

Subject card

Subject name and code	Introduction to molecular modeling, PG_00033260						
Field of study	Chemistry						
Date of commencement of studies	October 2024	Academic year of realisation of subject			2025/2026		
Education level	Bachelor's studies	Subject group			Optional subject group		
Mode of study	full-time studies	Mode of delivery			at the university		
Year of study	2	Language of instruction			Polish Some of the reference materials are available online in English only.		
Semester of study	3	ECTS credits			1.0		
Learning profile	academic	Assessment form					
Conducting unit	Laboratory of Carbohydrate Chemistry -> Department of Organic Chemistry -> Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Rafał Ślusarz					
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	0.0	0.0	0.0	15
	E-learning hours included: 0.0						
	Additional information: Methods: <ul style="list-style-type: none"> • multimedia presentation • analysis of critical events (cases) • discussion on the subject forum • work with the computer (on-line) 						
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	15		2.0		8.0	25
Subject objectives	Introduction of the student to the subject of molecular modeling.						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[CHEML3_W09] Describes the practical applications of IT tools (computer programmes) for chemical calculations and data analysis.	student illustrates changes occurring in systems, selects tools specialized in measurement, construction or analysis of collected data	[SW4] test/exam - oral or written
	[CHEML3_W08] Demonstrates knowledge of basic computational methods to solve problems in chemistry, physics, mathematics.	student calculates simple profiles of energy changes, constructs correct queries to bioinformatics databases, indicates the causes of conformation changes	[SW4] test/exam - oral or written
	[CHEML3_U10] Prepares papers on various fields of chemistry in Polish and English, using acquired knowledge and skills as well as various sources of scientific information.	student assesses the usefulness of types of representations in the presentation of results, proposes the best methods of visualization of chemical compounds, shows creativity in the preparation of chemical presentations	[SU4] test/exam - oral or written
[CHEML3_U05] Uses basic statistical methods and IT techniques to describe chemical processes and analyse experimental data.	student names the projection methods and defines the scope of the transmitted information in selected molecular systems	[SU4] test/exam - oral or written	
Subject contents	<ul style="list-style-type: none"> learning to visualize chemical structures in various computer programs preparation of two- and three-dimensional representations of structures of chemical compounds simple computer simulations of dynamics and geometry optimization of modeled chemical compounds 		
Prerequisites and co-requisites	A basic knowledge of English and a general understanding of the structure of chemical compounds is required.		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	multi-component online test; one test for each of the topics covered; the arithmetic average of all tests is calculated	51.0%	100.0%
Recommended reading	Basic literature	none	
	Supplementary literature	none	
	eResources addresses	Adresy na platformie eNauczenie: Wstęp do Modelowania Molekularnego - Moodle ID: 4036 https://mdl.ug.edu.pl/course/view.php?id=4036	
Example issues/ example questions/ tasks being completed	<ul style="list-style-type: none"> Assign colors to chemical elements according to IUPAC convention. What kind of coordinates contain information about bond lengths, valence and torsion angles? 		
Work placement	Not applicable		

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