COURSE DESCRIPTION

Applied chemometrics in experimental design, signal processing and pattern recognition

Academic year **2025-2026**

1. Programme-related data

1.1. Higher Education Institution	**Babeș-Bolyai University of Cluj-Napoca**
1.2. Faculty	**Faculty of Chemistry and Chemical Engineering**
1.3. Department	**Doctoral School of Chemistry**
1.4. Field	**Chemistry**
1.5. Level of study	**Doctoral studies (PhD)**
1.6. Degree programme / Qualification	**Doctoral studies – Doctoral School of Chemistry / PhD degree**
1.7. Form of education	**Full-time education**

2. Course-related data

2.1. Course title	**Applied chemometrics in experimental design, signal processing and pattern recognition**			Course code	**SDC-19-11**
2.2. Course coordinator	**Assoc. Prof. Dr. Habil. Augustin C. Moț**				**Label: 4**
2.3. Seminar coordinator	**Assoc. Prof. Dr. Habil. Augustin C. Moț**				
2.4. Year of study		2.5. Semester		2.6. Type of assessment	Exam
2.7. Course status	Optional			2.8. Course type	Specialisation subject

3. Total estimated time (hours per semester of teaching activities)

3.1. Number of hours per week	**3**	of which: 3.2. course	**2**	3.3. seminar/ laboratory/ project	**1**
3.4. Total of hours in the curriculum	36	of which: 3.5. course	24	3.6. seminar/ laboratory	**12**
Time allocation for individual study (IS) and self-taught activities (ST)					**hours**
Learning from textbooks, course materials, bibliography, and notes (IS)					**70**
Additional research in the library, on subject-specific electronic platforms, and on-site					**70**
Preparing seminars/ laboratories/ projects, assignments, reports, portfolios, and essays					**64**
Tutoring (professional guidance)					**6**
Examinations					**4**
Other activities					
3.7. Total hours of individual study (IS) and self-taught activities (ST)				**214**	
3.8. Total hours per semester				**250**	
3.9. Number of credits				**10**	

4. Prerequisites (where applicable)

4.1. curriculum-related	**Fundamental knowledge of statistics**
4.2 skills-related	**Basic use of MS Excel, Statistica, and Minitab**

5. Specific conditions (where applicable)

5.1. course-related	• A classroom equipped with a video projector is required • Students must attend the course with their mobile phones switched off
5.2. seminar/laboratory-related	• Students must attend seminars with their mobile phones switched off • Students must attend seminars at the scheduled date and time • Computers may be used only for the assigned seminar work • Bringing food into the seminar room is prohibited

6.1. Competencies resulting from the completion of the degree programme[1]

Professional competencies	
Competency code	**Competency**
PC1	Advanced expertise in chemistry and doctoral-level research topics
PC4	Planning, designing, and implementing an original scientific research project, in compliance with academic ethics and integrity
PC5	Applying and developing advanced research and analytical methods; critically interpreting data and formulating innovative solutions
Transversal competencies	
Competency code	**Competency**
TC2	Advanced scientific communication in Romanian and English; collaboration in interdisciplinary and multicultural settings
TC3	Advanced digital skills for research, data analysis, and dissemination; responsible use of digital tools.

6.2. Learning outcomes relevant to the degree programme (as referred to in the curriculum)[2]

Learning outcomes targeted by the subject		
Competency code	**Knowledge and comprehension**	**Specific academic skills**
PC1	Advanced and up-to-date knowledge in chemistry and the research field; critical understanding of the scientific literature.	Applies and synthesizes advanced concepts/theories to formulate research hypotheses; justifies the choice of scientific approaches.
PC4	Advanced research methodologies: experimental design, modern synthesis and characterization techniques, analysis and validation; principles of research project management.	Designs, plans and implements a research project; applies quality and safety procedures and documents stages and data with full traceability.
PC5	Advanced strategies for data analysis, interpretation, and integration; evaluation of methodological limitations, reproducibility, and scientific impact.	Critically analyses complex data, estimates uncertainty and formulates conclusions; proposes methodological improvements and directions for research/innovation.
TC2	Scientific terminology and communication in Romanian and English; the structure of scientific articles and presentations; good citation practices.	Writes and presents scientific results in Romanian/English coherently; provides well-argued responses to comments and peer reviews.
TC3	Digital tools for research, citation, and data processing (databases, specialized software, reference managers); responsible use of digital resources.	Uses discipline-specific digital tools effectively; manages citations; uses digital resources responsibly in research activities.

7. Subject-specific learning outcomes

Knowledge and comprehension
1. Advanced understanding of the principles of modern chemometrics and its role in advanced chemical research and analytical sciences.
2. Knowledge of multivariate experimental design methodologies (factorial designs, RSM, mixture designs) and their associated statistical foundations.

[1] The professional and/or transversal skills targeted by the subject for which the course description is prepared will be copied from the curriculum of the degree programme. For each competency, the complete entry, including the competency code, will be copied with the exact wording that appears in the curriculum, without any changes. If no competency is copied from either of the two categories, the row corresponding to that category is deleted from the table.

[2] The learning outcomes relevant for the degree programme and targeted by the subject for which the course description is prepared will be listed. The entries, copied without any changes from the Curriculum by subject type (Core Subject/Specialisation Subject/Complementary Subject), are listed under the corresponding competency.

3. Understanding of analytical signal processing methods, including filtering, transformations, and noise reduction.
4. Knowledge of multivariate analysis and pattern recognition methods (PCA, classification, multivariate regression) and model validation principles.
Specific academic skills
1. Ability to design and optimize complex experiments using experimental designs appropriate to analytical objectives.
2. Ability to preprocess and analyse complex chemical datasets, and to build and validate robust chemometric models.
3. Ability to critically interpret chemometric results and integrate them into doctoral research and scientific publications.

8. Contents

8.1. Course	**Teaching and learning methods**	**Remarks[3]**
8.1.1. Fundamentals of chemometrics and its role in doctoral research. The role of chemometrics in modern analytical sciences; types of chemical data and data structures; complete chemometric workflow (DoE, preprocessing, modelling, validation).	Lecture; Explanation; Discussion; Description; Problem-based learning	4 hours
8.1.2. Advanced experimental design. Fundamental DoE principles; full and fractional factorial designs; randomization, replication, blocking; screening vs. optimization.	Lecture; Explanation; Discussion; Description; Problem-based learning	4 hours
8.1.3. Response Surface & Mixture Design. Central Composite Design (CCD); Box–Behnken designs; mixture designs and constraints; simplex optimization.	Lecture; Explanation; Discussion; Description; Problem-based learning	4 hours
8.1.4. Analytical signal processing. Nature of instrumental noise; linear filters (Savitzky–Golay, smoothing); numerical derivatives; Fourier concepts in analytical chemistry.	Lecture; Explanation; Discussion; Description; Problem-based learning	4 hours
8.1.5. PCA and unsupervised pattern recognition. Concept of principal components; scores vs. loadings; preprocessing (autoscaling, centering); cluster analysis and chemical interpretation.	Lecture; Explanation; Discussion; Description; Problem-based learning	4 hours
8.1.6. Multivariate classification and calibration. Supervised classifiers; MLR, PCR, PLS; overfitting and validation; significant variable selection.	Lecture; Explanation; Discussion; Description; Problem-based learning	4 hours

Bibliography:

1. Richard G. Brereton, Chemometrics: Data Driven Extraction for Science, Wiley, 2018.
2. Alexey L. Pomerantsev, *Chemometrics in Excel*, Wiley, 2014.
3. Augustin C. Moț, Adrian-Ioan Dudu, Tiberiu Frentiu, Dorin Petreus, Erika-Andrea Levei, Zamfira Stupar, Maria Frentiu, Eniko Covaci, Cost-effective oxygen flask combustion and electrothermal vaporization capacitively coupled plasma microtorch optical emission spectrometry as a green and white method for multielemental determination in food, Journal of Analytical Atomic Spectrometry 41(1) (2026) 308–319.
4. Alexandra Gandea, Cezara Zagrean-Tuza, Eniko Covaci, Tiberiu Frentiu, Olivian Marincas, Emese Gal, Augustin C. Moț, Unravelling the bridge of polyphenol composition and mineralomics in Se biofortified edible Allium species, Journal of Food Composition and Analysis 135 (2024) 106648.
5. Bogdan Bosca, Augustin C. Mot, Novel simultaneous determination of alliin and allicin in Allium sp. using digital subtraction HPTLC, Journal of Chromatography B 1222 (2023) 123700.
6. Anca E. Anghel, Ibolya Balazs, Augustin C. Mot, Conventional versus Extended Standard Addition Method: Determination of Capsaicinoids in Topical Creams by High-Performance Liquid Chromatography – Diode Array Detection (HPLC-DAD), Analytical Letters 1 (2022) 1-16.

8.2. Seminar/ laboratory	**Teaching and learning methods**	**Remarks**
8.2.1. Complete chemometric workflow on real datasets. Exploratory Data Analysis; outlier detection; matrix structure of chemical data; guided mini-project.	Discussion; Description; Problem-based learning	2 hours

[3] For example, organisational aspects, recommendations for students, specific aspects relating to the course/seminar, such as inviting experts in the field, etc.

8.2.2. DoE applications. Building factorial designs in software; evaluation of main effects and interactions; interpretation of response surfaces; case study on analytical method optimization.	Discussion; Description; Problem-based learning	2 hours
8.2.3. Signal preprocessing and filtering. Smoothing vs. denoising; spectral derivatives; impact on multivariate models; method comparison.	Discussion; Description; Problem-based learning	2 hours
8.2.4. PCA applied to spectral data. PCA on large datasets; chemical interpretation of loadings; anomaly detection; individual mini-project.	Discussion; Description; Problem-based learning	2 hours
8.2.5. Supervised classification. Building classification models; sensitivity and specificity; external validation.	Discussion; Description; Problem-based learning	2 hours
8.2.6. PLS calibration on analytical data. Building PLS models; selection of number of factors; RMSEC, RMSEP, Q^2; evaluated final mini-project.	Discussion; Description; Problem-based learning	2 hours

Bibliography:

1. Richard G. Brereton, Chemometrics: Data Driven Extraction for Science, Wiley, 2018.
2. Alexey L. Pomerantsev, *Chemometrics in Excel*, Wiley, 2014.
3. Augustin C. Moț, Adrian-Ioan Dudu, Tiberiu Frentiu, Dorin Petreus, Erika-Andrea Levei, Zamfira Stupar, Maria Frentiu, Eniko Covaci, Cost-effective oxygen flask combustion and electrothermal vaporization capacitively coupled plasma microtorch optical emission spectrometry as a green and white method for multielemental determination in food, Journal of Analytical Atomic Spectrometry 41(1) (2026) 308–319.
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5. Bogdan Bosca, Augustin C. Mot, Novel simultaneous determination of alliin and allicin in Allium sp. using digital subtraction HPTLC, Journal of Chromatography B 1222 (2023) 123700.
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9. Evaluation

Type of activity	9.1 Evaluation criteria[4]	9.2 Evaluation methods[5]	9.3 Percentage in the final grade
9.4. Course	Accuracy of responses; correct acquisition and understanding of course topics	Written exam. Any attempt to cheat during the exam results in removal from the exam. Proven academic fraud is sanctioned by expulsion in accordance with UBB ECST regulations.	50%
9.5. Seminar/ laboratory	Accuracy of responses; correct acquisition and understanding of seminar topics	Practical test – computer-based test – conducted in the final week of teaching activity	50%
9.6 Minimum standard for passing			
Passing the course requires obtaining at least 50% of the points specified in the grading rubric in both the written exam and the practical test.			

[4] The evaluation criteria must directly reflect the learning outcomes targeted at the level of the degree programme respectively at the level of the subject. More specifically, the learning outcomes set out in the expected learning outcomes are assessed.

[5] Both final evaluation methods and ongoing evaluation strategies should be established.

10. SDG labels (Sustainable Development Goals)[6]

	○	Sustainable Development Generic Label

								
○	○	○	x	○	○	○	○	○
								No label applies
○	○	○	○	○	○	○	○	○

Date of entry:
05.02.2026

Signature of course coordinator

Assoc. Prof. Dr. Habil. Augustin C. Moț

Signature of seminar coordinator

Assoc. Prof. Dr. Habil. Augustin C. Moț

Date of approval in CDSC:

Signature of the Director of the DSC

Prof. dr. Niculina Daniela Hădade

[6] Select a single label which, according to the *Implementation of SDG labels in the academic process*, best matches the subject. If the subject addresses sustainable development in a generic manner (i.e. by presenting/introducing the general framework of sustainable development, etc.), then the Sustainable Development generic label may be applied. If none of the labels describe the subject, select the last option: *"No label applies."*