

Programming for Chemists

Course Workload		Assessment form (examination/ graded test/ ungraded test)
ECTS	Hours	
6	216	Credit

A course on the basics of Python, data structures, how to properly structure code and a repository, use package managers, Git. Linux, bash, working with the server.

Course structure:

1. Introduction to Programming

- 1.1. Basics of programming languages (Python and R)
- 1.2. Setting up the programming environment
- 1.3. Basic syntax and data types

2. Data Structures and Algorithms

- 2.1. Lists, dictionaries, and sets
- 2.2. Loops and conditionals
- 2.3. Functions and modules

3. Scientific Computing and Data Analysis

- 3.1. Numerical methods (e.g., solving equations, integration)
- 3.2. Data analysis and visualization (e.g., Matplotlib, Pandas)

4. Chemical Informatics

- 4.1. Handling chemical data (e.g., SMILES, InChI)
- 4.2. Accessing chemical databases (e.g., PubChem, ChemSpider)
- 4.3. Molecular file formats (e.g., SDF, MOL)

5. Simulations and Modeling

- 5.1. Basics of molecular dynamics simulations
- 5.2. Quantum chemistry calculations
- 5.3. Software tools (e.g., RDKit, Open Babel)

6. Automation and Scripting for Laboratory Work

- 6.1. Writing scripts for automating repetitive tasks
- 6.2. Parsing and processing laboratory data
- 6.3. Interfacing with laboratory equipment and software

7. Project Management and Version Control

7.1. Using Git and GitHub for version control

7.2. Collaborative programming practices
