Chemometrics 23.03 – 28.05.2021

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TEACHERS



Matthew MacLeod course responsible part I & II

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part III



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labs

COURSE LAYOUT

Part I Basic and Univariate Statistics Part II Design of Experiment Part III Multivariate Analysis

Consists of Lectures and Labs Each part ends with an exam Need to pass all parts

CHROMIUM IN GRASS

Two methods were compared for determination of chromium in grass. First method yielded a mean results of 1.48 mg/kg and for the second method it was 2.33 mg/kg. The standard deviation of the results were 0.28 and 0.31 mg/kg.

BASIC AND UNIVARIATE STATISTICS

- Hypothesis testing ANOVA
- Non-parametric tests Calibration and Quantification

CHROMATOGRAPHY METHOD

You are asked to develop a GC method for separating A and B. You can adjust the temperature in a range from 100 °C to 300 °C, the flow rate of the carrier gas from 0.1 mL/min to 2 mL/min and choose from different 30 m columns.

The client requires that the method you develop has a resolution >1.5. Since time is money, you also need to perform as many analysis a day as possible.

DESIGN OF EXPERIMENT

Factorial Design Mixture Design Green chemistry principles Design and Robustness Testing with MODDE Response surface designs Bayesian Statistics

SLEEP APNIA AND METABOLIC PROFILE

Sleep apnea may result in heart attack, stroke, diabetes, etc. while cardiovascular disease is associated with high blood pressure, diabetes, high blood cholesterol, poor diet, or excessive alcohol consumption.

Blood samples of 18 sleep apnea and 18 cardiovascular disease patients were analysed with LC-MS/MS for betaine, carnitine, choline, tma, tmao determined for. Can the metabolic profile can be used to differentiate between these diseases?

MULTIVARIATE ANALYSIS

Multilinear regression Classification methods Clustering methods Principal component analysis Advanced regression methods Applications of chemometrics in non-targeted HRMS



Software: R mainly and some Excel

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Altogether 14 labs

Exams involve calculations

