SPECTRUM FL

Software Guide

PerkinElmer®

Spectrum FL
Software Guide

Release History

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Welcome to Spectrum FL

System Overview

The Spectrum FL Software is an extensive and easy to operate software package for luminescence spectroscopy (fluorescence, phosphorescence, and bioluminescence).

Spectrum FL is operated under the MS Windows™ environment. In order to work with Spectrum FL a basic knowledge of Windows is necessary. When working with Windows for the first time, you should first review the Windows documentation.

It can be used to set up and collect data from the:

- FL 6500 (Pulse)
- FL 8500 (Continuous)

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

The manual is divided into the following areas:

Getting Started - A brief overview of Spectrum FL.

Method Setup - Select an application method to set up for your analysis.

Accessories Setup - A brief overview of the functions for the accessory setup tools.

Collecting Data - Controlling your instrument to collect spectra.

Data Analysis - Analyze the data collected using various processes.

Viewing Spectra - Working with windows and graph views.

Finding and Saving - File operations and navigation.

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

Processing Data - Working with your spectra and data.

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

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

Getting Started

Overview

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

- Login and Instrument Connection
- The Spectrum FL Workspace
- Managing Data
- Processing Data
- Publishing Results
- Exit and Save Options

Logging into Spectrum FL

Start Spectrum FL by clicking on its desktop icon 

or the Windows Start button and navigate to PerkinElmer Applications.

The Login Dialog

Spectrum FL can be configured to:

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

  OR

  Use your Windows login details.

If the Login dialog is displayed:

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

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

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

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

3. Click **OK**.

   Spectrum FL opens.

Selecting an Instrument at Login

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

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

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

Login and your Save Option on Exit

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

Additional Information

Passwords

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

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

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

Instrument Administration

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

Auto-Connect

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

Save Options on Exit

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

Unexpected Software Events and Power Failures (Spectrum ES only)

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

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

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

The Spectrum FL Workspace

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

NOTE: *Not all of the functions are available in every page of the Spectrum FL Workspace. For example, Data Explorer does not appear in the Method Setup screen.*

Panes

The Spectrum FL workspace window is divided into panes:

- The **Navigation Pane**, on the right, which contains shortcuts.
- The **Viewing Area**, in the center, which you use to display one or more spectra.
- The **Dialog Pane**, at the bottom, which you use to adjust parameters or enter information when, for example, setting up your instrument.
- The **Data Explorer**, on the left, which you use to manage your spectra.

The contents of the Dialog Pane reflect the shortcut selected in the Navigation Pane. You use the Data Explorer in conjunction with the Viewing Area.

Toolbars

The Spectrum FL workspace can include a number of global toolbars:

- The Method Setup Menu bar
- The Data Analysis Menu bar.
- The scan toolbars, namely the Instrument Settings bar and the Action bar and the Accessory bar. By default, these toolbars are located at the top of the workspace, under the Menu bar.
- The Status bar, located at the bottom of the workspace.

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

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

Additional Information:

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

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

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

Managing Data

Spectrum FL enables you to:

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

Using Familiar Windows Techniques

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

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

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

   OR

   Click  on the Graph bar.

   The Open File window is displayed.

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

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

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

3. Click **Open**.

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

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

Saving Spectra

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

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

Specify another default directory for saved spectra by selecting **Save As** or **Save All** from the File menu.

Organizing Samples Views using the Data Explorer

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

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

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

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

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

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

Using the Spectrum Browser

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

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

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

Additional Information

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

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

Processing Data

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

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

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

Publishing Results

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

You can also:

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

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

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

Additional Information

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

Exit and Save Options

When you want to Exit Spectrum FL:

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

   OR

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

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

   The Save Options dialog is displayed.

2. Select the appropriate option.

   If you have Spectrum FL Standard, select to:

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

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

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

   If you have Spectrum FL ES, select to:

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

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

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

   a. Return to workspace – Reload the previous workspace.

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

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

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

   Spectrum closes.

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

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

   Refer to **Assigning a New Default Workspace** for more information.

Method Setup

Spectra Scan

This Scan application is used for collecting various types of spectral data in a variety of modes (fluorescence, phosphorescence, and bioluminescence) and dimensions (single and 3D scans).

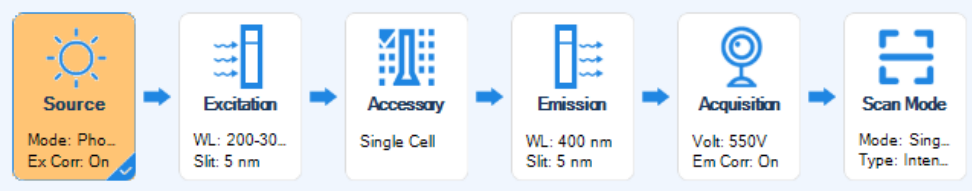
Data Collection Tab

Scan Type

There are five types of scans available from the Spectra Scan mode:

- An **Excitation Scan** is recorded using a fixed emission wavelength. The start and final wavelengths refer to the excitation monochromator.
- An **Emission Scan** is recorded using a fixed excitation wavelength. The start and final wavelengths refer to the emission monochromator.
- A **Synchronous (δλ) Scan**, where both monochromators are scanned simultaneously with a constant wavelength difference between the excitation and emission monochromators. This technique is used for rapid screening in environmental analysis, for example for differentiating between various types of crude oil (oil fingerprinting), since the technique greatly simplifies the spectra of complex mixtures with overlapping spectral components. In a synchronous scan, the start and final wavelengths always refer to the excitation monochromator and the emission monochromator always starts at a higher wavelength than the excitation monochromator.
- A **Synchronous (δE) Scan**, where both monochromators are scanned simultaneously with a constant energy difference between excitation and emission monochromators. The emission monochromator accelerates relative to the excitation monochromator. In a synchronous energy scan, a synchronous spectrum is recorded at a constant energy difference between excitation and emission monochromator. This technique can be used for the investigation of very complex mixtures where the spectral sensitivity at constant wavelength difference is too low. Scanning at constant energy difference between the monochromators has an advantage over the recording of spectra at constant wavelength difference by having a higher spectral resolution and lower background fluorescence.
- A **Pre-Scan** using either one or both monochromators can be used to determine the optimum excitation and emission wavelength for unknown samples. See **Performing a Pre-Scan**.
- A **Background Correction** scan Measures the current background intensity. This value is used for all subsequent reference measurements.

Instrument Settings



Source

Source Setup (FL 6500)

Source Mode: Pulse. This is set when you select your **Instrument Connection**.

Luminescence Mode: Select Fluorescence or Phosphorescence.

Fluorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click the check box to set Real-time Dark.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Phosphorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Flash Count: Enter a value from 1 to 10.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

NOTE: *The maximum frequency for each power is listed in the following table.*

Power	Maximum Frequency
20	200
40	200
80	100
120	50

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Bioluminescence (No additional settings required)

Source Setup (FL 8500)

Source Mode: Continuous. This is set when you select your **Instrument Connection**.

Luminescence: Select Fluorescence, Phosphorescence, or Bioluminescence.

Fluorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click the check box to set Real-time Dark.

NOTE: *A* ***Synchronous (δE) Scan*** *does not support* ***Real-time Dark*** *for the FL 8500.*

Chopper (Hz): Select a Chopper value of 10, 20, or 40 from the drop-down list.

Phosphorescence

Ex. Corr: Select On, Off, or File.

Chopper (Hz): Select a Chopper value: 10, 20, or 40 from the drop-down list.

Bioluminescence (No additional settings required)

Excitation

Scan Type setting: Excitation Scan, Synchronous (δλ) Scan, Synchronous (δE) Scan

Excitation Mono Setup

Excitation Start Wavelength (nm): Enter a value.

Excitation End Wavelength (nm): Enter a value.

Or click the **Full Range** button (190 - 900 nm)

Excitation Slit Width (nm): Select 1, 2.5, 5, 10 or 20 from the drop-down list.

Excitation Filter: Click the **Choose Filter** button or select a filter from the drop-down list.

NOTE: *Click this button to access the Filter Setting dialog which allows a user to read or modify the current filter configuration for the connected instrument. A user can also enter a custom name in the FilterCustom field.*

Scan Speed (nm/min): Select a value from the drop-down list.

NOTE: *As you move up in power, Scan Speed options will change.*

Accumulation Number: Enter a value from 1 to 100.

Scan Type setting: Emission Scan Type

Excitation Mono Setup

Excitation Wavelength (nm): Enter a value.

Excitation Slit Width (nm): Select 1, 2.5, 5, 10 or 20 from the drop-down list.

Excitation Filter: Click the Choose Filter button or select a filter from the drop-down list.

Accessory

Accessory Setup: Select an Accessory from the drop-down list.

Emission

Scan Type setting: Excitation Scan

Emission Mono Setup

Emission Wavelength (nm): Enter a value.

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list.

Emission Filter: Click the Choose Filter button or select a filter from the drop-down list.

Scan Type setting: Emission Scan

Emission Mono Setup

Emission Start Wavelength (nm): Enter a value.

Emission End Wavelength (nm): Enter a value.

Or click the Full Range button (190- 900 nm)

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list.

Emission Filter: Click the Choose Filter button or select a filter from the drop-down list.

Scan Speed (nm/min): Select a value from the drop-down list.

NOTE: *As you move up in power, Scan Speed options will change.*

Accumulation Number: Enter a value.

Scan Type setting: Synchronous (δλ) Scan

Emission Mono Setup

Delta Lambda (nm): Enter a value.

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list.

Emission Filter: Click the Choose Filter button or select a filter from the drop-down list.

Scan Type setting: Synchronous (δE) Scan

Emission Mono Setup

Delta Energy (cm-1): Enter a value.

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list.

Emission Filter: Click the Choose Filter button or select a filter from the drop-down list.

Acquisition

Detector Setup

Photomultiplier Voltage (V): Select Low (400), Medium (550), High (700), or Custom from the drop-down list. Select **Custom** to enter a value from 0 to 1250.

Response Width (nm): Select 0, 0.5, 0.75, 1, 2.5, 5, 10, or 20

NOTE: *In order to get a better repeatability data, it is suggested to set the response width at least to be value nearest (Excitation slit width +Emission slit width)/2. Eg. When set Excitation slit width to be 5 nm, Emission slit width to be 2.5 nm, it is suggested to set response width to be 5 nm.*

Em. Corr.: Select On, Off, or File from the drop-down list.

NOTE: *In the **Phosphorescence** Mode you need to enter two additional settings; a **Delay (us)** time value and a **Gate (ms)** time value.*

Gain

PMT: Select a gain of x1, x8, x64, x512, or Auto from the drop-down list.

NOTE: *The PMT Gain is a multiplier of the Photomultiplier Voltage.*

Scan Mode

Single Scan: Select Intensity, Polarization, or Anisotropy.

3D Scan

Scan Type setting: Excitation Scan

Enter the **Number of Scans** and the **Emission increment(nm)**.

Scan Type setting: Emission Scan

Enter the **Number of Scans** and the **Excitation increment(nm)**.

Scan Type setting: Synchronous (δλ) Scan

Enter the **Number of Scans** and the **Delta lambda increment(nm)**.

Scan Type setting: Synchronous (δE) Scan

Enter the **Number of Scans** and the **Delta energy increment(cm-1)**

Repeat Scan: Enter the **Number of Scans** and a **Repeat Option** (select **Repeat with time** or **Repeat with User Prompt**).

Auto Peak *(Displays only when Pre-Scan is selected as the Scan Type)*

Solvent: Select Water, Ethanol, Cyclohexane, Chloroform, Carbon tetrachloride, Other.

Raman Wavenumber (cm-1): This number is based on the **Solvent** selection. When selecting **Other** enter a value.

Rayleigh scatter check: Click the check box to select Rayleigh scatter check.

Raman scatter check: Click the check box to select Raman scatter check**.**

2nd order check: Click the check box to select 2nd order check.

Description Tab

Method Name: Type a name for your method.

Notes: Type notes specific to this method.

Signatures (ES version): Select Sign, Review, or Approve from the drop-down list.

Sample Table Tab

The Sample Table provides a listing of samples by **Sample ID**, **Description**, and **Type**. There is also an indicator to show if the sample has been measured or not. The right side contains buttons to control the samples.

For each sample row you can **Add**, **Insert**, **Remove**, and move the row **Up** or **Down**.

Format Sample Table: Opens a **Table Builder** dialog where you can add **Preparation** information, add custom **Columns**, and add **ID** information.

Setups…: Opens a Sample Table Setups dialog where you can **Save the current Sample Table**, **Delete**, **Set as current**, **Import**, **Export**, and with **Signatures**, Sign, Review and Approve the table.

Import or **Export** a sample table.

Fill Down or **Clear Measured** table rows.

Single Read

The Single Read application method enables measurements (intensity, concentration, polarization, anisotropy) to be made at fixed wavelengths. The data are saved on the hard disk in an Excel compatible file format.

Data Collection Tab

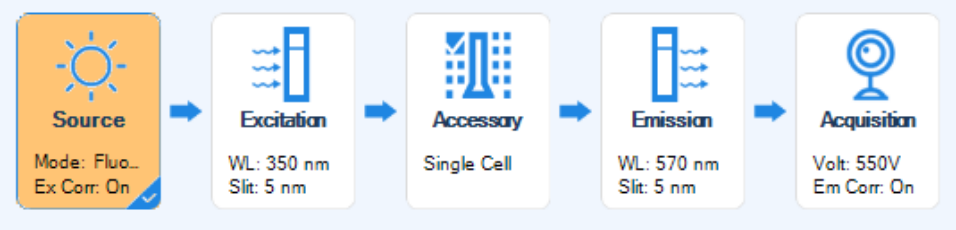
Calculation Mode

Select I**ntensity, Polarization, or Anisotropy**.

Background Correction: Measures the current background intensity. This value is used for all subsequent reference measurements.

Save Results: Saves the results after analysis.

Instrument Setting



Source

Source Setup (FL 6500)

Source Mode: Pulse. This is set when you select your **Instrument Connection**.

Luminescence: Select Fluorescence, Phosphorescence, or Bioluminescence.

Fluorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click the check box to set Real-time Dark.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Phosphorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Flash Count: Enter a value from 1 to 10.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

NOTE: *The maximum frequency for each power is listed in the following table.*

Power	Maximum Frequency
20	200
40	200
80	100
120	50

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Bioluminescence (No additional settings required)

Source Setup (FL 8500)

Source Mode: Continuous. This is set when you select your **Instrument Connection**.

Luminescence: Select Fluorescence, Phosphorescence, or Bioluminescence.

Fluorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click the check box to set Real-time Dark.

Chopper (Hz): Select a Chopper value of 10, 20, or 40 from the drop-down list.

Phosphorescence

Ex. Corr: Select On, Off, or File.

Chopper (Hz): Select a Chopper value: 10, 20, or 40.

Bioluminescence (No additional settings required)

Excitation

(Not applicable in the Bioluminescence Mode.)

Excitation Mono Setup

Excitation Wavelength (nm): Enter a value for the Excitation Wavelength.

Excitation Slit Width (nm): Enter a value for the Excitation Slit Width.

Excitation Filter: Click the **Choose Filter** button or select from the drop-down list.

Accessory

Accessory Setup: Select an Accessory from the drop-down list.

Emission

Emission Mono Setup

Emission Wavelength (nm): Enter a value.

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list.

Emission Filter: Click the Choose Filter button or select a filter from the drop-down list.

Acquisition

Detector Setup

Photomultiplier Voltage (V): Select Low (400), Medium (550), High (700), or Custom from the drop-down list. Select **Custom** to enter a value.

Intrgration Time (ms): Enter a value.

Em. Corr.: Select On, Off, or File from the drop-down list.

*NOTE: In the **Phosphorescence** Mode only enter a **Delay (us)** time value and a **Gate (ms)** time value.*

Gain

PMT: Select a gain of x1, x8, x64, x512, or Auto from the drop-down list.

Note: The PMT Gain is a multiplier of the Photomultiplier Voltage.

Description Tab

Method Name: Type a name for your method.

Notes: Type notes specific to this method.

Signatures (ES version): Select Sign, Review, or Approve from the drop-down list.

Time Drive

This application method allows a user to make luminescence (fluorescence, phosphorescence and bioluminescence) measurements at fixed wavelengths with well-defined intervals over a specified period of time.

Data Collection Tab

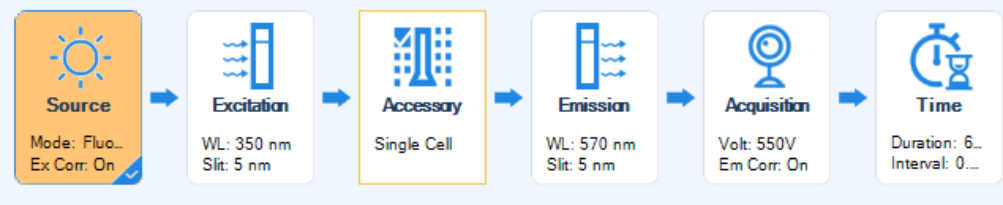
Immediate Mode: Click the check box to set Immediate Mode.

Backgroung Correction: Click the check box to set Background Correction.

Remote Start: Click the check box for remote start.

*NOTE: Select **Remote Start** if you wish to have data collection with a device which can provide external signal, for example a Rapid Mixing device. Data collection is initiated on receiving a trigger signal.*

Instrument Setting



Source

Source Setup (FL 6500)

Source Mode: Pulse. This is set when you select your **Instrument Connection**.

Luminescence: Select Fluorescence, Phosphorescence, or Bioluminescence.

Fluorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click the check box to set Real-time Dark.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Phosphorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Flash Count: Enter a value from 1 to 10.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

NOTE: The maximum frequency for each power is listed in the following table.

Power	Maximum Frequency
20	200
40	200
80	100
120	50

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Bioluminescence (No additional settings required)

Source Setup (FL 8500)

Source Mode: Continuous. This is set when you select your **Instrument Connection**.

Luminescence: Select Fluorescence, Phosphorescence, or Bioluminescence.

Fluorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click the check box to set Real-time Dark.

Chopper (Hz): Select a Chopper value of 10, 20, or 40 from the drop-down list.

Phosphorescence

Ex. Corr: Select On, Off, or File.

Chopper (Hz): Select a Chopper value: 10, 20, or 40.

Bioluminescence (No additional settings required)

Excitation

(Not applicable in the Bioluminescence Mode.)

Excitation Mono Setup

Excitation Wavelength (nm): Enter a value for the Excitation Wavelength.

Excitation Slit Width (nm): Enter a value for the Excitation Slit Width.

Excitation Filter: Click the **Choose Filter** button or select from the drop-down list.

Accessory

Accessory Setup: Select an Accessory from the drop-down list.

Emission

Emission Mono Setup

Emission Wavelength (nm): Enter a value.

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list.

Emission Filter: Click the Choose Filter button or select a filter from the drop-down list.

Acquisition

Detector Setup

Photomultiplier Voltage (V): Select Low (400), Medium (550), High (700), or Custom from the drop-down list. Select Custom to enter a value.

Response Time (sec): Enter a value.

Em. Corr.: Select On, Off, or File from the drop-down list.

NOTE: *In the **Phosphorescence** Mode only enter a **Delay (us)** time value and a **Gate (ms)** time value.*

Gain

PMT: Select a gain of x1, x8, x64, x512, or Auto from the drop-down list.

NOTE: *The PMT Gain is a multiplier of the Photomultiplier Voltage.*

Time

Time Drive Settings

Duration: Enter a Duration time. Select **Second** or **Minute**.

Data Interval: Enter a Data Interval value.

Event Marker Active: Click the check box to set the **Event Marker Active.**

NOTE: *Select **Event Marker Active** to mark events during a time drive run, for example marking the addition of a reagent to the sample. Timed events can be marked using press event button which located at the front of instrument. Once data acquisition starts, the data file with the extension *.td plus a second file using the same name but with the file extension *.tde will be displayed in the graph panel. This has a constant ordinate value -100 except for the marked events which result in a spike for each event.*

Delay Before Measure: Enter a delay time.

Description Tab

Method Name: Type a name for your method.

Notes: Type notes specific to this method.

Signatures (ES version): Select Sign, Review, or Approve from the drop-down list.

Sample Table Tab

The Sample Table provides a listing of samples by **Sample ID**, **Description**, and **Type**. There is also an indicator to show if the sample has been measured or not. The right side contains buttons to control the samples.

For each sample row you can **Add**, **Insert**, **Remove**, and move the row **Up** or **Down**.

Format Sample Table: Opens a **Table Builder** dialog where you can add **Preparation** information, add custom **Columns**, and add **ID** information.

Setups…: Opens a Sample Table Setups dialog where you can **Save the current Sample Table**, **Delete**, **Set as current**, **Import**, **Export**, and with **Signatures**, Sign, Review and Approve the table.

Import or **Export** a sample table.

Fill Down or **Clear Measured** table rows.

Advanced Tab

In a table format, **Add**, **Remove**, or **Clear** a process associated with the method.

Settings: If available modify any editable settings.

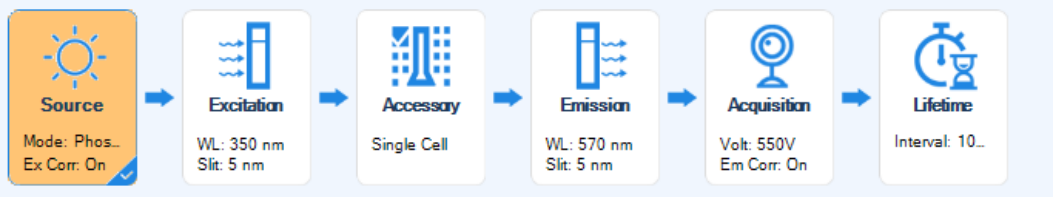
Lifetime

This application method measures the phosphorescence lifetime (delayed fluorescence) of sample.

Data Collection Tab

Remote Start: Select the check box if you have a remote start.

Instrument Setting



Source

Source Setup (FL 6500)

Source Mode: Pulse. This is set when you select your **Instrument Connection**.

Luminescence Mode: Select Phosphorescence (short) or Phosphorescence (long).

Ex. Corr: Select On, Off, or File from the drop-down list.

Flash Count: Enter a value from 1 to 10.

NOTE: *The Flash Count value in only necessary when the Luminescence Mode is Phosphorescence (long).*

Power (kW): Select a power value: 20, 40, 80, or 120 from the drop-down list.

Frequency (Hz): Select a frequency value: 50, 100, or 200 from the drop-down list.

NOTE: *The maximum frequency for each power is listed in the following table.*

Power	Maximum Frequency
20	200
40	200
80	100
120	50

Source Setup (FL 8500)

Source Mode: Continuous. This is set when you select your **Instrument Connection**.

Luminescence Mode: Select Phosphorescence (short) or Phosphorescence (long).

When you select Phosphorescence (long) enter an **Open Time (ms)**.

When you select Phosphorescence (short) select a **Chopper** value: 10, 20, or 40 Hz from the drop-down list.

Ex. Corr: Select On, Off, or File from the drop-down list

Excitation

Excitation Mono Setup

Excitation Wavelength (nm): Enter a value for the Excitation Wavelength.

Excitation Slit Width (nm): Enter a value for the Excitation Slit Width.

Excitation Filter: Click the **Choose Filter** button or select a value from the drop-down list.

Accessory

Accessory Setup: Select an Accessory from the drop-down list.

Emission

Emission Mono Setup

Emission Wavelength (nm): Enter a value.

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list.

Emission Filter: Click the Choose Filter button or select a filter from the drop-down list.

Acquisition

Detector Setup

Photomultiplier Voltage (V): Select Low (400), Medium (550), High (700), or Custom from the drop-down list. Select **Custom** to enter a value.

Response Time (sec): Enter a value.

Em. Corr.: Select On, Off, or File from the drop-down list.

Delay (us): Enter a Delay time value.
Gate (ms): Enter a Gate time value

Gain

PMT: Select a gain of x1, x8, x64, x512, or Auto from the drop-down list.

NOTE: *The PMT Gain is a multiplier of the Photomultiplier Voltage.*

Lifetime

Data Interval: Enter a Data Interval value.

NOTE: *Enter a Data Interval value only when Phosphorescence (long) is selected.*

Description Tab

Method Name: Type a name for your method.

Notes: Type notes specific to this method.

Signatures (ES version): Select Sign, Review, or Approve from the drop-down list.

Sample Table Tab

The Sample Table provides a listing of samples by **Sample ID**, **Description**, and **Type**. There is also an indicator to show if the sample has been measured or not. The right side contains buttons to control the samples.

For each sample row you can **Add**, **Insert**, **Remove**, and move the row **Up** or **Down**.

Format Sample Table: Opens a **Table Builder** dialog where you can add **Preparation** information, add custom **Columns**, and add **ID** information.

Setups…: Opens a Sample Table Setups dialog where you can **Save the current Sample Table**, **Delete**, **Set as current**, **Import**, **Export**, and with **Signatures**, Sign, Review and Approve the table.

Import or **Export** a sample table.

Fill Down or **Clear Measured** table rows.

Quantification

This application method is used for the determination of unknown concentration of a sample by assuming a relationship between fluorescence intensity of the unknown and concentration. The can be measured at a fixed excitation/emission wavelength (wavelength quantification) or on a peak height or area (scanning quantification).

Data Collection Tab

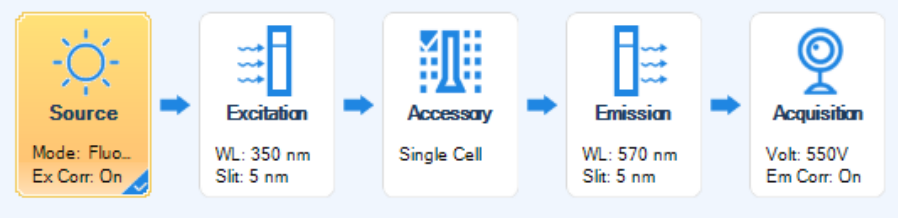
Quant Mode

Select **Wavelength Quant** or **Scan Quant.**

Settings

For each of the settings in the table (Setting1, Setting2, Setting3) select **Active** or **BG** by clicking in the check box.

Instrument Settings



Source

Source Setup (FL 6500)

Source Mode: Pulse. This is set when you select your **Instrument Connection**.

Luminescence: Select Fluorescence, Phosphorescence, or Bioluminescence

Fluorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Realtime Dark

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Phosphorescence

Ex. Corr: Select **On, Off, or File** from the drop-down list.

Flash Count: Enter a value from 1 to 10.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

NOTE: *The maximum frequency for each power is listed in the following table.*

Power	Maximum Frequency
20	200
40	200
80	100
120	50

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Bioluminescence (No additional settings required)

Source Setup (FL 8500)

Source Mode: Continuous. This is set when you select your **Instrument Connection**.

Luminescence: Select Fluorescence, Phosphorescence, or Bioluminescence

Fluorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Realtime Dark

Chopper (Hz): Select **10,** 20, or 40 from the drop-down list.

Phosphorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Chopper (Hz): Select **10,** 20, or 40 from the drop-down list.

Bioluminescence (No additional settings required)

Excitation

(Not applicable in the Bioluminescence Mode.)

Excitation Mono Setup

Excitation Wavelength (nm): Enter a value for the Excitation Start Wavelength.

Excitation Slit Width (nm): Enter a value for the Excitation Slit Width.

Excitation Filter: Click the **Choose Filter** button or select from the drop-down list.

Accessory

Accessory Setup: Select an Accessory from the drop-down list.

Emission

Scan Quant - Emission Mono Setup

Click the **Full Range** button or set your own values:

Emission Start Wavelength (nm): Enter a value.

Emission End Wavelength (nm): Enter a value.

Emission Slit Width (nm): 0.5, 1, 2.5, 5, 10 or 20

Emission Filter: Click the Choose Filter button or select a filter from the drop-down list.

Scan Speed: Enter a value in nm/min.

NOTE: *As you move up in power, Scan Speed options will change.*

Wavelength Quant - Emission Mono Setup

Emission Wavelength (nm): Enter a value.

Emission Slit Width (nm): 0.5, 1, 2.5, 5, 10 or 20

Emission Filter: Click the Choose Filter button or select a filter from the drop-down list.

Acquisition

Detector Setup

Photomultiplier Voltage (V): Select Low (400), Medium (550), High (700), or Custom from the drop-down list. Select Custom to enter a value.

Response Width (nm): Select 0, 0.5, 0.75, 1, 2.5, 5, 10, or 20 from the drop-down list.

Em. Corr.: Select On, Off, or File from the drop-down list.

NOTE: *In the **Phosphorescence** Mode only enter a **Delay (us)** time value and a **Gate (ms)** time value.*

Gain

PMT: Select a gain of x1, x8, x64, x512, or Auto from the drop-down list.

NOTE: *The PMT Gain is a multiplier of the Photomultiplier Voltage.*

Description Tab

Method Name: Type a name for your method.

Notes: Type notes specific to this method.

Signatures (ES version): Select Sign, Review, or Approve from the drop-down list.

Quant Tab

Component: View or modify the component type and **Units**.

Calibration

Type: Select the calibration type from the drop-down list (Calibration Curve or User Defined Curve).

Type of curve: Select the curve type from the drop-down list (Auto, Linear, Cubic, or Quadratic).

Force through zero: Click this check box to force the curve through zero.

Units

Correlation (r^2): Click this check box to select or enter a correlation value.

Standard tolerance (%): Click this check box to select or enter a standard tolerance value.

Control samples tolerance (%): Click this check box to select this setting.

Sample Table Tab

The Sample Table provides a listing of samples by **Sample ID**, **Description**, and **Type**. There is also an indicator to show if the sample has been measured or not. The right side contains buttons to control the samples.

For each sample row you can **Add**, **Insert**, **Remove**, and move the row **Up** or **Down**.

Format Sample Table: Opens a **Table Builder** dialog where you can add **Preparation** information, add custom **Columns**, and add **ID** information.

*NOTE: In the Design tab, by entering multiple **Replicates** or **Measurements** allow a user to get average quantification results for sample type. In addition, note that the **Concentration** column is a mandatory field for Standard and Control Type. If using the Calibration Curve type for quantification without force through zero, at least 2 standards need to be added.*

Setups…: Opens a Sample Table Setups dialog where you can **Save the current Sample Table**, **Delete**, **Set as current**, **Import**, **Export**, and with **Signatures**, Sign, Review and Approve the table.

Import or **Export** a sample table.

Fill Down or **Clear Measured** table rows.

Advanced Tab

In a table format, **Add**, **Remove**, or **Clear** a process associated with the method.

Settings: If available modify any editable settings.

Wavelength Program

This application method allows for a routine acquisition of time-dependent, multi-channel (multiple Excitation/Emission combinations).

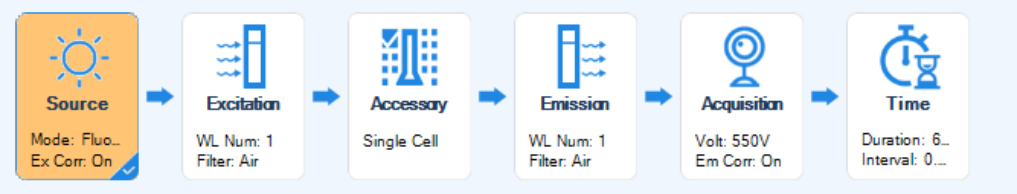
Data Collection Tab

Measured Num: Select a value from the drop-down list or enter a value.

Background Correction: Click the check box to set Background Correction.

Remote Start: Click the check box for remote start.

Instrument Setting



Source

Source Setup (FL 6500)

Source Mode: Pulse. This is set when you select your **Instrument Connection**.

Luminescence: Select Fluorescence, Phosphorescence, or Bioluminescence.

Fluorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click the check box to set Real-time Dark.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Phosphorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Flash Count: Enter a value from 1 to 10.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

NOTE: *The maximum frequency for each power is listed in the following table.*

Power	Maximum Frequency
20	200
40	200
80	100
120	50

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Bioluminescence (No additional settings required)

Source Setup (FL 8500)

Source Mode: Continuous. This is set when you select your **Instrument Connection**.

Luminescence: Select Fluorescence, Phosphorescence, or Bioluminescence.

Fluorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click the check box to set Real-time Dark.

Chopper (Hz): Select a Chopper value of 10, 20, or 40 from the drop-down list.

Phosphorescence

Ex. Corr: Select On, Off, or File.

Chopper (Hz): Select a Chopper value: 10, 20, or 40.

Bioluminescence (No additional settings required)

Excitation

(Not applicable in the Bioluminescence Mode.)

Excitation Setup

For each ID in the table enter:

Excitation Wavelength (nm): Enter a value for the Excitation Wavelength.

Excitation Slit Width (nm): Enter a value for the Excitation Slit Width.

Excitation Filter: Click the **Choose Filter** button or select a filter from the drop-down.

Accessory

Accessory Setup: Select an Accessory from the drop-down list.

Emission

Emission Setup

For each ID in the table enter:

Emission Wavelength (nm): Enter a value.

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list.

Emission Filter: Click the Choose Filter button or select a filter from the drop-down list.

Acquisition

Detector Setup

Photomultiplier Voltage (V): Select Low (400), Medium (550), High (700), or Custom from the drop-down list.

Select Custom to enter a value.

Integration Time (ms): Enter a value.

Em. Corr.: Select On, Off, or File from the drop-down list.

*NOTE: In the **Phosphorescence** Mode only enter a **Delay (us)** time value and a **Gate (ms)** time value.*

Gain

PMT: Select a gain of x1, x8, x64, x512, or Auto from the drop-down list.

NOTE: The PMT Gain is a multiplier of the Photomultiplier Voltage.

Time

Time Drive Settings

Duration: Enter a Duration time. Select **Second** or **Minute**.

Data Interval: Enter a Data Interval value.

Delay Before Measure: Enter a delay value.

Description Tab

Method Name: Type a name for your method.

Notes: Type notes specific to this method.

Signatures (ES version): Select Sign, Review, or Approve from the drop-down list.

Sample Table Tab

The Sample Table provides a listing of samples by **Sample ID**, **Description**, and **Type**. There is also an indicator to show if the sample has been measured or not. The right side contains buttons to control the samples.

For each sample row you can **Add**, **Insert**, **Remove**, and move the row **Up** or **Down**.

Format Sample Table: Opens a **Table Builder** dialog where you can add **Preparation** information, add custom **Columns**, and add **ID** information.

Setups…: Opens a Sample Table Setups dialog where you can **Save the current Sample Table**, **Delete**, **Set as current**, **Import**, **Export**, and with **Signatures**, Sign, Review and Approve the table.

Import or **Export** a sample table.

Fill Down or **Clear Measured** table rows.

Kinetics

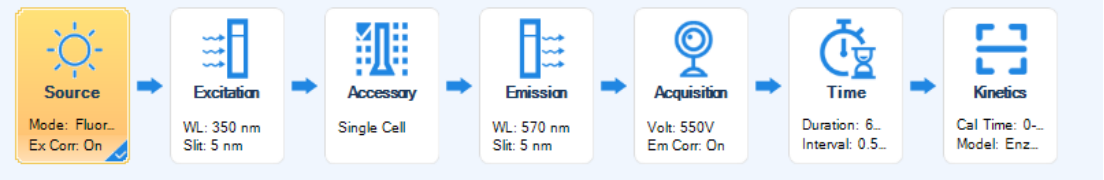
This is an application that is based on the Time Drive method. It allows for the automatic calculation of initial reaction rates and reaction velocities for enzyme kinetics

Data Collection Tab

Background Correction: Click the check box to set Background Correction.

Remote Start: Click the check box for remote start.

Instrument Setting



Source

Source Setup (FL 6500)

Source Mode: Pulse. This is set when you select your **Instrument Connection**.

Luminescence: Select Fluorescence, Phosphorescence, or Bioluminescence.

Fluorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click the check box to set Real-time Dark.

Power(kW): Select 20, 40, 80, or 120 from the drop-down list.

Frequency(Hz): Select 50, 100, or 200 from the drop-down list.

Phosphorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Flash Count: Enter a value from 1 to 10.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

NOTE: *The maximum frequency for each power is listed in the following table.*

Power	Maximum Frequency
20	200
40	200
80	100
120	50

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Bioluminescence (No additional settings required)

Source Setup (FL 8500)

Source Mode: Continuous. This is set when you select your **Instrument Connection**.

Luminescence: Select Fluorescence, Phosphorescence, or Bioluminescence.

Fluorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click the check box to set Real-time Dark.

Chopper (Hz): Select a Chopper value: 10, 20, or 40.

Phosphorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Chopper (Hz): Select a Chopper value: 10, 20, or 40.

Bioluminescence (No additional settings required)

Excitation

(Not applicable in the Bioluminescence Mode.)

Excitation Mono Setup

Excitation Wavelength (nm): Enter a value for the Excitation Wavelength.

Excitation Slit Width (nm): Enter a value for the Excitation Slit Width.

Excitation Filter: Click the **Choose Filter** button or select a filter from the drop-down.

Accessory

Accessory Setup: Select an Accessory from the drop-down list.

Emission

Emission Mono Setup

Emission Wavelength (nm): Enter a value.

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list.

Emission Filter: Click the Choose Filter button or select a filter from the drop-down list.

Acquisition

Detector Setup

Photomultiplier Voltage (V): Select Low (400), Medium (550), High (700), or Custom from the drop-down list. Select **Custom** to enter a value.

Response Time (sec): Enter a value.

Em. Corr.: Select On, Off, or File from the drop-down list.

NOTE: *In the **Phosphorescence** Mode only enter a **Delay (us)** time value and a **Gate (ms)** time value.*

Gain

PMT: Select a gain of x1, x8, x64, x512, or Auto from the drop-down list.

NOTE: The PMT Gain is a multiplier of the Photomultiplier Voltage.

Time

Time Drive Settings

Duration: Enter a Duration time. Select **Second** or **Minute**.

Data Interval: Enter a Data Interval value or select a value from the drop-down list.

Kinetics

Calculation Time (s): Enter a Start and End time.

Kinetics Model:

Select **Enzyme Kinetics** then select the following plots from the drop-down list: Michaelis-Menten Plot, Lineweaver-Burk Plot, Hofstee Plot, or Eadie-Hofstee Plot.
or
Select **Reaction Rate** then select one of the following from the drop-down list: Zero Order, Initial Rate, First Order, or Delta AU.

Description Tab

Method Name: Type a name for your method.

Notes: Type notes specific to this method.

Signatures (ES version): Select Sign, Review, or Approve from the drop-down list.

Sample Table Tab

The Sample Table provides a listing of samples by **Sample ID**, **Description**, and **Type**. There is also an indicator to show if the sample has been measured or not. The right side contains buttons to control the samples.

For each sample row you can **Add**, **Insert**, **Remove**, and move the row **Up** or **Down**.

Format Sample Table: Opens a **Table Builder** dialog where you can add **Preparation** information, add custom **Columns**, and add **ID** information.

*NOTE: In the **Enzyme Kinetics** Model, the **Concentration** field is mandatory to fill in the value of substrate concentration.*

Setups...: Opens a Sample Table Setups dialog where you can **Save the current Sample Table**, **Delete**, **Set as current**, **Import**, **Export**, and with **Signatures**, Sign, Review and Approve the table.

Import or **Export** a sample table.

Fill Down or **Clear Measured** table rows.

Quenching

This application method monitors the deactivation (quenching) of the excited state of fluorescence molecules in the presence of quencher molecules. The can be measured at a fixed excitation/emission wavelength (wavelength quenching) or on a peak height or area (scanning quenching) and yields the Stern-Volmer constant.

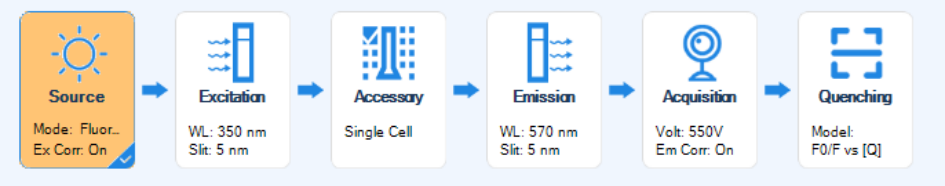
Data Collection Tab

Mode

Select the **Wavelength** or **Scan** mode.

Select the **Background Correction** check box to measure the current background intensity. This value is used for all subsequent reference measurements.

Instrument Setting



Source

Source Setup (FL 6500)

Source Mode: Pulse. This is set when you select your **Instrument Connection**.

Luminescence: Select **Fluorescence, Phosphorescence,** or **Bioluminescence.**

Fluorescence

Ex. Corr: Select On, Off, or File. (Does not apply for Bioluminescence)

Dark Apply (Does not apply for Bioluminescence)

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click the check box to set Real-time Dark.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

NOTE: *The maximum frequency for each power is listed in the following table.*

Power	Maximum Frequency
20	200
40	200
80	100
120	50

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Phosphorescence

Ex. Corr: Select On, Off, or File.

Flash Count: Enter a value from 1 to 10.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Bioluminescence (No additional settings required)

Source Setup (FL 8500)

Source Mode: View the source mode, Pulse or Continuous. This is set when you select your **Instrument Connection**.

Luminescence: Select **Fluorescence, Phosphorescence,** or **Bioluminescence.**

Fluorescence

Ex. Corr: Select On, Off, or File.

Dark Apply (Does not apply for Bioluminescence)

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click the check box to set Real-time Dark.

Chopper (Hz): Select a Chopper value: 10, 20, or 40.

Phosphorescence

Ex. Corr: Select On, Off, or File.

Chopper (Hz): Select a Chopper value: 10, 20, or 40.

Bioluminescence (No additional settings required)

Excitation

(Not applicable in the Bioluminescence Mode.)

Excitation Mono Setup

Excitation Wavelength (nm): Enter a value for the Excitation Wavelength.

Excitation Slit Width (nm): Enter a value for the Excitation Slit Width.

Excitation Filter: Click the **Choose Filter** button or select from the drop-down.

Accessory

Accessory Setup: Select an Accessory from the drop-down list.

Emission

Wavelength Mode - Emission Mono Setup

Emission Wavelength (nm): Enter a value.

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list.

Emission Filter: Click the Choose Filter button or select a filter from the drop-down list.

Scan Mode - Emission Mono Setup

Click the **Full Range** button or set your own values:

Emission Start Wavelength (nm): Enter a value.

Emission End Wavelength (nm): Enter a value.

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list.

Emission Filter: Click the **Choose Filter** button or select a filter from the drop-down list.

Scan Speed (nm): Select 30, 60, 240, 1200, or 2400 from the drop-down list.

NOTE: *As you move up in power, Scan Speed options will change.*

Acquisition

Detector Setup

Photomultiplier Voltage (V): Select Low (400), Medium (550), High (700), or Custom from the drop-down list. Select Custom to enter a value.

Wavelength Mode - Integration Time (ms): Enter a value.
Scan Mode - Response Width (nm): Select a value from the drop-down list.

Em. Corr.: Select On, Off, or File.

NOTE: *In the **Phosphorescence** Mode only enter a **Delay (us)** time value and a **Gate (ms)** time value.*

Gain

PMT: Select a gain of x1, x8, x64, x512, or Auto from the drop-down list.

NOTE: *The PMT Gain is a multiplier of the Photomultiplier Voltage.*

Quenching

Select a **Model** from the drop-down list: **F0/F vs [Q]** or (**F0/F-1)[Q] vs [Q]**.

Description Tab

Method Name: Type a name for your method.

Notes: Type notes specific to this method.

Signatures (ES version): Select Sign, Review, or Approve from the drop-down list.

Sample Table Tab

The Sample Table provides a listing of samples by **Sample ID**, **Description**, **Type**, and **Concentration**. There is also an indicator to show if the sample has been measured or not. The right side contains buttons to control the samples.

For each sample row you can **Add**, **Insert**, **Remove**, and move the row **Up** or **Down**.

Format Sample Table: Opens a **Table Builder** dialog where you can add **Preparation** information, add custom **Columns**, and add **ID** information.

NOTE: *The **Concentration** field is mandatory to fill in the quencher concentration. The 1st entry should be a sample without any quencher, so the concentration should be 0.*

Setups…: Opens a Sample Table Setups dialog where you can **Save the current Sample Table**, **Delete**, **Set as current**, **Import**, **Export**, and with **Signatures**, Sign, Review and Approve the table.

Import or **Export** a sample table.

Fill Down or **Clear Measured** table rows.

Quantum Yield

This application method measures the ratio of the number of photons emitted to the number of photons absorbed. This method provides the option of measuring either the relative or absolute fluorescence quantum yields. The absolute quantum yield require the use of the integrating sphere.

Data Collection Tab

Calc Mode

Select Absolute or Relative.

Absolute: If selecting Absolute then select a **Calc Method** of **Simplification** or **De Mello.**

Relative: If selecting **Relative** then select or deselect the **Background Correction** check box.

Instrument Setting

Source

Source Setup (FL 6500)

Source Mode: Pulse. This is set when you select your **Instrument Connection**.

Luminescence: Fluorescence.

Ex. Corr: Select On, Off, or File

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Realtime Dark

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

NOTE: *The maximum frequency for each power is listed in the following table.*

Power	Maximum Frequency
20	200
40	200
80	100
120	50

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Source Setup (FL 8500)

Source Mode: Continuous. This is set when you select your **Instrument Connection**.

Luminescence: Fluorescence.

Ex. Corr: Select On, Off, or File

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Realtime Dark

Chopper (Hz): Select a **Chopper** value of 10, 20, or 40 from the drop-down list.

Excitation

Excitation Mono Setup

Excitation Wavelength (nm): Enter a value for the Excitation Wavelength.
Excitation Slit Width (nm): Enter a value for the Excitation Slit Width.
Excitation Filter: Click the **Choose Filter** button or select a filter from the drop-down list.

Accessory

Accessory Setup: Select an Accessory from the drop-down list.

Emission

Emission Mono Setup

Click the **Full Range** button or set your own values:

Emission Start Wavelength (nm): Enter a value.

Emission End Wavelength (nm): Enter a value.

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list.

Emission Filter: Click the **Choose Filter** button or select a filter from the drop-down list.

Scan Speed: Select a value of 30, 60, 240, 1200, or 2400 from the drop-down list.

NOTE: *As you move up in power, Scan Speed options will change.*

Acquisition

Detector Setup

Photomultiplier Voltage (V): Select Low (400), Medium (550), High (700), or Custom from the drop-down list.
Select Custom to enter a value.
Response Width (nm): Select a value from the drop-down list.
Em. Corr.: Select On, Off, or File from the drop-down list.

Gain

PMT: Select a gain of x1, x8, x64, x512, or Auto from the drop-down list.

NOTE: *The PMT Gain is a multiplier of the Photomultiplier Voltage.*

Calculation

Select **Base 1** and/or **Base 2** and a table contains the following columns: **Name, Peak Start, Peak End, Peak Base 1,** and **Peak Base 2**.

Description Tab

Method Name: Type a name for your method.

Notes: Type notes specific to this method.

Signatures (ES version): Select Sign, Review, or Approve from the drop-down list.

Sample Table Tab

The Sample Table provides a listing of samples by **Sample ID**, **Description**, and **Type**. There is also an indicator to show if the sample has been measured or not. The right side contains buttons to control the samples.

For each sample row you can **Add**, **Insert**, **Remove**, and move the row **Up** or **Down**.

Format Sample Table: Opens a **Table Builder** dialog where you can add **Preparation** information, add custom **Columns**, and add **ID** information.

NOTE: *The column of Absorbance and Refractive is mandatory for Sample and Standard type, the column of Quantum Yield is mandatory for Standard type. Additionally, multiple measurement can allow relative Quantum Yield calculation in the Gradient mode. A different measurement number means a different absorbance level.*

Setups…: Opens a Sample Table Setups dialog where you can **Save the current Sample Table**, **Delete**, **Set as current**, **Import**, **Export**, and with **Signatures**, Sign, Review and Approve the table.

Import or **Export** a sample table.

Fill Down or **Clear Measured** table rows.

Absorbance

This application method uses the absorbance accessory to measure the absorbance of a sample. The absorbance can be measured/monitored at a number of fixed wavelengths (wavelength absorbance) or across the entire spectrum in the scanning absorbance option.

Data Collection Tab

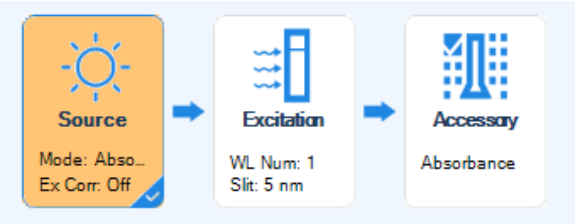
Scan Mode

Select **Wavelength** or **Scan**

Auto Filter Selection: Click the check box to select Auto Filter Selection.

Background Correction: This check box is automatically selected.

Instrument Settings



Source

Source Setup (FL 6500)

Source Mode: Pulse. This is set when you select your **Instrument Connection**.

Luminescence: Absorbance is automatically selected.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click this check box to select Real-time Dark.

Power (kW): Select 20, 40, 80, or 120 from the drop-down list.

NOTE: *The maximum frequency for each power is listed in the following table.*

Power	Maximum Frequency
20	200
40	200
80	100
120	50

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Source Setup (FL 8500)

Source Mode: Continuous. This is set when you select your **Instrument Connection**.

Luminescence: Absorbance is automatically selected.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click this check box to select Real-time Dark.

Chopper (Hz): Select 10, 20, or 40 from the drop-down list.

Excitation

Wavelength Mode

Excitation Setup

Excitation Wavelength (nm) table**:** Build a wavelength table. **Add** or **Remove** rows by using the buttons.

Excitation Slit Width (nm): Select 1, 2.5, 5, 10 or 20 from the drop-down list.

Excitation Filter: Click the **Choose Filter** button or select a filter from the drop-down list.

Scan Mode

Excitation Mono Setup

Excitation Start Wavelength (nm): Enter a value.

Excitation End Wavelength (nm): Enter a value.

Or click the **Full Range** button (190 - 900 nm)

Excitation Slit Width (nm): Select 1, 2.5, 5, 10 or 20 from the drop-down list.

Excitation Filter: Click the **Choose Filter** button or select a filter from the drop-down list.

Scan Speed (nm/min): Select 30, 60, 240, 1200, or 2400 from the drop-down list.

NOTE: As you move up in power, Scan Speed options will change.

Accessory

Accessory Setup

Accessory: Select an Accessory from the drop-down list: Absorbance or Water Jacket Absorbance Module with Stirrer.

Detector

PD Amp Level: Select **x1** through **x8** from the drop-down list.

Integration Time (ms): Enter an Integration Time.

When **Water Jacket Absorbance Module with Stirrer** is selected select a **Stirrer Speed** of **Stop, Low, Middle, or High** from the drop-down list**.**

Description Tab

Method Name: Type a name for your method.

Notes: Type notes specific to this method.

Signatures (ES version): Select Sign, Review, or Approve from the drop-down list.

Sample Table Tab

The Sample Table provides a listing of samples by **Sample ID**, **Description**, and **Type**. There is also an indicator to show if the sample has been measured or not. The right side contains buttons to control the samples.

For each sample row you can **Add**, **Insert**, **Remove**, and move the row **Up** or **Down**.

Format Sample Table: Opens a **Table Builder** dialog where you can add **Preparation** information, add custom **Columns**, and add **ID** information.

Setups...: Opens a Sample Table Setups dialog where you can **Save the current Sample Table**, **Delete**, **Set as current**, **Import**, **Export**, and with **Signatures**, Sign, Review and Approve the table.

Import or **Export** a sample table.

Fill Down or **Clear Measured** table rows.

Fast Filter

The Fast Filter method is used to specify the data collection conditions when using the Fast Filter accessory. The Fast Filter accessory enables rapid measurement of intracellular concentration. This accessory consists of two filter wheels. Up to two pairs of filters or polarizers can be fitted on each filter wheel: the filter wheels rotate rapidly and enable each filter to be in the beam coincident with source lamp. A data point is then measured. For example, if calcium changes are being monitored using FURA-2, a pair of filters (340 and 380 nm) are fitted in the excitation filter wheel and the emission is monitored at 510 nm using emission monochromator. The data for each run is saved in three time drive files with an extension of .td. The file name ending N, D or A is automatically added for the identification of the data type contained within that file:

*n.td= numerator for producing ratios of the measured data

*d.td= denominator for producing ratios of the measured data

*a.td= ratio of the intensity values of the above data

The polarizer filter set can be fitted to calculate the polarization or anisotropy of a sample. Fluorescence polarization is a very powerful technique for studying the rotational movement of molecules dynamically.

Polarization is calculated using the following equation:

$$Polarisation = \frac{Ivv - (GF \cdot Ivh)}{Ivv + (GF \cdot Ivh)}$$

Anisotropy is calculated using the following equation:

$$Anisotropy = \frac{Ivv - (GF \cdot Ivh)}{Ivv + (2GF \cdot Ivh)}$$

Where:

Ivv= Emission intensity with both excitation and emission polarisers vertical.

Ivh=Emission intensity with excitation polarizer vertical and emission polarizer horizontal.

GF= Grating factor

Data Collection Tab

Filter Mode

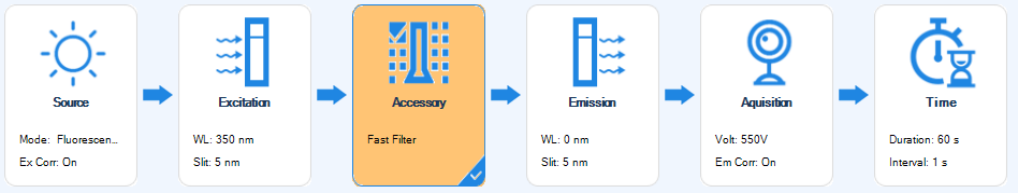
Select **Excitation FFA, Emission FFA, Polarisation, Anisotropy** or **GF**.

Immediate Mode: Click the check box to set Immediate Mode.

Background Correction: Click the check box to set Background Correction.

Remote Start: Click the check box for remote start.

Instrument Settings



Source

Source Setup (FL 6500)

Source Mode: Pulse. This is set when you select your **Instrument Connection**.

Luminescence: Fluorescence is automatically selected.

Ex. Corr: Select On, Off, or File

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Power (kW): Select 20, 40, 80, or 120 from the drop-down list.

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

NOTE: *The maximum frequency for each power is listed in the table.*

Power	Maximum Frequency
20	200
40	200
80	100
120	50

Source Setup (FL 8500)

Source Mode: Continuous. This is set when you select your **Instrument Connection**.

Luminescence: Fluorescence is automatically selected.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Chopper (Hz): Chopper control is not available when using the Fast Filter Accessory.

Excitation

Excitation Mono Setup

Excitation Wavelength (nm): Enter a value.

NOTE: *When the Excitation FFA has been selected, the excitation wavelength is fixed at zero order to allow the excitation wavelength to be defined solely by the Fast Filter, so the excitation wavelength is disabled*

Excitation Slit Width (nm): Select 1, 2.5, 5, 10 or 20 from the drop-down list.

Excitation Filter: Click the **Choose Filter** button or select a filter from the drop-down list.

Accessory

Accessory Setup

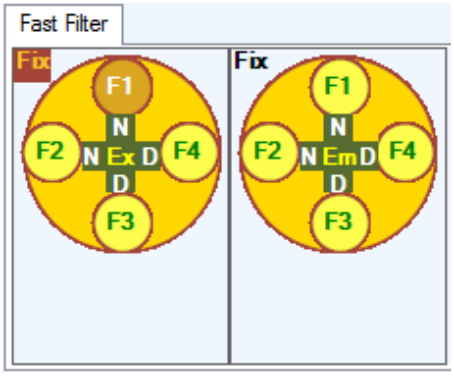
Accessory: Fast Filter is automatically selected.

Extra Accessory: Select an accessory from the drop-down list.

Fast Filter

Excitation FFA /Emission FFA

The fixed filter position can be selected via clicking the position ID in the below image. The Left image is for the Excitation filter, which is available for Emission FFA, and the right image is for the Emission filter which is available for Excitation FFA. The red highlighted position will be fixed during run a Excitation FFA or Emission FFA.



Ratio 1: Click the checkbox to enable the first ratio

Ratio 2: Click the checkbox to enable the second ratio

Name: Enter a name for the ratio in this box.

Numerator: Select a filter to use as the numerator for the ratio.

NOTE: *Selecting a filter for the numerator will cause the denominator value to be automatically set.*

Edit Filters: Click this to open and edit the filter information.

Save as Global: Saves the current Fast Filter Settings as the default.

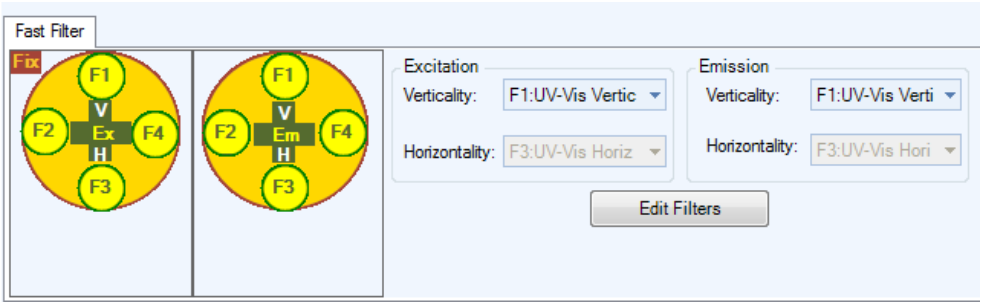
Load Global Setting: Reverts the Fast Filter Settings to the last saved global settings

Stirrer Control: Select a stirrer speed from the dropdown list.

Polarization/Anisotropy/GF

When selecting Polarization/Anisotropy mode, the excitation filter will be fixed at the filter position which has been specified as Excitation Vertical polarizer.

When selecting GF mode, the excitation filter will be fixed at filter position which has been specified as the Excitation Horizontal polarizer.



Excitation:

Verticality: Selecting a filter for Verticality Polarizer in Excitation filter wheel of Fast Filter.

NOTE: Selecting a filter for the Verticality will cause the Horizontality value to be automatically set.

Emission:

Verticality: Selecting a filter for Verticality Polarizer in Emission filter wheel of Fast Filter.

NOTE: Selecting a filter for the Verticality will cause the Horizontality value to be automatically set.

Edit Filters: Click this to open and edit the filter information.

Save as Global: Saves the current Fast Filter Settings as the default.

Load Global Setting: Reverts the Fast Filter Settings to the last saved global settings

Grating Factor:

GF Calculate: Enter the Grating factor in this textbox manually or calculated by pressing the "GF Calculate" button. This parameter is only available when selecting Polarization/Anisotropy.

Stirrer Control: Select a stirrer speed from the dropdown list.

Emission

Emission Mono Setup

Emission Wavelength (nm): Enter a value.

NOTE: When emission FFA has been selected, the emission wavelength is fixed at the zero order position, which selects the emission light according to the filters fitted.

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list.

Emission Filter: Click the **Choose Filter** button or select a filter from the drop-down list.

Detector

Photomultiplier Voltage (V): Select Low (400), Medium (550), High (700), or Custom from the drop-down list. Select Custom to enter a value.

Response Time (sec): Enter a value.

Em. Corr.: Select On, Off, or File from the drop-down list.

Gain

PMT: Select a gain of x1, x8, x64, x512, or Auto from the drop-down list.

NOTE: The PMT Gain is a multiplier of the Photomultiplier Voltage.

Time

Duration: Enter a Duration time. Select **Second** or **Minute**.

Data Interval: Enter a Data Interval value.

Delay Before Measure: Enter a delay time.

Description Tab

Method Name: Type a name for your method.

Notes: Type notes specific to this method.

Signatures (ES version): Select Sign, Review, or Approve from the drop-down list.

Sample Table Tab

The Sample Table provides a listing of samples by **Sample ID**, **Description**, and **Type**. There is also an indicator to show if the sample has been measured or not. The right side contains buttons to control the samples.

For each sample row you can **Add**, **Insert**, **Remove**, and move the row **Up** or **Down**.

Format Sample Table: Opens a **Table Builder** dialog where you can add **Preparation** information, add custom **Columns**, and add **ID** information.

Setups…: Opens a Sample Table Setups dialog where you can **Save the current Sample Table**, **Delete**, **Set as current**, **Import**, **Export**, and with **Signatures**, Sign, Review and Approve the table.

Import or **Export** a sample table.

Fill Down or **Clear Measured** table rows.

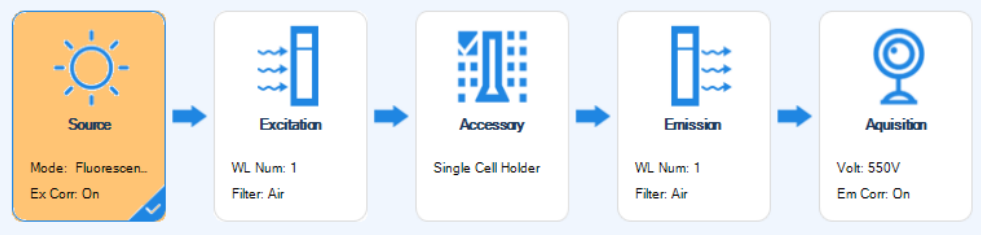
Microplate Reader

This Scan application is used for collecting various types of spectral data in a variety of modes (fluorescence, phosphorescence, and bioluminescence) using the Microplate Reader accessories.

Data Collection Tab

Measured Num: Enter the number of scans for each sample cell here.

Instrument Settings



Source

Source Setup (FL 6500)

Source Mode: Pulse. This is set when you select your **Instrument Connection**.

Luminescence Mode: Select Fluorescence, Phosphorescence or Bioluminescence.

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply:

Initial Dark: Click the check box to set Initial Dark.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

NOTE: *The maximum frequency for each power is listed in the following table.*

Power	Maximum Frequency
20	200
40	200
80	100
120	50

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Source Setup (FL 8500)

Source Mode: Continuous. This is set when you select your **Instrument Connection**.

Luminescence: Select Fluorescence, Phosphorescence or Bioluminescence.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Chopper (Hz): Chopper control is not available when using the Microplate Reader Accessory.

Excitation

Excitation Setup

Excitation Wavelength (nm): Enter a value for each ID in the table

Excitation Slit Width (nm): Select 1, 2.5, 5, 10 or 20 from the drop-down list for each ID in the table

NOTE: *The number of entries in the excitation setup is dependent on the number of measurements selected.*

Excitation Filter: Click the **Choose Filter** button or select a filter from the drop-down list.

Accessory

Accessory Setup

Accessory: Microplate Reader is automatically selected.

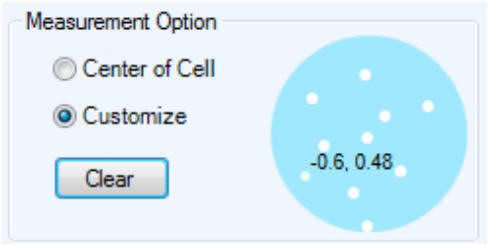
Extra Accessory: No extra accessories can be selected in this method type.

Measurement Option

Center of Cell: Measurements are taken from the centre of the cell on the microplate.

Customize: Enable custom settings for cell measurement.

The points of measurement are selected by clicking on the blue circle.



Clear: clears the selected points of measurement in the cell.

Calculation Mode

Average: the measured value is the average intensity of the points selected in customized measurements.

Sum: The measured value is the sum of intensities of the points selected in customized measurements.

NOTE: *Calculation Mode is only enabled when the* ***Customize*** *option is selected.*

Cycle Settings

Cycle Number: Set the number of cycles of the selected spots measured in a customized measurement.

Time Interval (s): Sets the time interval between selected points in a customized measurement.

Emission

Emission Wavelength (nm): Enter a value for each ID in the table.

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list for each ID in the table.

NOTE: The number of entries in the excitation setup is dependent on the number of measurements selected.

Excitation Filter: Click the **Choose Filter** button or select a filter from the drop-down list.

Detector

Photomultiplier Voltage (V): Select Low (400), Medium (550), High (700), or Custom from the drop-down list. Select Custom to enter a value.

Em. Corr.: Select On, Off, or File from the drop-down list.

Integration Time (ms): Enter an Integration Time.

PMT: Select a gain of x1, x8, x64, x512, or Auto from the drop-down list.

NOTE: The PMT Gain is a multiplier of the Photomultiplier Voltage.

Description Tab

Method Name: Type a name for your method.

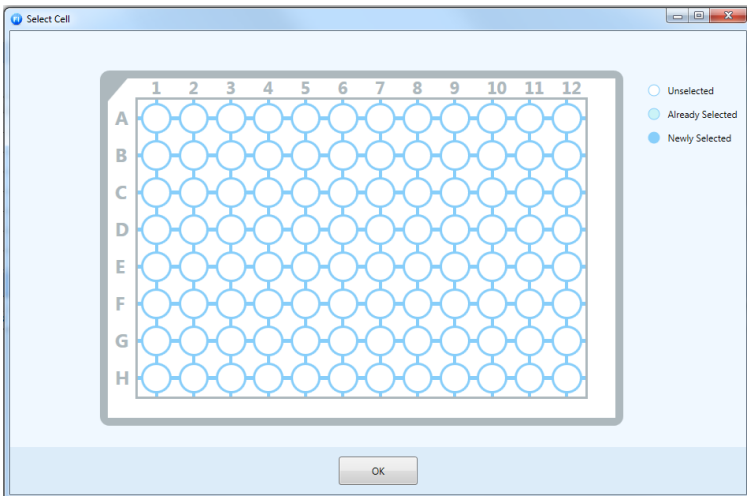
Notes: Type notes specific to this method.

Signatures (ES version): Select Sign, Review, or Approve from the drop-down list.

Sample Table Tab

The Sample Table provides a listing of samples by **Sample ID**, **Description**, and **Type**. There is also an indicator to show if the sample has been measured or not. The right side contains buttons to control the samples.

The **Position** tab opens the Microplate view, in the configuration which has been set in Options. Sample positions can be added here either by left clicking on the desired plate position or dragging a block in the image to select multiple lines and rows



For each sample row you can **Add**, **Insert**, **Remove**, and move the row **Up** or **Down**.

Format Sample Table: Opens a **Table Builder** dialog where you can add **Preparation** information, add custom **Columns**, and add **ID** information.

Setups…: Opens a Sample Table Setups dialog where you can **Save the current Sample Table**, **Delete**, **Set as current**, **Import**, **Export**, and with **Signatures**, Sign, Review and Approve the table.

Import or **Export** a sample table.

Fill Down or **Clear Measured** table rows.

Simple Read Method

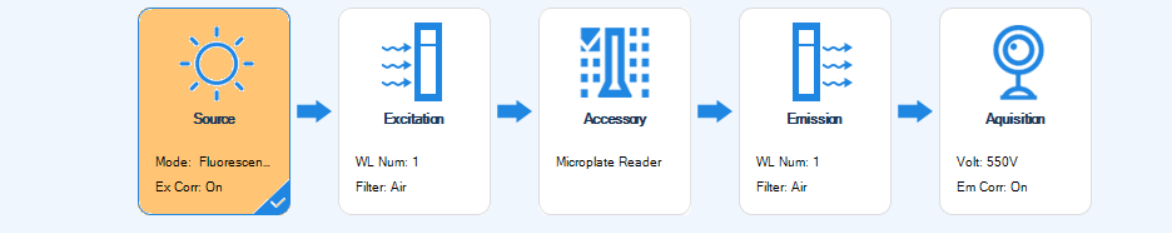
This Scan application is used for collecting tabular reading in Intensity, Polarization or Anisotropy. It can also be used for collecting reading in Intensity/Polarisation/Anisotropy based on ramp temperature.

Data Collection Tab

Measured Num: Enter the number of scans for each sample cell here.

Calculation mode: Select Intensity, Polarization, or Anisotropy.

Instrument Settings



Source

Source Setup (FL 6500)

Source Mode: Pulse. This is set when you select your **Instrument Connection**.

Luminescence: Select Fluorescence, Phosphorescence, or Bioluminescence.

Fluorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click the check box to set Real-time Dark.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

NOTE: *The maximum frequency for each power is listed in the following table.*

Power	Maximum Frequency
20	200
40	200
80	100
120	50

Phosphorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Flash Count: Enter a value from 1 to 10.

Power (kw): Select 20, 40, 80, or 120 from the drop-down list.

NOTE: *The maximum frequency for each power is listed in the following table.*

Power	Maximum Frequency
20	200
40	200
80	100
120	50

Frequency (Hz): Select 50, 100, or 200 from the drop-down list.

Bioluminescence (No additional settings required)

Source Setup (FL 8500)

Source Mode: Continuous. This is set when you select your **Instrument Connection**.

Luminescence: Select Fluorescence, Phosphorescence, or Bioluminescence.

Fluorescence

Ex. Corr: Select On, Off, or File from the drop-down list.

Dark Apply

Initial Dark: Click the check box to set Initial Dark.

Real-time Dark: Click the check box to set Real-time Dark.

Chopper (Hz): Select a Chopper value of 10, 20, or 40 from the drop-down list.

Phosphorescence

Ex. Corr: Select On, Off, or File.

Chopper (Hz): Select a Chopper value: 10, 20, or 40.

Bioluminescence (No additional settings required)

Excitation

Excitation Setup

Excitation Wavelength (nm): Enter a value for each ID in the table.

Excitation Slit Width (nm): Select 1, 2.5, 5, 10 or 20 from the drop-down list for each ID in the table.

NOTE: *The number of entries in the excitation setup is dependent on the number of measurements selected.*

Excitation Filter: Click the **Choose Filter** button or select a filter from the drop-down list.

Accessory

Accessory Setup

Accessory: select the **Single Cell Holder**, **Single Cell Peltier Holder** or **4-position multi-cell peltier holder** from the dropdown list.

Extra Accessory: select the **Auto Sipper** or **S10 Autosampler** from the dropdown list.

Emission

Emission Wavelength (nm): Enter a value for each ID in the table.

Emission Slit Width (nm): Select 0.5, 1, 2.5, 5, 10 or 20 from the drop-down list for each ID in the table.

NOTE: The number of entries in the excitation setup is dependent on the number of measurements selected.

Emission Filter: Click the **Choose Filter** button or select a filter from the drop-down list.

Detector

Photomultiplier Voltage (V): Select Low (400), Medium (550), High (700), or Custom from the drop-down list. Select Custom to enter a value.

Em. Corr.: Select On, Off, or File from the drop-down list.

Integration Time (ms): Enter an Integration Time.

PMT: Select a gain of x1, x8, x64, x512, or Auto from the drop-down list.

NOTE: The PMT Gain is a multiplier of the Photomultiplier Voltage.

Description Tab

Method Name: Type a name for your method.

Notes: Type notes specific to this method.

Signatures (ES version): Select Sign, Review, or Approve from the drop-down list.

Sample Table Tab

The Sample Table provides a listing of samples by **Sample ID**, **Description**, and **Type**. There is also an indicator to show if the sample has been measured or not. The right side contains buttons to control the samples.

For each sample row you can **Add**, **Insert**, **Remove**, and move the row **Up** or **Down**.

Format Sample Table: Opens a **Table Builder** dialog where you can add **Preparation** information, add custom **Columns**, and add **ID** information.

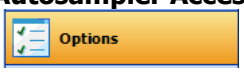
Setups…: Opens a Sample Table Setups dialog where you can **Save the current Sample Table**, **Delete**, **Set as current**, **Import**, **Export**, and with **Signatures**, Sign, Review and Approve the table.

Import or **Export** a sample table.

Fill Down or **Clear Measured** table row

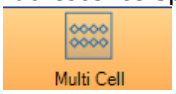
Accessories Setup

Accessories Overview

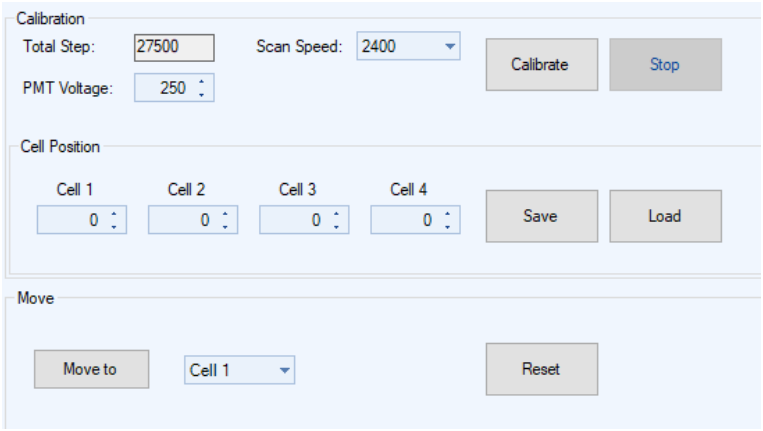
Some of the accessories for the FL6500/FL8500 Fluorescence Spectrometers require setup in the software; this includes the **Microplate Reader Accessory**, **Multi-Cell holder and Multi-Cell Peltier holder Accessories** and the **S10 Autosampler Accessory**. All the accessory setup options are accessed from the **Options** tab 

This section will give a brief overview of the functions for the accessory setup tools in Spectrum FL.

Multi-Cell Accessory Setup

The Multi-Cell setup menu is compatible with all the Multi-Cell accessories used in the FL6500/FL8500 Fluorescence Spectrometers. Multi-cell setup functions are accessed from the **Multi Cell** page 

under the **Options** tab.



Calibration

Total Step: the total number of motor steps the Multi-cell can travel. (Cannot be altered)

PMT Voltage (V): Enter a value between 0 and 1250V which could not make peak saturated.

Scan Speed (nm/minute): Select a value from the drop-down list.

Calibrate: Begins the automated calibration of the Mutli-Cell accessory.

Stop: Stops the automated calibration procedure (only available once the calibration has been started)

Cell Position

Cell 1, Cell 2, Cell 3, Cell 4: Values for cell position are entered here after calibration has finished. Values can also be entered manually.

Save: Save the current cell position values.

Load: Load the previous saved cell position values from the hardware.

NOTE: *In the ES version, only the user need permission of "Cell Changer Calibration" to Calibrate and Save the cell position.*

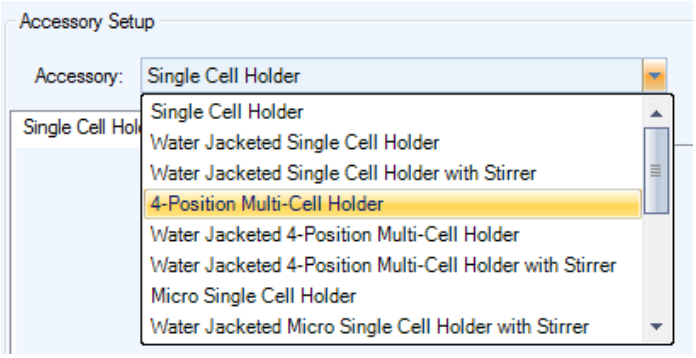
Move

Move to: Moves to the saved position of the cell selected from the dropdown list.

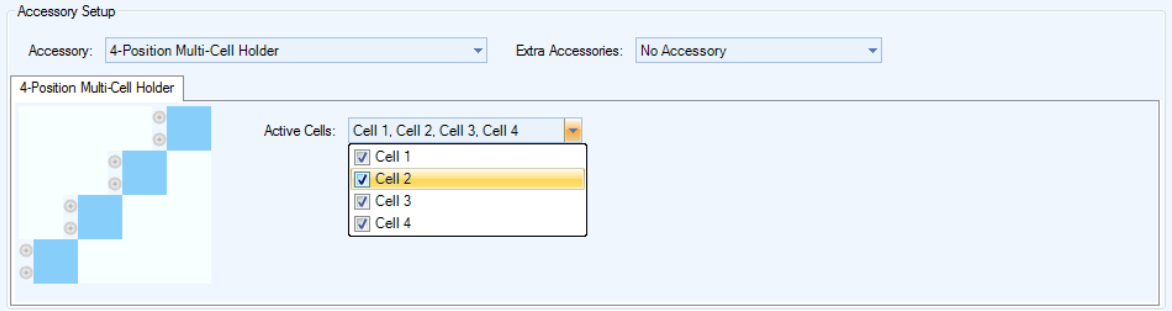
Reset: Returns the Multi-cell to its default position.

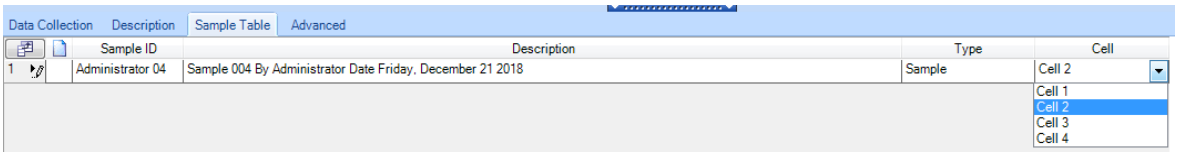
Multi-cell setup parameters in the method can be accessed when selecting a multicell accessory in the method.

Step 1: Select the cell changer accessory from **Accessory** drop-down list under Accessory block.

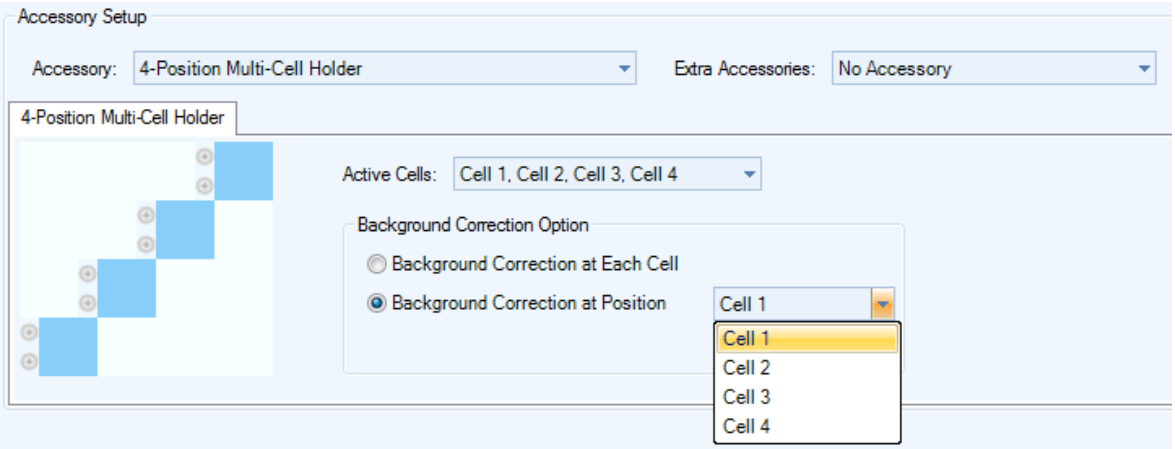


Step 2: Set the **Active Cell** by selecting or deselecting the check boxes to the left of the cell numbers. Only the actived cell(s) can be shown in the sample table for sample measurement.





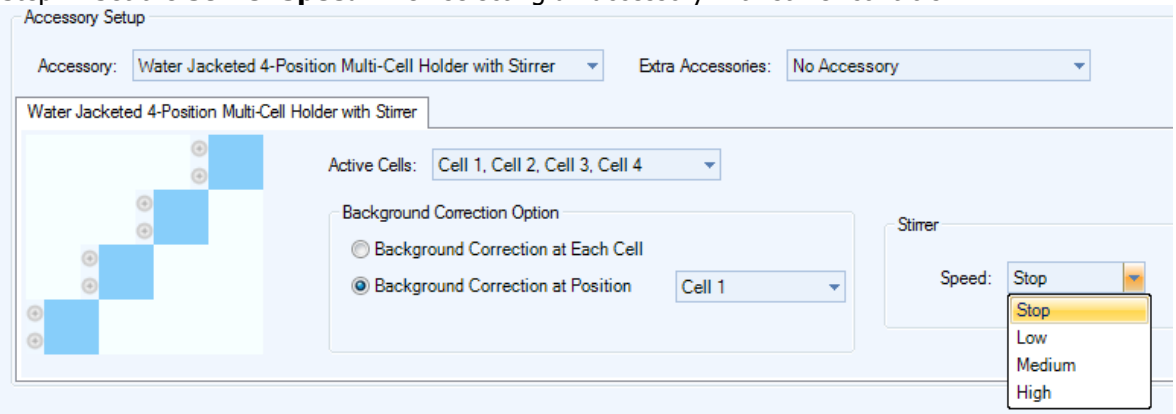
Step 3: When **Background Correct** is selected, a correction option can also be selected.



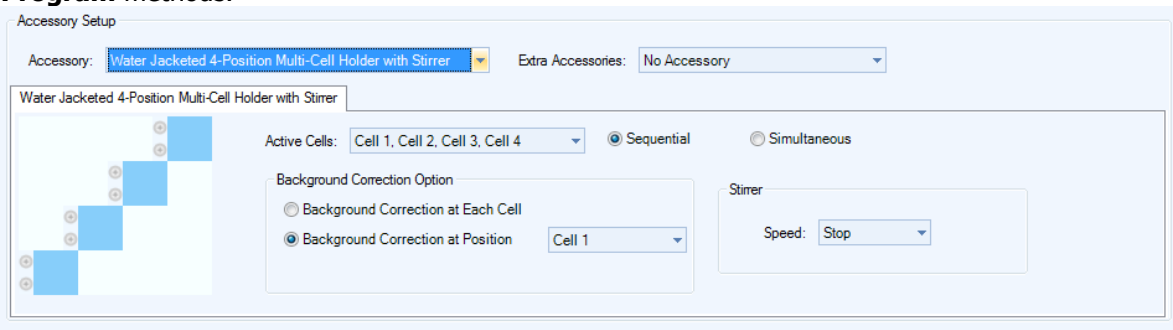
Background correction at each cell: Perform background correction for each cell position, and apply background data according to cell position number.

Background correction at Position: Perform background correction for specified cell position, and apply same background data for all samples.

Step 4: Set the **Stirrer Speed** when selecting an accessory with stirrer controls.



Step 5: Set option of **Sequential** or **Simultaneous** in **Time drive**, **Kinetic** or **Wavelength Program** methods.

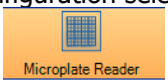


Sequential: scan sample sequentially which means start next sample measurement after scanning the previous sample completely.

Simultaneous: scan samples "simultaneously", which means after mearsurement is started, a maximum of four samples are analyzed in the same run.

Step 6: Cell position should be selected when running a method which uses a multi-cell changer accessory.

Microplate Reader Accessory Setup

The Microplate reader menu is used to align and provide image configuration selection. Microplate reader setup functions are accessed from the **Microplate Reader** 

page under the **Options** tab.

Plate Information

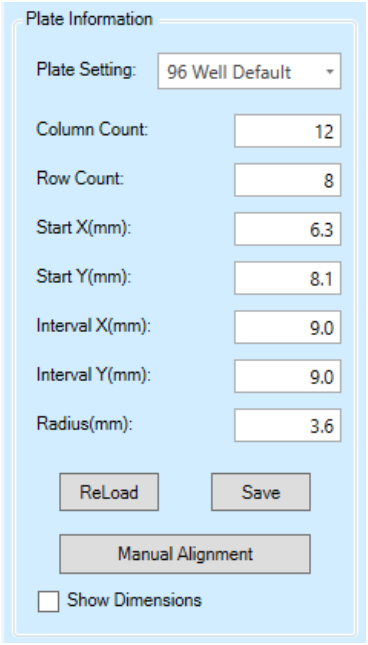


Plate Setting: Select a set of default Microplate dimensions or a previously saved custom dimensions.

Column Count: The number of columns present on the microplate. Values are set when a plate setting is selected, or can be entered manually.

Row Count: The number of rows present on the microplate.

Start X (mm): X-Axis start position of the Microplate Reader (Cell A1), calculated by distance from the edge of the plate.

Start Y (mm): Y-Axis start position of the Microplate Reader (Cell A1), calculated by distance from the edge of the plate.

Interval X (mm): The distance between the center point of two microplate cells on the X-axis.

Interval Y (mm): The distance between the centre point of two microplate cells on the Y-axis.

Radius (mm): The distance from the edge to the centre point of a Microplate Cell.

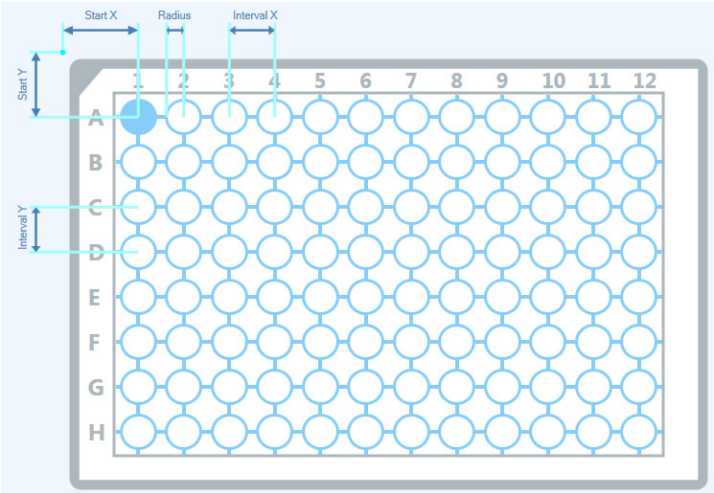
NOTE: *These values are populated when a default or saved plate dimensions are selected from the plate setting dropdown list. Details can also be entered manually.*

Reload: Reload the last saved entries for the selected plate setting

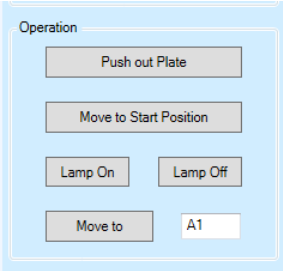
Save: Save the current plate information.

Manual Alignment: Opens the manual alignment wizard.

Show Dimensions: Click the check box to see a visible representation of the listed distances on the plate diagram.



Operation



Push out Plate: Moves the plate to a position from which it can be easily removed from the Microplate Reader Accessory.

Move to Start Position: Moves the plate to the start position (the upper right-most limit that theplate can move).

Lamp on: Activates the source lamp of the FL6500/FL8500 Fluorescence Spectrometer.

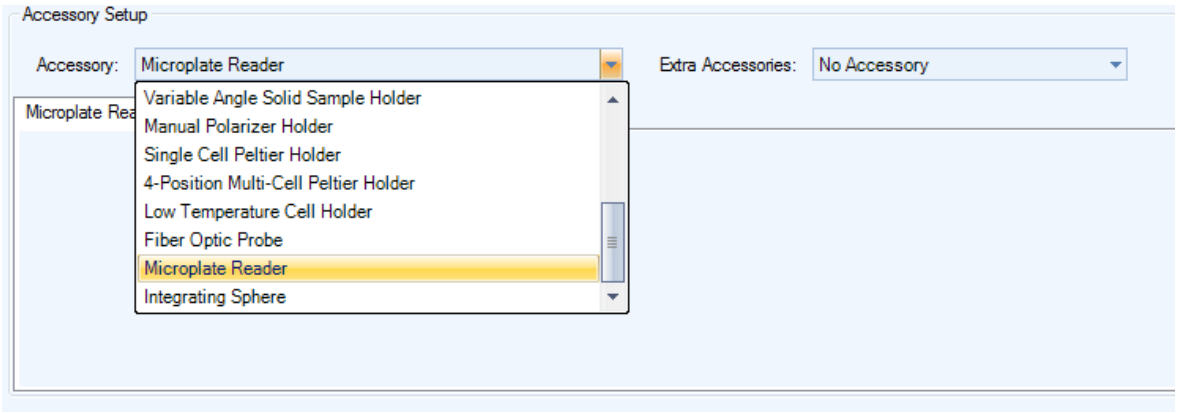
Lamp off: Deactivates the source lamp of the FL6500/FL8500 Fluorescence Spectrometer.

Move to: Moves the plate to the cell entered into the text box.

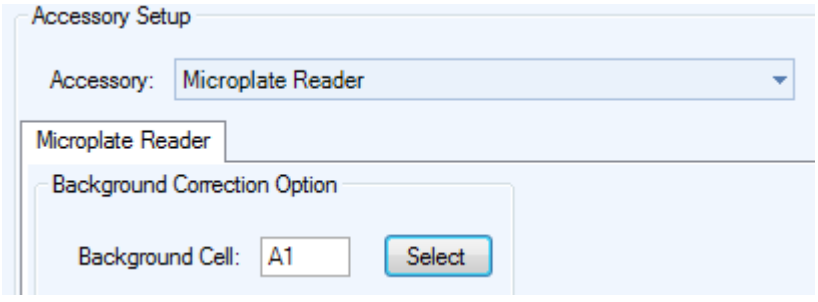
Microplate Reader parameters in the method can be accessed when "Microplate Reader" is selected in Accessory setup.

NOTE: *The description here only details the settings in methods except Microplate Reader Type.*

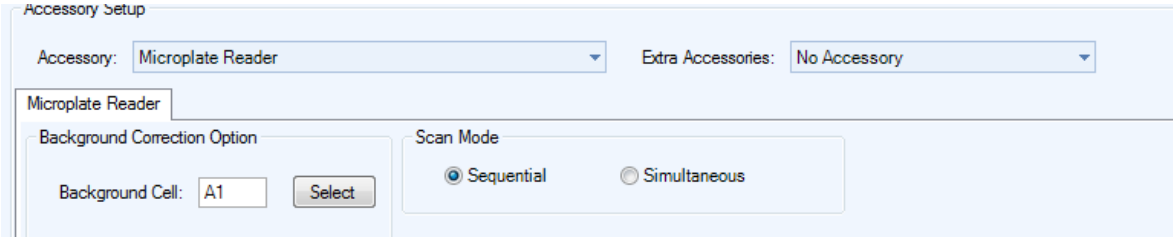
Step 1: Select **Microplate Reader** from **Accessory** drop-down list under Accessory block.



Step 2: When the **Background Correction** option is selected in the method, click the **Select** button and select **Background Well Position,** then left-click on the desired well position.



Step 3: Set the option of **Sequential** or **Simultaneous** in method of **Time drive**, **Kinetic** or **Wavelength Program**.



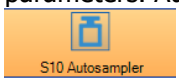
Sequential: scans samples sequentially, which the next sample measurement begins after the previous sample scan is completed.

Simultaneous: scan samples "simultaneously", which means after mearsurement is started, a maximum of 384 samples are analyzed in the same run.

Step 4: A well position should be selected when running a method which uses microplate Reader accessory.

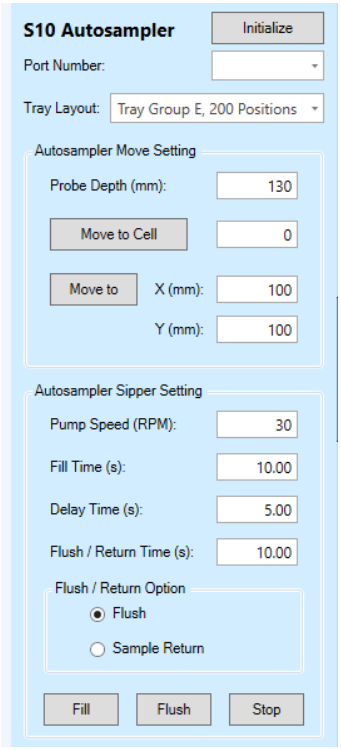
S10 Autosampler Acessory Setup

The S10 Autosampler menu is used to initialize the S10, manage movement settings and set sipper parameters. Autosampler setup functions are accessed from the **S10 Autosampler** page



under the **Options** tab.

S10 Autosampler



Initialize: Begins the initialization procedure of the S10.

Port Number: Select a correct COM port from the dropdown list. (Defaults to the COM port used to connect the Autosampler to the PC).

***NOTE:** The Max COM Port number is 9.*

Tray Layout: select a tray layout from the dropdown list. The selected layout will be shown in the display.

Autosampler Move Setting

Probe Depth (mm): enter a value (between 0 and 146) for the depth the autosampler probe descends.

Move to Cell: Enter a numerical position from the displayed layout and click "move to cell" to move the Autosampler to the specified location.

Move to X/Move to Y (mm): Enter a specified distance in the X and Y axes and click "move to" to move the Autosampler to the specified location.

Autosampler Sipper Setting

Pump Speed (RPM): set the pump speed (between 20 and 120) of the sipper function.

Fill Time (s): Enter a timespan that liquid is passed through the sample flow cell.

Delay Time (s): Enter a timespan to delay between sample filling and flushing of the flow cell.

Flush/Return Time (s): Enter a timespan that solvent is used to flush the flow cell after sampling and/or liquid is returned to the sample bay from the flow cell.

Flush/Return Option

Flush: sets the Autosampler and sipper to flush the flow cell after sampling.

Sample Return: sets the Autosampler and sipper to return sample from the flow cell.

Fill: Starts the sipper motor, moving fluid in the direction of the Flow Cell

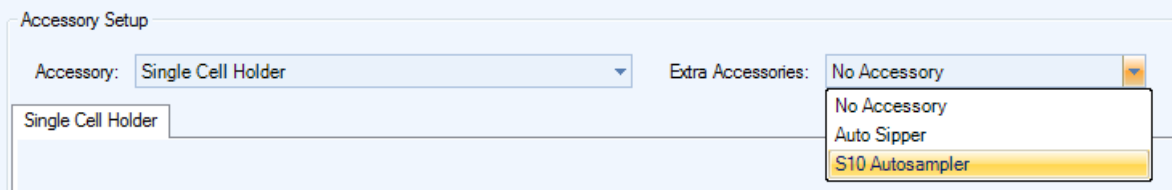
Flush: Starts the sipper motor, drawing fluid from the flow cell.

Stop: Stops the sipper motor.

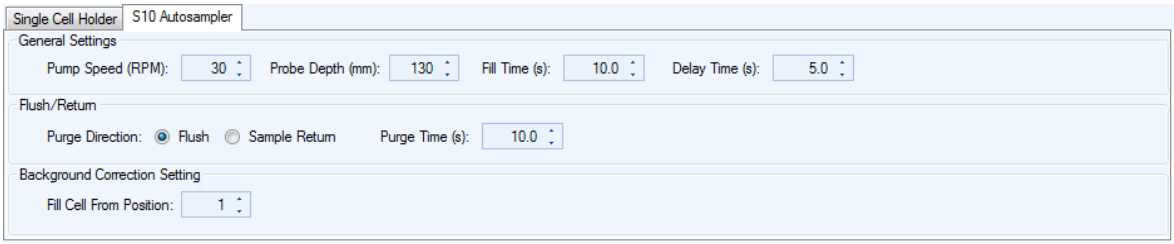
To access S10 Autosampler setup parameters in the method, follow this procedure:

S10 parameters in the method can be accessed when "S10 Autosampler" is selected in the Extra Accessory list. Normally, it will be compatible with single cell holder accessory.

Step 1: Select **Single Cell Holder** from the **Accesso**ry list drop-down list, then from the the **Extra Accessories** drop-down list select **S10 Autosampler**.

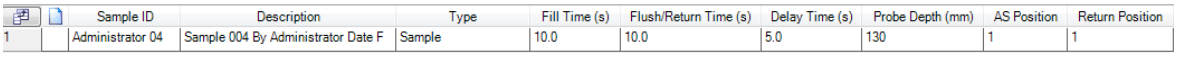


Step 2: Setup S10 Autosampler parameters as shown below:



Pump Speed (RPM)	Enter the pump speed (between 20 and 120) of the sipper function.
Probe Depth (mm)	Enter a value (between 0 and 146) for the depth the autosampler probe descends.
Fill Time (s)	Enter the amount of time that the pump pulls sample through for.
Delay Time (s)	Enter the amount of time between the end of filling and the start of data collection. This is to allow for bubbles, turbulence, etc.
Purge Direction	Select "Flush" for a forward flush which pulls sample into the waste; select "return" for a backwards flush which returns sample to the original reservoir. Flushing occurs after data collection;
Purge Time (s)	Allows you to set the time for flushing or returning the sample using the internal peristaltic pump.
Flush/Return	Allows you to control the sipper directly. Starts to flush the flow cell as set by the selection of Flush or Return and the Purge Time.
Fill Cell from Position	Allows you to specify the position for background solvent. Then when background measurement, the sample will be filled from here.

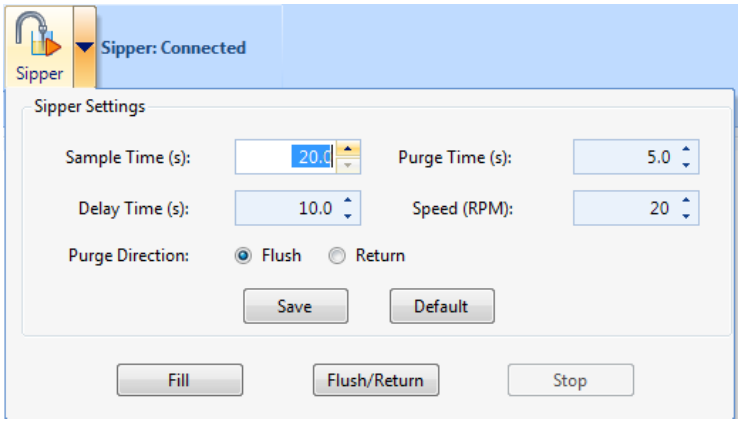
Step 3: Set customize parameter for **Fill Time**, **Flush/Return Time (s)**, **Delay Time**, **Probe Depth**, **AS Position,** and **Return Postion** (only available when select Sample Return) in sample table when run a method which select S10 Autosampler accessory.



		Sample ID	Description	Type	Fill Time (s)	Flush/Return Time (s)	Delay Time (s)	Probe Depth (mm)	AS Position	Return Position
1		Administrator 04	Sample 004 By Administrator Date F	Sample	10.0	10.0	5.0	130	1	1

Sipper Accessory Setup

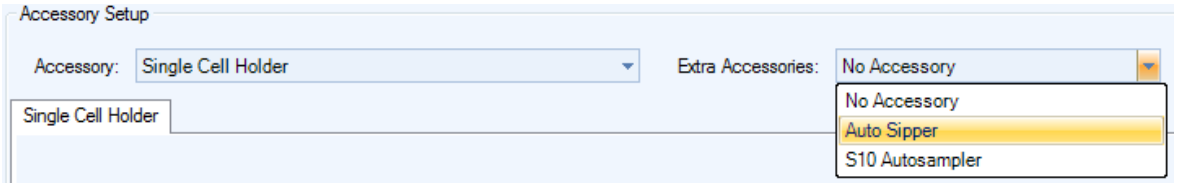
The sipper accessory can be auto-connected once the Sipper's USB port is recognized via the software. Sipper manual control dialog can be accessed via clicking the arrow button for Sipper accessory.



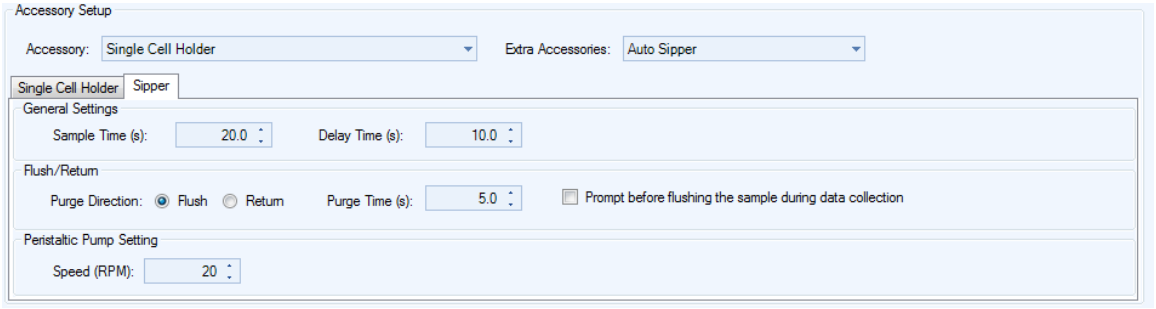
Sample Time (s)	Enter the amount of time that the pump pulls sample through for.
Delay Time (s)	Enter the amount of time between the end of filling and the start of data collection. This is to allow for bubbles, turbulence, etc.
Speed (RPM)	Enter the rotation speed in RPM.
Purge Direction	Select "Flush" for a forward flush which pulls sample into the waste; select "Return" for a backwards flush which returns sample to the original reservoir. Flush occurs after data collection;
Purge Time (s)	Allows you to set the time for flushing or returning the sample using the sipper.
Save	Save current setting which will be displayed next time. And moreover, it will be the default setting for the sipper when create a new method.
Default	Restore to default setting
Fill	Allows you to control the sipper directly. Starts to fill the flow cell as set by the Sample time.
Flush/Return	Allows you to control the sipper directly. Starts to flush the flow cell as set by the selection of Flush or Return and the Purge Time.
Stop	Allow you to stop Fill or Flush/Return

The Sipper's parameters in the method can be accessed when "Auto Sipper" is selected in the Extra Accessories list. Normally, it will be compatible with the single cell holder accessory.

Step 1: Select **Single Cell Holder** accessory from the **Accessory** drop-down list, and then select **Auto Sipper** from the **Extra Accessories** drop-down list.



Step 2: Setup **Auto Sipper** parameters in the method as shown below:



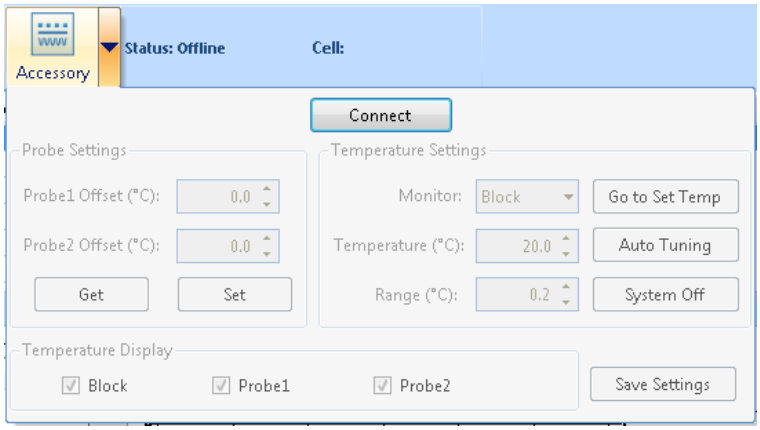
Sample Time (s)	Enter the amount of time that the pump pulls sample through for.
Delay Time (s)	Enter the amount of time between the end of filling and the start of data collection. This is to allow for bubbles, turbulence, etc.
Speed (RPM)	Enter the rotation speed in RPM.
Purge Direction	Select Flush for a forward flush which pull sample into waste, select Return for a backwards flush which return sample to the original reservoir. Flush occurs after data collection;
Purge Time (s)	Allow you to set the time for flushing or returning the sample using the sipper.
Prompt before flushing the sample during data collection	Select for a prompt to be called before flushing the sample at the end of data collection.

Step 3: Set customized parameters for **Fill Time**, **Flush/Return Time (s)**, and **Delay Time** in sample table when run a method which select Auto Sipper accessory.

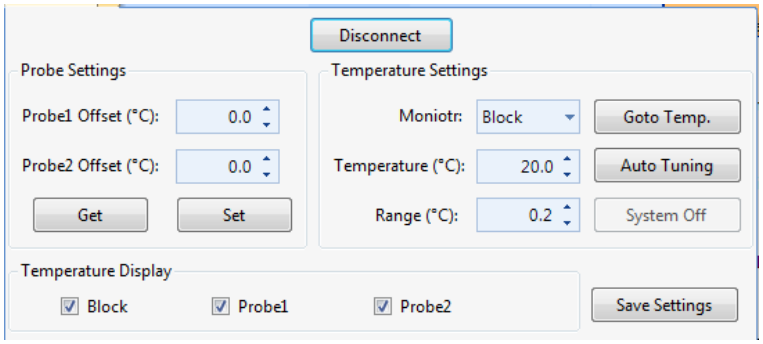
Fill Time(secs)	Flush/Return Time(secs)	Delay Time(secs)
20.0	5.0	10.0

Peltier Accessory Setup:

Step 1: Click the **Connect** button to connect Peltier Control.



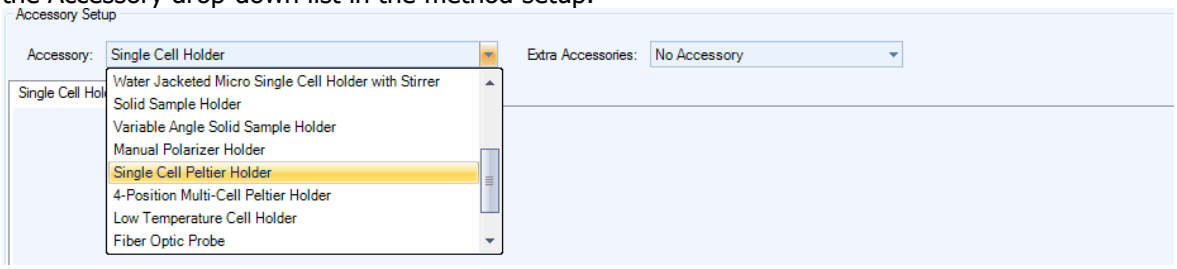
Step 2: You can manually control control the peltier using the following screen.



Probe Settings	This function is used to adjust temperature for Probe reading. It is only used for the manufacturing process, so do not modify the values except under help of PerkinElmer Service.
Get	Read the offset value from the hardware.
Set	Enter a new offset value and click "Set", this will set the new offset value into hardware.
Temperature settings	
Monitor	Select the temperature used to monitor during measurement. Options include: Block, Probe 1 or Probe 2.
Temperature (°C)	Enter the target temperature for the experiment. ***NOTE:*** *Starting temperature of experiment needs to be set up in the method window.*

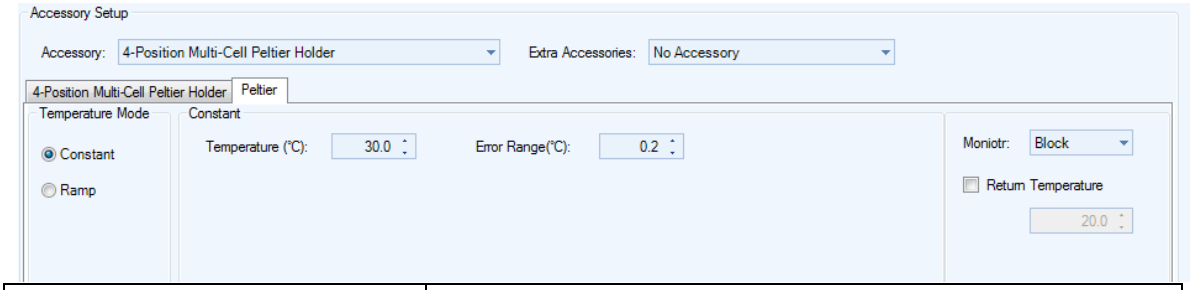
Range (℃)	Enter the error tolerance range.
Go to Temp	Peltier control starts heating up or cooling down to the set temperature, meanwhile the Set temperature can be read in hardware screen.
Auto Tuning	This function is used to minimize the temperature fluctuation at the target temperature. Click this button and wait until you see the warning of "Auto Tuning successful".
System Off	This function is used to stop the heating up or cooling down to the set Temperature in the Temperature Settings.
Temperature Display	Select which temperature will be displayed on the panel: Block, Probe 1 or Probe 2. Note that the selected temperature is only displayed in real time.
Save Settings	Save temperature settings and display mode. Save the Peltier Temperature and Temperature Display setting parameters. next time the software software is restarted.

Step 3: Select either **Single Cell Peltier Holder** or **4-Position Multi-Cell Peltier Holder** from the Accessory drop-down list in the method setup.



Step 4: Select **Temperature Mode** and setup the parameters according to below table.

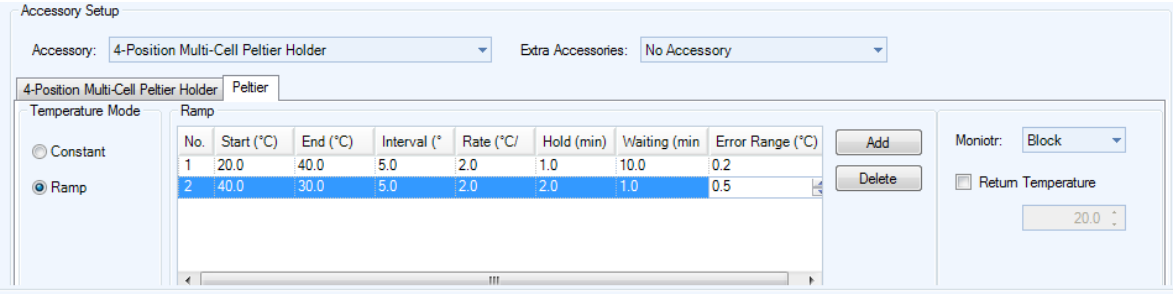
Constant Mode:



Constant mode	The measurement is only performed with isothermal state in the constant mode.
Temperature (℃)	Enter the target temperature for experiment.
Error Range (℃)	It shows the temperature tolerance between the target and monitored temperature. The measurement will start when the temperature tolerance reaches within the set error range. Example: Set the temperature at 20℃ and error range 0.2℃ and then the measurement will start when the temperature reaches between 19.8℃ and 20.2℃.

Monitor	Select temperature used to monitor during measurement. Options include: Block, Probe 1 or Probe 2.
Return Temperature	Allows user to input a safety temperature, to which, the system can be returned before inserting a new sample or at the end of experiment. If this option is unchecked, it will keep current temperature for Constant mode.

Ramp Mode:



Ramp mode	The Ramp mode can be set up according to desired temperature conditions. ***Note:*** *this option is only available in Spectra Scan method and Simple Read Method.*
Start (°C)	Enter the start temperature for the measurement.
End (°C)	Enter the end temperature for the measurement.
Interval (°C)	Enter the measurement interval temperature. For instance: when set at 5°C, the sample will be measured from start temperature to end temperature every 5°C.
Rate (°C/min)	Enter the heating (or cooling) temperature rate in each temperature range.
Hold (min)	Enter the holding time. For example, if you set 1 min, the measurement will start one minute after the temperature reaches at the set point.
Waiting (min)	Enter the waiting time at the end of current gradient. For example, in the grade 1 setting, the measurement will be start after holding 1 min at each interval temperature (20, 25, 30, 35, 40), and it will wait 10 min after measurement at 40°C, then start next grade or finish current method.
Error Range (℃)	It shows the temperature tolerance between the target and monitored temperature. The measurement will start when the temperature tolerance is measured within the set error range.

	Example: Set the temperature at 20°C and error range 0.2°C then, the measurement will start when the temperature is reached between 19.8°C and 20.2°C.
Add/Delete	Click on **Add and Delete** to edit the temperature range and the rate.
Monitor	Select the temperature used to monitor during measurement. Options include: Block, Probe 1 or Probe 2.
Return Temperature	Allows the user to input a safety temperature, which can be returned before inserting new sample or at the end of experiment. If this option is unchecked, it will go to start temperature for Ramp Cycle 1.

Collecting Data

Collecting Data

Data is collected based on the type of method that is setup.

- Spectra Scan
- Single Read
- Time Drive
- Lifetime
- Quantification
- Wavelength Program
- Kinetics
- Quenching
- Quantum Yield
- Absorbance
- Fast Filter
- Microplate Reader
- Simple Read

After selecting and setting-up a method. To collect data:

➢ Click **Run** in the Action Bar.

OR

Click **Run** in the Action menu.

The following points list some ways to use Spectrum FL to collect data using your instrument.

- Collecting data from a single sample.
- Collecting background spectra.
- Collecting data and running a process.

Backgrounds

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

The background spectrum is subtracted from the sample spectrum to eliminates features introduced by the instrument response, the sampling accessory or sample cell, and features introduced by atmospheric absorption.

If no valid background spectrum is available, a background spectrum must be collected before you begin to scan samples.

Data File Extension Summary

The following table lists the data file extensions:

	Data File Extension
Spectra Scan - Single Scan	.sp
Spectra Scan - 3D Scan	.sp3
Spectra Scan - Repeat Scan	.sp3
Spectra Scan - Ramp Scan	.sp3
Single Read	.wl
Time Drive	.td
Time Drive Event	.tde .tdex
Lifetime	.lt .ltx
Wavelength Program	.wl
Absorbance	.sp
Fast Filer	.td
Simple Read – Ramp Scan	.td

Data Analysis

Processing Data

These topics describe the range of processing commands that enable you to modify selected spectra.

Absorbance

%Transmittance

Data Tune-up

Baseline Correction

Interactive Baseline Correction

Difference

Normalization

Interpolate

Convert X

Smooth

Derivative

Arithmetic

Deconvolution

Polarization

Anisotropy

Peak Table

Peak Area/Height

Equations, available on the Data Analysis Navigation menu by default, requires you to set up one or more equations.

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

To invoke a process command:

➢ Select the appropriate command from the Process menu.
OR

Click the appropriate icon in the Process bar.

OR

Right-click on the curve you want to process in the Viewing Area pane, select **Process** from the shortcut menu, and then select the appropriate process command.

Absorbance

Use the Absorbance process command to transform one or more spectra whose ordinate scale is in transmittance (%T) units to spectra whose ordinate scale is in absorbance (A) units.

1. Display and select the spectrum or spectra that you want to transform to absorbance (A) units.

2. Select **Absorbance** from the Process menu, or click  on the Process bar.

   The selected spectra are transformed and displayed with absorbance (A) units.

NOTE: *Applying the Absorbance command to a spectrum in Spectrum FL Standard software does not generate a new result spectrum. However, the application of this data transform is logged in the spectrum History. In Spectrum FL ES software, a new spectrum is added to the Samples View (with _1 appended to the sample name) and the original spectrum is added to the Recycle Bin.*

Additional Information

The natural result of the Fourier transform of the interferogram is a spectrum in Transmission. This scale, however, is multiplicative. If a film of thickness n of a material has a transmission of 90% at a certain position, a film of thickness 2n will not have a transmission of 80%, but 90% of 90% transmission, that is, 81% transmission. When using a transmittance scale the noise level is independent of the energy level, so the influence of noise on the spectrum is greater at low transmittance levels than at high transmittance levels.

The Absorbance scale is a logarithmic transform of the multiplicative transmission scale that is additive. This means that absorbance spectra can be more reliably used for quantitative analysis (for example, Beer's Law).

% Transmittance

Use the Transmittance process command to transform one or more spectra whose ordinate scale is in absorbance (A) units to spectra whose ordinate scale is in transmittance (%T) units.

1. Display and select the spectrum or spectra that you want to transform to transmittance (%T) units.

2. Select **Transmittance** from the Process menu, or click  on the Process bar.

   The selected spectra are transformed and displayed with transmittance (%T) units.

NOTE: *Applying the Transmittance command to a spectrum in Spectrum FL Standard software does not generate a new result spectrum. However, the application of this data transform is logged in the spectrum History. In Spectrum FL ES software, a new spectrum is added to the Samples View (with _1 appended to the sample name) and the original spectrum is added to the Recycle Bin.*

Additional Information

The natural result of the Fourier transform of the interferogram is a spectrum in Transmission. This scale, however, is multiplicative. If a film of thickness *n* of a material has a transmission of 90% at a certain position, a film of thickness 2*n* will not have a transmission of 80%, but 90% of 90% transmission, that is, 81% transmission. When using a transmittance scale the noise level is independent of the energy level, so the influence of noise on the spectrum is greater at low transmittance levels than at high transmittance levels.

The Absorbance scale is a logarithmic transform of the multiplicative transmission scale that is additive. This means that absorbance spectra can be more reliably used for quantitative analysis (for example, Beer's Law).

Data Tune-up

Use the Data Tune-up command to smooth, and to perform a baseline correction to remove any slope from, one or more spectra using a single command.

CAUTION: *Use the Data Tune-up process with discretion. The Smoothing component of the process can remove important data and generate misleading results by reducing the number of data points in the spectrum.*
Spectra that have plateau regions adjacent to sharp peaks (typical for gas samples) are especially vulnerable to excessive smoothing.

1. Display and select the spectrum or spectra that you want to process.
2. Select **Data Tune-up** from the Process menu, or click  on the Process bar.

   The processed spectra are added to the Samples View and displayed in the Viewing Area.

Additional Information

The Smoothing component of the Data Tune-up process is a form of filtering that reduces noise, but also degrades the resolution of your spectra so that their features become broader. If you use too great a level of smoothing, bands are broadened excessively and resolution is lost.

The Baseline Correction component of the Data Tune-up removes slope and bow from your spectra, but cannot remove more complex baseline features.

Baseline Correction

Use the Baseline Correction process command to remove baseline features from one or more spectra.

1. Display and select the spectrum or spectra that you want to correct.
2. Select **Baseline Correction** from the Process menu, or click  on the Process bar.

   The corrected spectra are added to the Samples View and displayed in the Viewing Area.

Additional Information

You can use the Baseline Correction process to remove slopes in the baseline of your spectra.

You may want to correct the baseline of a sample spectrum before comparing it with reference spectra, or measuring peak intensities.

The Baseline Correction process attempts to correct spectra without distorting the band intensities or introducing discontinuities. There must be significant regions of the spectrum that can be regarded as baseline. The process detects baseline portions of the spectra, and then bridges the data across the peaks to form a smoothed approximation to the baseline which is then subtracted from the original spectra in absorbance.

The calculations are performed internally in absorbance to help preserve band intensities.

As well as the automatic Baseline Correction, an Interactive Baseline Correction is available. The Interactive Baseline Correction allows you select multiple base points to create a baseline that will be subtracted from the spectrum.

Interactive Baseline Correction

Interactive Baseline Correction (i-Baseline) enables to you to use the vertical cursor to specify where the base points of your spectrum lie. A smooth curve will be constructed through these points and subtracted from the spectrum. You can correct the baseline over the whole of the spectrum or the correction can be applied to a limited range of the spectrum.

You can run the Interactive Baseline process on multiple spectra. However, note that the same parameters will be used to correct the baselines of all the spectra selected. If you wish to use different parameters for each spectrum, you should process the spectra individually.

1. Display and select the spectrum or spectra that you want to correct.
2. Select **Interactive Baseline Correction** from the Process menu.

   OR

   Click  if you have made it available on the Process bar.

   The Interactive Baseline Correction dialog is displayed in the Viewing Area.

   Click **Overlaid** to display the source spectra and the derivative curve in a single graph display, or **Result** to display the derivative curves without the source spectra.

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the range of the other.
3. Select the spectrum you would like to display while defining the baseline from the drop-down list.

   If you selected more than one spectrum before selecting Interactive Baseline Correction, those spectra will be available in the drop-down list. Although only one spectrum is displayed, the same parameters will be used to correct the baselines of all the spectra. If you wish to use different parameters for each spectrum, you will need to process the spectra individually.
4. To select the base points to be used for the correction, move the Vertical Cursor to the first point you want to use.
5. To accept this value, double-click on the cursor or click the **Add** button.

   The value is added to the Base Points table and the new baseline is added to the display. A marker is placed on the spectrum to indicate a base point.

   If **Find Min in Range** is selected, range markers are added for each base point, and range Start and End columns are added to the Base Points table. The baseline point used will be the minimum value in the defined range.
6. To remove a base point, click on the row in the Base Point table you want to remove and then click **Remove**.

   The base point is removed from the baseline.
7. Repeat steps 4 and 5 to identify as many base points as you require.

   The baseline is updated in the Viewing Area, and another marker added, each time a new value is added. If only one point is added, a horizontal baseline is used; and if two points are added a linear baseline passing through the points is shown. If multiple base points are added, a curve intersecting the spectrum at these points is constructed using a cubic spline, and this curve is subtracted from the original spectrum

If **Restrict Range** is selected, an offset equal to the absorbance at the highest frequency base point is subtracted from the region between the start of the spectrum and the start of the selected region. An offset equal to the absorbance at the lowest frequency base point is applied to the region between the end of the selected range and the end of the spectrum.

8. Select **Overwrite** if you want to overwrite the source spectrum with the corrected spectrum.

   In Spectrum FL ES, Overwrite is not available.

9. When you are happy with the baseline, click **OK** to accept the result.

   The Baseline Correction dialog closes.

   If the Overwrite check box was not selected, the processed Source spectrum is added to the Samples View and displayed in the Viewing Area.

   If the Overwrite check box was selected, the processed Source spectrum replaces the source spectrum in the Samples View and is displayed in the Viewing Area. In Spectrum ES the source spectra are sent to the Recycle Bin.

   Processed spectra are not saved to disk automatically.

Additional Information

You may want to correct the baseline of a sample spectrum before comparing it with reference spectra, or measuring peak intensities.

The Baseline Correction process attempts to correct spectra without distorting the band intensities or introducing discontinuities. There must be significant regions of the spectrum that can be regarded as baseline. The process detects baseline portions of the spectra, and then bridges the data across the peaks to form a smoothed approximation to the baseline which is then subtracted from the original spectra in absorbance.

The calculations are performed internally in absorbance to help preserve band intensities.

You can also correct the baseline of you spectra automatically. See **Baseline Correction**.

Difference

Use the Difference command to perform a weighted subtraction of one spectrum from another.

1. Display and select the two spectra whose difference spectrum you want to calculate.

   If either or both of the selected source spectra are displayed in Absorbance (A), then both the source spectra and the difference spectrum are displayed in Absorbance. If both of the source spectra are displayed in Transmittance (%T), the difference spectrum is displayed in Transmittance.

   The calculation is always performed in Absorbance.

2. Select **Difference** from the Process menu.

   OR

   Click 

   if you have made it available on the Process bar.

   The Difference dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the two source spectra, and the lower graph contains the calculated difference spectrum.

   Change the relative sizes of the two graph displays in the Split view by dragging the bar between them. The mouse pointer changes to a two-headed arrow when it is positioned over the bar.

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the display of the other.

   Click **Overlaid** to display the source spectra and the difference spectrum in a single graph, or **Result** to display the difference spectrum without the source spectra.

3. If you want to subtract other source spectra, select the spectrum needed using the drop-down lists for **Source** and **Spectrum to subtract**.

   You can, for example, swap the spectra being subtracted, by clicking **Swap Source**, or select any spectrum available in the Samples View.

4. Enter any scaling **Factor** you want applied to the spectrum that is being subtracted, that is, **Spectrum to subtract**.

   This enables you to overcome, for example, the effect of differences in concentration or sample thickness between the two source spectra.

   OR

   Click **Auto**.

   The scaling factor is calculated automatically by performing a least squares fit of the two source spectra, over the range currently displayed in the graph.

   In Spectrum FL ES, Overwrite is not available.

5. Click **OK** to accept the result.

   This dialog is closed.

   If the **Overwrite** check box was not selected, the difference spectrum (that is, the processed Source spectrum) is added to the Samples View and displayed in the Viewing Area.

If the **Overwrite** check box was selected, the difference spectrum replaces the source spectrum in the Samples View and is displayed in the Viewing Area. In Spectrum FL ES the source spectra are sent to the Recycle Bin.

Processed spectra are not saved to disk automatically.

Additional Information

Typically, you calculate the difference between two spectra to remove the contribution of some components and see what remains. For example, you can:

- find the spectrum of a solute by subtracting the solvent spectrum from the solution spectrum
- find the spectrum of an unknown component of a mixture by subtracting the spectra of the known components
- subtract the background spectrum of a sampling accessory.

The Difference calculation is performed in absorbance because it is absorbance that varies linearly with concentration or path length. If the source spectra contain regions where the absorbance is very high, the noise level in these regions of the difference spectrum will be high.

Difference spectra are very sensitive to small changes in the shapes and positions of bands. Use identical instrument conditions to collect the two source spectra to be subtracted.

Normalization

Use the Normalization process command to set a common peak in one or more spectra to the same ordinate limit, which enables you to compare other peaks in these spectra.

1. Display and select the spectrum or spectra that you want to normalize.
2. Select **Normalization** from the Process menu.

   OR

   Click  on the Process bar.

   The Normalization dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the selected source spectra, and the lower graph display contains the converted spectra.

   Change the relative sizes of the two graph displays in the Split view by dragging the bar between them. The mouse pointer changes to a two-headed arrow when it is positioned over the bar.

   Click **Overlaid** to display the source spectra and the normalized spectra in a single graph display, or **Result** to display the normalized spectra without the source spectra.

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the display of the other.
3. In **Normalize ordinate to**, enter the value, or height, that the common peak should be normalized to.
4. Select the **Abscissa Position** where the common peak can be found in your source spectra.

   By default, the **Maximum ordinate value in the spectrum** of your spectra is selected.

   If you want to normalize your source spectra to a particular peak, click **Maximum ordinate value over defined range**, and then enter (or drag the vertical cursor in the source graph to) a **Start** value to the left, and an **End** value to the right, of the common peak.

   OR

   If you want to normalize your source spectra to an intensity at a particular wavelength, click **Defined position**, and then enter (or drag the vertical cursor in the source graph to) the appropriate value.
5. Select the **Zero Point** for the baseline of your normalized spectra.

   By default, the **Minimum ordinate value** found in your source spectra is set to zero in the normalized spectra.

   If you don't want a baseline correction applied, click **none**.

   OR

   If you want to zero your normalized spectra to the abscissa value at a particular wavelength, click **Selected abscissa point**, and then enter (or drag the vertical cursor in the source graph to) the appropriate value.
6. Select **Overwrite** if you want to overwrite the source spectrum with the corrected spectrum.

   In Spectrum FL ES, Overwrite is not available.

7. Click **OK** to accept the result.

   This dialog is closed.

   If the Overwrite check box was not selected, the normalized spectra are added to the Samples View and displayed in the Viewing pane.

   If the Overwrite check box was selected, the normalized spectra replace the selected spectra in the Samples View and are displayed in the Viewing Area. In Spectrum FL ES the source spectra are sent to the Recycle Bin.

   Processed spectra are not saved to disk automatically.

Additional Information

The Normalization process multiplies the ordinate value of each data point in a spectrum by a factor that scales a particular peak to a set limit. This enables you to compare the spectrum with spectra that include the same peak scaled to the same limit. All %T calculations are performed internally in Absorbance, to minimize any effect on the shape of the peaks.

Interpolation

Use the Interpolation process command to change the number of data points in one or more spectra and, if necessary, their range.

1. Display and select the spectrum or spectra that you want to interpolate.
2. Select **Interpolation** from the Process menu.

   OR

   Click  if you have made it available on the Process bar.

   The Interpolation dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the selected source spectra, and the lower graph display contains the converted spectra.

   Change the relative sizes of the two graph displays in the Split view by dragging the bar between them. The mouse pointer changes to a two-headed arrow when it is positioned over the bar.

   Click **Overlaid** to display the source spectra and the interpolated spectra in a single graph display, or **Result** to display the interpolated spectra without the source spectra.

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the range of the other.
3. If you want to use part of the **Full range** of your selected source spectra, click **Selected range**, and then enter (or drag the vertical cursor in the source graph to) the **Start** and **End** values for your range of interest.
4. If necessary, enter an appropriate new **Data point interval**.

   The default data interval maintains the number of points in the source spectra.
5. Select **Overwrite** if you want to overwrite the source spectrum with the corrected spectrum.

   In Spectrum FL ES, Overwrite is not available.
6. Click **OK** to accept the result.

   This dialog is closed.

   If the Overwrite check box was not selected, the interpolated spectra are added to the Samples View and displayed in the Viewing pane.

   If the Overwrite check box was selected, the interpolated spectra replace the selected spectra in the Samples View and are displayed in the Viewing Area. In Spectrum FL ES the source spectra are sent to the Recycle Bin.

   Processed spectra are not saved to disk automatically.

Additional Information

Use the Interpolation process command to:

- Save part of a spectrum
- Reduce the number of data points.

  The number of data points in a spectrum is included in the Sample section its History tab.

The Interpolation process adds data points to a spectrum by adding new points between the points that already exist, and removes data points from a spectrum by selecting every nth point in a spectrum and deleting it.

The number of data points needed in a spectrum depends on the width of the features in the spectrum. If the separation of the data points is smaller than is needed to define the features in the spectrum, the number of points can be reduced without reducing the amount of information in the spectrum.

Increasing the number of data points in a spectrum cannot increase the amount of information in the spectrum.

Convert X

Use the ConvertX process command to convert the abscissa units of your spectra to and from wavenumbers, microns, or nanometers.

1. Display and select the spectrum or spectra that you want to convert.
2. Select **ConvertX** from the Process menu.

   OR

   Click  if you have made it available on the Process bar.

   The ConvertX dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the selected source spectra, and the lower graph display contains the converted spectra.

   Change the relative sizes of the two graph displays in the Split view by dragging the bar between them. The mouse pointer changes to a two-headed arrow when it is positioned over the bar.

   Click **Overlaid** to display the source spectra and the converted spectra in a single graph display, or **Result** to display the converted spectra without the source spectra.

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the display of the other.
3. Select the **New abscissa unit** that you want to convert to.
4. If necessary, enter an appropriate **Data point interval**.

   The current data interval is selected by default. This maintains the number of points in the source spectra.
5. If you want the converted spectra to replace your source spectra, select the **Overwrite** check box.

   In Spectrum FL ES, Overwrite is not available.
6. Click **OK** to accept the result.

   This dialog is closed.

   If the Overwrite check box was not selected, the converted spectra are added to the Samples View and displayed in the Viewing Area.

   If the Overwrite check box was selected, the converted spectra replace the selected spectra in the Samples View and are displayed in the Viewing Area. In Spectrum FL ES the source spectra are sent to the Recycle Bin.

   Processed spectra are not saved to disk automatically.

Smooth

Use the Smooth process command to reduce the noise level in one or more spectra.

CAUTION: *Use the Smooth process with discretion. It can remove important data and generate misleading results by reducing the number of data points in the spectrum. Spectra that have plateau regions adjacent to sharp peaks (typical for gas samples, and some NIR and Raman spectra) are especially vulnerable to excessive smoothing.*

1. Display and select the spectrum or spectra that you want to smooth.
2. Select **Smooth** from the Process menu, or click  on the Process bar.
3. Select the **Smooth Factor** you wish to apply.
4. If you want the smoothed spectra to replace your source spectra, select the **Overwrite** check box.

   In Spectrum ES, Overwrite is not available.
5. Click **OK**.

   This dialog is closed.

   If the Overwrite check box was not selected, the smoothed spectra are added to the Samples View and displayed in the Viewing Area.

   If the Overwrite check box was selected, the smoothed spectra replace the selected spectra in the Samples View and are displayed in the Viewing Area.

Additional Information

Smoothing is a form of filtering that reduces noise, but also degrades the resolution of your spectrum so that the features in the spectrum become broader. If you use too great a level of smoothing, bands are broadened excessively and resolution is lost.

Smoothing should not change band areas or the position of symmetrical bands.

The Smooth process used is an adaptive procedure that estimates the signal-to-noise ratio of the data within a window and then applies an appropriate degree of smoothing. Areas with a high signal-to-noise ratio have no smoothing applied to them, and noisy areas are heavily smoothed.

The window size is appropriate for 4 cm^{-1} resolution data, which means that the smooth algorithm is unsuitable for spectra with very sharp peaks.

Derivative

Use the Derivative process command to generate a first, second, third or fourth order derivative curve from your selected spectrum.

1. Display and select the spectrum, or spectra, that you want to process.
2. Select **Derivative** from the Process menu.

   OR

   Click $\frac{d}{dx}$ if you have it available on the Process bar.

   The derivable dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the selected source spectra, and the lower graph contains the calculated derivative curves.

   Change the relative sizes of the two graph displays in the Split view by dragging the bar between them. The mouse pointer changes to a two-headed arrow when it is positioned over the bar.

   Click **Overlaid** to display the source spectra and the derivative curve in a single graph display, or **Result** to display the derivative curves without the source spectra.

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the range of the other.
3. Select the **Order** of the derivative, and the **Number of Points** to provide the required degree of smoothing.
4. If you want the calculated derivative curves to replace your source spectra, select the **Overwrite** check box.

   In Spectrum FL ES, Overwrite is not available.
5. Click **OK** to accept the result.

   This dialog is closed.

   If the Overwrite check box was not selected, the derivative curves are added to the Samples View and are displayed in the Viewing Area.

   If the Overwrite check box was selected, the derivative curves replace the selected spectra in the Samples View and are displayed in the Viewing Area. In Spectrum FL ES the source spectra are sent to the Recycle Bin.

   Processed spectra are not saved to disk automatically.

Additional Information

Derivative curves usually have sharper features than the original spectra, which can enable you to reduce the effects of overlapping bands and to suppress background effects. You can use derivative curves in quantitative methods to eliminate some baseline effects. For example, the amplitudes of features in derivative curves can be used in the same way as peak absorbances.

Order

The first derivative removes any baseline offset and linear slope.

The second derivative removes any parabolic baseline effects. These curves have sharp minima where there are maxima in the original spectrum, which can enable you to identify band positions in complex regions.

The third derivative removes any cubic baseline effects, and the fourth derivative any fourth order baseline effects. Both third and fourth order derivative curves can be difficult to interpret, and are only useful when the original spectra had a high signal-to-noise ratio.

Smoothing by varying the number of data points used for the slope calculation

Derivative curves emphasize narrow features, including noise, relative to broad ones. You can control this to some extent by varying the width (that is, the **Number of Points** used to calculate the slope) of the derivative function, which is equivalent to applying some smoothing to the derivative curve.

The Derivative process uses the Savitzky-Golay procedure to estimate the derivative of a smooth curve, constructed through the original data points of your original spectrum. It uses a number of neighboring data points to estimate the curve. As the number of data points used in the calculation is increased, the contribution of broader features increases relative to narrow features.

Raman data

Derivative is particularly useful to correct for spikes in your Raman data, for example, due to cosmic rays. It is also useful for removing baseline slope due to fluorescence.

Arithmetic

Use the Arithmetic process command to apply one or more of the following operations to your spectra:

+	addition	requires an operand
-	subtraction	requires an operand
x	multiplication	requires an operand
/	division	requires an operand
log	log base 10	
ln	log base e	
sqr	square	
sqrt	square root	

For example, you could multiply the ordinate values in a spectrum by a constant (such as 2), or divide one spectrum by another spectrum.

1. Display and select the spectrum that you want to process.
2. Select **Arithmetic** from the Process menu.

   OR

   Click  if you have made it available on the Process bar.

   The arithmetic dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the selected source spectrum, and the lower graph display will contain the processed spectrum.

   Change the relative sizes of the two graph displays in the Split view by dragging the bar between them. The mouse pointer changes to a two-headed arrow when it is positioned over the bar.

   Click **Overlaid** to display the source spectra and the interpolated spectra in a single graph display, or **Result** to display the processed spectrum without the source spectra.

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the range of the other.
3. Select the **Operator** you require from the drop-down list.
4. Enter the value of the **Constant** to apply to your spectrum.

   For example, **Current Sample x 2** multiplies the ordinate values in your spectrum by 2.

   OR (and provided you selected the +, -, x or / operator)

   Deselect the **Constant** button, and then select another spectrum from the **Operand** drop-down list; the browse option enables you to select any *.sp file available to your PC.

   The operation is performed and the **Arithmetic Result** graph display is updated.

   NOTE: *If you select log, ln, sqr, or sqrt the Operand field is not available because no other spectrum is required to complete these operations.*

   OR

   If the sample table contains a File Path custom column, click the **Column** button and select the name of the custom column from the drop-down list.

The operation is performed on the sample using the spectrum file in the custom column of the sample table.

5. Select **Overwrite** if you want to overwrite the source spectrum with the corrected spectrum.

   In Spectrum FL ES, Overwrite is not available.

6. Click **OK** to accept the result.

   This dialog is closed.

   If the Overwrite check box was not selected, the processed spectra are added to the Samples View and displayed in the Viewing Area.

   If the Overwrite check box was selected, the processed spectra replace the selected spectra in the Samples View and are displayed in the Viewing Area.

   In Spectrum FL ES, Overwrite is not available.

   Processed spectra are not saved to disk automatically.

Additional Information

Negative values in the logarithmic and square root operations

For logarithmic and square root operations, negative input values are set to zero.

Adding Spectra

If you add two spectra with the same units and the same range but with different data intervals, the resulting spectrum is constructed using the smaller data interval.

If you add two spectra with the same units and data intervals but with different ranges, the resulting spectrum is the sum of the overlapping regions only.

Subtracting Spectra

If you subtract two spectra with the same units and range but different data intervals, the resulting spectrum is constructed using the smaller data interval.

If you subtract two spectra with the same units and data intervals but different ranges, the resulting spectrum is the difference of the overlapping regions only.

Multiplying Spectra

If you multiply two spectra with the same units, data interval and range, the resulting spectrum is the product of the two spectra.

If you multiply two spectra with the same units and ranges but different data intervals, the resulting spectrum is constructed using the smaller data interval.

If you multiply two spectra with the same units and data intervals but different ranges, the resulting spectrum is the product of the overlapping regions only.

Dividing Spectra

If you divide two spectra with the same units, data interval and range, the resulting spectrum is the ratio of the two spectra.

If you divide two spectra with the same units and ranges but different data intervals, the resulting spectrum is the ratio constructed from the smaller data interval.

If you divide two spectra with the units and data intervals but different ranges, the resulting spectrum is the ratio of the overlapping regions only.

Deconvolution

Deconvolution applies a line-narrowing process so that interference between unresolved features is reduced. This means that you can see peaks that are present more easily. Deconvolution is used in estimating the positions and intensities of overlapping absorption bands.

1. Display and select the spectrum or spectra that you want to deconvolute.
2. Select **Deconvolution** from the Process menu.

   OR

   Click  on the Process bar.

   The Deconvolution dialog is displayed in the Viewing Area. This dialog contains interactive controls below a **Split** view; the upper graph display contains the selected source spectra, and the lower graph display contains the converted spectra.

   Change the relative sizes of the two graph displays in the Split view by dragging the bar between them. The mouse pointer changes to a two-headed arrow when it is positioned over the bar.

   Click **Overlaid** to display the source spectra and the normalized spectra in a single graph display, or **Result** to display the normalized spectra without the source spectra.

   If **Link graph ranges** is selected, changing the ordinate range displayed in one graph will also change the range of the other.
3. Enter the **Gamma** value, which defines the line-narrowing and can take values between 0 and 100; larger values give more narrowing.

   The reduction in linewidth for an ideal Lorentzian line is given by: 4 * Gamma * data interval. For spectra with a data interval of 1, typical gamma values are less than 3.
4. Select the smoothing **Length**.

   Length defines the smoothing that is applied to limit the noise generated by line-narrowing. It can take values between 0 and 95, with 95 corresponding to maximum smoothing. For spectra of different data intervals, equivalent smoothing is achieved for equal values of (100 length) x data interval.
5. Select the appropriate radio button for either **Bessel** or **Boxcar** smoothing.

   You should choose Bessel for real data.
6. Select **Overwrite** if you want to overwrite the source spectrum with the corrected spectrum.

   In Spectrum FL ES, Overwrite is not available.
7. Click **OK** to accept the result.

   This dialog is closed.

   If the Overwrite check box was not selected, the processed Source spectrum is added to the Samples View and displayed in the Viewing Area.

   If the Overwrite check box was selected, the processed Source spectrum replaces the source spectrum in the Samples View and is displayed in the Viewing Area. In Spectrum FL ES the source spectra are sent to the Recycle Bin.

   Processed spectra are not saved to disk automatically.

Additional Information

Deconvolution applies a line-narrowing process so that interference between unresolved features is reduced. This has traditionally been done by taking derivatives of the spectrum. For example the second derivative of a band has a narrow minimum at the frequency corresponding to the maximum of the original band. The disadvantage of derivative spectra is that secondary maxima and minima are generated along with the central features. Deconvolution achieves line-narrowing with minimal subsidiary features.

Deconvolution uses a method called Fourier self-deconvolution which operates on the Fourier transform of the spectrum. It can be thought of as involving two steps. A line narrowing filter removes broadening corresponding to a Lorentzian line shape. This filter is characterized by Gamma. Increasing the magnitude of Gamma produces narrower lines, but eventually leads to subsidiary features (sidelobes) around the narrowest bands. It also increases the noise. To reduce these undesired effects a smoothing function is applied. The degree of smoothing is controlled by a parameter called length. Increasing the length leads to a greater degree of smoothing. This reduces noise and sidelobes, but at the expense of some line broadening.

Deconvolution is an interactive routine to find the most appropriate combination of these parameters. It has to be used with caution since sidelobes from large bands can be confused with small overlapping bands.

Deconvolution works best with noise-free data where all the bands are Lorentzian and have the same width. Even with ideal data the line width cannot be reduced below the resolution at which the spectrum was collected. With real data, the degree of narrowing that can be achieved is limited either by noise or by the subsidiary features associated with the sharpest bands.

There is no correct result for real data. For example, small negative sidelobes may be perfectly acceptable when trying to identify band positions.

Polarization

Fluorescence polarization is used to study the rotational movement of small molecules in solution or suspension. For example the technique is used to measure the binding of coenzymes to proteins, in the study of antigen-antibody reactions, in determining low molecular weight haptens, and to measure cell membrane fluidity.

Select this option to calculate the polarization of a sample. Your instrument must have an excitation and an emission fast filter wheel fitted, and the positions of the horizontal and vertical polarizer for the excitation and the emission fast filter wheel must have been defined in the Status application.

1. Display and select the spectrum or spectra that you want to measure.
2. Select **Polarization** from the **Process** menu.

   OR

   Click  on the Process bar.

Anisotropy

Select this option to calculate the anisotropy of a sample. Your instrument must have an excitation and an emission fast filter wheel fitted, and the positions of the horizontal and vertical polarizer for the excitation and the emission fast filter wheel must have been defined in the Status application.

1. Display and select the spectrum or spectra that you want to measure.
2. Select **Anisotropy** from the **Process** menu.

   OR

   Click  on the Process bar.

Peak Table

Peak Table is a process command that automatically produces a table of the peaks in your spectrum or spectra. The parameters used to generate the Peak Table are defined on the Setup Peak Detection tab.

1. Display and select the spectrum or spectra that you want to process.
2. Select **Peak Table** from the Process menu.

   OR

   Click  if you have made it available on the Process bar.

The results are displayed on the Peak Table tab in the Viewing Area.

- 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.
- 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 results are also displayed on the Results Table tab.

Additional Information

The results of the Peak Area/Height process are also added to the Peak Table tab. Each time you run a Peak Table or Peak Area/Height process on a spectrum, a new row is appended to the results.

Peak Area/Height

Peak Area/Height is a process command that enables you to produce a table of the areas and heights of the peaks in your spectrum or spectra. You can auto-generate a peak table, or add peaks individually. You can use it to measure:

- Peak areas relative to a linear baseline, between two baseline points, or between two other points on the spectrum.
- Peak heights from a peak maximum to a baseline.
- The maximum height in a selected region.
- The ratio of two peaks.

You can run the Peak Area/Height process on multiple spectra. However, note that the same parameters will be used to produce the results for all the spectra selected. If you wish to use different parameters for each spectrum, you should process the spectra individually.

1. Display and select the spectrum or spectra that you want to process.
2. Select **Peak Area/Height** from the Process menu.

   OR

   Click  if you have made it available on the Process bar.

   The Peak Area/Height dialog is displayed in the Viewing Area.
3. Select the spectrum you would like to display while defining the peaks from the drop-down list.

   If you selected more than one spectrum before selecting Peak Area/Height, those spectra will be available in the drop-down list. Although only one spectrum is displayed, the same parameters will be used to generate the results for all the spectra. If you wish to use different parameters for each spectrum, you will need to process the spectra individually.
4. Select to display the **Area** or **Height** graph marker.
5. In the **Calculation** section, choose whether to calculate **Area**, **Height** or **Max Height**.

   Areas and heights are calculated in the same units as the spectrum. If you want to use units different from the current units of the spectrum, you must convert the spectrum to the correct units first.
6. Select the number of Bases.

   Select **Base 1**, **Base 2**. If one or more bases are selected, then **Min Bases** becomes available.

   If no bases are selected, the zero absorbance is used as the baseline. If Base 1 is selected, a horizontal baseline is drawn at that ordinate value. If Base 1 and Base 2 are selected, the baseline is drawn between the two points.

   Min Bases adds range markers for each base point. The base point used is the minimum value between the markers.
7. Click **Add** to add a peak (defined at the current Vertical Cursor position) to the table.

   OR

   Double click on the Vertical Cursor to add a peak to the table.

   OR

   Click **Auto** to automatically find the peaks and populate the table.

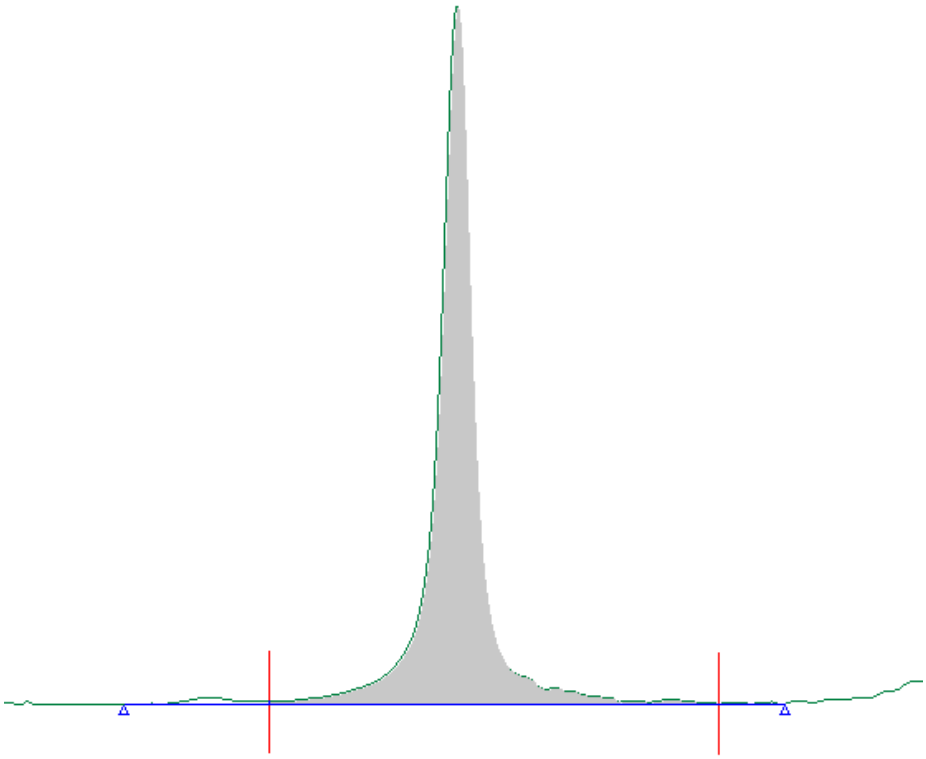
8. Use the graph markers to adjust the position of the baseline markers, the range over which the peak area or maximum height will be calculated, or the point on the curve at which the height will be determined, as required.
9. Select the results you want to be displayed in the Results Table.

   The options are the **X** and/or **Y** coordinates, **Height** and **Area**. The results added to the Results Table will be available as variables in Equations.
10. Click **OK** to exit the Peak Area/Height dialog.

    The Peak Table tab and Results Table tab are updated.

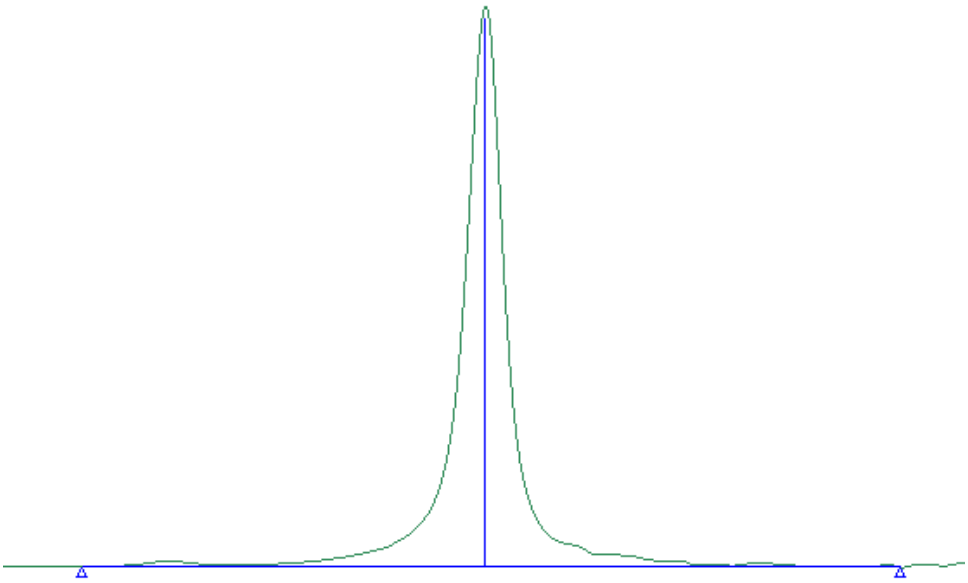
Area

An area is defined by a start and end abscissa value and two base points.



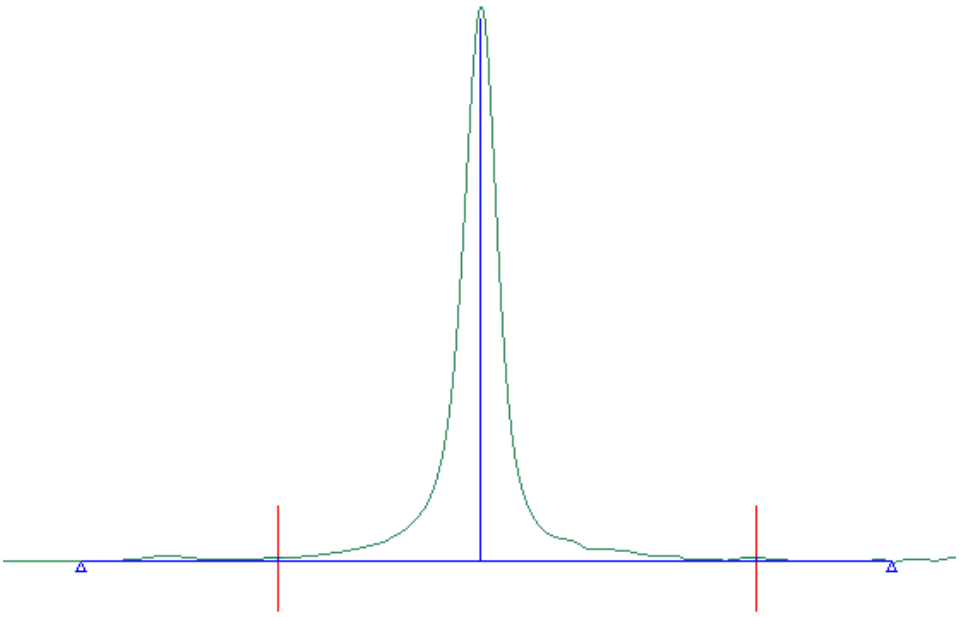
Height

Height is defined by an abscissa value (X in the table) and two base points. If no bases are selected, the Height is measured from the curve to zero absorbance. If one or two bases are selected, the max height is measured from the curve to the baseline.



Max Height

Max height is defined by a start and end abscissa value and two base points. The **Max Height** is the maximum peak height between the start and end abscissa values. If no bases are selected, the max height is measured from the curve to zero absorbance. If one or two bases are selected, the max height is measured from the curve to the baseline.



Defining a Ratio

The Ratio option is only available when two rows are selected in the table.

1. Click in the left-hand column of the peak row that you wish to be the numerator.

The row is highlighted.

2. Hold down the CTRL button on your keyboard, and then select the left-hand column of the peak row that you wish to be the denominator.

   Both rows are highlighted.

3. Click **Ratio**.

   A new row is added to the table, and automatically named [Peak Name Row 1]/[Peak Name Row 2].

NOTE: *If you modify the parameters of either peak row, then the ratio values are automatically updated.*

Removing a Row from the Table

➢ Select the row or rows in the table containing the peak positions that you want to remove, and then click **Remove**.

Peak Area/Height Results

The results are displayed on the Peak Table tab in the Viewing Area.

- 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 are 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, and the peak areas shaded and heights marked.

- 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 results are also displayed on the Results Table tab.

Additional Information

The results of the Peak Table process are also added to the Peak Table tab. Each time you run a Peak Table or Peak Area/Height process on a spectrum, a new row is appended to the results for that Samples View.

Equations

Equations are process commands that perform calculations on one or more spectra, or on the data obtained from other processes. An equation must be defined before it can be used.

To apply an equation that you have previously defined:

1. Display and select the spectrum or result that you want to process.
2. Select **Equations** from the Process menu, and then click on the name of the equation that you want to apply.

   OR

   Select the  icon labeled with the name of the equation that you want to apply from the Equations drop-down list on the Process bar.
   By default, an Equation icon and label is added to the Equations drop-down list on the Process bar each time a new equation is defined.

   The Results Table tab is updated. If the result amends the source spectrum, the processed spectrum is displayed in the Viewing Area and added to the Samples View.

Processed spectra are not saved to disk automatically.

Additional Information

Defining Equations

For further information about adding a new equation, see Setup Equations.

For further information about modifying an equation, see Setting up an Equation.

For further information about formatting the numeric results obtained by applying an equation, see Formatting Equation Results.

Viewing Spectra

Viewing Spectra

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

Optimizing the Viewing Area

Optimizing Graphs

Autorange X, Y, XY

Previous Range

Formatting a Graph

Graph Labels

Labeling Graphs using the Vertical Cursor

Label Peaks

Horizontal Cursor

Autoscale Y

Optimize

Panning, Zooming and Offsetting Spectra

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

Additional Information

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

The Data Explorer

In the Data Anaylsis mode use the **Data Explorer** together with the Viewing Area to organize your sample data in the Spectrum FL workspace.

- The **Data Explorer** pane is on the left of the Spectrum FL 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 FL Workspace. They have no explicit relationship with where, or whether, spectra are saved.*

- If you have Spectrum FL 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.
- The Viewing Area is in the center of the Spectrum FL 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 FL 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 FL 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 FL 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 FL 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 FL 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.*

Additional Information

Opening and Closing Panes

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

OR

Select Data Explorer from the View menu.

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

  OR

  Select Navigation Pane from the View menu.

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

  OR

  Select Dialog Pane from the View menu.

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

Resizing Panes

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

Optimizing the Viewing Area

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

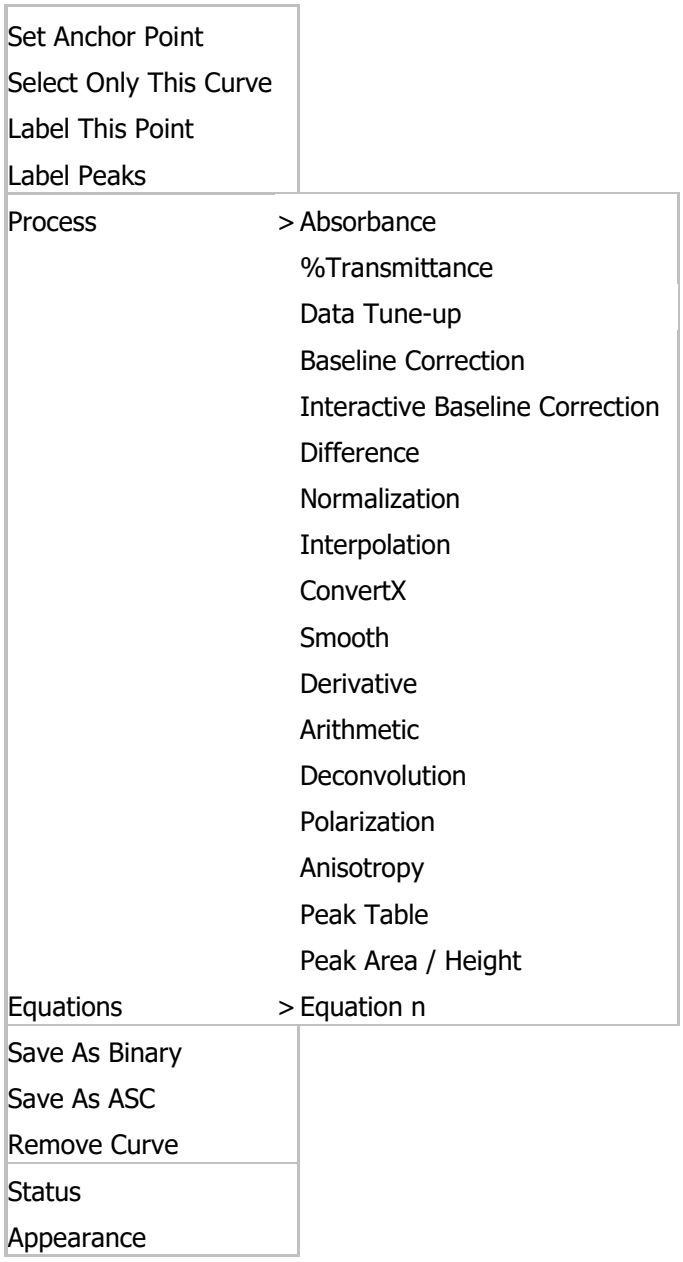
- Previous Range
- Full Scale
- Vertical Cursor
- Horizontal Cursor
- Split Display
- Set Anchor Point
- Add Text
- Add Range Marker
- Add Bitmap Image
- Print
- Copy to Clipboard
- Properties

Additional Information

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

Optimizing Graphs

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



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

Additional Information

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

Autorange

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

Autorange X

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

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

Autorange Y

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

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

Full Range

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

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

Additional Information

- Use the Previous Range command to undo the Autorange X command or Autorange Y command. Use the Previous Range command twice to undo the Autorange XY command; once to undo the Y component and once again to undo the X component.
- Use the Autoscale Y command to rescale every feature in your spectrum.
- Use the Optimize command to rescale every feature in your spectrum, excluding any noise spikes or unwanted peaks from atmospheric CO2 or water vapor.
- Use Cancel Offset command to fit any offset spectra onto the graph.

Previous Range

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

➢ Select Previous Range from the View menu.

OR

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

The graph is redisplayed.

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

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

Formatting a Graph

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

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

- Select **Format graph** from the View menu, or right-click on the graph and select **Properties** from the pop-up box.

  The Graph Properties dialog opens at the Axes tab.

The Graph Properties dialog has four tabs:

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

Additional Information

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

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

  The Graph Properties dialog opens at the Axes tab.

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

  The Graph Properties dialog opens at the Appearance tab.

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

Graph Title and Description

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

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

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

   OR

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

2. Select the General tab.

3. Enter your **Title** and/or **Description**.

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

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

   OR

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

   OR

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

Range and Units for the X and Y Axes

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

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

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

   OR

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

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

   The options available are:

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

3. To confirm changes without closing the dialog, click **Apply**.
   OR
   To close the dialog keeping only applied changes, click **Cancel**.

OR

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

Colors for Curves, Graph Elements, and Gridlines

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

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

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

   OR

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

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

   The options available are:

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

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

   OR

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

   OR

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

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

Advanced Curve Format Settings

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

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

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

   OR

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

2. Select the Advanced tab.

   The options available are:

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

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

   OR

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

   OR

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

Additional Information

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

Graph Labels

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

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

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

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

Additional Information

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

Text Labels

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

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

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

   OR

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

   The Label Properties dialog opens and displays the General tab. The options available are:

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

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

   OR

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

   OR

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

Additional Information

- **Moving a Text Label:** Select the graph label, and then drag it to its correct position on the graph.
- **Editing a Text Label:** Select the graph label, right-click and then select **Properties**. The Label Properties dialog is displayed, as described above.
- **Deleting a Text Label:** Select the graph label, right-click and then select **Remove**.
- **Adding a Bitmap Image:** You cannot paste a graphic element into a text label. You can, however, place an image, such as your company logo, into the graph using the Add Bitmap Image command.
- **Adding other Labels:** You can also add Point labels and Peak labels to your graph.

Point Labels

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

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

1. Select the position in the curve that you want to label, right-click and then select **Label this Point**.
   The Label Properties Dialog opens and displays the General tab. The options available are:

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

2. Select the **Advanced** tab.

   The options available are:

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

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

   OR

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

   OR

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

Point Labels Using the Vertical Cursor

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

   OR

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

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

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

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

3. Double-click the left mouse button.

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

Additional Information

- **Moving a Point Label:** Select the label, and then drag it to its correct position on the graph.
- **Editing a Point Label:** Select the label, right-click and then select **Properties**.

  The Label Properties dialog is displayed, as described above.
- **Deleting a Point Label:** Select the graph label, right-click and then select **Remove**.
- **Removing the Vertical Cursor:** Click  in the Graph toolbar.

  OR

  Right-click in the graph display and deselect **Vertical Cursor**.
- **Adding other Labels:** You can also add Text labels, Bitmap labels, and Peak labels to your graph.

Bitmap Labels

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

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

1. Right-click in a clear area of the graph display and select **Add Bitmap Image.**

   The Label Properties Dialog opens and displays the Bitmap tab.

   The options available are:

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

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

   OR

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

   OR

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

Additional Information

- **Moving a Bitmap Image:** Select the image, and then drag it to its correct position on the graph.
- **Editing a Bitmap Image:** Select the image, right-click and then select **Properties**. The Label Properties dialog is displayed, as described above.
- **Deleting a Bitmap Image:** Select the image, right-click and then select **Remove**.
- **Adding other Labels:** You can also add Text labels, Point labels, and Peak labels to your graph.

Labeling Graphs using the Vertical Cursor

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

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

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

   OR

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

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

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

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

3. Double-click the left mouse button.

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

Additional Information

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

  OR

  Click  in the Graph toolbar.

  OR

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

- **Moving a Point Label:** Select the label, and then drag it to its correct position on the graph.
- **Editing a Point Label:** Select the label, right-click and then select **Properties**. The Label Properties dialog is displayed, as described for Point labels.
- **Deleting a Point Label**: Select the graph label, right-click and then select **Remove**.

The Vertical Cursor in Process commands

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

Adding other Labels

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

Labeling Peaks

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

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

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

   OR

   Click  on the Graph Bar.

   OR

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

Additional Information

- **Clearing Peak Labels:** To remove all the peak labels from the selected spectrum, select **Label Peaks** from the View menu.

  OR

  Click  on the Graph Bar.

  OR

  Place your mouse pointer on the spectrum whose peaks you want to remove, right-click, and then select **Label Peaks**.
- **Moving a Peak Label:** Select the peak label, and then drag it to its correct position on the graph.
- **Deleting a Peak Label:** Select the peak label, right-click and then select Remove.
- **Adding other Labels:** You can also add Text labels, Point labels, and Bitmap labels to your graph.

Horizontal Cursor

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

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

   OR

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

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

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

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

Additional Information

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

  OR

  Click  in the Graph toolbar.

  OR

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

Autoscale Y

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

1. Select the spectra that you want to be fitted on to the graph display.
2. Select **Autoscale Y** from the Data Analysis toolbar.

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

Additional Information

Removing Autoscale Y

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

  The autoscaling is removed from the selected spectra.

Offset

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

Optimize

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

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

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

   The names of the selected spectra are underlined.

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

   The spectrum is rescaled.

   The ordinate range stays the same, but the abscissa range is rescaled to the next whole number.

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

Additional Information

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

Overlay/Split

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

Split

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

Overlay

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

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

Panning, Zooming and Offsetting Spectra

Use the techniques and tools described in these topics to:

- Zoom in on a region of the graph;
- Offset a spectrum so that its features can be seen more clearly;
- Pan a spectrum up and down or left and right;
- Expand or contract the X and Y scale around a fixed point.

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

Zooming to a Region of Interest

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

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

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

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

Additional Information

Changing the Size of a Grow Box

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

   The cursor changes to a two-headed arrow ⇿.

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

Moving a Grow Box

1. Position the mouse pointer inside the grow box.

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

Removing a Grow Box

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

Returning to the Previous Ranges

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

Offsetting Spectra

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

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

  OR

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

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

Additional Information

Autorange Y

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

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

   The spectra are underlined, indicating that they are selected.

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

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

Canceling Offsets and Restoring the Y Scale

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

   Any offsets are removed from the selected spectra.

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

Panning and Expanding

Moving Spectra to the Left or Right

- Move your mouse pointer close to the X axis and drag the horizontal pan pointer left or right to move your spectra.

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

Moving Spectra Up or Down

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

   OR

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

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

Using an Anchor Point

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

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

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

Expanding or Contracting the X or Y Scales

To expand or contract the X or Y scales around a fixed point:

1. Right-click in the graph and select **Set Anchor Point**.

   An anchor point is placed at the position of the mouse pointer.
2. Move your mouse pointer close to the X axis and drag the horizontal pointer right or left to expand or contract the X axis around the anchor point.

   OR
   Move your mouse pointer close to the Y axis and drag the vertical pointer up or down to expand or contract the Y axis around the anchor point.

NOTE: *In Split mode, all spectra are panned or expanded horizontally. However, each spectrum is treated separately when panned or expanded vertically, so be careful to place your anchor point in the graph for the correct spectrum.*

Finding and Saving

Finding and Saving

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

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

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

The following topics address these subjects in more detail:

- **Navigation**, which describes the Spectrum Browser, the Data Explorer, and the Results Table.
- **Samples Views**, which are the virtual folders displayed in the Data Explorer.
- **Opening, Removing and Deleting Files**, which describes opening files from disk, removing curves from a Samples View, and deleting files from disk.
- **Saving Spectra**, which describes the Save commands, setting up the default path to a Save location, and the Auto-Save option.
- **Exporting Spectra**, which describes how to save a spectra data sets in a format that can be read by a spreadsheet, LIMS, or another spectral application.

Additional Information

The Data Explorer Pane

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

Samples Views

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

Creating an Empty Samples View

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

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

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

Copying a Spectrum to a New Samples View

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

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

Removing a Samples View

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

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

  No files are deleted from disk.

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

Restoring Samples Views (Spectrum FL ES only)

- Right-click on the Recycle Bin in the Data Explorer pane and then select **Restore All**. Any Samples Views in the Recycle Bin will be recreated in the Data Explorer, together with any spectra they contained.

Additional Information

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

Opening, Removing, and Deleting Files

Opening a File

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

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

   OR

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

   The Open File dialog is displayed.

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

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

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

2. Click the filename you want to select.

   The file is selected, and all other files deselected.

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

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

3. Click **Open**.

   Your selected spectra are displayed in the selected Samples View.

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

Removing a Spectrum from a Samples View

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

   The spectrum is removed from the Samples View.

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

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

Alternatively:

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

  The spectrum is removed from the Samples View.

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

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

Removing all Selected Spectra from a Samples View

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

  All selected curves are removed from the Samples View.

  NO files are deleted from the hard disk.

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

Deleting a File from Disk

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

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

   OR

   Press CTRL+O.

   OR

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

   The Open File dialog is displayed.

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

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

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

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

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

Saving Spectra

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

The Save Command

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

1. Select the spectra you want to save.

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

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

   OR

   Press **CTRL+S**.

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

   The selected file, or files, are saved.

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

The Save All Command

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

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

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

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

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

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

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

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

   The Save File Path is amended for this spectrum.

   OR

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

   The Save File Path is amended for all the spectra.

5. Click **Save**.

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

The Save As Command

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

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

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

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

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

   The Save File Path is amended for this spectrum.

   OR

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

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

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

Additional Information

Auto-Save

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

Saving Files from the Graph tab

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

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

   The Save As dialog is displayed.

3. Browse to the location where you want the file to be saved.

   Initially the dialog displays the contents of C:\pefl_data\spectra. If you use the dialog more than once, the location of your last save is displayed.

4. Type or choose a filename.

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

5. Click **Save**.

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

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

   The Save As dialog is displayed.

3. Continue from step 3 above.

Exporting Reports

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

1. To generate a method report, select the **Method Setup** mode in navigation panel, select the method you are interested, then go to step 2.

   OR

   To generate an experiment report, select **Previous Results** mode in navigation panel, select the experiment you are interested, then go to step 2.

   OR

   To generate the report of a single spectrum, select the spectrum name in the **Data Explorer**, then go to step 2.

NOTE: *Check the appearance of the data that you will include in the report. Depending on the settings in the template you have selected, the appearance of the data in Spectrum FL may be duplicated in the report.*

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

   The Report dialog opens.

3. Select the **Reports Options** tab.
4. Select the **Save report** check box if you want to save the report(s).
5. Select **Show saved report** if you want the report(s) to be displayed when generated.
6. Select the **Print report** check box to print the report(s) to the currently active printer.
7. If necessary, click **Browse**, find the template file that you want to use to generate the report, and click **Open**.

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

   OR

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

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

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

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

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

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

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

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

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

    In Spectrum FL ES the report is saved in a secured and encrypted portable document format.

11. If necessary, browse to another (or create a new) folder for the generated report(s).

    By default, all reports are saved to C:\pefl_data\reports.

12. Select the sections to be included in the report from the **Section Name** list, which are derived from the template.

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

13. Click **Report**.

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

    The report is generated.

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

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

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

Additional Information for Spectrum FL ES

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

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

Opening an ES Report

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

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

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

2. Click the filename you want to select.

   The file is selected, and all other files deselected.

3. Click **Open**.

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

Exporting Spectra

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

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

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

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

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

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

5. Select the Format for your exported files.

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

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

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

6. Click **Export**.

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

   Your selected spectra are exported to the specified folder.

Additional information

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

Navigation

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

The Spectrum Browser

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

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

  OR

  Hover your mouse over the curve, right-click and then select **Select Only This Curve**. The curve is selected, and all other files deselected.

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

The Data Explorer

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

Publishing Results

Publishing Results

These topics describe the editing and printing options that enable you to publish your results.

Once you have processed and formatted your results, you can:

- Use the **Send To** command on the Data Analysis File menu to send your results to a WordPad or, if installed, a Microsoft® Word document, Microsoft Excel workbook data table. You can also send your results as an email attachment.
- Use the **Report** command on the File menu to output a report.
- Review a Print Preview and Print.
- Copy and Paste from the currently displayed tab in the Viewing Area to another location.

Additional Information

If you prefer to process and format your results outside Spectrum FL, you can:

- Use a File menu command to Export each spectrum as a comma separated value (*.csv), or JCAMP-DX (*.dx) file.
- Save your spectra as binary (*.sp) or ASCII (*.asc) files.

Send to WordPad or Word

Use the **Send To** command to copy the contents of the Viewing Area into an editable document.

1. Select the tab in the Viewing Area that contains the results or curves that you want to copy.
2. If the tab contains curves, format and label them until you are happy with their presentation.

   All your labels will be copied. If you copy into a Word document your labels are placed in text boxes.
3. Select **Send To** from the File menu, then **Word** or **WordPad**, and then select the document you require.

   The Microsoft® WordPad™ option copies into a rich text format (.rtf) file that you can edit using the WordPad accessory, which is a simple word processing program supplied with Windows.

   If Microsoft® Word™ is installed, the Word option copies into a native Word (.doc or .docx) file.

   The document sub-menu enables you to create a new document or to select any WordPad (.rtf) or Word (.doc or .docx) document that is open or minimized on your PC.

   Your results are copied into the selected document.
4. If you created a new document, open the minimized file.
5. Complete and publish your document.

Additional Information

Editable Objects Included in the Document

- When you send the Results Table tab or History tab, today's date is included in your document.
- When you send the Sample Table tab, today's date and the current time is included in your document.
- When you send a curve, the contents of the Results panel are included in your document.

Non-Editable Objects Included in the Document

By default, the Samples View includes the spectrum browser. When you send a graph display the contents of the spectrum browser are included in your document, which acts as a key to the graphic.

If you do not want this information to be included, hide the spectrum browser before sending:

1. Right-click in the Samples View, and then select Properties.

   The Graph Properties dialog is displayed.
2. Select the Advanced tab, select the **Hide Information Pane** option, and then click **OK**.

   The spectrum browser or Results pane is hidden.
3. Select **Send To** from the File menu, then **Word** or **WordPad**.

   Your results, but not the contents of the spectrum browser, are copied into the selected document.
4. Restore the Samples View by clearing the Hide Information Pane check box.

Send to Excel

Use the **Send To** command to copy the contents of the Viewing Area into an Excel workbook.

1. Select the tab in the Viewing Area that contains the results that you want to copy.
2. Select **Send To** from the File menu, then **Excel**, and then select the document you require.

   If Microsoft Excel is installed, the Excel option copies into a native Excel (.xls or .xlsx) file.

   The document sub-menu enables you to create a new workbook or to select any Excel workbook that is open or minimized on your PC.

   Your results are copied into new worksheets in the selected workbook. The number of worksheets created will depend on the tab currently displayed.
3. If you created a new worksheet, open the minimized file.
4. Complete and publish your file.

Additional Information

- When you send the Graph tab to Excel, the X and Y data of the spectrum or spectra are added to a new worksheet. Each worksheet is named after the spectrum.
- When you send the Results Table tab to Excel, the Results are added to a new worksheet named Results.
- When you send the Sample Table tab, the Sample Table is added to a new worksheet named Sample Table.
- When you send the Search tab, four worksheets are added to the workbook: Source Spectra Search Results, Search Hit List, and the X and Y data of the sample spectrum and the best hit spectrum. If your Search tab contains multiple source spectra, only the data for the row selected in Source Spectra Search Results will be sent.
- When you send the Compare tab, four worksheets are added to the workbook: Source Spectra Compare Results, List of Compared References, and the X and Y data of the sample spectrum and the best hit spectrum. If your Compare tab contains multiple source spectra, only the data for the row selected in Source Spectra Compare Results will be sent.
- When you send the History tab to Excel, four worksheets are added to the workbook: Sample, Instrument, History and Quality Checks, corresponding to the four sections of the History tab. If no Quality Checks were selected when the sample spectrum was collected, then the Quality Checks worksheet will not be created.

Send To Email

Before you use the Send To Email command, you will need to define the email settings on the Email tab.

Use the **Send To Email** command to copy the contents of the Viewing Area into an email.

1. Select the tab in the Viewing Area that contains the results or curves that you want to email.

   If the tab contains curves, format and label them until you are happy with their presentation.

   All your labels will be copied. If you copy into a Word document your labels are placed in text boxes.

2. Select **Send To** from the File menu, then **Email**.

   The Send Email dialog is displayed with your results added to the Attachments pane at the bottom of the dialog. The **Total Attachment Size** is shown in megabytes (MB). The **From** field is automatically populated with the User name entered on the Setup Email tab.

3. Enter the recipients email address in the **To** field.

4. If you want to remove any of the attached files, deselect the check box.

   The Total Attachment Size is updated.

5. If you wish to add any further attachments to the email, click **Add Attachments**, and then browse to the file(s) you would like to add.

   The Total Attachment Size is updated.

6. Complete your email message, and then click **Send**.

Additional Information

- If you selected the Samples View tab, you will receive an email with an rtf file attached that contains the spectra in a graph window, and the spectra attached as *.sp files.
- If you select the Graph view of an individual spectrum, the rtf file attached contains the spectrum in a graph window. The spectrum is also attached as an *.sp file.
- If you select the Results tab, the rtf file attached contains the date of the document and the content of the Results Table as a table. The spectra are also attached as *.sp files.
- If you select the History tab for the sample selected, the rtf file attached includes the date, the Sample data, Instrument Settings, and History. The spectrum is also attached as an *.sp file.
- If you select the Compare tab, the rtf file attached includes the user ID, the date of the document, the Compare results, the detail of the spectrum, and the graph display. The spectrum selected in the Compare Results is also attached as an *.sp file.
- If you select the Peak table tab, the rtf file attached includes the user ID, the date of the document, the peak table and the graph display with the peaks marked. The spectrum selected in the Results is also attached as an *.sp file.

Editable Objects Included in the Document

- When you send the Results Table tab or History tab, today's date is included in your document.

- When you send the Sample Table tab, today's date and the current time is included in your document.
- When you send a curve, the contents of the Results panel are included in your document.

Non-Editable Objects Included in the Document

By default, the Samples View includes the spectrum browser. When you send a graph display the contents of the spectrum browser are included in your document, which acts as a key to the graphic.

If you do not want this information to be included, hide the spectrum browser before sending:

1. Right-click in the Samples View, and then select **Properties**.

   The Graph Properties dialog is displayed.

2. Select the Advanced tab, select the **Hide Information Pane** option, and then click **OK**.

   The spectrum browser or Results pane is hidden.

3. Select **Send To** from the File menu, then **Email**.

   Your results, but not the contents of the spectrum browser, are copied into the selected document, which is added to the email.

4. Restore the Samples View by clearing the Hide Information Pane check box.

Print and Print Setup

Print

Use the **Print** command in the File menu to print a pre-formatted version of the contents of the Viewing Area.

This dialog also enables you to select a specific Printer and its Properties dialog.

Alternatively, if you want to print a graph display, right-click in the Graph tab and then select **Print**.

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

Print Preview

Use the **Print Preview** command in the File menu to review the printed output. The Print Preview dialog enables you to:

- Review a multi-page document.
- Amend the Page Setup, which includes the page Size, Orientation and Margins.
- Zoom in to a particular area of the document, and to use a Snapshot tool to select and copy a detail from the document to the Clipboard as a Windows metafile.

When you have finished reviewing the output, click **Print** from the File menu. This document is sent to your default printer using the current printer settings.

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

Exporting Reports

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

1. To generate a method report, select the **Method Setup** mode in navigation panel, select the method you are interested, then go to step 2.

   OR

   To generate an experiment report, select Previous Results mode in navigation panel, select the experiment you are interested, then go to step 2.

   OR

   To generate the report of a single spectrum, select the spectrum name in the **Data Explorer**, then go to step 2.

NOTE: *Check the appearance of the data that you will include in the report. Depending on the settings in the template you have selected, the appearance of the data in Spectrum FL may be duplicated in the report.*

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

   The Report dialog opens.

3. Select the **Reports Options** tab.
4. Select the **Save report** check box if you want to save the report(s).
5. Select **Show saved report** if you want the report(s) to be displayed when generated.
6. Select the **Print report** check box to print the report(s) to the currently active printer.
7. If necessary, click **Browse**, find the template file that you want to use to generate the report, and click **Open**.

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

   OR

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

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

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

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

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

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

   If you selected the Samples View in step 1, select the Include option next to the **Spectrum Name** if you want to generate an individual report for a spectrum. All the

spectra are selected by default. To select or deselect all the spectra, check or uncheck the **Select all single spectra reports** option.

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

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

    In Spectrum FL ES the report is saved in a secured and encrypted portable document format.

11. If necessary, browse to another (or create a new) folder for the generated report(s).

    By default, all reports are saved to C:\pefl_data\reports.

12. Select the sections to be included in the report from the **Section Name** list, which are derived from the template.

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

13. Click **Report**.

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

    The report is generated.

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

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

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

Additional Information for Spectrum FL ES

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

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

Setting up a Results File for Exporting

A file of accumulated results from each of the main spectral processing functions (Compare) can be collected by Spectrum FL for export as a *.csv file to another software application for further analysis.

1. Click the **Setup Results File** tab for the process whose results you want to record in an accumulated result file.

   There is a Setup Results File tab in each set of tabs displayed from the Setup menu or Navigation Pane.

2. Check the Create results file at this location checkbox.
3. If required, click **Browse** and select a different location for the result file.

   The file will be named automatically based on the process and, where applicable, the specific method being used to process the data.

4. Choose whether to **Overwrite** the data each time the process is run for a set of samples, or **Append** the new data to the existing data in the file.

Similar files can also be generated using the Setup Results File tab in Ready Checks and Instrument Verification. These collate the results for all the checks performed into a single file, except for Pharmacopoeia tests which are recorded separately.

Once the files have been created and contain some data, you can export them for further analysis.

Copying and Pasting

Use the Copy (CTRL+C) keyboard shortcut to place information on the Windows Clipboard, and the Paste (CTRL+V) keyboard shortcut to paste information from the Clipboard into another location.

The behavior of these keyboard shortcuts depends on the type of information that you are copying and pasting. If the keyboard shortcut is not enabled, you may be able to right-click and select a command.

NOTE: *If you have Microsoft® Word™, you can manage the clipboard using the Office Clipboard task pane. In Word 2003, select Office Clipboard from the Edit menu. In Word 2007, click the Clipboard dialog launcher in the Clipboard group on the Home tab.*

Samples View and Graph tab selected

To copy the graph display, including all labels and curves, whether selected or not:

- Right-click and then select **Copy to Clipboard**.

  The CTRL+C shortcut is not enabled.

NOTE: *The graph display is copied as a Windows metafile. You can paste spectra only into Windows applications that support metafiles*

Samples View and Results tab selected

To copy the Name and Description of the selected row:

- Right-click and then select **Copy**.

  ORadmin

  Press **CTRL+C**.
  A table containing the name and Description is copied.

Spectrum FL and [Sample Name] tab selected

To copy the graph display of a single spectrum, including all labels:

- Right-click and then select **Copy to Clipboard**.

  The CTRL+C shortcut is not enabled.

NOTE: *The graph display is copied as a Windows metafile. You can paste spectra only into Windows applications that support metafiles*

Spectrum FL and History tab selected

To copy the data from a panel:

1. Make sure that you have not selected a particular Setting or Value.

   If a Setting or Value is selected, the copy function is not enabled.

2. Right-click in a panel and then select **Copy**.

   OR

   Press CTRL+C.

   Each Settings and Value in the panel is copied as a paragraph with tab separators.

Sample Table selected

To copy a selected field as ASCII text, or the contents of a selected row as tab separated text:

- Right-click and then select **Copy**.

  OR

  Press CTRL+C.

NOTE: *You can use the Copy and Paste keyboard shortcuts and commands to help you complete a sample table with multiple rows for collecting spectra from a batch of samples. However, any duplicate Sample ID entries will be shaded pink and cannot be run. Make sure you have entered unique Sample ID entries before collecting data from your samples.*

Setup and Administration

Setup and Administration

These topics describe the range of Setup and Administration commands that enable you to:

- Administer the login names and passwords (if required) for each Spectrum FL user. To set up users, you must be logged into Spectrum FL as an Administrator.
- Administer the list of instruments available to Spectrum FL.
- Set up the connected Instrument.
- Set up instrument Ready Checks.
- Set up the custom Export of your spectra.
- Set up the email account that will be used for Send To Email.
- Set up how peaks in your spectra are detected and labeled.
- Setup the default graph View.
- Define, or edit, an Equation to perform calculations on one or more spectra, or on the data obtained from other processes.

Administration

Provided that you are logged into Spectrum FL Standard or Spectrum FL ES as an administrator, the Administration sub menu of the Setup menu enables you to:

- Setup a login name and password (if required) for each Spectrum FL user.

  Provided that you are logged into Spectrum FL ES as an administrator, the Administration sub-menu of the Setup menu also enables you to:

- Add new Groups and set the permissions for each group (except Administrators).
- Define the operations in the software that require a Signature from a pre-defined list.
- Administer the Users Audit Trail.
- Set a default workspace for a group.

Setting up Users, Groups, and Passwords

Each person using Spectrum must be set up as a user by a person who has permission to perform administration tasks.

➢ To set up users, select **Administration** from the Setup menu, and then click **Setup Users**.

The Users and Passwords Control dialog (Spectrum FL) or the Users, Groups, Signatures and Password Control dialog (Spectrum FL ES) is displayed.

NOTE: *When making any changes in the dialog, click Apply to accept the changes and keep the dialog open. Click OK to apply the changes and close the dialog.*

A user's access rights depend entirely on group memberships. Spectrum FL utilizes two pre-defined groups, namely the Administrators group and the Users group. You cannot use Spectrum FL to amend the access rights applied to these groups or to create new groups. The default Spectrum FL user named Administrator has membership of both the Administrators group and the Users group for Spectrum standard.

In Spectrum FL Enhanced Security (ES), the Administrators, Users, Reviewers and Approvers groups are predefined. The access rights applied to the Users, Reviewers and Approvers groups can be customized, and additional groups with particular access rights created. The access rights applied to the Administrators group cannot be customized.

The Administrators group exists for a range of PerkinElmer software applications. The Users group exists for the standard versions of a range of PerkinElmer software and for Spectrum FL ES.

A user defined for another standard PerkinElmer application will appear in the Users list for Spectrum FL, but that user must be enabled by a Spectrum FL administrator.

Default Users

The following user is pre-defined for Spectrum FL:

User	Password	Group Membership
Administrator	administrator	Administrators, Users

The following user is pre-defined for Spectrum FL ES:

User	Password	Group Membership
Administrator	administrator	Administrators

Default Groups

Spectrum FL Standard

The following groups are predefined for Spectrum FL. These groups cannot be deleted or other groups added.

Group	
Users	Members of the Users group cannot set up other users.
Administrators	Only members of the Administrators group have access to the Setup Users command.

Spectrum FL ES

The following groups are predefined for Spectrum FL ES. The Administrators group cannot be deleted. Other groups can be deleted or other groups added.

Group	
Administrators	Only members of the Administrators group have access to the Setup Users command. The permissions for the Administrators group cannot be changed.
Users	By default, members of the Users group can perform all functions in the software except those associated with Administrators and Return Workspace, Review and Approve. The permissions available are defined by the Administrator. Members of the Users group cannot set up other users.
Reviewers	Members of the Reviewers group are intended to act as reviewers of changes made by other users requiring an electronic signature. Members of the Reviewers group cannot set up other users.
Approvers	Members of the Approvers group are intended to act as approvers of changes made by other users requiring an electronic signature. Members of the Approvers group cannot set up other users.

Additional Information

The Administrators group applies across a range of PerkinElmer software applications.

Adding a New User to Spectrum FL

Use the Setup Users command to add a user to the list of users that are able to log in to Spectrum FL at this PC.

You cannot add a user unless you are logged into Spectrum FL as an administrator.

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users and Passwords Control dialog (Spectrum FL) or the Users, Groups, Signatures and Password Control dialog (Spectrum FL ES) is displayed.

2. Select the Password Control tab.

   If the **Login Type** is **Windows**, which is a global setting, click **Cancel**.

   Add new users using Windows User Management.

   Otherwise:

3. Select the Users tab and click **New**.

   The New User dialog is displayed.

4. Enter the **User name** and **Full name**.

5. If the **Login Type** is **PerkinElmer Login**, enter a user **Password**, and then enter this password again in the **Confirm password** field.

   The global properties of passwords, such as their minimum length, are defined on the Password Control tab. Passwords are case-sensitive, and can consist of letters, numbers and single spaces only.

6. By default, the **Status** of the user is **Enabled**, which allows the user to log in straightaway. If you want to enable the login later, select **Disabled**.

   When you enable a previously disabled user, you must enter a new password and confirm it.

7. If the **Login Type** is **PerkinElmer Login**, select whether the User must change their password at the next login.

NOTE: *In Spectrum FL ES User must change password at next login is mandatory.*

8. Click **OK**.

   The User name drop-down list is updated with the new user.

Adding and Deleting a Group (Spectrum FL Enhanced Security Only)

Use the Setup Users command to add a new group to those that users can be assigned to in Spectrum FL Enhanced Security at this PC.

NOTE: *It is not possible to create a new group within the Standard version of Spectrum FL.*

You cannot add a group unless you are logged into Spectrum FL as an administrator.

Administrators can assign permissions to the members of a group that control what they are able to do in a way that is tailored to your company's working practices. For example, you can set up permissions that allow members of a particular group to run a Compare process, but not to modify the Compare parameters, such as the Correlation value, or the spectra that are used as the Compare references.

If a group does not have permission to edit a group of options, those options will not be visible in the software. For example, if you do not have permission to run a Deconvolution Process, that option will not be displayed on the Process menu. If you do not have permission to perform any of the processes on the Process menu, then the menu will be hidden.

Adding a New Group

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users, Groups, Signatures and Passwords Control dialog is displayed.

2. Select the Groups tab and click **New**.

   The New Group dialog is displayed.

3. Enter the **Group name**.
4. Click **OK**.

   The new group is created.

5. Click **OK** to close the dialog, or select the Permissions and available Instruments for the group.

Deleting a Group

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users, Groups, Signatures and Passwords Control dialog is displayed.

2. Select the Groups tab.
3. Select the **Name** of the Group you want to delete from the drop-down list.
4. Click **Delete**.

   A confirmation dialog asks if you are sure that you want to delete the group.

5. Click **Yes**.

   The group is deleted.

NOTE: *Users that are not a member of a group are not able to access Spectrum FL. If you delete a group that has users assigned to it, check that all users are members of another group.*

Defining What Members of a Group Can Do

To define with what members of a group are able to do:

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users, Groups, Signatures and Passwords Control dialog is displayed.

2. Select the Groups tab.
3. Select the **Name** of the Group you want to modify from the drop-down list.
4. Click **Show Permissions** if the permissions are not displayed.

   The Permissions area shows the available permissions for the group.

   A tick indicates that the permission is selected for the group.

5. Select or deselect the **Permissions** for the members of the group.

   To select all the available permissions, select the **Permissions** option at the top of the list.

The following table lists the default permissions for the pre-defined groups in Spectrum FL:

Group	Default permissions
Administrators	The permissions of this group cannot be edited, and are not listed. Only members of the Administrators group are able to perform Administration tasks - setup users, groups and passwords.
Users	All tasks are enabled except Return Workspace, Review and Approve.
Reviewers	Review, Return Workspace, Import Sample Table Setups, Export Sample Table Setups, Import Instrument Setup, Export Instrument Setup, and Setup Equations only.
Approvers	Approve, Return Workspace, Import Sample Table Setups, Export Sample Table Setups, Import Instrument Setup, Export Instrument Setup, and Setup Equations only.

6. Select **Show Instruments**.
7. Select the instrument or instruments that you want the members of the group to be able to use.

   To select all the available instruments, check the **Instruments** option at the top of the list.

   NOTE: *When a new instrument is added to the Spectrum software, it will automatically be added to the instruments available for every group.*

8. Click **Apply** to apply the settings to the group and keep the dialog open, or **OK** to apply the settings and close the dialog.

Additional Information

An Administrator can define a default workspace (software settings, workspace layouts and objects such as equations, sample table setups, and instrument setups) for each group.

Assigning Users to, and Removing Users from, a Group

If you are an administrator, you can assign a Spectrum FL user to the Administrators group, the Users group, or both. You can assign a Spectrum FL Enhanced Security user to the default groups Administrators, Users, Approvers and Reviewers, or to any new groups created by an administrator.

To Assign a User to a Group

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users and Passwords Control dialog (Spectrum FL) or the Users, Groups, Signatures and Password Control dialog (Spectrum FL ES) is displayed.

2. Select the Users tab, and then the user's **Name** from the drop-down list.
3. Select the Group from the list of **Available groups for user** and then click **Add**.

   The Group is added to the **User is a member of list**, and removed from the **Available groups for user list**.

To Remove a User from a Group

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users and Passwords Control dialog (Spectrum FL) or the Users, Groups, Signatures and Password Control dialog (Spectrum FL ES) is displayed.

2. Select the User tab, then the user's **Name** from the drop-down list.
3. Select the Group from the list of **Available groups for user** and then click **Remove**.

   The Group is removed from the **User is a member of list**, and added to the **Available groups for user list**.

Enabling, Disabling, or Deleting a User

NOTE: *These procedures are not applicable when Login Type is set as Windows Login on the Password Control tab of the Users and Password Control dialog. In this case, add or delete users using Windows User Management.*

To Disable an Existing User

1. From the Setup menu, select **Administration** and then click **Setup Users** .

   The Users and Passwords Control dialog (Spectrum FL) or the Users, Groups, Signatures and Password Control dialog (Spectrum FL ES) is displayed.

2. Select the Users tab, select the user's **Name** from the drop-down list, and then click **Edit**.

   The Edit User dialog is displayed.

3. In the Status area, select **Disabled**, and then click **OK**.

   When this user attempts to login the error message 'Your user name has been locked or disabled. Please contact your system administrator' will be displayed.

NOTE: *To enable a previously disabled user, select Enabled on this dialog, and then enter a new Password and confirm it. The User must change password at next login selection is recommended.*

To Delete a User

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users and Passwords Control dialog (Spectrum) or the Users, Groups, Signatures and Password Control dialog (Spectrum FL ES) is displayed.

2. Select the Users tab, select the user's **Name** from the drop-down list, and then click **Delete**.

   A User Administration message will be displayed asking you to confirm that you wish to delete the user.

3. Click **Yes**.

   The user is deleted.

NOTE: *It is not possible to re-use a User name that has been deleted.*

NOTE: *It is not possible to delete the Administrator from the Administrators group.*

The workspace of a deleted user remains on the computer unless deleted manually using Windows Explorer. You may need to use the Windows Control Panel to select **Show hidden files and folders** before you are able to view the workspace files.

Signatures (Spectrum FL Enhanced Security Only)

Signatures are only available in Spectrum FL ES. An electronic signature as defined by 21 CFR Part 11 means a computer data compilation of any symbol or series of symbols executed, adopted, or authorized by an individual to be the legally binding equivalent of the individual's handwritten signature.

In Spectrum FL ES software, all operations that cause data to be collected, administer security or cause spectra and results data to be saved have an associated Signature Point that requires a signature. The list of Signature Points within the software is pre-defined, and includes:

- Loading and saving instrument settings files.
- Reporting on ready checks and instrument validation.
- Generating reports.
- Exporting data.
- Deleting graphs.
- Creating or making changes to equations.
- Approving and reviewing items that have been signed by other users.

When a Signature Point occurs in the software, a dialog will appear prompting you to enter your User name and Password, and then select a pre-defined Reason from the drop-down list, if required. In the Comments section you can add any additional information.

Members of the Administrators group are able to define whether a signature and comment is required for each Signature Point individually, or apply the same settings to all Signature Points. In addition, for each Signature Point they can define the list of Reasons.

NOTE: *If Signature required is not selected for a signature point, 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.*

For some signature points, a signature can be added on demand.

Defining the Settings for a Signature Point

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users, Groups, Signatures and Passwords Control dialog is displayed.

2. Select the Signatures tab.
3. Select the Signature Point **Name** from the drop-down list of available signature points.

   The following signature points are available in Spectrum:

Signature Point	Description
Approve	Occurs on demand. See Reviewing and Approving for more information.
Data	Occurs when data is added to the database, for example, when opening a spectrum that was collected on another system.
Data Export Collection	Occurs when data is exported immediately after data collection. See Setup Instrument - Data Collection.
Delete Graph	Occurs when a user deletes a spectrum or Samples View from the Data Explorer. The spectra are added to the Recycle Bin.
Equation	Occurs on demand, accessed via the Setup Equations tab. If you attempt to export an unsigned equation, you will be prompted for a signature first. If you import an equation, you will be prompted for a signature first. If you exit Spectrum and have unsigned Equations, the Equation will be signed for when you sign the workspace.
Instrument Validation	Occurs immediately after selecting to run a Instrument Validation.
Output	Signature is demanded just before the output of data. This is before saving, printing or exporting data, and includes saving a report using the **Report** command on the File menu.
Raman Instrument Setup	Occurs on demand, accessed via the Instrument Settings dialog, or when you exit Spectrum FL software. If you attempt to export an unsigned instrument setup, you will be prompted for a signature first. If you import an instrument setup, you will be prompted for a signature first. See Load and Save for more information.
Ready Check	Occurs immediately after selecting to run a Ready Check.
Return	Occurs on demand. See Reviewing and Approving for more information.
Review	Occurs on demand. See Reviewing and Approving for more information.
Sample Table Setup	Occurs on demand, or when you exit Spectrum software. If you attempt to export an unsigned sample table setup, you will be prompted for a signature first. If you import a sample table setup, you will be prompted for a signature first. See Sample Table Setups for more information.
Workspace	Occurs on demand, or when you exit Spectrum software. The signature applies to the whole workspace, and covers all currently unsigned activities logged for the user. See Signing for more information.

4. If a Signature is required for a Signature Point, select **Signature required**.
5. If you wish the user to be able to add comments, if required, select **Prompt for comments**.

   When the Signature Point dialog is displayed in the software, the user will be prompted to select a reason. The list of reasons is also defined on this tab.

6. To add a new reason, click **New** and enter the new Reason in the New Reason dialog.

   The reason is added to the list of reasons for the Signature Point.

   OR

   To delete a reason, select the Reason from the Reasons list and click **Delete**.

   You will be asked to confirm that you want to delete the reason. Click **Yes**.

   The Reason is deleted from the **Text** field. The changes are recorded in the Audit Trail.

   OR

   To edit a reason, select the Reason from the Reasons list, click **Edit** and modify the text in the Edit Reason dialog.

   The Edit Reason dialog closes and the updated reason appears in the **Text** field. The changes are recorded in the Audit Trail.

7. Repeat as many times as necessary to add reasons for the Signature Point.
8. When you have finished adding reasons for the Signature Point, reorder the reasons, if required.

   Items will appear in the Reason drop-down list in the order they are listed on the Signatures tab.

   a. Select the **Reason** that you wish to move the position of.
   b. Use the arrow keys on the right hand side of the list to move the **Reason** up or down as required.

9. Repeat steps 3 to 8 for each Signature Point **Name**.

Defining the Same Settings for all Signature Points

1. To define the same settings for all Signature Points, click **Update All**.

   The Update All Signature Points dialog is displayed.

2. In the Require Signature section, select either **All Points require a signature**, **No Points require a signature**, or **Do not change the current settings**.

   If **Do not change the current settings** is selected, no change will be made to the **Require Signature** settings.

3. In the Prompt for comments, select either **All Points require a prompt**, **No Points require a prompt**, or **Do not change the current settings**.

   If **Do not change the current settings** is selected, no change will be made to the **Prompt for Comments** settings.

4. Click **OK**.

   The Update All Signatures dialog closes and the Signature Points dialog is re-displayed.

Passwords

Passwords

During Login, users can be required to enter their **User name** and **Password**, or simply their User name. A password is not mandatory in Spectrum FL, but is mandatory in Spectrum FL ES.

1. From the Setup menu, select **Administration** and then click **Setup Users**.

The Users and Passwords Control dialog (Spectrum) or the Users, Groups, Signatures and Password Control dialog (Spectrum FL ES) is displayed.

2. Select the Password Control tab.
3. In the Login Type section, select:
    a. **PerkinElmer Login**, which requires the user to enter a User Name and Password.
    b. **No Passwords Login**, which requires the user to select their User Name from a drop-down list containing all Spectrum users (Spectrum FL Standard only).
    c. **Windows Login**, which requires that the PKIUsers group created during the installation of Spectrum has been populated by a Windows Administrator.

    See **Windows Login**.

NOTE: *The No Passwords Login setting alters the behavior of the Login dialog. When selected, the user can select their user name from a drop-down list. When de-selected, the user must enter their user name manually because, for security reasons, a drop-down list is not available.*

Changing or Setting a Password

NOTE: *This procedure is applicable only when Login Type is set as PerkinElmer Login on the Password Control tab of the Users and Password Control dialog. When Login Type is set as Windows Login, change passwords using Windows User Management.*

Changing your Password

You must change your password when prompted during login. This prompt occurs when an administrator mandates **User must change password at next login**, or when your password has expired.

You can also change your password during login, subject to the Minimum password age set for all users by an administrator.

1. At login, enter a valid **User name** and **Password**, and then click **Change Password**.

    The Change Password dialog opens.
2. Enter a **New password**, enter it again in the **Confirm password** field, and then click **OK**.
3. To complete the login, click **OK**.

NOTE: *You can always change your password when prompted during login. However, you cannot then change your password before the Minimum password age set by an administrator for all users has expired. In Spectrum FL, the Minimum password age: Allow changes after (days) is set to 1, so if you attempt to change your password, the following message is displayed: 'You have changed your password less than 1 days ago. You cannot change your password again.'*
To allow passwords to be changed within the first day, an administrator must set Minimum password age: Allow Changes Immediately.

To Set a new Password (Administrator only)

An administrator can set a new password for a user unable to login because their password is lost or forgotten:

1. From the Setup menu, select **Administration** and then click **Setup Users**.

The Users and Passwords Control dialog (Spectrum FL) or the Users, Groups, Signatures and Password Control dialog (Spectrum FL ES) is displayed.

2. On the Users tab, select the user from the **Name** drop-down list, then click **Edit**.

   The Edit User dialog is displayed.

3. Enter a new **Password** and then enter the password again in the **Confirm password** entry field.

NOTE: *Passwords are case sensitive, and can consist of letters, numbers and single spaces only.*

4. Select **Enabled** if you wish the user to be able to login straightaway, or **Disabled** if you wish to enable the login later.
5. If **Enabled** is selected, select whether the **User must change password at next login**.
6. Click **OK**.

   The new password is implemented.

Maximum and Minimum Password Age

NOTE: *These topics are only applicable when Login Type is set as PerkinElmer Login on the Password Control tab of the Users and Password Control dialog. When Login Type is set as Windows Login, administer passwords using Windows User Management.*

NOTE: *The settings on the Password Control tab apply to all users. It is not possible to define individual Password Controls for each user.*

Maximum Password Age

On the Password Control tab, Maximum password age defines the maximum number of days that users can retain the same password before they must change it. By default the password expires after 42 days. The minimum is 1 day and the maximum is 999 days.

The Maximum password age cannot be set less than or equal to the Minimum password age.

NOTE: *If you want to set the Maximum password age to 1 day the Minimum password age must be set to Allow changes immediately.*

If it is not necessary for users to change their password, select **Password never expires**.

Minimum Password Age

On the Password Control tab, Minimum password age defines the number of days that users must retain the same password before being allowed to change it. The default setting for **Allow changes after (days)** is 1. Setting Allow changes after (days) prevents users from changing their password several times in a short space of time in order to return to a previous password.

To allow users to change their password immediately, select **Allow changes immediately**.

The Minimum password age cannot be set greater than or equal to the Maximum password age. The minimum is 1 day and the maximum is 999 days.

NOTE: *If you want to set the Maximum password age to 1 day the Minimum password age must be set to Allow changes immediately.*

Password Length

NOTE: *These topics are only applicable when Login Type is set as PerkinElmer Login on the Password Control tab of the Users and Password Control dialog. When Login Type is set as Windows Login, administer passwords using Windows User Management.*

Minimum password length on the Password Control tab defines the minimum number of characters that must be used in the password. By default, the **At least (characters)** setting is 6. The minimum setting is 1 character, and the maximum is 16 characters.

Allow blank password (Spectrum FL only) means that users who have never logged in before (or who opted not to enter a password when they last changed their password) are not required to enter a password at login. In Spectrum FL ES, Allow blank password is not available as entering a password is mandatory.

NOTE: *If a blank password expires (the Maximum password age setting is not Password never expires), a second blank password cannot be used immediately unless the Password uniqueness setting is Do not keep a password History.*

Re-Using Passwords

NOTE: *These topics are only applicable when Login Type is set as PerkinElmer Login on the Password Control tab of the Users and Password Control dialog. When Login Type is set as Windows Login, administer passwords using Windows User Management.*

Password Uniqueness

Password uniqueness on the Password Control tab defines the number of new passwords that must be used before a previous password can be reused. For example, if the first password is 'spectrumid', and Number of passwords to remember is set to 24 (the default setting), a user must use 24 other passwords (in addition to their current password) before being able to use 'spectrumid' again.

The minimum **Number of passwords to remember** is 1 and the maximum is 24.

An additional Password uniqueness setting is Do not keep a password history, where no record of previous passwords is kept.

Password Records

By default, a record of previous passwords is made automatically.

Changes to passwords are logged. However the actual passwords are not visible; the word Hidden is displayed instead.

Select **Do not keep password history** (Spectrum FL only) if you do not wish to retain a record of the number of previous passwords.

Password Lockout

NOTE: *These topics are only applicable when Login Type is set as PerkinElmer Login on Password Control tab of the Users and Password Control dialog. When Login Type is set as Windows Login, administer passwords using Windows User Management.*

Limiting failed Login attempts using Lockout

This procedures enables you to lock out a user that persistently fails to log in correctly.

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users and Passwords Control dialog (Spectrum FL) or the Users, Groups, Signatures and Password Control dialog (Spectrum FL ES) is displayed.

2. Select the Password Control tab.

3. Click **Account Lockout**.

   The Account Lockout dialog is displayed.

4. Enter the **Number of failed logins allowed before lockout**.

   For example, if Number of failed logins allowed before lockout is set to 5 (the default value), the user is locked out on their fifth failed attempt until an administrator allows them access again (Permanent) or for a specified period of time (Duration).

   The minimum number of failed login attempts before a user is locked out is 1. The maximum number of allowed failed login attempts before a user is locked out is 10.

NOTE: *If Number of failed logins allowed before lockout is 1, then the user is locked out after their first incorrect login attempt. That is, an incorrect login attempt is not allowed; the user must login successfully at their first attempt or be locked out.*

5. Select the Lockout Duration as **Permanent, until administrator unlocks**, or **Duration (minutes)**. If you select Duration, enter the time (in minutes) for the lockout.

   Permanent means that the user will be unable to login again until an administrator has assigned a new password. Duration is grayed if Permanent is selected.

   Duration prevents the user being able to login again until the time specified has elapsed. If Duration is selected, the default is 60 minutes. The minimum Duration is 1 minute and the maximum Duration is 32767 minutes (22.75 days).

NOTE: *Details of failed login attempts are recorded in the Login History.*

Reinstating Locked Out Users

If Account Lockout is set to Permanent until Administrator unlocks and the user has failed to login correctly within the allowed number of attempts, an administrator must assign a new password before the user is able to login again.

If one or more users a has been locked out, when an administrator next logs in a list of Locked Out Users is displayed.

1. Highlight the name of the user that you wish to reinstate and then click **Edit**.

   The Edit User dialog is displayed.

NOTE: *If you click OK (rather than Edit) when the list of Locked Out Users is displayed, the list is closed. Any locked out users will remain locked out. The list will be re-displayed each time you log in until all locked out users have been assigned a new password.*

2. Enter a new Password and repeat it in the Confirm password field.

3. Click **OK**.

   The user is removed from the list of Locked Out Users.

4. Click **OK** to close the Locked Out Users dialog.

   The previously locked out user will now be able to log in using the new password.

   You can mandate a password change by selecting User must change password at next login.

NOTE: *In Spectrum FL ES User must change password at next login is mandatory.*

Users locked out for a specified duration can be unlocked by the administrator in the same manner.

Windows Login

It is possible for users to log in to Spectrum FL using their Windows User name and Password (instead of having a separate Spectrum FL User name and Password).

It is not possible to have some users that log in using their Windows User Name and Password while others use a separate Spectrum login.

NOTE: *Being logged in as a Windows administrator gives full read/write permissions to the system. To avoid negating the 21 CFR Part 11 compliance, end users (that is, individuals using Spectrum FL ES software and instruments to collect data), should run as Windows Users, never as Windows administrators.*

Adding Windows users to the PKIUsers group on a local PC:

To facilitate the use of Windows User names and Passwords, the PKIUsers group is created on the local PC during the installation of Spectrum FL. When Spectrum FL is installed and run on a local PC, the Windows administrator should add all the users who will access Spectrum to the PKIUsers group.

NOTE: *When Spectrum FL is used across a network, the Windows administrator should create a network group on an accessible domain and then add users to that group.*

1. Install Spectrum FL.
2. From the Windows Start menu navigate to **Control Panel.**
3. Select **Administrative Tools** and then **Computer Management**.

   The Computer Management dialog is displayed.

4. Select **Local Users and Groups.**
5. Select the **Groups** folder to see the list of available Groups on the PC, and then double-click **PKIUsers**.

   The PKIUsers Properties dialog is displayed. The Members list already contains Everyone. This group has been created for folder access only, not as a Windows user group as it contains no user members.

6. To add a user member to the Group, click **Add**.

   The Select Users, Computers, or Groups dialog is displayed.

7. To select a user from a different location (domain), click **Locations** and then select the required location for the user you wish to add.

8. To add a user to the group, enter the name of the user in the **Enter the object name to select** field and then click **Check Names**.

   Clicking Check Names will validate the name on the specified domain.

NOTE: *If you are not logged into this domain already, a login dialog will be displayed.*

9. Click **OK**.

   The Select Users, Computers, or Groups dialog is closed and the user is added as a member to the PKIUsers Properties dialog.

10. To add more users, repeat steps 6 to 9.

NOTE: *It is possible to add a user more than once if they are on more than one domain as each Location together with the User name and Password will be unique.*

All users added to the PKIUsers Group on the local PC, or added to a network users group, will be able to log in to Spectrum once a Spectrum administrator has defined the Login Type as Windows Login.

NOTE: *Any users added to the PKIUsers Group before logging into Spectrum FL for the first time will appear in the Name drop-down list on the Users tab of the Users and Passwords Control dialog. If users are added subsequently, click Update users on the Users tab to refresh the Name drop-down list.*

Defining the Spectrum FL Login Type as Windows Login

The Login Type (Windows Login, PerkinElmer Login or No Passwords Login) applies to all users. It is not possible to have some users that log in using their Windows Login while others use a separate Spectrum login.

1. Start Spectrum FL and log in as an administrator.
2. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users and Passwords Control dialog (Spectrum FL) or the Users, Groups, Signatures and Password Control dialog (Spectrum FL ES) is displayed.

3. Select the Password Control tab.
4. From the Login Type drop-down list select Windows Login.

   All the other information previously displayed on the tab is removed as the password controls are now from Windows rather than Spectrum FL.

   The Load Windows Users dialog is displayed.

5. Select the **Domain** and specify the **Group** of Windows users that you wish to add to the list of Spectrum FL users.

   The default selection is the PKIUsers group on the local PC.

6. Click **OK**.

   The Windows users will be loaded and you may be prompted to select a new Spectrum FL administrator.

NOTE: *If users are subsequently added to the PKIUsers group, to add these new Windows users to the list of Spectrum FL users a Spectrum FL administrator must click Update users on the User tab of the Users and Passwords Control dialog (Spectrum FL) or Users, Groups, Signatures and Passwords Control dialog (Spectrum FL ES).*

To assign users Spectrum FL group memberships, see Assigning a User to a Group.

If a user is not added to at least one group, an error message will be displayed when they try to log in informing them that they do not have access to the application.

Logging in to Spectrum FL using a Windows Login

If you have been set up to log in to Spectrum FL using your Windows login:

1. Start Spectrum FL.

   (Select Start, PerkinElmer Applications, Fluorescence).
2. Enter your Windows User name and Password.
3. If the Log on to field is not displayed, click **Options**.
4. Select the required Domain from the Log on to drop-down list.

   By default, the Domain last logged on to is displayed.

NOTE: *If all users are on the same Domain, there is no need to show the Log on to field as the correct Domain will be listed. To avoid confusion, this field can be hidden by clicking Options<<.*

Troubleshooting Windows Login

If you cannot login to Spectrum FL using your Windows Login, check that:

- Your Windows administrator has added your name to the PKIUsers Group.
- You have been assigned to at least one Group within Spectrum FL.
- You have entered the correct User Name and Password, and selected the correct Domain option from the Log on to drop-down list.
- PE21CFR is running. From the Start menu navigate to Control Panel, and then select Administrative Tools. Then select Services. In the Services dialog check that PE21CFR is still running. If this has been paused or stopped you will be unable to login to Spectrum.

Password expiry

If whilst logging into Spectrum FL you get a message that your password is about to expire, you can change your password. This change applies to Windows as well as Spectrum FL.

Removing a User from the PKIUsers group in Windows:

1. From the Windows Start menu navigate to **Control Panel.**
2. Select **Administrative Tools** and then **Computer Management**.

   The Computer Management dialog is displayed.
3. Double-click **Local Users and Groups**.
4. Double-click the **Groups** folder.

   The list of available Groups on the PC is displayed.

5. Double-click **PKIUsers**.

   The PKIUsers Properties dialog is displayed.

6. Select the appropriate user and then click **Remove**.

   The user is removed from the PKIUsers group.

Users Audit Trail (ES only)

Users Audit Trail (Spectrum Enhanced Security Only)

NOTE: *The Users Audit Trail is available in Spectrum ES only. It can be viewed by members of the Administrators group only.*

The Users Audit Trail records all changes to security settings in compliance with 21 CFR Part 11. All changes to users, groups and password settings are recorded. It also records when the Login History or Audit Trail have been exported and cleared.

1. Select **Users Audit Trail** from the Administration sub-menu of the Setup menu.

   The Login History, Audit Trail and Summary dialog is displayed.

2. Select the Audit Trail tab.

   The Audit Trail is displayed. For each change recorded, the following information is given in the Audit Trail:

   - **Function** – the item that was changed, for example, Add New User.
   - **Previous Value** – the state of the item before it was changed.
     Numbers refer to permissions or instruments; see Summary.
   - **Current Value** – the new state.
     Numbers refer to permissions or instruments; see Summary.
   - **Full Name** – the full name of the user who made the change.
   - **User Name** – the login user name of the user who made the change.
   - **Computer** – the name of the computer from which the change was made.
   - **Date Modified** – the date and time of the change.

Printing the Audit Trail

➢ To print the Audit Trail click **Print**.
All the information currently held in the Audit Trail is printed to the default printer.

Exporting the Audit Trail

1. To export the Audit Trail click **Export**.

   A Save As dialog is displayed.

2. Select the required destination and enter a filename.

   The Audit Trail is exported as a *.csv file that can be opened, for example, in Microsoft Excel.

Exporting the Audit Trail does not clear the Audit Trail entries from the dialog. However, you must export Audit Trail entries before they can be cleared.

Clearing the Audit Trail

➢ To clear the Audit Trail click **Clear Audit**.
You will be asked to confirm that you want to delete the Audit Trail log. All details are removed.

NOTE: *It is only possible to clear Audit Trail entries that have previously been exported. If the Audit Trail contains additional entries since it was last exported, only those entries that have been exported will be deleted. If none of the entries have been exported, a warning message will be displayed when you attempt to clear the Audit Trail.*

Additional Information

The Users Audit Trail is saved to the Security database, Users.mdb.

Login History (Spectrum FL Enhanced Security Only)

NOTE: *The Users Audit Trail is available in Spectrum FL ES only. It can be viewed by members of the Administrators group only.*

1. Select **Users Audit Trail** from the Administration sub-menu of the Setup menu.

   The Login History, Audit Trail and Summary dialog is displayed.

2. Select the Login History tab.

   The login history is displayed. This details every login attempt, since the history was last cleared, by:

   - **Full Name** – the full name of the user, or **Not Found** if the User Name entered did not exist.
   - **User Name** – the user name entered, whether correct or not.
   - **Computer** – the name of the computer
   - **Status – OK** indicates that the user logged in with the correct password; **Failed** indicates that a login was attempted with an incorrect password or User Name.
   - **Logged In** – date and time.
   - **Logged Out** – date and time.

Printing the Login History

➢ To print the Login History click **Print**.

All the information currently held in the Login History is printed to the default printer.

Exporting the Login History

1. To export the Login History click **Export**.

   A Save As dialog is displayed.

2. Select the required destination and enter a filename.

   The Login History is exported as a *.csv file and can be opened, for example, in Microsoft Excel.

NOTE: *Exporting the Login History does not clear the Login History details from the dialog. However, you must export Login History entries before they can be cleared. See* ***Clearing the Login History****.*

Clearing the Login History

- To clear the Login History, click **Clear History**.

  You will be asked to confirm that you want to delete the Login History log. All Login details are removed. The first Login details to appear after the Login has been cleared will be the date and time that you log out.

NOTE: *It is only possible to clear Login History entries that have previously been exported. If the Login History contains additional entries since it was last exported, only those entries that have been exported will be deleted. If none of the entries have been exported, a warning message will be displayed when you attempt to clear the Login History.*

The only limit to the size of the Login History is disk space, but we recommend that you review and archive it at regular intervals.

Summary (Spectrum FL Enhanced Security Only)

NOTE: *The Users Audit Trail is available in Spectrum FL ES only. It can be viewed by members of the Administrators group only.*

The document created by this command records a summary of the security status of the application.

1. Select **Setup Users Audit Trail** from the Administration sub-menu of the Setup menu.

   The Login History, Audit Trail and Summary dialog is displayed.

2. Select the Summary tab.

   The Summary records all information about the security settings:

   - **Application** – records the application for which this Summary applies.
   - **Password control** – records the Login type, Windows group, Maximum password age, Minimum password age, Minimum password length, Password uniqueness, Lockout count and Lockout duration settings.
   - **Permissions** – records the number of permissions, then lists each permission with a number that is used to identify the permission on the Users Audit Trail.
   - **Instruments** – records the number of instruments attached to the application. Each instrument is then listed with a number that is used to identify the instrument on the Users Audit Trail.
   - **Users** – records the number of users. It then records each User name, Full name, Status, Last Login, the Groups the user belongs to, the Permissions of that group and the Instruments the user has permission to use.
   - **Groups** – records the number of groups. For each Group it records the Group Name, the Users in the Group, the Permissions of that group and the Instruments the group has permission to use.

Printing the Summary

- To print the Summary click **Print**.

  All the information is printed.

Exporting the Summary

1. To export the Summary click **Export**.

   A Save As dialog is displayed.
2. Select the required destination and enter a filename.
3. Select to save the Summary as a *csv or as a *.txt file.
4. Click **Save**.

   The summary is exported as a *.csv file or *.txt file that can be opened, for example, in Microsoft Excel.

Assigning a New Group Workspace (Spectrum FL Enhanced Security Only)

A new workspace is created each time a user logs in to Spectrum FL (unless the user previously selected to reload their last workspace). By default, the new workspace is based on the software default workspace. However, members of the Administrators group in Spectrum FL can assign their current workspace as the default for a group.

Features that can be assigned to a group workspace include:

- Custom toolbars, reflecting the tasks frequently performed by a group of users
- Instrument Setups
- Sample Table Setups
- Equations
- Software settings, such as Instrument settings.

No spectra or data will be included in the default workspace.

Assigning the current workspace to existing groups

Before the workspace can be assigned as the default for a group, a user with the appropriate permissions should define the workspace, including toolbar layouts, Instrument Setups, Sample Table Setups, and Equations.

To set the current workspace as the default for a group:

1. Log in to Spectrum as an administrator.
2. Set up the workspace you want to assign to a group or groups.

   Refer to **Loading a Workspace** to load an existing workspace.
3. From the Setup menu, select **Administration** and then **Set Group Workspace**.

   The Set Group Default Workspace dialog is displayed. The dialog lists all the groups in Spectrum.
4. Select the **Include** check box for the group(s) you want to assign the workspace to.
5. Click **OK**.

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.

6. To sign the workspace, click **Sign**.

   The Sign 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 Workspace signature point.*

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

    The current workspace is saved as the new default workspace for the group(s) selected. The next time a new workspace is created on login by a member of that group, the new default will be used, unless that user is a member of more than one group. It will also be used if **Restore Default Workspace** is selected.

    If a user is a member of more than one group and one or more of those workspaces is modified, then the Choose Group Default Workspace dialog will prompt the user to select which group default to use to create a new workspace. This may be displayed when the user exits Spectrum and selects **Don't load spectra next time,** or when the user logs in to Spectrum.

Additional Information

User-defined objects

When a new group workspace is loaded, any user-defined objects such as Equations, Sample Table Setups and Instrument Setups are removed and replaced by the objects in the group workspace.

Common (Global) objects

When a new group workspace is loaded, any objects such as Equations, Sample Table Setups and Instrument Setups in the group workspace are loaded. Any objects in the appropriate common directory (defined during Spectrum installation) are also loaded. If any objects in the common directory have the same file name as an object in the workspace, then they are automatically renamed.

Instruments

The Instruments sub menu of the Setup menu enables you to:

- Select an instrument from the list of available instruments, or Work Offline.
- Auto-Connect to a particular instrument.

Provided you are logged into Spectrum FL as an administrator, you can also:

- Add an instrument to the list of instruments available to Spectrum FL.
- Remove an instrument from the list of available instruments.

Add Instrument

Use the Add Instrument command to install an instrument and make it available to Spectrum FL.

You cannot add or remove an instrument unless you are logged into Spectrum FL as an administrator.

To add an instrument:

1. Select **Instruments** from the **Setup** menu, and then click **Add Instrument**.

   The Add Instrument dialog is displayed.
2. Insert the Configuration Files CD that was shipped with the instrument.
3. Select the **Port Number** from the drop-down list or click **Use Default Port**.
4. Select the **Configuration File** by clicking the **Select** button.

   The Browse For Folder dialog appears.
5. Browse to the appropriate disk drive, highlight the configuration file and then click **Open**.
6. Click **OK**.

Remove Instrument

Use the Remove Instrument command to delete an instrument from the list of instruments available to Spectrum FL and to any other applicable PerkinElmer applications installed on this PC.

You cannot add or remove an instrument unless you are logged into Spectrum FL as an administrator.

1. Select **Instruments** from the Setup menu, and then click **Remove Instrument**.

   The Remove Instrument dialog is displayed.
2. Select the name of the instrument you want to remove from the drop-down list.
3. Click **OK**.

   A warning page is displayed. An additional warning is displayed if you select the instrument that is currently connected.
4. If you are certain that you want to delete this instrument from your system, click **Remove**.

   The instrument name is deleted from the list of instruments available.

   OR

   Click **Cancel** to exit close the Remove Instrument dialog.

Additional Information

It is not necessary to remove an instrument to select another instrument, or to disconnect the current instrument and work offline; use the Select Instrument command.

Select Instrument

Use the Select Instrument command to connect to an instrument if you are working offline, to free the current instrument and connect to another instrument, or to free the current instrument and work offline.

1. Select **Instruments** from the Setup menu, and then click **Select Instrument**.

   The Select Instrument dialog is displayed.

2. Select the name of the instrument you want to connect to from the drop-down list, and click **Connect**.

   If the instrument is not available (disconnected, or in use by another user) a warning is displayed.

   OR

   Click **work offline**.

Additional Information

Always connect to this instrument

This option enables you to select this instrument connection as your Spectrum FL log in default. When selected, the Auto-Connect option in the Setup menu is enabled.

Managing the List of Available Instruments

If the instrument you want to connect to is not in the drop-down list of available instruments; see Add Instrument.

If the drop-down list of available instruments contains superfluous instrument connections; see Remove Instrument. If you have other PerkinElmer software installed on your PC, remember that the instrument connection is removed from your system, not just the Spectrum FL software.

Auto-Connect

Use the auto-connect option to connect to a particular instrument automatically during log in, and skip the instrument connection dialog.

There are several ways to enable auto-connection to the instrument that is currently connected:

- Select the **Always connect to this instrument** check box in the Instrument Connection dialog during log in.

  This dialog will not be displayed if auto-connect is already enabled.

  OR

  Select the **Always connect to this instrument** check box in the Select Instrument dialog.

  OR

  Select the **Enable Auto-Connect** command from the Instruments sub menu of the Setup menu.

  When enabled, the auto-connect icon to the left of the command is highlighted in orange.

Export and Email

Setup Export and Email

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

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

   OR

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

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

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

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

Setup Export

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

1. Select **Preferences** from **Options** menu in the Navigation Pane.
   The **Export** and **Email** tabs are displayed in the left column.
2. Select the **Export** tab.

Header Options

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

File Options

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

Data Options

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

Additional Information

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

Setup Email

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

1. Select **Preference** from **Options** menu in the Navigation Pane.
   The **Export** and **Email** tabs are displayed in the left column.
2. Select the **Email** tab.

Server Information

1. Enter the **Outgoing mail server (SMTP)**.

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

   Simple mail transfer protocol (SMTP) is the standard for sending email messages across networks.

2. Select **Use Default Credentials**.

   OR

   Select **Enable SSL**.

   Choose this option if your mail administrator tells you to use a Secure Sockets Layer (SSL) connection.

3. Select either **HTML Body** or **Plain Text** for the mail output format.

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

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

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

User Information

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

Test Settings

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

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

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

Additional Information

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

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

Setup Peak Detection

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

➢ Select **Peak Detection**  in the **Data Analysis** section of the Navigation Pane. The **Setup Peak Detection** tab is displayed in the Dialog Pane.

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

Algorithm

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

Thresholds

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

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

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

Labeling

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

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

Refresh

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

View

Setup View

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

1. Select **View**  from the **Options** menu in the Navigation Pane.

   The Setup View tabs are displayed on the left.

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

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

Additional Information

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

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

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

Setup View Axes

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

1. Select **View**  from the **Options** menu in the Navigation Pane.

   The Setup View tabs are displayed in the Dialog Pane.

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

2. Select the **View Axes** tab.

X Axis

By default, the X axis is autoranged to the largest value and the smallest value in all the curves present. This panel allows you to enter a range of your choice.

Y Axis

By default, the Y axis is autoranged to the largest value and the smallest value in all the curves present. This panel allows you to enter a range of your choice. If you change the **Units** (**Auto**, **%T** or **A**), make sure that you select appropriate range values.

Display Mode

Select whether the graph display mode should **Overlay** curves (where the curves are displayed on

a common set of axes) or **Split** curves (where the curves are displayed on a common X, but separate Y, axes).

Setup View Appearance

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

1. Select **View**  from the **Options** menu in the Navigation Pane.

   OR

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

   The Setup View tabs are displayed in the Dialog Pane.

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

2. Select the **Setup View Appearance** tab.

Enable Gridlines

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

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

Text and Lines

Select the element, such as the Title or Background, of the graph display whose color you want to change, and then click **Color** to open the Color dialog. Select a **Basic** color, or one of the **Custom** colors you may have defined, and then click **OK**.

When you select a text element, the **Size** selector enables you to select a font size from the drop-down list.

Graph Color Palette

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

Setup View Advanced

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

1. Select **View**  from the **Options** menu in the Navigation Pane.

   The View tabs are displayed to the left.

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

2. Select the **View Advanced** tab.

Display Option

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

Curve Tool Tip Display

Deselect one or more of these check boxes to suppress elements in the tooltip that appears when the mouse pointer is near a curve or data point.

Data Points

Select whether to display data points in the curve, and if so, how they should be marked.

Line

Select the **Interpolation** algorithm (**Cubic**, **Linear**, or **None**) applied to the curve joining the data points.

Select a new **Size**, in pixels, from the drop-down list to amend the curve thickness, perhaps prior to copying the graph display to the clipboard or to emphasize a particular curve.

The **Style** options enable you to display the curve using a solid, dashed, or dotted line.

Setup Equations

Equations are process commands that perform calculations on one or more spectra, or on the data obtained from other processes.

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

➢ Select **Equations** from the **Process** menu.

OR

Select  in the **Setup** section of the Data Analysis - Navigation Pane.

The Setup Equations tab is displayed in the Dialog Pane.

Each of the equations you set up is appended to the Equations sub-menu in the Process menu, to the Equations drop-down list on the Process bar and to the Equations section of the Navigation pane.

NOTE: *The equations in the Common Equations Directory will be visible to all users. The Common Equations Directory is defined at Spectrum installation. The default is C:|pefl_data|equations*

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

Adding or Modifying an Equation

1. If you want set up a new Equation, and create a new row in the list of equations, click **Add**.

   OR

   Select a field in the row describing the equation you want to amend, and then click **Settings**.

   The Equations section of the Navigation pane opens with the Equation displayed in the Dialog pane.

2. Set up the Equation as described in Navigation Pane - Equations.

   The Equations Pane stays open so that you can continue with Result Formatting or select another Equation in the Equations pane. If you wish to return to the Setup Equations tab click **Back**.

   Your Equation is available in the Equations sub-menu in the Process menu.

Removing Equations

➢ Select the row containing the Equation that you want to remove, and then click **Remove**.
The Equation is removed from the table, the Equations sub-menu in the Process menu, and from the list in the Equations section of the Navigation pane.

You can select multiple rows. You will be prompted for confirmation for each Equation selected.

Importing Equations

To import an Equation:

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

   In Spectrum FL ES, if you attempt to import an unsigned Equation you may be prompted for a **Signature**.

   The Equation is added to the list of Equations on the Setup Equations tab.

Exporting Equations

To export an equation:

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

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

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

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

Running an Equation

- Display and select the spectrum or spectra that you want to process, select the Equation you want to apply and then click **Run**.

  The Results Table tab is updated. If the result amends the source spectrum, the processed spectrum is displayed in the Viewing Area and added to the Samples View.

  Processed spectra are not saved to disk automatically.

Signing, Reviewing or Approving an Equation (Spectrum FL ES only)

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

To Sign an Equation:

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

   The Sign Equation dialog is displayed. This contains the Audit Trail entries for that Equation, and any signatures added previously.
2. To sign the Equation, click **Sign**.

   The Sign dialog is displayed.
3. Enter your **User name** and **Password**.
4. Select the appropriate pre-defined **Reason** from the drop-down list, if applicable.

NOTE:	*A reason will required if the Administrator has defined Reasons on the Signatures tab for the Equation signature point.*

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

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

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

To Review or Approve an Equation:

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

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

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

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

   The Review or Approve dialog is displayed.

3. Enter your **User name** and **Password**.
4. Select the appropriate pre-defined **Reason** from the drop-down list, if applicable.

NOTE: *A reason will required if an administrator has defined Reasons on the Signatures tab for the Review or Approve signature points.*

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

   The Review Equation or Approve Equation entry is added to the Equation Audit Trail.

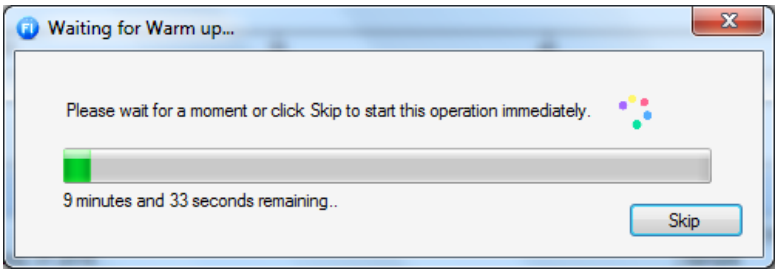
The Equation can now be exported for review or approval by another user, if it has not been approved, or to be added to a group default workspace by an administrator.

Global Setting

There are two settings on the Global Setting screen:

- Turn on/off warm up waiting time.

  There is 10 min. warm-up waiting time warning for the FL 8500 after connecting instrument. If it is unselected, no warm up waiting time **warning message** pops up.



- Enable auto logout (enter the number of minutes).

  The **Enable auto logout** option only available for ES version. When you select this option, the current user will be logged out automatically when there was no GUI interaction in specified period. When a user was auto logged out, the log in dialog will be shown in the screen to allow the latest user or administrator login back.

Audit Trail (ES only)

Audit Trail (Spectrum FL Enhanced Security only)

All data, settings and actions carried out by a user in Spectrum FL 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 user data. A new workspace, with a unique Workspace ID, is created each time a user starts Spectrum FL ES (unless the user selects to reload their current workspace next time, when they exit the software).

A Spectrum FL 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 FL. 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 FL 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 FL 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 FL 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 FL, which enables you to carry on with your work from where you left off when you next login to Spectrum FL at this PC.

   OR

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

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

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 FL 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 FL 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 FL ES Audit Trail is saved to the database FLMethodDB.mdf and FLResultDB.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 FL ES database(s) is:

- Windows 7/8/10 – C:\ProgramData\PerkinElmer\Fluorescence\xxxx.mdf

You can also configure Spectrum FL 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 FL 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, 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, 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 to 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, or a member of the Administrators group, 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 or by an Administrator. 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 FL 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, 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 FL 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 FL 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 FL.

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, such as 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.

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 Spectrum FL 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.

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 the **Sample Table** tab from the Method Setup 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, 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 FL 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.

1. Select the Preview option and then select **Run** from the Action menu, or click  .

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.

NOTE: *Clicking Run at any point runs the next unmeasured row in the Sample Table. You cannot highlight a row and run it from the Sample Table. If you want to run a specific sample, move the appropriate row to the top of the unmeasured samples in the table and click Run.*

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 FL 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 FL 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 in the column.

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

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.

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:\pefl_data\SampleTableSetups*

In Spectrum FL 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 FL 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

- 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.

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.

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 FL workspace.

  The Options section includes shortcuts to key items.

  The Equations section in Data Analysis 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 FL workspace.

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

Additional Information

Opening and Closing Panes

- To open or close the Dialog Pane, click the button at the center of the top 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 left 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.

Equations

Data Analysis - Navigation Pane - Equations

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

- Click Data Analysis in the Navigation pane then click **Equations** 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.

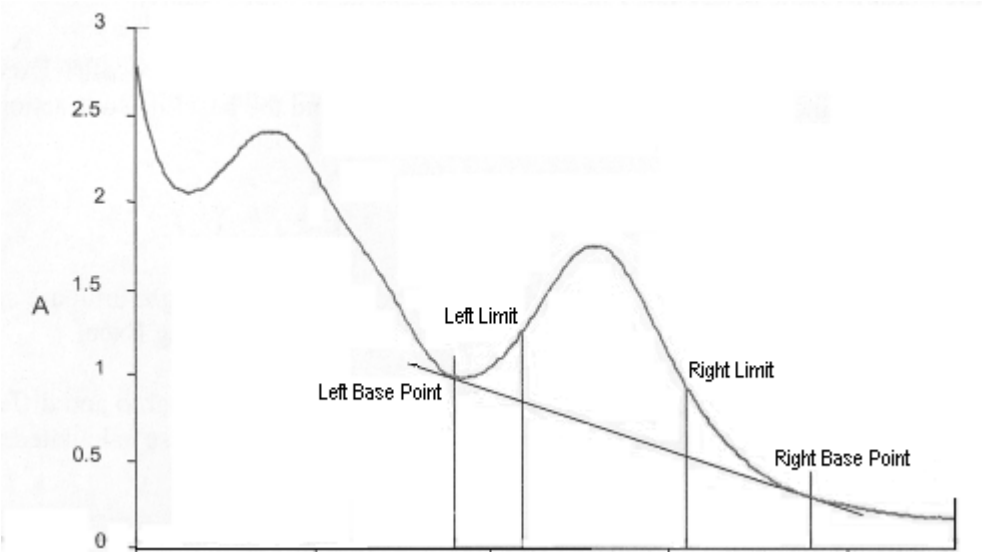
   Select whether to do nothing, or to label and/or highlight the result, as before.

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)]"**



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]"**.

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.

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]"**.

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]"**.

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]"**.

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)]**".

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.

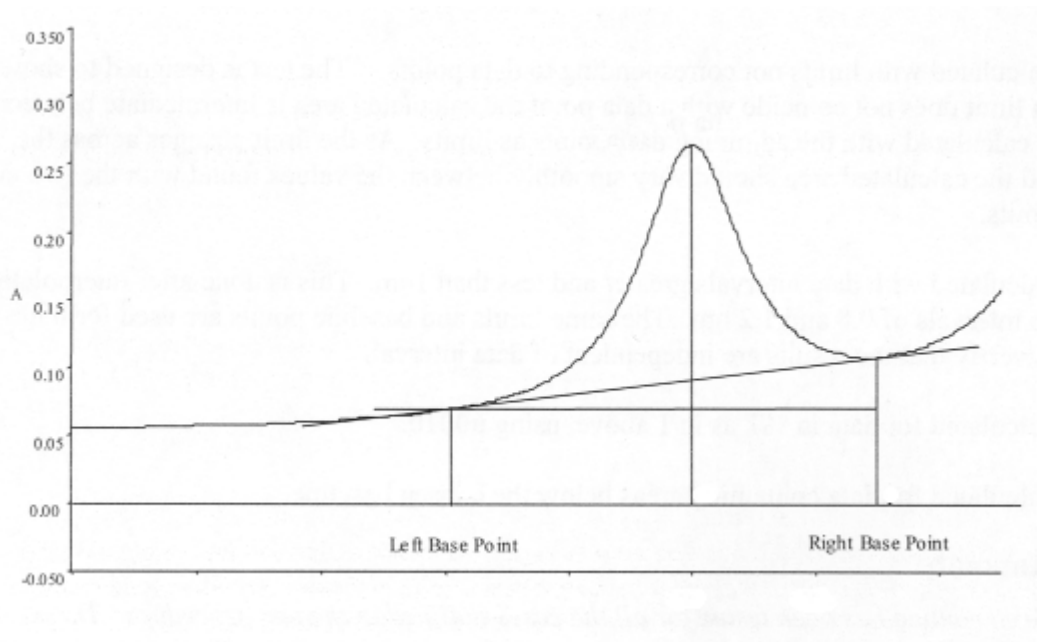
For example: **Height[All, Start[All]]** returns the height at the first wavelength in the list without pre-setting that value.

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]"**.

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)]"**.

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.

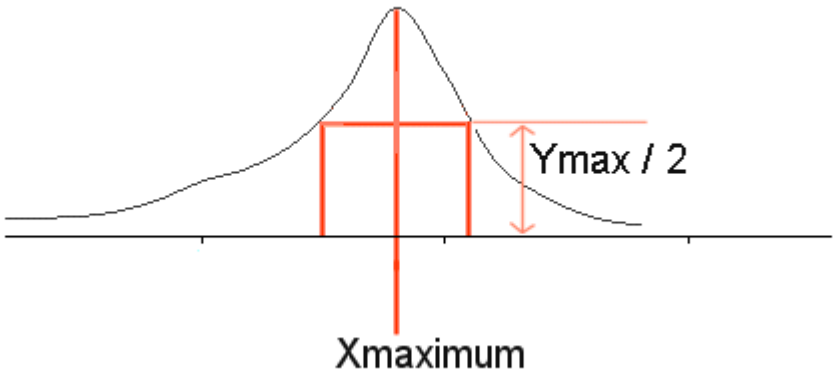
If when setting up the function, you enter 0 instead of interpolation in the syntax statement, the function returns the abscissa value of the nearest data point.

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)]**"

Width at half height

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



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 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 FL 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 FL 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.

Menus

The Data Analysis Menu Bar

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

- File
- View
- Process
- Setup
- Audit Trail (ES)
- Navigation
- Help

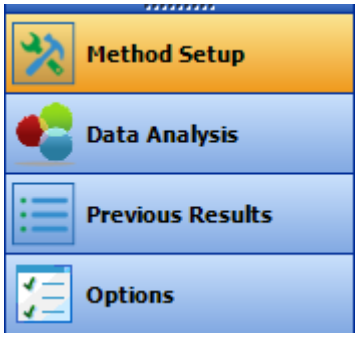
Additional Information

The Menu Bar cannot be turned off, floated or customized. It is placed at the top of the Spectrum FL workspace.

NOTE: *If you have Spectrum FL 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.*

Navigation Menu

These are the commands available on the Navigation menu.

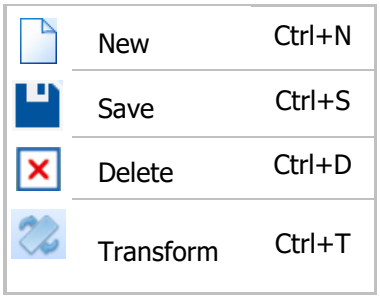


Additional Information

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.

Method Setup Method Menu

These are the commands available in the Method Setup Method 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**.

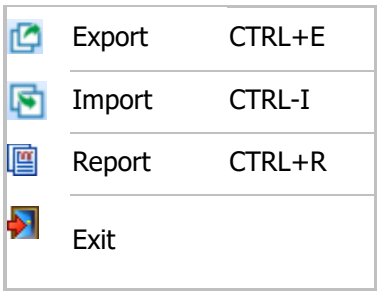
For more information about printing your results, see **Publishing Results**.

Send to Word, Send to WordPad and Send to Excel will only be available if you have the relevant software installed on your computer.

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

Method Setup File Menu

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



Additional information

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

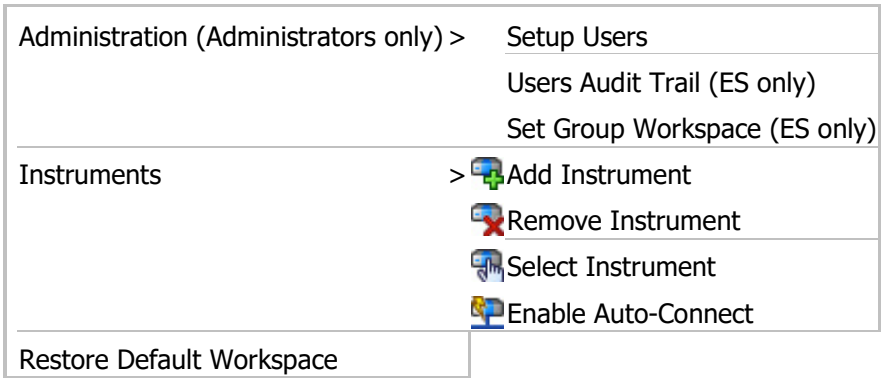
For more information about printing your results, see **Publishing Results**.

Send to Word, Send to WordPad and Send to Excel will only be available if you have the relevant software installed on your computer.

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

Setup Menu

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

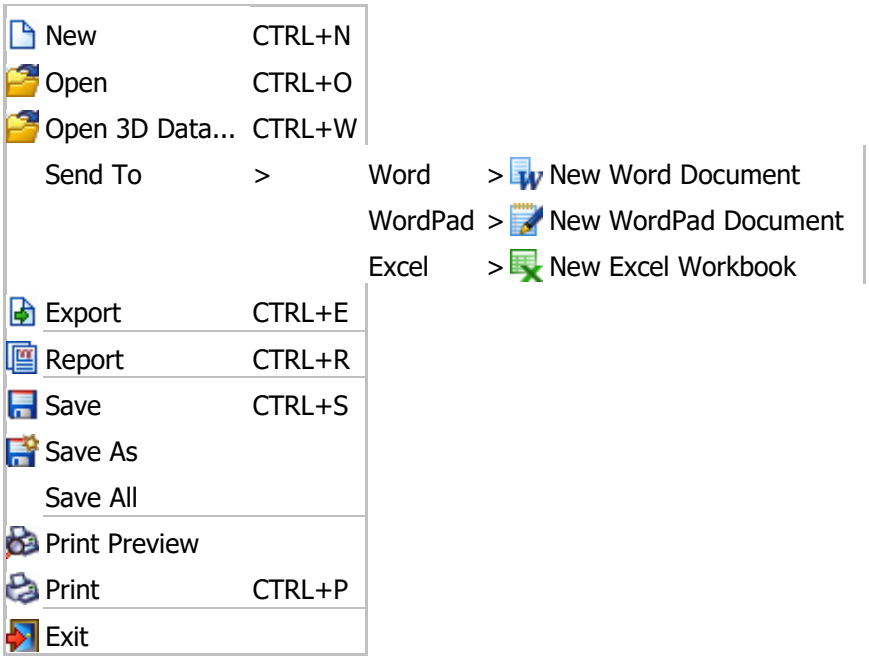


Additional Information

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

Data Analysis File Menu

These are the commands available in the Data Analysis 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**.

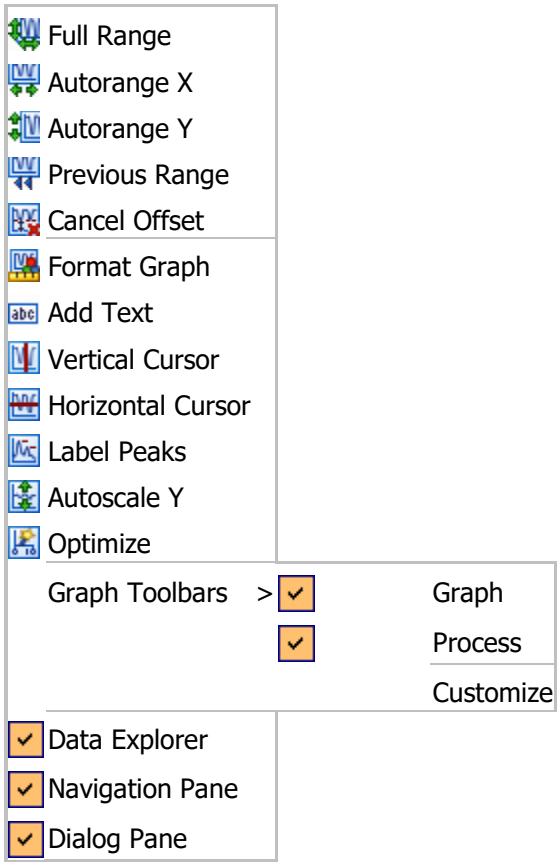
For more information about printing your results, see **Publishing Results**.

Send to Word, Send to WordPad and Send to Excel will only be available if you have the relevant software installed on your computer.

NOTE: *If you have Spectrum FL 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 Data Analysis View menu.



Additional Information

To view the Instrument Settings or Action 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.

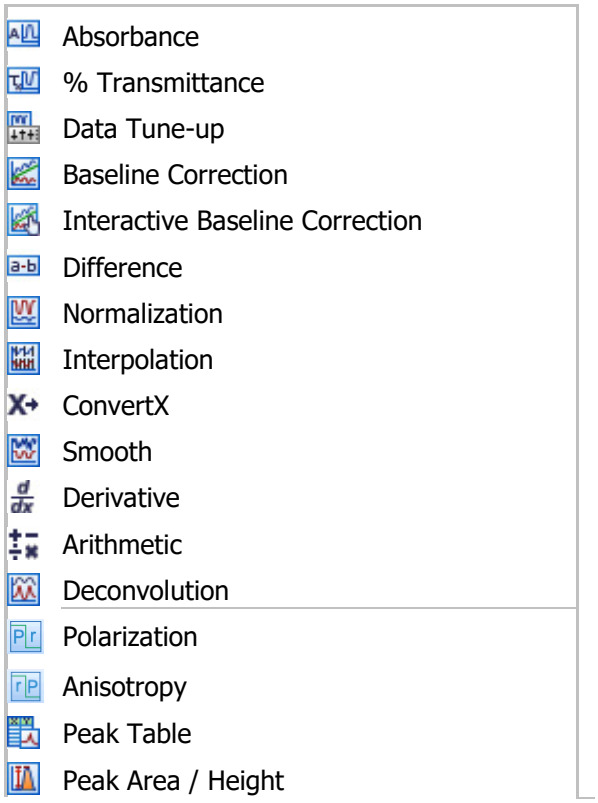
- Click the icon to the left of the name of the toolbar that you want to hide

  OR

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

Process Menu

These are the commands available in the Process menu.



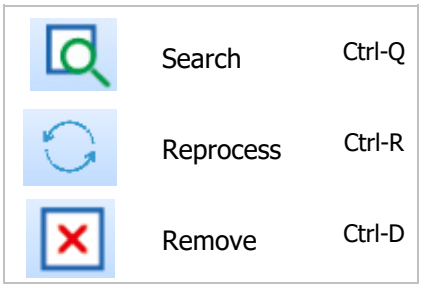
Additional Information

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

NOTE: *If you have Spectrum FL 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.*

Results Menu

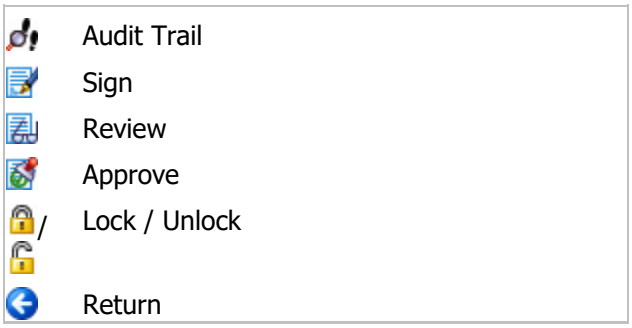
Use the actions in the Results menu to search, reprocess, or remove Previous Results displayed in the table.



Audit Trail Menu *(Spectrum FL Enhanced Security Only)*

The Audit Trail menu is only available in Spectrum FL 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.



Help Menu

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

Toolbars

The Spectrum FL workspace can include a number of global toolbars:

- The Scan toolbars, namely the Instrument Settings bar, the Action 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:

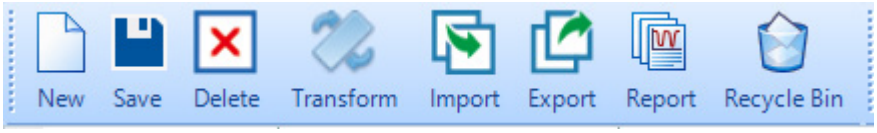
- The Graph bar. By default, this toolbar is located at the top of the Viewing Area.
- The Process bar. By default, this toolbar is located at the top of the Viewing Area.

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 Method Setup File Bar

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



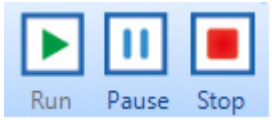
Additional Information

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.

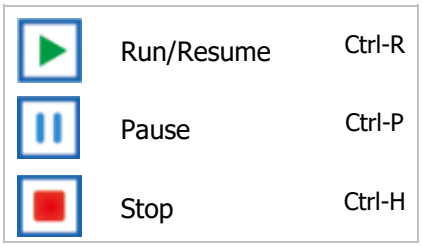
The Action Bar

Use the buttons in the Action bar, or from the Action menu, together with the messages given in the Prompts Display, to control your instrument.

Action Bar



Action Menu

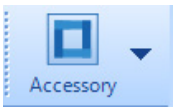


Additional Information

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 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.

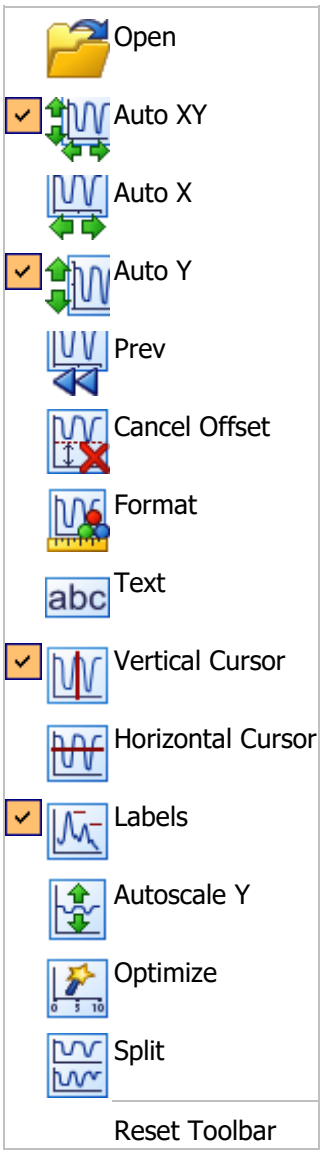


The following Accessories are available.

- Single Cell Holder
- Water Jacketed Single Cell Holder
- Water Jacketed Single Cell Holder w/ Stirrer
- Solid Sample holder
- Variable Angle Solid Sample Holder
- Micro Cell Holder
- Water Jacketed Micro Cell Holder w/ Stirrer
- Integrating Sphere
- Absorbance Module
- UV/Vis Automated Polarizer
- Rapid Mixing Accessory
- Fiber Optic Probe
- Vis Automated Polarizer
- Manual Polarizer Holder
- Microplate reader
- 4-Position Multi-Cell Holder
- Water Jacketed 4-Position Multi-Cell Holder
- Water Jacketed 4-Position Multi-Cell Holder w/ Stirrer
- Fast Filter
- Single Cell Peltier Holder
- 4-Position Multi-Cell Peltier Holder
- Auto Sipper
- S10 Autosampler

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.

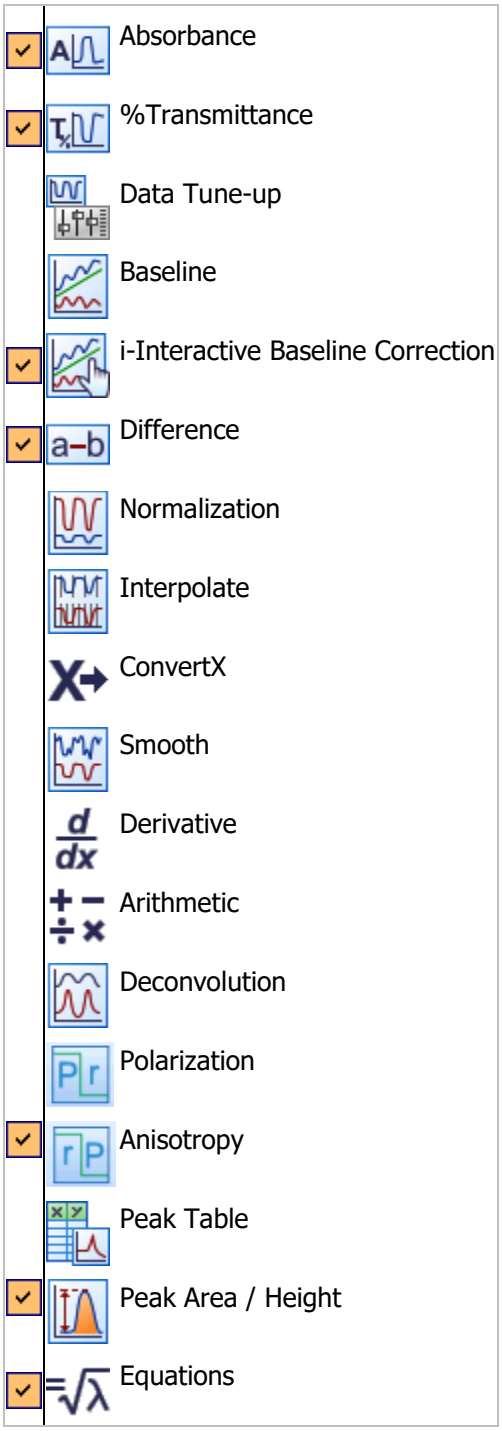


Additional Information

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

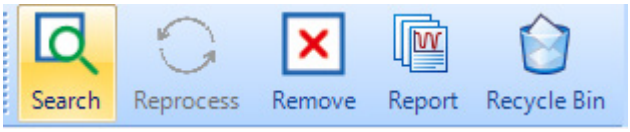
The  icon above indicates that the command is included in the factory default Process bar.

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 Previous Results File Bar

Use the Previous Results File bar to search for results, reprocess, display, and report previous results in the software.



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 Status Bar

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

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

When Spectrum FL 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.

Showing, Hiding and Moving 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 Action toolbars, or locking one of the Graph toolbars locks the Graph and Process toolbars.*

Restoring the Workspace

Spectrum FL 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 equations, instrument setups or sample table setups will be removed.

To restore the workspace to the system default:

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

   The Reset Layout dialog is displayed.

2. Click **OK** to restore.

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

Spectrum FL 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 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** and then select **Customize**.

   OR

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

   OR

   Right-click in an area next to the 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 Action 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 Action 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.

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