

# Bachelor's Degree in Chemistry

## Subject Guide

### 1. Information about the subject

|                             |                                |                            |                     |
|-----------------------------|--------------------------------|----------------------------|---------------------|
| <b>SUBJECT</b>              | Analytical Chemistry III       | <b>CODE</b>                | GQUIMI01-3-010      |
| <b>EDUCATIONAL OFFER</b>    | Bachelor's Degree in Chemistry | <b>CENTER</b>              | Facultad de Química |
| <b>TYPE</b>                 | Compulsory                     | <b>N° TOTAL CREDITS</b>    | 6.0                 |
| <b>PERIOD</b>               | Second Semester                | <b>LANGUAGE</b>            | Spanish             |
| <b>COORDINATORS/ES</b>      |                                | <b>EMAIL</b>               |                     |
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### 2. Context

This course is part of the **Fundamental Module** in the subject **Analytical Chemistry**, and with the course Analytical Chemistry II, both taught in the **third year** of the Degree in Chemistry, complete an integrated view of the theories and methods for solving a variety of real problems in chemical analysis. According to a recent study about the professional status of European Chemists, nearly 70% of them consider chemical analysis as either the main or an extremely important part of their job description. Analytical instrumentation is crucial to solve chemical problems in many different fields such as medicine, food science, materials science, environmental control etc. Therefore, a Chemist must understand the fundamentals of common analytical techniques and their capabilities and shortcomings. In this way, he/she will be able to select the appropriate technique or techniques to be used for solving a specific problem, design the analytical experiment to provide relevant data, and

ensure the data obtained are valid.

Analytical Chemistry III is divided into three blocks. **Block I** provides a complete description of **separation techniques**, such as chromatography and electrophoresis, which are crucial in today's laboratories. Taking into account the expanding role of bioanalytical chemistry in academic and industrial environments, **Block II** moves into the realm of **Bioanalysis**, giving an overview of immunoassays and biosensors. **Block III** then tackles the study of basic **chemometric** tools used in the selection and optimization of analytical methods, and to provide maximum relevant chemical information from the chemical data.

The course will be taught by professors from the Department of Physical and Analytical Chemistry, Area of Analytical Chemistry and is a **key subject** to the course Experimentation in Analytical Chemistry II (4th year)

### 3. Requirements

**Analytical Chemistry III** requires previous knowledge on the basic principles of Analytical Chemistry. To undertake this course it is mandatory to have passed the subject **Analytical Chemistry I (Key subject)** in the second year. It is also advisable to have completed Experimentation in Analytical Chemistry I (second year) and concurrently be taking Analytical Chemistry II (third year).

### 4. Competencies and learning results

The **generic competences** to be developed during this course (not in order of importance) are:

- Capacity for analysis and synthesis (CG-1).
- Solve problems effectively (CG-2).
- Oral and written communication in English (CG-7).
- Ability to learn autonomously (CG-9).
- Acquiring motivation for quality (CG-11).
- Sensitizing with subjects related to the environment. Develop an environmental awareness (CG-12).
- Develop critical reasoning (CG-17).
- Teamwork (CG-18).

As **subject-specific competences**, we identified the following as relevant for this course:

- Ability to apply the principles and procedures of chemical analysis for the separation, identification, determination, and characterization of chemical compounds (GE-6).
- Ability to relate the principles of analytical techniques and their applications (CE-15).
- Ability to apply metrology to chemical processes and products, including quality management (CE-18).
- Ability to demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of Chemistry (CE-19).
- Ability to apply such knowledge and understanding to the solution of qualitative and quantitative problems of a familiar nature (CE-20).
- Skills in the evaluation, interpretation and synthesis of chemical information and data (CE-22).
- Computational and data-processing skills, relating to chemical information and data (CE-24).
- Ability to interpret data derived from laboratory observations and measurements in terms of their significance, and relate them to appropriate theory (CE-30).
- Ability to correlate Chemistry with other disciplines (CE-34).
- Ability to perform calculations and error analysis, using correct magnitudes and units (CE-35).

**Learning outcomes** for this course will focus on developing a fundamental understanding of the following topics:

1. Understand the fundamental principles of, procedures used, and relevant terminology associated with separations techniques and bioanalysis.
2. Relate knowledge and understanding to critically evaluate the use and limitations of separation techniques and bioanalysis.
3. Develop the intellectual skills to integrate theory and practice related to separations techniques and bioanalysis to solve qualitative and quantitative analytical problems with familiar and unfamiliar contexts.
4. Apply knowledge regarding the principles discussed to extract chemical information using basic chemometrics.

## 5. Contents

### **BLOCK I: Analytical Separation Techniques**

#### **1. Non-chromatographic techniques for sample preparation.**

Introduction. Liquid sample preparation: dialysis, liquid-liquid extraction, solid-phase extraction, ion exchange, headspace analysis. Solid sample preparation: soxhlet extraction, supercritical fluid extraction. Fundamentals, instrumentation and applications.

#### **2. Introduction to chromatographic separations**

General description of chromatography. Classification of chromatographic methods. Theory of column chromatography: chromatographic resolution, column selectivity and efficiency, band broadening. Optimizing chromatographic separations. Planar

chromatography: stationary phases, chromatogram development, detection and applications.

### 3. Gas chromatography (GC)

Introduction. Components of a GC instrument: carrier gas and flow regulation, thermostatically controlled oven, sample injection systems, stationary phases and columns, principal GC detectors. Hyphenated techniques. Applications.

### 4. High-performance liquid chromatography (HPLC)

Introduction. Instrumentation: pumps and gradient elution, injection systems, columns and stationary phases. HPLC separation modes: partition, adsorption, ion exchange, size exclusion and affinity chromatography. HPLC detectors. HPLC-hyphenated techniques. Applications.

### 5. Chiral separations.

Introduction. Principles of chiral recognition. Chiral stationary phases: poly-saccharide-based stationary phases, Cyclodextrin, brush-type phases, protein-derived phases. Chiral derivatization. Applications

### 6. Electrophoresis

From zone electrophoresis to capillary electrophoresis. Theory of capillary electrophoresis: electrophoretic mobility and electro-osmotic flow. Instrumentation: Injection and detection systems. Capillary electrophoresis modes. Applications

## BLOCK II: Bioanalysis

### 7. Bioanalysis

**Introduction to Immunoassays.** The immunological reaction: reagents and characteristics. Classification of immunoassays. The precipitation reaction: immunodiffusion tests, turbidimetric and nephelometric immunoassays. **Immunoassays with labels:** Introduction. Assay configurations: competitive vs non-competitive, heterogeneous vs homogeneous assays. Binding theory: Scatchard plot and principles of quantitative immunoassays. Radioimmunoassays. Enzyme immunoassays: ELISA and EMIT. Fluorescence immunoassays.

Applications. **Chemical Sensors and Biosensors:** Introduction and definition. Classification of chemical sensors. General considerations for design. Electrochemical (bio)sensors. Optical (bio)sensors. Overview of applications.

### BLOCK III: Chemometrics

#### 8. Chemometrics

Experimental design and optimization: Introduction: why design experiments in analytical chemistry?. Factorial designs. Optimisation: basic principles and simplex optimization. Multivariate analysis: Introduction. Initial analysis. Pattern recognition and classification: principal components analysis, cluster analysis, discriminant analysis. Multivariate calibration. Analytical quality assurance: Quality control: basic concepts. Internal quality control: sampling strategies, control charts, method validation. External quality control.

#### 6. Methodology and working plan

The following teaching methods will be used in the course:

1. **Lectures:** In these sessions, the teacher will expose the core concepts of the course, with emphasis in those of special complexity. Slideshow and supplemental material will be made available via pdf files posted to Campus virtual. Regular attendance to these sessions is highly recommended. Study must be completed using the recommended bibliography.
2. **Classroom practices and seminars:** case studies and problem-solving applying concepts learned in class to "real-life" situations. Students will be provided in advance with the questions and problems to be discussed in these sessions. Active participation is recommended.
3. **Group tutoring classes.** Attendance to these sessions is **mandatory**. Homework assignments consisting of questions and/or problems will be posted on the course website in advance. In these sessions students will present the solutions, which will be discussed with the group. Active participation will be evaluated for quantity and quality.

The student is expected to dedicate significant effort both in and out class to be successful. The following table summarizes the expected dedication:

| Teaching method | Hours | % | Total Hours |
|-----------------|-------|---|-------------|
|-----------------|-------|---|-------------|

|                         |                               |     |       |    |
|-------------------------|-------------------------------|-----|-------|----|
| In-class activities     | Lectures                      | 46  | 30,67 | 60 |
|                         | Classroom practices/ Seminars | 7   | 4,67  |    |
|                         | Group tutorial sessions       | 4   | 2,67  |    |
|                         | Evaluation                    | 3   | 2     |    |
| Out-of-class activities | Individual work               | 90  | 60    | 90 |
|                         | Total                         | 150 |       |    |

## 7. Evaluation of the student's learning results

Grades in this course will reflect the student's ability to effectively communicate mastery of the goals and objectives outlined above. This will be assessed through:

1. **Exams:** There will be a three-hour exam, consisting in 10 points derived from all the course materials. It will account for 90% of the final course grade. Theoretical questions (6 points) and problem-solving exercises (4 points) will be included. It is necessary to obtain marks higher than 45% of the points in each part, with a total numeric grade higher than 5 to pass the course.
2. **Group tutoring sessions:** Quality and quantitative participation in these sessions will be assessed, accounting for 10% of the final course grade.

In **Extraordinary examination** (i.e. resits or retakes) an exam, similar to that described for ordinary examination, will account for 100% of the final course grade, with a total numeric grade higher than 5 to pass.

## **8. Resources, bibliography and complementary documentation**

### *Recommended Textbooks:*

**Block I.** *Principles of Instrumental Analysis*. 7th edition, by D.A. Skoog, F.J. Holler, S.R. Crouch. Cengage Learning 2018.

**Block II.** *Bioanalytical Chemistry*, by S.R. Mikelsen, E. Cortón. John Wiley & Sons 2004

**Block III.** *Statistics and chemometrics for Analytical Chemistry. 6th Edition*, by J.N. Miller, J.C. Miller. Pearson 2010.

### *Complementary Textbooks:*

*Chemical Analysis: Modern Instrumentation Methods and Techniques*. 2nd edition, by F. Rouessac, A. Rouessac. John Wiley & Sons 2007.

