

Chemometrics

Programme course

3 credits

Kemometri

TFKI11

Valid from: 2017 Spring semester

Determined by

Board of Studies for Chemistry, Biology
and Biotechnology

Date determined

2017-01-25

Main field of study

Chemical Engineering, Applied Mathematics, Chemistry

Course level

First cycle

Advancement level

G2X

Course offered for

- Chemical Analysis Engineering, B Sc in Engineering
- Chemistry

Entry requirements

Note: Admission requirements for non-programme students usually also include admission requirements for the programme and threshold requirements for progression within the programme, or corresponding.

Prerequisites

Statistical Tools for Chemical Analysis or Calculation tools for chemistry students

Intended learning outcomes

The overall aim of the course is to give the students theoretical and practical knowledge on how to apply experimental design (Chemometrics) in order to efficiently plan, perform and evaluate chemical experiments.

After completion of the course the students should be able to:

- Plan, conduct and evaluate screening experiments in order to identify design variables that affect response variables of interest. This part includes Factorial and Fractional factorial designs.
- Plan, conduct and evaluate experiments with the aim to optimise design variables with respect to one or several response variables. This part includes response surface modelling (Central Composite Design), Simplex optimisation and the Gradient method.
- Apply commercial Chemometrical software in order to plan and evaluate screening and optimisation experiments.

Course content

Experimental design, Screening designs, Optimisation designs, Design and analysis of such models, regression methods, optimisation of chemical analysis and processes.

Teaching and working methods

The course consists of theoretical lectures and computer exercises in which the theory is applied in practice.

Examination

PRA1 Project work with oral and written presentation 3 credits U, G

Grades are give as 'Fail' or 'Pass'.

Grades

Two-grade scale, U, G

Department

Institutionen för fysik, kemi och biologi

Director of Studies or equivalent

Magdalena Svensson

Examiner

Johan Dahlén

Education components

Preliminary scheduled hours: 30 h

Recommended self-study hours: 50 h

Course literature

Miller, J.N. and Miller, J.C., Statistics and Chemometrics for Analytical Chemistry

Common rules

Regulations (apply to LiU in its entirety)

The university is a government agency whose operations are regulated by legislation and ordinances, which include the Higher Education Act and the Higher Education Ordinance. In addition to legislation and ordinances, operations are subject to several policy documents. The Linköping University rule book collects currently valid decisions of a regulatory nature taken by the university board, the vice-chancellor and faculty/department boards.

LiU's rule book for education at first-cycle and second-cycle levels is available at http://stydokument.liu.se/Regelsamling/Innehall/Utbildning_pa_grund-_och_avancerad_niva.