COURSE DESCRIPTION

1. Program data

1.1 Higher education institution	**"ALEXANDRU IOAN CUZA" UNIVERSITY OF IASI**
1.2 Faculty	**CHEMISTRY**
1.3 Department	**DOCTORAL SCHOOL OF CHEMISTRY**
1.4 Field of study	**CHEMISTRY**
1.5 Cycle of studies	**DOCTORATE**
1.6 Study Programme/Qualification	**DOCTOR OF CHEMISTRY**

2. Discipline data

2.1 Name of the discipline			**EXPERIMENTAL TECHNIQUES AND DATA HANDLING IN CHEMISTRY– MODULE II**				
2.2 Course Activity Holder							
2.3 Owner of seminar activities							
2.4 Year of study	**I**	**2.5** Semester	**1**	**2.6** Type of evaluation	**C**	**2.7** Discipline regime	**OP**

** OB – Mandatory / OP – Optional*

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

3.1 Number of hours per week	**3**	of which: **3.2** course	**2**	**3.3.** Seminar	**1**
3.4 Total hours in the curriculum	**42**	of which: **3.5**. course	**28**	**3.6.** Seminar	**14**
Distribution of the time fund					hours
Study by textbook, course material, bibliography and others					20
Additional documentation in the library, on specialized electronic platforms and in the field					50
Preparation of seminars/laboratories, assignments, papers, portfolios and essays					20
Tutoring					4
Examination					4
Other activities					10

3.7 Total individual study hours	108
3.8 Total hours per semester	150
3.9 Number of credits	**6**

4. Preconditions (if applicable)

4.1 Curriculum	
4.2 Competences	

5. Conditions (if applicable)

5.1 Course Conduct	
5.2 Conduct of the laboratory	

6. Specific competences accumulated

Professional skills	Critical-constructive evaluation of projects and results of scientific research, assessment of the state of theoretical and methodological knowledge; identifying the priorities of knowledge and application to the field; Selection and application of principles, theories and advanced methods of knowledge, transfer of methods from one field to another, interdisciplinary approaches to solve theoretical and practical problems, new and complex; Use of advanced principles and methods for explaining and interpreting, from multiple perspectives, new and complex theoretical and practical situations/problems, specific to the field; Systematic, advanced knowledge of concepts, research methods, controversies and new hypotheses specific to the field; communication with specialists in related fields.
Transversal competence	Development of projects centered on creativity, as a basis for self-realization; Assuming responsibility and capacity to organize and manage the activity of professional groups, scientific research or organizations/institutions; Initiation and innovative development of complex theoretical and practical projects.

7. Objectives of the discipline (from the grid of specific competences accumulated)

7.1. General objective	The course aims to help the students of the doctoral school to easily identify advanced methods of mathematical processing of the experimental data obtained during the research, and their important role in disseminating the results. The course will introduce the main software methods and tools that could be used in experimental data processing. In addition, the course aims to inform doctoral students about the existence of an important variety of tools and programs that allow and facilitate the processing, visualization, and interpretation of databases obtained during research within doctoral activities.
7.2. Specific objectives	Upon successful completion of this discipline, students will be acquainted: ▪ what are the main techniques for generating complex and large databases; ▪ what are the main methods of obtaining correlations between experimental data; ▪ what are the tools used to facilitate the processing of databases; ▪ what are the main tools for visualization and graphical representation of experimental data ▪ how to ensure intellectual property requirements in the case of the use of specialized software;

8. Content

8.1	**Course**	**Teaching methods**	**Observations** (hours and bibliographic references)
1.	Experimental techniques for generating complex or large databases	Lecture, explanation, conversation, description, problematization	(4 ore, [1-4])
2.	Advanced methods of mathematical processing of raw experimental data	Lecture, explanation, conversation, description, problematization	(4 ore, [1-4])
3.	Correlation of experimental data using statistical methods and mathematical algorithms	Lecture, explanation, conversation, description, problematization	(4 ore, [1-4])
4.	Software tools to facilitate the processing of experimental data	lecture, explanation, conversation, description, Problematization	(4 ore, [5-7])
5.	Analysis of experimental data using modern tools	Lecture, explanation, conversation, description, problematization	(4 ore, [5-7])
6.	Modern tools for graphical representation of experimental data	Lecture, explanation, conversation, description, problematization	(4 ore, [5-7])

7.	Data reporting and intellectual property in the case of the use of specialized data processing programs	Lecture, explanation, conversation, description, problematization	(4 ore, [5-8])

Bibliography

1. Li, X, Dorman, F. L., Helm, P. A., Kleywegt, S., Simpson, A., Simpson, M. J., Jobst, K. J., Nontargeted screening using gas chromatography atmospheric pressure ionization mass spectrometry: recent trends and emerging potential. Molecules, 26, 6911, **2021**.
2. Fred, E., Szabo, C, Editor(s): Fred E. Szabo, The Linear Algebra Survival Guide, Academic Press, Pages 47-77, ISBN 9780124095205, https://doi.org/10.1016/B978-0-12-409520-5.50010-2, **2015**.
3. Pluskal,T., Castillo,S., Villar-Briones,A. and Oresic,M., MZmine 2: modular framework for processing, visualizing, and analyzing mass spectrometry-based molecular profile data, BMC Bioinformatics, 11, 395, **2010**.
4. Jollife, I.T., Cadima J., Principal component analysis: A review and recent developments. Philos Trans R Soc A, **2016**.
5. Norris, G., Duvall, R., Brown, S., Bai, S., EPA Positive Matrix Factorization (PMF) 5.0 Fundamentals and User Guide, Environmental Protection Agency Office of Researc and Development, Publushing House Whashington, DC 20460, **2014**.
6. Wiley's KnowItAll Software as a Spectral Interpretation Tool, https://sciencesolutions.wiley.com/whitepapers-case-studies/
7. Tools for Igor Pro® Users: https://www.wavemetrics.com/users/tools
8. Wiley Rights & Permissions Portal: https://www.wiley.com/en-us/permissions

8.2	**Seminar**	**Teaching methods**	**Observations** (hours and bibliographic references)
1.	Processing of complex data obtained by mass spectrometry techniques coupled with chromatographic techniques	The lecture, the explanation, the conversation Description, Problematization	(2 ore, [1-4])
2.	Raw experimental data processing: data mediation, data normalization, IR spectra processing, mass spectra processing	The lecture, the explanation, the conversation Description, Problematization	(2 ore, [1-4])
3.	Correlation matrix, principal component analysis, and positive matrix factorization in data processing	The lecture, the explanation, the conversation Description, Problematization	(2 ore, [1-4])
4.	Software programs involved in data processing optimization: KnowItAll, Igor Pro, Origin, SigmaPlot	The lecture, the explanation, the conversation Description, Problematization	(2 ore, [4-8])
5.	Use of specialized programs in data analysis KnowItAll, MZmine	The lecture, the explanation, the conversation Description, Problematization	(2 ore, [4-8])
6.	Possibilities of graphical representation of experimental data using Origin, ChemDraw, CorelDraw	The lecture, the explanation, the conversation Description, Problematization	(2 ore, [4-8])
7	Ways to ensure intellectual property requirements for the use of specialized programs	The lecture, the explanation, the conversation Description, Problematization	(2 ore, [4-8])

Bibliography

1. Fred, E., Szabo, C, Editor(s): Fred E. Szabo, The Linear Algebra Survival Guide, Academic Press, Pages 47-77, ISBN 9780124095205, https://doi.org/10.1016/B978-0-12-409520-5.50010-2, **2015**.
2. Pluskal,T., Castillo,S., Villar-Briones,A. and Oresic,M., MZmine 2: modular framework for processing, visualizing, and analyzing mass spectrometry-based molecular profile data, BMC Bioinformatics, 11, 395, **2010**.
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4. Norris, G., Duvall, R., Brown, S., Bai, S., EPA Positive Matrix Factorization (PMF) 5.0 Fundamentals and User Guide, Environmental Protection Agency Office of Researc and Development, Publushing House Whashington, DC 20460, **2014**.
5. Introduction to Igor Pro: https://www.wavemetrics.net/doc/igorman/I-01%20Intro.pdf
6. Tools for Igor Pro® Users: https://www.wavemetrics.com/users/tools
7. Origin user guide: https://www.originlab.com/doc/User-Guide
8. Wiley Rights & Permissions Portal: https://www.wiley.com/en-us/permissions

9. Corroborating the content of the discipline with the expectations of the representatives of the community, professional associations and representative employers in the field related to the program

After completing and promoting the discipline, the student will have the necessary knowledge to be able to select methods and tools for data processing and will know what to do to avoid the occurrence of a problem of ethics and integrity in research when using them for the preparation of a scientific manuscript.

10. Evaluation

Activity Type	**10.1 Evaluation criteria**	**10.2 Evaluation methods**	**10.3 Weight in final grade (%)**
10.4 Course	Correctness of answers – understanding and correct application of the issues dealt with in the course.	Colloquium –Lecture on the main experimental techniques for generating complex or large databases.	70
10.5 Seminar	Correctness of answers – the correct acquisition and understanding of the issues dealt with at the seminar.	Lecture on how to use data processing tools in research.	30
10.6 Minimum Performance Standard			
▪ Identification of the main methods and tools for processing and analyzing complex or large data; ▪ Choosing a suitable software tool in the processing of experimental data in the field of doctoral research; ▪ Knowledge of the ways to avoid the occurrence of a problem of ethics and integrity in research.			

Date of completion Course holder Seminar holder

28.09.2022

Date of approval

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