

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

|                      |  |
|----------------------|--|
| <b>Code</b>          | 42931                                    |
| <b>Name</b>          | Calibration, data processing and quality |
| <b>Cycle</b>         | Master's degree                          |
| <b>ECTS Credits</b>  | 2.0                                      |
| <b>Academic year</b> | 2022 - 2023                              |

**Study (s)**

| <b>Degree</b>  | <b>Center</b>        | <b>Acad. year</b> | <b>Period</b> |
|--|----------------------|-------------------|---------------|
| 2109 - Master's Degree in Experimental Techniques in Chemistry | Faculty of Chemistry | 1                 | First term    |

**Subject-matter**

| <b>Degree</b>  | <b>Subject-matter</b>   | <b>Character</b> |
|--|---|------------------|
| 2109 - Master's Degree in Experimental Techniques in Chemistry | 1 - Advanced laboratory of experimental techniques in chemistry | Obligatory       |

**Coordination**

| <b>Name</b>             | <b>Department</b>          |
|-------------------------|----------------------------|
| ESCUDER GILABERT, LAURA | 310 - Analytical Chemistry |
| SAGRADO VIVES, SALVADOR | 310 - Analytical Chemistry |

**SUMMARY**

Course dedicated to practical learning in the computer classroom, of advanced chemometric techniques, for use in various aspects of interest in the chemical laboratory such as the calibration of instruments, data processing, and quality assurance

**PREVIOUS KNOWLEDGE**

**Relationship to other subjects of the same degree**

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

**Other requirements**

Prior knowledge of chemistry and experimental work in the laboratory of chemistry taught in the degrees indicated in the recommended income profile for the student of the master's degree are required.

**COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)****2109 - Master's Degree in Experimental Techniques in Chemistry**

- To acquire basic skills to develop laboratory work in biomedical research.
- Be able to access the information required (databases, scientific articles, etc.) and to interpret and use it sensibly.
- Ser capaces de seleccionar y optimizar las variables instrumentales para obtener los mejores parámetros analíticos en las técnicas experimentales estudiadas.
- Ser capaces de emplear las herramientas básicas para el tratamiento de datos experimentales en el laboratorio.
- Realizar estudios relacionados con el análisis y/o la caracterización de sustancias químicas tales como: control de calidad, diseño de protocolos de trabajo para laboratorios, diseño e implementación de procesos de acreditación y validación, diseño y desarrollo de proyectos I+D+I, emisión de informes, certificaciones y/o dictámenes, etc.
- Ser capaces de planificar y gestionar los recursos disponibles de un laboratorio químico, teniendo en cuenta los principios básicos de la calidad, prevención de riesgos, seguridad y sostenibilidad.
- Seleccionar la instrumentación química comercializada apropiada para el estudio a realizar y de aplicar sus conocimientos para utilizarla de manera correcta.
- To prepare a clear and concise memory of the results of your work and the conclusions obtained.

**LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)**

At the end of the teaching-learning process, the student should be able to:

1. Use protocols of calibration and verification of instruments and validation of analytical procedures.
2. Use statistics related to the establishment of a model and its quality.
3. Extract information on quality parameters of a method and develop the corresponding experimental.
4. Characterize an analytical result.
5. Organize and characterize multivariate data.
6. Adjust protocols of multivariate analysis based on the objective of the problem.
7. Relationships between objects, variables, and objects-variables.
8. Calibrate, validate and apply multivariate regression models.
9. Regarding the Sustainable Development Goals (SDGs), it is expected that students will be able to



know in this subject how to apply the knowledge learned to guarantee an inclusive, equitable, and quality education and promote learning opportunities for everyone (SDG 4), to acquire a special sensitivity for sustainable management of water (SDG 6), raw materials and energy sources (SDG 7), as well as for an environmentally friendly and sustainable development (SDGs 11, 12, 13, 14 and 15), in addition to being able to design, select and/or develop efficient products, chemical processes, and analytical methodologies (SDG 7) that minimize their impact on the environment (SDGs 14 and 15), using alternative raw materials and reducing wastes (SDG 11).

## DESCRIPTION OF CONTENTS

### 1. Calibration of instruments and procedures for the quality assurance.

- Design, monitoring and evaluation of protocols of calibration and verification of instruments: gas chromatographs.
- Inference and descriptive in the validation of chemical analysis, environmental, industrial, food and sanitary procedures.
- Horwitz equation, uncertainty function and identification criteria.
- Characterization of analytical results obtained in procedures related with analysis environmental, industrial, food and health.

### 2. Techniques of multivariate analysis

- Exploratory analysis of environmental data through PCA.
- Characterization of the quality of drinking water using PCA
- Characterization of the quality of beach water using PCA
- Identification of food frauds by PLS
- Multi-component (Ca, Mg) in drinking water using PLS2
- Advanced estimate of one analyte from others by PLS

**WORKLOAD**

| ACTIVITY                             | Hours        | % To be attended |
|--------------------------------------|--------------|------------------|
| Laboratory practices                 | 20,00        | 100              |
| Development of individual work       | 6,00         | 0                |
| Study and independent work           | 12,00        | 0                |
| Readings supplementary material      | 6,00         | 0                |
| Preparation of evaluation activities | 6,00         | 0                |
| <b>TOTAL</b>                         | <b>50,00</b> |                  |

**TEACHING METHODOLOGY****Presential Activities**

Laboratory classes will begin with seminars in which Professor will perform a brief introduction of the objective, fundamentals and experimental practices methodology to perform.

The teacher will held in the laboratory the necessary explanations on operation of the instruments to be used in each practice prior to their use by students and will supervise its use during practices, to enhance knowledge on the techniques used.

Students will carry out the practice following the corresponding protocols or manual of practices.

Classroom activities performed in the laboratory, presentations and exhibitions of works will be part of the ongoing evaluation of the student (formative activities AF2 of verifica and teaching methodology MD1 of verifica)

Written examinations of the subject will be carried out on the date specified in the programming of the assessment tests (formative activities AF4 of verifica and teaching methdology MD1 of verifica).

The competences to acquire from the presential activities will be:

- Generals: CG1 and CG3
- Specific: CE2, CE3, CE4, CE5 y CE6

**Non-presential activities**

Students will conduct the non-presential activities requested by the teacher (memoirs, reports of practices, etc.) and they will deliver them on the specified date.

The competences to acquire from the presential activities will be:



- Specific: CE7

## EVALUATION

1. -Continuous evaluation of the student in classes and seminars (participatory assistance, material handling and equipment, organization of work, understanding and use of the screenplay of practices, performing calculations, team work, etc. )

Along the sessions, focus in the resolution of practical assays, the assistance and participation of the students will be evaluated individually (by oral answers or by writing questions planned by the professor, by planning questions which its answer will be relevant for all the group). Also, these questions will include the design of working protocols, the selection of variables and the tools for the data treatment (verifica competences CE2, CE3, CE5 and CE6). The practical sessions will be carried out in work groups (Competence of the verifica CG1), and will be based on the questioning of doubts and review of key aspects of the correct planning of the exam (without using the software). The competences to evaluate: specifics: CE2, CE3, CE4, CE5 and CE6

**WEIGHT 40 %**

2.- An assessment of non-classroom-based activities (memories and/or reports of practices delivered)

The reports performed by the students will include the main conclusions extracted from the laboratory work (working protocols, variable selection and data treatment; verifica competences CE2, CE5, CE6 and CE7) and it will be done by couples to improve the group working (consensus decision making: verifica competences CG1 and CE7)

**WEIGHT 30 %**

3. -Written examinations (Based on the results of learning the content and on the specific objectives of each subject)

The exam will consist in the resolution of questions and practical examples related to the studied techniques (verifica competences: CE2, CE4, CE5 and CE6).

**WEIGHT 30 %**





## REFERENCES

### Basic

- EURACHEM Quantifying Uncertainty in Analytical Measurement (2012)  
[https://www.eurachem.org/images/stories/Guides/pdf/QUAM2012\\_P1.pdf](https://www.eurachem.org/images/stories/Guides/pdf/QUAM2012_P1.pdf)
- Massart D.L., B.G.M. Vandeginste, L.M.C. Buydens, S. De Jong, P.J. Lewi y J. Smeyers-Verbeke. Handbook of Chemometrics and Qualimetrics: Part A y B, Elsevier, Amsterdam, 1997.
- Miller J.C. y J.N. Miller. Estadística y Quimiometría para Química Analítica. Pearson Education S.A. Madrid, 2002.
- Molins-Legua C., S. Meseguer-Lloret, Y. Moliner-Martínez y P. Campíns-Falcó. TRAC 2006 25, 282-290.
- Sagrado S., E. Bonet, M.J. Medina y Y. Martín. Manual Práctico de Calidad en los Laboratorios. Enfoque ISO 17025. AENOR 2005.