



Subject card

Subject name and code	Practical Bases of the Molecular Modelling, PG_00039064						
Field of study	Biotechnology						
Date of commencement of studies	February 2023		Academic year of realisation of subject		2022/2023		
Education level	second-cycle studies		Subject group		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	1		ECTS credits		3.0		
Learning profile	general academic profile		Assessment form		assessment		
Conducting unit	Department of Pharmaceutical Technology and Biochemistry -> Faculty of Chemistry						
Name and surname of lecturer (lecturers)	Subject supervisor		dr hab. inż. Marek Wojciechowski				
	Teachers		dr hab. inż. Marek Wojciechowski				
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_W04] has a structured knowledge of the application of informatics tools in biotechnology and molecular modeling of biomolecules		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		
	[K7_K02] is aware of the limitations and the necessity of continuous development of knowledge and technology; understands the need for education and constant training		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] is able to apply statistical methods, computer solutions, especially bioinformatics methods to design experiments and technologies, analyze experimental results and technological processes and solve problems in the field of biotechnology, is able to use biotechnological databases		Student is able to apply statistical and computer methods to plan computational experiments in the field of molecular modeling and analyze their results.		[SU1] Assessment of task fulfilment [SU4] Assessment of ability to use methods and tools		
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
	Practical test	60.0%	50.0%
	Theoretical exam	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: Praktyczne Podstawy Modelowania Molekularnego - 2023 - Moodle ID: 27463 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=27463	
Example issues/ example questions/ tasks being completed	- 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		