# COURSE DESCRIPTION

## 1. Programme Identification Data

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| **1.1** Higher Education Institution | **„ALEXANDRU IOAN CUZA” UNIVERSITY OF IAŞI** |
| **1.2** Faculty | **FACULTY OF CHEMISTRY** |
| **1.3** Department / Doctoral School | **DOCTORAL SCHOOL OF CHEMISTRY** |
| **1.4** Field of Study | **CHEMISTRY** |
| **1.5** Cycle of Studies | **DOCTORATE** |
| **1.6** Study Programme / Qualification | **ADVANCED UNIVERSITY STUDIES – DOCTORAL SCHOOL OF CHEMISTRY / PhD IN CHEMISTRY** |

## 2. Course Identification Data

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| **2.1** Course Title | | | **EXPERIMENTAL TECHNIQUES, PROCESSING AND INTERPRETATION OF RESEARCH RESULTS – MODULE II** | | | | |
| **2.2** Course coordinator (lectures) | | | **[NAME, ACADEMIC TITLE]** | | | | |
| **2.3** Seminar coordinator | | | **[NAME, ACADEMIC TITLE] (if applicable)** | | | | |
| **2.4** Year of study | **I** | **2.5** Semester | **1** | **2.6** Type of assessment | ***C** | **2.7** Disciple regime | ****OC** |

*[E – exam / C – colloquium] **[CC = Compulsory Course / OC = Optional Course]

## 3. Estimated Total Workload (hours per semester)

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|---|---|---|---|---|---|
| **3.1** Hours per week | **2.25** | **3.2** Lectures | **1.25** | **3.3.** Seminars | **1** |
| **3.4** Total hours according to the curriculum | **31.5** | **3.5** Lectures | **17.5** | **3.6.** Seminars | **14** |

| Time allocation | hours |
|---|---|
| Study based on textbooks, course materials, bibliographic sources, and other relevant resources | 10 |
| Additional research in the library, on specialized electronic platforms, and in the field | 15 |
| Preparation for seminars, assignments, papers, portfolios, essays | 10 |
| Academic tutoring | 4.5 |
| Assessment activities | 4 |
| Other activities | - |

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| **3.7** Total hours of individual study | 43.5 |
| **3.8** Total hours per semester | 75 |
| **3.9** Number of credits | **3** |

## 4. Preconditions (if applicable)

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| **4.1** Curriculum prerequisites | Graduation of a Master’s degree or an equivalent qualification. Enrollment in the doctoral study program in the field of Chemistry, in accordance with the regulations of the Doctoral School. |
| **4.2** Competences prerequisites | Basic competence in the use of scientific language specific to the field of Chemistry; the ability to analyze and interpret information from the scientific literature; competence in documenting and synthesizing scientific data; as well as competence in using a personal computer and data processing, analysis, and presentation applications (at least from the Microsoft Office suite). |

## 5. Conditions (if applicable)

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| **5.1** Conditions for lectures | Appropriate rooms for doctoral teaching equipped with multimedia equipment (video projector, PC), with access to the Internet, institutional IT infrastructure, and specialized software resources necessary for the processing, visualization, analysis, and interpretation of experimental data. |

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| | Compliance with institutional regulations regarding the organization of doctoral studies. |
| **5.2** Conditions for seminars | Appropriate rooms for doctoral teaching equipped with multimedia equipment (video projector, PC), with access to the Internet, institutional IT infrastructure, and specialized software resources necessary for the processing, visualization, analysis, and interpretation of experimental data.<br>Compliance with institutional regulations regarding the organization of doctoral studies. |

**6. Specific competences accumulated**

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| **Professional competences** | • Competence for critical and constructive evaluation of scientific research projects and results, with systematic reference to the current state of theoretical and methodological knowledge in the specialized field;<br>• Competence to select, adapt, and apply advanced research principles, theories, and methods, including through the use of interdisciplinary approaches, to address new and complex scientific problems;<br>• Competence to explain, analyze, and interpret experimental data and results from multiple perspectives in order to substantiate scientific conclusions;<br>• Systematic and in-depth knowledge of research concepts and methods, as well as the ability to communicate and engage in scientific dialogue with specialists in related fields. |
| **Transversal competence** | • Competence to develop creativity and initiative in the design and conduct of research projects;<br>• Competence to take responsibility for and organize research activities, both individually and within professional teams or structures;<br>• Competence to initiate, plan, and develop innovative theoretical and applied projects in academic and advanced research contexts. |

**7. Course Objectives**(derived from the acquired competences)

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| **7.1. General objective** | To develop the competence of doctoral students to identify, apply, and interpret advanced mathematical and statistical methods for the processing of experimental data obtained in scientific research, as well as to use specialized software tools for the rigorous analysis, visualization, and dissemination of research results. |
| **7.2. Specific objectives** | Upon completion of the course, the doctoral student will acquire the competence to:<br>• identify the main experimental techniques that generate complex and large datasets;<br>• apply appropriate methods to obtain and analyze correlations between experimental data;<br>• use software tools dedicated to the processing and management of experimental databases;<br>• apply methods and techniques for the visualization and graphical representation of experimental data, in accordance with the research objectives;<br>• comply with requirements related to intellectual property and the responsible use of specialized software in doctoral research activities. |

**8. Content**

| **8.1** | **Lecture Topics** | **Teaching methods*** | **Notes** (hours / references) |
|---|---|---|---|
| 1. | Experimental techniques for generating complex or large databases | Interactive lecture, explanation, conversation, demonstrative analysis, problematization | (4.5 hours, [1÷4]) |
| 2. | Advanced methods of mathematical processing of raw experimental data | Interactive lecture, explanation, conversation, demonstrative analysis, problematization | (4 hours, [1÷4]) |
| 3. | Correlation of experimental data using statistical methods and mathematical algorithms | Interactive lecture, explanation, conversation, demonstrative analysis, problematization | (4.5 hours, [1÷4]) |

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|---|---|---|---|
| 4. | Software tools to facilitate the processing of experimental data | Interactive lecture, explanation, conversation, demonstrative analysis, problematization | (4.5 hours, [5÷7]) |

*În cases of force majeure, teaching activities may be conducted online, in accordance with current legislation.

**Bibliography**


1. Li, X.; Dorman, F. L.; Helm, P. A.; et al. Nontargeted screening using gas chromatography atmospheric pressure ionization mass spectrometry: recent trends and emerging potential. Molecules, 26, 6911, **2021**. https://doi.org/10.3390/molecules26226911
2. Szabo, F. E. (Ed.) The Linear Algebra Survival Guide. Academic Press, Elsevier, **2015**.
3. Pluskal, T.; Castillo, S.; Villar-Briones, A.; Oresic, M. MZmine 2: modular framework for processing, visualizing, and analyzing mass spectrometry-based molecular profile data. BMC Bioinformatics, 11, 395, **2010**. https://doi.org/10.1186/1471-2105-11-395
4. Jolliffe, I. T.; Cadima, J. Principal component analysis: A review and recent developments. Philosophical Transactions of the Royal Society A, 374, 20150202, **2016**. https://doi.org/10.1098/rsta.2015.0202
5. Norris, G.; Duvall, R.; Brown, S.; Bai, S. EPA Positive Matrix Factorization (PMF) 5.0: Fundamentals and User Guide. U.S. Environmental Protection Agency, Office of Research and Development, Washington, DC, **2014**.
6. Wiley. KnowItAll® Software – Spectral Interpretation Tool. Disponibil online la: https://sciencesolutions.wiley.com/whitepapers-case-studies/, (accesat în scop educațional).
7. WaveMetrics. Tools for Igor Pro® Users. Disponibil online la: https://www.wavemetrics.com/users/tools, (accesat în scop educațional).


| **8.2** | **Seminar Topics** | **Teaching methods*** | **Notes** (hours / references) |
|---|---|---|---|
| 1. | Processing of complex data obtained by mass spectrometry techniques coupled with chromatographic techniques | Conversation, explanation, applicative analysis, problematization | (2 hours, [1÷4]) |
| 2. | Raw experimental data processing: data mediation, data normalization, IR spectrum processing, mass spectrum processing | Conversation, explanation, applicative analysis, problematization | (2 hours, [1÷4]) |
| 3. | Correlation Matrix, Principal Component Analysis and Positive Matrix Factorization in Data Processing | Conversation, explanation, applicative analysis, problematization | (2 hours, [1÷4]) |
| 4. | Software programs involved in optimizing data processing: KnowItAll, Igor Pro, Origin, SigmaPlot | Conversation, explanation, applicative analysis, problematization | (2 hours, [4÷7]) |
| 5. | Use of specialized data analysis programs KnowItAll, MZmine | Conversation, explanation, applicative analysis, problematization | (2 hours, [4÷7]) |
| 6. | Possibilities of graphical representation of experimental data using Origin, ChemDraw, CorelDraw | Conversation, explanation, applicative analysis, problematization | (2 hours, [4÷7]) |
| 7. | Ways to ensure intellectual property requirements for the use of specialised programmes | Conversation, explanation, applicative analysis, problematization | (2 hours, [4÷7]) |

*În cases of force majeure, teaching activities may be conducted online, in accordance with current legislation.

**Bibliography**


1. Szabo, F. E. (Ed.) The Linear Algebra Survival Guide. Academic Press, Elsevier, **2015**.
2. Pluskal, T.; Castillo, S.; Villar-Briones, A.; Oresic, M. MZmine 2: Modular framework for processing, visualizing, and analyzing mass spectrometry-based molecular profile data. BMC Bioinformatics, 11, 395, **2010**.
3. Jolliffe, I. T.; Cadima, J. Principal component analysis: A review and recent developments. Philosophical Transactions of the Royal Society A, 374, 20150202, **2016**.
4. Norris, G.; Duvall, R.; Brown, S.; Bai, S. EPA Positive Matrix Factorization (PMF) 5.0: Fundamentals and User Guide. U.S. Environmental Protection Agency, Office of Research and Development, Washington, DC, **2014**.
5. WaveMetrics. Introduction to Igor Pro. Disponibil online la: https://www.wavemetrics.net/doc/igorman/I-01%20Intro.pdf, (accesat în scop educațional).

6. WaveMetrics. Tools for Igor Pro® Users. Disponibil online la: https://www.wavemetrics.com/users/tools, (accesat în scop educațional).
7. OriginLab Corporation. Origin User Guide. Disponibil online la: https://www.originlab.com/doc/User-Guide, (accesat în scop educațional).

**9. Learning Outcomes**

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| **Knowledge and understanding** | • explain the fundamental principles of experimental techniques used in chemical research, with a focus on experimental data generation;<br>• describe the types and characteristics of experimental data obtained using different analytical and experimental techniques;<br>• understand the role of basic mathematical and statistical methods in the processing and interpretation of experimental data;<br>• recognize the importance of rigorous experimental data processing for the validity and reproducibility of research results. |
| **Application and analysis** | • apply appropriate procedures for the organization, processing, and filtering of raw experimental data;<br>• use statistical methods and mathematical tools for the analysis and correlation of experimental data;<br>• apply specialized software applications for the processing, visualization, and interpretation of experimental datasets;<br>• analyze experimental data in relation to research objectives and the experimental techniques used. |
| **Critical Assessment and Accountability** | • assess the quality and consistency of experimental data obtained using different experimental techniques;<br>• evaluate the impact of data processing methods on scientific interpretation and conclusions;<br>• demonstrate responsibility in the management, use, and reporting of experimental data in doctoral research;<br>• justify the need to comply with good practices in the processing and interpretation of experimental data. |
| **Academic Communication** | • communicate, orally and in writing, the results obtained from the processing and interpretation of experimental data in a coherent and well-reasoned manner;<br>• use scientific language specific to the field of Chemistry in the presentation of data and research results;<br>• actively participate in academic discussions on the interpretation and representation of experimental data;<br>• present datasets and experimental results clearly and in a structured manner in academic and scientific contexts. |

**10. Correlation of the course content with the expectations of community representatives, professional associations, and representative employers in the field related to the program.**

The content of the course *Experimental techniques, processing and interpretation of research results – Module II* is aligned with the requirements of the academic environment and scientific research by fostering the competence necessary for the selection and effective use of methods and tools for experimental data processing.
Upon successful completion of the discipline, the doctoral student will acquire the competence to select and apply appropriate methods and tools for data processing and interpretation, while adhering to the principles of ethics and research integrity in their use for the preparation and dissemination of scientific manuscripts.

**11. Assessment**

| **Activity** | **11.1 Assessment criteria** | **11.2 Assessment methods** | **11.3 Weight in final grade (%)** |
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| **11.4** Course | The correctness and coherence of the answers, as proof of the correct understanding and application of the issues dealt with in the course. | Colloquium – oral presentation on the main experimental techniques for generating complex or large databases. | 70 |

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| **11.5** Seminar | Correctness of answers and ability to apply data processing tools in research. | Presentation – presentation on the use of experimental data processing tools in research. | 30 |
| **11.6** Minimum Performance Standard | | | |
| In order to pass the discipline, the doctoral student must demonstrate:<br>• competence in identifying the main methods and tools for the processing and analysis of complex or large datasets;<br>• competence in selecting and using appropriate software tools for the processing of experimental data specific to the field of doctoral research. | | | |

Date of completion
26.09.2024

Course coordinator

Seminar coordinator

Date of approval

Director of the Doctoral School of Chemistry
Prof. univ. dr. habil. Cecilia ARSENE