Structure-Based Drug Design

BIOINF4371 (6 ECTS credits)

Summer 2020

Thu 4-6 p.m., C215, Sand 14

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Overview

The lecture conveys key concepts of structure-based computer-aided drug design (CADD). In the first part, required basics on pharmaceutical key concepts, the drug discovery process, and 3D structure modeling are introduced. In the second part we discuss protein-ligand interactions and strategies to model protein-ligand binding with a strong focus on algorithms for protein-ligand docking and on scoring functions to estimate binding affinities *in silico*. We will round off the lecture with selected topics from structure-based CADD.

Goals

- Understand the key concepts of modern drug discovery and structure-based CADD in particular.
- Understanding of fundamental methods and algorithms.
- Expertise in handling molecular data and applying state-of-the-art tools in structure-based CADD.
- Elucidation of protein-ligand interactions with docking.

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 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 pages.

Some 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

Key Dates

Apr. 16th

- First Lecture
- Hand-out of first assignment sheet

Jun. 18th

- Hand-out of projects

Jul. 9th

- Hand-in of project reports

Jul. 16th

- Project presentations

To be determined

- Oral exams