

# Course Specifications

Valid as from the academic year 2025-2026

# Molecular Simulations of Biosystems (C002727)

Course size	(nominal values; actual valu	es may depend on pro	igramme)		
Credits 3.0	Study time 80 h				
Course offerings and t	eaching methods in academic	year 2025-2026			
A (semester 1)	English	inglish Gent le		ture	
		sen			
Lecturers in academic	year 2025-2026				
Verstraelen, Toon			WE05	lecturer-in-charge	
Savvides, Savvas			WE10	co-lecturer	
Offered in the following programmes in 2025-2026				crdts	offering
Master of Science in Teaching in Science and Technology(main subject Biochemistry and				3	А
Biotechnology)					
Master of Science	e in Biochemistry and Biotechnol	ogy		3	A
Exchange programme in Biochemistry and Biotechnology (master's level)				3	А

#### Teaching languages

English

#### Keywords

Proteïnes en DNA, moleculaire dynamica, krachtvelden, uncertainty quantification, principal component analysis, high performance computing

#### Position of the course

The function of biological macromolecules is determined by their three-dimensional structure and dynamics. With molecular simulations, it is possible to calculate these microscopic properties and to link them to macroscopic variables, such as thermodynamic properties. Molecular modeling is increasingly used as a valuable tool by biologists and (bio)chemists. Due to the ever-increasing computer capabilities, these simulations have become accessible to end-users. In addition, simulations can often provide answers to fundamental scientific questions in a relatively inexpensive way, not requiring many (costly) chemical reactions or purifications. Within the academic world but also in the industry, modeling is frequently applied to biomolecules such as proteins, polynucleotides, pharmaceuticals, pesticides, etc.

Competence codes: Ma.WE.BB.1.1, Ma.WE.BB.1.3, Ma.WE.BB.2.1, Ma.WE.BB.2.4, Ma.WE.BB.2.6, Ma.WE.BB.3.2, Ma.WE.BB.3.5, Ma.WE.BB.4.3, Ma. WE.BB.6.1

#### Contents

In the lectures, the underlying principles are introduced of the techniques applied in the practical sessions; the aim is to understand, not to be able to reproduce. Moreover, the lectures are structured entirely in function of the computational applications. In the practical sessions, conventional packages in the field will be used: OpenMM, Jupyter Notebookes, NGLView, VMD, ... – all freely available for academic users.

1 Construction of a molecular model: the structure of a pdb file, visualization

- 2 Description of atomic/molecular interactions in biomolecular systems: classic (forcefields)
- 3 Molecular dynamics: minimization, equilibration, annealing
- 4 Analysis of dynamics: energy contributions, RMSD, normal mode analysis, principal component analysis

Students cary out their calculations at the VSC Tier-2 high performance cluster at

#### Ghent University.

#### Initial competences

Basic (bio)chemistry and Python programming

### **Final competences**

- 1 Understand and reproduce recent scientific literature, and implement these
- methods in own research.
- 2 Independently set up a computer simulation and perform a meaningful analysis.
- 3 Directly connect with the current research of different labs at home and abroad.

#### 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

#### Extra information on the teaching methods

The theory lessons are given in the form of lectures. Tutorials consist of solving computational projects under supervision and independently, in which the theory is applied.

#### Study material

#### Type: Slides

Name: Molecular Simulations of Biosystems Indicative price: Free or paid by faculty Optional: no Language : English Number of Slides : 160 Available on Ufora : Yes Online Available : Yes Available in the Library : No Available through Student Association : No

#### Type: Other

Name: OpenMM tutorial for the MSBS course Indicative price: Free or paid by faculty Optional: no Language : English Author : Jelle Vekeman en Toon Verstraelen Available on Ufora : No Online Available : Yes Available in the Library : No Available through Student Association : No Usability and Lifetime within the Course Unit : not applicable Usability and Lifetime within the Study Programme : intensive Additional information: https://github.com/molmod/openmm-tutorial-msbs

#### References

Martin J. Field, "A Practical Introduction to the Simulation of Molecular Systems", Cambrigde University Press Andreas Kukol, "Molecular Modeling of Proteins", Humana Press

#### Course content-related study coaching

Solving computational projects under supervision. Possibility to ask questions before, during and after the lesson, and online.

#### Assessment moments

end-of-term assessment

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

#### Oral assessment, Assignment

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

Oral assessment, Assignment

#### Examination methods in case of permanent assessment

# Possibilities of retake in case of permanent assessment

not applicable

#### Extra information on the examination methods

Projects: a project-paper is required and the project is defended in a short oral presentation.

# Calculation of the examination mark

100% project

# Facilities for Working Students

No additional facilities