

## 。 GDAŃSK UNIVERSITY OF TECHNOLOGY

## Subject card

Subject name and code	MOLECULAR MODELLING, PG_00038906								
Field of study	Chemistry								
Date of commencement of studies	,		Academic year of realisation of subject			2025/2026			
Education level	second-cycle studies		Subject gro	Subject group			Optional subject group		
Mode of study	Full-time studies		Mode of de	elivery		at the	at the university		
Year of study	1		Language of instruction			Polish	Polish		
Semester of study	2		ECTS credits			3.0			
Learning profile	general academic profile		Assessment form			assessment			
Conducting unit	Department of Pharm	aceutical Tech	nology and Bio	ochemistry -> F	aculty o	of Chen	nistry		
Name and surname	Subject supervisor		prof. dr hab. inż. Maciej Bagiński						
of lecturer (lecturers)	Teachers								
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Projec	t	Seminar	SUM	
	Number of study hours	15.0	0.0	30.0	0.0		0.0	45	
	E-learning hours inclu	uded: 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 45 hours			5.0		25.0		75	
Subject objectives	The aim of the course is to familiarize students with selected topics in the field of molecular modeling, which can be useful in carrying out the thesis and may also serve as the basis for specific items on the third level studies. The strategic objective will be achieved through assimilation of theoretical knowledge as well as practical execution of tasks within the project. Presented the content of education in the subject encouraged to broaden the knowledge by the use of electronic resources and indicated Recommended reading.								
Learning outcomes	Course outcome		Subject outcome			Method of verification			
	K7_W02		-has knowledge about the molecular properties of simple organic molecules as well as biopolymers -understands the nature of interactions between biomolecules and is able to analyze these interactions			[SW1] Assessment of factual knowledge			
	K7_U01		-can find literature source information about the tested model -can critically compare literature data with the results of molecular modeling simulations			[SU2] Assessment of ability to analyse information			
	K7_W05		-has knowledge about the molecular properties of simple organic molecules as well as biopolymers -understands the nature of interactions between biomolecules and is able to analyze these interactions			[SW1] Assessment of factual knowledge			

Subject contents	Introduction to the course and discuss its scope Biological and molecular systems as a matter of molecular modeling Molecular properties tested in silico Construction of molecular models Overview of molecular modeling Overview of software and Internet resources for molecular modeling Basic molecular mechanics and dynamics Force fields in molecular mechanics and dynamics Conformational analysis of molecular systems Electrostatic properties of molecular systems Analysis of intermolecular interactions Fundamentals of computer-aided molecular design Molecular Docking De novo design of ligands Test on the knowledge gained in the lecture							
Prerequisites	1. General Chemistry							
and co-requisites	1.1. Chemical bonding, intermolecular interactions							
	1.2. Properties of water, aqueous solutions							
	2. Organic and physical chemistry							
	2.1. Organic compounds							
	2.2. Thermodynamics							
	3. Biophysics							
	3.1. Molecular systems							
	3.2. Molecular properties of biopolymers							
	3.3. Eelectrostatics							
	4. Biochemistry							
	4.1. Construction of biopolymers (DNA, protein)							
Assessment methods	Subject passing criteria	Passing threshold	Percentage of the final grade					
and criteria	lecture (test)	60.0%	70.0%					
	project	60.0%	30.0%					
Recommended reading	Basic literature	<ol> <li>CH.I. Brookes III, M. Karplus. B.M. Pettitt, Proteins, perspective of dynamics, structure, and thermodynar Advances in Chemical Physics Volume LXXI, John W New York 1988</li> <li>D.W. Heermann, Podstawy symulacji komputerowy WNT, Warszawa 1997</li> </ol>						
		3. Ch. J. Cramer, Essentials of Computational Chemistry, theo and models, John Wiley & Sons, New York, 2002						
		4. D. Frenkel, B. Smit, Understanding molecular simulation, from algorithms to applications, Academic press, San Diego 2002						
		5. T. Schlick, Interdisciplinary Applied Mathematics, Vol. 21, Molecular Modeling and Simulation: An Interdisciplinary Guide, Springer, 2010 (e-book).						
		6. J. Czub, Molekularne aspekty aktywności biolog amfoterycyny B i jej pochodnych o podwyższonej badania z zastosowaniem metod chemii obliczenie doktorska, PG 2008. <u>http://www.pg.gda.pl/~chemn</u> <u>doktorat_Czub.pdf</u>						
	Supplementary literature	A number of scientific publications and teaching materials prepared by the teacher.						
	eResources addresses	Adresy na platformie eNauczanie:						

example questions/ tasks being completed	molecular dynamics
	molecular mechanics
	intermolecular interactions
	molecular docking
Work placement	Not applicable

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