Level: master

Course title: Rational drug design (IB-503)

Status: elective

ECTS: 6

Requirements: none

Learning objectives

Introduction to modern methods for the rational design of new biologically active molecules, potential drugs.

Learning outcomes

Upon successful completion of this course, the student is able to use the selected "Open Source" software for the rational drug design.

Syllabus

Theoretical instruction

Chemical and biochemical databases of interest for the development of new drugs. Molecular recognition as the basis for rational drug design. Analysis of protein-ligand interactions. The process of drug design when the structure of the target protein is unknown and pharmacophore modelling. Examples of molecular mimicry of known drugs and biomolecules. Drug design when the structure of the target protein is known (structure-based design). Molecular docking and virtual screening. Rational design of HIV-1 protease inhibitors.

Practical instruction

Identification and visualization of pharmacophore and ligand-receptor interactions in *Accelrys Discovery Studio Visualizer* and *Chimera*. Molecular docking using *AutoDock* and *AutoDock Vina*.

Weekly teaching load				Other:
Lectures: 2	Exercises: 2	Other forms of teaching: 1	Student research:	