COURSE DATA

Data Subject	
Code	34229
Name	Analytical chemistry II
Cycle	Grade
ECTS Credits	4.5
Academic year	2017 - 2018

Study (s)

Degree	Center	Acad. year	Period
1108 - Degree in Chemistry	Faculty of Chemistry	2	Second term

Subject-matter

Degree	Subject-matter	Character
1108 - Degree in Chemistry	6 - Analytical chemistry	Obligatory

Coordination

Name	Department
CERVERA SANZ, MARIA LUISA	310 - Analytical Chemistry

SUMMARY

Analytical Chemistry I dealt with the basics of Analytical Chemistry and classical qualitative and quantitative analysis. Analytical Chemistry II further develops basic training in Analytical Chemistry centred on instrumental analysis.

The development of analytical methods based on instrumental techniques has enabled Analytical Chemistry to meet the increasing needs of society and technological development. Today these methods are needed to tackle most analytical problems.

The course begins with the basic concepts of instrumental analysis and the classification of instrumental analysis techniques, especially optical spectral techniques.

It continues with the treatment of analytical results and calibration in instrumental analysis (univariate), including linear regression, straight line adjustment, and analytical parameters related to calibration. As well as conventional calibration, other calibration methods that are useful in certain cases are discussed.

The rest of the course involves the study of optical spectral analysis techniques, including techniques based on molecular absorption spectroscopy in the UV/V and IR zones, analytical luminescent techniques based on molecular emission spectroscopy and analytical techniques based on flame and non-flame atomic spectroscopy.

The knowledge and skills students acquire on this course will be reinforced in Laboratory of Analytical Chemistry II, where students will practice some of the analytical techniques studied.

The general aims of Analytical Chemistry II are to provide students with:

• an overview of the various types of instrumental analytical techniques before analysing in greater detail those that will be studied on this course.

• a solid foundation in the use of calibration methods in analytical chemistry to enable them to select the most suitable one for a given analytical problem and correctly treat the analytical results.

• the knowledge they need regarding the foundations, instruments, experimental methods and applications of optical spectral analysis techniques in order to select the best ones for solving a specific analytical problem.

• the skills they need to perform calculations in analytical problems in which instrumental analysis techniques are used.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

To successfully complete this course, students should have acquired knowledge from previous courses, especially from Analytical Chemistry I, which they completed in their first term.
Specifically, students will need basic knowledge of the analytical process and the chemistry of solutions.

OUTCOMES

1108 - Degree in Chemistry

- Develop capacity for analysis, synthesis and critical thinking.
- Show inductive and deductive reasoning ability.

- Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation.
- Solve problems effectively.
- Demonstrate ability to work in teams both in interdisciplinary teams and in an international context.
- Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate.
- Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional.
- Learn autonomously.
- Demonstrate the ability to adapt to new situations.
- Acquire a permanent sensitivity to quality, the environment, sustainable development and the prevention of occupational hazards.
- Demonstrate knowledge of the main aspects of chemical terminology, nomenclature, conventions and units.
- Interpret the variation of the characteristic properties of chemical elements according to the periodic table.
- Demonstrate knowledge of the main types of chemical reaction and their main characteristics.
- Demonstrate knowledge of the principles of thermodynamics and kinetics and their applications in chemistry.
- Demonstrate knowledge of the principles, procedures and techniques for the determination, separation, identification and characterisation of chemical compounds.
- Show knowledge of the metrology of chemical processes including quality management.
- Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry.
- Solve qualitative and quantitative problems following previously developed models.
- Recognise and analyse new problems and plan strategies to solve them.
- Evaluate, interpret and synthesise chemical data and information.
- Handle chemicals safely.
- Carry out standard experimental procedures involved in synthetic and analytical work, in relation to organic and inorganic systems.
- Handle the instrumentation used in the different areas of chemistry.
- Interpret data from observations and measurements in the laboratory in terms of their significance and the theories that underpin them.
- Evaluate the risks in the use of chemicals and laboratory procedures.
- Relate theory and experimentation.

- Recognise and evaluate chemical processes in daily life.
- Understand the qualitative and quantitative aspects of chemical problems.
- Develop sustainable and environmentally friendly methods.
- Relate chemistry with other disciplines.
- Students must be able to apply their knowledge to their work or vocation in a professional manner and have acquired the competences required for the preparation and defence of arguments and for problem solving in their field of study.
- Students must have the ability to gather and interpret relevant data (usually in their field of study) to make judgements that take relevant social, scientific or ethical issues into consideration.
- Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences.
- Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.
- Express oneself correctly, both orally and in writing, in any of the official languages of the Valencian Community.
- Have basic skills in the use of information and communication technology and properly manage the information obtained.

LEARNING OUTCOMES

The learning outcomes for this course, which are contained in the Degree document under Analytical Chemistry, are:

• To have the theoretical and practical knowledge needed to plan, apply and manage the most suitable analytical method for tackling environmental, health, industrial, food or any other problem related to chemical substances. (CG8, CG10, CE4, CE15, CE24, CE26)

• To demonstrate the principles, procedures and main instrumental technologies used in chemistry for the determination, separation, identification, characterization and behaviour of chemical compounds. (CE6, CE8, CE19, CE24)

• To clearly explain phenomena and processes related to Analytical Chemistry. (CG1, CG2, CE2, CE13)

• To understand and rigorously use bibliographical information and technology related to chemical analytical processes. (C14, CE16)

• To understand and be able to use the various forms of measurement for studying chemical processes and instrumental technologies used to determine the behaviour of chemical species. (CE1, CE10)

• To recognize and appreciate the behaviour of chemical substances for our daily lives. (CE23)

• To use technical information to choose the best method for solving a real problem. (CG3, CG4)

• To apply the quality criteria of the analytical results. (CG10)

• To demonstrate knowledge of sustainable analytical methods. (CE25)

• To have the theoretical and practical knowledge needed to manage chemical residues and safety procedures in the laboratory. (CE17, CE21)

• To clearly explain experimental phenomena using the theories that support them. (CE20, CE22)

• To develop experimental procedures for analysing organic and inorganic compounds. (CE18)

• To skilfully treat errors, handle error propagation of the magnitudes measured in the laboratory, and manage computer programs for processing experimental information. (CE16, CT3)

• To draft records, reports and normal work procedures used in a laboratory. (CG3, CG7, CG9, CE10, CT1)

• To demonstrate interpersonal skills also from the gender perspective. (CG6)

• To demonstrate sensitivity to environmental issues. (CG10)

• To demonstrate the ability to rigorously manage information. (CG7)

• To demonstrate leadership ability also from the gender perspective. (CG3)

• To effectively perform his or her tasks as a member of a team also from the gender perspective. (CG3)

• To solve problems rigorously. (CG4, CG6, CE14, CE15, CE24)

These learning outcomes should ensure that on successful completion of Analytical Chemistry II students will be able to:

- classify the most common instrumental analytical technologies.
- indicate the basic criteria for choosing an instrumental analytical technology.
- define and distinguish between systematic and random errors and describe their relationship with the analytical properties.
- express an analytical result correctly.
- implement simple hypothesis tests such as the rejection of anomalous results, the comparison of variances, the comparison of a result with a reference value and the comparison of two results.
- justify the need to use calibration in instrumental analysis.
- explain the characteristics of straight line adjustment for the simple and weighted least squares methods.
- indicate the most interesting calibration parameters and how they relate to the analytical characteristics of the instrumental methods.
- describe the various calibration methods (conventional, internal standard and standard addition) and establish their differences and applicability.
- solve analytical problems based on calibration technologies.
- explain the theoretical basis for the various analytical technologies studied.
- write and interpret the relationship between the analytical sign obtained in each analytical technique

and the concentration of the analyte.
- schematically design the instrumentation for the analytical technique studied, explaining the components and justifying why they are needed and where they are located in the context of the design.
- clarify the differences when different instrumentation designs exist for the same analytical technique or groups of techniques.
- describe the experimental method to follow for the analysis using the analytical techniques studied.
- identify the most common types of interference with the analytical techniques studied and the procedures that exist to correct them.
- provide representative examples of the applications for the analytical techniques studied.
- given a specific example of an application or a published article on an analytical method applied to a specific sample, justify its use, discuss its analytical characteristics, reasonably explain the steps to follow, and indicate how to perform the calculations.
- perform the calculations needed to solve analytical problems, correctly expressing the results and explaining the conclusions drawn.

DESCRIPTION OF CONTENTS

1. Introduction to Instrumental Analysis Techniques

Conceptual evolution of instrumental analysis. Classification of instrumental analysis techniques. Spectroscopic analysis techniques. Criteria for choosing the instrumental technique. Design and basic components of the instruments used in analytical spectroscopy.

2. Evaluation and Expression of Results

Systematic and random errors. Distribution functions. Confidence intervals and expression of results. Null and alternative hypotheses. Basic hypothesis tests: rejection of outliers, comparison of a data set with a reference value and comparison of two data sets.

3. Calibration

The concept of calibration and its importance in instrumental analysis. Conventional or external calibration. Linear regression. Simple and weighted least squares. Analytical parameters related to the calibration. Sensitivity, limits of detection, limits of quantification. Using a calibration curve to determine the concentration of an analyte in a sample. Calibration using an internal standard. Detecting and correcting matrix effects using standard addition calibration.

4. Introduction to Spectroscopic Analysis Techniques. UV/V Molecular Absorption

Introduction to spectroscopic analysis techniques. UV/V molecular absorption spectroscopy. Atomic and molecular spectra: use in instrumental analysis. Fundamentals of UV/V molecular absorption spectroscopy. Beer's Law and conditions of application. Factors that influence UV/V molecular absorption spectroscopy. Analytical use of UV/V spectrophotometry. Instrumentation and variables of interest. Experimental methodology. Interference and correction methods. Resolution of mixtures:

systems of linear equations. Use of derivative spectra. Analytical applications of major interest today. Criteria for reading publications on analytical methods based on UV/V spectrophotometry.

5. Molecular Emission Spectroscopy

Fundamentals of molecular emission spectroscopy. Excitation and emission spectra. Fluorescence and phosphorescence. Factors that influence fluorescence, phosphorescence and interferences. Analytical use of molecular luminescence. Instrumentation and variables of interest. Experimental methodology. Other techniques: analytical use of chemiluminiscence. Analytical applications. Criteria for reading publications on analytical methods based on molecular luminescence. Comparing the techniques of absorption and emission molecular spectroscopy.

6. Atomic Spectroscopy I

Fundamentals of atomic spectroscopy. The atomization process. Analytical use of atomic spectroscopy. Techniques based on flame atomization: atomic absorption and emission. Instrumentation and variables of interest. Experimental methodology. Types of interference and methods of correction.

7. Atomic Spectroscopy II

Electrothermal atomization techniques: instrumentation and variables of interest, experimental methodology, interference and correction. Atomic absorption techniques using cold vapour hydride generation: instrumentation and variables of interest, experimental methodology; interference and correction. Atomic fluorescence. Atomic emission using inductively coupled plasma atomization. Instrumentation and variables of interest, experimental methodology, interference and correction. Comparison of the atomic techniques. Analytical applications of the atomic techniques. Criteria for reading publications on analytical methods based on atomic spectrometry.

8. Infrared Molecular Absorption Spectroscopy

Fundamentals of infrared spectroscopy. Molecular vibrations and the theory of groups. Factors that affect vibrational coupling. Analytical use of infrared spectroscopy. Instrumentation and variables of interest. Experimental methodology. Sampling techniques and sample manipulation techniques. Fourier Transform Infrared Spectroscopy. Far infrared spectroscopy. Near infrared spectroscopy. Attenuated total reflectance. Analytical applications of major interest today. Criteria for reading publications on analytical methods based on infrared spectroscopy.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	38,00	100
Tutorials	7,00	100
Study and independent work	42,00	0
Preparation of evaluation activities	25,50	0
TOTAL	**112,50**	

TEACHING METHODOLOGY

This course will consist of classroom lectures for the theoretical concepts, problem-based learning sessions, group tutorials and conferences and/or seminars.

The lectures will present an overview of the topics contained on the course.

The problem-based learning sessions will provide the basis for solving problems or issues related to the theoretical contents.

The tutorials will be used to solve the theory-related problems or issues.

The seminars will be used to solve practical cases related to the instrumental analytical techniques discussed in the lectures.

In the programmed conferences where current topics will be tackled, at the end of the session, the students will answer a test with questions related to the content of the talk.

To grade the students' work, the professor may evaluate:

- assignments they have completed inside or outside the classroom

- classroom participation, including the standard of work presented, responses to questions asked, presentations, etc.

EVALUATION

Learning will be evaluated by taking into account all the aspects outlined in the Methodology section of this course guide.

FIRST CALL

Final grade:

Student activities (questions, exercises, evaluations, etc.)	Examination
30%	70%

The score obtained in the examination must be at least 4.5 in order to apply the average.

The minimum score obtained in student activities must be at least 5.0 in order to apply the average.

Attendance to the interdisciplinary conferences will be evaluated through a test, whose mark will be added as a 5% to the qualification of the ongoing assessment.

The minimum overall score to pass the course is 5.0.

Students who do not complete the minimum number of activities required by the lecturer or who obtain a score for those activities below 5.0 will be evaluated by examination only, which will count for 100% of their final grade. Students may also submit a request in writing to be evaluated only by examination.

SECOND CALL

In the second call the scores and final grade are obtained by applying the same criteria as in the first call.

REFERENCES

Basic

- SKOOG, D.A.; WEST, D.M.; HOLLER, F.J. Y CROUCH, S.R. Fundamentos de Química Analítica, 8ª edición. Madrid: Thomson-Paraninfo, 2005.ISBN: 9788497323338
- SKOOG, D.A.; HOLLER, F.J. Y NIEMAN, T.A. Principios de Análisis Instrumental, 5ª Edición. Madrid: McGraw-Hill, 2001. ISBN 8448127757
- HARRIS, D.C. Análisis Químico Cuantitativo, 3ª Edición. Barcelona: Reverté, 2007. ISBN 9788429172249
- HARVEY, D. Química Analítica moderna. Madrid: McGraw-Hill, 2002.ISBN 9788448136352
- HERNÁNDEZ, L. Y GONZÁLEZ-PÉREZ, C. Introducción al Análisis Instrumental. Barcelona: Ariel Ciencia, 2002. ISBN 8434480433

- MILLER, J.N. Y MILLER, J.C. Estadística y Quimiometría para Química Analítica. Madrid: Prentice Hall, Pearson Educación, 2002. ISBN 8420535141
- RÍOS CASTRO, A.; MORENO, M.C. Y SIMONET SUAU, B. M. (coords.) Técnicas espectroscópicas en Química Analítica, 2 vols. Madrid: Biblioteca de Químicas. Síntesis. Madrid, 2012. ISBN 9788499589312