Structure-Based Drug Design

BIO-4371 (6 ECTS credits)

Summer 2020

Online Course

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Course Format

- The weekly lectures will be broken down into smaller lessons
- Lessons will be recorded and made available as videos
- To discuss the lecture, a lecture hour is offered by the teacher
- The optional lecture hour will be held as a web conference
- An optional tutorial session will be offered as a web conference
- We will use Zoom and participation links will be published on ILIAS

Content

Starting with a broad introduction of the pharmaceutical drug development process, the lecture conveys key concepts of structure-based computer-aided drug design. Required basics on pharmaceutical key concepts are discussed followed by basic concepts for modeling of 3D structures. In the second part key physicochemical interactions between proteins and ligands are presented, forming the basis to discuss strategies to predict protein-ligand binding with a strong focus on algorithms for protein-ligand docking. Finally, the challenging task of estimating binding affinities *in silico* using so-called scoring functions is introduced

Competences

Knowledge of the drug development process and of pharmaceutical basics. Familiarity with protein-ligand structures and the ability to identify relevant interactions in 3D structures. Knowledge of basic theory and algorithmic techniques to model protein-ligand binding.

Requirements and Evaluation

- Individual work on assignment sheets and hand-in via ILIAS
- We will check for duplicate assignment solutions
- We reserve the right to distribute points across all identical solutions
- Students caught copying solutions can be excluded from the course

Finals and Grading

- Exam admission requires at least 50% of the achievable points
- Assignment points achieved in excess of 50% serve as a bonus
- A bonus improves the final grade but maximally by 10%
- Usually oral exams but written if too many students

Resources

Lecture videos and slides, additional materials, and web conference details will be provided on our ILIAS course pages.

Literature recommendations:

- Klebe, G.: Drug Design, Springer, 2013 (also in German)
- Leach, A.: Molecular Modeling. Principles and Applications, Prentice Hall, 2nd Ed., 2001
- Schlick, T.: Molecular Modeling and Simulation, Springer, 2nd Ed., 2010

Schedule

Publication of Lecture Slides and Videos

Weekly, Sunday 6 pm
First set published on April 19

Lecture Hour

Weekly, Thursday 4 pm

Publication of Assignments

Weekly, Thursday 10 am
Assignment 1 published on April 23

Tutorial Session

Weekly:
Plenum session, Thursday 5 pm
Individual session, booking on ILIAS

Final examinations

Will be held straight after the lecture period (July/August). Concrete exam format and schedule to be announced