Spectrum Quant Quantitative Analysis Software

Unleash the potential of your PerkinElmer FT-IR and NIR spectrometers with Spectrum® Quant software. Designed for novice and advanced spectroscopists who need to integrate accurate quantitative analysis into their IR or NIR analysis. Spectrum Quant combines very simple method development with a range of data processing options to ensure optimum quantitative analysis that can be achieved quickly and reliably. Spectrum Quant is designed by spectroscopists for spectroscopists. Like the highly popular Spectrum 10 Spectroscopy software for the PerkinElmer spectrometers, Spectrum Quant manages your data to enable you to easily work with multiple spectra, methods and results to maximize your productivity. The common design approach with Spectrum 10 enables quantitative methods to be easily incorporated into Spectrum 10, macros and Spectrum Touch methods, to provide simple turnkey analyzer operation with PerkinElmer IR and NIR systems.

PerkinElmer®

For the Better

Smart, simple quantitative analysis

Spectrum Quant is ideal for laboratories that need to deliver results efficiently, without the need for extensive software training or methods development. If you use Spectrum 10 to collect your IR or NIR data, Spectrum Quant requires virtually no additional training to get up and running (Figure 1). Method development can be fast-tracked thanks to the close linkage between the two packages. For example, when calibration spectra are collected using Spectrum 10, concentrations can be entered with sample information and all data automatically incorporated into a quantitative method using the smart method
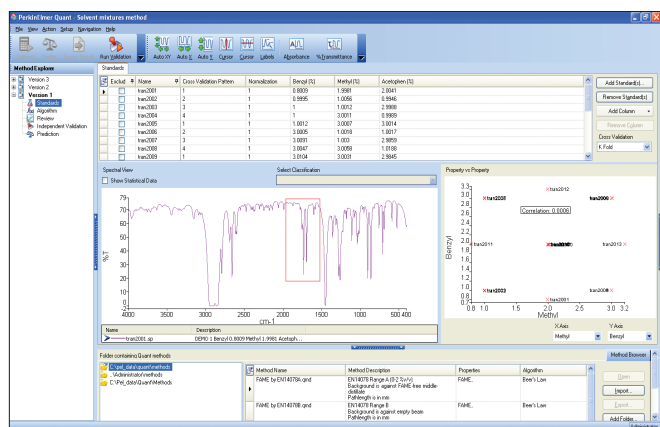

Figure 3. Interactive parameter setup from spectral displays.

Accelerated method optimization

Using Spectrum Quant means you can get the best results out of your valuable IR and NIR data. A range of quantitative analysis and data visualization options are available in a modular structure – from simple peak height/area analysis using the Beers Law module to powerful full spectrum multivariate methods such as partial least squares (PLS) or principal components regression (PCR) (Table 1).

Table 1. Spectrum 10 Quantitative Analysis modules.

Quantitative Technique	Software Module
Univariate analysis including peak height, area regression methods	Spectrum 10 with Beers Law Quant (LX108873)
Multivariate analysis with partial least squares and principal components regression (PLS1 and PCR+) with model diagnostics and validation	Spectrum Quant Algorithm Pack L1101024

Figure 1. Simple layouts allow you to manage Quant methods, data and results.

Wizard (Figure 2) or custom data fields settings in Spectrum 10 – minimizing the possibilities of transcription error. As the method is developed and refined using the powerful interactive Quant tools, the project is managed with the Method Explorer feature of the software. Method versions allow changes to be tracked and stored enabling you to converge on optimum choice of method parameters as quickly as possible. With Spectrum Quant you can get methods implemented quickly and easily.
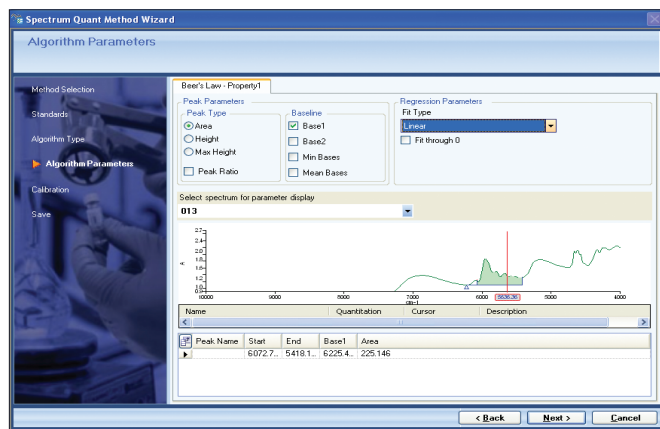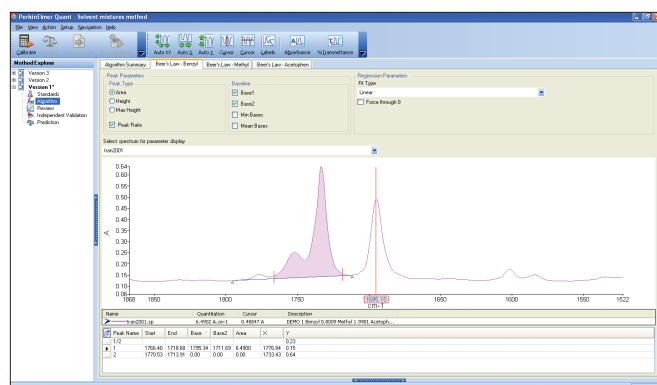
A suite of preprocessing algorithms are included to assist with common sampling variability issues and improve method robustness. Once calibration spectra are defined, the powerful graphical interaction allows calculation ranges (Figure 3), baselines and other parameters to be setup graphically using the spectra and cursors, and scatter plots can quickly reveal potential problems with spectral or concentration data in the calibration.
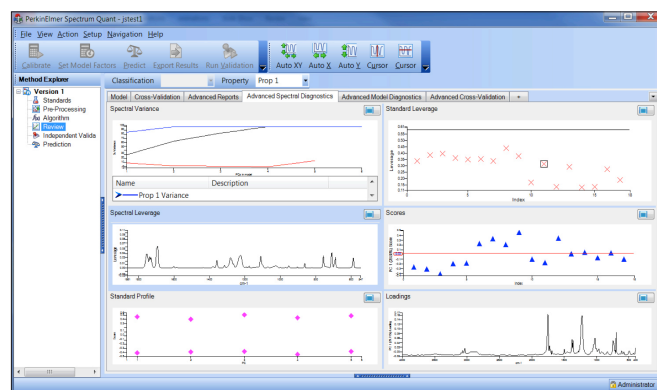

Figure 2. Quant method Wizard for simple method building from Spectrum 10.

Figure 4. Review plots for easier evaluation of statistical data.

Simple method development tools are available, like Property Correlation to find the most suitable peaks to use for a particular property or analyte, and a range of Review model diagnostic plots can provide rapid statistical analysis and confidence in the calibration model (Figure 4). Throughout the method development, a number of Validation options are available to test the method for self-consistency and its performance with independent samples. As methods are refined, the effects of parameter changes are easily seen as the validation plots and are instantly updated with each reiteration. The Method Explorer allows simple navigation between the method versions – providing updates to methods and results at a glance.

Figure 7. Conditional formatting of results and Quant Control Limits lets you setup PASS/FAIL criteria.

Figure 5. Incorporate Quant results in special macros.

Put your Quant methods into action

Once you are satisfied with a Quant method's performance using the simple validation tests, the Spectrum 10 suite provides convenient ways to analyze new samples. Run the samples directly from the Spectrum Quant module or from the main Spectrum 10 control software; single menu items or command buttons can be placed on the ribbon to perform single-click analysis of newly-acquired or saved data. Alternatively, use the powerful Macro-Editor to incorporate the Quant analysis into customized data collection and analysis procedures without the need for special manual coding (Figure 5).

Figure 6. For easy method implementation in the plant or warehouse with customization to local languages.

Using the unique Spectrum Touch interface allows simple touch/tap navigation through your analysis rather than the traditional point and click methods, to fully exploit modern touchscreen PC functionality (Figure 6). Performing multi-component analysis, even simultaneously on multiple spectra in Spectrum 10 is a single-click operation and exploring the results tables couldn't be easier with the sophisticated tabular/graphics display in Spectrum 10 and Quant. You can also specify control limits on calculated concentrations so that out-of-specification results can be visibly highlighted in results tables (Figure 7). With Spectrum Quant method integration you can concentrate on the results rather than the tasks.

Personalize your work space to suit your style

Figure 8. Transfer results to other applications for further processing or formatting.

With a familiar Microsoft® Outlook®-style interface, Spectrum Quant allows you to adjust your views to suit your preferences. Customizable Quant action and graphics toolbars can show your most-used tasks – while methods information, setups and navigators can be positioned in panes side by side – or pushed aside to avoid clutter as you would a normal work area.

You can send selected elements of the methods or results to other applications such as Microsoft® Word® for incorporating into your reports (Figure 8), or use the built-in Report Editor to customize Quant reports – or transfer results tables into third party spreadsheet and trending packages for specific views. Access control into the software is also provided via a separate customizable login screen.

Local language selection and Microsoft® support

Spectrum Quant is compatible with Windows® 7/8 with 64 bit support. Local language support is automatically selected from the Windows® locale setting, including English, Spanish, Chinese, Japanese, German, French and Portuguese versions.

Microsoft Gold Certified Partner

The Spectrum Quant software development site is a Microsoft® Gold certified partner. Spectrum team members have demonstrated the highest levels of technical excellence, marketplace impact and satisfaction of customers using Microsoft® products and services.

For a complete listing of our global offices, visit www.perkinelmer.com/ContactUs

010556A_01