GHENT UNIVERSITY

Course Specifications

Valid as from the academic year 2024-2025

Molecular Scale Modelling in Bio(medical) Engineering (E074500)

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

Credits 6.0 **Study time 180 h**

Course offerings in academic year 2025-2026

A (semester 1)	English	Gent

Lecturers in academic year 2025-2026

Mehdipour, Ahmadreza	TW17	lecturer-in-charge
Ghysels, An	TW06	co-lecturer

Offered in the following programmes in 2025-2026	crdts	offering
Master of Science in Biomedical Engineering	6	A
Master of Science in Biomedical Engineering	6	A

Teaching languages

English

Keywords

Nanoscale modeling, molecular dynamics simulations, computational drug design, drug delivery systems, machine learning

Position of the course

Computational modeling of biomedical processes such as drug-target interaction is one of the emerging fields in biomedicine, providing a complementary and quantitative tool to experiments which may be limited in temporal and spatial resolution. Molecular dynamics simulations and machine-learning based approaches are emerging as powerful methods for studying biomedical problems. This course covers the basics of these computational methods and their application in biomedicine.

Contents

1 Introduction to the Molecular scale modelling (Introductory practical session)
2 Drug development
  1 Introduction to structural biology (Practical session 1)
  2 Introduction (Recap) to statistical mechanic
  3 Molecular dynamics simulations (Practical session 2)
  4 Free energy calculation (Alchemical transformation)
  5 Docking (Practical session 3)
  6 Machine Learning/Artificial Intelligence (Practical session 4)
  7 Coarse graining (Theory)
  8 Coarse graining (applications): Drug delivery systems (Practical session 5)
3 Kinetics of life processes
  1 Theory I: Diffusion
  2 Theory II: Enhanced sampling methods
  3 Application: membrane transport (Practical session 6)

Initial competences

The students have studied molecular structure, thermodynamics and statistical mechanics. Competency in computer and programming.

Final competences

1 The student masters the basics of the molecular dynamics simulations and coarse-graining methods.
2 The student is able to use different Machine Learning and Artificial Intelligence

methods within the context of molecular modelling and drug design.

3 The student can apply various computer packages to model a biomolecular system using appropriate simulation methods and high-performance computing infrastructure.

4 The student can critically analyze and interpret simulation results and has a thorough understanding of the strengths and shortcomings of applied modeling approaches.

5 The student can present project results in writing as well as orally and critically assess them.

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, Independent work

Study material

None

References

Course content-related study coaching

Assessment moments

end-of-term and continuous assessment

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

Written assessment

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

Written assessment

Examination methods in case of permanent assessment

Presentation, Assignment

Possibilities of retake in case of permanent assessment

examination during the second examination period is possible

Extra information on the examination methods

- End of term evaluation (Written) (Individual)
- Assignment during the practical (Individual)
- Presentation assignment (an advanced subject to be presented in a short oral presentation) (Individual or group)

Calculation of the examination mark