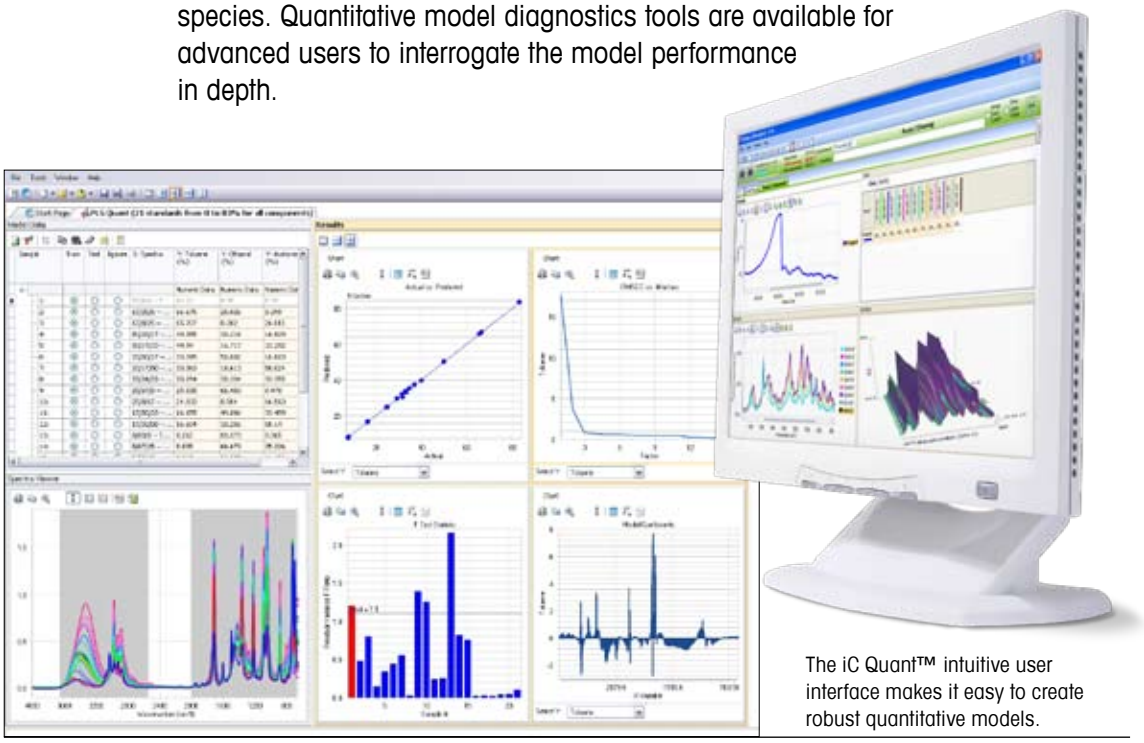
In Situ Spectroscopy

Predict Concentrations in Real Time

with iC Quant™ for iC Software

iC Quant™ provides quantitative information that allows scientists to speed the development and improve the quality of high value compounds. This is done with iC Quant™ by predicting the actual concentrations of key reaction species, even in a complex mixture, in real time to understand reaction performance.

iC Quant™ is a graphical add-on application for iC software that enables scientists to quickly and easily develop quantitative models without the need to be a specialist. Scientists record referee data with their iC experiments, which is then, with a click of a button, automatically transferred along with the associated spectra to iC Quant™ where a quantitative model is generated for each reaction species. Quantitative model diagnostics tools are available for advanced users to interrogate the model performance in depth.



The iC Quant™ intuitive user interface makes it easy to create robust quantitative models.

METTLER TOLEDO

Easy to Use

iC Quant™ is intuitive software designed to be used by any iC user and does not require any specialized knowledge in chemometrics. While iC Quant™ is rich in advanced functionality for the more experienced user, the interface is designed to simplify use by non-experts.

Simply Powerful

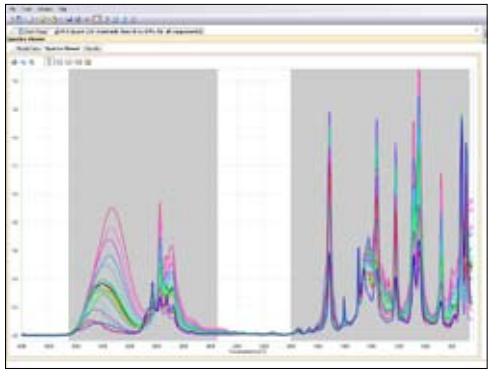
iC Quant™ is seamlessly integrated into iC software. Models are created or opened from the Start Page or from the menu bar. For prediction, iC Quant™ models are simply loaded from a quantitative analysis task pane. iC Quant™ displays component trends and associated quantitative values in real time as each spectrum is collected.

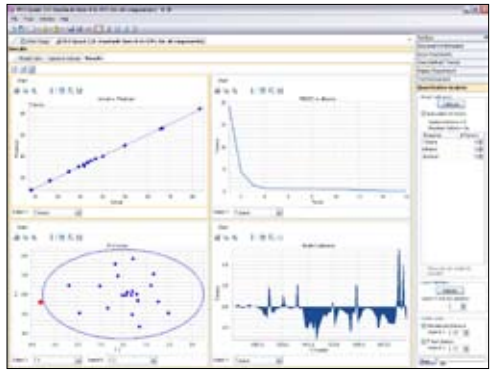
General Features

- Univariate or Multivariate model support
- Linked view display
- Seamless integration with iC software for prediction in real time
- 21 CFR 11 support with comprehensive Audit Trail
- Import legacy QuantIR files
- Supports calibration with data from multiple experiments
- Copy and paste offline referee data from Microsoft Excel
- Select Training or Test samples in a spreadsheet like editor
- Report customizable iC Quant™ results and diagnostics charts
- Interactive online documentation

Chemometrics Features

- Auto-select the number of factors for model calibration
- Linear Least Squares for univariate analysis
- Partial Least Squares (PLS) for multivariate analysis
- Transform variables before calibration
- Apply data treatments to variables
- Graphical selection of spectral regions
- Leave-n-out cross validation procedure
- Use probability values for outliers detection





Charts

- Results Charts – Actual vs. Predicted, RMSEC, PRESS
- Outliers Charts – F Test Statistics, Mahalanobis distance, Studentized Residuals vs. Leverage
- Diagnostics Plots – Scores, Loadings, Model coefficients, Residuals
- Auto update charts for different number of factors

www.mt.com/iC

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