



## Subject card

Subject name and code	Fundamentals Chemometry, PG_00045467						
Field of study	Chemical Technology						
Date of commencement of studies	February 2023	Academic year of realisation of subject			2022/2023		
Education level	second-cycle 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	1	Language of instruction			Polish		
Semester of study	1	ECTS credits			3.0		
Learning profile	general academic profile	Assessment form			exam		
Conducting unit	Department of Pharmaceutical Technology and Biochemistry -> Faculty of Chemistry						
Name and surname of lecturer (lecturers)	Subject supervisor	dr inż. Tomasz Laskowski					
	Teachers	dr inż. Julia Borzyszkowska-Bukowska dr 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	15.0	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	10.0		35.0		75
Subject objectives	A student:  designs, collects and controls the multidimensional data  creates graphical presentations of multidimensional data  selects variables necessary to describe the basic properties of the analyzed set of objects (samples)  uses principal component analysis to analyze the data sets  creates regression models depending on several variables and assess their relevance and appropriateness  classifies the analyzed objects according to the values of several variables						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	K7_K01	Student is able to state a chemometric problem and then solve it, step by step, using selected chemometric techniques and present the whole process in a form of a detailed report.	[SK2] Assessment of progress of work [SK5] Assessment of ability to solve problems that arise in practice
	K7_U05	Student learns the theory of correct analytical measurements, advances in usage of a spreadsheet and is finally introduced to the basics of R programming language, in order to process and analyze the data obtained.	[SU5] Assessment of ability to present the results of task [SU4] Assessment of ability to use methods and tools [SU2] Assessment of ability to analyse information [SU1] Assessment of task fulfilment
	K7_W04	Student learns some basic chemometric techniques and is able to properly select ones to be used, accordingly to the given scientific problem.	[SW3] Assessment of knowledge contained in written work and projects [SW1] Assessment of factual knowledge
Subject contents	The lectures will address , inter alia, following issues : - experimental designs with particular emphasis on factorial and minimal ones - collecting , archiving and preprocessing of multivariate data sets - graphical presentation of multidivariate data - principal component analysis (PCA) of multivariate data sets - multivariate mathematical models selection of descriptors and adequacy of model - object classification to predefined classes (supervised pattern recognition) - similarity analysis (natural clustering of the objects, unsupervised pattern recognition))		
Prerequisites and co-requisites	Subjects pre: mathematics, computer science Prerequisites: knowledge of basic statistical concepts, the ability to use a spreadsheet computer program ( eg Excel )		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	Test at the end of the semester or oral exam	60.0%	100.0%
Recommended reading	Basic literature	J.Mazerski: "Chemometria Praktyczna", ed. II., Wydawnictwo Malamut, Warszawa 202016 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		
Example issues/ example questions/ tasks being completed	Collect your own dataset, accordingly to the guides given by your supervisor. State a scientific problem for your data and solve it using chemometric techniques learned along the way.		
Work placement	Not applicable		