

Software **BW IQ™**

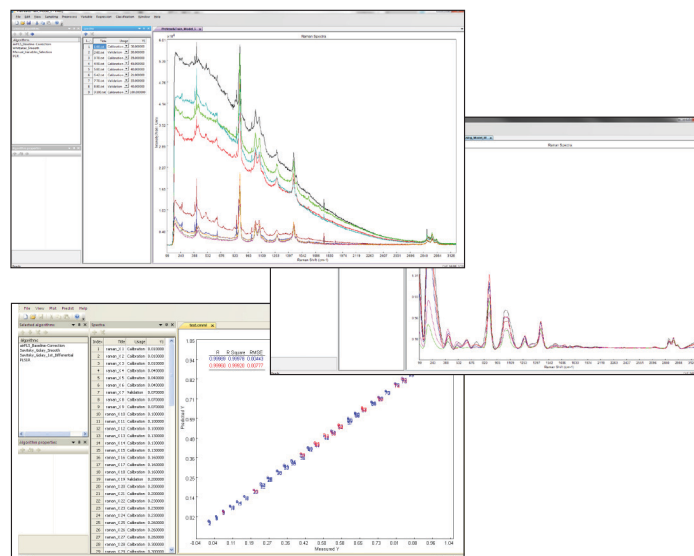
The Next Generation in Speed, Accuracy, and Performance



BW IQ™ chemometrics software package for use with the i-Raman® and other high resolution Raman products. BW IQ™ 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. BW IQ™ 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**



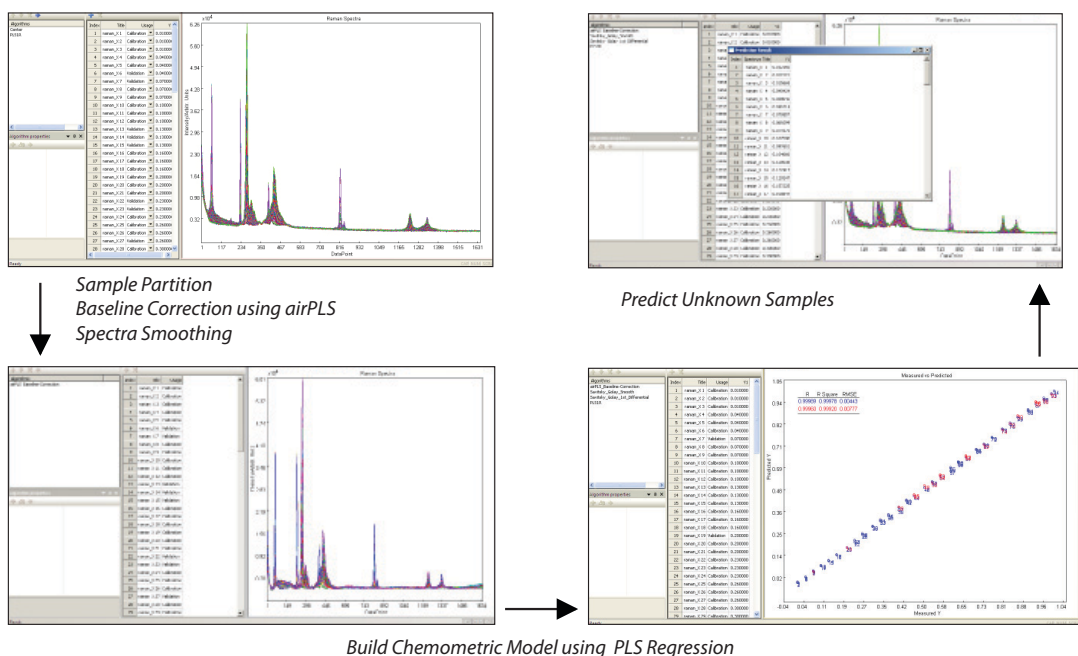
Key Features:

- 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



Advantage of airPLS compared to common baseline correction routines

