

**COURSE DATA****Data Subject**

<b>Code</b>	44994
<b>Name</b>	Estrategias analíticas para la resolución de problemas socio-económicos
<b>Cycle</b>	Master's degree
<b>ECTS Credits</b>	5.0
<b>Academic year</b>	2023 - 2024

**Study (s)**

<b>Degree</b>	<b>Center</b>	<b>Acad. year</b>	<b>Period</b>
2249 - M.D. in Chemistry	Faculty of Chemistry	1	First term

**Subject-matter**

<b>Degree</b>	<b>Subject-matter</b>	<b>Character</b>
2249 - M.D. in Chemistry	1 - Aplicaciones de la Química Analítica	Obligatory

**Coordination**

<b>Name</b>	<b>Department</b>
PEREZ GUAITA, DAVID	310 - Analytical Chemistry

**SUMMARY**

"Analytical Strategies for solving socio-economic problems" is part of the Applied Chemistry module and is intended to expand and complement the knowledge of Analytical Chemistry acquired in the Degree. Specifically, this course deepens student's knowledge of quality assurance of the analytical process; chemometric treatment of data as a tool for obtaining quality information, both qualitative (exploratory analysis) and quantitative; stages of preparation and treatment of samples introducing assisted systems and microextraction techniques and study of advanced instrumental analysis techniques including the sustainability of procedures, the use of automated systems, direct measurements and portable instrumentation.

Data treatment will focus on exploratory analysis through principal component analysis and classification problems applying discriminant analysis, ending with the use of multivariate regression through partial least squares. Advanced instrumental techniques such as the application of automation and sensors for the control of products and processes will be studied.



Finally, special importance will be given to applications so that the student acquires a practical and functional vision of the subjects studied.

## PREVIOUS KNOWLEDGE

### Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

### Other requirements

Previous knowledge of chemistry and mathematics that is taught in the degrees indicated in the recommended entry profile for the Master student is required.

## OUTCOMES

### 2249 - M.D. in Chemistry

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.
- Students should demonstrate self-directed learning skills for continued academic growth.
- Students should possess and understand foundational knowledge that enables original thinking and research in the field.
- Be able to solve complex chemistry problems, whether in the academic, research or industrial application areas at a specialization or masters-level.
- Possess the necessary skills to develop multidisciplinary activities within the field of chemistry at the master's level.
- Promote, in academic and professional contexts in the field of economic policy, ... technological, social or cultural progress within a society based on knowledge and respect for: a) fundamental rights and equal opportunities between men and women, b) the principles of equal opportunities and universal accessibility for people with disabilities and c) the values of a culture of peace and of democratic values.
- Possess the ability to plan and manage time and resources and gain experience in decision-making.
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- Gain experience in the use of information tools and in the management of the information obtained.
- Be able to defend positions in debates and colloquia in a rigorous and reasoned manner.
- Be able to design, conduct, analyse and interpret complex experiments and data, as a specialist.
- Gain skills and knowledge in advanced analytical techniques that can contribute to the economic and social development of the environment.
- Apply the advanced theoretical and practical knowledge gained in the different specialties of chemistry to R&D and innovation.
- Be able to conduct any type of research in the field of chemistry and/or the chemical industry, as a specialist.
- Be able to present and defend publicly the results obtained in scientific research or as a result of work in a chemical industry.

## LEARNING OUTCOMES

- Describe the fundamental aspects of European standards regarding the quality of analytical methods.
- Select and apply, among the main multivariate chemometric analysis techniques, the one that is / are most appropriate for the treatment of complex analytical data, and adequately interpret the results obtained.
- Explain the basis of the main advanced techniques for sample treatment, and describe the effect of the different experimental variables on the results.
- Describe the procedures for monitoring and controlling chemical processes, as well as the methods for control emissions and industrial chemical wastes.
- Detail the experimental methodology applied in methods of analysis of industrial interest, including the sample preparation, the analytical technique, the selection of experimental variables, the treatment of the records obtained and the interpretation of the results.
- Knowing how to apply the knowledge acquired to contribute to the Sustainable Development Goals (SDGs), such as the sustainable management of water, raw materials and energy sources (SDGs 6 and 7) and to develop a professional work with the least environmental impact and using alternative raw materials (SDGs 11, 14 and 15).

## DESCRIPTION OF CONTENTS

### 1. Quality criteria for analytical methods

Validation of analysis methods. Study of applicable standards.

**2. Application of multivariate analysis techniques to the study of analytical data**

Exploratory data analysis. Classification techniques. Multivariate regression. Study of practical cases.

**3. Advanced sample preparation and separation methods**

Use of assisted systems for sample preparation. Microextraction techniques. New developments.

**4. Analytical procedures for the control of chemical processes.**

Advanced instrumental analysis techniques. Sustainability of analytical procedures. Automatic and continuous equipment for product and process analysis.

**5. Study of methods of analysis of industrial interest**

Analysis of basic chemical products: raw materials, solvents,... Analysis of formulations: active principles, additives, contaminants,...

**WORKLOAD**

ACTIVITY	Hours	% To be attended
Theory classes	40,00	100
Tutorials	10,00	100
Study and independent work	75,00	0
<b>TOTAL</b>	<b>125,00</b>	

**TEACHING METHODOLOGY**

The course will be taught in asynchronous online mode. Among other training activities, applied practical problems will be solved in order to evaluate the student's understanding of the subject. In addition, use will be made of the Virtual Classroom platform, a virtual space where all the information considered appropriate for the development of teaching and control of student participation in the proposed activities is deposited.

**EVALUATION**

First call: The grade of the subject in the first call will be obtained from the marks obtained in the final exam and the continuous assessment activities carried out throughout the course. Exam and continuous assessment activities will be averaged according to the following percentages:



(a) On-site final exam: 70%.

(b) Continuous assessment activities: 30% (Presentation of assignments 15%, other activities 15%).

The minimum grade in each of the parts must be equal to or higher than 4.5 in order to be able to make the average. The minimum overall grade to pass the course will be 5.0.

Second call: The grade of the subject, in the second call, will be obtained by applying the same criteria as in the first call.

## REFERENCES

### Basic

- Eurolab España. P.P. Morillas y colaboradores. Guía Eurachem: La adecuación al uso de los métodos analíticos Una Guía de laboratorio para la validación de métodos y temas relacionados (1ª ed. 2016). Disponible en [www.eurachem.org](http://www.eurachem.org)
- International Organization for Standardization. (2017). Evaluación de la conformidad. Requisitos generales para la competencia de los laboratorios de ensayo y de calibración (ISO Standard No. 17025)
- Abu-Mostafa, Y.S.; Magdon-Ismail, M.; Lin, H.-T. Learning from Data: A Short Course; AMLbook.com: S.I., 2012; ISBN 978-1-60049-006-4
- Cámara C. (ed.), Fernández P., Martín Esteban A., Pérez-Conde C. i Vidal M. Toma y tratamiento de muestras. Editorial Síntesis, Madrid, 2002
- A. Ríos Castro, M. C. Moreno Bondi, B. M. Simonet Suau (coords.) Técnicas espectroscópicas en química analítica (vol. I y II). Editorial Síntesis, Madrid, 2012
- Skoog D. A., Holler, F. J., Crouch S.R., Principios de Análisis Instrumental. 7a ed., Cengage Learning, Ciudad de México, 2018

### Additional

- Sagrado S., E. Bonet, M. J. Medina i Y. Martín. Manual Práctico de Calidad en los Laboratorios. Enfoque ISO 17025. AENOR Ediciones 2005
- Hibbert D.B., Quality Assurance in the Analytical Chemistry Laboratory. Oxford University Press, Oxford, 2007
- 2002/657/CE: Decisión de la Comisión, de 12 de agosto de 2002, por la que se aplica la Directiva 96/23/CE del Consejo en cuanto al funcionamiento de los métodos analíticos y la interpretación de los resultados.



- Blanco M., Cerdà V., Temas avanzados de Quimiometría, Universitat de les Illes Balears, 2007
- Pawliszyn J. (ed.), Comprehensive Sampling and Sample Preparation, Academic Press, Oxford, 2012
- De la Guardia M., Garrigues S. (eds.), Handbook of Green Analytical Chemistry, John Wiley and sons, Chichester, 2012

