

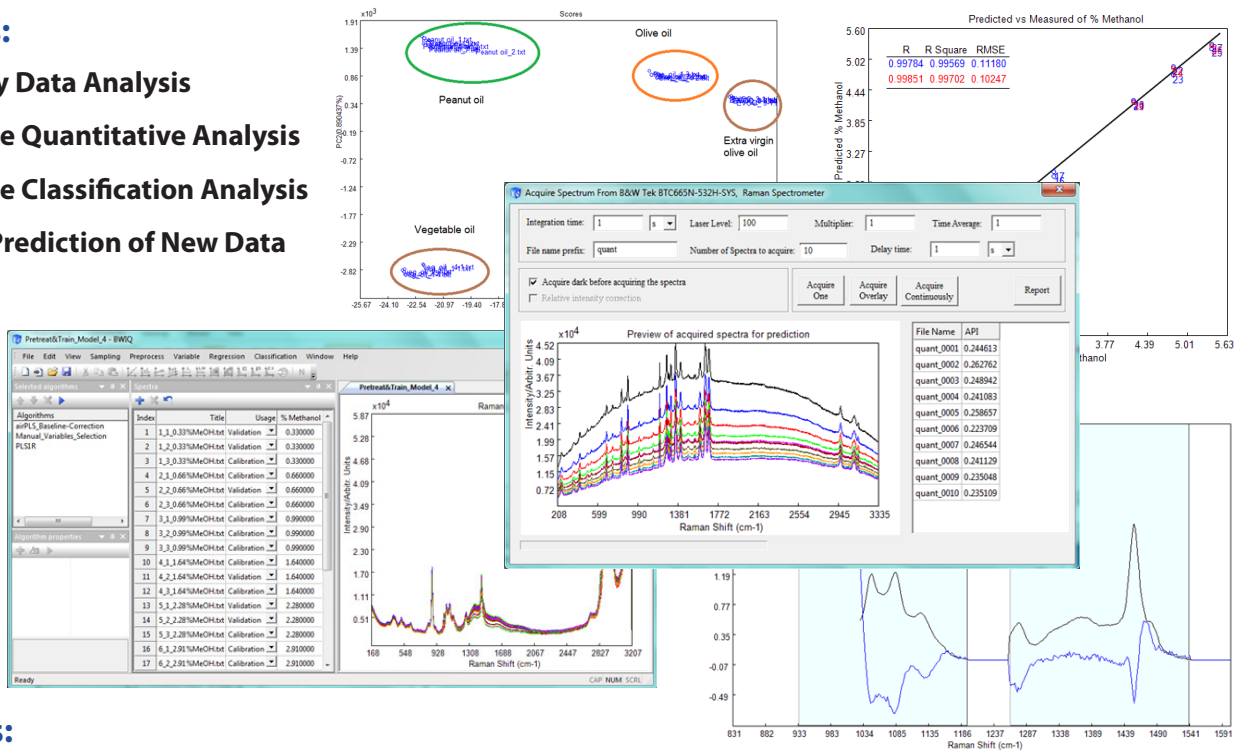
Graphical, Logical Chemometrics for Spectroscopic Data



BWIK[®] is a comprehensive multivariate analysis software package for analysis of spectral data including exploratory, qualitative analysis and quantitative regression methods. BWIK supports the classical chemometric methods for classification and regression including Partial Least Squares Regression (PLS), Principal Component Analysis (PCA) and Discriminant Analysis with Support Vector Machine (SVM) algorithms for non-linear datasets. It features an intuitive workflow from data import to prediction, with extensive graphics in support of model analysis and interpretation. BWIK includes preprocessing tools for optimal analysis of Raman, NIR, LIBS and other spectroscopic datasets. The BWIK chemometrics software package is ideal for online use with the i-Raman[®] series instruments for real-time prediction and offline use with high-resolution spectroscopic data.

Applications:

- Exploratory Data Analysis
- Multivariate Quantitative Analysis
- Multivariate Classification Analysis
- Real-time Prediction of New Data



Key Features:

- Full suite of regression and classification routines
- Extensive graphical display of data and results for evaluation of model performance metrics
- Easy import of BWSpec[®], spc, Matlab and csv data file formats
- Logical easy-to-follow work flow and progressive software structure
- Chemometric Modeling Markup Language (CMML) for easy model storage, sharing and use within operating software including BWAnalyst
- Innovative algorithms for baseline correction (airPLS) and spectral smoothing (Whittaker Penalized Least Squared)
- Real-time prediction with i-Raman series instruments
- Report function including model parameter summary

Main Functions:

- Exploratory data analysis through Principal Component Analysis (PCA)
- Regression analysis with various algorithms including MLR, PCR, PLS and Support Vector Machines (SVMR)
- Classification and discriminant analysis with algorithms including SIMCA, PCA-MD, PLS-DA, and Support Vector Machine Classification (SVC)
- Sample partition algorithms for sample selection including Kennard-Stone and SPXY
- Numerous spectral preprocessing algorithms, such as automatic baseline correction, smoothing, derivatives, and normalization
- Cross-validation and test set validation options
- Outlier detection using Y-residuals, Q-residuals, M-distance
- Full model details table viewable within model
- Portability of cmml model file use with BWIQ prediction engine in BWAnalyst software

System requirements:

The following hardware and software are recommended for optimal performance of BWIQ:

Operating Systems

- Windows 7, 8, or 10

Recommended Hardware

- Intel Core i7 or greater
- 4 GB RAM or more
- 1 GB hard drive space
- monitor with 1024 x 768 pixels or higher
- video card with high GDI+ drawing speed

Example applications:

- Quantitative analysis of API in pharmaceutical tablets
- Product contamination: quantitation of diethylene glycol in glycerin; methanol contamination in alcoholic beverages
- Quantitation of fatty acids in edible oils
- Real-time monitoring of glucose in nutrients; quantitation of glucose in aqueous solutions
- Sample classification: gasoline of different octane levels; alcohols; different edible oils

Example Software Work Flow

