

Training Course

***Chemometric Spectroscopy:
Basics and quantitative analysis
with practical examples using SL products***

in Norderstedt

The training course is designed as an introduction to multivariate calibration, but also helps you to refresh your existing knowledge in the field of chemometric spectroscopy in a systematic approach.

The complete workflow, from collecting spectroscopic data to the application of methods in practical routine work, is covered in theory and applied in practical exercises.

Participants will get to know the SL database and the most important functions of the SL product family. However, most topics are equally useful for users of other software packages.

Prior knowledge in instrumental analysis is necessary, but knowledge of chemometrics and its methods is not required.

The training course will be held in German (courses in English are available on request).

Instructor:

Dr. Heinrich Prüfer

Dipl. Chem., Managing Director at SensoLogic, has over 20 years of experience in chemometric methods and spectroscopy.

Topics:

1. The concepts of NIRS laboratory and industrial process analysis:
Common ground and differences
2. Modeling: Raw data make all the difference.
 - Examples for artefacts and their causes
 - Filtering or correction? What does "representative" mean in practice?
How many samples are necessary, and how should they be distributed?
 - Simple, duplicate or multiple sampling?
3. All inclusive: The SL database concept
 - Samples and reference data
 - Spectra, series and libraries
 - Transformations
 - Calibrations, methods and applications
4. The Emperor's new suit: Multivariate regression models become transparent
 - Functionality of multilinear models
 - Explanation of wavelength models and factor models -
Is it necessary to use more than one PLS?
 - Why do you need nonlinear calibration techniques?
5. Start small - win big: Derivatives and other techniques of data pre-processing
 - Linearisation and digital variance filter:
What are the effects of the most commonly used transformations?
 - How do you determine the best-suited transformation for your application?
 - Is it possible - and useful - to automate this decision?
 - Is there a universally well-suited transformation?
6. Cross-Validation & Co. –
Pre-testing and quality characterization of calibration models
 - How can you predict the performance of a calibration?
 - How important is the multiple correlation coefficient?

- How effective is cross-validation?
 - What other quality indices are useful?
7. Outlier diagnostics and side remarks on qualitative analysis
- Is it possible to evaluate the validity of measured spectra?
 - What are outliers? What do the outlier types T, H, D and S mean in the SL Calibration Workshop?
 - Outlier diagnostics in qualitative analysis: library and cluster models
8. Test, test, test – Validation
- What does "representative" mean for a validation set?
Is it the same as in the calibration set?
 - What is the preferred distribution in a validation set?
9. How can I trust? – Measurement uncertainty and other diagnostics for quality assurance with SL Predictor
- What methods of outlier diagnostics are useful for daily laboratory work?
 - How can you estimate the uncertainty of an individual measurement?
 - How do you identify a drift of measured values?
 - And what are the causes? Calibration, spectrometer or sampling?
10. The never-ending story: Calibration transfer and maintenance
- Three ways to the same end: Is it better to adjust the calibrations, to standardize spectra or to use only extremely robust calibrations?
 - What maintenance techniques are available?

Final discussion

Schedule:

1. Day: 1 pm – 6 pm
2. Day: 9 am – 5:30 pm
3. Day: 8:30 am – 12:00

Location: Norderstedt (Details to be agreed)

Course Fee: EUR 750,- + 19% VAT

Course fee includes course materials, refreshments, and lunch (on the second day).
On the first day, we would like to invite you to dinner.
Costs for travelling and accomodation are not included in the course fee.