SPECTRUM

User's Guide

PerkinElmer®

Setup Sample Area

If you have a RamanStation 400 Series instrument but do not have an automated stage, you can view the Live Video image from the Sample Area using the Setup Sample Area tab.

1. Select **Raman 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.

2. Select the Setup Sample Area tab.

Live Video

The Live Video view shows the live image from the video camera.

To move the scale bar:

- Click the scale bar with the left mouse button and drag to the new position.

  When you next click **Scan**, the scale bar will return to the default position.

Additional Information

Setup Sample Area Toolbar

Save Image	>	Save image with annotations	Saves the current Live Video image, including the scale bar, cross hairs and any markers, maps or line scans, as a *.bmp or *.jpg.
		Save image without annotations	Saves the current Live Video image as a *.bmp or *.jpg.
Toolbox	>	Align Video with Laser	Allows you to align the Laser and Video camera. This should ideally be performed by a PerkinElmer Service Engineer.

Illumination >	Off Low High	Illumination enables you to control the illumination LEDs on the base of the alignment camera assembly. You have the option to turn them **Off**, switch them to **Low** power, or switch them to **High** power.

Setup Microscope

Use the Setup Microscope tab (RamanMicro 200 Series/RamanMicro 300 Accessory with manual stage) to view the Live Video image from the microscope.

NOTE: The Setup Microscope tab is only available when Microscope is selected as the Accessory on the Setup Instrument Basic tab.

1. Select **Raman Instrument** from the Setup menu.

   OR

   Select  or  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.

2. Select the Setup Microscope tab.

Live Video

The Live Video view shows the live image from the video camera.

To move the scale bar:

- Click the scale bar with the left mouse button and drag to the new position. When you next click **Scan**, the scale bar will return to the default position.

NOTE: If you have a Raman microscope, the Microscope Objective selected on the Setup Instrument Basic tab is displayed next to the scale bar. For the scale bar dimensions to be correct you must ensure that you have selected the current Microscope Objective for your Accessory on the Setup Instrument Basic tab.

Additional Information

Setup Microscope Toolbar

Save > Image	Save image with annotations	Saves the current Live Video image as a *.bmp or *.jpg, with the scale bar.
	Save image without annotations	Saves the current Live Video image as a *.bmp or *.jpg.

Toolbox >	Align Video with Laser	Allows you to align the Laser and Video camera. This should ideally be performed by a PerkinElmer Service Engineer.

Setup Instrument - Data Collection

Use the Setup Instrument Data Collection tab to set up your Background options, enable repeat collections, to set up the Auto-Save option, and to set whether to display the Live tab in the Viewing Area during data collection.

1. Select **Raman Instrument** from the Setup menu.

   OR

   Select  ,  or  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.

2. Select the Setup Instrument Data Collection tab.

Background Collection

Background Collection

If, for example, the Standard Operating Procedures (SOPs) for your laboratory require you to collect a new background spectrum at a specified interval, select the appropriate Background Collection option. Then, as applicable, enter the number of samples after which a new background will be collected (1, by default), or an elapsed time after which a new background will be collected (1 minute, by default).

- As required

  Selected by default, a new background spectrum will not be collected 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 a new background is required by the instrument for some other reason.

- After number of samples

  A new background will be taken after the set number of samples.

- Before each sample point

  A background will be taken before every point in a high-throughput run.

- After elapsed time

  The background will "expire" after the set number of minutes. If a scan is in progress when the time runs out, it will be completed and a new background taken before starting the next collection.

Background Exposures

We recommend that you set the Background Exposures to **As samples** to reduce noise in the final spectrum. This collects that same number of background exposures as sample exposures.

If collection time is important, then a smaller **Specific number** of backgrounds can be acquired. Setting fewer background exposures than sample exposures will result in higher noise in the final spectrum. When using a smaller number of backgrounds, it is highly recommended that you use a value of more than 1 to avoid cosmic ray corruption in the background and thus in all collected spectra taken using that background.

Auto Processing

When selected, spectral processing options are applied to all spectra immediately after the scan. The raw data is not saved.

Baseline Correction

When you select **Baseline Correction**, the software will automatically correct the baseline of all collected spectra, resulting in a smooth horizontal baseline. Automatic baseline correction can be useful when your sample exhibits fluorescence.

Auto-Subtract Spectrum

When you select **Auto-Subtract Spectrum**, you can click the **Browse** button and then navigate to the spectrum file (.sp) that you want to subtract from all collected spectra.

Repeat Collections

NOTE: Repeat collections are not available for any shapes added to the Setup Sample Area XYZ Stage tab or Setup Microscope XYZ Stage tab, such as cell markers, markers, maps and lines.

This function allows the collection to be repeated for a fixed number of times, and can be very useful in, for example, reaction monitoring applications. The various options are:

- Single collection
- Repeat collections

  Enter the required number. If you select this option, **Cycle time** will become available.
- Cycle time

  When running **Repeat collections**, you can specify a delay between collections. For example, you may want a 10 second collection every minute. The delay is the time between the start of each collection and is NOT a delay between the end of one collection and the start of the next. This allows accurate and predictable start times for each collection.

NOTE: If the collection takes longer than the delay between collections (for example, if you attempt a 30 second collection every 30 seconds which will overrun due to the processing time of the collection) the cycle time is not achievable. An error message will be displayed during the scan and the data collection will stop. The Background Collection options can have an impact on the length of a data collection.

General Settings

Show Live Display

By default, the Viewing Area displays your spectrum on the Live tab during scanning. Once the spectrum has been collected, the spectrum is displayed in the tab.

If you prefer not to see the Live tab, deselect this option.

Auto-Save Options

Select **Save after each measurement** to automatically save each spectrum as it is collected, and then define the **Save Location** for all spectra. The default is C:\pel_data\spectra. Deselect this option if you want to explicitly select the spectra you want to save yourself.

NOTE: If you modify the default Save Location on the Setup Instrument Data Collection tab, then the Save Location on the Sample Table tab is also updated.

NOTE: In Spectrum ES, spectra are not saved to disk until the workspace is signed.

Select **Export** to automatically save each spectrum to the **File Format** selected in the drop-down lists. Then define the **Save Export Location**. The default Save Export Location is C:\pel_data\export. Deselect this option if you want to explicitly select the spectra you want to export yourself.

The File Formats available are Comma Separated Values (.csv), JCAMP-DX (.DX), ASCII (.ASC) and Custom Defined Format.

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). Custom Defined Format uses the settings defined on the Setup Export tab.

If you select a folder that you do not have write permissions for, or if the location maps to an external drive or network location that is no longer available, after the scan has completed an error message will be displayed saying the data could not be saved. The spectrum will be added to a Samples View in the Data Explorer, so you can save the spectrum file or export the data to a different location.

If you enter a folder location that does not exist, but in a location you have write permission for, when the scan has completed the folder will be created and the file saved to that location.

If you have Spectrum ES you may be prompted for an electronic signature for the Data Export Collection signature point before the data is exported.

Setup Instrument - Auto Name

Use the Setup Instrument Auto Name tab to set up a template for the Auto Name and Auto Description functions. These functions automatically enter names and descriptions for your samples.

1. Select **Raman Instrument** from the Setup menu.

   OR

   Select  ,  or  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.

2. Select the Setup Instrument Auto Name tab.

Auto-name

Enter an auto-name format for your samples using a mixture of text and placeholders for variables. When you want to insert a placeholder, select the variable you need from the drop-down list.

The list of available variables enables you to include the date in several formats, your User Name or User ID, and to identify both the instrument and computer. You can also enter a Barcode.

The most important variable is Counter, placeholder [nnn]. This counter is incremented by 1 for each subsequent sample, which enables you to distinguish one sample from the next.

An example sample name enables you to check that your auto name format is correct.

Auto-description

Enter an auto-description format for your sample using a mixture of text and placeholders for variables in the same manner as for an auto name format.

An example description enables you to check that your auto-description format is correct.

Setup Ready Checks

A Ready Check demonstrates that an aspect of the performance of your complete system, including sampling accessory, is fit-for-purpose. Ready checks provide a test for wavenumber precision and a check on noise, throughput and contamination. You can also verify that a Quant method is behaving as expected with your system.

Invoke a Ready Check from the Instrument Checks sub-menu in the Measurement menu.

Use the Setup Ready Checks tabs to set up the reporting options for Ready Checks and to set up a Ready Check.

1. Select **Ready Checks** from the Setup menu.

   OR

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

   The Ready Checks tabs are displayed in the Dialog Pane.

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

2. Select the Setup Abscissa Check tab, the Setup Noise Check tab, the Setup Throughput Check tab, the Setup Contamination Check tab, the Setup Quant Control Check tab, or the Setup Ready Checks tab.
3. Use the Setup Results File tab to configure a file of accumulated data for exporting to another software application for further data analysis.

Setup Ready Checks tab

Ready Checks	Select the Ready Checks that you would like to run when Check All is selected from the Ready Check list. The options are **Abscissa**, **Noise**, **Throughput**, **Contamination** and **Quant Control**.
Sampling	Select **Sample Area** to perform the checks using a reference sample placed by the user in the sample area. Select **Internal APV** to use the internal APV filter, located in the filter wheel, automatically inserted into the beam path. **NOTE:** If your instrument has an internal, automated filter wheel, but the beam path does not pass through it in the current configuration, the Sampling Option will be set to Sample Area. Internal APV will not be available until the beam path is directed through the filter wheel. If your instrument does not have an internal filter wheel, the Sampling options are not displayed. The Ready Checks use a reference sample placed by the user in the sample area. The spectrometer is supplied with a polystyrene reference card.

Report	Select the **Show report automatically** option to display a print preview of the Instrument Ready Checks Report (Filename: …\[date]\[instrument serial number][instrument name]_[Ready Check name]_Log([n]).rtf) automatically. Select the **Print report automatically** option to send the Instrument Ready Checks Report to your default printer automatically.
Spectra and Log Files	Browse to and select the folder where the spectra and log files created by your ready checks should be stored. The spectra and log files created by your ready checks are stored by default in C:\pel_data\Ready Checks\[date]. The spectra are saved with the filename …\[date]\[instrument serial number][instrument name]_[Ready Check name]([n]).sp. The background spectra are saved with the filename …\[date]\[instrument serial number][instrument name]_[Ready Check name]_Background([n]).sp
Load and Save...	Click this button to open the Ready Check Settings dialog. From this dialog, you can add the Ready Check Setup for the instrument you are using by clicking the **Save current settings** button. To save the Ready Check Setup (*.rcset) file to a folder on your PC, click **Export...**, select a filename and a location, and click **Save**. Click **Import...** to add a previously saved Ready Check Setup file to the list in the dialog, and click **Delete** to remove entries from the list. You can change the current settings by highlighting an entry in the list and clicking **Set as current**. This will be the setup that is used when Ready Checks are run from the Process menu. Click **Close** to close the dialog.

Additional Information

A documented Ready Check can be an element of the System Suitability checking required for regulatory compliance in some industries.

When you create a Ready Check, it is specific to the current instrument configuration. This configuration includes the instrument name, the instrument serial number, the current source, the current beamsplitter, the current detector, and the accessory name and part number. However, if you have manually selected a sampling configuration in the Accessory table on the Setup Instrument Basic tab, the setup being created will now be specific to that sampling configuration.

You can set up the Ready Checks to use the Automatic Precision Validator (APV) that is built into the instrument (if available). You can also use a reference sample placed in the accessory manually. This external reference standard can be either the polystyrene sample from an Instrument Performance Validation kit or your own standard. The polystyrene film in the APV is primarily intended for testing that the instrument is performing consistently, rather than for calibrating the wavenumber (abscissa) scale.

When deciding what tolerances to set for the Ready Checks, consideration should be given to the definition of fit-for-purpose for the individual application.

Setup Contamination Check

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.

1. Select **Ready Checks** from the Setup menu.

   OR

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

   The Ready Checks tabs are displayed in the Dialog Pane.

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

2. Select the Setup Contamination Check tab.

Setup Contamination Check tab

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.

NOTE: If you have a Spotlight 150, reference spectra must be collected with the apertures in the Validation Position.

To set up the contamination check for a particular instrument configuration and sample type, examine a typical sample spectrum, and select up to three strongly absorbing characteristic peaks. For each peak, place a check mark in the **Include** box, enter the **Start** and **End** wavenumber for the range in which the peak occurs, and then enter a value for **Nominal** absorbance (an expected value arising from noise or acceptable trace contamination) and for the absorbance **Limit** (beyond which the contamination check fails).

The default Nominal and Limit values are not indicative of values acceptable for your application. For example, you may need to set lower limits to avoid any cross-contamination between samples, or to avoid leaving any trace of a toxic material on the sampling accessory.

Additional Information

To set up the reporting options for your Ready Check, see Setup Ready Checks.

Setup Quant Control Check

Quant Control Check is a ready check that enables you to verify your system (Quant method, instrument and accessory) is performing as expected.

You can enter the known concentration of the control sample, and set a tolerance value for the result. The Quant Control Check collects the spectrum of the control sample and calculates the concentration using your chosen Quant method. If the result is within the tolerance limit, the control check will pass.

NOTE:	Only Quant+ and Beer's Law methods are supported.

1. Select **Ready Checks** from the Setup menu.

   OR

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

   The Ready Checks tabs are displayed in the Dialog Pane.

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

2. Select the Setup Quant Control tab.

Setup Quant Control Check tab

Quant Type	Select the **Quant Type** from **Quant+** and **Beer's Law**. The default is Quant+.
Quant Method	Browse to or type the filename and path of the Quant method that will be used for the Quant prediction. Quant+ methods have .md File name extensions. Beer's Law methods have .uqm file extensions.
Component	Select the Component that the Quant Control Check will test for. The component(s) listed will depend on the Quant method.
Nominal Value	Enter the concentration of the control sample.
Tolerance (±)	Set the tolerance in the Nominal Value.
Pathlength	Enter the Pathlength or the Normalization Factor for your analysis. This is only enabled if used in your Quant method. You can select to **Enter the Pathlength Manually**. The default is 1. Or, if **Enable pathlength** is selected on the Setup Pathlength tab, you can select to use the global **Pathlength Defined in Setup**. Refer to the Setup Pathlength tab for details.
Bias Correction	If the Quant+ method contains independent validation data, Bias Correction will be available. Select **None**, **Offset** or **Offset and slope**. If none of the Quant+ methods selected contains independent validation

	data, then the Bias Correction will not be available.

Additional Information

To set up the reporting options for your Ready Check, see Setup Ready Checks.

Setup Noise Check

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 (%T/cm-1)**.

1. Select **Ready Checks** from the Setup menu.

   OR

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

   The Ready Checks tabs are displayed in the Dialog Pane.

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

2. Select the Setup Noise Check tab.

Setup Noise Check tab

Enter the **Start (cm-1)** and **End (cm-1)** wavenumber for the range over which you wish the noise to be measured. For each statistic you wish to calculate, place a check mark in the **Include** box, and then enter a value for **Nominal** absorbance (an acceptable value arising from noise) and for the absorbance **Limit** (beyond which the noise check fails).

The default Nominal and Limit values are not indicative of values acceptable for your application. The values entered in the nominal and limit columns must be determined experimentally by you, using the accessory/sampling configuration defaults.

We recommend that you perform a series of tests several times over several days, to take into account variation in ambient temperature, length of time that the instrument has been switched on, humidity and other variables. Use these values to calculate the limits and nominal values for the check.

NOTE:	When you set the limit for the noise **Trend**, enter a positive number. This limit is applied independent of the direction of the slope.

Additional Information

To set up the reporting options for your Ready Check, see Setup Ready Checks.

Setup Abscissa Check

Abscissa Check is a ready check that enables you to validate the wavenumber precision.

1. Select **Ready Checks** from the Setup menu.

   OR

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

   The Ready Checks tabs are displayed in the Dialog Pane.

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

2. Select the Setup Abscissa Check tab.

Setup Abscissa Check tab

This enables you to set the **Nominal** abscissa value and **Lower** and **Upper** limits for the positions of up to three peaks measured in the abscissa test. For each peak position you wish to calculate, place a check mark in the **Include** box.

You can select the algorithm that is used to calculate the peak position from **Interpolated Peak** and **Center of Gravity**.

During the abscissa test, a spectrum is collected, and the wavenumber is measured at the specified peaks. If the measured wavenumber at each peak is within the upper and lower limits for that peak, the test passes.

Additional Information

If you intend to perform routine validation using internal reference materials, choose three peaks from the third column of the Certificate of Performance Validation (supplied with the optional IPV kit) as nominal reference values. For MIR, we recommend that you use the three peaks at nominally 3060.14, 1601.38 and 1028.42 cm^{-1}. As a guide for analytical applications involving the use of liquids and solids, ±0.5 cm^{-1} might be an appropriate tolerance.

NOTE: Peaks in the spectrum of polystyrene above 1800 cm^{-1} are broader than most of the peaks below 1800 cm^{-1}, and may therefore show more variation for a given noise level. The peaks at 1943 and 1802 cm^{-1} are subject to interference by water vapor and should not be used.

For NIR, we recommend that you use the peaks at 5669.3 cm^{-1} and 4571.6 cm^{-1}. As a guide for analytical applications involving the use of liquids and solids, ±1.5 cm^{-1} or ±1.0 cm^{-1} might be an appropriate tolerance.

Differences in temperature and beam geometry at the internal and sample compartment positions may give different peak positions. It is therefore important that routine Ready Checks are always performed using the sample position used for this calibration.

Spectra collected using the APV give peaks 10 cm^{-1} or more wide; the peak positions can be consistently measured to ±0.1 cm^{-1}, provided that the noise level is low enough.

The Interpolated Peak algorithm calculates peak position from maximum intensities. The Center of Gravity algorithm, used by the National Institute of Standards and Technology (NIST), calculates peak position from the shape of the peak. When using the Center of Gravity algorithm, the Peak Height which defines how much of a peak is used when calculating its center of gravity, is set to 0.5.

To set up the reporting options for your Ready Check, see Setup Ready Checks.

Setup Throughput Check

The Throughput check enables you to check for unexpected reduction of the transmittance, for example, as a results of fogged cell windows.

1. Select **Ready Checks** from the Setup menu.

   OR

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

   The Ready Checks tabs are displayed in the Dialog Pane.

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

2. Select the Setup Throughput Check tab.

Setup Throughput tab

This enables you to set the **Nominal** ordinate value and the **Lower Limit** at up to three abscissa positions. For each abscissa position you wish to measure at, place a check mark in the **Include** box. During the throughput test, the ordinate value is measured at the specified abscissa positions. If the measured ordinate value is above the lower limit, the test passes.

You need to **Import** a Reference Background spectrum in Energy units for the current instrument and accessory combination.

The values entered in the Nominal and Lower Limit columns must be determined experimentally by you, using the accessory/sampling configuration defaults.

We recommend that you perform a series of tests several times over several days, to take into account variation in ambient temperature, time that the instrument has been switched on, humidity and other variables. Use these values to calculate the limit and nominal values for the test.

Additional Information

To set up the reporting options for your Ready Check, see Setup Ready Checks.

Setup Instrument Verification

Instrument Verification is the procedure of demonstrating that your instrument is functioning correctly. When you create an instrument verification check, it is specific to the current instrument configuration. This configuration includes the instrument name, the instrument serial number, the current source, the current beamsplitter, and the current detector. Therefore, where the accessory includes a detector, such as the NIRA II/NIRM or the Fiber Optic Probe, the accessory should be installed for the test.

Use the Setup Instrument Verification tabs to set up the reporting options for Instrument Verification and to set up an Instrument Verification check.

1. Select **Instrument Verification** from the Setup menu.

   OR

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

   The Instrument Verification tabs are displayed in the Dialog Pane.

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

2. Select the Setup Instrument Verification tab, the Setup ASTM Level 0 Check tab, the Setup Noise Check tab, the Setup Ordinate Check tab, the Setup Abscissa Check tab or the Setup Pharmacopoeia Test tab (if available).
3. Use the Setup Results File tab to configure a file of accumulated data for exporting to another software application for further data analysis.

Setup Instrument Verification tab

Instrument Checks	Select the Instrument Checks that will be made when the Instrument Verification is run. The options are **Abscissa**, **Ordinate**, **Noise**, **ASTM (E1421-99) Level 0 (for MIR)** or **ASTM (E1944-98) Level 0** (for NIR) and **MIR Pharmacopoeia** (for MIR) or **NIR Pharmacopoeia** (for NIR). If **MIR Pharmacopoeia** or **NIR Pharmacopoeia** is selected, then select the pharmacopeia tests that you would like to run from the drop-down list.
Sampling	Select **Internal APV** to use the internal APV filter, located in the filter wheel, which is automatically inserted into the beampath. Select **Sample Area** to perform the instrument checks using a reference sample placed by the user in the sample area. **NOTE:** If your instrument has an internal, automated filter wheel, but the beam path does not pass through it at the current configuration, the Sampling option will be set to Sample Area. Internal APV will not be available until the beam path is redirected through the filter wheel.

	If your instrument does not have an internal filter wheel the Sampling options are not displayed. The ready checks use a reference sample placed by the user in the sample area. The spectrometer is supplied with a polystyrene and a Schott NG11 reference card. **NOTE:** Instrument Verification tests for a NIRA II/NIRM are performed with the NIRA II/NIRM in the Upper position, so it is important to have the Spectralon reference in position on the sample area or on top of any reference material placed on the sample area.
Report	Select the **Show report automatically** option to display a print preview of the Instrument Verification Report automatically. Select the **Print report automatically** option to send the Instrument Ready Checks Report to your default printer automatically. The report is saved with the filename …\[date]\[instrument serial number][instrument name]_[instrument verification check name]_Log([n]).rtf)
Spectra and Log Files	Browse to and select the folder where the spectra and log files created by your Instrument Verification checks should be stored. The spectra and log files created by your instrument verification checks are stored by default in C:\pel_data\Instrument Verification\[date]. The spectra are saved with the filename …\[date]\[instrument serial number][instrument name]_[Instrument verification test name].sp.

Additional Information

To setup up each instrument verification check, refer to the appropriate setup tab. See also, Instrument Verification for details of running the Instrument Verification procedure.

If you have Spectrum ES, to open the secured rich text format log file (*.srtf), select the **Open ES Report** option from the File menu and browse to and select the file. A *.rtf file will be created in the folder.

Setup Noise Check

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 (%T/cm-1)**.

1. Select **Instrument Verification**.

   OR

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

   The Instrument Verification Checks tabs are displayed in the Dialog Pane.

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

2. Select the Setup Noise Check tab.

Setup Noise Check tab

Enter the **Start (cm-1)** and **End (cm-1)** wavenumber for the range over which you wish the noise to be measured. For each statistic you wish to calculate, place a checkmark in the **Include** box, and then enter a value for **Nominal** absorbance (an acceptable value arising from noise) and for the absorbance **Limit** (beyond which the noise check fails).

The default Nominal and Limit values are not indicative of values acceptable for your application. The values entered in the nominal and limit columns must be determined experimentally by you, using the accessory/sampling configuration defaults.

We recommend that you perform a series of tests several times over several days, to take into account variation in ambient temperature, length of time that the instrument has been switched on, humidity and other variables. Use these values to calculate the limits and nominal values for the check.

NOTE:	When you set the limit for the noise **Trend**, enter a positive number. This limit is applied independent of the direction of the slope.

Additional Information

To set up the reporting options for your Instrument Verification Check, see Setup Instrument Verification.

Setup Abscissa Check

Abscissa Check is an Instrument Verification Check that enables you to validate the wavenumber precision.

1. Select **Instrument Verification** from the Setup menu.

   OR

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

   The Instrument Verification Checks tabs are displayed in the Dialog Pane.

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

2. Select the Setup Abscissa Check tab.

Setup Abscissa Check tab

This enables you to set the **Nominal** abscissa value and **Lower** and **Upper** limits for the positions of up to three peaks measured in the abscissa test. For each peak position you wish to calculate, place a checkmark in the **Include** box.

You can select the algorithm that is used to calculate the peak position from **Interpolated Peak** and **Center of Gravity**.

During the abscissa test, a spectrum is collected, and the wavenumber is measured at the specified peaks. If the measured wavenumber at each peak is within the upper and lower limits for that peak, the test passes.

Additional Information

If you intend to perform routine validation using internal reference materials, choose three peaks from the third column of the Certificate of Performance Validation (supplied with the optional IPV kit) as nominal reference values. For MIR, we recommend that you use the three peaks at nominally 3060.14, 1601.38 and 1028.42 cm^{-1}. As a guide for analytical applications involving the use of liquids and solids, ±0.5 cm-1 might be an appropriate tolerance.

NOTE:	Peaks in the spectrum of polystyrene above 1800 cm^{-1} are broader than most of the peaks below 1800 cm^{-1}, and may therefore show more variation for a given noise level. The peaks at 1943 and 1802 cm^{-1} are subject to interference by water vapor and should not be used.

For NIR, we recommend that you use the peaks at 5669.3 cm^{-1} and 4571.6 cm^{-1}. As a guide for analytical applications involving the use of liquids and solids, ±1.5 cm^{-1} or ±1.0 cm^{-1} might be an appropriate tolerance.

Differences in temperature and beam geometry at the internal and sample compartment positions may give different peak positions. It is therefore important that routine Instrument Validation Checks are always performed using the sample position used for this calibration.

Spectra collected using the APV give peaks 10 cm^{-1} or more wide; the peak positions can be consistently measured to ±0.1 cm^{-1}, provided that the noise level is low enough.

The Interpolated Peak algorithm calculates peak position from maximum intensities. The Center of Gravity algorithm, used by the National Institute of Standards and Technology (NIST), calculates peak position from the shape of the peak. When using the Center of Gravity algorithm, the Peak Height which defines how much of a peak is used when calculating its center of gravity, is set to 0.5.

To set up the reporting options for your Instrument Verification Checks, see Setup Instrument Verification.

Setup Ordinate Check

Abscissa Check is an Instrument Verification Check that enables you to validate the %T repeatability

1. Select **Instrument Verification.**

   OR

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

   The Instrument Verification Checks tabs are displayed in the Dialog Pane.

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

2. Select the Setup Ordinate Check tab.

Setup Ordinate Check tab

This enables you to set the **Nominal (%T)** ordinate value and **Lower Limit (%T)** and **Upper Limit (%T)** for the ordinate value at up to three abscissa positions. For each peak position you wish to calculate, place a checkmark in the **Include** box.

During the ordinate test, the ordinate value is measured at the specified abscissa positions. If the measured ordinate value is within the upper and lower limits, the test passes.

The values entered in the **Nominal** column must be determined experimentally by you, using the chosen instrument validation setup. We recommend that you perform a series of tests several times over several days, to take into account variation in ambient temperature, time that the instrument has been switched on, humidity and other variables. Use these values to calculate the limits and nominal values for the check.

Additional Information

In the MIR, the reference material for the ordinate check is Schott NG11 glass and the default abscissa positions are 3990 cm^{-1}, 3030 cm^{-1} and 200 cm^{-1}. In the NIR, the reference material for the ordinate check is polystyrene and the default abscissa positions for the ordinate check are 5669.3 cm^{-1} and 4571.6 cm^{-1}. The ordinate check spectrum can be collected using the appropriate filter in the filter wheel (Internal APV) or by inserting a reference in the sample area. See Setup Instrument Verification to set up the sampling type and the reporting options for your Instrument Verification Check.

If your instrument does not have an internal, automated filter wheel, use the Schott NG11 glass reference material is supplied with the instrument.

Schott NG11 glass

The sample provided for testing the ordinate performance is a piece of Schott NG11 glass with a nominal thickness of 1 mm. This is a very stable material, and has a series of broad spectral features with transmission between 70% and 0%. It can be used for checking that the instrument is performing consistently, but not for testing the accuracy of the transmittance scale, because accurate values for the transmittance of the glass sample are not available.

Setup ASTM Level 0 Check

When you create an ASTM test, it is specific to the current instrument configuration. This configuration includes the instrument name, the instrument serial number, the current source, the current beamsplitter, and the current detector. Therefore, where the accessory includes a detector, such as the NIRA II/NIRM or the Fiber Optic Probe, the accessory should be installed for the test.

ASTM Level Zero tests in the FT-IR range follow ASTM Designation E1421-99, titled "Standard Practice for Describing and Measuring Performance of Fourier Transform Infrared (FT-IR) Spectrometers: Level Zero and Level One Tests".

ASTM Level 0 tests in the FT-NIR range follow ASTM Designation E1944-98, titled "Standard Practice for Describing and Measuring Performance of Fourier Transform Near-Infrared (FT-NIR) Spectrometers: Level Zero and Level One Tests".

NOTE:	ASTM Level 0 tests are not defined for the FIR range.

1. Select **Instrument Verification** from the Setup menu.

   OR

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

   The Instrument Verification Checks tabs are displayed in the Dialog Pane.

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

2. Select the Setup ASTM Level O Check tab.

Setup ASTM (E1421-99) Level 0 Check tab

Set up the filename and path to the two reference spectra you wish to use for the ASTM E1421-99 tests.

The ASTM E1421-99 Level 0 tests are intended for the open beam instrument operating in the MIR range with a Sample Slide. Two reference spectra should be collected under the instrument conditions that will be used for each sampling configuration. Collect a single-beam energy spectrum (background) spectrum and a transmittance spectrum of a polystyrene sample named as, for example, Reference Background.sp and Reference Polystyrene.sp, respectively.

Then, during the ASTM Level Zero tests, spectra will be recorded and compared to the reference spectra.

The scan range should be at least 4050 to 150 cm-1 at a resolution of 4 cm-1. The ASTM method recommends scanning for 30 seconds, which with the TGS detector at the default scan speed of 0.2, is about 5 scans.

NOTE:	ASTM checks should be performed with CO2/H2O suppression switched off, so the reference spectra must be collected the same way. Ensure that **CO2/H20** is not selected on the Setup Instrument Advanced tab.

NOTE:	If you have a Spotlight 150, reference spectra must be collected with the apertures in the Validation Position.

The same polystyrene sample that is used to collect the polystyrene reference spectrum must be used when performing ASTM Level Zero tests, in the same sample position and orientation. The polystyrene spectrum can be collected using the polystyrene in the filter wheel (Internal APV), if available, or a polystyrene sample in the sample area. See Setup Instrument Verification to set up the sampling type.

Setup ASTM (E1944-98) Level 0 Check tab

Set up the filename and path to the two reference spectra you wish to use for the ASTM. Two reference spectra should be collected under the instrument conditions that will be used for each sampling configuration. Then, during the ASTM Level Zero tests, spectra will be recorded and compared to the reference spectra.

ASTM NIR in Transmission

The ASTM E1944-98 Level 0 tests in transmission are intended for the open beam instrument operating in the NIR range with a Sample Slide. Collect a single-beam energy spectrum (background) and a transmittance spectrum of a reference sample named as, for example, Energy Reference.sp and Check Sample Reference.sp, respectively.

The scan range should be at least 12550 to 3950 cm^{-1} at a resolution of 4 cm^{-1}. The ASTM method recommends scanning for 30 seconds, which with the TGS detector at the default scan speed of 0.2, is about 5 scans.

NOTE: ASTM checks should be performed with CO2/H2O suppression switched off, so the reference spectra must be collected the same way. Ensure that **CO2/H20** is not selected on the Setup Instrument Advanced tab.

NOTE: If you have a Spotlight 150, reference spectra must be collected with the apertures in the Validation Position.

The same reference sample that is used to collect this check sample reference spectrum must be used when performing ASTM Level Zero tests, in the same sample position and orientation. ASTM E1944 does not specify polystyrene, but the check sample reference spectrum can be collected using the 1.2 mm thick polystyrene film in the filter wheel (Internal APV), if available, or a 1.2 mm thick polystyrene sample card in the sample area. See Setup Instrument Verification to set up the sampling type.

ASTM NIR in Reflectance

The ASTM E1944-98 Level 0 tests in reflectance are used by spectrometers in the NIR mode with a NIRA II/NIRM or with the Fiber Optic Probe (FOP). Collect a energy reference spectrum collected using the open beam and a spectrum of a reference material collected using the sample area. The spectra could be named, for example, NIRA II/NIRM Energy Reference.sp and NIRA II/NIRM Check Sample Reference.sp, respectively.

The scan range should be at least 12550 to 3950 cm^{-1} at a resolution of 4 cm^{-1}. The ASTM method recommends scanning for 30 seconds, which with the TGS detector at the default scan speed of 0.2, is about 5 scans. However, for the NIRA II/NIRM or the FOP the default scan speed is 1.0, which corresponds to 26 scans in 30 seconds.

NOTE: ASTM tests are performed with CO_2/H_2O suppression switched off, so the reference spectra must be collected the same way. Ensure that **CO2/H20** is not selected on the Setup Instrument Advanced tab.

The same reference sample that is used to collect this check sample reference spectrum must be used when performing ASTM Level Zero tests, in the same sample position and orientation. ASTM E1944 recommends that a suitable reflectance material is used, for example, NIST SRM 1920. Internal APV is not really suitable for this text. See Setup Instrument Verification to set up the sampling type.

Additional Information

If the source, detector, beamsplitter or power supply is changed in your instrument, you must collect new reference spectra for subsequent ASTM Level Zero tests.

ASTM Designation E1421-99 and ASTM Designation E1944-98 are available from ASTM at:

American Society for Testing and Materials

100 Barr Harbor Drive

West Conshohocken

PA 19428

USA.

www.astm.org

Setup Pharmacopoeia Tests

The Setup Pharmacopoeia Test tab enables you to select pre-defined tests for the verification of your instrument performance to comply with the protocols specified in the British, Chinese, European, Indian, Japanese and United States pharmacopoeias. In addition, you can set up some generic tests based on these protocols that you can modify for your requirements.

To view the tab, you must have enabled the pharmacopoeia option in the Instrument Checks section of the Setup Instrument Verification tab.

The content of the Pharmacopoeia Test tab will depend on the Pharmacopoeia test selected from the drop-down list on the Setup Instrument Verification tab.

The validation tests are specific to the current instrument configuration: instrument type, the current source, the current beamsplitter, and the current detector.

1. Select **Instrument Verification** from the Setup menu.

   OR

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

   The Instrument Verification Checks tabs are displayed in the Dialog Pane.

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

2. Select the Setup Instrument Verification tab.
3. Select **MIR Pharmacopoeia** or **NIR Pharmacopoeia**.

   The option displayed will depend on the instrument you are connected to: MIR Pharmacopoeia for an MIR-range instrument or a dual-range instrument set to MIR mode; NIR Pharmacopoeia for an NIR-range instrument or a dual-range instrument set to NIR mode.
4. Select the test you would like to run from the drop-down list.

   The options for MIR are **Generic MIR Tests**, **European Tests**, **British Tests**, **Chinese Tests**, **Indian Tests** and **Japanese Tests**.

   The options for NIR are **Generic NIR Tests**, **United States Tests** and **Indian Tests**.
5. Select the Setup Pharmacopoeia Test tab.

   The tab is displayed. Within the tab, individual tabs are displayed for each test required by the pharmacopoeia. Refer to the table below for details of which tests are run for each pharmacopoeia.
6. For each test you would like to run, select the **Enable** check box on the tab.

   For the generic tests, all the tests are disabled by default. For the other options, all the tests are enabled by default.
7. If you selected Generic MIR or Generic NIR, select the additional options available, as described for the individual tests below.

MIR Tests

The MIR tests available are:

Pharmacopoeia	Resolution performance	Wavenumber Verification	Repeatability	Ordinate Units	Film Thickness
Generic	Yes	Yes	Yes	A/%T	–
European	Yes	Yes	No	A	35 μm
British	Yes	Yes	No	A	35 μm
Indian	Yes	Yes	No	A	35 μm
Japanese	Yes	Yes	Yes	%T	0.04 mm
Chinese	Yes	Yes	Yes	%T	0.04 mm

The default settings for each pharmacopoeia test will reflect those specified in the standard.

Resolution Performance

In the Resolution Performance test the spectrum of a polystyrene film of known thickness is collected over the wavelength range 4000–400 cm^{-1}.

In the Generic MIR tests, you can select the Ordinate units (A or %T), add rows to the table to add further peaks, and specify the peak positions and the minimum peak height.

To select which peaks will be included when the tests are run, select the **Include** check box for each row of the table.

If you selected Internal APV as the sampling option on the Setup Instrument Verification tab, the polystyrene filter in the internal filter wheel will be used for the test, but you should refer to the appropriate pharmacopoeia for the thickness specified.

A summary of the resolution performance tests for each pharmacopoeia included in Spectrum is given in the table below:

Pharmacopoeia	**Requirement 1**	**Requirement 2**
European/British/Indian	The difference between an absorption minimum at 2870 cm^{-1} and an absorption maximum at 2849.5 cm^{-1} must be greater than 0.33 A.	The difference between an absorption minimum at 1589 cm^{-1} and an absorption maximum at 1583 cm^{-1} (the minimum peak height) must be greater than 0.08 A.
Japanese	The depth of the trough from the maximum absorption at about 2850 cm^{-1} to the minimum at about 2870 cm^{-1} should be not less than 18% transmittance.	The depth of the trough from the maximum absorption at about 1583 cm^{-1} to the minimum at about 1589 cm^{-1} should be not less than 12% transmittance.
Chinese	The depth of the trough from the maximum absorption at about 2851 cm^{-1} to the minimum at about 2870 cm^{-1} should be greater than 18% transmittance.	The depth of the trough from the maximum absorption at about 1583 cm^{-1} to the minimum at about 1589 cm^{-1} should be greater than 12% transmittance.

The Chinese Pharmacopoeia also requires that seven peaks should be clearly resolved in the range 3110–2850 cm^{-1}, and that the nominal resolution of the instrument should be not less than 2 cm^{-1}.

During the test a background spectrum and a polystyrene sample spectrum will be collected. A log file is generated showing the results of the test that includes the sample spectrum and a table of the results. The spectra and log file are stored in the location specified on the Setup Instrument Verification tab.

CAUTION:	The Japanese and Chinese Pharmacopoeia (and Generic %T) resolution tests involve measuring the difference between two transmittance values. Because of this, the outcome of the test depends on the baseline level of the spectrum. Polystyrene samples for use as infrared standards have roughened faces to prevent the appearance of interference fringes, and scattering from these surfaces introduces a baseline offset to the spectrum. To avoid this spurious contribution to the resolution result, the test spectrum is baseline-corrected prior to the resolution calculation. A single baseline point at 2050 cm^{-1} is used for this process.

Wavenumber Verification

In the Wavenumber Verification test the spectrum of a polystyrene film is collected. The **Nominal** absorption position is compared to the actual absorbance maximum. The observed value must fall between the **Lower** and **Upper** limits each peak for the test to pass.

The exact peak positions and tolerances in the Limits table will depend on the pharmacopoeia. In the Generic test, you can add rows to the table to add further peaks, and specify the lower and upper limits.

To select which peaks will be included when the tests are run, select the **Include** check box for each row of the table.

If you selected Internal APV as the sampling option on the Setup Instrument Verification tab, the polystyrene filter in the internal filter wheel will be used for the test, but you should refer to the appropriate pharmacopoeia for the thickness specified.

During the test a background spectrum and a polystyrene sample spectrum will be generated. A log file is generated showing the results of the test that includes the sample spectrum and a table of the results. The spectra and log file are stored in the location specified on the Setup Instrument Verification tab.

Repeatability

The Repeatability limits can be adjusted to suit your instrument conditions for routine validation, but the Japanese Pharmacopoeia standard states that the difference in transmittance should be within 0.5% at wavenumbers from 3000 to 1000 cm^{-1}, and the abscissa variation within 1 cm^{-1} at about 1000 cm^{-1}. The Chinese Pharmacopoeia states that the error should be within 0.5% at wavenumbers near 3000 cm^{-1}, and the abscissa variation within 1 cm^{-1} at about 1000 cm^{-1}.

For the Generic MIR Repeatability Test you can increase the number of peaks measured. The default is to collect the polystyrene spectrum twice, but in the Generic MIR Repeatability test you can increase the number of repeats. For each wavenumber in the table, enter the nominal variation in the abscissa (cm-1) or ordinate (%T) vales. If the observed variation is less than the nominal variation for each peak, the test will pass.

During the test a background spectrum and the spectrum of a polystyrene sample will be generated at least twice, depending on the number of repeats selected. A log file is generated showing the results of the test that includes the sample spectrum and a table of the results. The spectra and log file are stored in the location specified on the Setup Instrument Verification tab.

NIR Tests

The NIR tests available are:

Pharmacopoeia	Wavelength Accuracy	Linearity	Noise	Repeatability	Ordinate Units
Generic	Yes	Yes	Yes	Yes	A/%T
USP	Yes	Yes	Yes	No	A
Indian	Yes	Yes	Yes	Yes	%T

Wavelength Accuracy (Wavelength Scale Verification)

In the Wavelength Accuracy test, a spectrum is collected, and the wavenumber is measured at the specified peaks. If the measured wavenumber at each peak is within the Upper and Lower limits for that peak, the test passes.

In the Indian NIR Wavelength Scale Verification and United States Wavelength Accuracy tests you can select the **Nominal** abscissa value and **Lower** and **Upper** limits for the positions of up to three peaks. In the Generic NIR Wavelength Accuracy test you can add rows to the table to specify further peaks.

For each peak position you wish to calculate, place a checkmark in the **Include** box.

You can select the algorithm that is used to calculate the peak position from **Interpolated Peak** and **Center of Gravity**. The Interpolated Peak algorithm calculates peak position from maximum intensities. The Center of Gravity algorithm calculates peak position from the shape of the peak. When using the Center of Gravity algorithm, the Peak Height, which defines how much of a peak is used when calculating its center of gravity, is set to 0.5.

The limits should be adjusted to suit your instrument conditions for routine validation. Refer to the appropriate pharmacopoeia for suitable reference materials.

During the test a background spectrum and a sample spectrum will be generated. A log file is generated showing the results of the test that includes the sample spectrum and a table of the results. The spectra and log file are stored in the location specified on the Setup Instrument Verification tab.

Linearity

In the photometric linearity test, spectra are collected from at least four reference materials and compared with stored reference reflectance spectra of the same samples. For each abscissa position specified, the measured versus the known absorbance values for the standards are plotted. A linear regression is then performed and the difference of the slope from 1 and the difference of the intercept from zero are reported. The reference spectra must be collected in absorbance.

The test is performed using at least four reference standards in the range 10% to 90% for analytes with absorbances below 1.0. Where analytes have absorbances which exceed 1.0 then a 2% or a 5% standard (or both) should be included. For details of suitable reflectance standards, refer to the appropriate pharmacopoeia.

You can define up to three abscissa positions at which to validate the standards. The defaults are 8333, 6250 and 5000 cm^{-1}. You can set the limits for the **Slope** and **Intercept.** The default value for the slope is 1+/-0.05 and the default for the intercept is 0+/-0.05. The values entered for the slope and intercept must be determined experimentally using your chosen instrument setup.

In the Generic NIR tests, you can add rows to the table to add further abscissa positions, and specify the positions and the limits for the slope and intercept.

For each reference in the Reference Spectra table, select the browse button in the **Spectrum File** column, and browse to your reference spectrum. To add new rows to the Reference Spectra table, edit the **No of Reference Materials** field. A minimum of 4 reflectance standards are required; a maximum of 10 spectra can be specified.

During the test a background spectrum will be generated, and then you will be prompted to insert a reference material. If no reference spectra are loaded an error message will be displayed during the test. A background spectrum and a spectrum for each reference are generated. A log file is generated showing the results of the test that includes the list of reference spectra, the plot of observed against nominal, and a table of the results at each position. The spectra and log file are stored in the location specified on the Setup Instrument Verification tab.

Noise Test

In the photometric Noise test a highly reflective (high flux) and a lower reflectivity (low flux) reference material are scanned with the material used as both the sample and the reference. You can set the range within which the noise is measured, the segment size over the range, and to set the Nominal value and upper Limit for the average RMS noise and maximum individual RMS noise for the High flux and Low flux noise tests.

Select the **Range** over which to calculate the noise. The default range is 8350 to 4450 cm^{-1}. You then select the **Segment Size (cm^{-1})** over which to calculate the noise. The default size is 300 cm^{-1}. The Noise is then calculated for successive segments of the defined size, over the specified range. There are 13 segments of 300 cm^{-1} over the range 8350 to 4450 cm^{-1}. The maximum number of segments allowed is 20.

High Flux is measured using a highly reflective reference material whilst Low Flux is measured using a lower reflectivity reference material. The reflectance standard is used as the sample and background reference. At reduced light flux, significant contributions are made to the noise from the optics, source, electronics and the detector. Low light flux occurs when a low reflectance or highly absorbing sample is measured.

The values entered in the Nominal column for High Flux and Low Flux must be determined experimentally by you, using the chosen instrument setup. We recommend that you perform a series of tests several times over several days, to take into account variation in ambient temperature, time that the instrument has been switched on, humidity and other variables. Use these values to calculate the limits and nominal values for the tests. Tolerance limits are dependent upon the definition of fit-for-purpose for the individual application. However the limits are set by the USP<1119> method at 0.0003 RMS, and 0.0008 Max for High Flux and 0.001 RMS and 0.002 Max for Low Flux.

During the test you will be prompted to insert a High Flux and Low Flux reference material. A background spectrum and a spectrum for each reference are generated. A log file is generated showing the results of the test that includes noise spectra, and a table of the nominal and observed Mean and Max RMS values for the High and Low Flux samples. The spectra and log file are stored in the location specified on the Setup Instrument Verification tab.

Repeatability

In the Indian NIR Wavelength Repeatability test you can specify up to three positions at which to determine the repeatability. The defaults are 7925, 5947 and 5167 cm^{-1}. You can then set the Abscissa Standard Deviation in cm^{-1}.

To select which peaks will be included when the tests are run, select the **Include** check box for each row of the table. The default **Number of repeats** is 5.

In the Generic NIR tests, you can add rows to the table to add further abscissa positions, and specify the abscissa and ordinate standard deviation in cm-1 and %T, respectively. In the Generic NIR tests, you can select the **Ordinate Units** (A or %T). You can then specify the **Test Limits Type** as **Standard deviation** or **Range**. The Standard Deviation or Limits for the Abscissa and Ordinate positions can then be specified. The default values are 1 cm^{-1} and 0.5%T respectively.

A background spectrum and a spectrum for each repeat are generated. A log file is generated showing the results of the test that includes the repeat spectra, and a table of the results. The spectra and log file are stored in the location specified on the Setup Instrument Verification tab.

Additional Information

To set up the reporting options for your Instrument Verification Checks, see Setup Instrument Verification.

The spectra generated, and the log file showing the results, are saved to the Instrument Verification **Spectra and Log Files** folder specified on the Setup Instrument Verification tab.

For the MIR tests if you select **Internal APV** as the Sampling position on the Setup Instrument Verification tab, the appropriate position in the filter wheel will be selected. For the NIR tests the Sampling position for the pharmacopoeia tests is always **Sample Area**.

MIR Pharmacopoeias

- European Pharmacopoeia 6.0, Chapter 2.2.24 - Absorption Spectrophotometry, Infrared.
- Indian Pharmacopoeia, 2010, Chapter 2.4.6, Infrared Absorption Spectrophotometry.
- Japanese Pharmacopoeia, Sixteenth Edition, General Tests Chapter 2.25, Infrared Spectrophotometry.
- Chinese Pharmacopoeia, 2010, Volume 1, Appendix V C.

NIR Pharmacopoeias

- USP<1119> Pharmacopeial Forum, Vol 24, No 4, July-Aug 1998, p 6463 - 6473. The test follows USP <1119> (United States Pharmacopoeia, Chapter 1119), Near-Infrared Spectrophotometry.
- Indian Pharmacopoeia, 2010, Chapter 2.4.6, Infrared Absorption Spectrophotometry.

Setup Laboratory Scheduler

Use the Setup Laboratory Action tab to schedule various checks to ensure that your spectrometer is working correctly. These include Ready Checks and Instrument Verification Tests, and, if you have a Spectrum Two spectrometer FT-IR/FT-NIR, Component Checks.

If you have a Spectrum Two FT-IR/FT-NIR spectrometer, use the Setup Power Save tab to set up the power save options so that the instrument is ready when you need to use it and in a low-power mode when you don't. You can set up power on and power off times for each day of the week independently.

NOTE: The Setup Power Save tab is only available if you have a Spectrum Two spectrometer.

1. Select **Laboratory Scheduler** from the Setup menu.

   OR

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

   The Laboratory Scheduler tabs are displayed in the Dialog Pane.

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

2. Select the Setup Laboratory Actions tab or, if you have a Spectrum Two instrument only, the Setup Power Save tab.

Setup Laboratory Actions

Use the Laboratory Actions tab to set the schedule for Instrument Checks and AVI Calibration for your spectrometer. If you have a Spectrum Two FT-IR/FT-NIR spectrometer, you can also use the tab to set up the actions for the diagnostic instrument component checks.

1. Select **Laboratory Scheduler** from the Setup menu.

   OR

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

   The Laboratory Scheduler tabs are displayed in the Dialog Pane.

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

2. Select the Setup Laboratory Actions tab.

Setup Laboratory Actions

The Setup Laboratory Actions tab enables you to select if, and when, your instrument will automatically perform certain checks.

Component Checks (Spectrum Two FT-IR/FT-NIR only)

Select **On Connection** to run diagnostic checks each time you connect to your Spectrum Two instrument.

Select **After elapsed time (days)** to run the component checks after a specified time interval. The default is 30 days. Then set an appropriate time of day for the checks to run. The default is 9.00 a.m.

If you do not wish to run the diagnostic checks automatically, select **On Demand**.

NOTE: You can run Component Checks on demand from the Measurement menu.

Ready Checks, Instrument Verification and AVI Calibration

For AVI Calibration, Ready Checks and Instrument Verification you can select to perform each process after a number of samples have been collected or after an elapsed time (in hours or days). Then enter a **Value** appropriate for the option you have selected. The default elapsed time in days is 30 days (at 9.00 am) and the default elapsed time in hours is 24 hours. The default number of samples is 10 samples.

If **Allow Cancel** is enabled, when the process is due a dialog will be displayed that allows you to **Cancel** the process.

The default option is **On Demand**, which means that the Scheduler will take no action.

NOTE: You can run Instrument Checks and Standardize (AVI Calibration) on demand from the Measurement menu.

Additional Information

When the Action is due, the Prompts Display will be updated, and the Scan icon will have a flag indicating the type of action due.

When a scheduled event is due the scan icon will be modified to indicate this. The Prompts Display will also show suitable instructions. Refer to the table below:

Action	Prompt	Scan Icon
Component Checks	Scheduled Component Checks Ensure Beam path is Clear Press [Scan] to Run	
Ready Checks	Scheduled Ready Checks Ensure Beam path is Clear Press [Scan] to Run	
Instrument Verification	Scheduled Verification Ensure Beam path is Clear Press [Scan] to Run	
AVI Calibration	Scheduled AVI Calibration Ensure Beam path is Clear Press [Scan] to Run	

Click the Scan icon to start the action and follow the instructions on-screen. If multiple actions are due at the same time, after each action is completed the Prompts Display and Scan icon will update for the next test.

The Ready Checks or Instrument Verification tests will be performed using the settings defined on the Setup Ready Checks or Setup Instrument Verification tabs, respectively. Only those tests selected will be run. Refer to Ready Checks and Instrument Verification for more information about running the procedure.

The AVI Calibration routine performed is the same as that available from the Adjustments Toolbox, accessed via the Setup Instrument Advanced tab.

The settings for the Laboratory Actions are associated with the User.

Setup Power Save (Spectrum Two FT-IR/FT-NIR only)

Use the Setup Power Save tab to set up Power Save mode options for your Spectrum Two FT-IR/FT-NIR spectrometer. This will increase the lifetime of your instrument and save energy, while still ensuring that the spectrometer is ready when you need to use it.

1. Select **Laboratory Scheduler** from the Setup menu.

   OR

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

   The Setup Laboratory Scheduler tabs are displayed in the Dialog Pane.

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

2. Select the Setup Power Save tab.

Power Save

You can use the Power Save options to select when your Spectrum Two instrument will automatically power on and enter a power-saving mode each day.

Select suitable **Power On** and **Power Off** times for each day and select the appropriate check box to **Activate** power save mode.

If power save mode has not been activated, the row in the table is grayed.

The power save options use the 24-hour clock. The default time for Power On is 8:00 and for Power Off is 18:00. You can use the up and down arrows to increase or decrease the time, or enter a time.

Additional Information

- 30 minutes before the instrument is due to enter power save mode a desktop alert will be displayed that will count down the remaining time. If you would like to continue working with your instrument beyond that time, you can choose to postpone the Power Off event. See Postponing Power Save Mode.
- If you are collecting data when the power save time is reached, the data collection will not be interrupted. When the scan is completed, or halted, the instrument will enter power save mode.
- When the instrument is in Power Save mode, the LED on the front of the instrument will flash orange and the Status bar will display **Power Save Mode**. The Scan toolbars will be disabled. The Setup Instrument tabs and the Setup Power Save tab can be viewed but are disabled.
- When the instrument is powered on, the instrument will initialize and the LED will display green. After initialization all the disabled functions will become active. The instrument will take 1-2 minutes to be accessible.
- The instrument's internal clock is synchronized to the last PC it was connected to. To update the instrument clock, after manually changing the PC time, or after automatic changes for Daylight Saving Time, connect to the instrument using either Spectrum (or AssureID) software.

Postponing Power Save Mode

If the Power Save Mode alert is displayed and you want to delay the instrument entering the power save mode, use the link **To postpone click here** to display the Delay Power Save dialog.

Enter the amount of time you would like to delay the power save by (in minutes) and then click **OK.** The maximum time you can postpone a power save by is 120 minutes.

Manually entering Power Save Mode

You can also enter power save mode immediately by selecting **Power Save Mode** from the Measurement menu, or by clicking  if available on the Measurement bar. This option is deactivated during data collection.

Alternatively, press the Power button on the front of the Spectrum Two instrument for two seconds to enter the manual Power Save Mode.

In this mode the instrument LED will display orange. To power up the spectrometer again, press and hold the Power button for approximately two seconds until the LED is green.

Setup Export and Email

Use the Setup Export and Setup Email tabs to set up the export of your spectra to a specified folder as data files that are accessible to other applications, using the Export command, or to set up the server and user information to enable you to send your data by email using the Send To Email command.

1. Select **Export and Email** from the Setup menu.

   OR

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

   The Setup Export and Email tabs are displayed in the Dialog Pane.

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

2. Select the Setup Export tab, or the Setup Email tab.

Setup Export

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

1. Select **Export and Email** from the Setup menu.

   OR

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

   The Setup Export and Email tabs are displayed in the Dialog Pane.

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

2. Select the Setup Export tab.

Header Options

Check the Header options to include spectral header information in the exported file. Then select which information to include from **General and Custom Fields**, **Instrument Settings**, **History Records** and **Quality Checks**. This information is the same as that displayed in the four sections of the History tab.

File Options

File Extension	Defines the file extension applied to exported data. The options are: CSV, DAT, TXT or XY.
File Encoding	Defines the file encoding used. The options are: Default, UTF8 or US ASCII.
List Separator	Defines the list separator used. The options are: Comma (","), Semi Colon (";"), Equals ("="), TAB or SPACE.
Decimal Separator	Defines the decimal separator used for the data. The options are: Point (".") or Comma (",").

Data Options

Decimal Places X	Defines the number of decimal places for the X axis. The options are: As in data set, 1 or 2.
Decimal Places Y	Defines the number of decimal places for the Y axis. The options are: As in data set, 1, 2, 3, 4, 5, or 6.
Sort data ascending	Check to sort the data in ascending order (of the X axis values).

Additional Information

To export your data using these settings, select Export from the File menu, and choose the **Custom Defined File** format.

Setup Email

Use the Setup Email tab to set up the email account that will be used in the Send To Email command. This must be set up for the Send To Email option to become available.

1. Select **Export and Email** from the Setup menu.

   OR

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

   The Setup Export and Email tabs are displayed in the Dialog Pane.

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

2. Select the Setup Email tab.

Server Information

1. Enter the **Outgoing mail server (SMTP)**.
2. Type the complete name of the server provided by your internet service provider (ISP) or mail administrator. In Microsoft Outlook this is the name of your Microsoft Exchange Server, which you can find in your account settings. Often the server name is smtp. followed by your domain name, for example, smtp.example.com. If you use a web-based mail application, you can usually accesses the server information via the application Help.

   Simple mail transfer protocol (SMTP) is the standard for sending email messages across networks.
3. Select **Use Default Credentials**.

   OR

   Select **Enable SSL**.

   Choose this option if your mail administrator tells you to use a Secure Sockets Layer (SSL) connection.
4. Select either **HTML Body** or **Plain Text** for the mail output format.

   If you select HTML Body, the message can contain formatting such as bold text or bullets.

NOTE:	For the email recipient to see these features, the recipients email application must support formatted messages.

   Plain Text does not support text formatting or image display in the message body.

User Information

Enter the **Email Address** you want to use to send emails from. If you selected **Enable SSL** rather the **Use Default Credentials** in Server Information, you will need to enter the **User Name** and **Password** that you use currently for that email account and then confirm the password.

Test Settings

Click **Test Settings** to check that your settings have been entered correctly. A message will be displayed in the Status bar to indicate that Spectrum is sending a test email, and then whether or not the test was successful. If the test is successful you will receive an email with the subject **Spectrum Software Setup Email - Test Confirmation** and the following message:

> This email has been sent to confirm that the Setup Email configuration in Spectrum software has been setup correctly.

If you selected **Enable SSL** and your email Server does not support secure settings (SSL) the test email will not be sent and a warning message will be displayed.

Additional Information

To email your data using these settings, select **Send To** from the File menu, and then select Email.

We recommend that you contact your organization's mail administrator if you are unclear about which settings to choose.

Setup Peak Detection

Use the Setup Peak Detection tab to edit the criteria used for peak detection and marking using the Peak Labels command.

- Select **Peak Detection** from the Setup menu.

  OR

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

  The Setup Peak Detection tab is displayed in the Dialog Pane.

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

Algorithm

By default, the peak positions are found using an **Interpolated peak** algorithm, which derives peak position from maximum intensities. Alternatively, you can select the **Center of gravity** algorithm, as used by NIST, which derives peak position from the shape of the peak.

Thresholds

The Thresholds section enables you to choose the thresholds used when detecting peak maxima or base points. The threshold used for the Interpolated Peak algorithm is %T (or %R); A (or Log 1/R); and A.U. (for any other units), depending on the type of spectrum examined.

The **Center of gravity peak height** threshold, which is only available when the Center of gravity algorithm is selected, enables you to set how much of a peak is used when calculating its center of gravity. Where peaks are well defined a value of 0.8 could be appropriate. However, where two poorly-defined peaks overlap to produce a shoulder, and the Center of gravity peak height threshold is set to include the overlap, the Center of gravity algorithm calculates a peak position shifted towards the shoulder unless this value is 0.2 or less.

Click **Reset** to return to the default threshold values: 2.00%T; 0.0088 A; 10.00 A.U.; 0.20 Pk Ht.

Labeling

The Labeling section enables you to set whether to label **All peaks found** or only a set number of the most intense peaks.

You can also select to mark the position of the **Peak maxima** and/or the peak **Base points**. For each position marked you can optionally include a text label with the **X Position** and/or the **Y Value**.

Refresh

Click **Refresh** to update any peak labels that are currently displayed after modifying any of the settings.

Setup Pathlength

Use the Setup Pathlength tab to set up a global pathlength. You can enter a pathlength manually, or determine the pathlength of your cell using either a pre-defined Quant method (Beer's Law or Quant+) or interference fringes. If enabled, the global pathlength is stored in the header of any spectrum collected. This global pathlength value will also be available as a variable (Setup Pathlength) in Equations, and can also be used in a Quant Control Ready Check or Quant Prediction. The global pathlength also means that you can run a process that utilizes a pathlength value, even when the spectra don't have a pathlength value saved in the header information of the file.

5. Select **Pathlength** from the Setup menu.

   OR

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

   The Setup Pathlength tab is displayed in the Dialog Pane.

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

Set the pathlength manually

1. Select **Enable Pathlength** on the Setup Pathlength tab.

   This adds a column **Pathlength (mm)** to the Sample Table.

2. Select **Set manually** as the Pathlength Determination option.

3. Enter the pathlength value in **Pathlength (mm)**.

   New samples added to the Sample Table will have the new global pathlength value. If you want to update existing entries in the Sample Table to the new pathlength value, select **Yes** when prompted.

Determine using Quant Method

You can use a Beer's Law or chemometric Quant+ method to determine the pathlength of your cell. The Quant method must first be defined in your Quant Builder software, and must return the pathlength value in millimeters (mm).

1. Collect or display the spectrum of a cell containing a suitable solvent for your analysis.

   The solvent should be that used when building the Quant method, and should be spectroscopy-grade and uncontaminated.

2. Ensure that the spectrum is selected in the Data Explorer.

3. Select **Enable Pathlength** on the Setup Pathlength tab.

   This adds a column **Pathlength (mm)** to the Sample Table.

4. Select **Determine using Quant method** as the Pathlength Determination option.

5. Select **Quant+** or **Beer's Law** as the Quant method type.

6. Browse to and select the file that you want to use as the Quant method.

7. If required, select the appropriate **Component** from the drop-down list.

   The Component drop-down list displays the components in your Quant method. The default is the first component in the method.

8. Click **Calculate**.

   The pathlength is calculated using the Quant method, and the Quant Analysis Details dialog is displayed.

   The dialog lists the pathlength determined, and the statistical properties of the analysis: **RMS Error**, **P2P error** (peak-to-peak error), **M Distance**, **Residual Ratio** and **Prediction Error**.

   High residual ratio values could be due to low-purity solvent or contaminated windows. High M Distance values can indicate that the pathlength is outside the range modeled in your Quant method.

   Refer to Quant for a description of the prediction properties. See the Quant Builder on-screen Help file for mathematical definitions of these terms.

9. If you wish to accept the results and use the new global pathlength value, click **OK**.

   New samples added to the Sample Table will have the new global pathlength value. If you want to update existing entries in the Sample Table to the new pathlength value, select **Yes** when prompted.

   OR

   To reject the results, click **Cancel**.

Determining the Pathlength using Interference Fringes

This method involves measuring the spectrum of the empty cell or of a film to produce a spectrum showing an interference fringe pattern and then using this fringe effect to calculate the pathlength of the cell or the thickness of the film.

NOTE:	This method cannot be used for wedged cells.

1. Collect or display the spectrum of the empty cell or film.

   The cell must be completely clean and dry. If the spectral resolution of the spectrum is not sufficient, fringes will not be visible.

2. Ensure that the spectrum is selected in the Data Explorer.

3. Select **Enable Pathlength** on the Setup Pathlength tab.

   This will add a column **Pathlength (mm)** to the Sample Table.

4. Select **Determine using interference fringes** as the Pathlength Determination option.

5. If you wish Spectrum to determine the number of fringes, select **Auto**.

   OR

   If you wish to enter the number of fringes manually, ensure that **Auto** is not selected.

6. Enter the **Start** and **End** points.

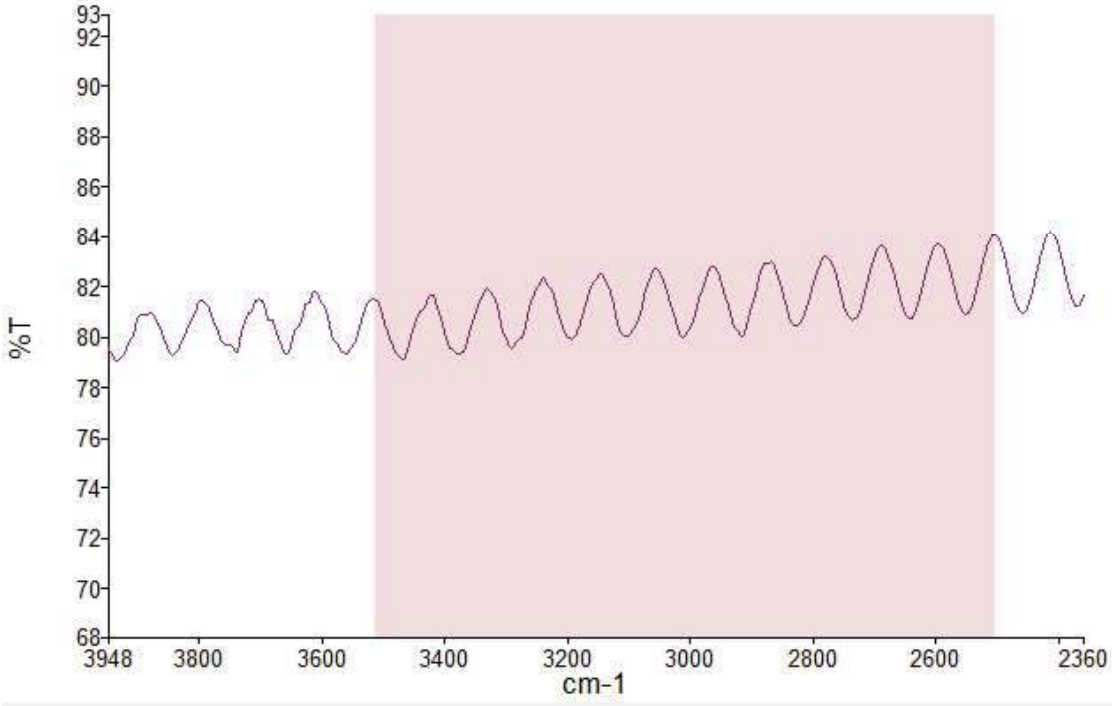
   OR

   Click on the shaded area in the Graph window and then drag the vertical cursors at each edge to select the region.

   You can also click and drag the shaded area up and down the ordinate axis. The Start and End values on the Setup Pathlength tab are updated.

If you selected Auto, Spectrum will determine the exact position of the first and last maxima (or minima) within the range selected and use those values for the calculation. If you did not select Auto, the Start and End points specified should be the frequency at which the first maximum (or minimum) occurs and the frequency at which the last maximum (or minimum) occurs. Both points should be maxima or both points should be minima.

You should select a wavelength range containing at least 10 fringes. It should be chosen to avoid common interferences and window cut-offs. For example:



7. If you selected Auto, then enter the **Peak Threshold** that Spectrum will use to identify the number of fringes in the selected wavenumber range.

   The Peak Threshold is displayed in the units of your spectrum. The default value is 0.5. The Peak Threshold should be set so that fringes are identified, but so that noise and atmospheric absorption or artefacts are ignored.

   OR

   If you did not select Auto, enter the **Number of Fringes** in the range selected.

8. Enter the **Refractive Index**, if required.

   For an empty cell the refractive index is that of air, which we will take as being 1.

9. Enter the **Angle of Incidence**, if required.

   This angle is measured relative to a line perpendicular to the surface. In the standard sample holder configuration the beam is perpendicular to the cell, so the angle of incidence is taken as 0.

10. When you have entered all the parameters, review the **Calculated Pathlength** value.
11. Click **Accept** if you wish the global pathlength to be updated to the new value.

    New samples added to the Sample Table will have the new global pathlength value. If you want to update existing entries in the Sample Table to the new pathlength value, select **Yes** when prompted.

The interference fringes method utilizes the equation pathlength (*d*) in mm = 10*N* / 2 (v1 - v2), where *N* is the number of fringes, and v1 and v2 are the wavenumbers of the Start and End fringe peaks (or troughs), respectively, if the angle of incidence is 0 and the Refractive index is 1.

Additional information

The interferences fringes method is the basis of the Tcalc function that you can add to an Equation.

Setup View

Use the Setup View tabs to select the default graph appearance properties that will be applied to all new graphs and to apply them to existing graphs.

1. Select **View** from the Setup menu.

   OR

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

   The Setup View tabs are displayed in the Dialog Pane.

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

2. Select the Setup View Axes tab, the Setup View Appearance tab or the Setup View Advanced tab.

Additional Information

The Setup View tabs define the graph appearance properties that will be applied to new graphs. To apply display options to the currently displayed graph, click **Refresh**. To apply display options to all graphs in the Samples View, click **Refresh All**. To return the View options to the factory default, click **Reset**.

NOTE:	**Reset** does not apply the factory default display options to existing graphs. To do this, use **Refresh** and **Refresh All**.

The Graph properties dialog enables you to customize the appearance of the graph currently displayed; see Formatting a Graph.

Setup View Axes

Use the Setup View tabs to select the graph appearance properties that will be applied to the selected graph or all graphs within that section.

1. Select **View** from the Setup menu.

   OR

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

   The Setup View tabs are displayed in the Dialog Pane.

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

2. Select the Setup View Axes tab.

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, or enhance the fingerprint region using the scale change at 2000 cm^{-1}.

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 change the **Units** (**Auto**, **%T** or **A**), make sure that you select appropriate range values.

Display Mode

Select whether the graph display mode should **Overlay** curves (where the curves are displayed on a common set of axes) or **Split** curves (where the curves are displayed on a common X, but separate Y, axes).

Setup View Appearance

Use the Setup View tabs to select the graph appearance properties that will be applied to the selected graph or all graphs within that section.

1. Select **View** from the Setup menu.

   OR

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

   The Setup View tabs are displayed in the Dialog Pane.

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

2. Select the Setup View Appearance tab.

Enable Gridlines

Select this check box if you want to see gridlines under your curves. The major and minor gridlines are elements whose color you can change in the Text and Lines panel.

The major and minor gridline intervals depend on the major and minor gridline intervals in 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.

Graph Color Palette

The palette defines the colors available to Spectrum to color curves open in the Samples Views. You can change the colors in the color palette; double-click on the color to open the Color dialog. Select a **Basic** color, or one of the **Custom colors** you may have defined, and then click **OK**.

Setup View Advanced

Use the Setup View tabs to select the graph appearance properties that will be applied to the selected graph or all graphs within that section.

1. Select **View** from the Setup menu.

   OR

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

   The Setup View tabs are displayed in the Dialog Pane.

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

2. Select the Setup View Advanced tab.

Display Option

Select one or more of **Hide X Axis Units**, **Hide Y Axis Units**, **Hide X Axis Numbers**, and **Hide Y Axis Numbers** to suppress the labels applied to the X and Y scales.

Curve 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.

Data 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.

Setup Compare

Before you use the Compare process:

- Select the spectra that you want your spectrum compared to, and set up Pass/Fail criteria. See Setup Compare References.
- Select which filters to apply, the wavenumber range over which the comparison should apply, and the number of comparisons to display on the Compare tab. See Setup Compare Parameters.

To set up Compare:

1. Select **Compare** from the Setup menu.

   OR

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

   The Setup Compare tabs are displayed in the Dialog Pane.

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

2. Select the Setup Compare References tab, or the Setup Compare Parameters tab.
3. Use the Setup Results File tab to configure a file of accumulated process data for exporting to another software application for further data analysis.

Setup Compare - References

Use the Setup Compare References tab to select which spectra your spectra should be compared with, and the Pass/Fail criteria for your results.

1. Select **Compare** from the Setup menu.

   OR

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

   The Setup Compare tabs are displayed in the Dialog Pane.

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

2. Select the **Setup Compare References** tab.

Managing the Compare Table

The table contains all spectra that your spectrum can be compared to.

Adding Spectra

1. Click **Add**.
2. Select the spectrum, or folder containing spectra, that you want to add.

   You can browse to and select any saved spectrum, or folder containing saved spectra, on your PC or network.

   A new row is added to the table.

Selecting Spectra for Compare

The table can contain all the spectra that you use for comparisons, but you do not need to include every row for every Compare.

- Select the **Include** check box for every row you want to include in a comparison, or deselect the **Include** check box for every row that you want excluded.

Removing Spectra

1. Select the row containing the spectra you want to remove.
2. Click **Remove**.

   The table row is deleted, but the spectra themselves are not deleted from your PC or network.

Pass/Fail Thresholds

Correlation

By default, the Pass/Fail result is based on a Correlation threshold, which expresses the degree of similarity between the two spectra.

By default, a Correlation of 0.98 is sufficient to match two spectra and deliver a 'Pass' result. Depending on your application, you many prefer to enter another Correlation threshold in any row in the table. Enter a value between 0.00 (no similarity) and 1.00 (identical).

If the Correlation threshold is exceeded, the result is reported in the results window as 'Pass'.

The higher the correlation threshold, the lower the chance of incorrect identification. But this also gives an increased chance of a false 'Fail' result, which lowers the efficiency of identification.

Discrimination

In most cases the Correlation threshold is sufficient to identify a material, but sometimes you may also wish to enter a Discrimination Threshold. This is an additional test to ensure that you discriminate between spectra. Both the Correlation and Discrimination thresholds must be satisfied to return a 'Pass' result.

If the Discrimination check box is selected, the default Discrimination threshold for any row is 0.05. Depending on your application, you many prefer to enter another Discrimination threshold for any row in the table. Enter a value between 0.00 and 1.00.

The Discrimination threshold ensures that the closest match is sufficiently separated from the next closest match. Its value is equal to the difference in the Correlation coefficients of the first two spectra reported on the Compare tab.

The Discrimination threshold you use depends on the available spectra in the table. If these spectra are very different from the tested spectrum, set the Discrimination threshold high. If the available spectra in the table are very similar to the tested spectrum, set the Discrimination threshold low.

Additional Information

To select which filters to apply, the wavenumber range over which the comparison should apply, and the number of comparisons to display on the Compare tab, see Setup Compare Parameters.

Setup Compare - Parameters

Use the Setup Compare Parameters tab to select the filters that are applied during a Compare.

1. Select **Compare** from the Setup menu.

   OR

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

   The Setup Compare tabs are displayed in the Dialog Pane.

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

2. Select the **Setup Compare Parameters** tab.

Filters

When you collect spectra with different instruments, on different days or under different conditions, there may be differences in the spectra that are not due to differences in your sample. These filters reduce or eliminate the differences from these sources.

Some regions of a spectrum contain information that is more reliable than other regions of the same spectrum. These filters reduce the influence of the less reliable information on the comparison.

When more than one filter is used, the total weighting is the product of the weightings of the individual filters.

Resolution Weighting	This filter emphasizes the influence of features with widths of approximately 8 to 16 cm^{-1} in mid infrared spectra, and 16 to 32 cm^{-1} in near infrared spectra. Bands with widths in this range tend to be the bands that correspond to real features in your spectrum. Bands with widths below this are often high frequency noise, and bands with widths broader than this are often baseline features. This filter is selected by default, and can be selected separately from any other filter.
Intensity Weighting	The signal-to-noise ratio of the spectrum varies with the abscissa scale. Data with a low signal-to-noise ratio is less reliable than data with a high signal-to-noise ratio. This option applies a *black body* filter that reduces the influence of data in the regions at the ends of the spectrum where the signal-to-noise ratio is lower. This filter is selected by default, and can only be selected with the Noise Weighting filter.

Noise Weighting	The noise level in a region of a spectrum that is near to totally absorbing is greater than other regions. This option applies a *black band* filter that reduces the influence of regions where the transmission is low because they have high noise in absorbance. This filter is selected by default, and can only be selected with the Intensity Weighting filter.
CO2 Blanking, H2O Weighting and H2O Blanking	Spectra collected on different days, and under different conditions may show the influence of different amounts of carbon dioxide and water vapor. These are not valid differences between spectra, and these filters reduce or eliminate these differences. The CO2 Blanking filter removes the influence of carbon dioxide on your spectrum, by excluding all data between 2390 and 2280 cm^{-1}. This filter is only selectable if Intensity and Noise Weighting are selected. This filter is not appropriate for near infrared spectra. The H2O Weighting filter reduces the influence of data between 7450 and 6950 cm^{-1}, 5600 and 5100 cm^{-1}, 4000 and 3500 cm^{-1}, and 1900 and 1300 cm^{-1}. Data in these regions is de-weighted by a factor of 8. This filter is only selectable if Intensity and Noise Weighting are selected. The H2O Blanking filter excludes all data between 7450 and 6950 cm^{-1}, 5600 and 5100 cm^{-1}, 4000 and 3500 cm^{-1}, and 1900 and 1300 cm^{-1}. This filter is only selectable if Intensity and Noise Weighting are selected.

Maximum number of comparisons

Enter the maximum number of results to display in the Compare tab in the Viewing Area.

Spectral Range

By default your spectrum is compared to a reference spectrum over the range where the spectra overlap.

If you are particularly interested in a region, or you want to exclude regions of a spectrum select **User Defined Range**, and then enter the **Start** and **End** values for the range over which you would like the spectra to be compared.

Additional Information

To select the spectra that you want your spectrum compared to, and set up Pass/Fail criteria, see Setup Compare References.

Setup Quant

Use the Setup Quant tabs to select which Quant methods should be used when the Quant process is run, and to select which results will be calculated and displayed on the Quant tab and on the Results Table tab.

1. Select **Quant** from the Setup menu.

   OR

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

   The Setup Quant tabs are displayed in the Dialog Pane.

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

2. Select the Setup Quant Methods tab, or the Setup Report Defaults tab.
3. Use the Setup Results File tab to configure a file of accumulated process data for exporting to another software application for further data analysis.

Setup Quant Methods

Use the Setup Quant Methods tab to select which Quant methods are available, and to specify which of the Quant methods should be used when the Quant process is run.

1. Select **Quant** from the Setup menu.

   OR

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

   The Setup Quant tabs are displayed in the Dialog Pane.

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

2. Select the Setup Quant Methods tab.

Adding a Quant method

1. Click **Add**, and then select the type of Quant method you want to open from the drop-down list.

   The options are: **Spectrum Quant** and **Quant+**.

   If you select Quant+, the options are: **PLS1**, **PLS2**, **PCR+**, **Beer's Law** and **Quant C**.

   A browse dialog is displayed.

2. Browse to and select the file that you want to add.

   Spectrum Quant methods all have *.qmd file extensions. Quant+ methods using the Beer's Law algorithm have *.uqm file extensions, while those using PCR+, Quant C, PLS1 and PLS2 algorithms have *.md file extensions.

3. Click **OK**.

   A new row is added to the Quant methods table.

   The Quant table displays the Quant method's **Name**, **Description**, the **Algorithm** and the **Properties** (or components) in the method.

   If the method contained pathlength information, the **Pathlength** field will be available in the **Parameters**. Define an appropriate pathlength for that method. You can enter the pathlength manually. The default is 1. Or, if **Enable pathlength** is selected on the Setup Pathlength tab, you can select to use the global **Pathlength Defined in Setup**. Refer to the Setup Pathlength tab for details. Or, if your spectra contain pathlength information, you can select to use the pathlength saved with the spectrum, by selecting **Pathlength in Spectrum header**.

   If the Quant method has Bias Correction enabled, then **Bias Correction** will be available in the **Parameters**. Select **None**, **Offset** or **Offset and Slope**.

   For QuantC methods, fields for normalization options will be displayed in the **Parameters**. The **Normalization** value normalizes the results by the value of the pathlength entered. If you select **Fixed Value**, the results will be normalized to sum to the value entered. If you select **Use Reference Band**, an internal standard that has a band that is not overlapped by the other components of the standards is used to overcome pathlength problems when the pathlength cannot be determined. It is the height of this band in each spectrum that is normalized.

Modifying the Quant method Settings

1. Click on the Quant method in the table that you would like to modify.
2. Click **Settings**.

   The Quant Settings dialog is displayed. It includes a **Summary** of the Quant method.

   The **Prediction Properties** section of the dialog lists all the components or properties that are included in the Quant method, and the **Units** of the calibration.
3. In the **Prediction Properties** table, select the **Include** check box next to each Component (for Beer's Law and Quant C methods) or Property (Quant+ methods) that you would like to include in the Quant prediction.
4. Click **OK**.

   The Properties section of the Quant methods table will be updated.

Selecting the Quant methods that are active

The table lists all the Quant methods that you have loaded, but only those methods selected will be used when you run the Quant process.

- Enable the checkbox in the **Include** column for each Quant method that you want to use when the Quant process is run.

Removing Quant methods

- Select the row containing the Quant method that you want to remove, and then click **Remove**.

  The Quant method is removed from the Quant table, but no files or folders are deleted from disk.

  You can select multiple rows. You will be prompted for confirmation for the methods selected.

Running a Quant prediction

- Click **Run**.

  The Quant process is performed, and the results are displayed on the Quant tab.

Quant Method Wizard

- Select **Quant Method Wizard** from the Quant sub-menu of the Process menu launch the Quant method Wizard.

  The Quant Method Wizard allows you to create a Quant method based on selected spectra. You can calibrate the method and view the results.

Setup Quant Report Defaults

The Setup Report Defaults tab enables you to select which prediction results will be displayed in the Results table and will be available as Equation variables.

1. Select **Quant** from the Setup menu.

   OR

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

   The Setup Quant tabs are displayed in the Dialog Pane.

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

2. Select the Setup Report Defaults tab.

Setup Report Defaults tab

The Display table lists all the possible statistical results of the Quant predication, grouped by Algorithm. For each property you are able to select whether the results will be available (for example, as an equation variable or a column in the Results Table) and if that property will be displayed by default.

Algorithm	The type of algorithm in the method. The algorithm types listed are BeersLaw, QuantPlusPCR, QuantPlusPLS1, QuantPlusPLS2 and QuantC.
Value	Lists the property- or method-related results that can be calculated for the algorithm. **NOTE:** Some properties of the algorithms are always displayed and made visible, and so are not listed in the table.
Calculate value	Select the results that you would like to be calculated. These will be available, either as variables in equations, displayed on the Quant tab, or available as columns in the Results Table. These results will not be displayed, unless the Display by default check box is selected. To select which columns are displayed in the Results Table, use the column chooser in the top left of the Results Table.
Display value by default	Select the check box of those results that you wish to have added to the Results Table by default.

Additional Information

The Value column lists results in with the prefix "Property" or "Method". Some Values provide information about the Quant prediction – for example, the Residual Ratio. Other values are determined for each Property in the Quant method – for example, the Prediction error.

See Quant for more information about the Quant results.

Setup Verify

Use the Setup Verify tabs to select which Verify methods are available for use when the process is run.

NOTE: Verify in Spectrum uses AssureID methods.

- Select **Verify** from the Setup menu.

  OR

  Select  in the Setup section of the Navigation Pane.

  The Setup Verify tab is displayed in the Dialog Pane.

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

- Use the Setup Results File tab to configure a file of accumulated process data for exporting to another software application for further data analysis.

Adding a Verify method

1. Click **Add**.
2. Select **From registered AssureID database**.

   The methods in all the AssureID databases are displayed. The active database is shown in bold characters.

   OR

   Select **From AssureID database file**, select the database (*.mdb) file that you want to open, and click **OK**.

   The methods in the selected database are displayed.
3. Highlight the method you want to use and click **OK**.

   The method appears in a new row in the Setup Verify table.

Removing a Verify method

- Highlight the method you want to remove from the table, click **Remove** and then click **OK**.

Viewing the details of a Verify method

1. Highlight the method and click **Details**.

   A dialog box is displayed showing information about the materials and the algorithm used by the method.
2. To close this dialog box, click **OK**.

Running a Verify method

Before running a Verify method, a sample spectrum must be selected in the Viewing Area.

1. Click **Run**.

   If the method contains more than one material, the Run Verify Method dialog appears.

2. From the drop-down list under Material Type, select the material you want to use to verify the sample's identity, or select **Unspecified**.

   If you select a material, the method will determine whether the sample matches the material you selected (authentication). If you select Unspecified, the method will determine whether the sample matches any of the materials in the method (identification).

   The Verify method is executed, and the results are displayed on the Verify tab.

Setting up a Verify step in a macro

If you include a Verify step in a macro, and you are using an AssureID method that contains more than one material, then you must select the material if authentication is required, or select **Unspecified** for identification of the sample. You can also select **Prompt User** if you want the user to be able to select the material type each time the macro is run. The default setting is Unspecified, which will be used by the method if the user does not select another material type when prompted.

Setup Adulterant Screen

NOTE: You can only set up Adulterant Screen materials if you have entered a valid license number for this feature during the installation of your software.

Use the Setup Adulterant Screen tab to configure methods for screening the spectrum of a sample for one or more specified substances of concern, such as adulterants added for economic advantage. The results of the screening process will be calculated and displayed on the Adulterant Screen tab and on the Results Table tab.

- Select **Adulterant Screen** from the Setup menu.

  OR

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

  The Setup Adulterant Screen tab is displayed in the Dialog Pane.

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

- Use the Setup Results File tab to configure a file of accumulated process data for exporting to another software application for further data analysis.

There are four tabs contained within the Setup Adulterant Screen tab. Use these tabs to configure the screening method for the material in your sample. Each method applies to a single material. The material is created or selected using the controls on the right side of the tab. You can set up screening methods for multiple materials using this tab, but you can only run one of these methods on your sample at a time.

NOTE: The settings on the four tabs contained within the Setup Adulterant Screen tab always refer to the material selected from the Material drop-down list.

Setting up Adulterant Screen in a Macro

You can set up an Adulterant Screen step in a macro by selecting the material in the Macro Settings dialog corresponding to the screening process you want to run, and selecting the various parameters and spectra in the same way as for a manual analysis. The process will be performed on the assumption that the material chosen corresponds to the sample being analyzed in the macro. If this is not true, then the results of the Adulterant Screen may be very inaccurate.

Configuring the Adulterant Screen Material

Create a new material

1. Click the Material box and select **New Material** from the drop-down list.

   The New Material dialog is displayed.

2. Enter a name and (optionally) a description for the new material, and click **OK**.

   The Material Spectra tab is automatically selected.

Change the name of an existing material

To change the name and description of an existing material:

1. Click the Material box and select **Edit Material Name.**
2. Make the changes required in the Edit Material dialog and click **OK.**

   The material details are updated.

Copy an existing material

If you want to create a similar material to one that already exists, you can copy a material with all its settings and give it a new title:

1. Click **Copy Material**.
2. Enter a new name and description in the Copy Material dialog, and click **OK.**

   A new material is created with the same settings as the material that was copied. It will have the default name *<original material name>_Copy*.

You can now make changes to the material as required, and rename it using the Edit Material Name option. This is helpful if you want to set up methods for several materials which use the same process parameters and/or adulterant spectra.

Import a material from AssureID

You can import a material from an AssureID method:

1. Click **Import material**.
2. Select **AssureID method.**

   A dialog is displayed which shows all the methods available in the registered database, and the materials in each method.
3. Check the checkbox next to the material you want to import.

   You can import more than one material at a time.
4. Click **OK.**

   The selected material is imported into the Setup Adulterant Screen tab. The Material Spectra tab displays the calibration and validation samples.

NOTE: Once a material has been imported, changes made in the Setup Adulterant Screen tab will not affect the material in the original AssureID method, and vice versa.

Remove a material

To remove the currently selected material:

1. Click **Remove Material**.
2. Click **OK.**

   The material is removed from the Setup Adulterant Screen tab.

Setup Material Spectra

The Material Spectra tab in the Setup Adulterant Screen tab is used to select spectra for calibration and validation of the Adulterant Screen method for the material shown in the Material selection box.

NOTE: The settings on the Material Spectra tab refer to the material selected from the

Material drop-down list.

Setting Up Calibration Samples

The calibration samples are used to generate a model to define the sample material. You can import them with a material from an AssureID method, or you can add them manually.

NOTE: We recommend that you select calibration and validation samples that represent all the sources of variation in your material. These could include batch-to-batch variation, sampling variation (including the presentation of the sample to the instrument), and differences between material from different suppliers.

To add calibration samples:

1. Click **Add**.
2. Select **Folder of Spectra** or **Spectrum**.
3. If you selected to add a folder of spectra, browse to the folder location in the Browse dialog and click **OK**.

   OR

   If you selected to add a spectrum file, select the file you want to add from the dialog and click **Open**.

   You can select multiple files by holding down the SHIFT key and clicking the files, or by holding down the CTRL key and clicking the first and last files in a block.

   The spectra are copied to a separate folder for use in the screening method, with the path shown in the table.

The added spectra are automatically included in the screening method, as indicated by the checked Include box.

- To exclude a spectrum file or folder from the method, uncheck the **Include** checkbox.

To change a spectrum file or folder:

1. Click the path of the file or folder in the list.
2. Click the "..." button that is displayed.

   You can select a different file or folder to be displayed at this position in the list.

To remove a spectrum file or folder completely from the method setup:

1. Click the file or folder to be removed.
2. Click **Remove.**
3. Click **OK**.

   The selected file or folder is removed from the method. You can select more than one file or folder to remove using the SHIFT and CTRL keys as described previously.

Setting Up Validation Samples

Validation samples are used to check whether the material model adequately describes the range of variation in the sample material. They may be imported with a material from an AssureID method, depending on the method settings. If they are not already included, then you need to set up the validation samples for the method.

By default, Spectrum will automatically select validation samples from the list of calibration samples. To select the validation samples manually:

1. Check the checkbox marked **Manually select Validation Samples**.
2. Select the validation samples in exactly the same way as adding calibration samples.

We recommend that you use approximately equal numbers of calibration and validation samples if possible.

Setup Adulterant Spectra

The Adulterant Spectra tab in the Setup Adulterant Screen tab allows you to select the spectra for the adulterants that you want to screen for in the Adulterant Screen material.

NOTE: An Adulterant Screen method must contain one spectrum for each adulterant you want to include in the screening process. For optimum results, we strongly recommend that the adulterant spectrum is collected from a pure sample of the adulterant, scanned using the same sampling technique and instrument settings as the sample spectrum.

NOTE: The settings on the Adulterant Spectra tab apply only to the material selected from the Material drop-down list.

To add an adulterant spectrum:

1. Click **Add**.
2. Select **Folder of Spectra** or **Spectrum**.
3. If you selected to add a folder of spectra, browse to the folder location in the Browse dialog and click **OK**.

   OR

   If you selected to add a spectrum file, select the file you want to add from the dialog and click **Open**.

   You can select multiple files by holding down the SHIFT key and clicking the files, or by holding down the CTRL key and clicking the first and last files in a block.

   The spectra are copied to a separate folder for use in the screening method, with the path shown in the table.

The added spectra are automatically included in the screening method, as indicated by the checked Include box.

- To exclude a spectrum file or folder from the method, uncheck the **Include** checkbox.

To change a spectrum file or folder:

1. Click the path of the file or folder in the list.
2. Click the "..." button that is displayed.

   You can select a different file or folder to be displayed at this position in the list.

To remove a spectrum file or folder completely from the method setup:

1. Click the file or folder to be removed.
2. Click **Remove.**

3. Click **OK**.

   The selected file or folder is removed from the method. You can select more than one file or folder to remove using the SHIFT and CTRL keys as described previously.

Setup Adulterant Screen Process Parameters

The Process Parameters tab in the Setup Adulterant Screen tab allows you to adjust the settings of the Adulterant Screen, including how the method will preprocess spectra, report results, and set pass/fail criteria.

> **NOTE:** The settings on the Process Parameters tab apply only to the material selected from the Material drop-down list.

Algorithm

- Number of factors: select the number of factors (principal components) used by the algorithm (values of 1–25 are available), or select **Automatic** to allow the software to determine this automatically.

  Principal components are common factors that account for the variance in the spectra.

  > **NOTE:** Reducing the number of factors can adversely affect the accuracy of the results by excluding sources of variation in the data.

- Baseline terms: select the order of the polynomial equation defining the baseline.

  Values of 0–10 are available. This option is useful if the baseline in the sample being analyzed is different from that in the calibration samples. The first term adjusts the vertical position of the baseline, the second term alters the slope, and the third term modifies the curvature.

Preprocessing

- Weighting: select a weighting option, which will be used to reduce the influence of regions of the spectrum which have a low signal-to-noise ratio.

  The options available are: **None**, **MIR**, **NIR**, **NIRA** and **Signal**. **MIR** and **NIR** should be used if you are working in transmittance in one of those regions of the spectrum. **NIRA** should be used if you are using a NIRA, NIRA II, or NIRM accessory to collect your sample spectrum. **Signal** is useful if your sample spectrum contains regions of high absorbance; where absorbance is high, noise is high and the spectrum is deweighted in these areas.

- First derivative: check the checkbox to use the first derivative of the sample spectrum in the Adulterant Screen.

  Using the first derivative spectrum removes any baseline offset in the sample spectrum and emphasizes narrow spectral features, but also reduces the signal-to-noise ratio.

  > **NOTE:** If you choose to use first derivative preprocessing, then only first derivative spectra will be displayed in the Adulterant Screen results.

Fail limits

- Enable limits: check the checkbox to set fail limits based on the thresholds in the method.

If this option is unchecked, then Spectrum will only report the details of the adulterants identified in the sample without designating the sample as a Pass or Fail.

NOTE: Only if both the level and confidence thresholds are met or exceeded will a sample be designated as a Fail, that is, the sample contains detectable levels of one or more of the selected adulterants. If a high level is reported but the confidence is below the threshold, then the sample will be designated as a Pass.

- Minimum concentration level of Adulterants: enter a value for the minimum total level of adulterant(s) that, in conjunction with the confidence, causes the sample to be designated as a Fail.
- Confidence: select a minimum level of confidence that, in conjunction with the minimum concentration level of adulterants, causes the sample to be designated as a Fail.

  Confidence is a measure of the reliability of the adulterant detection. The options are: Very Unlikely, Unlikely, Possible, Likely and Very Likely.

Results display

- Maximum number of hits: select a value for the maximum number of hits to be reported in the results.
- Maximum number of Adulterants: select the maximum number of adulterants to include in each hit.

  Values of 1–3 are available. For example, a value of 3 will cause the Adulterant Screen to search for results containing combinations of 1, 2 or 3 of the adulterants in the Adulterants Spectra tab. Including more adulterants will increase the time required to complete the process, but will give improved results when samples contain multiple adulterants.

Result limits

- Enable limits: check the checkbox to set limits on the results display.

  If this option is unchecked and only fail limits are enabled, then the details table will show all the hits that exceed the fail limits settings.

  If this option is checked, then the details table will show all the hits that exceed the result limits settings.

  If neither fail limits nor result limits are enabled, the details table will show all the hits up to the maximum number selected in Results display.

NOTE: If you enable the result limits, then the minimum level and confidence settings must be the same or lower than the fail limits. This is to ensure that a result which is designated as a Fail can be displayed.

- Minimum concentration level: enter a value for the minimum level of adulterant that will be reported in the results.

  Hits where one or more adulterants are below this level will not be displayed.
- Minimum confidence: select a minimum level of confidence for the detection of adulteration to be reported in the results.

  The options are: Very Unlikely, Unlikely, Possible, Likely and Very Likely.

Setup Adulterant Screen Wavenumber Range

The Wavenumber Range tab in the Setup Adulterant Screen tab allows you to select the range for comparison of the sample spectrum with the calibration and validation samples, and the adulterant spectra.

NOTE: The settings on the Wavenumber Range tab apply only to the material selected from the Material drop-down list.

Spectral Range

By default, your sample spectrum is compared to each reference spectrum (that is, each adulterant spectrum and each calibration and validation sample, if present) over the range where the spectra overlap.

If you are particularly interested in a region, select **Use defined range**, and then enter the **Start** and **End** values for the range over which you would like the spectra to be compared.

Blank Regions

If you want to exclude regions from the reference spectra:

1. Click **Add Region**.
2. Double-click an entry in the table to edit the value.

   Spectral features within the blank region will not be used in the calculation of the Adulterant Screen results.

To remove a blank region:

- Highlight the row and click **Remove**.

Setup Biodiesel (FAME)

The Biodiesel process command allows you to choose between ASTM D7371 and EN 14078 for the determination of fatty acid methyl esters (FAME) in biodiesel.

Before you use the Biodiesel process:

- Select the standard that you are using, either ASTM D7371 or EN 14078.
- Select the settings for your analysis, such as the Quant method(s) used.
- Select options to print or save the results of the analysis.

1. Select **Biodiesel** from the Setup menu.

   OR

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

   The Biodiesel (FAME) tabs are displayed in the Dialog Pane.

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

2. Select the Biodiesel (FAME) Settings tab, or the Biodiesel (FAME) Results Output tab.

Additional Information

References

ASTM D7371–07: Standard Test Method for Determination of Biodiesel (Fatty Acid Methyl Esters) Content in Diesel Fuel Oil Using Mid Infrared Spectroscopy (FT-IR-ATR-PLS Method).

EN 14078:2003 Determination of fatty acid methyl esters (FAME) in middle distillates (Infrared spectroscopy method).

Setup Biodiesel (FAME) Settings

Use the Biodiesel (FAME) Settings tab to choose between ASTM D7371-07 and EN 14078:2003 standards for the determination of FAME by IR. You can then set up your FAME analysis.

1. Select **Biodiesel** from the Setup menu.

   OR

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

   The Biodiesel (FAME) tabs are displayed in the Dialog Pane.

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

2. Select the Biodiesel (FAME) Settings tab.
3. Select the **Standard**, **ASTM D7371** or **EN 14078**.

   The options displayed on the tab will depend on the standard selected. ASTM D7371 is the default option.

Biodiesel ASTM D7371 Settings

Select the Quant+ methods that will be used for your FAME analysis, and the component for analysis. You can select a method for the low (0–10%), medium (10–30%) and, optionally, high (30–100%) concentration ranges.

Example methods for both the HATR and UATR Sampling Accessories are provided in the default directory: C:\Quant\PLS1\Methods.

Low concentration (0-10%) Quant Method	Browse button that enables you to browse to a partial least squares (PLS1) Quant+ method for the low concentration range.
Medium concentration(10-30%) Quant Method	Browse button that enables you to browse to a partial least squares (PLS1) Quant+ method for the medium concentration range.
High concentration (30-100%) Quant Method	Select the check box if you wish to include a high concentration (30-100%) Quant+ Method in your analysis. The Browse button enables you to browse to a partial least squares (PLS1) Quant+ method for the high concentration range.
Component	Select the Component for analysis for each method. The Component drop-down list contains the components used by each Quant+ method. The default is the first component in the method.

Use Bias Correction	If one, or more, of the Quant+ methods contains independent validation data, this check box will be enabled by default. If **Use Bias Correction** is selected, the process will correct for bias in both offset and slope. If enabled, bias correction will be applied to all the methods that contain independent validation data. If you do not want to use Bias Correction, clear the check box. If none of the Quant+ methods selected contains independent validation data, then the check box will not be available.
Generate Quant diagnostic spectra	If selected, diagnostic spectra (calculated and residual) are generated and saved to C:\Quant\PLS1\Analysis\[Quant Method]\SPECTRA\. The filename format is C[n][source spectrum name].sp or R[n][source spectrum name].sp for calculated and residual spectra, respectively, where n is a number relating to the position of the component in the Component drop-down list.

Bias Correction

Bias correction is used when there is a systematic difference between the spectra of the standards used to calibrate the method and the spectra that require analysis. For example, using a method calibrated on one instrument to predict spectra collected using a different instrument could produce results that are in error, but have a straight-line relationship to the correct values. In this case, Bias Correction allows you to correct for the offset and the slope of this line. Spectrum Quant+ enables you to validate your method by predicting a number of independent standards against a calibration. Use Bias Correction is only available if you have independent validation data in your method.

Additional Information

The Biodiesel FAME ASTM D7371 Analyser Quick Reference Guide and Biodiesel FAME ASTM D7371 Supervisor Standard Operating Procedure provide step-by-step instructions for using Spectrum to determine FAME according to ASTM D7371. They are also available from the Spectrum sub-menu of the PerkinElmer Applications group on the Windows Start menu.

The Spectrum Quant+ on-screen Help also provides more information on validating Quant methods and using Bias Correction.

Biodiesel EN 14708 Settings

Select the Beer's Law Method and settings that will be used for your FAME analysis, and the component for analysis.

Beer's Law Method	Browse button that enables you to browse to a Beer's Law method for the analysis. The default directory is C:\Pel_Data\Quant\Methods.
Component	The Component drop-down list contains the components used by the Beer's Law method. The default is the first component in the method.

Dilution Factor	Enter any Dilution Factor, where: Dilution Factor = (diluted volume)/(original volume) The field is blank by default.
Pathlength	Enables you to specify the pathlength of your liquid cell. Pathlength is only available if pathlength is specified in your Beer's Law method. The field is blank by default. You must ensure that the units for your value are consistent with your Beer's Law method.

Additional Information

The Biodiesel FAME EN 14078 Analyser Quick Reference Guide and Biodiesel FAME EN 14078 Supervisor Standard Operating Procedure provide step-by-step instructions for using Spectrum to determine FAME according to EN 14078. They are also available from the Spectrum sub-menu of the PerkinElmer Applications group on the Windows Start menu.

The Spectrum Beer's Law on-screen Help also provides more information on validating Beer's Law methods.

Additional Information

References

ASTM D7371–07: Standard Test Method for Determination of Biodiesel (Fatty Acid Methyl Esters) Content in Diesel Fuel Oil Using Mid Infrared Spectroscopy (FT-IR-ATR-PLS Method).

EN 14078:2003 Determination of fatty acid methyl esters (FAME) in middle distillates (Infrared spectroscopy method).

Setup Biodiesel (FAME) Results Output

Use the Biodiesel (FAME) Result Output tab to select to automatically print and/or save a report of the results, and to save the results of the analysis as a .csv file.

1. Select **Biodiesel** from the Setup menu.

   OR

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

   The Biodiesel (FAME) tabs are displayed in the Dialog Pane.

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

2. Select the Biodiesel (FAME) Results Output tab.

Printing

Select the check box to automatically print the analysis report to your default printer using the current printer settings.

Reporting

Select the check box to automatically save the analysis report as an .rtf file to the location specified as the **Report Files Folder**. The default is: C:\pel_data\Reports\Biodiesel

The file name will have the format …\[date]\[spectrum name]_[FAME Standard].rtf

Saving Results

Select the check box to automatically save the analysis results to a .csv file with the file name specified in **Results File Name**. The default is C:\pel_data\Results\Biodiesel\Results.csv

Each time the process is run the results are appended to the file.

Additional Information

References

ASTM D7371–07: Standard Test Method for Determination of Biodiesel (Fatty Acid Methyl Esters) Content in Diesel Fuel Oil Using Mid Infrared Spectroscopy (FT-IR-ATR-PLS Method).

EN 14078:2003 Determination of fatty acid methyl esters (FAME) in middle distillates (Infrared spectroscopy method).

Setup Libraries and Search

Before you use the Search process:

- Select the spectral libraries and files that you want to search. See Setup Spectral Libraries.
- Select the wavenumber range over which the comparison should apply, and the maximum number of comparisons to display on the Search tab. See Setup Search Parameters.

1. Select **Libraries and Search** from the Setup menu.

   OR

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

   The Setup Spectral Libraries tab and Setup Search tab are displayed in the Dialog Pane.

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

2. Select the Setup Spectral Libraries tab, or the Setup Search Parameters tab.
3. Use the Setup Results File tab to configure a file of accumulated process data for exporting to another software application for further data analysis.

Additional Information

Library Formats

You can utilize Spectral Libraries from a number of sources, including formats used by PerkinElmer, Thermo and Sadtler.

Browsing and Editing a Spectral Library

If you have write access to the contents of a spectral library, you can add or remove spectra, or amend any Additional Properties associated with spectra within it. See Navigation Pane - Spectral Libraries.

Setup Spectral Libraries

Use the Setup Spectral Libraries tab to select which folders or files are available as Spectral Libraries, and to specify which of the available spectral libraries should be included in the Search Process.

1. Select **Libraries and Search** from the Setup menu.

   OR

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

   The Setup Spectral Libraries tab and the Setup Search Parameters tab are displayed in the Dialog Pane.

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

2. Select the **Setup Spectral Libraries** tab.

   The Spectral Libraries table is displayed, which lists all the folders and files that have been setup as Spectral Libraries.

NOTE:	Libraries in the Common Search Library Directory will be visible to all users. The Common Search Library Directory is defined at Spectrum installation. The default is C:\pel_data\libs In Spectrum ES, libraries in the Common Search Library Directory are added to the Setup Spectra Libraries tab each time a new user workspace is created.

Managing the Spectral Libraries Table

Adding a Spectral Library

Either:

1. Click **Add**, and then select either **Library folder** or **Library files**.

   A user-defined spectral library is a folder containing one or more spectrum files.

   A commercial library is often a single file containing many spectra. You can load PerkinElmer libraries (*.dlb), Thermo Libraries (*.LBD), Sadtler libraries (*.idx, *.sdb, *.sdbx) and PerkinElmer OEM Libraries (*.spl).

   A browse dialog is displayed.

2. Browse to and select the library folder or file that you want to add.
3. Click **OK**.

   A new row is added to the Spectral Libraries table, and a new Spectral Libraries shortcut (such as  for a user-defined library) added to the Spectral Libraries section in the Navigation Pane.

NOTE:	By default, the **Include** check box is selected. If a folder containing spectrum files has been used previously by Spectrum as a spectral library its properties are preserved. These properties include the library's **Name**, **Description**, whether or not it is **Write Protected** (for a folder containing spectra saved in PerkinElmer format), and any Additional Properties applied to the spectra. If this folder or file has been never been used previously by Spectrum as a spectral library, a default

Name (such as 'Library 2') is applied, and the **Include** check box is selected.

OR

- Copy the file folder or file to the Global Search Library Location.

  The default Global Search Library Location is C:\pel_data\libs\. However, another path, such as to a folder on your network, may have been specified when Spectrum was installed.

Any folder or file containing compatible spectra placed in the Global Search Library Location is automatically included in the Spectral Libraries table, and an appropriate Spectral Libraries shortcut added to the Spectral Libraries section in the Navigation Pane.

Naming and Describing a Spectral Library

1. Double-click the **Name** field in the row describing the library, and then enter a more meaningful name.

   The label on the corresponding Spectral Libraries shortcut is updated.

2. Double-click the **Description** field in the row describing the library, and then enter a more meaningful description.

NOTE: The **Name** and **Description** are unique to the folder's or file's use in a spectral library. They have no relationship, for example, to the Name or Description applied to a spectrum when it was collected, or to a filename.

Including or Excluding Spectral Libraries

The table lists all the libraries that you can search, but you do not need to include all of them in every Search.

- Select the **Include** check box for every row you want to include in your Search.

  OR

  Deselect the **Include** check box for every row that you want to exclude from your Search.

Write Protecting Spectral Libraries

For a user-defined library containing spectra in PerkinElmer format, you can select whether or not the folder is **Write Protected**.

NOTE: This function is not available for Commercial Spectral Libraries or user-defined libraries containing spectra saved in other formats.

For every library whose content you wish to protect:

- Select the **Write Protected** check box.

  You, or any other Spectrum user, cannot amend the write-protected spectral library using the Library Editor.

For every library whose content you wish to be able to amend:

- Deselect the **Write Protected** check box.

  You, or any other Spectrum user, can amend the spectral library using the Library Editor.

NOTE: The **Write Protected** check box does not amend the read or write properties of the spectrum files within the folder as seen by Windows or by an external file management program, only the properties of the index file created when you defined the folder as a spectral library. If you revise the content of a spectral library folder outside Spectrum, make sure that it is not write-protected, and then use the Update function in the Library Editor to synchronize the index file with the revised content.

Commercial Spectral Libraries are locked so that their integrity cannot be compromised, as are spectra saved in other formats.

Removing Spectral Libraries

- Select the row containing the library that you want to remove, and then click **Remove**.

  OR

  In the Spectral Libraries section of the Navigation Pane, right-click the link to the Spectral Libraries (such as  for a user-defined library) that you want to remove, and then select **Remove Library** from the shortcut menu.

  The library is removed from the Spectral Libraries table, and its link removed from the Spectral Libraries section of the Navigation Pane, but no files or folders are deleted from disk.

Clearing Spectral Libraries

- Click the Clear button to remove all added Libraries from the Spectral Libraries table, and their links are removed from the Spectral Libraries section of the Navigation Pane, but no files or folders are deleted from disk.

Spectral Library Details

- Select the row containing the library that you want more details on, and then click the Details button to access The Library Browser. The library browser is used to browse, or to search the textural information within, or to open the Library Editor for the selected spectral library.

Additional Information

Sadtler (*.idx) Libraries

To use the Sadtler *.idx legacy format libraries with Spectrum you will need to install the Sadtler Control File found in the root directory of the Sadtler database CD. You do not need to install the control file for the newer *sdb and *.sdbx format libraries.

Copy the ir.ctl file to C:\Program Files\PerkinElmer\Spectrum

NOTE: The Program Files directory will depend upon the operating system language, and the drive Windows is installed on.

Follow the instructions supplied with your Sadtler database CD for the installation of the database files.

Search Parameters

To specify the **Maximum number of the best hits** that the Search process should display on the Search tab, and the **Spectral range** over which the Search process should apply, see Setup Search Parameters.

Setup Search Parameters

Use the Setup Search Parameters tab to specify the **Maximum number of the best hits** that a Search process should display on the Search tab, and the **Spectral range** over which the Search process should apply.

1. Select **Search** from the Setup menu.

   OR

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

   The Setup Search Parameters tab and Setup Spectral Libraries tab are displayed in the Dialog Pane.

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

2. Select the **Setup Search Parameters** tab.

Maximum number of search hits to display

When you run a Search process, each source spectrum is compared with the spectra in the included spectral libraries. Enter the maximum number of search hits to display in the Search tab when a Search process is run.

Spectral Range

By default your spectrum is compared to each reference spectrum (that is, each spectrum in your selected spectral libraries and files) over the range where the spectra overlap.

If you are particularly interested in a region, or if you want to exclude regions from the reference spectra, select **Use defined range**, and then enter the **Start** and **End** values for the range over which you would like the spectra to be compared.

Additional Information

Including Spectral Libraries

To select the spectral libraries and files that you want to search, see Setup Spectral Libraries.

Setup MultiSearch

NOTE: You can only see the Setup MultiSearch tab if you have entered a valid license number for this feature during the installation of your software.

MultiSearch uses the settings on the Search setup tabs, with some additional settings on the Setup MultiSearch tab.

Before you run the MultiSearch process:

1. Select **Libraries and Search** from the Setup menu.

   OR

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

   The four setup tabs are displayed in the Dialog Pane.

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

2. Select the spectral libraries and files that you want to search using the Setup Spectral Libraries tab.
3. Select the wavenumber range for your search and the number of results to display using the Setup Search Parameters tab.
4. Use the Setup Results File tab to configure a file of accumulated process data for exporting to another software application for further data analysis.
5. Click the **Setup MultiSearch** tab.

You can now choose to always include or exclude specific spectra from the MultiSearch process, and also restrict the search to a limited number of components.

Including and Excluding Spectra

You can choose to include up to ten spectra in the MultiSearch, which means that the calculation will assume that those spectra are present in the sample spectrum and then search for any other materials that are also present. You can also choose to exclude up to 1000 spectra from the search if you know that these materials are definitely not present in your sample.

NOTE: Included spectra can be chosen from any folder or library available on your system. Excluded spectra can also be chosen from any folder, but only from a library when its Include checkbox is checked in the Setup Spectral Libraries tab.

- Click the **Browse** button next to the Include section.
  A drop-down list will be displayed which contains the libraries in the Setup Spectral Libraries tab. You can also select spectra from a folder.

To include spectra from a folder:

1. Select the **Spectra** option in the drop-down list.
   An Open dialog will be displayed.
2. Choose the spectra you want to include in the MultiSearch process and click **OK**.

To include spectra from a library:

1. Select the library that contains the spectra you want to include.
   The library is opened in the Library Browser.

2. Select the spectra you want to include in the MultiSearch process.
   Use the search features of the Library Browser to find the spectra in the library.
3. When you have selected the spectra, click the **MultiSearch** button and choose the **Add to Includes** option.
   The Setup MultiSearch tab will be displayed with the selected spectra listed in the Include panel.

NOTE: To return to the Setup MultiSearch tab without selecting any spectra, click the **MultiSearch** button and select the **Go To Setup** option.

Use the same procedure for selecting spectra to exclude from MultiSearch, except that you should select the **Add to Excludes** option in the Library Browser.

Removing Included and Excluded Spectra

There are two ways of removing spectra from the Include and Exclude settings for MultiSearch:

- Uncheck the Include checkbox to remove the spectrum from the process without deleting it from the setup.
  OR
  Select the spectrum name and click the Remove button to delete the spectrum from the setup.

You can use the **Select All** check boxes to select or clear the Include checkboxes for all the spectra in the list.

Number of Components

MultiSearch can search for up to ten components in a mixture. You have two options for restricting this number, which can help to reduce the process time.

To search for a range of component numbers in the mixture:

1. Select the **Variable** option in the Setup MultiSearch tab.
2. Click the up and down arrows to select the **Minimum** and **Maximum** number of components to include in the process.
   MultiSearch will then report results for each number of components in this range.

To search for a single number of components:

1. Select the **Fixed** option in the Setup MultiSearch tab.
2. Click the up and down arrows to select the number of components.
   MultiSearch will then only report results for this number of components.

Hits with Negative Concentrations

Some results in MultiSearch may contain components with calculated levels that are negative. One way these could arise is if a spectrum included by default contains features not found in the sample spectrum, causing MultiSearch to identify an additional component present in a negative concentration to remove these features and minimize the residual spectrum. If you want to view all the hits, perhaps to investigate whether confusing results are occurring as a result of a poorly chosen included spectrum, then check the **Display hits with negative concentrations** check box.

By default, hits where one or more components have negative concentration levels are not displayed, which means that there may be fewer than the specified number of hits reported in some cases.

Fast Mode

Select the "Fast Mode" checkbox to increase MultiSearch processing speed with a possible compromise in accuracy of results.

This option uses a data interval for both reference spectrum (that is, each spectrum in your selected spectral libraries and files) and sample spectrum of 5 cm-1 for the Multi-Search processing. Note that this may affect accuracy, particularly for spectra with sharper features.

Setup Macros

Macros allow you to define instrument settings and collect data, apply previously defined processes, and output your data.

Each of the Macros you set up is appended to the Macros sub-menu in the Process menu, and added to the Macros sub-menu on the Process bar.

You can set up a Macro step-by-step, or from a processed spectrum.

Setting up a Macro Step-by-Step

1. Select **Macros** from the Setup menu, or click  in the Setup section of the Navigation Pane.

   The Dialog Pane lists all the Macros that are currently set up.

   NOTE: The Macros in the Common Macros directory will be visible to all users. The Common Macros directory is defined at Spectrum installation. The default is C:\pel_data\macros.

   In Spectrum ES, Macros in the Common Macros Directory are added to the Setup Macros tab each time a new user workspace is created.

2. If you want set up a new Macro, and create a new row in the list of Macros, click **Add**.

   OR

   If you want to amend a Macro, select a field in the row describing the Macro, and then click **Settings**.

   OR

   If you want set up a new Macro based on an existing Macro, select appropriate row describing the Macro, and then click **Copy**.

   The Setup Macros dialog is displayed, which lists the steps in the chain.

3. Amend the Macro's **Name** and **Description** as required.

   The Macro's name will be used in the Process menu, in the Macros sub-menu.

4. If required, select the Group that the Macro will be added to.

   Assigning a Macro to a group allows you to sort the Macros in the list on the Setup Macros tab. It is important to assign a Macro to a group if you are creating a Macro for Spectrum Touch, as this will determine how the Macro is displayed in that application. See Assigning Macros to Groups.

5. For each step in the Macro, select the **Process** to be applied, and then enter any **Settings** required.

   You can select the Macro step from one of the groups in the left pane. The Macro steps available are divided into the following groups: **Instrument and data collection**, **Processes**, **Search and Compare**, **Quantitation and Verification** and **Reporting and Output**. If you have Spectrum Touch you will have additional options. Expand the appropriate group and then click on the step. The step is added to the Macro. If the selected Process settings require any settings, the appropriate dialog is displayed below the Macro.

   You can change the type of Macro step. A Process selector appears when you hover over any cell in the Process column.

6. If the Macro step you have added will produce spectra, or results, ensure that **Visible** is selected if you want the spectra to be displayed in the Graph, or the results added to the Results Table when the Macro is run.
7. If available, select the **Overwrite input spectra** if you want to replace the input spectrum with the spectrum generated at this step.
8. Select another Macro step in the left pane.

   OR

   Select any cell in the preceding step, and then click **Add Step**.

   A new step is added, and the step numbers updated.

9. To remove a step, select any cell in the step, and then click **Remove Step(s)**.

   The step is removed, and the step numbers updated.

   If you select more than one cell in a column (by selecting while pressing SHIFT or CTRL), and then click **Remove Step(s)**, all the selected steps are removed.

10. To move a step, select any cell in the step, and then click **Up** or **Down**.
11. When you have completed the Macro, click **OK**.

    The Macros list is updated and the Macro Settings dialog closes.

    Your Macro is available in the Process menu, in the Macros sub-menu.

Setting up a Macro from a Processed Spectrum

If you have processed and saved a spectrum, and now want to set up a Macro that will process other spectra in a similar manner:

1. Select **Macros** from the Setup menu, or click  in the Setup section of the Navigation Pane.

   The Dialog Pane lists all the Macros that are currently setup.

2. Click **Add**.

   The Setup Macros dialog is displayed.

3. Amend the Macro's **Name** and **Description** as required.

   The Macro's name will be used in the Process menu, in the Macros sub-menu.

4. Click **Create Macro from File**.

   A Browse dialog is displayed.

5. Browse to and select the file that contains the processed spectrum, and then click **Open**.

   A Macro is created that reflects the processing history.

6. If necessary, amend the Macro as described in Setting up a Macro step-by-step.
7. When you have completed the Macro, click **OK**.

   The Macros list is updated and the Setup Macros Properties dialog closes.

Creating a Macro from an existing Macro

Creating a macro from an existing macro:

- Select the appropriate Macro in the list and then click **Copy**.

  A new Macro is added to the Setup Macros tab with the name Macro [n].

Assigning Macros to Groups

You can assign your Macros to a group. Select the group you would like to assign your Macro to from the **Group Name** drop-down list. The default is **Macros**. The groups available will depend on the groups associated with the Macros listed on the tab.

To create a new group:

1. Select **Create Macro Group** from the Group Name drop-down list.

   The Create Group dialog is displayed.

2. Enter a new Group Name.
3. Click **More details** if you want to modify the color of the group icon.

   This is the icon that will be displayed in the Setup Macro tab (and the icon displayed on the button in Touch software).

4. Click  to display a color selector.
5. Select a new color and then click **OK**.
6. Click **OK** to exit the Create Group dialog.

To modify the name or appearance of an existing group:

1. Select **Modify** from the Group name drop-down list.

   The Modify Group dialog is displayed.

2. Select the Group you want to modify from the Group list drop-down list.
3. If you want to change the name of the group, type a new **Group name**.
4. Click **More details** if you want to modify the color of the group icon.
5. Click  to display a color selector.
6. Select a new color and then click **OK**.
7. Click **OK** to exit the Modify Group dialog.

Importing Macros

To import a Macro:

1. Click **Import** and then browse to the Macro you want to import.
2. Click **Open**.

   In Spectrum ES, if you attempt to import an unsigned Macro you may be prompted for a signature.

   The Macro is added to the list of macros on the Setup Macros tab.

Running a Macro from the Setup Macros Tab

1. Display and select the spectrum or spectra that you want to process.
2. Select the appropriate Macro in the list and then click **Run**.

   The Macro runs. As each process in the Macro is completed, the Results Table tab is updated, and the processed spectrum is added to the Samples View and displayed in the Viewing Area. This enables you to examine the intermediate results in the Macro, as well its final results.

Exporting Macros

To export a Macro:

1. Select the Macro in the list that you wish to export and then click **Export**.

   In Spectrum ES, if you attempt to export an unsigned equation you may be prompted for a signature.

   The Save As dialog is displayed.
2. Enter an appropriate filename for the Macro.
3. If required, browse to the folder you wish to save the Macro to.
4. Click **Save**.

   The Macro is saved to the chosen location and the Save As dialog closes.

Deploying Macros on Other Systems

If you want to transfer a macro that contains data processing steps to a different system for an analyst to run, you need to copy all of the files used by the Macro to *exactly* the same locations on the analyst's PC, *with the same filenames*. If your Macro contains any of the steps listed below, copy the files as described:

- Macro workflow - export the Macro (*.prc) file to the global macros folder on the analyst's PC (usually at C:\pel_data\macros). Alternatively, copy the macro to the analyst's folder, from where it can be imported to the workspace and run using Spectrum or Spectrum Touch.

NOTE: The *.prc file contains details of the Instrument Settings and Data Collection steps.

- Difference - contains a spectrum for subtraction from the sample spectrum. Copy this to the same location on the analyst's PC as used in the original Macro.
- Arithmetic - may contain an operand spectrum with which to perform the operation on the sample spectrum. Copy this to the same location on the analyst's PC as used in the original Macro.

- Compare - copy the spectrum files or folders to the same location on the analyst's PC.

- Libraries and Search - unless the libraries used are supplied with Spectrum, you must copy them on to the analyst's PC (usually at C:\pel_data\libs). New copies of third-party libraries may need to be purchased to avoid infringing copyright.

NOTE: Ensure that the list of libraries in C:\pel_data\libs is exactly the same on both PCs.

- Quant - if you are transferring a Quant method in a *.qmd or *.uqm file, copy it to the same location on the analyst's PC (usually C:\pel_data\quant). If your Quant method uses a *.md file, you need to use the Quant Export tool to convert it to a *.qmz file, and then use the Quant Import Tool in Quant Utilities to transfer the method and all the associated data to the analyst's PC for use in Spectrum.

- Verify - open AssureID Method Explorer and select **File** > **Export** to transfer the AssureID method (*.amd) file to a memory stick. Copy the file to the analyst's PC, open AssureID Method Explorer and select **File** > **Import** to transfer the file into the active database.

- Output - copy the report template and logo filename (if used) into the same locations on the analyst's PC.

- User Application - copy the application to the same location on the analyst's PC.

- Touch screens (Touch Custom Prompt, Touch Background Scan, etc.) - the media file and SOP document (if used) need to be copied to the same locations on the analyst's PC. The images and icons used in the screens are included in the *.prc file.

Signing, Reviewing or Approving a Macro (Spectrum ES only)

NOTE: The Signatures drop-down list is not available if you have loaded a locked workspace.

To Sign a Macro:

1. Select the row containing the Macro you want to sign for and then select **Sign** from the **Signatures** drop-down list.

   The Sign Macro dialog is displayed. This contains the Audit Trail entries for that Macro, and any signatures added previously.

2. To sign the Macro, click **Sign**.

   The Sign dialog is displayed.

3. Enter your **User name** and **Password**.

4. Select the appropriate pre-defined **Reason** from the drop-down list, if applicable.

> **NOTE:** A reason will be required if an administrator has defined Reasons on the Signatures tab for the Macro signature point.

5. Enter any **Comment** required.
6. Click **OK**.

   The Sign Macro entry is added to the Macro Audit Trail.

To Review or Approve a Macro:

Users with the appropriate permissions can import a signed Macro to review or approve it. The options **Review** and **Approve** then become available from the Signatures drop-down list. A Macro can be signed or reviewed more than once, and by more than one reviewer. A Macro can be approved without being reviewed, but once it has been approved it becomes read-only and can no longer be reviewed or edited.

1. Select the row containing the Macro you want to review or approve, and then select **Review** or **Approve** from the **Signatures** drop-down list.

   The Review Macro or Approve Macro dialog is displayed. This contains the Audit Trail entries for that Macro, and any signatures added previously.

2. To review or approve the workspace, click **Review** or **Approve**.

   The Review or Approve dialog is displayed.

3. Enter your **User name** and **Password**.

4. Select the appropriate pre-defined **Reason** from the drop-down list, if applicable.

> **NOTE:** A reason will be required if an administrator has defined Reasons on the Signatures tab for the Review or Approve signature points.

5. Enter any **Comment** required.

6. Click **OK**.

   The review Macro or Approve Macro entry is added to the Macro Audit Trail.

The Macro can now be exported for review or approval by another use, if it has not been approved, or added to a group defualt workspace by an administrator.

> **NOTE:** In Spectrum ES an approved Macro is read-only and cannot be edited. However, you can create a copy which can be edited.

Additional Information

Instrument and Data Collection

Processing Data in a Macro

Enter any settings required by a process step in the same manner as an individual process command. See:

Adulterant Screen

Arithmetic

ATR Correction

Biodiesel

Compare

Convert X

Deconvolution

Derivative

Difference

Equations

Interpolation

Kramers–Kronig

Kubelka–Munk

Libraries and Search

Normalization

Peak Table

Quant

Smooth

Verify

Interactive Baseline Correction (Macro version)

Using Equations in Macros

You can import an existing equation into a Macro. Create an Equation process step, and then select Import on the Equation tab. A browser opens with the default location of the Equations folder displayed.

An Equation entered as a step in a Macro is not included in the Equations submenu in the Process menu. The Equation name is used as a label in the Results tab after the Macro has been applied.

Reporting and Output

See:

- Output
- Conditional Flow
- Custom Prompts
- User Applications

Touch Macros

If you have Spectrum Touch Developer software installed on your system, you can create special Macros known as Touch Apps which can be run on touch-screen computers. A number of extra features are available with the Spectrum Touch software to create these macros:

Touch Custom Prompt, Touch Sample Scan, Touch Background Scan and Touch Ready Checks.

Some examples of Touch Apps are supplied with your software. See About Touch Apps for more details about the steps in these Apps and how they are set up to carry out an analysis.

Setup Macros - Instrument and Data Collection

The Instrument setup and Data collection Macro steps allow you to use a Macro to collect spectra.

Instrument Setup

Add an **Instrument setup** step to a Macro, and then select from a previously saved set of instrument settings. Alternatively, select **Import instrument settings** and import a *.set file.

You can allow the Macro to be run using a different, but compatible, instrument to the one used to develop the Macro by selecting **Allow compatible instruments.** A compatible instrument has the same detector, source, beamsplitter and accessory as the one used to create the instrument settings. If this option is not selected, then when the Macro is run you must be connected to the same instrument that was used to create the instrument settings.

If you have Spectrum Touch Developer software installed on your PC, you can choose to activate two further options. Select **Show force bar** to monitor the force being exerted on the sample before collecting the spectrum, if an ATR accessory is being used. This option has no effect with other accessories. Select **Show spectrum** to display the background and sample spectra on the screen during monitoring and scanning.

Instrument Settings files are loaded or created on the Setup Instrument Basic tab. For details of how to save and export instrument settings, see Load and Save.

Data Collection

NOTE: If you create a Macro containing a Data Collection step, but do not include an Instrument Setup step, the current instrument settings will be used to collect the data.

Add a **Data collection** step and select either to use the current Sample Table or a previously saved Sample Table setup. The list includes all available files saved in Sample Table Setups. If you want to import another file, select **Import setup** and browse to the *.smt file (or *.ssmt file for Spectrum ES) you wish to import. For details of how to save and export sample table setups, see Setups.

If you select **Autonames**, then the Auto-name template and Auto-description template defined on the Setup Instrument Auto-Name tab will be used to enter a unique Sample ID and Description for your spectra. Also, if the **Enable Pathlength** option is selected on the Setup Pathlength tab, then the current pathlength will be used for all spectra collected.

Select an appropriate **Auto Save** location for the spectra that will be collected.

Your Sample Table setup can contain details of the column formatting, including Custom Columns. If you also wish to import details of the samples you wish to collect, for example if you are using a Laboratory Information Management System (LIMS), select **Load sample table content** and browse to a *.csv file. This will replace any rows in the current Sample Table or Sample Table setup. See Import CSV for more information on how to format a *.csv file.

The following four settings only apply to Macros run in Spectrum. They have no effect for Macros run in Spectrum Touch (Touch Apps):

If you select **Mandate all samples**, then the user must collect all the samples defined in the Sample Table before continuing with the next step in the Macro.

If you select **Show prompt at start of step**, a message will be displayed at the appropriate step in the Macro stating that a Data Collection step is in progress.

If you select **Show sample table,** the Sample Table tab will be displayed when the Data Collection step runs. If not, the Live tab will be displayed during the scan.

Macros usually process any spectra selected in the Graph when the macro is started. If you select **Only use data collected in this step in subsequent macro steps**, then Spectrum will discard any data selected in the Graph or collected in a previous macro Data Collection step. Only the data collected in this macro step will be used in subsequent macros steps, until superseded by a later Data Collection step with this option selected.

You can use this option to make sure that no spectra accidentally selected in the Graph are processed using the macro; or if you want to process and output data from a data collection step, clear it and then collect some more data for processing in a different way, as part of the same macro.

Allow Touch to import samples is only available if you have Spectrum Touch Developer software installed on your PC. If selected, you can choose to import a previously collected spectrum for analysis.

Setup Macros - Interactive Baseline Correction

Interactive Baseline Correction (i-Baseline) enables to you to specify where the base points of your spectrum lie. You can correct the baseline over the whole of the spectrum or the correction can be applied to a limited range of the spectrum.

1. Click the **Add** button to add a new base point to the table.

   The value is added to the Base Points table.

   If **Find Min in Range** is selected, range Start and End columns are added to the Base Points table. The baseline point used will be the minimum value in the defined range.

2. To remove a base point, click in the row in the Base Point table you want to remove and then click **Remove**.

   The base point is removed from the baseline.

3. Repeat steps 2 and 3 to identify as many base points as you require.

   If only one point is added, a horizontal baseline is used; and if two points are added a linear baseline passing through the points is used. If multiple base points are added, a curve intersecting the spectrum at these points is constructed using a cubic spline, and this curve is subtracted from the original spectrum.

   If **Restrict Range** is selected, an offset equal to the absorbance at the highest frequency base point is subtracted from the region between the start of the spectrum and the start of the selected region. An offset equal to the absorbance at the last frequency base point is applied to the region between the end of the selected range and the end of the spectrum.

Additional Information

You can also correct the baseline of your spectra automatically. See Baseline Correction.

Setup Macros – Report Designer Output

Report Designer Output is a process command that can be set up as part of a Macro.

NOTE:	Report Designer Output is only available as part of a Macro; it is not found in the Process menu.

1. Display the Macro Settings dialog, which lists the steps in the chain.
2. To add another step, select any cell in the preceding step, and then click **Add Step**.

   A Process selector appears when you hover over any cell in the Process column.
3. Select Report Designer Output from the **Process** drop-down list.

   The output setup tabs are displayed.

Reports Options and Report Edit tabs

Save report	Select this check box to save the process report in the folder specified.
Template filename	Browse button that enables you to specify the path for your XML report template.
Print report	Select this check box to print the report to the currently active printer.
Show saved report	Select this check box to display the report once it is generated and saved.
Report format	Select the **Report format** from the drop-down list. The options are *.rtf and *.pdf.
Folder for reports	Browse button that enables you to specify a folder location for your report. The default location for macro reports is C:\pel_data\reports.
Sections	Select the sections to be included in the report from the Section Name list, which is derived from the template.

Spectra Export tab

Export Format	Select the Export format from the drop-down list. The options are: *.csv, Custom, *.dx, *.asc and *.sp. Custom is the format set up on the Setup Export tab.
Export Spectra	Select this check box to enable the export of spectra in the selected format to the folder for exported results below.
Overwrite	Select this option to overwrite any existing spectra with the name.
Folder for exported spectra	Browse button that enables you to specify a folder location for your exported spectra. The default location is C:\pel_data\spectra.

Results Export tab

Export Format	Select the export format from the drop-down list. The options are: *.csv, *.xls and *.xlsx.
Export to folder	Select this check box to enable the export of results in the format specified to the folder for exported results.
Folder for exported results	Browse button that enables you to specify a folder location for your exported results.
Export to file	Select this check box to enable the export of results to the file specified in the appropriate export format.
Filename	Browse button that enables you to specify a filename for your results file.
Overwrite	Select Overwrite if you wish to overwrite the results file when the macro is run.
Append to file	Select Append to file if you wish to add the results to the file each time the macro is run.

Ready Checks Export tab

Export Format	Select the Export format from the drop-down list. The options are: *.csv, *.xls and *.xlsx.
Export to folder	Select this check box to enable the export of Ready Check results in the format specified to the folder for exported results.
Folder for exported results	Browse button that enables you to specify a folder location for your exported Ready Check results.
Overwrite	Select Overwrite if you wish to overwrite the Ready Check results file when the macro is run.
Append to file	Select Append to file if you wish to add the Ready Check results to the file each time the macro is run.

NOTE: The tabs below are available if you select the **Output** step when you are editing a macro that was created using Spectrum 10.4.3 or earlier.

Reports Options and Template tabs

Save report	Select this check box to save the process report in the folder specified.
Print report	Select this check box to print the report to the currently active printer.
Report format	Select the **Report format** from the drop-down list. The options are *.rtf and *.pdf.
Template filename	Browse button that enables you to specify the path for your XML report template. The default template for macro reports is MacroReportTemplate.xml.
Folder for reports	Browse button that enables you to specify a folder location for your report. The default location for macro reports is C:\pel_data\reports.
Logo filename	Browse button that enables you to specify the folder location for your company logo, which will be added to the header of the report.
Sections	Select the sections to be included in the report from the Section Name list, which is derived from the template.

Setup Macros - Conditional Flow

You can use conditional flow steps in your macro to add logic statements that allow looping and branching within a Macro.

Add a Conditional Flow step to the macro and then select the appropriate Logic statement. The Logic statements available are **IF**, **ELSE**, **ELSE IF**, **END** and **WHILE**.

For IF, ELSE IF and WHILE logic statements, you set up an Equation that defines a variable whose condition must equate to TRUE for the statement to proceed.

Each set of logic statements must contain an End step. The last step in a macro does not have to be an End step; you can continue with other macro steps.

IF	The Equation in an IF statement defines a variable whose condition must equate to TRUE for the statement to proceed. Performs the next steps up to ELSE or END if the Equation condition is TRUE.
ELSE	Performs the next steps up to IF, WHILE or END if the "If" Equation condition is FALSE.
ELSE IF	Performs the next steps up to IF, ELSE, WHILE or END if the Equation condition is TRUE.
WHILE	Repeats steps up to END while the Equation condition is TRUE.
END	Ends IF, ELSE IF, ELSE or WHILE.

IF ... ELSE ... END

IF	Performs the next steps up to Else if the IF condition is TRUE.
ELSE	Performs the steps following the Else statement if the IF condition is FALSE.
END	Ends IF or ELSE.

For example, you can set up a macro to collect a spectrum and then generate a Report only if the ordinate value at 2000 cm^{-1} is ≥60%T. If the value is <60%T, you can display a Custom Prompt telling the user that there is a problem with the sample:

1. Set up the Data Collection step.
2. Add a Conditional Flow step with the logic **IF**.
3. Enter the Equation **Yval[All,2000]≥60**.
4. Add an Output step and set up the reporting options.
5. Add a Conditional Flow step with the logic **ELSE**.
6. Add a Custom Prompt step, and set up a warning message.
7. Add a Conditional Flow step with the logic **END**.

In this example, the IF statement has used an Equation based on a simple Function. You set up an Equation for the IF statement that uses Variables generated using other Equations.

IF ... ELSE IF ... ELSE ... END

IF	Performs the steps up to Else If, if the IF condition is TRUE.
ELSE IF	Performs the steps up to ELSE, if the Else If condition is TRUE
ELSE	Performs the steps up to END, if the IF and ELSE IF conditions are FALSE.
END	Ends IF, ELSE IF or ELSE.

WHILE

The WHILE statement allows you to set up looping. The macro will perform the steps after the WHILE statement until the WHILE condition is FALSE.

For example, if you are using a UATR Sampling Accessory, you may have poor contact with the sample if the pressure arm is not deployed correctly. You might then want to set up a WILE statement after a Data Collection step to define appropriate limits for the ordinate value at a particular wavenumber value. You could then add a step to display a Custom Prompt instructing the user to lower the pressure arm to improve sample contact, followed by a repeat of the Data Collection step.

When the ordinate value indicates that a good-quality spectrum has been obtained, the WHILE statement will be FALSE, and any subsequent steps in the macro will then be executed.

Additional Information

You can "nest" logic statements. For example, you can add an "IF.. ELSE ... END" construct between IF and ELSE steps.

Setup Macros - Custom Prompts

You can add a step to your macro that will display a dialog to the user. The can contain any important warning message or instructions to help the user collect and process their data. When the user clicks **Continue** on the Custom Prompt dialog, the next step of the macro is run.

To set up a Custom Prompt:

1. Enter a **Caption** for the dialog.

   This will be displayed in the Title bar of the dialog.

2. Enter the **Prompt** text.

3. If you want to include an **Image** on the dialog, select one from the drop-down list.

   The options are **Information**, **Question**, **Warning**, **Error** and **None**.

4. If you want to include a Stop button on the dialog, select **Show Stop button**.

   This allows the user to halt the macro at the Custom Prompt step.

5. When you have completed the design for your custom prompt, click **Preview** to display the dialog.

Setup Macros - User Applications

The User Application option allows to select a third-party program to be run as part of a Macro.

You can browse to select the **Program Path** to any executable (*.exe) file to be run as part of the Macro step. You can then add any **Arguments** that will be used by the application. For example, you might include a file location for files that will be used by the third-party program.

If you wish to use data created during earlier Macro steps, you will need to include an Output step before the User Application step to output the files to a folder.

If the **Pause macro** check box is selected, the Macro will stop until the **OK** button is clicked to indicate that the user has completed the work in the third-party application.

The User Application option is also a way to create a launcher for a third-party executable that you use often. You can add the Macro icon to any toolbar in Spectrum to launch an application at a single click.

For information about adding or removing toolbar buttons or menu items, see Customizing Toolbars and Menus.

Setup Equations

Equations are process commands that perform calculations on one or more spectra, or on the data obtained from other processes.

You setup an equation using Functions and Operators, and can format the results using an If … Then … Else construction.

- Select **Equations** from the Setup menu.

  OR

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

  The Setup Equations tab is displayed in the Dialog Pane.

Each of the equations you set up is appended to the Equations sub-menu in the Process menu, to the Equations drop-down list on the Process bar and to the Equations section of the Navigation pane.

NOTE: The equations in the Common Equations Directory will be visible to all users. The Common Equations Directory is defined at Spectrum installation. The default is C:\pel_data\equations

In Spectrum ES, Equations in the Common Equations Directory are added to the Setup Equations tab each time a new user workspace is created.

Adding or modifying an Equation

1. If you want set up a new Equation, and create a new row in the list of equations, click **Add**.

   OR

   Select a field in the row describing the equation you want to amend, and then click **Settings**.

   The Equations section of the Navigation pane opens with the Equation displayed in the Dialog pane.

2. Set up the Equation as described in Navigation Pane - Equations.

   The Equations Pane stays open so that you can continue with Result Formatting or select another Equation in the Equations pane. If you wish to return to the Setup Equations tab click **Back**.

   Your Equation is available in the Equations sub-menu in the Process menu.

Removing Equations

- Select the row containing the Equation that you want to remove, and then click **Remove**.

  The Equation is removed from the table, the Equations sub-menu in the Process menu, and from the list in the Equations section of the Navigation pane.

  You can select multiple rows. You will be prompted for confirmation for each Equation selected.

Importing Equations

To import an Equation:

1. Click **Import** and then browse to the Equation you want to import.
2. Click **Open**.

   In Spectrum ES, if you attempt to import an unsigned Equation you may be prompted for a signature.

   The Equation is added to the list of Equations on the Setup Equations tab.

Exporting Equations

To export an equation:

1. Select the equation in the list that you wish to export and then click **Export**.

   In Spectrum ES, if you attempt to export an unsigned equation you may be prompted for a signature.

   The Save As dialog is displayed.
2. Enter an appropriate filename for the equation.
3. If required, browse to the folder you want to save the equation to.
4. Click **Save**.

   The equation is saved to the chosen location and the Save As dialog closes.

Running an Equation

- Display and select the spectrum or spectra that you want to process, select the Equation you want to apply and then click **Run**.

  The Results Table tab is updated. If the result amends the source spectrum, the processed spectrum is displayed in the Viewing Area and added to the Samples View.

  Processed spectra are not saved to disk automatically.

Signing, Reviewing or Approving an Equation (Spectrum ES only)

> **NOTE:** The Signatures drop-down list is not available if you have loaded a locked workspace.

To Sign an Equation:

1. Select the row containing the Equation you want to sign for and then select **Sign** from the **Signatures** drop-down list.

   The Sign Equation dialog is displayed. This contains the Audit Trail entries for that Equation, and any signatures added previously.

2. To sign the Equation, click **Sign**.

   The Sign dialog is displayed.

3. Enter your **User name** and **Password**.
4. Select the appropriate pre-defined **Reason** from the drop-down list, if applicable.

   > **NOTE:** A reason will required if the Administrator has defined Reasons on the Signatures tab for the Equation signature point.

5. Enter any **Comment** required.
6. Click **OK**.

   The Sign Equation entry is added to the Equation Audit Trail.

The Equation can now be exported for review or approval by a user with the appropriate permissions.

To Review or Approve an Equation:

Users with the appropriate permissions can import a signed Equation to review or approve it. The options **Review** and **Approve** then become available from the Signatures drop-down list. An Equation can be signed or reviewed more than once, and by more than one reviewer. An Equation can be approved without being reviewed, but once it has been approved it becomes read-only and can no longer be reviewed or edited.

1. Select the row containing the Equation you want to review or approve, and then select **Review or Approve** from the **Signatures** drop-down list.

   The Review Equation or Approve Equation dialog is displayed. This contains the Audit Trail entries for that Equation, and any signatures added previously.

2. To review or approve the workspace, click **Review** or **Approve**.

   The Review or Approve dialog is displayed.

3. Enter your **User name** and **Password**.
4. Select the appropriate pre-defined **Reason** from the drop-down list, if applicable.

   > **NOTE:** A reason will required if an administrator has defined Reasons on the Signatures tab for the Review or Approve signature points.

5. Enter any **Comment** required.

6. Click **OK**.

   The Review Equation or Approve Equation entry is added to the Equation Audit Trail.

The Equation can now be exported for review or approval by another user, if it has not been approved, or to be added to a group default workspace by an administrator.

Touch Macro Options

If you have Spectrum Touch Developer installed on your computer, an extra group of selectable steps is available in the Macros setup screen called Touch Macros. This allows you to select the steps that are specific to Touch Macros (also called Touch Apps), customize the screens that will appear, and set up the Ready Checks that will be carried out.

Each option contains a table and screen preview showing how the screen will appear when the macro is run. To customize the screens:

1. Click the item that you want to change in the table or on the screen preview.

   A yellow box appears around the item in each location.

2. Make the required changes in the table.

   To change the screen title, instruction title, instruction text and button caption, type the new text into the appropriate table entry.

   To change the image, browse to a new image file using the button on the right side of the image entry in the table.

The changes you make are shown in the screen preview.

1. Double-click the screen preview to view a full-size version.
2. To close the full-size screen preview, click **Close** in the top left corner.

Touch Custom Prompt

The Touch Custom Prompt is used to configure a step in the macro where instructions are being given to the analyst. Two Prompt Templates are available from the drop-down list: **Generic Prompt** and **Sample Preparation**.

Generic Prompt

The following features can be customized using this template:

- Prompt header - the main title on the screen
- Instructions title - the title of the set of instructions
- Instructions - the text for the instruction step(s)
- Next button text - the label on the button that moves on to the next step in the macro
- Prompt image file - the folder location of the image that you want to display
- Media file - the folder location of a media (*.wmv) file that can be viewed from the macro

Sample Preparation

The following features can be customized using this template:

- Prompt header - the main title on the screen
- Instructions title - the title of the set of instructions
- Instructions - the text for the instruction step(s)

- SOP button text - the label on the button that connects to a standard operating procedure
- Next button text - the label on the button that moves on to the next step in the macro
- Prompt image file - the folder location of the image that you want to display
- SOP file path - the folder location of the file containing the standard operating procedure document

Touch Sample Scan

The Touch Sample Scan is a step in the macro when a spectrum of the sample is collected by the spectrometer. Templates suitable for specific accessories are available from the Prompt Template drop-down list. The following features can be customized using these templates:

- Prompt header - the main title on the screen
- Instructions title - the title of the set of instructions
- Instructions - the text for the instruction step(s)
- Edit button text - the label on the button that allows you to edit the details of the current sample
- Background button text - the label on the button that forces a background spectrum to be collected
- Scan button text - the label on the button that collects a sample spectrum
- Prompt image file - the folder location of the image that you want to display

Touch Background Scan

The Touch Background Scan is a step in the macro when a background spectrum is collected by the spectrometer.

1. Select how frequently you want to collect a background using the Background Collection drop-down list.

   Choose **If necessary**, **After number of samples** or **After elapsed time (minutes)**.

   The counters for the number of samples and elapsed time options start at zero when the macro is run, and only apply while the macro is open. **If necessary** means that a new background will be collected only if there is no valid background for the current instrument settings.

2. Enter the number of samples or minutes between each background scan as appropriate in the text box.

3. Check the checkbox labeled **Force background for first sample** if you want to collect a background for the first sample in the macro's sample table.

Templates suitable for specific accessories are available from the Prompt Template drop-down list. The following features can be customized using these templates:

- Prompt header - the main title on the screen

- Instructions title - the title of the set of instructions
- Instructions - the text for the instruction step(s)
- Next button text - the label on the button that collects a background spectrum
- Prompt image file - the folder location of the image that you want to display

Touch Ready Checks

Ready Checks can be included in a Touch macro. You must first configure all the checks you want to run using Spectrum (see Setup Ready Checks). Then use the tabs on the Touch Ready Checks screen to set up how the checks are to be run in the macro.

Instrument Checks Setup

1. In the Touch Ready Checks screen, click the Instrument checks setup tab.
2. If you do not want to use the current settings, click **Import Settings**.
3. Browse to the Ready Check Setup file (*.rcset) that you want to use in the macro, and click **Open**.

Now select which Ready Checks you want to run and how often:

1. Check the **Include** checkbox next to each Ready Check you want to run during the macro.
2. For each check you want to run, choose **Hours**, **Samples**, or **Hours or Samples** in the Check Frequency column.
3. Enter the required Hourly Interval or Sample Interval as appropriate.

   If **Hours or Samples** is selected, then the Ready Check is repeated whenever one or other of the intervals has elapsed. The counters for these options start at zero when the macro is run, and only apply while the macro is open.

Now decide what to do if a Ready Check fails or contains an error:

1. Check the checkbox labeled **Proceed on error** to permit the analyst to continue with the macro if one or more tests fail.
2. Check the checkbox labeled **Allow repeats** to permit the analyst to repeat a failed test.

Touch Preview

The Touch screen for the Ready Checks can be configured using the Touch Preview tab, in a similar way to the Touch prompts described above. The following features can be customized using this prompt:

- Prompt header - the main title on the screen
- Halt button text - the label on the button that stops the running of the Ready Checks
- Scan button text - the label on the button that moves on to the next step in the macro
- Prompt image file - the folder location of the image that you want to display
- Progress icon file - the folder location of the icon to show that a Ready Check is in progress

- Pass icon file - the folder location of the icon to show that a Ready Check has passed
- Fail icon file - the folder location of the icon to show that a Ready Check has failed
- For each Ready Check:
  - Pre-check prompt - the text to display before the Ready Check runs
  - Post-check prompt - the text to display after the Ready Check has run
  - Pass message - the text to display if the Ready Check passes
  - Fail message - the text to display if the Ready Check fails
- In-progress message - the text to display while the Ready Check is running
- All checks pass message - the text to display if all Ready Checks have passed
- Failed checks message - the text to display if one or more Ready Checks have failed
- Rerun button text - the label on the button that reruns failed Ready Checks
- Report button text - the label on the button that displays a report of the results for the Ready Checks

You can click a button or Ready Check name in the preview screen to find the corresponding
features in the table.

To view a full-size version of the Touch screen:

➢ Double-click the preview screen.

To close the full-size preview, click **Close** in the top right corner.

User Images

You can customize the Login screen of Spectrum Touch macro to show a specific image for each user.

1. Copy the image into Program Files (x86)/PerkinElmer/Spectrum/Images (for 64-bit systems) or Program Files/PerkinElmer/Spectrum/Images (for 32-bit systems).

   The image must be a .png file. A small image works best, ideally 64 × 64 pixels.

2. Rename the image with the username of the user in Spectrum.

   For example, the image for the Administrator user would be Administrator.png.

The image will appear on the user's login button when the login screen is displayed in Spectrum Touch.

About Touch Apps

A Touch App can be set up in a similar way to a Macro, but the order of the steps is more important as it controls the workflow that the user of the App will follow. This can be illustrated using the following Touch App examples which are supplied with your software.

NOTE: We recommend that you display the Macro Settings dialog for the Touch App you are using while you are reading the description in the Help.

Compare Touch App Example - Polymer ID

The aim of this Touch App is to identify polymer samples by scanning the infrared spectrum using an ATR accessory, and then comparing the spectrum against a folder of spectral references.

The steps included in the App are described below. To view more information about each step, highlight the *Polymer ID* macro in the Macro Setup tab and click **Settings**. You can run the App from the Main Menu of Spectrum Touch or from the Macro Setup tab in Spectrum.

Touch Custom Prompt

This screen presents the analyst with a summary of the purpose of the App. The following configuration changes were made to the default settings:

- The Sample Preparation Prompt Template was used because, unlike the Generic Prompt Template, it includes an SOP button that can be linked to a Standard Operating Procedure (SOP) document.
- The Prompt Header, Instructions and Prompt image file were modified to be appropriate to the analysis.

An SOP document can be included by specifying a file under **SOP file path**. Since no file is selected, the SOP button will be disabled when the App is run.

Instrument setup

This step configures the instrument with appropriate settings to ensure that the scanned spectra have sufficient signal-to-noise ratio and are compatible with the reference spectra.

Before creating the App, the instrument was configured as desired, and the settings saved. When editing the App, these saved settings can be selected in the instrument setup step.

Data Collection

The Data Collection step must come before any background or sample scan steps, as it sets up the sample table properties and certain aspects of the data collection behavior. In this case, we have enabled the option **Allow Touch to import samples** so that the App can also be used with spectra that have already been measured and saved to disk.

Touch Background Scan

This step defines what information is shown to the analyst before starting the background scan, and also controls the frequency of background measurements. In this case, we have set the background interval to 30 minutes, and specified that a background should always be measured before the first sample in a batch. As with the Custom Prompt step at the start of the App, the step has been customized with an appropriate image and text.

Touch Sample Scan

This step determines the appearance of the prompt screen shown before scanning the sample spectrum, and is the ideal place to provide information about sample preparation, if any is required. In this case we have provided instructions for how to obtain representative spectra of hard and soft polymer samples.

When the analyst presses **Next** on this screen, the sample scan will start. All subsequent steps will have access to the spectrum measured in this step.

Compare

The only processing step in this App is a Compare step. The configuration of this step is exactly the same as in the Setup menu in Spectrum. In this case we have included a folder of polymer spectra in the Setup Compare References tab, and used the default settings in the Setup Compare Parameters tab.

Output

It is essential to include an output step in a Touch App, because it is this step that displays the results to the analyst. This App has been configured to produce a printable report. On the Report Options tab, **Save Report** has been selected. On the Report Template tab, **.pdf** has been chosen as the report format, and several sections of the template have been selected. It is recommended to use the default template and select the desired sections from the list. To see what information is contained in each section, select all of them and run the App. This will produce a full report from which you can select the sections that are relevant for your analysis.

Quant Touch App Example - Polystyrene Thickness

The aim of this Touch App is to estimate the thickness of a polystyrene film by comparing the measured peak height against a calibration developed in Spectrum Quant software.

The steps included in the App are described below. To view more information about each step, highlight the *Polymer thickness* macro in the Macro Setup tab and click **Settings**. You can run the App from the Main Menu of Spectrum Touch or from the Macro Setup tab in Spectrum.

Touch Custom Prompt

This screen presents the analyst with a summary of the purpose of the App. The following configuration changes were made to the default settings:

- The Sample Preparation Prompt Template was used because, unlike the Generic Prompt Template, it includes an SOP button that can be linked to a Standard Operating Procedure (SOP) document.
- The Prompt Header, Instructions and Prompt image file were modified to be appropriate to the analysis.

An SOP document can be included by specifying a file under **SOP file path**. Since no file is selected, the SOP button will be disabled when the App is run.

Instrument setup

This step configures the instrument with appropriate settings to ensure that the scanned spectra have sufficient signal-to-noise ratio for use with the Quant method.

Before creating the App, the instrument was configured as desired, and the settings saved. When editing the App, these saved settings can be selected in the instrument setup step.

Data Collection

The Data Collection step must come before any background or sample scan steps, as it sets up the sample table properties and certain aspects of the data collection behavior. In this case, we have enabled the option **Allow Touch to import samples** so that the App can also be used with spectra that have already been measured and saved to disk.

Touch Background Scan

This step defines what information is shown to the analyst before starting the background scan, and also controls the frequency of background measurements. In this case, we have set the background interval to 30 minutes, and specified that a background should always be measured before the first sample in a batch. As with the Custom Prompt step at the start of the App, the step has been customized with an appropriate image and text.

Touch Sample Scan

This step determines the appearance of the prompt screen shown before scanning the sample spectrum, and is the ideal place to provide information about sample preparation, if any is required.

When the analyst presses **Next** on this screen, the sample scan will start. All subsequent steps will have access to the spectrum measured in this step.

Quant

The only processing step in this macro is a Quant step. The configuration of this step is exactly the same as in the Setup menu in Spectrum. In this case, we have imported the Polystyrene film thickness method. To view the details of this method, open it in Spectrum Quant software.

Output

It is essential to include an output step in a Touch App, because it is this step that displays the results to the analyst. This App has been configured to produce a printable report. On the Report Options tab, **Save Report** has been selected. On the Report Template tab, **.pdf** has been chosen as the report format, and several sections of the template have been selected. It is recommended to use the default template and select the desired sections from the list. To see what information is contained in each section, select all of them and run the App. This will produce a full report from which you can select the sections that are relevant for your analysis.

Conditional Flow Touch App Example – Benzene

This Touch App contains a more complex macro that runs two quantitative methods and selects which results to report, based on the concentration of the sample. The analysis is for benzene in gasoline, using a transmission measurement through a liquid cell with KBr windows and a pathlength of 0.025 mm. If you have the correct type of cell, you can prepare suitable samples for analysis by adding benzene to isooctane, at levels between 0 and 5 % by volume. Alternatively, some example spectra have been provided (in C:\pel_data\spectra\Benzene example spectra) that can be imported into the App when it is running in Spectrum Touch.

The App carries out the following operations:

- Configuring the instrument
- Scanning the background spectrum
- Scanning the sample spectrum
- Running the low-concentration Quant method (result is "benzene_low")
- Running the high-concentration Quant method (result is "benzene_high")
- Reporting the results

A Conditional Flow structure is used in the App to decide which results to report to the analyst:

IF benzene_low > 1.3 and benzene_high > 1.3

– Report results from the high-concentration Quant method

ELSE

– Report results from the low-concentration Quant method

END

The setup of the important steps in the App is described in more detail in the table below. The numbers in the first column refer to the step number in the Macro Settings dialog. We recommend that you view the table with the Macro Settings dialog open on your screen.

Step	Step Name	Details
3	Data Collection	Because this Quant method requires pathlength normalization, the sample table used by the data collection step includes the column "Pathlength (mm)". This column was activated by using **Setup** > **Pathlength** to enable the Pathlength feature before the sample table was saved for use in the App.
6	Quant	A single Quant step can run multiple methods. In this App, two PLS1 Quant methods are used, BENZ_HI.MD and BENZ_LO.MD. To enable pathlength normalization, select the method. If the Quant method has been configured with pathlength normalization, a drop-down selector labeled **Pathlength** will appear in the Parameters box. Either enter a fixed pathlength in millimeters or select **Pathlength in Spectrum Header** to use the value entered by the user when the Touch App is run.

7-8	Equations	Two equations are used in steps 7 and 8 to define constants that will act as thresholds for the Mahalanobis (M) distance and residual ratio from the PLS1 predictions. High values for these quantities for an analysis show that the result from the Quant method is less accurate. The Visible checkbox is unchecked so that these values are not shown in the reported results.
9	Conditional Flow	This step begins the IF... ELSE... END routine that selects which results to report. The IF condition is specified as a Boolean expression using the same syntax as Equations. The <Variables> list shows the numerical variables available within the App that can be used in the Equation. Steps 10-13 will only occur when the IF condition (that both Quant methods return values greater than 1.3) is true.
10	Equation	The equation in this step, called "Range Used", reports to the user which of the two methods was used in this branch of the routine. Since equations must be numerical, the value is set to zero and the Results Formatting tab is used to set up conditional formatting that replaces the results with the text "High".
11-13	Equations	These steps set the outputs "Benzene", "M Distance" and "Residual Ratio" to the corresponding results of the high-concentration Quant method. Steps 12 and 13 also have conditional formatting to apply tests to the M distance and residual ratio to warn the user if they are above the thresholds set in steps 7 and 8.
14	Conditional Flow	This ELSE step begins the block of steps that occur only when the IF condition defined in step 9 is false, that is, one or both Quant methods return values less than or equal to 1.3.
15-18	Equations	These are the equivalent steps to 10-13 relating to the low-concentration Quant method. When you set up a structure like this, with the same equations defined in multiple branches of a conditional flow structure, you will receive a warning that the same equations have been defined multiple times. If you are certain that only one of the branches can occur at a time, dismiss the warning to continue developing the App.
19	Conditional Flow	This END step is needed to complete the conditional flow structure. All further steps in the App will occur regardless of the outcome of the IF condition. In this App, only an Output step is present.