

CH-630

Drug Discovery

Cavalli Andrea

Cursus	Sem.	Type
Chemistry and Chemical Engineering		Opt.

Language of teaching	English
Credits	2
Session	
Exam	Oral presentation
Workload	60h
Hours	28
Courses	14
TP	14
Number of positions	25

Frequency

Every year

Remark

Course start 29.9.2025 (recorded EuroTeQ course)

Summary

The course gives an overview of drug discovery. Computational methods in drug design and discovery, including methods for free energy and residence time, drug-target interactions, pharmacodynamics, pharmacokinetics, and drug delivery, biophysical methods, interaction including ITC, SPR, MST, and NMR.

Content

Basic concepts of drug discovery 1h

Structure-based methods in drug discovery (docking, compound libraries, and virtual screening) 1h

From static to dynamical docking 1h

Ligand-based methods in drug discovery (principal component analysis, support vector machine, machine learning, and QSAR) 2h

Physics-based methods in computational drug discovery (molecular dynamics, enhanced sampling methods, free energy and kinetics, and residence time) 2h

Basic concepts of pharmacodynamics (drug-target recognition and interaction) and pharmacokinetics (DM/PK and toxicology) 1h

Basics concepts of drug delivery 1h

Innovative approaches to drug delivery (micelles, nanoparticles, and vectors) 2h

Biophysical methods in drug discovery 1h

Drug-target interactions utilizing biophysical approaches (SPR, ITC, MST, and NMR) 2h

Note

EuroTeQ course

Next time September 29th 2025

The course materials are recorded videos, which can be accessed at any time after the course starts, so this material is time-independent. There will also be 3 hours of Q&A sessions and 14 hrs of practical work sessions which will be time-dependent. These will be rescheduled sessions as soon as they will be agreed by all the instructors.

Keywords

Drug Discovery, Medicinal Chemistry, Computational Chemistry, Drug Delivery, Biophysics, Drug-target interaction, Free Energy and Residence Time, Pharmacodynamics and Pharmacokinetics

Learning Prerequisites

Required courses

(Introductory knowledge of organic chemistry, biochemistry, genetics, computational sciences, and physics)

Learning Outcomes

By the end of the course, the student must be able to:

- Manage the most common software for docking simulations and molecular dynamics. The basics of Python scripting will also be part of the practical exercises.
- Develop knowledge in drug discovery and development, with a particular focus on computational methods, intelligent drug delivery, and biophysical approaches

Resources

Moodle Link

- <https://go.epfl.ch/CH-630>