Bachelor´s Degree in Chemistry

Subject Guide

1. Information about the subject

SUBJECT	Analytical Chemistry I	**CODE**	GQUIMI01-2-001
EDUCATIONAL OFFER	Bachelor´s Degree in Chemistry	**CENTER**	Facultad de Química
TYPE	Compulsory	**N° TOTAL CREDITS**	6.0
PERIOD	First Semester	**LANGUAGE**	Spanish
COORDINATORS/ES		**EMAIL**	
LECTURERS		**EMAIL**	
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2. Context

This is the first course in Analytical Chemistry and it is one of the fundamental courses taken by undergraduate chemistry students. Analytical Chemistry has been defined as the science for chemical measurements and focuses on the Techniques, Instrumentation, Methodologies, Procedures, Reagents, Quality Assurance, etc. related to the unit “Quantity of Matter” of the International System of Units. The symbol for such a unit is the MOL. Analytical Chemistry is closely related to Metrology and employs many concepts derived from it. According the Consultative Committee for the Quantity of Matter (CCQM) the fundamental areas of application of Analytical Chemistry are in the fields of Health (markers for clinical diagnostic), Food and Environmental quality, Forensic analysis, Raw and advanced materials, Pharmaceutical products, Biotechnology, Surface analysis and Chemical Metrology.

The subject Analytical Chemistry I is included in the Fundamental Module corresponding to Analytical Chemistry for the degree in Chemistry. It is a fundamental subject within the chemistry degree as it constitutes and introduction to one of the main disciplines in Chemistry. Moreover, the

contents of the subject are essential to understand a large part of the contents of other subjects in the chemistry degree.

This subject is taught in the second year of the degree in chemistry and is an initiation to the formative process in Analytical Chemistry. One of the objectives of this subject is to consolidate and homogenize the knowledge level of the students providing them with the basic analytical tools required to succeed in the rest of analytical chemistry subjects in the degree in chemistry. Hence, this subject needs to be passed to be able to register for the subjects Analytical Chemistry II and Analytical Chemistry III of the third course in the degree in Chemistry.

The subject will be taught by Nacho García Alonso and María Montes Bayón, from the Analytical Chemistry area of the Department of Physical and Analytical Chemistry.

3. Requirements

Students must have passed the following first-year courses: **General Chemistry**, **Laboratory Basic Operations and Computer Tools** and **Numerical Calculation and Applied Statistics**

4. Competencies and learning results

From the various abilities listed in the Project Book of the Chemistry Degree at the University of Oviedo, we highlight the following ones:

4.1 Specific competences and skills:

Students should acquire knowledge on:

- CE5. The different chemical reactions employed and their main characteristics.

- CE6. The principles and procedures employed in Analytical Chemistry for the quantification, identification and characterization of chemical compounds.

- CE13. To know and apply the basic principles of opto-spectroscopic techniques.

- CE14. To know and apply the basic principles of electrochemistry.

- CE15. To relate the basic principles of analytical techniques (titrimetric, gravimetric, optical and electrochemical) with its applications.

- CE18. The application of chemical metrology to processes and chemicals including the basic concepts of Quality Assurance.

- CE20. Solving qualitative and quantitative problems according to models developed previously.

- CE22. The ability to evaluate, interpret and synthesise chemical information.

- CE24. To process and compute data related to chemical information.

- CE35. To perform error and uncertainty calculations and correct use of units and magnitudes.

4.2 Broad competences and skills

Students should be able to:

- CG1. Carry out information analysis and synthesis.

- CG5. Capability for decision making.

- CG7. Use a foreign language, preferably English.

- CG9. Engage in autonomous learning activities.

- CG11. Acquire motivation for quality

- CG17. Develop critical thinking.

-CG18. Team working.

4.3 Overall learning outcome: Students should demonstrate knowledge and understanding of the facts, concepts, principles and theories related to Analytical Chemistry and its application to problem solving in chemical metrology.

5. Contents

1. **Introduction to Analytical Chemistry**. Definitions. Fields of application. Tools of the trade. Type of information obtained. Keywords in Analytical Chemistry. The analytical process. Methods in Analytical Chemistry. Methods for the measurement of the analytical signal. Methods for data treatment. Analytical Characteristics. The need for quality in the analytical laboratory. Keywords in Metrology and Quality Control: Traceability, uncertainty, validation.

2. **Analytical methods: an overview**. Introduction. Sampling methods. Digestion and extraction methods. Separation and preconcentration methods. Methods for the measurement of the analytical signal. Methods for data treatment. Methods for quality control.

3. **Statistics in Analytical Chemistry**. Introduction. Concepts of precision, accuracy and uncertainty. Combination of uncertainty sources: error propagation. Random error propagation of independent variables. Correction of systematic errors. Incorporating the reproducibility in the calculation of combined uncertainties. Validation of analytical methodologies: statistical tests. The use of certified reference materials. The comparison with alternative methods. The participation in proficiency testing exercises.

4. **Instrumental and methodological calibration in Analytical Chemistry**. Introduction. Instrumental calibration: Traceability of analytical instruments. Procedures for instrumental calibration: Examples. Methodological calibration: Preparation of a calibration graph. Types of methodological calibrations: Pure standards and standard additions. Internal standards. Correction of matrix interferences: use of internal standards. Signal behaviour: homoscedasticity and heteroscedasticity. Selection of the linear regression equation. Statistics from the linear regression equation: uncertainties of the slope and intercept. Limits of detection. Uncertainty propagation in linear regression.

5. **Absolute analytical methods**. Definition of absolute analytical methods. Applications of absolute analytical methods. Calibration requirements. Gravimetry. Titrimetry (volumetry). Coulometry. Isotope Dilution Mass Spectrometry.

6. **Gravimetric methods**. Introduction. Overview of gravimetric methods. The precipitation reaction: precipitation equilibria. Gravimetry by chemical precipitation: practical aspects. Factors affecting chemical precipitation. Analytical applications of gravimetry: precipitation.

Analytical applications of gravimetry: volatilization. Thermogravimetry. Other applications.

7. **Volumetric methods: Acid-base titrations. Complexometric titrations. Redox titrations**. Introduction. pH values for solutions of acids, bases and salts. Characteristics of the acid-base reaction. Changes in pH during the acid-base titration. Indicators. Selecting the right indicator. Potentiometric detection. Primary standards for acid-base titrations. Applications of acid base titrations. The coordination reaction: metal-ligand complexes. Theory of coordination chemistry (reminder). Secondary equilibria in coordination chemistry. Conditional stability constants and masking coefficients. Complexation titrations. EDTA as complexation reagent. Complexation titrations using EDTA. Detection of the end point. Applications. How to perform a redox reaction. Electrode potentials: measurements and significance. Calculating electrode potentials: Nerst equation. Relationship between cell potentials and stability constants for a redox reaction. Requirements for a redox titration. Reagents for redox titrations. Calculating potentials during redox titrations. Detection of the equivalence point. Selected applications.

8. **Introduction to optical methods: absorption, emission and fluorescence**. Relative analytical methods: a reminder. Introduction to optical methods. The nature of electromagnetic radiation. Interaction of radiation with atoms: electronic transitions. Interaction of radiation with molecules: electronic and vibrational transitions. Components of analytical instruments: lamps, monochromators, detectors. Instruments for absorption measurements. Instruments for emission measurements. Instruments for fluorescence measurements.

9. **Molecular Absorption and Fluorescence Spectroscopy**. Definitions. Quantitative laws for absorption measurements: Beer-Lambert law. Deviations from linearity: chemical and instrumental sources. Relationship between chemical structure and absorption. Instrumentation: single and double beam instruments. Spectrophotometry as detection technique for chromatography. Applications: Spectrophotometric determinations. Fluorescence: basic mechanisms for excitation and deactivation. Quantitative laws for fluorescence measurements. Instruments for fluorescence measurements. Applications of Fluorimetry.

10. **Atomic Absorption and Emission Spectrometry**. Atomic Absorption Spectroscopy. How to get atoms in the gas phase. Atomisation in flames. Population of ground and excited states in flames. Line broadening and monochromator bandwidths. Beer-Lambert law in Atomic Absorption. Typical Instrumentation. Interferences and correction methods. Atomic Emission Spectrometry. Effect of temperature on the population of excited states. Resonance and non-resonance lines. Autoabsorption. Comparative detection limits

11. **Introduction to electroanalytical methods**. Overview of electroanalytical methods. Electrochemical cells. Classification of electroanalytical methods. Instrumentation for potentiometry. Nernst and junction potentials. Indicator and reference electrodes. Electrode processes. Diffusion currents.

12. **Potentiometric methods. Voltamperometric methods**. Introduction. Direct potentiometry with ion selective electrodes. Potentiometric titrations. Analytical applications. Instrumentation for voltammetry. Working electrodes. Current-potential relationship. Techniques in voltammetry. Electrochemical detection in liquid chromatography.

6. Methodology and working plan

Lectures (CE, 49 hours): The lectures will analyze and develop, in a didactic manner, the contents of the program. Students will be encouraged to get involved by raising issues and questions during the lectures. It is highly recommended to attend regularly to the theoretical lectures. Lectures will be given both by Nacho García Alonso and María Montes Bayón.

Practical sessions (PA 7 hours/group): Students will analyze in detail the mathematical questions that are previously introduced in the lectures. They will also work out many numerical problems in order to apply the acquired knowledge to practical problems of interest. During the practical sessions, students are expected to play an active role with the support of the instructor. Practical sessions will be given by María Montes Bayón.

Group tutorials (PA 4 hours/group): The first part of these sessions will be open to discussions raised by the students on the basis of the materials and topics treated during the lectures. Students will carry out work about topics that will be previously suggested by the instructors. The selected topics will develop other aspects of the program showing how Analytical Chemistry can be put to work in the real world. Group tutorials will be given by María Montes Bayón.

7. Evaluation of the student's learning results

During the regular semester, the global grade will be based on:

(a) A written examination consisting of both theoretical questions and numerical problems will count 90% of the final grade. A minimum score of 4.5 out of 10 points will be required.

(b) Practical sessions and group tutorials. These activities, which will count 10% of the final grade (a minimum of 4.5 out of 10 points being required).

The weighted average of the two parts (a) and (b) should be equal or higher than 5.0. The date and time of the exam referred to in (a) will be those determined in the official academic calendar for the 2016-2017 course.

The grade of students who attend *extraordinary calls* will be that corresponding only to a written exam, a minimum of 5 out of 10 points will be required to pass the course.

8. Resources, bibliography and complementary documentation

The following books will be employed to prepare the theoretical and practical lectures and should be very useful for students willing to complement the notes taken during the lectures.

Fundamentos de Química Analítica*.* D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch. Ed. Thomson. 8ª Edición, Madrid, 2005

• ***Análisis Químico Cuantitativo****.* D.C. Harris. Ed. Reverté. 3ª Edición, Barcelona, 2007

• ***Principios de Análisis Instrumental.*** D.A. Skoog, F.J. Holler, T.A. Nieman. Ed. McGraw-Hill, 5ª Edición, Madrid, 2001

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Additionally, other specific bibliographic references that could help students to better understand the topics of study will be provided during the course.