
Cheminformatics

BIO 4372 (6 ECTS credits)

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.

Winter Semester 2019-20

Wed 8-10 am, C215, Sand 14

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Materials

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

Recommended but not required books

- Leach A.R. & Gillet V.J.:
An Introduction to Chemoinformatics
Springer, 2007
- Engel T. & Gasteiger J. (Eds.):
Chemoinformatics – Basic Concepts and Methods
Wiley-VCH, 2018
- Engel T. & Gasteiger J. (Eds.):
Chemoinformatics – Achievements and Future Opportunities
Wiley-VCH, 2018

Key Dates

Oct. 16th

- First Lecture
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Oct. 23rd

- Hand-out of first assignment sheet
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Jan. 8th

- Hand-out of projects
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Jan. 29th

- Hand-in of project reports
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Feb. 5th

- Project presentations
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Exam date(s) to be announced
