GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	MOLECULAR MODELLING, PG_00038906		
Field of study	Chemistry		
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
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 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	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

<table>
<tr><td>Prerequisites and co-requisites</td><td>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)</td></tr>
<tr><td>Assessment methods and criteria</td><td>
<table>
<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>project</td><td>60.0%</td><td>30.0%</td></tr>
<tr><td>lecture (test)</td><td>60.0%</td><td>70.0%</td></tr>
</table>
</td></tr>
<tr><td>Recommended reading</td><td>
<table>
<tr><td>Basic literature</td><td>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</td></tr>
<tr><td>Supplementary literature</td><td>A number of scientific publications and teaching materials prepared by the teacher.</td></tr>
<tr><td>eResources addresses</td><td></td></tr>
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<tr><td>Example issues/ example questions/ tasks being completed</td><td>molecular dynamics
molecular mechanics
intermolecular interactions
molecular docking</td></tr>
<tr><td>Work placement</td><td>Not applicable</td></tr>
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