

- Course title: **Numerical Analysis and Applied Statistics.**
- Course code: 5281
- Type of course: compulsory
- Level of course: fundamental
- Year of study: 2
- Semester: 2
- Number of credits allocated: 6
- Names of lecturers: Luis Antonio Sarabia and María Sagrario Sánchez.
- Objective of the course:
 - To understand and to manage computer and experimental design tools for the presentation and resolution of scientific problems, with particularly emphasis on those relating to chemistry.
 - To make computer simulations.
 - To know procedures for signal filtering in chemistry.
 - To work with specific software.
 - To design an efficient experiment for a well defined chemical problem.
 - To interpret experimental results in the context of the set problem.
- Prerequisites: It is recommended that students should have attended Mathematics I and Mathematics II before following this course.
- Course contents:
 - Numerical methods for optimization and modelling
 - Simulation: Monte Carlo and Markov chain Monte Carlo methods (MCMC)
 - Introduction to the theory and applications of Statistics.
 - Analysis and propagation of errors on experimental data.
 - Computational treatment of experimental data.
 - Introduction to experimental design.
- Recommended reading:
 - P. Sprent, N.C. Smeeton, Applied Nonparametric Statistical Methods (4th Ed.), Chapman & Hall/CRC, Boca Raton, 2007.
 - W.L. Martinez, A.R. Martinez, Computational Statistics handbook with MatLab, 2nd Ed., Chapman & Hall/CRC, Boca Raton, Florida, 2008.
 - Comprehensive Chemometrics, Ed. S. Brown, R. Tauler, B. Walczak Chapter 1.12: Response surface methodology, L.A. Sarabia, M.C. Ortiz, Elsevier, Amsterdam, 2009
 - Ullmann's. Modelling and simulation. Wiley VCH, Weinheim, 2007.
 - M.D. Rossetti, Simulation modelling and Arena, John Wiley & Sons, Hoboken. New Jersey, 2009.
- 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:
 - Continuous evaluation of the theoretical-practical sessions: 30%
 - Group and individual analysis, presentation and discussion of practices and problems: 10%
 - Written work and exams: 60%
- Language of instruction: Spanish and/or English