University of Gdańsk

Subject card

Subject name and code	Principles of the molecular modeling, PG_00193186		
Field of study	Biotechnology		
Date of commencement of studies	October 2025	Academic year of realisation of subject	2025/2026
Education level	Bachelor's studies	Subject group	Obligatory subject group in the field of study Optional subject group Subject group related to scientific research in the field of study
Mode of study	full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	Polish
Semester of study	2	ECTS credits	2.0
Learning profile	academic	Assessment form	credit
Conducting unit	Laboratory of Biophysics -> UG Institute of Biotechnology -> Intercollegiate Faculty of Biotechnology UG-MUG -> Rector		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Rajmund Kaźmierkiewicz, prof. UG	
	Teachers	dr hab. Rajmund Kaźmierkiewicz, prof. UG	

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	15.0	0.0	15.0	0.0	0.0	30

E-learning hours included: 0.0

Learning activity and number of study hours

Learning activity	Participation in didactic classes included in study plan	Participation in consultation hours	Self-study	SUM
Number of study hours	30	0.0	0.0	30

Subject objectives

The aim of the course is to familiarize course participants with practical information on creating computer models of chemical molecules, to acquire the ability to use available programs, to read and understand program instructions, to be able to plan activities leading to the creation of a realistic theoretical model of a phenomenon occurring in a cell, and to be able to critically evaluate and verification of results.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[BIOTECHL3_U03] The graduate applies mathematical and statistical methods to describe phenomena and analyze data and is able to use professional databases used in biotechnology.	The course participant is able to apply basic methods used for molecular modeling. They can dock small molecules and create models of protein complexes as well as protein–nucleic acid complexes. They also possess the ability to analyze molecular dynamics results.	[SU4] test/exam - oral or written

Subject contents

Familiarization with the capabilities of the Linux system and with programs and elementary concepts related to constructing, saving, reading and "manipulating" molecular models used in Molecular Mechanics. Calculation of electrostatic potential, energy minimization (optimization of molecular starting structures), use of a simplified energy function potential (so-called "soft" potential). in the ECEPP/3 force field, Applications of the molecular dynamics method in the AMBER force field. Monte-Carlo method, cluster analysis for a large number of conformations. Application of vibration analysis of normal molecules. Docking small molecules and creating models of protein and protein-nucleic acid complexes. Molecular dynamics using conformational freedom constraints derived from experimental results. (so-called restrains, constraints). Minimization and Simulated annealing. Using the penalty function. Detailed analysis of molecular dynamics results.

Prerequisites and co-requisites

Basic computer skills are required

<table>
<tr><td>Assessment methods and criteria</td><td colspan="2"><table>
<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>Written test with open questions and test cases</td><td>51.0%</td><td>50.0%</td></tr>
<tr><td>10 exercise reports</td><td>51.0%</td><td>50.0%</td></tr>
</table></td></tr>
<tr><td rowspan="3">Recommended reading</td><td>Basic literature</td><td>Textbook, "INTRODUCTION TO MOLECULAR MODELING", Rajmund Kaźmierkiewicz, Intercollegiate Faculty of Biotechnology UG-MUG, Gdańsk
2011</td></tr>
<tr><td>Supplementary literature</td><td>Understanding Molecular Simulation: From Algorithms to Applications (Second Edition), Daan Frenkel</td></tr>
<tr><td>eResources addresses</td><td></td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td colspan="2">1. What is the internal coordinate of a molecule? 2. Explain the concept of protein sequence overlap. 3. What number of internal coordinates should be used to fully describe: a) distances (bond lengths), b) valence angles, c) torsion angles in a methane molecule? 4. What program can be used to translate the Cartesian coordinates of a molecule into its internal coordinates? 5. What do you understand by the term conformation of a molecule, e.g. a protein? 6. Suggest at least two ways to experimentally verify the correctness of predictions of the conformation of any molecule. 7. Explain the term "empirical force field". 8. What can be useful for (in molecular modeling) the so-called "standard residue database", which is usually attached to the force field? 9. What are some examples of the names of empirical force fields, and what are the differences between the functions describing the potential energy of molecules in these force fields? 10. In what sense is the term "energy map" used in molecular mechanics, and how does it relate to the Ramachandran diagram? 11. Explain the concept of "contact map" between C carbon atoms, used to alternatively describe the conformation of a protein. 12. What is a "binding effect"? 13. What is "non-binding impact"? 14. For what purpose is the so-called effective range of interactions (cut-off) used in molecular mechanics? 15. One of the components of the energy of non-bonding interactions is often described using the Van der Waals formula. Write it and explain the meaning of the symbols in it. 16. Write a formula describing the potential energy of any molecule, e.g. water. 17. Name three types of force field parameters, give their brief description. 18. What do you understand by "limitations of conformational freedom"? 19. What are the "problems" with correctly considering electrostatic interactions in molecular mechanics? 20. Explain what "minimization" of the energy of a physical system, e.g. a molecule, is? 21. What is the "conjugate gradients" method used in molecular mechanics? 22. What is the difference between local minima on the surface described by the energy function and its global minimum?</td></tr>
<tr><td>Work placement</td><td colspan="2">Not applicable</td></tr>
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