**B&W TEK INC.**

Your Photonics Partner

Software

BWIQ™

The Next Generation in Speed, Accuracy, and Performance

BWIQ™ chemometrics software package for use with the i-Raman® and other high resolution Raman products. BWIQ™ is a multivariate analysis software package which can analyze spectral data and discover internal relationships between spectra and response data or spectra and sample classes. BWIQ™ combines traditional chemometric methods such as Partial Least Squares Regression (PLS) and Principal Component Analysis (PCA), with new methods such as B&W Tek's proprietary adaptive iteratively reweighted Penalized Least Squares (airPLS) algorithm for automatic baseline correction and Support Vector Machine (SVM) algorithms for non-linear datasets.

Applications:

* **Multivariable Quantitative Analysis**

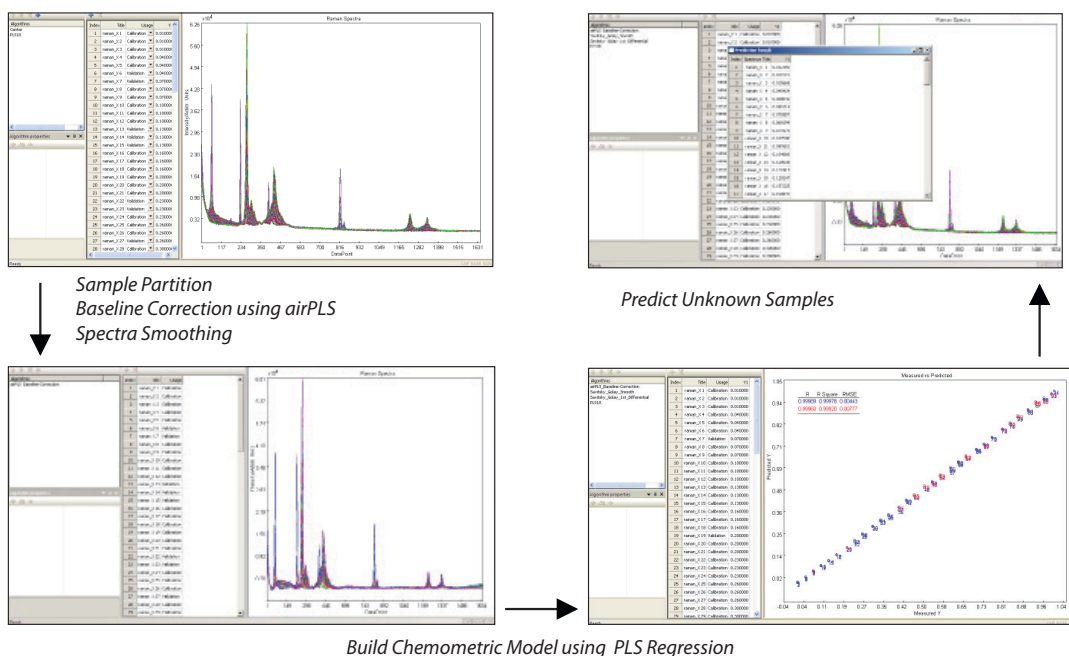* **Multivariable Classification Analysis**

* **Exploratory Analysis**
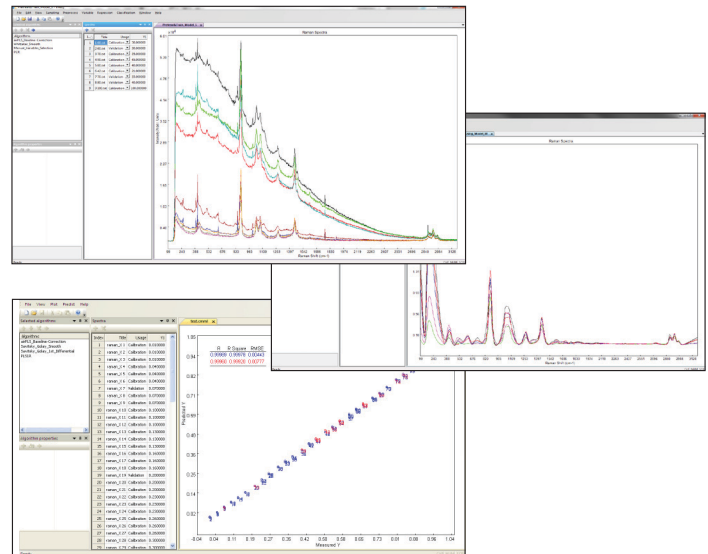
Key Features:

* Progressive structure and easy-to-follow work flow

* Wide variety of regression and classification routines

* Three different automatic sample partition algorithms

* High performance and accuracy with the help of BLAS and LAPACK

* High speed and less memory with sparse linear algebra algorithms

* Chemometric Modeling Markup Language (CMML) for easy model storage and sharing

* Innovative algorithms airPLS for baseline correction and Whittaker Penalized Least Squared algorithm for spectra smoothing

Main Functions:

- Automatic sample partition algorithms for sampling process

- Various spectra preprocess algorithms, including automatic baseline correction airPLS (adaptive iteratively reweighted Penalized Least Squares); smoothing algorithms and spectra differential; as well as mean centering and auto scaling

- Intuitive variable selection based on spectra as well as correlative coefficient.

- Exploratory data analysis through Principle Component Analysis (PCA)

- Regression analysis through various algorithms including MLR, PCR, PLS1, PLS2

- Support Vector Machine Regression for non-linear datasets

- Classification with cluster analysis and discriminant analysis with algorithms including SIMCA, PCA-MD, PLS-DA, SVC

Example Software Work Flow

Sample Partition
Baseline Correction using airPLS
Spectra Smoothing

Predict Unknown Samples

Build Chemometric Model using PLS Regression

Advantage of airPLS compared to
common baseline correction routines

- airpls
- irls
- als
- rbe