



Subject card

Subject name and code	Chemometrics, PG_00036535						
Field of study	Chemistry						
Date of commencement of studies	October 2021	Academic year of realisation of subject			2024/2025		
Education level	first-cycle studies	Subject group			Obligatory subject group in the field of study 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	4	Language of instruction			Polish		
Semester of study	7	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	dr hab. inż. Tomasz Laskowski					
	Teachers	dr inż. Julia Borzyszkowska-Bukowska dr hab. inż. Tomasz Laskowski					
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	Student: <ul style="list-style-type: none">• designs, collects, and controls multidimensional data,• creates graphical presentations of multidimensional data,• selects the variables necessary to describe the basic properties of the analyzed set of objects (samples),• uses principal component analysis to analyze data,• creates multivariate regression models and determine their significance and adequacy,• classifies the examined objects according to the value of many explanatory variables.						
Learning outcomes	Course outcome	Subject outcome		Method of verification			
	[K6_U03] can make detailed documentation of the results of self-conducted experiments and prepare a report describing these results	The student is able to correctly prepare a summary documentation of the results of the experiments and prepare a study containing a discussion of these results		[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools			
	[K6_U04] can use professional vocabulary, can prepare and communicate technical information in the form of text documents, spreadsheets, charts and technological schema	The student is able to use professional vocabulary and prepare and transfer technical informations.		[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU5] Assessment of ability to present the results of task			
	K6_W02	A student possesses knowledge on basic and advanced chemometric techniques, particularly regarding the mathematics fueling the methods used.		[SW1] Assessment of factual knowledge			

Subject contents	<p>The lectures will include following issues:</p> <ul style="list-style-type: none"> • experimental design with particular regard to factor and minimum design, • data collection, archiving and pre-processing, • methods of graphic presentation of multidimensional data, • application of the principal components analysis to multidimensional data sets, • mathematical modeling of relationships with particular emphasis on the rules of models creation and assessment of their adequacy, • classification, i.e. determining the rules of belonging of objects to predefined classes, • similarity analysis, i.e. searching for natural clusters of objects. <p>As part of the laboratory, students will independently carry out chemometric analysis of their multidimensional data sets using various chemometric techniques.</p>														
Prerequisites and co-requisites	Prerequisite subjects: mathematics, computer science. Prerequisites: knowledge of basic concepts of statistics, skills in using a spreadsheet computer program (e.g. Excel)														
Assessment methods and criteria	<table border="1" data-bbox="448 512 1487 651"> <thead> <tr> <th data-bbox="448 512 794 546">Subject passing criteria</th> <th data-bbox="794 512 1141 546">Passing threshold</th> <th data-bbox="1141 512 1487 546">Percentage of the final grade</th> </tr> </thead> <tbody> <tr> <td data-bbox="448 546 794 580">practical exercises</td> <td data-bbox="794 546 1141 580">60.0%</td> <td data-bbox="1141 546 1487 580">40.0%</td> </tr> <tr> <td data-bbox="448 580 794 613">compilation of results</td> <td data-bbox="794 580 1141 613">60.0%</td> <td data-bbox="1141 580 1487 613">10.0%</td> </tr> <tr> <td data-bbox="448 613 794 651">lecture test</td> <td data-bbox="794 613 1141 651">60.0%</td> <td data-bbox="1141 613 1487 651">50.0%</td> </tr> </tbody> </table>			Subject passing criteria	Passing threshold	Percentage of the final grade	practical exercises	60.0%	40.0%	compilation of results	60.0%	10.0%	lecture test	60.0%	50.0%
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Recommended reading	Basic literature	J.Mazerski: "Chemometria Praktyczna", Wydawnictwo Malamut, Warszawa 2009. J. Koronacki, J. Mielniczuk: Statystyka dla studentów kierunków technicznych i przyrodniczych. WN-T, W-wa 2001													
	Supplementary literature	E. Steiner: "Matematyka dla chemików", Wydawnictwo Naukowe PWN, Warszawa 2001. S. Brandt: Analiza danych, Wydawnictwo Naukowe PWN, Warszawa 1998													
	eResources addresses	Adresy na platformie eNauczenie: Chemometria - Chemia - zimowy 24/25 - Moodle ID: 37188 https://enauczenie.pg.edu.pl/moodle/course/view.php?id=37188													
Example issues/ example questions/ tasks being completed	<ol style="list-style-type: none"> 1. Design a series of measurements whose results will allow you to create a model of relationship between yield the chemical synthesis and its conditions: temperature, time and catalyst content. 2. Based on the attached results of the regression analysis, determine an adequate model of a relationship 3. Evaluate the prognostic capacity of the obtained model. 														
Work placement	Not applicable														

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