GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Molecular modeling, PG_00066121		
Field of study	Chemistry		
Date of commencement of studies	February 2025	Academic year of realisation of subject	2024/2025
Education level	second-cycle studies	Subject group	Specialty 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	1	ECTS credits	3.0
Learning profile	general academic profile	Assessment form	exam
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 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

eNauczanie source addresses:
Moodle ID: 44582 Modelowanie molekularne
https://enauczanie.pg.edu.pl/moodle/course/view.php?id=44582

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	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 laboratory 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_W03] recognizes and describes phenomena in the field of physics, including elements of quantum mechanics, solid state physics and nuclear physics, necessary to predict the course of physical phenomena and to solve technical problems	The student knows and understands the basic equations of physics covering molecular interactions and the equations describing the force fields in molecular modeling that are used to perform calculations.	[SW1] Assessment of factual knowledge
[K7_U04] develops and transmits technical information in the form of text documents, spreadsheets, graphs, technological diagrams and multimedia presentations, and prepares a speech including a multimedia presentation	The student is able to apply molecular modeling methods in practice to study molecular properties and is able to analyze these properties quantitatively using mathematical methods.	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU5] Assessment of ability to present the results of task
[K7_W01] recognizes problems of modern chemistry, including properties and obtaining chemical compounds, necessary for making calculations, including the dependence of the compound's structure and its reactivity	The student is able to use molecular modeling methods such as molecular dynamics to learn about the molecular properties of biomolecules. The student understands the basics of designing chemical compounds with desired properties.	[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	1. General Chemistry 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 and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
lecture (test)	60.0%	70.0%
project	60.0%	30.0%

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, 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. http://www.pg.gda.pl/~chemmbag/doktorat_Czub.pdf**
Supplementary literature	A number of scientific publications and teaching materials prepared by the teacher.
eResources addresses	

Example issues/ example questions/ tasks being completed	Test contains open questionas for examle issues: molecular dynamics molecular mechanics intermolecular interactions molecular docking
Work placement	Not applicable

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