

Subject card

Subject name and code	Practical computational chemistry., PG_00148499						
Field of study	Bioinformatics						
Date of commencement of studies	October 2025		Academic year of realisation of subject		2027/2028		
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	3		Language of instruction		Polish		
Semester of study	5		ECTS credits		3.0		
Learning profile	academic		Assessment form				
Conducting unit	Laboratory of Quantum Chemistry -> Department of Theoretical Chemistry -> Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. Iwona Anusiewicz				
	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						
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		0.0		0.0	30
Subject objectives	Acquiring the knowledge of the possibilities of solving specific chemical problems using a computer and modern computational programs.						
Learning outcomes	Course outcome		Subject outcome		Method of verification		
	[BIOINL3_U02] Graduate is able to apply knowledge of natural sciences and science to formulate, analyze and solve problems related to bioinformatics		Student determines a chemical problem in terms of the possibility of solving it theoretically, assesses the physicochemical and spectral properties of molecules using computational methods, determines the mechanism of a chemical reaction based on the designated activation barriers and parameters characterizing the rate constant.		[SU2] presentation/project/paper/report		
	[BIOINL3_W02] Has the scientific knowledge necessary to understand the basic processes in living organisms.		Student defines chemical problems that can be solved theoretically, explains the theoretical approach used to solve specific chemical problems, describes the method of preparing data and interpreting the results, characterizes the computational methods used nowadays to predict the structure and physicochemical properties of molecules and study the mechanisms of chemical reactions		[SW2] presentation/project/paper/report		
Subject contents	preparation of input data for chemical calculations and numerical and graphical interpretation of results, determining the geometrica structure of molecules, obtaining spectral characteristics of molecules (simulation of IR, NMR, UV spectra), determining physicochemical properties (enthalpy, free enthalpy, entropy, specific heat, dipole and quadrupole moments, polarizability and hyperpolarizability),modeling of chemical reactions (studying the mechanism, determining activation barriers, determining the rate constant).						

Prerequisites and co-requisites	basic skills in computer usage		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	based on the reports containing the solutions of the assigned tasks	51.0%	100.0%
Recommended reading	Basic literature	none	
	Supplementary literature	Exploring chemistry with electronic structure methods (J.B. Foresman, Æ. Frisch)	
	eResources addresses	Adresy na platformie eNauczanie:	
Example issues/ example questions/ tasks being completed	Calculate the barrier height of the CH ₃ CN--> CH ₃ NC isomerization process.		
Work placement	Not applicable		

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