

Comparative Study of Drug Discovery Approaches and Technologies (J000527)

Cursusomvang (nominale waarden; effectieve waarden kunnen verschillen per opleiding)

Studiepunten 6.0

Studietijd 150 u

Aanbodsessies en werkvormen in academiejaar 2025-2026

A (semester 1)

Engels

Gent

hoorcollege

groepswork

zelfstandig werk

Lesgevers in academiejaar 2025-2026

Van Calenbergh, Serge

FW01

Verantwoordelijk lesgever

Hertleer, Carla

FW02

Medewerker

Mehdipour, Ahmadreza

TW17

Medelesgever

Aangeboden in onderstaande opleidingen in 2025-2026

[International Master of Science in Sustainable Drug Discovery](#)

stptn

aanbodsessie

6

A

[Uitwisselingsprogramma Faculty of Pharmaceutical Sciences](#)

6

A

Onderwijstalen

Engels

Trefwoorden

drug discovery approaches and technologies, lead discovery

Situering

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).

Inhoud

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

Begincompetenties

General and Organic Chemistry, Biochemistry, physiology

Eindcompetenties

- 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.

Creditcontractvoorwaarde

Toelating tot dit opleidingsonderdeel via creditcontract is mogelijk na gunstige beoordeling van de competenties

Examencontractvoorwaarde

Dit opleidingsonderdeel kan niet via examencontract gevolgd worden

Didactische werkvormen

Groepswerk, Werkcollege, Hoorcollege, Zelfstandig werk

Toelichtingen bij de didactische werkvormen

hoorcollege 27,5u

werkcollege 10u

zelfstandig werk of groepswerk 5u

Studiemateriaal

Type: Slides

Naam: Slides Comparative

Richtprijs: Gratis of betaald door opleiding

Optioneel: nee

Taal : Nederlands

Aantal slides : 400

Oudst bruikbare editie : 2024

Beschikbaar op Ufora : Ja

Online beschikbaar : Nee

Beschikbaar in de bibliotheek : Nee

Beschikbaar via studentenvereniging : Nee

Referenties

Vakinhoudelijke studiebegeleiding

Guidance of students in discussing and presenting a relevant paper

Evaluatiemomenten

periodegebonden en niet-periodegebonden evaluatie

Evaluatievormen bij periodegebonden evaluatie in de eerste examenperiode

Vaardigheidstest, Schriftelijke evaluatie met open vragen

Evaluatievormen bij periodegebonden evaluatie in de tweede examenperiode

Werkstuk

Evaluatievormen bij niet-periodegebonden evaluatie

Participatie, Werkstuk

Tweede examenkans in geval van niet-periodegebonden evaluatie

Examen in de tweede examenperiode is niet mogelijk

Eindscoreberekening

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.