University of Gdańsk

Subject card

Subject name and code	Practical Computational Chemistry, PG_00193536		
Field of study	Bioinformatics		
Date of commencement of studies	October 2026	Academic year of realisation of subject	2028/2029
Education level	Bachelor's 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	3	Language of instruction	Polish
Semester of study	5	ECTS credits	3.0
Learning profile	academic	Assessment form	credit
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, prof. UG	
	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	45.0	75

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 advanced 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

<table>
<tr><td>Subject contents</td><td colspan="3">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).</td></tr>
<tr><td>Prerequisites and co-requisites</td><td colspan="3">basic skills in computer usage</td></tr>
<tr><td>Assessment methods and criteria</td><td colspan="3"><table><tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr><tr><td>based on the reports containing the solutions of the assigned tasks</td><td>51.0%</td><td>100.0%</td></tr></table></td></tr>
<tr><td rowspan="3">Recommended reading</td><td>Basic literature</td><td colspan="2">none</td></tr>
<tr><td>Supplementary literature</td><td colspan="2">Exploring chemistry with electronic structure methods (J.B. Foresman, Æ. Frisch)</td></tr>
<tr><td>eResources addresses</td><td colspan="2"></td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td colspan="3">Calculate the barrier height of the CH_3CN--> CH_3NC isomerization process.</td></tr>
<tr><td>Work placement</td><td colspan="3">Not applicable</td></tr>
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