SPECTRUM

User's Guide

PerkinElmer®

Release History

Release Date	Version
September	10.6

Any comments about the documentation for this product should be addressed to:

User Assistance
PerkinElmer, Inc.
710 Bridgeport Avenue
Shelton, CT 06484-4794
U.S.A.

Or emailed to: info@perkinelmer.com

Notices

Copyright Information

Produced in the U.S.A..

Trademarks

Contents

Welcome to Spectrum

Spectrum is a PerkinElmer software package for collecting, viewing and processing spectral data.

It can be used to set up and collect data from a range of PerkinElmer FT-IR spectrometers, including the:

- Spectrum Two FT-IR/FT-NIR spectrometers
- Frontier FT-IR/FT-NIR and FT-IR/FT-FIR spectrometers
- Frontier FT-IR and FT-NIR spectrometers
- Frontier Optica FT-IR
- Spectrum 400 FT-IR/FT-NIR and Spectrum 400 FT-IR/FT-FIR spectrometers
- Spectrum 100 FT-IR and Spectrum 100N FT-NIR spectrometers
- Spectrum 100 Optica FT-IR spectrometer
- Spectrum 65 FT-IR spectrometer
- Spectrum One FT-IR and Spectrum One NTS FT-NIR spectrometers.

You can also control the Spotlight 150 and 200 microscopes.

However, the following instruments are NOT supported by this release:

- Spectrum GX and Spectrum BX spectrometers.

It can be used to set up and collect data from a range of PerkinElmer Raman systems, including the:

- RamanStation 400 Series instruments
- RamanFlex 400 Series instruments
- RamanMicro 200 Series instruments
- RamanMicro 300 Series accessory
- Raman IdentiCheck instruments.

To familiarize yourself with Spectrum we suggest you work through the on-screen tutorials. Select **Tutorials** from the Help menu.

NOTE: The tutorials are designed to be displayed full-screen at a resolution of at least 1280 x 768. If the vertical resolution of your display is lower, the tutorial should play, but the playback controls may be obscured. You can exit a tutorial at any time by pressing the ESC key.

The Spectrum Help System

NOTE: When you are working in Spectrum, press F1 at any point to display an appropriate Help topic.

The help system is divided into the following areas:

Getting Started - A brief overview of Spectrum.

Finding and Saving - File operations and navigation.

Viewing Spectra - Working with windows and graph views.

Collecting Data - Controlling your instrument to collect spectra.

Publishing Results - How to cut and paste, print your screen, or export data to another application.

Processing Data - Working with your spectra and data.

Setup and Administration - Adapting Spectrum to your needs and preferences.

Workspace Reference - Links to help about particular commands, tools and features.

Getting Started

Getting Started

These topics provide a brief overview of the essential features of Spectrum:

Spectrum Tutorials

To familiarize yourself with Spectrum we suggest you work through the on-screen tutorials. Select **Tutorials** from the Help menu.

NOTE: The tutorials are designed to be displayed full-screen at a resolution of at least 1280 x 768. If the vertical resolution of your display is lower, the tutorial should play, but the playback controls may be obscured. You can exit a tutorial at any time by pressing the ESC key.

More about Spectrum

This Help system provides more detailed information about Spectrum in the following chapters:

Logging into Spectrum

Start Spectrum by clicking on its desktop icon, or via the Windows Start dialog.

The Login Dialog

Spectrum can be configured to:

- Open after you have entered a valid User name in a Login dialog. Password control is optional.

  OR

  Use your Windows login details.

If the Login dialog is displayed:

1. Enter your User name and, if required, Password.

   For a new installation of Spectrum (where no users have been set up and no other PerkinElmer applications are installed), log in as the default Administrator. We suggest that you set up at least one User and one other Administrator. See Setting up Users, Groups and Passwords.

   The security component does not distinguish between Spectrum version 6 and Spectrum version 10 (or later). If Spectrum 6 is (or has been) installed, enter your existing User name and Password.

2. If you want to change your password for any reason, click **Change Password**, enter and confirm your new password, and then click **OK**.

3. If you are a new user, have been given a new password, or your password has expired, you may be required to change your password.

4. Click **OK**.

   Spectrum opens.

5. If required, select which group workspace you want to load and then click **OK.**

   If the group workspace you are currently using has not been changed, then Use Existing Configuration will also be available. The group default workspace selected is loaded.

   The Choose Group Default Workspace is displayed in Spectrum ES when a new workspace is created and the default workspace of one or more groups of which you are a member has been updated since you last used Spectrum.

   Any new workspace created subsequently will be based on the group workspace you have selected. The Choose Group Default Workspace dialog will not be displayed again until one of the group workspaces is updated.

   Refer to Assigning a New Default Workspace for more information.

Selecting an Instrument at Login

- You can use Spectrum online to control an instrument, or offline to simply review or process data.

  Working offline releases a networked instrument for use by another user.

- If your PC is connected to your instrument via a cross-over cable, it is automatically made available to Spectrum.

- To make an instrument available to Spectrum, select Add Instrument from the Instruments sub menu of the Setup menu.

Login and your Save Option on Exit

When you exit or close Spectrum, you can save all your data for reload when you next log in. If you were connected to an instrument, this instrument becomes your default instrument when you next log in.

Additional Information

Passwords

If you have forgotten your password, ask an administrator to set a new password for you. You may have to change this password when you next log into Spectrum.

To learn more about password control, and the rules that can apply to passwords, see Passwords.

To learn more about how Spectrum can utilize Windows logins and passwords automatically, see Windows Login.

Instrument Administration

To learn how to select, add, or remove a networked instrument from Spectrum, refer to Instruments.

Auto-Connect

To learn more about how you can auto-connect to a instrument when you log into Spectrum, refer to Auto-Connect.

Save Options on Exit

To learn more about exiting or closing Spectrum, refer to Save Options on Exit.

Unexpected Software Events and Power Failures (Spectrum ES only)

In the event of a sudden power failure or software "crash", some of the workspace data may be left unsigned.

When the software is next started, it compares the current workspace setup with the signed information held in the database and, if a difference is found, the user is given the option to reload the previously saved workspace. A new entry is added to the Audit Trail to indicate that the workspace has been recreated. The user can then work on the data and apply an electronic signature to it.

If the workspace is not reloaded, the old data is left unmodified and a new workspace is created.

The Spectrum Workspace

After you log in to Spectrum, your workspace window is displayed. It can include a number of panes and toolbars.

Panes

The Spectrum workspace window is divided into panes:

- The Viewing Area, in the center, which you use to display one or more spectra.
- The Data Explorer, on the left, which you use to manage your spectra.

  You use the Data Explorer in conjunction with the Viewing Area.
- The Navigation Pane, on the right, which contains shortcuts grouped in a Setup pane.
- The Dialog Pane, at the bottom, which you use to adjust parameters or enter information when, for example, setting up your instrument.

  The contents of the Dialog Pane reflect the shortcut selected in the Navigation Pane.

Opening and Closing Panes

- To open or close the Data Explorer, click the button at the center of the left edge of the Viewing Area.

  OR

  Select **Data Explorer** from the View menu.
- To open or close the Navigation Pane, click the button at the center of the right edge of the Viewing Area.

  OR

  Select **Navigation Pane** from the View menu.
- To open or close the Dialog Pane, click the button at the center of the bottom edge of the Viewing Area.

  OR

  Select **Dialog Pane** from the View menu
- To open or close the Data Explorer, Navigation and Dialog panes simultaneously, hold down the SHIFT key and click the button that opens or closes any of these panes.

Resizing Panes

- Open the pane, and then drag the edge of the pane containing the button (not the button itself) to the width or height required.

Toolbars

The Spectrum workspace can include a number of global toolbars:

- The Menu bar.
- The Scan toolbars, namely the Instrument Settings bar and the Measurement bar and the Accessory bar. By default, these toolbars are located at the top of the workspace, under the Menu bar.
- The Status bar, located at the bottom of the workspace.

A pane can include one or more local toolbars. For example, the Viewing Area can include the following Graph toolbars:

- The Graph bar. By default, this toolbar is located at the top left of the Viewing Area.
- The Process bar. By default, this toolbar is located at the top right of the Viewing Area.

Additional Information

You can show, hide, re-arrange, or float many toolbars to suit your preferred manner of working.

You can also easily customize your global and local toolbars so that they include the tools you need and exclude the tools you do not use. For example, you can decrease the apparent complexity of the application by excluding unused icons from the Process bar. See Personalizing Toolbars.

You can revert to a default workspace, or preserve your current workspace for your next session.

Scanning a Sample

By default, the Scan toolbars (that is, the Instrument Settings bar and the Measurement bar) at the top of the workspace include the tools you need to collect a spectrum from a sample.

NOTE: The exact configuration of the default toolbars will depend on your instrument.

To collect a spectrum:

1. Check and set the instrument parameters, such as the **Start** and **End** points of the scan range (in wavenumbers, such as mid IR 4000 cm^{-1} to 400 cm^{-1} or near IR 10000 cm^{-1} to 4000 cm^{-1} or in Raman Shift, such as 3200 cm^{-1} to 100 cm^{-1}), the **Number of Scans** or **Accumulations** required, and a unique **Sample ID** and **Description**.

   By default, sensible values for the scan and instrument parameters are entered in the Instrument Settings toolbar; the values applied depend on your instrument and accessory. The **Sample ID** and **Description** are supplied by the Auto-Name function.

   To amend any value, select the parameter and enter your new value.

2. If you are connected to an FT-IR spectrometer and a background scan is required, the **Scan** button includes a small background flag. Clear the instrument beam path or insert a suitable background material, as applicable, and then click  to collect a background spectrum.

   The background spectrum is displayed, and then the Viewing Area is prepared for data collection from your sample.

   By default, the Measurement bar includes **Scan**, **Halt**, **Background** and **Monitor** buttons. You can also select these commands from the Measurement menu.

3. Place your sample in the instrument and then click  to begin scanning your sample.

   By default, during scanning the scan data is displayed on the Live tab in the Viewing Area.

   If you are connected to a Raman spectrometer and a background scan is required, the background spectrum is collected, and then the Viewing Area is prepared for data collection from your sample.

   The completed spectrum is displayed on the Graph tab, and added to the current Samples View in the Data Explorer.

4. If, for any reason, you want to stop scanning your sample, click  .

   If you halt the scan, no data will be saved.

Additional Information

Toolbars

- If there is insufficient space to display all the buttons on a toolbar two small arrows are displayed in the button on its right edge (or bottom edge, if the toolbar is vertical). Click  to reveal the buttons and then select the button required.
- The settings on the Accessory Toolbar depend on the current sampling accessory.

Parameter Values

➢ If you need to revert to the factory default settings, or amend the default values used, open the Navigation pane, select the Setup menu, click **Instrument** or **Raman Instrument** and then select the Setup Instrument Basic tab in the Dialog pane.

Press the **F1** key to display information about these settings, or see Setup Instrument - Basic.

The Prompts Display

The Prompts Display in the Measurement bar provides hints and prompts for data collection that may be mirrored in your FT-IR instrument display.

If required, you can hide the Prompts Display.

➢ Click  at the end of the Measurement bar, select **Add or Remove Buttons**, then **Measurement**, and then deselect the **Prompts Display** option.

Spotlight 150

For more information on collecting sample spectra with the Spotlight 150, see Scanning a Sample with the Spotlight 150.

Triggered Fiber Optic Probe

The Scan options on the Measurement menu and Measurement bar are disabled if you have selected a Triggered Fiber Optic Probe as your accessory on the Setup Instrument Basic tab. The Scan icons are grayed out, and contain a representation of the fiber probe  . A Scan can only be started by pressing the trigger on the probe. Refer to the *Raman Triggered Fiber Optic Probe* leaflet supplied with the probe for configuration and usage details.

Markers, Maps and Line Scans for Raman

If you have a motorized stage, you can collect data by adding Markers, Cell Markers, Maps and Line Scans. For details of collecting spectra using these objects, refer to Using Markers, Using Cell Markers, Using Maps and Using Line Scans.

Any objects added to the Setup Sample Area XYZ tab or Setup Microscope XYZ tab, such as cell markers, markers, maps and lines will be scanned when **Scan** is clicked. These will take priority over any samples added to the Sample Table. Samples in the Sample Table will only be run when there are no unscanned objects.

Batch Scanning

Spectrum includes features that simplify the collection of spectra from groups, or batches, of samples. A batch could include, for example, several similar samples.

Auto-Name

The default Auto-Name function enables you to set up a naming convention that is applied to your spectra automatically.

Depending on your instrument, Auto-Name can enable you to collect spectra from one sample after another by following the prompts in the instrument display and using the Go button. There is no need to return to your PC. This feature is useful when using accessories that enable you to start and stop scanning remotely from the instrument.

Alternatively, follow the prompts in the Prompts display on the Measurement bar.

The Sample Table

You may prefer to setup data collection for a batch of samples in a Sample Table, which enables you to enter meaningful Sample IDs and Descriptions for a specified number of samples.

The following procedure outlines how to use a Sample Table to collect spectra from a batch of samples into a new Samples View:

1. Open the Data Explorer.

   The Data Explorer enables you to organize your spectra into Samples Views.

   By default, the Data Explorer contains one Samples View, but you can create as many as you need.

2. To create a Samples View, select **New** from the File menu.

   A Samples View is appended to Data Explorer.

3. If you wish, right-click and **rename** the Samples View.

   Samples Views are virtual folders that are a useful way to organize your spectra in the Spectrum workspace. They do not reflect the path to saved spectra.

4. In the Data Explorer, click **Sample Table**.

   OR

   Select **Sample Table** from the Measurement menu.

   The Sample Table is displayed in the Viewing Area, with table management controls to the right.

5. Click **Clear Measured** to remove any completed rows that you do not need.

   No spectra are deleted from the application.

   The Sample Table now contains one empty row for the next sample.

6. Enter, or select from the drop-down list, the number of samples needed to complete your batch and then click **Add**.

   A table row is created for every sample in the batch.

   By default, the Auto-Name function creates a **Sample ID** and **Description** for each row.

7. If necessary, click in the appropriate cell and enter a meaningful **Sample ID** and **Description** for each sample in the batch, amending any default entries.

   Each **Sample ID** must be unique.

8. To move a table row to another position in the sample table, click the row selector cell in the first column and then click **Up** or **Down**. Click **Insert** to add a row, or **Remove** to delete a row.

   Select a number of rows by clicking the row selector cells in conjunction with the SHIFT or CTRL keys.

   If the Auto-Name function is enabled, the Sample IDs are updated automatically.

9. When you are happy with the Sample Table, the Instrument Settings to be used and, if necessary, have collected a valid background spectrum, place the first sample in the instrument.

10. Select the Samples View and then click  .

    The spectrum collected from the first sample is displayed in the Viewing Area, and added to the current Samples View.

11. Follow the Prompts Display in Spectrum, or on your instrument display, if applicable, until you have collected a spectrum from every sample in the batch.

    Each spectrum is added to the Samples View.

Additional Information

Auto-Name is especially useful when using an accessory that enables you to start and halt scanning remotely, such as the Triggered NIR Fiber Optic Probe.

Managing Data

Spectrum enables you to:

- Use familiar Windows techniques to find, select, open and save files.
- Automatically save spectra to a default location as they are collected.
- Organize different spectra into Samples Views to help facilitate data collection and processing.
- Select spectra from a Samples View for presentation.

Using Familiar Windows Techniques

File menu commands enable you to open and save files using familiar Windows techniques.

For example, to view a spectrum file stored on your PC:

1. Select **Open** from the File menu.

   OR

   Click  on the Graph bar.

   The Open File window is displayed.

2. Browse to, and select, the appropriate *.sp file.

   To display summary information about a spectrum, place the mouse pointer over its filename.

   To select more than one file, hold down the CTRL key while selecting each file. To select a range of files, hold down the SHIFT key as you select the first and last file.

3. Click **Open**.

   The spectrum is displayed in the Viewing Area on a graph tab.

   The spectra in the current Samples View are listed in a table embedded under the graph referred to as the Spectrum Browser.

Saving Spectra

Unless you have specified another default directory, the **Save** command in the File menu saves your selected spectra to C:\pel_data\spectra\

The Auto-Save option, which is enabled by default, automatically saves each spectrum collected from a sample to this default directory. If you want to disable Auto-Save, refer to Setup Instrument Data Collection.

One way to discover whether a spectrum has been saved is to select the Results Table tab in the Viewing Area, which lists the spectra in the current Samples View. By default, a column in the table indicates whether each spectrum has been saved.

Specify another default directory for saved spectra by selecting **Save As** or **Save All** from the File menu, or when setting up a Sample Table.

Organizing Samples Views using the Data Explorer

Samples Views are virtual folders that are a useful way to organize open spectra in the Spectrum workspace. They do not reflect the actual location of any saved spectra.

A Samples View can contain links to the spectra associated with a batch of samples, or an experiment, and the results generated by any processes applied to them.

To see the Samples Views currently in use, open the Data Explorer on the left side of the Spectrum interface. Each folder represents a Samples View.

The contents of the Viewing Area, arranged on one or more tabs, reflect the currently selected Samples View or link.

To create a new Samples View, select **New** from the File menu. You can drag and drop a copy a link from one Samples View to another.

You can right-click and Delete a Samples View, or any of the links it contains, without deleting any saved spectra from disk. If you Rename a link, a new spectrum it is not automatically saved to disk.

Using the Spectrum Browser

When you are viewing a Samples View selected using the Data Explorer, the graph tab includes a table known as the spectrum browser, which enables you to select the spectra you want to work with.

Each selected spectrum is marked by a  and its curve drawn in full color. Any unselected spectra are drawn dimmed.

- To select more than one spectrum, press the CTRL key as you select the next spectrum.
- To select a block of spectra, press the SHIFT key as you select the first and last spectrum in the block.
- To select all the spectra in the Samples View, press CTRL+A.

Additional Information

To learn more about saving spectra, and setting up paths to directories, see Saving Spectra.

To learn more about opening files, removing spectra from view, and deleting spectra from disk, see Opening, Removing and Deleting Files.

Processing Data

The Process menu in Spectrum includes a number of commands that enable you to process one or more of your spectra.

For example, you can convert curves between Absorbance units (A) and Transmittance units (%T). You can also perform an automatic Baseline Correction or an Interactive Baseline Correction on your selected spectra, and Compare a spectrum with one or more reference spectra. The Arithmetic command enables you to apply one or more operations to, for example, divide one spectrum by another or to multiply the ordinate values in a spectrum by a constant.

For more complex spectral calculations, Spectrum enables you to set up Equations, and to link processes and equations into Macros. Once setup, Equations and Macros are added to sub-menus in the Process menu, so are always available for reuse or modification.

You can include Quant, Verify, Compare and Search processes in a Macro. You can also include Adulterant Screen and MultiSearch in a Macro if you have the appropriate license.

If you use any of these tools frequently, you may want to show it on the Process bar.

NOTE: Before using a process ensure that it is appropriate for your data. For example, some processes may not be suitable for Raman data.

Publishing Results

Spectrum enables you to format and label the curves in Viewing Area and then send the prepared graph to WordPad or, if installed, to a Microsoft Word document for publishing.

You can also:

- Review a Print Preview and Print.
- Copy and Paste from the currently displayed tab in the Viewing Area to another location.

NOTE: Formatting and Labeling are not saved to disk with spectra, and are not preserved when you Exit Spectrum.

- Use the Report command on the File menu to output a report.

Additional Information

You can also Export spectra to another data management application or for processing.

Exit and Save Options

When you want to Exit Spectrum:

1. Select **Exit** from the File menu.

   OR

   Click Close (X) at the top right of the Spectrum window.

   If you have Spectrum ES, you will be prompted to sign the workspace on exit.

   The Save Options dialog is displayed.

2. Select the appropriate option.

   If you have Spectrum Standard, select to:

   a. Save any unsaved data, and open Spectrum with your default settings and layout next time, which enables you to preserve your current workspace for when you next login to Spectrum at this PC.

   b. Save any unsaved data, and reload the current spectra, settings and layout next time, which enables you to carry on with your work from where you left off when you next login to Spectrum at this PC.

   c. Exit without saving any unsaved data, layout or settings information, which restores the default workspace when you next login to Spectrum at this PC.

   If you have Spectrum ES, select to:

   a. Reload spectra next time – Save any unsaved data, and reload the current spectra, settings and layout next time, which enables you to carry on with your work from where you left off when you next login to Spectrum at this PC.

   b. Don't load spectra next time – Clear for reload next time, which will load a new workspace, with a new Workspace ID, next time you login to Spectrum at this PC.

   If you have Spectrum ES and have loaded a workspace created by another user, select to:

   a. Return to workspace – Reload the previous workspace.

   b. Exit the software. The previous workspace is restored next time you login to Spectrum at this PC.

3. If required, select which group workspace you want to load and then click **OK.**

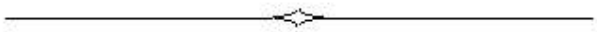
   If the group workspace you are currently using has not been changed, then Use Existing Configuration will also be available.

   Spectrum closes.

   The Choose Group Default Workspace is displayed in Spectrum ES when **Don't load spectra next time** is selected and the default workspace of one or more groups of which you are a member has been updated since you last created a new workspace in Spectrum.

   Any new workspace created subsequently will be based on the group workspace you have selected. The Choose Group Default Workspace dialog will not be displayed again until one of the group workspaces is updated.

   Refer to Assigning a New Default Workspace for more information.



Finding and Saving

Finding and Saving

The Open, Save, and Export commands that you use to open spectra and save spectra to disk are available in the File menu.

Some of these file management commands are also available via keyboard shortcuts and shortcut menus. To display a shortcut menu, right click your mouse on the object of interest.

It is important to distinguish between the commands you use to manage stored files, and the Samples Views that you use to organize spectra in the Spectrum workspace.

The following topics address these subjects in more detail:

Navigation, which describes the Spectrum Browser, the Data Explorer, and the Results Table.

Samples Views, which are the virtual folders displayed in the Data Explorer.

Opening, Removing and Deleting Files, which describes opening files from disk, removing curves from a Samples View, and deleting files from disk.

Saving Spectra, which describes the Save commands, setting up the default path to a Save location, and the Auto-Save option.

Exporting Spectra, which describes how to save a spectra data sets in a format that can be read by a spreadsheet, LIMS, or another spectral application.

Additional Information

The Data Explorer Pane

The Data Explorer pane provides a visual representation of the spectra and curves generated by scanning samples and processing your data. You can create Samples Views in the Data Explorer pane, and copy spectra between Samples Views via shortcut menu commands and drag-and-drop operations.

Samples Views

A Samples View is a virtual folder that you use to manage your spectra. The currently selected Samples View is displayed in the Viewing Area. All the available Samples Views are displayed in the Data Explorer pane and listed in the Navigation menu.

Creating an Empty Samples View

Use the **New** command on the File menu to create an empty Samples View.

1. Open the Data Explorer pane.
2. Select **New** from the File menu, or press CTRL+N.

   A new Samples View is added to the Data Explorer and given the default name Samples View n, where n is an incremented integer.
3. To give the Samples View another name, right-click on the folder name and select **Rename**, and then enter your preferred name in the editing box.

Copying a Spectrum to a New Samples View

1. Open the Data Explorer, right-click the name of the spectrum you want to copy, and select **Copy to New Folder**.

   A new Samples View containing a copy of the spectrum is added to the Data Explorer and given the default name Samples View n, where n is an incremented integer.
2. To give the Samples View another name, right-click on the folder name and select **Rename**, and then enter your preferred name in the editing box.

Removing a Samples View

- Right-click on the Samples View name in the Data Explorer pane and then select **Delete**.

  The Samples View is removed, together with all its contents.

  No files are deleted from disk.

NOTE: If you have Spectrum ES, you may be prompted to enter an electronic signature for the Delete Graph signature point. The contents of the Samples View will be stored in the Recycle Bin.

Restoring Samples Views (Spectrum ES only)

- Right-click on the Recycle Bin in the Data Explorer pane and then select **Restore All**.

  Any Samples Views in the Recycle Bin will be recreated in the Data Explorer, together with any spectra they contained.

Additional Information

For further information about organizing spectra using Samples Views, see Data Explorer.

Opening, Removing and Deleting Files

Opening a File

Use the **Open** command on the File menu to open any file that can be used with Spectrum.

1. Select **Open** from the File menu, or press CTRL+O.

   OR

   In the Data Explorer pane, select a Samples View, right-click and then select **Open Spectrum**.

   The Open File dialog is displayed.

   By default, all the binary spectra (*.sp files) in the C:\ pel_data\spectra folder are displayed. You can also open interferograms (*. ig files), JCAMP files (*.dx), Omnic files (*.spa), GRAM files (*.spc), or spectra saved as data points in a PerkinElmer ASCII text format (*.asc files).

   By default, your spectra are displayed with thumbnail previews. To discover more about the spectrum, hover your mouse pointer over a thumbnail (or icon in the Tiles, Icons, or List views). In the Details view you can choose to display the columns Analyst, Spectrum Description, Ordinate, Abscissa, Scan Start, Scan End and Scan Interval.

> **NOTE:** The properties of a Samples View are separate from the properties of any graph it contains.

2. Click the filename you want to select.

   The file is selected, and all other files deselected.

   To select a block of files, hold down SHIFT and click the first and the last filenames in the block.

   To select or deselect a file, leaving the others selected, hold down CTRL as you click the filenames.

3. Click **Open**.

   Your selected spectra are displayed in the selected Samples View.

> **NOTE:** If you have Spectrum ES, and you are opening non-ES data, then you may be prompted to enter an electronic signature for the Data signature point.
>
> The spectrum will be added to the database.

Removing a Spectrum from a Samples View

1. Open the Data Explorer pane, and then select the Samples View.
2. Right-click the link you want to remove, and then click **Delete.**

   The spectrum is removed from the Samples View.

   If the spectrum has been saved, the file is NOT deleted.

> **NOTE:** If you have Spectrum ES, you may be prompted to enter an electronic signature for the Delete Graph signature point. The spectrum will be stored in the Recycle Bin.

Alternatively:

- Right-click the spectrum you want to remove in the Viewing Area, and then click **Remove Curve.**

  The spectrum is removed from the Samples View.

  If the spectrum has been saved, the file is NOT deleted.

> **NOTE:** If you have Spectrum ES, you may be prompted to enter an electronic signature for the Delete Graph signature point. The spectrum will be stored in the Recycle Bin.

Removing all Selected Spectra from a Samples View

- Open the Data Explorer pane, right-click the Samples View, and then press the **Delete** key.

  All selected curves are removed from the Samples View.

  NO files are deleted from the hard disk.

> **NOTE:** If you have Spectrum ES, you may be prompted to enter an electronic signature for the Delete Graph signature point. The contents of the Samples View will be stored in the Recycle Bin.

Deleting a File from Disk

Use the **Open** command on the File menu to delete a saved file.

1. Select **Open** from the File menu,

   OR

   Press CTRL+O.

   OR

   In the Data Explorer pane, select a Samples View, right-click and then select **Open Spectra**.

   The Open File dialog is displayed.

   By default, all the binary spectra (*.sp files) in the C:\pel_data\spectra folder are displayed. You can also view interferograms (*.ig files), spectra saved as data points in a PerkinElmer ASCII text format (*.asc files), or any type of file (*.* files).

   By default, your each spectrum is displayed with a thumbnail previews. To discover more about the spectrum, hover your mouse pointer over a thumbnail (or filename in the List and Detail views).

2. Right-click the filename you want to delete from disk, and then click **Delete**.

   You can select a number of filenames to delete using the SHIFT and CTRL keys, right-click on any selected filename, and then click **Delete**.

   The selected spectra are deleted from disk. The spectrum will not be removed from the Samples View.

Saving Spectra

The Viewing Area's Results Table tab includes, by default, a column that indicates whether or not a particular spectrum has been saved.

The Save Command

Use the **Save** command to save selected spectra using their current filename and file format.

1. Select the spectra you want to save.

   You can use the Data Explorer to select a single spectrum from a Samples View. Alternatively, you can use the spectrum browser to select one or more spectra from the selected Samples View.

2. Select **Save** from the File menu.

   OR

   Press CTRL+S.

   If you have Spectrum ES, you will be prompted to enter an electronic signature for the Output step.

   The selected file, or files, are saved.

   If a spectrum has not been saved before, the **Save As** dialog is displayed.

The Save All Command

Use the **Save All** command to specify new filenames, or to specify a new default path for all Samples Views.

1. Select **Save All** from the File menu.

   The Save All Spectra dialog is displayed, which tabulates all the spectra in all the Samples Views.

2. In the Save column, select (check) all the spectra you want to save, and deselect (uncheck) all the spectra that should not be saved.

   The icon to the right of the check box indicates whether a spectrum has already been saved.

3. Amend any Filenames that you want to change, remembering that some characters cannot be used in filenames.

   If you amend a filename, the icon to its left indicates that the file has not been saved.

4. To amend the path used to store a particular spectrum, hover your mouse pointer over the Save File Path entry for the spectrum, and the click the  button that appears. Select the directory in the Browse for Folder dialog and then click **OK**.

   The Save File Path is amended for this spectrum.

   OR

   To amend the path used to store these spectra, click the  button on the right of the directory field at the bottom of the dialog, select the directory in the Browse for Folder dialog and click **OK**. the directory field is updated. Then click **Apply to all**.

   The Save File Path is amended for all the spectra.

5. Click **Save**.

If you have Spectrum ES, you will be prompted to enter an electronic signature for the Output step.

The Save As Command

Use the **Save As** command to specify new filenames, or to specify a new default path for the selected Samples View.

1. In the Data Explorer pane, select the Samples View that contains the spectra you want to save.
2. Select **Save As** from the File menu.

   The Save Spectra As dialog is displayed, which tabulates all the spectra in the selected Samples View.
3. In the **Save** column, select (check) all the spectra you want to save, and deselect (uncheck) all the spectra that should not be saved.

   The icon to the right of the check box indicates whether a spectrum has already been saved.
4. Amend any Filenames that you want to change.

   If you amend a filename, the icon to its left indicates that the file has not been saved.
5. To amend the path used to store a particular spectrum, hover your mouse pointer over the Save File Path entry for the spectrum, and the click the  button that appears. Select the directory in the Browse for Folder dialog and then click **OK**.

   The Save File Path is amended for this spectrum.

   OR

   To amend the path used to store these spectra, click the  button on the right of the directory field at the bottom of the dialog, select the directory in the Browse for Folder dialog and click **OK**. the directory field is updated. Then click **Apply to all**.

   The Save File Path is amended for all the spectra.
6. Click **Save**.

   If you have Spectrum ES, you will be prompted to enter an electronic signature for the Output step.

Additional Information

Auto-Save

The Auto-Save option saves each spectrum after data collection automatically. This option is selected by default; see Setup Instrument Data Collection.

Saving Files from the Graph tab

You can save a spectrum in either binary (*.sp) or ASCII (*.asc) format using shortcut menu commands. This method allows you to save the file with any filename and to any location.

1. Hover your mouse pointer over a spectrum and right-click to display a shortcut menu.
2. Select **Save as Binary** or **Save as ASC**.

   The Save As dialog is displayed.
3. Browse to the location where you want the file to be saved.

   Initially the dialog displays the contents of C:\pel_data\spectra. If you use the dialog more than once, the location of your last save is displayed.
4. Type or choose a filename.

   You do not need to include the filename extension because the extension that is displayed in the file selector is added automatically.
5. Click **Save**.

If a Samples View is selected so that the spectrum browser is displayed:

1. Hover your mouse pointer over the curve names in the spectrum browser, and right-click when the name of the spectrum you want to save is underlined.
2. Select **Save as Binary** or **Save as ASC**.

   The Save As dialog is displayed.
3. Continue from step 3 above.

Exporting Reports

Reports in Spectrum are generated from templates prepared using PerkinElmer's Report Designer software. You can either prepare these templates in advance or create one when required and use it to generate a report immediately.

1. To generate a multi-spectrum report, select the Samples View name in the Data Explorer.

   OR

   To generate multiple single-spectrum reports, select the Samples View name in the Data Explorer.

   OR

   To generate the report of a single spectrum, select the spectrum name in the Data Explorer.

2. Check the appearance of the data that you will include in the report.

   Depending on the settings in the template you have selected, the appearance of the data in Spectrum may be duplicated in the report.

3. Select **Report** from the File menu.

   The Report dialog opens.

4. Select the Reports Options tab.

5. Select the **Save report** check box if you want to save the report(s).

6. Select **Show saved report** if you want the report(s) to be displayed when generated.

7. Select the **Print report** check box to print the report(s) to the currently active printer.

8. If necessary, click **Browse**, find the template file that you want to use to generate the report, and click **Open**.

   Templates created in Report Designer have a *.tplx filename.

   OR

   Click **Create** and Report Designer will open so that you can create a new template.

   You can also select a template and then click **Edit** if you want to make any changes in Report Designer before you generate a report. Remember to save the template in Report Designer before you generate the report. See the on-screen Help in Report Designer for further details.

   In Spectrum ES, you can also select a template from a list of those used previously in the workspace.

9. Select the type of report(s) you want to generate from the options available.

   The report options available will depend on the items included in the selected template and on the data selected in Spectrum. For example, if the template only contains items related to data for multiple spectra (that is, all the spectra in the Samples View), then the single spectrum report option is disabled. If you have selected a single spectrum name in the Data Explorer in step 1, then the multiple spectra report option is disabled.

   Select the Include option next to the **Samples View Name** if you want to generate a report for all the spectra in the Samples View.

If you selected the Samples View in step 1, select the Include option next to the **Spectrum Name** if you want to generate an individual report for a spectrum. All the spectra are selected by default. To select or deselect all the spectra, check or uncheck the **Select all single spectra reports** option.

10. Select the Report Edit tab.
11. Select the **Report format** from the drop-down list.

    In Spectrum Standard the options are rich text format (*.rtf) and portable document format (*.pdf).

    In Spectrum ES the report is saved in a secured and encrypted portable document format.
12. If necessary, browse to another (or create a new) folder for the generated report(s).

    By default, all reports are saved to C:\pel_data\reports.
13. Select the sections to be included in the report from the **Section Name** list, which are derived from the template.

    To select all or deselect all the possible sections, check or uncheck the **Select all** check box.
14. Click **Report**.

    If you have Spectrum ES, you may be prompted to enter an electronic signature for the Output step.

    The report is generated.

    The filename generated for saved multiple spectra reports is derived from the Samples View name. The file name for an individual spectrum report is derived from the Samples View name and the Sample ID.

    Each time a report file is generated, a number is appended to the name.

    No output will be produced if the file cannot be created.

Additional Information for Spectrum ES

You can only generate reports in Spectrum ES if you have the appropriate permission. Similarly, you can only open Report Designer to create or edit a template if you have the appropriate permission.

You can only select a template if it has the correct status. The acceptable status levels are shown in the drop-down list in the Report Options tab. If you are a user with the appropriate permission, you can change these settings, but otherwise you will only be able to select templates which meet these criteria. The status for each template is shown in the dialog when you click **Browse** to find a template.

Opening an ES Report

Use the **Open ES Report** command on the File menu to open a secure (checksummed) report file in Spectrum ES.

1. Select **Open ES Report** from the File menu, or press CTRL+T.

   By default, all the secured PDF report files (*.spdf files) in the C:\ pel_data\reports folder are displayed. You can also open secured RTF report files (*.srtf files).

2. Click the filename you want to select.

   The file is selected, and all other files deselected.

3. Click **Open**.

   A *pdf or *.rtf file is created in the reports folder, opened and displayed in the default application for PDF or RTF files. The *.srtf and *.spdf files remain unchanged.

Exporting Spectra

Use the Export command save your spectra to a specified folder as data files that are accessible to other applications.

1. Select **Export** from the File menu.

   The Export Data dialog opens. By default, all the spectra available in the Data Explorer pane are displayed.

2. Deselect any spectra that you do not want to export.

3. If necessary, click  to browse to another (or to create a new) folder for the exported files, and then click **Apply to All** to specify that this folder should be used (rather than the current default directory).

4. If your selected folder already contains files with the same names that you wish to overwrite, tick the Overwrite files check box.

5. Select the Format for your exported files.

   Custom Defined File uses the settings defined on the Setup Export tab.

   Comma Separated Value (*.csv) is a common file format that can be read into, for example, a Microsoft Excel spreadsheet or a Laboratory Information Management System (LIMS).

   JCAMP-DX (*.DX) is a standard file format for spectral data specified by the International Union of Pure and Applied Chemistry (IUPAC).

6. Click **Export**.

   If you have Spectrum ES, you will be prompted to enter an electronic signature for the Output step.

   Your selected spectra are exported to the specified folder.

Additional information

You can also save spectra in the binary *.sp (*.ig for interferograms) or the plain text ASCII (*.asc) file formats.

Navigation

The Viewing Area, in the center, shows all the curves in the current Samples View on the Graph tab.

The Spectrum Browser

The Graph tab includes a table, or spectrum browser, that enables you to select which curves you want to work with. The names of the selected spectra are marked by a ➤, and are drawn in full color; any unselected curves are not marked and are drawn dimmed.

- To select a curve in the spectrum browser, click its name.

  OR

  Hover your mouse over the curve, right-click and then select **Select Only This Curve**.

  The curve is selected, and all other files deselected.
- To select a block of curves, hold down SHIFT and click the first and the last name in the block.
- To select or deselect a curve, leaving the others selected, hold down CTRL as you click the name of the curve.
- To select all the curves in the Samples View, press CTRL+A.

The Data Explorer

The Data Explorer pane, on the left, provides a visual representation of all the Samples Views containing all that the spectra that are currently open.

Viewing Spectra

Viewing Spectra

These topics describe how to format your results so that they are presented as clearly as possible:

Optimizing the Viewing Area

Optimizing Graphs

Autorange X, Y, XY

Previous Range

Formatting a Graph

Graph Labels

Labeling Graphs using the Vertical Cursor

Label Peaks

Horizontal Cursor

Autoscale Y

Optimize

Panning, Zooming and Offsetting Spectra

NOTE: Your formatting is not stored when you save your curve as a *.sp file, or preserved if you select **Save for reload next time** when you Exit Spectrum.

Additional Information

You can print or publish your formatted results. See Publishing Results.

Optimizing the Viewing Area

When you are working in the Viewing Area, right click in a clear area to display a shortcut menu containing a selection of useful commands:

- Previous Range
- Full Scale
- Vertical Cursor
- Horizontal Cursor
- Split Display
- Set Anchor Point
- Add Text
- Add Bitmap Image
- Print
- Copy to Clipboard
- Properties

Additional Information

If you right click on a particular curve, a shortcut menu containing a different selection of useful commands is displayed.

Optimizing Graphs

When you are working in the Viewing Area, right click on a curve to display a shortcut menu containing a selection of useful commands:

- Set Anchor Point
- Select Only This Curve
- Label This Point
- Label Peaks
- Process >
  - Absorbance
  - %Transmittance
  - Data Tune-up
  - Baseline Correction
  - Interactive Baseline Correction
  - Difference
  - Normalization
  - Interpolation
  - ConvertX
  - Smooth
  - Derivative
  - ATR Correction
  - Arithmetic
  - Kubelka–Munk

	Kramers–Kronig
	Deconvolution
	Biodiesel
	Peak Table
	Peak Area / Height
	Quant
	Compare
	Search
Equations	> Equation n
Macros	> Macro n
Save As Binary	
Save As ASC	
Remove Curve	
Status	
Appearance	

NOTE: If you are using the Viewing Area to display a particular curve, rather than a Samples View, the shortcut menu does not include Process commands.

Additional Information

If you right click away from a curve, rather than on a curve, a shortcut menu containing a different selection of useful commands is displayed.

Autorange

Use the **Autorange X**, **Autorange Y**, and **Full Range** commands to rescale the axes so that your selected spectra fill the graph, making their features easier to see.

Autorange X

1. Select the spectra that you want to be fitted on to the graph.
2. Select **Autorange X** from the View menu, or click **Auto X** on the Graph toolbar (hidden by default).

   The Y range stays the same, but the X range is set to the Start and End data points of the selected spectra.

Autorange Y

1. Select the spectra that you want to be fitted on to the graph.
2. Select **Autorange Y** from the View menu, or click **Auto Y** on the Graph toolbar (hidden by default).

   The X range stays the same, but the Y range is set to the minimum and maximum of the selected spectra.

Full Range

1. Select the spectra that you want to be fitted on to the graph.
2. Select **Full Range** from the View menu, or click **Auto XY** on the Graph toolbar (hidden by default).

   The X range is set to the Start and End data points, and the Y range is set to the minimum and maximum, of the selected spectra.

Additional Information

Use the Previous Range command to undo the Autorange X command or Autorange Y command. Use the Previous Range command twice to undo the Autorange XY command; once to undo the Y component and once again to undo the X component.

Use the Autoscale Y command to rescale every feature in your spectrum.

Use the Optimize command to rescale every feature in your spectrum, excluding any noise spikes or unwanted peaks from atmospheric CO_2 or water vapor.

Use Cancel Offset command to fit any offset spectra onto the graph.

Previous Range

Use the **Previous Range** command to undo a command that changes the X or Y range displayed by the graph. The range may have been changed by zooming using a grow box, or by using the Autorange X, Autorange Y or Full Range (Auto XY) commands.

- Select **Previous Range** from the View menu.

  OR

  Right-click in a clear area of your graph and then select **Previous Range**.

  The graph is redisplayed.

If you have applied a series of commands that affect the ranges displayed, you can use the Previous Range command to undo them one by one.

NOTE: To undo the Full Range (Auto XY) command, use the Previous Range command twice; once to undo the X component and once again to undo the Y component.

Formatting a Graph

Use the Graph Properties dialog to customize the graph display, or to change how the curves are displayed.

NOTE: The properties of a graph display are separate from the properties of any curve it contains.

- Select **Format graph** from the View menu, or click **Format** in the Graph toolbar.

  The Graph Properties dialog opens at the Axes tab.

The Graph Properties dialog has four tabs:

- Use the General tab to apply a title and description to your graph.
- Use the Axes tab to change the range and units applied to the X and Y axes.
- Use the Appearance tab to enable gridlines; and to apply color to text, to line elements, and to the curves.
- Use the Advanced tab to change whether, and how, data points are displayed; whether units or numbers are suppressed on the graph axes; the information associated with the curve tooltip; and the interpolation, size (width), and style applied to the curves.

Additional Information

When you are customizing a graph display, perhaps prior to copying it to the clipboard or sending it to a WordPad or Word document, you may prefer to use shortcut menus. For example:

- To amend the X or Y axes, place the mouse pointer in a clear area of the graph, right-click and then select **Properties**.

  The Graph Properties dialog opens at the Axes tab.

- To change the color of a selected curve, right-click on the curve and then select **Appearance**.

  The Graph Properties dialog opens at the Appearance tab.

The Graph properties dialog enables you to customize the display of the graph currently displayed. To set up the default settings for all new graphs, see the Setup View topics.

Graph Title and Description

Use the General tab in the Graph Properties dialog to apply or edit the title or the description of a curve or graph display.

NOTE:	The properties of a graph display are separate to the properties from any curve it contains.

1. Select **Format graph** from the View menu, or click **Format** in the Graph toolbar.

   OR

   Right-click in the graph display and select **Properties** (of the graph display) or **Appearance** (of a curve).

2. Select the General tab.
3. Enter your **Title** and/or **Description**.

   The Title is displayed at the top center of the graph, using the font size and color specified on the Appearance tab.

4. To confirm changes without closing the dialog, click **Apply**.

   OR

   To close the dialog keeping only applied changes, click **Cancel**.

   OR

   To confirm all changes and close the dialog, click **OK**.

Range and Units for the X and Y Axes

Use the Axes tab in the Graph Properties dialog to change the range and units applied to the X and Y axes of a graph or Samples View.

NOTE: The properties of a graph display are separate from the properties of any curve it contains.

1. Select **Format graph** from the View menu, or click **Format** in the Graph toolbar (hidden by default).

   OR

   Right-click in the graph display and select **Properties** (of the graph) or **Appearance** (of a curve).

2. If it was not selected by default, select the Axes tab.

   The options available are:

Properties of	Select whether your changes on this tab apply to All Curves or only to a selected curve.
Display Mode	Select whether the graph display mode should be Overlay (where the curves are displayed on a common set of axes) or Split (where the curves are displayed on a common X, but separate Y, axes). If a curve is selected in the Data Explorer pane, this field is not applicable as only one curve is shown.
Y Axis	By default the Y axis is autoranged to the largest value and the smallest value in all the curves present. This panel allows you to enter a range of your choice. If you select another unit make sure that you select appropriate range values.
X Axis	By default the X axis is autoranged to the largest value and the smallest value in all the curves present. This panel allows you to enter a range of your choice, enhance the fingerprint region using the scale-change at 2000 cm^{-1} convention, if appropriate, and to label the X axis units.

3. To confirm changes without closing the dialog, click **Apply**.

   OR

   To close the dialog keeping only applied changes, click **Cancel**.

   OR

   To confirm all changes and close the dialog, click **OK**.

Additional Information for Mid IR

2000cm-1 scale change is a particular feature of the abscissa scale that enables you to see peaks in the region 2000 to 450 cm^{-1} more clearly. It expands the abscissa scale below 2000 cm^{-1} such that each scale interval on the X axis represents half the value it did above 2000 cm^{-1}

The Graph properties dialog enables you to customize the display of the graph currently displayed. To set up the default settings for all new graphs, see the Setup View topics.

Colors for Curves, Graph Elements and Gridlines

Use the Appearance tab in the Graph Properties dialog to customize the color of a curve and of other elements in the graph display.

NOTE: The properties of a graph display are separate from the properties of any curve it contains.

1. Select **Format graph** from the View menu, or click **Format** in the Graph toolbar (hidden by default).

   OR

   Right-click in the graph display and select **Properties** (of the graph) or Appearance (of a curve).

2. If it was not selected by default, select the **Appearance** tab.

   The options available are:

Enable Gridlines	Select this check box if you want to see gridlines under your curves. You can change the color of the major and minor gridlines in the Text and Lines panel. The major and minor gridline intervals depend on the graph display.
Text and Lines	Select the element, such as the title or background, of the graph display whose color you want to change, and then click **Color** to open the Color dialog. Select a **Basic** color, or one of the **Custom** colors you may have defined, and then click **OK**. When you select a text element, the Size selector enables you to select a font size from the drop-down list; select **Auto** to revert to the default font size.
Curves	Select whether your changes on this tab apply to **All Curves** or only to a selected curve. Click **Color** to open the Color dialog. Select a **Basic** color, or one of the **Custom** colors you may have defined, and then click **OK**.

3. To confirm changes without closing the dialog, click **Apply**.

   OR

   To close the dialog keeping only applied changes, click **Cancel**.

   OR

   To confirm all changes and close the dialog, click **OK**.

The Graph properties dialog enables you to customize the display of the graph currently displayed. To set up the default settings for all new graphs, see the Setup View topics.

Advanced Curve Format Settings

Use the Advanced tab in the Graph Properties dialog to change whether, and how, data points are displayed; whether units or numbers are suppressed on the graph axes; the information associated with a curve tool tip; and the interpolation, size (line thickness), and style applied to curves.

NOTE: The properties of a graph display are separate from the properties of any curve it contains.

1. Select **Format graph** from the View menu, or click **Format** in the Graph toolbar (hidden by default).

   OR

   Right-click in the graph display and select **Properties** (of the graph) or **Appearance** (of a curve).

2. Select the Advanced tab.

   The options available are:

Properties of	Select whether your changes on this tab apply to All Curves or only to a selected curve.
Hide	Select one or more of **Hide X Axis Units**, **Hide Y Axis Units**, **Hide X Axis Numbering**, and **Hide Y Axis Numbering** to suppress the labels applied to the X and Y scales. Select **Hide Information Pane** to suppress the curve selector that would otherwise, for example, be copied to the clipboard with the graph display.
Tool Tip Display	Deselect one or more of these check boxes to suppress elements in the tooltip that appears when the mouse pointer is near a curve or data point.
Points	Select whether to display data points in the curve, and if so, how they should be marked.
Line	Select the **Interpolation** algorithm (Cubic, Linear, or none) applied to the curve joining the data points. Select a new **Size**, in pixels, from the drop-down list to amend the curve thickness, perhaps prior to copying the graph display to the clipboard or to emphasize a particular curve. The **Style** options enable you to display the curve using a solid, dashed, or dotted line.

3. To confirm changes without closing the dialog, click **Apply**.

   OR

   To close the dialog keeping only applied changes, click **Cancel**.

   OR

   To confirm all changes and close the dialog, click **OK**.

Additional Information

The Graph properties dialog enables you to customize the display of the graph currently displayed. To set up the default settings for all new graphs, see the Setup View topics.

Graph Labels

Use the Label Properties dialog to add, edit or customize labels on the graph.

NOTE: The properties of a graph display are separate from the properties of any curve it contains.

The tabs displayed in the dialog depend on which type of label you are working with:

- Text label, which enables you to place text at any position on the graph.
- Point label, which enables you to use your mouse pointer, or the vertical cursor, to label particular points on your curve(s), such as when you want to compare the position and/or intensities of features.
- Bitmap label, which enables you to place an image, such as your company logo, on the graph display.

Additional Information

The graph title label and axis labels are properties of the graph format.

Text Labels

Use the Label Properties dialog to add a text label to the graph display.

NOTE: Labels are not stored when you save your curve as an *.sp file, or preserved if you select **Save for reload next time** when you Exit Spectrum.

1. Select **Add Text** from the View menu, or click **Text** in the Graph toolbar.

   OR

   Right-click in the graph display and select **Add Text.**

   The Label Properties dialog opens and displays the General tab.

   The options available are:

Text	Type the text for the label. Use the ENTER key to enter a new line. The size of the label is auto-fitted to your text.
Orientation	Select whether the label text should be horizontal or vertical. A vertical label reads from bottom to top, which matches the Units label on the Y axis.
Font Size	Select the size of the label text.
Insert	Enables you to insert one or more variables into the Text field, including the current <Date> and <Time>
Draw Border	Select this check box if you want a box drawn around the label.
Color	If you want to change the color of the label text and any border, click **Color** to open the Color dialog. Select a **Basic** color, or one of the **Custom** colors you may have defined, and then click **OK.** The label background is transparent, so the color of the graph background shows through.

2. To confirm changes without closing the dialog, click **Apply.**

   OR

   To close the dialog keeping only applied changes, click **Cancel.**

   OR

   To confirm all changes and close the dialog, click **OK.**

Additional Information

Moving a Text Label

- Select the graph label, and then drag it to its correct position on the graph.

Editing a Text Label

- Select the graph label, right-click and then select **Properties.**

  The Label Properties dialog is displayed, as described above.

Deleting a Text Label

- Select the graph label, right-click and then select **Remove.**

Adding a Bitmap Image

You cannot paste a graphic element into a text label. You can, however, place an image, such as your company logo, into the graph using the Add Bitmap Image command.

Adding other Labels

You can also add Point labels and Peak labels to your graph.

Point Labels

Use point labels to compare the position and/or intensities of features. A point label includes a tie-line to, and the X value of, a particular position on the curve.

NOTE: Labels are not stored when you save your curve as an *.sp file, or preserved if you select **Save for reload next time** when you Exit Spectrum.

1. Select the position in the curve that you want to label, right-click and then select **Label this Point**.

   The Label Properties Dialog opens and displays the General tab.

   The options available are:

Text	By default, this contains <X Value>. Edit the text as needed. Use the ENTER key to enter a new line. The size of the label is auto-fitted to your text.
Orientation	Select whether the label text should be horizontal or vertical. A vertical label reads from top to bottom, which matches the Units label on the Y axis.
Font Size	Select the size of the label text.
Insert	Enables you to insert one or more variables into the Text field. The <Curve Name> and <Description> are taken from the Results table; you can also insert X and Y values and their units.
Draw Border	Select this check box if you want a box drawn around the label.
Color	If you want to change the color of the label text and any border, click **Color** to open the Color dialog. Select a **Basic** color, or one of the **Custom** colors you may have defined, and then click **OK**. The label background is transparent, so the color of the graph display background shows through.

2. Select the Advanced tab.

   The options available are:

Show Tie Line	This default option draws a line between a label and the peak.
Label Position	Relative to tie point (default): Label pans as the graph is panned. Relative to screen: Label stays in a fixed position on the screen as the graph is panned. If the tie line is shown, it is redrawn automatically.

3. To confirm changes without closing the dialog, click **Apply**.

   OR

   To close the dialog keeping only applied changes, click **Cancel**.

   OR

   To confirm all changes and close the dialog, click **OK**.

Point Labels Using the Vertical Cursor

1. Select **Vertical Cursor** from the View menu, or click  in the Graph toolbar.

   OR

   Right-click in a clear area of the graph display and select **Vertical Cursor**.

   The Vertical Cursor is displayed on the graph, with its position on the X axis value displayed at its base.

2. Drag the cursor line to a point of interest.

   Position the mouse pointer over the Vertical Cursor until the mouse cursor changes to a double-headed arrow ⇿. Hold down the left mouse button and then move the mouse left or right to drag the cursor to the new position. Release the mouse button.

3. Double-click the left mouse button.

   A label is applied to each curve crossed by the vertical cursor.

Additional Information

Moving a Point Label

- Select the label, and then drag it to its correct position on the graph.

Editing a Point Label

- Select the label, right-click and then select **Properties**.

  The Label Properties dialog is displayed, as described above.

Deleting a Point Label

- Select the graph label, right-click and then select **Remove**.

Removing the Vertical Cursor

- Click  in the Graph toolbar.

  OR

  Right-click in the graph display and deselect **Vertical Cursor**.

Adding other Labels

You can also add Text labels, Bitmap labels, and Peak labels to your graph.

Bitmap Labels

Use the Add Bitmap Image command to add a graphic, such as your company logo, to the graph display.

NOTE: Labels are not stored when you save your curve as an *.sp file, or preserved if you select **Save for reload next time** when you Exit Spectrum.

1. Right-click in a clear area of the graph display and select **Add Bitmap Image.**
   The Label Properties Dialog opens and displays the Bitmap tab.
   The options available are:

Filename	Click Browse and select the *.bmp file that you want to apply to the graph. You cannot crop or resize this image within Spectrum.
Transparent Background	Select this check box if you want the graph background color to replace any white areas in your image.

2. To confirm changes without closing the dialog, click **Apply.**
   OR
   To close the dialog keeping only applied changes, click **Cancel.**
   OR
   To confirm all changes and close the dialog, click **OK.**

Additional Information

Moving a Bitmap Image

- Select the image, and then drag it to its correct position on the graph.

Editing a Bitmap Image

- Select the image, right-click and then select **Properties.**
  The Label Properties dialog is displayed, as described above.

Deleting a Bitmap Image

Select the image, right-click and then select **Remove.**

Adding other Labels

You can also add Text labels, Point labels, and Peak labels to your graph.

Labeling Graphs using the Vertical Cursor

Use the Vertical Cursor command to place a vertical line on the graph display that you can drag horizontally along the X axis. You can label the position of the cursor in your spectra at any point, which enables you to compare the position and/or intensities of features.

NOTE: Labels are not stored when you save your curve as a *.sp file, or preserved if you select **Save for reload next time** when you Exit Spectrum.

1. Select **Vertical Cursor** from the View menu, or click  in the Graph toolbar.

   OR

   Right-click in the graph display and select **Vertical Cursor**.

   The Vertical Cursor is displayed on the graph, with its position on the X axis value displayed at its base.

2. Drag the cursor line to a point of interest.

   Position the mouse pointer over the Vertical Cursor until the mouse cursor changes to a double-headed arrow ⇿. Hold down the left mouse button and then move the mouse left or right to drag the cursor to the new position. Release the mouse button.

3. Double-click the left mouse button.

   A Point label is applied to each curve crossed by the vertical cursor.

Additional Information

Removing the Vertical Cursor

- Select **Vertical Cursor** from the View menu.

  OR

  Click  in the Graph toolbar.

  OR

  Right-click in the graph display and deselect **Vertical Cursor**.

Moving a Point Label

- Select the label, and then drag it to its correct position on the graph.

Editing a Point Label

- Select the label, right-click and then select **Properties**.

  The Label Properties dialog is displayed, as described for Point labels.

Deleting a Point Label

- Select the graph label, right-click and then select **Remove**.

The Vertical Cursor in Process commands

For some process commands, including Interpolation, the vertical cursor is displayed by default, as an aid to selecting the **Start** and **End** values for your **Selected range**.

Adding other Labels

You can also add Text labels, Bitmap labels, and Peak labels to your graph.

Labeling Peaks

Use the Label Peaks command to label the peaks in your selected spectra Peaks according to the criteria set up in Setup Peak Detection.

NOTE: Labels are not stored when you save your curve as a *.sp file, or preserved if you select **Save for reload next time** when you Exit Spectrum.

1. Select the spectrum whose peaks you want to label.
2. Select **Label Peaks** from the View menu.

   OR

   Click  on the Graph Bar.

   OR

   Place your mouse pointer on the spectrum whose peaks you want to label, right-click, and then select **Label Peaks**.

Additional Information

Clearing Peak Labels

To remove all the peak labels from the selected spectrum:

- Select **Label Peaks** from the View menu.

  OR

  Click  on the Graph Bar.

  OR

  Place your mouse pointer on the spectrum whose peaks you want to remove, right-click, and then select **Label Peaks**.

Moving a Peak Label

- Select the peak label, and then drag it to its correct position on the graph.

Deleting a Peak Label

- Select the peak label, right-click and then select **Remove**.

Adding other Labels

You can also add Text labels, Point labels, and Bitmap labels to your graph.

Horizontal Cursor

Use the Horizontal Cursor command to place a horizontal line on the graph display that you can drag vertically along the Y axis.

1. Select **Horizontal Cursor** from the View menu, or click  in the Graph toolbar.

   OR

   Right-click in the graph display and select **Horizontal Cursor**.

   The Horizontal Cursor is displayed on the graph, with its position on the Y axis value displayed at its end.

2. Drag the cursor line to a point of interest.

   Position the mouse pointer over the Horizontal Cursor until the mouse cursor changes to a double-headed arrow ⇳. Hold down the left mouse button and then move the mouse up or down to drag the cursor to the new position. Release the mouse button. The Y axis value is updated.

Additional Information

Removing the Horizontal Cursor

- Select **Horizontal Cursor** from the View menu.

  OR

  Click  in the Graph toolbar.

  OR

  Right-click in the graph display and deselect **Horizontal Cursor**.

Autoscale Y

Use the Autoscale Y command to display your selected spectra so that each spectrum fills the graph vertically, which enables you to compare spectra of different intensities.

1. Select the spectra that you want to be fitted on to the graph display.
2. Select **Autoscale Y** from the View menu, or click **Autoscale Y** on the Graph toolbar.

   The selected spectra are scaled, vertically, so that the spectra completely fill the graph. The ordinate scale is removed because the spectra are on different scales.

Additional Information

Removing Autoscale Y

- Select **Autoscale Y** from the View menu, or click **Autoscale Y** on the Graph toolbar.

  The autoscaling is removed from the selected spectra.

Offset

Removing Autoscale Y also removes any vertical offset applied to the selected spectra.

Optimize

Use the **Optimize** command to rescale your graph, while ignoring any large noise spikes or peaks from atmospheric CO_2 or water vapor.

These unwanted features can dominate the spectrum, making peaks in regions of interest difficult to see.

1. Select the spectra that you want to be fitted on to the graph.

   The names of the selected spectra are underlined.

2. Select **Optimize** from the View menu.

   The spectrum is rescaled.

> **NOTE:** The Optimize command changes the way your spectra are displayed in the Viewing Area. Your data is not changed.

Additional Information

Use the Autorange X command to rescale every feature in your spectrum, including any spikes or peaks from atmospheric CO_2 or water vapor.

Overlay/Split

Use the Overlay/Split command to switch between the overlay display mode and the split display mode when displaying two or more curves.

Split

Split Display mode displays each curve in its own coordinate system. It formats the graph such that all the spectra are autoscaled and automatically offset, one above the other. Any spectra that are added to the graph later are also autoscaled and offset.

Overlay

Overlay display mode formats the graph such that the spectra are displayed on top of each other, in the same coordinate system.

In Overlay mode, you can vertically offset one spectrum from another, which may enable you to see its features more easily.

Panning, Zooming and Offsetting Spectra

Use the techniques and tools described in these topics to:

- Zoom in on a region of the graph;
- Offset a spectrum so that its features can be seen more clearly;
- Pan a spectrum up and down or left and right;

NOTE: These techniques only change the way the spectra are displayed, they do not modify the data in any way.

Zooming to a Region of Interest

Use the mouse to draw a grow box in the graph. You can be move and resize this grow box. Once the box surrounds the region of interest, you can zoom in by double-clicking inside the grow box. The region of interest is displayed on the whole graph display:

1. Position the mouse pointer at the top-left corner of the region of interest.
2. Hold down the left mouse button and drag the mouse diagonally until the grow box covers the region of interest.
3. Release the left mouse button.

   A grow box has been drawn around the region of interest.
4. Double-click inside the grow box.

   The graph is zoomed to display only the region of interest.

Additional Information

Changing the Size of a Grow Box

1. Position the mouse pointer on the border of the grow box.

   The cursor changes to a two-headed arrow ⇿.

   You can resize the box diagonally by positioning the pointer at a corner, or in one direction only by positioning the pointer at an edge.
2. Hold down the left mouse button and drag the mouse until the grow box is the size you require.
3. Release the mouse button.

Moving a Grow Box

1. Position the mouse pointer inside the grow box.

   The cursor changes to a four- headed arrow  .
2. Hold down the left mouse button and drag the grow box to the required position.
3. Release the mouse button.

Removing a Grow Box

- Position the mouse pointer outside the grow box and click.

Returning to the Previous Ranges

- Select **Previous Range** from the View menu, or click  on the Graph Bar.

Offsetting Spectra

In Overlay mode, you can vertically offset one spectrum from another, which may enable you to see its features more easily. If you select one or more spectra, they will be offset relative to the other spectra. If you select all the spectra, they are panned vertically rather than offset.

- Use the ↑ or ↓ keys to move the spectrum.

  OR

  Move your mouse pointer close to the Y axis and drag the vertical pan pointer to move the spectrum.

  The Y range start and end values for the graph change, but the X range values do not. The numbers on the Y scale disappear when you introduce an offset.

Additional Information

Autorange Y

When you introduce an offset, you may find that one or more spectra have moved off the top or bottom of the graph.

- Select the spectra that you want to fit on to the graph.

  The spectra are underlined, indicating that they are selected.

- Select Autorange Y from the View menu or from the Graph Bar.

  The spectra are fitted onto the graph, and the offset is maintained.

Canceling Offsets and Restoring the Y Scale

- Select the spectra whose offset you want to cancel.
- Select **Cancel Offset** from the View menu.

  Any offsets are removed from the selected spectra.

> **NOTE:** If spectra are removed so that the graph contains only one spectrum, any offset is automatically removed and the Y scale is restored.

Panning

Moving Spectra to the Left or Right

- Move your mouse pointer close to the X axis and drag the horizontal pan pointer left or right to move your spectra.
- The X range start and end values for the graph change, but the Y range does not.

Moving Spectra Up or Down

1. Select the spectra you want to move.
2. Use the ↑ or ↓ keys to move the spectra.

   OR

   Move your mouse pointer close to the Y axis and drag the vertical pan pointer to move the spectra.

   The Y range start and end values for the graph change, but the X range does not.

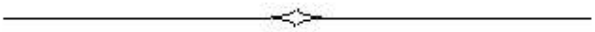
   NOTE: In Overlay mode, if you have one or more spectra selected from a larger number of spectra in the graph, the selected spectra are offset.

Using an Anchor Point

1. Select the spectra you want to move.
2. Right-click in the graph and select **Set Anchor Point**.

   An anchor point is placed at the position of the mouse pointer.
3. Drag the anchor point horizontally or vertically to move the selected spectra.

   NOTE: In Overlay mode, if you have one or more spectra selected from a larger number of spectra in the graph, the selected spectra are offset as you drag up or down.



Collecting Data with your FT-IR

Collecting Data

These topics describe how to use Spectrum to collect data using your instrument.

Collecting background spectra.

Collecting data from a single sample.

Collecting data from a batch of samples.

Collecting data and running a process.

Monitoring data collection while optimizing your sample setup.

Checking that the instrument is fit-for-purpose using Ready Checks.

Backgrounds

When collecting data to generate sample spectra, a first step is to collect a background spectrum from the instrument with no sample present.

The sample spectrum is ratioed against the background spectrum to eliminate features introduced by the instrument response, the sampling accessory or sample cell, and features introduced by atmospheric absorption.

If no valid background spectrum is available, a background spectrum must be collected before you begin to scan samples. When a background spectrum is required, the **Scan** icon in the Measurement toolbar changes from  to  , and the Prompts Display (which is included in the Measurement toolbar by default), prompts 'Ensure beampath is clear, press [Scan] to continue'.

- When the beam path is clear, select **Scan** from the Measurement menu, or click  .

  A background spectrum is collected, but is not displayed or saved.

Manually Renewing the Background Spectrum

You are not prompted for a new background spectrum unless none has been collected; you have changed the sampling accessory; you have applied an instrument setting that invalidates the background scan (such as a higher resolution or scan speed); or is required by the instrument for some other reason.

You can collect a background spectrum at any time that the beam path is clear.

- Make sure that the beam path is clear and then select **Background** from the Measurement menu, or click  .

  The background spectrum is renewed.

Explicitly Collecting a Background Spectrum

You can explicitly collect a background spectrum so that, for example, it can be used when processing another spectrum.

1. Make sure the beam path is clear.
2. Select **Instrument** from the Setup menu.

   OR

   Select  in the **Setup** section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

NOTE:	To see the tabs, you may have to resize the Dialog Pane.

3. Select the Setup Instrument Basic tab.
4. In the Settings Pane, set the **Scan Type** to **Background**.
5. When the beam path is clear, select **Scan** from the Measurement menu, or click  .

This spectrum can be used, manipulated and stored in the same ways as any other spectrum.

Once the background scan has been completed, the Scan Type is reset to Sample.

Additional Information

For information on collecting backgrounds with a relevant Spotlight instrument, see the appropriate user guide.

Scanning a Sample

Provided a valid background spectrum is available, to scan a single sample:

1. Place your sample in the instrument or accessory.
2. Check and set the instrument parameters, such as the **Start** and **End** points of the scan range, the **Number of Scans** required, and a unique **Sample ID** and **Description**.

   By default, sensible values for the scan and instrument parameters are entered in the Instrument Settings toolbar or Measurement toolbar, and the Setup Instrument Basic tab. The **Sample ID** and **Description** are supplied by the Auto-Name function.

   To amend any value, select the parameter and enter your new value.

NOTE: Spectrum automatically remembers the settings you last used.

3. When you are happy with your setup, click  .

   OR

   Select **Scan** from the Measurement menu.

   OR

   If available on your instrument, press the Go button.

   The sample is scanned, and displayed in the Viewing area.

   The completed spectrum is added to the current Samples View in the Data Explorer.

4. If for any reason you want to stop scanning, click  .

   OR

   Select **Halt** from the Measurement menu.

   If you halt the scan, no data will be saved.

Additional Information

Collecting a background

If a background scan is required the Scan button includes a small background flag  .

- Clear the instrument beam path, and then click **Scan** to collect a background spectrum.

  The background spectrum is displayed briefly, and then the Viewing area is prepared for data collection from your sample.

Detailed Instrument Settings

If you want to amend a more detailed instrument setting, use the Setup Instrument dialog.

Batch Scanning

By default, the instrument settings automatically suggest a name for your samples.

Depending on your instrument, Auto-Name can enable you to collect spectra from one sample after another by following the prompts in the instrument display and using the Go button. There is no need to return to your PC. This feature is useful when using accessories that enable you to start and stop scanning remotely from the instrument.

The Sample Table

You may prefer to setup data collection for a batch of samples in a Sample Table, which enables you to enter meaningful Sample IDs and Descriptions for a specified number of samples before you begin scanning. If necessary, you can amend the Sample Table (by adding, deleting or editing rows) to address any issues that arise during data collection.

Additional Information

- All your spectra are added to a new Samples View.
- Batch scanning does not hinder Previewing data collection on the Live tab before collecting the final spectrum from a sample.

Scanalyze

You can use the Scanalyze command on the Measurement bar to collect a spectrum from a sample or batch of samples and then run a Compare, Search or Quant analysis as one action.

1. Check and set the instrument parameters, such as the **Start** and **End** points of the scan range (in wavenumbers, such as 4000 cm^{-1} to 400 cm^{-1}), the **Number of Scans** required, and a unique **Sample ID** and **Description**.

   By default, sensible values for the scan and instrument parameters are entered in the Instrument Settings toolbar; the values applied depend on your instrument and accessory. The **Sample ID** and **Description** are supplied by the Auto-Name function.

   To amend any value, select the parameter and enter your new value.

2. Ensure that the correct process parameters are entered on the appropriate setup tabs.

3. If a background scan is required, the **Scan** button includes a small background flag. Clear the instrument beam path, or insert a suitable background material, and then click  to collect a background spectrum.

   The background spectrum is displayed briefly, and then the Viewing Area is prepared for data collection from your sample.

   By default, the Measurement bar includes **Scan**, **Halt**, **Background** and **Monitor** buttons. You can also select these commands from the Measurement menu.

4. Place your sample in the instrument, click  and then select the process you would like to run.

   OR

   Select **Scanalyze** from the Measurement menu.

   The options are **Scan and Compare**, **Scan and Search**, **Scan and Quant** and **Scan and Verify**.

   During scanning the scan data is displayed on the Live tab in the Viewing Area. The Results pane includes columns for the Sample Name (ID) and Description and additional columns that depend on the results associated with the process selected and the settings defined. You can change the results displayed in the table using the column selector in the top left corner of the table. The results are refreshed during the scan.

   When the scan is completed, the Compare, Search, Quant or Verify tab is displayed. The spectrum is added to the Graph tab in the Viewing Area and to the current Samples View.

   A column selector allows you to choose which results columns are displayed. For Scan and Compare, the Best Hit and the result (Pass/Fail) are displayed by default. For Scan and Search, the Search Best Hit and associated Search Score are displayed by default. For Scan and Quant, the results shown by default depend on the type of Quant Method selected and the settings on the Setup Quant tab. For Scan and Verify, the method name and the specified material are displayed by default with the identified material and, if applicable, the result (Pass/Fail).

5. If, for any reason, you want to stop scanning your sample, click  .

Additional Information

Each process is run using the current setup.

- Before running **Scan and Search**, you will need to set up spectral libraries and search parameters.
- Before running **Scan and Quant**, you will need to set up Quant.
- Before running **Scan and Compare**, you will need to set up compare references.
- Before running **Scan and Verify**, you will need to add a Verify method.

Monitoring

Monitoring enables you to continuously monitor the currently detected signal at the instrument as raw data (single beam), the current interferogram, or as a total infrared energy reading. This enables you to immediately observe the effect of making an adjustment, such as to the force applied to the sample when using a UATR accessory.

- Select **Monitor** from the Measurement menu, or click  .

  The Live tab is displayed in the Viewing area for the current Samples View.

Energy

Select **Energy** to monitor the level of infrared energy reaching the detector in your instrument or accessory. This is useful for optimizing the sample and accessory. The horizontal bars and corresponding values represent the current energy level and the maximum level detected since monitoring began. If the bars reach the edge of the screen, the scale is automatically reset so that the bars are half the width of the screen.

Sample

Select **Sample** to preview the sample spectrum ratioed against the current background spectrum.

Single Beam

A single-beam spectrum is monitored without ratioing against a background spectrum.

This is useful when purging, as you can see the features due to water vapor and CO_2 gradually being removed. Clearly, to avoid introducing negative bands, the purge conditions must be the same for the background as for the sample(s).

Interferogram

The maximum data range for interferograms is determined by the current resolution setting and interferogram sidedness.

Force Gauge

If the currently installed accessory is an HATR or Universal ATR with the pressure arm fitted, the Live tab includes a Force Gauge, which displays the force applied by the arm. If too much force is applied, the green bar flashes red as an over-pressure warning.

CAUTION: Where an over-pressure clutch is fitted to the UATR pressure arm, it significantly reduces the risk of crystal breakage, but should never slip in day-to-day use. In particular, DO NOT use the over-pressure clutch as a substitute for the scan Preview option and the Force Gauge. The pressure applied by the arm when the clutch slips is rather greater than should be necessary to achieve optimum transmission of between 40% and 80%, and is sufficient for the Force Gauge to generate a red over-pressure warning.

Additional Information

- To stop monitoring, select **Halt** from the Measurement menu, or click  .
- To stop monitoring and scan the sample, select **Scan** from the Measurement menu, or click  .

Ready Checks

A Ready Check demonstrates that an aspect of the performance of your complete system, including sampling accessory, is fit-for-purpose.

- Select **Ready Checks** from the Instrument Checks sub-menu in the Measurement menu, and select Contamination, Quant Control, Noise, Throughput, Abscissa or Run Selected.

  The Ready Checks dialog is displayed. Follow the prompts on-screen.

  The **Run Selected** option allows you to run multiple Ready Checks. The Ready Checks selected on the Setup Ready Checks tab will be run in the order displayed on the tab.

  If necessary, click the link that enables you to see a print preview of the Instrument Ready Checks Report.

  If you have Spectrum ES, you may be prompted for a signature before the report is generated.

Additional Information

Contamination Check is a Ready Check applicable to sampling accessories that include a component, such as a top plate, that may require cleaning between samples. This includes the UATR and HATR accessories, and the NIRA II/NIRM. The check compares a reference background spectrum (taken when the accessory was perfectly clean) with a background spectrum taken after your sample has been removed. The ratioed spectrum is then examined in absorbance for any sample residue. Before use, you must set up the Contamination Check by making sure that a suitable reference background spectrum is available, and by entering details for up to three peaks that are characteristic of the substance thought to pollute the crystal.

The Quant Control Check enables you to verify your Quant Method before scanning your samples. The concentration of the Component is calculated using the Quant Method selected, compared with the Nominal Value and the result displayed. If the Observed Value is within the Tolerance limit, then the Ready Check result will be PASS. If the Observed Value is outside the Tolerance limit, then the Ready Check result will be FAIL.

The Abscissa Check collects a spectrum and measures the wavenumber at the specified peaks. If the wavenumber value is within the Upper and Lower Limits, the test passes.

The Throughput Check collects a spectrum and measures the ordinate value at each of the specified abscissa positions. If the measured ordinate value is above the lower limit, the test passes.

The Noise Check is a Ready Check that enables you to measure RMS (%T) and Peak-to-Peak (%T) noise over a range and report the baseline Trend.

A documented Ready Check can be an element of the System Suitability checking required for regulatory compliance in some industries. You can set up Ready Checks such that the detailed Instrument Ready Checks Report is displayed or printed automatically.

Instrument Verification

Instrument Verification is the procedure of demonstrating that your instrument is functioning correctly.

To perform an Instrument Verification:

- Select **Instrument Verification** from the Instrument Checks sub-menu in the Measurement menu.

  The Instrument Verification dialog is displayed. Follow the prompts on-screen. The Instrument Verification checks that are selected on the Setup Instrument Verification tab will be run.

  If necessary, click the link that enables you to see a print preview of the Instrument Ready Checks Report to see the detailed results.

  If you have Spectrum ES, you may be prompted for a signature before the report is generated.

NOTE: If performing an Instrument Verification Check with a NIRA or a Fiber Optic Probe, ensure that the Spectralon reference is placed on the sample area of the NIRA and that the Fiber Optic Probe is holstered during background scans. Instrument Verification checks are run with the NIRA in the Upper position. When running a reference sample with the NIRA, the Spectralon reference must be placed on top of the reference material on the sample area.

Additional Information

The Abscissa Check collects a spectrum and measures the wavenumber at the specified peaks. If the wavenumber value is within the Upper and Lower Limits, the test passes.

The Ordinate Check collects a spectrum and measures the ordinate value at each of the specified abscissa positions. If the measured ordinate value is above the lower limit, the test passes..

The Noise Check is a ready check that enables you to measure RMS (%T) and Peak-to-Peak (%T) noise over a range and report the baseline Trend.

The ASTM check collects two spectra and compares them to two reference spectra. The check consists of a Background, ASTM Noise and ASTM Abscissa check.

The Pharmacopoeia Test will run tests for the verification of instrument performance as defined in the some of the national pharmacopoeias. For details refer to the Setup Pharmacopoeia Test tab.

You can set up Instrument Verification such that the detailed Instrument Verification report is displayed or printed automatically.

Component Checks (Spectrum Two Only)

The Component Checks ensure that the main components of your instrument are in good working order and, where necessary, suggest appropriate actions.

NOTE: The first time you connect to your Spectrum Two spectrometer, the Component Checks will run automatically. You can then select whether to run these component checks each time you connect to the instrument on the Setup Laboratory Actions tab.

To run the Component Checks on demand:

- Select **Component Checks** from the Instrument Checks sub-menu in the Measurement menu.

  The Component Checks dialog is displayed and the tests are run. Each item is assigned a pass ✓ or fail status ✗. If the Component Checks identify a problem, further information or instructions will be provided in the Recommended Action section.

Recommended Actions

If the Component Checks identify that a user-maintainable part needs to be replaced, for example the source or desiccant, a link to the appropriate Replacement Wizard will be displayed. The Replacement Wizard will provide step-by-step instructions for replacing the part. Before starting the replacement procedure, you will need the appropriate parts:

Part Number	Spares Kit
L1600243	Source Replacement Kit
L1600244	Desiccant Replacement Kit

If the Component Checks identify a problem that may require investigation by a PerkinElmer Service Representative, refer to the support website for information on how to proceed:

www.perkinelmer.com/SpectrumTwoSupport

Your PerkinElmer Service Representative may require the log file created during the Component Checks:

- To access the file, click **Export the saved log file.**

  Save the log file to a convenient location.

Additional Information

You can also access the source or desiccant replacement wizards from the Adjustments Toolbox, which is available from the Setup Instrument Advanced tab.

Humidity Shield (Spectrum Two Only)

The Humidity Shield enables you to view the current internal humidity of your Spectrum Two spectrometer. The function uses a humidity sensor inside the spectrometer.

NOTE: The humidity is also checked during the Component Checks available from the Measurement menu.

To view the Humidity Shield:

- Select **Humidity Shield** from the Measurement menu.

  OR

  Select  in the Measurement bar.

  The Humidity Shield dialog is displayed, showing the Current Internal Humidity (%).

  If the humidity is normal the number will appear green.

  If the humidity is high the number will appear yellow. You are recommended to change the desiccant.

  If the humidity is critical the number will appear red. Replace the desiccant immediately to avoid instrument damage.

  NOTE: If the humidity of your instrument reaches high or critical levels, the humidity sensor will display a warning message on the Status bar.

  If the Humidity Shield recommends that the desiccant should be replaced, you can click **Replace Desiccant** to access a wizard that will take you through the procedure, step-by-step. You will need to have the Desiccant Replacement Kit (L1600244) ready when you start the wizard.

  The expiry date of the desiccant is based on the date the desiccant was last changed. It gives an indication of when the desiccant is expected to expire in normal conditions (up to five years). However, if your spectrometer is switched off for long periods of time, or used or stored in an environment that has high levels of humidity, then you are advised to use the Humidity Shield to check the humidity of your instrument more frequently.

Additional Information

You can access the Desiccant Replacement Wizard from the Adjustments Toolbox, which is available from the Setup Instrument Advanced tab.

Collecting Data Using the Spotlight 150 Microscope

When associated with a Frontier system, Spectrum software allows you to collect spectra using the Spotlight 150 microscope, which has a manually-operated stage and allows scanning at a single point on your image.

Click an option to find more information about collecting and analyzing data using this microscope.

Collecting backgrounds

Scanning a sample

Collecting Backgrounds with the Spotlight 150

When collecting data to generate sample spectra, a first step is to collect a background spectrum from the instrument with no sample present.

The sample spectrum is ratioed against the background spectrum to eliminate features introduced by the instrument response, the sampling accessory and features introduced by atmospheric absorption.

If no valid background spectrum is available, a background spectrum must be collected before you begin to scan samples. When a background spectrum is required, the **Scan** icon in the Measurement toolbar changes from  to  .

NOTE: If you change the instrument parameters, such as Resolution, the Sampling Mode or the Aperture dimensions (or calibrate the Apertures), then you will need to collect a new background.

Collecting a background spectrum

1. Check and set the instrument parameters, such as the **Start** and **End** points of the scan range (in wavenumbers, such as 4000 cm^{-1} to 400 cm^{-1}), the **Number of Scans** required, and a unique **Sample ID** and **Description**.

   By default, sensible values for the scan and instrument parameters are entered in the Instrument Settings toolbar; the values applied depend on your instrument and accessory. The **Sample ID** and **Description** are supplied by the Auto-Name function.

   To amend any value, select the parameter and enter your new value.

2. Select the appropriate Sampling Mode for your experiment.

3. Move the stage so that the area on the sample from which you want to collect spectra is in the center of the video image.

   You may need to adjust the Illumination to view the sample.

4. Set the infrared aperture to an appropriate size for the feature you wish to measure.

   See Setting an Aperture.

5. Remove the sample and select a suitable substrate for your background measurement.

   If you are sampling in transmittance, you may simply chose move the stage to an area away from the sample and focus on the surface of the substrate using the microscope focus controls. If you are sampling in reflectance, you may want to use an appropriate reference, such as the gold mirror supplied with your Spotlight 150.

6. If required, adjust the Illumination.

7. If you are examining the sample in transmittance mode, then you may need to adjust the position of the lower cassegrain using the Correction controls to maximize the energy reaching the detector, see Maximizing the Energy.

   If you are working in reflectance, you do not need to maximize the energy provided that the infrared focus is the same as the visible focus.

8. Select **Background** from the Measurement menu, or click  .

   A background spectrum is collected, but is not displayed or saved.

Additional Information

The calibrated rules on the microscope sample stage may help you to relocate an area of interest if you have moved the sample stage.

For more information on collecting backgrounds with Spectrum software, see Backgrounds.

For more information on collecting sample spectra with the Spotlight 150, see Scanning a Sample with the Spotlight 150.

Scanning a Sample with the Spotlight 150

1. Collect a background spectrum as described in Collecting Backgrounds with the Spotlight 150.

   NOTE: If you change the Sampling Mode or the Aperture dimensions (or calibrate the Apertures) before collecting your sample spectrum, then you will need to collect a new background.

2. Move the current aperture to the part of the sample where you want to collect a spectrum.
3. Focus on the sample using the microscope focus controls.
4. If required, adjust the Illumination.
5. Click  to begin scanning your sample.

   By default, during scanning the sample data is displayed on the Live tab in the Viewing Area.

   The completed spectrum is displayed on the Graph tab, and added to the current Samples View in the Data Explorer.

6. If, for any reason, you want to stop scanning your sample, click  .

Additional Information

The microscope settings used for the last successful scan are retained when you exit Spectrum software, and will be available when you next login to the software at this PC.

For information on collecting a background spectra with a Spotlight 150, see Collecting Backgrounds with the Spotlight 150.

For more information on scanning samples with Spectrum software, see Scanning a sample.

Collecting Data Using the Spotlight 200 Microscope

Spectrum software allows you to collect data using the Spotlight 200 microscope, which has an automated stage to allow surveys to be taken of large areas of your sample. You can select points, lines or areas on your image at which to collect spectra. You can also use the software to automatically recognize particles and layers in your sample, and set up the spectral analysis.

Click an option to find more information about collecting and analyzing data using this microscope.

Viewing and Saving Images Using the Spotlight 200 Microscope

Once your microscope is initialized, the Stage View and Camera View panes for your microscope can be viewed by clicking **Microscope** in the Data Explorer.

Camera View

The Camera View pane displays the entire field of view of the camera in your microscope, which is approximately 450 µm wide and 360 µm high. Use this pane to optimize the imaging of your sample. You can also use it for point scanning of spectra from features of interest.

You cannot rescale this image; to view larger or smaller areas of your sample, use the Stage View pane.

Obtaining an optimized image

1. Place your sample on to the microscope stage and adjust the stage position in the X and Y directions using the joystick.
2. Use the joystick to adjust the Z-axis until the sample's features can be seen in the Camera View.
3. Click the **Auto-Illumination** button.
   The illumination level will be optimized.
4. Click the **Auto-Focus** button.
   The Auto-Focus routine will be performed to focus the sample image.
5. If you are working in transmittance mode, click the **Maximize Energy** button.
   The lower cassegrain will be adjusted to maximize the energy reaching the detector.
6. If necessary, adjust the Brightness and Contrast of the image in the Setup Microscope Advanced tab.
   You may need to click the Auto-Illumination button again after changing these settings.

NOTE: The image is displayed with the current aperture settings shown as a red, dashed rectangle. These are used when collecting spectra from your sample. The aperture properties (height, width and rotation) for the most recent scan are displayed in the bottom left corner of the Camera View. The current sampling position ("C") and background position ("B") for collecting spectra are also shown on the image.

Saving an Image

1. Click the **Save Image** button.
2. Select either **Save Image** or **Save Image with Markers**.
   If you select the Save Image with Markers option, the saved image will include any markers and apertures shown on the image in the Camera View.
3. Enter a name for your image file, choose a format, and click **Save**.
   The file format options available are *.bmp and *.png.

Stage View

The Stage View pane allows you to view either the whole stage or a part of it that is larger than the area shown in the Camera View. You can also zoom in on a very small area of the stage. You can set positions at which to collect spectra using markers, lines or maps. To make best use of the Stage View, we recommend that you collect an image survey of your sample.

Viewing the Stage

Initially, the Stage View covers the entire area of the stage, with the current Camera View at the center. In most cases, this area will be far larger than your sample, and an image survey of such a large area would take a long time to collect. Therefore, you will probably need to reduce the Stage View area before collecting an image survey.

1. Select **Stage View Range** from the Microscope menu.
   OR
   Click the **Stage View**  button on the Stage View toolbar.
2. Choose an area to view from the four predefined options available (1000, 2000, 5000 or 10000 µm squares).
   OR
   Click **Format**, enter the left, right, bottom and top limits of the Stage View in micrometers, and click **OK**.
   The Stage View dimensions change to fit the selected area.

You can now collect an image survey of a portion of your sample, centered on the area covered in the current Camera View.

There are two other options in the Stage View Range menu which may be useful when setting the viewing area:

Previous Range - returns to the previous Stage View area.

Full Range - returns the Stage View to the entire stage area.

Collecting an Image Survey and Saving the Stage View

An image survey is a mosaic of adjacent camera images which give an image of a larger area.

- Select **Image Survey** from the Microscope menu.
  OR
  Click the **Image Survey**  button on the Stage View toolbar.
  Spectrum will begin collecting and building the image survey in the Stage View pane.

  You can stop the process at any time by clicking the **Halt**  button on the Stage View toolbar.

Once you have collected an image survey, you can still change the area shown in the Stage View:

- To zoom in on an area, click and drag a rectangle on the image survey with the mouse, and then double-click inside it.
- To zoom out, select a different area to display from the options in the Stage View Range menu.

NOTE: If you zoom out, then the area outside the image survey will be shown in white because no images have been recorded at these locations. However, you can still collect spectra from these white regions.

To save the Stage View:

1. Click the **Save View**  button.
2. Select either **Save View** or **Save View with Markers**.
   If you select the Save View with Markers option, the saved image survey will include any markers and apertures shown on the image in the Camera View.
3. Enter a name for your image file, choose a format, and click **Save**.
   The file format options available are *.bmp and *.png.

Subtracting a Background Image

If your camera image always displays an optical artefact or a variation in illumination, this can cause a repeating pattern to appear when you collect an image survey. This effect may be reduced using a background image. Spectrum records an image and subtracts it from future image surveys.

1. Move the camera view to a region of the sample with no features.
   You can use a mirror if you are working in reflectance mode.
2. Adjust the focus so that the visible image is less sharp.
3. Click the **Collect Background Image**  button.
   This button will be shaded to indicate that the background image is being applied. You can now collect an image survey with the background image subtracted from each individual image.
4. When you have finished imaging your sample, click the  button again to stop subtracting the background image.
   A background image will depend on the appearance of your sample image, so it should be re-recorded for each sample.

Navigating Around the Stage

The stage origin is the reference point from which all other positions on the stage are measured. By default, it is at the center of the stage. If you are examining a large sample under the microscope, it can be useful to set the stage origin to be near to an area of particular interest, especially if this is some distance from the center. You can then use this as a reference point to quickly find the area again.

NOTE: While the stage is moving to a new position, the current position marker "C" is replaced by "D" on the Stage View.

1. Use the joystick to position the Camera View at a point at or near the features you want to examine.
2. Select **Set Stage Origin** from the Microscope menu.
   OR
   Click the **Set Origin**  button on the Stage View toolbar.
   The stage origin is set to the new position, and the coordinates displayed in the bottom left of the Stage View pane are set to zero.

The Stage Move menu provides a number of commands to help you navigate around the stage and examine your sample thoroughly. These commands can be found under the Microscope menu or by clicking the **Stage Move**  button on the Stage View toolbar.

Click a command below to view more information:

- ***To Origin***

  Once you have set the Stage Origin to a point at or near a region of interest on your sample, use the **To Origin** command to return the Camera View to that position.

- ***To Selected Marker***

  Once a marker is added to the Stage View and selected by clicking it (when it will turn blue), use this command to move the Camera View to the marker location.

- ***To Background Position***

  Use this command to move the Camera View to the position selected for the collection of background spectra.

- ***To Load Position***

  This command moves the stage down and toward the user to make it easier to place samples on to the stage.

- ***To Previous Position***

  Use this command to return the Camera View to its previous position.

- ***To Center View***

  Use this command to move the Camera View to the center of the Stage View area.

- ***To Center Stage***

  Use this command to move the Camera View to the center of the sample stage.

  NOTE: The center of the stage may not be visible in the Stage View.

- ***To Coordinate***

  Use this command to move to any point on the stage. Enter the number of micrometers from the origin in the x, y and z directions, and click **OK**. The dialog box displays the limits of travel along each axis.

Collecting Spectra Using the Spotlight 200 Microscope

If there are only a few areas of your sample where you want to collect spectra, you can quickly and easily do this once you have obtained an image. You need to select a position for the background spectrum and set the apertures to be used when scanning your sample.

1. Use the joystick to position the camera over or near to the feature you want to scan and click the **Set Origin** button on the Stage View toolbar.
   This will help you to easily find the position again after you move the stage.
2. Move the camera to a suitable region of your sample and click the **Set Background Position** button on the Stage View toolbar.
   The crosshairs in the center of the Camera View are now marked "B" to show that this is the Background position. A similar marker is also displayed in the Stage View.
3. Click the **Stage Move** button on the Stage View toolbar, and select **To Origin**.
   The Camera View will return to the position of the stage origin.
4. Move the sample stage using the joystick so that the current position crosshairs are on the feature you want to scan.
5. To set the aperture size, move the mouse pointer to one of the sides of the aperture indicator (the red, dashed rectangle).
   The mouse pointer changes to a two-headed arrow ⇔, ⇕, ⤢ or ⤡.
6. Drag the edges of the aperture indicator so that it fits around the feature you want to scan.
   It is best to make the aperture slightly smaller than the feature to correct for diffraction of the infrared beam.
7. To set the aperture rotation, move the mouse pointer to a corner of the aperture indicator.
   The mouse pointer changes to a curly arrow ↺.
8. Drag the corner of the rectangle left or right to rotate the apertures.

> **NOTE:** You can also set the apertures using the Setup Microscope Advanced tab.

9. To check that the apertures are the correct size and shape, click **Test** in the Setup Microscope Advanced tab.
   The apertures will move into position in the Camera View. Click **Park** to retract the apertures.
10. Click .
    The stage will move to the background position and collect a background scan with the selected apertures. Depending on the settings in the Setup Microscope Data Collection tab, you may be asked to confirm whether or not the stage should move to the background position.

> **NOTE:** If you have not selected the correct background position, click **Cancel** to halt the data collection.

11. When the stage returns to the current position, click to scan the feature you selected.
    The spectrum is saved in a new Samples View in the Data Explorer as normal.

NOTE: To add further spectra to the same Samples View, you must select the Samples View before collecting the spectra, otherwise each spectrum will be saved in separate Samples Views. Position the Camera View as required, select the Samples View in the Data Explorer, and then click  .

Setting Up Markers Using the Spotlight 200 Microscope

If your sample contains many points from which you want to collect spectra, it is quicker and easier to collect the spectra using markers rather than collecting each one manually. You can place single markers on your sample for scanning at a single point, or you can place a collection of markers in a line or map to cover a larger section of the sample.

To add a marker:

1. Obtain a focused image of your sample, and collect an image survey.
2. Select **Add Marker** from the Microscope menu.
   OR
   Click the **Add Marker**  button in the Stage View toolbar and select the **Add Marker** option.
   A blue cross appears at the current position, both in the Camera View and the Stage View. A set of marker properties appears in the pane underneath the Stage View.
3. Click and drag the marker to the desired position in the Camera View, or in the Stage View if you want to move it a greater distance from the current position. As you move around the Stage View, any markers that are close to the current position will also be visible in the Camera View.
4. Adjust the marker's apertures by dragging the edges and corners of the red rectangle, or by changing the values of width, height and rotation in the properties pane.
   You can also change the marker's coordinates in the properties pane.
5. Repeat steps 2-4 to add other markers as required.
   You can assign a different ID to each marker using the properties pane to help distinguish them in the results and the Data Explorer.

To add a line:

1. Obtain a focused image of your sample, and collect an image survey.
2. Select **Add Line** from the Microscope menu.
   OR
   Click the **Add Marker**  button in the Stage View toolbar and select the **Add Line** option.
   A graduated blue line appears at the center of the Stage View. The first point in the line is marked by a blue square. A set of line properties appears in the pane underneath the Stage View.
3. Click and drag the blue square to the location in the Stage View where you want to start scanning the line.
4. In the properties pane, choose the number of **Points** in the line, the **Spacing** and the angle of **Rotation** from the first point.
   You can also adjust the Spacing and Rotation by clicking and dragging each end of the line on the Stage View.
5. Adjust the apertures to be used for scanning the points in your line by dragging the edges and corners of the red rectangle, or by changing the values of width, height and rotation in the properties pane.
6. Select whether you want to display the individual spectra from the line in Spectrum using the **Display in graph** option.
   We do not recommend trying to display more than 300 spectra as this may cause operating problems with the software. If you choose not to display the spectra, then the line will be completely removed from the results display.
7. If required, enter a new ID for the line in the properties pane.

To add a map:

1. Obtain a focused image of your sample, and collect an image survey.
2. Select **Add Map** from the Microscope menu.
   OR
   Click the **Add Marker** button in the Stage View toolbar and select the **Add Map** option.
   A grid of blue crosses is displayed at the center of the Stage View. The first point to be scanned is marked by a red, dashed rectangle that indicates the aperture size and rotation. A set of map properties appears in the pane underneath the Stage View.
3. Click and drag the top left corner of the map to the location in the Stage View where you want to start scanning the map.
4. In the properties pane, choose the number of **Points** in the x and y directions of the map, and the **Spacing** between points in each direction.
   You can also adjust the Spacing by clicking and dragging a corner or edge of the map on the Stage View.
5. Adjust the apertures to be used for scanning the points in your map by dragging the edges and corners of the red rectangle, or by changing the values of width, height and rotation in the properties pane.
6. Select whether you want to display the individual spectra from the map in Spectrum using the **Display in graph** option.
   We do not recommend trying to display more than 300 spectra as this may cause operating problems with the software. If you choose not to display the spectra, then the map will be completely removed from the results display.
7. If required, enter a new ID for the map in the properties pane.

Moving Between Markers

You can use the left and right arrows on either side of the properties pane to move between each marker. The stage will move to place the marker position at the center of the Camera View.

Scanning Markers

Once you have set your markers, the software will scan all of them in sequence.

To scan all markers:

1. Click .
   Background spectra will be collected for each of the different aperture sizes of your markers, according to the Background Options settings in the Setup Microscope Data Collection tab.
2. Click .
   Spectrum will scan each marker in sequence, and display the results in the Image tab of the Image View.

You can also choose to perform certain processes on each spectrum, while the next spectrum is being collected.

For example, click the arrow next to the Scan Markers button and select **Scan and Compare.** Spectrum will now run a Compare process on each spectrum after it is collected, using the settings in the Setup Compare tabs. The Scan Markers button in the Scan toolbar will change to display  , so the default setting for scanning markers will now include running a Compare process until you select a different scanning option.

Removing Markers

To remove an individual marker, line or map:

1. Select the marker, line or map you want to remove on the image survey. The selected item will be shown in blue.
2. Click the **Remove Marker**  button in the Stage View toolbar. The selected item will be removed.

To remove all markers:

- Click the **Remove All Markers**  button in the Stage View toolbar.

Saving the Markers Layout

To save the current markers layout:

1. Click the **Save Layout** button on the Setup Microscope Data Collection tab.
2. Enter a name for the markers layout file, and click **OK.**

You can reuse this layout for future samples.

Viewing Results from a Microscope Experiment

The results from a microscope experiment to scan markers, lines or maps on an image are automatically displayed in an Image View. This is a virtual folder, very similar to a Samples View, which organizes all the results from a series of scans into one location in the Data Explorer.

The Image View includes:

- The spectrum for each marker; click a spectrum sub-node and then click the **History** tab to view all the information on that spectrum.
- An Image View tab that displays all the spectra collected during the experiment.
- A Results Table tab that summarizes the results for all the spectra in the Image View.
- An Image tab from which you can examine the results from your experiment with reference to the image locations where scans were collected.

The first three items in this list behave in the same way as the equivalent items in a Samples View, except that you cannot perform further data processing from these tabs. The Image tab is unique to microscope experiments, and allows you to examine the results in a number of different ways.

Image Tab Layout

The Image tab contains three panes:

- The top left pane displays the image of your sample, showing the regions identified (if any) and the markers that have been scanned.
- The top right pane displays a series of tabs which list the name and color for each marker, and the results of any processing operations performed on the spectra.
- The bottom pane displays the spectrum for each marker and, depending on the data processing being performed, other relevant spectral data.

Data Displayed While the Experiment is in Progress

While background spectra are being collected, the software continues to display the microscope view, with the background spectra displayed in the lower pane. The Image tab is displayed once scanning of the markers has commenced. The tab displays the image or image survey, with the first marker to be scanned (in red) and the remaining markers (in grey).

As each marker is scanned, a line is added to the tables in the appropriate tabs. Initially, this assigns a color to each marker which corresponds to the color shown in the image. This color may change later if any processing is performed on the spectrum. The next marker to be scanned is then shown in red.

By default, the latest spectrum to be collected is shown in the bottom pane.

- To hide the spectrum viewing pane in the Image tab, uncheck the **Show graph** checkbox.
- To stop the screen from updating during the data collection, uncheck the **Auto-View** checkbox.
  This can be useful if you want to examine any spectra already collected, as otherwise they are replaced by each new spectrum as it is collected and processed.

NOTE: The Live tab is included in the Image View while the spectra are being scanned. During data collection, it may not be possible to change the tab being viewed if the system is busy.

Image Display

The image being scanned is displayed in the top left of the Image tab. It shows the marker, line and map locations and, where applicable, any regions identified using an Analyze Image process. Where regions have been identified, there are several options for controlling their appearance:

1. Check the **Show Regions** checkbox to display the regions found by the Analyze Image process.
2. Use the drop-down list to select whether to display the regions in **Outline** or in **Overlay** (solid color).
   The apertures are always displayed.

Results Display

Using the Scan Markers button, you can either simply collect the spectra from the markers on the image, or in addition run certain processes such as Search, Compare and Verify, based on the settings in the setup tabs for each process. These processes produce different sets of results in the Image tab, which can be selected using the **Display results for process** drop-down list. This list shows the various processes performed on the data in the order that they were run.

Viewing Results from Data Collection

You can choose to view only the data collected during the scanning of the markers:

- Select **None** in the **Display results for process** drop-down list.

The four tabs on the right pane list the various markers scanned during the experiment.

- **All** - lists each marker scanned (including those in lines and maps) with their assigned colors and names, and the segments for any lines scanned.
- **Markers** - lists the individual markers in order of scanning, with their assigned colors and names.
- **Lines** - lists the segments and markers in a line with their assigned color and name. If more than one line was scanned, use the **Object ID** drop-down selector to view the markers for each line in turn.
- **Maps** - lists the markers in a map with their assigned color and name. If more than one map was scanned, use the **Object ID** drop-down selector to view the markers for each map in turn.

As you click each tab, the markers shown on the image change accordingly. The All tab shows the entire image with all the marker locations. The other tabs zoom in on the selected items.

The tabs also list the aperture areas for each marker, and their percentages relative to the area of the image.

To change the color of a marker:

1. Position the mouse pointer over the **Color** entry in the table for the marker you want to change.
2. Click the drop-down arrow that appears.
   A color palette is displayed.
3. Click the new color.

You can change the marker colors using any of the four tabs. All the markers in a line or map are automatically set to the same color.

To view the spectra for markers:

- Select rows in the table by clicking the row selector buttons on the left side of the table.
  The spectrum displayed in the bottom pane changes accordingly, and the marker in the image turns blue to show that it is selected. You can select more than one marker by holding down CTRL and selecting multiple lines in a table.

Viewing Process Results

- Select the process name from the options available in the **Display results for process** drop-down list.

The tables in each tab list the results of the selected process for each marker. Above these tables, a Components table is displayed. This table summarizes the results of the process. For example, if you have selected Scan and Search, the Components table lists all the spectra identified by the Search process and assigns a color to each. The markers in the image are then colored according to these results, so you can see whether multiple markers have given the same result for the process. This applies to maps and lines as well; where two adjacent markers in a line have different results, the line changes color halfway between the markers.

Similar tables are produced for the other available processes.

Where applicable, areas for each type of marker which correspond to a particular result are reported as a percentage of the entire image area. The All tab sums the areas for all markers, lines and maps. The Markers tab sums the areas for all markers. The Lines and Maps tabs sum the areas for the selected line or map.

After running a process, you can change the color of a component which changes the colors of the markers identified as that component:

1. Position the mouse pointer over the **Color** entry in the Components table for the marker you want to change.
2. Click the drop-down arrow that appears.
   A color palette is displayed.
3. Select the new color.

NOTE: When you are viewing the results of a process such as Search, you can only change the colors in the Components tables. These changes are then applied to all the tabs.

You can select a particular component in the Components table to only display markers whose spectra match that component:

- Click the row selector button on the left side of the Components table for the component you are investigating.
  Spectrum will highlight the related markers in the lower table, and the image will show those markers in color, with the rest shown as colorless. The graphs of the related markers will be displayed in the bottom pane.

NOTE: In some processes, the bottom pane displays additional spectra. For example, running Search causes the identified library spectrum to be displayed with the sample spectra.

Further Processing of Spectra

You can run further processes on your spectra using the commands in the Process menu. These results are added to the results tables in the Image tab, and the process is added to the **Display results for process** drop-down list.

NOTE:	The processing operation is performed on the set of spectra currently selected in the Image View tab. Processing from the Image View tab is not allowed as any processing has to be applied to all markers.

If a process changes the spectra, then the processed spectra are added to the results unless the Overwrite option is selected, in which case the spectra are overwritten and the new process replaces the previous option in the **Display results for process** drop-down list. For example, if a Smooth process is run without the Overwrite option being checked, then the drop-down list will contain the entries None and Smooth. If the Overwrite option is checked, then the list will only contain Smooth because the original spectra have been overwritten.

To run further processes on the a set of spectra, ensure they are selected in the Image tab when you run the process. In the first example above, you have the option to process the original spectra or the smoothed spectra, depending on which one is displayed when you run the process.

Saving and Retrieving the Image View

Once you have collected and processed the data as required, you can choose to save the contents of the Image View to allow it to be easily retrieved in the future for reporting or further analysis.

1. Select **File** > **Save Image View**.
2. Select a location and a filename for the file, and click **Save**.
   The Image View file will be saved as an *.xml file.

To retrieve the data:

1. Select **File** > **Open Image View**.
2. Select the file and click **Open**.
   The Image View is opened.

You can retrieve an Image View and carry out further processing after you have disconnected from the microscope.

Additional Information

If you have chosen to save *.lsc or *.fsm files when scanning lines and maps respectively, then these will be available in the same location as the spectra *.sp files once the experiment is complete. You can only view *.lsc and *.fsm files using SpectrumIMAGE Viewer. This software application can be installed using the separate CD supplied.

Automatic Image Analysis Using the Spotlight 200 Microscope

The Analyze Image option performs the following tasks automatically: identifying features or regions in your sample, selecting marker positions within each region, and setting the aperture sizes for each marker. For samples with many distinctive surface features, this can save you a lot of time. Four analysis processes are available for different types of sample features: Detect Particles, Detect Inclusions, Detect Layers and Characterize Layers.

Analyzing an Image

1. Obtain a focused image of your sample, and collect an image survey.
2. Select **Analyze Image** in the Microscope menu.
   The software will run the process you last used on the Stage View image.
   OR

   Click the **Analyze Image**  button in the Stage View or Camera View toolbars, and select the process you want to run.
   Spectrum searches your sample for features, as shown by a green band moving down the image survey. The Analyze Image results view is then displayed.
3. Examine the results and make adjustments to the settings as needed to identify the regions of interest in your image.
   The settings are described below.
4. Click **OK**.
   The microscope view screen is displayed, showing the markers on each feature. These can now be adjusted further and then scanned.

NOTE: To return to the microscope view without saving the results of an image analysis, click **Cancel**.

Viewing the Image Analysis Results

By default, the Analyze Image results view is split to show the source image on the left and the results of the analysis on the right. You can display only the result image by clicking **Result** in the toolbar on the left of the panel underneath the images.

The Result image displays each feature or region identified by the image analysis in a different color. The software also selects the largest rectangular area within each region and sets this as the aperture size for scanning that feature. These apertures are shown as a red, dashed rectangle with a set of crosshairs at the center. You can adjust them by clicking and dragging the edges of the rectangle.

You can also adjust the view of your image analysis using the settings in the panel underneath. Each time you change these settings, the analysis process is repeated and the results are displayed, so you can see the effects of your change very quickly.

Source Image

If you want to change the image being analyzed, select the image you want to use and the process will rerun immediately.

Process Type

If your sample contains particles on its surface that you want to identify, select **Detect Particles.** If it contains defects or areas of contamination within its structure, select **Detect Inclusions.** This process collects a spectrum from a "clean" area of the surface to use as a reference in detecting inclusions, which appears as an extra marker in the Result image. If the sample is a layered structure, then select **Detect Layers** to mark individual layers in the sample for analysis. **Characterize Layers** automatically sets up a line scan across the layers identified in the sample so that all the layers can be analyzed.

Result Image

There are several settings that you can adjust to help view the results of the analysis more clearly. Click a setting to view more information.

Reverse Contrast

Check the checkbox to display the negative of the image. This can help with visualizing dark features.

Show Apertures

Check the checkbox to view the apertures selected for each detected region or feature as a red, dashed rectangle on the result image.

Overlay

Select this option to display the detected feature or region in solid color over the image.

Outline

Select this option to display the detected features or regions outlined in the assigned color.

Opacity

Use the slider to change the opacity of the colored features or regions displayed. Reducing the opacity allows you to view the detected regions without obscuring the details of the image.

Particles

There are two options for adjusting the number of particles and inclusions shown in the results from the Detect Particles and Detect Inclusions processes.

To display a selected number of particles or inclusions:

- Click **Largest Particles** and enter a number in the text box, and press ENTER. The Result image will display the selected number of particles or inclusions in order of size, starting with the largest.

To only include particles or inclusions that lie within a certain size range:

1. Click **Filter Particle Size.**
2. Drag the markers at each end of the slider to select the target size range. The selected range is shown in green. The Result image is updated.

Advanced Settings

If you are still not satisfied with the results of the image analysis, you can adjust the advanced settings and make the detection of features in the image more or less sensitive.

- Check the **Use Advanced Settings** checkbox.

NOTE: In Spectrum ES, you need the correct permissions to change the advanced settings.

Click on the options below to learn more about the advanced settings for each process type.

Advanced Particle/Inclusion Settings

Minimum Area

The minimum number of pixels that must be occupied by the object for it to be detected. Reduce the value if the analysis is not finding small particles or inclusions, and increase it if the analysis is detecting too many features.

Minimum Contrast

Controls the contrast needed for the detection of particles or inclusions. Reduce this value if features similar in color or contrast to the surface material are not detected by the analysis, and increase it if the analysis is incorrectly detecting other surface features or optical artifacts as particles or inclusions.

Threshold

Affects the determination of the edge of a particle. Reduce this value if the identified regions are smaller than the particles in the image, and increase it if the edges of the regions are outside the edges of the particles.

Split Factor

Determines whether particles or inclusions touching or overlapping each other are split or kept together as a single object. By default, no additional splitting is applied. Increase the value if you want the process to separate features which are overlapping.

Advanced Laminate Settings

Layer Width

Controls the number of separate layers detected between the layer boundaries in the image by changing the sensitivity of the analysis. Reduce the value to detect fewer layers, and increase it to detect more layers.

Binning Level

Controls the sensitivity of detecting layer boundaries. Reduce the value to increase the sensitivity, which will require longer processing times and may also increase the influence of image artifacts on the results. Increase the value to reduce the sensitivity, which may give less precise detection of boundaries.

Minimum Length

Defines the minimum length of a detected layer as a fraction of the longest dimension of the image. Objects shorter than this length will not be detected. Reduce this value if small layers are not being detected, and increase it if too many features are being detected as layers.

Signal Fraction

Determines the minimum image signal needed for a layer to be detected. Reduce the value to lower the signal threshold, and increase it to set a higher threshold.

Width Coefficient

Determines the width of the angle around the principal axis of the sample's layered structure where boundaries are detected. Reduce the value to reduce the angle, which may detect smaller fragments as separate layers. Increase the value to widen the angle, which reduces the resolution and may detect fewer layer boundaries.

Kernel Radius

Determines the extent of processing performed on the image, which affects the detection of boundaries and edges. Reduce the value to reduce the processing, which may cause many small layers to be detected. Increase the value to increase the processing, which may detect fewer layers due to less sensitive detection of boundaries.

Kernel Shift

Determines the distance between image lines processed during the analysis. Reduce the value to reduce the distance, which requires longer processing times and may lead to many small regions being detected. Increase the value to increase the distance, which reduces processing times but may detect fewer boundaries.

Using the Automated ATR with the Spotlight 200 Microscope

The Automated ATR Objective accessory is available for use with the Spotlight 200 microscope. The infrared beam is directed on to the sample surface through a germanium crystal. The beam is then reflected from the surface to give a spectrum of the sample. Spectrum can control the automated ATR objective to automatically scan markers, lines and maps on selected areas of your sample. The accessory includes a weighbridge that fits onto the microscope stage; this allows a known pressure to be applied by the crystal each time a spectrum is collected, which helps you to obtain repeatable results. The weighbridge reports its measurements to the microscope using wireless communication, powered by an internal battery.

Refer to the *Spotlight 200 User's Guide* for more information on using the automated ATR objective to analyze samples.

NOTE: The manual ATR objective can also be used with the Spotlight 200 for collecting spectra. You can scan markers automatically once you have manually lowered the crystal. However, there is no weighbridge available to control the applied pressure.

Controlling the Automated ATR

If your microscope is equipped with an automated ATR objective, then a  button is displayed in the Accessory bar once the microscope has initialized. An indicator for the weighbridge battery will also be displayed in the Status bar at the bottom of the screen, showing when the battery charge is at the correct level (), becoming low (), or when the battery needs replacing immediately ().

NOTE: Refer to the *Spotlight 200 User's Guide* for information on how to change the weighbridge battery.

Spectrum will automatically control the position of the ATR crystal when collecting spectra, but you can control it yourself if required. The  button in the Accessory bar lowers the ATR crystal, ready to scan a spectrum. Once you lower the crystal, you can no longer view the live image in the Camera View. To raise the crystal, click the  button.

NOTE: You can also control the crystal position using the **Raise** and **Lower** buttons in the ATR section of the Setup Microscope Basic tab.

Data Collection Options

- On the Setup Microscope Data Collection tab, select one of the **Automated ATR** options.
  These options only relate to the collecting of spectra using markers.

Use Marker Height will collect a spectrum from the z-coordinate of the marker position in the Camera View or Stage View. It is therefore important that the ATR crystal is in contact with the sample at this position.

Determine Height Using Pressure will apply the selected Auto-Pressure level set in the Setup Microscope Basic tab before collecting the spectrum of a marker. The software will attempt to apply the requested pressure a number of times before collecting a spectrum with the closest achievable pressure.

Setting the ATR Auto-Pressure

To ensure that good spectra are collected using the automated ATR objective, the pressure applied by the crystal onto the sample must be set correctly. If it is too low, a weak and noisy spectrum will be collected. If it is too high, the sample may be damaged. The weighbridge measures the pressure applied by the crystal, and allows Spectrum to control the value for each scan collected using the ATR.

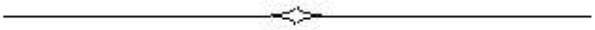
To find the correct Auto-Pressure setting for your sample:

1. Select the **ATR** sampling mode.
2. Place your sample on the stage, with the weighbridge installed.
3. Use the Camera View to obtain a focused image of the sample's surface.
4. Click  .
   The ATR crystal will lower to collect a background spectrum in air.
5. Select **Monitor** from the Measurement menu, or click  .
   The software will ask if you want the ATR crystal to make contact with the sample.
6. Click **Yes**.
   The stage moves upward slowly until the ATR crystal just touches the sample.
7. When the stage is in contact with the sample, select the **Sample** monitoring option.
8. Raise the stage until a spectrum is observed in the Live tab.
9. Observe the appearance of the spectrum and increase or decrease the pressure as required by making small changes to the stage height.
   The applied Sample Force is shown in the Stage View pane. A value of 100% is equal to 200 g of force applied across the area of the crystal, or a pressure of approximately 25 kg/mm^2.

   NOTE: The applied pressure will eventually level off as the spring in the ATR objective begins to compress.

10. When you have obtained a satisfactory system, note the Sample Force percentage value in the Stage View and click  .
    The ATR crystal will be raised and the Monitor screen will be closed.
11. Set the Auto-Pressure slider to the correct percentage value.
    When you next scan a marker in ATR mode with the **Determine Height Using Pressure** option selected, this pressure will be applied before the spectrum is collected (providing the Auto-Pressure setting has not been changed).

NOTE: You can use a similar method to select the height of a marker which gives a good spectrum before collecting data with the **Use Marker Height** option selected. Adjust the height of the stage using the **Adjust Up** and **Adjust Down** buttons on the Accessory bar while monitoring the spectrum. Once a suitable height is found, add markers to your image; they will all have a z-position corresponding to the selected stage height.



Collecting Data with your Raman Instrument

Collecting Data

These topics describe how to use Spectrum to collect data using your instrument.

Collecting data from a single sample.

Collecting data from a batch of samples.

Collecting data and running a process.

Monitoring data collection while optimizing your sample setup.

Scanning a Sample

To scan a single sample:

1. Place your sample in the instrument or accessory and locate the position of interest.

   NOTE: If you have a motorized stage, refer to Moving the Stage to a Position of Interest.

2. Check and set the instrument parameters, such as the **Start** and **End** points of the scan range (in Raman Shift, for example, 3200 cm^{-1} to 100 cm^{-1}), the **Accumulations** required, and enter a unique **Sample ID** and **Description**.

   By default, sensible values for the scan and instrument parameters are entered in the Instrument Settings toolbar. The **Sample ID** and **Description** are supplied by the Auto-Name function.

   To amend any value, select the parameter and enter your new value.

   NOTE: Spectrum automatically remembers the settings you last used.

3. If required, adjust the **Exposure Time (s)** for your sample.

   You may find it useful to Monitor your sample before scanning to check the Exposure time and laser power are appropriate for your sample.

4. When you are happy with your setup, click  .

   OR

   Select **Scan** from the Measurement menu.

   OR

   If you are using a triggered probe, press the trigger.

   OR

   If you are using the RamanStation 400 Series remote from the PC, press the control button on the instrument.

   If a background is required, it will be collected before the sample scan. The completed spectrum is added to the current Samples View in the Data Explorer.

5. If for any reason you want to stop scanning, click  .

   OR

   Select **Halt** from the Measurement menu.

   If you halt the scan, no data will be saved.

   If you have a motorized stage (some RamanStation 400 Series instruments or Raman microscopes) the data collection will use any Sampling Pattern or Focus options set on the Setup XYZ Stage tab for your instrument.

Additional Information

If you have a motorized stage, you can collect data by adding Markers, Cell Markers, Maps and Line Scans. For details of collecting spectra using these objects, refer to Using Markers, Using Cell Markers, Using Maps and Using Line Scans.

Collecting a Background

If a background scan is required it will be collected before the sample scan, and then the Viewing area is prepared for data collection from your sample.

Detailed Instrument Settings

If you want to amend the detailed instrument settings, use the Setup Raman Instrument dialog.

Triggered Fiber Optic Probe

The Scan options on the Measurement menu and Measurement bar are disabled if you have selected a Triggered Fiber Optic Probe as your accessory on the Setup Instrument Basic tab. The Scan icons are grayed out, and contain a representation of the fiber probe  . A Scan can only be started by pressing the trigger on the probe. Refer to the *Raman Triggered Fiber Optic Probe* leaflet supplied with the probe for configuration and usage details.

Markers, Maps and Line Scans

If you have a motorized stage, you can also collect data using Markers, Maps and Line Scans. See Setup XYZ Stage for more information.

Any shapes added to the Setup Sample Area XYZ tab or Setup Microscope XYZ tab, such as cell markers, markers, maps and lines will be scanned when  is clicked. These will take priority over any samples added to the Sample Table. Samples in the Sample Table will only be run when there are no unmeasured shapes.

Batch Scanning

By default, the instrument settings automatically suggest a name for your samples.

Depending on your instrument, Auto-Name can enable you to collect spectra from one sample after another by using the instrument scan button, providing that you do not need to change the laser power or exposure time between samples. There is no need to return to your PC. This feature is also useful when using accessories that enable you to start and stop scanning remotely from the instrument or when you do not need to change instrument settings between samples.

The Sample Table

You may prefer to setup data collection for a batch of samples in a Sample Table, which enables you to enter meaningful Sample IDs and Descriptions for a specified number of samples before you begin scanning. If necessary, you can amend the Sample Table (by adding, deleting or editing rows) to address any issues that arise during data collection.

Additional Information

- All your spectra are added to a new Samples View.
- Batch scanning does not hinder Previewing data collection on the Live tab before collecting the final spectrum from a sample.

Scanalyze

You can use the Scanalyze command on the Measurement bar to collect a spectrum from a sample or batch of samples and then run a Compare, Search, Quant or Verify analysis as one action.

1. Check and set the instrument parameters, such as the **Start** and **End** points of the scan range (in wavenumbers, such as mid IR 4000 cm^{-1} to 400 cm^{-1} or near IR 10000 cm^{-1} to 4000 cm^{-1}), the **Number of Scans** required, and a unique **Sample ID** and **Description**.

   By default, sensible values for the scan and instrument parameters are entered in the Instrument Settings toolbar; the values applied depend on your instrument and accessory. The **Sample ID** and **Description** are supplied by the Auto-Name function.

   To amend any value, select the parameter and enter your new value.

2. Ensure that the correct process parameters are entered on the appropriate setup tabs.

3. If a background scan is required, the Scan button includes a small background flag. Clear the instrument beam path, or insert a suitable background material, and then click  to collect a background spectrum.

   The background spectrum is displayed briefly, and then the Viewing Area is prepared for data collection from your sample.

   By default, the Measurement bar includes **Scan**, **Halt**, **Background** and **Monitor** buttons.

   You can also select these commands from the Measurement menu.

4. Place your sample in the instrument, click  and then select the process you would like to run.

   OR

   Select **Scanalyze** from the Measurement menu.

   The options are **Scan and Compare**, **Scan and Search**, **Scan and Quant** and **Scan and Verify**.

   During scanning the scan data is displayed on the Live tab in the Viewing Area. The Results pane includes columns for the Sample Name (ID) and Description and additional columns that depend on the results associated with the process selected and the settings defined. You can change the results displayed in the table using the column selector in the top left corner of the table. The results are refreshed during the scan.

   When the scan is completed, the Compare, Search, Quant or Verify tab is displayed. The spectrum is added to the Graph tab in the Viewing Area and to the current Samples View.

   A column selector allows you to choose which results columns are displayed. For Scan and Compare, the Best Hit and the result (Pass/Fail) are displayed by default. For Scan and Search, the Search Best Hit and associated Search Score are displayed by default. For Scan and Quant, the results shown by default depend on the type of Quant Method selected and the settings on the Setup Quant tab. For Scan and Verify, the method name and the specified material are displayed by default with the identified material and, if applicable, the result (Pass/Fail).

5. If, for any reason, you want to stop scanning your sample, click  .

Additional Information

Each process is run using the current setup.

- Before running **Scan and Search**, you will need to set up spectral libraries and search parameters.
- Before running **Scan and Quant**, you will need to set up Quant.
- Before running **Scan and Compare**, you will need to set up compare references.
- Before running **Scan and Verify**, you wil need to add a Verify method.

Monitoring

Monitoring enables you to observe Raman spectra in real time. This allows you to immediately observe the effect of making an adjustment to the Laser power or Exposure time.

- Select **Monitor** from the Measurement menu, or click  .

  The Live tab is displayed in the Viewing area for the current Samples View.

Laser power

- Enter the **Laser power** (%) for your experiment, or adjust using the slider.

  Occasionally, samples may be damaged by the laser. This can be avoided by turning the laser power down.

  The laser power should be determined using a meter if an accurate power value is critical to your experiment.

Exposure time

- Adjust the **Exposure time** for your experiment.

  Adjust the scan time to collect a well-resolved spectrum that maximizes signal quality and minimizes noise. This option is only available if a number of exposures was selected in Accumulations on the Setup Instrument Basic tab.

Additional Information

- To stop monitoring, select **Halt** from the Measurement menu, or click  .
- To stop monitoring and scan the sample, select **Scan** from the Measurement menu, or click  .

Preview

When the Preview option is selected on the Sample Table, and you select **Scan** from the Measurement menu or click  , the Live tab is displayed to help you monitor the scan conditions before initiating data collection.

Triggered Fiber Optic Probe

Monitor is not available if you have selected a Triggered Fiber Optic Probe as your accessory on the Setup Instrument Basic tab. The Monitor icon is grayed out, and contains a representation of the probe  . However, Preview is available. Refer to the *Raman Triggered Fiber Optic Probe* leaflet supplied with the probe for configuration and usage details.

Publishing Results

Publishing Results

These topics describe the editing and printing options that enable you to publish your results.

Once you have processed and formatted your results, you can:

- Use the Send To command on the File menu to send your results to a WordPad or, if installed, a Microsoft® Word document, Microsoft Excel workbook, or TIBCO® Spotfire® data table. You can also send your results as an email attachment.
- Use the Report command on the File menu to output a report.
- Review a Print Preview and Print.
- Copy and Paste from the currently displayed tab in the Viewing Area to another location.

Additional Information

If you prefer to process and format your results outside Spectrum, you can:

- Use a File menu command to Export each spectrum as a comma separated value (*.csv), or JCAMP-DX (*.dx) file.
- Save your spectra as binary (*.sp) or ASCII (*.asc) files.

Send to WordPad or Word

Use the **Send To** command to copy the contents of the Viewing Area into an editable document.

1. Select the tab in the Viewing Area that contains the results or curves that you want to copy.
2. If the tab contains curves, format and label them until you are happy with their presentation.

   All your labels will be copied. If you copy into a Word document your labels are placed in text boxes.
3. Select **Send To** from the File menu, then **Word** or **WordPad**, and then select the document you require.

   The Microsoft® WordPad™ option copies into a rich text format (.rtf) file that you can edit using the WordPad accessory, which is a simple word processing program supplied with Windows XP.

   If Microsoft® Word™ is installed, the Word option copies into a native Word (.doc or .docx) file.

   The document sub-menu enables you to create a new document or to select any WordPad (.rtf) or Word (.doc or .docx) document that is open or minimized on your PC.

   Your results are copied into the selected document.
4. If you created a new document, open the minimized file.
5. Complete and publish your document.

Additional Information

Editable Objects Included in the Document

- When you send the Results Table tab or History tab, today's date is included in your document.
- When you send the Sample Table tab, today's date and the current time is included in your document.
- When you send a curve, the contents of the Results panel are included in your document.

Non-Editable Objects Included in the Document

By default, the Samples View includes the spectrum browser. When you send a graph display the contents of the spectrum browser are included in your document, which acts as a key to the graphic.

If you do not want this information to be included, hide the spectrum browser before sending:

1. Right-click in the Samples View, and then select **Properties**.

   The Graph Properties dialog is displayed.

2. Select the Advanced tab, select the **Hide Information Pane** option, and then click **OK**.

   The spectrum browser or Results pane is hidden.

3. Select **Send To** from the File menu, then **Word** or **WordPad**.

   Your results, but not the contents of the spectrum browser, are copied into the selected document.

4. Restore the Samples View by clearing the Hide Information Pane check box.

Send to Excel

Use the **Send To** command to copy the contents of the Viewing Area into an Excel workbook.

1. Select the tab in the Viewing Area that contains the results that you want to copy.
2. Select **Send To** from the File menu, then **Excel**, and then select the document you require.

   If Microsoft Excel is installed, the Excel option copies into a native Excel (.xls or .xlsx) file.

   The document sub-menu enables you to create a new workbook or to select any Excel workbook that is open or minimized on your PC.

   Your results are copied into new worksheets in the selected workbook. The number of worksheets created will depend on the tab currently displayed.
3. If you created a new worksheet, open the minimized file.
4. Complete and publish your file.

Additional Information

- When you send the Graph tab to Excel, the X and Y data of the spectrum or spectra are added to a new worksheet. Each worksheet is named after the spectrum.
- When you send the Results Table tab to Excel, the Results are added to a new worksheet named Results.
- When you send the Sample Table tab, the Sample Table is added to a new worksheet named Sample Table.
- When you send the Search tab, four worksheets are added to the workbook: Source Spectra Search Results, Search Hit List, and the X and Y data of the sample spectrum and the best hit spectrum. If your Search tab contains multiple source spectra, only the data for the row selected in Source Spectra Search Results will be sent.
- When you send the Compare tab, four worksheets are added to the workbook: Source Spectra Compare Results, List of Compared References, and the X and Y data of the sample spectrum and the best hit spectrum. If your Compare tab contains multiple source spectra, only the data for the row selected in Source Spectra Compare Results will be sent.
- When you send the History tab to Excel, four worksheets are added to the workbook: Sample, Instrument, History and Quality Checks, corresponding to the four sections of the History tab. If no Quality Checks were selected when the sample spectrum was collected, then the Quality Checks worksheet will not be created.

Send to Spotfire

Use the **Send To** command to copy the contents of the Viewing Area into a Spotfire data table.

NOTE: This option is only available if you have TIBCO® Spotfire® installed on your computer.

1. Select the tab in the Viewing Area that contains the results that you want to copy.
2. Select **Send To** from the File menu, and then **Spotfire**.

   Each section of the Viewing Area is displayed in a dialog.
3. Select the set of results you want to view in Spotfire and click OK.

   The results are opened as a new *.dxp file in Spotfire.

Additional Information

The results selected to be sent to Spotfire are temporarily saved as a *.csv file at C:\ProgramData\PerkinElmer\Spectrum\Users\[username]\Spotfire\SendTo. We recommend that you save this file in another location if you want to keep it for use again later.

Send To Email

Before you use the Send To Email command, you will need to define the email settings on the Setup Email tab.

Use the **Send To Email** command to copy the contents of the Viewing Area into an email.

1. Select the tab in the Viewing Area that contains the results or curves that you want to email.

   If the tab contains curves, format and label them until you are happy with their presentation.

   All your labels will be copied. If you copy into a Word document your labels are placed in text boxes.

2. Select **Send To** from the File menu, then **Email**.

   The Send Email dialog is displayed with your results added to the Attachments pane at the bottom of the dialog. The **Total Attachment Size** is shown in megabytes (MB). The **From** field is automatically populated with the User name entered on the Setup Email tab.

3. Enter the recipients email address in the **To** field.

4. If you want to remove any of the attached files, deselect the check box.

   The Total Attachment Size is updated.

5. If you wish to add any further attachments to the email, click **Add Attachments**, and then browse to the file(s) you would like to add.

   The Total Attachment Size is updated.

6. Complete your email message, and then click **Send**.

Additional Information

- If you selected the Samples View tab, you will receive an email with an rtf file attached that contains the spectra in a graph window, and the spectra attached as *.sp files.
- If you select the Graph view of an individual spectrum, the rtf file attached contains the spectrum in a graph window. The spectrum is also attached as an *.sp file.
- If you select the Results tab, the rtf file attached contains the date of the document and the content of the Results Table as a table. The spectra are also attached as *.sp files.
- If you select the History tab for the sample selected, the rtf file attached includes the date, the Sample data, Instrument Settings, History and Quality Checks. The spectrum is also attached as an *.sp file.
- If you select the Compare tab, the rtf file attached includes the user ID, the date of the document, the Compare results, the detail of the spectrum, and the graph display. The spectrum selected in the Compare Results is also attached as an *.sp file.
- If you select the Peak table tab, the rtf file attached includes the user ID, the date of the document, the peak table and the graph display with the peaks marked. The spectrum selected in the Results is also attached as an *.sp file.

Editable Objects Included in the Document

- When you send the Results Table tab or History tab, today's date is included in your document.
- When you send the Sample Table tab, today's date and the current time is included in your document.
- When you send a curve, the contents of the Results panel are included in your document.

Non-Editable Objects Included in the Document

By default, the Samples View includes the spectrum browser. When you send a graph display the contents of the spectrum browser are included in your document, which acts as a key to the graphic.

If you do not want this information to be included, hide the spectrum browser before sending:

1. Right-click in the Samples View, and then select **Properties**.

   The Graph Properties dialog is displayed.

2. Select the Advanced tab, select the **Hide Information Pane** option, and then click **OK**.

   The spectrum browser or Results pane is hidden.

3. Select **Send To** from the File menu, then **Email**.

   Your results, but not the contents of the spectrum browser, are copied into the selected document, which is added to the email.

4. Restore the Samples View by clearing the Hide Information Pane check box.

Send to KnowItAll

Use the **Send To** command to send your spectrum to the KnowItAll application.

1. Select the tab in the Viewing Area that contains the results or curves that you want to send to KnowItAll.
2. Select **Send To** from the File menu, then **KnowItAll**, and then select the option you require from the sub-menu, for example, SearchIt or AnalyzeIt.

Print and Print Setup

Print

Use the **Print** command in the File menu to print a pre-formatted version of the contents of the Viewing Area.

This dialog also enables you to select a specific Printer and its Properties dialog.

Alternatively, if you want to print a graph display, right-click in the Graph tab and then select **Print.**

If you have Spectrum ES, you may be prompted to enter an electronic signature for the Output signature point.

Print Preview

Use the **Print Preview** command in the File menu to review the printed output. The Print Preview dialog enables you to:

- Review a multi-page document.
- Amend the Page Setup, which includes the page Size, Orientation and Margins.
- Zoom in to a particular area of the document, and to use a Snapshot tool to select and copy a detail from the document to the Clipboard as a Windows metafile.

When you have finished reviewing the output, click **Print** from the File menu. This document is sent to your default printer using the current printer settings.

If you have Spectrum ES, you may be prompted to enter an electronic signature for the Output signature point.

Exporting Reports

Reports in Spectrum are generated from templates prepared using PerkinElmer's Report Designer software. You can either prepare these templates in advance or create one when required and use it to generate a report immediately.

1. To generate a multi-spectrum report, select the Samples View name in the Data Explorer.

   OR

   To generate multiple single-spectrum reports, select the Samples View name in the Data Explorer.

   OR

   To generate the report of a single spectrum, select the spectrum name in the Data Explorer.

2. Check the appearance of the data that you will include in the report.

   Depending on the settings in the template you have selected, the appearance of the data in Spectrum may be duplicated in the report.

3. Select **Report** from the File menu.

   The Report dialog opens.

4. Select the Reports Options tab.

5. Select the **Save report** check box if you want to save the report(s).

6. Select **Show saved report** if you want the report(s) to be displayed when generated.

7. Select the **Print report** check box to print the report(s) to the currently active printer.

8. If necessary, click **Browse**, find the template file that you want to use to generate the report, and click **Open**.

   Templates created in Report Designer have a *.tplx filename.

   OR

   Click **Create** and Report Designer will open so that you can create a new template.

   You can also select a template and then click **Edit** if you want to make any changes in Report Designer before you generate a report. Remember to save the template in Report Designer before you generate the report. See the on-screen Help in Report Designer for further details.

   In Spectrum ES, you can also select a template from a list of those used previously in the workspace.

9. Select the type of report(s) you want to generate from the options available.

   The report options available will depend on the items included in the selected template and on the data selected in Spectrum. For example, if the template only contains items related to data for multiple spectra (that is, all the spectra in the Samples View), then the single spectrum report option is disabled. If you have selected a single spectrum name in the Data Explorer in step 1, then the multiple spectra report option is disabled.

   Select the Include option next to the **Samples View Name** if you want to generate a report for all the spectra in the Samples View.

If you selected the Samples View in step 1, select the Include option next to the **Spectrum Name** if you want to generate an individual report for a spectrum. All the spectra are selected by default. To select or deselect all the spectra, check or uncheck the **Select all single spectra reports** option.

10. Select the Report Edit tab.
11. Select the **Report format** from the drop-down list.

    In Spectrum Standard the options are rich text format (*.rtf) and portable document format (*.pdf).

    In Spectrum ES the report is saved in a secured and encrypted portable document format.
12. If necessary, browse to another (or create a new) folder for the generated report(s).

    By default, all reports are saved to C:\pel_data\reports.
13. Select the sections to be included in the report from the **Section Name** list, which are derived from the template.

    To select all or deselect all the possible sections, check or uncheck the **Select all** check box.
14. Click **Report**.

    If you have Spectrum ES, you may be prompted to enter an electronic signature for the Output step.

    The report is generated.

    The filename generated for saved multiple spectra reports is derived from the Samples View name. The file name for an individual spectrum report is derived from the Samples View name and the Sample ID.

    Each time a report file is generated, a number is appended to the name.

    No output will be produced if the file cannot be created.

Additional Information for Spectrum ES

You can only generate reports in Spectrum ES if you have the appropriate permission. Similarly, you can only open Report Designer to create or edit a template if you have the appropriate permission.

You can only select a template if it has the correct status. The acceptable status levels are shown in the drop-down list in the Report Options tab. If you are a user with the appropriate permission, you can change these settings, but otherwise you will only be able to select templates which meet these criteria. The status for each template is shown in the dialog when you click **Browse** to find a template.

Setting Up a Results File for Exporting

A file of accumulated results from each of the main spectral processing functions (Compare, Libraries and Search, MultiSearch, Quant, Adulterant Screen and Verify) can be collected by Spectrum for export as a *.csv file to another software application, such as TIBCO Spotfire, for further analysis.

1. Click the **Setup Results File** tab for the process whose results you want to record in an accumulated result file.

   There is a Setup Results File tab in each set of tabs displayed from the Setup menu or Navigation Pane.

2. Check the **Create results file at this location** checkbox.

3. If required, click **Browse** and select a different location for the result file.

   The file will be named automatically based on the process and, where applicable, the specific method being used to process the data.

4. Choose whether to **Overwrite** the data each time the process is run for a set of samples, or **Append** the new data to the existing data in the file.

Similar files can also be generated using the Setup Results File tab in Ready Checks and Instrument Verification. These collate the results for all the checks performed into a single file, except for Pharmacopoeia tests which are recorded separately.

Once the files have been created and contain some data, you can export them to Spotfire for further analysis (providing you have TIBCO Spotfire installed on your system).

Exporting Data to Spotfire

Use the Export to Spotfire command to export a file of accumulated process or instrument check data to Spotfire, and view the data using a predefined display template.

NOTE: This option is only available if you have TIBCO® Spotfire® installed on your computer.

1. Select **Export to Spotfire** from the File menu.

   The Export to Spotfire dialog is displayed, showing all the data files that are available for exporting to Spotfire.

2. Click the process or instrument check data file that you want to view in Spotfire.

3. If necessary, click **Browse** to browse to another (or to create a new) folder for the exported files.

4. Similarly, select a template file with which to view the data.

   A number of default templates are supplied with Spotfire that are designed for visualizing data from different processes. These can be customized in Spotfire to suit your own needs.

   NOTE: You must enter a valid license number during installation to use these templates.

5. Click **Export**.

   The data file is exported to Spotfire, which automatically opens and displays the data using the selected template.

Additional Information

You can set up data files for exporting to Spotfire using the Setup Results File tabs of Ready Checks, Instrument Verification and each of the main spectral data processing options (Compare, Search, MultiSearch, Quant, Adulterant Screen and Verify). Once a file has been created and contains some data, it is displayed in the Export to Spotfire dialog.

The template files used in Spotfire must have their data linked to the source data file. Open the template file in Spotfire, click **Edit** > **Data Table Properties** and select the **Linked to source** option for storing data in the General tab.

Copying and Pasting

Use the Copy (CTRL+C) keyboard shortcut to place information on the Windows Clipboard, and the Paste (CTRL+V) keyboard shortcut to paste information from the Clipboard into another location.

The behavior of these keyboard shortcuts depends on the type of information that you are copying and pasting. If the keyboard shortcut is not enabled, you may be able to right-click and select a command.

NOTE: If you have Microsoft® Word™, you can manage the clipboard using the Office Clipboard task pane. In Word 2003, select **Office Clipboard** from the Edit menu. In Word 2007, click the Clipboard dialog launcher in the Clipboard group on the Home tab.

Samples View and Graph tab selected

To copy the graph display, including all labels and curves, whether selected or not:

- Right-click and then select **Copy to Clipboard**.

  The CTRL+C shortcut is not enabled.

  NOTE: The graph display is copied as a Windows metafile. You can paste spectra only into Windows applications that support metafiles.

Samples View and Results tab selected

To copy the Name and Description of the selected row:

- Right-click and then select **Copy**.

  OR

  Press CTRL+C.

  A table containing the name and Description is copied.

Spectrum and [Sample Name] tab selected

To copy the graph display of a single spectrum, including all labels:

- Right-click and then select **Copy to Clipboard**.

  The CTRL+C shortcut is not enabled.

  NOTE: The graph display is copied as a Windows metafile. You can paste spectra only into Windows applications that support metafiles.

Spectrum and History tab selected

To copy the data from a panel:

1. Make sure that you have not selected a particular Setting or Value.

   If a Setting or Value is selected, the copy function is not enabled.

2. Right-click in a panel and then select **Copy**.

   OR

   Press CTRL+C.

   Each Settings and Value in the panel is copied as a paragraph with tab separators.

Sample Table selected

To copy a selected field as ASCII text, or the contents of a selected row as tab separated text:

- Right-click and then select **Copy**.

  OR

  Press CTRL+C.

NOTE: You can use the Copy and Paste keyboard shortcuts and commands to help you complete a sample table with multiple rows for collecting spectra from a batch of samples. However, any duplicate Sample ID entries will be shaded pink and cannot be run. Make sure you have entered unique Sample ID entries before collecting data from your samples.