UCLouvain

| birc2106 | Chemometrics |
| 3 credits | 22.5 h + 15.0 h | Q1 |

Teacher(s)	Govaerts Bernadette ;				
Language :	French				
Place of the course	Louvain-la-Neuve				
Main themes	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. 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 Multivariate statistical methods in chemistry: principal component analysis, partial least squares (PLS) clustering, discriminant analysis and its application to multivariate calibration in analytical chemistry 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 1 - 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				
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	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. 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 Multivariate statistical methods in chemistry: principal component analysis, partial least squares (PLS), clustering, discriminant analysis and its application to multivariate calibration in analytical chemistry				

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	4 . Applications with the JMP software				
Inline resources	Moodle				
Bibliography	Documentation obligatoire disponible sur Moodle - Transparents de théorie et d'exemples liés au cours - Enoncés d'exercices - Formulaire Documentation facultative disponible sur Moddle - Documents méthodologiques divers				
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. This course can be given in English.				
Faculty or entity in charge	AGRO				

Programmes containing this learning unit (UE)						
Program title	Acronym	Credits	Prerequisite	Aims		
Master [120] in Biomedical Engineering	GBIO2M	3		٩		
Master [120] in Mathematical Engineering	MAP2M	3		٩		
Master [120] in Chemistry	CHIM2M	3		٩		
Master [120] in Chemistry and Bioindustries	BIRC2M	3		٩		