

Course Specifications

From the academic year 2016-2017 up to and including the

Course size (nominal values; actual values may depend on programme)
Credits 4.0 Study time 120 h Contact hrs 45.0 h

Course offerings and teaching methods in academic year 2018-2019

A (semester 1)	English	lecture	15.0 h
		seminar: practical PC	30.0 h
		room classes	

Lecturers in academic year 2018-2019

Vincze, Laszlo	WE06	lecturer-in-charge
----------------	------	--------------------

Offered in the following programmes in 2018-2019

	crdts	offering
Master of Science in Chemistry	4	A
Exchange Programme in Chemistry (master's level)	4	A

Teaching languages

English

Keywords

Experimental design, design of experiments, data analysis, signal processing, univariate calibration, pattern recognition

Position of the course

Compulsory subject in the first year Master of Chemistry, second semester, just before starting the Master proof in the second year (first and second semester).

Builds on a general course "statistics", e.g. partim "Mathematics II" in the first year Bachelor of Chemistry.

Objective: theoretical and practical introduction to chemometrics, possibly to be applied in the Master proof

Contents

Introduction: measurements, uncertainty, error, detection limit

Experimental design, design of experiments, DOE

One or more factors (e.g. (concentration of) reagents, temperature, pH, ...) influence a process (e.g. synthesis, separation, analysis, production, ...) to be optimised for one or more parameters (e.g. high yield and/or purity, baseline separation, high sensitivity, low production costs, minimal environmental pollution, ...). Experimental design will learn us (1) how and which experiments are to be planned, and (2) the conclusions to be drawn from these experiments: which factor(s) influence the process, which factors are correlated, what are the optimum conditions, ...

Data analysis

Create relevant information from the measurements (experiments).

Signal processing Sequential signals, (e.g. spectrum, chromatogram) are measured digitally. The quality of the information obtained depends on the processing of the raw measurement data, e.g. filtering, first and second derivative.

Univariate calibration The measurement of one variable (e.g. absorption, emission, ... for one wavelength, retention time, ...) is determined by one factor (e.g. species concentration).

Pattern recognition Multiple variables that are not necessarily independent, can define a physical or chemical reality that can not be measured directly. The concentration or presence of molecules, elements, ..., a spectrum, ... are examples of multiple variables that define e.g. the nature of environmental pollution (urban, industrial, ...), the identity of a chemical species, ...

Initial competences

The student has acquired credits for the course units "Chemistry I: Structure of Matter"

and "Chemistry II: Changes in Matter", "Introduction to Organic Structures", "Mathematics II: Fundamental Methods in Mathematics and Statistics", "Spectroscopic Methods of Analysis", and "Analytical separation methods", or has required knowledge by equivalent course units, to be proven by credits.

Final competences

- 1 Know the principles of common chemometrical methods.
- 2 Recognize problems to be solved (preferably) by chemometrics.
- 3 Ability to apply chemometrics for specific cases.
- 4 Use of professional statistical software.
- 5 Interpretation of the results and drawing relevant conclusions (i.e. data reduction).
- 6 Overcome one's initial hesitation to learn and apply advanced chemometrical methods.

Conditions for credit contract

Access to this course unit via a credit contract is determined after successful competences assessment

Conditions for exam contract

This course unit cannot be taken via an exam contract

Teaching methods

Lecture, seminar: practical PC room classes

Learning materials and price

Richard G. Brereton

Chemometrics. Data Analysis for the Laboratory and Chemical Plant

J. Wiley, Chichester, 2003, ISBN: 978-0-471-48978-8 or 0-471-48978-6

<http://eu.wiley.com/WileyCDA/WileyTitle/productCd-0471489786.html>

Cost: € 103.90 in 2016 (+ 12%/year)

Minerva

Software (licence free of charge for use in the PC class and on Citrix server at athena.ugent.be or athenax.ugent.be)

References

Course content-related study coaching

Minerva: exercises: Q & A

Personally by appointment

Evaluation methods

end-of-term evaluation and continuous assessment

Examination methods in case of periodic evaluation during the first examination period

Written examination with open questions, open book examination, oral examination

Examination methods in case of periodic evaluation during the second examination period

Written examination with open questions, open book examination, oral examination

Examination methods in case of permanent evaluation

Skills test

Possibilities of retake in case of permanent evaluation

examination during the second examination period is not possible

Extra information on the examination methods

Periodical evaluation:

- open book (SPSS instructions): PC exercises: applications
- closed book questions: theory
- written and oral questioning

Non-periodical evaluation:

- during classroom problem solving sessions: PC exercises: applications

Calculation of the examination mark

Periodical evaluation (80%)

Non-periodical evaluation (20%) during classroom problem solving sessions: PC exercises

Students who are absent without any well-justified reason or who do not participate in all evaluation methods (seminars) of the continuous assessment, get a non-deliberable examination mark.

The marks resulting from the permanent evaluation are retained in the second examination period, as the second examination period only consists of a periodic evaluation.