GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	MOLECULAR MODELING OF BIOMOLECULES, PG_00063476		
Field of study	MODELOWANIE MOLEKULARNE BIOMOLEKUŁ		
Date of commencement of studies	October 2024	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	2	Language of instruction	Polish Polish
Semester of study	3	ECTS credits	2.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Pharmaceutical Technology and Biochemistry -> Faculty of Chemistry -> Wydziały Politechniki Gdańskiej		
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. inż. Maciej Bagiński	
	Teachers	prof. dr hab. inż. Maciej Bagiński	

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	15.0	0.0	0.0	15.0	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	2.0	18.0	50

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 in the field of drug design 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 implementation of tasks in the laboratory.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K7_U04] predicts the interaction of biomolecules and biologically active compounds on living organisms and the course of processes involving them based on knowledge in biology, biotechnology and related fields and computer methods of data analysis, modeling and simulation	- understands the molecular structure of biomolecules - understands the relationships between biological molecules - understands cause-and-effect pathways at the molecular level	[SU3] Ocena umiejętności wykorzystania wiedzy uzyskanej w ramach przedmiotu [SU2] Ocena umiejętności analizy informacji
[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	-- has knowledge of basic molecular methods - is able to use some molecular modeling methods in practice - is able to analyze the results of molecular modeling for biomolecules	[SW3] Ocena wiedzy zawartej w opracowaniu tekstowym i projektowym [SW1] Ocena wiedzy faktograficznej

Subject contents	• - Introduction and definition what it is a molecular dynamics and its historical background. • - Definition and characteristics of static and dynamics molecular properties of biomolecules (biopolymers and small organic molecules). • - Definition and characteristics of inter- and intra-molecular interactions. • - Areas and limitations of application of molecular modeling with regard to advancement of different methods. • - Force-fields definition and examples. • - Molecular mechanics and dynamice. • - Overview of molecular mechanics and dynamics software. • - Electrostatic interactions and solvation models applied in molecular modeling. • - Examples of application of molecular dynamics (biopolymers). • - Examples of application of molecular dynamics in simulations of model biological membranes. • - Free energy calculations. • - Molecular docking. • - Modeling of interactions between ligands and molecular targets. • - Computer-aided drug design as well as design other small molecules exhibited required molecular properties. • - AI methods in drug design - Learning molecular modeling software - Performing a series of simple simulations to learn practical applications of molecular modeling - Analyzing the results obtained from simple simulations - Performing a given design simulation for a final exam
Prerequisites and co-requisites	Students have to complete previously courses: physical chemistry, mathematics, biochemsitry and biophysics.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
test - lecture	60.0%	70.0%
laboratory - practical test	60.0%	30.0%

Recommended reading

Basic literature

1. **CH.I. Brookes III, M. Karplus. B.M. Pettitt, Proteins, a theoretical perspective of dynamice, structure, and thermodynamics, Advances in Chemical Physics Volume LXXI, John Wiley & Sons, New York 1988**
2. **D.W. Heermann, Podstawy symulacji komputerowych w fizyce, WNT, Warszawa 1997**
3. **Ch. J. Cramer, Essentials of Computational Chemistry, theories 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 biologicznej amfoterycyny B i jej pochodnych o podwyższonej selektywności badania z zastosowaniem metod chemii obliczeniowej. Praca doktorska, PG 2008.**
7. Simone Brogi, Teodorico Castro Ramalho, José L. Medina-Franco, Kamil Kuca and Marian ValkoIn silico methods in drug design and discovery. Frontiers in Chemistry, 2020 (DOI: 10.3389/978-2-88966-057-5).
8. Marco Tutone and Anna Maria Almerico, Computational Approaches Drug Discovery and Design in Medicinal Chemistry and Bioinformatics, MDPI 2021 (ISBN: 978-3-0365-2779-6; 978-3-0365-2778-9).
9. Rebecca C. Wade and Outi M. H. Salo-Ahen, Molecular Modeling in Drug Design, MDPI 2019 (ISBN: 978-3-03897-615-8)
10. Jerzy Leszczynski, Handbook of Computational Chemistry, Springer 2012 (ISBN: 978-94-007-0711-5; 978-94-007-0712-2; 978-94-007-0710-8) 5.Giovanni Ciccotti, Mauro Ferrario and Christof Schuette, Molecular Dynamics Simulation, MDPI 2014 (ISBN: 978-3-906980-65-2; 978-3-906980-66-9). 6.Gerhard Klebe, Drug design, Springer 2013 (DOI 10.1007/978-3-642-17907-5).

Supplementary literature: List of scientific papers prepared by the academic teacher given at particular lecture.

eResources addresses:

Example issues/ example questions/ tasks being completed	molecular dynamics molecular mechanics drug design molecular docking hydratation in molecular modeling
Practical activites within the subject	Not applicable

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