


4.00 credits

30.0 h

Q2

Teacher(s)	Desmet Lieven ;
Language :	French
Place of the course	Louvain-la-Neuve
Prerequisites	<i>The prerequisite(s) for this Teaching Unit (Unité d'enseignement – UE) for the programmes/courses that offer this Teaching Unit are specified at the end of this sheet.</i>
Main themes	The purpose of the course is to familiarize students with the concepts of chemometrics.
Learning outcomes	
Evaluation methods	The evaluation will be partly based on the ongoing work of the students and partly on a final written exam. The ongoing work will be accounted for in the final note only if you have obtained at least a score of 45% in the written exam.
Teaching methods	This course is a lecture course of 30h involving applied exercises during the lecture time. It currently is planned to be a classroom course. The entirety of this course will be dispensed in a computer room, insisting on (1) theoretical aspects that are necessary to understand the presented methods and (2) application exercises based on concrete case studies. The practical sessions will use the R software, based on RMarkdown documents.
Content	This course intends to complement the competencies of students for the treatment (pre-processing and statistical data analysis) of chemical data through the application of multivariate methods. It will be based on real case studies from industry and research to illustrate the importance of using such tools for the pre-processing, the exploration, the visualisation, and the modelling of data from analytical chemistry. The course will explain and apply the main pre-processing steps, as well as the most common exploratory, regression and discrimination methods (PCA, clustering, PCR, PLS, LDA, ...).
Inline resources	Every student must be registered on the Moodle course LCHM1320. The communications between the professor and the students will be made mostly via this channel.
Bibliography	<ul style="list-style-type: none"> • Wehrens, R. (2011). <i>Chemometrics with R</i>. Heidelberg, Germany: Springer. • Varmuza, K., & Filzmoser, P. (2016). <i>Introduction to multivariate statistical analysis in chemometrics</i>. CRC press. • Husson, F., Lê, S., & Pagès, J. (2011). <i>Exploratory multivariate analysis by example using R</i> (Vol. 15). Boca Raton: CRC press. • James, G., Witten, D., Hastie, T., & Tibshirani, R. (2013). <i>An introduction to statistical learning</i> (Vol. 112, p. 18). New York: springer.
Other infos	The slides of the course will be made available on Moodle.
Faculty or entity in charge	CHIM

Programmes containing this learning unit (UE)				
Program title	Acronym	Credits	Prerequisite	Learning outcomes
Minor in Chemistry	MINCHIM	4		
Additional module in Chemistry	APPCHIM	4	LCHM1381	