This course syllabus is discontinued or replaced by a new course syllabus.



# **Course Syllabus**

School of Science and Technology

# Chemometrics, Statistics for Chemists, Second Cycle, 7.5 Credits

Course Code: KE104A Subject Area: Field of Science

Main Field of Study: Chemistry Credits: 7.5

Subject Group (SCB): Chemistry

Education Cycle:Second CycleProgression:A1FEstablished:2016-11-30Last Approved:2018-03-28Valid from:Autumn semester 2018Approved by:Head of School

## **Aims and Objectives**

#### General aims for second cycle education

Second-cycle courses and study programmes shall involve the acquisition of specialist knowledge, competence and skills in relation to first-cycle courses and study programmes, and in addition to the requirements for first-cycle courses and study programmes shall

- further develop the ability of students to integrate and make autonomous use of their knowledge
- develop the students' ability to deal with complex phenomena, issues and situations, and
- develop the students' potential for professional activities that demand considerable autonomy, or for research and development work.

(Higher Education Act, Chapter 1, Section 9)

#### **Course Objectives**

Knowledge and understanding

After completing the course, the student should be able to

- Demonstrate knowledge to choose statistical methods for a given question and corresponding dataset,
- Demonstrate knowledge of univariate statistics that can be used on data sets,
- Apply multivariate statistical methods in the interpretation of data using basic methods of data reduction analysis, hierarchical cluster analysis, principal component analysis, and regression methods for classification (Partial Least Squares),
- Understand how visualization of data sets can complement statistical methods, and
- Present proposals for chemical / analytical sampling strategies and project planning.

#### Proficiency and ability

After completing the course, the student should be able to

- Systematize scattered information into structures for statistical analysis,
- Apply basic univariate statistics,
- Select and apply multivariate statistical methodology for a given problem,
- Identify problems and transpose them into graphic or tabular outputs,
- Structure and analyze multi-dimensional data using computer programs for multivariate methods and critically review the result, and
- Apply multivariate principles for study planning.

After completing the course, the student should

- Be able to characterize a scientific problem and critically review the relevant information regarding the task.
- Perform a data analysis with statistical methods and chemometrics, and
- Present the results based on univariate or multivariate statistical methods in written and orally.

#### **Main Content of the Course**

The course requires a basic but solid understanding of mathematical operations and general statistics.

The course provides a basic understanding of the application of mathematical and statistical methods in the planning and implementation of measurements and analysis with the help of univariate and multivariate statistical problem solving. The course includes introductory statistics, univariate and multivariate statistics for data analysis and interpretation as well as experimental design. Furthermore, computer based laboratory exercises are conducted using examples with relevance to environmental chemistry. Pivot charts, box-whisker plots, hierarchical cluster analysis, principal component analysis (PCA) as well as partial least square (PLS) are focus areas that are treated during the course.

Examples are handled with software tools (R).

# **Teaching Methods**

Lectures, exercises, individual computer software projects and seminars.

Students who have been admitted to and registered on a course have the right to receive tuition and/or supervision for the duration of the time period specified for the particular course to which they were accepted (see, the university's admission regulations (in Swedish)). After that, the right to receive tuition and/or supervision expires.

### **Examination Methods**

Theoretical part, 4 Credits. (Code: 0100) Written exam.

Practical Parts, 3.5 Credits, (Code: 0200)

Exercises and project are reported in writing and orally at seminars.

Absence from Mandatory Course Component

If a student is absent from a mandatory course component, the examiner determines if the student will be able to make up for the component during another scheduled class of the same kind. Otherwise, the student is referred to the next time the course is offered. As an exception the examiner may decide on substitute assignments. These shall then be carried out before or shortly after the end of the course.

For further information, see the university's local examination regulations (in Swedish).

#### **Grades**

According to the Higher Education Ordinance, Chapter 6, Section 18, a grade is to be awarded on the completion of a course, unless otherwise prescribed by the university. The university may prescribe which grading system shall apply. The grade is to be determined by a teacher specifically appointed by the university (an examiner).

According to regulations on grading systems for first- and second-cycle education (vice-chancellor's decision 2010-10-19, reg. no. CF 12-540/2010), one of the following grades is to be used: fail, pass, or pass with distinction. The vice-chancellor or a person appointed by the vice-chancellor may decide on exceptions from this provision for a specific course, if there are special reasons.

Grades used on course are Fail (U), Pass (G) or Pass with Distinction (VG).

Theoretical part

Grades used are Fail (U), Pass (G) or Pass with Distinction (VG).

Practical Parts

Grades used are Fail (U) or Pass (G).

Grade on full course

As a grade of the course as a whole, the grade from the theory part is given, provided that the practical moments are approved.

The course grading is translated to the ECTS grading scale.

For further information, see the university's local examination regulations (in Swedish).

## Specific entry requirements

A first-cycle qualification comprising of at least 180 credits in Natural Science in which at least 60 credits are for specialized study in the main field of Chemistry, and Chemistry, Second Cycle, 30 Credits are needed. The applicant must also have qualifications corresponding to the course English 6/B from the Swedish Upper Secondary School.

For further information, see the university's admission regulations (in Swedish).

## **Transfer of Credits for Previous Studies**

Students who have previously completed higher education or other activities are, in accordance with the Higher Education Ordinance, entitled to have these credited towards the current programme, providing that the previous studies or activities meet certain criteria.

For further information, see the university's local credit transfer regulations (in Swedish).

#### **Other Provisions**

The language of the course is English.

## **Reading List and Other Teaching Materials**

#### **Required Reading**

Miller, James N. & Miller, Jane C. Sixth edition Statistics and Chemometrics for Analytical Chemistry Harlow, England: Pearson Education Limited

#### **Additional Reading**

Eriksson Lennart (Senaste upplagan)

Multi- and Megavariate Data Analysis Basic Principles and Applications

Boca Raton F: CRC Press, Books can be borrowed from the School of Science and Technology (MTM)

## Additions and Comments on the Reading List

Kompendier och digitalt material tillkommer. Written instructions and digital materials to be added.