



Subject card

Subject name and code	AI in the chemistry lab, PG_00069259						
Field of study	Chemistry						
Date of commencement of studies	February 2025		Academic year of realisation of subject		2025/2026		
Education level	second-cycle studies		Subject group				
Mode of study	Full-time studies		Mode of delivery		at the university		
Year of study	1		Language of instruction		Polish		
Semester of study	2		ECTS credits		3.0		
Learning profile	general academic profile		Assessment form		assessment		
Conducting unit	Department of Physical Chemistry -> Faculty of Chemistry -> Wydziały Politechniki GdańskieJ						
Name and surname of lecturer (lecturers)	Subject supervisor		dr hab. inż. Adam Kłoskowski				
	Teachers						
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	The aim of the course is to introduce students to the R programming language for data processing, analysis and visualization (including chemical data). The course focuses on developing practical skills necessary for working with data from laboratory experiments, instrumental analyses and environmental studies. Students will learn to use the R programming language for independent data processing, statistical, chemometric and/ or chemoinformatic analysis and creation of professional (including interactive) graphs. After completing the course, the student should: 1) know the basics of the R language and the basic functions and their application in the analysis of chemical data, 2) be able to use the appropriate R packages supporting statistical, chemometric and data visualization analysis (e.g. tidyverse, ggplot2, plotly, shiny, etc.), 3) be able to independently import, process and prepare data for further analysis, 4) be able to perform basic and advanced statistical, chemometric and/or chemoinformatic analysis, 5) be able to create clear and professional graphs illustrating research results, 6) be able to prepare an automated data analysis report in the form of a PDF, Word or HTML document.						
Learning outcomes	Course outcome		Subject outcome		Method of verification		
	[K7_W01] recognizes problems of modern chemistry, including properties and obtaining chemical compounds, necessary for making calculations, including the dependence of the compound's structure and its reactivity		The student recognizes the problems of modern chemistry, including the properties and preparation of chemical compounds, necessary to perform calculations, including the dependence of the compound's structure and its reactivity		[SW1] Assessment of factual knowledge		
	[K7_U04] develops and transmits technical information in the form of text documents, spreadsheets, graphs, technological diagrams and multimedia presentations, and prepares a speech including a multimedia presentation		The student prepares and conveys technical information in the form of text documents, spreadsheets, graphs, technological diagrams and multimedia presentations, and prepares a speech including a multimedia presentation		[SU3] Assessment of ability to use knowledge gained from the subject [SU1] Assessment of task fulfilment		
	[K7_K02] is able to cooperate and work in a group, taking on different roles		The student is able to cooperate and work in a group, assuming different roles in it.		[SK2] Assessment of progress of work [SK1] Assessment of group work skills		

Subject contents	The content covered in the lab includes the following areas: 1) Introduction to R and RStudio history, capabilities, applications, R syntax, data types, data structures, simple data operations, 2) Introduction to working with data in R loading and saving data: data import and export (CSV, Excel, txt), data cleaning, handling missing data, filtering, sorting, merging sets, 3) Basic statistical analysis of research results mean, median, standard deviation, Student's t-tests, correlations, etc., 4) Introduction to chemometrics and chemoinformatics in R correlation analysis, similarity analysis, dimensionality reduction methods, etc., 5) The tidyverse package the foundation of modern data analysis, data transformation and manipulation using dplyr and tidyr, 6) Data visualization theory and best practices: principles of creating scientific graphs (plot, ggplot2), graph types (scatter plot, line plot, histogram, box plot, bar plot, pie chart, etc.), coloring, layered chart structure, personalization, faceting, interactive data presentation (shiny and plotly), 7) First scripts in R writing simple functions and user scripts. 8) Review of selected applications of R language in the analysis of real chemical and environmental data: analysis of spectroscopic, toxicological and environmental monitoring data, etc., 9) Project comprehensive analysis and visualization of real chemical data independent execution of the full workflow: data import, statistical analysis, visualization, report.		
Prerequisites and co-requisites			
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
		60.0%	50.0%
		50.0%	50.0%
Recommended reading	Basic literature	<ul style="list-style-type: none">Przemysław Biecek. Przewodnik po pakiecie R. Oficyna wydawnicza GIS. 2014. ISBN: 9788389020987.Gillespie Colin Lovelace Robin. Wydajne programowanie w R. Praktyczny przewodnik po lepszym programowaniu. Helion 2018, ISBN: 9788375413526.	
	Supplementary literature	Marek Gagolewski. Programowanie w języku R: Analiza danych, obliczenia, symulacje. Wydawnictwo Naukowe PWN 2016. ISBN: 9788301189396 Jared P. Lander. Język R dla każdego. Zaawansowane analizy i grafika statystyczna. Pearson Addison-Wesley 2018. ISBN: 978-83-7541-336-6	
	eResources addresses		
	Example issues/ example questions/ tasks being completed	Example theoretical topics: - Explain the difference between a vector and a list in R. - What are the basic data structures in R? Give examples. - How do I create and call variables in R? - Explain the difference between the read.csv() and read.table() functions. - How does the mutate() function work in the dplyr package? - What functions in dplyr are used to filter and group data? - How can I combine functions with dplyr using the pipe %>% operator? - What does "layered plot construction" mean in ggplot2? - What is faceting and what is it used for? - What is the difference between plot() and ggplot()? - How do I create a simple function in R? - What is a for loop and how can I replace it with apply() functions? - How can I store and call my own scripts? - How to prepare a data analysis report in R using R Markdown?	
Work placement	Not applicable		

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