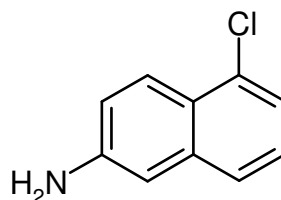
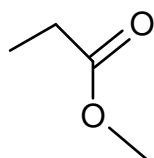
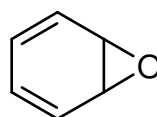
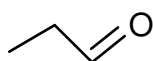
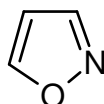


**3rd Assignment** to be handed in until 01.12.2014

your name:

1. Report the appropriate SMILES for the following compounds. No computer generated SMILES please ! (30 points)



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

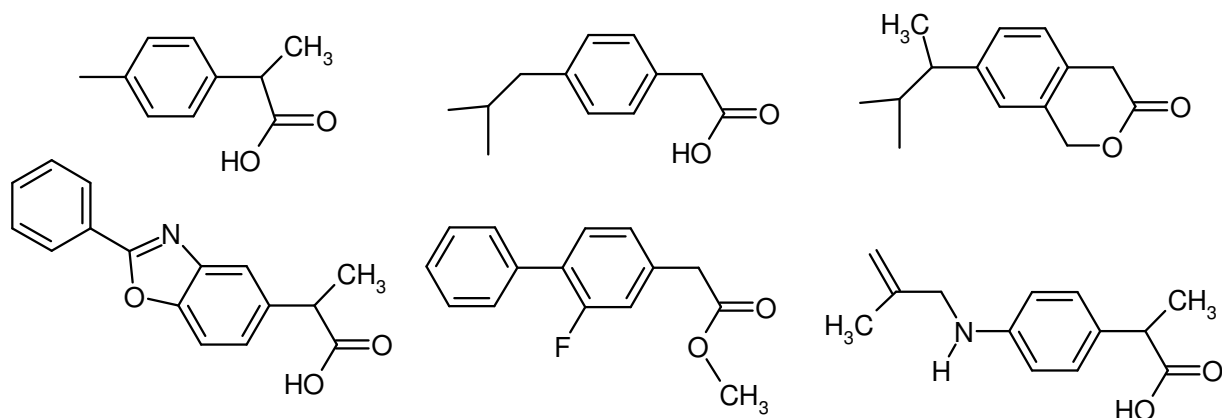
CC(=O)N1CCC(C(=O)N)C1

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  $\text{H}_3\text{C-OH}$  as well as  $\text{H}_3\text{C-CH}_2\text{-O-CH}_3$  (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)

