UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Computational approaches for Structure-Based Drug Design

2526-124R-SCGA.24

Title

Computational approaches for Structure-Based Drug Design

Teacher(s)

Stefano Motta

Language

English

Short description

This course introduces in-silico strategies for the rational design of drug candidates. The course is aimed at PhD students interested in studying small-molecules targeting proteins, DNA or other types of receptors. Program: Introduction to the Drug Design process, Structures of proteins acting as small-molecule receptors, Retrieving 3D structure from PDB and AlphaFold and 3D visualization, Small molecule databases, Hints on Ligand-based Drug Design, The basis of Molecular Modelling: Force Fields, Structure-based Drug Design: Molecular Docking, Virtual Ligand Screening, Molecular Dynamics simulation methods, Optimization of the drug: Pharmacophore models, Chemical Library preparation based on pharmacophore, Optimization of hit compounds, Prediction of the main physico-chemical and ADME properties. During the course real-world case studies showcasing successful

applications of structure-based drug design in the development of therapeutic agents will be presented.

Final evaluation: Students will be required to deliver a presentation based on a scientific article chosen in agreement with the teacher of the course. The presentation will serve as a starting point for an in-depth discussion on the computational approaches employed in the study. This format is designed to foster critical thinking and enhance understanding of the methodologies covered during the course.

CFU / Hours

2 CFU - 16 Hours (Lecture)

Teaching period

I semester

Sustainable Development Goals