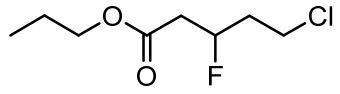
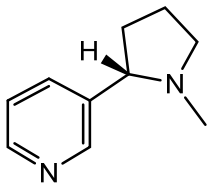
CM5239 Tutorial 1 – SMILES and MOL File

(1) Write down the SMILES notations of the following compounds.

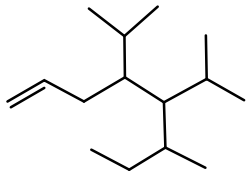
(a)



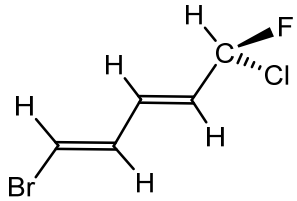
(b)



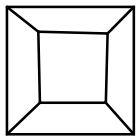
(c)



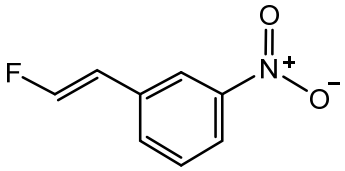
(d)



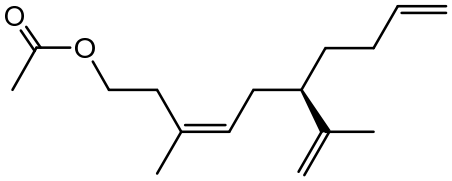
(e)



(f)



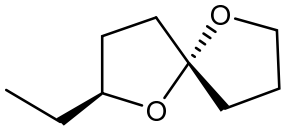
(g)



(h)

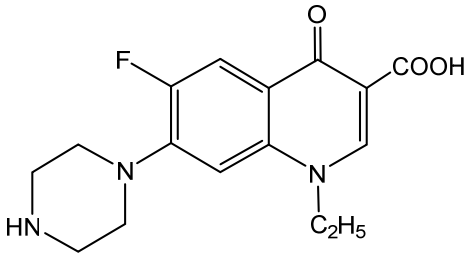
$Cu^{2+}SO_4^{2-}$

(i)



(2) "O1C=C[C@H]([C@H]1O2)c3c2cc(OC)c4c3OC(=O)C5=C4CCC(=O)5" is the SMILES notation for aflatoxin B1. Draw the chemical structure of this compound.

(3) Draw the structure of Norfloxacin using ChemDraw or PubChem (Search – 3D Conformer – Draw (use sketcher tool). Create and download a mol file of the molecule. Examine the file as a text file and identify various blocks and syntaxes of the mol file.



Norfloxacin

(4) Construct the bond block of the molfile of 3-methoxy-4-hydroxybenzaldehyde based on the following atom block.

-1.9046	0.0000	2.6331	H	0	0	0	0	0	0	0	0	0	0	0
-1.4024	0.0000	1.6512	C	0	0	0	0	0	0	0	0	0	0	0
-0.0865	0.0000	-0.8110	C	0	0	0	0	0	0	0	0	0	0	0
-0.0045	0.0000	1.6023	C	0	0	0	0	0	0	0	0	0	0	0
-2.1555	0.0000	0.4801	C	0	0	0	0	0	0	0	0	0	0	0
-1.5033	0.0000	-0.7595	C	0	0	0	0	0	0	0	0	0	0	0
0.6576	0.0000	0.3652	C	0	0	0	0	0	0	0	0	0	0	0
-3.2548	0.0000	0.5090	H	0	0	0	0	0	0	0	0	0	0	0
1.7572	0.0000	0.3343	H	0	0	0	0	0	0	0	0	0	0	0
0.7853	0.0000	2.8422	C	0	0	0	0	0	0	0	0	0	0	0
0.2888	0.0000	3.9710	O	0	0	0	0	0	0	0	0	0	0	0
1.8904	0.0000	2.6984	H	0	0	0	0	0	0	0	0	0	0	0
-2.2875	0.0000	-1.8833	O	0	0	0	0	0	0	0	0	0	0	0
0.4423	0.0000	-2.0923	O	0	0	0	0	0	0	0	0	0	0	0
-1.7079	0.0000	-2.6616	H	0	0	0	0	0	0	0	0	0	0	0
1.8620	0.0000	-2.1810	C	0	0	0	0	0	0	0	0	0	0	0
2.2855	0.9186	-1.7068	H	0	0	0	0	0	0	0	0	0	0	0
2.0525	0.0000	-3.2844	H	0	0	0	0	0	0	0	0	0	0	0
2.2855	-0.9186	-1.7068	H	0	0	0	0	0	0	0	0	0	0	0