Symbion QT

…Expert Chemometrics Made Easy

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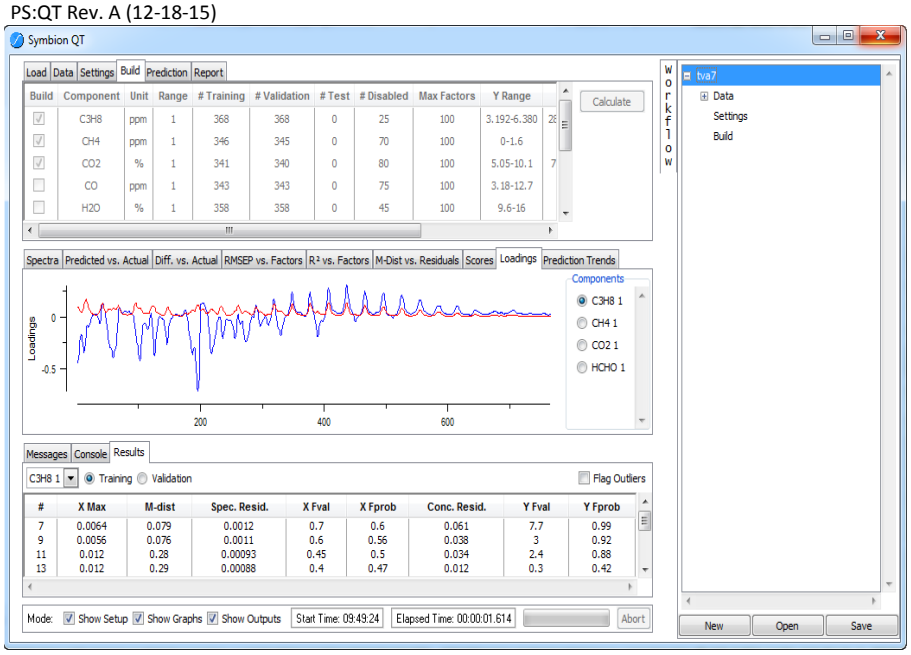

Symbion QT represents a new approach to chemometrics, one which places the chemometrics engine in the background and focusses instead on streamlining the process of building and deploying chemometric models.

The *QT* Model Builder employs a step by step workflow approach which guides beginner and expert alike through the process of assembling and processing the data needed to build and evaluate calibrations. The resulting calibrations are fully validated and documented and ready for deployment.

The entire *QT* package has been developed from the ground up to provide a completely natural, non-intrusive development environment which frees the user to focus directly on meeting project requirements without being encumbered by overly complex software. It can function either as a free standing multivariate analysis program, or it can be combined with any of the Symbion instrumentation software packages to constitute a fully integrated environment for data collection, automated model development, and on-line process monitoring.

For the chemometrician, Symbion QT leverages scarce human resources by eliminating many of the clerical steps normally required to enter data and build models. For example, a data table comprising several hundred spectra - along with the required metadata and reference values – can be built in a matter of seconds. In addition, QT's flat workflow inspired user interface makes it the ideal platform for training non-specialists such as chemical engineers, bench chemists, and lab technicians to carry out many of the tasks required by modern chemometrics. The result can be a major advance in resource scalability.

The Symbion QT Model Builder

For the non-specialist and expert alike, Symbion QT delivers the broad capabilities of modern chemometrics without the need for specialized training. The QT experience is like having an expert guiding you at every step of the process.

Automated Data Input: Symbion QT can be employed as a stand-alone chemometrics package or integrated with Symbion LX, DX, or RX so as to fully automate the data collection and table building process. The user simply enters the Batch, Sample, Expected Value, and Units in the appropriate Symbion window during data collection. When the desired data are gathered into QT, the requisite information automatically populates the data table, taking only a few seconds for even hundreds of spectra, and substantially reducing the operator's clerical workload and potential for error.

Data Inspection: A full complement of visualization tools enable the user to scroll through his data so as to identify interferences and regions of non-linearity or other artifacts to be avoided.

Type Assignment: While still on the data input page, one can assign individual spectra to categories such as "Calibrate", "Test", or "Validate".

Streamlined Model Set-up: The next tab on the home page opens the "Settings" screen, allowing the assignment of all of the parameters for any number of individual methods on this one screen. Examples include Y range, X range, min. and max. values for each, maximum number of factors, and a selection of preprocessing functions and metrics. Separate methods can be defined for distinct X and Y ranges so as to handle interferences and nonlinearities.

Rapid and Flexible Model Building: To build the desired set of methods, one simply selects the "Build" tab. This displays all of the current settings for each selected method. Pressing "Calculate" then builds the selected methods.

The results of the build are immediately displayed in two new windows, each with a series of tabs, allowing you view a range of plots and tabular information, including all of the metrics specified under "Settings". Clicking on a component's name updates the current display to present the information for that component.

The flat, tabular format, allows the user to rapidly compare all of his methods and examine the results for statistical outliers and bad data files. The results of this analysis can then be fed back to refine individual methods.

Automatic Model Optimization: The first step in model optimization is the intelligent examination of the raw data and of trial models, as outlined above. However, Symbion QT also includes an automatic model optimization capability utilizing parametric based variable selection. This enables the rapid comparison of builds employing different combinations of X axis ranges and preprocessing functions.

Reporting: In addition to reporting results, QT provides a high-level perspective for assessing the internal conformity of models and the performance of a given model when tested against plant data.

The Symbion QT Predictor

Once a model has been optimized and validated, the result is saved out in XML format so that it comprises a completely self-contained prediction system.

Prediction: The Predictor can be employed from the main QT platform by simply selecting the appropriate tab in the QT home window. This allows the chosen models to be used to predict the values of selected files. A range of statistical metrics are available for evaluating the results**.**

Real-time deployment: The combination of Symbion QT with any of the Symbion process analytical programs (Symbion DX, RX, or RTM) constitutes a fully integrated system for continuous on-line process analysis. In addition to this real-time monitoring capability, the Symbion Replay Mode can be used to replay previously acquired time-dependent data sets using any number of models. This capability enables the evaluation of trial models using actual process data.

Symbion *QT* Features:

During development:

- A clean user-oriented approach to model development
- Integrated Work-flow environment
- Automated model optimization
- Rapid, flexible assembly of training, test, and validation data sets
- Auto-generation of reports to document every step of method development and deployment
- Incorporation of external variables such as temperature, pressure, and flow into models
- Compatible with diverse data formats and instruments
- Supports PLS, PCR, and PCA

During deployment:

- Rapid, simultaneous execution of multiple models by means of multi-threading
- Full integration into the Symbion suite of analytical software
- Replaying of pre-acquired data using new or refined models
- Full Life-Cycle Optimization™ utilizing automated internal diagnostics

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