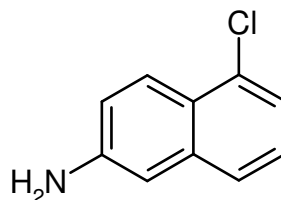
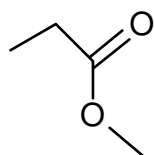
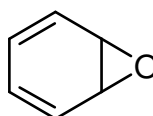
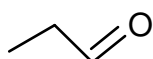
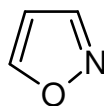


3rd Assignment to be handed in until 25.11.2019

your name:

1. Report the appropriate SMILES for the following compounds. Computer generated SMILES will be not accepted! (30 points)



2. Draw the according structure of the given SMILES. Please add all hydrogens. (40 Points)

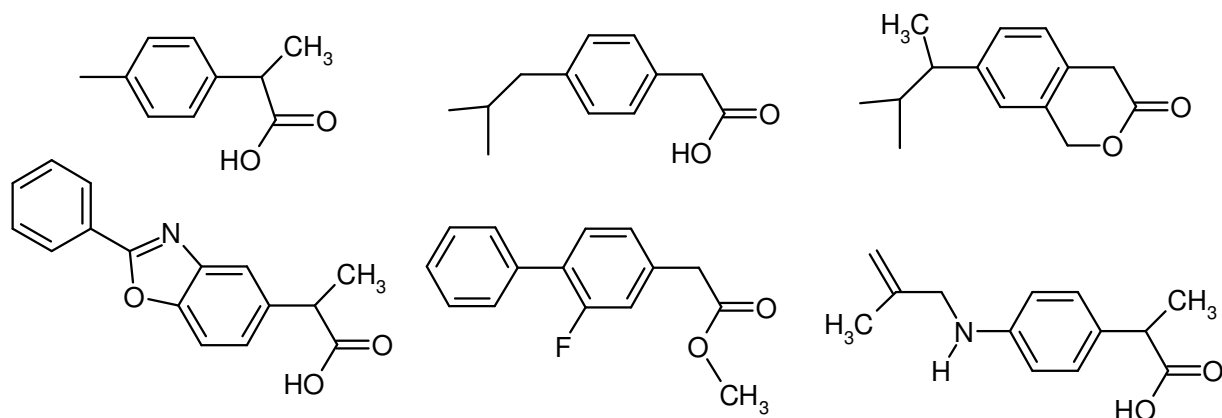
CC(=O)N1CCC(C(=O)N)C1

FS(=O)(=O)Nc1ccc(C)cc1

CC(C)Cc1ccc(C(C)C(=O)O)c(Cl)c1

c1ccccc1C2=C(c3ccc(NC)cc3)COC2(=O)

3. Find the maximum common substructure of the following compounds and report its corresponding SMILES. Keep in mind that „CO“ matches H₃C-OH as well as H₃C-CH₂-O-CH₃ (only non-hydrogen atoms are considered) (20 points)



4. Which of the compounds A or B should bind more selectively to a given target? Please give a short explanation why! Also mark the rotatable bonds. (10 points)

