

GDAŃSK UNIVERSITY

Subject card

Subject name and code	MOLECULAR MODELLING, PG_00038906								
Field of study	Chemistry								
Date of commencement of studies	February 2024		Academic year of realisation of subject			2024/2025			
Education level	second-cycle studies		Subject group			Optional subject group			
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								
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	ided: 0.0		;					
Learning activity and number of study hours	Learning activity	Participation i classes incluc plan		Participation in consultation hours		Self-study		SUM	
	Number of study hours	45		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_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			
	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_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			

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 and co-requisites	 General Chemistry General Chemistry Chemical bonding, intermolecular interactions Properties of water, aqueous solutions Organic and physical chemistry Organic compounds Thermodynamics Biophysics Molecular systems Molecular properties of biopolymers Electrostatics 						
	4. Biochemistry4.1. Construction of biopolymers (DNA, protein)						
Assessment methods and criteria	Subject passing criteria project lecture (test)	Passing threshold 60.0% 60.0%	Percentage of the final grade 30.0% 70.0%				
Recommended reading	Basic literature	 Chiefe (1997) CH.I. Brookes III, M. Karplus. B.M. Pettitt, Proteins, a theoretical perspective of dynamics, structure, and thermodynamics, Advances in Chemical Physics Volume LXXI, John Wiley & Sons, New York 1988 D.W. Heermann, Podstawy symulacji komputerowych w fizyce, WNT, Warszawa 1997 Ch. J. Cramer, Essentials of Computational Chemistry, theories and models, John Wiley & Sons, New York, 2002 D. Frenkel, B. Smit, Understanding molecular simulation, from algorithms to applications, Academic press, San Diego 2002 T. Schlick, Interdisciplinary Applied Mathematics, Vol. 21, Molecular Modeling and Simulation: An Interdisciplinary Guide, Springer, 2010 (e-book). J. Czub, Molekularne aspekty aktywności biologicznej amfoterycyny B i jej pochodnych o podwyższonej selektywności badania z zastosowaniem metod chemii obliczeniowej. Praca doktorska, PG 2008. <u>http://www.pg.gda.pl/~chemmbag/</u> doktorat. Czub.pdf 					
	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