SPECTRUM

User's Guide

PerkinElmer®

Audit Trail (ES only)

Audit Trail (Spectrum Enhanced Security only)

All data, settings and actions carried out by a user in Spectrum ES are saved to a database, grouped into user environments known as workspaces. A workspace is an collection of software settings, custom layouts, objects such as equations and macros, and user data. A new workspace, with a unique Workspace ID, is created each time a user starts Spectrum ES (unless the user selects to reload their current workspace next time, when they exit the software).

A Spectrum database has a default maximum size of 5 GB. When it reaches this size, a new database is automatically created. Refer to Additional Information below for the default location of the database.

Any activity that affects the way data is collected or stored is recorded in the workspace Audit Trail. Entries are written to the Audit Trail at the point where a change that has been made affects the recording of data. For example, changes to instrument settings are only applied to the instrument when the Scan button is pressed, and so that is when the change is recorded in the Audit Trail. This means that any changes made to settings that are subsequently cancelled without being used are not recorded.

Some changes to the Audit Trail may require a "signature" from the user. Details of the signature will be added to the Audit Trail. These signature points are predefined and cannot be added to, but members of the Administrators group can define which actions will require a signature. Refer to Signatures for more information.

When the Audit Trail dialog is displayed, the Audit Trail of the current workspace is shown by default. However, you can use the filters on the Audit Trail dialog to view other workspaces in the database(s). Members of the Users group can only view workspaces they have created. However, members of the Administrators group can view the Audit Trail for all workspaces. Also, members of the groups Reviewers and Approvers can view the Audit Trail of workspaces that have been locked by other users for review or approval.

You can select a saved workspace in the Audit Trail and then load it in Spectrum. This means that you can continue working on a previously saved workspace. Also, if you have Review or Approve permissions you can check work completed by another user. Refer to Reviewing and Approving for more information.

Members of the Administrators group can load any workspace, although the workspace will be read-only.

Viewing the Audit Trail

To view the Audit Trail of a workspace:

- Select **Audit Trail** from the Audit Trail menu.

  The Audit Trail dialog is displayed. The current workspace is displayed by default.

  If **Show details** is selected, the lower part of the dialog shows the detailed Audit Trail for the selected workspace.

  To exit the Audit Trail dialog, click **Close**.

Selecting the Workspace

You can use the filtered list of available workspaces to select the one you want to view. The Audit Trail for the current workspace is displayed by default.

Members of the Users group an only view workspaces they have created. Members of the Administrators group can view all workspaces.

Members of the Reviewers and Approvers groups can select For Review or For Approval, as applicable, to display workspaces that have been locked by their creator, indicating that they are ready for review and/or approval. All other user workspaces are hidden.

To select a workspace:

1. From the **Database selection** drop-down list select the database that contains the workspace(s) you would like to view.

   The drop-down list contains any Spectrum ES databases at the database location. Refer to Additional Information below for the default location of the database.

2. Select the appropriate filter from the **Workspace selection** drop-down list.

   The options are **Current Workspace**, **When created**, **Last modified**, **Signed**, **Reviewed**, **Approved**, **Returned**, **For Review**, and **For Approval**.

   Current Workspace is selected by default.

3. Enter or select the start date and time in the **From** field.

   Click the drop-down arrow to display a calendar and select the date. Or click in the field and use the up and down arrows to increase or decrease a value, respectively, or type a new value.

   This option filters the list of workspaces so that only those with a Time and Date stamp including and after the time and date entered will be displayed. For example, if **Last modified** is selected as the **Workspace selection**, only those workspaces last modified at times including and after the **From** entry will be displayed.

   If **Current Workspace** is selected as the Workspace selection, **From** is not available.

4. To display workspaces created by a particular user select the user name from the **Creator ID** drop-down list.

   OR

   To display workspaces created by all users in the database select **All** from the **Creator ID** drop-down list.

   Creator ID is only available if you have the appropriate permissions, which depend on the Workspace selection. **Current User** is selected by default.

   Members of the Users group can only view workspaces they have created. Members of the Administrators group can view all workspaces. Also, members of the groups Reviewers and Approvers (or any other groups with Review or Approve permissions) with For Review or For Approval selected as the Workspace selection can display workspaces by other users. Those workspaces must have been locked by their creator, indicating that they are ready for review and/or approval.

5. Select the maximum number of workspaces you want to display.

   The workspaces with the most recent Time and Date stamps will be displayed.

   If **Current Workspace** is selected, **Number of workspaces** is not available.

   The list of workspaces is now filtered by your selections.

6. Click the left mouse button in the row of the Workspaces table for the workspace you would like to view.

   The Audit Trail displayed is updated the selected workspace.

Audit Trail

The Audit Trail area, in the lower part of the screen, shows a chronological list of activities performed within the workspace (with the most recent at the top). You can select which columns to display in the table using the column selector in its top left corner.

The available columns are:

- **Category –** provides an overview of the type of action that has been audited. For example, Setup or Administration.
- **Subcategory –** provides the sub-menu grouping. For example, if the category is Setup, an example sub-category is Instrument and Accessory; or, if the category is Administration, an example sub-category is Users.
- **Audit –** the audit entry indicates what type of setting was changed. For example, for a Setup category with a sub-process Instrument and Accessory, the Audit entry would be Instrument Settings, if one of the instrument settings was changed.
- **Audited items –** provides the detail of which setting was changed. For example, the Scan Type.
- **Old Value –** the previous value applied to the configuration that was changed. For example, the Scan Type was Background.
- **New Value –** the value applied when the configuration change was made. For example, the Scan Type is Sample.
- **Time and date –** the date and time of the change.
- **Workspace ID –** the unique ID of the current workspace.

The following additional columns are relevant for Audited items that required a signature:

- **Sign point –** the type of signature point, for example, Sign Workspace. For a list of the signature points in Spectrum ES, and how to set up signature points, refer to Signatures.
- **Signature –** the signature of the user (this is the same as the User name).
- **Signature (full name) –** the full user name of the user.
- **Reason –** the reason given for the signature. The reasons available for a signature point are defined by the administrator; refer to Signatures.
- **Comment –** any comment by the user added at the signature point.
- **Signature time and date –** the time and date of the signature point.

Loading a Workspace

You can load an existing workspace and continue work. Only the user who created the workspace, or an administrator, can open a workspace. If a workspace has been locked, then users that are members of a group with Review and/or Approve permissions can load the workspace to review or approve it.

A locked workspace is read-only. An approved workspace is also read-only. However, login information is still recorded in the Audit Trail.

1. Select the Workspace ID of the workspace you would like to load and then click **Load Workspace**.

   The Load workspace dialog is displayed.

2. Click **OK** to confirm.

   Any unsaved data in the current workspace will be saved. If a signature is required, the Sign workspace dialog will be displayed for you to enter a signature. The workspace closes. Spectrum then reloads with the selected workspace displayed.

NOTE: When a workspace is loaded, the Audit Trail displays the details of that workspace only. To view the details of other workspaces, you must return to your own workspace. Refer to Exiting the workspace.

Exiting the workspace

After completing work on your own workspace:

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

   OR

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

   The Save Options dialog is displayed.

2. Select **Reload spectra next time**.

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

   OR

   Select **Don't load spectra next time**.

   This means a new workspace loads next time you login to Spectrum.

After completing work on another user's workspace:

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

   OR

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

   The Save Options dialog is displayed.

2. Select **Return to workspace** to reload the previous workspace.

   OR

   Select **Exit the software.**

   The previous workspace is restored next time you login to Spectrum at this PC.

Saving the Audit Trail

1. To save the Audit Trail of the currently displayed Workspace, click **Save.**

   A Save As dialog is displayed.

2. Select the required destination and then enter a filename.

   The Audit Trail is exported as a *.csv file that can be opened in a spread-sheeting application, for example, Microsoft® Excel™.

Printing the Audit Trail

1. To print the Audit Trail of the currently displayed Workspace, click **Print.**

   The Print Preview dialog is displayed.

2. Review the printed output, and then select **Print** from the File menu.

Additional Information

The Spectrum ES Audit Trail is saved to the database Spectrum10ES*.mdf. A Spectrum database has a default maximum size of 6 GB. When it reaches this size, a new database is automatically created.

The default location of the Spectrum ES database(s) is:

- Windows XP – C:\Documents and Settings\All Users\Application Data\PerkinElmer\Spectrum\Spectrum10ES*.mdf

  OR

- Windows 7/8 – C:\ProgramData\PerkinElmer\Spectrum\Spectrum10ES*.mdf

You can also configure Spectrum ES to access the database over a network. For more information, refer to the Spectrum ES Administrator's Guide (part number L1050100) available on the manuals CD supplied with your software.

A new workspace may be based on the system default, or on a group default. Refer to Assigning a New Default Workspace for more information.

Signing

The ability to formally sign at signature points is available in Spectrum Enhanced Security (ES) software only. Only the user that created the workspace, or a member of the Administrators group, can sign the workspace. A user's signature applies to the whole workspace, and covers all currently unsigned activities logged for the user in the Spectrum ES Audit Trail.

You will be prompted to enter an electronic signature when performing an action that requires a signature, such as exporting data, or when you exit the software. You can also sign the workspace at any time by selecting **Sign** from the Audit Trail menu.

Objects such as Equations, Macros, Instrument Setups and Sample Table Setups contain their own Audit Trail, and are not signed as part of signing the workspace. To sign one of these objects, select **Sign** from the Signatures drop-downs on the Setup Equations and Setup Macros tabs, and the Sample Table Setups and Instrument Setups dialogs, as applicable. Refer to the on-screen Help accessed from those dialogs for more information.

Signing the Workspace (Audit Trail Menu)

1. Select **Sign** from the Audit Trail menu.

   The Sign Workspace dialog is displayed. The upper part of the dialog shows the Audit Trail. The lower part, if displayed, shows the signatures in the current workspace. To display the Signature Details list, ensure that **Show signature details** is selected.

2. To sign the workspace, 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 an administrator has defined Reasons on the Signatures tab for the Workspace signature point.

5. Enter any **Comment** required.

6. Click **OK**.

Additional information

Signature points are predefined and cannot be added to, but members of the Administrators group can define which actions will require a signature. If no signature is required, then the software will ignore the signature point and you will not be prompted for a signature. However, if any Reasons have been set up for the signature point, you will still be prompted to select one. Refer Signatures for more information.

A signed (and locked) workspace, or a signed object, can be reviewed and approved by users that are members of a group with Reviewer or Approve permissions. Refer to Reviewing and Approving for more information.

Lock/Unlock Workspace (Spectrum Enhanced Security only)

When a user has completed work on a workspace, it should be presented for sign-off by users with the required authority. The workspace must be locked to indicate that it is ready for review and to make it visible in the Audit Trail to users with Review and/or Approve permissions.

Only the user that created the workspace can lock or unlock the workspace.

Lock Workspace

The Lock workspace option enables the user to make a workspace available for review and approval by users with the appropriate permissions. Lock is not available if the workspace is already locked.

When a workspace is locked it becomes read-only. Users with Review or Approve permissions can load the workspace and then review or approve it, but they cannot make changes to content.

To lock a workspace:

1. Display the workspace you want to lock.

   You can lock the current workspace, or load a previously saved workspace.

2. Select **Lock** from the Audit Trail menu.

   The Sign Workspace dialog is displayed. The upper part of the dialog shows the Audit Trail. The lower part, if displayed, shows the signatures in the current workspace. To display the Signature Details list, ensure that **Show signature details** is selected.

3. Click **Sign**.

   The Sign dialog is displayed.

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

5. 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 Workspace signature point.

6. Enter any **Comment** required.

7. Click **OK**.

   The workspace Status is changed to Locked. Users with Review and/or Approve permissions can then view the workspace under For Review or For Approval in the Audit Trail dialog. Refer to Reviewing and Approving.

Unlock Workspace

Unlock is not available if the workspace is not locked. A workspace can be unlocked only by the user that locked it. A workspace cannot be unlocked once it has been approved (workspace Status Approved).

To unlock a workspace:

1. Display the workspace you want to unlock.
2. Select **Unlock** from the Audit Trail menu.

   The workspace Status is changed to Unlocked. The workspace is no longer visible under For Review or For Approval in the Audit Trail.

Reviewing and Approving Workspaces

Reviewing and approving, or returning, workspaces is a function of Spectrum Enhanced Security (ES) software only and can be performed only by someone with the appropriate permission(s). It is up to the administrator to set the correct privileges to ensure that only the appropriate people can "sign-off" data.

We use the term "Review" to mean that the person has looked at the data and has agreed that it is correct. This is along the lines of a peer review and any number of people can review data as determined by your internal procedures.

We use the term "Approve" to mean that a person with the "authority" has signed off the data as fit-for-purpose and, again, details of who is allowed to do this should be documented in your internal procedures. When a workspace has been approved, it will be read-only. You will be able to view the data but no changes can be made.

When work has been completed on a workspace, the user must lock it to indicate that it is ready for review and/or approval. A user with Review or Approve permissions can then load the workspace to check the data. The ability to load a workspace created by another user means that a reviewer or approver can check the work at any time: the user does not have to be present. If you are working over a network, a reviewer or approver can load a workspace created by another user while that user is logged in to Spectrum ES at another PC.

After checking the workspace, reviewers and approvers can add an electronic signature using the **Return**, **Review** or **Approve** option from the Audit Trail menu. (The items displayed will depend on the permissions of the user.) A workspace can be reviewed multiple times, and by multiple users. A workspace can be approved without being reviewed. However, when a workspace has been approved it will be read-only and can no longer be reviewed. If a reviewer or approver views the data and does not agree that it is correct, then if they have the Return Workspace permission they can "Return" the workspace to the user with a description of the problem.

Some objects such as Equations, Macros, Instrument Setups and Sample Table Setups contain their own Audit Trail. They are reviewed or approved separately from the workspace using the **Review** or **Approve** option in the Signatures drop-down on the appropriate dialog. Refer to the on-screen Help accessed from those dialogs for more information.

Reviewing or Approving the Workspace (Audit Trail Menu)

Workspaces that have been locked by a user ready for review are visible in the Audit Trail to users with Review or Approve permissions (assigned by default for members of the groups Reviewers and Approvers).

To review or approve a workspace:

1. Select **Audit Trail** from the Audit Trail menu.

   The Audit Trail dialog is displayed.

2. Use the filters to display the workspace that you want to review.

   Select **For Review** or **For Approval** as the Workspace selection. Then select the Creator ID of the appropriate user from the drop-down list, or **All** to see workspaces from all users.

   NOTE: In the list of Workspaces the Login ID of the last user to access the workspace will be shown. This may be the creator of the workspace, or a reviewer.

3. Select the workspace, and then click **Load Workspace**.
4. Click **OK** to confirm that you want to load the workspace.

   If you have unsigned data in your current workspace, then you are asked to sign the workspace.

   The workspace closes. Spectrum will then be reloaded with the selected workspace displayed. The loaded workspace is read-only, although login information will be saved to the Audit Trail.

5. When you have finished checking the workspace, if the contents are correct select **Review** or **Approve** from the Audit Trail menu.

   The Review Workspace or Approve Workspace dialog is displayed. The upper part of the dialog shows the Audit Trail. The lower part, if displayed, shows the signatures in the current workspace. To display the Signature Details list, ensure that **Show signature details** is selected.

   OR

   When you have finished checking the data, if the data is not correct, return the workspace to the user.

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

   The Review or Approve dialog is displayed.

7. Enter your **User name** and **Password**.
8. 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.

9. Enter any **Comment** required.
10. Click **OK**.

    If the workspace was reviewed it is still visible to users under For Review or For Approval in the Audit Trail. A workspace can be reviewed more than once by the same reviewer and by several reviewers. The user that created the workspace, and the administrator, can see the workspace under Reviewed.

    If the workspace was approved it is no longer visible to users under For Review or For Approval in the Audit Trail. The user that created the workspace, and the administrator, can see the workspace under Approved. The workspace is now read-only.

11. Exit the workspace.

    You can review or approve, as applicable, multiple workspaces without exiting Spectrum software. Refer to Exiting the workspace for more information.

Returning the Workspace

If a reviewer or approver identifies a problem with the workspace, and does not want to review or approve the workspace until this has been corrected, then they can Return the workspace to the user. If enabled for the Return Workspace signature point, they can add a comment describing the problem.

Return is only available from the Audit Trail menu if the reviewer or approver has the Return Workspace permission (assigned by default for members of the groups Reviewer and Approver) and a locked workspace has been loaded.

1. Select **Return** from the Audit Trail menu.

   The Return Workspace dialog is displayed.

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

3. 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 Return Workspace signature point.

4. Enter any **Comment** required.

5. Click **OK**.

   The workspace is no longer visible to users with Review or Approve permissions (assigned by default for members of the groups Reviewers and Approvers) under For Review or For Approval in the Audit Trail. The user that created the workspace, and the administrator, can see the workspace under Returned.

Additional information

Refer to Signatures for more information about the signature points in Spectrum.

Workspace Reference

Workspace Reference

These reference topics describe the elements of the Spectrum user interface:

Viewing Area

Data Explorer

Navigation Pane

Dialog Pane

Menus

Toolbars

Additional Information

- The View menu includes options that enable you to select whether a toolbar is shown  or hidden.
- For information about manipulating toolbars and resetting the workspace layout, see Showing, Hiding and Moving Toolbars.
- For information about manipulating toolbar buttons, see Personalizing Toolbars.
- You cannot customize the Status bar.

Viewing Area

The Viewing Area contains one or more tabs, depending on the item you have selected in the Data Explorer, whether an instrument is connected, and whether or not the instrument is scanning.

Additional tabs may be displayed showing the results of some processes: Search, Compare, Quant and Peak Table.

Offline

Item Selected	Tab
[Samples View name]	Graph tab [Samples View name]
	Results Table tab
[spectrum name]	Graph tab [spectrum name]
	History tab

Instrument Connected

Not Scanning

Item Selected	Tab
Sample Table	Sample Table
[Samples View name]	Graph tab [Samples View name]
	Results Table tab
[spectrum name]	Graph tab [spectrum name]
	History tab

Scanning

Item Selected	Tab	Option
[Samples View name]	Live tab	Energy
		Sample
		Single Beam
		Interferogram
		Force Gauge
	Graph tab [Samples View name]	
	Results Table tab	

Graph Tab

When you are viewing a single spectrum, the Graph tab displays the curve and a Results pane.

When you are viewing a Samples View selected using the Data Explorer, the graph tab contains a table (or 'spectrum browser') that enables you to select which curves you want to display from that Samples View.

Additional Information

Optimizing and Formatting Graphs

- To learn more about optimizing graphs, and preparing them for publication by formatting and adding labels, see Viewing Spectra.
- The Results pane includes columns for the Name (ID), Description, an icon to indicate whether the curve has been saved, and an icon to indicate whether any warnings were generated by Quality Checks.

  A column chooser in the top left corner enables you to select which columns are displayed. You can also resize any column by dragging it borders, or move a column by dragging its header.

History Tab

Use the History tab to view information about the way in which a spectrum was collected and, if applicable, was processed.

When the spectrum is saved, this information is stored in the file header.

1. Select the spectrum in the Data Explorer Pane.

   The spectrum is displayed in the Viewing Area.

2. Select the **History** tab.

   Information about the spectrum is displayed categorized by Sample, Instrument, History, and Quality Checks.

   The fields displayed depend on your instrument configuration and the amount of processing that has been applied to the spectrum.

Additional Information

When exporting your data using the **Custom Defined Format**, include the information displayed on the History tab in the header of the exported file using the Header Options on the Setup Export tab.

Amending the Sample History

The information in the History tab is collected automatically and cannot be edited, or was entered in the sample table as the spectrum was collected.

You can, however, amend the current Sample Description and Comment using the Status dialog:

1. Select the Graph tab.
2. Place the mouse pointer over the curve, right-click, and then select **Status**.

   The Status dialog opens with the Sample tab displayed.

   The Status dialog includes a useful subset of the History information.
3. Edit the **Description** and **Comments** fields as required.
4. Close the Status dialog.
5. To update the History tab, save, close and then reload the spectrum.

Results Table Tab

To view a table that summarizes all the spectra in the currently selected Samples View:

- Select the Results Table tab.

  The Results Table includes a row for each spectrum in the Samples View, and columns for the Name (ID), Description, an icon to indicate whether the curve has been saved, and an icon to indicate whether any warnings were generated by Quality Checks.

If the Results Table becomes overly complex, consider hiding (or resizing) the columns containing intermediate results:

- To select which columns are displayed, use the column chooser in the top left of the table.
- To resize a column, drag its borders.
- To move a column, select and drag its header.

You can delete an Equation result column from the Results Table in Standard software:

- To delete an Equation result column, right click the mouse button in the column and then select **Delete** from the shortcut menu.

Processes and Equation Results

- If you apply a process to a spectrum that generates a new spectrum, the new spectrum is appended to the Samples View, and a new row is added to the Results Table.
- If you apply a process to a spectrum that generates a numeric result, such as an Equation, a new column is added to the Results Table, and the result is entered into the corresponding cell.

Search

- The full list of best hits, ranked by score, is displayed in the Search tab.
- By default, the highest scoring result is displayed in a set of columns in the Results Table.
- If you apply a Search process to more than one spectrum, the Results Table includes a row for each spectrum, and the highest scoring result for each spectrum is recorded in the corresponding cells in the Search columns.
- If you apply another Search process to a spectrum, another row is created in the Search tab, and another set of Search columns is created in the Results Table.

If you decide that the highest scoring best-hit for a sample is inappropriate, you can accept another hit:

1. Select the **Search** tab, and then make sure the appropriate row is selected in the Source Spectra Search Results table.

   When a Samples View is selected, the Source Spectra Search Results table in the Search tab refers to every sample in the Samples View. If you select a sample from the Samples View, the Search tab refers to the selected sample.

2. Select your preferred row from the List of Searched Library References table, and then click **Accept as best hit**.

   The corresponding search result cells in the Results Table tab are updated to refer to the accepted result.

You can also delete all the Search results for a particular sample:

1. Select the **Search** tab, and then make sure the appropriate row is selected in the Source Spectra Search Results table.
2. Right-click in the Source Spectra Search Results table, and then select Delete Selected Result from the shortcut menu.

   The corresponding search result cells in the Results Table tab are updated.

Macros Results

- For a Macro, the Samples View and Results Table are updated as each process in the chain is completed.

  This enables you to examine all the intermediate spectra and results.
- Processes such as Smooth, which you can set to overwrite the source spectrum when used alone, cannot be set to overwrite the source spectrum when used within a Macro. However, for spectra, or results, generated during a macros step to be added to the Samples View and displayed in the Viewing Area, or the Results Table, **Visible** should be enabled for the macro step in the Macro Settings dialog.
- If you apply a Macro to more than one spectrum, the Macro is applied step-by-step to each spectrum.

Quant Results

- The Results table lists the **Sample Name**, the **Method Name**, and any results associated with the Method, such as the Total M-distance.

  You can select which columns to display in the table using the column selector in its top left corner.
- Your Quant results for each Spectrum are also tabulated in the upper left quadrant of the Quant tab.
- The full details for each result are displayed in the top right quadrant Quant tab.
- If you apply another Quant process to a spectrum, another row is created in the Quant tab, and another set of Quant columns is created in the Results Table.

Repeat Collections (Raman Only)

If you have one or more repeat collections selected on the Setup Instrument Data tab, one sample in the Sample Table will generate a number of rows in the Results Table, each with [_nnn] appended to the original Sample ID.

Live Tab

While Scanning

By default, the Live tab is displayed during scanning to provide a progress monitor. When the spectrum is complete, the Graph tab is displayed.

If you are connected to a Raman instrument, the upper toolbar provides the progress of the current measurement (%). The lower progress bar provides the overall progress of the data collection, which might consist of a several markers, or a number of repeat collections; for example, scan 1 of 3.

If you do not want the Live tab to be displayed during scanning, deselect (uncheck) the **Show live display** option in the Instrument Setup dialog.

While Monitoring

The Live tab is used to display a range of monitoring tools.

While Previewing

When the Preview option is selected on the Sample Table, the Live tab is displayed to help you monitor the scan conditions before initiating data collection. This is useful with accessories such as the Universal ATR and the HATR, where a Force Gauge is enables you to achieve optimum transmission and minimize any risk of crystal breakage. It is also useful for Raman data collection where the Exposure time and Laser power may need to be adjusted.

Sample Table

Use the Sample Table tab to specify the Sample IDs and Descriptions for a batch of similar samples.

The Sample Table is available whenever an instrument is connected. You cannot build a Sample Table when working offline.

Displaying the Sample Table

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

  OR

  Open the Data Explorer pane, and then select **Sample Table**.

  The Sample Table is displayed in the Viewing Area.

Save Location

This field displays the current default path to saved spectra.

- To amend this default path, click  , browse to and select your preferred location, and then click **OK**.

  The Save Location on the Setup Instrument Data Collection tab is also updated.

NOTE: In Spectrum ES if you do not have the appropriate permission, then you will not be able to modify the Save Location.

Preview

The Preview option initiates the monitor mode for the sample, which helps you optimize the scan conditions before initiating data collection. This is useful with accessories such as the Universal ATR and the HATR, where the force applied to the sample by the pressure arm can be important, or for Raman data collection where the Exposure time and Laser power may need to be adjusted.

1. Select the Preview option and then select **Scan** from the Measurement menu, or click  .

   Data collection is monitored in the Live tab while you prepare the sample, or make adjustments.

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

   The sample is scanned.

Sample ID and Description

The Sample ID and Description fields in the Instrument Settings bar correspond to the first 'unmeasured' row in the Sample Table.

Any default entries in the Sample ID and Description fields rows depend on the Setup Instrument Auto-Name settings.

- To amend a Sample ID or Description, double-click the field and enter new text.

  To avoid replacing all the text, click to place your editing cursor within the highlighted text.

Right-click to select Copy (CTRL+C) and Paste (CTRL+V) commands.

You cannot use a Sample ID more than once. Any duplicate entries are highlighted in pink and data collection from this sample will not be executed.

Sample Rows

By default, the Sample Table contains a row for each completed measurement, and another row for the next measurement.

To set up a batch of samples, build a table with the appropriate number of 'unmeasured' rows.

Selecting Rows

- Select, or deselect, a complete row in the Sample Table by clicking the first (leftmost) column in the row. The most recently modified row is marked, and any selected rows (or cells) are highlighted.

  To select a block of rows, hold down SHIFT and click the first and the last cells in the block, or drag a highlight up or down the table.

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

Adding Rows

To add a number of rows to the bottom of the Sample Table:

1. Enter the number of rows to be added.
2. Click **Add**.

   OR

   Right-click anywhere within the table and then select **Add**.

NOTE: If you have Spectrum ES, you will not be able to add rows to the Sample Table if you do not have the appropriate permissions.

Moving and Inserting Rows

Move rows to amend the order in which the samples are measured. Insert a row to place a sample in a particular position in the batch.

- Select the unmeasured rows you want to move, and then click **Up** or **Down** (or right-click and select **Up** or **Down**).
- To insert a new row above the selected row, click **Insert** (or right-click and select **Insert**).

Removing and Clearing Rows

You may want to clean up the Sample Table so that it only refers to the current batch of samples.

- Select any rows that are not needed and then click **Remove**.
- To remove all the rows for completed measurements, click **Clear Measured**.

NOTE: Removing or Clearing rows in the Sample Table does not affect the Samples Views and links set up in the Data Explorer.

Custom Columns

Selecting Columns

- Select, or deselect, a complete column in the Sample Table by clicking the column title bar. Any selected columns are highlighted.

  To select a block of columns, hold down SHIFT and click the first and the last column titles in the block, or drag a highlight left or right across the table.

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

Adding Columns

NOTE: If you have Spectrum ES, you will not be able to add columns to the Sample Table if you do not have the appropriate permissions.

To add a column to the Sample Table:

1. Click **Add Column**.

   OR

   Right-click any column title and then select **Insert Column**.

   The Add a custom column dialog is displayed.

2. Enter a title for the column in the **Name** field.

   The column name cannot be blank. An existing column name cannot be used. All-numeric column titles are not allowed.

3. Select the **Type** of custom column, and define any settings for that type.

   The options are **Data Entry, File Path, Numeric, List** or **Image**.

   Data Entry custom columns allow both numeric and text entries if you select **Text**. If you have a barcode reader and you wish to enter barcodes in this column, select **Barcode**. You can then optionally enter a **Barcode Prefix** that will filter which barcodes are entered in the column. For more details, see Barcode Reader.

   File Path custom columns allow the user to select a spectrum from disk that can then be used in a processing step, such as Arithmetic.

   List custom columns allow you to create a list of options for the user. Only items within the list can be selected in the Sample Table column. Add new entries to the List using the **Add** button on the Add a custom column dialog. Change the order of the list using the **Up** and **Down** buttons. To delete an entry from the list, highlight the item and click **Remove**.

   Numeric custom columns can be set to display a number of **Decimal places** or **Significant figures**. Only numeric entries are allowed in the column.

   Image custom columns contain a browse button that allows you to navigate to an image. *.bmp, *.jpg and *.gif files can be opened.

4. If you wish to force users to complete a column entry before running a sample, select **Mandatory**.

5. Click **OK**.

   The Sample Table will be updated to include the column you have added. Any Mandatory entries will be highlighted in red until data is entered. If you try to run a sample row containing fields highlighted in red, the scan will not be completed and a warning message will be displayed.

Moving and Inserting Columns

Move columns to amend the order in which the data is displayed.

- Select the column you want to move, and then click and drag the column. The new location is indicated by arrows.
- To insert a new column to the left of the selected column, right-click and select **Insert Column**.

Editing custom columns

1. Right-click the title of the column you wish to modify and select **Edit Column**.

   The Edit custom columns dialog is displayed.
2. To rename to column, select **Edit Name** and edit the **Name** field.
3. To change the **Type**, select a new option from the drop-down list.

   If you select a new type, any data you have entered in the column will be lost.
4. Click **OK**.

Making Custom Columns Read only

After you have entered data in a custom column, you can make that data read only.

1. Right-click the title of the column you wish to modify and select **Edit Column**.

   The Edit custom columns dialog is displayed.
2. Select **Read only**.
3. Click **OK**.

   The entries in the column in the Sample Table now cannot be edited.

Setups

You can save the Sample Table, or load a previously saved Sample Table. To access the Sample Table Setups dialog, click **Setups**.

The Sample Table Setups dialog contains a list of Sample Table settings that have been saved. To save the current Sample Table as a setup, click **Save current Sample Table**. You can select a previously saved Sample Table and make this the current Sample Table using **Set as Current**. To delete a Sample Table setup, click select the appropriate row in the table and then click **Delete**.

The Sample Table setups list is specific to the User currently logged in to Spectrum. You can **Export** your Sample Table Setup (as a *.smt file, or secured *.ssmt file) or **Import** an existing file.

Sample Table setups can also be loaded and used as part of a Macro.

NOTE: The setups in the Common Sample Table Setups Directory will be visible to all users. The Common Sample Table Setups Directory is defined at Spectrum installation. The default is C:\pel_data\SampleTableSetups

In Spectrum ES, Sample Table Setups in the Common Sample Table Setups Directory are added to the Sample Table Setups dialog each time a new user workspace is created.

Signing, Reviewing or Approving a Sample Table Setup (Spectrum ES only)

To Sign a Sample Table Setup:

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

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

2. To sign the Sample Table Setup, 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 an administrator has defined Reasons on the Signatures tab for the Sample Table Setup signature point.

5. Enter any **Comment** required.

6. Click **OK**.

   The Sign Sample Table Setup entry is added to the Sample Table Setup Audit Trail.

The Sample Table Setup can now be exported for review or approval by a user with the appropriate permissions.

To Review or Approve a Sample Table Setup:

Users with the appropriate permissions can import a signed Sample Table Setup to review or approve it. The options **Review** and **Approve** then become available from the Signatures drop-down list. A Sample Table Setup can be signed or reviewed more than once, and by more than one reviewer. A Sample Table Setup 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 Sample Table Setup you want to review or approve, and then select **Review or Approve** from the **Signatures** drop-down list.

   The Review Sample Table Setup or Approve Sample Table Setup dialog is displayed. This contains the Audit Trail entries for that Sample Table Setup, 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 Sample Table Setup or Approve Sample Table Setup entry is added to the Sample Table Setup Audit.

The Sample Table Setup 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.

Import CSV

You can import a CSV file containing sample information into the Sample Table.

1. Ensure that the Sample Table setup displayed contains the appropriate columns for the samples you wish to add.

   The CSV file import will enter data into the columns defined on the Sample Table. It will not create new columns, or reorder existing columns.

2. Create a CSV that contains the data you wish to import into the Sample Table.

   It is advisable to produce a test CSV file to check that the columns are set up correctly, before importing a lot of sample data.

   The CSV file should contain entries that correspond to the columns in the Sample Table setup, in the correct order. You will need to include empty columns as a placeholders for any Image custom columns. Any data entered in this column will not be imported into the Image column.

   You should not include placeholders for the leftmost column that indicates whether a measurement has been completed, the column that indicates whether the curve has been saved or the column that indicates whether any warnings were generated by Quality Checks.

   If you include any text that will be entered into a List custom column but that does not match one of the predefined entries, the field will be left blank when the CSV file is imported. If you include any text that will be entered into a Numeric custom column, the field will be left blank. Only numeric entries can be imported into a Numeric custom column.

   If you want to include entries in your CSV file that contain a comma, you can put the entry in quotation marks. For example, "2,00","1,00".

   Any blank rows in the CSV file will be ignored when the file is imported.

3. Click **Import CSV**.

   The Import CSV dialog is displayed.

4. Browse to and select the *.CSV file you wish to import and then click **Open**.

5. Click **Yes**. to overwrite the existing samples in the Table with those in the *.CSV file.

   OR

   Click **No** to cancel the import.

Additional Information

- The Sample IDs entered in Sample Table are used in the Prompts Display, which is included in the Measurements bar by default. The Prompts Display is analogous to the instrument display on some spectrometers.
- By default, the Sample Table includes columns to indicate that a measurement has been completed, Sample (ID), Description, an icon to indicate whether the curve has been saved, and an icon to indicate whether any warnings were generated by Quality Checks.

  A field chooser in the top left corner enables you to select which columns are displayed in the table. You can also resize any column by dragging its borders, or move a column by dragging its header.
- Custom column entries are available as Variables on the Equations tab.
- Data entered for samples that have not been scanned, including custom column entries, will only be retained upon exiting and reopening the software if you select **Save for reload next time** on the Save Options dialog before closing the software.

- If **Enable Pathlength** is selected on the Setup Pathlength tab, a column **Pathlength (mm)** will be added to the Sample Table. See Setup Pathlength for more information.

Raman Instrument

If you are connected to a Raman instrument with a motorized stage you can set up two types of data collection. You can add samples to the Sample Table for "point-and-shoot measurements", where you select a region of your sample, set up the measurement parameters and then click Scan to collect data at the current stage location. Or you can use the controls on the Setup Sample Area XYZ Stage or Setup Microscope XYZ Stage tabs to set up multiple-location data collections using, for example, Markers, Maps and Line Scans.

Objects added to the Setup XYZ Stage tabs are not included in the Sample Table, and will be scanned in preference to any samples added the Sample table. For more information see Setup XYZ Stage tab.

If you are connected to a Raman instrument with a motorized stage and collecting data using the Sample Table, any Sample Pattern selection made on the Setup XYZ Stage tab will still apply.

Barcode Reader

You can use a barcode reader to enter data into the Sample Table. In standard operation, each barcode will be entered into the next empty cell in the column of the Sample Table, just like typing in a cell and pressing the ENTER key.

You can configure your PerkinElmer supplied barcode reader (part number L9004196) to only enter barcode data into Data Entry custom columns set to **Barcode** data entry. If you enter a **Barcode Prefix**, only barcodes with that prefix will be entered into the column. To configure the barcode reader you will need to scan a sequence of barcodes as described in the hard-copy leaflet (part number L1050245) that was supplied with you barcode reader.

You could, for example, define a custom column for the Part Number of a material with the prefix **LX**, for the Supplier ID with the prefix **Z**, and for the Lot number with the prefix **9**. When you scan a number of barcodes in succession, Spectrum will determine whether each input is a barcode, check the prefix and then enter the barcode in the next empty cell in the appropriate column. For example, any barcode beginning LX will be entered into the first available cell in the Part Number column.

NOTE: You can also set up the Sample ID and Description auto-name placeholders as barcodes on the Setup Instrument Auto-Name tab for PerkinElmer FT-IR instruments or the Setup Instrument Auto-Name tab for PerkinElmer Raman instruments.

Peak Table Tab

When you run a Peak Table or Peak Area/Height process, the results are displayed on the Peak Table tab.

- The upper left quadrant of the Peak Table tab lists each spectrum.

  You can select which columns to display in the table using the column selector in its top left corner.

  To view this table in detail, it may be helpful to drag the borders between the quadrants.

- The List of Peaks for each spectrum is tabulated in the upper right quadrant of the Peak Table tab.

  You can select which columns to display in the table using the column selector in its top left corner.

  To view this table in detail, it may be helpful to drag the borders between the quadrants.

- Your source spectrum or spectra are displayed in a graph below the results tables with the peak X and Y positions labeled.

  The peak areas will be shaded and the height will be marked on the peaks if a Peak Area/Height process was run.

- Use the shortcut menu to **Copy** the Peak Table to the clipboard, or use the **Send To** command to copy the contents of the Viewing Area into a Word or WordPad document.

The Data Explorer

Use the Data Explorer together with the Viewing Area to organize your sample data in the Spectrum workspace.

- The Data Explorer pane is on the left of the Spectrum workspace.

  It contains Samples Views and links that help you organize the spectra that you open, collect, process, or publish.

  NOTE: Samples Views are virtual folders that are a useful way to organize your spectra in the Spectrum Workspace. They have no explicit relationship with where, or whether, spectra are saved.

- If you have Spectrum ES, the Data Explorer will also contain a Recycle Bin. Any spectra that are deleted from a Samples View will be stored in the Recycle Bin.
- When you are connected to an instrument, the Data Explorer also enables you to open the Sample Table, which you use to set up data collection from a batch of samples.
- If you are connected to a Spotlight 200 microscope, the Data Explorer also includes a Microscope option that displays the Camera View and Stage View. If you have scanned a series of markers in an image, then the Data Explorer includes an Image View (similar to a Samples View) that contains the image, spectra and results tables.
- The Viewing Area is in the center of the Spectrum workspace.

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

This organization is preserved when you Exit Spectrum provided that you choose to **Save for reload next time.**

Working with Samples Views

Creating a New Samples View

- Select **New** from the File menu.

Adding a Saved Spectrum in a Samples View

1. Select the Samples View, right-click, and then select **Open spectrum.**

   The Open File dialog is displayed.
2. Browse to, and select, the spectrum you want, and then click **Open.**

Renaming a Samples View

1. Select the Samples View, right-click, and then select **Rename.**

   The Rename Samples View dialog is displayed.
2. Enter a valid name, and then click **OK.**

   If the name is not valid, an advisory message is displayed in the dialog.

Deleting a Samples View

- Select the Samples View, right-click, and then select **Delete**.

  The Samples View, and any links it contains, are deleted from the Data Explorer. Any saved spectra are not deleted from disk.

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

Working with Sample Links

Creating New Links

New links are added automatically as you collect, open and process spectra. The contents of a Samples View reflect the work you have done on this sample.

Copying a Link into a New Samples View

- Select the link, right-click, and then select **Copy to New Folder**.

Renaming a Sample

1. Select the link, right-click, and then select **Rename**.

   The Rename Sample dialog is displayed.
2. Enter a valid name, and then click **OK**.

   If the name is not valid, an advisory message is displayed in the dialog.

Deleting a Link

- Select the link, right-click, and then select **Delete**.

  The link is deleted from the Data Explorer. If saved, the spectrum is not deleted from disk.

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

Copying a Link from one Samples View into Another

- Select the link, and drag it to the Samples View you want to copy to.

  If a link of the same name already exists in the Samples View, a suffix is added to the new link name.

Working with the Recycle Bin (Spectrum ES only)

Restoring a Sample

- Right-click on the sample link in the Recycle Bin and then select **Restore**.

  The sample link is restored in the Samples View. If the Samples View had been deleted previously, it is recreated and the samples link added.

Restoring Samples Views

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

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

  NOTE: If you have Spectrum ES, the contents of the Samples View will be added to the Recycle Bin.

Repeat Collections (Raman Instruments Only)

If you select Repeat Collections on the Setup Instrument Data Collection tab, for each sample scanned Spectrum will perform the number of repeat scans specified. The spectra are grouped in a Samples View named [Sample ID] where the Sample ID is from the Sample Table. The file name of each spectrum is the Sample ID with a number *_nnn* appended corresponding to each repeat collection. For example, [Sample ID]_[nnn].sp.

NOTE: You can only run one repeat collection at a time. You cannot run repeat collections of shapes added to the Setup Sample Area XYZ tab or Setup Microscope XYZ tab, such as markers, maps and line scans. If there are any shapes that have not been run, you will not be able to start a Repeat Collection until they have been measured or deleted.

Cell Markers and Markers (Raman Instruments Only)

The spectra for each marker scanned will be added to a new Samples View, named Markers *nnn*. Each spectrum is called [Sample Name].sp using the Sample Name specified in the Marker Settings on the Setup Sample Area XYZ Stage tab or Setup Microscope XYZ Stage tab.

The spectra for each cell marker scanned will be added to a new Samples View named [Base Sample ID], as specified in the Cell Marker Settings on the Setup Sample Area XYZ Stage tab or Setup Microscope XYZ Stage tab. The Base Sample Name is the file name under which the spectrum for each cell marker will be saved with a number representing the position in the well plate appended. For example, [Base Sample ID]_[Row][Column].sp.

If the Base Sample ID has already been used, a number *_nnn* is appended to give the spectrum a unique file name. For example [Base Sample Name]_A2_001.sp.

Line Scans and Maps (Raman Instruments Only)

The spectra for each line scan or map will be added to a new Samples View named [Base Sample Name], as specified in the Line Scan Settings or Map Settings on the Setup Sample Area XYZ Stage tab or Setup Microscope XYZ Stage tab.

The Base Sample Name is the file name under which each spectrum in the line scan will be saved with a number representing the position in the line appended. For example, [Base Sample Name]_(2).sp for position 2 of a line scan, or [Base Sample Name]_(1)(3).sp for row 1 column 3 of a map.

If the Base Sample Name has already been used, a number *_nnn* is appended to give the spectrum a unique file name. For example [Base Sample Name]_(2)_001.sp.

NOTE: Spectra for line scans and maps will only be added to a Samples View if you selected **Display in graph** in the Line Scan Settings or Map Settings on the Setup Sample Area XYZ Stage tab or Setup Microscope XYZ Stage tab. If your line scan or map will generate more than 200 spectra, you will not be able to select this option.

Additional Information

Opening and Closing Panes

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

  OR

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

  OR

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

Resizing Panes

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

The Navigation Pane

Use the Navigation Pane together with the Dialog Pane to, for example, set up your instrument.

- The Navigation Pane is on the right of the Spectrum workspace.

  The Setup section includes shortcuts to key items from the Setup menu.

  The Spectral Libraries section includes shortcuts to the spectral libraries and files currently included on the Setup Spectral Libraries tab.

  The Equations section includes shortcuts to the Equations currently listed on the Setup Equations tab. Selecting an Equation in the pane displays the settings of that equation, which can be edited.

- The Dialog Pane is at the bottom of the Spectrum workspace.

  The contents of the Dialog Pane, arranged on one or more tabs, reflect the shortcut selected in the Navigation Pane.

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

Additional Information

Opening and Closing Panes

- To open or close the Dialog Pane, click the button at the center of the bottom edge of the Viewing Area.

  OR

  Select **Dialog Pane** from the View menu.

- To open or close the Navigation pane, click the button at the center of the right edge of the Viewing Area.

  OR

  Select **Navigation Pane** from the View menu.

- To open or close the Data Explorer, Navigation and Task Dialog panes simultaneously, hold down the SHIFT key and click the button that opens or closes any of these panes.

Resizing Panes

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

Navigation Pane - Setup

Click **Setup** in the Navigation Pane to display shortcuts to key items from the Setup menu.

- Click  to set up your Instrument.

  This shortcut is not available when you are working offline.

  OR

- Click  ,  or  to set up your Raman Instrument.

  This shortcut is not available when you are working offline.

  OR

- Click  to set up your Spotlight 200 microscope.

  This shortcut is not available when you are working offline.

  OR

- Click  to set up Ready Checks.

  This shortcut is not available when you are working offline.

  OR

- Click  to set up Instrument Verification.

  This shortcut is not available when you are working offline.

  OR

- Click  to set up the Laboratory Scheduler.

  This shortcut is not available when you are working offline.

  OR

- Click  to set up the Export and Email functions.

  OR

- Click  to set up Peak Detection.

  OR

- Click  to set up the default display options for the graph View.

  OR

- Click  to set up a global Pathlength.

  OR

- Click  to set up the Compare function.

  OR

- Click  to define or edit an Equation.

  OR

- Click  to set up Spectral Libraries and Search Parameters (including MultiSearch).

  OR

- Click  to set up the Biodiesel process.

  OR

- Click  to set up the Verify process.

  OR

- Click  to set up the Adulterant Screen process.

  OR

- Click  to set up the Quant process.

  OR

- Click  to define or edit a Macro.

After you click a shortcut, the Dialog Pane at the bottom of the Spectrum workspace, is opened (or updated) to display one or more tabs appropriate for the setup task.

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

Additional Information

Changing the Order of the Options in the Navigation Pane

- To change the order of items in the Navigation Pane, click the icon you want to move using the left mouse button, and then drag it to the new position.

Opening and Closing Panes

- To open or close the Dialog Pane, click the button at the center of the bottom edge of the Viewing Area.

  OR

  Select **Dialog Pane** from the View menu.

- To open or close the Navigation pane, click the button at the center of the right edge of the Viewing Area.

  OR

  Select **Navigation Pane** from the View menu.

- To open or close the Data Explorer, Navigation and Task Dialog panes simultaneously, hold down the SHIFT key and click the button that opens or closes any of these panes.

Resizing Panes

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

Navigation Pane - Spectral Libraries

Spectral Libraries contain the reference spectra utilized by the Search process.

- Click **Spectral Libraries** in the Navigation pane to display shortcuts to the spectral libraries that have been set up in the Spectral Libraries Table.

NOTE: The Search process utilizes the spectral libraries that you **Include** in the Search setup, which need not be every Spectral Library shown in the Spectral Libraries section of the Navigation Pane.

The type of library (user-defined or commercial), and its location (local or networked), are indicated by the link icon.

- A user-defined spectral library is a folder containing a number of reference spectra.
- A commercial library is often a single file that includes many reference spectra (that is, a database).

The Spectral Library Icons

- Click  to access a user-defined library stored in a local folder.

  OR

- Click  to access a user-defined library stored or shared on the network.

  OR

- Click  to access a commercial library stored locally.

  OR

- Click  to access a commercial library stored or shared on the network.

  The Dialog Pane at the bottom of the Spectrum workspace, is opened (or updated) to display the library browser.

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

NOTE: You can add spectra to an unprotected library by dragging and dropping spectra from a Samples View or Graph onto the library icon or into the Library Pane.

The Library Browser

The library browser is displayed in the Dialog pane after you click on a shortcut in the Spectral Libraries section of the Navigation pane. Use the library browser to browse, or to search the textural information within, the selected spectral library.

Library Pane

The left pane lists all the spectra in the library.

- Click  **View** to select how the spectra in the library are represented in this pane.

Select from **Details**, **Icons**, **List**, or **Thumbnails**.

In the **Details** view, to sort the library in ascending, or descending, order by any column, click in the column heading. The columns displayed in the Details view are **Name** and **Description**. You can also display the **Size**, **Type**, **Date Created**, **Date Modified** and any custom fields in the library. The icon in the top left corner of the list enables you to select which columns are displayed.

Additional Properties Pane

The right pane, which is open by default, lists any Property information associated with a particular spectrum, such as one or more physical properties (melting point, concentration of a component), CAS number, or image of a structural unit.

If no Property information is available, you can close this pane.

- Click **Additional Info** to open, or to close, the properties pane.

  To sort the library in ascending, or descending, order by **Property** or **Information**, click in the column heading.

Find Tools

Use the Find tools to search the textural information associated with the spectra in the spectral library, including any textural properties information.

1. Enter the text you want to search for in the **Find Text** field.

   For example, you could enter a CAS number (provided that property has been added to the library).

   The **Find** button is enabled.

2. If necessary, to filter your search, select one of the **Find Options**.

   You can select from **All searchable fields**, **Name**, **Size**, **Type**, **Date Created**, and **Date Modified**.

3. Click **Find**.

   The Library pane is updated to list only those spectra that include the specified text.

   The **Clear** button is enabled, and the **Find** button disabled.

To clear the Search:

- Click **Clear**.

  The Library pane is updated to list the complete spectral library.

  The **Find Text** field is cleared, and the **Find** and **Clear** buttons are disabled.

Shortcut Menu

To display the shortcut menu for a particular spectral library, right-click on its icon in the Spectral Libraries area of the Navigation pane.

Remove Library	Deletes the spectral library icon from the Spectral Libraries area, and removes the library from the Setup Spectral Libraries tab. No files are deleted.
Administer Library	Opens the Library Editor.

The Library Editor

Use the Library Editor to review the spectral library in detail.

For a user-defined library, you can also add or remove spectra, and define and amend Additional Properties, such as physical properties for the sample material.

To display the Library Editor:

- Click **Administer** in the Library browser.

  OR

  Right-click on the Spectral Library in the Spectral Libraries area of the Navigation pane, and then select **Administer Library** from the shortcut menu.

  The Library Editor is displayed.

Library Content tab

The Library Content tab lists the spectra in the library, provides a dynamic preview of the currently selected spectrum, and lists the Peak Positions for that spectrum. Hover over a particular peak in the preview to display its position in a pop-up label.

The columns in the Library Contents list include **Name**, **Size**, **Type**, **Date Created**, and **Date Modified**. The icon in the top left corner of the list enables you to select which columns are displayed.

You can sort in ascending, or descending, order by any column by clicking the column heading.

You can zoom and label the preview of the selected spectrum using the graph tools provided. However, any annotations are lost when the Library Editor is closed.

Summary tab

As well as providing some summary information about the library, and a the path to its **Location**, the Summary tab enables you to edit the library **Name** and **Description**, and to select whether to **Write protect** the library.

Adding a spectrum to the library

1. Click  **Add Entry.**

   OR

   Select **Add Entry** from the Edit menu.

   A browse dialog is displayed.
2. Select the spectrum you want to add to the library and then click **Open.**

Removing a spectrum from the library

1. Select the spectrum on the Library Content tab.
2. Click  **Remove.**

   OR

   Select **Remove** from the Edit menu.

Additional Properties

If any Additional Properties have been defined (such as one or more physical properties, the CAS number, or an image of a structural unit), an additional column is defined for each property in the Library Content tab

By default, the column is displayed, but can be displayed or hidden using the column selector in the top left corner of the list.

To add a Property column:

1. Select the spectrum on the Library Content tab.
2. Click  **Add Property.**

   OR

   Select **Add Property** from the Edit menu.
3. Complete the **Add Property** dialog.
4. Click **OK.**

To amend a Property entry:

- Double-click in the appropriate cell, complete the **Enter data** dialog, and then click **OK.**

  You can enter property data as text, or browse to a suitable image file.

To remove a Property column:

1. Double-click the column header to select the column.
2. Click  **Remove.**

   OR

   Select **Remove** from the Edit menu.

Updating the Library

If the library content has been amended outside Spectrum by, for example, adding or deleting spectrum files, synchronize the library content with the index file created when you defined the folder as a spectral library.

To synchronize the Library:

1. Make sure the Write Protected check box for the library on the Setup Spectral Libraries tab is not selected.
2. Click **Update** in the Library Editor.

Print and Print Preview

To print a graph containing information about one or more spectra in the Library:

1. Select the spectrum or spectra that you want to print in the table on the Library Content tab.

   To select more than one row in the table, select while pressing SHIFT or CTRL.

   Use the column selector at the top left of the table to show or hide the information you want printed.
2. Check that the report will be printed as you intend by clicking **Print Preview** (or selecting **Print Preview** from the File menu).
3. In either the **Library Editor** or the **Print Preview** window, click **Print.**

   OR

   Select **Print** from the File menu.

   A report containing the graph is printed, with the data displayed in the corresponding row in the Library Content tab appended. If you selected more than one spectrum, the spectra are printed in a single graph with the row data printed in a table beneath.

Shortcut menus

The graph in the Library Editor includes a selection of tools and a shortcut menu that enable you to optimize and label the graph, and copy it to the Windows clipboard to be pasted into, for example, Word.

- To access the shortcut menu, right-click in the graph.

NOTE: To avoid infringing (c), spectra, images, and text taken from commercial libraries cannot be copied.

Closing the Library Editor

1. Click  **Close Editor.**

   OR

   Select **Close Editor** from the File menu.
2. Select **Save and close library editor** to confirm any changes you have made.

   OR

   Close without saving to disregard any changes you have made.
3. Click **OK.**

Additional Information

Opening and Closing Panes

- To open or close the Dialog Pane, click the button at the center of the bottom edge of the Viewing Area

  OR

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

  OR

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

Resizing Panes

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

Navigation Pane - Equations

The Equations section in the Navigation pane displays shortcuts to the Equations listed in the Setup Equations tab. New Equations are added using the Setup Equations tab.

- Click **Equations** in the Navigation pane to display shortcuts to the Equations currently listed on the Setup Equations tab.

You setup an equation using Functions and Operators, and can format the results using an If … Then … Else construction.

Setting up an Equation

1. Click  in the Equations section of the Navigation pane to access a user-defined equation.

   The Dialog Pane at the bottom of the Spectrum workspace, is opened (or updated) to display the settings of that equation.
2. Select the Equation tab.
3. Amend the **Equation name** and **Equation description** as required.

   The Equation name will be used in the Equations sub-menu in the Process menu.
4. Enter the **Equation**, either by typing directly or by clicking on items in the **Operators**, **Functions** and **Variables** lists.

   Every function has a number of required or optional arguments, as shown in the syntax popup displayed when the function is selected.

   Often, the first argument is <spectrum>, set to **All** by default, which means that the function is applied to all selected spectra. If you want the equation to address a particular type of sample select another of the Variables or, to address a specific spectrum, click **Browse** and then select the spectrum required. All numeric entries in the Results Table are available in the Variables List, including numeric values from Custom columns set up in the Sample Table. If Enable Pathlength is selected on the Setup Pathlength tab, the global pathlength defined there will be available as a Variable (Setup_Pathlength).
5. Click **Check** to make sure that the syntax used in the equation is correct.

The Equation list on the Setup Equations tab is updated, but the dialog pane stays open so that you can continue with Result Formatting. 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.

Formatting Equation Results

You can highlight the numeric result delivered by your equation in a different font or color, depending on its value. Essentially, you apply an If … Then … Else … condition.

1. Click  in the Equations section of the Navigation pane to access a user-defined equation.

   The Dialog Pane at the bottom of the Spectrum workspace, is opened (or updated) to display the settings of that equation.
2. Select the Results Formatting tab.
3. Set up the 'If' condition by entering a constant or selecting a result (usually you select the result of the equation you are working on), followed by an Operator

(such as 'greater than'), and then a Criterion (such as a constant or the result from another equation).

The criteria available are **<>**, **<=**, **>=**, **<**, **>**, **=**, **Not Between**, and **Between**. The **Not Between** and **Between** operators require two criteria, so you must complete the **Criterion** and the **Criterion 2** fields.

4. Setup the 'Then' conditional formatting, which specifies what happens when the 'If' section is true. Select whether to do nothing, or to label and/or highlight the result.

   To do nothing, select **No formatting**.

   To label your result, select **Replace result with text** or **Add text to result**, which opens a text field for you to enter your label. If no label is required, select **Only change font**.

   To highlight your result, you can amend its font attributes and/or the color of the cell or row in which it is displayed. Click **Change Font** to amend attributes such as Font, Font styles (italic, bold) and Size, and to apply Effects such as Color, Strikeout and Underline. Use the **Fill color** drop-down selector to choose a background color, and select the **Apply to row** check box if you want this color to apply to the table row containing your result.

5. Setup the 'Else' conditional formatting, which specifies what happens when the 'If' condition is false.

   Select whether to do nothing, or to label and/or highlight the result, as before.

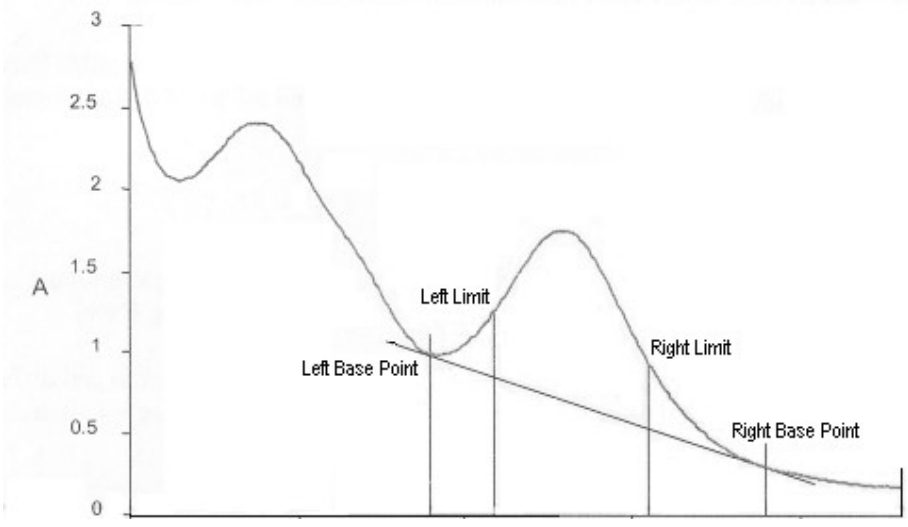
6. If you wish to return to the Setup Equations tab click **Back**.

Function Reference

The Area function

Use the **Area** function to calculate the area under a curve between two set points. The syntax of the function is **"Area[<spectrum variable>, Left Limit, Right Limit, Left Base Point(optional), Right Base Point(optional)]"**

For example: **Area(All, 3100,3000,3150,2930)** calculates the area between abscissa positions 3100 cm^{-1} and 3000 cm^{-1} above a baseline with base points at 3150 cm^{-1} and 2930 cm^{-1}.



The area reported is between the **Left Limit** and **Right Limit**, either relative to a zero baseline or relative to a linear baseline intersecting the spectrum at the specified baseline points. If no baseline points are specified, the area reported is that above zero. If only one baseline point is specified, a horizontal baseline is constructed from that point.

The Yval function

Use the **Yval** function to obtain the ordinate value at a specified abscissa position.

The syntax of the function is **"Yval[<spectrum variable>, Abscissa position]"**.

For example: **Yval[All, 3100]** returns the ordinate value for each spectrum at 3100 cm^{-1}.

The Yval function is useful for calculating net absorbance from the difference in absorbance at two positions. The Yval function also enables you to determine the amplitude of a band on a varying sloping background.

The PeakX function

Use the **PeakX** function to find the position of a peak or valley within a specified range.

The syntax of the function is **"PeakX[<spectrum variable>, Start Range, End Range, Peak Threshold, 1=Peak/-1=Base, 1=Interpolated(default)/0=sampled position (optional)]"**.

A peak is identified by a valley that exceeds the selected threshold on either side. **PeakX** gives the abscissa position of a peak or valley over the specified range. If there is more than one peak that exceeds the threshold the routine returns the value of the first peak or valley it finds.

For example: **PeakX[All, 3500, 3000, 0.1, 1, 0]** returns the first peak between 3500 cm^{-1} and 3000 cm^{-1} over the 0.1 threshold, and the abscissa value of the sampled data point (as opposed to the peak position on a smooth curve fitted between the sampled data points).

The Ymax function

Use the **Ymax** function to find the maximum ordinate value within a specified range, instead of measuring the height at a fixed position. When processing many spectra, the Ymax function enables you to address any shifts in the location of the maximum.

The syntax of the function is **"Ymax[<spectrum variable>, Start Range, End Range]"**.

For example: **Ymax[All, 3150, 3000]** returns the maximum ordinate value between 3150 cm^{-1} and 3000 cm^{-1}.

The Ymin function

Use the **Ymin** function to find the minimum ordinate value within a specified range. When processing many spectra, the Ymin function enables you to address any shifts in the location of the minimum.

The syntax of the function is **"Ymin[<spectrum variable>, Start Range, End Range]"**.

For example: **Ymin[All, 3150, 3000]** returns the minimum ordinate value between 3150 cm^{-1} and 3000 cm^{-1}.

The XYmax function

Use the **XYmax** function to return the abscissa position of the maximum ordinate value found by interpolation over a specified range.

The syntax of the function is **"XYmax[<spectrum variable>, Start Range, End Range]"**.

For example: **XYmax[All, 3150, 3000]** returns the abscissa position for the maximum ordinate value between 3150 cm^{-1} and 3000 cm^{-1}.

The XYmin function

Use the **XYmin** function to return the abscissa position of the minimum ordinate value found by interpolation over the specified range.

The syntax of the function is **"XYmin[<spectrum variable>, Start Range, End Range]".**

For example: **XYmin[All, 3150, 3000]** returns the abscissa position for the minimum ordinate value between 3150 cm^{-1} and 3000 cm^{-1}.

The Height function

Use the **Height** function to calculate the ordinate value at a specified abscissa position relative to an optional baseline.

The syntax of the function is "**Height[<spectrum variable>, Abscissa position, Left Base Point(optional), Right Base Point(optional)]**".

For example: **Height[All, 3000, 3050, 2950]** returns the height at 3000 cm^{-1} corrected for a baseline drawn between 3050 cm^{-1} and 2950 cm^{-1}.

If you specify one base point, a horizontal baseline is calculated from that point. If you specify no base points then the height is not corrected for a baseline.

The Interval function

Use the **Interval** function to calculate the data interval of the spectrum.

The syntax of the function is **"Interval[<spectrum variable>]".**

For example: **Interval[All]** return the data interval of each spectrum.

The Npts function

Use the **Npts** function to calculate the number of data points in the spectrum.

The syntax of the function is **"Npts[<spectrum variable>]".**

For example: **Npts[All]** returns the number of data points in each spectrum.

The End function

Use the **End** function to find the last abscissa point in the spectrum.

The syntax of the function is **"End[<spectrum variable>]".**

For example: **End[All]** returns the last abscissa point in each spectrum.

You can also nest the End command within a command in place of its end value.

For example: **XYmax[All, Start[All], End [All]]** returns the abscissa value for the maximum ordinate anywhere in each spectrum without having to set start and end limits.

If you use the End command with Wavelength Programmed data the last wavelength in the list is returned.

For example: **Height[All, End[All]]** returns the height at the last wavelength in the list without pre-setting that value.

The Start function

Use the **Start** function to find the first abscissa point in the spectrum.

The syntax of the function is **"Start[<spectrum variable>]".**

For example: **Start[All]** returns the first abscissa point in each spectrum.

You can also nest the Start command within a command in place of its start value.

For example: **XYmax[All, Start[All], End [All]]** returns the abscissa value for the maximum ordinate anywhere in each spectrum without having to set start and end limits.

If you use the End command with Wavelength Programmed data the last wavelength in the list is returned.

For example: **Height[All, Start[All]]** returns the height at the first wavelength in the list without pre-setting that value.

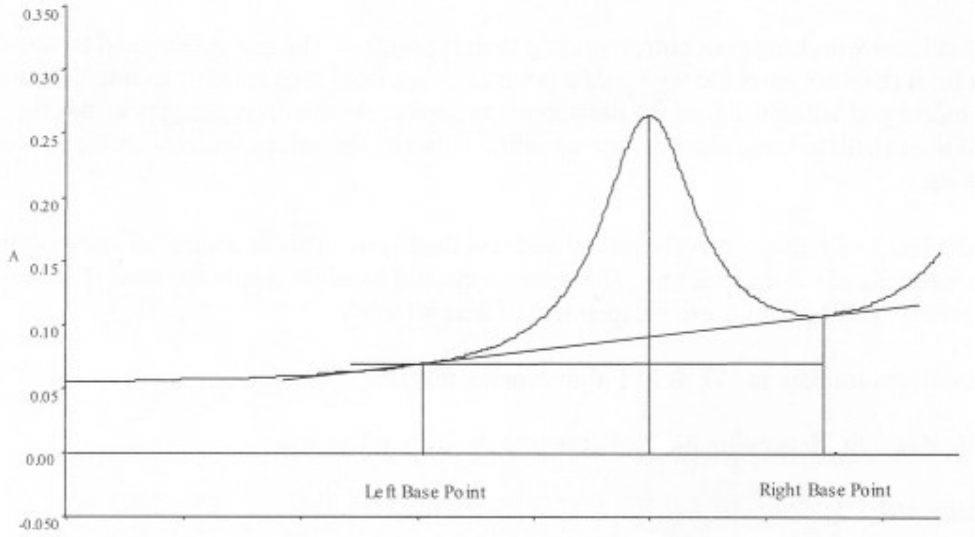
The MaxHt command

Use the **MaxHt** function to determine the height of the tallest peak in a range, relative to a baseline if required. The MaxHt function is useful for obtaining absorbance values for quantitative applications.

The syntax of the function is **"MaxHt[<spectrum variable>, Start Range, End Range, Left Base Point, Right Base Point]".**

For example: **MaxHt[All, 3150, 3050, 3200, 300]** returns the height of the tallest peak between 3150 cm^{-1} and 3050 cm^{-1}, corrected for the baseline constructed between 3200 cm^{-1} and 3000 cm^{-1}, using cubic interpolation between the data points.

When the **Left Base Point** and **Right Base Point** are given the same value, a horizontal baseline is used, as shown below.



The Mean, SD, and RMS functions

The **Mean**, **SD** (Standard deviation) and **RMS** (Root mean square deviation) functions are standard statistical functions. When you apply them to spectral data they return the average, standard deviation or RMS deviation ordinate value over all wavelengths.

You can use the Mean and SD functions to evaluate the results from repeated measurements to estimate their precision and uncertainty. Use the RMS function in a similar manner to determine variability, for example as a measure of the noise in a region of a spectrum.

The syntax of these commands is **"[<spectrum variable> or <number variable>]".**

You can apply the Mean, SD and RMS functions to spectra or to a numeric result from another equation.

For instance, if you replicated your experiments and had an equation to find the area of a peak in each, you could calculate the Mean of the peak areas.

The Trend function

Use the **Trend** function to measure a slow variation, that is a variation described as drift rather than as noise.

The **Trend** function calculates the slope of a linear fit to the spectrum. You can apply the function to the complete spectrum or to a region within it, defined by **Start Range** and **End Range**.

The syntax of the function is **"Trend[<spectrum variable>, Start Range (optional), End Range (optional)]"**.

For example: **Trend[All, 3500, 3000]** calculates the slope of a linear fit to all data between 3500 cm^{-1} and 3000 cm^{-1}.

The Exp, Log, Sqr, Sqrt and Ln functions

Use the Exp (Exponent), Log (Logarithm), Sqr (Square), Sqrt (Square Root), and Ln (Logarithm base e, or natural logarithm) as standard mathematical tools that you can apply to spectra or to the numeric results from another equation.

NOTE: If you try to take the log, natural log (Ln), or square root (Sqrt) of a negative number, a value of zero is returned.

The Log function returns the base <n> logarithm of a number or a spectrum. The syntax of the Log function is **"Log[<spectrum variable> or number, base]"**.

For example, **Log[All, 10]** would return the logarithm (base 10) of all your spectra.

The XVal function

Use the **XVal** function to determine the abscissa value at a specified Y value. The function uses interpolation by default, which returns the actual abscissa value at the specified Y value.

If when setting up the function, you enter 0 instead of interpolation in the syntax statement, the function returns the abscissa value of the nearest data point.

The XVal function returns the first abscissa value at the specified Y value. If the spectrum has more than one abscissa value at the specified Y value (such as when there is more than one peak in the spectrum), the Search from Start / End options in the syntax statement are useful. Select whichever end of the spectrum ensures that the required value is returned.

The syntax of the function is "**XVal[<spectrum variable>, Ordinate value, Start Range, End Range, 1=Search from Start(default)/-1=Search from End(optional), 1=Interpolated(default)/0=sample position (optional)]**"

NOTE: If you include the Interpolated parameter in the function, you must include the Search from parameter. **XVal[All, 1.2, 3500, 2500, 1]** would search the spectrum from the end using default interpolation, but **XVal[All, 1.2, 3500, 2500, 1]** where no value has been entered for the Search from parameter (only a space between 2 commas) would return an incorrect syntax message.

Examples:

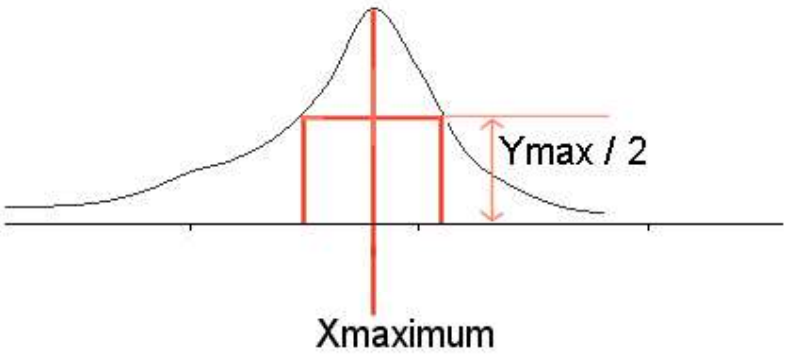
XVal[All, 1.2, 3500, 2500, 1, 1] would return the abscissa value for all spectra at the Y value of 1.2, between 3500 cm^{-1} and 3000 cm^{-1}. It would start the search from 3500 cm^{-1}, and return an interpolated abscissa value, rather than the value from the nearest data point, for each spectrum.

XVal[All, 1.1, 3500, 3000, -1, 0] would return the abscissa value for all spectra at the Y value of 1.1, between 3500 cm^{-1} and 3000 cm^{-1}. It would start the search from 3000 cm^{-1} (Search from End), and would return the abscissa value from the nearest data point, rather than an interpolated value, for each spectrum.

XVal[All, 1.2, 3500, 3000] would return the abscissa value for all spectra at the Y value of 1.2, between 3500 cm^{-1} and 3000 cm^{-1}. It would start the search from 3500 cm^{-1} (by default), and return an interpolated abscissa value (by default) for each spectrum.

Width at half height

You can use the XVal function to calculate the width of a peak at half its height:



XVal[All,Ymax[All, 2535, 2545]/2,XYMax[All, 2535, 2545],2545]-XVal[All,Ymax[All,2535,2545]/2,XYMax[All,2535,2545],2535]

This equation would look at the peak between 2535 $cm^{-1}$and 2545 cm^{-1}. The width at half height will be reported for all spectra. The functions Ymax and XYMax are used to calculate XVal. Ymax calculates the maximum ordinate value within the range. XYMax calculates the abscissa position of the ordinate maximum.

In the first part of the equation - XVal[All, Ymax[All, 2535, 2545] / 2, XYMax[All, 2535, 2545], 2545] -

2545 means the first XVal is looked for starting from 2545 cm^{-1}.

In the second part of the equation - XVal[All, Ymax[All, 2535, 2545] / 2, XYMax[All, 2535, 2545], 2535] - 2535 means the first XVal is looked for starting from 2535 cm^{-1}.

To calculate the width at half height for any data, use the equation above and simply replace the values (2535, 2545).

The YShift function

Use the YShift function to find the ordinate value difference at the selected position between two linear best fit lines fitted to the data points either side of a specified x position over a fixed width.

The syntax of the function is "**YShift[<spectrum>, x position at which to calculate shift, x width from position for Linear Fit**]".

The RCoeff function

Use the **RCoeff** function to calculate the correlation coefficient.

The syntax of the function is "**RCoeff[<spectrum variable>,Start Range(optional), End Range(optional)]**"

If you do not specify Start Range and End Range values, the complete spectrum is used.

The Ri function

Use the **Ri** function to calculate the refractive index of your sample.

The syntax of the function is "**Ri[<spectrum variable>, Start Range, End Range, Thickness, Num Fringes (-1=Auto), Angle of Incidence, Thickness Units: 1=Å/2= μ m, Peak Threshold(optional)]**"

The Tcalc function

Use the **Tcalc** function to calculate the thickness of your sample.

The syntax of the function is **"Tcalc[<spectrum variable>, Start Range, End Range, Refractive Index, Num Fringes(-1=Auto), Angle of Incidence, Result Units: 1=Å/2= μ m, Peak Threshold(optional)]"**

Additional Information

If you add an Equation step to a Macro, there are two additional settings on the Equation tab that are relevant to Equations that generate spectral results.

If you want the spectrum generated by an Equation to be used as the input spectrum for the next step, you should enable the option **Use for next step**.

If **Use for next step** is selected, you can also select to **Overwrite input spectra**. The Equation will generate a new spectrum and overwrite the input spectrum. The new spectrum generated will then be used by the next step. Any numerical results calculated for the input spectrum will be retained.

The Dialog Pane

Use the Dialog Pane together with the Navigation Pane to, for example, set up your instrument.

- The Dialog Pane is at the bottom of the Spectrum workspace.

  The contents of the Dialog Pane, arranged on one or more tabs, reflect the shortcut selected in the Navigation Pane.

- The Navigation Pane is on the right of the Spectrum workspace.

  The Navigation Pane contains a Setup area, which includes shortcuts to key items from the Setup menu.

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

Additional Information

Opening and Closing Panes

- To open or close the Dialog Pane, click the button at the center of the bottom edge of the Viewing Area

  OR

  Select **Dialog Pane** from the View menu.

- To open or close the Navigation pane, click the button at the center of the right edge of the Viewing Area

  OR

  Select **Navigation Pane** from the View menu.

- To open or close the Data Explorer, Navigation and Task Dialog panes simultaneously, hold down the SHIFT key and click the button that opens or closes any of these panes.

Resizing Panes

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

The Menu Bar

These reference topics describe the menus available in the Menu Bar:

File

View

Measurement

Microscope

Process

Setup

Audit Trail (ES)

Navigation

Help

Additional Information

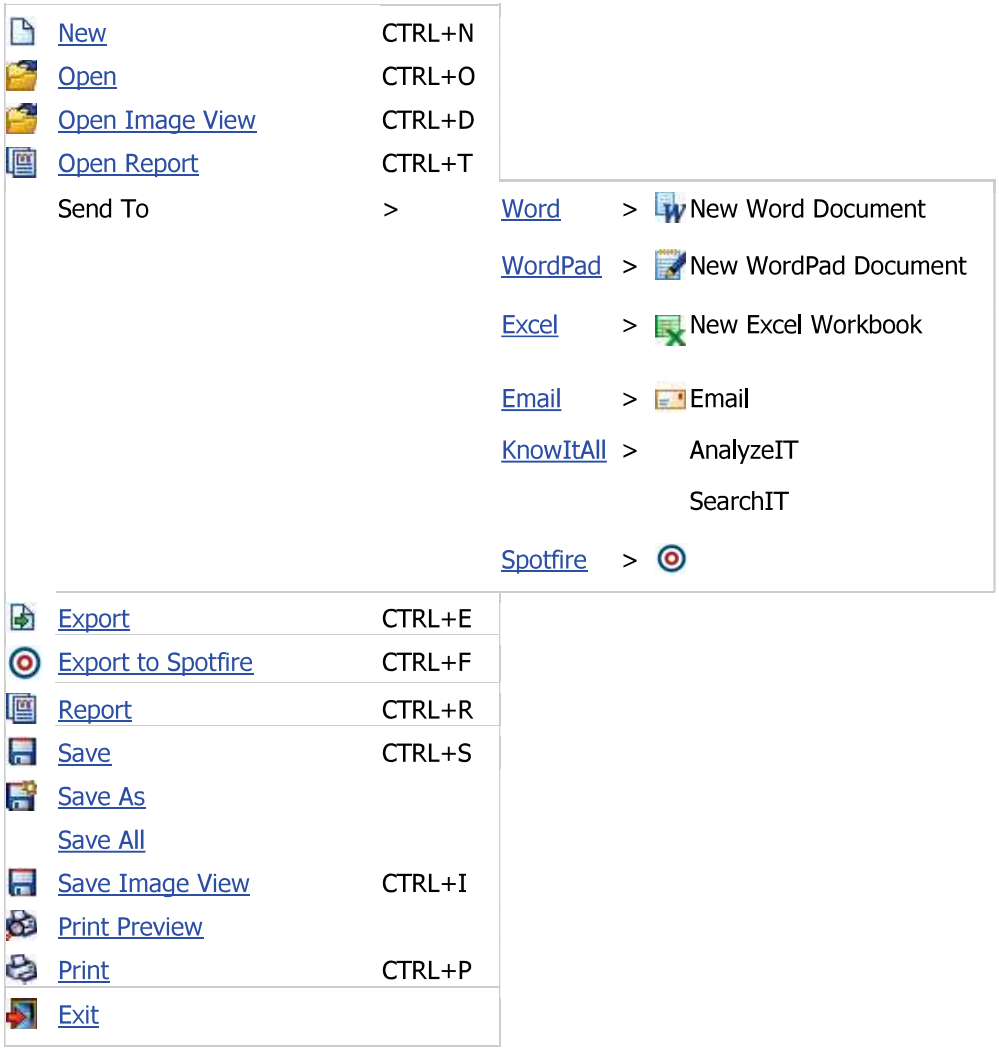
The Measurement and Microscope items are not shown when running in the offline mode. They are only shown when connected to an instrument.

The Menu Bar cannot be turned off, floated or customized. It is placed at the top of the Spectrum workspace, either above or below the Instrument Settings and/or Measurement toolbars.

NOTE: If you have Spectrum ES, and you do not have permission to perform any of the functions on the menu, the menu will not be displayed. If you have permissions for some, but not all, of the functions, the menu will be displayed showing only those items for which you have permission.

File Menu

These are the commands available in the File menu. To learn more about a command, click on its name.



Additional information

For more information about opening and saving files, see Finding and Saving.

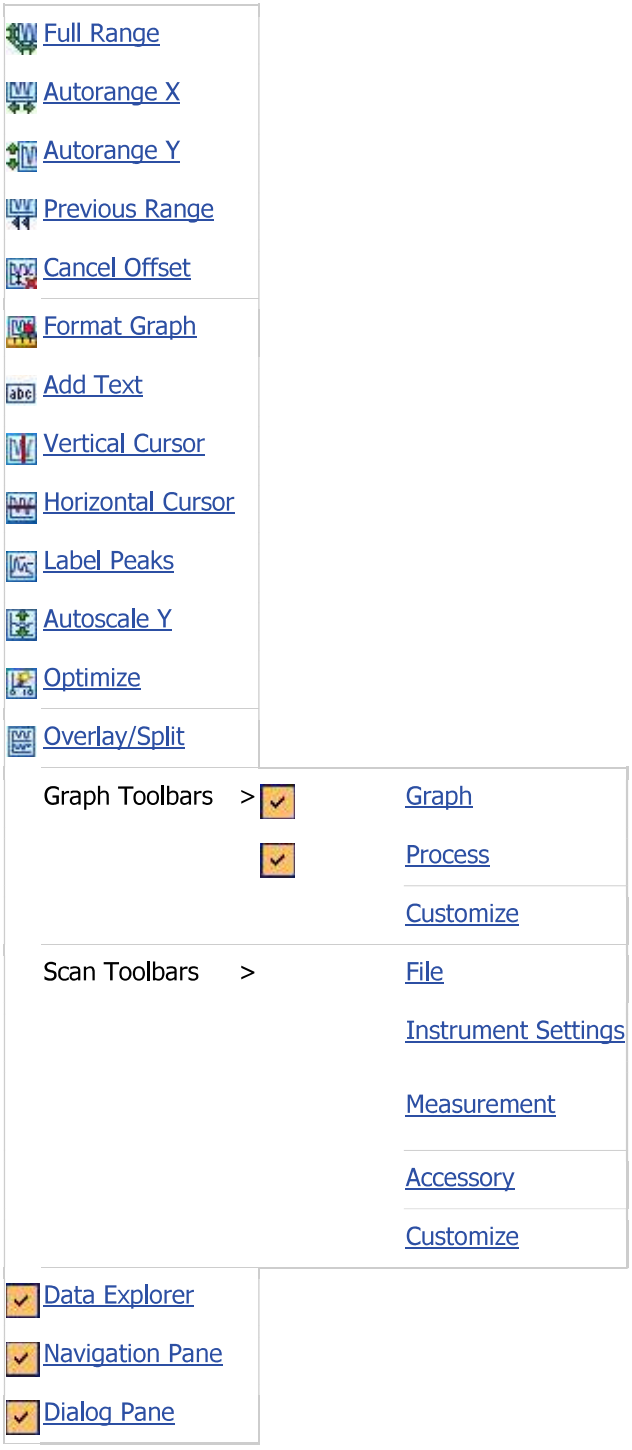
For more information about printing your results, see Publishing Results.

Send to Excel, Send to Word, Send to Spotfire and Send to KnowItAll will only be available if you have the relevant software installed on your computer. To see the Send to Email option, you first need to set up your email account settings on the Setup Email tab.

NOTE: If you have Spectrum ES, some items on this menu may not be available if you do not have the appropriate permissions.

View Menu

These are the commands available in the View menu. To learn more about a command, click on its name.



Additional Information

To view the Instrument Settings or Measurement toolbars, you must be connected to an instrument.

Viewing Graphs

The menu items referring to how curves are displayed can also be available on the Graph Toolbar.

A selection of the commands are also made available in vertical toolbars displayed by the spectra when some processes are run.

For more information about viewing graphs, see Optimizing Graphs.

Showing or Hiding Interface Elements

The menu items referring to toolbars and panes enable you to quickly show or hide parts of the Spectrum interface. For a toolbar,  indicates that the toolbar is visible. For the Data Explorer, Navigation and Dialog Panes,  indicates that the pane is open.

The toolbars displayed by default will depend on the options you selected at installation.

You can organize your workspace by hiding a toolbar, or by showing a toolbar that had been hidden.

- Click the  icon to the left of the name of the toolbar that you want to hide

  OR

  Click the shaded area to the left of the name of the toolbar that you want to show.

Measurement Menu

These are the commands available in the Measurement menu. To learn more about a command, click on its name.

If you are connected to an FT-IR instrument:

- Scan
- Scan Markers (Spotlight 200 only) > Scan Markers
  - Scan and Compare
  - Scan and Search
  - Scan and MultiSearch
  - Scan and Verify
- Scanalyze > Scan and Compare
  - Scan and Search
  - Scan and Quant
  - Scan and Verify
- Halt
- Background
- Monitor
- Sample Table
- Instrument Checks > Ready Checks > Run Selected
  - Abscissa
  - Noise
  - Throughput
  - Contamination
  - Quant Control
  - Instrument Verification
  - Component Checks

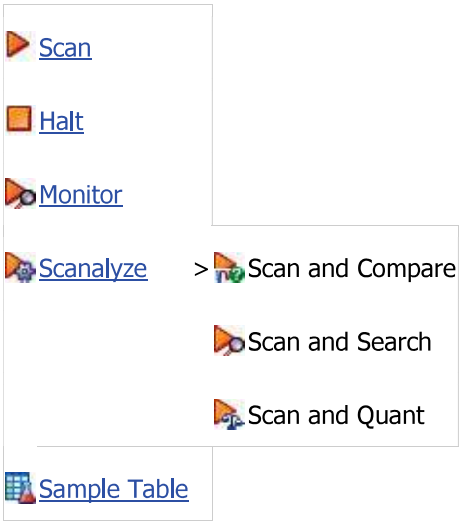
(Spectrum Two only)

Standardize (AVI)

Humidity Shield (Spectrum Two only)

Power Save Mode (Spectrum Two only)

If you are connected to a Raman instrument:



Additional Information

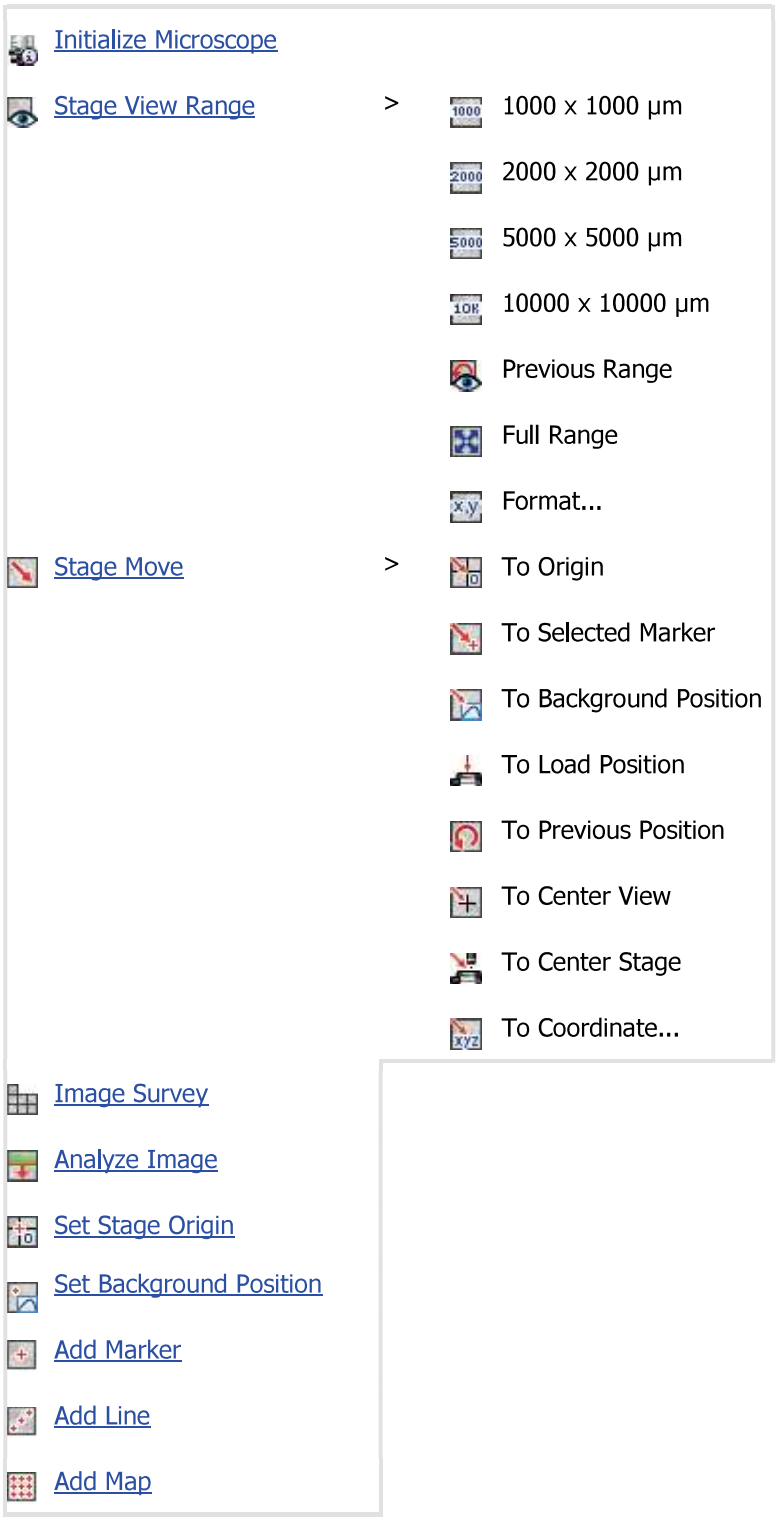
For more information about making measurements, refer to Collecting Data.

If you are connected to a Raman instrument with a Triggered Probe selected as the Accessory, the Scan and Monitor icons will indicate that there is a probe connected and will be disabled. The Scan and Preview functions can only be started using the trigger on the probe. This is to prevent accidental exposure to the laser beam when working at a distance from the PC.

NOTE: If you have Spectrum ES, some items on this menu may not be available if you do not have the appropriate permissions. If you do not have permission to access any of the items on the menu, the menu will not be displayed.

Microscope Menu

These are the commands available in the Microscope menu. To learn more about a command, click on its name.

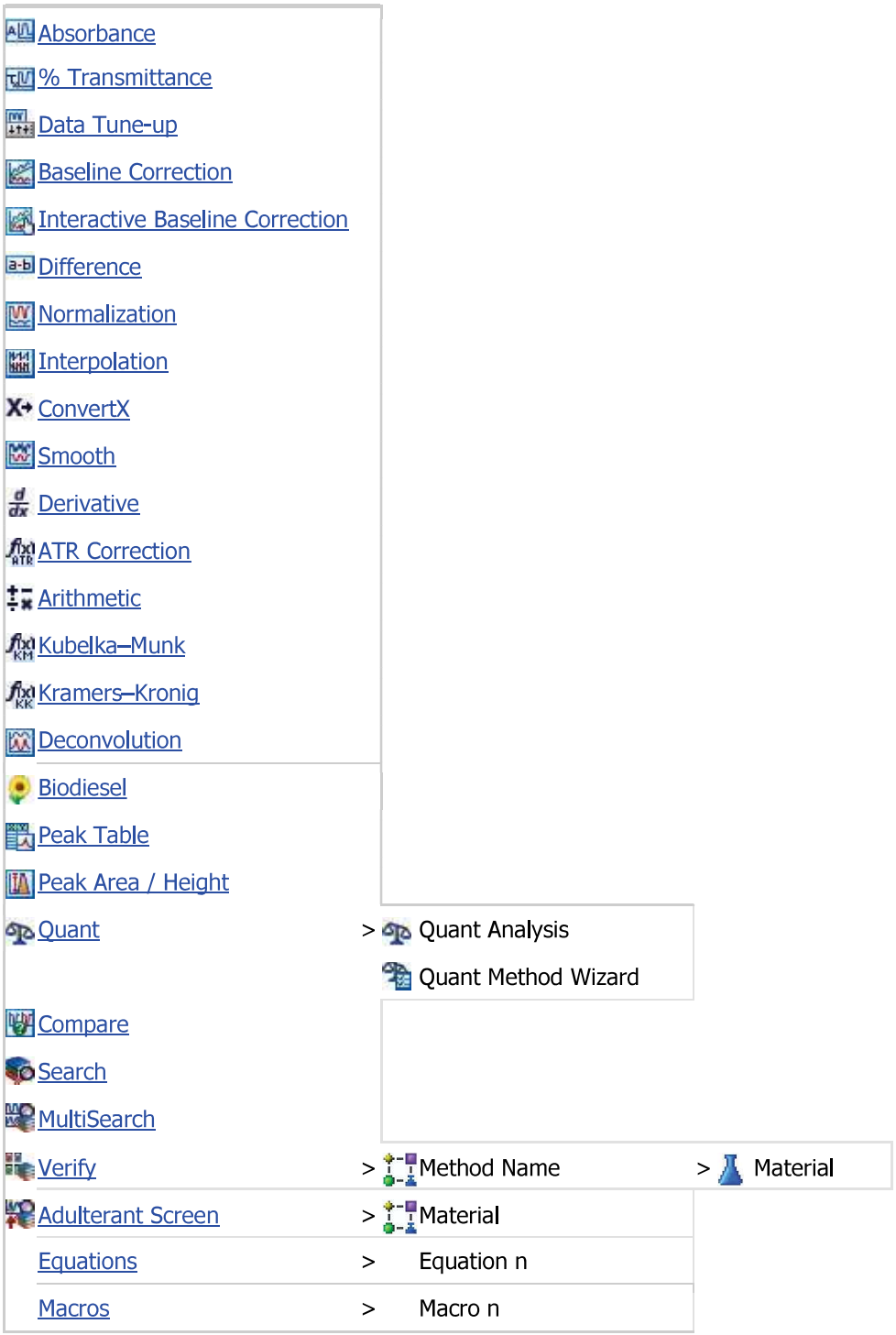


Additional Information

These options are also available on the toolbar in Stage View.

Process Menu

These are the commands available in the Process menu. To learn more about a command, click on its name.



Additional Information

These commands are also available from a shortcut menu in the Viewing Area, and may be included in the Process Bar.

If you have installed the Biodiesel Analyzer, **Biodiesel** is available on the Process menu.

NOTE: If you have Spectrum ES, some items on this menu may not be available if you do not have the appropriate permissions. If you do not have permission to access any of the items on the menu, the menu will not be displayed.

Setup Menu

These are the commands available in the Setup menu. To learn more about a command, click on its name.

	Administration (Administrators only)	>	Setup Users
			Users Audit Trail (ES only)
			Set Group Workspace (ES only)
	Instruments	>	Add Instrument
			Remove Instrument
			Select Instrument
			Enable Auto-Connect
	Instrument/Raman Instrument		
	Microscope (Spotlight 200 only)		
	Ready Checks		
	Instrument Verification		
	Laboratory Scheduler		
	Export and Email		
	Peak Detection		
	View		
	Pathlength		
	Quant		
	Compare		
	Libraries and Search (including MultiSearch)		
	Verify		
	Adulterant Screen		
	Biodiesel		
	Equations		
	Macros		
	Restore Default Workspace		

Additional Information

If you install the Biodiesel Analyzer, **Biodiesel** is available on the Setup menu.

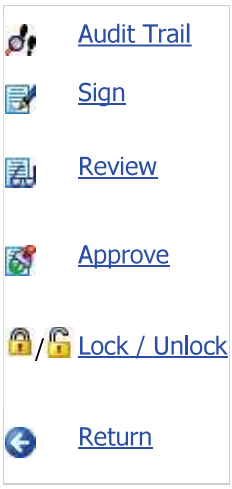
The options available in the Administration sub-group of the Setup menu depend on whether you have Spectrum Standard or Spectrum Enhanced Security installed. To view the Administration sub-menu you must have administrator rights.

To access the Add Instrument and Remove Instrument options on the Instruments sub-menu, you must have administrator rights.

Audit Trail Menu (Spectrum Enhanced Security Only)

The Audit Trail menu is only available in Spectrum ES. The commands available will depend on your permissions and the current status (for example, Locked or Unlocked) of the workspace.

To learn more about a command, click on its name.



Navigation Menu

These are the commands available on the Navigation menu. To learn more about a command, click on its name.

Sample Table
Samples View n

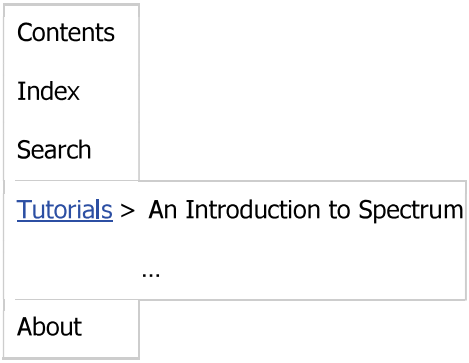
Additional Information

The Sample Table item is only available when an instrument is connected.

The number of folder items available mirrors the number of Samples Views displayed in the Data Explorer pane. Use the Folder items to select the current Samples View.

Help Menu

These are the commands available on the Help menu. To learn more about a command, click on its name.



Additional Information

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

Toolbars

The Spectrum workspace can include a number of global toolbars:

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

The Viewing Area pane can include one or more local Graph toolbars:

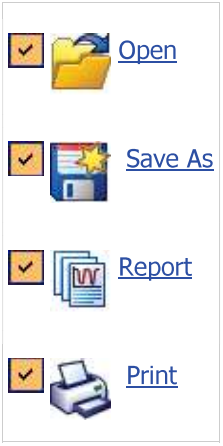
- The Graph bar. By default, this toolbar is located at the top of the Viewing Area.
- The Process bar. By default, this toolbar is located at the top of the Viewing Area.

Additional Information

- The View menu includes options that enable you to select whether a toolbar is shown  or hidden.
- For information about manipulating toolbars and resetting the workspace layout, see Showing, Hiding and Moving Toolbars.
- For information about manipulating toolbar buttons, see Personalizing Toolbars.
- You cannot customize the Status bar.

The File Bar

Use the File bar to create new sample views, open spectra in the software, to save spectra and publish data to other formats and applications.



Additional Information

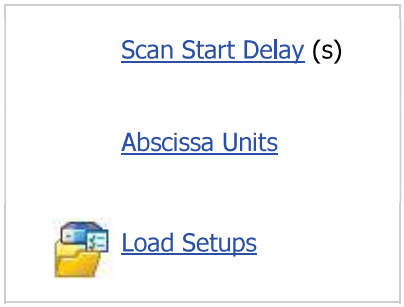
The commands displayed by default on the toolbar will depend on the option you selected at installation. You may decide to include other view commands that you use frequently. See Personalizing Toolbars.

The Instrument Settings Bar

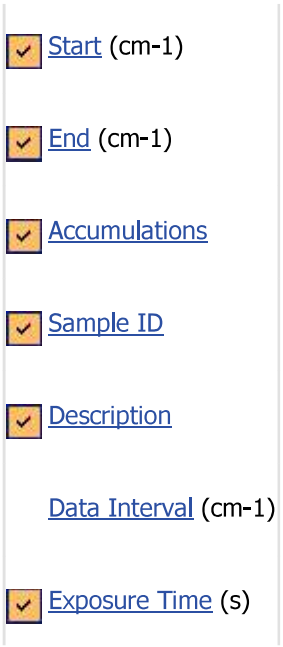
Use the Instrument Settings bar to review and, if necessary, to edit the scan settings and the sample information for the current scan.

If you are connected to an FT-IR instrument:

- ☑ Start (cm-1)
- ☑ End (cm-1)
- ☑ No of Scans / Scan Time
- ☑ Sample ID
- ☑ Description
- Mode
- Scan Type
- Resolution (cm-1)
- Ordinate Units
- AVI Calibration
- CO2/H2O
- Phase Correction
- Apodization
- Scan Speed (cm/s)
- Data Interval (cm-1)
- B-Stop
- J-Stop



If you are connected to a Raman instrument:



Additional Information

The icon above indicates that the command is included in the factory default Instrument Settings bar. The commands displayed by default on the toolbar will depend on the option you selected at installation. You may decide to include other view commands that you use frequently. See Personalizing Toolbars.

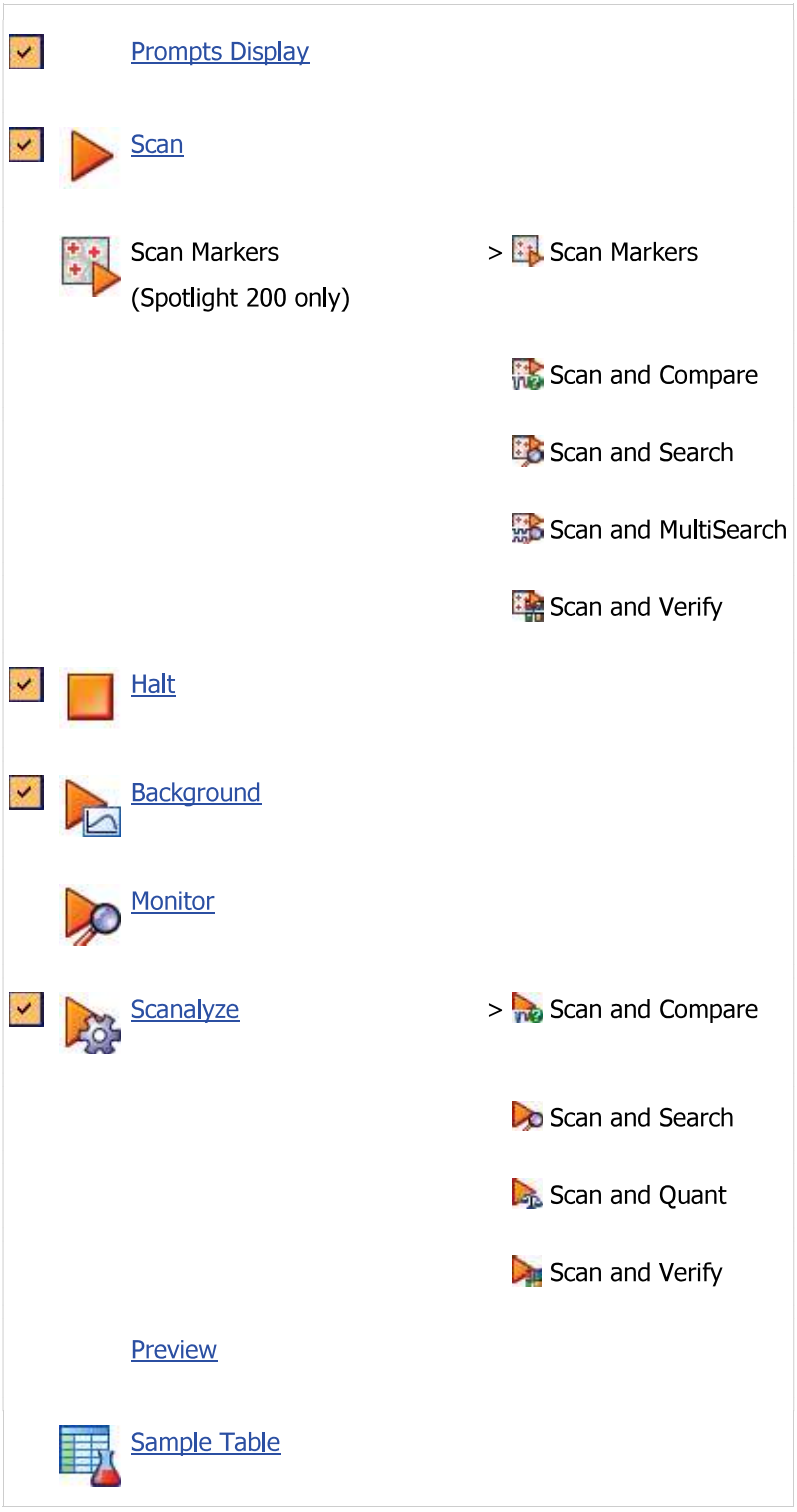
For detailed information about instrument settings, see Setup Instrument or Setup Raman Instrument.

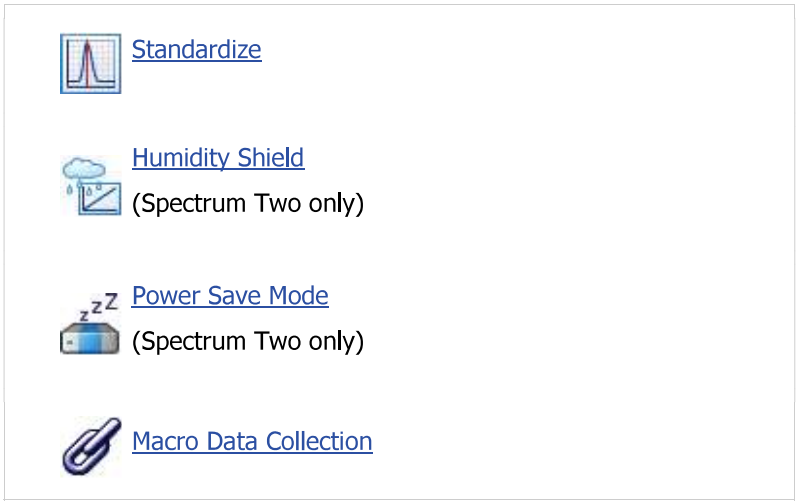
For information about setting up sample identities, see Sample Table.

The Measurement Bar

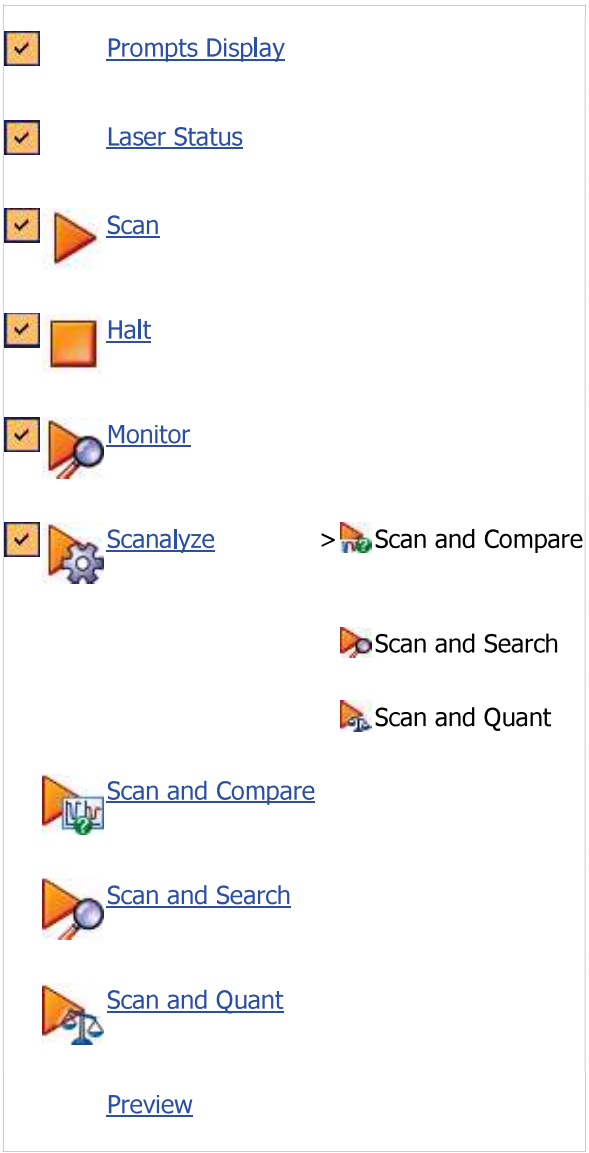
Use the buttons in the Measurement bar, together with the messages given in the Prompts Display, to control your instrument.

If you are connected to an FT-IR instrument:





If you are connected to a Raman instrument:



 Sample Table

Additional Information

The commands displayed by default on the toolbar will depend on the option you selected at installation. You may decide to include other view commands that you use frequently. See Personalizing Toolbars.

You can also add Instrument Checks and Ready Checks commands to the Measurement bar.

FT-IR Instrument

The Prompts Display is analogous to the instrument display available on some spectrometers. This can be useful when working with multiple samples and the Sample Table.

Macro Data Collection is only available when running a Data Collection step of a macro.

The Spectrum Two **Power Save Mode** option is disabled during data collection.

Raman Instrument

The Raman Laser Status icon provides information about the current state of the laser. It also provides important safety information about your system. For example:

-  Laser off
-  Laser stabilizing
-  Laser on, shutter closed
-  Laser on, safety interlock breached
-  Class 1 system, laser on, shutter open or ready to open
-  Class 3B system, laser on, shutter open or ready to open.

If you are connected to a Raman instrument with a Triggered Probe selected as the Accessory, the Scan  and Monitor  icons will indicate that there is a probe connected and will be disabled. The Scan and Preview functions can only be started using the trigger on the probe. This is to prevent accidental exposure to the laser beam when working at a distance from the PC.

The Accessory Bar

The Accessory Bar contains controls appropriate to the accessory currently installed in the instrument. The toolbar includes an icon that identifies the accessory installed. If you change the sampling accessory, the Accessory bar will automatically be updated with the new accessory controls.

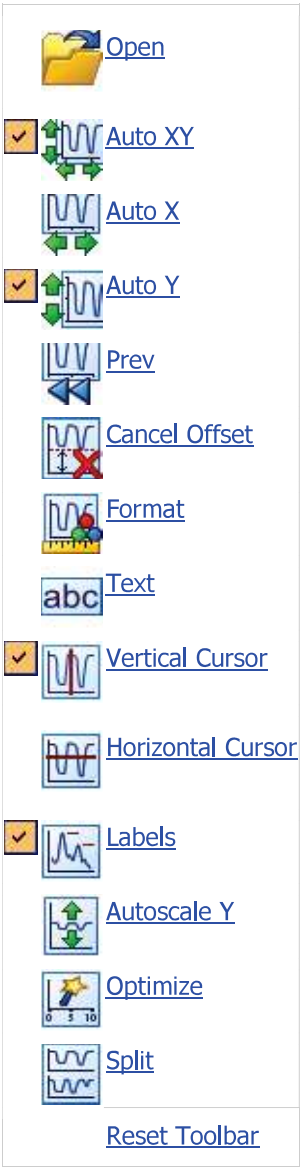
Additional Information

If your instrument configuration includes a Spotlight microscope, the Accessory bar will contain the Microscope icon. If you click  then the Setup Microscope tabs are displayed.

You can personalize toolbars by adjusting their appearance and by showing, hiding and re-arranging buttons. See Personalizing Toolbars.

The Graph Bar

Use the Graph bar to optimize how your spectra are displayed, particularly prior to printing, or cutting and pasting into another application.

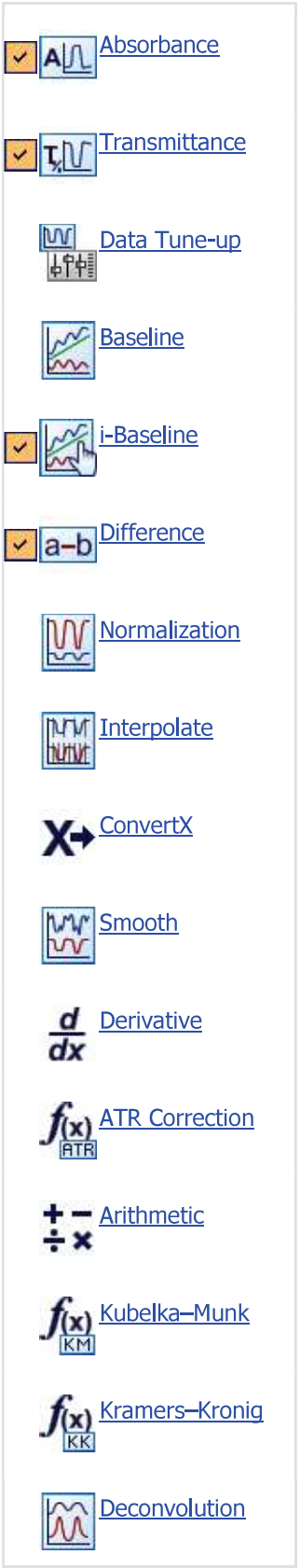


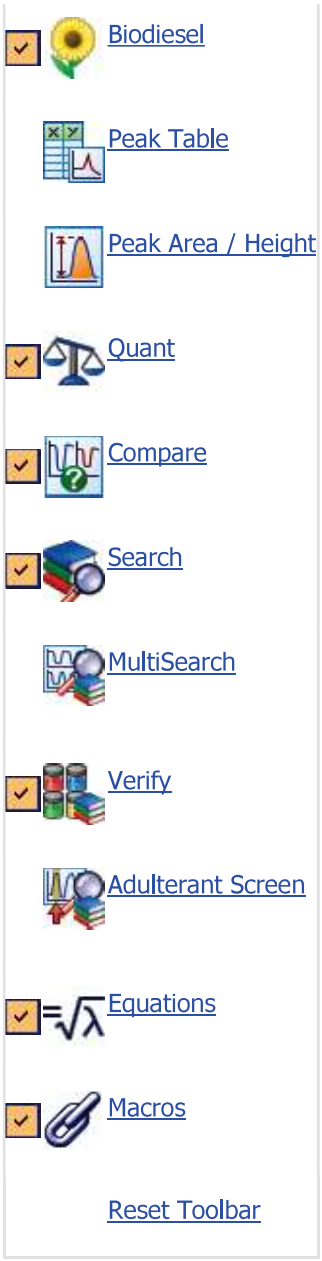
Additional Information

The commands displayed by default on the toolbar will depend on the option you selected at installation. You may decide to include other view commands that you use frequently. See Personalizing Toolbars.

The Process Bar

Use the Process bar to select a process to apply to your selected spectrum.





Additional Information

The  icon above indicates that the command is included in the factory default Process bar.

If you have the Biodiesel Analyzer installed, the process **Biodiesel** and the Macros **Biodiesel HATR** and **Biodiesel UATR** will be included in the default Process bar.

You may decide to include other process commands that you use frequently. See Personalizing Toolbars.

These commands are also available from a shortcut menu in the Viewing Area, and from the Process Menu.

The Status Bar

The Status bar is a global toolbar that is displayed at the bottom of the Spectrum workspace.

The Status bar reports the name of the user who is currently logged in, and whether Spectrum is working Offline or is connected to an instrument.

When Spectrum is connected to an instrument, the Status bar reports whether:

- The connection to a networked instrument is healthy.
- The instrument is Idle or Scanning.
- The instrument requires servicing, or its desiccant requires changing.
- The J-stop card needs changing for the current resolution. This is relevant for spectrometers that do not have an automated, internal J-stop.
- The Mode of your dual-range spectrometer has been changed since you last used the instrument.

The Status Bar also reports:

- The current status of the Microscope if a Spotlight is connected to the instrument. For example, if the microscope is initializing or an aperture calibration is in progress. Also the status of the battery in the microscope weighbridge (if fitted to the stage).
- The current status of the Raman laser, if you are connected to a Raman instrument. For example, Off, Stabilizing, On with shutter closed, On with shutter open or On with laser safety interlock breached.
- The current status of the Raman detector, if you are connected to a Raman instrument. For example, whether the detector is cooling, and the current temperature of the detector.

Showing, Hiding and Moving Toolbars

Showing and Hiding Toolbars

You can organize your workspace by hiding a toolbar, or by showing a toolbar that had been hidden.

- In the View menu, click the  icon to the left of the name of the toolbar that you want to hide

  OR

  Click the shaded area to the left of the name of the toolbar that you want to show.

NOTE:	The Menu and Status bars cannot be hidden.

Moving, or Floating, a Toolbar

When a toolbar is unlocked, a dotted drag handle is displayed, usually on its left edge. This handle enables you to change the position of a toolbar, or to float it in a separate window.

- Place your mouse pointer over the drag handle on the toolbar you want to move and drag it to its new position.

Locking Toolbars

Locking a toolbar protects it from some inadvertent changes. A locked toolbar can be hidden, and its buttons re-arranged or reset, but it cannot be customized or dragged to a new location.

- Right-click the  button to the right of the toolbar and then click **Lock The Toolbars**.

  The toolbars are locked when  is displayed to the left of this command.

NOTE:	The toolbars are grouped so that, for example, locking one of the Scan toolbars locks the Instrument Settings and Measurement toolbars, or locking one of the Graph toolbars locks the Graph and Process toolbars.

Restoring the Workspace

Spectrum Standard

Restore Default Workspace will return your workspace, including instrument settings and other default parameters, toolbar buttons and the layout, to the system default. No macros, equations, instrument setups or sample table setups will be removed.

To restore the workspace to the system default:

1. Select **Reset Layout** from the Setup menu.

   The Reset Layout dialog is displayed.

2. Click **OK** to confirm the reset.

   Spectrum closes briefly, and then opens with the system default layout.

Spectrum ES

Restore Default Workspace will return your workspace, including instrument settings and other default parameters, toolbar buttons and the layout, to the group or system default. Any user macros, equations, instrument setups or sample table setups will be removed.

To restore the workspace to the group or system default:

1. Select **Restore Default Workspace** from the Setup menu.

   The Restore Default Workspace dialog is displayed.

2. Click **OK** to confirm the reset.

   If you are a member of a group with a group default workspace, then the group workspace will be loaded. If not the system default will be loaded.

   If you are a member of more than one group, the Set Group Workspace dialog is displayed.

3. Select which group workspace you want to load.

   Members of the Administrators group can select the system default.

4. Click **OK**.

   Any unsaved data in the current workspace will be saved. If a signature is required, the Sign workspace dialog will be displayed for you to enter a signature. The workspace closes. Spectrum then reloads with the selected workspace displayed.

Additional Information

- For information about manipulating toolbar buttons, see Personalizing Toolbars.
- For information about adding or removing toolbar buttons or menu items, see Customizing Toolbars and Menus.
- You cannot personalize or customize the Status bar.

Personalizing Toolbars

You can personalize toolbars by adjusting their appearance and by showing, hiding and re-arranging buttons.

NOTE: The toolbars are grouped so that, for example, changing the appearance of the Graph toolbars changes the appearance of both the Graph Toolbar and the Process Toolbar.

Displaying and Positioning Text

By default, toolbars are displayed with command names placed under below the command icon.

1. In the View menu, select **Graph Toolbars** or **Scan Toolbars**, and then select **Customize**.

   OR

   Right-click the  button to the right of a toolbar and then click **Customize**.

   The Customize dialog is displayed.
2. Select the **Toolbars Text** tab.

   By default, the Show both text and images in toolbars option is enabled (checked) and the Text below image option is selected.
3. If you want to display the toolbar buttons without text, deselect (uncheck) the Show both text and images in toolbars option.

   OR

   Select one of the text display options.
4. Click **Close**.

Changing the Icon Size

1. In the View menu, select **Graph Toolbars** or **Scan Toolbars**, and then select **Customize**.

   OR

   Right-click the  button to the right of a toolbar and then click **Customize**.

   The Customize dialog is displayed.
2. Select the **Options** tab.

   By default, the Large Icons in Toolbars option is enabled (checked).
3. If you want to display the toolbar buttons with smaller icons, as used in the menus, disable (uncheck) the Large Icons in Toolbars option.
4. Click **Close**.

Showing and Hiding Buttons

The toolbars are, by default, populated by standard sets of buttons (that is, icons or text entry fields), which depend on the Installation Type selected when Spectrum was installed. You can organize your workspace by hiding any buttons that you do not use very often, or by showing a button that had been hidden.

- Click the  button to the right of the toolbar you want to modify, select **Add or Remove Buttons**, the name of the toolbar, and then click the  icon to the left of the name of the button that you want to hide,

  OR

  Click the shaded area to the left of the name of the button that you want to show.

Re-arranging Buttons on a Toolbar

You can arrange the buttons in the toolbars to suit your preferred method of working.

1. Hold down the ALT key and select the edge of the button you want to move.

   The button is surrounded by a black box.

2. Drag the button to its new position on the toolbar.

   The button is placed at the position of the cursor.

Resetting a Toolbar

- Click the  button to the right of the toolbar you want to reset, select **Add or Remove buttons**, the name of the toolbar, and then click **Reset Toolbar**.

  The toolbar is reset to include all the icons available for that toolbar.

Additional Information

- For information about manipulating toolbars and resetting the workspace layout, see Showing, Hiding and Moving Toolbars.
- For information about adding or removing toolbar buttons or menu items, see Customizing Toolbars
- You cannot customize the Status bar.

Customizing Toolbars and Menus

Adding Buttons to a Toolbar

You can customize a toolbar by adding buttons that are not simply hidden in the current setup. For example, you can add a button that is usually displayed in another toolbar.

1. In the View menu, select **Graph Toolbars** (if you want to customize the Graph toolbar or Process toolbar) or **Scan Toolbars** (if you want to customize the File toolbar, Instrument Settings toolbar or Measurement toolbar), and then select **Customize**.

   OR

   Right-click the  button to the right of the toolbar, click **Add or Remove Buttons** and then click **Customize**.

   The Customize dialog is displayed.

2. Select the **Commands** tab, and then click **Rearrange Commands**.

   The Rearrange Commands dialog is displayed.

3. Select the **Toolbar** option, select the toolbar you want to customize, and then click **Add**.

   The Add Command dialog is displayed.

4. Select from the **Categories** of command available, and then select the **Command** you want to add.

   You can select any available command from the All Commands category.

5. Click **OK**.

   The command is added to the list of commands that you can rearrange.

6. Position the command in the toolbar by clicking **Move Up** and **Move Down**.

7. If you want to insert a separator 'below' a button (as listed in the dialog, usually to the right of the button when the toolbar is displayed), click **Modify Selection** and select the **Begin a Group** option.

8. Click **Close**.

9. Click **Close** to shut the Customize dialog.

NOTE: Although you can use the Rearrange Commands dialog to delete a command from a toolbar, you may prefer to simply hide it.

Creating a New Toolbar

You can create a new toolbar containing any of the available commands, such as those needed for a particular task. You could hide the toolbar when it is not needed.

You associate a new toolbar with either the Graph toolbars (that is, the Graph toolbar and the Process toolbar) or with the Scan toolbars (that is, the Accessory toolbar, File toolbar, Instrument Settings toolbar and the Measurement toolbar).

1. In the View menu, select **Graph Toolbars** or **Scan Toolbars**, and then select **Customize**.

   OR

Right-click the  button to the right of a toolbar and then click **Customize**.

The Customize dialog is displayed.

2. Select the **Toolbars** tab, and then click **New**.

   The New Toolbar dialog is displayed.

3. Enter a **Toolbar name** and its default **Location**, and then click **OK**.

   The New Toolbar dialog closes, and an empty toolbar is added to Spectrum.

   The toolbar name will be added to the appropriate sub-menu in the View menu, which enables you to show or hide it.

4. If you want the toolbar to be hidden by default, deselect the checkmark to the left of its name in the Toolbars pane.

5. To populate your toolbar, continue from Step 2 in Adding Buttons to a Toolbar.

   OR

   Click **Close**.

Customizing the Menu Bar

NOTE: The menu system is very flexible, but there are some restrictions. For example, some sub-menus are treated separately and not every command is available.

You cannot add a new menu to the Menu bar, or add a command that does not exist. However, you can simplify a menu by not displaying a command that you never you use, display a command in another menu, or rearrange a menu to make a useful command more prominent.

1. In the View menu, select **Scan Toolbars**, and then select **Customize**.

   OR

   Right-click in the Menu bar and then click **Customize**.

   The Customize dialog is displayed.

2. Select the **Commands** tab, and then click **Rearrange Commands**.

   The Rearrange Commands dialog is displayed.

3. Select the **Menu Bar** option, and then select the menu or sub-menu that you want to customize.

   If any of the existing commands in the menu can be modified, they are listed in the Commands pane.

4. If you want to add a command to the menu, click **Add**, select the command from the Add Command dialog, and then click **OK**.

   The command is added to the list of commands that you can rearrange.

5. Position a selected command in the menu by clicking **Move Up** and **Move Down**, or remove it by clicking **Delete**.

6. If you want to insert a separator below a command, click **Modify Selection** and select the **Begin a Group** option.

7. Click **Close**.

8. Click **Close** to shut the Customize dialog.

Additional Information

- For information about manipulating toolbars and resetting the workspace layout, see Showing, Hiding and Moving Toolbars.
- For information about manipulating toolbar buttons, see Personalizing Toolbars.
- You cannot customize the Status bar.

Glossary

A

Absorbance: Traditionally, the absorbance scale has been used for quantitative work on spectra. The transmittance scale has been used for interpretation.

Alignment: In this context, alignment is the adjustment of the interferometer mirror angles to optimize the amplitude of the interferogram centerburst.

Apodization: The true interferogram of a light source is infinite in length. A spectrometer can only measure a finite part of the interferogram; this means that unwanted oscillations or sidelobes are produced on either side of narrow bands in the spectrum. Apodization is a mathematical function that removes the sidelobes.

ATR: Attenuated Total Reflectance. ATR correction makes a spectrum collected with an ATR accessory similar to a transmittance spectrum so the two types of spectrum can be compared.

AVI: Absolute Virtual Instrument. AVI correction measures the current instrument performance relative to an absolute standard (the methane cell in the filter wheel) and an ideal lineshape function, and applies a correction.

B

Baseline correction: Baseline correction removes baseline features from your spectrum, such as a baseline slope caused by scattering.

Beamsplitter: The beamsplitter is a plate with approximately equal transmittance and reflectance, used to generate and recombine the two beams in the interferometer.

C

CO2/H2O Suppression: An atmospheric correction routine that also overcomes non-linearity due to resolution; temperature dependence; and the effects on lineshape and calibration caused by J-stop and the sample or accessory.

D

Data Interval: The data interval, or digital resolution, refers to the abscissa spacing of data points in a spectrum or interferogram. The unit for the spectral data interval is the wavenumber (cm-1) and for interferogram data it is the number of interferogram data points collected.

Derivative: Derivative spectra usually have sharper features than the original spectra. In quantitative analysis, they are sometimes used to reduce the effects of overlapping bands. The elimination of some baseline effects in derivative spectra can be useful in quantitative methods. Second-derivative spectra have sharp minima where there are maxima in the original spectrum and so can be used to identify band positions in complex regions.

Difference: A weighted subtraction of one spectrum from another.

F

FT-IR: Fourier Transform - Infra Red. A generic term, but usually refers to a spectrometer optimized for the mid-infrared region.

FT-NIR: Fourier Transform - Near Infra Red. A spectrometer optimized for the near-infrared region.

I

Interpolate: If the features in a spectrum are sufficiently wide, fewer datapoint may be needed to define them. Interpolate adds and removes datapoints to create a copy of a spectrum constructed from a smaller dataset.

J

J-stop: Jacquinot stop. The aperture setting that restricts beam divergence to the maximum acceptable for the required resolution.

N

Normalize: A function used to set a common peak in several spectra to the same ordinate limit so that other peaks within the spectra can be compared.

O

Optimize: A display function, rather than a data transform, that ignores dominant noise spikes or peaks from atmospheric carbon dioxide or water vapor, so that you display features of interest more easily.

R

Reference material: A material (stable, homogeneous) one or more properties of which are sufficiently well-established to be used for the calibration of apparatus, the assessment of a measurement method, or for assigning values to materials.

S

Spectrum: Proprietary software used to control a PerkinElmer spectrometer; and to display, process, and store the data sets (a spectrum or series of spectra) collected.

Spectrum file: A file that contains a spectrum. Spectrum files have the extension *.sp

T

Transmittance: Traditionally, the transmittance scale has been used for interpretation of spectra. The absorbance scale has been used for quantitative work.

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