Using Pre-Treatments Effectively for Chemometric Analysis of NIR Spectra

Learn how to interpret and optimize derivatives and use them with other pretreatments to minimize multiplicative scatter effects in NIR measurements for sensitive quantitative measurements

Who Should Attend

Scientists and technicians who are concerned with getting the best performance from calibrations. Anyone who employs NIR or MIR Spectroscopy in an analytical lab. The course employs minimal vector mathematical notation, and a knowledge of basic algebra and statistics will be helpful. Prior use or knowledge of NIR methods is recommended.

Key Topics You'll Learn About

- Segment-Gap and Savitzky-Golay Polynomial Fit methods of calculating derivatives
- How Convolution Functions elucidate the calculation of derivatives
- How to evaluate the degree of smoothing in calculation of derivatives
- Some methods of calculating derivatives actually **improve the signal/noise ratio in spectra**
- Standard Normal Variate (SNV) and Multiplicative Scatter Correction (MSC) Pretreatments adjust for optical path differences between samples
- Extended Multiplicative Scatter Correction – what it is, how to use it
- Spectral Pretreatments make spectral bands and analytical relationships clearer
- Statistics to evaluate and compare various calibrations

How You'll Benefit from This Course

- Take the "Black Box Approach" out of your chemometric analyses
- Learn how to evaluate spectra and advantages of derivatives
- Learn how to evaluate various methods of calculating derivatives
- Learn how SNV and MSC pretreatments work and how to combine them with derivatives
- Learn about the features of EMSC
- Learn how the pretreatments affect the precision of NIR measurement results

About the Instructor

David W. Hopkins has been a NIR Consultant for more than 15 years, and has more than 40 years experience in spectroscopy. He has contributed to many projects in NIR applications in pharmaceutical, petrochemical, chemical, and food/agricultural industries, as well as development of NIR instrumentation. Dr. Hopkins has published papers and scientific articles, and has presented lectures at many international meetings. He has presented training courses in Using NIR Spectroscopy under the auspices of the American Chemical Society and Applied Chemometrics. He earned his Ph.D. from the University of California, San Diego.

Course Agenda

The course will be kept informal, with plenty of opportunities for questions and discussion. Participants will receive a course book for taking notes and to keep as a useful reference.