

Subject card

Subject name and code	Introduction to molecular modeling, PG_00033259						
Field of study	Chemistry						
Date of commencement of studies	October 2025		Academic year of realisation of subject		2026/2027		
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		
Semester of study	3		ECTS credits		2.0		
Learning profile	academic		Assessment form		credit		
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	0.0	0.0	30.0	0.0	0.0	30
	E-learning hours included: 0.0						
	Additional information:						
	• experiment designing • analysis of critical events (cases) • conducting experiments • blended learning (on-line and stationary classes) Methods: • problem study with issues for independent learning • discussion in the course forum • exercises in the computer lab (stationary)						
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	30		5.0		15.0	50
Subject objectives	Introduction of the student to the subject of molecular modeling.						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[CHEML3_U09] Is able to learn independently.	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	[SU2] presentation/project/paper/report
	[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	[SW2] presentation/project/paper/report
	[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	[SW2] presentation/project/paper/report
	[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	[SU2] presentation/project/paper/report
Subject contents	• 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
	student prepares a report for each exercise performed; each such report is assessed separately; the final grade is the arithmetic mean of the partial grades obtained	51.0%	100.0%
Recommended reading	Basic literature	none	
	Supplementary literature	none	
	eResources addresses		
Example issues/ example questions/ tasks being completed	• identify and measure all valence angles in an aspirin molecule • prepare 1,2-dichloroethane z-matrix • draw up and interpret selected bond-rotation energy profile		
Work placement	Not applicable		

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