UCL Université catholique de Louvain

LBIRC2106

2015-2016

Chemometrics

3.0 credits	22.5 h + 15.0 h	1q

Teacher(s) :	Govaerts Bernadette ;
Language :	Français
Place of the course	Louvain-la-Neuve
Inline resources:	Icampus
Prerequisites :	Material: Basic Elements of statistics: descriptive statistics, elements of probability, statistical distributions, inference in normal populations (tests and confidence intervals for one and two means or variances) , ANOVA 1, simple and multiple regression . Courses : LBIR1203 and LBIR1304 : Probability and Statistics 1 and 2
Main themes :	1 . Statistics for measurement methods: reminders of Metrology (error types, quantification of error uncertainty, error propagation'), variance components estimation by ANOVA, control charts, simple linear calibration. 2 . Experimental design in product and process development: Methodology , multiple regression and multiple response optimization , factorial designs and derivatives, screening designs, response surface designs , mixture designs and optimal designs 3 . Multivariate statistical methods in chemistry: principal component analysis , partial least squares (PLS) , clustering, discriminant analysis and its application to multivariate calibration in analytical chemistry 4 . Applications with the JMP software
Aims :	Contribution à l'activité du référentiel 1.1, 1.2, 1.4, 2.1, 2.2, 2.3, 3.4, 3.5, 3.6 At the end of the course students will be able to : - Explain the interest of statistical tools in the work of the chemical engineer - Explain the purpose and usage of each statistical tool seen in the course. select the one adapted to a given situation and calculate related parameters. - Demonstrate their understanding of main course concepts by solving methodological exercises - Use JMP software to apply the methods presented in the course. - Interpret the results of a statistical analysis in the context of a case study in chemistry or life science. For specific tools - Use statistical tools to quantify the precision of a measurement method - Organise an experiment with the design of experiment methodology from the design selection to the statistical analysis - Summarize / visualize large data sets (eg from spectral analytical methods) using multivariate statistical tools *The contribution of this Teaching Unit to the development and command of the skills and learning outcomes of the programme(s) can be accessed at the end of this sheet, in the section entitled "Programmes/courses offering this Teaching Unit".*
Evaluation methods :	Written exam (17pts/20) containing - Methodological exercices to verify the intergration of course main concepts - Questions on the selection and application of methods adapted to given practical situations - Interpretation of JMP software outputs Tests (3pts/20) Case studies on JMP during the semester
Teaching methods :	Lectures (22.5h) - Methods presentation on the basis of real-life situations - Formal but intuitive discussion of theoretical concepts and formulae for most methods - Interpretation of software outputs - Interactive lectures: students are encouraged to participate during the course Computer labs (15h) - Case studies on JMP, methodological exercises, and JMP Output interpretation. Synthesis Exercise Student are invited to prepare an abstract of the course that they are allowed to use during the exam.
Content :	1 . Statistics for measurement methods : reminders of Metrology (error types, quantification of error uncertainty, error propagation'), variance components estimation by ANOVA, control charts, simple linear calibration. 2 . Experimental design in product and process development : Methodology , multiple regression and multiple response optimization , factorial designs and derivatives, screening designs, response surface designs , mixture designs and optimal designs 3 . Multivariate statistical methods in chemistry : principal component analysis , partial least squares (PLS) , clustering, discriminant analysis and its application to multivariate calibration in analytical chemistry

	4 . Applications with the JMP software
Bibliography :	On I- Campus ' Course slides ' Exercises and case studies Selection of methodological Documents Book (optional) : Chemometrics : Data Analysis for the Laboratory and Chemical Plant - R. G. Brereton - Wiley
Other infos :	Accessibility to a public who does not speak the language of instruction ' No, the lectures and course material are in French. Equivalent activities : - No course strictly equivalent at UCL - LSTAT2320 course on experimental designs is partly equivalent.
Faculty or entity in charge:	AGRO

Programmes / formations proposant cette unité d'enseignement (UE)				
Intitulé du programme	Sigle	Credits	Prerequis	Acquis d'apprentissage
	STAT9CE	3	-	
Master [120] in Statistics: Biostatistics	BSTA2M	3	-	
Master [120] in Chemistry	CHIM2M	3	-	
Master [120] in Chemistry and Bioindustries	BIRC2M	3	-	
	STAT2FC	3	-	