Essential FTIR™

15th Edition.

1. Contents

2. Product Overview

Essential FTIR is a program that provides a potent environment for the acquisition, manipulation and presentation of infrared data. Infrared data, whether in the form of interferograms, raw energy spectra, transmission spectra or absorbance spectra, may be represented as arrays consisting of an ***x*** vector (e.g. frequency) and a ***y*** vector (e.g. absorbance). ***Essential FTIR*** can be used to manipulate process and analyze these vectors. Though a large number of tools and options for the manipulation of such data are available, ***Essential FTIR*** achieves simplicity by relying on a small number of organizing principles.

While this manual is intended as a reference for ***Essential FTIR***, it will also focus on a tutorial based approach, offering new users a chance to familiarize themselves with the many tools and functions offered by the program. Taking each topic in a logical sequence, from opening and saving data, through manipulating, editing and transforming spectra, to presenting graphics, this manual aims to provide a complete guide to the functionality of this scientific software. Some familiarity with FTIR operation and data handling will be assumed, as it is beyond the scope of this manual to provide a 'first principles' explanation of all the concepts encountered when exploring FTIR data, though as much detail will be provided as possible throughout.

3. Installation

Essential FTIR is installed via its ***setup file***. This may be obtained from the software CD, or from a download. In either case the procedure for installing the software is the same. In this example we will assume that the software was downloaded to a location on your hard disk. Once the ***setup*** file is located, installation is initiated either by double clicking the appropriate icon, or by right-clicking the icon and selecting ***Open*** from the context menu.

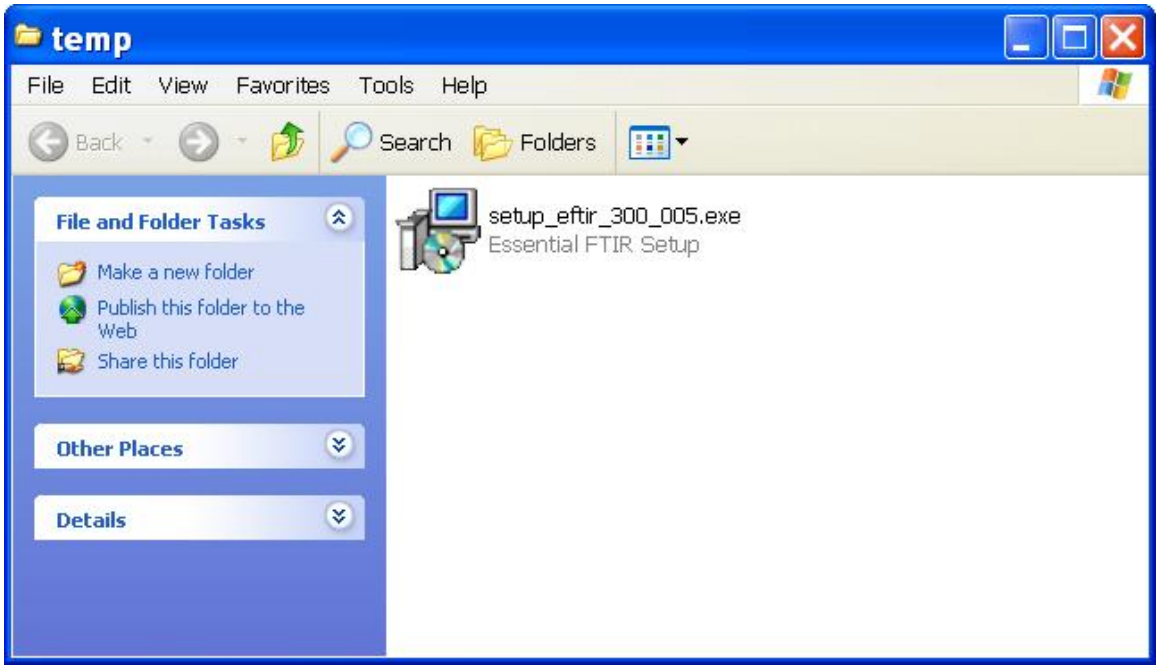


Figure 3-1 *Essential FTIR setup icon*

Initializing the installation delivers the window illustrated in Figure 3-2

Figure 3-2 *Setup introduction screen*

Clicking ***Next*** continues the installation. The installation program will then display the license agreement, as shown in Figure 3-3. This should be accepted before clicking ***Next***.

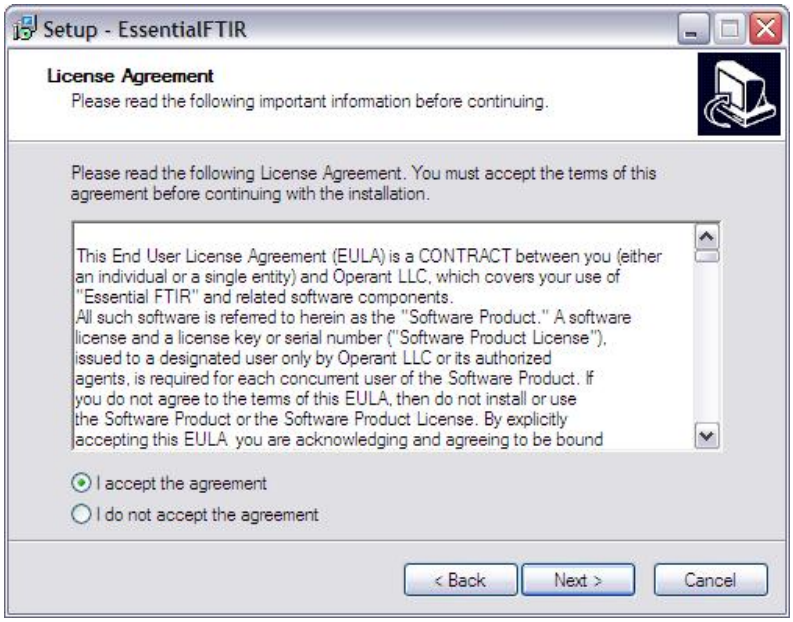


Figure 3-3 *License agreement*

Once the license agreement is accepted, the ***install*** button is displayed as shown in the next figure.

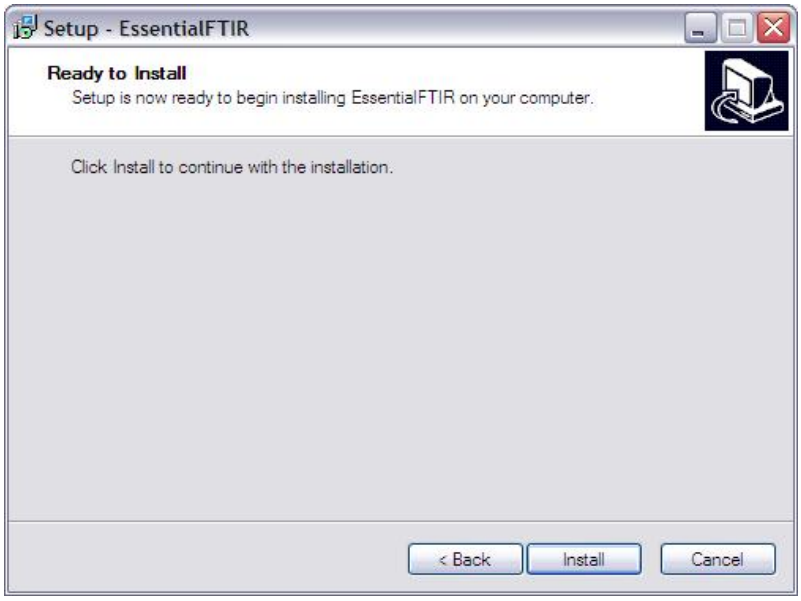


Figure 3-4 *Ready to install screen*

Once the ***install*** button is pressed the installation will proceed. On concluding the installation the ***setup*** program will display the window shown in Figure 3-5.

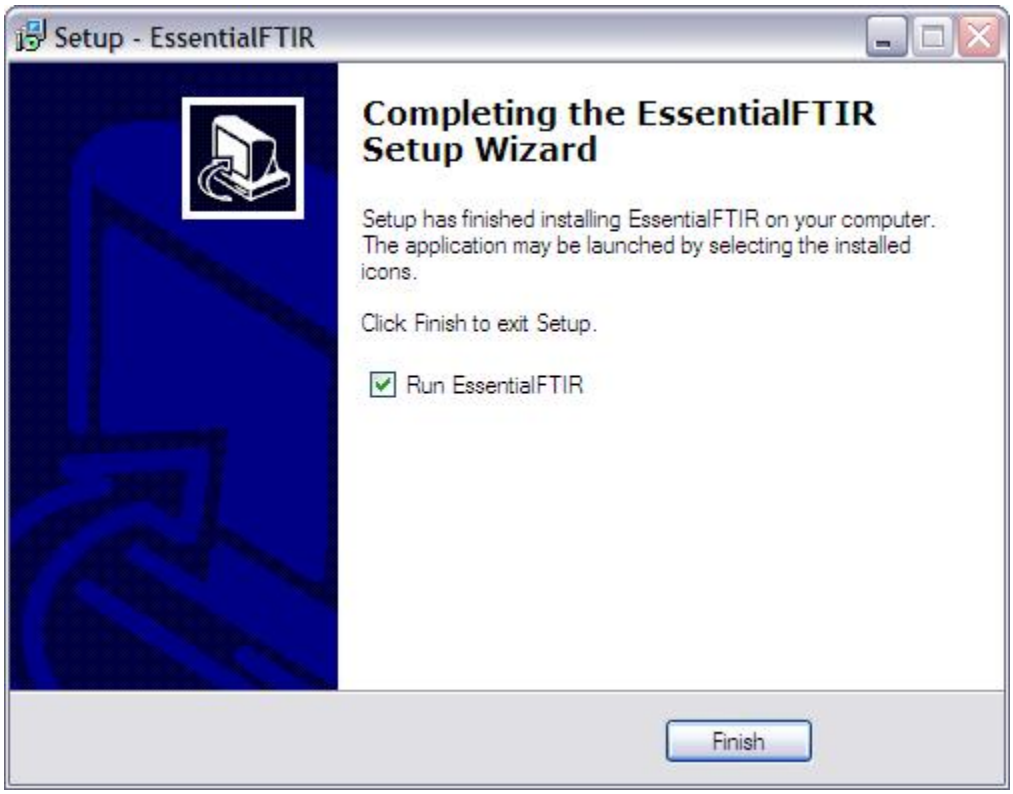


Figure 3-5 *Setup complete notification*

A check-box is displayed in this window, which allows running of ***Essential FTIR*** immediately upon clicking the ***Finish*** button, which concludes the installation. If this box remains unchecked you may choose to start the program either from the ***Programs*** menu, or by double clicking the shortcut icon. These methods of starting ***Essential FTIR*** are shown in the following figures.

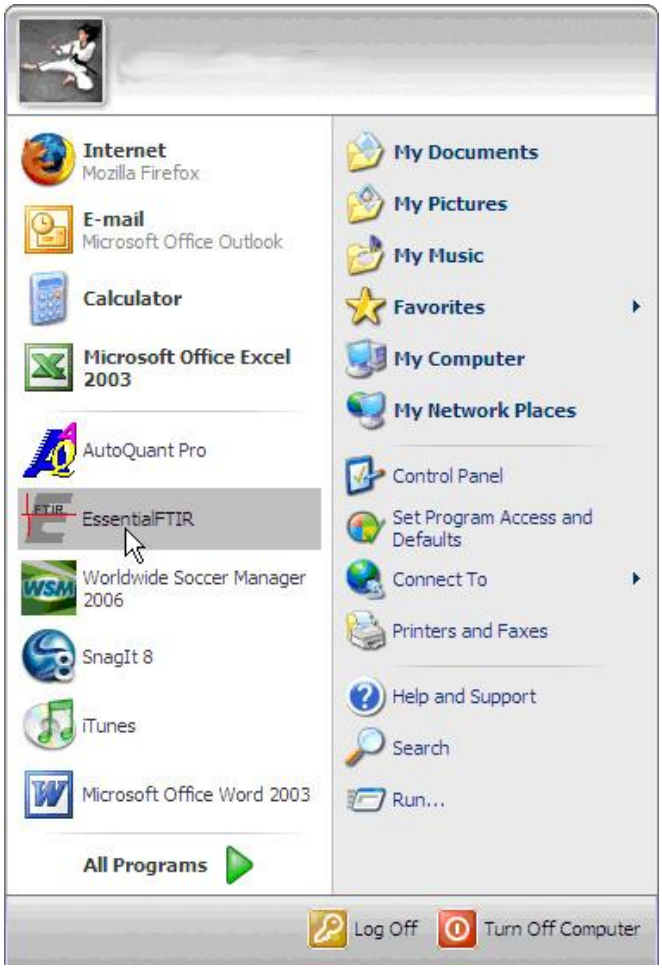


Figure 3-6 *Program Menu*

Figure 3-7 *Desktop shortcut*

Essential FTIR is now installed and ready for use. In the next chapter, we'll begin to explore the program.

4. Getting Started

The Essential FTIR Main Window

When starting the program you are presented with the ***Essential FTIR*** front end, which we will refer to as the ***Desktop***. This desktop is illustrated with its default settings in Figure 4-1.

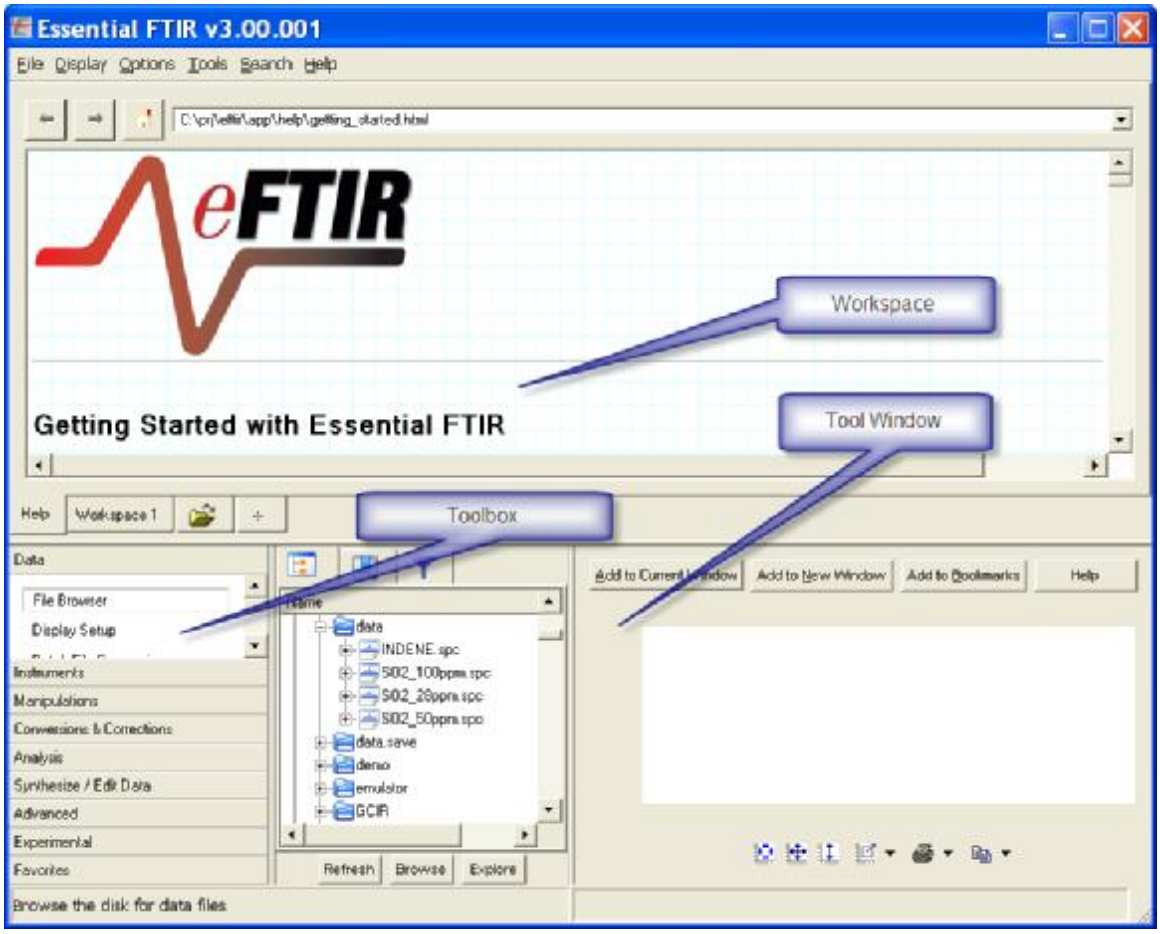


Figure 4-1 *Essential FTIR desktop*

At the highest level, the ***Workspace*** contains the data on which operations may be performed. Multiple workspaces may be opened, though only a single workspace may be active at any one time. A workspace may be viewed as a container which holds the data to be manipulated. Many spectra may be displayed in a ***Workspace***, but only one spectrum may be active at a time, and this active spectrum is displayed along with associated header information. The ***Toolbox*** contains ***Tools*** which are used to perform operations on spectra. In Figure 4-1, the Essential FTIR startup screen is shown. This screen can be

changed to display any HTML document, to do so, use the Options / Setup / Miscellaneous menu selection. In the ***Toolbox*** in the lower left, the 'File Browser' tool is selected.

In order to edit or manipulate a spectrum, it is often necessary to define a ***Region*** upon which to perform operations. A ***Region*** is defined in ***Essential FTIR*** by clicking and dragging over a portion of a spectrum in a manner familiar to Windows users. Regions may be named, saved and stored for later use, further simplifying many complex operations.

Workspaces

In Figure 4-2, one of the example files that is installed with Essential FTIR has been added to a Workspace.

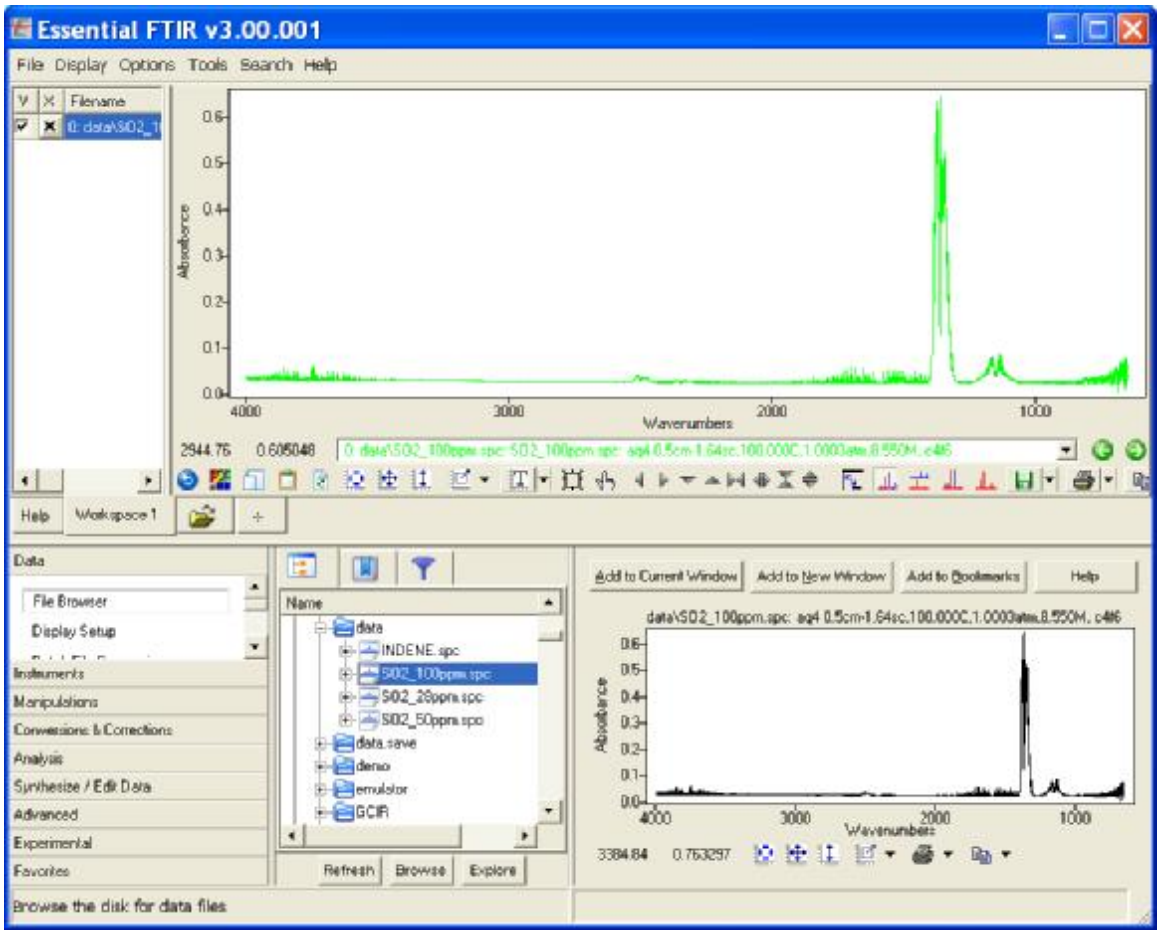


Figure 4-2 *The* Essential FTIR *desktop*

The Workspace, Toolbox, and Tool Window are separated by resizing bars. When passing over boundaries between desktop elements, the cursor will assume the re-sizing arrows. This change in cursor appearance is shown in Figure 4-3. Depending on the Windows theme you have installed, the resizing bars may appear differently than as shown.

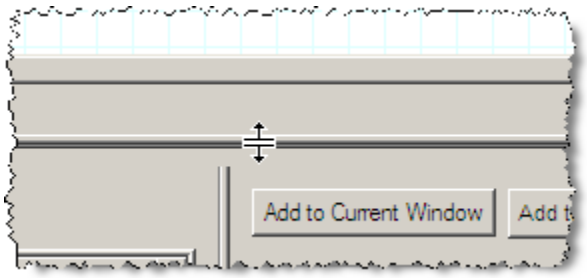


Figure 4-3 *Resizing cursor*

The ***Workspace*** window may comprise a number of ***Workspaces***, which are selected as active by tabs. These tabs are shown in detail in Figure 4-4.

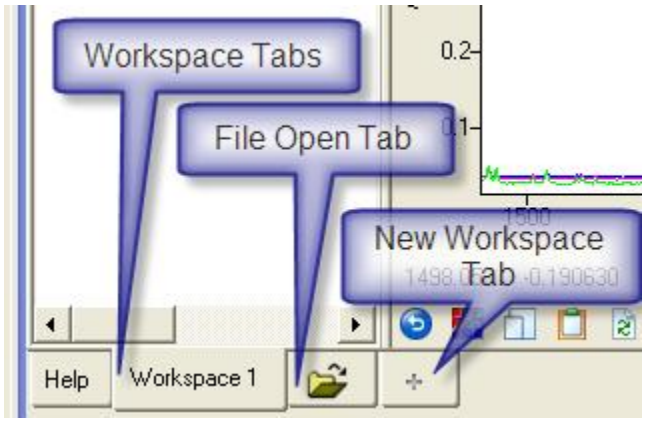


Figure 4-4 Workspace tabs

By default, the initial active ***Workspace*** Window is occupied by the ***Help*** interface. We will discuss changing default settings in the ***Options*** section in chapter five – The ***Essential FTIR Menus***, where instructions are presented which enable you to display a pre defined page on startup, or no page. Clicking on a ***Workspace Selection Tab*** renders that workspace active. The ***Workspace*** is a flexible environment where we may view spectra, and review any changes to our data that we make using the tools offered by the program. There are two special tabs, labeled in Figure 4-4 as the 'File Open Tab' and the 'New Workspace Tab'. The 'File Open Tab' will open a file open dialog box, allowing data to be added to the workspace. The 'New Workspace Tab' will open a new Workspace. These two special tabs are convenient shortcuts allowing quick loading of data.

Right-Clicking on a Data Workspace tab brings up this menu of choices:

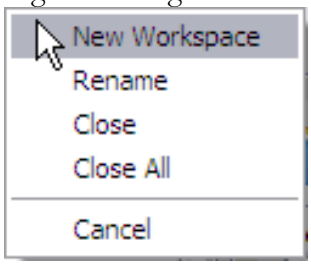


Figure 4-5 *Workspace tab context menu*

We will look now in detail at an active ***Workspace*** with some example data loaded.

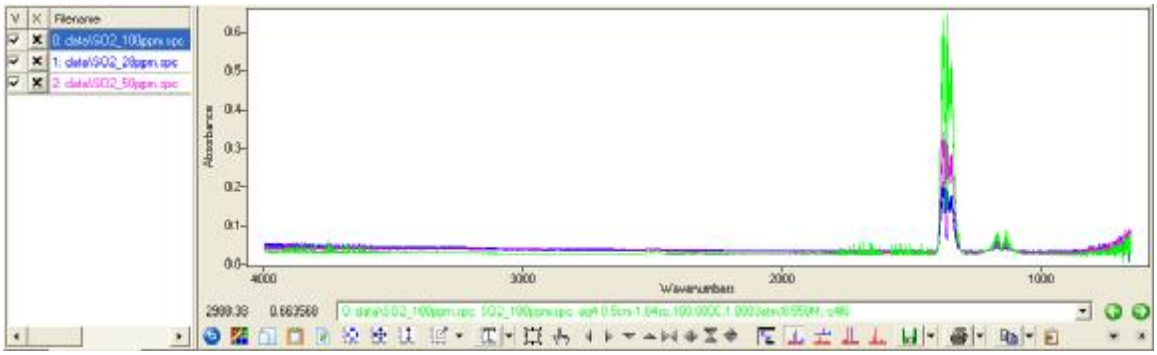


Figure 4-6 The active Workspace

Figure 4-6 shows an active ***Workspace***, with three sulfur dioxide absorbance spectra displayed. These spectra are supplied with ***Essential FTIR***, and may be loaded by navigating to the directory containing them using the ***File Browser Tool***. On the left of the ***Workspace*** we see a browser panel. Let's resize this panel by dragging its splitter bar to view it in detail.

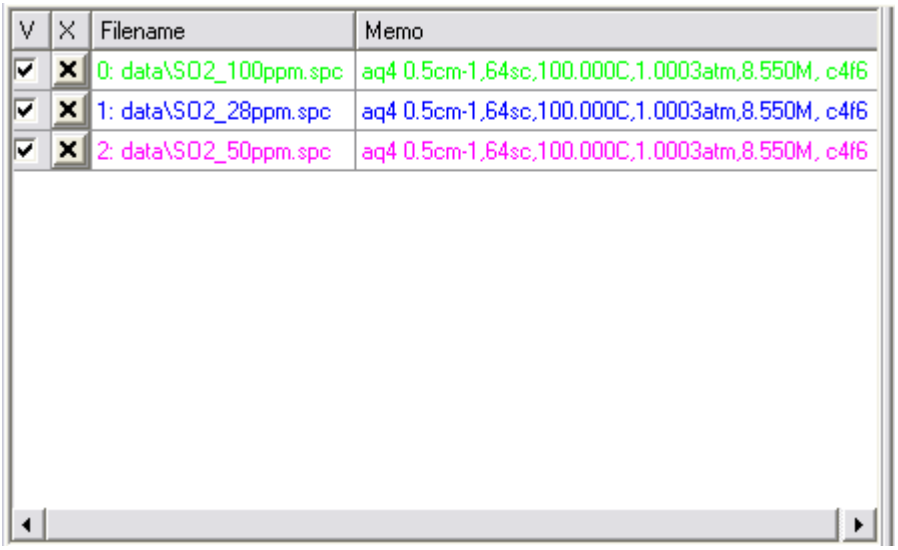


Figure 4-7 *Workspace browser panel*

The browser panel consists of four columns. The first column is labeled ***V***, and consists of a column of check-boxes – one for each loaded data file. The ***V*** is short for ***visible***, and by default the visibility box is checked. Clearing this check-box renders the associated spectrum invisible, though the data is not removed from the ***Workspace***.

The next column is labeled ***X***, and also consists of a button for each data file. Clicking on the button associated with a data file will clear that spectrum from the workspace.

The next column is labeled ***Filename***, and contains the name of the data file. The final column is labeled ***Memo***, and contains any information held in the memo field of the data file.

Right-clicking in this panel summons the context menu shown in Figure 4-8.

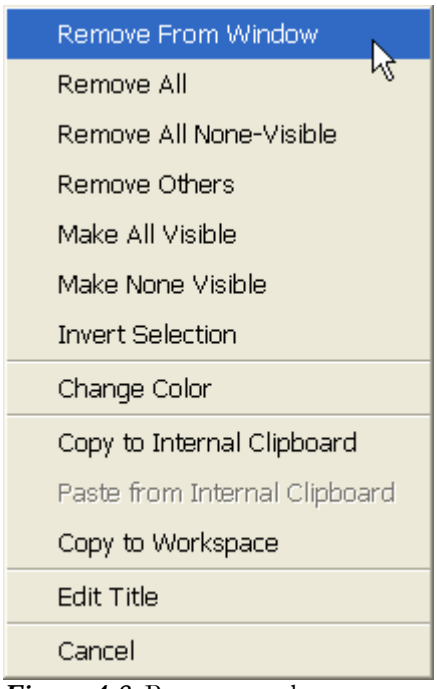


Figure 4-8 Brower panel context menu

The menu may be used as a shortcut when selecting, removing or otherwise handling data in the window.

The ***Workspace*** data display window is shown in Figure 4-9.

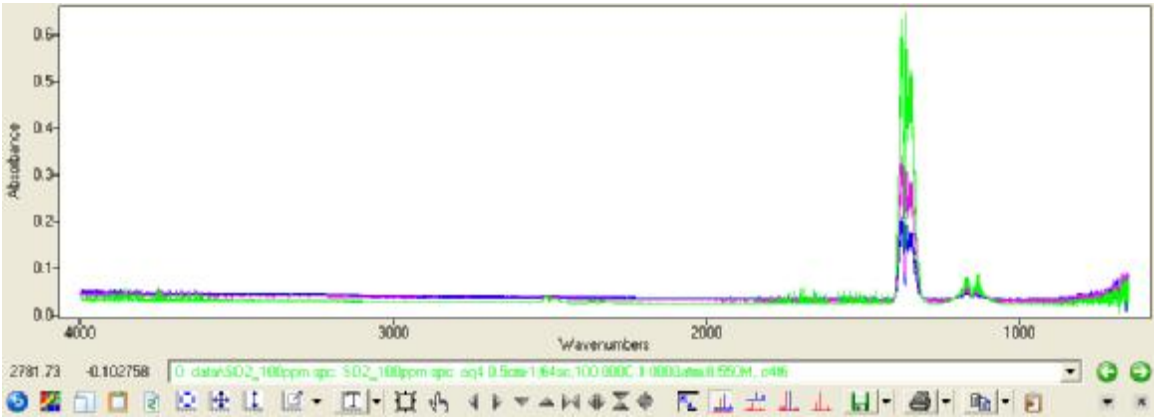


Figure 4-9 *The* Workspace *data display window*

Expanding / Zooming

The data display can be zoomed-in on by drawing a box with the mouse. Select a corner of the area you want to zoom in on, press and hold the left mouse button, and move the mouse to define the new display area.

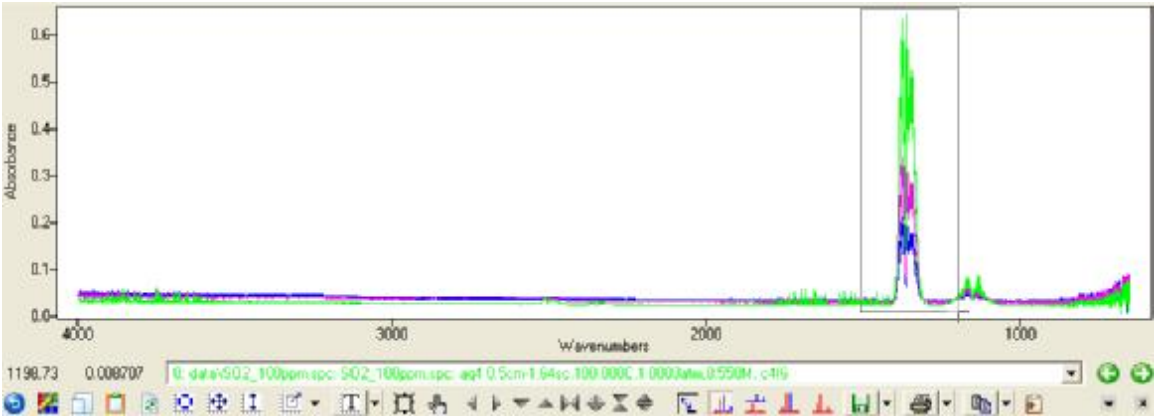


Figure 4-10 zooming in on the data

Figure 4-10 shows the box being drawn by the user. When the left mouse button is released, the display will be adjusted to show only the area within the box, as in Figure 4-11.

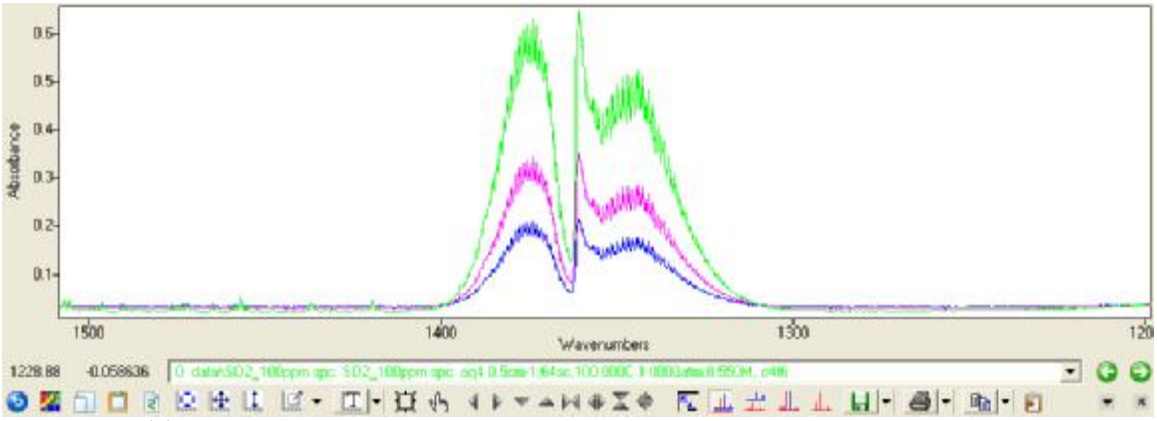


Figure 4-11 The zoomed-in display.

The data display can be quickly returned to the full limits, or 'autoscaled' by clicking the left mouse button (that is, press and release the left mouse button without moving the mouse). There are many other ways to control the display, which are attached to the display icons that will be discussed below.

Graphic Display Controls

The display consists of a Cartesian plot of the data files. The ***y***-axis is dependent upon the type of data currently active in the ***Workspace***. The ***x***-axis may be labeled in wavenumbers, nanometers or microns – or data points when viewing interferograms. Changing the axes

labels is discussed in the ***Display* menu** section of chapter four. Two rows of buttons and other items are clustered below the display window. These items are known as the ***Graphic Display Controls***, and are shown in more detail in Figure 4-12.

Figure 4-12 *Graphic display controls*

These controls may be used to manipulate the data display. Some of these features are replicated in the ***Display* menu** discussed in chapter four. . In the upper left corner of the panel are two numbers. These numbers represent the position of the cursor on the data display with reference to the Cartesian axes of the active data file. The number on the left represents the position of the cursor on the ***x***-axis, while the number on the right shows the location on the ***y***-axis. Next we see a drop down list. This list contains all data files currently loaded in the active ***Workspace***. Selecting a data file from the drop down list will make that file the active sample in the ***Workspace.***

All the remaining items are buttons. These form four distinct sets:

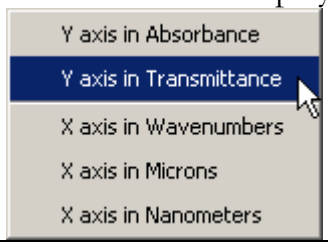
1. The ***File*** buttons
2. The ***Display Limit*** buttons
3. The ***Axis Navigation*** buttons
4. The ***Display Type*** buttons

We will examine the function of each member of the four sets.

File buttons

	Designates the previous spectrum in the Workspace as active
	Designates the next spectrum in the Workspace as active
	Undo changes to the data
	Allows you to change the color of the active spectrum (see Display menu in chapter four)
	Copies the active spectrum to the internal clipboard. This spectrum will then be available for pasting into another Workspace
	Pastes from the internal clipboard (not the Windows clipboard)
	Creates a copy of the active spectrum in the current workspace - Cloning
	Save spectra to disk
	Print the data window
	Export the data window as a graphics file
	Export the data in the window as data files

Display Limit buttons

	Manually set the display limits. This allows fine control of the display.
	Autoscale the data display
	Auto-scales the y-axis without changing the x-axis
	Undoes the previous expansion – you may choose from a list of previous expansions to undo from a drop-down menu, summoned by clicking the "down" arrow on the Undo button
	Force the units of the data in the display to be the same. Clicking on this button will display this menu: 
	Enables you to define the axis limits of the display by left-clicking and dragging a box around the desired area, known as "expand" or "zoom"
	Enables you to drag all visible spectra around the data display, known as "roll"

Axis Navigation buttons

 Moves all visible spectra to the left

 Moves all visible spectra to the right

 Moves all visible spectra down

 Moves all visible spectra up

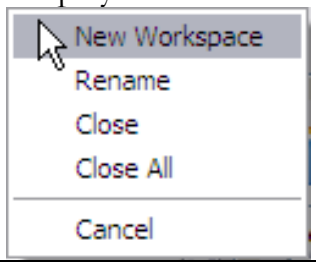
 Zooms out on x-axis

 Zooms in on x-axis

 Zooms out on y-axis

 Zooms in on y-axis

Display Type buttons

	Toggles full screen display mode on and off
	Displays data in Overlay mode – all spectra retain their relative proportions
	Displays data in Stacked mode – all spectra are displayed in a separate display area, with the active spectrum lowest in the stack
	Displays data in Superimpose mode, with spectral features matched on the y axis
	Displays data in Paged mode – only the active spectrum is displayed. Navigating through the spectra loaded into the Workspace will display each in turn
	Displays the menu shown in below. 
	Closes the workspace

Many of the functions provided by these buttons are also accessible via the menu system, described in chapter four of this manual.

The last feature of the ***Workspace*** that we will note in this section is that of the ***Workspace*** tab context menu. This menu is summoned by right-clicking on a ***Workspace*** tab, and is shown in Figure 4-13.

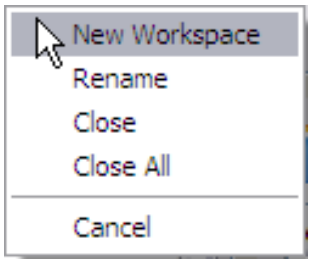


Figure 4-13 Workspace *tab context menu*

This contains five items. The ***New Workspace*** option creates a new ***Workspace***, selectable by its tab. The ***Rename*** option allows you to provide a meaningful name for a ***Workspace***. The ***Close*** option exits the currently active ***Workspace***. The ***Close All*** option dismisses all open workspaces. The Cancel option dismisses the context menu without further action.

At the lower left of the Essential FTIR desktop we find the ***Toolbox Selection*** window, as shown in Figure 4-14. This element of the desktop allows you to choose a set of ***Tools*** relevant to their needs.

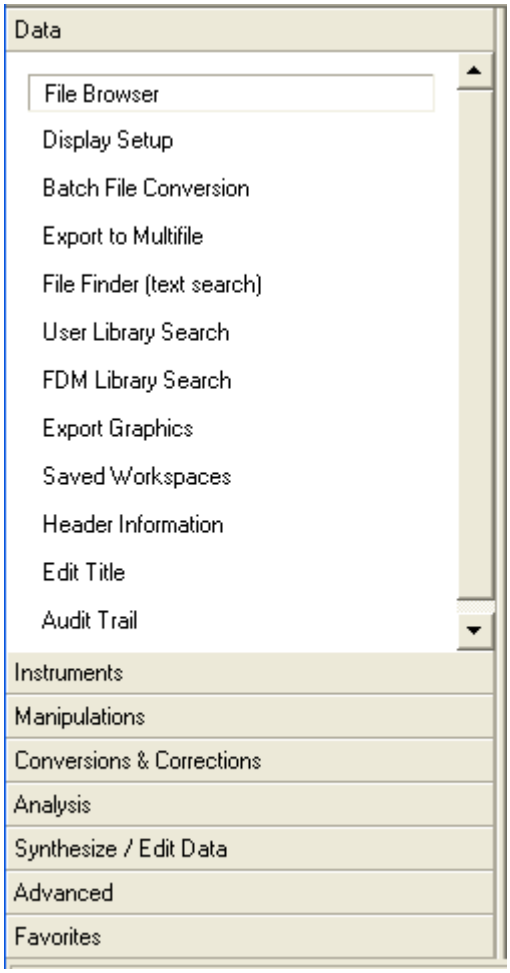


Figure 4-14 *Toolbox selection window*

The items on the toolbox selection window form a two stage hierarchy. At the highest level, the toolboxes are represented as gray tabs. Each of these tabs represents a collection of tools, grouped according to their function. For example, the clicking the ***Data*** tab reveals tools that will handle files, acquire new data, convert between file types and other data handling functions. Similarly, the other tabs contain tools relevant to their labels. We will discuss the toolboxes in detail in chapter five – ***Toolboxes and Tools.***.

The final element of the desktop is the ***Tool Window***, an example of which is illustrated in Figure 4-15. This element is context sensitive – when a tool is selected the appropriate tool window is displayed.

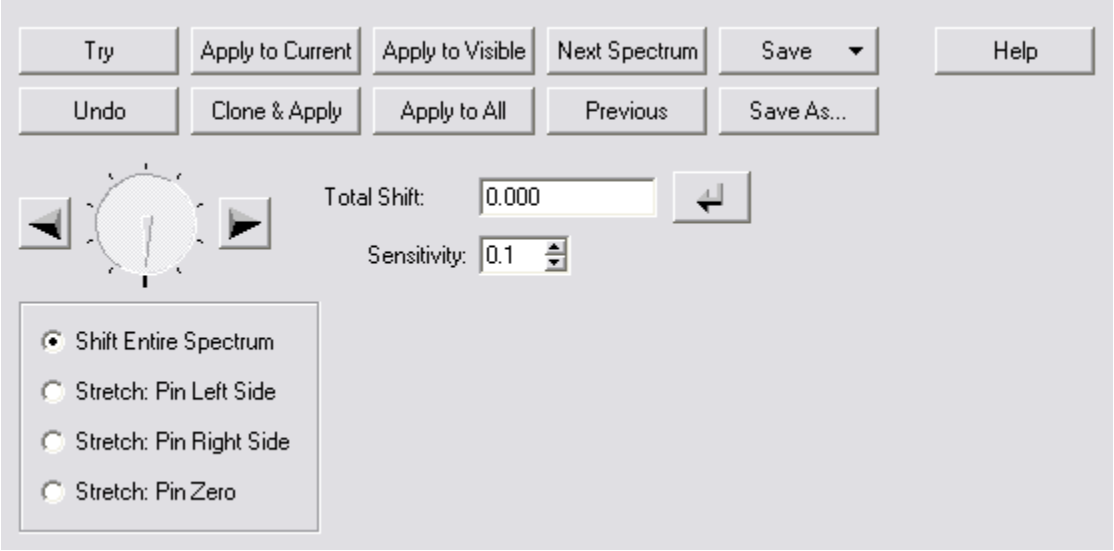


Figure 4-15 *X-Shift Tool Window*

Many tools require user input, for example when making an adjustment to the x-axis vector of a spectrum using the ***X-Shift*** tool, it is necessary to define the amount of shift applied, and whether to "stretch" the spectrum or shift the whole axis.

As an example of a typical operation often carried out in Essential FTIR, let's look at how to locate, open and correct the baseline of an absorbance spectrum. We may locate a spectrum using the ***File Browser*** tool contained in the ***Data*** toolbox. If we assume that the desired spectrum is located in the folder "data" and has the filename "SO2_28ppm", then we should click on the file to highlight it as shown in Figure 4-16.

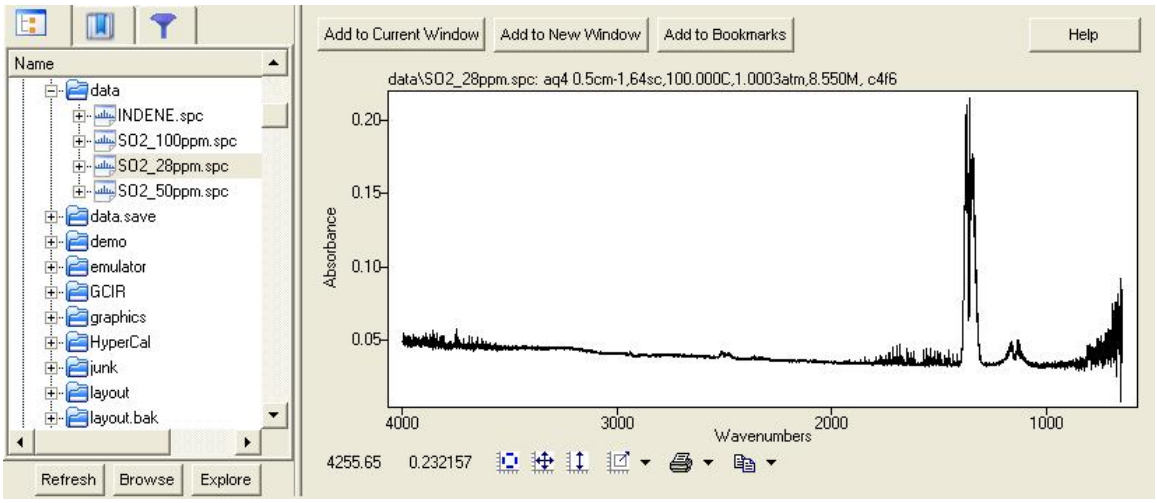


Figure 4-16 *Choosing a file for display*

Once the highlighted file is displayed in the lower right hand window, clicking the 'Add to Current Window' button will load the spectrum into the workspace.

Now that the spectrum is held in the workspace we are free to perform manipulations upon the data. On inspecting the sulfur dioxide absorbance spectrum we notice that the ***y*** axis has

a slope, with the high end at 4000cm^{-1}. Two tools are included in the ***Manipulations*** toolbox which may be used to correct this problem – the ***Manual Baseline Correction*** and ***Auto Baseline Correction*** tools. In this case we will use the ***Auto Baseline Correction tool***, as shown in Figure 4-17.

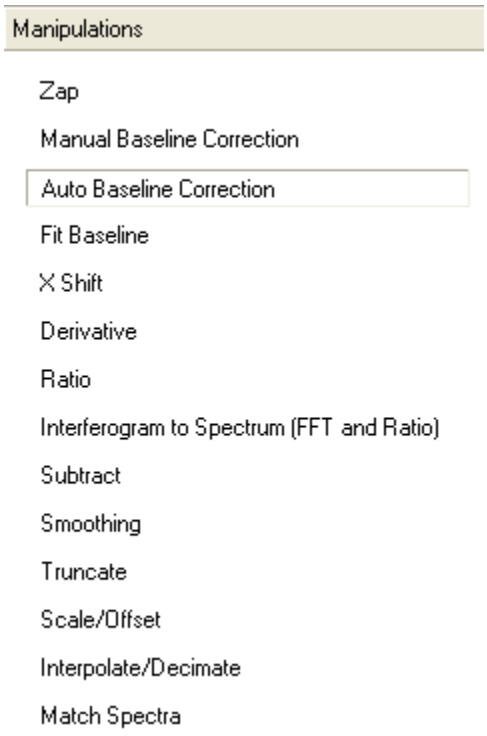


Figure 4-17 *Manipulations toolbox*

Clicking on the ***Manipulations*** tab of the ***toolbox selection window*** reveals the tools included in the ***Manipulations*** toolbox. Highlighting the ***Auto Baseline Correction*** tool on the menu reveals the ***tool window*** for that function. This window is shown in Figure 4-18.

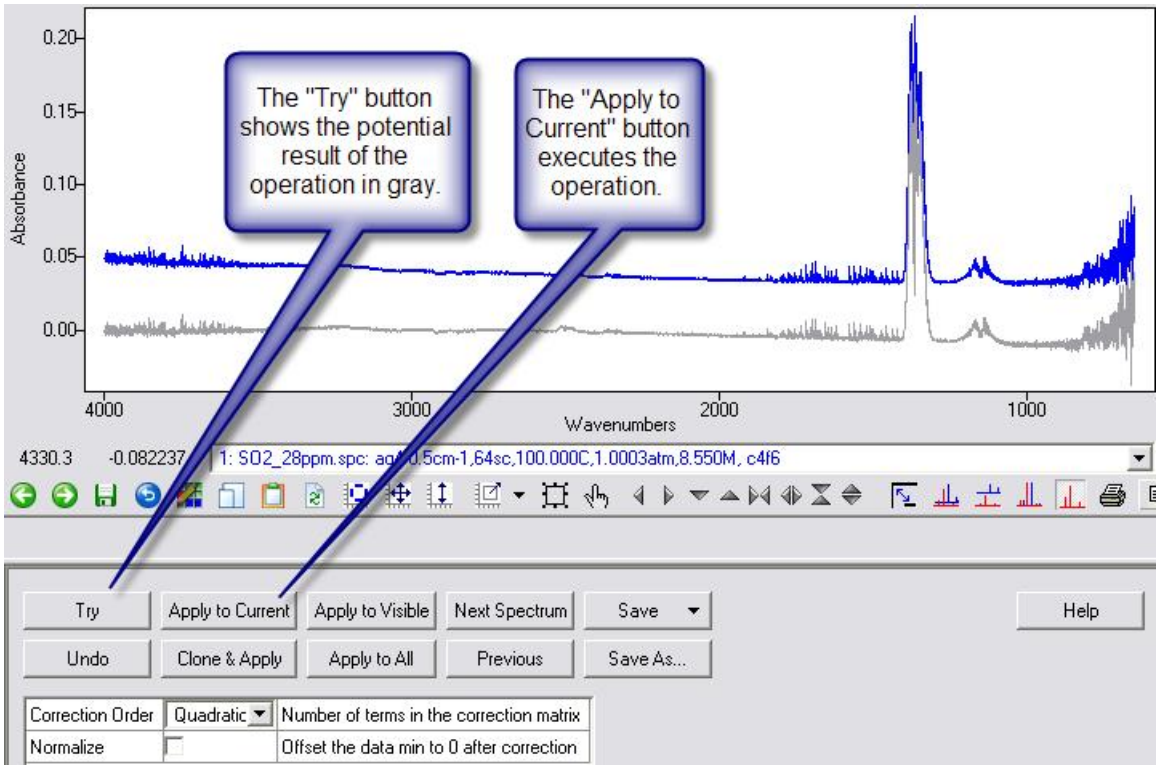


Figure 4-18 *Using auto baseline correction*

In this example the baseline of the sulfur dioxide spectrum varies between approximate absorbance values 0.05 at the high end and 0.00 at the low end. Options available are "Correction Order" and "Normalize". We have chosen "Quadratic" as the correction order so as to remove any curve present in the sloping baseline. The "Normalize" checkbox remains unchecked as increasing noise levels toward the lower extremes of the spectrum result in "noise data points" well below zero, and normalizing to zero including these data points would result in lifting the entire spectrum so as to place the lowest point on the ***y*** axis at zero. Clicking the ***Try*** button displays the projected result of the operation in gray in the workspace window. Clicking the ***Apply to Current*** button performs the operation and replaces the visible spectrum with the corrected data. This data is NOT saved automatically however, and closing the window or removing the data results in the spectrum being stored unsaved. In order to save the corrected spectrum we must click the ***Save As…*** button, which delivers the dialog box shown in Figure 4-19.

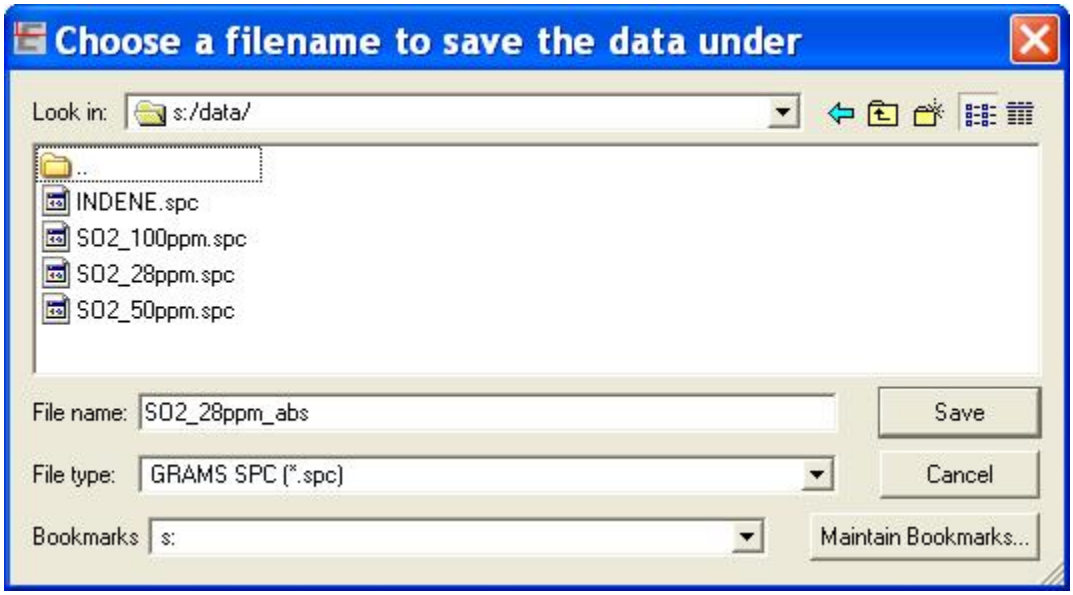


Figure 4-19 Save As… *dialog box*

After clicking the Save button on the dialog box, the data is saved to the selected folder. In the example above we have renamed the file with the prefix "New". If a different filename is not supplied the file will be over written.

We have now covered all the basic elements of manipulating a spectrum in ***Essential FTIR***:

- Locating and opening a data file
- Selecting an appropriate tool
- Carrying out the operation
- Saving the resultant file to disk

One more concept must be explored before we go on to examine in detail the tools and features offered by ***Essential FTIR***.

Creating and Working with Spectral Regions

The idea of ***Regions*** is central to the operation of the software. A region may be defined as: ***"Region* – A portion of the *x* -axis of a spectrum designated by the user to be operated upon, or designated by the user to be representative of that spectrum for the purposes of that operation."**

In ***Tools*** that work with ***Regions***, ***Regions*** may be defined by right-clicking in the active ***Workspace*** window. One right-click defines a ***Region Marker*** – a vertical line delineating the edge of a ***Region***. This ***Region Marker*** may be repositioned by left-clicking and dragging, in a manner analogous the that previously described for re-sizing desktop elements. Right-clicking in the ***Workspace*** window a second time completes the ***Region***

with a second marker, and the portion of the spectrum selected is shaded. The result of this operation is shown in Figure 4-20, using the ***Zap*** Tool as an example.

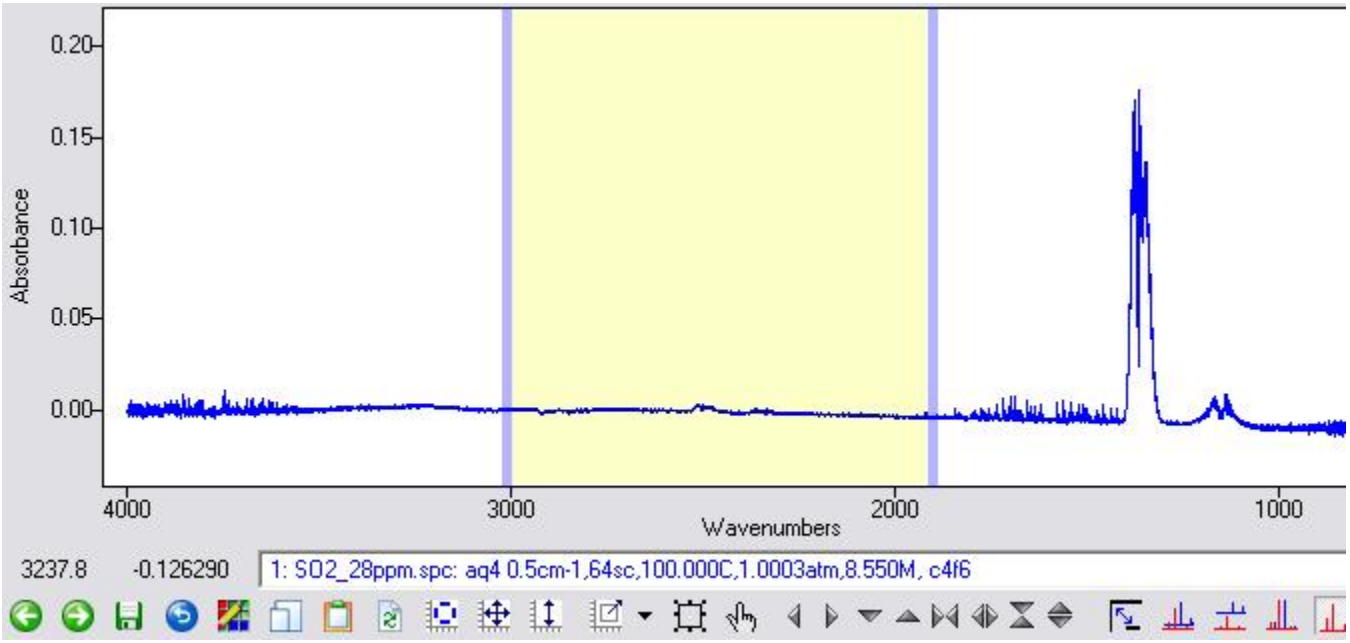


Figure 4-20 Region *markers*

The numerical values of the ***Region*** defined in this way are recorded in a Region Table, as shown in Figure 4-21.

	Wavenumber...	Wavenumber...
1	3013.517	1902.522

Figure 4-21 Region *Table*

Part of the power of the ***Regions*** concept is that regions defined as described earlier may be saved to disk as a ***Regions*** file. This may be achieved by right-clicking on the region table and selecting ***Save Table*** from the resulting context menu or by clicking the '***Wavenumber...***' column headers of the region table. The context menu is shown in Figure 4-22.

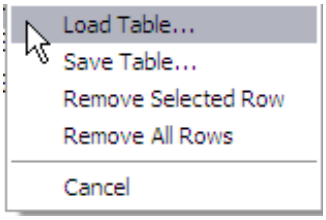


Figure 4-22 Region table context menu

These ***Regions*** may then be loaded as needed, for example as part of an automated batch processing routine – easily configured in ***Essential FTIR*** with no requirement for

programming. This process is described in chapter five in the section on the ***Batch Processor Tool***.

When defining a ***Region*** from which includes an endpoint of the data, it is not necessary to painstakingly position the cursor on the final data point. If you select a point outside of the data range ***Essential FTIR*** will use the final point of the data.

The above summary gave us a general overview of operations in ***Essential FTIR***. Many operations may be carried out in series, before the final result is saved. In following chapters we will examine each feature of ***Essential FTIR*** in detail.

5. The Essential FTIR Menus

In common with most programs running under Microsoft Windows, ***Essential FTIR*** uses a combination of menus and buttons to provide the mechanics of the user interface. ***Essential FTIR*** employs some redundancy in this regard – some options and functions are accessible via either the menus or buttons, allowing you to access features in a manner comfortable and intuitive to the individual. In this section we will examine the features unique to the menu system – features accessible via the button interface will be detailed in the chapter relevant to that button.

The Essential FTIR menus are shown in Figure 5-1

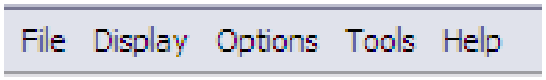


Figure 5-1 *The EFTIR menus*

The menu concept is familiar to most computer users. The ***Essential FTIR*** menu is located at the top left of the desktop, and comprises five headings, each containing sub-elements relevant to that heading. We will examine each heading and sub-element in turn. It is worth noting that each menu sub-element has a corresponding keyboard shortcut, which is activated by pressing ***ctrl x***, or ***alt x***, where ***ctrl*** or ***alt*** is the "control" or "alternative" key, and ***x*** represents the corresponding shortcut key. The actual shortcut keys are listed on the menus to the right of the sub-element, where available. For example, pressing ***ctrl O*** will deliver the ***Open File*** dialog box.

The File Menu

Clicking on the File heading displays the menu shown in Figure 5-2.

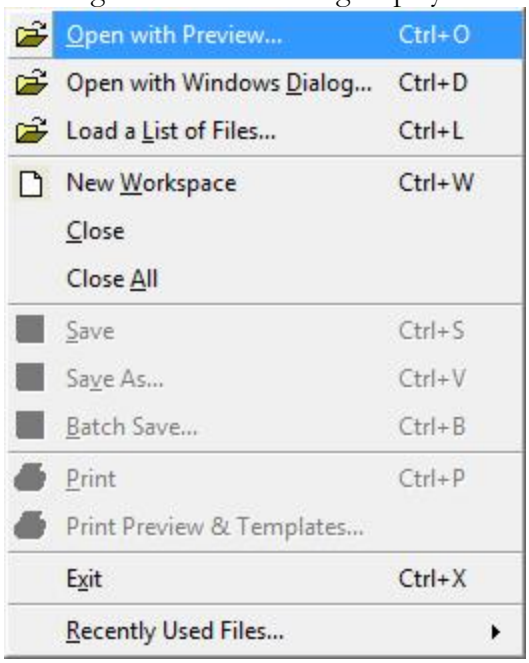


Figure 5-2 *File menu*

Clicking ***Open with Preview*** on the file menu displays the dialog box shown in Figure 5-3.

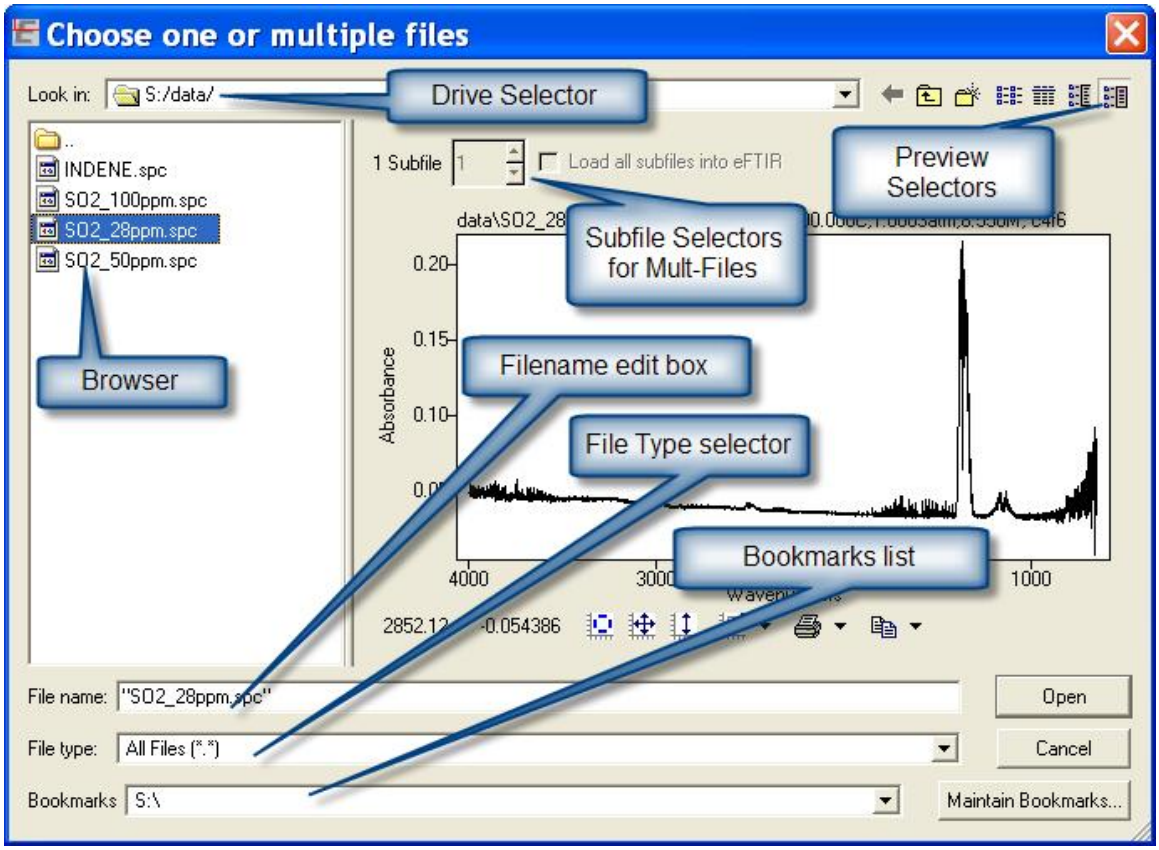


Figure 5-3 *Open file dialog box*

The ***Open with Preview*** dialog box consists of a drop down menu which allows you to specify a drive, a browser window, a filename edit box, a file format drop down menu, an ***Open*** button and a ***Cancel*** button. On the upper right hand side of the window contains the folder viewing option buttons, which are shown in Figure 5-4. These buttons are common to most file handling dialog boxes in Microsoft Windows. Examining the options from left to right we have:

- Back button
- Up one level button
- New folder button
- List view
- Detail view

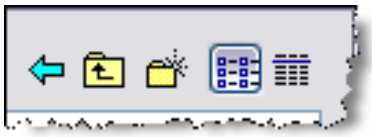


Figure 5-4 *Folder viewing options*

Folders visible in the browser window may be double clicked to show the contents. Once the desired file is located, clicking the ***Open*** button loads the file into the active workspace. Clicking ***Cancel*** dismisses the dialog box without further effects.

Clicking ***Open with Windows Dialog*** will display the Windows operating system's file open dialog, as shown in this figure. This dialog is useful when you are working with networked drives because it is much faster than the Preview dialog.

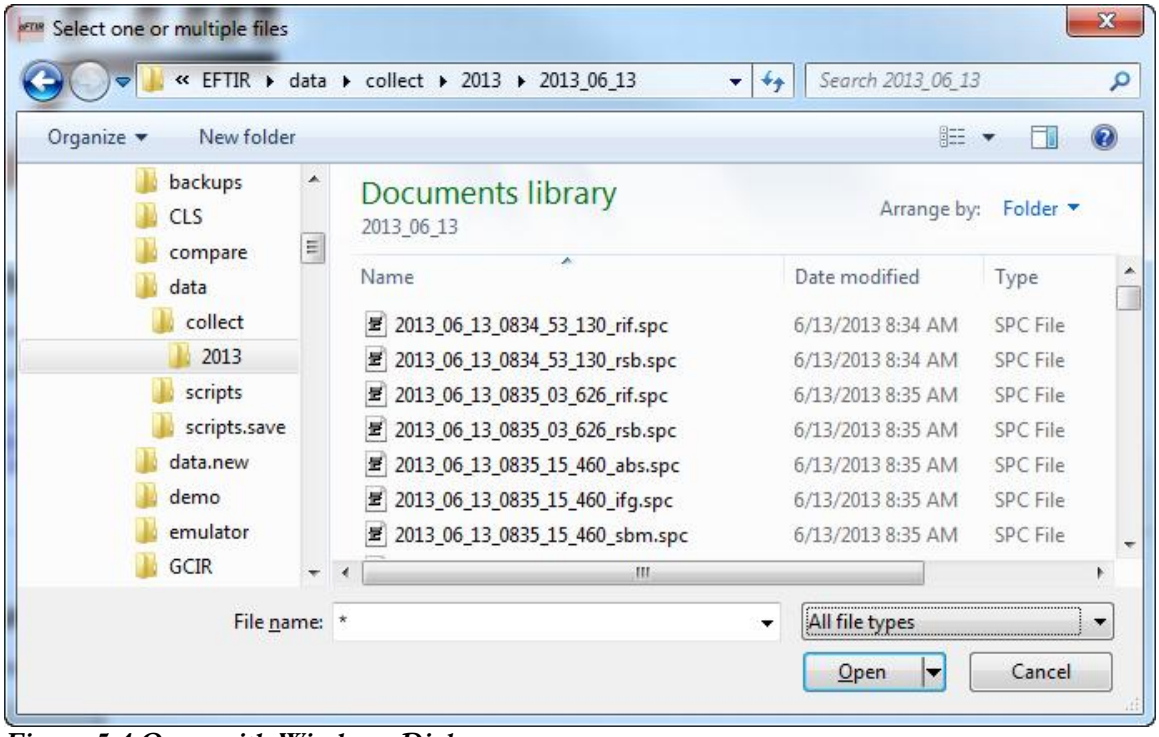


Figure 5-4 Open with Windows Dialog

The ***Load a List of Files*** selection will load files from a list contained in an ASCII text file. The file must contain one filename per line. If the filenames do not contain the full path to the file, Essential FTIR will then look in the folder that the text file is in. If any files cannot be found, the user is prompted for the location of the files. This feature is useful when it is necessary to handle groups of files. Also, see the 'Workspace' tool for another way to manage groups of files.

Clicking ***New Workspace*** opens a new workspace window. These windows are tabbed and may be renamed for clarity by right-clicking the workspace tab and using the context menu. ***Essential FTIR*** context menus are examined in Chapter six – Context Menus. By default multiple workspaces are numbered sequentially.

Clicking ***Close*** dismisses the active workspace.

Clicking ***Close All*** dismisses all visible workspaces.

Clicking ***Save*** will save the datafile in its current location, with its current name.

Clicking ***Save As*** summons the ***File Save*** dialog box

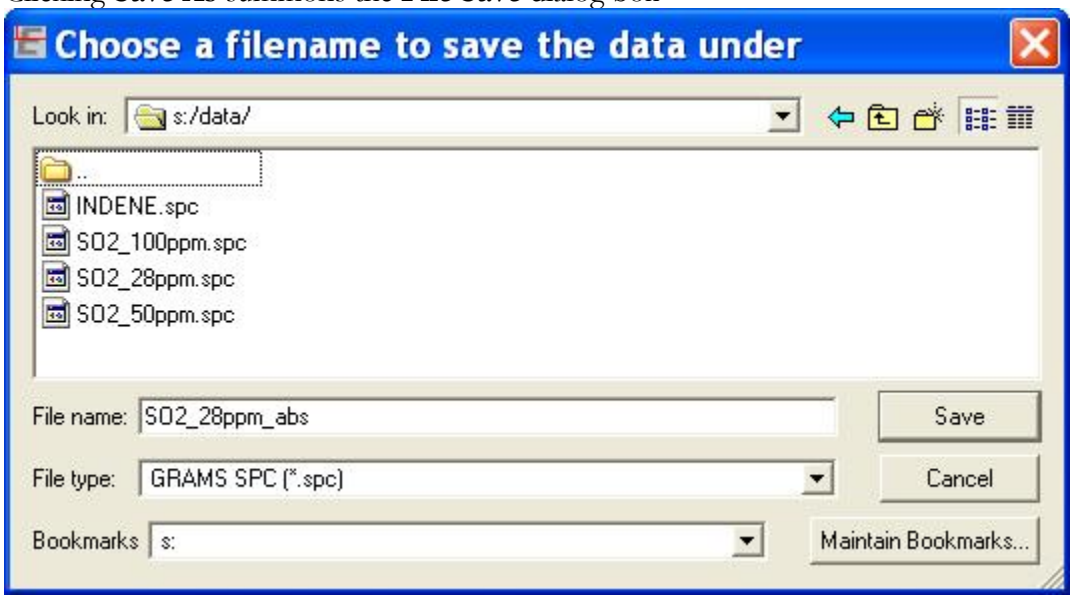


Figure 5-5 File Save dialog box

The 'File type' list allows the file to be saved in the formats that Essential FTIR can write to.

Clicking ***Batch Save*** brings up this dialog box, which allows saving all of the data with flexible file relocation and renaming options:

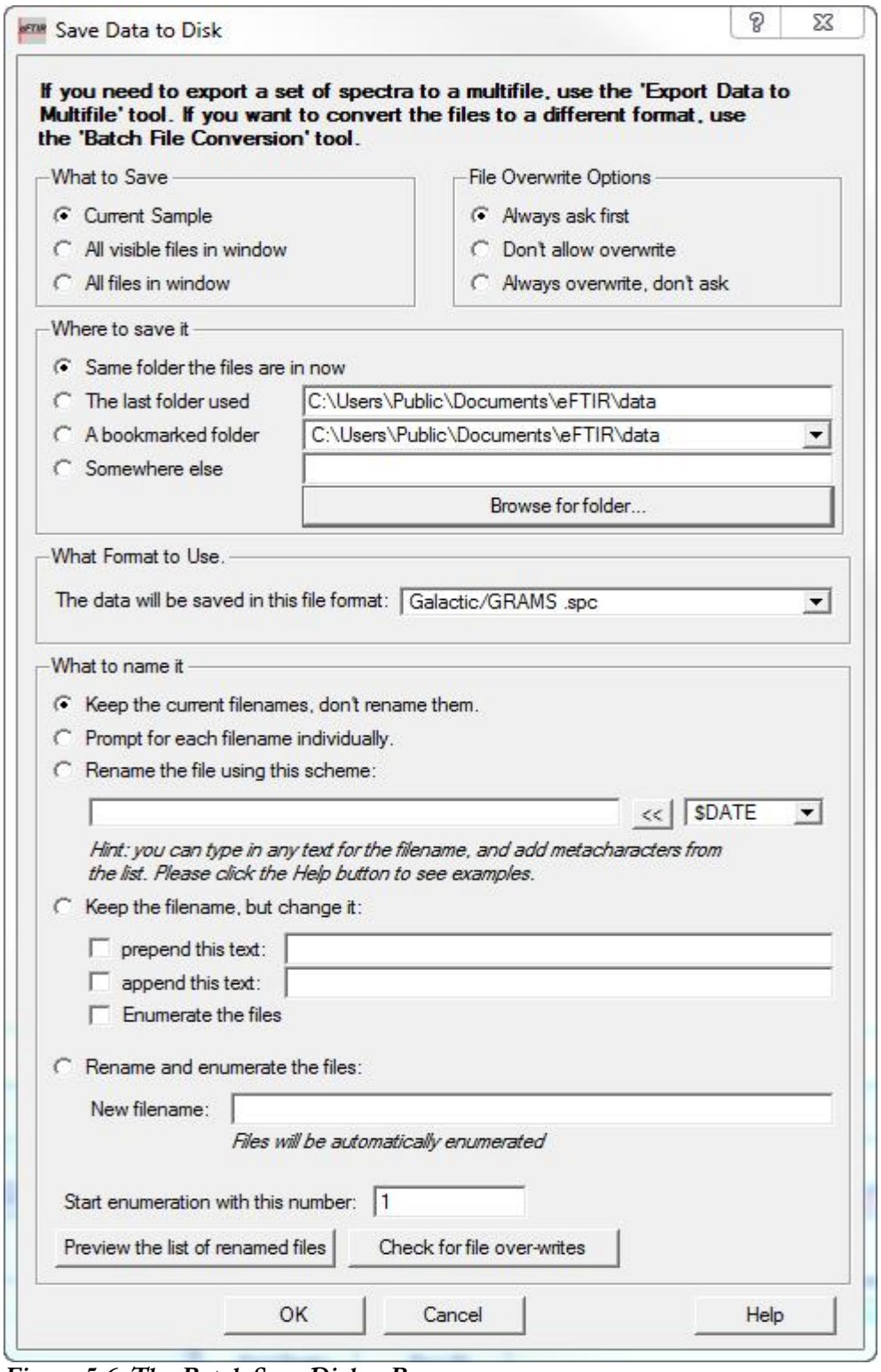


Figure 5-6 The Batch Save Dialog Box

There are four sections to this dialog:

1. What to Save: choose which files will be saved.
2. Where to Save It: choose where to put the saved files.
3. What Format to use: the files can be saved in any of the formats that Essential FTIR can write to.
4. What to name it: there are five naming strategies to provide flexibility in creating copies of files.
5. File Overwrite Options: to allow or disallow overwriting of existing files.

At the bottom of the 'What to name it' section are two important buttons:

Preview the list of renamed files	Presents a list of the new filenames for review
Check for file over-writes	Check to see if saved files will overwrite existing files.

The ***Print*** menu selection may be used to print the contents of the active workspace window using the default Print template. Clicking the ***Print*** button displays the dialog box shown in Figure 5-7.

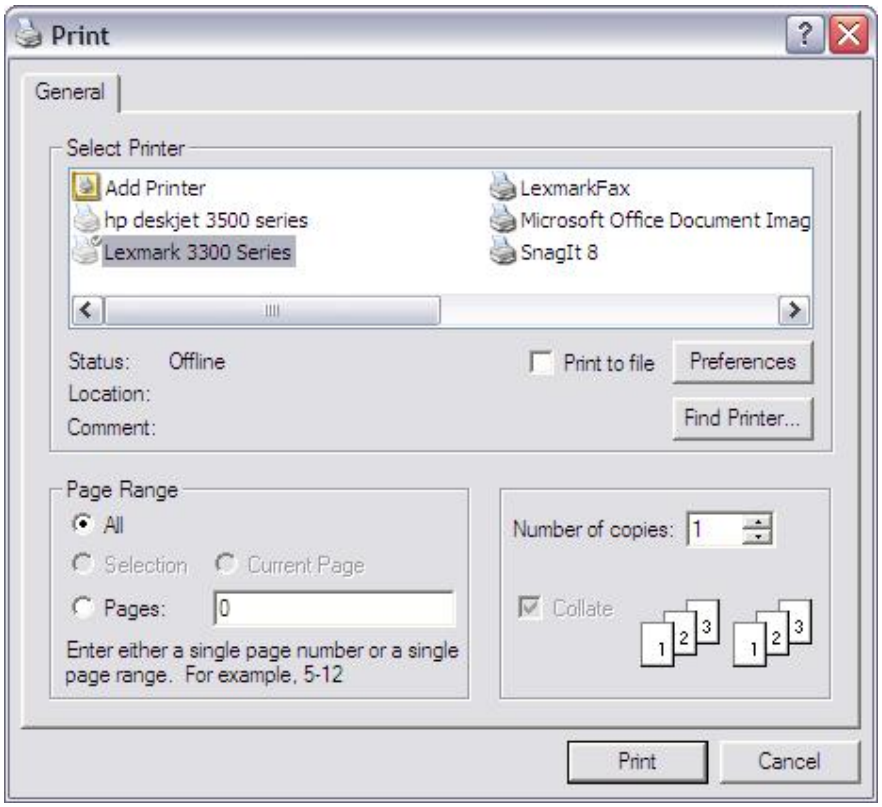


Figure 5-7 Print… *dialog box*

The printers installed on the computer are listed in the window at the top of the dialog box. An option of printing to a file is offered via a check box. The ***Preferences*** button allows you to define the printing parameters, depending upon the printer selected, while the ***Find Printer*** button allows searching of network printers. The page range is redundant in this printing application, as only the active workspace is printed. The option to print multiple copies is given on the lower right hand side of the dialog box. Clicking ***Print*** results in the contents of the active workspace window being printed, while clicking ***Cancel*** dismisses the dialog box without further action.

The ***Print Preview and Templates*** menu selection will bring up the Print Template Editor. This Editor is discussed in the 'Print Template Editor' section of this manual.

Clicking ***Exit*** closes ***Essential FTIR***.

The Display Menu

Clicking on the Display heading yields the menu shown in Figure 5-8

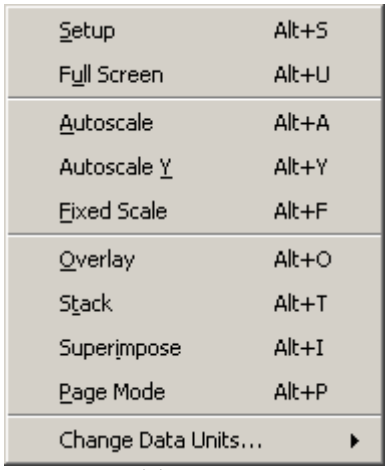


Figure 5-8 The Display Menu

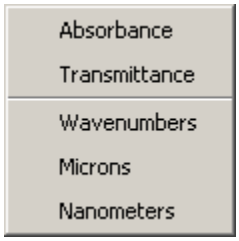


Figure 5-9 *The Change Data Units Menu*

Clicking ***Setup*** results in the ***Display Settings*** parameter box being shown in the ***Tool Parameters Window***, as illustrated in Figure 5-10. This parameter box is also accessible from both the ***Data Toolbox*** and the ***Options*** menu.

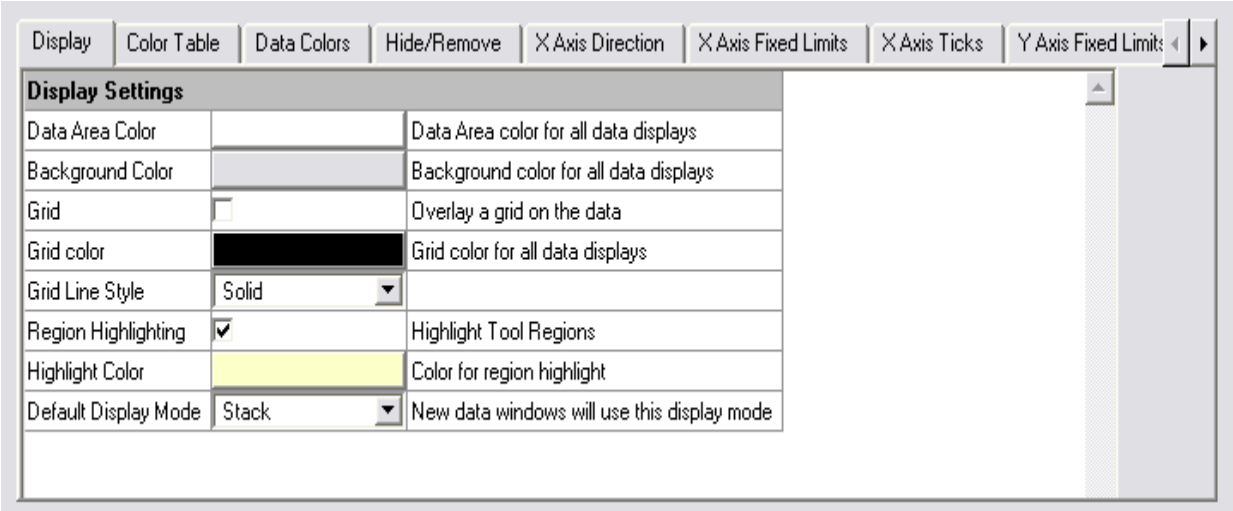


Figure 5-10 Display Settings

The ***Display Settings*** parameters are split into tabs, shown across the top of the window. In Figure 5-10 the first tab, labeled ***Display*** is highlighted. Taking each of the tabs in turn:

Display

Provides fundamental options for the spectrum display. The ***Data Area Color*** button allows you to choose the color of the backdrop to the spectra. Clicking the ***Data Area Color*** button displays the ***Select color*** dialog box shown in Figure 5-11. This dialog box is common to all functions in ***Essential FTIR*** which allow color specification.

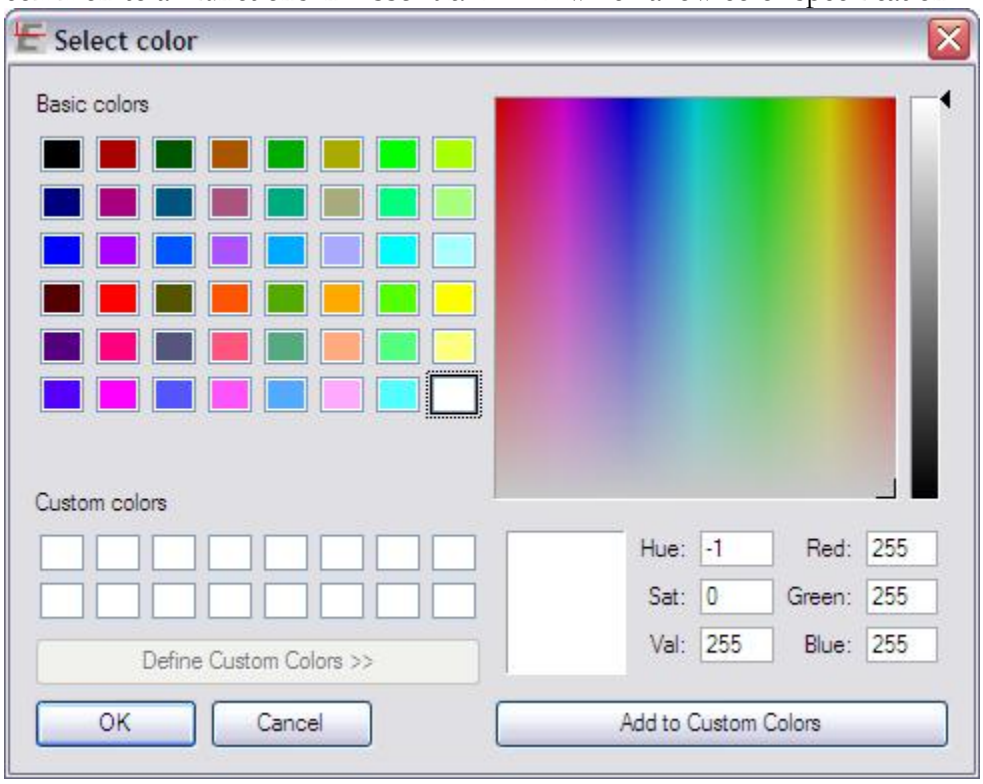


Figure 5-11 Select Color *dialog box*

The ***Select Color*** dialog box comprises a number of elements. A pre-defined selection of colors are displayed on the top left hand side of the dialog, while you may specify an intermediate shade using the custom color picker on the right hand side. These may then be added to the ***Custom Colors*** palette on the lower left of the dialog by clicking the ***Add to Custom Colors*** button.

The ***Background Color*** button summons a dialog box like that shown in Figure 5-11, and allows you to set the frame color for the workspace window. An example of the use of these two options together is shown in Figure 5-12, where both the data area and the frame have custom colors defined.

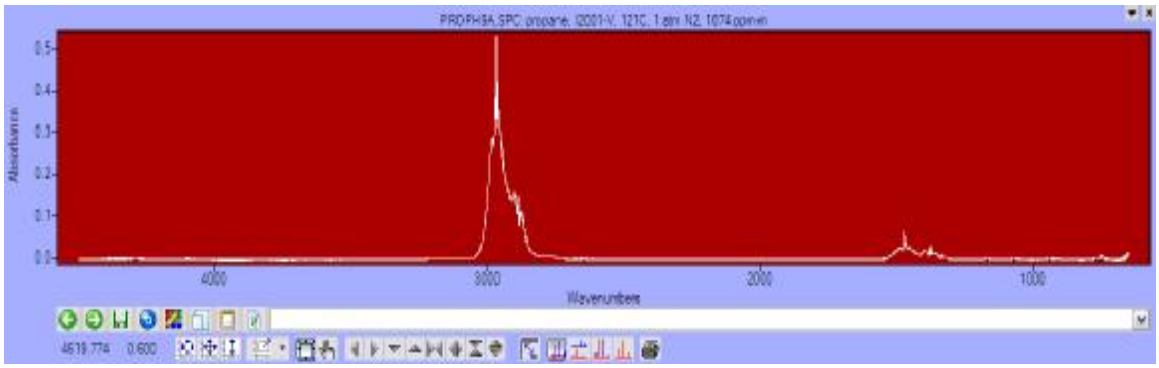


Figure 5-12 *Data area and background color changes*

The ***Grid*** check-box imposes a grid onto the data area, which may be toggled on and off. The ***Grid Color*** button summons the ***Select Color*** dialog box. The ***Grid Line Style*** drop down menu offers a number of choices for the type of grid-lines. The options are ***Solid, Dash, Dot, Dash-Dot*** and ***Dash-Dot-Dot***.

The ***Region Highlighting*** check-box specifies whether regions currently selected for the ***Tools*** in use for the displayed spectrum are shown on the data area. Regions are discussed in detail in chapter five – ***Toolboxes and Tools***. The Highlight Color button summons the dialog box shown in Figure 5-11, and is used to set the color used to shade the region. Hence the workspace shown in Figure 5-13, with dotted yellow gridlines, and a region defined in the ***Zap*** tool may be configured – this is illustrated in Figure 5-13.

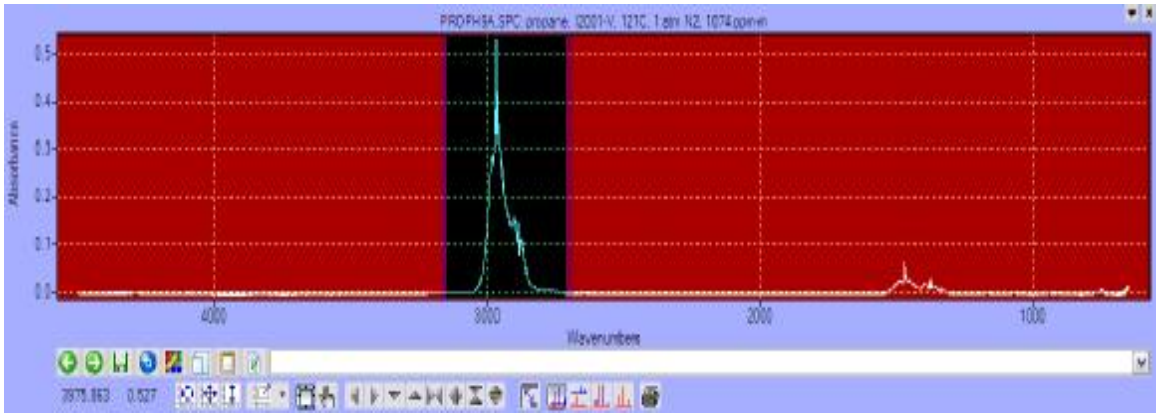


Figure 5-13 *Altered display configuration*

The "Default Display Mode" allows you to chose which display mode will be in effect for new data workspaces.

Color Table

Colors used to display spectra are chosen sequentially from this table:

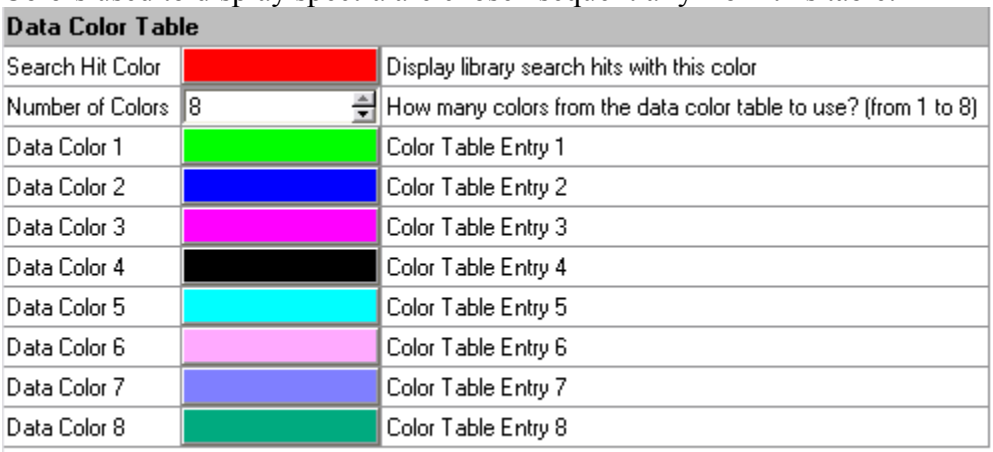


Figure 5-14 The Data Color Table

In this example, we have chosen that the color table consist of 16 colors, and then selected the colors individually for each. So the first spectrum displayed will be green, the second will be blue, and so on. After 8 spectra are displayed, 'Data Color 1' will be used again.

The 'Search Hit Color' allows you display the library search hits in a unique color.

Data Colors

Allows you to set colors for each data file visible in the workspace, via the ***Select Color*** dialog box. Each data file has a corresponding color button, as shown in Figure 5-15. Multiple rows can be selected in the table, and then changing the color of one spectrum will change the color for all the selected spectra.

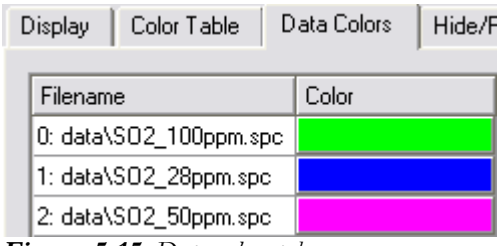


Figure 5-15 *Data colors tab*

Hide/Remove

The ***Hide/Remove*** tab is used to manipulate the visibility of data displayed in the workspace. There are six options available in the ***Hide/Remove*** tab, as detailed in Figure 5-16

Figure 5-16 Hide/Remove *tab*

The options are:

- Make All Visible - Renders all data loaded into the active workspace visible.
- Make Non Visible - Hides all data in the active workspace.
- Invert Selection - Hides visible data and shows hidden data.
- Remove Invisible - Closes data files not visible in the active workspace.
- Remove all Data - Closes all data in the active workspace
- Close all Workspaces – Exits all workspaces on the desktop.

These options are similar to those given when using the context menu for the data window file list, shown in Figure 4-8.

X-Axis Direction

Enables you to choose ascending or descending values for the x-axis from left to right. The ***X-Axis Direction*** tab is shown in Figure 5-17

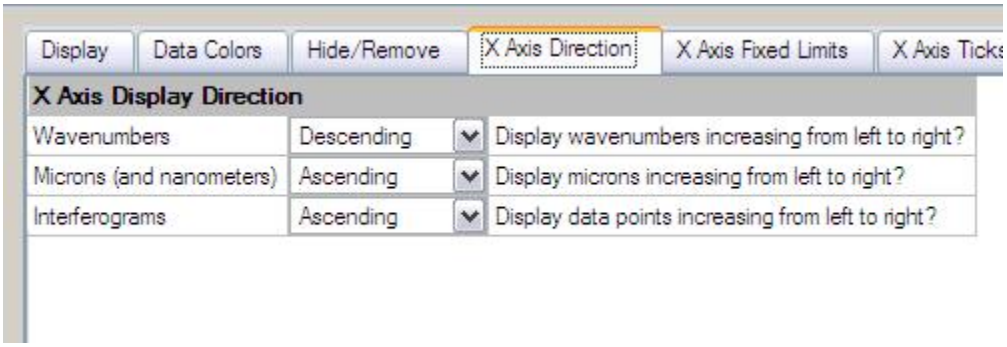


Figure 5-17 X-Axis Direction *tab*

Depending on the format of the data in the workspace, three options may be selected from the drop down menus:

- Wavenumbers
- Microns (and nanometers

- Interferograms

The drop down menus for each file type offer a choice between ascending or descending left to right values. The default for infrared spectra is to display the *x*-axis such that energy (frequency) increases from left to right, which is why wavenumbers are displayed with high values on the left.

X-Axis Fixed Limits

Allows you to specify and apply fixed limits for the x-axis, as shown in Figure 5-18

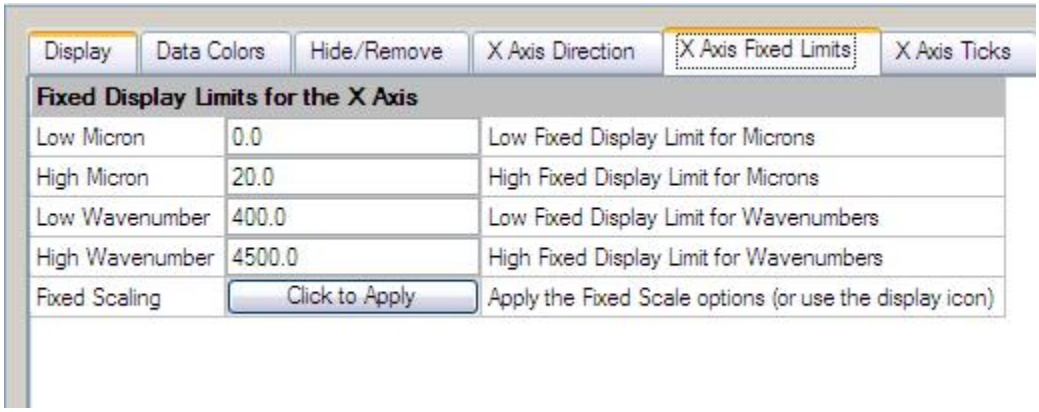


Figure 5-18 X-Axis Fixed Limits *tab*

The edit boxes allow entry of desired axis limits for both microns and wavenumber scales, while the ***Click to Apply*** button applies those fixed limits to the data visible in the workspace.

X-Axis Ticks

Allows setting of tick markers on the x-axis, as shown in Figure 5-19

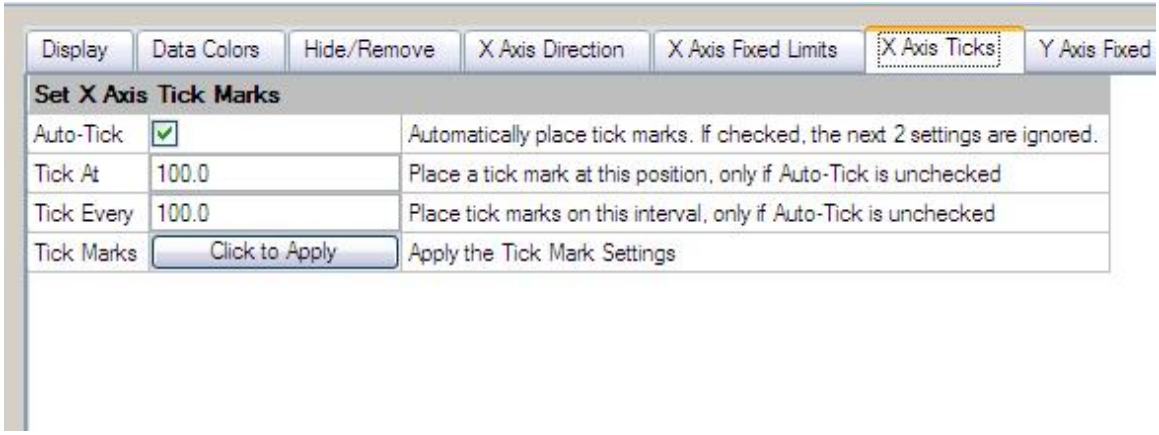


Figure 5-19 X-Axis Ticks

The ***Auto-Tick*** check-box overrides the edit boxes below it. The ***Click to Apply*** button implements the changes to the tick mark settings.

Y-Axis Fixed Limits

Allows you to define fixed y-axis limits on the display, as shown in Figure 5-20. The ***x*** and ***y*** axis fixed limits settings define what happens when you click the fixed limits button on the data window tools. Fixed limits allow data to be viewed in a consistent way, regardless of the actual limits of the data.

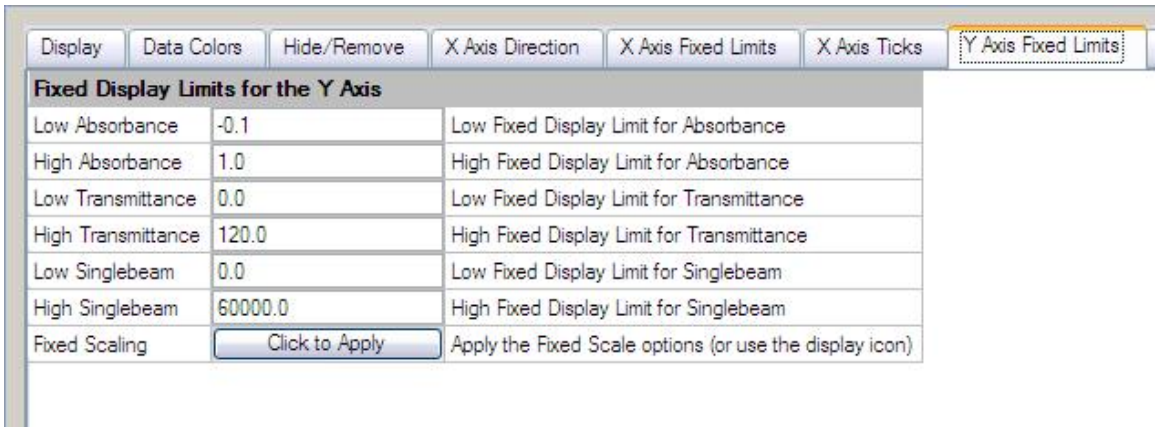


Figure 5-20 Y-Axis Fixed Limits

The tab consists of six edit boxes, which hold the fixed limit values for the low and high display values for absorbance, transmittance and single-beam data. A ***Click to Apply*** button executes any changes made.

Y-Axis Ticks

Allows you to set y-axis tick marks in a manner analogous to the x-axis ticks tab detailed above. The Y-Axis Ticks tab is shown in Figure 5-21

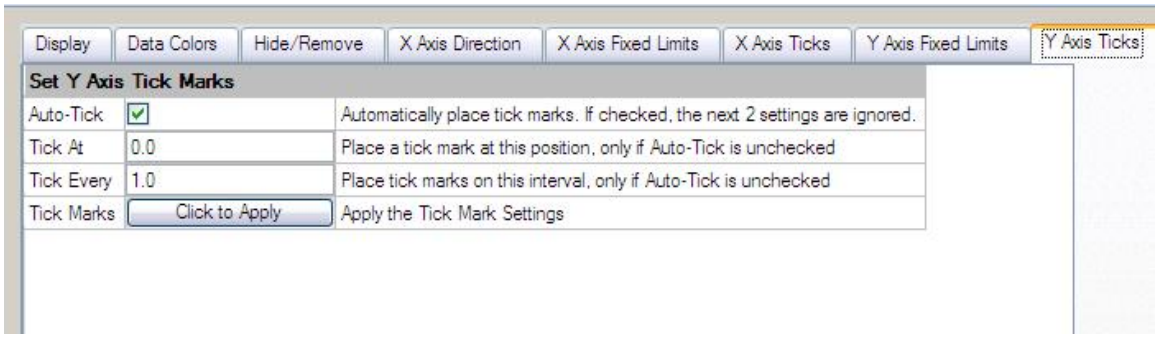


Figure 5-21 Y-Axis Ticks

As before, the ***Auto-Tick*** check-box overrides any subsequent settings.

Plot Labels

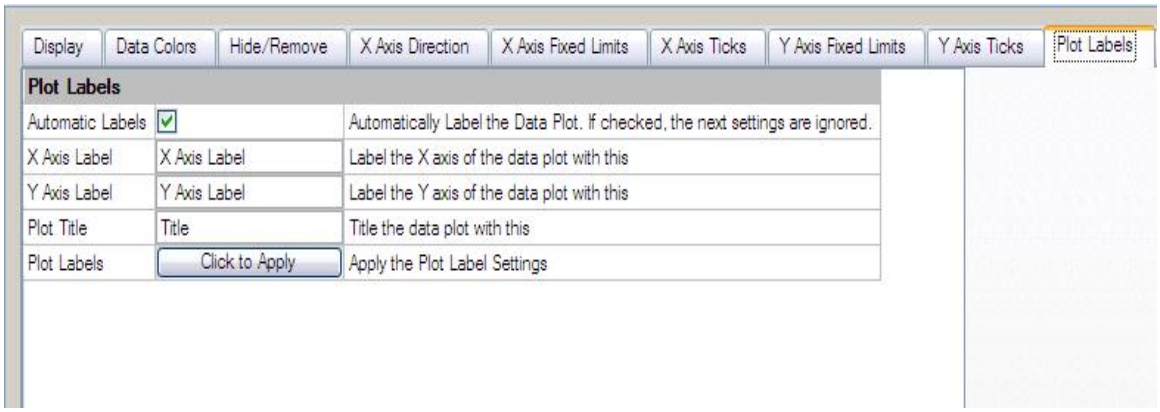


Figure 5-22 Plot Labels

Five options exist in the ***Plot Labels*** options –

1. ***Automatic Labels*****:** A check-box allows automatic labeling of axes, ignoring the settings below.
2. ***X Axis Label***: Title for the X-axis
3. ***Y Axis Label***: Title for the Y-axis
4. ***Plot Title***: Title for the whole plot
5. ***Plot Labels***: The **Click to Apply** button executes the plot labels for the active ***Workspace***.

Printing

The ***Printing*** tab enables print options for the workspace to be set, as shown in Figure 5-23

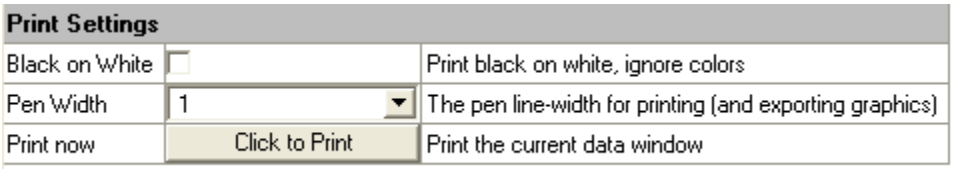


Figure 5-23 Printing tab *options*

The ***Black on White*** check-box may be checked to select black on white printing, with colors disregarded. The drop down menu labeled ***Pen Width*** is used to select the weight of the lines representing the data. The workspace may be sent to a printer using the ***Click to Print*** button.

The subsequent options available on the ***Display*** menu are also accessible via two other methods – the ***Setup*** menu item on the ***Options*** menu, and the ***Graphic Control*** buttons underneath the display area of the ***Workspace***.

Reports

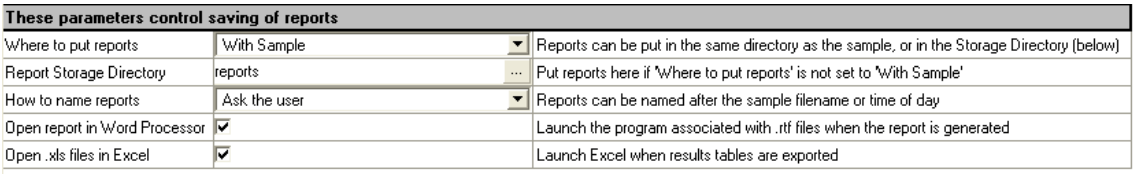


Figure 5-24 Report Settings

The Reports tab controls how and where reports are saved to disk. Some of the tools in Essential FTIR generate information that can be used to automatically create reports. These tools will have a button labeled 'Report' on them. The reports are generated in RTF format, which stands for 'Rich Text Format'. This format can be read and written by Microsoft Word, but more importantly, it can be read and written by Write, also known as WordPad, which is installed with all windows systems.

- ***Where to put reports***: reports can be out into the Essential FTIR reports folder, or can be stored in the same folder as the datafile used to generate the report.
- ***Report Storage Directory***: If the reports are not stored in the same folder as the datafile, use this option to tell Essential FTIR where to put the reports.
- ***How to Name Reports***: The choices are 'Sample Based', in which case the .rtf file will have the same base filename as the FTIR sample datafile used to generate the report; 'Time-Stamped' gives the reports a filename based on the time the report was generated, and 'Ask the User' will prompt the user for a filename.
- ***Open Report in Word Processor***: after the .rtf file is generated, it can automatically be displayed in a word processor. The word processor program that is used depends on your system configuration, eFTIR merely launches the program that Windows has associated with the .rtf file extension.
- ***Open .XLS files in Excel:*** Tables of data can be exported from Essential FTIR into the Excel spreadsheet .xls file format. Optionally, Excel can be automatically launched to display the .xls file.

Display Modes

We now return to the discussion of the ***Display Menu***. After the ***Setup*** menu item, the next element of the ***Display*** menu is the ***Full Screen*** option. Clicking this option toggles between docked and full screen display of the active workspace.

The ***Autoscale*** menu item automatically sets the display limits of the workspace to encompass all points of the active spectrum.

The ***Autoscale Y*** option expands the y-axis to encompass all data without altering the x-axis display settings.

The ***Fixed Scale*** option sets the x and y axes to the limits specified in the ***X-Axis Fixed limits*** and ***Y-Axis Fixed Limits*** on the ***Setup*** dialog – see Figure 5-18 and Figure 5-20.

The final four options concern the way in which active data are displayed in the workspace. Selecting ***Overlay*** results in spectra being plotted on common *x* and *y* axes – hence they are overlaid, as illustrated in Figure 5-25

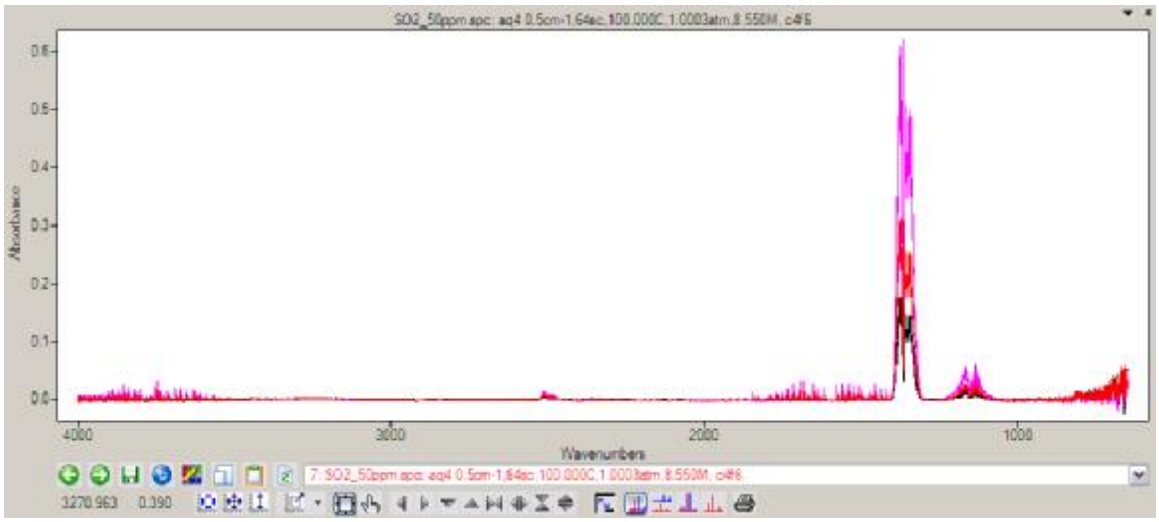


Figure 5-25 *Data in* Overlay *display mode*

The ***Stacked*** option displays the data vertically stacked sets of coordinates, as shown in Figure 5-26

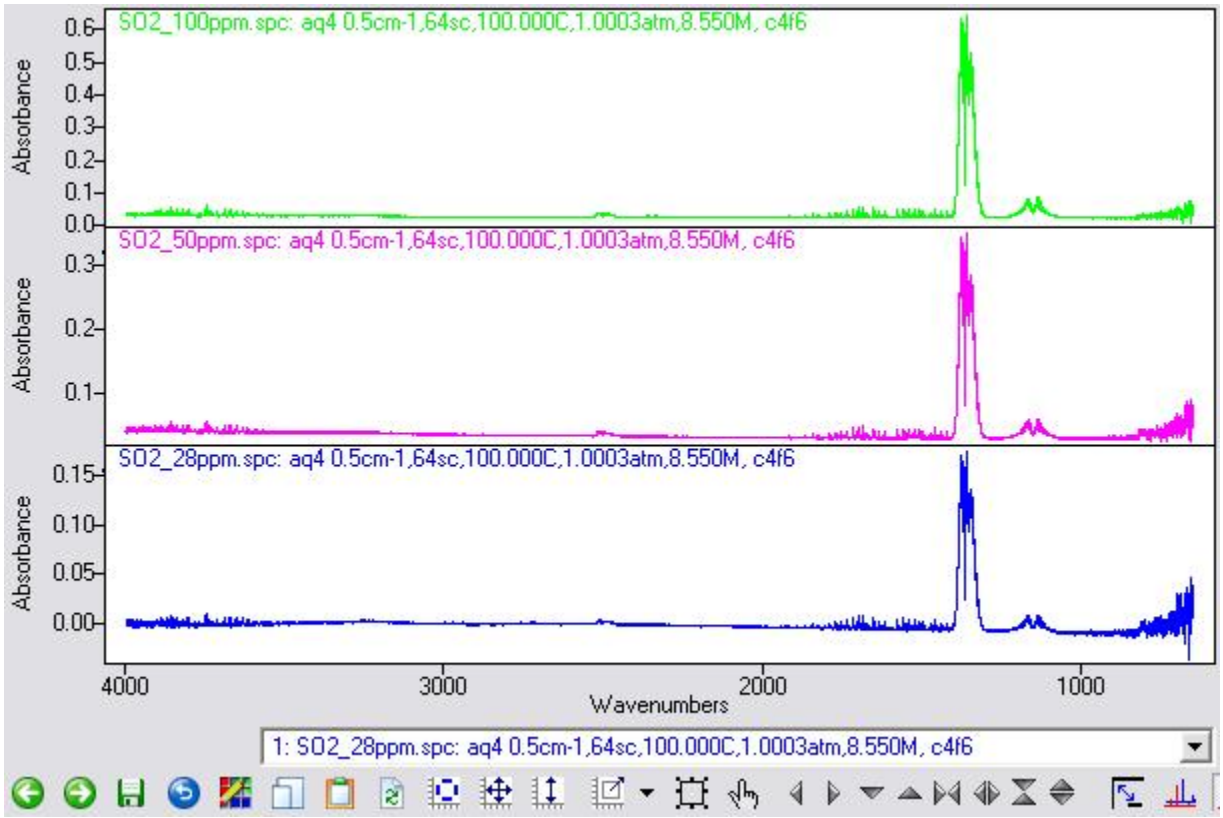


Figure 5-26 *Data in* Stacked *display mode.*

Displaying the data in ***Superimpose*** mode matches the *y* axis magnitude of all active data. This feature is useful for comparing spectra collected at different path lengths or concentrations. An example is shown in Figure 5-27

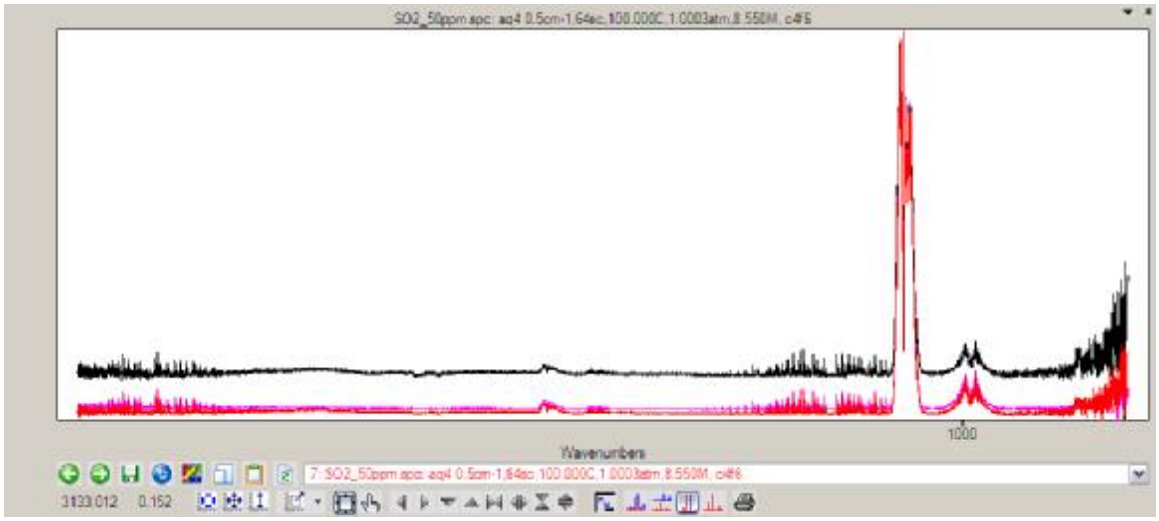


Figure 5-27 *Data in* Superimpose *display mode*

When viewing data in ***Superimpose*** mode, the *y* axis will automatically re-scale as the *x* axis limits are changed. For example, in Figure 5-28 the area between 1000cm^{-1} and 1300cm^{-1} is selected using the cursor in the display window. Notice that the visible absorbance features

are re-scaled so as to match each others magnitude as closely as possible. No tick-marks are placed on the ***y***-axis because they would only apply to the active sample, and may be misinterpreted as they do not apply to the other spectra in the display.

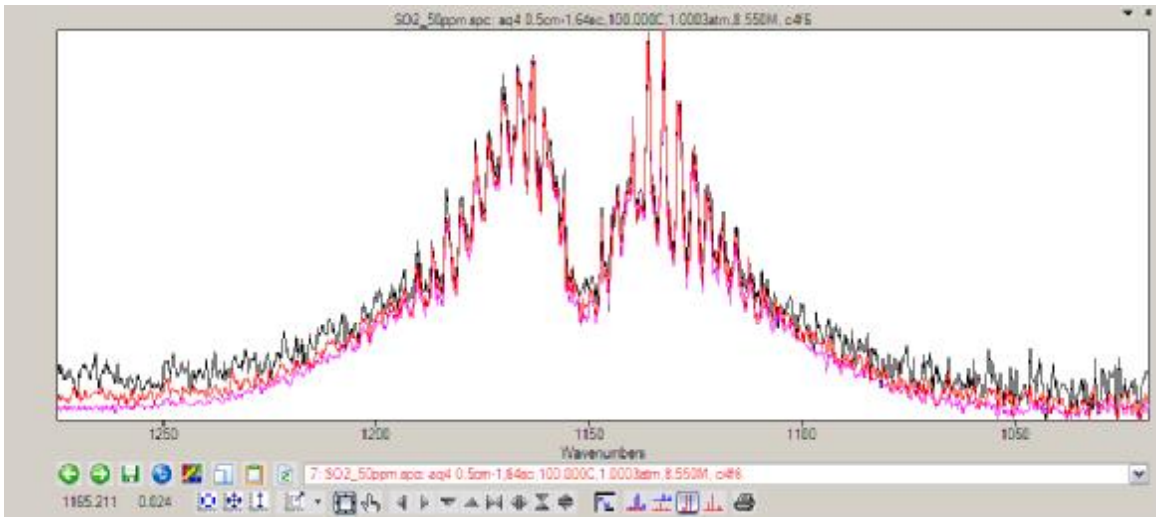


Figure 5-28 *Superimposition with zoomed* x*-axis*

Selecting ***Paged*** mode displays only the active spectrum in the workspace window. Any spectra loaded into the workspace may be selected as active, either by selecting the file in the workspace browser to the left of the display window, or by selecting it from the list box on the display window or by cycling through the spectra in the workspace using the arrow buttons. Paged mode is illustrated in Figure 5-29

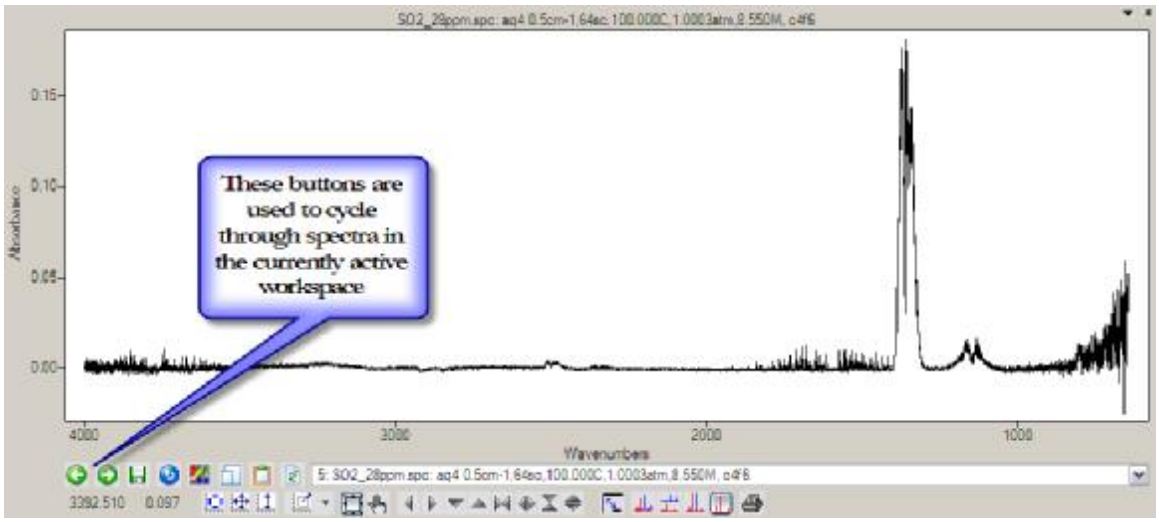


Figure 5-29 *Selecting spectra for display in* Paged *mode*

The ***Change Display Units*** menu item has a submenu:

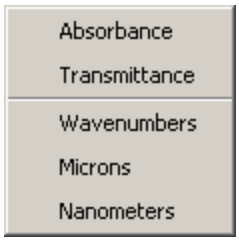


Figure 5-30 Change Display Units.

These choices allow you to force conversion of all the data in a window to share the same units, when such a conversion is possible. This is useful when you have a mixture of absorbance and transmittance data, or a mixture of data calibrated in wavenumbers and wavelengths. Using these menu choices will convert all of the data in the window so they can displayed on the same scale with the same units.

The Options Menu

The ***Options*** menu contains the interface for the ***Setup*** parameters. Selecting Setup from the Options menu delivers the interface shown in Figure 5-31

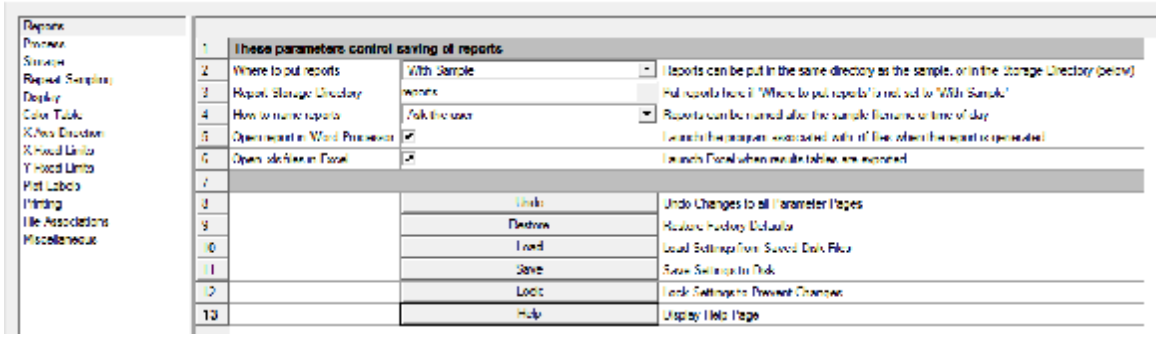


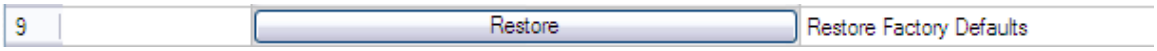
Figure 5-31 Setup *parameters*

The ***Setup*** parameters are displayed as a workspace tab. On the left hand side of this ***Setup*** tab is a secondary menu. This menu comprises options for the collection of data, data processing, instrument alignment, and data storage. In addition, options concerning data display and printing are available. These display options may also be accessed via the ***Display*** settings.

The interface for the ***Setup*** menu is located in the main window of the ***Setup*** tab, on the right hand side. This section of the tab is known as the ***Parameters Page***. The appearance of the particular page is dependant upon which option is currently selected as active. An option is selected by left-clicking on that item in the menu. Once the desired set of parameters is displayed, you may execute changes in those parameters using the drop down menus and edit boxes provided. Each parameter is placed on a numbered row, and we will use these numbers to reference each parameter.

On each of the ***Parameter Pages***, a series of options exist which are common to all pages. We will deal with these options first. With the Reports option selected, as in Figure 5-31, we see that rows 8 – 13 are occupied by a series of buttons. The functions of these buttons are:

The ***Undo*** button rolls back all changes to parameters in the page since the last save.

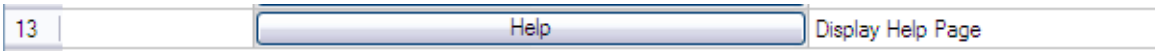


The ***Restore*** button rolls back all parameters in the page to factory default settings

The ***Load*** button summons a dialog box used to locate and load a file containing pre-defined settings for the parameters on that page. The settings file is in ***.ini*** format – see ***Save***.

The ***Save*** button enables you to save the parameters defined in that page to disk. The parameters are saved in a ***.ini*** file.

The ***Lock*** button toggles a "safe" mode on and off, where the parameters in that page are grayed out to prevent changes.



The ***Help*** button is used to display help topics relevant to the parameters page.

As the above buttons are common to all parameter pages, we will not refer to them each time we encounter them, but concentrate on elements unique to each page. Taking each page in turn from top to bottom we have:

Process Options

The Process parameters page is shown in Figure 5-32. These settings pertain to the Fast Fourier Transform (FFT), and control the processing of data from interferogram to a final data type of your choosing.

1	**These parameters control data processing**		
2	Final Data Type	SingleBeam	Process sample data to this data type
3	Starting Wavenumber	500.0	From 0 to 7899 wavenumbers. The first wavenumber value to save in the FFT'd data
4	Ending Wavenumber	4500.0	From 0 to 7899 wavenumbers. The last wavenumber value to save in the FFT'd data
5	Zero Filling	1	Increase the resolution of the processed data through zero-filling
6	Apodization	triangle	The apodization function to use with the FFT
7	Phase Correction	magnitude	The phase correction method to use with the FFT
8	Advanced options	Advanced...	FFT options that don't need to change often.
9			
10		Undo	Undo Changes to all Parameter Pages
11		Restore	Restore Factory Defaults
12		Load	Load Settings from Saved Disk Files
13		Save	Save Settings to Disk
14		Lock	Lock Settings to Prevent Changes
15		Help	Display Help Page

Advanced FFT Settings. Change these with care.Instrument settings may over-ride these when collecting data.

Advanced FFT Settings. Change these with care.
Instrument settings may over-ride these when collecting data.

1	**Advanced FFT Settings**		
2	Laser Wavelength	0.63299	The wavelength of the laser in microns (default 0.63299 for HeNe laser)
3	Laser Sampling Interval	1.0	How often samples are taken relative to the laser zero-crossings
4	Sampling Direction	Forward	Is data collected during forward or reverse mirror travel?
5	Interferogram Symmetry	Single-Sided	When the ADC is turned on
6	Normalize Singlebeam	☐	After the FFT, scale the singlebeam to normalize it
7	Interferogram Baseline Correction	Offset	How to correct the Interferogram Baseline
8	Mertz Points	256	How many interferogram points to use in Mertz Phase Correction
9	Truncate the Interferogram	☑	Limit the spectral resolution by truncating the interferogram before the FFT
10	Truncate Points	2048	If 'Truncate the Interferogram' is checked, this many points will be used. Use the calculator to set.
11	Limit Resolution	Limit Resolution...	Use a calculator to determine 'Truncate Points' to attain a specified resolution

OK Cancel

Figure 5-32 Process and Advanced Process *parameters*

Parameters unique to the page begin at row 2:

2. ***Final Data Type***: Sets the level of processing of the data. The data type is selected from a drop down menu, in a hierarchy of increasing processing from ***Interferogram***, ***Single Beam***, ***Transmittance*** or ***Absorbance***.
3. ***Starting Wavenumber***: Sets the lower limit of the wavenumber range to be computed in the fast Fourier transform.
4. ***Ending Wavenumber***: Sets the upper limit of the wavenumber range to be computed in the fast Fourier transform.

5. ***Zero Filling***: Sets the interpolation factor via a drop down menu for smoothing of acquired data. The interpolation factor may take the values 1, 2, 4, 8, or 16. Zero filling increases the resolution of the data by Fourier interpolation.
6. ***Apodization sets*** the type of apodization function to use in the fast Fourier transform to remove truncation artifacts. ***Triangle, Boxcar, Beer-Norton Med, Beer-Norton Weak, Beer-Norton Strong, Happ-Genzel, Bessel, Cosine, Blackman-Harris 3 Term and Blackman-Harris 4 Term*** are selectable via a drop down menu.
7. ***Phase Correction:*** Sets the type of phase correction function to be used. ***Mertz*** and ***Magnitude*** are selectable via drop down menus. Another choice of ***None*** is available. When ***None*** is selected, the complex un-phase-corrected singlebeam is returned. The real and imaginary data points are interspersed, with the real being in the even numbered array positions and the imaginary in the odd. When selecting ***None,*** select 0 for the starting wavenumber and the Nyquist frequency for the last wavenumber, in order to see the full bandwidth complex spectrum.

Advanced Process Parameters are accessed by clicking on the 'Advanced' button.

2. ***Laser Frequency:*** Used to define the nominal frequency of the HeNe laser used as a clock in a Fourier transform infrared spectrometer. The actual laser wavelength will remain unaffected by any changes to the ***Laser Frequency parameter*** – historically this number was manipulated to correct for shifts in the *x*-axis. It is recommended that the ***X-Shift*** tool is used for this purpose.
3. ***Laser Sampling Interval:*** The available settings are 0.25, 0.5, 1.0, 2.0, 4.0 and 8.0. The bandwidth (full spectral range) of the interferogram data is determined by the Laser Frequency and the Laser Sampling Interval. For instance, if the laser frequency is 0.63299, the wavenumber bandwidth is 10000 / 0.63299 / 2 , or 7899 cm-1 (the division by 2 is called for by the Nyquist theorem). However, if data is sampled more often, say twice every laser cycle, the bandwidth is twice that, or 15798 cm-1. The value of 0.25 corresponds to taking 4 samples every laser cycle, 0.5 to 2 samples, 1.0 to 1 sample, and so on.
4. ***Sampling Direction:*** The available settings are ***Automatic Detection, Forward, Reverse, or Both***. An infrared spectrometer can take data when the mirror is moving forward, backward, or in both directions. Essential FTIR will automatically detect when the data is Bi-Directional (Both) or not. In the case where the data is not bi-directional, it is assumed to be Forward. This setting is can be used to manually tell the program how to handle the data. After the FFT is done, the audit trail will contain information about what the software used for interferogram direction. When collecting and processing data from an instrument, this setting is typically taken from the instrument and such an instrument setting will over-ride whatever is specified here.
5. ***Interferogram Symmetry:*** The available settings are ***Automatic Detection, Single-Sided and Double-Sided***. Single sided interferograms are sometimes called 'asymmetric' and double sided 'symmetric'. An infrared spectrometer can initiate data collection such that the ZPD is placed in the middle or near the beginning of the interferogram. This setting can be used to tell the software how to handle the data, because single and double sided interferograms are apodized

differently. Like the Sampling Direction setting,, the audit trail will contain information about what the software used for interferogram symmetry. When collecting and processing data from an instrument, this setting is typically taken from the instrument and such an instrument setting will over-ride whatever is specified here.

6. ***Normalize Singlebeam:*** After the data is FFT'd, some software will scale the data by the inverse of the number of FFT points. This setting is here so the you can produce data compatible with data from other software.

7. ***Interferogram Baseline Correction:*** An interferogram may contain a DC offset, usually originating from the spectrometer electronics. The baseline must be brought to zero or there will be a discontinuity between the interferogram and the zero-filled portion. This discontinuity will create a sine wave in the singlebeam after the FFT. The choices for baseline correction are offset and linear. Offset baseline correction subtracts off the average value of the interferogram, removing a DC offset.. Linear baseline correction subtracts off a straight line calculated by performing a linear regression through the entire interferogram. The linear baseline correction will get rid of a DC offset and a higher order term, as could happen if the DC offset is not constant and slowly drifts.

8. ***Mertz Points:*** Mertz phase correction uses a small portion of the interferogram centered on the ZPD. The phase changes very slowly with wavenumber, so only a low resolution interferogram is needed. This option allows control of the resolution of the interferogram used to calculate the Mertz phase correction. The default of 256 points is probably sufficient for most data.

9. ***Truncate Points:*** This is a 'read-only' field; it cannot be changed by direct editing. Click *the 'Limit Resolution'* button to set this value. The interferogram can be truncated before the FFT is performed, to achieve a specific optical resolution.

10. ***Limit Resolution:*** Clicking this button bring up the 'Limit Resolution' calculator, explained in the next section.

Limit Resolution Calculator

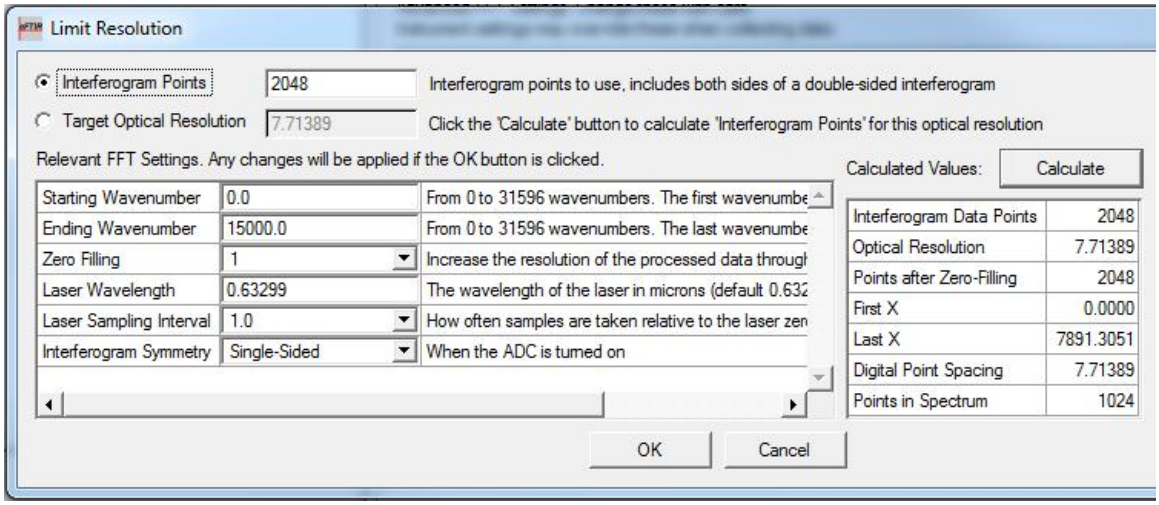


Figure 5-33 *The Limit Resolution Calculator*

The interferogram can be truncated before the FFT to produce a spectrum with an exact optical resolution. The interferogram can also be zero-filled to produce an exact digital resolution (data point spacing). This is useful to make spectra match exactly, and is a better way of matching spectra than decimating or interpolating the singlebeam spectra after the FFT.

Either a specific number of points or a target resolution can be specified. On the left side, the FFT settings that affect resolution can be set. Clicking the 'Calculate' button will fill in the grid on the left side with the values calculated from the settings on the left side.

Clicking the 'OK' button will copy any changes made to the table of 'Relevant FFT Settings' table back to the 'Interferogram To Spectrum' settings. Also, the 'Truncate Interferogram' check box will be checked, and the 'Truncate Points' field will be filled with the 'Interferogram Data Points' value.

For a given resolution and laser wavelength the number of points on either side of the ZPD is given by

$$\text{floor}\left(\frac{2\cdot 10^{7}}{\lambda_{.laser}\cdot \text{Resolution}}\right)$$

Where the interferogram is sampled every zero-crossing, the laser wavelength is in nm, and the resolution is in cm-1.

Storage Options

The Storage parameters page is shown in Figure 5-33

1	**These parameters control saving of collected data**		
2	Save these Sample Data Types	abs, trn, sbm, ifg ...	Which Sample data types to save
3	Save these Background Data Types	sbm, ifg ...	Which Background data types to save
4	Root Storage Folder	junk ...	Where to put collected data
5	Time-Stamped Folders	☐	Store data in time-stamped sub-folders of the root storage folder
6	Enable Backups	☑	Enable automatic backup of collected data
7	Root Backup Folder	backup ...	Where to put backup data (if backups are enabled)
8	File Naming Scheme	Sequentially Numbered ▼	How to name newly collected files
9	Filename Prefix	mf5	Prepend this to all new filenames
10	Filename Seed	Seed is 8395 ...	Starting number for sequentially numbered files
11	Prompt For Filename	☑	Ask the user where to save the data after data is collected

Figure 5-33 Storage *parameters*

The storage parameters begin at row 2.

2. ***Save these Sample Data Types***: Offers the choice of saving any of four kinds of data. On the right of the row, notice the edit button labeled with three periods (**…**). Clicking this button summons a dialog containing four check boxes. These are labeled ***Absorbance***, ***Transmittance***, ***Single Beam*** and ***Interferogram***. Checking ***Interferogram***, while leaving the other options unchecked, will save only the raw interferogram to disk. Adding the ***Single Beam*** option will additionally save the Fourier transform of the interferogram to disk. Checking the ***Transmittance*** box will enable saving of the ratio of the single beam against the current or selected background. Finally, and as is recommended, if all boxes are checked the ***Absorbance*** spectrum (negative logarithm of the transmittance spectrum) will also be saved.
3. ***Save these Background Data Types***: When recording background spectra, two options are available for data storage. These are Interferogram and Single Beam. Again, it is recommended that all data types be saved to disk.
4. ***Root Storage Directory***: Defines the default directory to which data is saved. Clicking the edit button (…) summons a dialog allowing you to specify or create a folder for data collection.
5. ***Enable Backups***: Toggles on or off automated backing up of data – see line 6. If backups are enabled, new data is automatically copied to the backup directory as it is generated.
6. ***Root Backup Directory***: Enables you to set the directory for backups of collected data. This may be on a different drive from the original data, thus providing insurance against disk failure.
7. ***File Naming Scheme***: A drop down menu allows specification of the system for naming consecutively collected files. Three options are available – ***Time Stamped***, where files are named according to the time of acquisition (on the computer clock), ***Sequentially Numbered***, where each file is named with an number which is incremented each time a spectrum is acquired, and

Sequentially Numbered in 8.3 Format., where the incremental numbering is observed in accordance with the old DOS format. This results in eight-character filenames (padded with leading zeros) and three character file extensions, hence the term 8.3.

8. ***Filename Prefix***:: The editable text box in row 8 accepts a string, which is used as a prefix for file names, unless the File Naming Scheme is set to 'Time-Stamped' For instance, if the filename prefix is 'br' and the filenaming scheme is 'Sequentially Numbered in 8.3 Format', the first filename will be 'br000001', the second 'br000002', and so on.
9. ***Filename Seed***: Provides the starting number for sequentially numbered data files. Note that if the 8.3 format detailed in option 7 is applied, an absorbance file with the seed "1" will become *00000001.abs*
10. ***Prompt for Filename***: Checking this box instructs the program to offer a file naming and saving dialog box after each data file is collected.

The ***Storage*** settings collectively control the names of acquired data files. As an example, consider the results of settings where option ***7*** is set to ***Sequentially Numbered in 8.3 Format***, option ***8*** is set to "test", option ***9*** is set to "1" and option ***11*** is set to ***Use .spc Extension.*** The name of the fourteenth file acquired under this scheme would be: test0014.spc

Repeat Sampling Options

1	**These parameters control frequency and duration of repeat sampling**		
2	Sample Fast	☑	Sample as fast as possible; ignore Sampling Frequency
3	Sampling Frequency	00:00:00	Start a sample this often (HH:MM:SS); only if 'Sample Fast' is unchecked
4	How long to sample	Forever	How many repeat samples to collect
5	Sampling Duration	00:00:00	Collect samples for this long (HH:MM:SS); only if 'How long to sample' is 'Time-limited'
6	Number of Samples	10	Collect this many samples; only if 'How long to sample' is 'Sample-limited'
7	Max Spectra	50	The maximum number of spectra in the collection window
8	Save to a multifile	☑	Save the data into a GRAMS multifile
9	Start Now	☐	Start collection when 'Start' is clicked, otherwise wait for the Starting Time (below)
10	Starting Time	18:00:00	Start data collection at this time (HH:MM:SS), in 24-hour time. Only if 'Start Now' is unchecked

Figure 5-34 The Repeat Sampling settings

Sample Fast:. Collects spectra immediately upon finishing the previous collection, regardless of other settings specifying wait times.

Sampling Frequency: The edit box is used to specify a time interval for sampling. The interval may be input in an HH:MM:SS format, where HH is hours, MM is minutes and SS is seconds. This parameter is ignored if '***Sample Fast'*** is selected.

How long to sample. The choices are '***Forever***', meaning to sample indefinitely, '***Time-Limited'***, and '***Sample-Limited'***. ***'Forever'*** means to collect data indefinitely. '***Time-Limited***' means to sample for the length of time specified by ***Sampling Duration***. '***Sample Limited'*** means to sample until the number of spectra specified by the '***Number of Samples'*** setting is reached.

Sampling Duration: An edit box in HH:MM:SS format allows specification of duration for sampling. The instrument will sample continuously according to the ***Sampling Frequency*** parameter until the duration is reached. This parameter is overridden by the previous ***Sample Forever*** setting. Note, this is not a clock time, but a length of time for data collection.

Max Spectra. During Repeat Sampling, every spectrum is displayed. When collecting hundreds, or even tens of thousands of spectra, the program would quickly run out of memory unless the number of spectra held in memory is restricted. This setting determines the maximum number of spectra that will be displayed at one time. In the figure, the setting is 50. After 51 spectra are collected, the 1st spectra will be removed from the display so that the 51st can be displayed. This setting does not have any affect on the saving and storage of data, only on the display of the most recent data.

Save to a multifile: The spectra collected by Repeat Sampling can be saved in s single file containing multiple spectra, known as a 'multifile'.

Start Now: Start the Repeat Sampling data collection immediately, when the green 'Start' button is pressed.

The next five options on the menu – ***Display***, ***X-Axis Direction***, ***X Fixed Limits***, ***Y Fixed Limits*** and ***Printing*** are discussed in detail in the ***Display*** section, from Figure 5-8 to Figure 5-22.

File Associations

1	**Set File Associations for so Windows can use Essential FTIR to display files**		
2	File Associations	Click To Set	Set the windows file assocations for spectral data to this program

Figure 5-35

File Associations tells Windows to use Essential FTIR to be the file handler for spectral data files. Windows 'File Associations' are made by associating the file extension, which is the part of the filename after the '.', such as .spc. Windows uses can associated a particular application with a particular filename extension, and use that application to handle a file when that file is clicked on in windows file explorer.

Miscellaneous Options

The final option we are concerned with in this section is the miscellaneous parameters. These parameters are shown in Figure 5-36.

1	**Miscellaneous program control settings that don't fit elsewhere**		
2	Time Format	%H:%M:%S	The template for displaying time of day. See Python strftime() docs
3	Date Format	%m/%d/%Y	The template for displaying dates. See Python strftime() docs
4	NaN Handling	Replace with zero	How to handle data that contains IEEE NaNs?
5	Startup Help	☑	Show a help screen when the program starts up
6	Startup Help Screen	getting_started ...	Display this help screen at startup

Figure 5-36 Miscellaneous *parameters*

The Miscellaneous options run from row 2 to row 7.

1. ***Time Format***: The format in which the time is displayed – see table below.
2. ***Date Format***: The format in which the date is displayed – see table below
3. ***NaN Handling.*** Sometimes spectra contain 'NaN's, which are a representation of missing or invalid values. This option tells eFTIR how to handle these values, because a having NaNs in a spectrum will cause problems when doing math on the spectrum. The NaNs can be replaced with zeros, or can be be replaced with values interpolated from the nearest valid numbers.
4. ***Startup Help***: This check-box selects whether a ***Help*** workspace window is summoned upon starting ***Essential FTIR***. If the box is left unchecked then no help page will be shown when starting the software.
5. ***Startup Help Screen***: The edit button (**…**) is used to choose which help page is loaded upon starting the program, assuming the ***Startup Help*** check-box in row 6 is selected. This option enables customization of the information shown to you on starting Essential ***FTIR***. The help pages are in the standard HTML format. With this option the software can be customized to display information specific to the site or application.

The date and time formats may be set using the scheme shown below, in conjunction with options 2 and 3.

%a	Locales abbreviated weekday name.
%A	Locales full weekday name.
%b	Locales abbreviated month name.
%B	Locales full month name.
%c	Locale's appropriate date and time representation.
%d	Day of the month as a decimal number [01,31].
%H	Hour (24-hour clock) as a decimal number [00,23].
%I	Hour (12-hour clock) as a decimal number [01,12].
%j	Day of the year as a decimal number [001,366].
%m	Month as a decimal number [01,12].
%M	Minute as a decimal number [00,59].
%p	Locale's equivalent of either AM or PM.
%S	Second as a decimal number [00,61].
%U	Week number of the year (Sunday as the first day of the week) as a decimal number [00,53]. All days in a new year preceding the first Sunday are considered to be in week 0.
%w	Weekday as a decimal number [0(Sunday),6].

%W	Week number of the year (Monday as the first day of the week) as a decimal number [00,53]. All days in a new year preceding the first Sunday are considered to be in week 0.
%x	Locale's appropriate date representation.
%X	Locale's appropriate time representation.
%y	Year without century as a decimal number [00,99].
%Y	Year with century as a decimal number.
%Z	Time zone name (or by no characters if no time zone exists).
%%	A literal "%" character.

The Tools Menu

The ***Tools*** menu contains the ***Essential FTIR*** features which give the program its power. The Tools menu is shown in Figure 5-37.

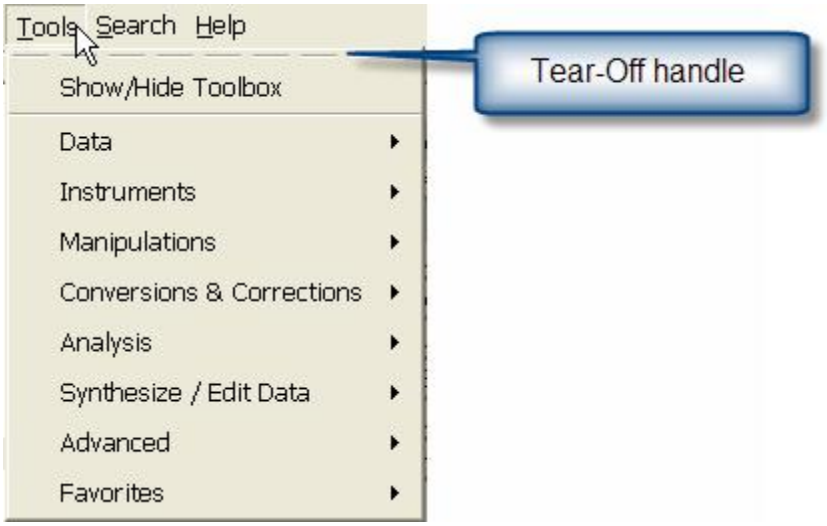


Figure 5-37 Tools *menu*

Note the dashed line called the 'Tear-Off Handle'. Clicking on this line in the menu will make the menu float as a separate window above the application, making all the menu choices available all the time, without having to pull down the menu.

The ***Toolboxes*** and ***Tools*** presented by the ***Tools*** menu may be accessed either using this menu, or by using the ***Toolbox Selection Window.*** The methods of access are equivalent, though there are differing schools of thought on which method is more intuitive. The menu system is a familiar feature of software running on Microsoft Windows systems, and many users find that this familiarity allows them to feel comfortable with ***Essential FTIR*** more quickly. However, the ***Toolbox Selection Window*** is designed to make all tools accessible with a minimum of mouse movement, and once you are familiar with this interface it is usually the faster method of access.

As with other program features where redundancy is employed in an effort to provide you with the most intuitive and comfortable access options, we must make a choice concerning

which section is most appropriate in which to present the features. As it will be necessary to present a section on the ***Toolbox Selection Window***, we will provide a detailed description of all ***Toolboxes*** and ***Tools*** in that section. The only feature unique to the Tools menu is the Show/Hide Toolbox option, which allows toggling of the Toolbox selection window. This feature may be used to create more room at the bottom of the screen for tools,if you intend to access features solely using the menu bars.

The Help Menu

The Help menu is shown in figure Figure 5-38.

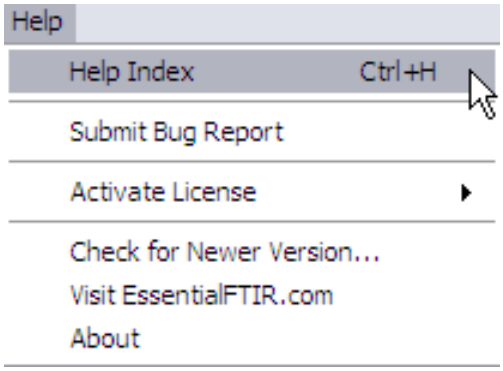


Figure 5-38 Help *menu*

The ***Help*** menu provides a number of features. The first item on the menu, the ***Help Index***, allows you to display a page containing ***Links*** to instructions and information on the functions of Essential FTIR. This Help is a separate file named 'eftir.chm', and is displayed in the standard Windows help file viewer:

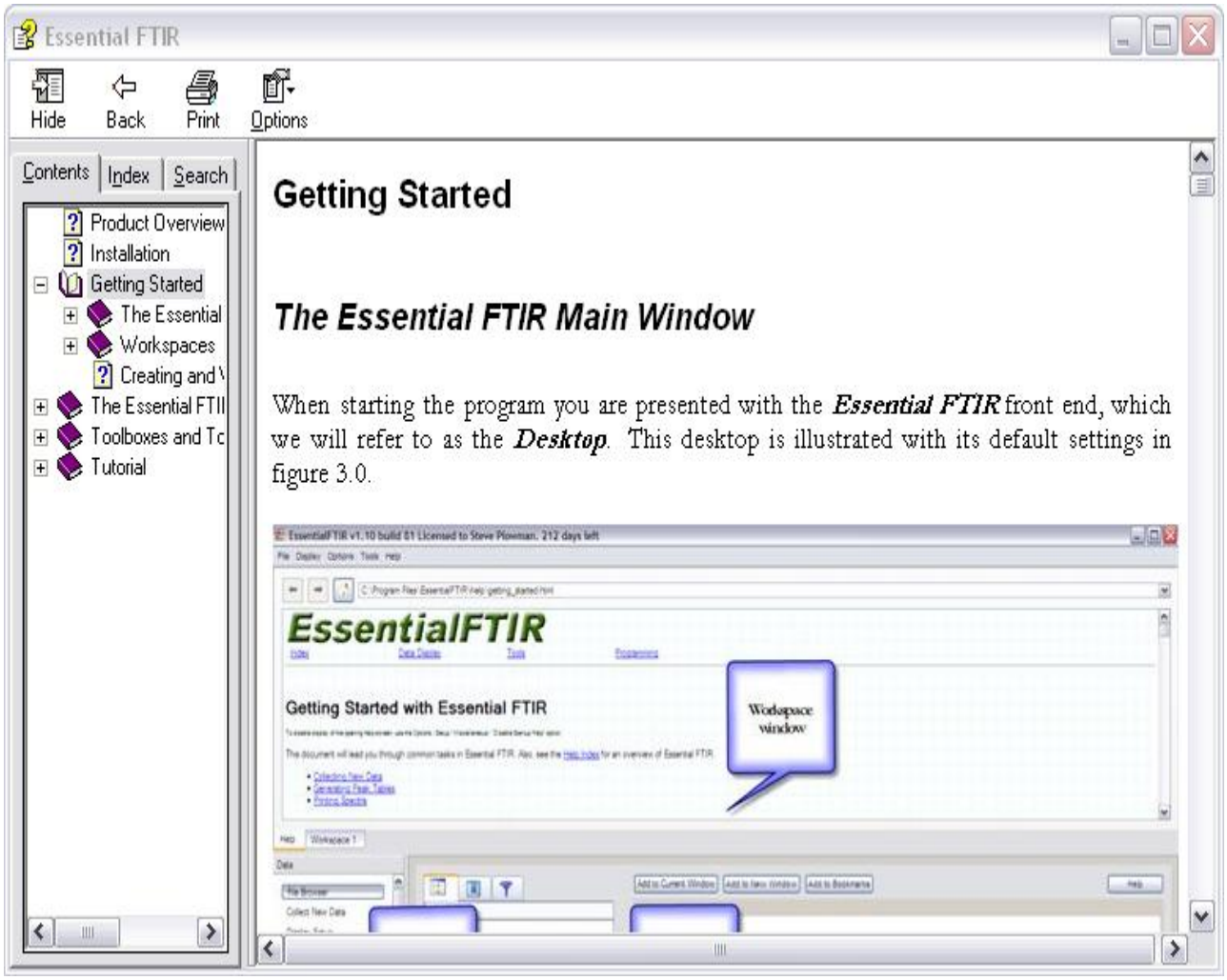


Figure 5-39 The Help File.

The ***Submit Bug Report*** option may be used should you encounter any irregularities or problems with ***Essential FTIR***. The computer used must be connected to the internet in order to use the option. This feature allows the producers to react quickly to any problems.
The ***Activate License*** feature is used whenever a user needs to upgrade a license for ***Essential FTIR*** – for example, when switching from a trial version to the fully licensed product. Two options exist for activation – ***Internet Activation*** or ***Manual Activation***. These options require a user name and a code for activation – these will be provided to license holders.

The ***Check for Newer Version*** option contacts the ***Essential FTIR*** website – www.essentialFTIR.com - to determine if a later version of the program is available, and if such a version is found you will be prompted to download and install the updated version. This will not affect any previously collected data. This option assumes that an internet connection is present on the computer running ***Essential FTIR***.

The ***Visit Essential FTIR.com*** option may be used to connect to the official ***Essential FTIR*** website – www.essentialFTIR.com -, which contains information and downloads relevant to the program,

Finally, the ***About Essential FTIR*** option provides information on version number, build number, copyright and other information regarding the software.

6. Instruments: Collecting data from a spectrometer

Collecting Data

Although different instruments will have different capabilities and settings, Essential FTIR uses a common interface for setting instrument parameters and collecting data. This section of the manual will discuss the common features for all instrument data collection.

A data collection tool has a 'Start' button which initiates data acquisition, sometimes referred to as 'scanning', or 'collecting a scan'.

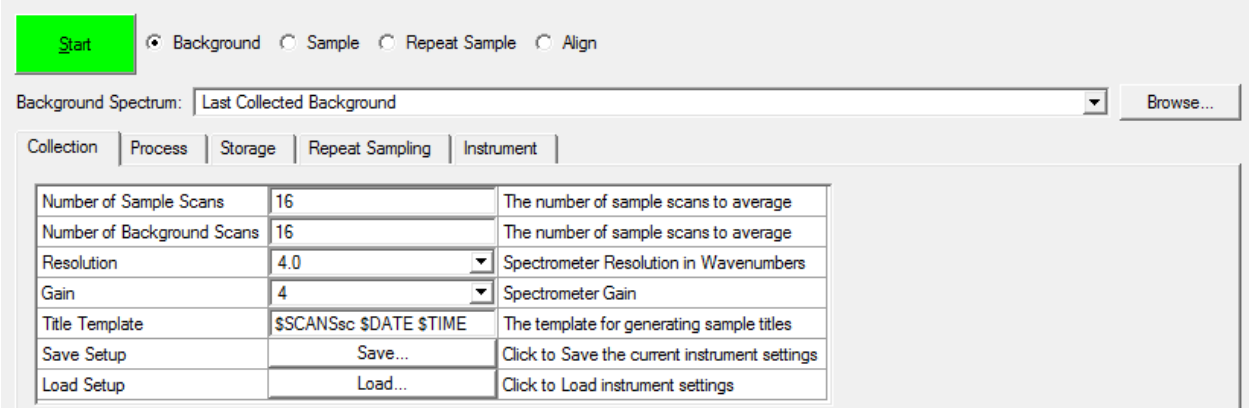


Figure 6-1 A typical data collection tool, showing the 'Collection' settings tab.

To the right of the Start button are four radio buttons, which modify the action performed by the Start button.

- Background: Collect a background spectrum
- Sample: Collect a sample spectrum
- Repeat Sample: Collect samples repeatedly, under program control
- Align: Collect single-scan interferograms repeatedly. This is used to optimize the instrument, for instance to adjust an accessory or tweak the electronics.

Below the green Start button is a drop down list labeled 'Background Spectrum'. A stored background can be used by clicking the Browse button and selecting a stored spectrum. 'Last Collected Background' is selected in the list, so Essential FTIR will automatically use the last background when processing sample data.

Below the background selection list is a series of tabs, each of which contains a table of parameters that control aspects of the instrument, data processing, and data storage.

All supported instruments will have at least these tabs, as shown in Figure 6-1

- Collection
- Process
- Align
- Storage
- Repeat Sampling

In addition, if the instrument has settings that don't fit into the above categories, there may be an additional tab labeled:

- Instrument

At this stage, it will be helpful to briefly summarize the steps involved in collecting valid FTIR data.

- A background spectrum must be collected or loaded from disk. FTIR is a single beam technique; therefore background data is needed in order to interpret the sample data. This is apparent from Beer's law, which states that $T = I_0 / I$, where T is the fraction of infrared energy of a given wavelength reaching the detector, I_0 is the background single beam spectrum and I is the sample spectrum.
- Depending upon the final data type selected from the ***Collection*** parameters, the interferogram may be Fourier transformed from the time domain to the frequency domain to create a single beam sample spectrum.
- The ratio of the single beam sample spectrum and the background spectrum may then be computed to give the fractional transmittance spectrum.
- Finally, the negative logarithm of this transmittance spectrum may be computed to give an absorbance spectrum. The absorbance spectrum is linearly related to the concentration of absorbing species whereas the transmittance spectrum is logarithmically related.

A background spectrum is collected by selecting the ***Background*** radio button and pressing ***Start***. A previously saved background spectrum may also be loaded from disk using the ***Browse*** button. Once the background single beam spectrum is collected, and the final data type (interferogram, single beam, transmittance or absorbance spectrum) is selected, the radio buttons should be used to select either ***Sample*** or ***Repeat Sample***. The repeat sample parameters may be set as shown in chapter five. An example of the use of the ***Collect New Data*** tool is given in Tutorial chapter.

The Collection Tab

The collection tab is shown in Figure 6-1. This table of settings gathers the most commonly changed instrument settings. Each line of the settings table has three columns: a label, a visual control for changing the setting, and a brief description of the purpose of the value.

Number of sample scans	When collecting Sample data, this number of individual scans will be averaged.
Number of background scans	When collecting a Background spectrum, this number of individual scans will be averaged.
Resolution	The optical resolution of the data that will be collected. The available values will depend on the instrument. A typical range of values is 0.5 to 32 cm-1.
Gain	A gain multiple, for increasing the signal gain of the instrument
Title Template	This template will be expanded to produce a title for all spectra. See the 'Title Template' section below for more information. The title is stored with the spectrum in the data file.
Save Setup	Allows saving of all instrument parameters, allowing you to configure the instrument for different experiments, and recall those settings at a later time.
Load Setup	Recall instrument settings that were previously saved with the 'Save Setup' button.

Title Templates

A title template can contain any text, but some of the text is special 'meta-text', which is replaced with information about the spectrum when the data is acquired from the instrument. These are the available meta-text strings:

$SCANS	Will be replaced with the number of averaged scans
$GAIN	Will be replaced with the gain setting
$RES	Will be replaced with the resolution setting
$DATE	Will be replaced with the current data, formatted according to the data formatting settings in the Tools/Options/Miscellaneous screen.
$TIME	Will be replaced with the current time, formatted according to the data formatting settings in the Tools/Options/Miscellaneous screen.

For instance, for the settings shown in Figure 6-1, and a title template of "Intake sample: $SCANS scans; gain $GAIN; resolution $RES", the resulting title assigned to a new spectrum would be "Intake sample: 16 scans; gain 4; resolution 4.0".

Process

The Process settings are identical to those documented in the section about the Options / Process menu. Please refer to that section of the manual for more information.

Storage

The storage parameters are show in Figure 6-2

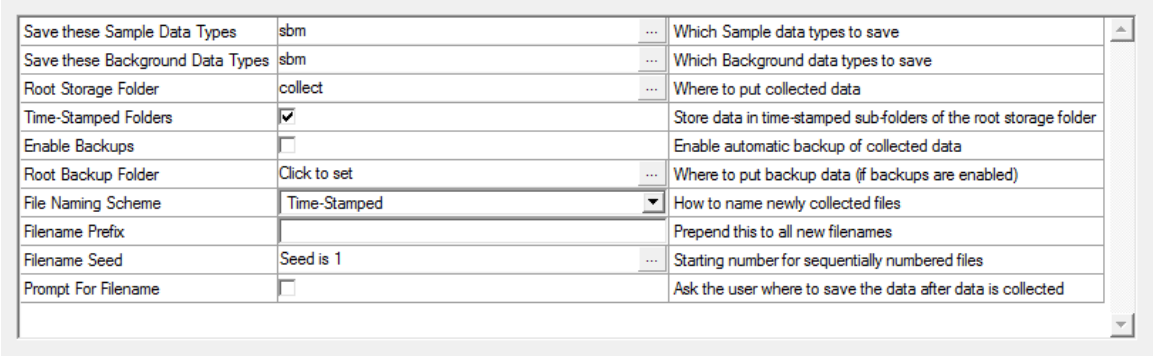


Figure 6-2 The data collection Storage settings

These settings are identical to those documented in the section about the Options / Storage menu. Please refer to that portion of the manual for more information.

Repeat Sampling

The Repeat Sampling parameters page is shown in figure Figure 6-3.

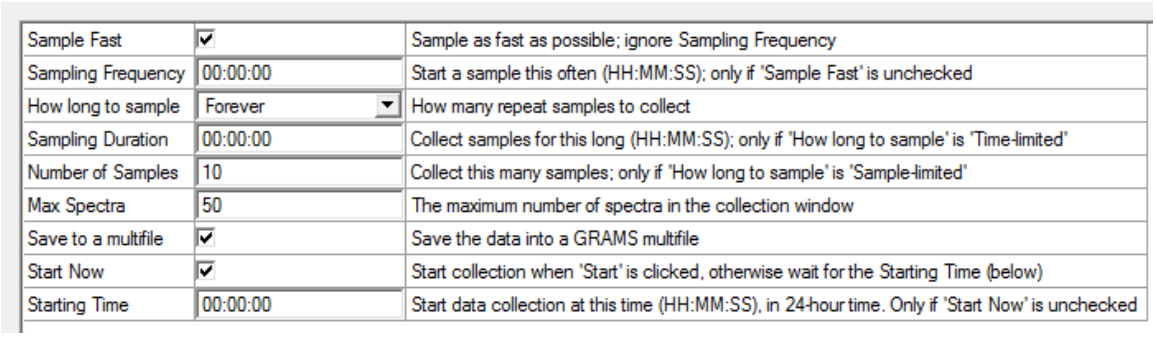


Figure 6-3 Repeat Sampling *parameters*

These parameters are documented in the Repeat Sampling section of the 'Options Menu' chapter of this manual.

If 'Start Now' is unchecked, you can enter a time when data collection should begin. When the green Start button is clicked, this dialog will be displayed:

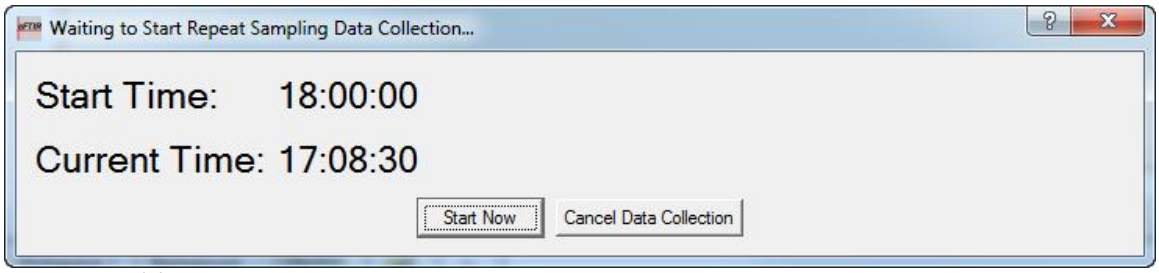


Figure 6-4 The Delayed Start dialog

The start time is displayed, along with the current time. This 'Delayed Start' feature allows for un-attended data collection to begin at a designated time.

7. Printing and Print Templates

Printing of spectra is done using Print Templates. Print Templates control the layout of the page. In addition to spectra, the template can include logos, text, tables of data, and legends. Print Templates can be created and edited by using the Print Template Editor (PTE), which is accessed through the File menu. A default template is installed with Essential FTIR, and when you bring up the PTE the first time, it should appear as Figure 7-1

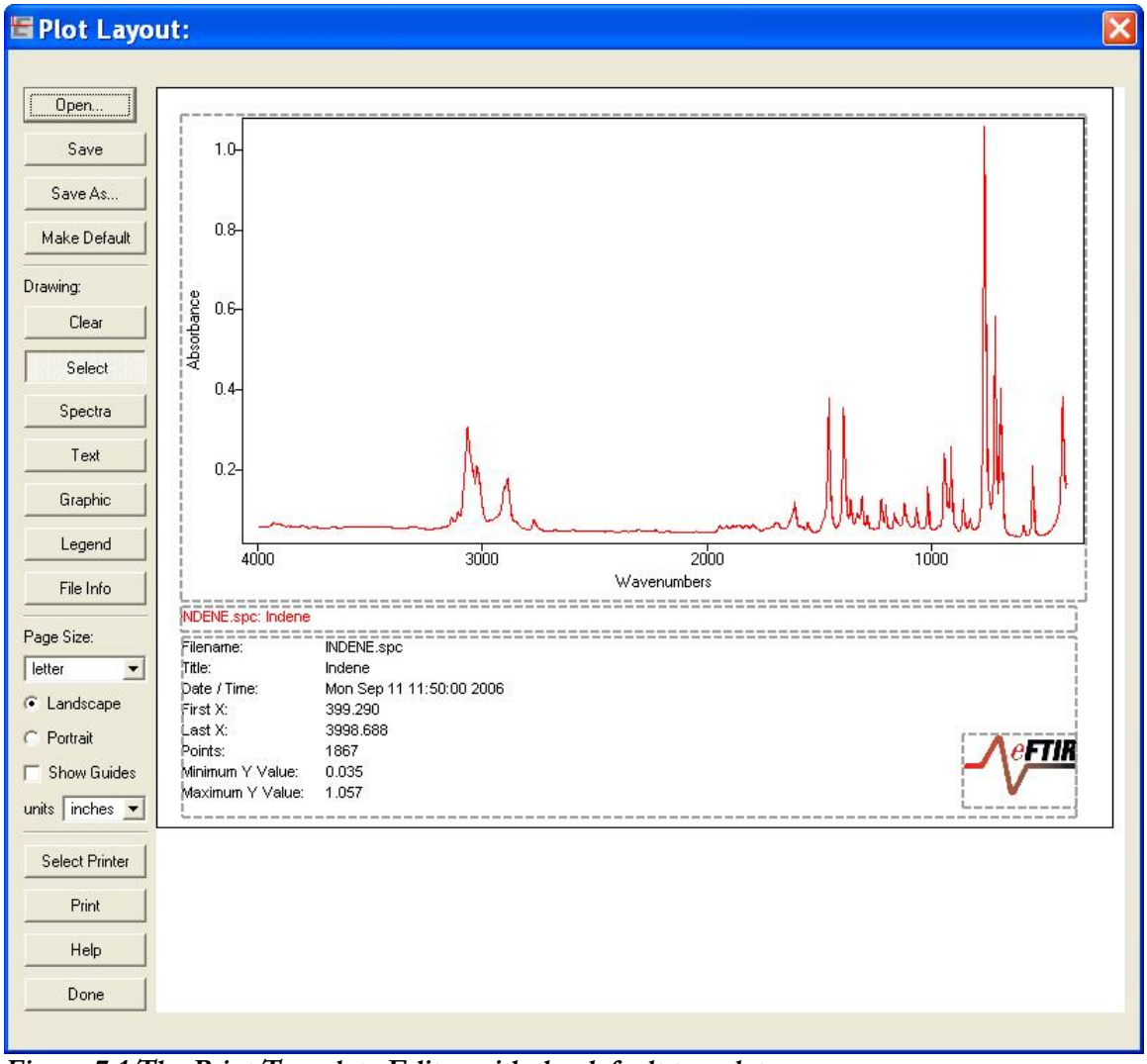


Figure 7-1 The Print Template Editor with the default template.

The PLE allows spectra to be printing in a user-customized format. Corporate Logos, page orientation, legends, and custom text can be added to the page. The page above uses these page elements: Spectra, Legend, File Info, and Graphic.

The buttons on the left side perform these actions:

Open an existing plot template file

Save the template using its current filename

Save the template to a new file

Clear all elements on the template

Select an element on the template for moving or resizing

Draw a new spectral display box on the template

Draw a new text box on the template

Draw a new graphics box on the template

Draw a new legend on the template

Draw a new File Information table on the template.

Select the page size of the template.

Select the page orientation of the template

Show grid lines on the template, to help lay out the elements

The units for the grid lines, either inches or centimeters.

Select the printer to use for printing the template

Print the template as shown.

Creating a template involves placing elements on the page using the mouse. Elements are placed in boxes. The boxes are drawn using the mouse.

Select the type of element by clicking the Spectra, Text, Graphic, Legend, or File Info buttons.
Move the mouse into the template area.
Press and hold the left mouse button.
Drag the box to define the area of the element on the page
Release the mouse button.

After an element is drawn on the page, right-clicking the mouse on the element will bring up a menu of choices relevant to that element.

For instance, after drawing a Text element on the page, the element will display like this:

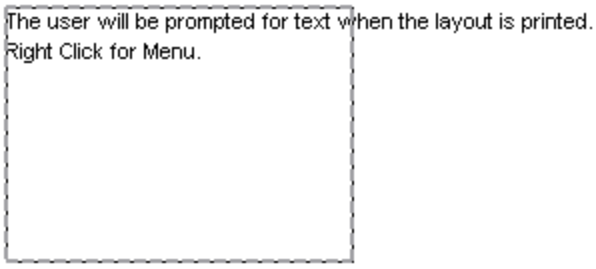


Figure 7-2 A Text Box in the PLE

Right clicking will produce this menu:

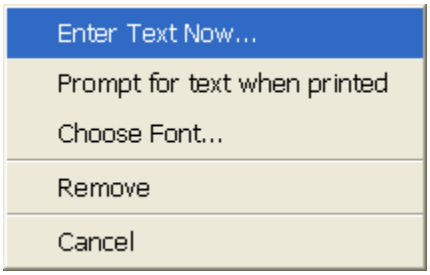


Figure 7-3 Text Box Context Menu

By default, a Text box will prompt the user to enter text when the template is used to produce a printout. This feature allows you to insert custom text at the time of printing. However, you can enter text that will be a part of every printout produced with this template by choosing 'Enter Text Now…'.

Other elements have their own menu choices. 'Remove' and 'Cancel' are common to all elements.

8. Toolboxes and Tools

In this section we will examine the toolbox window. The toolbox window is pictured in Figure 8-1.

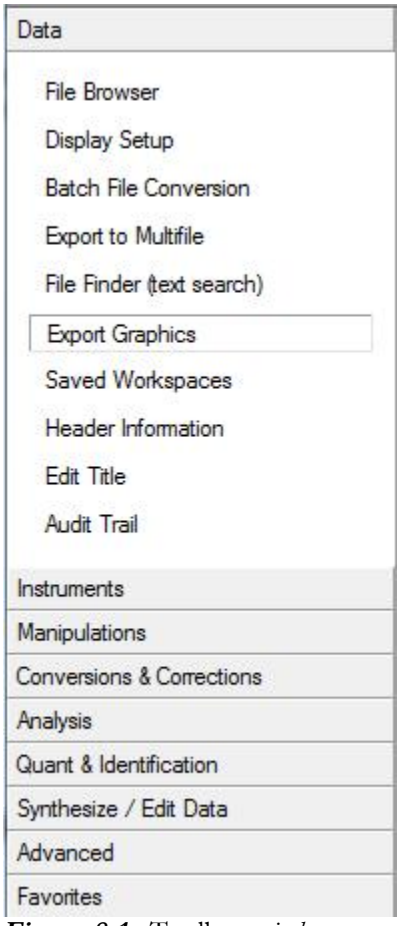


Figure 8-1 Toolbox *window*

The ***Toolbox*** window is the heart of ***Essential FTIR***. It is from this window that you may choose and apply many features to enhance, interpret and analyze spectral data. The features offered by the ***Toolbox*** are also available from the ***Tools*** menu. However, the ***Toolbox*** is designed to offer maximum utility with a minimum of cursor movement, and many users find the Toolbox a more ergonomic way to access the tools offered by ***Essential FTIR***.

The ***Toolbox*** window organizes the ***Tools*** into categories. The categories are:

- ***Data***
- ***Instruments***
- ***Manipulations***

- ***Conversions & Corrections***
- ***Analysis***
- ***Synthesize / Edit Data***
- ***Advanced***
- ***Favorites***

Each ***Toolbox*** is selectable by clicking on the appropriate tab in the ***Toolbox Selection Window***, and each individual ***Tool*** is accessed by clicking on its label.. We will examine each ***Toolbox*** and its contents in turn.

The Favorites

The Favorites Toolbox gives a user a place to organize the tools they most often, and to specify a particular tool that should be made active every time Essential FTIR is started. Also, the name 'Favorites' can be changed to something else, for instance 'Technician Tools'.

When you first open the Favorites tool box, you will see a button labeled 'Add Tools to this Toolbox':

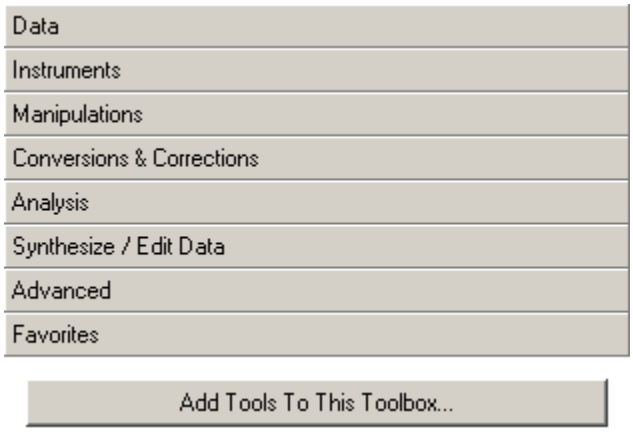


Figure 8-2 The Favorites

Clicking the button will bring up this Dialog box:

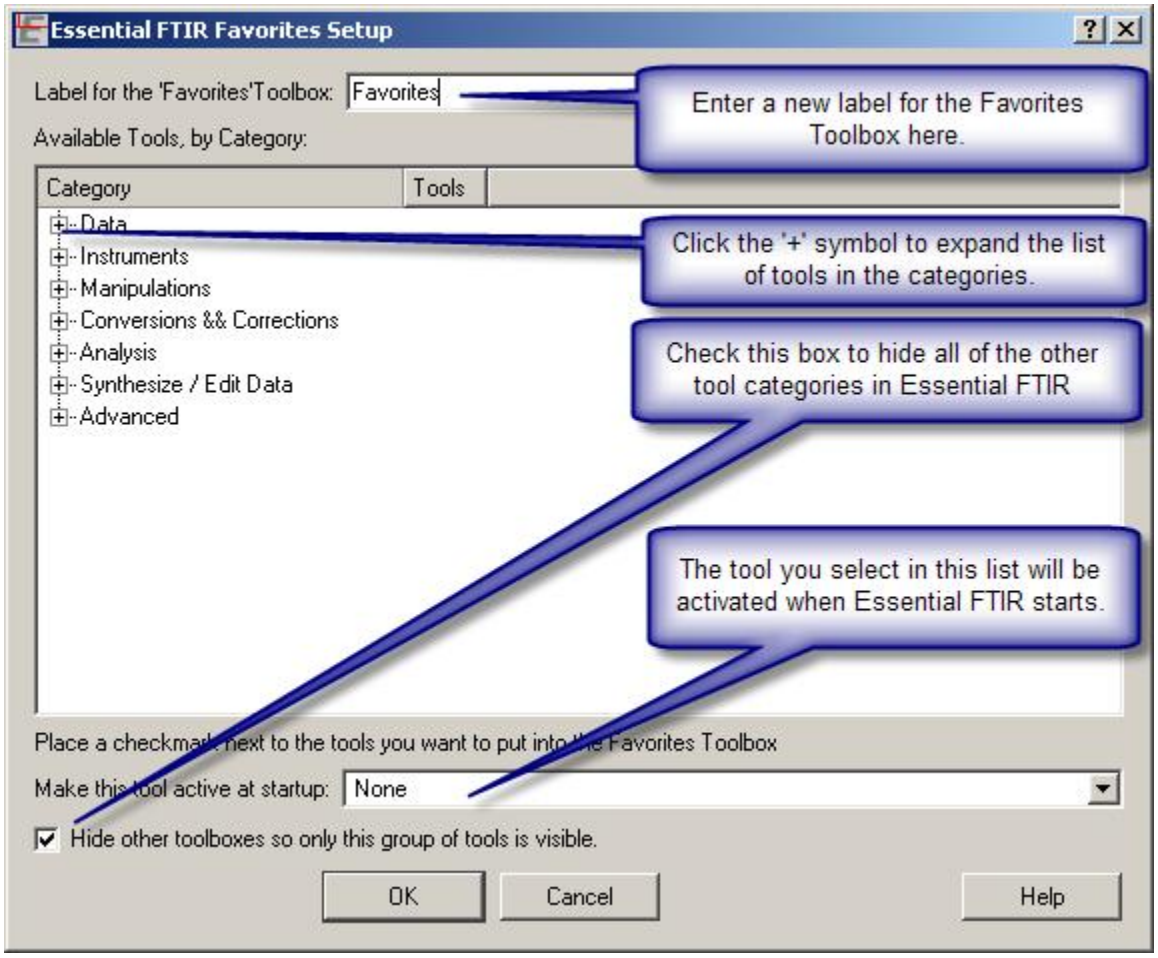


Figure 8-3 Setting up the Favorites

In this next picture, the name of the 'Favorites' has been changed, some tools have been selected by placing check marks next to them, and one of the tools has been chosen as the startup tool:

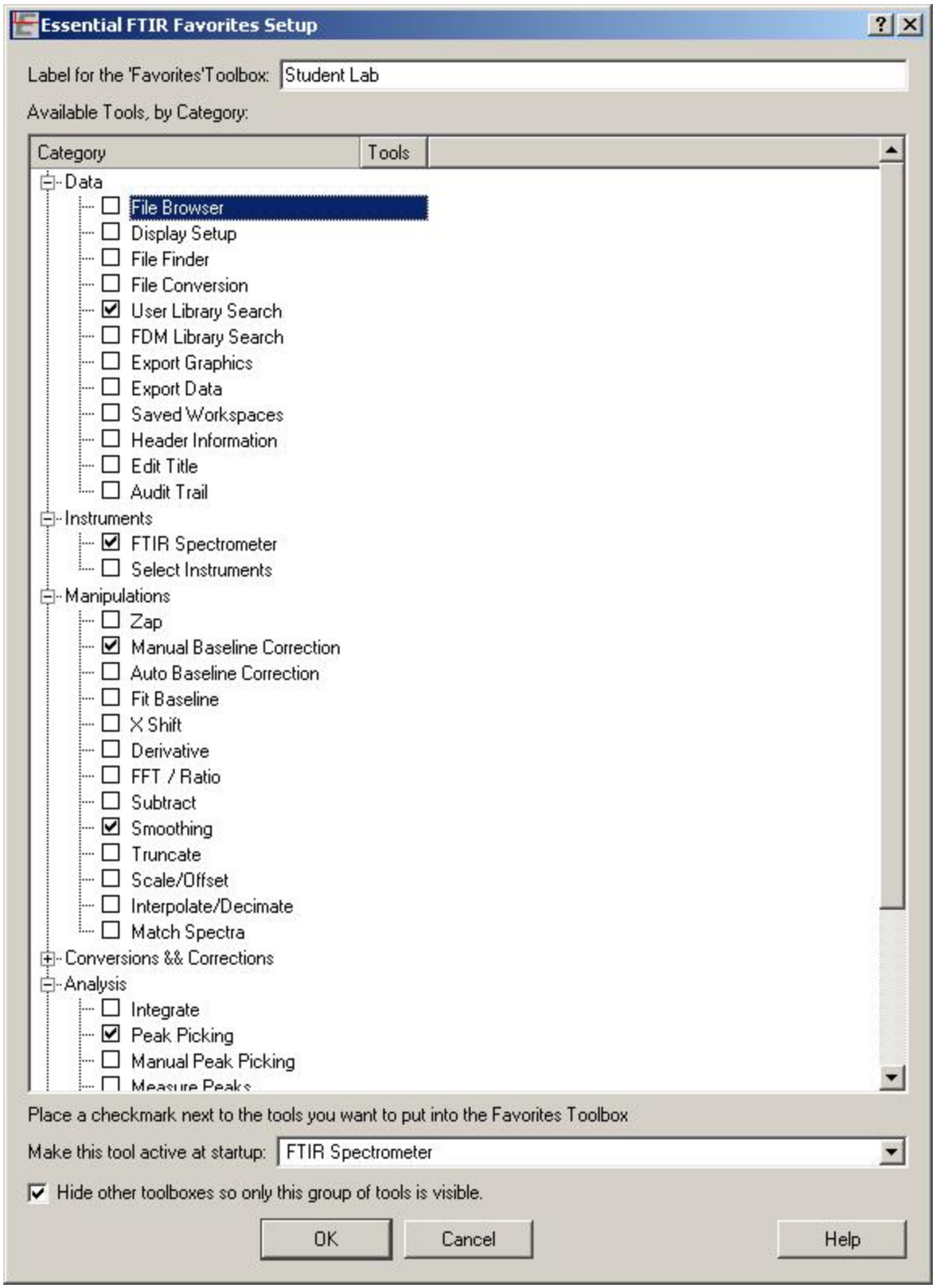


Figure 8-4

The 'Favorites' button will display the label 'Student Lab', the 'Student Lab' toolbox will have five tools: 'FTIR Spectrometer', 'User Library Search', 'Manual Baseline

Correction', and 'Peak Picking'. In addition, when the program starts, the 'FTIR Spectrometer' tool will be displayed right away. Because the 'Hide other toolboxes' button is checked, only these tools will be available.

Changes to the 'Favorites' toolbox require that Essential FTIR be closed and restarted to be applied. When you click 'OK' on the dialog, you will see this message:

Figure 8-5

When Essential FTIR is restarted, the toolbox will look like this, and will start up with the 'FTIR Spectrometer' data collection tool.

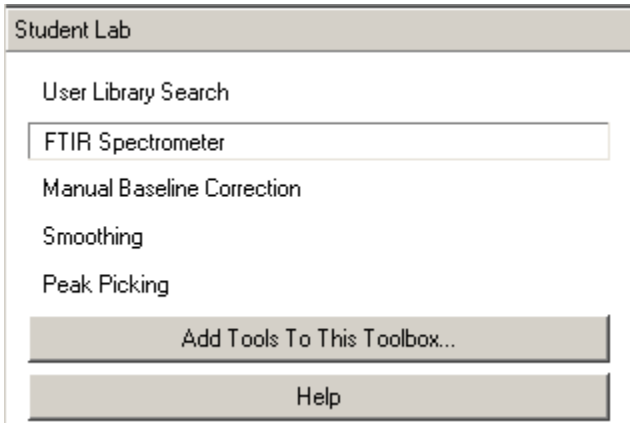


Figure 8-6

The 'Favorites' Tool is a way to tailor the program to display only those tools that are relevant to a particular task. It can make the software easier to use by gathering the tools you use most often into one group.

The Data Toolbox

The first ***Toolbox*** in the list is labeled ***Data***. The ***Data*** section houses all the ***Tools*** concerning data location, data loading, data acquisition, library searching, file and graphics exporting and file header information. We will examine each ***Tool*** in detail.

File Browser

The first ***Tool*** in the ***Data Toolbox*** is the ***File Browser***, which is shown together with its associated ***Tool Parameters Window*** in Figure 8-7.

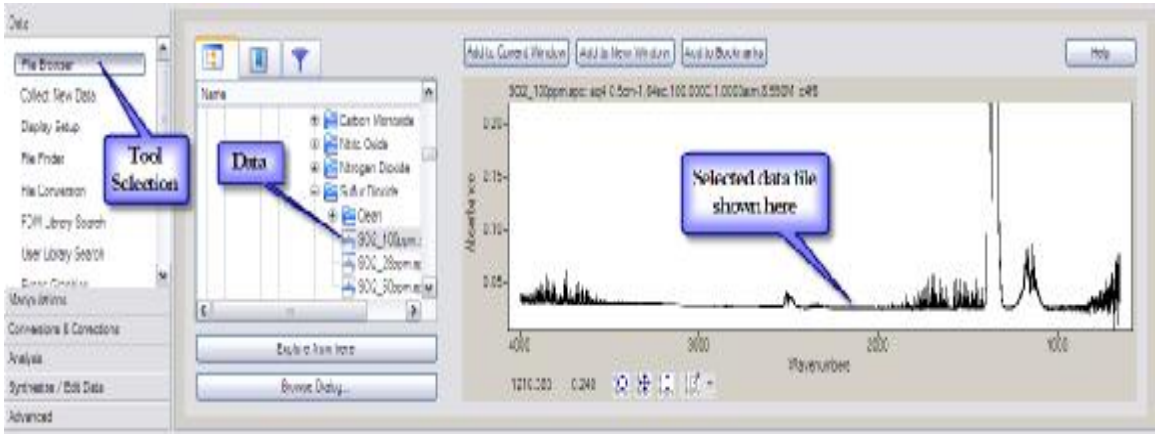


Figure 8-7 File Browser Tool

Figure 8-7 the extreme left of the window is taken up by the ***Data Toolbox***. The central portion of the window is occupied by the ***File Browser*** itself. This tool allows you to browse files in a way familiar to most users of Microsoft Windows. By selecting a drive – either a local disk or removable volume – and navigating to the desired folder the data may be loaded directly into the active ***Workspace***. If no ***Workspace*** is currently open then one will be created. Two additional options exist for navigation, you may either use the ***Explore from Here*** button – which launches the Windows file browser – or by clicking the ***Browse Dialog*** button, which summons a traditional Microsoft Windows "open file" dialog. A single click on a recognized data file displays that file in the browser pane on the right of the window. The data file may be loaded into the ***Workspace***, either by clicking the ***Add to Current Window*** button, or by double-clicking the data file. Additionally, the selected file may be loaded into a new ***Workspace*** by clicking the ***Add to New Window*** button.

Multiple files may be selected in the standard manner – by holding the *Shift* key while selecting the first and last files, or, for if the desired files are discontinuous, by holding the *ctrl* key while selecting the files. The multiple files selected may be loaded by right-clicking on the files and selecting either the ***Load all selected files in a new window*** or ***Load all selected files in current window*** options from the context menu. The ***Add to Window*** buttons function as normal.

The directory may also be labeled as a favorite by clicking on the ***Add to Bookmarks*** button. At the top of the File Browser are three tabs. By default, the first tab is active – the ***Browse Files*** tab. The second option is the ***Load Files from Bookmarks*** tab, shown in Figure 8-8.

Figure 8-8 Load Files from Bookmarks *tab*

The tab displays a list of options for browsing, including a list of ***Bookmarked*** files, defined using the ***Add to Bookmarks*** button described above.

The third option available is the ***Manage File Filters*** tab, shown in Figure 8-9.

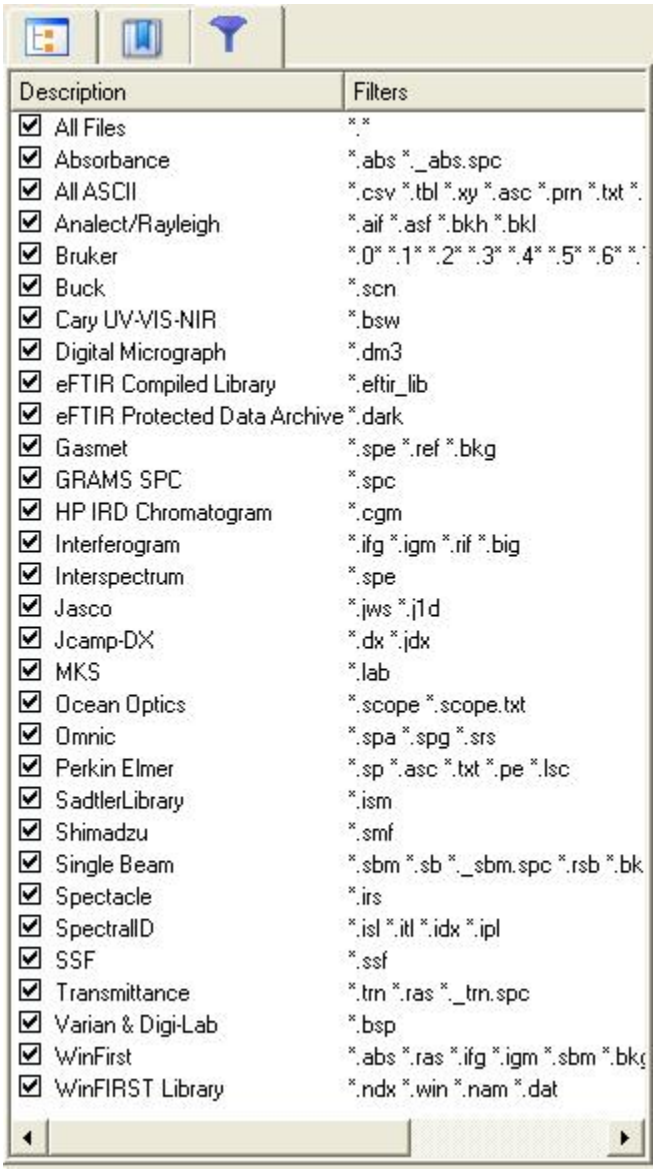


Figure 8-9 Manage File Filters *tab*

This option allows you to filter the files displayed in the browser window by format. As in most cases it would be counter productive to list files not compatible with ***Essential FTIR***. A list of file formats is displayed, selectable via a checkbox next to each format.

Display Setup

The ***Display Setup Tool*** is identical to that detailed in Figure 5-11 through Figure 5-24. Please refer to that section of the manual for information on this ***Tool***.

Batch File Conversion

The ***Batch File Conversion Tool*** is a utility that enables you to change the format of data files. The ***Batch File Conversion*** parameters window is shown in Figure 8-10.

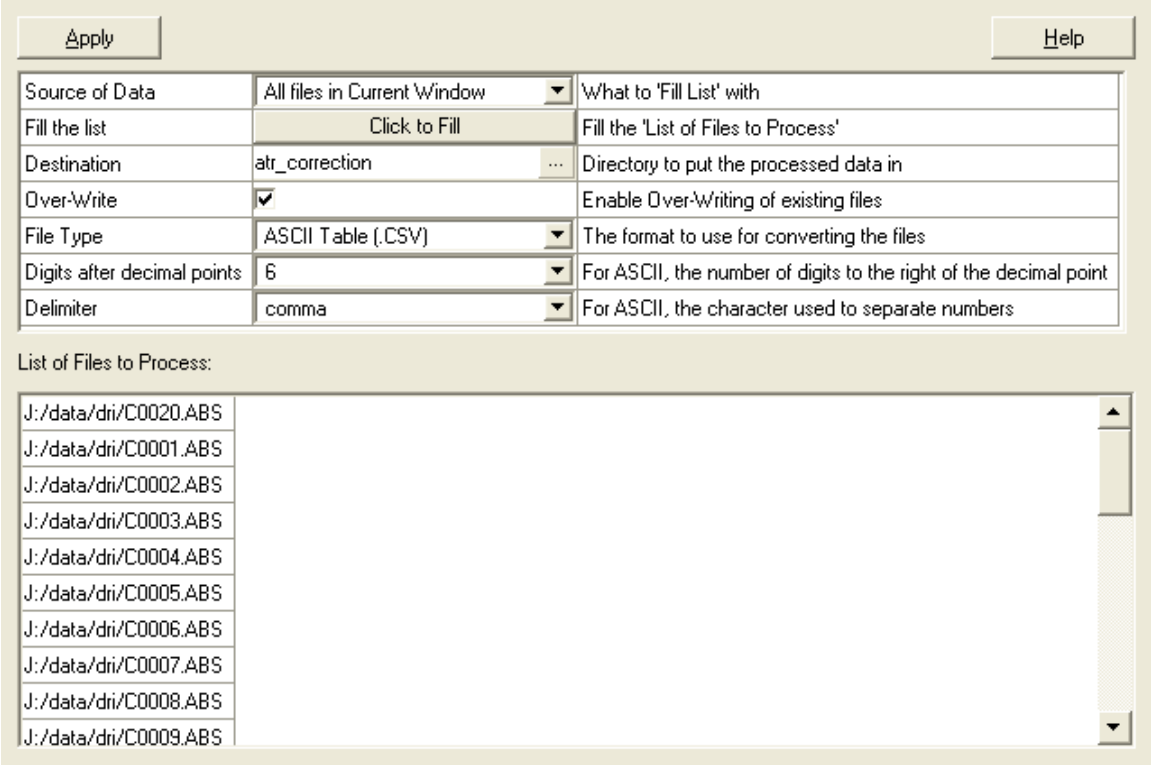


Figure 8-10 File Conversion *utility*

At the top of the ***File Conversion*** parameters window are five inputs. Taking each in turn:

- ***Source of Data***: A drop down menu allows the selection of a number of options for source data. You may choose ***Pick Files From Disk***, ***All Visible Files In Current Window***, ***All files in Current Window*** or ***Entire Directory***.
- ***Fill the list:*** The ***Fill the list*** button populates the window at the bottom of the parameters screen with the chosen files. If the ***Pick Files From Disk*** or ***Entire Directory*** options are chosen then clicking the ***Fill the list*** button summons a file browser dialog box.
- ***Destination:*** The ***Destination*** option enables you to select a destination directory. By clicking the edit button (**…**) a browser dialog is summoned that allows selection of a folder or the creation of a new folder to accept the incoming converted files.
- ***Over-Write:*** A check box toggles between states of over-writing any files of the same name as the incoming files already present in the destination folder.
- ***File Type:*** Specifies the format of the result of the conversion. You may choose between Galactic, Perkin-Elmer, JCAMP-DX, Excel, Matlab, or ASCII formats.

File Conversion Example

In this example, an entire directory of JCamp-DX files will be converted to Galactic .spc format.

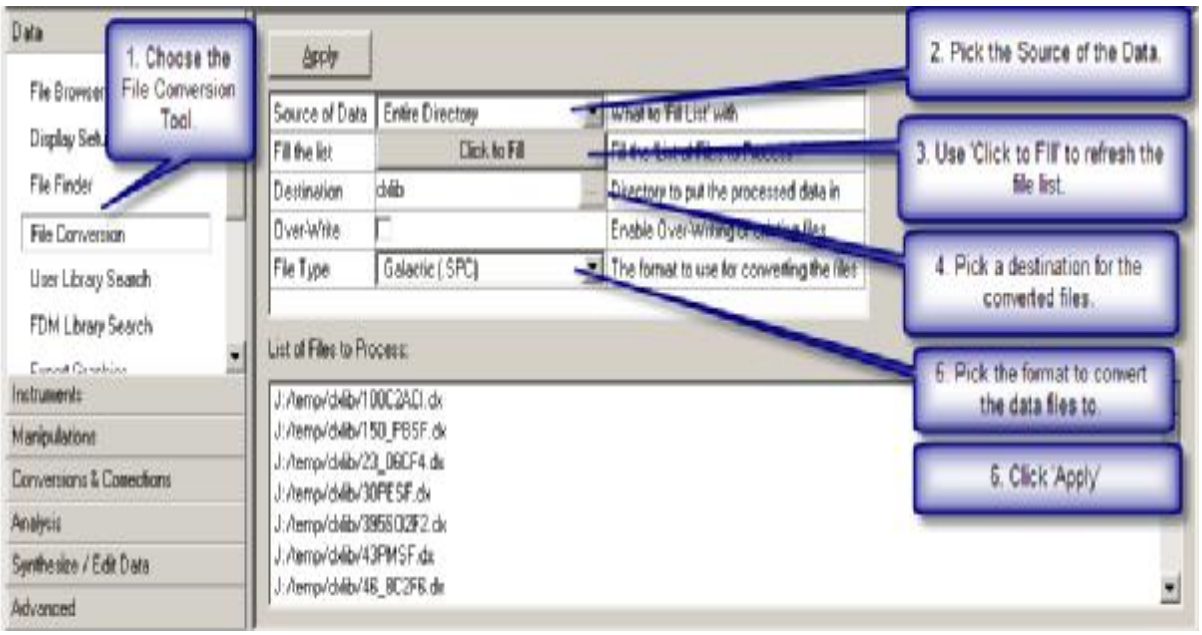


Figure 8-11

1. Select the File Conversion Tool in the 'Data' category.
2. Pick the source of the data. The choices are:

   "Visible Files in Current Window"
   "All files in Current Window"
   "Pick Files From Disk"
   "Entire Directory"

3. The 'Click to Fill' button can be used to refresh the list of files to convert.
4. Pick a destination folder for the converted files. In this case, note that the source and destination are the same.
5. Pick the format the files will be converted to. The choices are:

   "PE (.SP)"
   "Galactic (.SPC)"
   "JCAMP-DX (.DX)"
   "ASCII Table (.CSV)"
   "Excel (.XLS)"
   "Matlab (.MAT)"
   "Spectra-Calc (fixed-point .SPC)"

   Fixed-point .SPC is a Galactic format .SPC file, with the spectra stored in an older

integer format that was in use when the Grams program was known as ‘Spectra Calc’. This is useful if you have array basic programs that only work with this older format.

6. Click ‘Apply’

In this example, a folder of JCamp-DX files is converted to Galactic .spc format in-place, meaning the source and destination folders are the same.

Also, take a look at the ‘Export Data’ tool. This ‘File Conversion’ tool exports single spectra to individual Files. The ‘Export Data’ tool can export multiple spectra to a single multi-dimensional file (known as a ‘multifile’).

Export To Multifile

This tool gathers multiple spectra and stores them together in a single file, known as a 'multifile'. While the 'Batch File Conversion' tool converts files that contain single spectra between file formats, 'Export to Multifile' groups similar spectra into a single file. This is useful if you are using Excel or Matlab to analyze spectra.

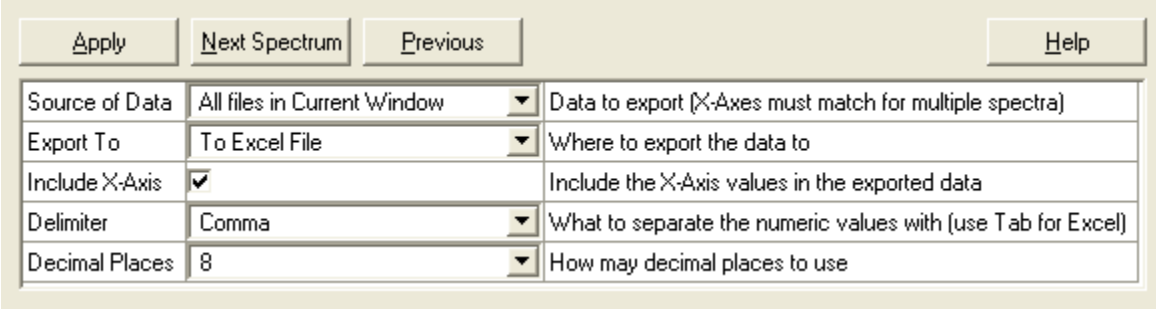


Figure 8-12 Export to Multifile

The 'Source of Data' selection is described in the 'Batch File Conversion' tool discussion, above. The 'Export To' choices are Excel, Matlab, .CSV (comma-separated ASCII files), clipboard, or GRAMS multifile.

Three buttons are situated at the top of the parameters window. The ***Apply*** button executes the settings in the window. ***Next Spectrum*** makes the adjacent spectrum in the ***Workspace*** active. The ***Previous*** button renders the preceding spectrum in the ***Workspace*** active.

Five option rows are available. The row labeled ***Source of Data*** includes a drop down menu, which is used to select the data to be exported. The current spectrum, all visible spectra in workspace and all files in the workspace are the three options given.

The ***Export To*** option offers a drop down menu providing choices on the format of the exported data. The options are:

- To the Windows clipboard, from where the data may be pasted into other programs.
- To Comma Separated Values file (.csv)
- Pasted into Excel
- To Excel files (.xls)
- To Matlab files (.mat)
- To GRAMS multifile (.spc)

The ***Include X-Axis*** checkbox should be checked if *x* axis data (wavenumber, in the case of absorbance files) is required.

When the data is exported to the clipboard or to CSV file, the data is in ASCII text format. Two options are specifically for exporting ASCII text. The row labeled ***Delimiter*** is used to define the character used to delimit the data – that is, to separate individual data points. Tab

should be chosen as a general rule, but other circumstances may dictate the use of a comma or other character. The choices available from the drop down menu are:

- Comma
- Tab
- Space

Although CSV stands for 'Comma-Separated-Values, the actual separator will be the chosen delimiter.

The final row is labeled ***Decimal Places***. This also only applies to ASCII text (the clipboard and CSV files). A drop down menu allows specification of the number of decimal places to include in the exported numeric data. The data may be exported in scientific format, or with decimal places numbering 1-9.

For export to a multifile, all the spectra in the list of files must have the same resolution and spectral limits. If the spectra in the list of files do not match, this dialog will be displayed:

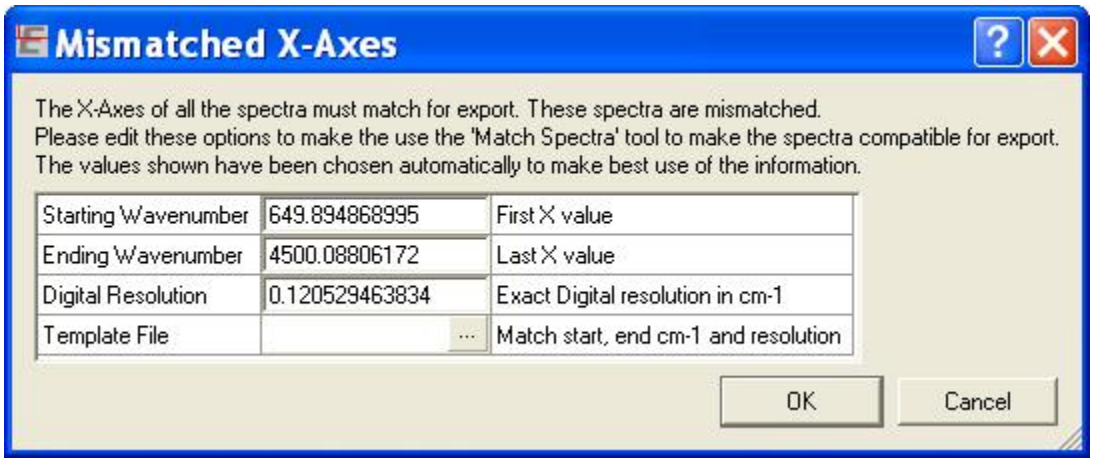


Figure 8-13: matching spectral limits and resolution

By clicking 'OK', the data in the multifile will automatically be converted to match these settings.

An example of the output of the ***Export Data Tool***, set to export a single absorbance spectrum visible in the ***Workspace*** to Microsoft Excel, is provided in Figure 8-14.

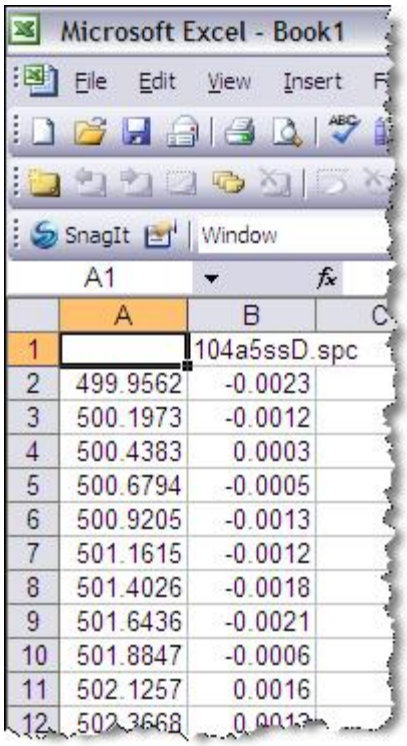


Figure 8-14 *Exporting Data to Microsoft Excel*

The filename of the spectrum exported is visible in the cell 1B of the worksheet.

Also, take a look at the 'File Conversion' tool. The 'File Conversion' tool exports single spectra to individual Files. The 'Export Data' tool exports multiple spectra to multi-dimensional files.

File Finder

The ***File Finder*** is, as its name implies, a method for searching disks for specific files or sets of files. The parameters window for the File Finder Tool is shown in Figure 8-15.

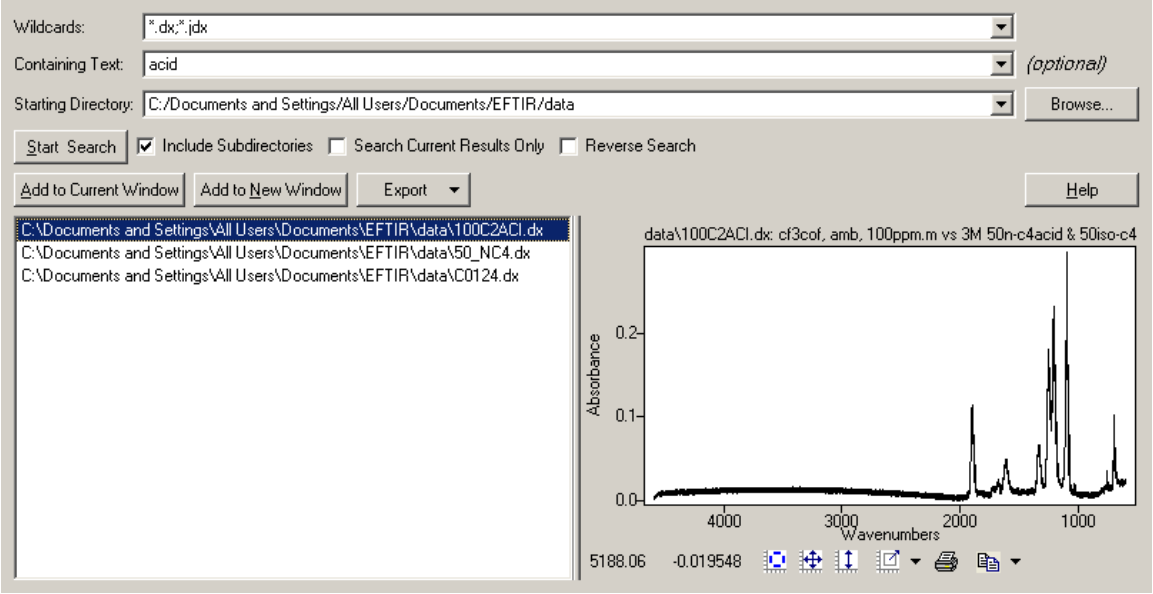


Figure 8-15 File Finder Tool

The ***Tool*** has three main parts. In the upper portion of the ***File Finder*** window are three drop down menus for the entry of wild card characters, text and the directory to search. On the bottom left is a browser, used to select files identified by the search. The display window in the bottom right of the screen shows any file highlighted in the browser window.

Addressing each of the ***File Finder*** elements in turn, let's examine the three drop down menus. The first – ***Wildcards*** – enables selection of file extensions to search for. In the example used in Figure 8-15 the file extensions ***.dx and .jdx*** are included in the search, which are the file extensions used by JCamp-DX. The wildcard characters * is used to signify that the portion in front of the file extension is not relevant. In the second drop down menu text may be entered or selected from previous searches. This text is then included as part of the search. The search is not case sensitive, the text 'acid' will match both 'acid', 'Acid' and 'ACID'. Entering text to search for is optional, if no text is provided then the Finder will find all files with the given extension(s). The third drop down menu is used to select drives, directories and folders for searching. The search folders may also be specified using the ***Browse*** button. This drop down list is pre-populated with book-marked folders. If 'Search Current Results Only' is checked, then only the files listed in the file list box are searched. This provides a way to narrow down the search using multiple search texts. If 'Reverse Search' is checked, only files that ***do not*** contain the search text are listed.

Pressing the ***Start Search*** button begins the search. Subdirectories are included in the search by checking the box next to the ***Start Search*** button. Once the search is concluded the browser portion of the window is populated with a list of the files found. These may be viewed in the display window by clicking once on the file. Multiple files may be selected in

this list using the mouse in combination with the shift and control keys. The selected files found may be loaded to the active ***Workspace*** by clicking the ***Add to Current Window*** button, or loaded to a new ***Workspace*** by clicking the ***Add to New Window*** button.

Export Graphics

The ***Export Graphic Tool*** allows the ***Essential FTIR*** user to export presentation quality graphics via a variety of formats. The ***Export Graphics*** parameters window is shown in Figure 8-16.

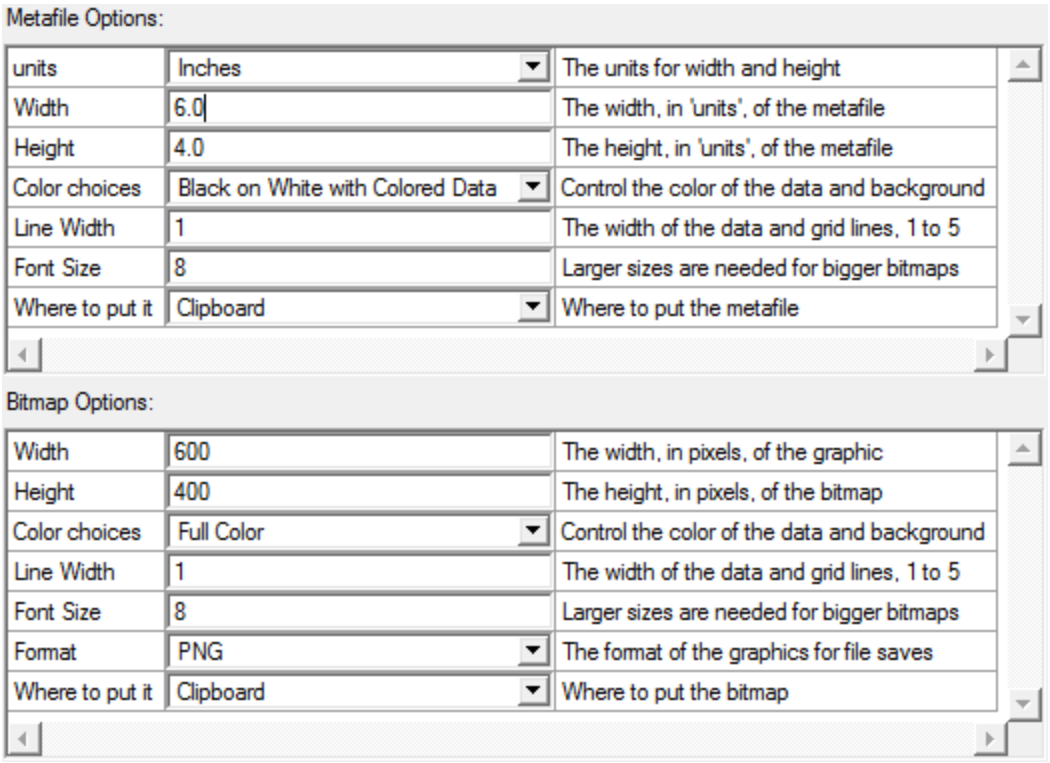


Figure 8-16 Export Graphics

The ***Export Graphics Tool*** has two main options, export to Metafile or Bitmap format. These two choices have different options, so there are two tables of options, one for each format. The resulting graphic can be written to a file, or placed on the Windows clipboard for pasting the graphic into other program.

The Bitmap parameter window contains four rows. The row labeled ***Format***, contains a drop down menu that is used to select the output format for the ***Workspace*** graphic. The available choices are:

- Portable Network Graphics (.png) - commonly used on internet web pages.
- Bitmap (.bmp) – a Windows specific picture format.
- Joint Photographic Expert Group (.jpg) – the "standard" compressed image format.

- X Pix Map (.xpm) - used mostly on Unix systems with the X Window System.

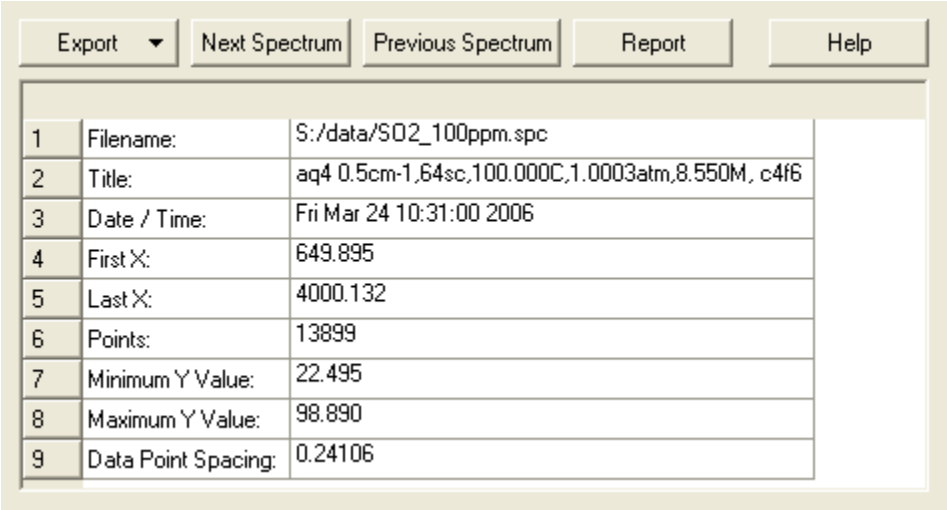
The ***Width*** row contains an edit box which allows you to set the width in units of pixels of the exported graphic. The ***Height*** row works in an analogous way. The ***Black On White*** option may be used to export the graphic as a grayscale picture, ignoring colors.

Saved Workspaces

The ***Saved Workspaces*** Tool allows you to save or load a ***Workspace*** window. Three buttons are available. The ***Save All Windows*** button summons a dialog box enabling you to navigate to the desired folder before saving all ***Workspaces***. The Save Current Window button summons a dialog box which allows you to browse to the desired directory before saving the active ***Workspace***. The ***Load a Workspace*** button summons a browser dialog box which is used to navigate to a saved ***Workspace***, which may then be opened by clicking on the ***Open*** button on the browser dialog box. A ***Workspace*** is the window or windows open in ***Essential FTIR*** and the data that they contain. If there are data that you work with often, or if you want to return to particular data later, this tool allows you to save the state of the program and restore it later without having to load all the separate data files. Please refer to chapter three for a full discussion of ***Workspaces***.

Header Information

The ***Header Information Tool*** is used to display information contained in the file header of the active spectrum. The ***Header Information*** parameters window is shown in Figure 8-17.



1	Filename:	S:/data/SO2_100ppm.spc
2	Title:	aq4 0.5cm-1,64sc,100.000C,1.0003atm,8.550M, c4f6
3	Date / Time:	Fri Mar 24 10:31:00 2006
4	First X:	649.895
5	Last X:	4000.132
6	Points:	13899
7	Minimum Y Value:	22.495
8	Maximum Y Value:	98.890
9	Data Point Spacing:	0.24106

Figure 8-17 Header Information Tool

The header information is displayed in rows. The data may be inserted into documents from the Windows clipboard via the ***Export to Clipboard*** button. The ***Next Spectrum*** and ***Previous Spectrum*** buttons are used to navigate between spectra in the active ***Workspace***.

Edit Title

The ***Edit Title Tool*** is used to amend the information contained in the ***Title*** row of the file information header. The ***Title*** is a memo field where you may store information regarding the data. The ***Title*** should not be confused with the ***Filename***. The parameters window is shown in Figure 8-18.

Figure 8-18 Edit Title

The ***Title*** for the active spectrum in the currently active ***Workspace*** is displayed in the edit box. Any changes made to the title may be executed using the ***Apply*** button. The ***Next Spectrum*** and ***Previous*** buttons are used to navigate between spectra in the ***Workspace***. The ***Undo*** button provides an option to roll back any changes made. The ***Help*** button is used to summon the help ***Workspace***. The ***Save*** button saves the file in its current location, while the ***Save As*** button summons a browser dialog box enabling you to select a filename and folder for the modified file.

Audit Trail

In ***Essential FTIR***, a record of all changes to the data is automatically generated, and this record (audit trail) is automatically saved with the spectrum when you save the data. This information may be viewed using the ***Audit Trail Tool***, which records any changes made to the spectral data. In the example shown in Figure 8-19, a region of the data has been lined-out using the Zap tool.

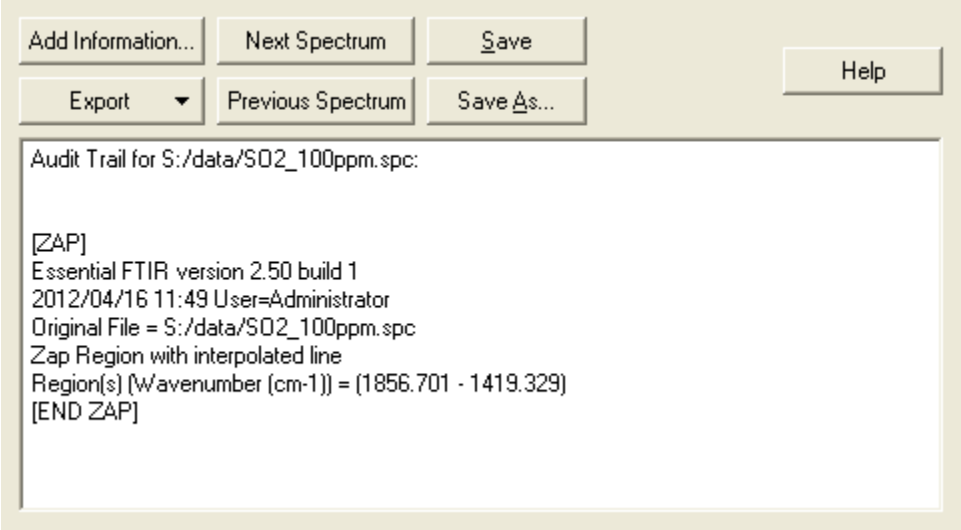


Figure 8-19 Audit Trail

The ***Audit Trail*** window shows details of changes made to the active spectrum in the ***Workspace***. The ***Export*** button may be used to export the text to the usual choices of Clipboard, Excel, or ASCII file. ***Next Spectrum*** and ***Previous Spectrum*** buttons are used to navigate between spectra in the ***Workspace***.

You can add information to the audit trail by clicking on the Add Information button.

The Manipulations Toolbox

The ***Data Toolbox*** provides all the options necessary to locate, open, view, edit information and save spectral data. The role of the ***Manipulations Toolbox*** is to provide the features needed to perform operations on the spectra. The contents of the Manipulations Toolbox are shown in Figure 8-20.

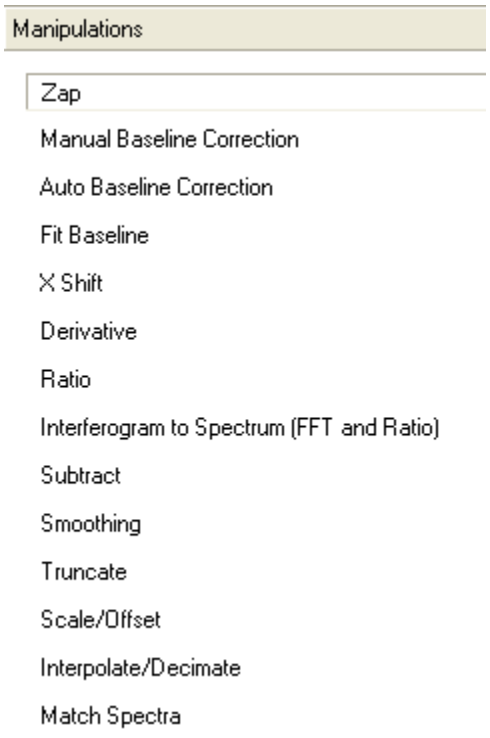


Figure 8-20 *The* Manipulations Toolbox

Many of the ***Tools*** we are about to encounter use the concept of ***Regions***. In the context of Essential FTIR we may define a region as:

***"Region* – A portion of the *x* -axis of a spectrum designated by the user to be operated upon, or designated by the user to be representative of that spectrum for the purposes of that operation."**

A detailed treatment of the Regions concept is given in chapter three. ***Regions*** may be defined by right-clicking in the active ***Workspace*** window. One right-click defines a

Region Marker – a vertical line delineating the edge of a ***Region***. This ***Region Marker*** may be repositioned by left-clicking and dragging. Right-clicking in the ***Workspace*** window a second time completes the ***Region*** with a second marker, and the portion of the spectrum selected is shaded. The numerical values of the Region defined in this way are recorded in a Region Table, as shown in Figure 8-21.

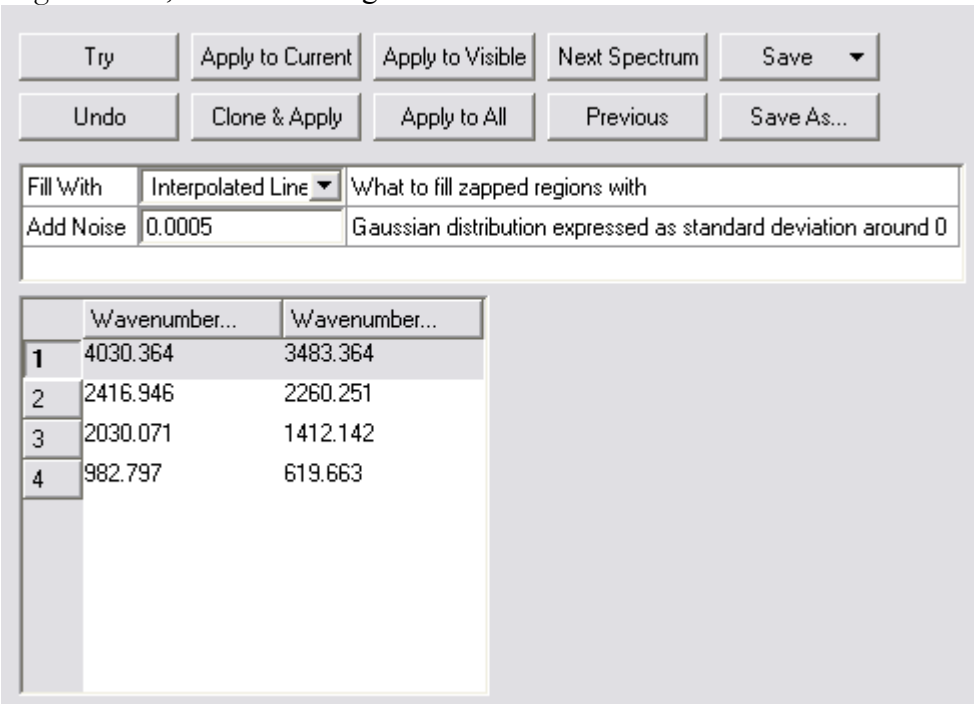


Figure 8-21 Region Table

The ***Region***(s) listed in the ***Region Table*** may be saved or loaded via the context menu summoned by right-clicking in the ***Region Table***, as shown in Figure 8-21, or by clicking on the ***Wavenumber*** column headers. The menu may also be used to remove rows from the table. In this way once regions have been defined and found successful, they may be retrieved later for use in similar circumstances. Please refer to chapter three for a full discussion of the ***Regions*** concept.

Different tools in the Manipulations Toolbox (and indeed the ***Analysis*** and ***Synthesize / Edit Data Toolboxes***) use ***Regions*** in different contexts. For instance, the ***Zap Tool*** is an example of a feature which uses the ***Region*** as a simple definition of a portion of the *x*-axis of the active spectrum to be operated upon. Put simply, the selected ***Region*** is "zapped", leaving the remainder of the spectrum unchanged. This is not the case with all ***Tools***.

Take the ***Manual Baseline Correction Tool*** for example. A ***Region*** selected is not the only portion of the spectrum operated upon; rather that ***Region*** is taken to be *representative* of the whole spectrum. The distinction will become clear as we examine each ***Tool*** in turn.

Zap

The ***Zap Tool*** is used primarily to remove unwanted portions of a spectrum. For example, if a reference absorbance spectrum representing a compound is contaminated it is desirable to remove those absorbance peaks not attributable to the compound of interest. Figure 8-22 shows the ***Zap*** parameter window, together with the ***Workspace*** display.

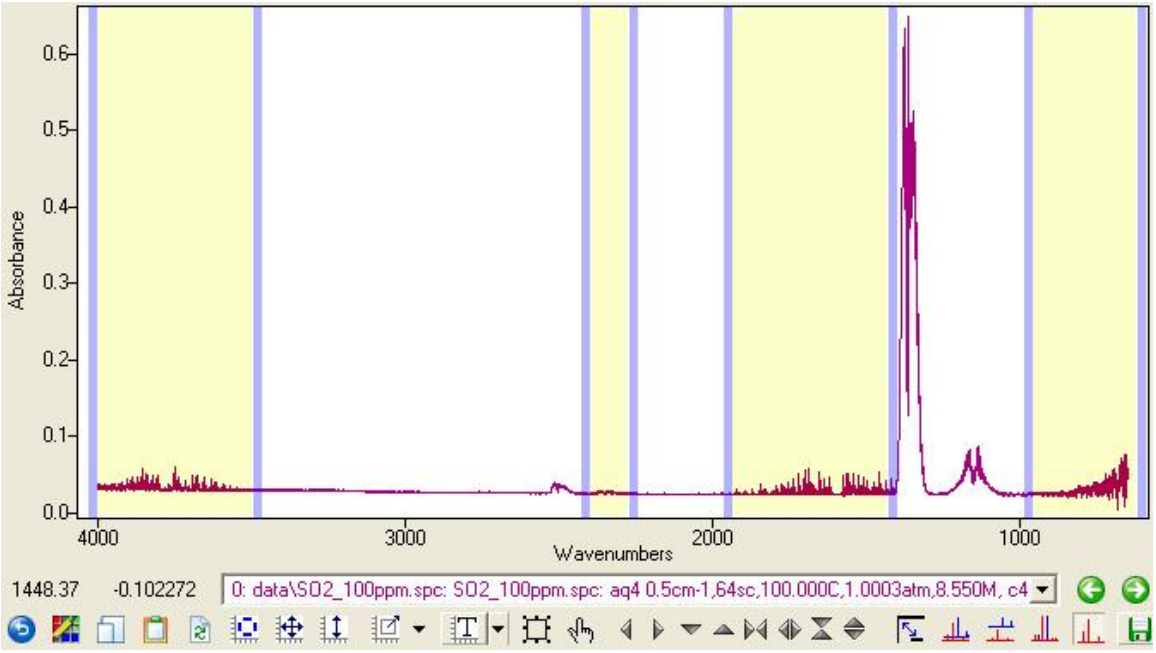
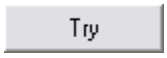
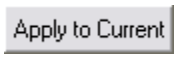


Figure 8-22 Zap Tool *parameters and* Workspace *window*

The ***Zap*** parameters window comprises three main elements. At the top of the window are eight buttons:

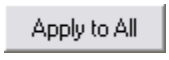


The ***Try*** button allows you to apply the current ***Zap*** settings without committing to them. The parameters will be applied to a gray "ghost" spectrum, overlaying the actual data.

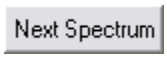


The ***Apply To Current*** button is used to execute the ***Zap*** operation on the spectrum. The original spectrum is replaced in the ***Workspace*** by the modified data.

The ***Apply to Visible*** button will execute the Zap operation on all of the visible spectra in the workspace.



The ***Apply to All*** button will execute the Zap operation an all of the spectra in the workspace, whether they are visible or not.

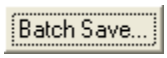


The ***Next Spectrum*** button Selects the next spectrum in the Workspace as active.

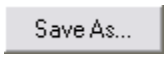
The ***Undo*** button allows you to roll back changes made to the spectrum. A menu is summoned with the options to undo any one of a list of changes, or to undo all changes to the spectrum.

The ***Clone and Apply*** button creates a copy of the active spectrum before performing the ***Zap*** operation upon the copy, thus preserving the original spectrum. The new spectrum becomes the active spectrum in the ***Workspace***.

The ***Previous*** button navigates to the preceding spectrum in the active ***Workspace***.



The ***Batch Save*** brings up the batch save dialog, with many options for saving multiple spectra, with many renaming options.



The ***Save As…*** button summons a navigation dialog box enabling you to select or create a folder to contain the modified spectrum.

The above buttons are known as the ***Toolbox Buttons***, and are common to many ***Tools*** in the ***Manipulations Toolbox*** and other ***Toolboxes***. Users will be referred to this section for information on the buttons whenever they are relevant.

The center of the ***Zap*** parameters window contains an options table with two rows. The table is shown in Figure 8-23.

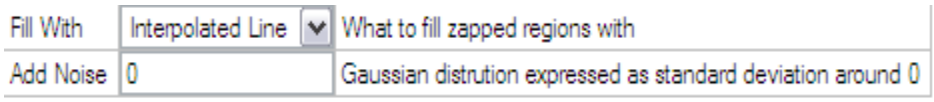


Figure 8-23 *Zap options table*

The first row of the ***Zap*** options table contains a drop down menu with five options – to fill with an interpolated line, fill with zeros, fill with the mean value, fill with the left-most value or to fill with the right-most value. The second row allows you to add noise to the ***Zap Region***(s) to avoid an unnatural looking flat line.

The spectrum shown in the workspace in Figure 8-22 is a gaseous sulfur dioxide absorbance spectrum at 0.5cm^{-1} resolution, with 64 co-added scans, with the 10m gas cell heated to 100C, and regulated to a pressure of 1 atmosphere. We will use this spectrum, sometimes in combination with others, throughout our examination of the ***Manipulations Toolbox***.

Note the four ***Regions*** selected in Figure 8-24. The sulfur dioxide spectrum is contaminated with water and carbon dioxide – two very common atmospheric contaminants in gas-phase samples. The ***Regions*** are chosen so as to remove the absorbencies due to the contaminants. This contamination is made more obvious in the expanded view shown in Figure 8-24.

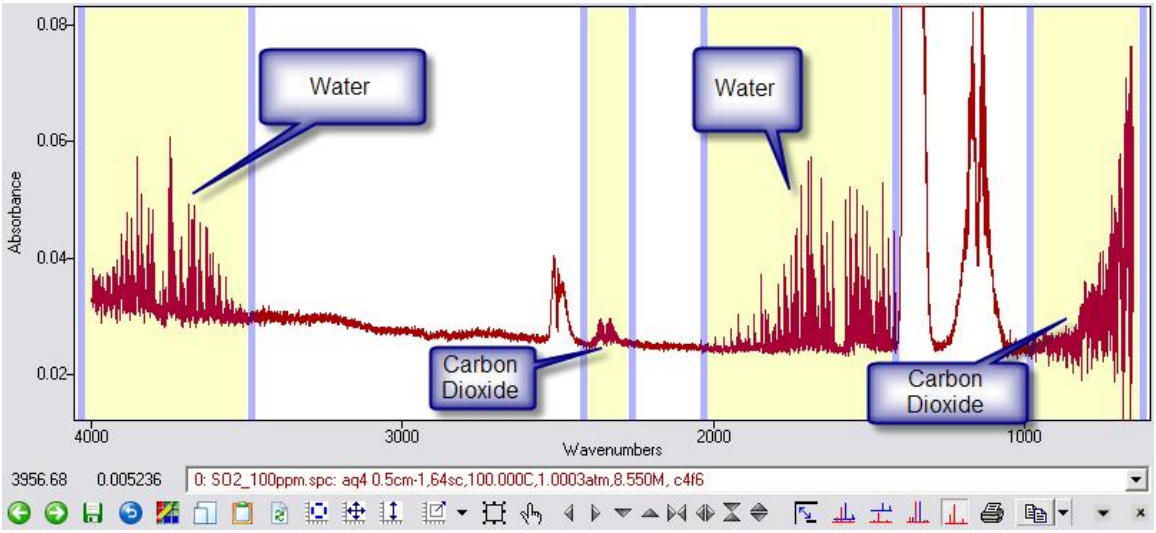


Figure 8-24 *Contamination from H_2O and CO_2 in SO_2*

This contamination, while at relatively low levels, can still prejudice the results of a library search, or bias a least squares fitting routine for quantification. If we press the ***Try*** button to test the effects of the operation on the spectrum, we see the result in Figure 8-25.

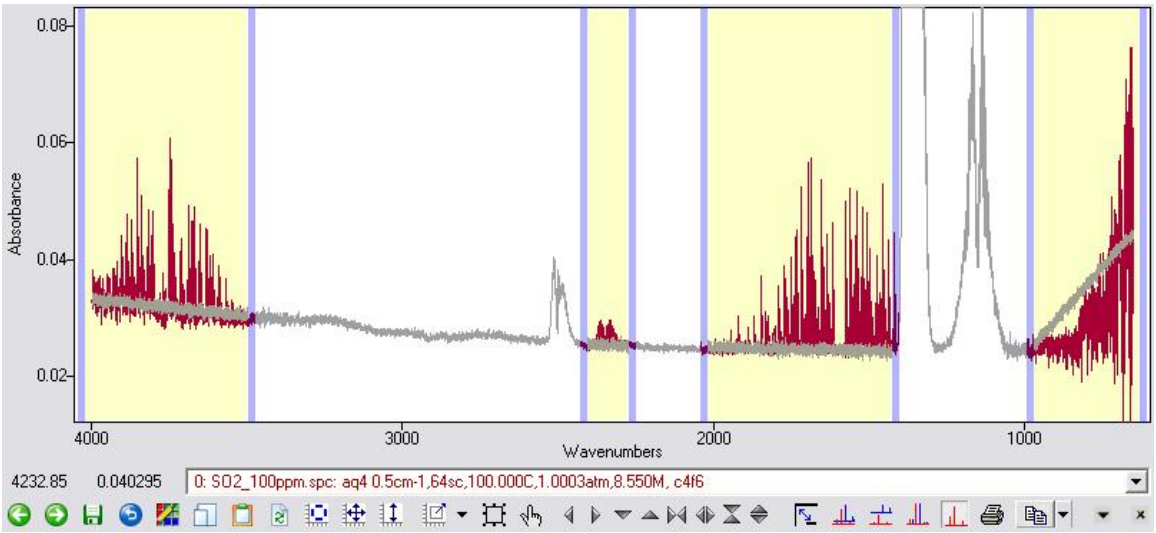


Figure 8-25 *Applying the* Zap *with the* Try *button*

We see that the interferences have been replaced with a flat line, interpolated between the ***Region Markers***. Should we wish, we may apply synthetic noise to the ***Zap*** Regions, to render the spectrum more "natural" in appearance. In Figure 8-26 we see the result of

applying the operation using the ***Interpolated Line*** option and applying noise at a level of 0.00085 absorbance units.

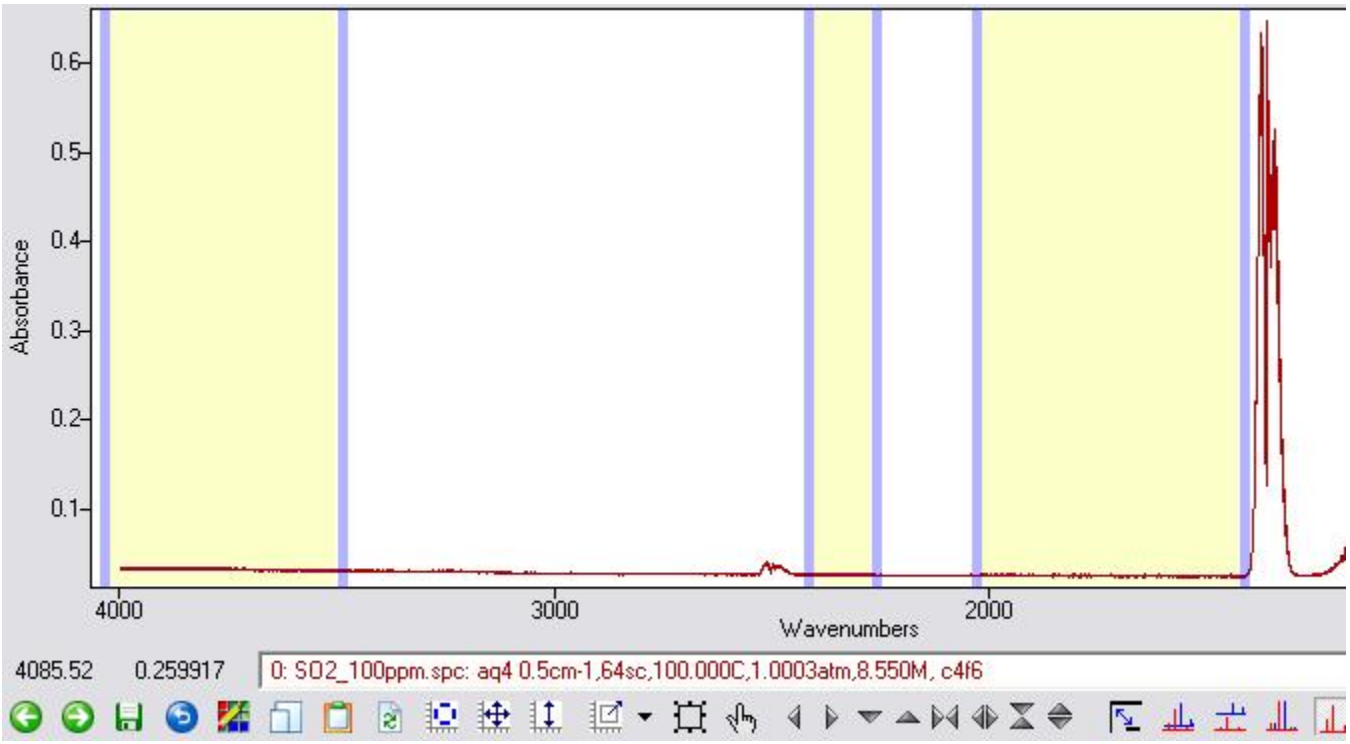


Figure 8-26 Applied Zap

The spectrum is now free of contamination. Notice that some artifacts have been introduced to the baseline, notably the slope on the baseline below 1000cm^{-1}. We will remove these artifacts with the next tool.

Manual Baseline Correction

The ***Manual Baseline Correction*** Tool is used to remove defects from the baseline of a absorbance spectrum. The associated parameters window and Workspace is shown in Figure 8-27.

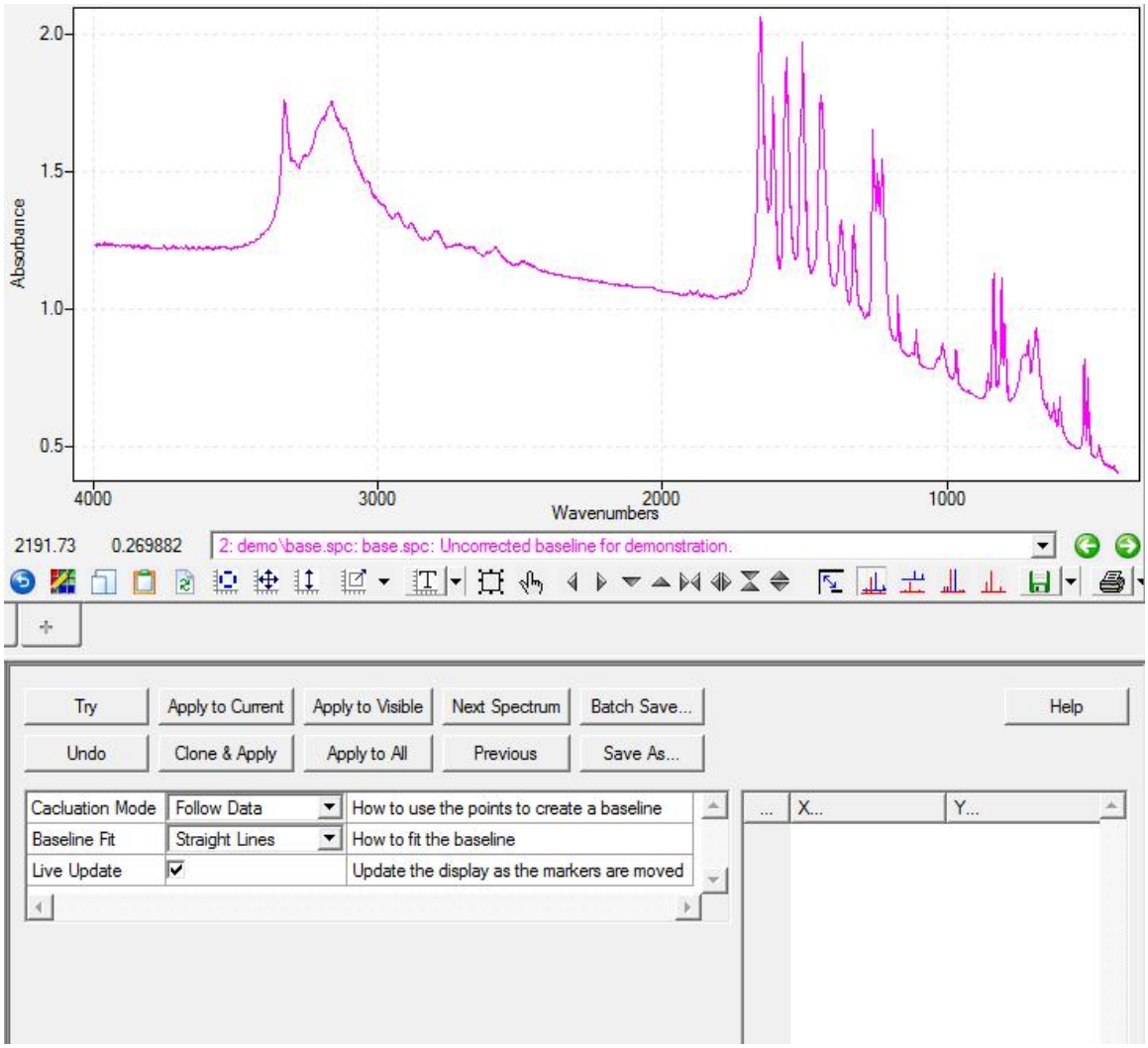


Figure 8-27 Manual Baseline Correction *parameters*

The ***Manual Baseline Correction*** window comprises three parts. The first consists of the ***Toolbox Buttons***, identical to those of the ***Zap*** parameters window detailed in the previous section. The middle portion contains the processing options, and the right side of the window is taken up with a ***Region Table***.

In this tool, the user selects points that will define a new baseline that is subtracted from the spectrum. This new baseline can be either straight line segments, or a smooth curve, which behavior is controlled by the 'Baseline Fit' option.

The 'follow data' option determines the behavior of the region markers, and the resulting baseline correction. If 'Follow Data' is checked, the region markers will be forced to fall on the spectrum. If unchecked, the region markers can be placed anywhere in the X,Y coordinate space.

If the 'Live Update' option is checked, the results of the calculation can be viewed in real time as the region markers are placed and moved. In practice, some may be necessary to achieve the goal of removing baseline artifacts, so this live update can speed the process. In Figure 8-28, we have selected new baseline points with 'Follow Data' checked, and 'Baseline Fit' set to 'Cubic Spline'. After clicking 'Apply', the result in Figure 8-29 is obtained.

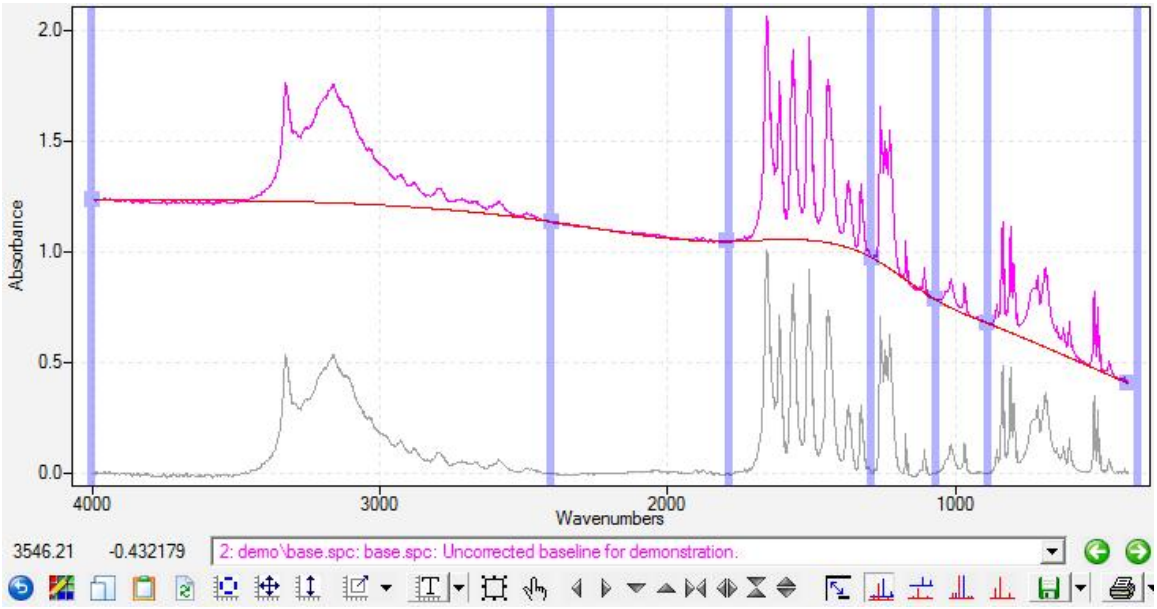


Figure 8-28 Baseline Correction

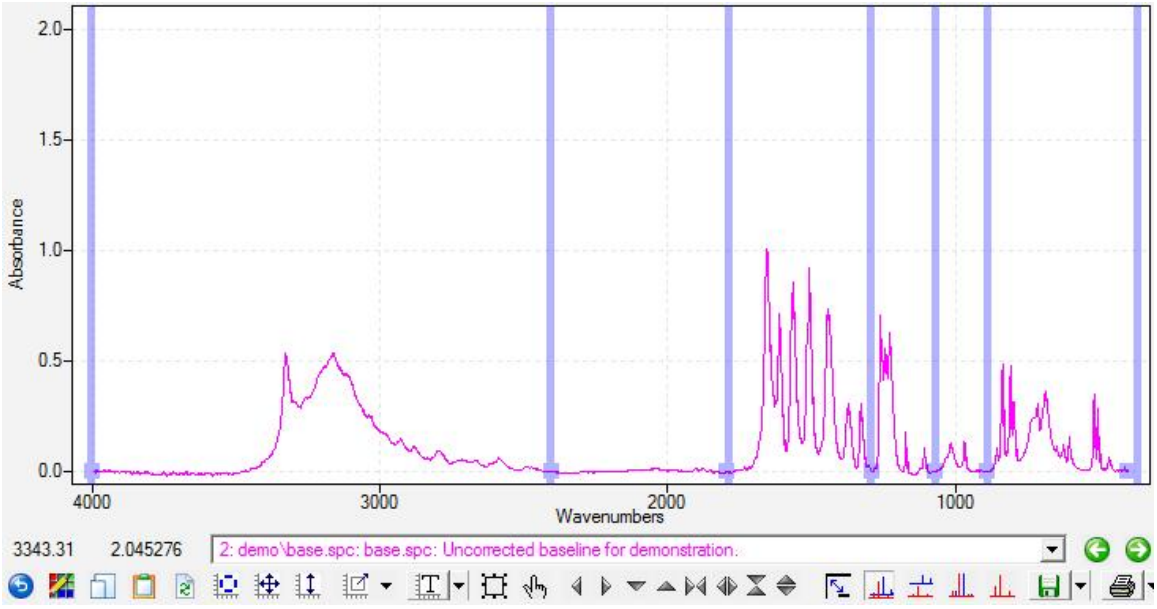


Figure 8-29 Applied Baseline Correction

Auto Baseline Correction

The ***Auto Baseline Correction Tool*** is used to repair simple baseline defects without the requirement of defining ***Regions***. The **Auto Baseline Correction** parameters window is shown in Figure 8-30.

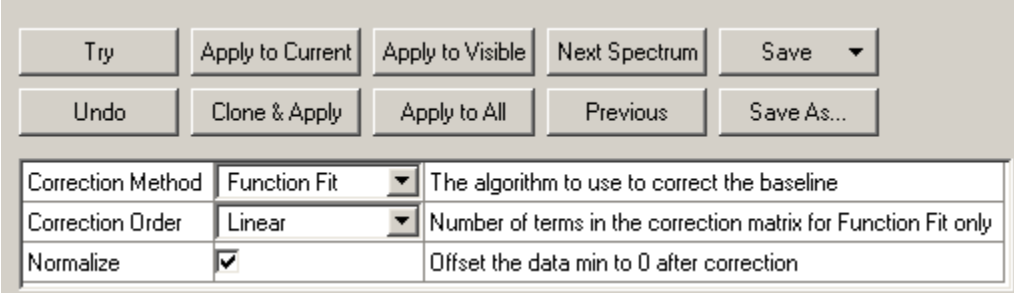


Figure 8-30 Auto Baseline Correction *parameters*

Again, the eight common ***Toolbox Buttons*** are present. You should refer to the section on the ***Zap Tool*** for detailed information on the functions of these buttons. Below the buttons is a two row options box.
The Correction Method specifies the way the baseline correction is done. Two options are available:

- ***Function Fit*** – Fit a polynomial of first through fourth order by solving a linear regression equation.
- ***GIFTS Auto-Leveling***- baseline slope and offset are removed by fitting a straight line to the data and iteratively discarding points that do not fit the line well.

The second row, labeled ***Correction Order*** is used to specify the order of the polynomial used to correct the spectrum when the 'Function Fit' correction method is specified. Three options are available from the drop down menu.

- ***Linear*** - corrects the spectrum baseline with reference to a 1st order polynomial
- ***Quadratic*** -corrects the spectrum baseline with reference to a 2nd order polynomial
- ***Offset*** - does not use a polynomial, but offsets the data so as to place the mean value of the spectrum at zero.

The check-box labeled ***Normalize*** sets the minimum *y*-axis data point to zero after correction. If noise is present to a significant degree in any part of the spectrum (as is often the case in the high and low extremes of the *x*-axis) then this option is not desirable. An example of the ***Auto Baseline Correction Tool*** in action is given in Figure 8-31.

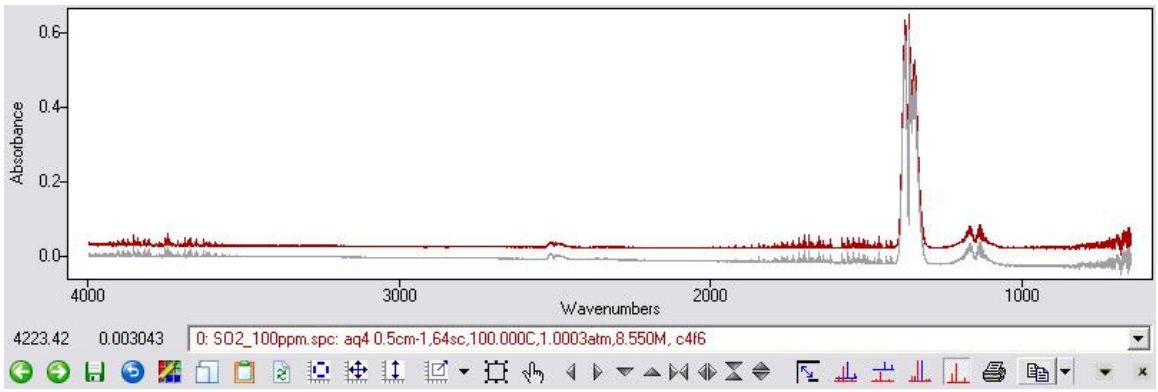


Figure 8-31 Auto Baseline Correction *example*

The example given in Figure 8-31 uses the sulfur dioxide spectrum we have used previously. The parameters were as set out in Figure 8-30. The gray spectrum was invoked by pressing the ***Try*** button.

Fit Baseline

The ***Fit Baseline Tool*** is like a combination of the Zap tool (above) and the Manual Baseline Correction tool (above). Unlike the Zap tool, the region markers are not used pair-wise to define separate distinct regions for zapping. The region markers define points to use to fit a new baseline, as in the Manual Baseline Correction tool. Unlike the Manual Baseline Correction, those points defined by the region markers are not pulled to zero to 'correct' the baseline. Rather, the region markers define points to use in fitting a cubic spline, which spline is then used to generate new points over the total area defined by the region markers.

This tool is useful in creating synthetic backgrounds from single beam spectra. In open-path spectroscopy, often the sample spectrum is made to serve as its own background by smoothing or lining-out (i.e. zapping) regions of interest. This tool makes it easier to fit a curve to the regions of interest.

In the following figure, a singlebeam spectrum has been loaded and zoomed into the region of interest. In this case, we want to analyze the spectrum for ammonia.

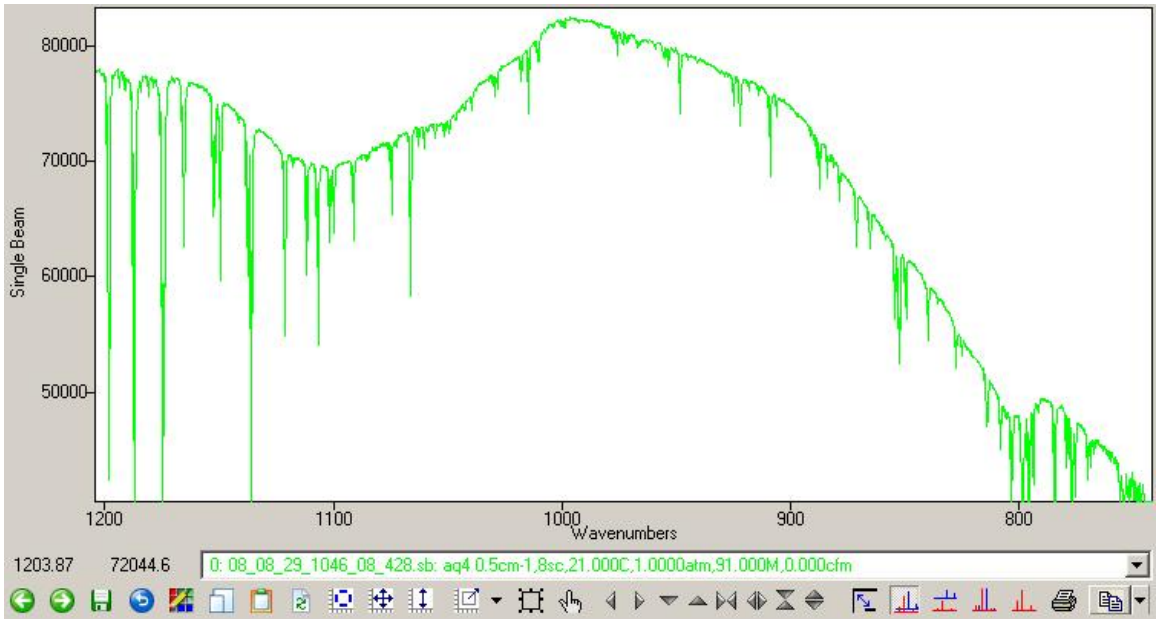


Figure 8-32 A singlebeam spectrum

Now the user has laid down region markers:

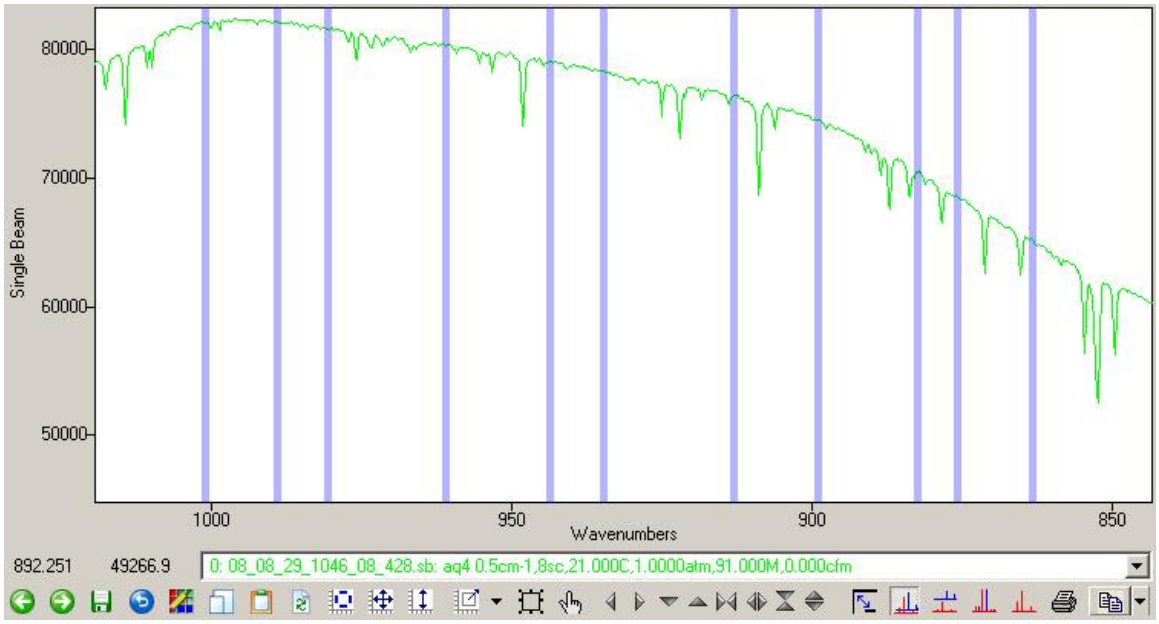


Figure 8-33 Region Markers for Fit Baseline

After clicking the 'Apply' button, the data over the area defined by the region markers is replaced with an interpolated curve:

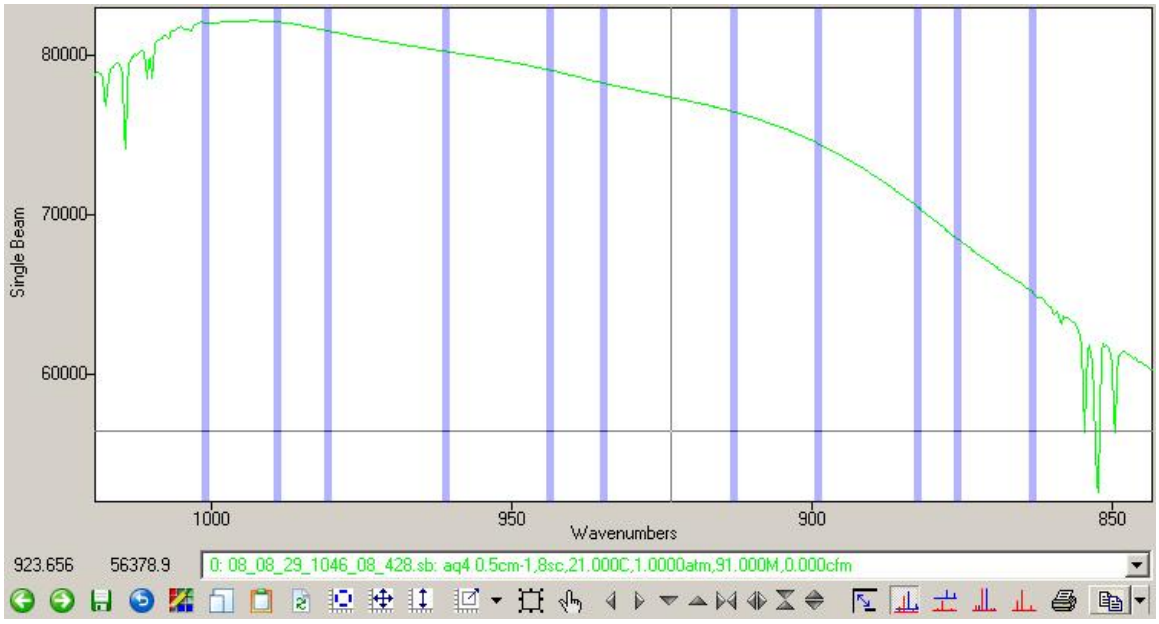


Figure 8-34 Applied Fit Baseline

The modified singlebeam spectrum can now be used as its own background. Using the FFT/Ratio tool, this absorbance spectrum is produced by ratioing the singlebeam in Figure 8-32 against the 'Fit Baseline' result in Figure 8-34, which can now be used to analyze the spectrum for ammonia.

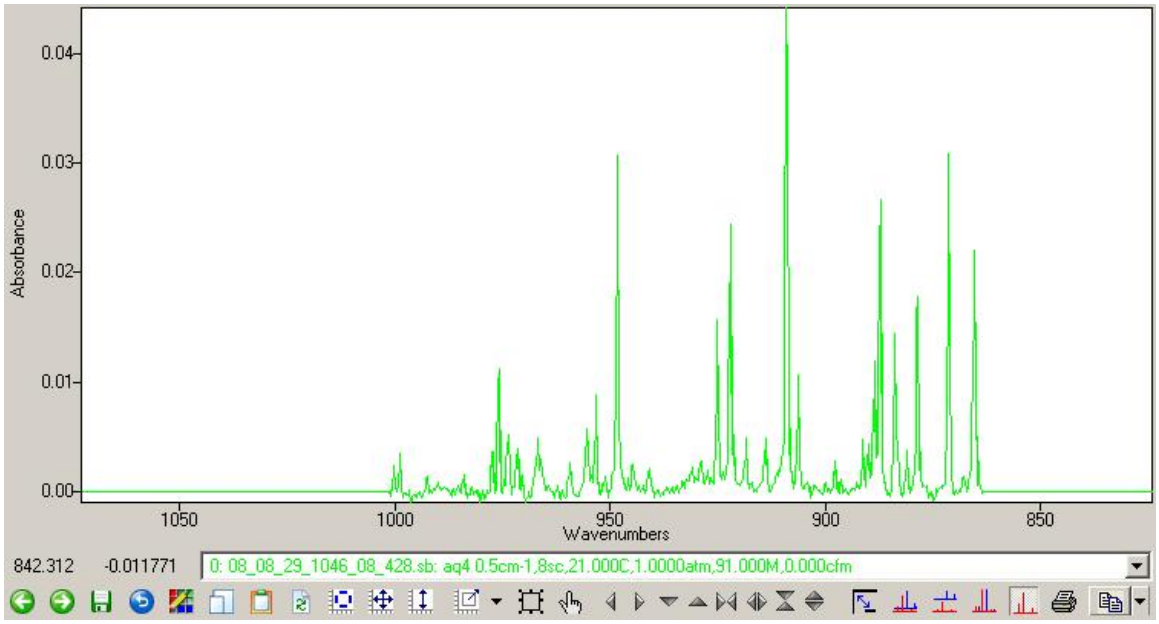


Figure 8-35 An absorbance spectrum produced by ratio with itself.

X-Shift

It is often useful in FTIR to employ library spectra in the course of a measurement. Often however, these library spectra were acquired on an instrument other than the spectrometer used to obtain the sample spectra. While this is theoretically not a problem, when spectral features are very narrow (as is often the case with gas phase spectra) then any small uncertainties in the *x*-axis of either sample or library spectra are readily apparent. These discrepancies, or *x*-shifts, can cause problems for quantitative analysis. The ***Essential FTIR X-Shift Tool*** provides a simple and powerful method of correcting these *x*-shifts.

The parameters window for the X-Shift Tool is shown in Figure 8-36.

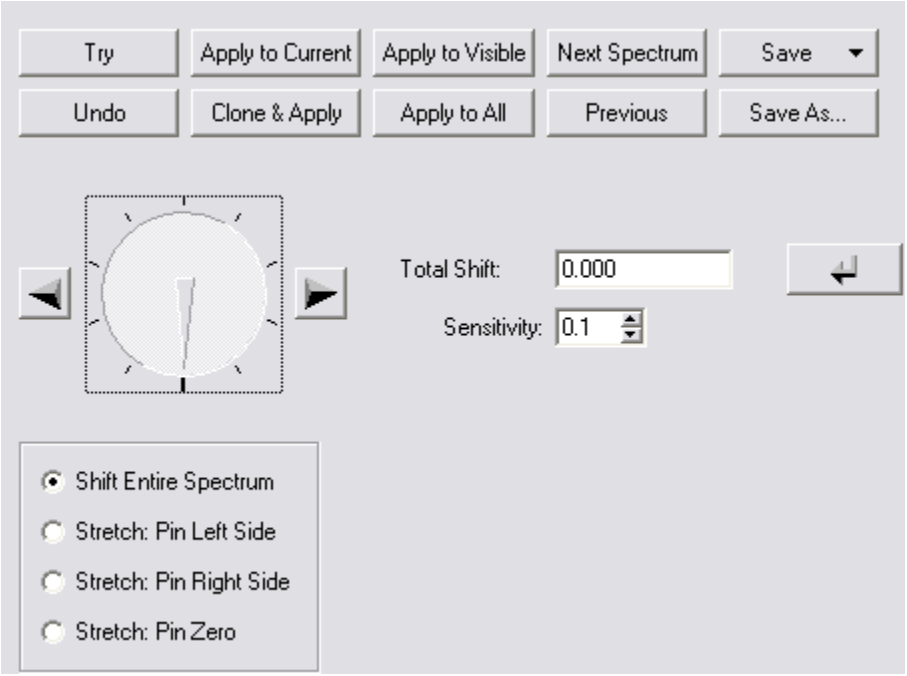


Figure 8-36 X-Shift *parameters*

The common ***Toolbox Buttons*** are present. Below these buttons three main features are evident – a ***Clock Dial***, a series of radio buttons and two edit boxes, together with a ***Return*** button.

The ***X-Shift Tool*** provides three methods of shifting a spectrum. Clicking on the arrows on either side of the ***Clock Dial*** shifts the active spectrum in the direction indicated by the arrows. The degree to which the active spectrum is shifted by a given rotation of the ***Clock Dial*** is set using the ***Sensitivity*** box - using the up and down arrows sensitivity to rotation may be set between $100cm^{-1}$ and $0.001cm^{-1}$. The ***Clock Dial*** provides an interactive way of shifting a spectrum – the *x*-shift applied is shown by a "ghost" gray spectrum. Clicking ***Apply*** will execute the shift. The third method is to enter a number directly in the 'Total Shift' edit box and then pressing the 'enter' key or clicking the 'return key' icon to the right of the edit box. An example showing carbon monoxide spectra with relatively *x*-shifted absorbance bands is given in Figure 8-37.

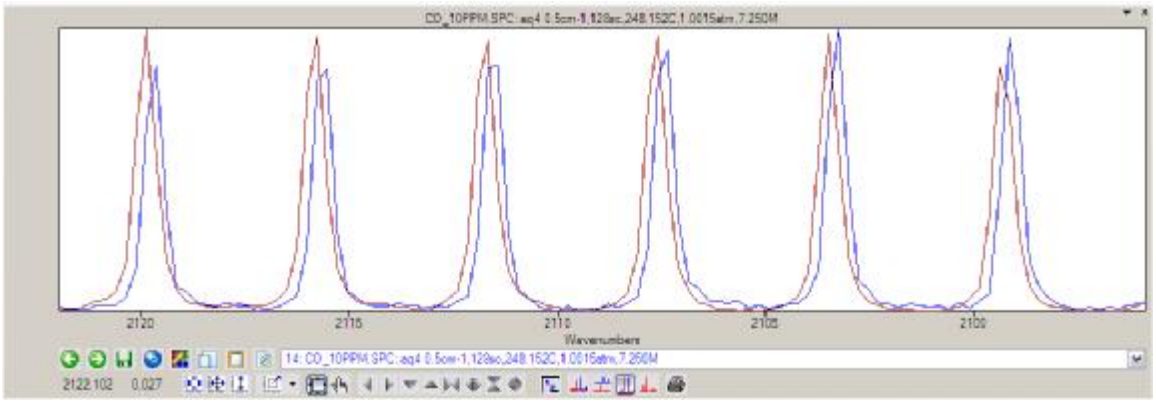


Figure 8-37 *Relatively shifted carbon monoxide peaks*

We see that in order to match correctly the absorbance bands shown in Figure 8-37 must be shifted. Figure 8-38 shows how this is accomplished.

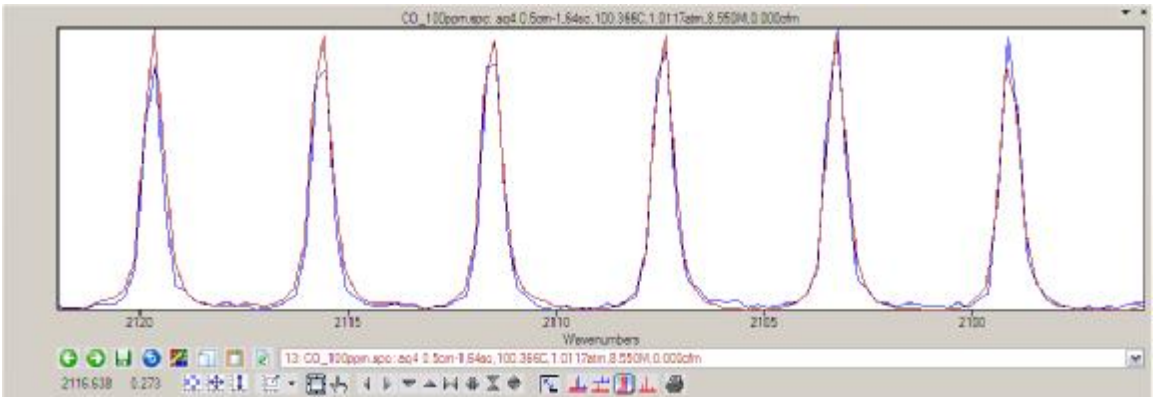


Figure 8-38 X-*Shift corrected carbon monoxide*

The ***Clock Dial*** is used with a ***Sensitivity*** setting of 0.01cm^{-1} to shift the active spectrum to match the carbon monoxide spectrum, as judged by the gray "ghost" spectrum. We see from the ***Total Shift*** box that the degree of shift necessary to match the two spectra is -0.230cm^{-1}. The ***Total Shift*** box may be used in place of the ***Clock Dial*** to shift spectra, simply by entering the numerical value for the desired shift. As with other tools, clicking the ***Apply*** button executes the change, and the spectrum may be saved.

Derivative

The ***Derivative Tool*** may be used to show the n^{th} order derivative of a spectrum, where n may take the values 1-4. The ***Derivative*** parameters window is shown in Figure 8-39.

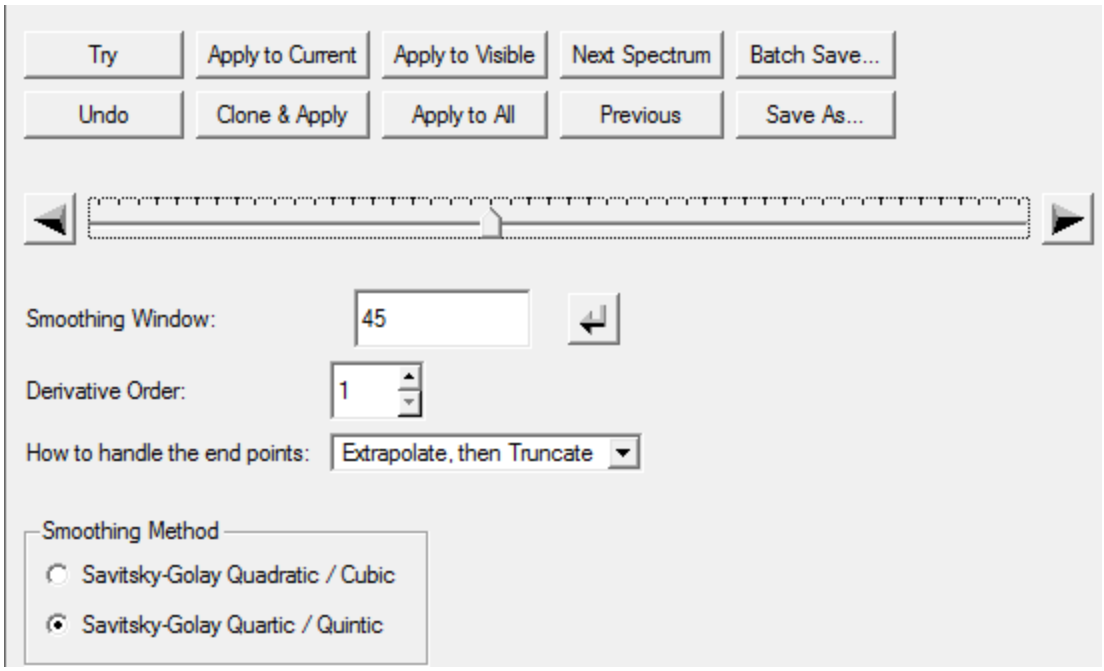


Figure 8-39 The Derivative Tool

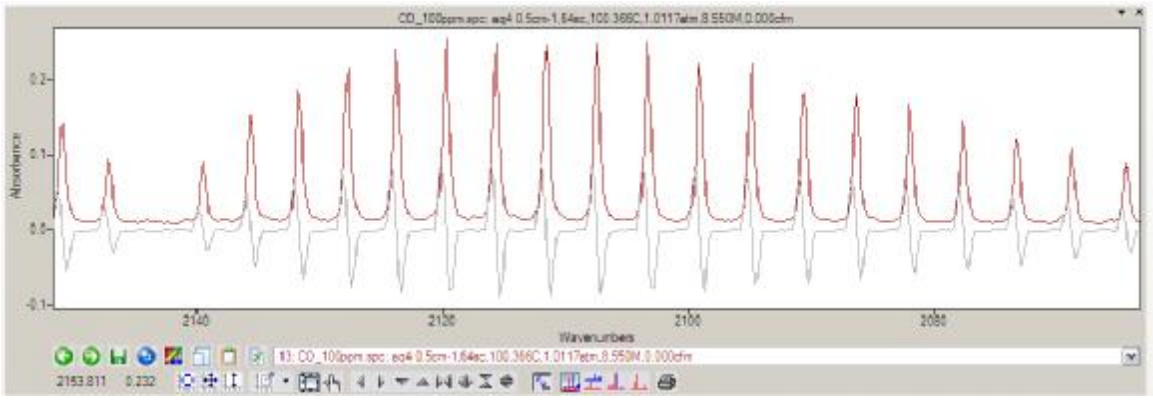


Figure 8-40 Derivative *parameters and result*

We see from Figure 8-39 that along with the usual ***Toolbox Buttons*** the ***Derivative Tool*** uses a slider bar to select the order of the derivative to be applied. In this case we have selected a 1st order derivative, which is often used to precisely locate the *x*-axis position of the *maxima* and *minima* of absorbance features.

Ratio

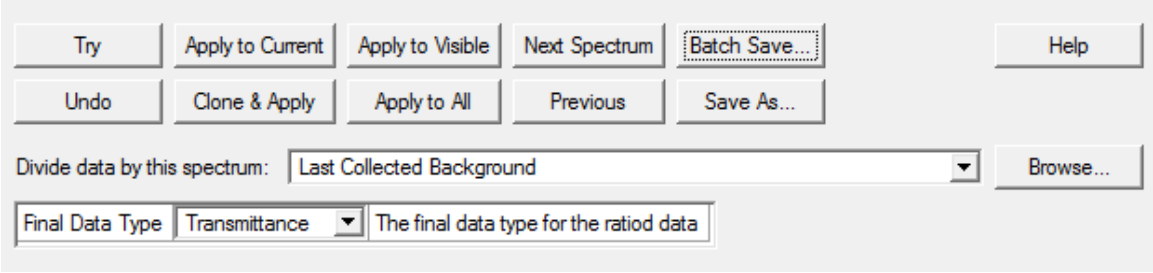


Figure 8-41 The Ratio Tool

FTIR is a ratio technique. Typically, a sample spectrum is derived from two singlebeam spectra: the background singlebeam and the sample singlebeam. Dividing the sample singlebeam by the background singlebeam yields a Transmittance spectrum. This ratio of sample by background divides out features that are both spectra (such as CO2 or Water vapor), leaving only the spectral features of the sample.

The ratio tool in Essential FTIR can be used to ratio any two spectra. Usually these will be two singlebeam spectra to produce a Transmittance spectrum, but the tool is more general-purpose. Any spectrum can be divided by any other spectrum, regardless of the data types of the two, providing there is overlap in the x-axes of the two.

If the endpoints of the two spectra do not match, the intersection of the two spectra is used automatically. If the data point spacing of the two spectra do not match, the background (that is, the divisor) is automatically interpolated to the data point spacing of the sample (that is, the numerator).

Interferogram to Spectrum (FFT / Ratio)

An absorbance spectrum usually represents the final stage in spectral processing. An FTIR spectrum begins life as an interferogram. In order to glean information regarding the infrared absorbance at any given frequency the interferogram must be Fourier transformed to yield a single beam spectrum. This single beam sample spectrum is then divided by a background single beam spectrum. This ratio forms a transmittance spectrum. An absorbance spectrum is the negative logarithm of this transmittance spectrum, as infrared transmission is logarithmically related to the concentration of the absorbing species at a characteristic wavelength, whereas the absorbance spectrum is linearly proportional to this concentration.

There may arise circumstances where a user might wish to convert between these data types, and the ***Interferogram to Spectrum Tool*** provides a method to achieve this. Note that the parameters for the ***Tool*** are duplicated on the ***Collect Tool*** and in the ***Settings***, and changing the parameters in one place will also change the parameters in the other. The

parameters window for the ***FFT Interferogram to Spectrum Tool*** is shown in Figure 8-42.

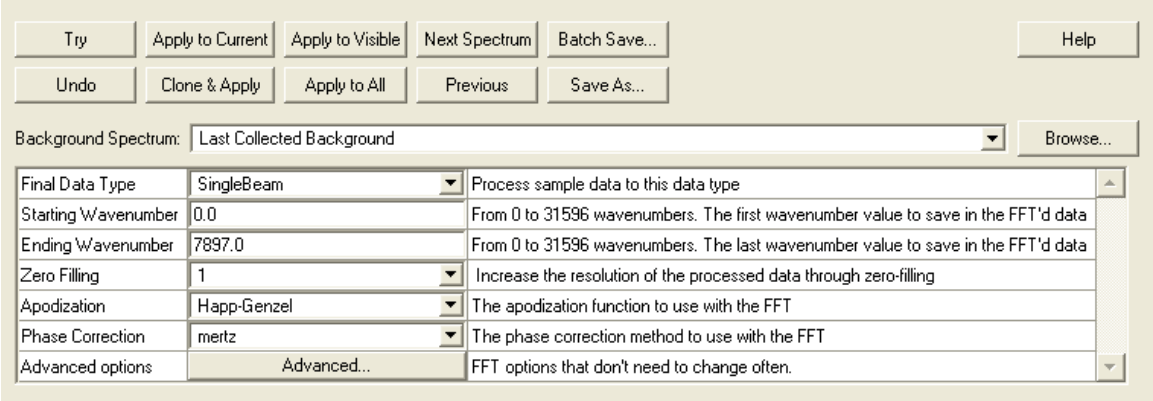


Figure 8-42 Interferogram to Spectrum *parameters window*

Ignoring the common ***Toolbox Buttons***, we see that the parameters window shows a drop-down menu labeled ***Background Spectrum***. This feature allows you to specify any interferogram or single beam spectrum for the purposes of division, to produce a transmittance spectrum from two single beam spectra.

If the background spectrum is an interferogram, it will automatically be processed to a singlebeam using the same parameters, before it is used in the ratio. Note that the spectrum in the 'Background Spectrum' box is always read from disk, even if it is in an Essential FTIR workspace. Therefore, if you modify a spectrum in a workspace for use as a background in this tool, please save it to disk so that the changes you made will take effect.

The main feature of the parameters window is the options box, containing seven rows of options. Examining each option in turn:

1) ***Final Data Type***: A drop down menu allows selection of absorbance, transmittance, single beam or interferogram.
2) ***Starting Wavenumber***: An edit box allows specification of the lowest wavenumber to be processed.
3) ***Ending Wavenumber***: An edit box allows specification of the highest wavenumber to be processed.
4) Zero Filling: A drop down menu allows selection of the degree of interpolation in the processed spectrum. Positive integer values between 0 and 3 are allowed.
5) ***Apodization***: The apodization function used to remove processing artifacts from the fast Fourier transform (FFT). ***Triangle, Boxcar, Beer-Norton Med, Beer-Norton Weak, Beer-Norton Strong, Happ-Genzel, Bessel, Cosine, Blackman-Harris 3 Term, Blackman-Harris 4 Term and Cosine 3*** are selectable via a drop down menu.
6) ***Phase Correction***: You may select either Mertz or magnitude methods of phase correction.

7) ***Advanced:*** Refer the 'Process' section of Chapter 6 for a discussion of the advanced settings. Click here to go to that section. Pay close attention to the advanced settings, or the calculated spectrum will not be correct.

The ***FFT / Ratio Tool*** can also be used to simply ratio two single beam spectra. If the active spectrum is a single beam, then this ***Tool*** may be used to ratio it against a background spectrum.

The ***FFT /Ratio Tool*** can also be used to change a spectrum between Transmittance and Absorbance, although the 'Y axis conversion' tool is better suited for this task. The FFT / Ratio tool always tries to convert from the starting data type of the active spectrum to whatever the final data type is.

Subtract

The ***Subtract Tool*** is used to remove unwanted absorbance features from a sample absorbance spectrum by subtracting a reference spectrum from the sample spectrum. This reference spectrum is known as the ***Subtrahend***. The parameters window for the ***Subtract Tool*** is shown in Figure 8-43.

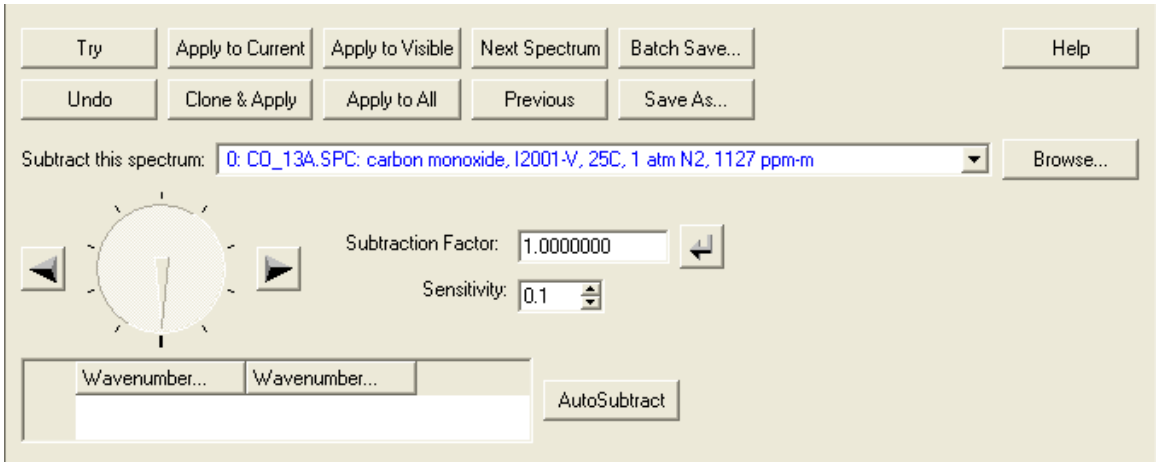


Figure 8-43 Subtract *parameters window*

The ten common ***Toolbox Buttons*** are present. Below these is a drop down window, used to select the ***Subtrahend*** from a list of spectra in the ***Workspace***. If the desired ***Subtrahend*** is not present in the ***Workspace*** then the ***Browse*** button may be used to locate and load it.

A ***Clock Dial*** interface, similar to that used in the ***X-Shift Tool*** is available to interactively adjust the degree of subtraction applied to the active spectrum. The indicator in the dial may be adjusted using the arrow buttons on each side. The ***Sensitivity*** box is used to set the degree of subtraction applied when the ***Clock Dial*** indicator is advanced by one tick mark. The ***Subtraction Factor*** box shows the multiple of the ***Subtrahend*** applied to the subtraction, for instance if the ***Total Subtraction*** box reads 0.5000 then the ***Subtrahend*** is multiplied by 0.5 and subtracted from the active spectrum. A subtraction may also be applied by entering a factor in the ***Subtraction Factor*** box and clicking the Return button.

The subtraction may be automated by setting wavenumber limits. This is achieved by right-clicking in the Workspace window to set Regions for evaluation of the subtraction. Pressing the ***Auto Subtract*** button then applies the Subtrahend to the active spectrum, automatically removing the interfering absorbance peaks over the wavenumber range specified.

Smoothing

The ***Smoothing Tool*** is used to convolve the active spectrum with a choice of smoothing coefficients. Smoothing may be undertaken for a variety of reasons, such as the need to improve the quality of a least squares fit for a low resolution spectrum, or removing large absorbance features from a single beam spectrum to create a background spectrum for use in open path FTIR analysis. The ***Smoothing Tool*** parameters window is shown in Figure 8-44.

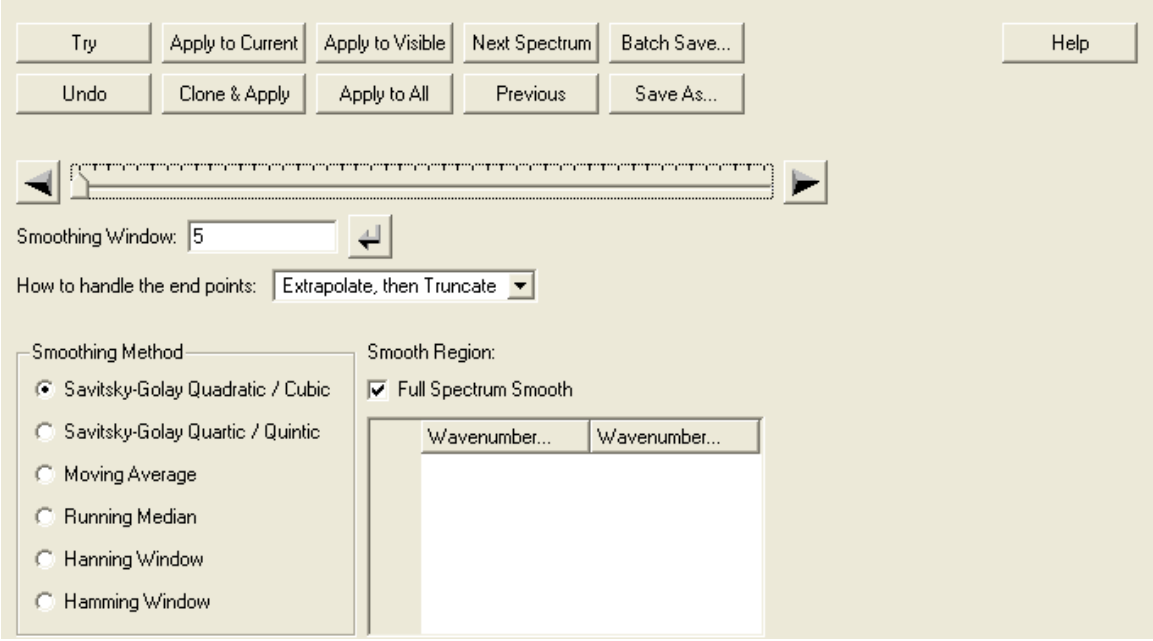


Figure 8-44 Smoothing Tool *parameters window*

The common ***Toolbox Buttons*** are all present, beneath which is a slider bar, which may be used to select the number of smoothing points. Alternatively, the number may be directly entered into the edit box labeled ***Smoothing Window***. Pressing the ***Return*** button will apply the change.

Five smoothing algorithms are available, selectable via the radio buttons on the left of the window. To the right of these is a ***Regions*** window. When the ***Full Spectrum Smooth*** check-box is un-checked, a single ***Region*** may be selected by right-clicking on the active spectrum in the ***Workspace***, and will be visible in the ***Smooth Region*** window. The smoothing will then be applied over the specified range.

An example of using the ***Smoothing*** feature to create a background spectrum for open path FTIR is shown in Figure 8-45.

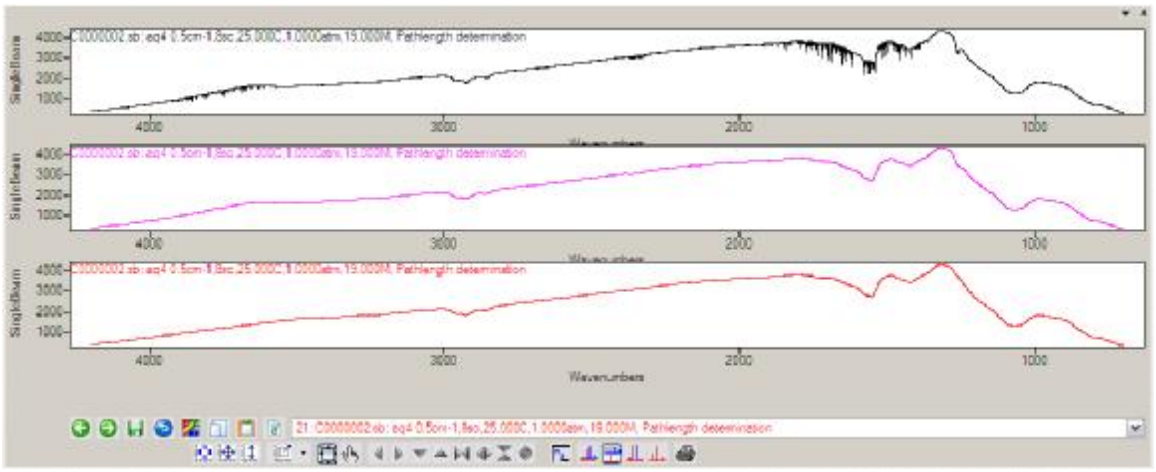


Figure 8-45 *Application of* Smoothing Tool

The uppermost spectrum shown in Figure 8-45 is an untreated open path single beam spectrum. The center of the figure shows the same spectrum after the smoothing parameters shown in Figure 8-44 have been applied. The lower spectrum has the wide features removed using the ***Zap*** feature. This would not be possible without the intermediate smoothing step, as the true "zero" background of the single beam is obscured by water and carbon dioxide bands.

Truncate

The ***Truncate Tool*** enables you to trim a spectrum, retaining only the data range defined by the ***Region***. This ***Region*** is set in the usual way – by right-clicking on the active spectrum in the ***Workspace*** to define ***Region Markers***. Figure 8-46 shows the parameters window, together with an example Workspace.

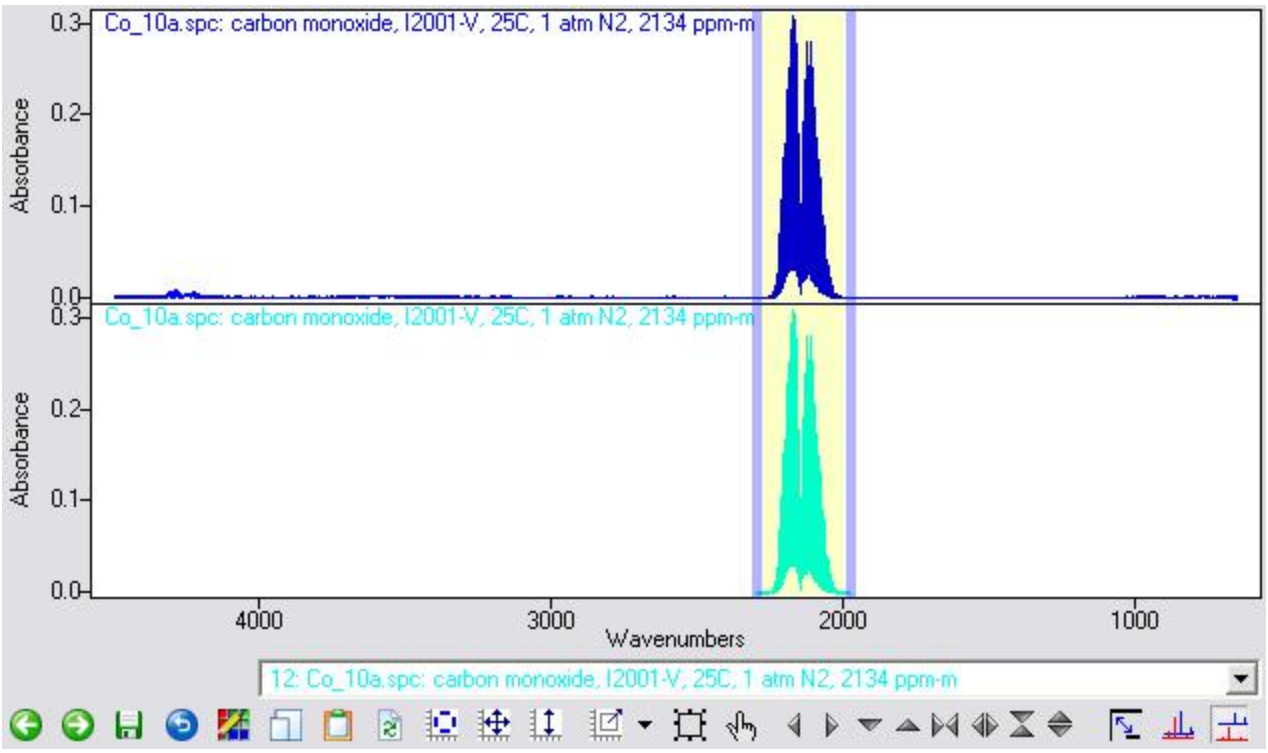


Figure 8-46 Truncate Tool

The ***Truncate Tool*** parameters window contains the common ***Toolbox Buttons***. Below these buttons lies a ***Regions*** window, which displays the data range marked for retention after the truncation. In the example shown in Figure 8-46, a carbon monoxide spectrum has the main absorbance feature captured by the ***Region*** markers. In ***Stacked*** display mode the ***Clone and Apply*** button was used to truncate the spectrum and display the result in the lower data display. This truncated spectrum may now be saved as a new file, or saved over the original data.

Scale / Offset

The ***Scale / Offset*** tool may be used to perform arithmetic operations on spectra using a constant. The Scale / Offset parameters window is shown in Figure 8-47.

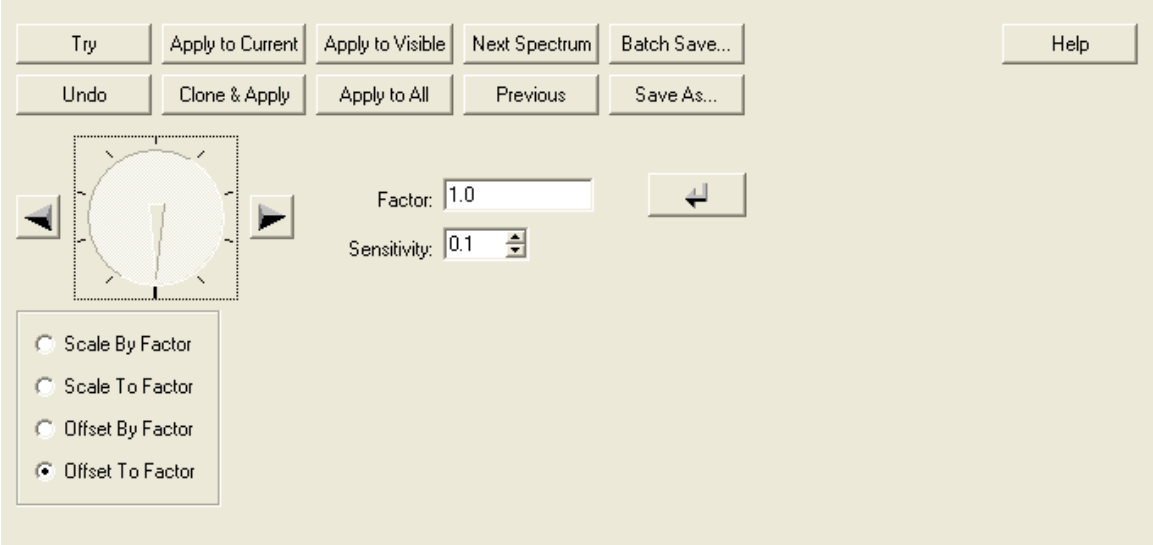


Figure 8-47 Scale / Offset *parameters*

The ***Toolbox Buttons*** are present. Below these buttons lies a ***Clock Dial*** interface, which allows application of the operations interactively. The ***Factor*** edit box contains the value dialed in. This value may also be entered directly into the edit box. The ***Return*** key executes the operation as a ***Try*** – delivering a gray "ghost" spectrum showing the result of the operation. The ***Sensitivity*** box is used to set the magnitude of the change in the ***Factor*** applied when the ***Clock Dial*** indicator is advanced by one tick mark.

Four radio button occupy the lower left of the parameters window. Dealing with each button in turn:

- ***Scale By Factor:*** The data will be scaled according to the constant displayed in the ***Factor*** edit box.
- ***Scale To Factor:*** The dynamic range of the data will be re-scaled from n, where n is the constant specified in the ***Factor*** edit box.
- ***Offset By Factor:*** Adds the constant specified in the ***Factor*** edit box to the data.
- ***Offset To Factor:*** Sets the minimum value in the spectrum to the value specified in the ***Factor*** edit box.

Interpolate / Decimate

The ***Interpolate / Decimate Tool*** enables you to alter the digital resolution of a spectrum. Digital resolution is the actual distance between data points in a spectrum, the 'point spacing', also referred to as 'delta X'.. It is not the same thing as Optical Resolution, although it can affect the apparent optical resolution of the data. The ***Interpolate / Decimate*** parameters window is shown in Figure 8-48.

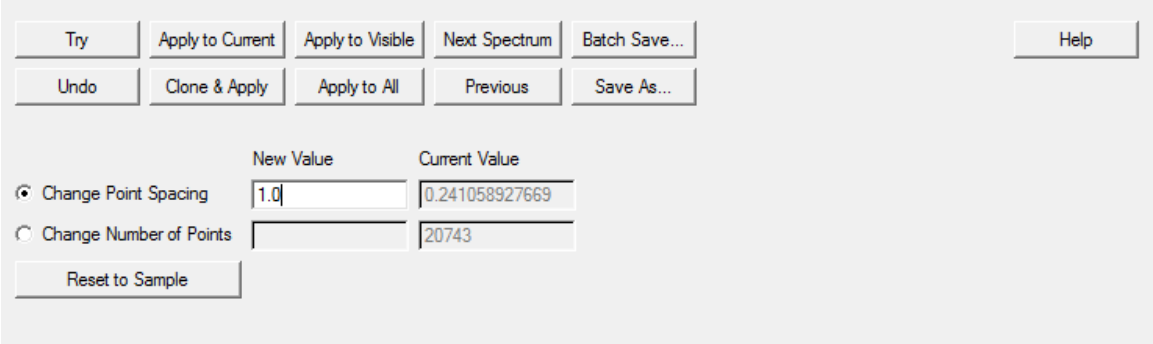


Figure 8-48 Interpolate / Decimate *parameters window*

The parameters window houses the usual ***Toolbox Buttons***. You can enter the point spacing directly in the edit box to the right of the 'Change Point Spacing' radio button, or you can enter the number of points that will be in the resulting spectrum, and the point spacing will be calculated from that. The formula used to calculate the point spacing is:

deltaX = (lastX – firstX) / (points -1)

where lastX is the x-value of the last point in the spectrum, and firstX is the x-value of the first point in the spectrum.

The 'Reset to Sample' button will set the New Values to be the same as the Current Values.

The cubic spline interpolation method is used. It is important to note that while decimating data usually yields a spectrum resembling a reference spectrum acquired at the new resolution, interpolating a spectrum does not add new information to the data, and therefore will not re-generate narrow absorption features not captured by the original data acquisition parameters. That is, interpolating a spectrum to a higher resolution does not increase the optical resolution of the spectrum.

Match Spectra

A common task in handling spectra is make all of their starting and ending values and digital resolution match each other, or some standard set of parameters. This tool makes it easy to do this to groups of spectra at a time.

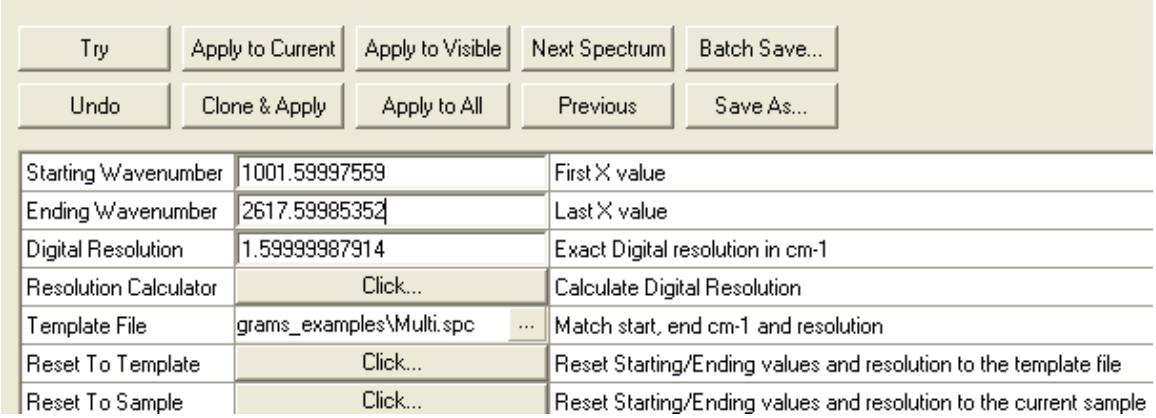


Figure 8-49
The Match Spectral window

A very powerful and convenient feature of this tool allows you to select a spectrum as the 'template'. When you choose a template spectrum, the starting and ending wavenumbers and the digital resolution of this spectrum are put into the table and will be applied to spectra that you perform this operation with.

The Conversions & Corrections Toolbox

Many different methods of sampling are available to the infrared spectroscopist. The sample matrix usually dictates the sampling method - attenuated total reflectance, diffuse reflectance and transmission are the most commonly used methods. These techniques deliver data with differing characteristics. The ***Conversion & Corrections Toolbox*** houses a set of ***Tools*** that may be used to convert between the characteristic data sub-types acquired using different sampling methods, or to correct a spectrum so that it may be compared – "apples to apples" – with a spectrum acquired using a different sampling technique. We will examine each tool and its applications in turn.

Y-Unit Conversions

This tool converts the Y-Axis units between various common infrared spectroscopy units.
The ***Kubelka-Munk*** conversion is used when handling diffuse reflectance spectra, and provides a more linear relationship with concentration than absorbance spectra.

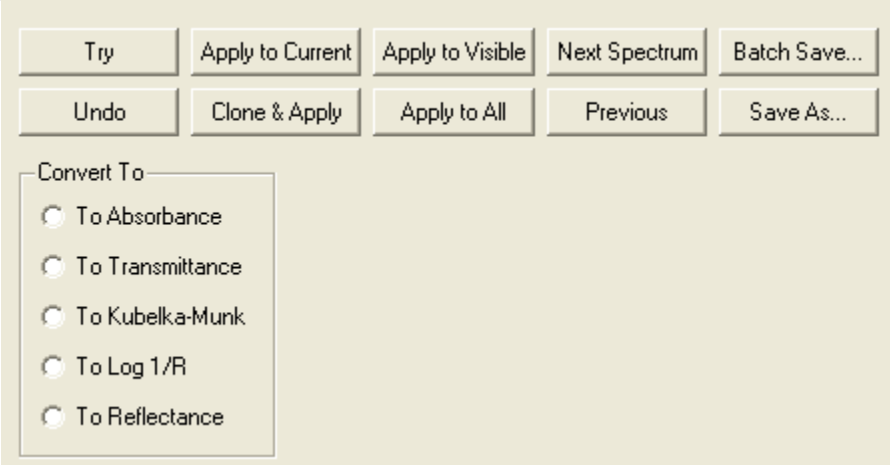


Figure 8-50

X-Unit Conversions

Historically, wavenumbers (cm^{-1}) are used as the *x*-axis units for infra red spectra. Wavenumbers are a convenient unit for infrared data, but sometimes it is desirable to use wavelength units, such as nanometers or micrometers The ***X-Unit Conversion*** parameters window is shown in Figure 8-51.

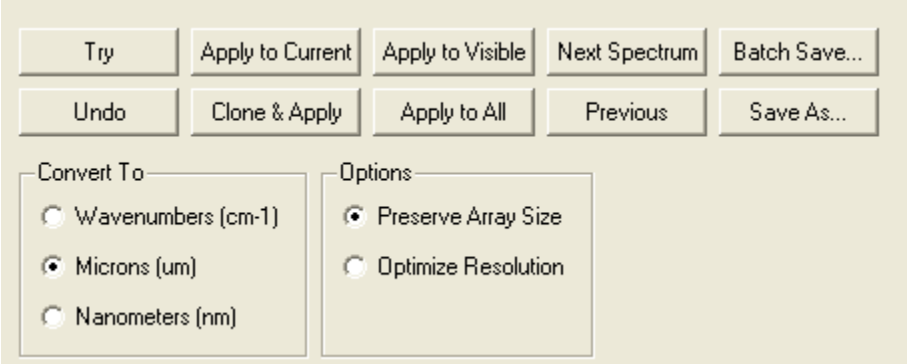


Figure 8-51 X-Unit *Conversion parameters*

The ***Toolbox Buttons*** are used to try, apply and save the transformed spectrum. Three options are available through the conversion options – wavenumbers cm^{-1}, nanometers (nm) and micrometers (μm).

The application of a conversion will impact on the number of data points contained in the converted spectrum, as converting from wavenumbers to linear units requires linearization - that is, wavenumbers are cm^{-1}, or reciprocal centimeters, 1/cm. The two systems of units are inversely related. Two options are provided which enable you to manage the size of the resultant array – ***Preserve Array Size*** and ***Optimize Resolution***, which are selected using the radio buttons on the right of the parameters window. The ***Optimize Resolution*** option creates a new data array that is approximately a factor of ten larger than the original. When using this option the high wavenumber end of the array is used to calculate the *x*-axis spacing necessary to preserve all spectral features. At the low wavenumber end of the spectrum, points are interpolated between the existing points. Thus, the ***Optimize Resolution*** option preserves spectral features at the high wavenumber end of the spectrum.

The ***Preserve Array Size*** option creates a new data array that will contain the same number of points as the original. Resolution must be degraded in order to satisfy this condition. Data points are interpolated at the low wavenumber end of the spectrum and averaged at the high wavenumber end of the spectrum.

It is important to note that when using either option, converting back and forth between formats will quickly increase the data array size to unmanageable proportions very quickly – the ***Undo*** button should be used to convert back to the original *x*-axis units.

Advanced ATR Correction

When using attenuated total reflectance (ATR) sampling techniques, spectra take on characteristics which are dependent on the angle of the infrared beam incident on the ATR crystal, the refractive index of the crystal and on the refractive index of the sample.

In order to compare a reference spectrum acquired using traditional transmission spectroscopy, it is necessary to correct the ATR data before making any quantitative calculations. The ***ATR Correction Tool*** may be used to carry out this correction. The ***ATR Correction*** parameters are shown in Figure 8-52.

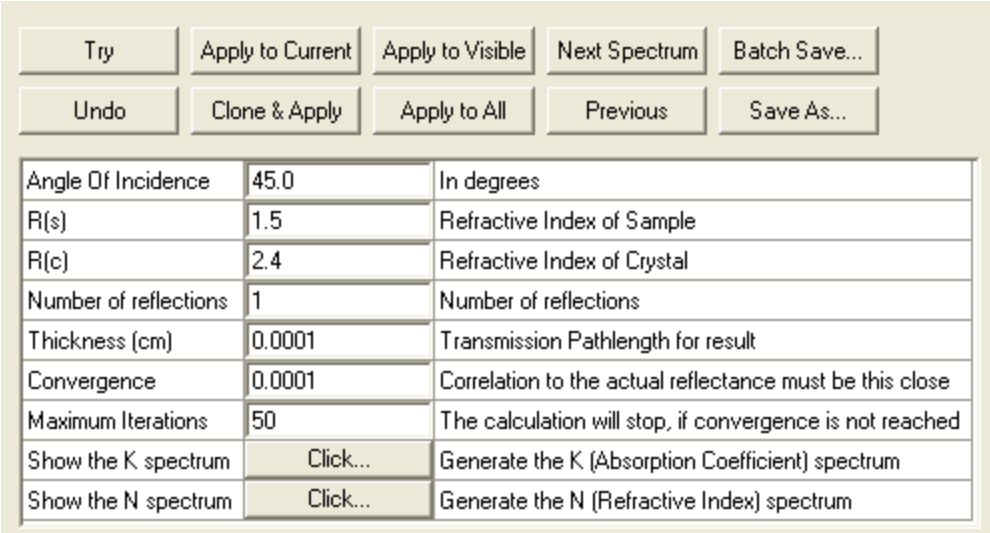


Figure 8-52 ATR Correction *parameters*

The usual collection of Toolbox Buttons are available. Below these buttons, a three row options box contains the following options:

- ***Angle Of Incidence***: The angle at which the infrared radiation strikes the ATR crystal.
- ***R(s)***: The refractive index of the sample.
- ***R(c)***: The refractive index of the ATR crystal.
- ***Number of reflections***: How many bounces the beam makes in the ATR accessory.
- ***Thickness***: The equivalent thickness of the transmission sample.
- ***Convergence***: The ATR correction is an iterative calculation. The calculated reflectance spectrum is compared to the actual measure reflectance spectrum, and the calculate stops when sequential results differ by this amount.
- ***Maximum Iterations***: If convergence is not obtained, stop after this many iterations and return the best result.
- ***Show the K Spectrum***: The algorithm generates a spectrum of the Absorption Coefficient. After the correction is run, clicking this button will display the K Spectrum.

- ***Show the N Spectrum***: just like 'Show the K Spectrum', for the Refractive Index spectrum.

The refractive index of the ATR crystal should be supplied in the literature from the accessory manufacturer, as should the angle of incidence (many ATR accessories now boast adjustable incidence angles). Powders of organic materials and aqueous solutions possess refractive indices of approximately 1.7. A table of common crystal materials is provided in the on-line help for this feature.

Kramers-Kronig

Absorbance spectra generated using reflectance spectroscopy differ in character from data acquired using traditional transmission spectroscopy. In order to quantitatively compare absorption data from the two sampling techniques it is necessary to employ a ***Kramers-Kronig*** transformation. This transformation has many applications in the field of non-linear optics, as it relates the imaginary and real parts of a function. Essential FTIR uses the Maclaurin series to compute the ***Kramers-Kronig*** transformation. There are no parameters to enter for the ***Tool***, simply use the ***Toolbox Buttons*** to apply and save the data. A warning box may be generated if the data contains zeros; if this is the case then use the ***Scale / Offset*** tool to remove these before computing the transform.

Raman Shift

The ***Raman Shift Tool*** may be employed to correct for differences exhibited in Raman spectra acquired on different instruments at different excitation frequencies. The parameters window for the ***Raman Shift*** feature is shown in Figure 8-53.

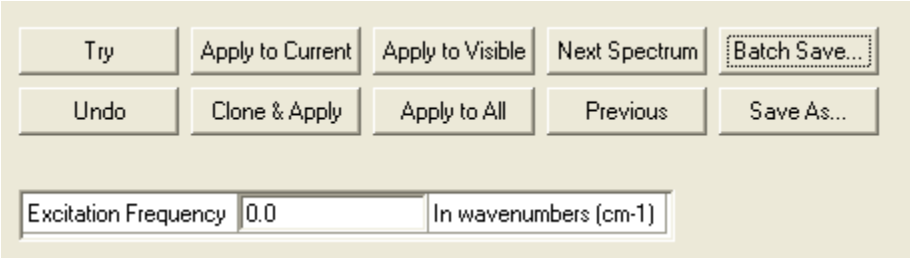


Figure 8-53 Raman Shift *parameters*

The edit box labeled Excitation Frequency is used to enter the frequency of the laser used in the Raman experiment. The Toolbox Buttons are used to try, apply and save the result.

Normalization

Normalization is used to remove variation from data to bring spectra into line with each other.

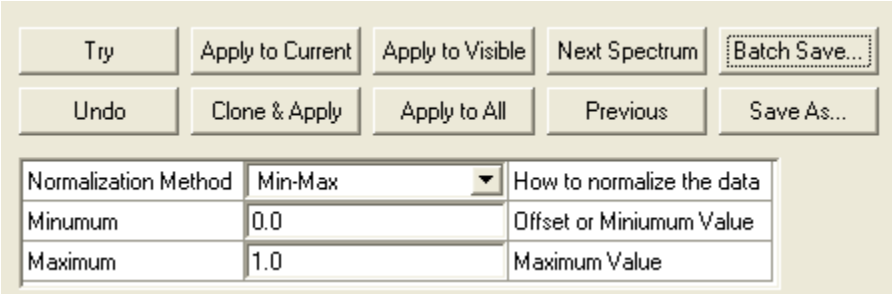


Figure 8-54 The Normalization Tool

The options for ‘Normalization Method’ are:

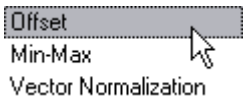


Figure 8-55 Normalizaton Methods

Offset: change the minimum value in the spectrum to the value given as ‘Minimum’. This will offset the baseline of the spectrum.

Min-Max: The baseline of the spectrum is set to the ‘Minimum’, as in Offset Normalization, and then the spectrum is scaled so that its maximum value is that given as ‘Maximum’. This changes the baseline and the dynamic range of the spectrum.

Vector Normalization: The average Y-value of the spectrum is subtracted from the spectrum (this is called ‘centering’ the spectrum). Then the spectrum is divided by the square root of the sum of the squares of the Y-values. This makes the vector norm of the spectrum equal to 1.

The Analysis Toolbox

In some applications, particularly in quality control and quality assurance, it is valuable to have the capability to carry out qualitative and quantitative tests on data, in a manner that minimizes human involvement. The role of the ***Analysis Toolbox*** is to provide this capability. We will examine each ***Tool*** in turn.

Integrate

The ***Integrate Tool*** may be used to calculate and assign a numerical value to the area beneath an absorbance feature. The ***Integrate Tool*** parameters window is shown in Figure 8-56.

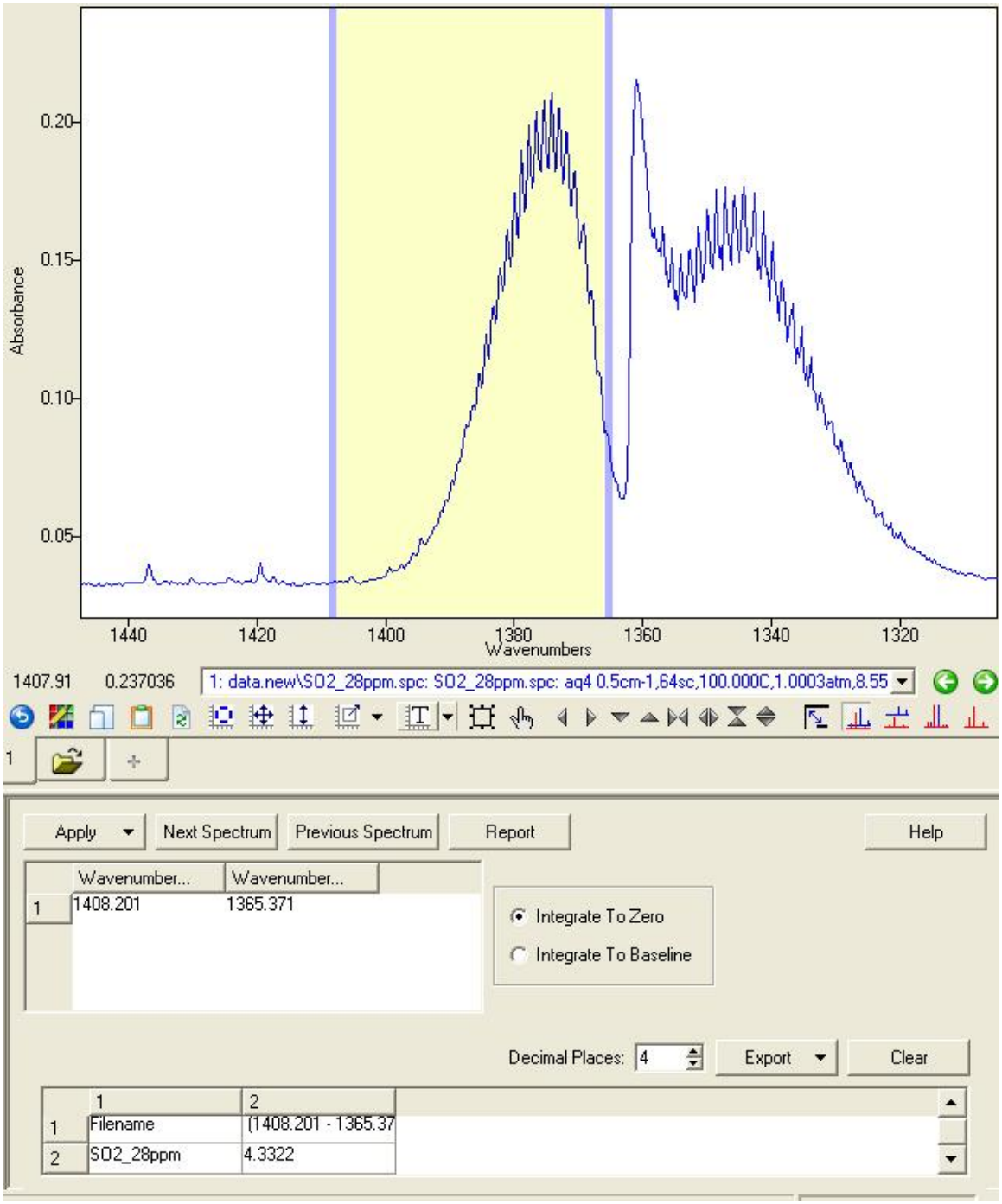


Figure 8-56 *Integration parameters*

Three of the set of ***Toolbox Buttons*** are present in the ***Integrate Tool*** parameters window – ***Apply***, ***Next Spectrum*** and ***Previous Spectrum,*** and a ***Report*** button. Below these buttons is a ***Regions*** window, which displays the ***Region***(s) to be integrated, which are set by right-clicking on the active spectrum in the ***Workspace***. An options box immediately to the right of the ***Regions*** window provides two options, selectable via radio buttons. The first option – ***Integrate To Zero*** – computes the numerical area defined by the data and the ***Region Marker's*** intersection point with the zero line. The second option – ***Integrate To Baseline*** – calculates the numerical value of the area defined by the data and the ***Region Marker's*** intersection point with the baseline. The baseline is calculated in a local way, by drawing a straight line between the ***Region Markers*** at their intersection with the data.

Once the ***Apply*** button is clicked, the numerical integral (evaluated in arbitrary units) is displayed in the area at the bottom of the parameters window, together with the filename and the limits of integration. The ***Decimal Places*** edit box allows you to set the desired precision of the measurement. The data may be pasted to the clipboard using the ***Export*** button, and erased using the ***Clear*** button.

The ***Report*** button will generate a word-compatible document including the spectral display and results table. How the report file is named, and where it is saved, are controlled by the Report settings from the Options/Setup menu selection. Using these settings, the file can also be loaded automatically in the editor for viewing and editing.

Peak Picking

When comparing one spectrum with another, it is useful to have some repeatable definition of what constitutes an absorbance peak. When operating on absorbance features of low intensity, this line can become blurred due to the increasing noise component of the data. The ***Peak Picking Tool*** allows you to set parameters to define unambiguously the peaks present in a spectrum. Figure 8-57 shows the ***Peak Picking*** parameters window.

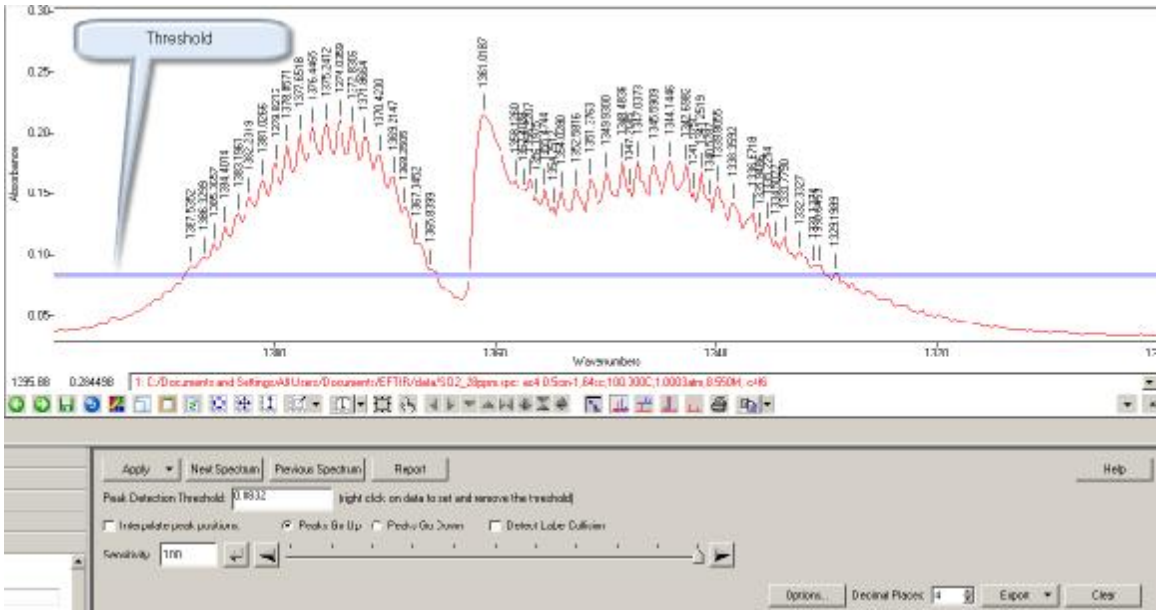


Figure 8-57 Peak Picking *parameters*

The ***Workspace*** window in Figure 8-57displays a sulfur dioxide spectrum at 1000ppm-m which has been expanded to the region of interest. In the parameters window itself are four of the set of eight ***Toolbox Buttons***.

Below these buttons is an edit box labeled ***Peak Detection Threshold***. This value may be entered directly, or defined by right-clicking on in the ***Workspace*** and dragging the resulting horizontal gray line to the desired position. The threshold is identified in Figure 8-57 by a call out box. This ***Threshold*** will exclude any peaks which do not meet or exceed the ***Threshold*** value, defined in absorbance units. We see that only the Q-branch of the SO_2 spectrum is identified by the ***Threshold*** and ***Sensitivity*** settings used.

The next feature is the ***Sensitivity*** edit box, which should not be confused with the ***Threshold.*** The Sensitivity value may be input directly to the edit box, or interactively entered using the slider bar to the right of the edit box. The slider bar may be clicked and dragged, or the buttons on either end of the bar used to position the indicator to the desired position. The ***Sensitivity*** value determines how far an absorbance feature must differ from its local baseline before being considered a peak. The sensitivity is interpreted as the percentage of the peaks to keep, based on their height above the local baseline.

If the ***Interpolate Peak Positions*** check box is checked, The five points surrounding the peak are interpolated using a cubic spline to a digital resolution 100 times greater, and the peak position and height are determined using the interpolated data.

The Peaks Go Up and Peaks Go Down radio buttons allow you to over-ride the program's default sense of whether the data's peaks go up or down. For instance, if the data is Absorbance the program will assume the peaks go up, and if Transmittance, the peaks go down. You can over-ride this behaviour with these radio buttons.

The Detect Label Collision check box adjusts the positions of the peak labels so that they do not obscure other labels. For the same peaks as the figure above, the display will look like this:

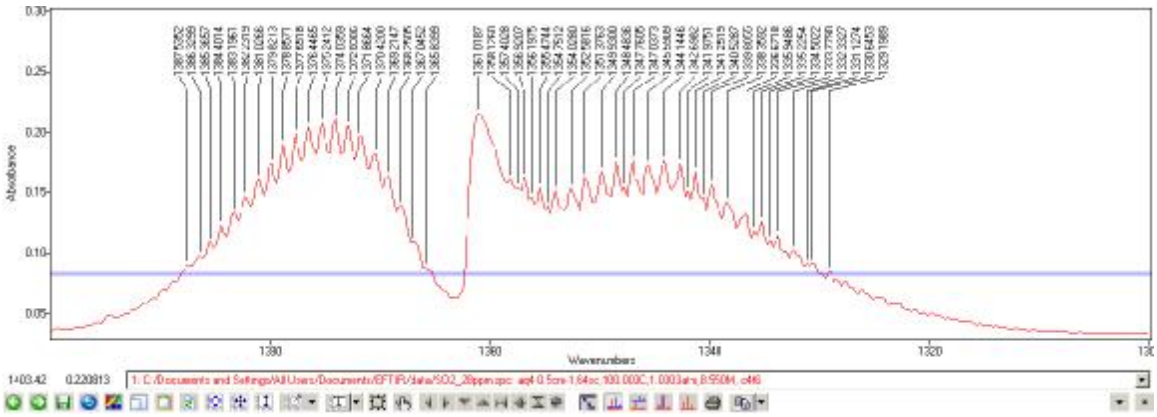


Figure 8-58 Peak Labels with 'Detect Label Collision' checked

At the bottom of the parameters window is a ***Peak Table***. The ***Peak Table*** displays the results of applying the currently set ***Peak Picking*** parameters. The peaks so defined are also displayed as annotations to the active spectrum in the ***Workspace*** window. As with the ***Integration Tool***, the precision of the numerical data generated may be specified using the ***Decimal Places*** edit box. The data in the ***Peak Table*** may be exported to the clipboard or Excel using the ***Export*** button, or removed using the ***Clear*** button.

The 'Options' button will bring up this dialog:

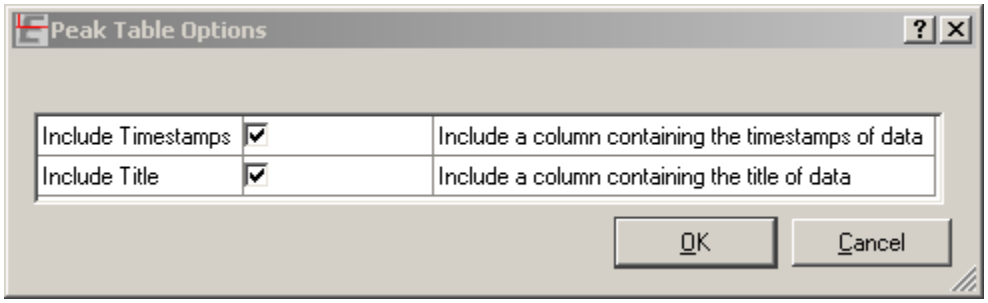


Figure 8-59 Peak Table Column Options

This will determine which information is included in the tables. The 'Include Timestamps' setting is useful when doing studies of peak height versus time.

The 'Apply' button has a drop-down menu that allows you to batch process many files at once.

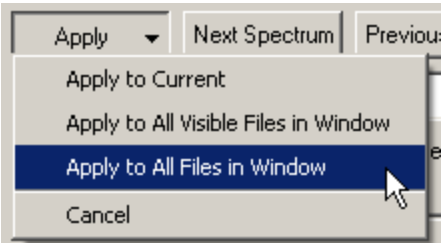


Figure 8-60

Manual Peak Picking

Sometimes automatic peak picking is not the right tool. When data is very noisy, or the peaks of interest are small relative to other peaks, or the baseline is curved, or the peaks of interest are small peaks superimposed on a broad absorbance band, manual peak picking is necessary.

For instance, automatic peak picking will do a poor job on this spectrum:

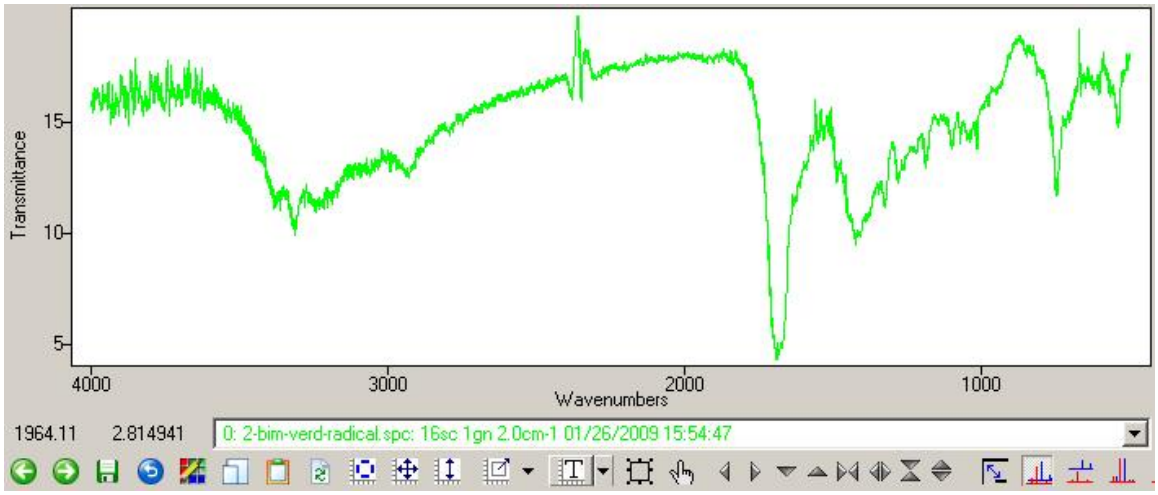


Figure 8-61

With manual peak picking, one can zoom and expand in and out of the regions of interest and manually label peaks and remove the peak labels.

To pick a peak manually, hold the mouse over or near the peak to be labeled, and click the right mouse button. The peak label will be added to the display, as in this figure:

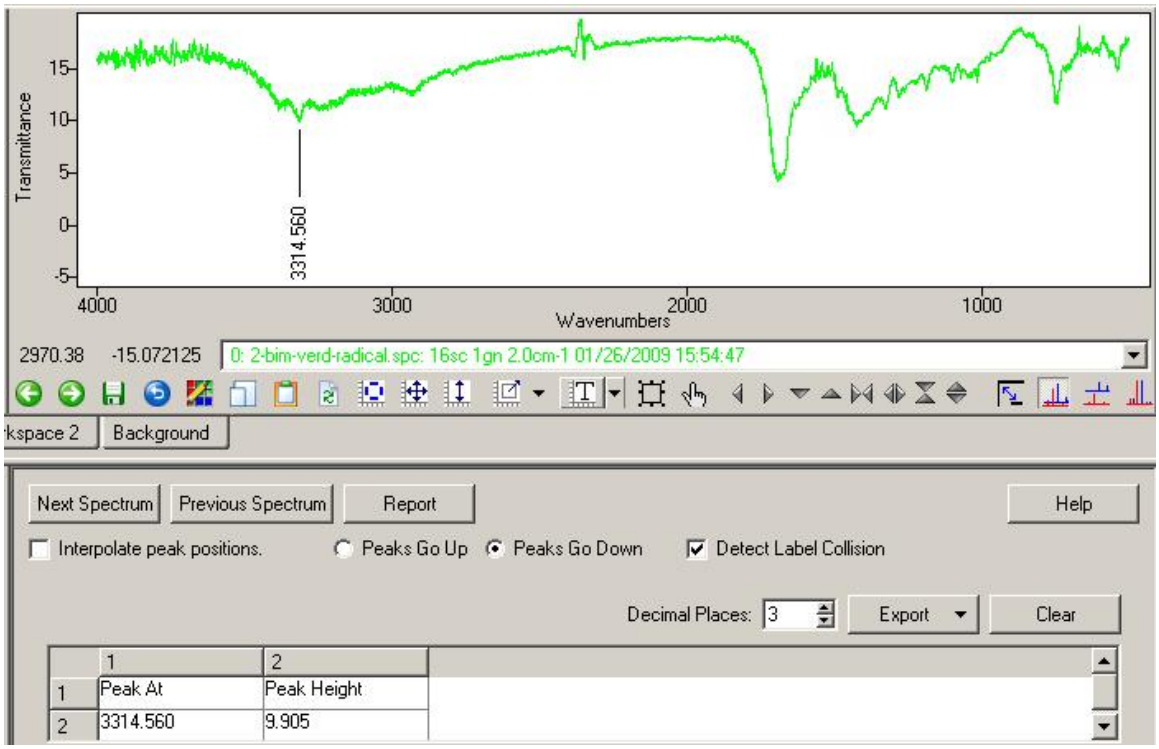


Figure 8-62 Manual Peak Picking

The peak is also added to the peak table at the bottom of the tool.

Peak labels can be removed from the display and the peak table by holding the mouse over the peak label in the data display and right clicking. When the mouse is over a peak label the cursor will change as shown in this figure:

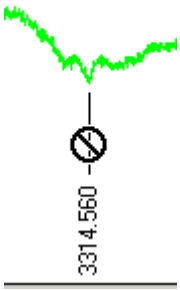


Figure 8-63 Removing a peak label

And right clicking will remove that peak label.

Using the manual peak picking tool allows you do things that are not possible with automatic peak picking, as in the next figure.

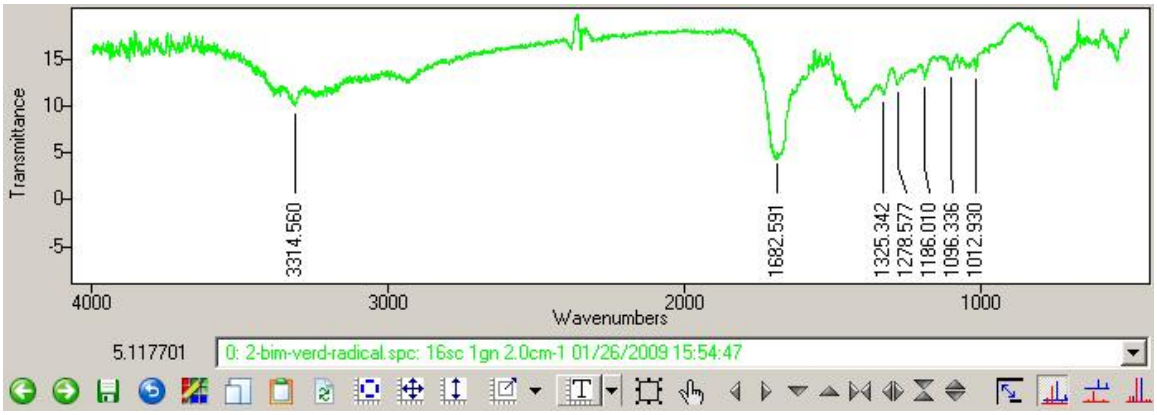


Figure 8-64 This is not possible with automatic peak picking.

The 'Interpolate Peak Postions', 'Peaks go up', 'Peaks go down', and 'Detect Label collision' buttons work as described in the section on automatic Peak Picking, above.

Measure Peaks

It is sometimes useful to manually assign a defined peak position to an absorbance feature, and to be able to measure the width of a peak. This task may be accomplished using the ***Measure Peaks Tool***. The left and right extremes of the peak are defined by you. You must also set the center of the absorbance feature to be measured. Figure 8-65 shows the ***Measure Peaks*** parameters window.

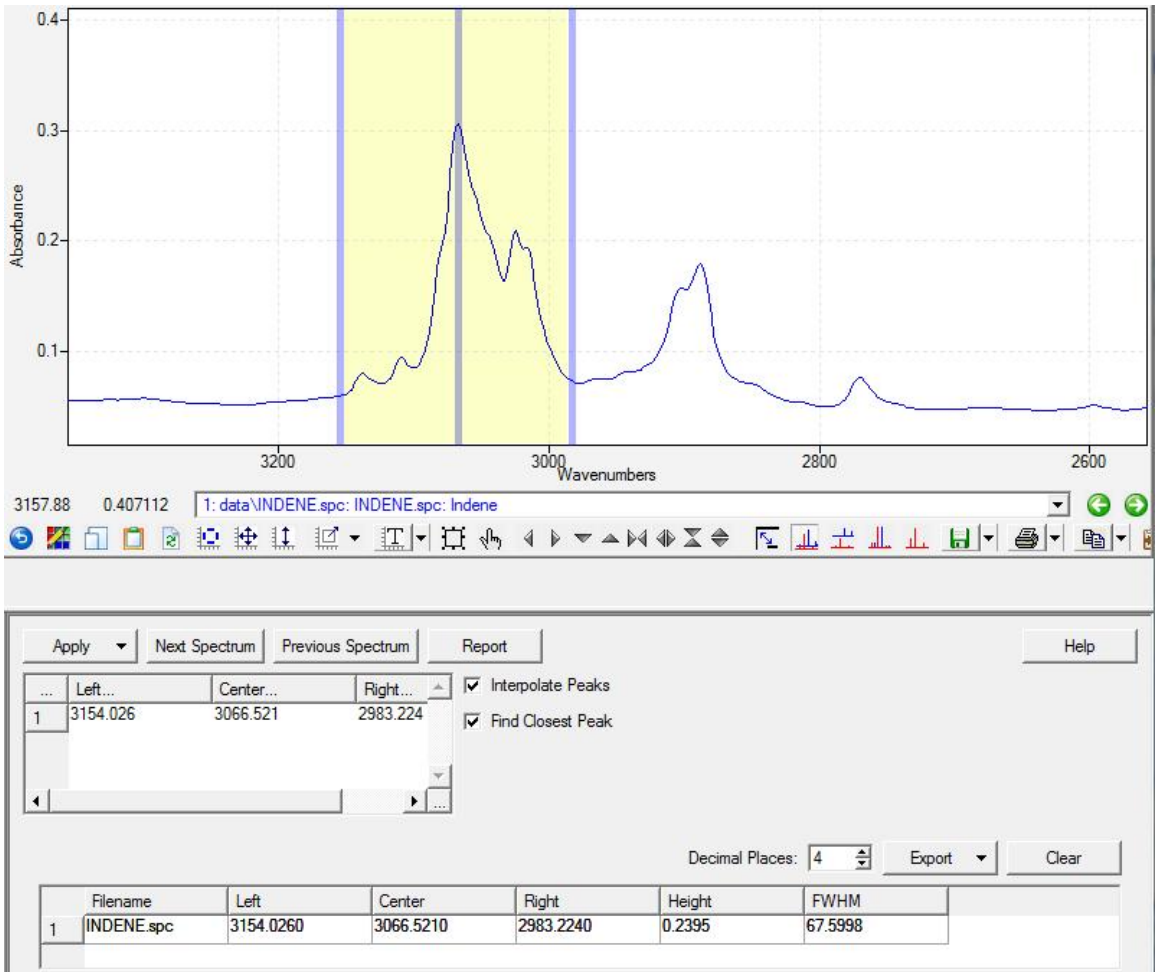


Figure 8-65 Measure Peaks *parameters*

Three ***Toolbox Buttons*** are present. Immediately below these buttons is a ***Regions Window***, displaying the left, right and center of the peak as specified by the user defined **Regions**. Clicking the ***Apply*** button results in the peak data being displayed in the results table at the bottom of the page. The results data include the filename, the ***Regions*** used, peak height, and FWHM, which is the Full Width at Half Maximum. The degree of precision may be set using the ***Decimal Places*** edit box. The data may be placed on the clipboard using the ***Export*** button, or erased using the ***Clear*** button.

The peak height is measured to a baseline drawn between the left and right points. The FWHM is the width of the peak at half of this height.

Two options are available that affect the calculation.

If 'Interpolate Peaks' is checked, the peak data is interpolated to a 10 times higher resolution before calculating the peak height and width.

If 'Find Peak' is checked, the center peak position is taken as the nominal position of the peak, and the actual peak position is found as the closest peak to the nominal position. This is important because the peak may shift over a series of files. This has the advantage of accounting for any small variations of the position of the peak maximum which may be missed by measuring only the peak height at a single value.

Data Point Picker

Essential FTIR's peak picking is easy and accurate, but is sometimes not the right tool. If you are interested in just knowing the Absorbance value at a certain point in the spectrum where there may not be a peak, or to find the the value of a peak shoulder, the Data Point Picker is a useful tool.

Consider this spectrum, and assume you need to know the position of the shoulder on the larger peak. The gray spectrum is the overlaid, inverted, 2nd derivative of the spectrum, which can be a visual aid in picking out the exact position of such small spectral features.

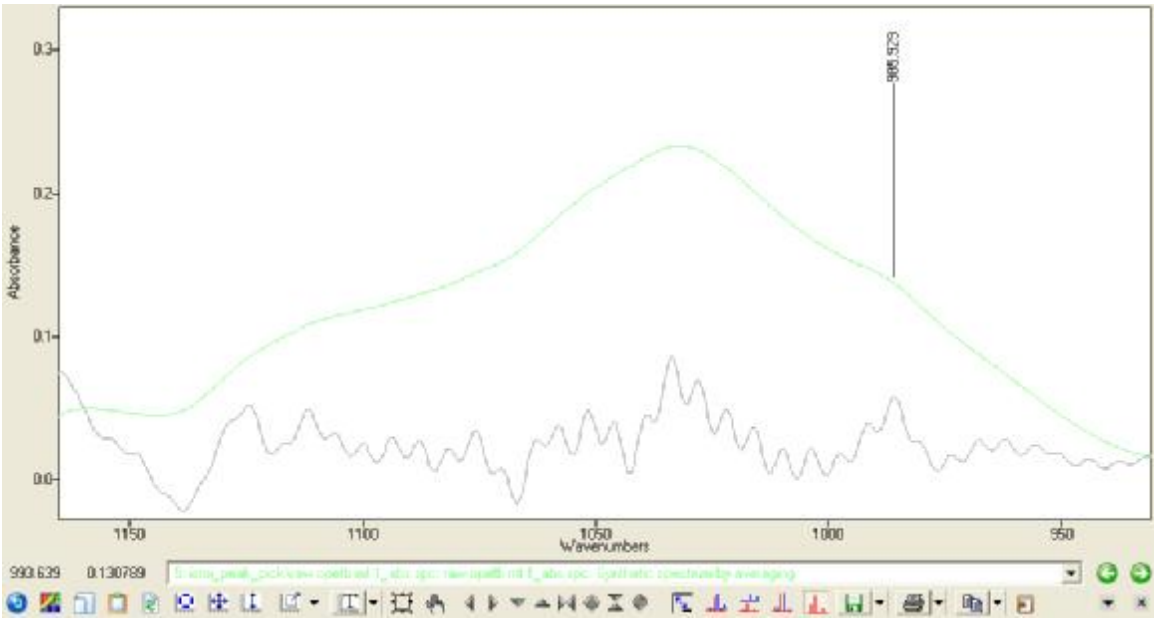


Figure 8-66 Point Picking

The buttons on this tool are very similar to the Peak Picking tool, with the addition of the 'Overlay inverted 2nd derivative' check box.

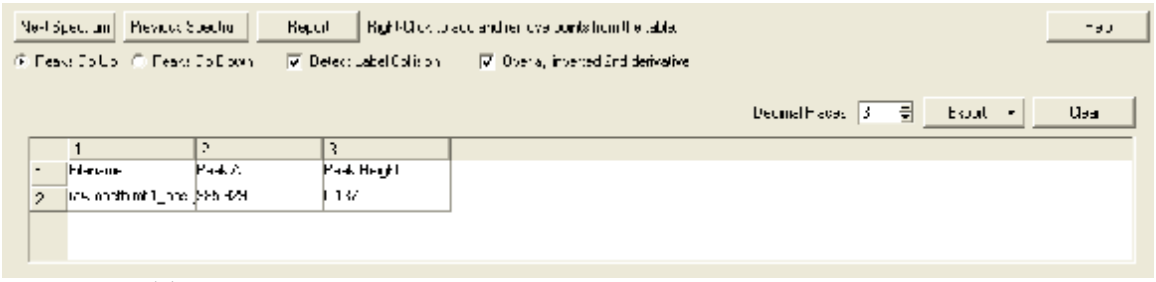


Figure 8-67 The results of Data Point Picking.

Signal to Noise Calculator

This tool calculates Root noise in a noise band area. Typically this is used to verify instrument performance using a standard sample.

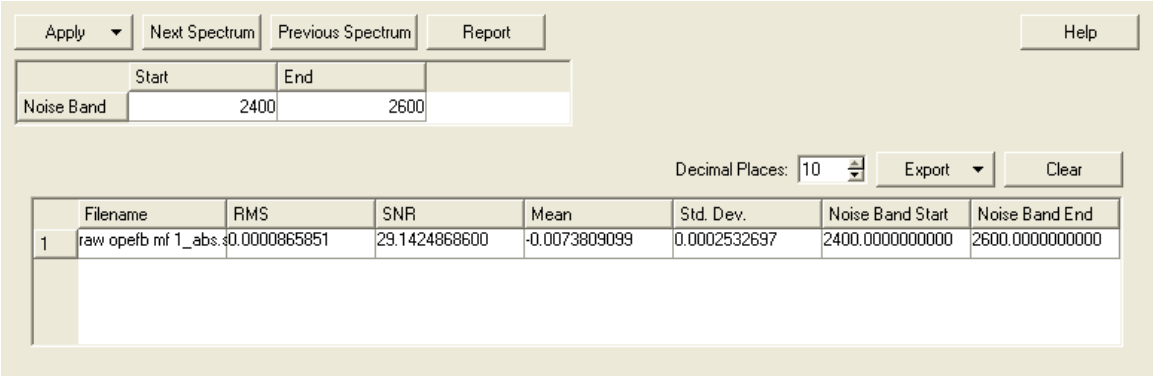


Figure 8-68 The signal-to-noise calculator

- RMS: Root Mean Square of the data values in the noise band.
- SNR: The mean value in the data in the noise band divided by the standard deviation of the data in the noise band.
- Mean: The mean value of the data in the noise band.
- Std Dev: The standard deviation of the data in the noise band.

The Quant & Identification Toolbox

Spectral Library Search

The infrared spectrum of a pure substance is unique, and can be thought of as a molecular fingerprint. The spectrum can be compared against known spectra of compounds to identify unknown substances. The ***Spectral Library Search*** tool in Essential FTIR automates the process of comparing a sample spectrum against collections of known spectra. For each spectrum in the library, a number known as the 'metric' or 'score' or 'hit quality index' (HQI) is produced. This number is a measure of how well the library spectrum matches the sample. The results are ordered (sorted) by the HQI and presented in a list, known as the 'hit list'.

Interpreting Library Search Results

A library search will always produce a result and a top hit. That does not mean that the top hit identifies the sample. For one, a spectrum of the sample may not even be in the search libraries. Also, noise and artifacts can make dissimilar spectra the top hit, and likewise give similar spectra a poor HQI.

Library Search attempts to do what a human analyst does visually by reducing the comparison to a single number, but should not be a substitute for careful visual comparison of the sample with the proposed matches in the hit list. Library search is useful to very quickly narrow down the possible identification of a sample, but should not be relied on to produce definitive results. ***Always compare the spectra visually, don't rely on the HQI alone.*** The shapes and relative heights of peaks may be slightly different, but missing or extra peaks in either spectrum require further analysis.

User Libraries

Users may build their own libraries of spectra for searching. In ***Essential FTIR***, a user library is nothing but a disk directory containing individual data files. Users may add and remove spectra from 'libraries' simply by using Windows file explorer to move files in and out of these directories. The files can be in any format that ***Essential FTIR*** supports.

Search is faster if all the spectra in the library have the same resolution and spectral data limits. You can use the 'Match Spectra' tool to make the data have the same resolution and spectral limits. Spectra in libraries can be in Absorbance or Transmittance, but spectra are always automatically converted to Absorbance before the spectra are compared.

Commercial Libraries

Commercial libraries of infrared spectra are available from many vendors, offering hundreds of thousands of high-quality spectra for different applications. A list of library vendors is on the Essential FTIR website at http://www.essentialFTIR.com/libraries.html.

The Spectral Library Search tool

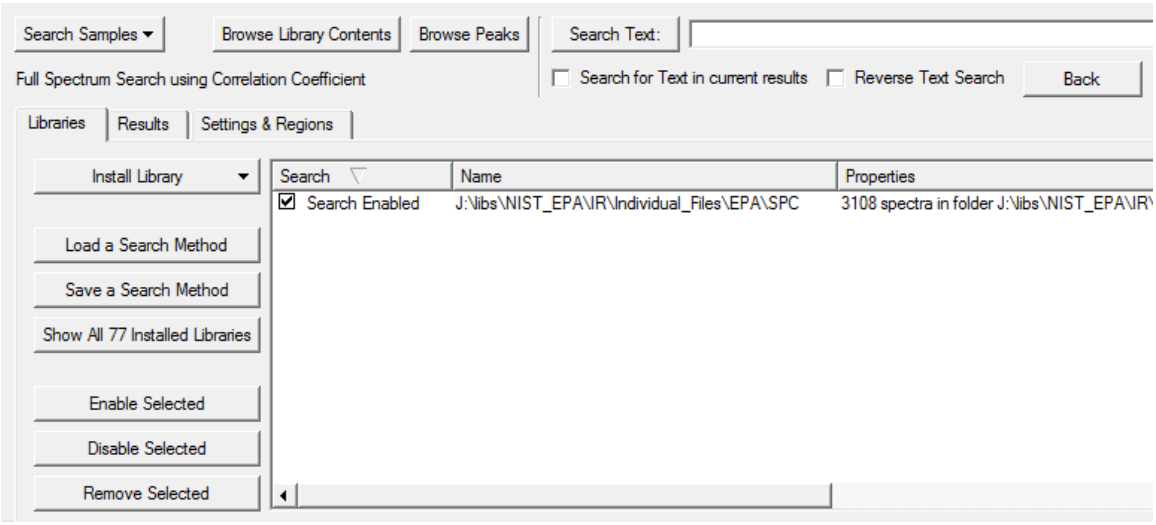


Figure 8-69 The spectral Library Search tool showing the 'Libraries' tab active

The tool consists of a row of buttons that perform search actions, as shown below. Below the buttons are three tabs that allow selecting which libraries to use, how the search will be performed, and the search results. Each of these action buttons will be discussed.

Search Samples ▾	Perform a library search. The drop-down menu allows multiple samples to be searched at the same time.
Browse Library Contents	A list of all the spectra in the selected libraries will be displayed in the 'Results' tab.
Browse Peaks	Absorbances in the library spectra can be searched using integrated areas of peaks.
Search Text:	Search the library for given text.

Figure 8-70 The action buttons on the Library Search Tool.

Search Samples

Clicking this button will initiate a search of one or more samples against the selected libraries. This button has a drop-down menu with these choices:

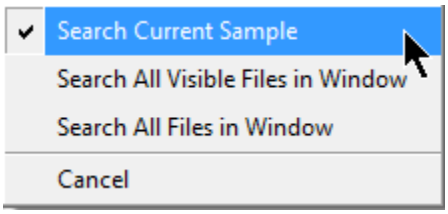


Figure 8-71 The sample search choices

The ability to 'batch search', to search more than one sample with a single click, is a powerful time-saving feature.

The results of the library search are discussed below, in the section about the ***Results Tab***.

Browse Library Contents

Clicking this button will fill the Results list with the names of all the spectra in the selected libraries. The spectra are listed in the order they are within the library.

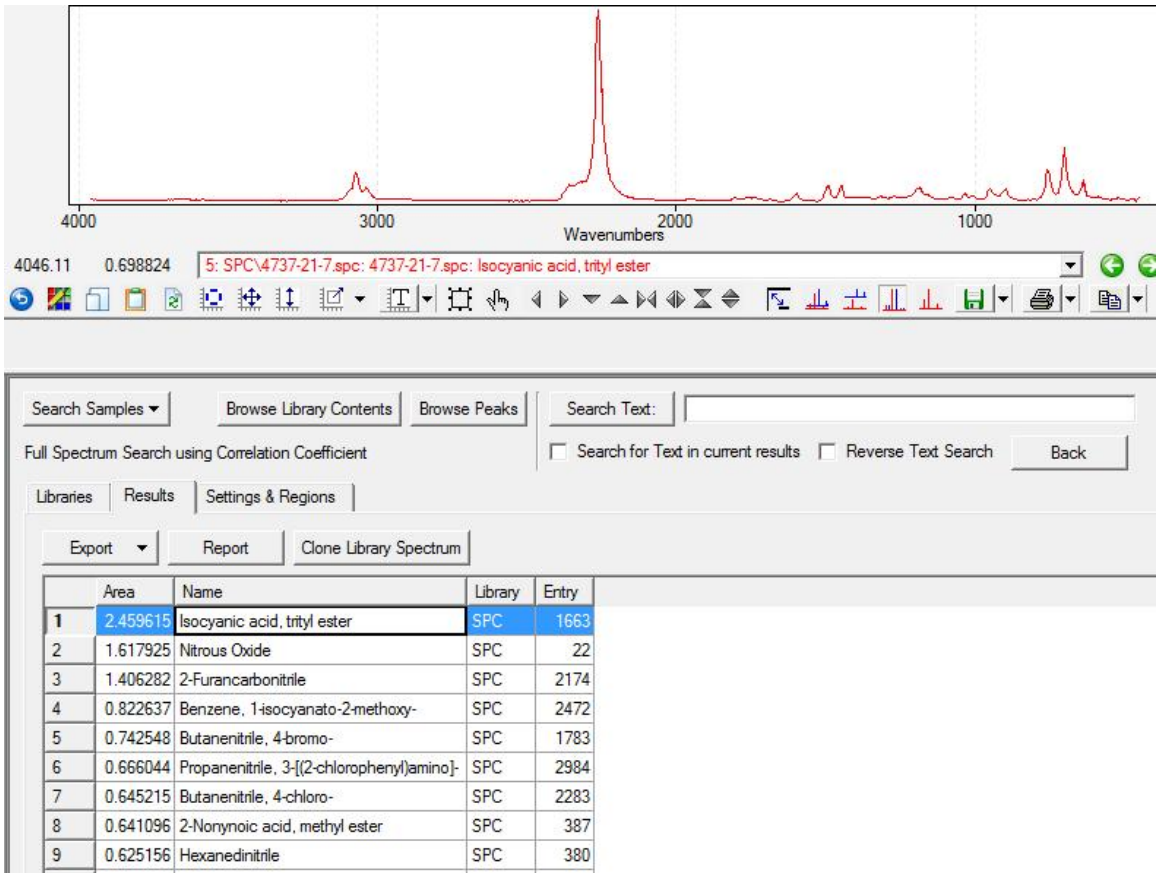
		Library	Name	Entry
1	⊟	SPC	Benzene, 1-chloro-4-nitro-	0: 100-00-5.spc
2			Benzene, 1-methoxy-4-nitro-	1: 100-17-4.spc
3			Acetophenone, 4'-nitro-	2: 100-19-6.spc
4			Benzeneethanol, 4-nitro-	3: 100-27-6.spc
5			Benzene, 1-ethoxy-4-nitro-	4: 100-29-8.spc
6			1,2-Ethanediamine, N,N-diethyl-	5: 100-36-7.spc
7			Ethanol, 2-(diethylamino)-	6: 100-37-8.spc
8			Cyclohexene, 4-ethenyl-	7: 100-40-3.spc
9			Benzyl chloride	8: 100-44-7.spc
10			3-Cyclohexene-1-carboxaldehyde	9: 100-50-5.spc
11			Benzaldehyde	10: 100-52-7.spc

Figure 8-72 The contents of the library. Clicking on an entry in the list will display the spectrum.

Browse Peaks

Browse Peaks allows you to search for absorbance peaks in a library, independent of any sample. To use it, define one or more regions (see Creating and Working with Spectral Regions) using the right mouse button. The summed integrated areas of the defined regions will be calculated for all the spectra in the selected libraries, and displayed in descending order in the results list.

For example, assume that you want to find all nitrile compounds in a library. Define a spectral region from 2265 to 2234 wavenumbers, and click "Browse Peaks". Here's the results:



	Area	Name	Library	Entry
1	2.459615	Isocyanic acid, trityl ester	SPC	1663
2	1.617925	Nitrous Oxide	SPC	22
3	1.406282	2-Furancarbonitrile	SPC	2174
4	0.822637	Benzene, 1-isocyanato-2-methoxy-	SPC	2472
5	0.742548	Butanenitrile, 4-bromo-	SPC	1783
6	0.666044	Propanenitrile, 3-[(2-chlorophenyl)amino]-	SPC	2984
7	0.645215	Butanenitrile, 4-chloro-	SPC	2283
8	0.641096	2-Nonynoic acid, methyl ester	SPC	387
9	0.625156	Hexanedinitrile	SPC	380

Figure 8-73 The results of 'Browse Peaks'

The hit list now shows the library contents sorted by integrated area in the nitrile region.

Search Text

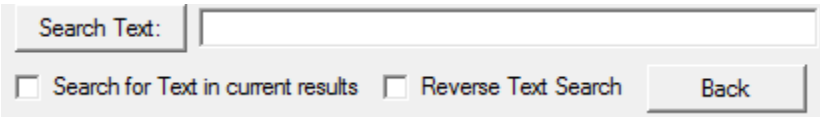


Figure 8-74 Text Search

Enter text into the edit field to the right of the "SearchText" button and then click the button or press the 'Enter' key. The library will be searched for all text that matches what you have entered. The search is not case-sensitive.

The "Search for Text in current results" check box allows you to narrow a search down with sequential searches. The "Reverse Text Search" searches for all text that does not match the text you entered.

When narrowing a text search down using sequential searches, you may hit a dead-end, and need to back up. The "Back" button resets the results in the hit list to the results of the last spectral, peak, or browse results so you can start over.

The Libraries tab

The Libraries tab has seven buttons and a list of libraries.

Install Library ▾	Displays a menu of choices, see below.
Load a Search Method	Load a saved search method.
Save a Search Method	Save the current list of libraries and search settings
Show All 77 Installed Libraries	Show a list of all the currently installed libraries
Enable Selected	Enable search for the libraries that are selected in the list of libraries.
Disable Selected	Disable search for the libraries that are selected in the list of libraries.
Remove Selected	Remove the selected libraries from the list. This does not remove the libraries from the computer, only from the list of displayed libraries.

Figure 8-75

Install Library

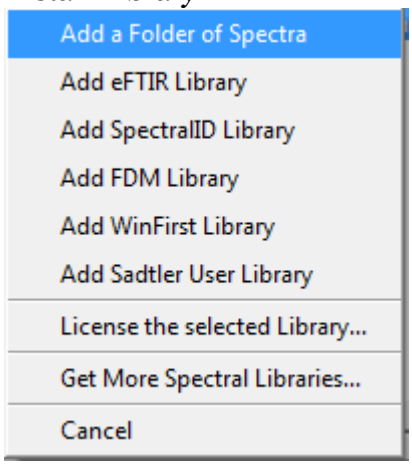


Figure 8-76The 'Install Library' menu.

Add a Folder of Spectra: a 'choose directory' dialog will be displayed. The directory (folder) of spectra will be added to the list of libraries. Please see the 'Folder of Spectra' section below for notes about creating and maintaining such libraries.

Add eFTIR library: An eFTIR library has the file extension .eftir_lib. This format contains spectra and information about those spectra into a single file. Some library vendors distribute data in this format. If you have an interest in supporting this format, please contact Essential FTIR.

Add Spectral ID Library: Spectral ID libraries are the format used by the GRAMS software. All commercial library vendors support this format.

Add FDM Library: These are libraries distributed by Fiveash Data Mangement.

Add WinFirst library: these are libraries that were distributed by Mattson Instruments. Add Sadtler User Library: Sadtler is a distributer of commercial libraries. Their software allowed users to create libraries using the user's own data.

License the Selected Library: Use this to install a license for an eFTIR library or a FDM library.

Get More Spectral Libraries: this will launch a web browser and navigate to the Libraries page on the EssentialFTIR.com website.

The Results Tab

In this example, a spectrum of Indene is searched against a folder of spectra. The folder of spectra contains the individual spectral data files that comprise the EPA vapor phase library. The results of the search are displayed in a sorted list, known as the 'hit list', with the best match, or 'hit', at the top. The spectrum of the top hit is displayed automatically after the search is complete..

Libraries | Results | Settings & Regions

Export | Report | Clone Library Spectrum

	Sample	Metric	Name	Library	Entry
1	indene.spc	0.985733	Indene	SPC	2992: 95-13-6.spc
2		0.827723	Benzo[b]thiophene	SPC	2993: 95-15-8.spc
3		0.758490	Benzonitrile, 2-methyl-	SPC	1770: 529-19-1.spc
4		0.752572	1,2-Diphenylethylamine	SPC	1227: 25611-78-3.spc
5		0.741952	Azulene	SPC	1266: 275-51-4.spc
6		0.739270	Isothiazole, 4-phenyl-	SPC	2965: 936-46-9.spc
7		0.736037	o-Terphenyl	SPC	2797: 84-15-1.spc
8		0.730445	1,1'-Biphenyl, 3-methyl-	SPC	2353: 643-93-6.spc
9		0.717683	Naphthalene, 1-(chloromethyl)-	SPC	2814: 86-52-2.spc
10		0.711833	1,1'-Biphenyl, 4-methyl-	SPC	2355: 644-08-6.spc

Figure 8-77 The search results. Clicking on an entry in the list will display its spectrum.

The Metric is a measure of how well the library spectrum matches the sample. In this case, the Correlation Coefficient algorithm was used (search algorithms are discussed below). The Correlation Coefficient offers a value that has statistical significance. A value of 1.0 would indicate a perfect match. The 0.98 value for the best hit is a good match.

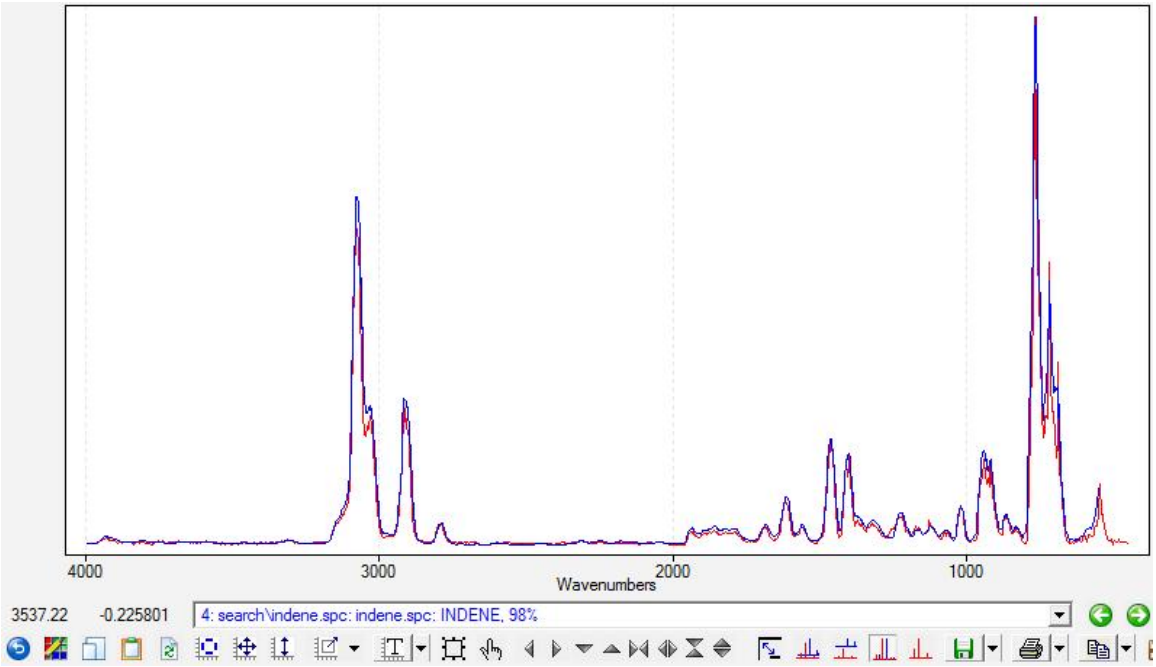


Figure 8-78 The Indene sample spectrum is in blue, the library spectrum in red

It is always necessary to visually compare the best hit to the sample spectrum, so, after a search, the best hit is automatically overlaid on the sample spectrum. Please see the section 'Interpreting Library Search Results' earlier in this chapter. In this example, the best hit is a good visual match to the sample spectrum, because there are no missing or extra peaks in either the sample or library spectrum.

Above the hit list are three buttons:

Export	Export the hit list to the clipboard, a text file, or to Excel.
Report	Generate a report based on the spectral display and the information in the hit list.
Clone Library Spectrum	Make a copy of the currently displayed library spectrum. To avoid confusion and congestion, one library spectrum a time is displayed. 'Cloning' the library spectrum makes a copy of it so that it persists in the spectral display window.

Settings and Regions

The Search Options

Search Algorithm	Choose how the search is performed. See below for details.
Derivative Search	Perform the search on the first derivative of the data. See below.
Region Search	Restrict the search to selected regions of the spectra.
Number of hits	How many hits to display in the hit list

The Report Options

Report Hits	How many hits to report in the printed report.
Report Scores	Do or do not include the search metric in the reports.

Search Algorithm

Different algorithms are available for the library search. The algorithm is the method that is used to do a point-by-point comparison of a sample spectrum with a library spectrum. The result of this comparison is always a single number, referred to as the 'metric' or 'search metric'.

Any of the algorithms offered will perform a satisfactory search. However, special situations exist where one algorithm may be favored over another. The options available for selection from the drop down menu are:

Correlation Coefficient: This is the most widely used search algorithm because it gives the best results. The equation is:

$$HQI = \frac{\left(x - \bar{x}\right)\left(y - \bar{y}\right)}{\sqrt{\sum\left(\left(x - \bar{x}\right)^2 \sum\left(y - \bar{y}\right)^2\right)}}$$

Where *x* and *y* are the data points on the sample and library spectra, and *x-bar* and *y-bar* are the means of the data. It is the covariance of the spectra divided by the product of their standard deviations. A higher number indicates a better match.

The other search algorithms yield relative scores, but Correlation Coefficient yields an absolute result with statistical meaning. 1.0 means a perfect correlation and -1.0 is a perfect anti-correlation. Generally, a result of 0.98 or better is a good match, but a visual confirmation is always necessary.

The Correlation Coefficient is not affected by baseline slope and offset. All other algorithms here are affected by baseline artifacts. The Correlation Coefficient is similar to Euclidean Distance, except that spectra are mean-centered before multiplying them.

This mean-centering will correct for negative dips in the spectrum, and other baseline artifacts.

Euclidean Distance – This algorithm is similar to the Correlation Coefficient. A smaller number indicates a better match. This algorithm is not as sensitive to differences in spectra, so it is useful when the sample is a mixture. The equation for ***Euclidean Distance*** is:

$$HQI = \sqrt{2} \times \sqrt{1 - \frac{(X \times Y)}{\sqrt{X \times X} \times \sqrt{Y \times Y}}}$$

Where X is the library spectrum and Y is the sample spectrum.

Absolute Difference – The simplest of the algorithms. This method emphasizes peak heights and does not enhance spectral differences as much as the others. The equation for ***Absolute Distance*** is:

$$HQI = \frac{\sum_{i=1}^{n} |x_i - y_i|}{n}$$

Where x and *y* are corresponding points on the sample and library spectra. A smaller number indicates a better match.

Squared Difference (also known as Least Squares)

The equation for is:

$$HQI = \frac{\sum_{i=1}^{n} (x_i - y_i)^2}{n}$$

HQI is the sum of the squares of the residuals, *y* is the library data and *x* is the sample data. A smaller number indicates a better match.

First Derivative Search

When this option is checked, the first derivatives of the sample and library spectra are compared. The first derivative of a spectrum removes baseline artifacts, so it is very useful when baseline slope and offset are present or there are slowly varying, broad background features. This is useful when searching Raman or Near Infrared spectra.

Region Searching

Region Search permits searching of library spectra over a defined region or regions (multiple regions can be used). The region is set by right-clicking on the sample spectrum in the *Workspace* to set the two extremes of the region to be used in the search. The region is then displayed in the *Region Table* at the right of the window. Please refer to the section Creating and Working with Spectral Regions for a detailed discussion of *Regions*.

Region searching is useful when the sample spectrum is a mixture. It can limit the search to spectral regions that are the result of one component of a mixture.

If your sample spectrum has totally absorbing bands, better results will be obtained if those bands are excluded from the search.

Folders of Spectra used as Search Libraries

By definition, a Search Library contains edited and curated spectra, meaning that the user acts as the editor / collector to ensure quality, integrity and internal consistency. All the spectra in a Search Library should share these properties:

- X-axis data type (for instance, wavenumbers)
- Y-axis data type (for instance, absorbance)
- Starting and Ending X values (the endpoints of the spectra)
- The data point spacing (digital resolution, also known as 'delta X')

Spectra that share these values are said to be 'compatible'. Essential FTIR will automatically match the spectra endpoints and data point spacing for the search, so these two properties are not critical. Problems can arise when the X and Y data types of the sample and the library spectra do not match, or if the library folder contains spectra of different types.

Essential FTIR has tools to make the spectra in a folder compatible. The 'Batch Processor' tool in the 'Advanced' category, and the 'Match Spectra' tool in the 'Manipulations' category are especially useful for ensuring compatibility.

Sometimes the units in a spectral datafile are mis-assigned. For instance, the spectra are in absorbance, but the datafile header may say that the data has 'arbitrary' units. This situation can be handled by using the 'Change Header Fields' operation in the Batch Processor.

Note that the majority of commercial FTIR libraries are in units of wavenumbers vs. absorbance. Better search results are obtained with absorbance units vs. transmittance. However, Essential FTIR does not force or assume the use of any particular units for a folder of spectra.

If the sample and library spectrum are of different Y-axis types, such as the sample being in Transmittance and the library being in Absorbance, Essential FTIR will automatically perform the conversion for the purpose of the search. When library spectra are later retrieved for visual comparison with the sample spectrum, they will be converted to match the sample data type.

For mismatched X-axis types, Essential FTIR is less forgiving. The sample's X units must match the library spectra X units or an error will be recorded. Search errors are placed at the top of the hit list so they can be noted and corrected.

FDM Library Search

Fiveash Data Management (FDM, ***www.fdmspectra.com***) makes libraries of spectral reference data available to users of Essential FTIR. FDM Library Search is documented in a separate manual. Clicking the 'Help' button in the FDM Search Tool will display the FDM documentation.

QC Compare

A common feature of QA/QC procedures is the comparison of materials, whether raw or finished product or any intermediate stage. The ***QC Compare Tool*** compares a sample spectrum against reference spectra. The reference spectra can reside in a directory on disk, a spectral library, or as data loaded into a window. For example, a user could save a set of spectra representing a day of manufacturing to a directory, the contents of which are then compared against the reference standard.

The QC Compare tool has several tabs which contain the settings which comprise a 'method'. A 'method' is the collection of data and parameters to be used for a comparison.

Figure 8-79 shows the ***QC Compare*** Methods tab:

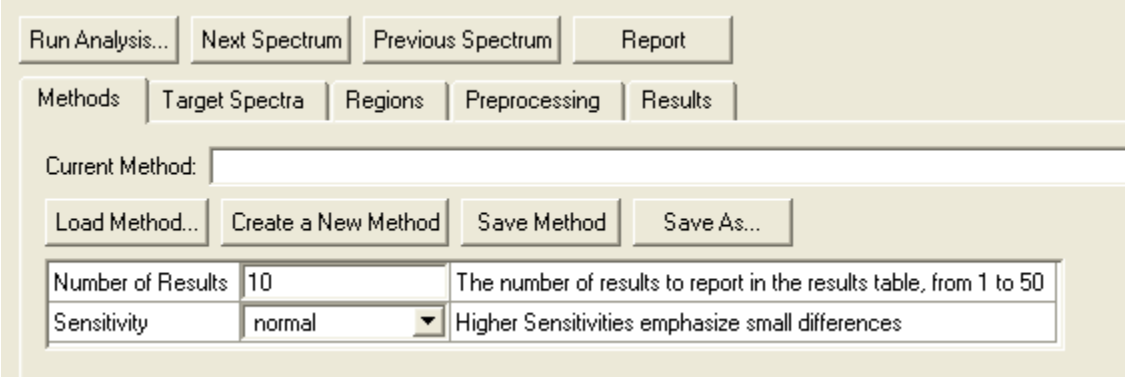


Figure 8-79 QC Compare *methods tab*

The Buttons:

- Load Method: brings up a file open dialog box to load a method that has been saved earlier.
- Create New Method: start a new, clean, method.
- Save Method: save the existing method to disk.
- Save As: save the existing method under a new filename.

The Parameters:

- Number of Results: display only the top N results, regardless of how many spectra are compared. In this case, the 10 best results will be reported.
- Sensitivity: The Comparison is done using a correlation coefficient calculation, but the correlation can be made more sensitive, to pick out small differences in the spectra. The choices are: Normal, High, and Super.

The Target Spectra Tab:

Figure 8-80

Reference spectra are included and removed from the method using the controls on this tab. Clicking on the 'Add Targets' button reveals a drop-down menu:

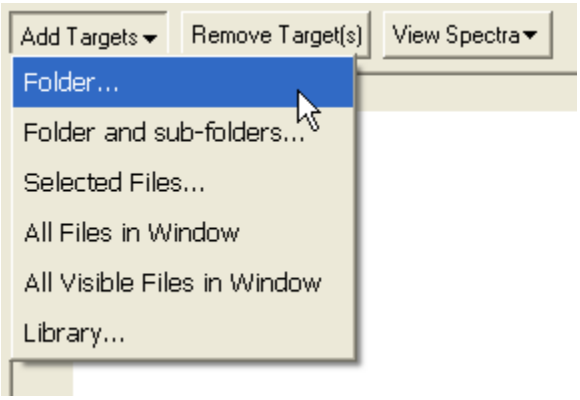


Figure 8-81

The 'Target' sources are comprehensive, and include being able to use library spectra for the comparison. Multiple sources of target spectra can be added. Commercial spectral libraries can also be used in the analysis.

The Regions Tab:

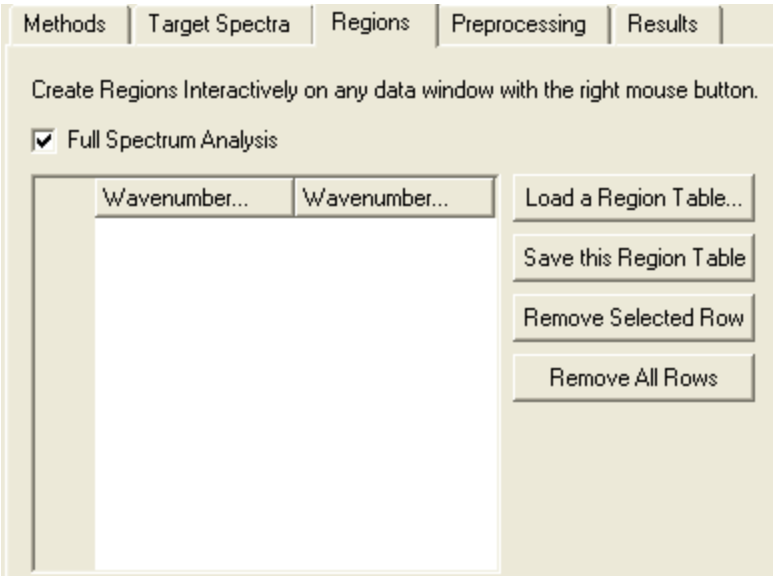


Figure 8-82

The comparison can be restricted to user-specified regions. This can make the comparison more accurate by excluding, for instance, Carbon Dioxide or Water from the analysis.

The Preprocessing Tab

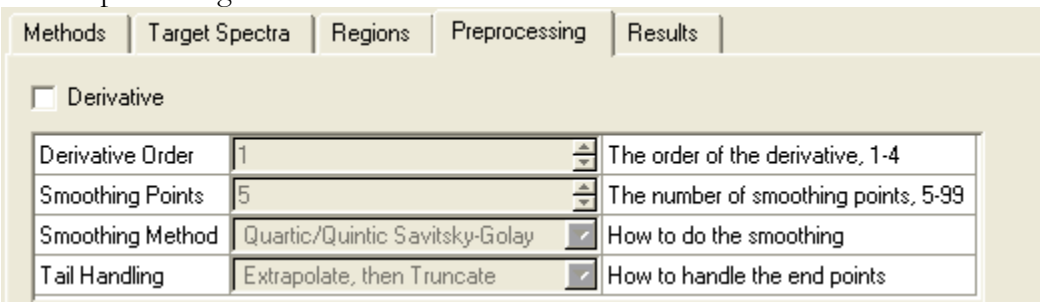


Figure 8-83 QC Compare Preprocessing options

The data can be optionally be preprocessed before the comparison using the first or second derivative. This can improve results, and is indeed necessary for most Near Infrared spectra.

Upon clicking the ***Analyze*** button, ***Essential FTIR*** begins to compare the data against the active spectrum in the ***Workspace***. The results of the comparison are ranked in order of their correlation coefficient, as listed in the ***Results Window***. The results are displayed along with the associated filename, directory and memo field. This results table may be placed on the clipboard, saved to a file, or exported to Excel using the ***Export*** button.

Beers Law Quant

This chapter will explain how to use the Beer's Law Quant tool in Essential FTIR. It serves as both user documentation and a tutorial. In this tutorial we will build a method from scratch. A sample method named 'glycine_in_water.eftir_quant' is installed with Essential FTIR. The spectral data included in this method will be used.

Background

Beer's law (also known as the Beer-Lambert law) states that as the concentration of a substance increases, it will absorb more light. The equation is expressed:

$A = abC$	Absorbance is linearly proportional to the concentration
where:	
A	Absorbance
a	The absorptivity constant, a measure of how strongly a substance absorbs at a specified wavelength
b	The pathlength or thickness of the sample
C	The concentration of the substance

For a fixed pathlength, the equation reduces to $A = kC$, where k is a constant.
The absorbance 'A' in the equation is also called the measured response, or just response. In practice it is either the absorbance at a fixed wavelength, the maximum absorbance within a specified region, or the integrated area of a specified region. For this reason, Beer's Law Quant is called a univariate quantitative analysis, because a single number is extracted from the data and used in quantitation.
A rule of thumb in spectroscopy is that the linear relationship expressed in Beers' law is usually obeyed by samples with absorbances less than .8.
Beer's Law assumes that the absorbance at a frequency results from only one substance. If there are interfering substances with overlapping absorbances, there will be errors in the calibration and subsequent prediction. In the case of interferences, CLS or PLS must be used.
In the this discussion, the terms wavelength, wavenumber, and frequency are used interchangeably for the X units of the spectra. The terms 'spectral region' and 'band' are synonymous. The 'measured response' is the number that is extracted from a band for use in the quantitation.

Developing a Method

A Quant Method is a *model* that describes the behavior of the substances of interest. A method can model a mixture of substances, as long as those substances don't interfere, meaning that they each have a unique spectral region where the absorbance is due to only one substance.

A method is developed by preparing a set of standards. The concentrations of the standards should span the expected range of concentrations that will be encountered when analyzing unknown samples.
A quantitative analysis method can be divided into three parts: selection of analytical wavelengths, calibration using standards, and measurement of samples of unknown concentrations.

Selection of Wavelengths

A spectral region, also called the analytical band, or just band, has to be selected for each substance in the method. The measured response within that band may be either the absorbance at a fixed wavelength, the absorbance maximum found within that region (that is, the peak), or the integrated area of the region.
When using single absorbances at a fixed wavelength, only one data point is used. There is more possible error, due to instrument drift or interferents, when using a single point. A single point measurement is often used when the absorbance of interest is a shoulder sitting on an interfering band. Using the absorbance peak within a region is more robust and can be used when there are non-overlapped bands which shift with changing concentration. Many points are used in calculating integrated areas, so the calibration model should be more robust because it is less susceptible to an error in measuring a spectrum at a single point.
The best analytical wavelengths for an analyte correspond to absorbance peaks which don't overlap the peaks found in spectra of other substances found in the mixture. Essential FTIR leaves the selection of analytical regions to the spectroscopist because this situation does not always occur, and the correct choice of band is critical to making good quantitative predictions.
Usually a baseline correction is applied to the analytical band. The baseline correction can be 'None', 'Offset', or 'Linear', and the 'Linear' baseline correction is most commonly used. The baseline region can be different from the analytical band, and usually is wider than the analytical band.
In addition, it may be necessary to define a reference band. The reference band is used in situations where the pathlength is unknown or varying, such as with polymer films. The ratio of the analytical band measurement and the reference band measurement will correct for deviations in the pathlength. A baseline correction region for the reference band may also be used.
Region selection is critical to developing a model that fits the data.

Calibration using the standards

The standards are used to generate the calibration by fitting a curve to the Absorbance and Concentration data for the standards. The calibration coefficients are then stored with the method and are used to calculate the concentration of unknown samples.
Standards can be single substances or a mixture of substances, but the concentrations of the components in the standard must be known.

During the calibration step, the method must be validated by evaluating how good the fit to the standards is. This is done both visually, by looking at plots of the calibration curve, and by statistics generated by the curve fitting mathematics.
During the validation step, outliers can be spotted and removed from the method. An outlier can result from an error in the spectrum and/or an error in concentration.
During the validation step, it will become apparent if a linear, quadratic, or cubic curve fit should be used. It's up to the method developer to determine the equation that describes the data. In the real world, there can be deviations from ideal adherence to Beer's law. These cases can sometimes be handled by using second and third order polynomials fits, providing there are enough standards. The minimum number of standards needed depends on the order of the equation, the curve fit, which is used. For a linear first-order equation $y = ax + b$, a minimum of two standards, or one standard and the origin, are needed. For a second order quadratic fit, $y = ax^2 + bx + c$, at least three standards (or two and the origin) are needed. For a third order cubic fit, four standards (or three and the origin) are necessary. (In Essential FTIR, the method developer can choose force the curve to pass through the origin. This serves as a virtual standard saying that there is zero absorbance when the concentration of a substance is zero).

Measurement of Samples of Unknown Concentrations

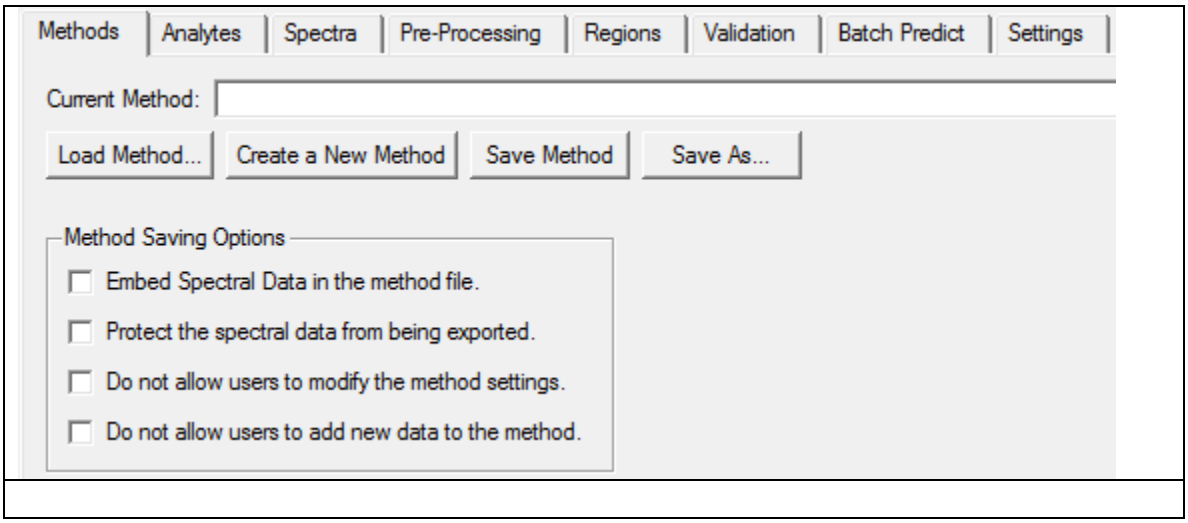
Once a robust calibration has been developed, it can be applied to samples of unknown concentration. The absorbance spectrum of the sample is collected, and the quant method extracts the measured response from the spectrum, and uses the calibration coefficients to calculate the predicted concentration of the substances in the method.

Tutorial

Start eFTIR and navigate to the 'Beer's Law Quant' tool, which is in the 'Quant & Identification' toolkit. At the top of the tool is a row of tabs:

These tabs organize the information and activities that will be used to develop and use a quant method.

The Methods tab



The Methods tab buttons

Load Method...	Load a previously saved method. Method files have the extension '.eftir_qaunt'
Create a New Method	Clear any previously loaded method from memory, creating an empty method.
Save Method	Save the current method.
Save As...	Save the current method under a different filename.

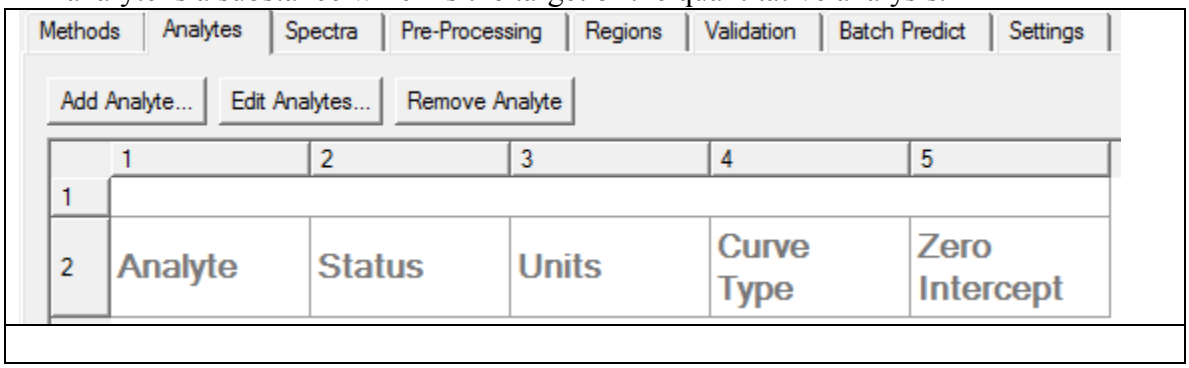
Method Saving Options

The spectral data used in the method can be stored in the method file itself, or left on disk as external datafiles. If the data are embedded in the method file, they can also be protected from export. These options effectively confer ownership rights of the data to the developer of the method.

☐ Embed Spectral Data in the method file.	The spectra will be included in the method file.
☐ Protect the spectral data from being exported.	The spectra cannot be exported from eFTIR
☐ Do not allow users to modify the method settings.	The method user cannot modify the method. All the method are locked except for the option to add new data to a deployed method.
☐ Do not allow users to add new data to the method.	The method user cannot add new data to the method. Sometimes new data become available that needs to be added to a deployed method. Checking this option keeps the method locked against added new data after deployment.

The Analytes tab

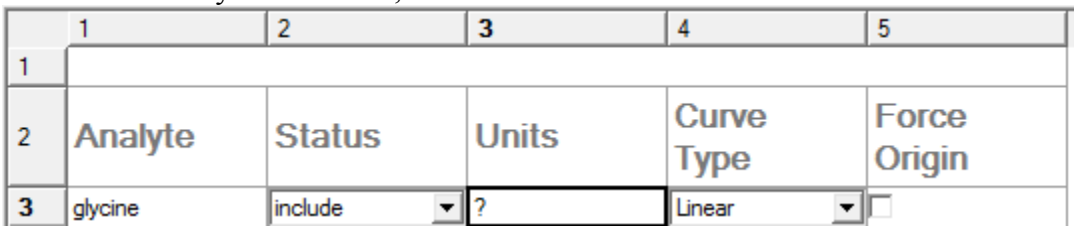
An analyte is a substance which is the target of the quantitative analysis.



The Analytes tab buttons

Add Analyte...	Add an analyte to the method.
Edit Analytes...	Edit the properties of one or more selected analytes.
Remove Analyte	Remove one or more selected analytes from the method.

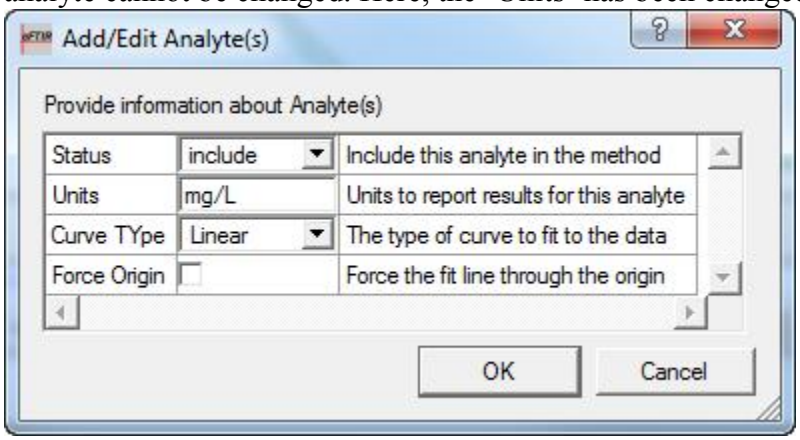
The first step in developing a method is to click 'Add Analyte'. In this example, we are analyzing for glycine in water. After clicking the button, you will be prompted for the name of the analyte. After that, the table will look like this:



Analyte	The name of the analyte
Status	Either include or exclude, determining if the analyte is actually being used.
Units	The units of concentration of the analyte in the method standards.
Curve Type	The choices are Linear, Quadratic and Cubic. This determines the type of line that is fit to the standards. What to use depends on what is learned during the Validation step.
Force origin	The curve can be forced to go through the origin (0,0). In theory, with a Linear curve, only one standard is needed for an analyte if Force Origin is checked.

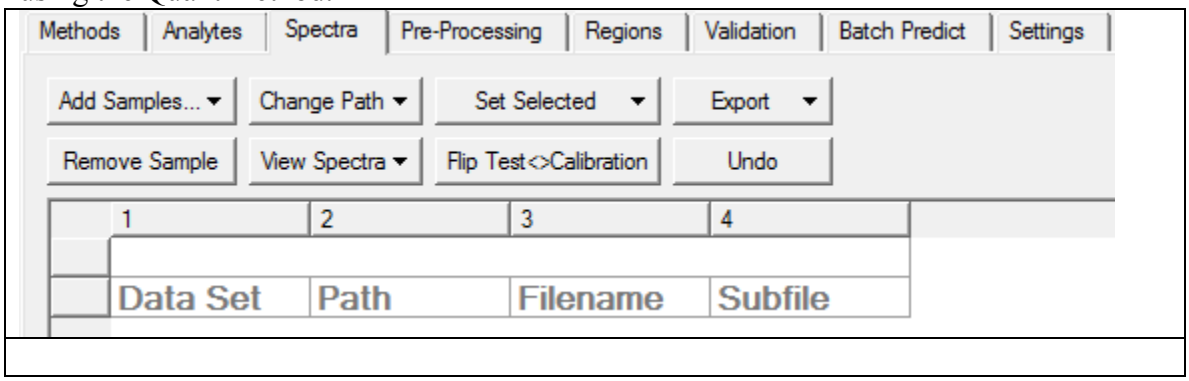
For Curve Type, you must have a minimum of 2 standards for Linear, 3 for Quadratic and 4 for Cubic. Using 'Force Origin' counts as a standard, because the origin will be a data point used in the calibration.

Selecting a row or rows in the Analyte table and clicking 'Edit Analytes…' will bring up this dialog which allows changing the properties of the analyte. Note that the name of the analyte cannot be changed. Here, the 'Units' has been changed to 'mg/L'.



The Spectra tab

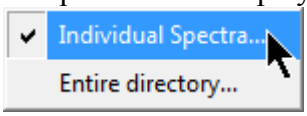
The words 'Spectra' and 'Standard' are synonymous here. A Standard is a Spectrum containing known quantities of all of the analytes that have been added to the method. The word 'Sample' is used to mean a spectra unknown concentrations that are predicting using the Quant method.



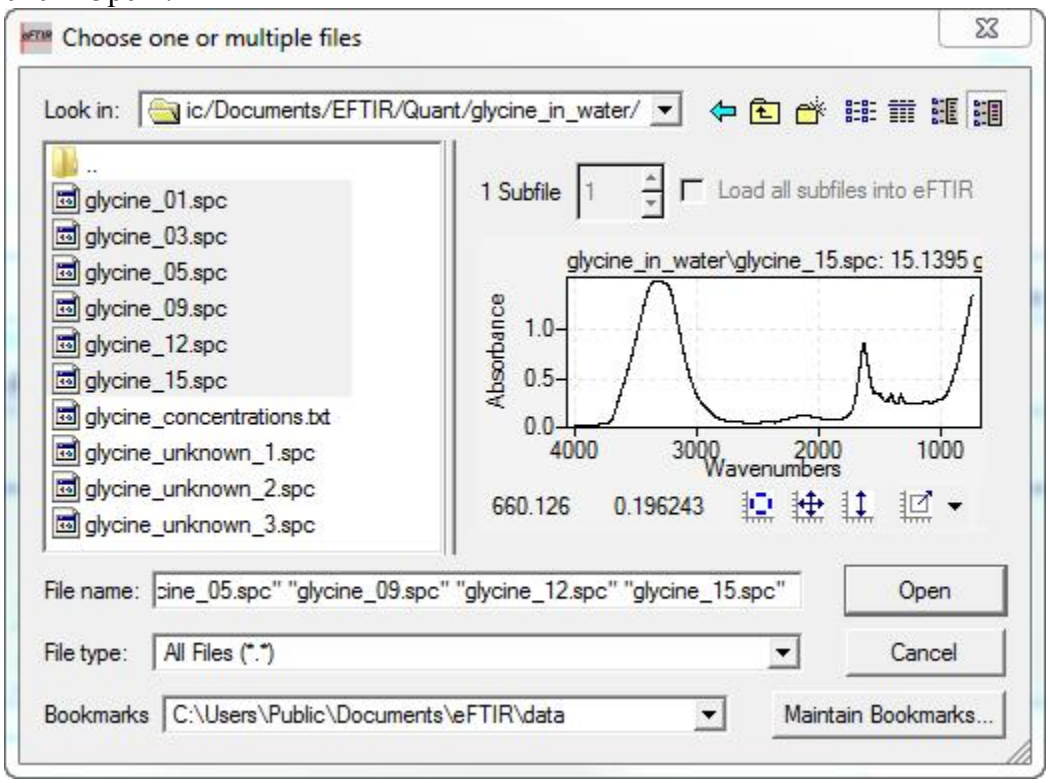
The Spectra tab buttons

Add Samples...	Add spectral files to the method.
Remove Sample	Remove one or more selected spectra from the method
Change Path	Change the disk path to the selected samples.
View Spectra	View the spectra
Set Selected	Change the 'Data Set' that the selected samples belong to.
Flip Test<>Calibration	Flip the 'Data Set' assignment for all samples in the method. This is useful for testing and validating the method.
Export	Export the Spectra table to Excel,
Undo	Will attempt to undo the last change to the standards table.

After adding an Analyte to the method, the next step is to add spectra. Clicking the 'Add Samples' button displays this menu:



Choose 'Individual Spectra', then the 'Choose one or multiple files' dialog will open. Navigate to the eFTIR Quant directory. On Windows 7 this will be usually be C:\Users\Public\Documents\EFTIR. On Windows XP it will usually be C:\Documents and Settings\All Users\Documents\EFTIR. The installed samples are in the 'glycine_in_water' sub-folder. Choose the files glycine_01 through glycine_15.spc, and click 'Open'.

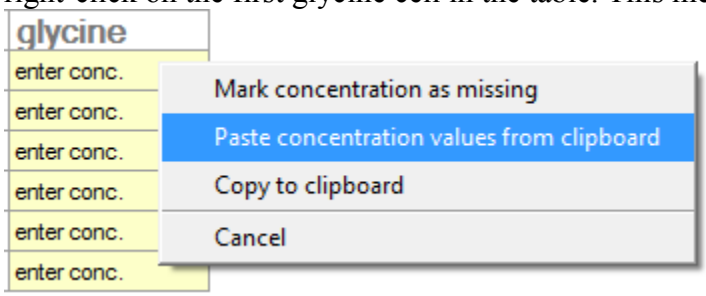


The Spectra table will now look like this:

	Data Set	Path	Filename	Subfile	glycine
1	calibration	C:/users/Public/Documents/EFTIR/Quant/glycine_in_water	glycine_in_water\glycine_01.spc	0	enter conc.
2	calibration	C:/users/Public/Documents/EFTIR/Quant/glycine_in_water	glycine_in_water\glycine_03.spc	0	enter conc.
3	calibration	C:/users/Public/Documents/EFTIR/Quant/glycine_in_water	glycine_in_water\glycine_05.spc	0	enter conc.
4	calibration	C:/users/Public/Documents/EFTIR/Quant/glycine_in_water	glycine_in_water\glycine_09.spc	0	enter conc.
5	calibration	C:/users/Public/Documents/EFTIR/Quant/glycine_in_water	glycine_in_water\glycine_12.spc	0	enter conc.
6	calibration	C:/users/Public/Documents/EFTIR/Quant/glycine_in_water	glycine_in_water\glycine_15.spc	0	enter conc.

Notice the 'enter conc.' Text in the glycine column. The concentration of glycine in each of the standards must be entered here. It's OK if you don't have the concentration for all standards, which can happen when you have multiple analytes in a method. Just leave the concentration entry for that standard alone, and the software will know that that standard

does not apply to the analyte with a missing concentration. Any non-numeric entry for a concentration value will mark that value as 'missing'.
Rather than enter all of those concentrations, you can paste them from the clipboard. In the same directory as the standards is a file named "glycine_concentrations.txt". Open this file in a text editor, and copy all the text in the file to the Windows clipboard. Then right-click on the first glycine cell in the table. This menu will appear:



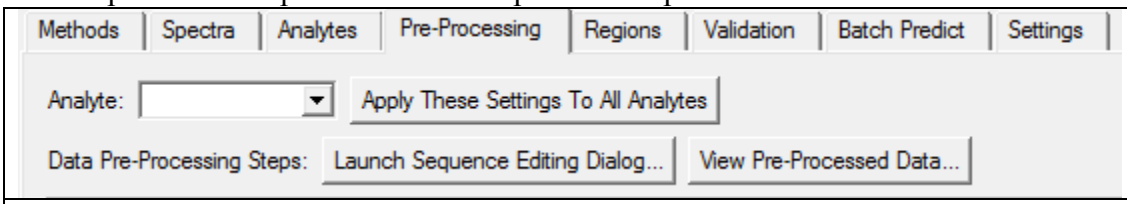
Select 'Paste Concentration values from clipboard'.
The concentration values will be pasted into the table:

glycine
1
3
5
9
12
15

You can use this same paste method to paste multiple columns of concentrations, or individual columns, or single numbers. Just highlight the first cell that you want the data to go into, and the software will parse the clipboard text into the table.

The Pre-Processing tab

Preprocessing is operations that are performed on the standards before calibration. The same operations are performed on samples before prediction.



The Pre-Processing buttons

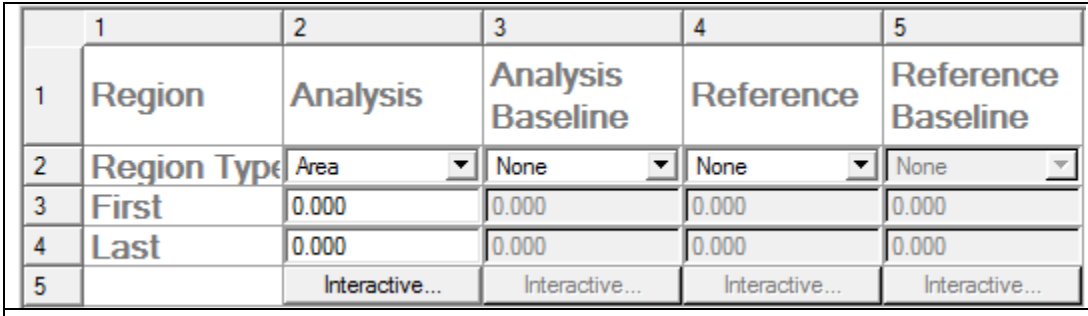
Analyte:	Choose the analyte to assign preprocessing for.
Launch Sequence Editing Dialog...	Launch the preprocessing dialog
View Pre-Processed Data...	Apply the preprocessing to the data and view the result

Apply These Settings To All Analytes	Apply the pre-processing assigned to the selected analyte to all analytes.

The Pre-Processing Dialog

Clicking the 'Launch Sequence Editing Dialog' button will bring up a dialog very similar to the Batch Processing Sequence dialog available in the 'Advanced' section of the Essential FTIR manual, except that the available processing options are limited to those that are useful for quantitative analysis. The only pre-processing options for quant are Smoothing and Derivative. Smoothing is used to enhance information in noisy data. Derivatives are used to remove baseline artifacts. Also, if the analytical region overlaps a band from some other component, the derivative may help avoid the interference from the overlapping band.

The Regions tab



Assigning analytical regions to the analyte standards is perhaps the most difficult thing about setting up a quant method. A region of the spectra must be found where absorbance increases with concentration, and where the other analytes in the method do not have absorbances that will interfere with the analyte.
In addition, the analysis region can be baseline corrected using a wider region than the analysis region.
A reference region can be assigned, which can also have its own baseline correction region. A reference region is useful when the pathlength of the samples is varying. As pathlength increases, absorbance will increase, and the calculated concentration based on that absorbance will increase. By ratioing one peak or area against another, the effect of varying pathlength is corrected.

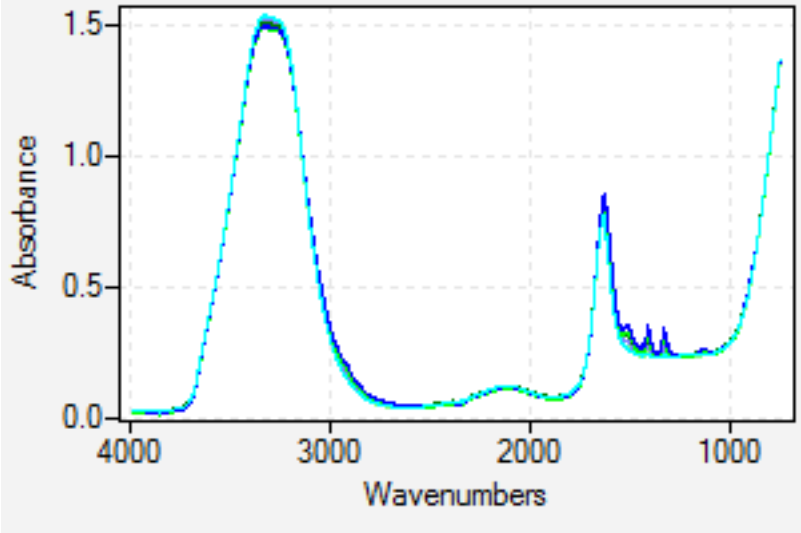
The Regions Buttons

Analyte:	Choose the analyte to work with
View Spectra	View spectra from the method to help with region selection
Getting Started...	Displays a brief help hint about how to

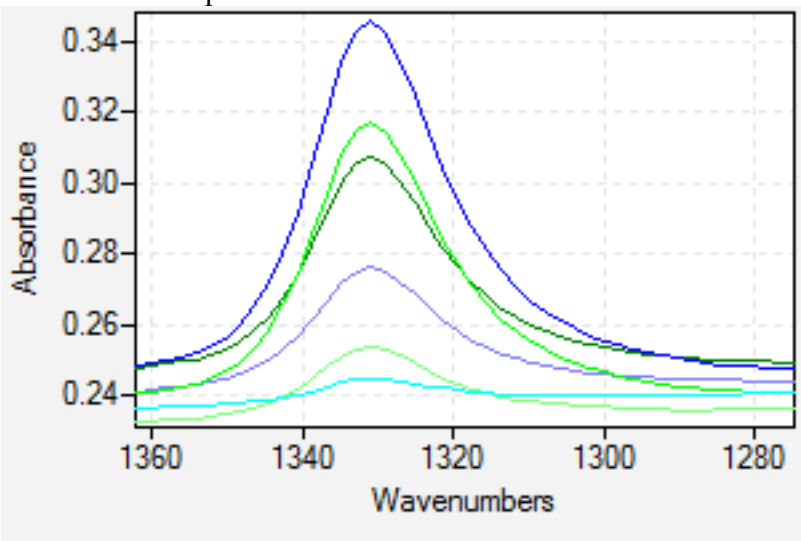
	assign analysis regions to an analyte.

Assigning regions to an analyte

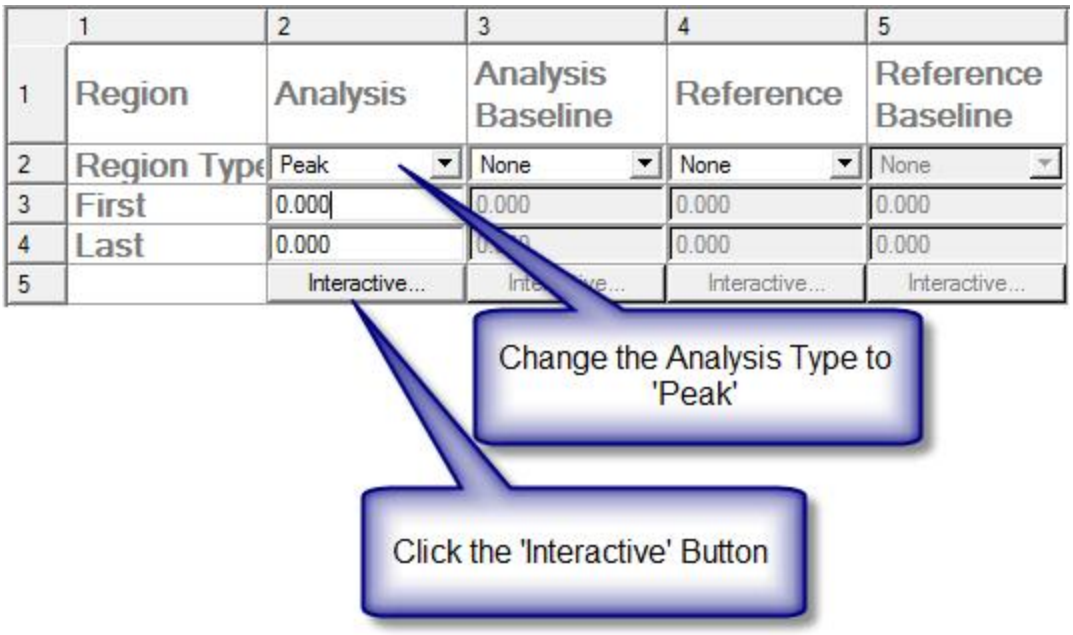
First, click the 'View Spectra' button to display some or all of the methods' spectra.



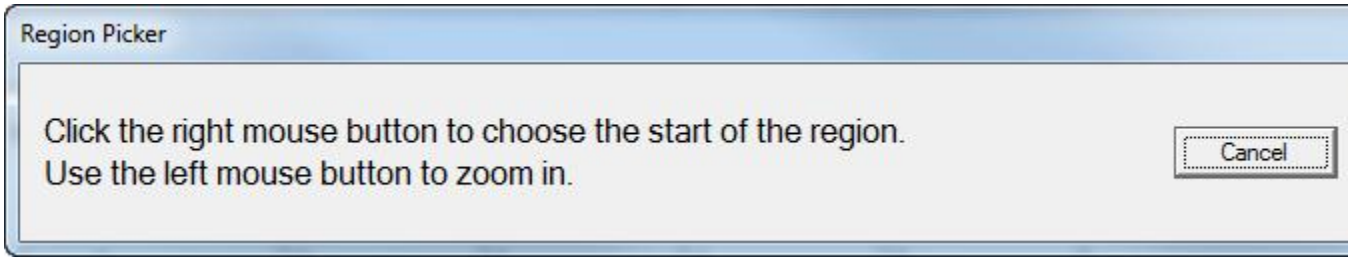
Zoom in on the peak at 1330 cm-1:



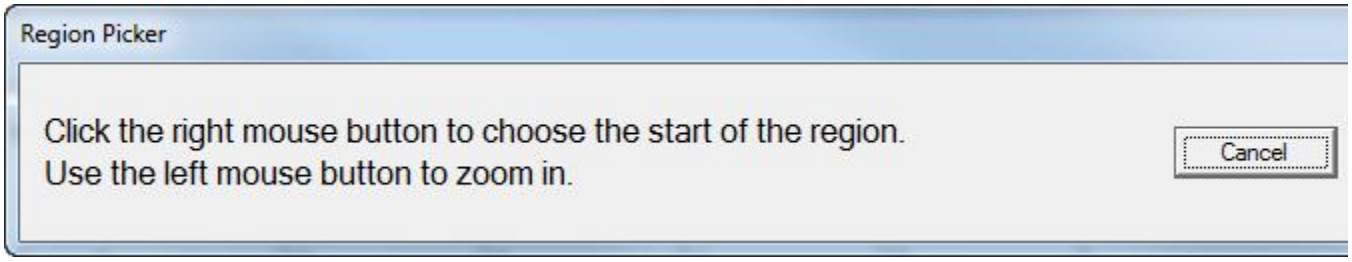
This is the peak we will use to quantitate glycine in water.
Change the Analysis type to 'Peak', and then click the 'Interactive' button in that column.



This dialog will appear:



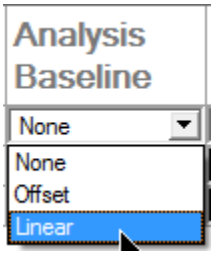
Move the mouse into the data display, and right-click the mouse when the cursor is at about 1324 wavenumbers in the display. An X,Y cursor readout is in the lower left corner of the display window. All of the display controls on the data window are active, and you can use the left mouse button to zoom in on the data.
After right-clicking, a marker will appear in the data window, and the selected wavenumber value will be entered into the table. The dialog text will change to prompt you to pick the second point for the region:



Move the mouse until it is at about 1336 wavenumbers, and right click. This second value will be entered into the table, and the table will look something like this:

	1	2	3	4	5
1	Region	Analysis	Analysis Baseline	Reference	Reference Baseline
2	Region Type	Peak	None	None	None
3	First	1323.971	0.000	0.000	0.000
4	Last	1335.899	0.000	0.000	0.000

After initially selecting the region, the markers can be moved interactively, or the numbers in the table can be edited directly, so you don't have to be too fussy about selecting the exact values because they can be easily tweaked once there are First and Last entries in the table. Note that we could have just edited the cells in the table directly, but it is easier and more interactive to use the mouse within the data window.
Now a baseline correction region must be entered. Change the 'Analysis Baseline' to 'Linear':

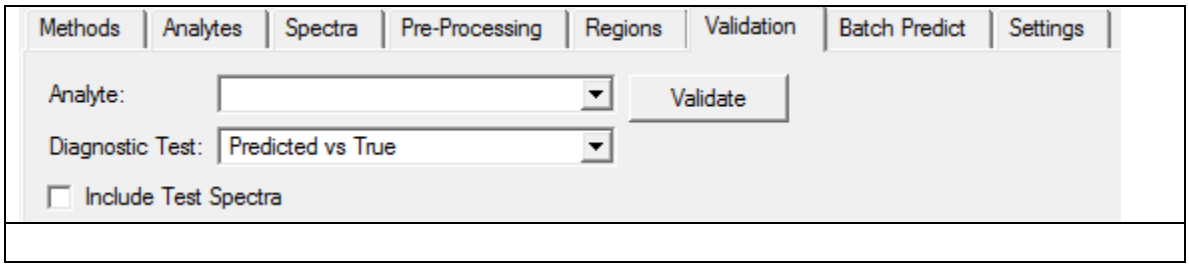


Then click on the Interactive button and select First and Last baseline points at 1228 and 1363 wavenumbers. The table will then look something like this:

	1	2	3	4	5
1	Region	Analysis	Analysis Baseline	Reference	Reference Baseline
2	Region Type	Peak	Linear	None	None
3	First	1323.706	1229.114	0.000	0.000
4	Last	1336.779	1363.256	0.000	0.000
5		Interactive...	Interactive...	Interactive...	Interactive...

The Validation Tab

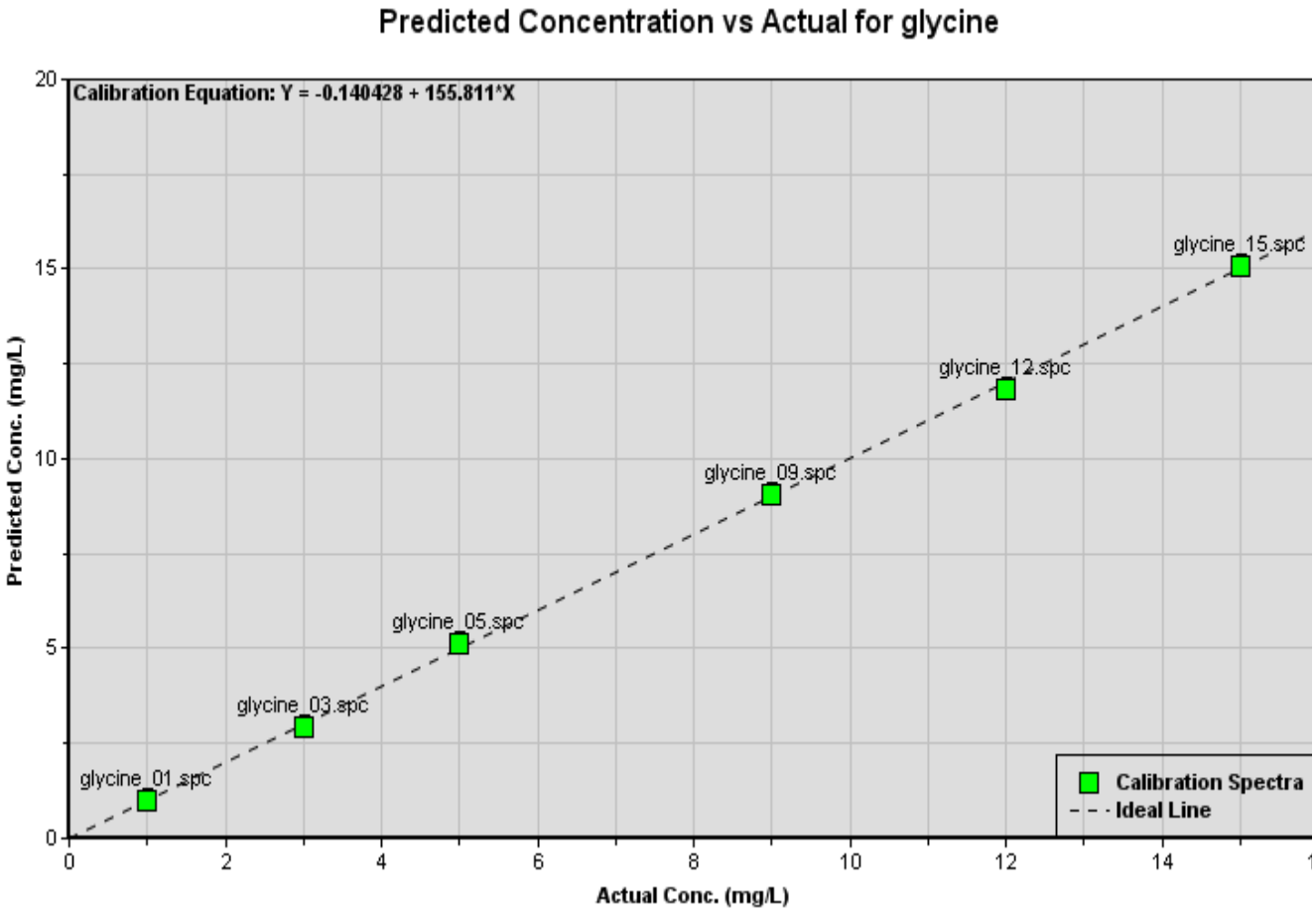
After assigning an analysis region for each analyte, the method must be validated. Validation ensures that the method (the standards, concentrations, curve type, and analysis regions) correctly models the variation of absorbance with concentration.



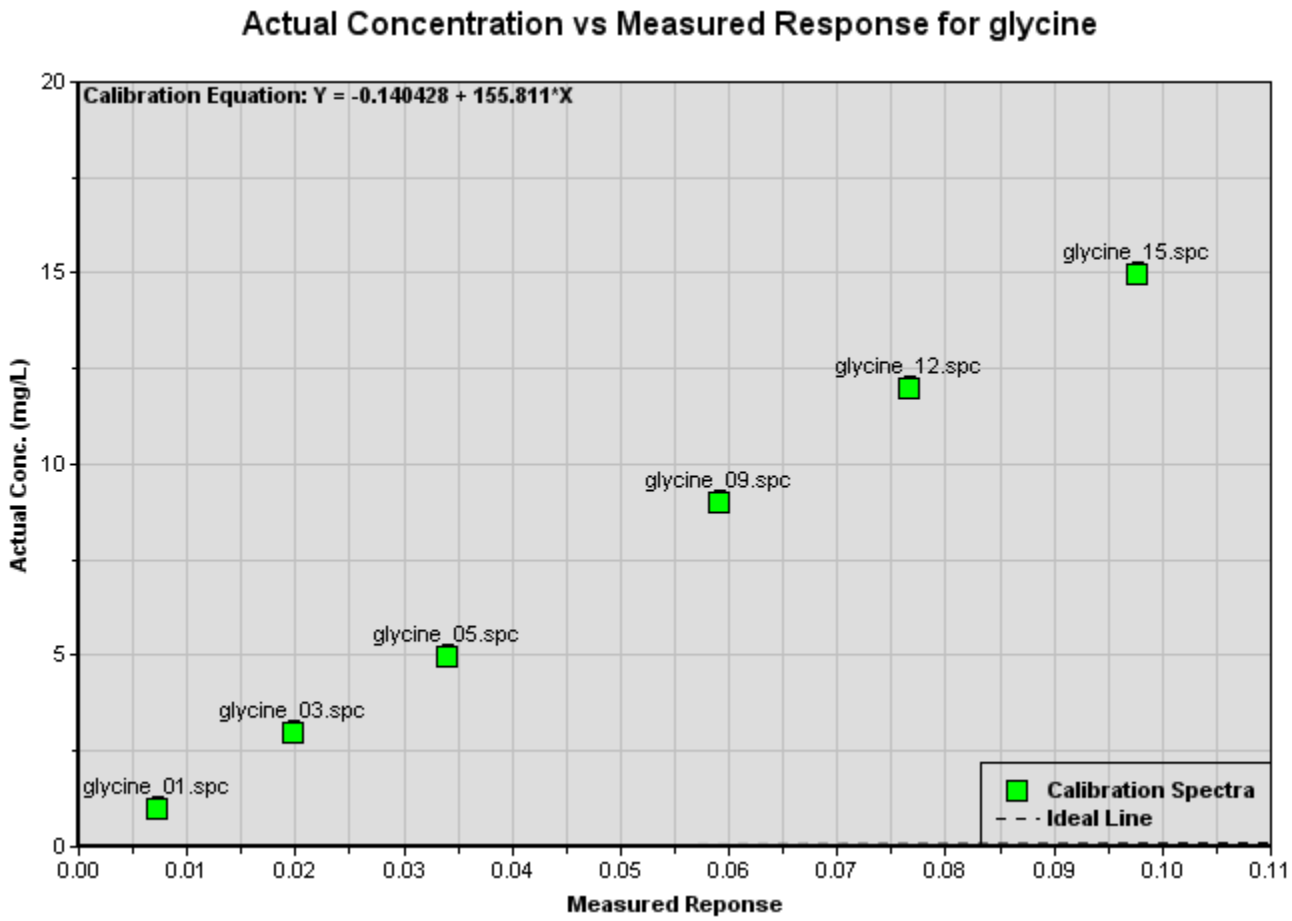
The validation buttons

Analyte:	Select the analyte to validate
Diagnostic Test: Predicted Concentration vs Actual	What type of chart to display
Include Test Spectra	If there are test spectra in the method, should they be included in the chart
Validate	Perform the validation

In this example for glycine in water, the graph of Predicted Concentration vs. Actual is generated:

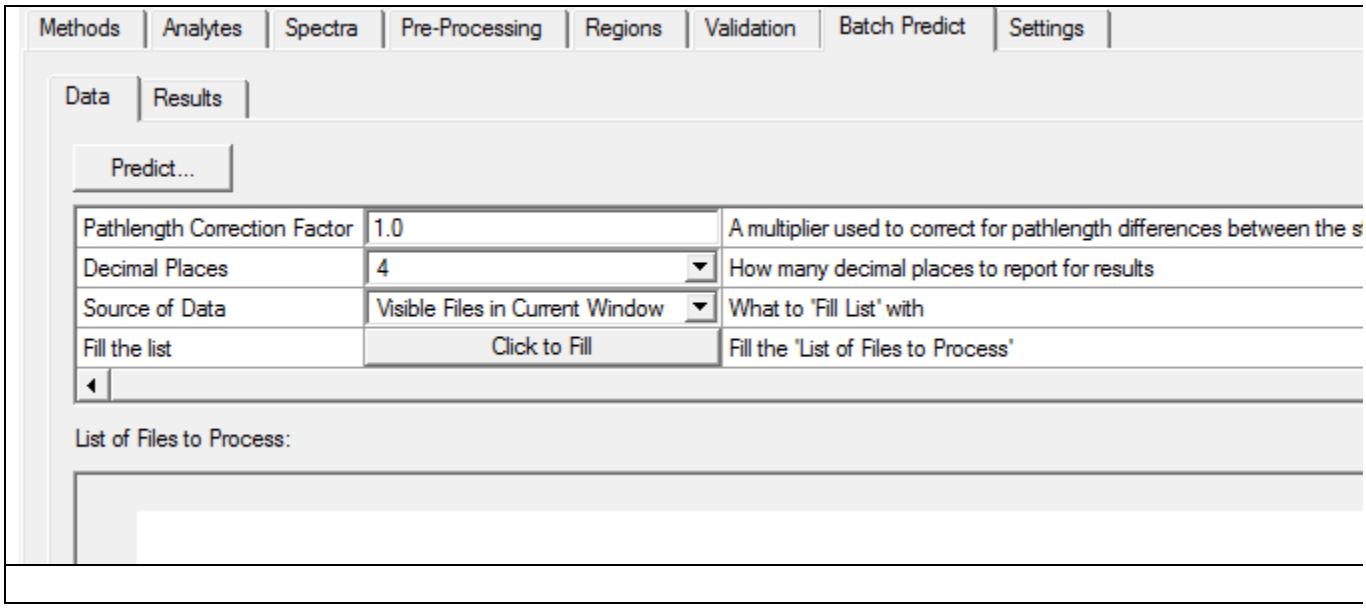


The dashed line is the expected line for a linear fit.
A useful plot to look at is the ‘Actual Concentration vs. Measured Response.



The Batch Predict tab

The Batch Predict tab is used to run samples with unknown concentrations of analytes against the method to predict the quantities of the analytes in the samples. The Batch Predict tab contains two tabs itself, labeled Data and Results. On the Data tab, select the source of the data you want to analyze. The results will be displayed on the Results tab. Included with the example glycine in water quant method are three unknowns, named glycine_unknown_1, _2, and_3. They are installed into the same directory as the method. Load them into a window, and then click ‘Predict’.



After the prediction is performed, the results will automatically display on the 'Results' tab.

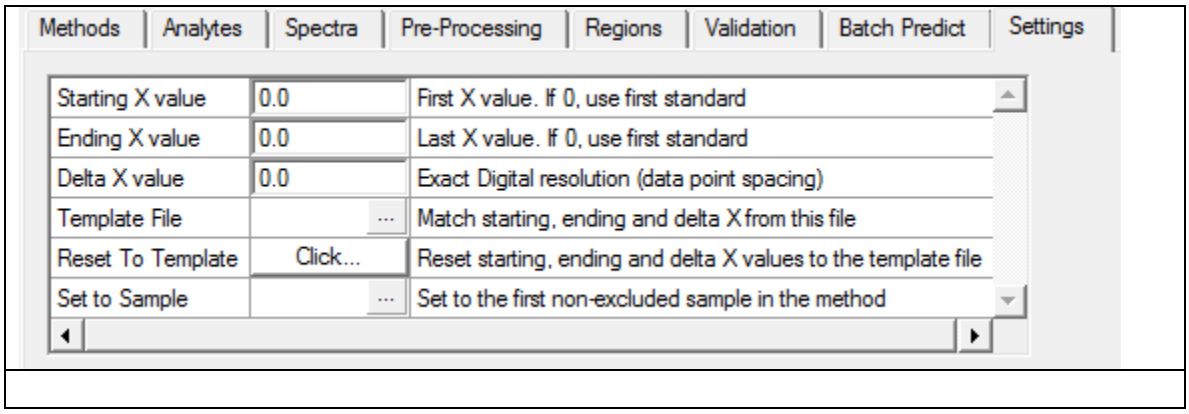
	1	2	3
1	File	glycine (mg/L)	Std Error
2	glycine_in_water\glycine_unknown_1.spc	7.9927	0.1371
3	glycine_in_water\glycine_unknown_2.spc	17.1203	0.1371
4	glycine_in_water\glycine_unknown_3.spc	4.8738	0.1371

Note that unknown 2 is highlighted in red. This is because the result for this unknown has been extrapolated, meaning that the predicted concentration is greater than the most concentrated standard included in the method. An extrapolated result is not as reliable as an interpolated result, such as when the predicted concentration lies between the concentrations of two standards in the method.

The Batch Predict buttons

Export		The results table can be exported to the clipboard, Excel, or to a file.
Clear		The results table will be cleared.

The Settings tab



Ideally, all of the Standards in the method would have the same resolution and wavelength/wavenumber range. If they don't, they need to be interpolated to a common resolution and range. When the first standard is added to the method, these numbers are filled in using that standard. If you need to change them, you can do it on this table. Usually this action is not needed, as the Standards will all be collected on the same instrument at the same time using the same data collection settings.

Partial Least Squares (PLS)

PLS is an add-on package for Essential FTIR. It is documented in a separate manual. Clicking the 'Help' button in the PLS tool will display the PLS documentation.

Classical Least Squares (CLS)

CLS is an add-on package for Essential FTIR. It is documented in a separate manual. Clicking the 'Help' button in the CLS tool will display the CLS documentation.

Custom Quant Application

Custom Quant Application allows the creation of a custom, simplified, user interface to Essential FTIR's quantitative analysis. The user interface is simplified to allow only the selection of an analysis method, loading or collecting sample data, and running the analysis. Custom Quant Application makes repeated running of samples easier and less error-prone by removing the possibility of changing any options that may affect the results, and increases productivity by focusing on the simple task of collecting and analyzing sample data.

Custom Quant Application can work with any Beer's Law, PLS, CLS, or QC Compare methods created in Essential FTIR.

Here is an example of how a custom application looks when it is running. This is all that the operator sees. The logo and caption of the screen can be changed to anything.

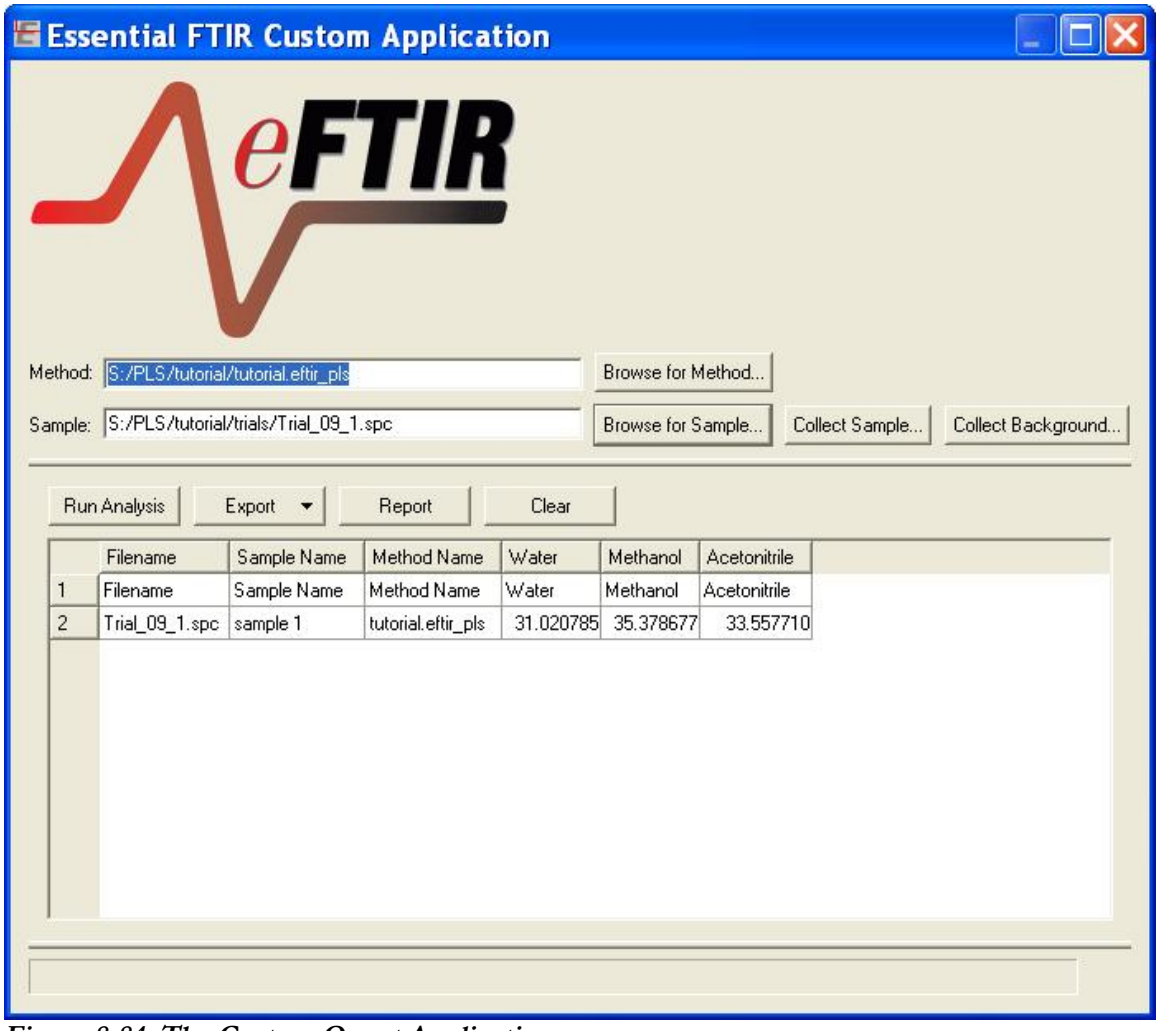


Figure 8-84 The Custom Quant Application

To create a Custom Quant Application, start with the ‘Application’ tab.

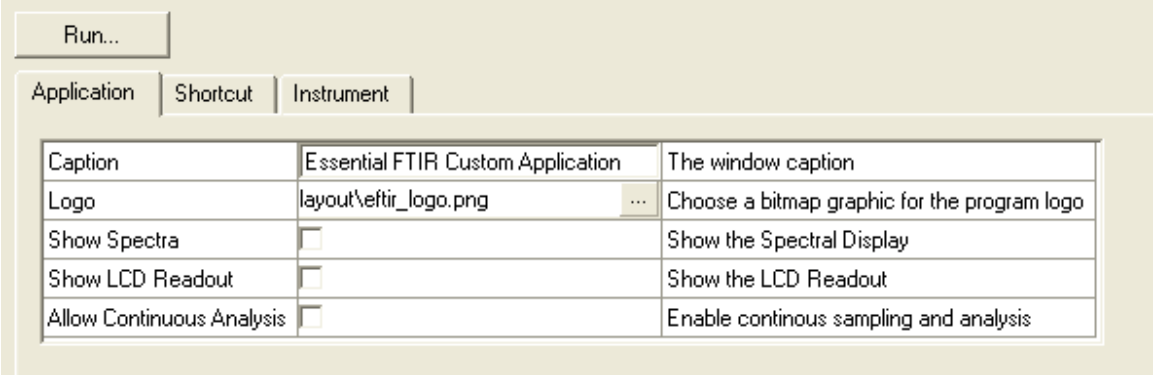


Figure 8-85

On the application tab, select the Caption and Logo that you want to use.
The other options further customize the screen:
Show Spectra: If this is checked, the user will see the spectra that are loaded or collected. If unchecked, the spectra will not be displayed.
Show LCD Readout: A large readout of calculated values can be displayed, which is useful when continuously monitoring a single value.
Allow Continuous Analysis: Adds the ability to continuously and automatically collect and analyze samples, rather than having to manually collect and analyze single samples.
If all three of these are checked, the Custom Quant Application interface will look like this:

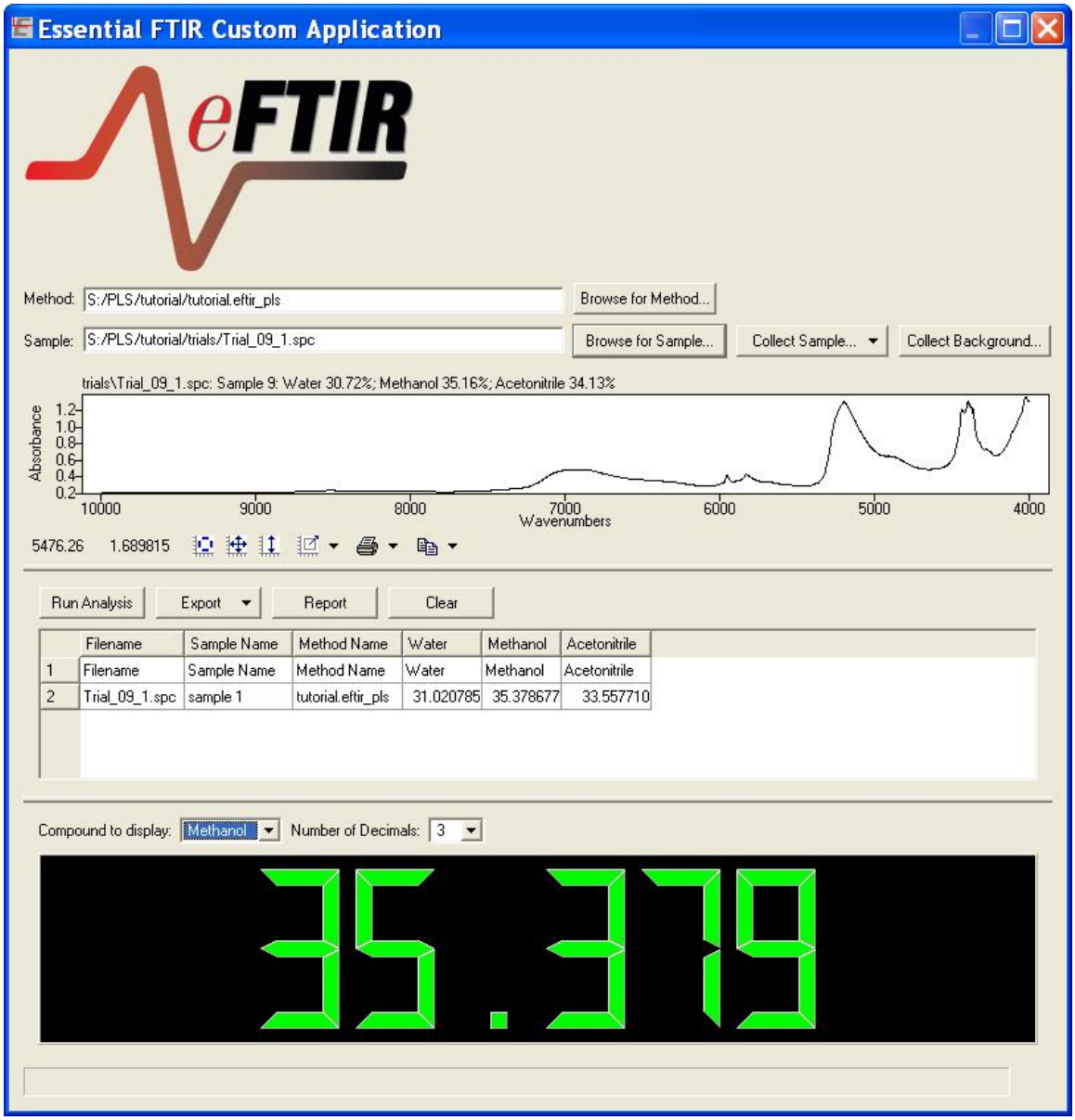


Figure 8-86 Custom Quant Application with spectrum, results table, and readout visible

The three sections of the spectrum, the results table, and LCD readout, are separated by splitter bars that allow the sections to be resized.

The next tab, labeled ‘Shortcut’, can be used to create a desktop shortcut that will launch the Custom Quant Application directly.

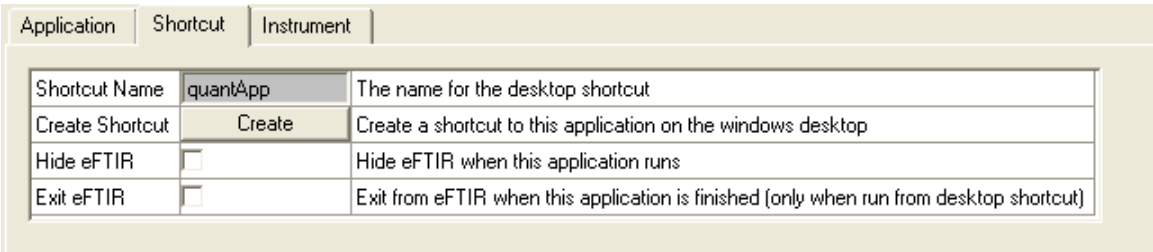


Figure 8-87

Shortcut Name	The Desktop shortcut will be labeled with this name
Create Shortcut	Click this button to create the shortcut
Hide eFTIR	If checked, Essential FTIR is hidden while the custom application runs.
Exit eFTIR	If checked, eFTIR closes when the quant application is closed.

By using 'Hide eFTIR' and 'Exit eFTIR', the user of the Custom Quant Application never sees Essential FTIR at all, only this custom interface is seen by the user at any time.

The Instrument Tab chooses which instrument, and set of instrument parameters, to use when collecting data in the Custom Quant Application. The 'Instrument Options' file has to first be created using the Instrument's data collection tool, and then selected here.

The Synthesize / Edit Data Toolbox

In this section we turn out attention to a set of features likely to be of interest to the research scientist – the ***Synthesize / Edit Data Tools***. These routines have a wide variety of applications, and may be used to offer solutions to problems that seem intractable using any of the more "traditional" ***Tools***. We will examine each feature in turn.

Add Peaks to Data

The Add Peaks to Data parameters window is shown in Figure 8-88

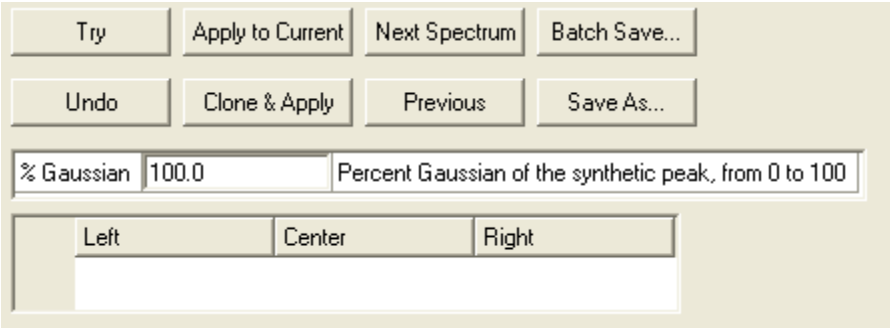


Figure 8-88 Add Peaks to Data parameters

The Toolbox Buttons are positioned at the top of the parameters window. Below these buttons is an edit box, labeled ***% Gaussian***. This value, from 0 – 100%, determines the Gaussian proportion of the synthetic peak. Any remainder of the peak will be Lorentzian – for example, if the value 45% is entered, the synthetic peak will be 45% Gaussian and 55% Lorentzian in character. The range of the peak is defined by Regions, selected by right-clicking on the active spectrum in the workspace and dragging to the desired locations. This range in turn dictates the full width at half maximum (FWHM) of the peak. Clicking within the region markers allows dragging of the peak maximum to the desired absorbance value. Figure 8-89 shows the process of shaping the peak.

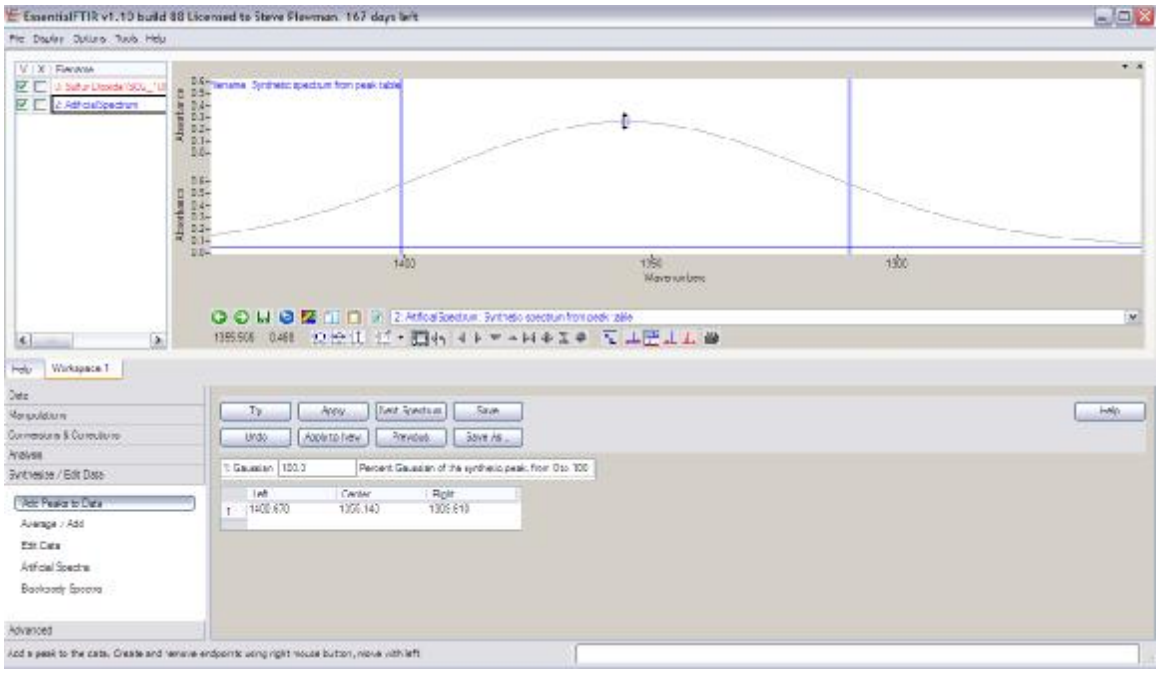


Figure 8-89 *Shaping a synthetic peak*

The ***Regions*** defined in Figure 8-89 dictate the extent of the peak over the wavenumber axis. The cursor is visible in the center of the peak, and has assumed the double-arrow form, which is used to left-click and drag the peak center to the desired height. The limits of the synthetic peak are shown in the display window. Figure 8-90 shows a synthetic absorbance feature generated in this way.

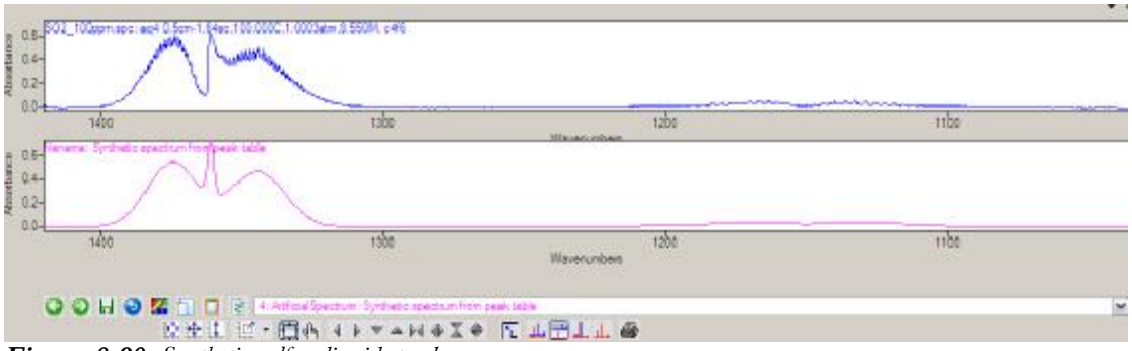


Figure 8-90 *Synthetic sulfur dioxide peaks*

The upper spectrum in Figure 8-90 represents sulfur dioxide. The lower spectrum is a synthetic version created by first summoning a "flat line" absorbance spectrum using the ***Artificial Spectra*** tool discussed later in this section. Peaks were then added to this spectrum to create a reasonable facsimile of the original spectrum. An arbitrary level of detail is possible by overlaying peaks.

Average / Add

It is often desirable to average or co-add a large collection of spectra together, to eliminate noise and to bring out low intensity absorbance features. The ***Average / Add Tool*** provides this capability. Figure 8-91 shows the parameters window for this ***Tool***.

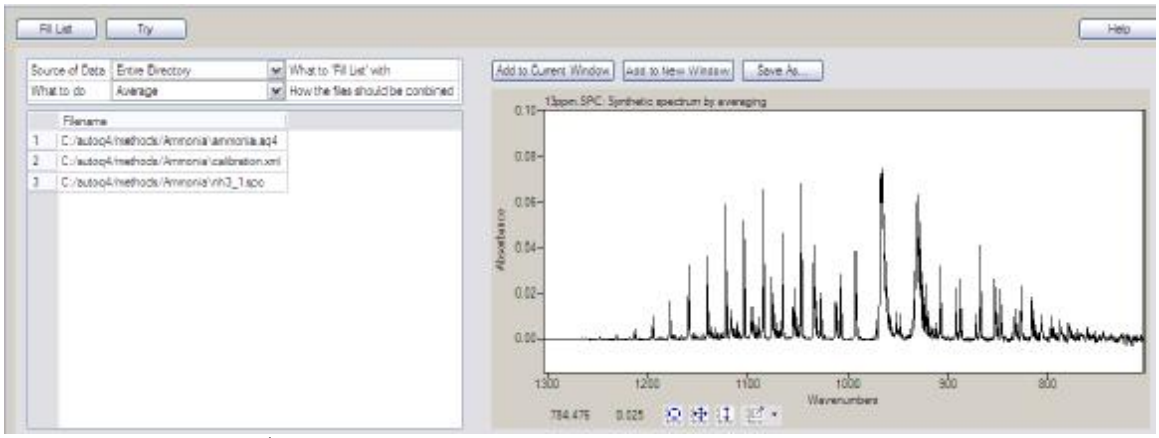
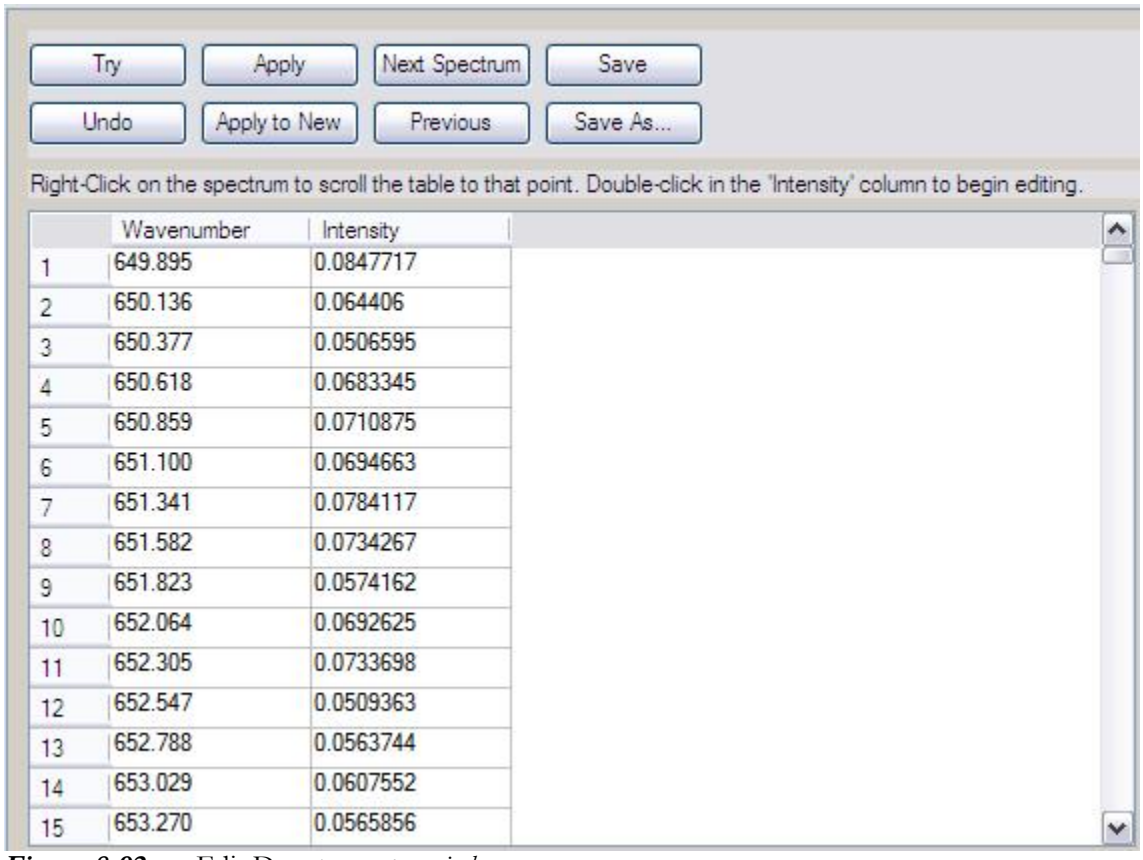


Figure 8-91 Average / Add *parameters window*

The ***Fill List*** button is used to populate the file window in the lower left of the window. The ***Try*** button performs the operation and shows the result in the preview window, in the lower right of the screen. In the upper left of the window is the options box. There are two options, each selectable via drop down menus. The first option is ***Source of Data***. The options available are ***Visible Files in Current Window***, ***All Files in Current Window***, ***Pick Files from Disk*** and ***Entire Directory***. The second option determines what to do with the data once the list is filled. The options are ***Average***, ***Add*** and ***Add with weights***. Once the ***Try*** button has been pressed and the result displayed in the preview window, the processed spectrum may be saved, added to the current ***Workspace***, or added to a new ***Workspace*** using the buttons above the preview window.

Edit Data

The ***Edit Data Tool*** allows direct access to the numerical data in the array representing a spectrum in a familiar spreadsheet format. The ***Edit Data*** parameters window is shown in Figure 8-92.



	Wavenumber	Intensity
1	649.895	0.0847717
2	650.136	0.064406
3	650.377	0.0506595
4	650.618	0.0683345
5	650.859	0.0710875
6	651.100	0.0694663
7	651.341	0.0784117
8	651.582	0.0734267
9	651.823	0.0574162
10	652.064	0.0692625
11	652.305	0.0733698
12	652.547	0.0509363
13	652.788	0.0563744
14	653.029	0.0607552
15	653.270	0.0565856

Figure 8-92 Edit Data *parameters window*

The full complement of ***Toolbox Buttons*** is available. Beneath these buttons is the data array, contained within an editable spreadsheet interface. Right clicking on the data in the ***Workspace*** scrolls the numerical data to that point, and double clicking on a cell in the ***Intensity*** column of the spreadsheet renders the cell active for editing. In this way, data may be directly edited by the user.

Use the left mouse button to select data in the table and then right-click to bring up a menu that allows copying the selected contents to the Windows clipboard.

Artificial Spectra

The ***Artificial Spectra*** feature may be used to generate purely synthetic spectra. If precise line positions are known then it is theoretically possible to create highly realistic absorbance spectra using this ***Tool***. A simple example of an artificial spectrum, together with the parameters used to generate it are shown in Figure 8-93.

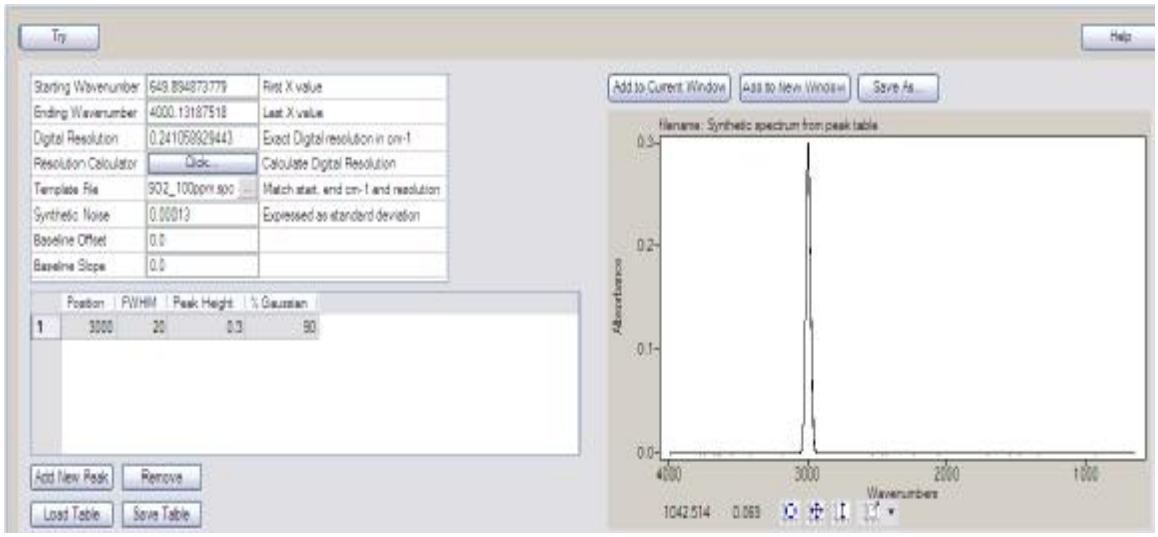


Figure 8-93 *Synthetic spectrum generated with the* Artificial Spectra Tool

The ***Try*** button is used to show the results of the current parameters in the preview window. Below the ***Try*** button is an options box, with eight rows. Examining each in turn:

- ***Starting Wavenumber:*** Defines the low wavenumber value for the spectrum.
- ***Ending Wavenumber:*** Defines the high wavenumber value for the spectrum.
- ***Digital Resolution:*** Specifies the digital resolution for the spectrum**.**
- ***Resolution Calculator:*** Calculates the digital resolution for the spectrum based on other entered parameters.
- ***Template File:*** Allows you to select a template for the synthetic spectrum, via a browser window summoned by the edit button (**…**). The synthetic spectrum will be matched to the template in terms of starting and ending wavenumber, and resolution.
- ***Synthetic Noise:*** Specifies the magnitude of synthetic noise added to the artificial spectrum in absorbance units.
- ***Baseline Offset:*** Specifies the amount by which the baseline should be offset from zero in absorbance units.
- ***Baseline Slope:*** Defines the gradient of the baseline.

Below the options box is a ***Peak Table***, into which values for peak center position, full width at half maximum (FWHM), peak height and the percentage of the peak defined by a Gaussian curve. As with the ***Add Peaks to Data Tool***, any remainder is generated as Lorentzian. Below the ***Peak Table*** are four buttons. The ***Add New Peak*** button generates a new row in the ***Peak Table***, into which new values may be entered. The ***Remove*** button

erases the selected peak. The ***Save Table*** button enables you to save the table to disk, while the ***Load Table*** button allows you to load a pre-fabricated table from disk.

Once the ***Try*** button has been pressed and the result displayed in the preview window, the processed spectrum may be saved, added to the current ***Workspace***, or added to a new ***Workspace*** using the buttons above the preview window.

Blackbody Spectra

There are occasions, particularly when working with data generated using open-path FTIR, when a comparison of black body spectra is useful. The ***Blackbody Spectra Tool*** provides the capability to generate synthetic black body spectra. Figure 8-94 shows the parameters window for the ***Blackbody Spectra Tool***.

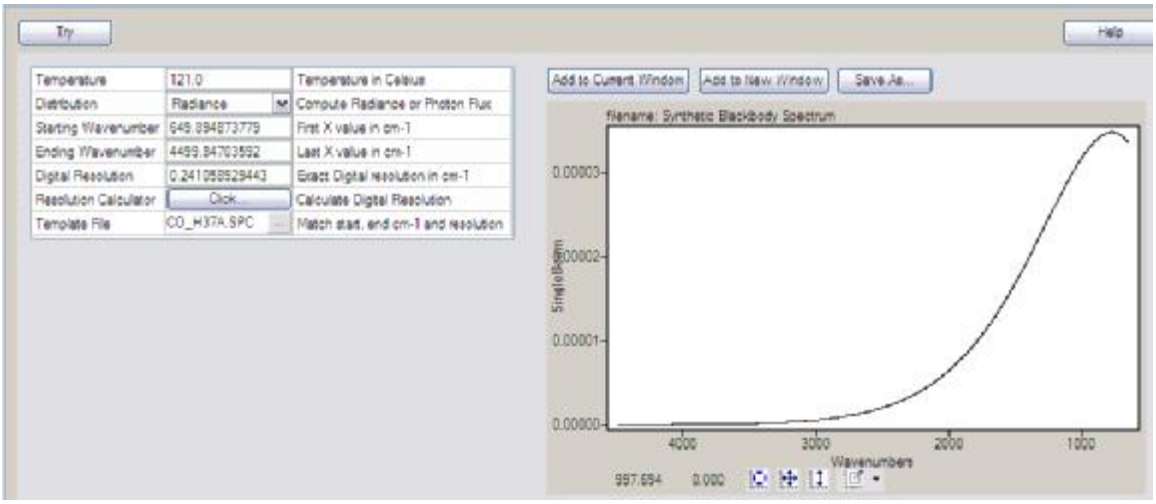


Figure 8-94 Blackbody Spectra *parameters window*

The options box for the ***Tool*** has seven rows. Dealing with each in turn:

1. ***Temperature:*** The temperature in degrees Celsius at which the black body curve is to be calculated
2. ***Distribution:*** The distribution of the synthetic curve. Options of ***Photons*** or ***Radiance*** are available from the drop-down menu.
3. ***Starting Wavenumber:*** The lowest wavenumber in the curve.
4. ***Ending Wavenumber:*** The highest wavenumber in the curve.
5. ***Digital Resolution:*** Specifies the exact digital resolution of the black body spectrum.
6. ***Resolution Calculator:*** The button associated with this feature summons a calculator which enables you to calculate the precise value based on laser wavelength and optical resolution.
7. ***Template File:*** Summons a browser dialog which allows specification of a spectrum file to act as a template for the synthetic black body. The new spectrum will match the resolution and starting and ending wavenumber values of the template file.

The ***Try*** button on the upper left of the window applies the current options to a synthetic spectrum, which is displayed on the right side of the window. The buttons labeled ***Add to Current Window***, ***Add to New Window*** and ***Save As*** may be used to display the spectrum in the current active ***Workspace***, display in a new ***Workspace,*** or save the file to disk.

Change Header Fields

Sometimes spectra are recorded with incorrect information. For instance, the data in a file may be Absorbance, but the information in the header file be set to Transmittance, so the data will be displayed incorrectly. This tool allows you to change the header of the data file. It does not change the data itself at all, it just changes the information about that data so that the data can be correctly displayed and interpreted. For instance, choosing 'Transmittance' for the Y units does not change the data values to Transmittance.
It only changes the header field associated with the data.

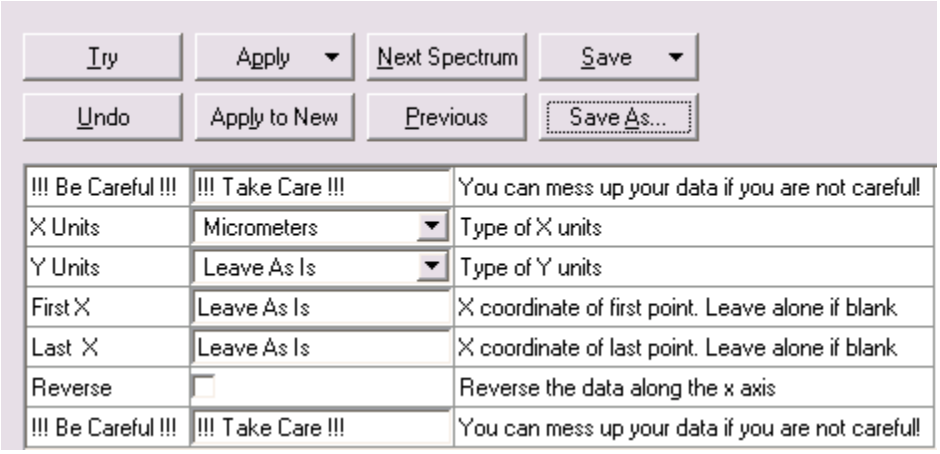


Figure 8-95 The Change Header Fields window

Please take heed of the !!!Be Careful!!! entries in the options table. This capability is provided as a convenient way to correct problems in data file headers. Do not do this unless you are very sure about what you are doing; you can render your data meaningless!

The Advanced Toolbox

The final toolbox in the collection is called the ***Advanced Toolbox***. This collection of ***Tools*** is home to the more flexible and powerful elements of Essential FTIR. The Advanced Toolbox is shown in Figure 8-96

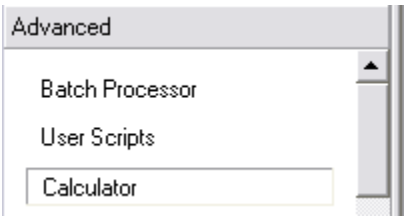


Figure 8-96 *The* Advanced Toolbox

We will explore each ***Tool*** in turn.

Batch Processor

The ***Batch Processor Tool*** is used to identify a group of spectral files, perform a pre-defined set of operations upon the selected data, and save the modified data to a specified directory. The ***Tool*** is used to automate any repetitive tasks that may arise in the course of data processing. The parameters window for the ***Batch Processor Tool*** is shown in Figure 8-97.

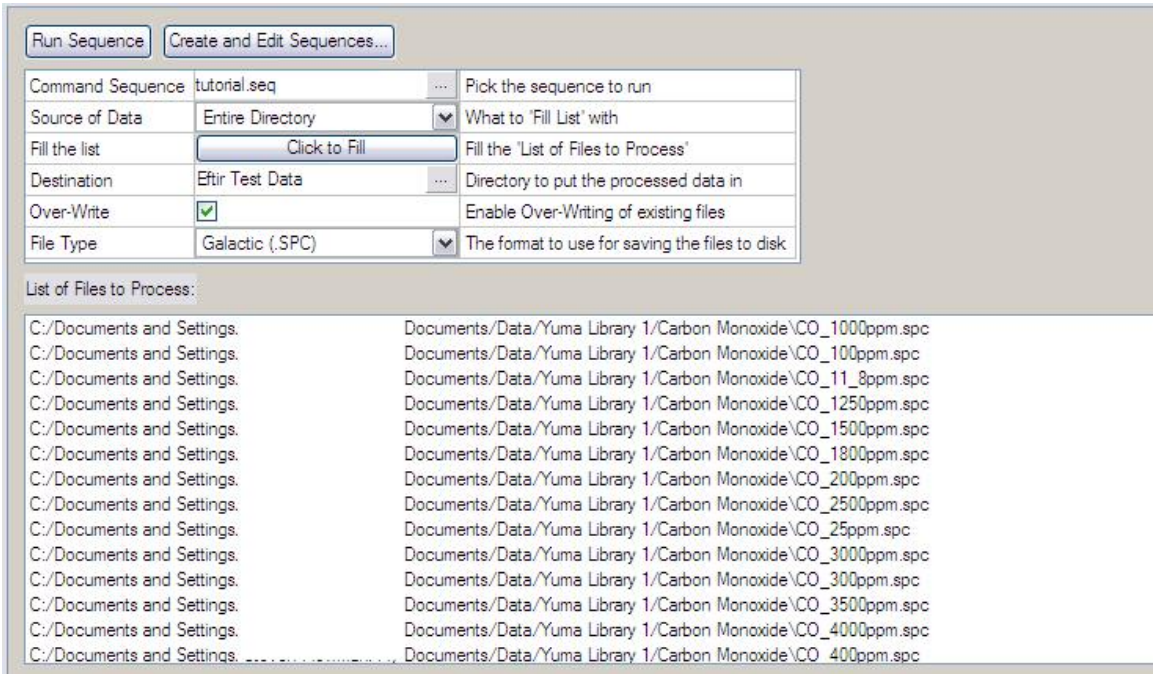


Figure 8-97 Batch Processor *parameters*

The Batch Processor Tool uses the concepts of ***Regions*** and ***Sequences***, which are defined and saved to disk for later use. Two buttons are located in the upper left of the parameters

window. The ***Run Sequence*** button is used to execute the currently set parameters in the options box. The button labeled ***Create and Edit Sequences*** summons the ***Build Batch Processing Sequence*** dialog box, which is shown in Figure 8-98.

Editing Batch Sequences

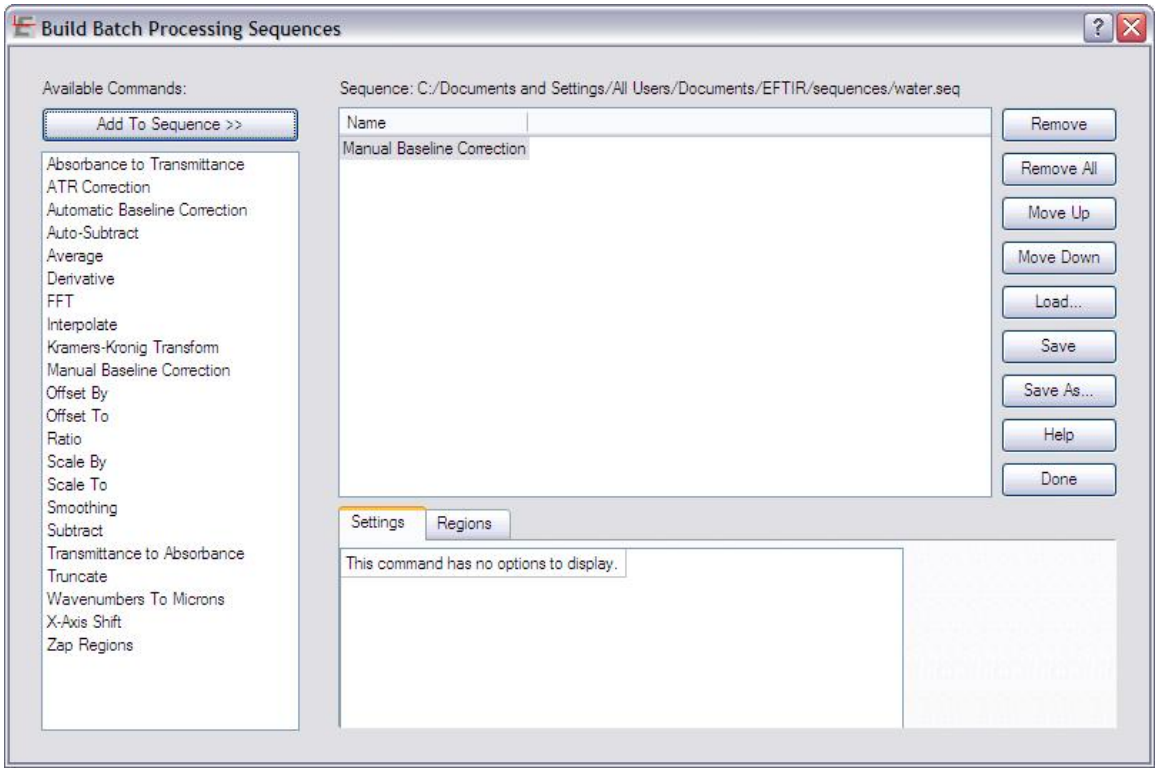


Figure 8-98 Build Batch Processing Sequence *dialog box*

The ***Build Batch Processing Sequence*** dialog box consists of four main areas – the ***Tools*** list, the ***Sequence***, the ***Settings*** and ***Regions*** window, and the button panel. We will examine each area in turn.

The Tools list

The panel on the left lists all ***Tools*** available to the ***Batch Processor***. Each ***Tool*** may be selected with a mouse click and added to the ***Sequence*** window by clicking the ***Add To Sequence*** button. Alternatively, these steps may be combined by double clicking a ***Tool*** in the list, which adds that ***Tool*** to the ***Sequence*** without using the ***Add To Sequence*** button.

The Sequence window

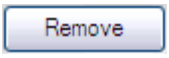
The upper central area is called the ***Sequence*** window. In this area all operations to be carried out on the spectra selected for ***Batch Processing*** are listed.

The Settings and Regions window

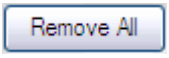
The window occupying the lowest portion of the dialog box is called the ***Settings* and *Regions*** window. There are two tabs; the ***Settings*** tab and the ***Regions*** tab. Under the ***Settings*** tab, the options and settings associated with the ***Tool*** currently selected in the ***Sequence*** window are displayed. The ***Regions*** tab displays the ***Regions*** to be used by the currently selected ***Tool***, if applicable. The ***Load Regions*** button allows the loading of a pre-defined set of ***Regions*** for the operation currently selected.

The *Buttons* panel

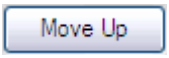
The Buttons panel comprises nine buttons. Taking each in turn:



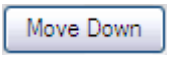
Removes the currently selected operation from the ***Sequence***.



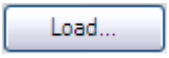
Removes all operations from the ***Sequence***.



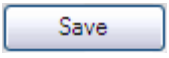
Shifts the selected operation up one position in the order of operations.



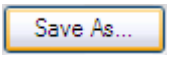
Shifts the selected operation down one position in the order of operations.



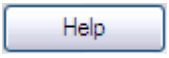
Summons a dialog box allowing you to load a pre-defined ***Sequence***.



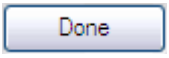
Saves the ***Sequence*** currently being edited.



Displays a ***Save As*** dialog box for the ***Sequence*** currently being edited.



Displays the ***Essential FTIR Help*** files for the ***Batch Processor***.



Dismisses the dialog box.

Batch processing options

Six options are available, as shown in Figure 8-97. Taking each option in turn:

1. ***Command Sequence***: The path to the Sequence file currently loaded.

2. ***Source of Data***: Defines the source of the unprocessed data. There are four options – ***Pick Files From Disk***, ***All Files in Current Window***, ***All Visible Files in Current Window*** and ***Entire Directory***.

3. ***Fill The List***: Populates the list with the source files.

4. ***Destination***: Defines the destination directory for the processed files. The ***Edit*** button (**…**) summons a browser dialog box enabling you to create or choose this directory.

5. ***Over-Write***: A check box selects whether to over-write files in the destination directory
6. ***File Type***: A drop down menu allows you to specify the format of the processed files.

Once all options have been adjusted to your satisfaction, clicking the ***Run*** button executes the currently loaded sequence.

User Scripts

Python is a programming language used in the creation of ***Essential FTIR***. The ***User Scripts Tool*** enables you to select and run Python scripts (.py files). The ***User Script*** parameters window is shown in Figure 8-99.

This document only talks about the user interface of this tool. For technical details about how to write scripts for eFTIR, a separate document named 'eftirScripting.html' is installed in the Essential FTIR program directory. That document can be viewed by clicking the 'Help' button.

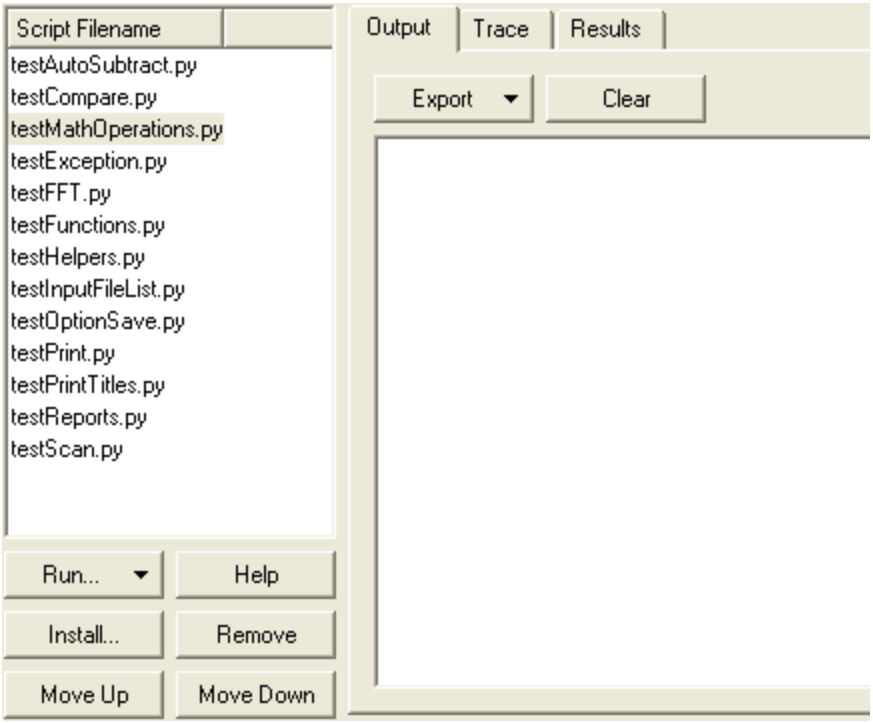


Figure 8-99 User Scripts

The screen shot above shows the sample scripts that are installed along with eFTIR.

The parameters window has six buttons. The ***Run*** button executes the currently selected Python script. The ***Install*** button is used to install a Python plug-in. The ***Remove*** button erases a script. The ***Move Up*** and ***Move Down*** buttons shift the selected script up and down the list of scripts. The ***Help*** button summons the help files for this feature.

Figure 8-99 shows the test scripts that are automatically installed with Essential FTIR. The scripts are installed as Python source code files into the 'scripts' directory, which is usually located at "C:\Documents and Settings\All Users\Documents\EFTIR\scripts.

Examining these scripts is a good place to start learning how to write scripts for Essential FTIR.

The Run button has this drop-down menu attached to it:

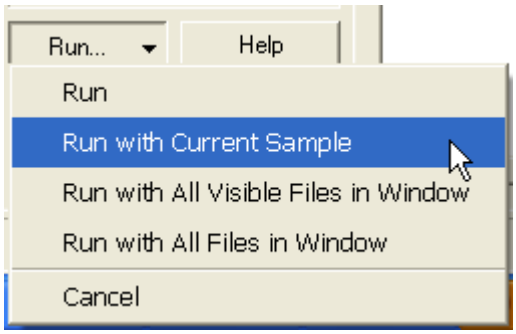


Figure 8-100

This allows selection of data that the script will act on. The affect this has, and whether or not the script requires data to be delivered to it this way, depends on how the script is written. To take advantage of passing data into the script from the user interface requires the script be written to utilize such data.

The tabs on this tool:

Figure 8-101

capture output from the script. The eFTIR_Scripting document (eftirScripting.html) tells how scripts can use this. Briefly, 'Output' captures Python 'print' statements, 'Trace' captures program trace statements, usually for debugging, and 'Results' can display data in a table format.

Calculator

The calculator provides a way to manipulate spectra quickly, easily, and directly using arithmetic and algebraic expressions.

The tool buttons are a subset of the usual buttons. In addition, there are the buttons you would see on a standard four-function calculator. The 'Data' list box lists all of the available data you can work on. The 'Functions' list box is a list of the available math functions, and the 'Final Data Type' allows changing the data type of a result.

You do not have to type anything, these buttons and lists are to help users become familiar with the calculator, but it is really much easier to just type expressions into the calculator and press the Enter key to evaluate those expressions.

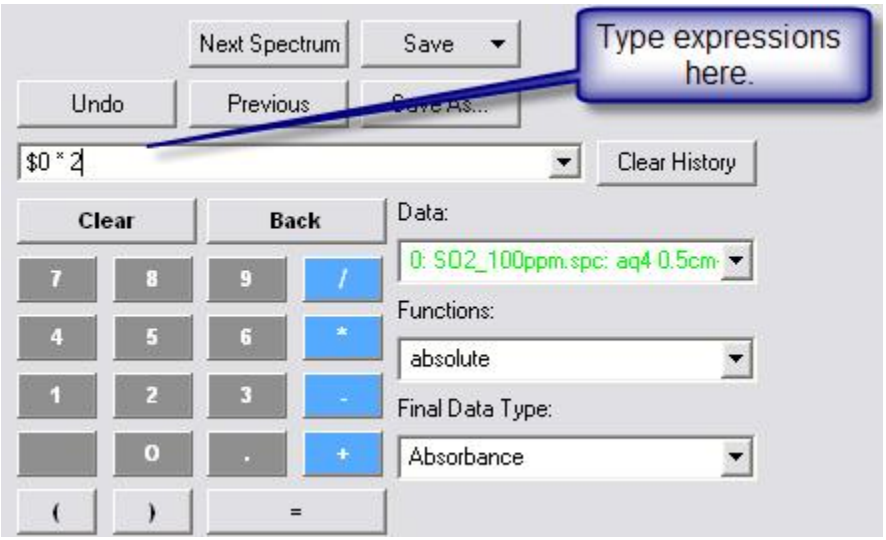


Figure 8-102 The Calculator

Referring to data in the calculator. Data is referred to by its 'index number', which is the number you see wherever spectra is displayed in eFTIR.

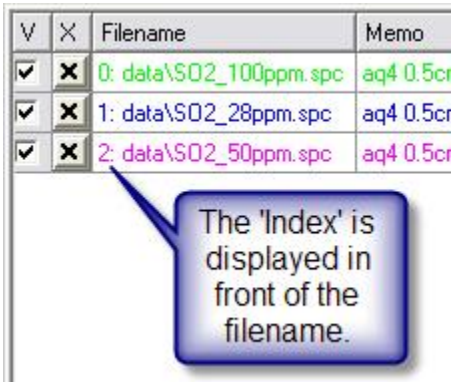


Figure 8-103

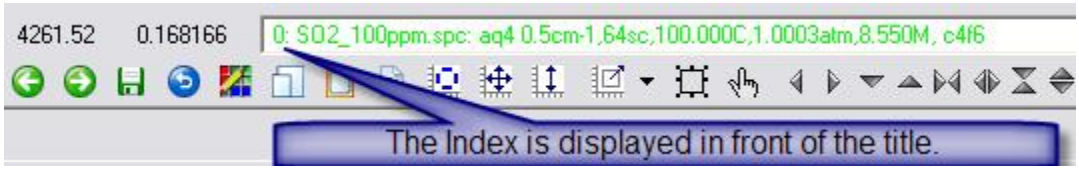


Figure 8-104

To use a spectrum in the calculator, enter '$N', where 'N' is the Index of the spectrum. For instance, type in '$0 * 2' and press the Enter key (or click on the button with the equals sign), and spectrum 0 will be multiplied by 2 and redisplayed.

The results of any expression are assigned to the first spectrum in the expression. For instance the result of '$0 * 2' will be assigned to '$0'. This is true no matter how complicated the expression is. For example '(2 * $0) / (($1+$2+$3)/3) will multiply spectrum 0 by 2 and then divide it by the average of spectra 1,2,and3, and place the result back into spectrum 0.

Undo: All calculator functions can be undone using the 'Undo' button.

Simple Arithmetic.

Numbers can be used directly:

- 2 * 2
- 3 / 4
- etc…

Spectra can b added, multiplied, and divided by, and subtracted from, other spectra.

- To multiply spectra: $1 * $2
- To divide spectra: $1 / $2
- To subtract spectra: $1 - $2
- To add spectra: $1 + $2

Entering multiple expressions. Multiple expressions can be entered in the calculator and separated with semicolons ';'. For instance, '$0 * $1; $0 * $2' will multiply spectrum 0 by spectrum 1, and then divide spectrum 0 by spectrum 2.

Applying the calculation to other spectra. Use the 'Next Spectrum' and 'Previous' buttons to increment the target spectrum of the calculation. For instance, if the expression is:
$0 * 2, and you click the 'Next Spectrum' button, the expression will be changed to $1 * 2.

Using a spectrum as a constant in a calculation. A spectrum index can be held constant in an expression by referring to it with the '#' sign instead of the '$' sign. For instance, if you want to subtract the same spectrum from a series of spectra, use the expression $0 - #10. Clicking the 'Next Spectrum' button will change the expression to $1 - #10.

Using math functions. Standard math functions are available. The functions can operate on the entire spectrum. These are the functions available now:

Standard Math Functions:

absolute	absolute($0) returns the absolute value of each element
ceil	ceil($0) returns array of elementwise least whole number >= x.
exp	exp($0) returns array of elementwise e**x.
e	2.718281828
fabs	fabs($0) returns array of elementwise absolute values.
floor	floor($0) returns array of elementwise least whole number <= x.
floor_divide	Floor divide the arguments elementwise.
fmod	fmod($0,$1) is remainder($0,$1)
log	log($0) returns array of elementwise natural logarithms.
log10	log10($0) returns array of elementwise base-10 logarithms.
min	return the minimum value in array $0.
max	return the maximum value in array $0.
multiply	Multiply the arguments elementwise.
negative	negative($0) == -x elementwise.
pi	3.141592654
power	power($0, y) : returns returns array of values in $0 raised to the yth power
remainder	returns remainder of division elementwise
sqrt	sqrt($0) returns array of elementwise square roots.
sum	Sum the array

Available Essential FTIR functions:

deriv1	take the first derivative. Optional arguments are the number of points to use in the convolution (default 5, can be 5 - 99) and the order of the polynomial (default 1, can be 0 for Quadratic/Cubic or 1 for Quartic/Quintic). examples: deriv($0) is equivalent to deriv1($0, 5, 1)
deriv2	take the second derivative. Optional arguments are the same as for deriv1
smooth	perform Savitsky-Golay smoothing. Optional arguments are the number of points to in the smoothing (default 5) and the order of the smoothing polynomial (as in deriv1).

Interpolation Rules. When using multiple spectra in a calculation, the starting and ending wavelengths and digital point spacing of spectra must match when they are used together in a calculation. If it is necessary to make the spectra compatible, this matching is done automatically. The spectra are matched to the highest resolution (minimum point spacing) of all spectra in the expression. This can have the side effect of changing the resolution of the target spectrum, but doing it this way ensures that no information is lost.

Changing the data type of the result: Set the 'Final Data Type' before executing the expression. For instance, if $1 and $2 are two singlebeam spectra, set the Final Data Type to Transmittance and then execute the expression '$1/$2'.

If you forget to set the Final Data Type: If you just enter '$0' as the expression, and choose the data type you want $0 to be, and then click the 'equals' button, the data type of $0 will be changed. This is very useful when you have forgotten to change the data type of a spectrum in a calculation; you can easily change it later.

Some examples: Some complex manipulations can be done with the calculator, including many interactive features that are built in to Essential FTIR.

Bringing the minimum of a spectrum to zero	$0 – min($0)
Normalizing a spectrum to be between 0 and 1	$0 – min($0); $0 / max($0)
Inverting data	$0 * -1
Converting transmittance to absorbance	-log10($0)
Converting absorbance to transmittance	power(10, (-1*$0))

Common Error Messages

Index out of range.	You will see this error when you use a spectrum index that does not exist. For instance, if there is no spectrum with the index '10', and you refer to $10 in a calculation, you will get this error
name 'N' is not defined	an uknown function was called: N($0)
Math domain error	Usually this is a divide by zero, or logarithm of a negative number.
unexpected EOF while parsing	Usually an incomplete statement such as '$0+'

9. Tutorial

This section is intended to aid the inexperienced user in performing a set of tasks. As with most skills, the surest way to learn is to follow along, and it is anticipated that you will grow more confident in the use of Essential FTIR after completing this tutorial. We will work through various common procedures - acquiring data, correcting the spectra for contamination and baseline defects, analysis of the spectrum and the building of a batch-sequence for the automated processing of a directory of similar files. While following along, you may wish to substitute alternative values for some of the parameters. Understanding of the ***Tools*** employed in this section will be enhanced by observing the results. The spectra acquired for use in this section are supplied with this manual, and it is suggested that you begin to follow along immediately after the data acquisition section.

The screen shots in this tutorial were generated using an earlier version of Essential FTIR, but the changes are mostly cosmetic and do not impact the actions outlined here.

Data Acquisition

The first step in any analysis is to ensure that the spectrometer used has adequate throughput, and to diagnose any issues that may exist with the hardware. This task is accomplished using the ***Align*** screen, shown .

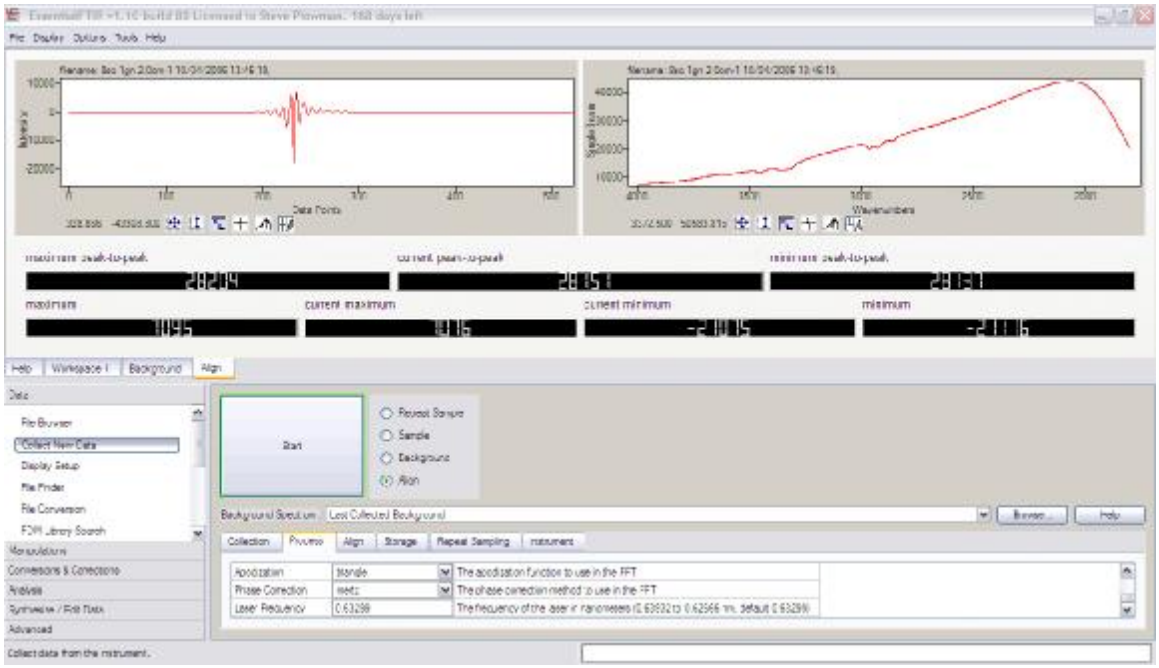


Figure 9-1 *The* Align *Screen*

The ***Align*** screen is viewed by selecting the ***Collect New Data Tool*** from the ***Data Toolbox***, then selecting the ***Align*** tab from the parameters window. In this example the instrument is scanning at a resolution of 0.5cm^{-1}.

Note the numbers visible between the display windows and the parameters windows. These numbers relate to the magnitude of the interferogram produced by each scan. Looking at the top row of the numbers, the values indicate the maximum peak to peak value of the interferogram magnitude, the current value and the lowest value. The bottom row of numbers indicate the maximum (positive values), current maximum, minimum (negative values) and minimum.

Once satisfied that the instrument is functioning correctly, the next stage is to take a background spectrum. The procedure for this step will vary, according to the instrument and sampling technique employed by the user. In our example we have used a 10 meter gas cell, which was purged with dry nitrogen – as a homo-nuclear diatomic molecule, N_2 is invisible to infrared radiation.

Once the cell was purged, the radio button labeled ***Background*** was selected, and the ***Start*** button was pressed. Note that the ***Start*** button changes from green to red upon beginning data acquisition, and the ***Start*** label changes to ***Stop***. The acquisition may be terminated at any time by pressing this ***Stop*** button. The background was taken at 0.5cm^{-1} resolution, using 8 co-added scans, over the wavenumber region 4000cm^{-1} to 1800cm^{-1}. The result is shown in Figure 9-2.

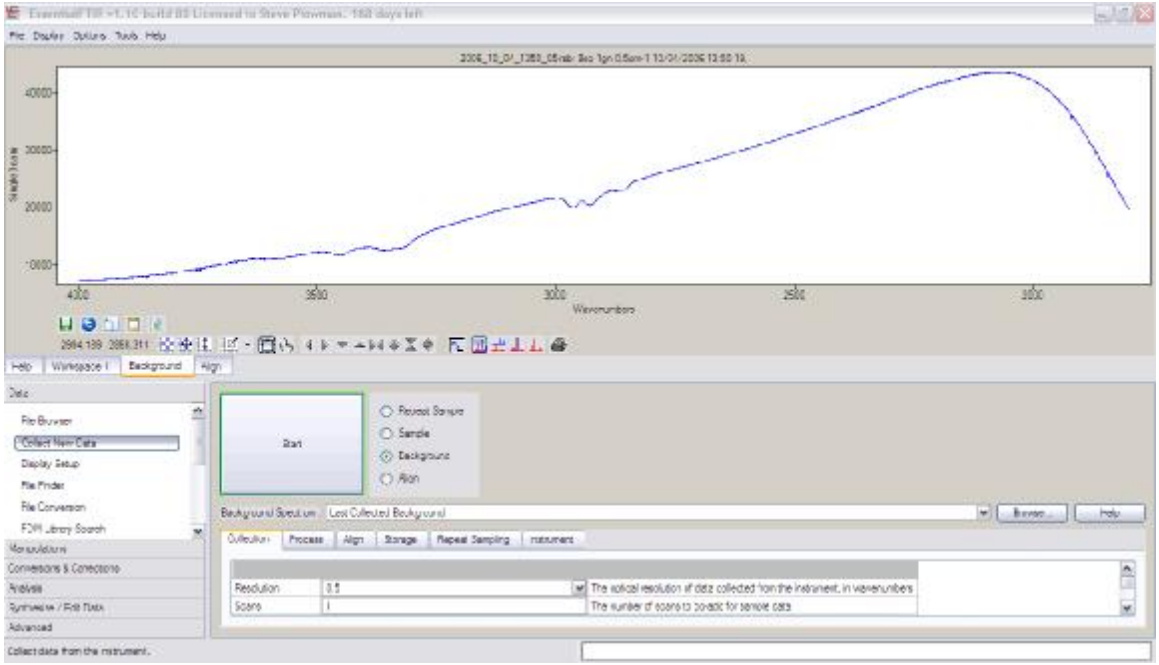


Figure 9-2 *Background spectrum*

After viewing the background spectrum, and ensuring that it appears free of contamination, the radio button labeled ***Sample*** was selected. The target analyte used for this example was carbon dioxide, at a concentration of 18%, in nitrogen balance gas. Sample gas was

introduced to the gas cell at a flow rate of 1.5lmin^{-1}, and the ***Start*** button was pressed. Once satisfied that the absorbance spectra were being generated correctly, the radio button labeled ***Repeat Sampling*** was selected, and the ***Start*** button pressed. A spectrum from the ***Repeat Sampling*** stage is shown in Figure 9-3.

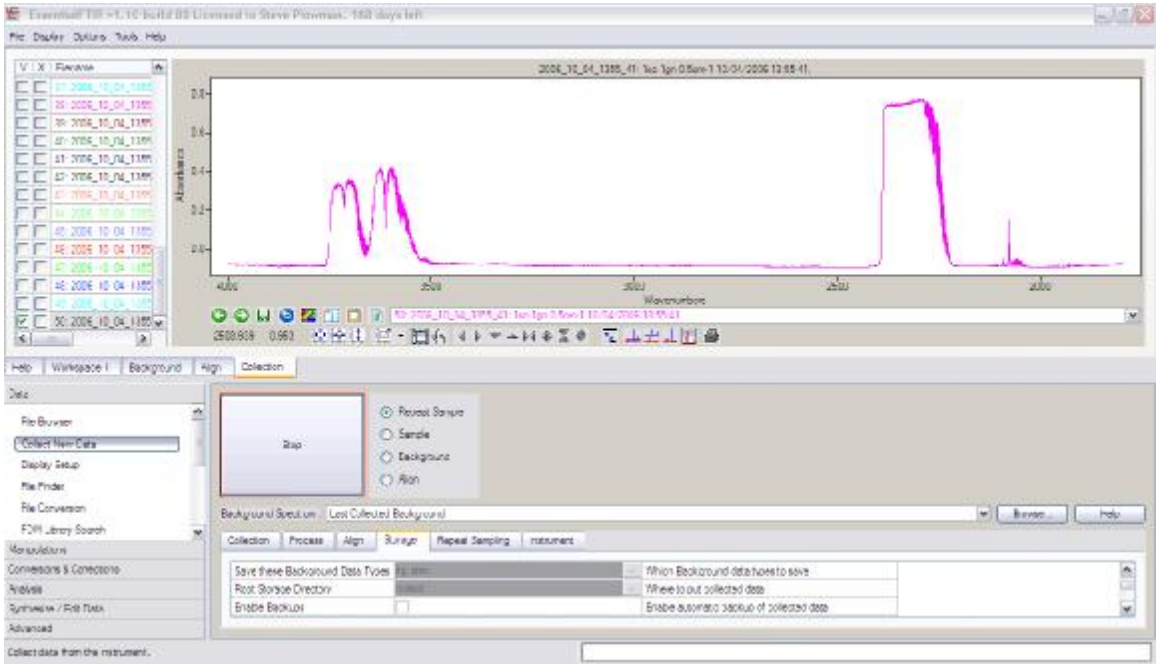


Figure 9-3 Repeat Sampling

The acquisition will now run as specified in the ***Repeat Sampling*** parameters window, on the lower right of Figure 9-3. These parameters, along with all others involved in data collection, are discussed in detail in chapter four. In this example, the check-box labeled ***Sample Forever*** was checked, and the run continued until manually terminated using the ***Stop*** button. We now have some data to work with. Let's explore the absorbance spectra further.

Processing the Data

Now that we have some data, the first step is to ensure that it is representative of the target analyte. Ideally, with perfectly clean samples and a baseline that never drifts, this would not be necessary. In the real world, baselines do drift over time, and samples do contain contamination. If the spectrum is to be used as a quantitative standard, any impurities could bias results low when looking for the contaminant as a target analyte. If, when recording such reference spectra, you are unsure regarding which spectral features are foreign to the target analyte, the surest corroboration is to pull up a library spectrum of that compound and compare the two qualitatively.

Turning to our data, let's load the first absorbance file in the collect directory, with the filename *2006_10_04_1353_46.abs*. This filename indicates that the collection parameters

specified ***Time and Date Stamped*** for the acquisition, and that the collection began in 2006, on October 4th, at 1353 hours and 46 seconds, as measured by the clock on the data collection computer. Using the ***File Browser Tool*** in the ***Data Toolbox***, navigate to the directory holding the files and click once on the file. The file will be displayed in the preview window at the lower right of the screen. Once satisfied that the correct file is selected, click the ***Add to Current Window*** button. This action will load the file into the ***Workspace***. The ***Workspace*** display window showing the file is pictured in Figure 9-4

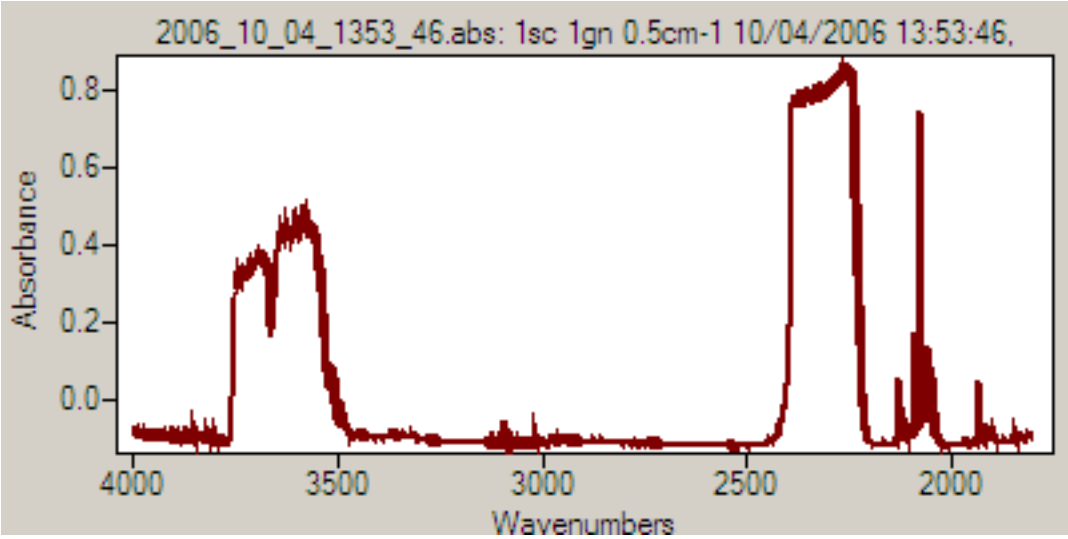


Figure 9-4 Workspace *display showing spectrum* 2006_10_04_1353_46.abs

Figure 9-4 was generated using the ***Export Graphics Tool***, located in the ***Data Toolbox***. The first thing to notice is that the baseline appears sloped. This gradient is most pronounced at the edges. Secondly, some water contamination is evident, particularly at the left and center portions of the spectrum. We will remove this contamination using the ***Zap*** Tool from the ***Manipulations Toolbox***.

Selecting ***Zap*** from the ***Manipulations Toolbox*** delivers the screen shown in Figure 9-5.

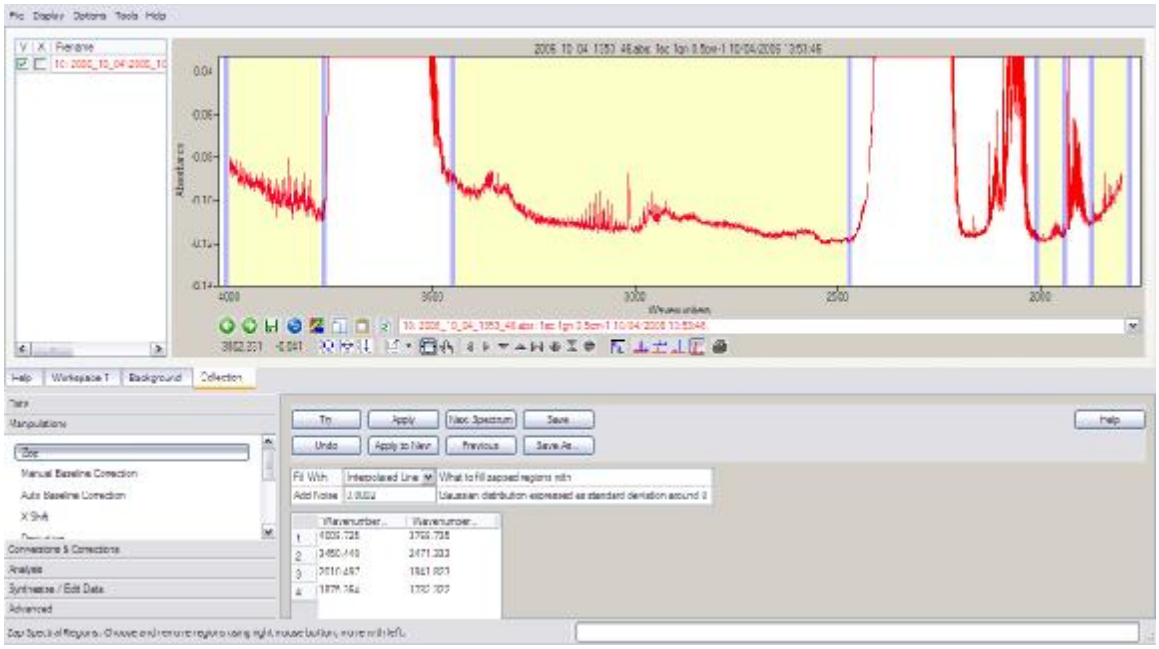


Figure 9-5 Zap *parameters for 18% CO_2*

The baseline is zoomed to show the ***Zap*** sections clearly. The ***Regions*** selected for the ***Zap Tool*** are displayed graphically on the data display, and numerically on the ***Regions*** window toward the lower left of the screen. For a full discussion of ***Regions***, please see chapter three. Once you have defined these ***Regions*** (or similar ***Regions***, feel free to experiment, the Undo button is always available) then we may save them as a ***Regions*** file. Right click on the numeric ***Regions*** window, and select the ***Save Table*** option from the context menu. Note that this menu is also available by left clicking on the ***Wavenumber*** column heading of the ***Regions*** window. Now that the ***Regions*** are saved, we may call them in to use as a set when building automated ***Sequences***. We will save ***Regions*** for all operations we perform on this spectrum, so that we may automate the process for the remainder of the data in the directory.

Clicking the ***Try*** button results in a gray "ghost" spectrum showing the potential results of the operation. In our example, the ***Interpolated Line*** option is used, and noise has been added to the data at a level of 0.0015 absorbance unit, which was a value that closely resembled the actual noise level. This method of noise approximation is a useful semi-quantitative way of evaluating noise in a baseline. Clicking the Apply button performs the operation, as shown in Figure 9-6.

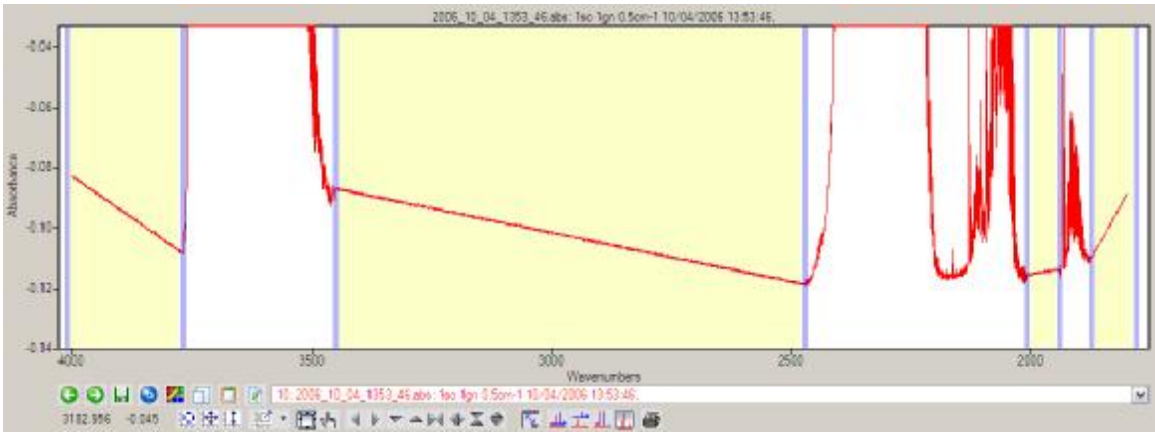


Figure 9-6 *Zapped CO_2 spectrum*

Now that we have removed any unwanted absorbance, we may address the baseline defects introduced by the ***Zap*** process. In this example, let's use the ***Manual Baseline Correction Tool***, which is found in the ***Manipulations Toolbox***.

The ***Manual Baseline Correction Tool*** uses the parameters screen shown under the data display in Figure 9-7.

Figure 9-7 Manual Baseline Correction

The gray spectrum shows the result of applying the ***Regions***. Again, use the ***Try*** button to experiment with ***Regions*** – remember that the object is to ensure that all portions of the baseline that should be at zero on the ***y***-axis are at zero. Zoom in on portions of the spectrum by left-clicking and dragging a box in the data display, and zoom out by double-clicking. Once satisfied, click **Apply** to perform the operation. Save the ***Regions*** with a different name to those used for the ***Zap*** operation.

Automating the Processing Steps

Now that the spectrum has been corrected, let's build a sequence to automate the procedure for the rest of the data in the directory. Select the ***Advanced Toolbox*** from the ***Toolbox Selection Window***. The first item on the list is the ***Batch Processor***, discussed in detail in

chapter five. Click the ***Create Sequence*** button to summon the sequence editor dialog box. Press the ***Remove All*** button on the right side of the dialog to clear the sequence. Now we need to add in the operations we wish to perform on the spectra. First, highlight the ***Zap Regions*** item on the browser window on the left of the dialog. Pressing the ***Add to Sequence >>*** button will now place the operation in the sequence editor window.

Notice the tabs at the bottom of the dialog, labeled ***Settings*** and ***Regions***. First select the ***Regions*** tab, and click the ***Load Region Table*** button. Select the appropriate table from the browser and click ***Open***.

Next, select the ***Settings*** tab. As before for the ***Zap Tool***, we will choose ***Interpolated Line,*** and a noise level of 0.0015 absorbance units. The first step is now configured. Figure 9-8 shows the sequence editor window for the ***Zap Tool***.

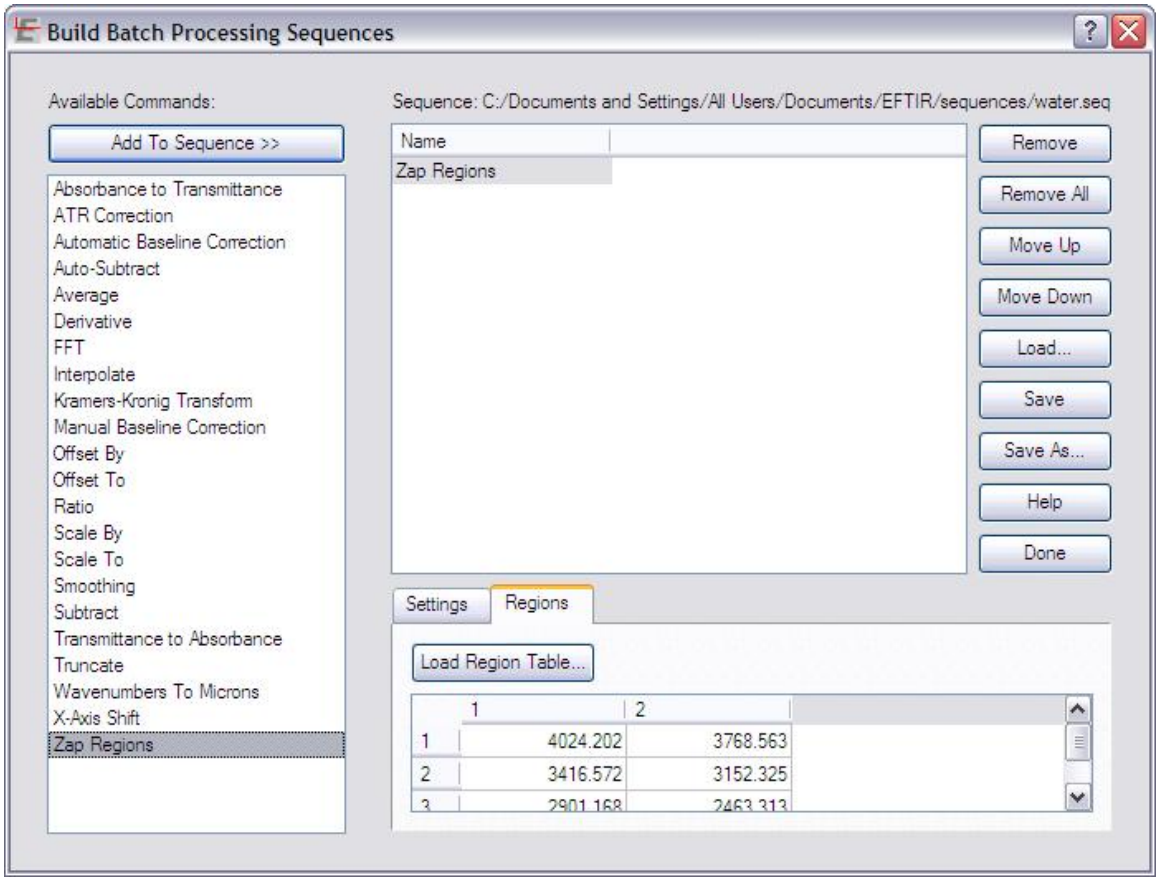


Figure 9-8 *Sequence editor window*

Now we must configure the ***Manual Baseline Correction Tool*** for the automated sequence. As before, select the ***Tool*** from the list on the left, and press ***Add to Sequence***. We should then load the appropriate ***Region*** table, which we saved while performing the operation manually. Once this is done, press the ***Save As*** button to save the sequence file. Clicking ***Done*** will then dismiss the dialog.

We have now configured our sequence. We must now tell ***Essential FTIR*** where to find the data we wish to process, and where to put the processed files. Figure 9-9 shows the options for the ***Batch Processor Tool***. In this example we have opted to ***Pick Files From Disk***, which summons an "open file" dialog, which we use to browse to the files of interest. If files of different type are available in a directory, e.g. absorbance and interferogram data, then they may be filtered using the ***File Type*** drop down menu on the dialog. Select the files you wish to process (*Shift*-Clicking the first and last files will select all). Press the ***Open*** button on the dialog to open the files. Clicking the ***Click to Fill*** button populates the list at the bottom of the screen, which shows the files to be processed.

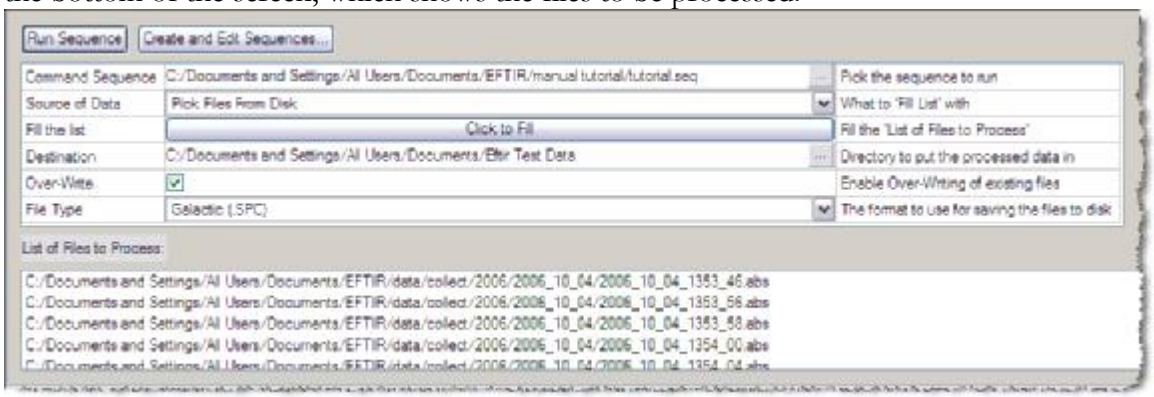


Figure 9-9 Batch Processor *options*

We tell the program where to put the files using the ***Destination*** option. The Destination button summons a dialog used to navigate to, and / or create a destination directory. Set the options you desire with regard to final file type and over-writing, and we are ready to go.

After ensuring that the correct sequence is loaded by inspecting the ***Command Sequence*** option, clicking ***Run Sequence*** will execute our process. While the ***Batch Processor*** is running the window shown in Figure 9-10 will appear.

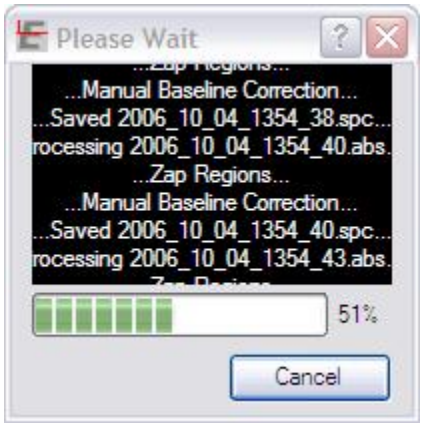


Figure 9-10 *Running the* Batch Processor

Once the indicator reaches 100% the window will be dismissed and we may browse our results. Let's load up a file from the result directory and take a look. Figure 9-11 shows the result spectrum with the filename 06_10_04_1356_06.spc

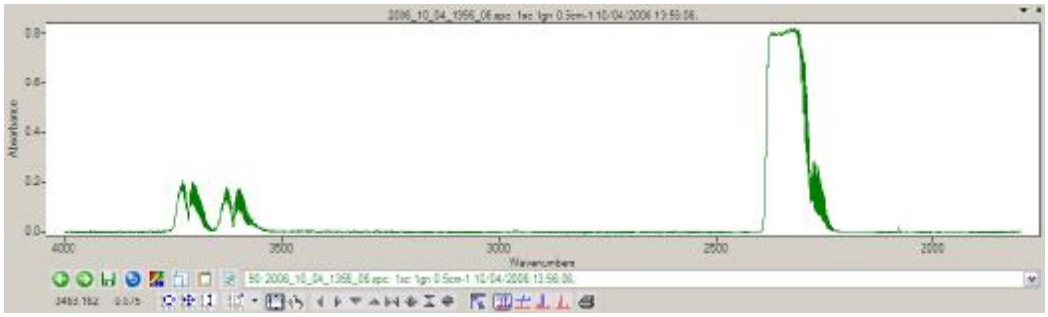


Figure 9-11 *Result of batch sequence*

The sequence has removed the interfering absorbance, and corrected the baseline defects. As a final stage, let's analyze this carbon dioxide spectrum in more detail.

Select the ***Analysis Toolbox*** from the selection window, and choose the ***Integrate Tool*** from the list. This ***Tool*** will allow us to assign a rigorous numerical value to the area under an absorbance feature. The parameters window, together with the ***Regions*** chosen, are shown in Figure 9-12.

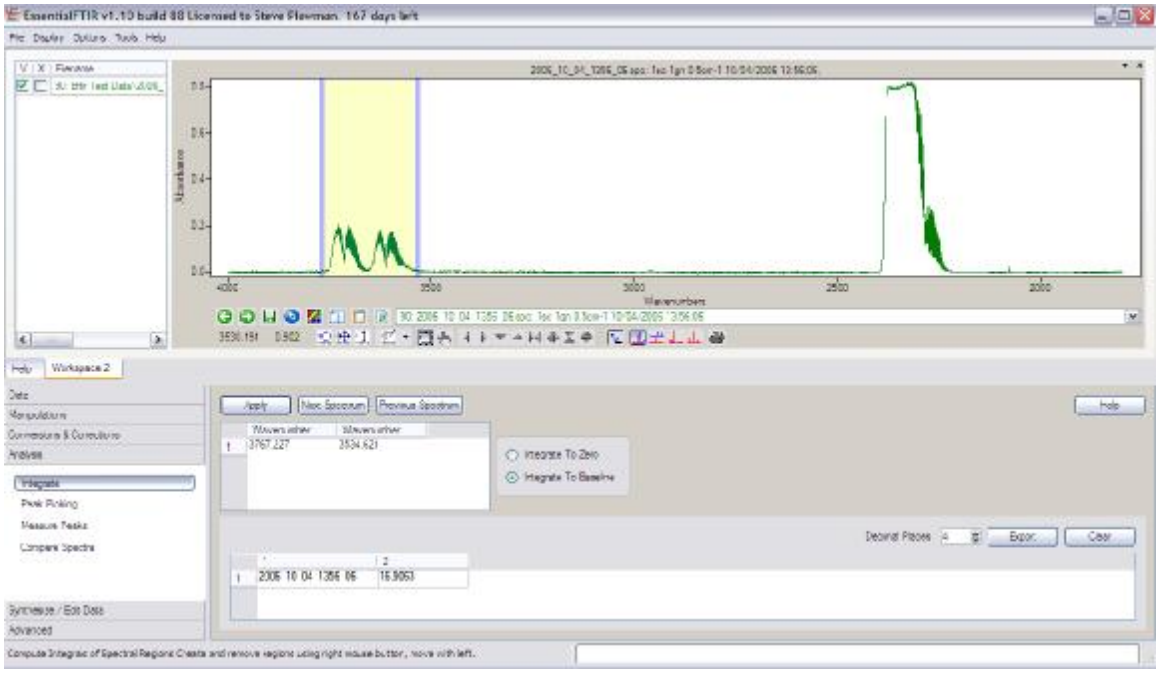


Figure 9-12 *The* Integrate Tool

Select the areas bordering an absorbance feature as a ***Region***. In this example, we have chosen to ***Integrate to Baseline***, but now that the baseline is corrected, this should be equivalent to using the other option, ***Integrate to Zero***. Clicking ***Apply*** shows the filename and the numerical value of the integral in the lower spreadsheet window. This data may now be transferred to another program, using the ***Export*** button.

Essential FTIR is a potent tool for the acquisition, manipulation and analysis of infrared data. The software boasts many features, all of which will show their value over a long period of use. The new user should feel free to experiment with the different ***Tools*** and options in order to become more familiar with the capabilities of the software.

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