



Subject card

Subject name and code	PRACTICAL BASES OF THE MOLECULAR MODELING, PG_00063485						
Field of study	Biotechnology						
Date of commencement of studies	October 2025	Academic year of realisation of subject			2025/2026		
Education level	second-cycle studies	Subject group			Optional subject group Specialty 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			3.0		
Learning profile	general academic profile	Assessment form			assessment		
Conducting unit	Department Of Pharmaceutical Technology And Biochemistry -> Faculty Of Chemistry -> Wydział Politechniki Gdańskiej						
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. inż. Marek Wojciechowski					
	Teachers						
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	30.0	0.0	0.0	45
	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	45	10.0		20.0		75
Subject objectives	The goal of this lecture is to familiarize students with basics of modern molecular modeling of biomolecules and their interactions. The lectures cover modeling of small molecules, macromolecules and their complexes. Students get acquainted with capabilities of popular modeling tools. They learn methods of complex data analysis and presenting results in a clear form.						
Learning outcomes	Course outcome	Subject outcome			Method of verification		
	[K7_K02] is aware of the potential risks and opportunities associated with the development of science and technology for the natural environment and society	Student is aware of the rapid development of this field of science and is aware of the need to constantly update his knowledge in the field of molecular modeling			[SK5] Assessment of ability to solve problems that arise in practice		
	[K7_U06] plans research and designs biotechnological products and processes taking into account legal regulations and bioethical principles	Student is able to apply statistical and computer methods to plan computational experiments in the field of molecular modeling and analyze their results			[SU4] Assessment of ability to use methods and tools [SU1] Assessment of task fulfillment		
	[K7_W04] selects methods of data analysis, including bioinformatics, statistical and molecular modeling, useful for solving technological and scientific problems in biotechnology and related fields	The student is familiar with the theoretical basis of the most important computational techniques used in molecular modeling and knows the basic programs in which they can be used			[SW3] Assessment of knowledge contained in written work and projects		
Subject contents	Building and visualization of molecules. Common molecular data formats. Molecular surfaces. Empirical model of interactions. Molecular mechanics and forcefields. Conformational analysis. Molecular dynamics. Monte Carlo method. Sparse models of interactions. Molecular docking and intermolecular interactions. Protein structure modeling.						
Prerequisites and co-requisites	No requirements						
Assessment methods and criteria	Subject passing criteria	Passing threshold			Percentage of the final grade		
	Theoretical exam	60.0%			50.0%		
	Practical test	60.0%			50.0%		
Recommended reading	Basic literature	Educational materials provided by the lecturer					

	Supplementary literature	A. R. Leach Molecular Modelling Principles and Applications,
	eResources addresses	Adresy na platformie eNauczanie:
Example issues/ example questions/ tasks being completed	<ul style="list-style-type: none"> - force fields in molecular modeling - stochastic methods in molecular modeling - the problem of boundary conditions in molecular modeling - the basic steps of protein structure prediction 	
Work placement	Not applicable	

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