

# Drug Design 2

## BIOINF 4372 (6 ECTS credits)

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### Overview

The lecture gives an overview of ligand-based computer-aided drug design. Introduction to cheminformatics key techniques conveys basic skills to understand and solve relevant tasks and problems. Special focus is put on quantitative structure-activity relationships derived from small molecule data. Prior participation in the lecture *Structure-Based Drug Design* (formerly *Drug Design I*) is recommended, although the contents are mostly independent.

### Goals

- Get an overview of Drug Design principles.
- Learn to analyze and interpret chemical information.
- Acquire cheminformatics key techniques and skills.
- Understanding computational challenges in ligand-based drug design and important algorithms to solve them.

### Requirements

- Participation in the weekly problem sessions (date and location tba).
- Individually work on weekly assignment sheets.
- Work on a small research project in a team of 2-3 students. Results have to be documented by a report and an in-class presentation of the project.

### 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 and the project separately are required for admission to the final exam.
- Points achieved in excess of 50% in assignments and projects will serve as a bonus to the final exam, which can improve the final grade up to a maximum of 10%.
- Depending on the number of participants, the final exam can be either a written or an oral exam.

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Summer 2017

Thu 10-12, A104, 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 pages.

Recommended, though not required, textbooks are:

- Klebe:  
*Wirkstoffentwurf*, Spektrum, 2009
- Leach & Gillet:  
*An Introduction to Chemoinformatics*, Springer, 2007
- Jensen:  
*Introduction to Computational Chemistry*, Wiley, 2007

### Key Dates

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**April, 20<sup>th</sup>**

First Lecture,  
hand-out of first assignment sheet

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**June, 1<sup>st</sup>**

Hand-out of the projects

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**July, 20<sup>th</sup>**

Hand-in of project reports

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**July, 27<sup>th</sup>**

Project presentations

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**TBD**

Oral exams

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