

Chemometric Analysis for Spectroscopy

Bridging the Gap between the State and Measurement of a Chemical System

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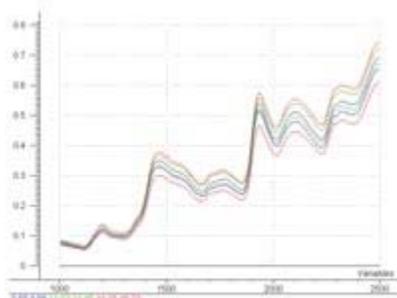
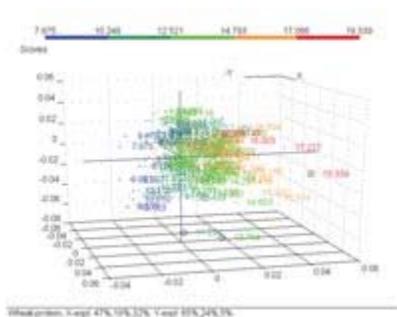


Figure 1. NIR spectra 1000-2500 nm of wheat samples. [Click to enlarge.](#)

Chemometrics is the use of mathematical and statistical methods to improve the understanding of chemical information and to correlate quality parameters or physical properties to analytical instrument data. Patterns in the data are modeled; these models can then be routinely applied to future data in order to predict the same quality parameters. The result of the chemometrics approach is gaining efficiency in assessing product quality. It can lead to more efficient laboratory practices or automated quality control systems. The only requirements are an appropriate instrument and software to interpret the patterns in the data.

The science of chemometrics gives spectroscopists many efficient ways to solve the calibration problem for analysis of spectral data. Chemometrics can be used to enhance methods development and make routine use of statistical models for data analysis. Spectroscopists use software packages like The Unscrambler® for spectroscopic data analysis, modeling, classification and prediction to meet process monitoring and quality assurance needs. The spectroscopists' chemometrics requirements are:

- Proper application of spectroscopic data pre-processing, to reduce and correct interferences such as overlapped bands, baseline drifts, scattering, and pathlength variation. Figure 1 shows NIR spectra of wheat samples that scatter effect is severe due to packing and size variation. Multiplicative Scatter Correction (MSC) pretreatment is recommended to build reliable relationship between wheat protein content and spectral data, for scatter correction.



[Click to enlarge.](#)

- Strong calibration and diagnostics means of sample selection and variable selection, statistic result calculation to build representative and reliable models. Figure 2 shows potential sample outliers (circled) identified by sample residual, leverage and Hotelling T2. Sample outliers usually affect negatively on model performance, and need to be kept-out.

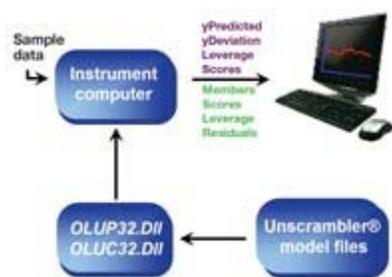
- Model validation and integration means to supply rigorous prediction, measurement QC and real-time product quality and process monitoring.

Spectroscopists need to use the following methods within a chemometrics software package to explore their data:

- Principal Component Analysis (PCA)
- Regression (PLS, PCR, MLR, 3-way PLS) and Prediction
- SIMCA and PLS-DA Classification

- Design of Experiments
- ANOVA and Response Surface Methodology
- Multivariate Curve Resolution (MCR)
- Clustering (K-Means)

In conclusion, Chemometrics is the bridge between connecting the state of a chemical system to the measurements of the system. It has become an essential part in the modern chemical and biomedical industries. Chemometrics software has been widely used by product development scientists, process engineers, PAT specialists, and QA/QC scientists to build reliable model, ensure product quality, classify raw material, and to monitor process end point in real-time as shown in Figure 3.



Scheme of utilizing Unscrambler® models for real-time prediction/classification. Not only the predicted value/membership, but also data QC results are reported to ensure the prediction can be trusted. [Click to enlarge.](#)

For more information, contact Dongsheng Bu, PhD, Principal Scientist, CAMO Software, at dbu@camo.com or by phone at 732-602-8886 x32.

AT A GLANCE

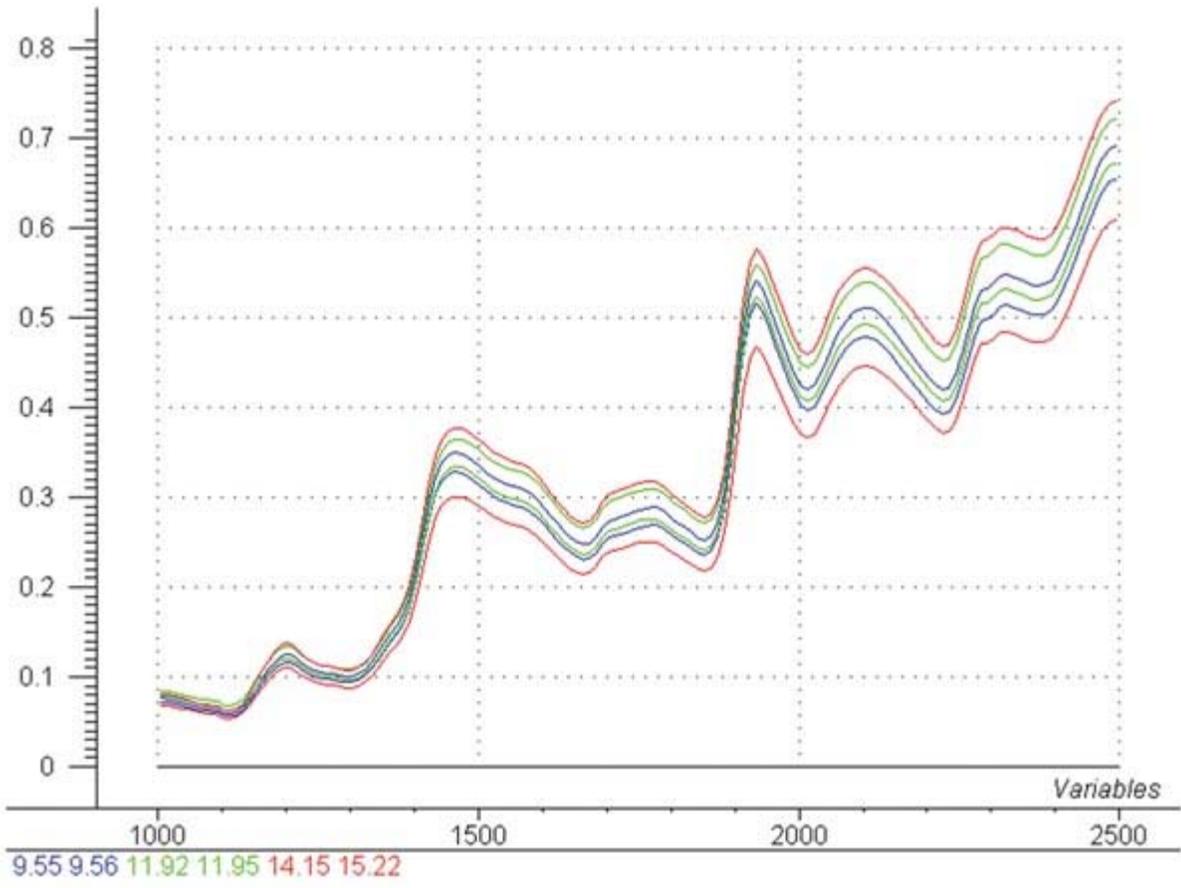
- Chemometrics uses mathematical and statistical methods to improve understanding of chemical information
- Chemometrics gives spectroscopists efficient ways to solve the calibration problem for analysis of spectral data
- Spectroscopists use software packages for data analysis, modeling, classification and prediction
- Chemometrics has become an essential part in the modern chemical and biomedical industries

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Sample data



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