Cheminformatics
BIO 4372 (6 ECTS credits)

Winter Semester 2018-19

Tue 2-4 pm, A104, Sand 1

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Overview

After a short motivation and recapitulation of basic chemistry knowledge we will discuss problems arising in chemistry where informatics can provide solutions. Methods to represent and store chemical information *in silico* will allow us to discuss approaches to compare and search chemical data efficiently, both in 2D and 3D. Introducing so-called descriptors as an abstract representation to encode chemical molecules will lead us to the field of Quantitative Structure-Activity Relationship (QSAR), where the aim is to learn and predict molecular properties. We will motivate the content by showing real-world applications, mainly taken from Drug Design as arguably the main application area of cheminformatics.

Goals

- Understand the need for informatics in chemistry.
- Learn to process, analyze, and interpret chemical information.
- Understand computational challenges and key algorithms to solve them.
- Acquire cheminformatics key techniques and skills practically.

Requirements

- Participation in the weekly problem sessions.
  The date will be determined in the first lecture.
- Individually work on assignment sheets.
- Work out of a small research project in a team of 2-3 students.
  Documentation by a scientific report and presentation is required.

Evaluation

- We will check for duplicate assignment solutions and reserve the right to distribute points across all identical solutions.
- Students caught copying solutions can be excluded from the course!
- 50% of the achievable points in the assignments as well as the project are required for admission to the final exam.
- Points achieved in excess of 50% in assignments and projects will serve as a bonus to improve the final exam grade up to a maximum of 10%.
- Depending on the number of participants, the final exam can be either written or oral.

Materials

Slides will be handed out at the beginning of each lecture. All materials will be made available within the ILIAS course page.

Recommended, though not required, textbooks are:

- Leach A.R. & Gillet V.J.:
  An Introduction to Chemoinformatics
  Springer, 2007
- Gasteiger J. & Engel T. (Eds.):
  Chemoinformatics – A Textbook
  Wiley-VCH, 2003
- Bajorath J. (Ed.):
  Chemoinformatics for Drug Discovery
  Wiley, 2014

Key Dates

Oct. 16th
- First Lecture
- Hand-out of first assignment sheet

Dec. 11th
- Hand-out of projects

Jan. 22nd
- Hand-in of project reports

Jan. 29th
- Project presentations

To be determined
- Oral exams