

Drug Design (C003088)

Course size *(nominal values; actual values may depend on programme)*

Credits 3.0

Study time 80 h

Course offerings and teaching methods in academic year 2025-2026

A (semester 2)

English

Gent

lecture

seminar

Lecturers in academic year 2025-2026

Savvides, Savvas

WE10

lecturer-in-charge

Mehdipour, Ahmadreza

TW17

co-lecturer

Offered in the following programmes in 2025-2026

Master of Science in Teaching in Science and Technology(main subject Biochemistry and Biotechnology)

crdts

offering

3

A

Master of Science in Bioinformatics(main subject Systems Biology)

3

A

Master of Science in Biochemistry and Biotechnology

3

A

Exchange programme in Biochemistry and Biotechnology (master's level)

3

A

Teaching languages

English

Keywords

protein-protein and protein-ligand interactions, biochemical-biophysical basis of protein-protein and protein-drug interactions, thermodynamics and kinetics of biomolecular interactions, rational drug-design, protein engineering, biologics, small-molecule and protein-based therapeutics.

Position of the course

- The course aims to expose the student to the principles that underlie molecular interactions in biological systems in terms of the affinity and specificity of binding in the context of protein-drug interactions. These concepts are approached from a thermodynamic, kinetic, and structural perspective, and in particular how they relate to the physicochemical properties of water as a universal solvent. Through well chosen case-studies the course will demonstrate the practical applications of such detailed molecular knowledge in structure-based drug design, protein engineering and design, and protein-based therapeutics (antibody and non-antibody protein scaffolds). Finally the course covers the main methods currently used in the development of small-molecule and protein-based therapeutics.

This course contributes to the following program competences: Ma.WE.BB.1.1; Ma.WE.BB.1.2; Ma.WE.BB.1.4; Ma.WE.BB.1.5; Ma.WE.BB.2.1; MA.WE.BB.2.2., Ma.WE.BB.2.6; Ma.WE.BB.3.5; Ma.WE.BB.4.2; MA.WE.BB.7.RES.1, MA.WE.BB.7.RES.2

Contents

- Overview of the drug discovery process: Overview of certain rationally designed drugs and their mode of action. Lead identification and lead optimization. Towards the concept of affinity in protein-drug interactions. Indirect methods: IC50 plots and the Cheng Prusov equations. Direct methods: Isothermal Titration Calorimetry (ITC) and Surface Plasmon Resonance (SPR).
- ITC and SPR: Historical background. Instrumentation and Principles of measurement. Experimental design. Data analysis. Informational content of ITC/SPR data. Case studies: (1) Specificity of Citrate binding to the Histidine Autokinase CitA receptor. (2) Structural and thermodynamic basis for the

emergence of drug resistance. HIV protease inhibitors

- Structure based drug design: Introduction. Key Point considerations and difficulties. Prediction of binding energetics. Case study: Anti-HIV protease: Amprenavir and Nelfinavir development
- Protein-Protein interactions: Introduction and overview. Optimization of interacting surfaces. SPR in determining kinetic binding constants k_{on} and k_{off} . Case study: Receptor-cytokine interactions
- Therapeutic targeting of protein-protein interactions

Initial competences

Biochemistry, structure-function relationships of proteins, enzymology

Final competences

- 1 To obtain insights into the process of therapeutic compounds.
- 2 To obtain insights into the forces, thermodynamics, and kinetics of (bio) molecular binding.
- 3 To obtain insights into protein engineering in the context of biotechnology and drug-design.
- 4 To obtain insights into protein engineering, and protein-based therapeutics.
- 5 To be able to critically read research articles in the field of protein engineering and structure-based drug design.

Conditions for credit contract

Access to this course unit via a credit contract is determined after successful competences assessment

Conditions for exam contract

This course unit cannot be taken via an exam contract

Teaching methods

Seminar, Lecture

Study material

Type: Slides

Name: Slides, review- and research articles'

Indicative price: € 10

Optional: no

Additional information: via Ufora

References

X

Course content-related study coaching

Appointment with the lecturer

Assessment moments

continuous assessment

Examination methods in case of periodic assessment during the first examination period

Examination methods in case of periodic assessment during the second examination period

Examination methods in case of permanent assessment

Assignment

Possibilities of retake in case of permanent assessment

examination during the second examination period is possible

Extra information on the examination methods

The exam will be completed independently by each student against a specified deadline and will be submitted online according to specified instructions and format.

Calculation of the examination mark

Evaluation methods: Assignment 100%

