

Comparative Study of Drug Discovery Approaches and Technologies (J000527)

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

Credits 6.0 **Study time 150 h**

Course offerings and teaching methods in academic year 2025-2026

A (semester 1)	English	Gent	lecture
			group work
			independent work

Lecturers in academic year 2025-2026

Hertleer, Carla	FW02	staff member
Van Calenbergh, Serge	FW01	lecturer-in-charge
Mehdipour, Ahmadreza	TW17	co-lecturer

Offered in the following programmes in 2025-2026

	crdts	offering
International Master of Science in Sustainable Drug Discovery	6	A
Exchange Programme Faculty of Pharmaceutical Sciences	6	A

Teaching languages

English

Keywords

drug discovery approaches and technologies, lead discovery

Position of the course

There is not a general applicable method or recipe to discover small-molecule drugs. Depending on the pre-existing knowledge of the target disease (phenotypic hits, target/pathway involvement/validation, structural knowledge of the target, etc.) different routes may be followed towards new lead compounds. This course aims at exposing the students to state-of-the-art approaches and technologies that may be used to discover or design small-molecule pharmacological agents (lead generation).

Contents

The course will involve the following topics:

- Why small molecules are still a big deal
- Phenotypic drug discovery vs target-based drug discovery
- High-throughput screening and physical methods to assess affinity and binding kinetics
- Searching compounds and synthesis methods with SciFinder
- Introduction to computational drug design
 - Ligand-based approaches
 - Quantitative structure-activity relationship (QSAR)
 - Pharmacophore modeling
- Bioinformatics approaches (target recognition and structural modeling)
 - Sequence alignments and searches
 - Target identification and prediction
 - PDB database, Machine learning- and template-based protein structure prediction
- Structure-based approaches
 - Druggability assessment (druggable pockets)

- Docking and virtual screening
 - Molecular dynamics simulation
 - Fragment-based drug discovery
 - Targetted covalent inhibitors
 - PROTACs
- Prodrugs
- Optional: hot topic in drug discovery

Initial competences

General and Organic Chemistry, Biochemistry, physiology

Final competences

- 1 To possess critical insights into methods and technologies used for identifying and designing small-molecule therapeutics.
- 2 To decide which technologies are suited to tackle particular challenges.
- 3 To obtain insights into the forces, thermodynamics, and kinetics of (bio) molecular binding.
- 4 To be able to critically read research articles in the field of structure-based drug design and to present these.

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

Group work, Seminar, Lecture, Independent work

Extra information on the teaching methods

lecture 27,5h

seminar 10h

independent or group assignment 5h

Study material

Type: Slides

Name: Slides Comparative

Indicative price: Free or paid by faculty

Optional: no

Language : Dutch

Number of Slides : 400

Oldest Usable Edition : 2024

Available on Ufora : Yes

Online Available : No

Available in the Library : No

Available through Student Association : No

References

Course content-related study coaching

Guidance of students in discussing and presenting a relevant paper

Assessment moments

end-of-term and continuous assessment

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

Skills test, Written assessment with open-ended questions

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

Assignment

Examination methods in case of permanent assessment

Participation, Assignment

Possibilities of retake in case of permanent assessment

examination during the second examination period is not possible

Calculation of the examination mark

The permanent activities, culminating in an oral presentation and/or a written report are responsible for 10% of the course score.

The permanent examination at the end of the semester is responsible for the other 90% of the points.

Students who eschew period aligned and/or non-period aligned evaluations for this course unit may be failed by the examiner.