

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 Pharm	Department of Pharmaceutical Technology and Biochemistry -> Faculty of Chemistry							
Name and surname	Subject supervisor	ıbject supervisor dr hab. inż. Tomasz Laskowski							
of lecturer (lecturers)	Teachers								
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	' 		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	earning activity Participation is classes included plan				Self-study SUM		SUM	
	Number of study hours	45		5.0		25.0		75	
Subject objectives	Student: 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 determitheir significance and adequacy, classifies the examined objects according to the value of many explanatory variables.								
Learning outcomes	Course outcome Subject of				ect outcome		Method of verification		
	[K6_U03] can make detailed documentation of the results of self-conducted experiments and prepare a report describing 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			

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Subject contents	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. As part of the laboratory, students will independently carry out chemometric analysis of their multidimensional data sets using various chemometric techniques.					
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	Subject passing criteria	Passing threshold	Percentage of the final grade			
and criteria	practical exercises	60.0%	40.0%			
	compilation of results	60.0%	10.0%			
	lecture test	60.0%	50.0%			
Recommended reading	Basic literature	J.Mazerski: "Chemometria Praktyczna", Wydawnictwo Malamut,Warszawa 2009J.Koronacki, J.Mielniczuk: Statystyka dla studentów kierunkówtechnicznych i przyrodniczych. WN-T, W-wa 2001				
	Supplementary literature	E.Steiner: "Matematyka dla chemików", Wydawnictwo Naukowe PWN,Warszawa 2001S.Brandt: Analiza danych, Wydawnictwo Jaukowe PWN, Warszawa1998				
	eResources addresses	Adresy na platformie eNauczanie:				
Example issues/ example questions/ tasks being completed	 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. Based on the attached results of the regression analysis, determine an adequate model of a relationship Evaluate the prognostic capacity of the obtained model. 					
Work placement	Not applicable					

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