Assignment 23.10.2025

Get Familiar with SMILES and RDKit

Install RDKit

!pip install rdkit

SMILES (Basics)

- Get a rough understanding of what Simplified Molecular Input Line Entry System (SMILES) are.
- https://en.wikipedia.org/wiki/Si mplified_Molecular_Input_Line_ Entry_System
- Try to write (without a computer) the SMILES for some simple molecules, e.g.
  - Water
  - Carbon dioxide
  - Alcohol (ethanol)
  - Methane, ethane, propane, butane
  - Propanol, iso-propanol

SMILES with RDKit

• Create SMILES for alcohol (ethanol)

• Draw a sketch of the molecule using RDKit

• What happens if you input an illegal SMILES?

Get Familiar with Lipophilicity.xlsx

- Read Lipophilicity.xlsx
- For each SMILES in the file
  - Create molecule
  - Add hydrogens
  - Count number of atoms
- For all molecules in the file find the 10 most frequent atoms
- For all molecules in the file find the 10 most frequent atom-atom bonds