KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
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Course title	ECTS code
Statistics and chemometrics in chemical analytics	13.3.0865

Name of unit administrating study

null

Studies

faculty	field of study		
Wydział Chemii	Chemia	type	pierwszego stopnia
		form	stacjonarne
		specialty	chemia żywności
		specialization	wszystkie

Teaching staff

prof. dr hab. Tomasz Puzyn; mgr Jarosław Wieczorek; dr hab. Łukasz Haliński; mgr Marcin Kaczor; dr inż. Karolina Jagiełło; mgr Aleksandra Moniakowska; dr inż. Anna Malankowska; mgr Jarosław Wieczorek; dr Agnieszka Gajewicz-Skrętna; mgr Marcin Kaczor; mgr Klaudia Block-Łaszewska; mgr inż. Małgorzata Rybczyńska; Filip Stoliński; dr Alicja Mikołajczyk; mgr Maciej Gromelski

Forms of classes, the realization and number of hours

Forms of classes

Auditorium classes, Laboratory classes, Lecture

The realization of activities

classroom instruction

Number of hours

Lecture: 30 hours, Laboratory classes: 15 hours, Auditorium classes: 15 hours

ECTS credits

6
classes - 60 h
tutorial classes – 20 h
student's own work – 70 h

Total: 150 h - 6 ECTS

The academic cycle

2022/2023 summer semester

Type of course

obligatory

Language of instruction

polish

Teaching methods

- multimedia-based lecture
- •During the auditorium classes students will solve tasks with the application of statistical test
- •In the computational laboratory students will conduct hands on exercises, based on the instructions prepared by the teacher

Form and method of assessment and basic criteria for eveluation or examination requirements

Final evaluation

Graded credit

Assessment methods

Lectures – final test
Laboratories – colloquia and written reports
Auditorium classes – colloquia

The basic criteria for evaluation

	All colloquia as well as written reports organized during lab and/or auditorium classes need to have a positive grade Final test: Written part (obligatory): single choice test with 15 questions (1 point per question) plus three open questions (5 points per each) – max. 30 points in total. Positive grade if the number of points > 50%. For students having between 40% and 50% from the written part, oral part is obligatory. Students with the number of points < 40% do not pass the exam. Oral part (obligatory for students having between 40% and 50% from the written part and facultative for students with > 50%): discussion on three problems related to the topic, selected by the teacher Students are allowed passing the test twice (two attempts). All colloquia organized during lab and auditorium classes need to have a positive grade as well as written reports Its obligatory to have a positive final grade from the lab exercises before passing the final test

Method of verifying required learning outcomes

Required courses and introductory requirements

A. Formal requirements

Chemistry
Mathematics

B. Prerequisites

Aims of education

Achieving basic skills in statistic calculations by the students
Presenting the applications of chemometrics in green chemistry to the students
Achieving basic skills in chemometric methods by the students (performing basic analyses and interpreting the results)
Familiarizing the students with the available chemometric software

Course contents

The course discusses the basic statistical theory that is frequently used in chemometric analysis: general population and statistical sample, characteristic of a single series of results, testing statistical hypothesis
Introduction to chemometrics: multivariate data, difference between statistics and chemometrics, review of the basic software
Methods of the initial data controlling, e.g.: problem of lacking data, outlying objects, variables transformation, distribution normalization, correlation, and covariation analysis
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). Examples of applying these methods in green chemistry and technology.
Modeling phenomena and processes with regression and classification techniques: linear regression (LR), multiple linear regression (MLR), principal component regression (PCR), partial least square regression (PLS), linear discriminant analysis (LSA), k-nearest neighbors classifier (k-NN); artificial neural networks (ANN) for solving classification and regression problems; methods of optimal variables selection (stepwise regression, genetic algorithms); validation of classification and regression models. Examples of applying these methods in green chemistry and technology.

Bibliography of literature

Literature required to pass the course

• A. Łomnicki: Wprowadzenie do statystyki dla przyrodników. Wydawnictwo Naukowe PWN, Warszawa 2003.
• J. Mazerski: Podstawy chemometrii. Gdańsk: Wydawnictwo Politechniki Gdańskiej, 2000
• P. Konieczka, J. Namieśnik i in.: Ocena i kontrola jakości wyników analitycznych. Centrum Doskonałości Analityki i Monitoringu Środowiskowego, Gdańsk 2004.

A.1. Literatura wykorzystywana podczas zajęć

• Skrypt do ćwiczeń laboratoryjnych przygotowywany przez pracowników Pracowni Chemometrii Środowiska

Extracurricular readings

• J. B. Czermiński, A. Iwasiewicz i in.: „Metody statystyczne w doświadczalnictwie chemicznym”, Wydawnictwo Nau-kowe PWN, Warszawa 1992 lub wersja starsza tej książki zatytułowana „Metody statystyczne dla chemików”.
• Praca zbiorowa pod redakcją H. Kassyk-Rokickiej: „Statystyka. Zbiór zadań”. Polskie Wydawnictwo Ekonomiczne, Warszawa 1997.
• S. D. Brown, R. Tauler, B. Walczak (red): Comprehensive chemometrics: Chemical and biochemical data analysis. Amsterdam: Elsevier, 2009
• R. Kramer: Chemometric techniques for quantitative analysis. New York: Marcel Dekker, Inc, 2005
• D. Zuba, A Parczewski (red.): Chemometria w analityce: wybrane zagadnienia. Kraków: Wydawnictwo Instytutu Eks-pertyz Sądowych, 2008
• JM. Dobosz: Wspomagana komputerowo statystyczna analiza danych. Warszawa: Akademicka Oficyna Wydawnicza EXIT, Warszawa 2004

The learning outcomes (for the field of study and	**Knowledge**

specialization)	At the end of the course every student: knows basic statistical parameters used to characterize a single series of result knows basis statistical distributions (e.g., t-Student) knows basis statistical tests, their applications and limitations knows basic classification of chemometric methods and provides examples of theirs applications in green chemistry knows basic software packages to be used for chemometric analyses explains theoretical background (algorithm) of the most important chemometric methods, including: HCA, PCA, LR/MLR, LDA, kNN
	Skills
	At the end of the course every student: calculates basis statistical parameters used to characterize a single series of results prepares the histogram for assessing the distribution of a single series of results uses statistical tests to solve various problems uses KNIME environment for chemometric analyses correctly prepares data for further analysis performs HCA and PCA analyses and correctly interprets the results develops regression and classification models, validates the models correctly and applies the models for predictions applies methods of chemometric optimization
	Social competence
	At the end of the course every student: is convinced that the use of a computer and chemometrics strengthens the potential of data analysis can critically evaluate experimental results and understand the necessity of their control understands the need of deeper learning of chemometric methods
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