- Course title: **Chemometrics and Experimentation in Analytical Chemistry**.
- Course code: 5289
- Type of course: compulsory
- Level of course: fundamental
- Year of study: 3
- Semester: 2
- Number of credits allocated: 6
- Names of lecturers: Mª Cruz Ortiz, Ana Herrero and Silvia Sanllorente.
- Objective of the course: to express measurement uncertainty; to implement analytical quality assurance and good practice in the laboratory; to understand, interpret and apply international quality performance regulations on analytical methodology; to prepare working standard protocols; to design and interpret interlaboratory and proficiency tests; to assign uncertainty related to steps of analytical procedures; to optimize uncertainty measurements when analysing complex matrices; to use multivariate methods for analyte identification and quantification.
- Prerequisites: It is recommended that students should have attended Instrumental Analysis and Numerical analysis and applied Statistics before following this course.
- Course contents: implementation of analytical procedures for the determination of synthetic and complex samples according to regulatory norms; validation of chemical measurements; comparison of two analytical procedures; multiple comparisons; ANOVA; linear calibration; detection capability of analytical methods; calculation of uncertainty levels in analytical procedures; reliability and robustness of analytical procedures; introduction to multivariate analysis.
- Recommended reading:
    - Analytical Chemistry: The approved text to the FECS curriculum analytical chemistry, R. Kellner, J.M.Mermet, M. Otto and H.M. Widmer, 1998, Wiley-VCH, Weinheim.
    - Avances en Quimiometría práctica, R.Cela (Coordinador), 1994, Servicio de publicaciones e Intercambio científico de la Universidade de Santiago de Compostela, Santiago de Compostela
    - Handbook of Chemometrics and Qualimetrics; Part A and Part B in Data Handling in Science and Technology, D.L. Massart, B.G.M. Vandeginste, L.M.C. Buydens, S. de Jong, P.J. Smeyeers-Verbeke 1997, Elsevier, Amsterdam.
    - Applied Statistics, L. Sach, 1982, Springer-Verlag, New York.
    - Quality of Analytical Measurements: Statistical Methods for Internal Validation, M.C. Ortiz, L.A. Sarabia, M.S. Sánchez, A. Herrero in "Comprehensive Chemometrics", volume 1, S. Brown, R. Tauler, B. Walczak (Editores), 2009, Amsterdam, Elsevier.
    - Sample preparation techniques in Analytical Chemistry, S. Mitra (Editor), 2003, Wiley, Hoboken (NJ).
- Teaching methods:
    - Lectures: teachers explain the contents of the lessons.
    - Seminars: students and teacher discuss the problems and other points raised in class.
    - Practicals: students apply their knowledge to solve laboratory experiments.
- Assessment methods:
    - Written work and exams: 60%
    - Group and individual analysis, presentation and discussion of practices and problems: 30%
    - Group and individual work: 10%
- Language of instruction: Spanish and/or English