Course: Chemometry

credits: 5

Course code	CHVH24CHEMOMETR1
Name	Chemometry
Study year	2025-2026
ECTS credits	5
Language	Dutch, with parts in English
Coordinator	-

Modes of delivery	Lecture Practical / Training Tutorial
Assessments	Chemometrie 1 Practicum - Other assessment Chemometrie 1 Theorie - Computer, organised by STAD examinations

Learning outcomes

You apply univariate and multivariate sequential optimization and interpret the results, using the following search methods: Binary, Fibonacci and (modified) Simplex.

You can do matrix arithmetic (scalar product, matrix product, determinant, inverse, transposed).

You numerically determine maxima and minima of functions within optimization and discuss the results found in relation to chemical and experimental significance.

You perform univariate and multivariate simultaneous optimization and interpret the results, including through application of Response Surface Methodology (with screening and detail designs, such as factorial and Central Composite designs)

You can perform and interpret appropriate analysis of variance (ANOVA) based on the experimental design

You apply the acquired theoretical knowledge about spectrometry, potentiometry and optimization in an independent, safe and responsible way during the execution of an experiment, and communicate about this with a logbook and/or results form according to the applicable guidelines.

Content

Chemometrics is the application of statistical and mathematical methods and techniques in chemistry. It is used to obtain and process measurement data for optimization, calibration, interpretation of data, etc. The focus of this module is on optimization. You will learn to collect chemical information, measurement data, in a structured way and thus efficiently find out the influence of variables and an optimum of a chemical experiment. For example, you can increase the yield of a reaction. From the beginning you will learn how to use factorial design, you will learn to apply matrix arithmetic so that you can solve regression problems and calculate the influence of variables.

In practice, you will use the knowledge gained in spectrometry, potentiometry and experimental design in experiments in which you apply these techniques. The processing of the experiment requires an elaboration using an ANOVA and an interpretation of the results.

Included in programme(s)

Chemistry

School(s)

Institute for Life Science & Technology

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