## **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)

 $NH_2$  O O CI

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<sub>3</sub>C-OH as well as H<sub>3</sub>C-CH<sub>2</sub>-O-CH<sub>3</sub> (only non-hydrogen atoms are considered) (20 points)

$$CH_3$$
 $HO$ 
 $CH_3$ 
 $HO$ 

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)