Spectrum 10 Spectroscopy Software

PerkinElmer Spectrum™ 10 is the infrared spectroscopy software platform for the range of PerkinElmer FT-IR spectrometers. Designed for busy industrial and academic laboratories that require both efficient operation and wide-ranging capabilities, this comprehensive package sets the standard in FT-IR software for simplicity and efficiency in data collection, processing, and generating results. The software’s specially designed interface combines single-click commands functions with powerful data and results management. Its “layered simplicity” is a breakthrough in spectroscopy software. Unlike other packages, which often trade-off ease-of-use for advanced capability, Spectrum 10 provides both – making it the ideal software for novices and advanced spectroscopists alike.

Make Your Everyday Tasks Faster And Easier

Focus on the results, not the tasks

Clicking many times to perform frequent operations can be frustrating. To avoid this repetition, we’ve made some software enhancements to make your work easier:

1. Common operations including fully automated procedures can be placed on the toolbar and reduced to a single-click or keyboard shortcut. The unique “Scanalyse” feature scans spectra and updates results real-time so you can assess your results almost instantly even as the data is being scanned.

2. Setups can be viewed and adjusted using a separate Setup panel area away from data.

3. Operations which generate multiple results are automatically set up to order the results in a logical layered output avoiding the need to click through multiple windows.

4. Report layouts can be tailored to local requirements with the interactive Report Designer module, while multiple results, trends, and patterns can be visualized in more meaningful ways for ease of interpretation with unique connectivity to TIBCO Spotfire® visualization software. Spectrum 10 provides unsurpassed ability to visualize, and collaborate results in a multitude of ways.

No matter how you work, you’ll find the Spectrum 10 desktop design provides the fastest access to spectral data and results, including audit trail information.
Take control of your FT-IR

Our popular instrument software for the Spectrum Two and Frontier™ instruments has been enhanced to provide instant access to both instrument commands and parameters you frequently adjust with a unique Instrument Toolbar. For example, this can be helpful in the factory warehouse installation where you typically only need to define a sample scan time. The on-screen toolbar can be set up to include just a scan button, instrument status indicator, and setup field for scan time. You will not have to navigate complex instrument setups, making operating your instrument more efficient and reproducible.

Automatically configure accessories

The plug-and-play feature of our software allows for smart sampling accessory recognition. When a PerkinElmer intelligent accessory is changed or added to your FT-IR, the software automatically re-configures the FT-IR to accommodate the new accessory. Numerous intelligent, live graphics status indicators such as accessory type provide instant confirmation of the correct settings allowing you to quickly continue with your measurements.

Figure 1. Configurable instrument toolbar lets you display just the operations and settings you need to change.

Figure 3. You can reduce multiple operations to 1-click procedures using the simple macros facility.

Need to occasionally check advanced instrument settings? No problem. The setup pane can be raised to reveal full parameter setups, subdivided logically into basic and advanced setups. More importantly, this advanced information can be retained on-screen if required while data is collected and manipulated. Thanks to the intelligent layered screen arrangement, advanced settings can be viewed without obscuring the live data window. In addition, our sophisticated 7-day Laboratory Scheduler for Spectrum Two and Frontier instruments enables you to predefine when you need to automatically run regular instrument checks, so the instrument can be setup and ready to run whenever you need it, day or night.

Customize your workbench

Spectrum 10 is fully customizable in both operator functions, software appearance and reports. You can ensure the commands you need are at your fingertips. Enhanced configurability is added to the spectrum graph area, allowing setup of all aspects of the drawing area so you can get your presentation or report just right.

For Faster, Easier FT-IR Solutions

Whether you need to screen for minor impurities or adulterants, identify unknown materials, or verify your product’s composition, Spectrum 10 provides the tools you need – all fully integrated, set up, and ready to go. Spectrum 10 not only gets results faster this way, but it provides an easier route to derive information by its seamless interface with other applications. For example, you can easily display a set of quantitative predictions in a radar display using TIBCO Spotfire® or Microsoft® Excel® to highlight anomalous samples, or calculate statistical functions such as standard deviations from a set of results data.

Figure 2. Simplified layout means you can easily manage data, associated results and setup information.
For Better Laboratory Practice
The sophisticated Sample Table layer enables multiple sample information to be entered prior to scanning and is especially convenient when used with the instrument ‘Go’ button on the Frontier or Touchscreen PC/barcode combination with the Spectrum Two. Custom data entry fields can be included to mandate input of additional information before scanning is allowed and supplementary data can be text, numeric (e.g. concentration information) or even graphical data enabling the spectral data to be permanently tagged with information such as chemical structures and other relevant images. In addition, during quantitative methods building component concentrations entered into the Sample Table are retained with the spectral data and can be transferred directly to the Quant method development software. This avoids transcription errors and saves time during method development.

Workbench Layers Help You Manage Your Work
Spectrum 10’s design is a result of extensive feedback requesting a software that can provide comprehensive functionality without losing its simplicity of operation. One outstanding feature is how simple it is to interpret data and results with our workbench layers. These allow you to easily:

- **Work with multiple spectra** and see multiple results in a single table without navigating numerous results pages. For example, you can perform peak height calculations to determine contamination levels on 50 spectra with a single-click, then select the results and transfer them into TIBCO Spotfire® or Microsoft® Excel® for trending and statistical analysis with one additional click.

- **Navigate multiple spectra** and associated results using the Data Explorer Tree – much simpler than using multiple windows. Data Tree structures can be retained for the next time you log on so you can quickly return to your workbench arranged as you left it.

- **Activate other applications** for further manipulation. The ‘Send To’ function places selected spectra and reports directly into new Microsoft® Word®, WordPad® documents or other software. Results tables can also be easily transferred to spreadsheet packages or to stunning visual results dashboards using the Send to TIBCO Spotfire® capability. Or “Send To Email” instantly sends data or reports directly to specified email recipients. Other spectroscopic software packages tend to place single results in locations which prohibit easy manipulation of multiple results. With Spectrum 10 you can more easily present and communicate your data the way you want.

- **View** the instrument toolbar, numeric results, and their setups at the same level, or push aside the setups and navigators just as you would tools on a normal workbench to minimize clutter and focus on live data or results.

- **For Better Laboratory Practice**
  - For Better Laboratory Practice
    - The sophisticated Sample Table layer enables multiple sample information to be entered prior to scanning and is especially convenient when used with the instrument ‘Go’ button on the Frontier or Touchscreen PC/barcode combination with the Spectrum Two. Custom data entry fields can be included to mandate input of additional information before scanning is allowed and supplementary data can be text, numeric (e.g. concentration information) or even graphical data enabling the spectral data to be permanently tagged with information such as chemical structures and other relevant images. In addition, during quantitative methods building component concentrations entered into the Sample Table are retained with the spectral data and can be transferred directly to the Quant method development software. This avoids transcription errors and saves time during method development.

- **Navigate multiple spectra** and associated results using the Data Explorer Tree – much simpler than using multiple windows. Data Tree structures can be retained for the next time you log on so you can quickly return to your workbench arranged as you left it.

- **Activate other applications** for further manipulation. The ‘Send To’ function places selected spectra and reports directly into new Microsoft® Word®, WordPad® documents or other software. Results tables can also be easily transferred to spreadsheet packages or to stunning visual results dashboards using the Send to TIBCO Spotfire® capability. Or “Send To Email” instantly sends data or reports directly to specified email recipients. Other spectroscopic software packages tend to place single results in locations which prohibit easy manipulation of multiple results. With Spectrum 10 you can more easily present and communicate your data the way you want.

- **View** the instrument toolbar, numeric results, and their setups at the same level, or push aside the setups and navigators just as you would tools on a normal workbench to minimize clutter and focus on live data or results.
Comprehensive Data Processing To Meet All Your Application Needs

Spectrum 10 includes a full suite of standard IR data processing commands designed specifically for spectroscopic processing. From simple spectral transforms to advanced qualitative and quantitative analysis, the data analysis modules work seamlessly together from the Spectrum 10 platform and can be called on-demand or run from pre-configured workflows for improved productivity. In addition, a unique Equations Editor enables you to quickly define non-standard process commands and make them single-click buttons on the toolbar or components in macro programs. No programming knowledge is required to use the smart equations or macro editors – customizing data commands is fast and intuitive.

Sample Verification of known materials is performed using the highly popular and acclaimed COMPARE™ software which includes specialized data filters to minimize effects of sampling variations and FT-IR noise distribution to improve accuracy and robustness of results. In addition, the Verify command can be used where known sample variability needs to be modelled using SIMCA (Soft Independent Modelling by Class Analogy) methods developed in the PerkinElmer AssureID materials verification software.

Screening for adulterants the innovative Adulterant Screen™ module is specifically designed for screening for suspected adulterants in ingredients and products. This unique tool combines the benefits of SIMCA by handling known sample variability in the calibration while providing additional information on levels of suspected adulterants with added statistical significance. This approach greatly simplifies method development while providing maximum sensitivity for low level contaminants.

For improved collaboration, more insights

Built-in options allow you to view your results the way you want to help collaborate and help gain deeper insights into your products and processes. The interactive Report Designer allows simple customization of single reports while direct visualization of multiple data trends and patterns is provided by the Send To TIBCO Spotfire® command. You get more time to understand your results with Spectrum 10.
Identification of unknown compounds and mixtures is accomplished with the standard Search function. This performs rapid comparison with commercial databases and user-generated spectral databases with the ability to interrogate the libraries with additional sample data such as physical properties. As with the other integrated data handling functions, Search parameters and reporting is easily configured from the Spectrum 10 setup sidebar, or combined with spectrum processing commands in macros. Alternatively, the Send To KnowItAll® function places data directly into the KnowItAll® software, allowing access to the most comprehensive collection of spectral databases available.

High performance Quantitative Analysis of mixtures is a key advantage of our FT-IR spectrometers due to their high performance source and electronics design. Spectrum 10 provides a range of quantitative algorithm options to suit the application, from simple peak height or area threshold measurement to full spectrum partial least squares predictions. Method development is made simple using Quant module, allowing methods to be developed and refined. In all cases quantitative method optimization is assisted by comprehensive graphical Review features in the software to allow rapid method evaluation. In addition, multiple-file, multi-model prediction has never been easier. A separate workbench layer is generated for all results, allowing both single-click multiple predictions with easy transfer of results to spreadsheets for trending and statistical analysis.

Create meaningful Results Dashboards to gain faster insights. All major quantitative and qualitative analyses results in Spectrum 10 can be displayed in a multitude of ways thanks to built-in connectivity to TIBCO Spotfire® visualization software. For example, the highly popular IR Compare command for verifying a product’s ID displays a number showing the degree of similarity between its IR spectrum and the best match in a reference library. In addition the operator or lab manager can see this result and with a single command show a dashboard to display how this Compare score has been changing over time to reveal if there is process drift, if the reference library is likely to require updating, or simply view statistical trends like number of pass/fail results tracked by operator, on a monthly basis. Or even view potential relationships with other analytical results like quantitative concentrations - or explore categorical relationships with other data associated with sample – like supplier information. For example, is there a link between a sudden change in analysis results and supplier, operator or packaging? This unique capability is made possible by addition of special export options within the Spectrum 10 commands which automatically save results and metadata to files which are displayed in the TIBCO Spotfire® software.

For More Confidence In Analysis
Validation of instrument performance and data integrity is standard with Spectrum 10 and performed at multiple levels. Low level interferogram integrity checking and other checks are applied automatically throughout the data processing chain through to final spectrum Quality Checks. These can be supplemented with the Spectrum 10 Instrument Verification suite which performs predefined instrument Operational Qualification, ASTM® and a suite of built-in pharmacopoeial tests. To verify system fitness for purpose for a given application, the configurable Ready Checks can include accessory contamination, throughput and even chemometric quantitative prediction control checks using a control sample. Only such multiple level validation checking ensures the highest confidence in analysis.

For improved insights into the system’s longer term performance and help pre-empt potential issues, validation commands output can also be trended and analyzed statistically with the powerful TIBCO Spotfire® option. The results is greater confidence in instrument performance and uptime.
The Spectrum 10 family of IR spectroscopy software products is designed for operational simplicity with power to address the most challenging IR analyses. All software modules work with the Spectrum 10 platform to provide an integrated approach to working with IR data.


**Adulterant Screen** - module designed for simple yet sensitive detection of economic adulterants in IR/NIR spectra. Standard and ES compatible

**Quant Advanced Algorithms Pack** - enables development of multivariate quantitative methods using principal components regression, partial least squares and spectral curve-fitting algorithms. Standard and ES versions

**Touch Developer software** - provides ability to create and run custom macros featuring an interface designed for simple Touch-screen operation

**Workflow Developer software** - a powerful developer package specially designed to allow creation of Touchscreen workflows which combine results of sample verification, adulterant screening and quantitative analysis in a logical an intelligent way. No special programming required. Standard version only.

**AssureID** - enables development of SIMCA product verification methods which can be run in Spectrum 10, macros, or AssureID workflows. Standard and ES versions

**Timebase** - For running time resolved or hyphenated experiments using FT-IR and FT-NIR spectrometers

**SpectrumIMAGE** - Controller for PerkinElmer Spotlight IR Imaging systems, featuring highly automated microscope control and IR image analysis functions

**Touch Applications Methods** - pre-built Touch methods, incorporating workflows, documentation and starter calibrations are available for a number of common methods including Trans-fat analysis, Lubricant analysis, Dairy powder analysis and environmental hydrocarbon analysis using standard methodology.

**Spectrum 10 ES For Regulatory Compliance**

Spectrum 10 ES provides additional security and data integrity features for achieving compliance with 21 CFR Part 11. In addition to enhanced access control features, ES software additionally and automatically stores data, experimental parameters and audit trail information in a secure SQL database. Data operating parameters and events can quickly and easily be recovered for inspection using a special query editor in the “Audit Trail” feature in the ES software. In addition, e-signature points can be added at appropriate defined events defined by the system administrator and included in the audit trail. In addition, comprehensive software validation documentation including test data and results are available to support the system validation process.

**Local Language Selection and Microsoft® Support**

Spectrum 10 is compatible with Windows® 7 and Windows® 8. Local language support is automatically selected from the Windows® locale setting, including English, Spanish, Chinese, Japanese, German and French, Portuguese versions. Local language support includes software interface, on-line Help and built-in tutorial programs.