



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2026 – 11:51 AM UTC

PDB ID : 6ZZX / pdb_00006zzx
EMDB ID : EMD-11588
Title : Structure of low-light grown *Chlorella ohadii* Photosystem I
Authors : Caspy, I.; Nelson, N.; Nechushtai, R.; Neumann, E.; Shkolnisky, Y.
Deposited on : 2020-08-05
Resolution : 2.70 Å (reported)
Based on initial model : 6IJO

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

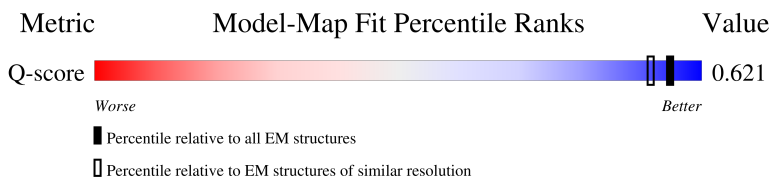
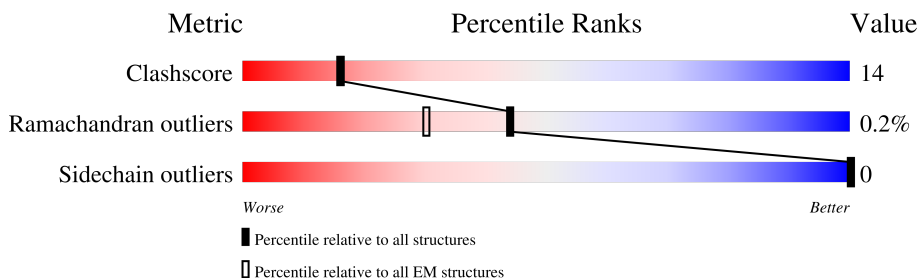
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



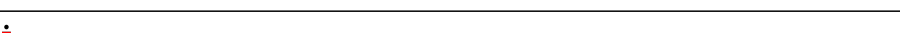
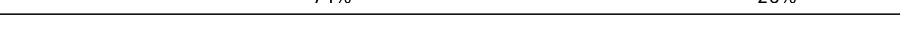
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	741	 74%26%
2	B	731	 79%21%
3	C	80	 78%22%
4	D	143	 79%21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	64	
6	F	165	
7	G	99	
8	H	94	
9	J	41	
10	K	86	
11	L	157	
12	M	31	
13	I	35	
14	O	87	
15	1	192	
15	a	192	
16	3	241	
17	4	207	
18	5	229	
19	6	231	
20	7	221	
21	8	219	
22	2	215	
23	9	183	

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
24	CL0	A	1011	X	-	-	-
25	CLA	1	601	X	-	-	-
25	CLA	1	602	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	1	603	X	-	-	-
25	CLA	1	605	X	-	-	-
25	CLA	1	606	X	-	-	-
25	CLA	1	607	X	-	-	-
25	CLA	1	608	X	-	-	-
25	CLA	1	612	X	-	-	-
25	CLA	1	615	X	-	-	-
25	CLA	2	601	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	603	X	-	-	-
25	CLA	2	604	X	-	-	-
25	CLA	2	605	X	-	-	-
25	CLA	2	606	X	-	-	-
25	CLA	2	607	X	-	-	-
25	CLA	2	608	X	-	-	-
25	CLA	2	612	X	-	-	-
25	CLA	2	615	X	-	-	-
25	CLA	2	621	X	-	-	-
25	CLA	3	601	X	-	-	-
25	CLA	3	602	X	-	-	-
25	CLA	3	605	X	-	-	-
25	CLA	3	606	X	-	-	-
25	CLA	3	607	X	-	-	-
25	CLA	3	610	X	-	-	-
25	CLA	3	612	X	-	-	-
25	CLA	3	613	X	-	-	-
25	CLA	3	616	X	-	-	-
25	CLA	3	618	X	-	-	-
25	CLA	4	601	X	-	-	-
25	CLA	4	602	X	-	-	-
25	CLA	4	603	X	-	-	-
25	CLA	4	604	X	-	-	-
25	CLA	4	605	X	-	-	-
25	CLA	4	606	X	-	-	-
25	CLA	4	607	X	-	-	-
25	CLA	4	608	X	-	-	-
25	CLA	4	610	X	-	-	-
25	CLA	4	611	X	-	-	-
25	CLA	4	612	X	-	-	-
25	CLA	4	615	X	-	-	-
25	CLA	4	616	X	-	-	-
25	CLA	4	617	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	5	601	X	-	-	-
25	CLA	5	602	X	-	-	-
25	CLA	5	603	X	-	-	-
25	CLA	5	604	X	-	-	-
25	CLA	5	605	X	-	-	-
25	CLA	5	606	X	-	-	-
25	CLA	5	607	X	-	-	-
25	CLA	5	608	X	-	-	-
25	CLA	5	609	X	-	-	-
25	CLA	5	612	X	-	-	-
25	CLA	5	614	X	-	-	-
25	CLA	5	615	X	-	-	-
25	CLA	6	601	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	604	X	-	-	-
25	CLA	6	605	X	-	-	-
25	CLA	6	606	X	-	-	-
25	CLA	6	607	X	-	-	-
25	CLA	6	608	X	-	-	-
25	CLA	6	612	X	-	-	-
25	CLA	6	615	X	-	-	-
25	CLA	6	618	X	-	-	-
25	CLA	7	601	X	-	-	-
25	CLA	7	602	X	-	-	-
25	CLA	7	603	X	-	-	-
25	CLA	7	604	X	-	-	-
25	CLA	7	605	X	-	-	-
25	CLA	7	606	X	-	-	-
25	CLA	7	607	X	-	-	-
25	CLA	7	608	X	-	-	-
25	CLA	7	610	X	-	-	-
25	CLA	7	612	X	-	-	-
25	CLA	8	602	X	-	-	-
25	CLA	8	605	X	-	-	-
25	CLA	8	606	X	-	-	-
25	CLA	8	607	X	-	-	-
25	CLA	8	608	X	-	-	-
25	CLA	8	609	X	-	-	-
25	CLA	8	611	X	-	-	-
25	CLA	8	612	X	-	-	-
25	CLA	8	615	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	8	618	X	-	-	-
25	CLA	8	620	X	-	-	-
25	CLA	9	602	X	-	-	-
25	CLA	9	604	X	-	-	-
25	CLA	9	605	X	-	-	-
25	CLA	9	606	X	-	-	-
25	CLA	9	607	X	-	-	-
25	CLA	9	609	X	-	-	-
25	CLA	9	612	X	-	-	-
25	CLA	A	1012	X	-	-	-
25	CLA	A	1013	X	-	-	-
25	CLA	A	1101	X	-	-	-
25	CLA	A	1102	X	-	-	-
25	CLA	A	1103	X	-	-	-
25	CLA	A	1104	X	-	-	-
25	CLA	A	1105	X	-	-	-
25	CLA	A	1106	X	-	-	-
25	CLA	A	1107	X	-	-	-
25	CLA	A	1108	X	-	-	-
25	CLA	A	1109	X	-	-	-
25	CLA	A	1110	X	-	-	-
25	CLA	A	1111	X	-	-	-
25	CLA	A	1112	X	-	-	-
25	CLA	A	1113	X	-	-	-
25	CLA	A	1115	X	-	-	-
25	CLA	A	1116	X	-	-	-
25	CLA	A	1117	X	-	-	-
25	CLA	A	1118	X	-	-	-
25	CLA	A	1119	X	-	-	-
25	CLA	A	1120	X	-	-	-
25	CLA	A	1121	X	-	-	-
25	CLA	A	1122	X	-	-	-
25	CLA	A	1123	X	-	-	-
25	CLA	A	1124	X	-	-	-
25	CLA	A	1125	X	-	-	-
25	CLA	A	1126	X	-	-	-
25	CLA	A	1127	X	-	-	-
25	CLA	A	1128	X	-	-	-
25	CLA	A	1129	X	-	-	-
25	CLA	A	1130	X	-	-	-
25	CLA	A	1131	X	-	-	-
25	CLA	A	1132	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	1133	X	-	-	-
25	CLA	A	1134	X	-	-	-
25	CLA	A	1135	X	-	-	-
25	CLA	A	1136	X	-	-	-
25	CLA	A	1137	X	-	-	-
25	CLA	A	1138	X	-	-	-
25	CLA	A	1139	X	-	-	-
25	CLA	A	1140	X	-	-	-
25	CLA	A	1141	X	-	-	-
25	CLA	B	1021	X	-	-	-
25	CLA	B	1022	X	-	-	-
25	CLA	B	1023	X	-	-	-
25	CLA	B	1201	X	-	-	-
25	CLA	B	1202	X	-	-	-
25	CLA	B	1203	X	-	-	-
25	CLA	B	1204	X	-	-	-
25	CLA	B	1205	X	-	-	-
25	CLA	B	1206	X	-	-	-
25	CLA	B	1207	X	-	-	-
25	CLA	B	1208	X	-	-	-
25	CLA	B	1209	X	-	-	-
25	CLA	B	1210	X	-	-	-
25	CLA	B	1211	X	-	-	-
25	CLA	B	1212	X	-	-	-
25	CLA	B	1213	X	-	-	-
25	CLA	B	1214	X	-	-	-
25	CLA	B	1215	X	-	-	-
25	CLA	B	1216	X	-	-	-
25	CLA	B	1217	X	-	-	-
25	CLA	B	1218	X	-	-	-
25	CLA	B	1219	X	-	-	-
25	CLA	B	1220	X	-	-	-
25	CLA	B	1221	X	-	-	-
25	CLA	B	1222	X	-	-	-
25	CLA	B	1223	X	-	-	-
25	CLA	B	1224	X	-	-	-
25	CLA	B	1225	X	-	-	-
25	CLA	B	1226	X	-	-	-
25	CLA	B	1227	X	-	-	-
25	CLA	B	1228	X	-	-	-
25	CLA	B	1229	X	-	-	-
25	CLA	B	1230	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	1231	X	-	-	-
25	CLA	B	1232	X	-	-	-
25	CLA	B	1235	X	-	-	-
25	CLA	B	1236	X	-	-	-
25	CLA	B	1237	X	-	-	-
25	CLA	B	1238	X	-	-	-
25	CLA	B	1239	X	-	-	-
25	CLA	B	1240	X	-	-	-
25	CLA	F	1301	X	-	-	-
25	CLA	F	1302	X	-	-	-
25	CLA	G	1601	X	-	-	-
25	CLA	G	1602	X	-	-	-
25	CLA	G	1603	X	-	-	-
25	CLA	H	1701	X	-	-	-
25	CLA	H	1702	X	-	-	-
25	CLA	H	1703	X	-	-	-
25	CLA	J	1901	X	-	-	-
25	CLA	K	1401	X	-	-	-
25	CLA	K	1402	X	-	-	-
25	CLA	K	1403	X	-	-	-
25	CLA	K	1404	X	-	-	-
25	CLA	L	1501	X	-	-	-
25	CLA	L	1502	X	-	-	-
25	CLA	L	1503	X	-	-	-
25	CLA	L	1504	X	-	-	-
25	CLA	O	1801	X	-	-	-
25	CLA	O	1802	X	-	-	-
25	CLA	O	1803	X	-	-	-
25	CLA	a	601	X	-	-	-
25	CLA	a	602	X	-	-	-
25	CLA	a	603	X	-	-	-
25	CLA	a	605	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	608	X	-	-	-
25	CLA	a	611	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	a	615	X	-	-	-
26	CHL	1	604	X	-	-	-
26	CHL	1	609	X	-	-	-
26	CHL	1	610	X	-	-	-
26	CHL	1	611	X	-	-	-
26	CHL	1	613	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CHL	2	609	X	-	-	-
26	CHL	2	610	X	-	-	-
26	CHL	2	613	X	-	-	-
26	CHL	3	603	X	-	-	-
26	CHL	3	604	X	-	-	-
26	CHL	3	608	X	-	-	-
26	CHL	3	611	X	-	-	-
26	CHL	4	609	X	-	-	-
26	CHL	4	613	X	-	-	-
26	CHL	4	618	X	-	-	-
26	CHL	5	610	X	-	-	-
26	CHL	5	611	X	-	-	-
26	CHL	5	613	X	-	-	-
26	CHL	5	617	X	-	-	-
26	CHL	5	618	X	-	-	-
26	CHL	6	609	X	-	-	-
26	CHL	6	610	X	-	-	-
26	CHL	6	611	X	-	-	-
26	CHL	6	613	X	-	-	-
26	CHL	6	617	X	-	-	-
26	CHL	6	619	X	-	-	-
26	CHL	7	609	X	-	-	-
26	CHL	7	611	X	-	-	-
26	CHL	7	613	X	-	-	-
26	CHL	7	615	X	-	-	-
26	CHL	7	617	X	-	-	-
26	CHL	8	601	X	-	-	-
26	CHL	8	603	X	-	-	-
26	CHL	8	604	X	-	-	-
26	CHL	8	610	X	-	-	-
26	CHL	8	613	X	-	-	-
26	CHL	9	601	X	-	-	-
26	CHL	9	603	X	-	-	-
26	CHL	9	608	X	-	-	-
26	CHL	9	610	X	-	-	-
26	CHL	9	613	X	-	-	-
26	CHL	A	1114	X	-	-	-
26	CHL	a	604	X	-	-	-
26	CHL	a	606	X	-	-	-
26	CHL	a	609	X	-	-	-
26	CHL	a	610	X	-	-	-
26	CHL	a	613	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	NEX	F	4001	X	-	-	-
40	RRX	3	506	X	-	-	-
40	RRX	J	4002	X	-	-	-
43	LUT	2	507	X	-	-	-
43	LUT	4	501	X	-	-	-
43	LUT	7	501	X	-	-	-
46	QTB	a	504	X	-	-	-
50	XAT	2	501	X	-	-	-
50	XAT	7	502	X	-	-	-
50	XAT	9	504	X	-	-	-
50	XAT	9	507	X	-	-	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 56369 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5824	3815	988	1001	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	ALA	SER	conflict	UNP W8SY74
A	437	ILE	MET	conflict	UNP W8SY74

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5796	3807	980	994	15		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP W8SUA3
B	5	LEU	-	insertion	UNP W8SUA3
B	241	ALA	VAL	conflict	UNP W8SUA3
B	402	ALA	GLU	conflict	UNP W8SUA3
B	403	GLN	ALA	conflict	UNP W8SUA3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			601	367	104	119	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1124	716	196	208	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	188	ALA	VAL	conflict	UNP A0A2P6TKF8
D	320	ILE	VAL	conflict	UNP A0A2P6TKF8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	64	Total	C	N	O	S	0	0
			509	323	91	95			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	44	GLN	THR	conflict	UNP A0A2P6U4S6
E	48	LEU	MET	conflict	UNP A0A2P6U4S6
E	96	VAL	GLU	conflict	UNP A0A2P6U4S6
E	97	ALA	GLU	conflict	UNP A0A2P6U4S6
E	98	ALA	VAL	conflict	UNP A0A2P6U4S6

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1277	830	216	228	3		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	346	LEU	MET	conflict	UNP A0A2P6TPV8
F	348	ASN	LYS	conflict	UNP A0A2P6TPV8
F	351	ALA	GLU	conflict	UNP A0A2P6TPV8
F	352	ASP	GLY	conflict	UNP A0A2P6TPV8
F	360	LYS	GLN	conflict	UNP A0A2P6TPV8
F	364	ALA	ASP	conflict	UNP A0A2P6TPV8
F	367	GLU	ASN	conflict	UNP A0A2P6TPV8
F	430	ALA	SER	conflict	UNP A0A2P6TPV8
F	431	ALA	SER	conflict	UNP A0A2P6TPV8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	432	THR	MET	conflict	UNP A0A2P6TPV8
F	433	ALA	THR	conflict	UNP A0A2P6TPV8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	99	Total	C	N	O	S	0	0
			727	466	127	130	4		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1229	ALA	SER	conflict	UNP A0A2P6TZI8
G	1272	LEU	MET	conflict	UNP A0A2P6TZI8
G	1285	ILE	VAL	conflict	UNP A0A2P6TZI8
G	1313	ILE	LEU	conflict	UNP A0A2P6TZI8
G	1317	SER	HIS	conflict	UNP A0A2P6TZI8
G	1320	GLY	GLN	conflict	UNP A0A2P6TZI8
G	1321	LEU	VAL	conflict	UNP A0A2P6TZI8
G	1324	ASN	VAL	conflict	UNP A0A2P6TZI8

- Molecule 8 is a protein called Photosystem I reaction center subunit VI-chloroplastic-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	94	Total	C	N	O	S	0	0
			729	457	132	139	1		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	92	ILE	VAL	conflict	UNP A0A2P6TPU7
H	102	GLY	LEU	conflict	UNP A0A2P6TPU7
H	105	ALA	SER	conflict	UNP A0A2P6TPU7
H	106	ALA	SER	conflict	UNP A0A2P6TPU7
H	109	ARG	SER	conflict	UNP A0A2P6TPU7
H	?	-	ILE	deletion	UNP A0A2P6TPU7
H	113	VAL	LYS	conflict	UNP A0A2P6TPU7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	41	Total	C	N	O	S	0	0
			316	212	46	57	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	86	Total	C	N	O	S	0	0
			613	390	106	115	2		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	74	ALA	GLU	conflict	UNP A0A2P6U0J1
K	103	LEU	ILE	conflict	UNP A0A2P6U0J1
K	105	CYS	VAL	conflict	UNP A0A2P6U0J1
K	107	ILE	VAL	conflict	UNP A0A2P6U0J1
K	108	VAL	ILE	conflict	UNP A0A2P6U0J1
K	112	LYS	ARG	conflict	UNP A0A2P6U0J1
K	113	SER	GLY	conflict	UNP A0A2P6U0J1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	157	Total	C	N	O	S	0	0
			1165	758	192	211	4		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	350	TYR	PHE	conflict	UNP A0A2P6TC44
L	364	ASP	ASN	conflict	UNP A0A2P6TC44
L	?	-	ALA	deletion	UNP A0A2P6TC44
L	421	ASP	GLU	conflict	UNP A0A2P6TC44
L	443	LEU	ILE	conflict	UNP A0A2P6TC44

- Molecule 12 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O	S	0	0
			239	163	36	39	1		

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	35	Total	C	N	O	S	0	0
			270	183	37	47	3		

- Molecule 14 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	87	Total	C	N	O	S	0	0
			679	453	109	115	2		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	192	Total	C	N	O	S	0	0
			1405	900	237	261	7		
15	a	192	Total	C	N	O	S	0	0
			1405	900	237	261	7		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	166	SER	LEU	conflict	UNP A0A2P6TT36
1	167	LYS	GLU	conflict	UNP A0A2P6TT36
1	171	THR	VAL	conflict	UNP A0A2P6TT36
1	194	THR	ASN	conflict	UNP A0A2P6TT36
1	196	ALA	GLN	conflict	UNP A0A2P6TT36
1	204	SER	ALA	conflict	UNP A0A2P6TT36
1	210	MET	LEU	conflict	UNP A0A2P6TT36
a	166	SER	LEU	conflict	UNP A0A2P6TT36
a	167	LYS	GLU	conflict	UNP A0A2P6TT36
a	171	THR	VAL	conflict	UNP A0A2P6TT36
a	194	THR	ASN	conflict	UNP A0A2P6TT36
a	196	ALA	GLN	conflict	UNP A0A2P6TT36
a	204	SER	ALA	conflict	UNP A0A2P6TT36
a	210	MET	LEU	conflict	UNP A0A2P6TT36

- Molecule 16 is a protein called Glutathione reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	241	Total	C	N	O	S	0	0
			1844	1194	302	337	11		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	314	CYS	GLY	conflict	UNP A0A2P6TMT4
3	329	ILE	VAL	conflict	UNP A0A2P6TMT4
3	339	THR	SER	conflict	UNP A0A2P6TMT4
3	359	LYS	ASN	conflict	UNP A0A2P6TMT4
3	405	GLY	ALA	conflict	UNP A0A2P6TMT4
3	429	GLU	ALA	conflict	UNP A0A2P6TMT4
3	484	THR	ARG	conflict	UNP A0A2P6TMT4
3	485	ILE	ARG	conflict	UNP A0A2P6TMT4
3	486	LEU	ARG	conflict	UNP A0A2P6TMT4
3	487	LYS	ALA	conflict	UNP A0A2P6TMT4

- Molecule 17 is a protein called Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	4	207	Total	C	N	O	S	0	0
			1631	1056	277	294	4		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5	229	Total	C	N	O	S	0	0
			1786	1146	310	317	13		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	32	LYS	ASP	conflict	UNP A0A2P6U4K1
5	38	VAL	ALA	conflict	UNP A0A2P6U4K1
5	40	ALA	SER	conflict	UNP A0A2P6U4K1
5	42	GLY	ALA	conflict	UNP A0A2P6U4K1
5	113	SER	GLY	conflict	UNP A0A2P6U4K1
5	127	ILE	LEU	conflict	UNP A0A2P6U4K1
5	195	VAL	ILE	conflict	UNP A0A2P6U4K1

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	231	Total	C	N	O	S	0	0
			1787	1168	295	314	10		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	83	CYS	ALA	conflict	UNP A0A2P6TPR7
6	94	LEU	MET	conflict	UNP A0A2P6TPR7
6	196	ILE	VAL	conflict	UNP A0A2P6TPR7
6	201	ALA	GLY	conflict	UNP A0A2P6TPR7
6	250	GLN	ASN	conflict	UNP A0A2P6TPR7

- Molecule 20 is a protein called Lhca7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	7	221	Total	C	N	O	S	0	0
			1698	1090	294	308	6		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	8	219	Total	C	N	O	S	0	0
			1669	1073	285	305	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	103	GLU	ASP	conflict	UNP A0A2P6TZ50

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	2	215	Total	C	N	O	S	0	0
			1666	1074	277	309	6		

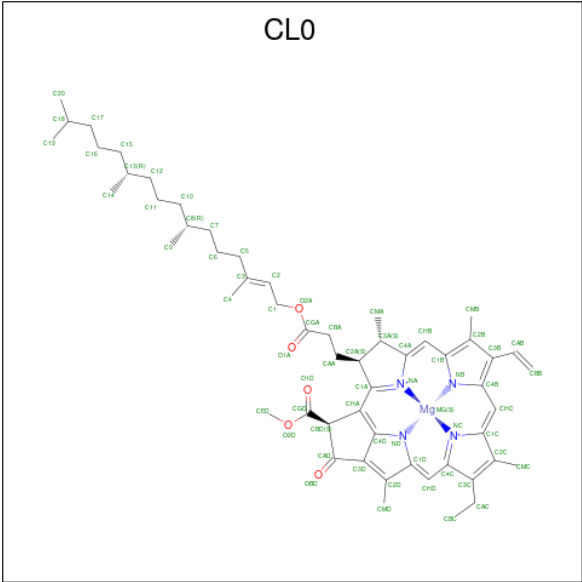
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	64	ASP	GLU	conflict	UNP A0A2P6TMX4
2	97	PRO	ASN	conflict	UNP A0A2P6TMX4

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

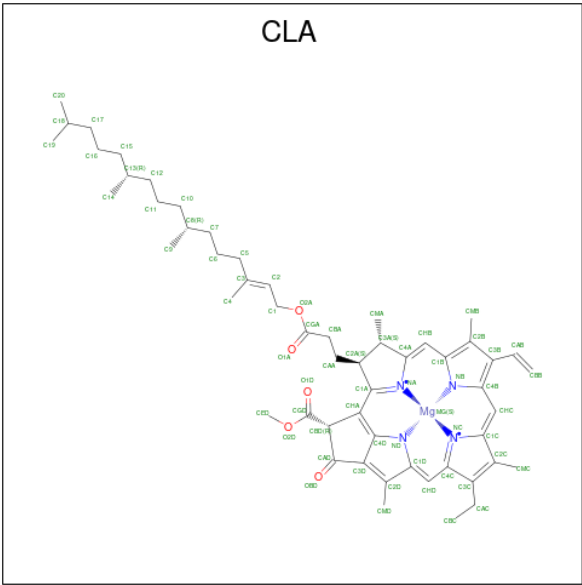
Mol	Chain	Residues	Atoms					AltConf	Trace
23	9	183	Total	C	N	O	S	0	0
			1406	909	237	254	6		

- Molecule 24 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 55	C 45	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	B	1	Total	C	N	O		0
			64	55	4	5		
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	F	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	K	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
25	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	5	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	7	1	Total 44	C 34	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

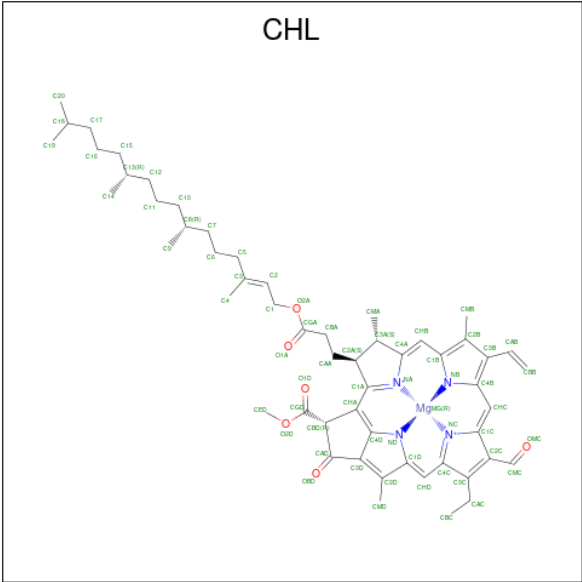
Mol	Chain	Residues	Atoms					AltConf
25	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
25	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	7	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	8	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	2	1	Total 52	C 42	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 26 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	a	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
26	a	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	a	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
26	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
26	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

Continued on next page...

Continued from previous page...

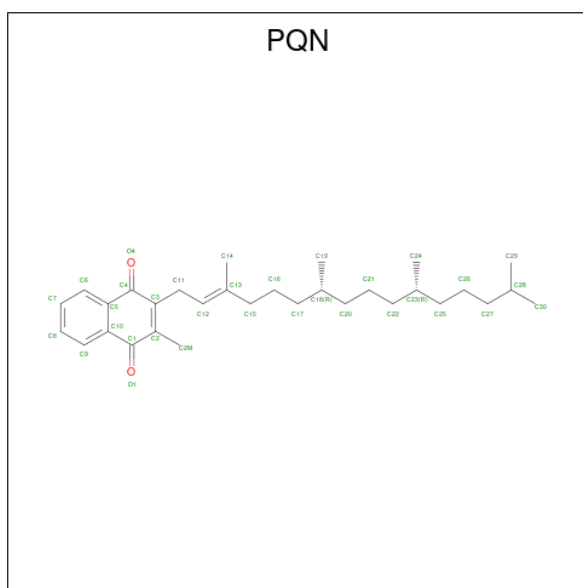
Mol	Chain	Residues	Atoms					AltConf
26	3	1	Total 61	C 50	Mg 1	N 4	O 6	0
26	4	1	Total 52	C 41	Mg 1	N 4	O 6	0
26	4	1	Total 56	C 45	Mg 1	N 4	O 6	0
26	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
26	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
26	5	1	Total 51	C 40	Mg 1	N 4	O 6	0
26	5	1	Total 56	C 45	Mg 1	N 4	O 6	0
26	5	1	Total 47	C 36	Mg 1	N 4	O 6	0
26	5	1	Total 51	C 40	Mg 1	N 4	O 6	0
26	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
26	6	1	Total 56	C 45	Mg 1	N 4	O 6	0
26	6	1	Total 51	C 40	Mg 1	N 4	O 6	0
26	6	1	Total 51	C 40	Mg 1	N 4	O 6	0
26	6	1	Total 43	C 34	Mg 1	N 4	O 4	0
26	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
26	7	1	Total 62	C 51	Mg 1	N 4	O 6	0
26	7	1	Total 56	C 45	Mg 1	N 4	O 6	0
26	7	1	Total 61	C 50	Mg 1	N 4	O 6	0
26	7	1	Total 51	C 40	Mg 1	N 4	O 6	0
26	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
26	8	1	Total 61	C 50	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

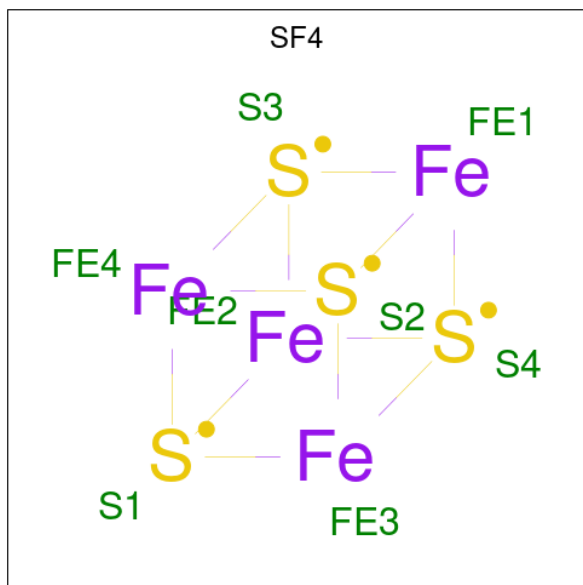
Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	8	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
26	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 27 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



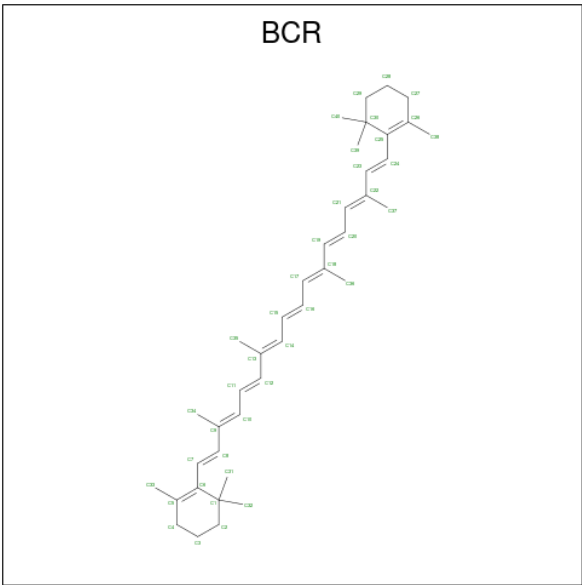
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			33	31	2	
27	B	1	Total	C	O	0
			33	31	2	

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



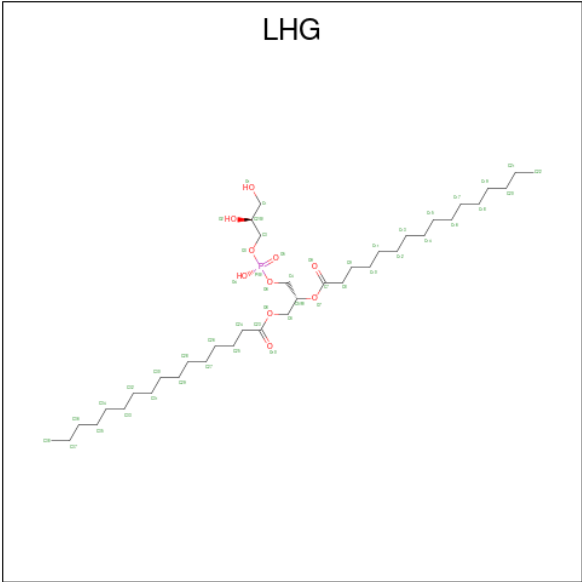
Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total	C	0
			40	40	
29	A	1	Total	C	0
			40	40	
29	A	1	Total	C	0
			40	40	
29	A	1	Total	C	0
			40	40	
29	A	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	B	1	Total	C	0
			40	40	
29	G	1	Total	C	0
			40	40	
29	H	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
29	J	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	I	1	Total C 40 40	0
29	O	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	4	1	Total C 40 40	0
29	5	1	Total C 40 40	0
29	5	1	Total C 40 40	0
29	6	1	Total C 40 40	0
29	6	1	Total C 40 40	0
29	7	1	Total C 40 40	0
29	8	1	Total C 40 40	0

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



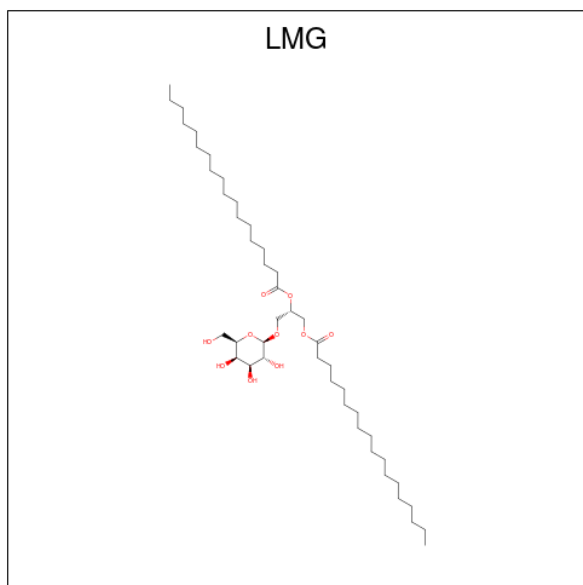
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			49	38	10	1	
30	A	1	Total	C	O	P	0
			49	38	10	1	
30	A	1	Total	C	O	P	0
			46	35	10	1	
30	B	1	Total	C	O	P	0
			49	38	10	1	
30	B	1	Total	C	O	P	0
			49	38	10	1	
30	F	1	Total	C	O	P	0
			36	25	10	1	
30	F	1	Total	C	O	P	0
			43	32	10	1	
30	1	1	Total	C	O	P	0
			35	24	10	1	
30	1	1	Total	C	O	P	0
			49	38	10	1	
30	a	1	Total	C	O	P	0
			35	24	10	1	
30	3	1	Total	C	O	P	0
			49	38	10	1	
30	4	1	Total	C	O	P	0
			32	21	10	1	
30	4	1	Total	C	O	P	0
			49	38	10	1	
30	5	1	Total	C	O	P	0
			49	38	10	1	

Continued on next page...

Continued from previous page...

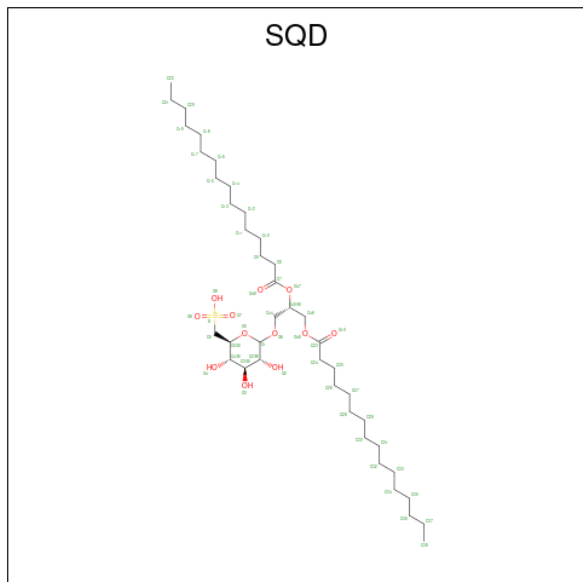
Mol	Chain	Residues	Atoms				AltConf
30	6	1	Total	C	O	P	0
			37	26	10	1	
30	6	1	Total	C	O	P	0
			49	38	10	1	
30	7	1	Total	C	O	P	0
			37	26	10	1	
30	7	1	Total	C	O	P	0
			36	25	10	1	
30	7	1	Total	C	O	P	0
			35	24	10	1	
30	8	1	Total	C	O	P	0
			37	26	10	1	
30	2	1	Total	C	O	P	0
			49	38	10	1	
30	2	1	Total	C	O	P	0
			49	38	10	1	
30	9	1	Total	C	O	P	0
			49	38	10	1	
30	9	1	Total	C	O	P	0
			33	22	10	1	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



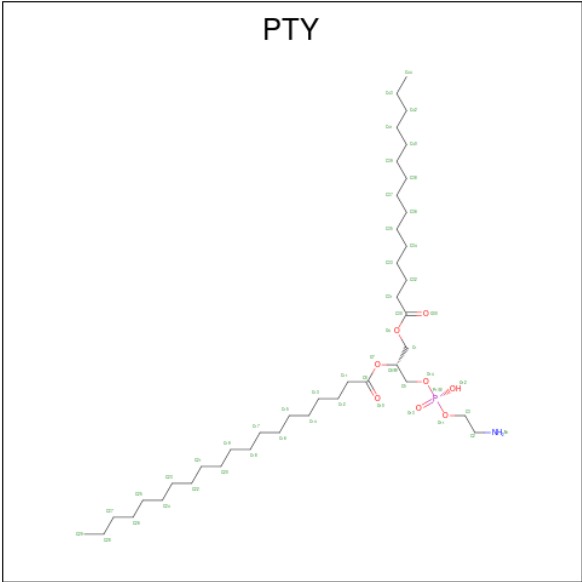
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			42	32	10	

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



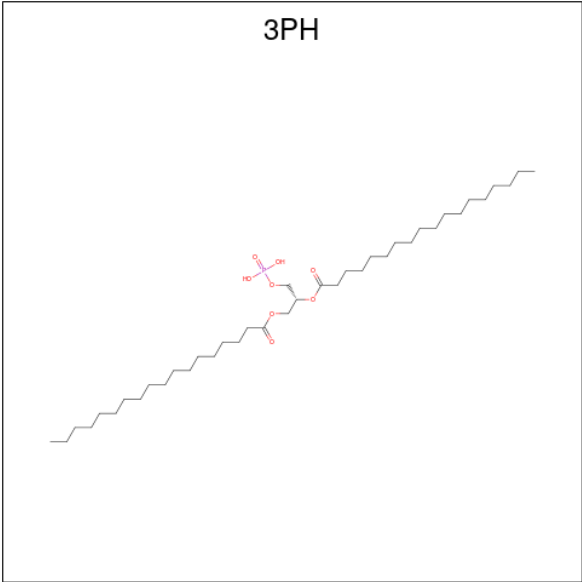
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O	S	0
			54	41	12	1	
32	G	1	Total	C	O	S	0
			46	33	12	1	
32	H	1	Total	C	O	S	0
			45	32	12	1	
32	I	1	Total	C	O	S	0
			54	41	12	1	
32	7	1	Total	C	O	S	0
			39	26	12	1	

- Molecule 33 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



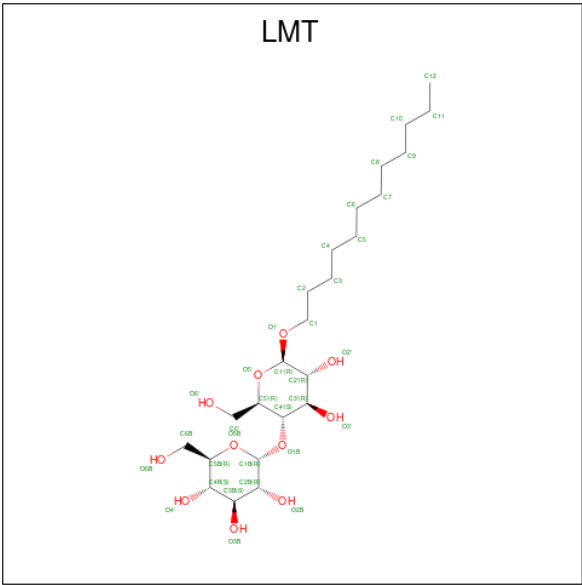
Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
33	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
33	G	1	Total	C	N	O	P	0
			28	18	1	8	1	
33	G	1	Total	C	N	O	P	0
			28	18	1	8	1	
33	J	1	Total	C	N	O	P	0
			28	18	1	8	1	
33	a	1	Total	C	N	O	P	0
			38	28	1	8	1	
33	a	1	Total	C	N	O	P	0
			38	28	1	8	1	
33	3	1	Total	C	N	O	P	0
			38	28	1	8	1	
33	5	1	Total	C	N	O	P	0
			38	28	1	8	1	
33	7	1	Total	C	N	O	P	0
			33	23	1	8	1	
33	9	1	Total	C	N	O	P	0
			48	38	1	8	1	

- Molecule 34 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O	P	0
			33	24	8	1	

- Molecule 35 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



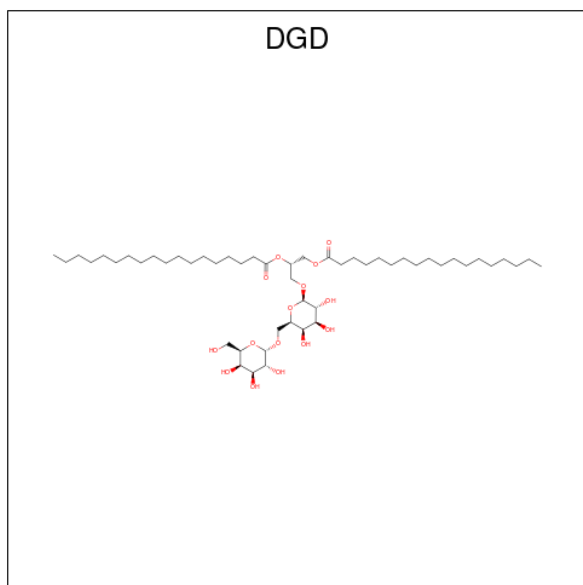
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			35	24	11	
35	B	1	Total	C	O	0
			35	24	11	
35	1	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

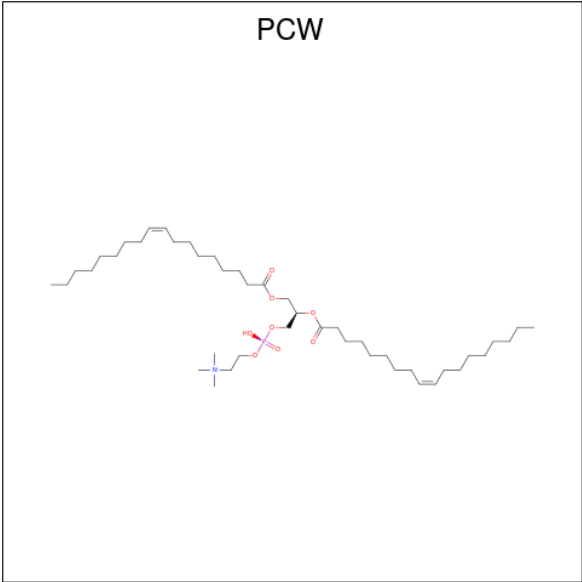
Mol	Chain	Residues	Atoms			AltConf
35	2	1	Total	C	O	0
			35	24	11	

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



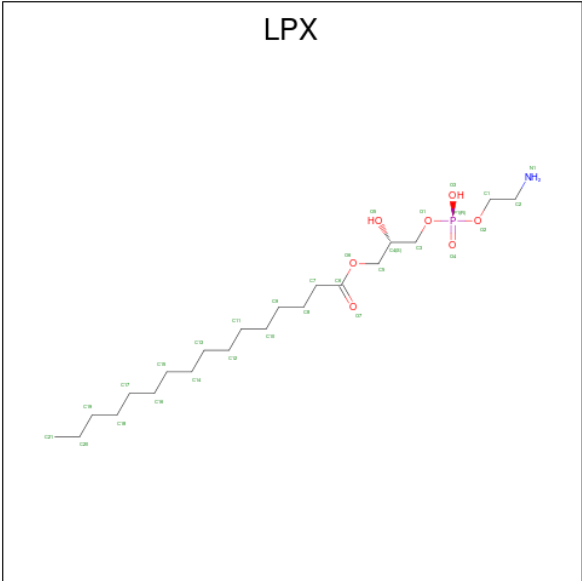
Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			66	51	15	
36	7	1	Total	C	O	0
			50	35	15	
36	8	1	Total	C	O	0
			59	44	15	
36	8	1	Total	C	O	0
			46	31	15	

- Molecule 37 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



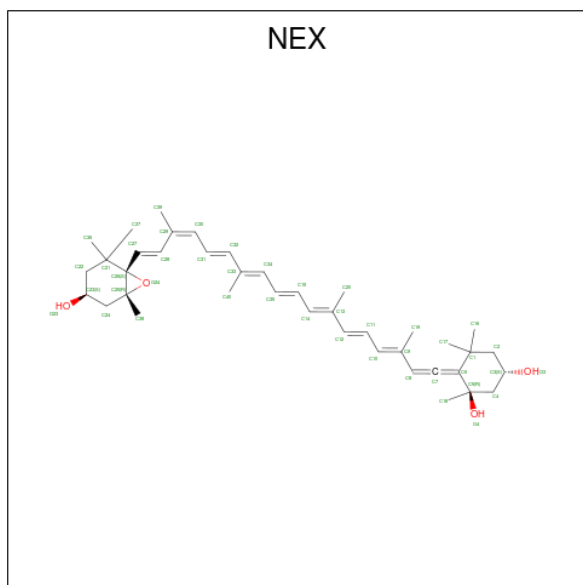
Mol	Chain	Residues	Atoms					AltConf
37	B	1	Total	C	N	O	P	0
			39	29	1	8	1	
37	K	1	Total	C	N	O	P	0
			36	26	1	8	1	
37	K	1	Total	C	N	O	P	0
			41	31	1	8	1	
37	6	1	Total	C	N	O	P	0
			36	26	1	8	1	

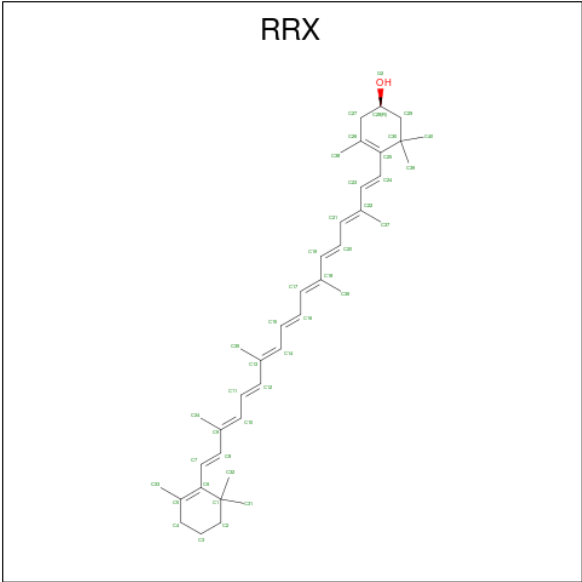
- Molecule 38 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



Mol	Chain	Residues	Atoms					AltConf
38	F	1	Total	C	N	O	P	0
			30	21	1	7	1	

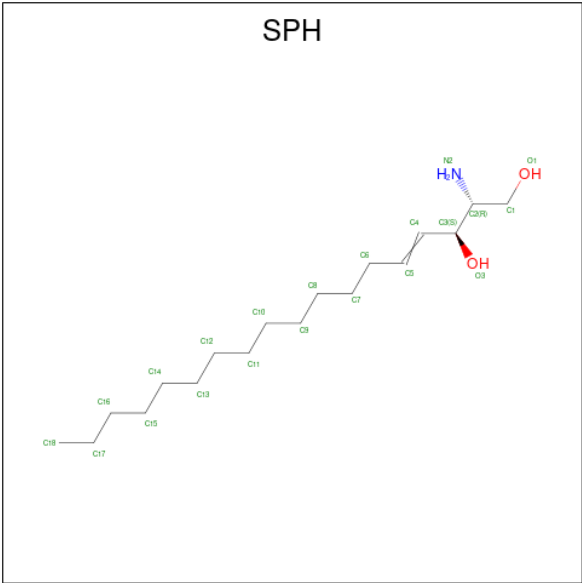
- Molecule 39 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).





Mol	Chain	Residues	Atoms			AltConf
40	J	1	Total	C	O	0
			41	40	1	
40	3	1	Total	C	O	0
			41	40	1	

- Molecule 41 is SPHINGOSINE (CCD ID: SPH) (formula: C₁₈H₃₇NO₂).



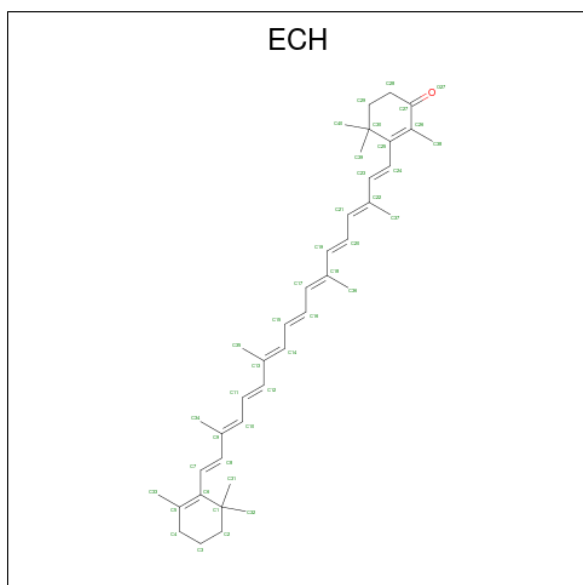
Mol	Chain	Residues	Atoms				AltConf
41	J	1	Total	C	N	O	0
			21	18	1	2	
41	4	1	Total	C	N	O	0
			21	18	1	2	

Continued on next page...

Continued from previous page...

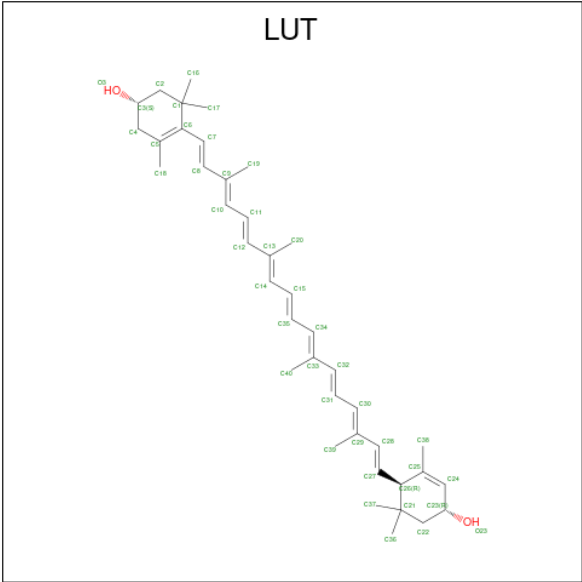
Mol	Chain	Residues	Atoms				AltConf
41	6	1	Total	C	N	O	0
			21	18	1	2	
41	9	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 42 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $C_{40}H_{54}O$).



Mol	Chain	Residues	Atoms			AltConf
42	M	1	Total	C	O	0
			41	40	1	

- Molecule 43 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



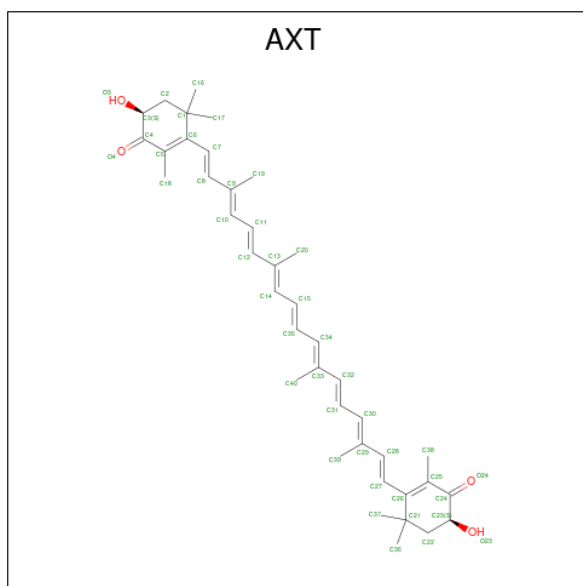
Mol	Chain	Residues	Atoms			AltConf
43	1	1	Total	C	O	0
			42	40	2	
43	1	1	Total	C	O	0
			42	40	2	
43	a	1	Total	C	O	0
			42	40	2	
43	a	1	Total	C	O	0
			42	40	2	
43	a	1	Total	C	O	0
			42	40	2	
43	3	1	Total	C	O	0
			42	40	2	
43	3	1	Total	C	O	0
			42	40	2	
43	4	1	Total	C	O	0
			42	40	2	
43	4	1	Total	C	O	0
			42	40	2	
43	5	1	Total	C	O	0
			42	40	2	
43	5	1	Total	C	O	0
			42	40	2	
43	5	1	Total	C	O	0
			42	40	2	
43	6	1	Total	C	O	0
			42	40	2	
43	6	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

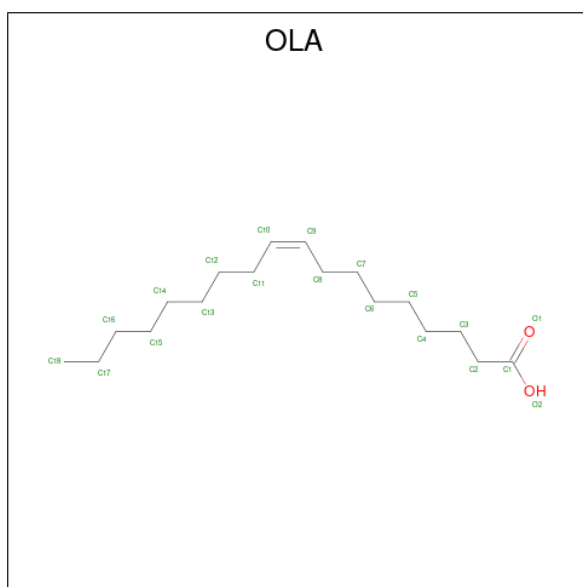
Mol	Chain	Residues	Atoms			AltConf
43	7	1	Total	C	O	0
			42	40	2	
43	8	1	Total	C	O	0
			42	40	2	
43	8	1	Total	C	O	0
			42	40	2	
43	2	1	Total	C	O	0
			42	40	2	
43	2	1	Total	C	O	0
			42	40	2	
43	9	1	Total	C	O	0
			42	40	2	
43	9	1	Total	C	O	0
			42	40	2	

- Molecule 44 is ASTAXANTHIN (CCD ID: AXT) (formula: $C_{40}H_{52}O_4$).



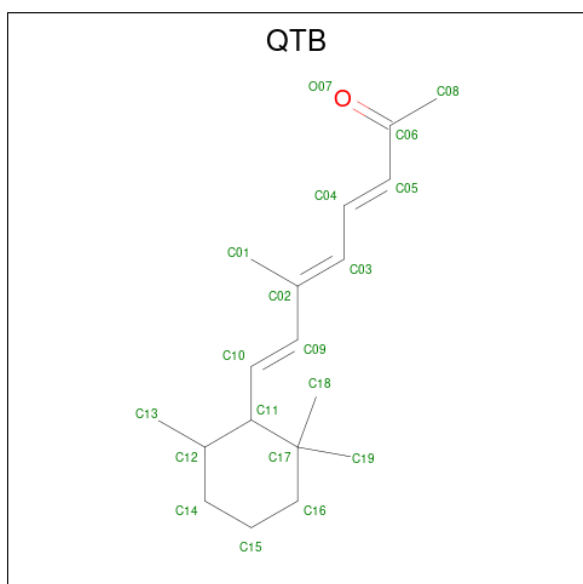
Mol	Chain	Residues	Atoms			AltConf
44	1	1	Total	C	O	0
			43	40	3	
44	7	1	Total	C	O	0
			43	40	3	

- Molecule 45 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



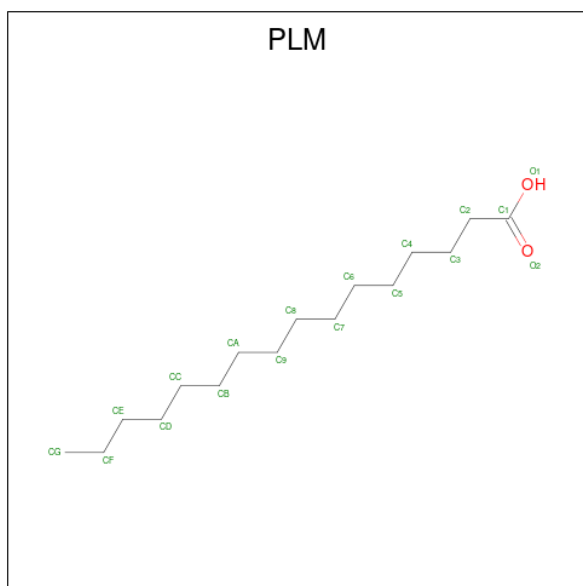
Mol	Chain	Residues	Atoms			AltConf
45	1	1	Total	C	O	0
			20	18	2	
45	a	1	Total	C	O	0
			20	18	2	
45	8	1	Total	C	O	0
			20	18	2	
45	8	1	Total	C	O	0
			20	18	2	

- Molecule 46 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (CCD ID: QTB) (formula: C₁₈H₂₈O).



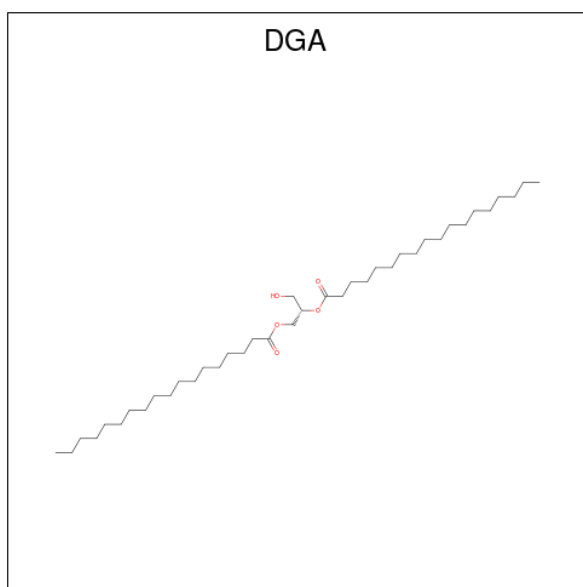
Mol	Chain	Residues	Atoms			AltConf
46	a	1	Total	C	O	0
			19	18	1	

- Molecule 47 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



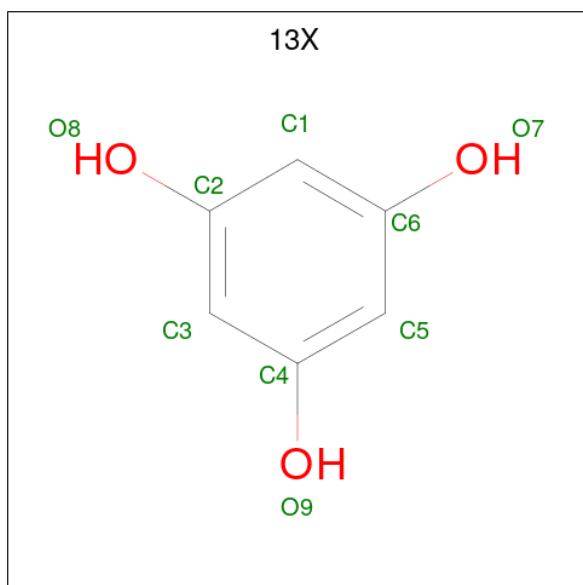
Mol	Chain	Residues	Atoms			AltConf
47	a	1	Total	C	O	0
			17	16	1	
47	4	1	Total	C	O	0
			18	16	2	
47	4	1	Total	C	O	0
			17	16	1	
47	5	1	Total	C	O	0
			18	16	2	
47	6	1	Total	C	O	0
			18	16	2	
47	8	1	Total	C	O	0
			17	16	1	
47	8	1	Total	C	O	0
			18	16	2	

- Molecule 48 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



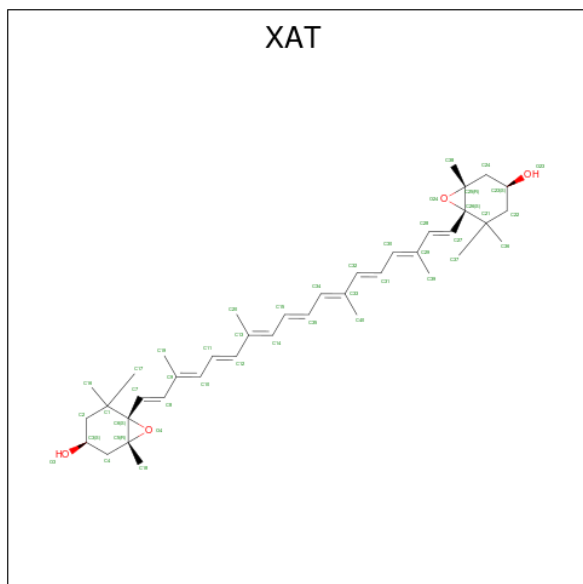
Mol	Chain	Residues	Atoms			AltConf
48	3	1	Total	C	O	0
			24	19	5	
48	5	1	Total	C	O	0
			23	18	5	
48	8	1	Total	C	O	0
			40	35	5	
48	2	1	Total	C	O	0
			37	32	5	

- Molecule 49 is benzene-1,3,5-triol (CCD ID: 13X) (formula: $C_6H_6O_3$).



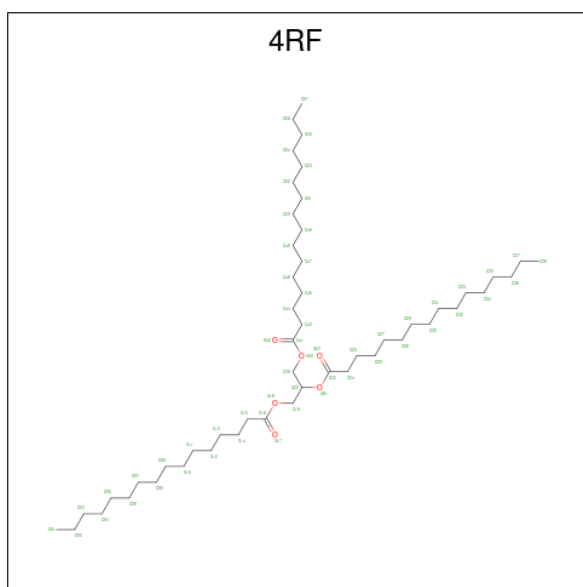
Mol	Chain	Residues	Atoms			AltConf
49	6	1	Total	C	O	0
			9	6	3	

- Molecule 50 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



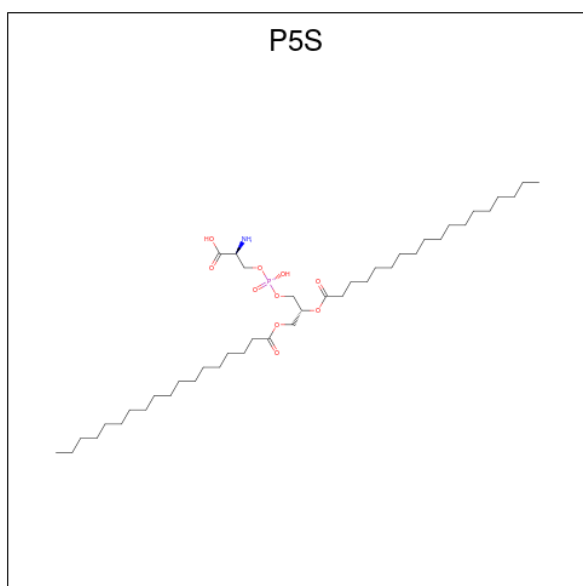
Mol	Chain	Residues	Atoms			AltConf
50	7	1	Total	C	O	0
			44	40	4	
50	2	1	Total	C	O	0
			44	40	4	
50	9	1	Total	C	O	0
			44	40	4	
50	9	1	Total	C	O	0
			44	40	4	

- Molecule 51 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: C₅₁H₉₈O₆).



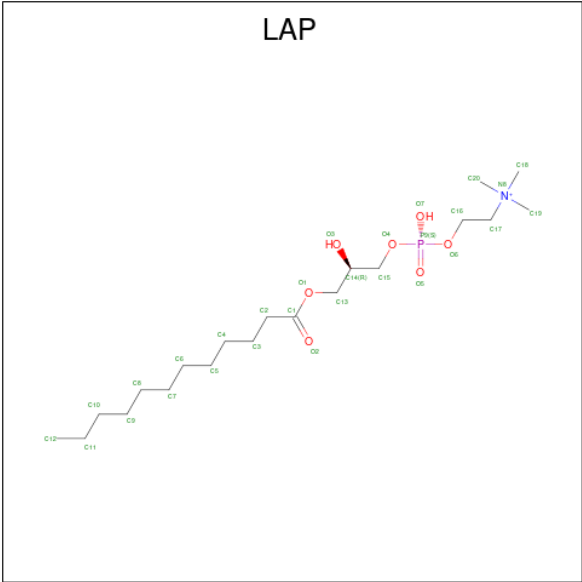
Mol	Chain	Residues	Atoms			AltConf
51	7	1	Total	C	O	0
			37	31	6	

- Molecule 52 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



Mol	Chain	Residues	Atoms					AltConf
52	8	1	Total	C	N	O	P	0
			37	25	1	10	1	

- Molecule 53 is [2-((1-OXODODECANOXY-(2-HYDROXY-3-PROPANYL))-PHOSPHONATE-OXY)-ETHYL]-TRIMETHYLAMMONIUM (CCD ID: LAP) (formula: C₂₀H₄₃NO₇P).



Mol	Chain	Residues	Atoms					AltConf
53	8	1	Total	C	N	O	P	0
			29	20	1	7	1	

- Molecule 54 is water.

Mol	Chain	Residues	Atoms		AltConf
54	A	20	Total	O	0
			20	20	
54	A	1	Total	O	0
			1	1	
54	B	2	Total	O	0
			2	2	
54	B	2	Total	O	0
			2	2	
54	B	5	Total	O	0
			5	5	
54	B	6	Total	O	0
			6	6	
54	B	4	Total	O	0
			4	4	
54	B	3	Total	O	0
			3	3	
54	B	1	Total	O	0
			1	1	
54	B	1	Total	O	0
			1	1	
54	C	1	Total	O	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
54	C	1	Total O 1 1	0
54	D	1	Total O 1 1	0
54	D	1	Total O 1 1	0
54	E	1	Total O 1 1	0
54	F	1	Total O 1 1	0
54	F	1	Total O 1 1	0
54	F	1	Total O 1 1	0
54	G	1	Total O 1 1	0
54	G	2	Total O 2 2	0
54	H	1	Total O 1 1	0
54	J	1	Total O 1 1	0
54	K	3	Total O 3 3	0
54	L	1	Total O 1 1	0
54	L	1	Total O 1 1	0
54	M	1	Total O 1 1	0
54	1	5	Total O 5 5	0
54	a	1	Total O 1 1	0
54	3	4	Total O 4 4	0
54	3	1	Total O 1 1	0
54	4	3	Total O 3 3	0
54	4	1	Total O 1 1	0

Continued on next page...

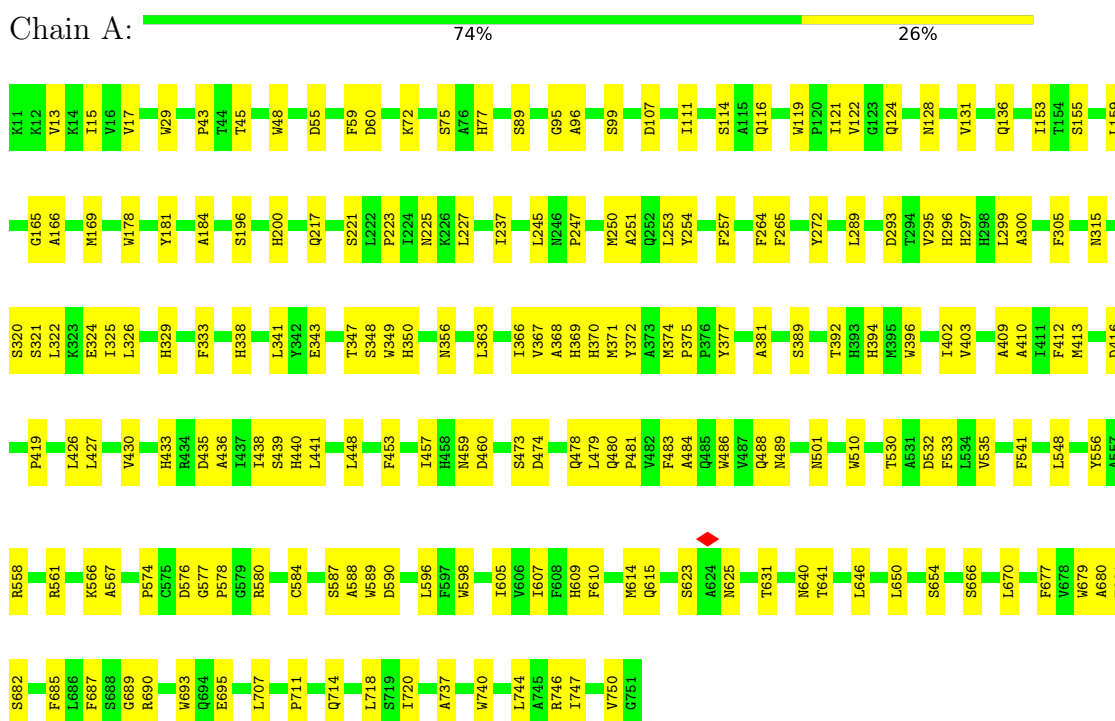
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
54	5	3	Total 3	O 3	0
54	6	7	Total 7	O 7	0
54	7	2	Total 2	O 2	0
54	8	1	Total 1	O 1	0
54	8	1	Total 1	O 1	0
54	2	4	Total 4	O 4	0
54	9	1	Total 1	O 1	0
54	9	1	Total 1	O 1	0

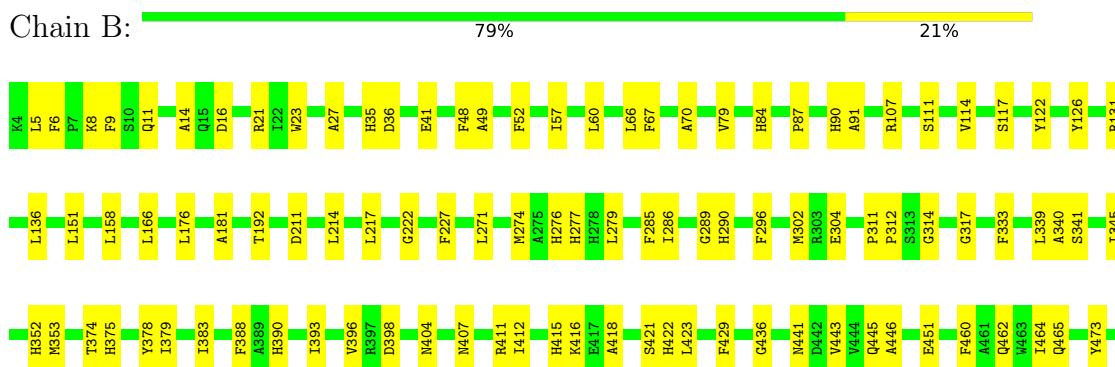
3 Residue-property plots

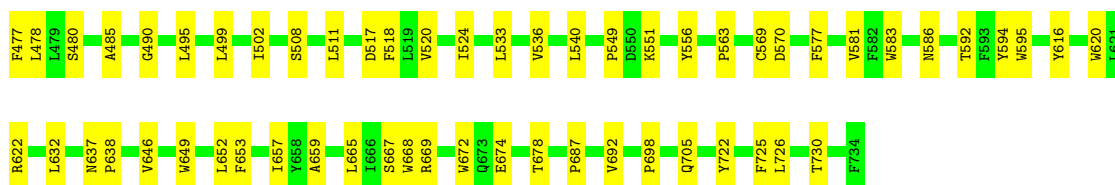
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





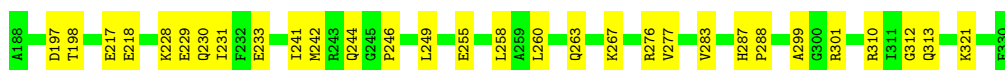
• Molecule 3: Photosystem I iron-sulfur center

Chain C: 78% 22%



• Molecule 4: Photosystem I reaction center subunit chloroplastic

Chain D: 79% 21%



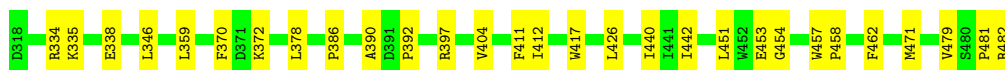
• Molecule 5: Photosystem I reaction center subunit IV

Chain E: 80% 20%



• Molecule 6: PSI-F

Chain F: 82% 18%



• Molecule 7: Photosystem I reaction center subunit chloroplastic

Chain G: 84% 16%

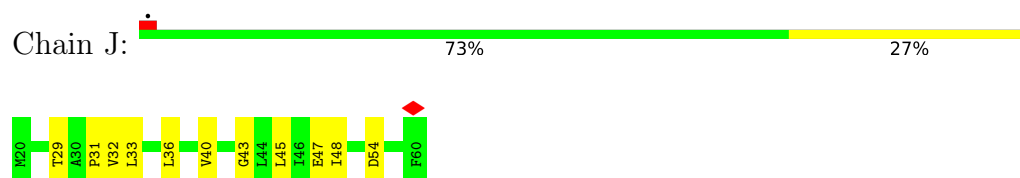


• Molecule 8: Photosystem I reaction center subunit VI-chloroplastic-like

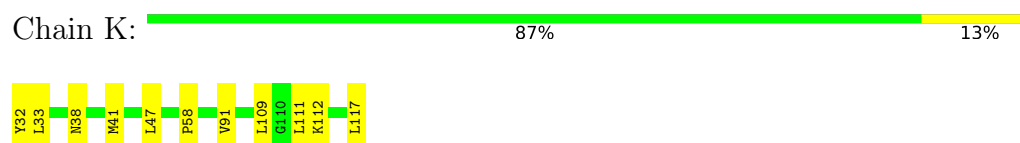
Chain H: 5% 68% 32%



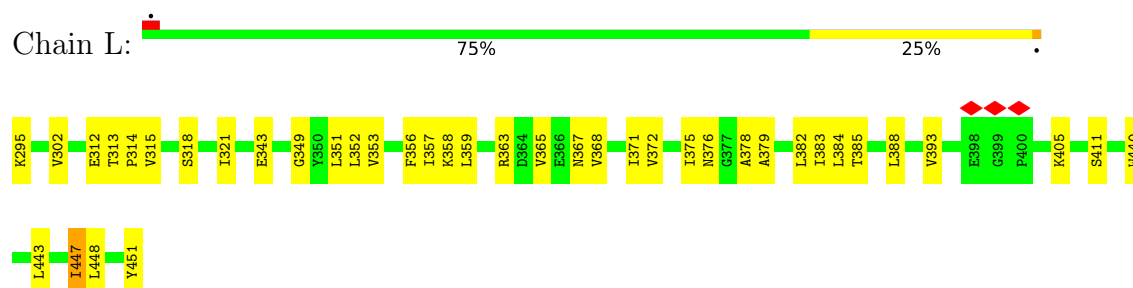
- Molecule 9: Photosystem I reaction center subunit IX



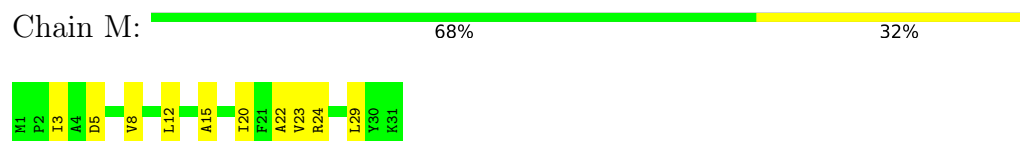
- Molecule 10: Photosystem I reaction center subunit chloroplastic



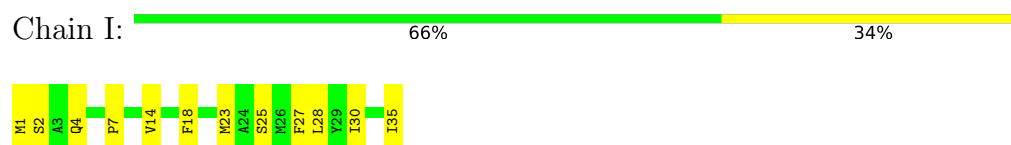
- Molecule 11: Photosystem I reaction center subunit XI



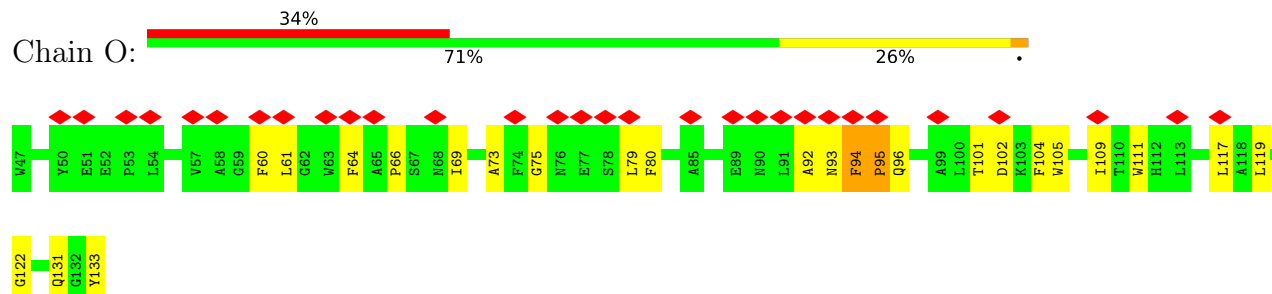
- Molecule 12: Photosystem I reaction center subunit XII



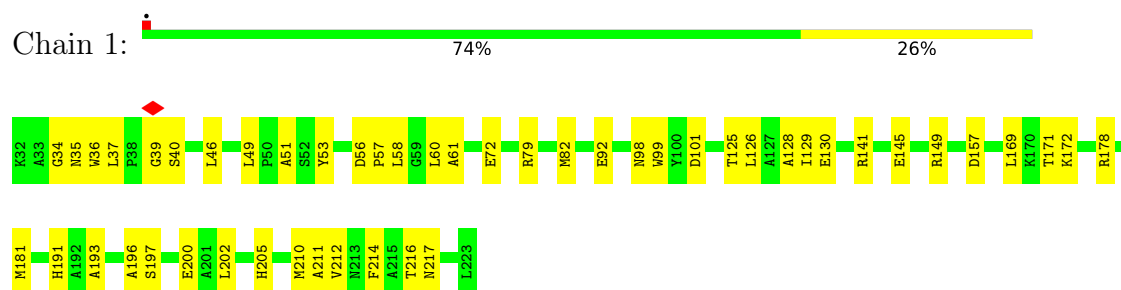
- Molecule 13: Photosystem I reaction center subunit VIII



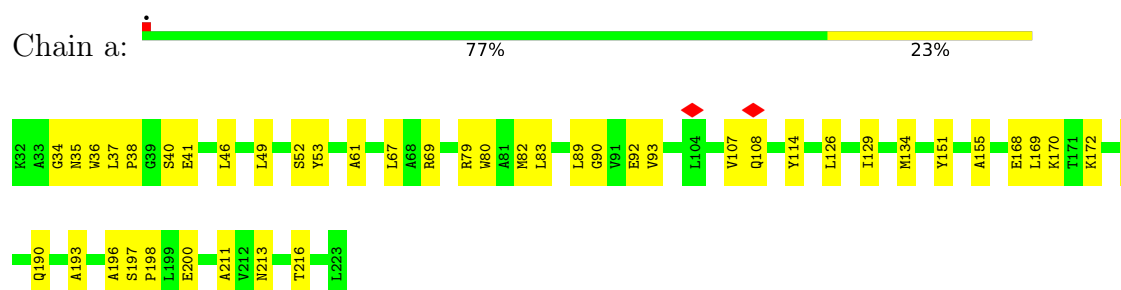
- Molecule 14: Photosystem I subunit O



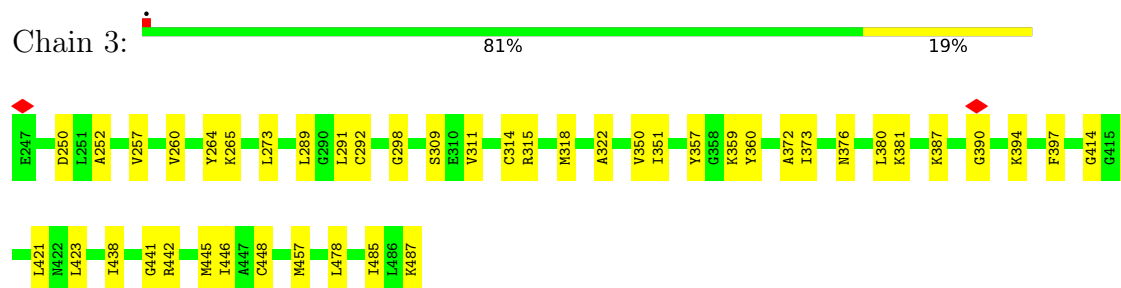
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



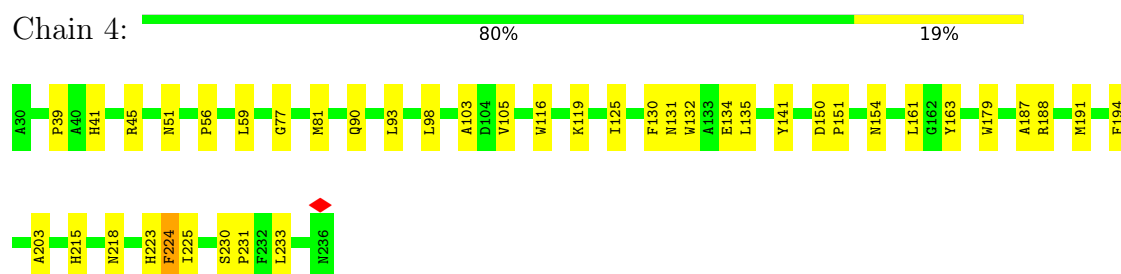
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



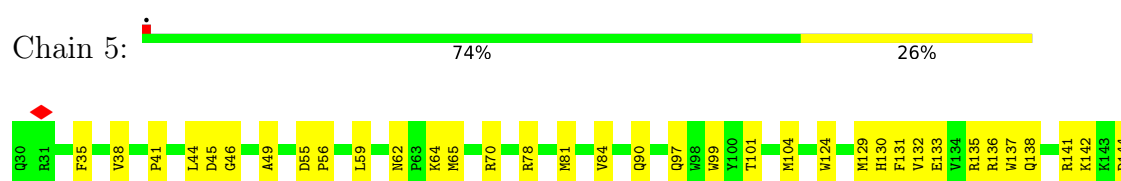
- Molecule 16: Glutathione reductase



- Molecule 17: Lhca4

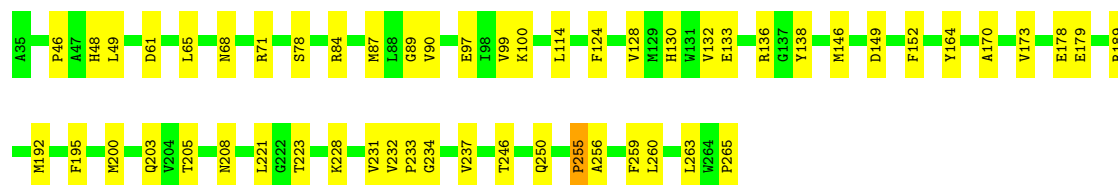
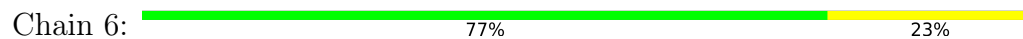


- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

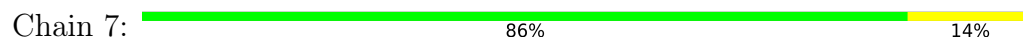




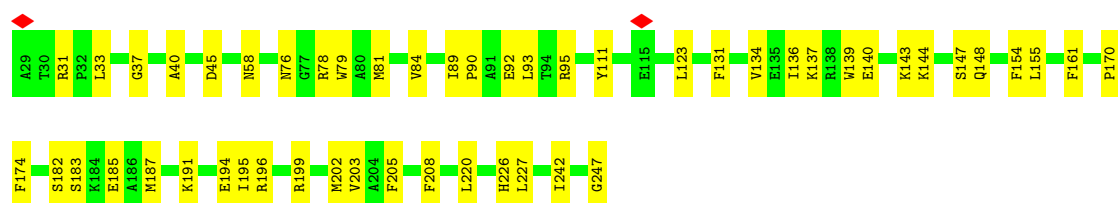
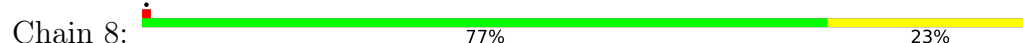
- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



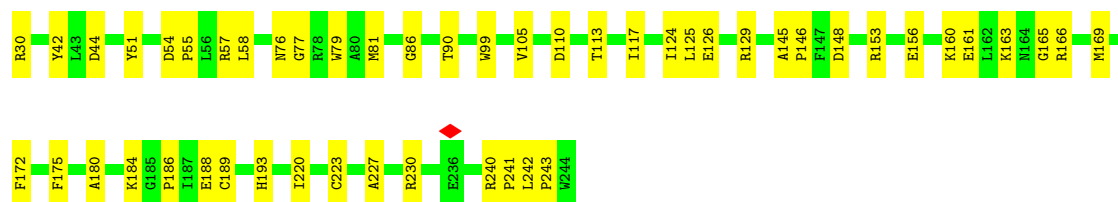
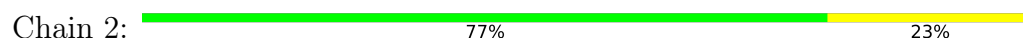
- Molecule 20: Lhca7



- Molecule 21: Chlorophyll a-b binding protein, chloroplastic



- Molecule 22: Chlorophyll a-b binding protein, chloroplastic



- Molecule 23: Chlorophyll a-b binding protein, chloroplastic



L394	T395	R396	N414	P423	G427
------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	185138	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.05	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0112	Depositor
Map size ($\text{\AA}$)	394.56, 394.56, 394.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82199997, 0.82199997, 0.82199997	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, PLM, PCW, ECH, 4RF, LUT, SF4, LAP, BCR, 13X, SPH, 3PH, PTY, P5S, CLA, LMT, QTB, SQD, OLA, RRX, XAT, LMG, CL0, PQN, CHL, DGA, LPX, LHG, AXT, NEX

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	0.16	0/6022	0.39	0/8215
2	B	0.16	0/6006	0.39	1/8205 (0.0%)
3	C	0.14	0/611	0.35	0/828
4	D	0.13	0/1150	0.41	0/1551
5	E	0.13	0/520	0.39	0/705
6	F	0.15	0/1309	0.36	0/1771
7	G	0.13	0/743	0.31	0/1007
8	H	0.15	0/744	0.43	0/1000
9	J	0.13	0/322	0.33	0/439
10	K	0.13	0/622	0.32	0/844
11	L	0.16	0/1195	0.40	0/1635
12	M	0.14	0/244	0.32	0/330
13	I	0.15	0/276	0.43	0/373
14	O	0.18	0/703	0.49	0/956
15	1	0.15	0/1443	0.35	0/1960
15	a	0.16	0/1443	0.41	0/1960
16	3	0.16	0/1896	0.38	0/2573
17	4	0.15	0/1681	0.39	0/2285
18	5	0.14	0/1842	0.31	0/2505
19	6	0.15	0/1845	0.37	0/2515
20	7	0.16	0/1748	0.37	0/2372
21	8	0.17	0/1717	0.36	0/2330
22	2	0.14	0/1708	0.35	0/2318
23	9	0.15	0/1444	0.32	0/1957
All	All	0.15	0/37234	0.38	1/50634 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	222	GLY	N-CA-C	5.41	119.41	110.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5824	0	5675	171	0
2	B	5796	0	5576	137	0
3	C	601	0	576	15	0
4	D	1124	0	1129	21	0
5	E	509	0	507	8	0
6	F	1277	0	1296	21	0
7	G	727	0	724	14	0
8	H	729	0	705	26	0
9	J	316	0	332	9	0
10	K	613	0	639	10	0
11	L	1165	0	1181	37	0
12	M	239	0	255	10	0
13	I	270	0	287	12	0
14	O	679	0	661	26	0
15	1	1405	0	1370	43	0
15	a	1405	0	1370	41	0
16	3	1844	0	1805	37	0
17	4	1631	0	1575	35	0
18	5	1786	0	1736	50	0
19	6	1787	0	1760	43	0
20	7	1698	0	1640	28	0
21	8	1669	0	1619	50	0
22	2	1666	0	1657	48	0
23	9	1406	0	1385	34	0
24	A	65	0	72	6	0
25	1	528	0	523	41	0
25	2	615	0	568	40	0
25	3	576	0	555	31	0
25	4	768	0	685	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	5	642	0	564	29	0
25	6	624	0	591	29	0
25	7	566	0	525	30	0
25	8	573	0	480	34	0
25	9	379	0	338	22	0
25	A	2532	0	2566	196	0
25	B	2583	0	2685	168	0
25	F	105	0	88	7	0
25	G	155	0	130	8	0
25	H	156	0	130	7	0
25	J	42	0	30	2	0
25	K	200	0	161	12	0
25	L	205	0	168	11	0
25	O	134	0	95	6	0
25	a	496	0	443	22	0
26	1	284	0	248	26	0
26	2	165	0	137	7	0
26	3	236	0	223	18	0
26	4	174	0	154	15	0
26	5	271	0	217	15	0
26	6	333	0	284	23	0
26	7	296	0	267	21	0
26	8	296	0	265	19	0
26	9	273	0	233	23	0
26	A	66	0	69	8	0
26	a	264	0	205	29	0
27	A	33	0	46	7	0
27	B	33	0	46	5	0
28	A	8	0	0	0	0
28	C	16	0	0	1	0
29	3	120	0	158	11	0
29	4	40	0	53	8	0
29	5	80	0	103	8	0
29	6	80	0	106	8	0
29	7	40	0	52	9	0
29	8	40	0	53	3	0
29	A	200	0	264	23	0
29	B	280	0	371	34	0
29	G	40	0	53	5	0
29	H	40	0	53	4	0
29	I	40	0	52	2	0
29	J	40	0	53	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	K	80	0	106	7	0
29	L	120	0	159	6	0
29	O	40	0	52	1	0
30	1	84	0	114	5	0
30	2	98	0	148	11	0
30	3	49	0	74	1	0
30	4	81	0	108	4	0
30	5	49	0	74	2	0
30	6	86	0	118	5	0
30	7	108	0	126	3	0
30	8	37	0	44	1	0
30	9	82	0	110	7	0
30	A	144	0	213	8	0
30	B	98	0	148	6	0
30	F	79	0	101	2	0
30	a	35	0	40	2	0
31	A	42	0	54	0	0
32	7	39	0	41	1	0
32	A	54	0	77	8	0
32	G	46	0	55	4	0
32	H	45	0	53	3	0
32	I	54	0	77	4	0
33	3	38	0	49	3	0
33	5	38	0	49	3	0
33	7	33	0	39	0	0
33	9	48	0	72	4	0
33	A	34	0	41	4	0
33	B	42	0	60	2	0
33	G	56	0	62	2	0
33	J	28	0	29	2	0
33	a	76	0	98	4	0
34	A	33	0	39	3	0
35	1	35	0	46	2	0
35	2	35	0	45	5	0
35	A	35	0	45	1	0
35	B	35	0	45	2	0
36	7	50	0	58	3	0
36	8	105	0	126	7	0
36	B	66	0	96	4	0
37	6	36	0	44	3	0
37	B	39	0	50	1	0
37	K	77	0	99	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	F	30	0	43	2	0
39	F	44	0	54	4	0
40	3	41	0	56	1	0
40	J	41	0	56	3	0
41	4	21	0	37	0	0
41	6	21	0	37	1	0
41	9	21	0	37	2	0
41	J	21	0	37	1	0
42	M	41	0	54	5	0
43	1	84	0	110	6	0
43	2	84	0	110	11	0
43	3	84	0	110	7	0
43	4	84	0	110	10	0
43	5	126	0	165	12	0
43	6	84	0	110	10	0
43	7	42	0	55	5	0
43	8	84	0	110	11	0
43	9	84	0	110	17	0
43	a	126	0	165	13	0
44	1	43	0	52	3	0
44	7	43	0	52	10	0
45	1	20	0	33	2	0
45	8	40	0	66	1	0
45	a	20	0	33	2	0
46	a	19	0	0	0	0
47	4	35	0	62	3	0
47	5	18	0	31	3	0
47	6	18	0	31	1	0
47	8	35	0	62	6	0
47	a	17	0	31	0	0
48	2	37	0	56	6	0
48	3	24	0	30	3	0
48	5	23	0	28	3	0
48	8	40	0	65	5	0
49	6	9	0	6	0	0
50	2	44	0	56	3	0
50	7	44	0	56	3	0
50	9	88	0	112	7	0
51	7	37	0	49	6	0
52	8	37	0	40	2	0
53	8	29	0	42	4	0
54	1	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2	4	0	0	0	0
54	3	5	0	0	0	0
54	4	4	0	0	0	0
54	5	3	0	0	0	0
54	6	7	0	0	0	0
54	7	2	0	0	0	0
54	8	2	0	0	0	0
54	9	2	0	0	0	0
54	A	21	0	0	1	0
54	B	24	0	0	0	0
54	C	2	0	0	0	0
54	D	2	0	0	0	0
54	E	1	0	0	0	0
54	F	3	0	0	0	0
54	G	3	0	0	0	0
54	H	1	0	0	0	0
54	J	1	0	0	0	0
54	K	3	0	0	0	0
54	L	2	0	0	0	0
54	M	1	0	0	0	0
54	a	1	0	0	0	0
All	All	56369	0	56465	1606	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 1606 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:295:LYS:N	14:O:133:TYR:HH	1.63	0.94
50:9:504:XAT:H32	50:9:507:XAT:H10	1.50	0.94
1:A:396:TRP:CD1	25:A:1126:CLA:HAB	2.04	0.92
18:5:161:GLU:OE2	18:5:183:GLN:NE2	2.05	0.89
11:L:356:PHE:HB2	11:L:372:VAL:HG13	1.55	0.89

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/741 (100%)	709 (96%)	30 (4%)	0	100	100
2	B	729/731 (100%)	697 (96%)	32 (4%)	0	100	100
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	D	141/143 (99%)	129 (92%)	12 (8%)	0	100	100
5	E	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
6	F	163/165 (99%)	154 (94%)	9 (6%)	0	100	100
7	G	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
8	H	92/94 (98%)	80 (87%)	11 (12%)	1 (1%)	11	29
9	J	39/41 (95%)	39 (100%)	0	0	100	100
10	K	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
11	L	155/157 (99%)	144 (93%)	10 (6%)	1 (1%)	21	44
12	M	29/31 (94%)	29 (100%)	0	0	100	100
13	I	33/35 (94%)	29 (88%)	4 (12%)	0	100	100
14	O	85/87 (98%)	66 (78%)	16 (19%)	3 (4%)	3	6
15	1	190/192 (99%)	174 (92%)	15 (8%)	1 (0%)	24	48
15	a	190/192 (99%)	171 (90%)	19 (10%)	0	100	100
16	3	239/241 (99%)	225 (94%)	13 (5%)	1 (0%)	30	54
17	4	205/207 (99%)	184 (90%)	19 (9%)	2 (1%)	12	32
18	5	227/229 (99%)	214 (94%)	13 (6%)	0	100	100
19	6	229/231 (99%)	213 (93%)	15 (7%)	1 (0%)	30	54
20	7	219/221 (99%)	207 (94%)	11 (5%)	1 (0%)	24	48
21	8	217/219 (99%)	207 (95%)	10 (5%)	0	100	100
22	2	213/215 (99%)	197 (92%)	16 (8%)	0	100	100
23	9	181/183 (99%)	171 (94%)	10 (6%)	0	100	100
All	All	4636/4684 (99%)	4348 (94%)	277 (6%)	11 (0%)	44	68

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	118	PRO
14	O	93	ASN
14	O	95	PRO
15	1	36	TRP
17	4	224	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	600/600 (100%)	600 (100%)	0	100	100
2	B	588/588 (100%)	588 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	121/121 (100%)	121 (100%)	0	100	100
5	E	55/55 (100%)	55 (100%)	0	100	100
6	F	126/126 (100%)	126 (100%)	0	100	100
7	G	71/71 (100%)	71 (100%)	0	100	100
8	H	71/71 (100%)	71 (100%)	0	100	100
9	J	35/35 (100%)	35 (100%)	0	100	100
10	K	66/66 (100%)	66 (100%)	0	100	100
11	L	122/122 (100%)	122 (100%)	0	100	100
12	M	23/23 (100%)	23 (100%)	0	100	100
13	I	30/30 (100%)	30 (100%)	0	100	100
14	O	66/66 (100%)	66 (100%)	0	100	100
15	1	134/134 (100%)	134 (100%)	0	100	100
15	a	134/134 (100%)	134 (100%)	0	100	100
16	3	186/186 (100%)	186 (100%)	0	100	100
17	4	165/165 (100%)	165 (100%)	0	100	100
18	5	185/185 (100%)	185 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	6	187/187 (100%)	187 (100%)	0	100	100
20	7	176/176 (100%)	176 (100%)	0	100	100
21	8	168/168 (100%)	168 (100%)	0	100	100
22	2	173/173 (100%)	173 (100%)	0	100	100
23	9	141/141 (100%)	141 (100%)	0	100	100
All	All	3692/3692 (100%)	3692 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
18	5	76	ASN
22	2	76	ASN
18	5	189	ASN
21	8	71	ASN
22	2	209	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

403 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	1113	-	64,68,73	1.40	6 (9%)	76,107,113	1.94	18 (23%)
25	CLA	1	608	-	64,68,73	1.39	8 (12%)	76,107,113	1.89	16 (21%)
25	CLA	K	1401	-	50,54,73	1.58	6 (12%)	59,90,113	1.98	14 (23%)
33	PTY	G	5002	-	27,27,49	1.04	2 (7%)	28,31,54	1.07	1 (3%)
25	CLA	A	1111	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	16 (19%)
45	OLA	1	803	-	19,19,19	0.57	0	19,19,19	1.02	0
29	BCR	I	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.45	15 (26%)
25	CLA	B	1231	-	69,73,73	1.35	6 (8%)	82,113,113	1.83	16 (19%)
25	CLA	2	615	-	60,64,73	1.46	7 (11%)	71,102,113	2.02	19 (26%)
49	13X	6	805	-	9,9,9	0.92	0	12,12,12	0.36	0
29	BCR	A	4004	-	41,41,41	1.63	4 (9%)	56,56,56	4.47	18 (32%)
30	LHG	4	801	-	48,48,48	0.39	0	51,54,54	1.01	2 (3%)
43	LUT	8	501	-	42,43,43	2.44	1 (2%)	51,60,60	1.75	15 (29%)
43	LUT	3	502	-	42,43,43	2.48	1 (2%)	51,60,60	1.82	15 (29%)
26	CHL	8	610	-	50,64,74	1.38	8 (16%)	46,102,114	1.85	11 (23%)
26	CHL	1	611	-	50,64,74	1.40	9 (18%)	46,102,114	1.97	12 (26%)
25	CLA	8	607	30	50,54,73	1.57	6 (12%)	59,90,113	2.04	13 (22%)
25	CLA	3	602	-	50,54,73	1.59	8 (16%)	59,90,113	2.02	17 (28%)
35	LMT	1	804	-	36,36,36	1.14	6 (16%)	47,47,47	1.03	3 (6%)
29	BCR	3	503	-	41,41,41	1.60	4 (9%)	56,56,56	4.47	13 (23%)
25	CLA	5	606	-	54,58,73	1.53	8 (14%)	64,95,113	2.07	17 (26%)
40	RRX	J	4002	-	42,42,42	5.02	24 (57%)	56,58,58	2.71	21 (37%)
25	CLA	A	1101	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	21 (25%)
43	LUT	a	501	-	42,43,43	2.46	1 (2%)	51,60,60	1.93	13 (25%)
25	CLA	B	1204	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	20 (24%)
26	CHL	a	610	-	42,56,74	1.53	9 (21%)	36,92,114	2.06	11 (30%)
25	CLA	B	1238	-	69,73,73	1.35	8 (11%)	82,113,113	1.87	17 (20%)
43	LUT	6	501	-	42,43,43	2.43	1 (2%)	51,60,60	1.81	12 (23%)
25	CLA	A	1106	1	69,73,73	1.34	8 (11%)	82,113,113	1.94	19 (23%)
30	LHG	F	5001	-	42,42,48	0.42	0	45,48,54	1.11	2 (4%)
25	CLA	4	610	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	18 (21%)
25	CLA	A	1138	-	69,73,73	1.35	7 (10%)	82,113,113	1.78	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	H	1703	-	59,63,73	1.45	7 (11%)	70,101,113	1.98	17 (24%)
37	PCW	K	5002	-	35,35,53	1.33	4 (11%)	41,43,61	1.08	2 (4%)
25	CLA	5	609	18	55,59,73	1.53	8 (14%)	64,96,113	2.02	17 (26%)
25	CLA	O	1802	-	59,63,73	1.47	7 (11%)	70,101,113	2.05	21 (30%)
33	PTY	G	5003	-	27,27,49	1.04	2 (7%)	28,31,54	1.08	1 (3%)
25	CLA	7	602	-	48,52,73	1.61	6 (12%)	57,88,113	2.02	14 (24%)
25	CLA	2	604	-	60,64,73	1.46	7 (11%)	71,102,113	2.01	17 (23%)
26	CHL	6	610	-	50,64,74	1.44	9 (18%)	46,102,114	1.85	12 (26%)
45	OLA	a	805	-	19,19,19	0.57	0	19,19,19	1.00	0
25	CLA	5	605	-	50,54,73	1.60	8 (16%)	59,90,113	2.04	15 (25%)
29	BCR	K	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.49	14 (25%)
25	CLA	9	605	-	64,68,73	1.43	7 (10%)	76,107,113	1.93	19 (25%)
29	BCR	6	504	-	41,41,41	1.63	4 (9%)	56,56,56	4.59	17 (30%)
33	PTY	a	802	-	37,37,49	1.02	4 (10%)	40,42,54	1.11	2 (5%)
25	CLA	a	607	-	62,66,73	1.43	7 (11%)	73,104,113	1.96	18 (24%)
43	LUT	2	507	-	42,43,43	2.48	1 (2%)	51,60,60	2.48	15 (29%)
36	DGD	8	802	-	60,60,67	1.17	6 (10%)	74,74,81	1.09	6 (8%)
30	LHG	8	801	25	36,36,48	0.44	0	39,42,54	1.17	3 (7%)
25	CLA	B	1225	-	69,73,73	1.35	7 (10%)	82,113,113	1.81	17 (20%)
25	CLA	A	1107	1	59,63,73	1.49	7 (11%)	70,101,113	1.96	17 (24%)
25	CLA	A	1102	25	59,63,73	1.46	6 (10%)	70,101,113	2.05	16 (22%)
25	CLA	5	603	18	60,64,73	1.45	7 (11%)	71,102,113	1.98	18 (25%)
25	CLA	6	607	30	59,63,73	1.47	7 (11%)	70,101,113	1.95	17 (24%)
25	CLA	H	1702	8	50,54,73	1.58	6 (12%)	59,90,113	2.10	14 (23%)
26	CHL	8	613	-	45,59,74	1.49	9 (20%)	40,96,114	2.11	12 (30%)
25	CLA	A	1103	-	69,73,73	1.33	6 (8%)	82,113,113	1.90	16 (19%)
25	CLA	A	1121	-	64,68,73	1.41	6 (9%)	76,107,113	1.99	18 (23%)
32	SQD	A	5005	-	52,54,54	0.78	0	62,65,65	0.85	2 (3%)
25	CLA	A	1115	-	64,68,73	1.40	7 (10%)	76,107,113	1.93	18 (23%)
25	CLA	A	1120	-	53,57,73	1.53	7 (13%)	61,93,113	2.17	19 (31%)
30	LHG	F	5002	-	35,35,48	0.43	0	38,41,54	1.21	3 (7%)
26	CHL	6	611	-	45,59,74	1.54	9 (20%)	40,96,114	2.08	12 (30%)
25	CLA	G	1601	-	54,58,73	1.53	7 (12%)	64,95,113	2.05	19 (29%)
29	BCR	L	4002	-	41,41,41	1.60	4 (9%)	56,56,56	4.49	15 (26%)
25	CLA	1	606	-	61,65,73	1.43	7 (11%)	72,103,113	2.05	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	a	608	-	59,63,73	1.46	7 (11%)	70,101,113	1.97	16 (22%)
43	LUT	5	502	-	42,43,43	2.42	1 (2%)	51,60,60	1.81	10 (19%)
25	CLA	9	607	-	51,55,73	1.57	7 (13%)	60,91,113	2.07	17 (28%)
25	CLA	L	1502	-	64,68,73	1.40	7 (10%)	76,107,113	1.96	19 (25%)
47	PLM	8	806	-	15,16,17	0.39	0	14,15,17	0.88	0
25	CLA	2	605	-	64,68,73	1.42	8 (12%)	76,107,113	1.94	22 (28%)
43	LUT	9	502	-	42,43,43	2.42	1 (2%)	51,60,60	1.72	13 (25%)
25	CLA	3	613	-	65,69,73	1.39	7 (10%)	77,108,113	1.91	19 (24%)
47	PLM	8	807	-	17,17,17	0.57	0	17,17,17	1.12	0
32	SQD	I	5001	-	52,54,54	0.79	0	62,65,65	0.83	2 (3%)
25	CLA	A	1141	-	49,53,73	1.60	8 (16%)	58,89,113	2.10	14 (24%)
32	SQD	G	5001	-	44,46,54	0.82	0	54,57,65	0.87	2 (3%)
25	CLA	5	614	18	50,54,73	1.59	7 (14%)	59,90,113	1.99	15 (25%)
25	CLA	8	620	-	49,53,73	1.61	8 (16%)	58,89,113	2.04	16 (27%)
29	BCR	G	4001	-	41,41,41	1.61	4 (9%)	56,56,56	4.57	15 (26%)
27	PQN	B	2002	-	34,34,34	0.38	0	43,45,45	1.06	3 (6%)
29	BCR	5	503	-	41,41,41	1.61	4 (9%)	56,56,56	4.50	15 (26%)
30	LHG	2	802	-	48,48,48	0.39	0	51,54,54	1.13	4 (7%)
25	CLA	A	1118	-	59,63,73	1.46	7 (11%)	70,101,113	1.98	18 (25%)
25	CLA	6	603	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	17 (20%)
25	CLA	B	1229	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	21 (25%)
25	CLA	8	615	21	50,54,73	1.57	7 (14%)	59,90,113	2.10	17 (28%)
25	CLA	5	608	-	49,53,73	1.61	7 (14%)	58,89,113	1.95	13 (22%)
26	CHL	a	606	-	50,64,74	1.41	9 (18%)	46,102,114	1.88	11 (23%)
26	CHL	1	613	-	42,56,74	1.48	8 (19%)	36,92,114	2.10	12 (33%)
26	CHL	8	603	21	60,74,74	1.41	9 (15%)	58,114,114	1.75	13 (22%)
30	LHG	7	801	25	36,36,48	0.44	0	39,42,54	1.12	3 (7%)
26	CHL	4	618	-	50,64,74	1.57	9 (18%)	46,102,114	1.88	13 (28%)
29	BCR	B	4006	-	41,41,41	1.62	4 (9%)	56,56,56	4.41	13 (23%)
26	CHL	6	613	-	45,59,74	1.52	8 (17%)	40,96,114	2.03	11 (27%)
25	CLA	4	611	-	60,64,73	1.44	7 (11%)	71,102,113	2.00	20 (28%)
26	CHL	5	611	-	45,59,74	1.73	9 (20%)	40,96,114	2.02	11 (27%)
25	CLA	A	1110	-	58,62,73	1.47	8 (13%)	68,99,113	2.02	18 (26%)
25	CLA	7	610	-	64,68,73	1.41	6 (9%)	76,107,113	1.92	20 (26%)
25	CLA	B	1205	-	69,73,73	1.34	7 (10%)	82,113,113	1.96	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	8	618	21	64,68,73	1.40	6 (9%)	76,107,113	1.98	17 (22%)
43	LUT	1	503	-	42,43,43	2.47	1 (2%)	51,60,60	2.16	17 (33%)
25	CLA	A	1137	-	64,68,73	1.40	8 (12%)	76,107,113	1.95	22 (28%)
26	CHL	6	609	19	60,74,74	1.16	7 (11%)	58,114,114	1.65	11 (18%)
50	XAT	9	507	-	41,47,47	0.70	1 (2%)	54,74,74	1.99	15 (27%)
25	CLA	B	1232	-	49,53,73	1.60	7 (14%)	58,89,113	2.01	14 (24%)
25	CLA	2	621	22	69,73,73	1.37	7 (10%)	82,113,113	1.93	17 (20%)
29	BCR	B	4005	-	41,41,41	1.61	4 (9%)	56,56,56	4.46	13 (23%)
25	CLA	1	615	15	50,54,73	1.59	6 (12%)	59,90,113	2.03	12 (20%)
43	LUT	9	501	-	42,43,43	2.44	1 (2%)	51,60,60	1.83	13 (25%)
25	CLA	6	605	-	50,54,73	1.59	8 (16%)	59,90,113	2.04	14 (23%)
25	CLA	2	608	-	49,53,73	1.60	7 (14%)	58,89,113	2.01	13 (22%)
43	LUT	7	501	-	42,43,43	2.47	1 (2%)	51,60,60	1.96	12 (23%)
43	LUT	2	502	-	42,43,43	2.47	1 (2%)	51,60,60	1.82	13 (25%)
25	CLA	B	1207	-	64,68,73	1.40	6 (9%)	76,107,113	1.89	17 (22%)
25	CLA	3	601	16	69,73,73	1.36	6 (8%)	82,113,113	1.84	17 (20%)
43	LUT	a	503	-	42,43,43	2.45	1 (2%)	51,60,60	2.15	14 (27%)
25	CLA	7	607	30	63,67,73	1.42	7 (11%)	74,105,113	1.96	15 (20%)
25	CLA	A	1119	-	69,73,73	1.36	6 (8%)	82,113,113	1.79	15 (18%)
25	CLA	B	1209	-	69,73,73	1.35	8 (11%)	82,113,113	1.88	17 (20%)
25	CLA	A	1117	-	69,73,73	1.36	7 (10%)	82,113,113	1.97	15 (18%)
25	CLA	6	604	19	69,73,73	1.34	7 (10%)	82,113,113	1.87	21 (25%)
48	DGA	8	804	-	39,39,43	1.18	3 (7%)	41,41,45	1.58	3 (7%)
25	CLA	4	602	-	56,60,73	1.50	6 (10%)	65,97,113	2.01	19 (29%)
25	CLA	6	601	-	64,68,73	1.40	7 (10%)	76,107,113	1.94	19 (25%)
25	CLA	4	603	17	60,64,73	1.44	8 (13%)	71,102,113	1.94	18 (25%)
25	CLA	4	607	-	59,63,73	1.47	7 (11%)	70,101,113	2.00	18 (25%)
26	CHL	1	604	-	60,74,74	1.55	9 (15%)	58,114,114	1.74	12 (20%)
26	CHL	2	613	-	45,59,74	1.40	9 (20%)	40,96,114	2.14	11 (27%)
25	CLA	B	1234	-	58,69,73	1.51	7 (12%)	55,99,113	2.18	13 (23%)
25	CLA	A	1104	1	69,73,73	1.35	8 (11%)	82,113,113	1.87	20 (24%)
25	CLA	L	1504	-	54,58,73	1.54	7 (12%)	64,95,113	2.05	16 (25%)
30	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	1.01	3 (5%)
43	LUT	6	502	-	42,43,43	2.41	1 (2%)	51,60,60	1.86	11 (21%)
25	CLA	a	615	15	50,54,73	1.60	7 (14%)	59,90,113	2.02	14 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	2	606	-	50,54,73	1.59	7 (14%)	59,90,113	2.02	14 (23%)
25	CLA	A	1128	-	69,73,73	1.37	7 (10%)	82,113,113	1.88	14 (17%)
25	CLA	J	1901	9	46,50,73	1.65	6 (13%)	53,85,113	2.11	14 (26%)
25	CLA	a	605	-	59,63,73	1.47	7 (11%)	70,101,113	2.01	17 (24%)
41	SPH	J	5002	-	19,20,20	0.69	1 (5%)	18,21,21	0.92	0
37	PCW	6	803	-	35,35,53	1.32	4 (11%)	41,43,61	1.14	2 (4%)
26	CHL	2	609	22	60,74,74	1.44	9 (15%)	58,114,114	1.64	12 (20%)
25	CLA	A	1108	-	69,73,73	1.35	8 (11%)	82,113,113	1.83	18 (21%)
25	CLA	B	1022	54	69,73,73	1.37	7 (10%)	82,113,113	1.85	18 (21%)
25	CLA	B	1203	2	69,73,73	1.35	6 (8%)	82,113,113	1.83	18 (21%)
36	DGD	8	803	-	47,47,67	0.82	1 (2%)	61,61,81	1.10	4 (6%)
25	CLA	L	1501	11	54,58,73	1.53	7 (12%)	64,95,113	2.07	16 (25%)
26	CHL	6	617	19	37,51,74	1.63	8 (21%)	30,86,114	2.32	10 (33%)
43	LUT	8	502	-	42,43,43	2.42	1 (2%)	51,60,60	1.79	12 (23%)
25	CLA	1	601	-	64,68,73	1.41	7 (10%)	76,107,113	1.91	17 (22%)
24	CL0	A	1011	-	58,73,73	3.20	17 (29%)	60,113,113	2.83	17 (28%)
28	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
25	CLA	B	1208	-	58,62,73	1.39	6 (10%)	71,100,113	2.01	18 (25%)
30	LHG	3	801	25	48,48,48	0.40	0	51,54,54	1.05	3 (5%)
25	CLA	A	1116	-	64,68,73	1.40	8 (12%)	76,107,113	1.91	18 (23%)
25	CLA	L	1503	-	49,53,73	1.61	8 (16%)	58,89,113	2.02	14 (24%)
29	BCR	B	4003	-	41,41,41	1.62	4 (9%)	56,56,56	4.48	17 (30%)
35	LMT	A	5008	-	36,36,36	1.16	5 (13%)	47,47,47	1.01	2 (4%)
25	CLA	1	607	30	69,73,73	1.35	7 (10%)	82,113,113	1.84	18 (21%)
25	CLA	B	1236	-	57,61,73	1.48	8 (14%)	67,98,113	2.00	19 (28%)
33	PTY	B	5005	-	41,41,49	0.95	4 (9%)	44,46,54	1.14	2 (4%)
30	LHG	1	801	25	34,34,48	0.45	0	37,40,54	1.17	3 (8%)
30	LHG	6	801	25	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
29	BCR	B	4001	-	41,41,41	1.61	4 (9%)	56,56,56	4.45	14 (25%)
26	CHL	7	613	-	55,69,74	1.51	9 (16%)	52,108,114	1.72	9 (17%)
34	3PH	A	5007	-	32,32,47	1.03	4 (12%)	35,37,52	1.23	2 (5%)
29	BCR	5	504	-	41,41,41	1.62	4 (9%)	56,56,56	4.70	17 (30%)
25	CLA	4	617	-	49,53,73	1.60	6 (12%)	58,89,113	2.07	16 (27%)
50	XAT	9	504	-	41,47,47	0.65	1 (2%)	54,74,74	6.35	15 (27%)
50	XAT	2	501	-	41,47,47	0.69	1 (2%)	54,74,74	2.00	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	4	612	17	66,70,73	1.37	6 (9%)	78,109,113	1.97	17 (21%)
25	CLA	B	1201	-	69,73,73	1.35	7 (10%)	82,113,113	4.03	22 (26%)
25	CLA	5	615	18	50,54,73	1.59	6 (12%)	59,90,113	2.02	15 (25%)
25	CLA	A	1013	-	69,73,73	1.34	6 (8%)	82,113,113	1.78	18 (21%)
26	CHL	1	610	-	42,56,74	1.43	7 (16%)	36,92,114	2.05	10 (27%)
25	CLA	K	1404	10	49,53,73	1.60	8 (16%)	58,89,113	2.05	14 (24%)
28	SF4	C	3002	3	0,12,12	-	-	-		
26	CHL	5	617	18	41,55,74	1.51	9 (21%)	35,91,114	2.13	12 (34%)
43	LUT	3	501	-	42,43,43	2.45	1 (2%)	51,60,60	1.81	15 (29%)
43	LUT	a	502	-	42,43,43	2.44	1 (2%)	51,60,60	1.82	13 (25%)
25	CLA	4	604	-	64,68,73	1.41	7 (10%)	76,107,113	1.94	17 (22%)
33	PTY	3	802	-	37,37,49	1.00	4 (10%)	40,42,54	1.11	2 (5%)
25	CLA	9	602	-	50,54,73	1.59	7 (14%)	59,90,113	2.00	16 (27%)
25	CLA	3	607	30	69,73,73	1.36	7 (10%)	82,113,113	1.82	16 (19%)
25	CLA	A	1130	-	60,64,73	1.45	7 (11%)	71,102,113	1.97	17 (23%)
25	CLA	A	1133	-	69,73,73	1.35	6 (8%)	82,113,113	1.81	16 (19%)
26	CHL	a	604	-	55,69,74	1.67	9 (16%)	52,108,114	1.90	12 (23%)
29	BCR	A	4003	-	41,41,41	1.62	4 (9%)	56,56,56	4.59	17 (30%)
25	CLA	3	618	16	50,54,73	1.59	7 (14%)	59,90,113	2.02	15 (25%)
25	CLA	5	601	18	64,68,73	1.40	7 (10%)	76,107,113	1.97	21 (27%)
25	CLA	G	1603	-	49,53,73	1.59	6 (12%)	58,89,113	2.03	16 (27%)
43	LUT	1	501	-	42,43,43	2.45	1 (2%)	51,60,60	1.82	15 (29%)
25	CLA	B	1023	-	69,73,73	1.35	6 (8%)	82,113,113	1.85	18 (21%)
47	PLM	6	804	-	17,17,17	0.57	0	17,17,17	1.13	1 (5%)
29	BCR	A	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.43	17 (30%)
25	CLA	8	606	-	61,65,73	1.43	7 (11%)	72,103,113	1.94	16 (22%)
43	LUT	4	502	-	42,43,43	2.43	1 (2%)	51,60,60	1.82	11 (21%)
25	CLA	4	616	-	54,58,73	1.53	6 (11%)	64,95,113	2.04	17 (26%)
25	CLA	7	612	-	64,68,73	1.42	6 (9%)	76,107,113	1.91	16 (21%)
30	LHG	9	801	-	32,32,48	0.47	0	35,38,54	1.20	3 (8%)
26	CHL	a	613	-	40,54,74	1.46	8 (20%)	34,90,114	2.17	10 (29%)
25	CLA	A	1129	-	54,58,73	1.53	7 (12%)	64,95,113	2.06	17 (26%)
25	CLA	a	611	-	54,58,73	1.54	7 (12%)	64,95,113	2.04	16 (25%)
29	BCR	L	4001	-	41,41,41	1.59	4 (9%)	56,56,56	4.46	15 (26%)
25	CLA	4	605	-	50,54,73	1.59	7 (14%)	59,90,113	2.03	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	BCR	B	4007	-	41,41,41	1.60	4 (9%)	56,56,56	4.50	15 (26%)
25	CLA	9	612	-	69,73,73	1.36	7 (10%)	82,113,113	1.87	17 (20%)
38	LPX	F	5003	-	29,29,29	1.02	2 (6%)	31,33,33	0.94	1 (3%)
25	CLA	F	1301	-	54,58,73	1.52	6 (11%)	64,95,113	2.07	17 (26%)
40	RRX	3	506	-	42,42,42	5.05	24 (57%)	56,58,58	2.83	20 (35%)
46	QTB	a	504	-	19,19,19	2.59	4 (21%)	23,26,26	2.96	10 (43%)
25	CLA	B	1230	-	62,66,73	1.42	7 (11%)	73,104,113	1.99	19 (26%)
30	LHG	7	802	-	35,35,48	0.45	0	38,41,54	1.08	2 (5%)
33	PTY	J	5001	-	27,27,49	1.17	4 (14%)	30,32,54	1.21	2 (6%)
25	CLA	8	605	-	59,63,73	1.48	8 (13%)	70,101,113	2.00	19 (27%)
25	CLA	9	604	23	64,68,73	1.42	6 (9%)	76,107,113	1.94	19 (25%)
25	CLA	B	1220	-	64,68,73	1.40	6 (9%)	76,107,113	1.89	17 (22%)
25	CLA	B	1227	-	54,58,73	1.54	7 (12%)	64,95,113	2.08	19 (29%)
25	CLA	7	604	20	69,73,73	1.36	6 (8%)	82,113,113	1.91	18 (21%)
25	CLA	B	1226	-	69,73,73	1.38	7 (10%)	82,113,113	1.84	16 (19%)
25	CLA	2	601	-	64,68,73	1.40	7 (10%)	76,107,113	2.04	18 (23%)
26	CHL	3	608	-	37,51,74	1.70	9 (24%)	30,86,114	2.19	10 (33%)
30	LHG	4	802	-	31,31,48	0.47	0	34,37,54	1.24	3 (8%)
43	LUT	4	501	-	42,43,43	2.46	1 (2%)	51,60,60	1.93	10 (19%)
25	CLA	B	1219	2	63,67,73	1.42	6 (9%)	74,105,113	1.93	16 (21%)
43	LUT	5	505	-	42,43,43	2.48	1 (2%)	51,60,60	2.12	11 (21%)
48	DGA	3	803	-	23,23,43	1.43	3 (13%)	25,25,45	1.36	2 (8%)
45	OLA	8	808	-	19,19,19	0.58	0	19,19,19	1.02	0
41	SPH	6	806	-	19,20,20	0.66	0	18,21,21	1.08	1 (5%)
36	DGD	B	5003	-	67,67,67	1.30	7 (10%)	81,81,81	1.03	3 (3%)
30	LHG	B	5001	25	48,48,48	0.40	0	51,54,54	0.99	3 (5%)
44	AXT	1	502	-	44,44,45	3.01	16 (36%)	54,62,64	1.91	13 (24%)
37	PCW	K	5001	-	40,40,53	1.29	4 (10%)	46,48,61	1.09	2 (4%)
25	CLA	4	608	-	55,59,73	1.52	7 (12%)	64,96,113	2.07	17 (26%)
26	CHL	3	611	-	55,69,74	1.46	9 (16%)	52,108,114	1.72	12 (23%)
47	PLM	4	804	-	17,17,17	0.58	0	17,17,17	1.06	0
25	CLA	7	608	-	59,63,73	1.46	7 (11%)	70,101,113	2.00	17 (24%)
50	XAT	7	502	-	41,47,47	0.68	1 (2%)	54,74,74	1.95	10 (18%)
26	CHL	5	610	-	60,74,74	1.19	8 (13%)	58,114,114	1.70	11 (18%)
25	CLA	B	1221	-	69,73,73	1.36	8 (11%)	82,113,113	1.91	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	1224	-	69,73,73	1.37	8 (11%)	82,113,113	1.88	18 (21%)
25	CLA	1	602	-	49,53,73	1.61	7 (14%)	58,89,113	2.02	16 (27%)
30	LHG	B	5002	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
25	CLA	9	609	23	50,54,73	1.58	7 (14%)	59,90,113	2.04	16 (27%)
25	CLA	B	1216	-	69,73,73	1.35	6 (8%)	82,113,113	1.81	17 (20%)
25	CLA	2	612	-	54,58,73	1.53	7 (12%)	64,95,113	2.01	16 (25%)
43	LUT	5	501	-	42,43,43	2.44	1 (2%)	51,60,60	1.79	13 (25%)
25	CLA	1	605	-	69,73,73	1.34	7 (10%)	82,113,113	1.94	20 (24%)
25	CLA	B	1206	2	69,73,73	1.36	6 (8%)	82,113,113	1.89	14 (17%)
47	PLM	4	803	-	15,16,17	0.39	0	14,15,17	0.89	0
25	CLA	A	1012	-	69,73,73	1.37	8 (11%)	82,113,113	1.89	17 (20%)
28	SF4	C	3003	3	0,12,12	-	-	-	-	-
25	CLA	A	1131	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	16 (19%)
25	CLA	8	611	-	54,58,73	1.52	7 (12%)	64,95,113	2.06	17 (26%)
29	BCR	L	4003	-	41,41,41	1.62	4 (9%)	56,56,56	4.52	14 (25%)
25	CLA	A	1127	-	69,73,73	1.35	6 (8%)	82,113,113	1.81	17 (20%)
25	CLA	B	1218	-	59,63,73	1.46	6 (10%)	70,101,113	2.10	19 (27%)
25	CLA	B	1235	-	69,73,73	1.35	7 (10%)	82,113,113	1.91	19 (23%)
29	BCR	J	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.43	14 (25%)
26	CHL	9	608	-	42,56,74	1.60	9 (21%)	36,92,114	2.09	11 (30%)
25	CLA	6	612	-	54,58,73	1.53	7 (12%)	64,95,113	2.05	17 (26%)
25	CLA	a	602	-	54,58,73	1.53	7 (12%)	64,95,113	2.05	19 (29%)
26	CHL	4	613	-	46,60,74	1.47	9 (19%)	40,97,114	2.08	12 (30%)
25	CLA	9	606	-	59,63,73	1.47	8 (13%)	70,101,113	1.93	17 (24%)
25	CLA	8	608	-	56,60,73	1.49	6 (10%)	65,97,113	2.04	17 (26%)
33	PTY	a	803	-	37,37,49	1.01	4 (10%)	40,42,54	1.09	2 (5%)
25	CLA	B	1217	-	60,64,73	1.45	9 (15%)	71,102,113	2.03	21 (29%)
33	PTY	5	802	-	37,37,49	1.00	4 (10%)	40,42,54	1.17	2 (5%)
25	CLA	6	618	-	50,54,73	1.59	6 (12%)	59,90,113	2.00	15 (25%)
36	DGD	7	806	-	51,51,67	0.96	3 (5%)	65,65,81	1.04	3 (4%)
25	CLA	B	1237	-	69,73,73	1.35	6 (8%)	82,113,113	1.84	16 (19%)
25	CLA	B	1239	-	69,73,73	1.34	8 (11%)	82,113,113	1.86	19 (23%)
25	CLA	H	1701	-	59,63,73	1.46	6 (10%)	70,101,113	2.00	16 (22%)
30	LHG	9	802	-	48,48,48	0.39	0	51,54,54	1.14	3 (5%)
25	CLA	K	1403	10	53,57,73	1.54	6 (11%)	61,93,113	2.15	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CHL	A	1114	-	60,74,74	1.23	9 (15%)	58,114,114	1.74	11 (18%)
41	SPH	4	805	-	19,20,20	0.65	0	18,21,21	1.09	1 (5%)
25	CLA	B	1215	-	64,68,73	1.39	7 (10%)	76,107,113	1.87	16 (21%)
51	4RF	7	807	-	36,36,56	1.08	6 (16%)	39,39,59	1.16	3 (7%)
44	AXT	7	504	-	44,44,45	2.44	17 (38%)	54,62,64	2.37	18 (33%)
29	BCR	A	4002	-	41,41,41	1.61	4 (9%)	56,56,56	4.25	13 (23%)
25	CLA	B	1202	-	69,73,73	1.34	8 (11%)	82,113,113	1.86	18 (21%)
25	CLA	F	1302	-	59,63,73	1.47	8 (13%)	70,101,113	1.98	18 (25%)
25	CLA	1	612	15	69,73,73	1.36	6 (8%)	82,113,113	1.86	17 (20%)
26	CHL	a	609	15	47,61,74	1.41	8 (17%)	41,98,114	1.99	11 (26%)
26	CHL	3	604	16	60,74,74	1.49	9 (15%)	58,114,114	1.88	12 (20%)
29	BCR	H	4001	-	41,41,41	1.61	4 (9%)	56,56,56	7.48	21 (37%)
25	CLA	A	1125	-	69,73,73	1.35	8 (11%)	82,113,113	1.86	21 (25%)
25	CLA	4	615	17	64,68,73	1.42	7 (10%)	76,107,113	1.86	16 (21%)
53	LAP	8	810	-	28,28,28	1.25	2 (7%)	33,35,35	1.02	1 (3%)
29	BCR	6	503	-	41,41,41	1.62	4 (9%)	56,56,56	4.41	13 (23%)
31	LMG	A	5004	-	42,42,55	0.86	2 (4%)	50,50,63	1.08	2 (4%)
26	CHL	5	613	-	50,64,74	1.30	7 (14%)	46,102,114	1.98	13 (28%)
26	CHL	4	609	17	60,74,74	1.29	9 (15%)	58,114,114	1.73	12 (20%)
32	SQD	H	5001	-	43,45,54	0.84	0	53,56,65	0.90	2 (3%)
25	CLA	A	1112	-	59,63,73	1.47	6 (10%)	70,101,113	2.07	16 (22%)
25	CLA	B	1212	-	61,65,73	1.43	6 (9%)	72,103,113	2.02	20 (27%)
25	CLA	5	602	-	56,60,73	1.51	6 (10%)	65,97,113	2.00	19 (29%)
25	CLA	6	602	-	56,60,73	1.50	7 (12%)	65,97,113	2.01	17 (26%)
25	CLA	3	610	16	61,65,73	1.43	7 (11%)	72,103,113	1.97	19 (26%)
25	CLA	3	616	-	60,64,73	1.45	7 (11%)	71,102,113	2.02	20 (28%)
25	CLA	B	1228	-	69,73,73	1.35	7 (10%)	82,113,113	1.90	19 (23%)
42	ECH	M	4001	-	42,42,42	0.85	2 (4%)	55,58,58	2.04	15 (27%)
30	LHG	5	801	-	48,48,48	0.38	0	51,54,54	1.10	3 (5%)
25	CLA	a	603	-	69,73,73	1.37	7 (10%)	82,113,113	1.92	16 (19%)
25	CLA	6	608	-	59,63,73	1.46	7 (11%)	70,101,113	2.02	17 (24%)
25	CLA	7	606	-	58,62,73	1.49	6 (10%)	69,100,113	1.95	16 (23%)
25	CLA	2	602	-	56,60,73	1.51	7 (12%)	65,97,113	2.00	18 (27%)
25	CLA	A	1136	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	19 (23%)
25	CLA	8	609	21	64,68,73	1.40	8 (12%)	76,107,113	1.98	20 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	a	612	15	61,65,73	1.44	7 (11%)	72,103,113	1.91	16 (22%)
37	PCW	B	5004	-	38,38,53	1.31	4 (10%)	44,46,61	1.08	2 (4%)
25	CLA	a	601	-	64,68,73	1.41	7 (10%)	76,107,113	1.94	20 (26%)
25	CLA	B	1214	-	63,67,73	1.42	7 (11%)	74,105,113	1.98	17 (22%)
26	CHL	7	609	20	56,70,74	1.43	9 (16%)	53,109,114	1.79	11 (20%)
35	LMT	2	804	-	36,36,36	1.16	6 (16%)	47,47,47	1.07	3 (6%)
30	LHG	2	801	25	48,48,48	0.36	0	51,54,54	1.04	2 (3%)
30	LHG	7	803	-	34,34,48	0.45	0	37,40,54	1.17	3 (8%)
29	BCR	8	503	-	41,41,41	1.61	4 (9%)	56,56,56	4.41	13 (23%)
30	LHG	1	802	-	48,48,48	0.40	0	51,54,54	1.01	4 (7%)
25	CLA	K	1402	-	64,68,73	1.42	8 (12%)	76,107,113	1.94	17 (22%)
25	CLA	7	605	-	47,52,73	1.65	7 (14%)	55,88,113	1.94	14 (25%)
45	OLA	8	809	-	19,19,19	0.58	0	19,19,19	1.00	0
26	CHL	9	613	-	36,50,74	1.65	9 (25%)	29,85,114	2.25	9 (31%)
25	CLA	B	1240	30	69,73,73	1.37	8 (11%)	82,113,113	1.90	18 (21%)
25	CLA	4	601	-	64,68,73	1.40	6 (9%)	76,107,113	1.96	20 (26%)
29	BCR	3	504	-	41,41,41	1.60	4 (9%)	56,56,56	4.49	16 (28%)
29	BCR	B	4004	-	41,41,41	1.61	4 (9%)	56,56,56	4.42	14 (25%)
25	CLA	A	1140	-	59,63,73	1.47	8 (13%)	70,101,113	2.01	19 (27%)
26	CHL	3	603	16	60,74,74	1.41	9 (15%)	58,114,114	1.76	13 (22%)
27	PQN	A	2001	-	34,34,34	0.38	0	43,45,45	1.15	3 (6%)
29	BCR	A	4005	-	41,41,41	1.59	4 (9%)	56,56,56	4.39	13 (23%)
29	BCR	B	4002	-	41,41,41	1.60	4 (9%)	56,56,56	4.50	14 (25%)
33	PTY	9	803	-	47,47,49	0.90	4 (8%)	50,52,54	1.12	2 (4%)
26	CHL	9	610	-	45,59,74	1.52	10 (22%)	40,96,114	1.98	11 (27%)
26	CHL	8	604	21	56,70,74	1.59	9 (16%)	53,109,114	1.89	13 (24%)
25	CLA	G	1602	7	64,68,73	1.41	7 (10%)	76,107,113	1.93	19 (25%)
25	CLA	5	612	18	69,73,73	1.34	7 (10%)	82,113,113	1.87	19 (23%)
26	CHL	2	610	-	42,56,74	1.47	9 (21%)	36,92,114	2.09	11 (30%)
25	CLA	A	1124	-	59,63,73	1.48	7 (11%)	70,101,113	1.96	19 (27%)
25	CLA	8	602	-	56,60,73	1.50	6 (10%)	65,97,113	2.04	18 (27%)
25	CLA	B	1021	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	17 (20%)
25	CLA	O	1803	-	45,49,73	1.67	7 (15%)	54,84,113	2.11	17 (31%)
25	CLA	A	1132	-	69,73,73	1.34	7 (10%)	82,113,113	1.91	18 (21%)
25	CLA	O	1801	-	41,46,73	1.77	8 (19%)	47,80,113	2.07	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CHL	6	619	19	60,74,74	1.25	8 (13%)	58,114,114	1.80	12 (20%)
29	BCR	3	505	-	41,41,41	1.60	4 (9%)	56,56,56	4.45	15 (26%)
30	LHG	6	802	-	36,36,48	0.43	0	39,42,54	1.26	3 (7%)
32	SQD	7	805	-	37,39,54	0.89	0	47,50,65	0.94	3 (6%)
25	CLA	5	604	18	69,73,73	1.36	7 (10%)	82,113,113	1.88	16 (19%)
25	CLA	A	1109	25	69,73,73	1.36	7 (10%)	82,113,113	1.92	18 (21%)
33	PTY	A	5006	-	33,33,49	1.07	4 (12%)	36,38,54	1.12	2 (5%)
35	LMT	B	5006	-	36,36,36	1.15	6 (16%)	47,47,47	0.96	1 (2%)
26	CHL	9	601	-	60,74,74	1.38	8 (13%)	58,114,114	1.64	11 (18%)
25	CLA	B	1223	-	69,73,73	1.36	8 (11%)	82,113,113	1.92	19 (23%)
30	LHG	A	5003	-	45,45,48	0.40	0	48,51,54	1.05	3 (6%)
25	CLA	7	601	20	64,68,73	1.41	7 (10%)	76,107,113	1.95	18 (23%)
25	CLA	8	612	-	54,58,73	1.52	6 (11%)	64,95,113	2.01	15 (23%)
47	PLM	5	804	-	17,17,17	0.59	0	17,17,17	1.12	0
25	CLA	A	1134	1	64,68,73	1.41	8 (12%)	76,107,113	1.99	20 (26%)
25	CLA	3	606	-	69,73,73	1.35	6 (8%)	82,113,113	1.85	15 (18%)
25	CLA	6	615	54	69,73,73	1.36	6 (8%)	82,113,113	1.92	19 (23%)
25	CLA	7	603	20	69,73,73	1.36	7 (10%)	82,113,113	1.92	20 (24%)
52	P5S	8	805	-	35,36,53	1.18	3 (8%)	37,43,60	1.22	2 (5%)
25	CLA	B	1213	-	59,63,73	1.45	7 (11%)	70,101,113	2.00	17 (24%)
26	CHL	5	618	-	45,59,74	1.47	8 (17%)	40,96,114	2.06	12 (30%)
25	CLA	2	607	30	69,73,73	1.36	6 (8%)	82,113,113	1.89	19 (23%)
29	BCR	7	503	-	41,41,41	1.59	4 (9%)	56,56,56	4.47	17 (30%)
25	CLA	A	1126	-	69,73,73	1.37	8 (11%)	82,113,113	1.90	20 (24%)
26	CHL	8	601	21	55,69,74	1.67	9 (16%)	52,108,114	1.89	13 (25%)
29	BCR	O	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.80	15 (26%)
30	LHG	A	5001	-	48,48,48	0.39	0	51,54,54	1.11	3 (5%)
25	CLA	B	1210	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	20 (24%)
25	CLA	A	1139	-	59,63,73	1.47	8 (13%)	70,101,113	1.98	17 (24%)
25	CLA	4	606	-	54,58,73	1.54	8 (14%)	64,95,113	2.08	17 (26%)
25	CLA	6	606	19	69,73,73	1.35	6 (8%)	82,113,113	1.92	19 (23%)
47	PLM	a	804	-	15,16,17	0.39	0	14,15,17	0.92	0
48	DGA	5	803	-	22,22,43	1.45	3 (13%)	24,24,45	1.34	2 (8%)
25	CLA	5	607	-	64,68,73	1.41	7 (10%)	76,107,113	1.95	19 (25%)
33	PTY	7	804	-	32,32,49	1.07	4 (12%)	35,37,54	1.20	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	BCR	K	4002	-	41,41,41	1.61	4 (9%)	56,56,56	4.46	17 (30%)
25	CLA	3	605	-	69,73,73	1.36	7 (10%)	82,113,113	1.87	17 (20%)
25	CLA	3	612	16	54,58,73	1.50	6 (11%)	64,95,113	2.06	16 (25%)
29	BCR	4	503	-	41,41,41	1.60	4 (9%)	56,56,56	4.53	11 (19%)
26	CHL	9	603	-	60,74,74	1.28	9 (15%)	58,114,114	1.75	11 (18%)
26	CHL	1	609	15	60,74,74	1.25	9 (15%)	58,114,114	1.80	12 (20%)
48	DGA	2	803	-	36,36,43	1.22	3 (8%)	38,38,45	1.36	3 (7%)
26	CHL	7	611	-	50,64,74	1.38	9 (18%)	46,102,114	2.00	12 (26%)
26	CHL	7	617	20	60,74,74	1.28	9 (15%)	58,114,114	1.78	12 (20%)
25	CLA	B	1211	-	59,63,73	1.47	8 (13%)	70,101,113	2.00	19 (27%)
25	CLA	A	1135	-	55,59,73	1.53	8 (14%)	64,96,113	2.10	20 (31%)
25	CLA	A	1105	-	61,65,73	1.43	6 (9%)	72,103,113	1.97	17 (23%)
26	CHL	7	615	20	45,59,74	1.49	9 (20%)	40,96,114	2.08	12 (30%)
39	NEX	F	4001	-	40,46,46	2.71	11 (27%)	50,70,70	4.73	15 (30%)
25	CLA	A	1122	-	64,68,73	1.41	7 (10%)	76,107,113	1.89	18 (23%)
25	CLA	2	603	22	64,68,73	1.41	6 (9%)	76,107,113	2.05	21 (27%)
25	CLA	A	1123	-	69,73,73	1.37	8 (11%)	82,113,113	1.91	17 (20%)
25	CLA	B	1222	-	62,66,73	1.42	7 (11%)	73,104,113	1.96	18 (24%)
25	CLA	1	603	-	69,73,73	1.35	8 (11%)	82,113,113	1.86	16 (19%)
30	LHG	a	801	-	34,34,48	0.46	0	37,40,54	1.12	3 (8%)
41	SPH	9	804	-	19,20,20	0.66	0	18,21,21	1.09	0

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
25	CLA	A	1113	-	1/1/14/20	14/33/109/115	-
25	CLA	1	608	-	1/1/14/20	12/33/109/115	-
25	CLA	K	1401	-	1/1/11/20	4/17/93/115	-
33	PTY	G	5002	-	-	9/30/30/53	-
25	CLA	A	1111	-	1/1/15/20	17/39/115/115	-
45	OLA	1	803	-	-	6/17/17/17	-
29	BCR	I	4001	-	-	15/29/63/63	0/2/2/2
25	CLA	B	1231	-	1/1/15/20	15/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	2	615	-	1/1/13/20	8/29/105/115	-
49	13X	6	805	-	-	-	0/1/1/1
29	BCR	A	4004	-	-	12/29/63/63	0/2/2/2
30	LHG	4	801	-	-	30/53/53/53	-
43	LUT	8	501	-	-	1/29/67/67	0/2/2/2
43	LUT	3	502	-	-	2/29/67/67	0/2/2/2
26	CHL	8	610	-	5/5/18/26	6/27/125/137	-
26	CHL	1	611	-	4/4/18/26	4/27/125/137	-
25	CLA	8	607	30	1/1/11/20	5/17/93/115	-
25	CLA	3	602	-	1/1/11/20	5/17/93/115	-
35	LMT	1	804	-	-	12/21/61/61	0/2/2/2
29	BCR	3	503	-	-	12/29/63/63	0/2/2/2
25	CLA	5	606	-	1/1/12/20	8/21/97/115	-
40	RRX	J	4002	-	1/1/11/25	12/29/65/65	0/2/2/2
25	CLA	A	1101	-	1/1/15/20	22/39/115/115	-
43	LUT	a	501	-	-	5/29/67/67	0/2/2/2
25	CLA	B	1204	-	1/1/15/20	19/39/115/115	-
26	CHL	a	610	-	3/3/16/26	2/18/116/137	-
25	CLA	B	1238	-	1/1/15/20	10/39/115/115	-
43	LUT	6	501	-	-	3/29/67/67	0/2/2/2
25	CLA	A	1106	1	1/1/15/20	18/39/115/115	-
30	LHG	F	5001	-	-	27/47/47/53	-
25	CLA	4	610	-	1/1/15/20	22/39/115/115	-
25	CLA	A	1138	-	1/1/15/20	6/39/115/115	-
25	CLA	H	1703	-	1/1/13/20	11/27/103/115	-
37	PCW	K	5002	-	-	17/39/39/57	-
25	CLA	5	609	18	1/1/12/20	9/23/99/115	-
25	CLA	O	1802	-	1/1/13/20	13/27/103/115	-
33	PTY	G	5003	-	-	13/30/30/53	-
25	CLA	7	602	-	1/1/11/20	5/13/89/115	-
25	CLA	2	604	-	1/1/13/20	11/29/105/115	-
26	CHL	6	610	-	4/4/18/26	4/27/125/137	-
45	OLA	a	805	-	-	6/17/17/17	-
25	CLA	5	605	-	1/1/11/20	2/17/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	K	4001	-	-	10/29/63/63	0/2/2/2
25	CLA	9	605	-	1/1/14/20	12/33/109/115	-
29	BCR	6	504	-	-	12/29/63/63	0/2/2/2
33	PTY	a	802	-	-	20/41/41/53	-
25	CLA	a	607	-	1/1/13/20	13/31/107/115	-
43	LUT	2	507	-	1/1/12/27	19/29/67/67	0/2/2/2
36	DGD	8	802	-	-	19/48/88/95	0/2/2/2
30	LHG	8	801	25	-	28/41/41/53	-
25	CLA	B	1225	-	1/1/15/20	6/39/115/115	-
25	CLA	A	1107	1	1/1/13/20	9/27/103/115	-
25	CLA	A	1102	25	1/1/13/20	9/27/103/115	-
25	CLA	5	603	18	1/1/13/20	16/29/105/115	-
25	CLA	6	607	30	1/1/13/20	10/27/103/115	-
25	CLA	H	1702	8	1/1/11/20	8/17/93/115	-
26	CHL	8	613	-	3/3/17/26	1/21/119/137	-
25	CLA	A	1103	-	1/1/15/20	17/39/115/115	-
25	CLA	A	1121	-	1/1/14/20	18/33/109/115	-
32	SQD	A	5005	-	-	21/49/69/69	0/1/1/1
25	CLA	A	1115	-	1/1/14/20	16/33/109/115	-
25	CLA	A	1120	-	1/1/11/20	6/20/96/115	-
30	LHG	F	5002	-	-	19/40/40/53	-
26	CHL	6	611	-	3/3/17/26	4/21/119/137	-
25	CLA	G	1601	-	1/1/12/20	9/21/97/115	-
29	BCR	L	4002	-	-	11/29/63/63	0/2/2/2
25	CLA	1	606	-	1/1/13/20	11/30/106/115	-
25	CLA	a	608	-	1/1/13/20	10/27/103/115	-
43	LUT	5	502	-	-	3/29/67/67	0/2/2/2
25	CLA	9	607	-	1/1/11/20	8/18/94/115	-
25	CLA	L	1502	-	1/1/14/20	12/33/109/115	-
47	PLM	8	806	-	-	6/14/14/15	-
25	CLA	2	605	-	1/1/14/20	18/33/109/115	-
43	LUT	9	502	-	-	3/29/67/67	0/2/2/2
25	CLA	3	613	-	1/1/14/20	12/35/111/115	-
47	PLM	8	807	-	-	5/15/15/15	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SQD	I	5001	-	-	23/49/69/69	0/1/1/1
25	CLA	A	1141	-	1/1/11/20	7/15/91/115	-
32	SQD	G	5001	-	-	19/41/61/69	0/1/1/1
25	CLA	5	614	18	1/1/11/20	8/17/93/115	-
25	CLA	8	620	-	1/1/11/20	8/15/91/115	-
29	BCR	G	4001	-	-	11/29/63/63	0/2/2/2
27	PQN	B	2002	-	-	7/23/43/43	0/2/2/2
29	BCR	5	503	-	-	13/29/63/63	0/2/2/2
30	LHG	2	802	-	-	37/53/53/53	-
25	CLA	A	1118	-	1/1/13/20	10/27/103/115	-
25	CLA	6	603	-	1/1/15/20	12/39/115/115	-
25	CLA	B	1229	-	1/1/15/20	12/39/115/115	-
25	CLA	8	615	21	1/1/11/20	9/17/93/115	-
25	CLA	5	608	-	1/1/11/20	4/15/91/115	-
26	CHL	a	606	-	4/4/18/26	6/27/125/137	-
26	CHL	1	613	-	3/3/16/26	1/18/116/137	-
26	CHL	8	603	21	4/4/20/26	9/39/137/137	-
30	LHG	7	801	25	-	25/41/41/53	-
26	CHL	4	618	-	4/4/18/26	4/27/125/137	-
29	BCR	B	4006	-	-	15/29/63/63	0/2/2/2
26	CHL	6	613	-	3/3/17/26	0/21/119/137	-
25	CLA	4	611	-	1/1/13/20	9/29/105/115	-
26	CHL	5	611	-	3/3/17/26	3/21/119/137	-
25	CLA	A	1110	-	1/1/12/20	9/26/102/115	-
25	CLA	7	610	-	1/1/14/20	13/33/109/115	-
25	CLA	B	1205	-	1/1/15/20	13/39/115/115	-
25	CLA	8	618	21	1/1/14/20	17/33/109/115	-
43	LUT	1	503	-	-	7/29/67/67	0/2/2/2
25	CLA	A	1137	-	1/1/14/20	10/33/109/115	-
26	CHL	6	609	19	4/4/20/26	9/39/137/137	-
50	XAT	9	507	-	1/1/12/26	7/31/93/93	0/4/4/4
25	CLA	B	1232	-	1/1/11/20	8/15/91/115	-
25	CLA	2	621	22	1/1/15/20	16/39/115/115	-
29	BCR	B	4005	-	-	15/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	1	615	15	1/1/11/20	7/17/93/115	-
43	LUT	9	501	-	-	2/29/67/67	0/2/2/2
25	CLA	6	605	-	1/1/11/20	6/17/93/115	-
25	CLA	2	608	-	1/1/11/20	7/15/91/115	-
43	LUT	7	501	-	1/1/12/27	6/29/67/67	0/2/2/2
43	LUT	2	502	-	-	2/29/67/67	0/2/2/2
25	CLA	B	1207	-	1/1/14/20	18/33/109/115	-
25	CLA	3	601	16	1/1/15/20	13/39/115/115	-
43	LUT	a	503	-	-	4/29/67/67	0/2/2/2
25	CLA	7	607	30	1/1/13/20	8/31/107/115	-
25	CLA	A	1119	-	1/1/15/20	18/39/115/115	-
25	CLA	B	1209	-	1/1/15/20	15/39/115/115	-
25	CLA	A	1117	-	1/1/15/20	16/39/115/115	-
25	CLA	6	604	19	1/1/15/20	14/39/115/115	-
48	DGA	8	804	-	-	23/41/41/45	-
25	CLA	4	602	-	1/1/12/20	8/24/100/115	-
25	CLA	6	601	-	1/1/14/20	11/33/109/115	-
25	CLA	4	603	17	1/1/13/20	6/29/105/115	-
25	CLA	4	607	-	1/1/13/20	11/27/103/115	-
26	CHL	1	604	-	4/4/20/26	9/39/137/137	-
26	CHL	2	613	-	3/3/17/26	1/21/119/137	-
25	CLA	B	1234	-	-	19/37/87/115	0/5/5/9
25	CLA	A	1104	1	1/1/15/20	18/39/115/115	-
25	CLA	L	1504	-	1/1/12/20	9/21/97/115	-
30	LHG	A	5002	-	-	37/53/53/53	-
43	LUT	6	502	-	-	4/29/67/67	0/2/2/2
25	CLA	a	615	15	1/1/11/20	4/17/93/115	-
25	CLA	2	606	-	1/1/11/20	4/17/93/115	-
25	CLA	A	1128	-	1/1/15/20	19/39/115/115	-
25	CLA	J	1901	9	1/1/10/20	4/12/88/115	-
25	CLA	a	605	-	1/1/13/20	10/27/103/115	-
41	SPH	J	5002	-	-	12/21/21/21	-
37	PCW	6	803	-	-	22/39/39/57	-
26	CHL	2	609	22	4/4/20/26	9/39/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	1108	-	1/1/15/20	15/39/115/115	-
25	CLA	B	1022	54	1/1/15/20	12/39/115/115	-
25	CLA	B	1203	2	1/1/15/20	13/39/115/115	-
36	DGD	8	803	-	-	18/35/75/95	0/2/2/2
25	CLA	L	1501	11	1/1/12/20	7/21/97/115	-
26	CHL	6	617	19	3/3/15/26	0/12/110/137	-
43	LUT	8	502	-	-	5/29/67/67	0/2/2/2
25	CLA	1	601	-	1/1/14/20	12/33/109/115	-
24	CL0	A	1011	-	3/3/20/25	11/37/135/135	-
28	SF4	A	3001	1,2	-	-	0/6/5/5
25	CLA	B	1208	-	1/1/13/20	11/25/101/115	-
30	LHG	3	801	25	-	32/53/53/53	-
25	CLA	A	1116	-	1/1/14/20	13/33/109/115	-
25	CLA	L	1503	-	1/1/11/20	9/15/91/115	-
29	BCR	B	4003	-	-	7/29/63/63	0/2/2/2
35	LMT	A	5008	-	-	10/21/61/61	0/2/2/2
25	CLA	1	607	30	1/1/15/20	16/39/115/115	-
25	CLA	B	1236	-	1/1/12/20	9/25/101/115	-
33	PTY	B	5005	-	-	19/45/45/53	-
30	LHG	1	801	25	-	23/39/39/53	-
30	LHG	6	801	25	-	33/53/53/53	-
29	BCR	B	4001	-	-	11/29/63/63	0/2/2/2
26	CHL	7	613	-	4/4/19/26	4/33/131/137	-
34	3PH	A	5007	-	-	17/34/34/49	-
29	BCR	5	504	-	-	12/29/63/63	0/2/2/2
25	CLA	4	617	-	1/1/11/20	6/15/91/115	-
50	XAT	9	504	-	1/1/12/26	13/31/93/93	0/4/4/4
50	XAT	2	501	-	2/2/12/26	0/31/93/93	0/4/4/4
25	CLA	4	612	17	1/1/14/20	17/36/112/115	-
25	CLA	B	1201	-	1/1/15/20	20/39/115/115	-
25	CLA	5	615	18	1/1/11/20	9/17/93/115	-
25	CLA	A	1013	-	1/1/15/20	16/39/115/115	-
26	CHL	1	610	-	3/3/16/26	1/18/116/137	-
25	CLA	K	1404	10	1/1/11/20	8/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SF4	C	3002	3	-	-	0/6/5/5
26	CHL	5	617	18	3/3/16/26	0/17/115/137	-
43	LUT	3	501	-	-	2/29/67/67	0/2/2/2
43	LUT	a	502	-	-	2/29/67/67	0/2/2/2
25	CLA	4	604	-	1/1/14/20	9/33/109/115	-
33	PTY	3	802	-	-	17/41/41/53	-
25	CLA	9	602	-	1/1/11/20	4/17/93/115	-
25	CLA	3	607	30	1/1/15/20	15/39/115/115	-
25	CLA	A	1130	-	1/1/13/20	11/29/105/115	-
25	CLA	A	1133	-	1/1/15/20	23/39/115/115	-
26	CHL	a	604	-	4/4/19/26	5/33/131/137	-
29	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
25	CLA	3	618	16	1/1/11/20	4/17/93/115	-
25	CLA	5	601	18	1/1/14/20	12/33/109/115	-
25	CLA	G	1603	-	1/1/11/20	5/15/91/115	-
43	LUT	1	501	-	-	3/29/67/67	0/2/2/2
25	CLA	B	1023	-	1/1/15/20	16/39/115/115	-
47	PLM	6	804	-	-	8/15/15/15	-
29	BCR	A	4001	-	-	13/29/63/63	0/2/2/2
25	CLA	8	606	-	1/1/13/20	13/30/106/115	-
43	LUT	4	502	-	-	1/29/67/67	0/2/2/2
25	CLA	4	616	-	1/1/12/20	8/21/97/115	-
25	CLA	7	612	-	1/1/14/20	13/33/109/115	-
30	LHG	9	801	-	-	16/37/37/53	-
26	CHL	a	613	-	3/3/16/26	7/15/113/137	-
25	CLA	A	1129	-	1/1/12/20	9/21/97/115	-
25	CLA	a	611	-	1/1/12/20	8/21/97/115	-
29	BCR	L	4001	-	-	12/29/63/63	0/2/2/2
25	CLA	4	605	-	1/1/11/20	4/17/93/115	-
29	BCR	B	4007	-	-	7/29/63/63	0/2/2/2
25	CLA	9	612	-	1/1/15/20	13/39/115/115	-
38	LPX	F	5003	-	-	11/31/31/31	-
25	CLA	F	1301	-	1/1/12/20	8/21/97/115	-
40	RRX	3	506	-	1/1/11/25	10/29/65/65	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	QTB	a	504	-	1/1/5/10	2/11/28/28	0/1/1/1
25	CLA	B	1230	-	1/1/13/20	11/31/107/115	-
30	LHG	7	802	-	-	19/40/40/53	-
33	PTY	J	5001	-	-	20/31/31/53	-
25	CLA	8	605	-	1/1/13/20	12/27/103/115	-
25	CLA	9	604	23	1/1/14/20	8/33/109/115	-
25	CLA	B	1220	-	1/1/14/20	14/33/109/115	-
25	CLA	B	1227	-	1/1/12/20	12/21/97/115	-
25	CLA	7	604	20	1/1/15/20	17/39/115/115	-
25	CLA	B	1226	-	1/1/15/20	11/39/115/115	-
25	CLA	2	601	-	1/1/14/20	11/33/109/115	-
26	CHL	3	608	-	3/3/15/26	0/12/110/137	-
30	LHG	4	802	-	-	22/36/36/53	-
43	LUT	4	501	-	1/1/12/27	6/29/67/67	0/2/2/2
25	CLA	B	1219	2	1/1/13/20	10/32/108/115	-
43	LUT	5	505	-	-	9/29/67/67	0/2/2/2
48	DGA	3	803	-	-	14/25/25/45	-
45	OLA	8	808	-	-	5/17/17/17	-
41	SPH	6	806	-	-	9/21/21/21	-
36	DGD	B	5003	-	-	22/55/95/95	0/2/2/2
30	LHG	B	5001	25	-	33/53/53/53	-
44	AXT	1	502	-	-	10/29/71/75	0/2/2/2
37	PCW	K	5001	-	-	20/44/44/57	-
25	CLA	4	608	-	1/1/12/20	4/23/99/115	-
26	CHL	3	611	-	4/4/19/26	11/33/131/137	-
47	PLM	4	804	-	-	9/15/15/15	-
25	CLA	7	608	-	1/1/13/20	10/27/103/115	-
50	XAT	7	502	-	2/2/12/26	0/31/93/93	0/4/4/4
26	CHL	5	610	-	4/4/20/26	11/39/137/137	-
25	CLA	B	1221	-	1/1/15/20	9/39/115/115	-
25	CLA	B	1224	-	1/1/15/20	21/39/115/115	-
25	CLA	1	602	-	1/1/11/20	6/15/91/115	-
30	LHG	B	5002	-	-	28/53/53/53	-
25	CLA	9	609	23	1/1/11/20	6/17/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	1216	-	1/1/15/20	15/39/115/115	-
25	CLA	2	612	-	1/1/12/20	9/21/97/115	-
43	LUT	5	501	-	-	1/29/67/67	0/2/2/2
25	CLA	1	605	-	1/1/15/20	20/39/115/115	-
25	CLA	B	1206	2	1/1/15/20	20/39/115/115	-
47	PLM	4	803	-	-	6/14/14/15	-
25	CLA	A	1012	-	1/1/15/20	13/39/115/115	-
28	SF4	C	3003	3	-	-	0/6/5/5
25	CLA	A	1131	-	1/1/15/20	14/39/115/115	-
25	CLA	8	611	-	1/1/12/20	6/21/97/115	-
29	BCR	L	4003	-	-	10/29/63/63	0/2/2/2
25	CLA	A	1127	-	1/1/15/20	13/39/115/115	-
25	CLA	B	1218	-	1/1/13/20	7/27/103/115	-
25	CLA	B	1235	-	1/1/15/20	19/39/115/115	-
29	BCR	J	4001	-	-	11/29/63/63	0/2/2/2
26	CHL	9	608	-	3/3/16/26	6/18/116/137	-
25	CLA	6	612	-	1/1/12/20	10/21/97/115	-
25	CLA	a	602	-	1/1/12/20	8/21/97/115	-
26	CHL	4	613	-	3/3/17/26	6/23/121/137	-
25	CLA	9	606	-	1/1/13/20	6/27/103/115	-
25	CLA	8	608	-	1/1/12/20	5/24/100/115	-
33	PTY	a	803	-	-	23/41/41/53	-
25	CLA	B	1217	-	1/1/13/20	12/29/105/115	-
33	PTY	5	802	-	-	22/41/41/53	-
25	CLA	6	618	-	1/1/11/20	8/17/93/115	-
36	DGD	7	806	-	-	13/39/79/95	0/2/2/2
25	CLA	B	1237	-	1/1/15/20	20/39/115/115	-
25	CLA	B	1239	-	1/1/15/20	16/39/115/115	-
25	CLA	H	1701	-	1/1/13/20	8/27/103/115	-
30	LHG	9	802	-	-	26/53/53/53	-
25	CLA	K	1403	10	1/1/11/20	9/20/96/115	-
26	CHL	A	1114	-	4/4/20/26	9/39/137/137	-
41	SPH	4	805	-	-	10/21/21/21	-
25	CLA	B	1215	-	1/1/14/20	16/33/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	4RF	7	807	-	-	19/39/39/59	-
44	AXT	7	504	-	-	14/29/71/75	0/2/2/2
29	BCR	A	4002	-	-	9/29/63/63	0/2/2/2
25	CLA	B	1202	-	1/1/15/20	16/39/115/115	-
25	CLA	F	1302	-	1/1/13/20	10/27/103/115	-
25	CLA	1	612	15	1/1/15/20	18/39/115/115	-
26	CHL	a	609	15	3/3/17/26	3/24/122/137	-
26	CHL	3	604	16	4/4/20/26	8/39/137/137	-
29	BCR	H	4001	-	-	12/29/63/63	0/2/2/2
25	CLA	A	1125	-	1/1/15/20	26/39/115/115	-
25	CLA	4	615	17	1/1/14/20	12/33/109/115	-
53	LAP	8	810	-	-	15/30/30/30	-
29	BCR	6	503	-	-	16/29/63/63	0/2/2/2
31	LMG	A	5004	-	-	4/37/57/70	0/1/1/1
26	CHL	5	613	-	4/4/18/26	5/27/125/137	-
26	CHL	4	609	17	4/4/20/26	10/39/137/137	-
32	SQD	H	5001	-	-	8/40/60/69	0/1/1/1
25	CLA	A	1112	-	1/1/13/20	15/27/103/115	-
25	CLA	B	1212	-	1/1/13/20	10/30/106/115	-
25	CLA	5	602	-	1/1/12/20	10/24/100/115	-
25	CLA	6	602	-	1/1/12/20	9/24/100/115	-
25	CLA	3	610	16	1/1/13/20	13/30/106/115	-
25	CLA	3	616	-	1/1/13/20	11/29/105/115	-
25	CLA	B	1228	-	1/1/15/20	15/39/115/115	-
42	ECH	M	4001	-	-	5/29/66/66	0/2/2/2
30	LHG	5	801	-	-	33/53/53/53	-
25	CLA	a	603	-	1/1/15/20	16/39/115/115	-
25	CLA	6	608	-	1/1/13/20	9/27/103/115	-
25	CLA	7	606	-	1/1/13/20	10/25/101/115	-
25	CLA	2	602	-	1/1/12/20	14/24/100/115	-
25	CLA	A	1136	-	1/1/15/20	16/39/115/115	-
25	CLA	8	609	21	1/1/14/20	16/33/109/115	-
25	CLA	a	612	15	1/1/13/20	10/30/106/115	-
37	PCW	B	5004	-	-	23/42/42/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a	601	-	1/1/14/20	7/33/109/115	-
25	CLA	B	1214	-	1/1/13/20	18/32/108/115	-
26	CHL	7	609	20	4/4/19/26	8/35/133/137	-
35	LMT	2	804	-	-	5/21/61/61	0/2/2/2
30	LHG	2	801	25	-	29/53/53/53	-
30	LHG	7	803	-	-	22/39/39/53	-
29	BCR	8	503	-	-	16/29/63/63	0/2/2/2
30	LHG	1	802	-	-	33/53/53/53	-
25	CLA	K	1402	-	1/1/14/20	8/33/109/115	-
25	CLA	7	605	-	1/1/11/20	3/13/89/115	-
45	OLA	8	809	-	-	11/17/17/17	-
26	CHL	9	613	-	3/3/15/26	2/10/108/137	-
25	CLA	B	1240	30	1/1/15/20	11/39/115/115	-
25	CLA	4	601	-	1/1/14/20	9/33/109/115	-
29	BCR	3	504	-	-	11/29/63/63	0/2/2/2
29	BCR	B	4004	-	-	9/29/63/63	0/2/2/2
25	CLA	A	1140	-	1/1/13/20	10/27/103/115	-
26	CHL	3	603	16	4/4/20/26	9/39/137/137	-
27	PQN	A	2001	-	-	7/23/43/43	0/2/2/2
29	BCR	A	4005	-	-	13/29/63/63	0/2/2/2
29	BCR	B	4002	-	-	16/29/63/63	0/2/2/2
33	PTY	9	803	-	-	27/51/51/53	-
26	CHL	9	610	-	3/3/17/26	4/21/119/137	-
26	CHL	8	604	21	4/4/19/26	11/35/133/137	-
25	CLA	G	1602	7	1/1/14/20	11/33/109/115	-
25	CLA	5	612	18	1/1/15/20	21/39/115/115	-
26	CHL	2	610	-	4/4/16/26	2/18/116/137	-
25	CLA	A	1124	-	1/1/13/20	7/27/103/115	-
25	CLA	8	602	-	1/1/12/20	5/24/100/115	-
25	CLA	B	1021	-	1/1/15/20	16/39/115/115	-
25	CLA	O	1803	-	1/1/10/20	2/10/86/115	-
25	CLA	A	1132	-	1/1/15/20	17/39/115/115	-
25	CLA	O	1801	-	1/1/9/20	0/6/78/115	-
26	CHL	6	619	19	5/5/20/26	8/39/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	3	505	-	-	11/29/63/63	0/2/2/2
30	LHG	6	802	-	-	25/41/41/53	-
32	SQD	7	805	-	-	10/34/54/69	0/1/1/1
25	CLA	5	604	18	1/1/15/20	11/39/115/115	-
25	CLA	A	1109	25	1/1/15/20	19/39/115/115	-
33	PTY	A	5006	-	-	12/37/37/53	-
35	LMT	B	5006	-	-	9/21/61/61	0/2/2/2
26	CHL	9	601	-	4/4/20/26	10/39/137/137	-
25	CLA	B	1223	-	1/1/15/20	12/39/115/115	-
30	LHG	A	5003	-	-	25/50/50/53	-
25	CLA	7	601	20	1/1/14/20	14/33/109/115	-
25	CLA	8	612	-	1/1/12/20	8/21/97/115	-
47	PLM	5	804	-	-	3/15/15/15	-
25	CLA	A	1134	1	1/1/14/20	14/33/109/115	-
25	CLA	3	606	-	1/1/15/20	13/39/115/115	-
25	CLA	6	615	54	1/1/15/20	16/39/115/115	-
25	CLA	7	603	20	1/1/15/20	22/39/115/115	-
52	P5S	8	805	-	-	23/42/42/59	-
25	CLA	B	1213	-	1/1/13/20	12/27/103/115	-
26	CHL	5	618	-	3/3/17/26	3/21/119/137	-
25	CLA	2	607	30	1/1/15/20	12/39/115/115	-
29	BCR	7	503	-	-	11/29/63/63	0/2/2/2
25	CLA	A	1126	-	1/1/15/20	22/39/115/115	-
26	CHL	8	601	21	4/4/19/26	5/33/131/137	-
29	BCR	O	4001	-	-	13/29/63/63	0/2/2/2
30	LHG	A	5001	-	-	32/53/53/53	-
25	CLA	B	1210	-	1/1/15/20	20/39/115/115	-
25	CLA	A	1139	-	1/1/13/20	11/27/103/115	-
25	CLA	4	606	-	1/1/12/20	7/21/97/115	-
25	CLA	6	606	19	1/1/15/20	15/39/115/115	-
47	PLM	a	804	-	-	4/14/14/15	-
48	DGA	5	803	-	-	14/24/24/45	-
25	CLA	5	607	-	1/1/14/20	12/33/109/115	-
33	PTY	7	804	-	-	14/36/36/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	K	4002	-	-	10/29/63/63	0/2/2/2
25	CLA	3	605	-	1/1/15/20	16/39/115/115	-
25	CLA	3	612	16	1/1/12/20	6/21/97/115	-
29	BCR	4	503	-	-	15/29/63/63	0/2/2/2
26	CHL	9	603	-	4/4/20/26	9/39/137/137	-
26	CHL	1	609	15	4/4/20/26	10/39/137/137	-
48	DGA	2	803	-	-	26/38/38/45	-
26	CHL	7	611	-	4/4/18/26	5/27/125/137	-
26	CHL	7	617	20	4/4/20/26	9/39/137/137	-
25	CLA	B	1211	-	1/1/13/20	11/27/103/115	-
25	CLA	A	1135	-	1/1/12/20	9/23/99/115	-
25	CLA	A	1105	-	1/1/13/20	4/30/106/115	-
26	CHL	7	615	20	3/3/17/26	6/21/119/137	-
39	NEX	F	4001	-	1/1/12/25	13/27/83/83	0/3/3/3
25	CLA	A	1122	-	1/1/14/20	19/33/109/115	-
25	CLA	2	603	22	1/1/14/20	10/33/109/115	-
25	CLA	A	1123	-	1/1/15/20	13/39/115/115	-
25	CLA	B	1222	-	1/1/13/20	8/31/107/115	-
25	CLA	1	603	-	1/1/15/20	13/39/115/115	-
30	LHG	a	801	-	-	22/39/39/53	-
41	SPH	9	804	-	-	13/21/21/21	-

The worst 5 of 2247 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	3	506	RRX	C26-C25	15.98	1.61	1.34
40	J	4002	RRX	C26-C25	15.93	1.61	1.34
40	3	506	RRX	C5-C6	15.36	1.60	1.34
43	3	502	LUT	C24-C25	15.36	1.51	1.33
43	7	501	LUT	C24-C25	15.32	1.51	1.33

The worst 5 of 5239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H	4001	BCR	C23-C22-C21	26.56	160.78	119.01
50	9	504	XAT	C20-C13-C14	-26.26	80.27	122.82
50	9	504	XAT	C12-C13-C14	26.16	160.15	119.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	F	4001	NEX	C17-C1-C6	-26.13	87.08	110.47
29	H	4001	BCR	C37-C22-C21	-26.11	80.51	122.82

5 of 394 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	1011	CL0	ND
24	A	1011	CL0	NA
24	A	1011	CL0	NC
25	A	1012	CLA	ND
25	A	1013	CLA	ND

5 of 4645 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	1102	CLA	C1A-C2A-CAA-CBA
25	A	1102	CLA	C3A-C2A-CAA-CBA
25	A	1103	CLA	C3A-C2A-CAA-CBA
25	A	1103	CLA	CAD-CBD-CGD-O1D
25	A	1103	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

372 monomers are involved in 1151 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1113	CLA	8	0
25	1	608	CLA	6	0
25	K	1401	CLA	5	0
33	G	5002	PTY	1	0
25	A	1111	CLA	7	0
45	1	803	OLA	2	0
29	I	4001	BCR	2	0
25	B	1231	CLA	7	0
25	2	615	CLA	3	0
29	A	4004	BCR	3	0
30	4	801	LHG	4	0
43	8	501	LUT	6	0
43	3	502	LUT	4	0
26	8	610	CHL	2	0
26	1	611	CHL	4	0
25	8	607	CLA	2	0
25	3	602	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	1	804	LMT	2	0
29	3	503	BCR	2	0
25	5	606	CLA	3	0
40	J	4002	RRX	3	0
25	A	1101	CLA	5	0
43	a	501	LUT	5	0
25	B	1204	CLA	6	0
26	a	610	CHL	2	0
25	B	1238	CLA	2	0
43	6	501	LUT	5	0
25	A	1106	CLA	6	0
25	4	610	CLA	5	0
25	A	1138	CLA	8	0
25	H	1703	CLA	5	0
37	K	5002	PCW	1	0
25	5	609	CLA	1	0
25	O	1802	CLA	5	0
33	G	5003	PTY	1	0
25	2	604	CLA	12	0
26	6	610	CHL	2	0
45	a	805	OLA	2	0
25	5	605	CLA	2	0
29	K	4001	BCR	4	0
25	9	605	CLA	4	0
29	6	504	BCR	4	0
33	a	802	PTY	2	0
25	a	607	CLA	2	0
43	2	507	LUT	7	0
36	8	802	DGD	3	0
30	8	801	LHG	1	0
25	B	1225	CLA	4	0
25	A	1107	CLA	1	0
25	A	1102	CLA	2	0
25	5	603	CLA	2	0
26	8	613	CHL	4	0
25	A	1103	CLA	8	0
25	A	1121	CLA	1	0
32	A	5005	SQD	8	0
25	A	1115	CLA	8	0
25	A	1120	CLA	3	0
30	F	5002	LHG	2	0
26	6	611	CHL	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	G	1601	CLA	2	0
29	L	4002	BCR	2	0
25	1	606	CLA	2	0
25	a	608	CLA	1	0
43	5	502	LUT	4	0
25	9	607	CLA	2	0
25	L	1502	CLA	5	0
47	8	806	PLM	1	0
25	2	605	CLA	3	0
43	9	502	LUT	8	0
25	3	613	CLA	6	0
47	8	807	PLM	5	0
32	I	5001	SQD	4	0
32	G	5001	SQD	4	0
25	5	614	CLA	1	0
25	8	620	CLA	2	0
29	G	4001	BCR	5	0
27	B	2002	PQN	5	0
29	5	503	BCR	4	0
30	2	802	LHG	6	0
25	A	1118	CLA	2	0
25	6	603	CLA	5	0
25	B	1229	CLA	6	0
25	8	615	CLA	2	0
25	5	608	CLA	1	0
26	a	606	CHL	8	0
26	1	613	CHL	6	0
26	8	603	CHL	5	0
26	4	618	CHL	4	0
29	B	4006	BCR	5	0
26	6	613	CHL	3	0
25	4	611	CLA	2	0
26	5	611	CHL	1	0
25	A	1110	CLA	4	0
25	7	610	CLA	7	0
25	B	1205	CLA	6	0
25	8	618	CLA	4	0
43	1	503	LUT	2	0
25	A	1137	CLA	4	0
26	6	609	CHL	7	0
50	9	507	XAT	5	0
25	B	1232	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	2	621	CLA	2	0
29	B	4005	BCR	6	0
25	1	615	CLA	2	0
43	9	501	LUT	9	0
25	2	608	CLA	1	0
43	7	501	LUT	5	0
43	2	502	LUT	4	0
25	B	1207	CLA	4	0
25	3	601	CLA	7	0
43	a	503	LUT	4	0
25	7	607	CLA	2	0
25	A	1119	CLA	8	0
25	B	1209	CLA	5	0
25	A	1117	CLA	7	0
25	6	604	CLA	3	0
48	8	804	DGA	5	0
25	4	602	CLA	1	0
25	6	601	CLA	7	0
25	4	603	CLA	2	0
26	1	604	CHL	6	0
26	2	613	CHL	1	0
25	B	1234	CLA	8	0
25	A	1104	CLA	2	0
25	L	1504	CLA	2	0
30	A	5002	LHG	3	0
43	6	502	LUT	5	0
25	a	615	CLA	2	0
25	A	1128	CLA	5	0
25	J	1901	CLA	2	0
25	a	605	CLA	3	0
41	J	5002	SPH	1	0
37	6	803	PCW	3	0
26	2	609	CHL	4	0
25	A	1108	CLA	8	0
25	B	1022	CLA	4	0
25	B	1203	CLA	1	0
36	8	803	DGD	4	0
26	6	617	CHL	1	0
43	8	502	LUT	5	0
25	1	601	CLA	7	0
24	A	1011	CL0	6	0
25	B	1208	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	3	801	LHG	1	0
25	A	1116	CLA	8	0
25	L	1503	CLA	5	0
29	B	4003	BCR	2	0
35	A	5008	LMT	1	0
25	1	607	CLA	4	0
25	B	1236	CLA	6	0
33	B	5005	PTY	2	0
30	1	801	LHG	2	0
30	6	801	LHG	5	0
29	B	4001	BCR	5	0
26	7	613	CHL	10	0
34	A	5007	3PH	3	0
29	5	504	BCR	4	0
50	9	504	XAT	3	0
50	2	501	XAT	3	0
25	4	612	CLA	4	0
25	B	1201	CLA	6	0
25	5	615	CLA	1	0
25	A	1013	CLA	8	0
26	1	610	CHL	3	0
25	K	1404	CLA	1	0
26	5	617	CHL	2	0
43	3	501	LUT	3	0
43	a	502	LUT	4	0
25	4	604	CLA	6	0
33	3	802	PTY	3	0
25	3	607	CLA	1	0
25	A	1130	CLA	7	0
25	A	1133	CLA	8	0
26	a	604	CHL	9	0
29	A	4003	BCR	4	0
25	5	601	CLA	4	0
25	G	1603	CLA	4	0
43	1	501	LUT	4	0
25	B	1023	CLA	8	0
47	6	804	PLM	1	0
29	A	4001	BCR	4	0
25	8	606	CLA	4	0
43	4	502	LUT	6	0
25	4	616	CLA	2	0
25	7	612	CLA	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	9	801	LHG	3	0
26	a	613	CHL	7	0
25	A	1129	CLA	4	0
29	L	4001	BCR	3	0
25	4	605	CLA	3	0
29	B	4007	BCR	4	0
25	9	612	CLA	7	0
38	F	5003	LPX	2	0
25	F	1301	CLA	3	0
40	3	506	RRX	1	0
25	B	1230	CLA	8	0
33	J	5001	PTY	2	0
25	8	605	CLA	2	0
25	9	604	CLA	4	0
25	B	1220	CLA	12	0
25	B	1227	CLA	4	0
25	7	604	CLA	4	0
25	B	1226	CLA	5	0
25	2	601	CLA	6	0
26	3	608	CHL	1	0
43	4	501	LUT	4	0
25	B	1219	CLA	5	0
43	5	505	LUT	4	0
48	3	803	DGA	3	0
41	6	806	SPH	1	0
36	B	5003	DGD	4	0
30	B	5001	LHG	5	0
44	1	502	AXT	3	0
37	K	5001	PCW	2	0
25	4	608	CLA	4	0
26	3	611	CHL	6	0
47	4	804	PLM	3	0
25	7	608	CLA	1	0
50	7	502	XAT	3	0
26	5	610	CHL	5	0
25	B	1221	CLA	5	0
25	B	1224	CLA	10	0
25	1	602	CLA	1	0
30	B	5002	LHG	1	0
25	9	609	CLA	3	0
25	B	1216	CLA	6	0
25	2	612	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	5	501	LUT	4	0
25	1	605	CLA	6	0
25	B	1206	CLA	5	0
25	A	1012	CLA	10	0
28	C	3003	SF4	1	0
25	A	1131	CLA	6	0
25	8	611	CLA	4	0
29	L	4003	BCR	1	0
25	A	1127	CLA	8	0
25	B	1218	CLA	3	0
25	B	1235	CLA	4	0
29	J	4001	BCR	5	0
26	9	608	CHL	2	0
25	6	612	CLA	2	0
25	a	602	CLA	3	0
26	4	613	CHL	5	0
25	9	606	CLA	4	0
33	a	803	PTY	2	0
25	B	1217	CLA	4	0
33	5	802	PTY	3	0
36	7	806	DGD	3	0
25	B	1237	CLA	2	0
25	B	1239	CLA	2	0
25	H	1701	CLA	2	0
30	9	802	LHG	4	0
25	K	1403	CLA	3	0
26	A	1114	CHL	8	0
25	B	1215	CLA	4	0
51	7	807	4RF	6	0
44	7	504	AXT	10	0
29	A	4002	BCR	4	0
25	B	1202	CLA	4	0
25	F	1302	CLA	4	0
25	1	612	CLA	11	0
26	a	609	CHL	5	0
26	3	604	CHL	6	0
29	H	4001	BCR	4	0
25	A	1125	CLA	10	0
25	4	615	CLA	3	0
53	8	810	LAP	4	0
29	6	503	BCR	4	0
26	5	613	CHL	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	4	609	CHL	6	0
32	H	5001	SQD	3	0
25	A	1112	CLA	3	0
25	B	1212	CLA	3	0
25	5	602	CLA	4	0
25	6	602	CLA	3	0
25	3	610	CLA	2	0
25	3	616	CLA	3	0
25	B	1228	CLA	4	0
42	M	4001	ECH	5	0
30	5	801	LHG	2	0
25	a	603	CLA	2	0
25	6	608	CLA	4	0
25	7	606	CLA	2	0
25	2	602	CLA	2	0
25	A	1136	CLA	4	0
25	8	609	CLA	4	0
25	a	612	CLA	5	0
37	B	5004	PCW	1	0
25	a	601	CLA	5	0
25	B	1214	CLA	5	0
26	7	609	CHL	4	0
35	2	804	LMT	5	0
30	2	801	LHG	5	0
30	7	803	LHG	3	0
29	8	503	BCR	3	0
30	1	802	LHG	3	0
25	K	1402	CLA	3	0
25	7	605	CLA	3	0
45	8	809	OLA	1	0
26	9	613	CHL	3	0
25	B	1240	CLA	4	0
25	4	601	CLA	6	0
29	3	504	BCR	5	0
29	B	4004	BCR	8	0
25	A	1140	CLA	5	0
26	3	603	CHL	5	0
27	A	2001	PQN	7	0
29	A	4005	BCR	9	0
29	B	4002	BCR	4	0
33	9	803	PTY	4	0
26	9	610	CHL	6	0

Continued on next page...

Continued from previous page...

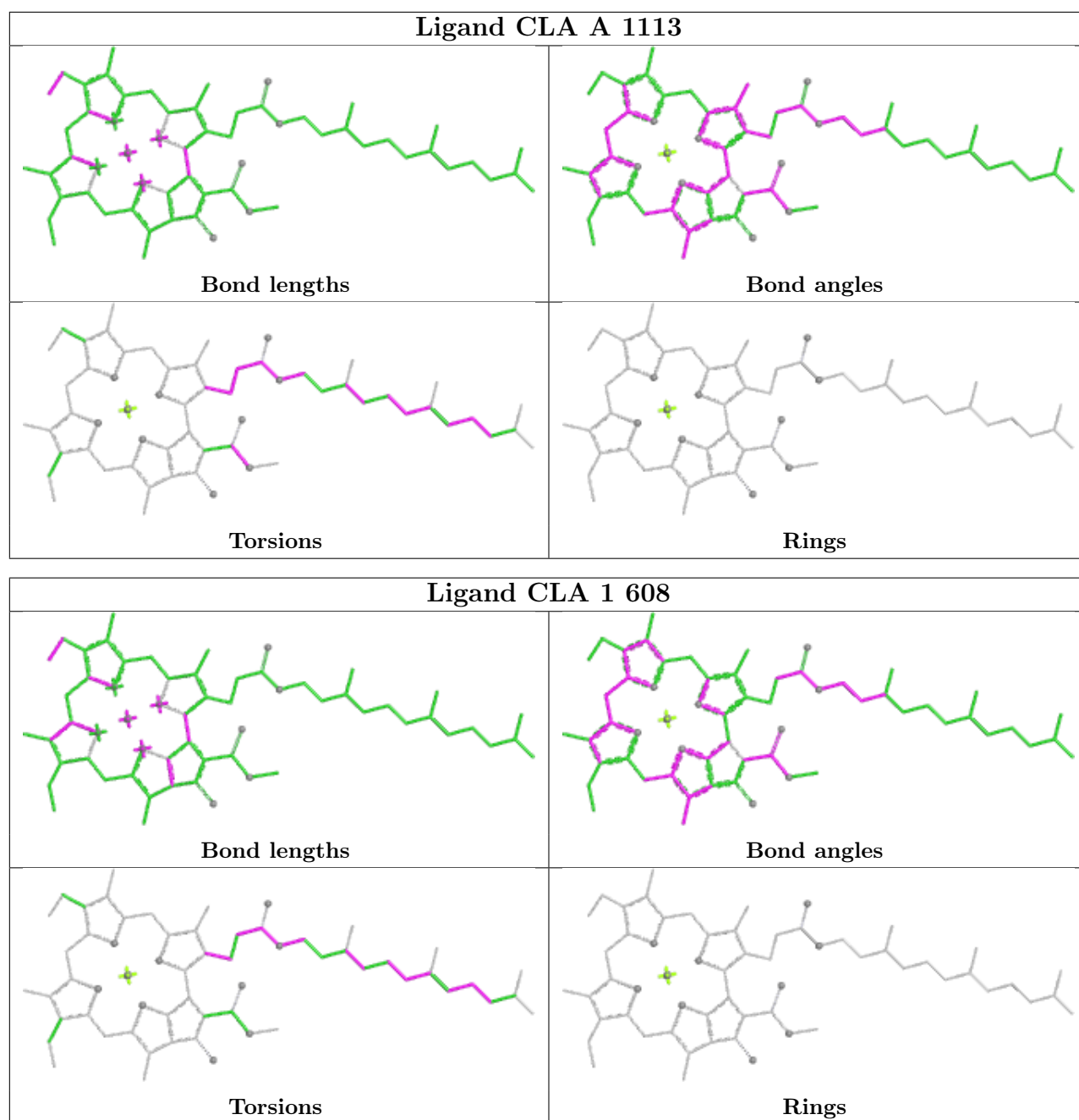
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	8	604	CHL	3	0
25	G	1602	CLA	2	0
25	5	612	CLA	9	0
26	2	610	CHL	2	0
25	A	1124	CLA	4	0
25	8	602	CLA	5	0
25	B	1021	CLA	7	0
25	A	1132	CLA	3	0
25	O	1801	CLA	1	0
26	6	619	CHL	7	0
29	3	505	BCR	4	0
32	7	805	SQD	1	0
25	5	604	CLA	3	0
25	A	1109	CLA	7	0
33	A	5006	PTY	4	0
35	B	5006	LMT	2	0
26	9	601	CHL	7	0
25	B	1223	CLA	3	0
30	A	5003	LHG	2	0
25	7	601	CLA	3	0
25	8	612	CLA	5	0
47	5	804	PLM	3	0
25	A	1134	CLA	2	0
25	3	606	CLA	6	0
25	6	615	CLA	6	0
25	7	603	CLA	4	0
52	8	805	P5S	2	0
25	B	1213	CLA	2	0
26	5	618	CHL	4	0
25	2	607	CLA	4	0
29	7	503	BCR	9	0
25	A	1126	CLA	12	0
26	8	601	CHL	5	0
29	O	4001	BCR	1	0
30	A	5001	LHG	3	0
25	A	1139	CLA	4	0
25	4	606	CLA	3	0
25	6	606	CLA	1	0
48	5	803	DGA	3	0
25	5	607	CLA	2	0
29	K	4002	BCR	3	0
25	3	605	CLA	5	0

Continued on next page...

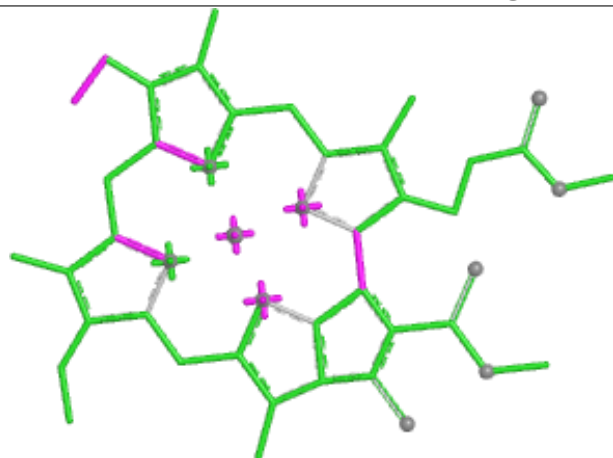
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	3	612	CLA	2	0
29	4	503	BCR	8	0
26	9	603	CHL	6	0
26	1	609	CHL	8	0
48	2	803	DGA	6	0
26	7	611	CHL	1	0
26	7	617	CHL	5	0
25	B	1211	CLA	1	0
25	A	1135	CLA	3	0
25	A	1105	CLA	5	0
26	7	615	CHL	1	0
39	F	4001	NEX	4	0
25	A	1122	CLA	5	0
25	2	603	CLA	5	0
25	A	1123	CLA	4	0
25	B	1222	CLA	5	0
25	1	603	CLA	4	0
30	a	801	LHG	2	0
41	9	804	SPH	2	0

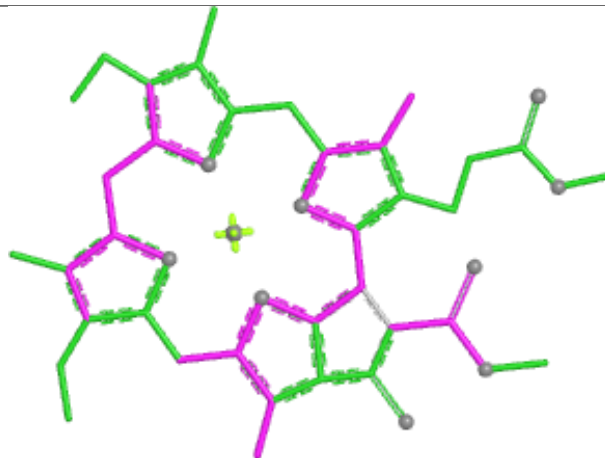
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



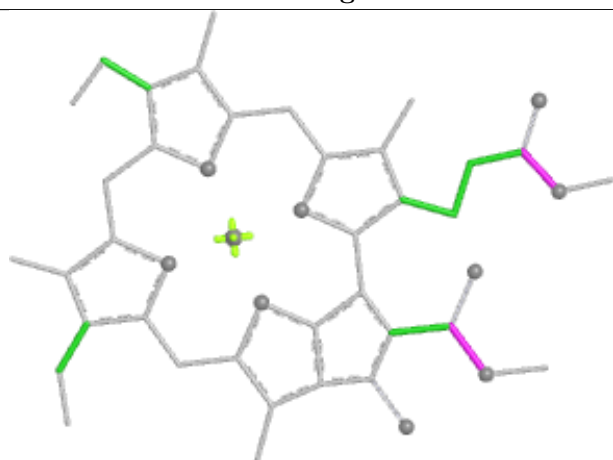
Ligand CLA K 1401



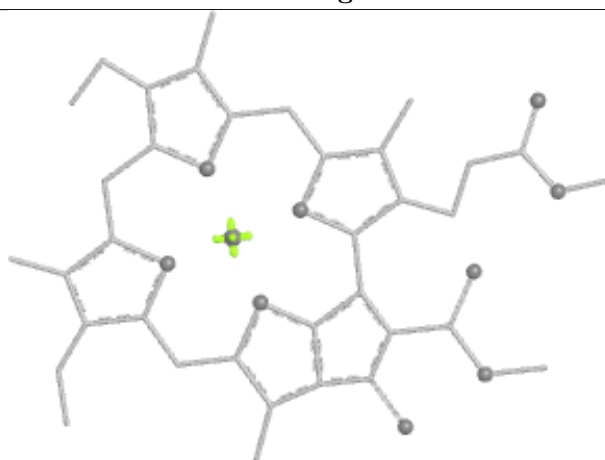
Bond lengths



Bond angles

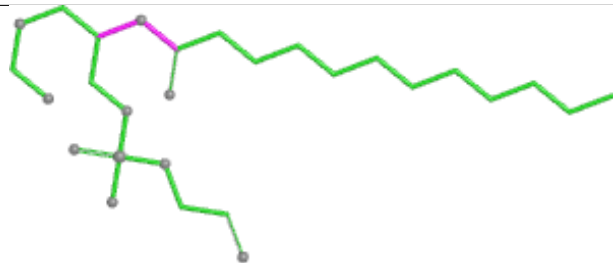


Torsions

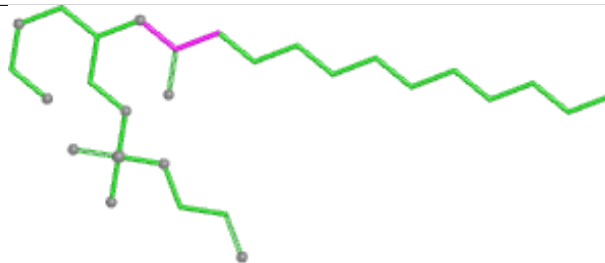


Rings

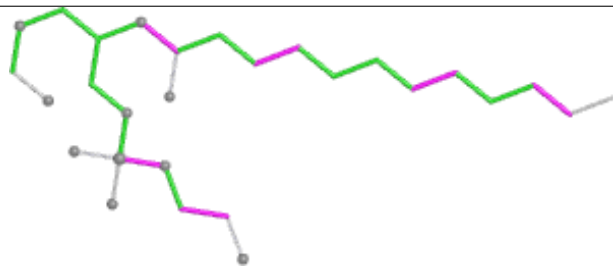
Ligand PTY G 5002



Bond lengths



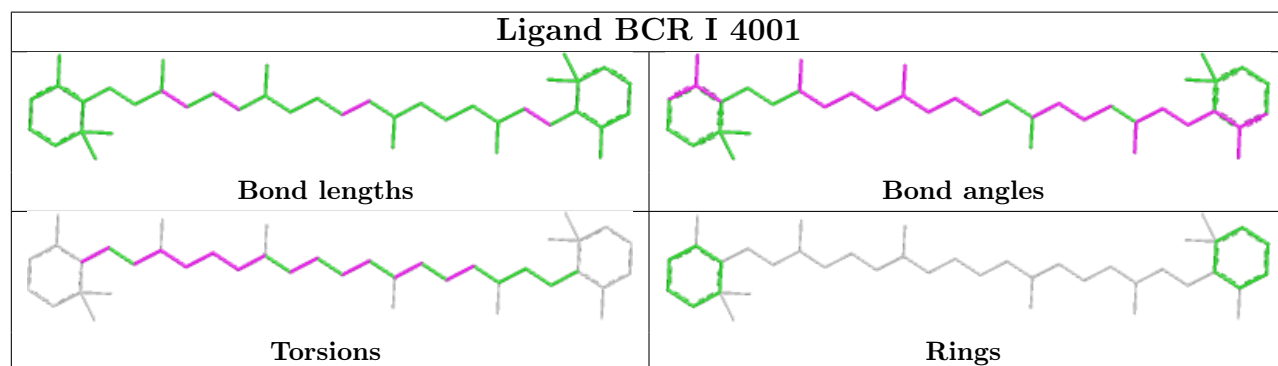
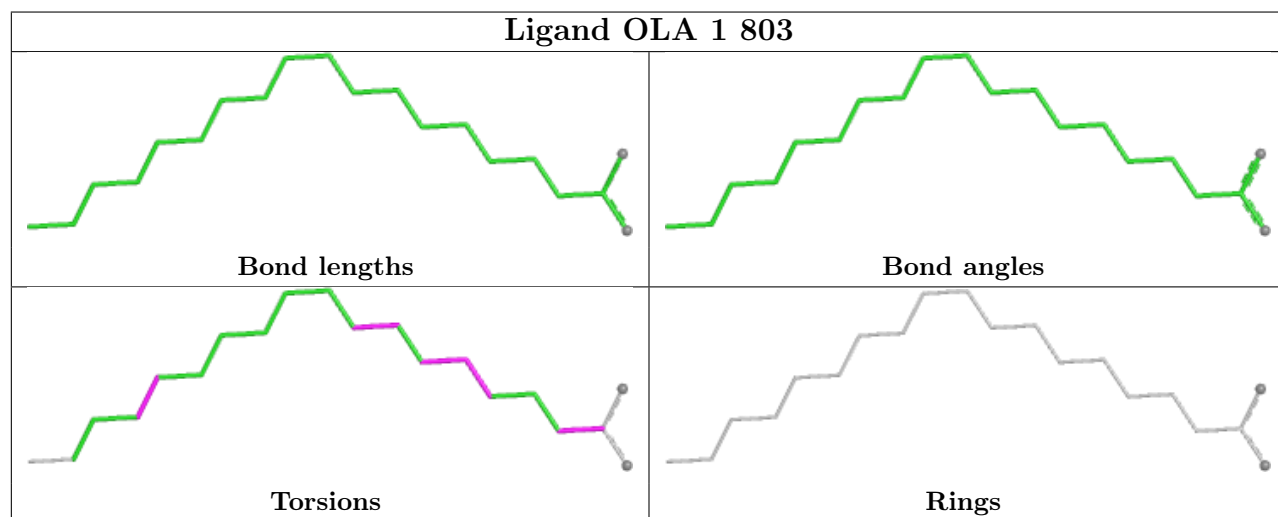
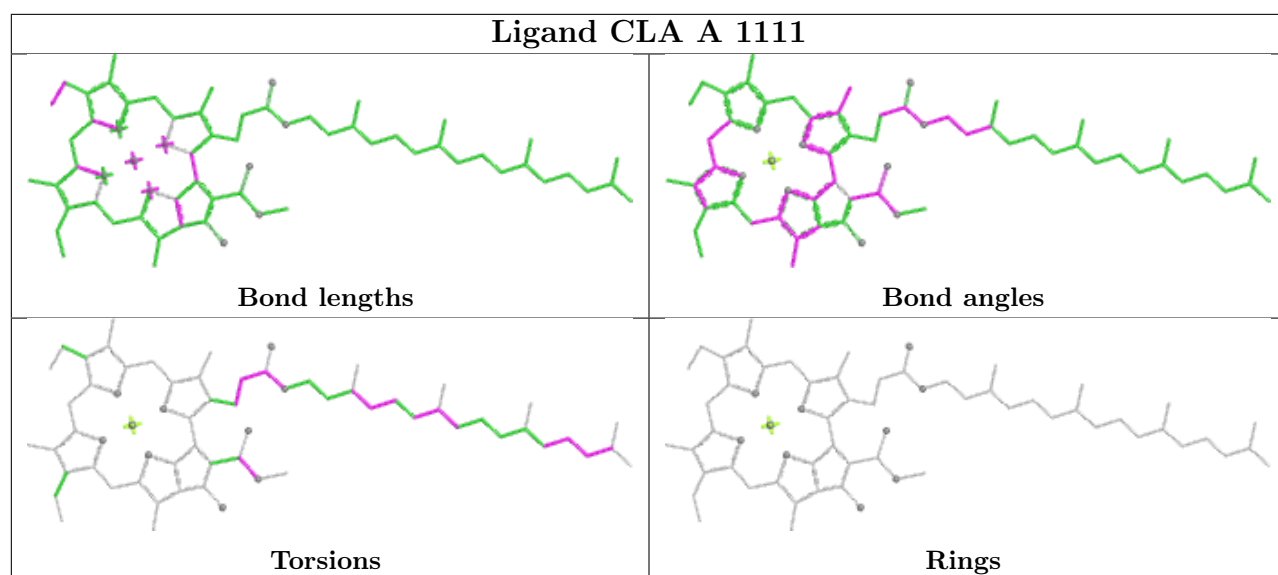
Bond angles

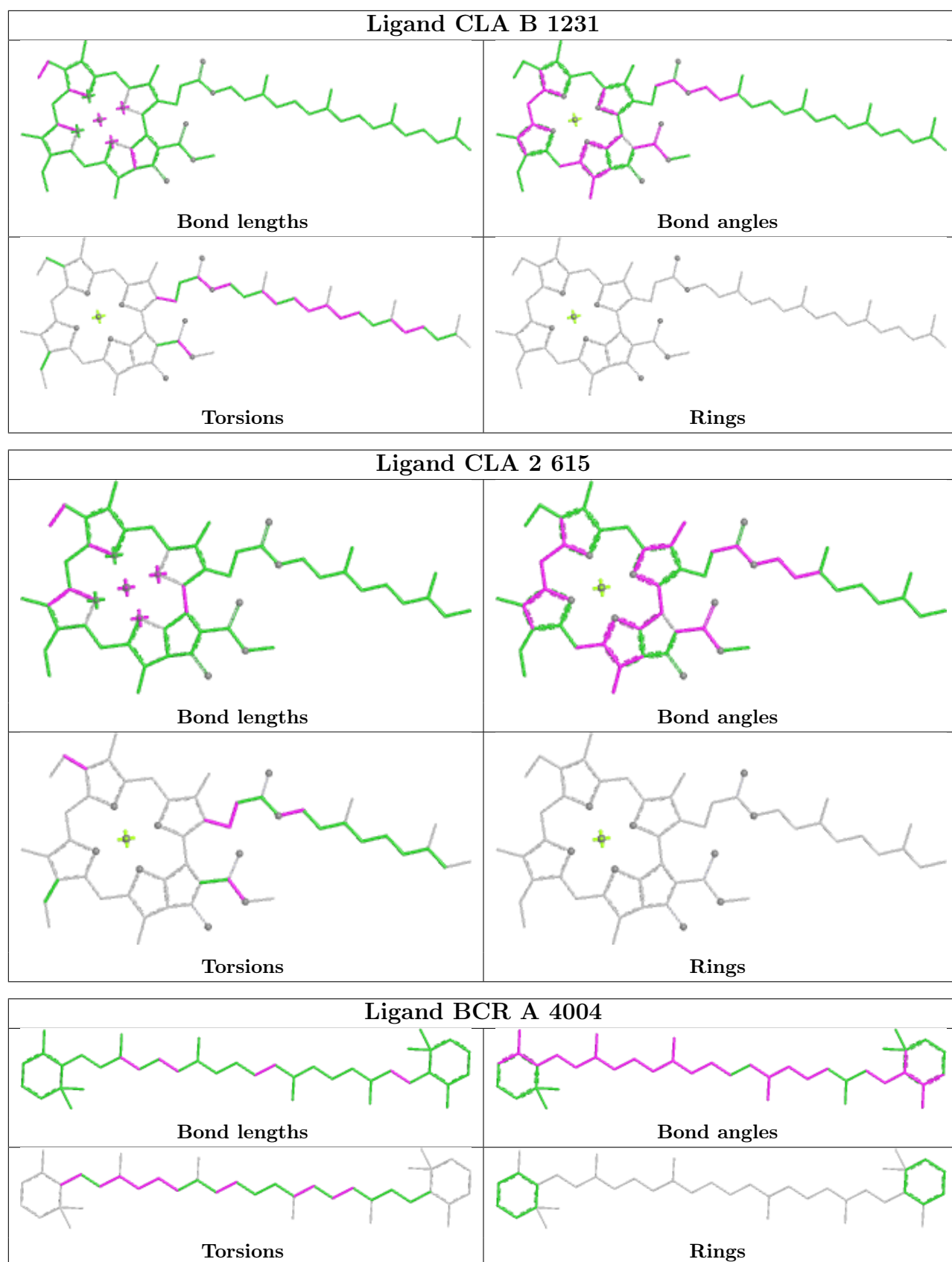


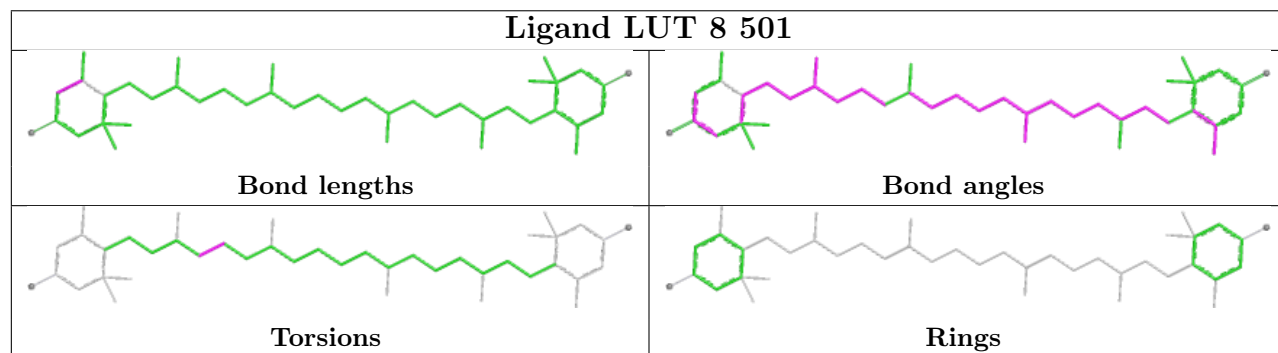
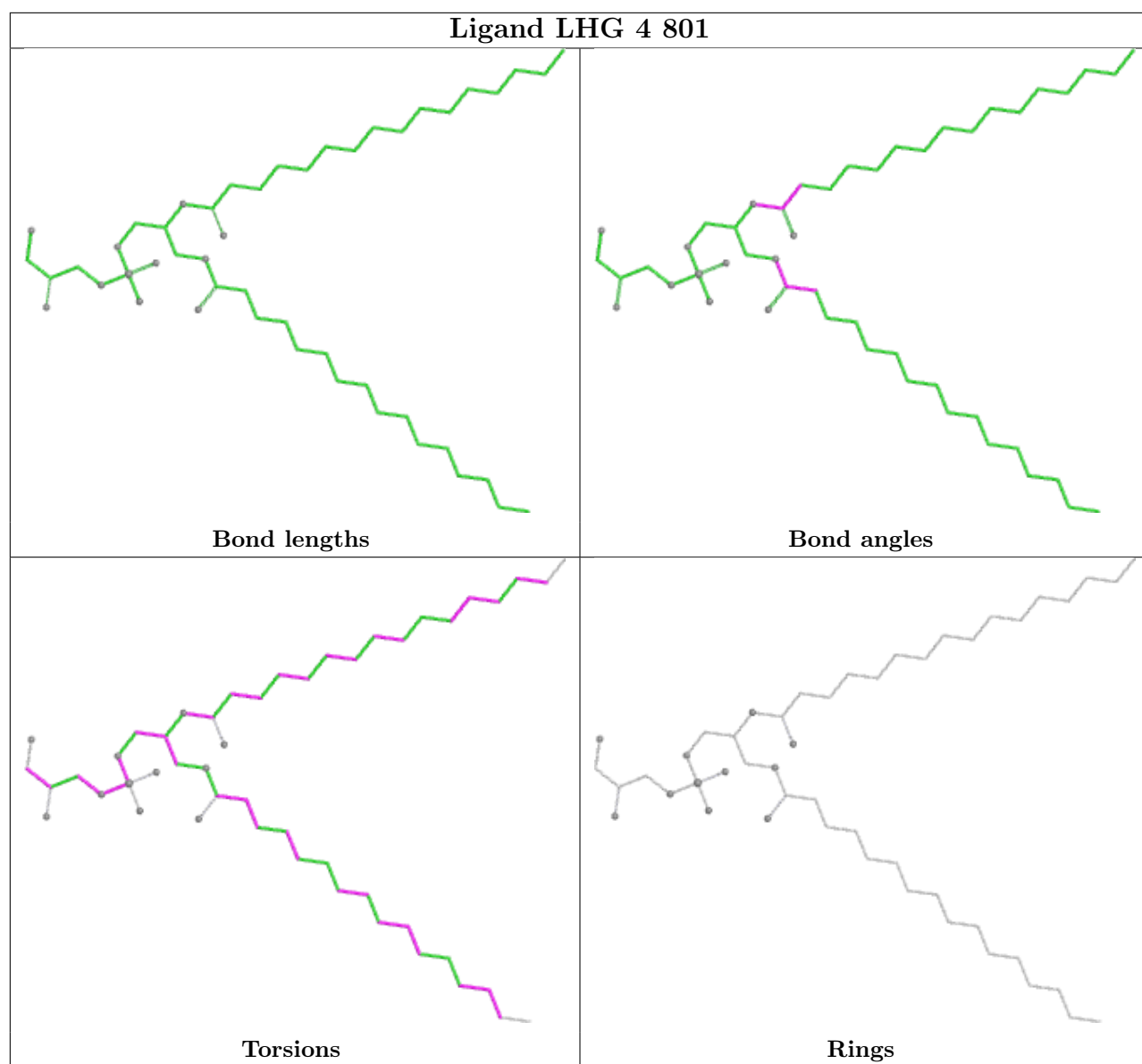
Torsions

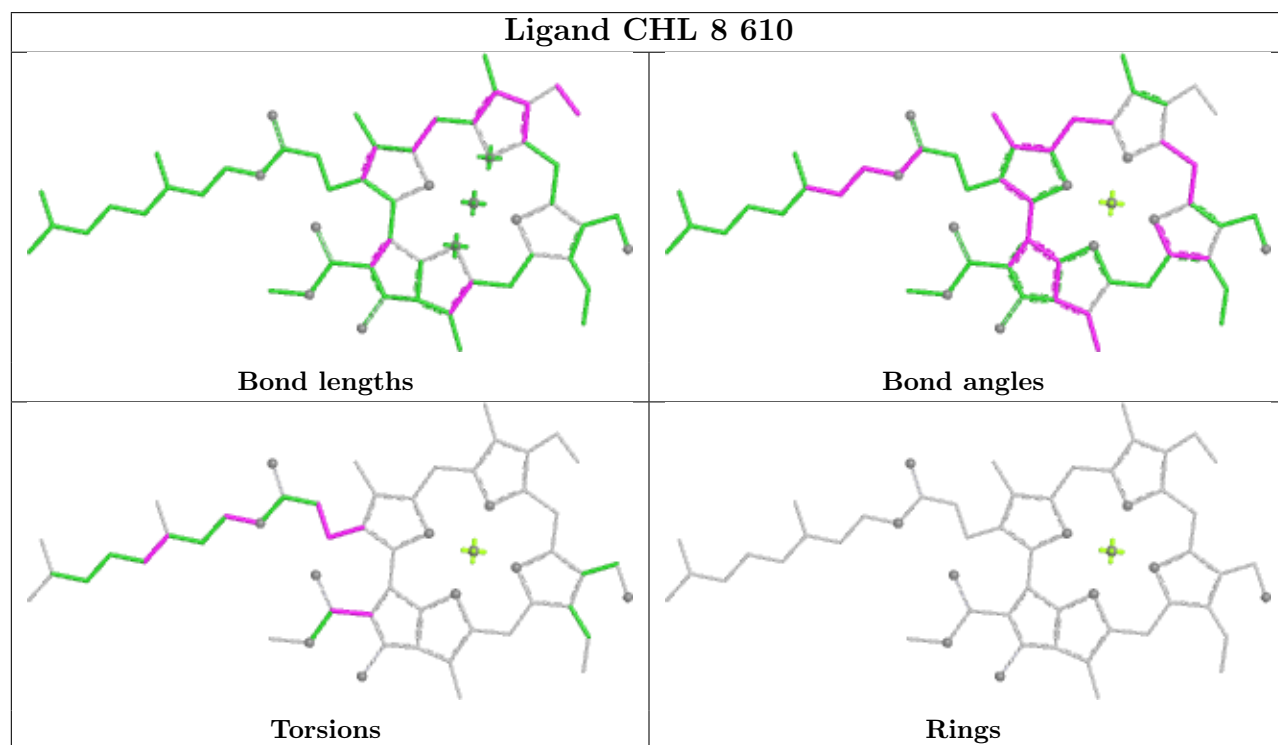
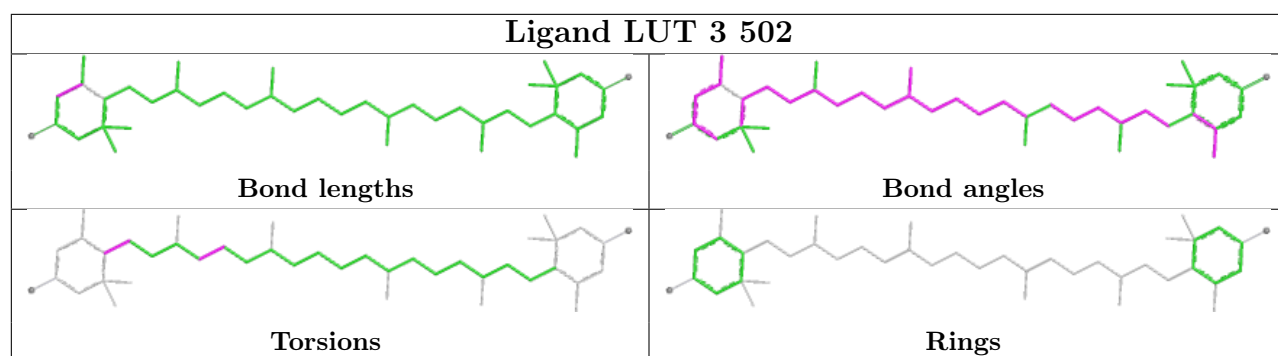


Rings

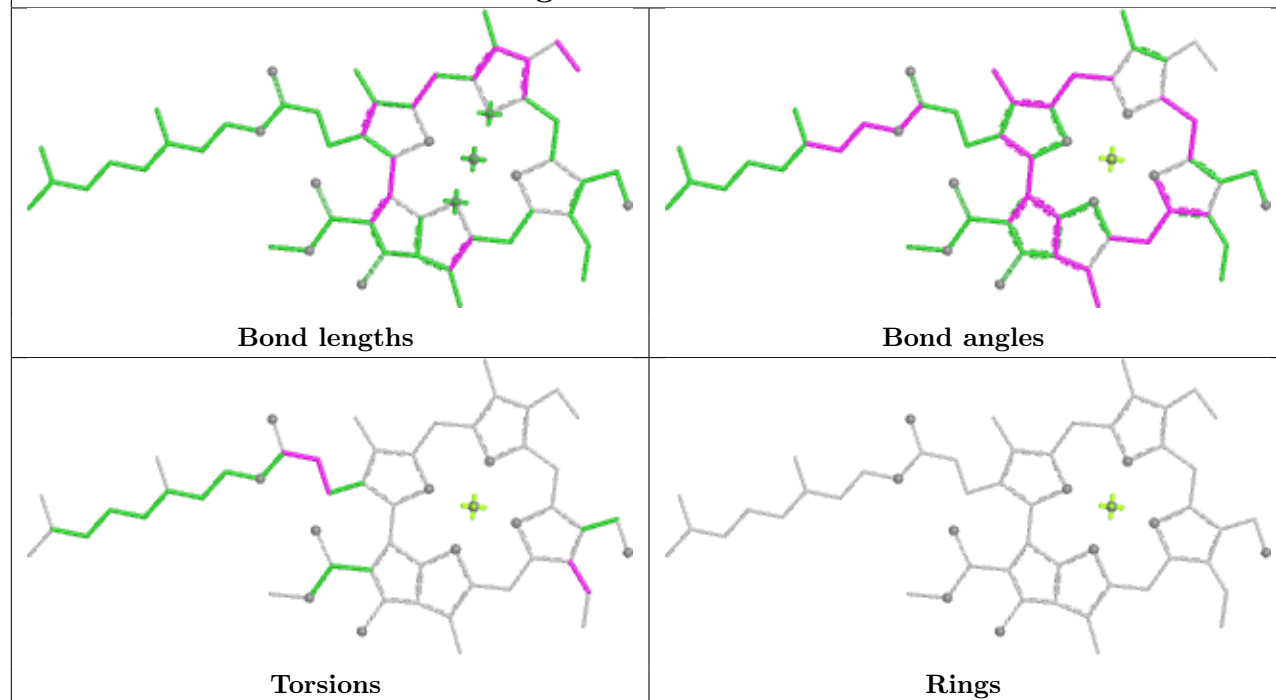




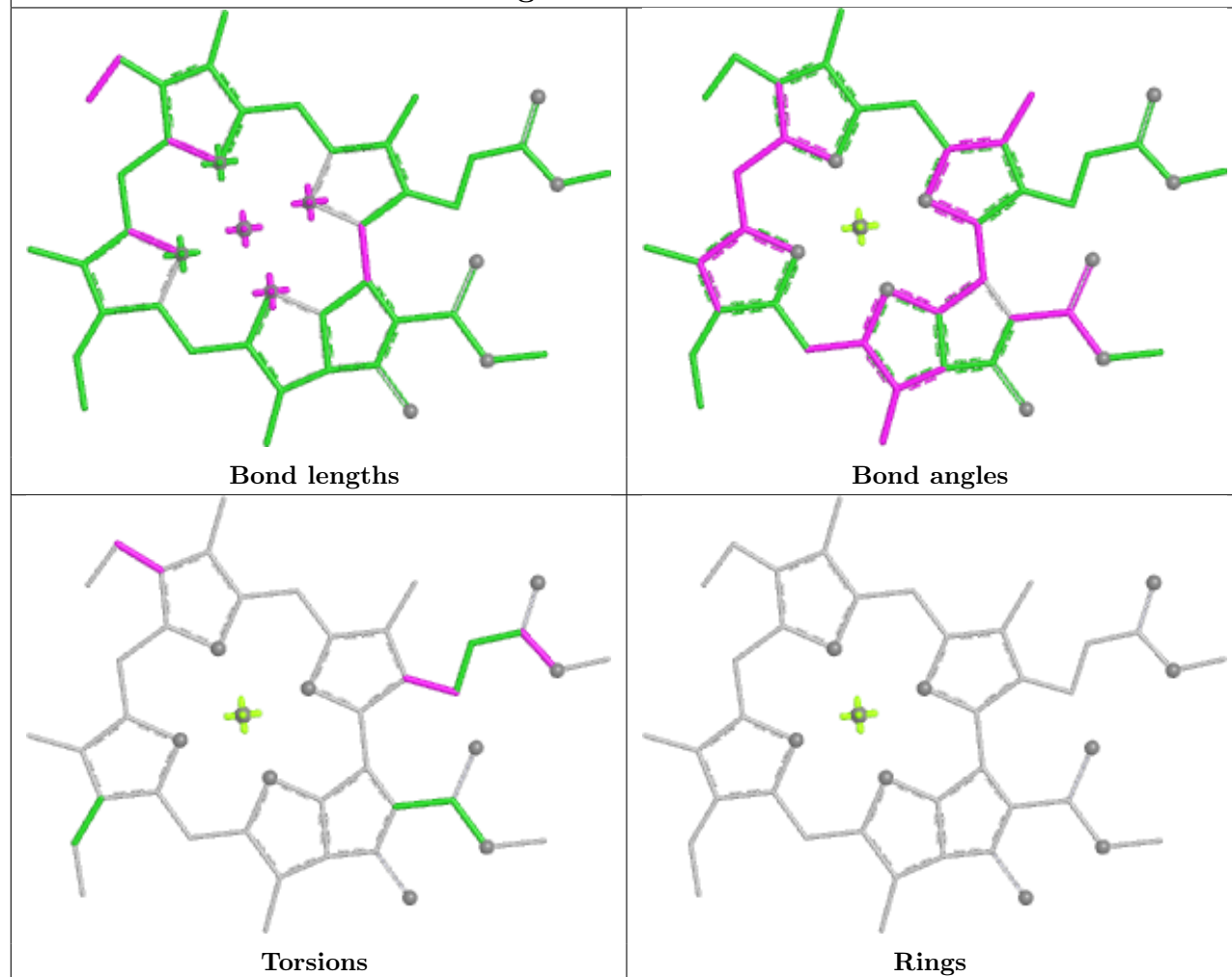




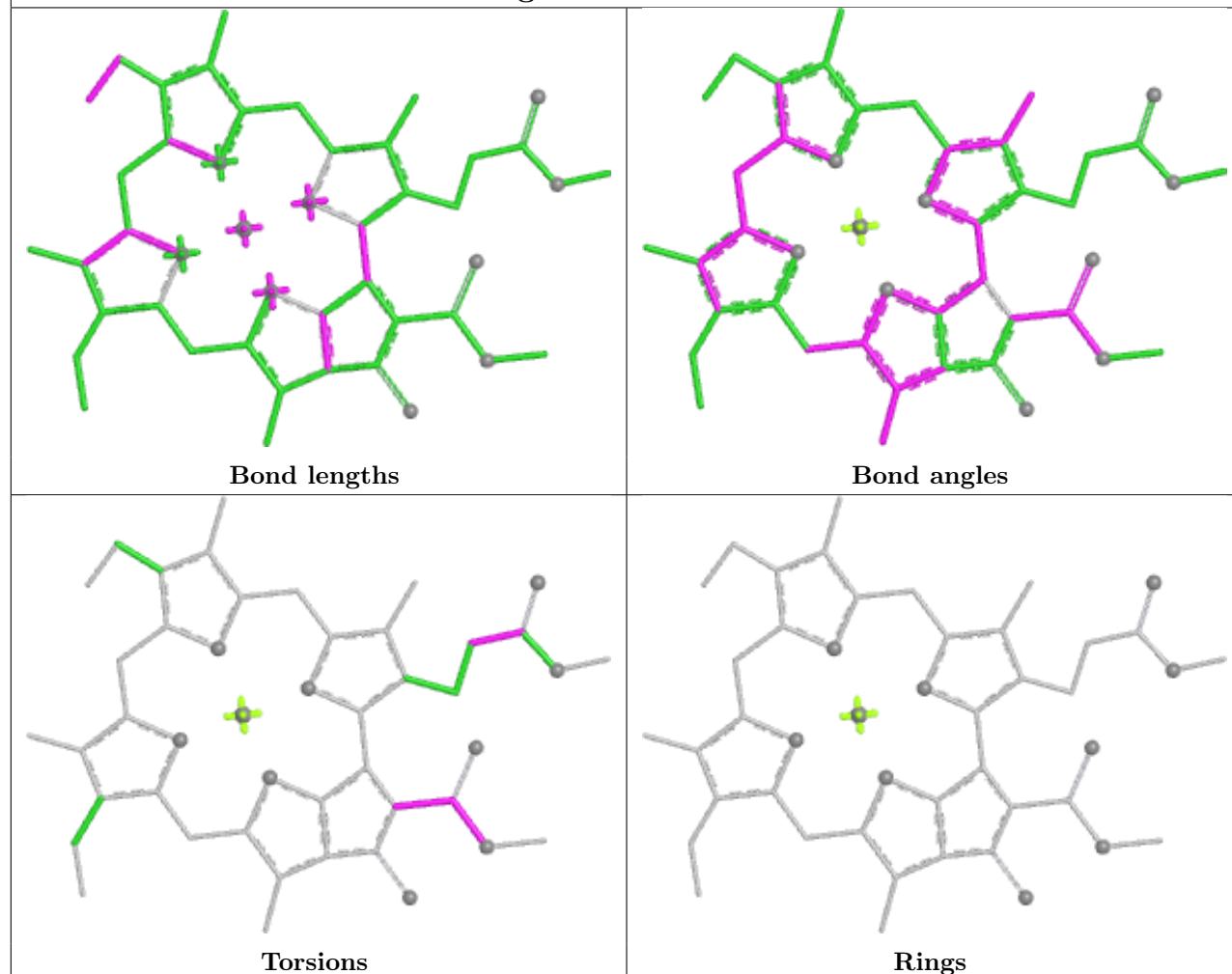
Ligand CHL 1 611



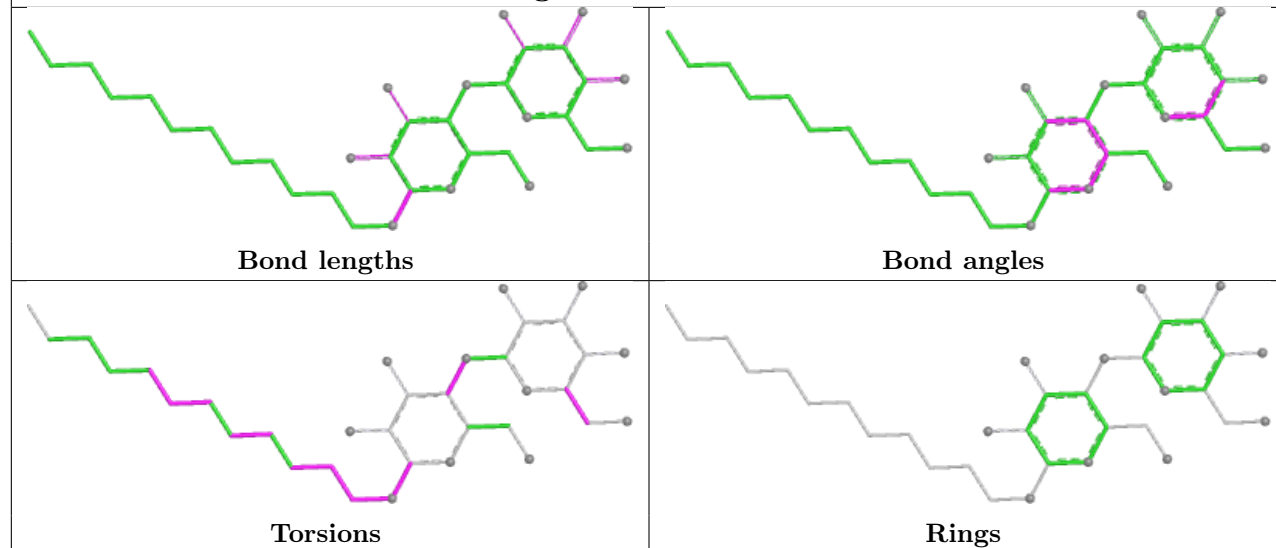
Ligand CLA 8 607

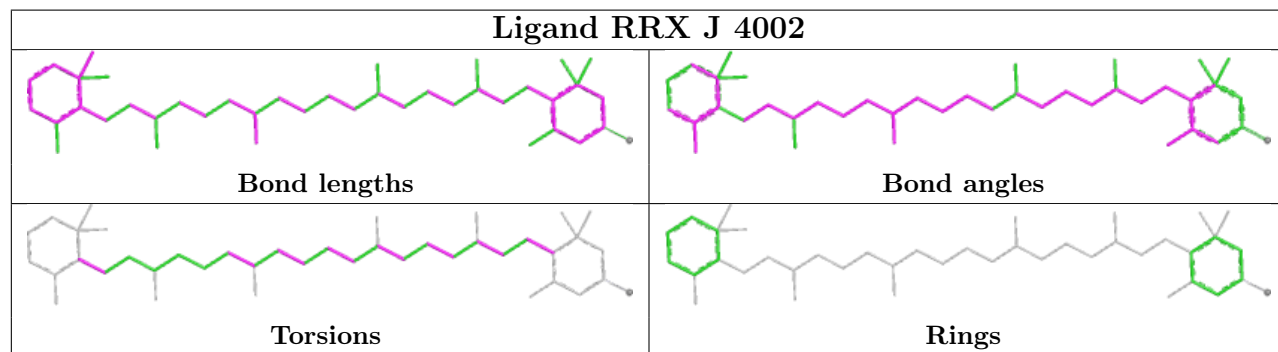
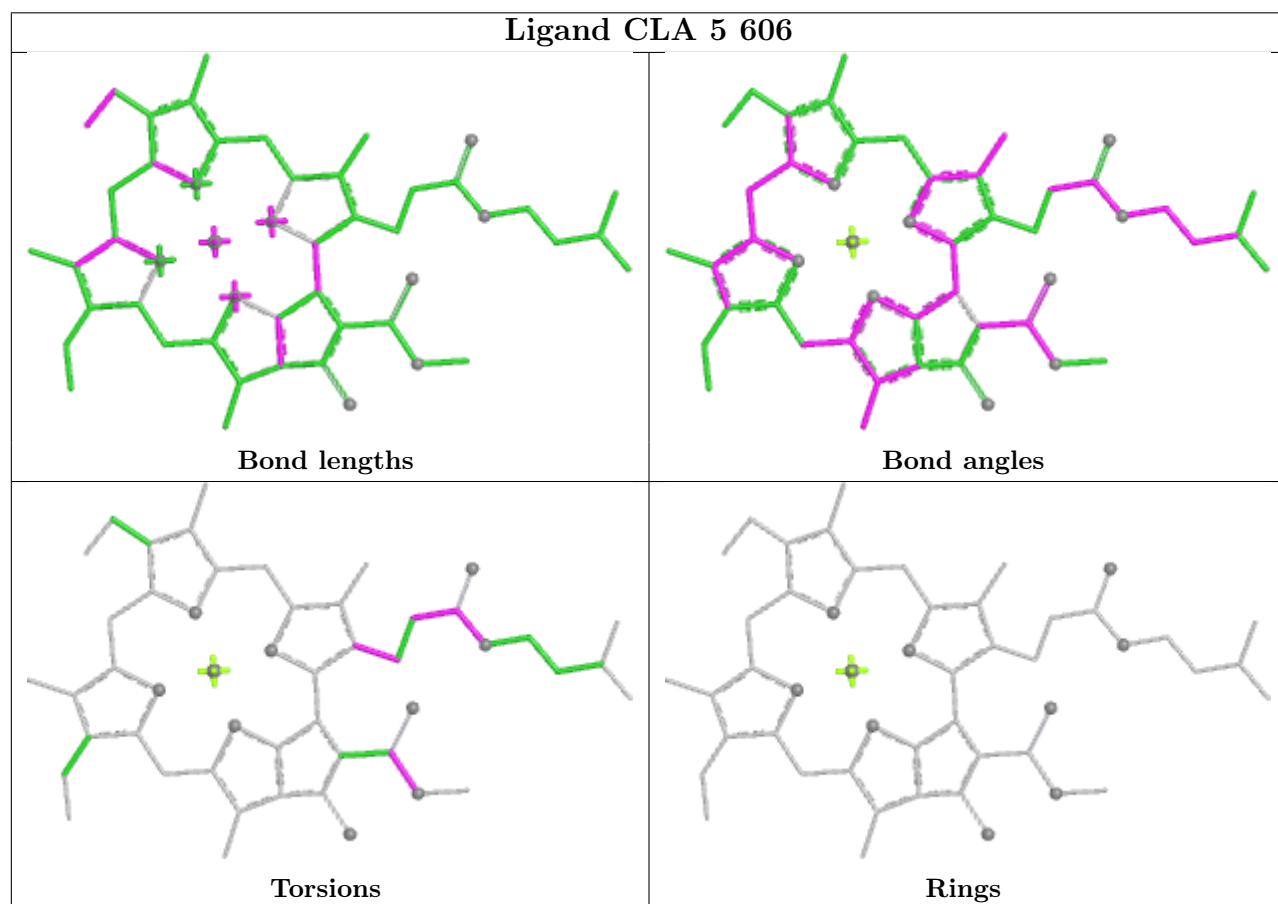
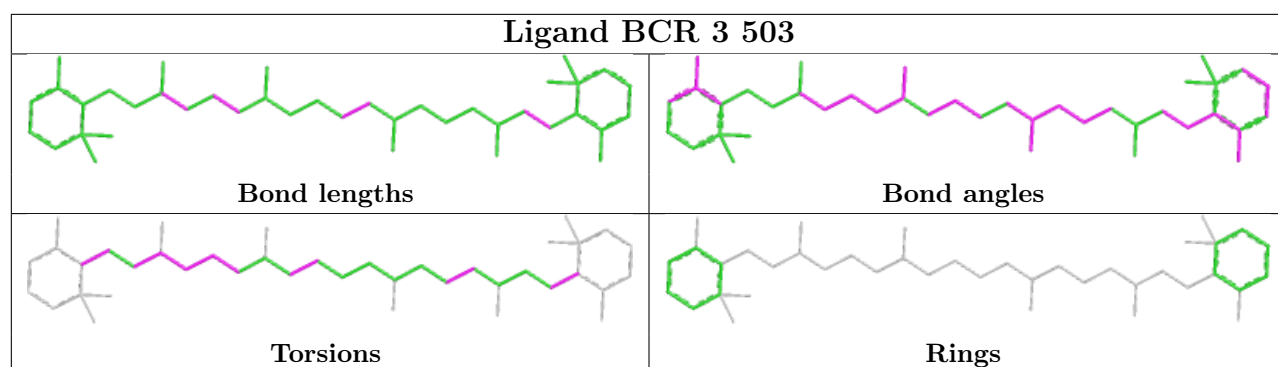


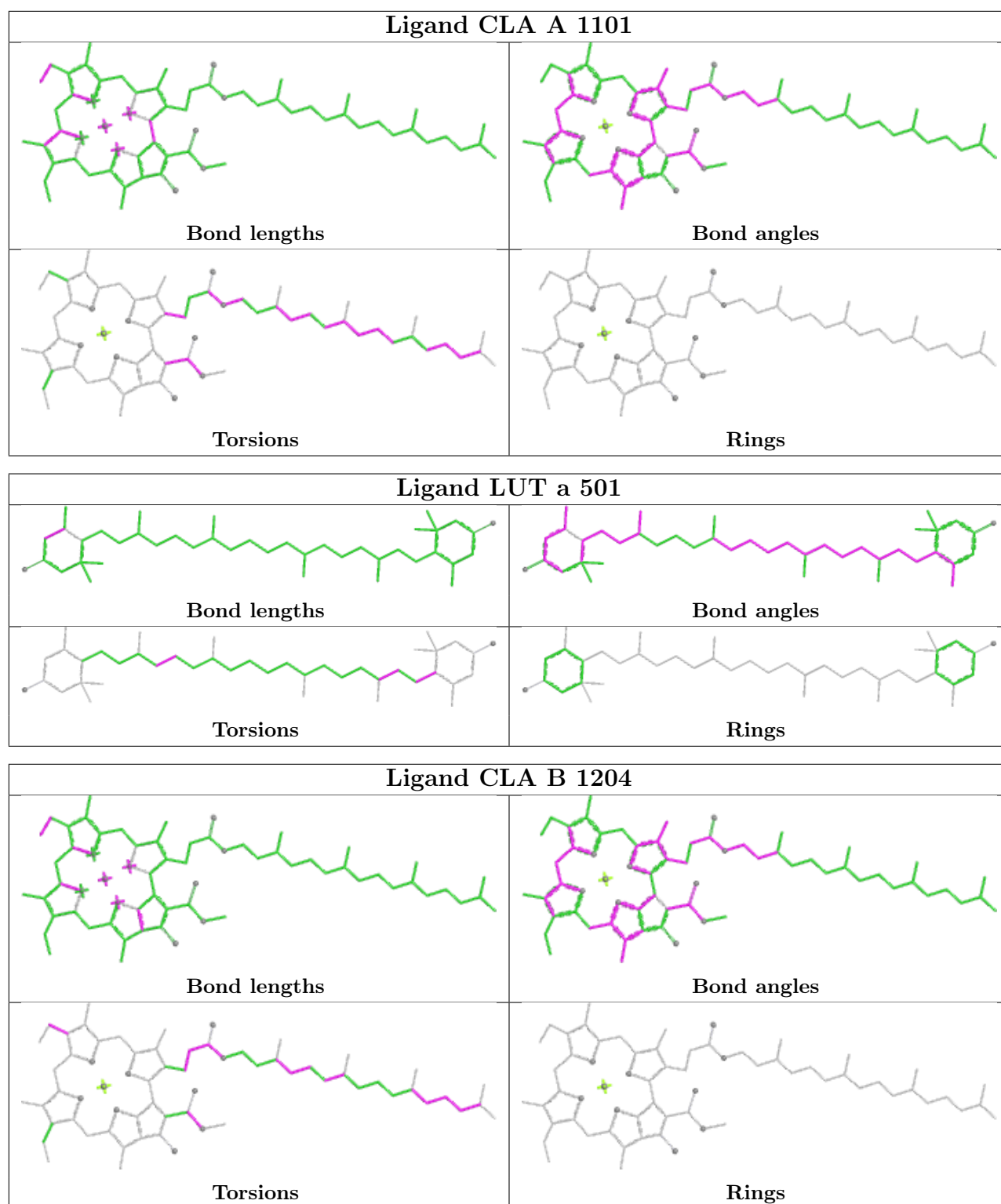
Ligand CLA 3 602



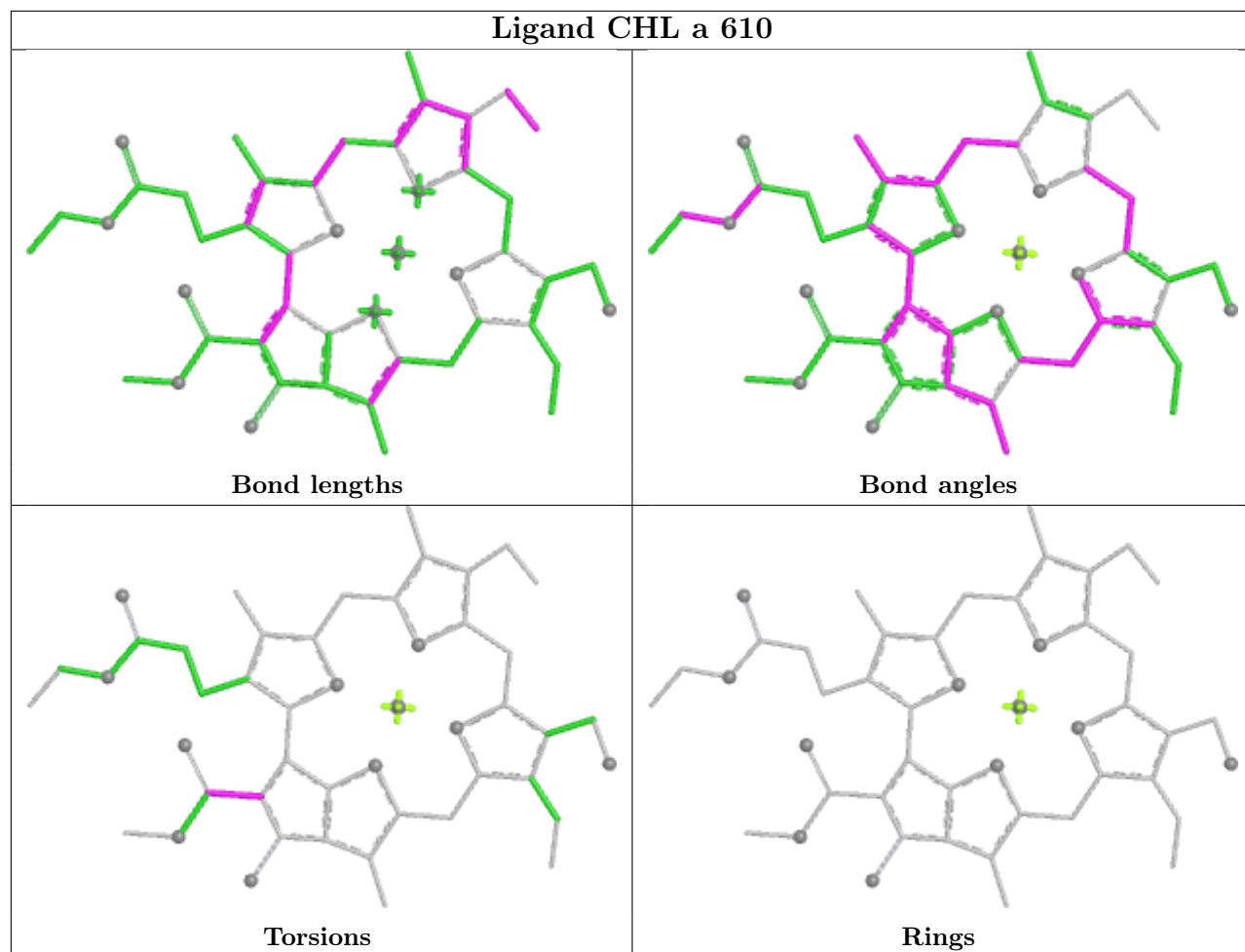
Ligand LMT 1 804



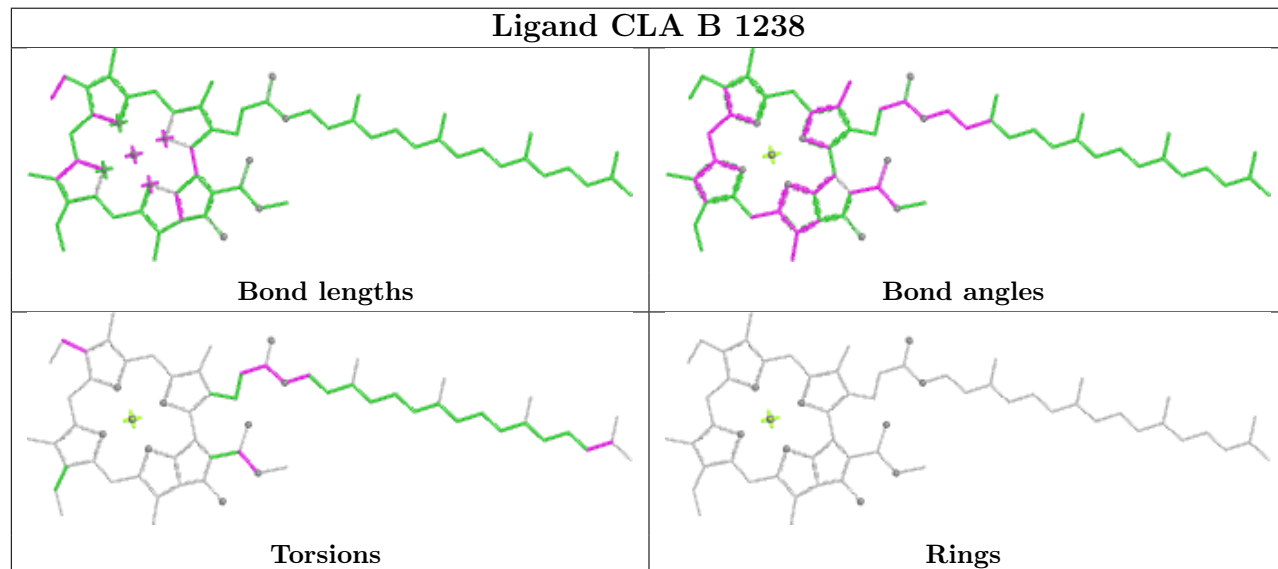


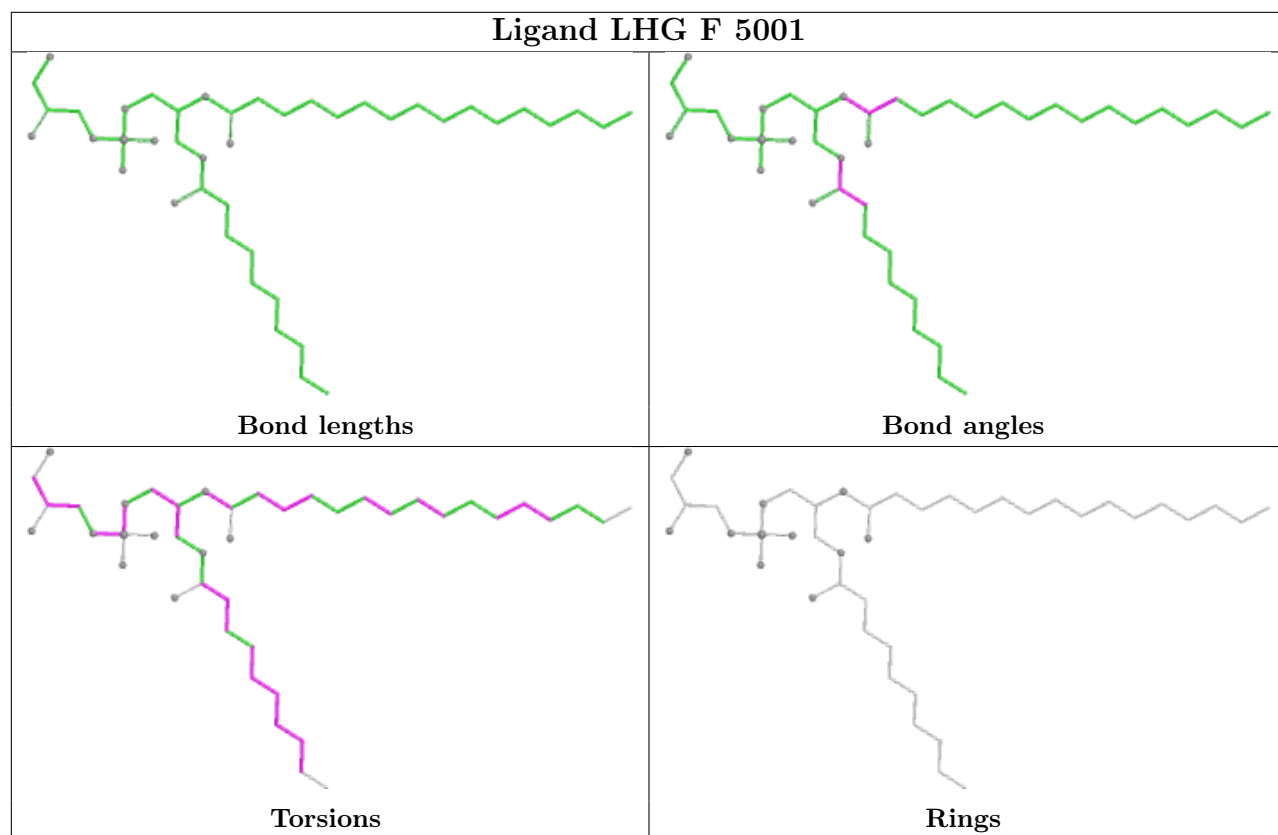
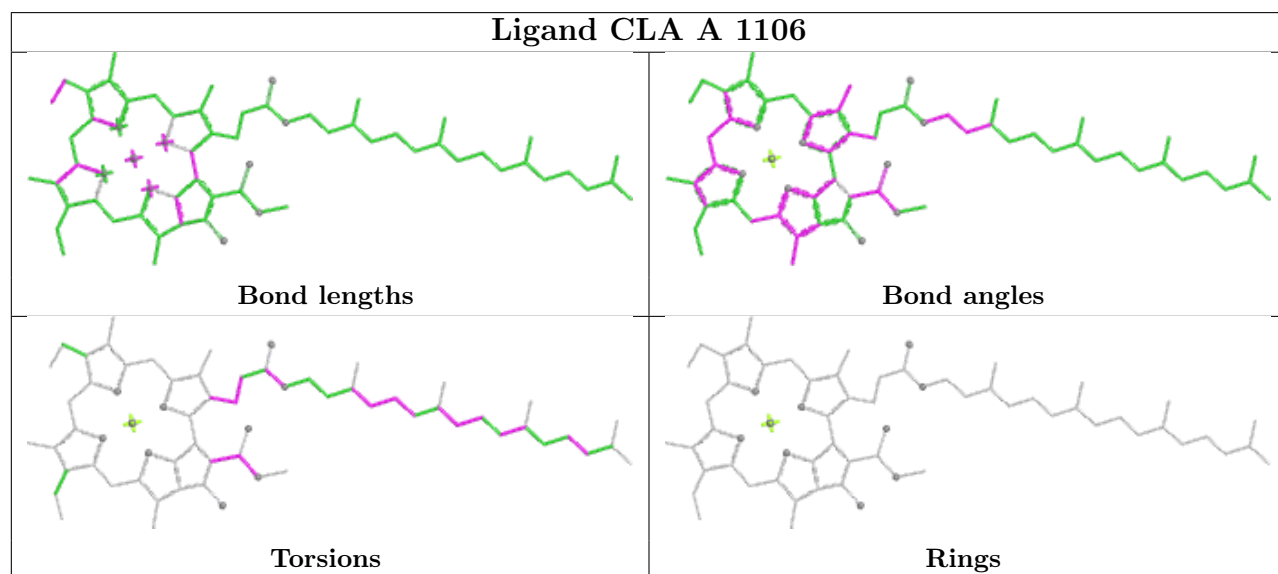
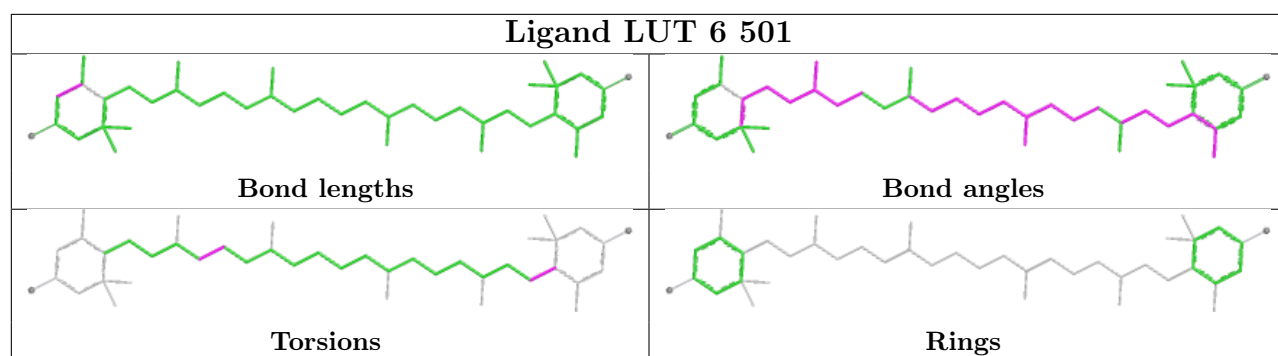


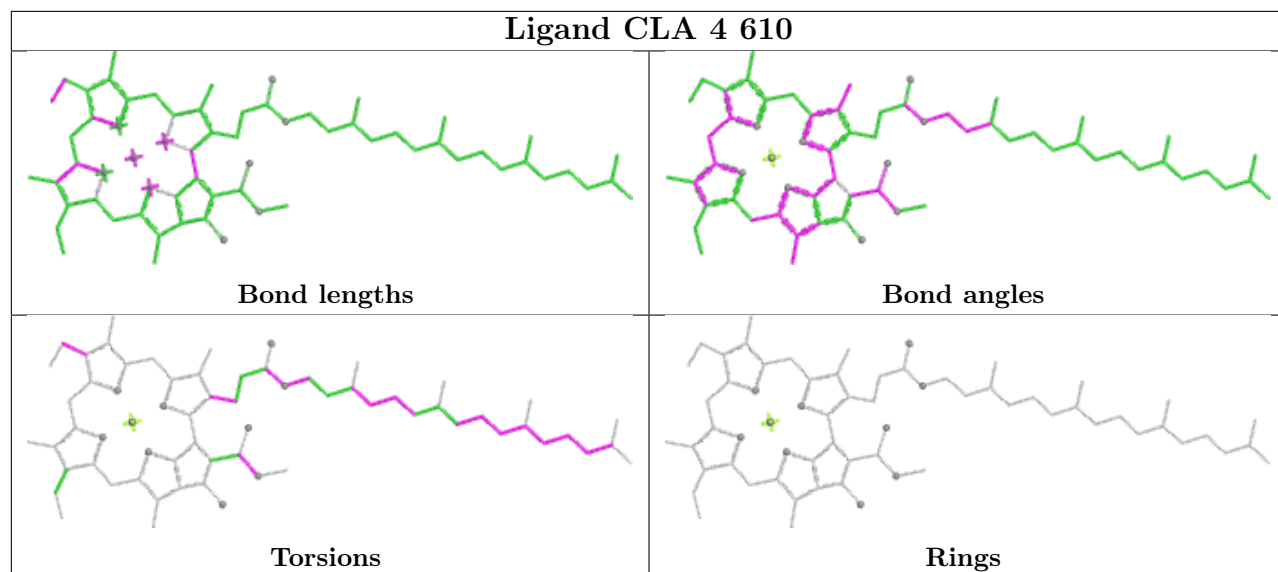
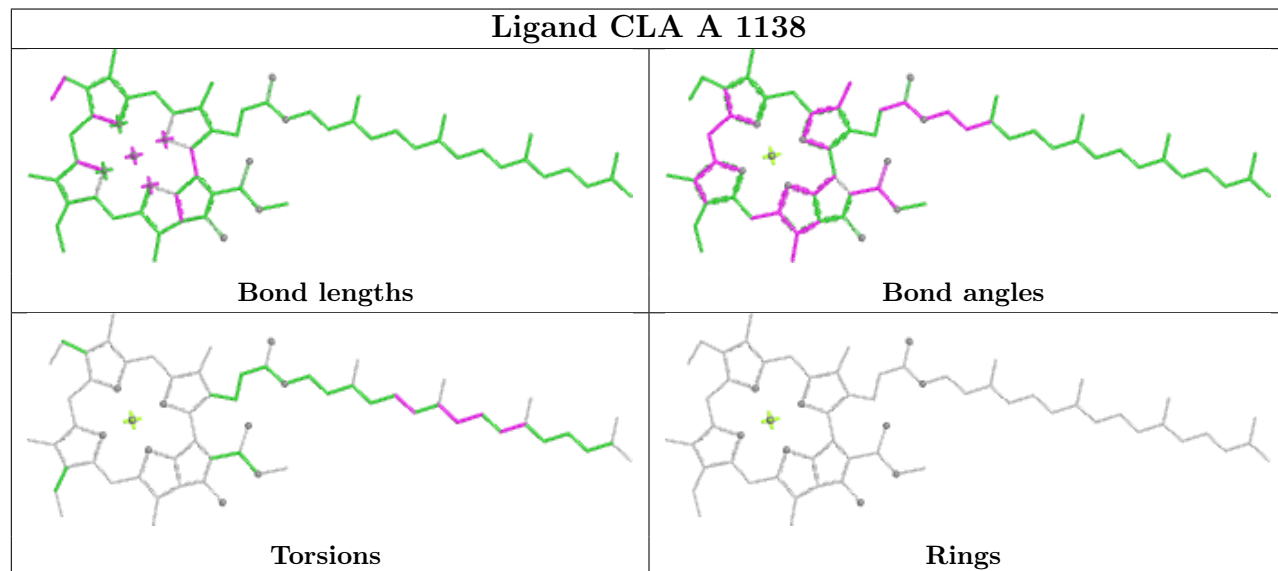
Ligand CHL a 610

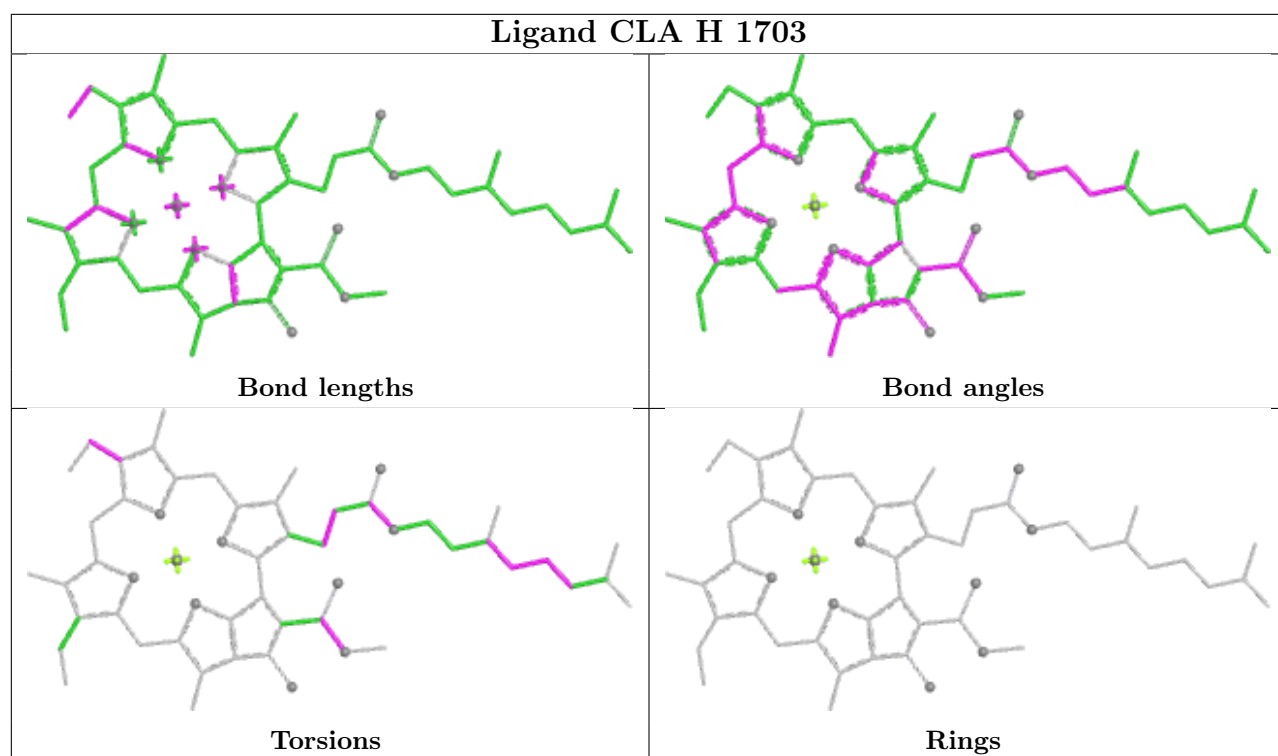


Ligand CLA B 1238

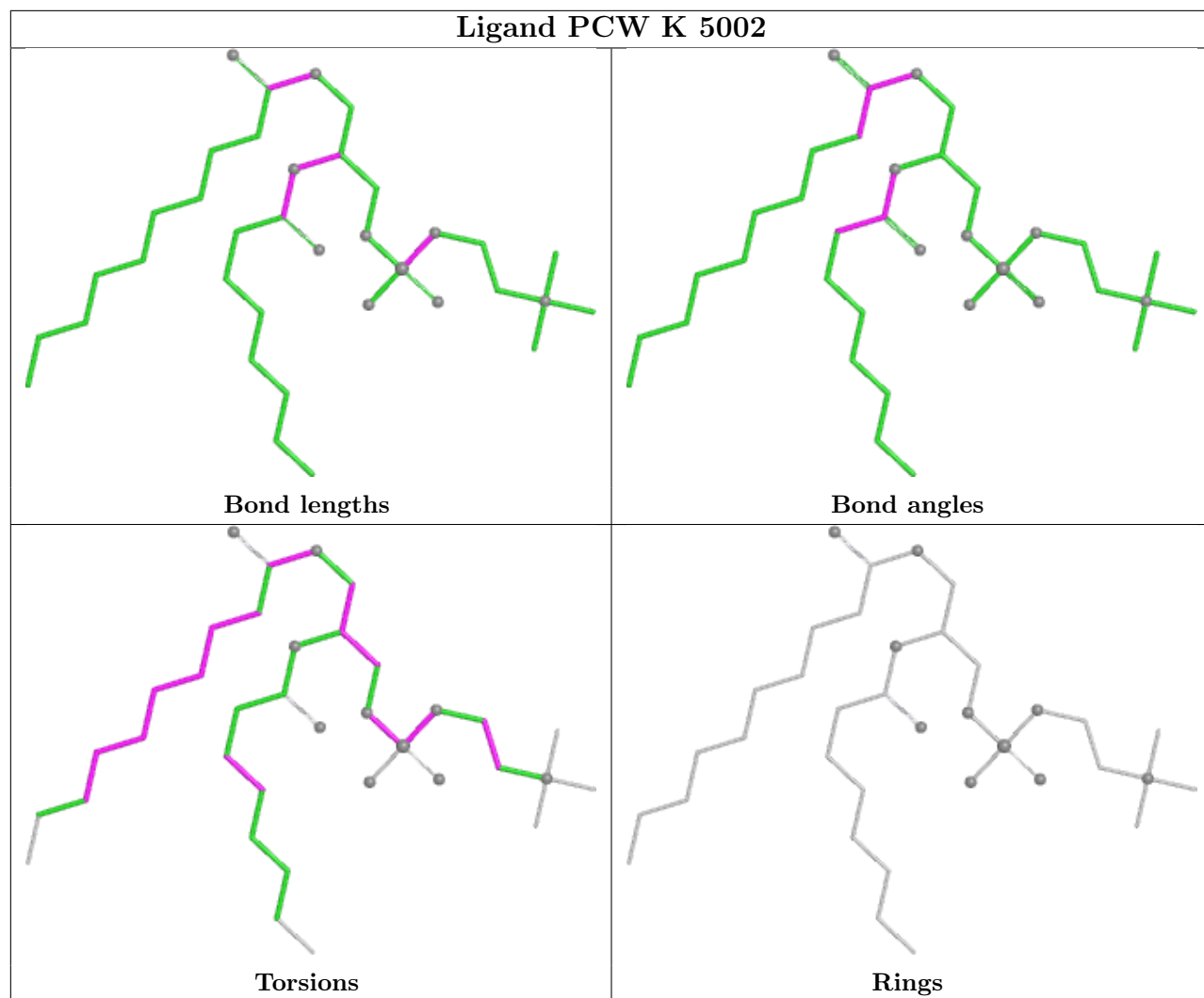




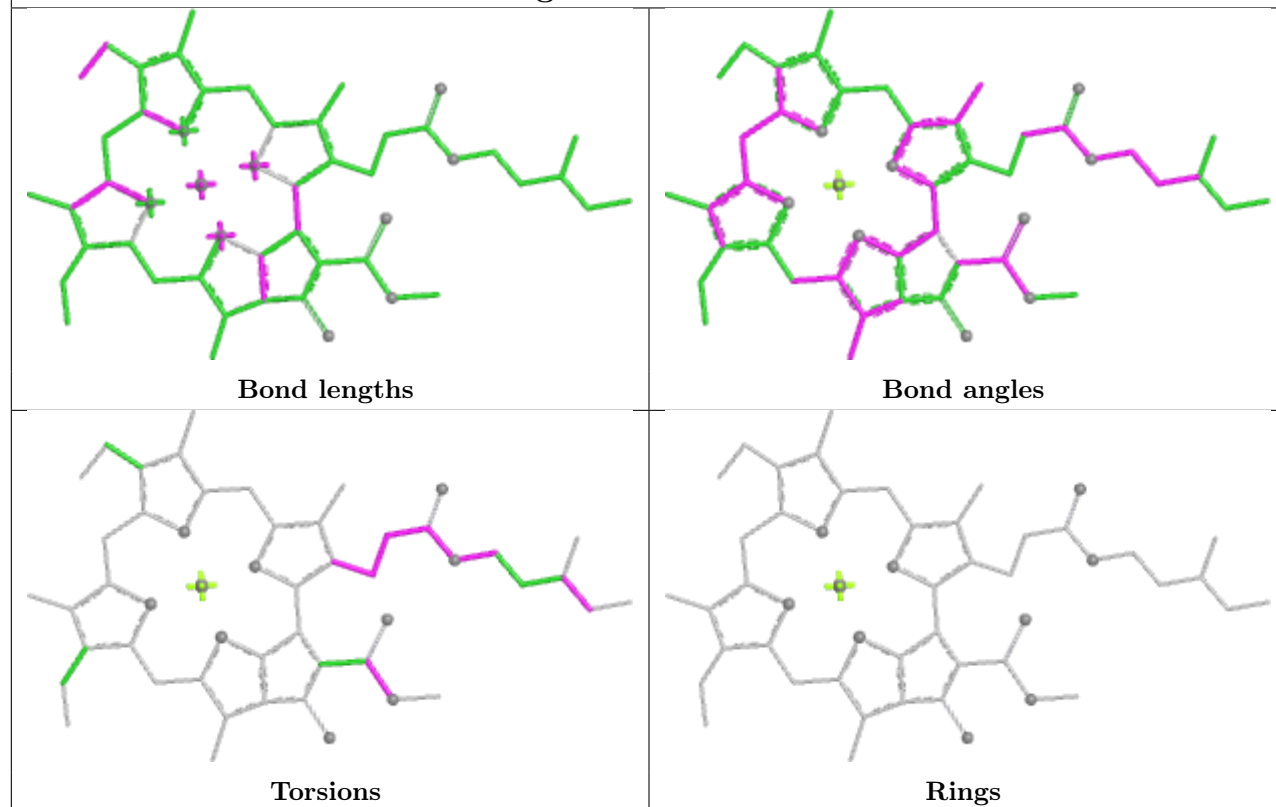
Ligand CLA 4 610**Ligand CLA A 1138**



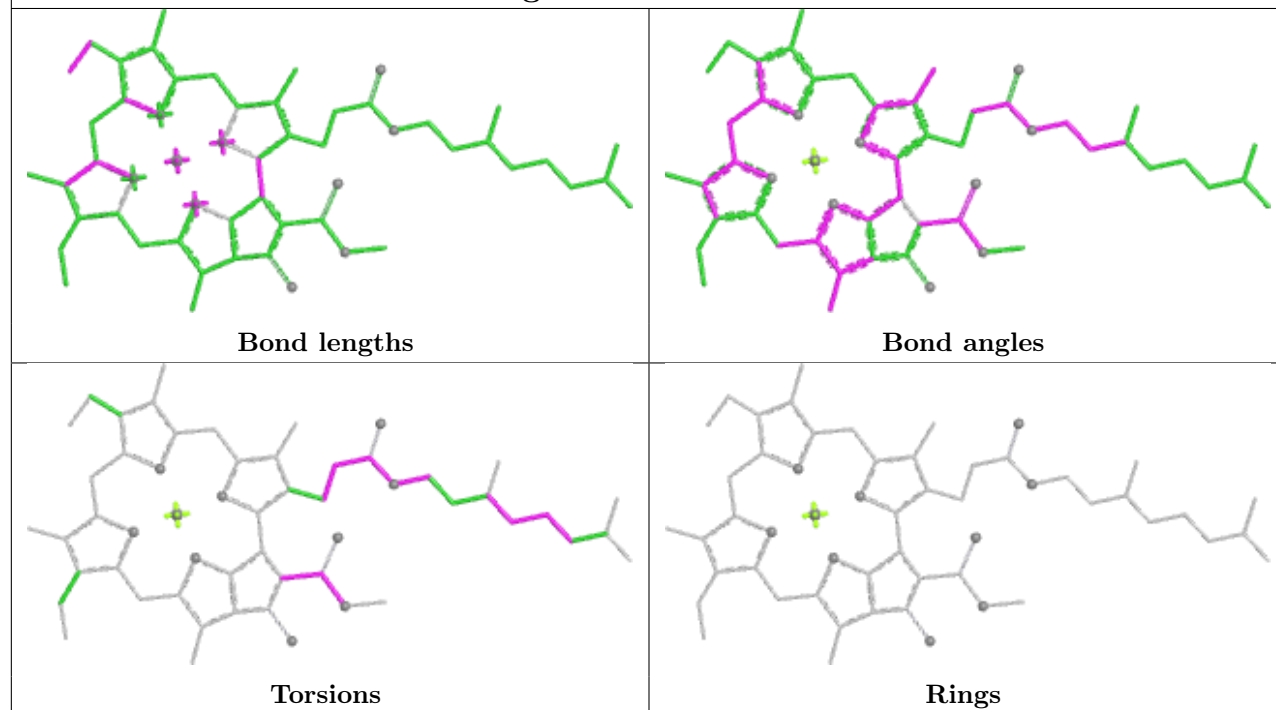
Ligand PCW K 5002

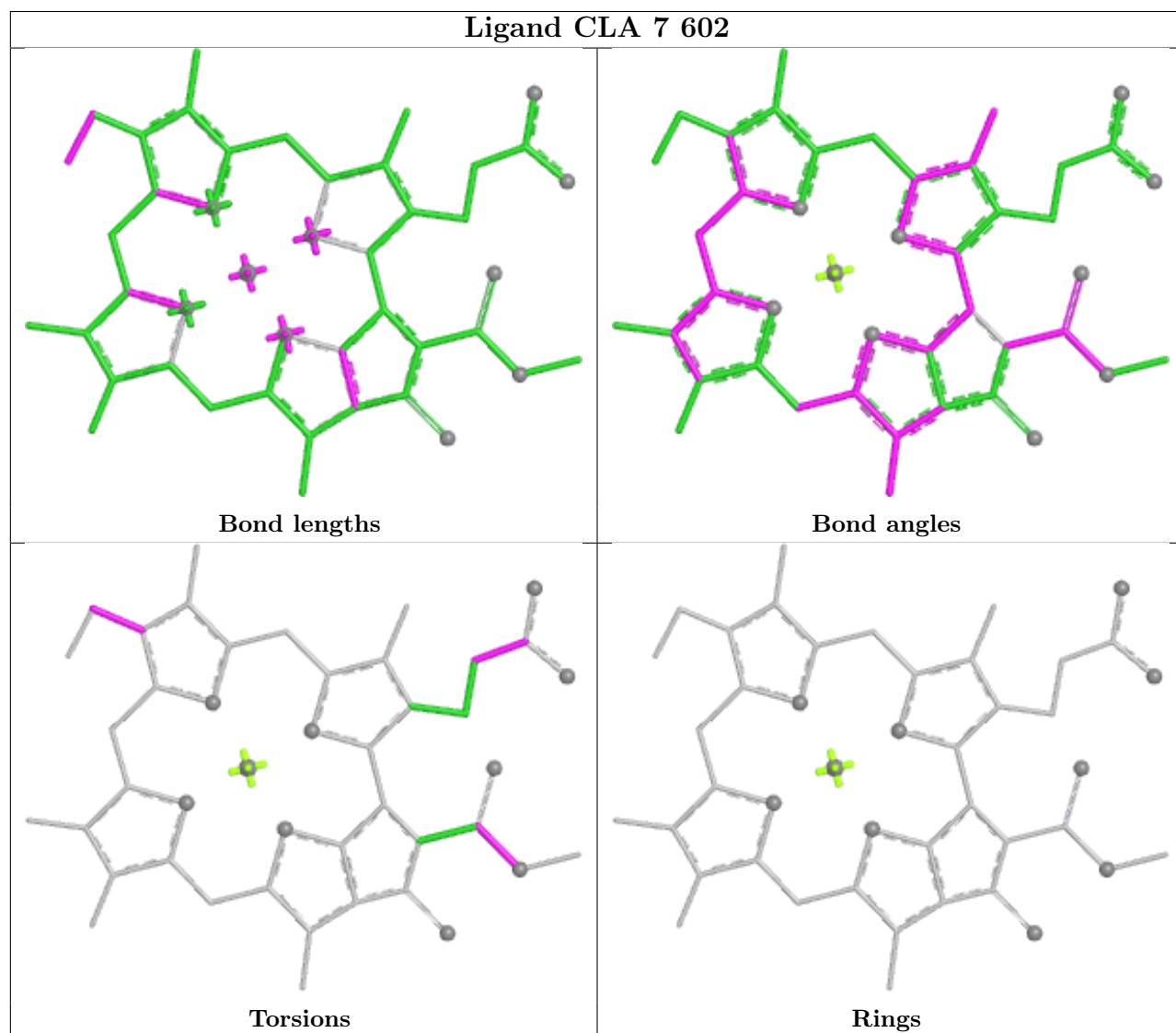
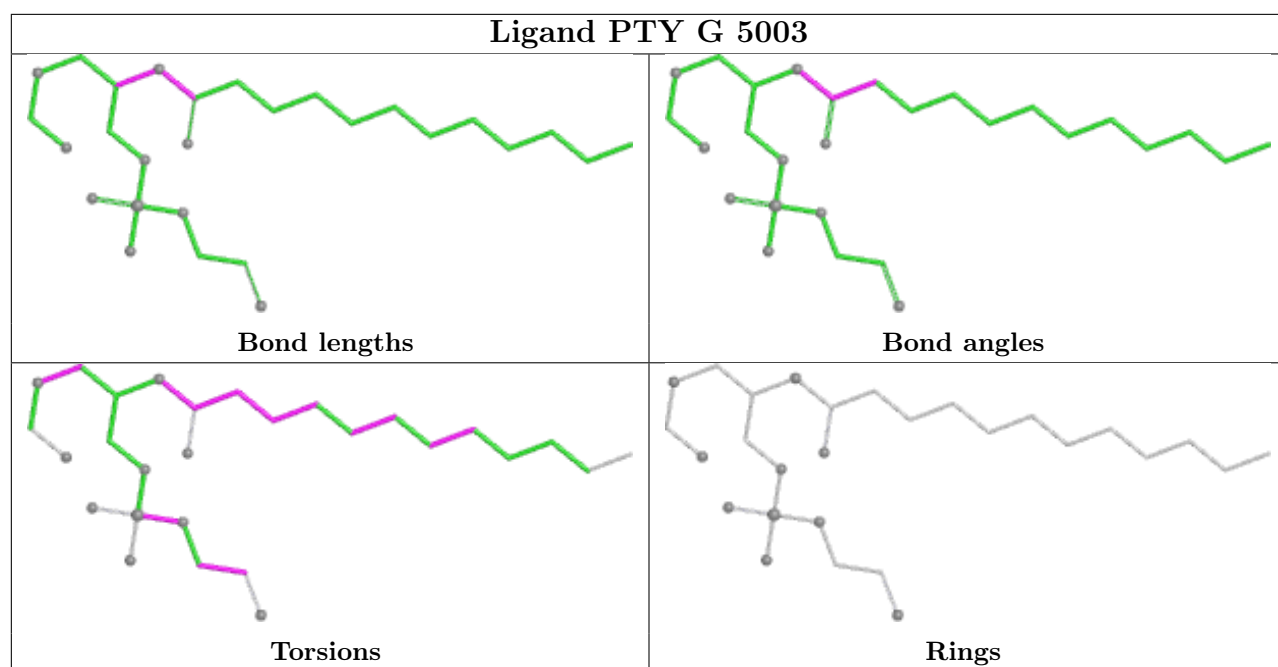


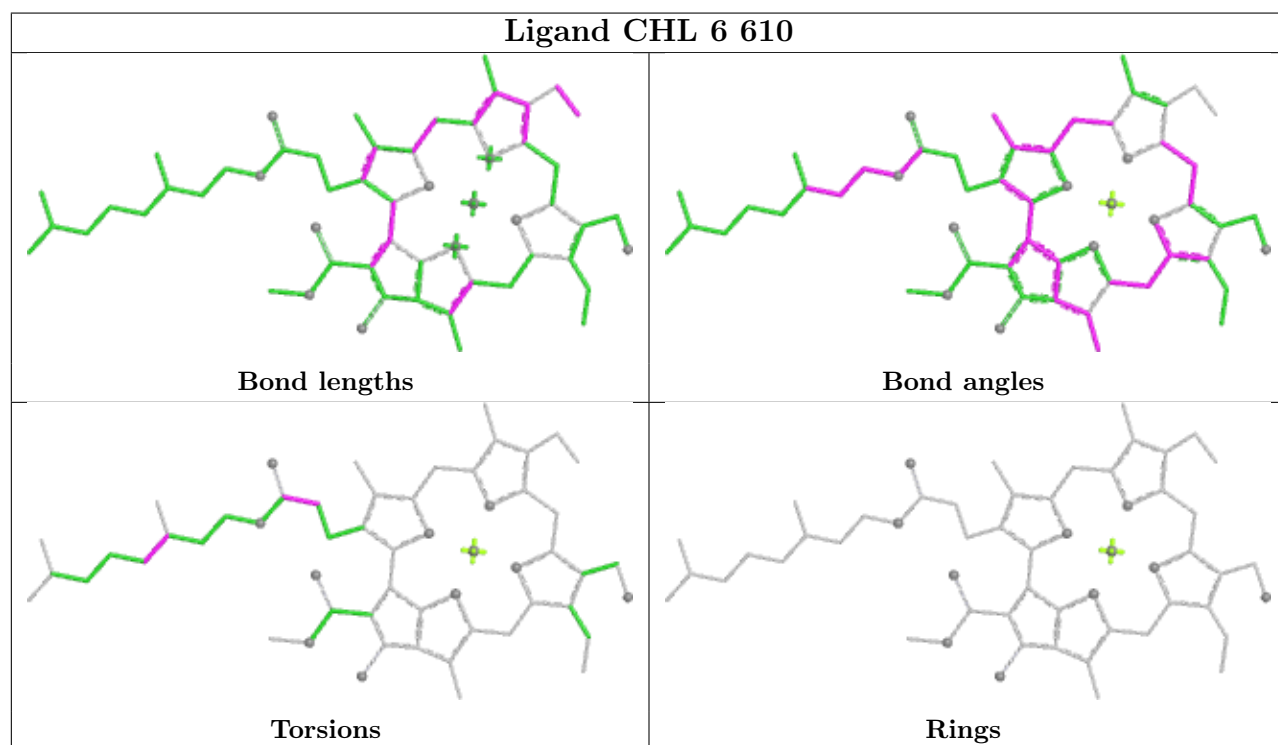
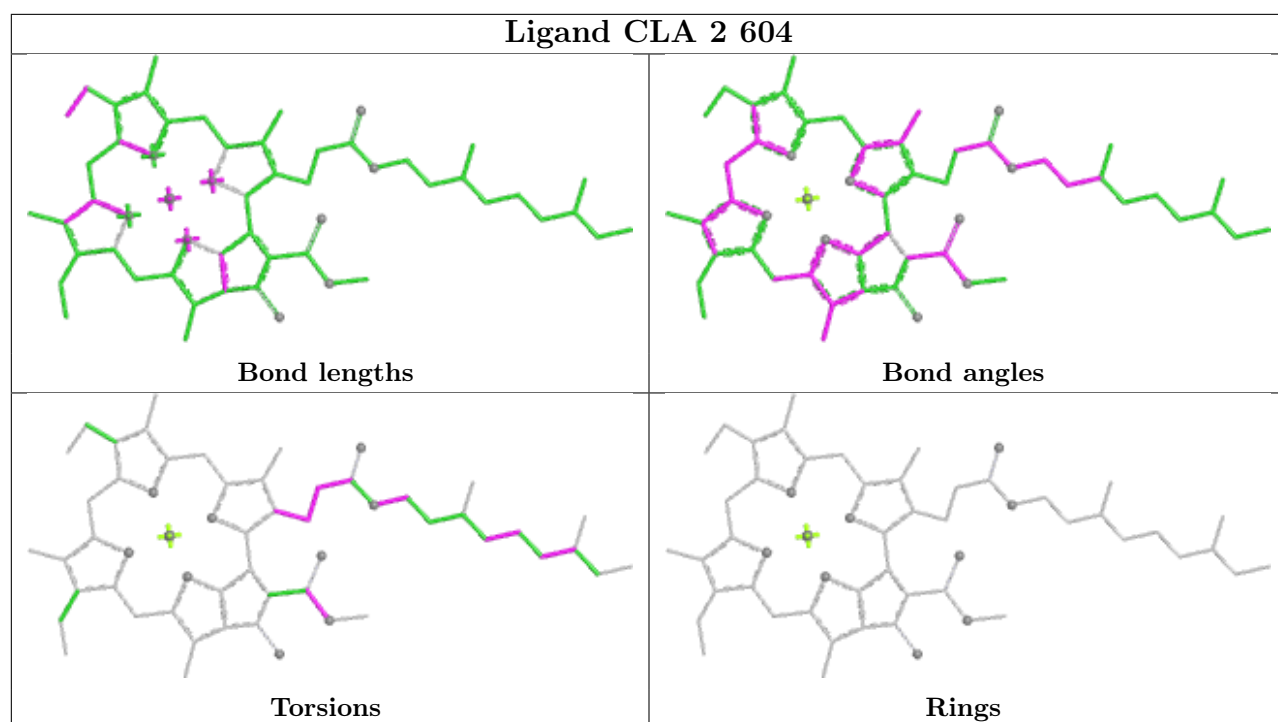
Ligand CLA 5 609

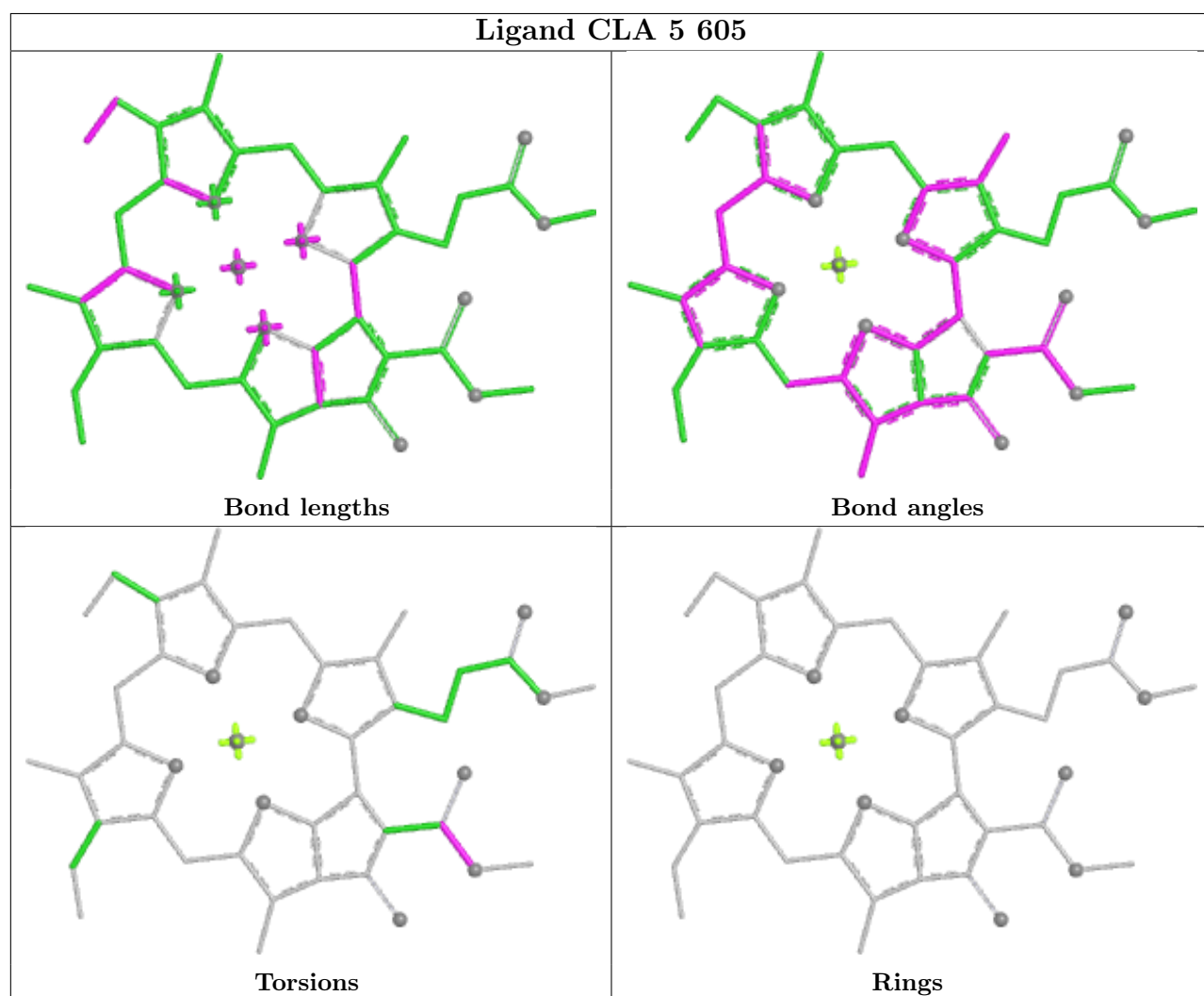
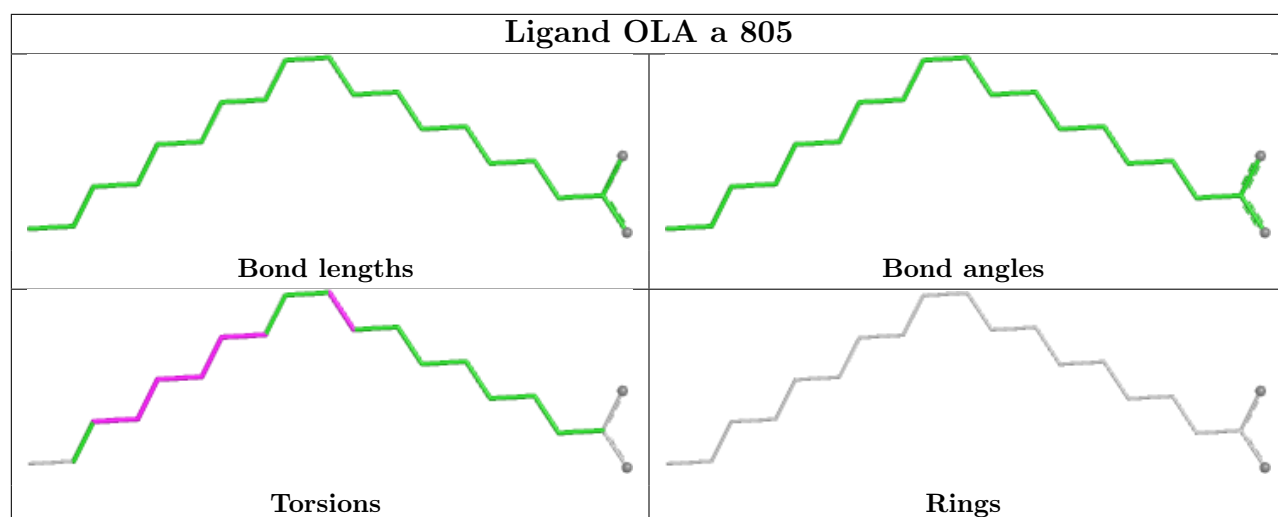


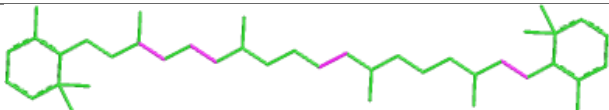
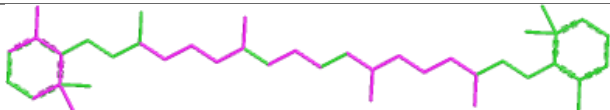
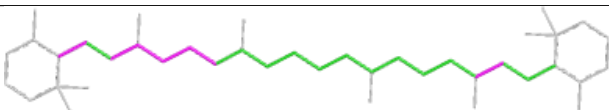
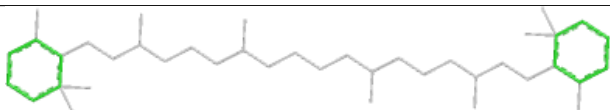
Ligand CLA O 1802

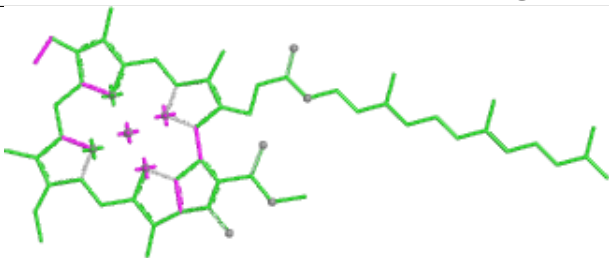
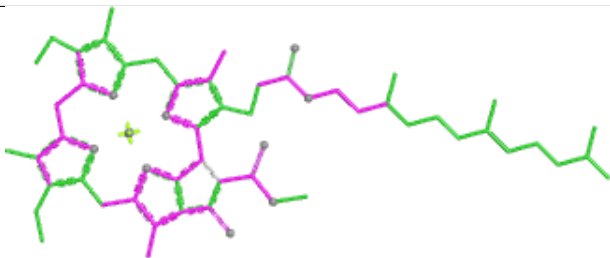
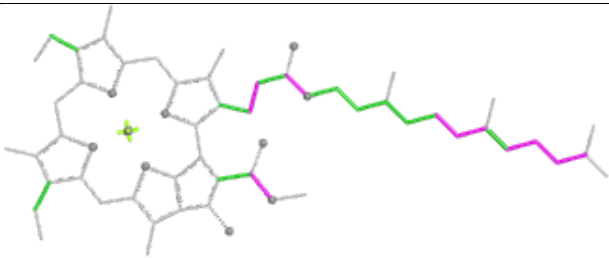
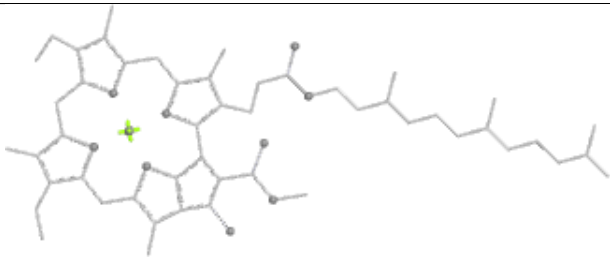


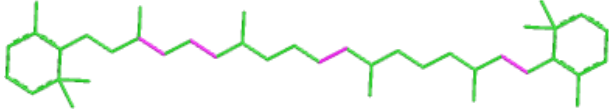
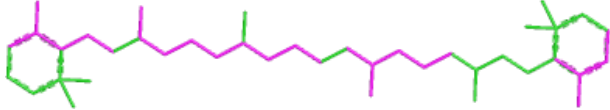
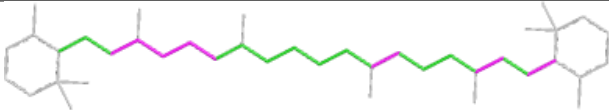
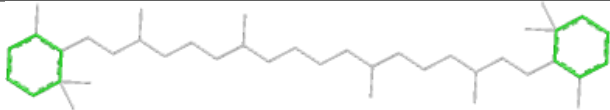


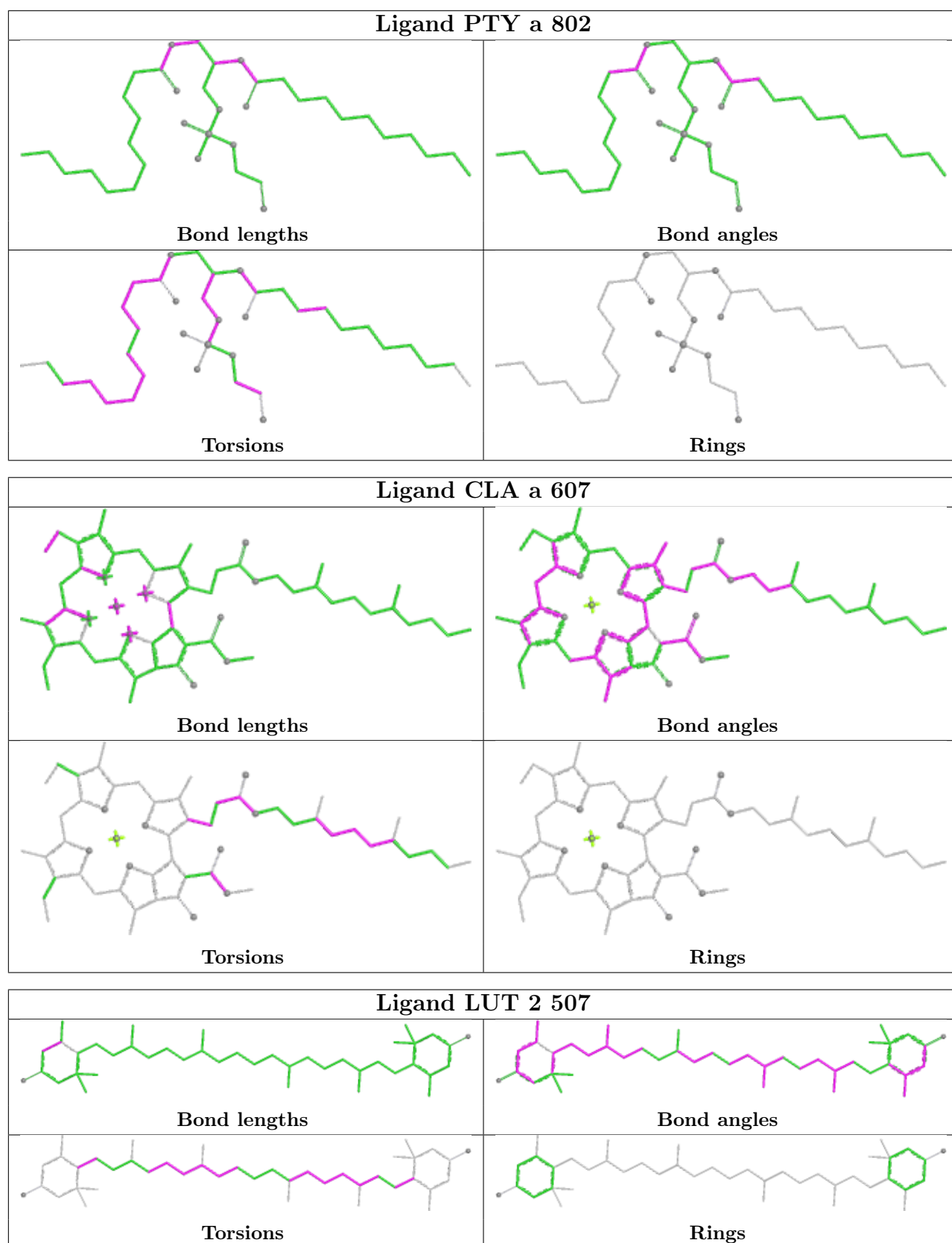


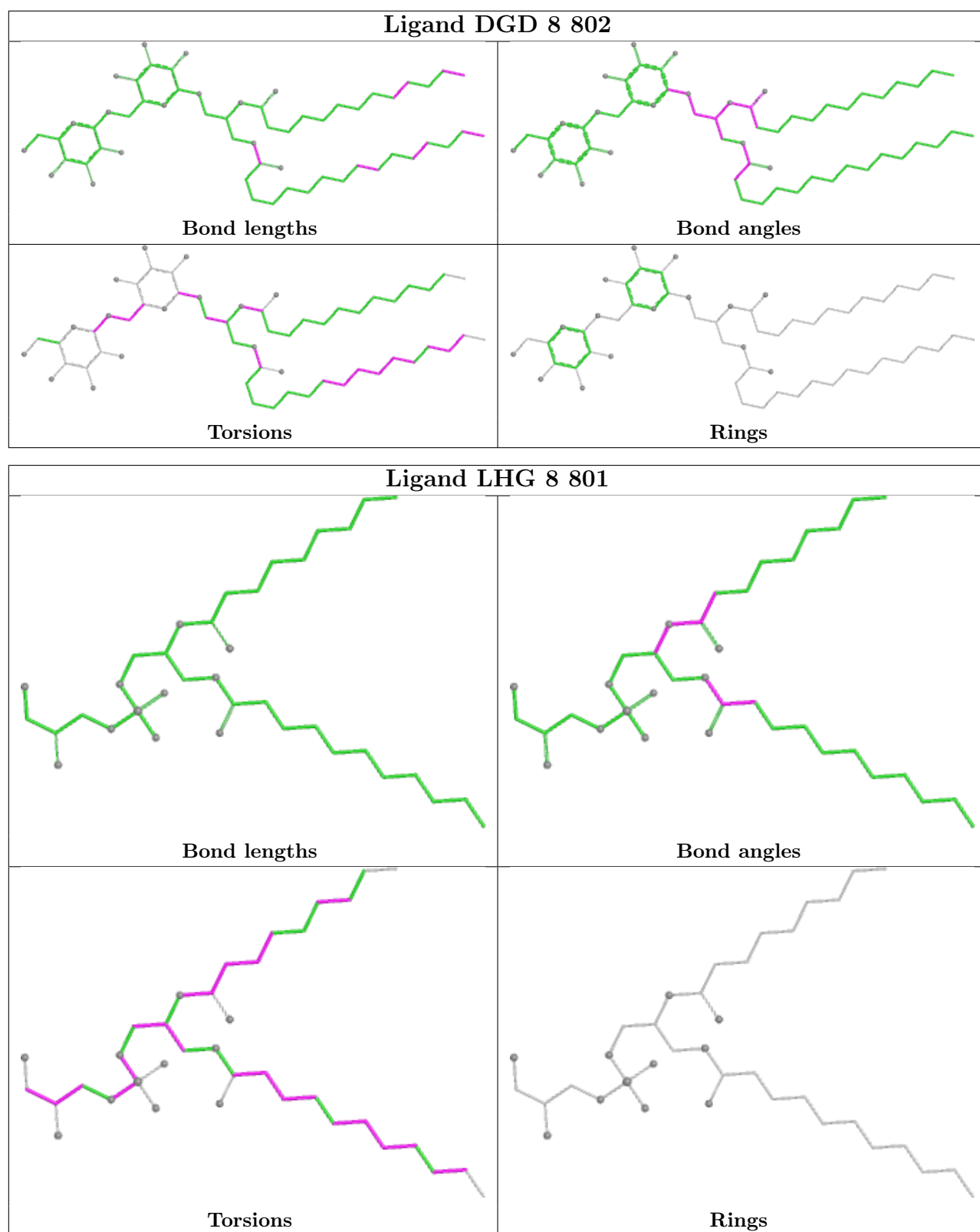


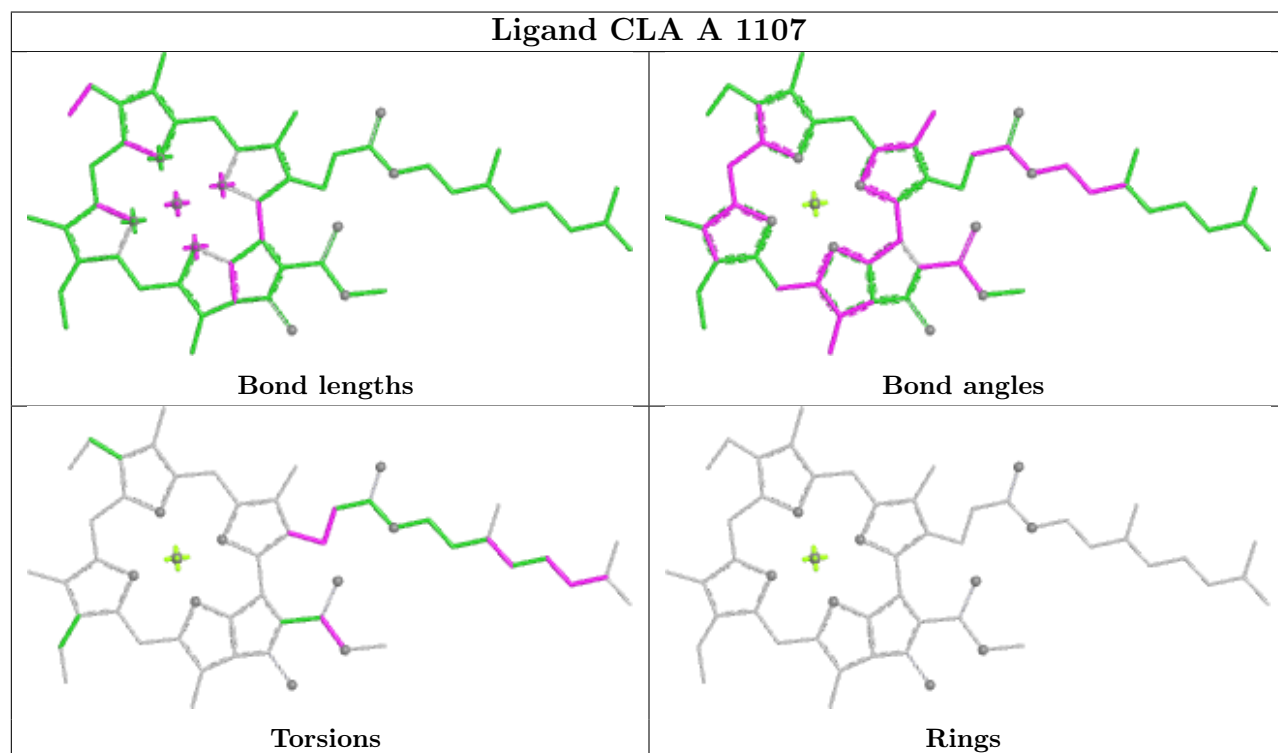
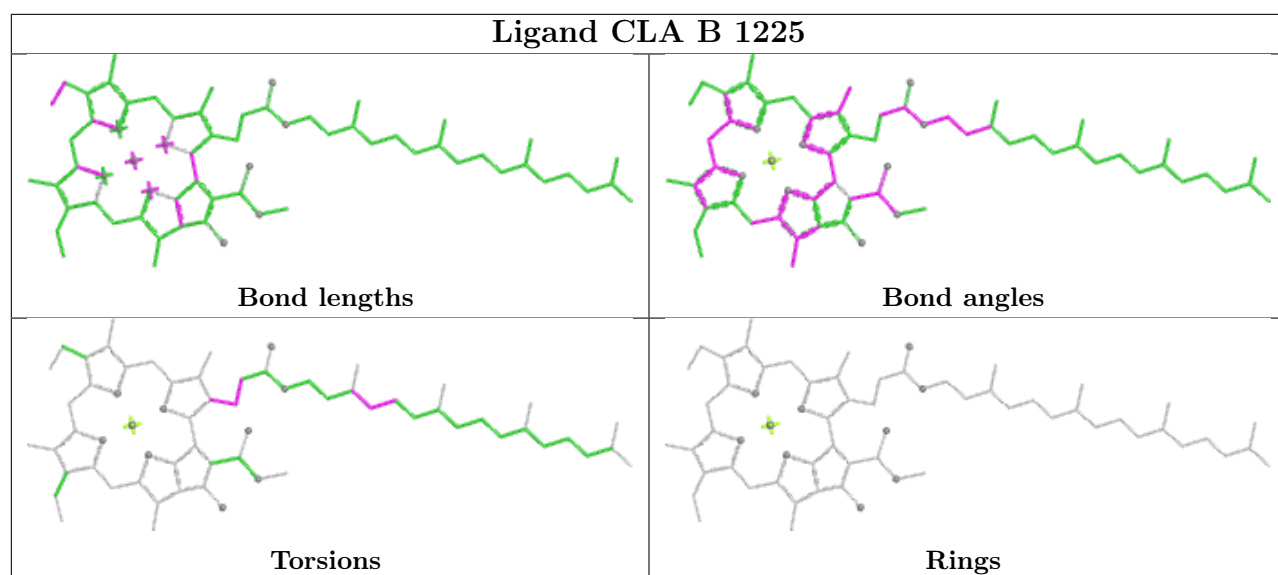
Ligand BCR K 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 9 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

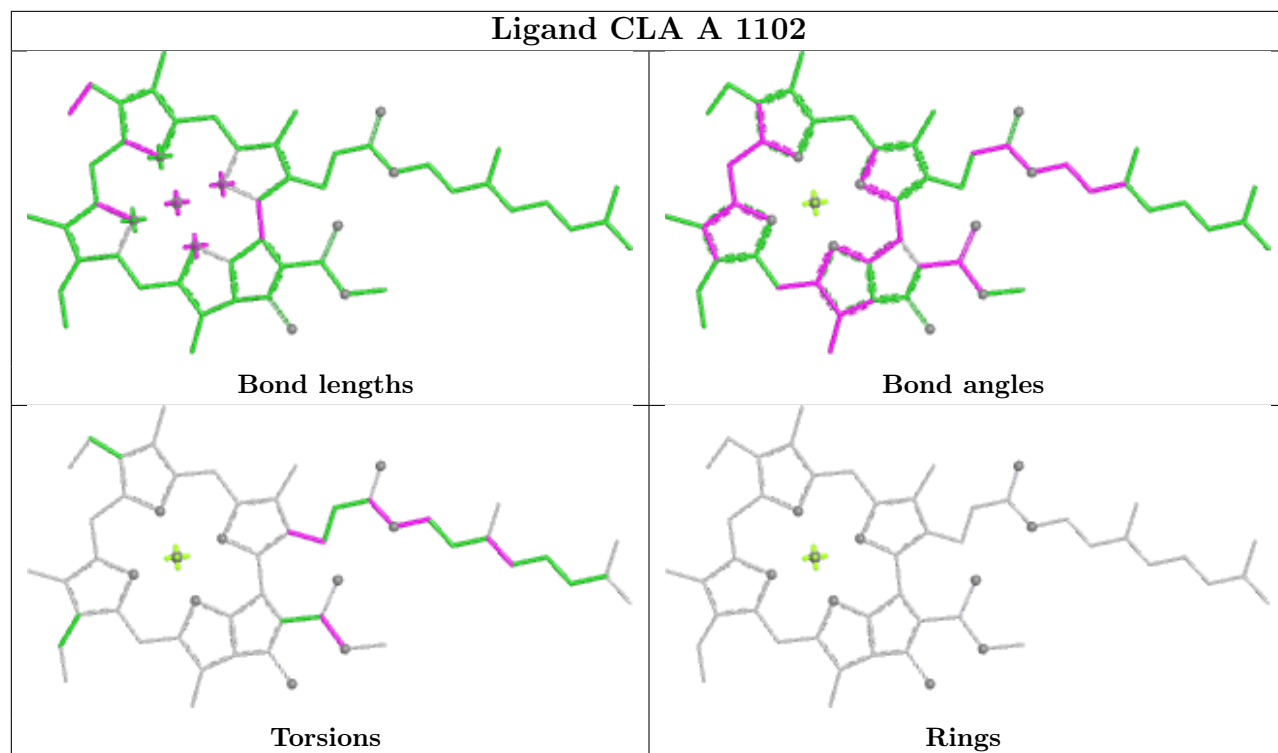
Ligand BCR 6 504	
	
Bond lengths	Bond angles
	
Torsions	Rings



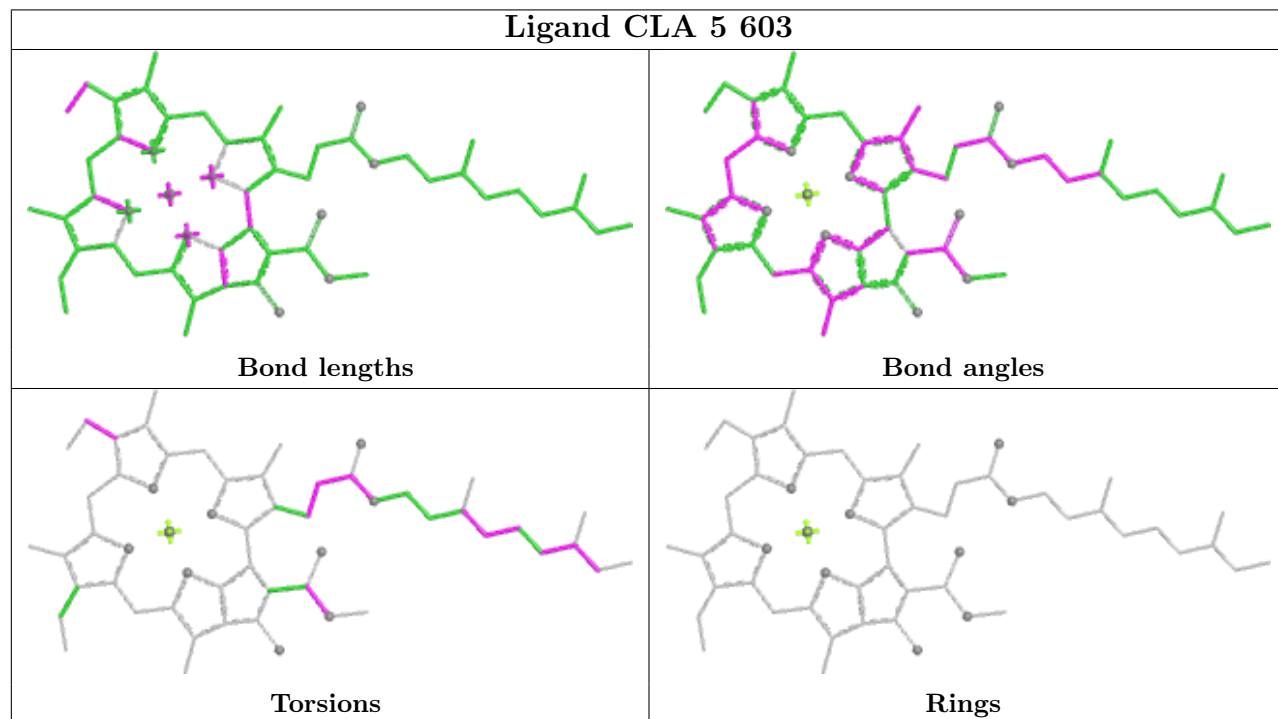


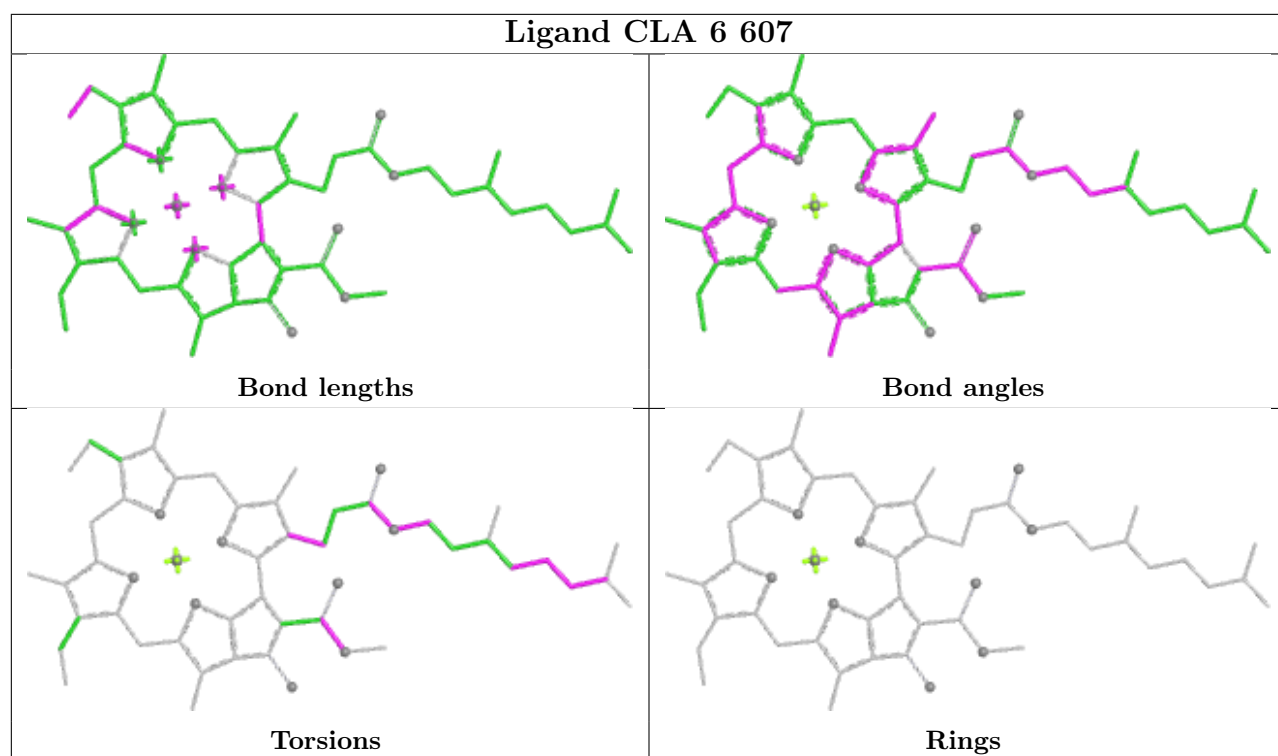


Ligand CLA A 1102

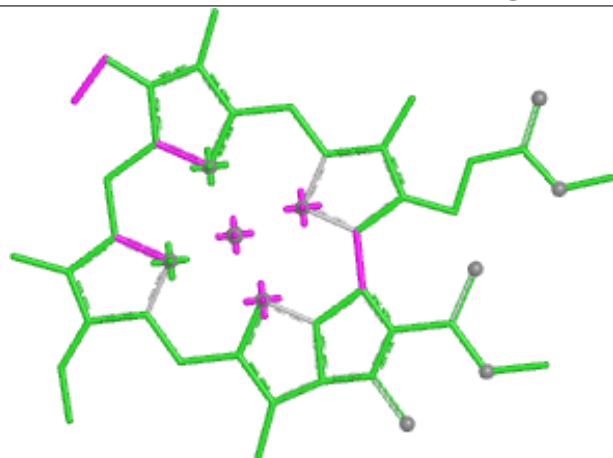


Ligand CLA 5 603

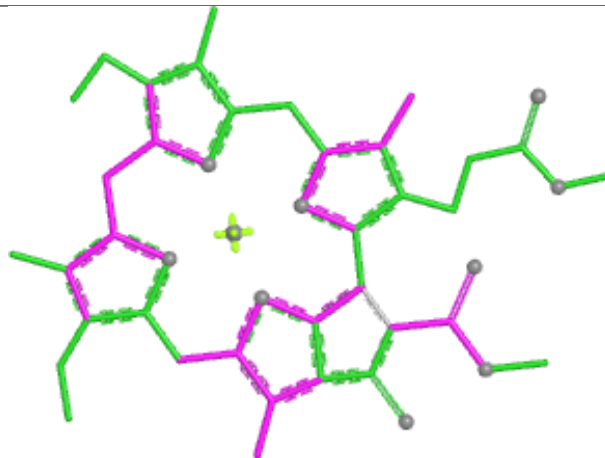




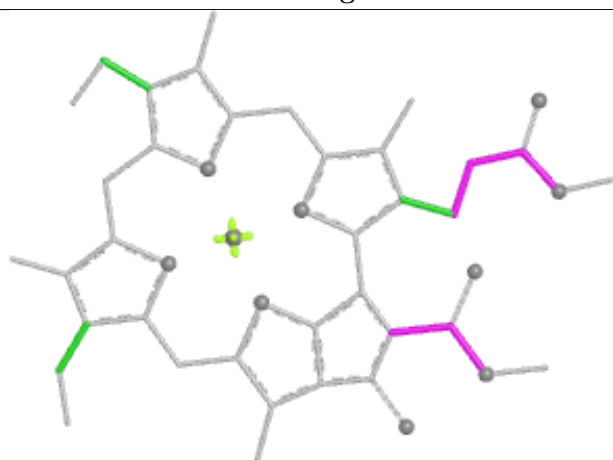
Ligand CLA H 1702



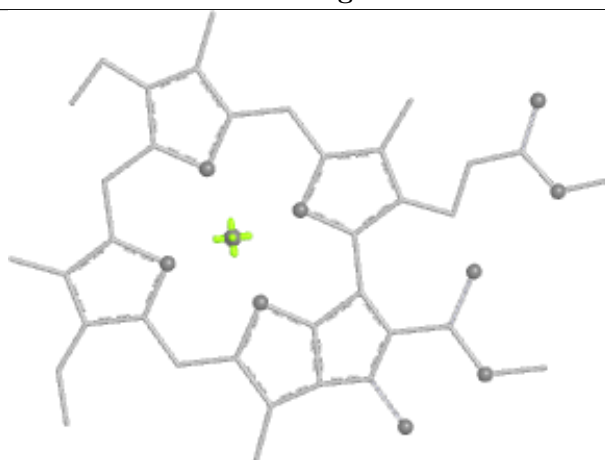
Bond lengths



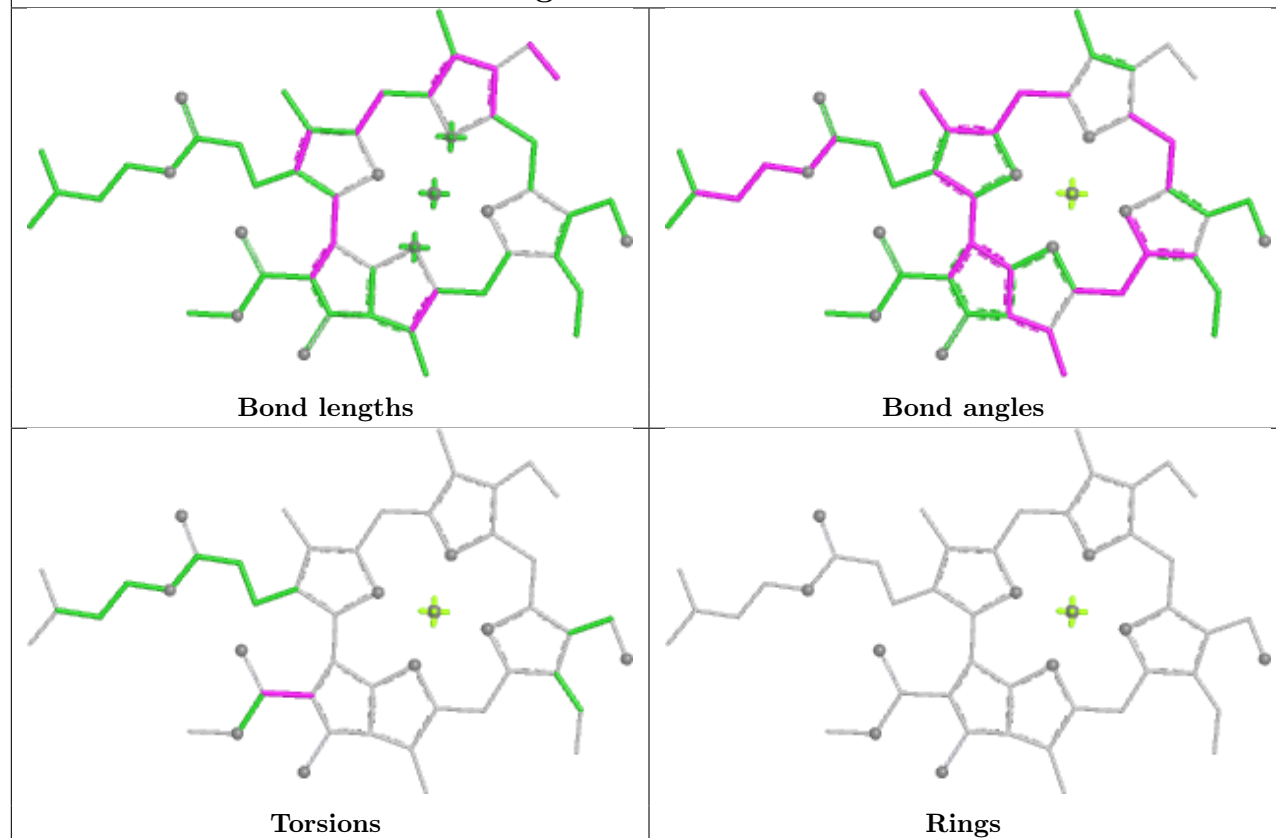
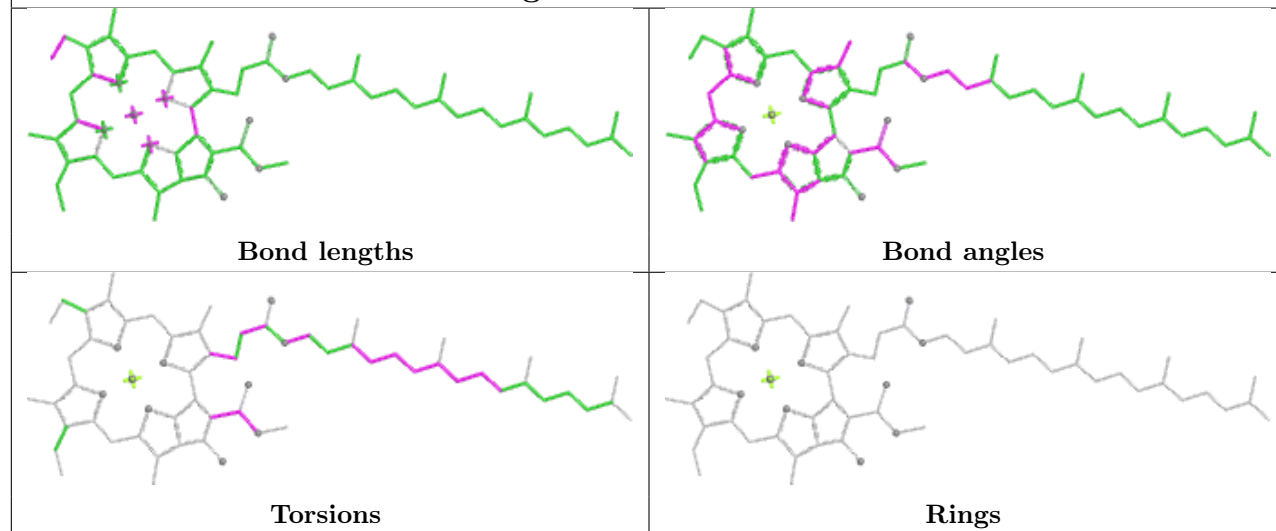
Bond angles

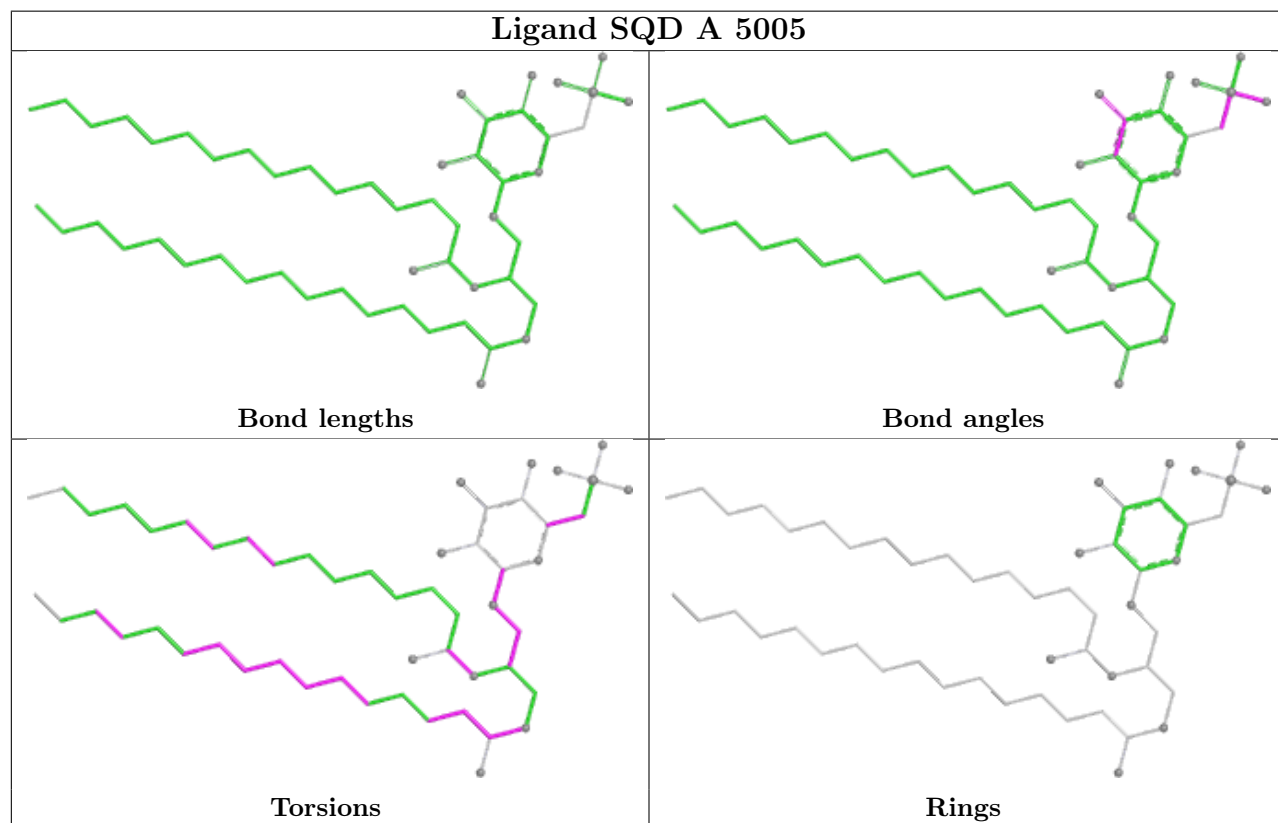
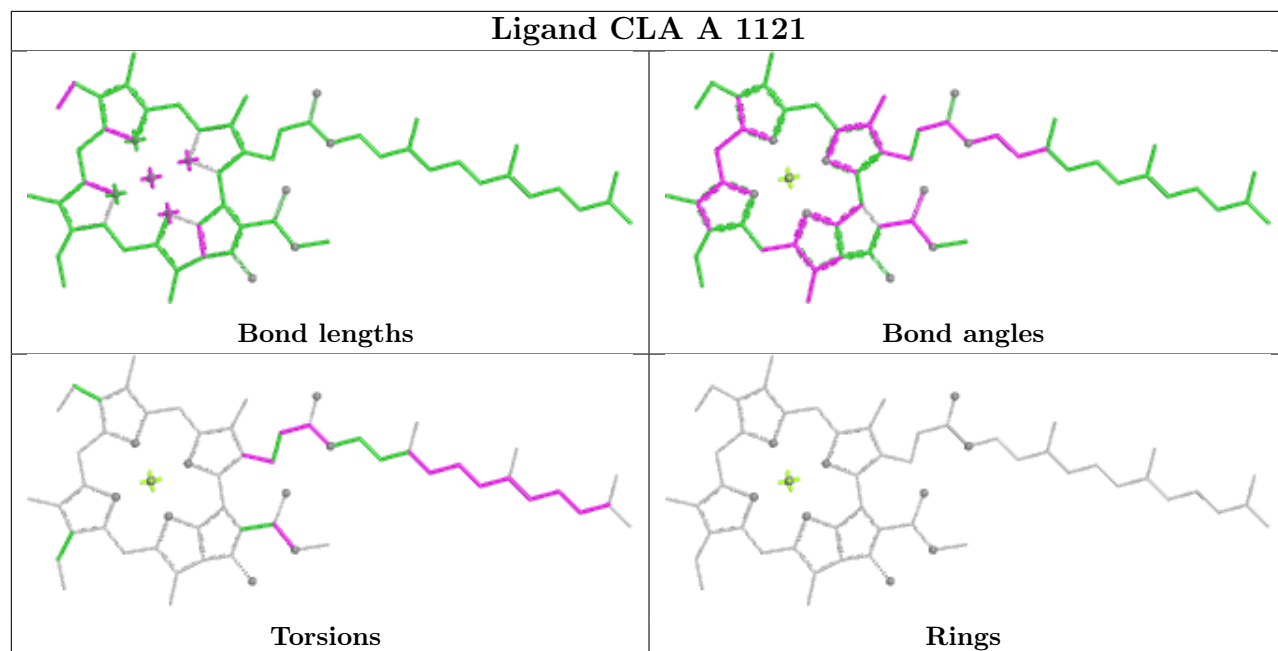


Torsions

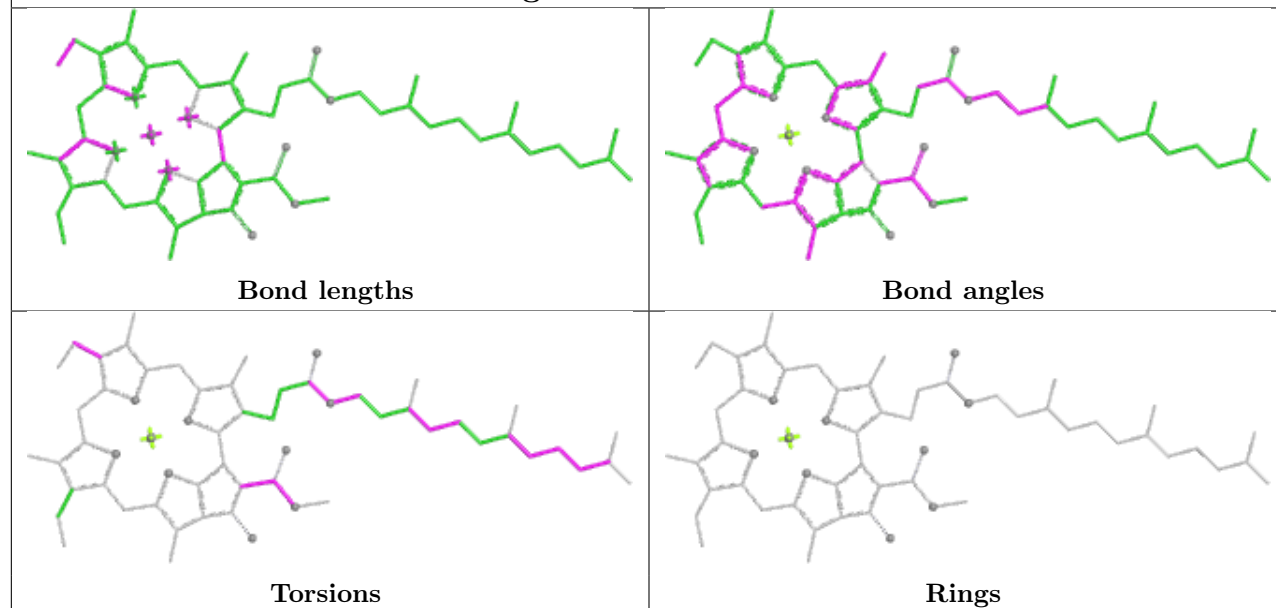


Rings

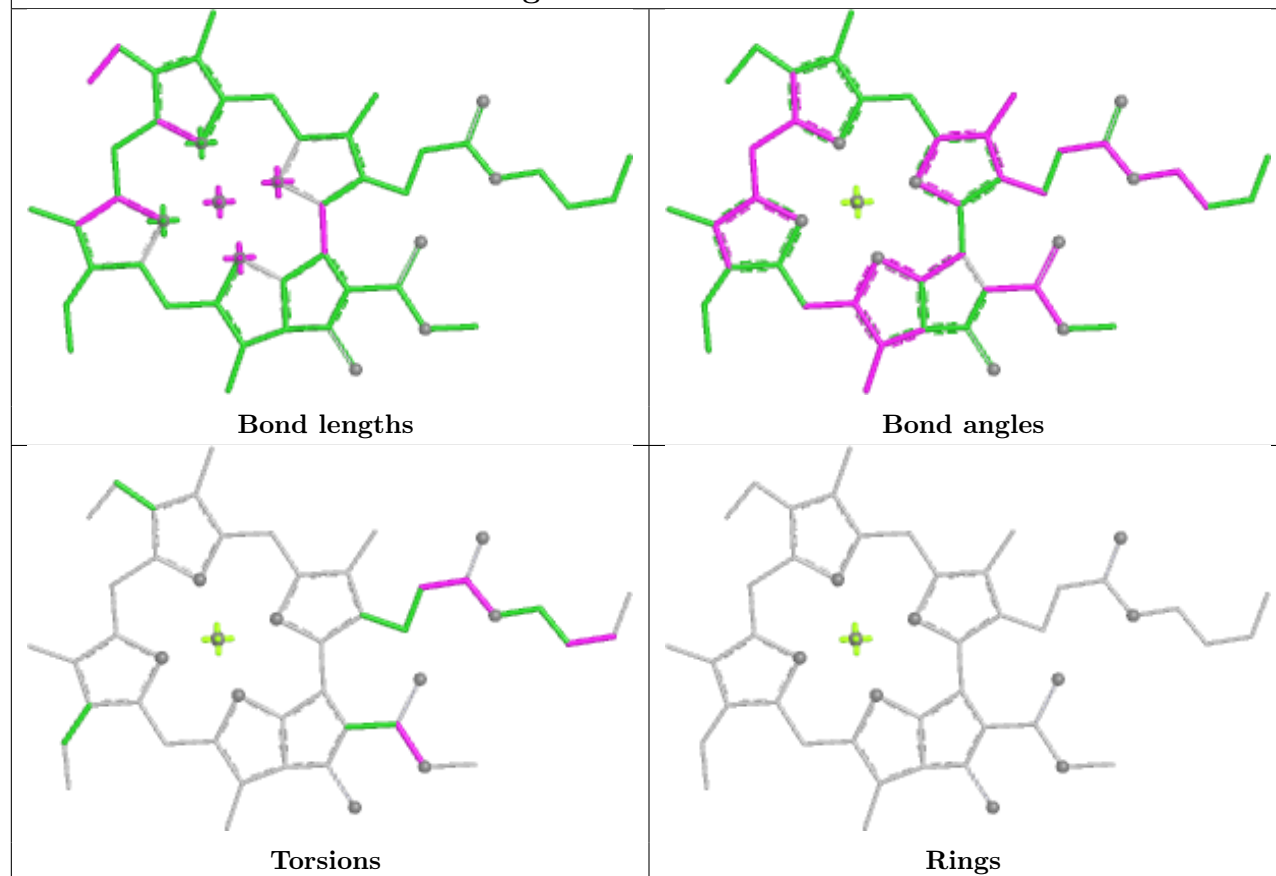
Ligand CHL 8 613**Ligand CLA A 1103**

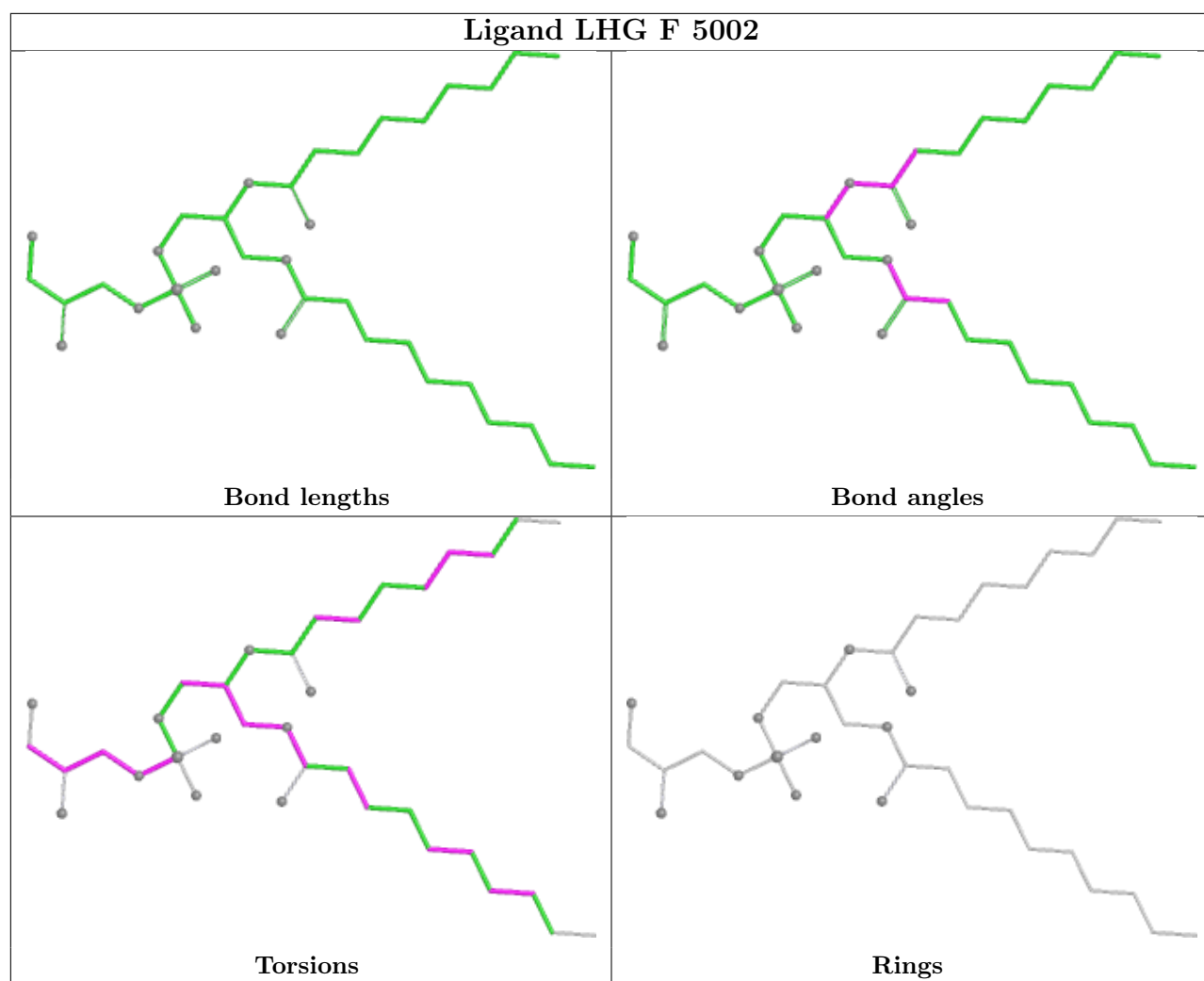


Ligand CLA A 1115

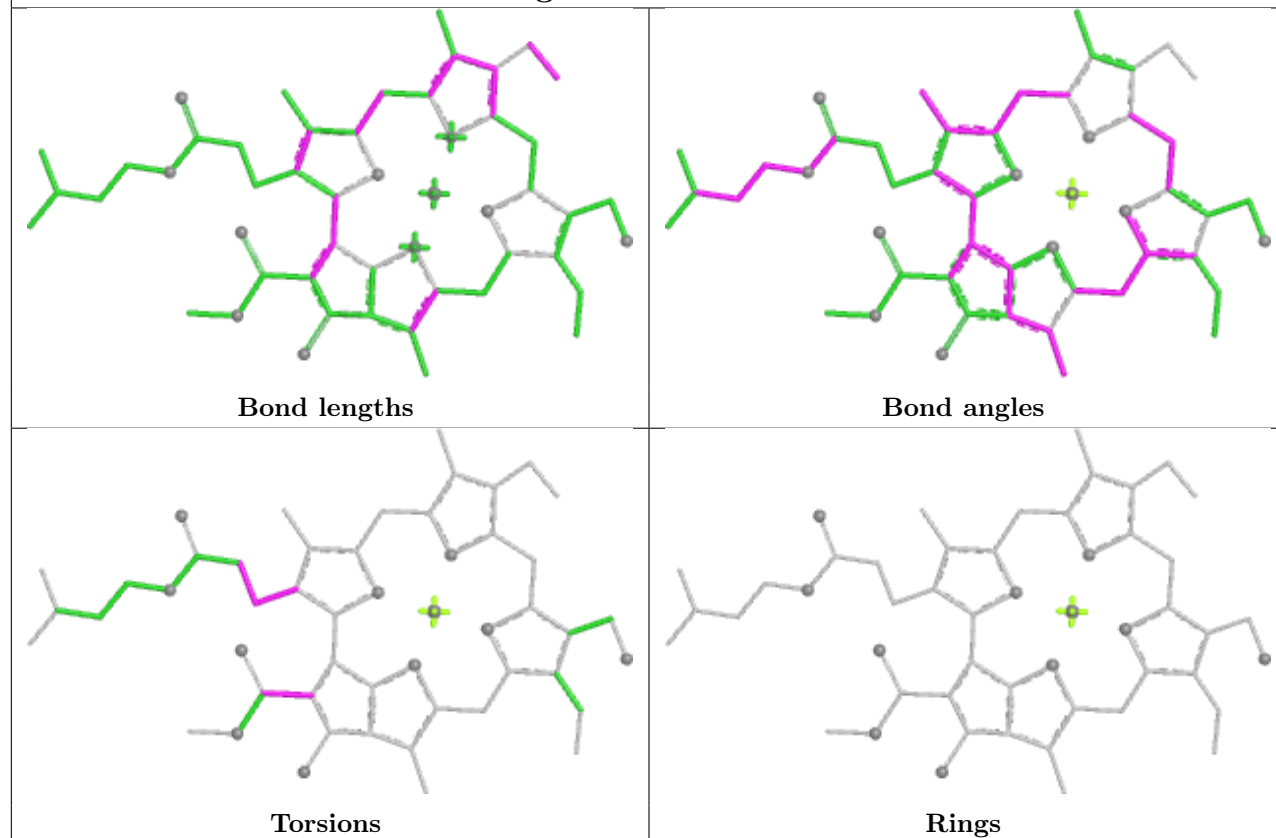


Ligand CLA A 1120

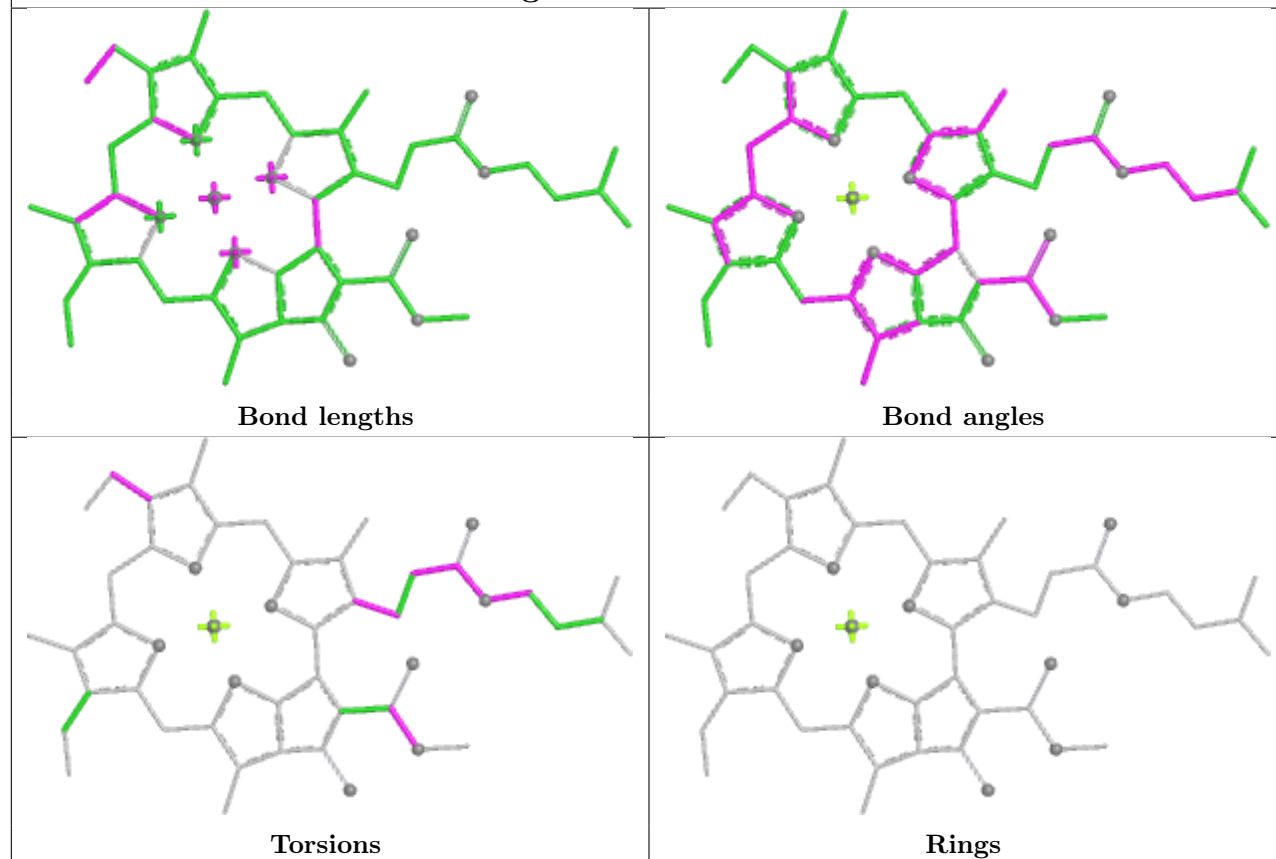


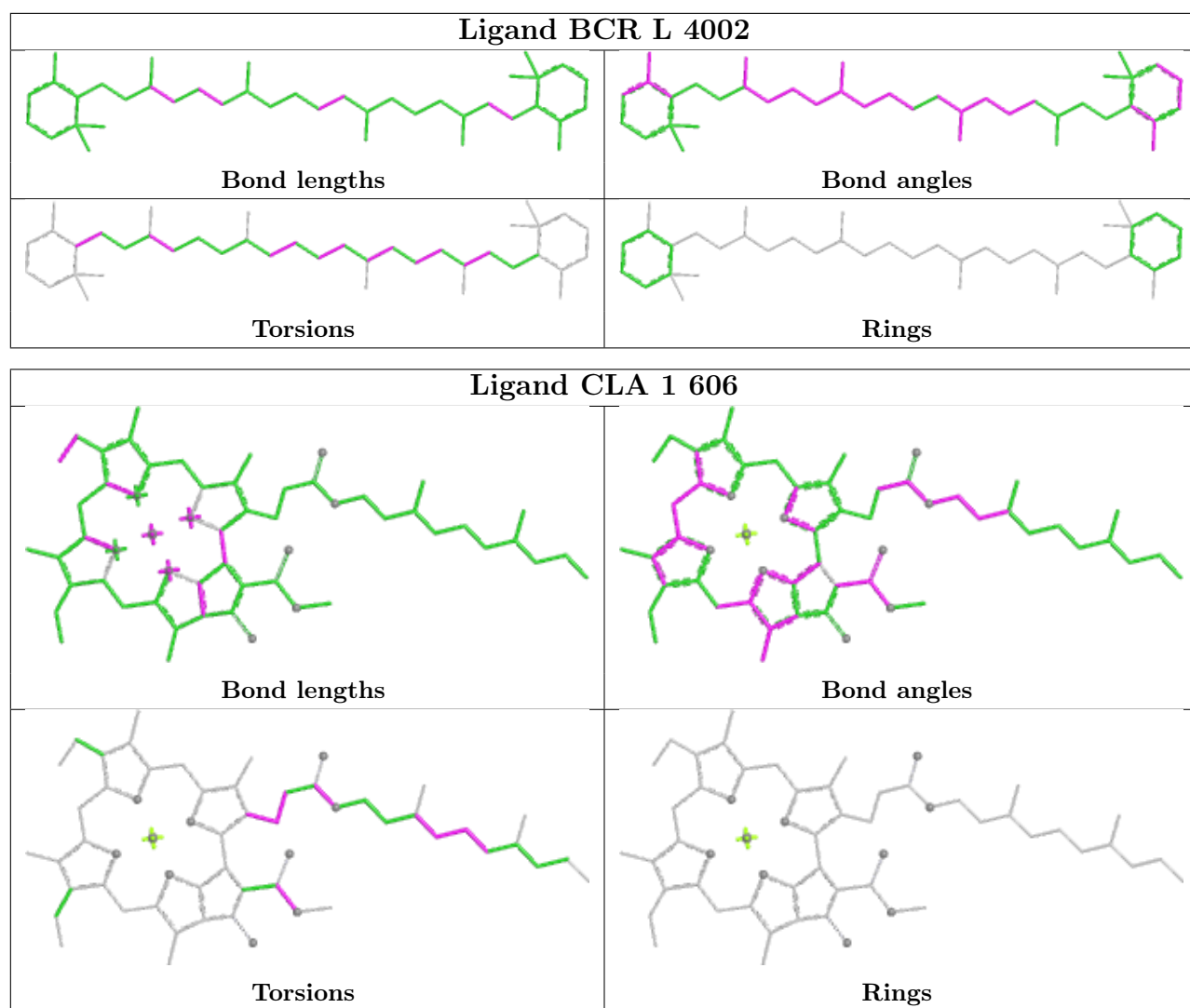


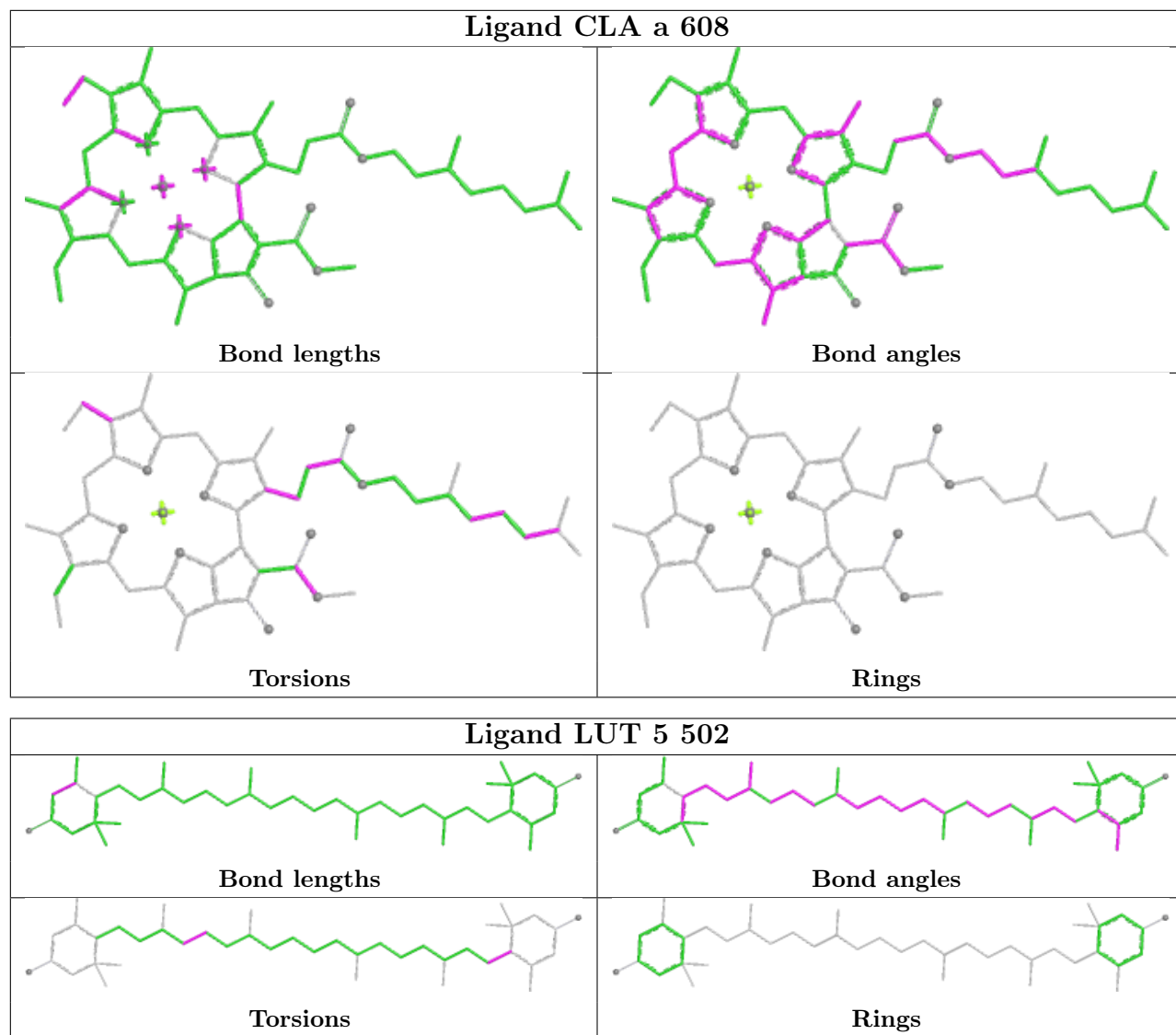
Ligand CHL 6 611



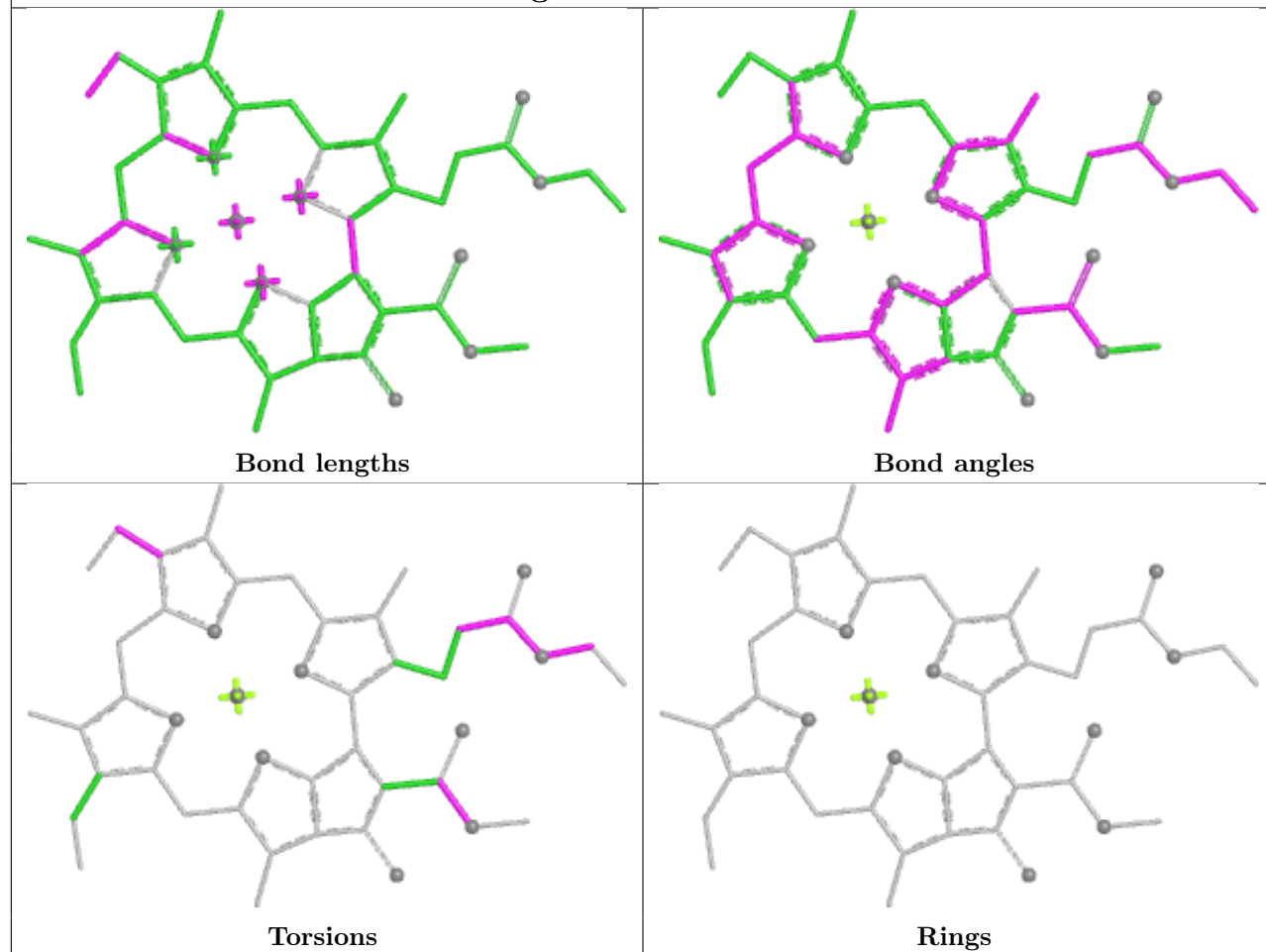
Ligand CLA G 1601



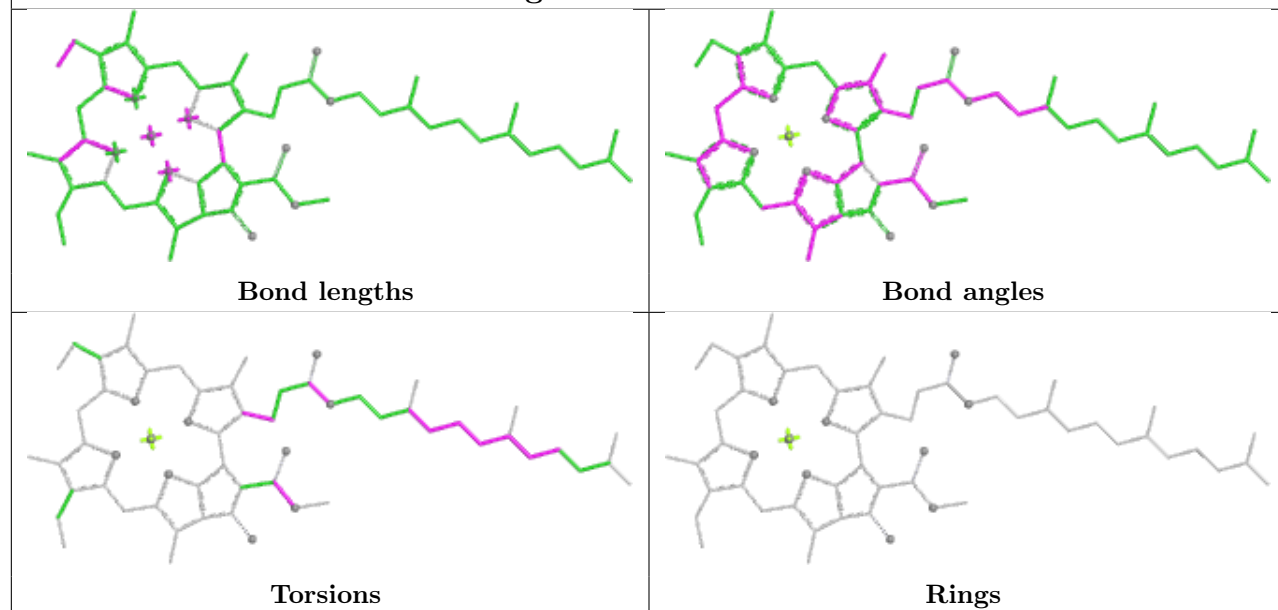


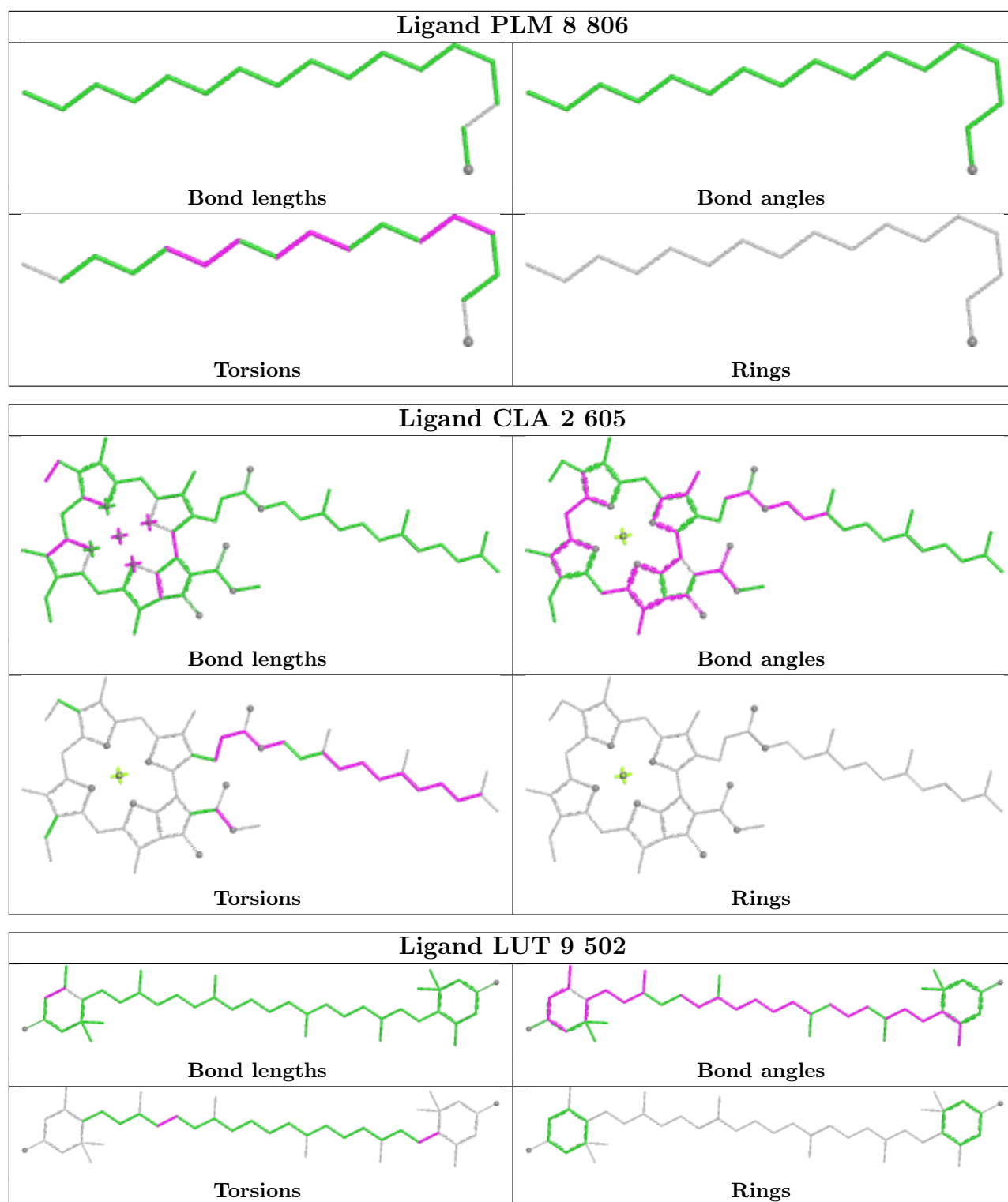


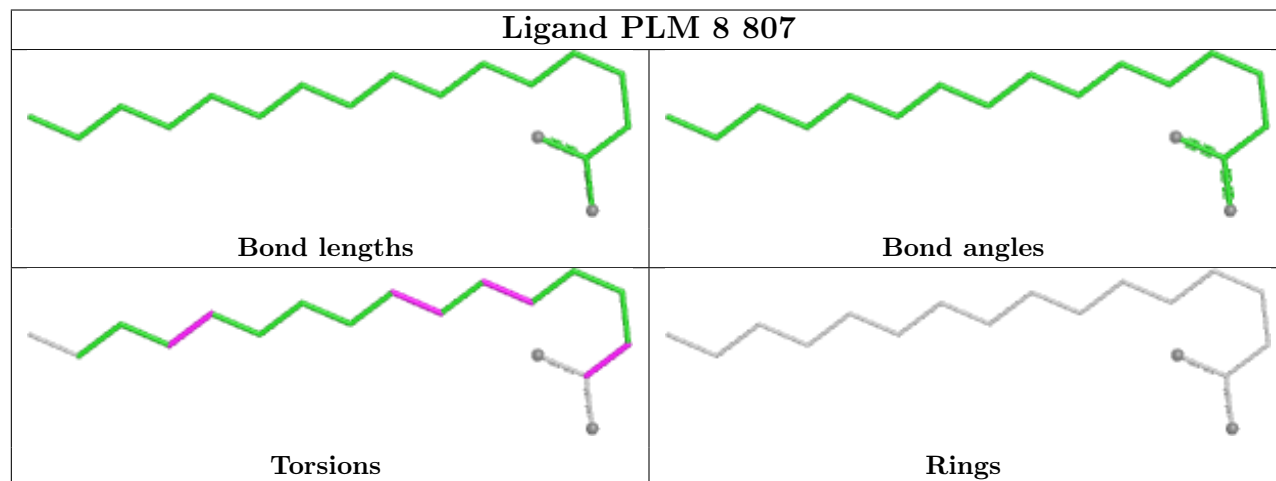
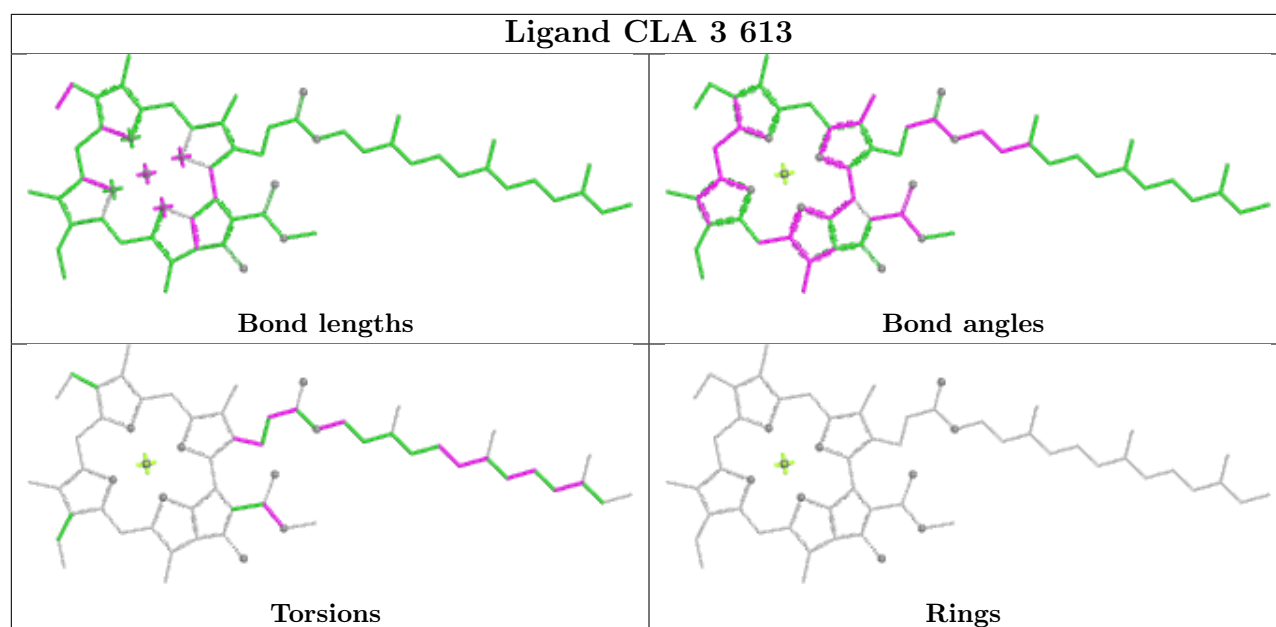
Ligand CLA 9 607

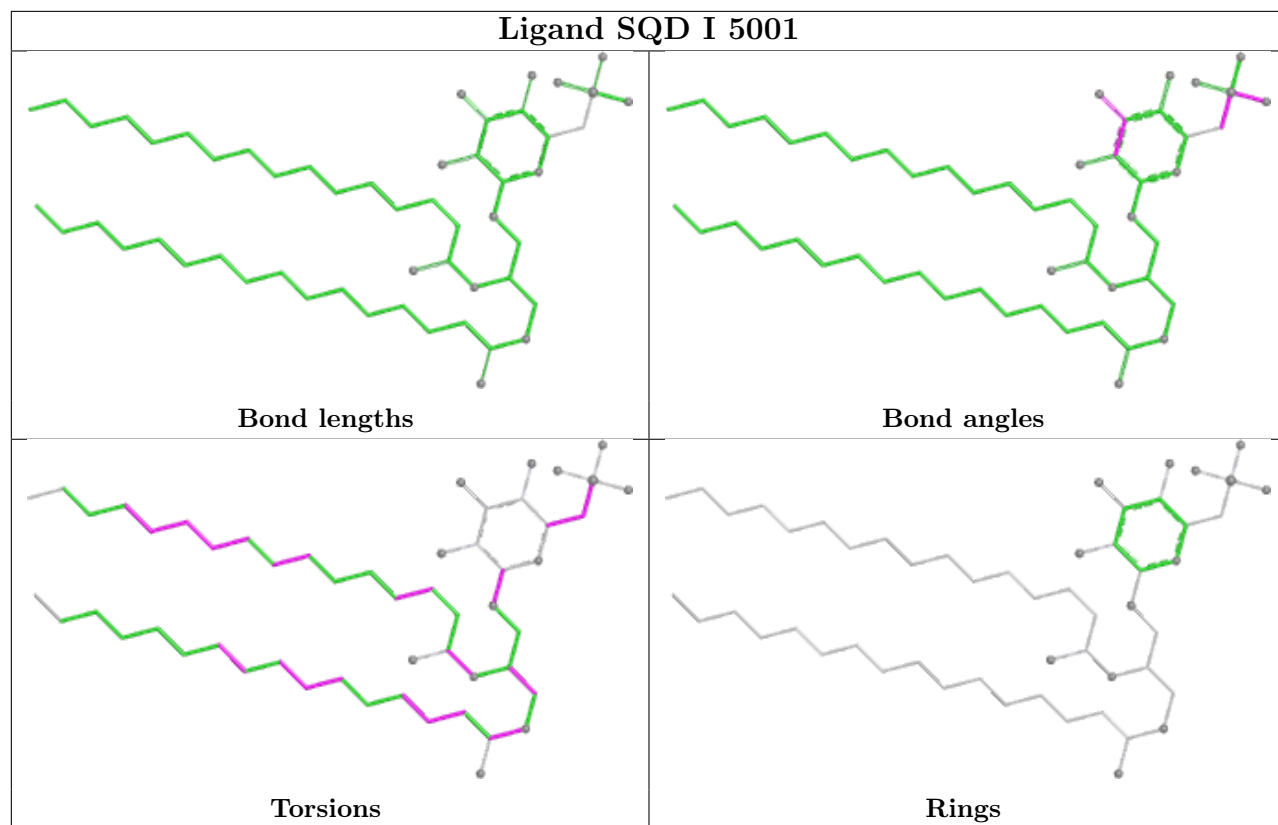


Ligand CLA L 1502

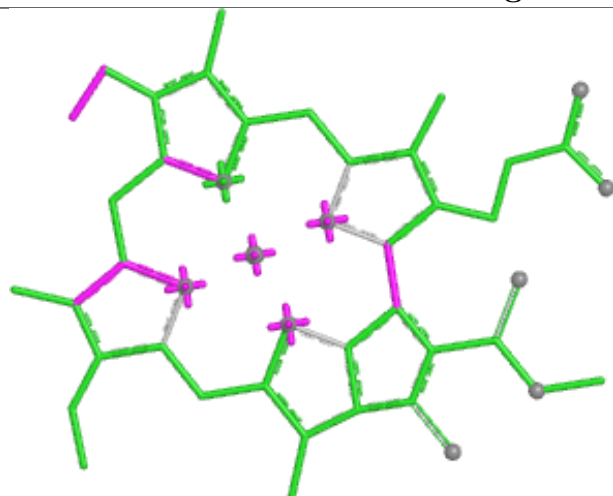




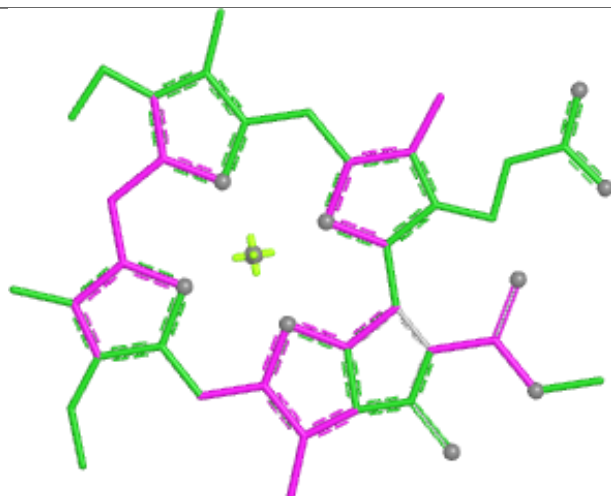




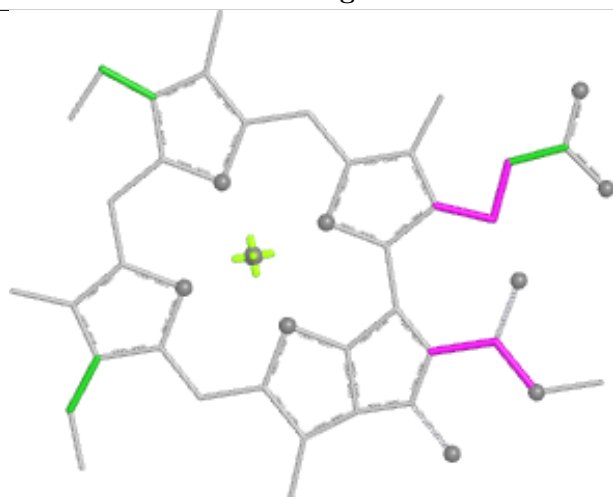
Ligand CLA A 1141



Bond lengths



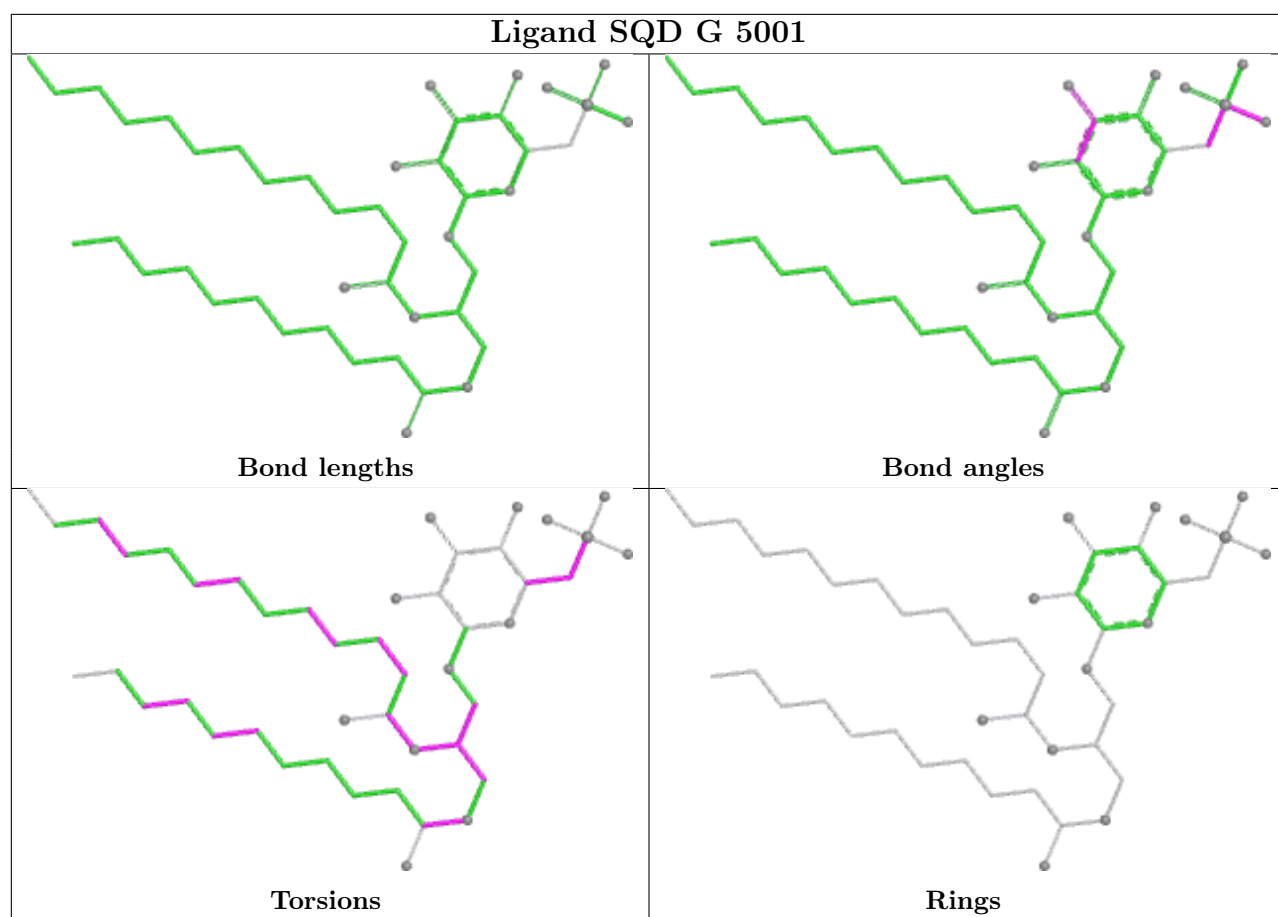
Bond angles



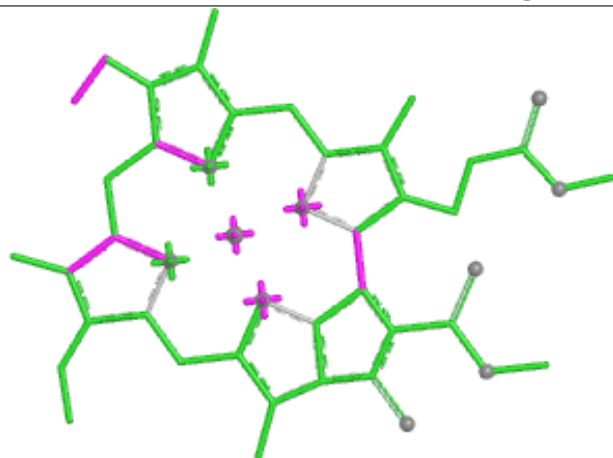
Torsions



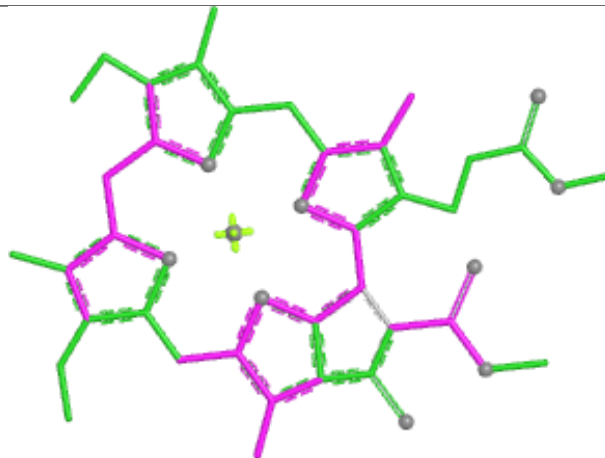
Rings



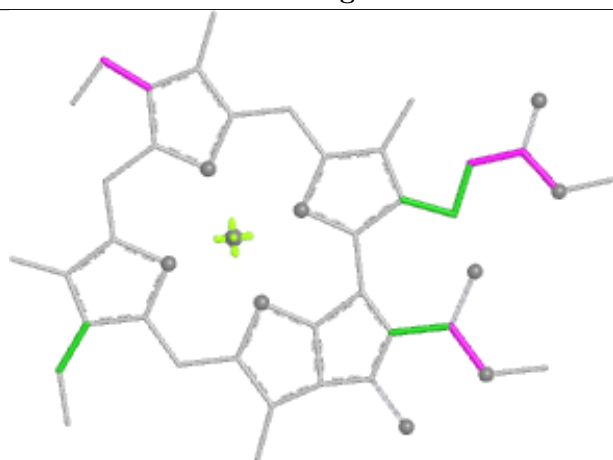
Ligand CLA 5 614



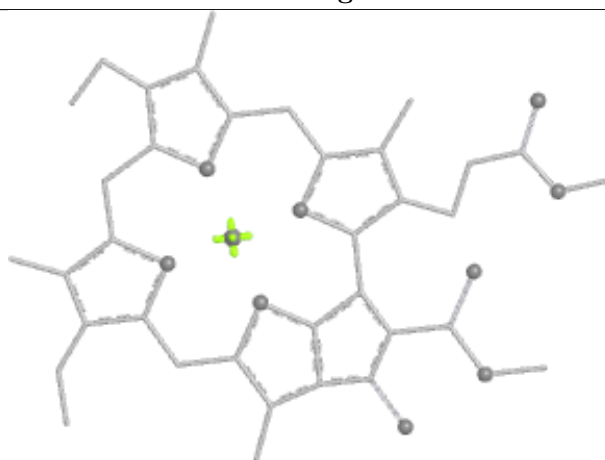
Bond lengths



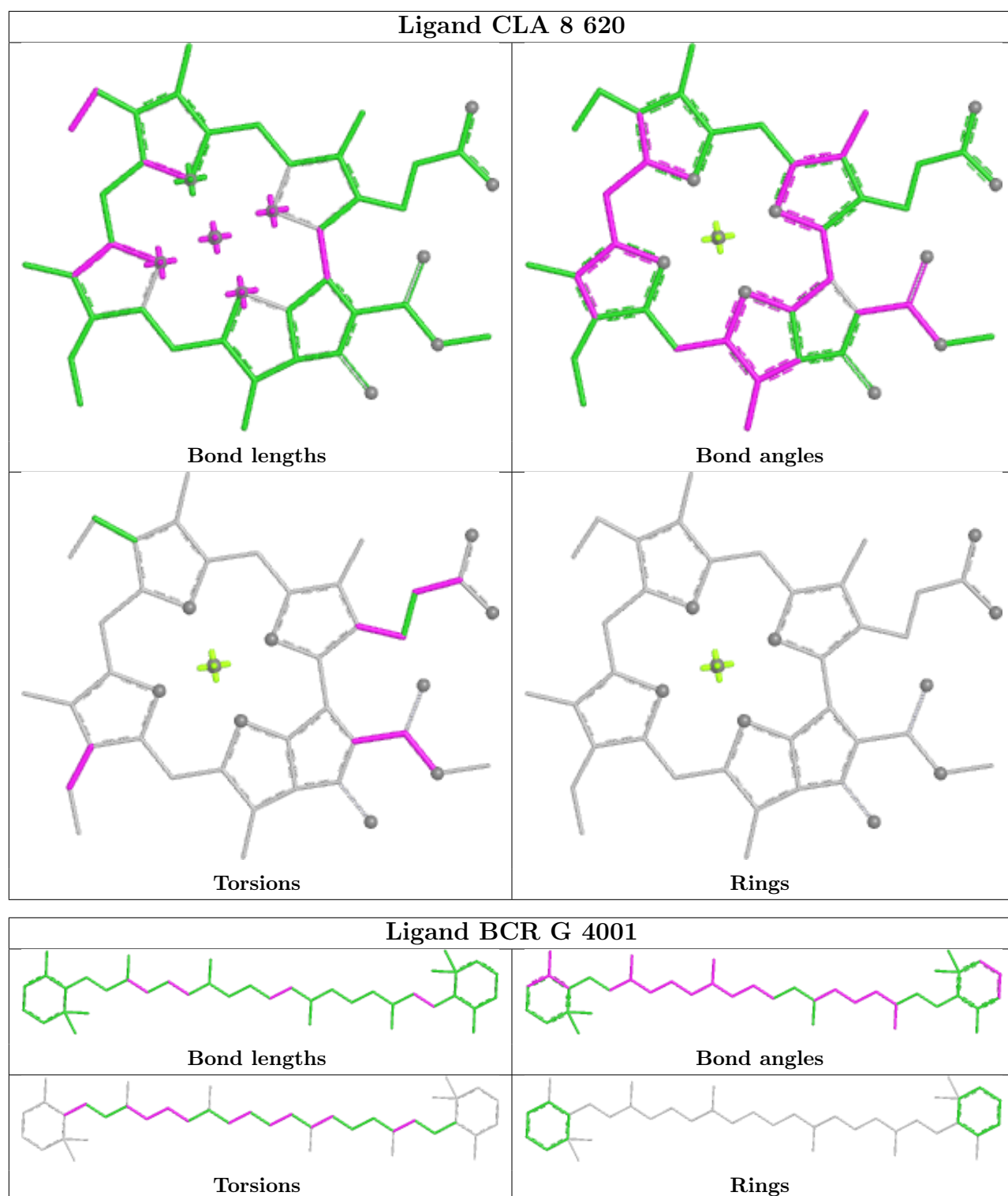
Bond angles

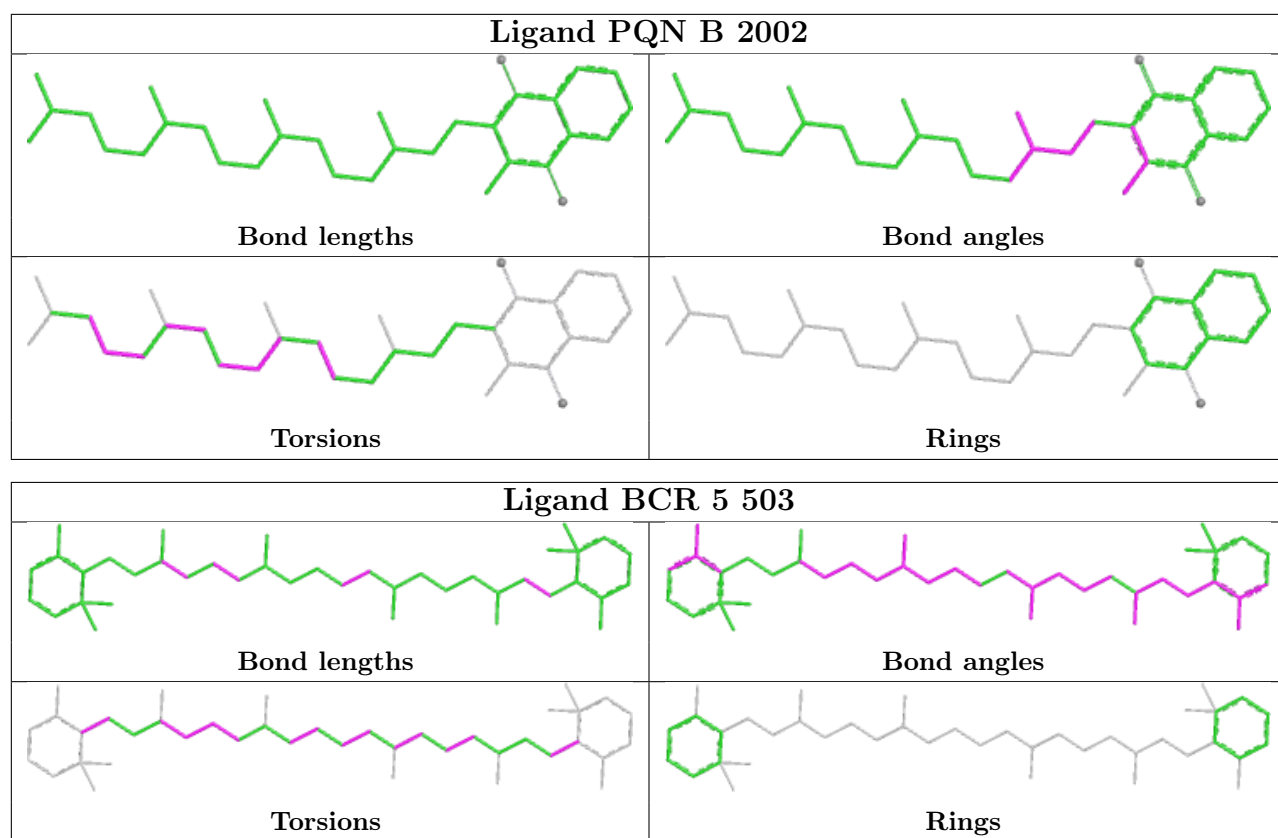


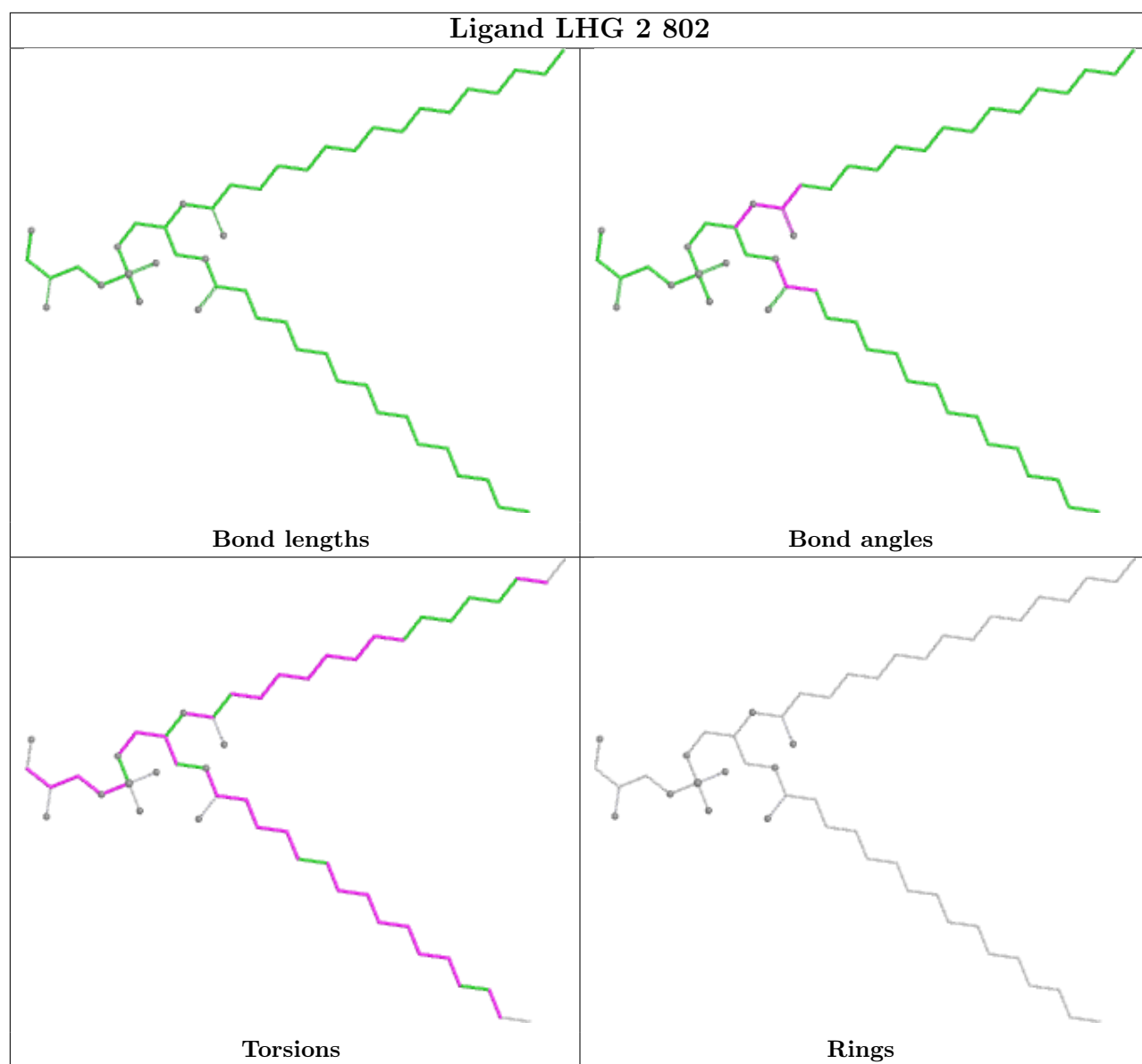
Torsions



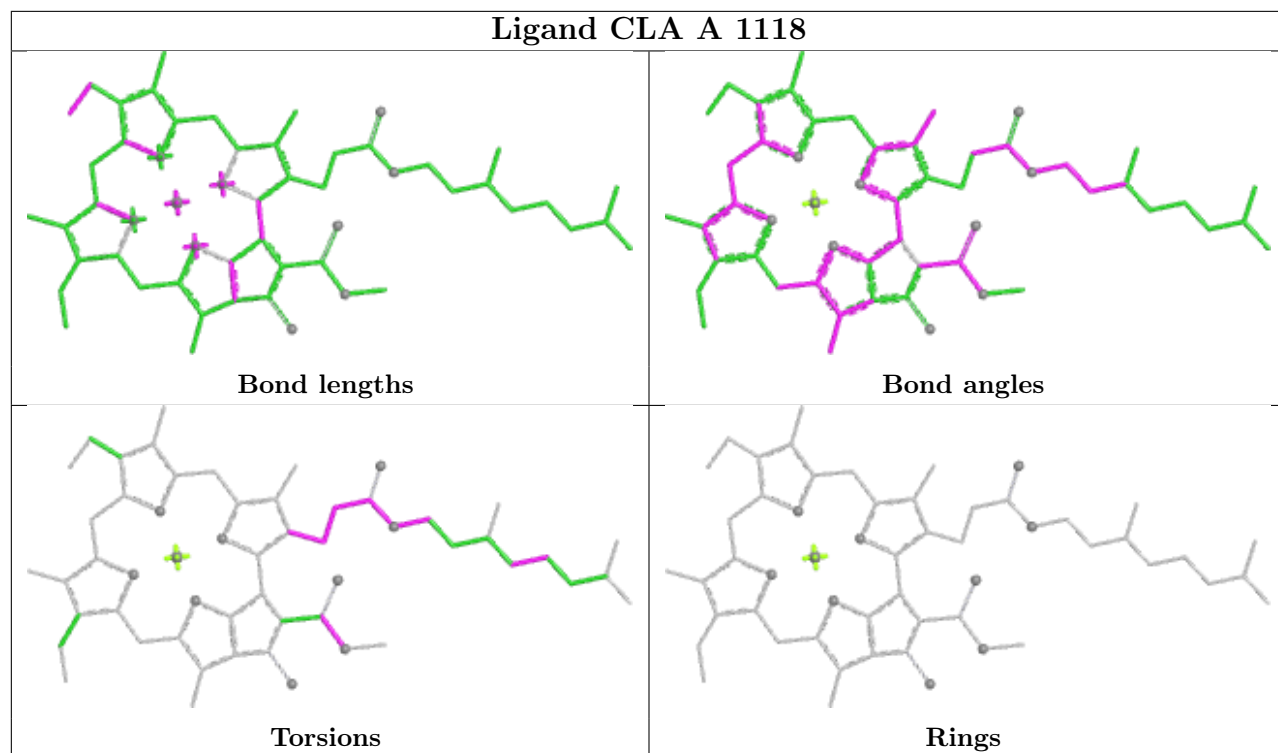
Rings



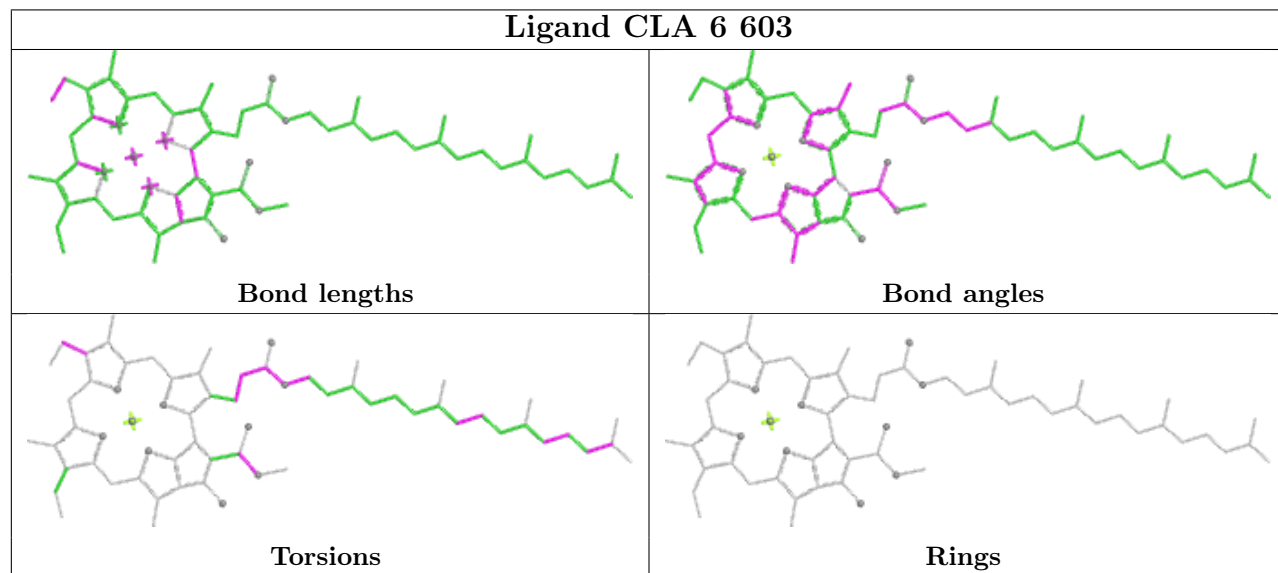


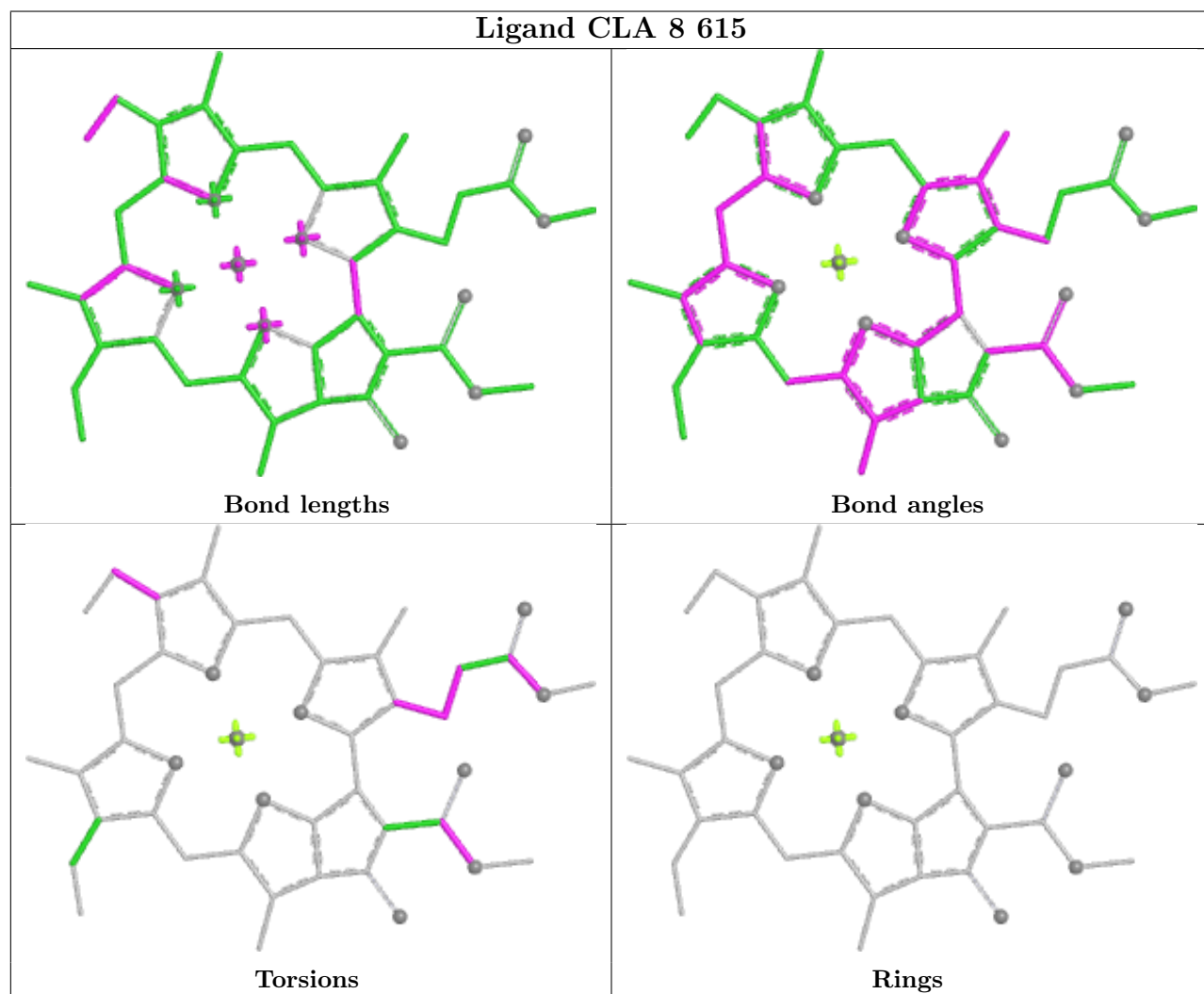
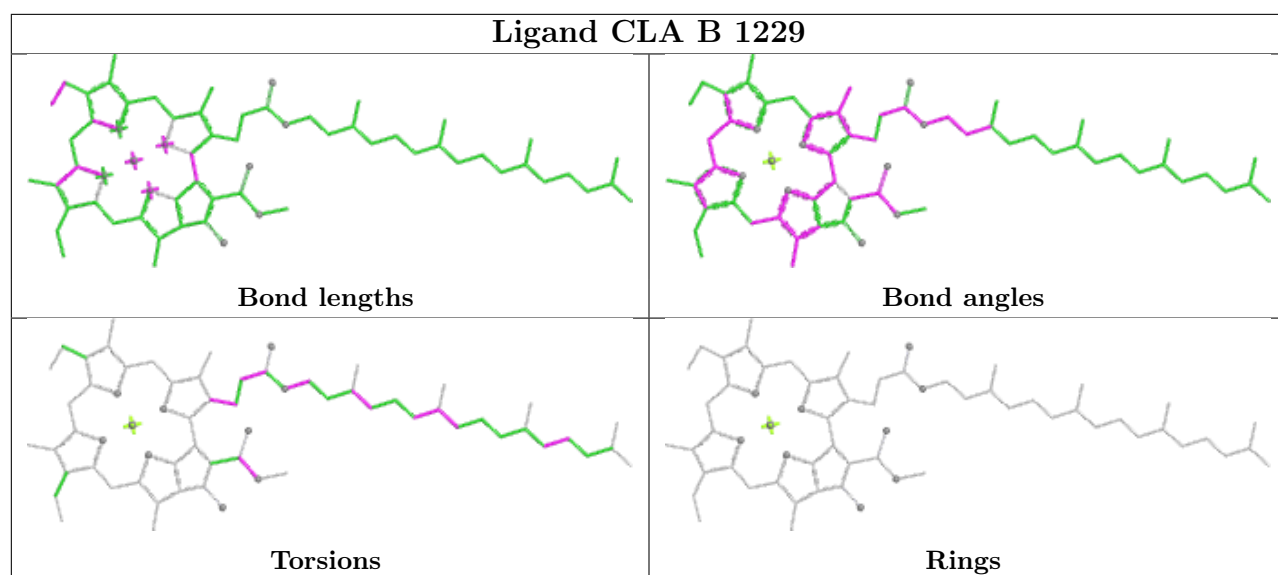


Ligand CLA A 1118

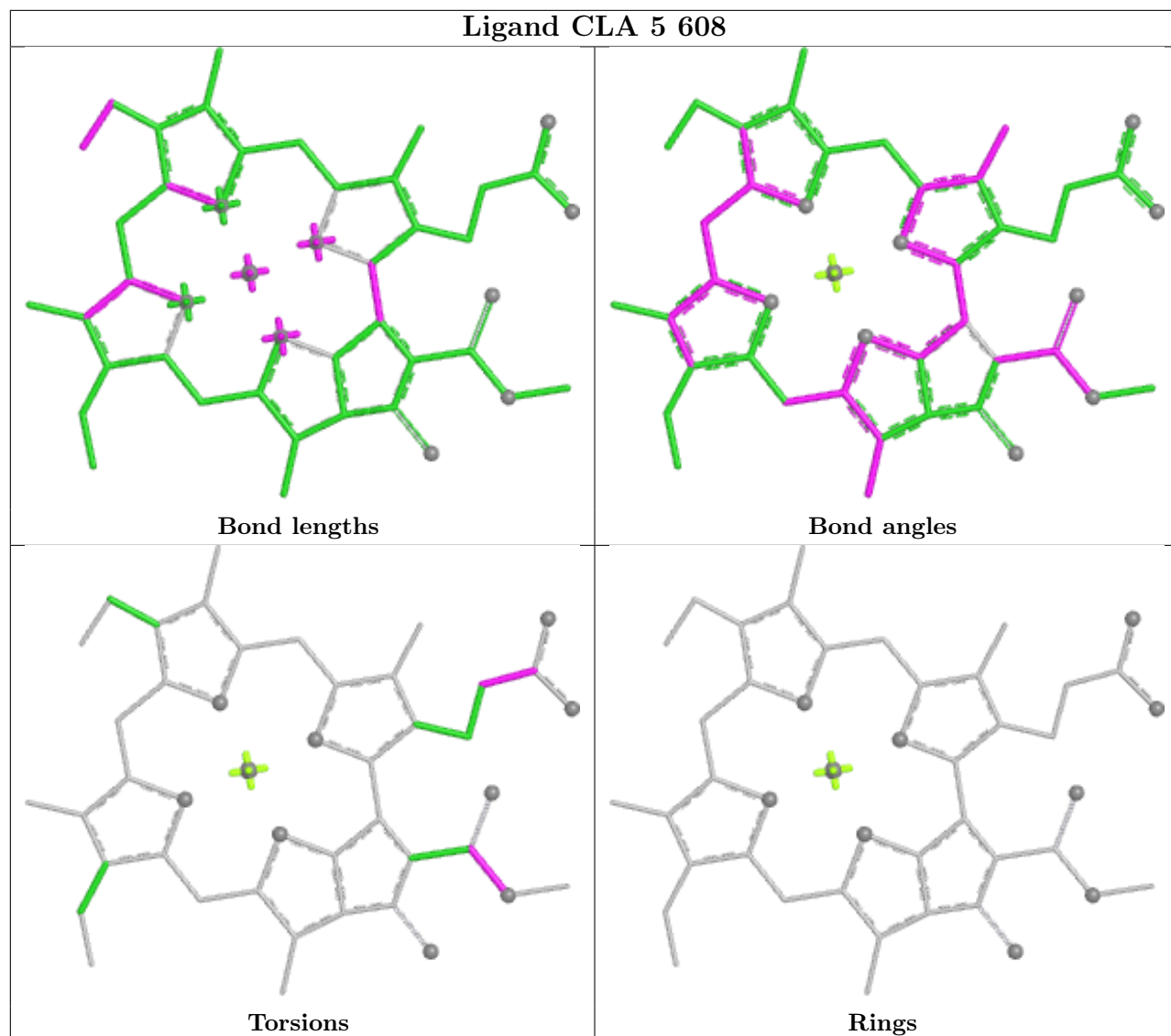


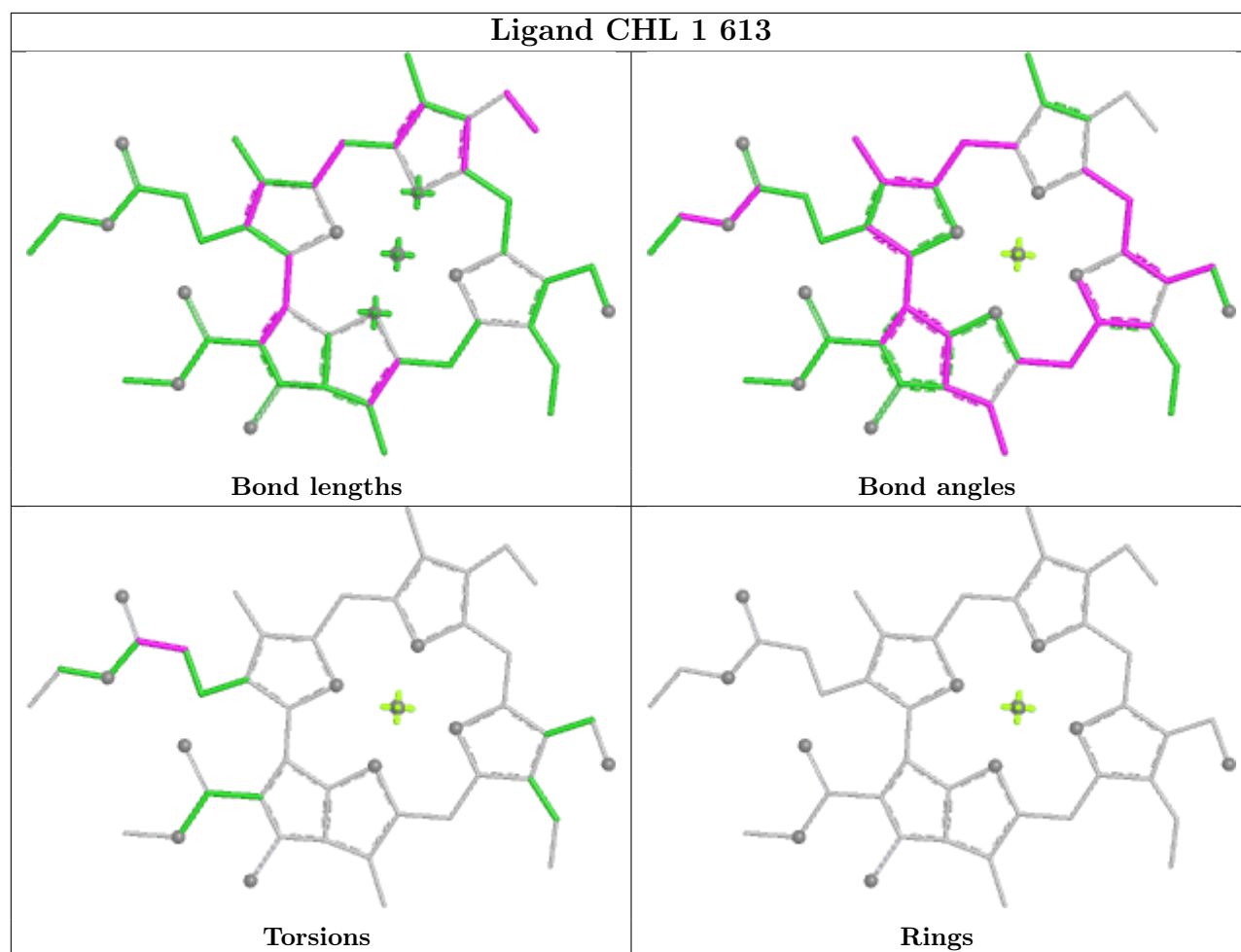
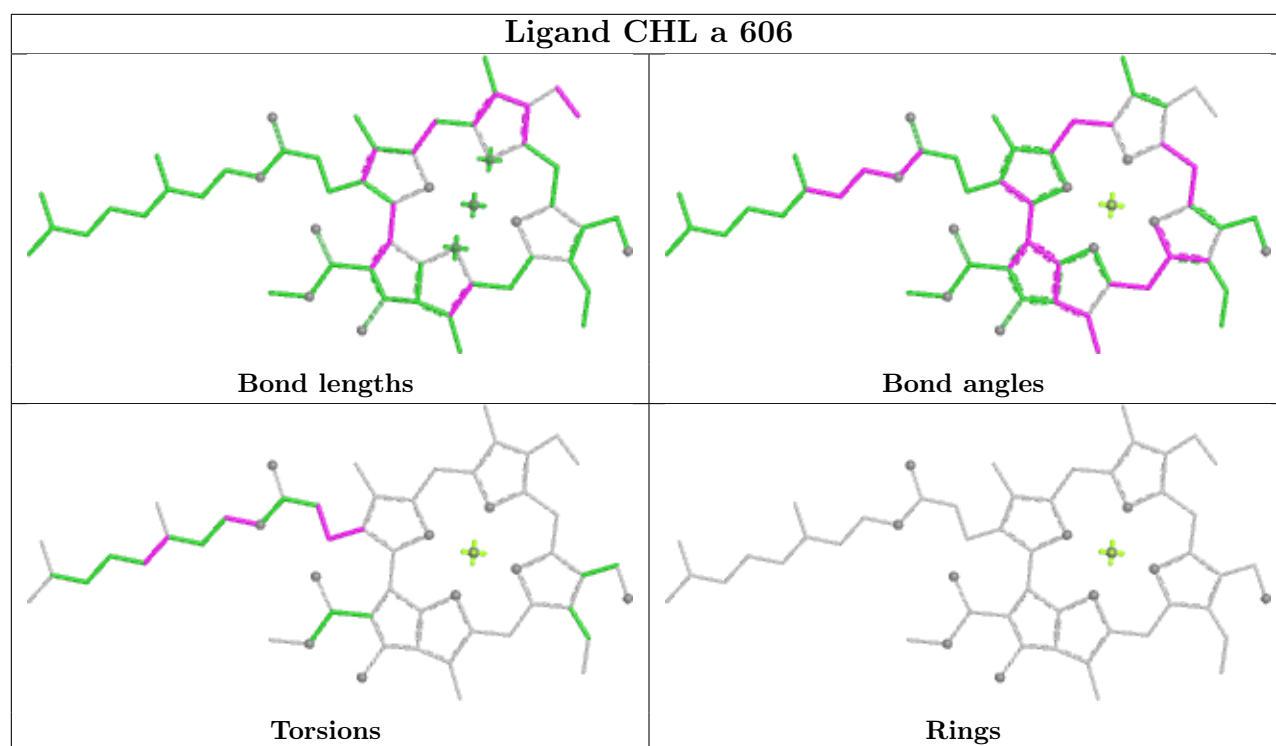
Ligand CLA 6 603

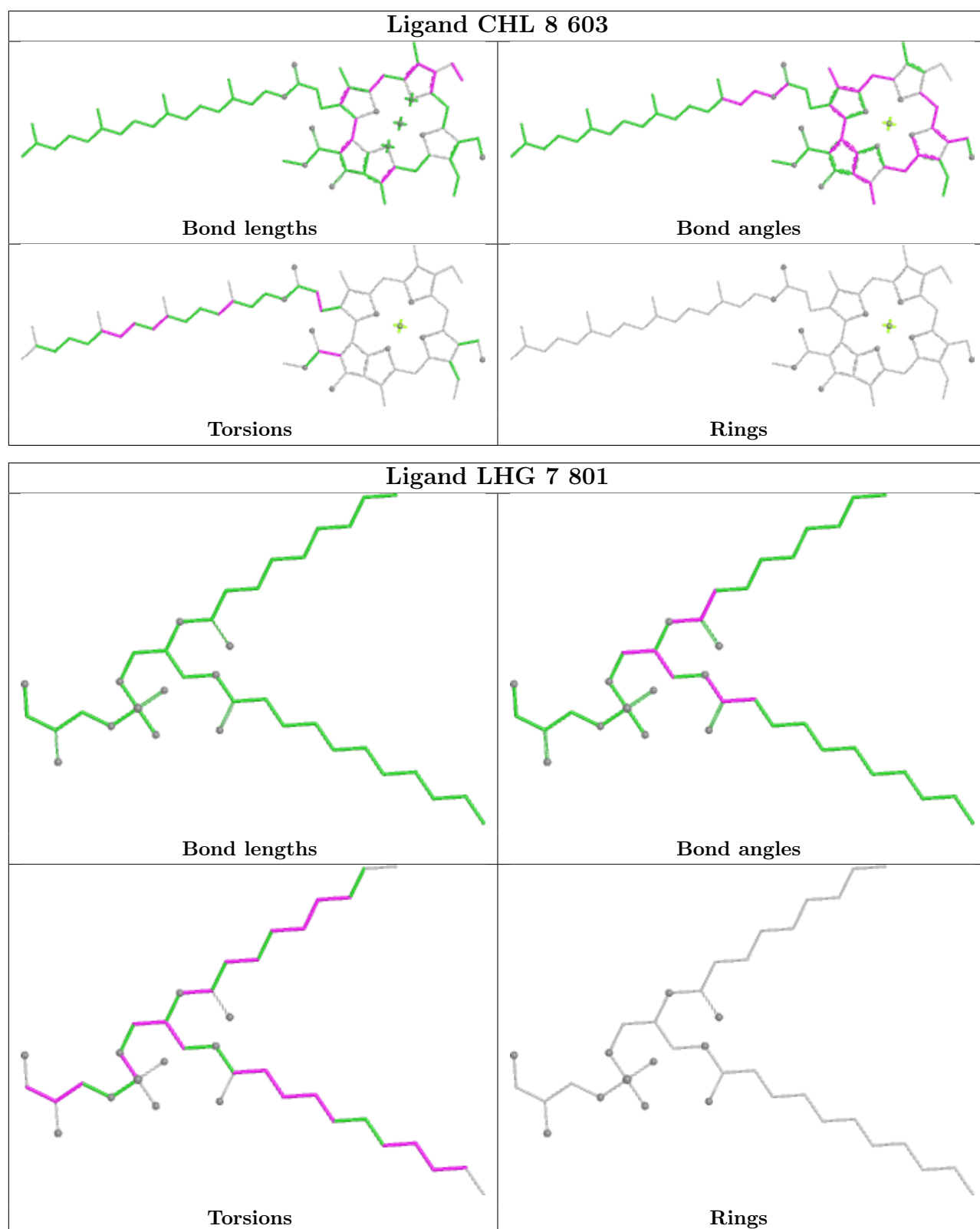


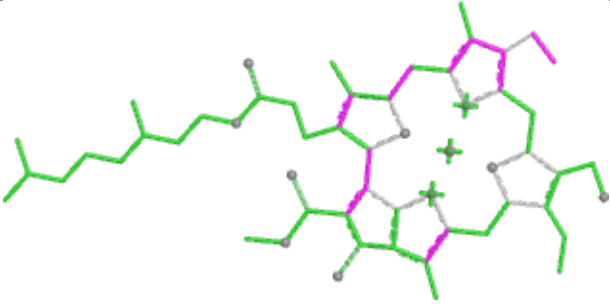
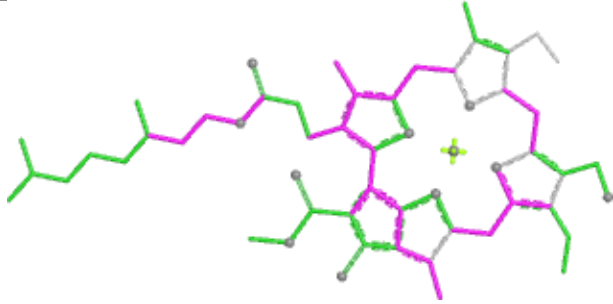
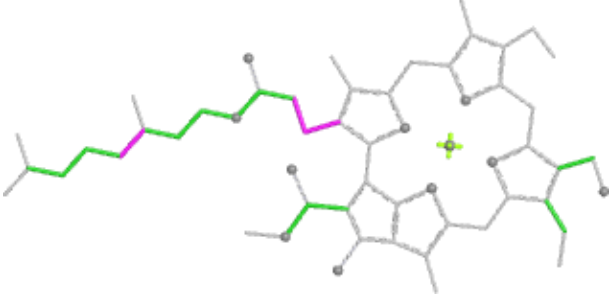
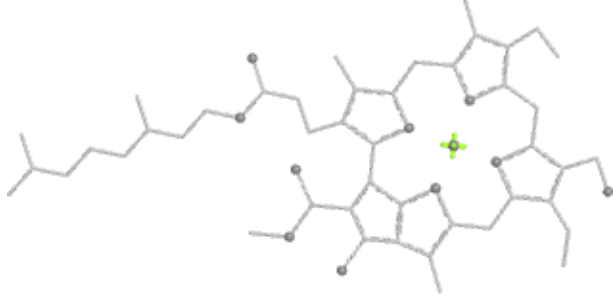
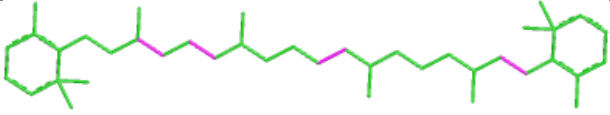
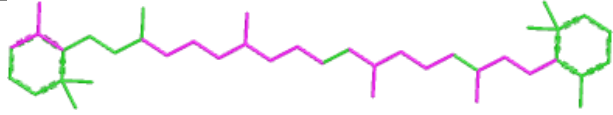
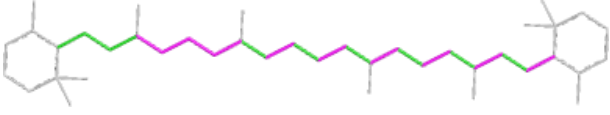
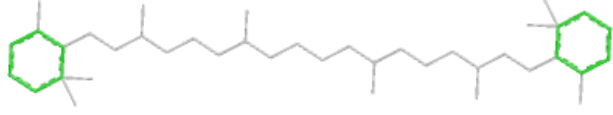


Ligand CLA 5 608

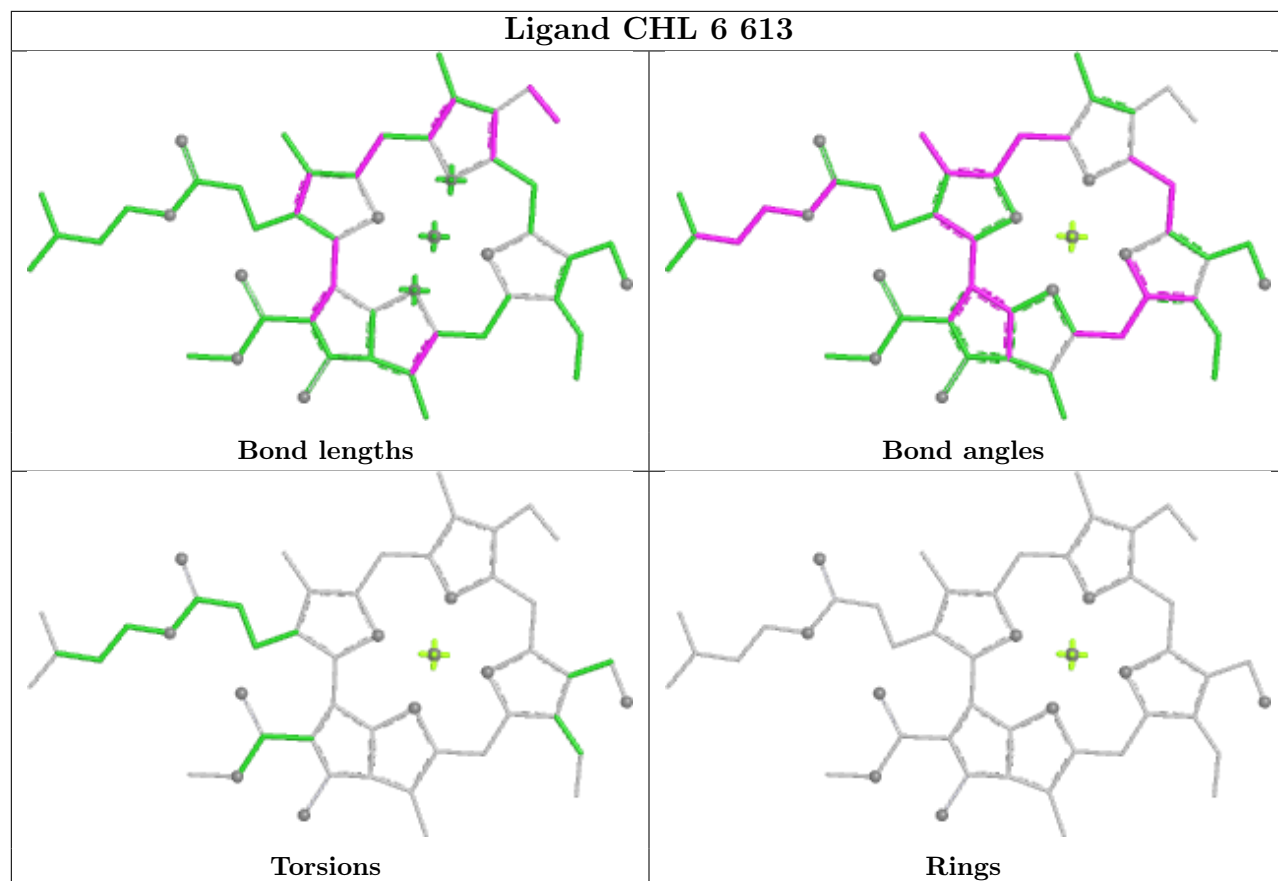




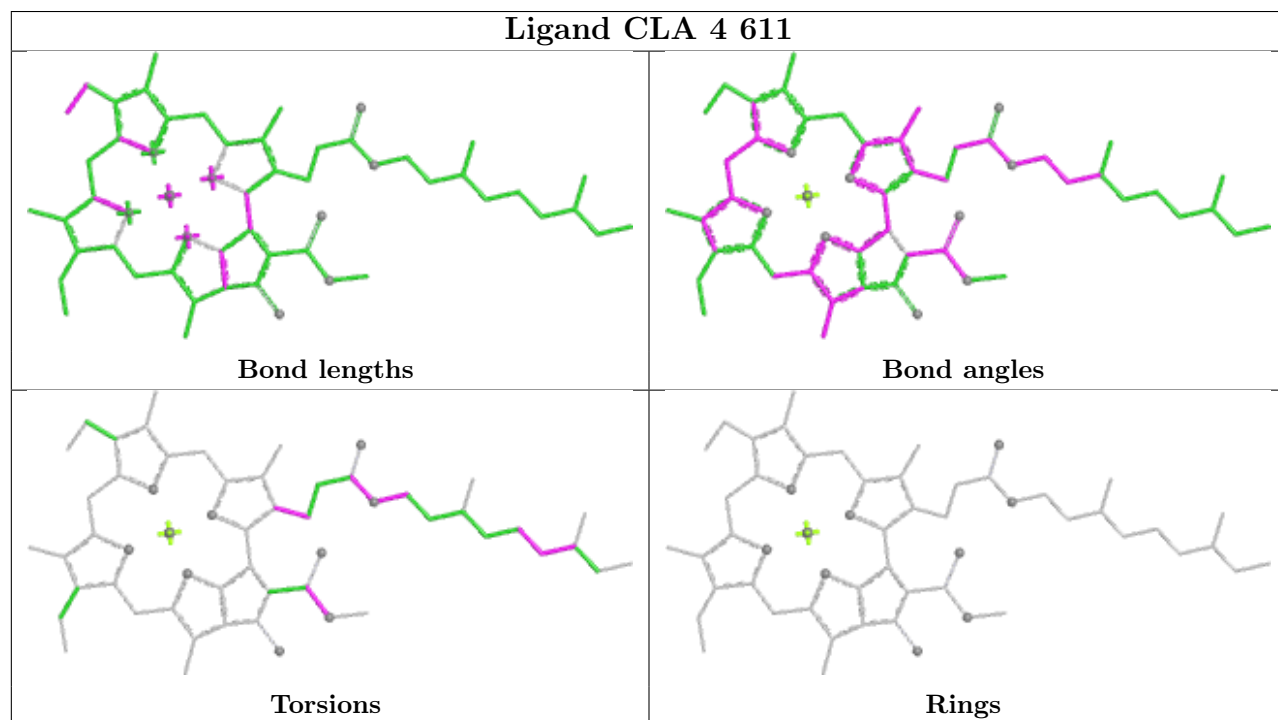


Ligand CHL 4 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 4006	
 Bond lengths	 Bond angles
 Torsions	 Rings

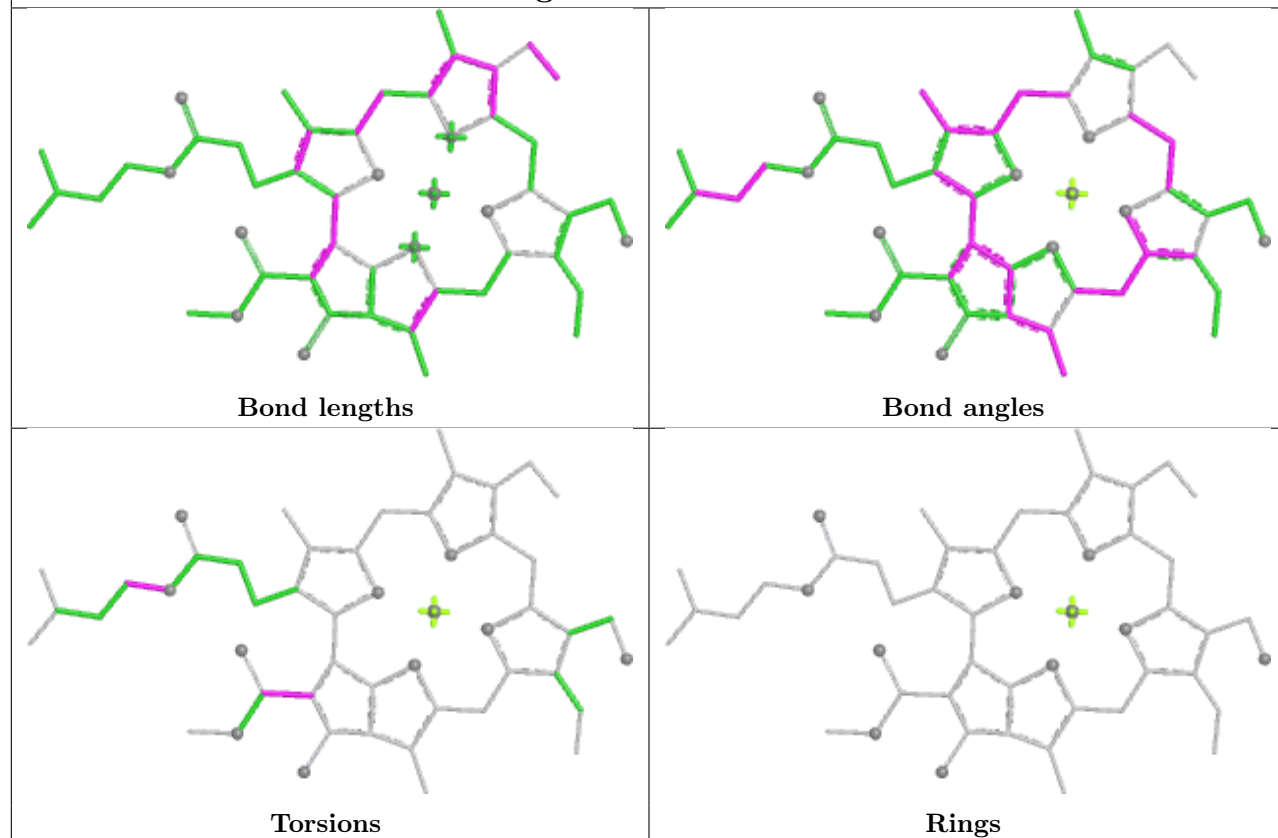
Ligand CHL 6 613



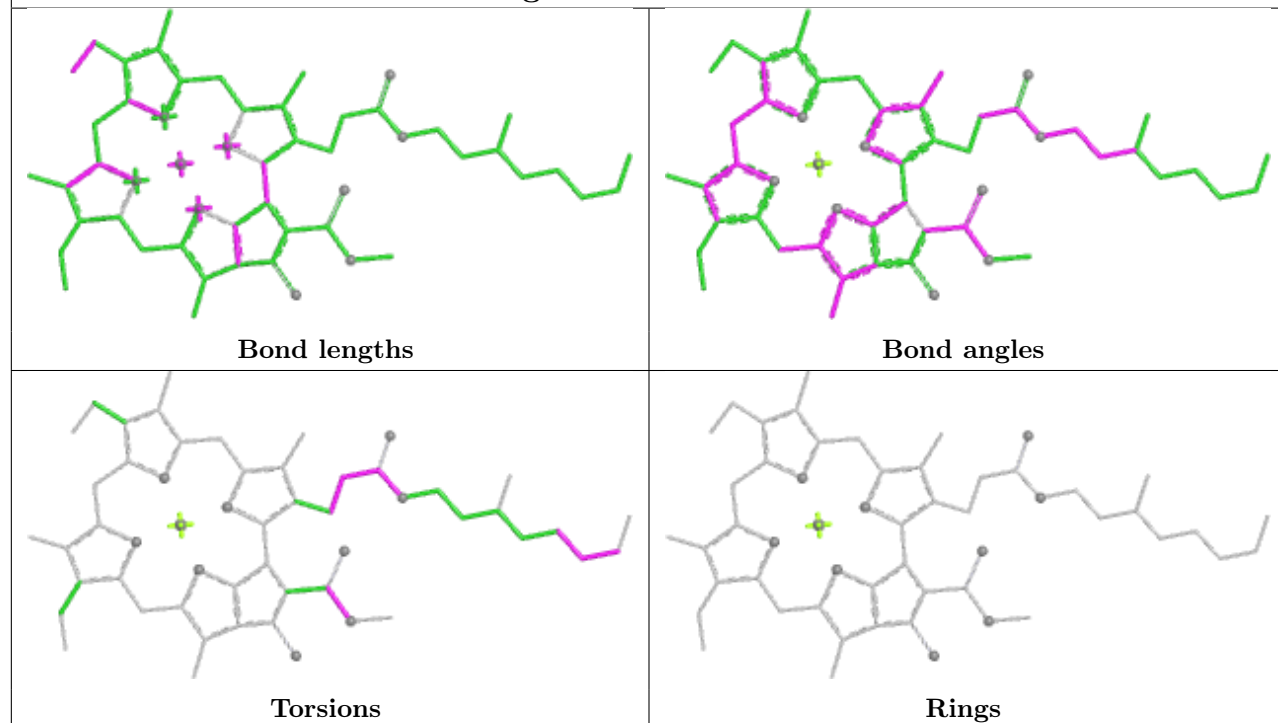
Ligand CLA 4 611

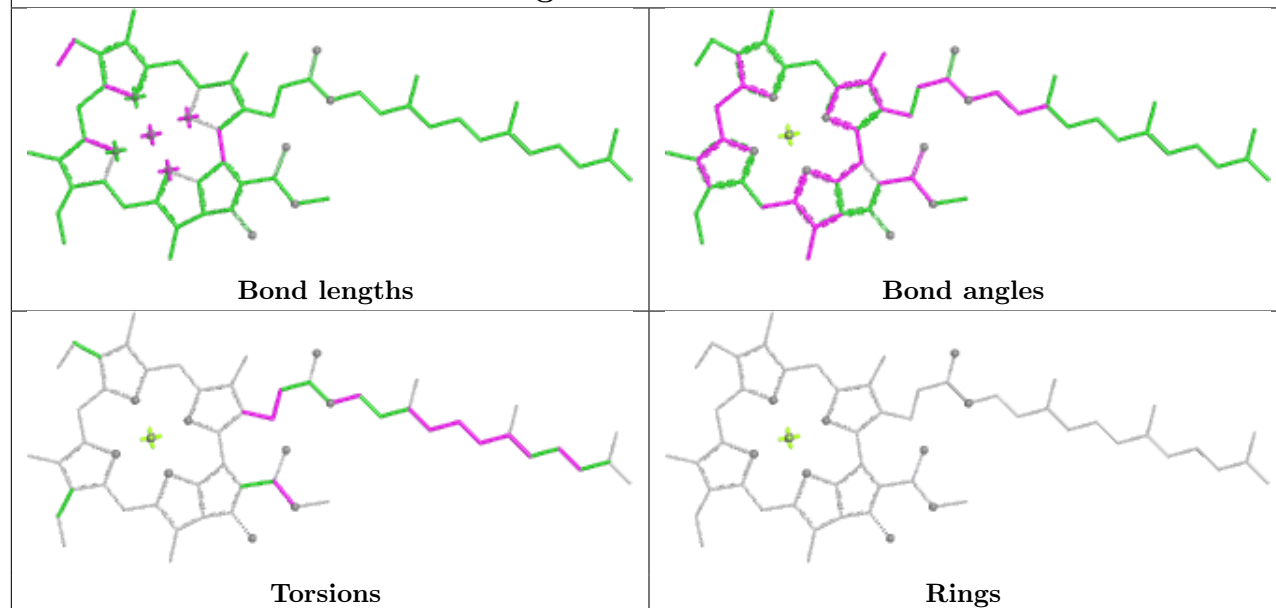
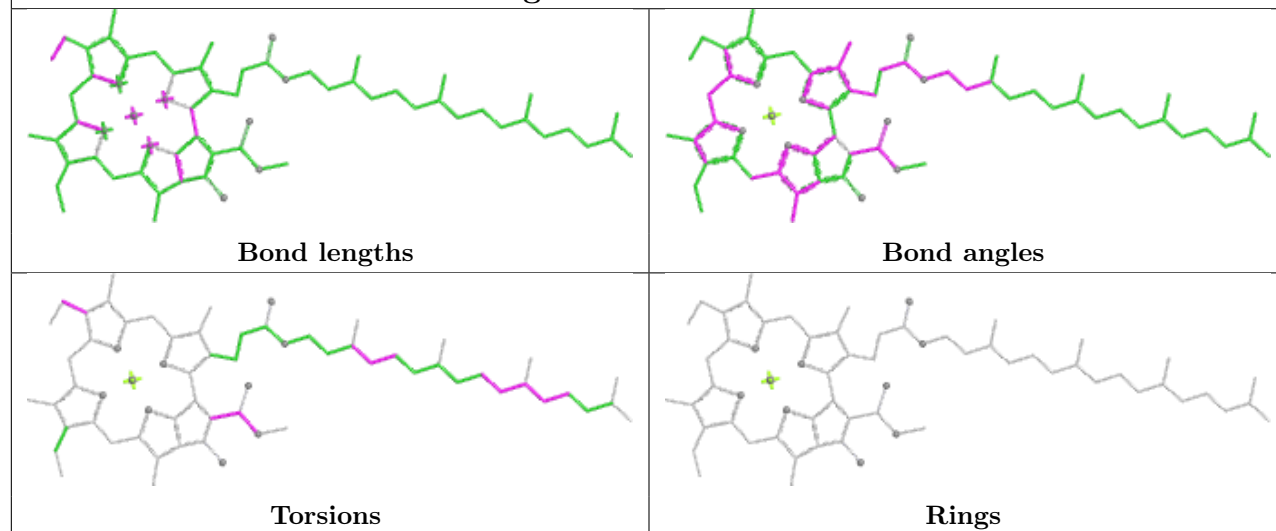


Ligand CHL 5 611

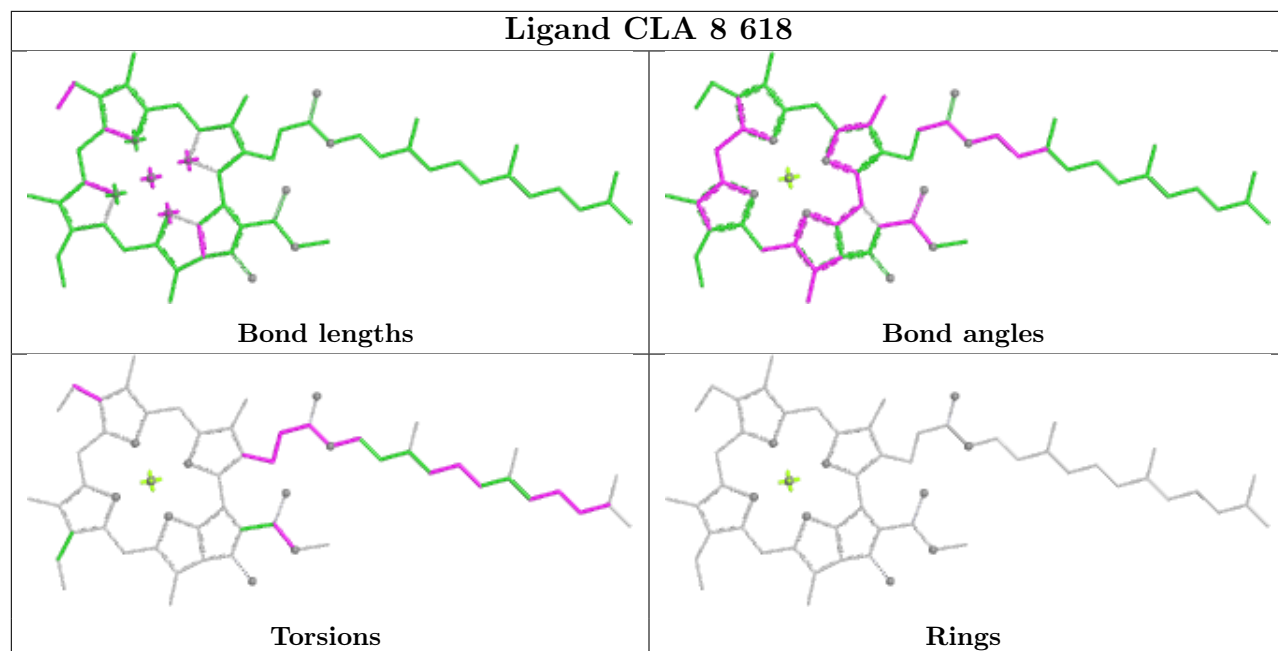


Ligand CLA A 1110

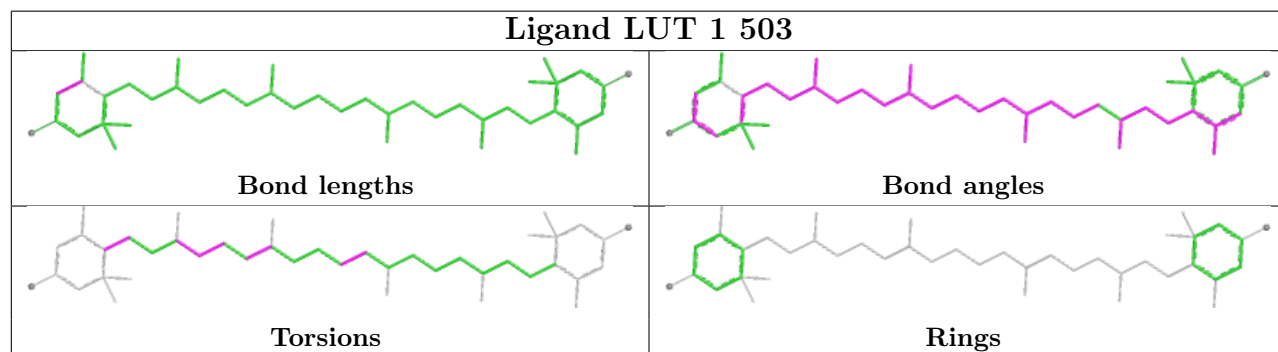


Ligand CLA 7 610**Ligand CLA B 1205**

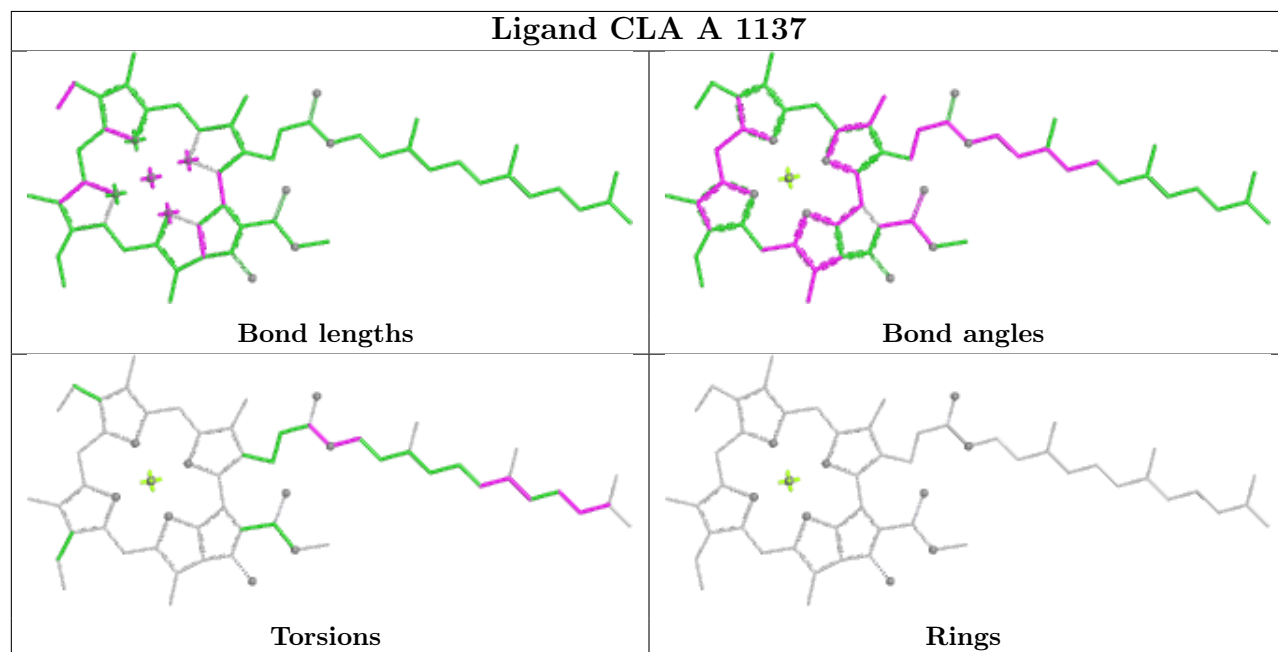
Ligand CLA 8 618

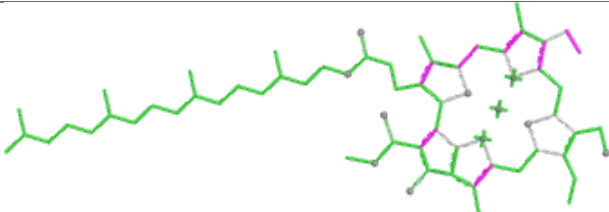
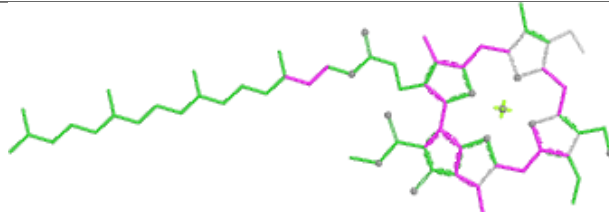
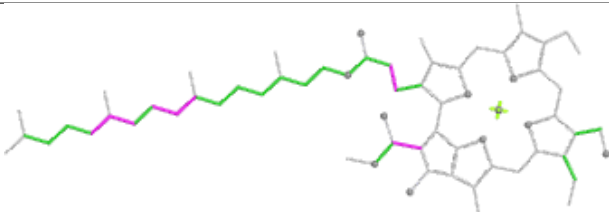
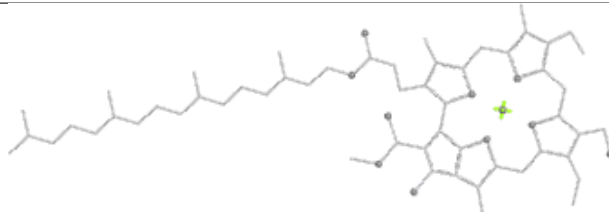


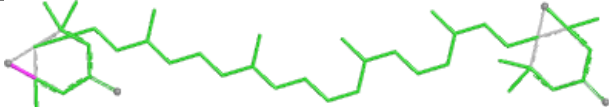
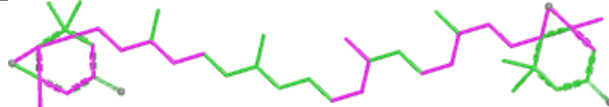
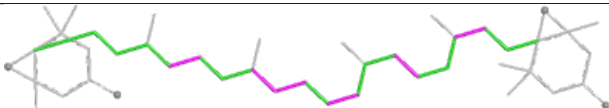
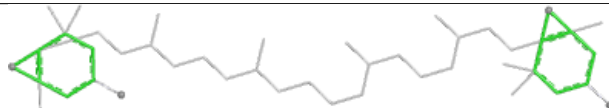
Ligand LUT 1 503



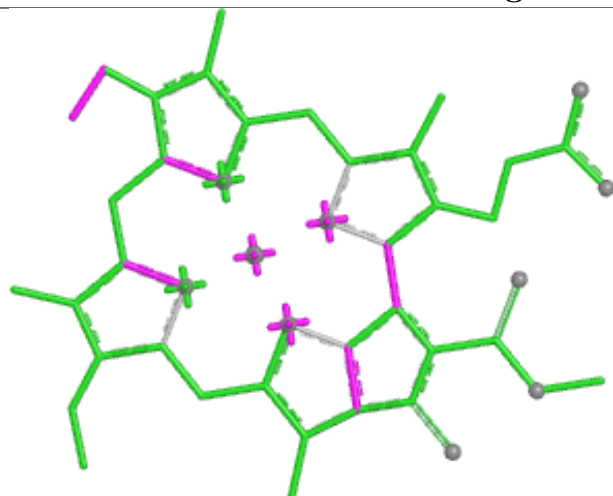
Ligand CLA A 1137



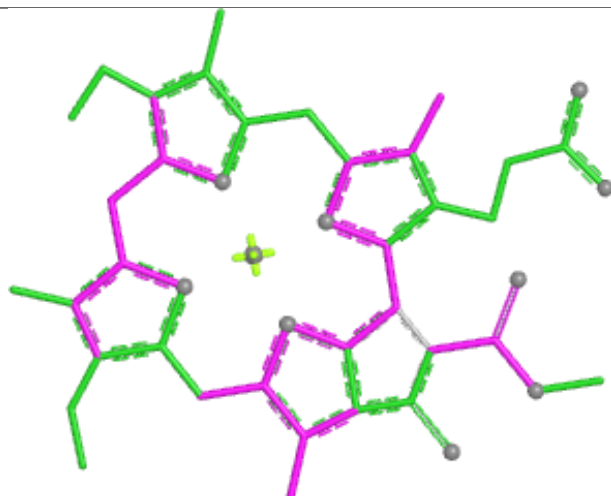
Ligand CHL 6 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT 9 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

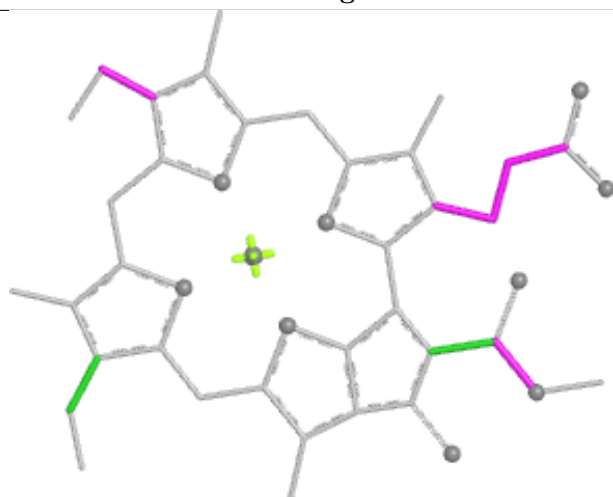
Ligand CLA B 1232



Bond lengths



Bond angles

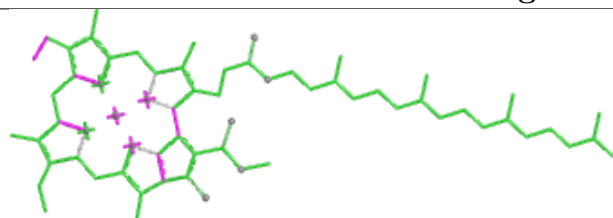


Torsions

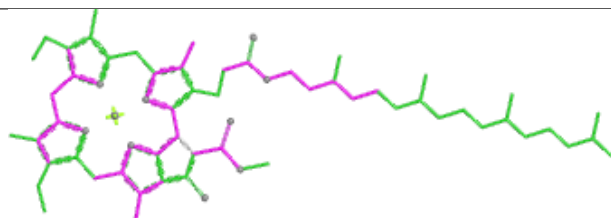


Rings

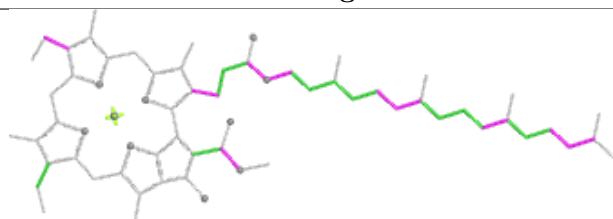
Ligand CLA 2 621



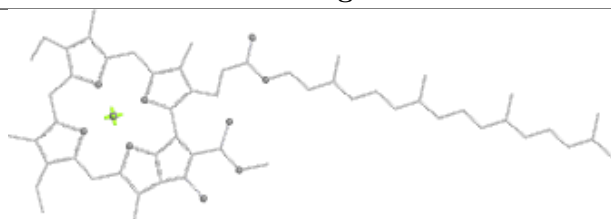
Bond lengths



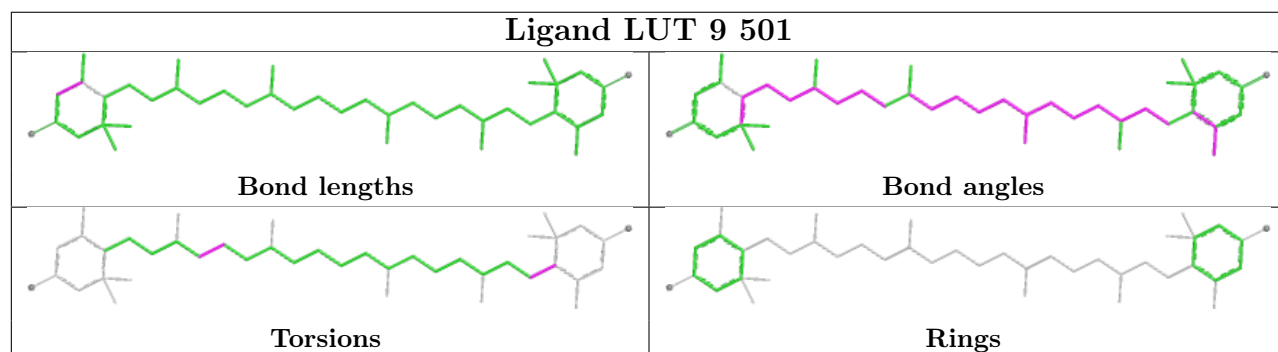
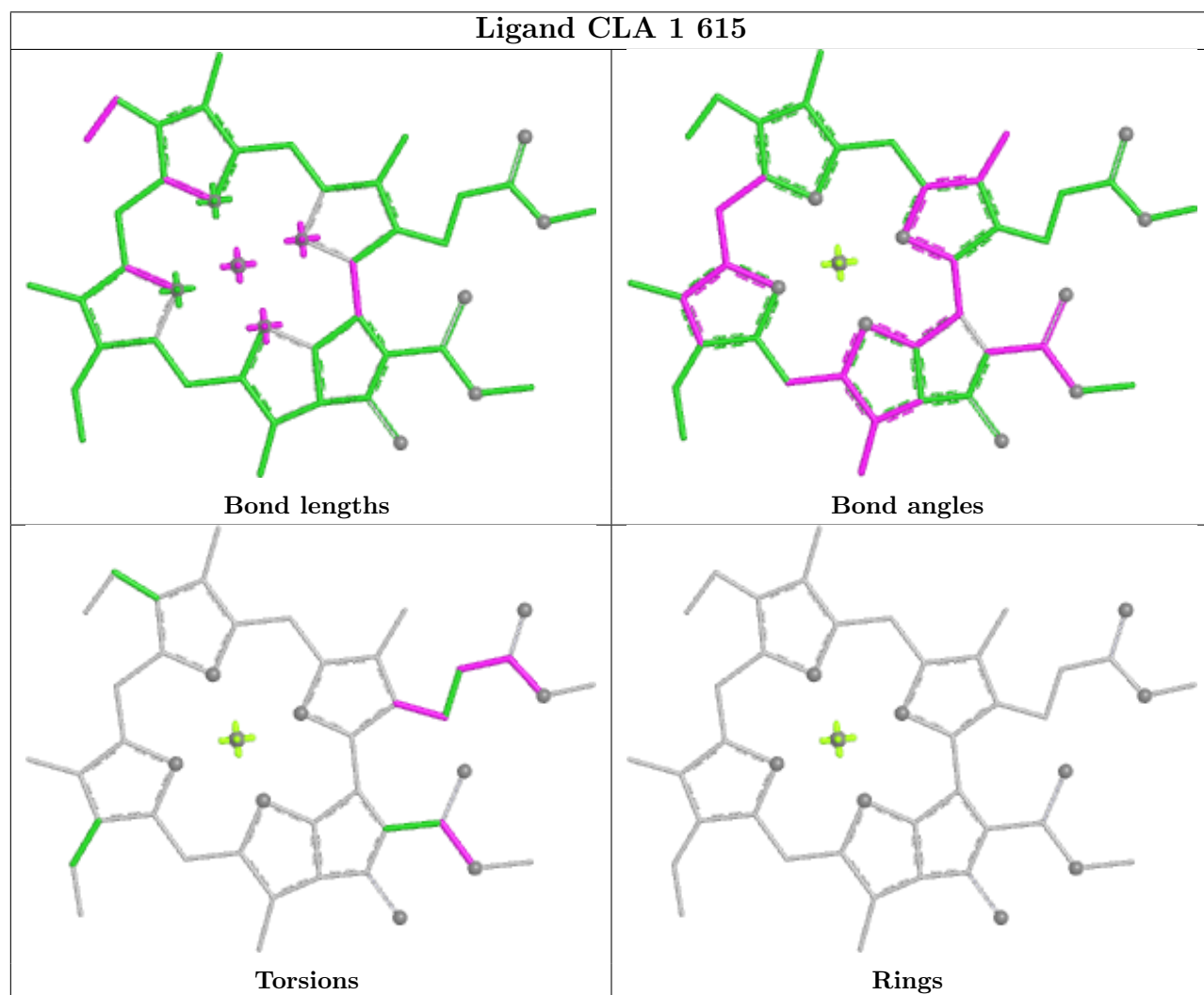
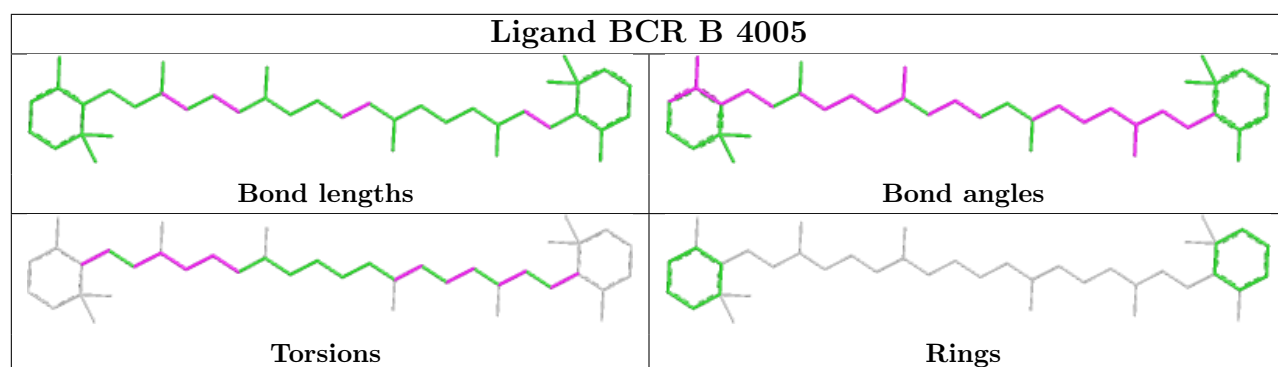
Bond angles



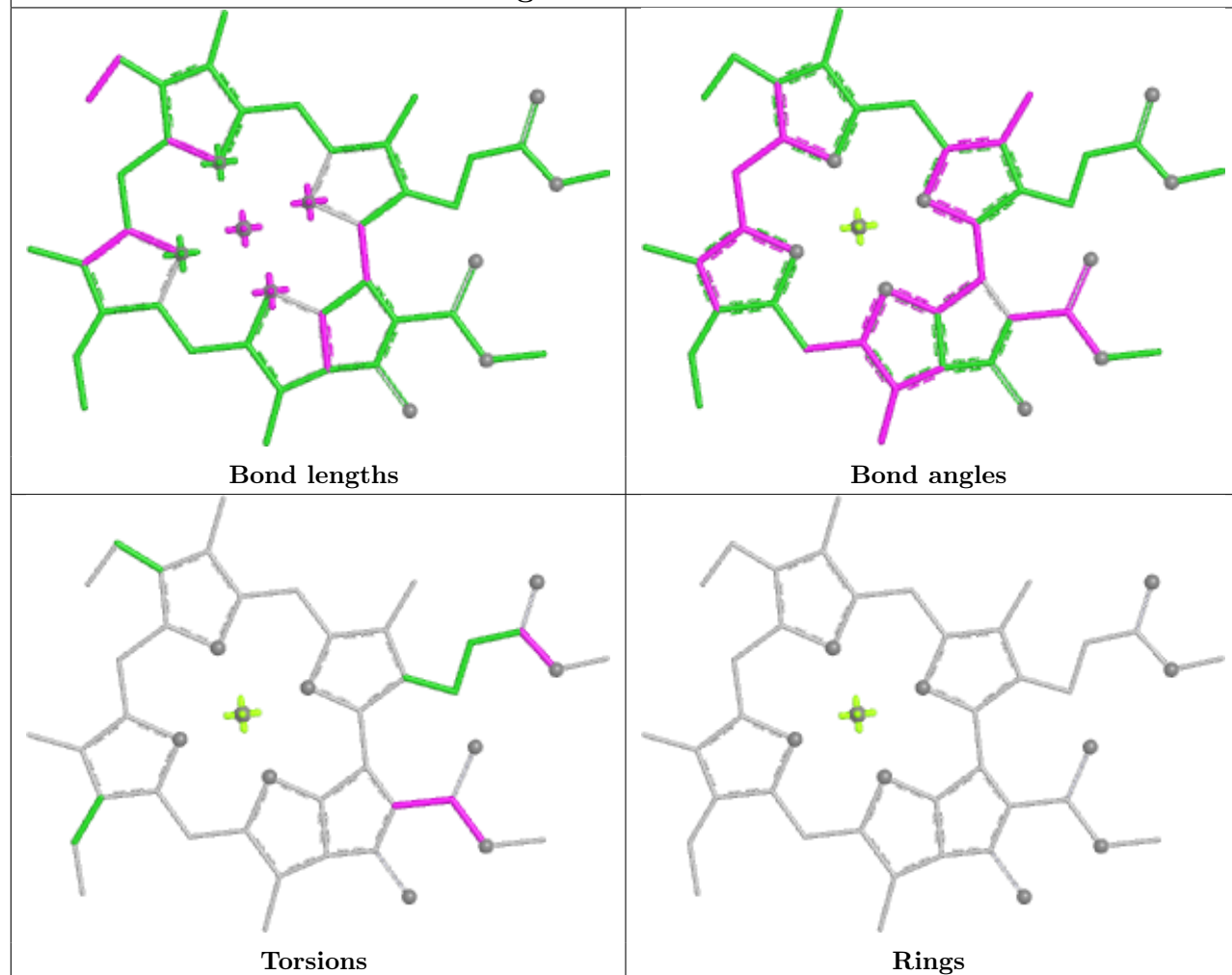
Torsions



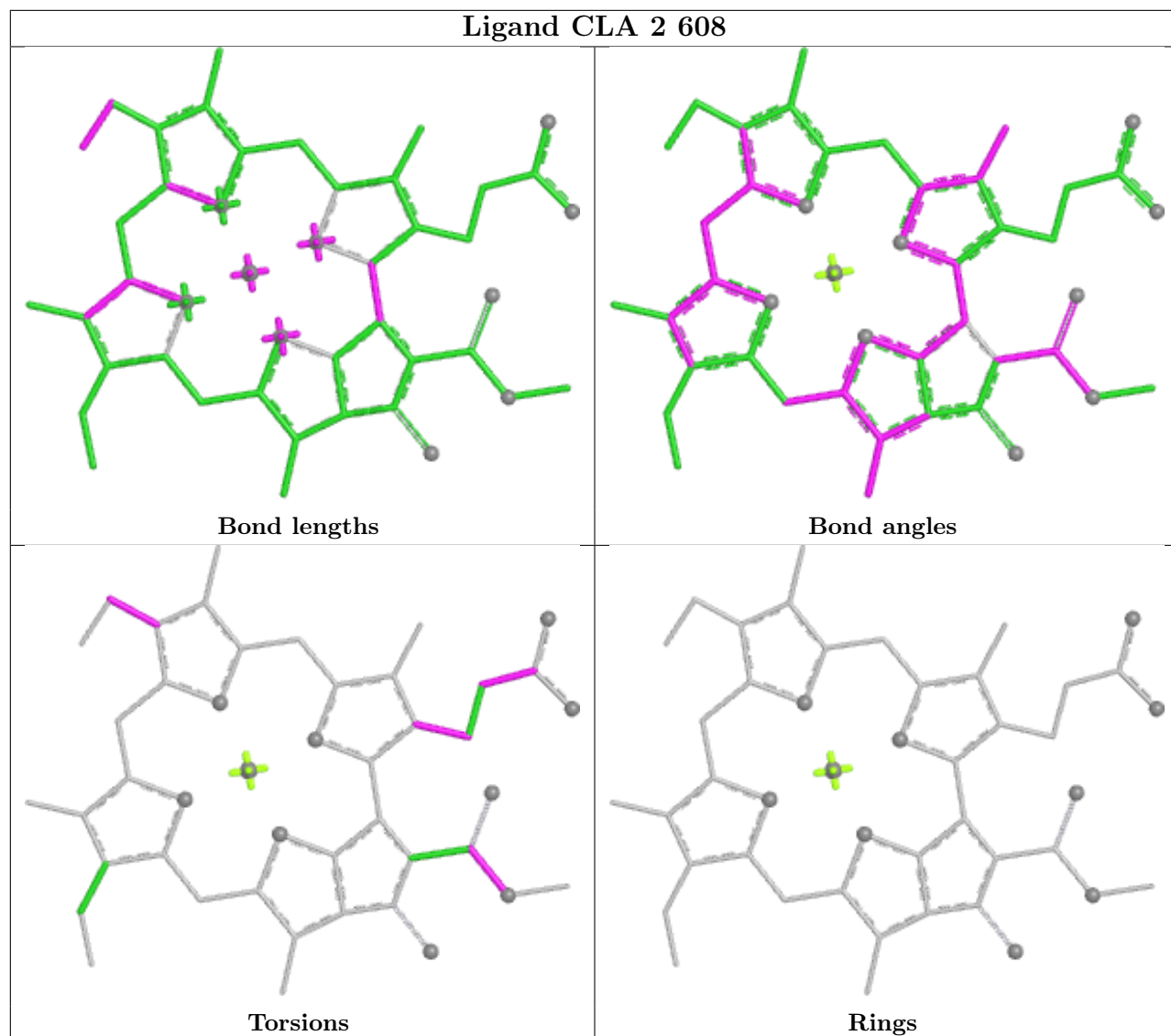
Rings



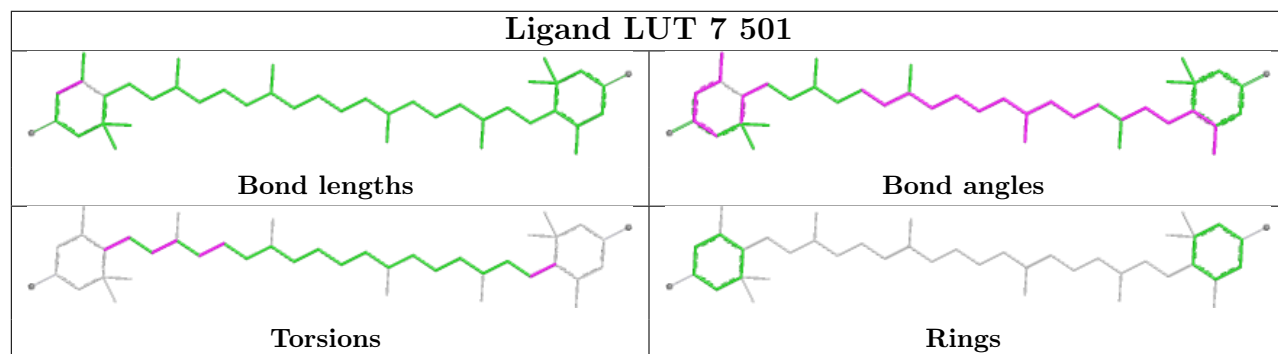
Ligand CLA 6 605

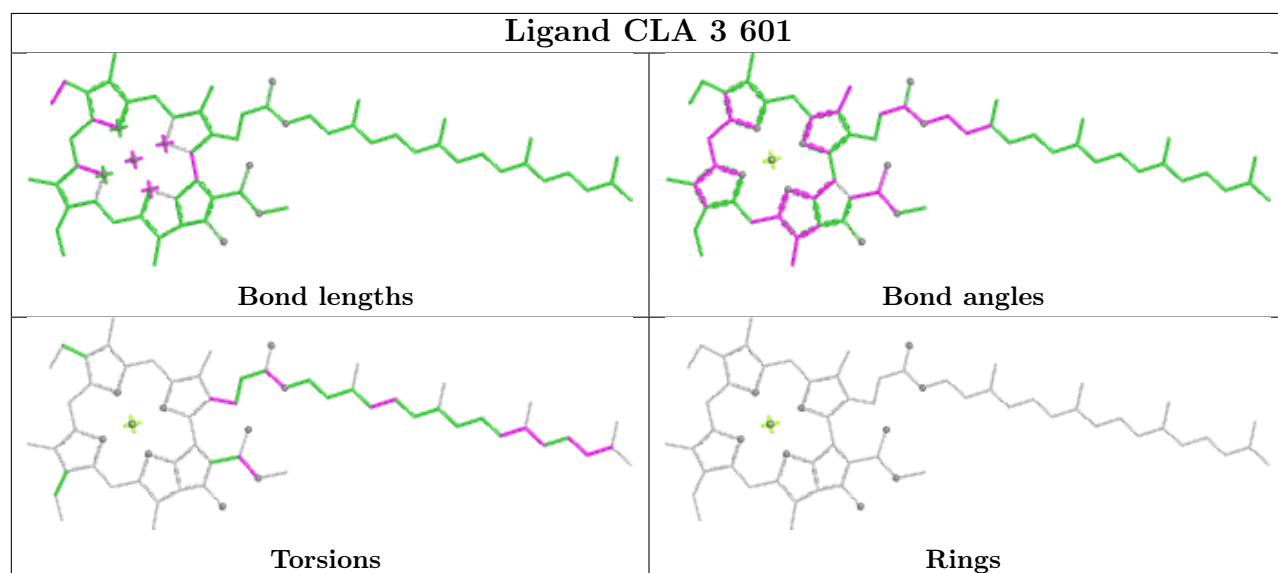
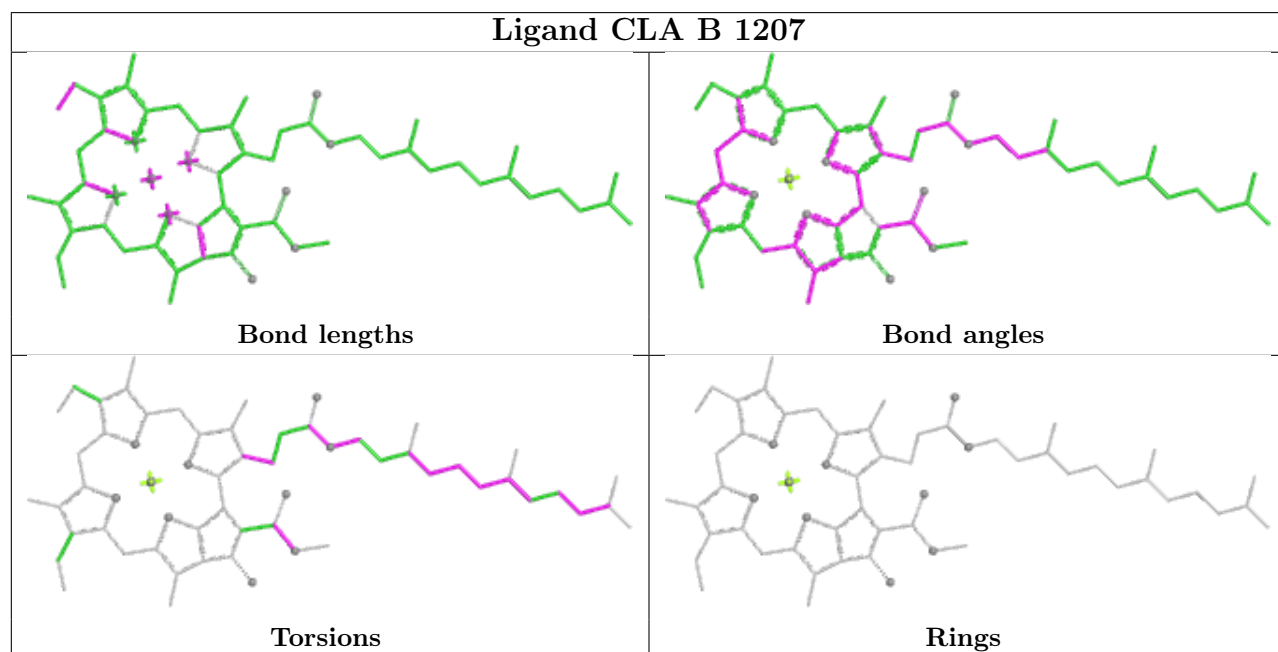
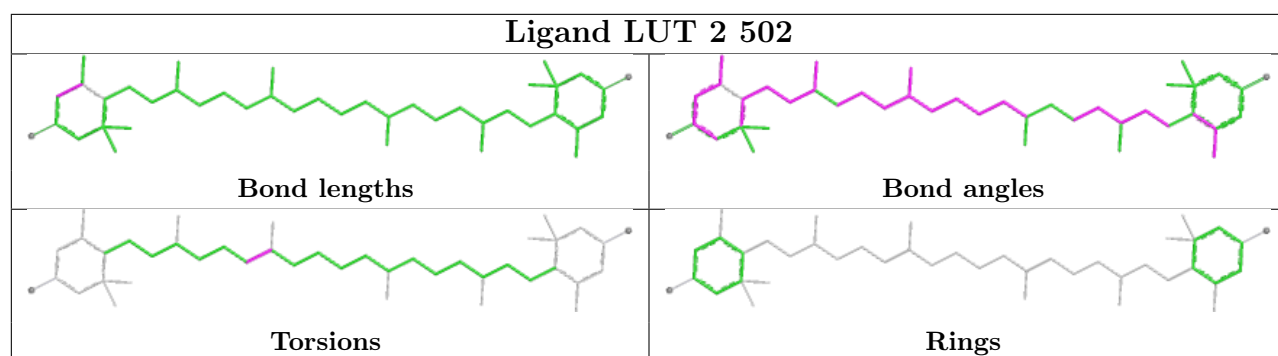


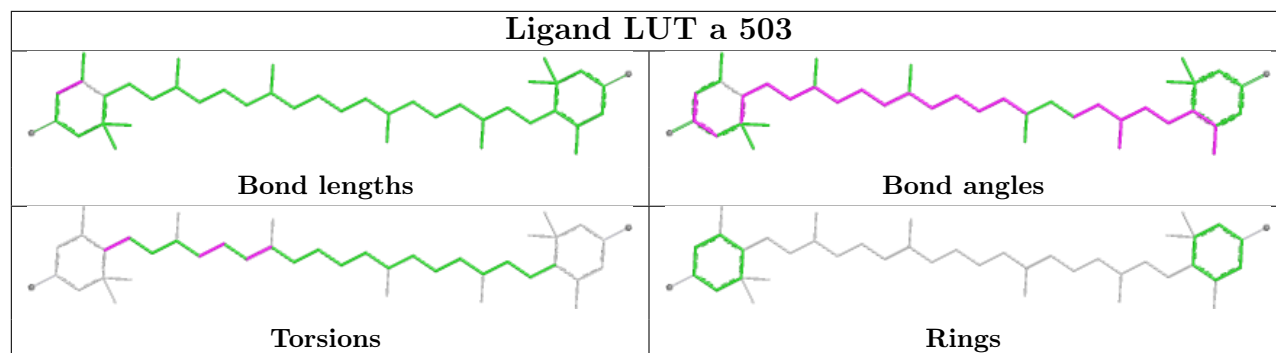
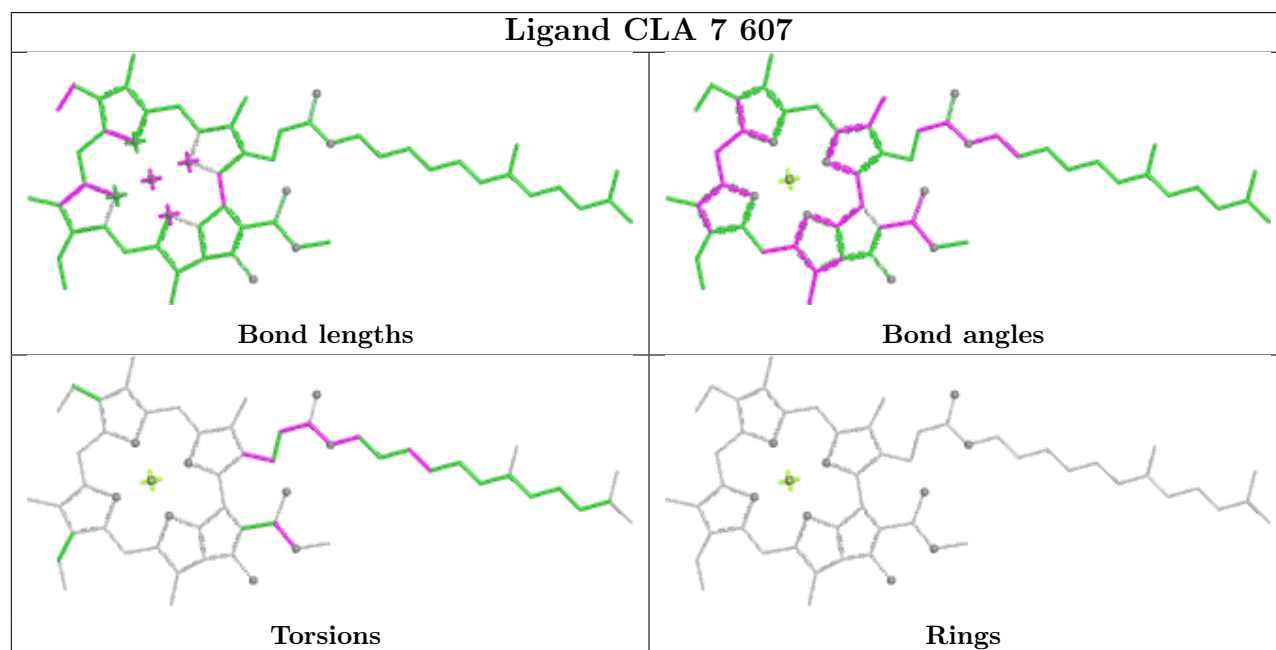
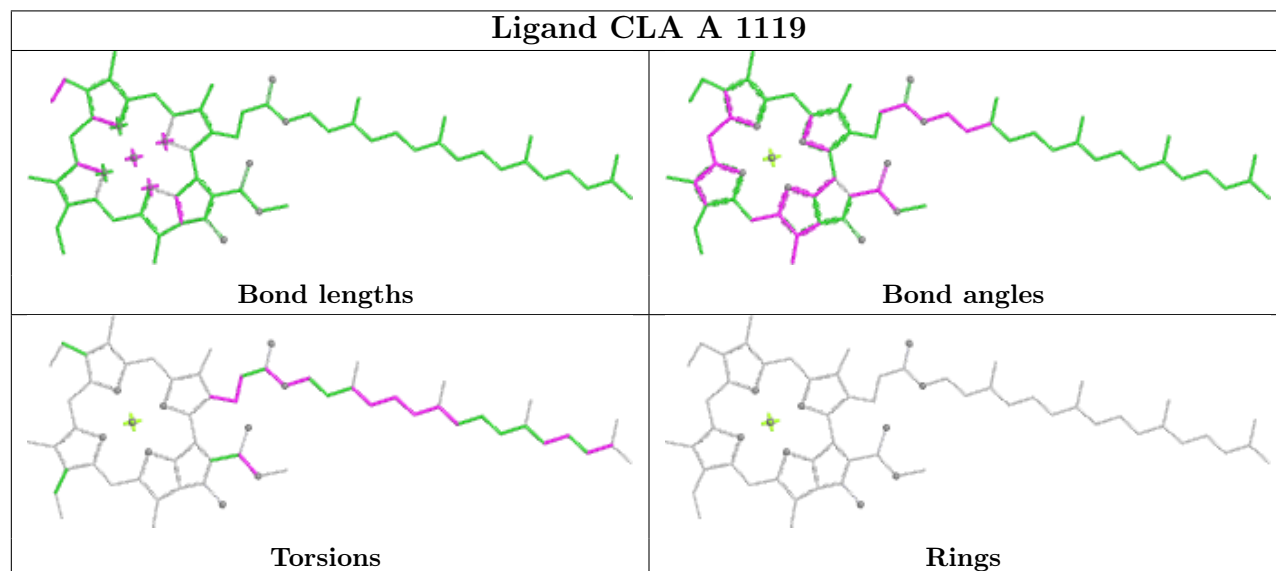
Ligand CLA 2 608

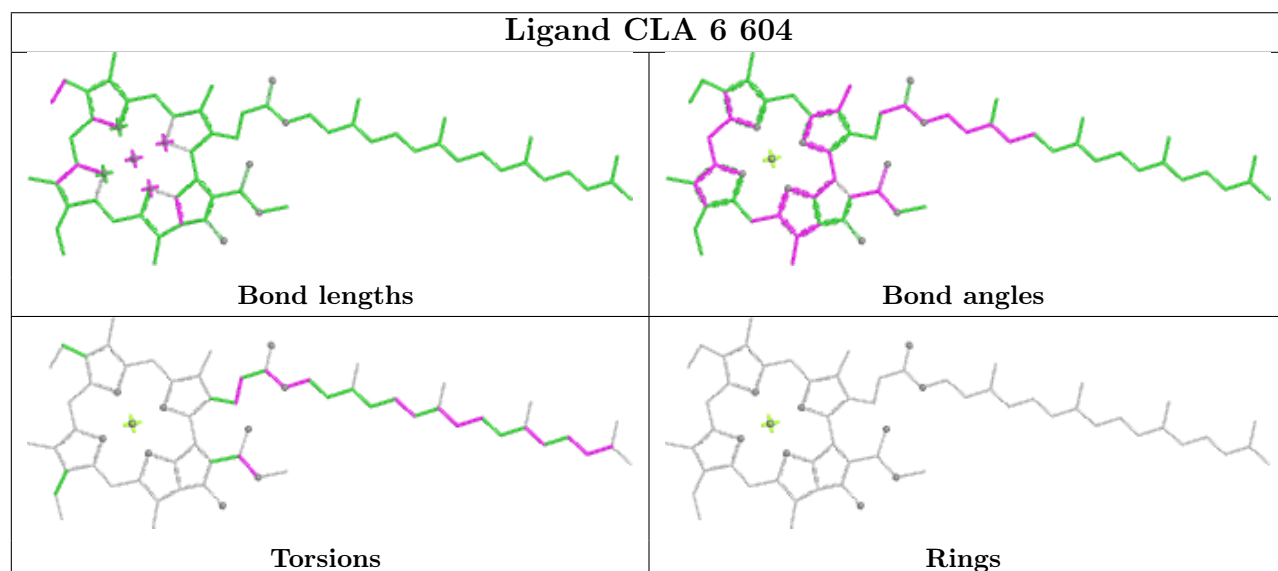
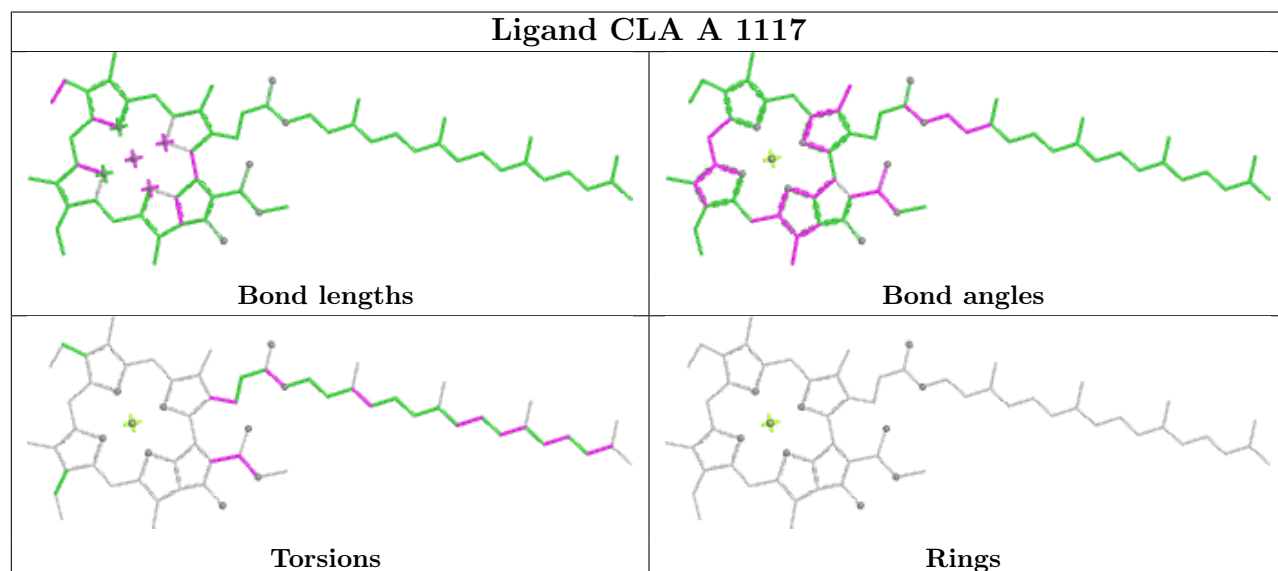
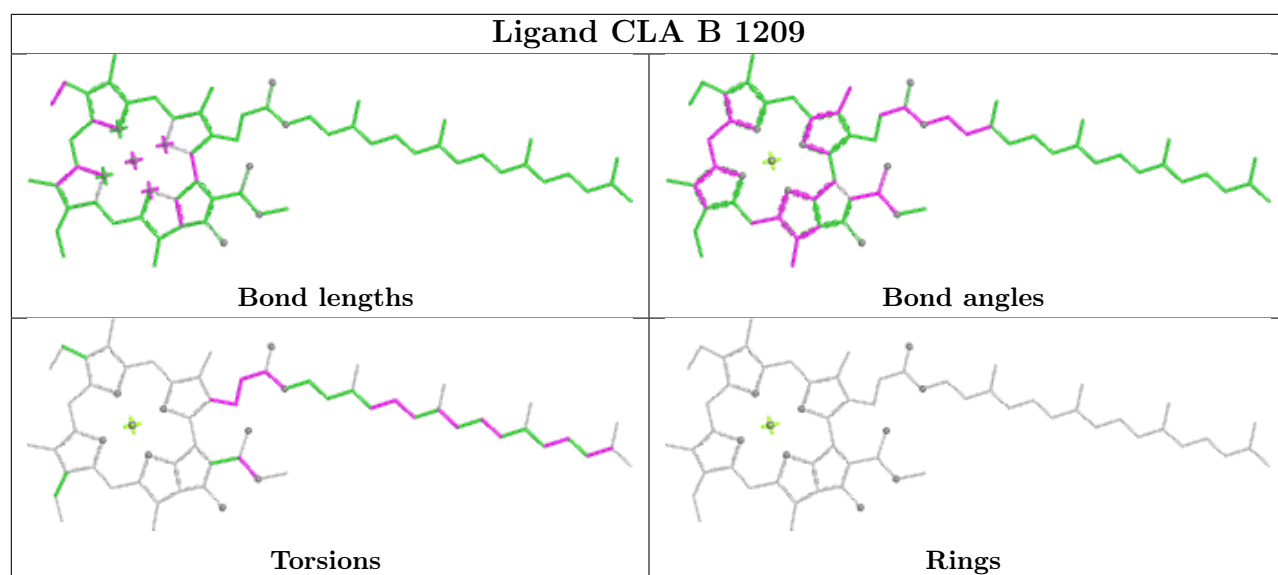


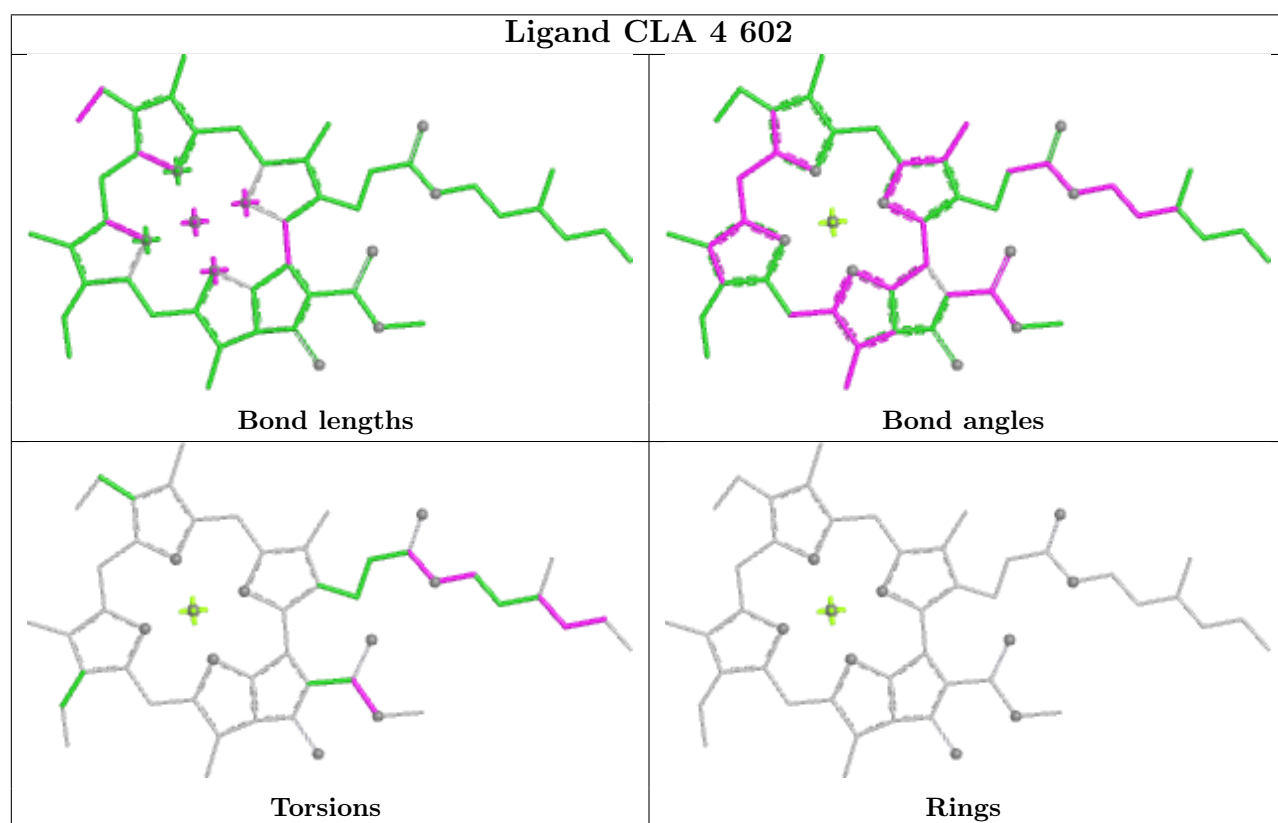
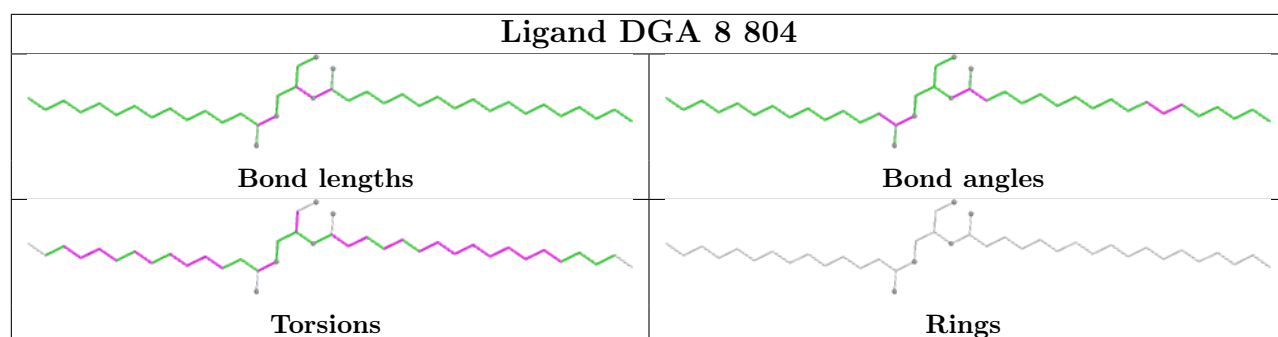
Ligand LUT 7 501



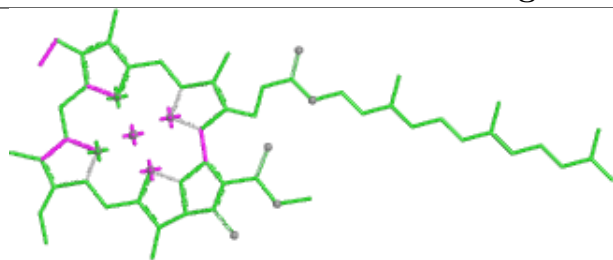


Ligand LUT a 503**Ligand CLA 7 607****Ligand CLA A 1119**

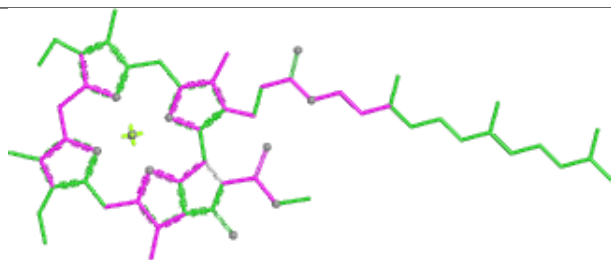




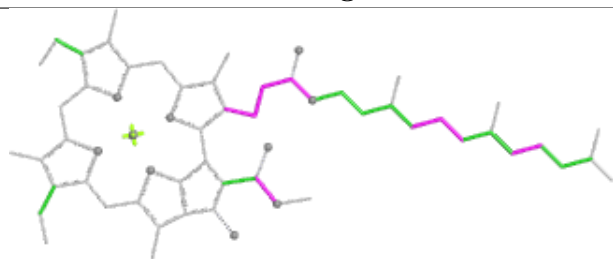
Ligand CLA 6 601



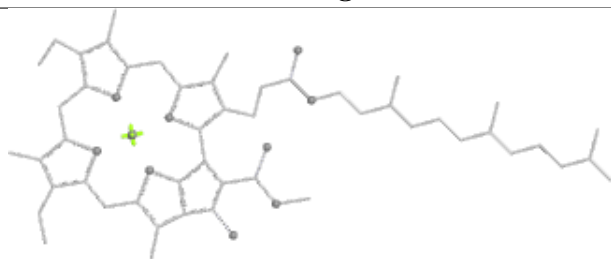
Bond lengths



Bond angles

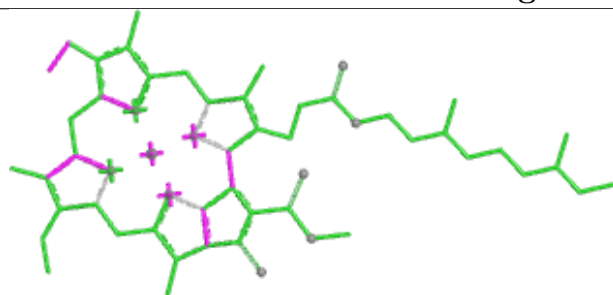


Torsions

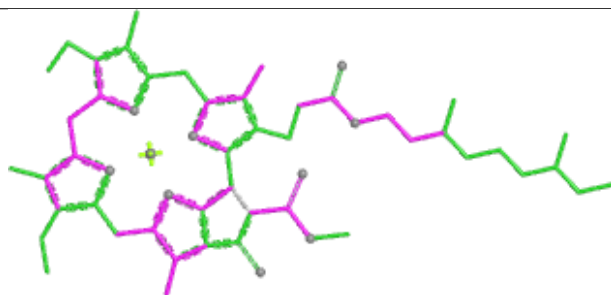


Rings

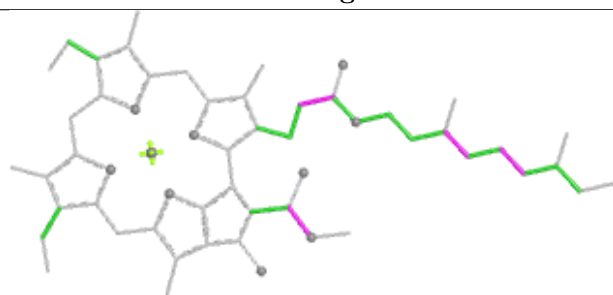
Ligand CLA 4 603



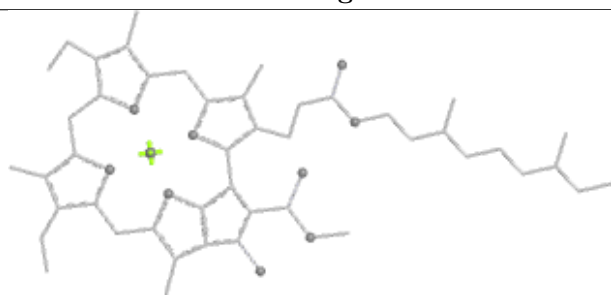
Bond lengths



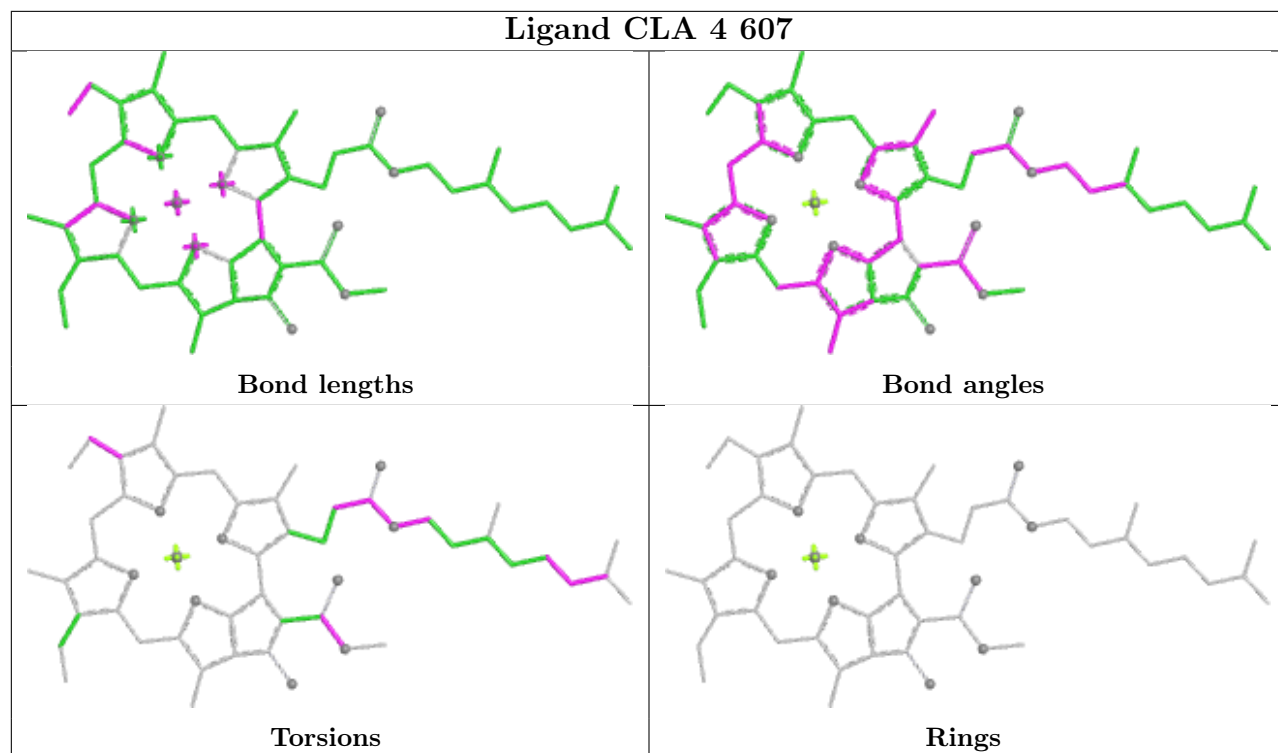
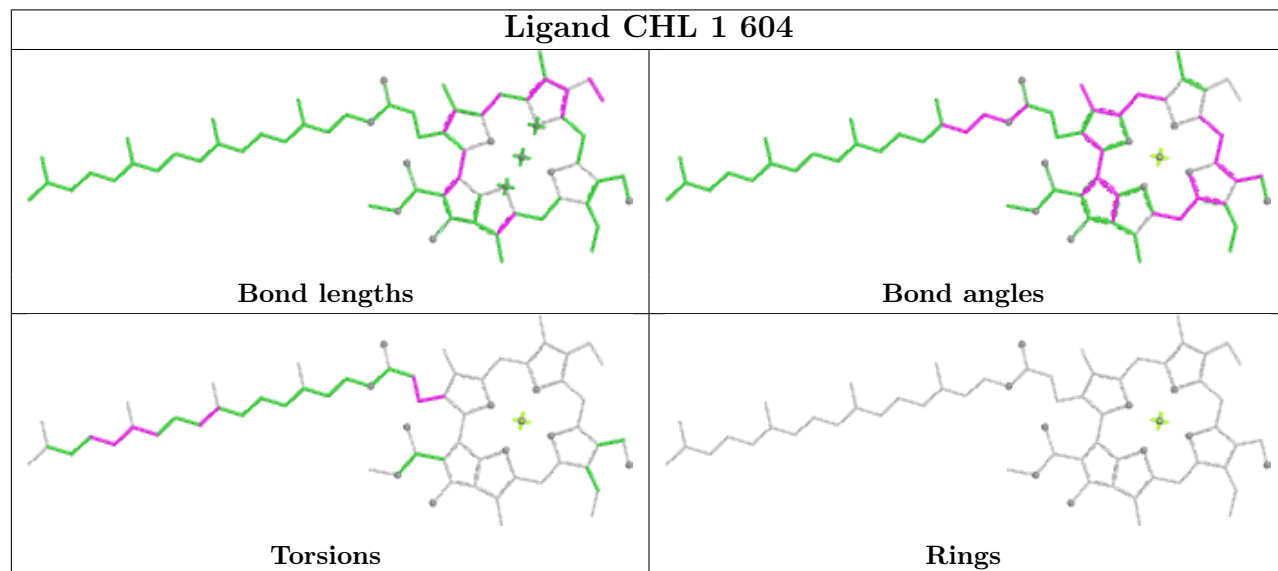
Bond angles



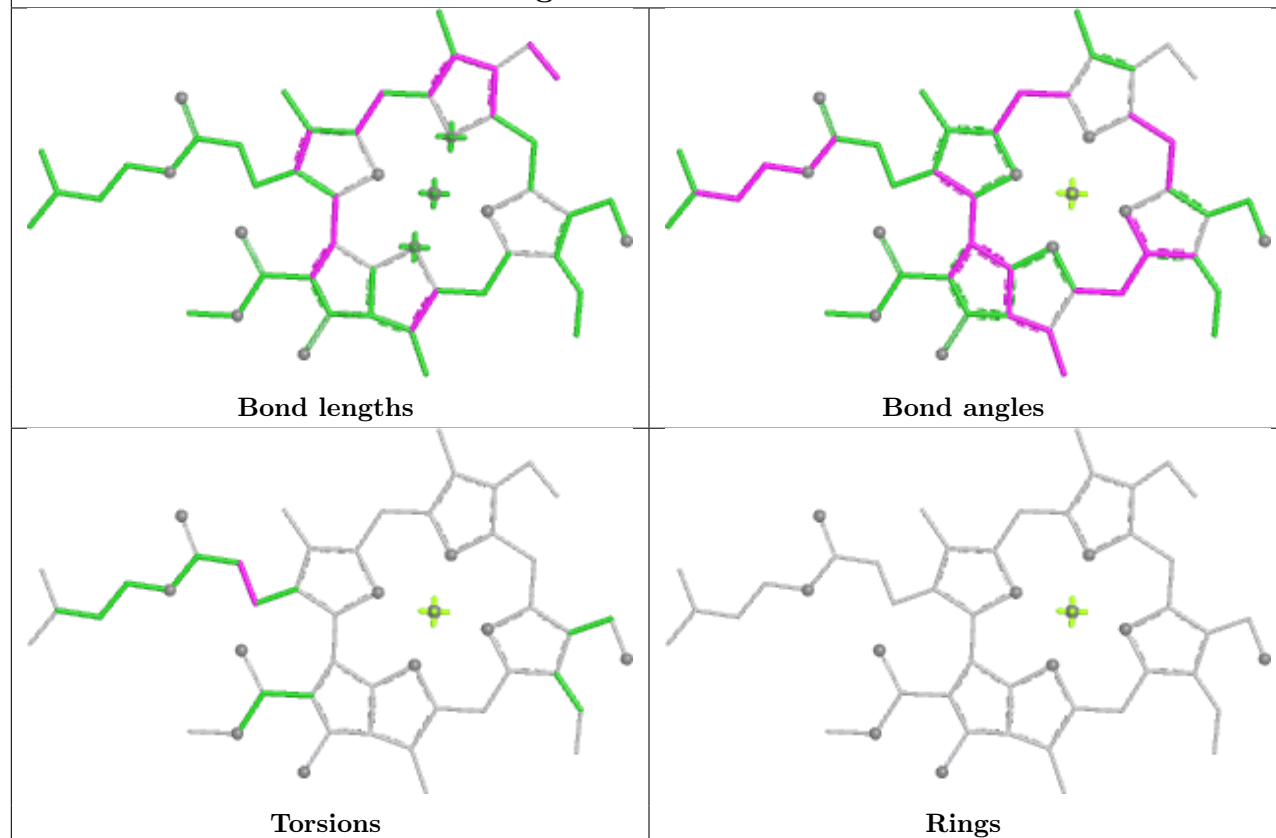
Torsions



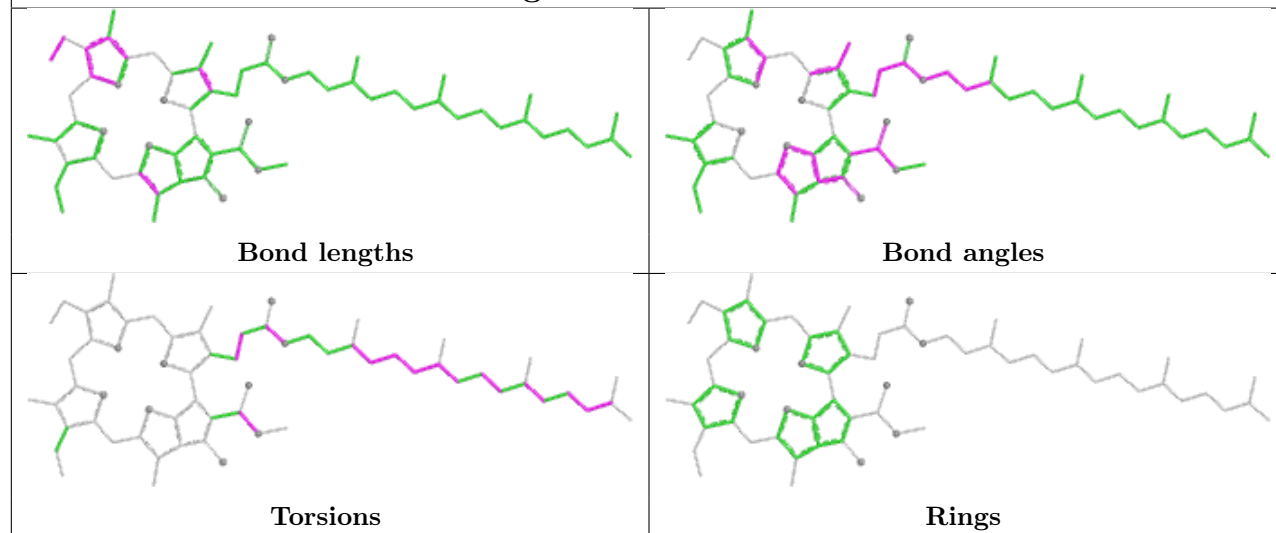
Rings

Ligand CLA 4 607**Ligand CHL 1 604**

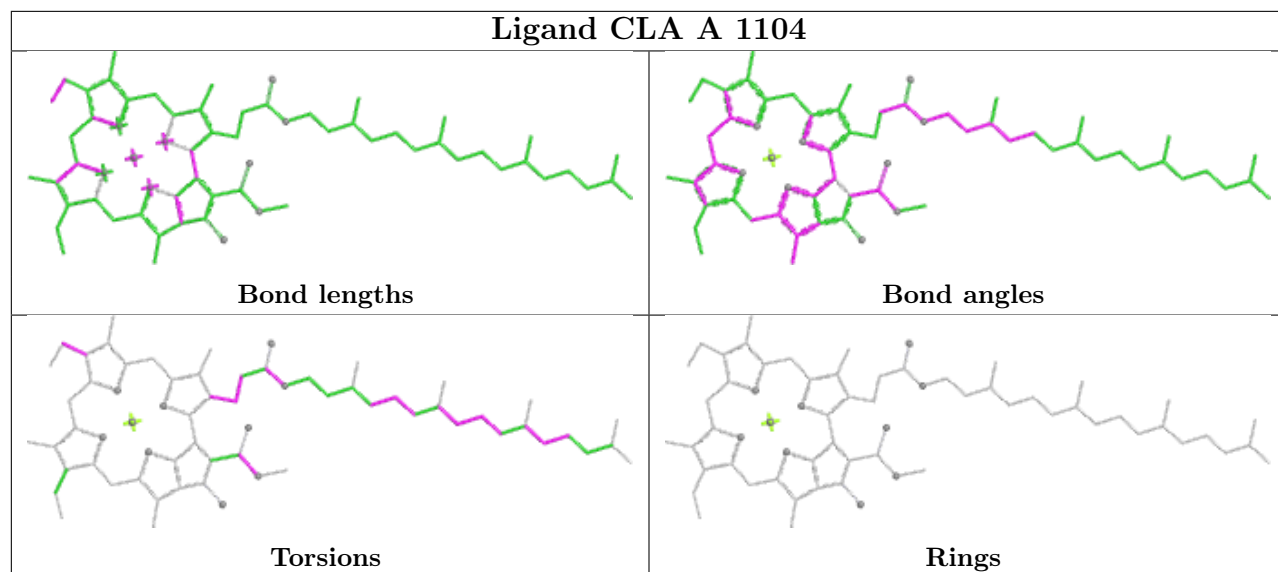
Ligand CHL 2 613



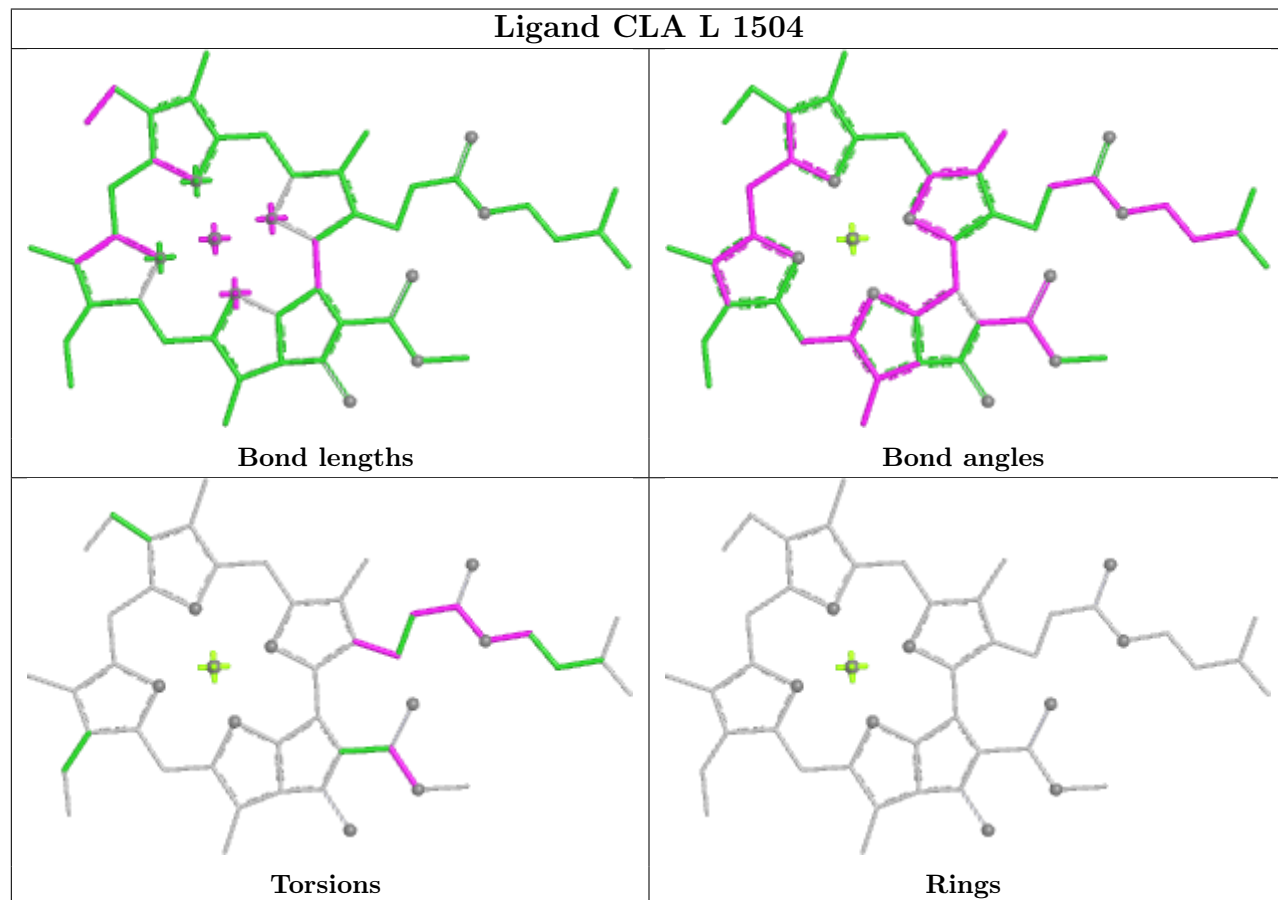
Ligand CLA B 1234

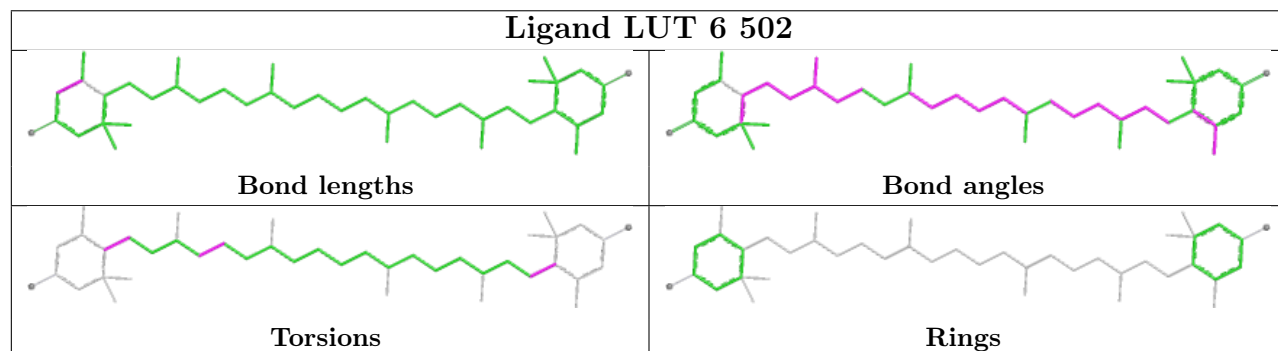
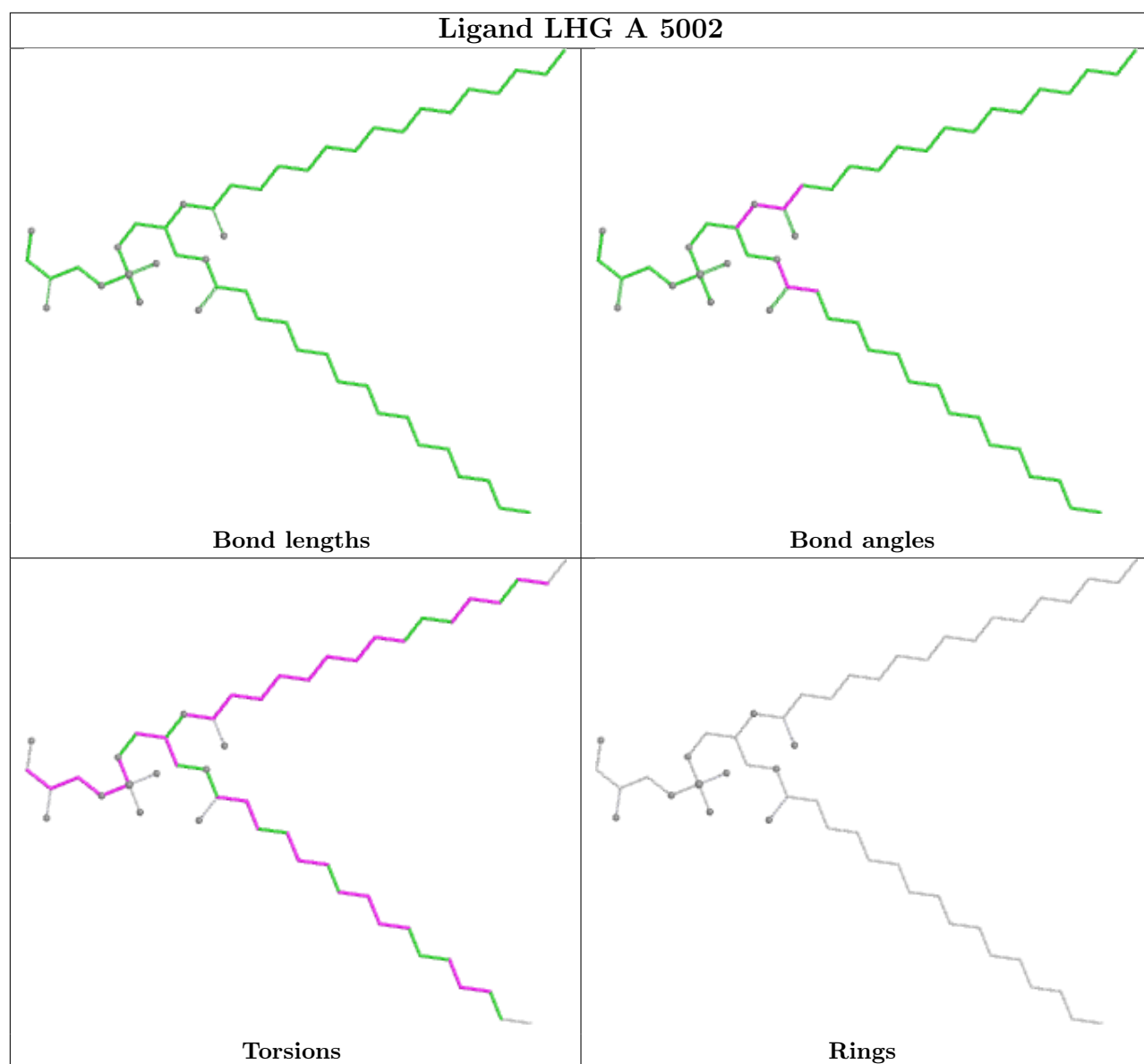


Ligand CLA A 1104

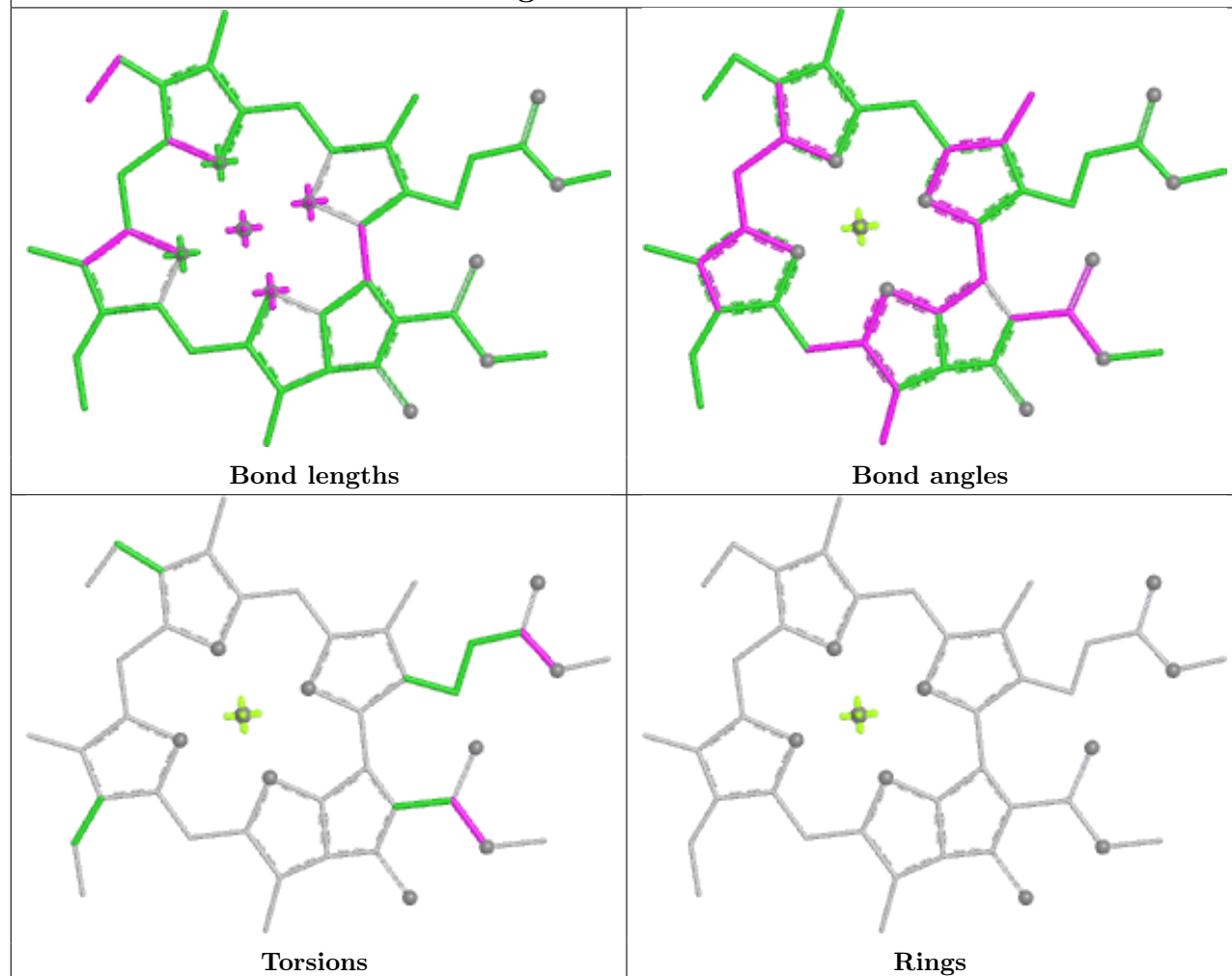


Ligand CLA L 1504

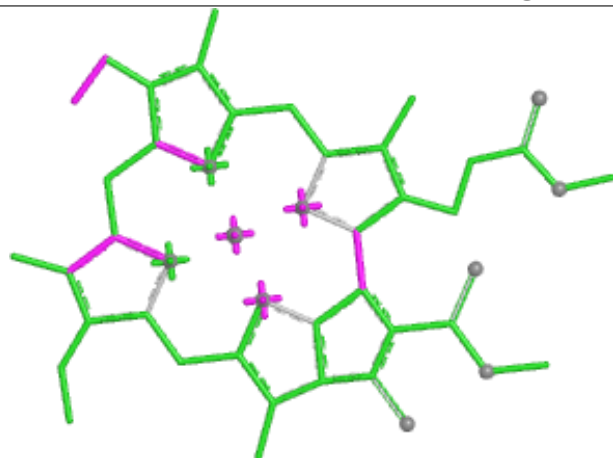




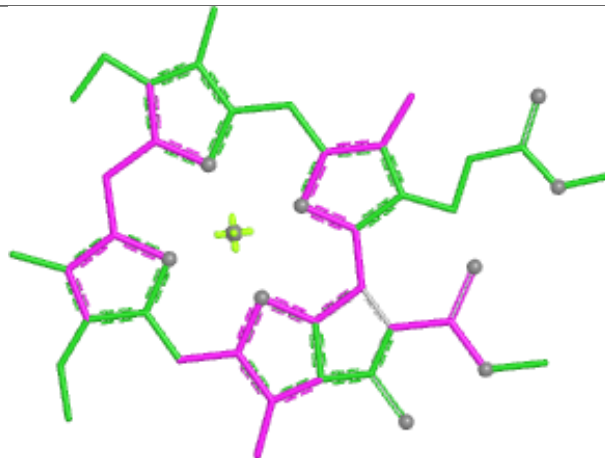
Ligand CLA a 615



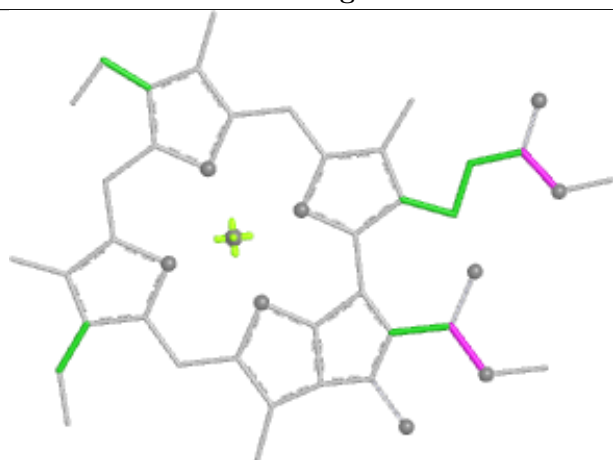
Ligand CLA 2 606



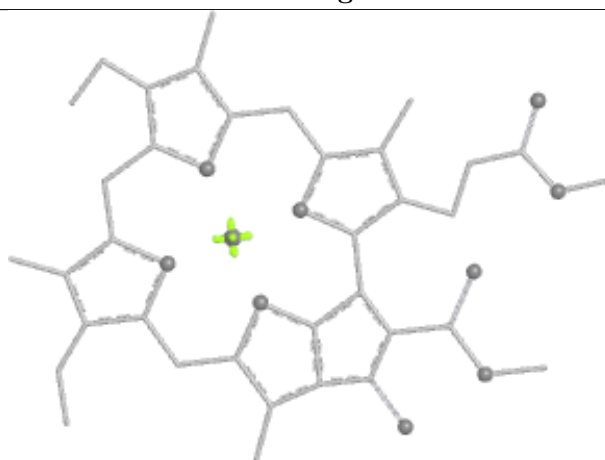
Bond lengths



Bond angles

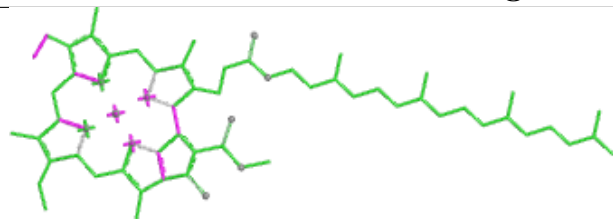


Torsions

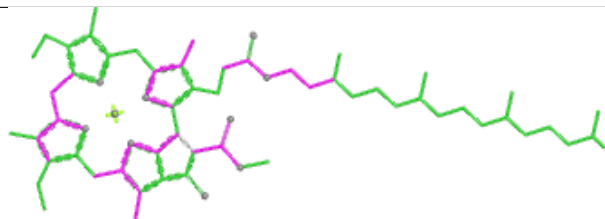


Rings

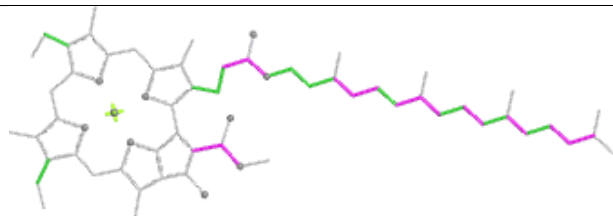
Ligand CLA A 1128



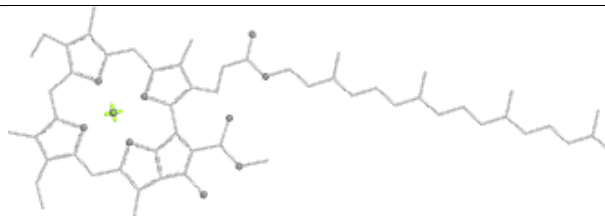
Bond lengths



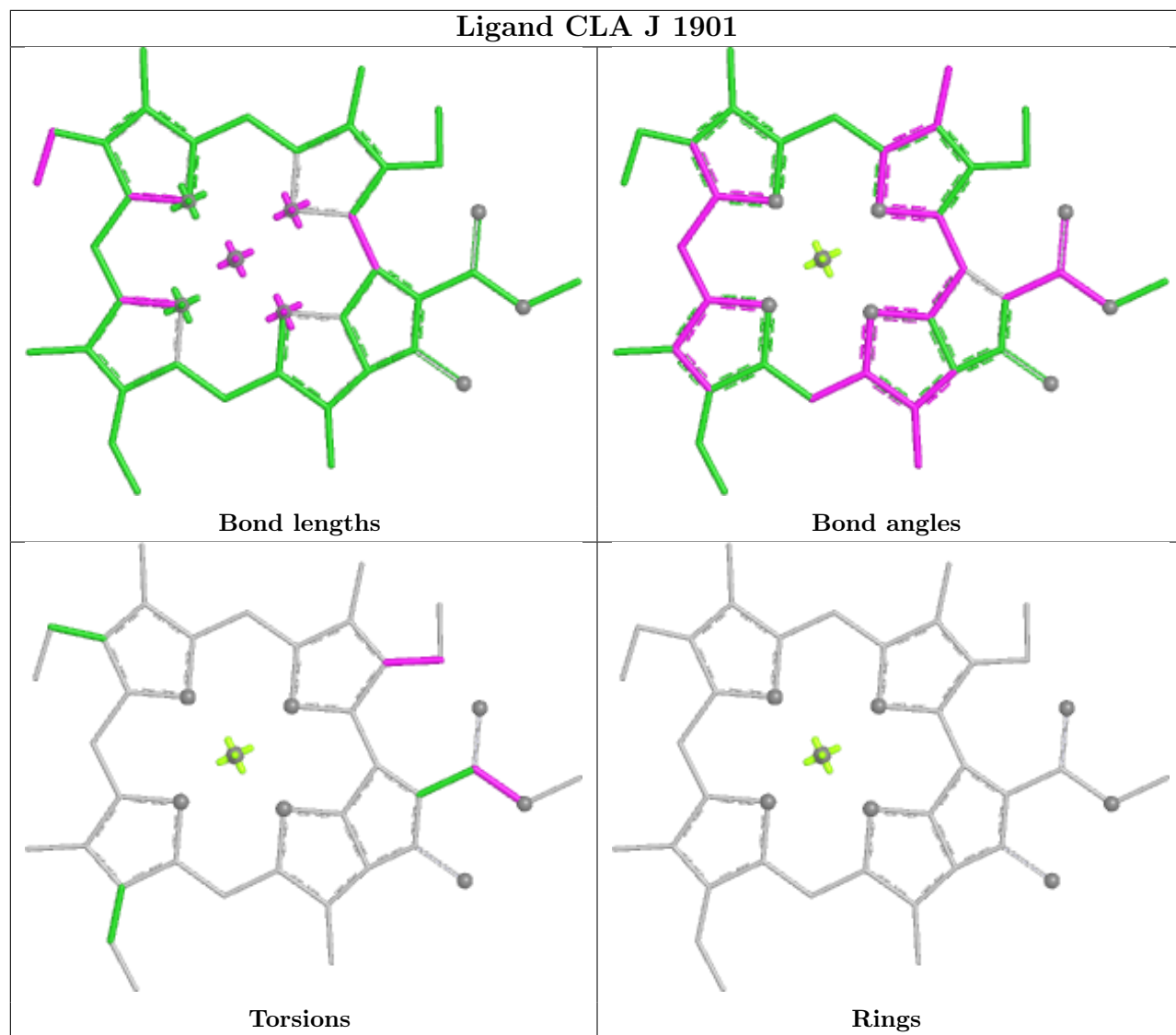
Bond angles

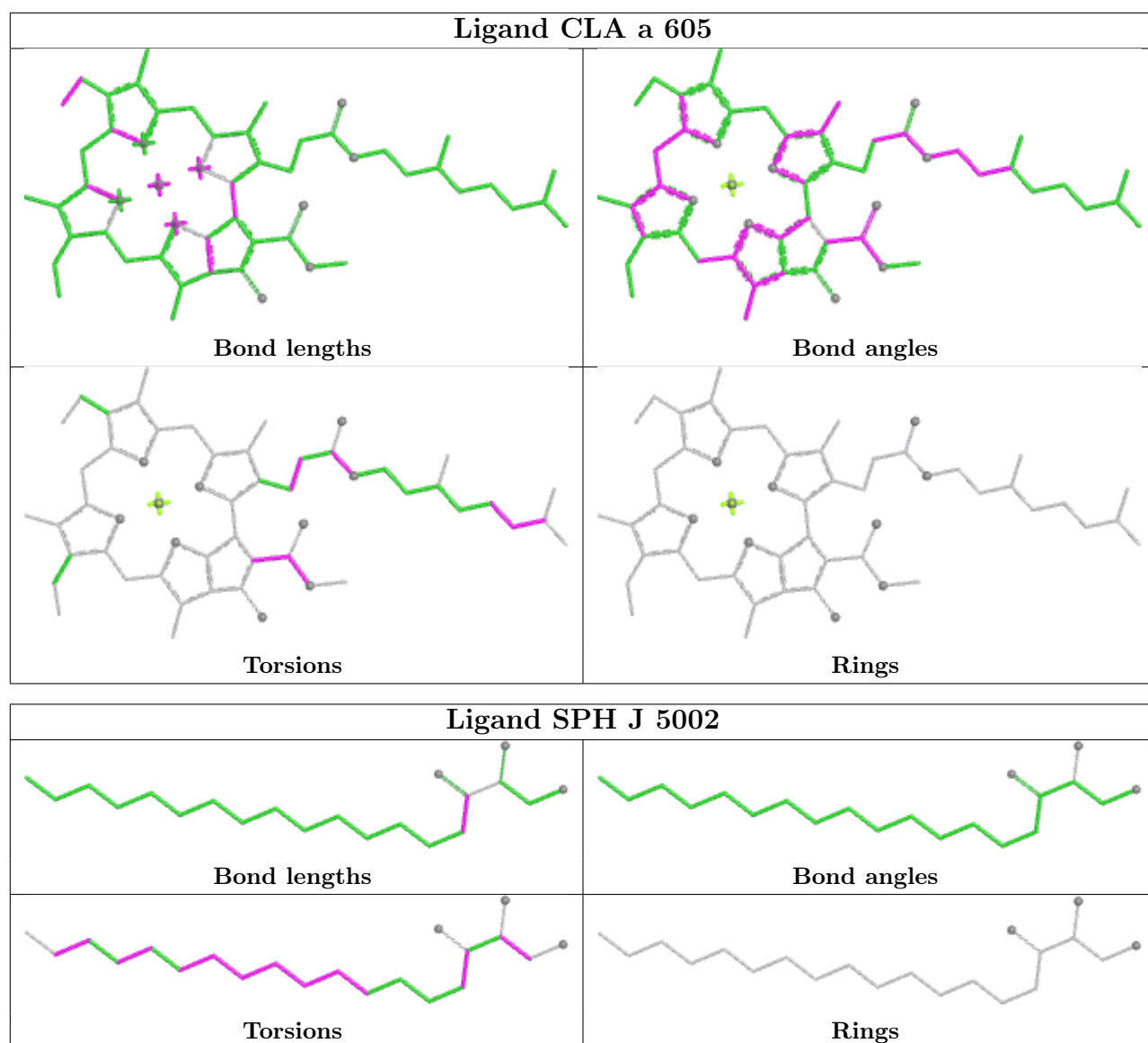


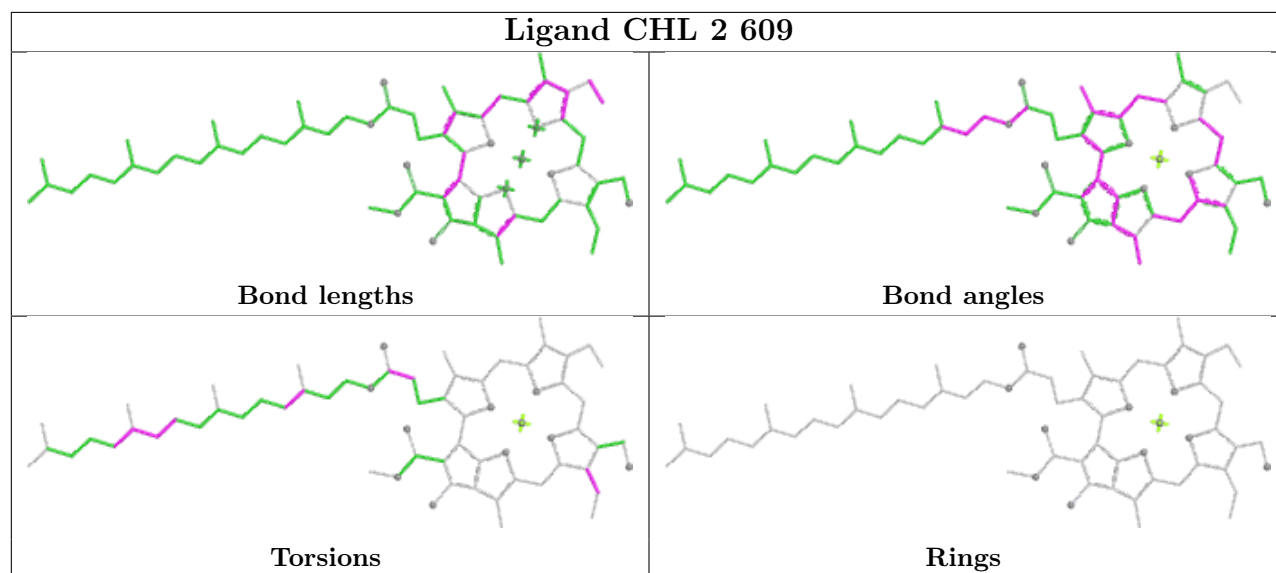
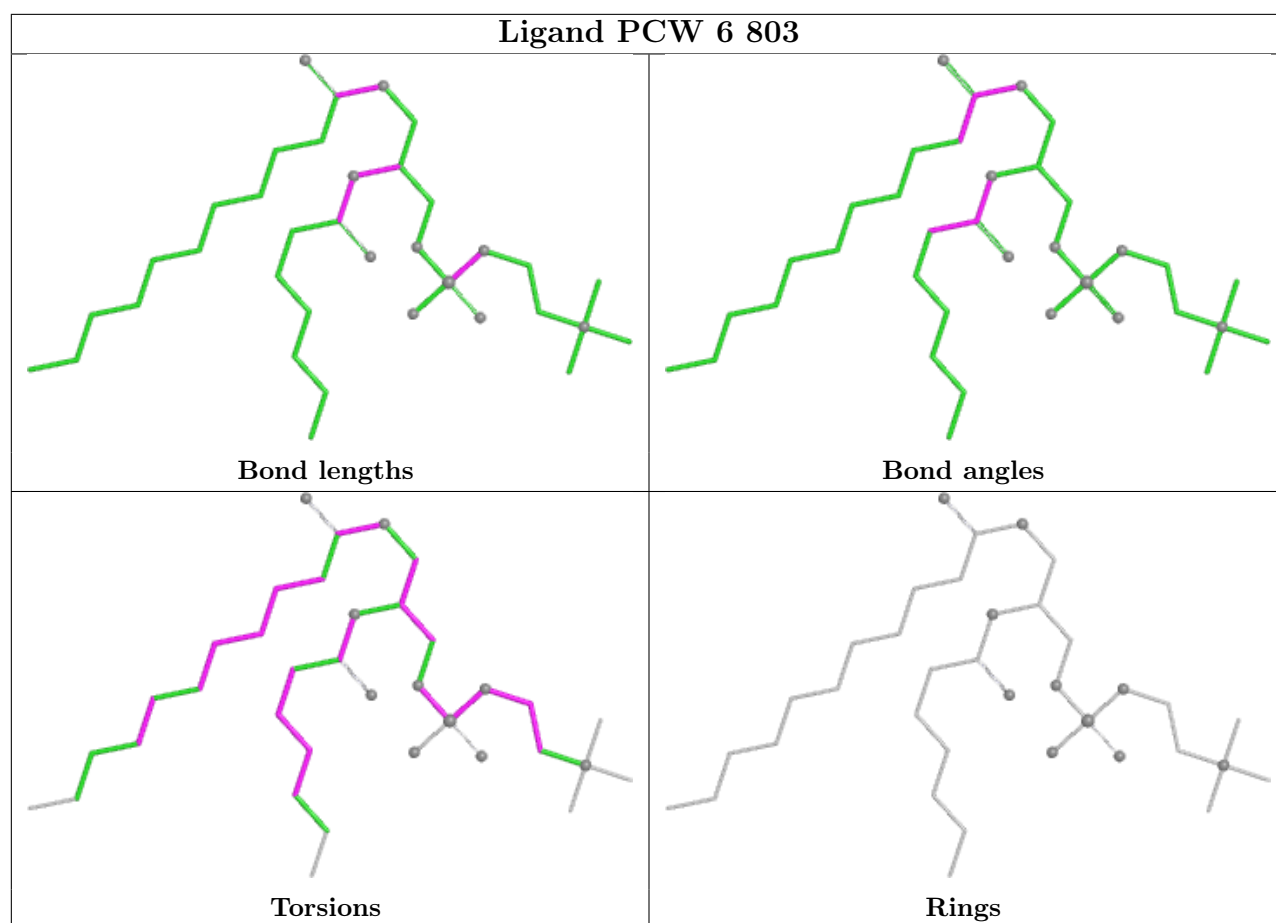
Torsions

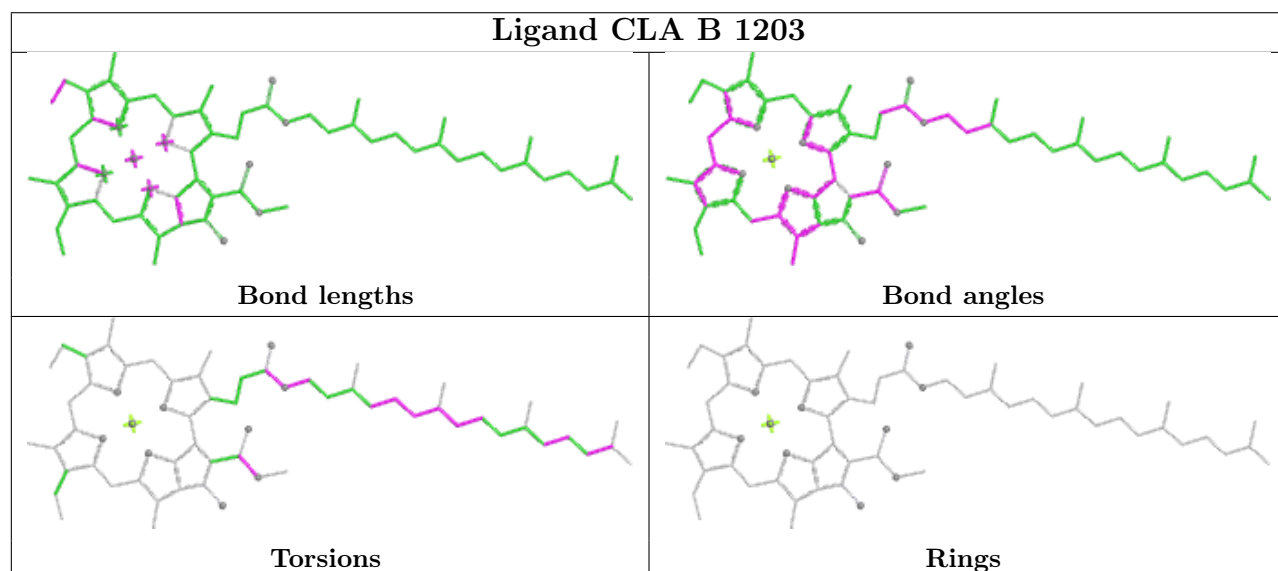
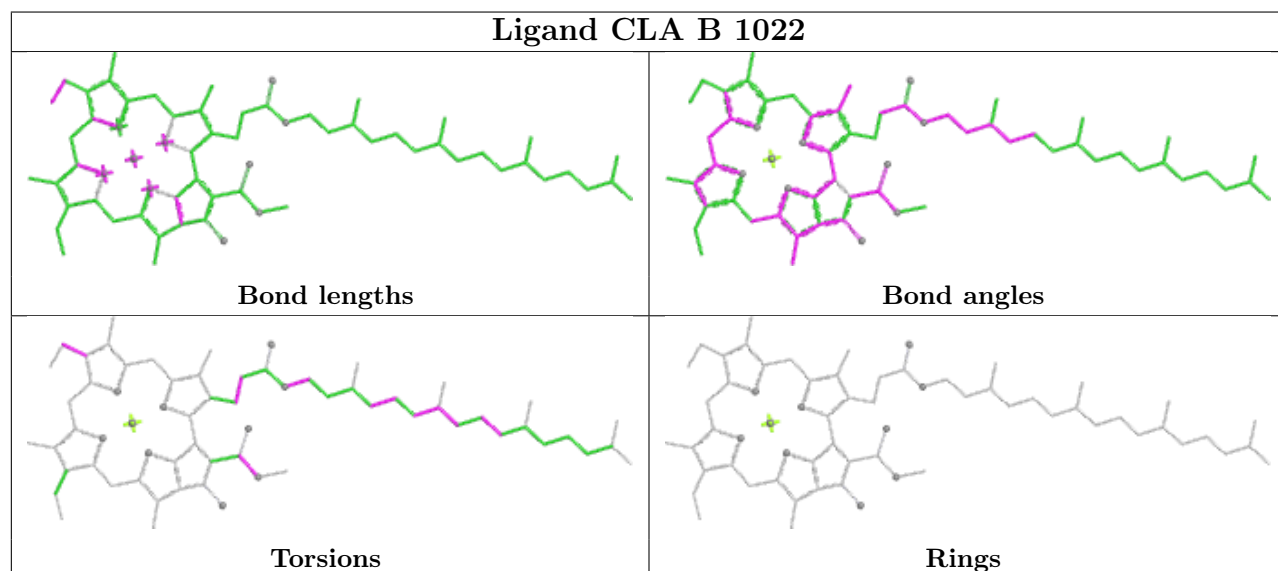
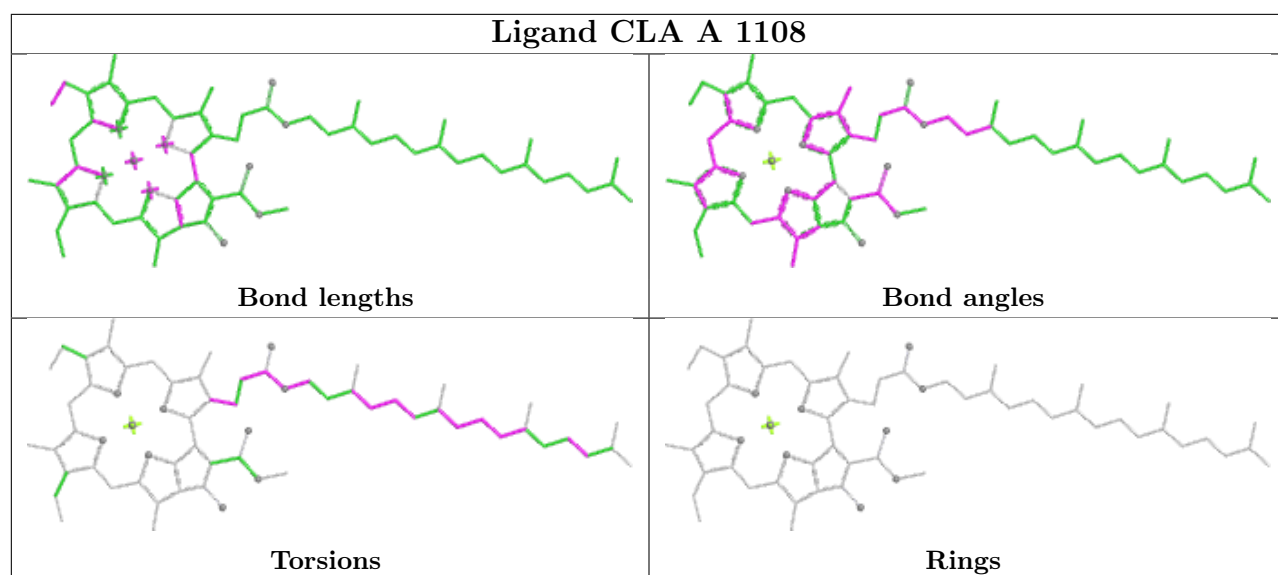


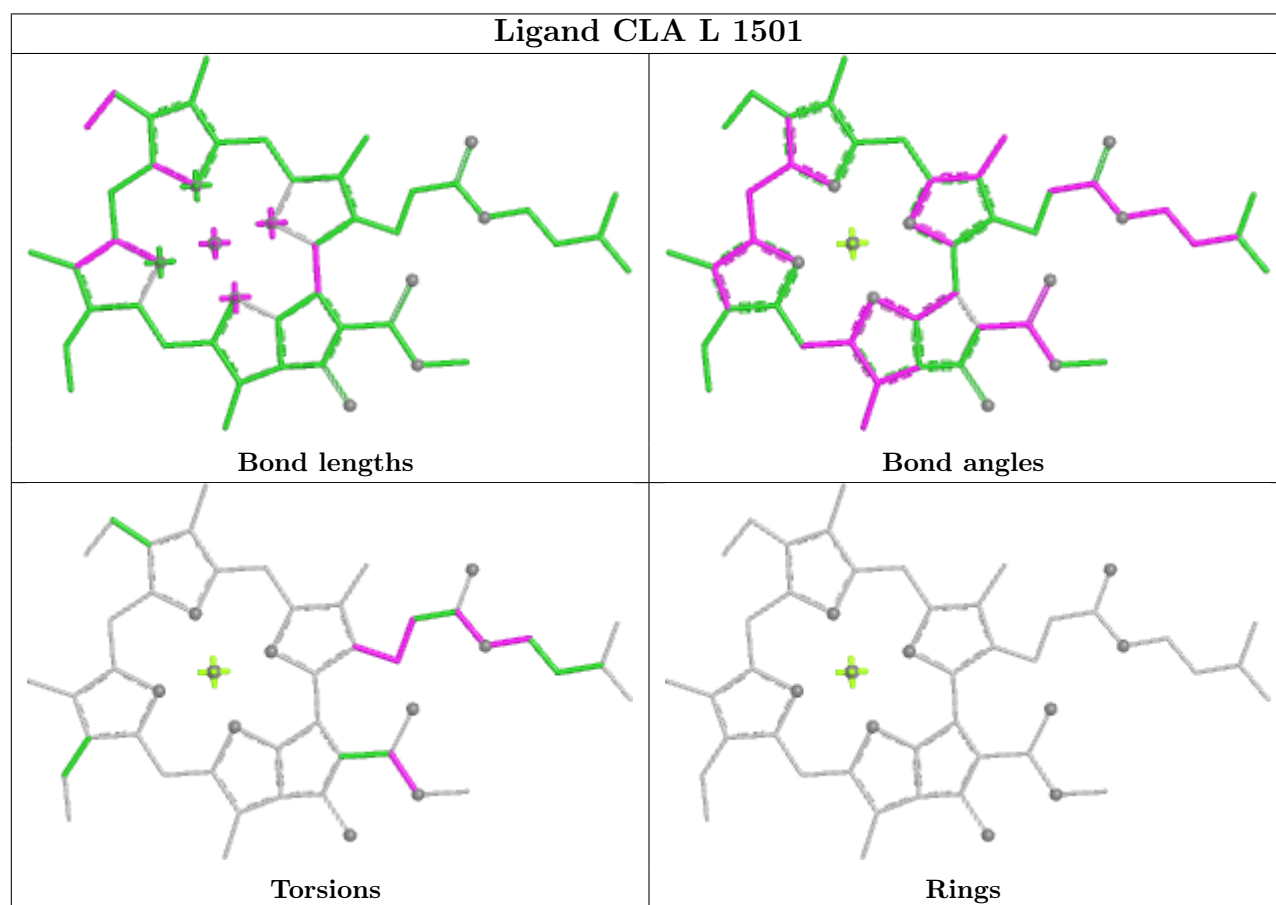
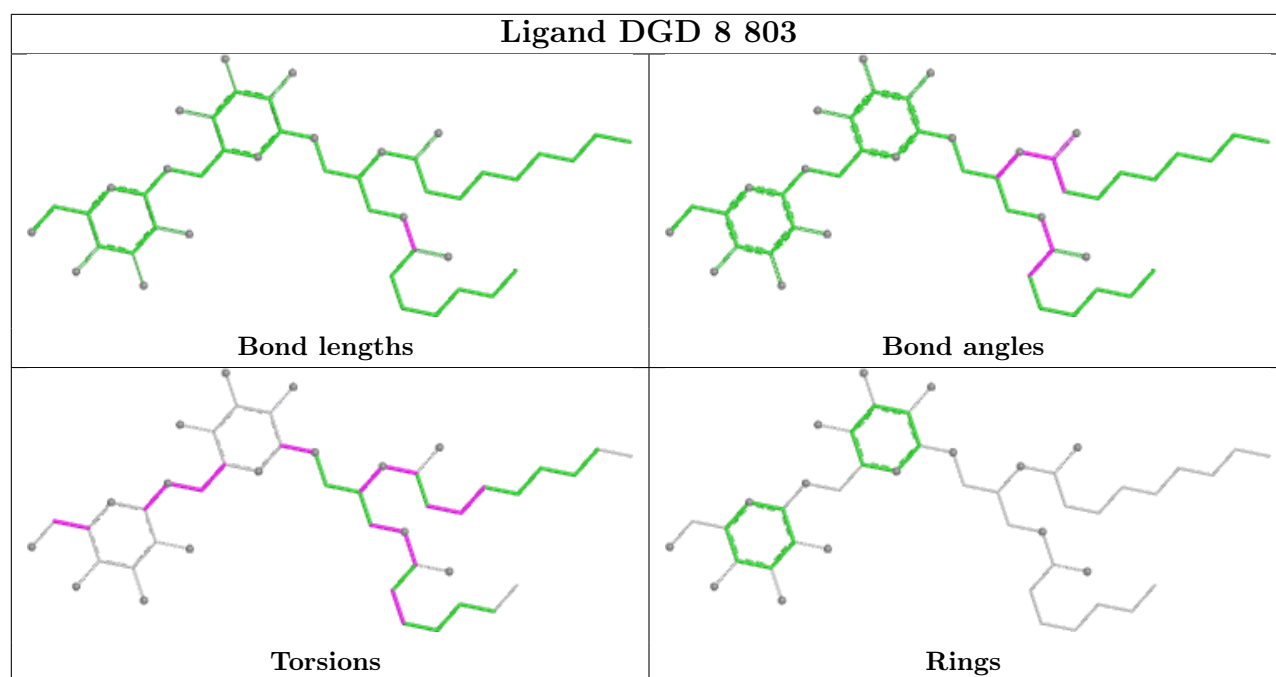
Rings



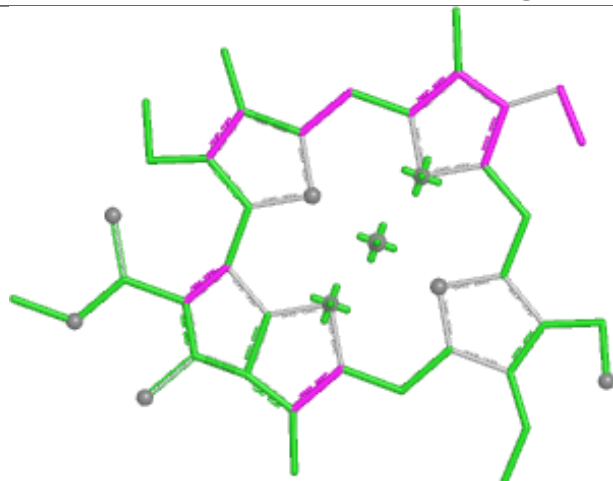




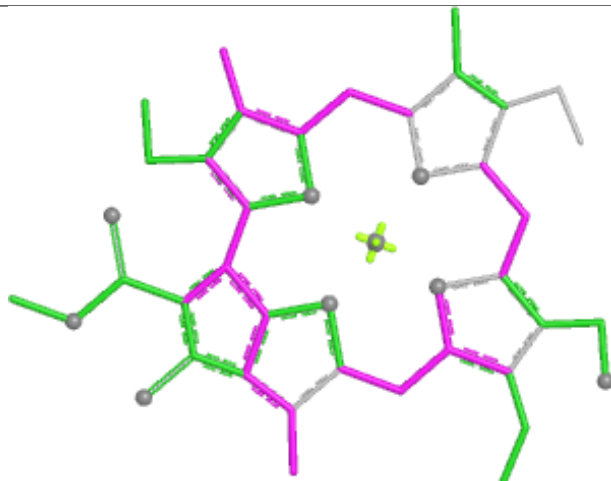




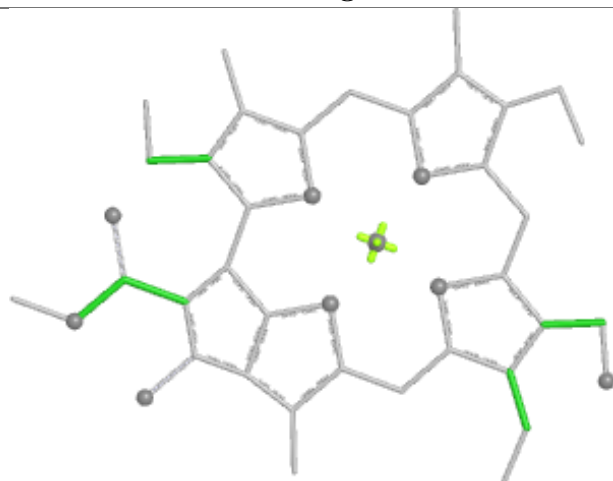
Ligand CHL 6 617



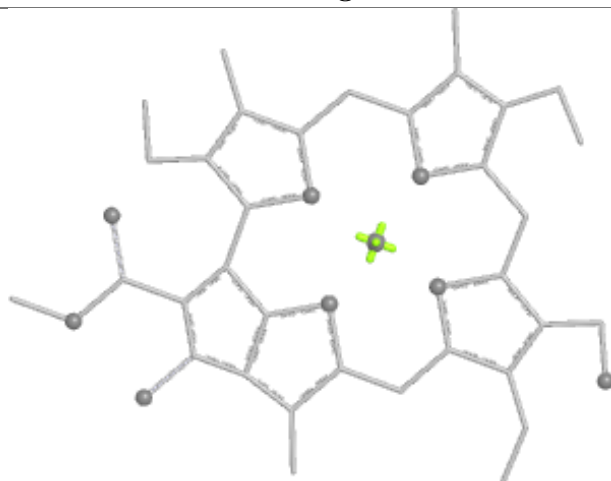
Bond lengths



Bond angles

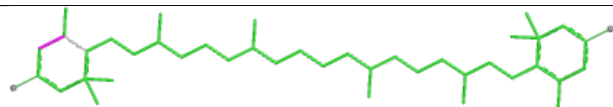


Torsions

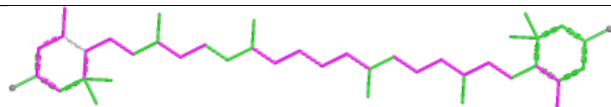


Rings

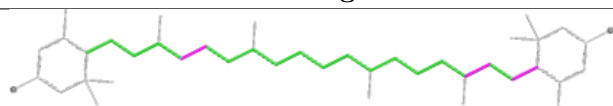
Ligand LUT 8 502



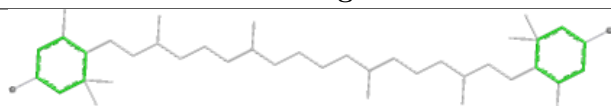
Bond lengths



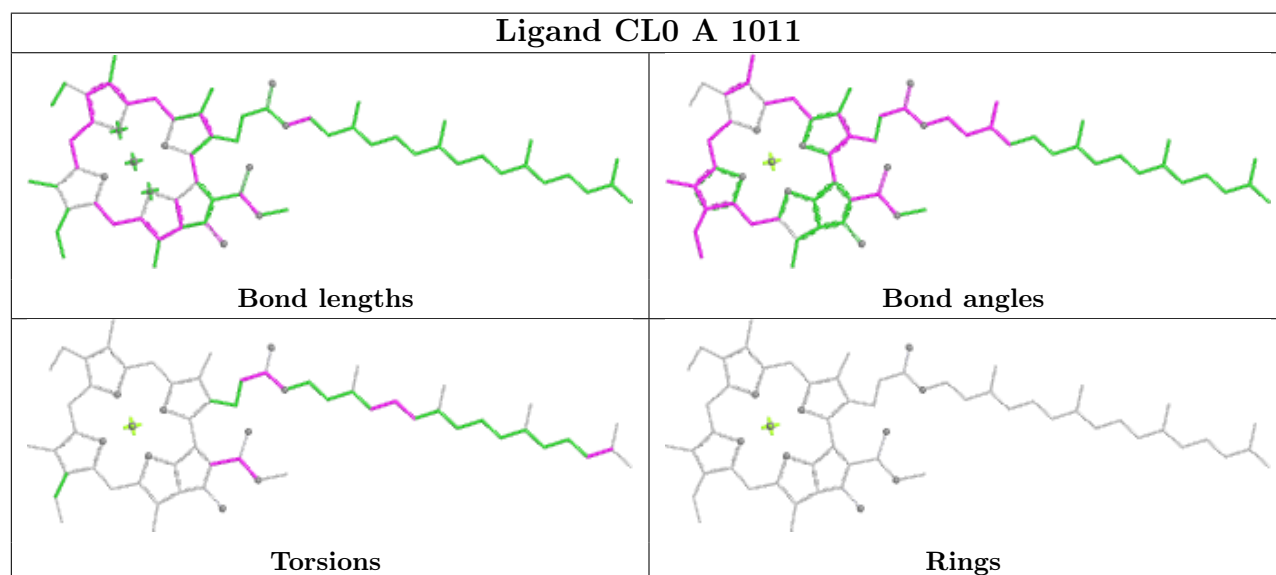
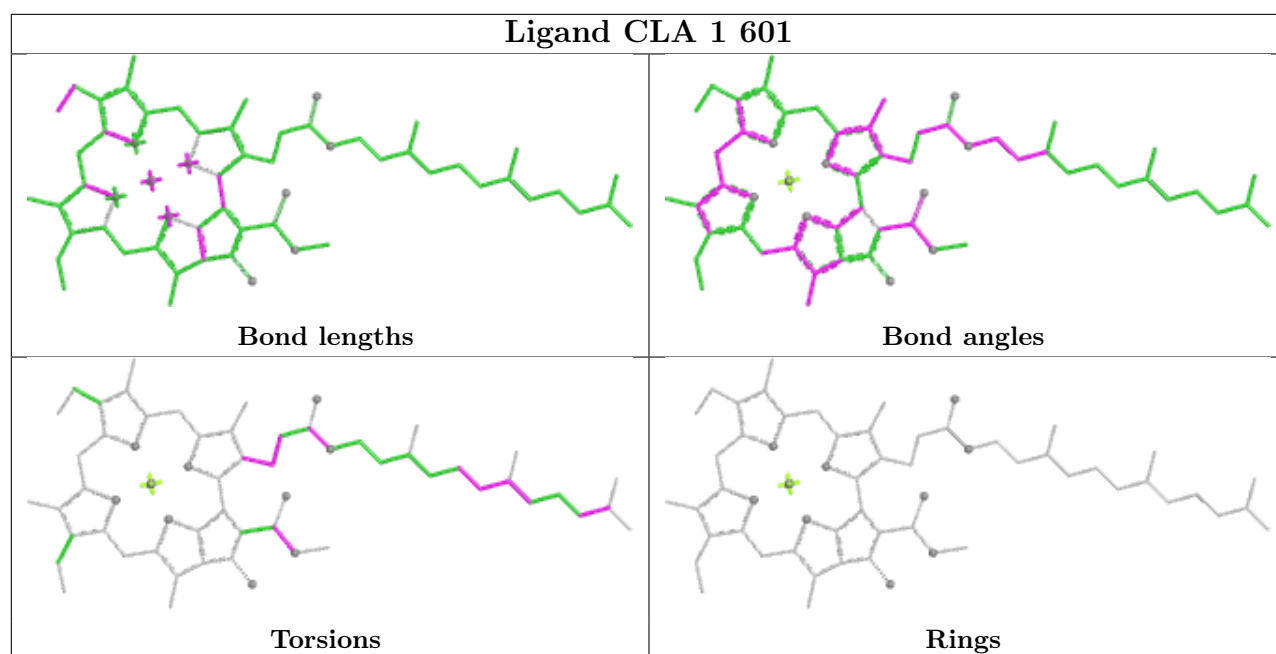
Bond angles

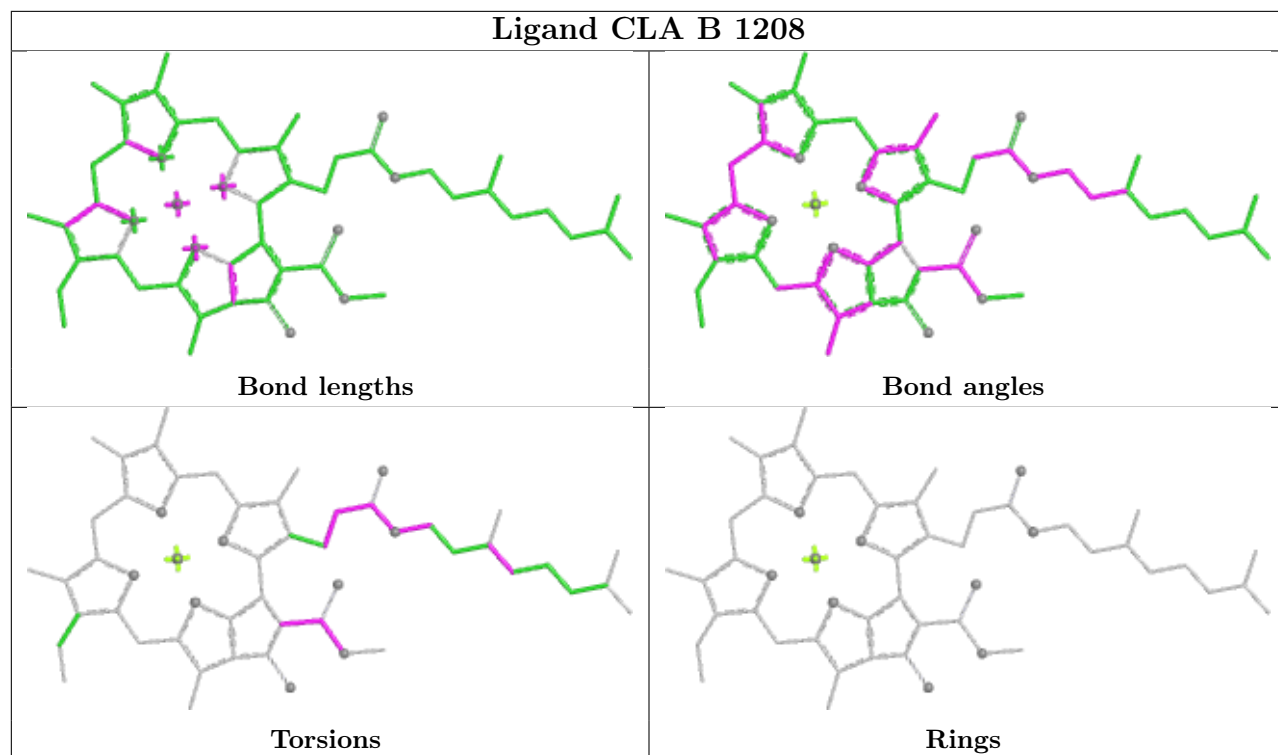


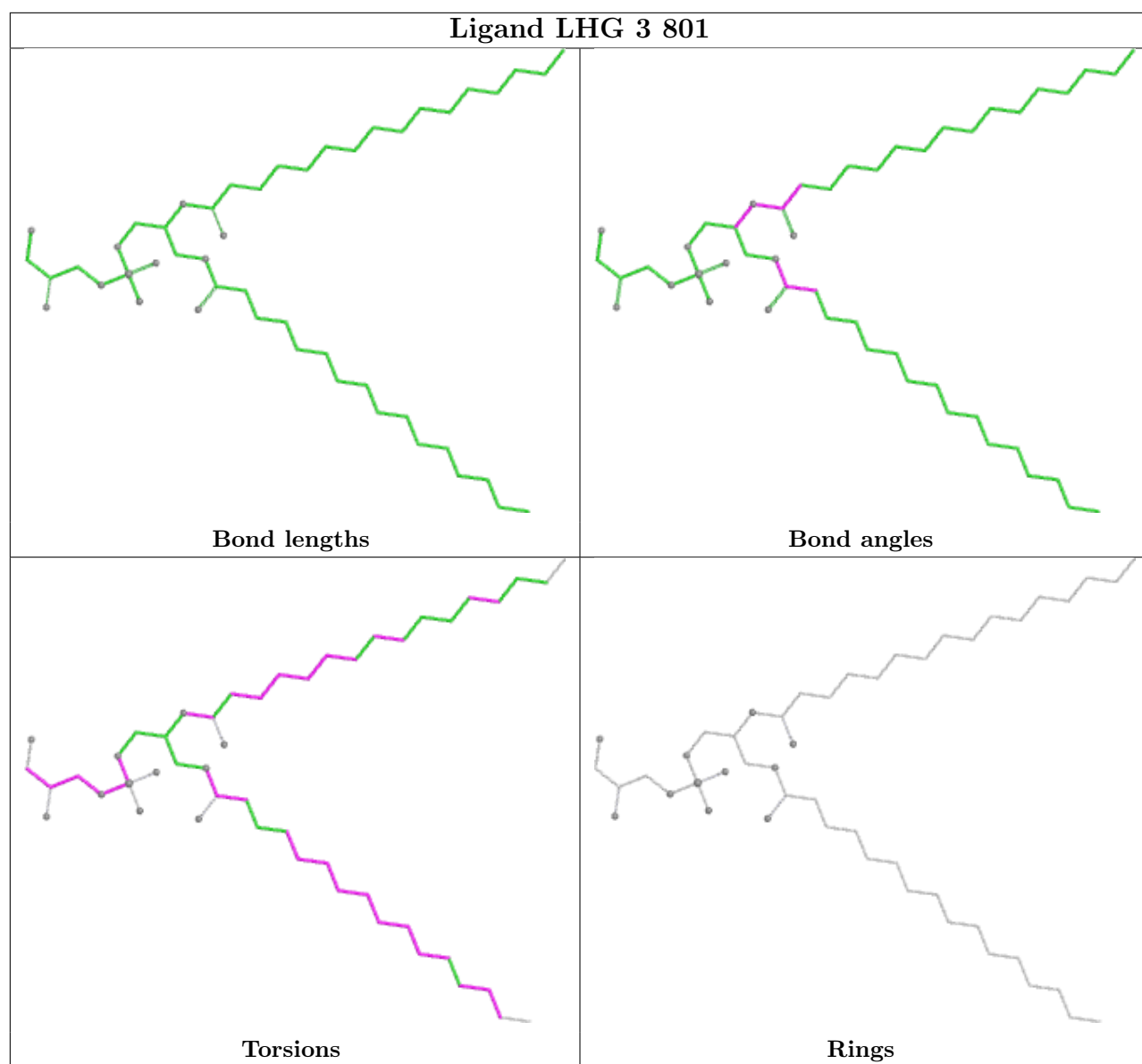
Torsions



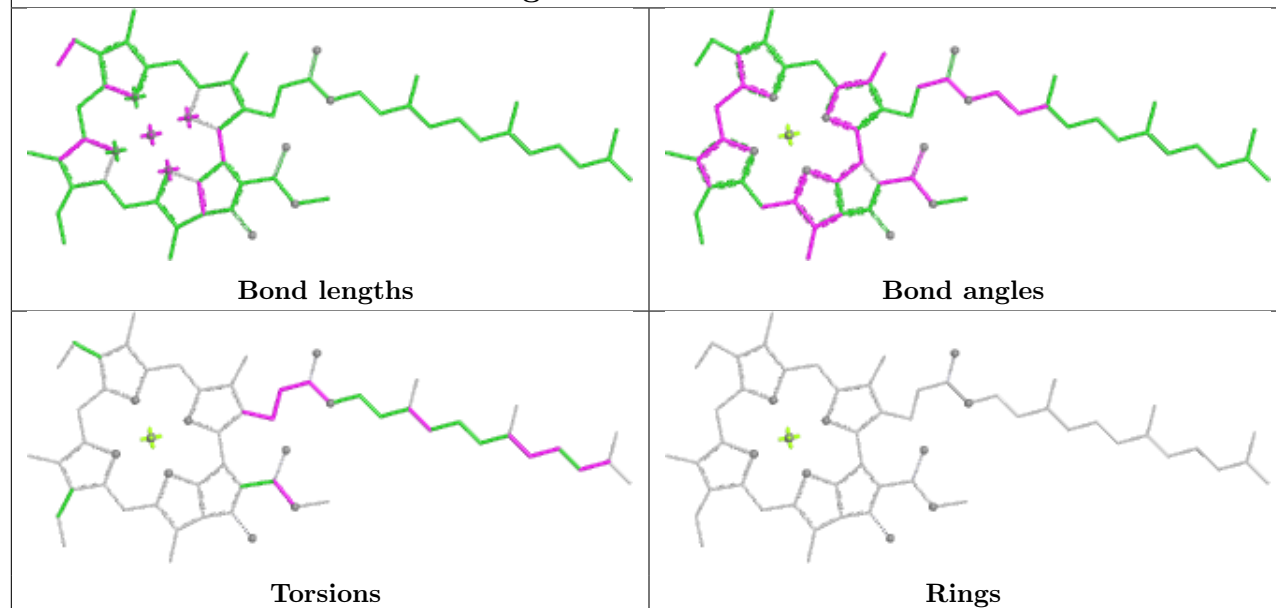
Rings



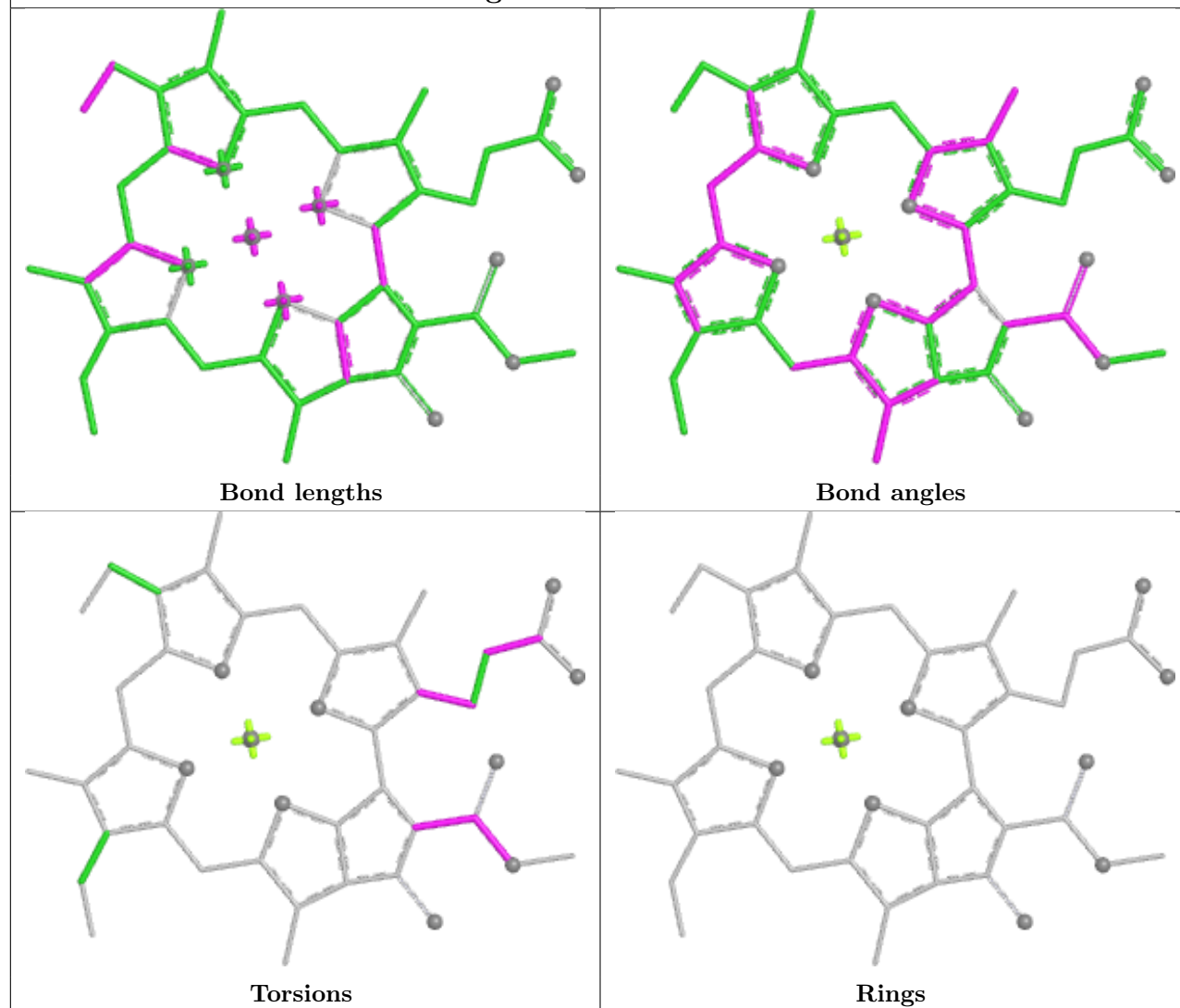


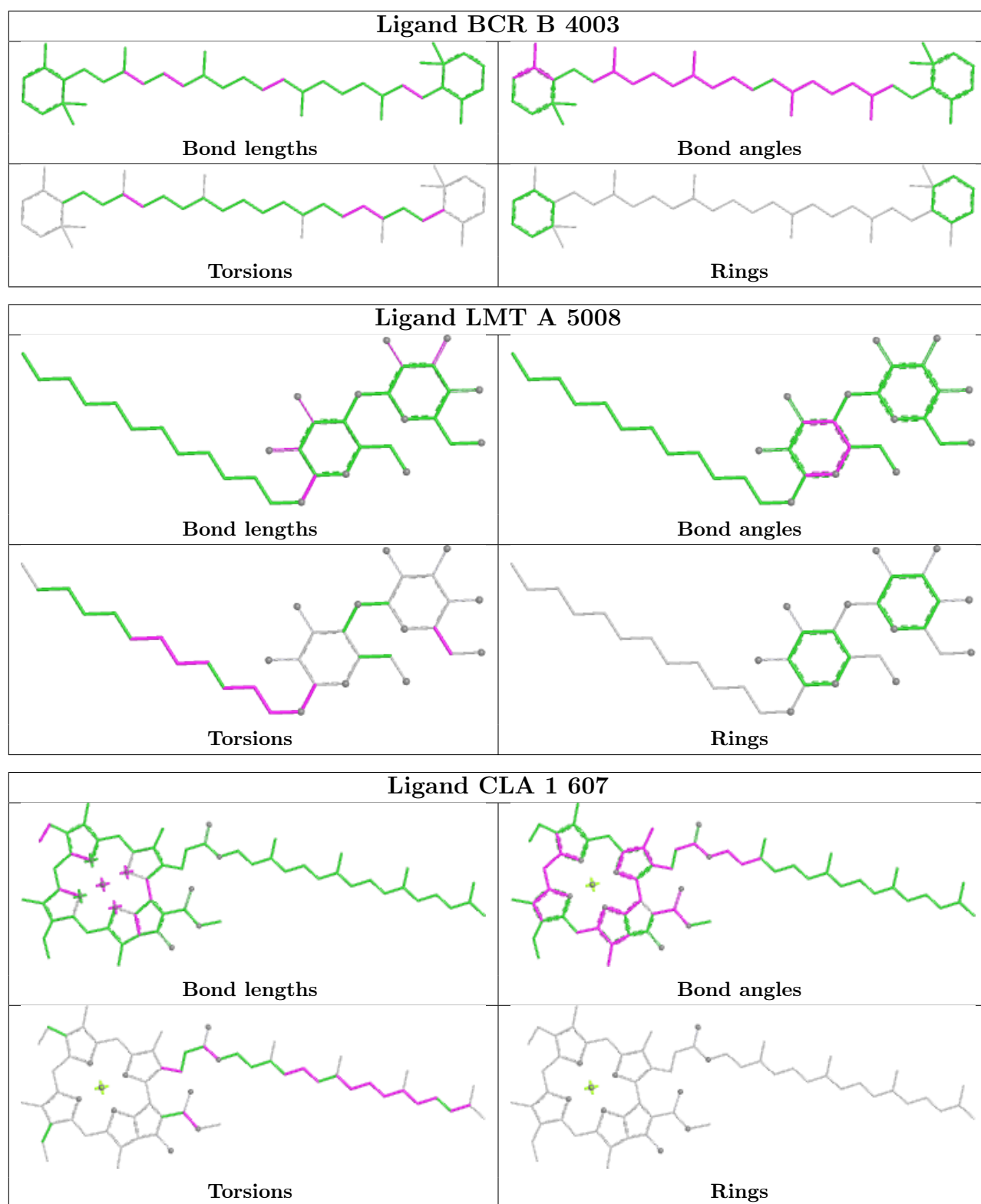


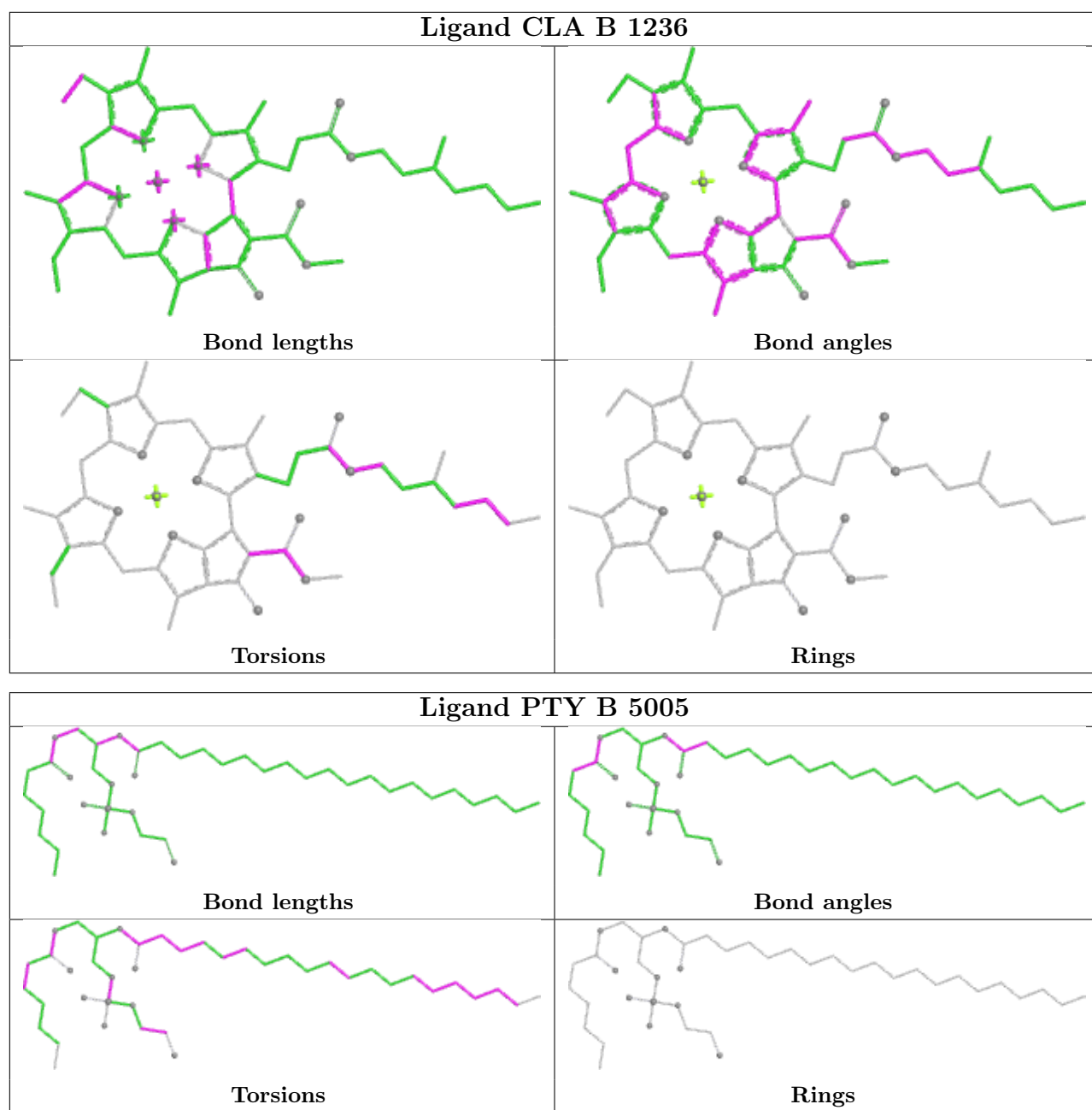
Ligand CLA A 1116

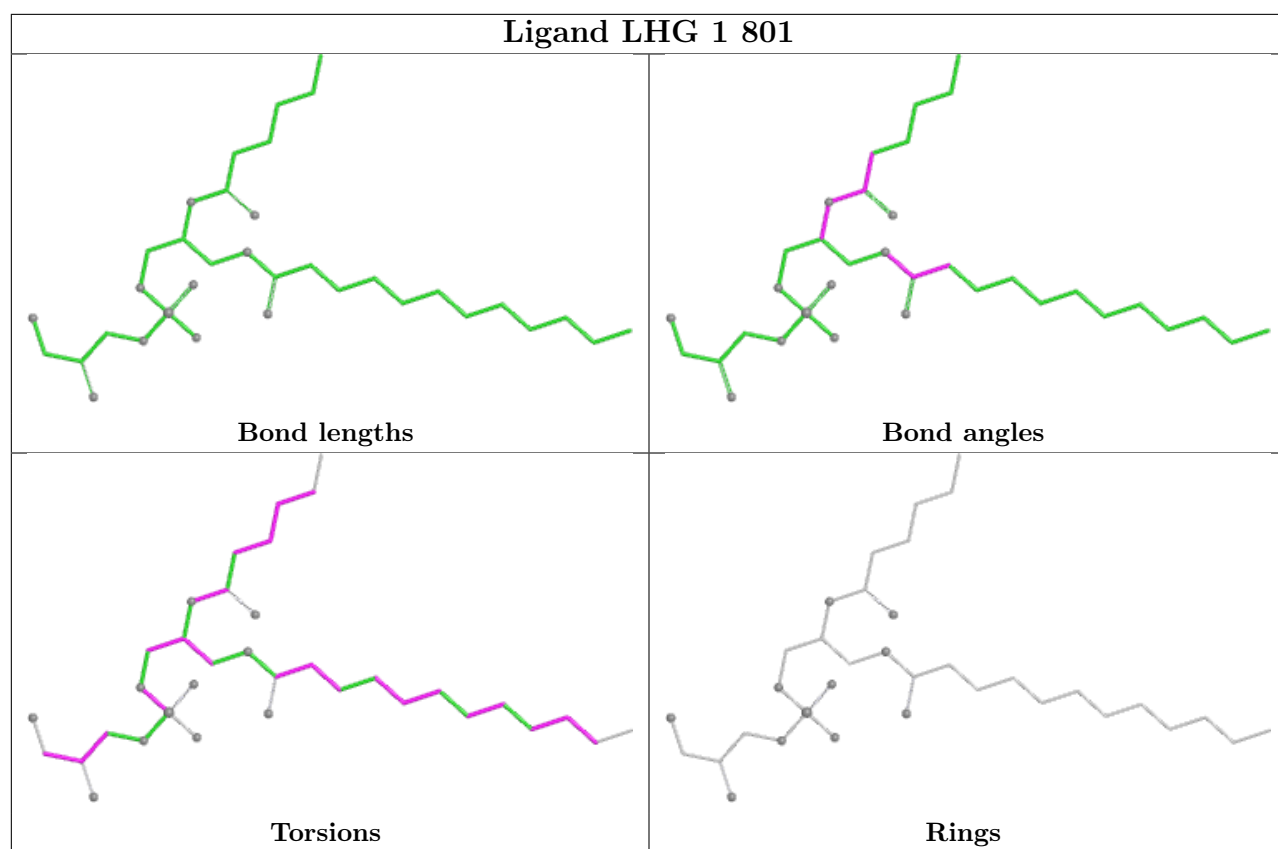


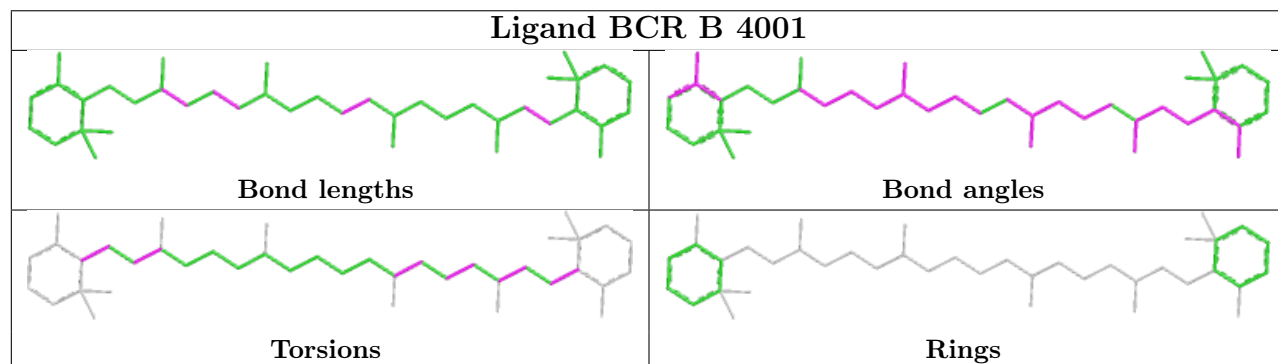
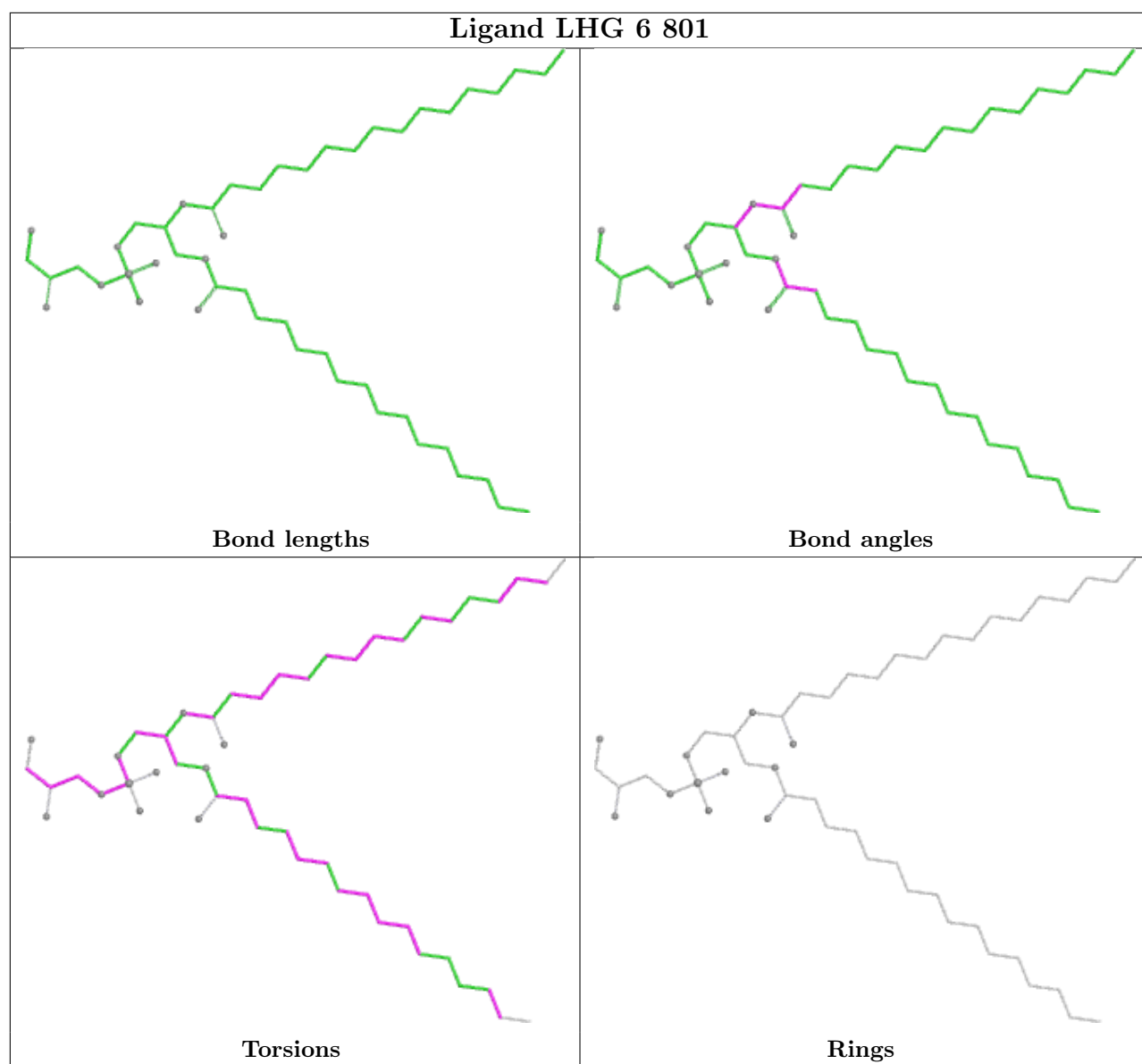
Ligand CLA L 1503

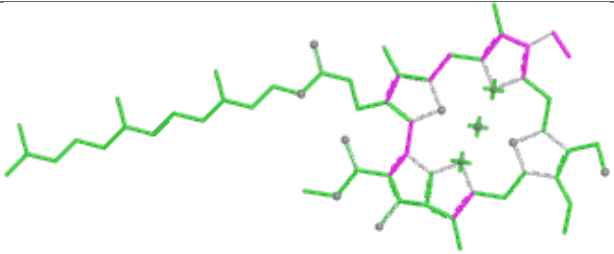
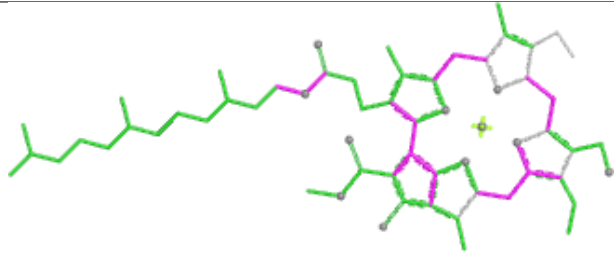
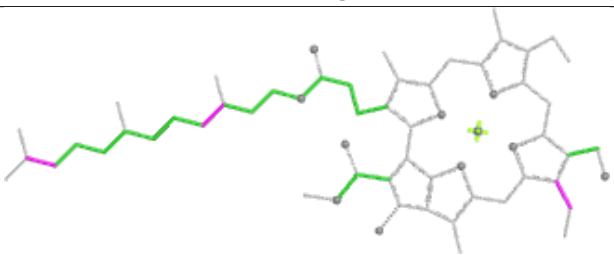
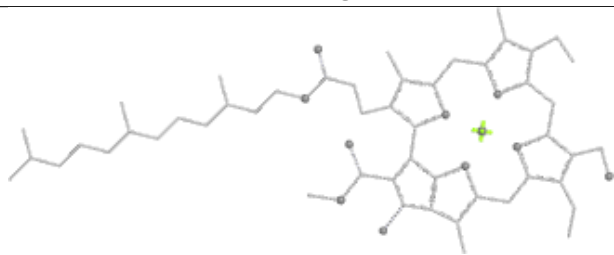


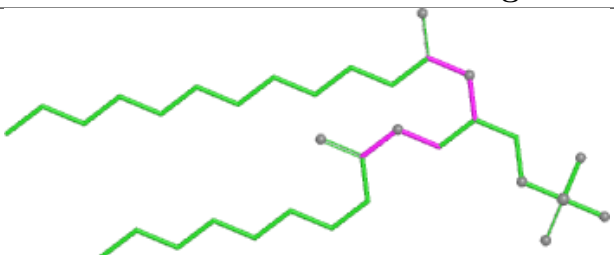
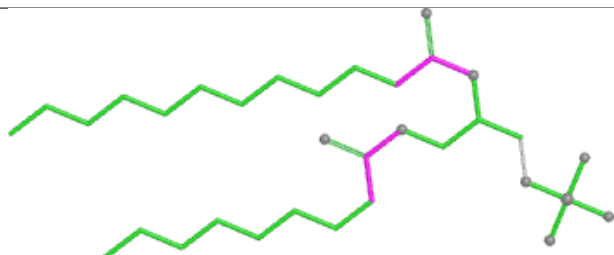
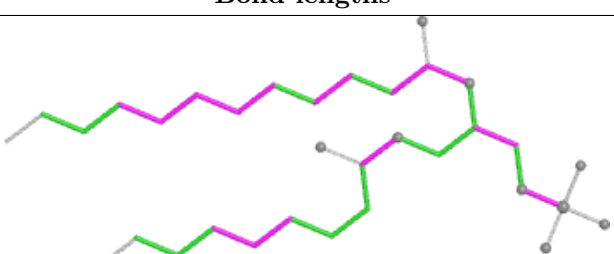
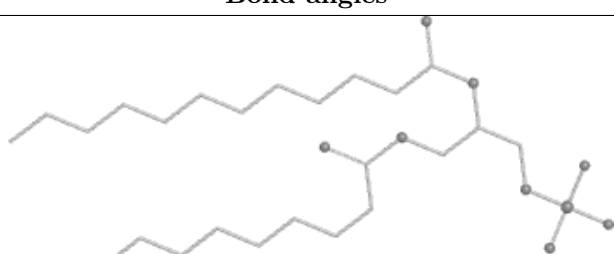


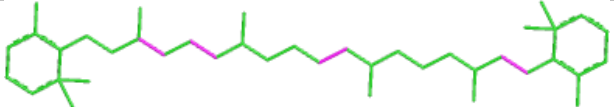
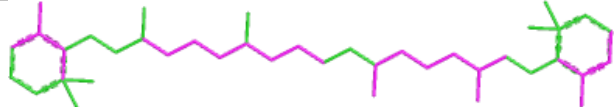
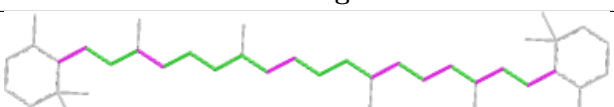
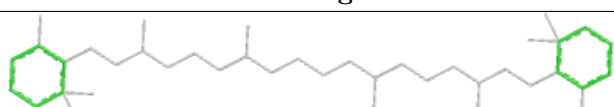




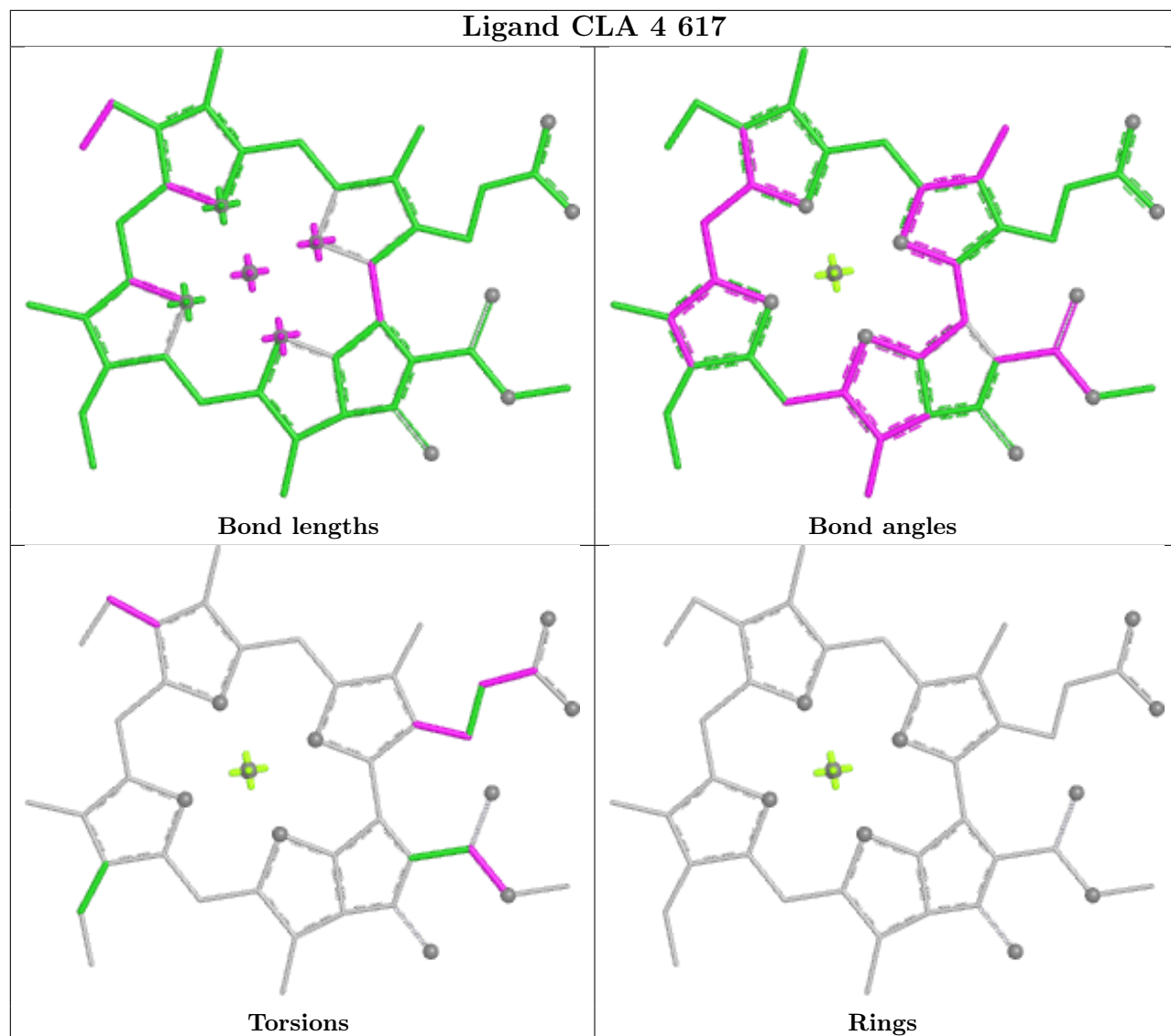


Ligand CHL 7 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

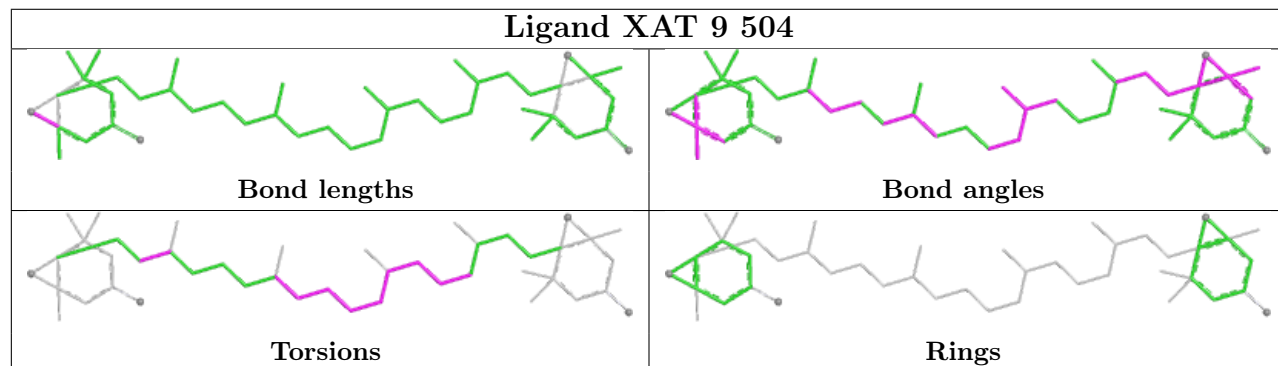
Ligand 3PH A 5007	
	
Bond lengths	Bond angles
	
Torsions	Rings

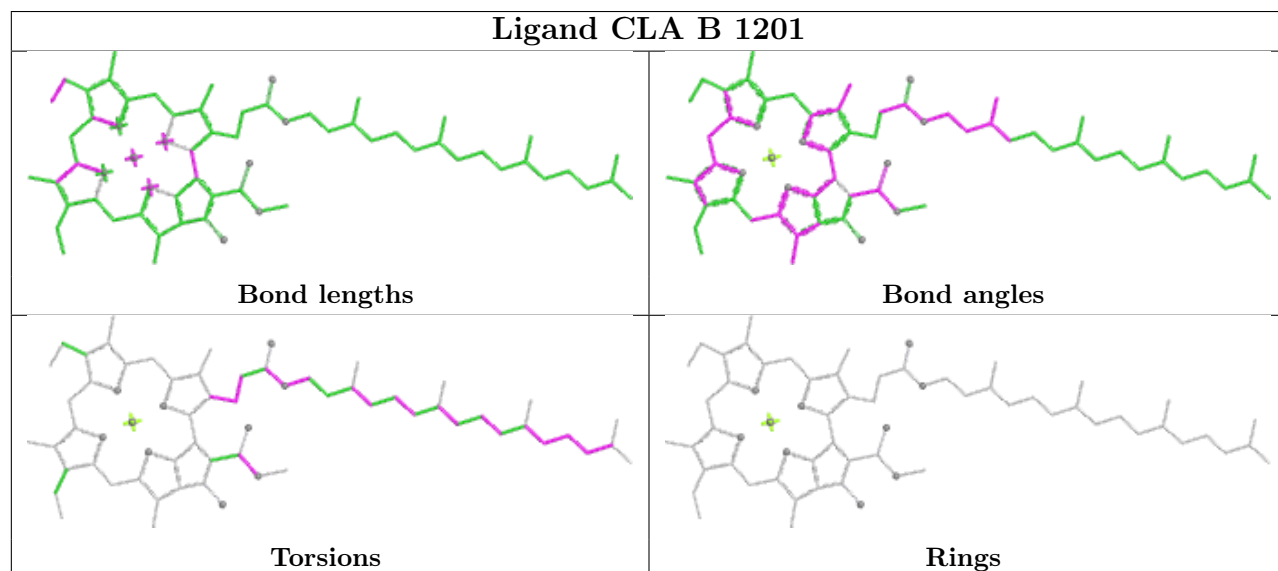
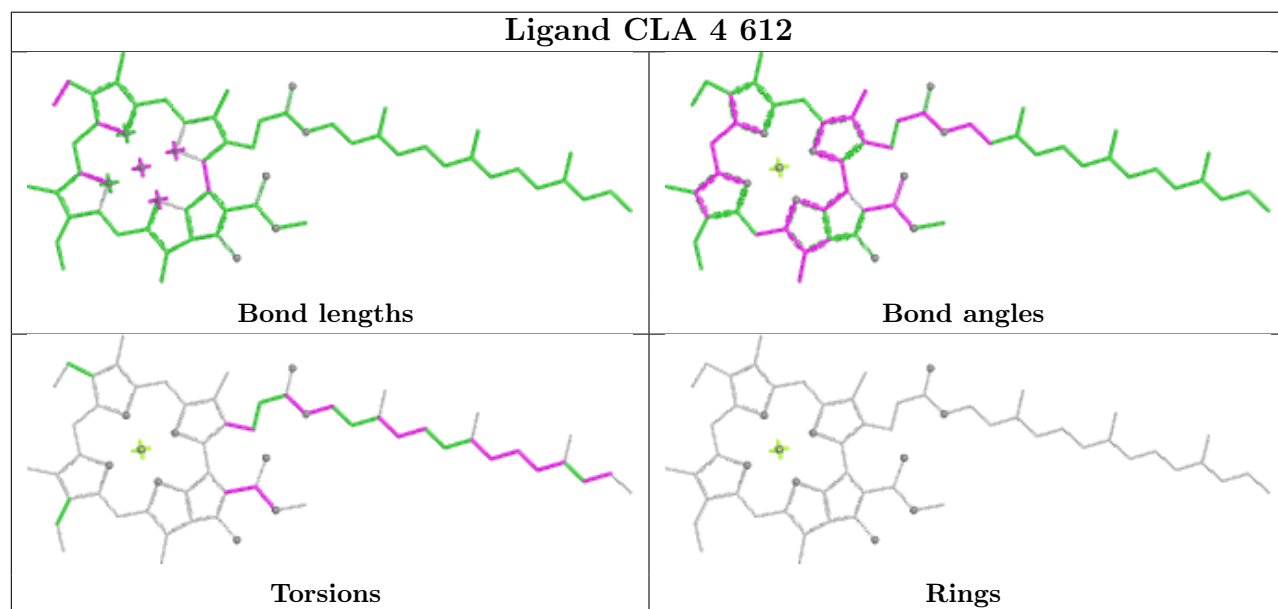
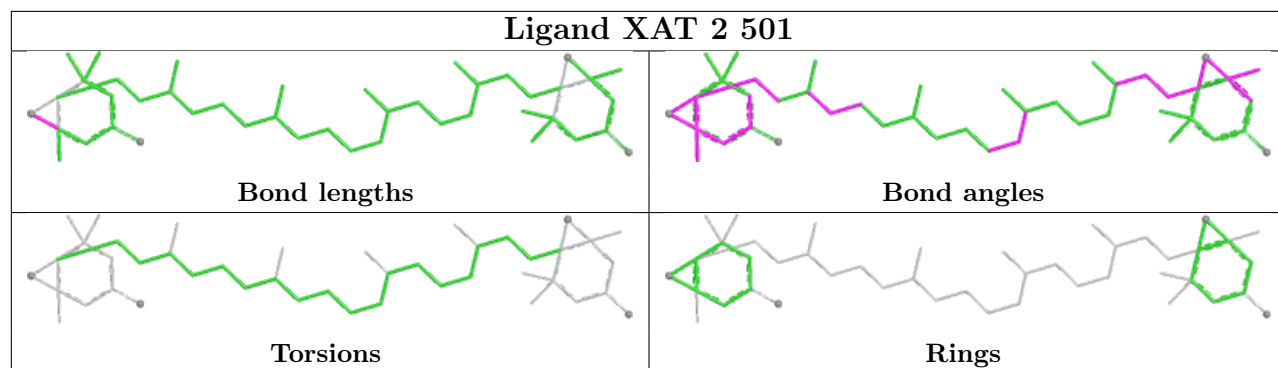
Ligand BCR 5 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 617

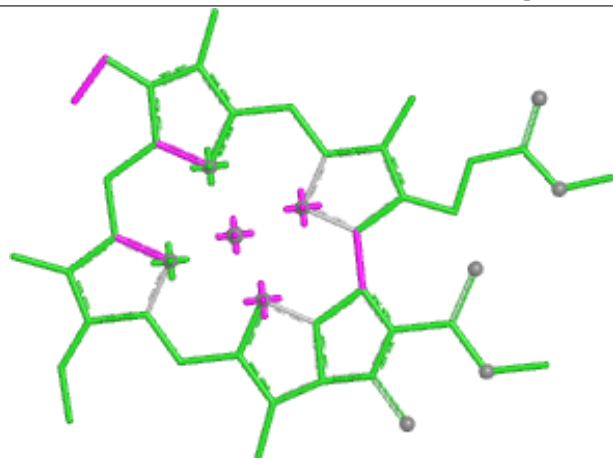


Ligand XAT 9 504

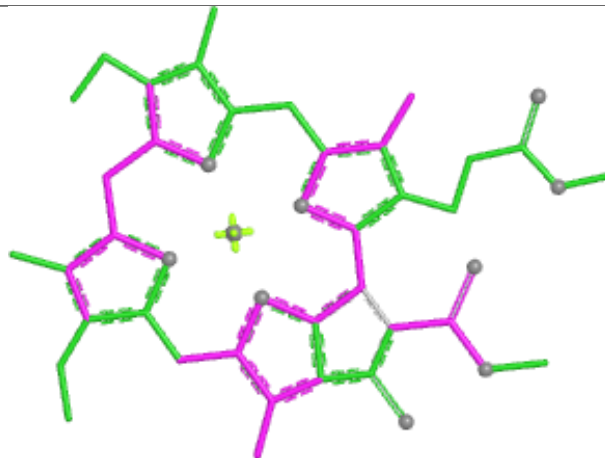




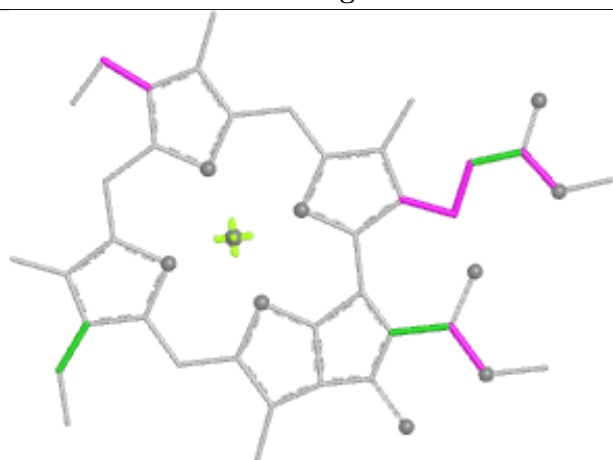
Ligand CLA 5 615



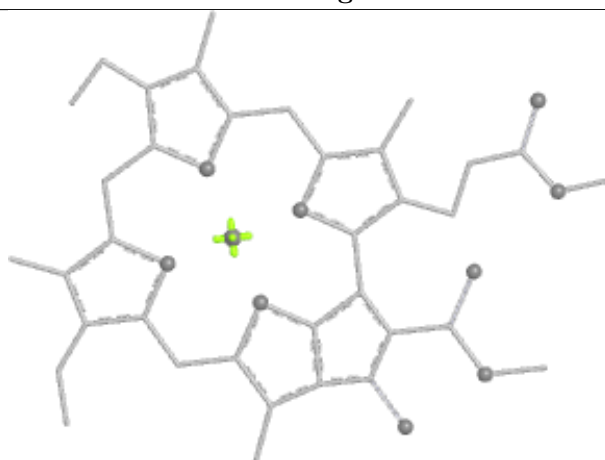
Bond lengths



Bond angles

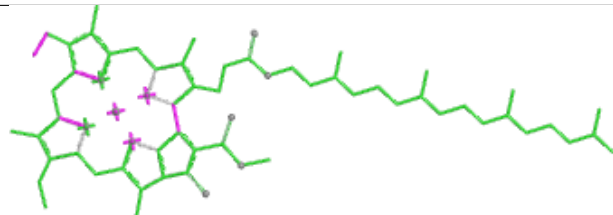


Torsions

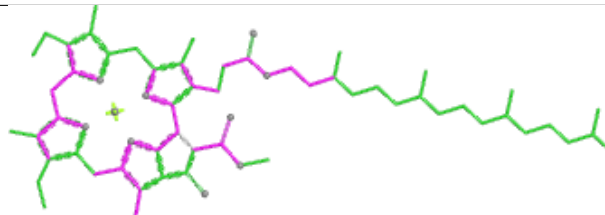


Rings

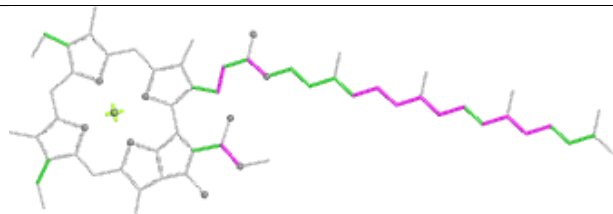
Ligand CLA A 1013



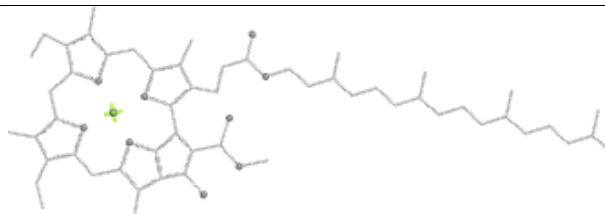
Bond lengths



Bond angles

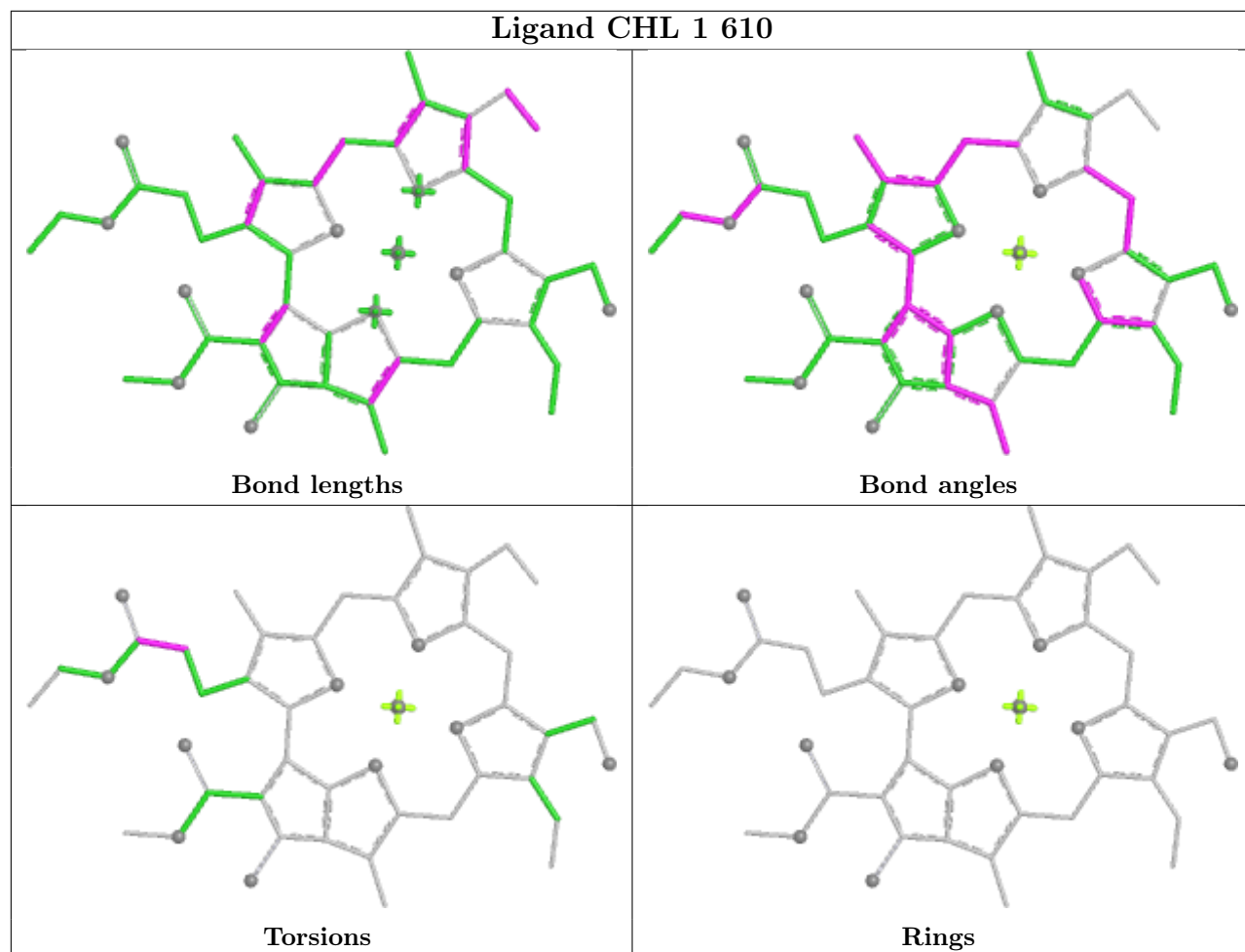


Torsions

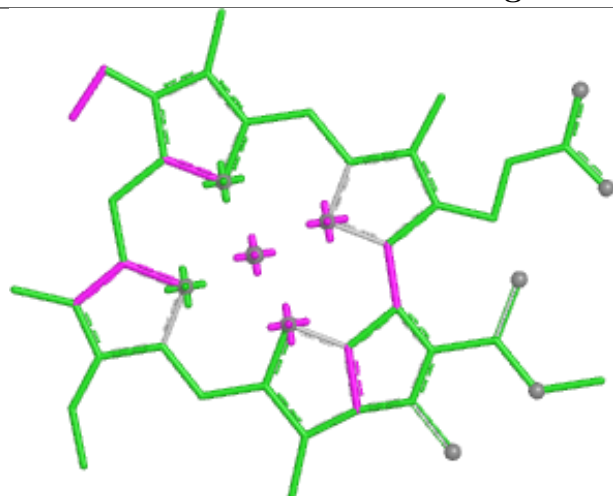


Rings

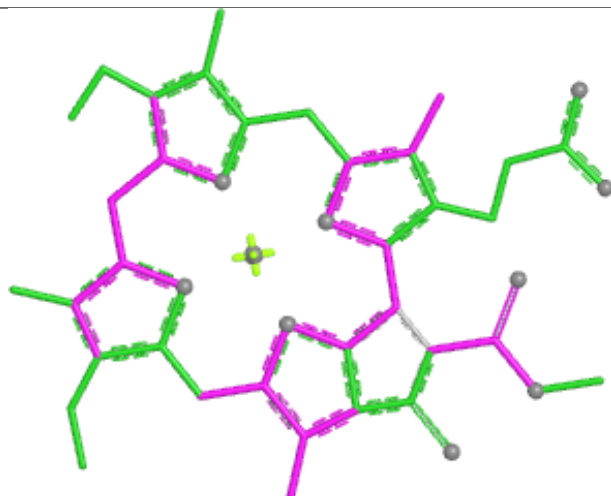
Ligand CHL 1 610



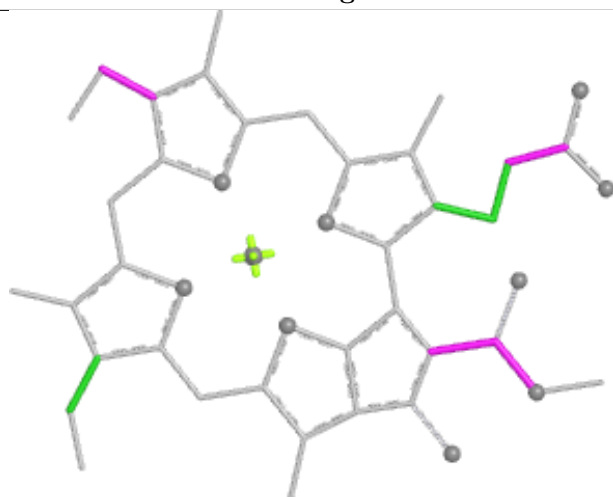
Ligand CLA K 1404



Bond lengths



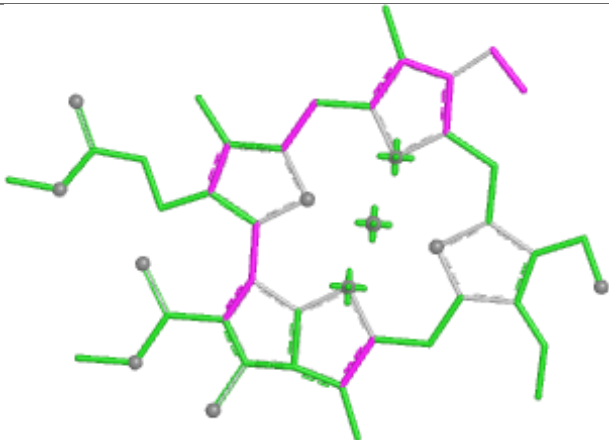
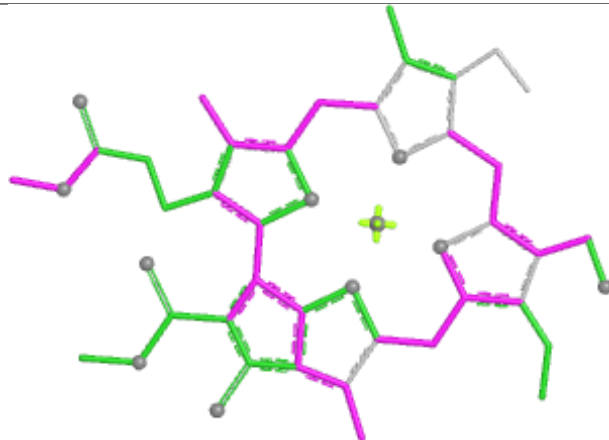
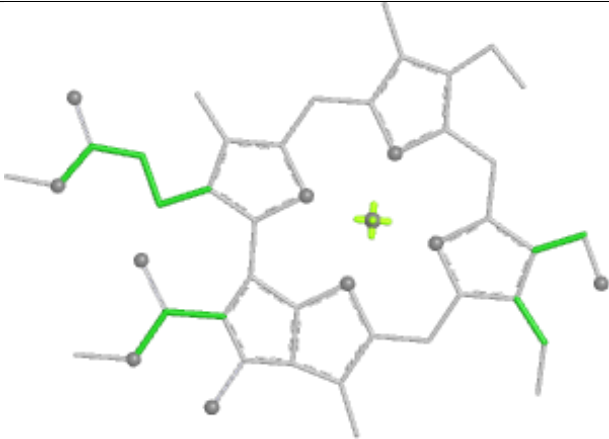
Bond angles

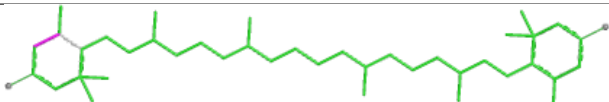
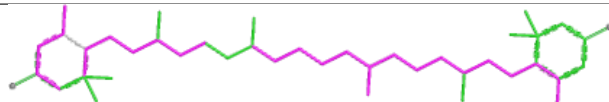
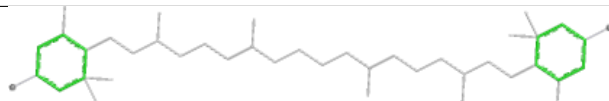


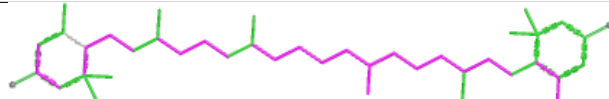
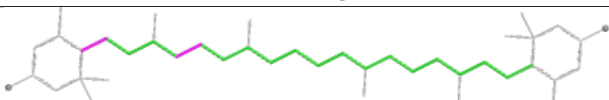
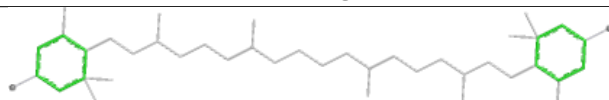
Torsions

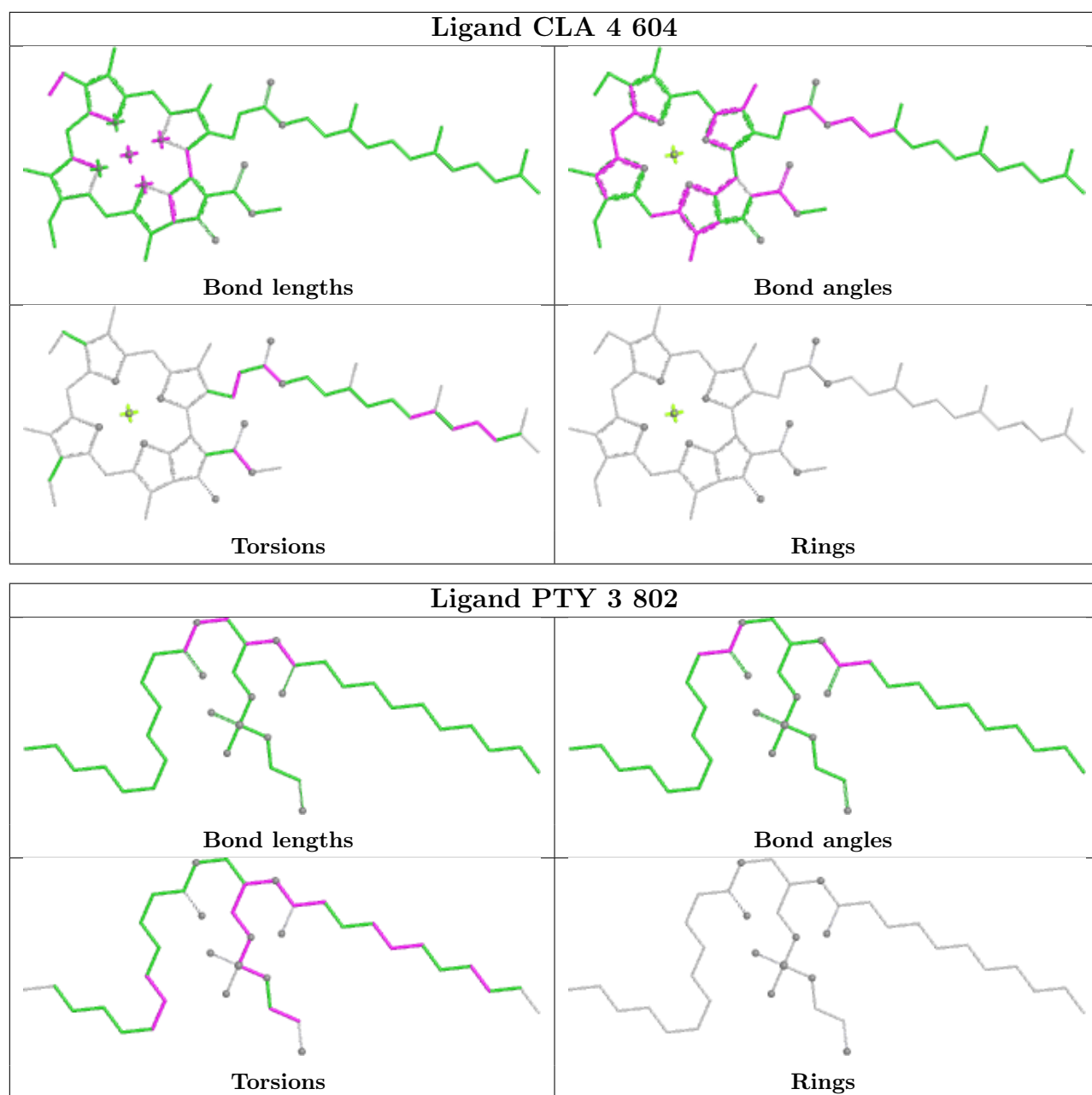


Rings

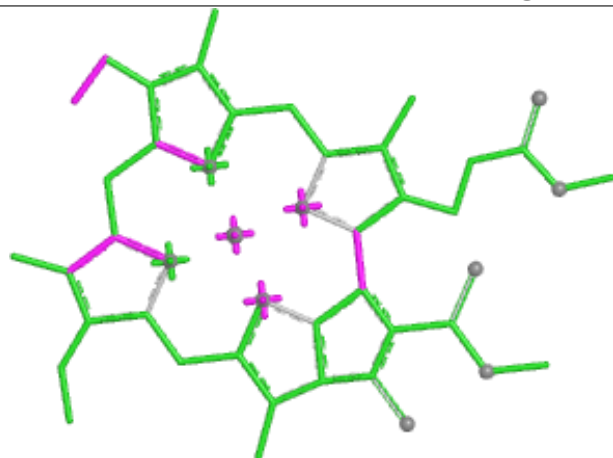
Ligand CHL 5 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 3 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

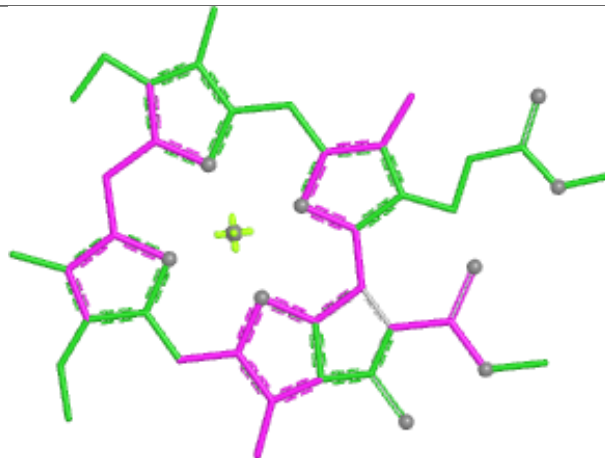
Ligand LUT a 502	
	
Bond lengths	Bond angles
	
Torsions	Rings



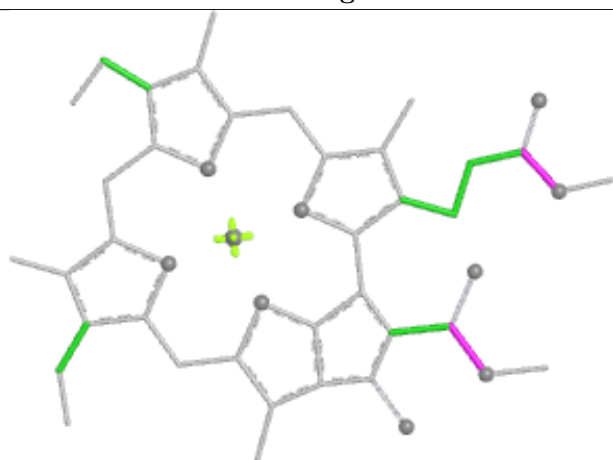
Ligand CLA 9 602



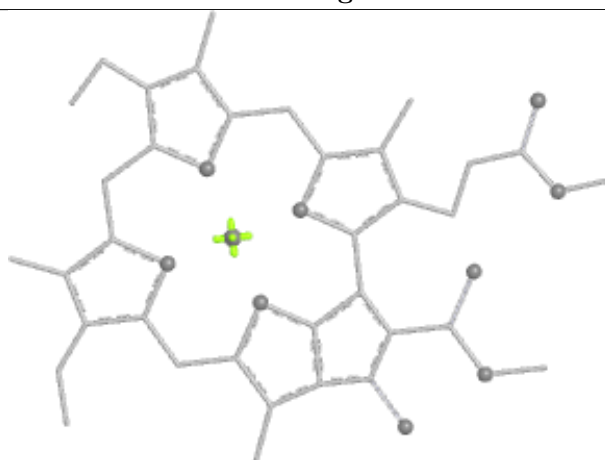
Bond lengths



Bond angles

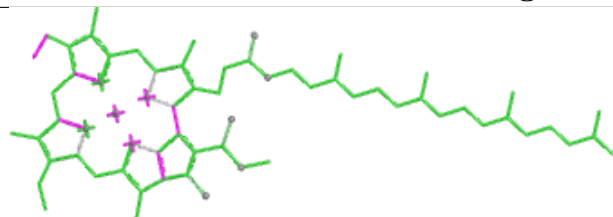


Torsions

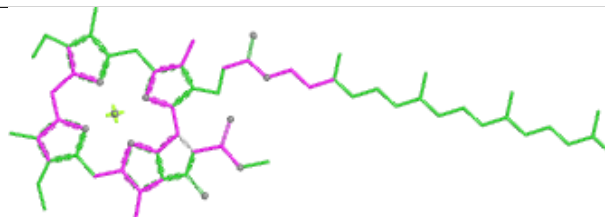


Rings

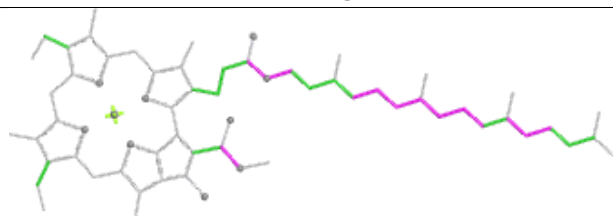
Ligand CLA 3 607



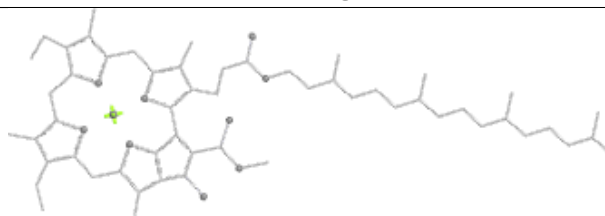
Bond lengths



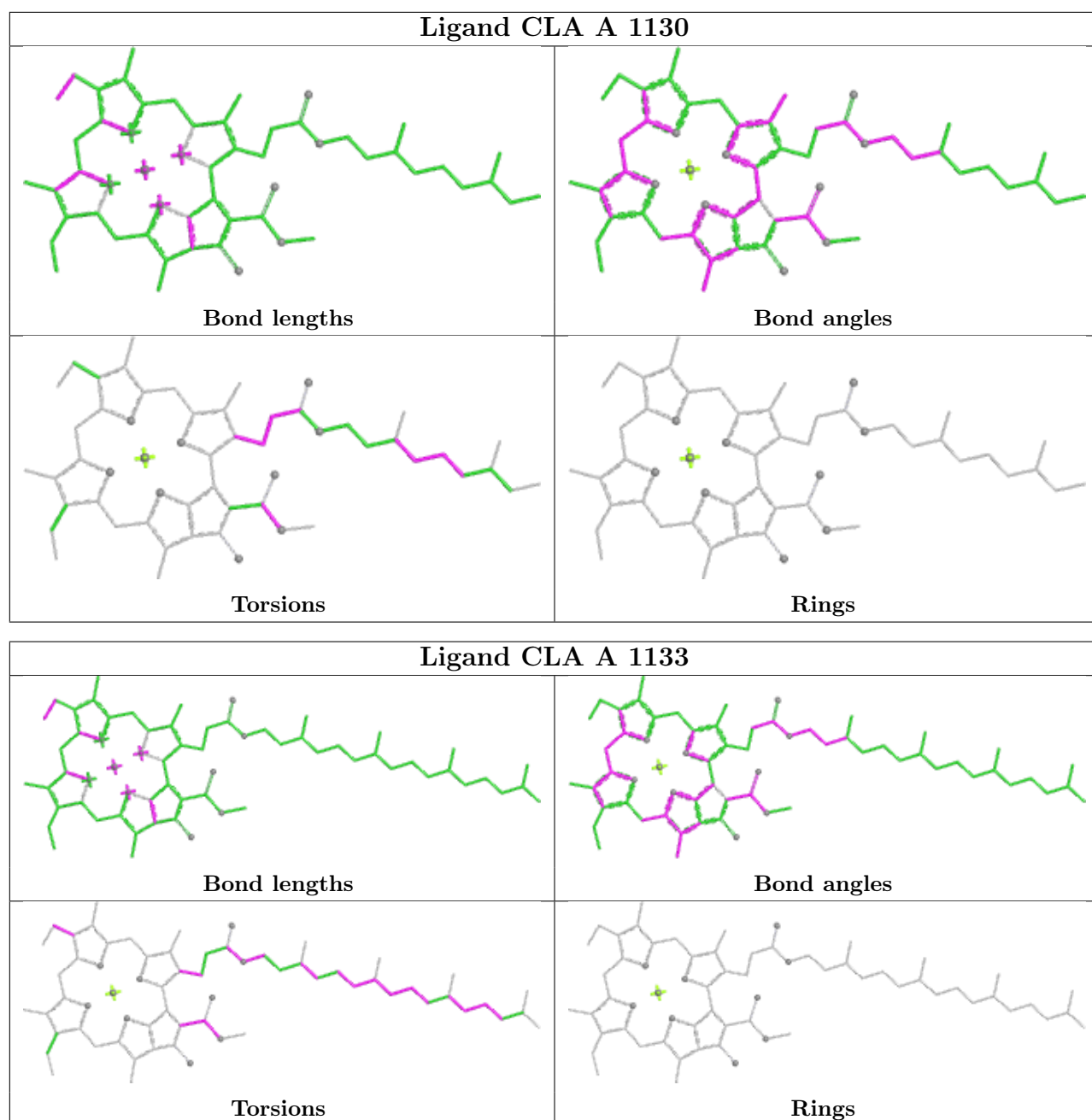
Bond angles

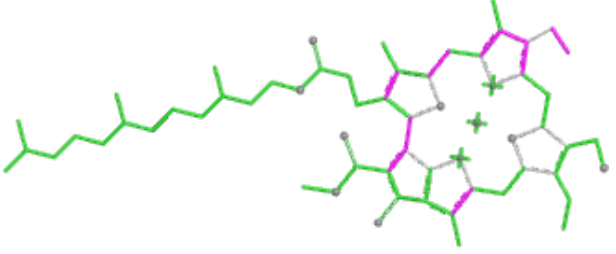
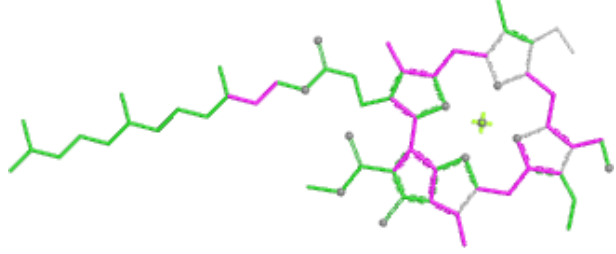
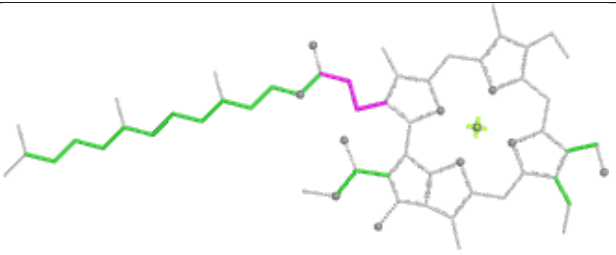
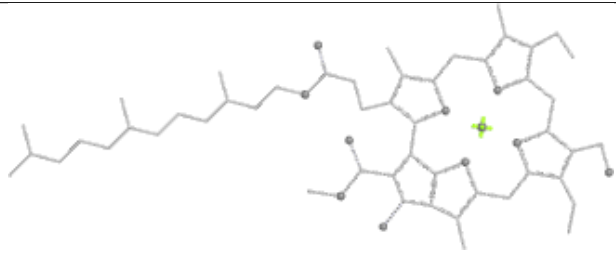
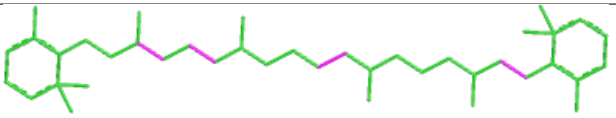
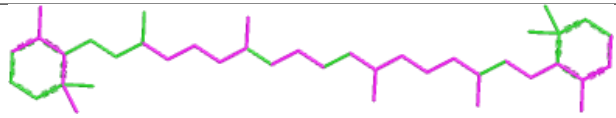
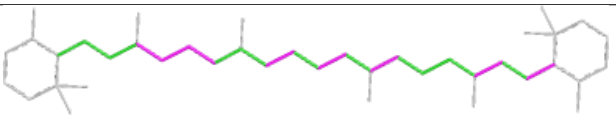
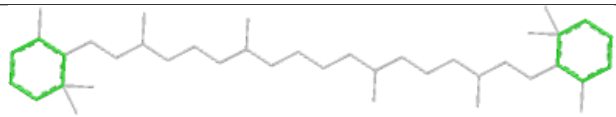


Torsions

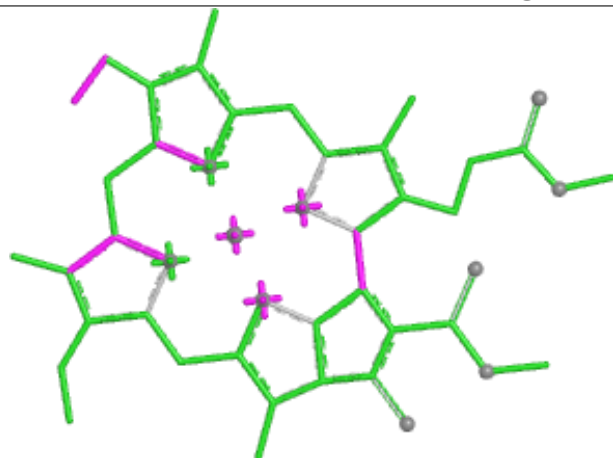


Rings

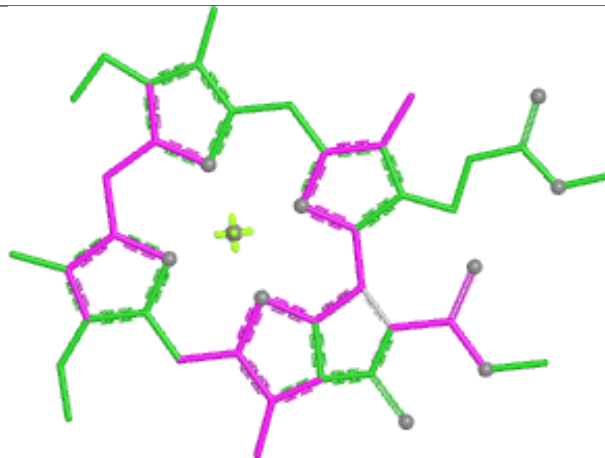


Ligand CHL a 604	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 4003	
 Bond lengths	 Bond angles
 Torsions	 Rings

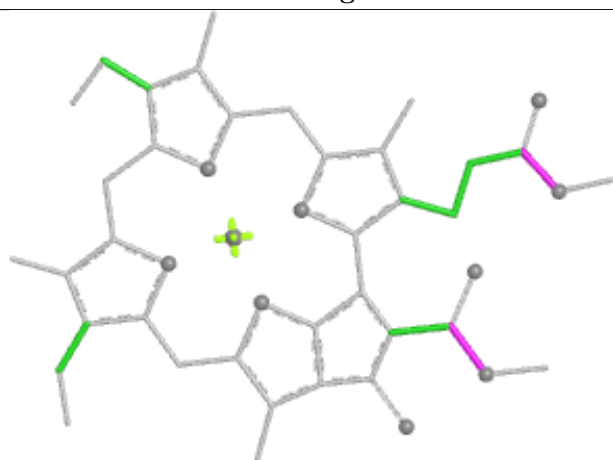
Ligand CLA 3 618



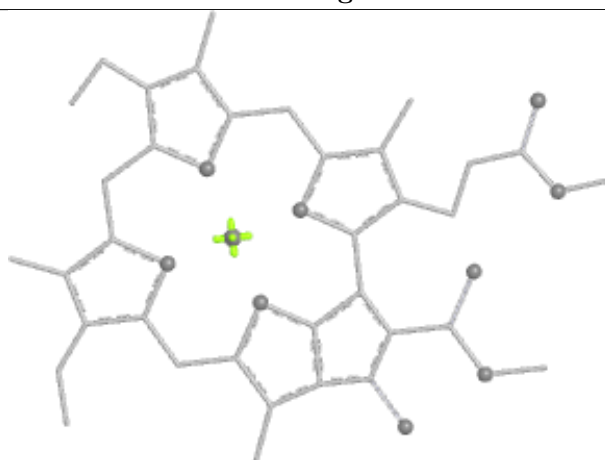
Bond lengths



Bond angles

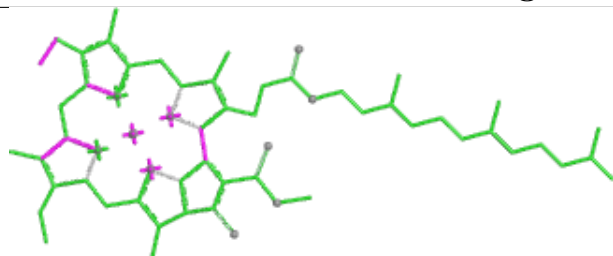


Torsions

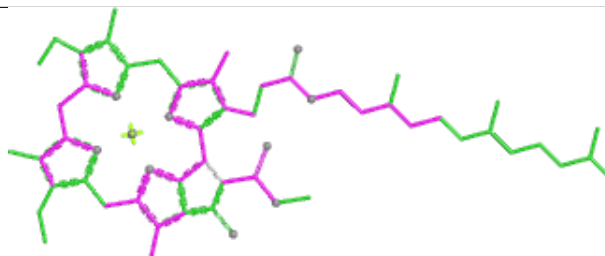


Rings

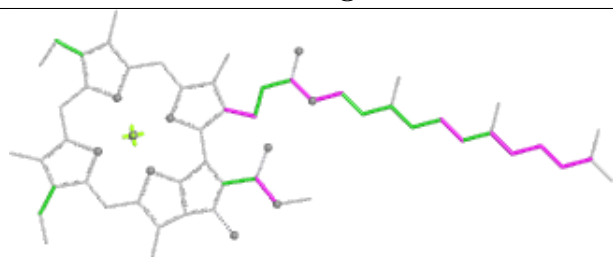
Ligand CLA 5 601



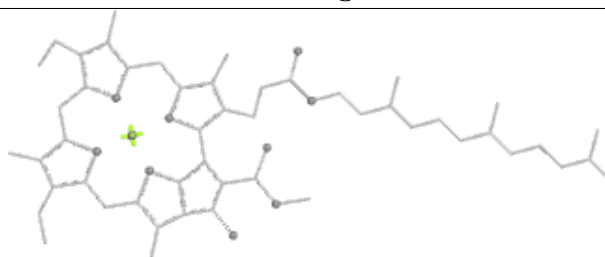
Bond lengths



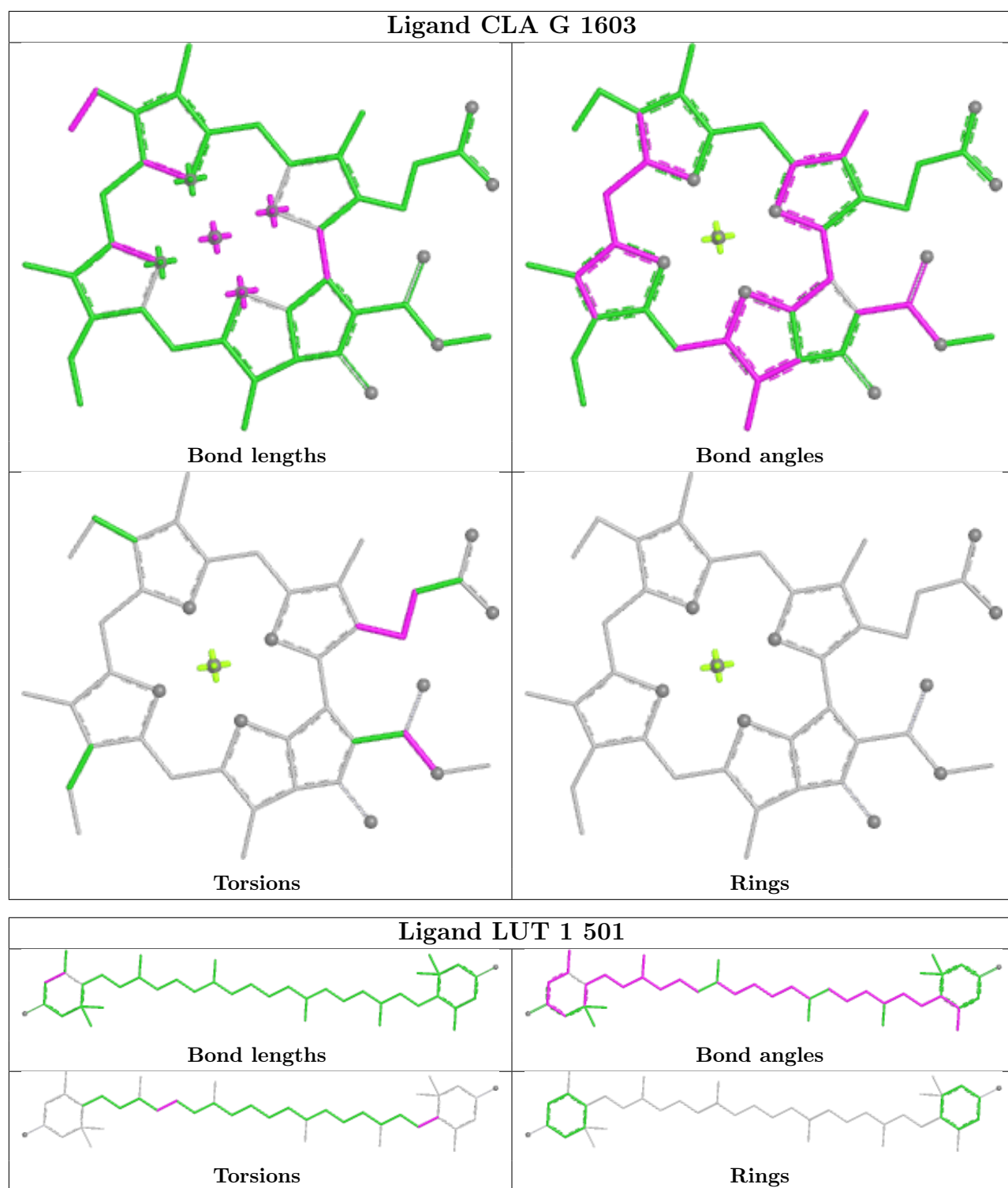
Bond angles

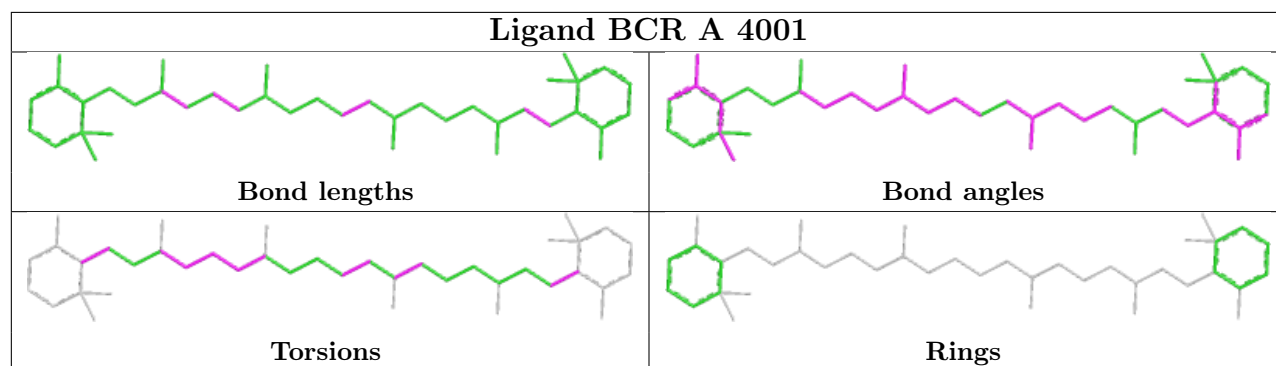
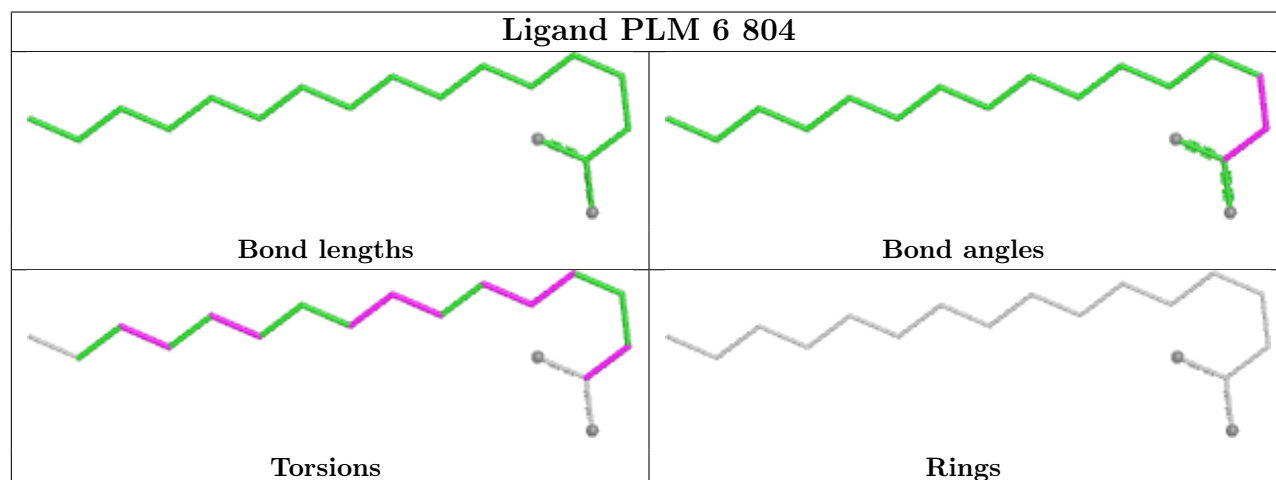
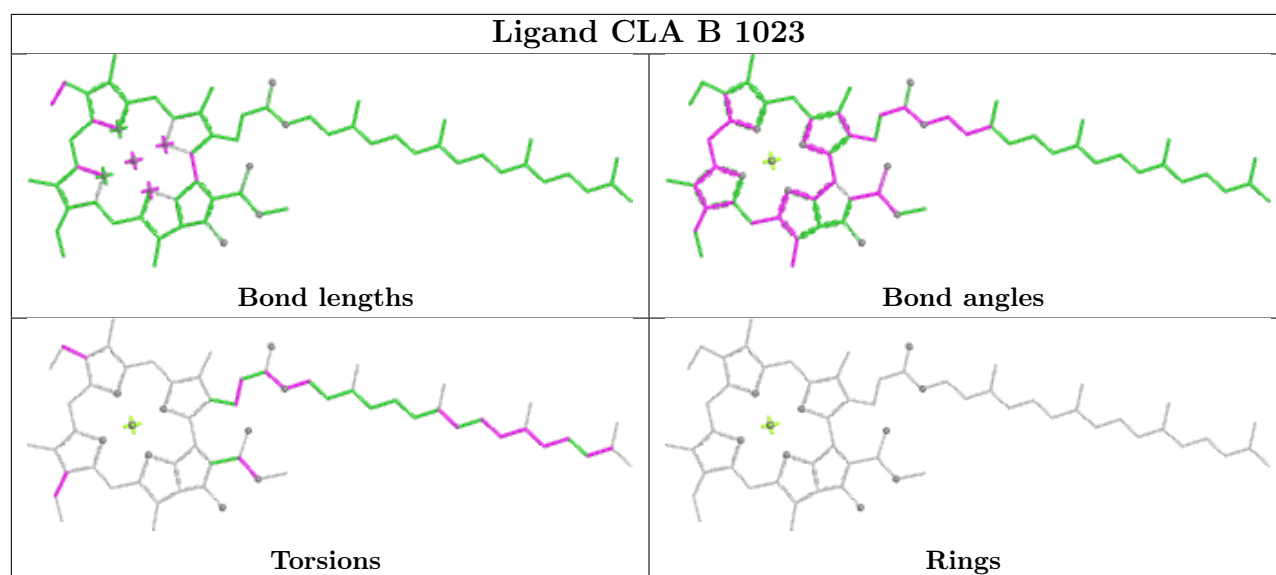


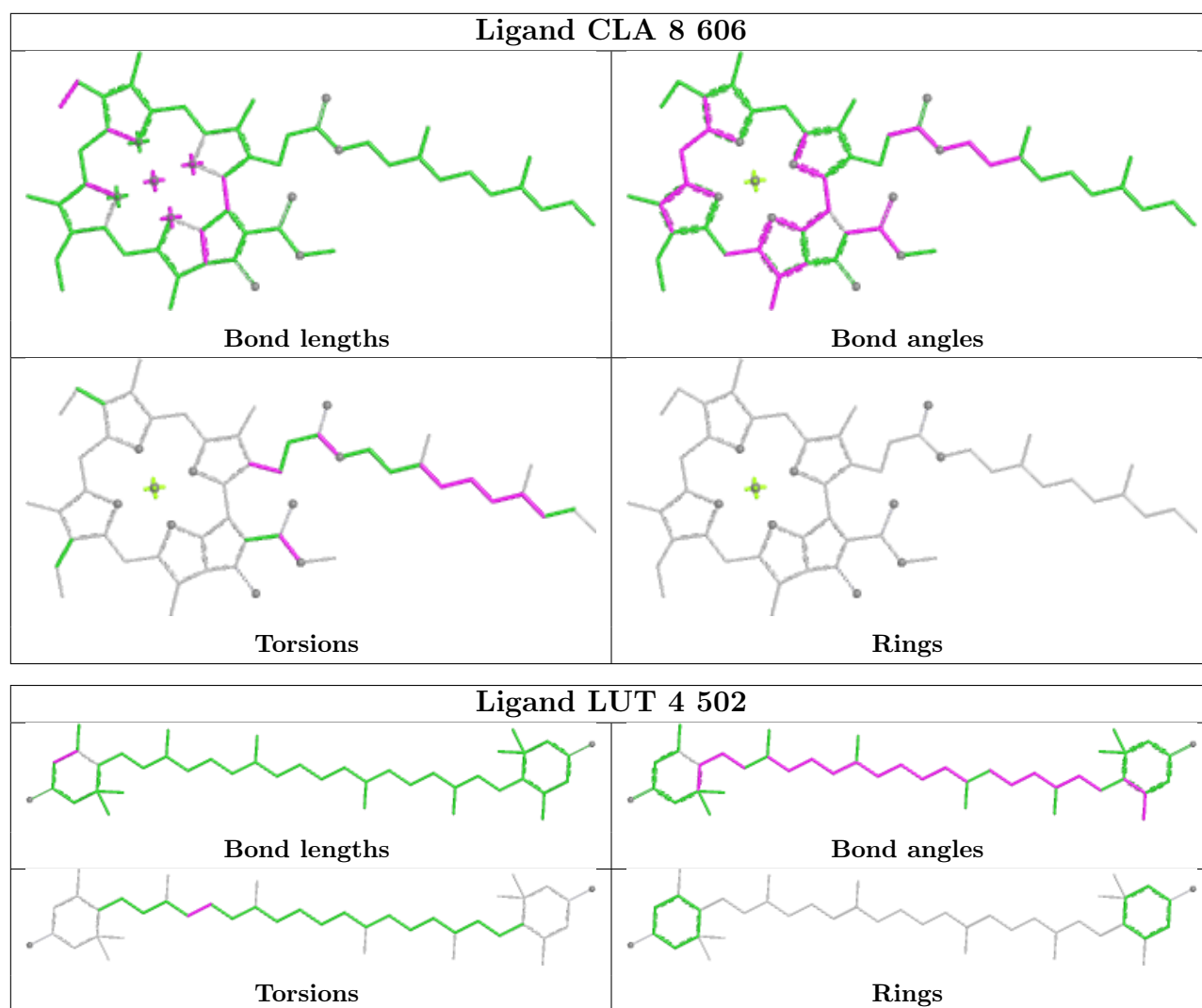
Torsions



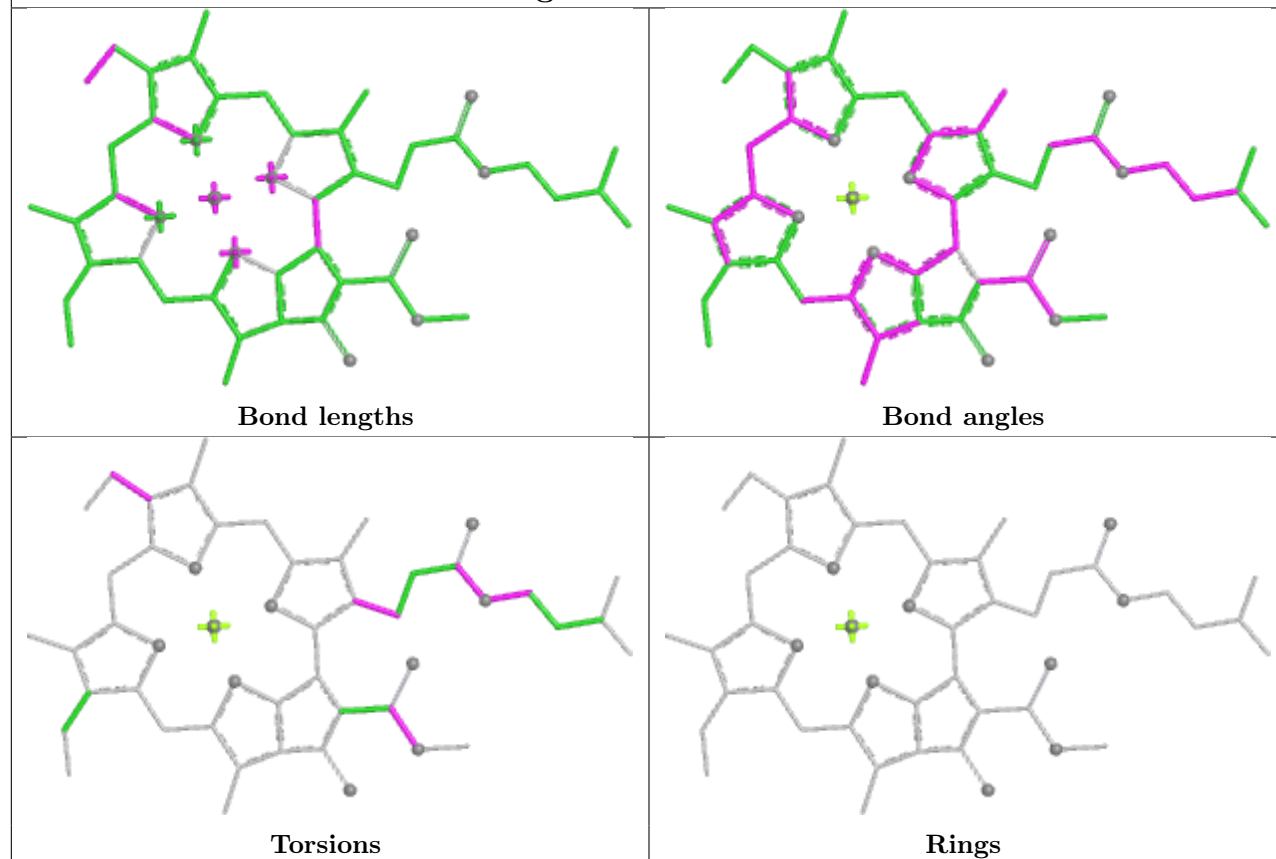
Rings



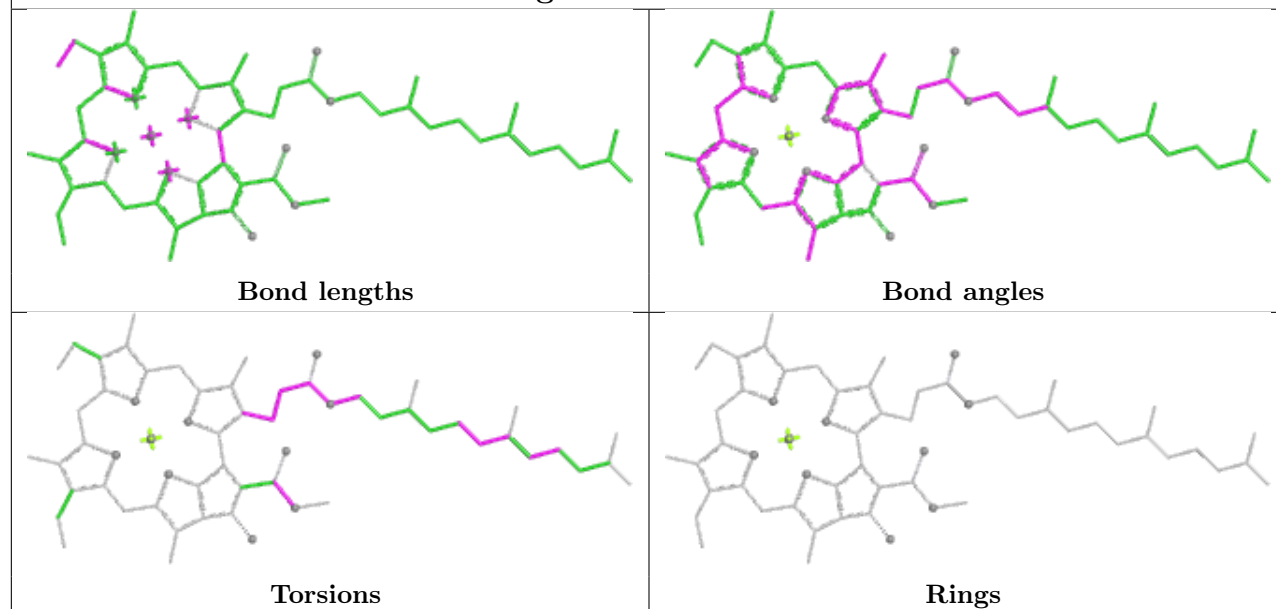


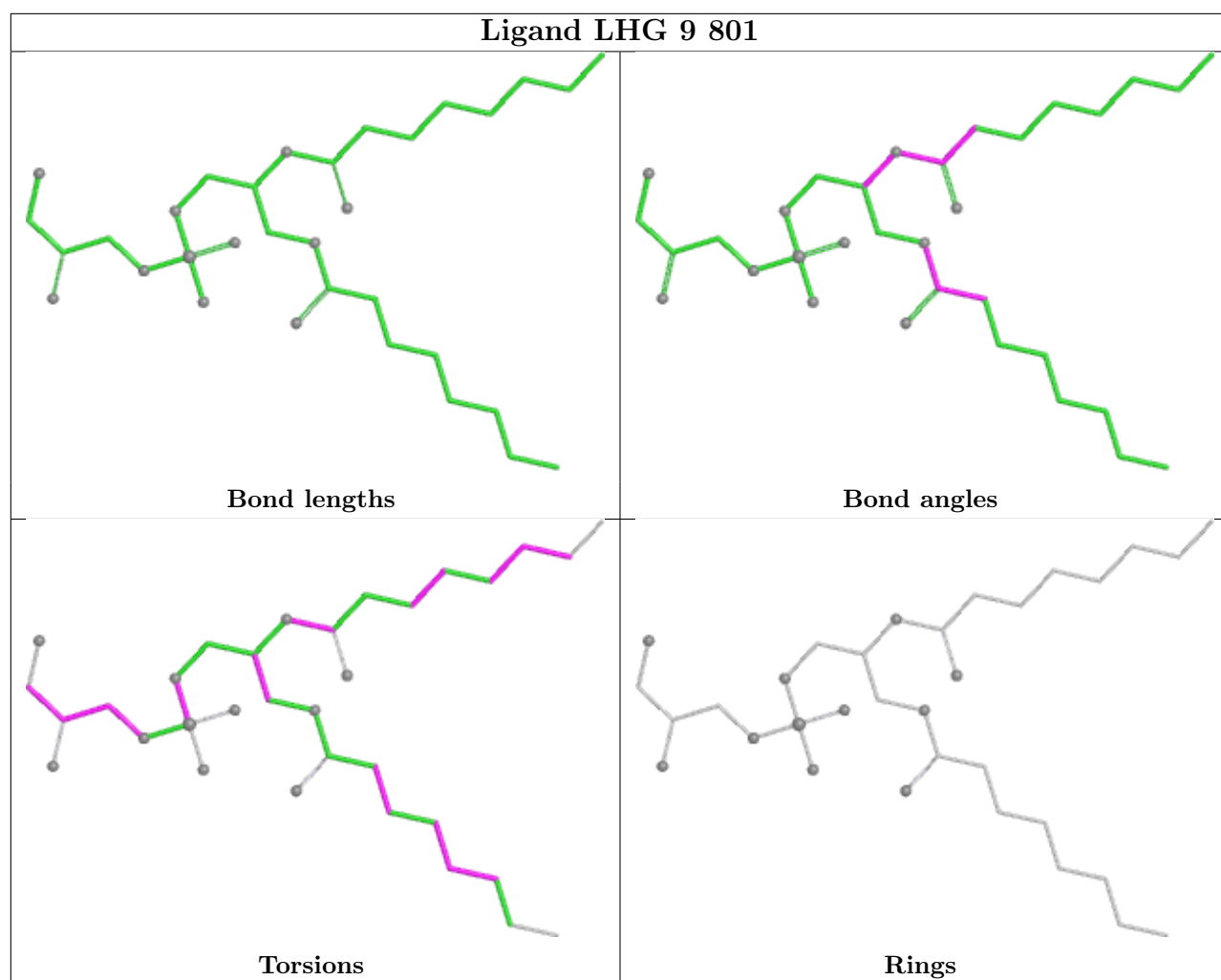


Ligand CLA 4 616

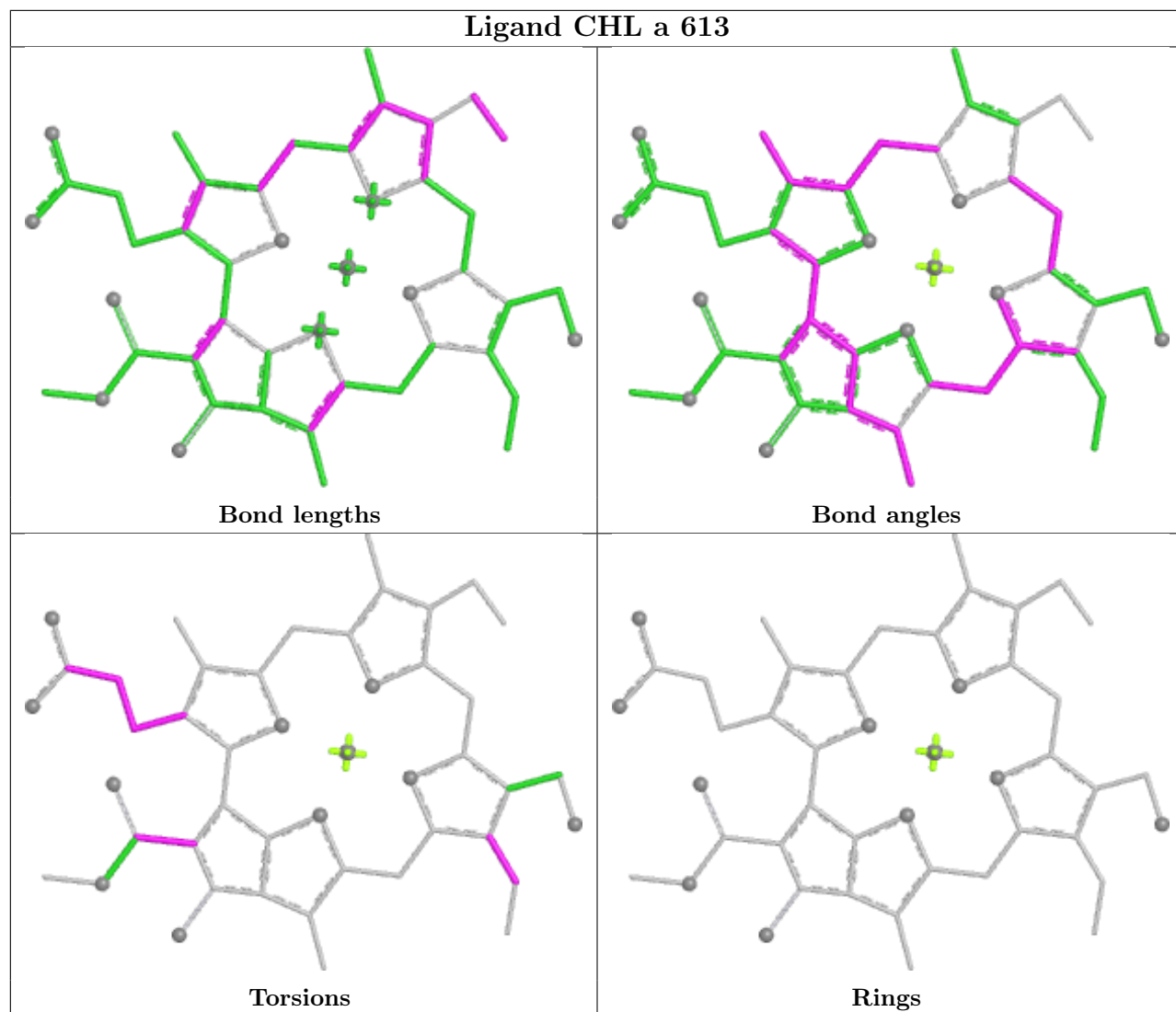


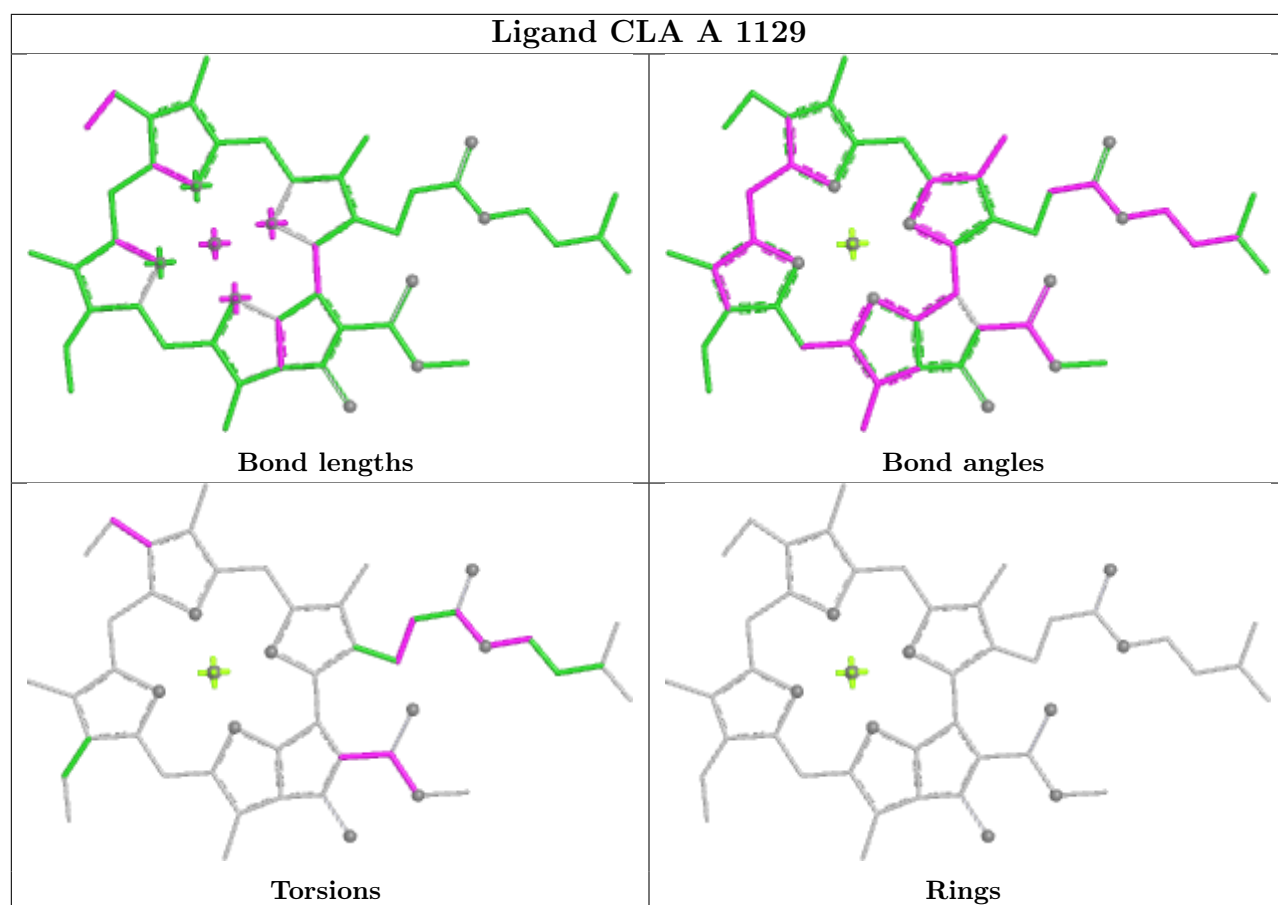
Ligand CLA 7 612

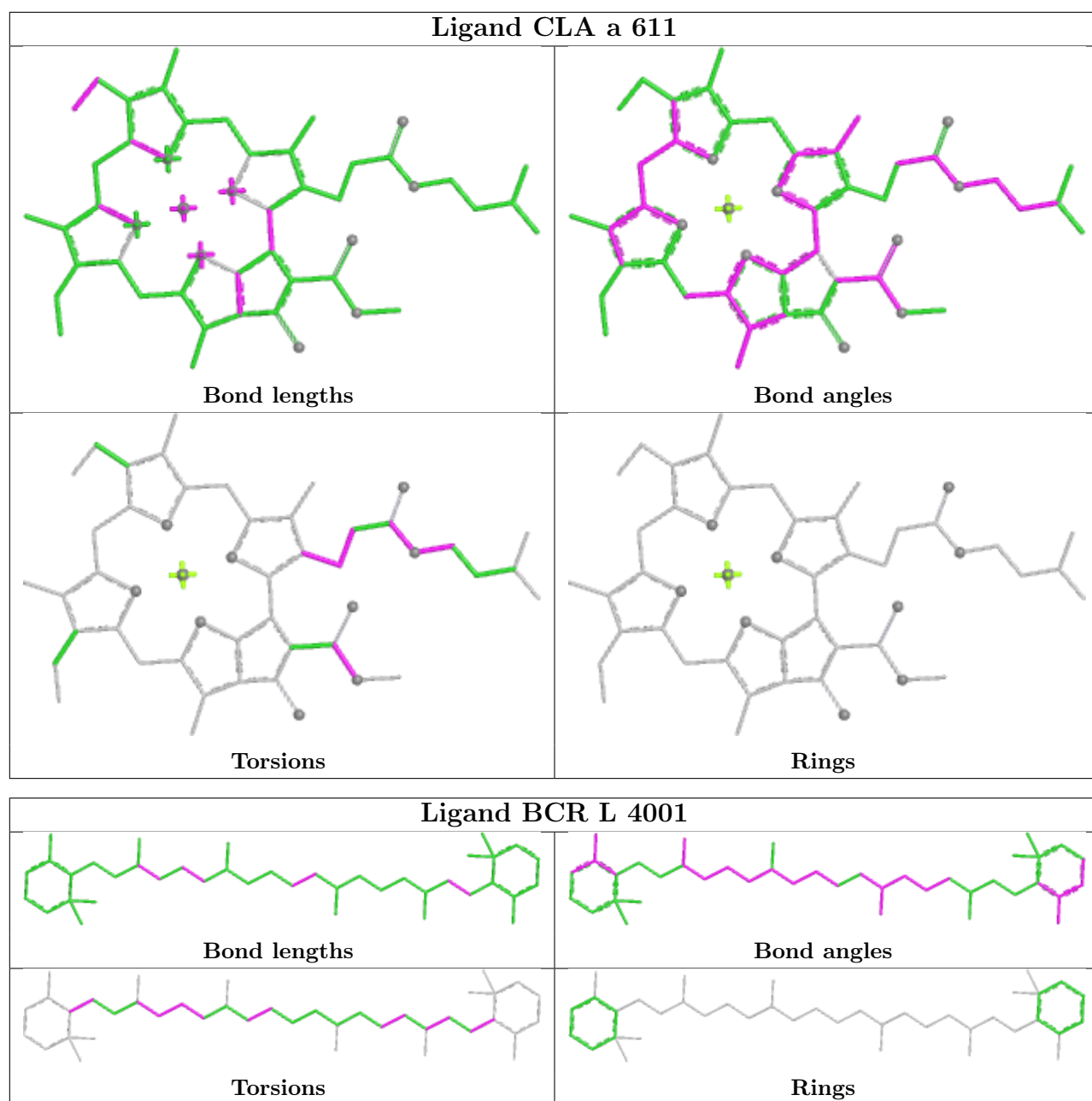




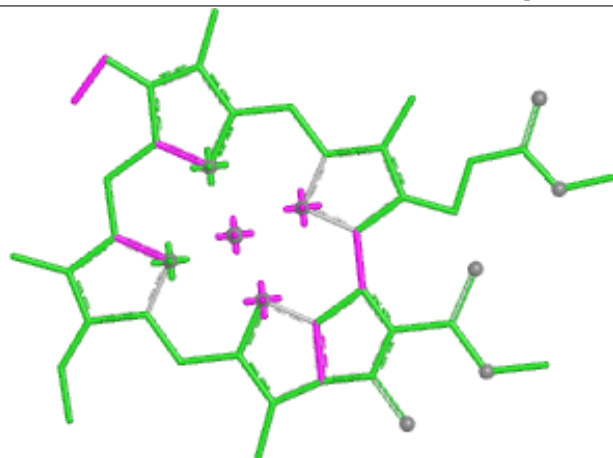
Ligand CHL a 613



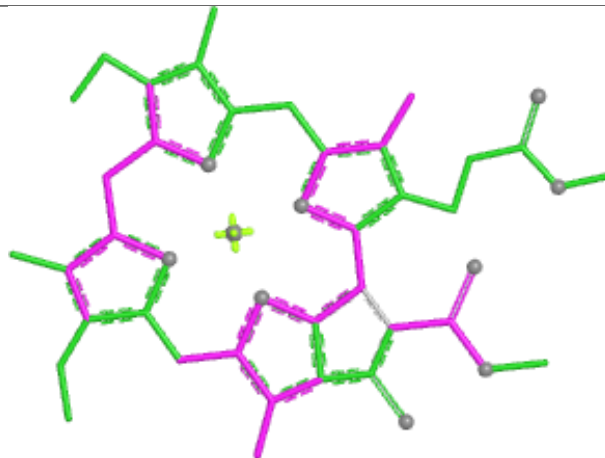




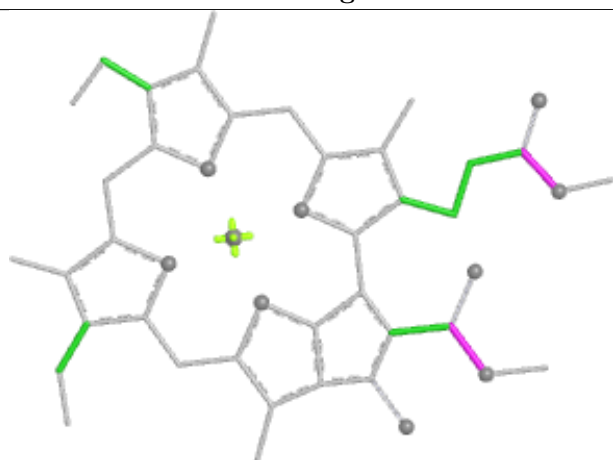
Ligand CLA 4 605



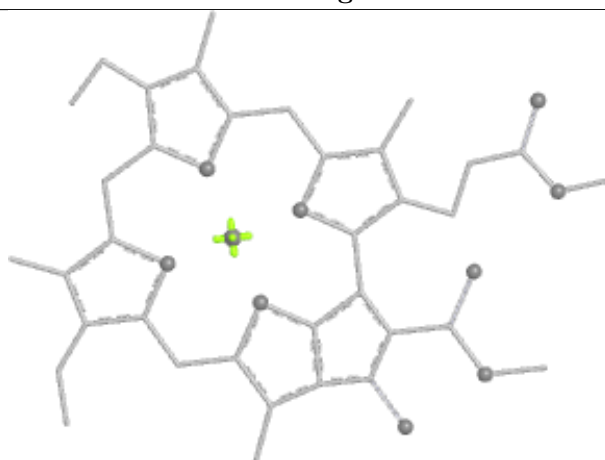
Bond lengths



Bond angles

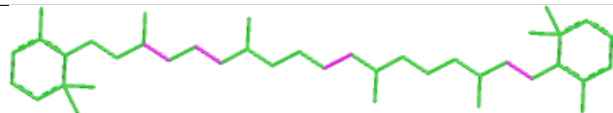


Torsions

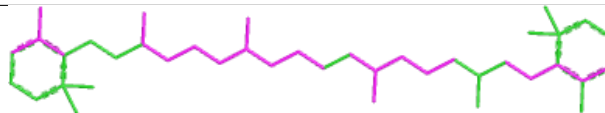


Rings

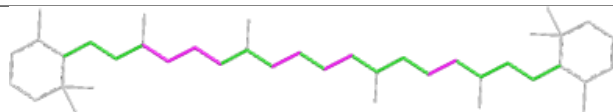
Ligand BCR B 4007



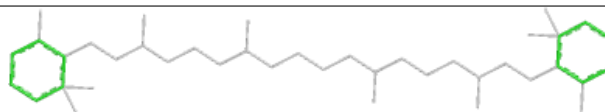
Bond lengths



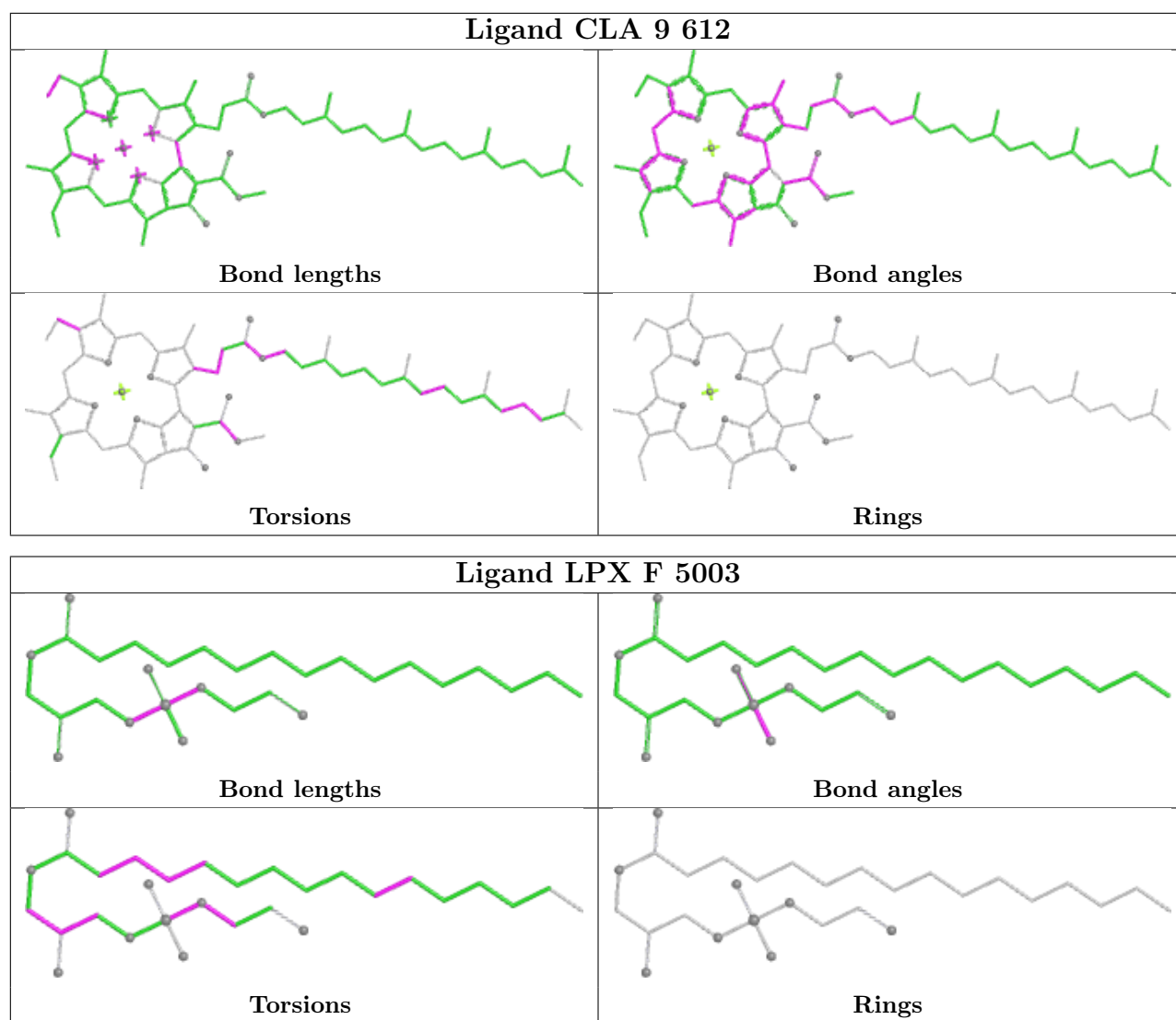
Bond angles

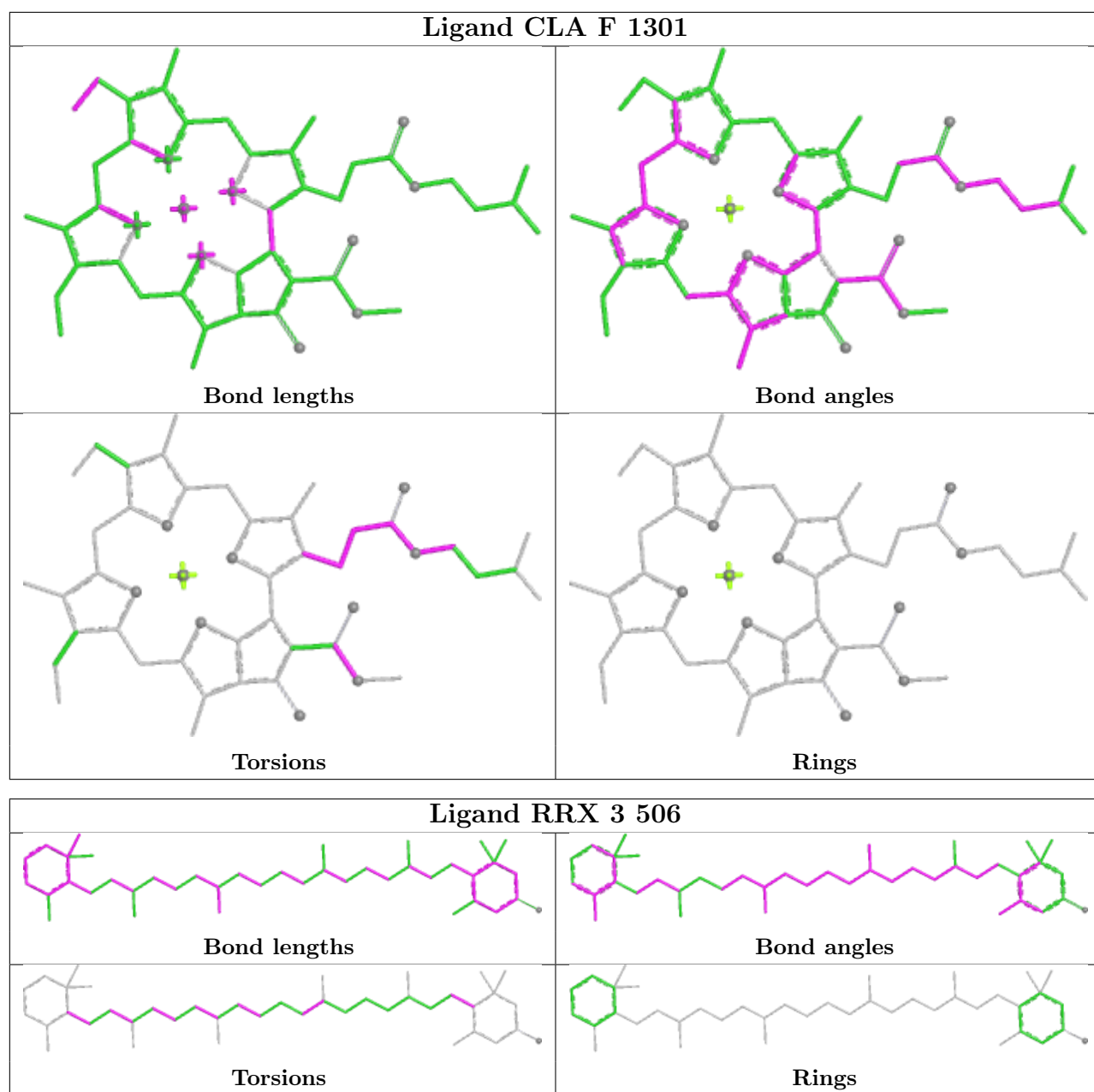


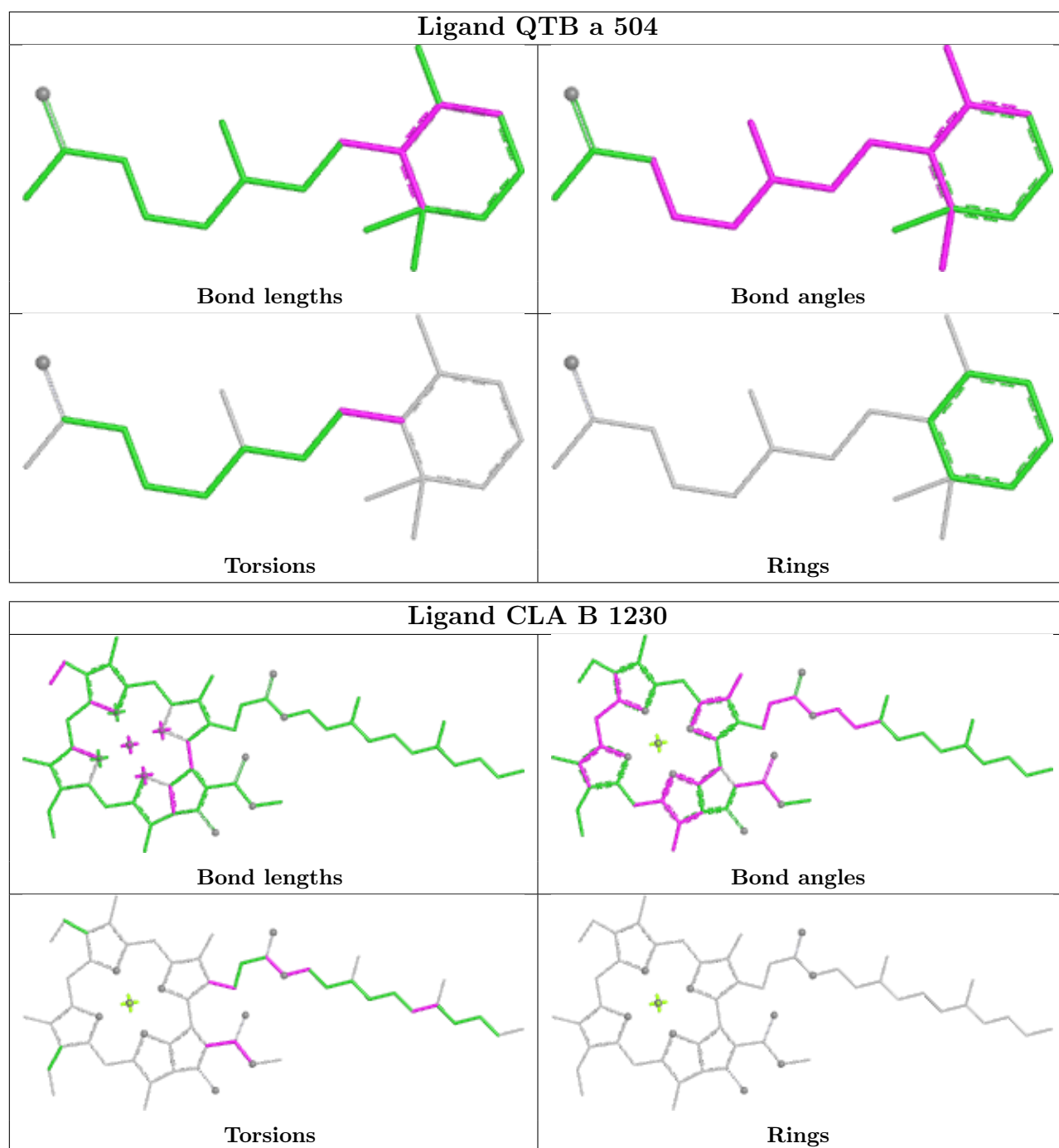
Torsions

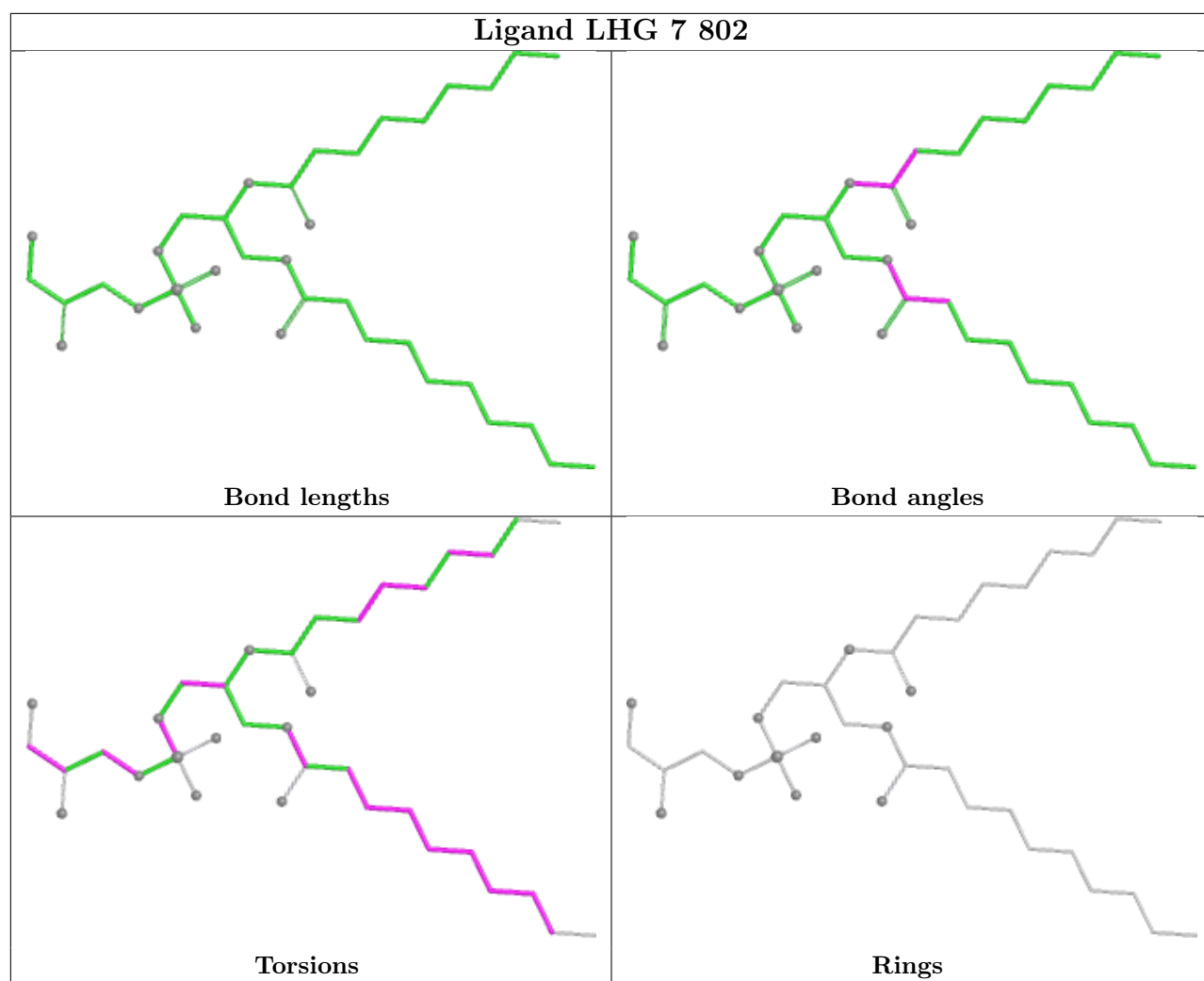


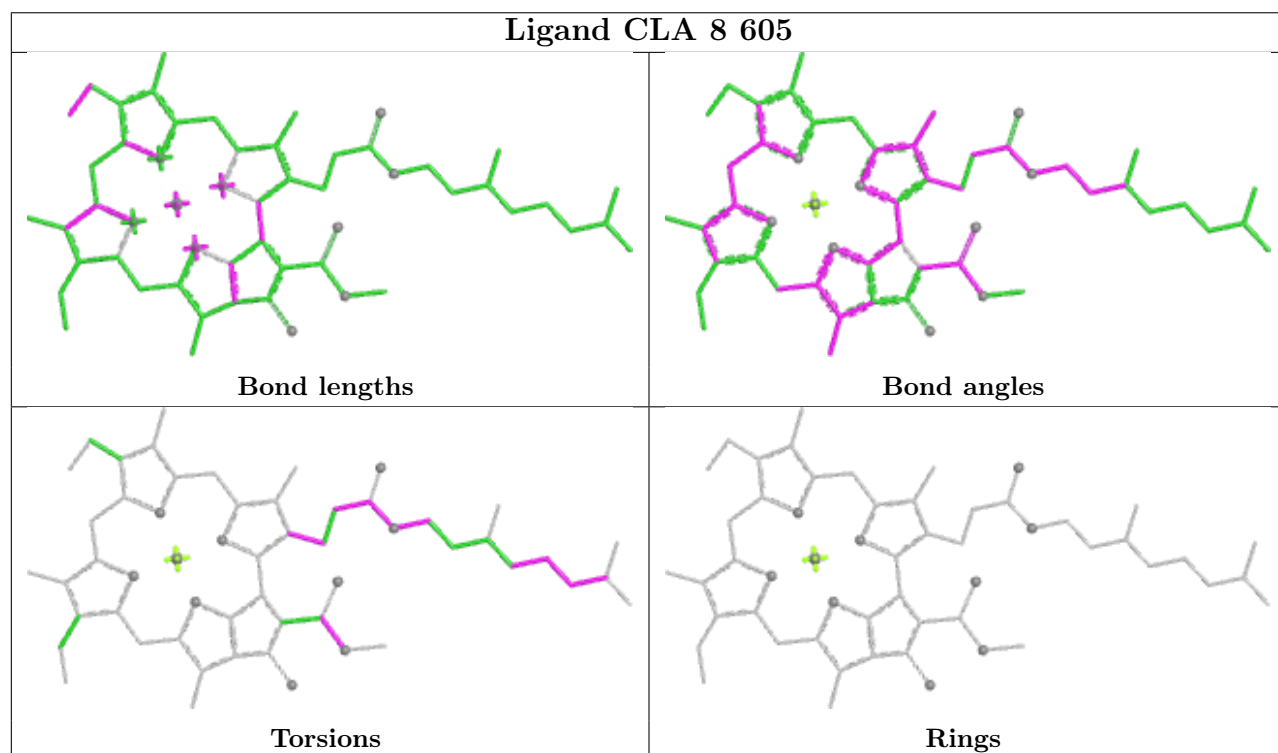
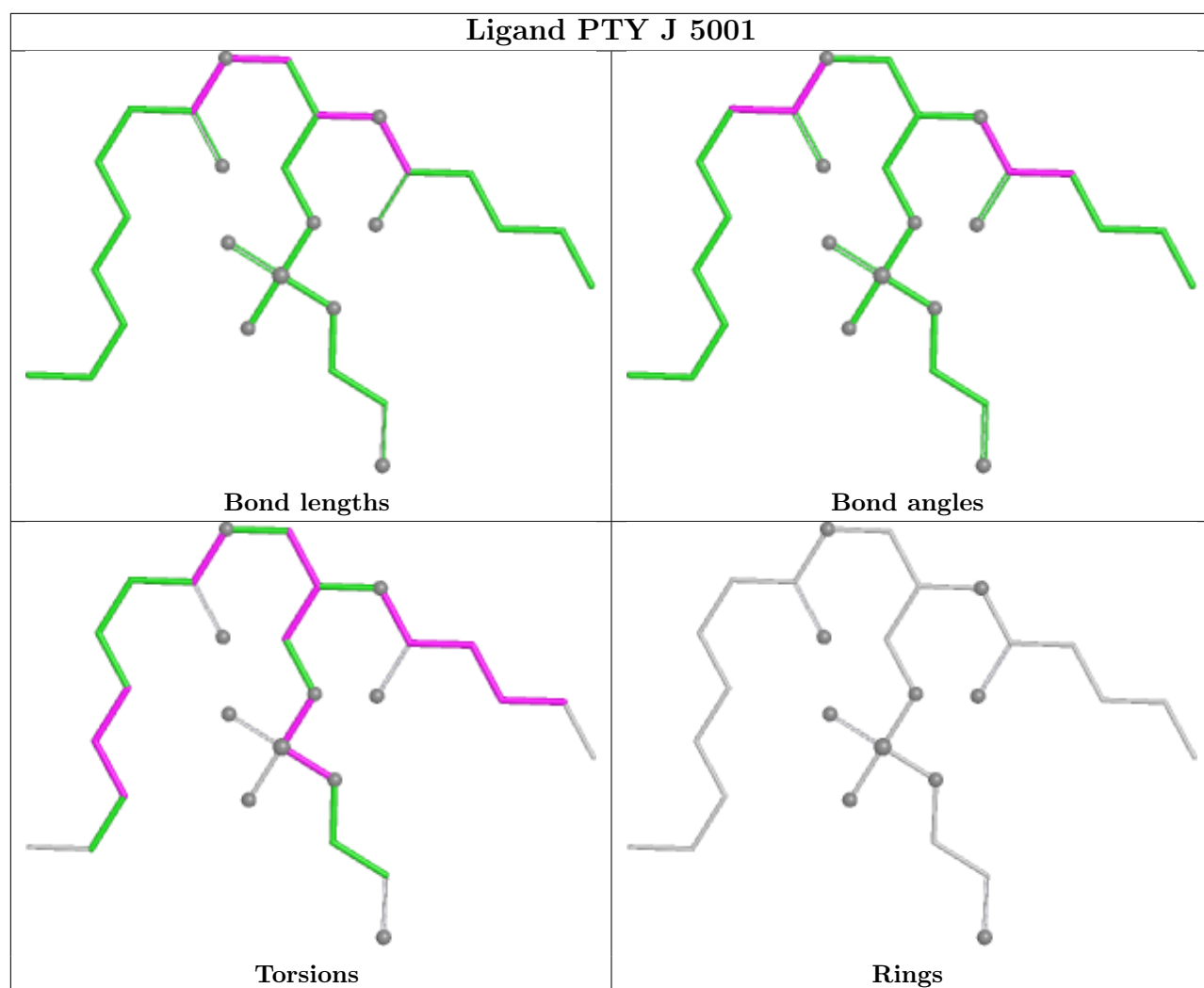
Rings

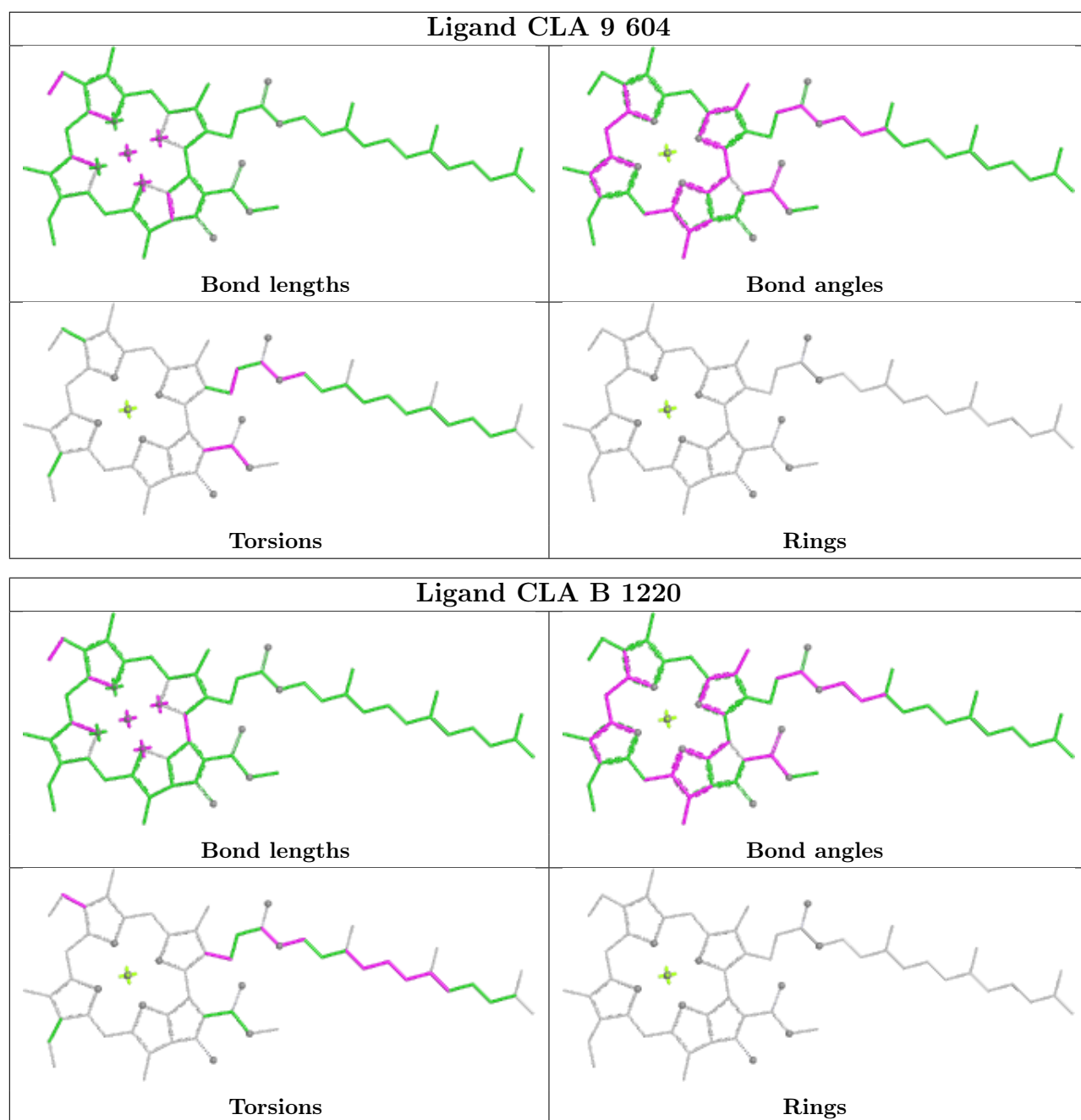




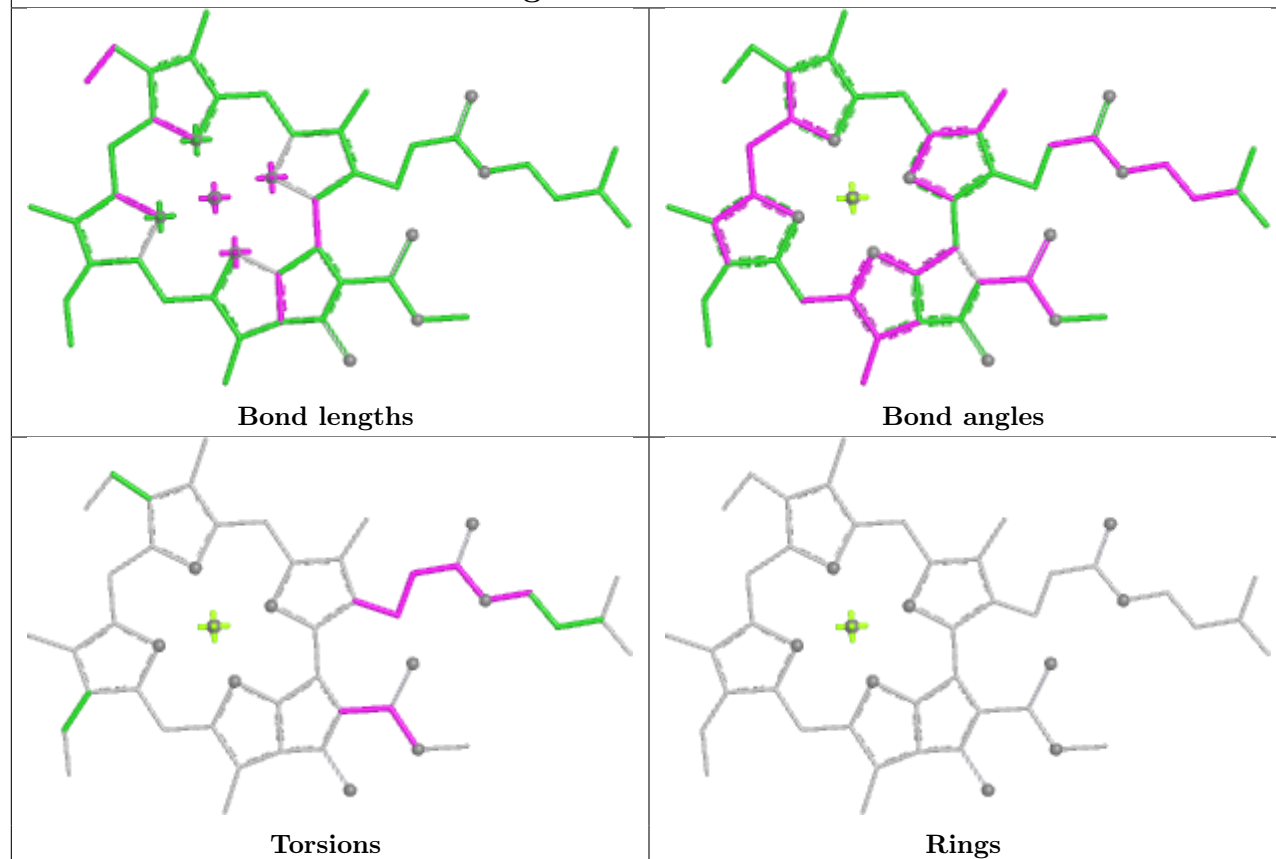




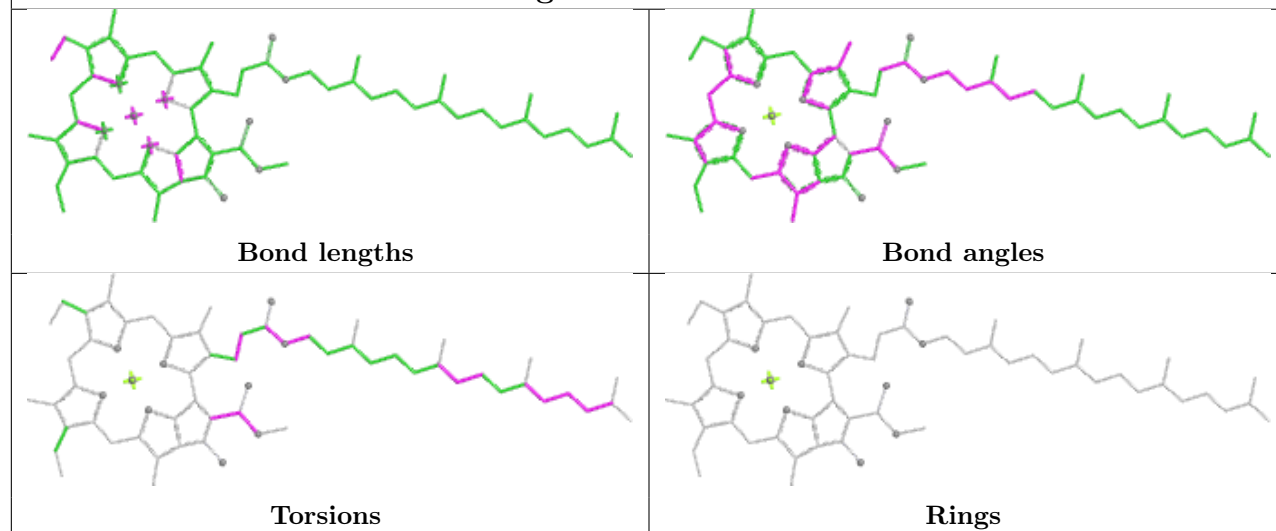


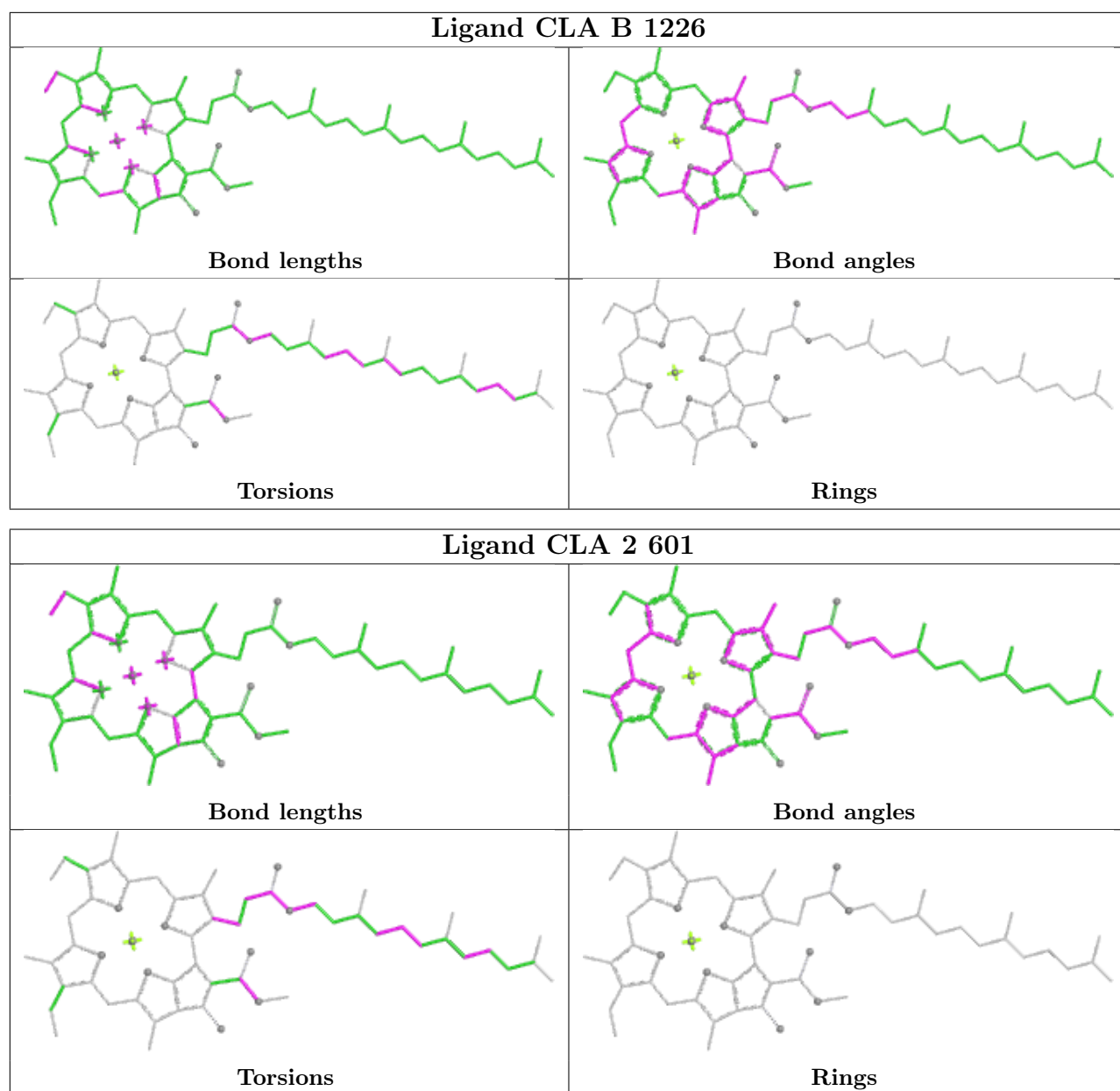


Ligand CLA B 1227

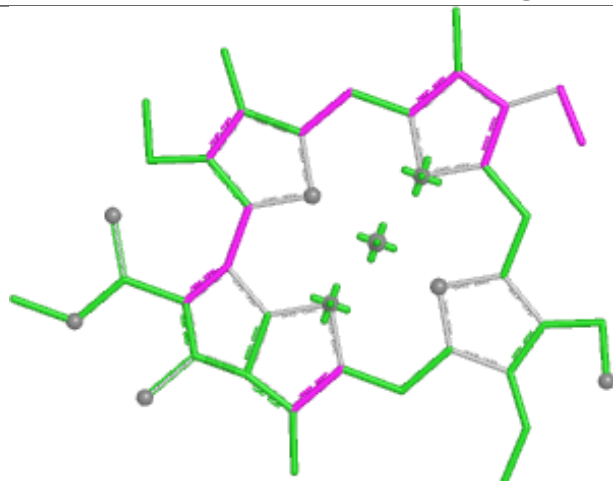


Ligand CLA 7 604

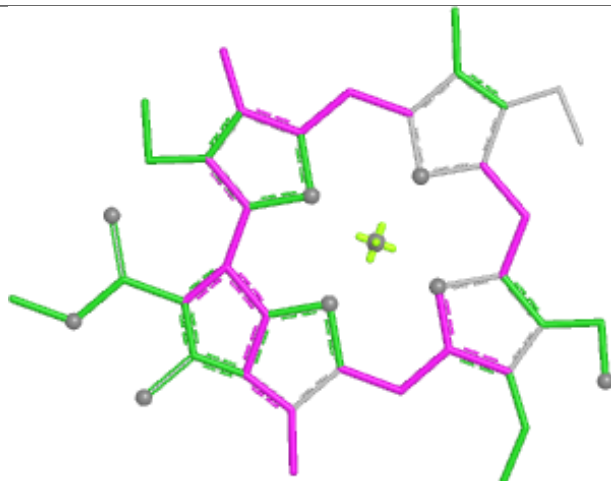




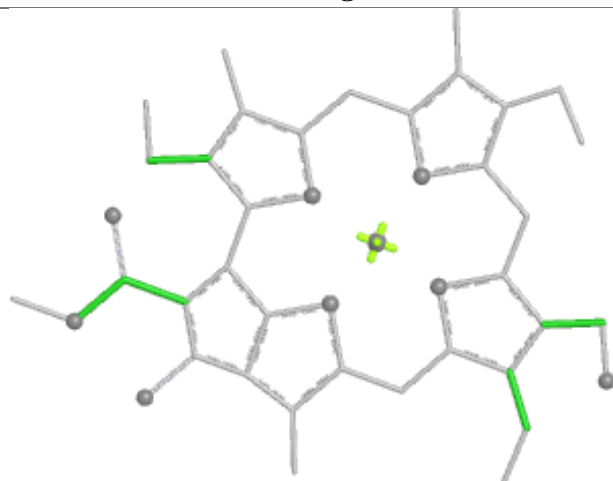
Ligand CHL 3 608



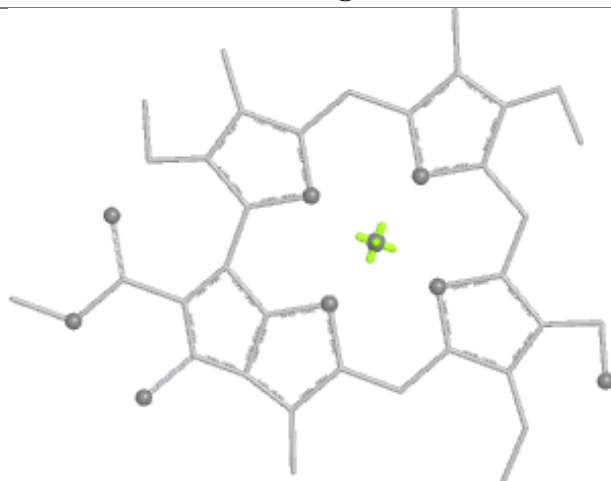
Bond lengths



Bond angles

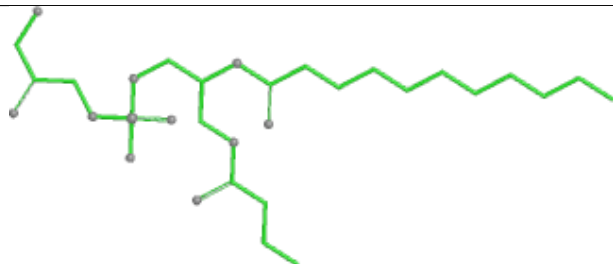


Torsions

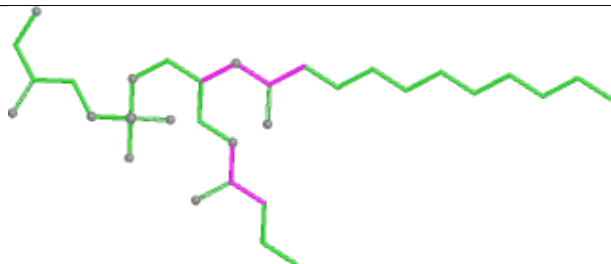


Rings

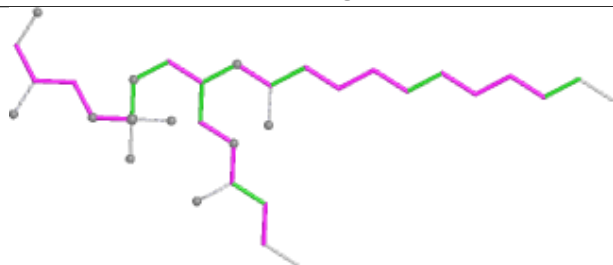
Ligand LHG 4 802



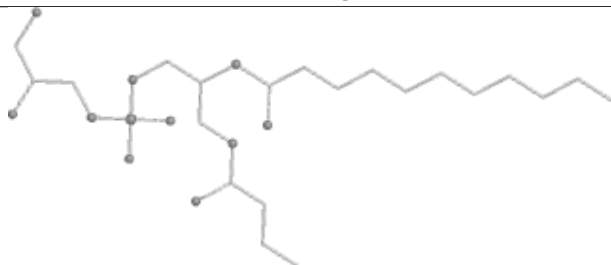
Bond lengths



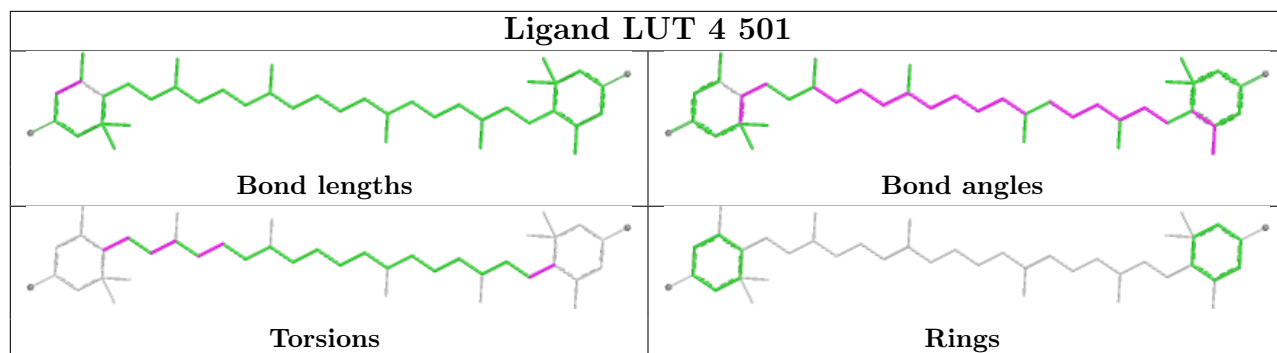
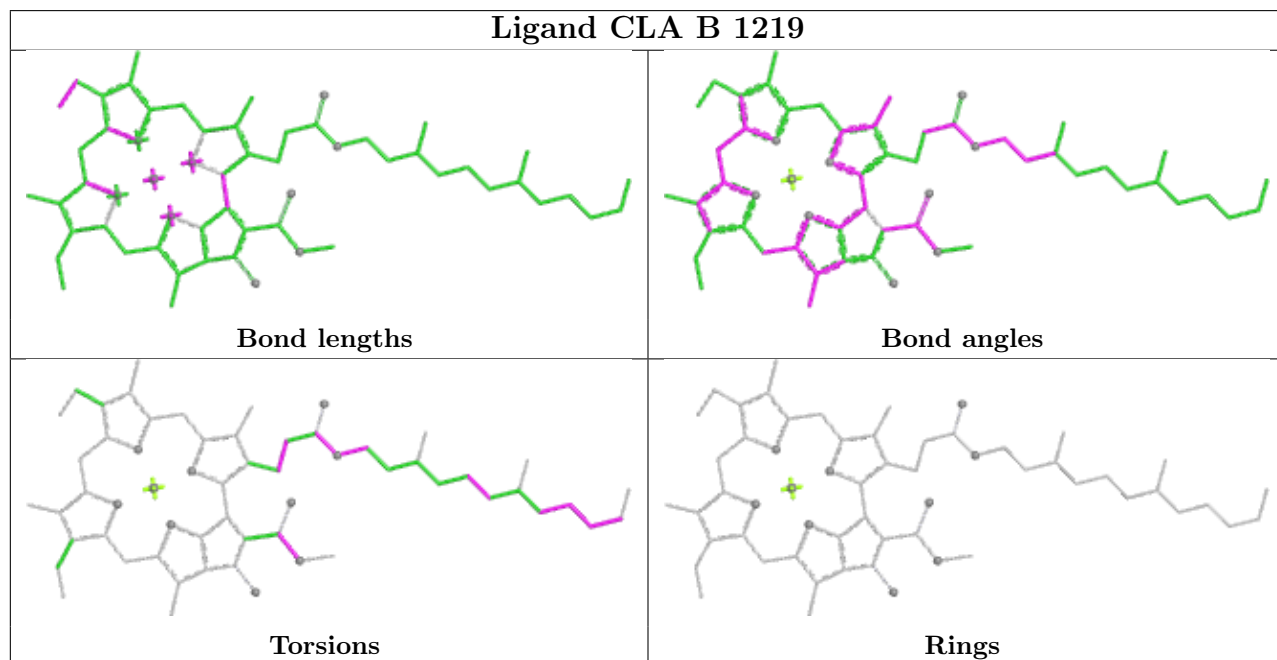
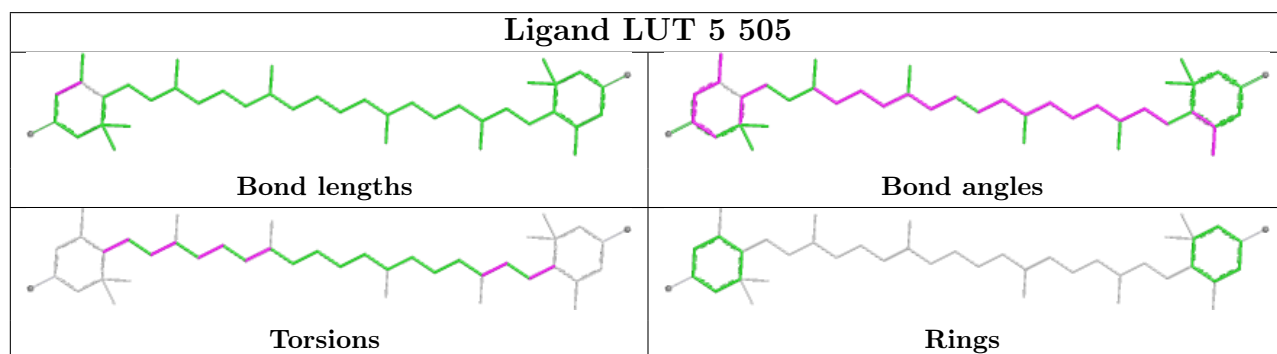
Bond angles

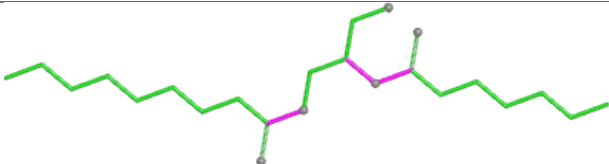
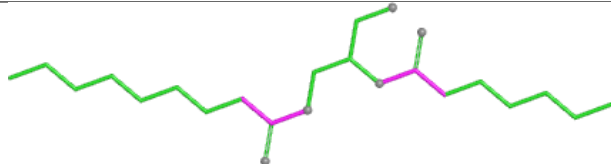
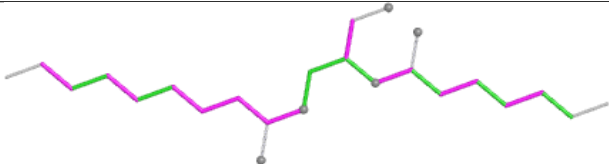
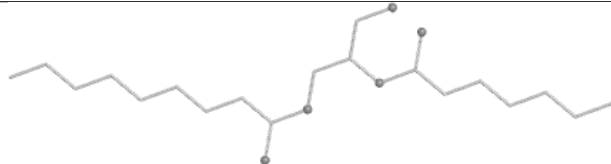


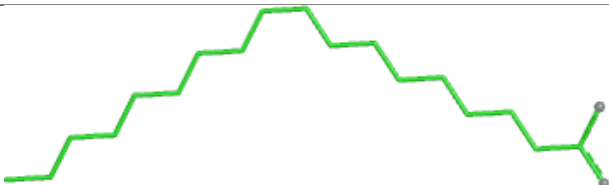
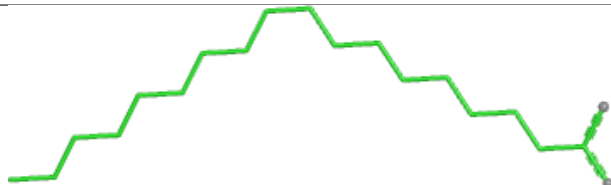
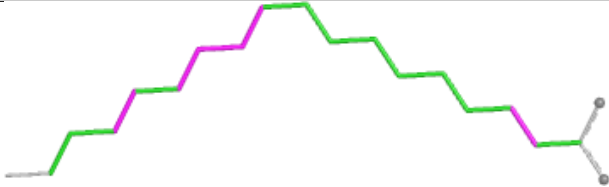
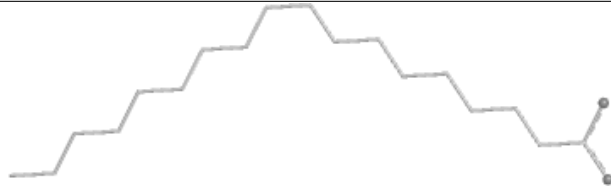
Torsions

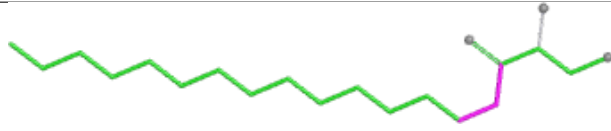
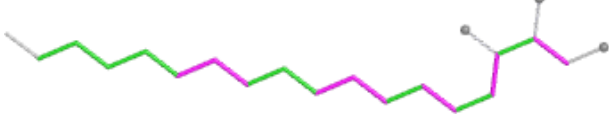
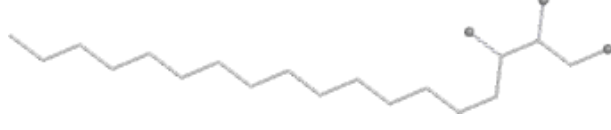


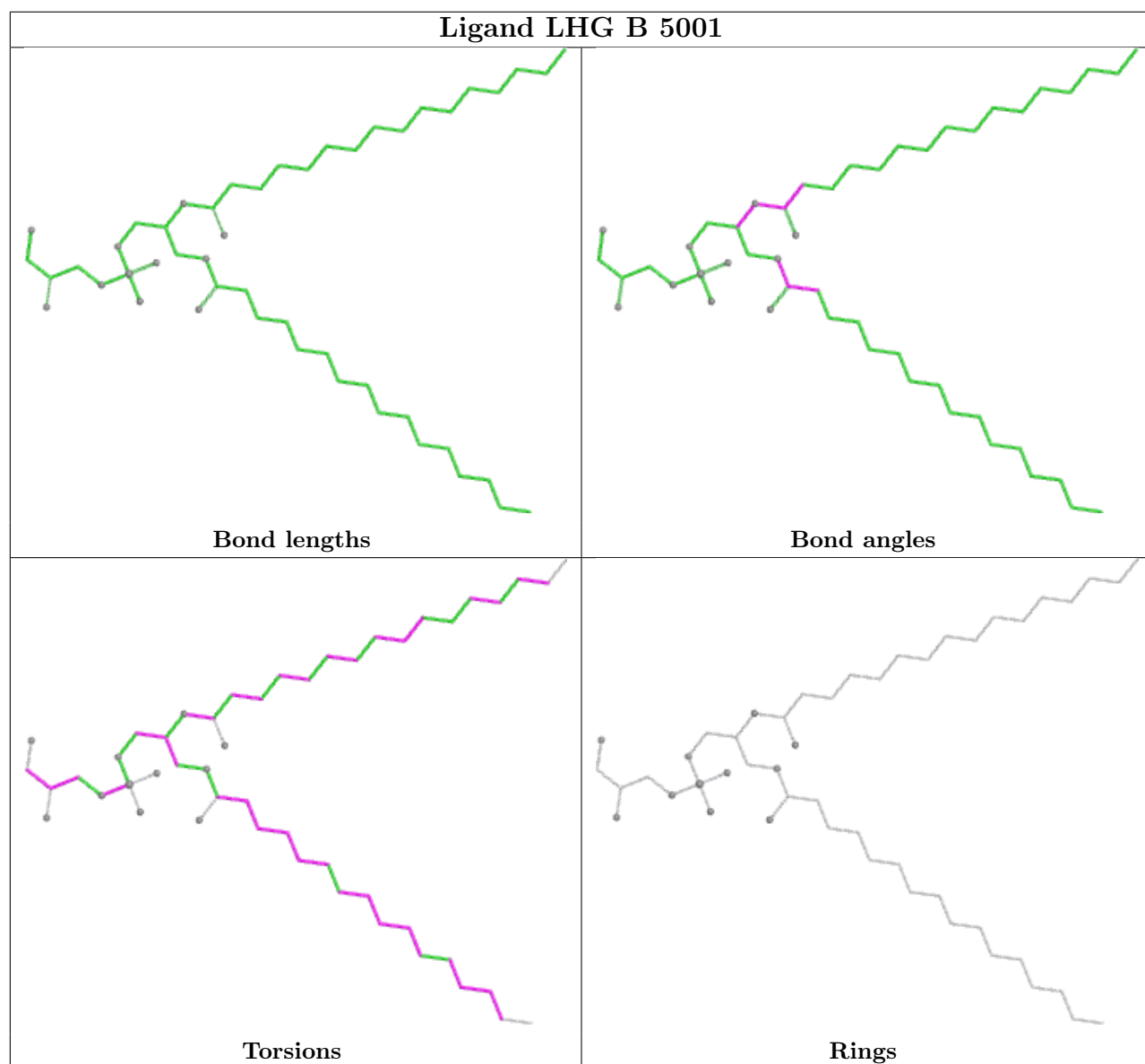
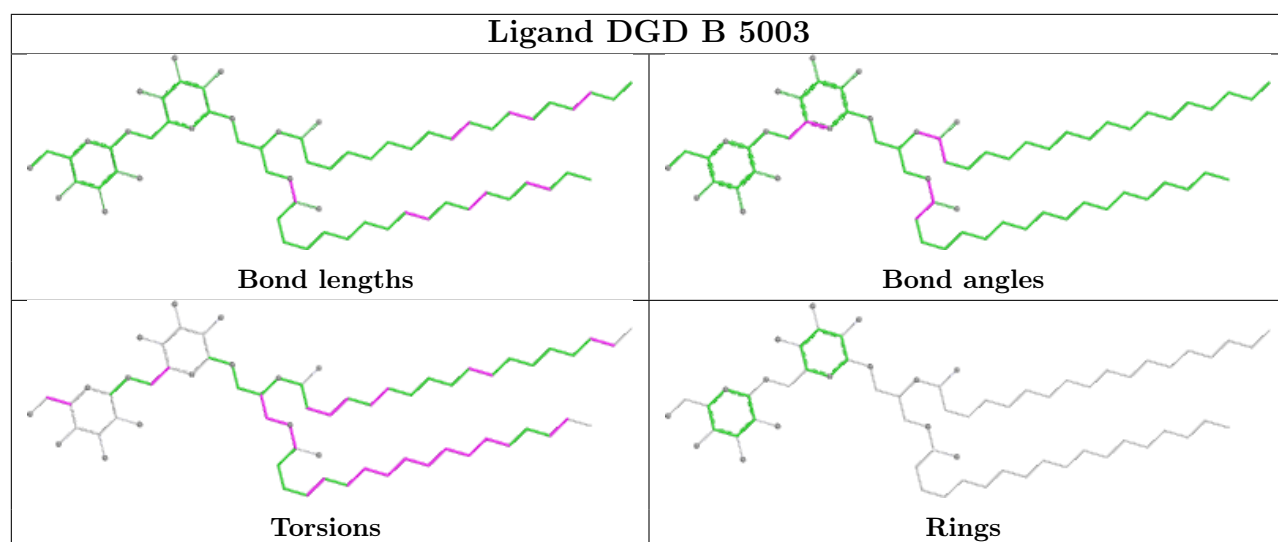
Rings

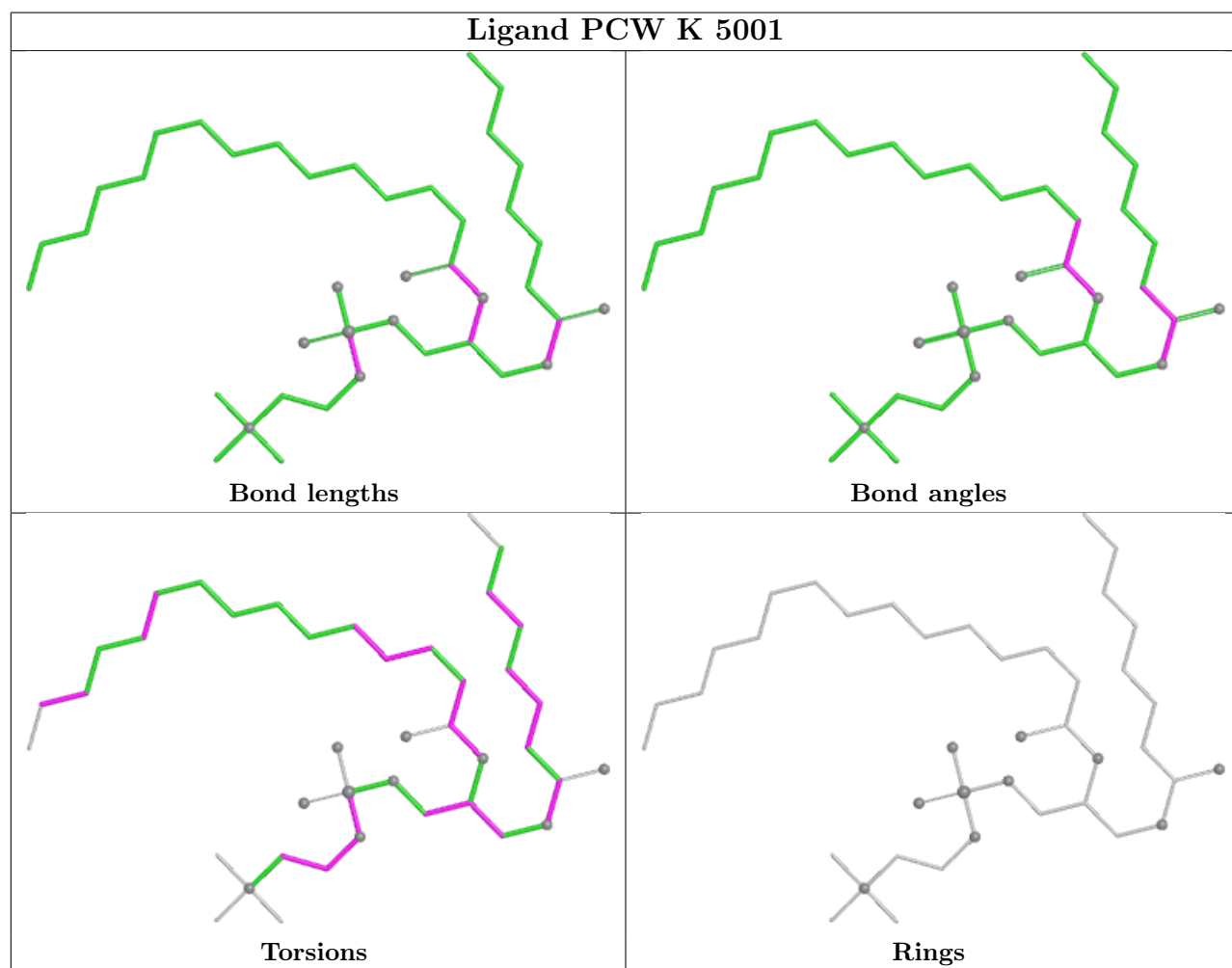
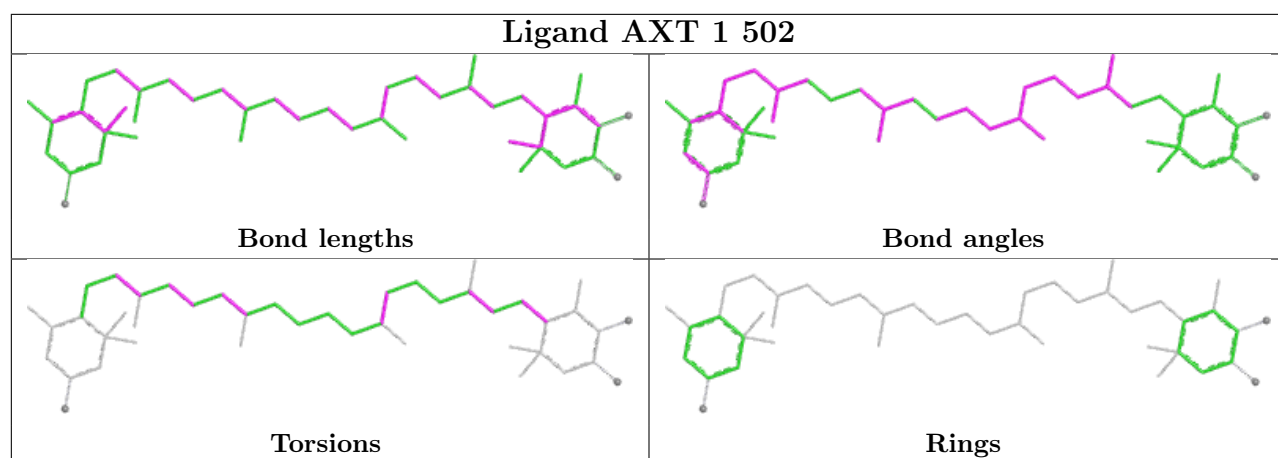
Ligand LUT 4 501**Ligand CLA B 1219****Ligand LUT 5 505**

Ligand DGA 3 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

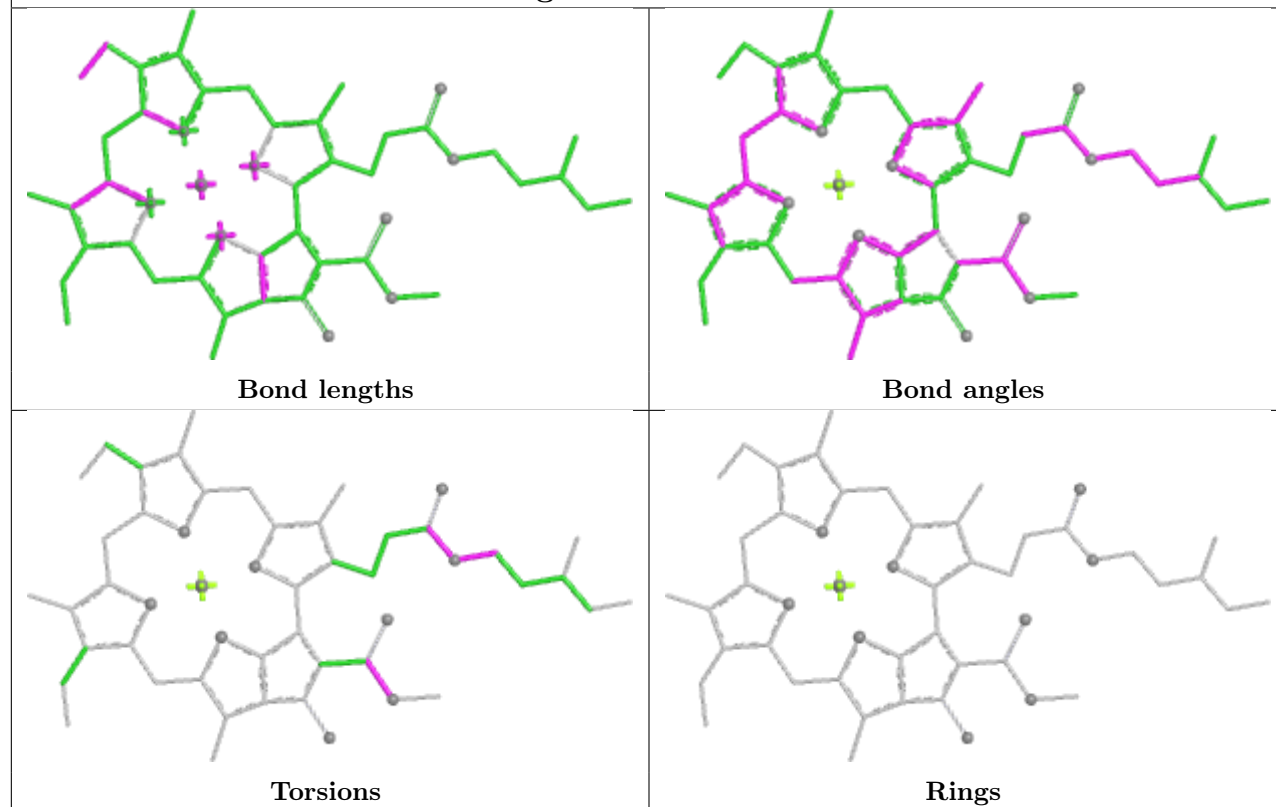
Ligand OLA 8 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPH 6 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

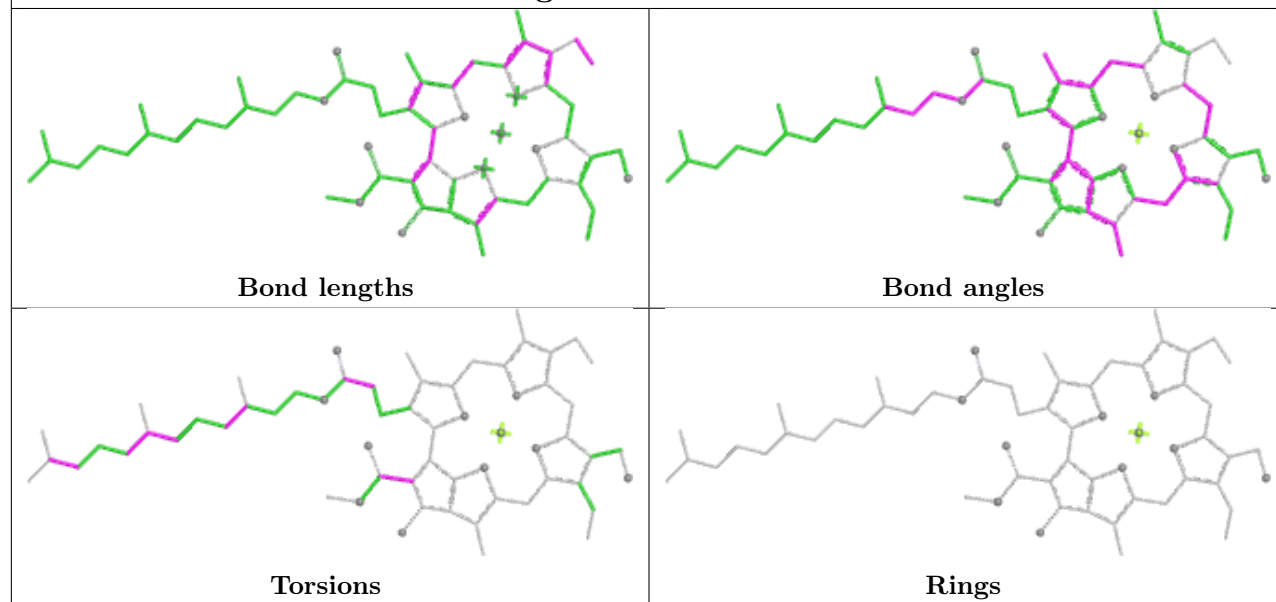


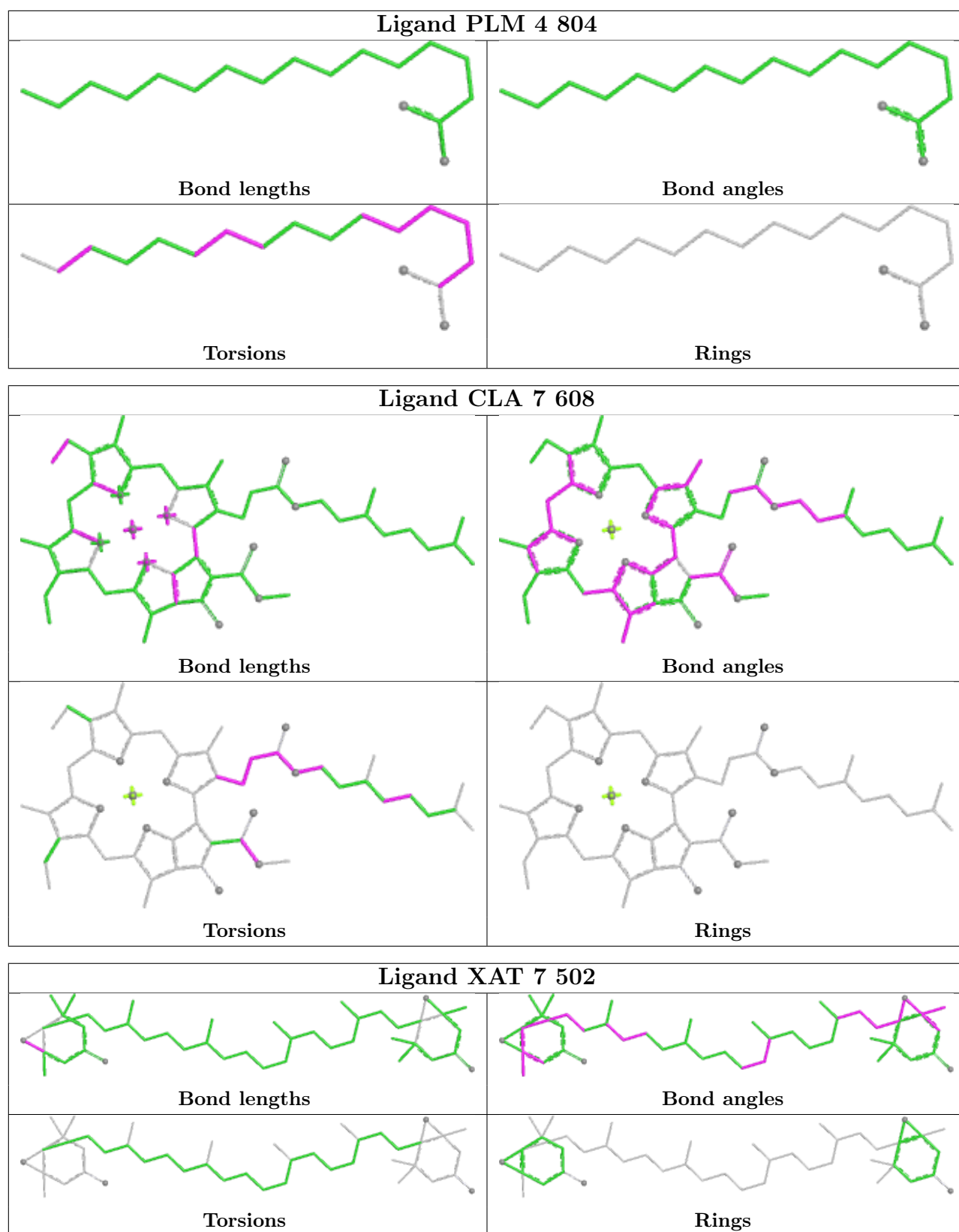


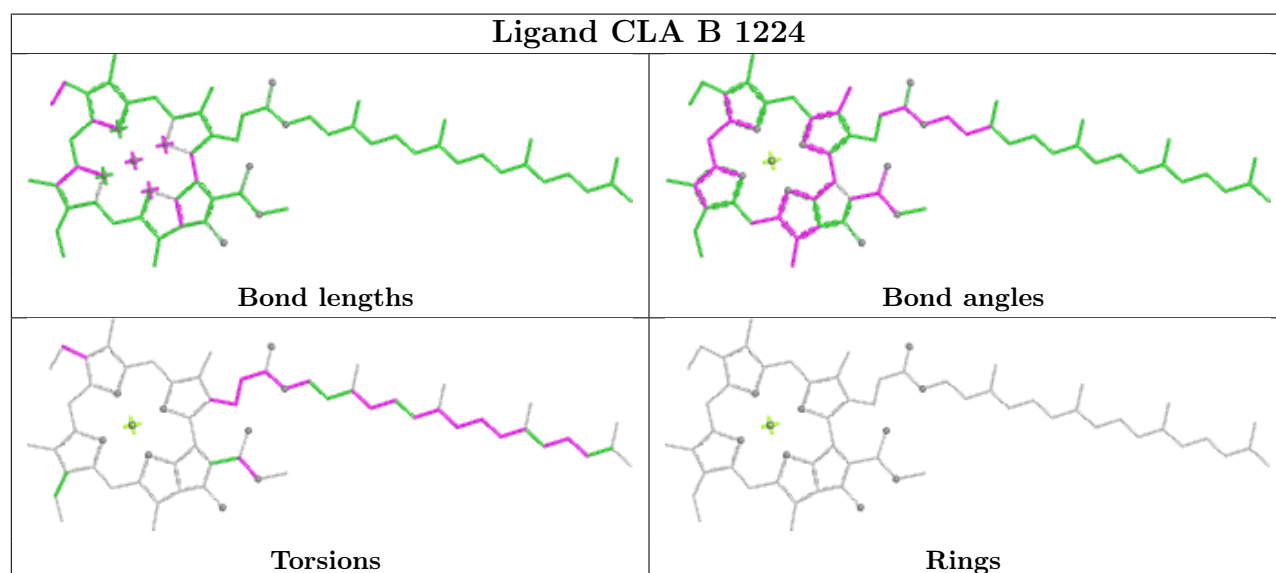
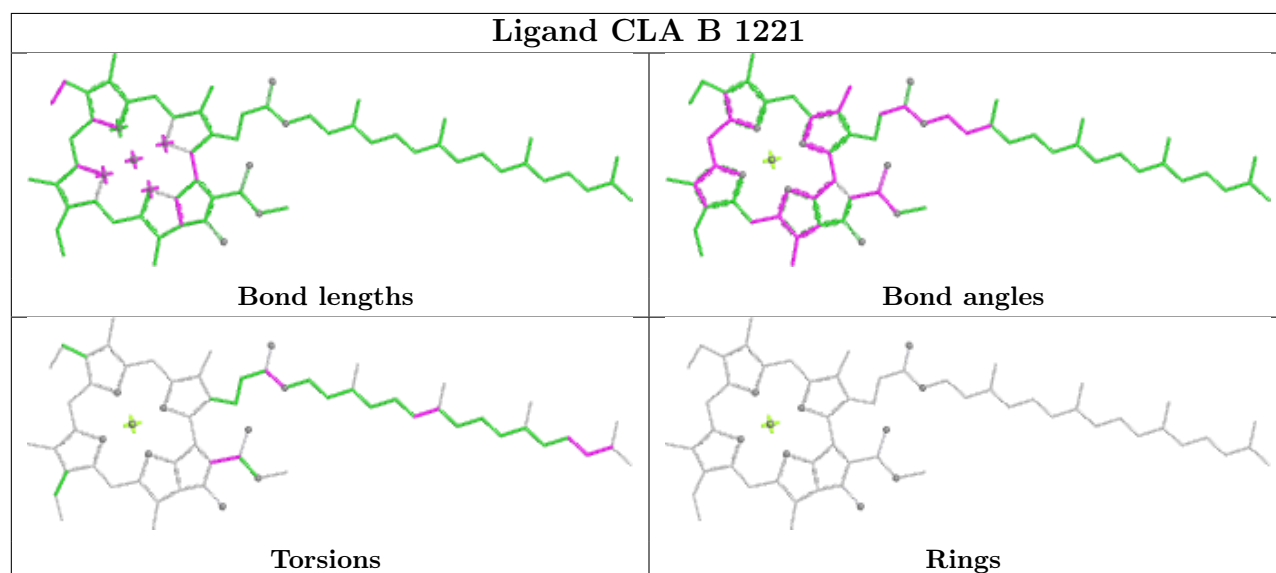
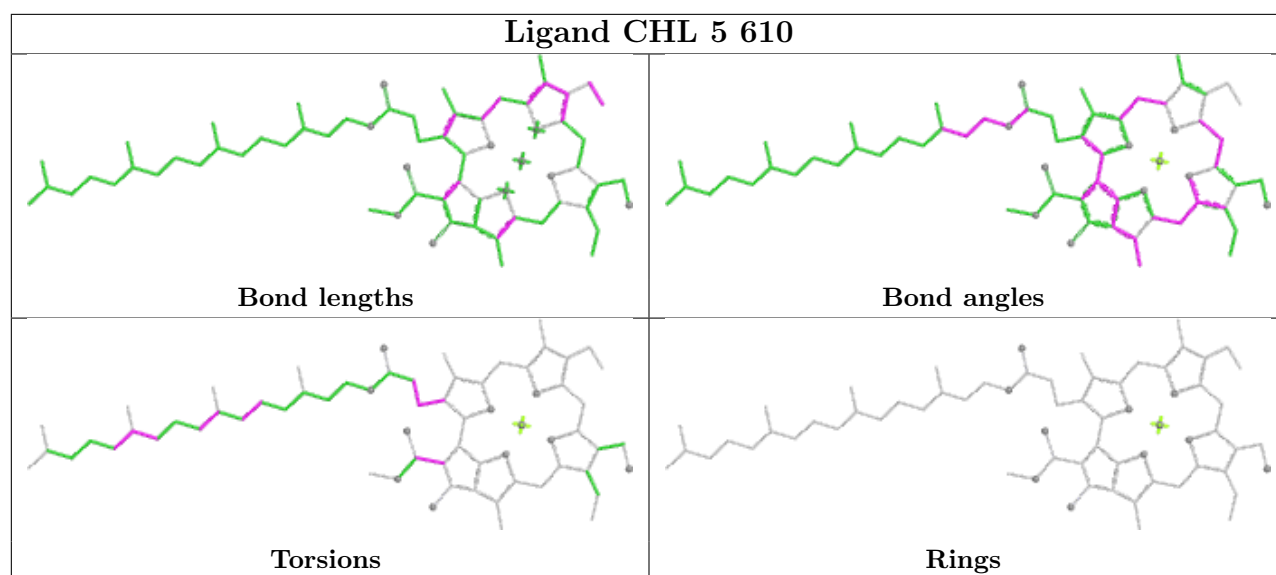
Ligand CLA 4 608



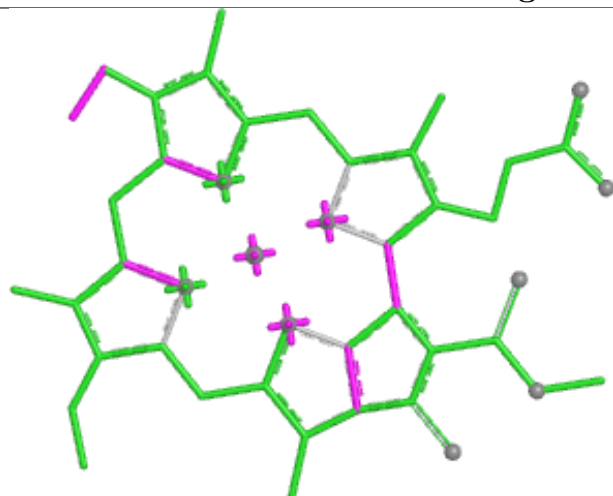
Ligand CHL 3 611



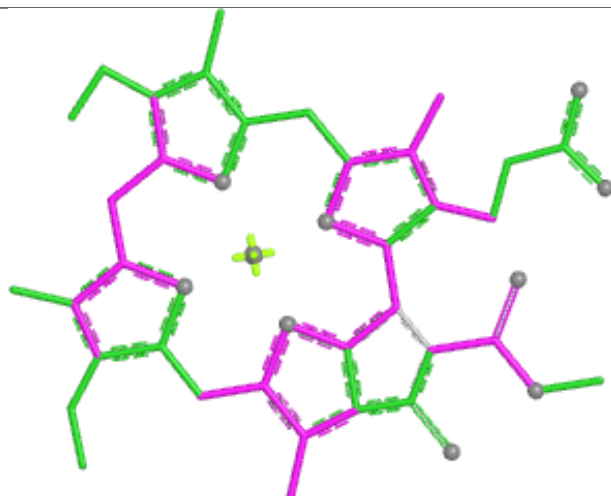




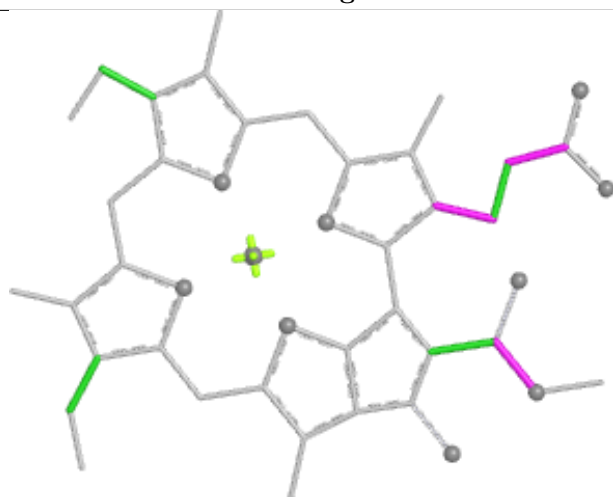
Ligand CLA 1 602



Bond lengths



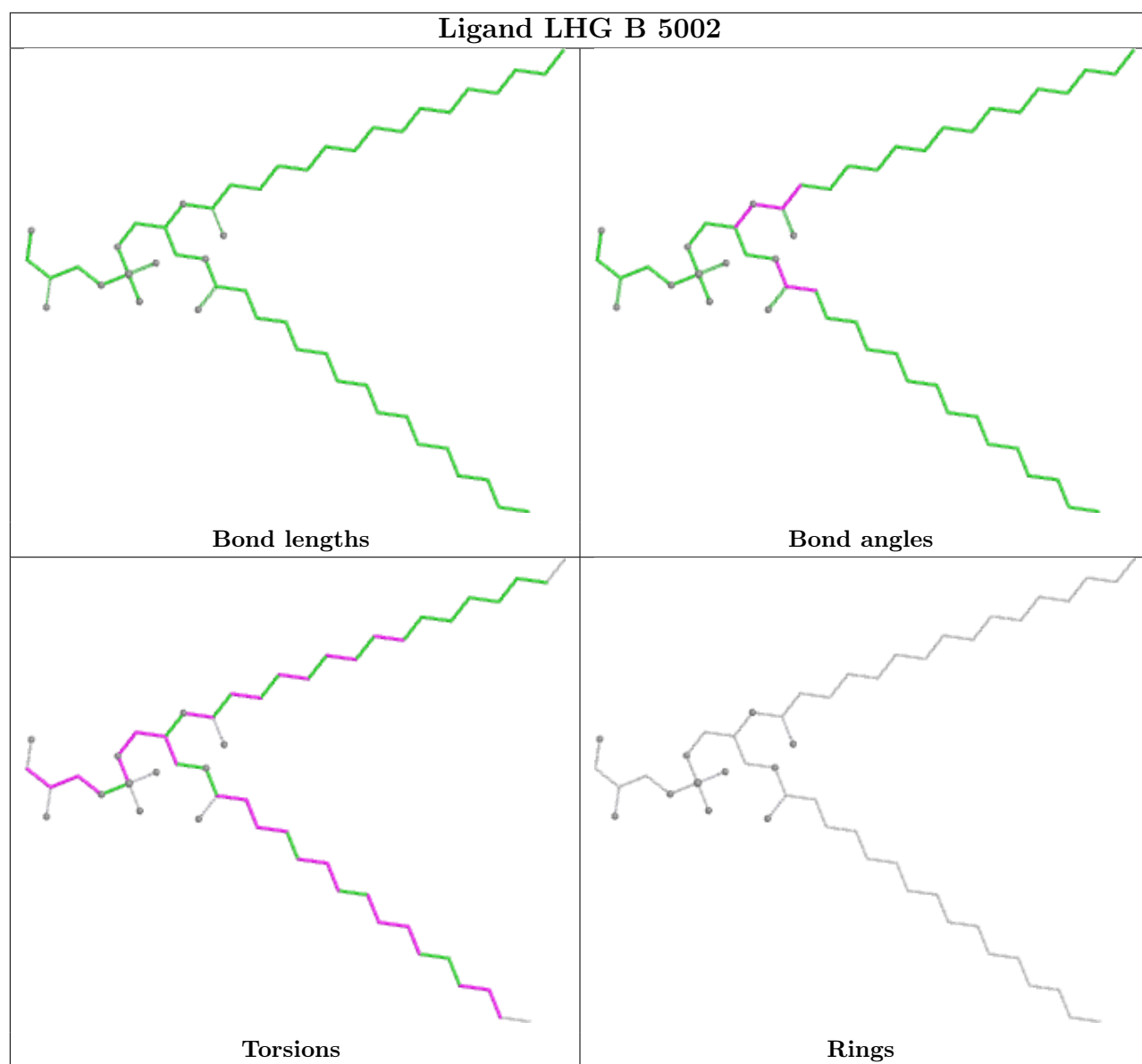
Bond angles



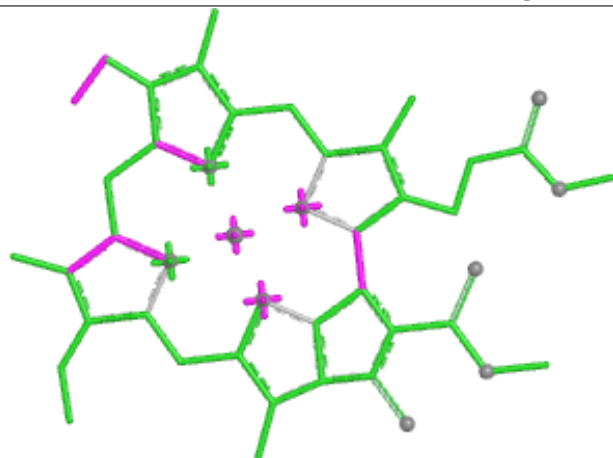
Torsions



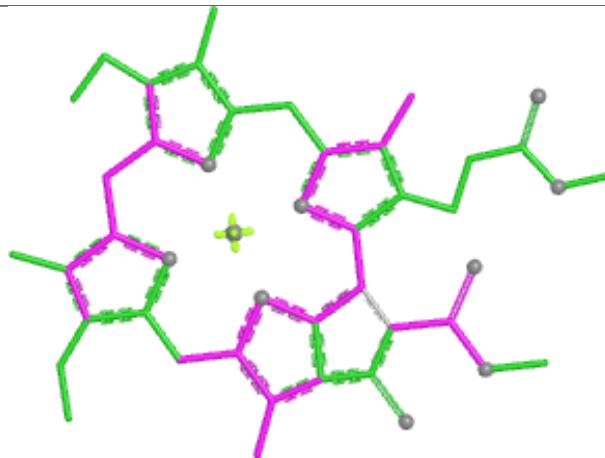
Rings



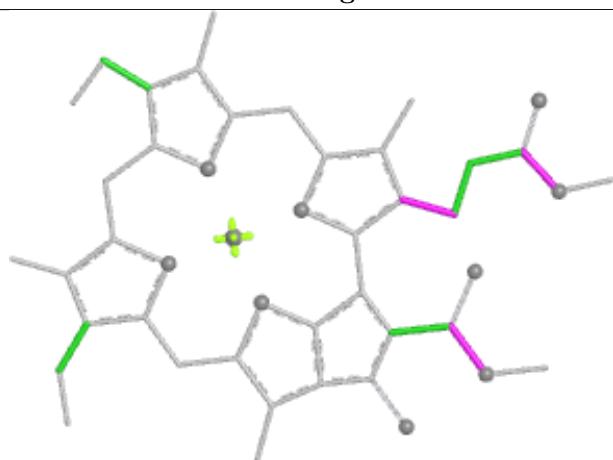
Ligand CLA 9 609



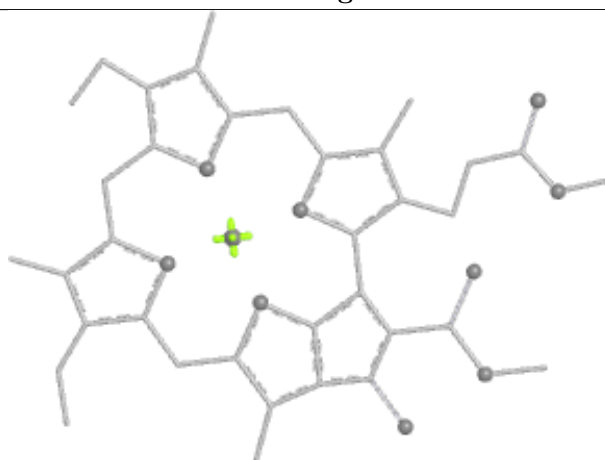
Bond lengths



Bond angles

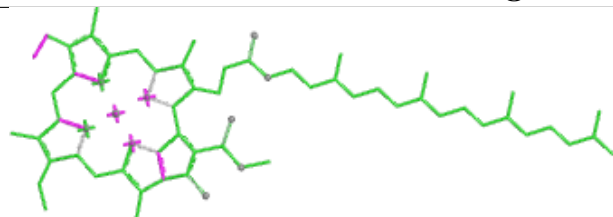


Torsions

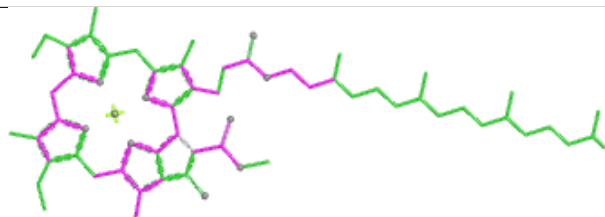


Rings

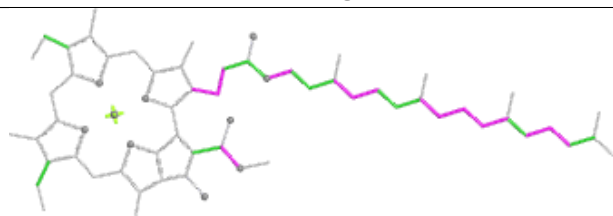
Ligand CLA B 1216



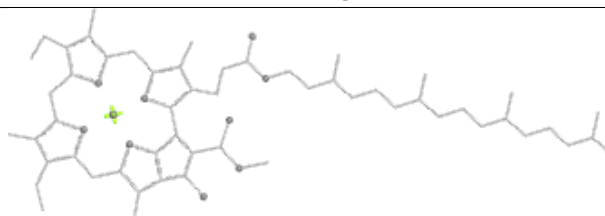
Bond lengths



Bond angles

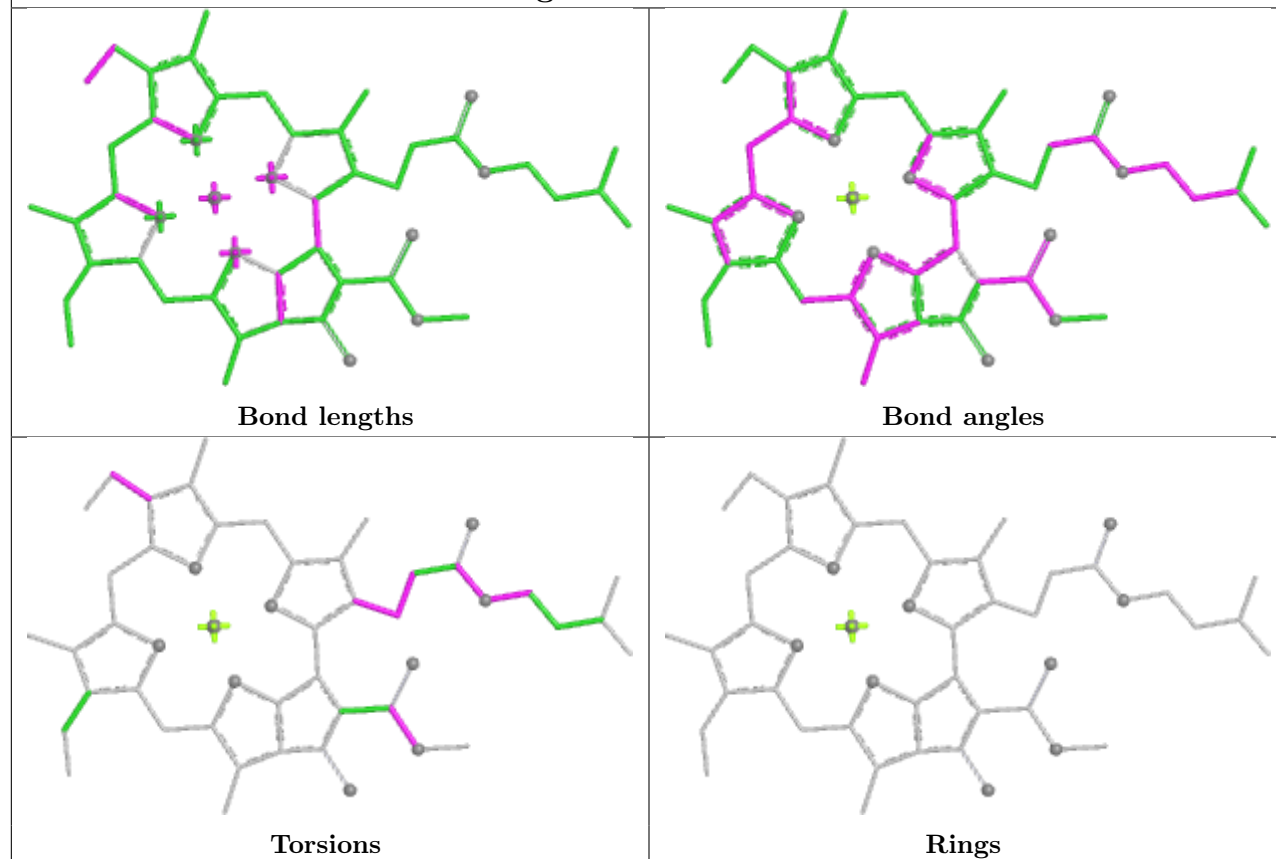


Torsions

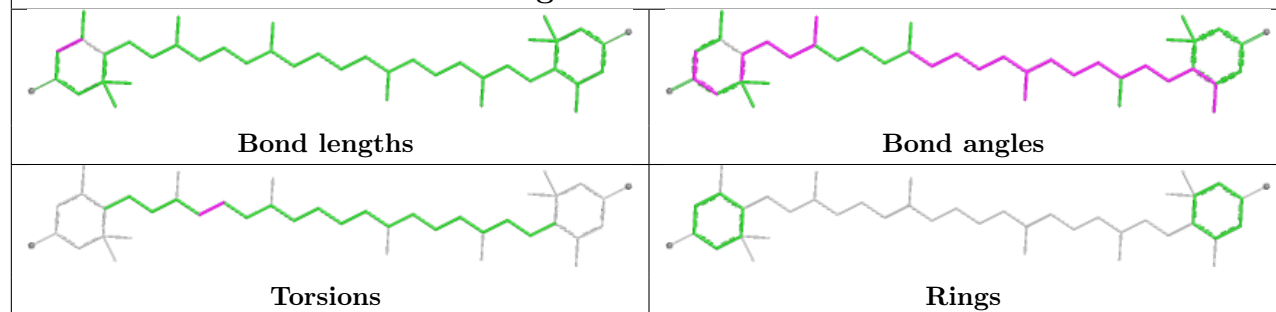


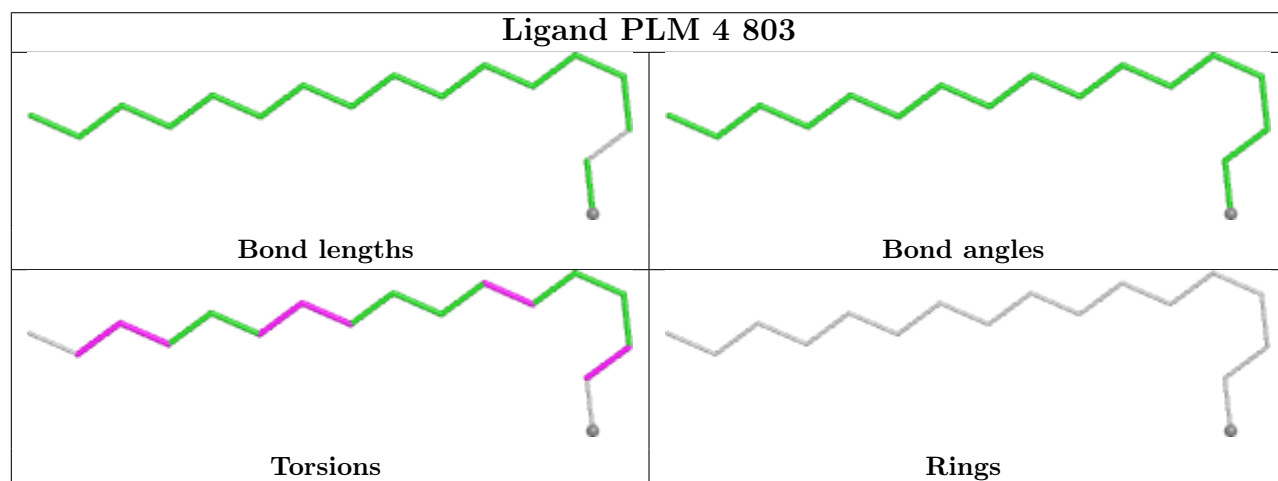
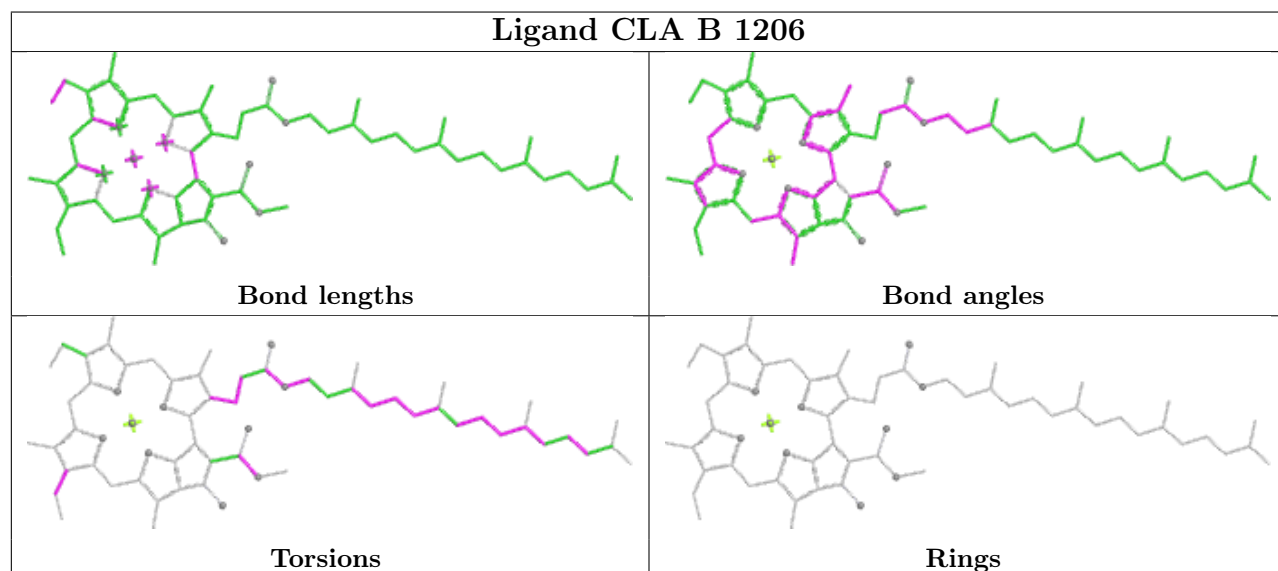
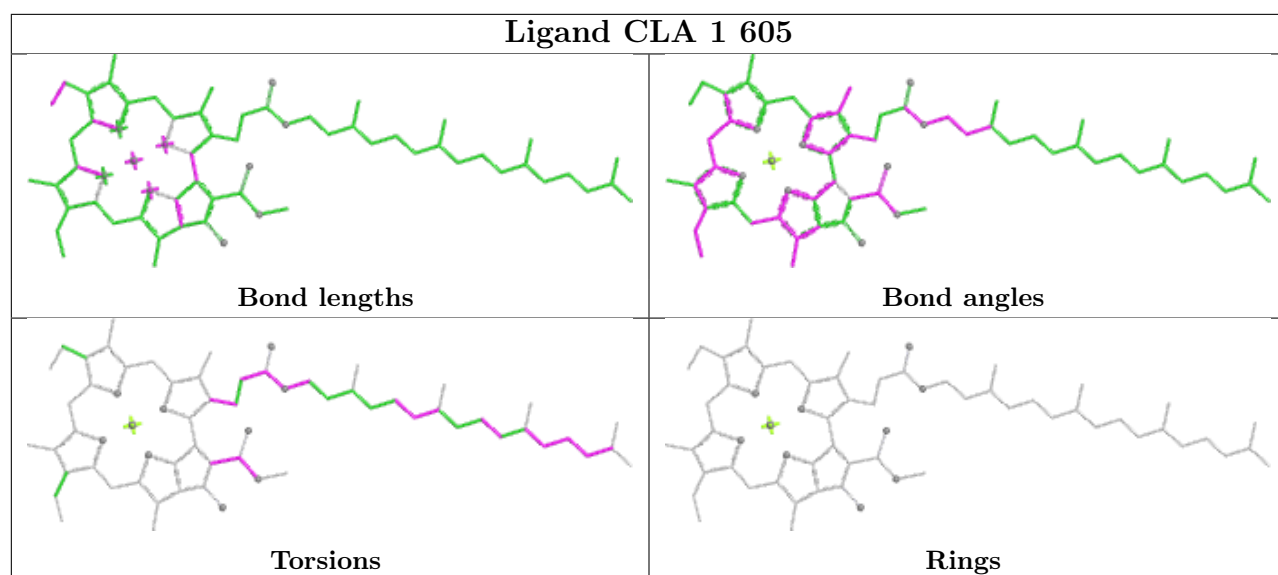
Rings

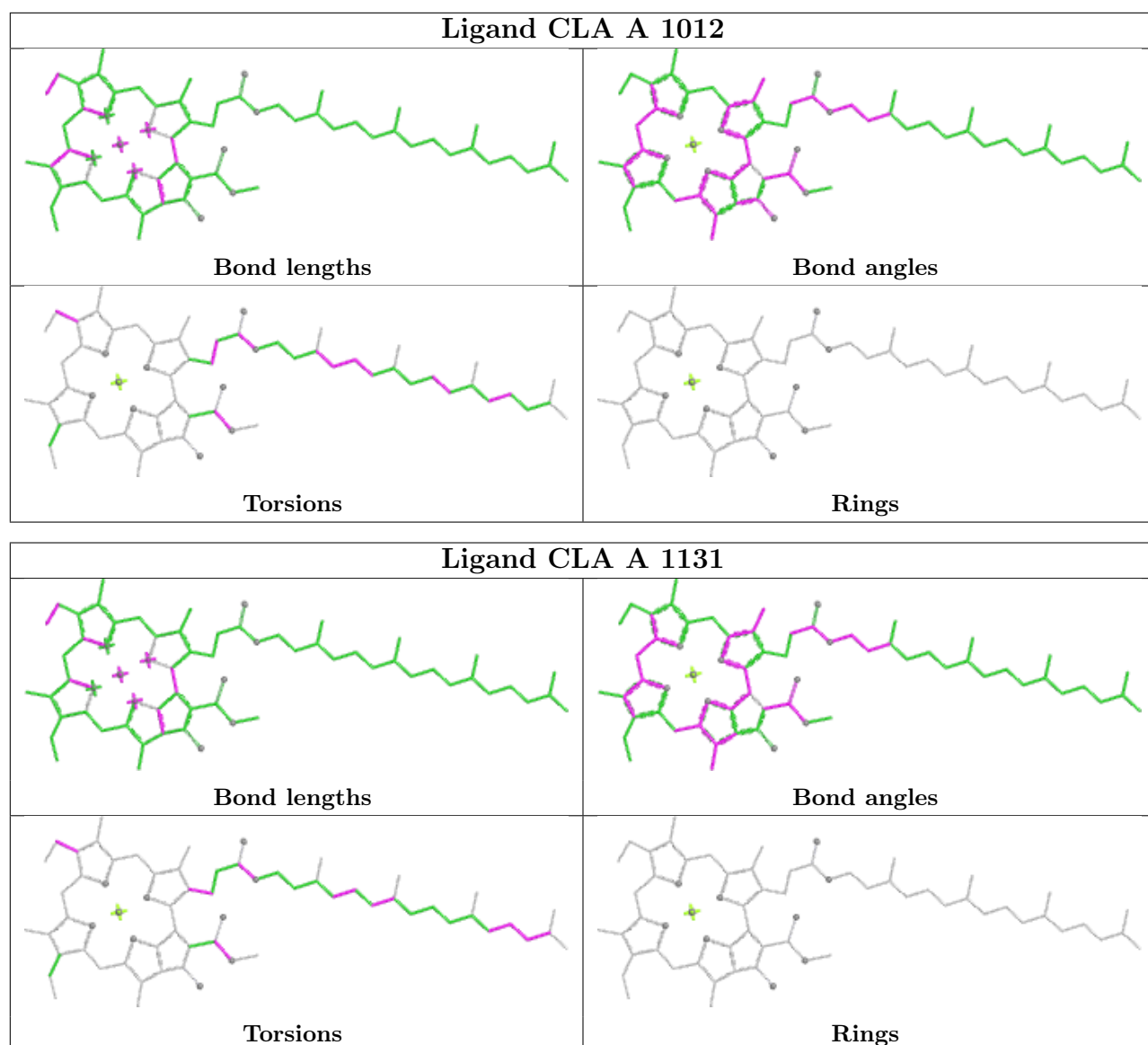
Ligand CLA 2 612

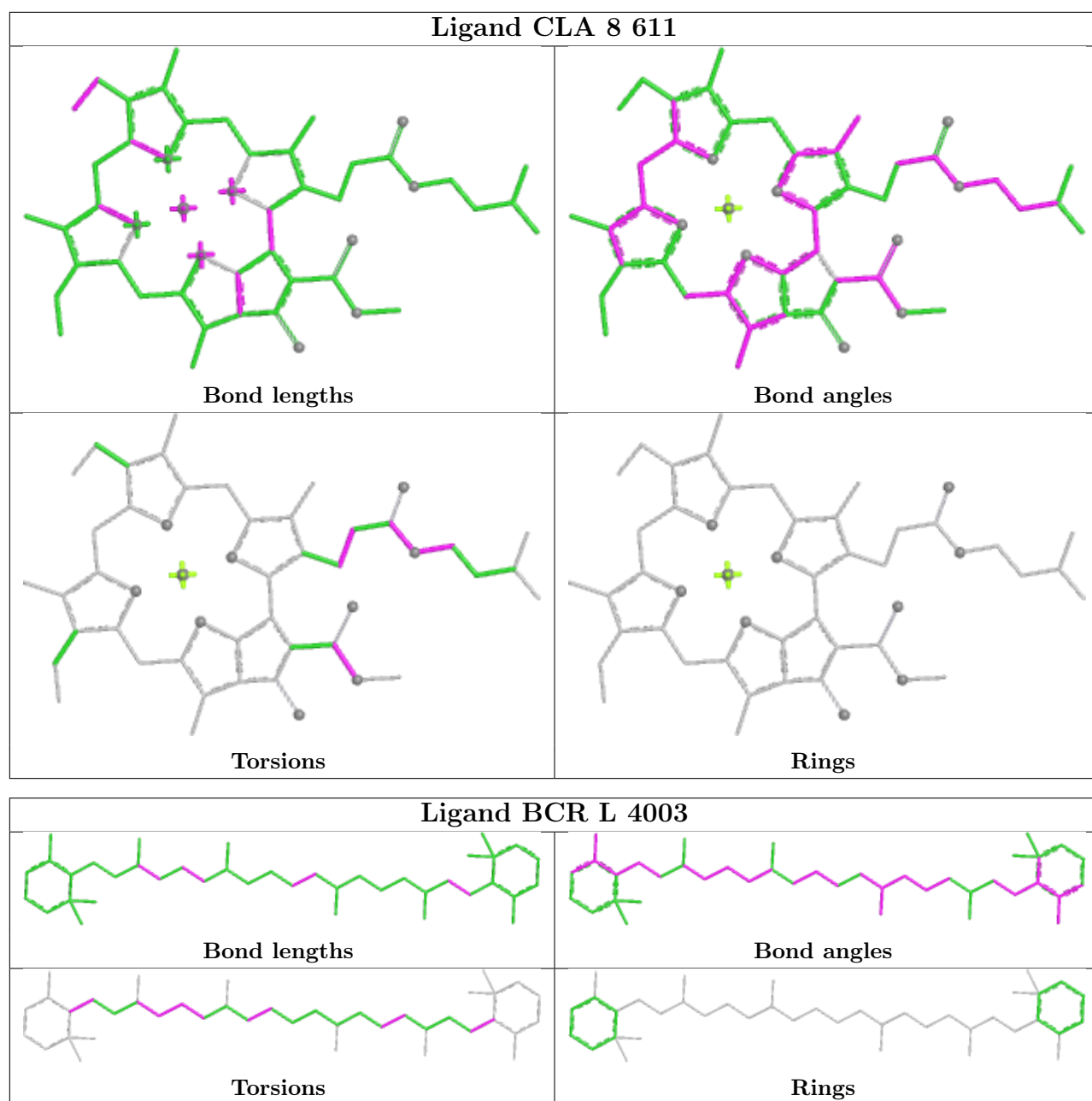


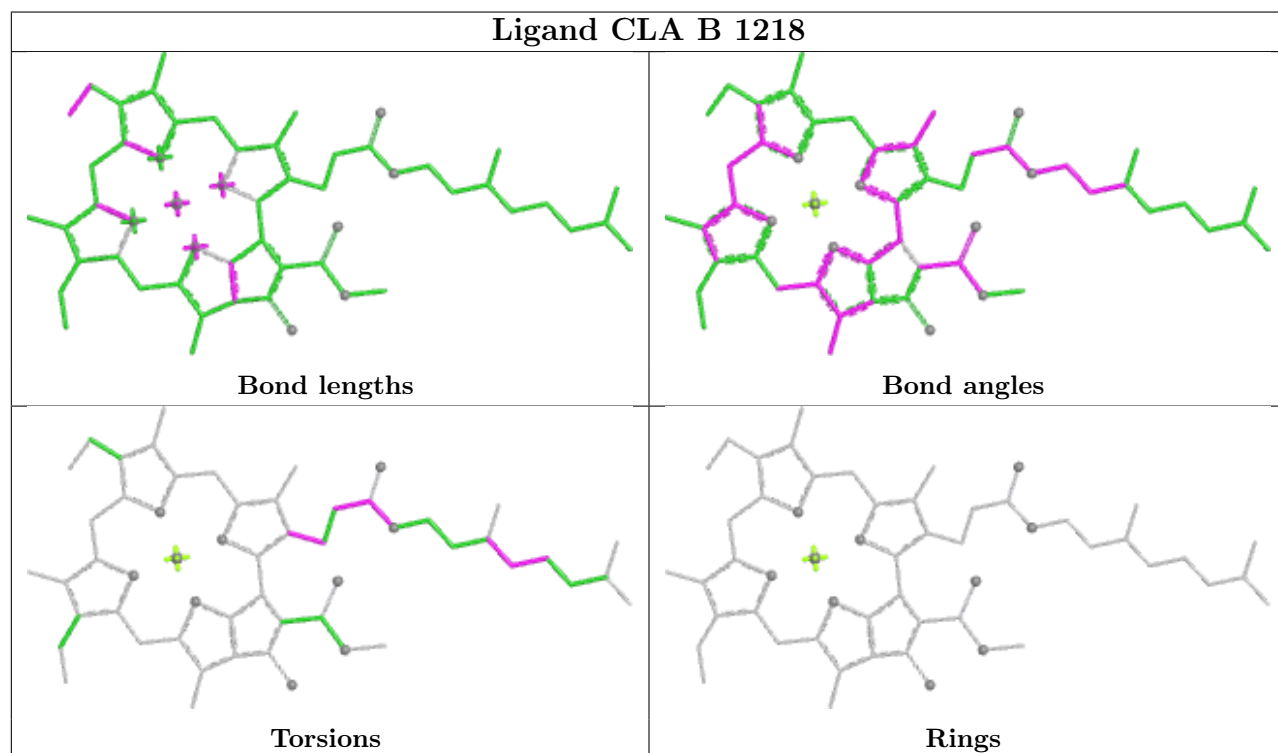
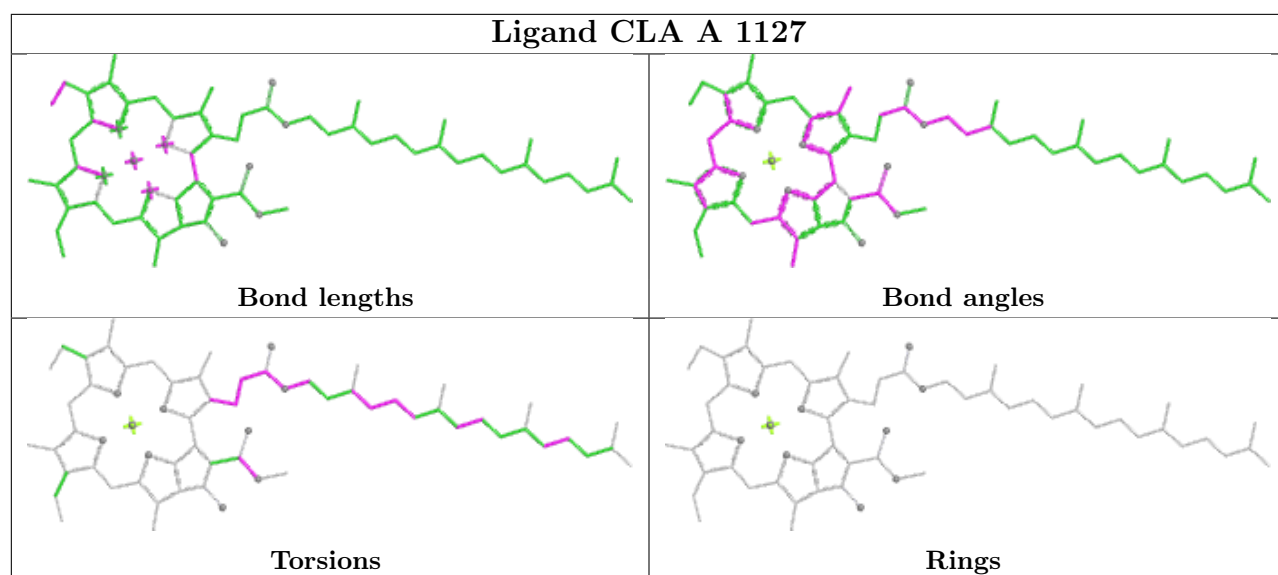
Ligand LUT 5 501

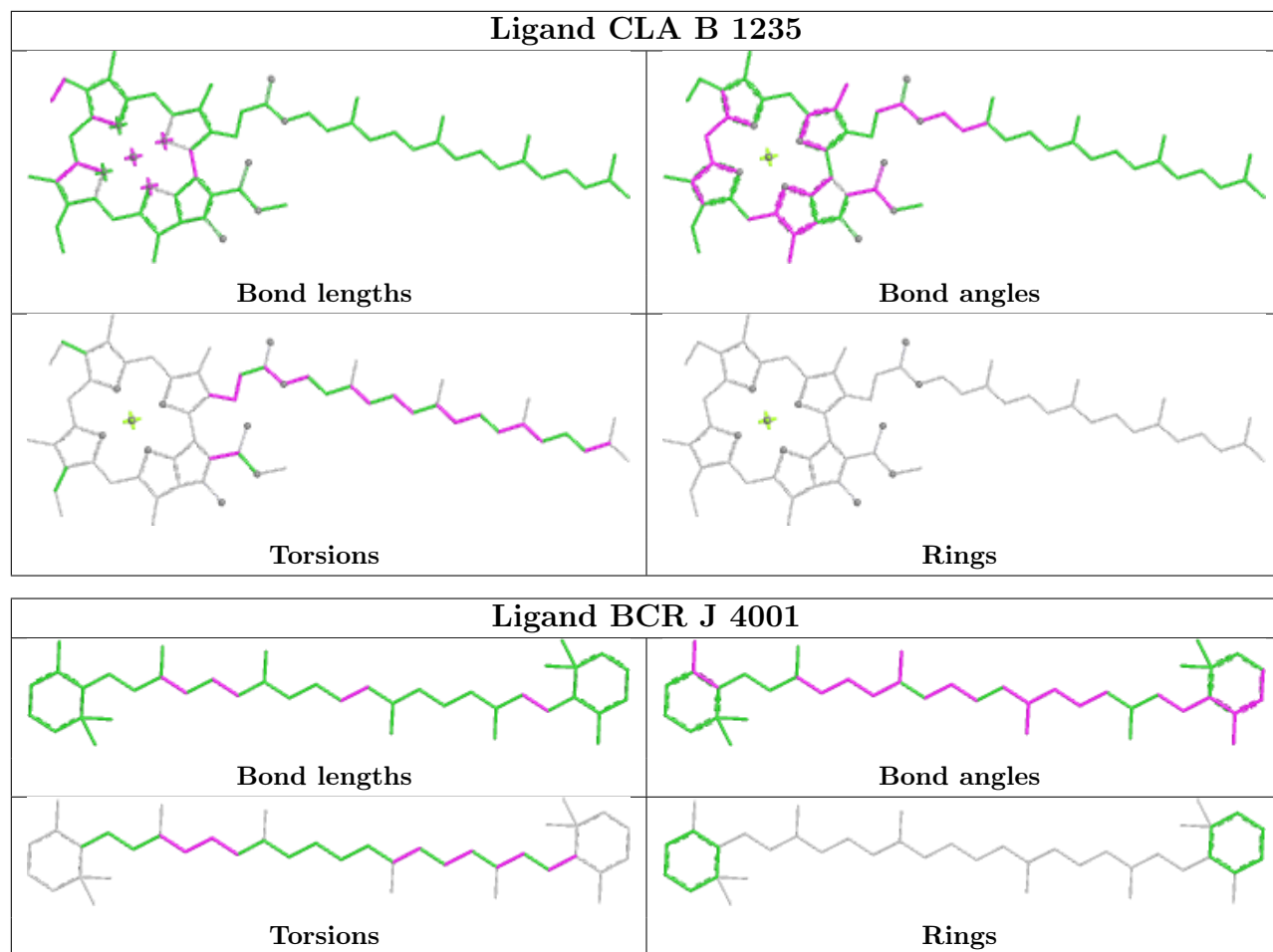




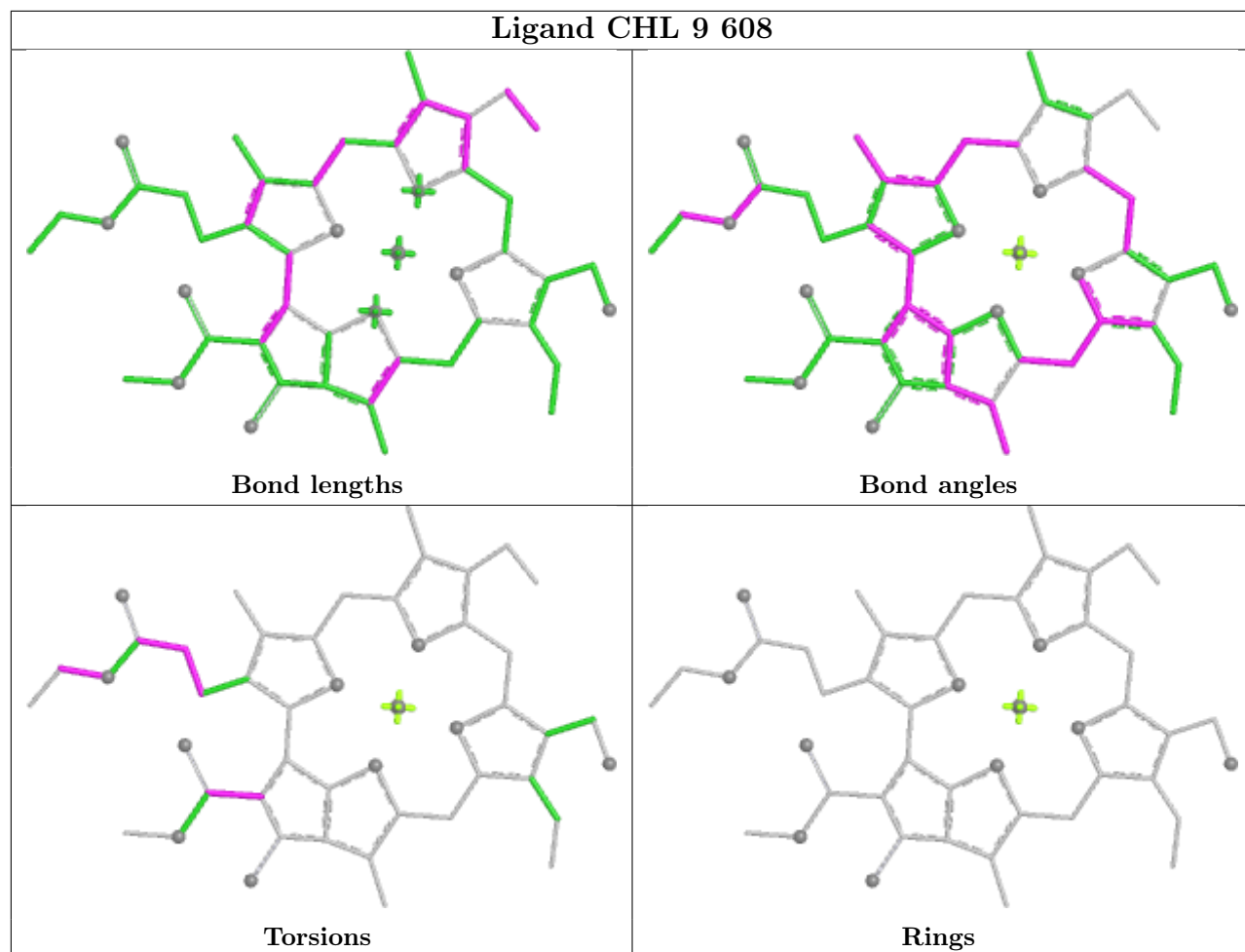




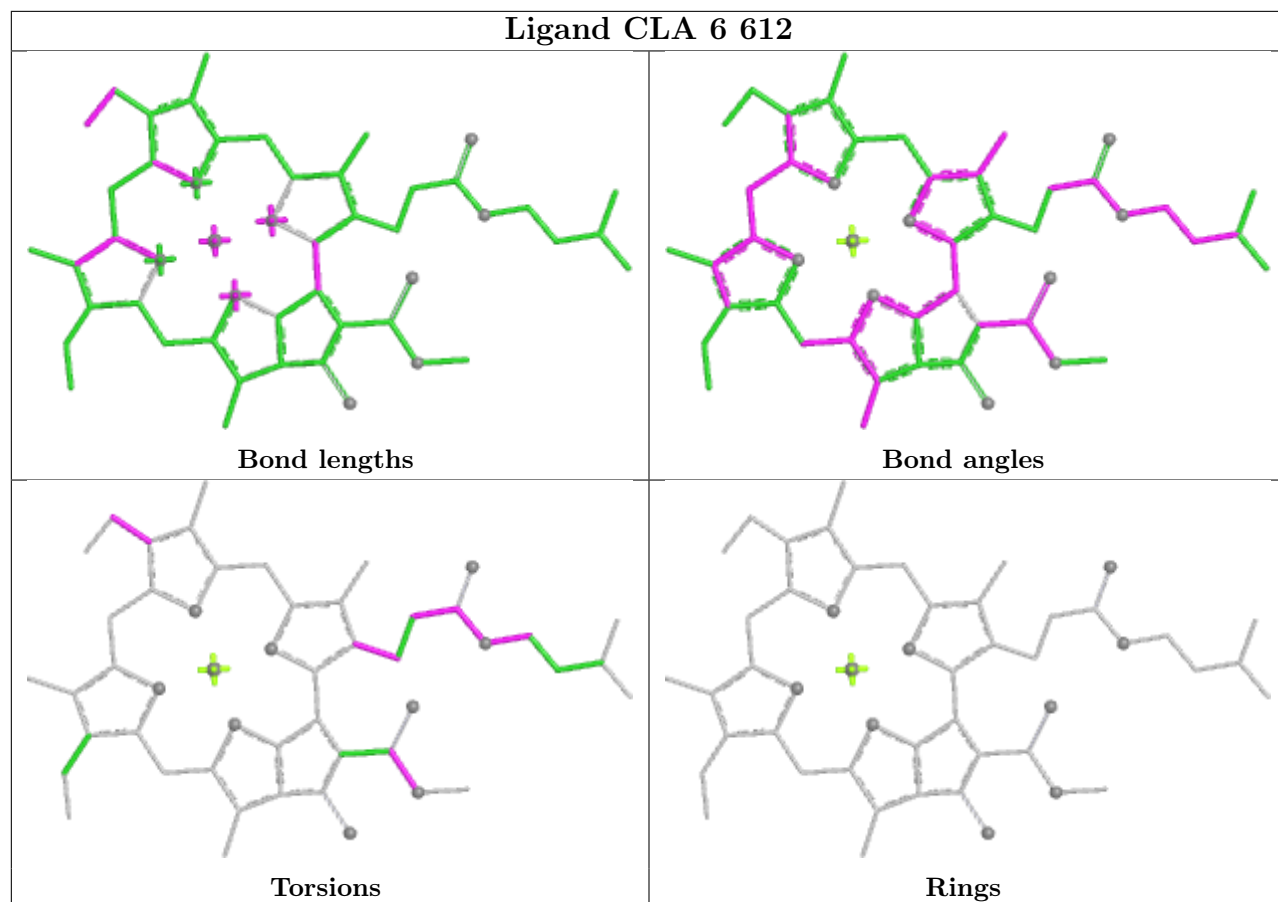




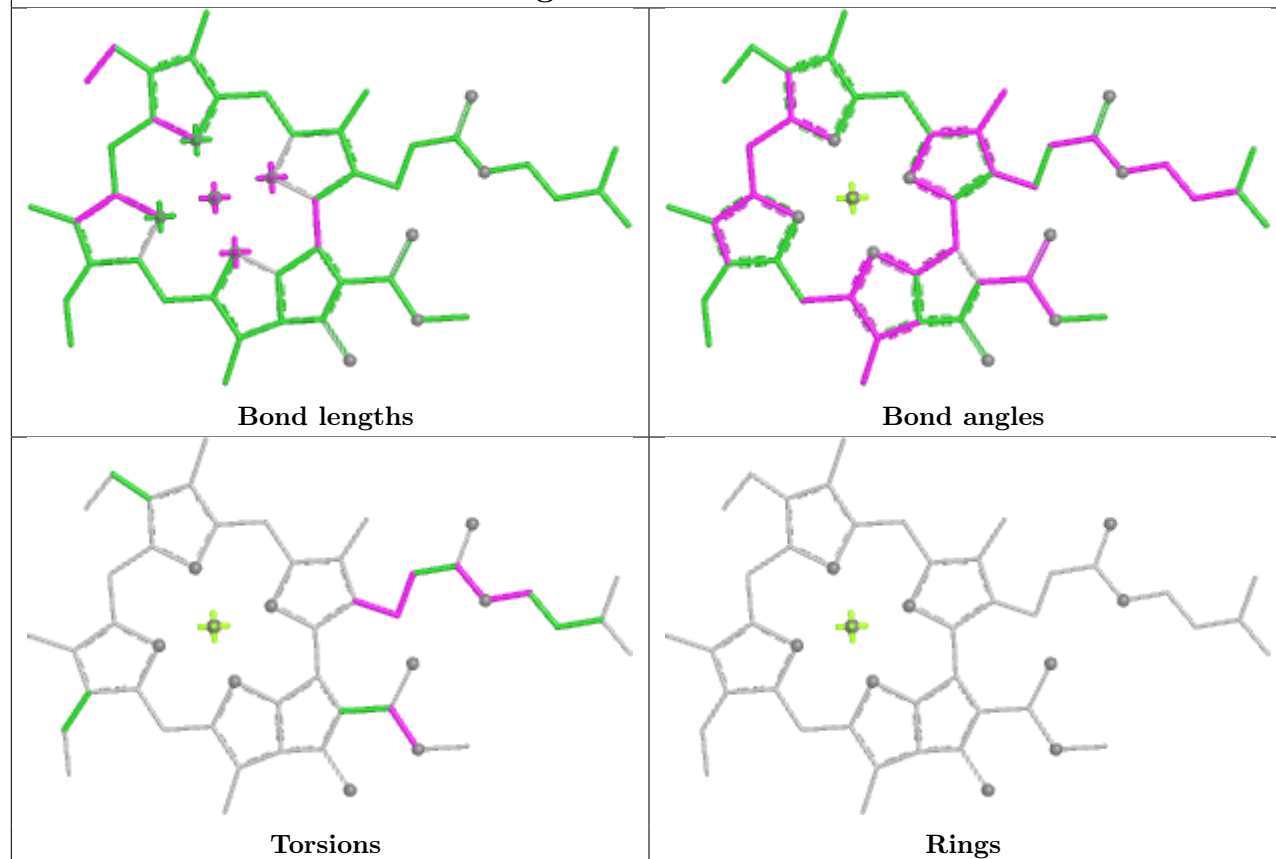
Ligand CHL 9 608



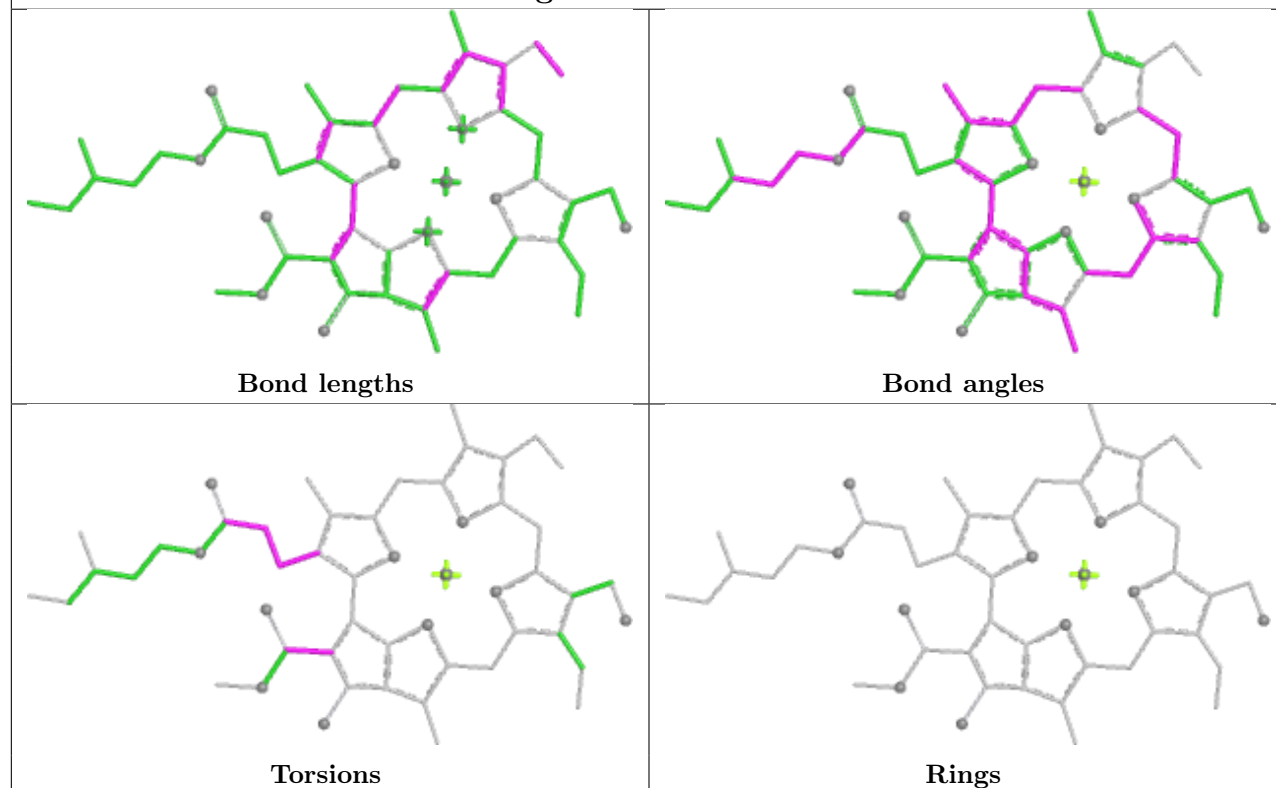
Ligand CLA 6 612



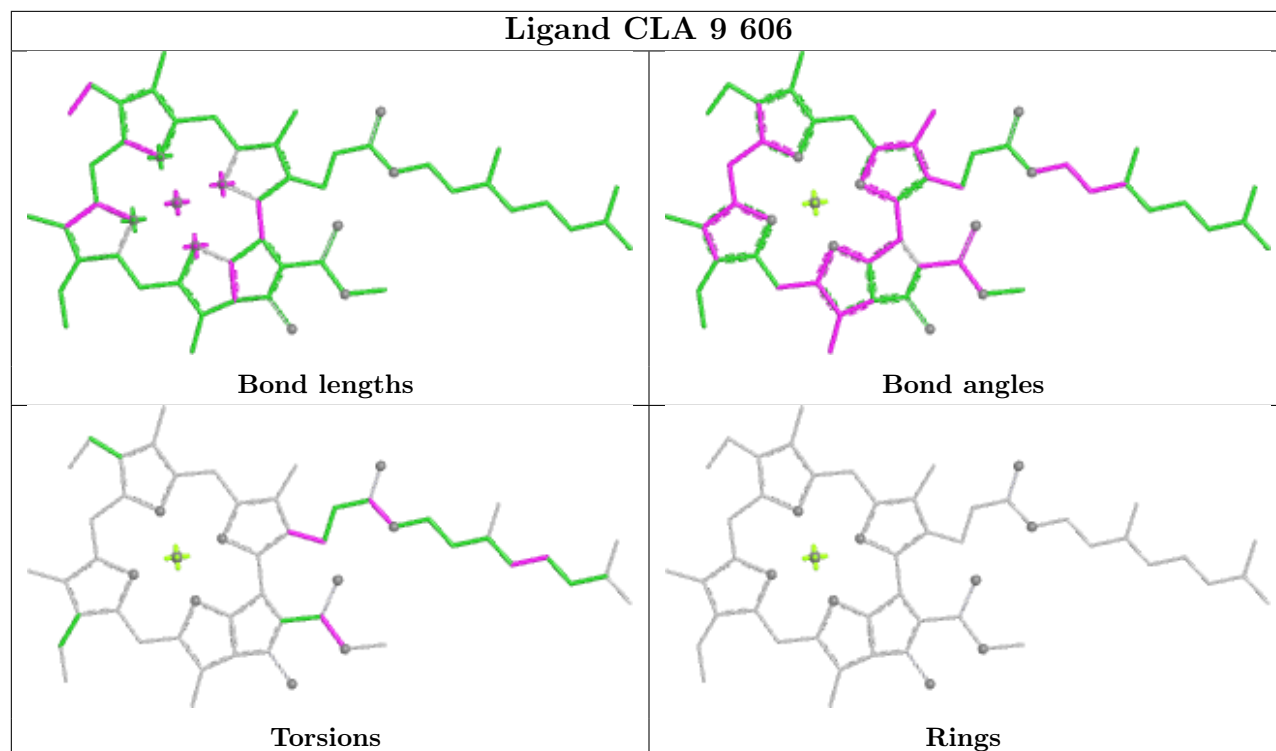
Ligand CLA a 602



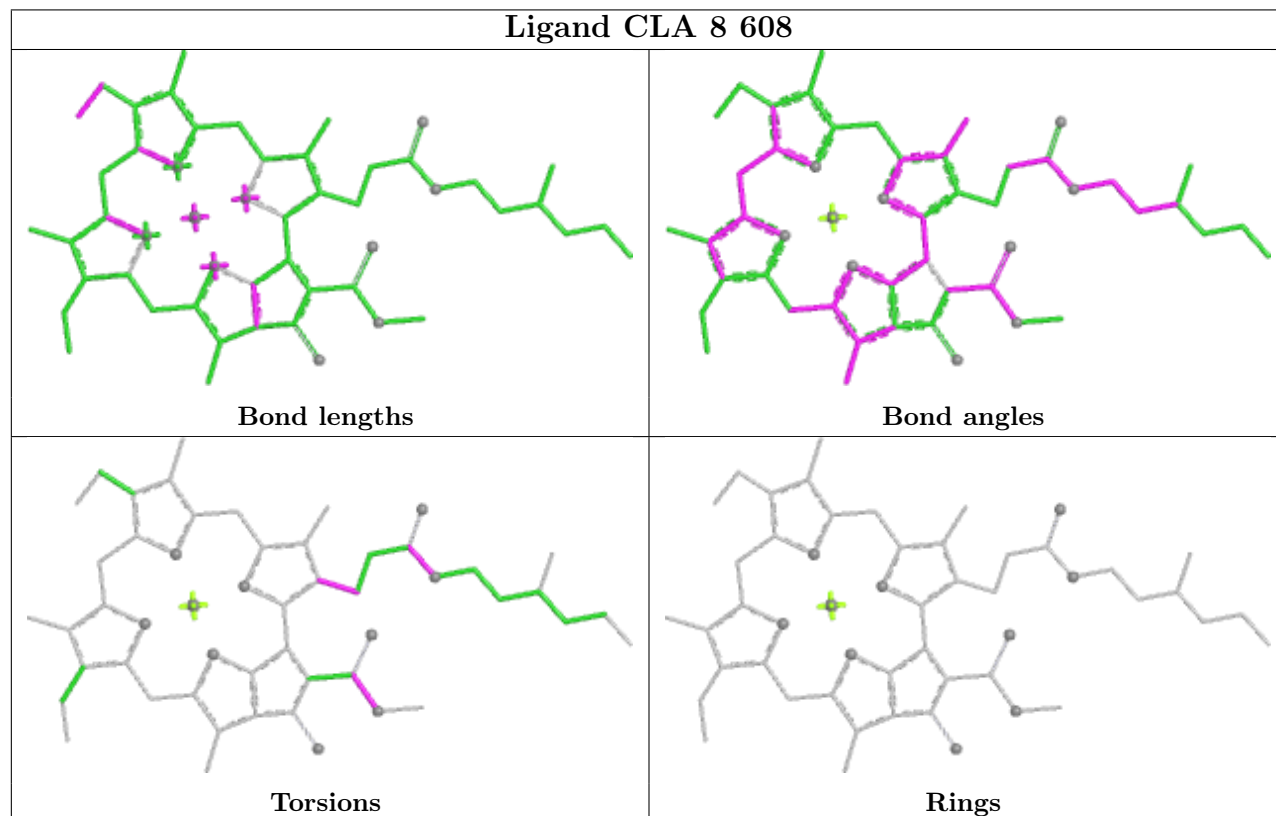
Ligand CHL 4 613

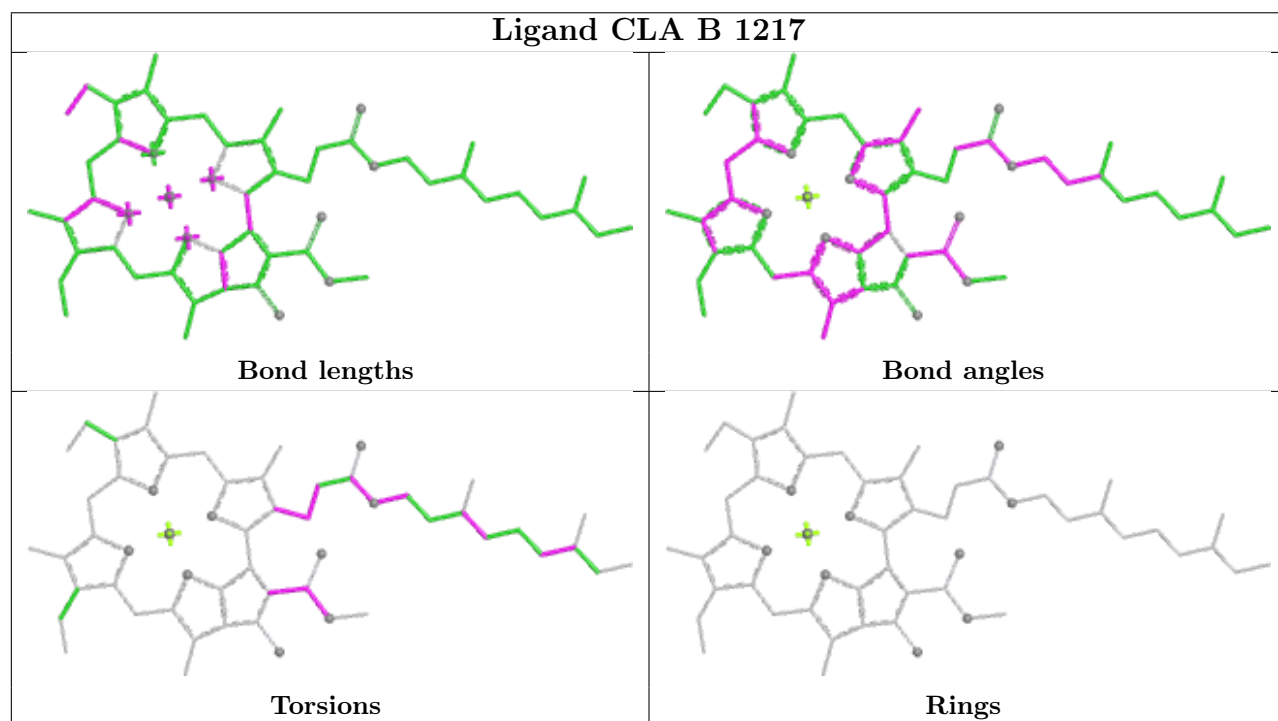
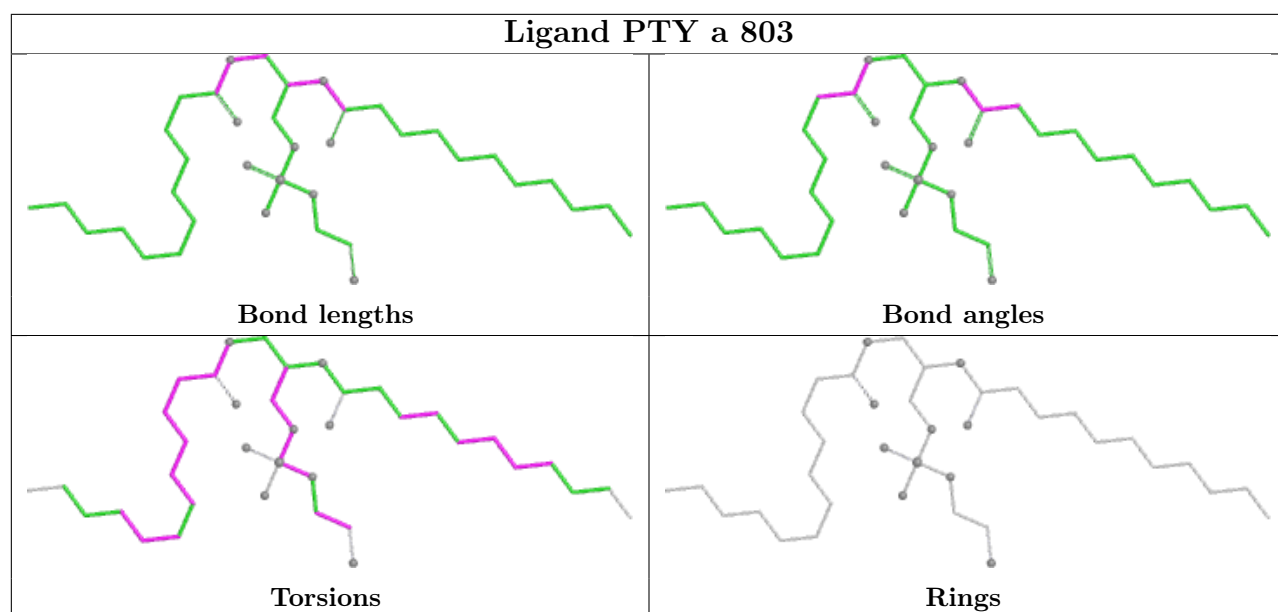


Ligand CLA 9 606

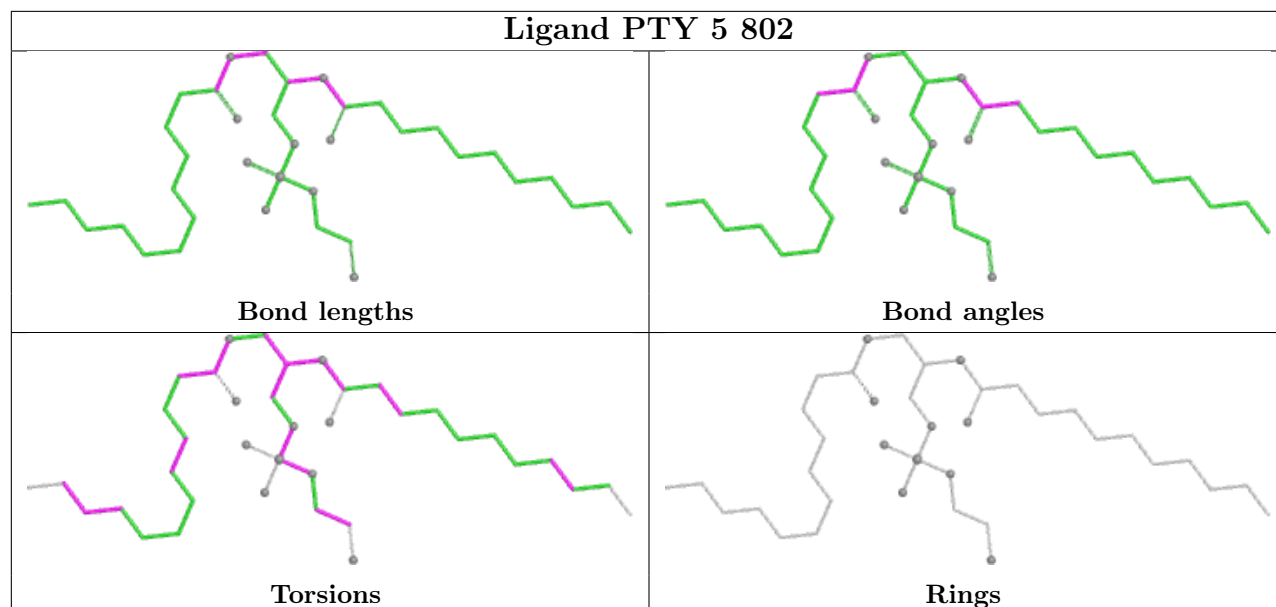


Ligand CLA 8 608

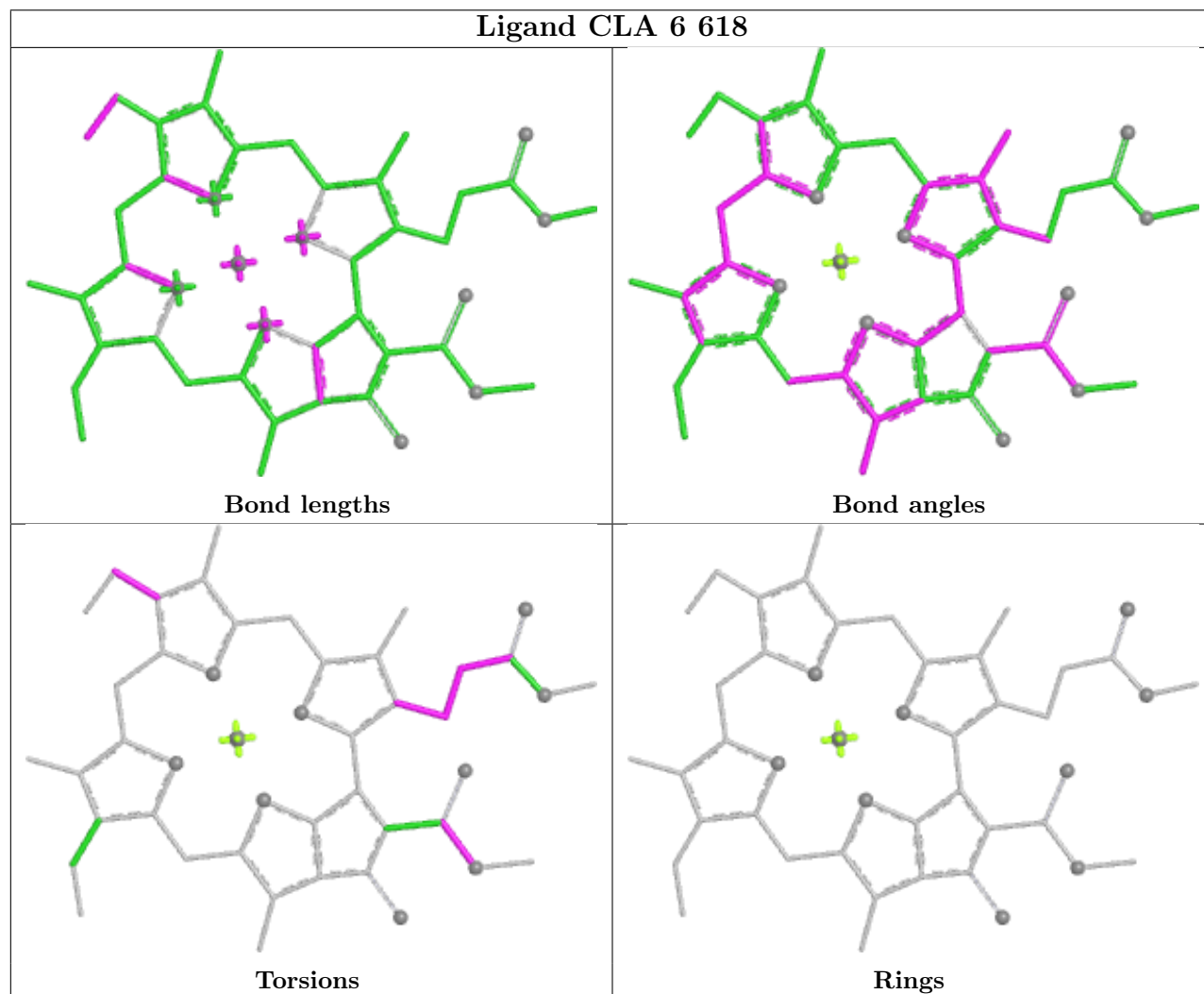


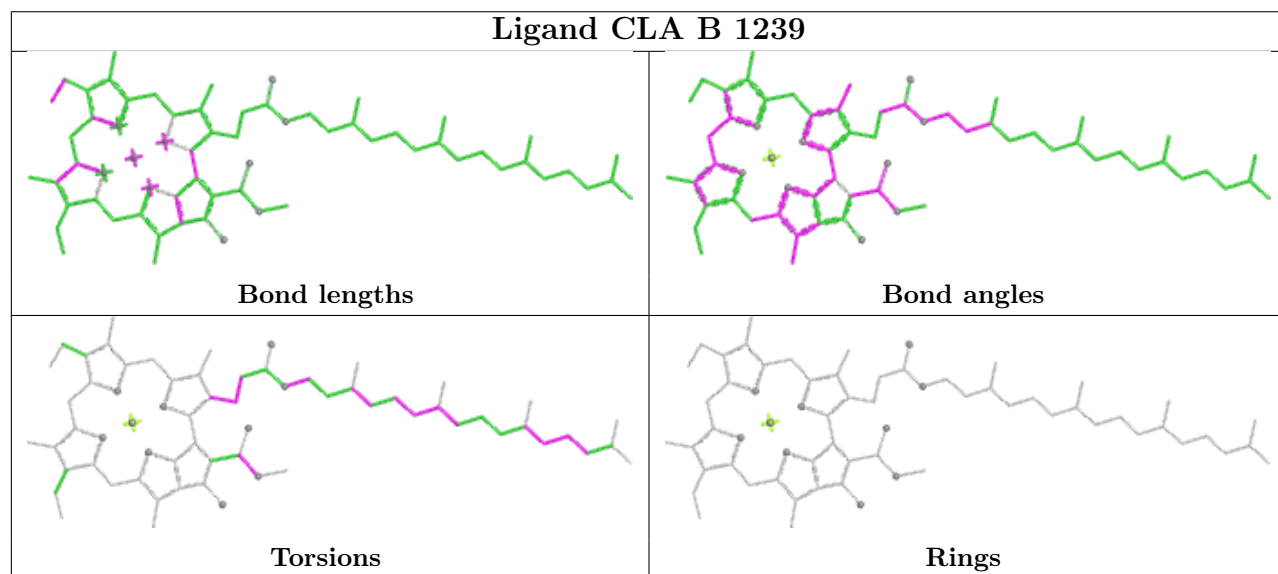
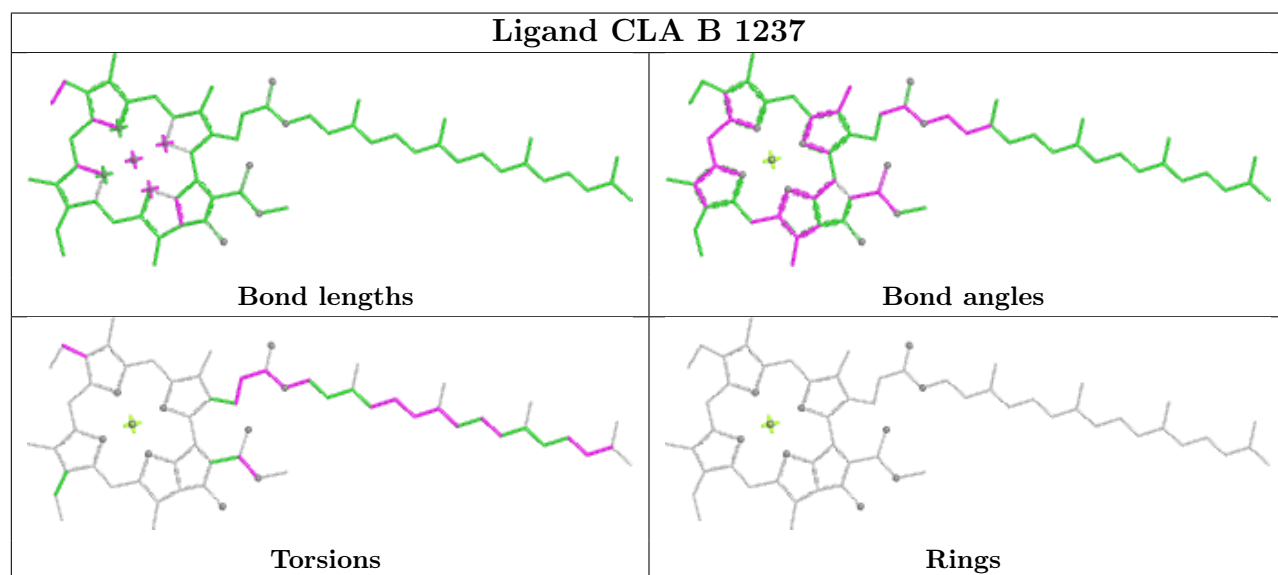
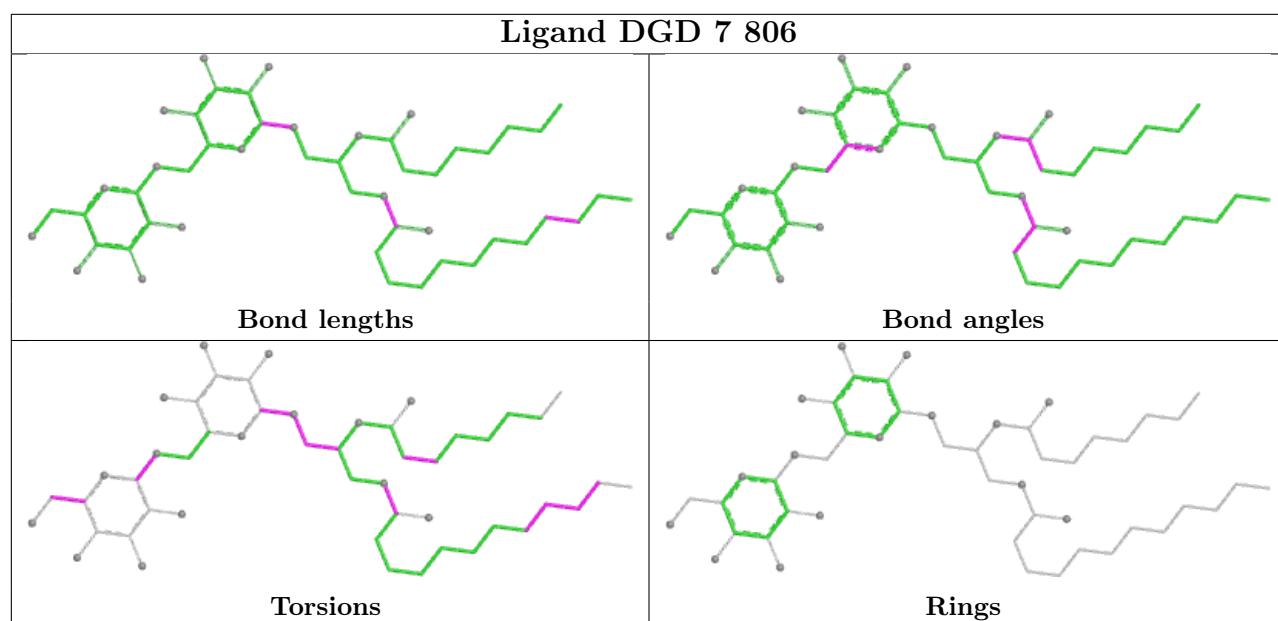


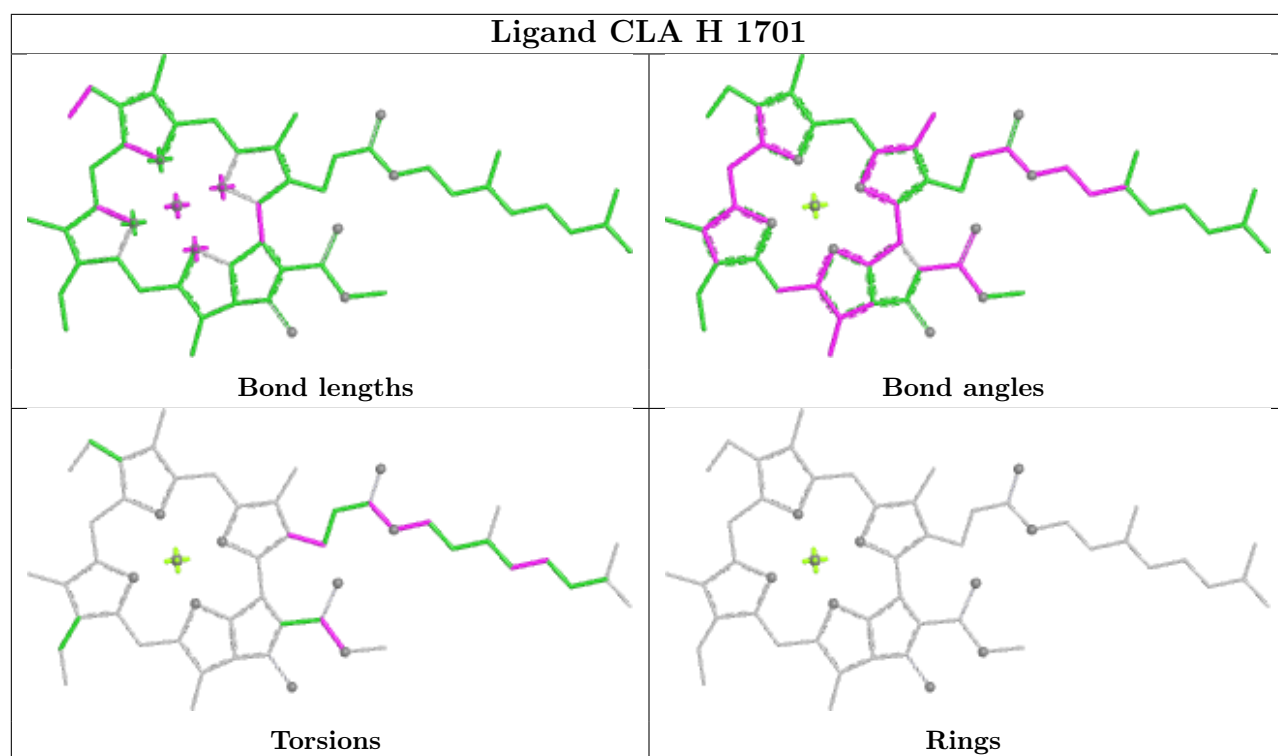
Ligand PTY 5 802

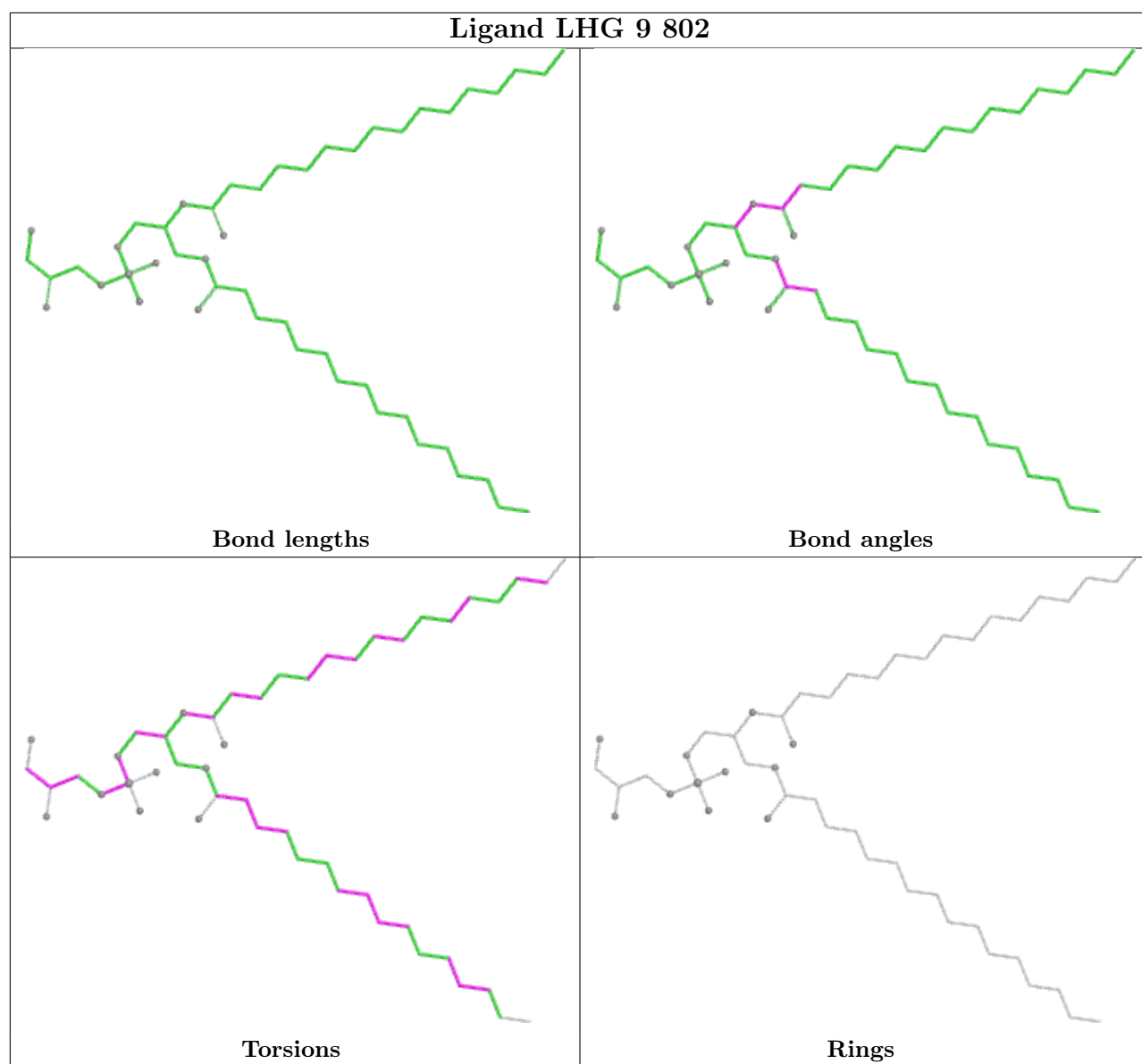


Ligand CLA 6 618

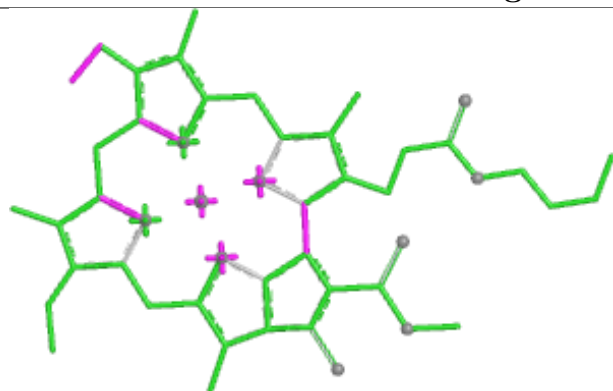




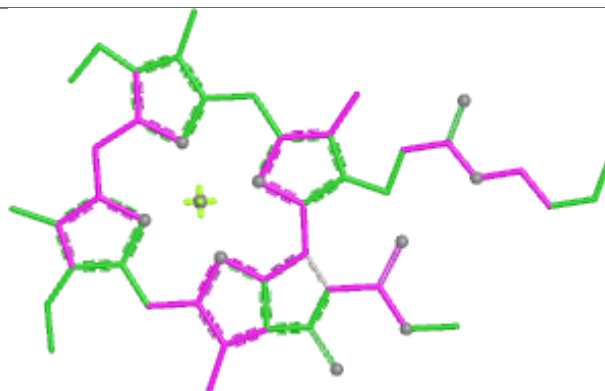




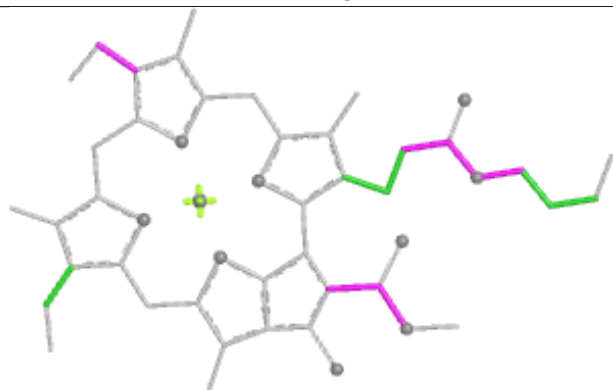
Ligand CLA K 1403



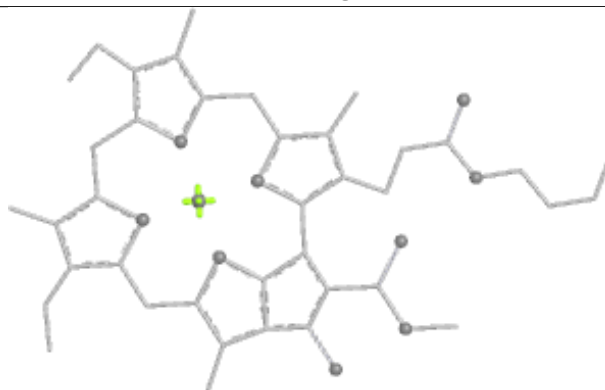
Bond lengths



Bond angles

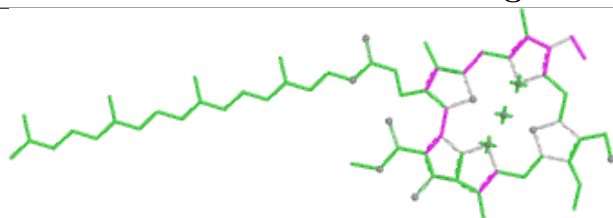


Torsions

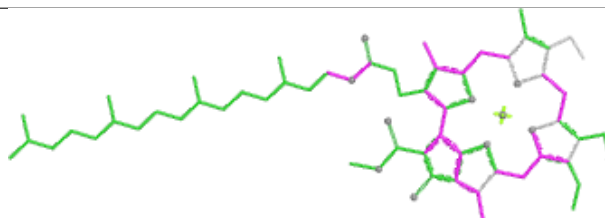


Rings

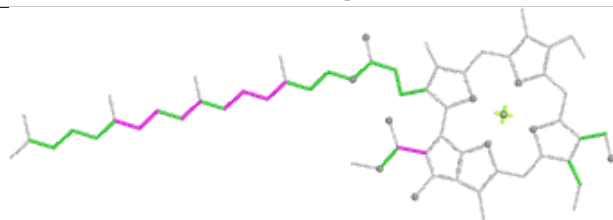
Ligand CHL A 1114



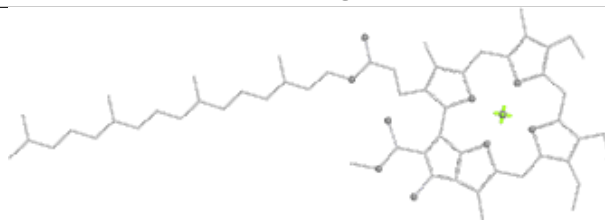
Bond lengths



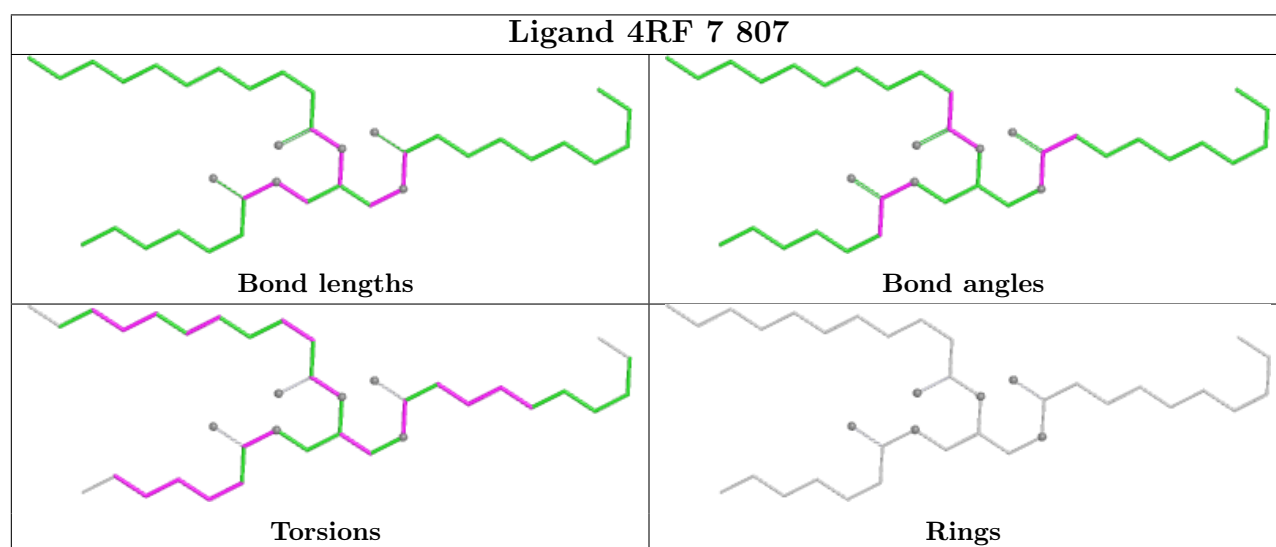
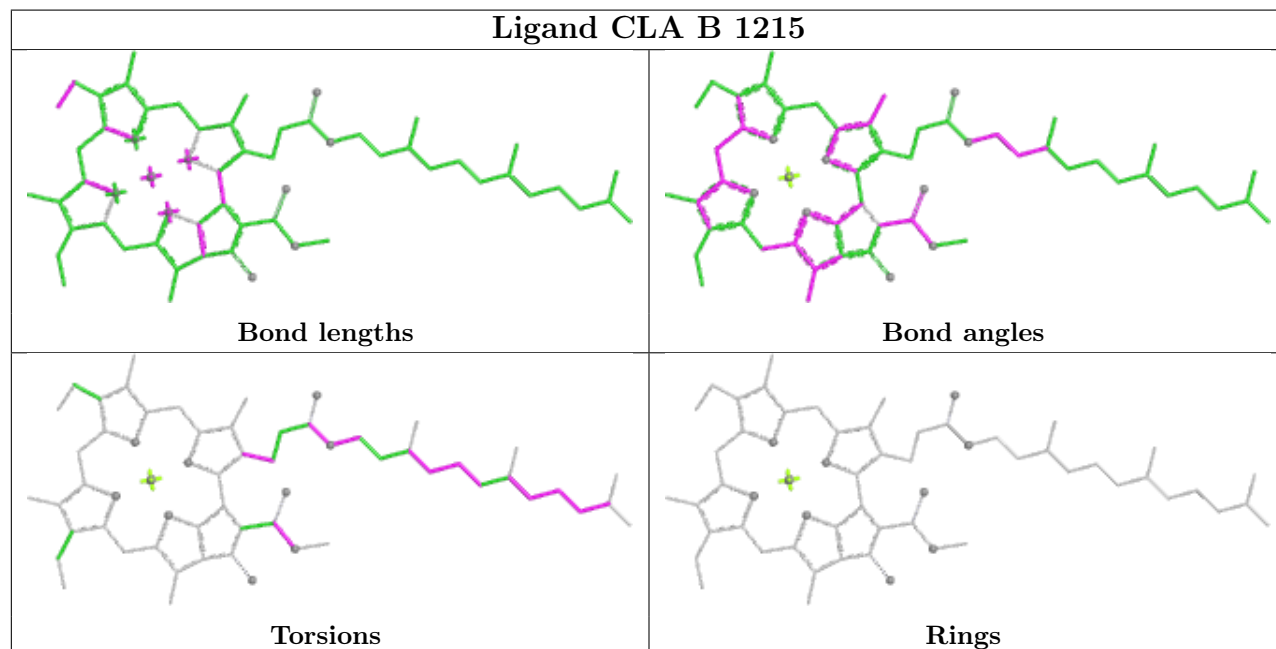
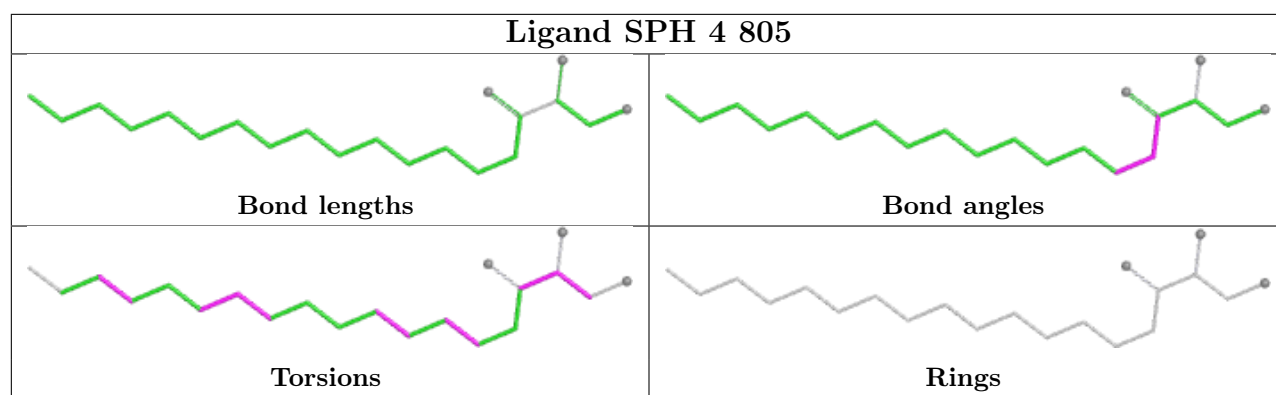
Bond angles

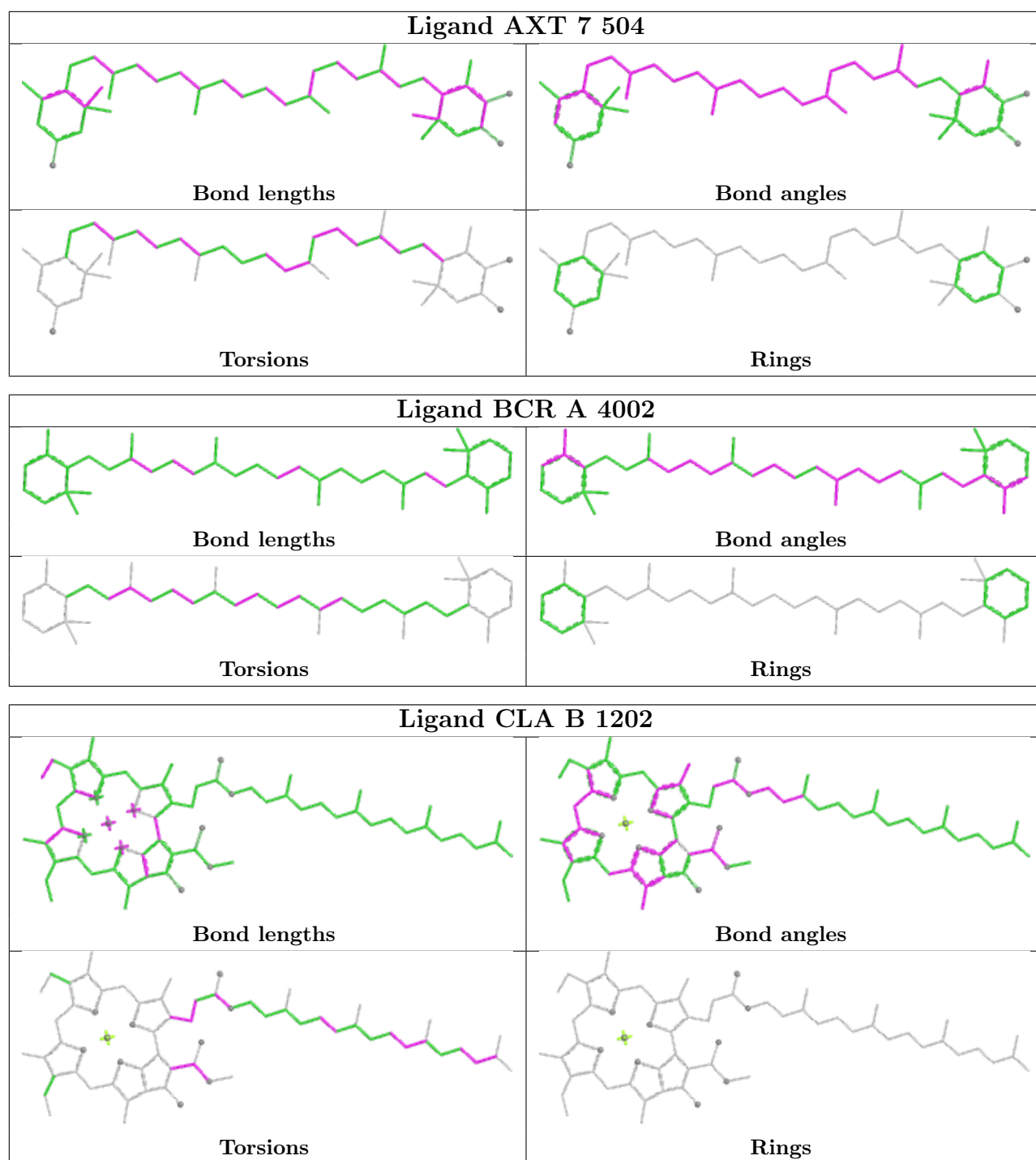


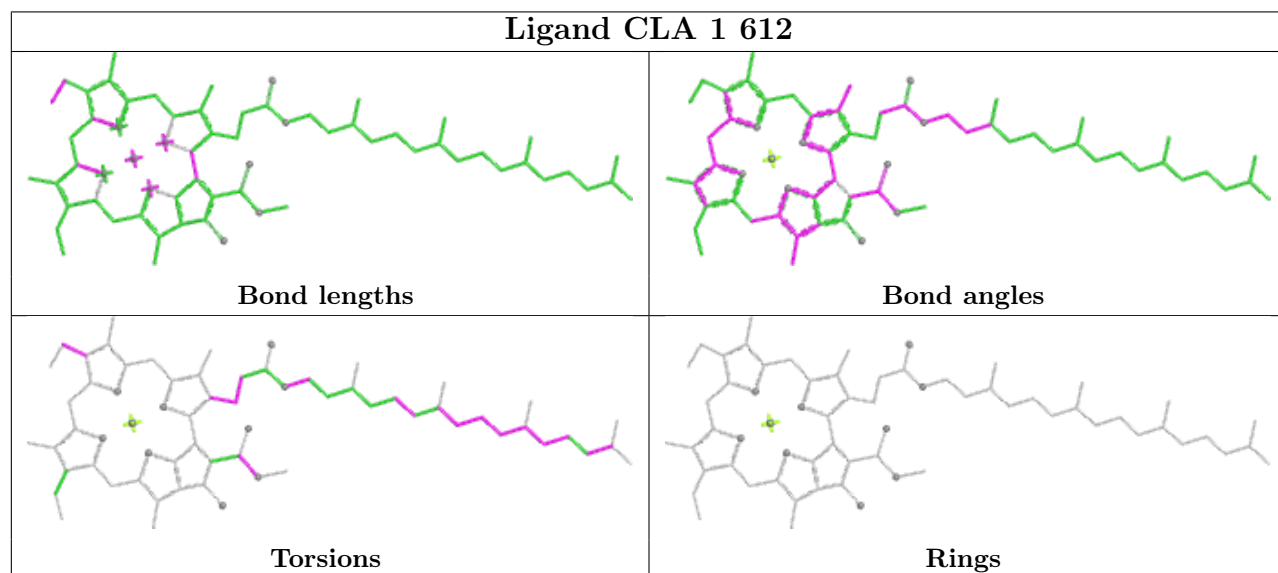
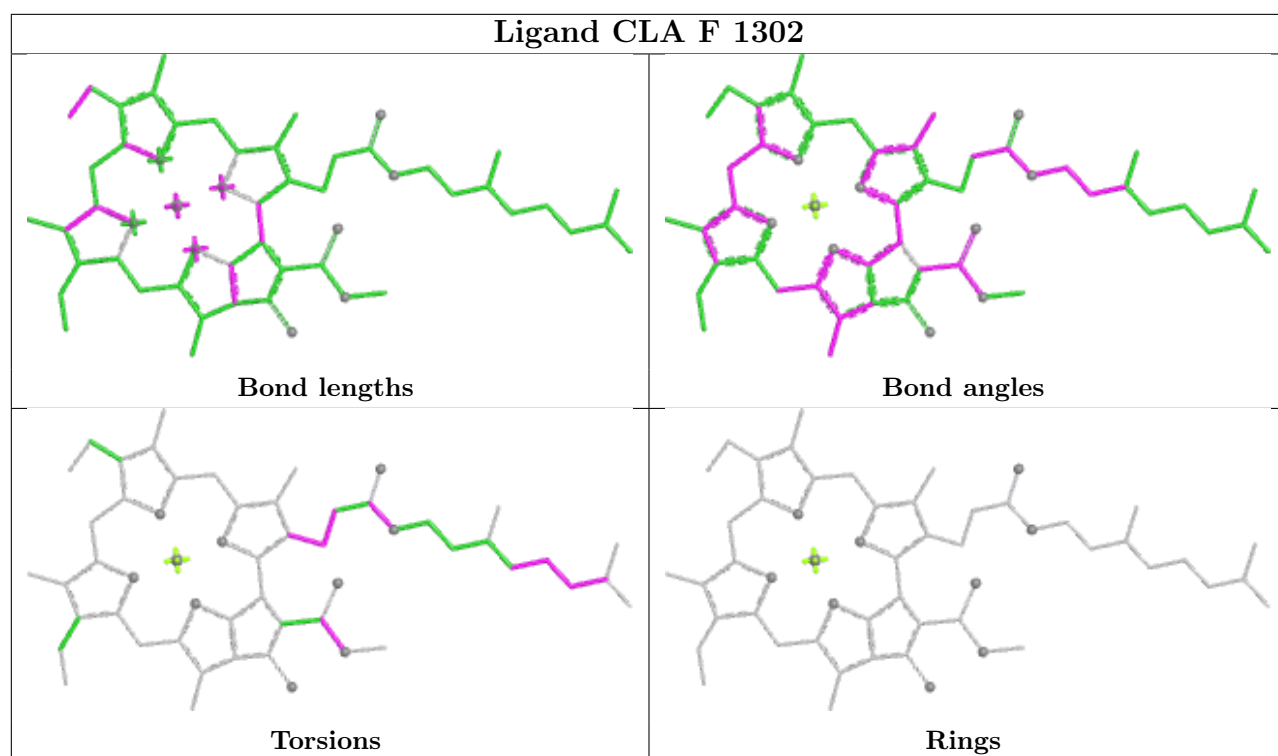
Torsions

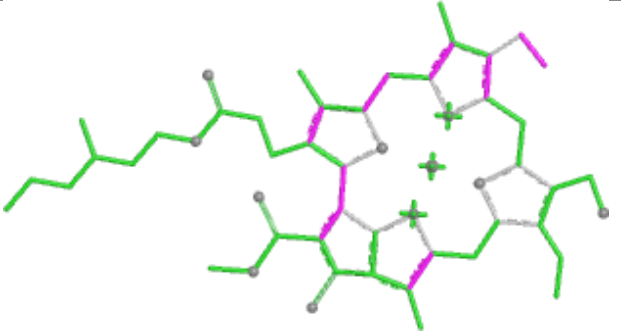
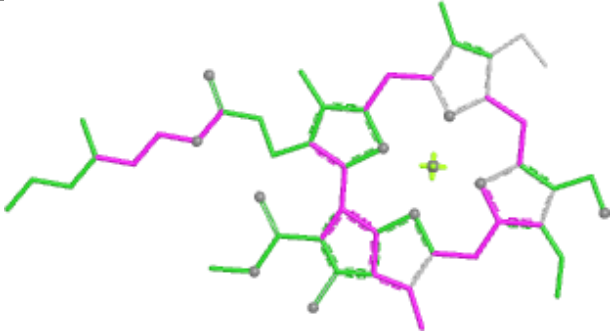
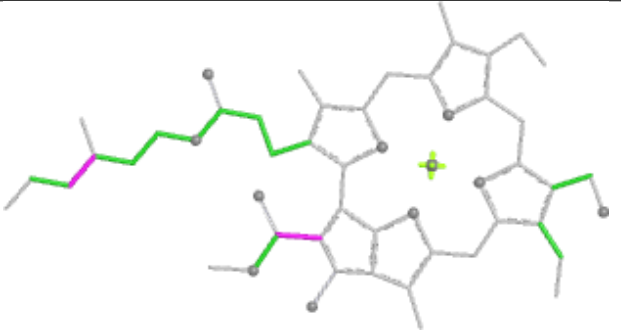
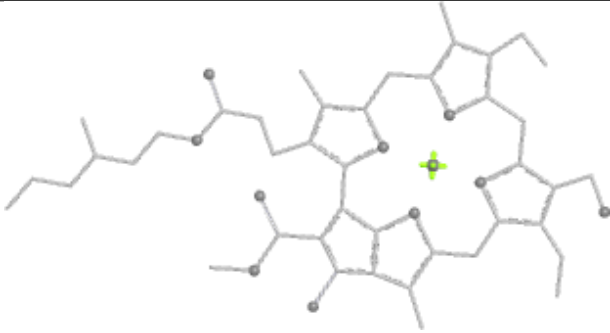
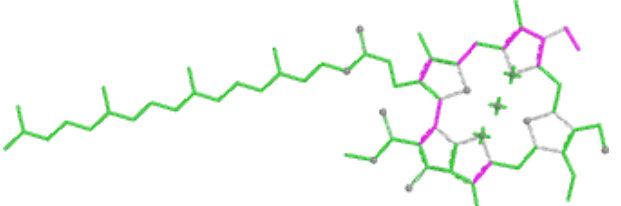
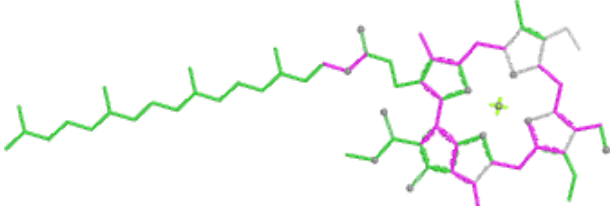
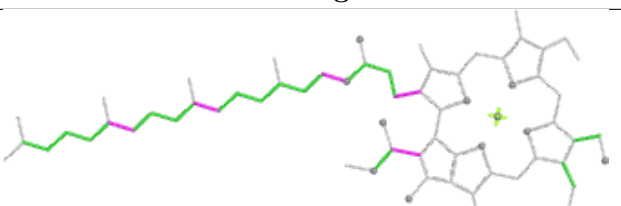
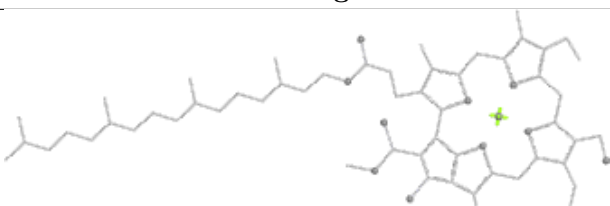
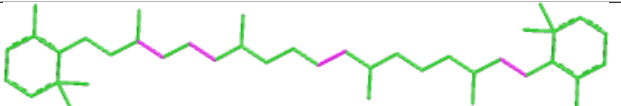
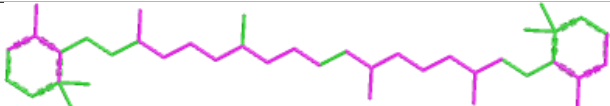
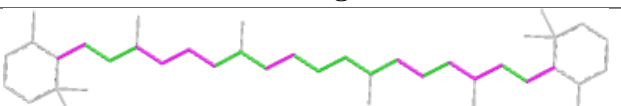
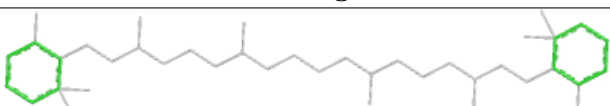


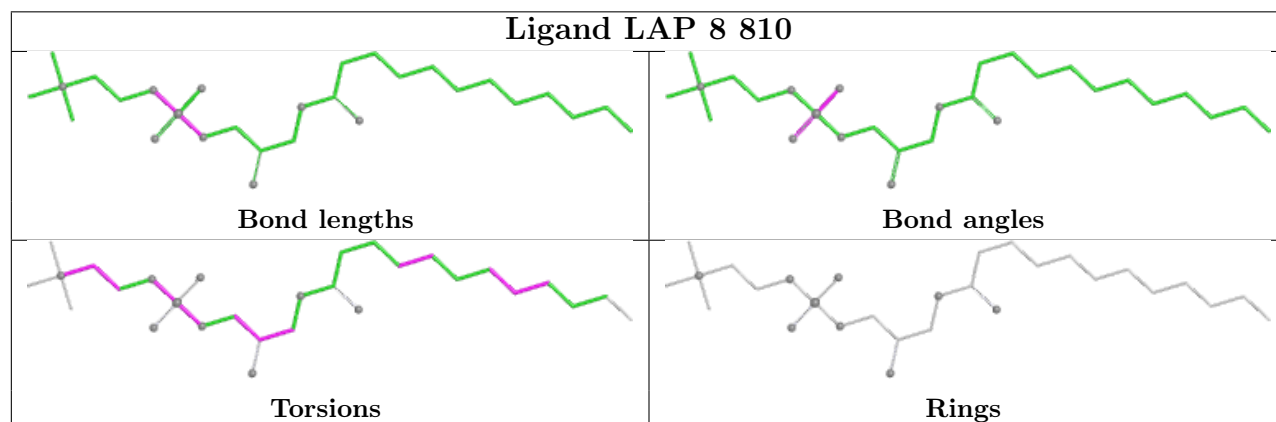
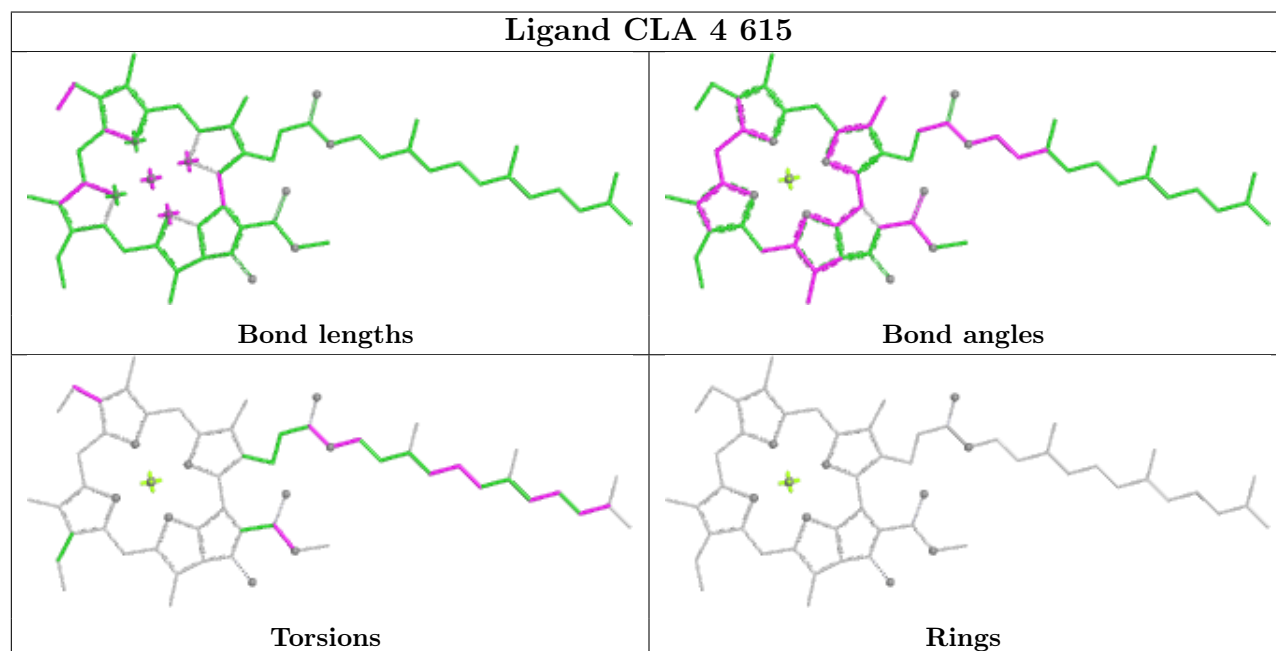
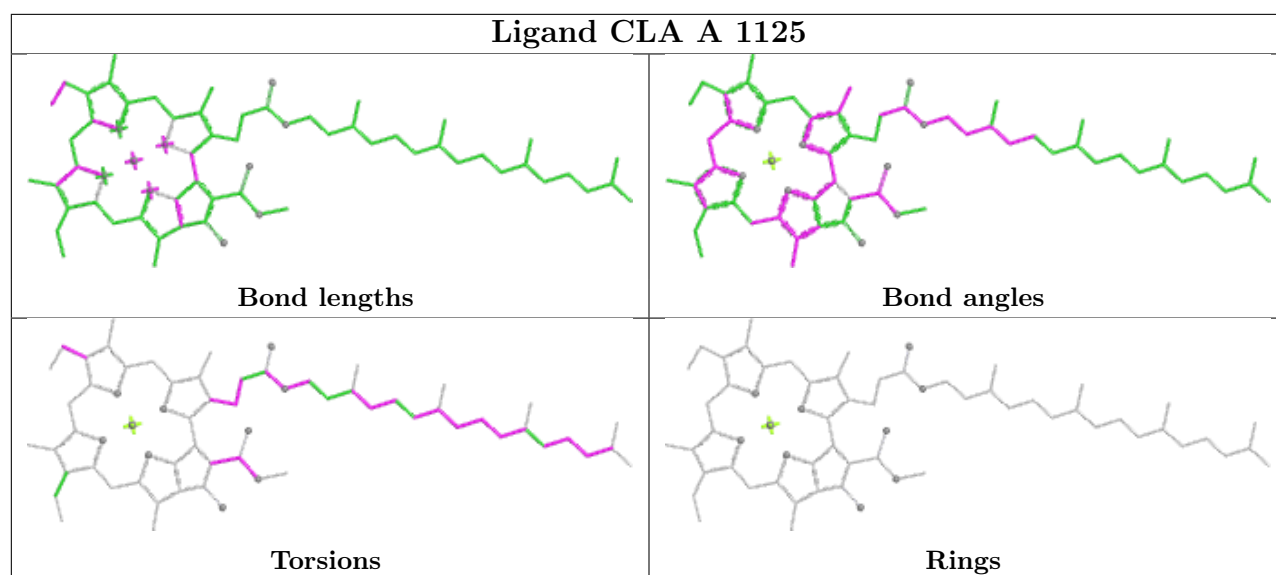
Rings

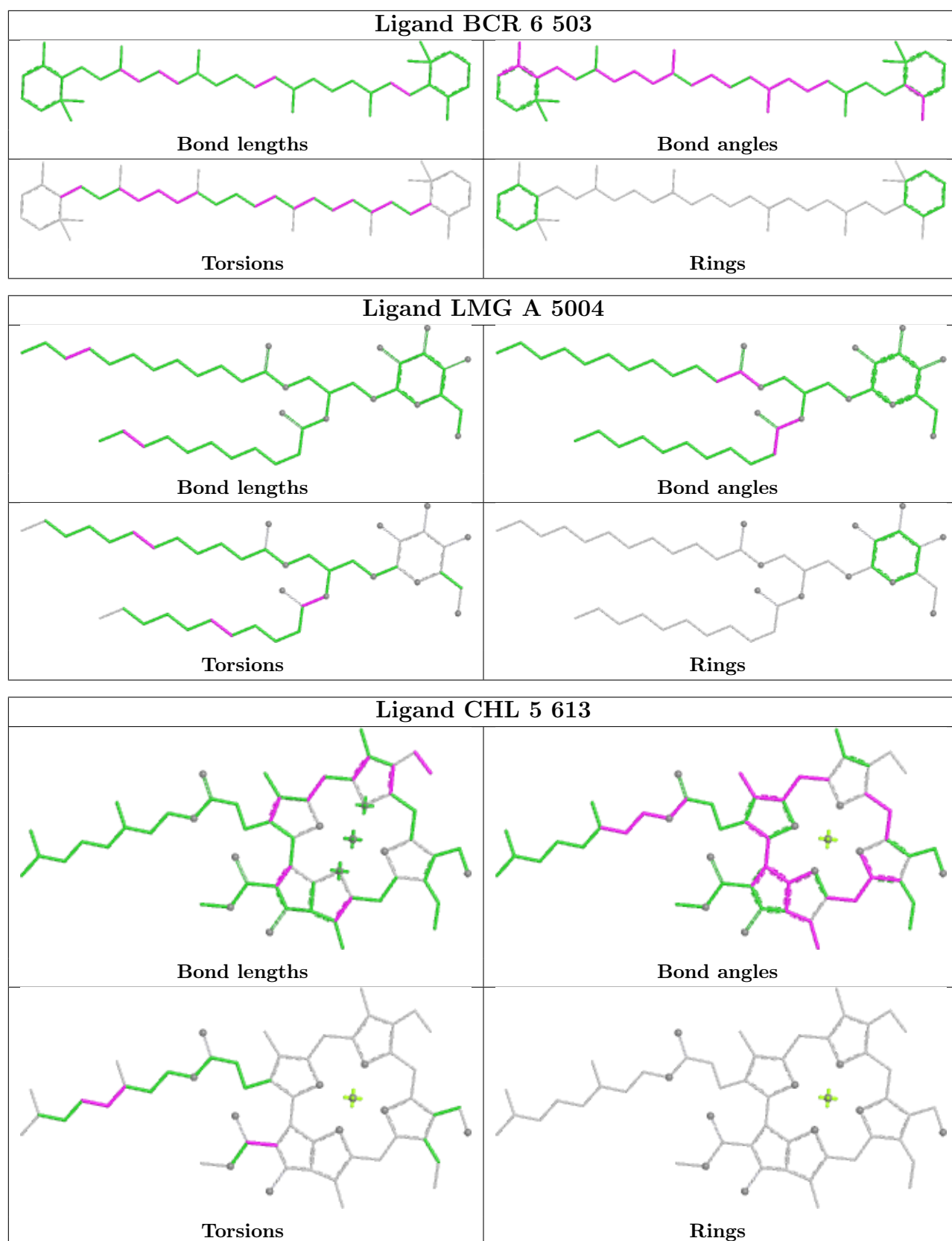


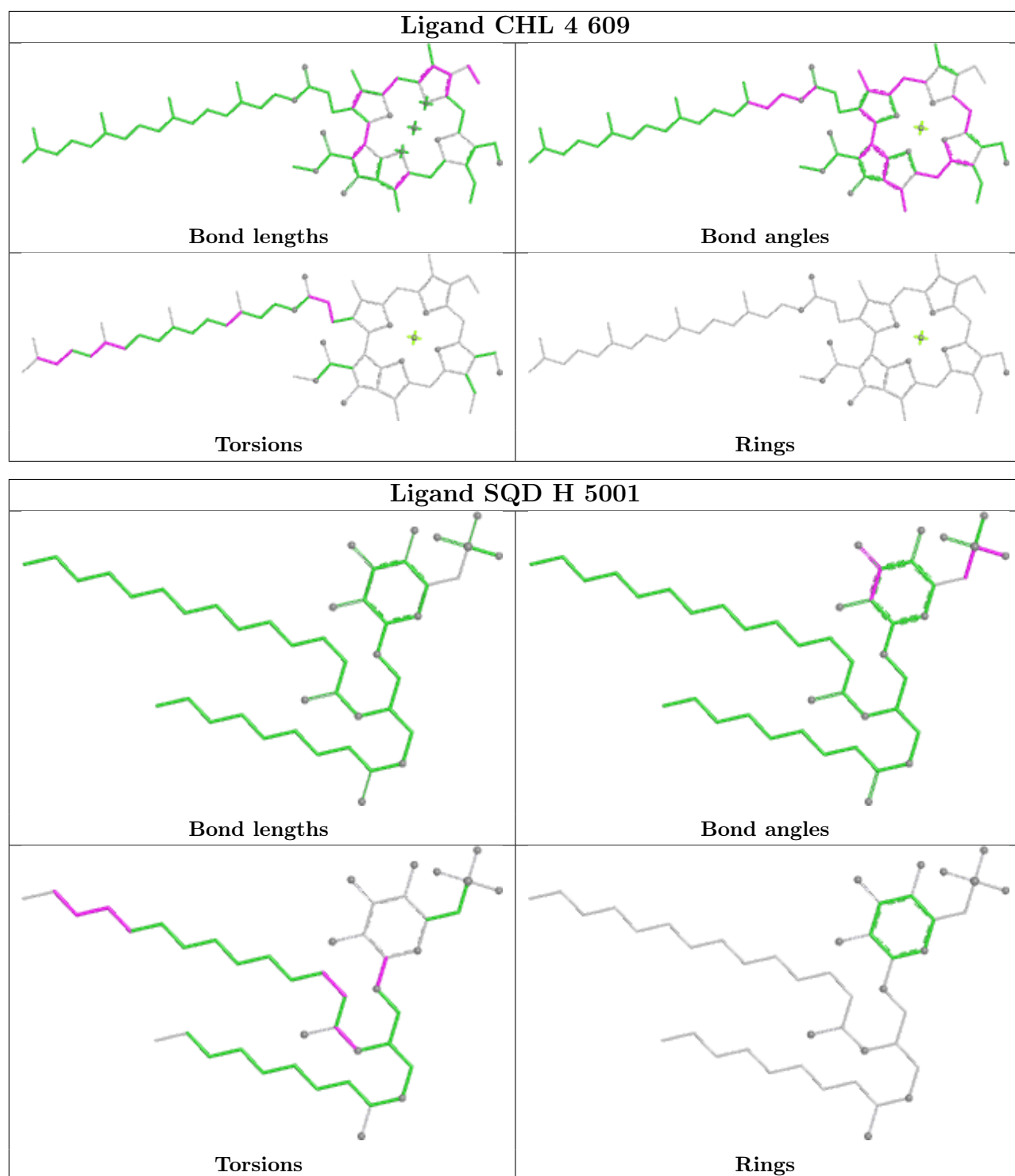


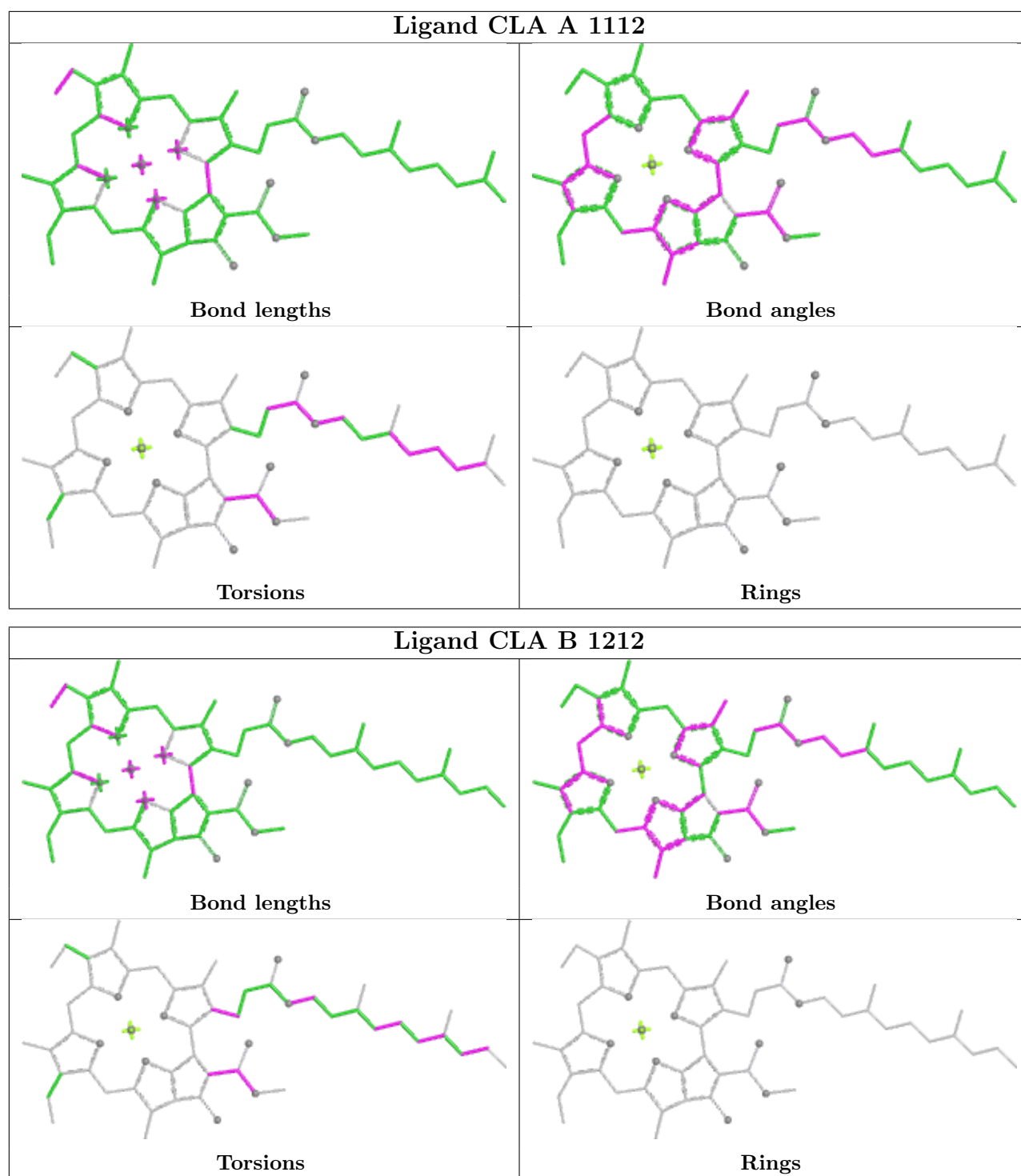


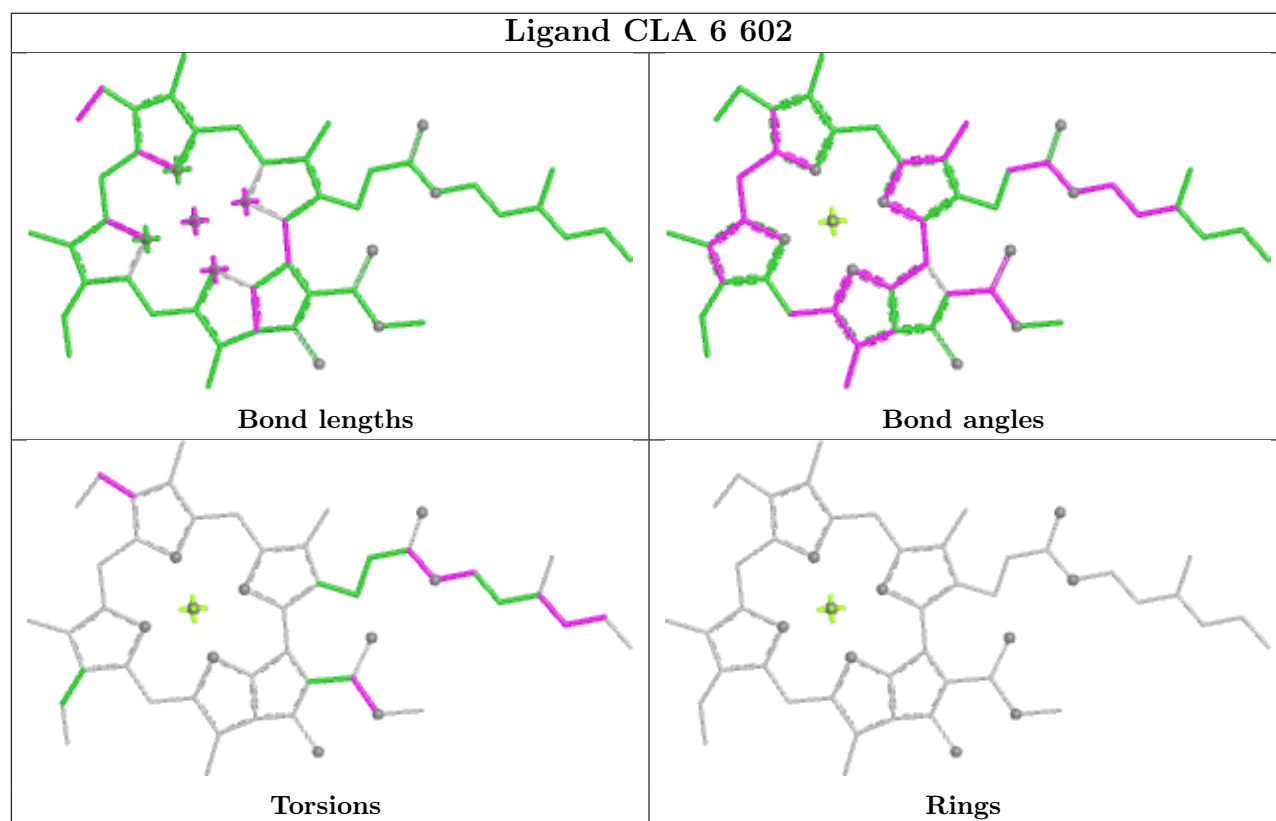
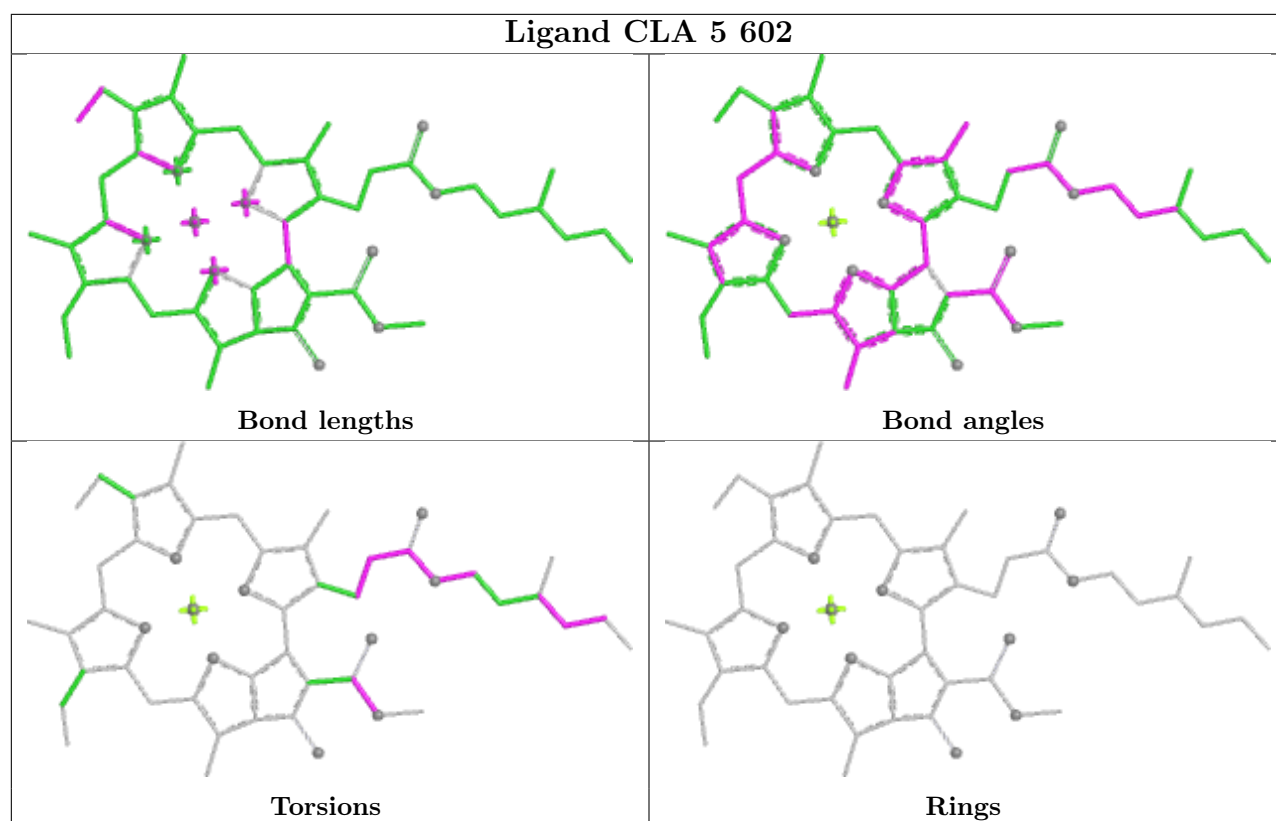
Ligand CHL a 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL 3 604	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 4001	
 Bond lengths	 Bond angles
 Torsions	 Rings

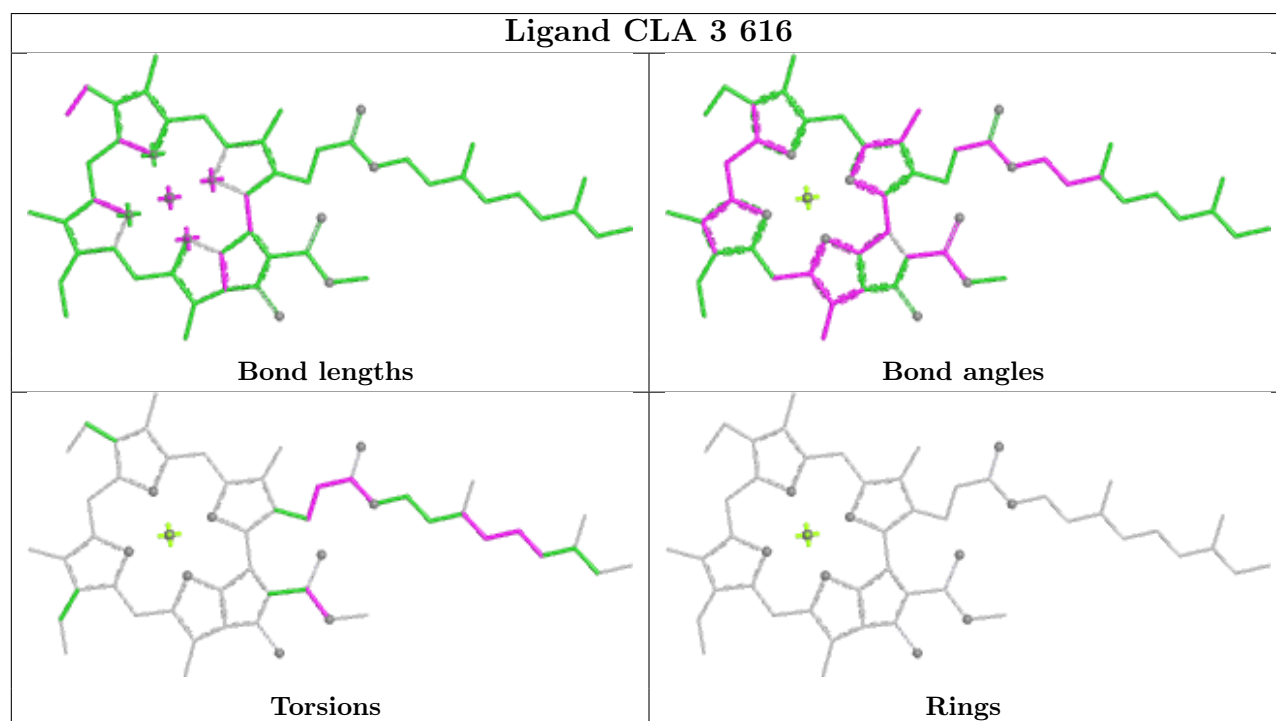
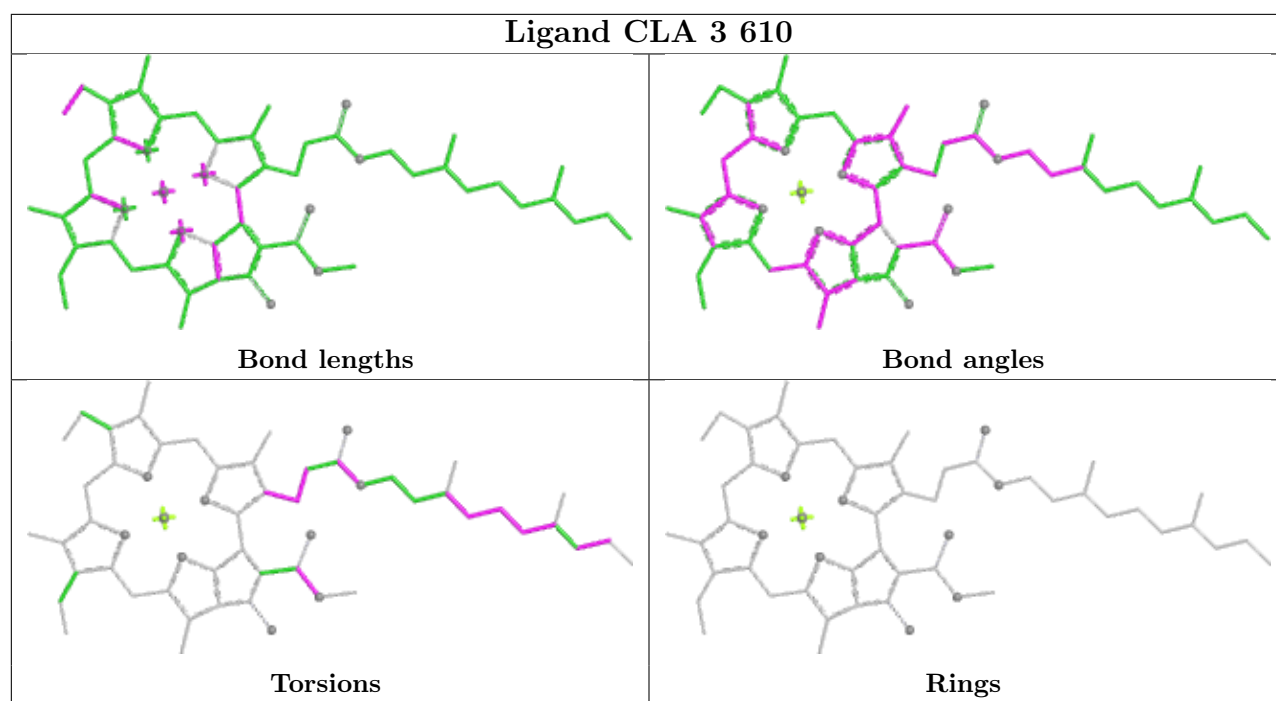


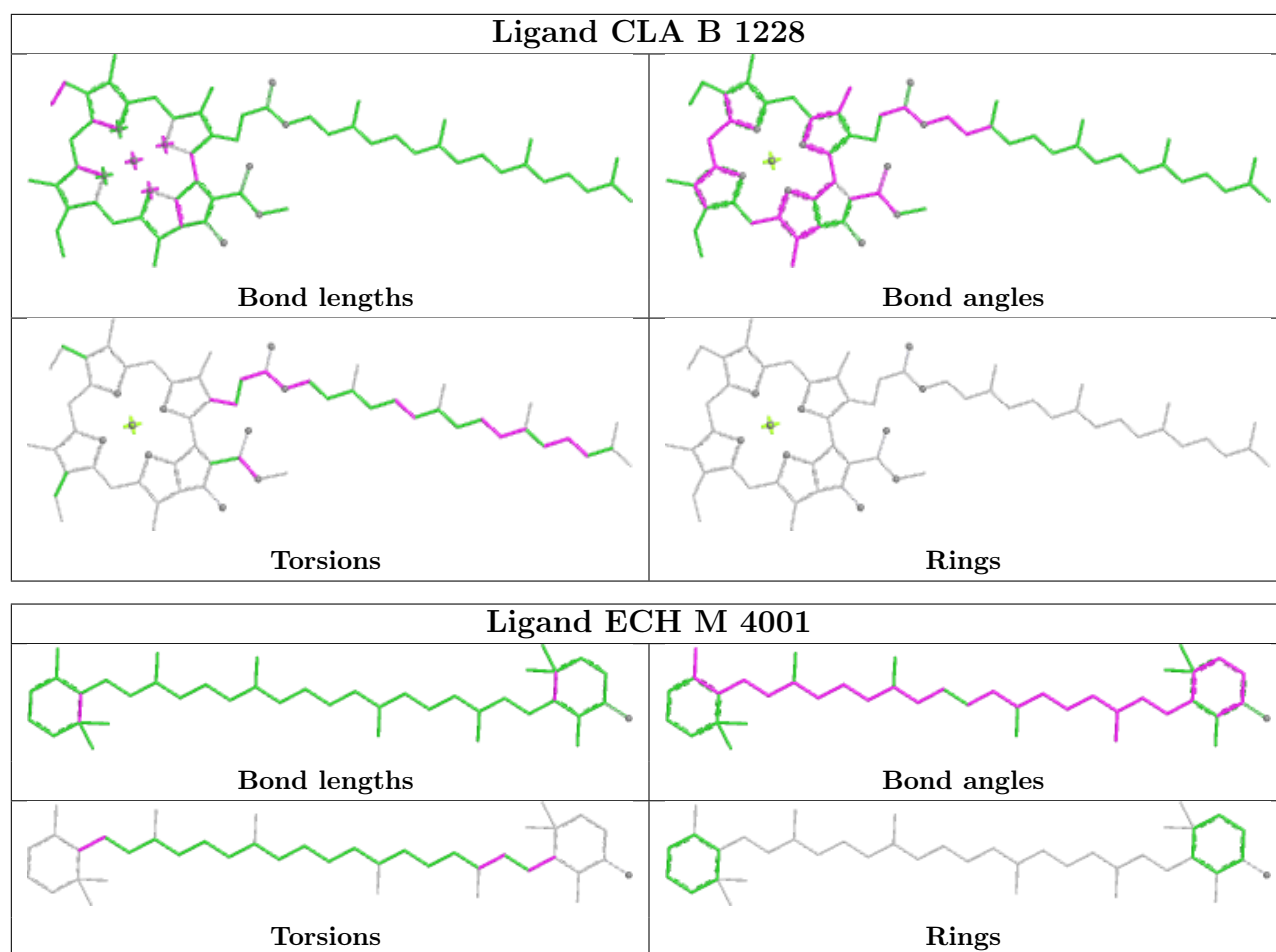


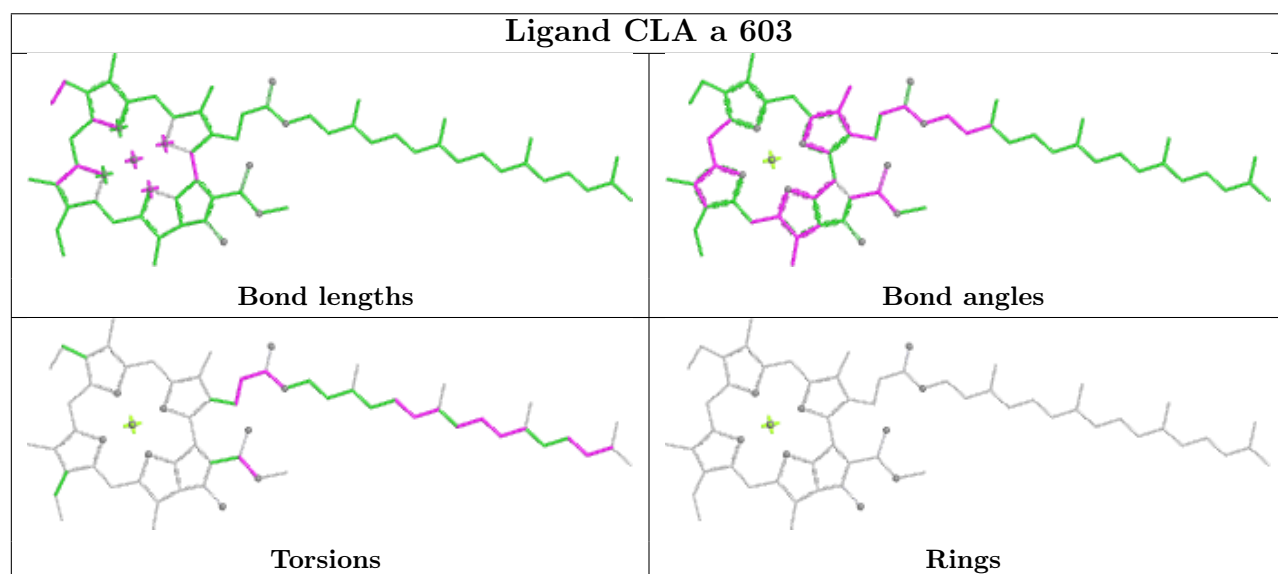
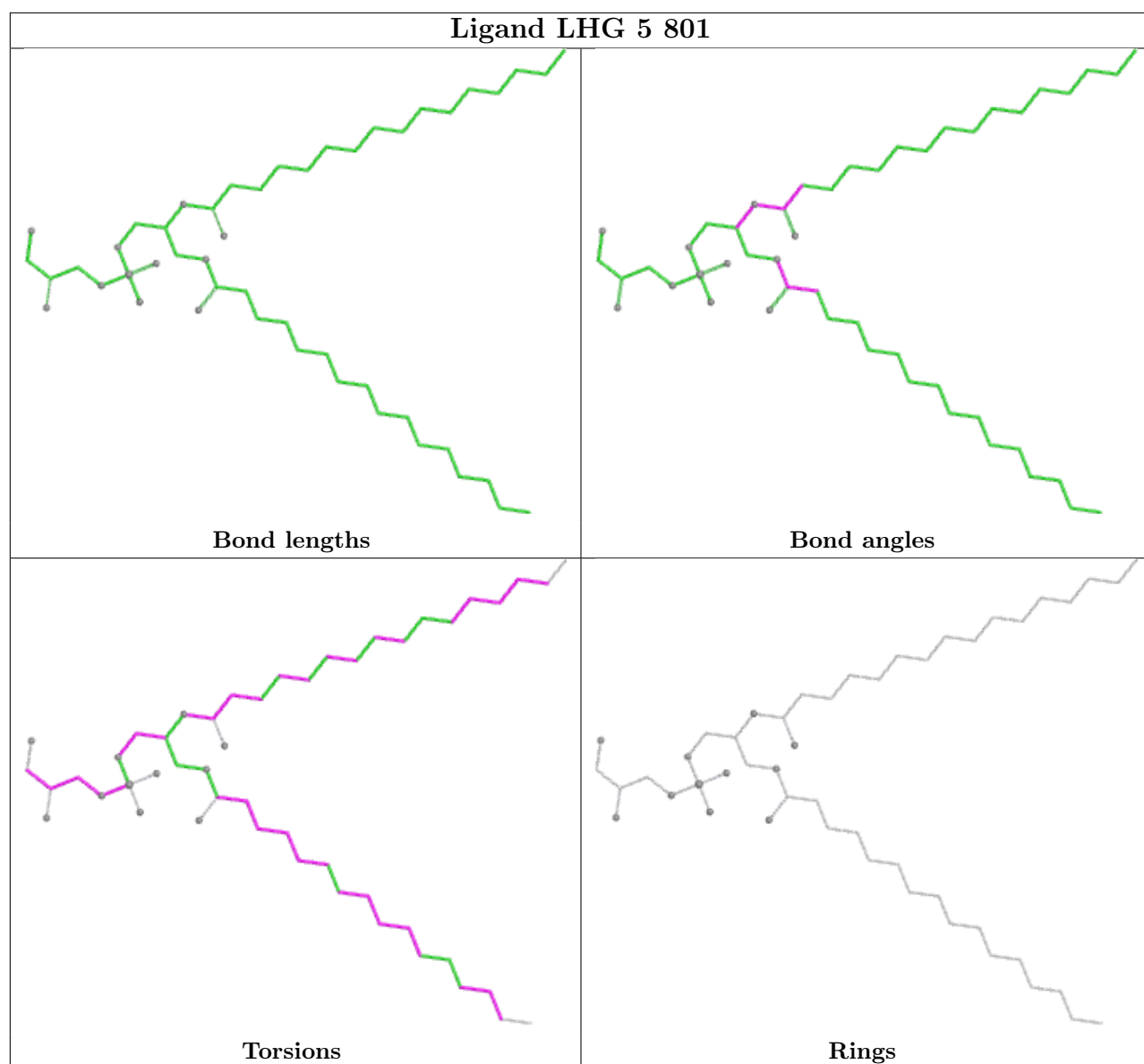




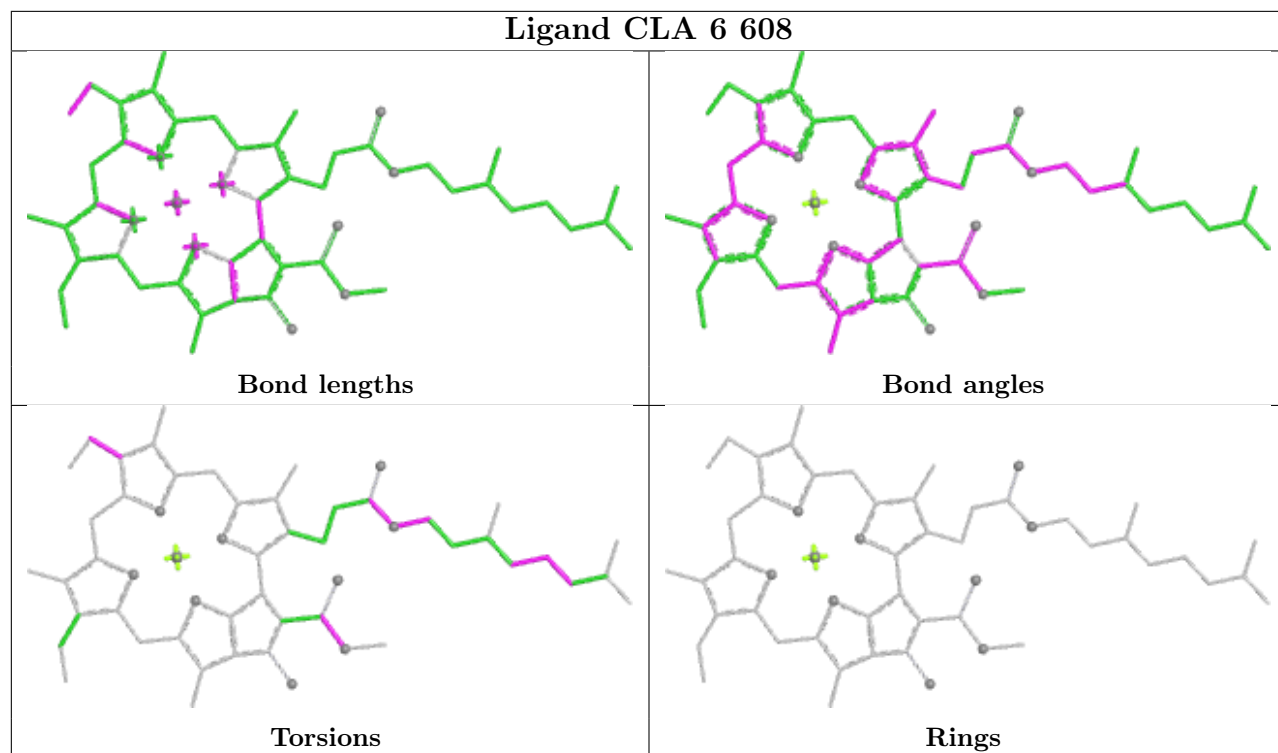




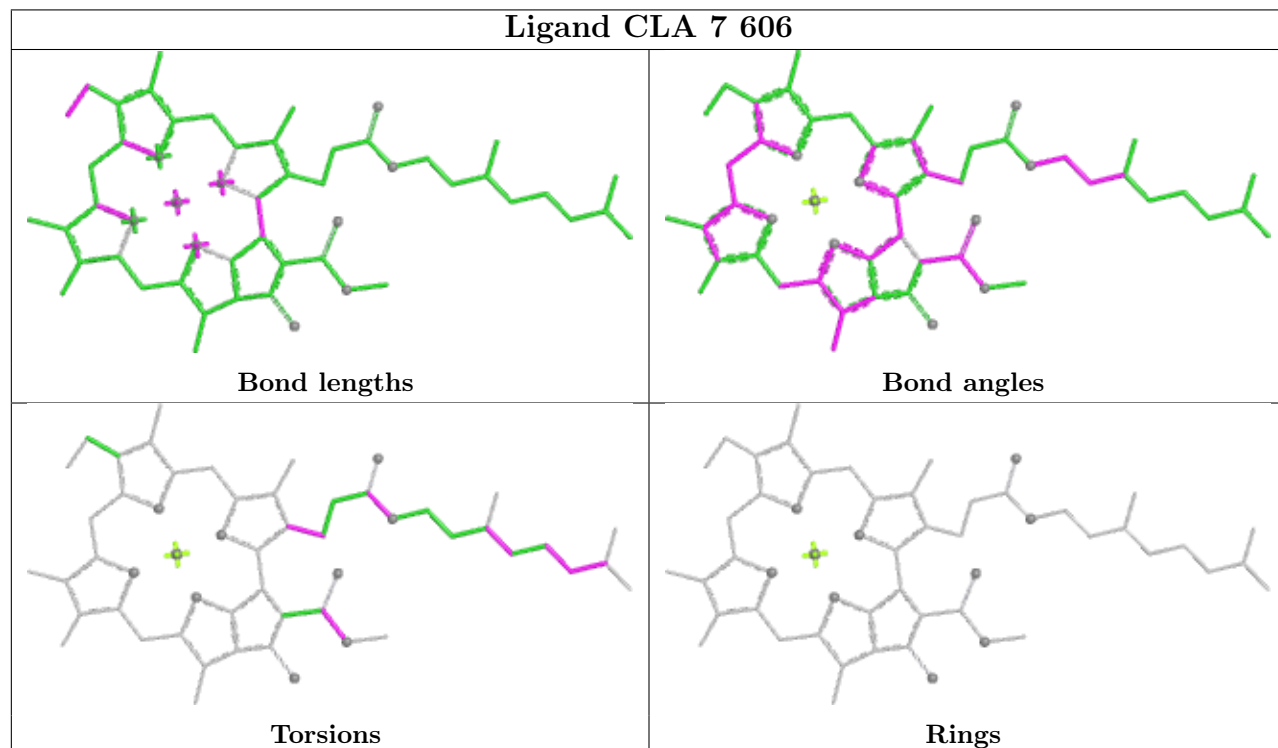




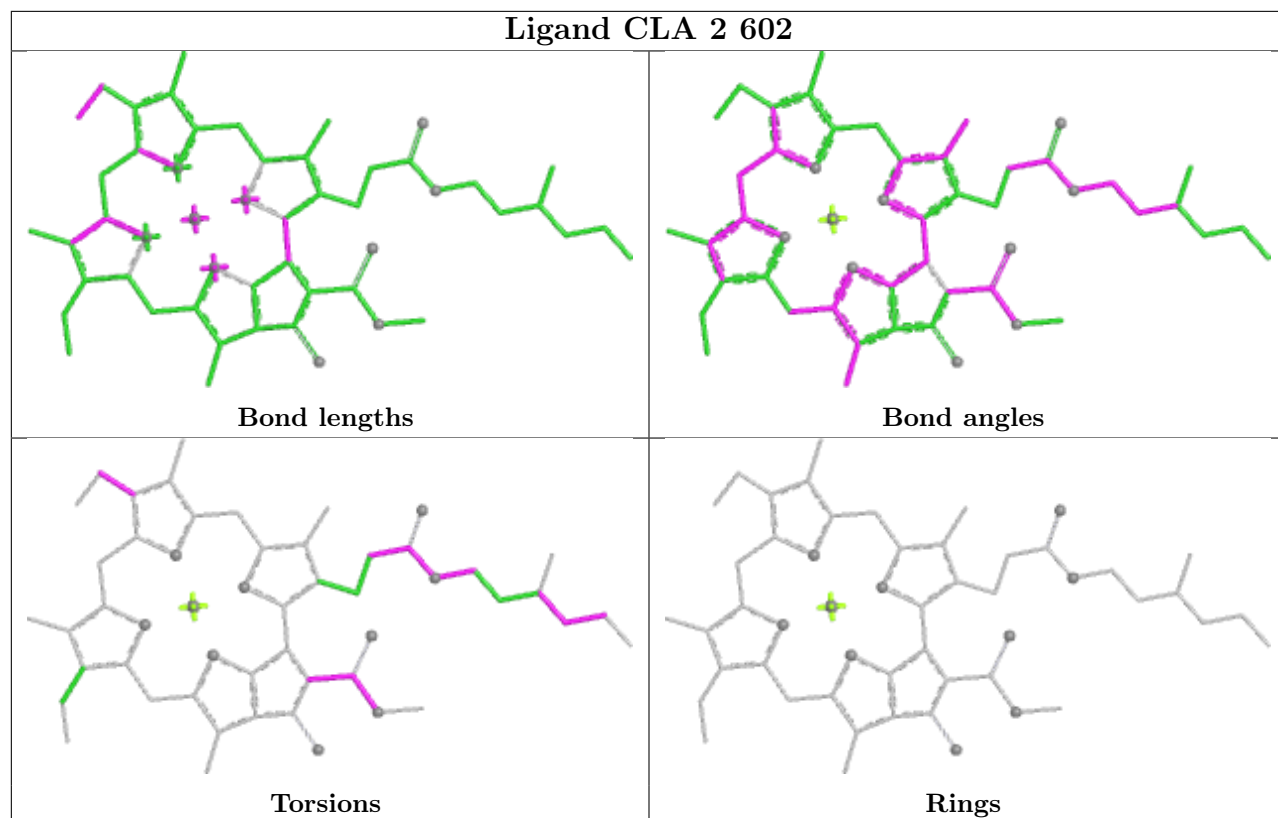
Ligand CLA 6 608



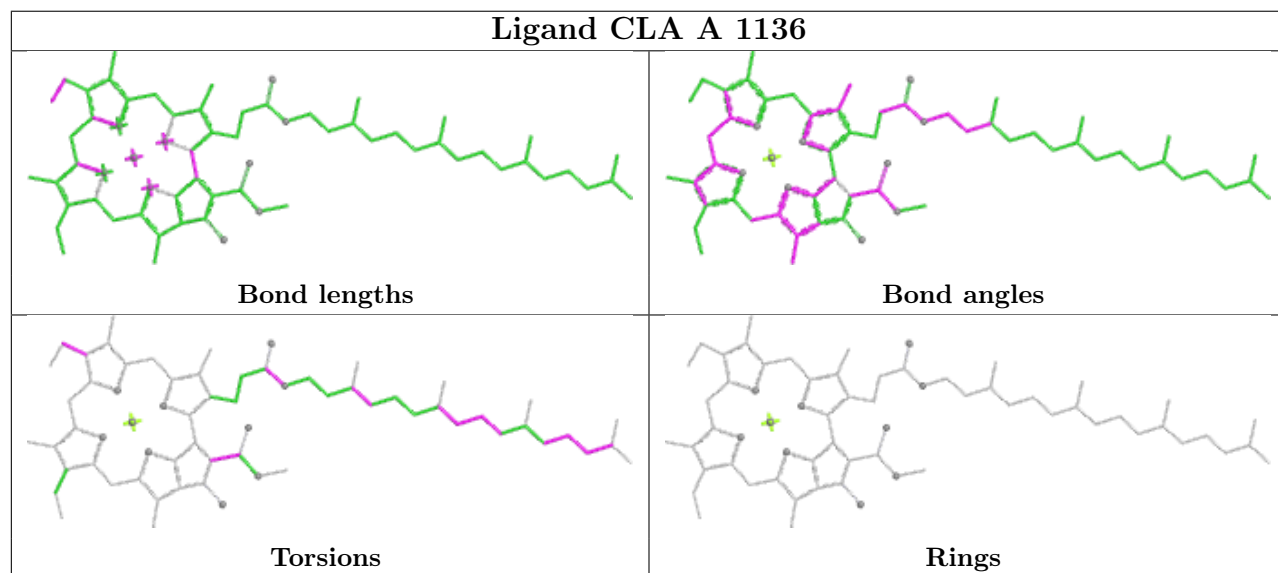
Ligand CLA 7 606

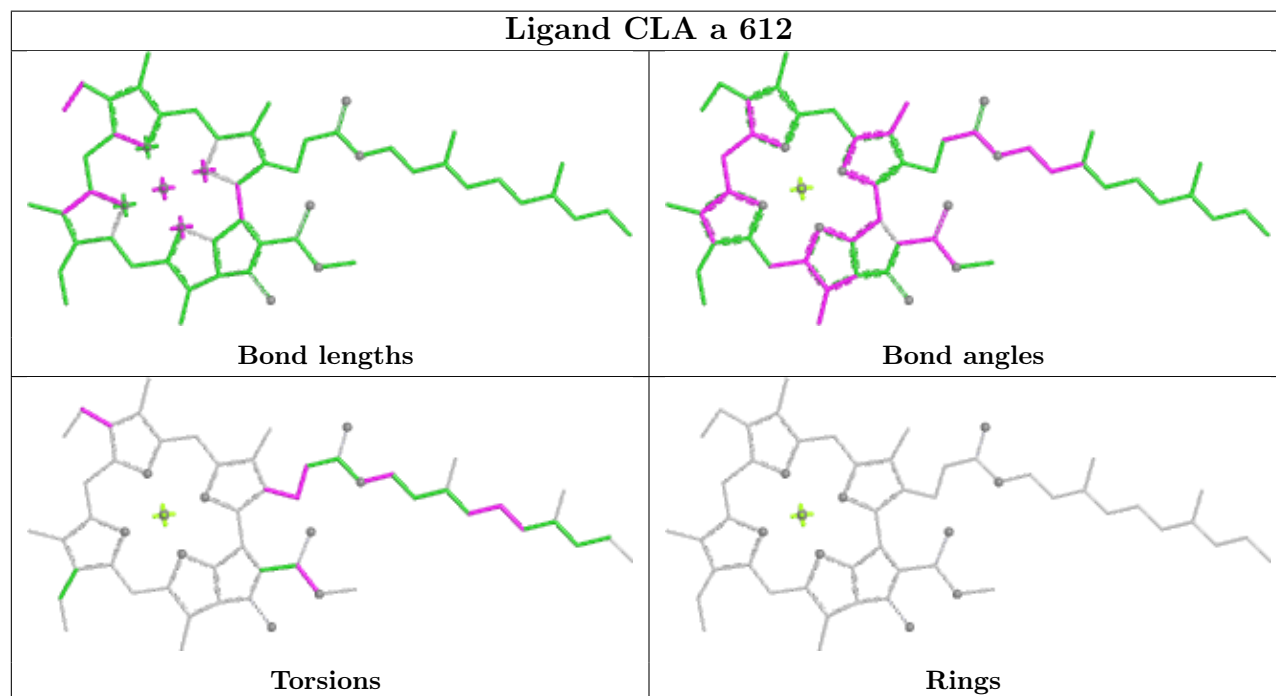
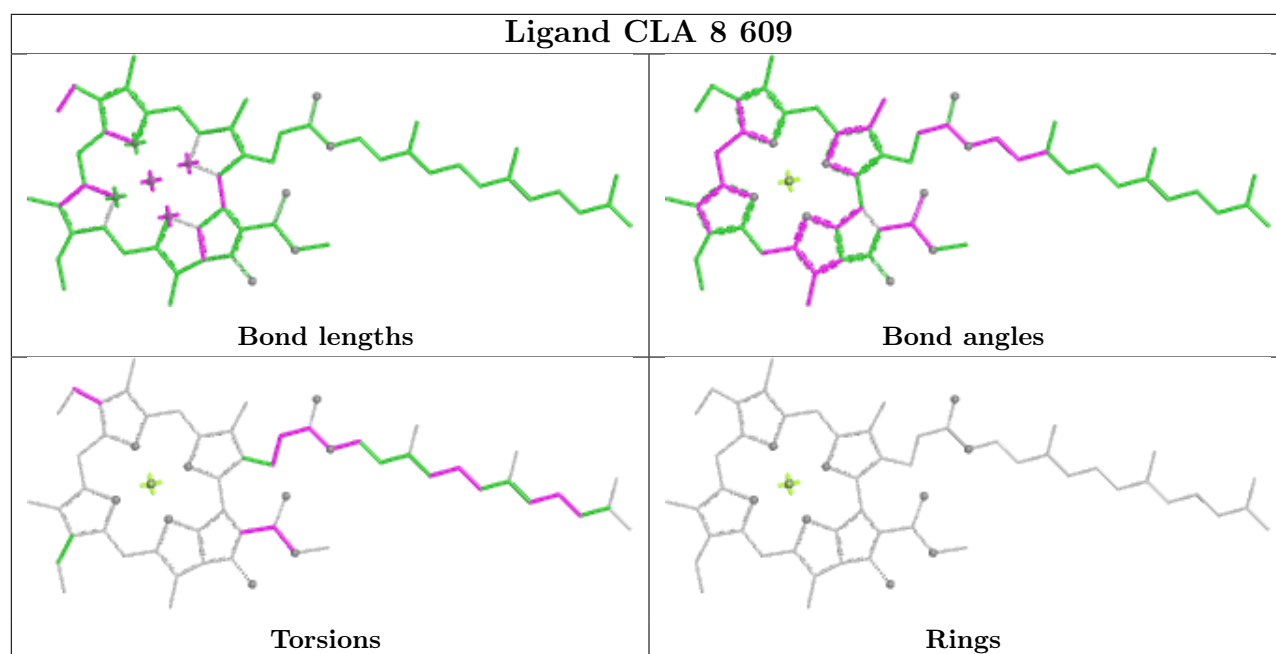


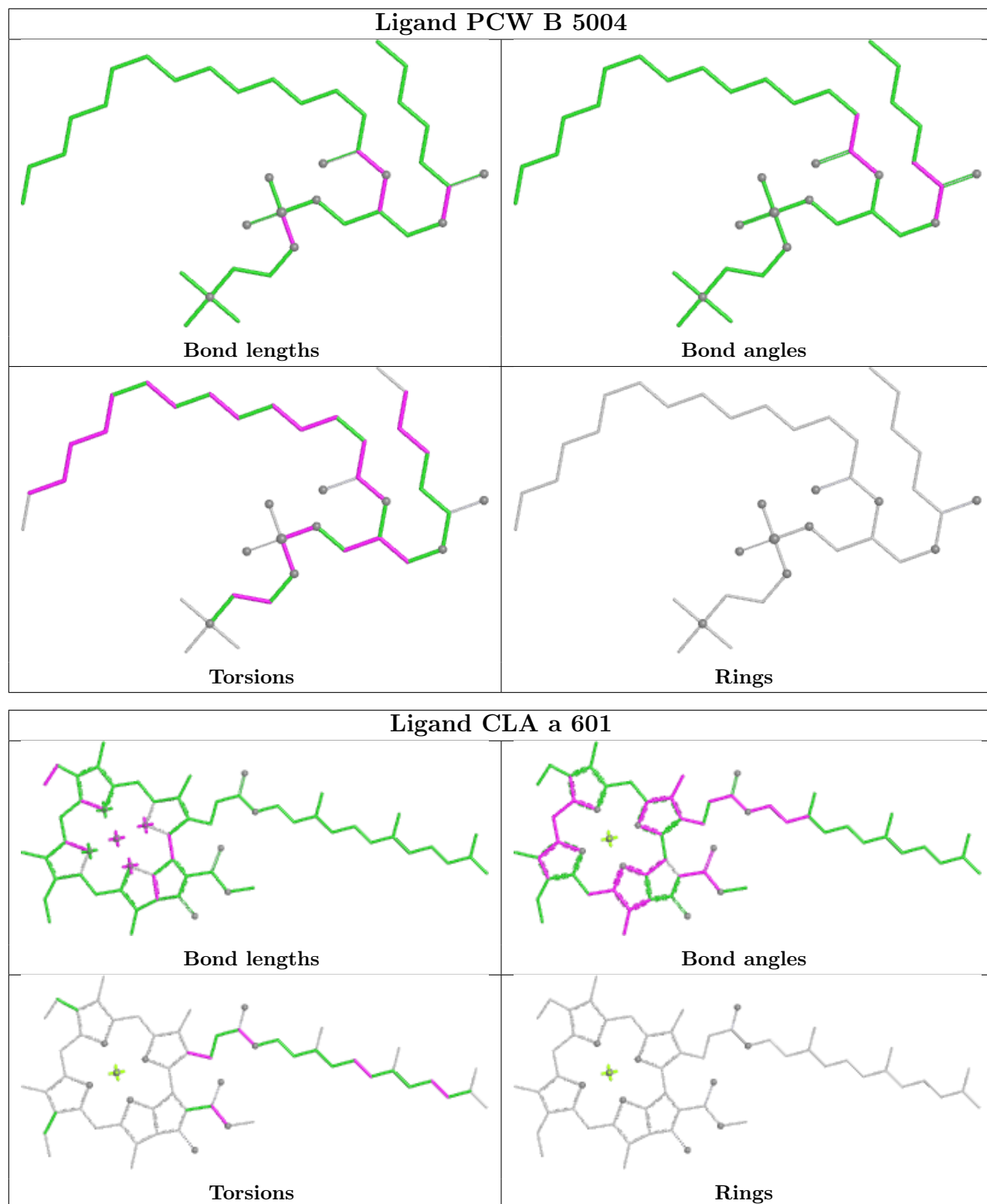
Ligand CLA 2 602

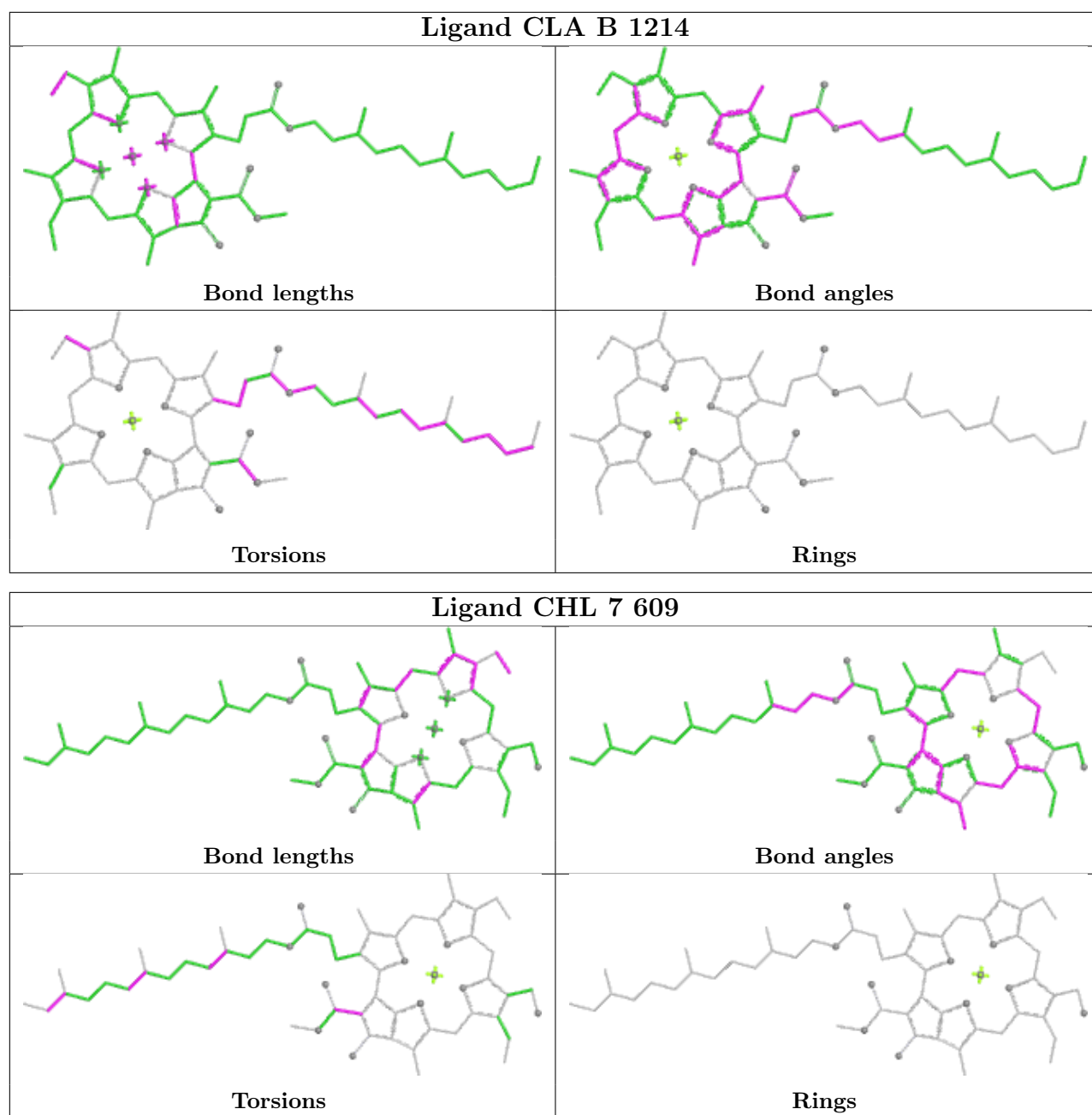


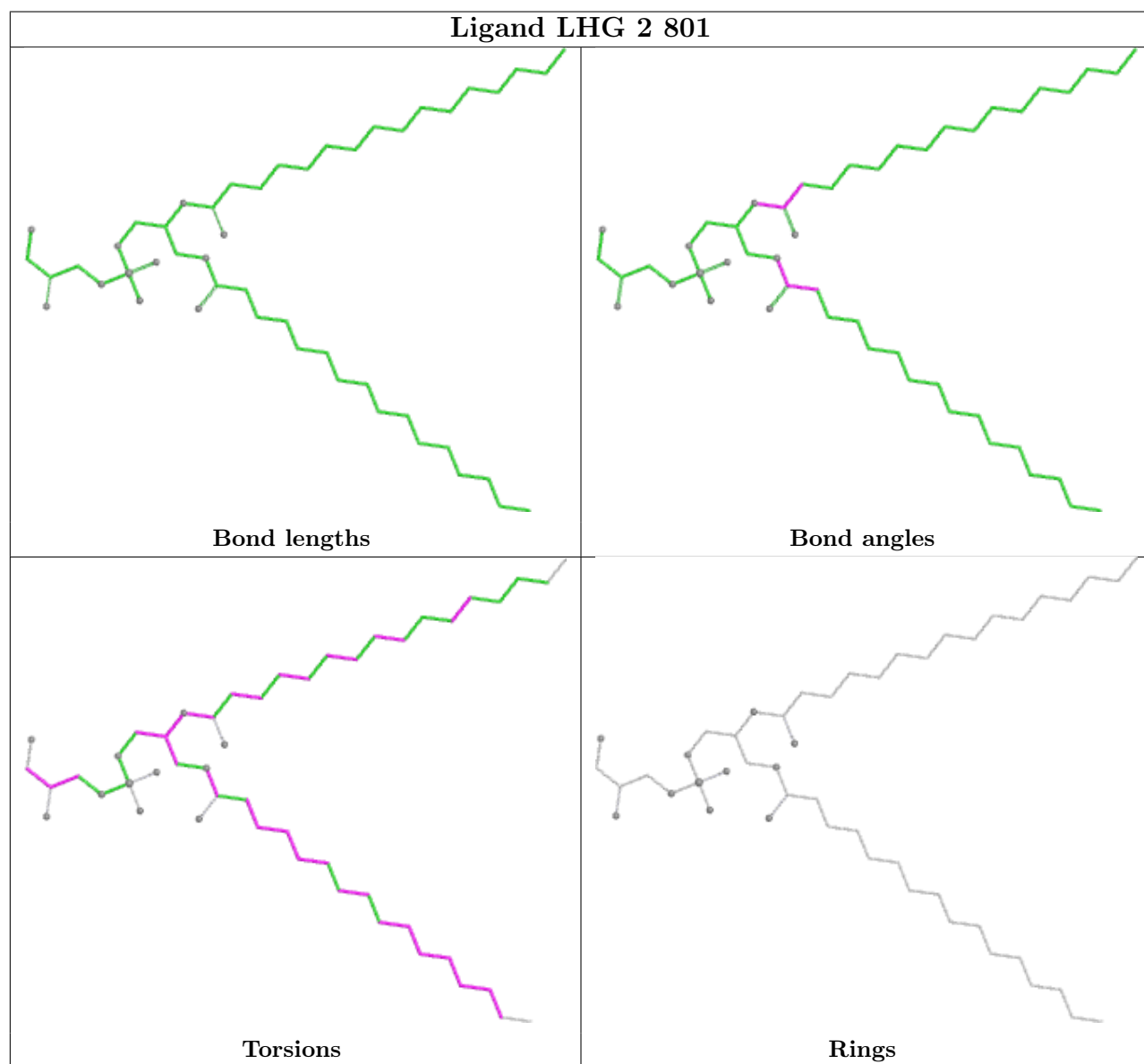
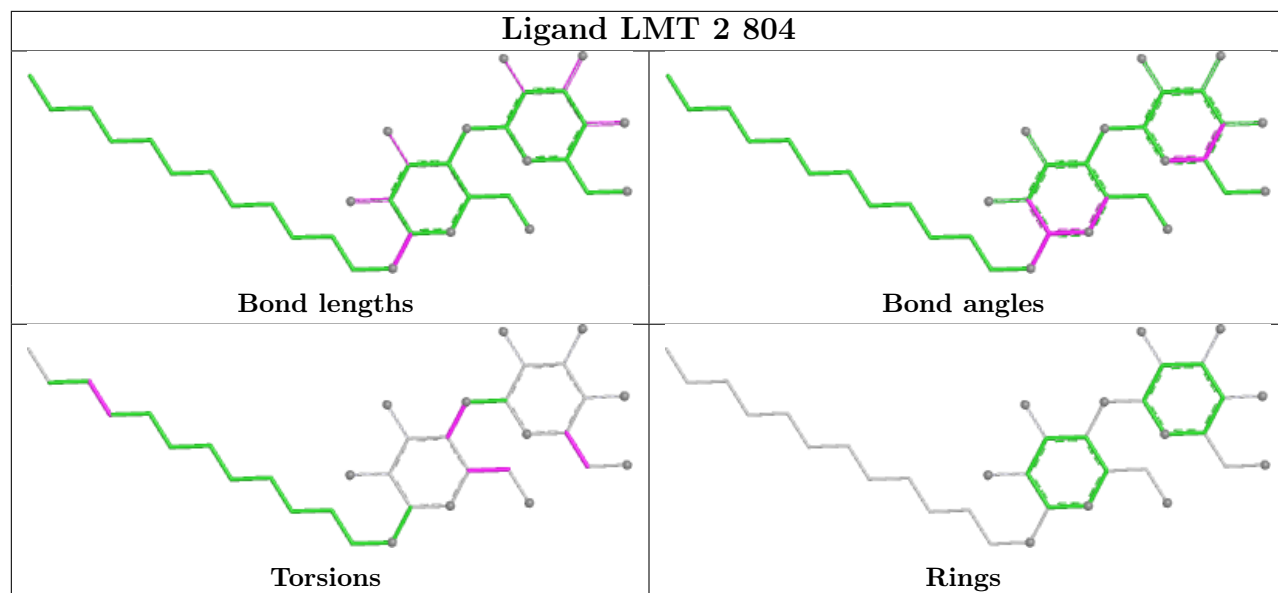
Ligand CLA A 1136

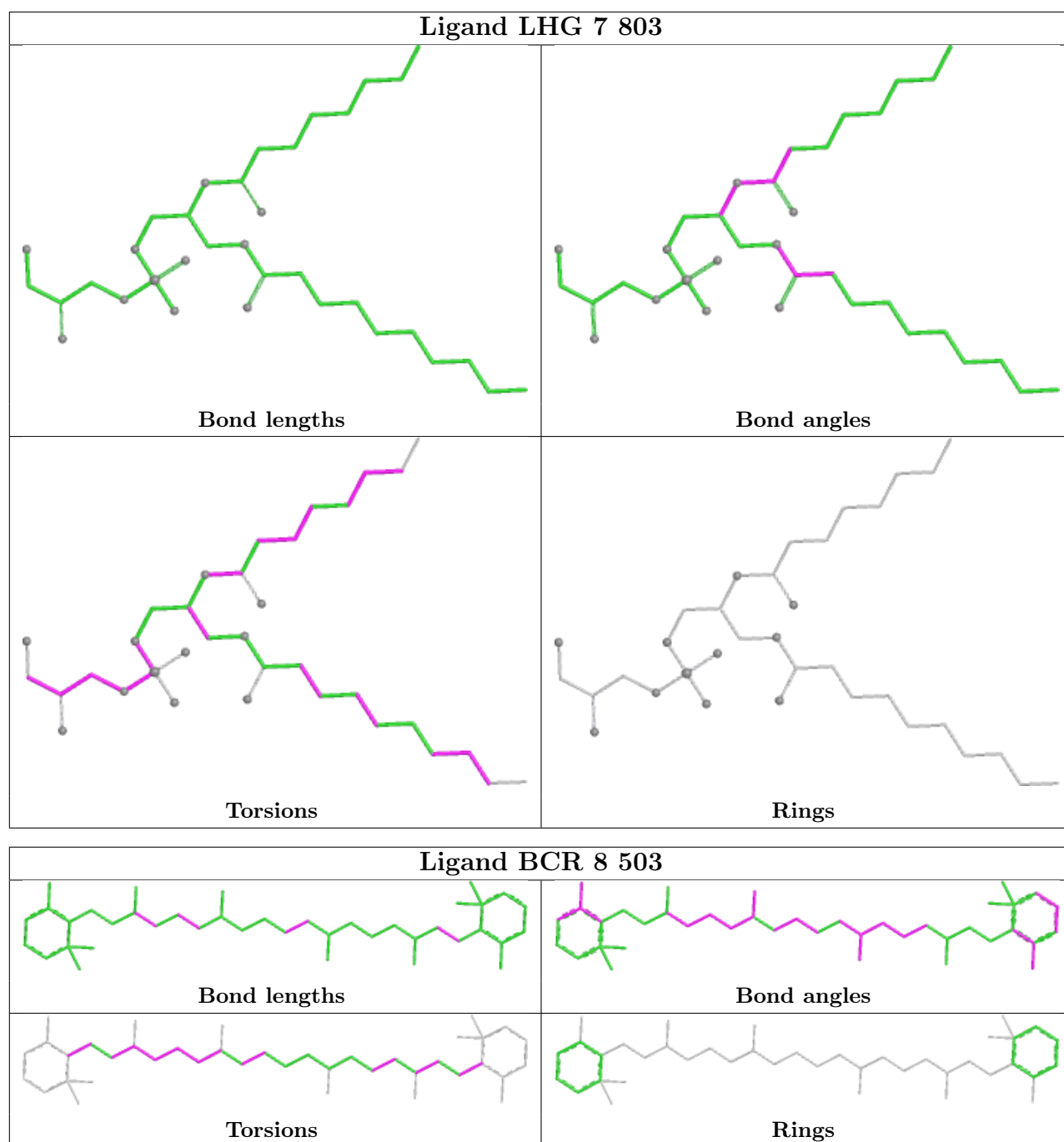


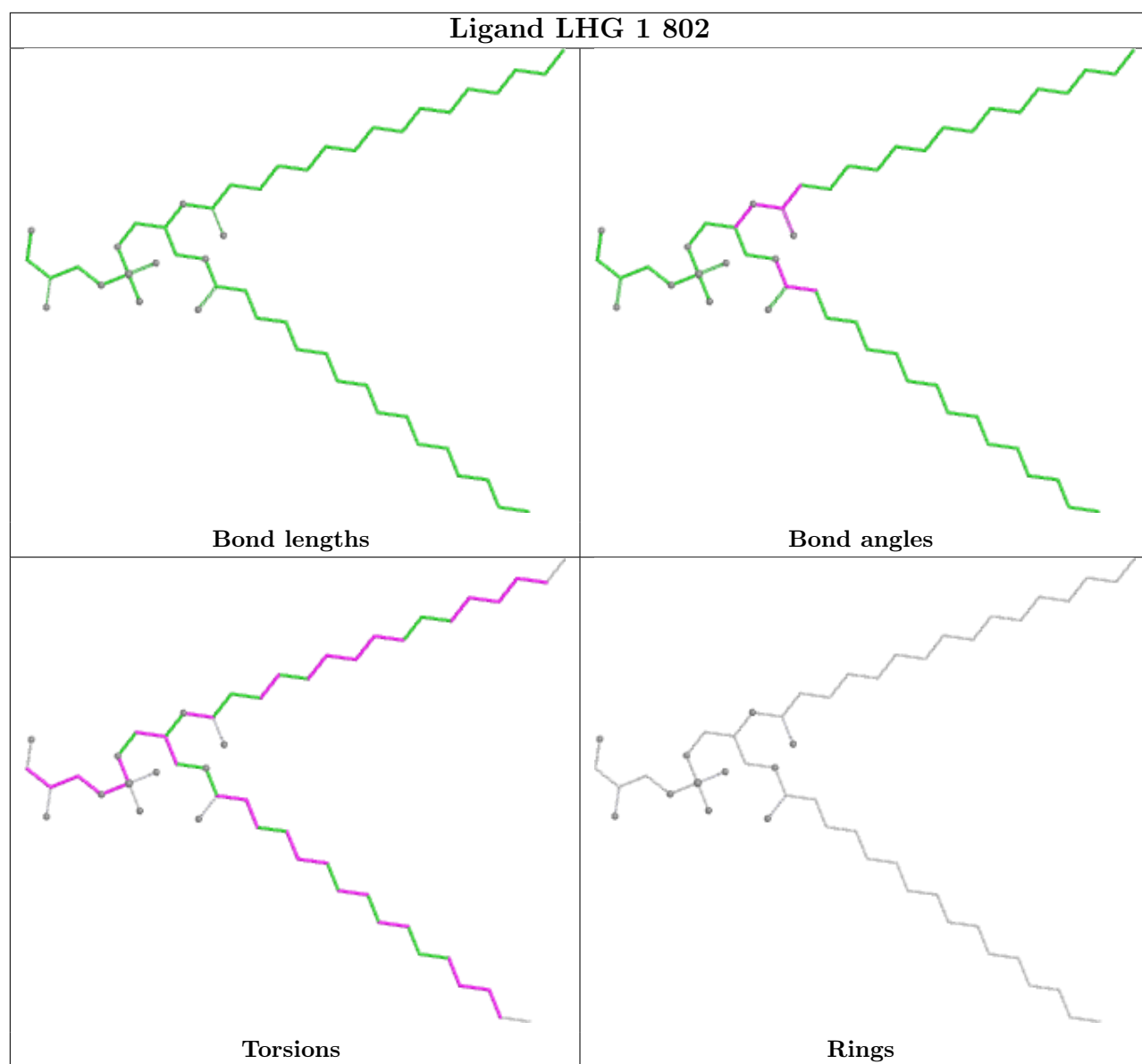




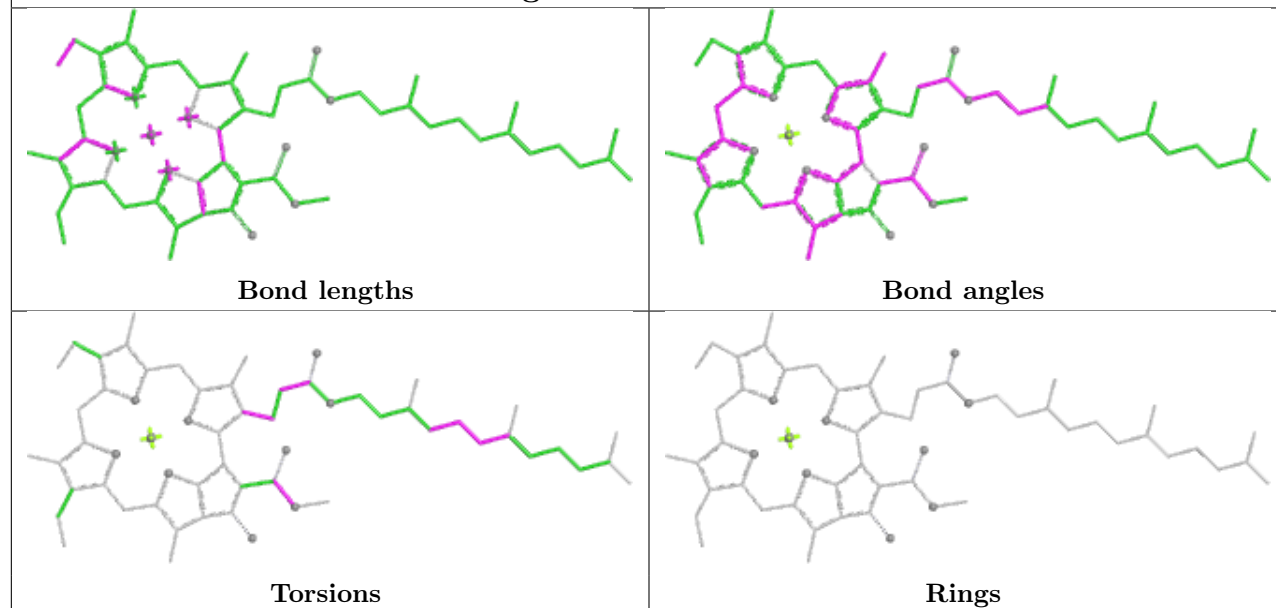




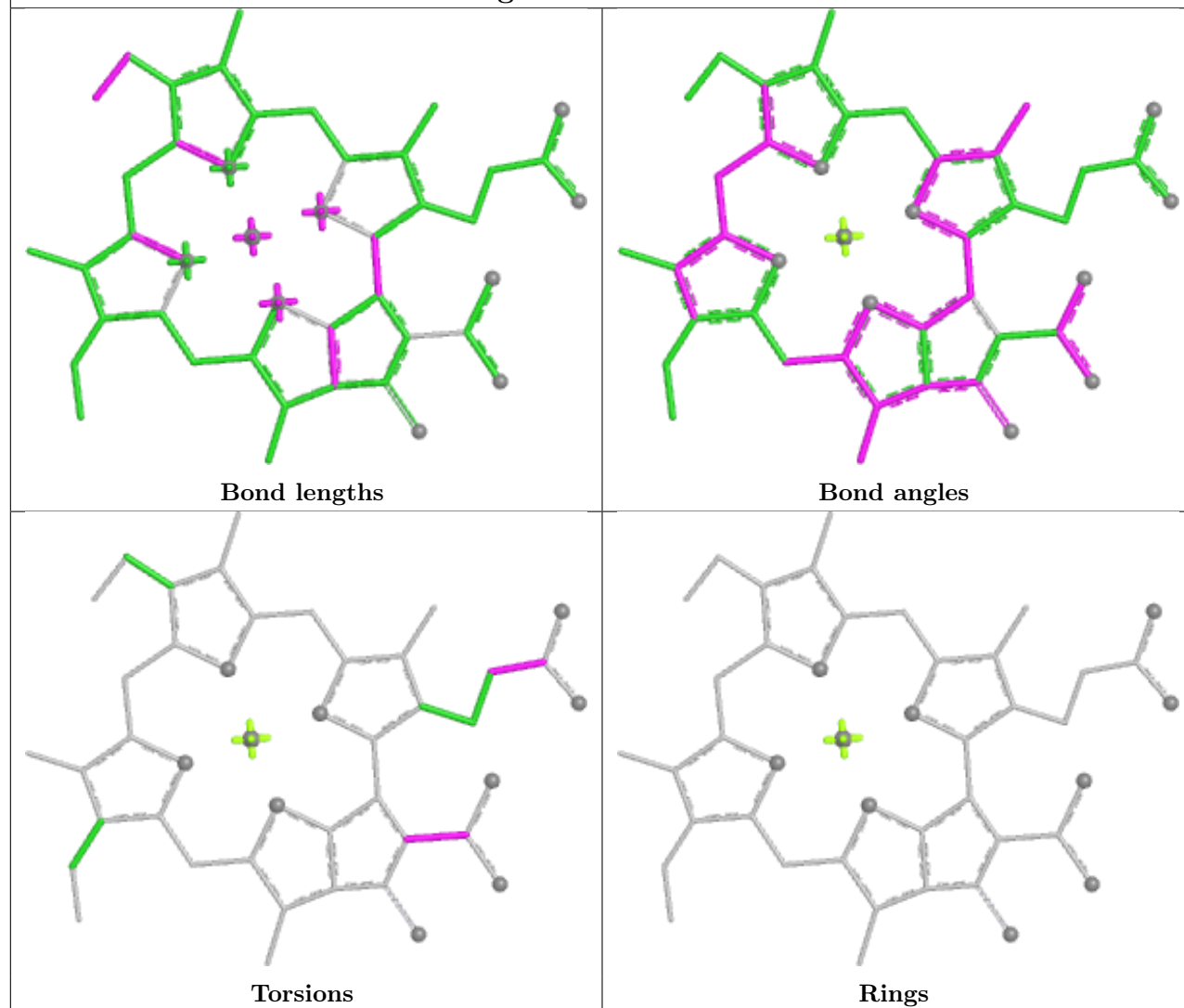


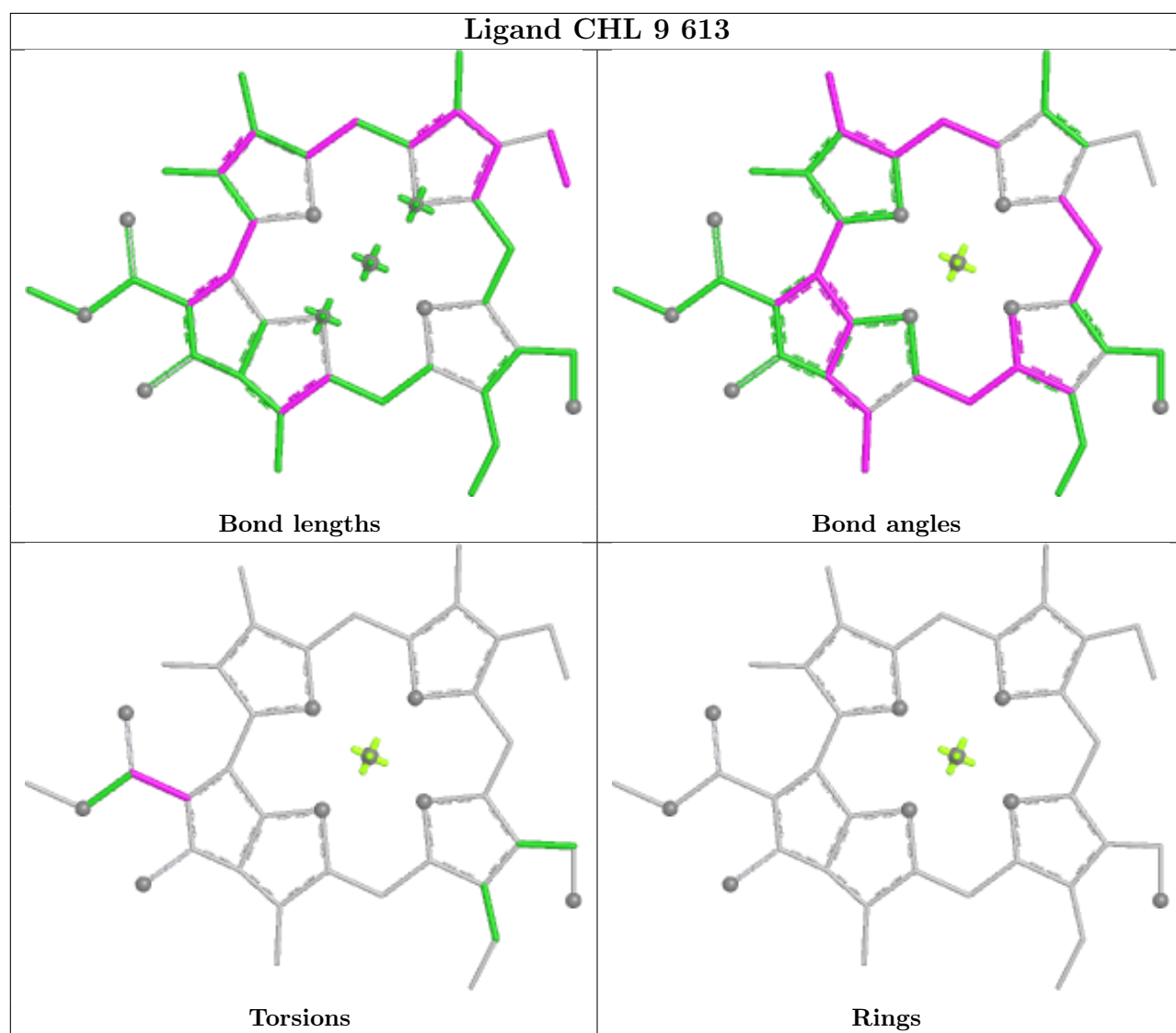
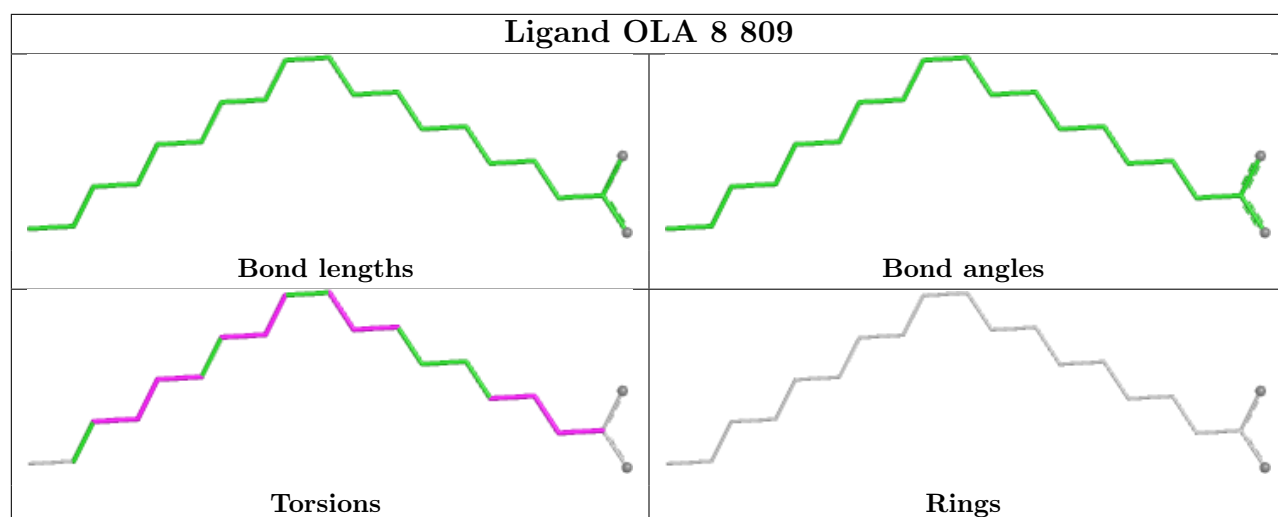


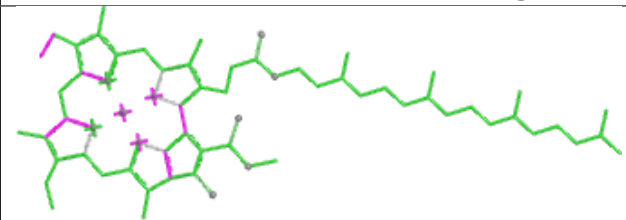
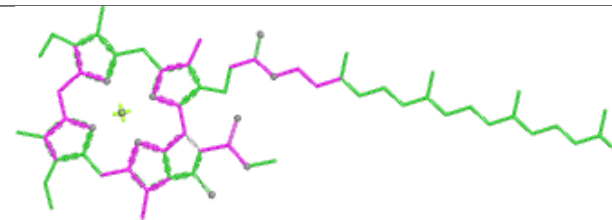
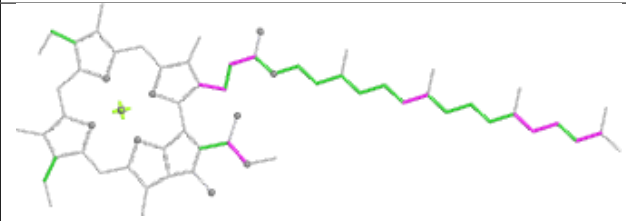
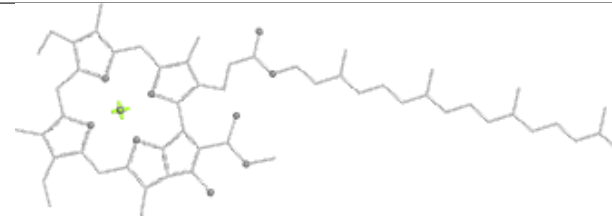
Ligand CLA K 1402

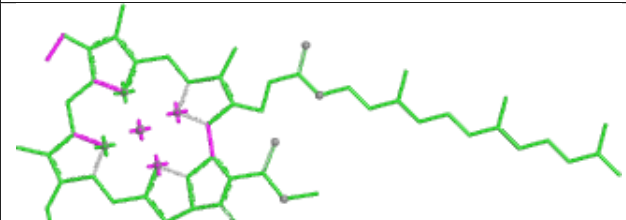
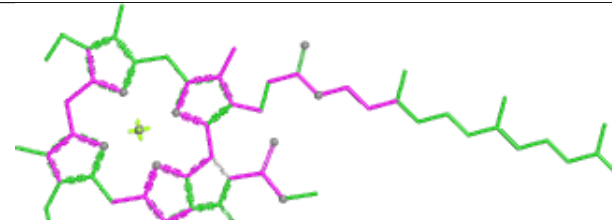
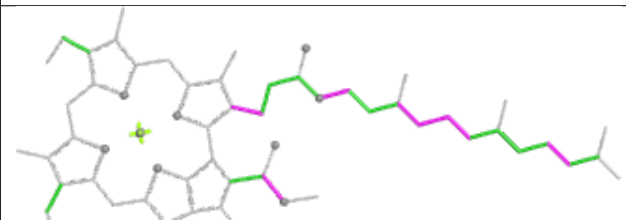
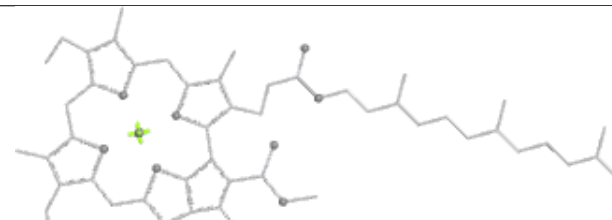


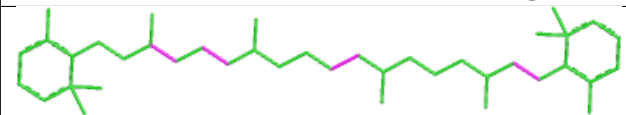
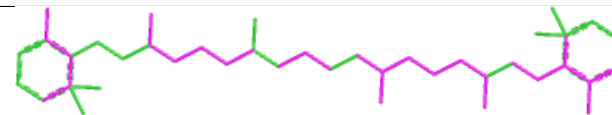
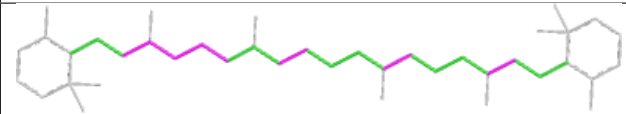
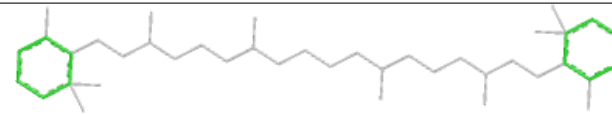
Ligand CLA 7 605

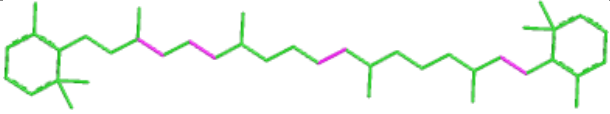
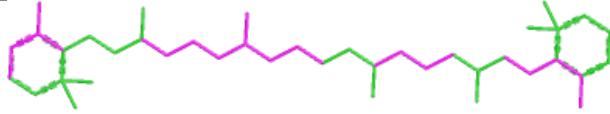
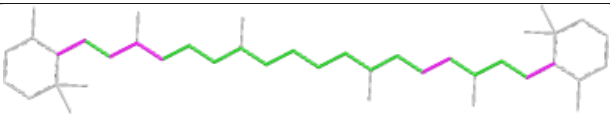
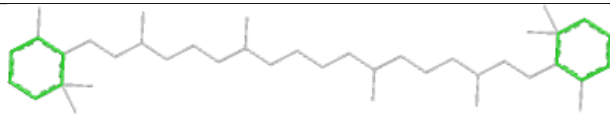
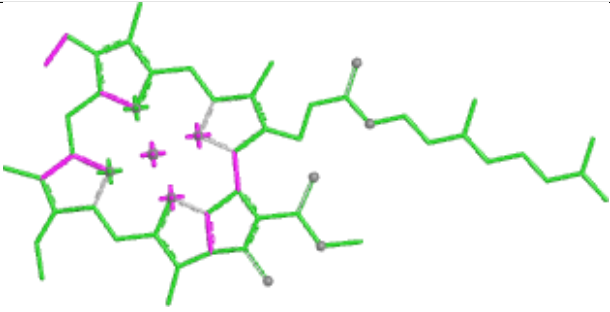
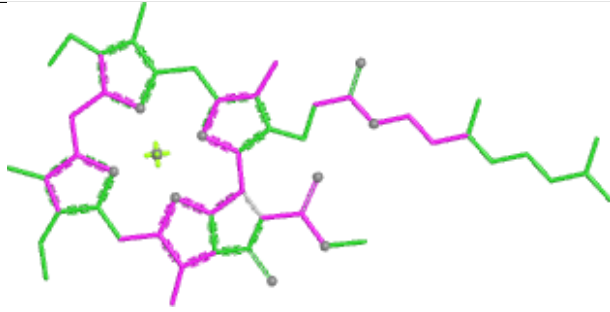
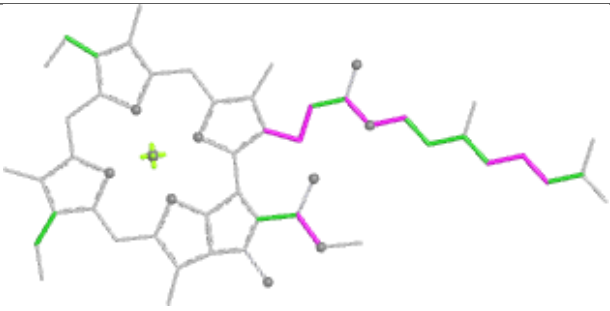
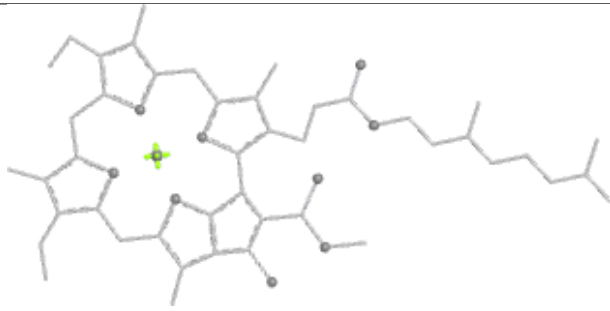
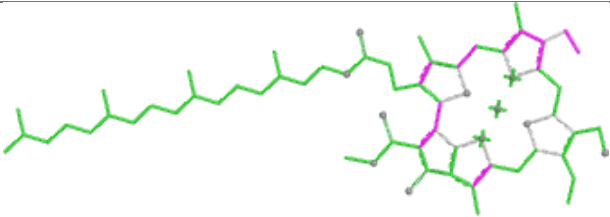
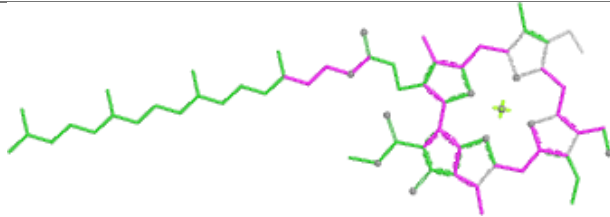
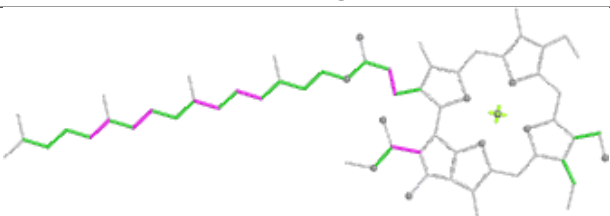
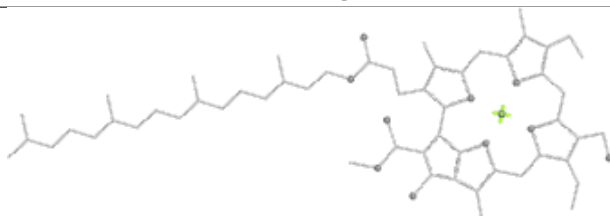


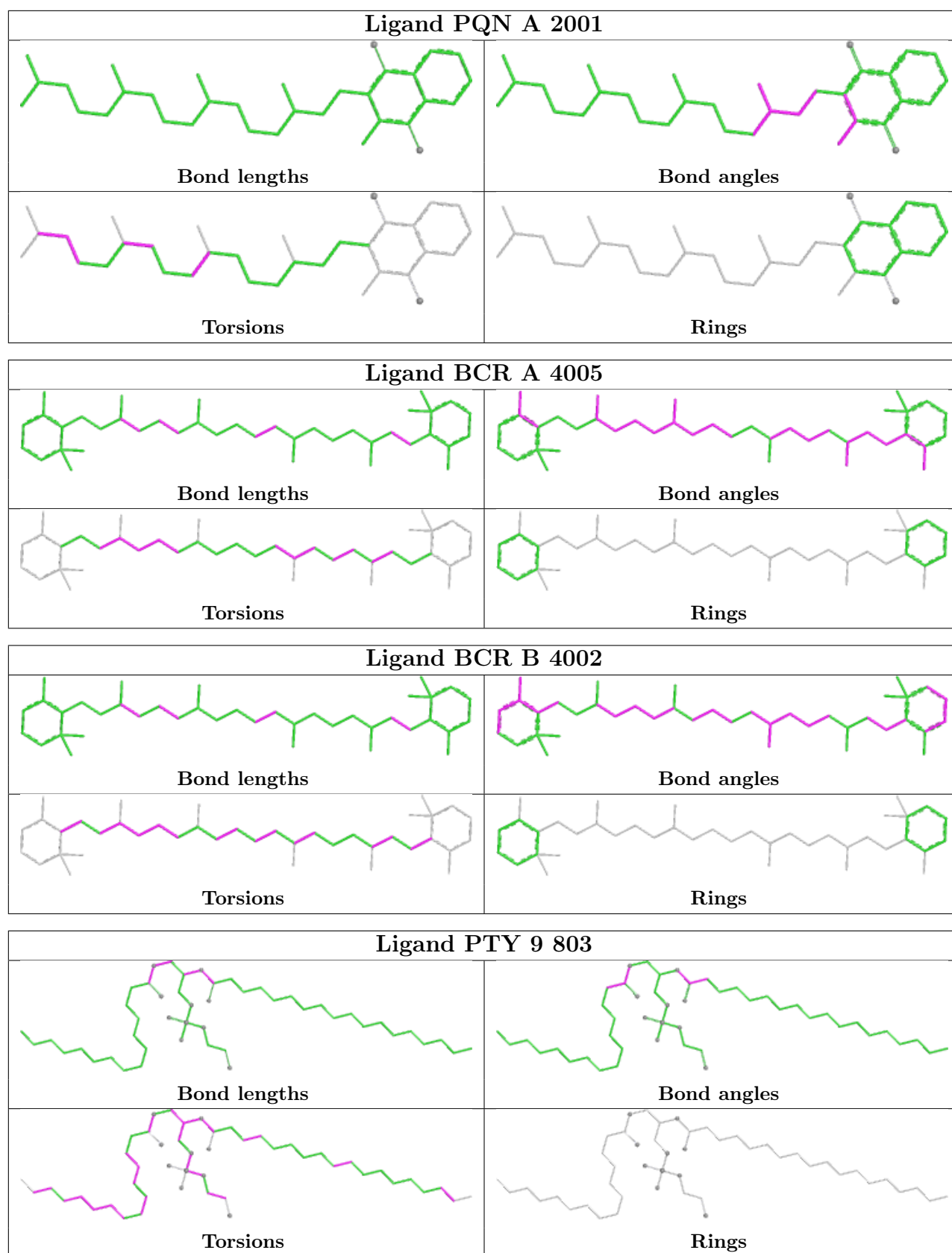


Ligand CLA B 1240	
	
Bond lengths	Bond angles
	
Torsions	Rings

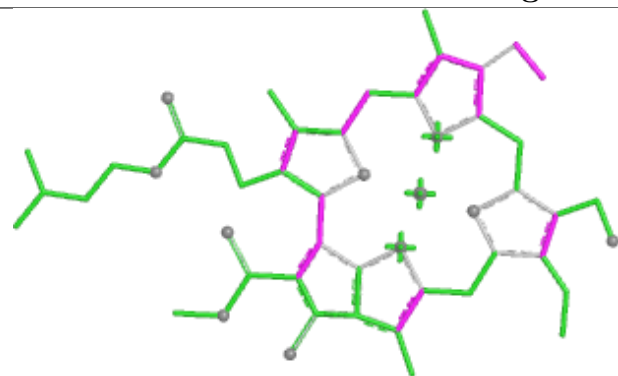
Ligand CLA 4 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 3 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

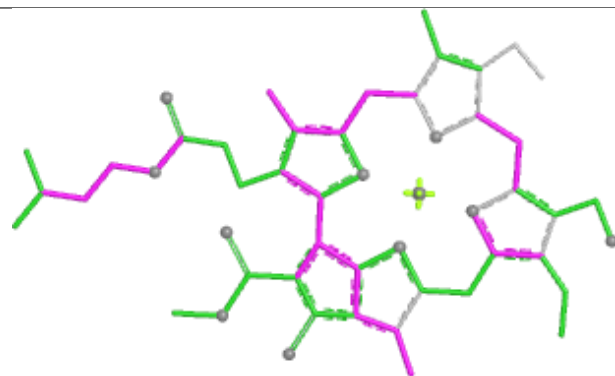
Ligand BCR B 4004	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 1140	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL 3 603	
 Bond lengths	 Bond angles
 Torsions	 Rings



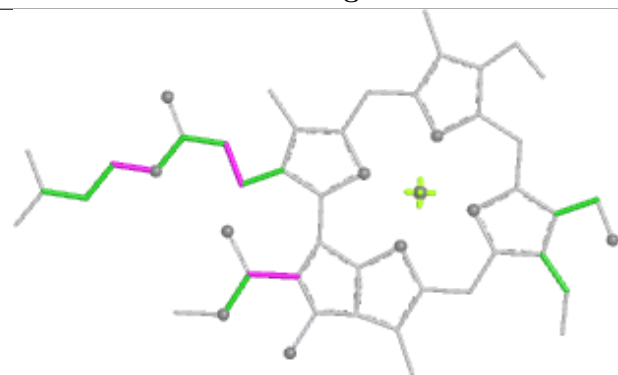
Ligand CHL 9 610



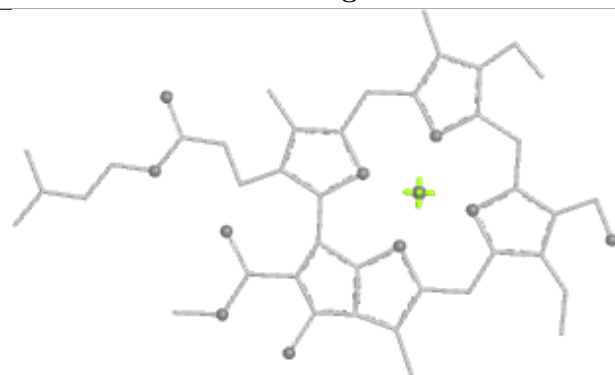
Bond lengths



Bond angles

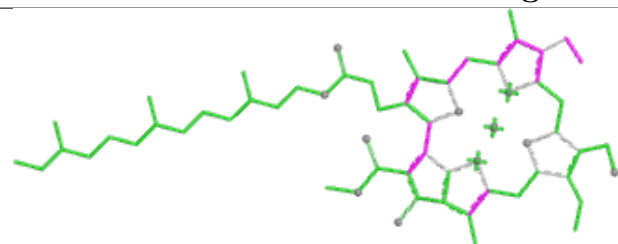


Torsions

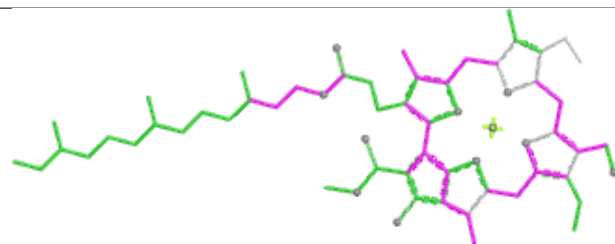


Rings

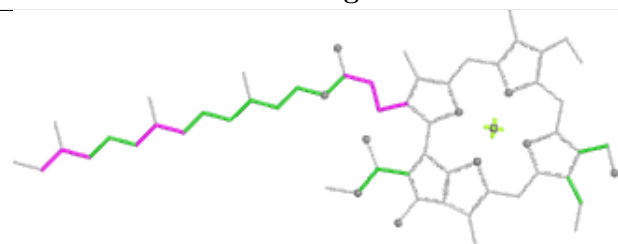
Ligand CHL 8 604



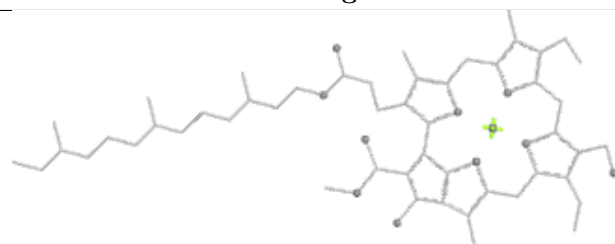
Bond lengths



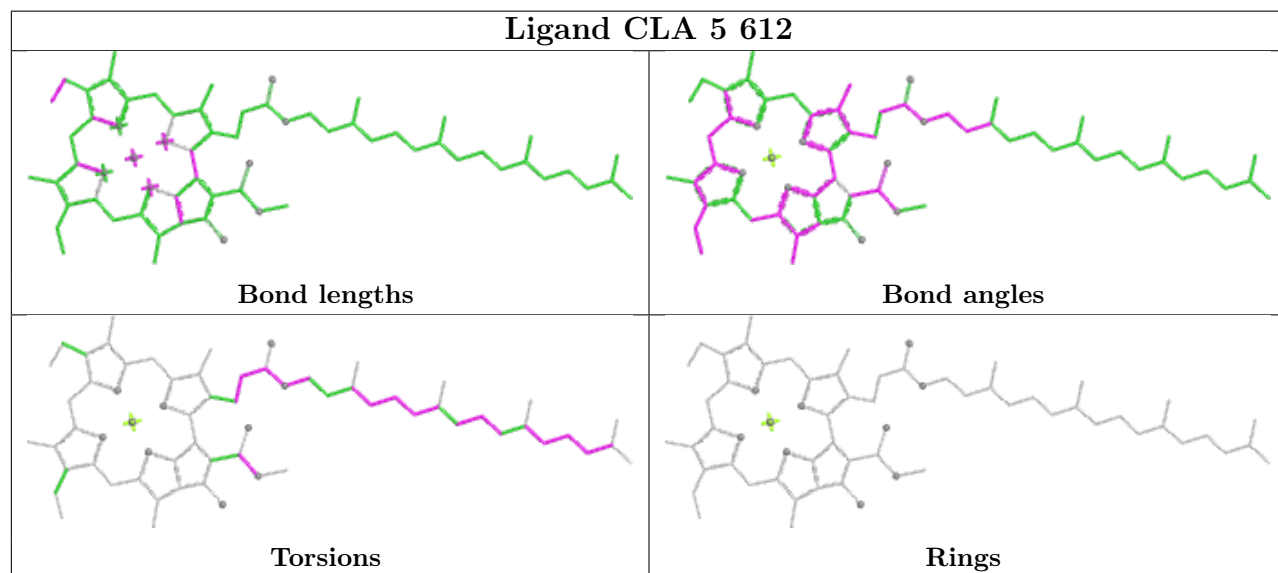
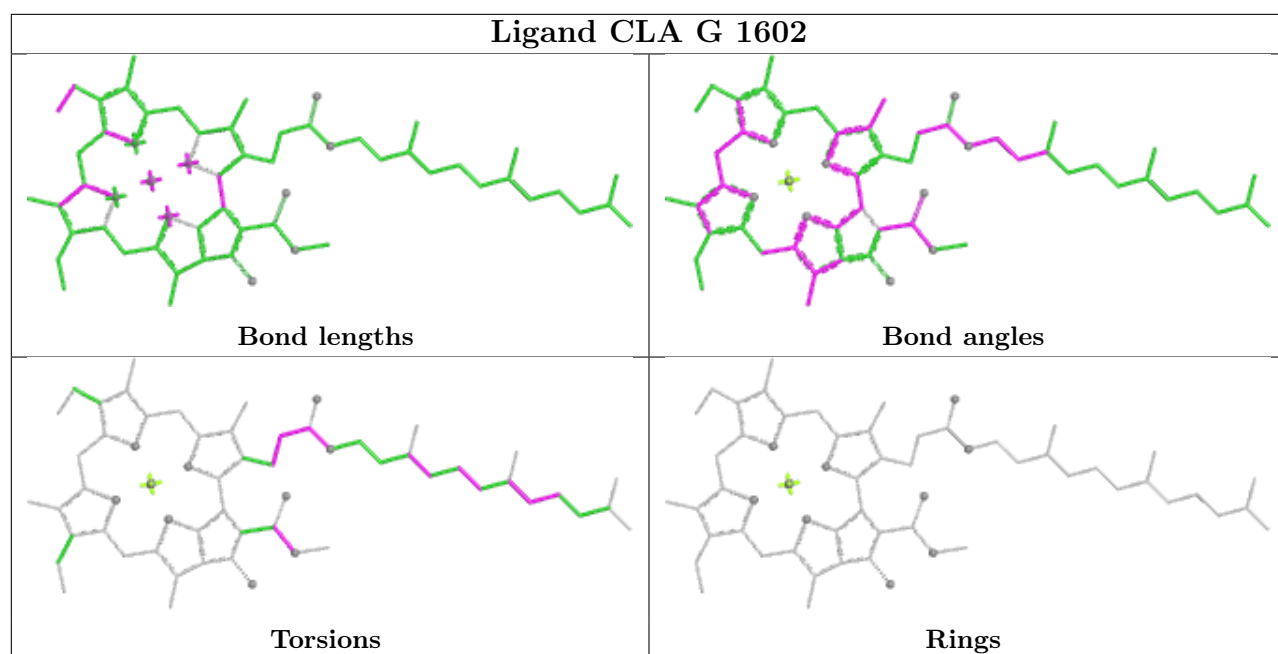
Bond angles



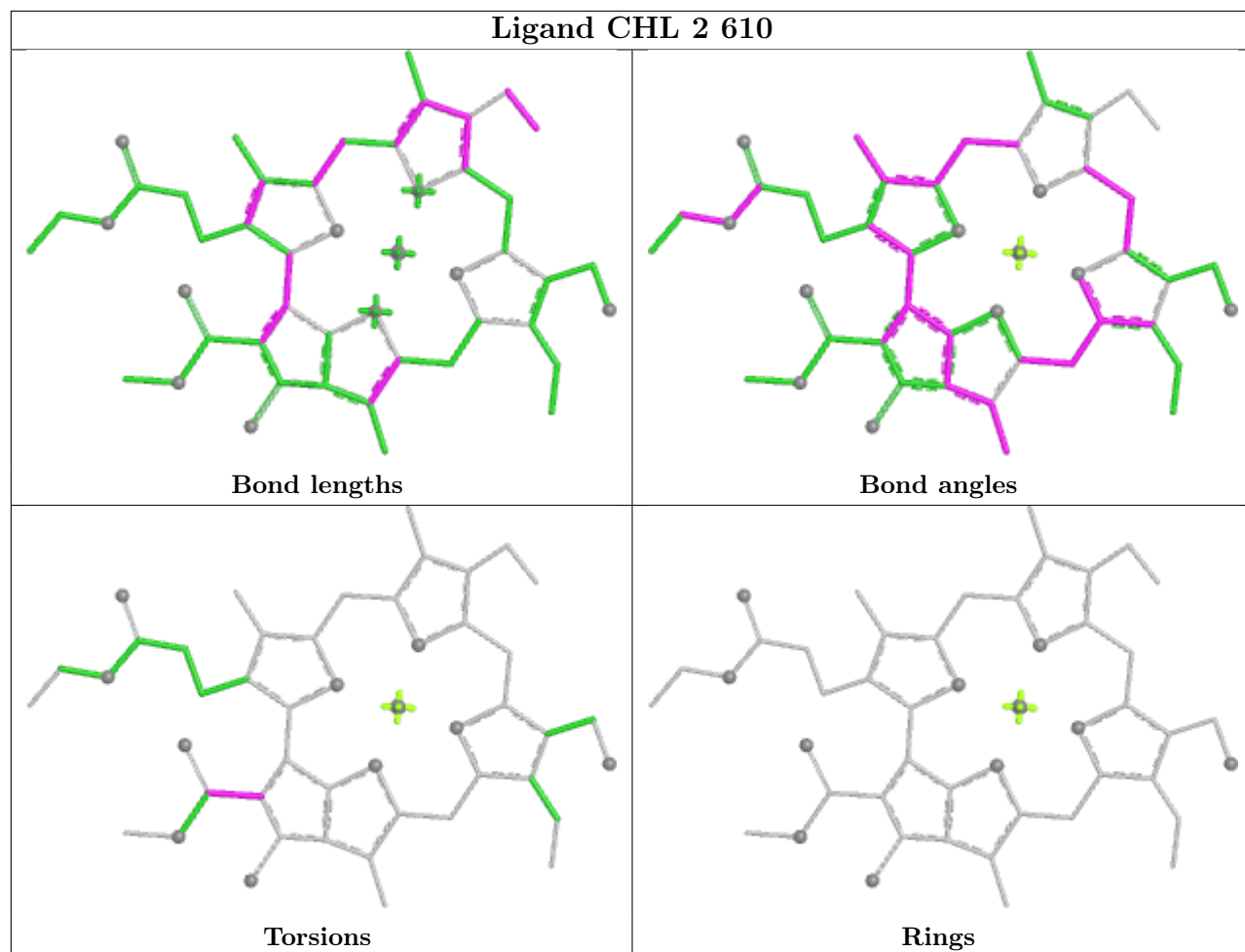
Torsions



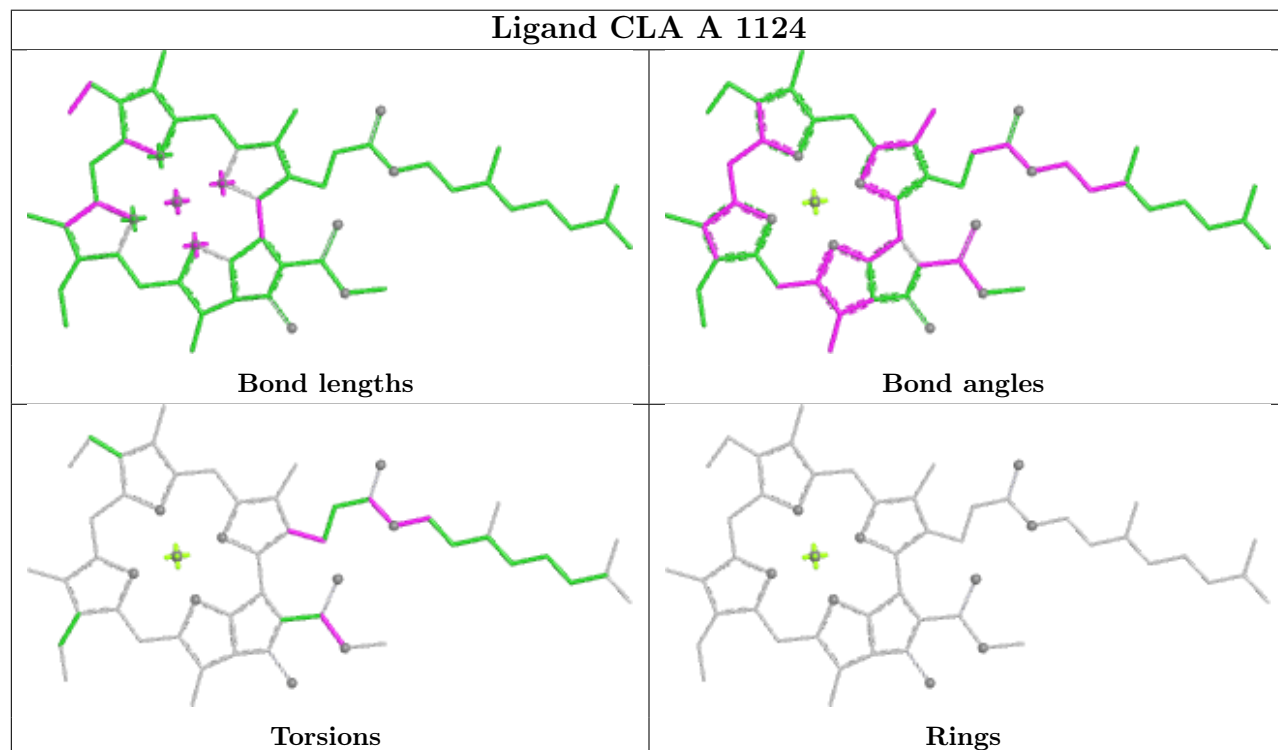
Rings



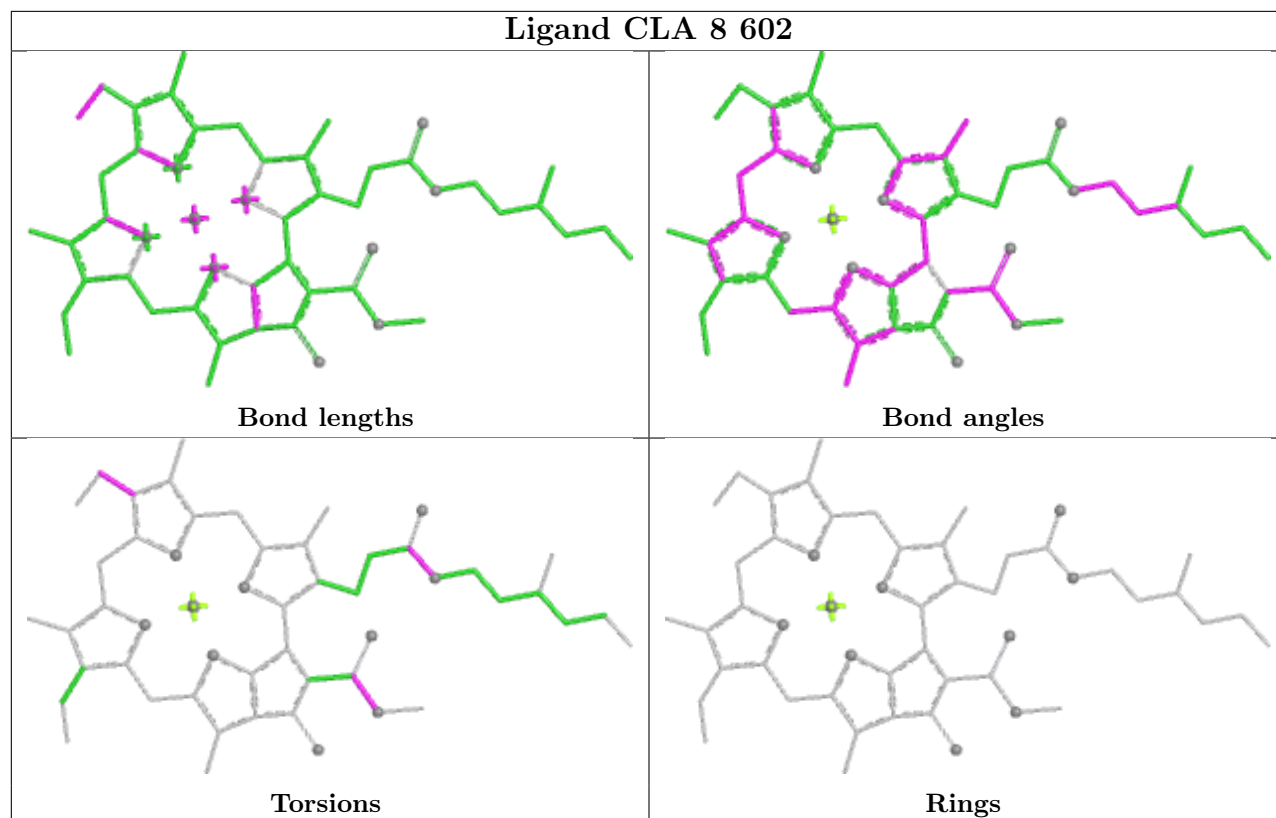
Ligand CHL 2 610



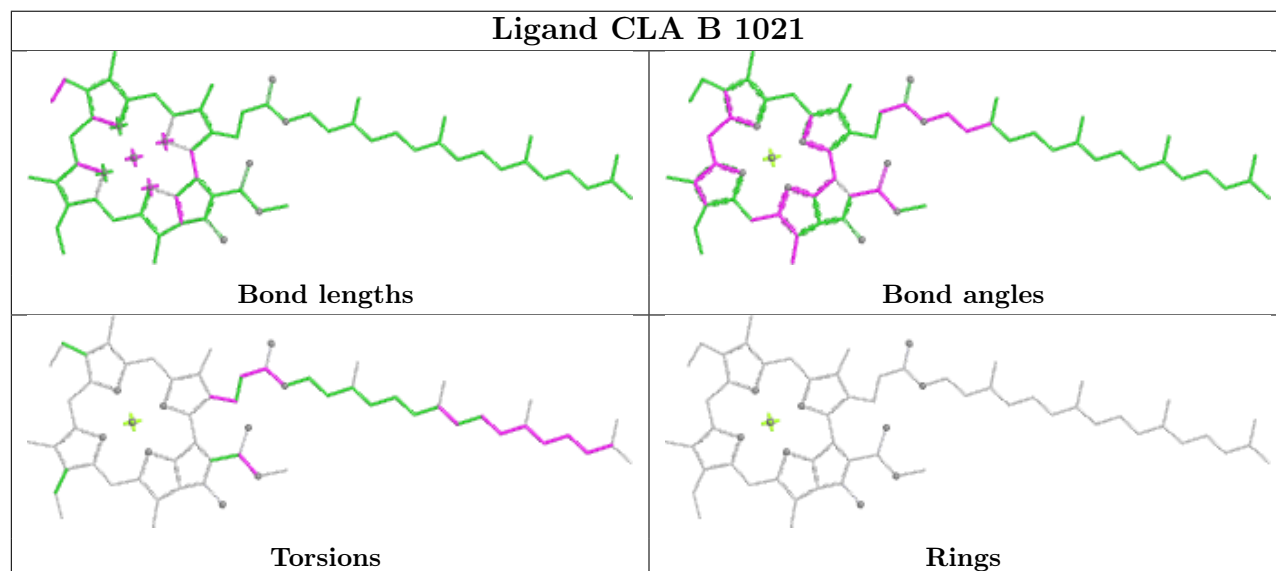
Ligand CLA A 1124



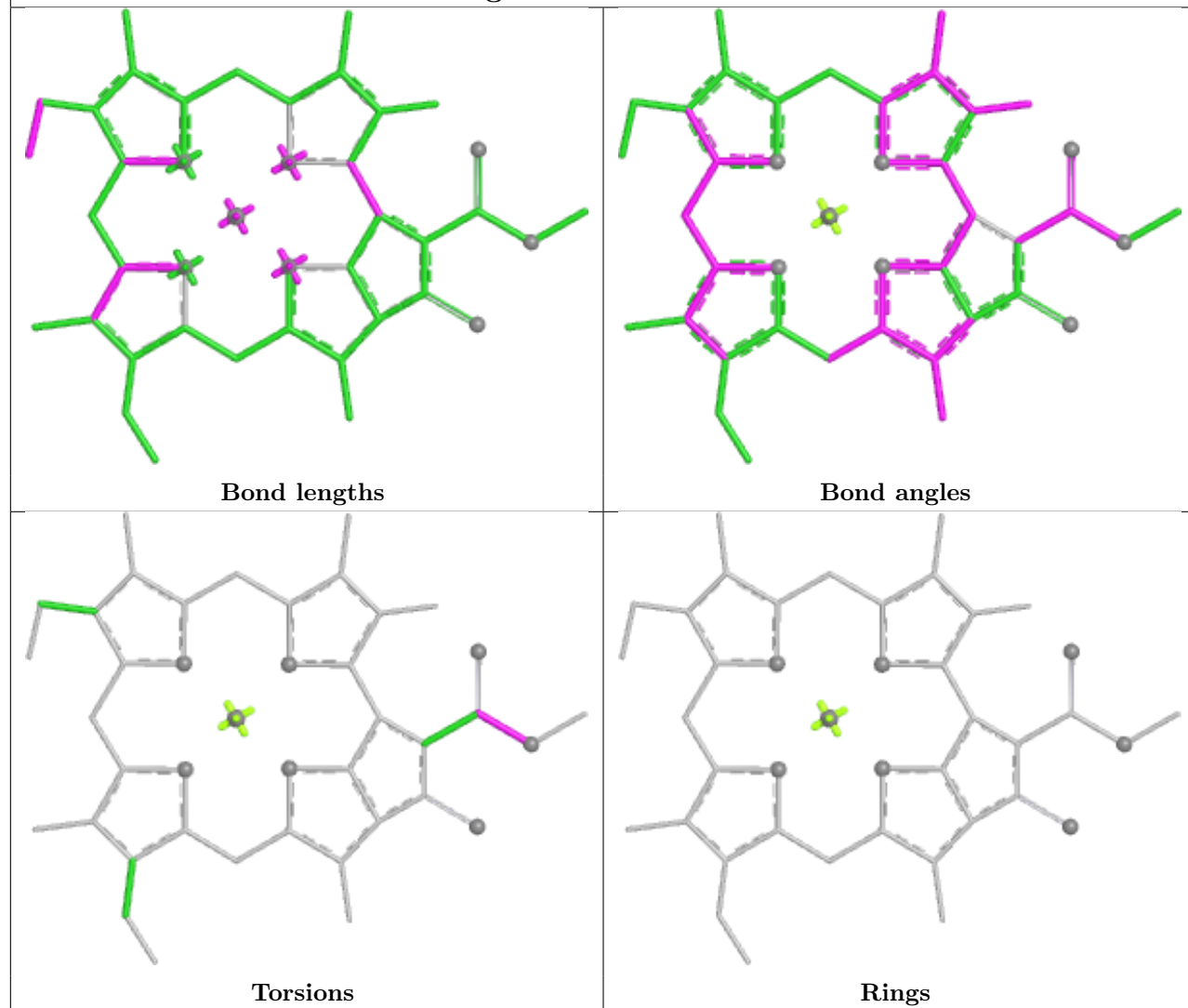
Ligand CLA 8 602



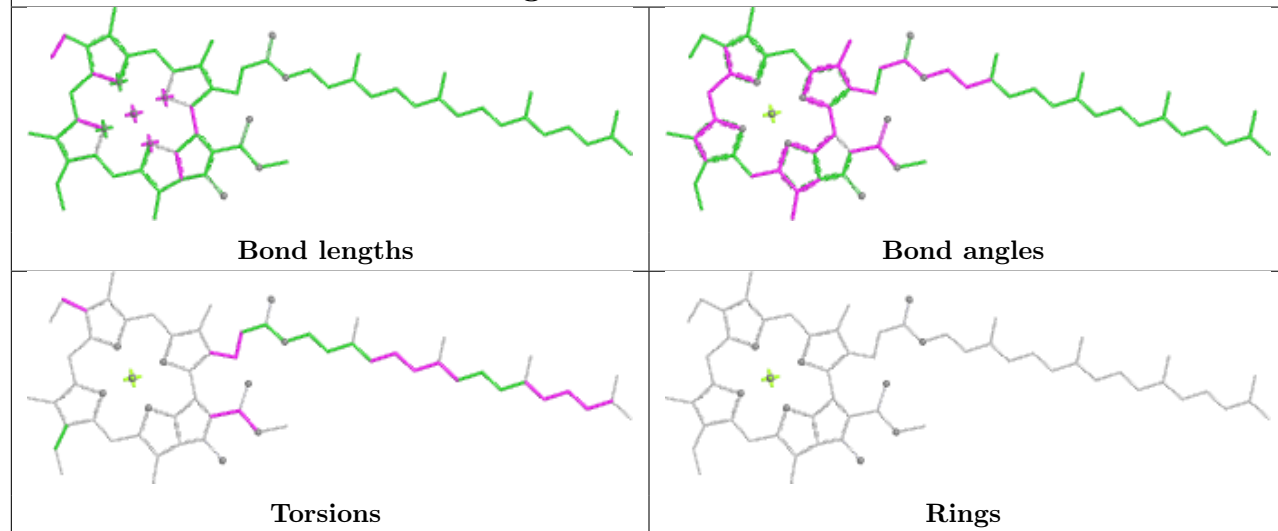
Ligand CLA B 1021



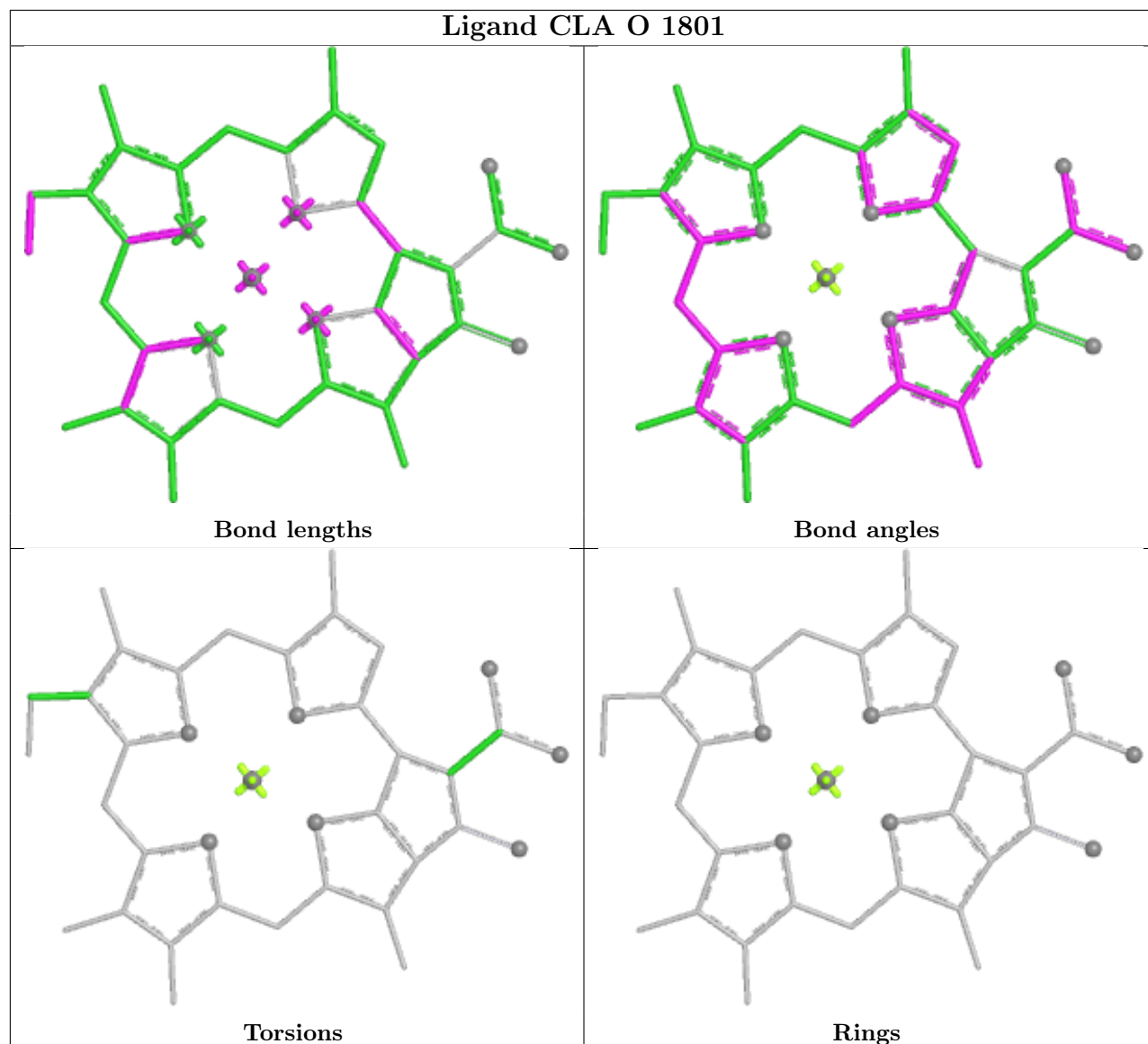
Ligand CLA O 1803



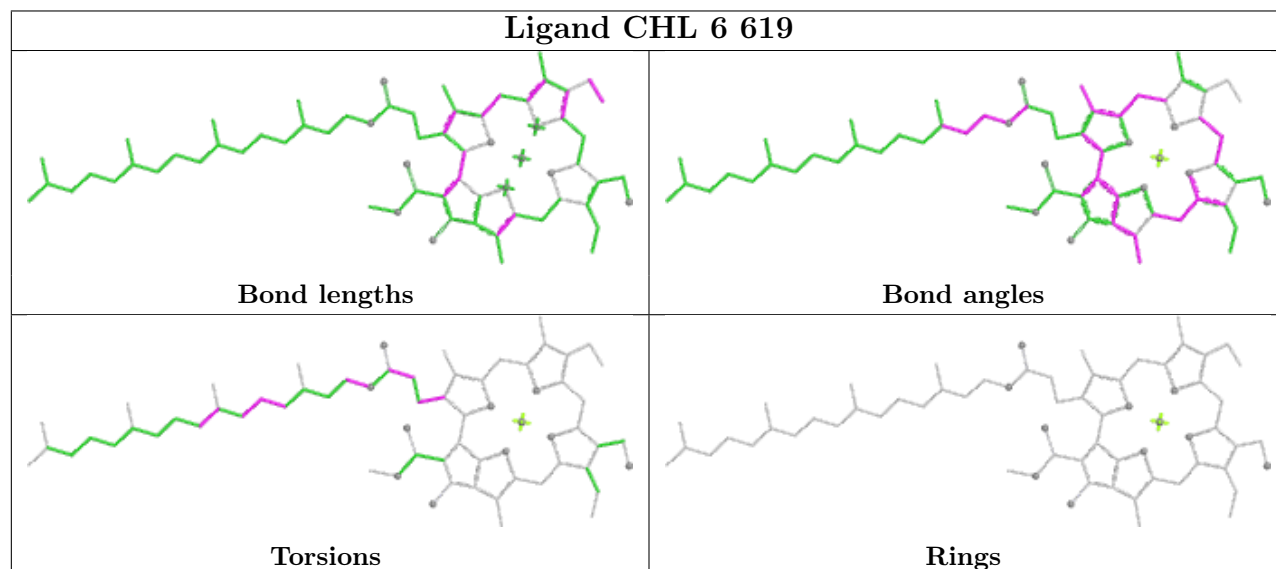
Ligand CLA A 1132

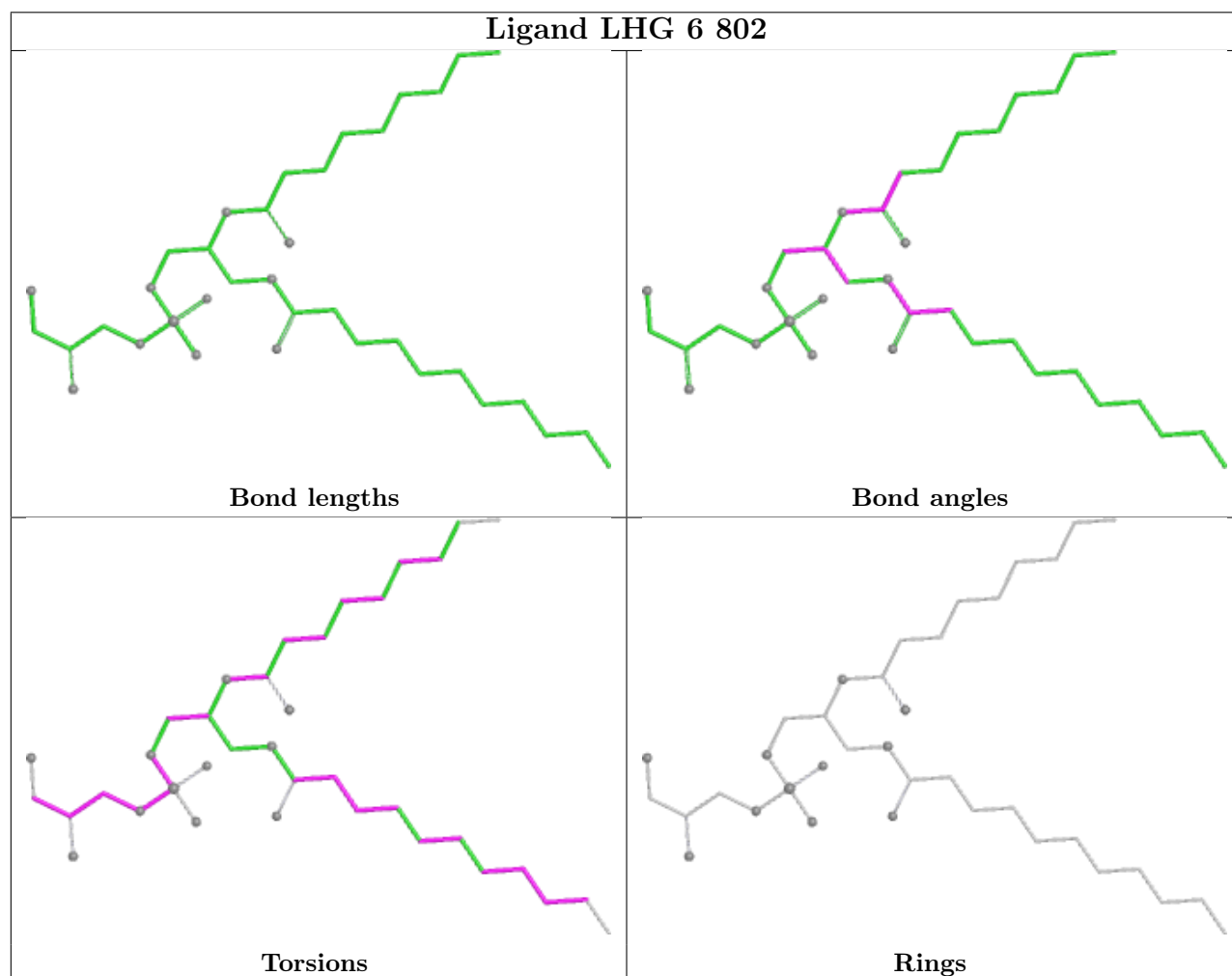
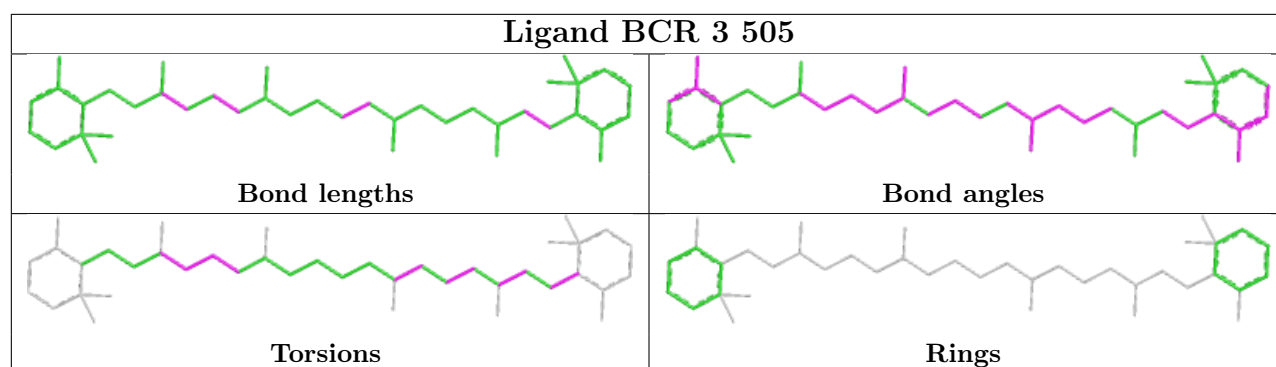


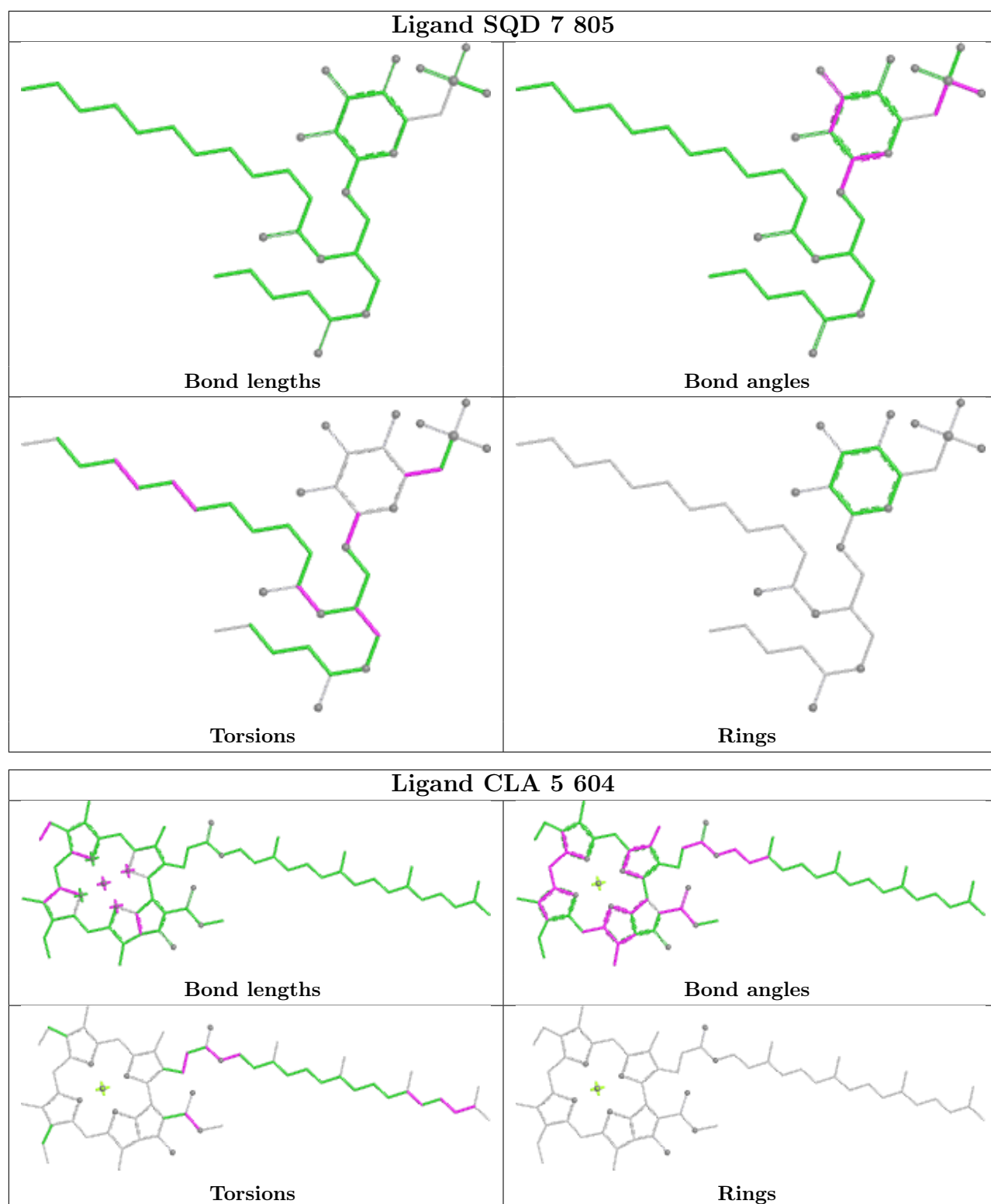
Ligand CLA O 1801

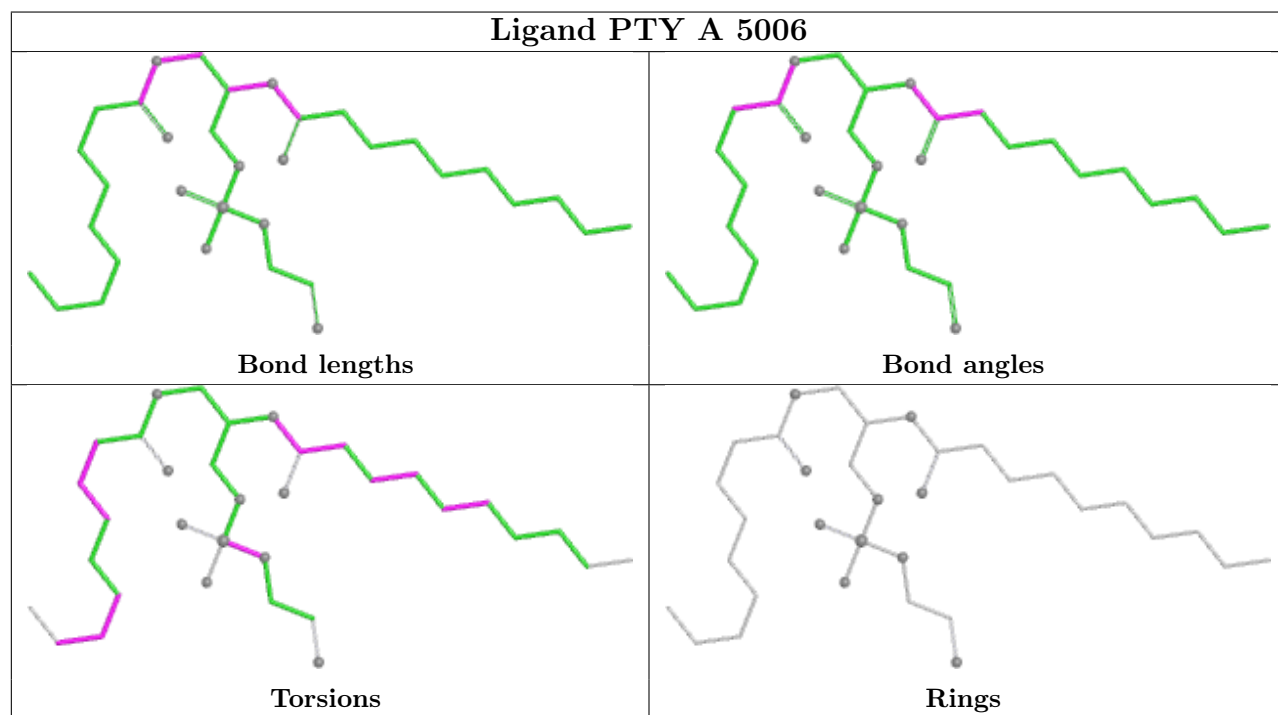
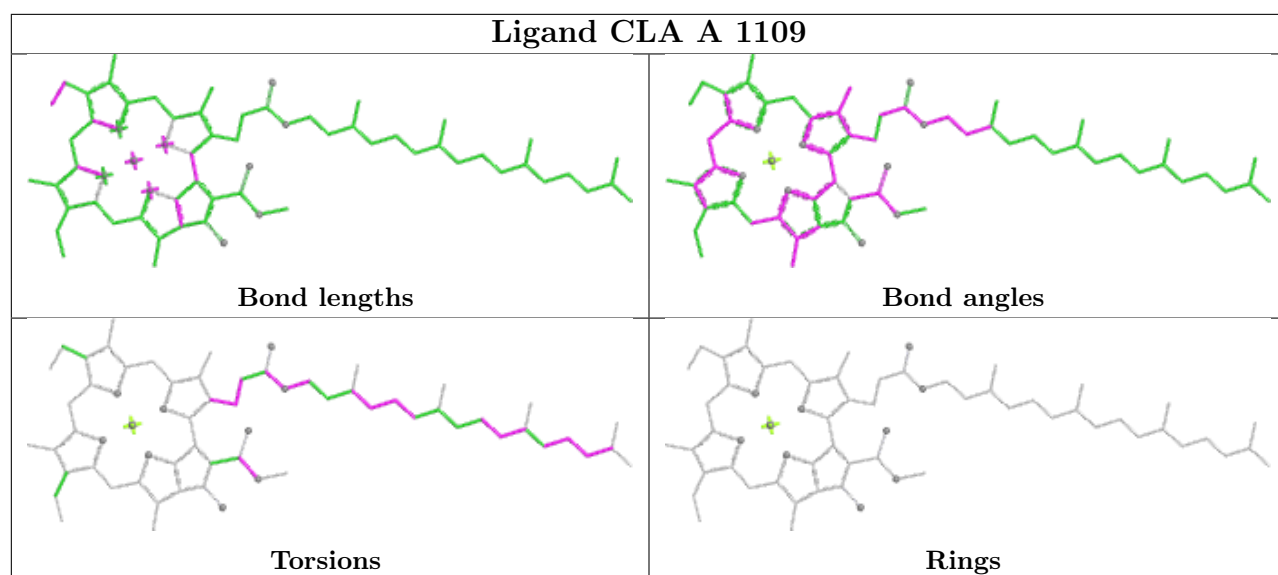


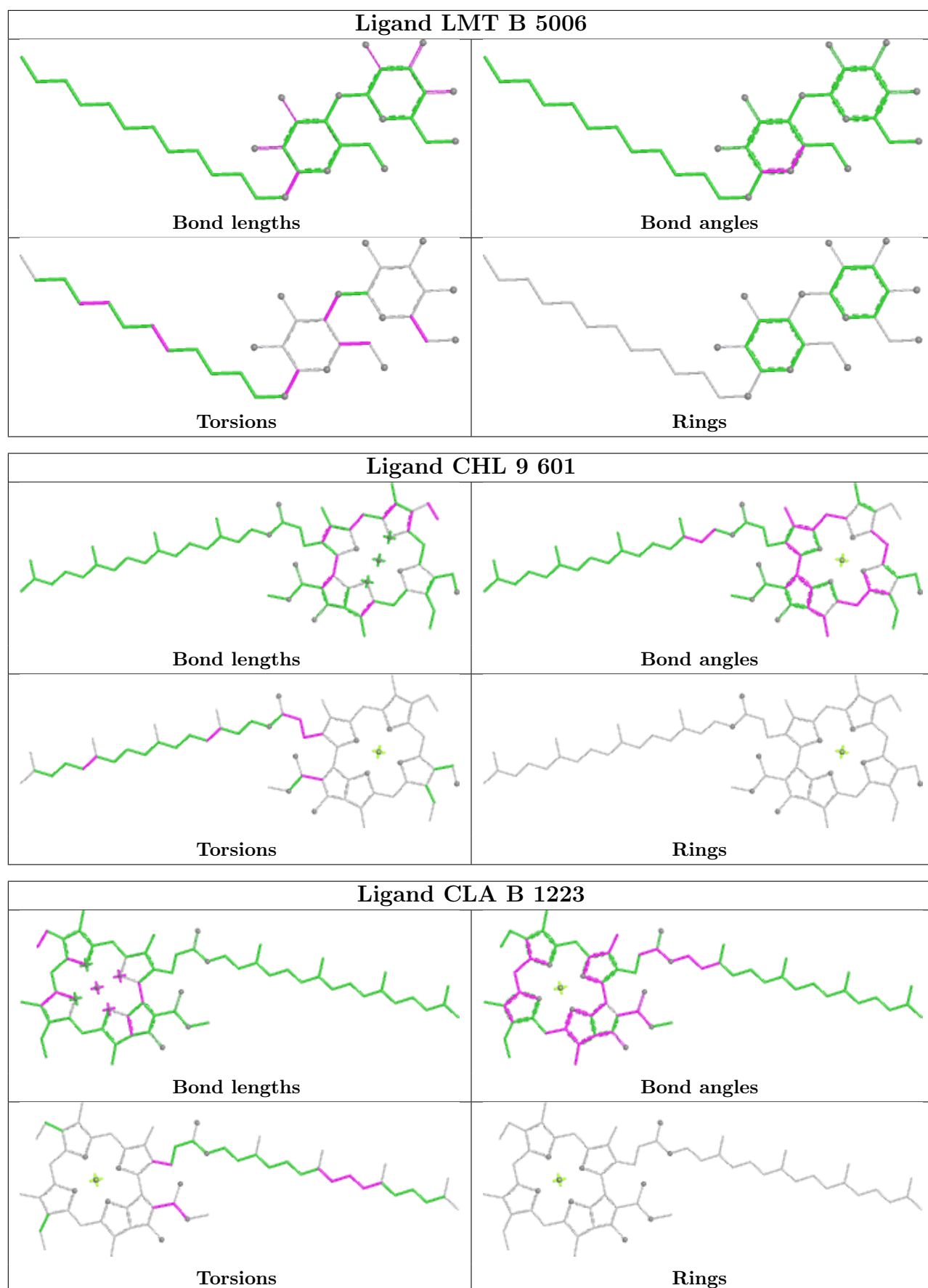
Ligand CHL 6 619

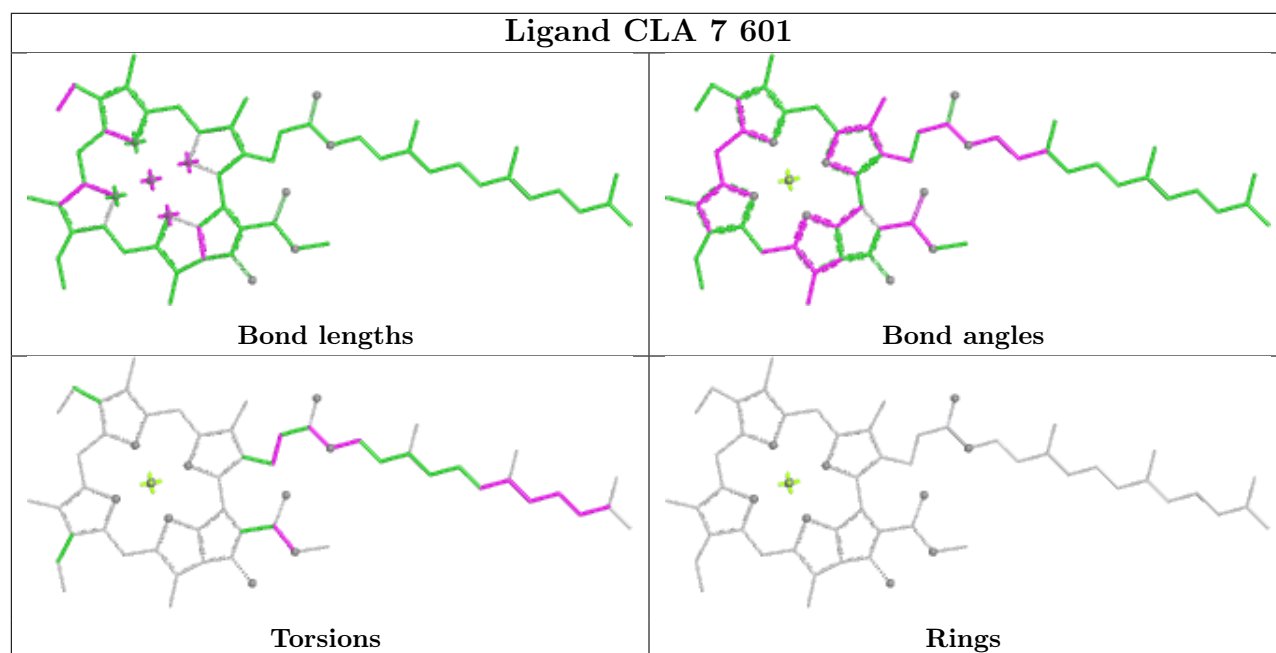
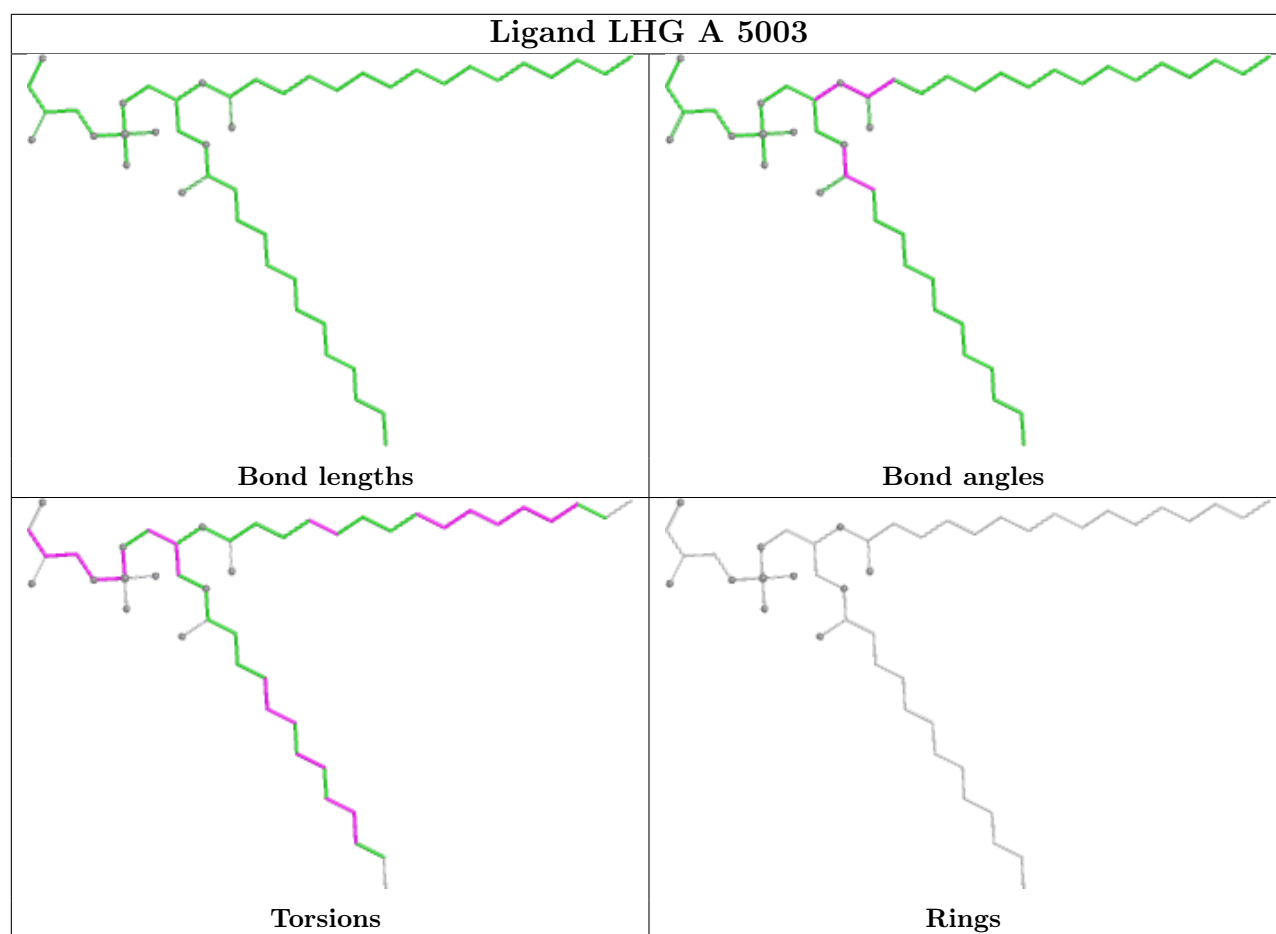




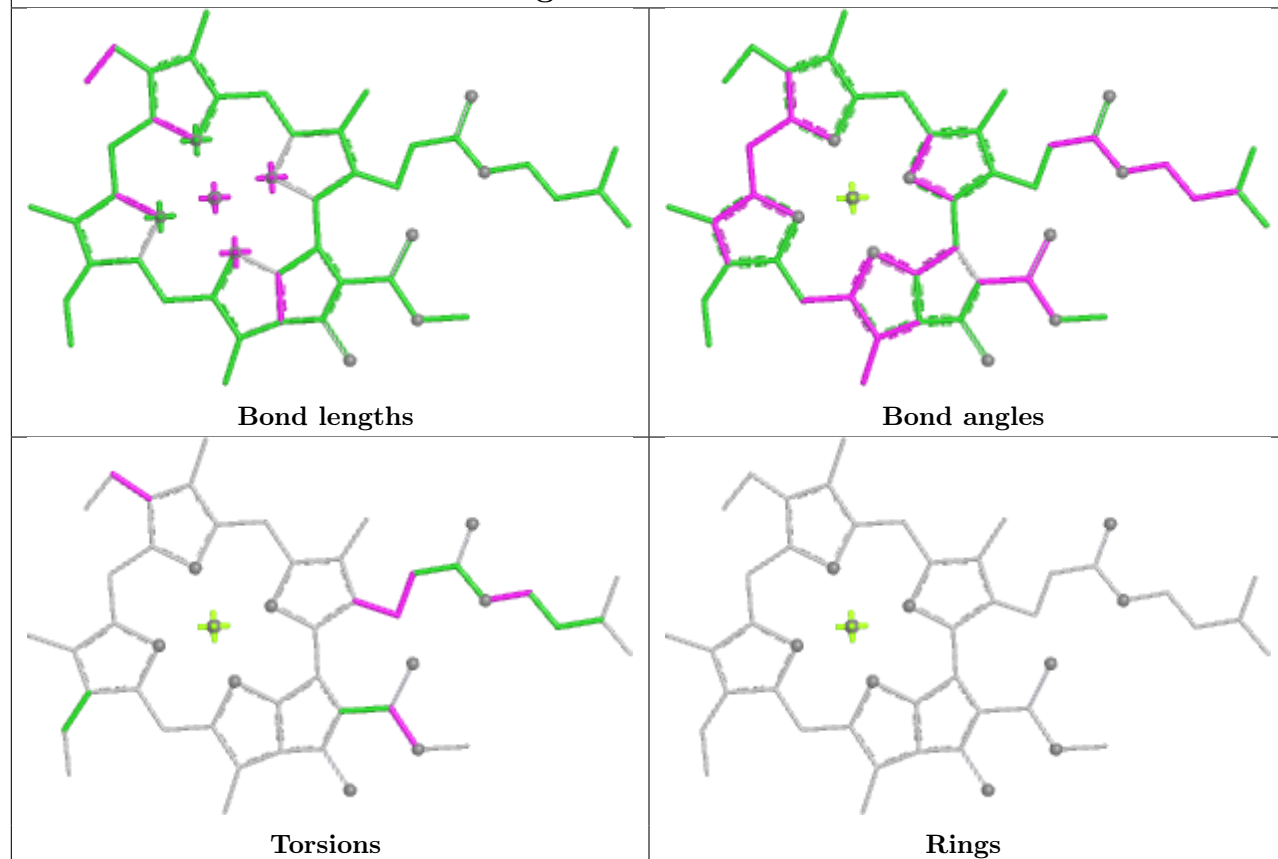




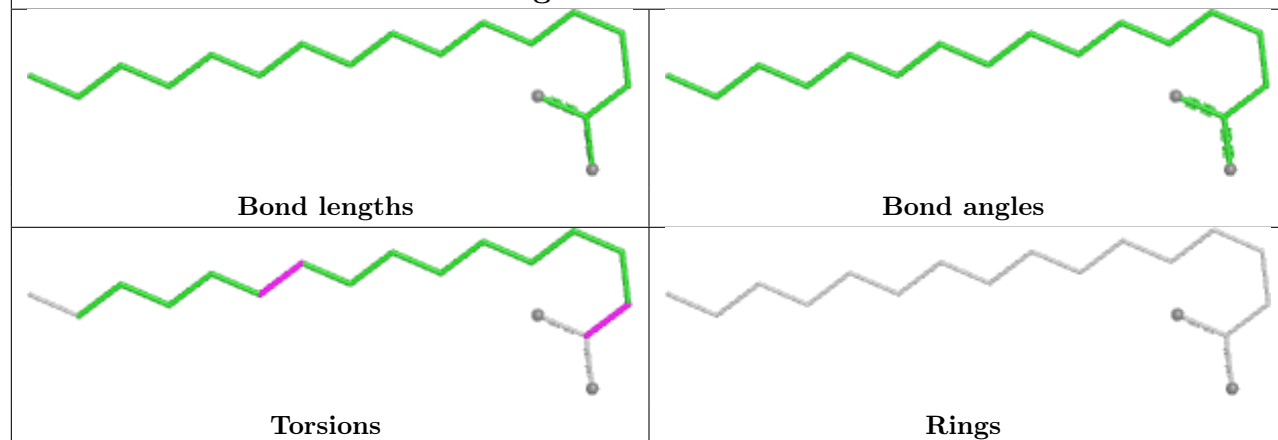


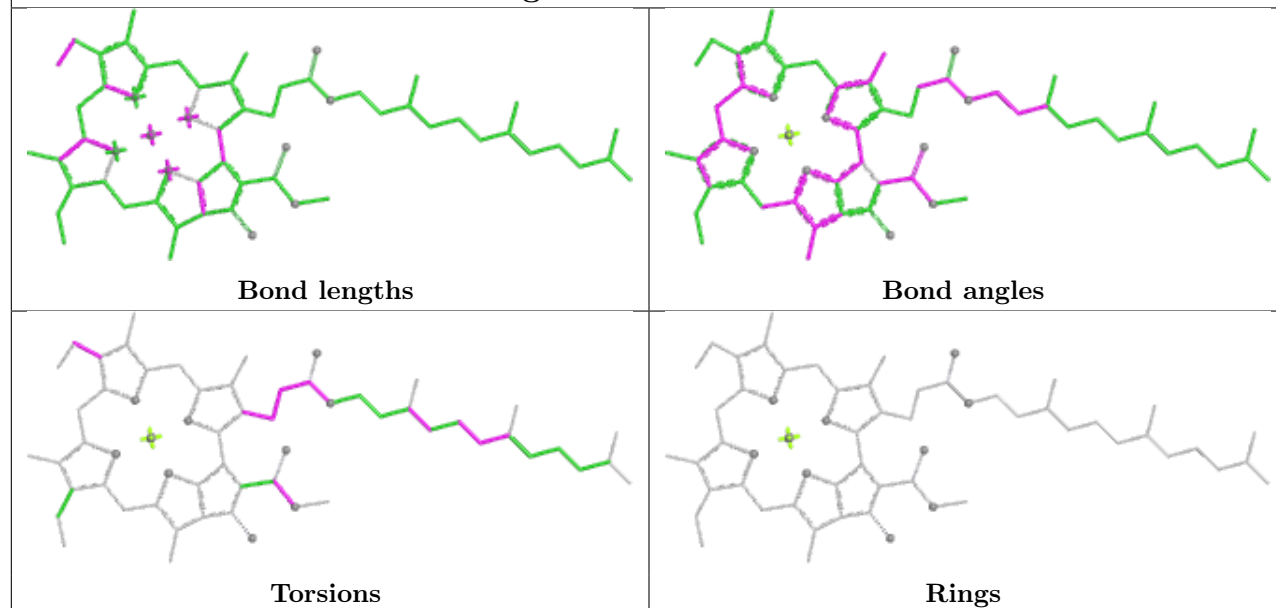
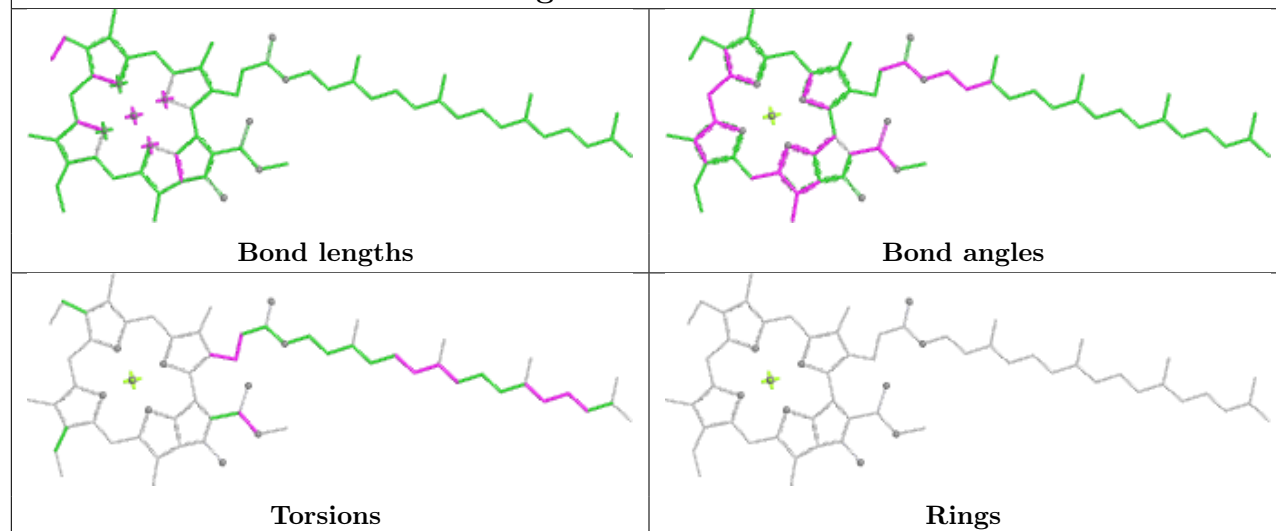


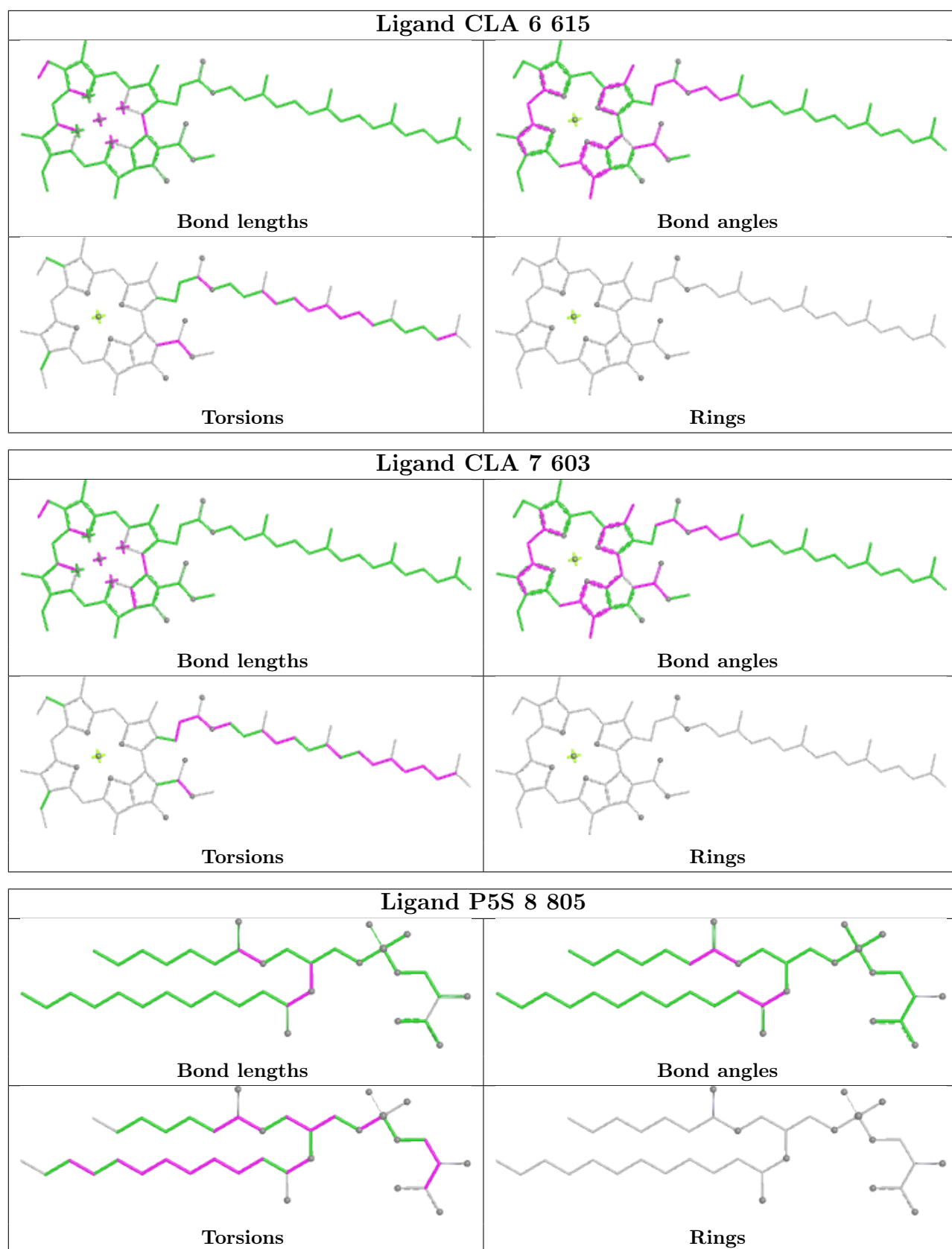
Ligand CLA 8 612

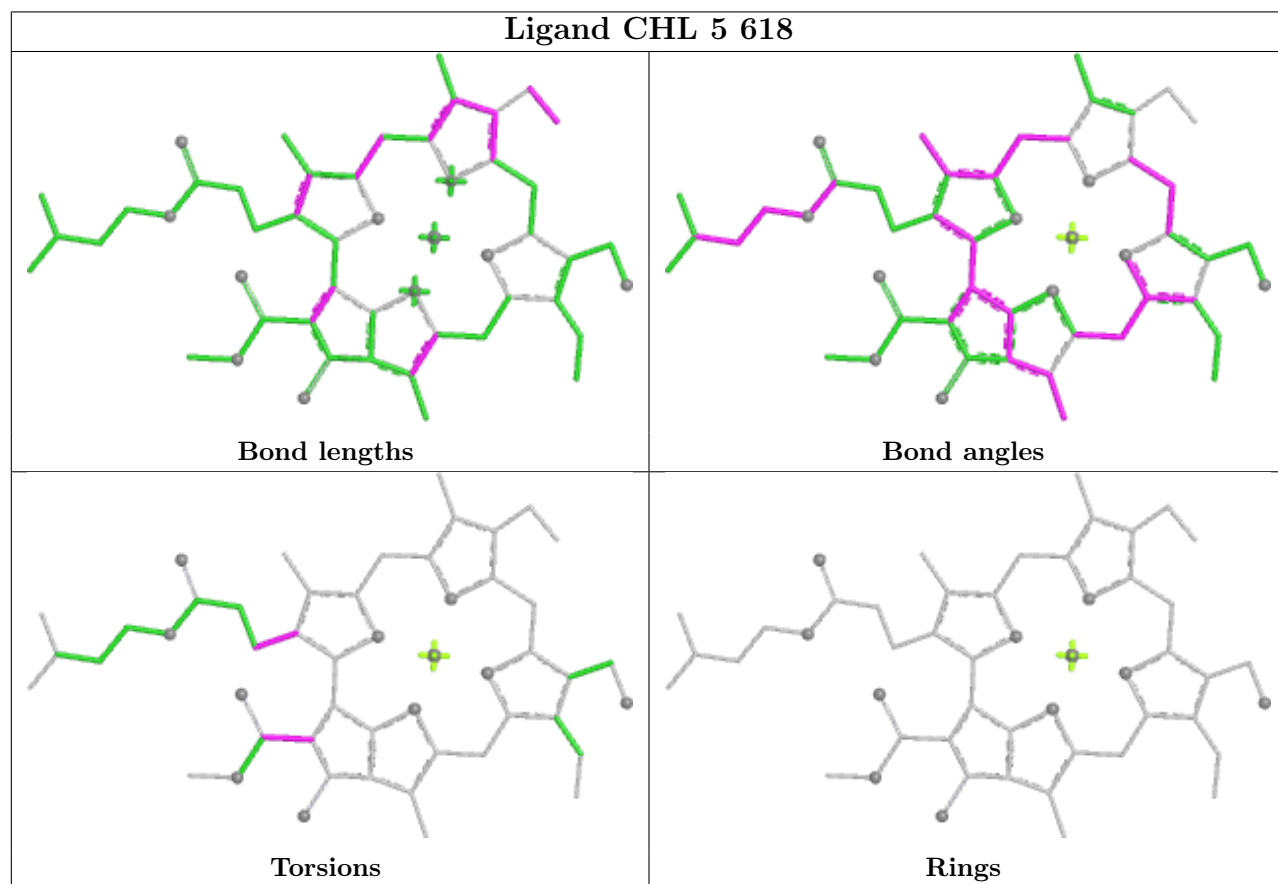
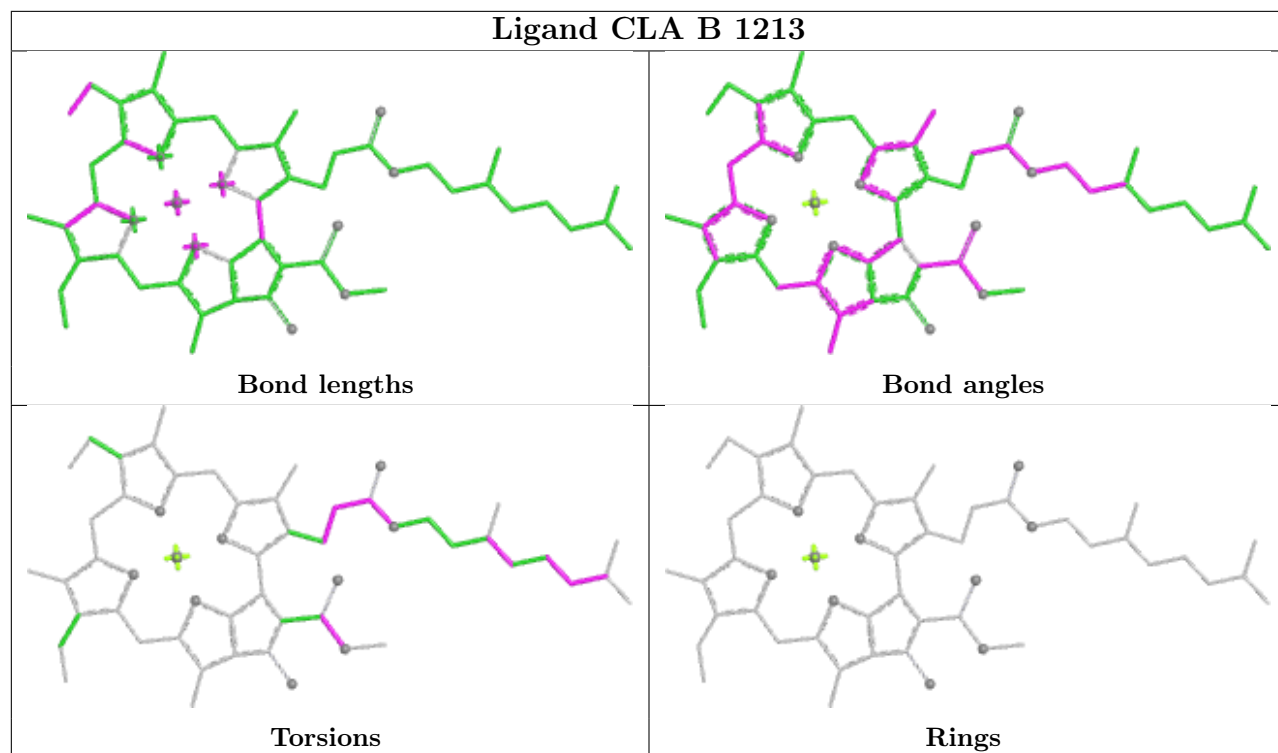


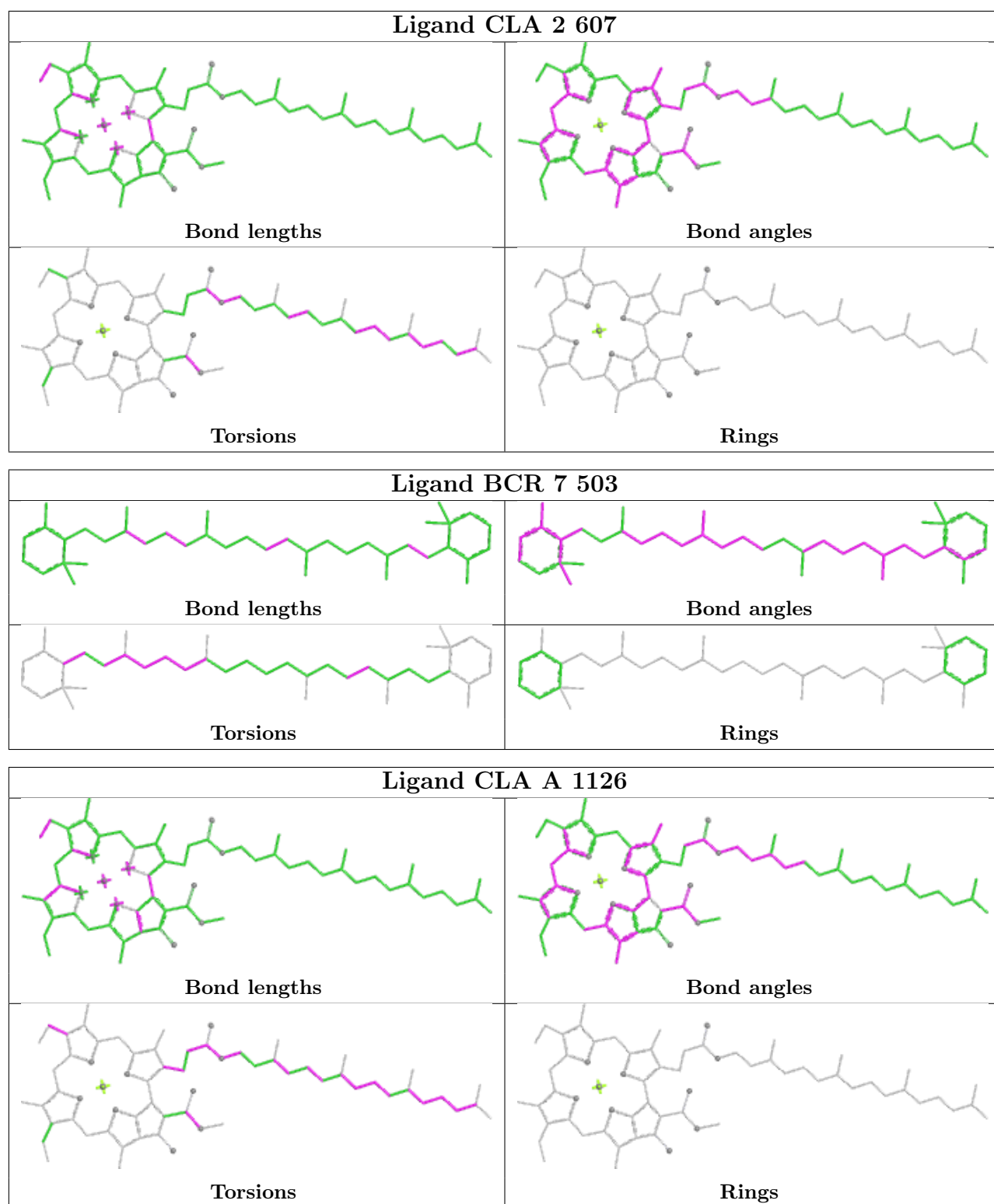
Ligand PLM 5 804

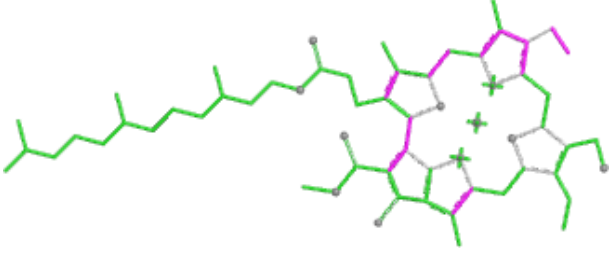
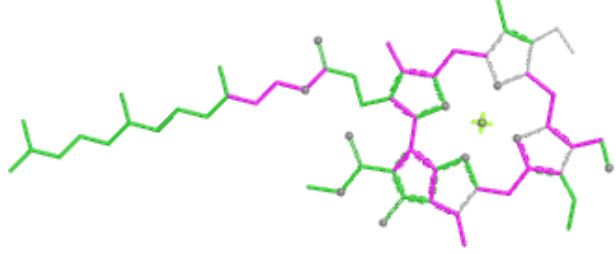
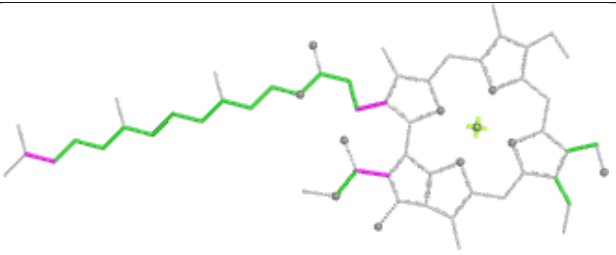
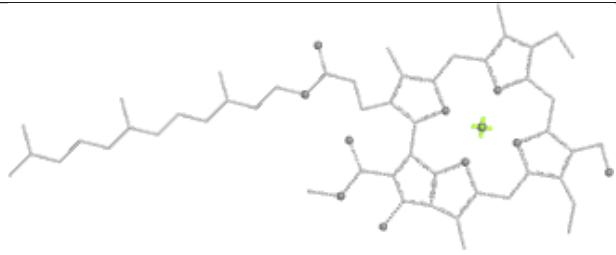
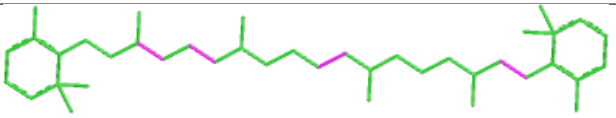
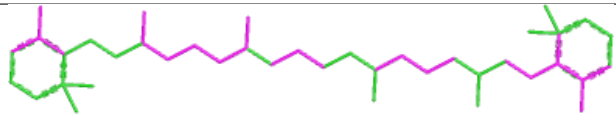
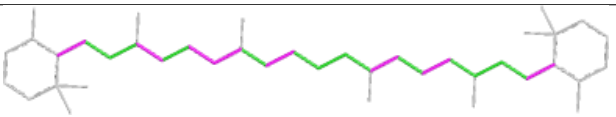
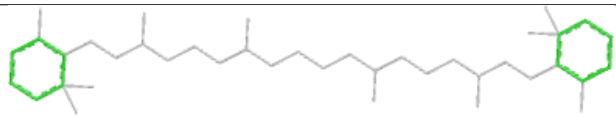


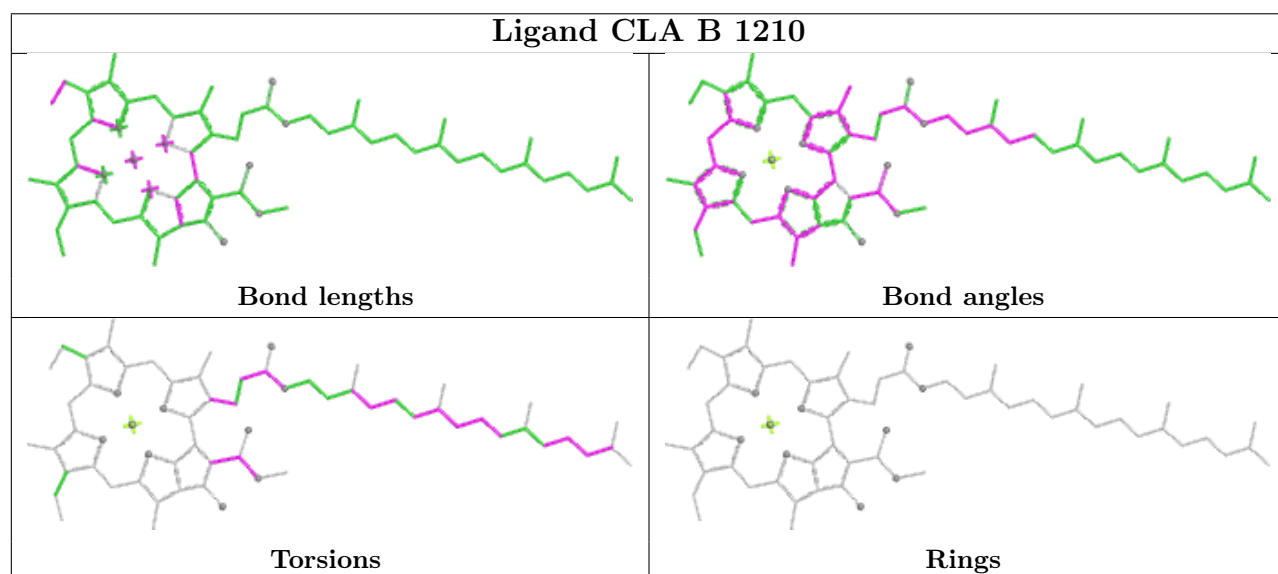
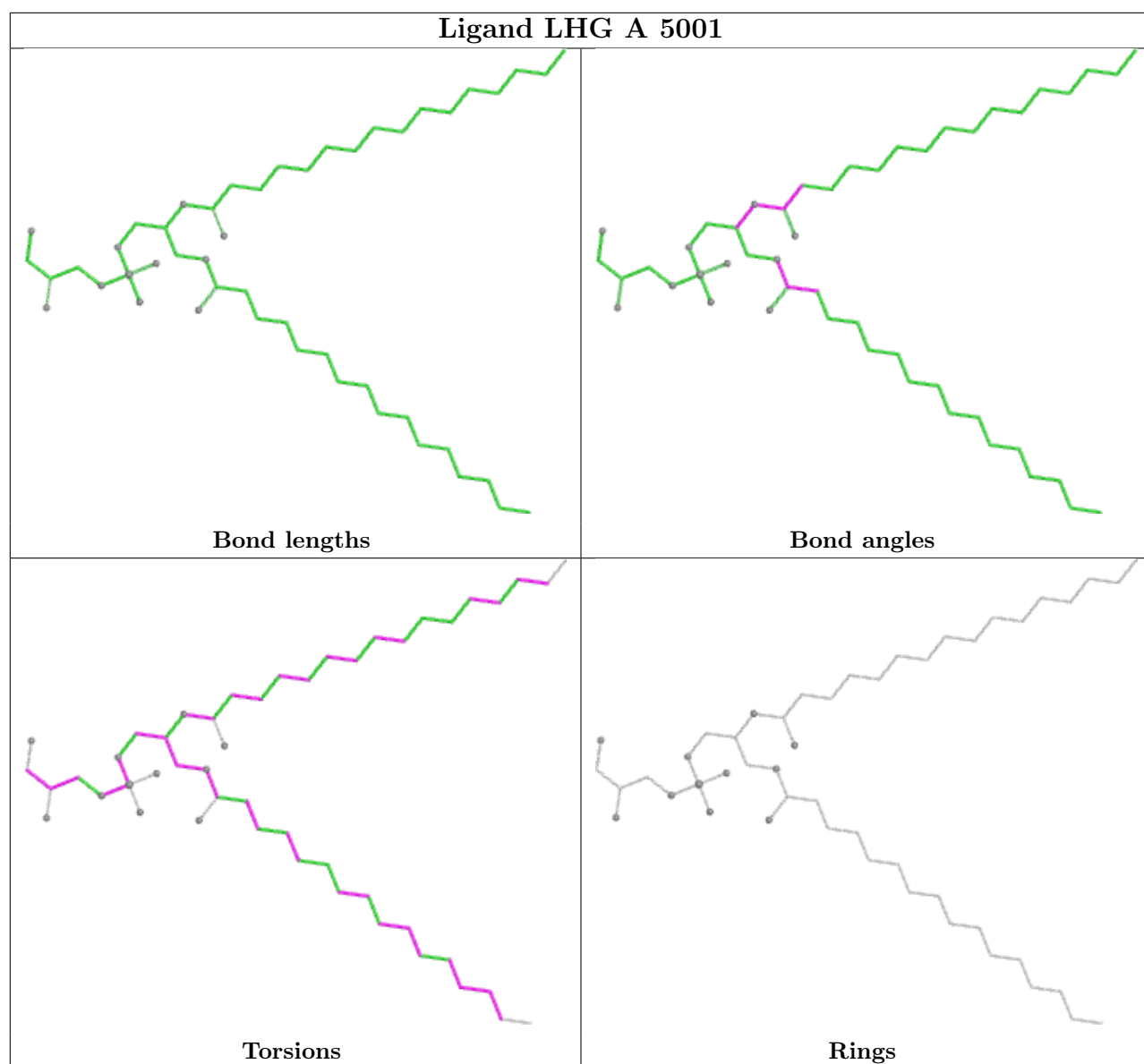
Ligand CLA A 1134**Ligand CLA 3 606**



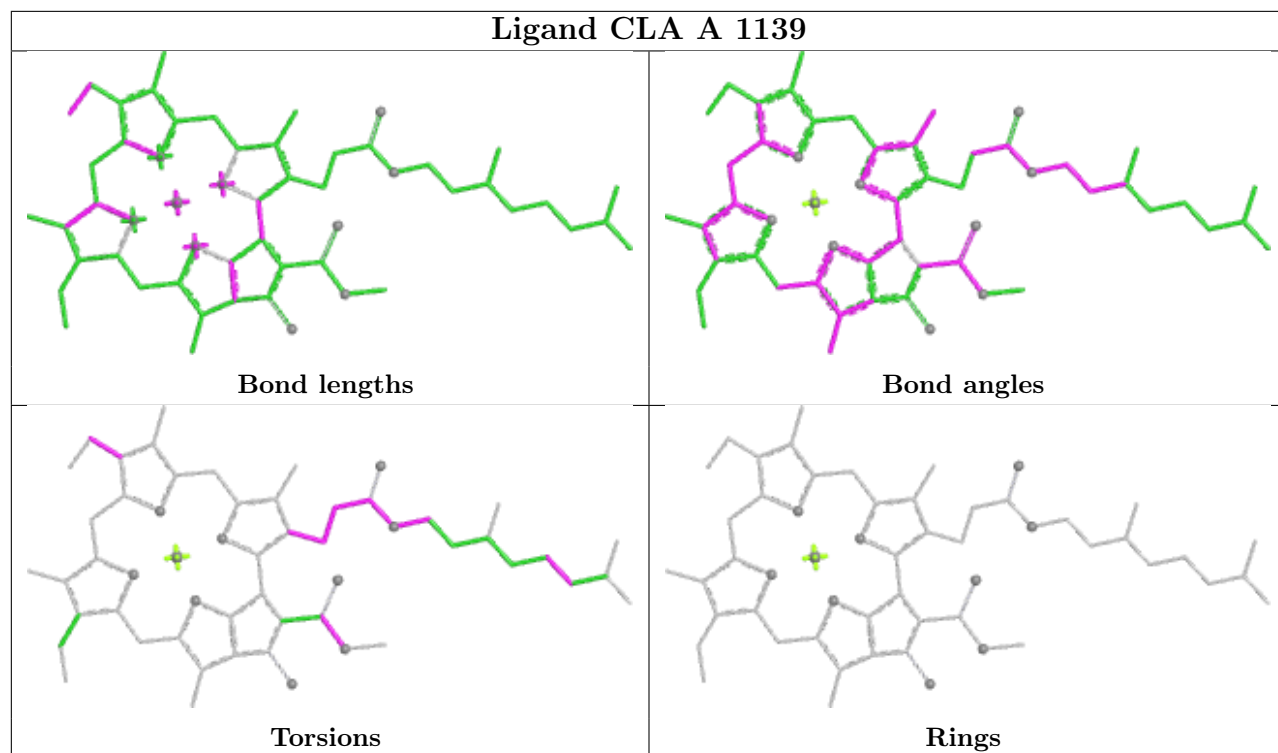




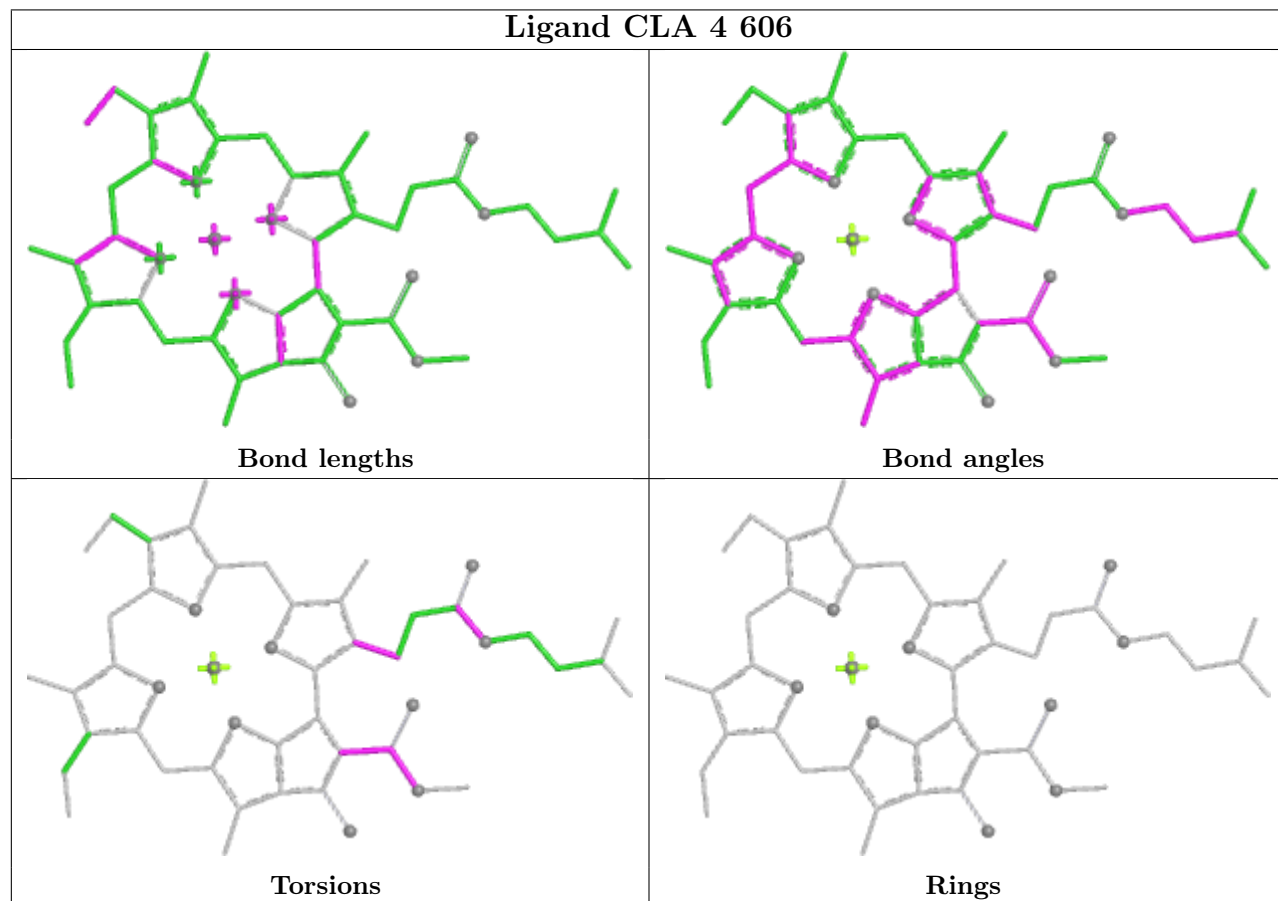
Ligand CHL 8 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR O 4001	
 Bond lengths	 Bond angles
 Torsions	 Rings

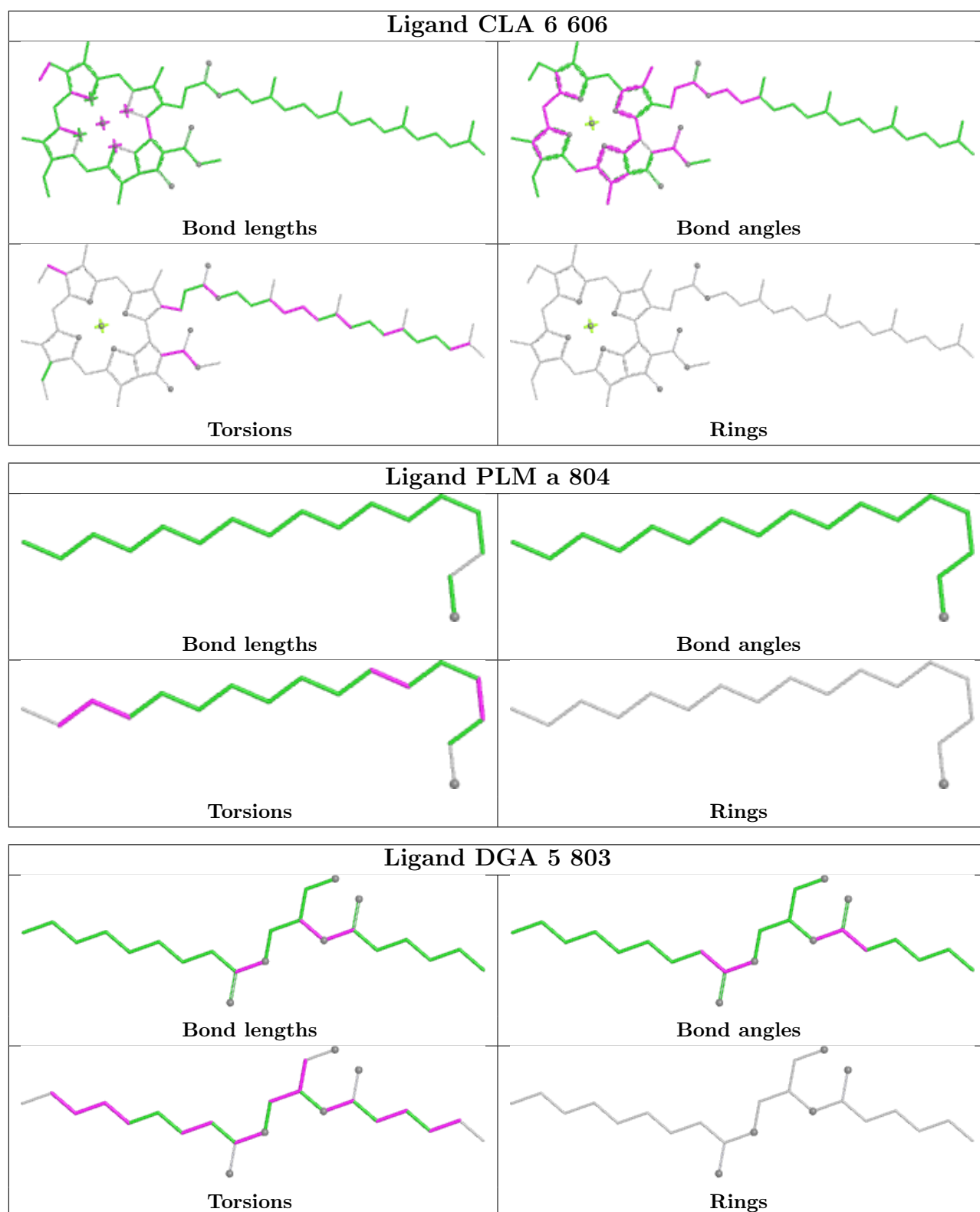


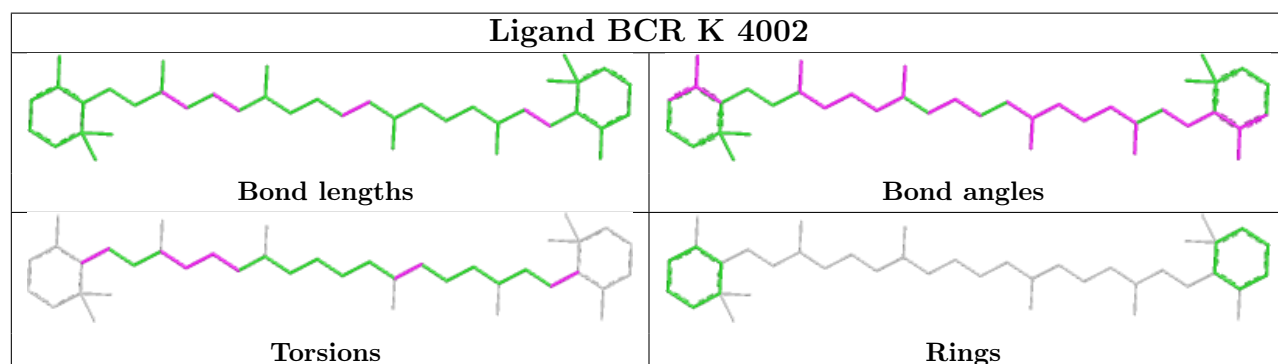
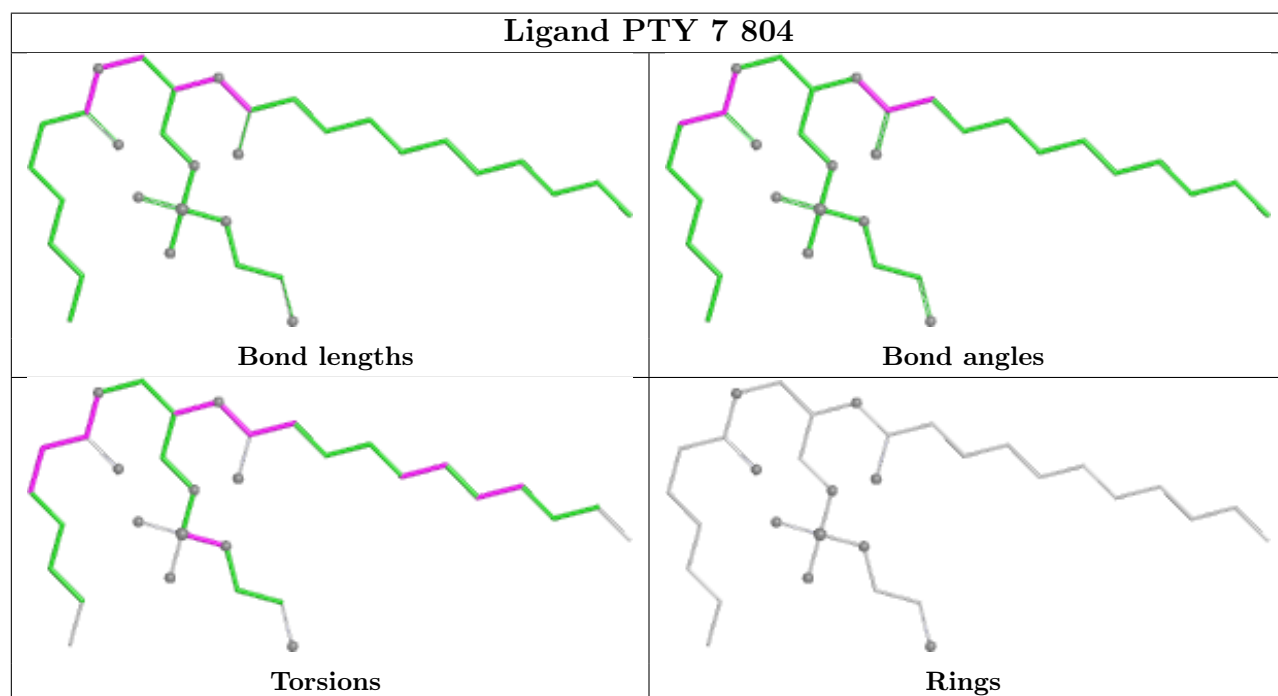
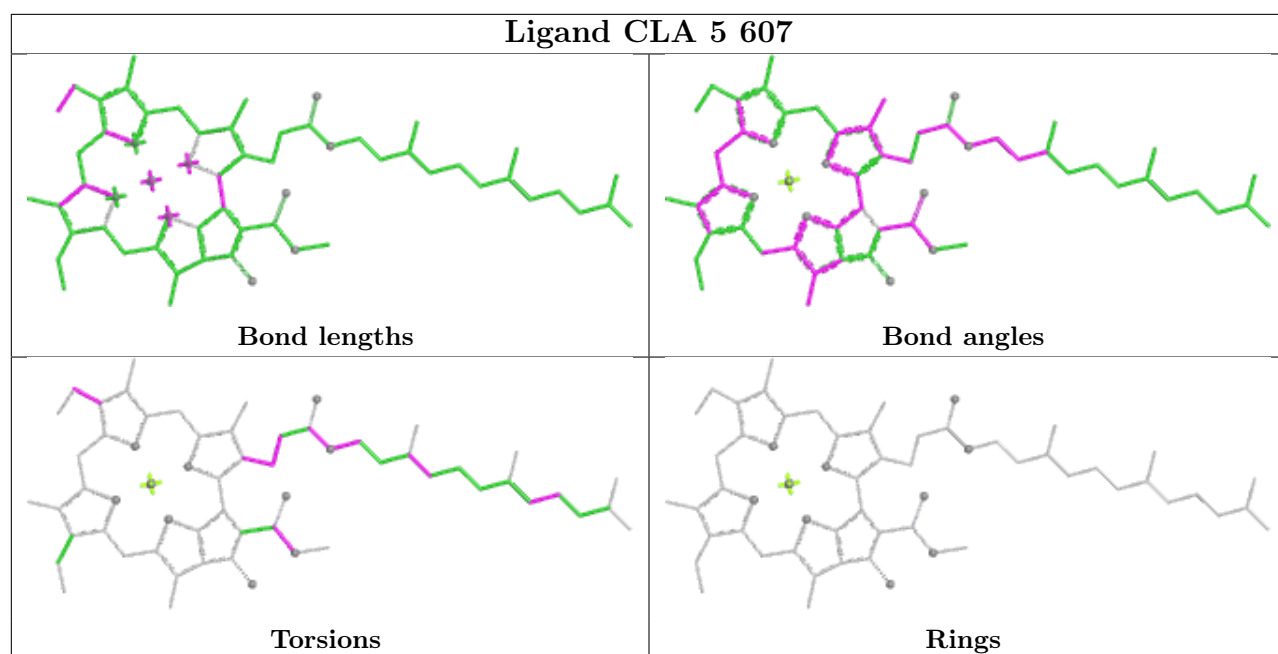
Ligand CLA A 1139

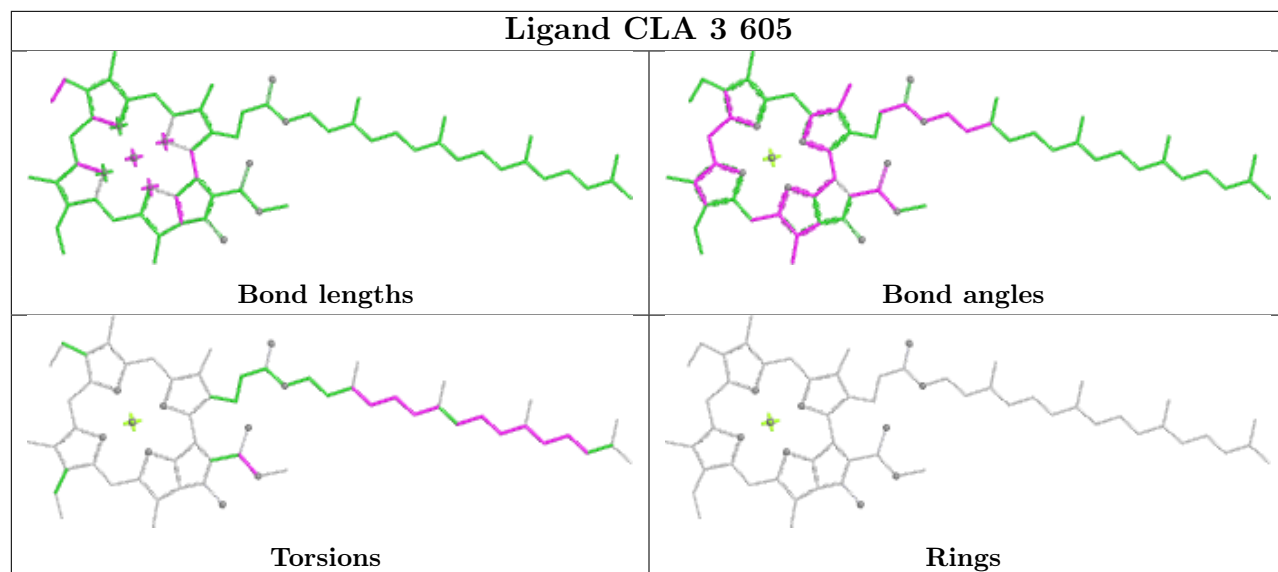
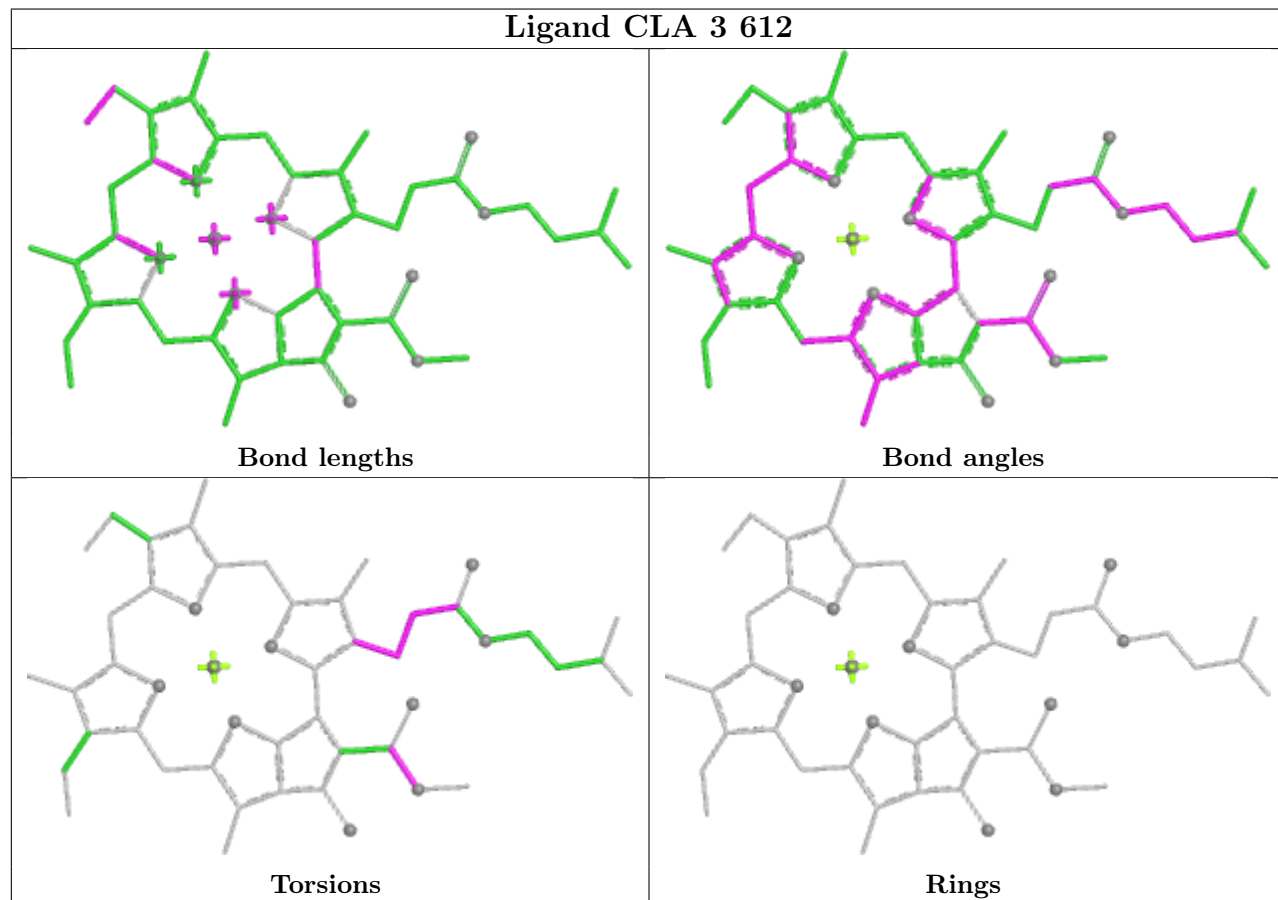


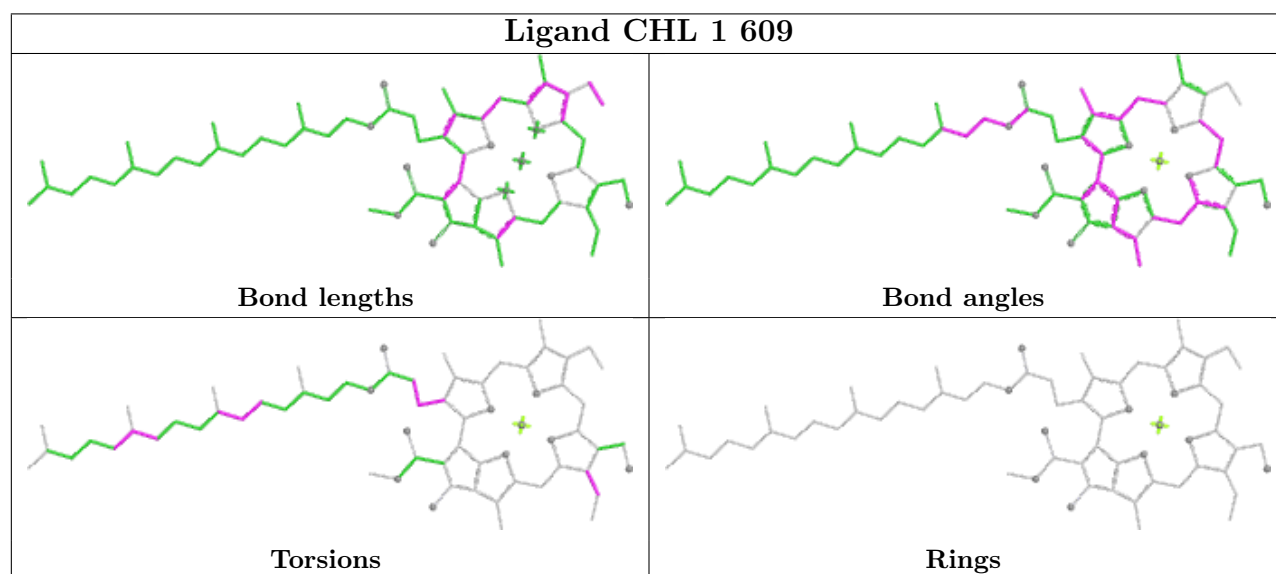
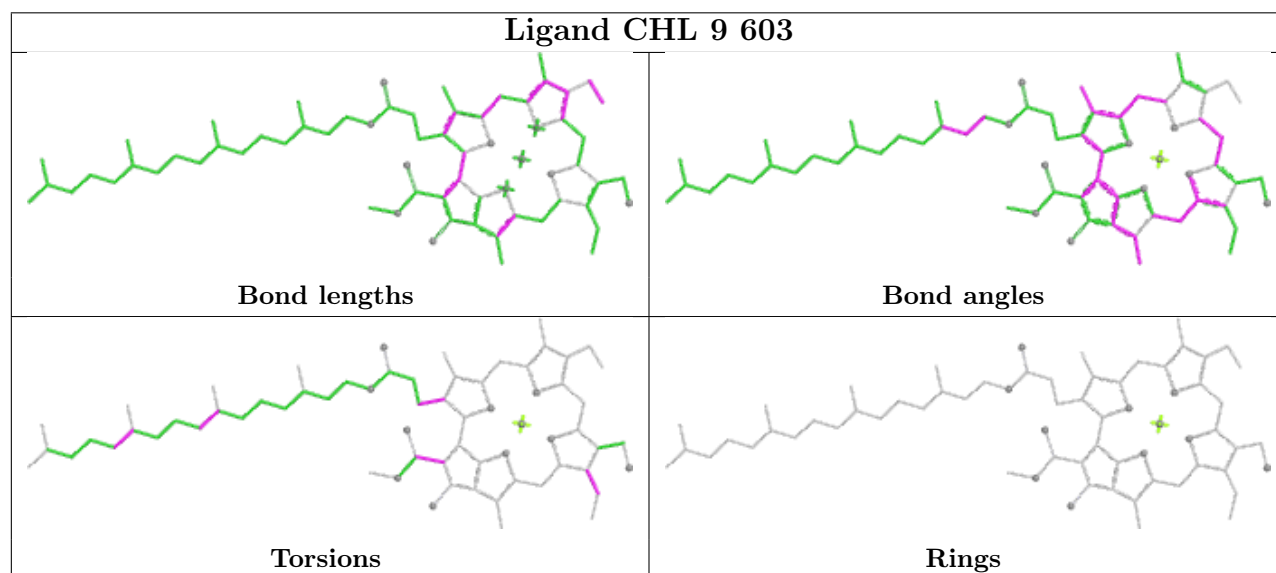
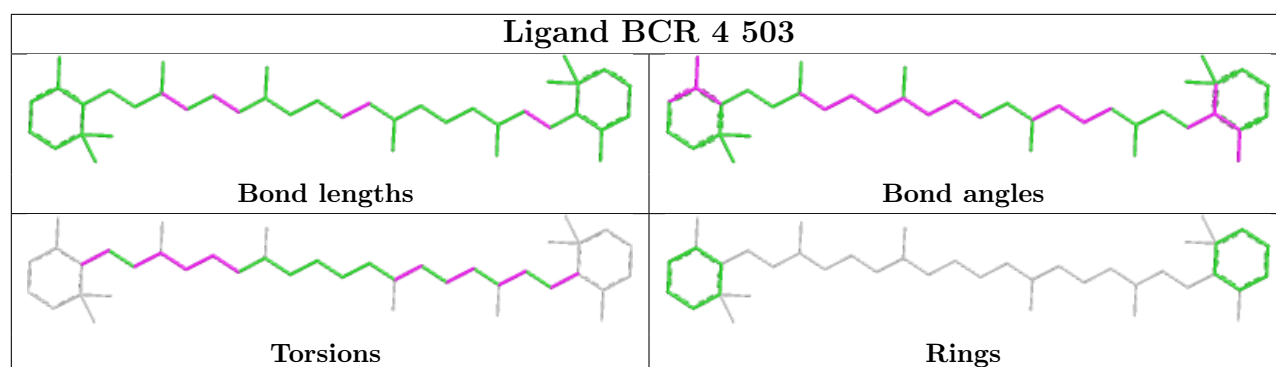
Ligand CLA 4 606

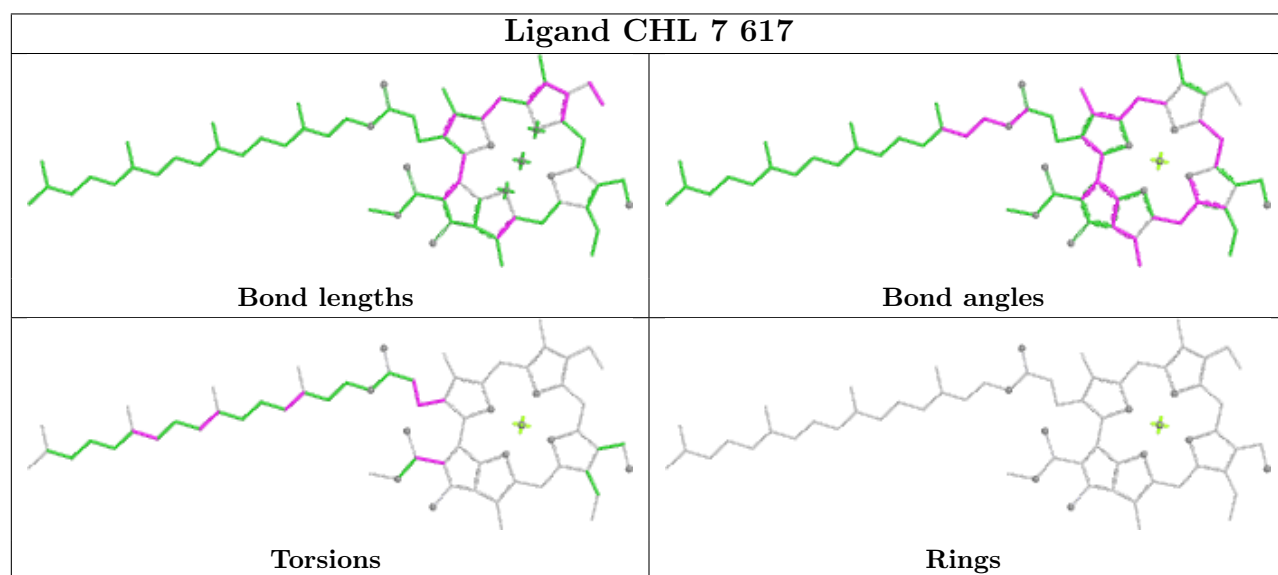
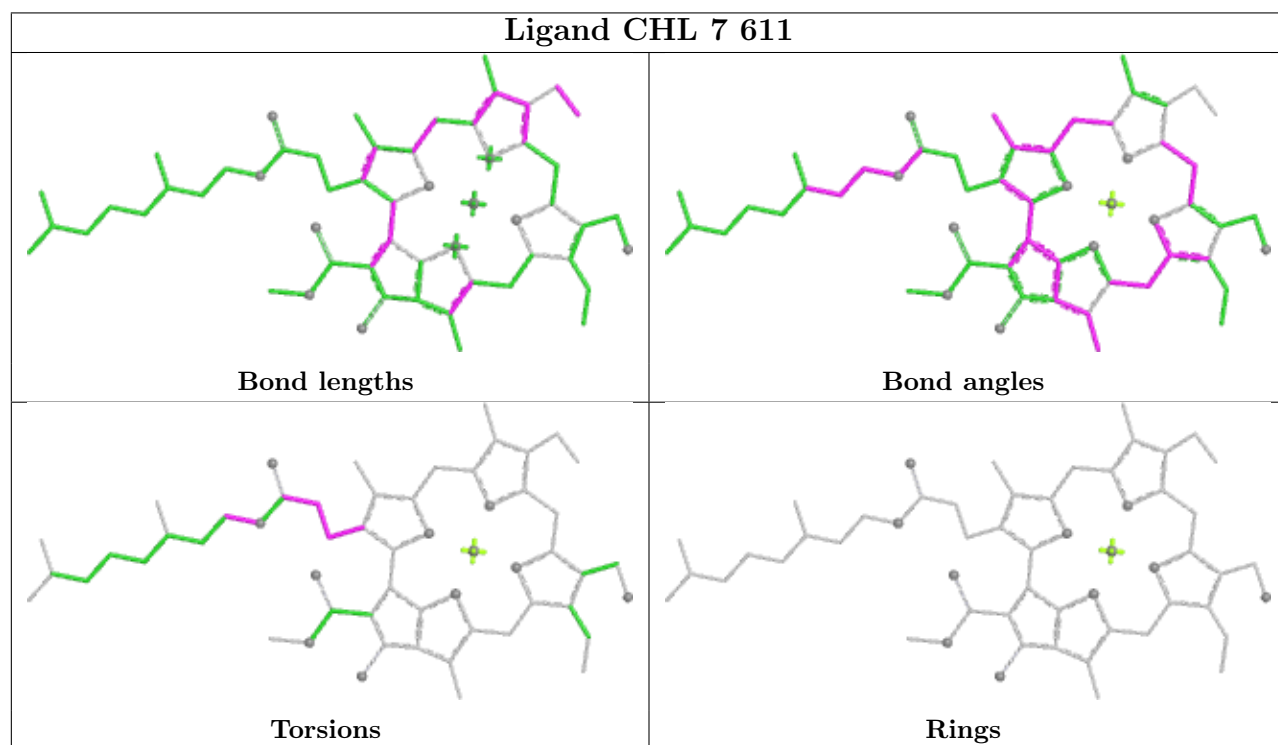
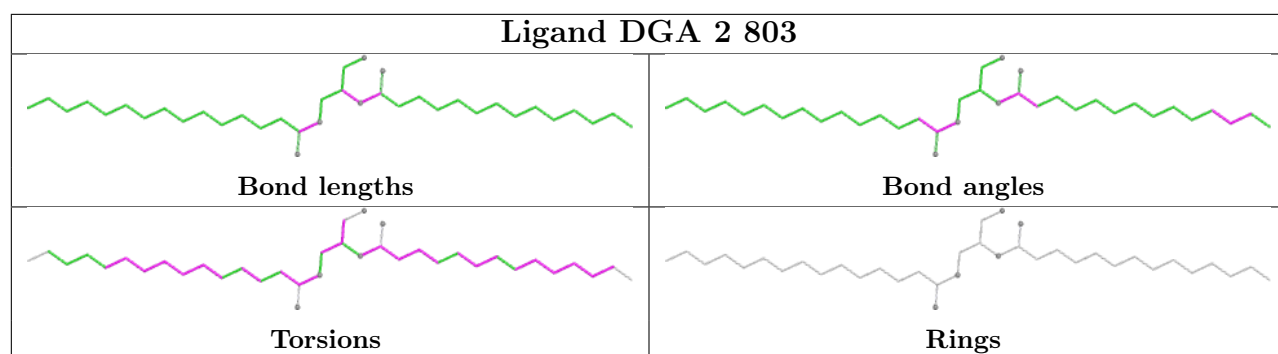




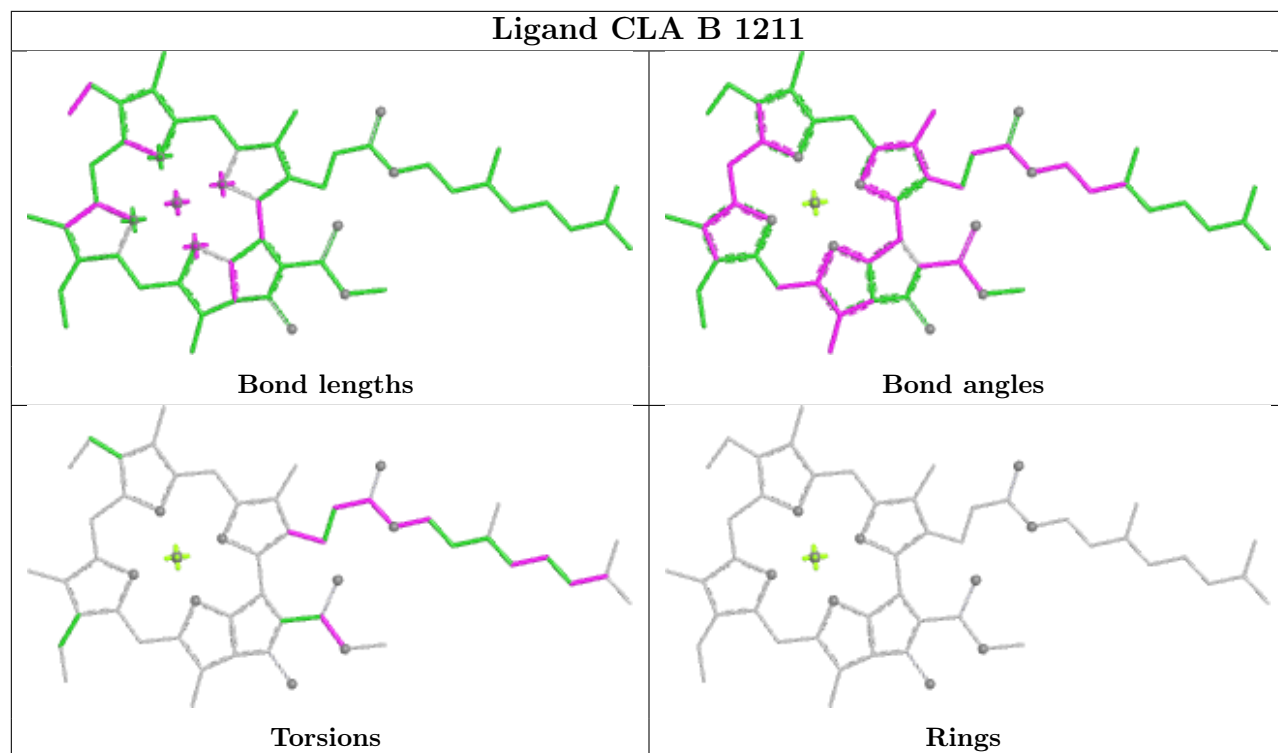


Ligand CLA 3 605**Ligand CLA 3 612**

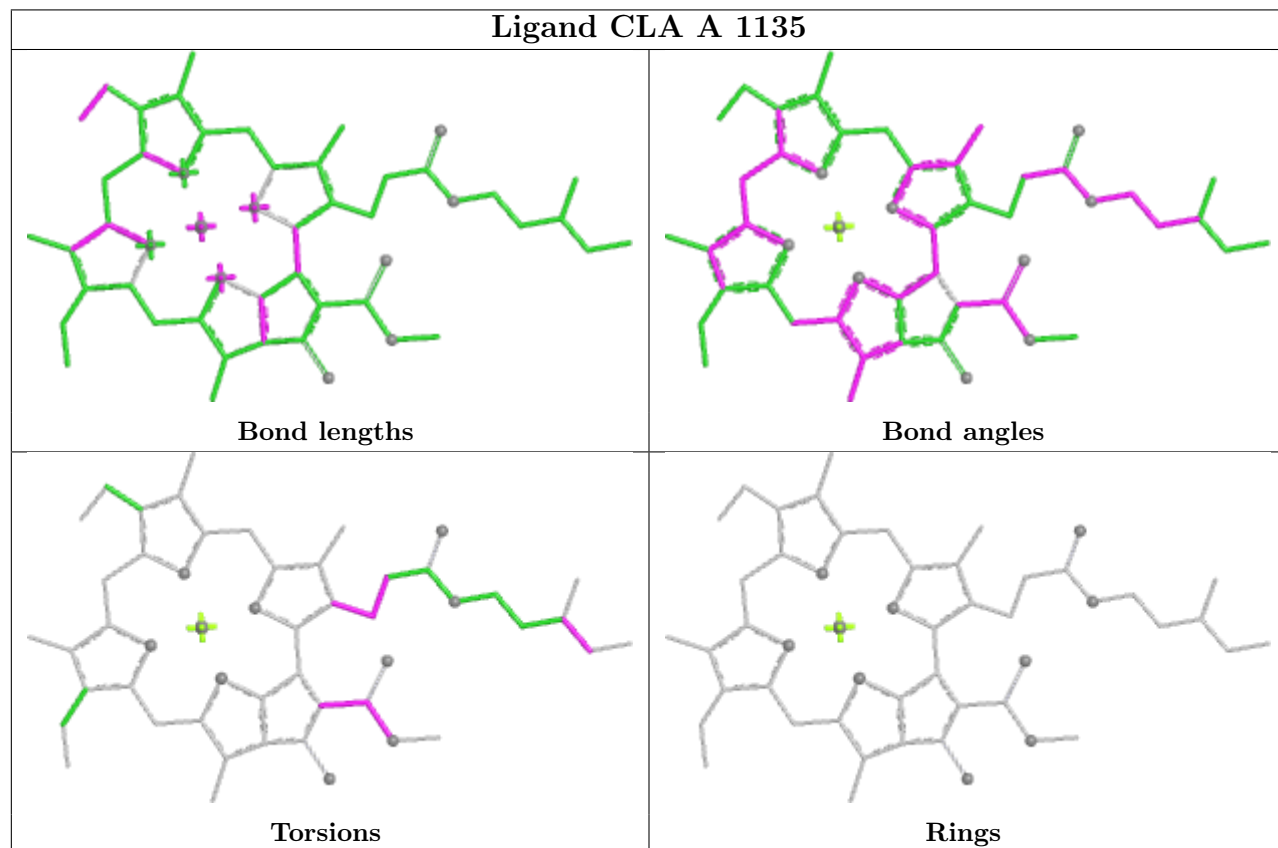


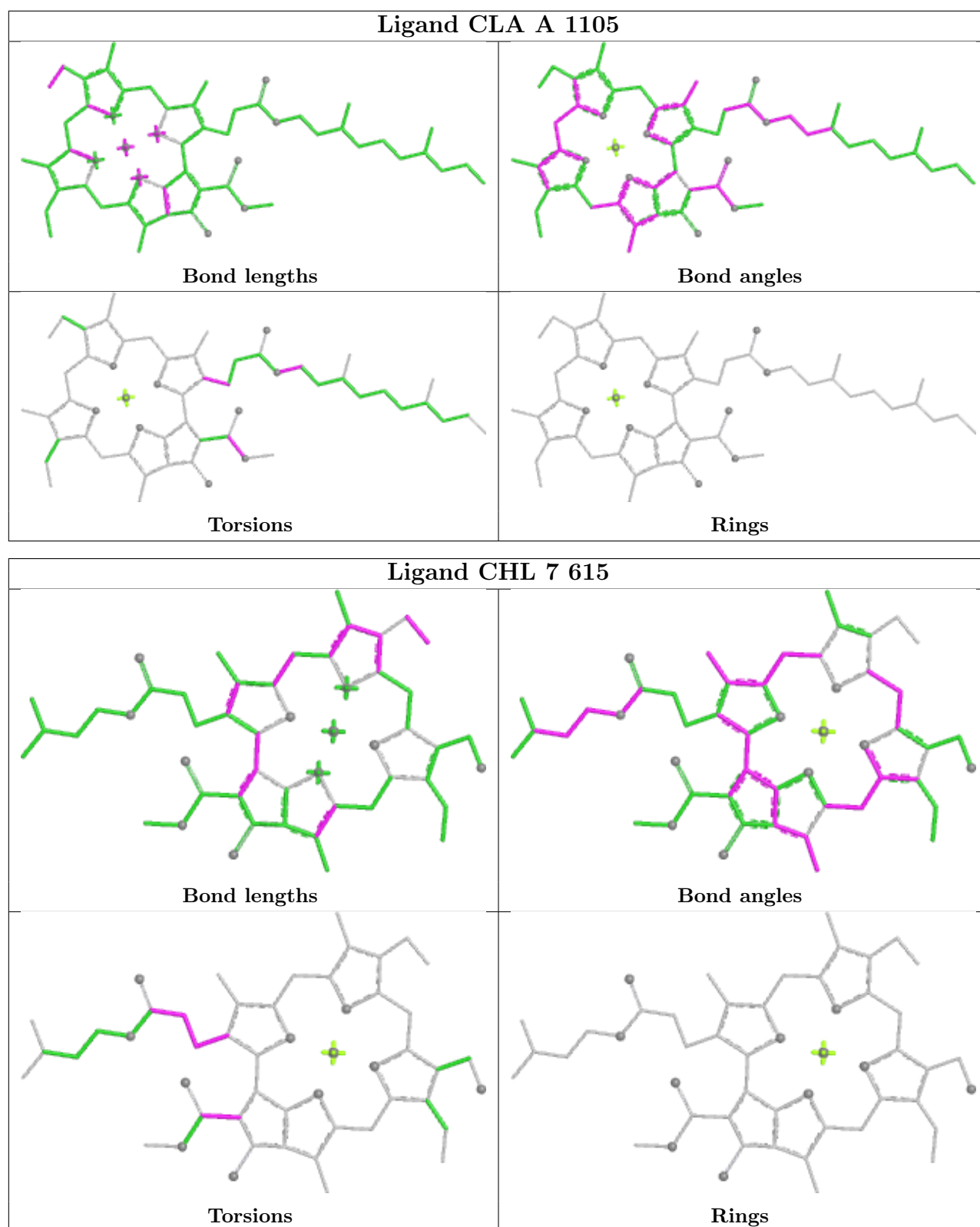


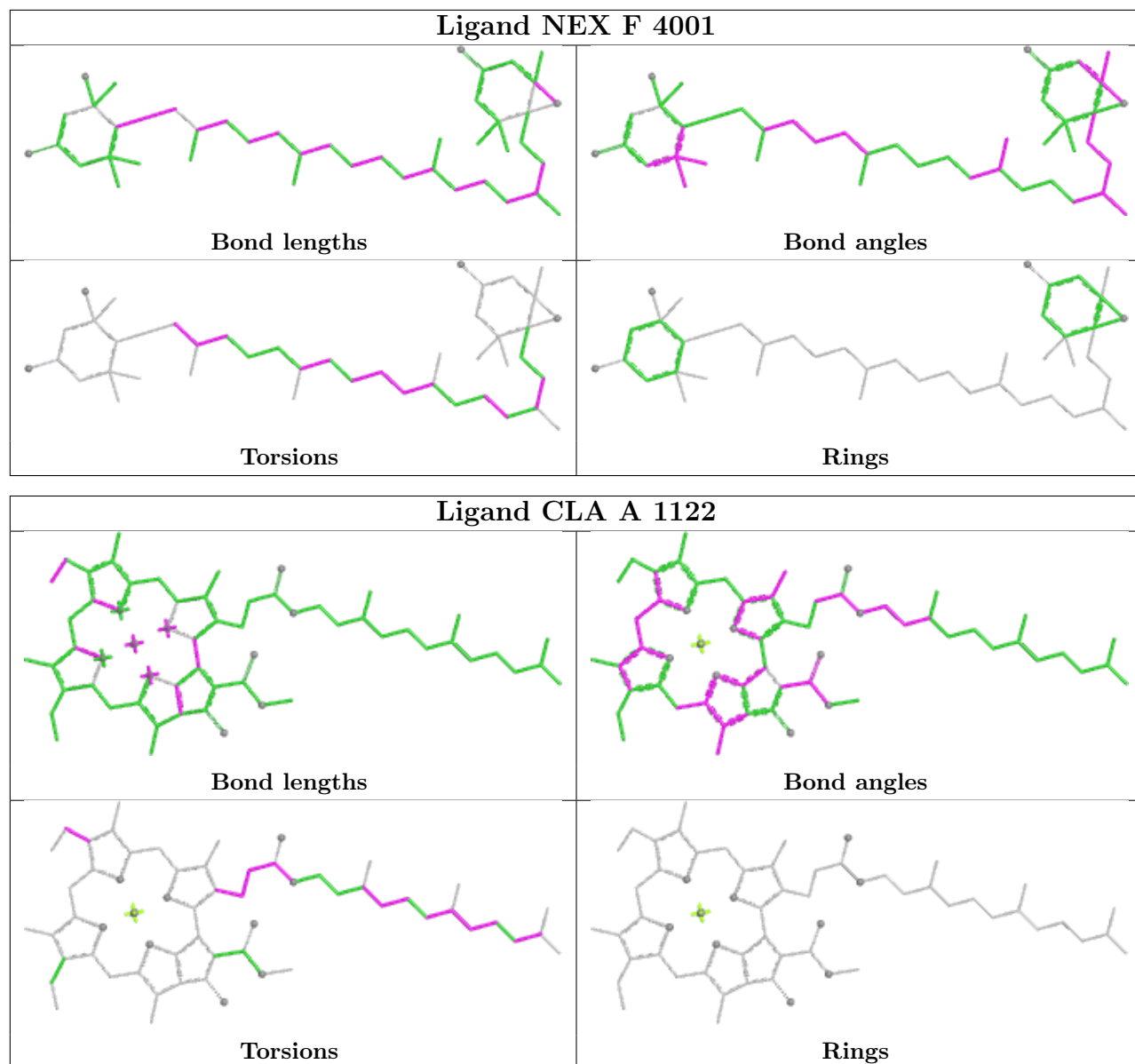
Ligand CLA B 1211

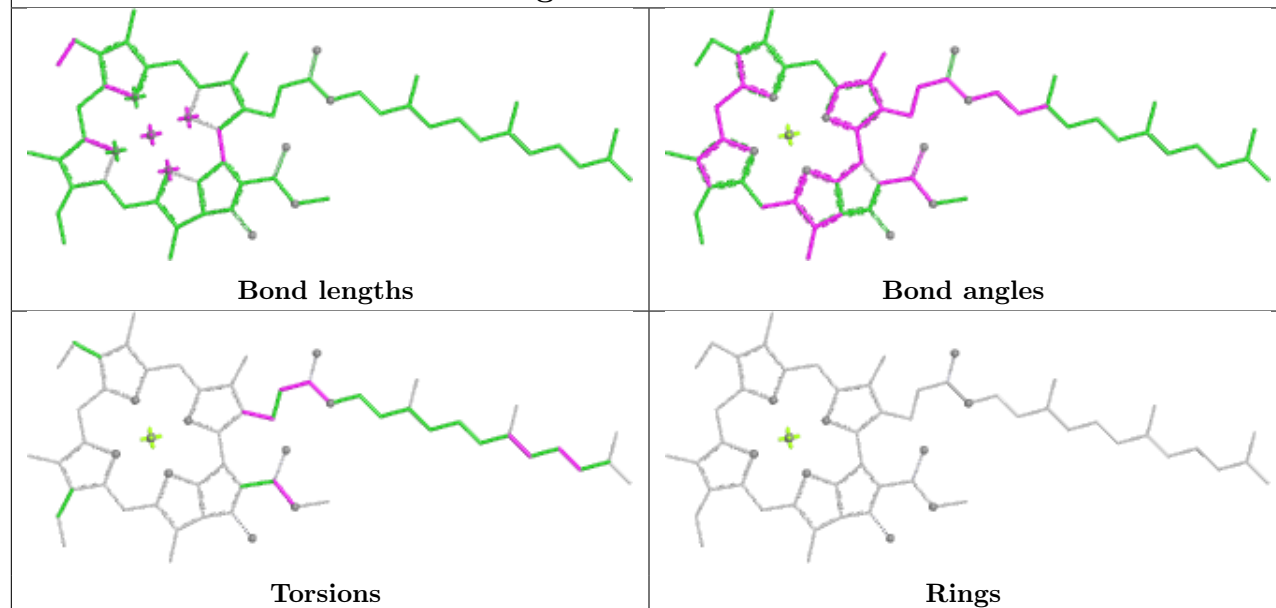
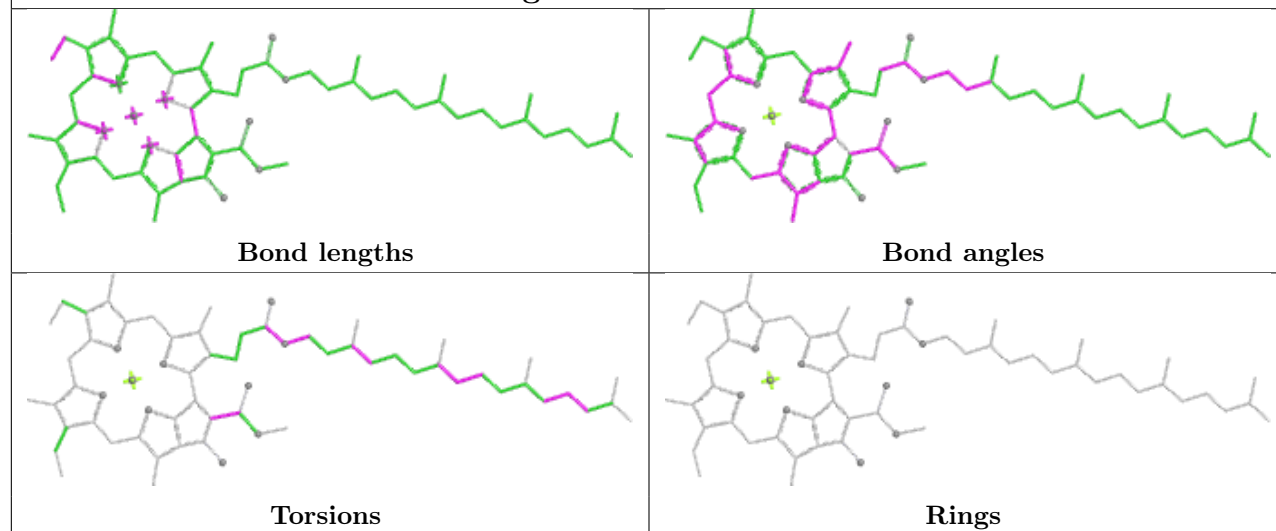


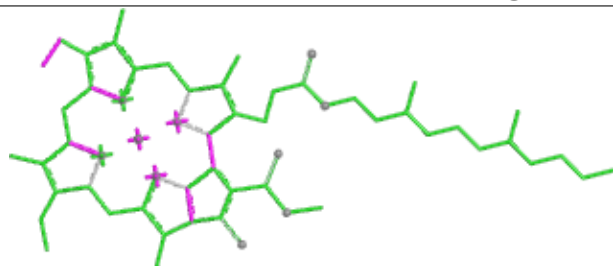
Ligand CLA A 1135



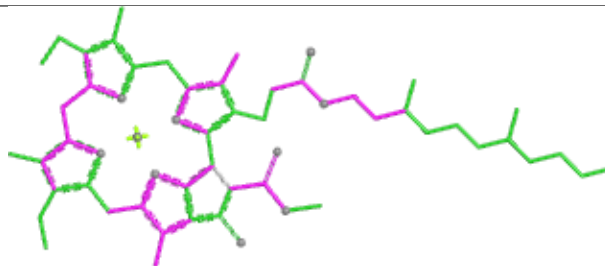




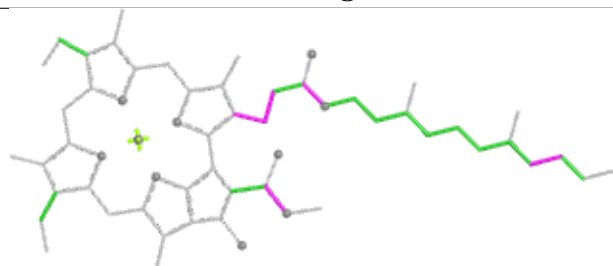
Ligand CLA 2 603**Ligand CLA A 1123**

Ligand CLA B 1222

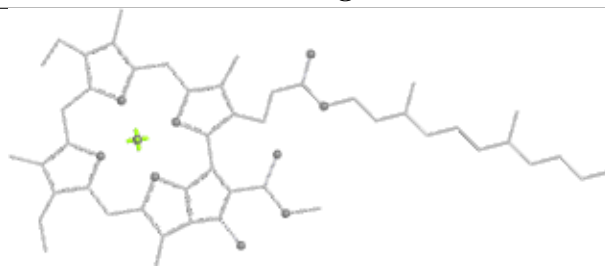
Bond lengths



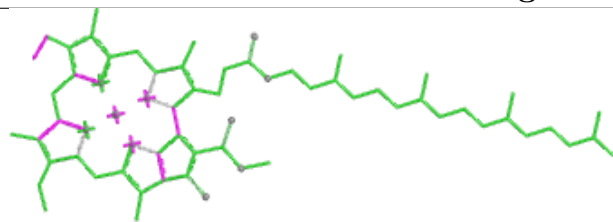
Bond angles



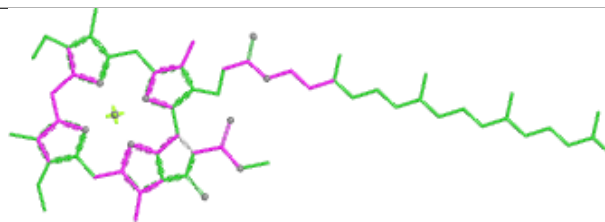
Torsions



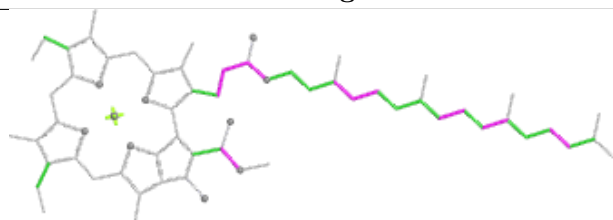
Rings

Ligand CLA 1 603

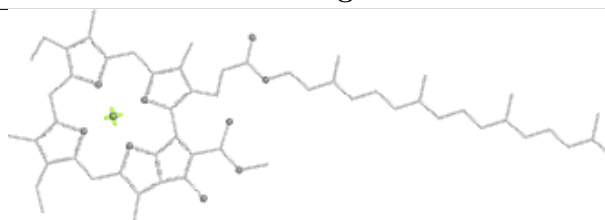
Bond lengths



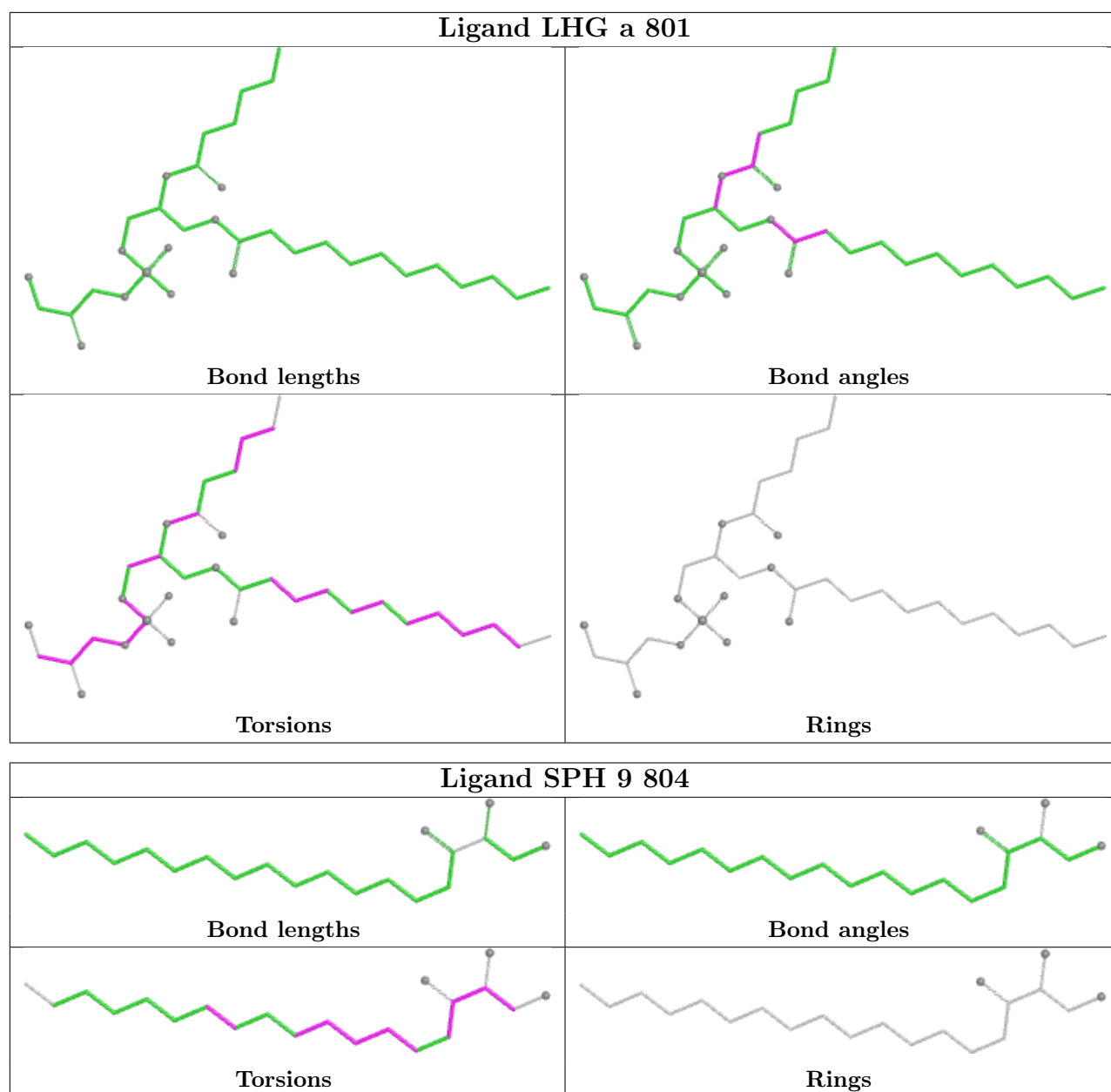
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11588. These allow visual inspection of the internal detail of the map and identification of artifacts.

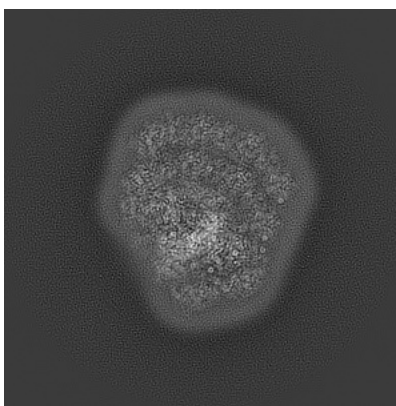
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

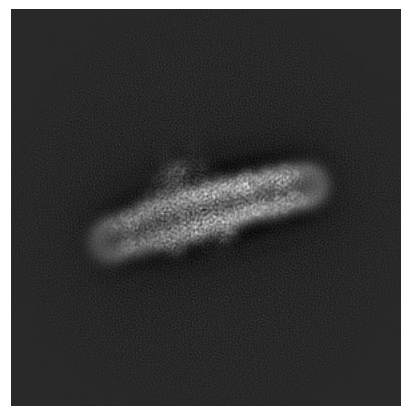
6.1.1 Primary map



X

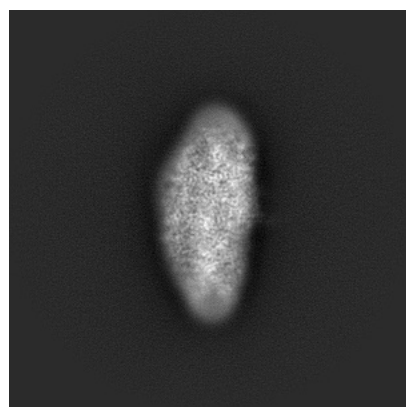


Y

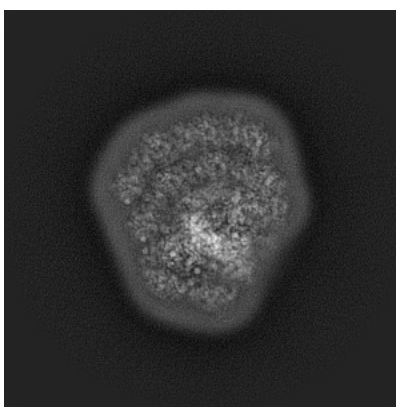


Z

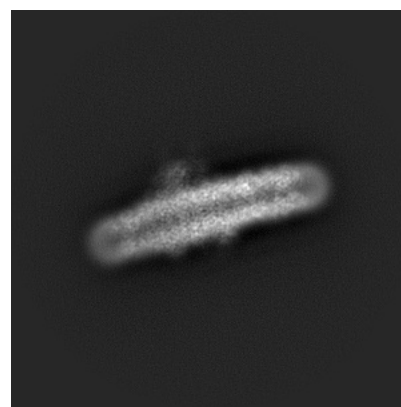
6.1.2 Raw map



X



Y

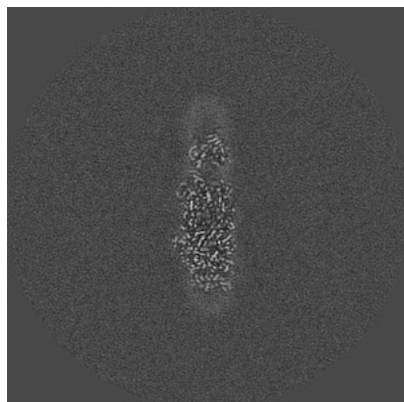


Z

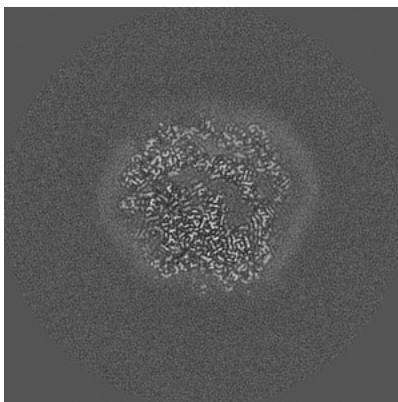
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

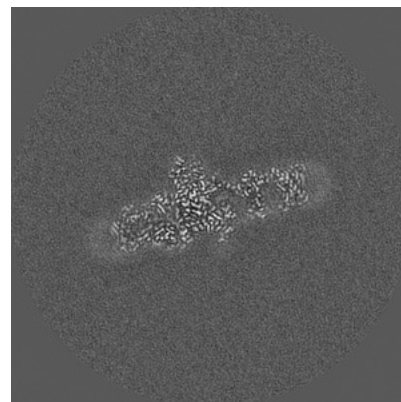
6.2.1 Primary map



X Index: 240

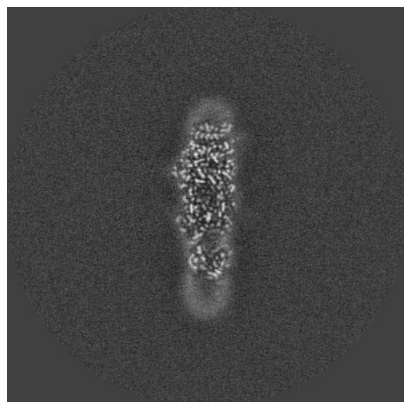


Y Index: 240

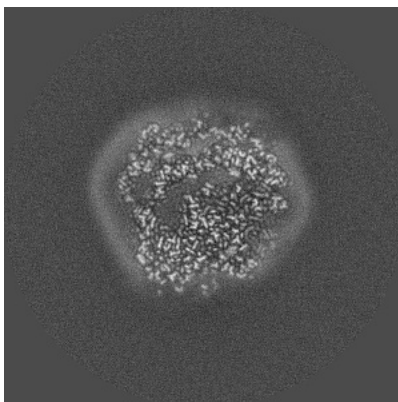


Z Index: 240

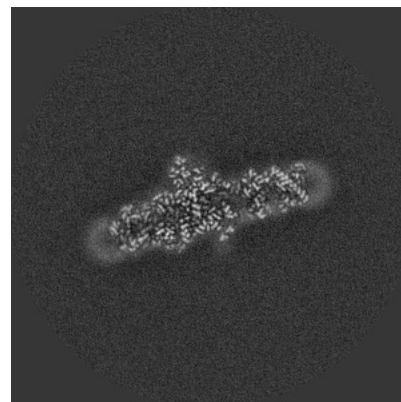
6.2.2 Raw map



X Index: 240



Y Index: 240

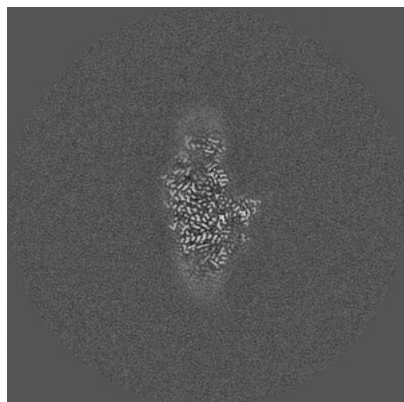


Z Index: 240

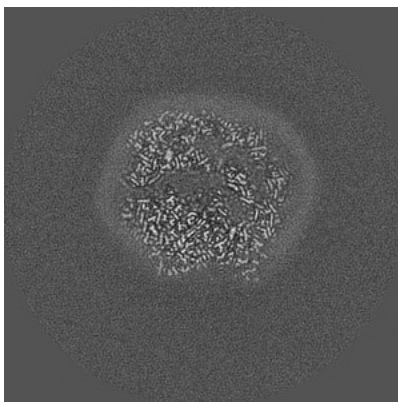
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

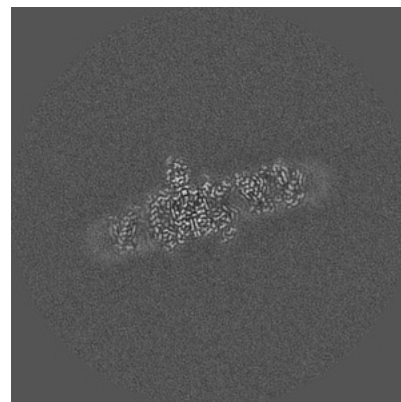
6.3.1 Primary map



X Index: 208

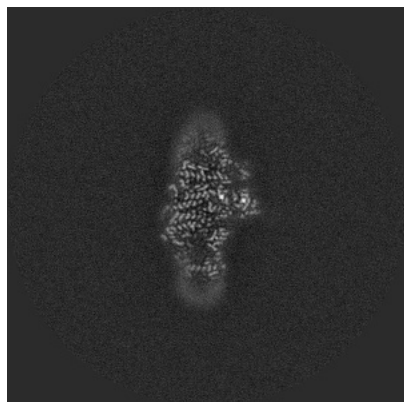


Y Index: 248

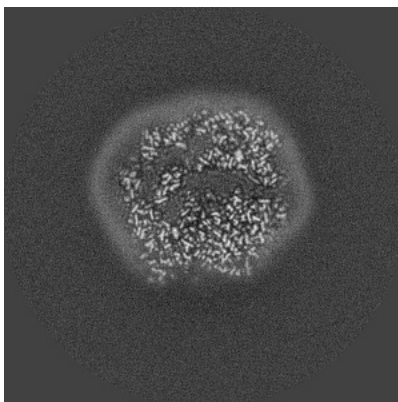


Z Index: 227

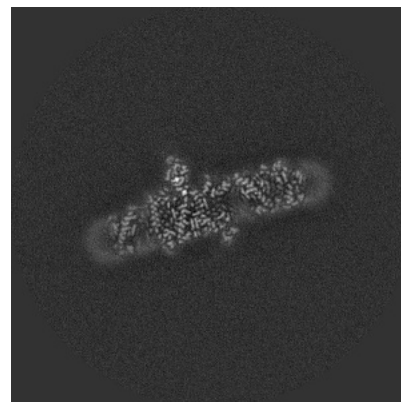
6.3.2 Raw map



X Index: 207



Y Index: 248

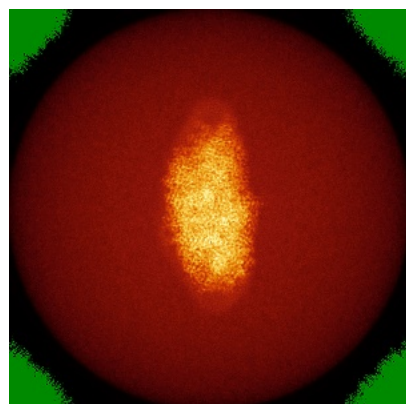


Z Index: 253

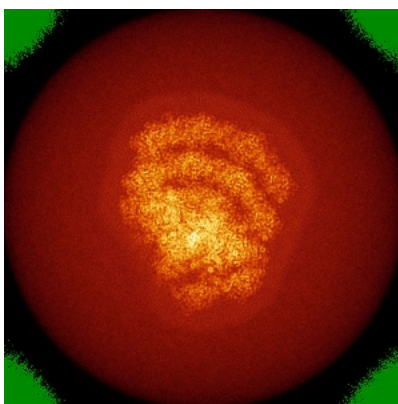
The images above show the largest variance slices of the map in three orthogonal directions.

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

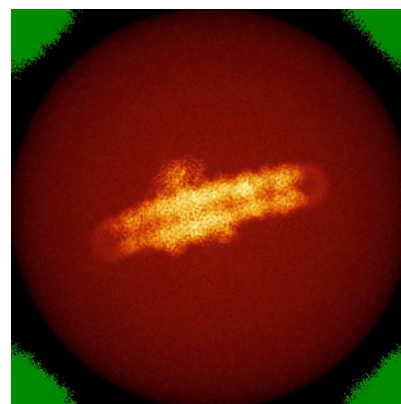
6.4.1 Primary map



X

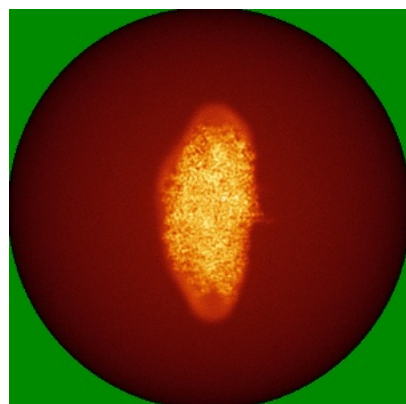


Y

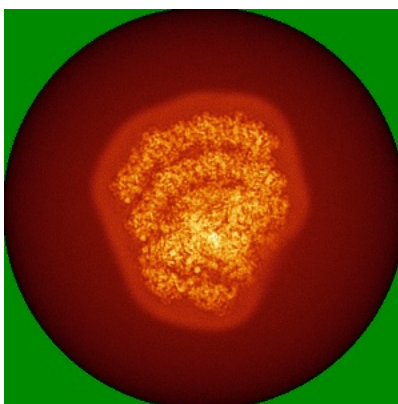


Z

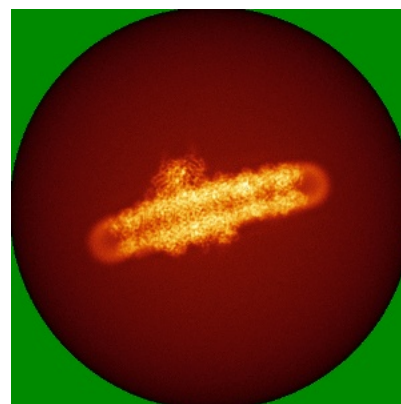
6.4.2 Raw map



X



Y

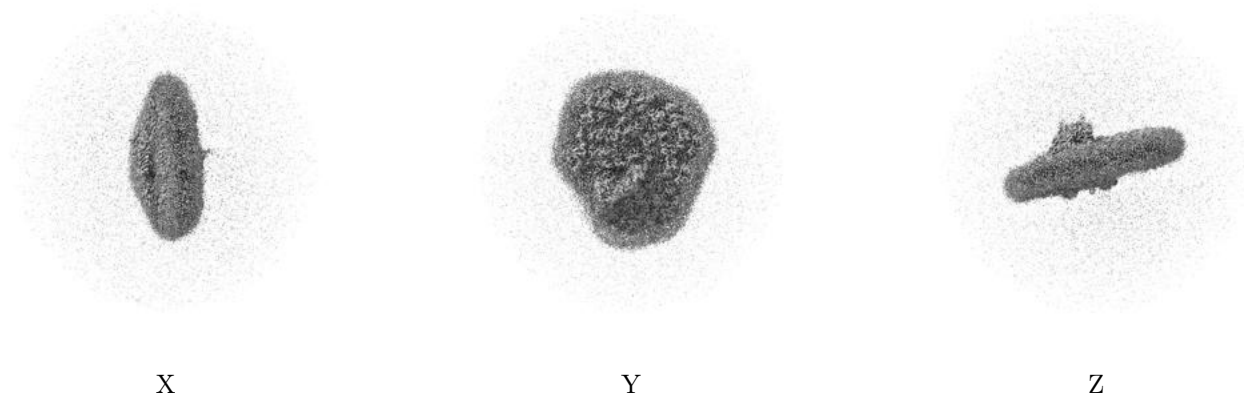


Z

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

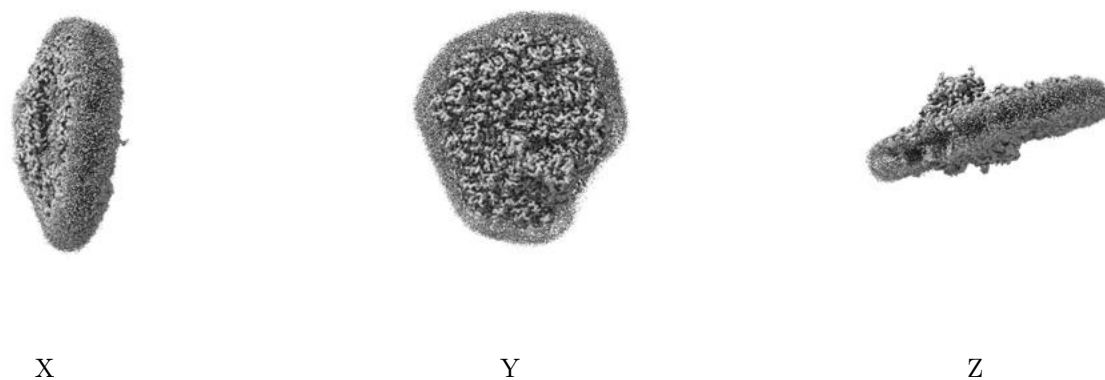
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

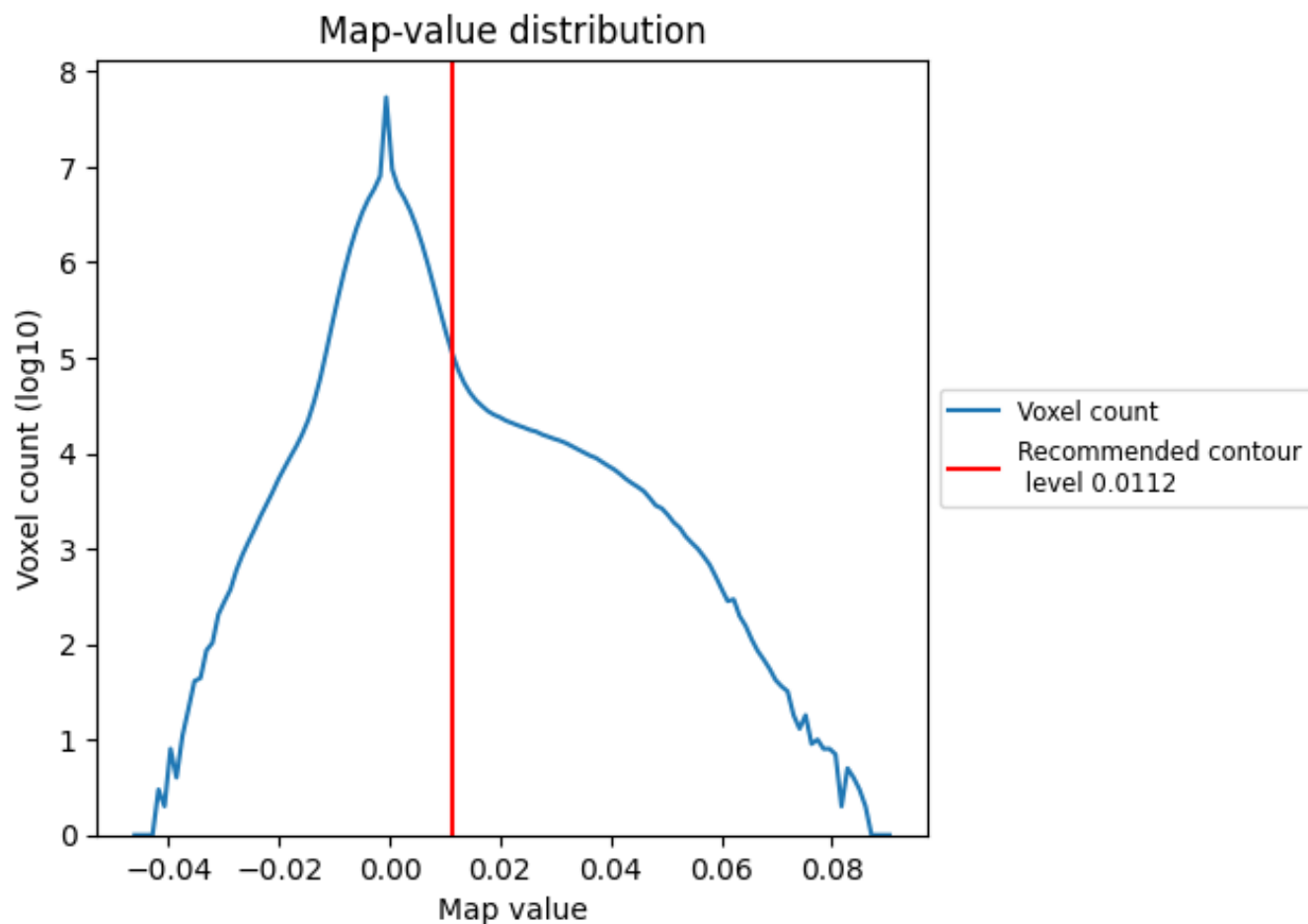
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

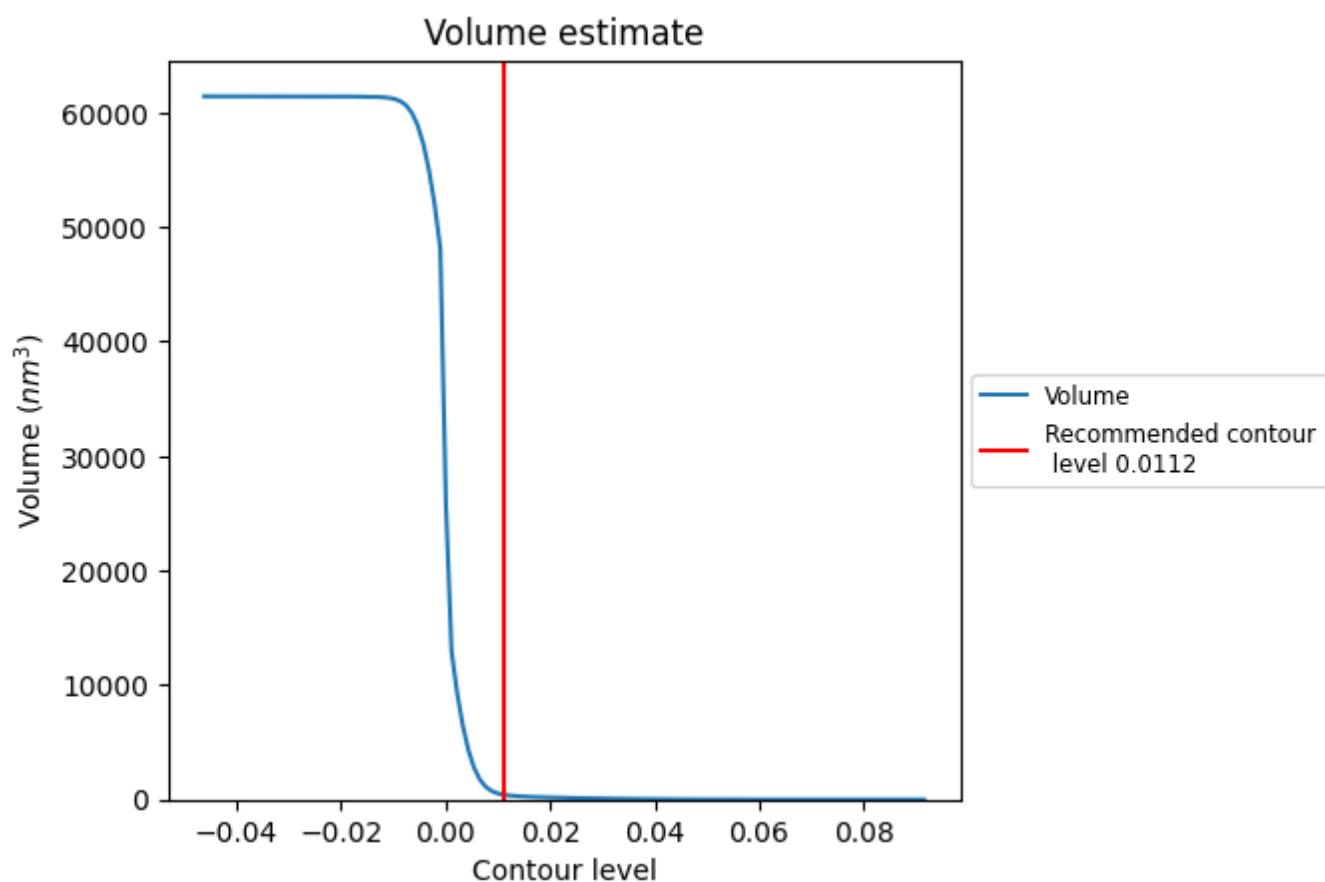
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

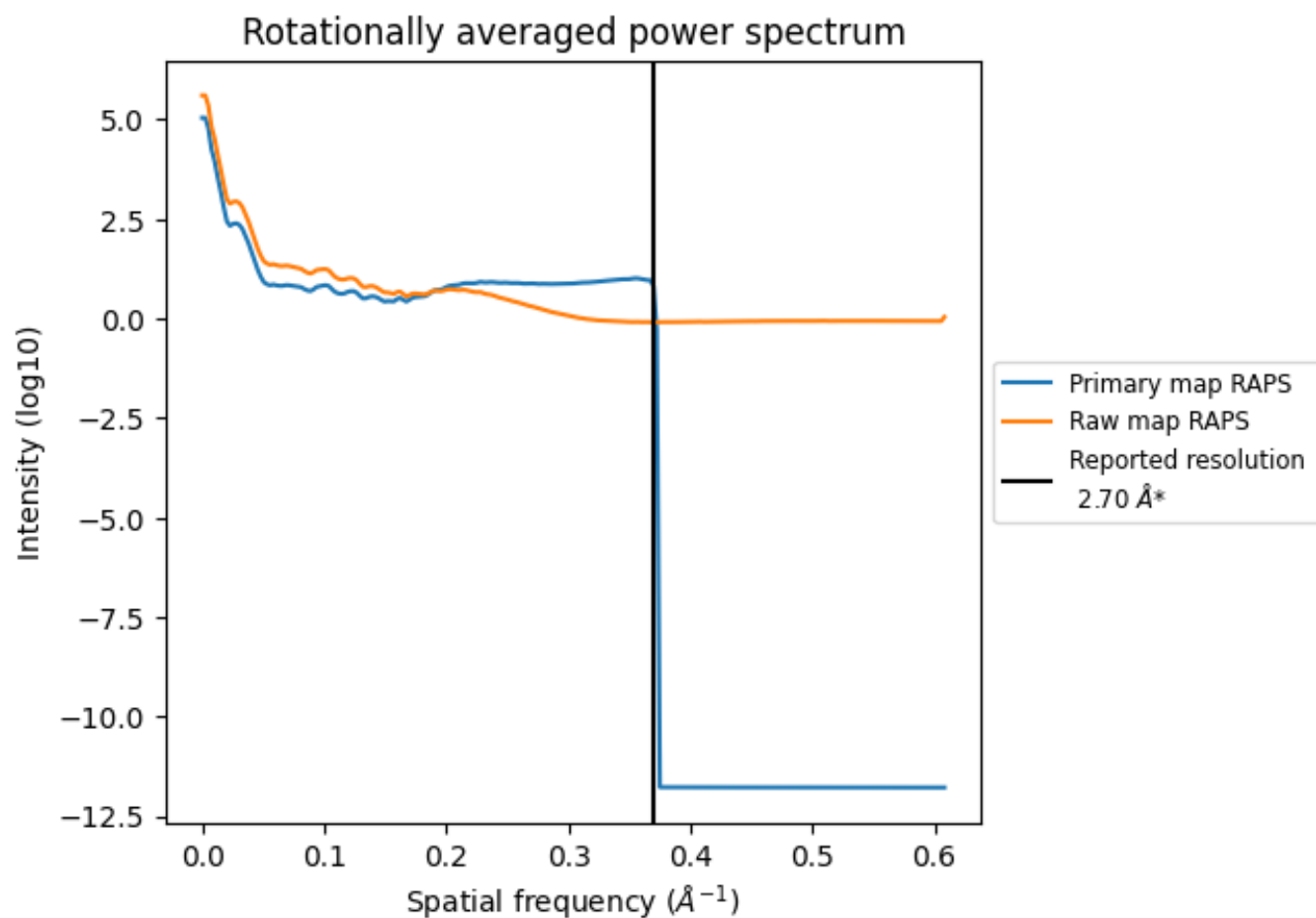
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 418 nm³; this corresponds to an approximate mass of 378 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 ⓘ

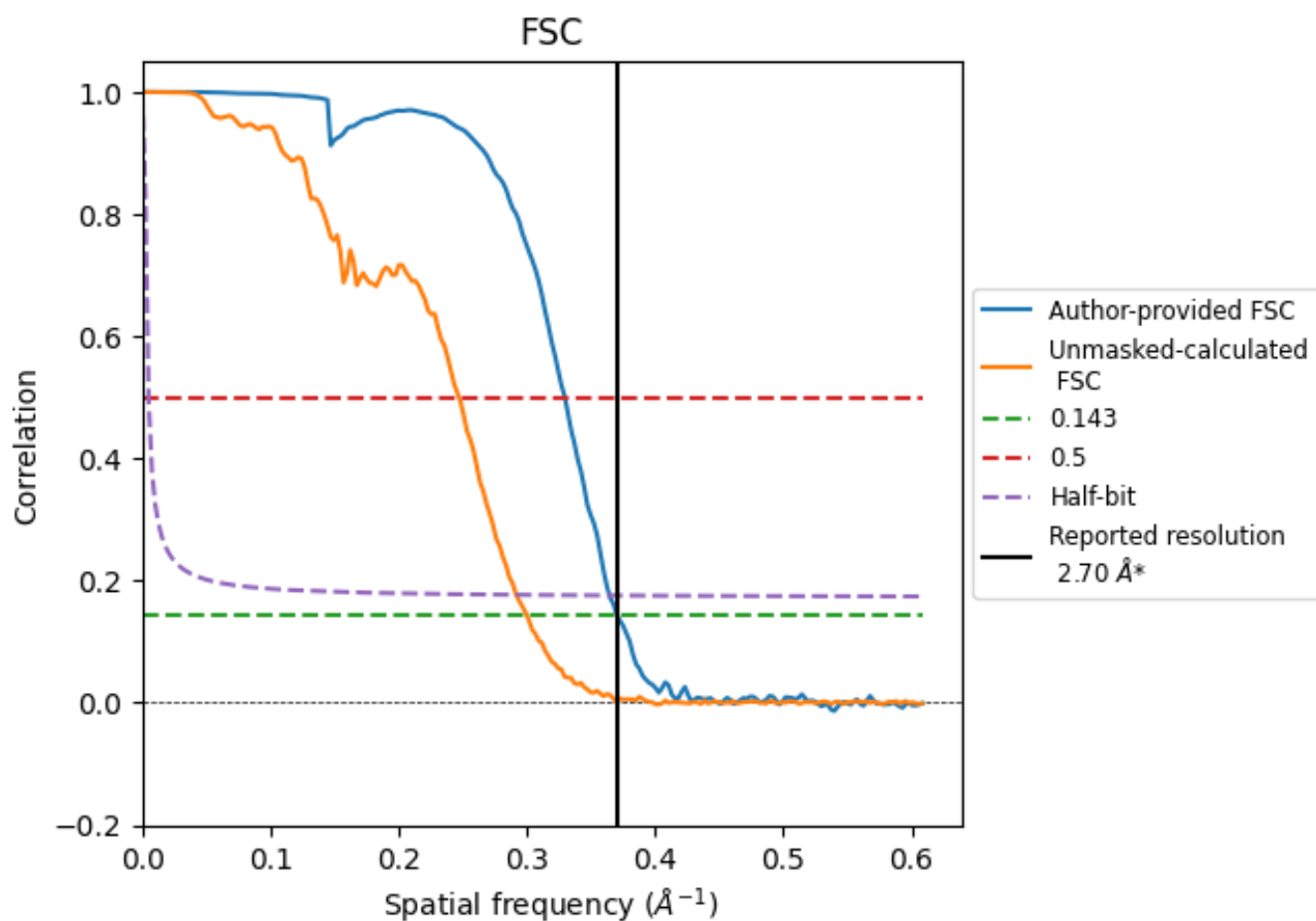


*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.370 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

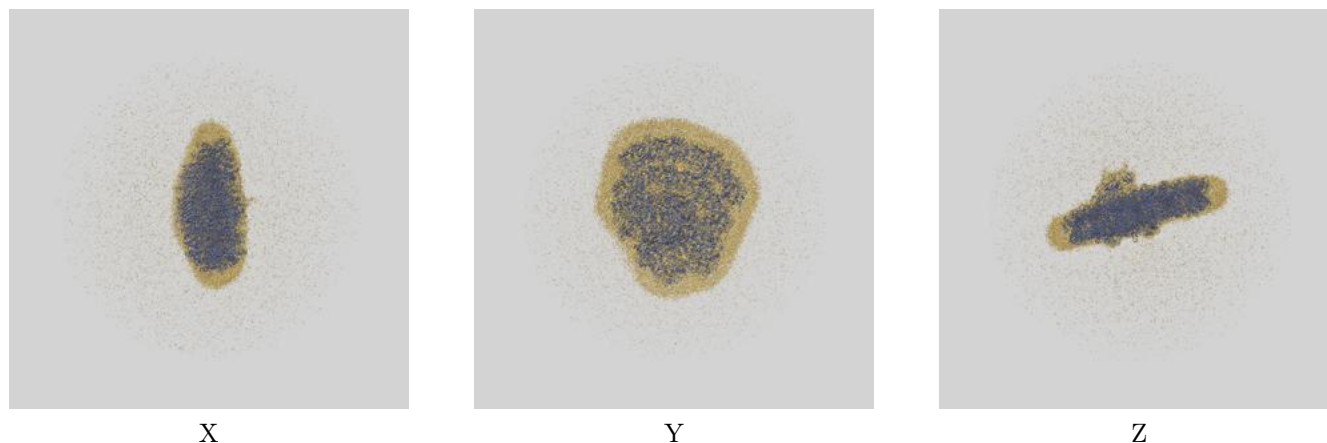
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.03	2.74
Unmasked-calculated*	3.33	4.05	3.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.33 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

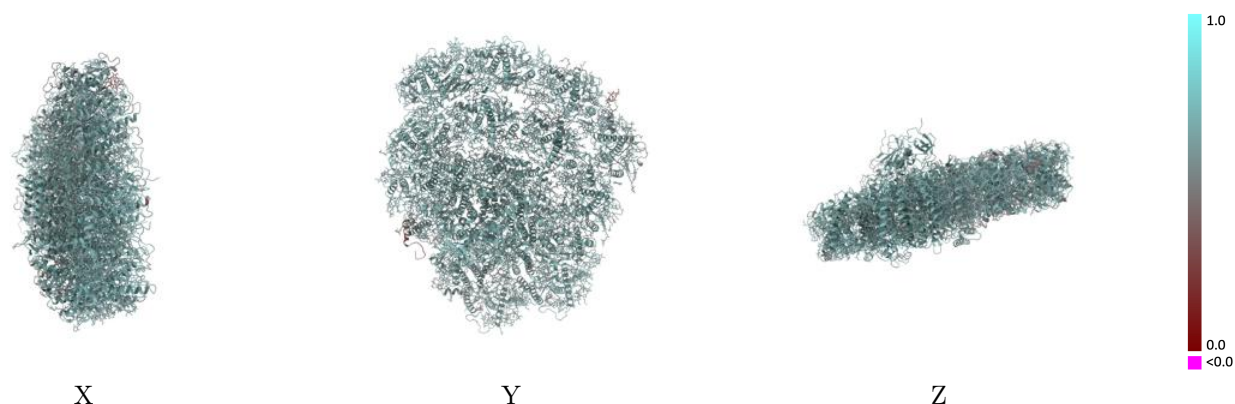
This section contains information regarding the fit between EMDB map EMD-11588 and PDB model 6ZZX. Per-residue inclusion information can be found in [section 3](#) on [page 55](#).

9.1 Map-model overlay [i](#)



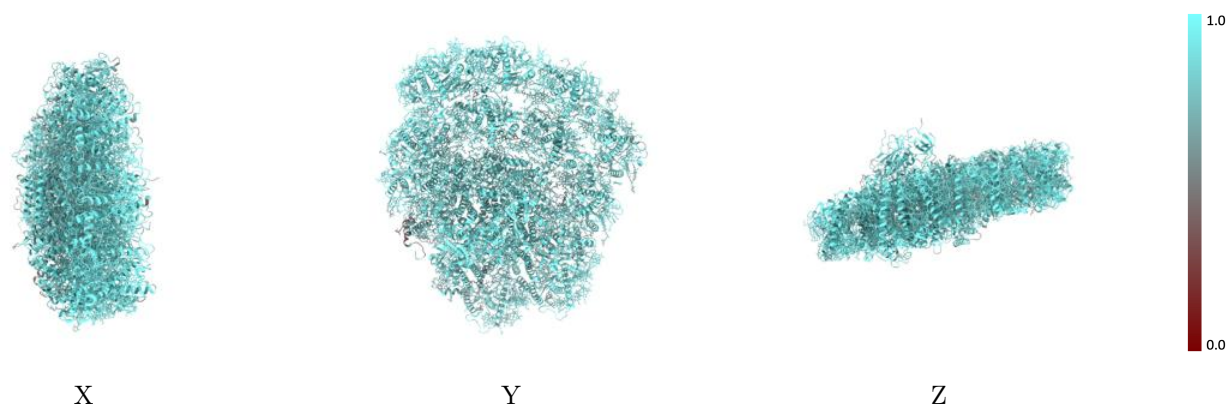
The images above show the 3D surface view of the map at the recommended contour level 0.0112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



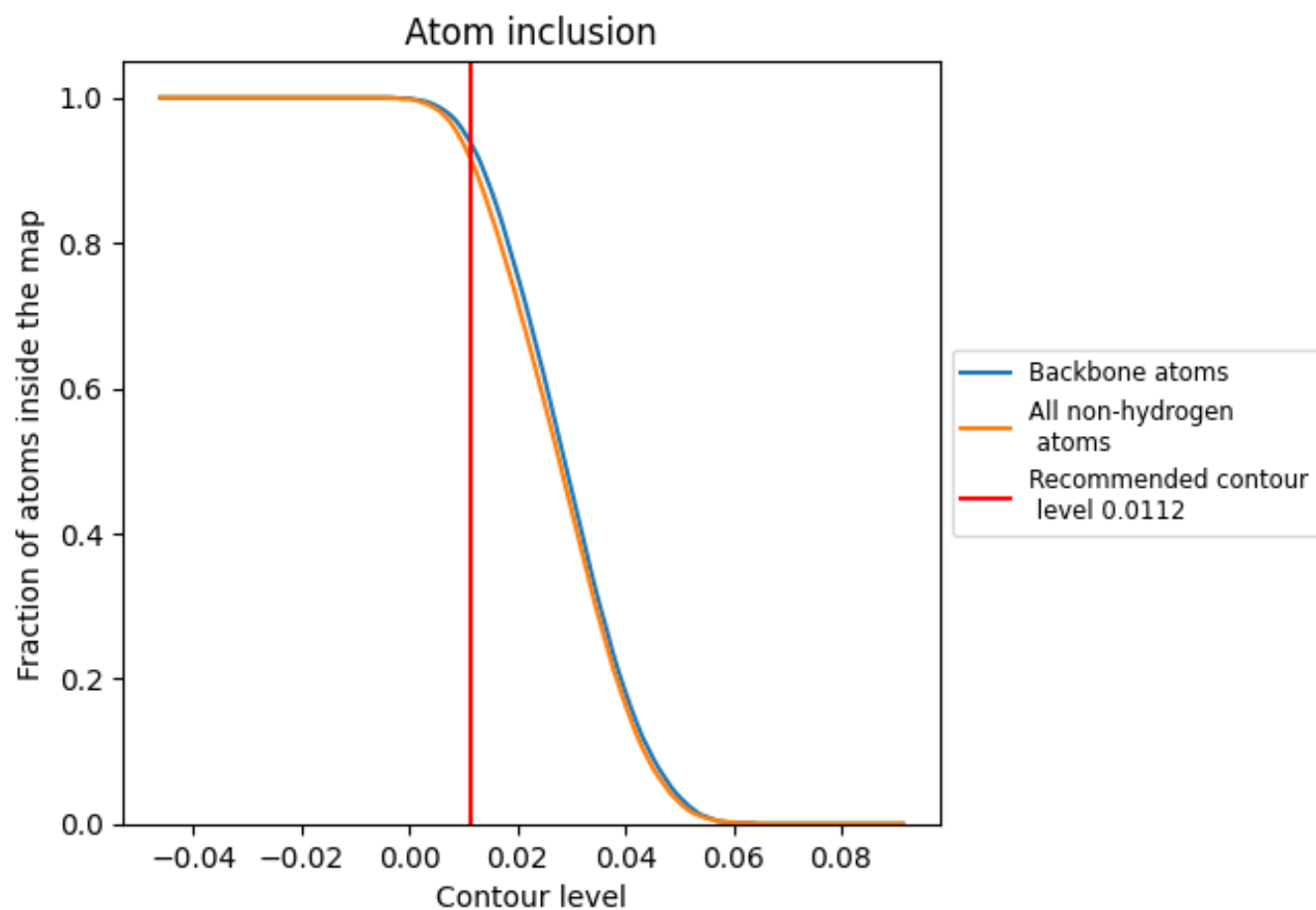
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0112).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.0112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9180	0.6210
1	0.9060	0.6130
2	0.8860	0.6000
3	0.9370	0.6350
4	0.8970	0.5980
5	0.9340	0.6190
6	0.9200	0.6190
7	0.9090	0.6200
8	0.9050	0.6190
9	0.9160	0.6190
A	0.9560	0.6480
B	0.9600	0.6500
C	0.9780	0.6530
D	0.9320	0.6250
E	0.9310	0.6160
F	0.9120	0.6210
G	0.8990	0.6170
H	0.7480	0.5440
I	0.9010	0.6100
J	0.9020	0.6260
K	0.8960	0.6010
L	0.8820	0.5930
M	0.9640	0.6330
O	0.5450	0.4140
a	0.8550	0.5770

