KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI
Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego
UNIA EUROPEJSKA
EUROPEJSKI FUNDUSZ SPOŁECZNY

**Course title**

Chemometrics

**ECTS code**

13.3.0755

**Name of unit administrating study**

null

**Studies**

| faculty | field of study | | |
|---|---|---|---|
| Faculty of Chemistry | Chemical Business | type | all |
| | | form | all |
| | | specialty | all |
| | | specialization | all |

**Teaching staff**

prof. dr hab. Tomasz Puzyn

**Forms of classes, the realization and number of hours**

**Forms of classes**

Laboratory classes, Lecture

**The realization of activities**

classroom instruction

**Number of hours**

Lecture: 15 hours, Laboratory classes: 30 hours

**ECTS credits**

3
classes - 45 h
tutorial classes – 5 h
student's own work – 25 h

Total: 75 h - 3 ECTS

**The academic cycle**

2024/2025 winter semester

**Type of course**

obligatory

**Language of instruction**

polish

**Teaching methods**

- multimedia-based lecture
- •Students will conduct hands on exercises in the computational laboratory, 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
- Examination

**Assessment methods**

Assessment methods
•Written/oral final test (as described below)
•Colloquia that must be passed before each laboratory exercise
•Written reports

**The basic criteria for evaluation**

The basic criteria for evaluation or exam requirements

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).
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**

General chemistry

**B. Prerequisites**

Mathematics (linear algebra)
Statistics

## Aims of education

Aims of education

- Familiarizing the students with the possible application of chemometrics algorithms
- Acquiring by the students the skills of collecting, archiving and evaluating of the multivariable data
- 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

Course contents

Lecture:

1. Introduction to chemometrics: specificity of multidimensional data; differences between statistics and chemometrics; area of interest in chemometrics; division of chemometric methods; review of the basic software (including MATLAB, Statistica, Origin, SPSS, QSARINS, KNIME).
2. Methods of analyzing the internal structure of the multidimensional chemical data: similarity of objects in the multivariable feature space; hierarchical cluster analysis (HCA) as an example of a similarity analysis method; principal component analysis (PCA) as an example of the projection search method. Examples of applying these methods in various areas of chemistry.
3. Modeling phenomena and processes with regression and classification methods: linear regression of single and multiple variables (LR and MLR), principal component regression (PCR) and partial least squares regression (PLS); linear discriminant analysis (LDA), a non-linear classifier of k-nearest neighbors (kNN); methods for selecting the optimal set of variables in the model (using the genetic algorithm); validation of regression and classification models. Examples of applying these methods in various areas of chemistry.

B. Computer lab:

1. Introduction to chemometric calculations in the KNIEM software environment. The rules of working with a computer.
2. Hierarchical cluster analysis (HCA).
3. Principal Component Analysis (PCA).
4. Linear regression of single and multiple variables (LR / MLR).

## Bibliography of literature

Bibliography of literature

Literature required to pass the course:

S. D. Brown, R. Tauler, B. Walczak (ed): Comprehensive chemometrics: Chemical and biochemical data analysis. Amsterdam: Elsevier, 2009
R. Kramer: Chemometric techniques for quantitative analysis. New York: Marcel Dekker, Inc, 2005

Extracurricular readings:

J. Leszczynski, A. Kaczmarek-Kedziera, T. Puzyn, M. G. Papadopulos, H. Reis, M. Shukla (ed): Handbook of Computational Chemistry (2nd Edition). Springer 2016. Volume 5: Chemoinformatics, Puzyn T (ed.).
T. Puzyn, J. Leszczynski, M. T. D. Cronin (ed): Recent Advances in QSAR Studies: Methods and Applications. Springer 2010. ISBN: 978-1-4020-9782-9.
K. Roy, S. Kar, R. Narayan Das (ed): A Primer on QSAR/QSPR Modeling - Fundamental Concepts. Springer 2015. ISBN: 978-3-319-17281-1.

## The learning outcomes (for the field of study and specialization)

### Knowledge

Knowledge

At the end of the course every student:
understands the need for reliable documentation of the results,
knows the basic division of chemometric methods, lists the use of particular groups of these methods in the analysis of chemical data;
knows basic software packages to be used for chemometric analyses;
knows the theoretical background (algorithm of operation) of the most important chemometric methods, including HCA, PCA, LR, MLR, PCR, PLS.

### Skills

Skills

At the end of the course every student:
uses the KNIME environment for chemometric analyses;
correctly prepares data for further chemometric analysis;
performs HCA and PCA analyses and correctly interpret the obtained results;

| | |
|---|---|
| | develops regression model (LR / MLR method), validates the models correctly and applies the models for predictions. |
| | **Social competence** |
| **Contact** | |
| tomasz.puzyn@ug.edu.pl | |