Faculty of Biological, Agronomic and Environmental Engineering

BIRC2106   Chemometrics

[22.5h+15h exercises] 3 credits

This course is taught in the 2nd semester

Teacher(s):   Bernadette Govaerts
Language: French
Level: Second cycle

Aims

This course gives an introduction to statistical tools for chemistry and analytical chemistry : experimental design, statistical tools for the laboratory and multivariate chemometrics methods.
At the end of the course, the student should recognise the situations where statistical methods are useful in chemistry and will be trained to apply them efficiently.

Main themes

Statistic and measure uncertainty: error types, quantification of error uncertainty, bias analysis, estimation of variance components, control charts, simple linear calibration.
Experimental design in product and process development : methodology, factorial designs, screening designs, design for response surface analysis, mixture designs, multiresponse optimisation.
Multivariate methods in chemistry : principal components analysis, clustering, discriminant analysis and partial least squares with application to multivariate calibration.
The exercises will apply the methodology presented in the course on case studies and with a dedicated statistical software.

Other information (prerequisite, evaluation (assessment methods), course materials recommended readings, ...)

Pré-requis Cours BIR 1203 et Chimie Analytique
Divers Ouvrages de référence proposés :
D.L. Massart, B.G.M. Vandeginste, L.M.C. Buydens, S. De Jong, P.J. Lewi, J. Smeyers-Verbeke. Handbook of chemometrics and qualimetrics. Elsevier; Part A, 1997; Part B, 1998.
G.E.P. Box, N.R. Draper. Empirical model-building and response surfaces. Wiley, 1987.
Brereton R.G., Chemometrics: Data Analysis for the Laboratory and Chemical Plant, Wiley.

Other credits in programs

BIR22/1C	Deuxième année du programme conduisant au grade de bio-ingénieur: Chimie et bio-industries (Sciences, technologie & qualité des aliments)	(3 credits)	Mandatory
BIR22/2C	Deuxième année du programme conduisant au grade de bio-ingénieur : Chimie et bio-industries (Ingénierie biomoléculaire et cellulaire)	(3 credits)	Mandatory
BIR22/3C	Deuxième année du programme conduisant au grade de bio-ingénieur : Chimie et bioindustries (Nanobiotechnologies, matériaux et catalyse)	(3 credits)	Mandatory
BIR22/4C	Deuxième année du programme conduisant au grade de bio-ingénieur : Chimie et bio-industries (Technologies environnementales: eau, sol, air)	(3 credits)	Mandatory
FSA3DA	Diplôme d'études approfondies en sciences appliquées	(3 credits)	
STAT21MS/ST	Première année du master en statistique, orientation générale, à finalité spécialisée (sciences et technologie)	(3 credits)	
STAT22MS/ST	Deuxième année du master en statistique, orientation générale, à finalité spécialisée (sciences et technologie)	(3 credits)	