

## **Basic Chemometrics for NIR**

This half-day course will cover the chemometric techniques most commonly used in developing NIR calibrations. The topics that will be covered, in order of presentation, are

1. Calibration by multiple linear regression
2. Choosing a training set
3. Spectral pre-treatments
4. Tuning and validation
5. Principal component analysis
6. Quantitative calibration using PLS and PCR
7. Qualitative calibration using discriminant analysis and regression methods

This is not a hands-on course, there isn't time in half a day for practical sessions. The emphasis will be on understanding how these basic chemometric tools work, and the issues involved in using them for NIR calibration.

The course will run from 08.15 until 12.00, with a break for coffee/soda from 10.00 to 10.15. If things go to plan this will happen between items 4 and 5 on the list.

## **Advanced Chemometrics for NIR**

This half-day course may be taken as a continuation of the basic course, or on its own. It will assume some knowledge of the material in the basic course. It will cover some of the more sophisticated methodology that has been used for NIR calibration. Essentially this means looking at non-linear methods. The topics to be covered, in order of presentation are:

1. Nonlinear calibration, local versus global approaches
2. Artificial neural networks
3. Support vector machines
4. Local regression methods such as LWR, LOCAL, CARNAC
5. Qualitative calibration using KNN and SIMCA

As with the basic course, the emphasis will be on explaining how these methods work, and discussing some of the issues involved in using them for NIR calibration.

The course will run from 13.00 until 16.45, with a break for coffee/soda from 14.45 to 15.00. If things go to plan this will happen between items 3 and 4 on the list.

## **About the Instructor**

Tom Fearn is Professor of Applied Statistics at University College London, UK. He has worked in NIR since 1978, and received the Tomas Hirschfeld award for contributions to near infrared spectroscopy in 2001. His publications include joint authorship of the books Practical NIR Spectroscopy, with Osborne and Hindle, and A User Friendly Guide to Multivariate Calibration and Classification, with Næs, Isaksson and Davies. He is chemometrics editor of the Journal of Near Infrared Spectroscopy and writes the Chemometric Space column in NIR News.