

Subject card

Subject name and code	Basics of the molecular modeling, PG_00153667						
Field of study	Biotechnology						
Date of commencement of studies	October 2024	Academic year of realisation of subject			2024/2025		
Education level	undergraduate studies		Subject group				
Mode of study	full-time studies		Mode of delivery		at the university		
Year of study	1		Language of instruction		Polish Some content is provided in English. Also, most of the program instructions are written in English.		
Semester of study	2		ECTS credits		2.0		
Learning profile	academic		Assessment form				
Conducting unit	Pracownia Biofizyki -> Instytut Biotechnologii UG -> Intercollegiate Faculty of Biotechnology UG-MUG						
Name and surname of lecturer (lecturers)	Subject supervisor		dr hab. Rajmund Kaźmierkiewicz				
	Teachers						
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		10.0		20.0	60
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 is able to use basic mathematical and statistical methods to describe phenomena and analyse data; analyse basic data in professional databases used in biotechnology		The course participant has basic skills in using basic mathematical and statistical methods to describe phenomena and analyze data enabling the description of simple relationships in biological processes using methods used in molecular modeling.		[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						
Assessment methods and criteria	Subject passing criteria		Passing threshold		Percentage of the final grade		
	Written test with open questions and test cases		51.0%		50.0%		
	10 exercise reports		51.0%		50.0%		

Recommended reading	Basic literature	Textbook, "INTRODUCTION TO MOLECULAR MODELING", Rajmund Kaźmierkiewicz, Intercollegiate Faculty of Biotechnology UG-MUG, Gdańsk 2011
	Supplementary literature	Understanding Molecular Simulation: From Algorithms to Applications (Second Edition), Daan Frenkel
	eResources addresses	Adresy na platformie eNauczanie:
Example issues/ example questions/ tasks being completed	<p>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?</p>	
Work placement	Not applicable	

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