

Subject card

Subject name and code	Exploratory analysis of multidimensional chemical space, PG_00054859						
Field of study	Chemistry						
Date of commencement of studies	October 2026		Academic year of realisation of subject		2026/2027		
Education level	Master's 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	1		Language of instruction		English		
Semester of study	1		ECTS credits		3.0		
Learning profile	academic		Assessment form		exam		
Conducting unit	Laboratory of Environmental Chemoinformatics -> Department of Environmental Chemistry and Radiochemistry -> Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor		dr Artur Mirocki				
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	30.0	0.0	0.0	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		5.0		40.0	75
Subject objectives	Course objectives are: - Achieving advanced skills in exploratory analysis of multidimensional chemical space (performing analyses and interpreting the results) - Familiarizing the students with the available software allowing to perform the multidimensional analysis - Familiarizing the students with Python scripts used to data analysis						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[CHEMMU2_U04] Applies acquired knowledge of chemistry and related scientific disciplines.	At the end of the course every student is convinced that the use of a computer and exploratory analysis strengthens the potential of data analysis and can critically evaluate experimental results and understand the necessity of their control	[SU4] test/exam - oral or written
	[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	Pod koniec kursu każdy student rozumie potrzebę głębszego poznania metod wielowymiarowej analizy danych	[SK4] test/exam - oral or written
	[CHEMMU2_W07] Selects experimental and theoretical techniques to the extent necessary to understand the description and modelling of medium complexity chemical processes.	At the end of the course every student uses Python environment for multidimensional analyses of chemical space	[SW4] test/exam - oral or written
	[CHEMMU2_W04] Applies the acquired knowledge to an in-depth description of the properties of chemical connections, methods of their synthesis and analysis.	At the end of the course every student explains theoretical background (algorithm) of the advanced methods, including HCA, PCA	[SW4] test/exam - oral or written
	[CHEMMU2_W11] Demonstrates general knowledge about the current trends in the development of chemistry as a science and the latest discoveries in this field.	At the end of the course every student knows classification of advanced methods of data analysis and provides examples of their applications in multidimensional chemical problems	[SW4] test/exam - oral or written
Subject contents	Course contents: • Introduction to multivariate data, review of the basic software allowing to perform the multidimensional analysis • Advanced methods of analyzing the internal structure of the data: similarity in the multivariable feature space, methods of similarity analysis, dimensionality reduction, hierarchical cluster analysis (HCA), principal component analysis (PCA), k-Means clustering, fuzzy c-Means clustering, Self-organizing maps, Gaussian Mixture models, and other deep learning algorithms Density-based spatial clustering of applications with noise. • Examples of applying these methods in chemical data analysis.		
Prerequisites and co-requisites			
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	test	51.0%	100.0%
Recommended reading	Basic literature	R. Kramer: Chemometric techniques for quantitative analysis. New York: Marcel Dekker, Inc, 2005	
	Supplementary literature	S. D. Brown, R. Tauler, B. Walczak (red): Comprehensive chemometrics: Chemical and biochemical data analysis. Amsterdam: Elsevier, 2009	
		scientific publication in the field	
	eResources addresses		
Example issues/ example questions/ tasks being completed			
Work placement	Not applicable		

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