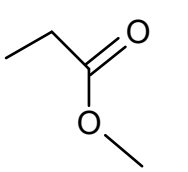
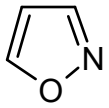
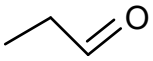
Exercise to the lecture „Modern Methods in Drug Discovery“ WS24/25

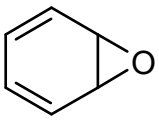
3rd Assignment

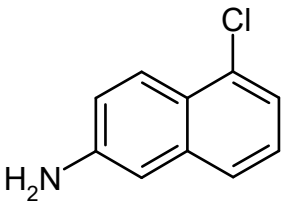
1. Aim of this exercise is that you are able to construct and modify SMILES without the help of a graphical editor (which may rearrange the sequence of your input). Thus use the SMILES viewer as control for your hand made SMILES strings, only:
https://pubchem.ncbi.nlm.nih.gov/edit3/index.html
Type your SMILES into a text editor and then copy/paste them to the input window.
Hit the “NEW” button to delete the input before each new try. (30 points)











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

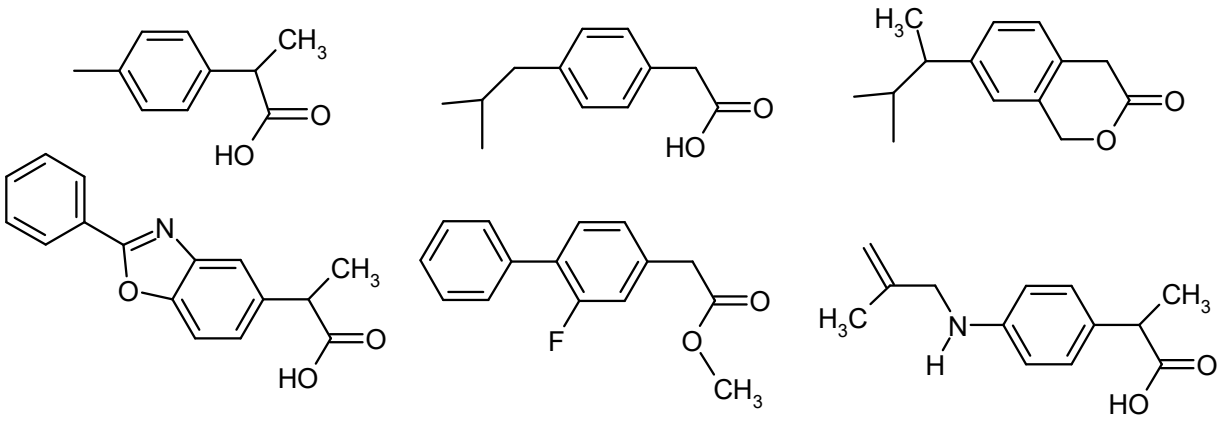
CC(=O)N1CCC(C(=O)N)C1

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

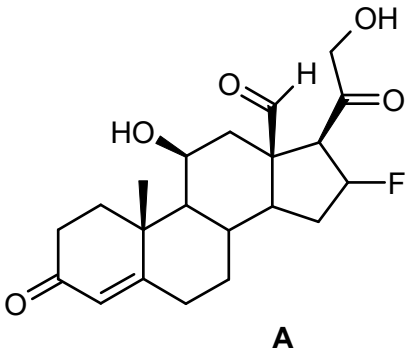
CC(C)Cc1ccc(C(C)C(=O)O)c(Cl)c1

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

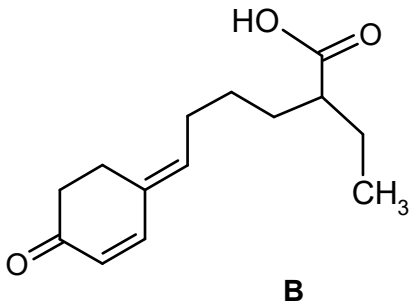
3. Find the maximum common substructure of the following compounds by visual inspection and report the corresponding SMILES string that would match all compounds. Keep in mind that „CO“ matches H_3C-OH as well as H_3C-CH_2-O-CH_3 (only non-hydrogen atoms are considered) (20 points)



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



A



B