

Training session

Spectroscopic data analysis

Learn the basis of Chemometrics methods
for spectral data processing

Objectives

This training session on multivariate data analysis is intended for people wishing to:

- Learn the basic methods of Chemometrics
- Become autonomous in spectral data processing
- Assimilate the key steps of spectroscopic data analysis methodology

During the training, the method principles are introduced by a geometric approach. Emphasis is placed on the practical use of the methods and the interpretation of the results.

Application exercises are proposed for each method. Training can be held on various chemometrics software: Unscrambler® (Camo Analytics), SIMCA® (Umetrics Sartorius), PLS_Toolbox® (Eigenvector Research Inc.) or software under Matlab® environment (MathWorks).

Information



No prerequisites



3 days



R&D, quality control, product development, process optimization, ...



In-house sessions



Spectroscopic data



Researchers, scientists and engineers



Agriculture / food, Petrochemical, Pharmaceutical, Biotechnology, Chemistry, Environment...

Program

Day 1: Exploratory analysis

- Introduction - Chemometrics
 - ✓ Principal Components Analysis (PCA)
 - ✓ Theoretical principle
 - ✓ Interpretation
 - ✓ Detection of outliers
 - ✓ Application on data set and software



Day 2: Quantitative predictive modeling and pre-processing

- Linear multivariate regression models (MLR, PCR, PLS)
 - ✓ Theoretical principle
 - ✓ Model validation methods
 - ✓ Detection of outliers
 - ✓ Optimization
 - ✓ Application on data set and software
- Pre-processing of spectroscopic data
 - ✓ Correction of additive effects
 - ✓ Correction of multiplicative effects
 - ✓ Application on data set and software

Day 3: Methods of discrimination

- Principle of identification
- PLS-DA (PLS - Discriminant Analysis)
- SIMCA (Soft Independent Modeling of Class Analogies)



In-house sessions

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