60626 - Chemometry

Información del Plan Docente

Academic Year	2016/17
Academic center	100 - Facultad de Ciencias
Degree	542 - Master's in Chemical Research
ECTS	3.0
Course	1
Period	First semester
Subject Type	Optional
Module	---

1.Basic info

1.1.Recommendations to take this course

1.2.Activities and key dates for the course

2.Initiation

2.1.Learning outcomes that define the subject

2.2.Introduction

3.Context and competences

3.1.Goals

3.2.Context and meaning of the subject in the degree

3.3.Competences

3.4.Importance of learning outcomes

4.Evaluation

5.Activities and resources

5.1.General methodological presentation

The learning process that is designed for this subject is based on the following:

Development theory sessions and practical case studies where student participation and initiative is encouraged. For it will be used:
1. Exhibition in master classes: to offer a vision of a type problem and its resolution applying chemometric tools
2. Resolution practice cases. Involves the selection and discussion of chemometric methodology together with justification - interpretation of results
3. Selection of cases proposed by the students. Supervision and monitoring of student pro-autonomy and activity.

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5.2.Learning activities

5.3.Program

MODULE I: Measurement strategies and isolation of analytical uncertainty

Accuracy of the method and uncertainty of the result. Uncertainty in the case of normal distribution. Propagation of uncertainties. Tolerances. Estimation of uncertainty from modeling the measurement function. Experimental isolation of sources of uncertainty. Experimental uncertainty calculation

MODULE II: Design and optimization of experiments

Introduction to design of experiments. Factorial designs two and three levels. Fractional factorial designs. Optimization strategies. Robust optimization methods

MODULE III: Recognition of information

Unsupervised models: Principal Component Analysis (PCA). Study of latent variables and systems interpretation. Supervised models

MODULE IV: Multiple calibration and multivariate

Calibration models and, multiple and multivariate regression models. Multiple linear regression (MLR). Principal Component Regression (PCR). Regression Partial Least Squares (PLS).

5.4.Planning and scheduling

5.5.Bibliography and recomended resources

BIBLIOGRAPHY

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2. BLANCO M., CERDA V. Editores. *Temas avanzados de Quimiometría* . Universidad de as Islas Baleares, Palma, 2007

3. VANDEGINSTE B.G.M., MASSART D.L., BUYDENS L.M.C., DE JONG S., LEWI P.J., SMEYERS-VERBEKE J . *Handbook of chemometrics and qualimetrics: part A and B* . Elsevier. Amsterdam, 1997

4. BRERETON R.G. *Chemometrics. Data analysis for the laboratory and chemical plant* . Wiley, Chichester, 2003

5. MARTENS H. & NAES T.; Multivariate Calibration. Wiley, Chichester April 1991