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 2022	Academic year of realisation of subject	2022/2023
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	prof. dr hab. inż. Maciej Bagiński	

Lesson type and method 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 aim of the course is to familiarize students with the basic and selected issues in the field of molecular modeling, which may be useful in the performance of a diploma thesis in the field of computer-aided moolecular design as well as may constitute the basis for specialized subjects at the third level of studies. The strategic goal will be achieved through the acquisition of theoretical and practical knowledge performance of tasks within the laboratory (project).

Learning outcomes

Course outcome	Subject outcome	Method of verification
[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:n - developing the achievements of the profession,n- observing and developing rules of professional ethics and acting to comply to these rulesn	-can work together in a group and implement a project, can prepare and analyze a report on the implementation of such a project	[SK1] Assessment of group work skills [SK2] Assessment of progress of work
[K7_U01] can apply mathematical knowledge to formulate and solve complex and non-typical problems related to the field of study by:n- appropriate selection of source information and its critical analysis, synthesis, creative interpretation and presentation,n- application of appropriate methods and toolsn	-has knowledge about molecular properties simple organic molecules as well as biopolymers - understand the nature of the interactions between biomolecules and can analyze such impacts	[SU3] Assessment of ability to use knowledge gained from the subject
[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.	-can understand the mathematical apparatus used in molecular modeling and can apply modeling methods to specific molecular systems -understands the nature of interactions between biomolecules and can analyze such impacts	[SW1] Assessment of factual knowledge

Subject contents

- Introduction. Definition of molecular modeling and its genesis.

- Definitions and characteristics of static and dynamic molecular properties of biomolecules (biopolymers and low molecular weight organic compounds).

- Definitions and characteristics of molecular interactions within and intermolecular.

- Scopes of application of molecular modeling broken down into the degree of advancement of the methods.

- Force fields - definition and examples.

- Mechanics and molecular dynamics.

- Overview of molecular mechanics and dynamics software.

- Electrostatic interactions and solvation models in molecular modeling.

- Examples of applications of molecular dynamics (biopolymers).

- Examples of applications of molecular dynamics to simulate biological membranes.

- Free energy calculations.

- Molecular docking.

- Modeling of ligand interactions with molecular targets.

- Computer aided design of drugs and other desired particles molecular properties.

<table>
<tr><td>Prerequisites and co-requisites</td><td colspan="2">Students should have basic knowledge of physical chemistry, mathematics, biochemistry, and biophysics.</td></tr>
<tr><td>Assessment methods and criteria</td><td colspan="2"><table>
<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>test</td><td>60.0%</td><td>70.0%</td></tr>
<tr><td>laboratory - project</td><td>60.0%</td><td>30.0%</td></tr>
</table></td></tr>
<tr><td rowspan="3">Recommended reading</td><td>Basic literature</td><td>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. http://www.pg.gda.pl/~chemmbag/doktorat_Czub.pdf</td></tr>
<tr><td>Supplementary literature</td><td>Publications the references of which are on the slides.</td></tr>
<tr><td>eResources addresses</td><td></td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td colspan="2">molecular dynamics

molecular docking

drug design

intermolecular interactions</td></tr>
<tr><td>Work placement</td><td colspan="2">Not applicable</td></tr>
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