GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Fundamentals of molecular modeling, PG_00053379		
Field of study	Biomedical Engineering, Biomedical Engineering, Biomedical Engineering		
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 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 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 of lecturer (lecturers)	Subject supervisor	prof. dr hab. inż. Maciej Bagiński	
	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	3.0	27.0	75

Subject objectives	The content of the lecture includes the definition and application of various molecular modeling methods to study the molecular properties of biological systems, including the interactions between the components of these supramolecular systems; in addition, the lecture discusses the outlines of computer-aided molecular design of molecules with desired properties; practical implementation in the form of a project will include a simulation task for a small biological system.

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[K7_W01] knows and understands, to an increased extent, mathematics to the extent necessary to formulate and solve complex issues related to the field of study	The student knows and understands the basic equations covering molecular interactions and equations describing force fields in molecular modeling, which are used to perform calculations.	[SW1] Assessment of factual knowledge
	[K7_U01] can apply mathematical knowledge to formulate and solve complex and non-typical problems related to the field of study by: - appropriate selection of source information and its critical analysis, synthesis, creative interpretation and presentation, - application of appropriate methods and tools	The student is able to practically apply molecular modeling methods in the study of molecular properties and is able to quantitatively analyze these properties using mathematical methods.	[SU1] Assessment of task fulfilment [SU3] Assessment of ability to use knowledge gained from the subject [SU2] Assessment of ability to analyse information
	[K7_K01] is ready to create and develop models of proper behaviour in the work and life environment; undertake initiatives; critically evaluate actions of their own, teams and organisations they are part of; lead a group and take responsibility for its actions; responsibly perform professional roles taking into account changing social needs, including: - developing the achievements of the profession, - observing and developing rules of professional ethics and acting to comply to these rules	Through a joint project, the student is able to develop patterns of appropriate behavior and interactions with others in a professional environment. They also learn responsibility and fulfilling professional roles.	[SK5] Assessment of ability to solve problems that arise in practice [SK3] Assessment of ability to organize work

Subject contents	1. Introduction. The definition of molecular modeling and its origins. 2. Definitions and characterization of static and dynamic molecular properties of biomolecules (biopolymers and low molecular weight organic compounds). 3. Definitions and characteristics of intra- and intermolecular molecular interactions. 4. Scopes of application of molecular modeling divided into levels of advancement of methods. 5. Force fields - definition and examples. 6. Molecular mechanics and dynamics. 7. Overview of molecular mechanics and dynamics software. 8. Electrostatic interactions and solvation models in molecular modeling. 9. Examples of applications of molecular dynamics (biopolymers). 10. Examples of applications of molecular dynamics to the simulation of biological membranes. 11. Free energy calculations. 12. Molecular docking. 13. Protein folding. 14. Homology modeling of proteins. 15. Modeling interactions of ligands with molecular targets. 16. Computer-aided design of drugs and other particles (including new materials) with desired molecular properties.
Prerequisites and co-requisites	mathematics, basics of physics and chemistry
Assessment methods and criteria	

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

Recommended reading	Basic literature	1. 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. 2. D.W. Heermann, Fundamentals of computer simulations in physics, WNT, Warsaw 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, Molecular aspects of the biological activity of amphotericin B and its derivatives with increased selectivity - research using computational chemistry methods. Doctoral thesis, PG 2008.
	Supplementary literature	Publications as illustrations of individual lectures.
	eResources addresses	Adresy na platformie eNauczanie:
Example issues/ example questions/ tasks being completed	description of force fieldsmolecular mechanicsmolecular dynamicsmolecular electrostatic potential	
Work placement	Not applicable	

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