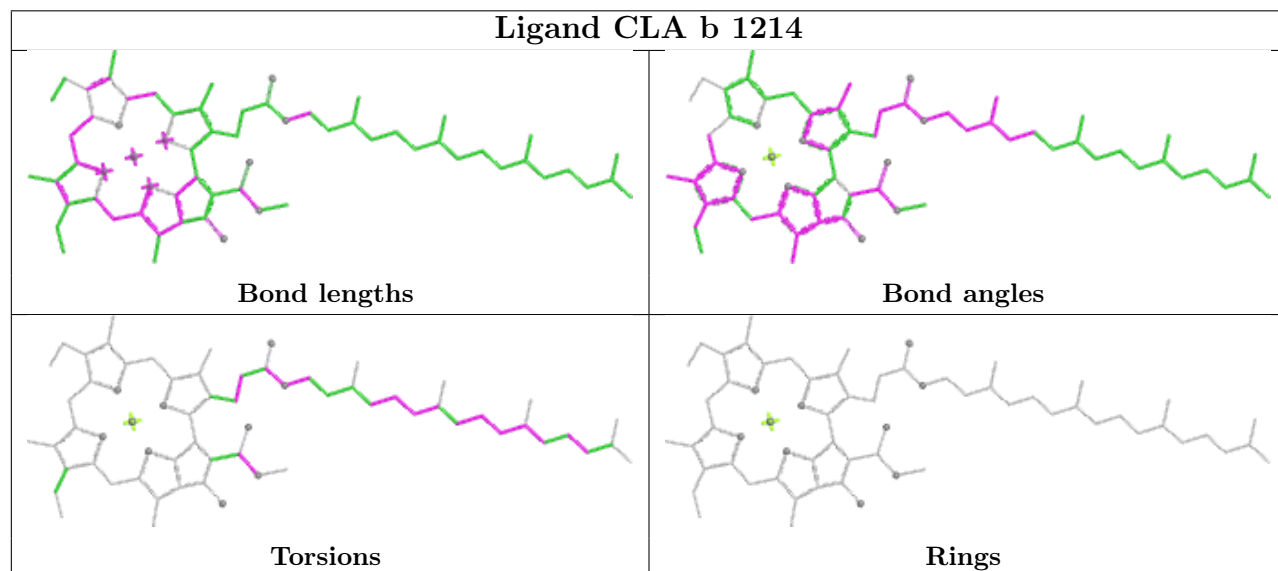
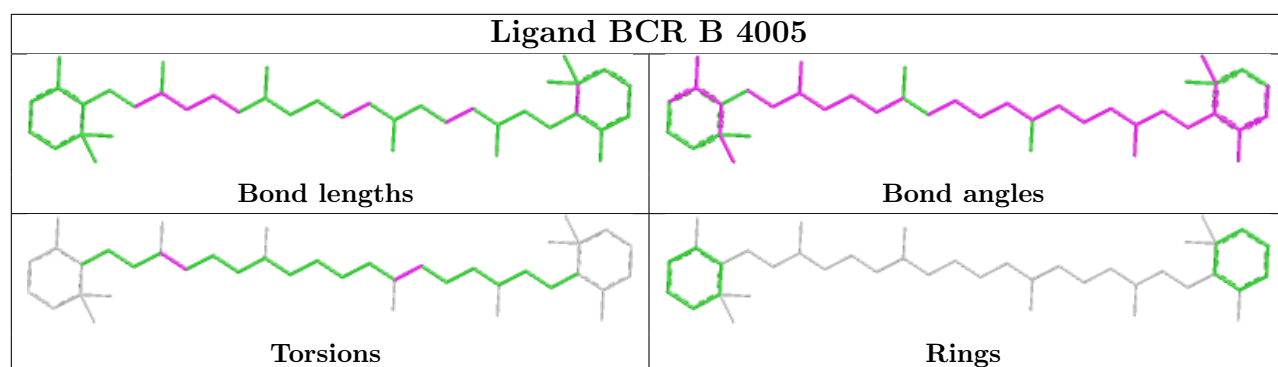




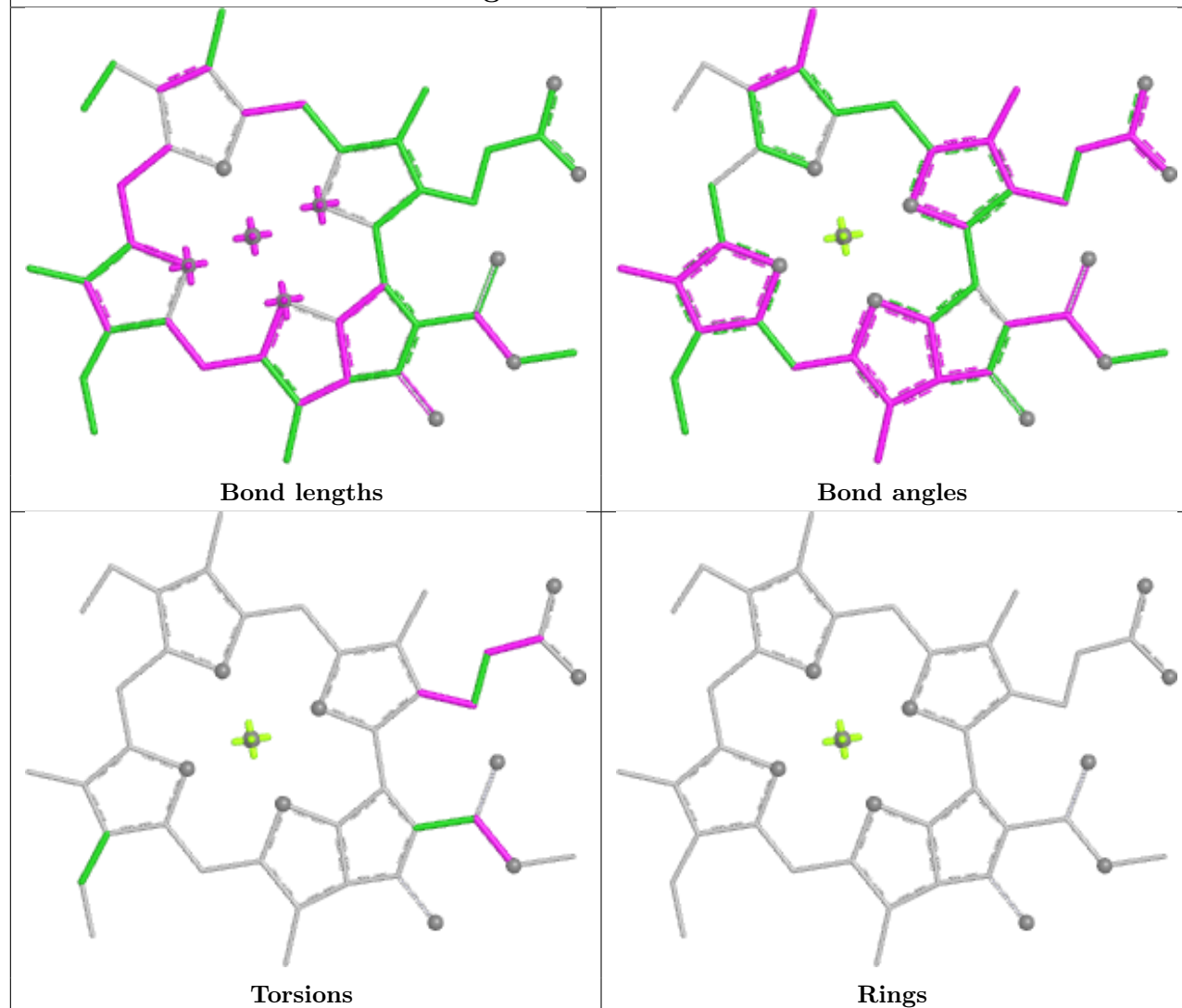




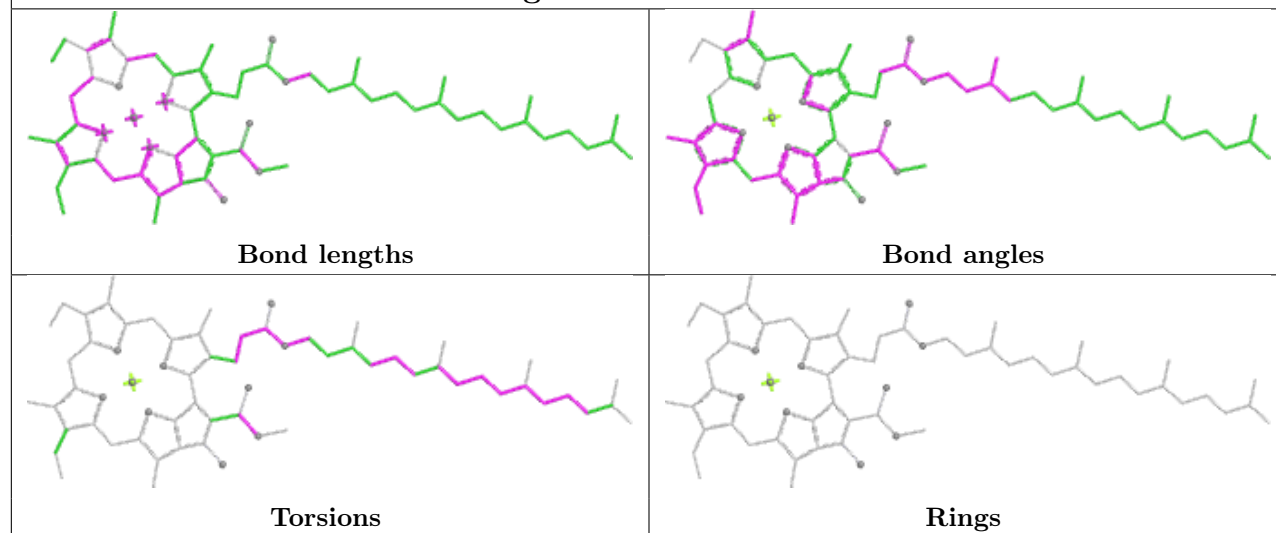


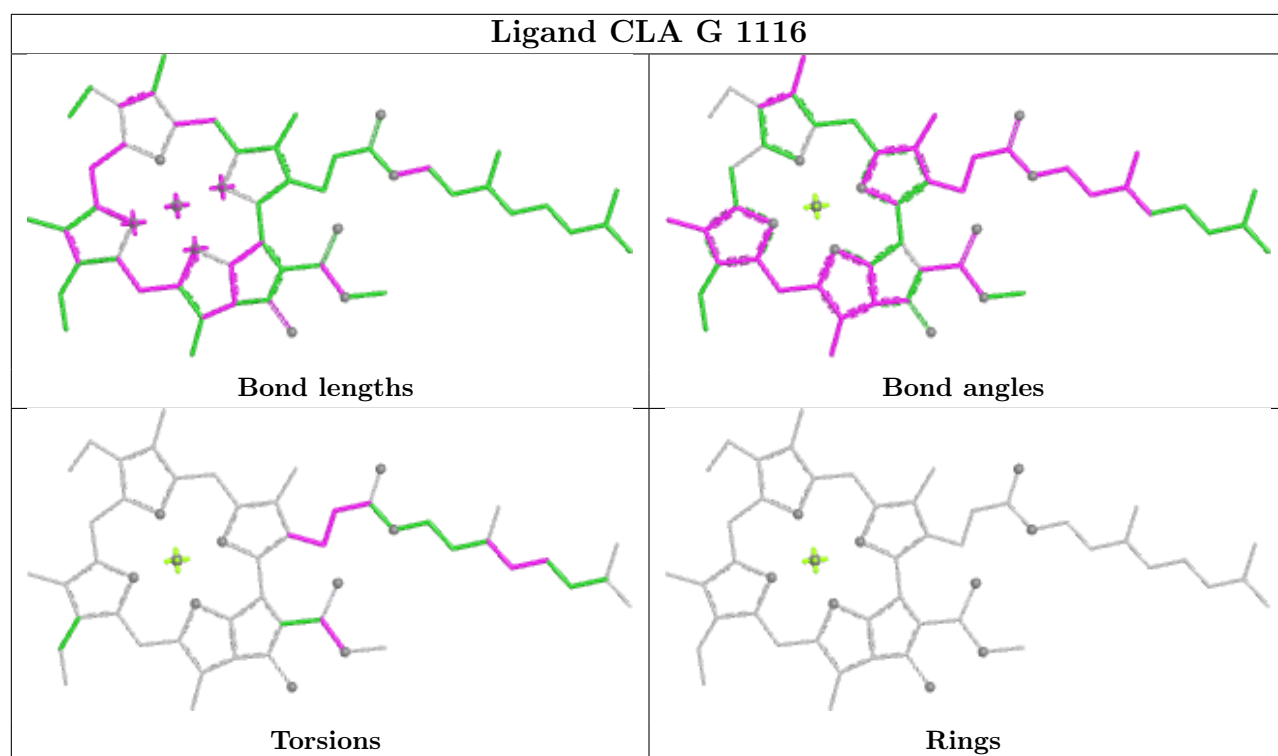


Ligand CLA G 1110

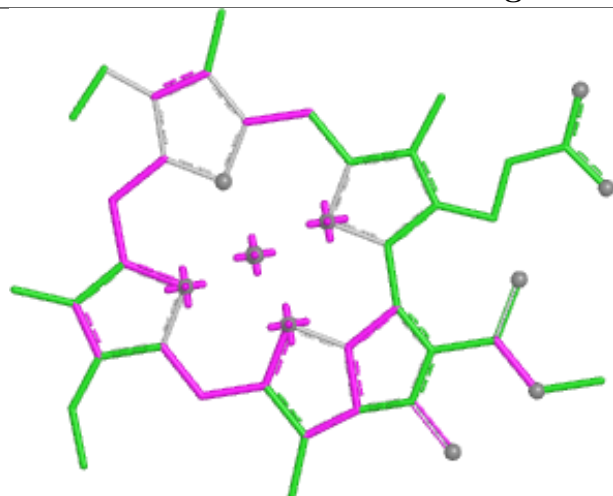


Ligand CLA B 1211

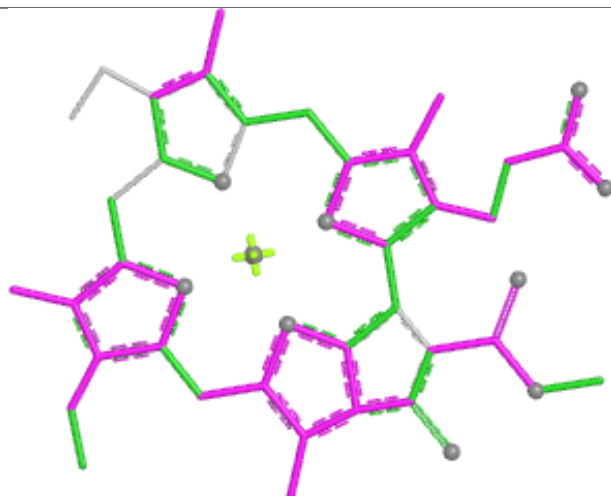




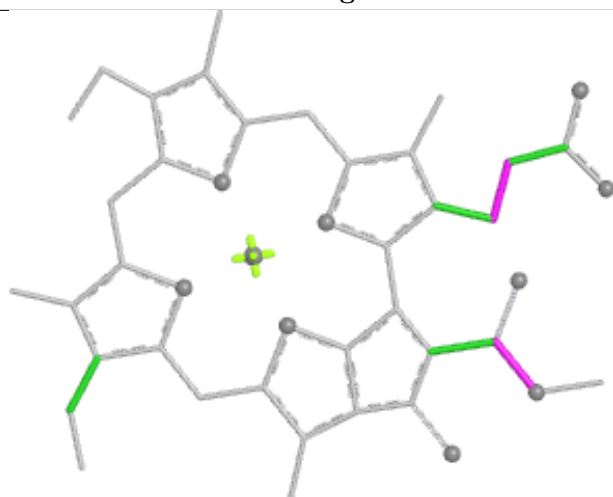
Ligand CLA A 1139



Bond lengths



Bond angles

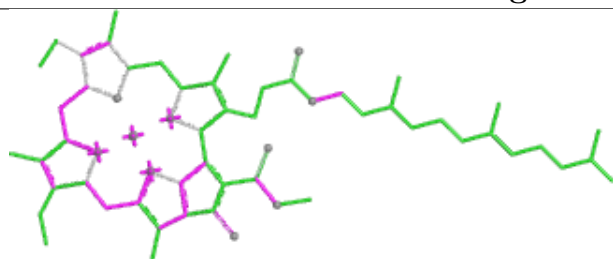


Torsions

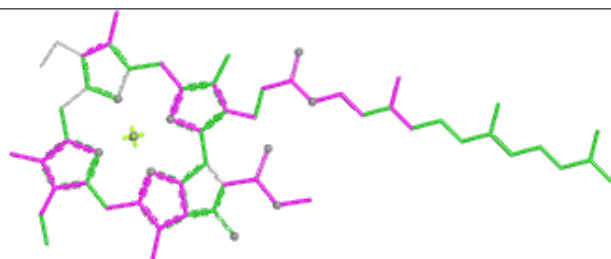


Rings

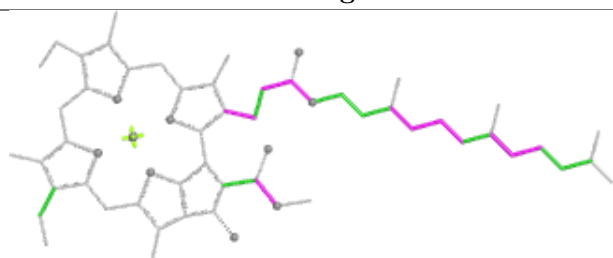
Ligand CLA a 1138



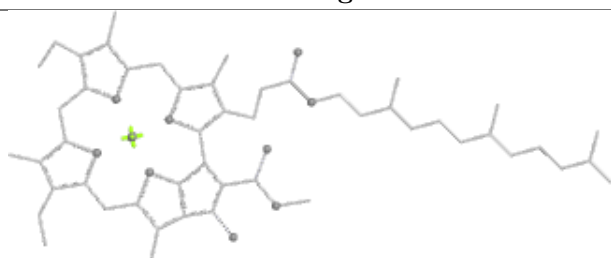
Bond lengths



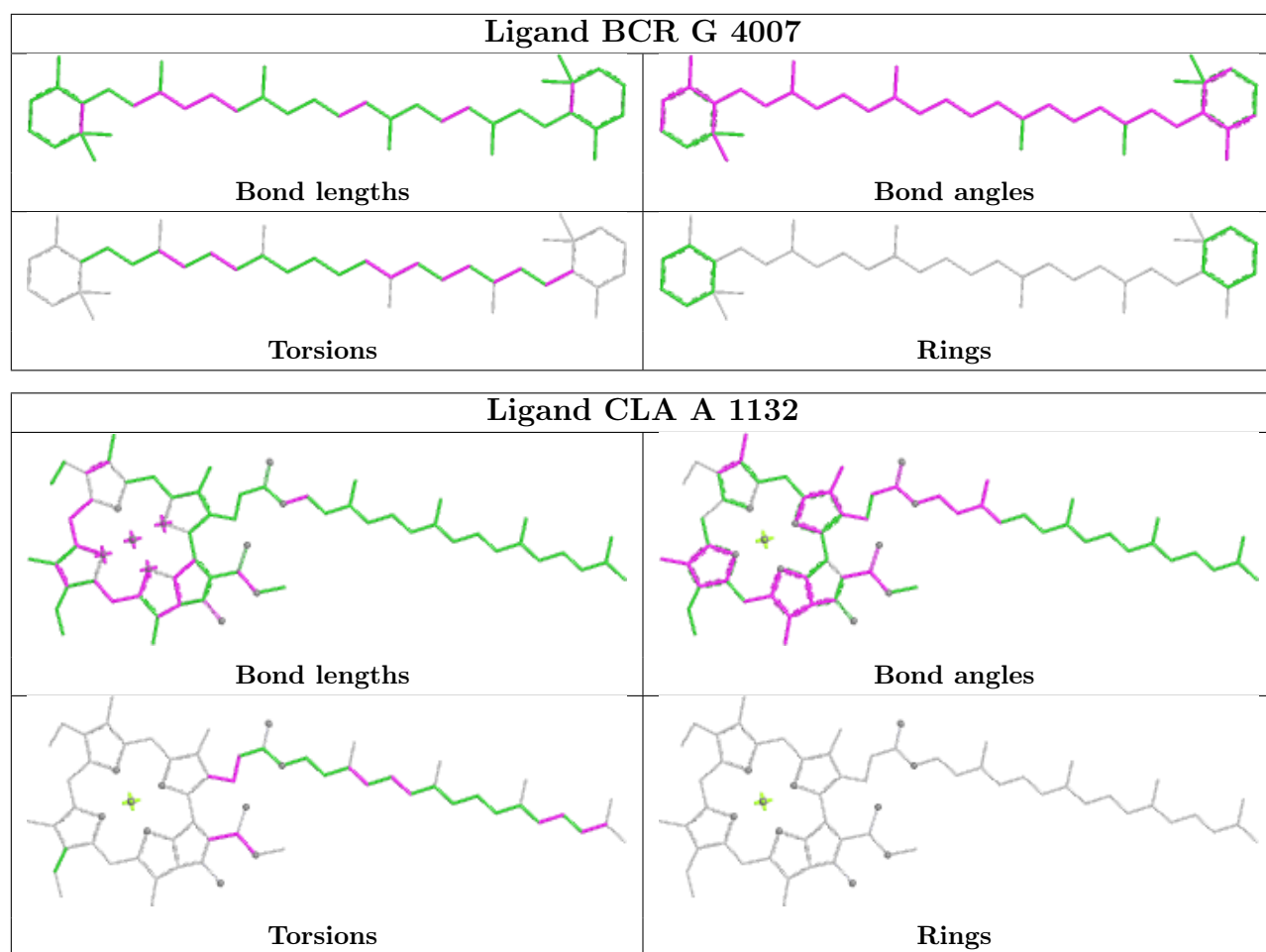
Bond angles

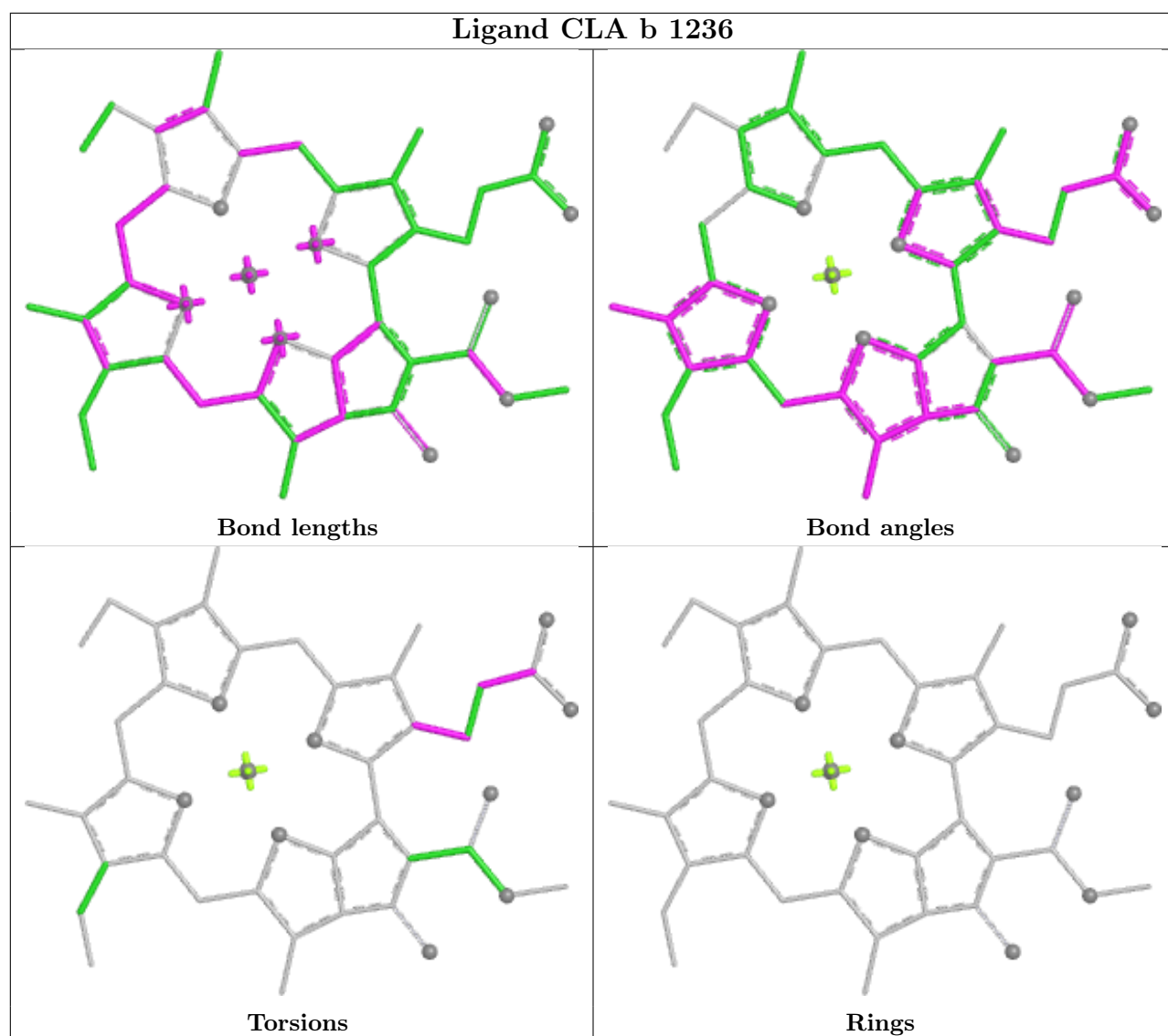


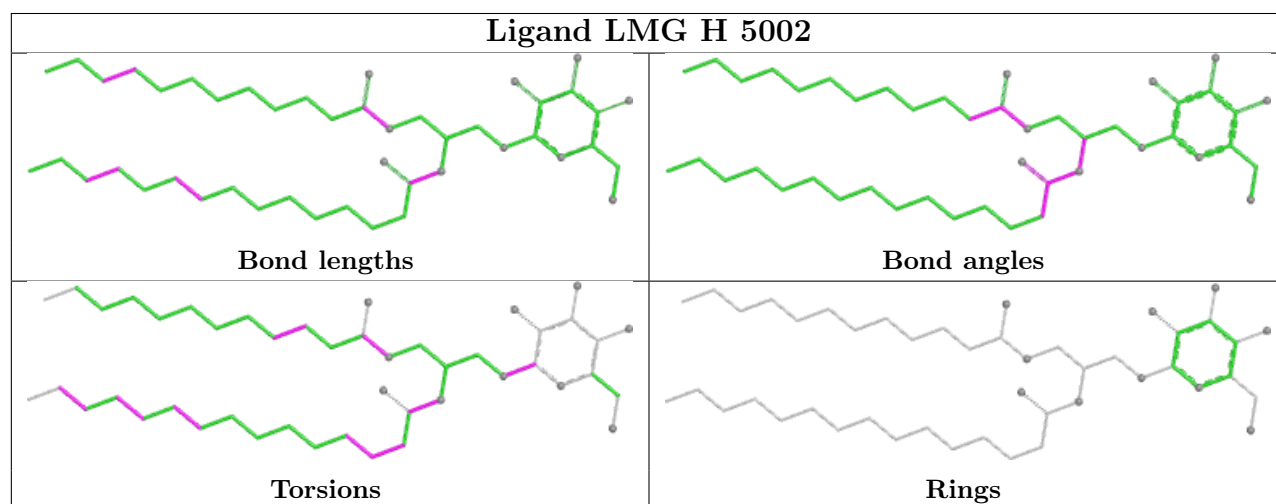
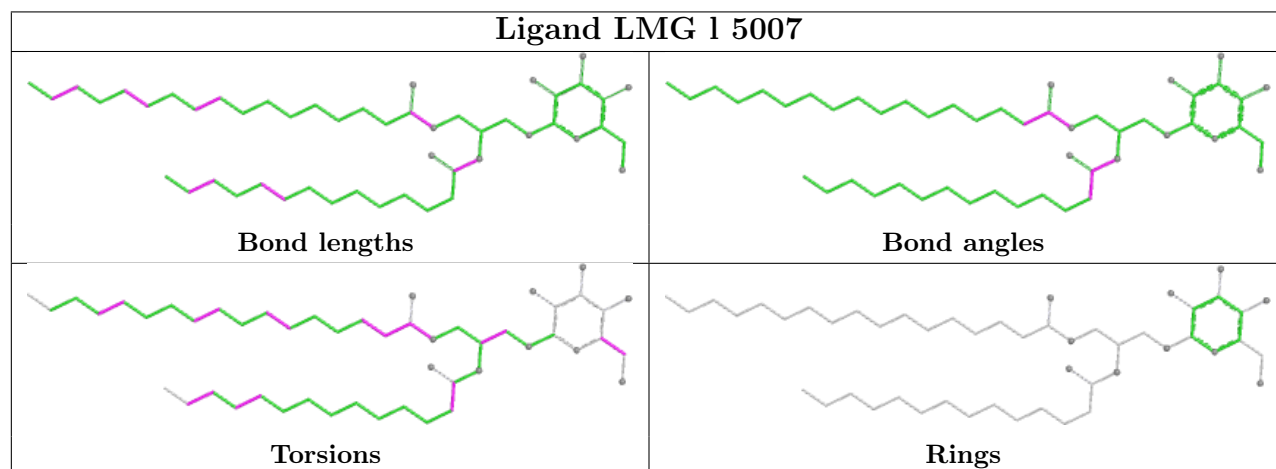
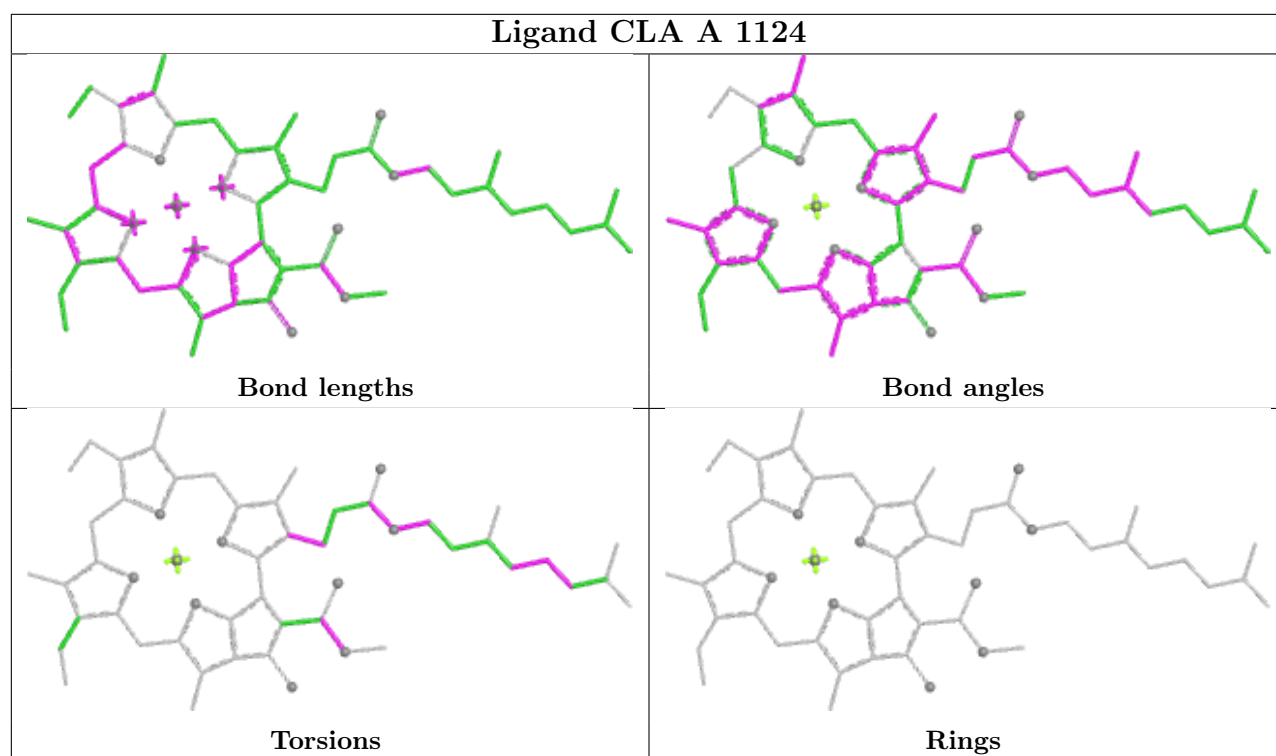
Torsions

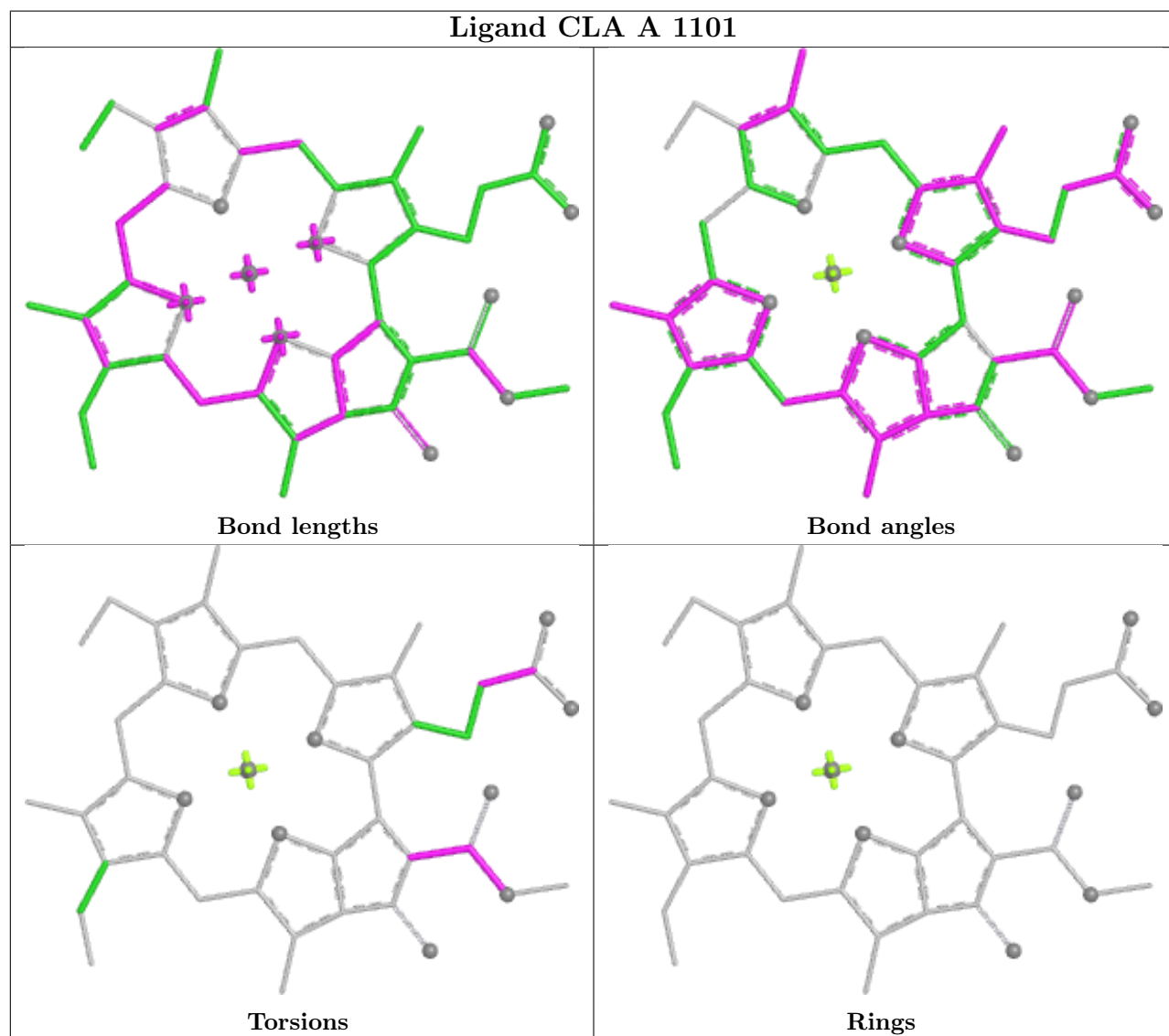
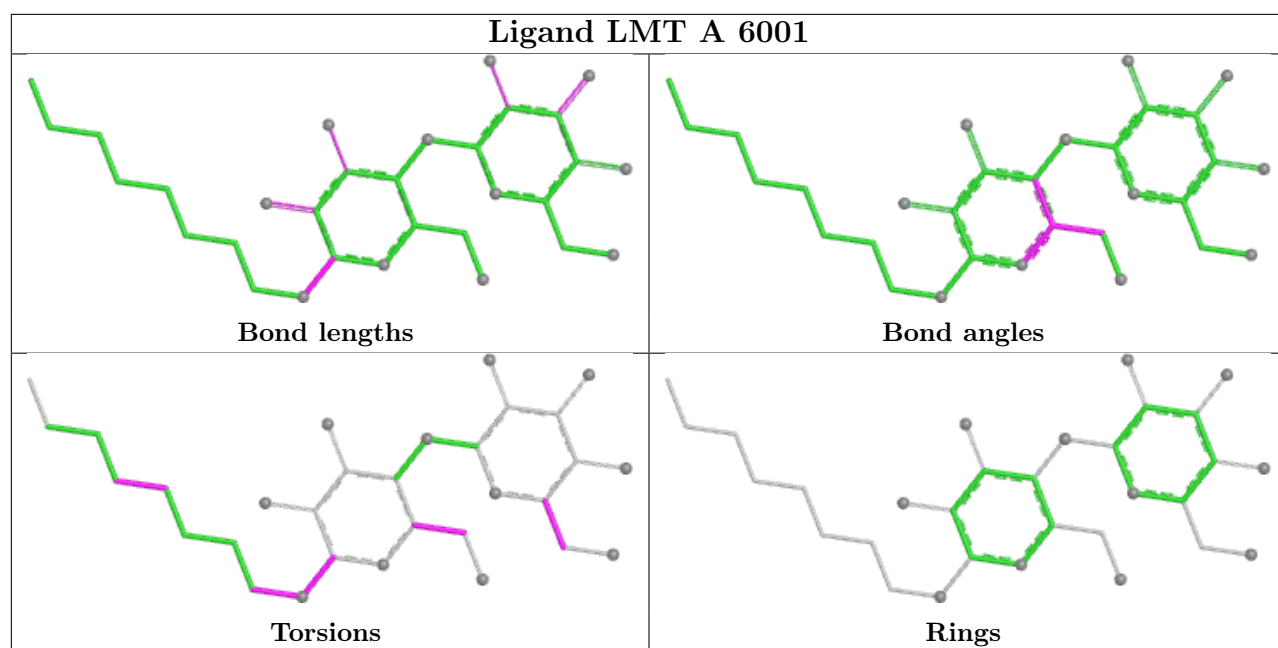


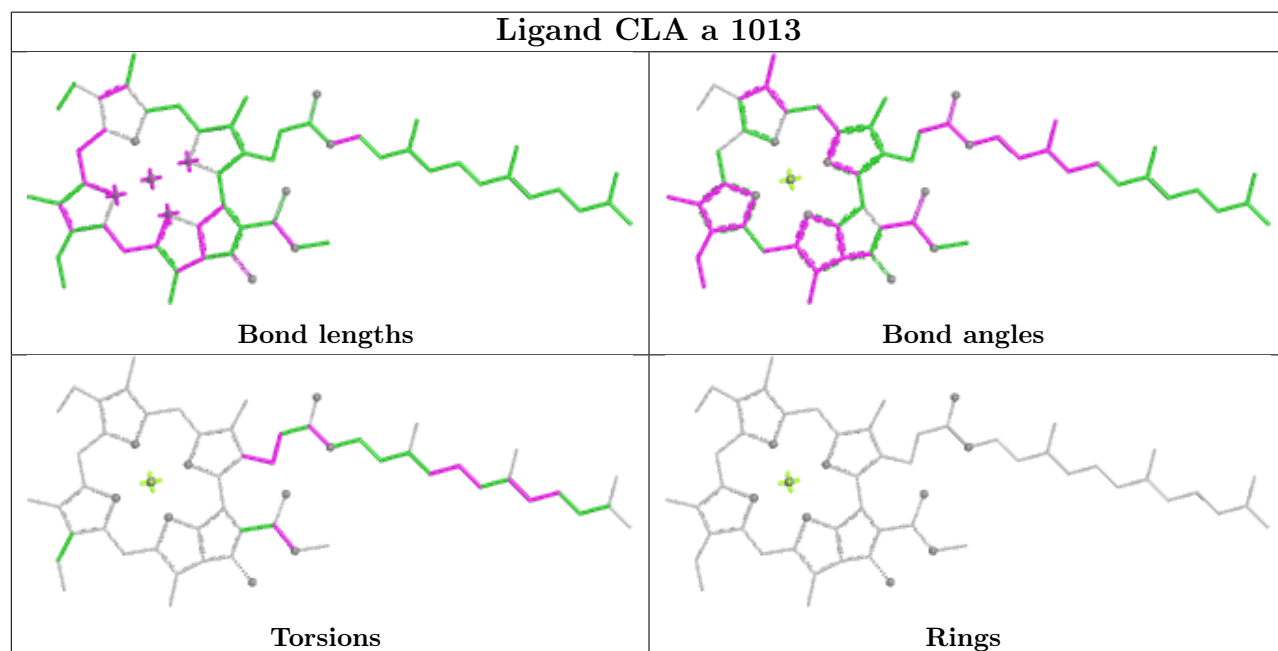
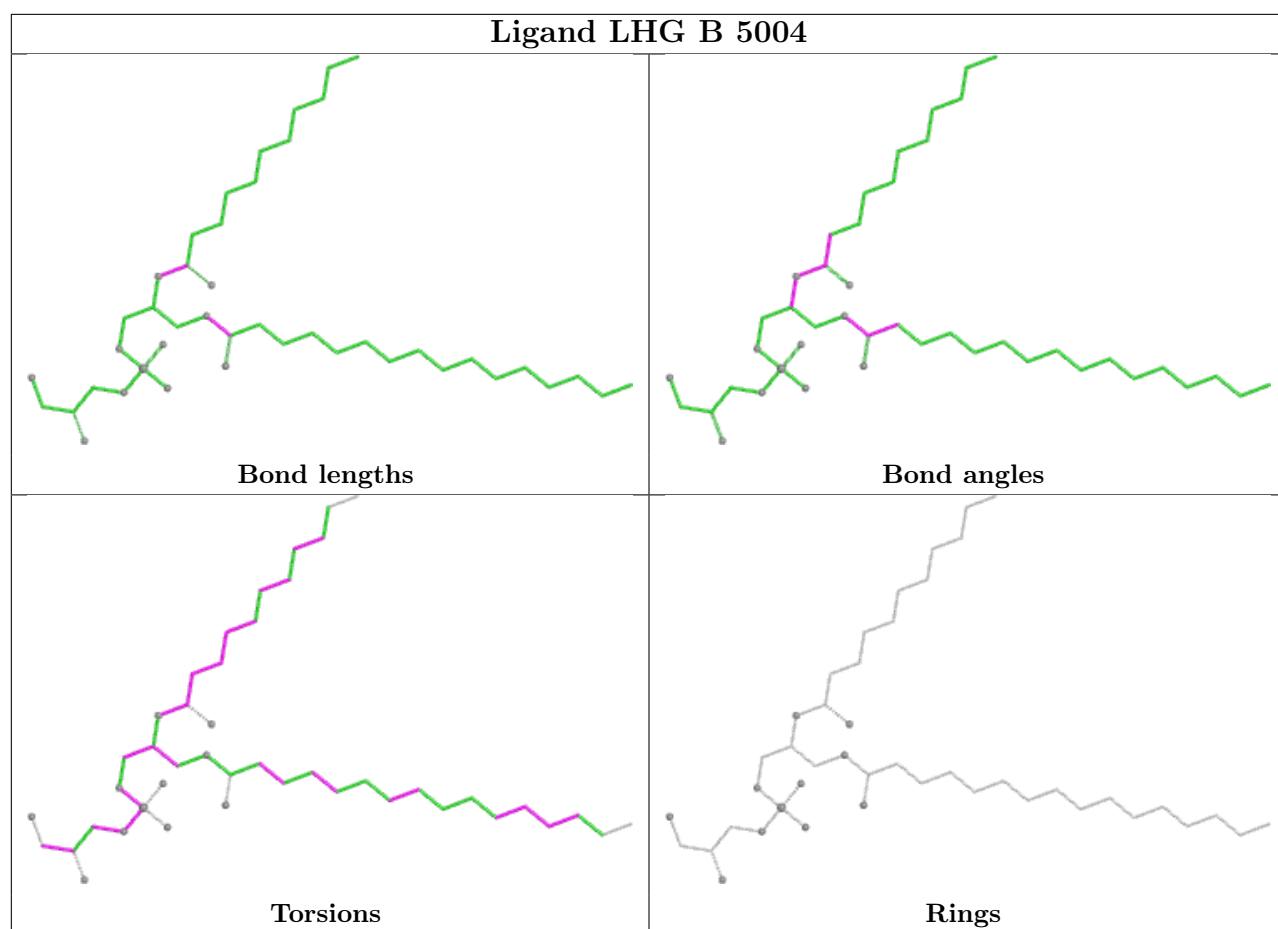
Rings

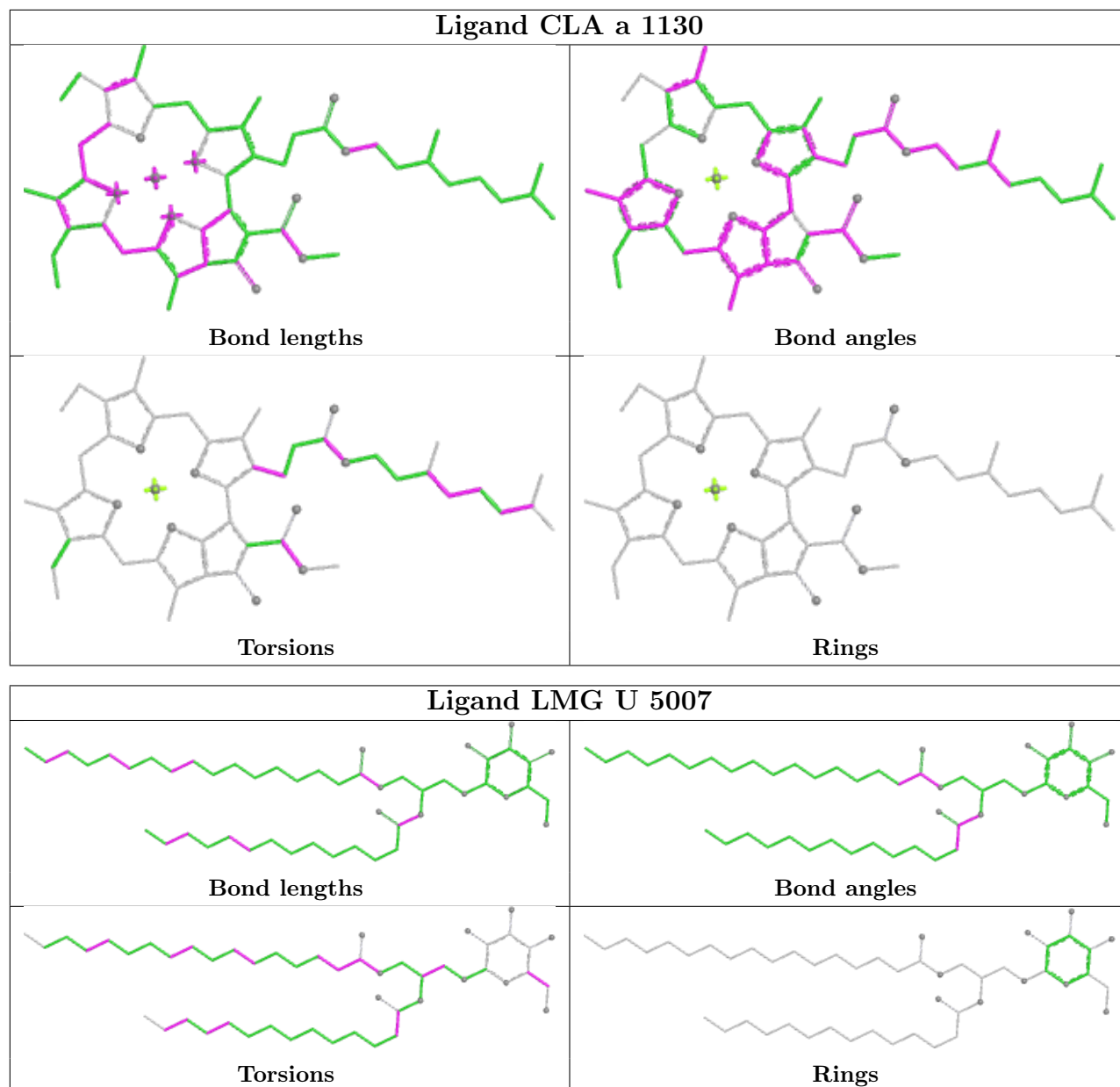


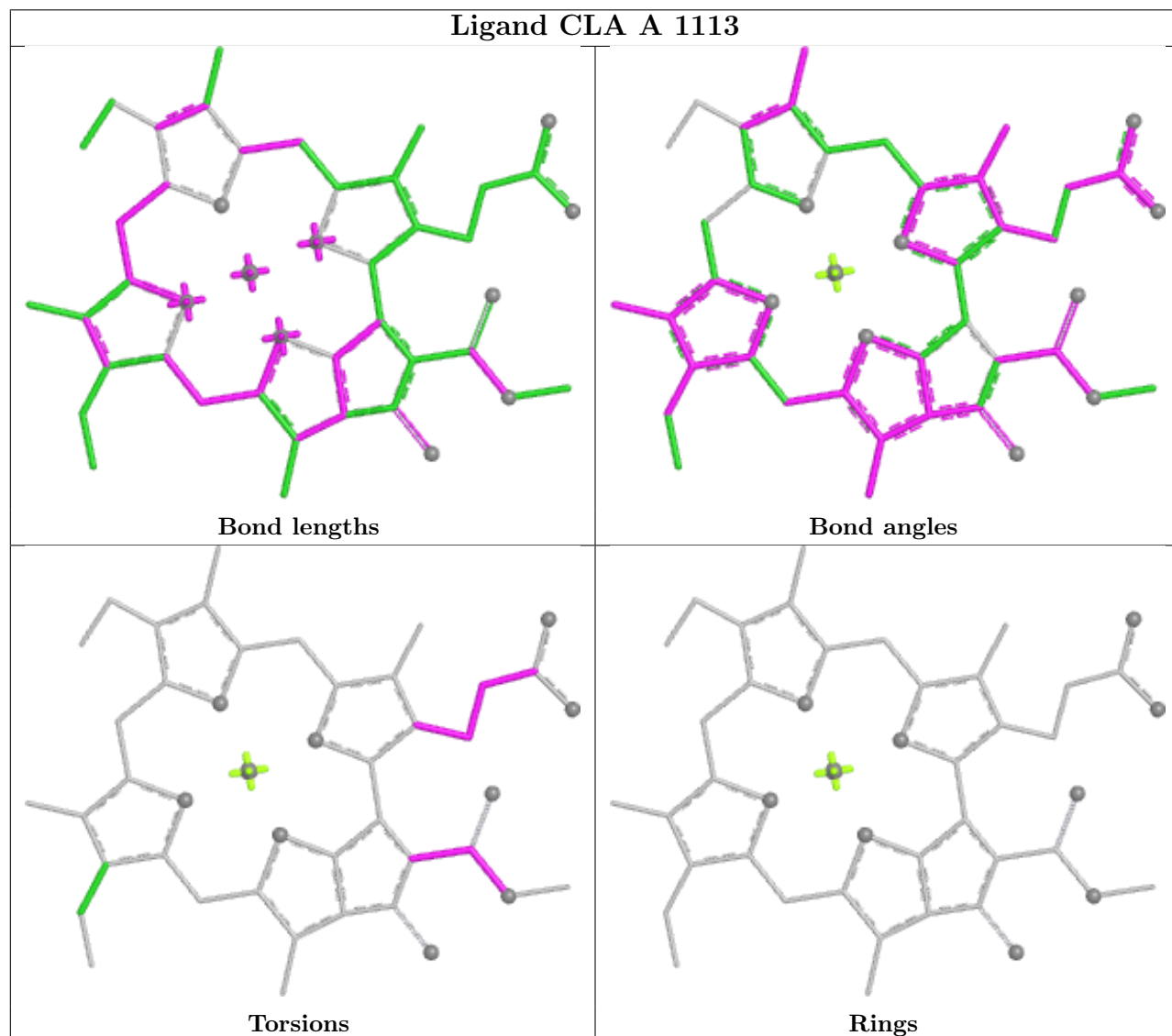
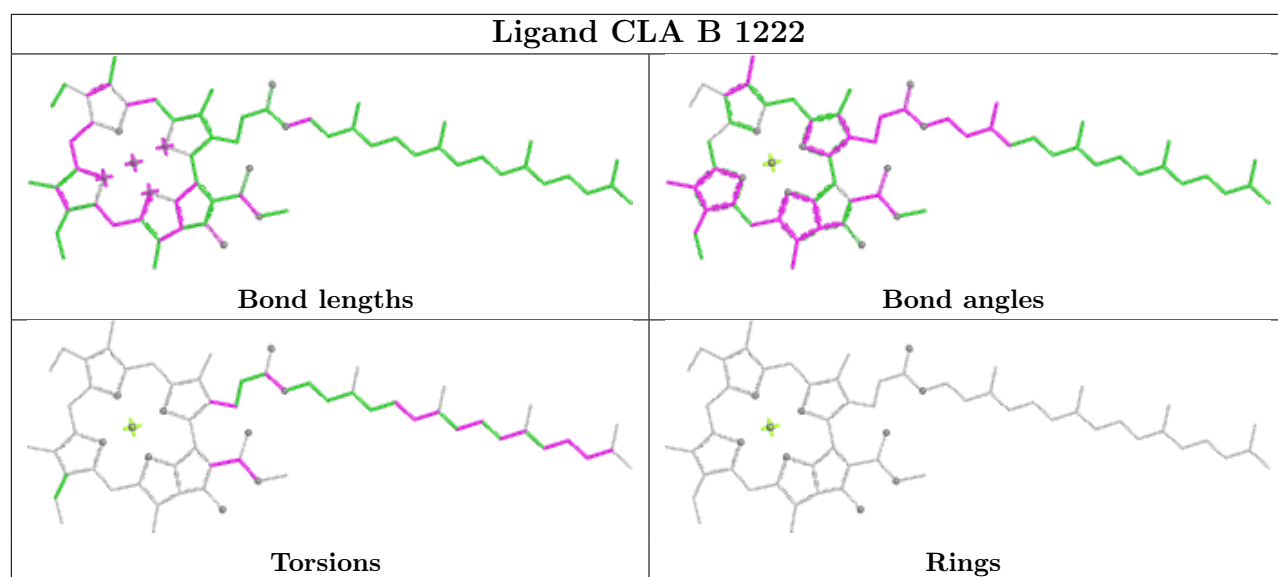


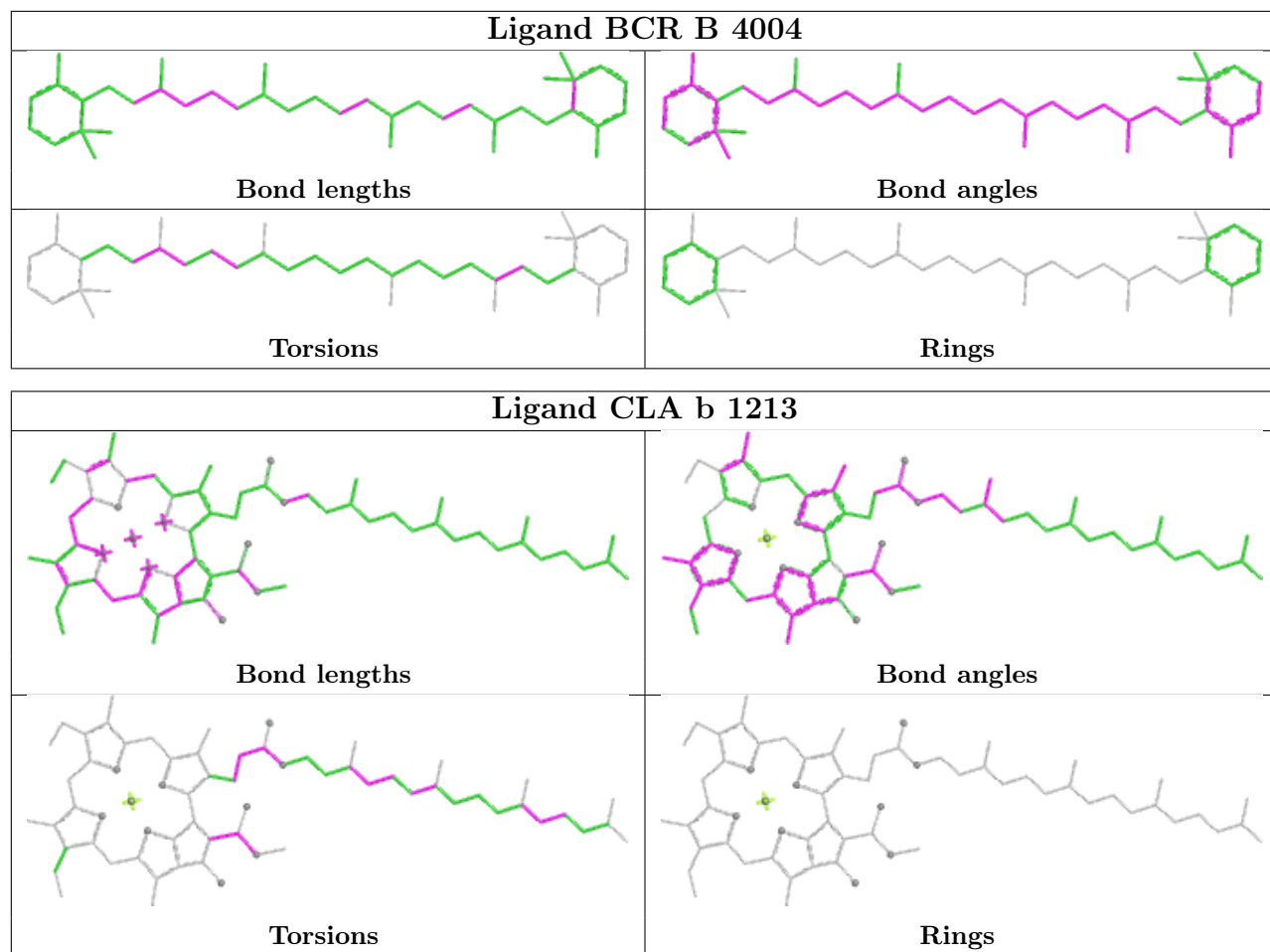




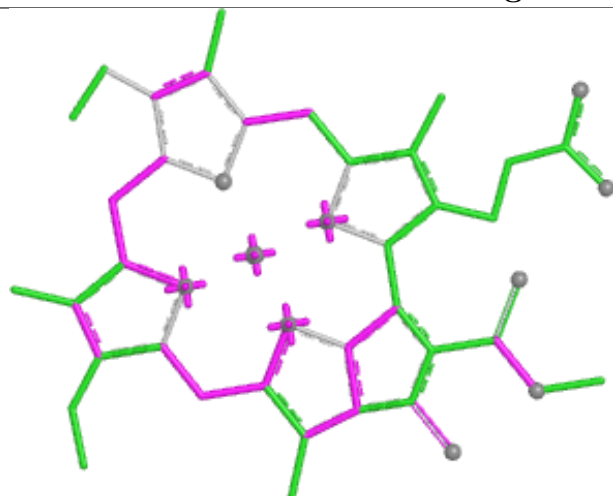




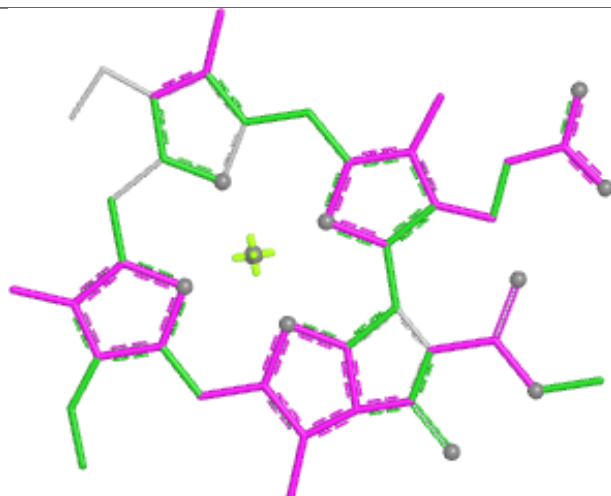




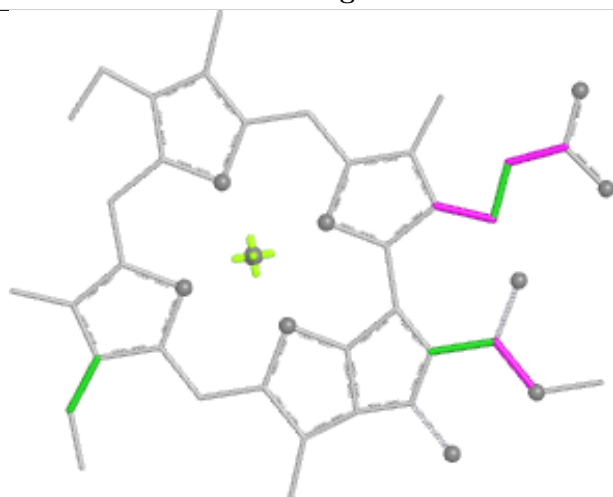
Ligand CLA A 1110



Bond lengths



Bond angles

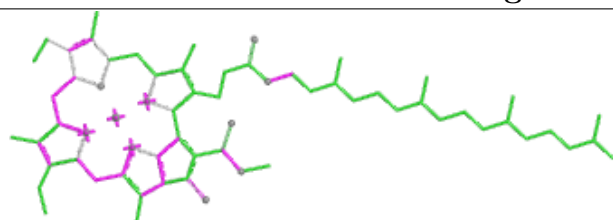


Torsions

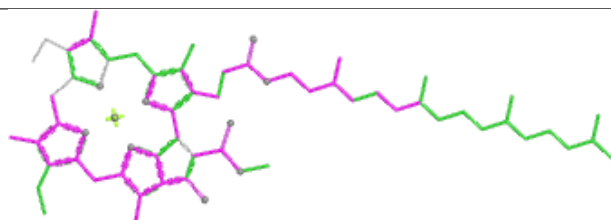


Rings

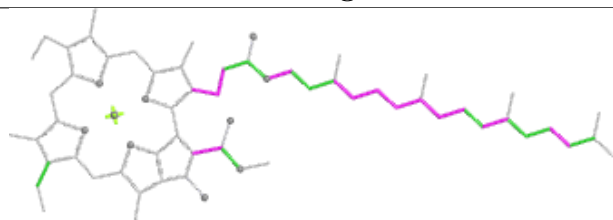
Ligand CLA H 1022



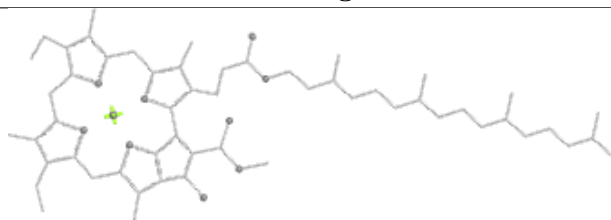
Bond lengths



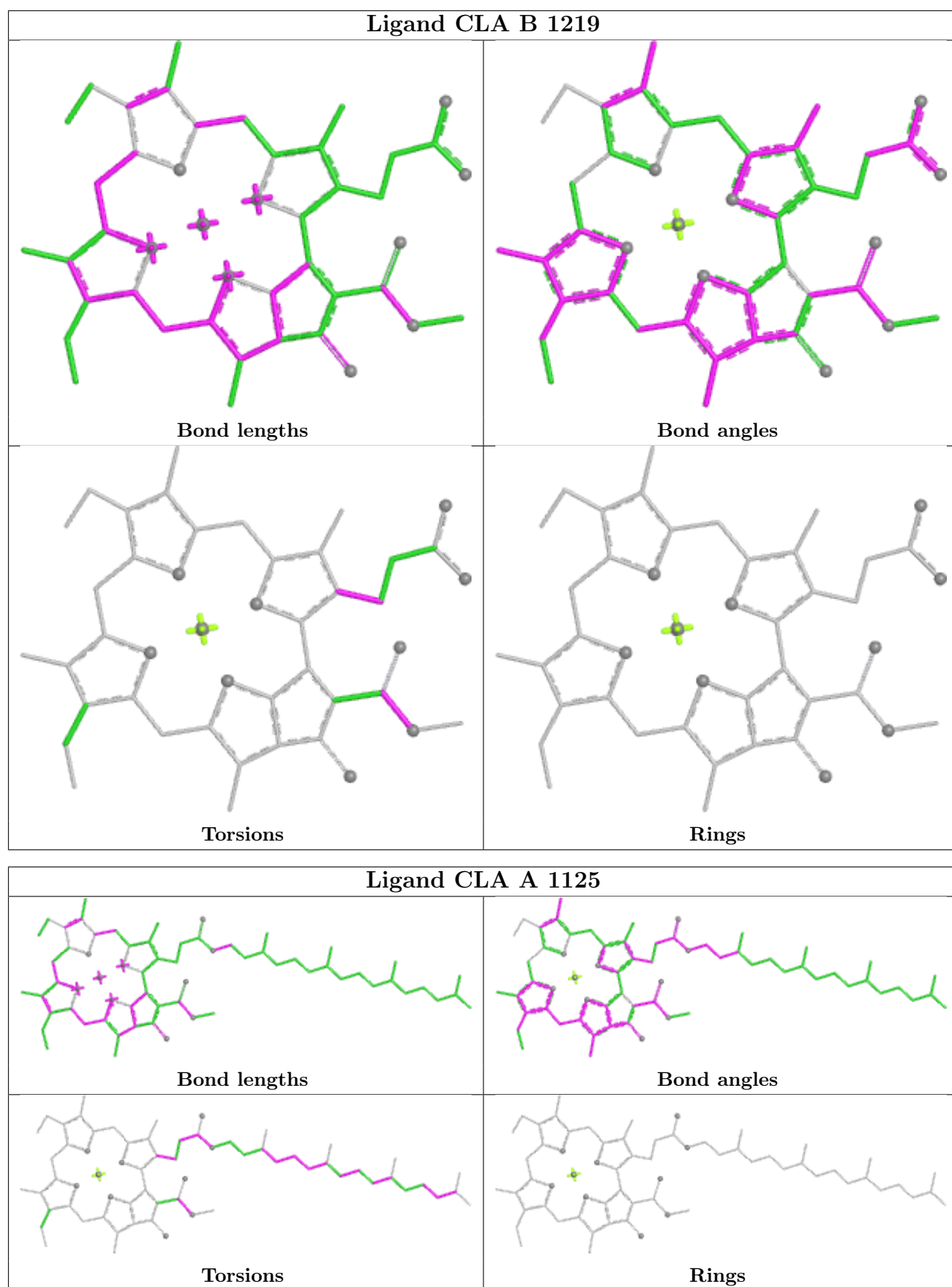
Bond angles

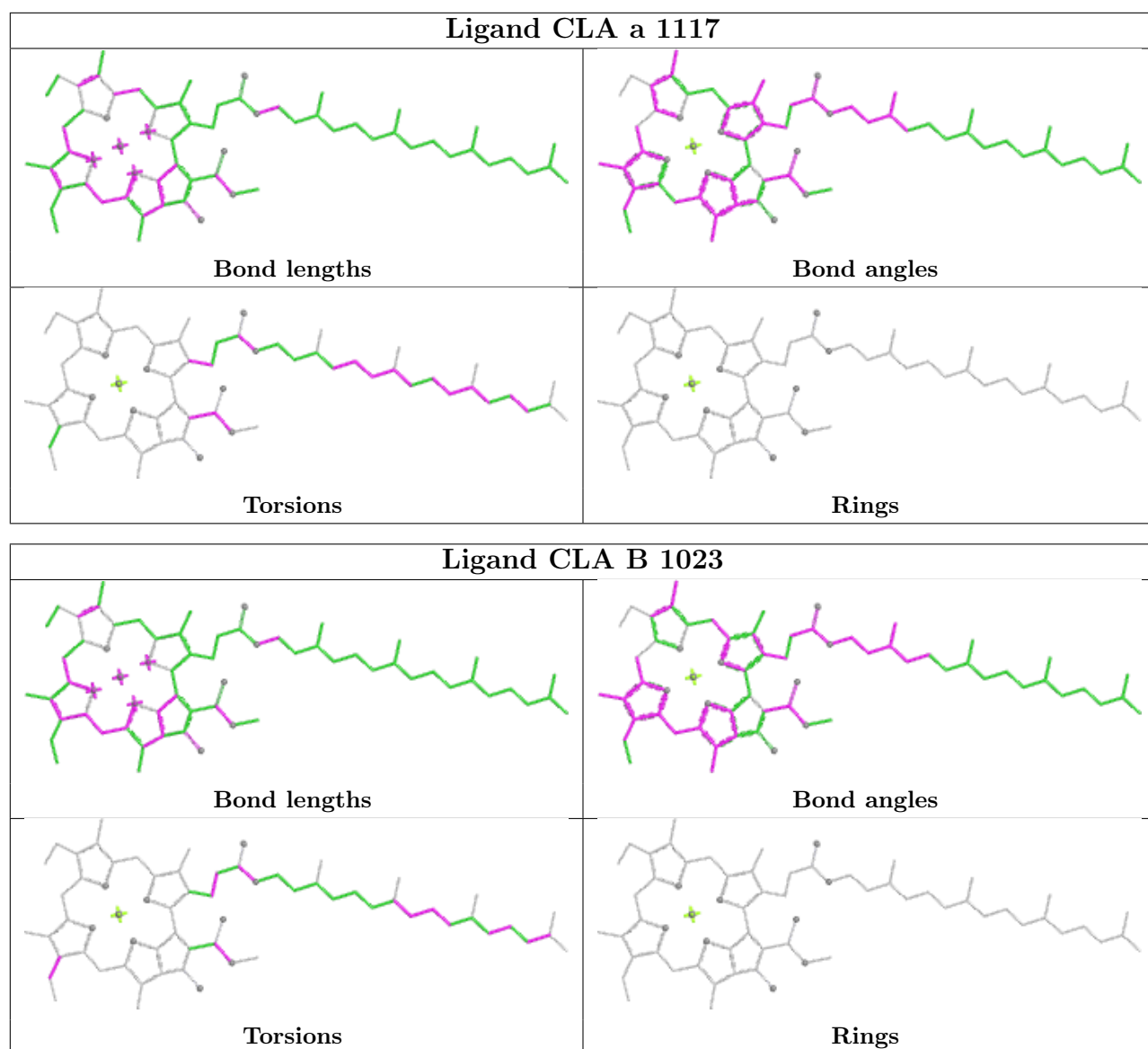


Torsions

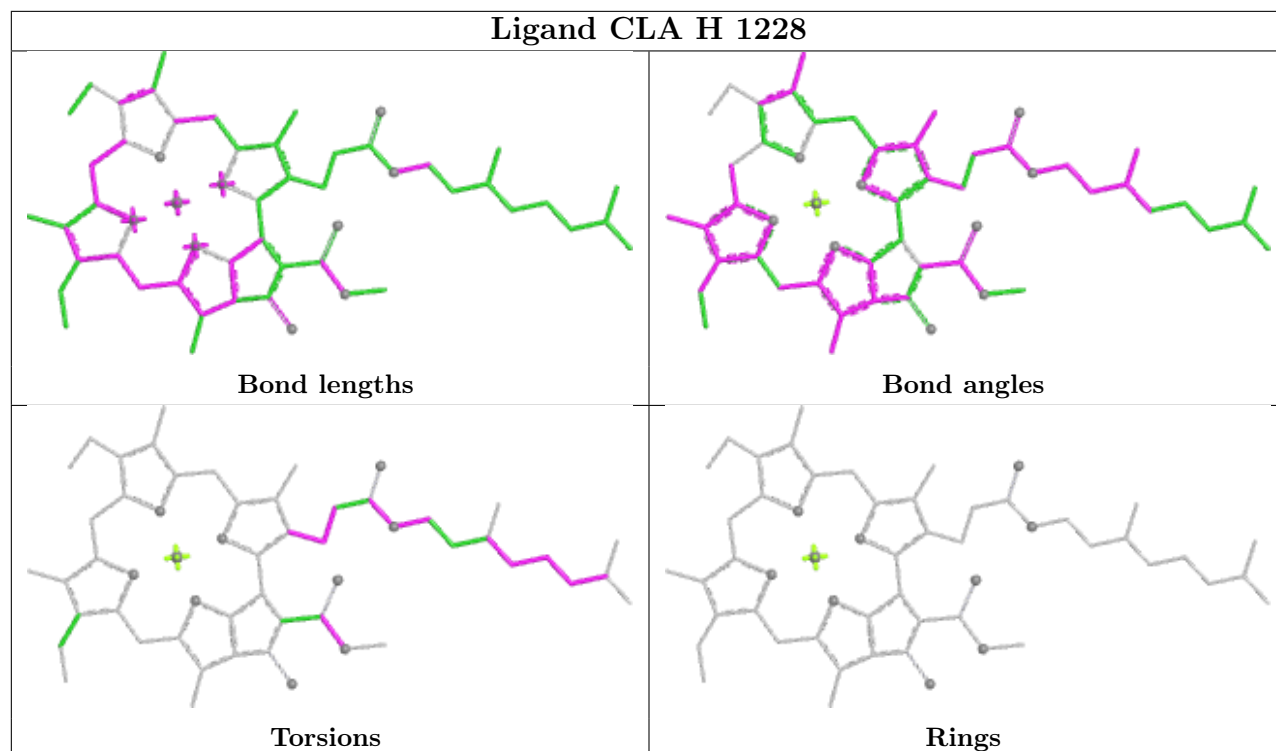


Rings

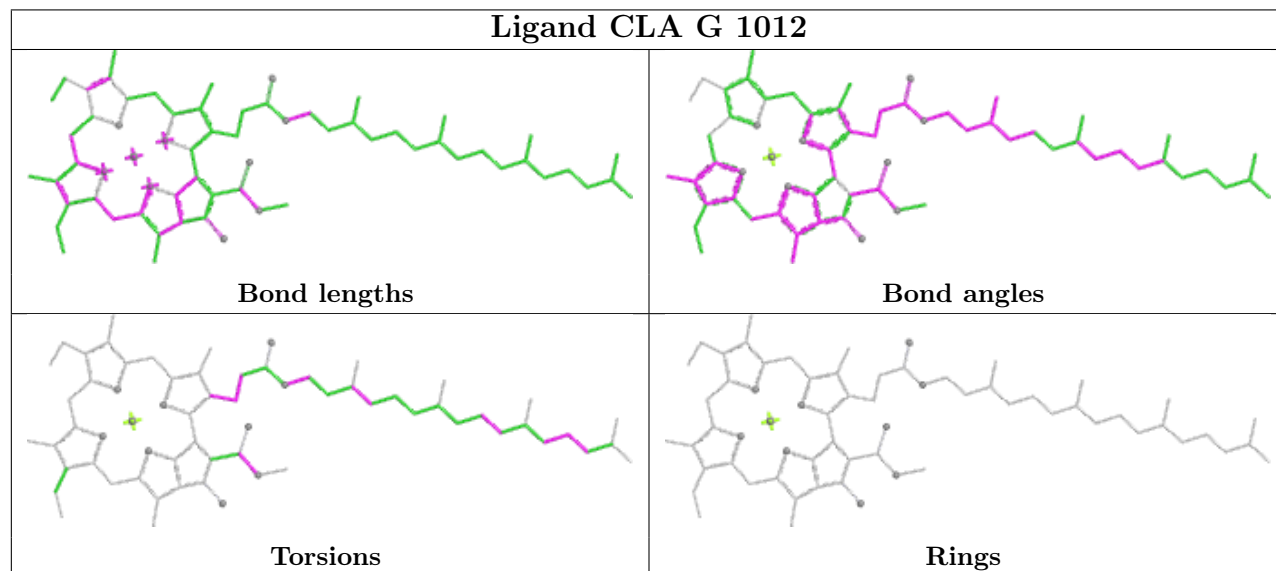


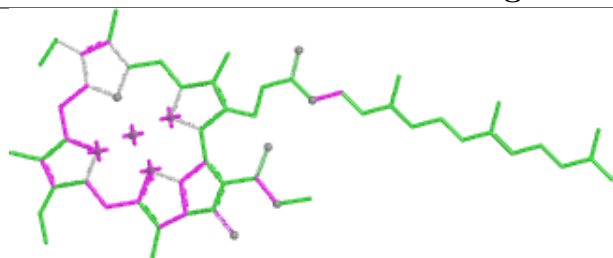
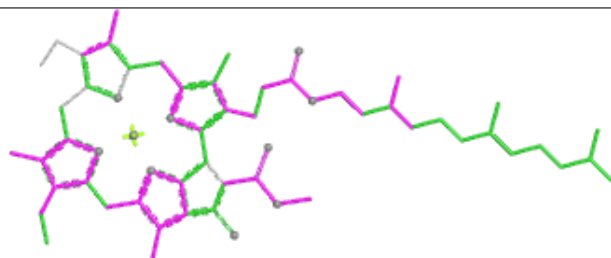
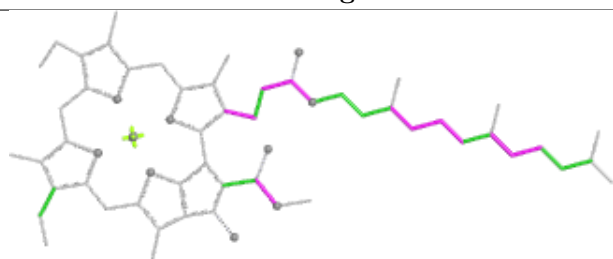
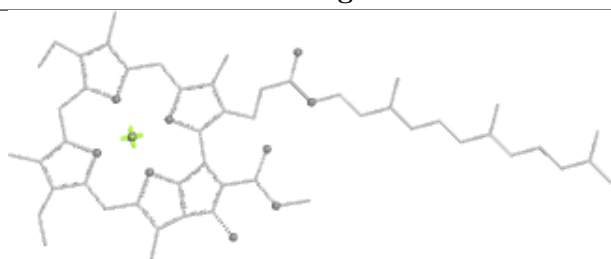
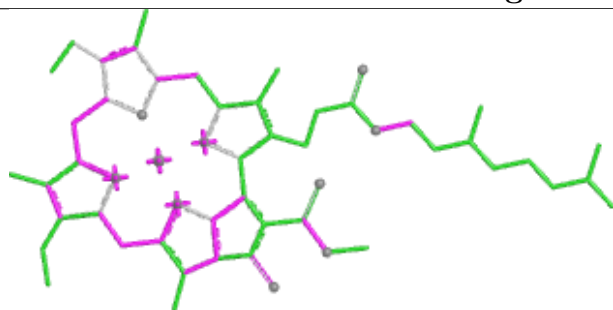
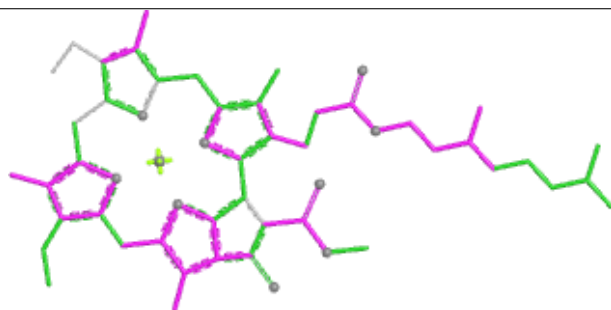
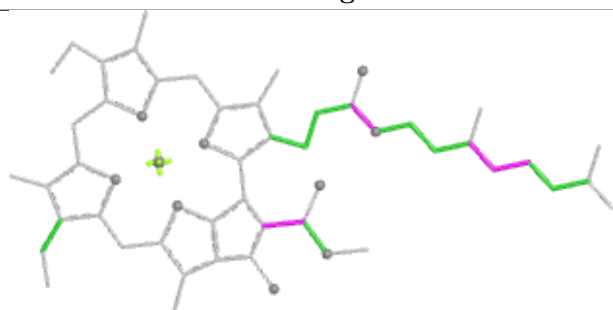
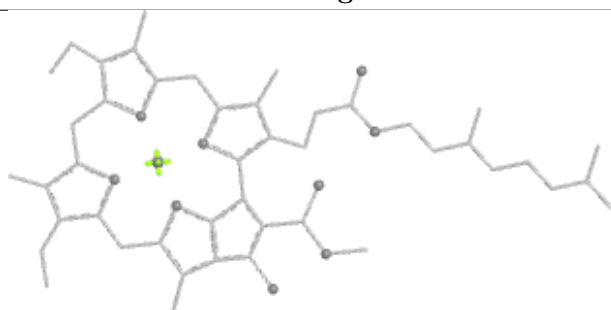


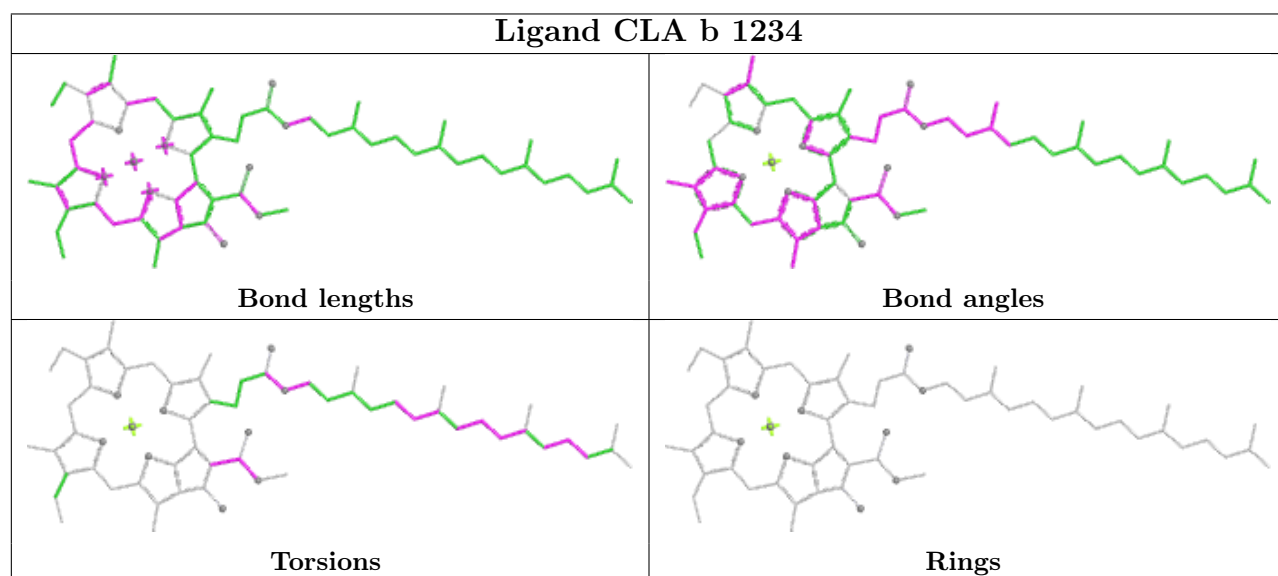
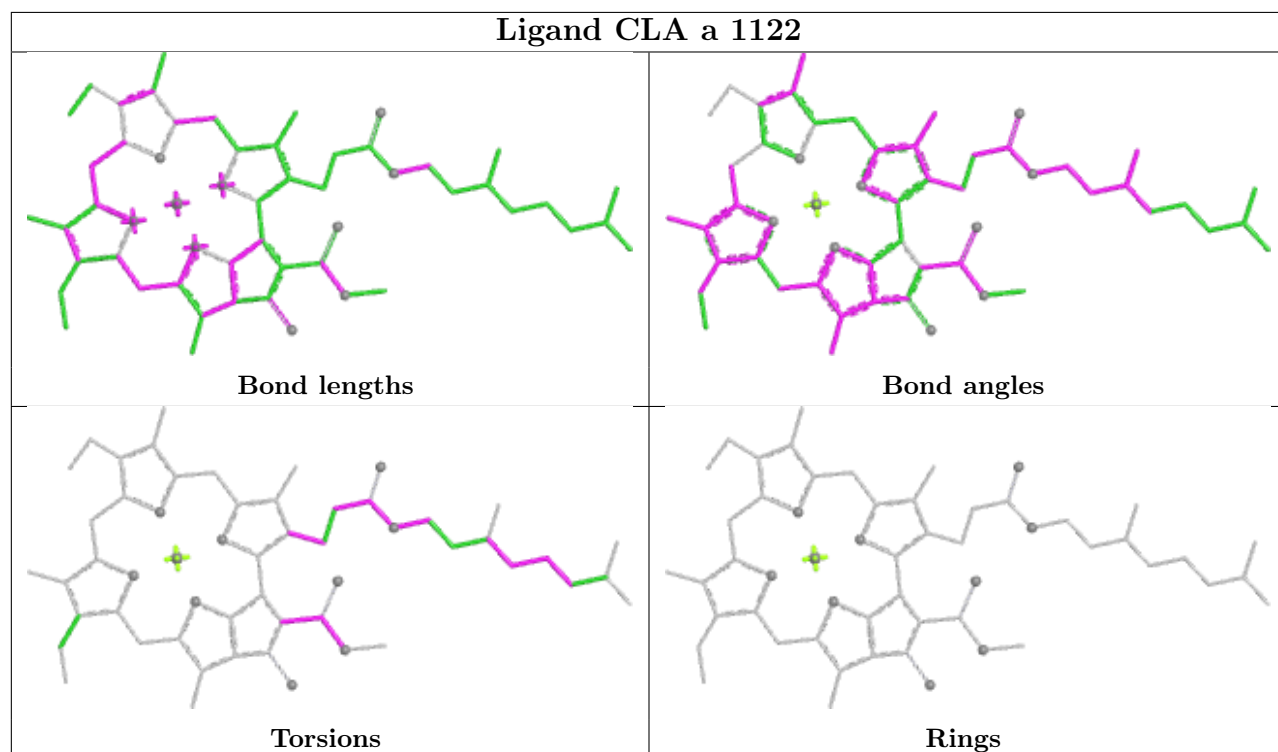
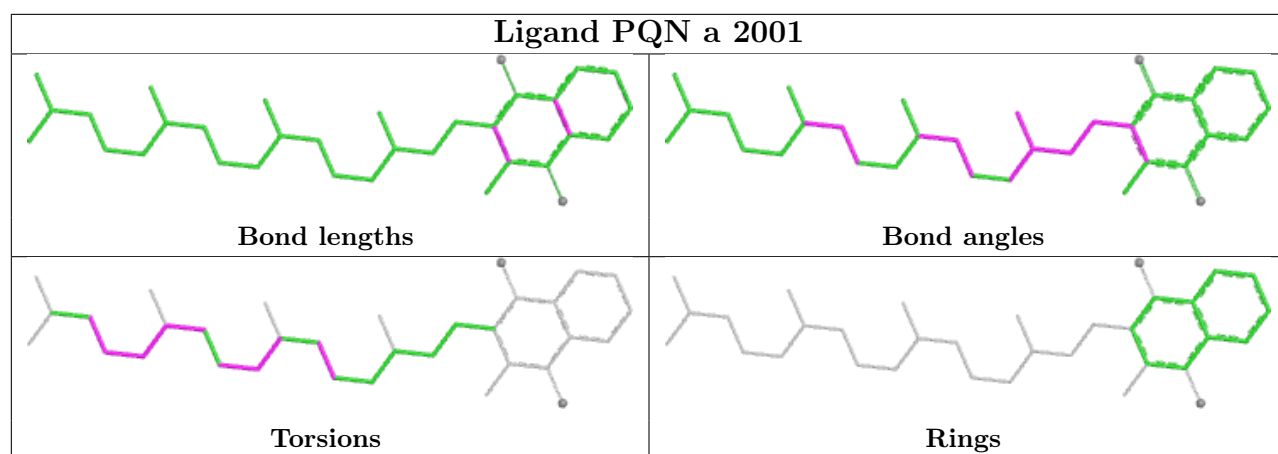
Ligand CLA H 1228



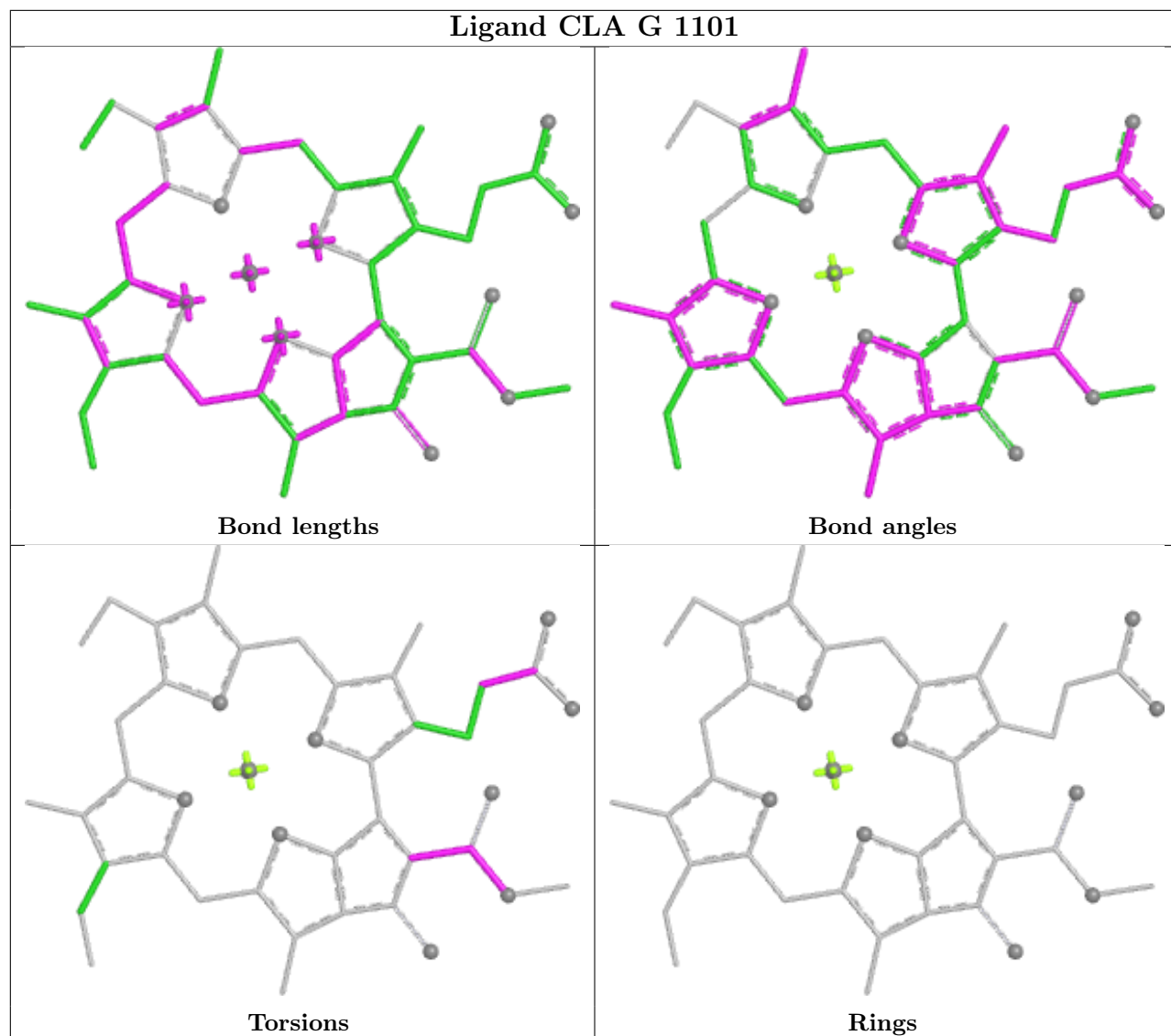
Ligand CLA G 1012



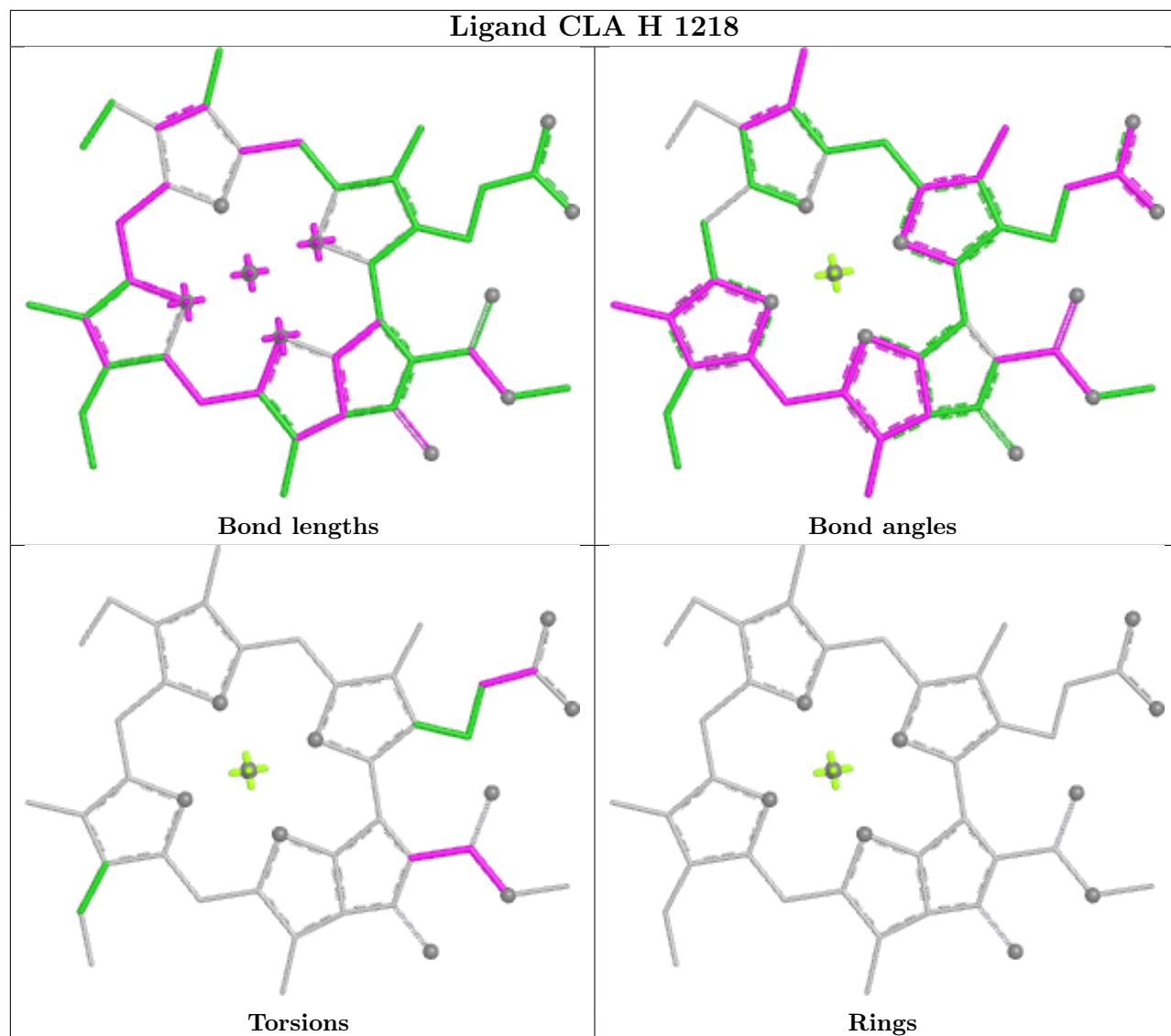
Ligand CLA G 1138**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 1201****Bond lengths****Bond angles****Torsions****Rings**

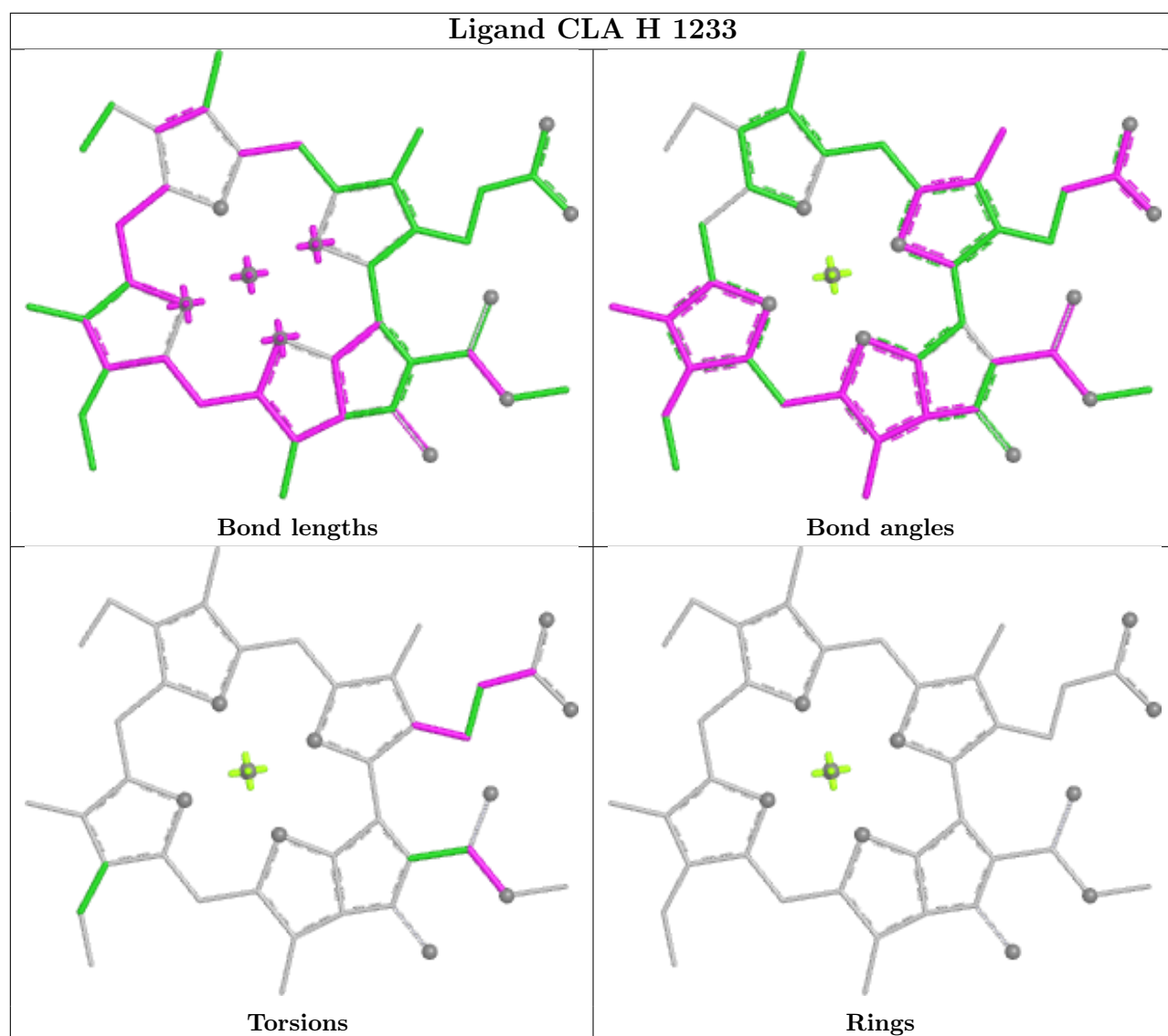


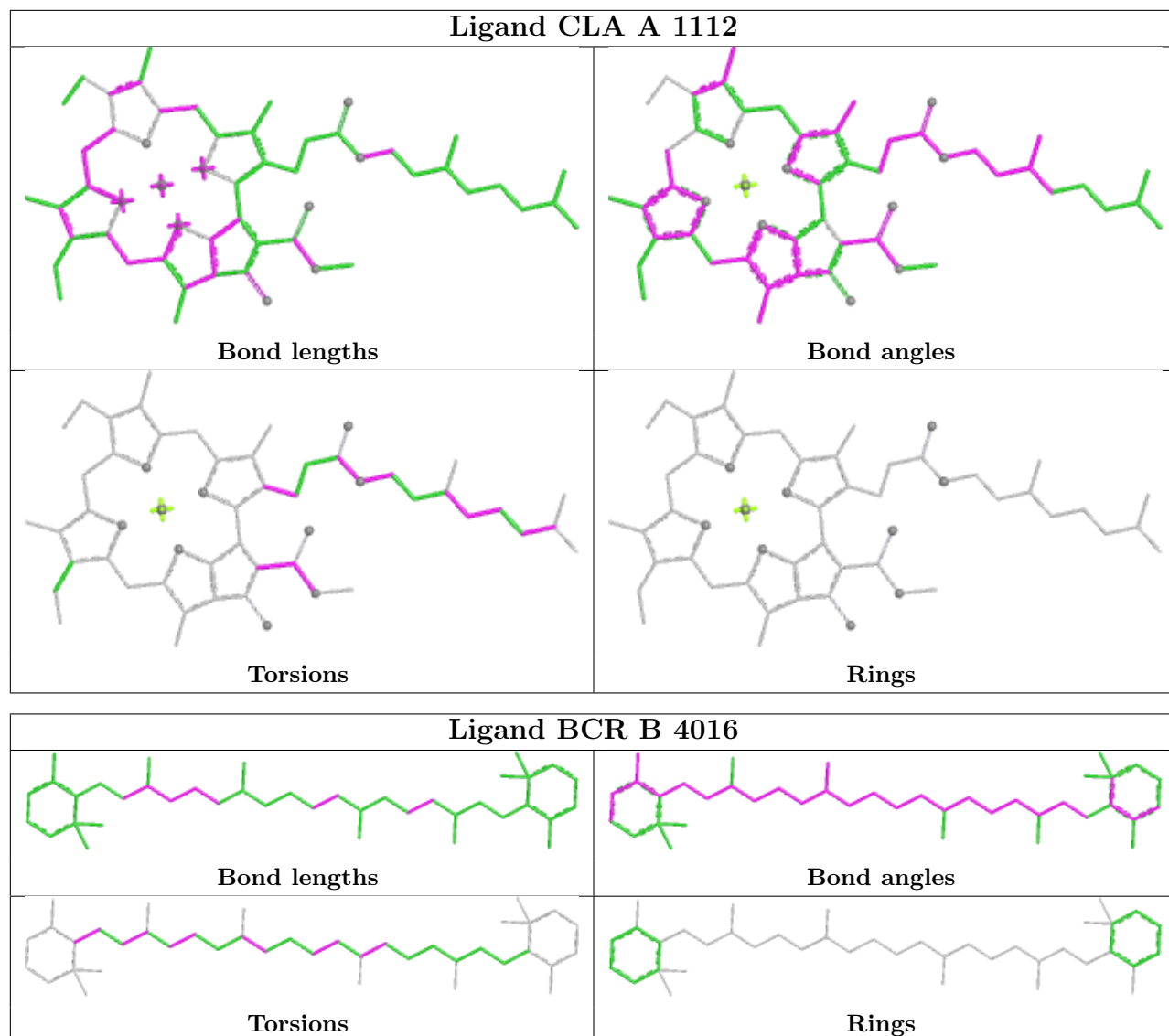
Ligand CLA G 1101



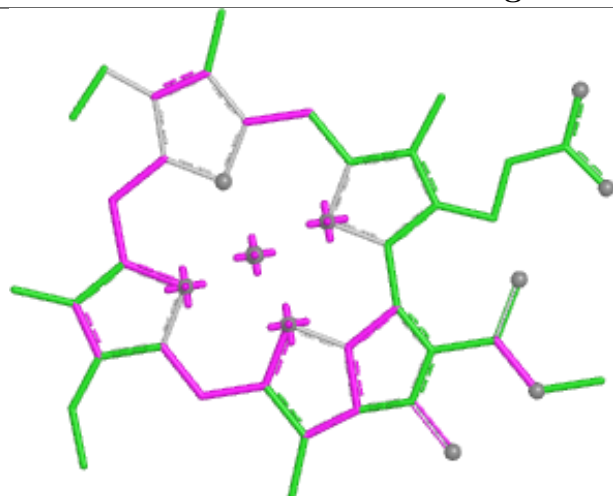
Ligand CLA H 1218



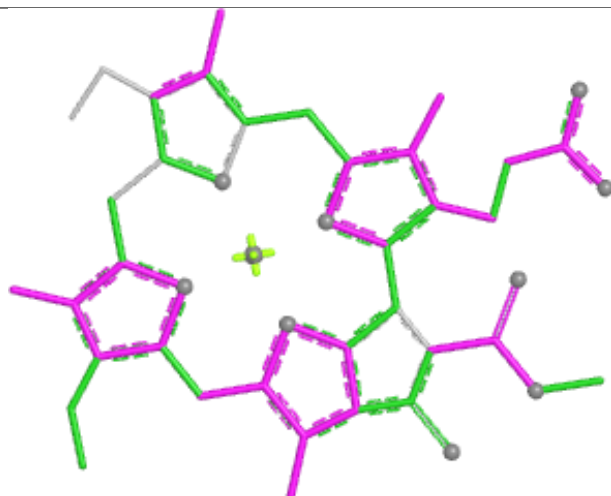




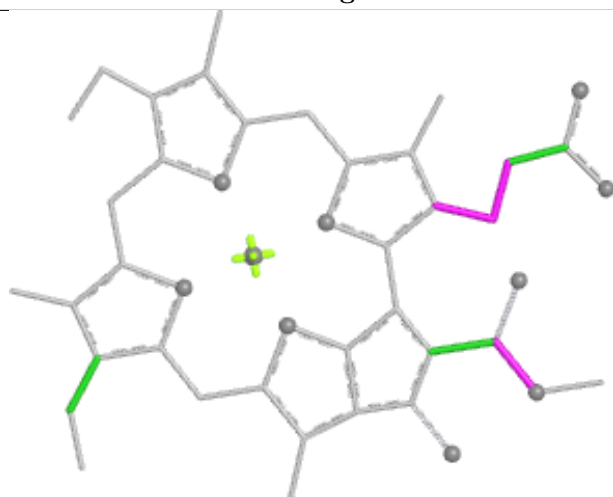
Ligand CLA H 1212



Bond lengths



Bond angles

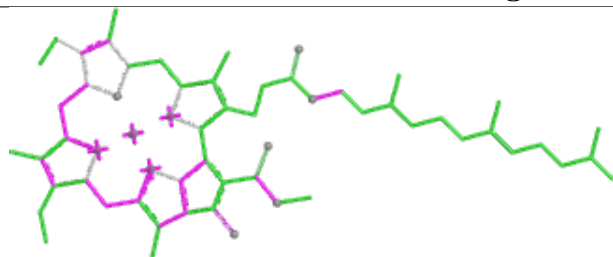


Torsions

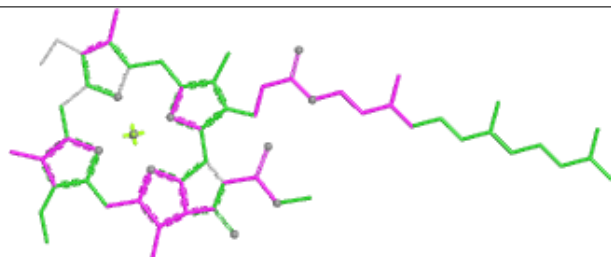


Rings

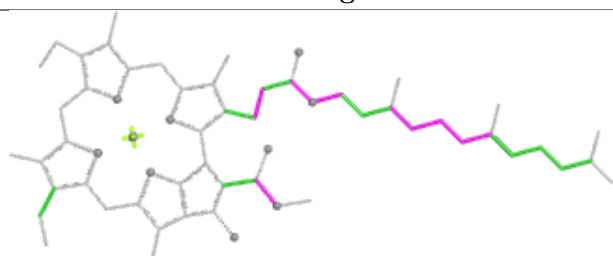
Ligand CLA A 1131



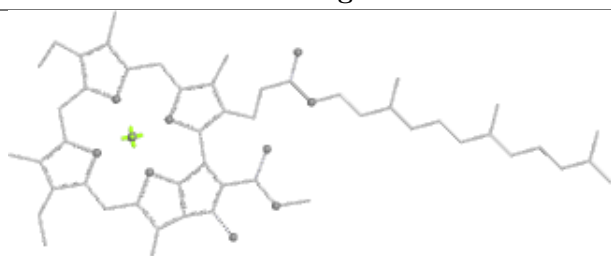
Bond lengths



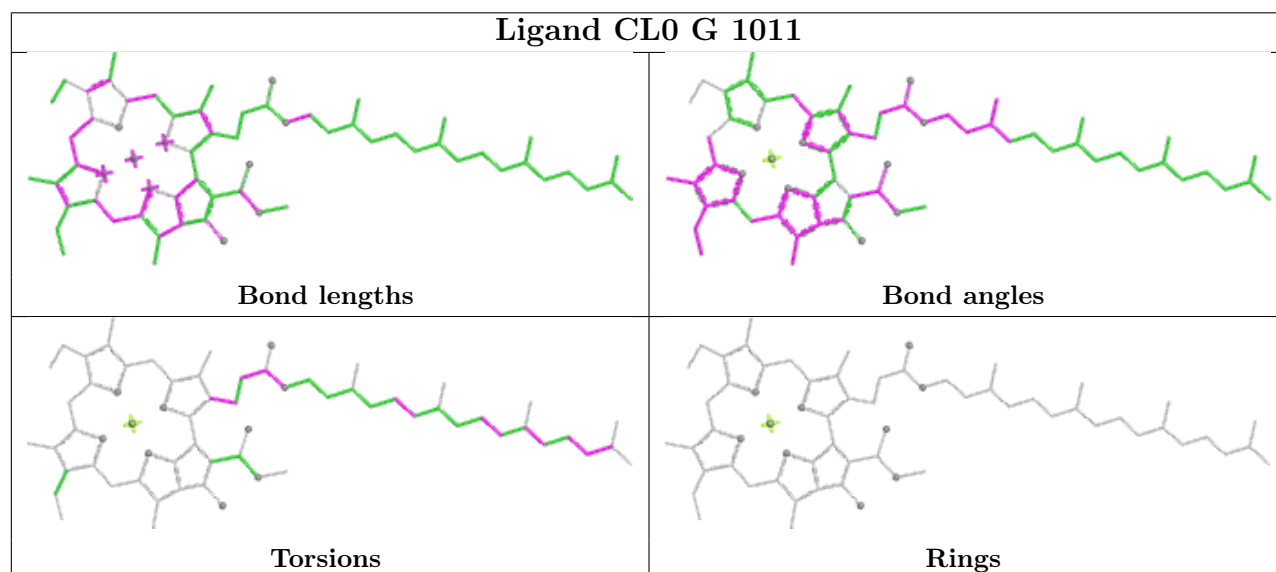
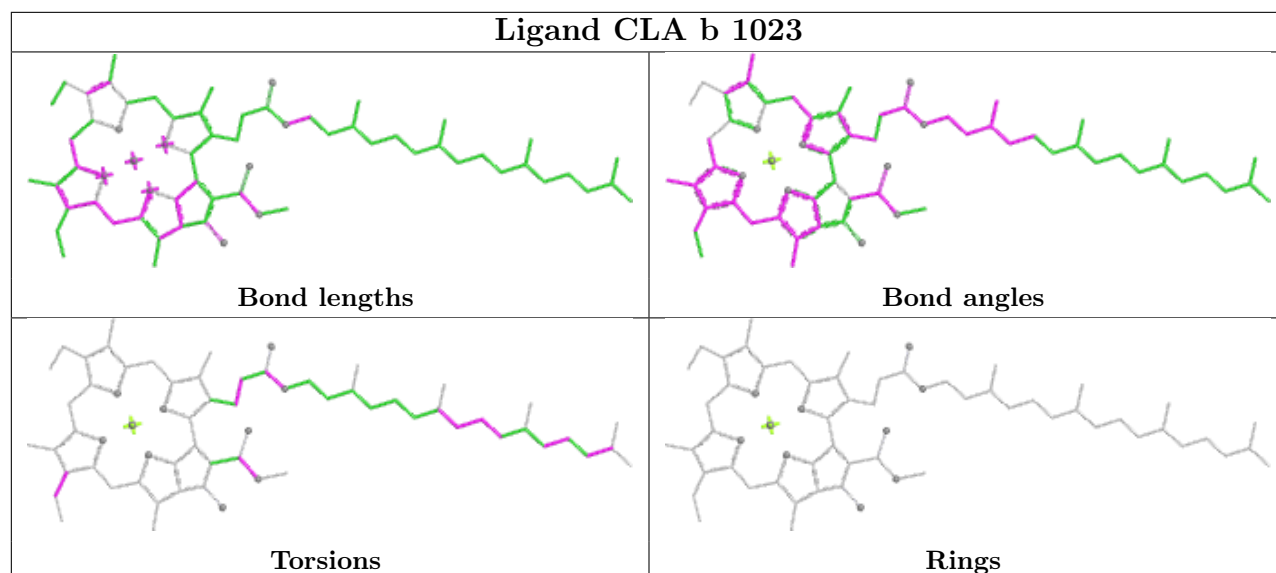
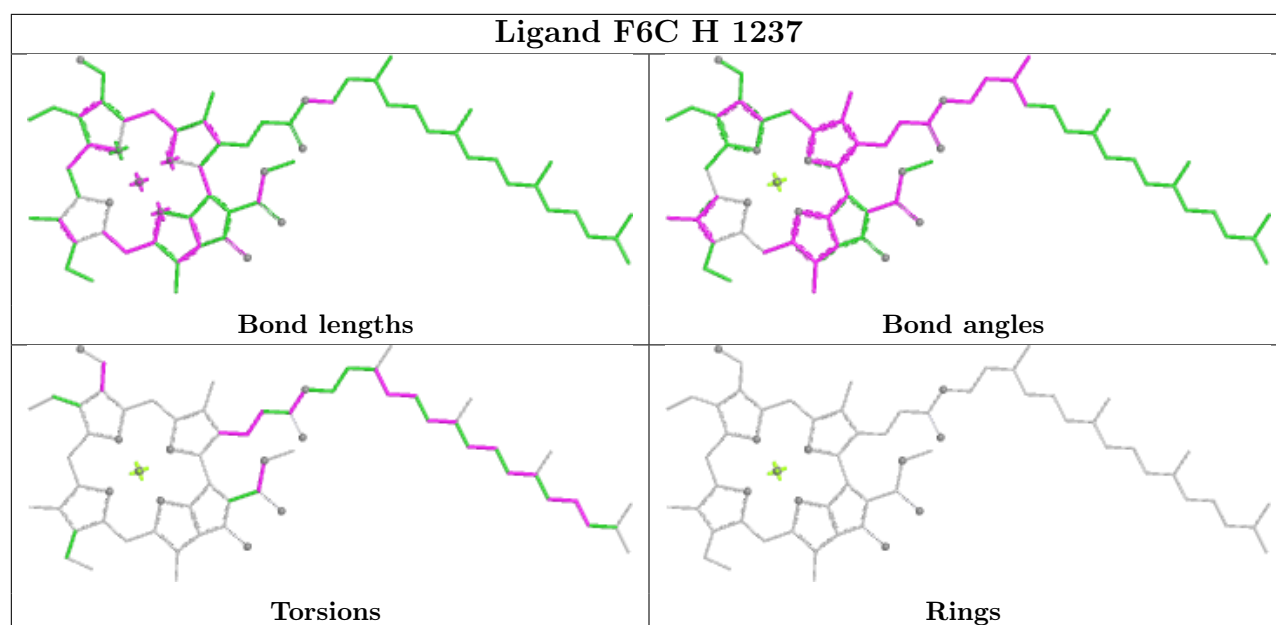
Bond angles

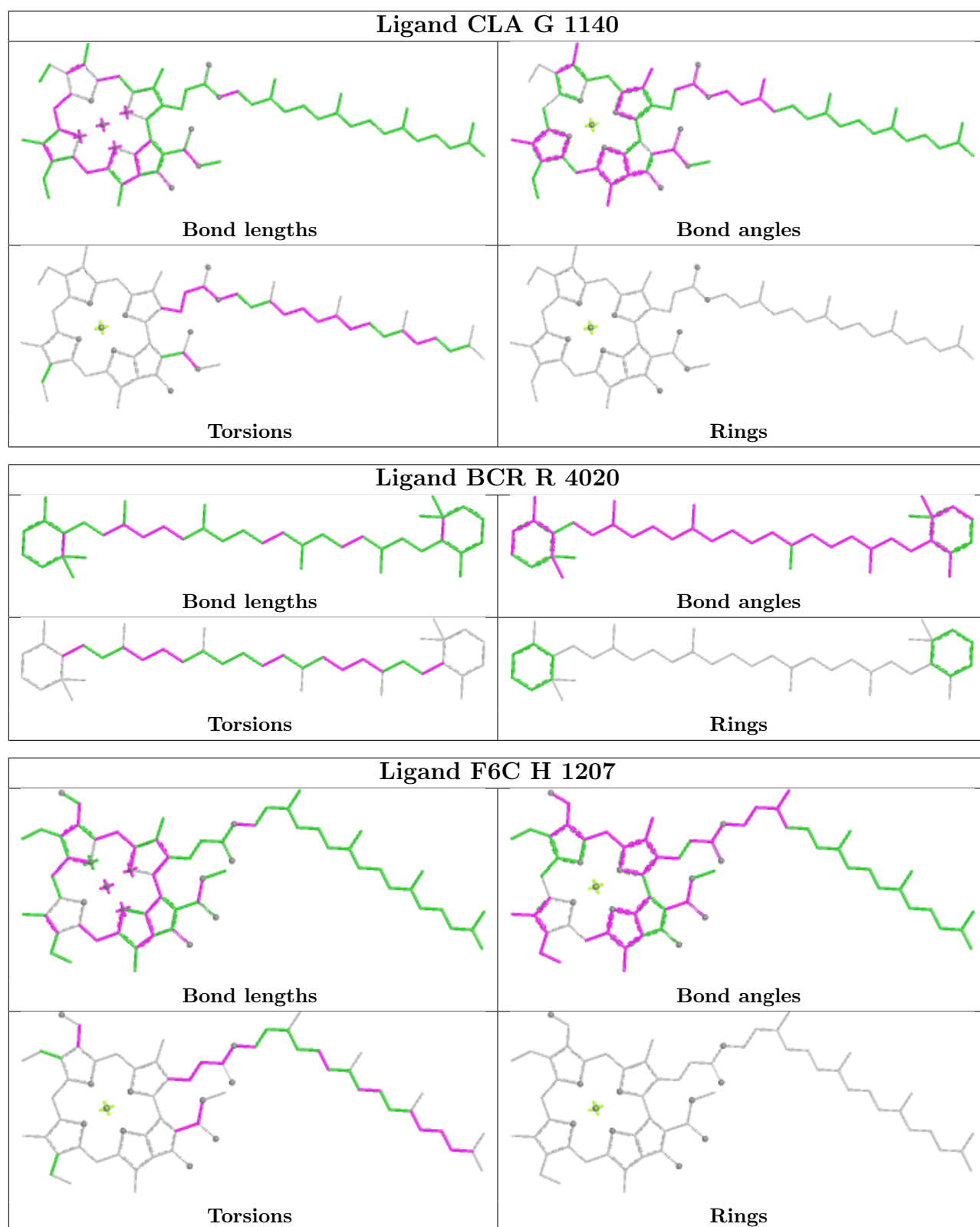


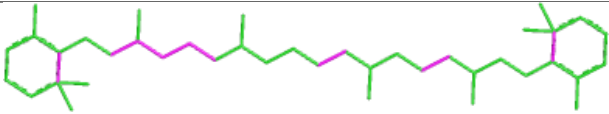
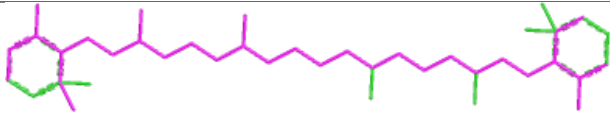
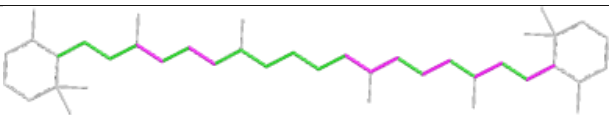
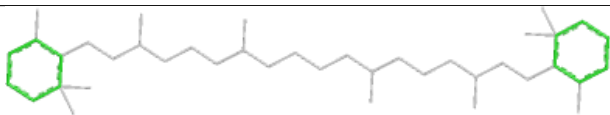
Torsions

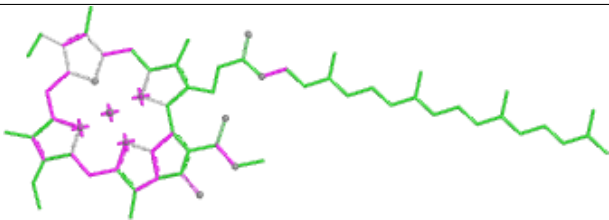
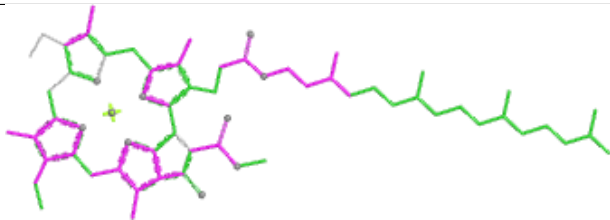
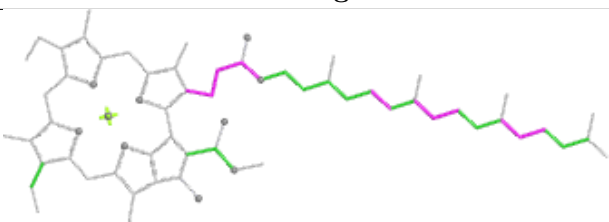
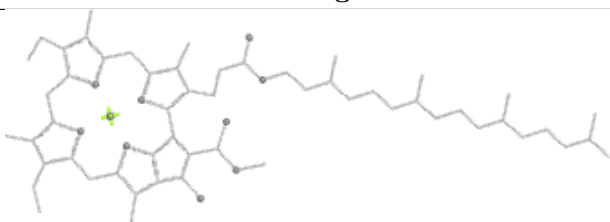


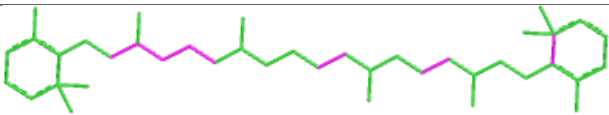
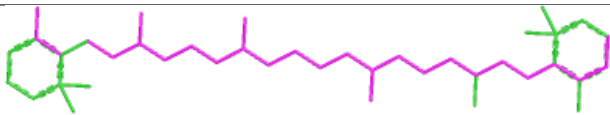
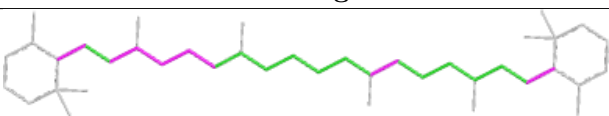
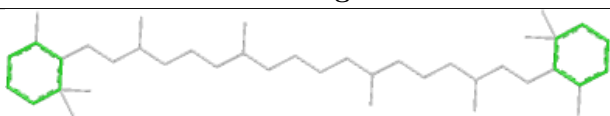
Rings

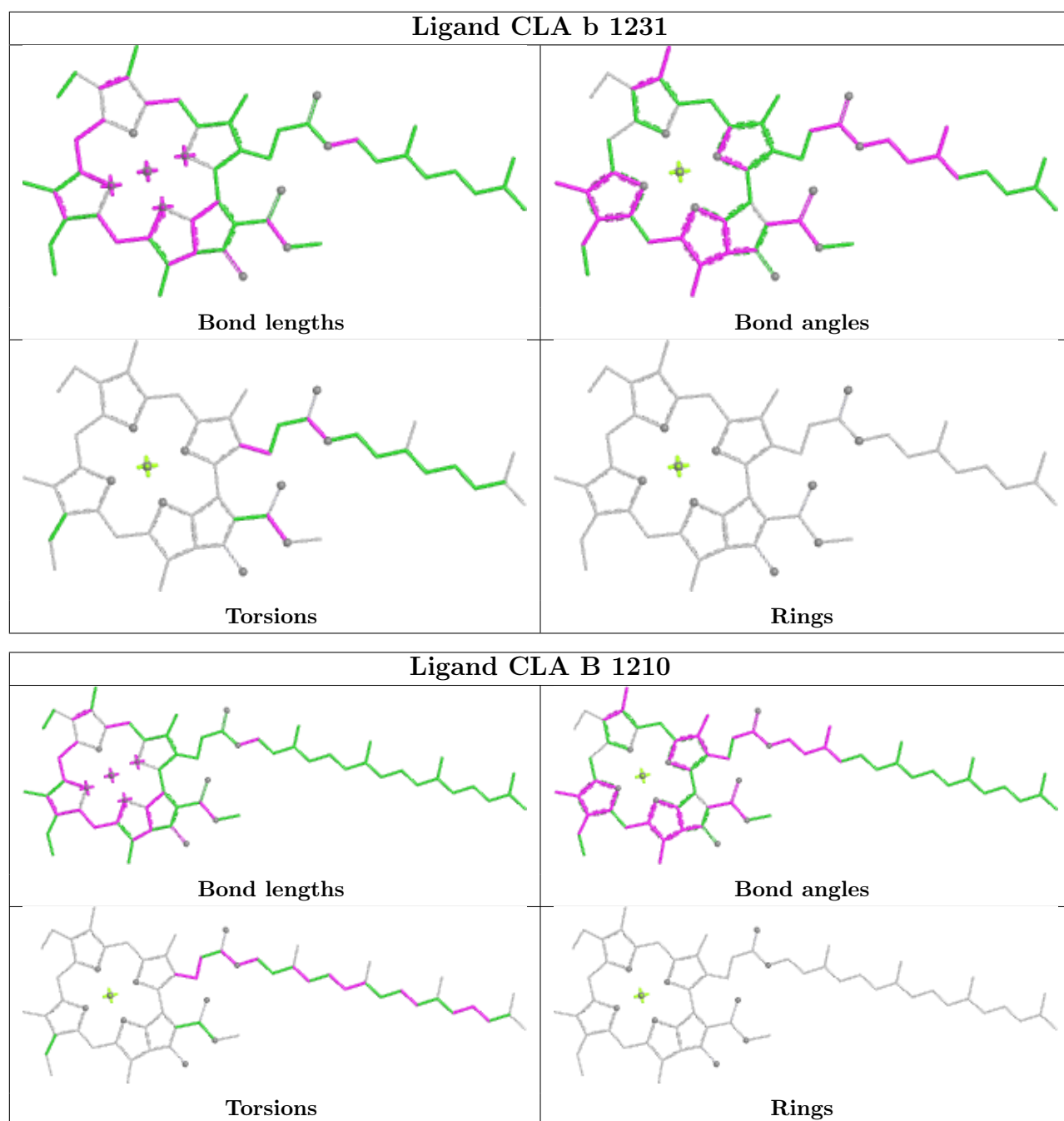


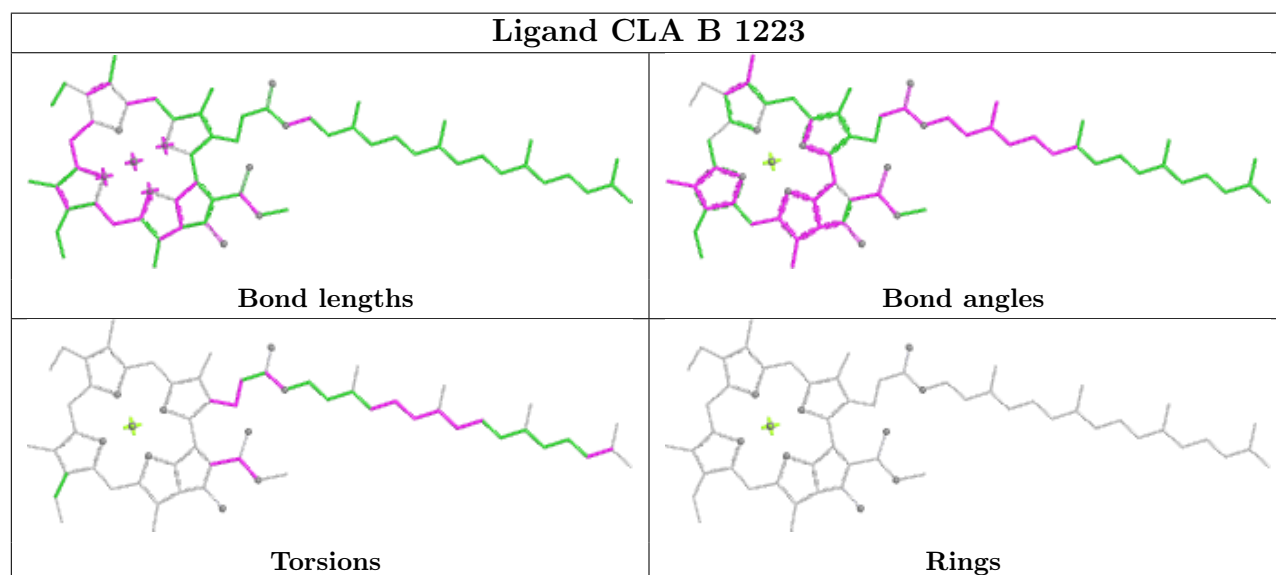
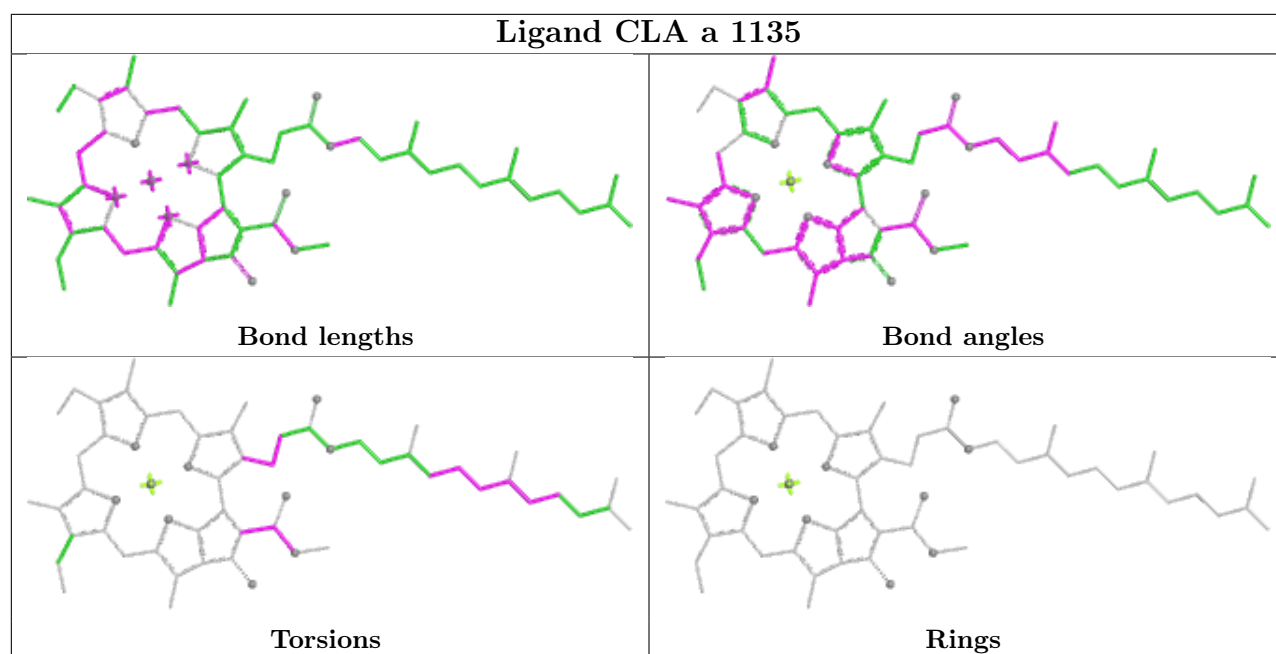


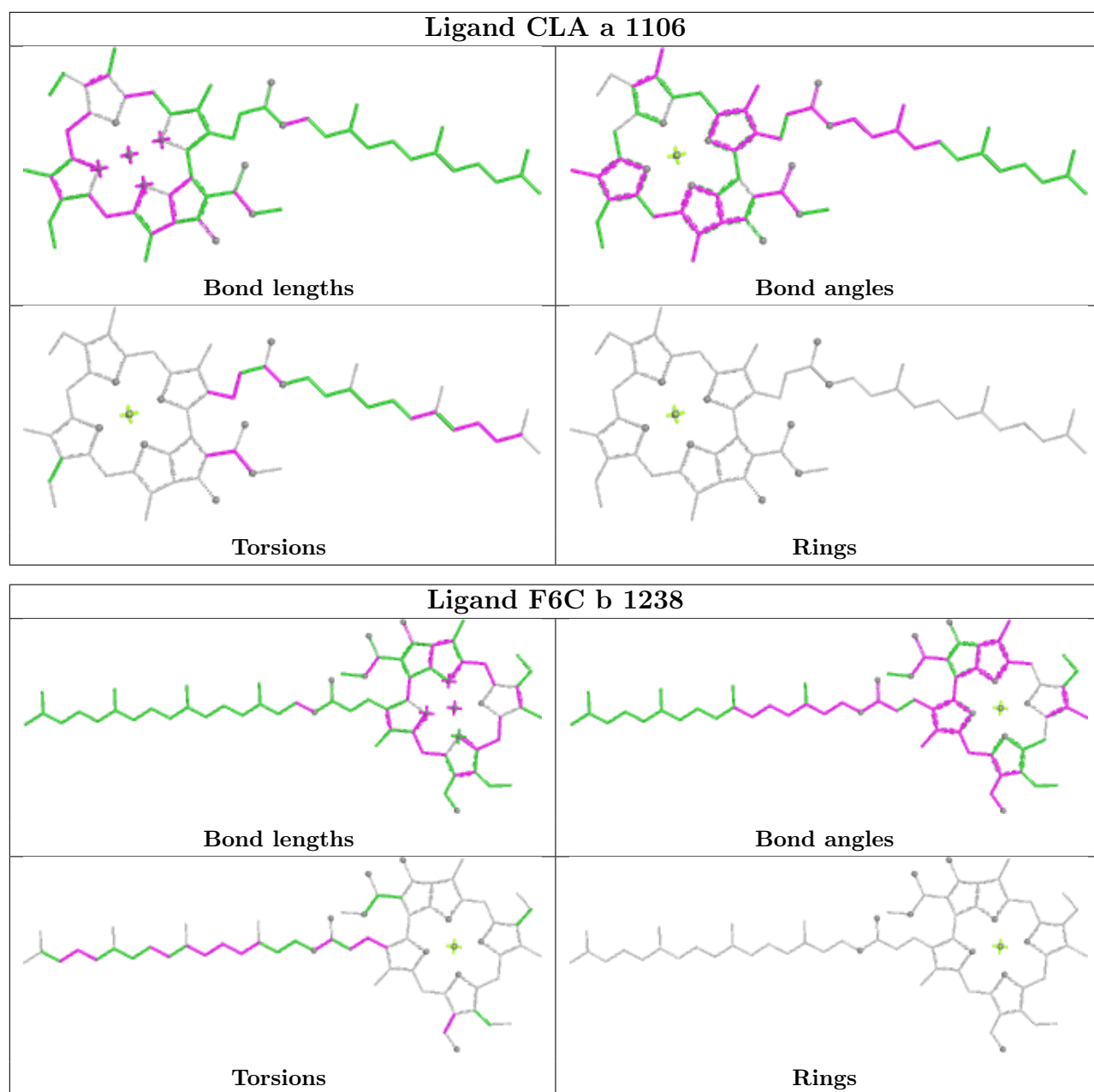
Ligand BCR a 4007	
	
Bond lengths	Bond angles
	
Torsions	Rings

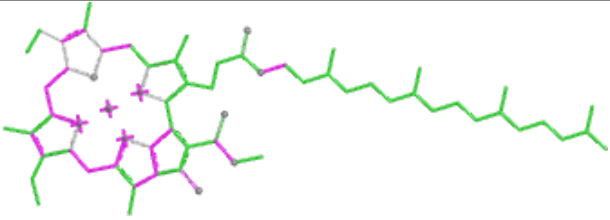
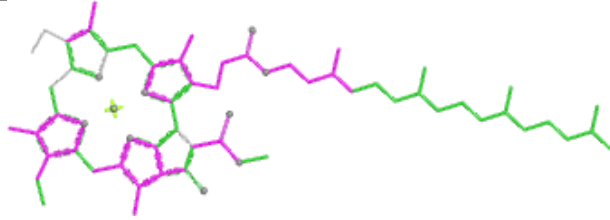
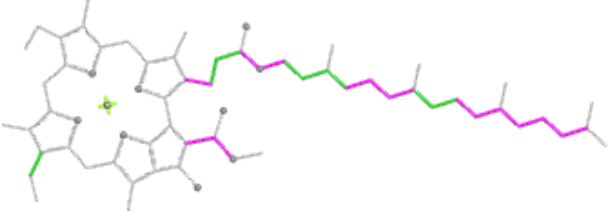
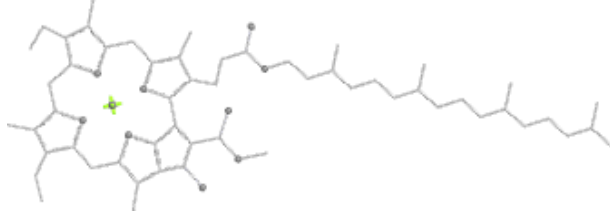
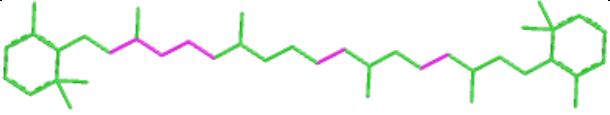
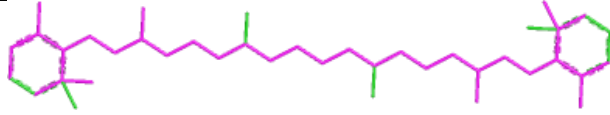
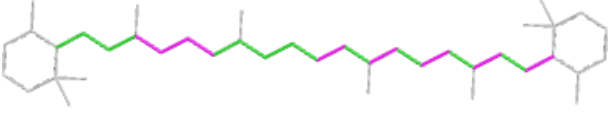
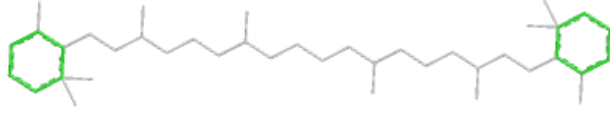
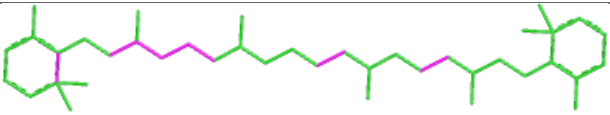
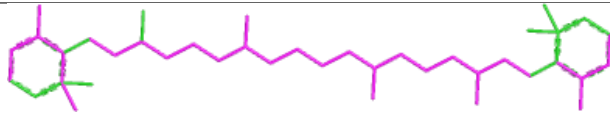
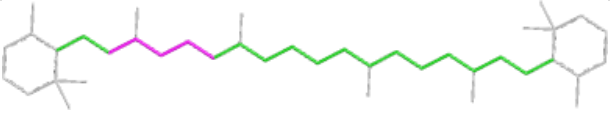
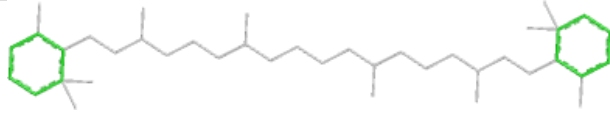
Ligand CLA a 1127	
	
Bond lengths	Bond angles
	
Torsions	Rings

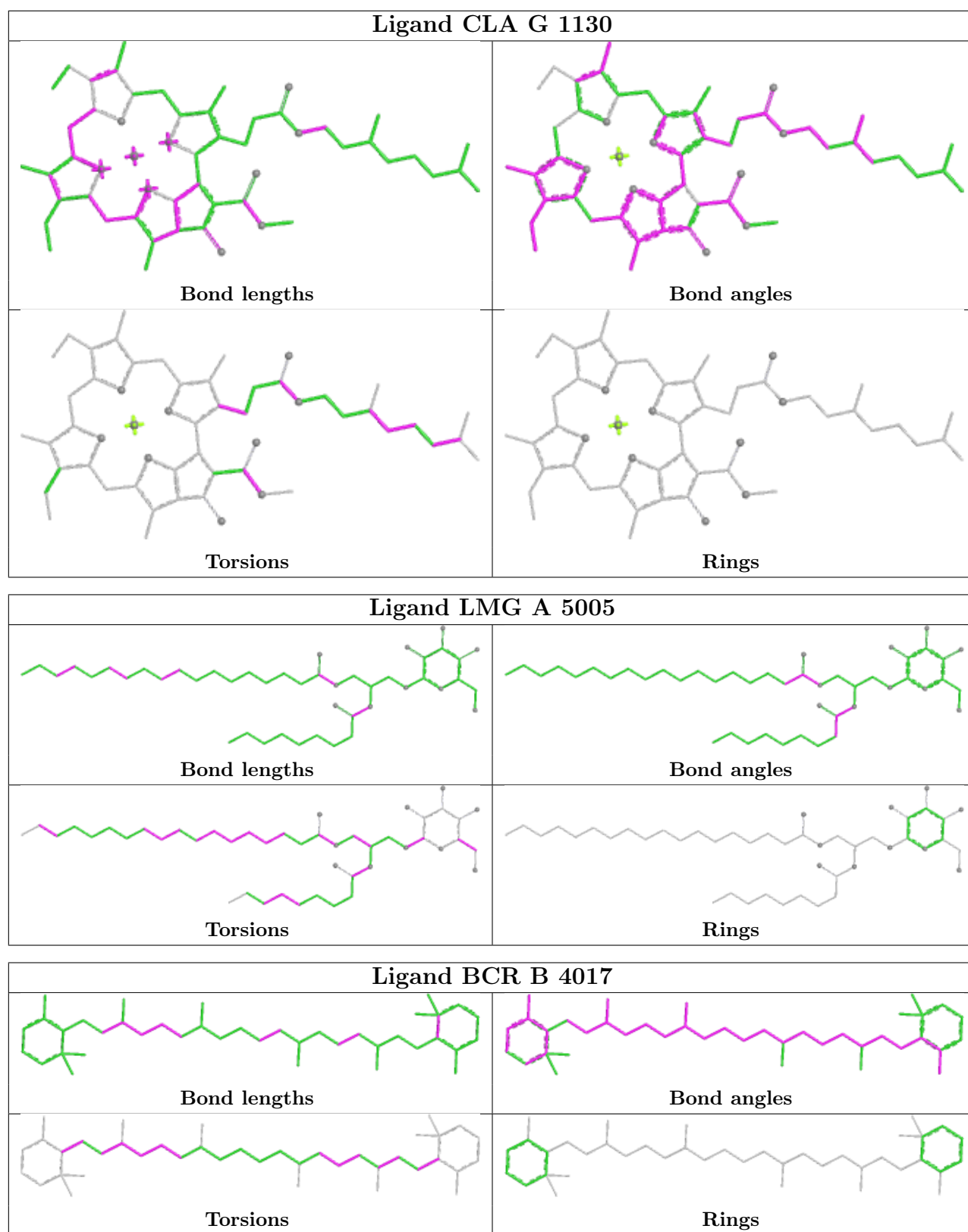
Ligand BCR G 4008	
	
Bond lengths	Bond angles
	
Torsions	Rings

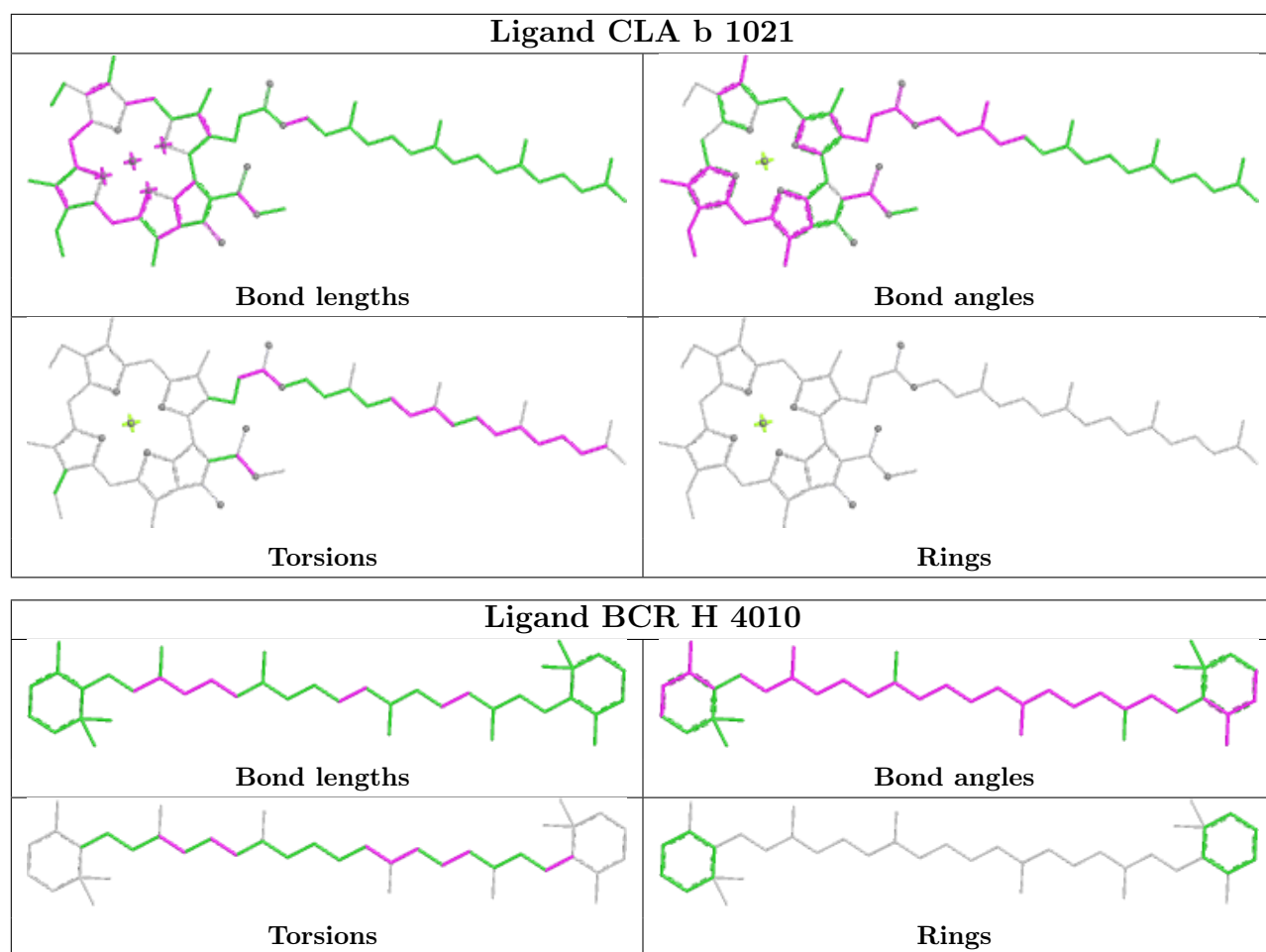




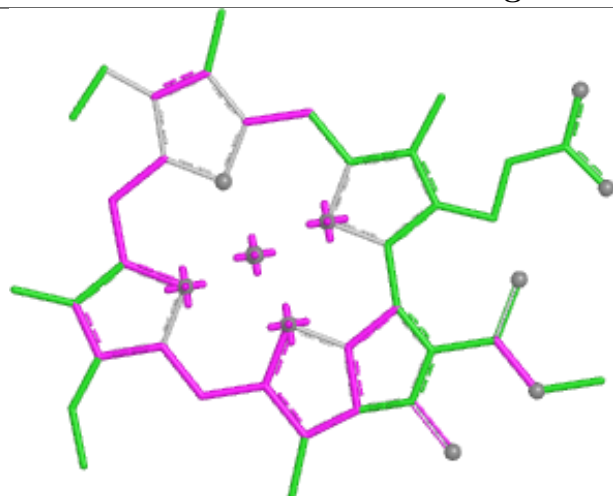


Ligand CLA G 1115	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR U 4019	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR I 4022	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

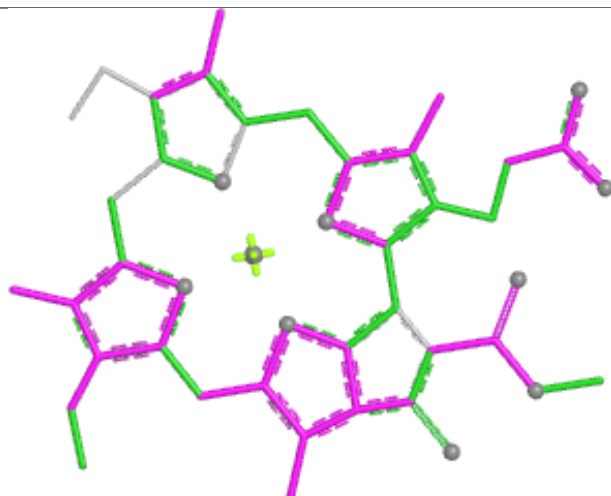




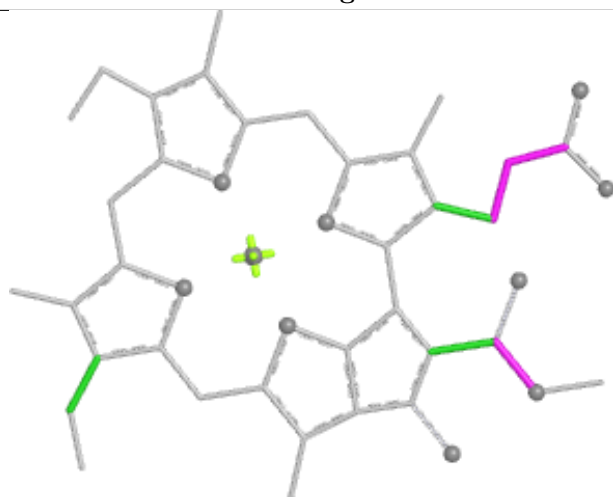
Ligand CLA G 1134



Bond lengths



Bond angles

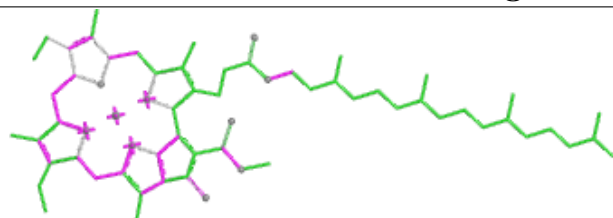


Torsions

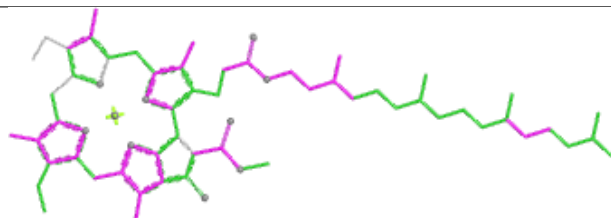


Rings

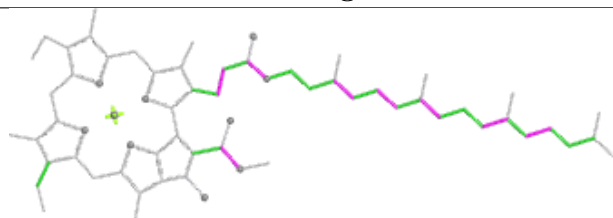
Ligand CLA U 1501



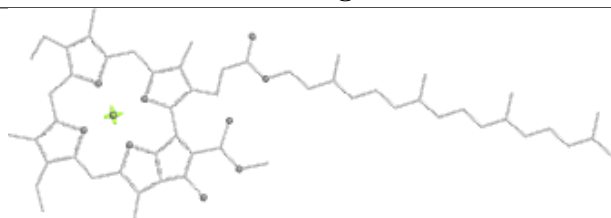
Bond lengths



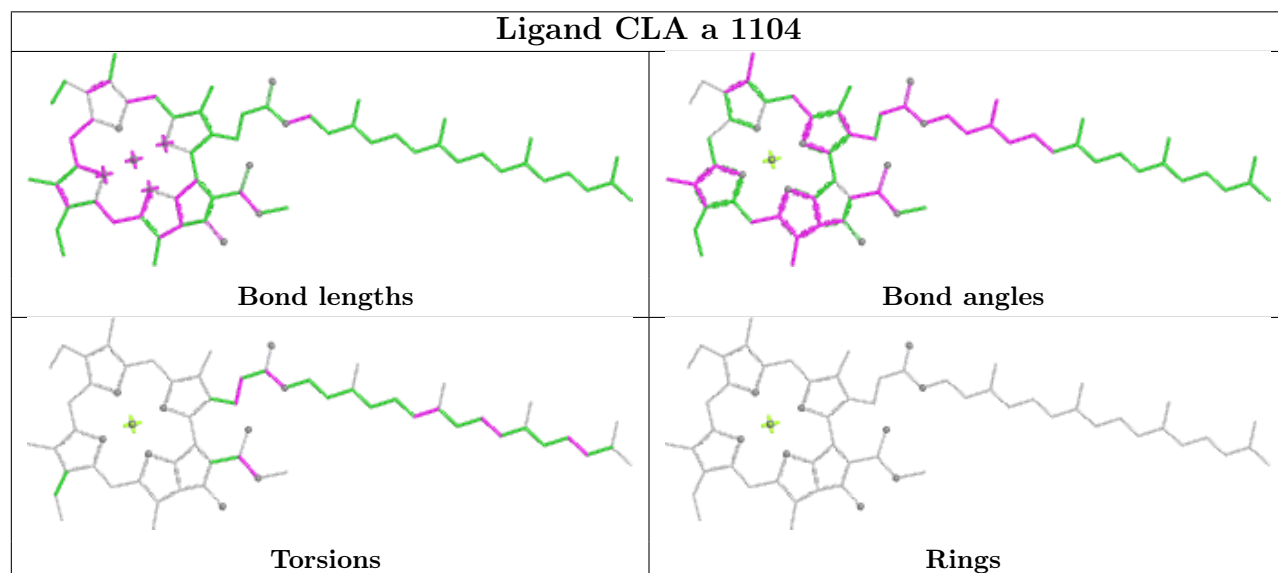
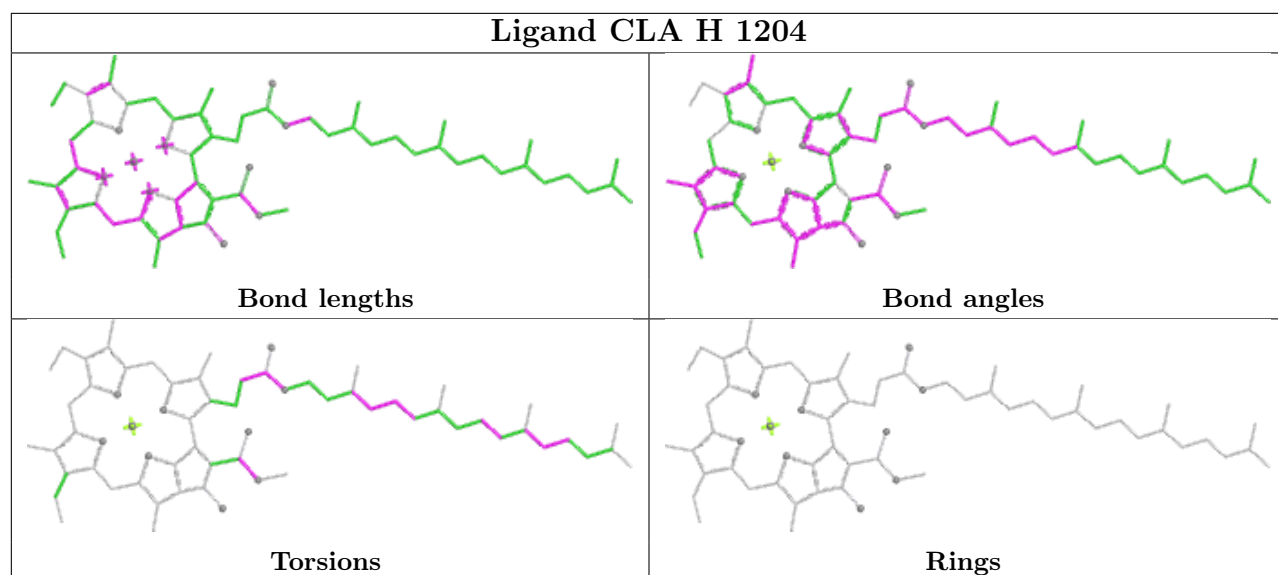
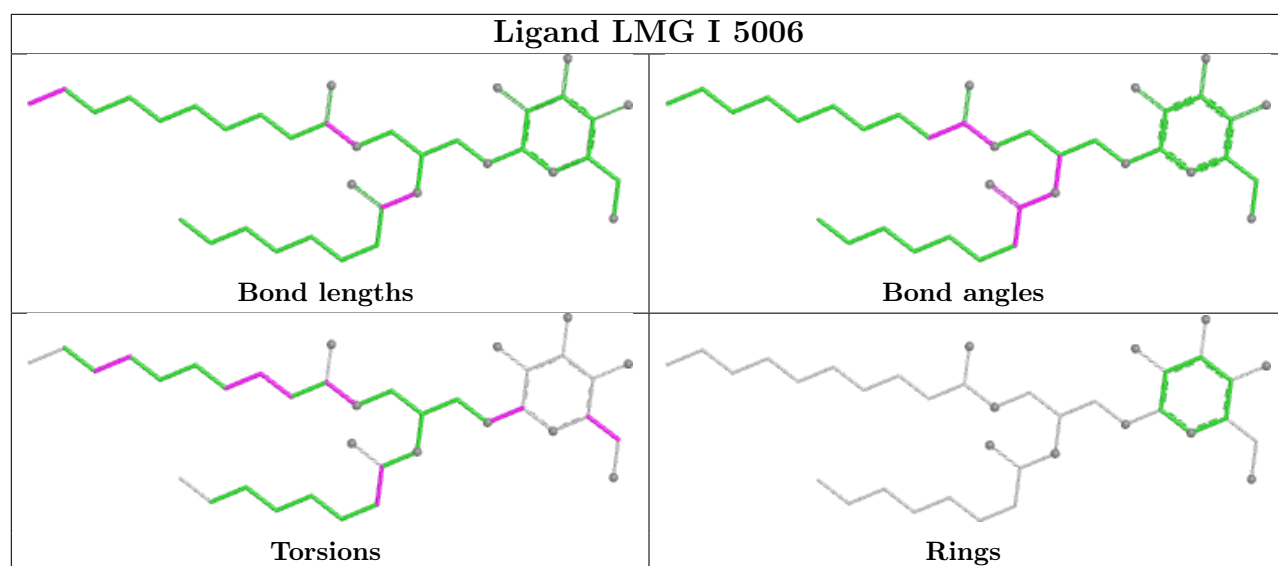
Bond angles

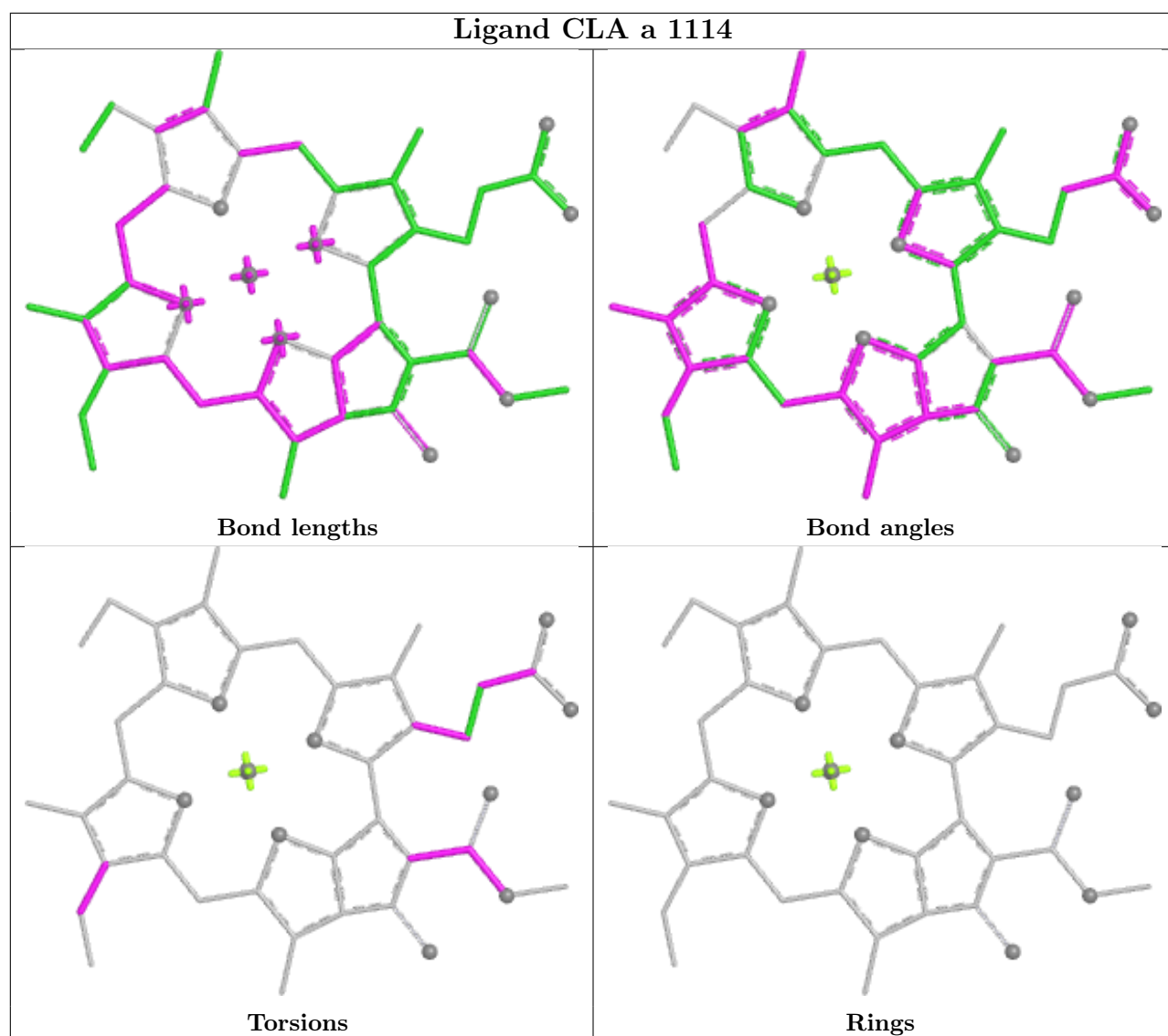


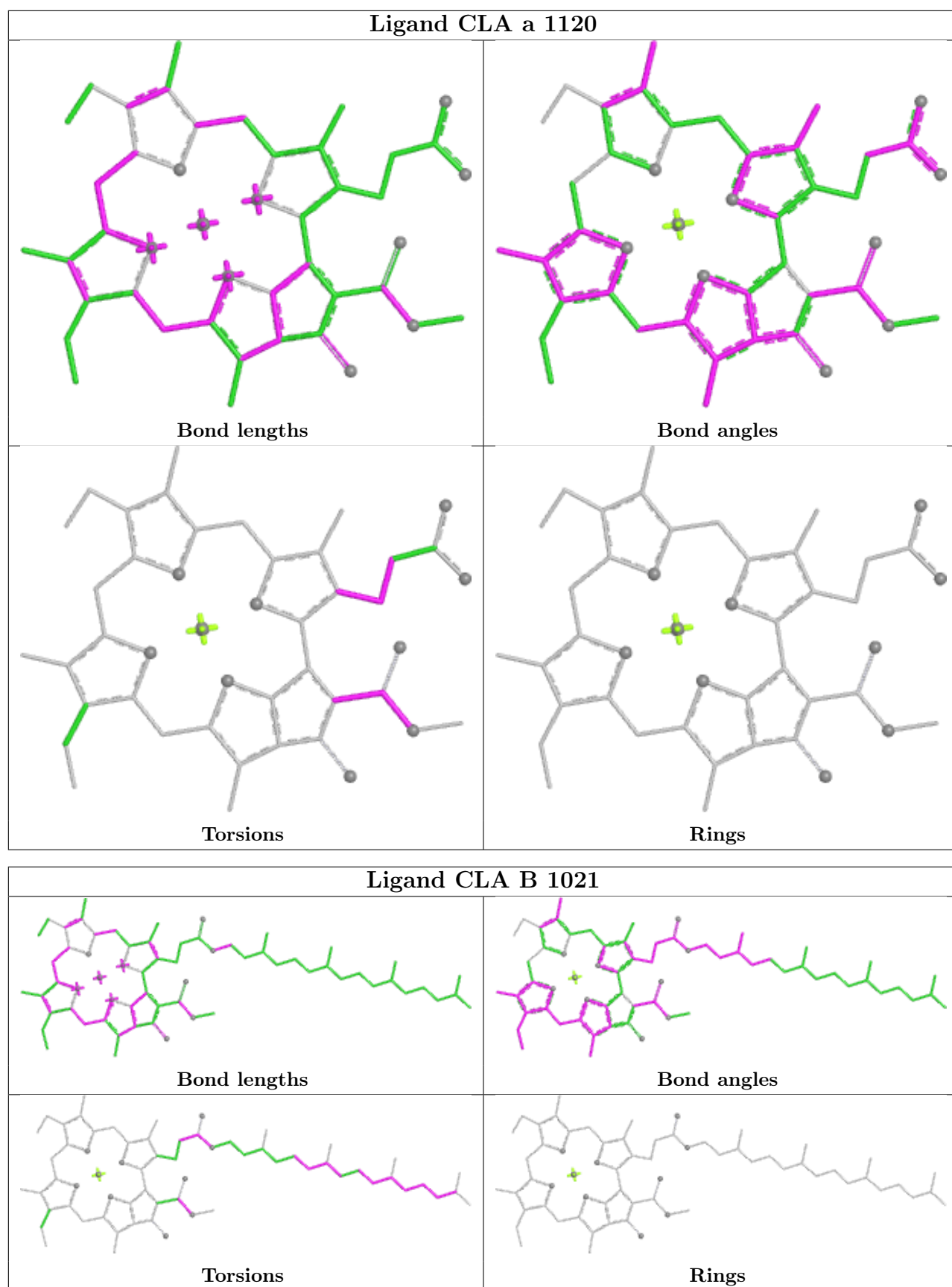
Torsions

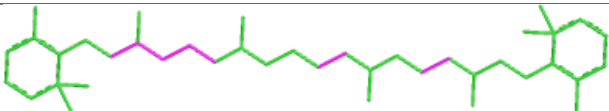
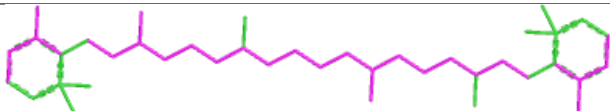
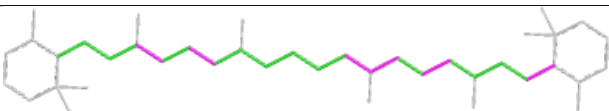
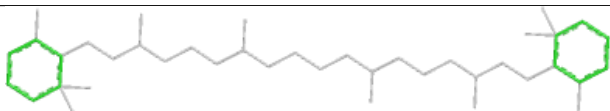


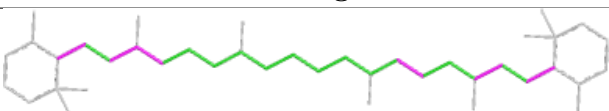
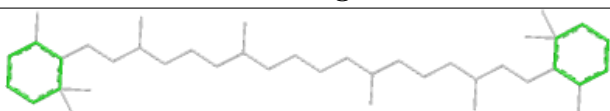


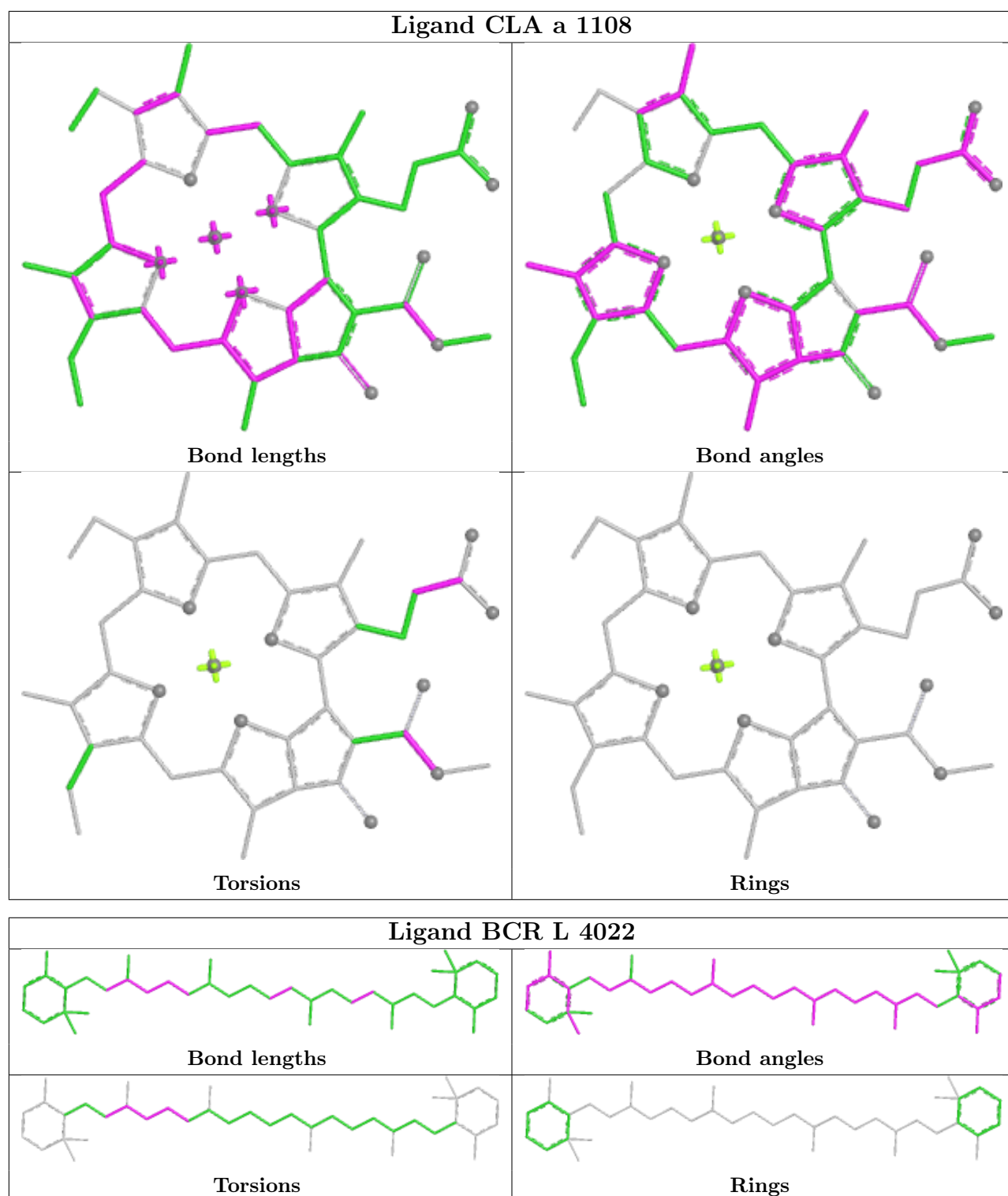
Rings

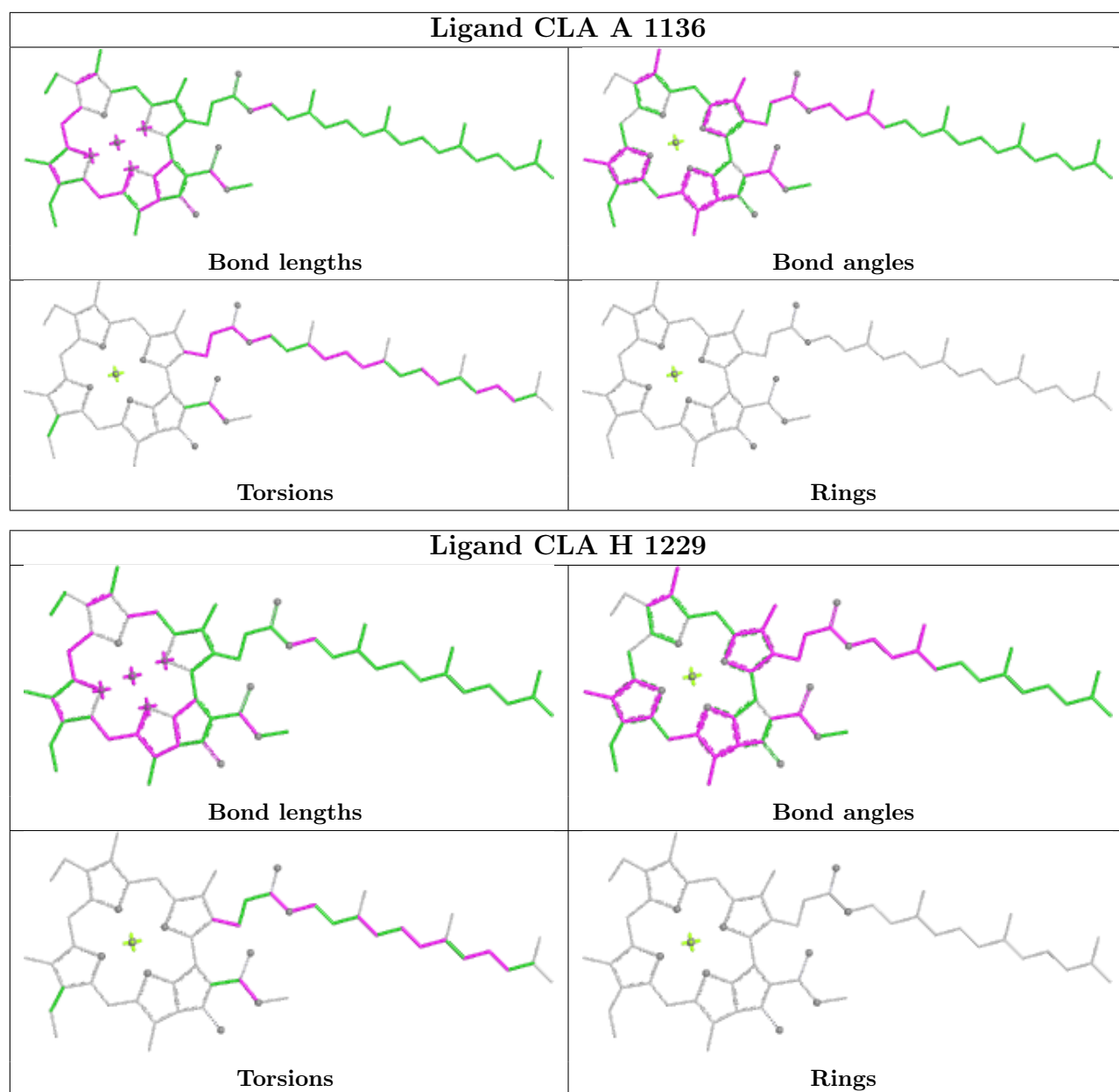


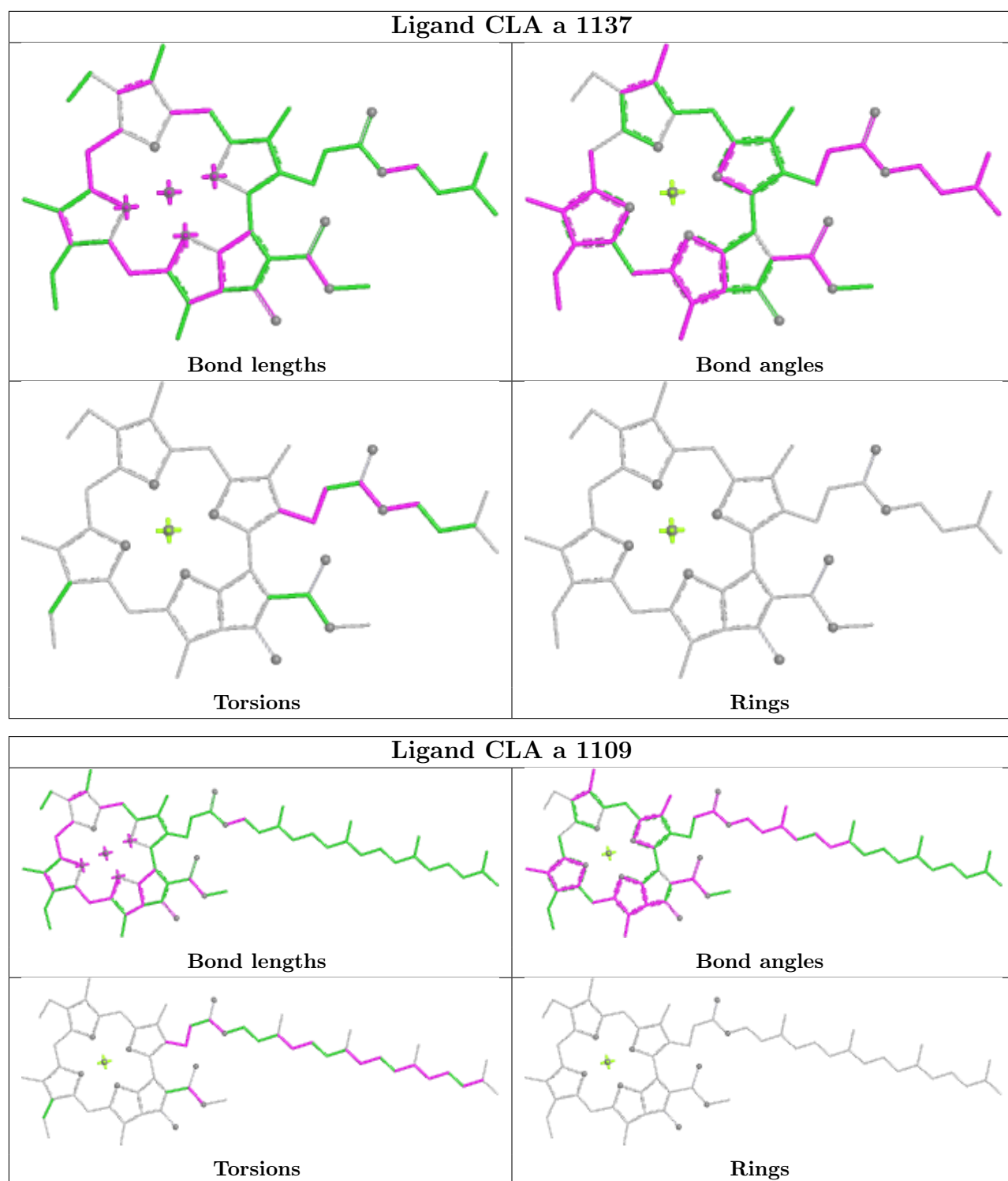


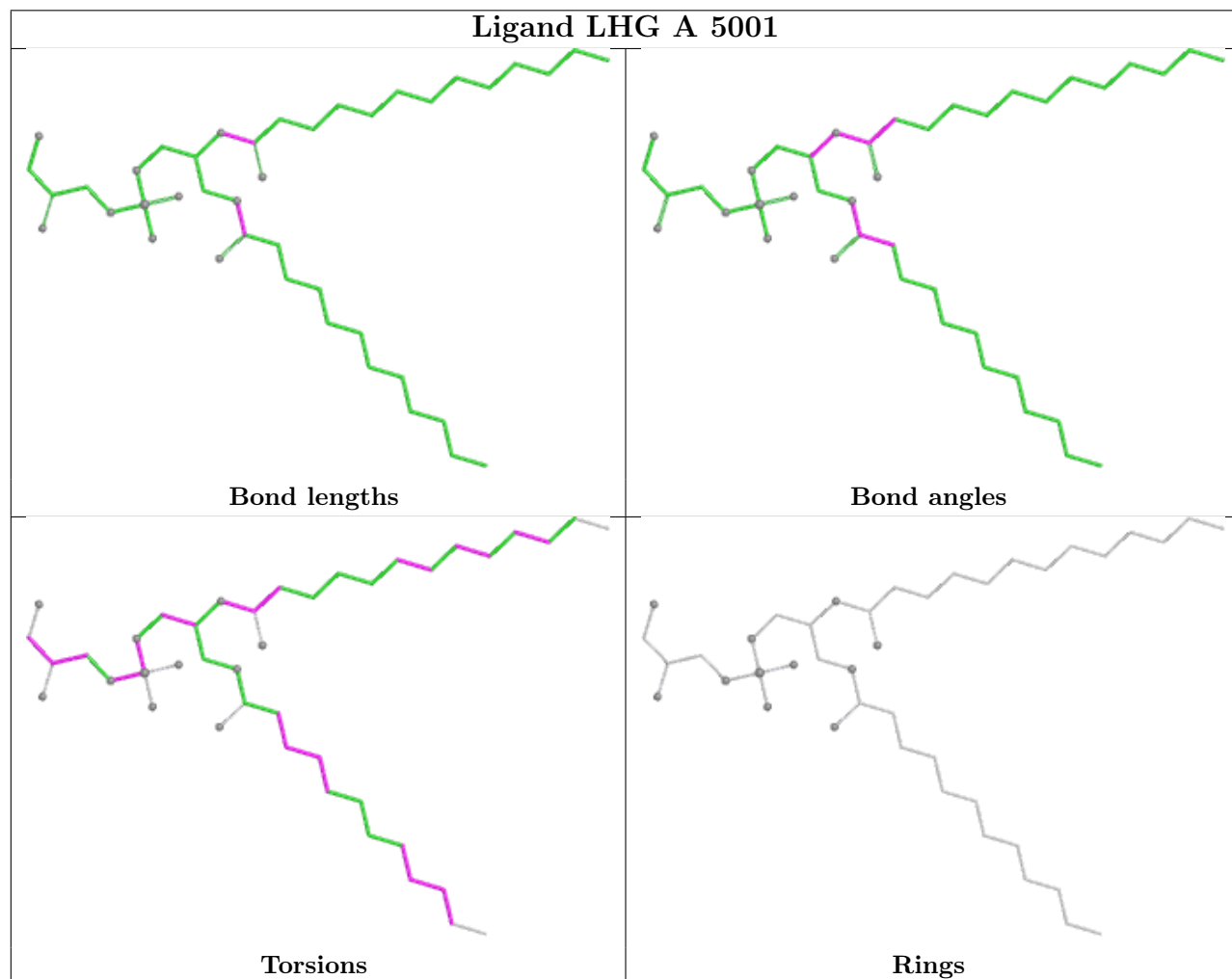
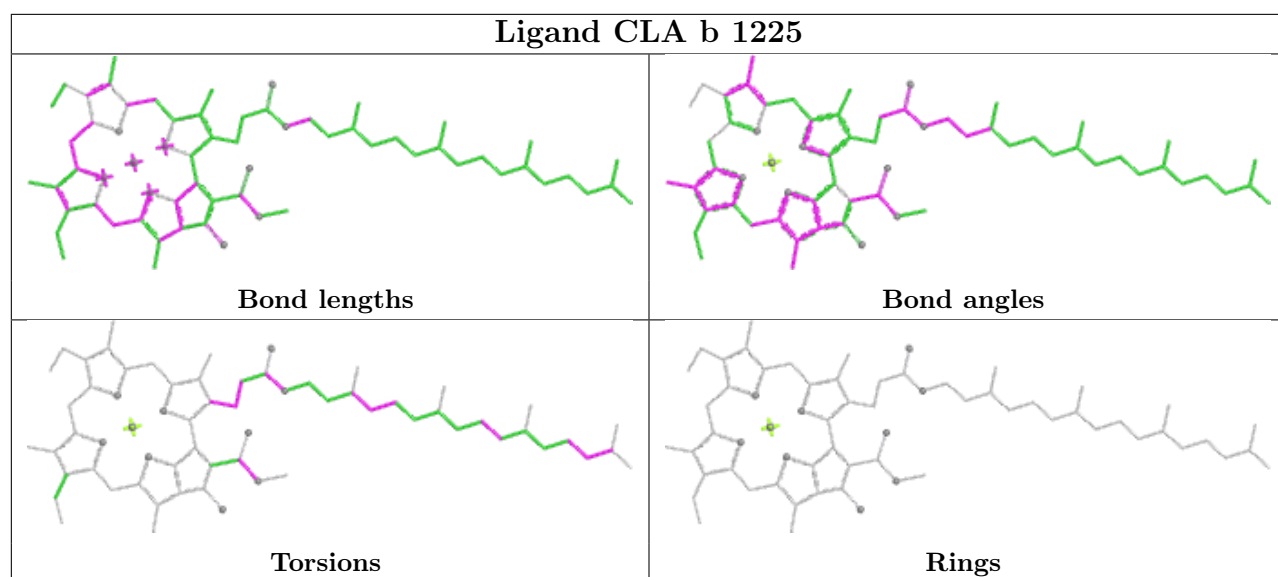


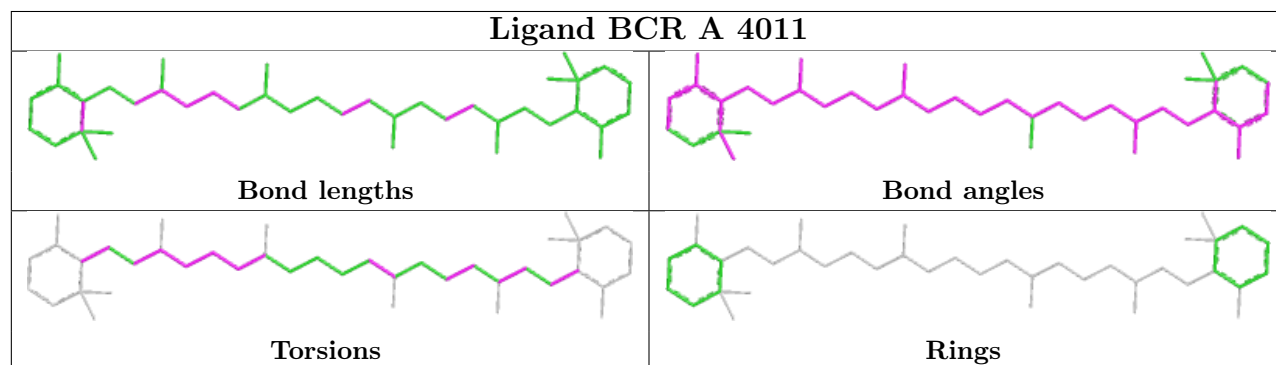
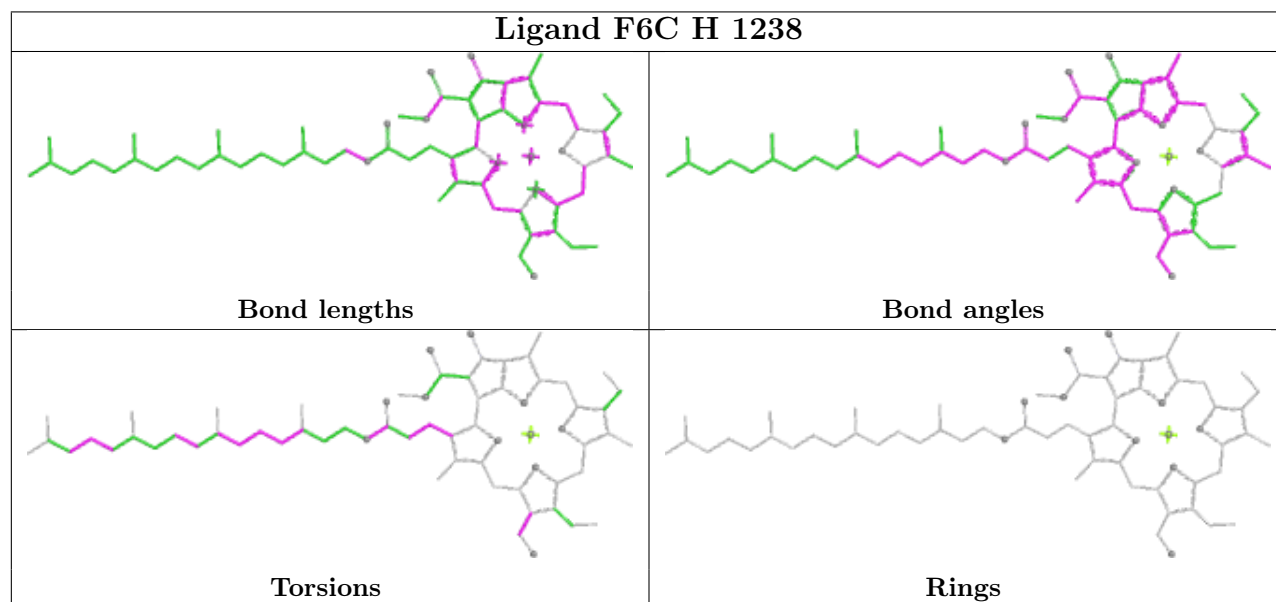
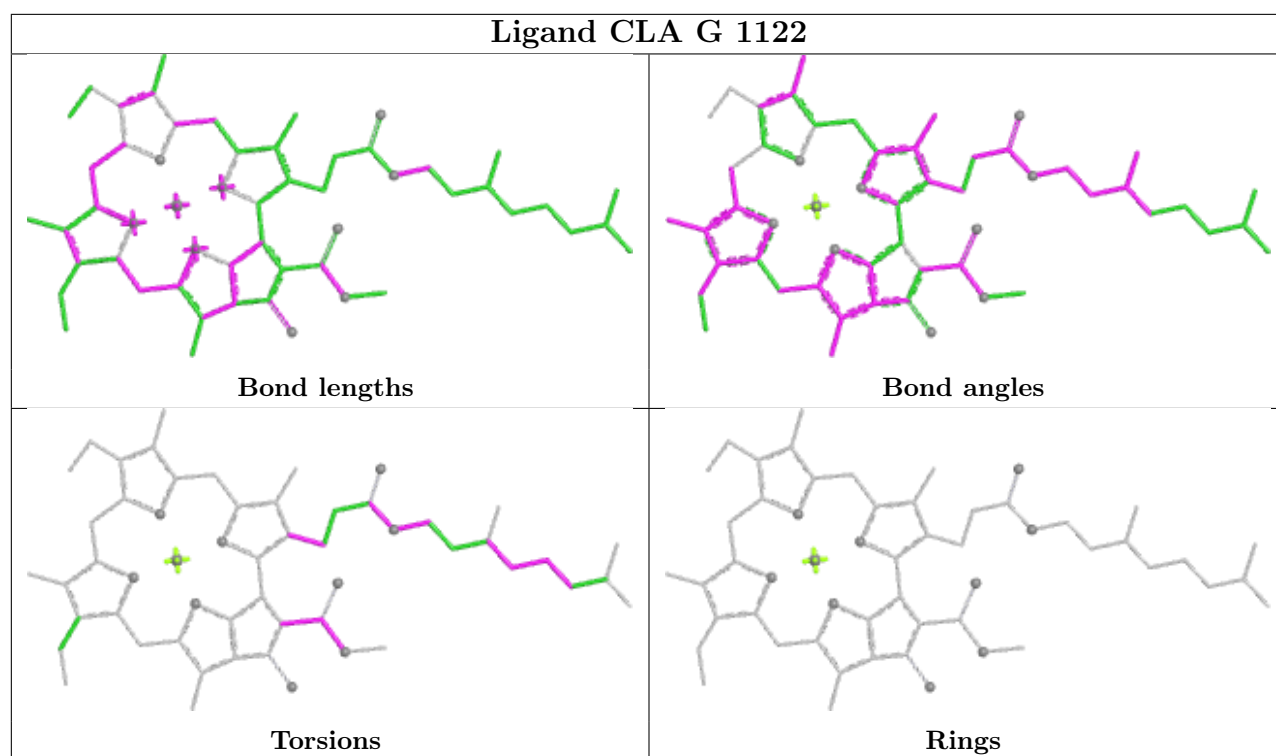
Ligand BCR b 4010					
	Bond lengths				
	Torsions				
Rings					
Ligand BCR b 4006					
	Bond lengths				
	Torsions				
Rings					

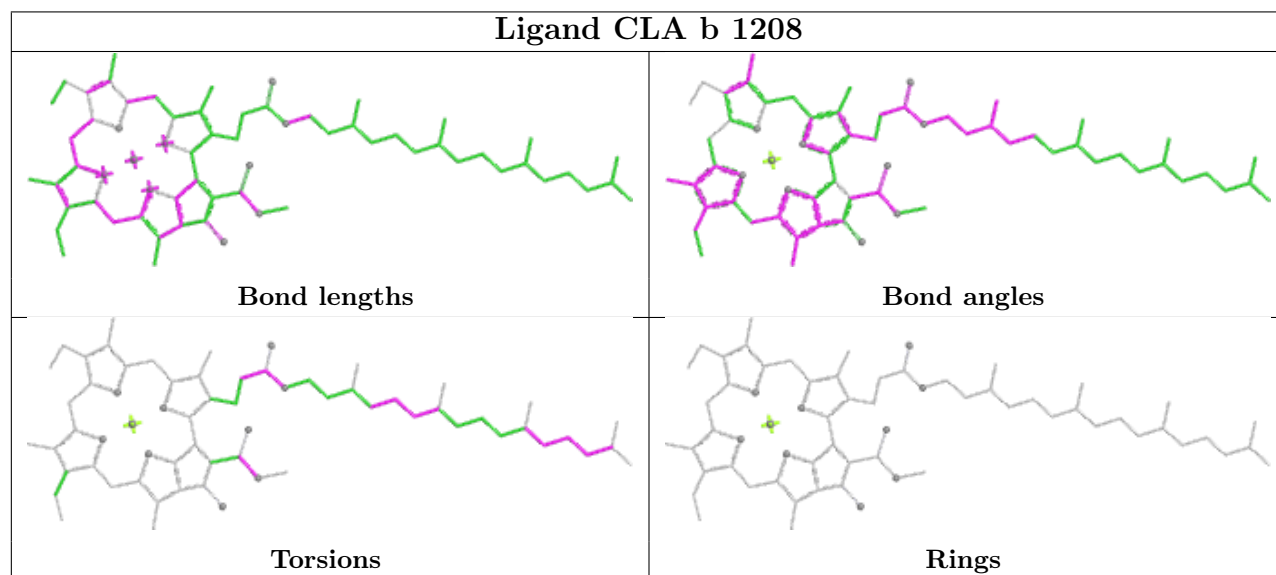
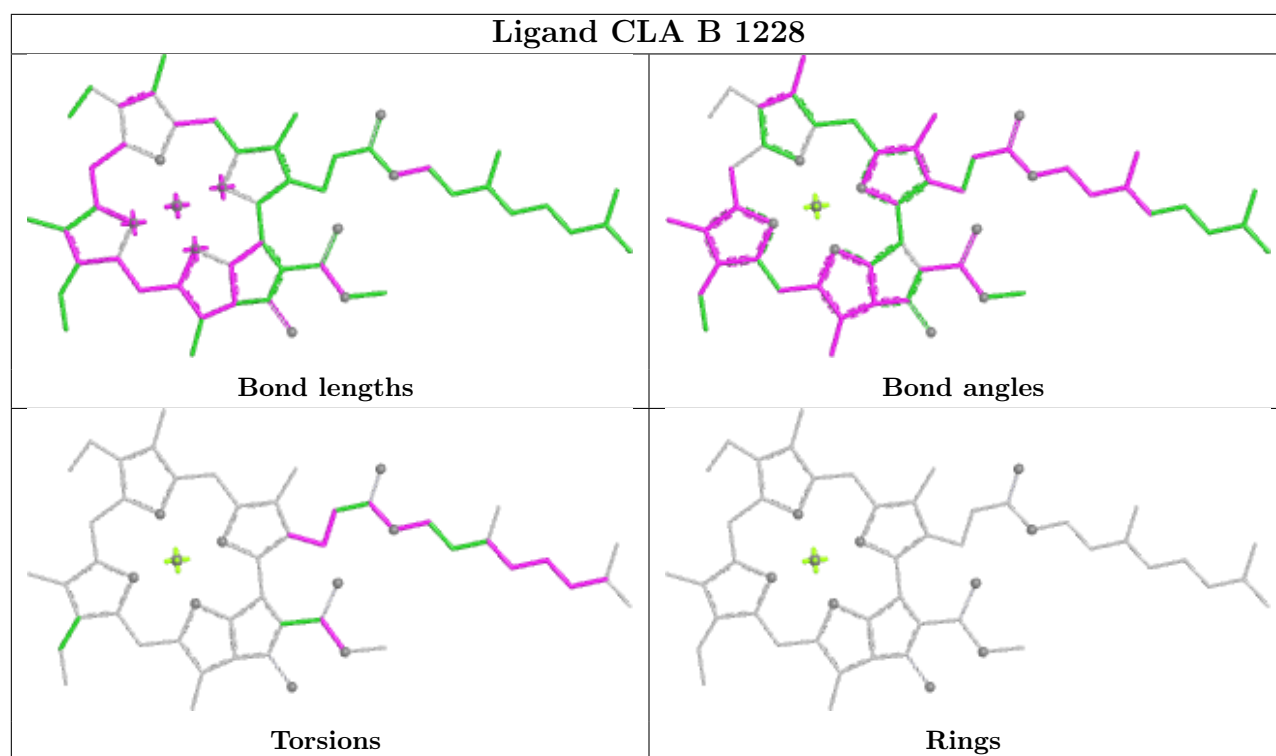




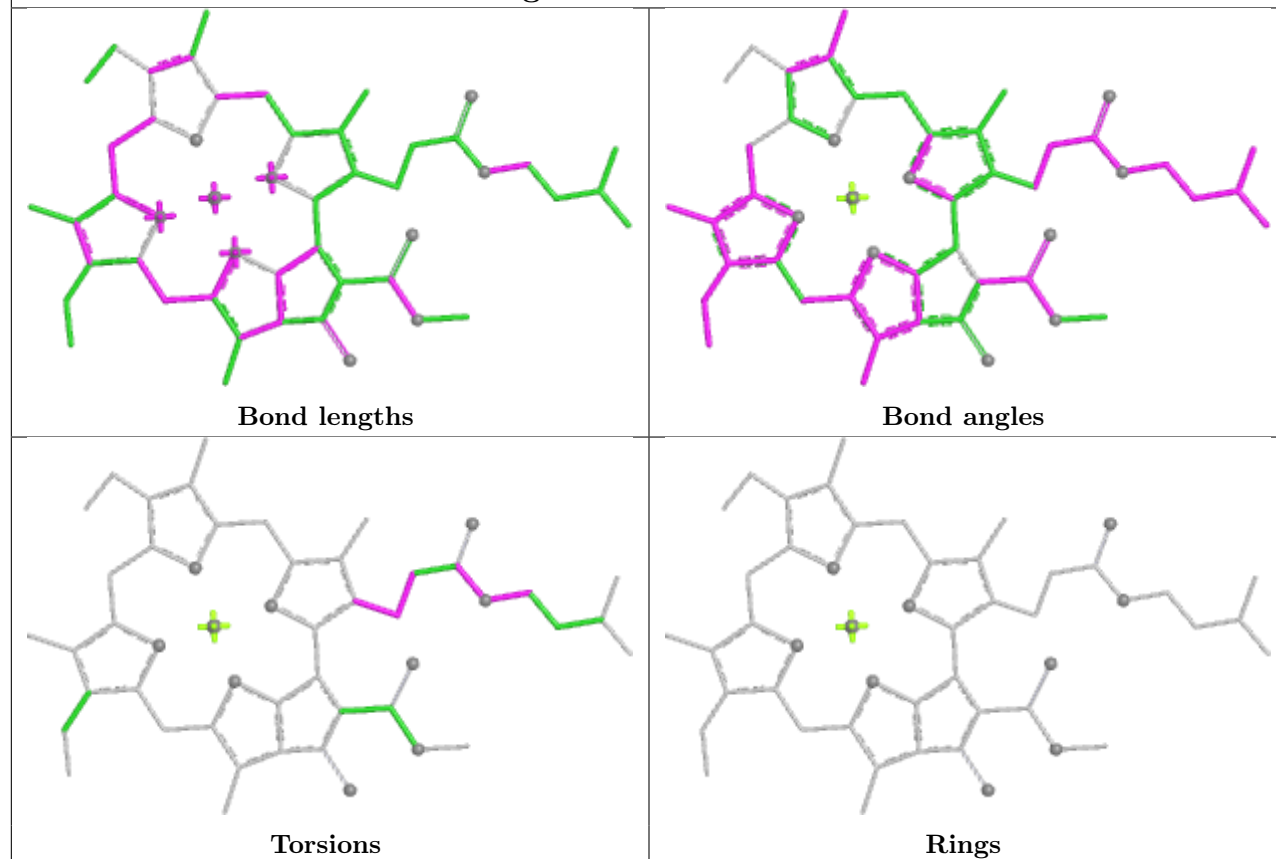




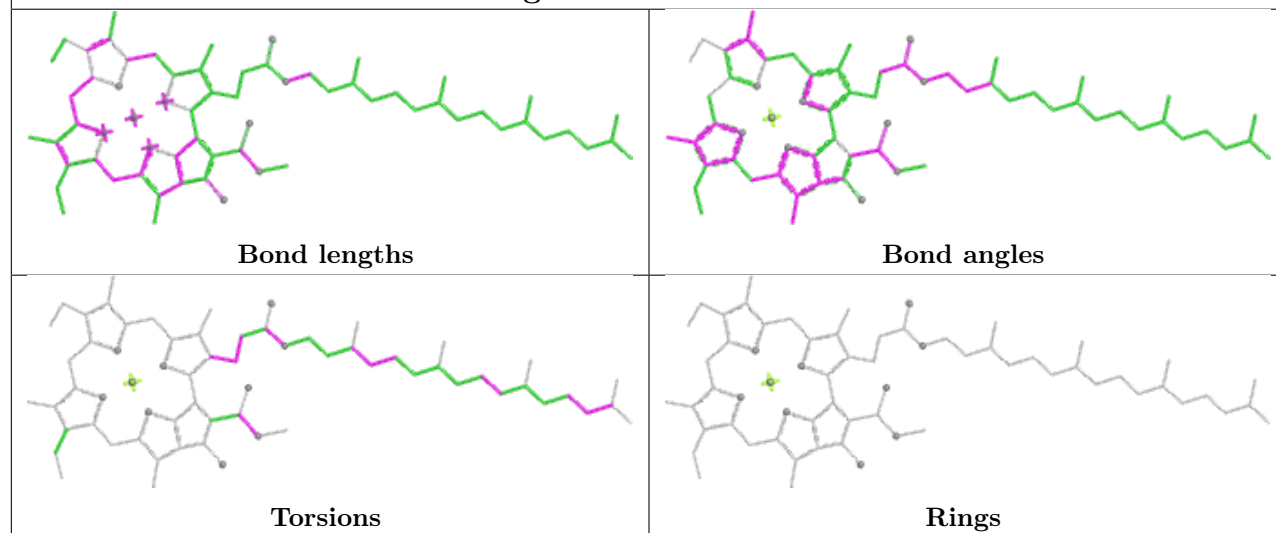


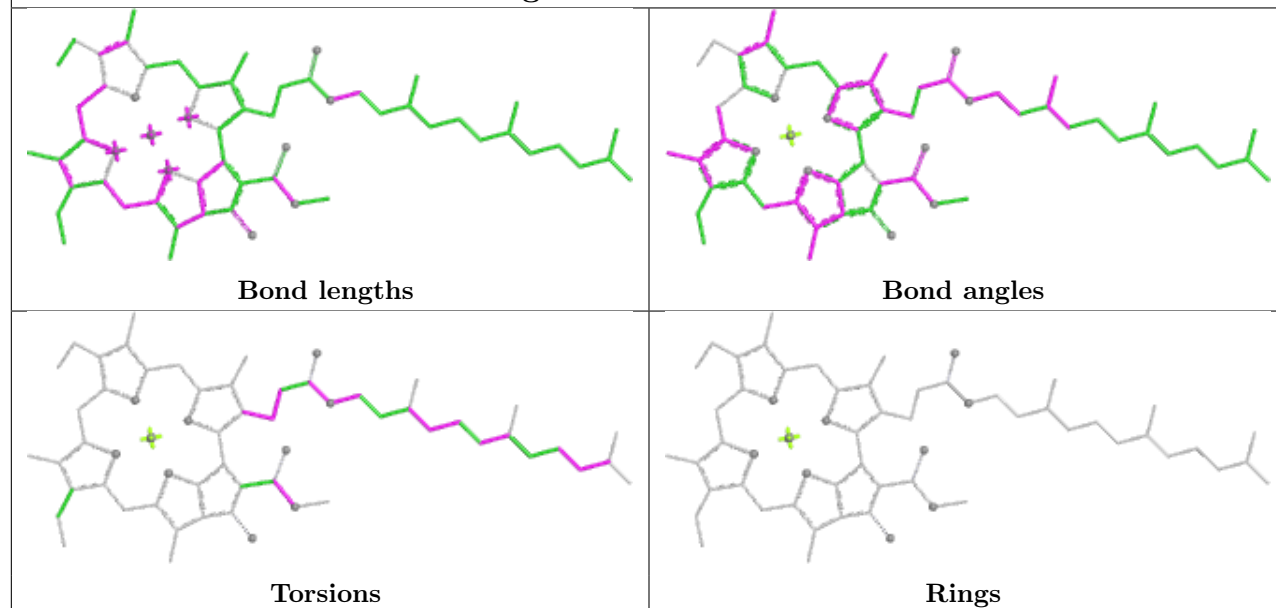
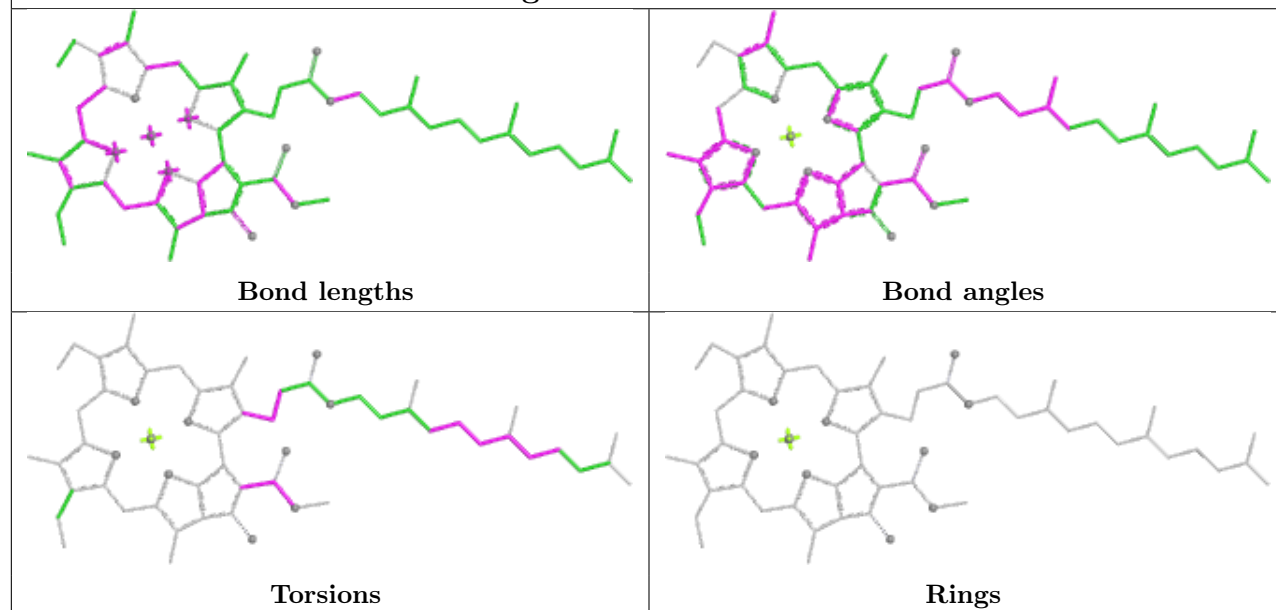


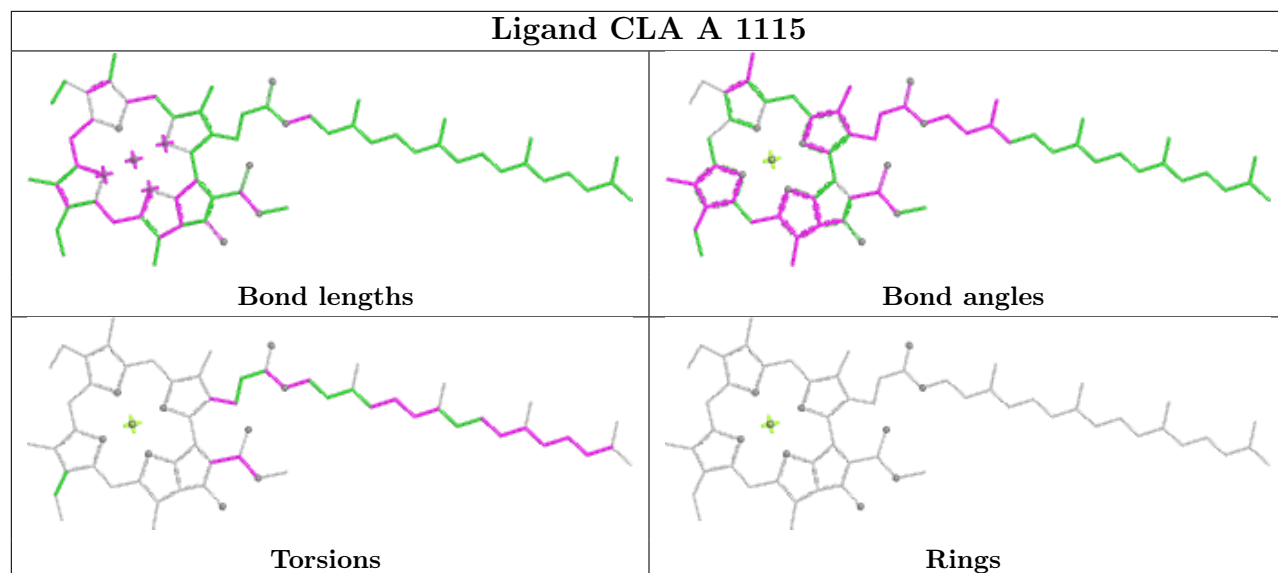
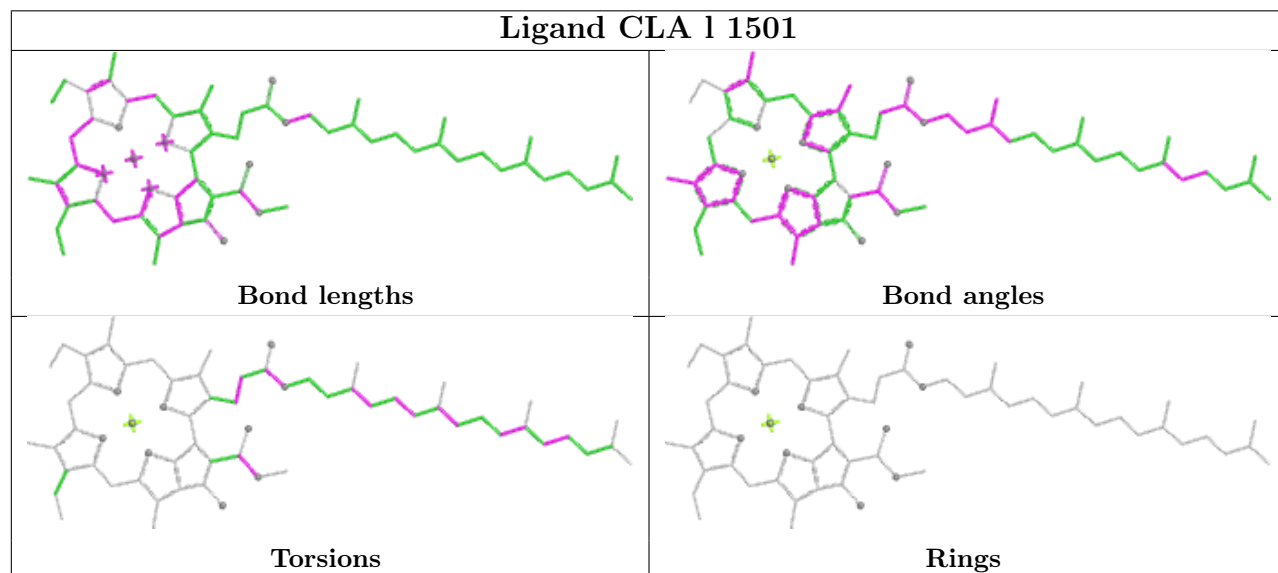
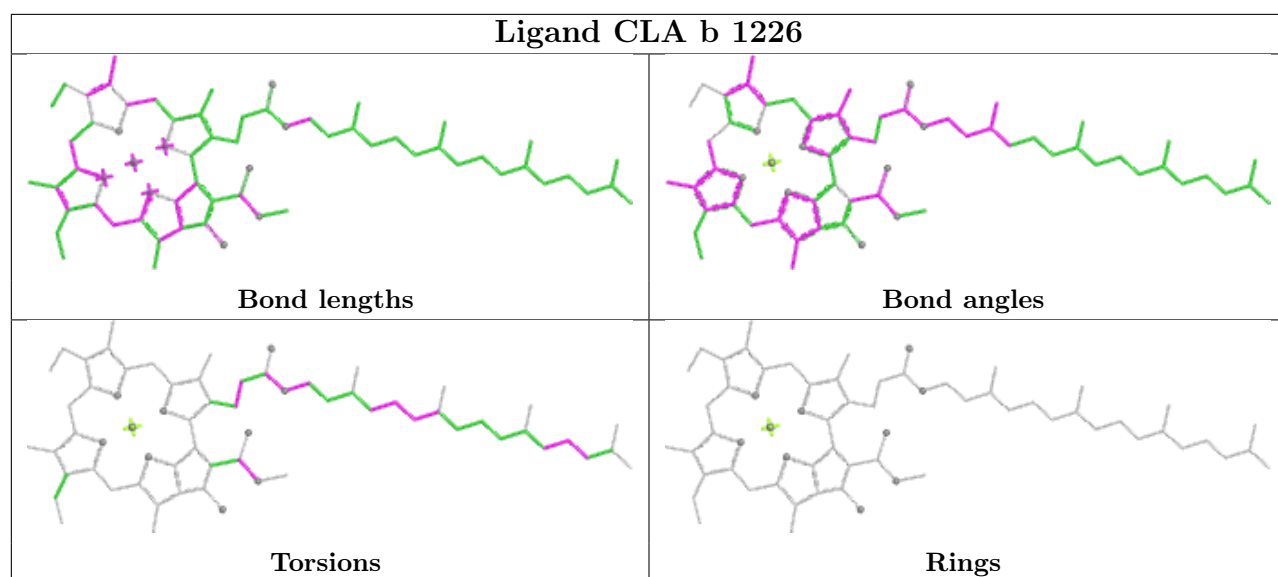
Ligand CLA A 1137

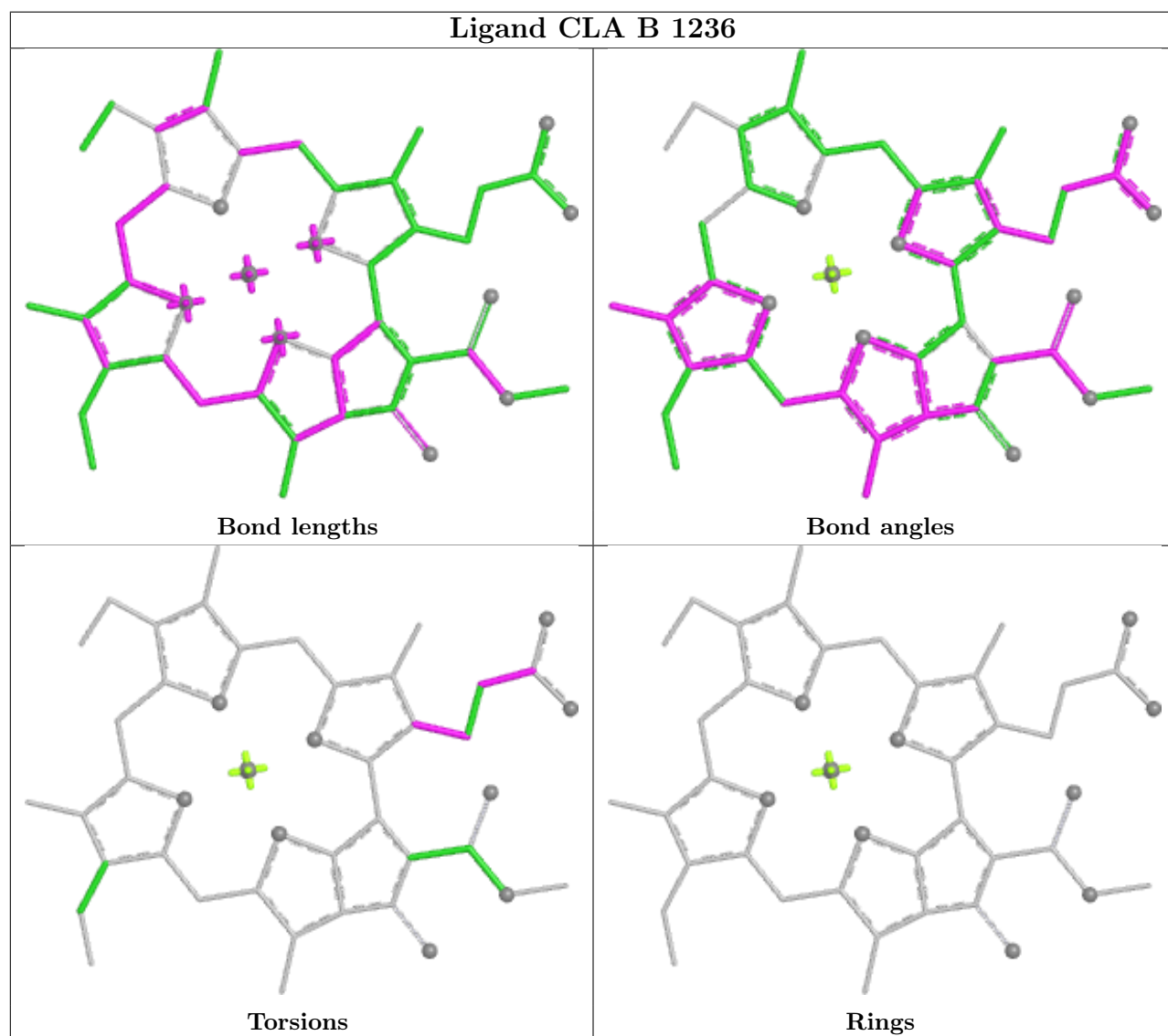
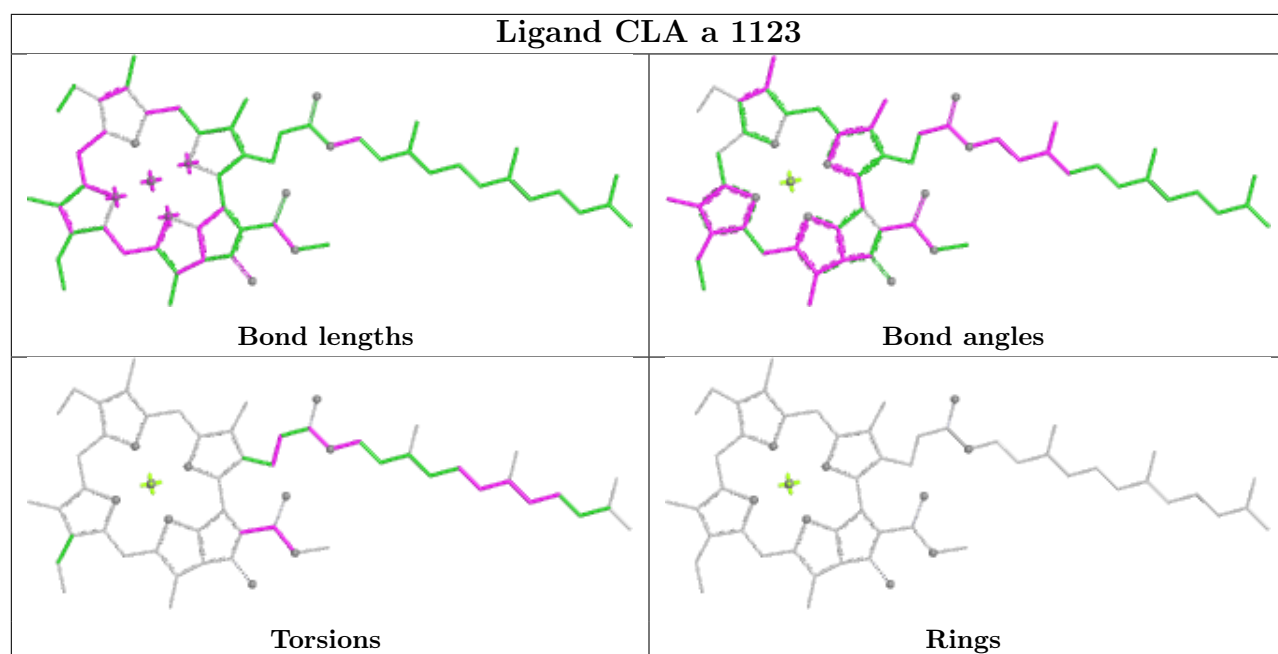


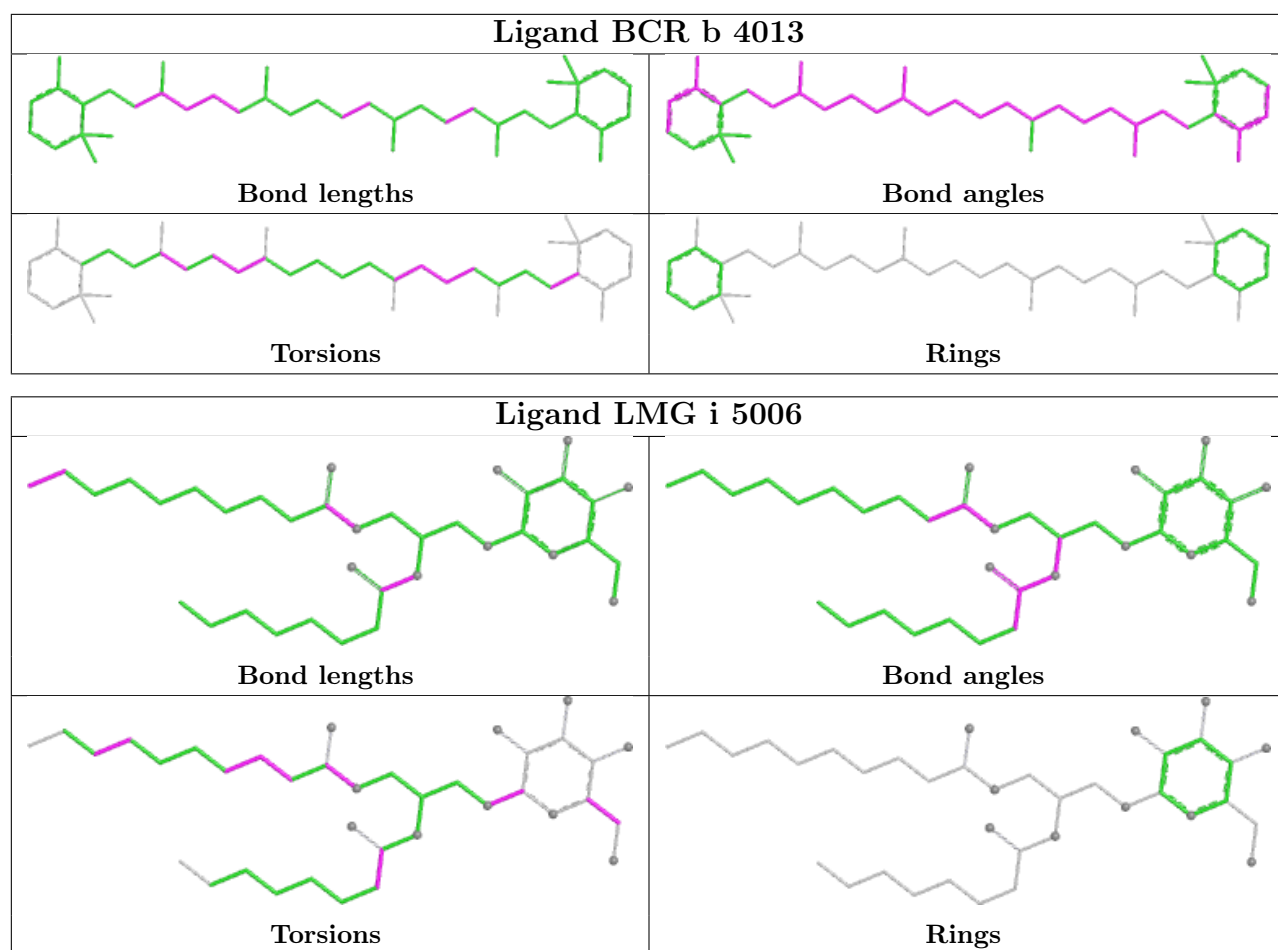
Ligand CLA B 1225

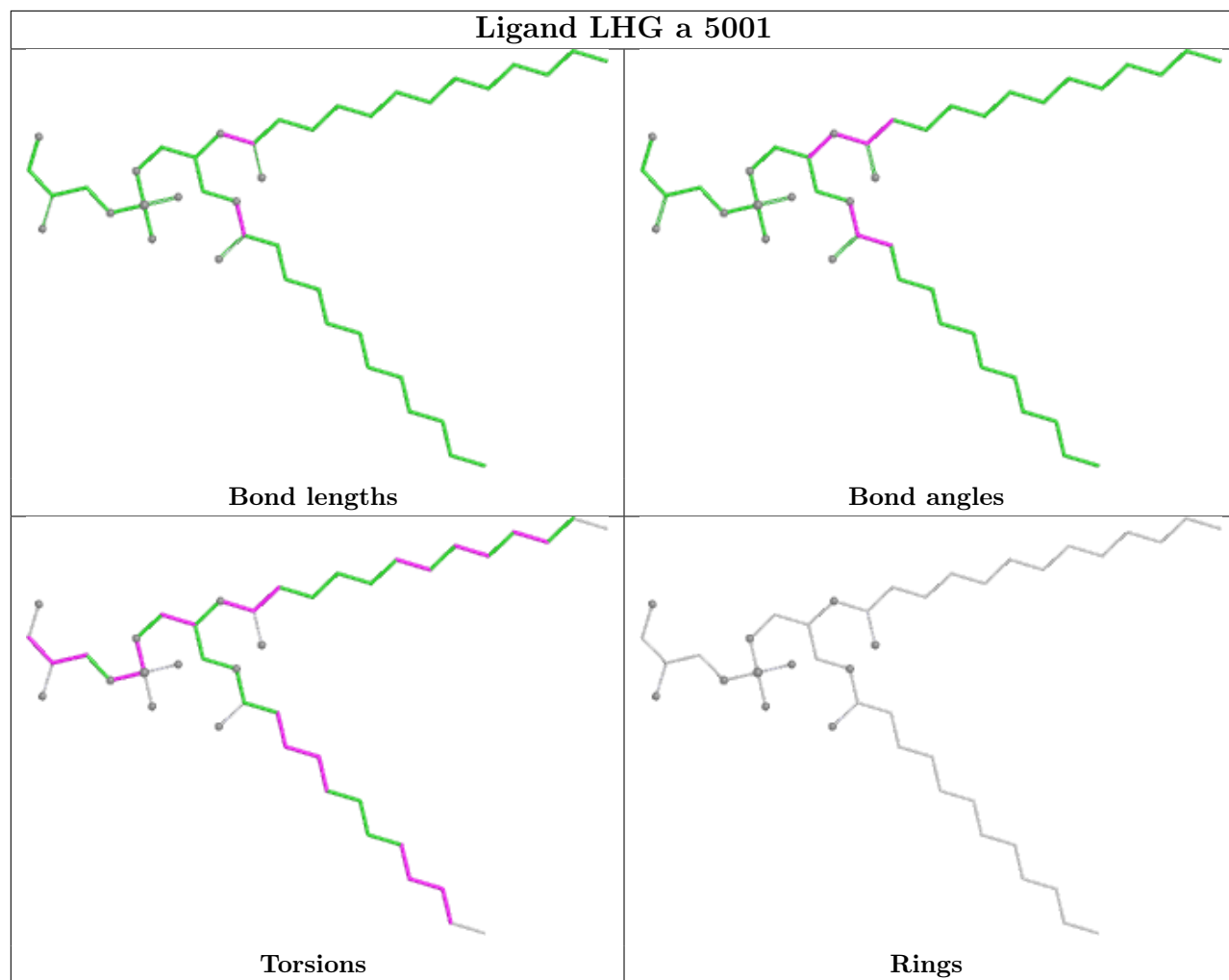


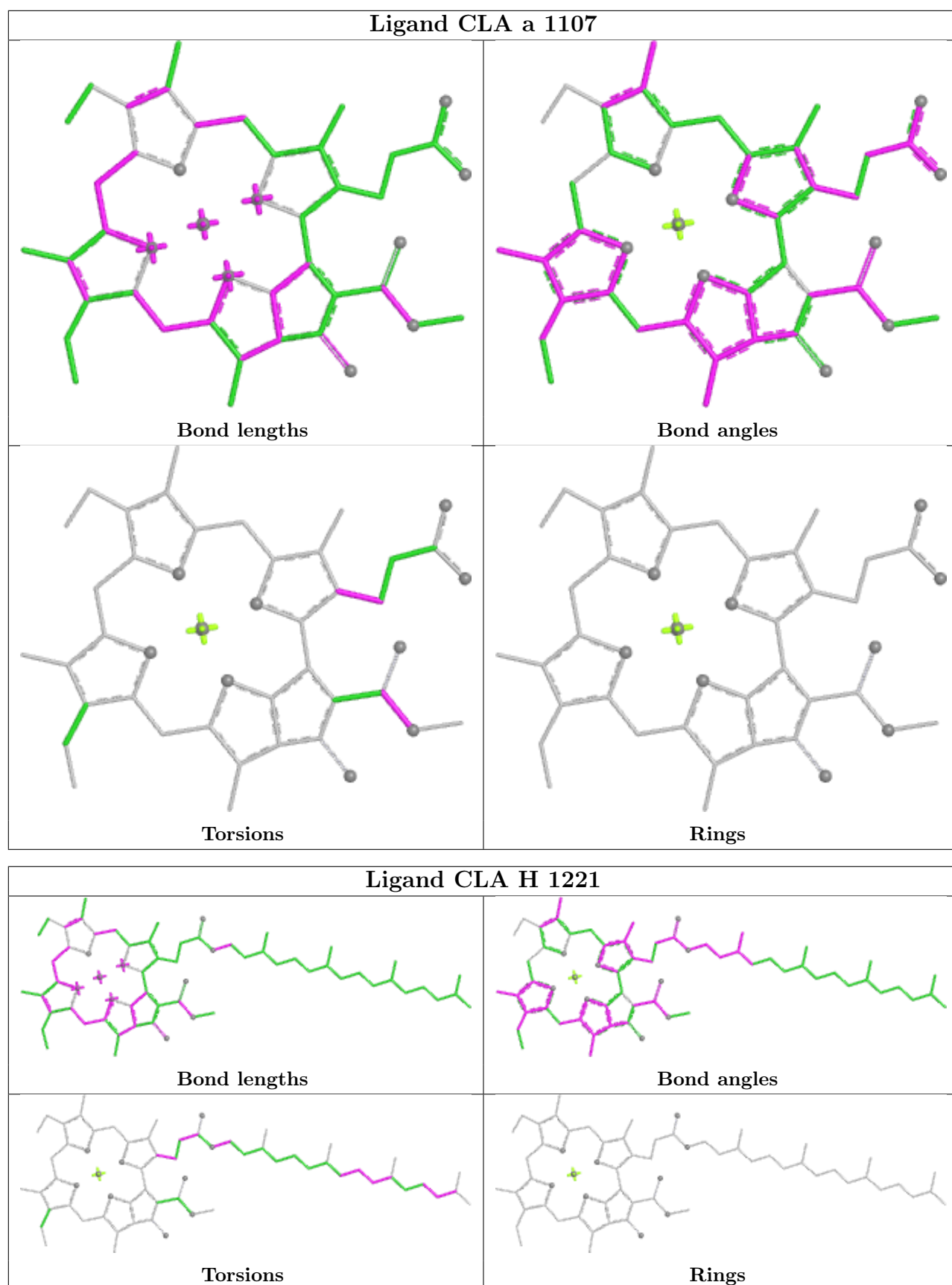
Ligand CLA H 1215**Ligand CLA G 1135**

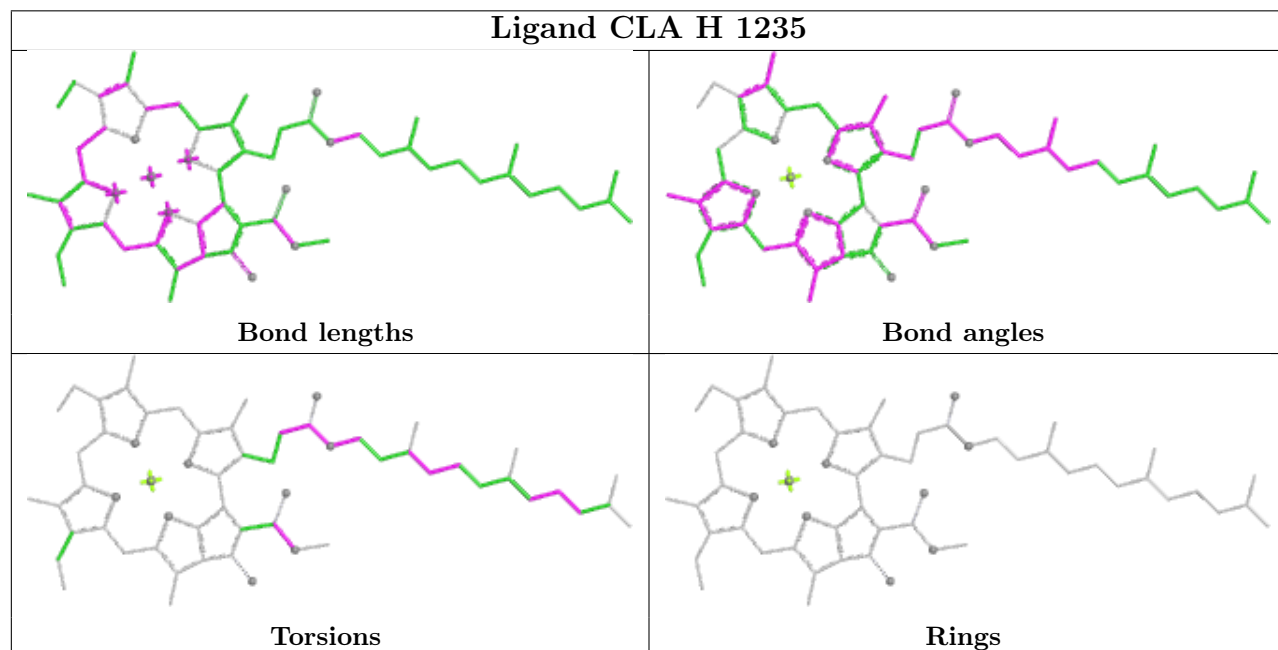
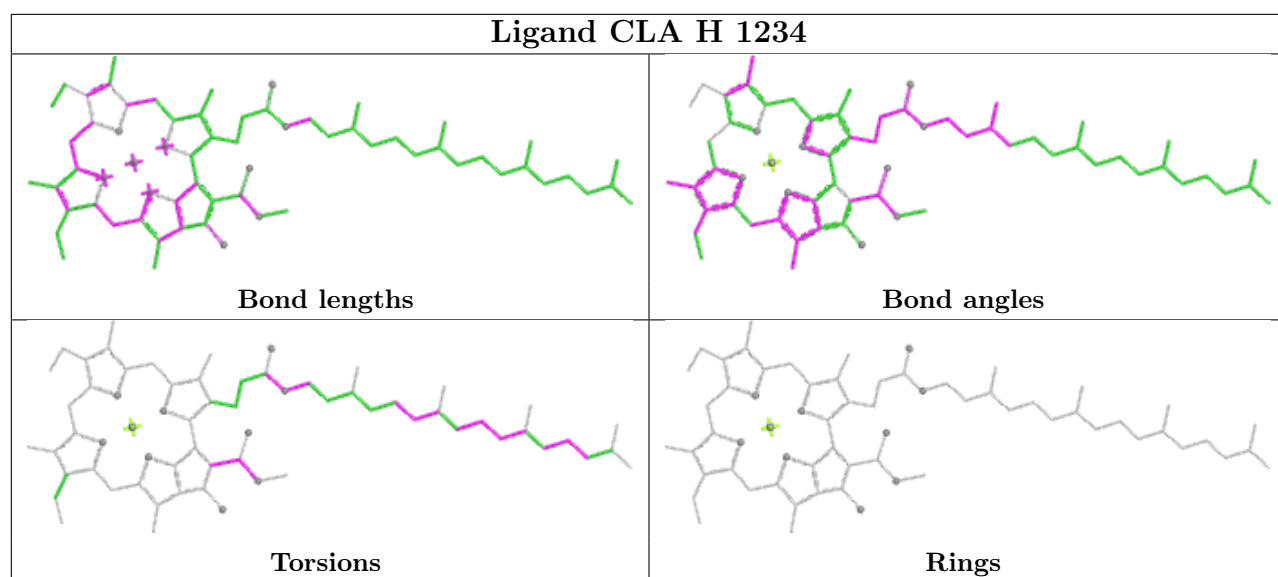


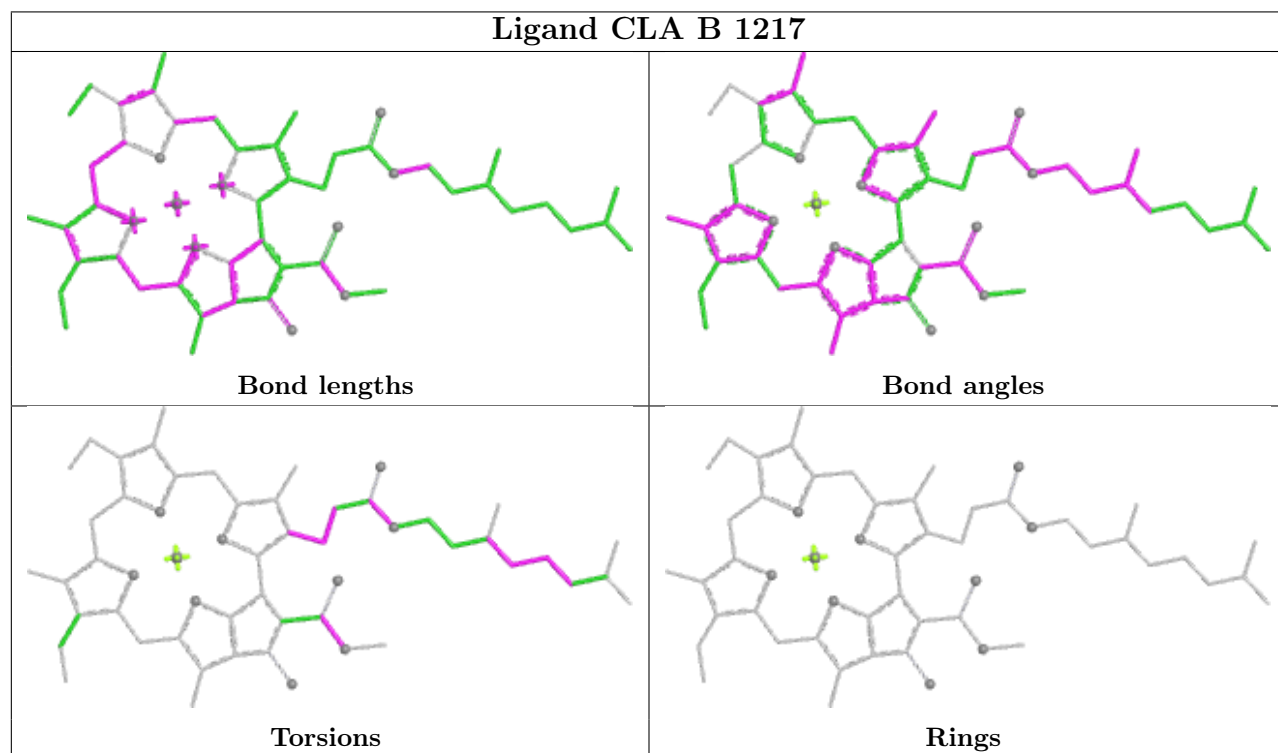
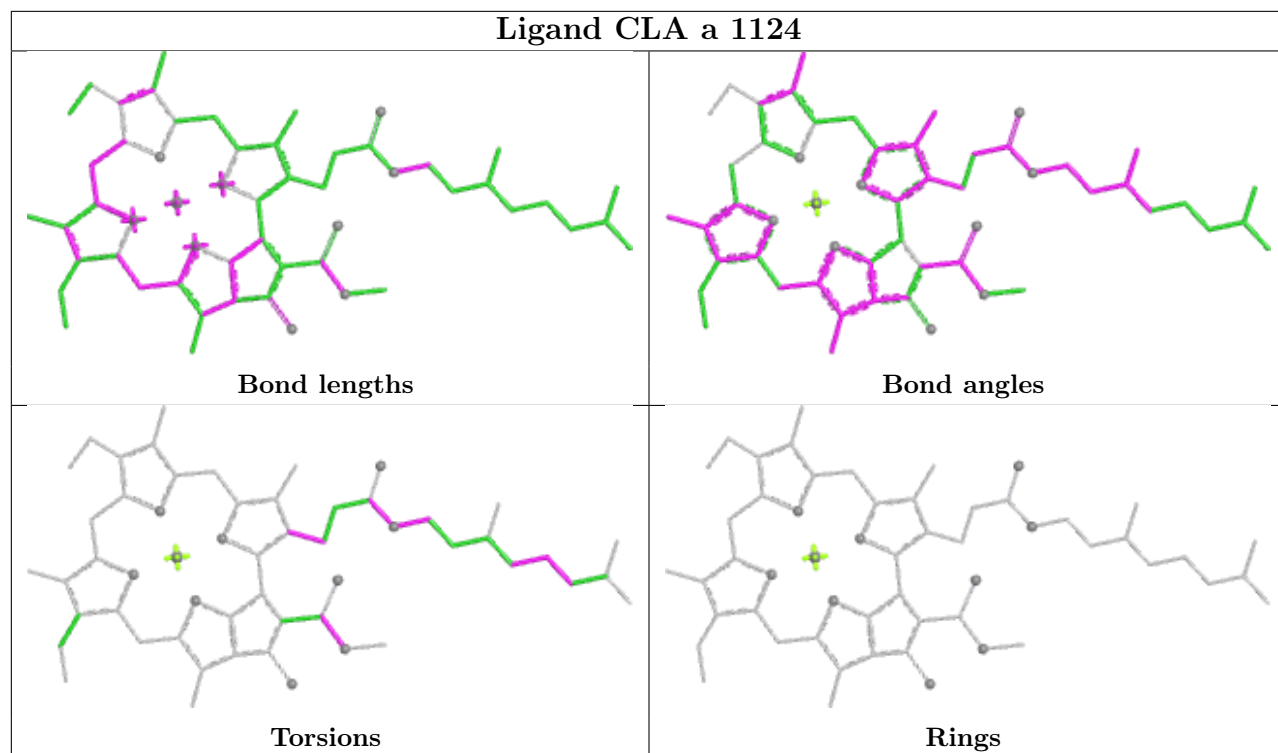


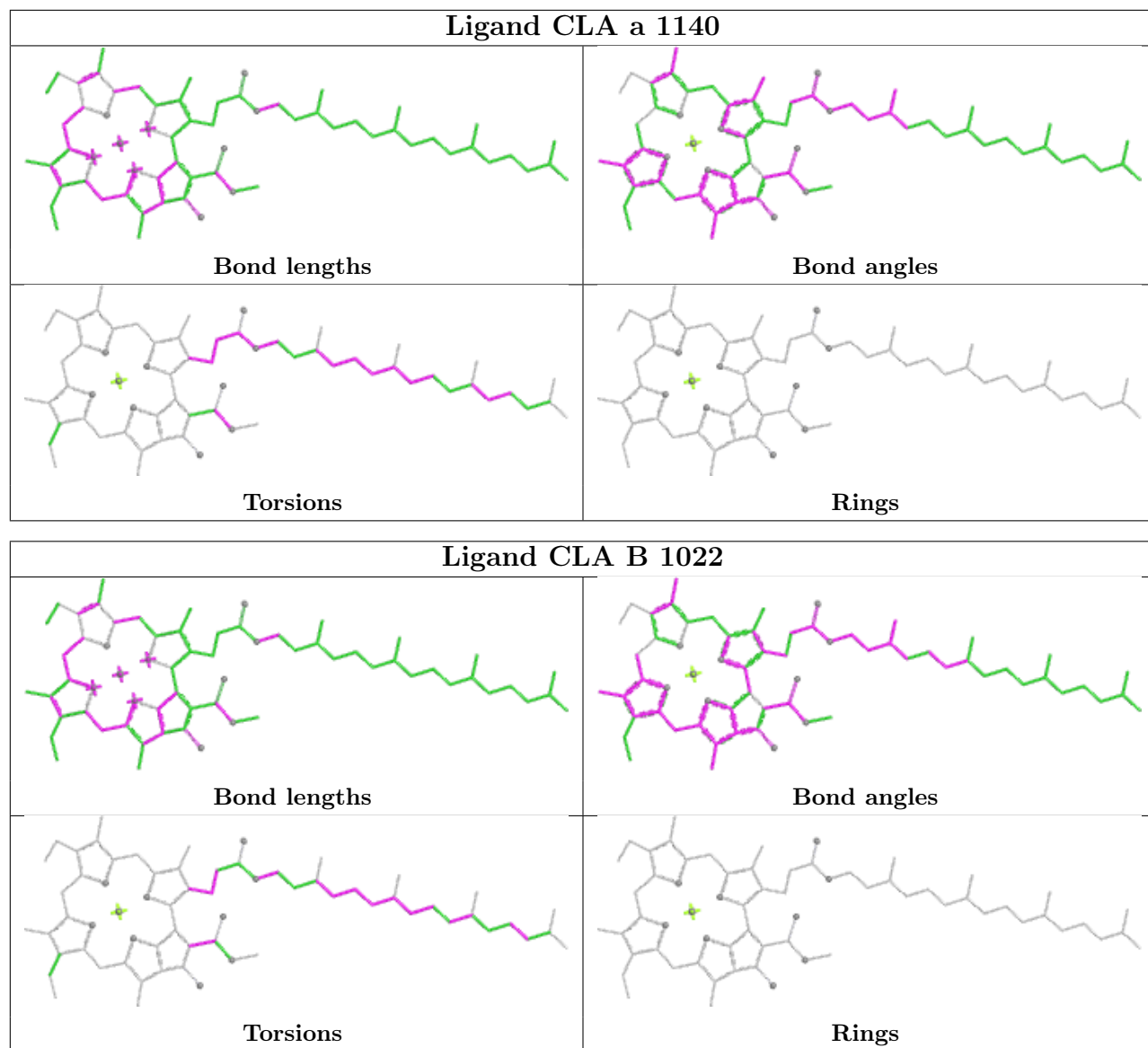


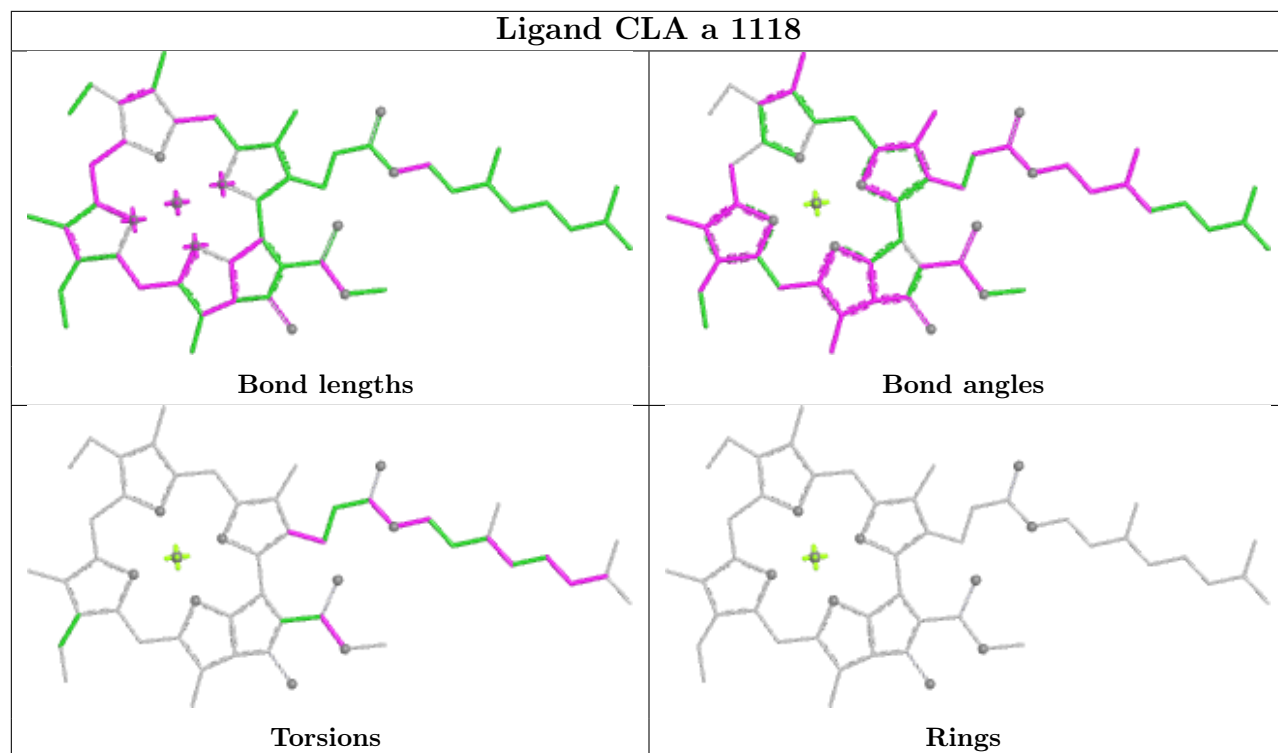


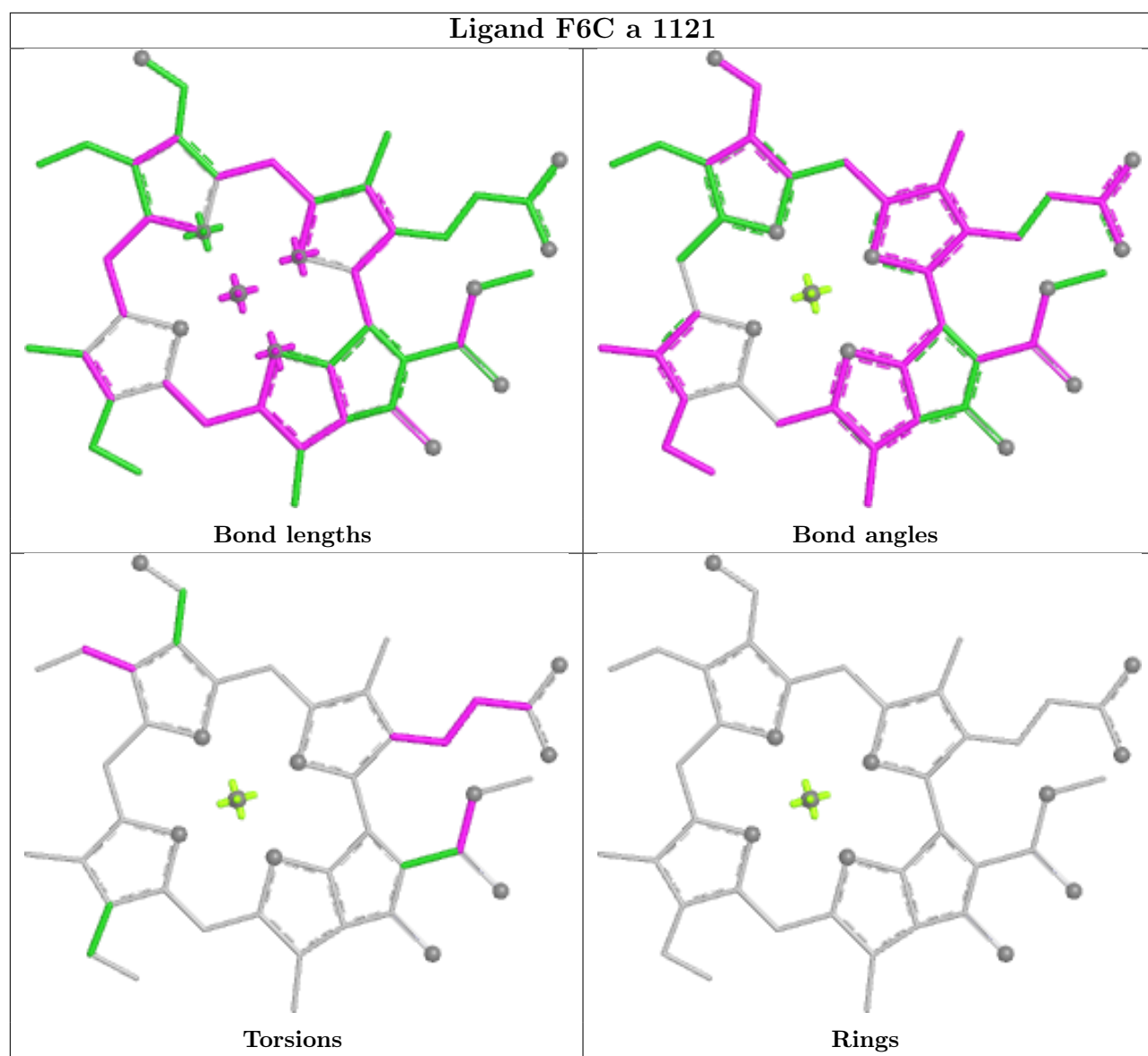


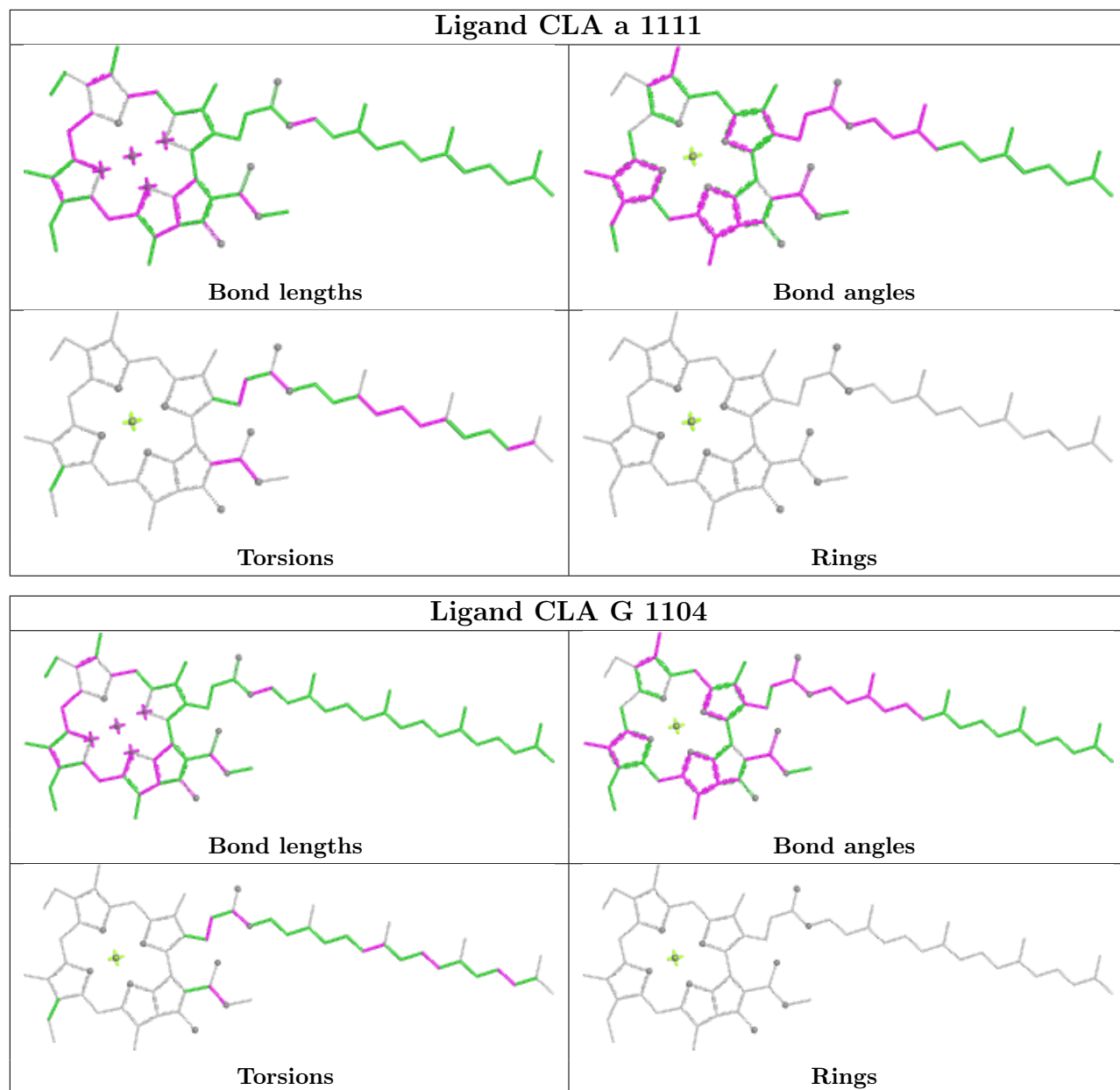


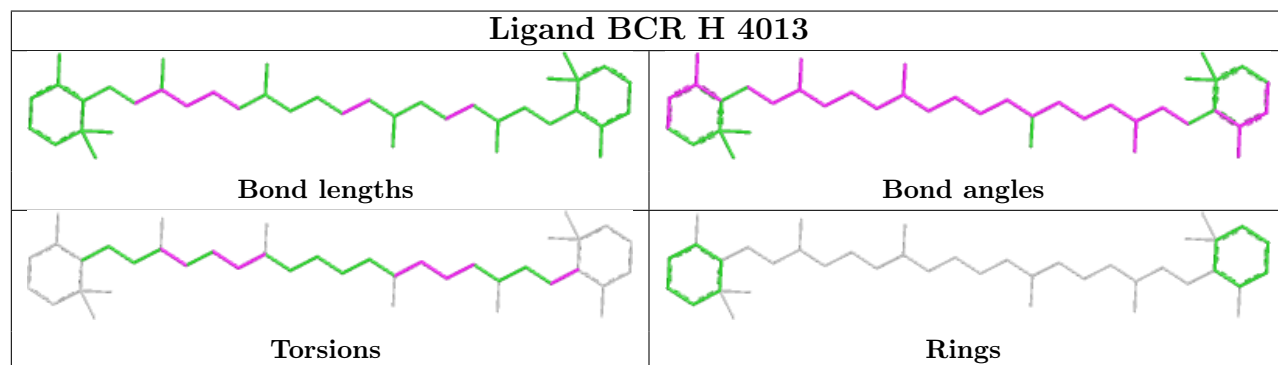
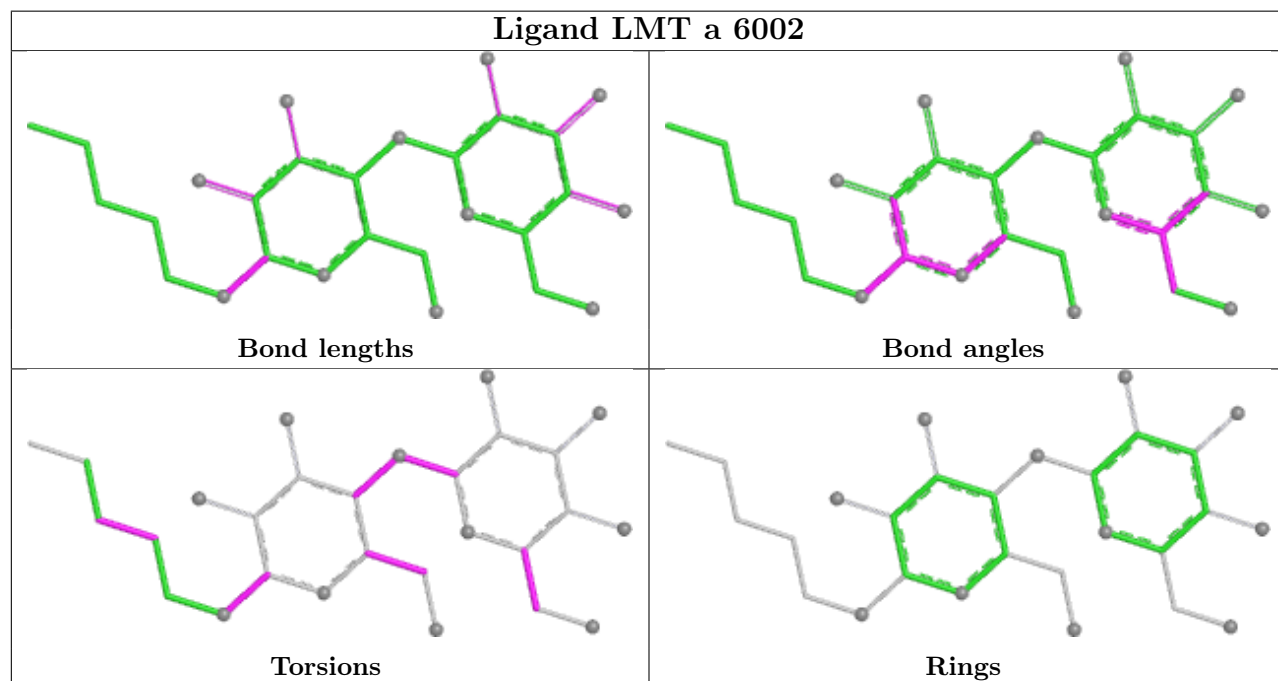
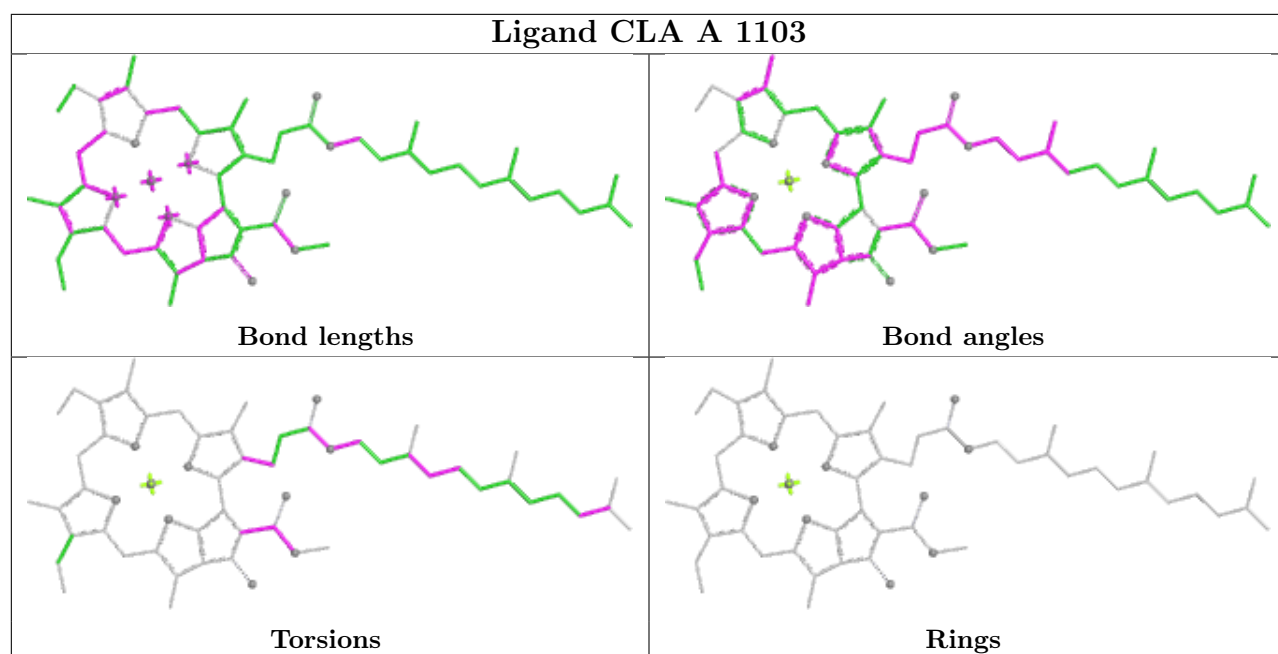


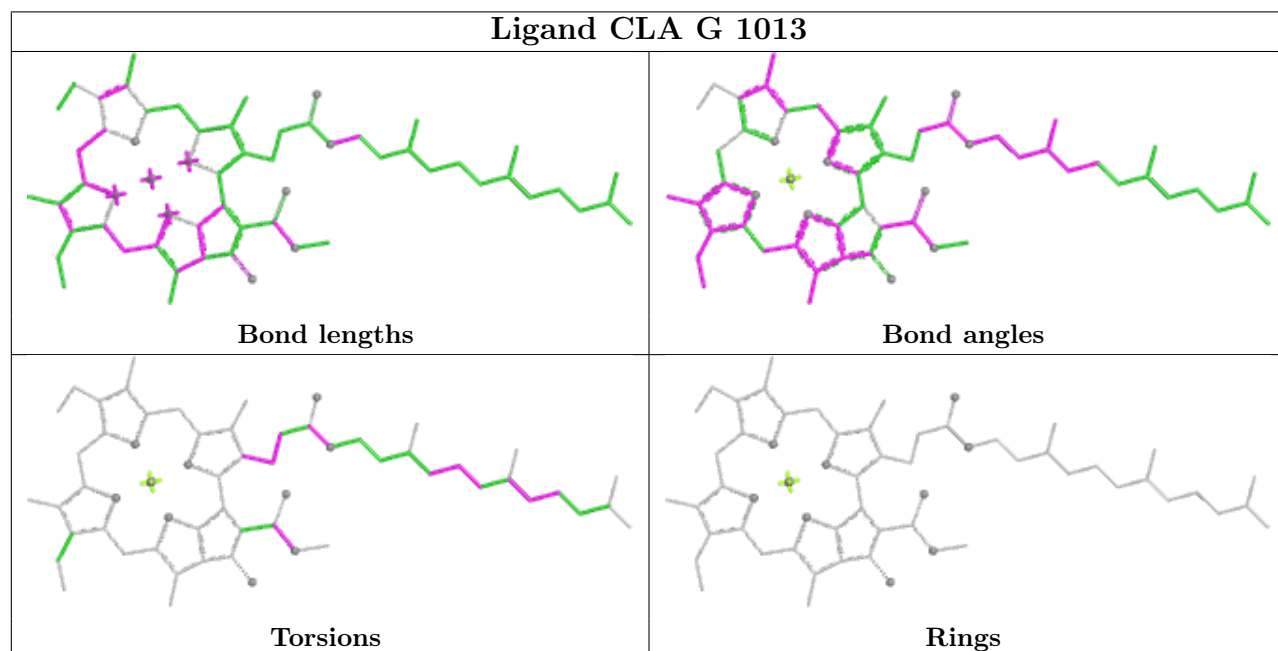
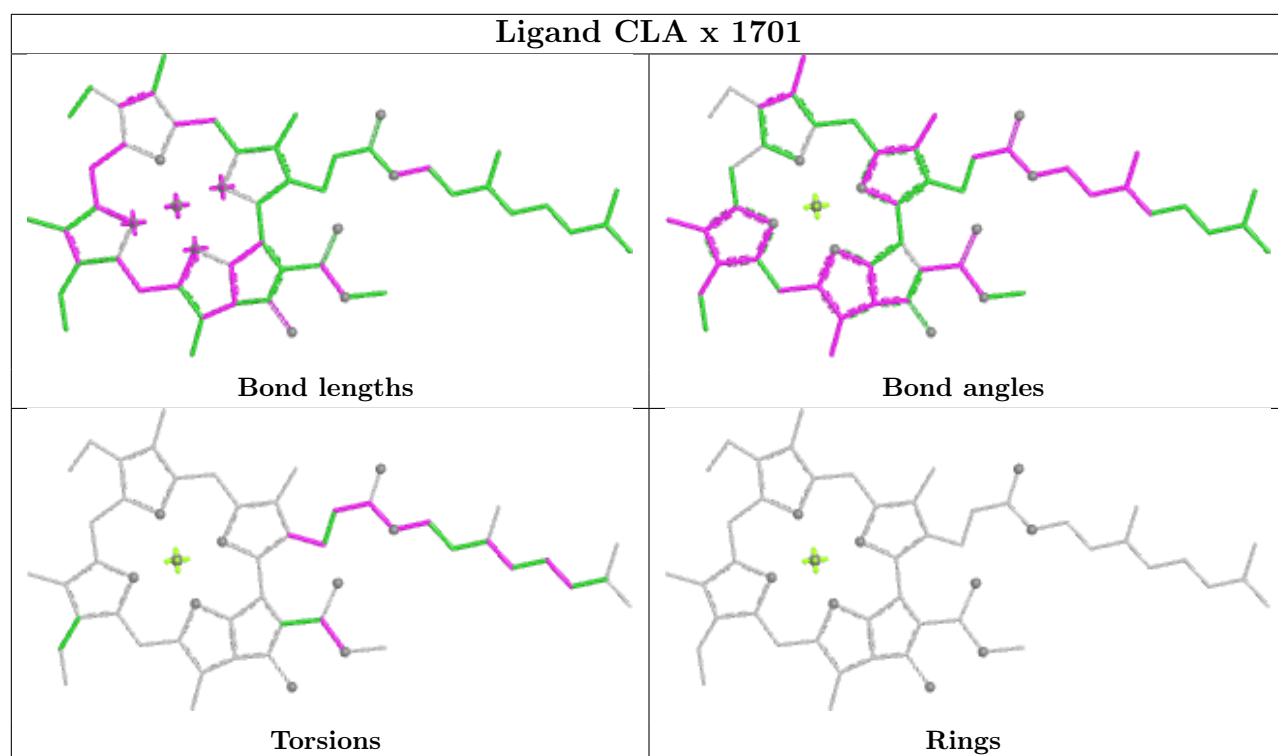




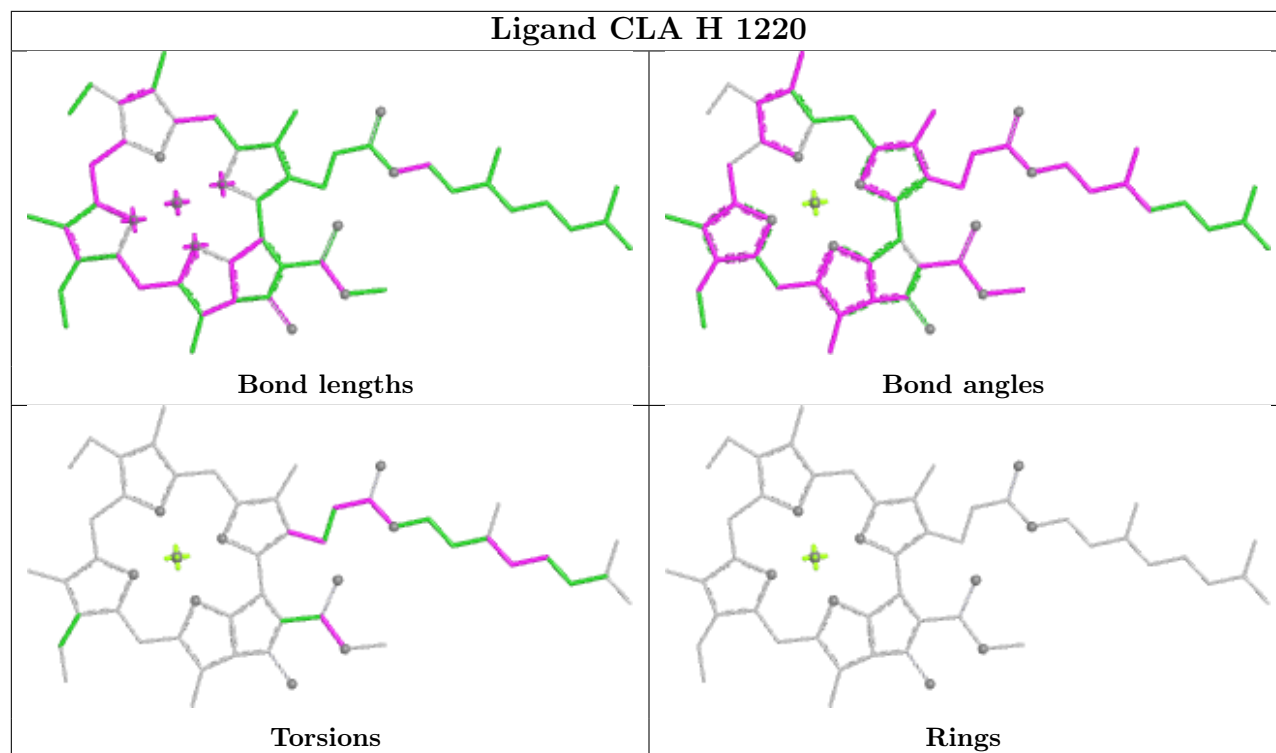




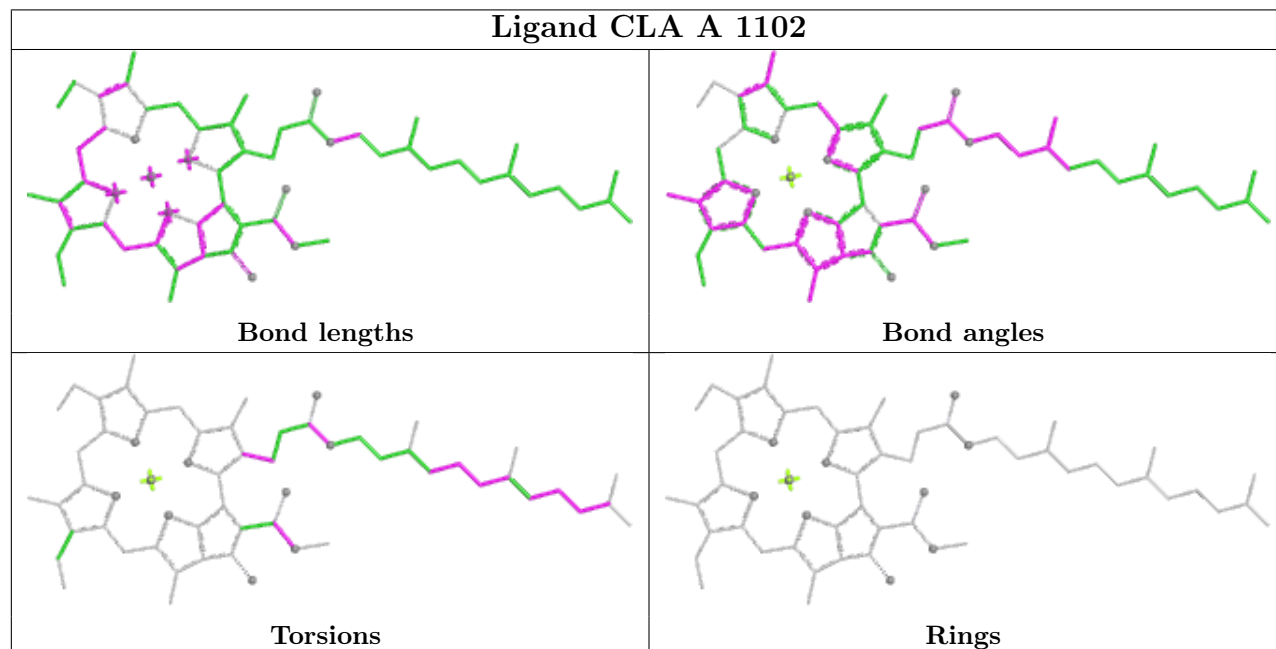


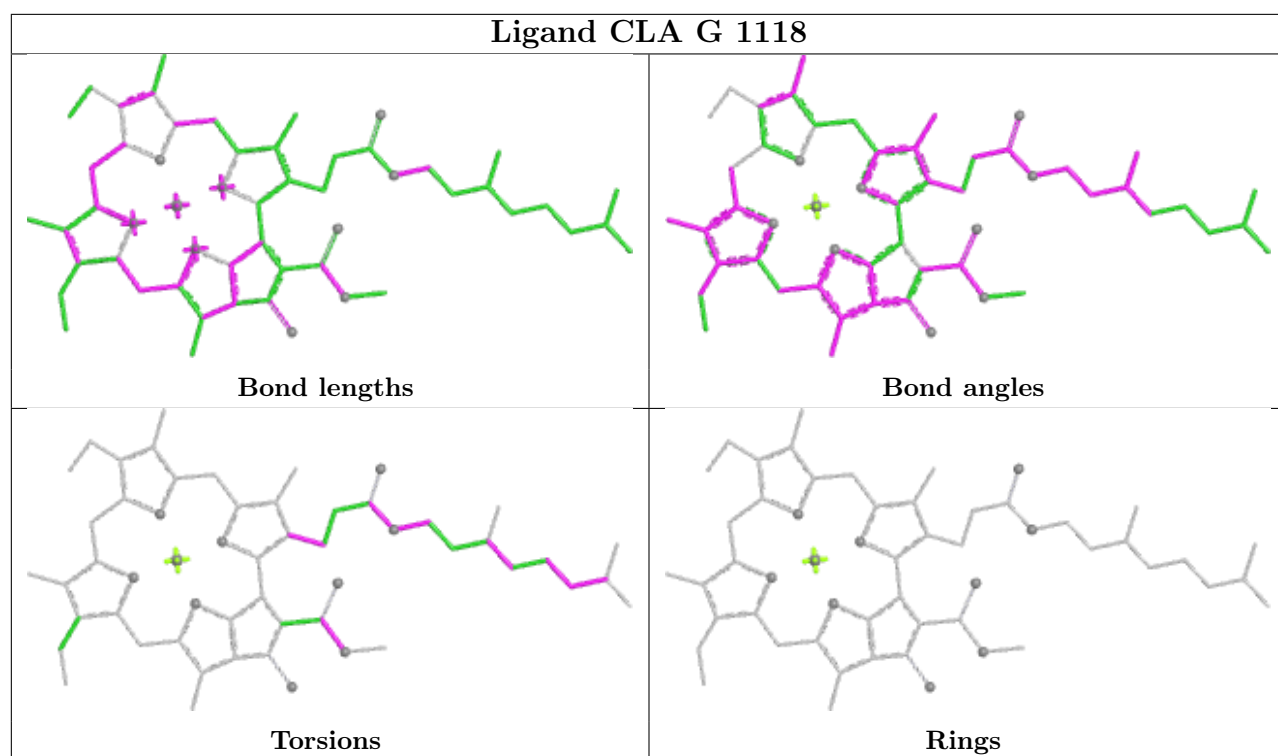


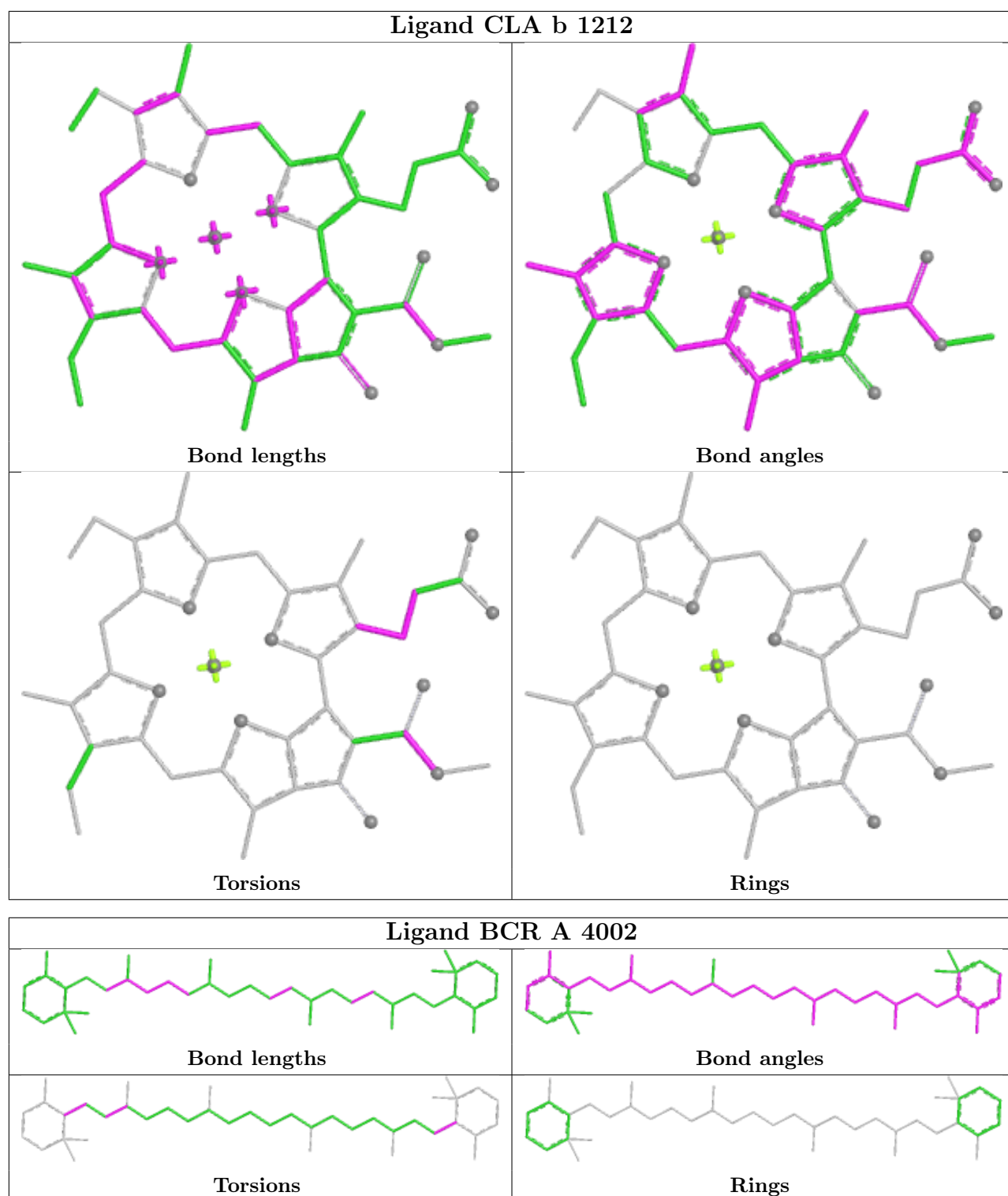
Ligand CLA H 1220



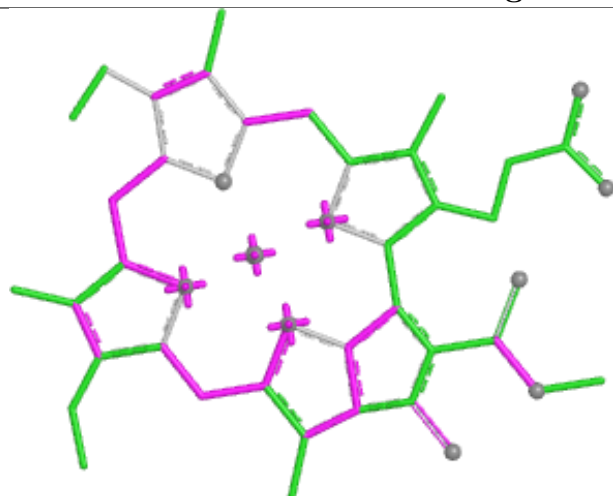
Ligand CLA A 1102



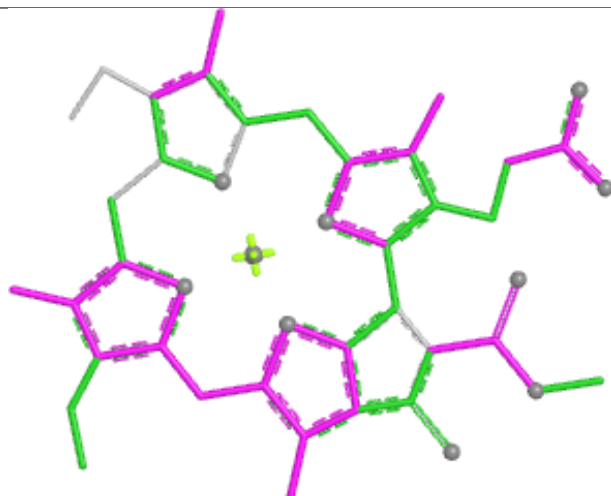




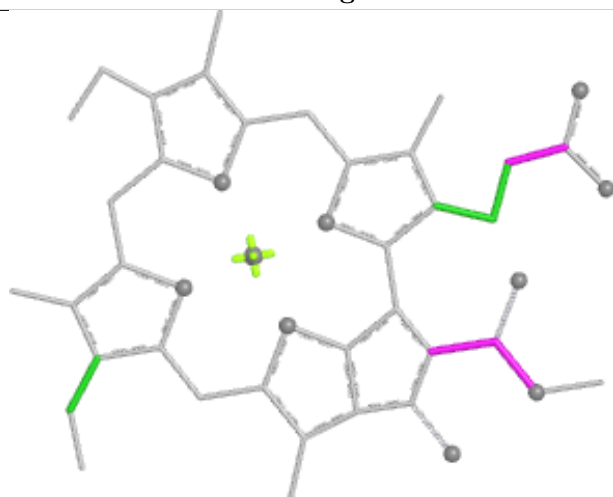
Ligand CLA B 1218



Bond lengths



Bond angles

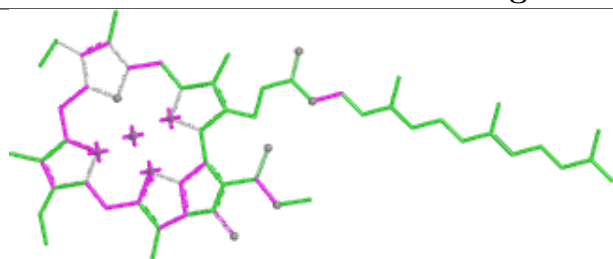


Torsions

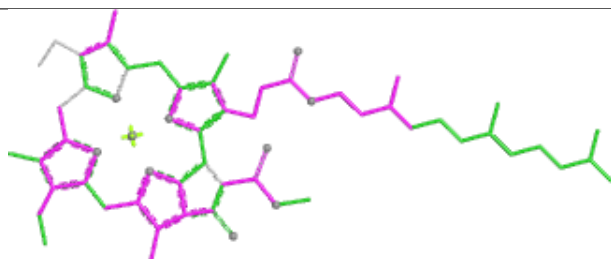


Rings

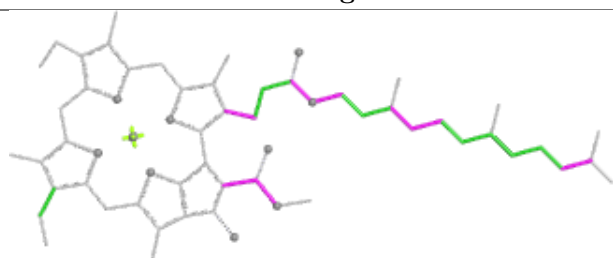
Ligand CLA a 1103



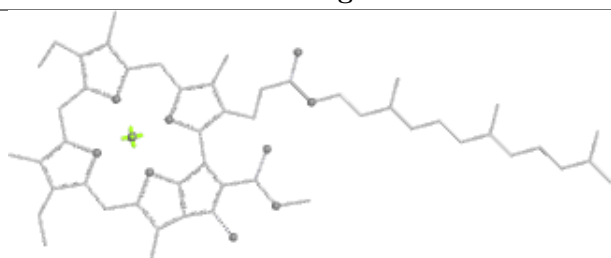
Bond lengths



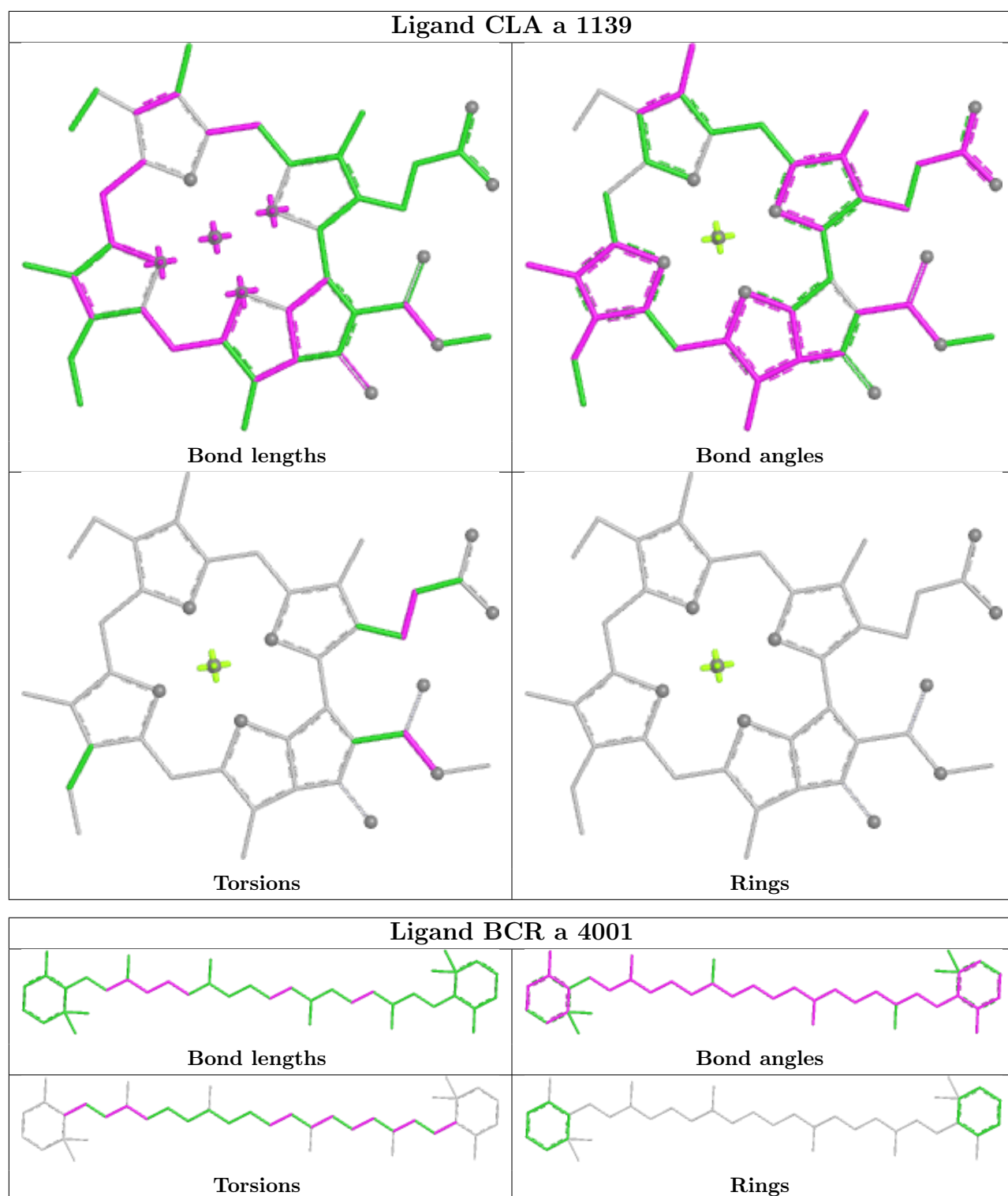
Bond angles

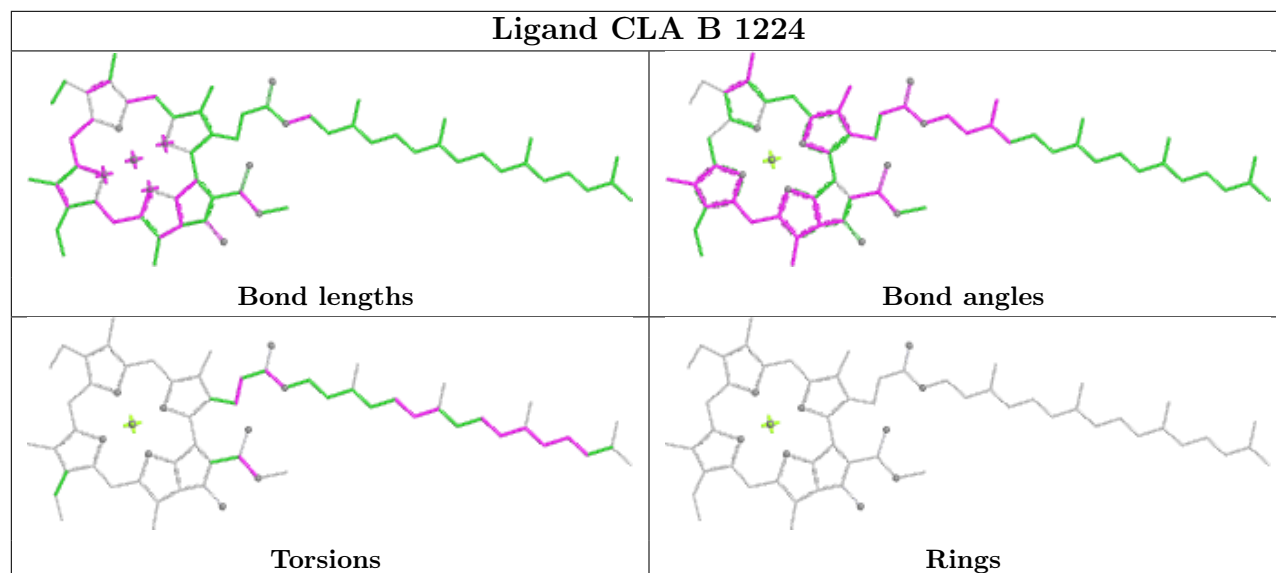
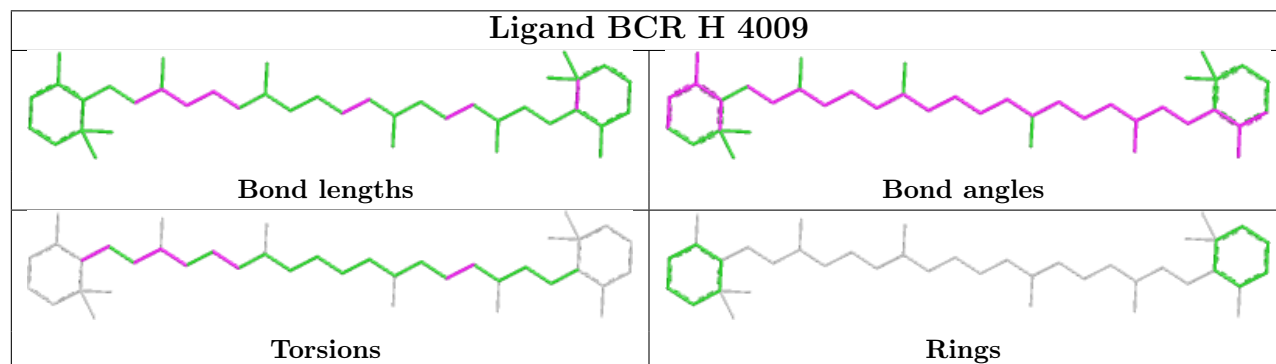
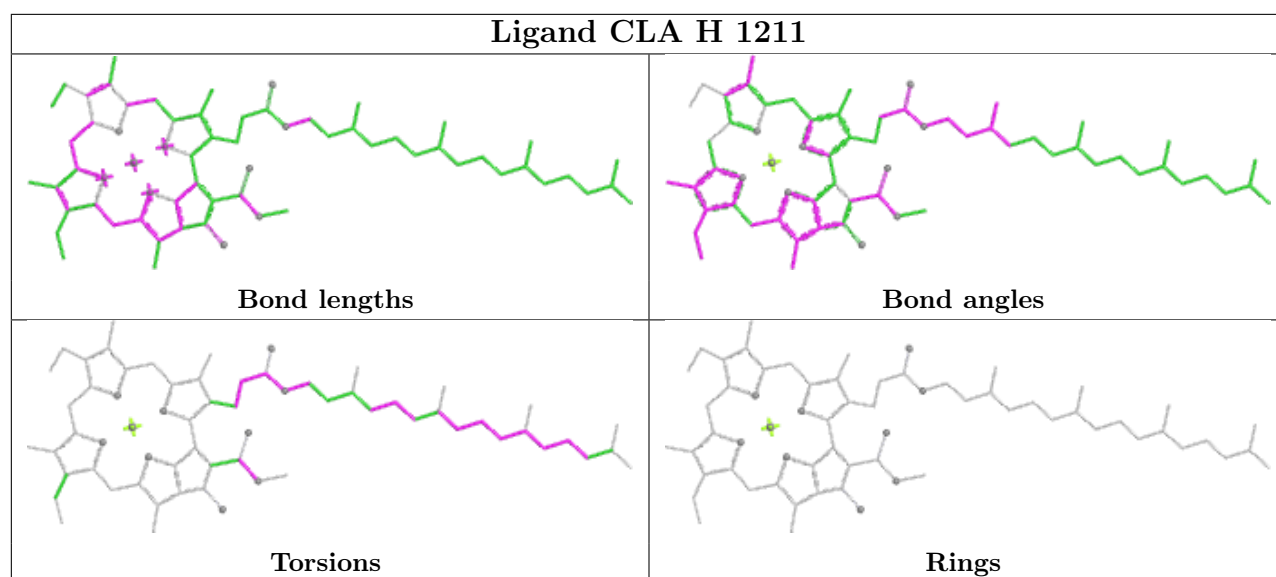


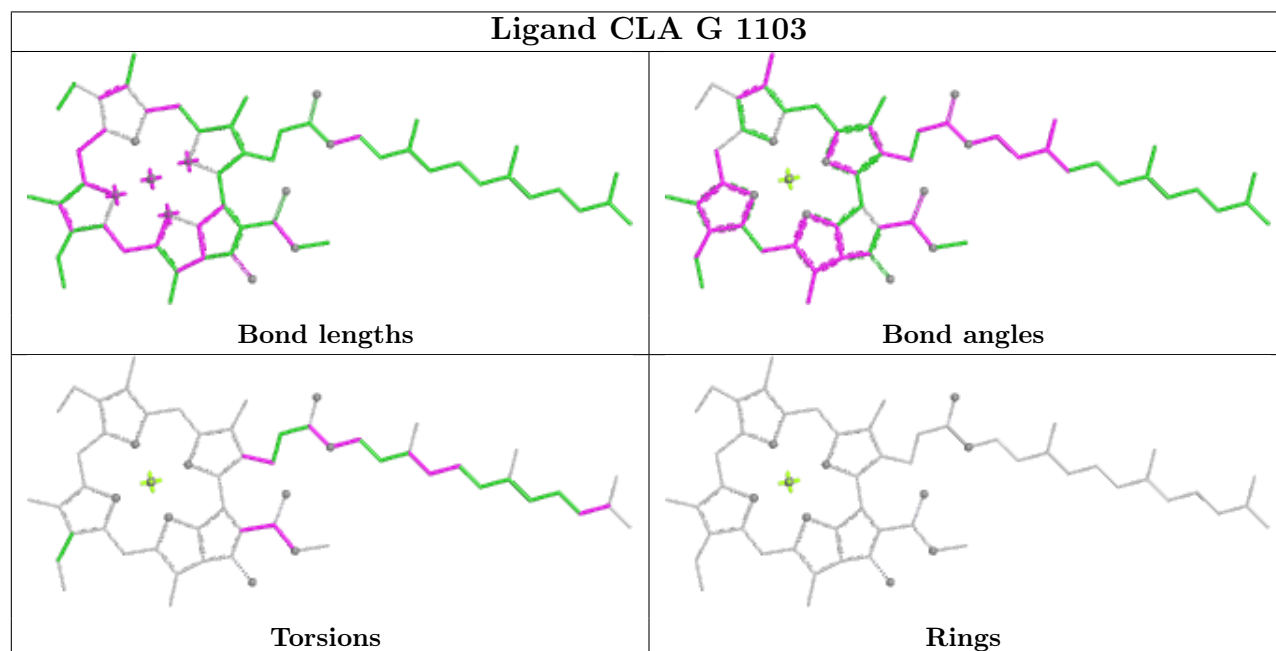
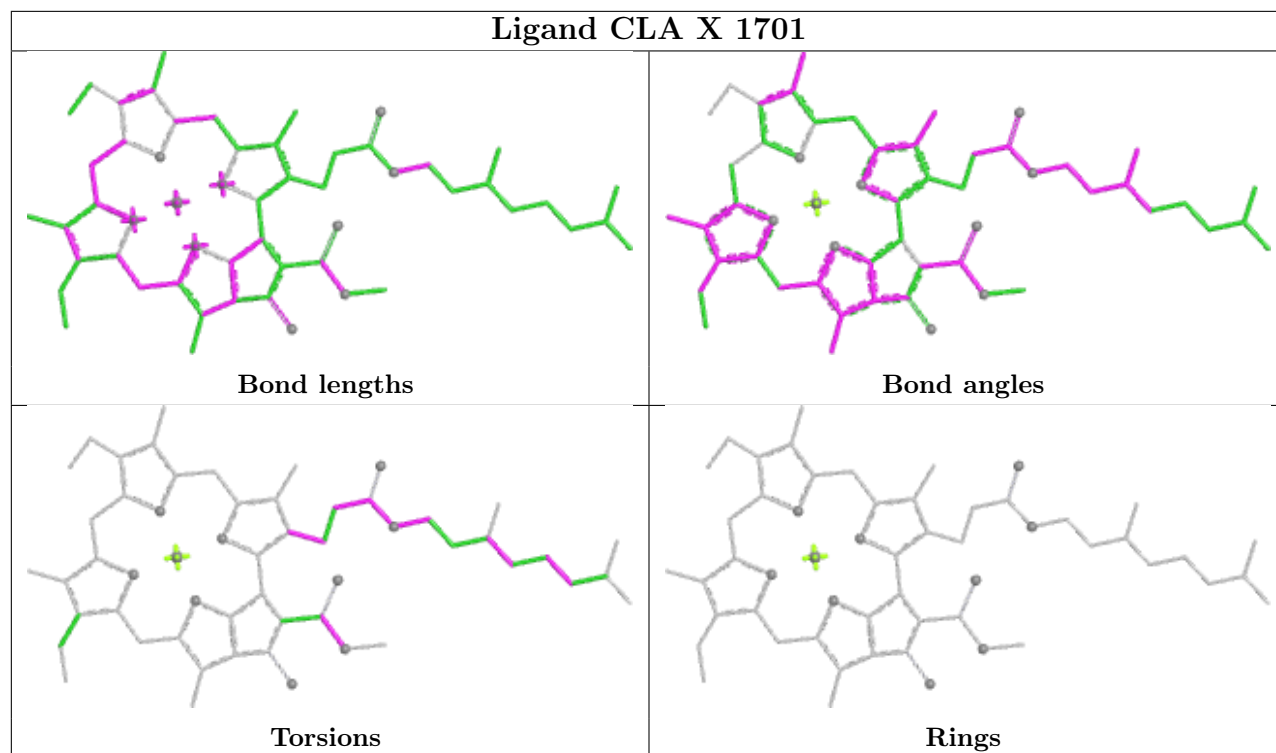
Torsions

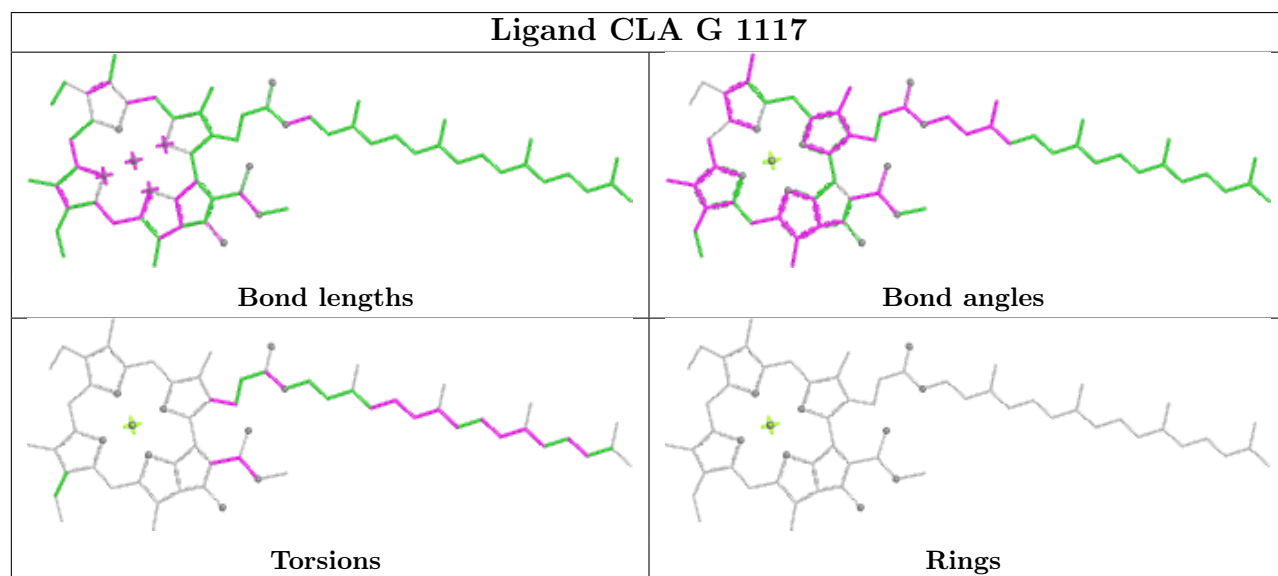
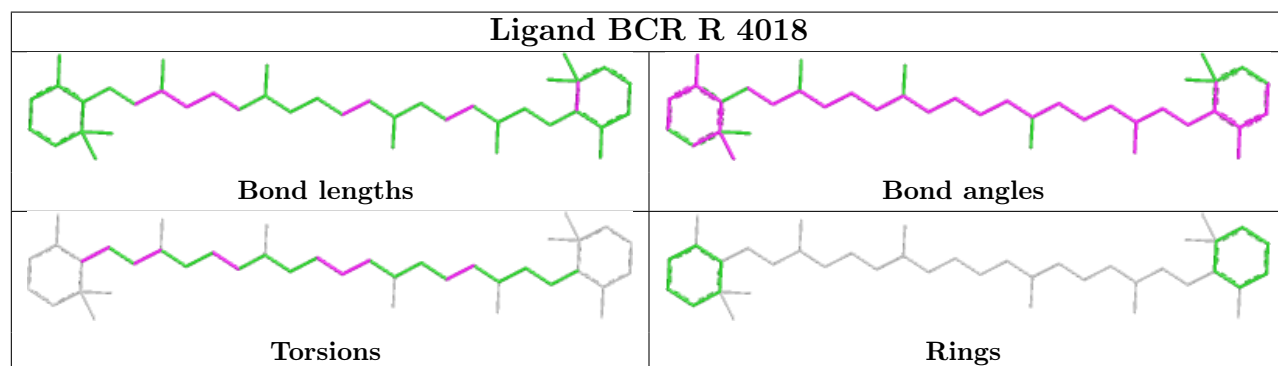
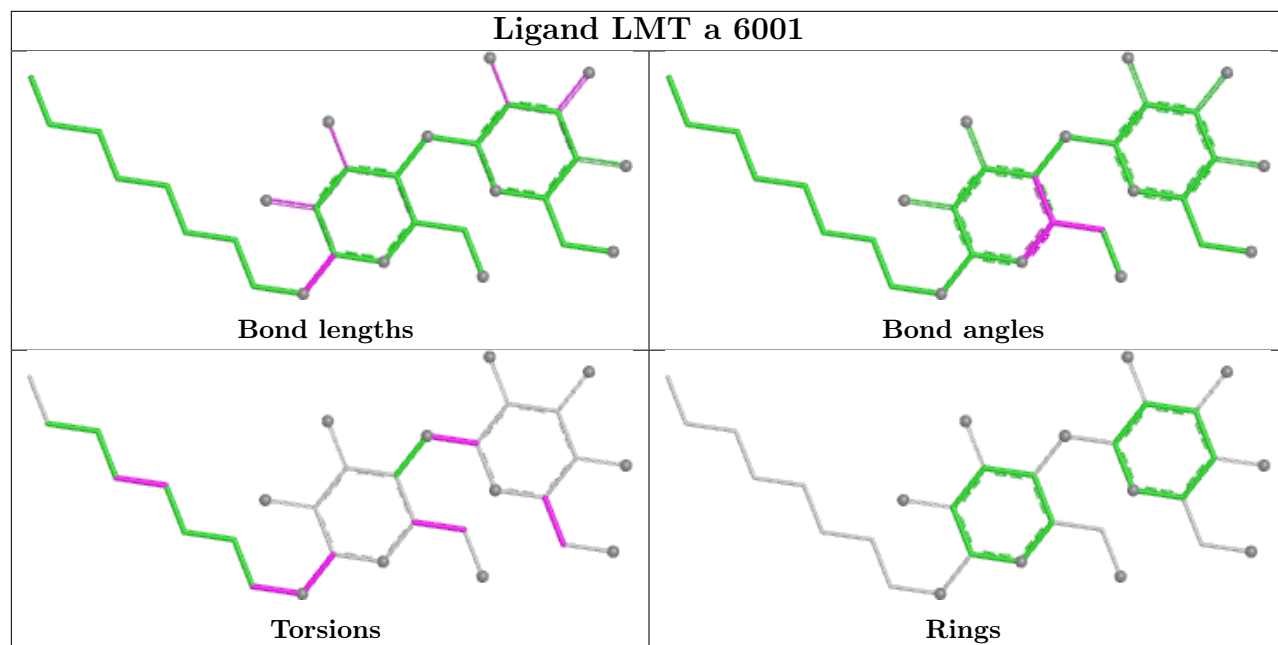


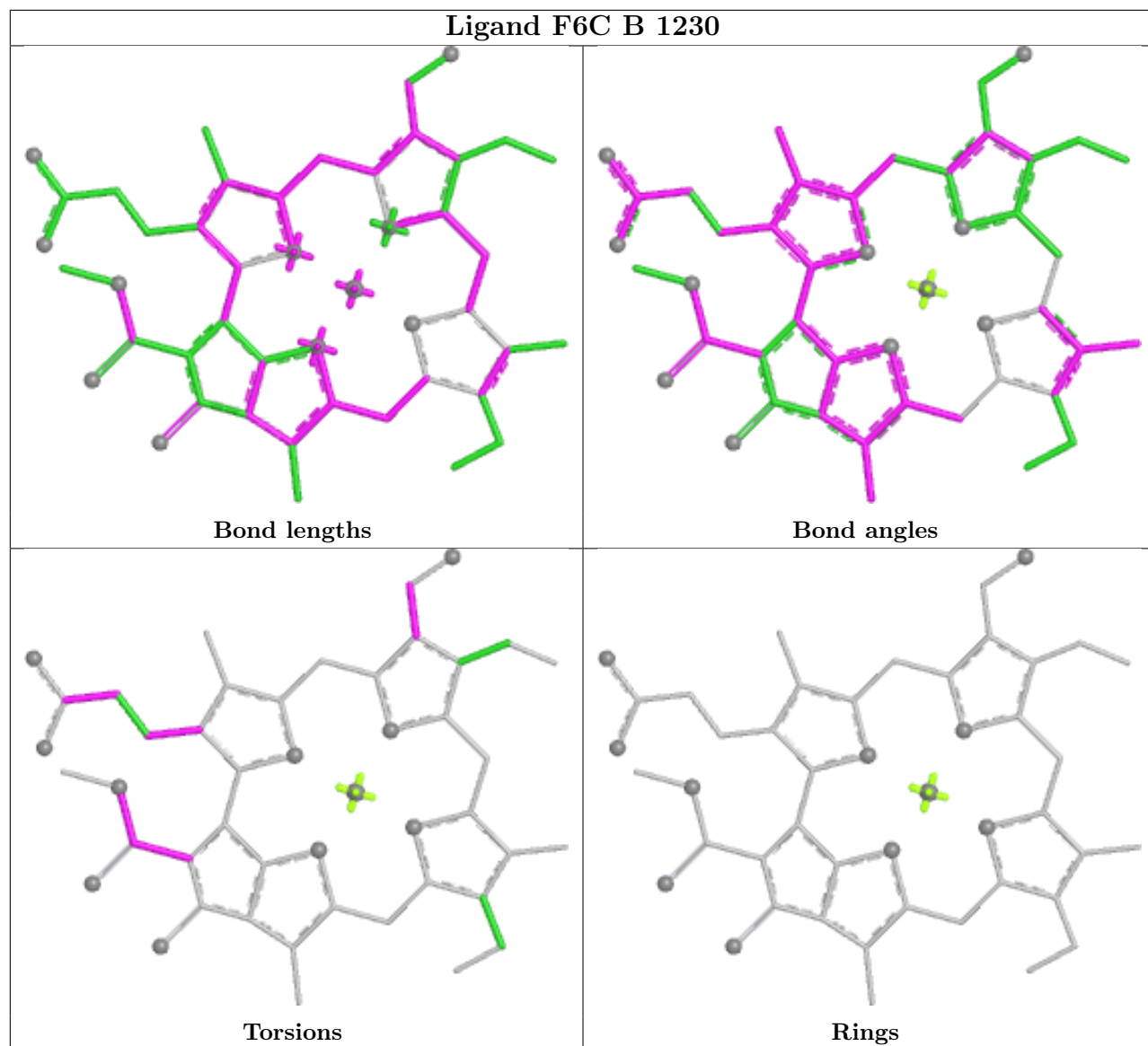
Rings



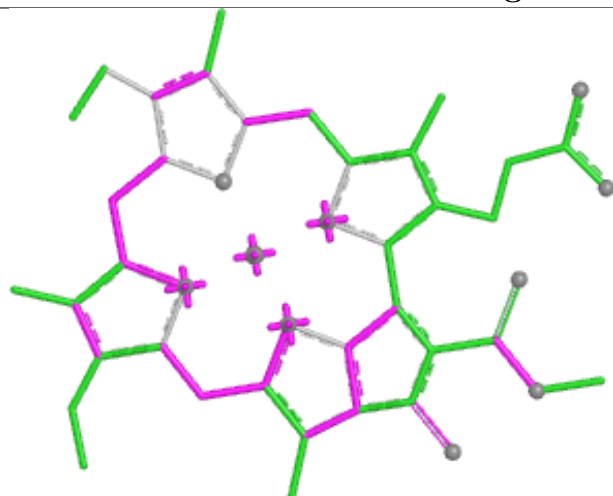




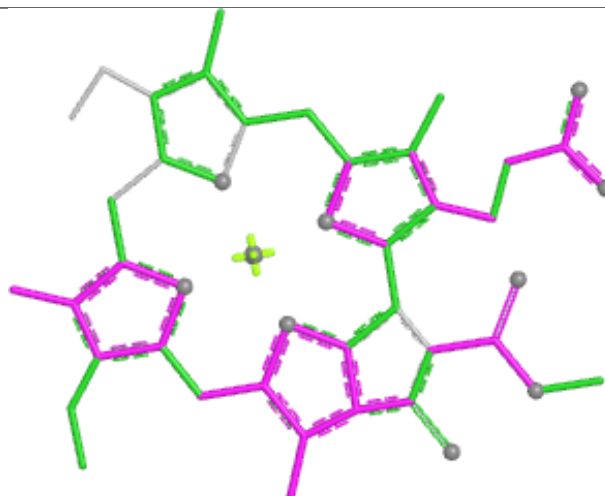




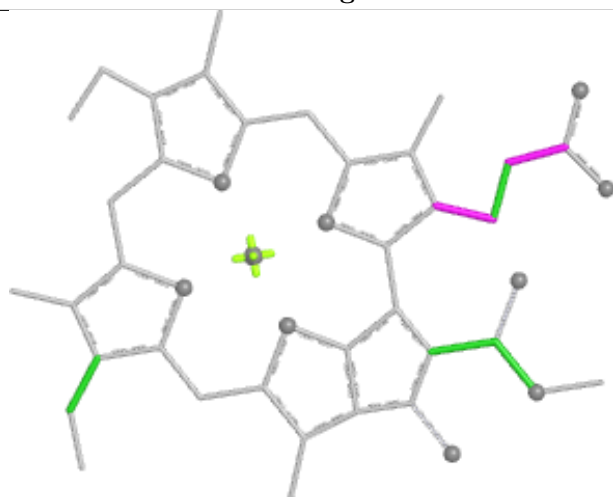
Ligand CLA H 1236



Bond lengths



Bond angles

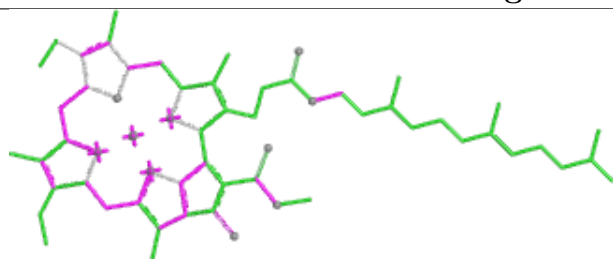


Torsions

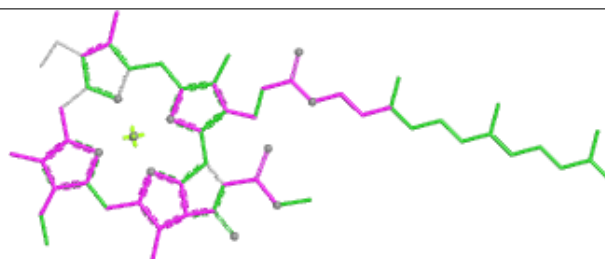


Rings

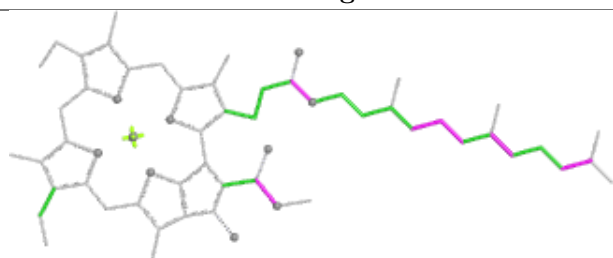
Ligand CLA A 1133



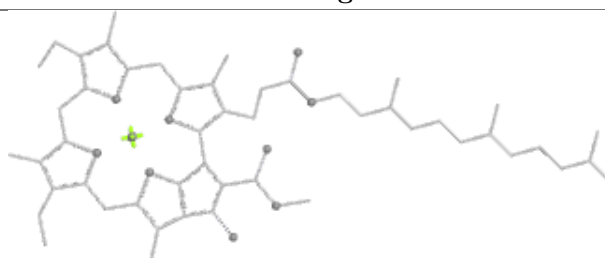
Bond lengths



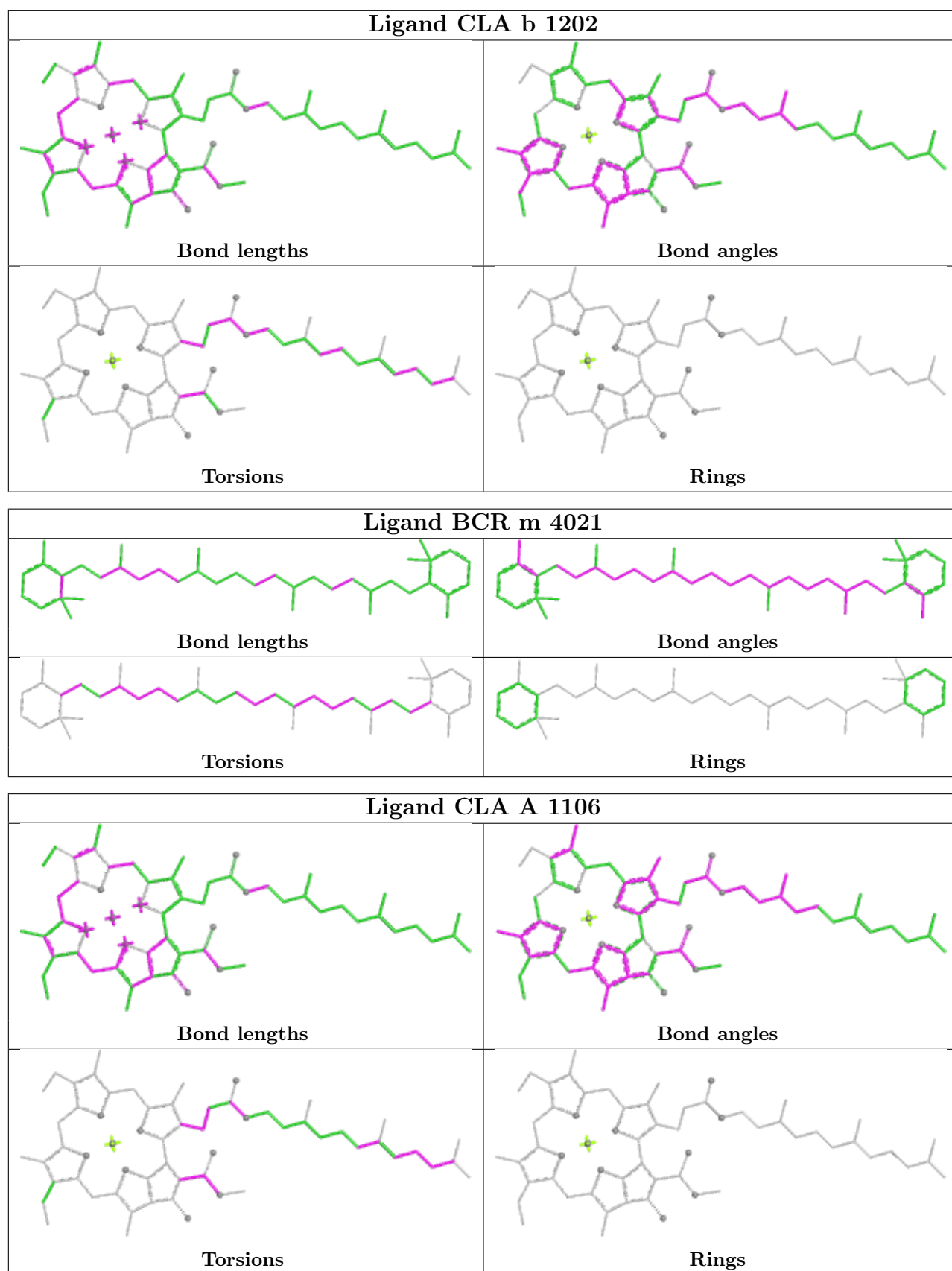
Bond angles

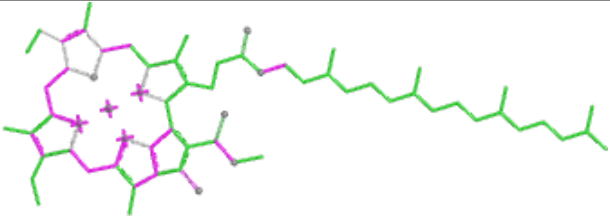
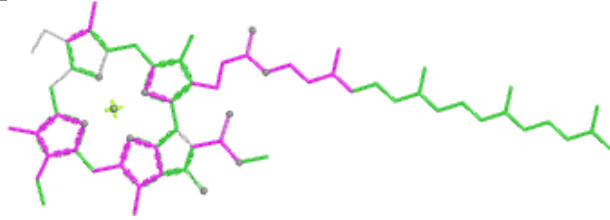
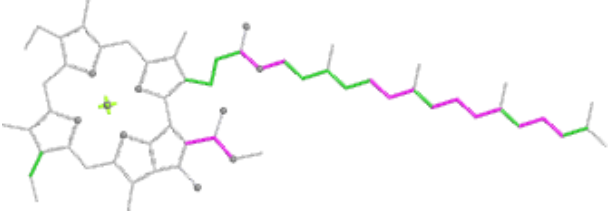
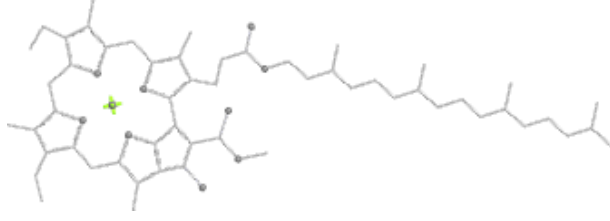
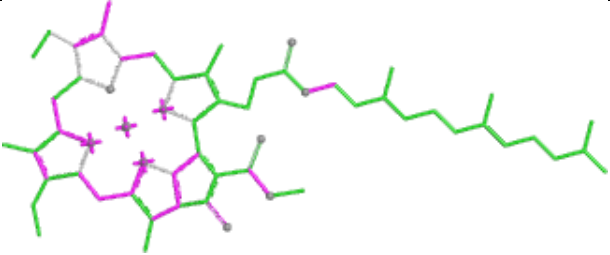
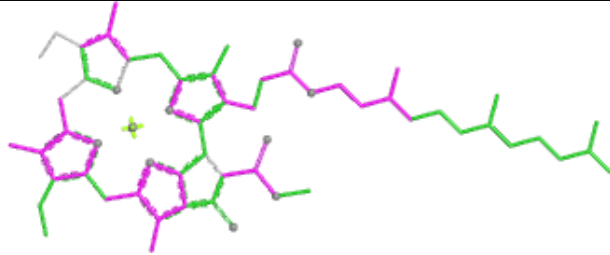
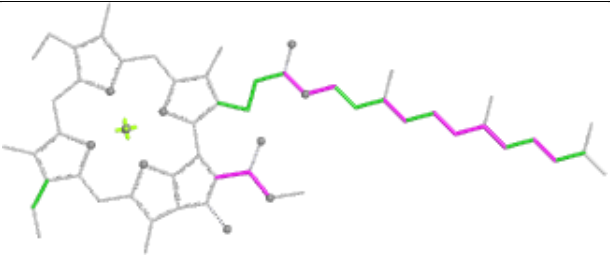
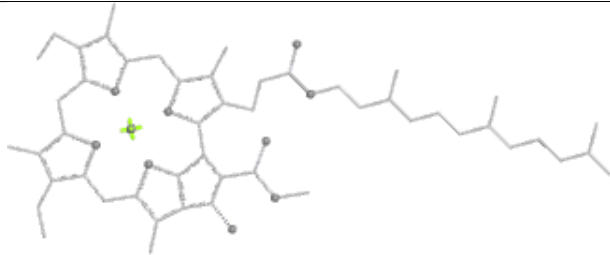
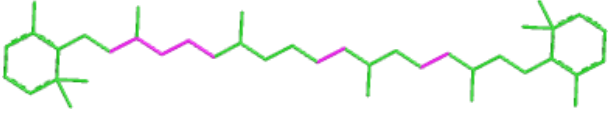
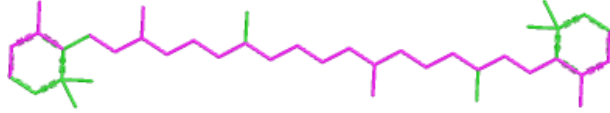
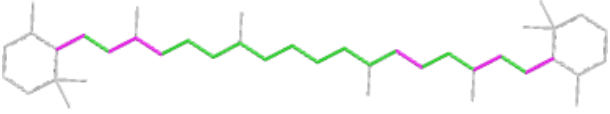
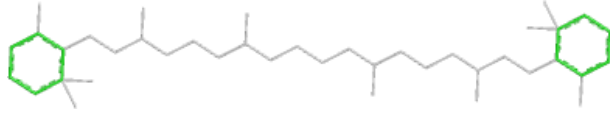


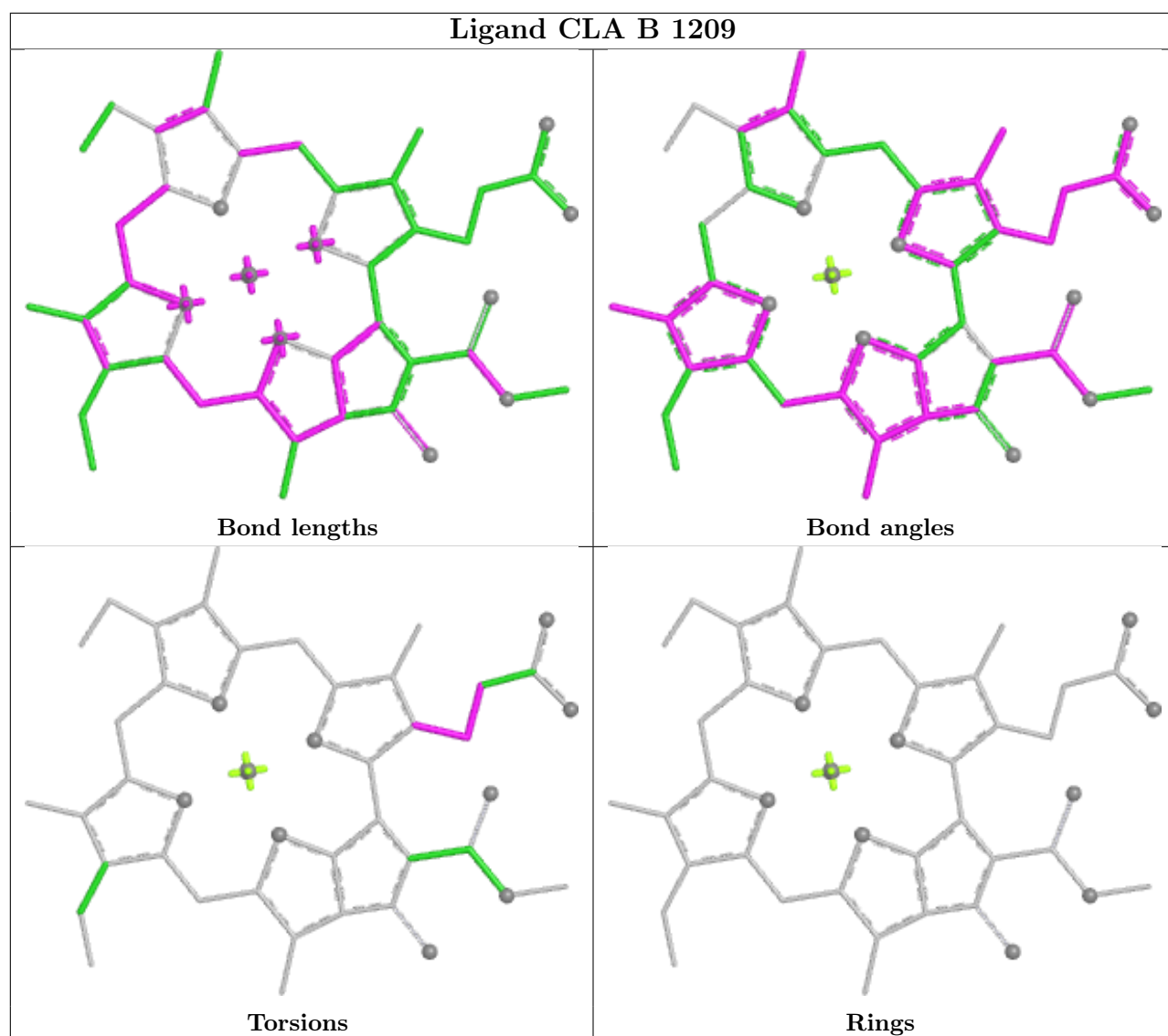
Torsions

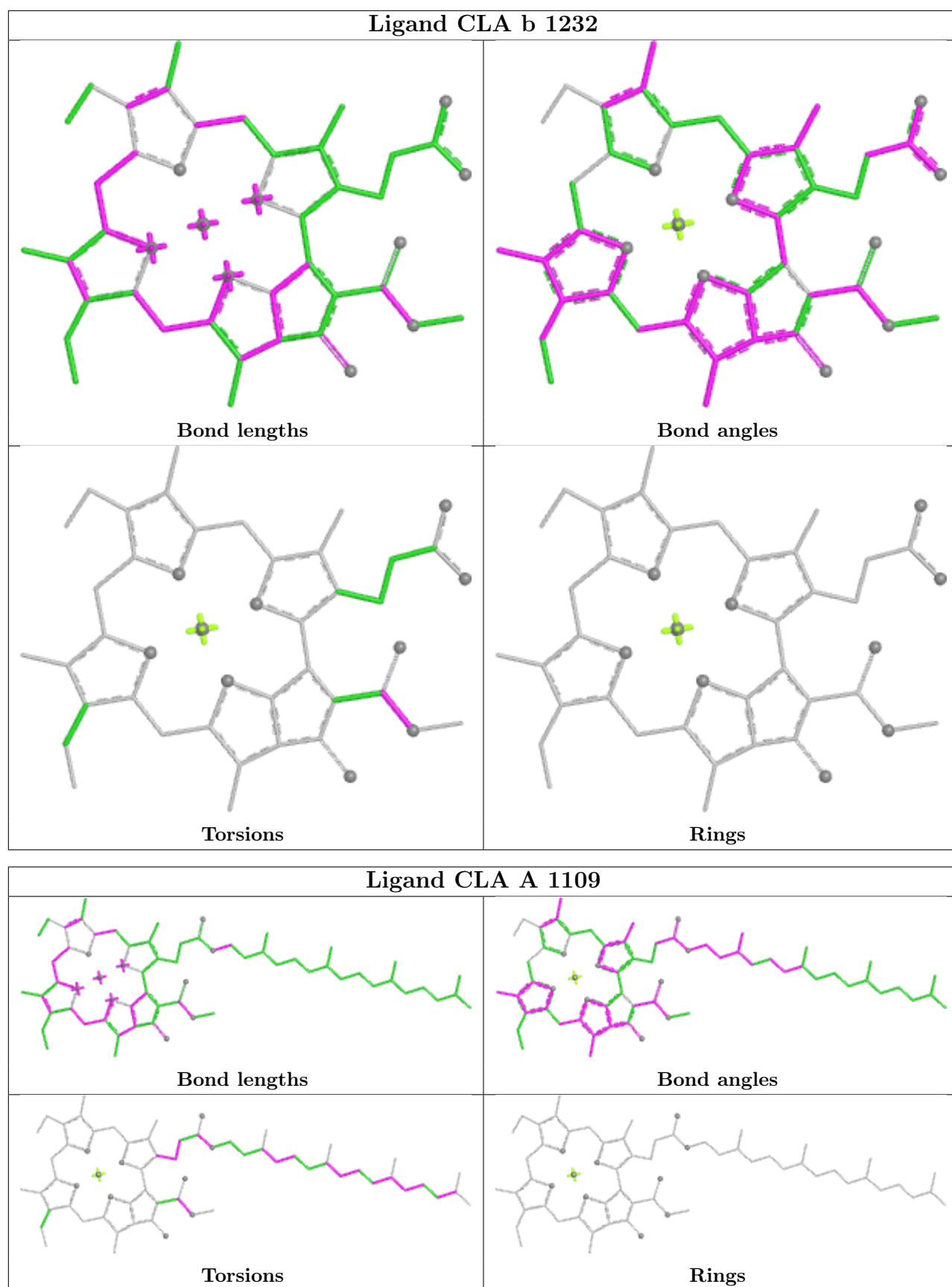


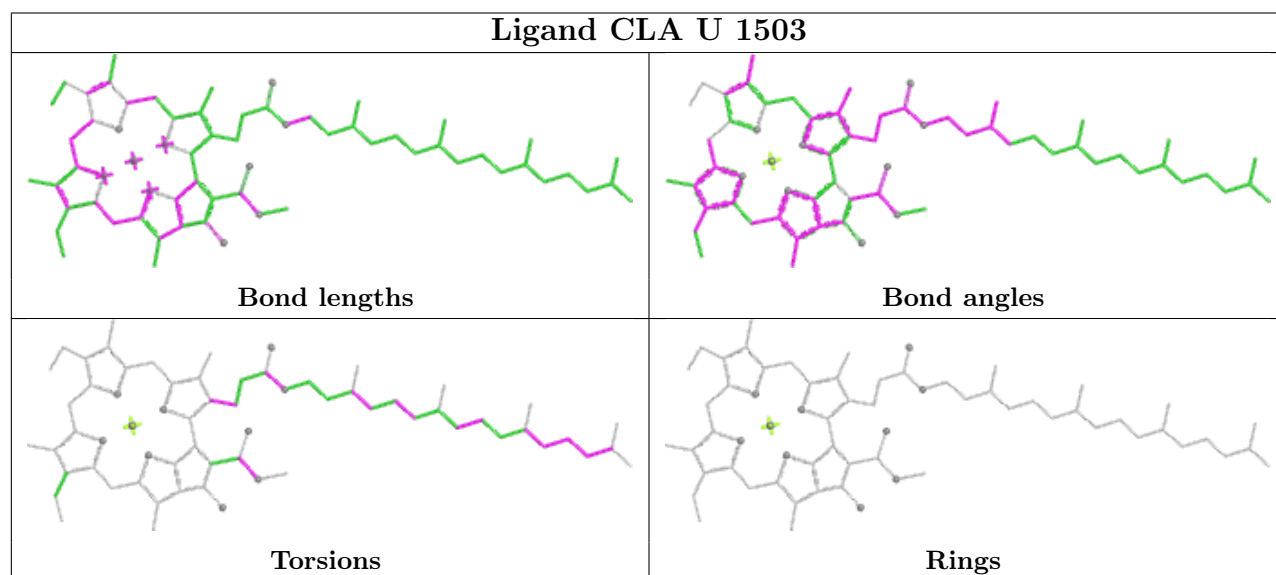
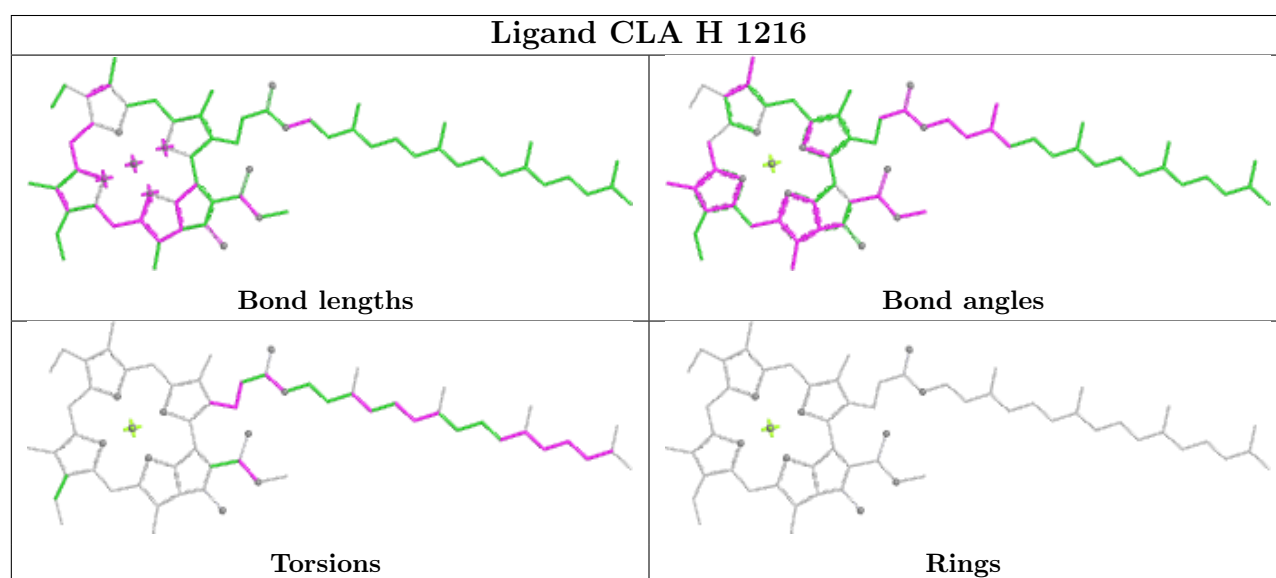
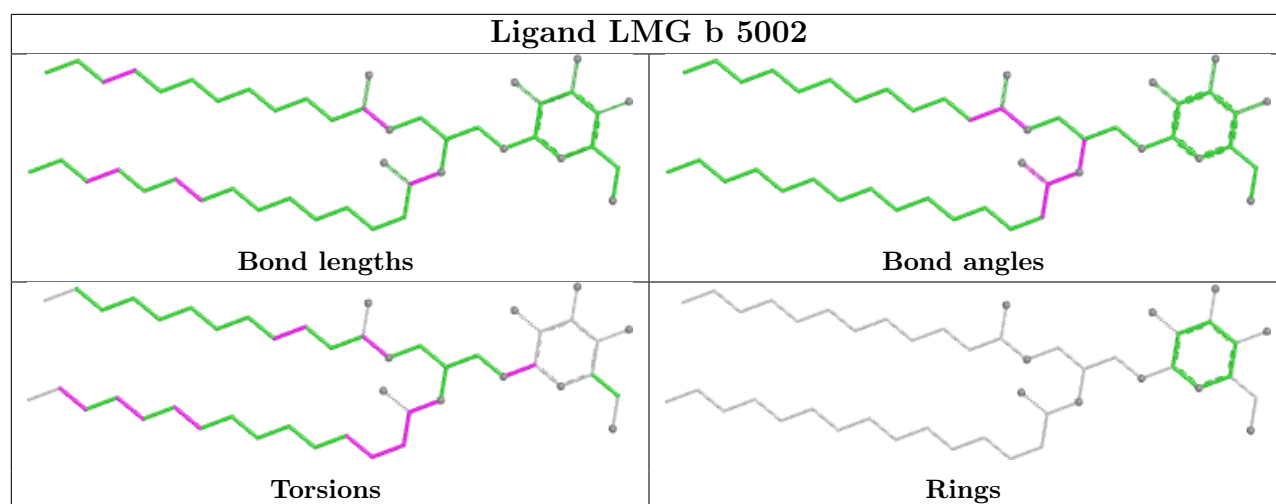
Rings

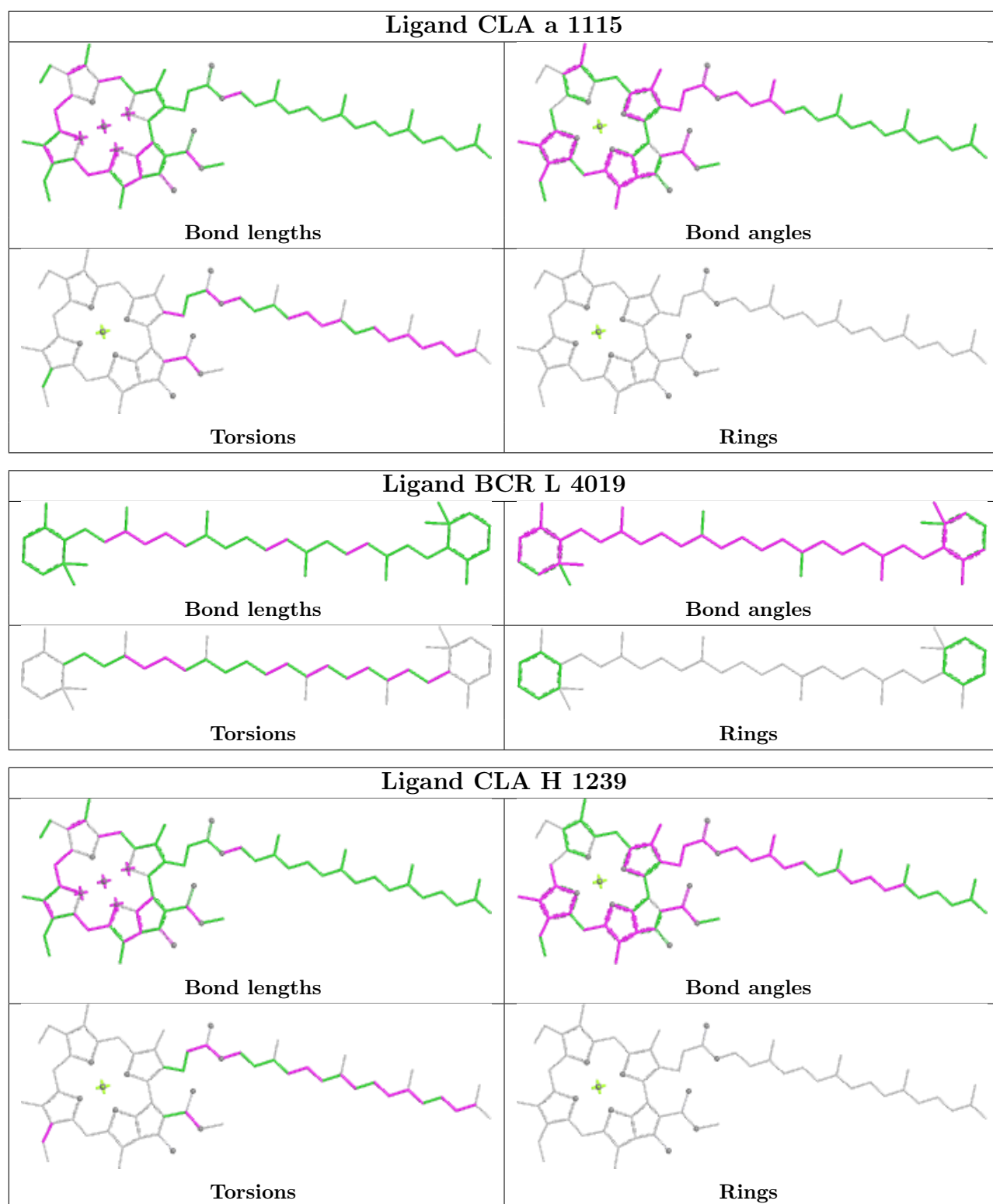


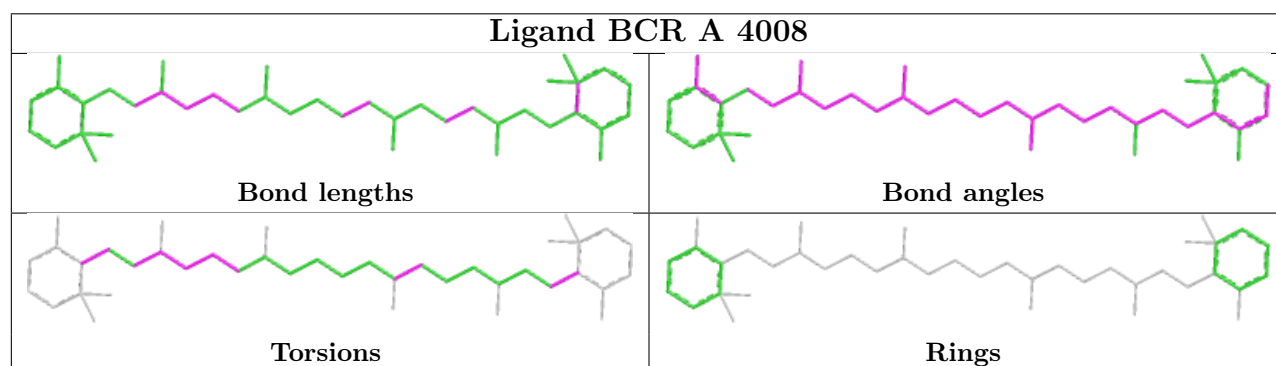
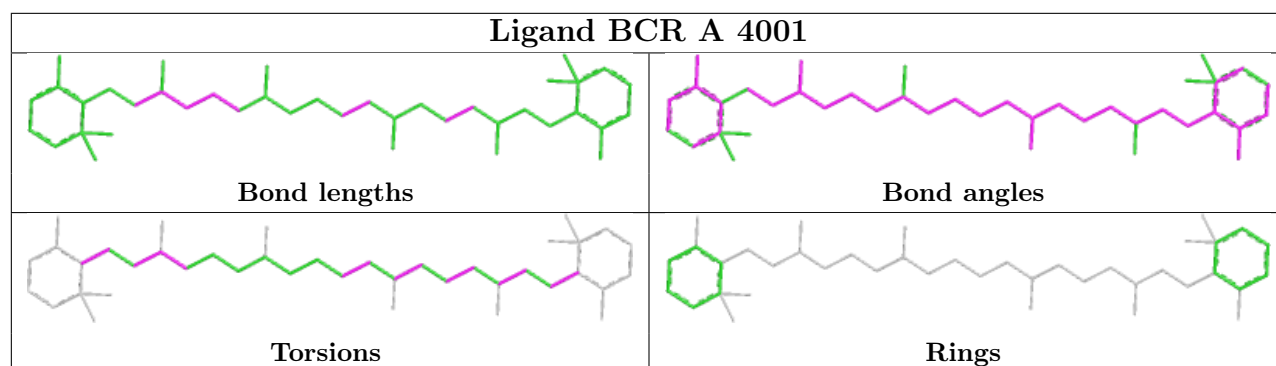
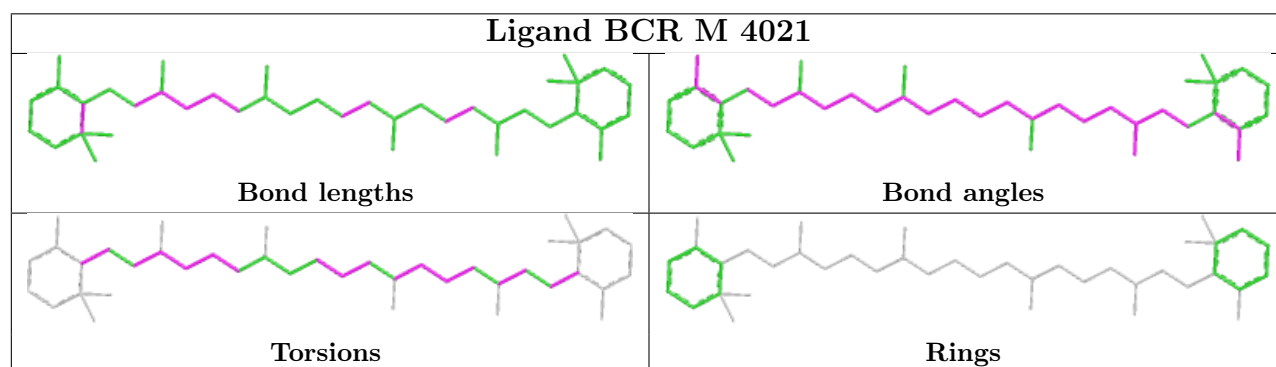
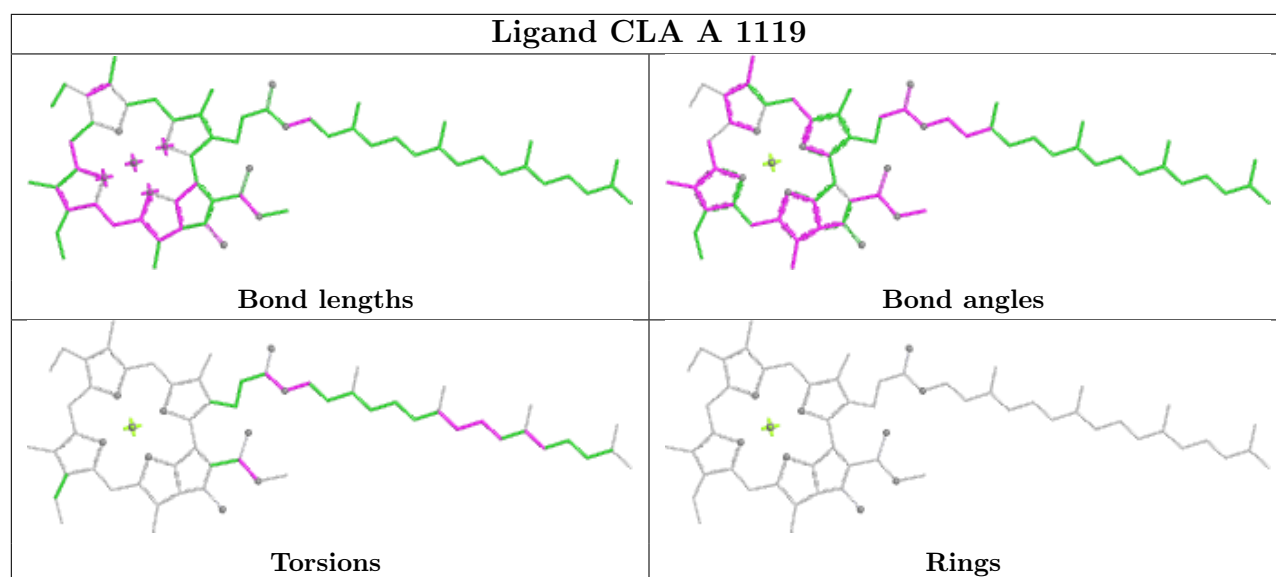
Ligand CLA B 1234	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA a 1128	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR B 4006	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

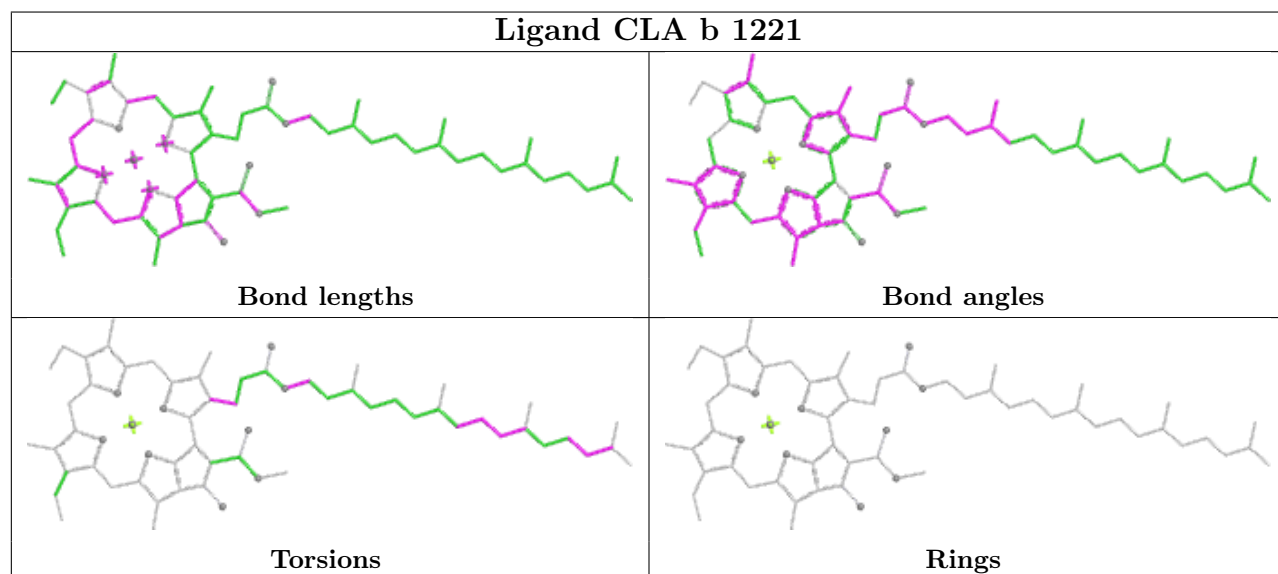
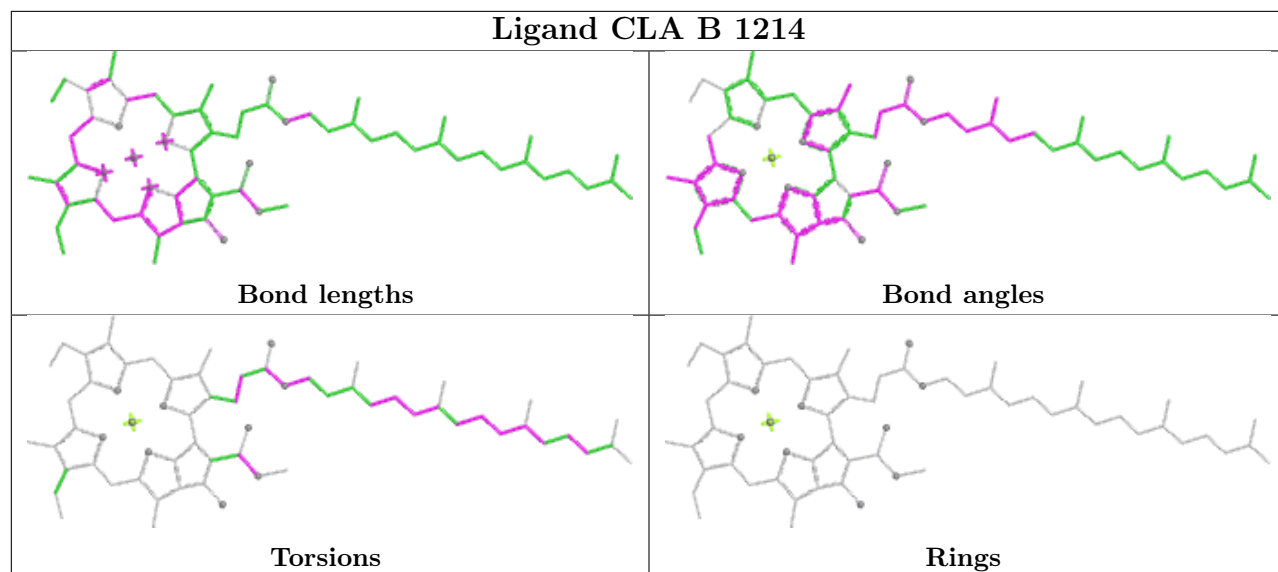


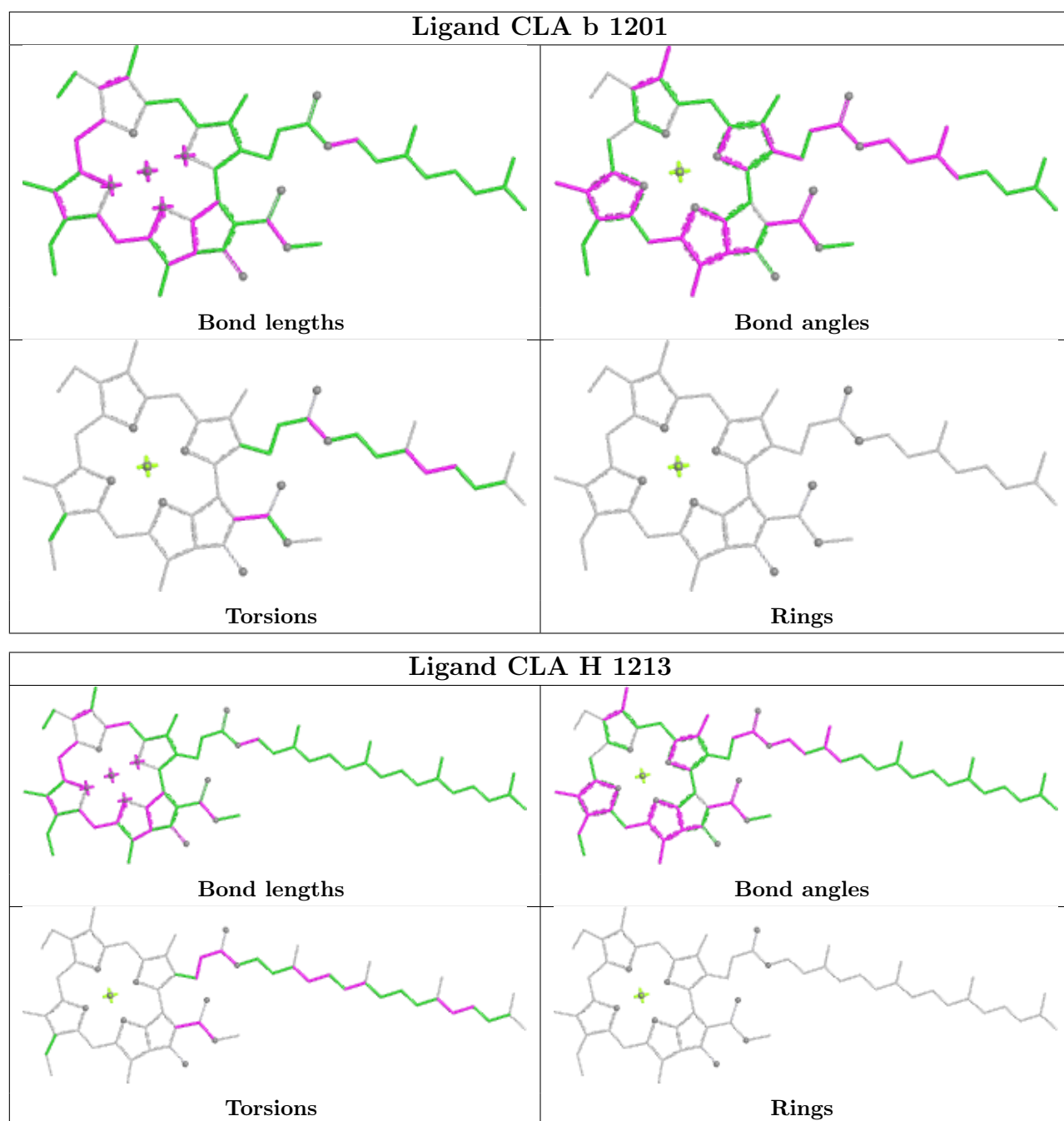


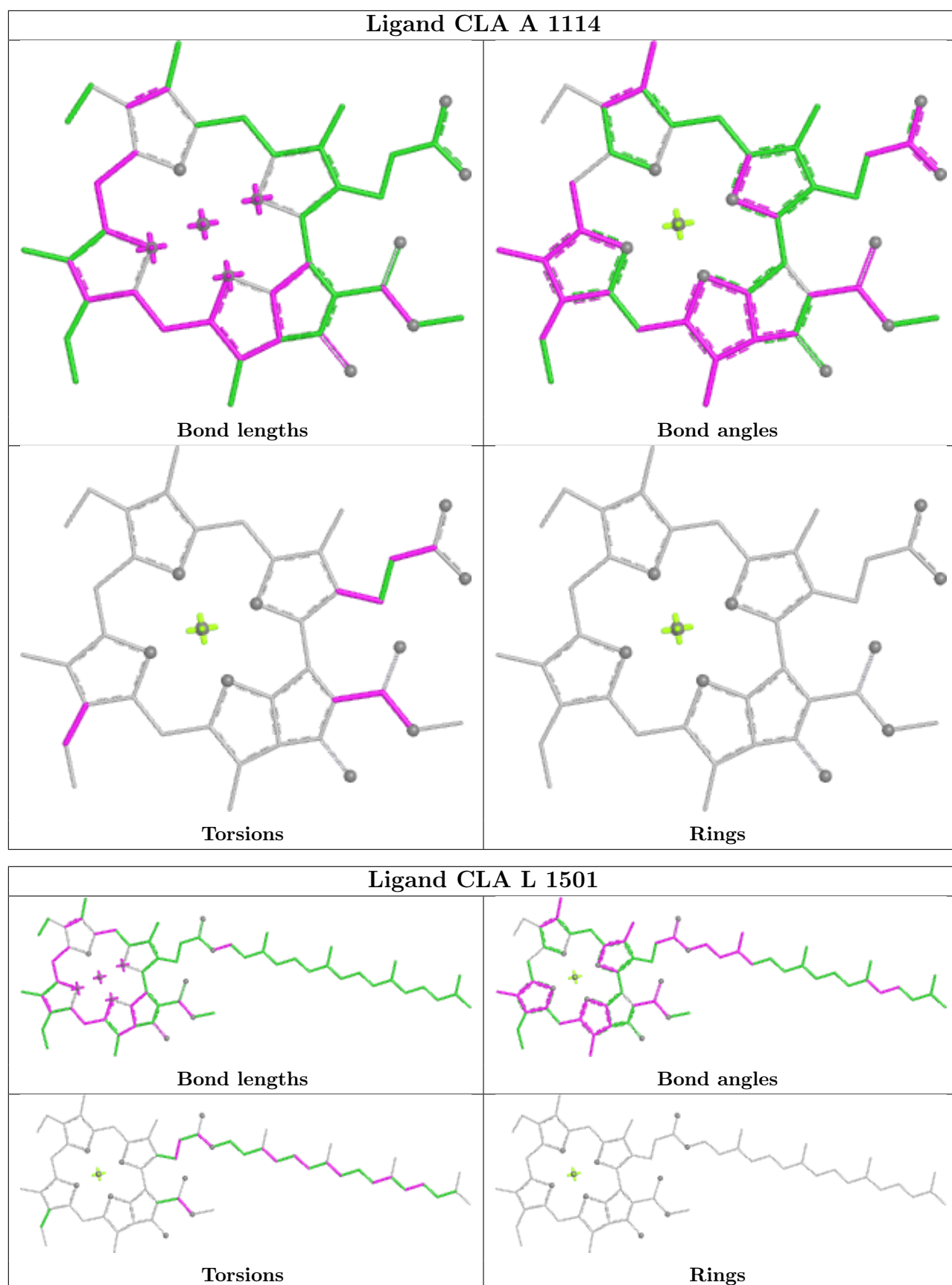


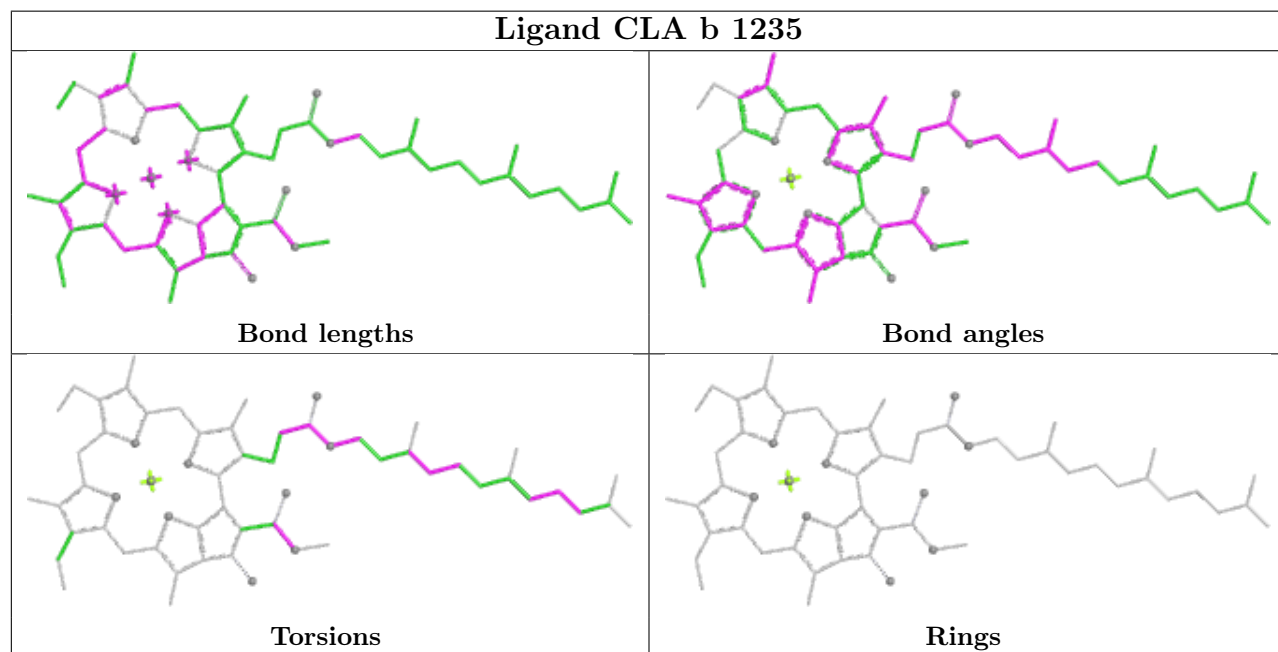
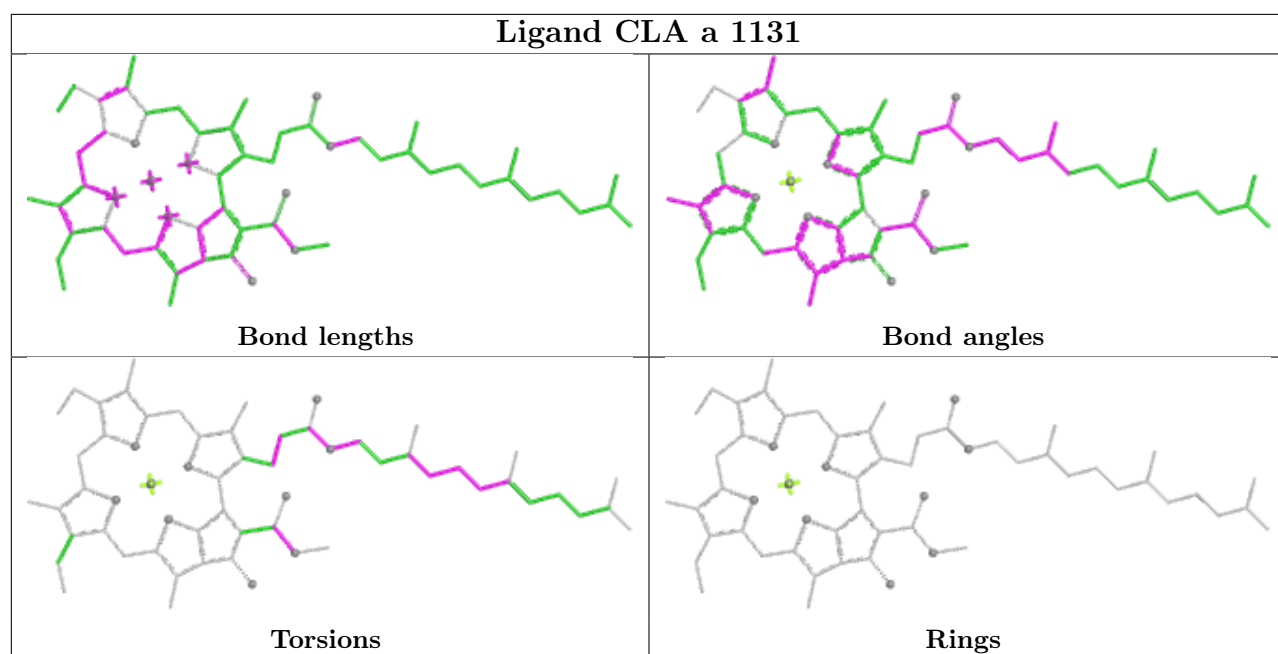


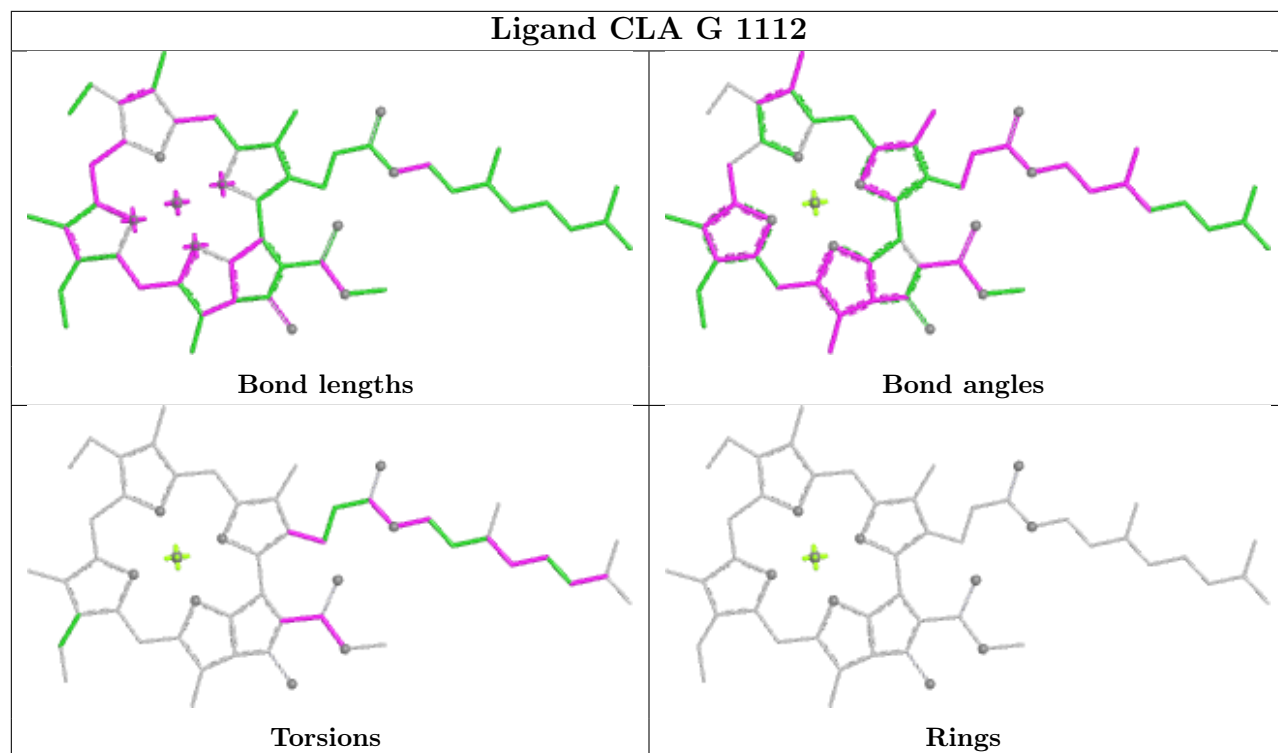


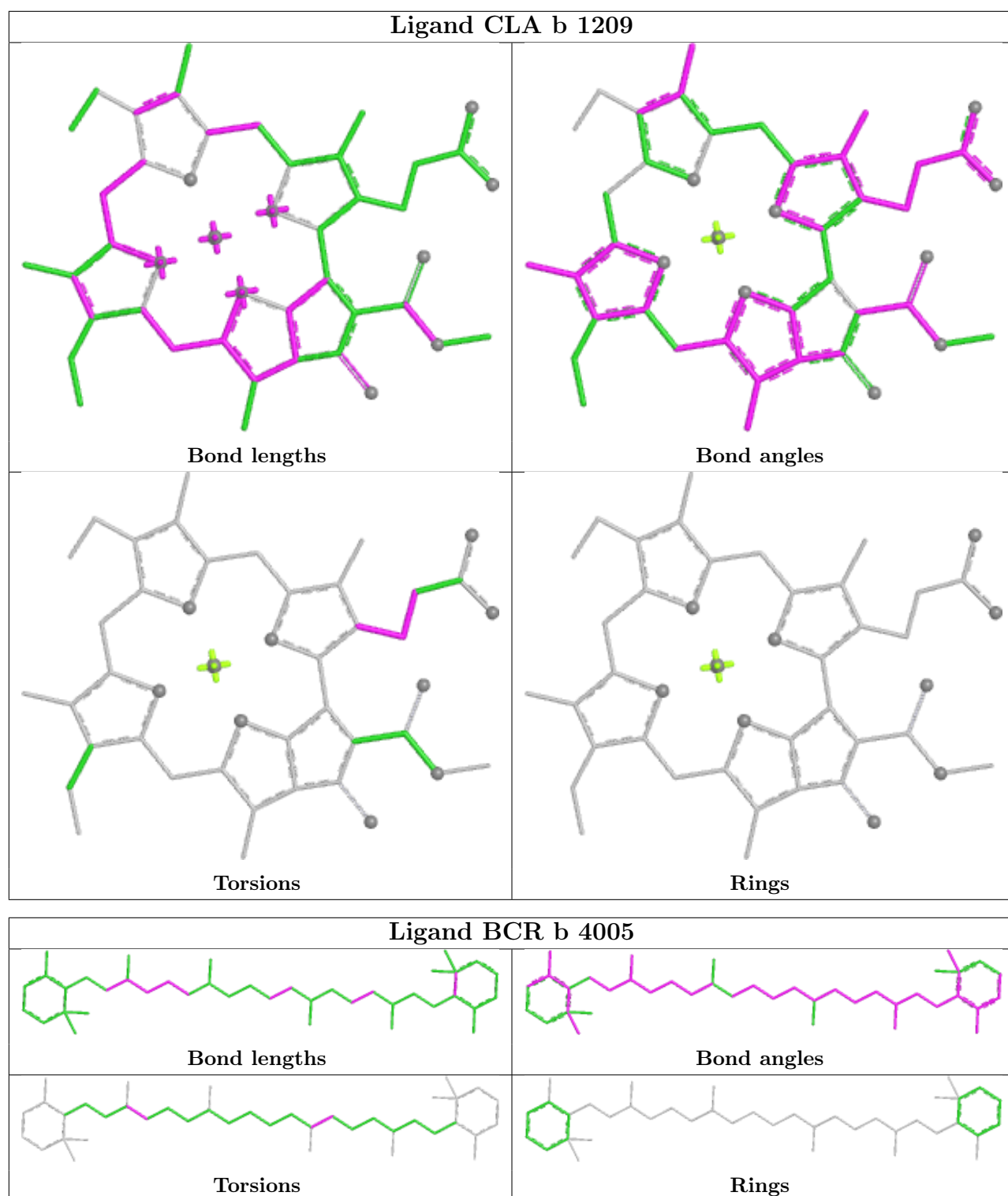


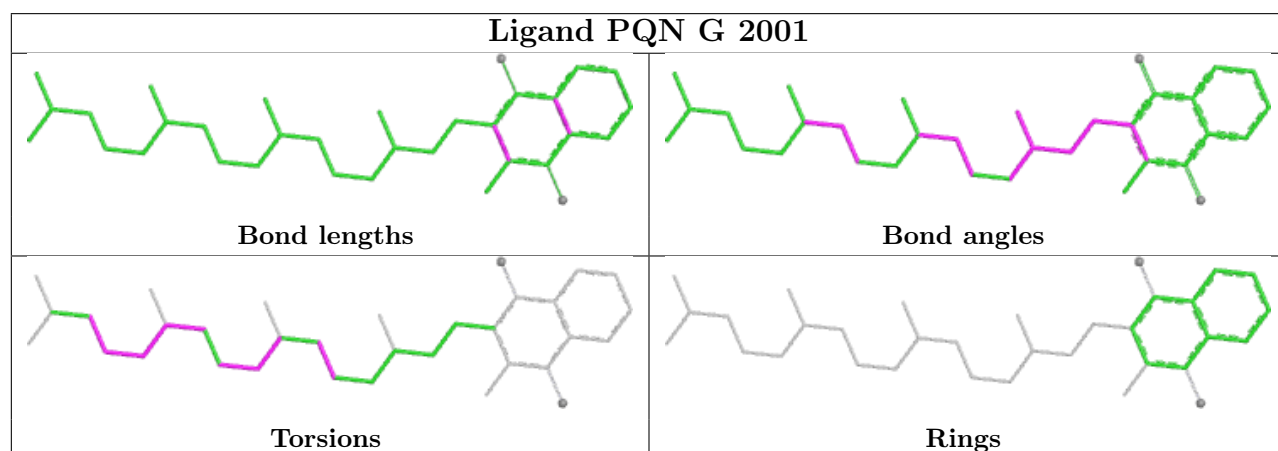
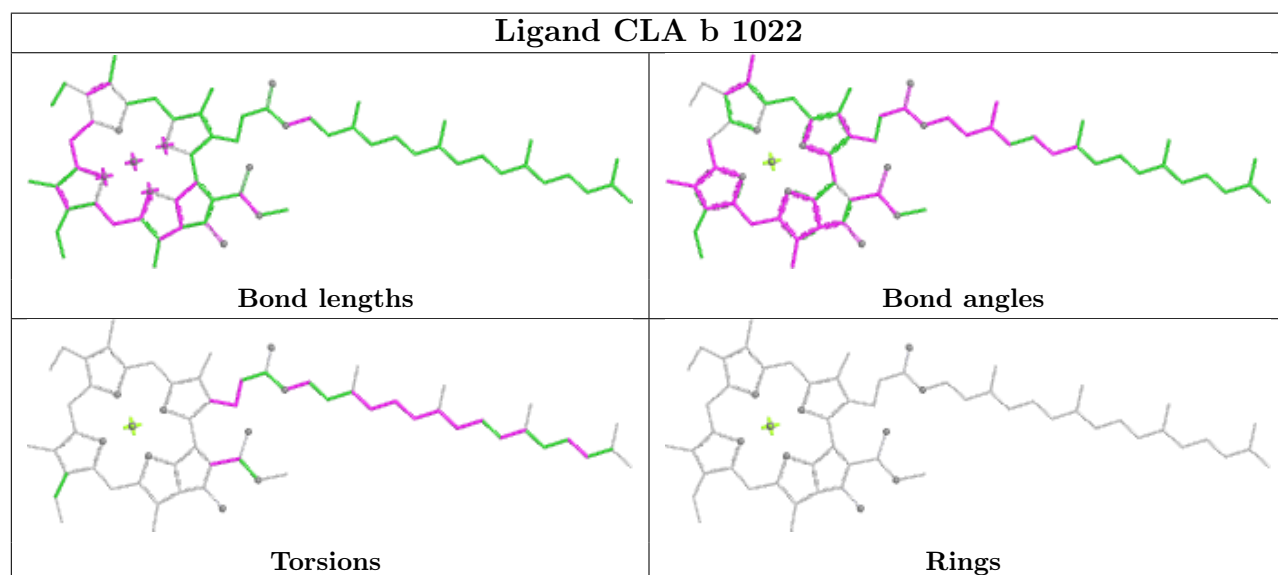
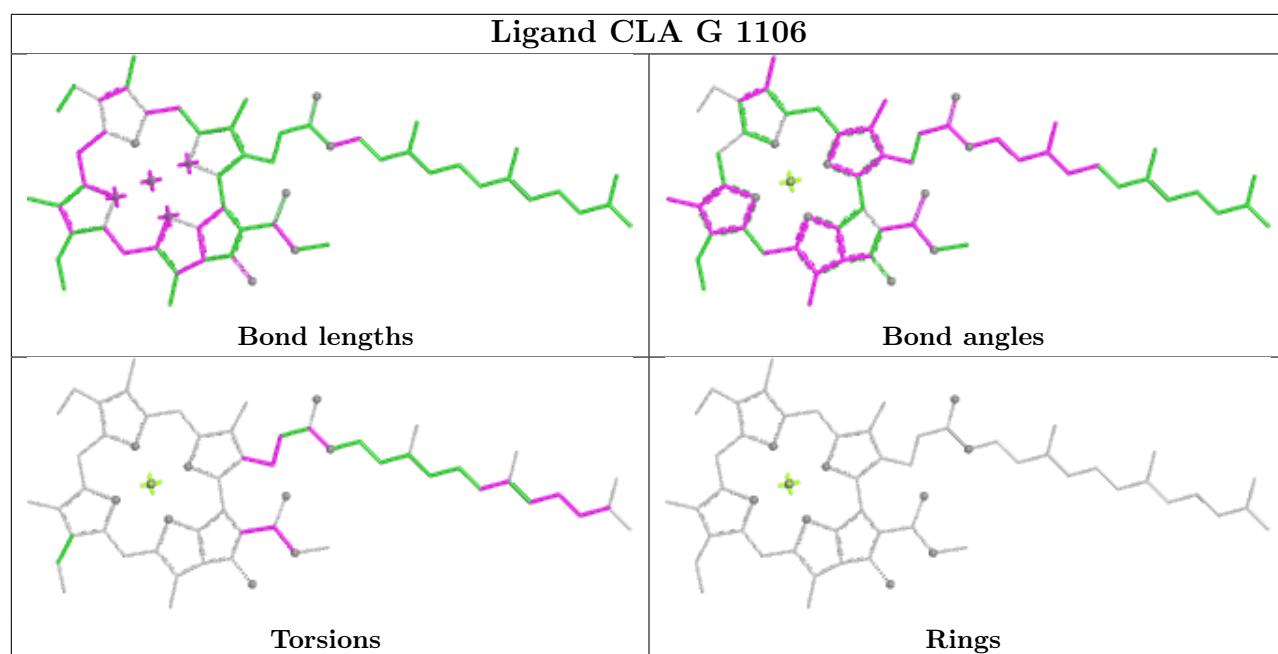


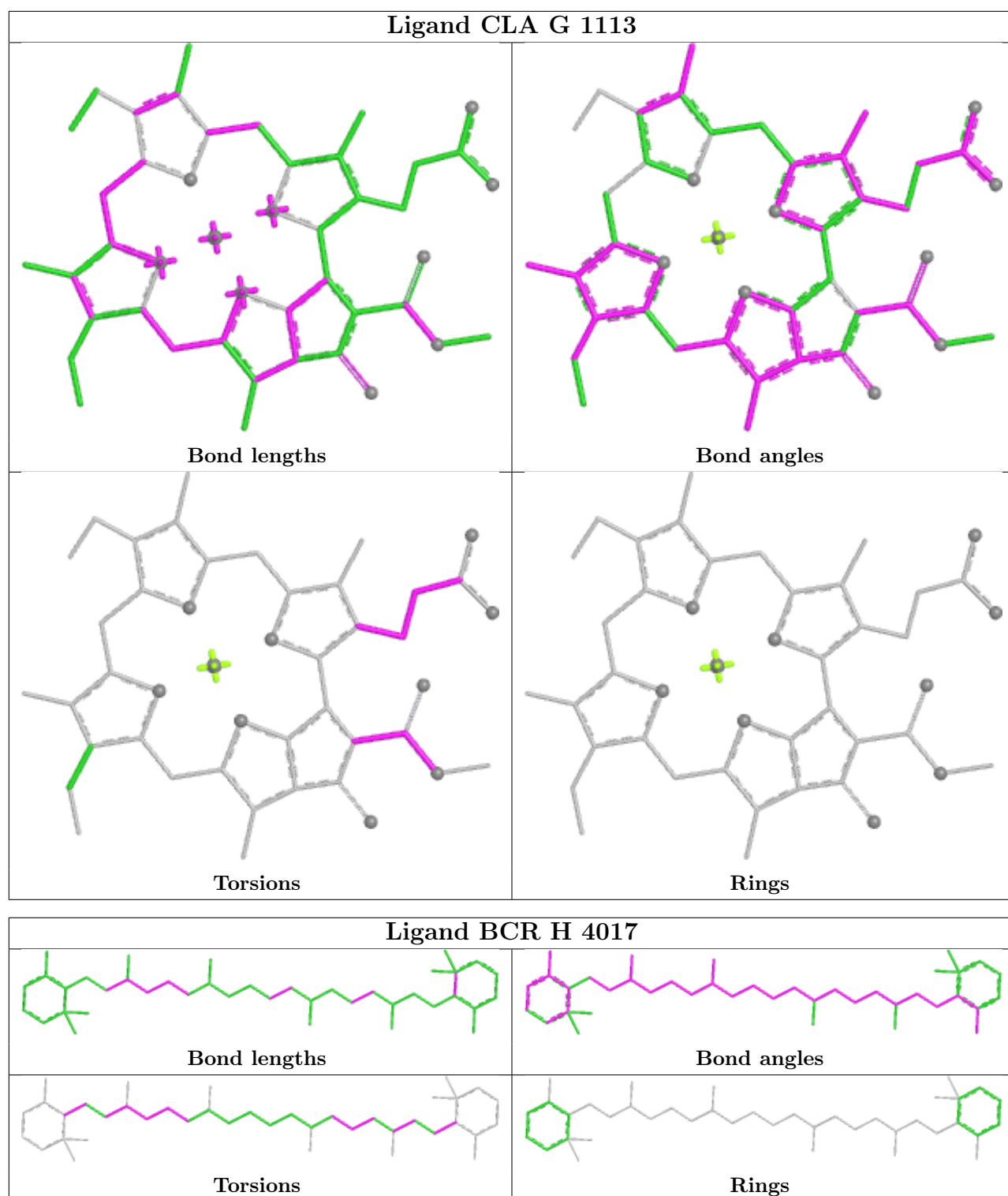


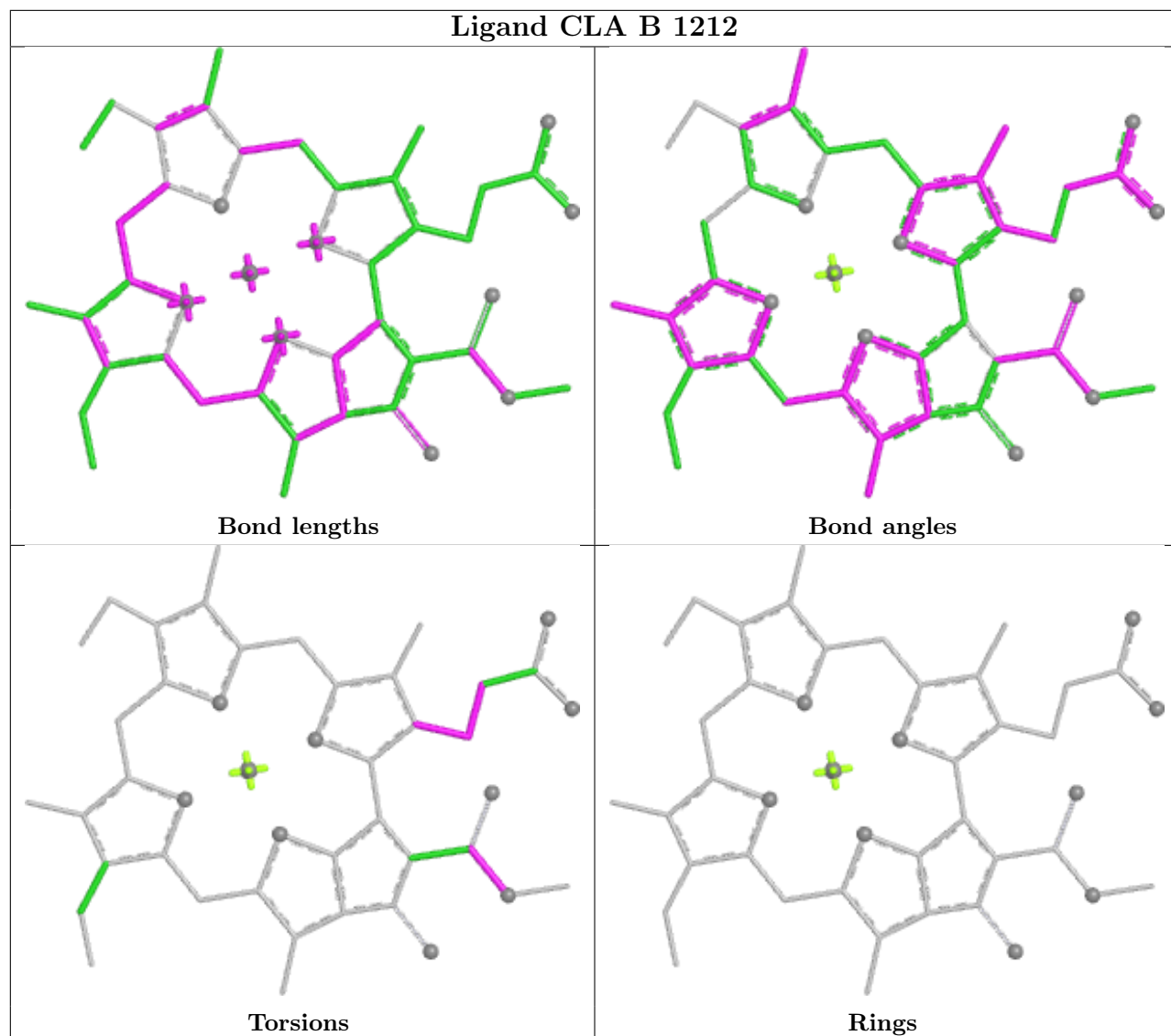




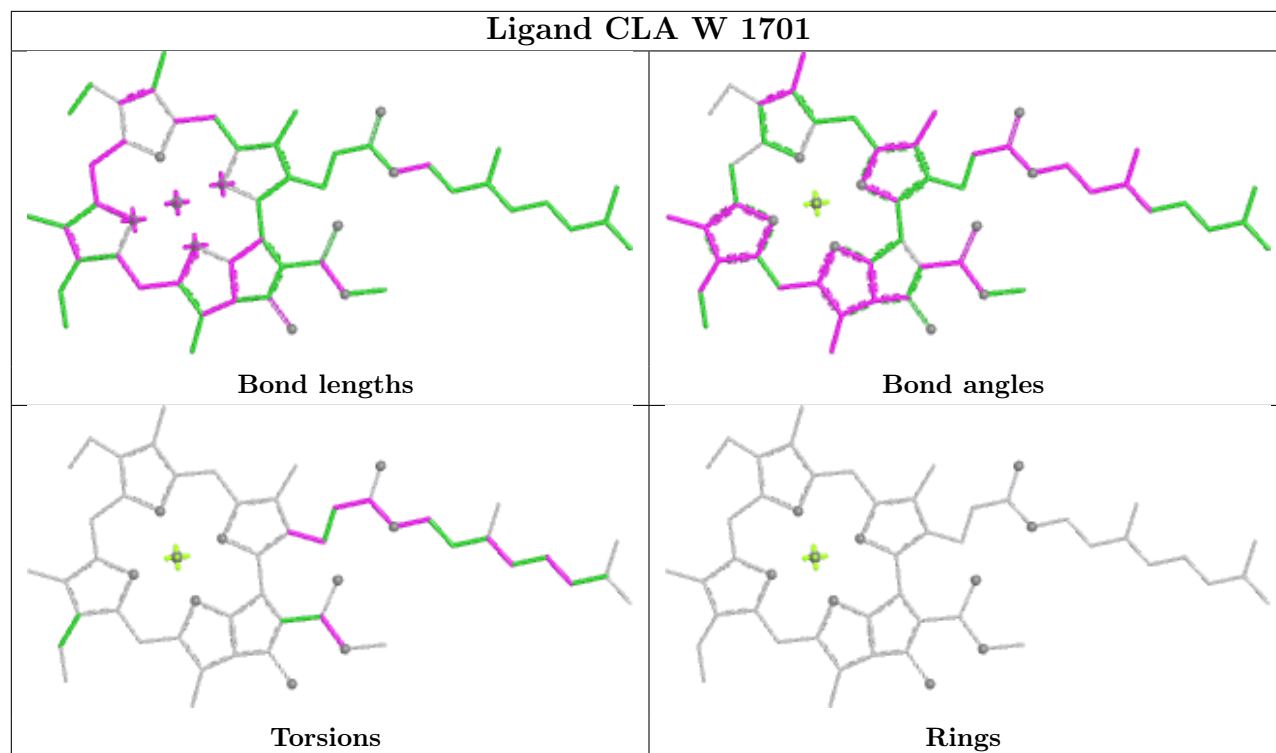




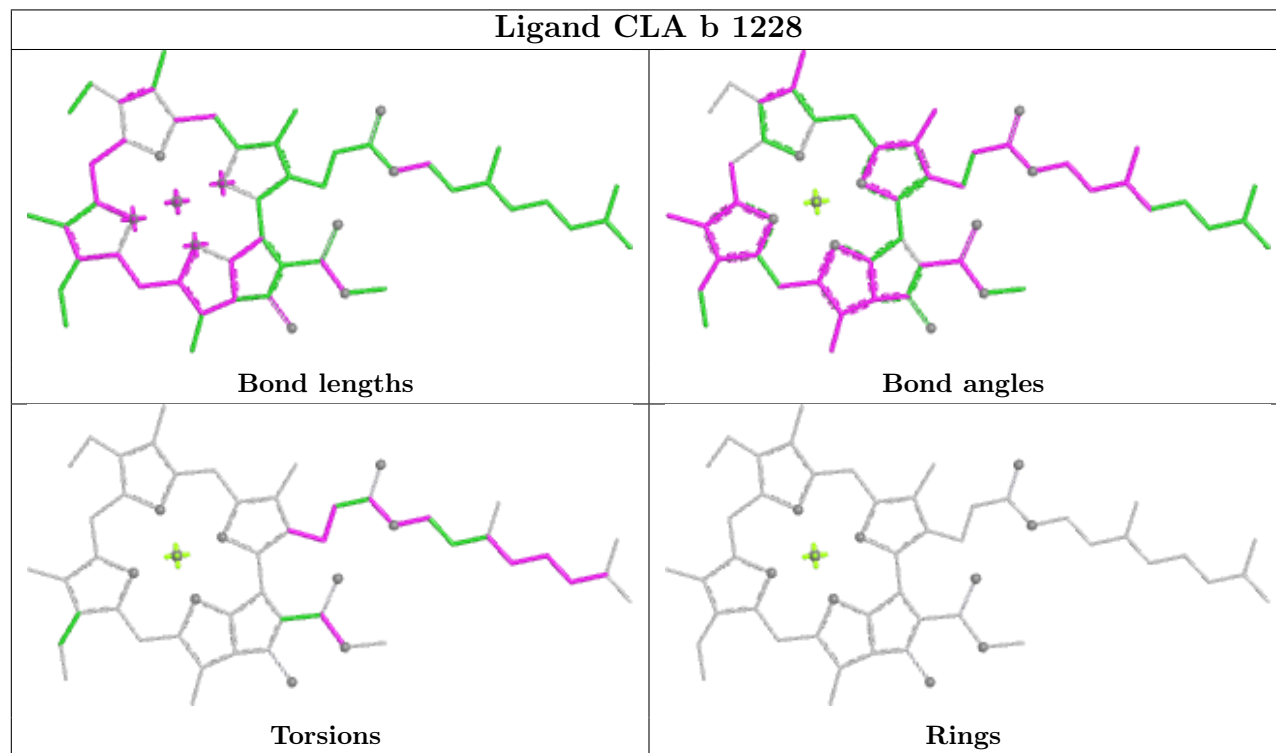


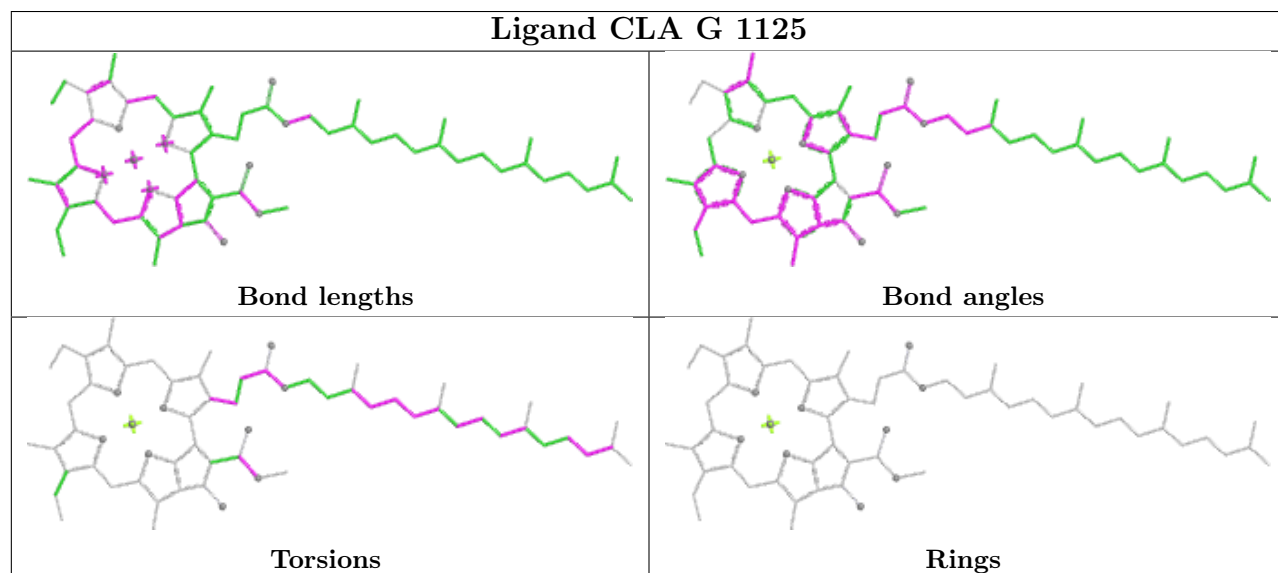
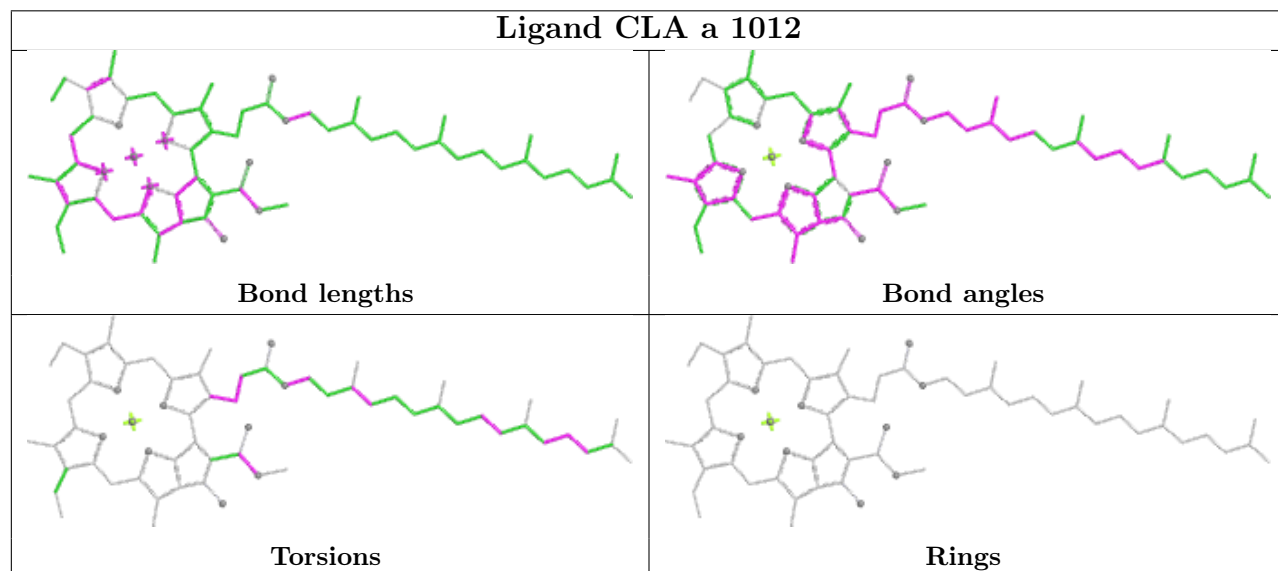
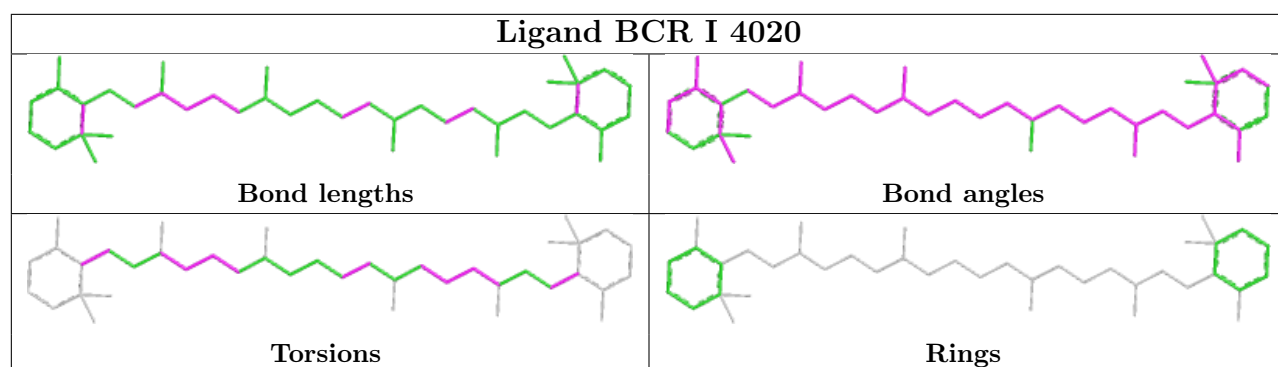


Ligand CLA W 1701

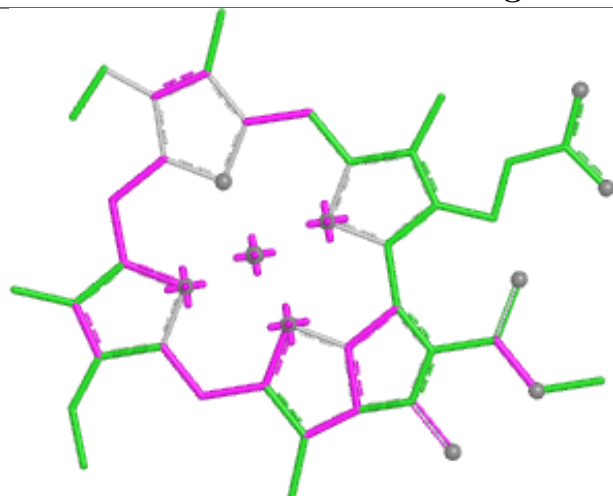


Ligand CLA b 1228

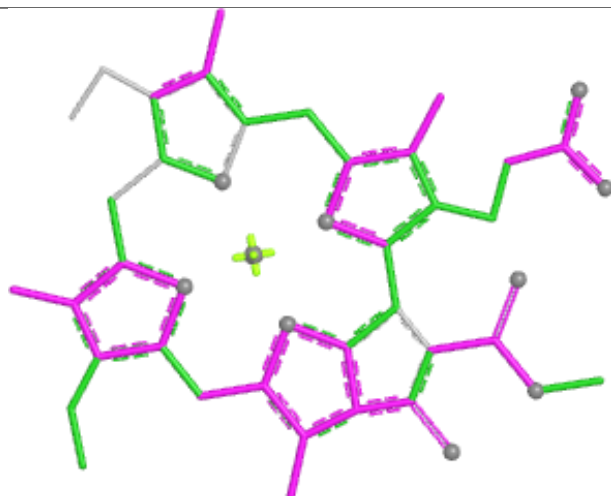




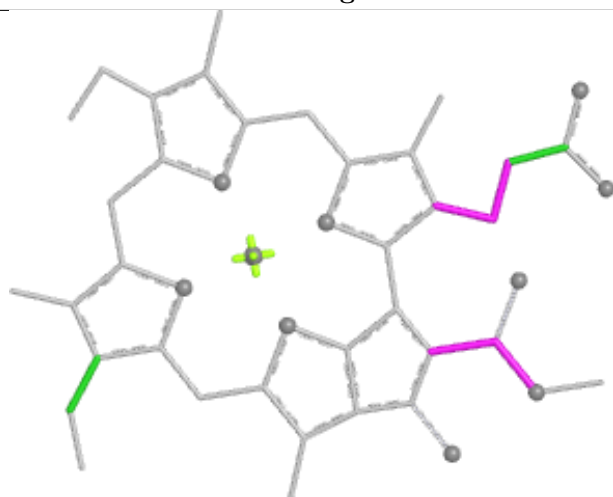
Ligand CLA G 1120



Bond lengths



Bond angles

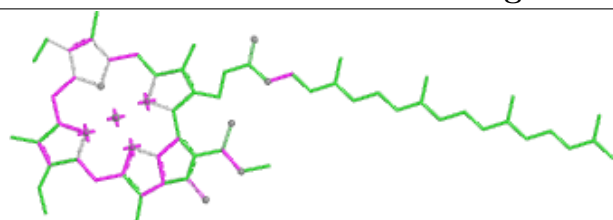


Torsions

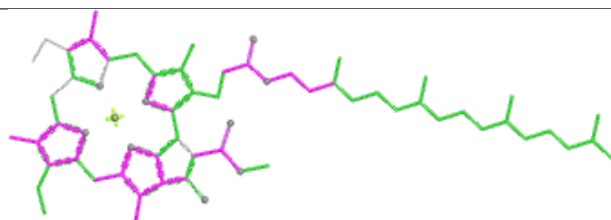


Rings

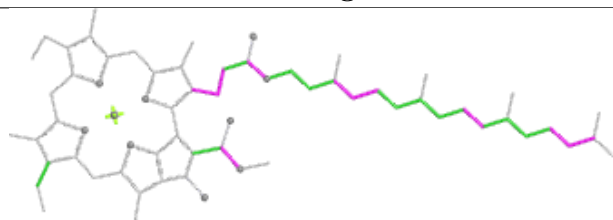
Ligand CLA H 1225



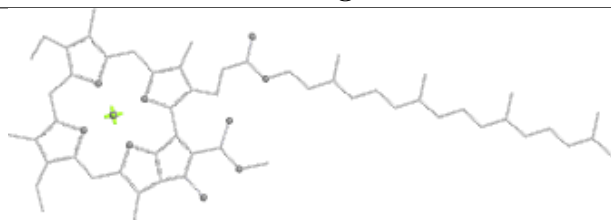
Bond lengths



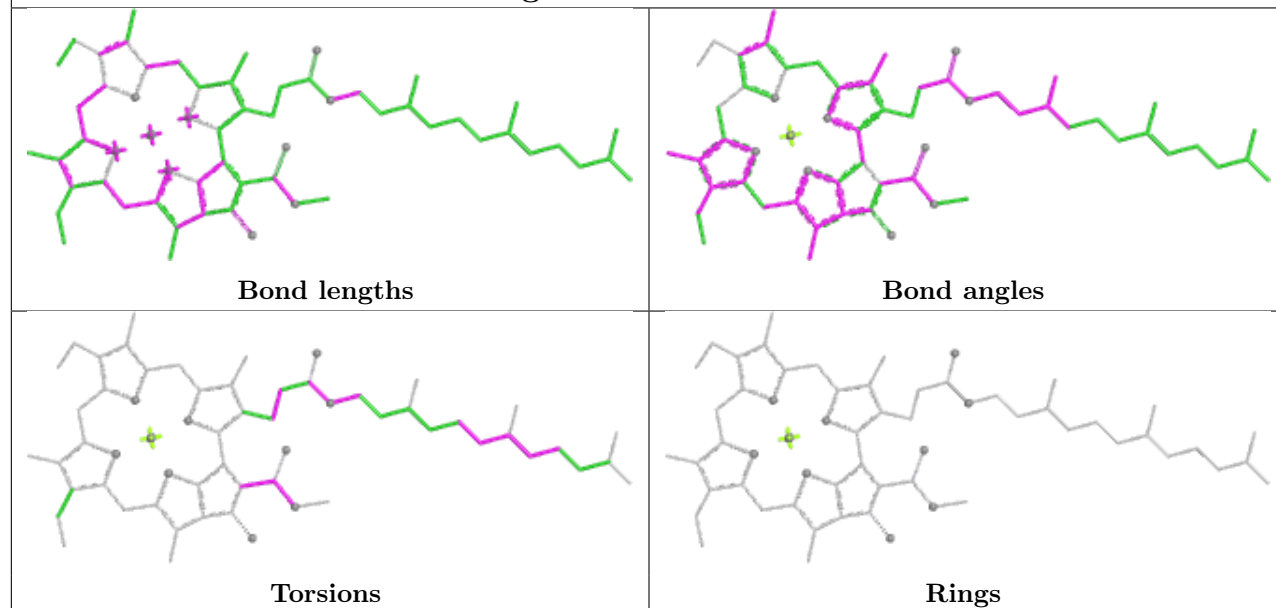
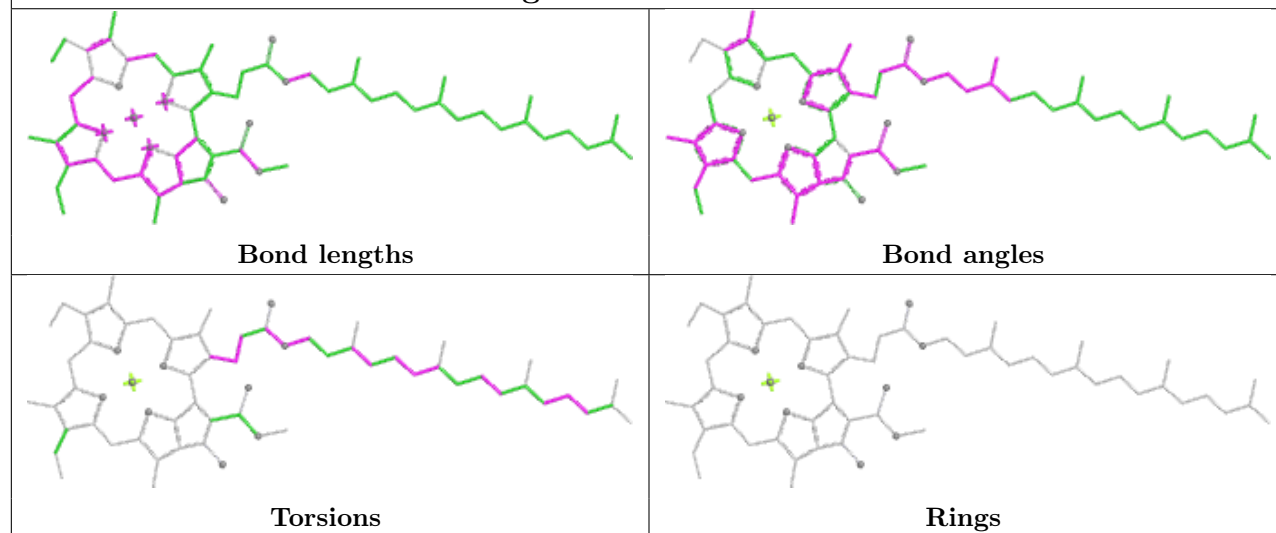
Bond angles

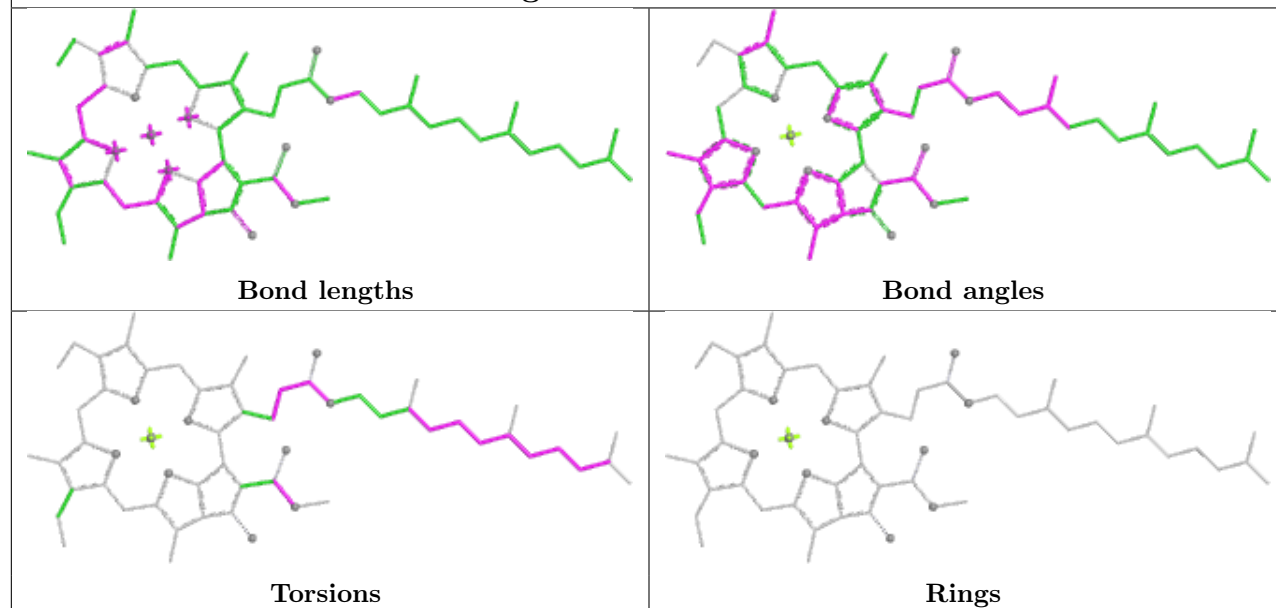
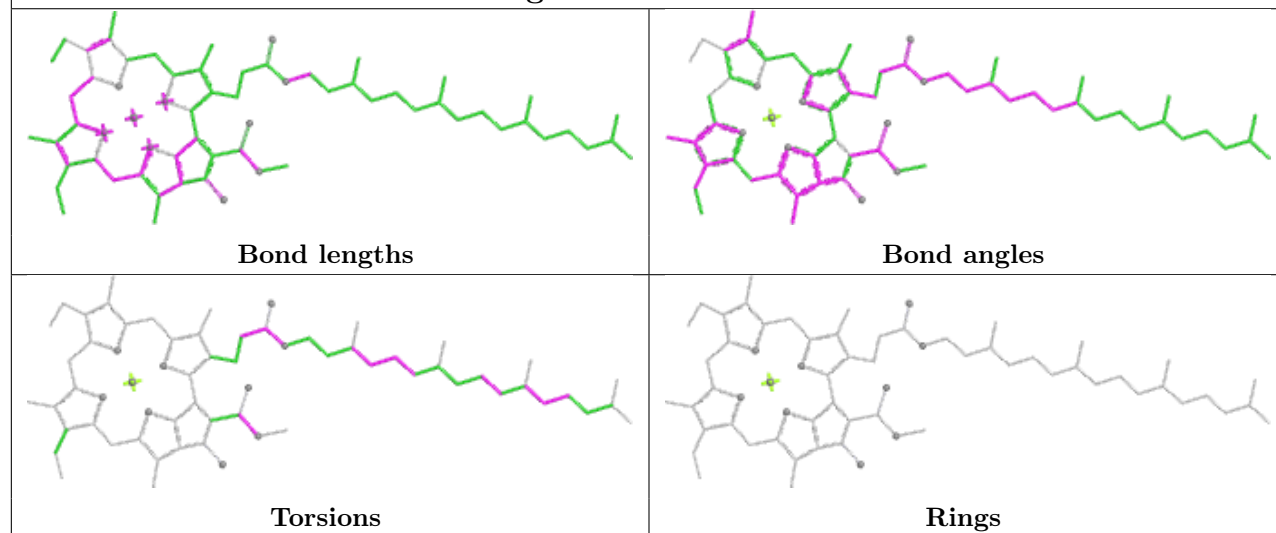


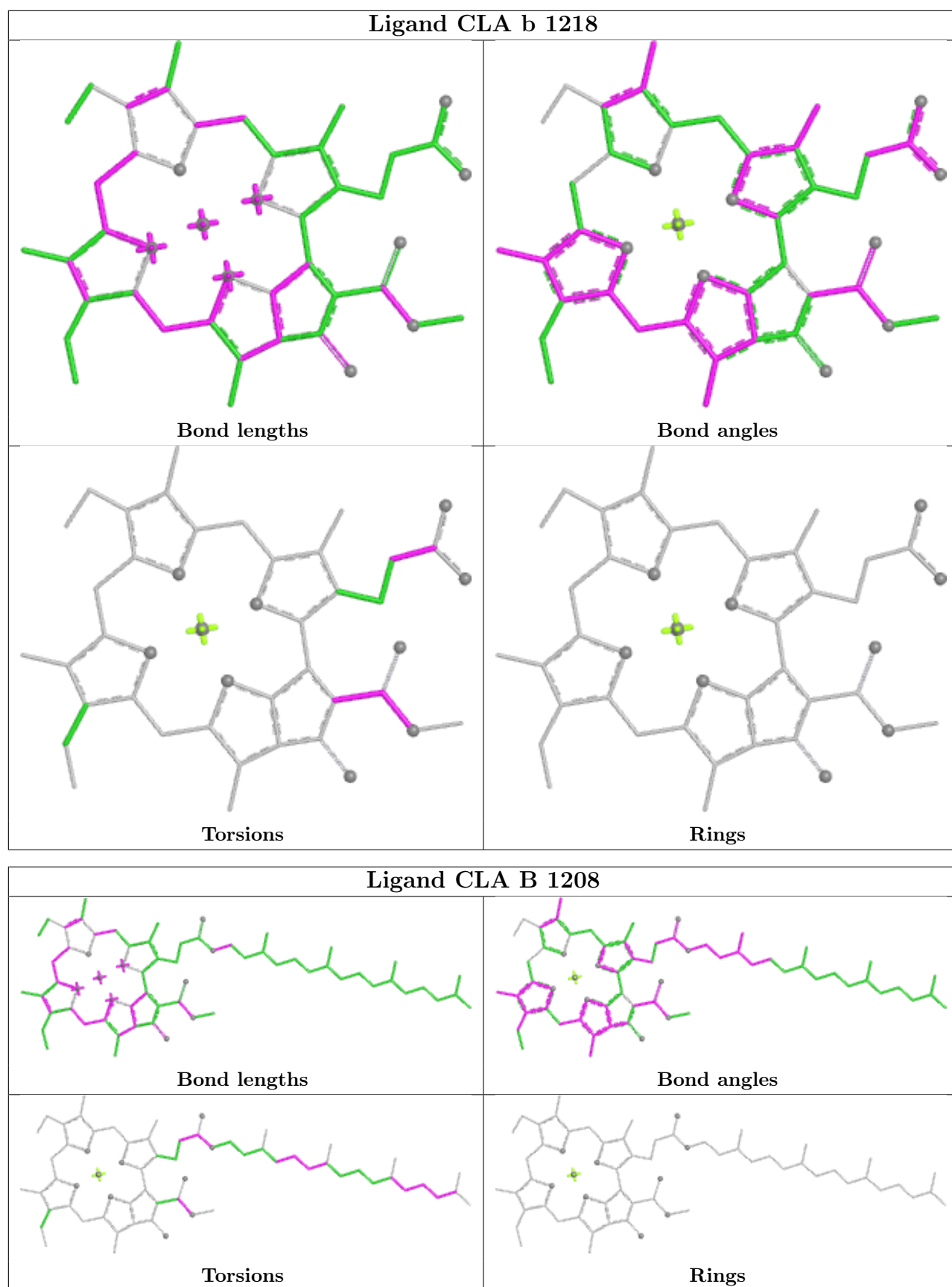
Torsions

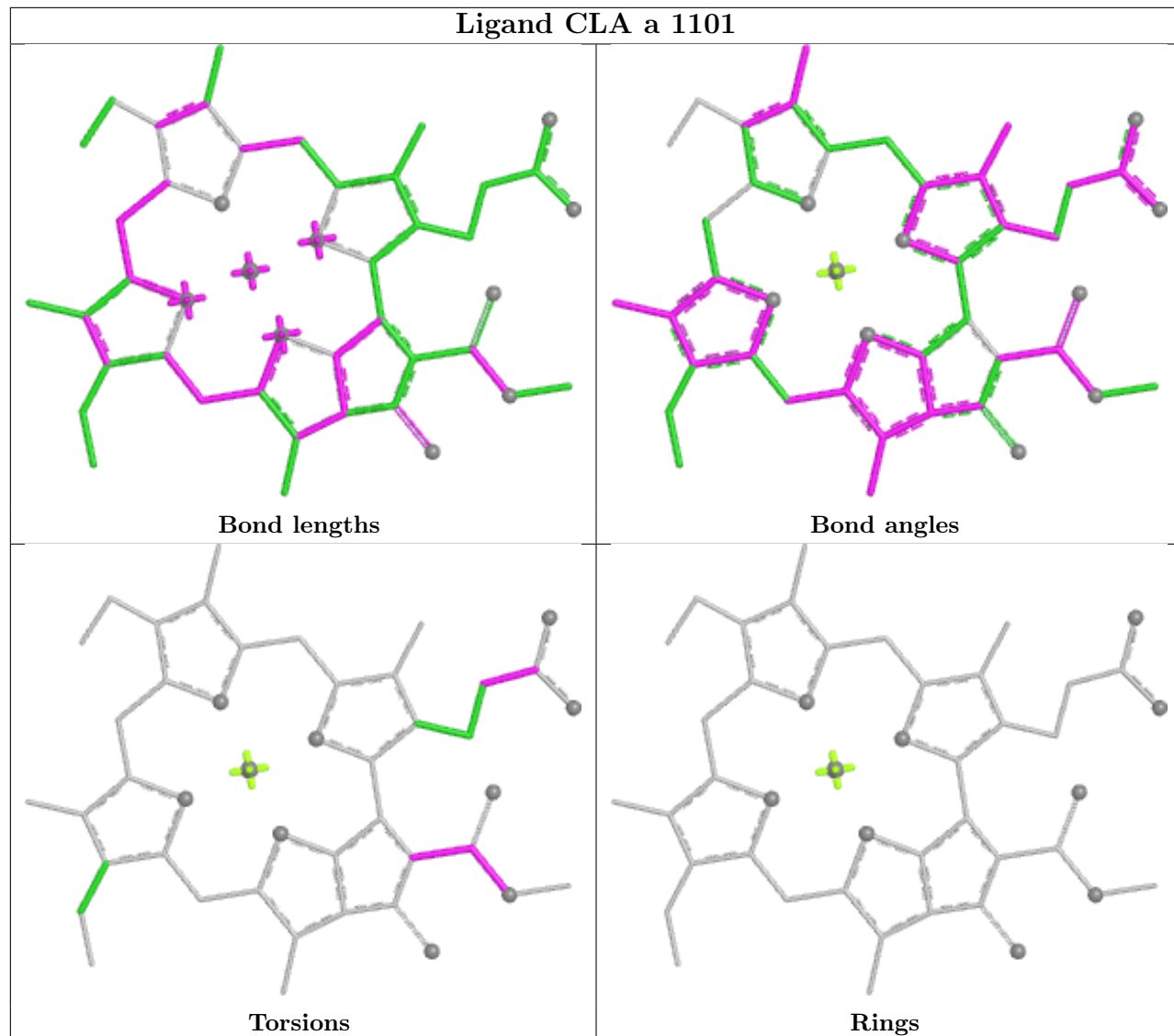
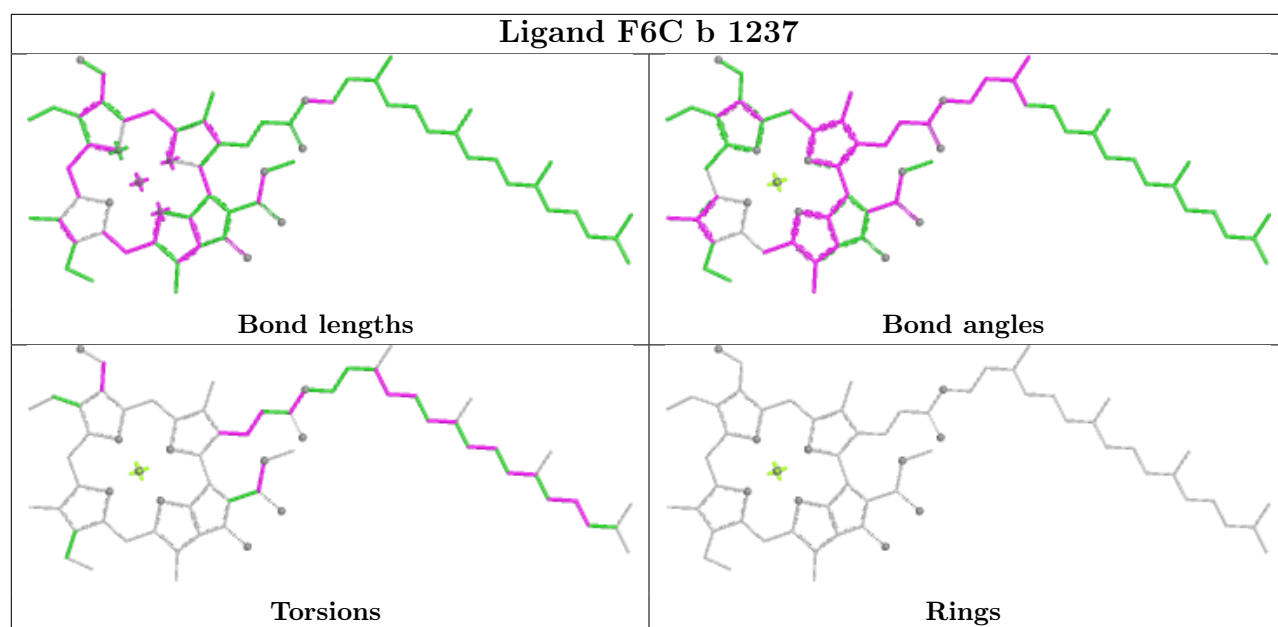


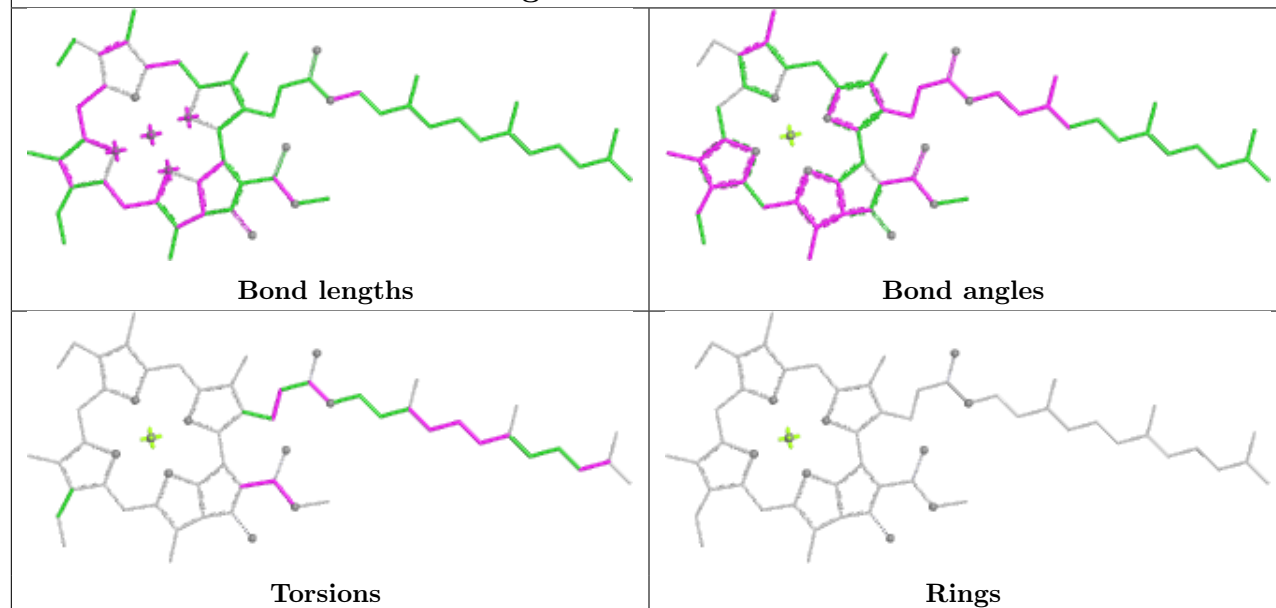
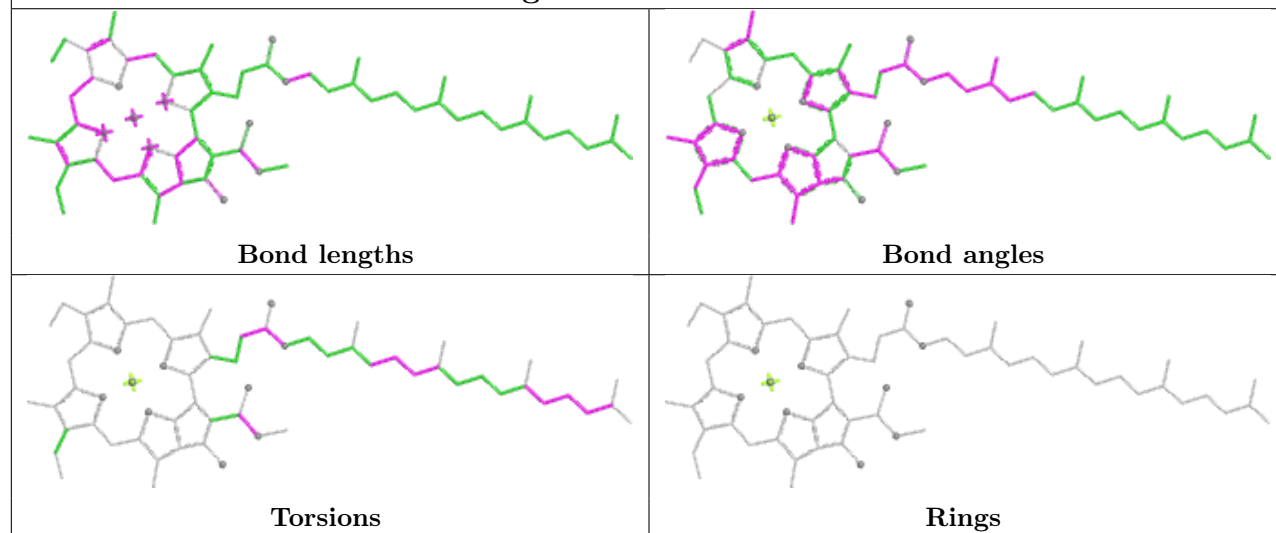
Rings

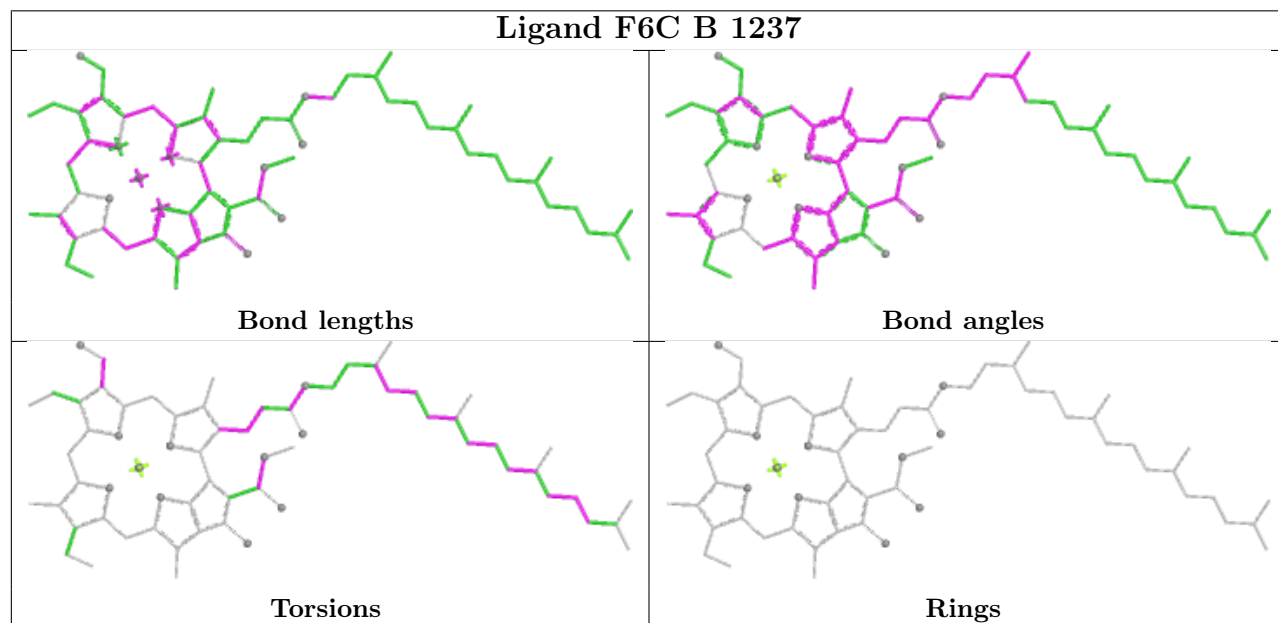
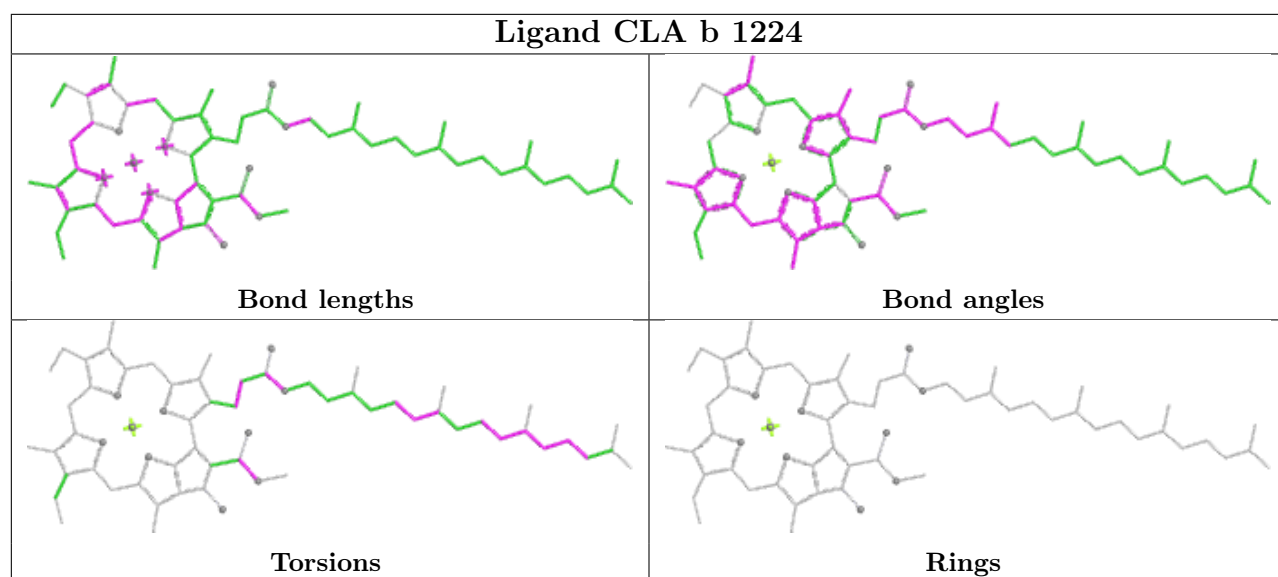
Ligand CLA G 1123**Ligand CLA H 1210**

Ligand CLA G 1126**Ligand CLA b 1204**

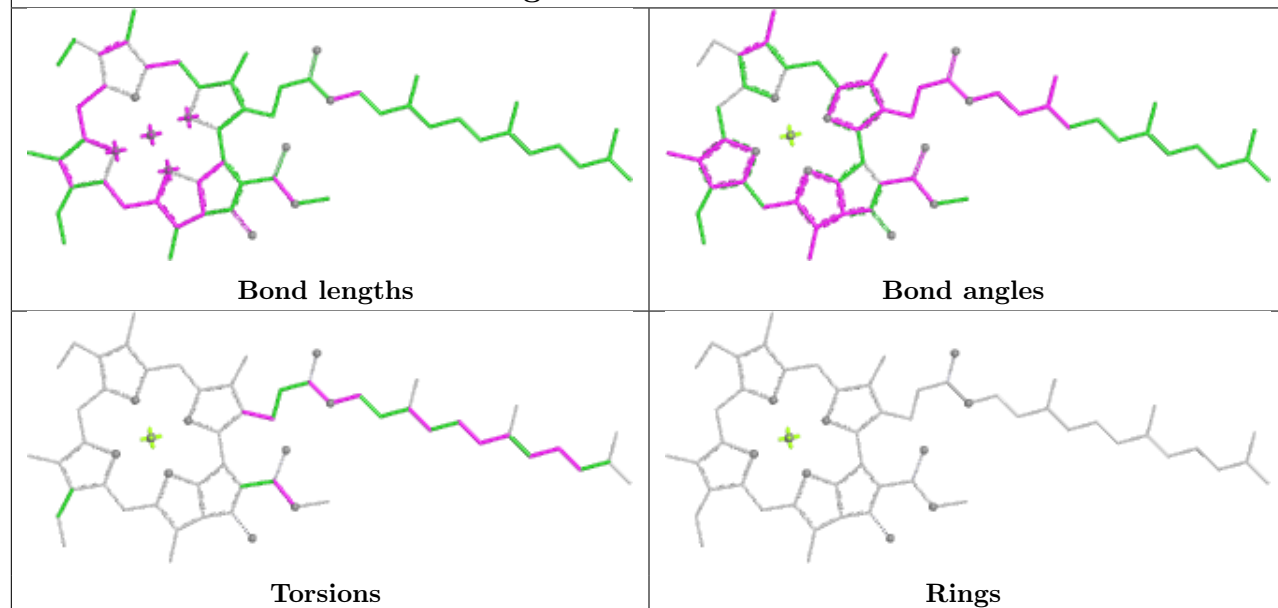




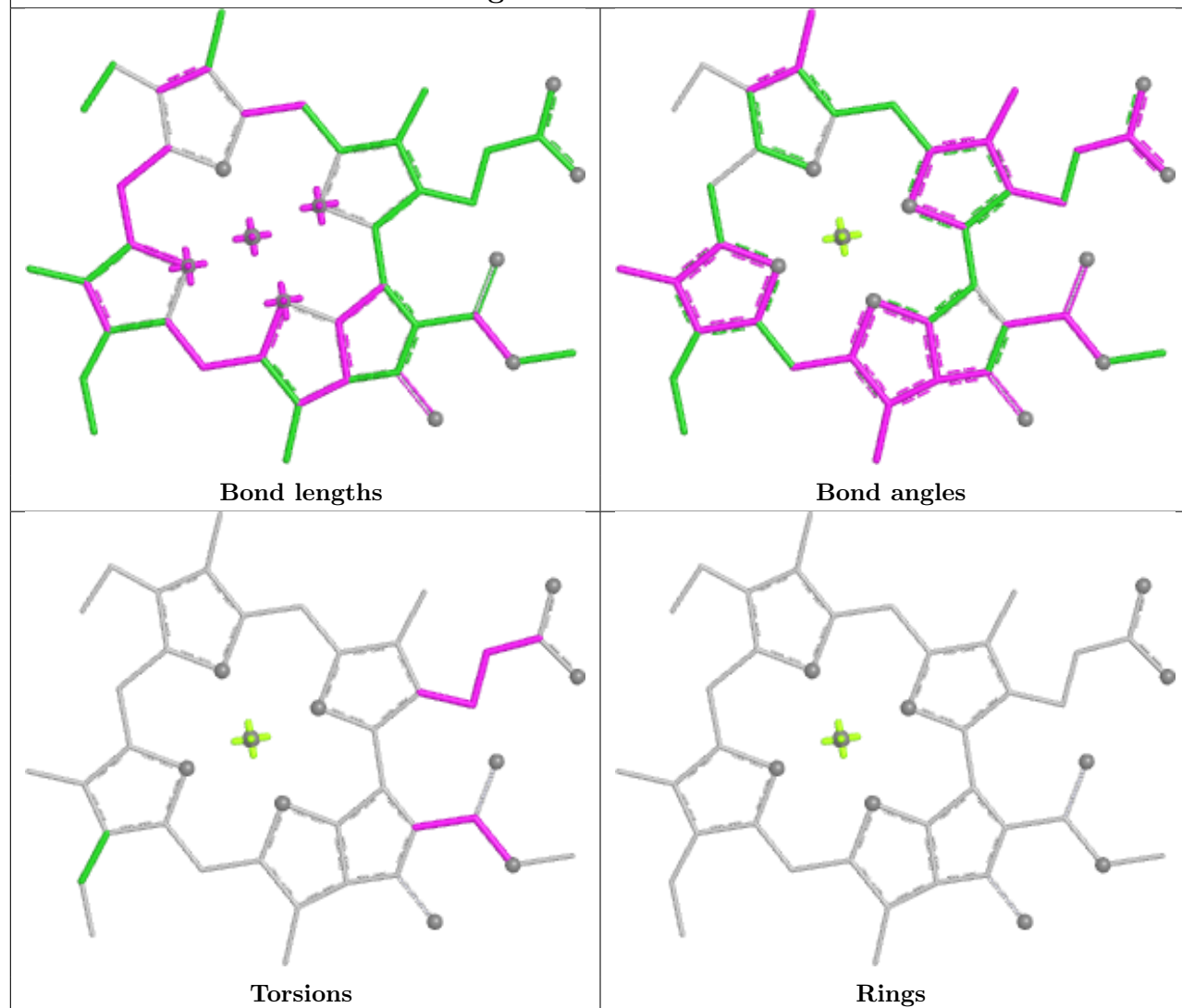
Ligand CLA G 1111**Ligand CLA H 1208**



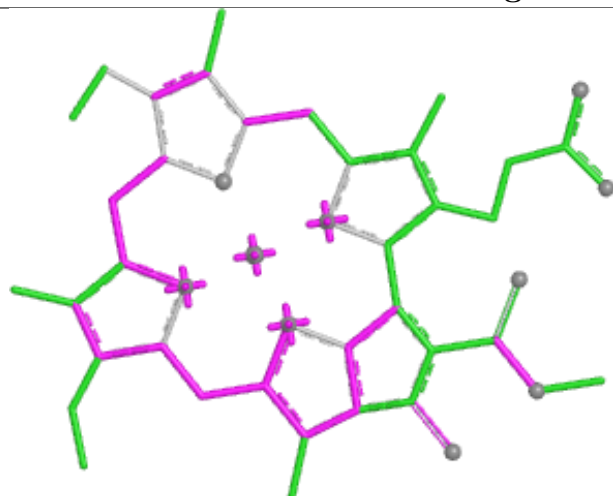
Ligand CLA B 1229



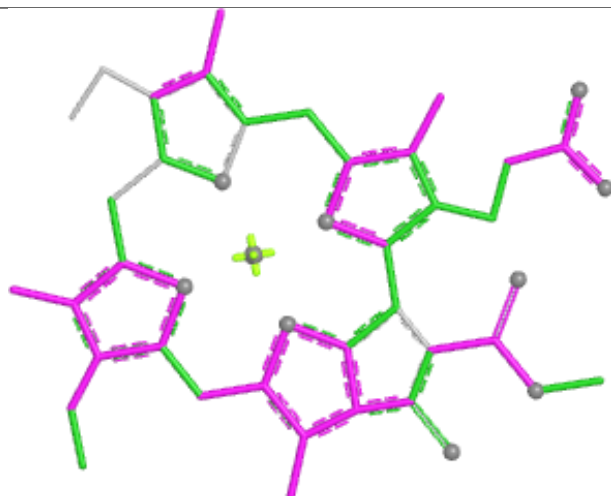
Ligand CLA a 1113



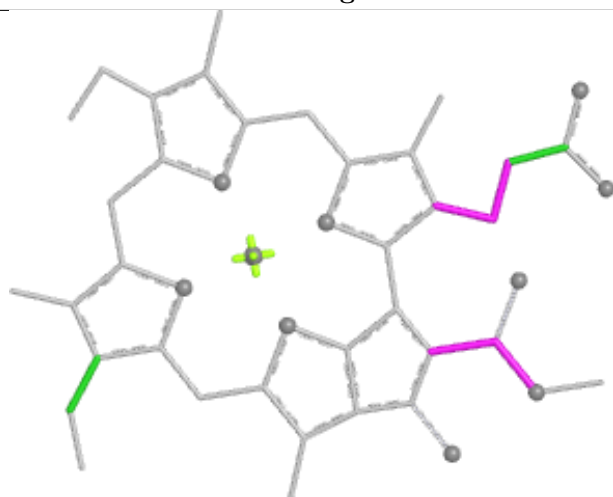
Ligand CLA K 1401



Bond lengths



Bond angles

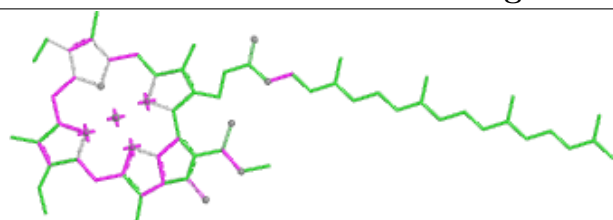


Torsions

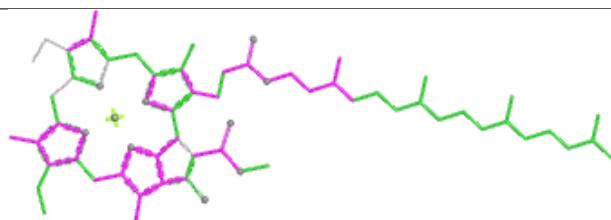


Rings

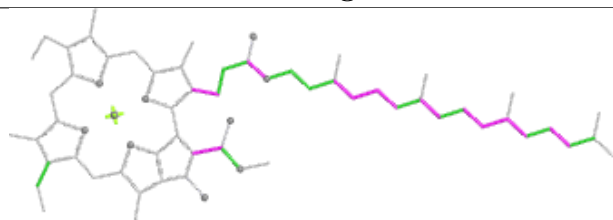
Ligand CLA H 1203



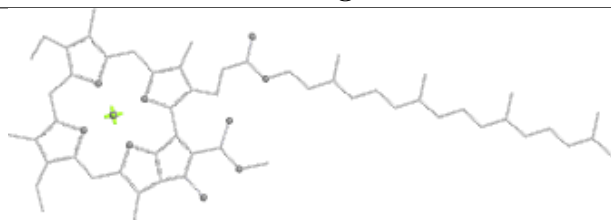
Bond lengths



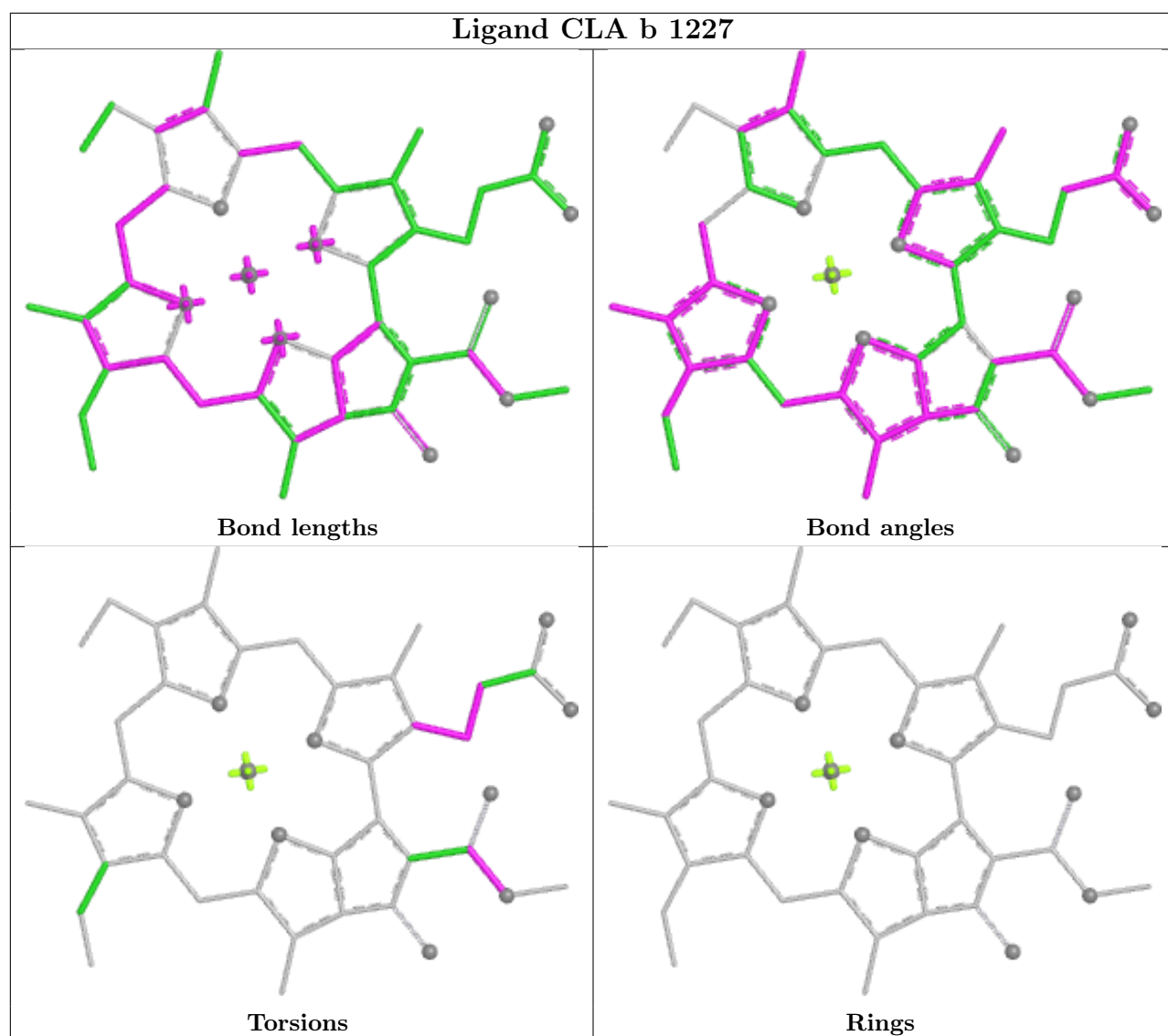
Bond angles

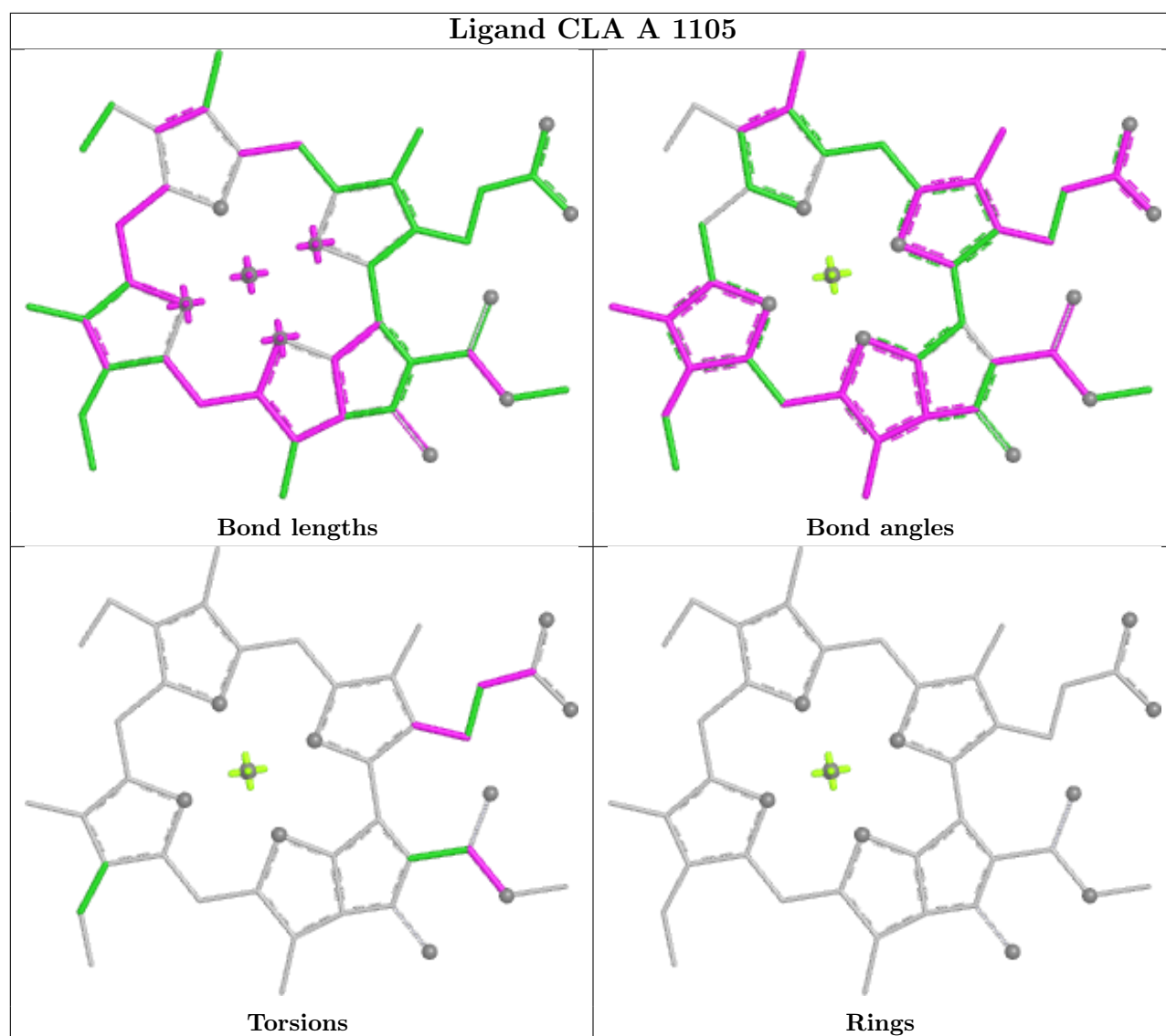


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	T	1
9	k	1
9	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	49:UNK	C	69:VAL	N	9.76
1	k	49:UNK	C	69:VAL	N	9.75
1	K	49:UNK	C	69:VAL	N	9.75

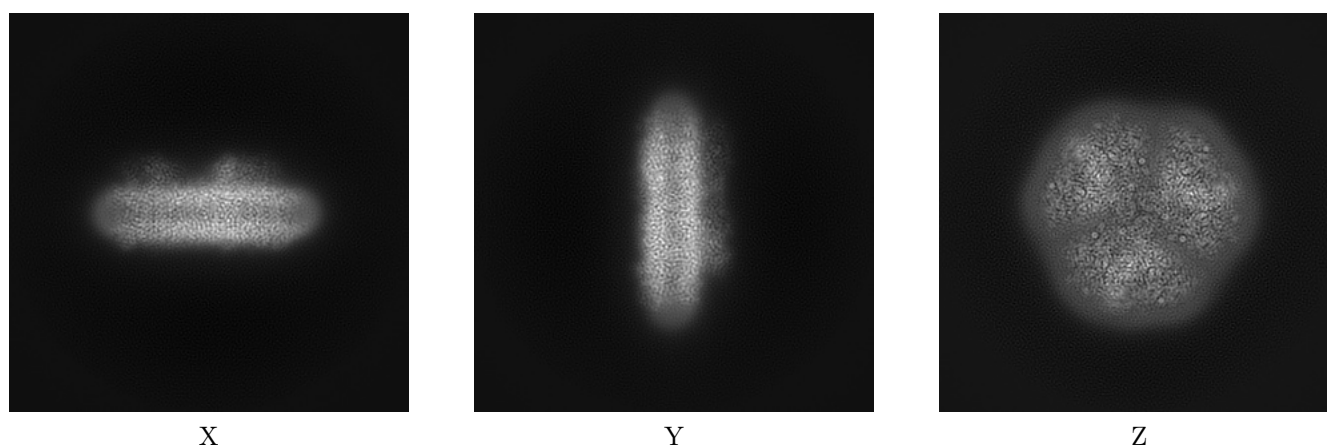
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23563. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

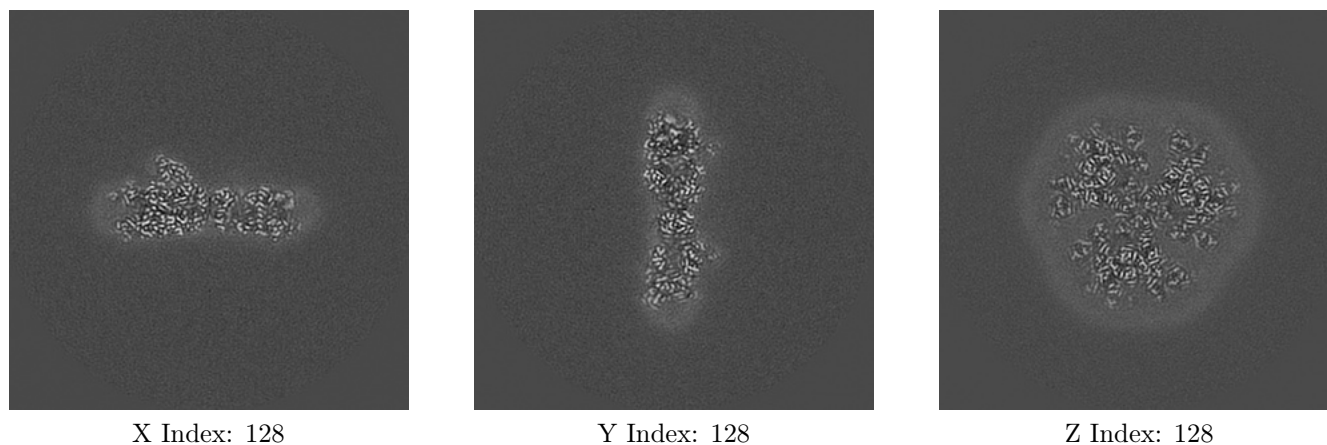
6.1.1 Primary map



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

6.2 Central slices [i](#)

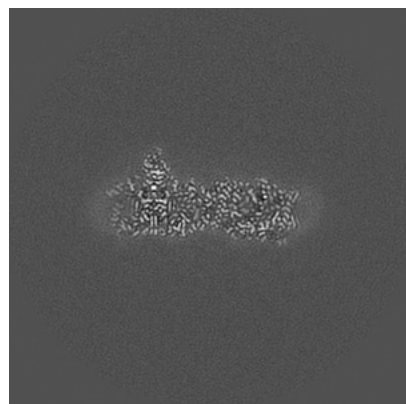
6.2.1 Primary map



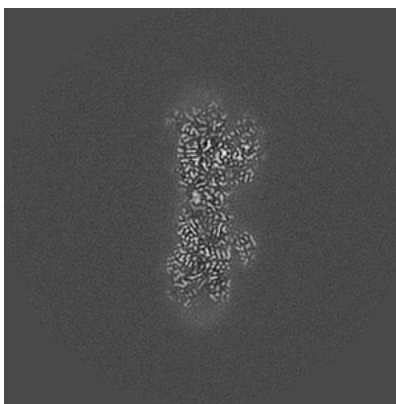
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

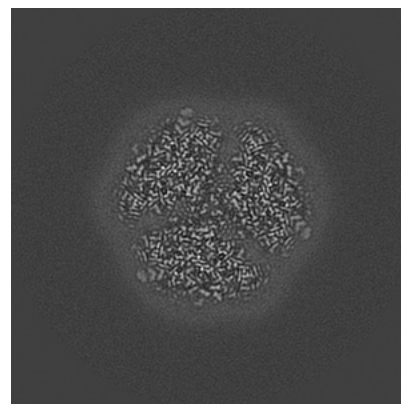
6.3.1 Primary map



X Index: 121



Y Index: 140

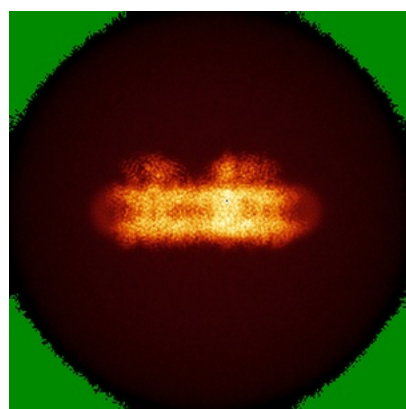


Z Index: 120

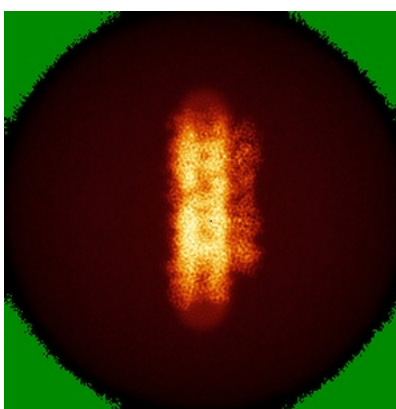
The images above show the largest variance slices of the map in three orthogonal directions.

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

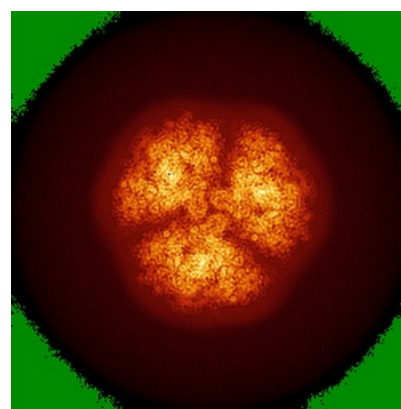
6.4.1 Primary map



X



Y

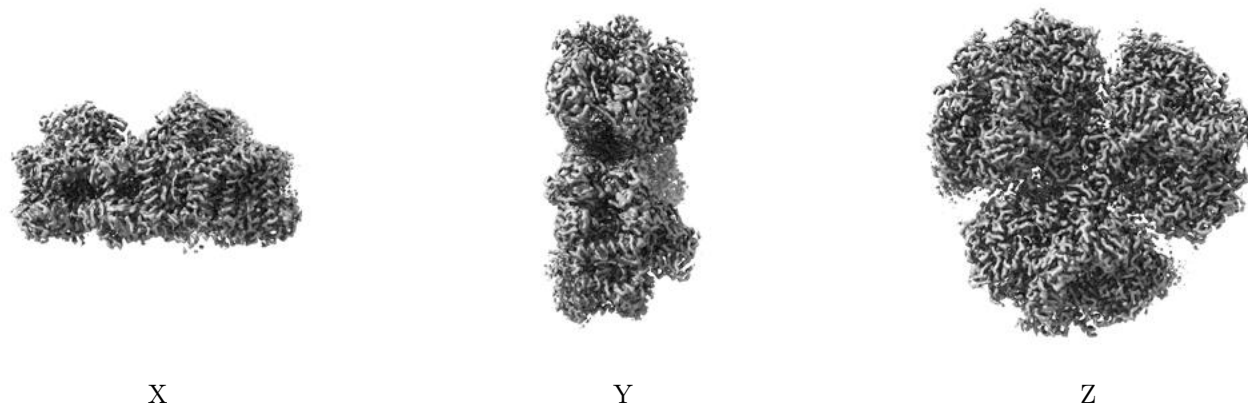


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

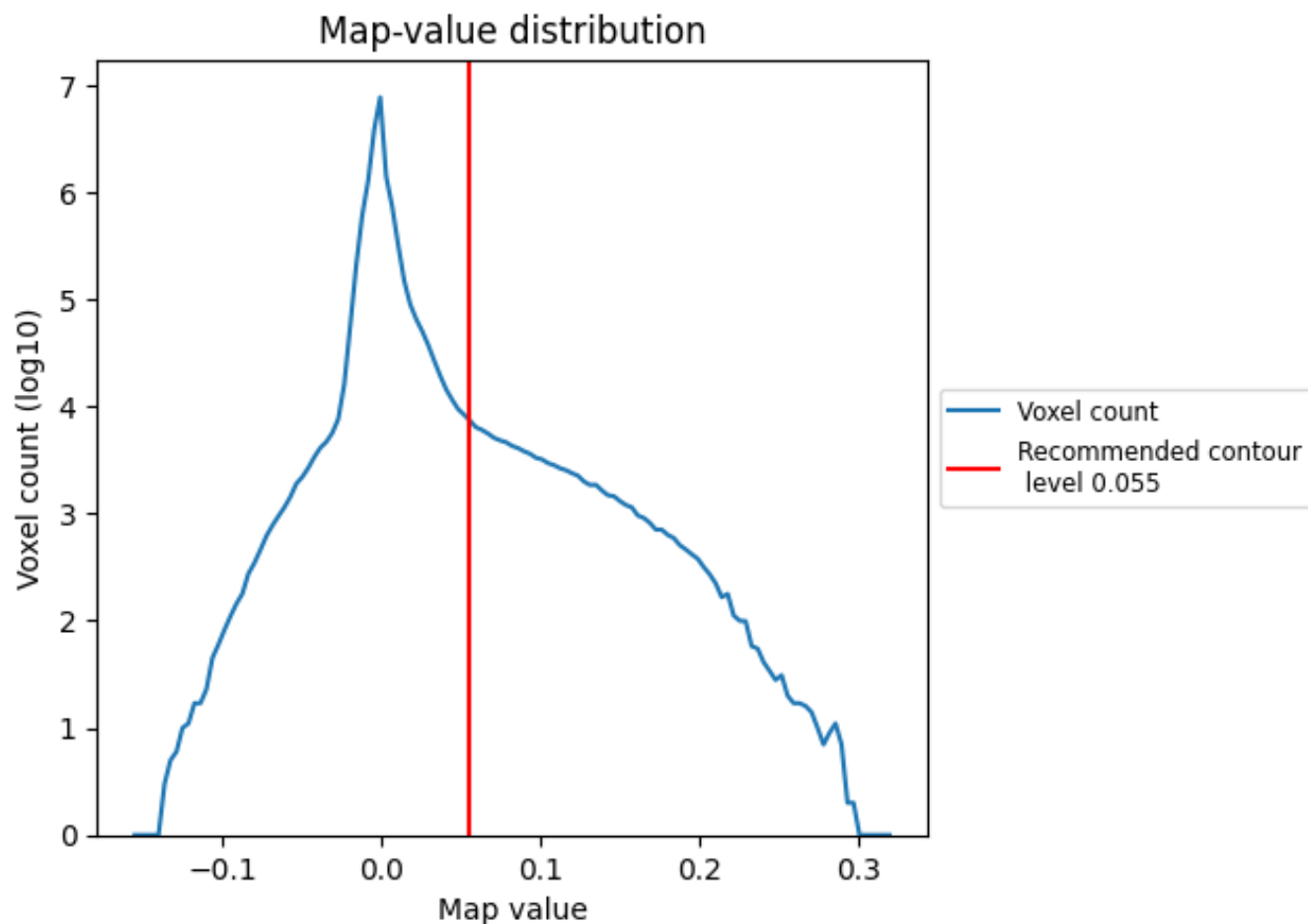
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

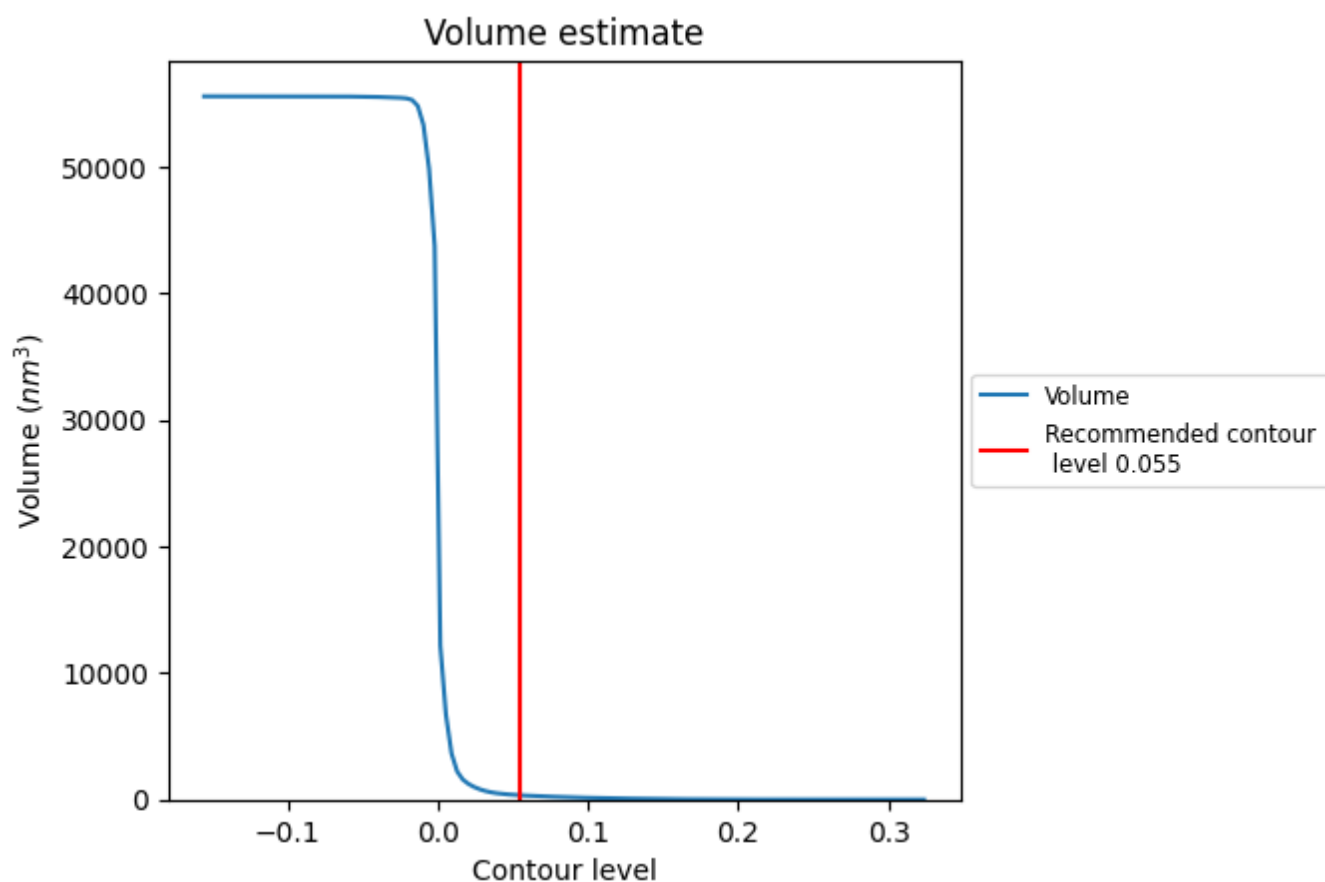
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

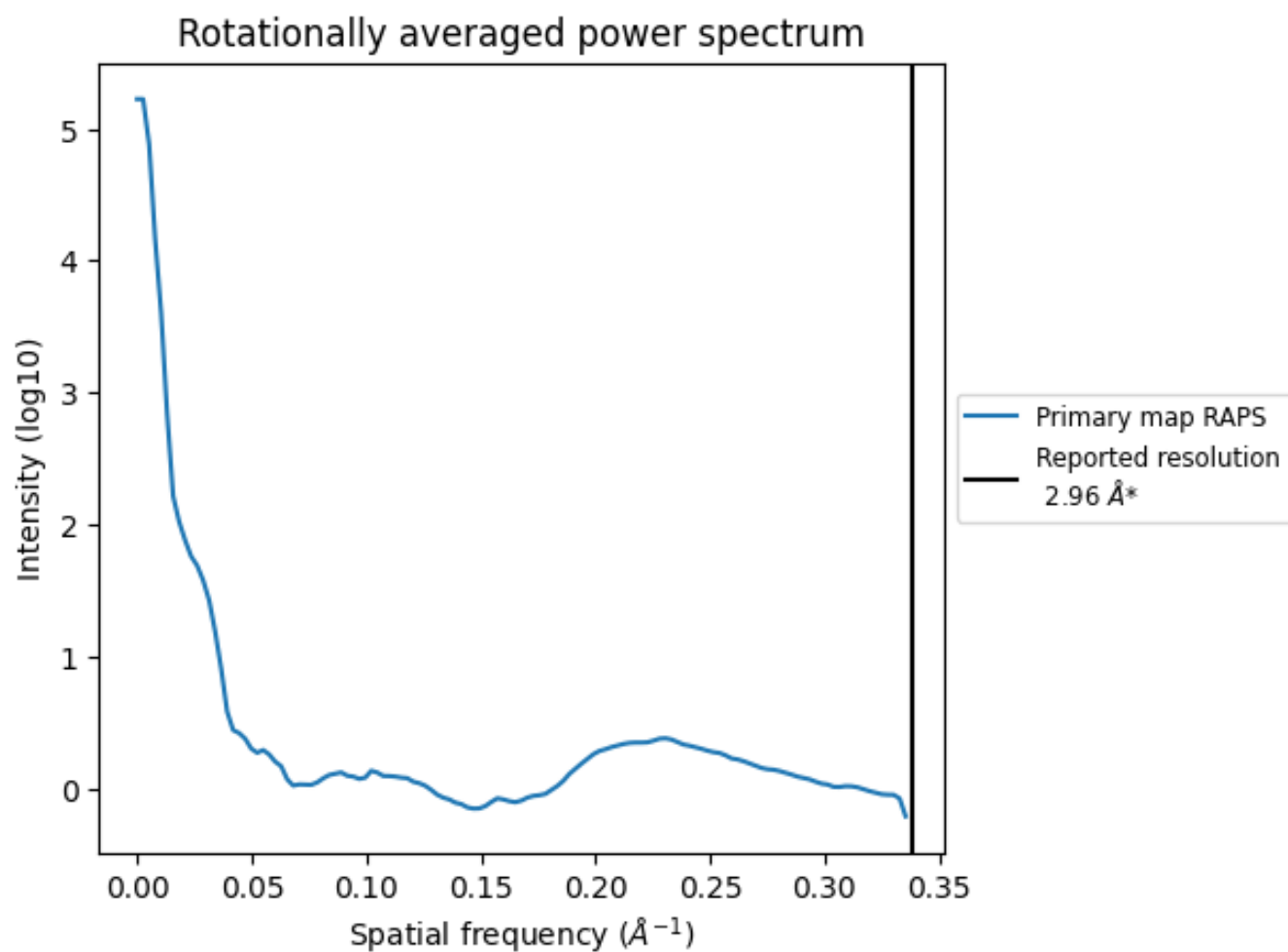
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339 nm³; this corresponds to an approximate mass of 306 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 ⓘ

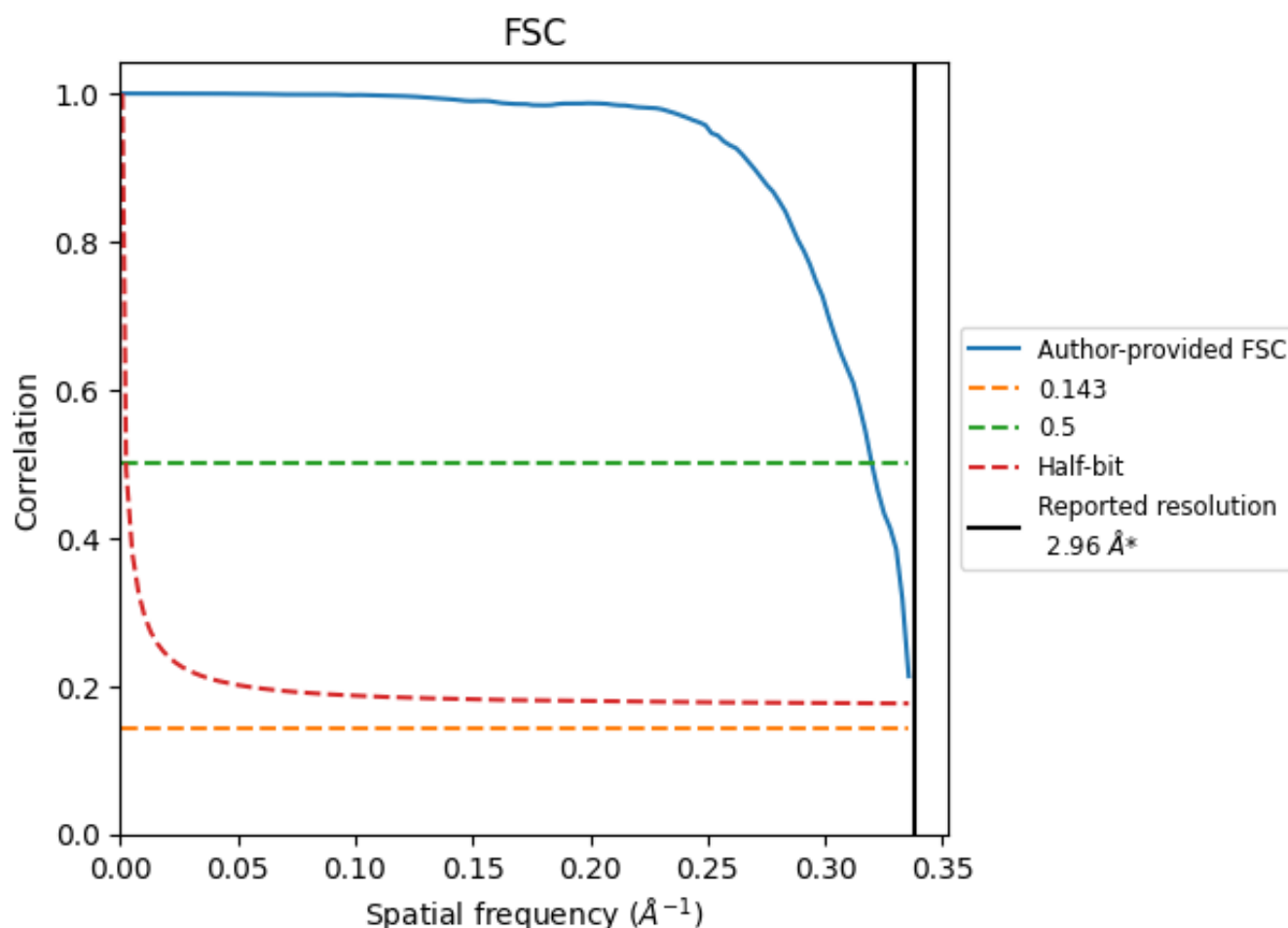


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 Å⁻¹

8.2 Resolution estimates [i](#)

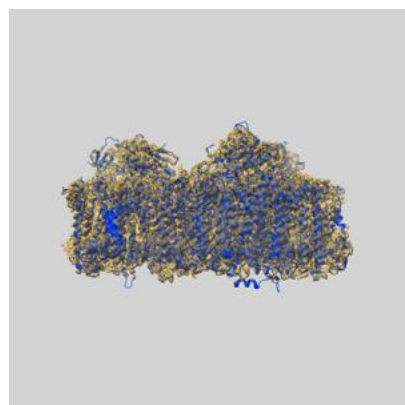
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	-	3.13	-
Unmasked-calculated*	-	-	-

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

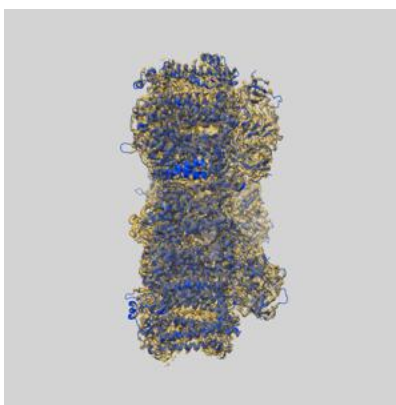
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23563 and PDB model 7LX0. Per-residue inclusion information can be found in section [3](#) on page [37](#).

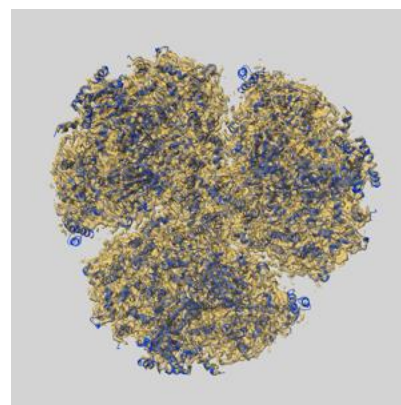
9.1 Map-model overlay [i](#)



X



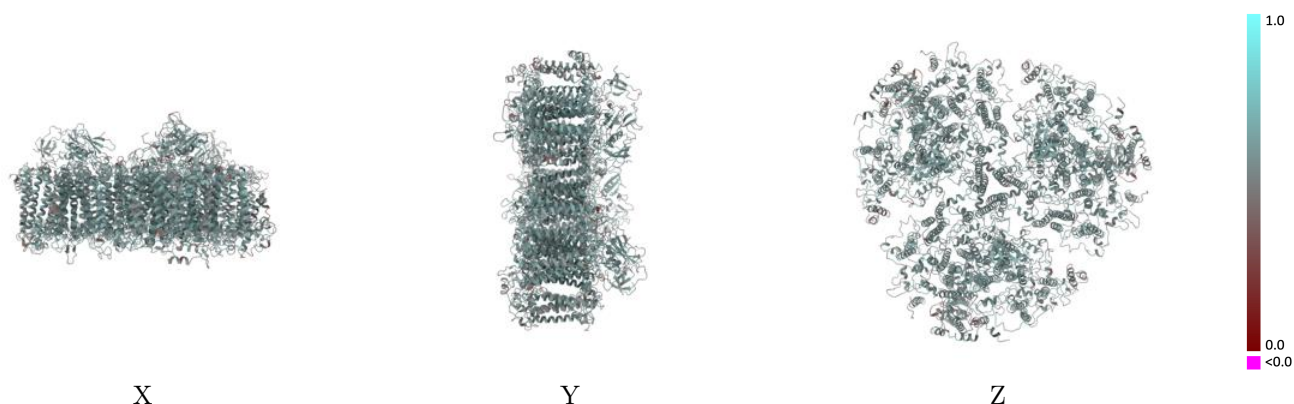
Y



Z

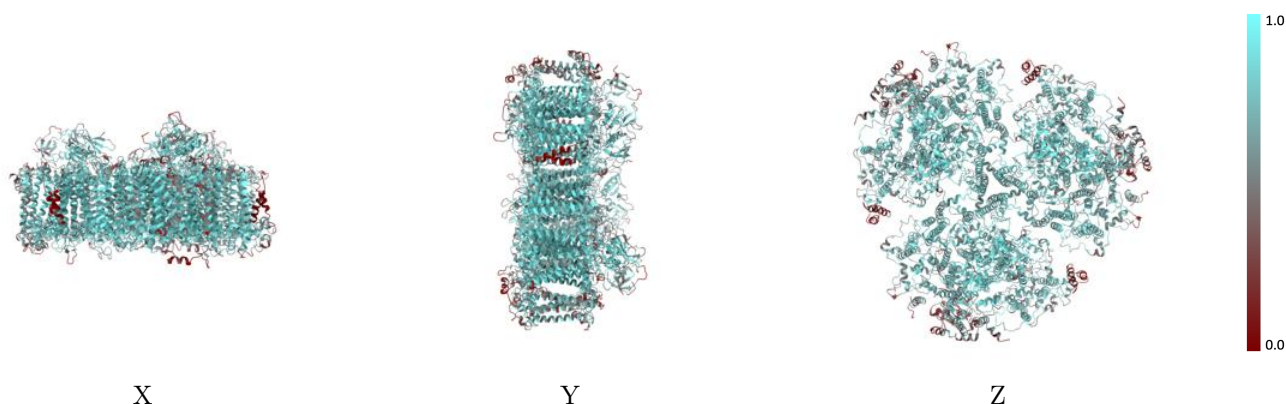
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



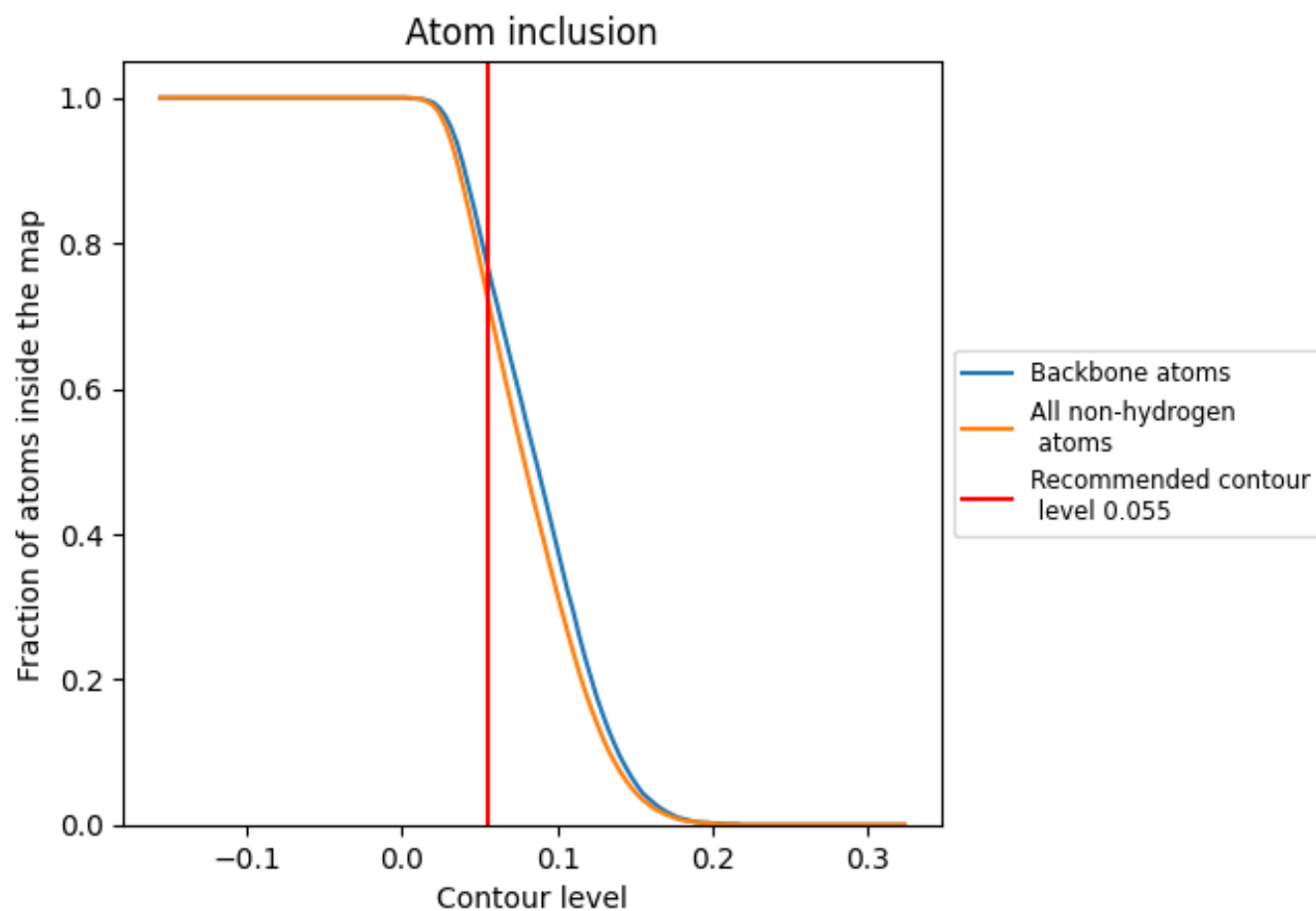
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.055).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 73% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7260	 0.5650
A	 0.7680	 0.5740
B	 0.7700	 0.5740
C	 0.7790	 0.5640
D	 0.6530	 0.5490
E	 0.5630	 0.5200
F	 0.3940	 0.4990
G	 0.7700	 0.5750
H	 0.7680	 0.5770
I	 0.7960	 0.5720
J	 0.4490	 0.4770
K	 0.0920	 0.4640
L	 0.7760	 0.5720
M	 0.7000	 0.5480
N	 0.7850	 0.5550
O	 0.6520	 0.5470
P	 0.5610	 0.5160
Q	 0.3970	 0.5010
R	 0.7830	 0.5670
S	 0.4580	 0.4730
T	 0.0710	 0.4560
U	 0.7790	 0.5690
V	 0.7110	 0.5530
W	 0.4910	 0.4970
X	 0.4810	 0.4960
a	 0.7690	 0.5770
b	 0.7650	 0.5770
c	 0.7870	 0.5610
d	 0.6450	 0.5480
e	 0.5400	 0.5100
f	 0.3960	 0.4930
i	 0.7920	 0.5750
j	 0.4410	 0.4730
k	 0.1050	 0.4620
l	 0.7700	 0.5720



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Chain	Atom inclusion	Q-score
m	 0.7000	 0.5580
x	 0.4780	 0.4930