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Win-IR Pro System Reference Manual

091-0834H

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Preface

ABOUT THE DOCUMENTATION

This book, the *Win-IR Pro System Reference Manual* (Bio-Rad part # 091-0834), explains:

- the basic concepts of the Win-IR Pro system, including the screens, document types, spreadsheets, etc.
- how to use the menus and menu entries to process data that you have collected or have imported into the Win-IR Pro system

It also covers adding new accounts to your PC, importing data collected on other systems, and other relevant tasks.

The README.RTF file contains updates made since this book was printed. It is installed in C:/Program Files/Win-IR_Pro. Use WordPad (supplied with Windows NT 4.0) to open and read this. Print a copy of this file and store it with this manual for future reference.

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The *Win-IR Pro Installation and Configuration Manual* (091-0837) tells about the PC that is used to control the spectrometer and the printers that are supported by the software.

Each spectrometer supported by Win-IR Pro has its own manual covering hardware, site requirements (power, purge gas, cooling), maintenance, data collection, and similar topics. This manual is supplied with the spectrometer.

Typographic conventions

Text in this font indicates a

- a box label
- a choice from a menu
- an item to be typed in

Context and specific instructions tell you which it is.

Text in small caps are keyboard keys; for example, NUMLOCK.

Key combinations, written as CTRL+A means press and hold the CTRL key, and then press the A key. Release them at the same time.

Note

Unless it is otherwise specified, you may use either upper-case or lower-case letters.

WHAT YOU SHOULD ALREADY KNOW

This book assumes that you are familiar with the basic features and operations of Microsoft Windows NT on your PC. In particular, you should know :

- how to start Windows NT on your PC
- choosing
- clicking
- double-clicking
- dragging

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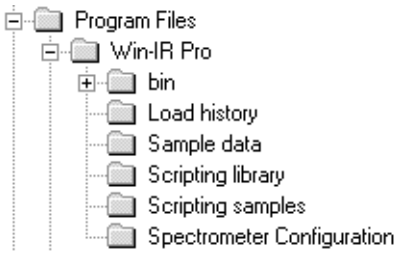
- formatting disks
- copying files
- Task bar
- Windows NT Explorer

If you are not familiar with these concepts, review the Windows NT documentation that you received with your Windows NT software.

INSTALLATION

The Windows NT and Win-IR Pro software are installed at the factory by Bio-Rad. If you need to re-install Windows NT, follow the instructions that came with the Windows NT disks. You should reboot your PC after installing, or re-installing, Win-IR Pro.

The Win-IR Pro software is in the Win-IR_Pro sub-directory of the Program Files directory as shown below.



bin	contains the executable files and other files necessary to run Win-IR Pro
Load history	contains records of the installation process. They are mostly of use to Bio-Rad Customer Service.
Sample data	contains a number of spectra that you can copy and use to practice working with Win-IR Pro. They are identified in the Appendix H.
Scripting library	contains software and files necessary for the execution of the scripting language.
Scripting samples	contains a number of examples of scripts that you can copy and use for development of your own scripts.
Spectrometer Configuration	contains software and files defining the hardware configuration of the spectrometer.

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Use the Folder subentry in the New entry in the File menu in the Windows NT Explorer to create your own directories to store the data that you collect. Do not store your files in the Win-IR Pro directory or in its sub-directories; the contents of these directories can be altered by Win-IR Pro software installations.

If you need to re-install Win-IR Pro, follow the instructions in the *Win-IR Pro Installation and Configuration Manual* (091-0837).

CUSTOMER SUPPORT

If you have a problem concerning Win-IR Pro that is not addressed in the accompanying documentation, please call or fax us at:

Tel: 1-800-333-4246 (U. S. only)
1-617-234-7086
Fax: 1-617-234-7188

or write to us at:

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Training

Training courses are available at the Bio-Rad Digilab Division headquarters in Cambridge, Massachusetts, on a periodic basis. These courses are most valuable after you have working experience with your instrument. Upon completing the course you will be able to operate the instrument at an advanced level.

Bio-Rad maintains an application laboratory to conduct a continuing effort in methods development. The laboratory can help as users as they explore new techniques with which they are unfamiliar. Application Laboratory personnel also provide information regarding technical advances in the FT-IR field. Bio-Rad encourages users to feel free to communicate with this group, as your input can be valuable to us in determining how we can best serve you.

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There is a Users' Group to further technical exchanges. Bio-Rad holds the National Users' Group Conference every summer at Cambridge, Massachusetts, headquarters of Digilab Division. On a more irregular basis, Regional Users' Group conferences are also held. Information pertaining to these conferences are mailed to all customers well in advance of the conference date.

For details on any of the above topics, contact your local Bio-Rad office or call Bio-Rad Digilab Division Headquarters in Cambridge, Massachusetts:

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1
Basic Concepts and Operations

BASIC CONCEPTS

In this chapter we define and discuss the basic concepts of Win-IR Pro.

Win-IR Pro: Bio-Rad's software package that allows you to collect spectra, to manipulate them, to perform quantitative analyses, to search libraries for spectral identification, and to print these spectra, reports, etc. To start Win-IR Pro, from the Taskbar, select Start / Programs / Win-IR-Pro (Common) / Win-IR_Pro. Win-IR Pro follows the Windows NT standards for both local and network use. Networking is integrated into Win-IR Pro.

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Windows NT allows multiple copies of Win-IR Pro to be memory-resident at the same time. Because Win-IR Pro controls the spectrometer, it is not desirable to have more than one copy resident in memory. To see how many copies are memory resident, look at the Taskbar to see if there is duplication.

If there is more than one copy, put the cursor on the one to be closed and click the right mouse button to get this menu.



Select Close to stop that copy of Win-IR Pro. See your Windows NT documentation for more details, if required.

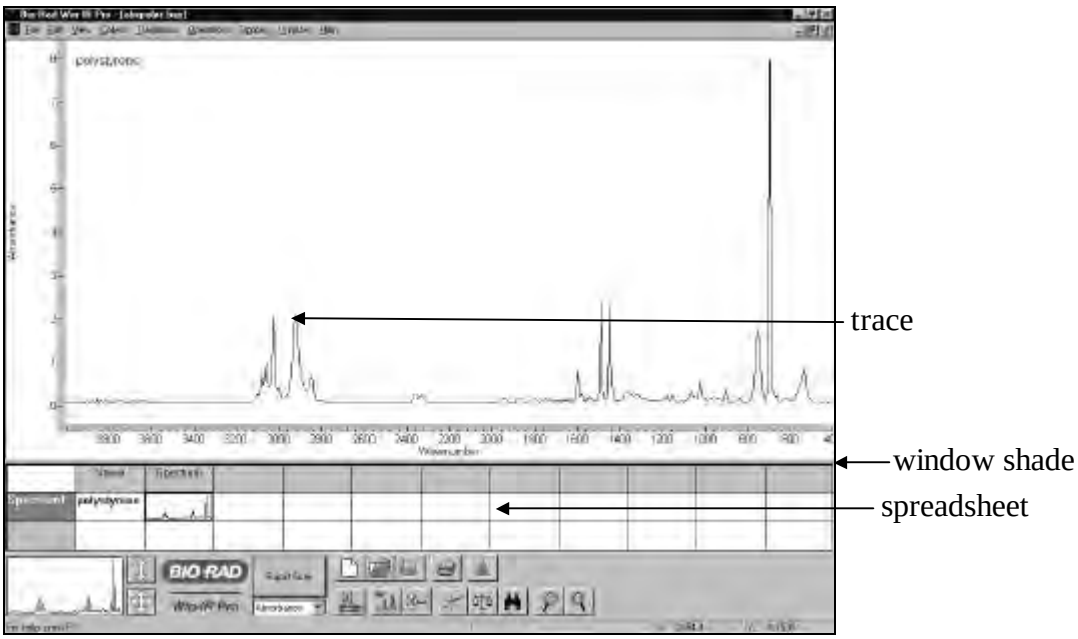
Screen: the sum of all text and graphical information visually presented to the user on the computer monitor. It may also refer to the physical part of the monitor on which this information is presented.

Cursor: The cursor (sometimes called a pointer) is a visual indication of what you are pointing to. It moves as you move your mouse. The appearance of the cursor changes depending upon where in the document you are pointing, what document you are into, what options you have selected, etc. These changes are described in the sections which discuss the Win-IR Pro functions they are associated with.

CAUTION
The Windows NT cursor must be set to Windows Default for the Win-IR Pro cursor to assume the proper shapes. If your cursor does not behave as described in this manual, it is likely that the Windows NT cursor has been changed. See Chapter 16 for details of restoring the Windows NT cursor to its default setting.

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Document: The document is the basic building block of the Win-IR Pro system. Documents can contain one or many spectra. When a document is opened the information contained within it can be presented as traces on a display window, a spreadsheet, or both. Each spectrum has a trace, a spreadsheet row, and associated properties and history. For example,



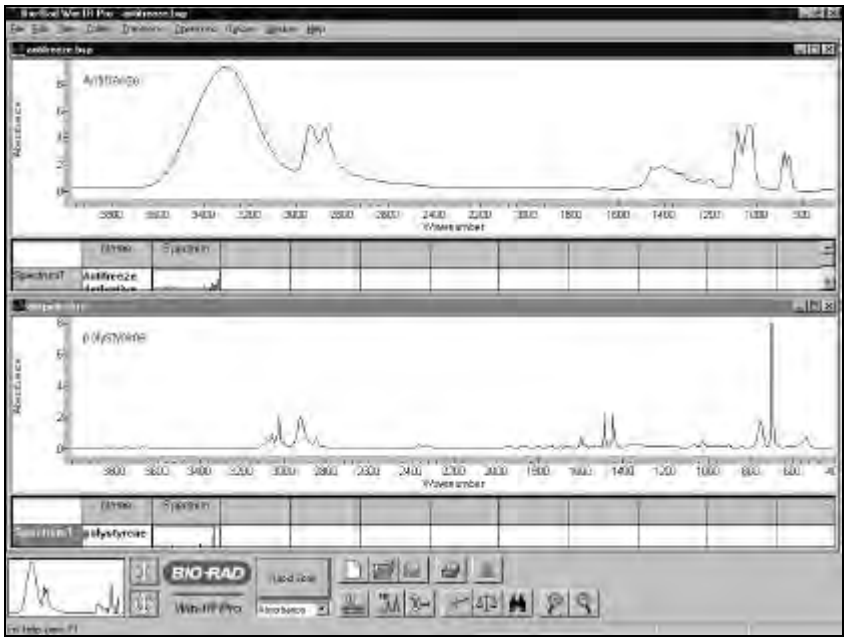
Note

See Chapter 3 for a complete description of this screen and its components.

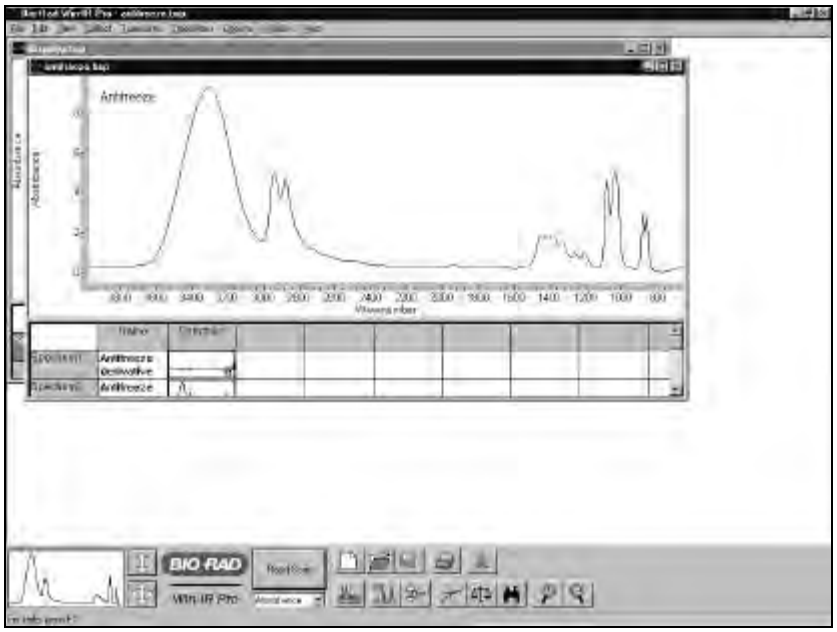
There is a multiple document interface; that is, more than one document can be open at one time. This makes it possible to easily transfer data between documents.

Because Win-IR Pro adheres to Windows NT standards, the document windows can be moved and resized in the normal manner. Document windows can also be tiled horizontally

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or cascaded using the Window menu (see Chapter 13 for details).



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File: The portion of the computer disk memory in which the document is stored. Files are accessed by name. Each file is a document. Existing files are opened by selecting Open from the File menu. New files are created by selecting New from the File menu. See Chapter 4 for details. Windows NT allows you to have filenames longer than eight characters; see your Windows NT documentation for details on filenames, restricted characters, etc.

Note

Do not use the character **[** or the character **]** in file names. Win-IR Pro uses these square brackets internally to indicate subfiles.

Do not use file names with embedded periods, for example, liquid.37.bsp.

Directory: A directory may be thought of as a special kind of file which contains other files and/or directories (often called sub-directories).

Note

Do not use the character **(** or the character **)** in directory names. Although Windows NT supports the use of these characters, Win-IR Pro does not. Using parentheses in directory names will make some transforms inoperative.

Create directories to store your files. Do not store them in the Win-IR Pro directory or its sub-directories; their contents are subject to change by Bio-Rad.

Spectrum: A set of number pairs representing the wavenumber and intensity at that wavenumber. Less rigorously, spectrum may be used for any set of data pairs with even X-axis spacing, such as interferograms. Trace (see below) is a somewhat more general term.

Properties: The data items of a spectrum, including the spectrum data set itself, the spectrum history, and derived and user input. Collect conditions are properties primarily for data imported from the 3200-series; otherwise, they would be sub-properties of history. You can see these properties by selecting Property Browse Bar from the View

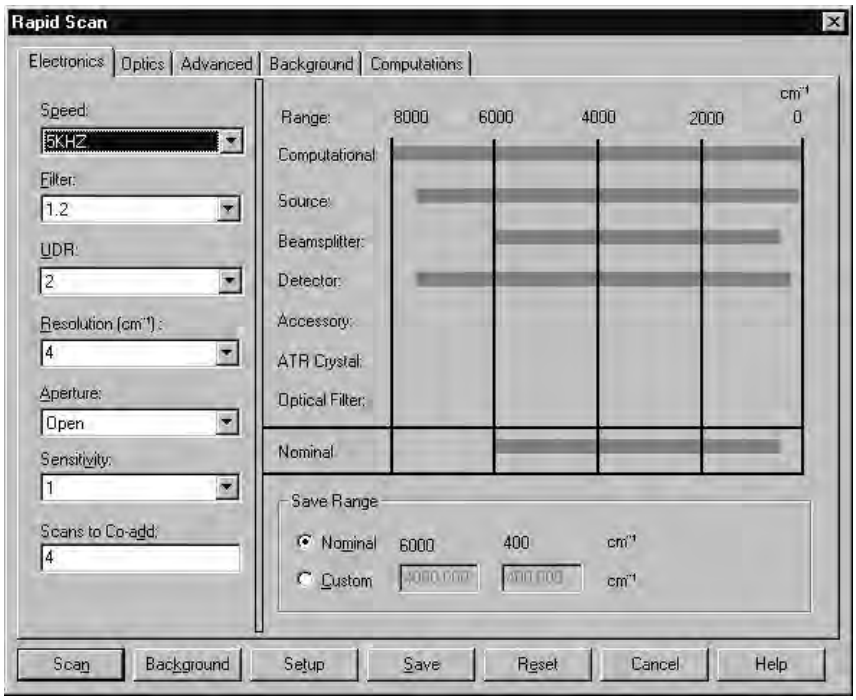
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menu (Chapter 8). You can add properties to the spectrum using the right mouse button as described later in this chapter.

History: A record of the conditions under which the spectrum was collected and of any subsequent manipulations or modifications of the spectrum. You can see the history by selecting History from the View menu (Chapter 8), or by double-clicking in a history cell in the spreadsheet.

Tab Pages: Sometimes there is more information, choices, or entries than can be clearly and conveniently presented in one dialog box. In this case, closely related items are grouped together in a special kind of dialog box called a tab page. You can rapidly go from one page to another by clicking the tab with the desired page label. You can think of these tabs as the tabs on file folders or index cards; they serve the same purpose.

An example—the Rapid Scan dialog box—is shown below. The tabs are Electronics, Optics, Advanced, Background, and Computations. Each tab is attached to the corresponding page. Clicking a tab brings its page to the front; you can then view and/or alter entries as required.



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Spreadsheet: Presents information about each trace in the document in a two-dimensional array. Each row in the array represents information for a particular trace. Each column presents a particular piece of information about that trace, that is a property or sub-property. The left-most column is the **ID column** or **Spectrum ID**.

The spreadsheet is discussed in detail in Chapter 4.

TRACE

Trace: The trace is the display of the spectrum on the monitor screen. Colloquially, this may also be spoken of as the spectrum.

Zoom: Zooming is the magnification of a portion of a trace. You can select portions of the spectrum to view in the main window, or with the Radar Box, described below.

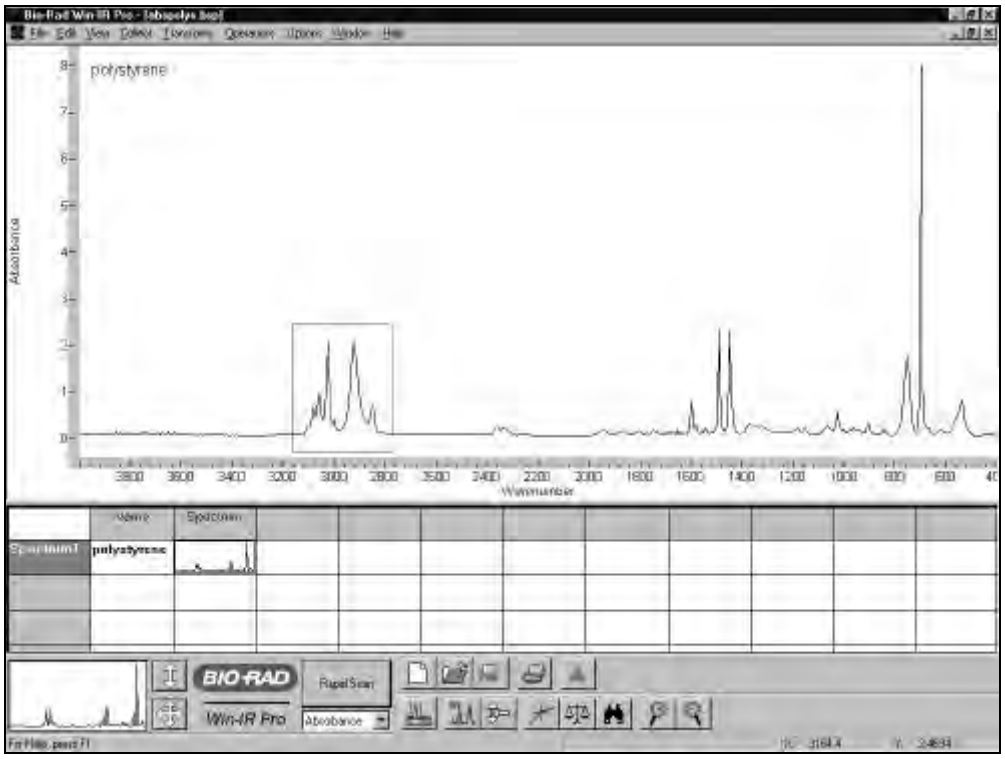
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Normally, when the cursor is not on the trace it looks like ; use the cursor to alter the position and the portion of the trace that appears in the trace display.

Note

If the cursor is placed on the trace, the magnifying glass disappears; the cursor is then used to scale the trace, not zoom it.

Place the cursor at the corner of a rectangle that outlines the portion of the spectrum you want to display. Hold down the left mouse button and draw the rectangle.

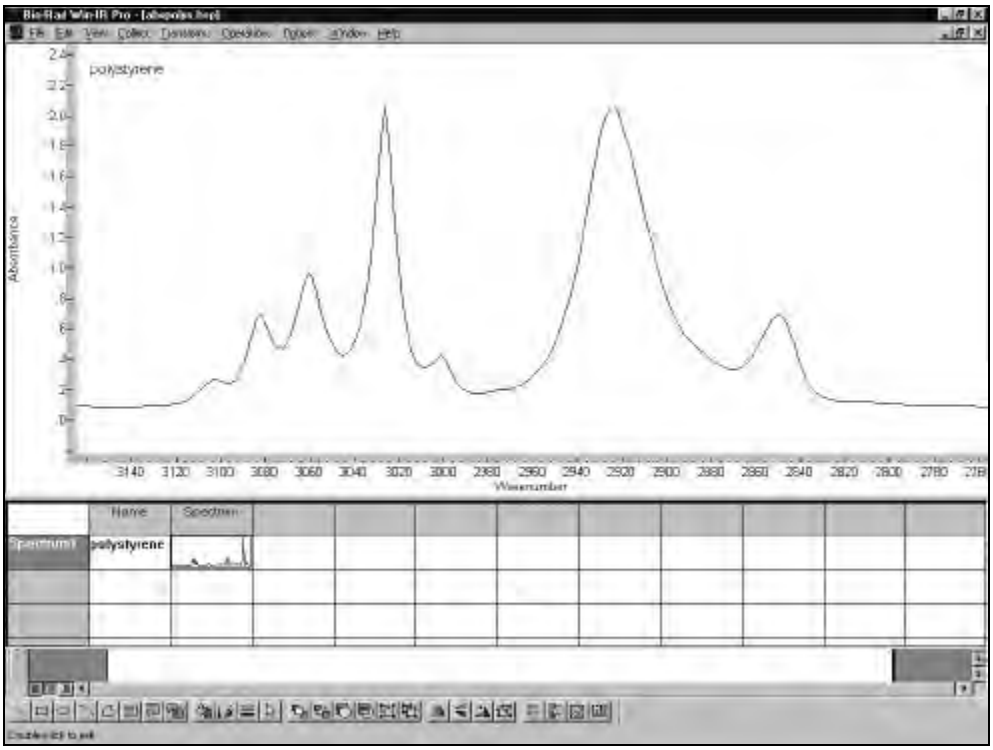


Release the mouse button. The display immediately changes.

Note

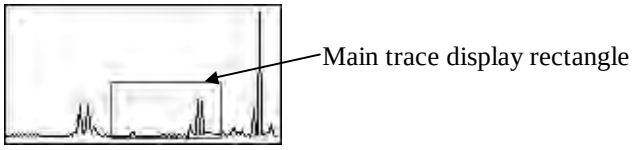
If you want to abort the zoom, draw the rectangle so that it is smaller than about 5 mm on a side. When you release the mouse button zooming will not take place.

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The radar box (lower left) also reflects the change in the display.

Radar Box: The radar box is at the lower left of the window. It displays the entire spectrum, independent of what portion of the spectrum is displayed in the main trace window. The main trace display rectangle shows the portion of the spectrum shown in the main display. If you change the main display by zooming, autoscaling, altering X (and/or Y) limits, this rectangle will change to reflect what is visible in the main display.

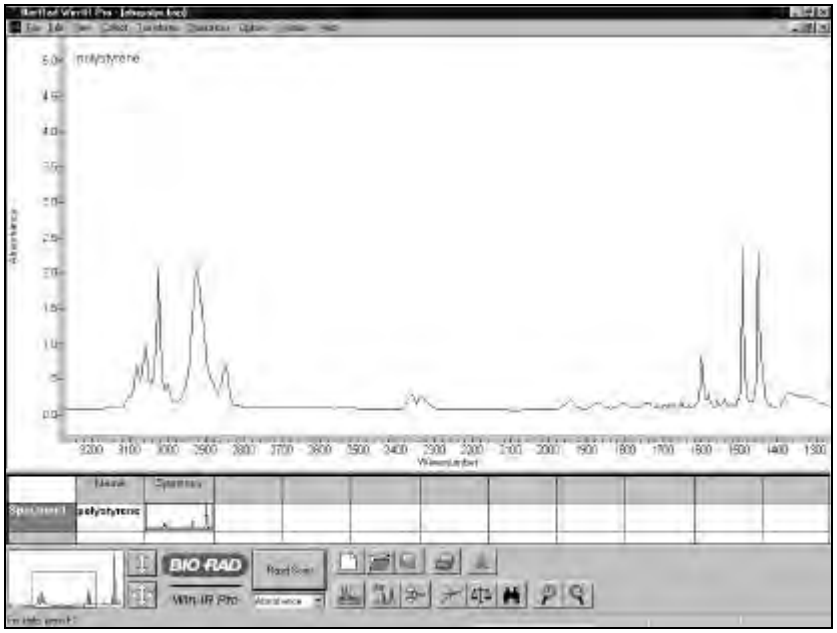


Note

If more than one spectrum is selected, the radar box will display the last one that was selected.

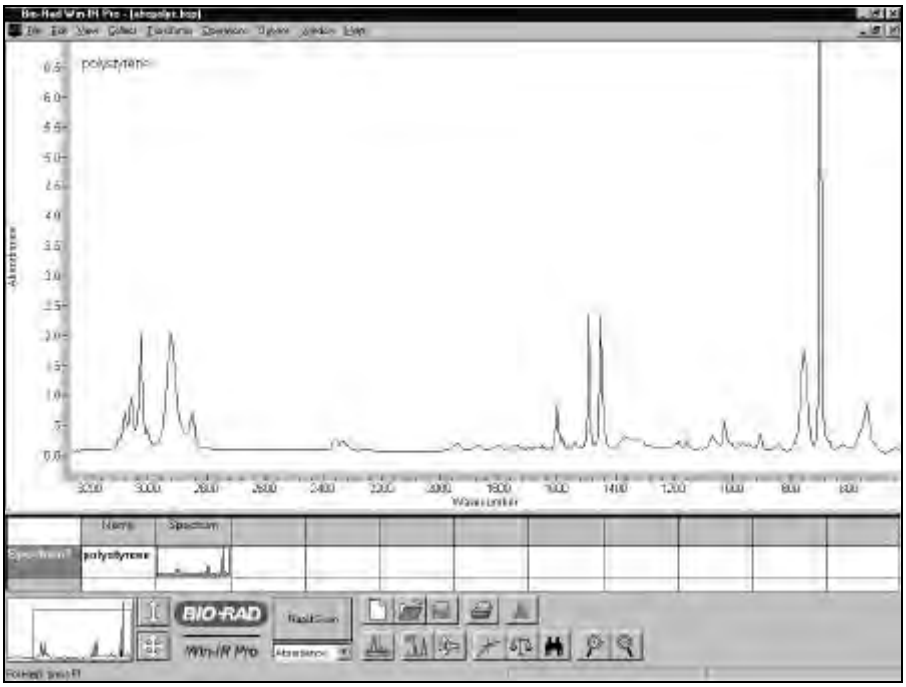
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Zooming with the radar box: Place the cursor on the edge of the main trace display rectangle in the radar box. The cursor will change to ⇔ at the vertical edges, ⇕ at the horizontal edges, and ⤡ or ⤢ at the corners. Hold down the left mouse button and drag the edge of the rectangle; the main display changes as you modify this rectangle. Release the mouse button to stop altering the display. In the example below, the main trace display rectangle in the radar box was altered; the main trace display shows this change.



Scrolling with the radar box: Place the cursor inside the main trace display rectangle in the radar box. The cursor will change to ✥. Hold down the left mouse button and drag the rectangle; the main display changes as you drag this rectangle. Release the mouse button to stop altering the display. In the example below, the main trace display rectangle in the radar box was dragged; the main trace display shows this change.

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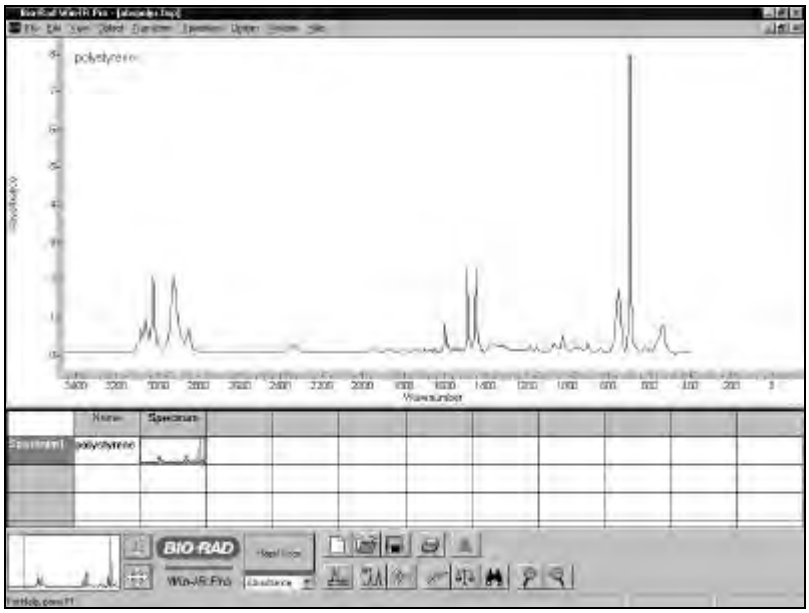
Note

You can move the main trace display box so that none of the spectrum is visible in the main display. The easiest way to recover from this is to click the button.

X-Axis

X-axis Scroll: Scrolling is the movement of the trace with respect to the window (it can also be considered as moving a window about the trace to view portions of the trace). Place the cursor in the middle third of the X-axis ruler; the cursor changes shape to ⟺. Hold down the left mouse button and move the cursor along the X-axis ruler. The trace and the X-axis ruler will move with the cursor. Release the mouse button when you are satisfied with the new position of the trace. In the example below, the trace has been shifted to the left.

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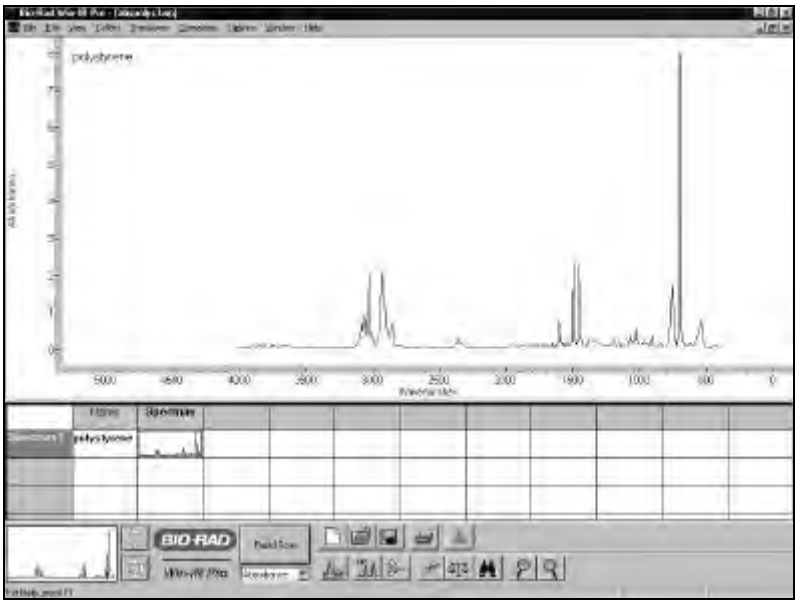


Note

In three-dimensional views, the cursor also changes as described above. However, its use there is not recommended, use the other methods described for that particular view.

X-axis Expanding/Compressing: In this procedure, the trace is anchored at one end of the display and it can be stretched out or compressed to see more details, or to see more of the spectrum. Place the cursor in the left (or right) third of the X-axis scale; the cursor changes shape to ⟹‖ (or ‖⟹). Hold down the left mouse button and move the cursor along the X-axis ruler. When you move the cursor to the left (right), the trace expands; when you move the cursor to the right (left) the trace compresses. The X-axis ruler changes to correspond with the new trace display. Release the mouse button when you are satisfied with the new position of the trace. In the example below, the cursor was put in the left third, and the trace compressed.

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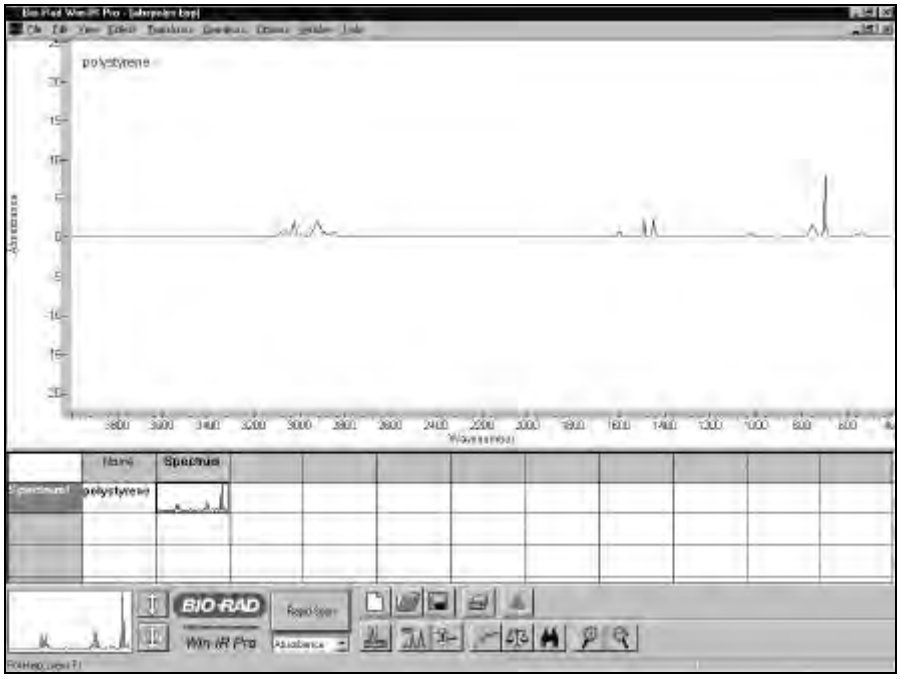
Note

In three-dimensional views, the cursor also changes as described above. However, its use there is not recommended, use the other methods described for that particular view.

X-axis Units: The default unit for the X axis is wavenumber (cm^{-1}). In some applications, it is useful to have the X-axis units be microns (or nanometers). You can change the X-axis units by selecting Wavenumbers, Microns, or Nanometers from the Transforms / More Transforms submenu. See Chapter 10 for details.

Y-axis Rescale: You can interactively change the Y-axis scaling of the trace. Place the cursor on the trace; the magnifying glass in the cursor disappears. Hold down the left mouse button; the cursor changes to a double-headed arrow. Holding down the left mouse button you can drag the trace, changing the Y-axis scale. Release the mouse button and the new values appear on the Y axis.

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Y-axis Relabel: You can change the Y-axis trace label. Place the cursor on the trace (but not in a region of the trace where a peak has been defined, see Chapter 2) or in the in the Spectrum column of the trace you want to relabel. Click the right mouse button. This menu appears:



Select Properties. The Core Spectrum Information dialog box appears

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Type in the new Y-axis label, and click OK.

Alternatively, in the spreadsheet, place the cursor in the Spectrum column of the trace you want to relabel, and double-click. The Core Spectrum Information dialog box appears. Type in the new Y-axis label, and click OK. For more details, see Chapter 4.

Notes

This changes the *label* of the Y-axis, not its units.

Peak Direction is discussed in Chapter 2.

Y-axis Scroll: Scrolling is the movement of the trace with respect to the window (it can also be considered as moving a window about the trace to view portions of the trace). Place the cursor in the middle third of the Y-axis ruler; the cursor changes shape to ⟦. Hold down the left mouse button and move the cursor along the Y-axis ruler. The trace and the Y-axis ruler will move with the cursor. Release the mouse button when you are satisfied with the new position of the trace. In the example below, the trace has been shifted to the left.

Y-axis Expanding/Compressing: In this procedure, the trace is anchored at one end of the display and it can be stretched out or compressed to see more details, or to see more of the spectrum. Place the cursor in the upper (or lower) third of the Y-axis scale; the cursor changes shape to ⟦ (or ⟦). Hold down the left mouse button and move the cursor along the Y-axis ruler. When you move the cursor up (down), the trace expands;

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when you move the cursor down (up) the trace compresses. When you release the mouse button, the Y-axis ruler changes to correspond with the new trace display.

Vertical Lines

Often it is useful to have a vertical line drawn on the screen. This allows you to examine a number of traces to see if there is a shift in the position of the peaks. To draw a vertical line, place the cursor at the desired x-value location in the x-axis scale or the regions ruler and click the right mouse button. This menu appears:



Click New and select Vertical Line.

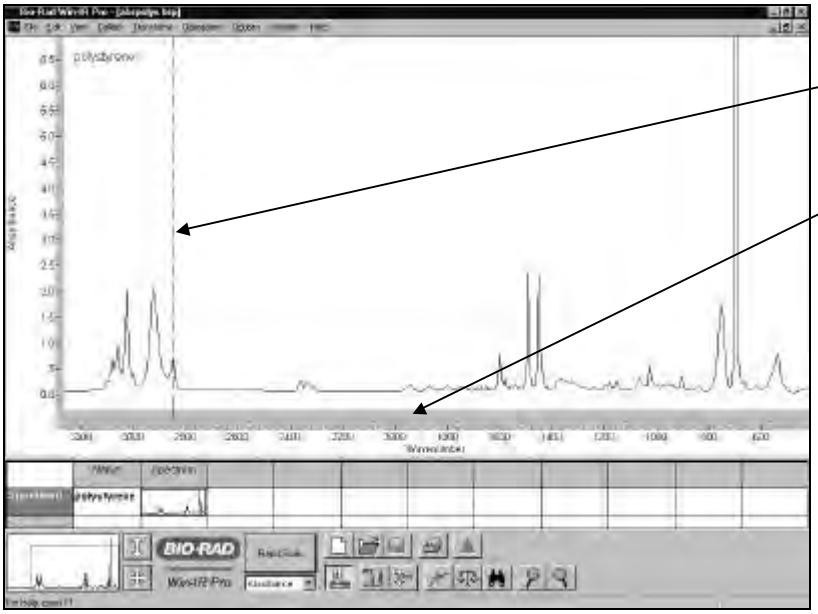


A vertical line is drawn through the x-value position of the cursor.

Note

If the regions ruler is not visible, it will automatically be selected when the vertical line is chosen.

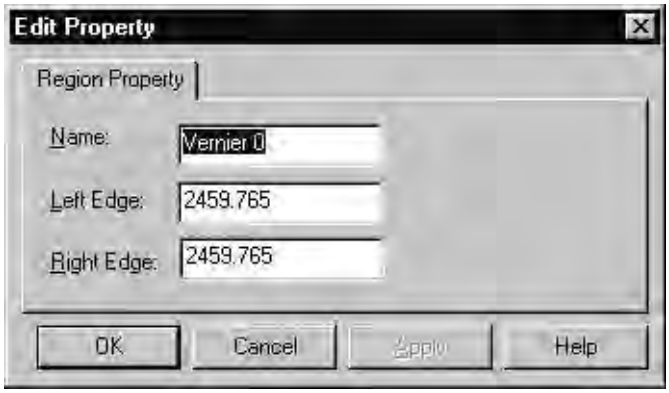
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If you want to know the exact position of the vertical line, place the cursor on the line in the regions ruler and click the right mouse button. The following menu appears.



Select Properties; the Edit Property dialog box appears.



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Either Left Edge or Right Edge gives the exact position of the line.

Moving the line: place the cursor over the extension of the line into the ruler. Hold down the left mouse button and drag the line to the desired position. Release the mouse button.

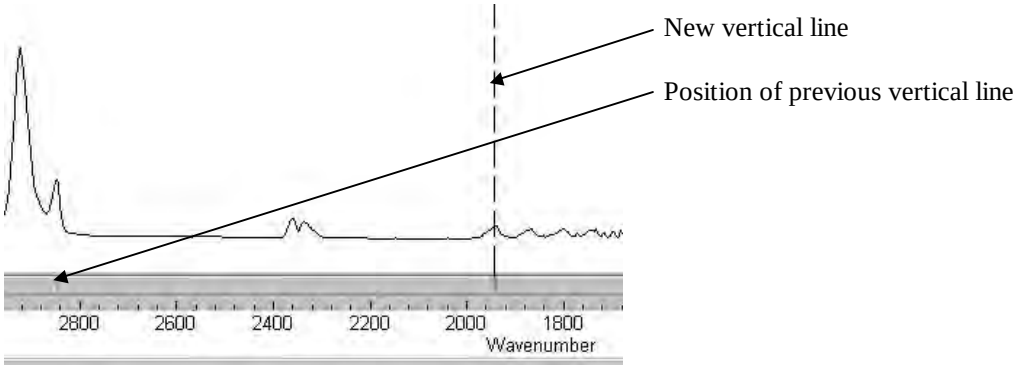
Deleting the line: place the cursor on the line in the regions ruler and click the right mouse button. The following menu appears.



Select Delete. This deletes the selected line.

Alternatively, place the cursor over the extension of the line into the ruler. Click the left mouse button to select the line. Press the DELETE key on the keyboard.

If you select more than one vertical line, only the last one selected is displayed. Previously selected lines are indicated by short lines in the ruler; if you place the cursor over one of these and click the left mouse button, this vertical line will be displayed, replacing the existing line.



Position Labels

You can label the x- and y-coordinates of a point on a trace. First, select the trace. To label a point, place the cursor in the window at the desired x-value location at any y-

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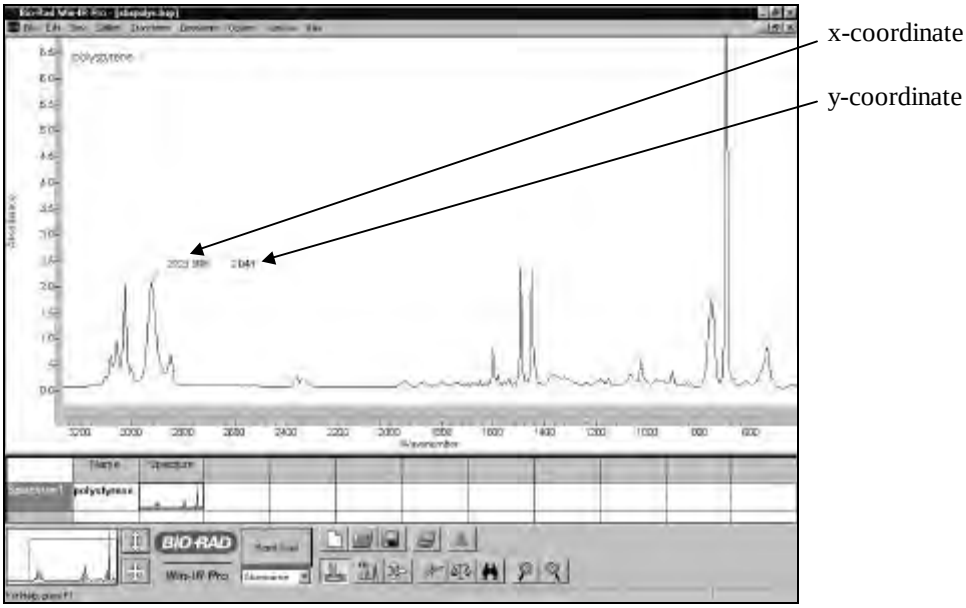
value point (except in a defined peak) and click the right mouse button. This menu appears:



Click New and select Position Label.



The point is labeled with its x- and y-coordinates.

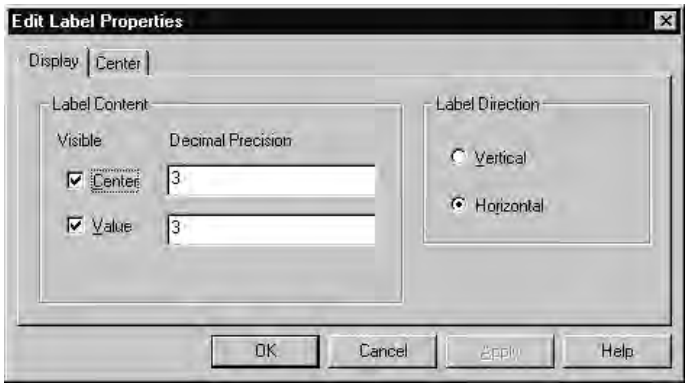


Editing Position Labels: place the cursor on the x-coordinate, y-coordinate, or the line joining them to the trace. The cursor changes to . Click the right mouse button; this menu appears:

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Select Properties. The Edit Label Property dialog box appears.



On the Display tab page.

Label Content: determines what is in the position label.

> Visible: select Center to have the x-coordinate shown; select Value to have the y-coordinate shown. The default is to have both shown.
>
> Decimal Precision: how many numbers (0 - 8) are displayed after the decimal point. The default is 3.

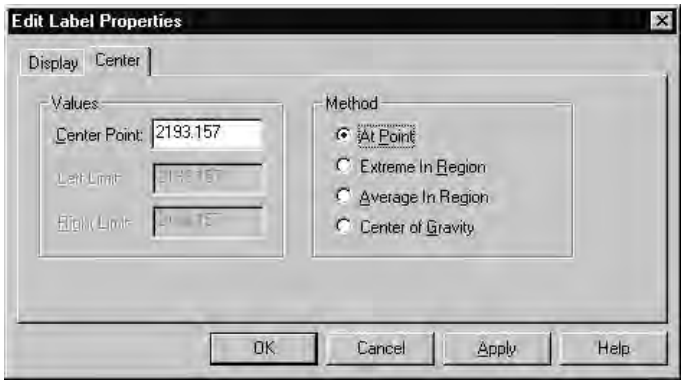
Label Direction: orientation of the label; either Vertical or Horizontal (default).

If you want to find out the exact attachment point or change it, click the Center tab.

Note

You can also change the attachment point by putting the cursor on it, holding down the left mouse button, dragging it to the desired location, and releasing the mouse button.

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Method: how the attachment point is determined.

At Point: attachment point is at value entered in Center Point.

Extreme in Region: attachment point is the extreme (maximum for absorbance spectra, minimum for transmittance spectra) in the region defined by the values entered in Left Limit and Right Limit.

Average in Region: the attachment point is at the arithmetic mean of the Left Limit and Right Limit of the region.

Center of Gravity: the attachment point is determined by the average of the x-values in the region defined by the values entered in Left Limit and Right Limit weighted by the spectrum height at each x-value.

$$peak_location = \frac{\sum_i x_i y_i}{\sum_i y_i}$$

where y_i is the height of the spectrum at wavenumber x_i; all x_i are inside the defined region.

OK: return to main screen and implement values set in the dialog box.

Cancel: return to main screen; do not implement any changes made since last clicking the Apply button.

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Apply: immediately implement changes entered in dialog box. This button is enabled only if changes are entered in the dialog box. Changes made through the Apply button cannot be reversed by using the Cancel button.

Help: enter the on-line Help system.

Moving Position Labels: you may want to move the position label, especially if labels overlap or interfere with each other. Place the cursor on the x-coordinate or the y-coordinate of the position label. The cursor changes to . Hold down the left mouse button and drag the position label as desired. Release the mouse button.

Deleting Position Labels: place the cursor on the attachment point, the line, or one of the coordinates and click the right mouse button. The following menu appears.



Select Delete. This deletes the selected position label.

Alternatively, place the cursor on the x-coordinate, y-coordinate, or the line joining them to the trace. The cursor changes to Click the left mouse button to select the position label. Press the DELETE key on the keyboard.

REGIONS

In some instances, you want to perform an operation on a part (or parts) of the trace, for example, deconvolution. There are two ways to define a region—by using the right mouse button, or by selecting Operations / Drag Region.

Defining a region with the right mouse button: To define a region:

1. In the regions ruler, place the cursor at the x-coordinate that will be the center of the region in the x-axis scale or the regions ruler.

2. Click the right mouse button. This menu appears:

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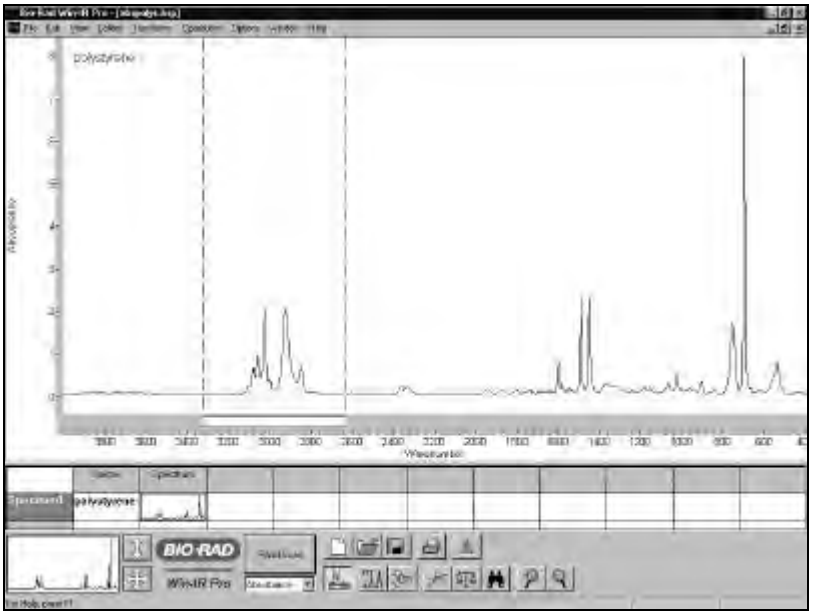
3. Select New / Region.



This creates a region centered at the x-coordinate of the cursor and extending 10% of the displayed x-axis in either direction from the center. . The region is defined by the vertical dashed lines. The white bar at the bottom of the region means that this region is active and selected.

Note

If the regions ruler is not visible, it will automatically be selected when the vertical line is chosen.

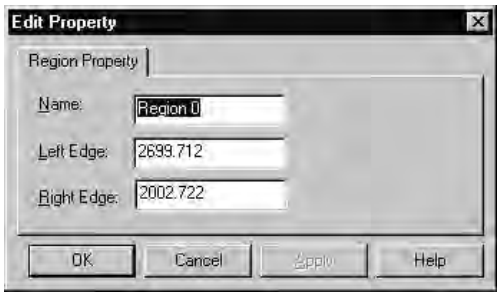


You can determine the exact limits of the region by placing the cursor in the white area of the regions ruler and clicking the right mouse button. Select Properties from the menu that appears.

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The Edit Properties dialog box appears with the desired information.



4. The limits of this region can be modified. See "Modifying a Region," below.

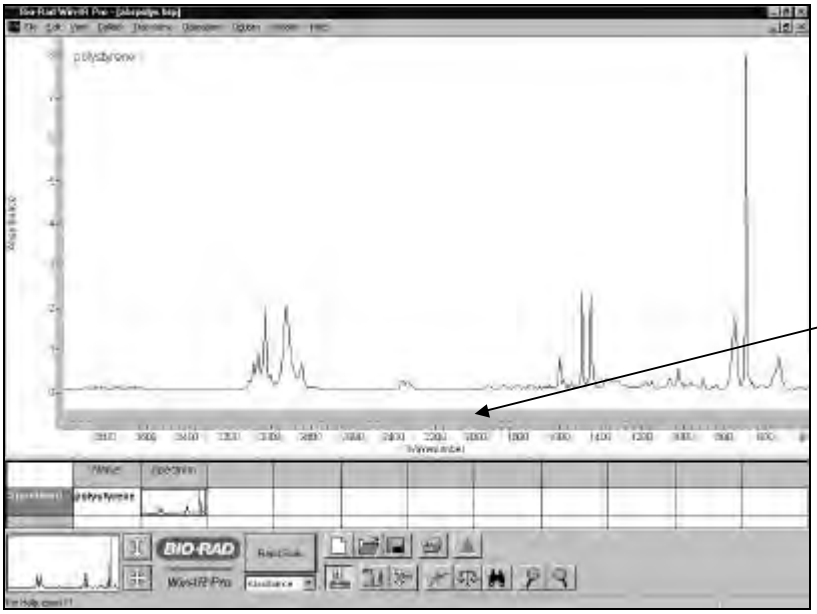
5. You can create additional regions, as desired.

Defining a region with the ruler:

1. If the ruler is not present, select Drag Region from the Operations menu. A check mark (√) appears in front of Drag Regions if it is selected. Or, press the  toggle button at the bottom of the screen; the button remains depressed until it is clicked again. Drag Regions (region selection) is now enabled. A blank rectangle (the ruler) appears at the bottom of the trace display, just above the x-axis scale.

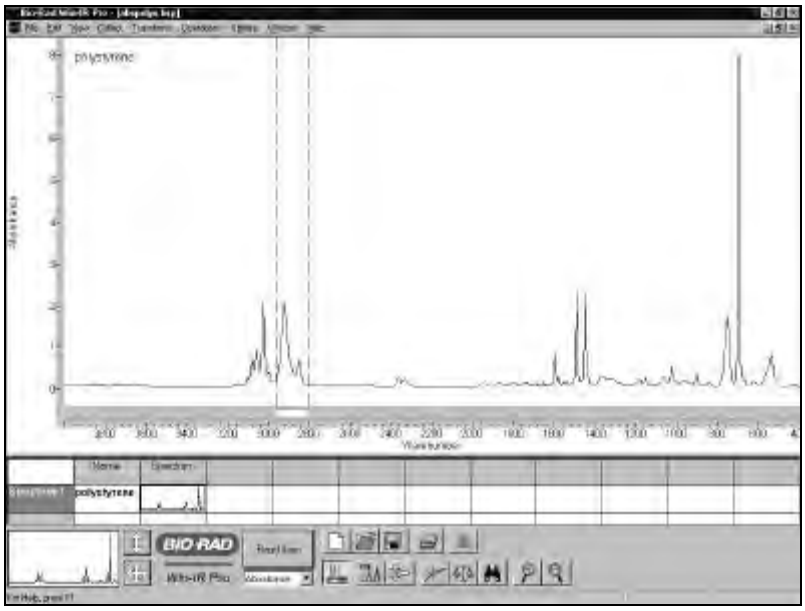
2. Put the cursor into the ruler at one end of the region to be selected. The cursor changes to .

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3. Hold down the left mouse button and drag the cursor to the other end of the region being defined. Release the button. The region is defined by the vertical dashed lines. The white bar at the bottom of the region means that this region is active and selected.

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4. Repeat this procedure to define additional regions, if desired.

Modifying a region:

1. Select the region to be modified by putting the cursor on the ruler inside that region and clicking the left mouse button.

2. Place the cursor at the edge of the region to be moved. The cursor changes to ⟷.

3. Hold down the left mouse button and drag the edge of the region to the new desired position. Release the mouse button.

Deleting a region:

1. Select the region to be deleted by putting the cursor on the ruler inside that region and clicking the left mouse button.

2. Place the cursor in the white area of the regions ruler and click the right mouse button. The following menu appears.

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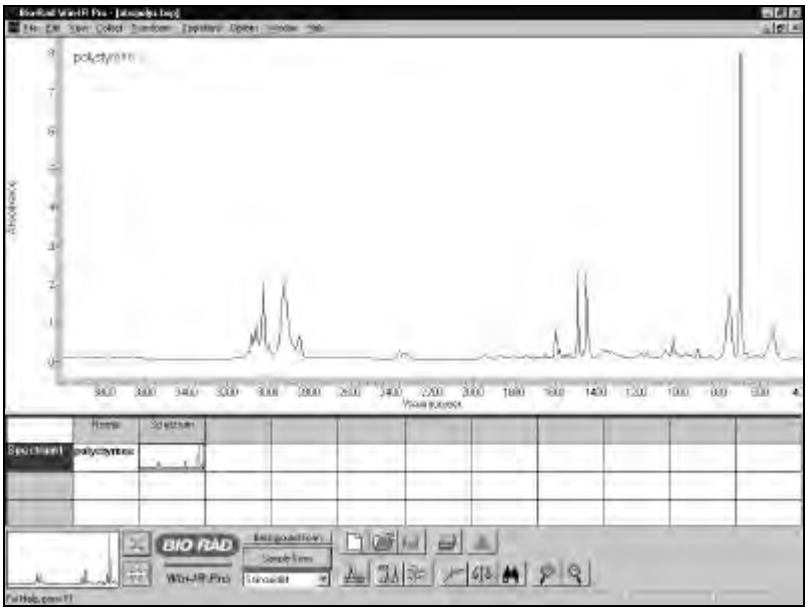
Select Delete. This deletes the selected region.

OR

After selecting the region, press the DELETE key on the keyboard or the DEL key on the numeric keypad (NUM LOCK off).

PROPERTIES

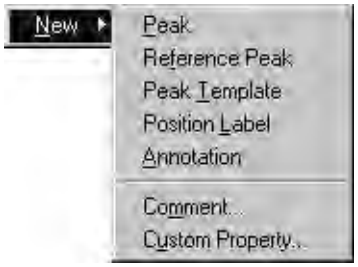
You can add properties and their values to any spectrum in a document using the right mouse button. Consider, for example, this spectrum:



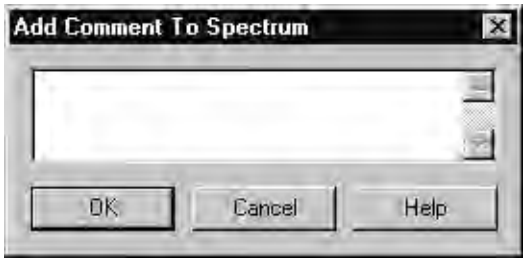
Adding Comments

1. Place the cursor in the trace window. Click the right mouse button; from the New submenu, select Comment.

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The Add Comment to Spectrum dialog box appears.



2. Put the cursor in the scroll box and type in whatever comment is desired. Any text, including comment text from a previous session may be altered and/or deleted.

3. Click the OK button to save the new comment text. A column headed Comment is added to the spreadsheet and the value for this spectrum is the text of the comment. You may have to resize the spreadsheet cell (see Chapter 4 for details) to view all the text). If you do not want this column in the spreadsheet, remove it with View / Remove Columns (see Chapter 8 for details).

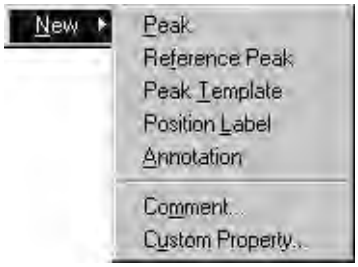
   Click Cancel to leave the text, if any, as it was before this session.

   Click Help to enter the on-line help system.

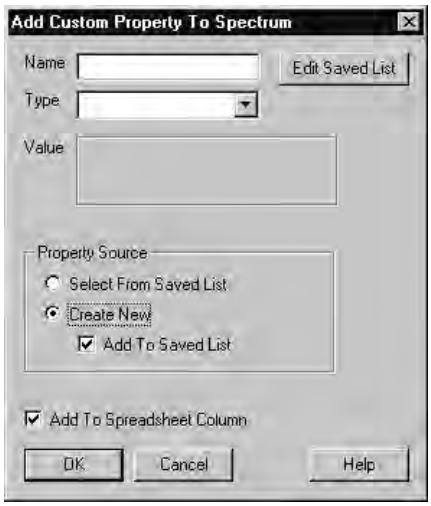
Adding Custom Properties

1. Place the cursor in the trace window. Click the right mouse button; from the New submenu, select Custom Property….

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The Add Custom Property to Spectrum dialog box appears. The default selection (Property Source) is to create a new property.



2. To add a new property, select the parameters as follows:

Name: the name of the property to be added.

Type: the type of property;select the appropriate type from the pull-down menu. The types are:

Text: a character string.
Number: a numerical value (double-precision)
Time: the time and date at which this property was created.
Chemical Structure: a graphical display of the molecule.

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Value: once Name and Type are entered, this box becomes active. Enter the value of the property. The type of Value must match Type.

Property Source: where the property to be added to the spectrum comes from.
Select From Saved List: pick a property from the existing list (see section below).
Create New: create a new property with a value.
Add to Saved List: if selected, the new property is added to the list of properties which can be added to a spectrum.

Add to Spreadsheet Column: select this option if a column for this property is to be added to the spreadsheet when the property creation process is completed.

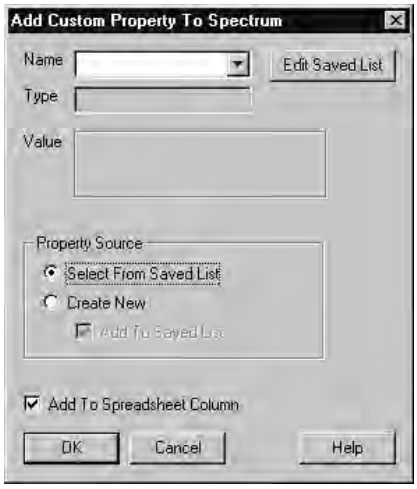
Click OK to add the new property to the spectrum and (if selected) to the saved list and to the spreadsheet.

Click Cancel to leave the text, if any, as it was before this session.

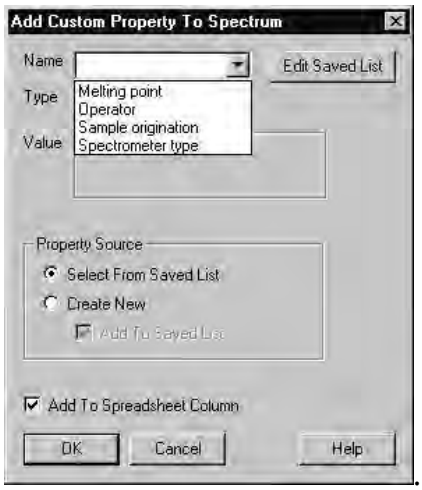
Click Help to enter the on-line help system.

3. To add a property to the spectrum from the saved list, first select the Select From Saved List option from the Property Source choice. The dialog box then becomes:

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Name: use the pull-down menu to select the name of the property to be added to the spectrum



Type: the property type for the selected property automatically appears in this box. The types are:

Text: a character string.
Number: a numerical value (double-precision)
Time: the time and date at which this property was created.
Chemical Structure: a graphical display of the molecule.

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Value: once Name is selected, this box becomes active. Enter the value of the property. The type of Value must match Type.

Property Source: where the property to be added to the spectrum comes from.

Select From Saved List: pick a property from the existing list; this option should be selected,

Create New: create a new property with a value (see above section).

Add to Saved List: this is disabled for items already in the saved list.

Add to Spreadsheet Column: select this option if a column for this property is to be added to the spreadsheet when the property creation process is completed. .

Click OK to add the saved property to the spectrum and (if selected) to the spreadsheet.

Click Cancel to leave the text, if any, as it was before this session.

Click Help to enter the on-line help system.

3. Edit Saved List: click this button to bring up the list of existing saved properties for the purpose of deleting one or more of them from the list. The Edit Saved List dialog box appears



Highlight all properties to be removed from the saved list using the standard ctrl+left-mouse-click procedure.

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Click OK to remove the selected properties from the saved list and return to the Add Custom Property to Spectrum dialog box.

Click Cancel to leave the saved list as it was and return to the Add Custom Property to Spectrum dialog box.

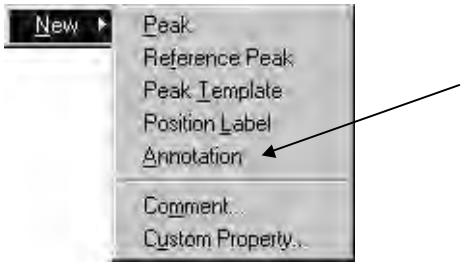
Click Help to enter the on-line help system.

ANNOTATIONS

You can place text annotations on the display ; each annotation can be connected to a point on the spectrum—for example, a peak, a group of peaks, or some interesting feature of the spectrum.

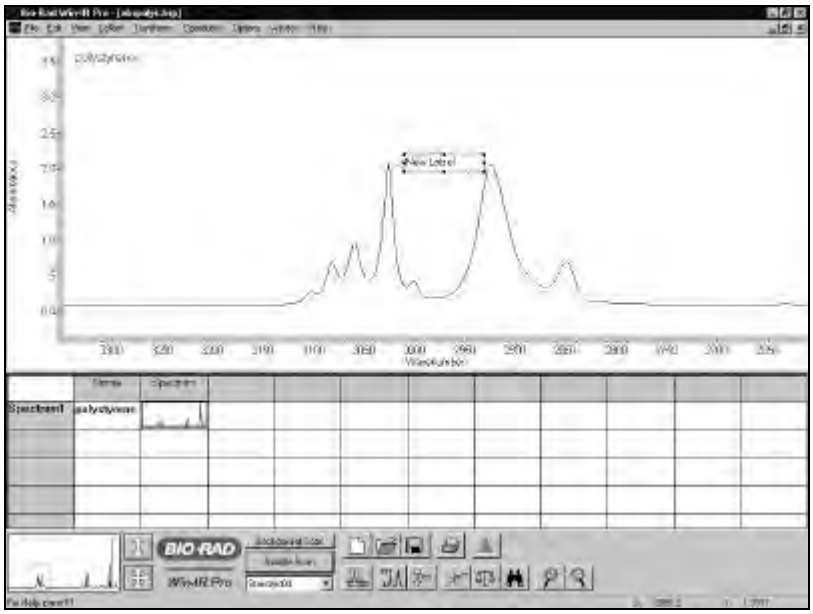
Create Annotation

1. Place the cursor near the feature to be annotated. Click the right mouse button. From the New entry, select Annotation.

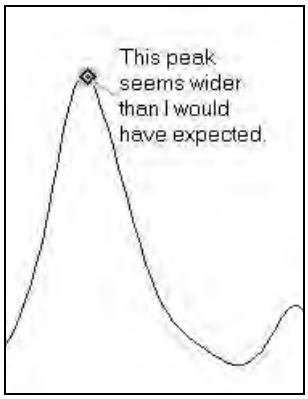


An annotation box containing the text New Label appears. This box is connected to the spectral trace by a line. The point at which this line touches the trace is called the attachment point.

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2. Place the cursor in the label box and double click the left mouse button; the cursor changes to a vertical insertion bar. You can now replace the text New Label by highlighting it and typing in new text. Enter and edit text as you would in a word processor such as Word.



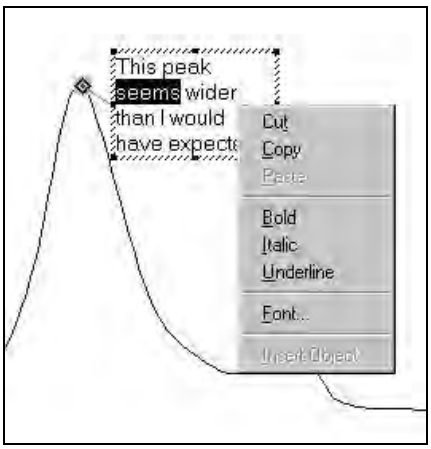
Format the Annotation Text

1. Place the cursor in the label box; double-click the left mouse button.

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2. Highlight the selected text.

3. Place the cursor in the label box and click the right mouse button. The formatting menu appears.



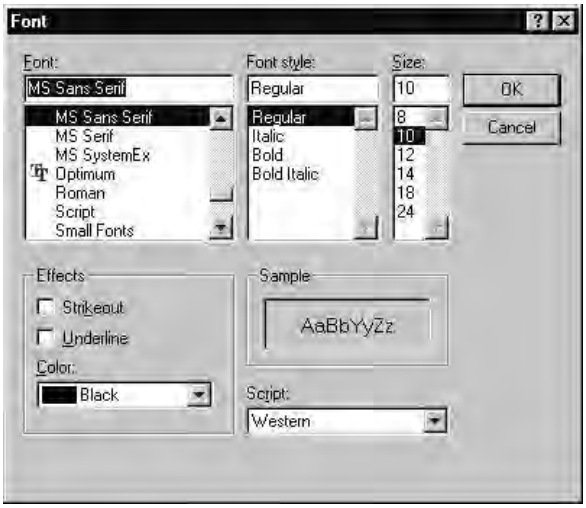
4. Select the format to be performed.

Note

Although they are not shown, the usual shortcut control key combinations are implemented in this menu.

Copy	copy the highlighted item to the clipboard.
Cut	copy the highlighted item to the clipboard, then delete the highlighted item.
Paste	paste the clipboard into the label box at the vertical insertion mark
Bold	make the highlighted text **boldface**.
Italic	make the highlighted text *italic*.
Underline	underline the highlighted text.
Font	causes the Font dialog box to appear.

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You can select the Font, Font style, Size, Effects and Color for the highlighted text. The appearance of the text with these selections is shown in the Sample box. Script is normally Western.

Insert Object allows insertion of an ActiveX object such as a graphic, Excel spreadsheet, etc.

Resize the Label Box

1. Make sure the box is selected; it will be a rectangle whose edges are short diagonal segments with a small square at each of the corners and in the center of each side of the rectangle.



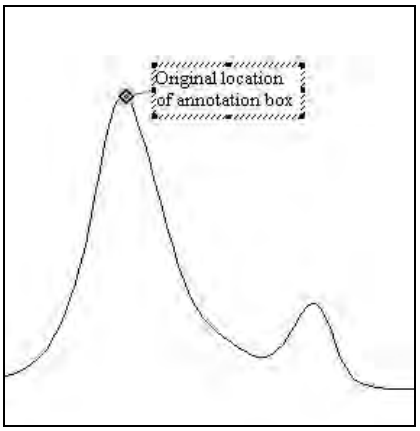
2. Place the cursor on one of the small squares and hold down the left mouse button. The cursor changes to a double-headed arrow showing in what direction the box can be resized.

3. Drag the box to the desired size; release the left mouse button.

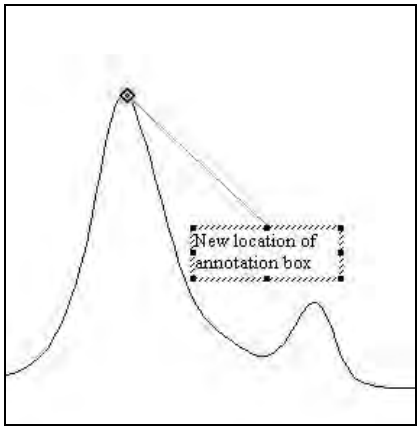
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Move the Label Box

1. Place the cursor inside the box. Hold down the left mouse button; the cursor will change to a four-headed arrow.



2. Holding down the left mouse button, drag the box to the desired position. Release the left mouse button. The attachment point does not change.



Delete the Label Box

1. Make sure the box is selected; it will be a rectangle whose edges are short diagonal segments with a small square at each of the corners and in the center of each side of the rectangle.

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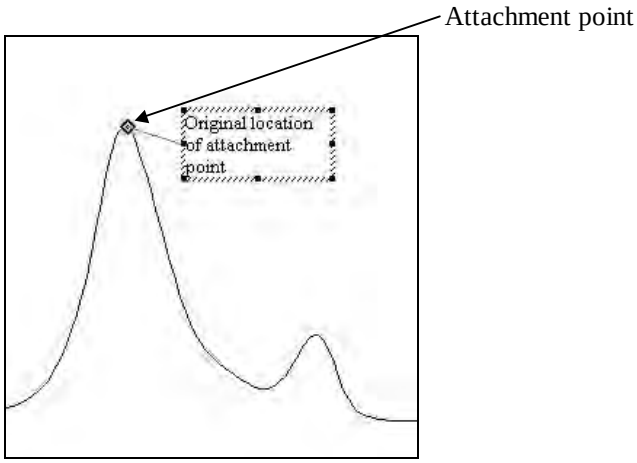
2. Place the cursor in the label box and click the right mouse button. The following menu appears.



Select Delete. This deletes the selected annotation.

Move the Attachment Point

1. Click on the label box area or on the attachment line. The attachment point is now displayed.

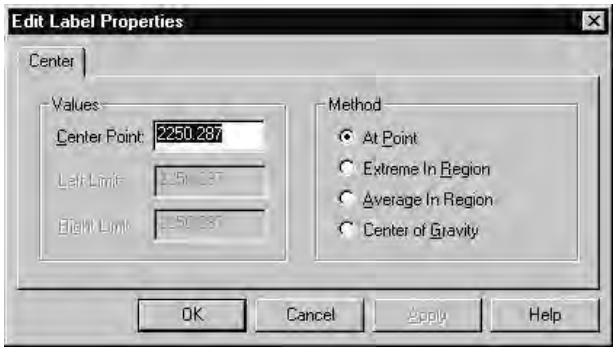


2, If you want to know the exact position of the attachment, place the cursor on the attachment point, the line, or in the label box and click the right mouse button. The following menu appears.



3. Select Properties; the Edit Label Properties dialog box appears.

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Method: how the attachment point is determined.

At Point: attachment point is at value entered in Center Point.

Extreme in Region: attachment point is the extreme (maximum for absorbance spectra, minimum for transmittance spectra) in the region defined by the values entered in Left Limit and Right Limit.

Average in Region: the attachment point is at the arithmetic mean of the Left Limit and Right Limit of the region.

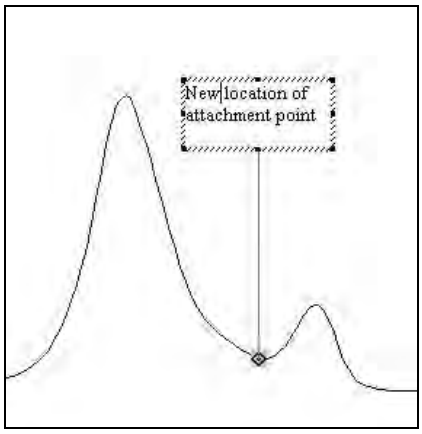
Center of Gravity: the attachment point is determined by the average of the x-values in the region defined by the values entered in Left Limit and Right Limit weighted by the spectrum height at each x-value.

$$peak_location = \frac{\sum_i x_i y_i}{\sum_i y_i}$$

where y_i is the height of the spectrum at wavenumber x_i; all x_i are inside the defined region.

You can also change the attachment point by putting the cursor on it, holding down the left mouse button, dragging it to the desired location, and releasing the mouse button.

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PRINTING THE SCREEN IMAGE

At times, you will want to capture the image on the screen in order to print it. This includes documents with multiple trace displays, contour and perspective displays, etc. The word processor WordPad and the graphic editor Paint are included with Windows NT. However, you can use most word processors and graphic editors to perform the same functions.

Note

Some keyboards and/or computers require you to press the SHIRT + PRINT SCRN keys, rather than just the PRINT SCRN key. Consult the documentation that came with your computer.

To print the screen image using WordPad:

1. Set the Win-IR Pro display as desired. Press the PRINT SCRN key on the keyboard. This copies the screen image to the Windows NT clipboard.

2. From the Taskbar select Start / Programs / Accessories / WordPad. The WordPad application starts.

3. Select Paste from the Edit menu.

4. If necessary, size the screen image so it fits on the page. The details of sizing an image in Write are given in its Help menu.

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5. If you want to have the maximum size of the screen image, select Print Setup from the File menu. Then, set Orientation to Landscape. Click the OK button.

6. Select Print from the File menu. Click the OK button.

To print the screen image using Paint:

1. Set the Win-IR Pro display as desired. Press the PRINT SCRN key on the keyboard. This copies the screen image to the Windows NT clipboard.

2. From the Taskbar select Start / Programs / Accessories / Paint. The Paint application starts.

3. Select Paste from the Edit menu.

4. You can use the tools in Paint to edit the screen image, crop it, add text, etc. The details of using Paint are given in its Help menu.

7. If you want to have the maximum size of the screen image, select Print Setup from the File menu. Then, set Orientation to Landscape. Click the OK button.

8. Select Print from the File menu. If you have not cropped the screen image, click the Properties button; then select the Advanced tab page. If the Graphic icon is not expanded, click the Graphic icon; then highlight Scaling. Set Scaling to 60% (Portrait) or 77% (Landscape) to get the printed image on a single page. These values will be different if you cropped the screen image. Experiment to find the best scaling factor. Click the OK button, to return to the Print dialog box, then click OK to start printing.

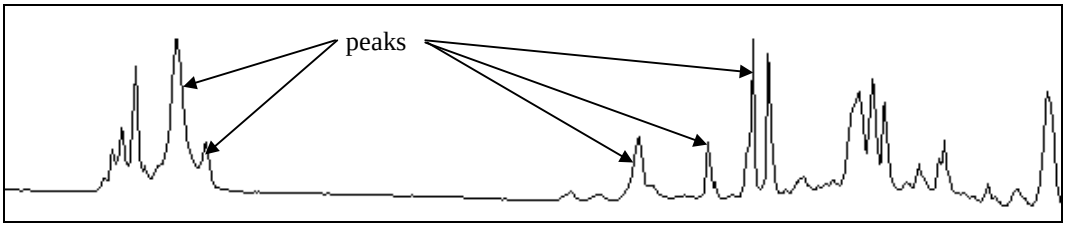
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2
Peaks

DEFINITION

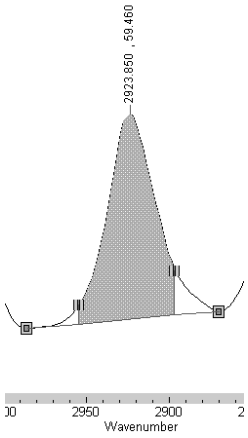
A peak is a local maximum in a spectrum indicating that there is absorbance in the sample at that wavenumber. Some, but not all, of the peaks in the example below are indicated.



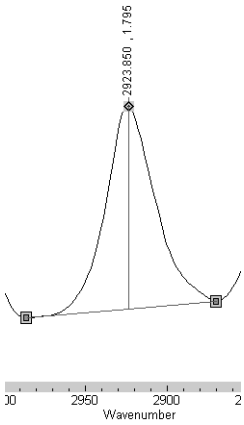
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PEAK DISPLAY

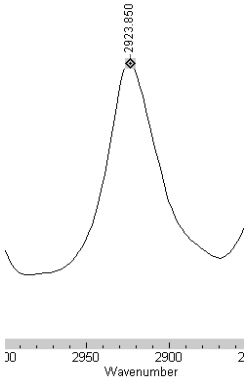
A defined peak can be displayed in three ways: area (default), height, or center. Which one you choose depends upon which properties of the peak you are working with.



Area (default)



Height



Center

Note

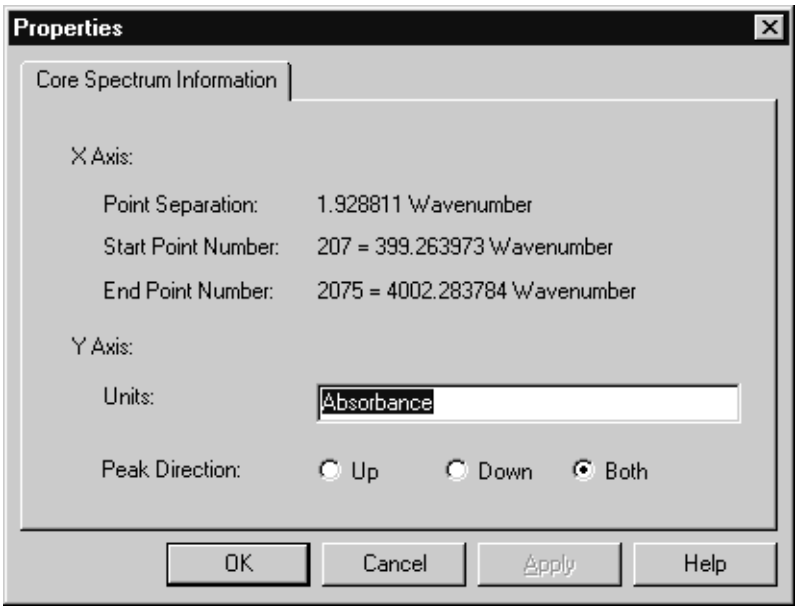
Only one number is displayed for center because the numbers would identical. However, see Reference Position for Center Value, later in this chapter.

Reference Peaks and Peak Templates are discussed later in this chapter.

Peak Direction

In absorbance and absorbance-like spectra, peaks point upwards, in transmission spectra peaks point downwards, in some spectra—for example single-beam—they may point in both directions. To make sure that you can define peaks properly for the spectrum you are using, place the cursor on the spectra where no peak has been defined. Click the right mouse button and select Properties. The Properties dialog box appears.

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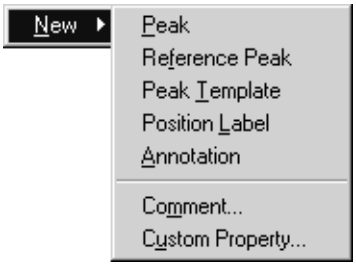
Select the Peak Direction desired and click the OK button. You can now define peaks as appropriate for this spectrum.

Defining peaks

1. Place the cursor on the peak to be defined and click the right mouse button. This menu appears:

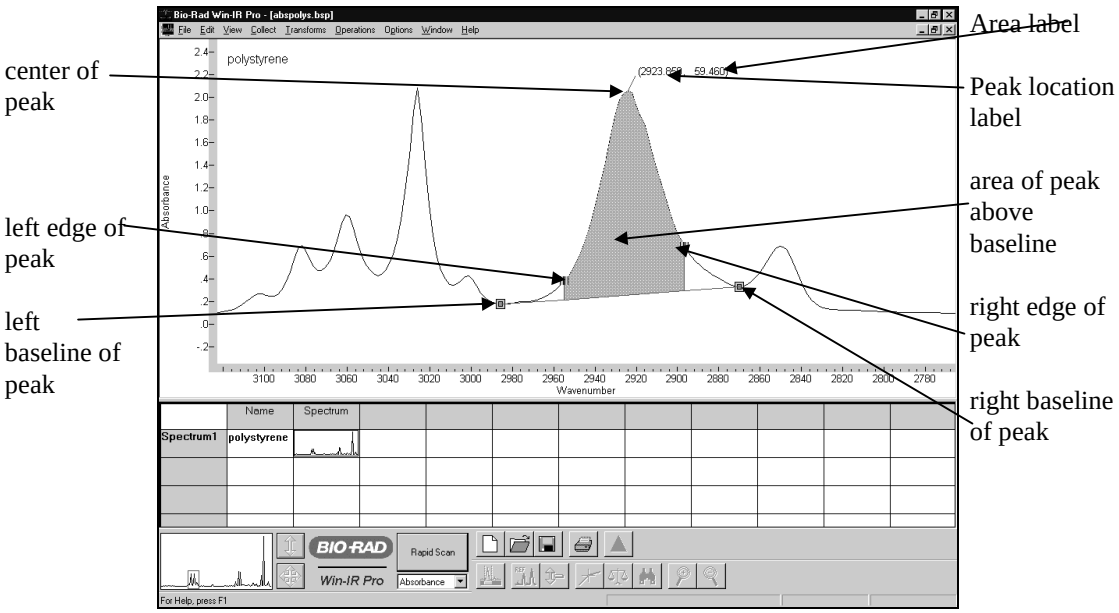


2. Select New / Peak.



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The peak is selected.



This display is the peak area. The center of the peak is at the maximum; the baseline edges are at the minima between the selected peak and the adjacent peaks (whether selected or not); each peak edge is halfway between the corresponding baseline edge and the centerline along the x axis.

You can manually adjust the peak edges and the baseline edges (but not the center of the peak) in area mode.

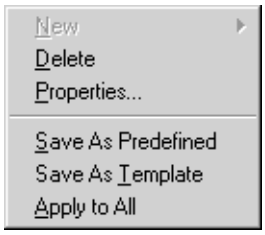
Peak edges

Place the cursor on the peak edge box ▮ whose position you wish to change. There are two methods of moving this box.

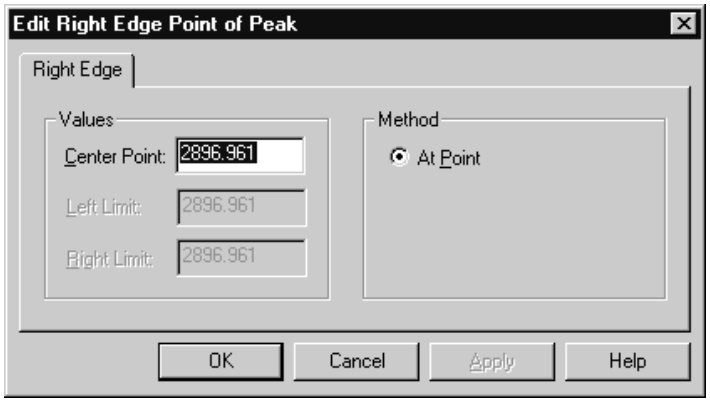
Interactive: hold down the left mouse button and drag this box to the desired position; then, release the mouse button.

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Menu: put the cursor on the peak right edge box and click the right mouse button; this menu appears.



Select Properties. The Edit Right Edge Point of Peak dialog box appears.



Type the desired value in the Center Point box. The method for peak edges is At Point.

OK: implement new values and return to main screen.

Cancel: ignore all changes made to values since last clicking the Apply button and return to main screen.

Apply: implement new values; remain in Edit Right Edge Point of Peak dialog box. These changes cannot be undone with the Cancel button.

Help: enter the on-line Help system.

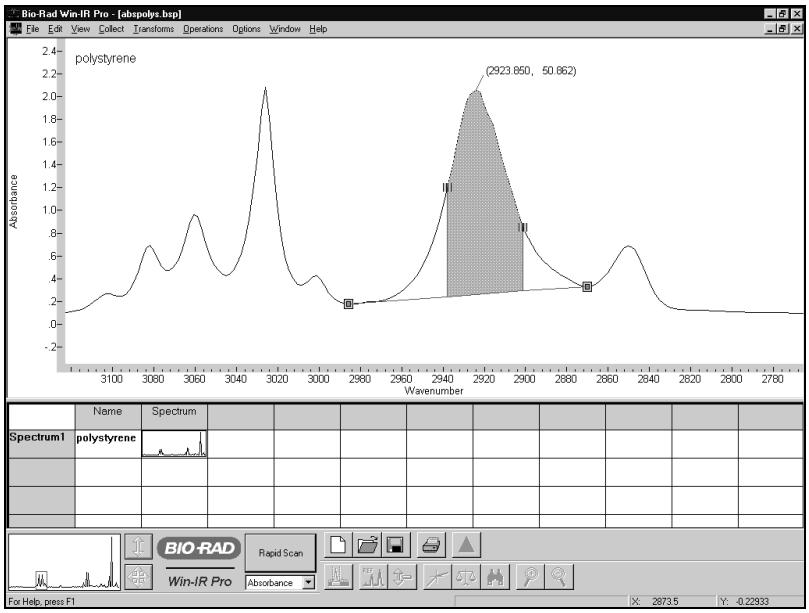
Note

This is the dialog box for the Right Edge Point; there is a similar dialog box for the Left Edge Point.

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You can also put the cursor on the peak label, click the right mouse button, and select Properties. Then, click on the Right Edge (or Left Edge) tab. The same tab page as above appears.

In the example below, both peak edges have been changed to make the peak narrower. The area has decreased and the new value is displayed.



Baseline edges

The box ▣ showing the location of the baseline edge can be split (into a left ◧ and right ◨ box) to define a region; the baseline edge is the point of extreme value (minimum for absorbance spectra, maximum for transmittance spectra) in that region. To define each baseline region, place the cursor on the baseline edge box (or split) whose position you wish to change. There are two methods of moving this box.

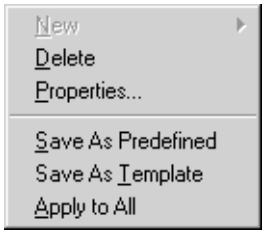
Interactive: hold down the left mouse button and drag this box to the desired position; then, release the mouse button.

Note

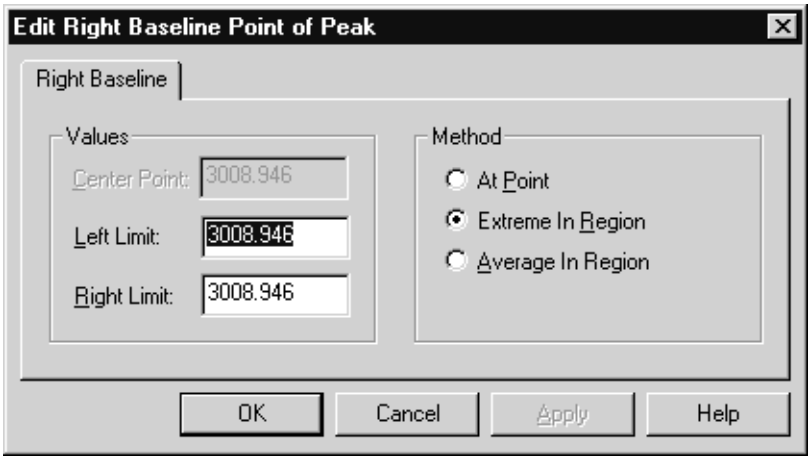
The split box cannot be dragged over its corresponding other half.

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Menu: click the right mouse button; this menu appears.



Select Properties. The Edit Right Baseline Point of Peak dialog box appears.



Method

At Point: the right baseline is defined by a single point.

Extreme in Region: if the baseline box is split, the right baseline is defined by the extreme value of the spectrum in that region (minimum for absorbance spectra, maximum for transmittance spectra).

Average in Region: if the baseline box is split, the x-position of the right baseline point (x) is the arithmetic mean of the x-positions of the left and right limits of the baseline region. The y-position of the right baseline point (y) is the average of the y-position values in the region. The (x,y) point is not necessarily on the spectrum. This technique reduces the effect of noise within the baseline region.

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Values

Type the desired value(s) in the Left Limit and/or Right Limit box(es).

Notes

These are the left and right limits of the region in which the baseline point will be located; they are not the left and right baseline points.

The same dialog box appears whether you put the cursor on the left or right half of the baseline edge box.

OK: implement new values and return to main screen.

Cancel: ignore all changes made to values since last clicking the Apply button and return to main screen.

Apply: implement new values; remain in Edit Property dialog box. These changes cannot be undone with the Cancel button.

Help: enter the on-line Help system.

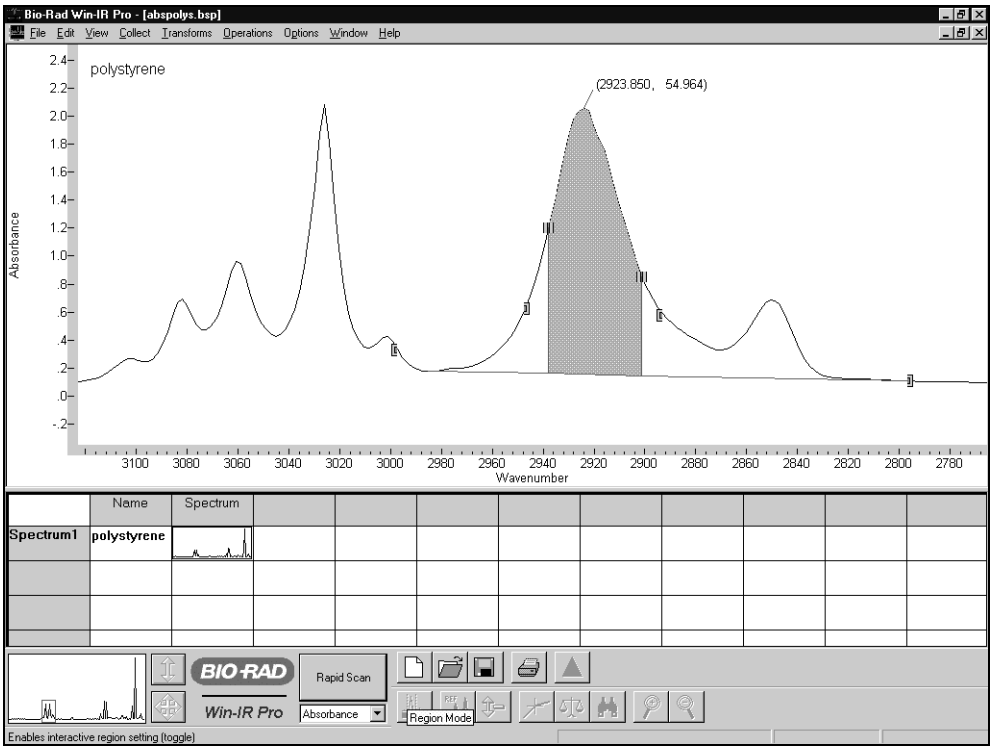
Note

This is the dialog box for the Edit Right Baseline Point of Peak; there is a similar dialog box for the Left Baseline Point of Peak.

You can also put the cursor on the peak label, click the right mouse button, and select Properties. Then, click on the Right Baseline (or Left Baseline) tab. The same tab page as above appears.

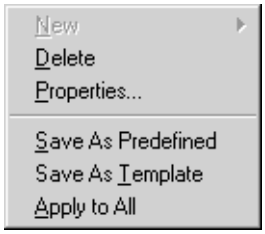
In the example below, both baseline edges have been changed. The baseline has changed and so has the area of the peak above the baseline.

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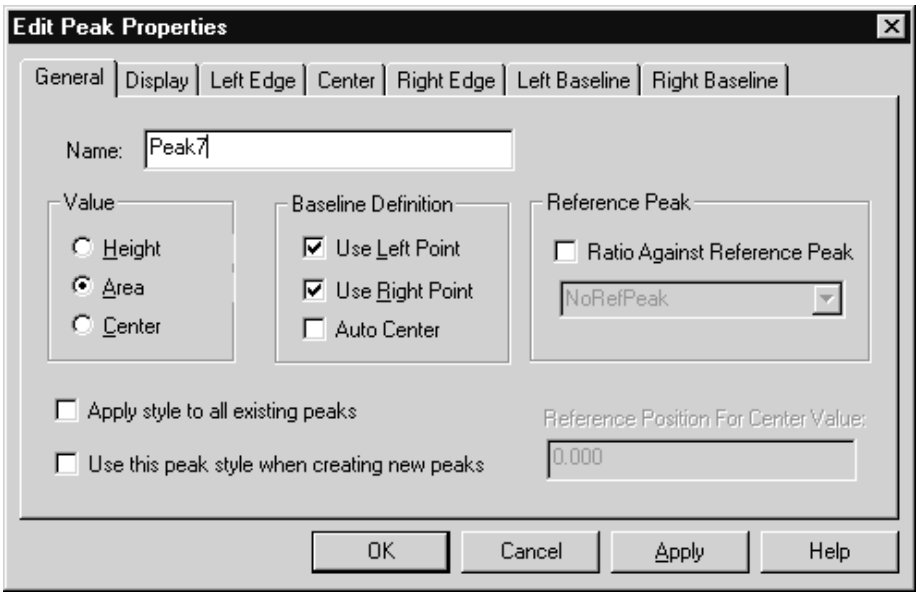
Height display: allows you to move the peak from the maximum point between the edges (for example, the peak might be shifted because two peaks are convolved). You can also adjust the baseline, but not the peak edges in height mode.

To access height mode, put the cursor under the peak or on the label and click the right mouse button; this menu appears.



Select Properties. The Edit Peak Properties dialog box appears. Click on the General tab.

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Name: the name labeling the peak. The default is of the form Peakn, where n is the order in which the peak was defined. You can give the peak any name you want. If you select Name on the Display tab page (see below), then the peak name is displayed as part of the label to the left of the parentheses holding the location and value.

Value: select display mode for peak.

Height
Area
Center

Baseline Definition:

select both left and right—the baseline is a straight line connecting the two baseline points

select none—the baseline is the x-axis

select only left or right—the baseline is a horizontal line through the selected baseline point.

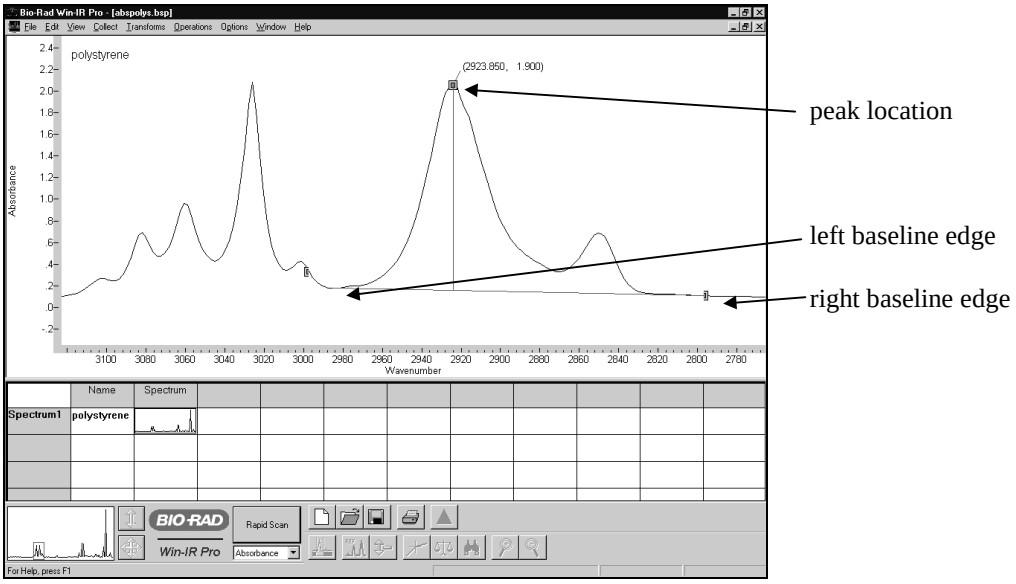
Use Left Point: baseline is a horizontal line through the left baseline point.

Use Right Point: baseline is a horizontal line through the right baseline point.

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Auto Center: moves the right half box of the left baseline point to the x-position of the center of the peak; moves the left half box of the right baseline point to the x-position of the center of the peak. These half boxes move if the center of the peak moves. If the baseline boxes have not been split, then selecting Auto Center splits the boxes and moves them as above. This option is most useful in kinetics documents (see Chapter 3 for details).

In the example below, height mode is selected, and both baseline points are used. The second peak label now displays height; see below for details on modifying the labels.

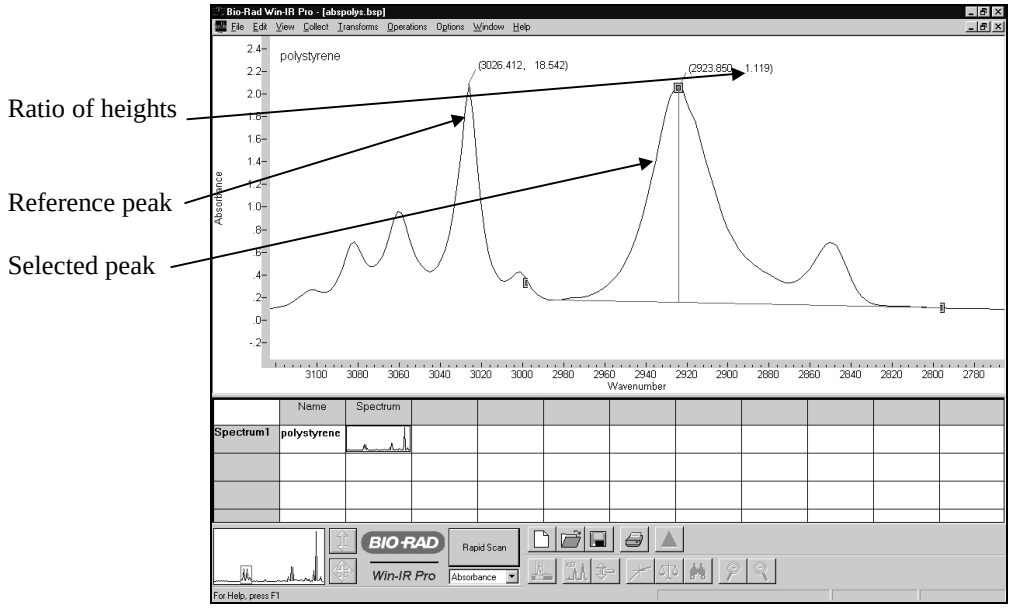


Reference Peak: reference peaks are those whose areas and/or heights will be used as a standard against which other peaks will be ratioed. Reference peaks are discussed later in this chapter.

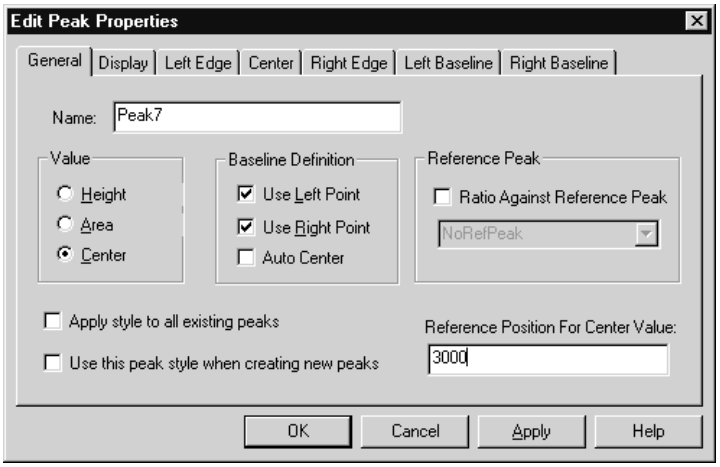
Ratio Against Reference Peak: if selected, the Value part of the peak label will be the ratio of the area (height) of this peak to the area (height) of the reference peak selected from the pull-down menu. Which ratio appears depends upon whether Area or Height is selected in the Value part of this dialog box; no ratio is calculated if Center is selected. It does not matter which Value of the reference peak has been selected.

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In the example below, a reference peak was inserted at 3026.412 wavenumbers; the height of the selected peak was ratioed to the height of the reference peak.

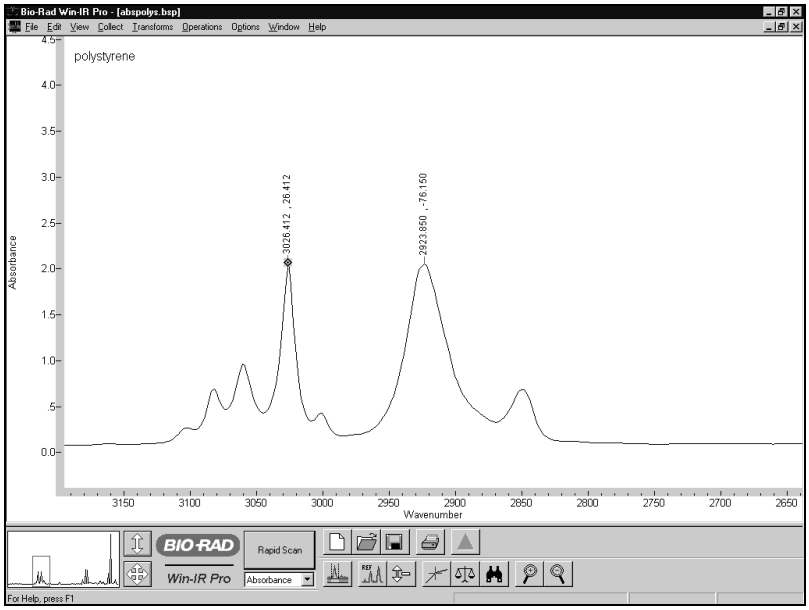


Reference Position For Center Value: this displays the wavenumber of the peak relative to a value that you select. This is of most use in image files, but is displayed here to show the format. Value must be set to Center for this feature to be enabled.



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In this example, the reference has been set to 3000 cm^{-1}. Both the absolute wavenumber and the relative wavenumber of the center of the peak are displayed.



Apply style to all existing peaks: if this is selected, then when Apply or OK is clicked, all existing peaks, in any trace in this document, will use the style defined for this peak. Style includes such parameters as Value, Baseline Definition, Label Content, Label Direction, etc.

Use this peak style when creating new peaks: if this is selected, then when Apply or OK is clicked, all subsequently created peaks, in any trace in this type of document (multi-spectral, kinetics, etc.), will use the style defined for this peak. Style includes such parameters as Value, Baseline Definition, Label Content, Label Direction, etc.

OK: implement new values and return to main screen.

Cancel: ignore all changes made to values since last clicking the Apply button and return to main screen.

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Apply: implement new values; remain in Edit Peak Properties dialog box. These changes cannot be undone with the Cancel button.

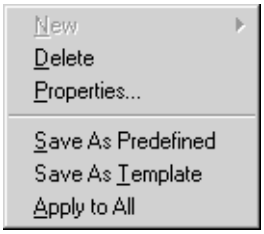
Help: enter the on-line Help system.

Center Point of Peak (location)

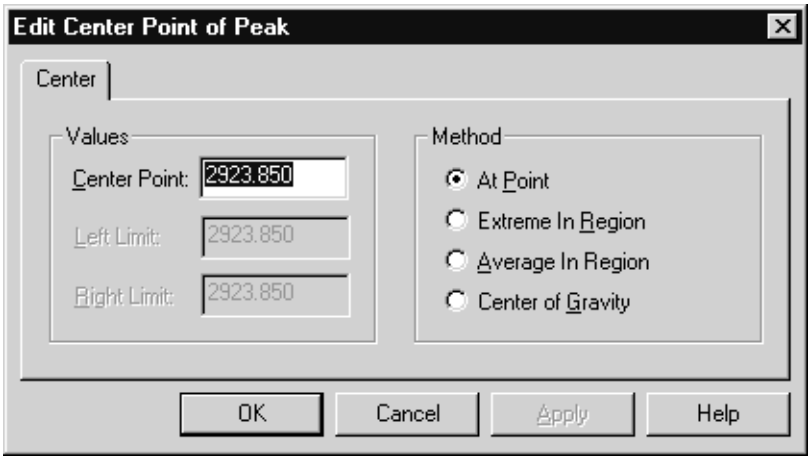
Place the cursor on the peak center box ◈. There are two methods of moving this box.

Interactive: hold down the left mouse button and drag this box to the desired position; then, release the mouse button.

Menu: put the cursor on the peak center box and click the right mouse button; this menu appears.



Select Properties. The Edit Center Point of Peak dialog box appears.



Method: how the peak location is determined.

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At Point: peak location is at value entered in Center Point.

Extreme in Region: peak location is the extreme (maximum for absorbance spectra, minimum for transmittance spectra) in the region defined by the values entered in Left Limit and Right Limit.

Average in Region: the peak location is at the arithmetic mean of the Left Limit and Right Limit of the region.

Center of Gravity: the peak location is determined by the average of the x-values in the region defined by the values entered in Left Limit and Right Limit weighted by the spectrum height at each x-value.

$$peak_location = \frac{\sum_i x_i y_i}{\sum_i y_i}$$

where y_i is the height of the spectrum at wavenumber x_i; all x_i are inside the defined region.

OK: implement new value and return to main screen.

Cancel: ignore all changes made to values since last clicking the Apply button and return to main screen.

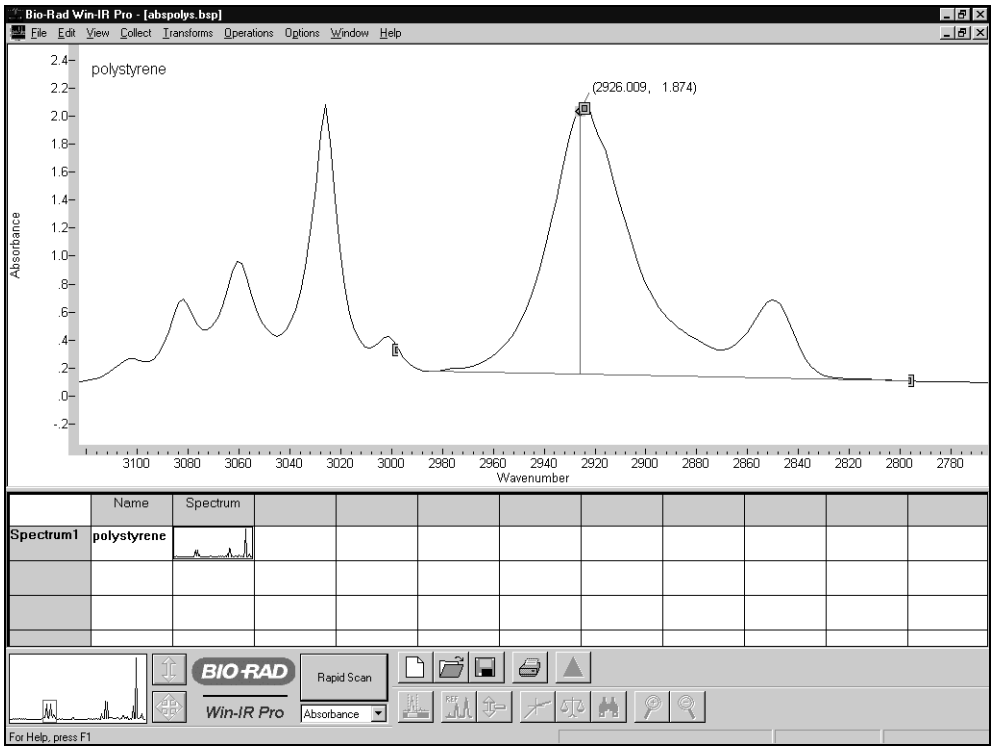
Apply: implement new values; remain in Edit Center Point of Peak dialog box. These changes cannot be undone with the Cancel button.

Help: enter the on-line Help system.

You can also put the cursor on the peak label, click the right mouse button, and select Properties. Then, click on the Center tab. The same tab page as above appears.

In the example below, the peak has been shifted slightly to the left (higher wavenumber).

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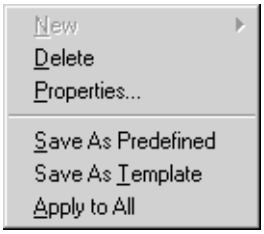


Baseline edges: are adjusted exactly the same as when the area is displayed; see above for details.

DISPLAY PROPERTIES

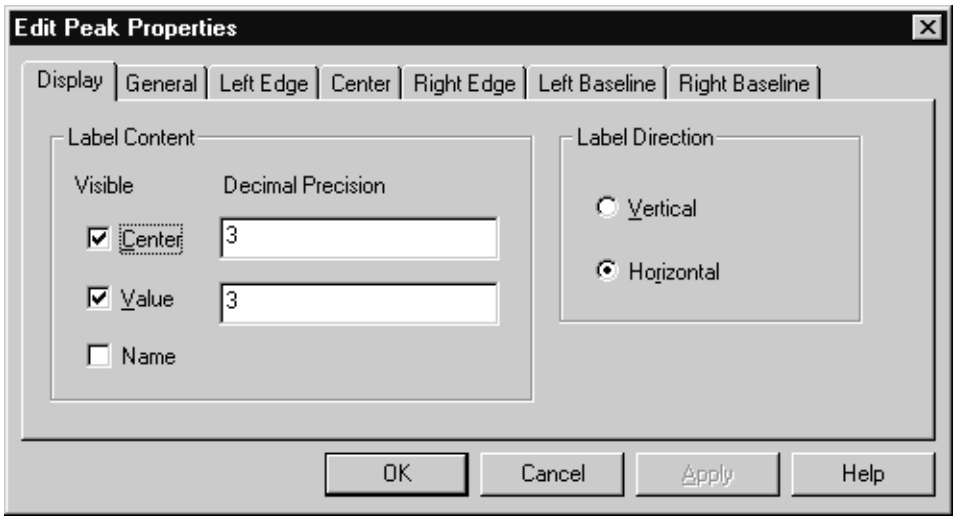
A number of the properties of the peak labels can be changed. This can be done regardless of what value is displayed.

To modify the peak labels, put the cursor under the peak or on the label and click the right mouse button; this menu appears.



Select Properties. The Edit Peak Properties dialog box appears. Click on the Display tab.

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Label Content: select the material to be displayed for each label.

Visible: if selected (default), this label is displayed, otherwise the label is not displayed. If Center is not displayed, Value will be displayed in the its position.

Center: the position of the center of the peak.

Value: the area, height, or center of the peak as selected on the General tab page.

Name: the name of the peak as entered on the General tab page (default is Peakn—Peak1, Peak2, etc.).

Decimal Precision: how many decimal places are displayed; the default is 3. If a value less than 3 is selected, the number is rounded (not truncated.

Content: select what is to be displayed. The first label is Wavenumber; the second is Height, Area, or Center depending upon what Value has been selected on the General tab page.

Label Direction: select the orientation of the label.

Vertical: from bottom to top

Horizontal: from left to right (default)

OK: implement new value and return to main screen.

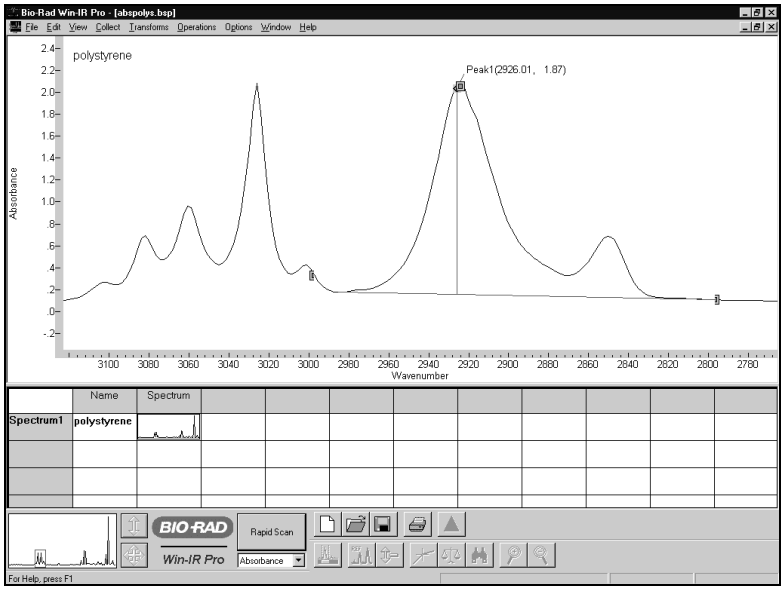
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Cancel: ignore all changes made to values since last clicking the Apply button and return to main screen.

Apply: implement new values; remain in Edit Peak Properties dialog box. These changes cannot be undone with the Cancel button.

Help: enter the on-line Help system.

In the example below, Wavenumber and Height are displayed horizontally to 2 decimal places; Name is also visible.



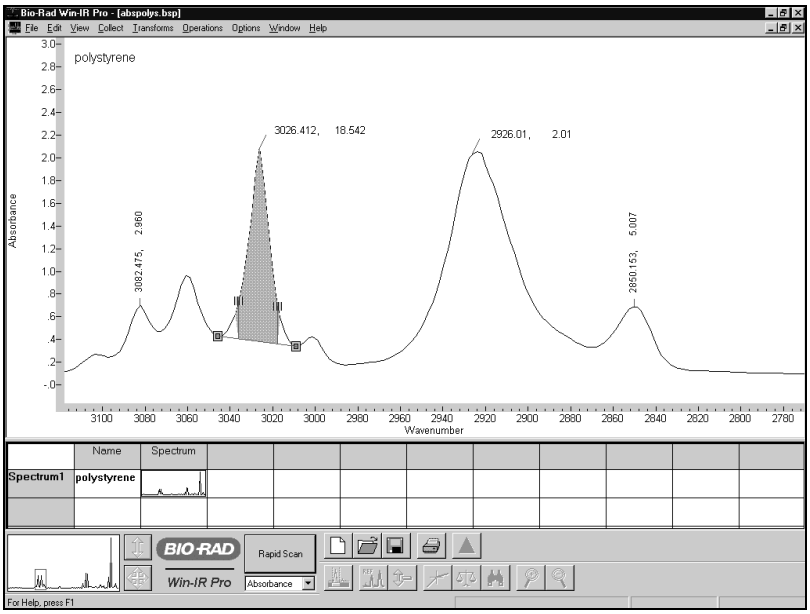
Moving Peak Labels

You may want to move the peak label, especially if labels overlap or interfere with each other. Place the cursor on the peak label. The cursor changes to . Hold down the left mouse button and drag the peak label as desired. Release the mouse button.

MULTIPLE PEAK SELECTION

You can select as many peaks as desired by this process. The mode and display for each peak is independent of the others.

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To modify peak parameters, make the peak active by putting the cursor on its label and clicking the left mouse button.

Note

If you click the cursor on an already defined peak, it will highlight the existing peak, not define a new one.

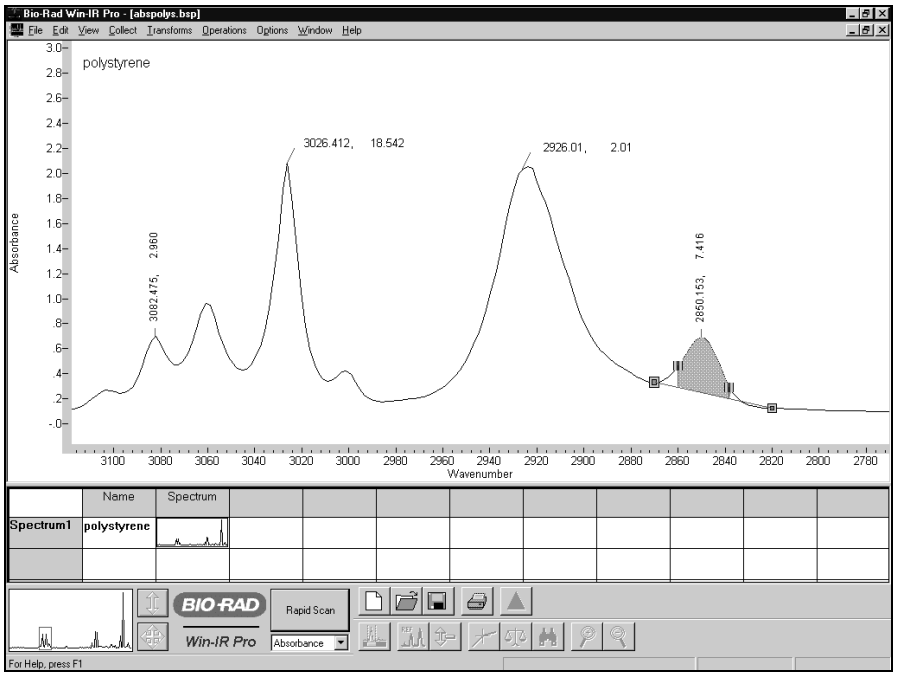
After peaks have been picked, they and/or their parameters can be added to the spreadsheet using Edit / Peak List. See Chapter 7 for details.

REMOVING PEAKS

Individual peak can be removed from the peak table (deselected). . methods of deleting

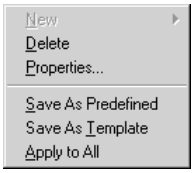
1. Place the cursor in the area under the peak and click the left mouse button to make this peak active.

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2. There are two methods of deleting a selected position label:

   Click the right mouse button; this menu appears



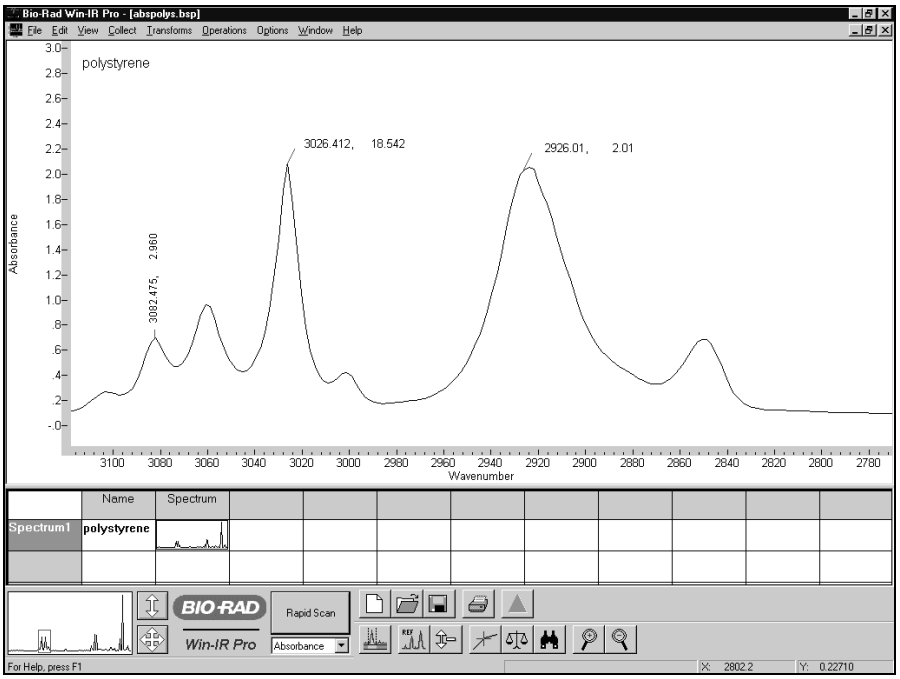
   Select Delete.

   OR

   Press the DELETE key on the keyboard.

The peak is no longer labeled and is removed from the peak table.

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See View / Property Browse Bar (Chapter 8) and Edit / Peak List (Chapter 7) for details of the peak table.

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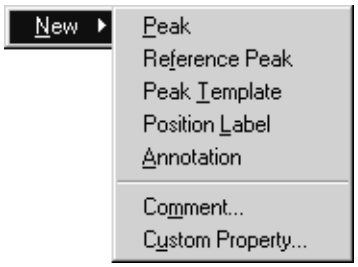
REFERENCE PEAKS

A reference peak is defined in a spectrum so that the area (height) of other peaks in the spectrum can be normalized to the area (height) of the reference peak. To define a reference peak:

1. Place the cursor on the peak to be defined as a reference peak and click the right mouse button. This menu appears:



2. Select New / Reference Peak.

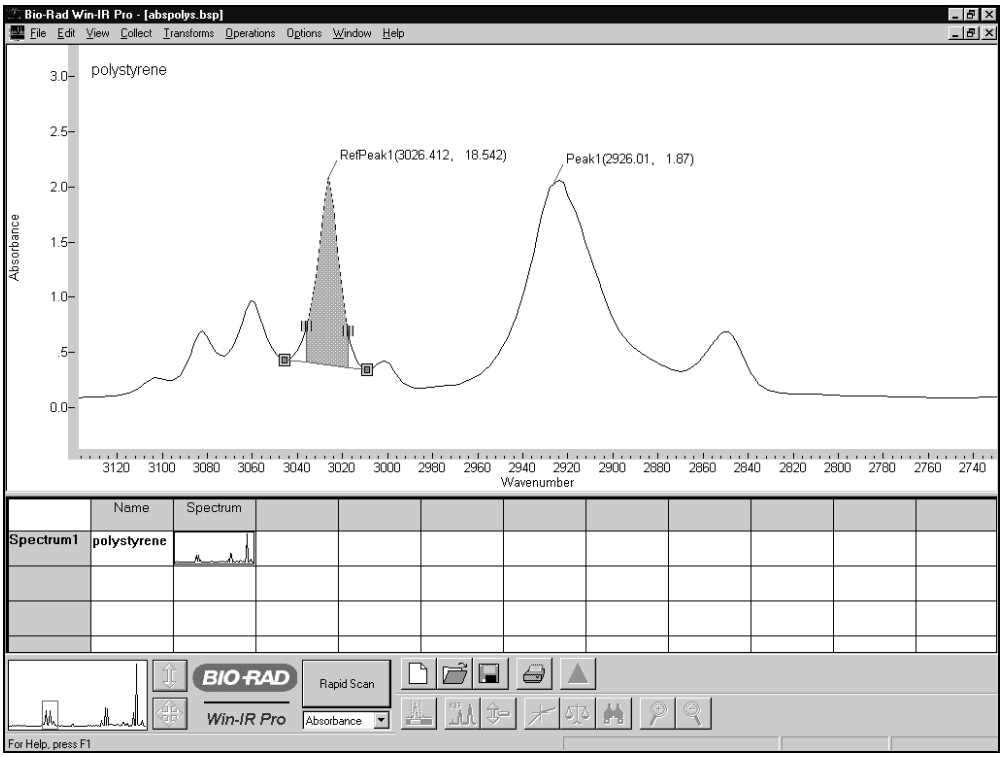


The reference peak will be selected. In this example, we have edited the reference peak's properties to make Name visible. The default name for reference peaks is RefPeakn—RefPeak1, RefPeak2, etc.

Note

Because Reference Peaks look like Peaks in the display, we recommend that you always select Name for your Reference peaks to help distinguish them from the regular peaks of the spectrum.

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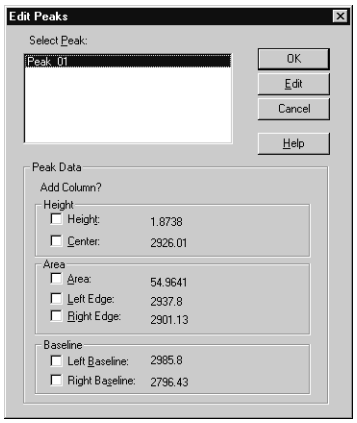
Reference peaks are manipulated exactly the same as peaks. You can alter the center, edges, and baselines. You can choose to display area, height, or center. You can specify what and how will be in the label.

Differences between Peaks and Reference Peaks

Some features in Win-IR Pro do not treat reference peaks in the same way as they treat peaks. Some major examples are shown below.

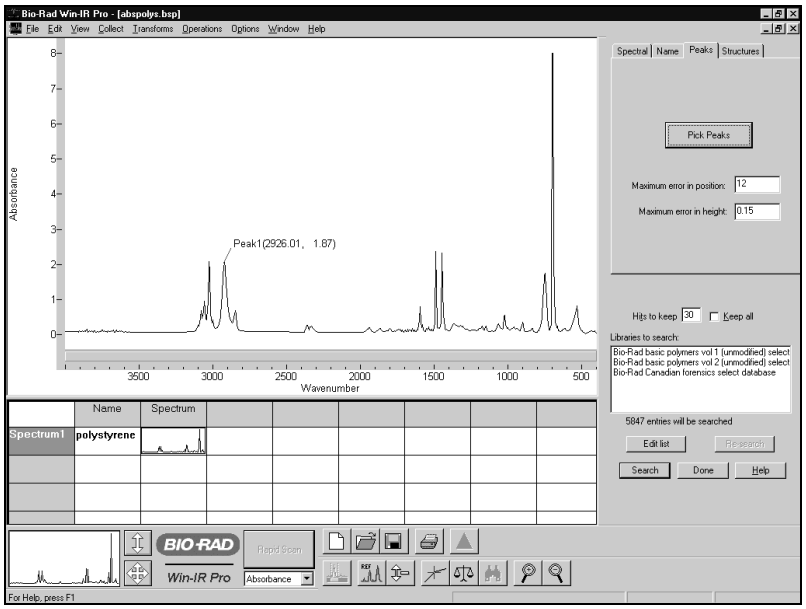
Edit / Peak List: reference peaks do not appear in the peak list (see Chapter 7). The peak list for the example above looks like.

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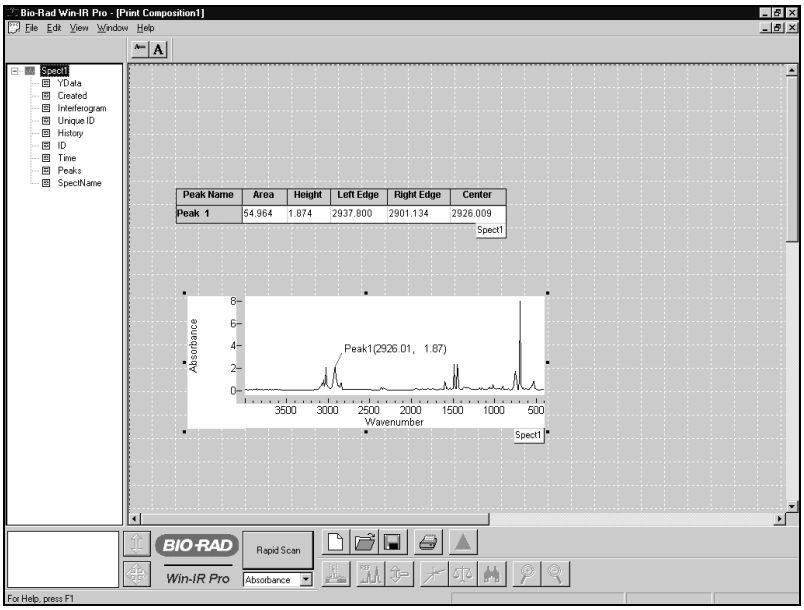
The peak is shown, but the reference peak is not.

Operations / Search: in Peaks search, the reference peaks are neither displayed nor considered (see Chapter 11).



File / Print Composition: Reference peaks are not included in either peak lists or in the display of the spectrum (see Chapter 15).

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PEAK TEMPLATES

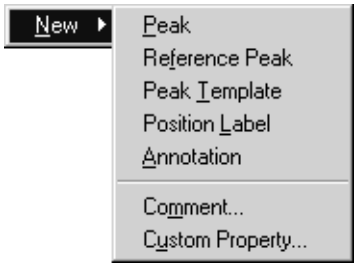
A peak template defines a peak for all spectra in the document. One use of this could be to observe what happens to a set of peaks in a time-varying system; this would typically be used with kinetics. Another possible use is to look at peaks in a number of different samples to observe what effects the sampling conditions had on this peak. To define a peak template:

1. Place the cursor on the peak to be defined as a peak template and click the right mouse button. This menu appears:

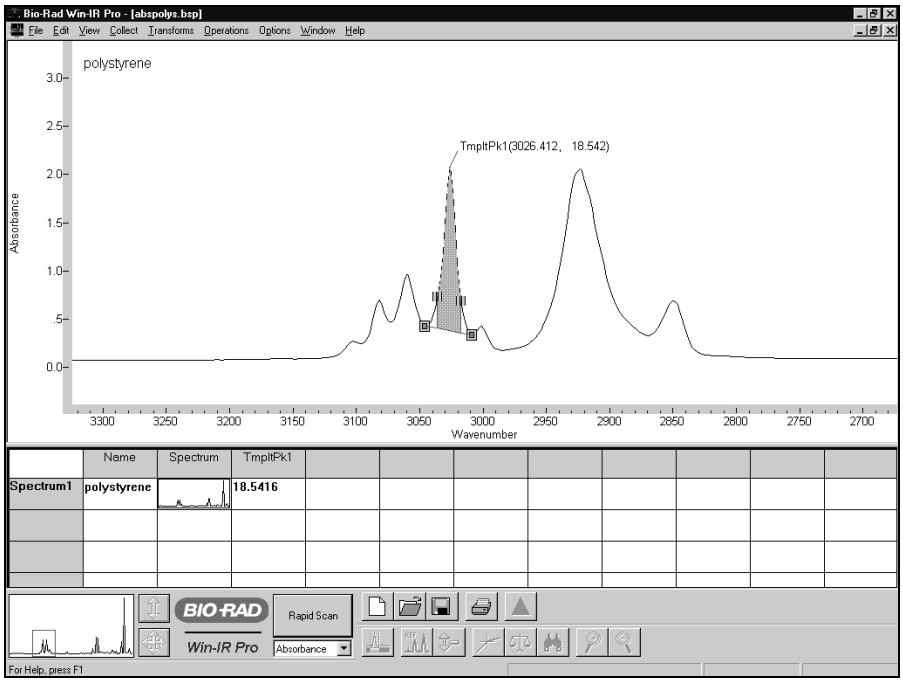
   

2. Select New / Peak Template.

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The peak template will be selected. In this example, we have edited the reference peak's properties to make Name visible. The default name for peak templates is TmpltPkn—TmpltPk1, TmpltPk2, etc.

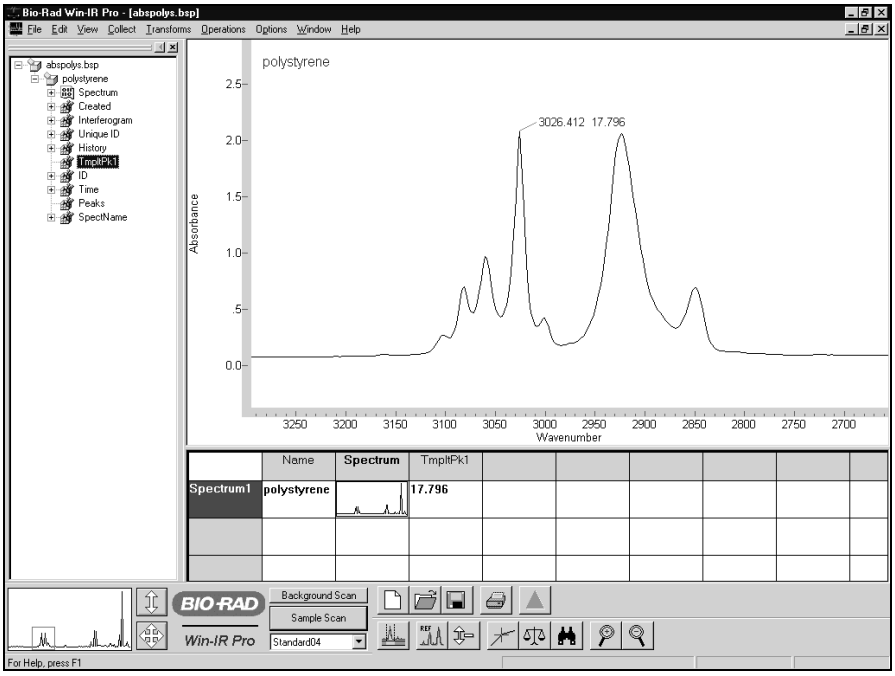


Peak templates are manipulated exactly the same as peaks. You can alter the center, edges, and baselines. You can choose to display area, height, or center. You can specify what and how will be in the label.

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Peak Templates and the Document

Peak templates are a property of the document. As shown above, their Value appears in a column in the spreadsheet. The column heading is the Name of the peak template. An entry for each peak template is created in the property browse bar. However, the property browse bar is not automatically selected when a peak template is defined; to see the property browse bar, select View / Property Browse Bar.



If a peak template is modified (for example, baselines, edges, center, etc. are changed), the same modification is automatically made for all spectra in the document.

When a new spectrum is added to the document, the peak template is automatically added to this spectrum's trace. The Value of the peak template is put into the corresponding spreadsheet cell.

If you delete a peak template, the corresponding column in the spreadsheet is also automatically deleted; the peak template entry is deleted from the property browse bar. Peak template numbers not reset. If you define a new peak template, its number will be the next in sequence after the highest numbered previous peak template.

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Differences between Peaks and Peak Templates

Some features in Win-IR Pro do not treat peak templates in the same way as they treat peaks. As with reference peaks,

Edit / Peak List: peak templates do not appear in the peak list (see Chapter 7

Operations / Search: in Peaks search, the peak templates are neither displayed nor considered (see Chapter 11).

File / Print Composition: peak templates are not included in either peak lists or in the display of the spectrum (see Chapter 15).

PREDEFINED PEAKS

Predefined peaks allow you to save the parameters of a peak, peak template, or reference peak and then use those parameters to define a peak, peak template, or reference peak in the same or another document. The peak parameters are saved in a file; the default file is C:\USERS\DEFAULT\Win-IR_Pro\Peaks.Def. You can change the file in which the predefined peaks are stored by selecting Options / Configuration (see Chapter 12 for details). If you change the file name after predefining some peaks, then those peaks will not be found; you must move the old file to the new location.

Note

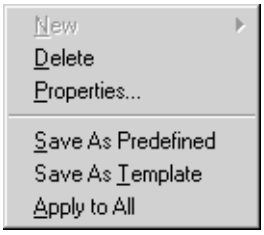
It does not matter whether the original is a peak, peak template, or reference peak; it can be used to define any (or all) of these.

To save a peak as predefined,

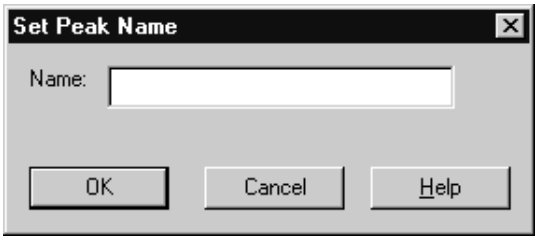
1. You must already have defined a peak (peak template, reference peak). If you want the peak saved under a name other than its existing default name, use the General tab page of the Edit Peak Properties dialog box to change the name.

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2. Put the cursor on the peak label and click the right mouse button.

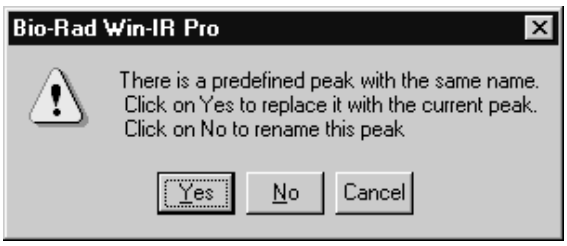


3. Select Save As Predefined. The peak will be saved under its existing name. If the peak has no name (for example, if you deleted the name), then the Save Peak Name dialog box appears.



Enter a meaningful value for Name.

4. If the name of the peak already exists in the predefined peak file, this message appears.



Yes: replace the existing predefined peak with the new one.
No: return to the Set Peak Name dialog box.
Cancel: return to the main screen without predefining a peak.

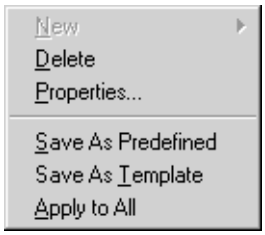
You can predefine as many peaks (peak templates, reference peaks) as desired.

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GLOBAL PEAK PREFERENCES

You can globally set the style of the peak labels—that is, are the labels to be horizontal or vertical, what values are to be displayed, how many decimal points should be shown, what mode is the peak to be (height, area, center), etc. After you have selected a peak with the desired style.

1. Select the peak that is to be used as your standard. Put the cursor on the peak label and click the right mouse button. This menu appears.



2. If you select Save as Template, then all subsequently created peaks, in any trace in this type of document (multi-spectral, kinetics, etc.), will use the style defined for this peak. Style includes such parameters as Value, Baseline Definition, Label Content, Label Direction, etc.

3. If you select Apply to All, then all existing peaks, in any trace in this document, will use the style defined for this peak. Style includes such parameters as Value, Baseline Definition, Label Content, Label Direction, etc.

Note

You can select both options, if desired.

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3
Main Screen and Document Types

OVERVIEW

Documents are used to collect and manipulate spectra. Each document can contain more than one spectrum; any number of documents can be open at any one time.

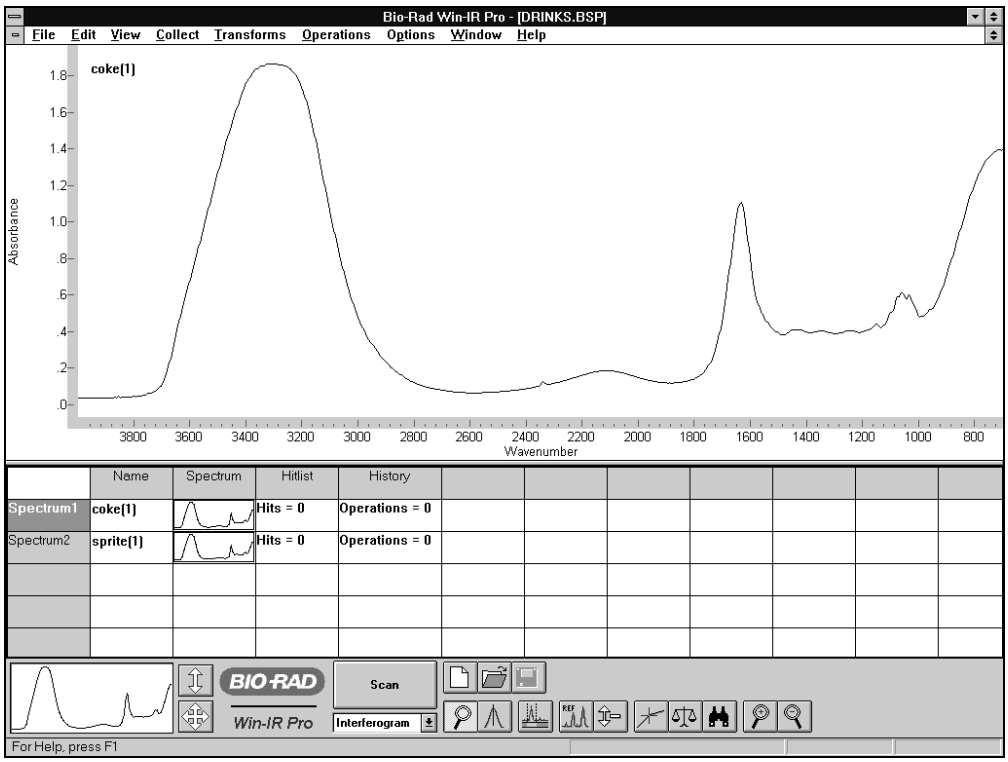
Documents

There are three basic formats for Win-IR Pro documents—multi-spectra, kinetics, and image.

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When spectra are collected into a Multi-Spectral Document, the latest spectrum is put at the top of the spreadsheet. As spectra are collected into a Kinetics Document, the latest one collected is put at the bottom of the spreadsheet.

Multi-Spectral Documents: this type of document may contain a number of spectra. They do not necessarily have to have any systematic relationship to each other. Therefore, these spectra are accessed either through their location in the document (View / Go To, discussed in Chapter 8), or, more commonly, by selecting a spectrum in the spreadsheet which displays a row of information for each spectrum in the document. The spreadsheet is discussed briefly in this chapter and, in much more detail, in Chapter 4. Multi-Spectral Documents can contain interferograms, single-beam spectra, ratioed spectra, and chromatograms. These may have been collected under Win-IR Pro or imported from the 3200 series data systems or from Win-IR or GRAMS. A typical Multi-Spectral Document is shown below.



This document contains two spectra; Spectrum 1 has been selected.

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The following documents may be thought of as special types of Multi-Spectral documents.

Background Documents: contain a background single-beam spectrum collected for use in ratioing the sample single-beam spectrum to obtain a transmittance, absorbance, etc. spectrum. Background spectra for either Multi-Spectral Documents (*.bkg) or Kinetics Documents (*.kbg) are stored in this way.

Note

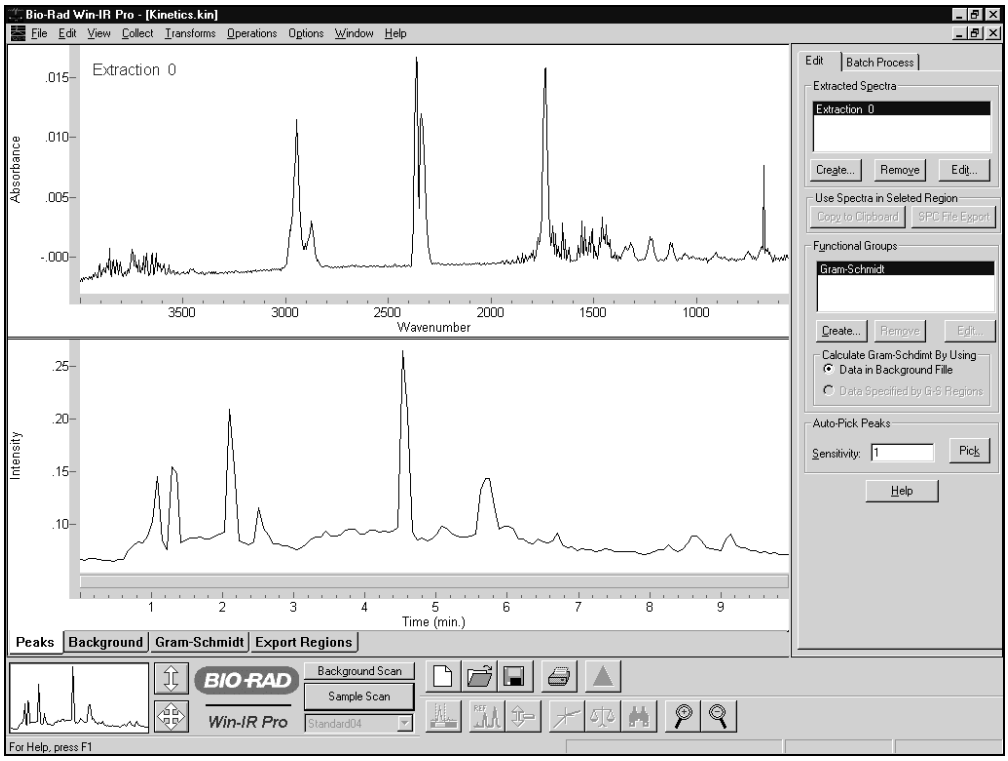
When you archive documents, it is a good idea to also archive their background spectra to allow for future reprocessing (see Chapters 5 and 11 for details about reprocessing spectra).

Calibration Documents: contain spectra either collected directly into them or copied into them from other documents. They also contain the concentrations of the components for each spectrum as well as a least-squares calibration of the concentrations to the spectra (see Chapter 11 for details).

Library Documents: may be thought of as a collection of chemically related spectra collected under standard conditions. Bio-Rad supplied libraries are read-only and are accessed through Operations / Search. You can browse a library by using File / Open, but you cannot search it that way.

Kinetics Documents: the spectra in this type of document are all explicitly related to each other. They are the spectra of a system or process as it evolves in time. Some examples of this include gas chromatography (GC), thermogravimetric analysis (TGA), and kinetics spectra. Individual spectral in this type of document are accessed through the spreadsheet (the default is for the spreadsheet to be hidden) or through the chromatogram (seen in the lower part in the example below). Details of the kinetics document are discussed later in this chapter.

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Views

Some data presentations appear to be documents, but are actually views of the data. They are presented in document format to allow consistent use of the viewing and manipulation features of Win-IR Pro.

Search Hit List: presents the sample spectrum above the row of column labels in the spreadsheet. The hits are listed below, one spectrum per row, in decreasing goodness of fit, that is, the best hit is at the top of the list. Search hit lists are discussed in Chapter 11.

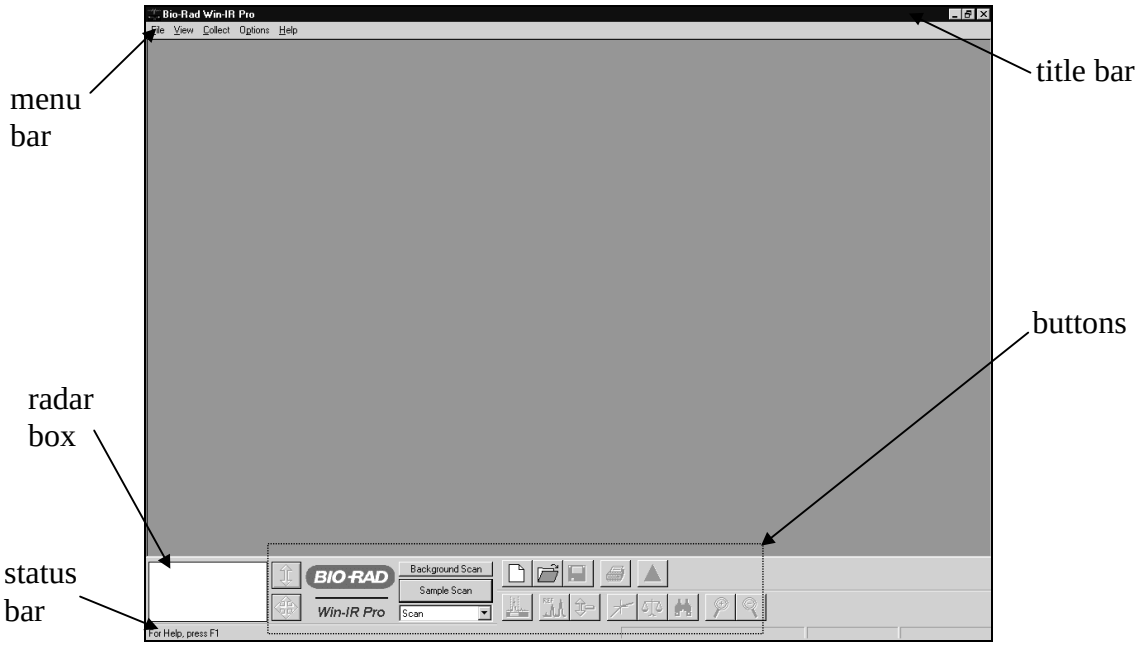
Three-dimensional views: are generated from sets of kinetics spectra (View / 3D; see Chapter 8), from in-phase/quadrature spectra or series of spectra (Operations / 2D-IR, see Chapter 11) or from PAS spectra (Operations / Spectral Arithmetic / 3D Interpolation, see Chapter 11). These views allow for a two-dimensional presentation (by contours, colors, and isometrics) of the three-dimensional data.

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COMMON FEATURES

There are many features, such as buttons, menus, etc. that are common to all types of documents.

Before any documents are opened, the screen looks like this.



There are two major actions you can take now.

Collect data which will automatically open a document of the proper type depending upon your choice from the Collect menu. This operation is discussed in the manual that came with your spectrometer.

Open (File / Open) an existing document for collection, manipulation, printing.

Notes

Multiple documents of one or more types can be open simultaneously.

Multiple views of one document can also be open simultaneously.

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Once any document is opened (using File / Open, for example), the full menu bar is displayed.

Title Bar

The title bar controls the usual Windows operations. If the document window is maximized, the name of the active document is displayed in the title bar.



Menu Bar



Each menu in the menu bar (File, Edit, etc.) is described in detail in its own chapter later in the book. The contents of the menus can change depending upon the type of the active document.

If no document is open, then only the menu subset below is displayed:



Status Bar

The text in the left side of the status bar gives a brief description of the results of clicking the button that the cursor is on. For example,



If the cursor is in the spectrum display window (and has been clicked), the X and Y coordinates of the cursor are shown in the right side of the status bar. For example,

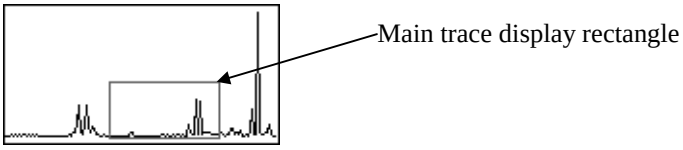


The status bar also shows the progress of an action—such as collecting data, errors, and other information as appropriate. It may be hidden using the View menu. This toggles of the √ beside its name in the menu.

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Radar Box

The radar box is at the lower left of the window. It displays the entire spectrum independent of what portion of the spectrum is displayed in the main trace window. The main trace display rectangle shows the portion of the spectrum shown in the main display. If you change the main display by zooming, autoscaling, altering X (and/or Y) limits, this rectangle will change to reflect what is visible in the main display.



The main trace display rectangle can be moved and resized by placing the cursor on it, holding down the left mouse button and dragging it. The main display changes as you modify this rectangle. Release the mouse button to stop altering the display. An example of this is shown in Chapter 1.

If you want to display a portion of the spectrum outside the current display, put the cursor in the radar box, hold down the left mouse button, draw a box around the portion to be displayed, and release the button.

Note

If a number of spectra are visible in the main display, the last one selected is shown in the radar box.

Buttons

The buttons at the bottom of the screen are used as shortcuts for commonly performed operations. Some are equivalent to a selection of an item from a menu. The details are discussed in the chapter for that menu.



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Autoscaling Buttons



Autoscales the trace in the Y direction. This is the same as selecting Autoscaled from the View menu.



Autoscales the trace in both the X and Y directions. This is the same as selecting Entire Spectrum from the View menu.

Scan



Collect data using rapid scan according to the named collect selected from the pull-down menu. If no scan is defined, the parameters of the current spectrum are used. Data collection and processing proceed as far as is specified by the Computation tab page of the collect.



Collect a background using rapid scan according to the named collect selected from the pull-down menu. If no scan is defined, the parameters of the current spectrum are used.



This is the Named Collects pull-down menu. Select the collect desired for scanning and, optionally, further manipulation. The creation and editing of named collects are discussed in your spectrometer manual.

File Buttons



Opens a new document of the type currently active. This is similar to selecting New from the File menu, except that with the menu you have a choice of document type.



Opens an existing document. This is the same as selecting Open from the File menu.



Saves the currently active document. This is the same as selecting Save from the File menu.



Prints the currenlty active document. Equivalent to selecting Print from the File menu.

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Raman Laser Button



Turns the Raman laser power on and off. To set the power level, you must select Raman Laser from the Collect menu.

Spectrum Buttons



Allows you to use the cursor to interactively define spectrum regions for future operations. Same as selecting Drag Region from the Operations menu.



Shortcut: Defines the currently selected spectrum as the reference spectrum for spectral subtraction. (Select Define Reference from the Transforms menu to choose any spectrum to be the reference spectrum.)



Shortcut: Allows you to perform interactive spectral subtraction using the currently defined reference spectrum. (Select Spectral Subtraction from the Transforms menu to choose any spectrum to be the reference spectrum.)



Allows you to perform interactive baseline subtraction to the active spectrum. Same as selecting Baseline Correct... from the Transforms menu.



Allows you to perform simple quantitative analysis on the active spectrum. Same as selecting Quantitative Analysis / Simple from the Operations menu.



Allows you to begin searching libraries for a match to the active spectrum. Same as selecting Search from the Operations menu.



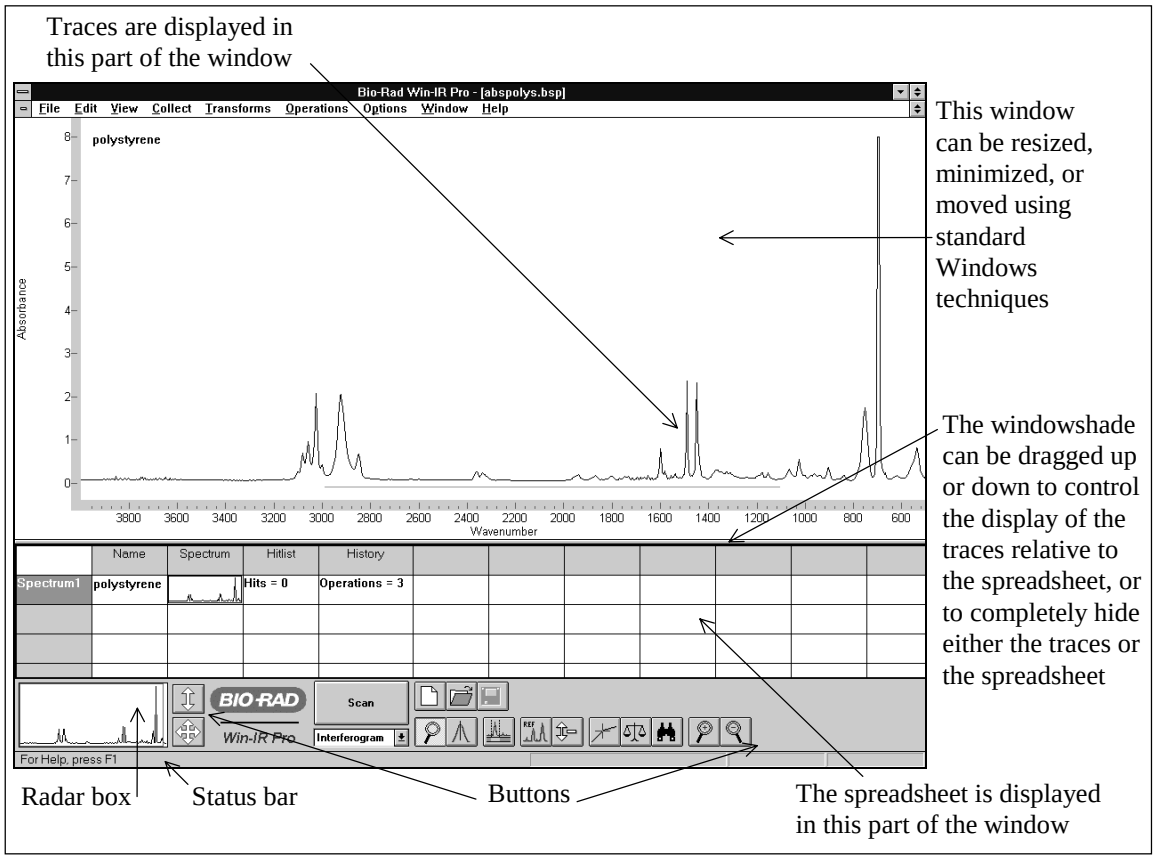
Approximately doubles the height of the y-axis of the trace. Same as selecting Zoom In from the View menu.



Approximately halves the height of the y-axis of the trace. Same as selecting Zoom Out from the View menu.

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MULTI-SPECTRAL DOCUMENT WINDOW



The multi-spectral document window can contain multiple spectra. It has a trace display and a spreadsheet display. The spreadsheet can be hidden by selecting Maximize traces from the Window menu (or press F11 on the keyboard). The traces can be hidden by selecting Maximize spreadsheet from the Window menu (or press F12 on the keyboard).

You can adjust the division of the document window by placing the cursor on the bar between the trace display and the spreadsheet. The cursor changes to ⇳. Hold down the left mouse button and drag the bar up to increase the spreadsheet display area or down to increase the trace display area. When the partition is satisfactory, release the mouse button.

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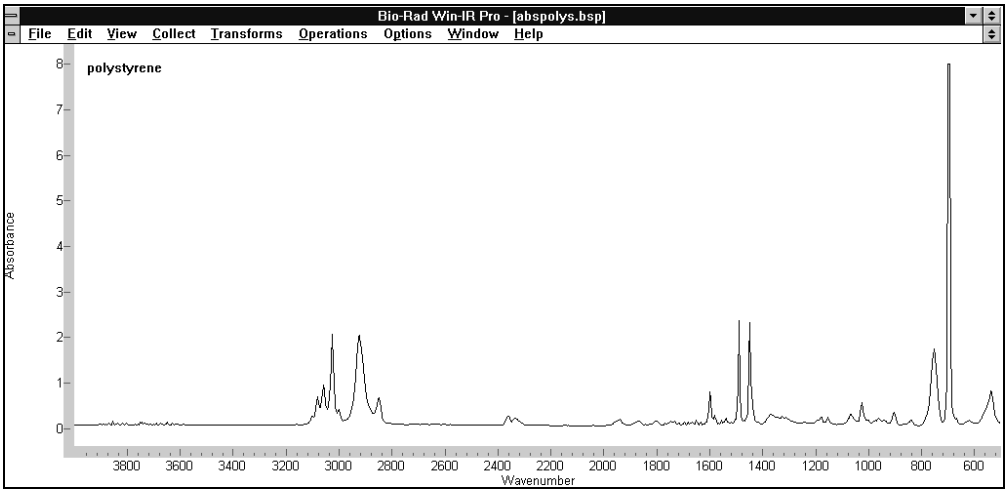
Certain operations (for example, by selecting Trace Control Bar from the View menu), cause a dialog box to appear on the right-hand side of the window. In this case, the trace display is automatically resized. However, the spreadsheet display is not resized; if the columns are full, a horizontal scroll bar appears at the bottom of the spreadsheet display.

Spectra within a document can be selected either through the trace display or through the spreadsheet; see below for details. A spectrum selected through the spreadsheet is always both visible and selected for operations. Spectra in the trace display can be made visible but not selected for operations; this is true even if the spectra were originally selected through the spreadsheet.

Locking/Unlocking a Spectrum into Display

Spectra can be locked into the main display (or unlocked) using Lock Selected (or Unlock Selected) from the View menu (see Chapter 6).

Trace Display



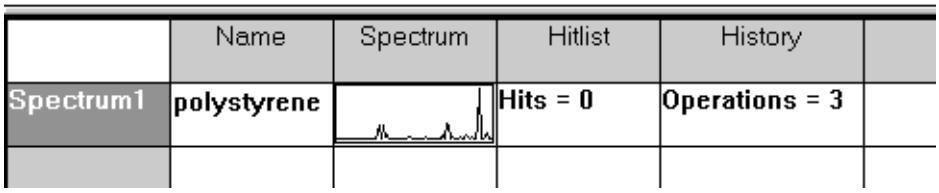
The trace(s) is displayed in the upper part of the window. The label in the upper left (polystyrene in this example) is the text in the Name column of the spreadsheet.

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Spectrum Selection using the Trace Display
A spectrum (or set of spectra) selected for operations are displayed in green; unselected traces are displayed in other colors.

- Single spectrum selection: place the cursor on the trace and click the left mouse button. If you click on another trace, that spectrum becomes selected and the first spectrum is deselected. This does not affect their visibility.
- Multiple spectra selection: place the cursor on the trace and click the left mouse button; the spectrum is selected. Place the cursor on the trace of any other spectrum, hold down the CTRL key and click the left mouse button; this second spectrum is also selected. This process can be repeated as desired. Using control-click, any spectrum can be toggled between selected and deselected without affecting the status of any of the other spectra.

Spreadsheet

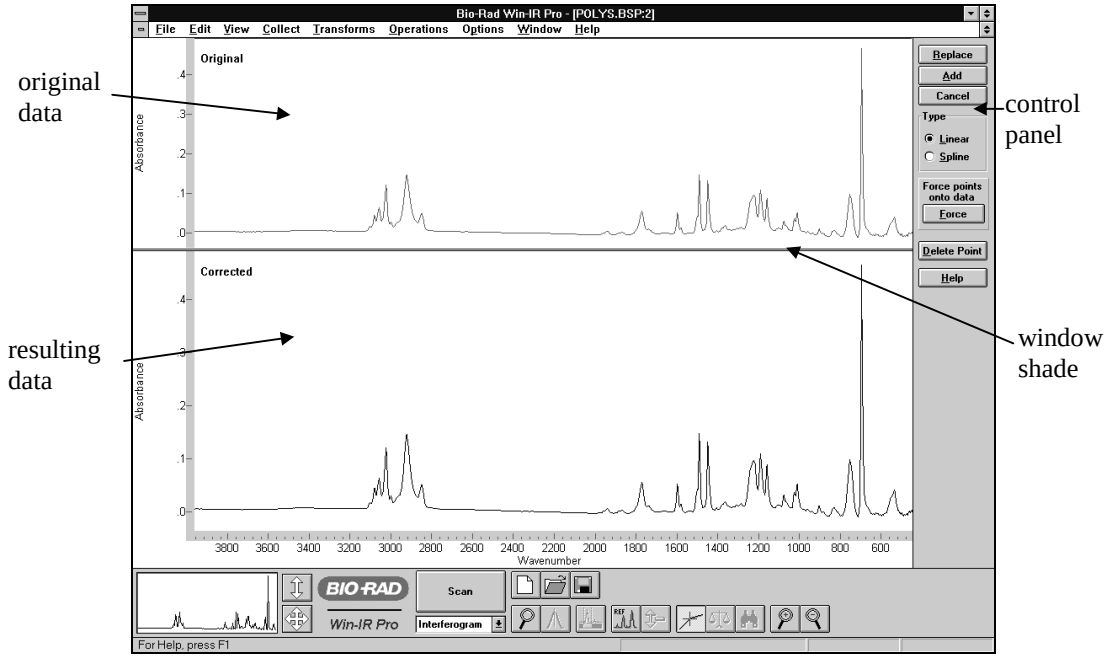


The spreadsheet presents information about each trace in the document, one row per trace. It provides direct access to each trace in a multi-spectral document. If there are too many spectra in the document to fit in the spreadsheet box, a vertical scroll bar automatically appears to allow access to all spectra. Details of the spreadsheet are given in the chapter “Introduction to the Spreadsheet.”

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General Layout of Transforms Programs

When invoked, many of the transforms (see Chapter 8) present a common appearance. They split the screen and place a control panel sidebar on the right side of the window. Below, Baseline Correct is used as an example.



The original trace is in the upper half of the split screen; the modified trace is in the lower half of the split screen. (Since nothing has been done yet, the two traces are currently identical.) After completing the transform, you can replace the original trace with the transformed one (click Replace), add the transformed trace to the document along with whatever traces were originally there (click Add), or cancel the entire procedure (click Cancel). All three choices return you to the main screen. Details of each transform are in Chapter 8.

Note

Zooming, scrolling, and the radar box are still active in these programs.

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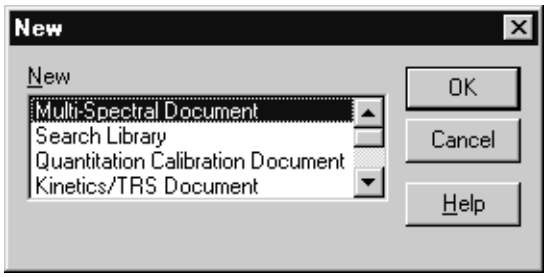
SEARCH LIBRARY DOCUMENT WINDOW

You can create and edit your own search libraries; you cannot edit the search libraries supplied by Bio-Rad. Before you can create a Search Library document, you must define the parameters of the library. Select New from the File menu; the New dialog box appears.

Note

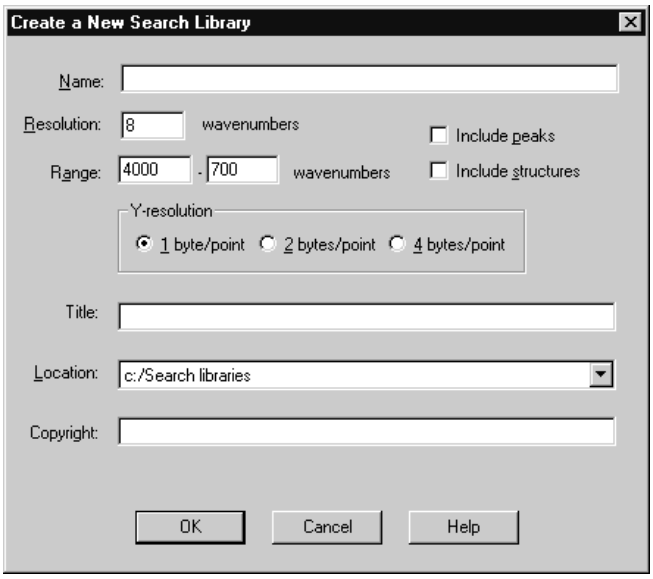
In order to create a search library, you must have at least 9 Megabytes free on your hard disk for temporary files, etc. Most of this memory is released when the library is made read-only and/or closed.

You need an additional 3 Megabytes each if you include peaks and structures (see below).

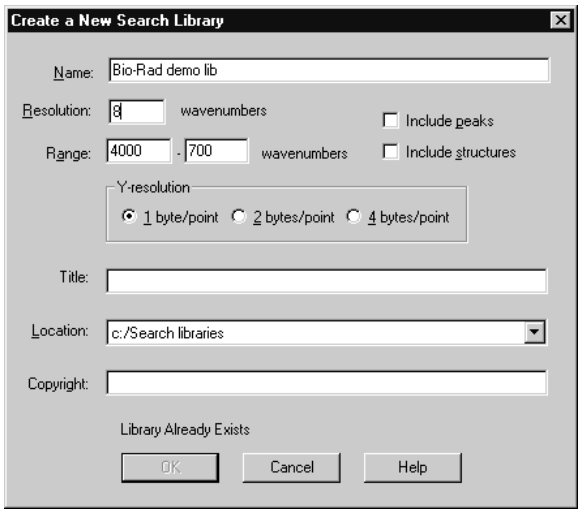


Now select Search Library and click OK. The Create a New Search Library dialog box appears.

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Name: the filename under which the Search Library will be stored. This name must conform to all Windows NT file names convention. Do not use the name of an existing library. If you enter the name of an existing library, the OK button will be disabled and the message Library Already Exists will appear above it.



Delete this Name entry and the OK button is re-enabled; the message disappears.

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Resolution: the resolution (data point spacing, in cm^{-1}) of the spectra in the library. If a spectrum was collected at a lower resolution, points will be interpolated. If a spectrum was collected at a different resolution, it will be resampled and it will either be smoothed or have points interpolated. Normally, there is no reason to have the library at a higher resolution than that of the spectra. Setting a higher resolution increases the space needed for the library and also increases the search time. We recommend that the resolution be set at 4 cm^{-1}.

Note

Digital resolution is the spacing between points in the data file (typically, a library). Interpolating values between existing points increases the digital resolution.

Optical resolution of a spectrum a function of the collecting instrument and the collection parameters. Once a spectrum is collected, its resolution is fixed and cannot be improved.

Range: the upper and lower limits (in cm^{-1}) of the library spectra. If you add a spectrum to the library whose range exceeds those limits, it is truncated. If you add a spectrum to the library whose range falls inside those limits, it is extended with zeros to the limits. The default range is 4000 to 700 cm^{-1}.

Include peaks: if checked, any peak tables in the spectra being copied will also be copied into the Search Library.

Include structures: if checked, any [molecular] structures in the spectra being copied will also be copied into the Search Library.

Caution
If you create a library without structures or peaks they cannot be added later.

If you later want to add structures or peaks, you must create a new library—including those features—and copy the spectra into that library. You can then enter structures or peaks into the newly created libraries.

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Y-resolution: the number of bytes (8 bits/byte) that will be used for the Y-axis scale. The default is 1; this value is recommended for library searches. Increasing the Y-resolution increases the size of the Search Library document.

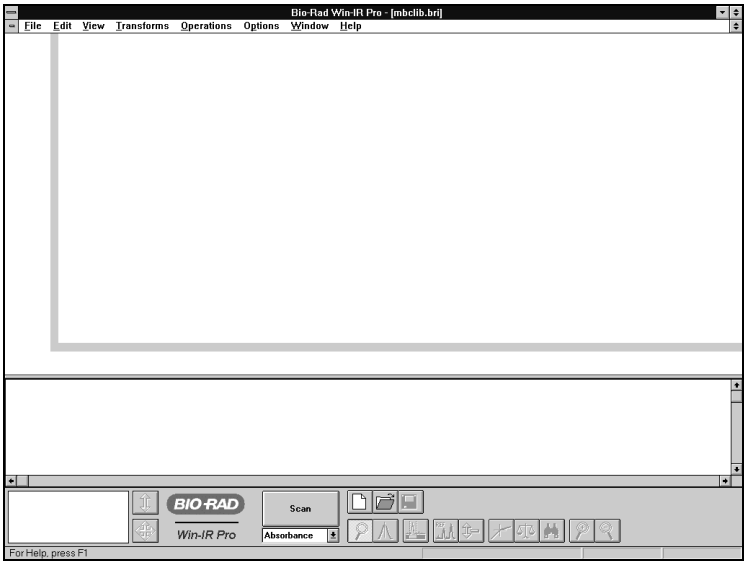
Y-resolution	Y-axis range
1 byte/point	0-255
2 bytes/point	0-511
4 bytes/point	0-1023

Title: a text string describing the contents of the Search Library. This will appear in the description when this library is highlighted in the Search Library Selection dialog box (see Chapter 11).

Location: the directory in which the search library will be stored. Click on the pull-down menu arrow and select a directory pathname. The default value is c:\Search libraries. Additional pathnames can be added to this list through the Search Library Path dialog box (see Search, Chapter 11 for details).

Copyright: a text string which will appear for each entry in the library. This will be the contents of the copyright column in the hit list after a search.

After the values are entered, click the OK button. An empty Search Library document is opened.



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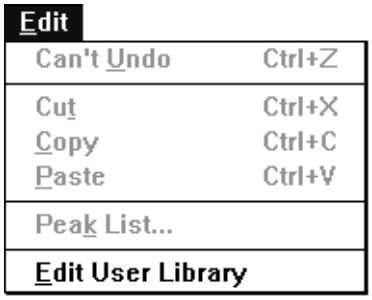
The empty Search Library document looks like a Multi-spectral document except that the Collect menu is absent. You cannot collect into a Search Library document. Spectra must be collected elsewhere and copied into the Search Library document.

When a Search Library document is created, it can be both read from and written to; you can add spectra, delete them, etc.. If you want to make it read-only, deselect Edit User Library from the Edit menu.

Notes

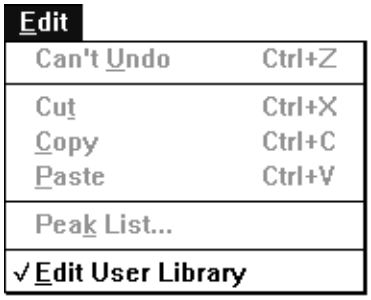
Writeable libraries are significantly larger than the read-only form. The library size decreases when the library is made read only again. If there is not enough room to make a library writeable, switch to File Manager, delete files, compress files, or move them to another disk, and try again.

When you make a library writeable, it cannot be accessed from any other copy of Win-IR Pro that is running. Any attempt to do so will result in a message saying that the library is not accessible. When the library is made read-only or closed, it can then be read by any number of copies of Win-IR Pro.



The library is read-only.

The library can be searched.



The library is writeable.

The library can be searched.

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Once the library is writeable, you can add spectra and edit their rows in the spreadsheet. Spectra can be copied using the Edit / Copy and Edit / Paste commands, or they can be dragged from a spreadsheet in another document into the Search Library document's spreadsheet (see Chapter 4 for details).

After a spectrum is copied into the Search Library document, its row in the spreadsheet can be edited. The usual columns in a search library document are: Name, Spectrum (a small plot of the spectrum), Copyright, and Chem Structure.

Caution

If you delete a spectrum from the library, it is marked as deleted and the spectrum is set to 0 (zero) over the entire range; the slot originally used by this spectrum is still assigned—it is not automatically removed or overwritten by another entry. When this library is searched, this entry is skipped. However, if you edit the name of a spectrum marked as deleted (for example, double-clicking in the name cell of this entry), the spectrum will no longer be considered as deleted but as a zero-value spectrum; it will be searched. The methods of the comparison algorithms will often give a high hit quality index for a zero-valued spectrum and it will appear high in the hit list.

Once you have deleted a spectrum, adding a new spectrum to the library should fill the slot marked as deleted.

When you have completed added spectra to the Search Library document and (optionally) editing their spreadsheet rows, make the Search Library document read-only by selecting √ Edit User Library from the Edit menu.

Saving the Library

Unlike the rest of Win-IR Pro, libraries are edited as if they were a data base program—all changes are saved immediately to the file whose name you specified in the Create a New Search Library dialog box. Therefore, the File / Save entry is disabled (grayed out).

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When you are finished the current session of editing the library, close it by selecting Close from the File menu. This will make the library read-only, make any final saves necessary, and close the library. You can now use this library in searches; see Chapter 11 for details.

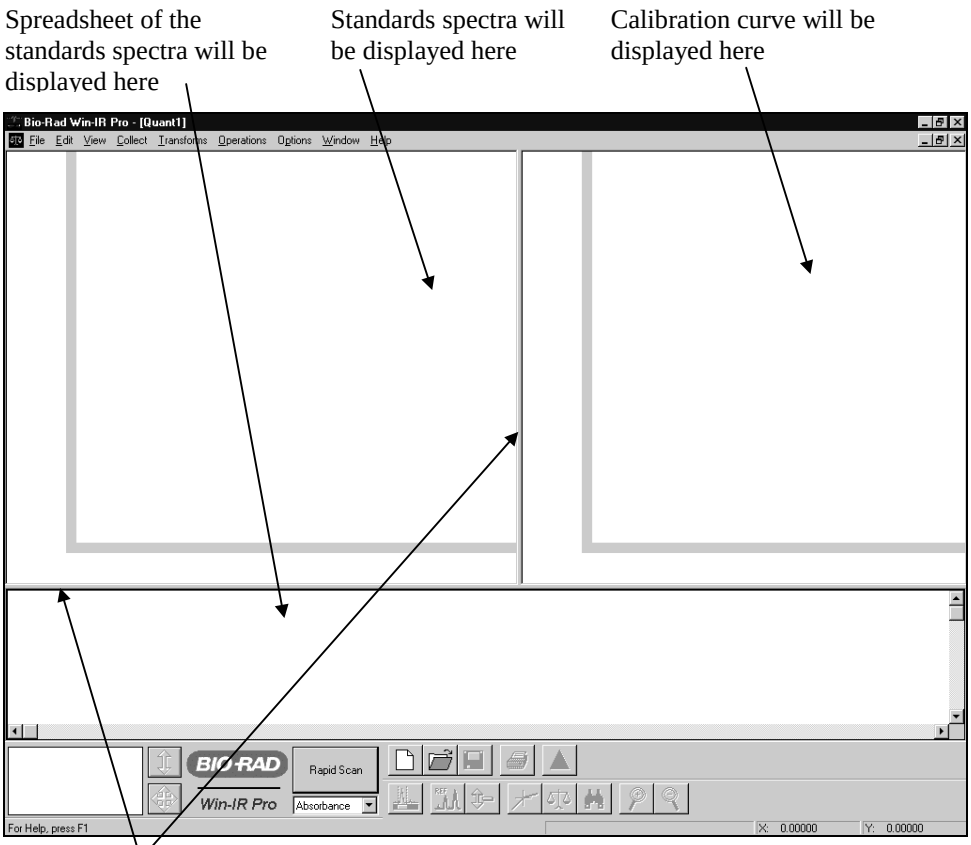
Note

If you create a library and save it, you can open it at a later time and add additional spectra using the procedure above. You can also delete spectra from your library by selecting that spectrum and pressing the Delete key. See Chapter 4 for details of the spreadsheet operations.

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QUANTITATION CALIBRATION DOCUMENT WINDOW

When a new quantitation document is opened, it looks like this:



windowshades—move horizontal windowshade to view/hide spreadsheet; move vertical windowshade to partition screen between standards spectra and calibration curve

The Quantitation Calibration Document window has the same structure as the Multi-Spectral Document window with the addition of a calibration curve window on the right. An example of the creation of the calibration curve is given in the “Quantitative Analysis” section of Chapter 11. The following is a brief overview of quantitative analysis calibration. A more complete discussion of the theory and practice is given in Appendix I.

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1. Create standard samples using known concentrations of compounds. These compounds are those expected to be in samples to be analyzed, and whose concentrations in those samples is to be determined.

2. Collect the spectra of these standard samples either directly into document, or copy previously collected standards spectra into it, using Win-IR Pro's Edit / Copy and Edit / Paste menu entries..

3. Select a feature of the spectrum—usually a peak—that changes when the concentrations change.

4. Enter the concentrations of each component each spectrum into the document.

5. Do a least squares fit between the concentrations and the spectral features you have selected; this is normally linear, following Beer's Law that absorption is a linear function of concentration. Sometimes, the chemistry or physics of the situation may cause a deviation from linearity, especially at higher concentrations; in that case, the data are fitted to a quadratic curve (see Appendix I).

Note

Normally, the calibration equation should be overdetermined. That is, there should be more standards spectra than are required for a mathematical fit to the calibration curve (exact fits are provided by 2 standards for a linear, and 3 for a quadratic calibration curve). This allows statistical and random noise to be averaged out.

6. Use this calibration curve to determine the component concentrations of the unknown samples (see Chapter 11)

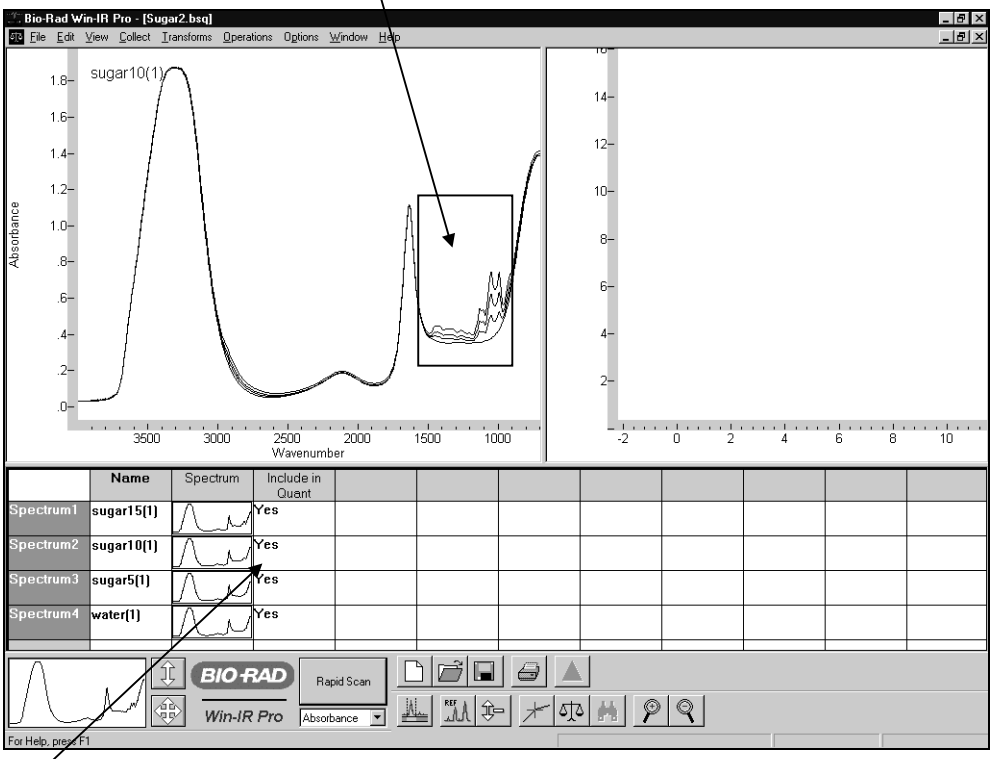
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After the document contains standards spectra, it looks like this.

Note

The horizontal windowshade has been raised slightly to view the entire spreadsheet.

In this example, this is the region of the spectra that changes with the changes in concentration



By default, all spectra are initially included in calculating the calibration curve. Double-click in the cell to exclude any spectrum. The contents change to No

Use the right mouse button menu to define a Component. Once this is done, you can use all the peak editing tools available to define the peak parameters—select Properties from the right mouse button menu. You can adjust the center, edges, and/or baselines of the component. These edits are done exactly the same as for any peak. You can also decide whether the calibration will be based upon peak area, peak height, ratio of peak areas,

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or ratio of peak heights. Use the General tab page of the Edit Peak Properties dialog box to define whether area or height is to be used.

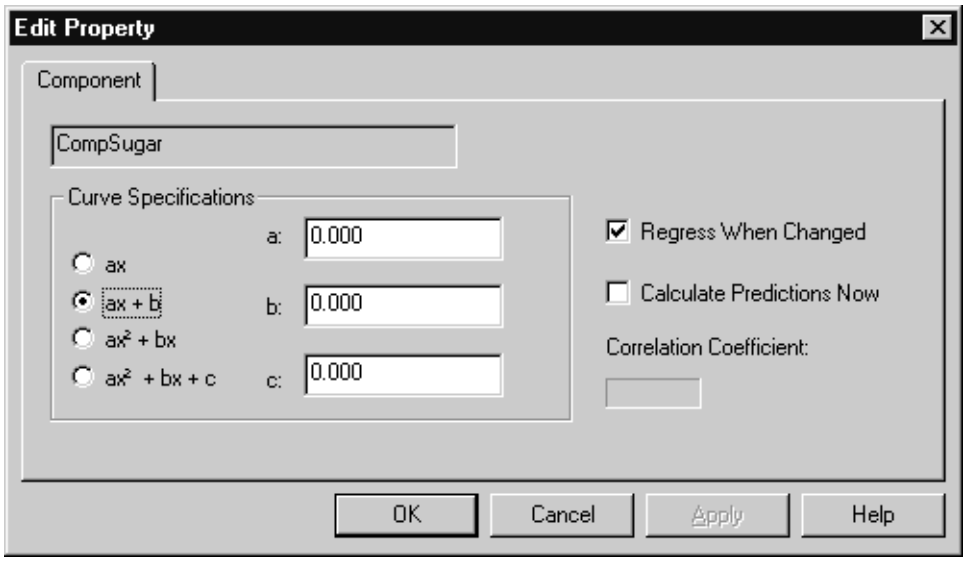
Note

If a ratio of height or area is to be used, first define the reference peak against which the component is to be ratioed; then use the General tab page of the Edit Peak Properties dialog box.

Calibration Curve Window: to control the details of the calibration curve.

1. Put the cursor in the right hand side of the screen and click the right mouse button.

2. Select Properties from the menu. The Edit Property dialog box appears.



Component: identifies the component of the spectra being used to establish the correlation curve.

Curve Specifications: select the equation for the curve that is to be fitted to the data points. The Apply button is enabled; click the Apply button for a new calibration curve. The coefficients of the equation will change and be

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displayed in a, b, c.

If you want to fit data to a predetermined curve, select the type of equation and enter the values of the coefficients.

Regress When Changed: if selected, the equation coefficients will change if the curve type is changed and Apply is clicked. The Correlation Coefficient will be displayed with the calibration curve.

Calculate Predictions Now: when selected, his creates a new column in the spreadsheet; CompSugar (Predicted) in this example shown below. These are the concentration values calculated from the calibration curve for the absorbance values in the standards spectra. Note that, as expected, they are close to the nominal values.

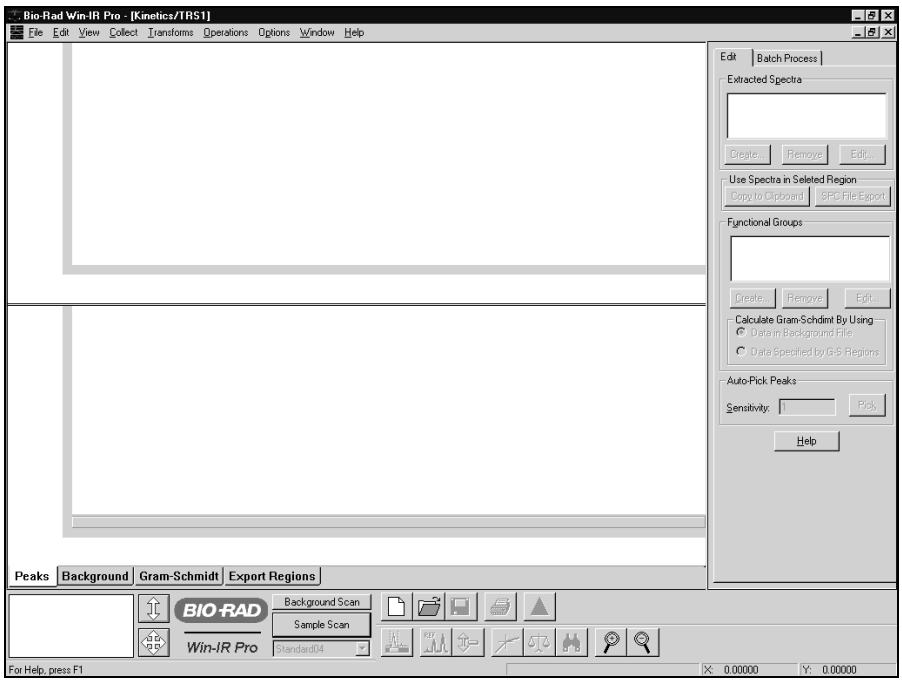
Correlation Coefficient: displays the calculated correlation coefficient.

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KINETICS DOCUMENT WINDOW

This document is used to collect kinetics data and step-scan TRS data.

A new kinetics document looks like this.



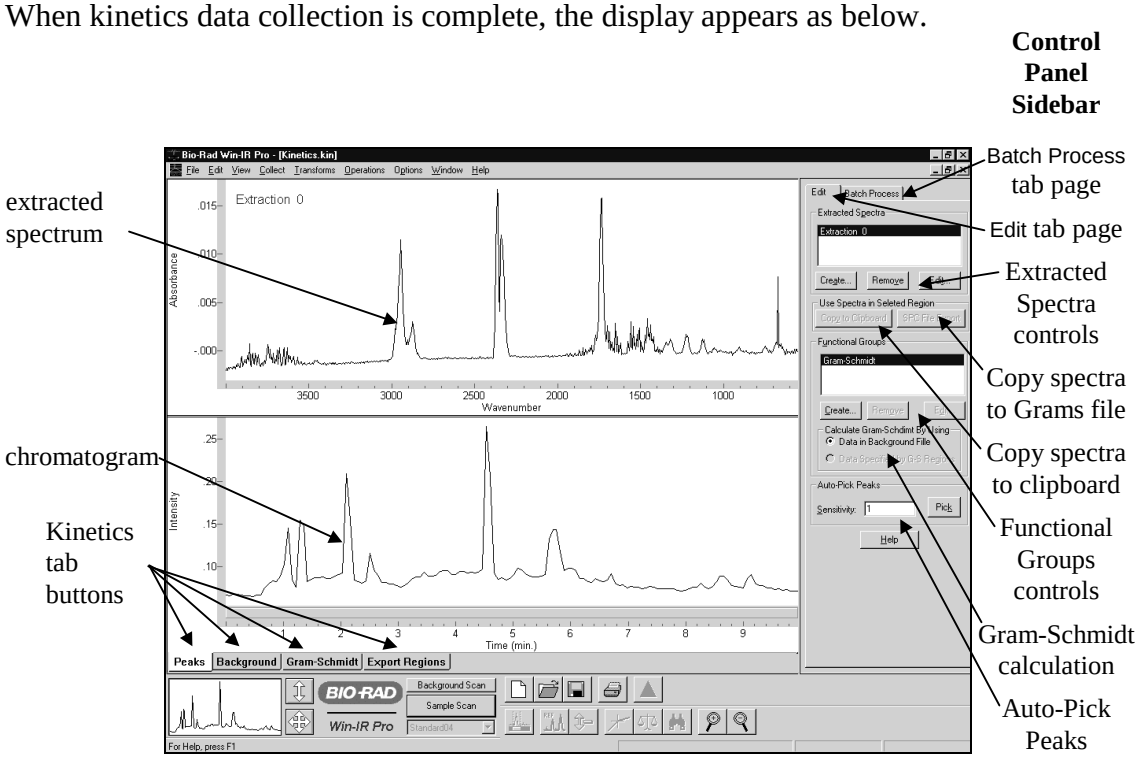
Collect data into this document following the instructions in the spectrometer manual supplied with your particular spectrometer.

Note

A kinetics background is collected into a separate kinetics background document. It may be collected either before or after collecting the kinetics data. It must exist before you ratio the kinetics data.

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When kinetics data collection is complete, the display appears as below.



Trace Display: The last spectrum collected is displayed in the upper part of the document window. The Gram-Schmidt chromatogram is displayed in the lower part of the document window.

Tab Buttons: These buttons control the activation of the ruler bars in the trace windows. They also control the type of spectrum or Gram-Schmidt basis vectors selected from a region.

Peaks: activates the ruler bar in the lower window. When you define a region by dragging the cursor, an extracted spectrum is created by co-adding the individual spectra in this region.

Background: activates the ruler bar in the lower window. When you define a region by dragging the cursor, a background spectrum is created by co-adding

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the individual spectra in this region. This background can be used as the background for any extracted spectrum in the document. .

Gram-Schmidt: activates the ruler bar in the lower window. When you define a region by dragging the cursor, it defines the interferograms from which the Gram-Schmidt basis vectors are calculated. If you define more than one region, information from all the interferograms in all the regions are used to calculate the Gram-Schmidt basis vectors. .

Export Regions: activates the ruler bar in both the upper and lower windows. In the lower window, define a region to define the spectra to be copied when you select Edit / Copy. You can then Edit / Paste the spectra into a .bsp document. You can also paste the defined spectra into a Grams file. In both the lower and upper windows, the spectra and wavenumber range of those spectra in the defined region can be used to display the information in 3D or to perform the generalized 2D algorithm calculation.

Control Panel: The lower part of the control panel (Functional Groups) initially selects the Gram-Schmidt chromatogram which is based upon the entire spectrum.

The upper part of the control panel (Extracted Spectra) initially selects the last spectrum collected. It is labeled Extraction 0. The Extraction Template is chosen to be Extract at time, and the time of the end of the data collection is displayed in the Time box.

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Kinetics Document Control Panel—Edit page

Both functional groups and extracted spectra can be defined on the edit page.

Functional Groups: there are two mechanisms to define and label functional groups

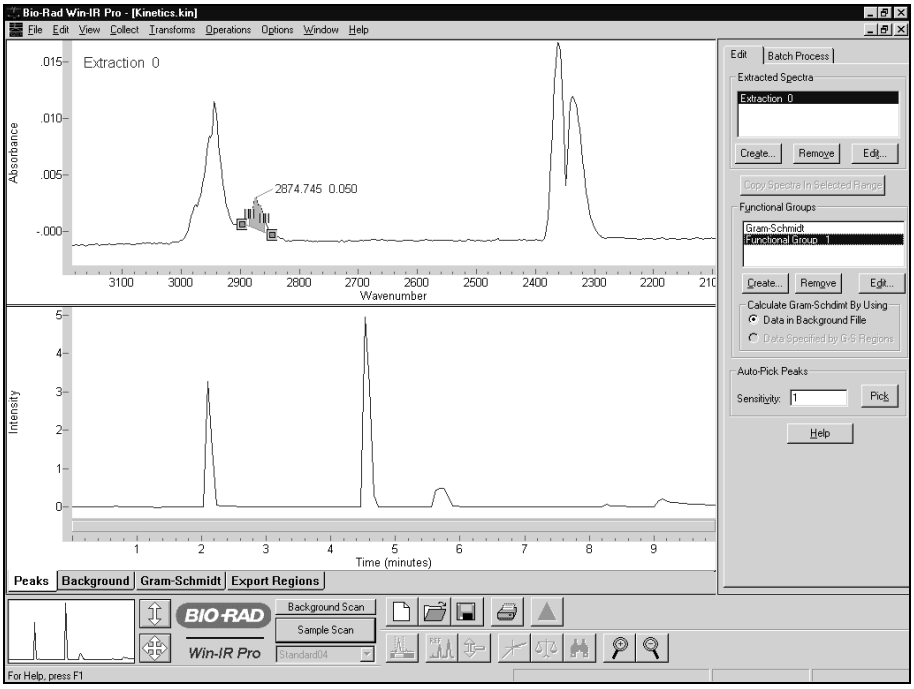
- use the right mouse button in the extracted spectra part of the window
- use the Functional Groups part of the control panel.

The functional groups defined are displayed in the lower part of the document window.

To create a functional group using the right mouse button:

1. Zoom in on the area of interest in the upper part of the document window.

2. Put the cursor on the peak that specifies the functional group. Click the right mouse button and select Functional Group from the submenu. The functional group so defined appears in the lower part of the document window. Its name, Functional Group 1, appears in the control panel sidebar.



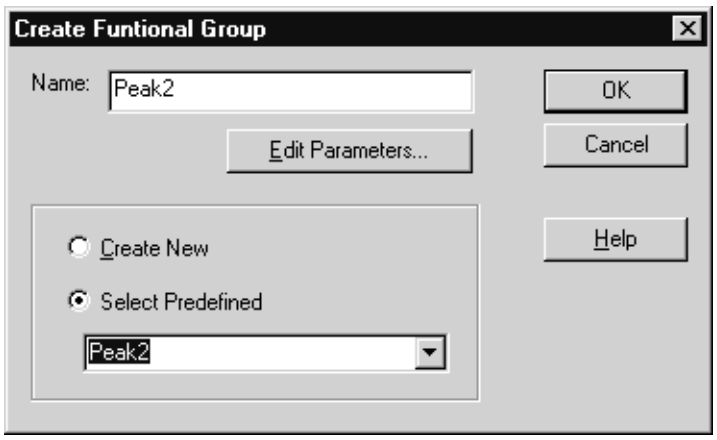
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Note

The other choices—Peak, Reference Peak, Region, Vertical Line, and Position Label function exactly the same as for multi-spectral documents. See Chapter 2 for details.

To create a functional group using the control panel sidebar:

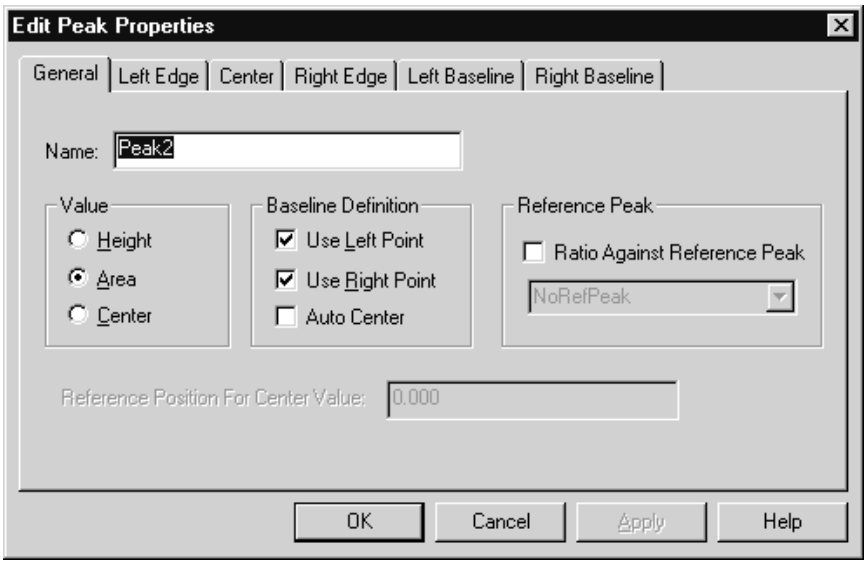
1. Press the Create button; the Create Functional Group dialog box appears.



   In this example, a predefined peak exists. If you want to use another predefined peak, select it from the pull-down menu. You can accept the existing name of the predefined peak or enter a different one in the Name: window. Then, click the OK button to create a functional group.

2. If you do not want to use a predefined peak to create the functional group, select Create New and click the Edit Parameters button. The Edit Peak Properties dialog box appears.

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3. You can accept the default name or enter your choice for the functional group.

4. In the dialog box, use the tab pages to enter values to define the peak, or the region about the peak, for which the functional group chromatogram will be displayed in the lower part of the document. These are described in detail in Chapter 2. Some special items

Center

At Point: the chromatogram is calculated for the specific chosen point of the spectrum. Win-IR Pro will find the actual value on the x-axis (in wavenumbers) for that peak and replace the approximate value you have entered.

At Extreme in Region: the more common method is to define a region about a peak; then, Win-IR Pro will find the x-value of the maximum excursion from zero in that region and use that value.

Note

If kinetics or TRS bands go negative, use Extreme in Region to track the absorbance at a single point. Unlike Win-IR Pro at Release 2.3 and earlier, the extreme in

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region is the maximum excursion from zero, whether this excursion is positive or negative.

Edges
Left Edge: upper value for functional group chromatogram region.
Right Edge: lower value for functional group chromatogram region.

Baselines
Baseline Left: value defining the baseline at wavenumbers higher than the region.
Baseline Right: value defining the baseline at wavenumbers less than the region.

Note

In some cases, as in this example, the structure of the spectrum does not allow for reasonable left and right baselines to be defined. In this case, Win-IR Pro will choose to set both baseline values equal to the one that is reasonable.

OK: return to the Create Functional Group dialog box with the new values selected for the parameters.

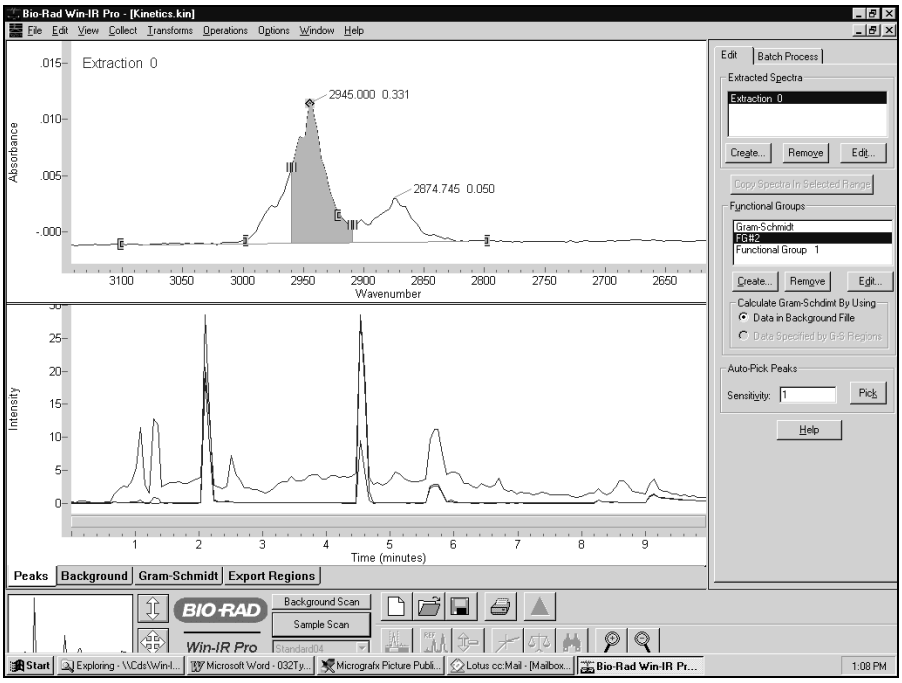
Cancel: returns to the Create Functional Group dialog box with the values in effect since the last use of the Apply button.

Apply: when this button is clicked, the existing set of values is saved. The Cancel button does not return the parameters to their original values.

Help: enters the on-line help system.

5. Click the OK button to define the functional group. Click the Cancel button to return to the Kinetics document without creating a new functional group. The example here has been named FG #12.

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Modifying Functional Groups: There are three methods to modify the definition of a functional group, or to change the label and/or the parameters displayed. See Chapter 2 for details of each method.

1. Select the peak in the extracted spectrum that defines the functional group. Use the cursor to interactively change the center, edges, and/or baselines as desired.

2. Select the peak in the extracted spectrum that defines the functional group. Put the cursor on the label or in the active area under the peak and click the right mouse button. Select Properties from the sub-menu. The Edit Peak Properties dialog box appears. Use the tab pages to alter the properties.

3. In the control panel sidebar, highlight the name of the functional group to be edited. Click the Edit button. The Edit Peak Properties dialog box appears. Use the tab pages to alter the properties.

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Removing Functional Groups: There are two methods for removing a functional group.

1. Select the peak in the extracted spectrum that defines the functional group. Put the cursor on the label or in the active area under the peak and click the right mouse button. Select Delete from the sub-menu.

2. In the control panel sidebar, highlight the name of the functional group to be removed. Click the Remove button.

The functional group is removed from the list and its chromatogram is no longer displayed in the lower part of the window.

Notes

You cannot remove the Gram-Schmidt chromatogram. If you do not wish it to be displayed, select Hide Gram-Schmidt Chromatogram from the View menu. The Gram-Schmidt label disappears from the list and the chromatogram is no longer displayed.

To redisplay the label and the Gram-Schmidt chromatogram, select Show Gram-Schmidt Chromatogram from the View menu.

The Hide/Show Gram-Schmidt Chromatogram menu entry is available only in an opened kinetics document.

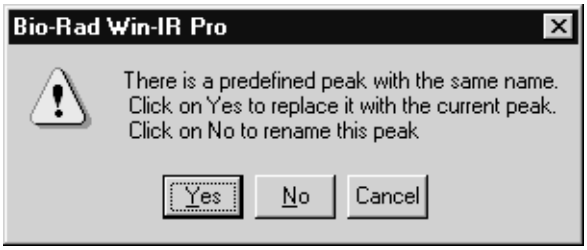
Global Functional Groups: you can save the parameters of the functional group so that this functional group can be used for all kinetics documents (global functional group). To define a global functional group:

1. Create a functional group using one of the methods described above.

2. Select the peak in the extracted spectrum that defines the functional group. Put the cursor on the label or in the active area under the peak and click the right mouse button. Select Save as Predefined from the sub-menu. The predefined peak will be saved using the existing name of the peak.

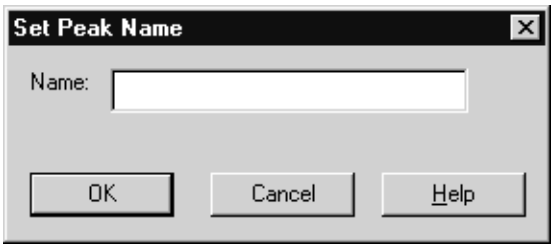
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If there is an already existing predefined peak with this name, the Bio Rad Win IR Pro dialog box appears.



3. Yes: replaces the existing predefined peak with the newly defined one.

   No: The Set Peak Name dialog box appears.



4. Give the global functional group a meaningful name and click the OK button.

   If you decide not to create a global functional group, click the Cancel button.

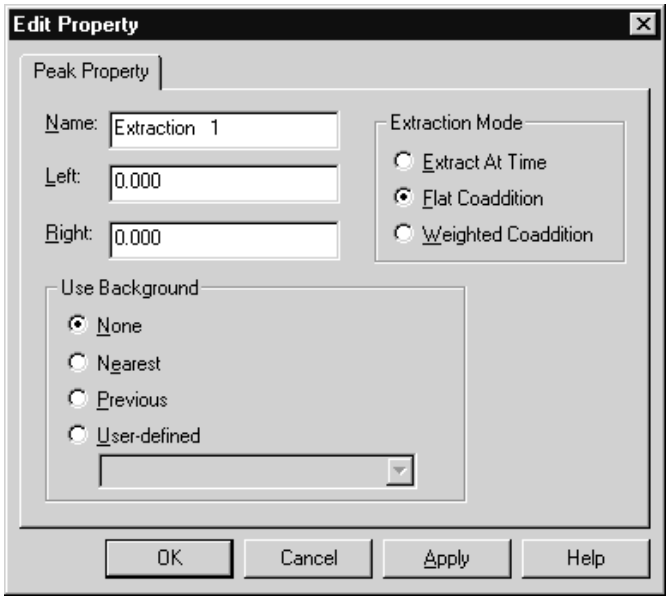
Extracted Spectra: the upper part of the control panel allows you to define and label extracted spectra. The spectra defined here are displayed in the upper part of the document window.

Note

Before extracting spectra, you usually want to extract a background or backgrounds. Click the Background tab button and use the cursor in the lower window ruler to define the background extractions.

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Creating an extracted spectrum: if you wish to type in values, you must create a label. Press the Create button; the Edit Property dialog box appears.



You can use the extraction number or enter a name for the extracted spectrum.

Extraction Mode: defines the point, or region, of the chromatogram from which a spectrum will be extracted and which will be displayed in the upper part of the document.

> Extract At Time: extract the spectrum at the specific defined time. Enter the Left Edge (time for which you want the spectra extracted).
>
> Flat Coaddition: extract the average spectrum in the defined region, co-adding the spectra in the region with equal weight.
>
> Weighted Coaddition: extract the weighted average spectrum in the defined region. Each spectrum in the region is multiplied by the value of the chromatogram for that spectrum. The result is normalized.
>
> If one of the coaddition methods is selected, you can define the region by entering the edges.

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Name: the name by which the extracted spectrum will be labeled.

Left Edge: lower time value for extracted spectrum region.
Right Edge: upper time value for extracted spectrum region.

Use background: select the background to be used for the extracted spectrum.

None: no background is used.

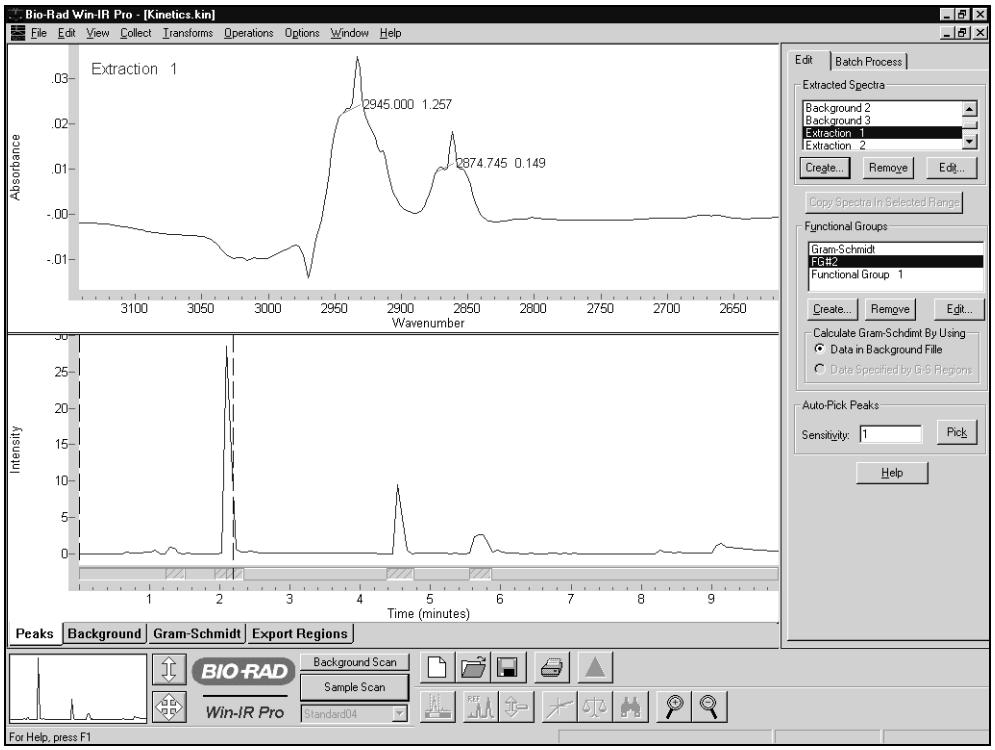
Nearest: use the background that is closest to the selected extract time or, if there is more than one background within a coaddition region, use the earliest background (the leftmost one) within the region.

Previous: use the closest background earlier than the selected extract time or the left edge of the coaddition region. If there is no background defined to the left of the selected time or region, no background is used (same as selecting None).

User-Defined: select a background from the pull-down menu.

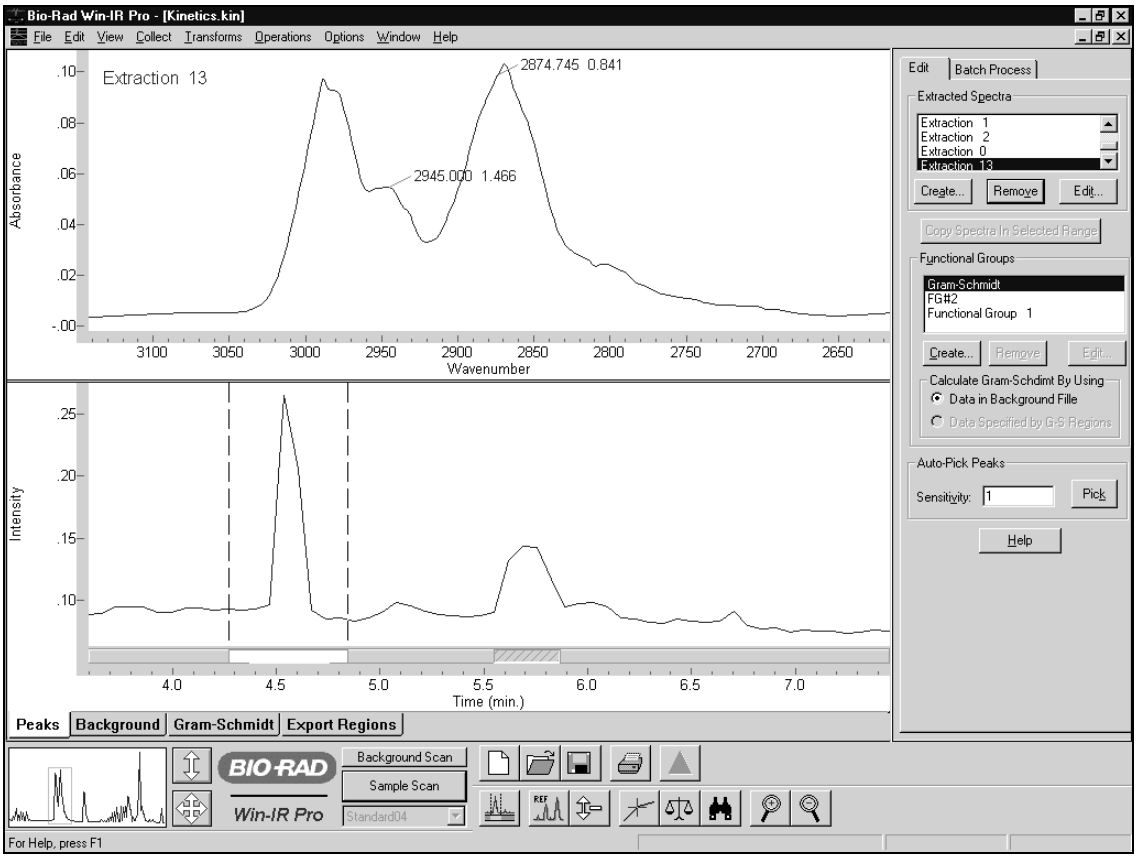
Press the OK button. Wait until the spectrum is extracted and displayed before proceeding. In the example below, extraction is for a specific time; for clarity of presentation, only the extracted spectrum and the Gram-Schmidt chromatogram are shown.

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Alternatively, an extracted spectrum can be created by placing the cursor in the ruler of the lower display. Click the Peaks tab button. Hold down the left mouse button and drag to create a region, or click to extract an individual scan-set. In the example below, we zoomed in on a region of interest.

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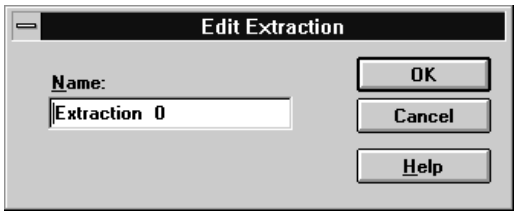


You can now name the extracted spectrum as discussed above by using the Edit button.

Removing an extracted spectrum: put the cursor on the label of the spectrum to be removed and click the left mouse button; this highlights the label. Press the Remove button. The extracted spectrum is removed from the list and its trace is no longer displayed in the upper part of the window.

Relabeling an extracted spectrum: extracted spectra, when created via the ruler, are labeled as Extraction 1, etc. To relabel an extracted spectrum, highlight the spectrum label, then press the Edit button. The Edit Extraction dialog box appears.

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Type in the new name for the spectrum. Then click OK.

Cancel returns you to the main screen without relabeling the functional group.

Help enters the on-line Help system.

Copying Extracted Spectra to the Clipboard

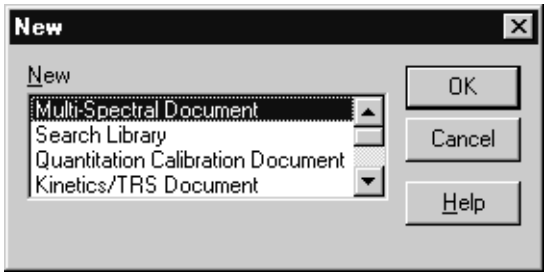
You can copy the extracted spectra into a multi-spectral document using the following procedure.

1. Click the Export Regions tab button.

2. In the lower part of the kinetics document window, define one or more extract regions. Select all regions from which spectra are to be copied using the ctrl-click combination.

3. Click the Copy to Clipboard button on the control panel sidebar.

4. Select New from the File menu. The New dialog box appears.



5. Select Multi-Spectral Document. Click OK.

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6. Select Paste from the Edit menu. The selected spectra are pasted into this new document.

Notes

The time at which each spectrum was collected (extracted) is also copied into the new document.

None of the spectra pasted into this new document are named. We recommend that you name them, so that they are identified meaningfully.

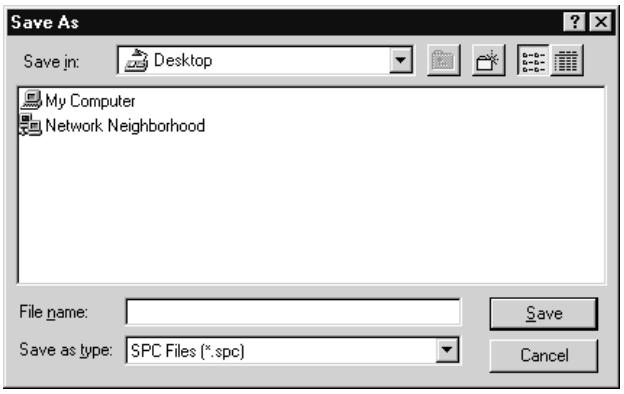
Exporting Extracted Spectra to a .SPC File

You can copy the extracted spectra into a .spc file using the following procedure.

1. Click the Export Regions tab button.

2. In the lower part of the kinetics document window, define one or more extract regions. Select all regions from which spectra are to be exported using the ctrl-click combination.

3. Click the SPC File Export button on the control panel sidebar. The Save As dialog box appears.



4. Use standard Windows NT procedures to navigate to a directory and enter a file name. The name must have a .spc extension.

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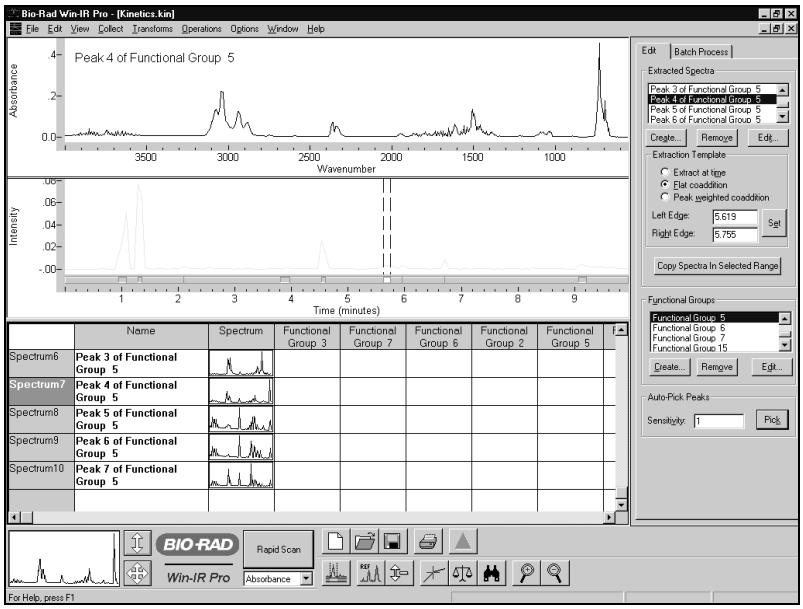
Notes

The time at which each spectrum was collected (extracted) is also copied into the new document.

None of the spectra pasted into this new document are named. We recommend that you name them, so that they are identified meaningfully.

Auto-Pick Peaks

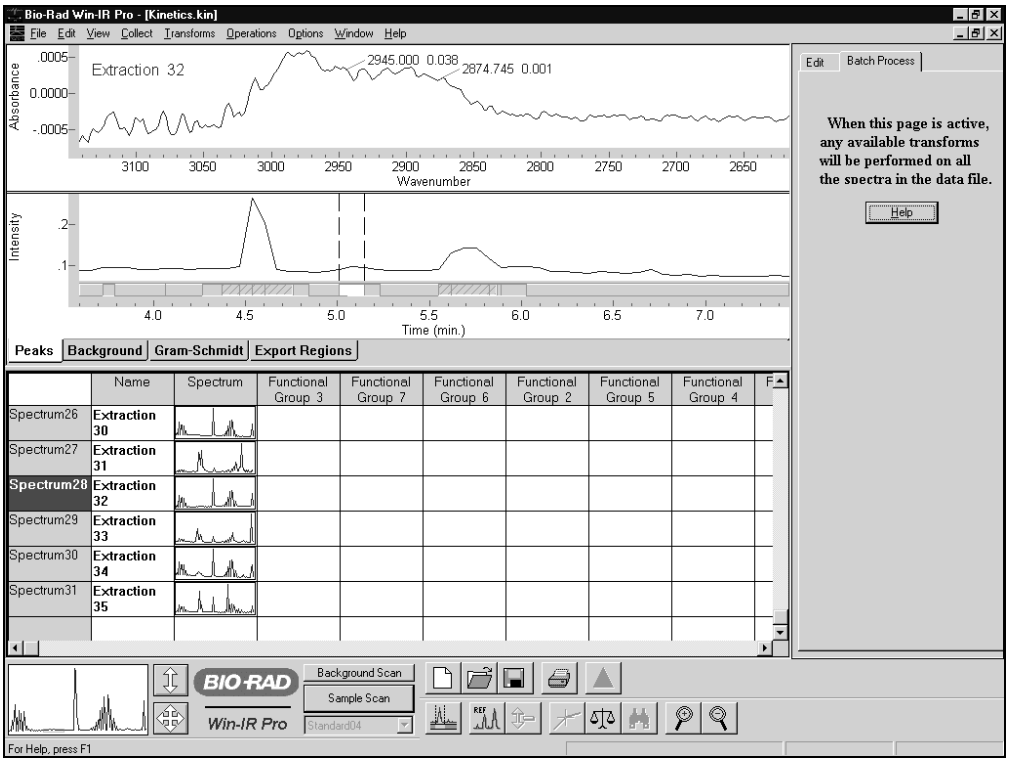
When the Pick button is pressed, all the peaks meeting the sensitivity criterion in the spectra associated with the selected (highlighted) functional groups are picked. This means that each peak label appears in the Extracted Spectra scroll box, for example, Peak 4 of Functional Group 5. These peaks can be accessed through the scroll box and through the spreadsheet (discussed later in this section). The peaks can be de-selected from either the scroll box or the spreadsheet. Enter the sensitivity in the Sensitivity text box; the higher the number, the more peaks that are picked.



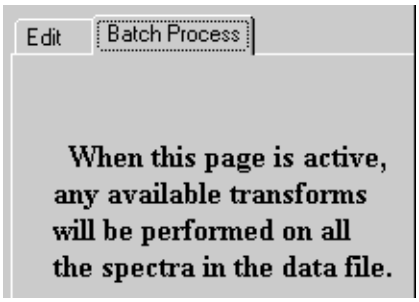
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Kinetics Document Control Panel—Batch Process page

Click on the Batch Process tab in the sidebar control panel. The screen now shows



The text on this tab page reads:



Select an entry from the Transforms menu; entries that cannot work on the kinetics spectra are disabled.

Set the parameters; the same parameters will be used for all the spectra in the file.

Select Replace or Add; this will be done for all the spectra in the file.

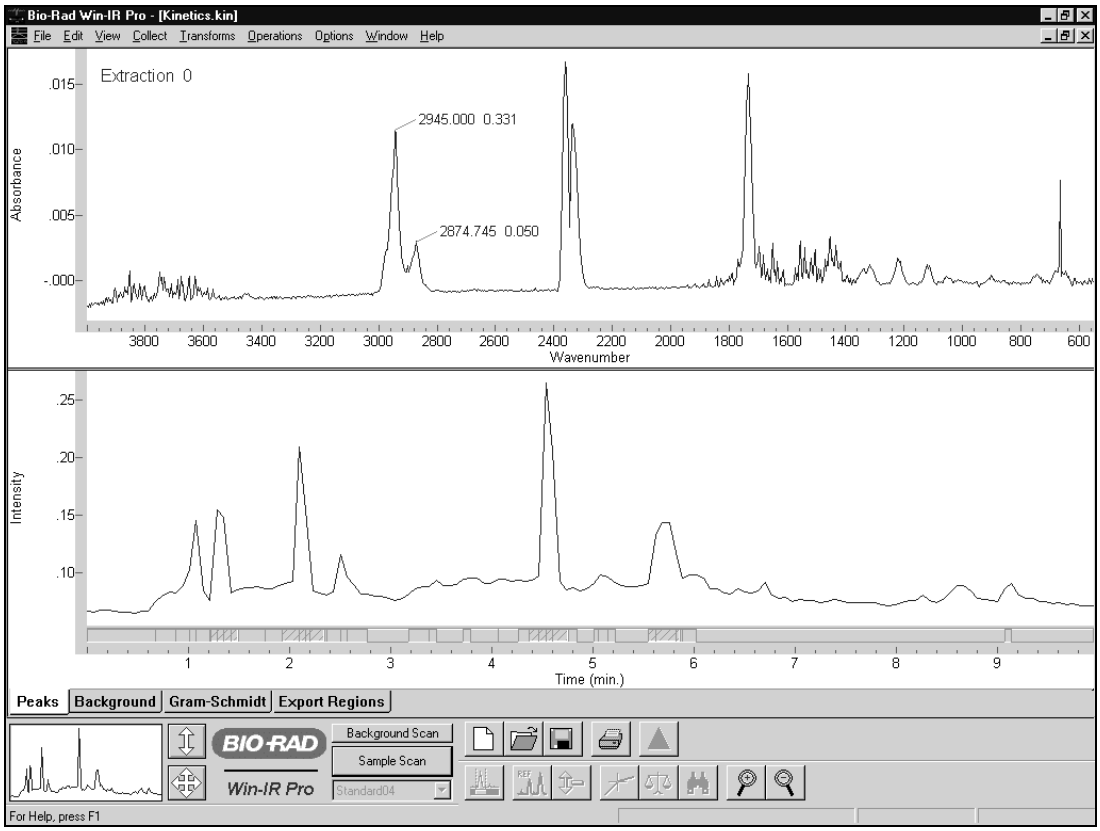
After the transforms are completed, the new spectra will replace the original ones, or be added to the spreadsheet, as you selected.

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Other Kinetics Document Features

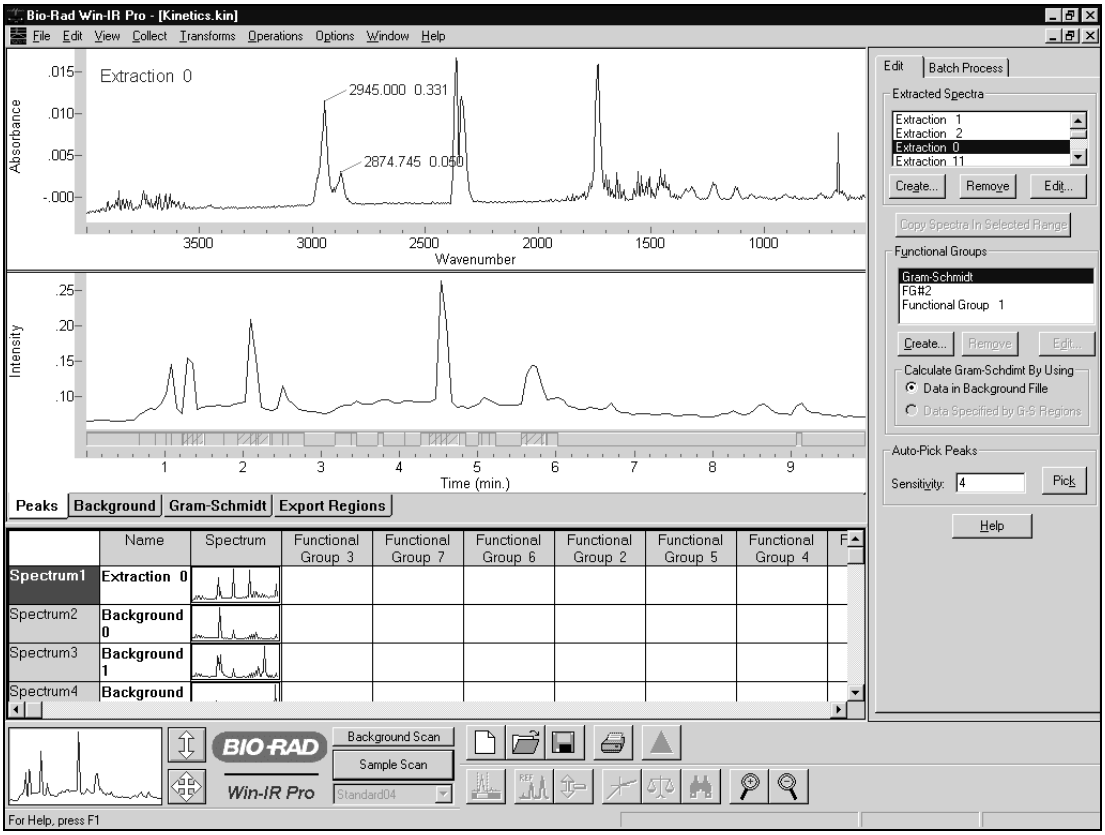
There are a number of menu entries in the View menu specific to Kinetics documents.

Kinetics Edit Bar: displays the control panel sidebar. If this is de-selected, the kinetics document looks like:



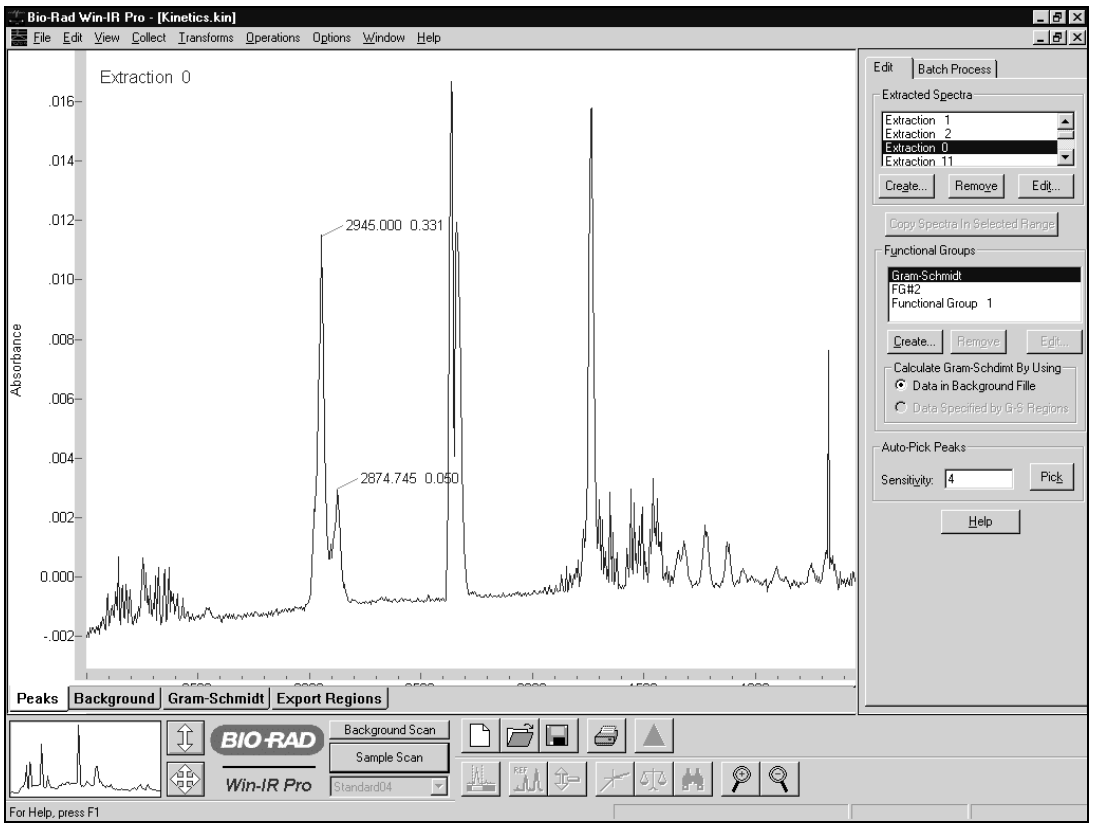
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Spreadsheet: select this to view the spreadsheet. The spreadsheet allows direct access to the extracted spectra (see Chapter 4 for details of the spreadsheet). The kinetics document looks like:



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Chromatogram Edit Window: if selected, shows the lower traces (chromatograms); if de-selected, this display is hidden and the kinetics document looks like:



Hide Gram-Schmidt Chromatogram: hides the Gram-Schmidt chromatogram display. When this is selected, the entry changes to Show Gram-Schmidt Chromatogram.

Show Peaks: if peaks are labeled (see Chapter 11), selecting this option hides the label display. When this is selected, the entry changes to Show Peaks.

Printing Chromatograms

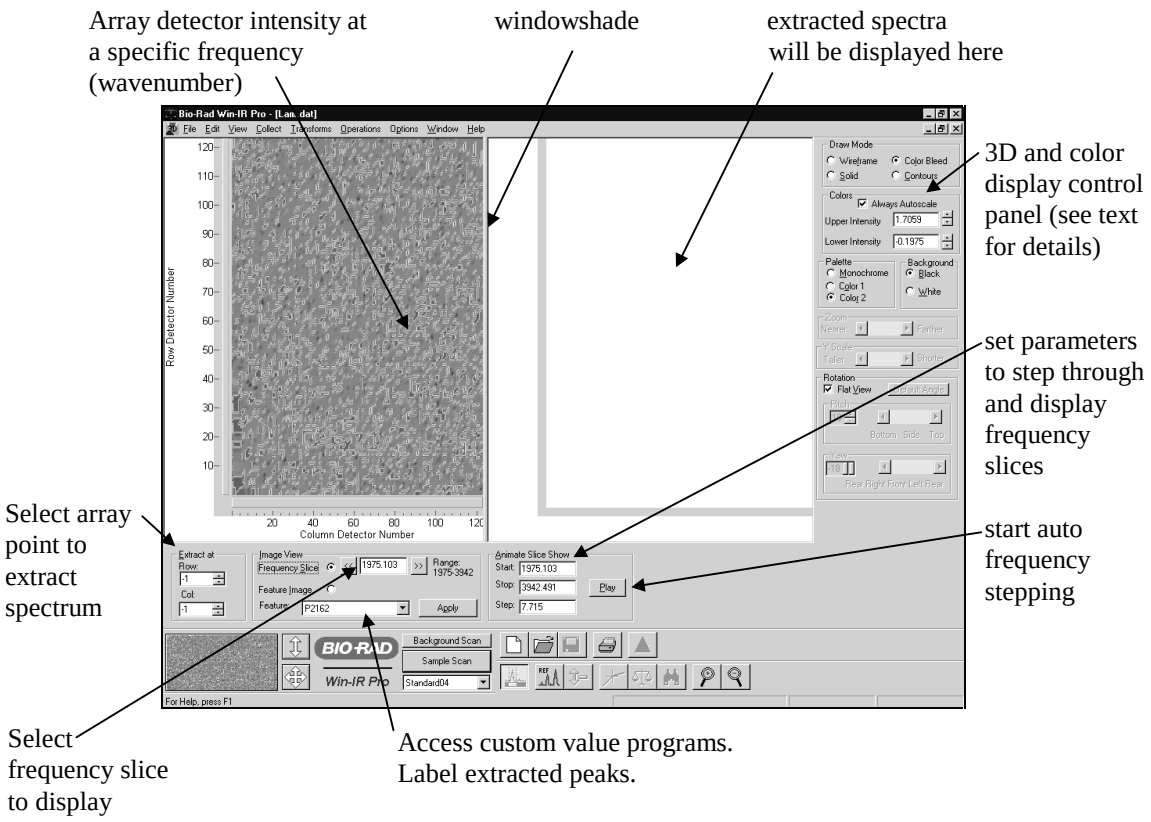
It is possible to print chromatograms by copying them into a Multi-spectral document. Details of this process are given in Chapter 16 , “Frequently Asked Questions.”

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IMAGE DOCUMENT WINDOW

This document allows you to manipulate data collected with an image array detector.

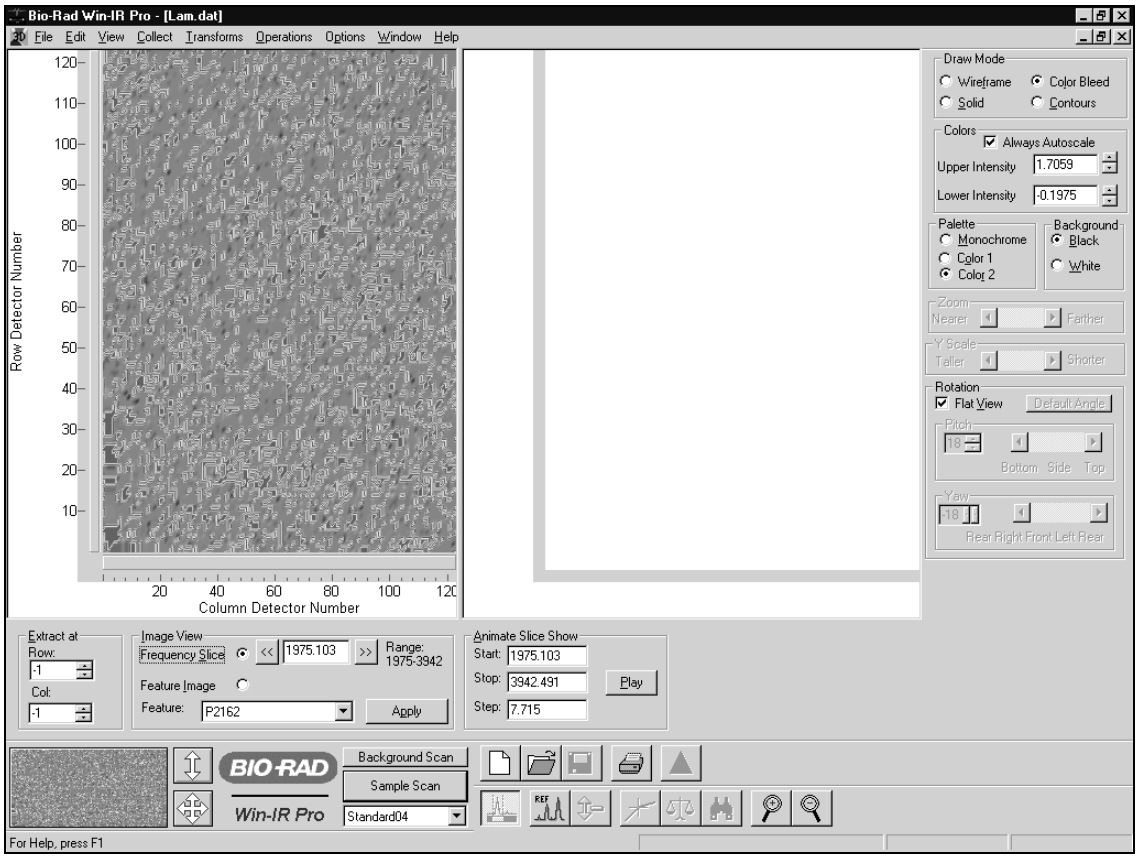
When an image file (.dat) is opened, the screen initially looks like this.



Note

It is possible to open the raw image data collect files (.seq) if required. For details on how to do this, see Open in Chapter 6.

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After the file is opened, Frequency Slice displays the lowest wavenumber at which collection was made (here, 1975.103 cm^{-1}). To the right of that, Range displays the frequency range (in wavenumbers) for which data was collected. On the right. In Animate Slice Show, Step shows the difference (in wavenumbers, here 7.715) between frequency slices; this is roughly the same as the resolution of the data collection.

You can use zooming in the left-hand part of the Image document. We recommend that you do not use the expansion/compression feature in this part of the document.

The radar box works as described earlier in this chapter.

Note

The Extract Spectrum at boxes show values of -1 indicating that no spectrum has been extracted.

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Frequency Slices

The view in the left-hand side uses the x- and y-axes for detector column and rows. The z-axis, represent by color, is the intensity of the spectrum at a particular frequency. This frequency is shown in the Frequency Slice box. You can display a different slice by clicking on the << button (one step lower) or the >> button (one step higher). You can also change the frequency slice by typing a number in the box, followed by the ENTER key on the keyboard. The intensity for that frequency slice will then be displayed.

Note

Win-IR Pro will round your entry down to the next lower valid frequency.

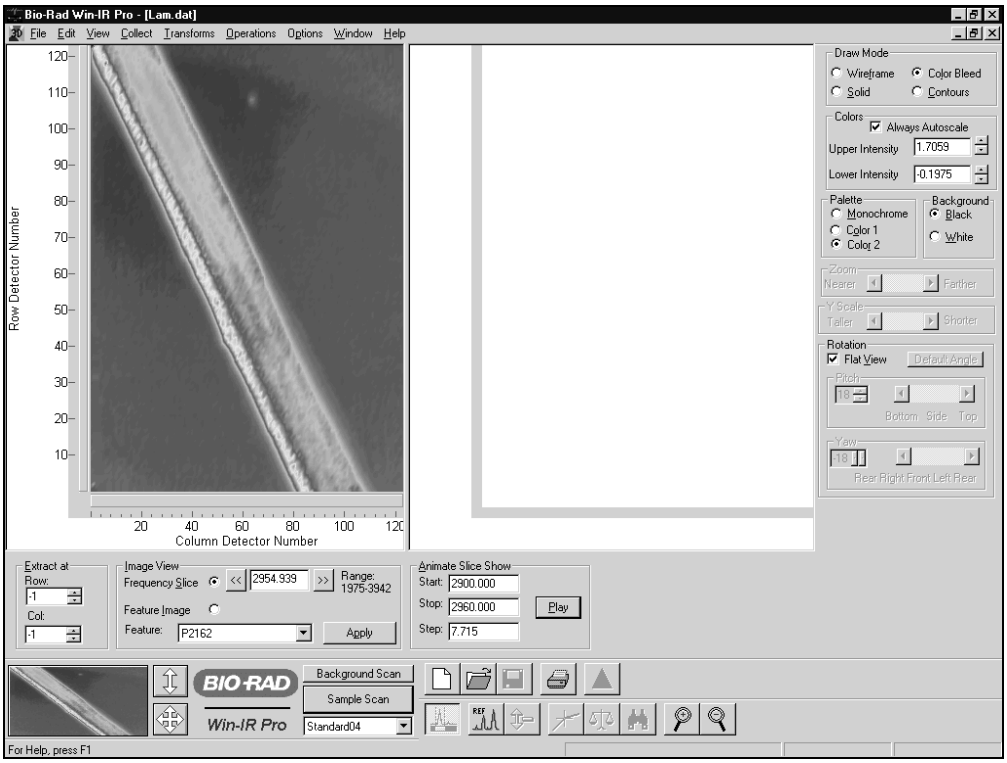
You can observe the system automatically step through a range of values using the Animate Slice Show controls.

Start: enter the lowest value of frequency you wish to observe.
Stop: enter the highest value of frequency that you wish to observe.
Step: this is the difference between frequencies. Normally, it would be left at the default; if you want to move through the frequency slices faster, you could set it at a multiple of the default value.

Play: click this button to observe the frequency slices in the left-hand side of the document. The frequency of the slice being viewed in given in the Frequency Slice box. After the animation is finished, you are viewing the highest slice. If you want to stop the animation before it has completed, press any key on the keyboard.

The example below shows the end of an animation. Start was set to 2900; Stop to 2960; Step to 7.715 (the default). The first slice was actually at 2893.217, (2900 rounded down to the nearest valid frequency); the last slice shown was at 2954.935 (the last valid frequency below 2960).

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Extracting a Spectrum

Spectra can be extracted by one of three methods.

1. Put the cursor on the desired point in the array and click the left mouse button. The spectrum is extracted for that point and displayed in the right hand box.

2. Put the cursor on the x-axis at the desired point and click the left mouse button. Then, put the cursor on the y-axis at the desired point and click the left mouse button. The intersection of the lines defines the point at which the spectrum is to be extracted.

3. In the Extract Spectrum at area of the lower control bar, enter the row and column that defines the point at which the spectrum is to extracted. These values can either be typed in or entered using the spin arrows to the right of the Row: and Col: boxes.

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Notes

The extraction point can be changed by putting the cursor on the line in the ruler (either x or y), holding down the left mouse button, and dragging the line to the new position.

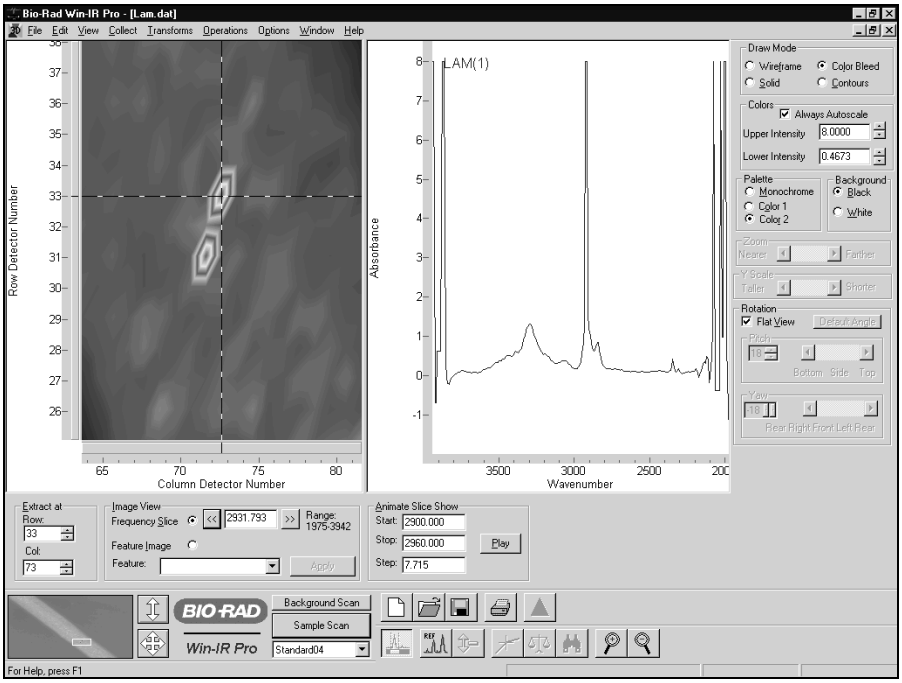
The example below shows a spectrum extracted at the selected point. The selection process used was:

1. Step through the frequency slices (either manually or automatically) until a structure of interest is seen. In this case, it was at approximately 2932 cm^{-1}.

2; Zoom in on an area of interest to make it easier to select the point at which extraction is to be done.

3. Put the cursor on the point on interest and click the left mouse button.

The display now looks like:



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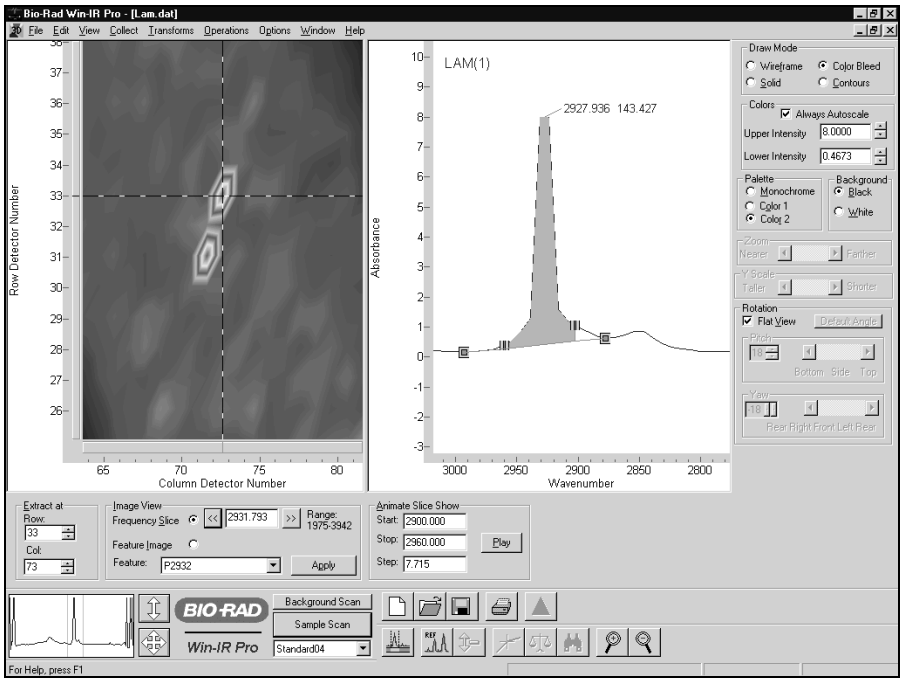
Note

You can use all the normal zoom, scroll, etc. features discussed earlier in Chapters 1 and 3, in the extracted spectrum part of the document.

Zoom in on the extracted spectrum and, using the right mouse button menu New / Image Peak entry, define an image peak at ~2932 cm^{-1}. The default name TmpItPk1 is displayed in the Peak: box. You can edit this image peak and re-label this peak with any name using the Properties entry on the right mouse menu (see Chapter 2 for details of peak editing). In this example, we will change the image peak name to P2932.

Note

Changing the name of the peak cannot be done using the Feature box; you must use the standard peak editing procedures.



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Note

This image peak is defined for all extracted spectra. If there were predefined image spectra, they could be used to define an image peak using Operations / New / Image Peak (see Chapter 11 for details).

The array on the left hand side of the screen currently shows the total spectral intensity for each detector. To see the area under the 2932 cm^{-1} peak at each detector in the array:

1. Put the cursor in the peak area, or on the peak label, and click the right mouse button.

2. Select Properties from the right mouse button menu. The Edit Peak Properties dialog box appears.

3. Click the General tab.

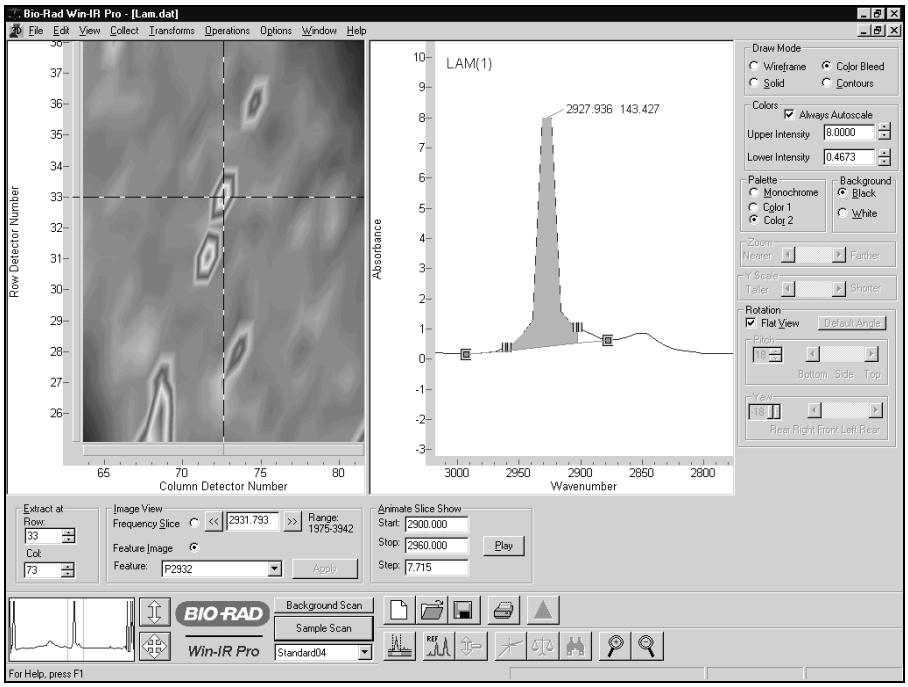
4. Select Area. Click the OK button.

5. Select Feature Image.

6. Click the Apply button.

Calculating Feature Image is displayed in the status bar during this process. The display is shown below. After the redisplay, the Apply button is disabled.

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To view peak height in the array, instead of peak area:

1. Put the cursor in the peak area, or on the peak label, and click the right mouse button.

2. Select Properties from the right mouse button menu. The Edit Peak Properties dialog box appears.

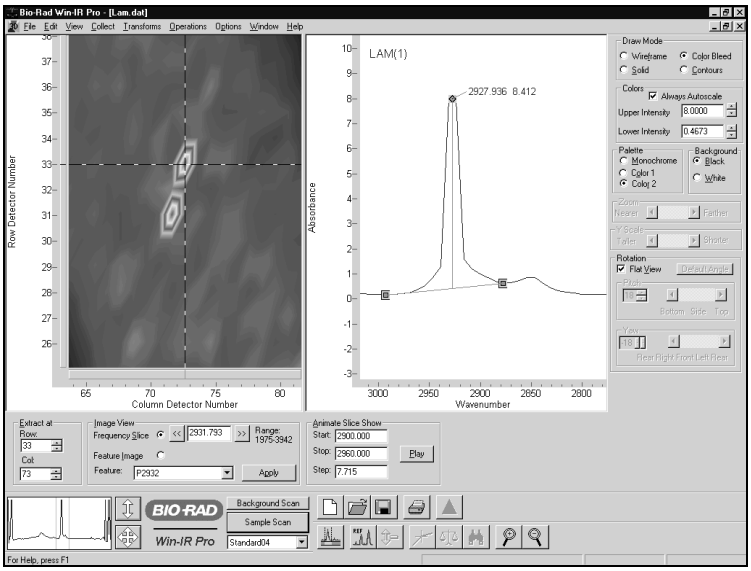
3. Click the General tab.

4. Select Height. Click the OK button.

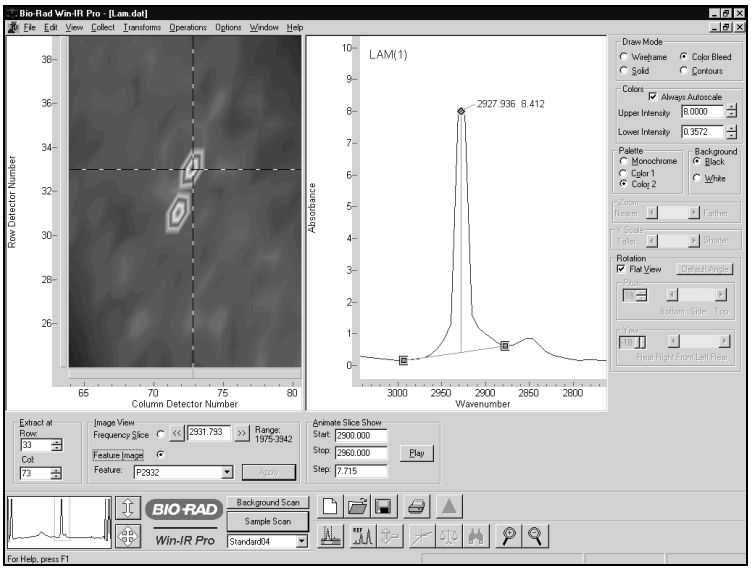
5. Select Feature Image.

The display now looks like this; the Apply button is enabled once again.

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Click the Apply button; when calculations are completed, the peak height at each array detector is displayed in the left hand side of the screen.



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Printing: to print the extracted spectrum

1. Put the cursor on the extracted spectrum and click the left mouse button.
2. Select File / Print or click the  button on the main screen.

Copying the Extracted spectrum: to copy the extracted spectrum

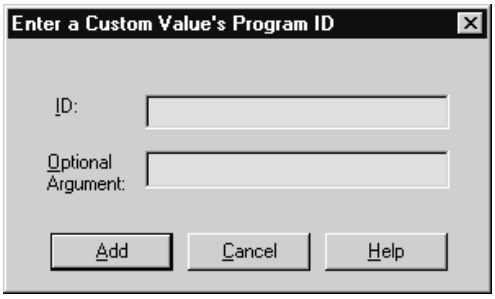
1. Put the cursor on the extracted spectrum and click the left mouse button.
2. Select Edit / Copy.
3. Access a multi-spectral document either through File / Open, File / New, or the Window menu.
4. Select Paste from the Edit menu to put the spectrum into this document. It can now be treated like any other spectrum.

Custom Value Programs

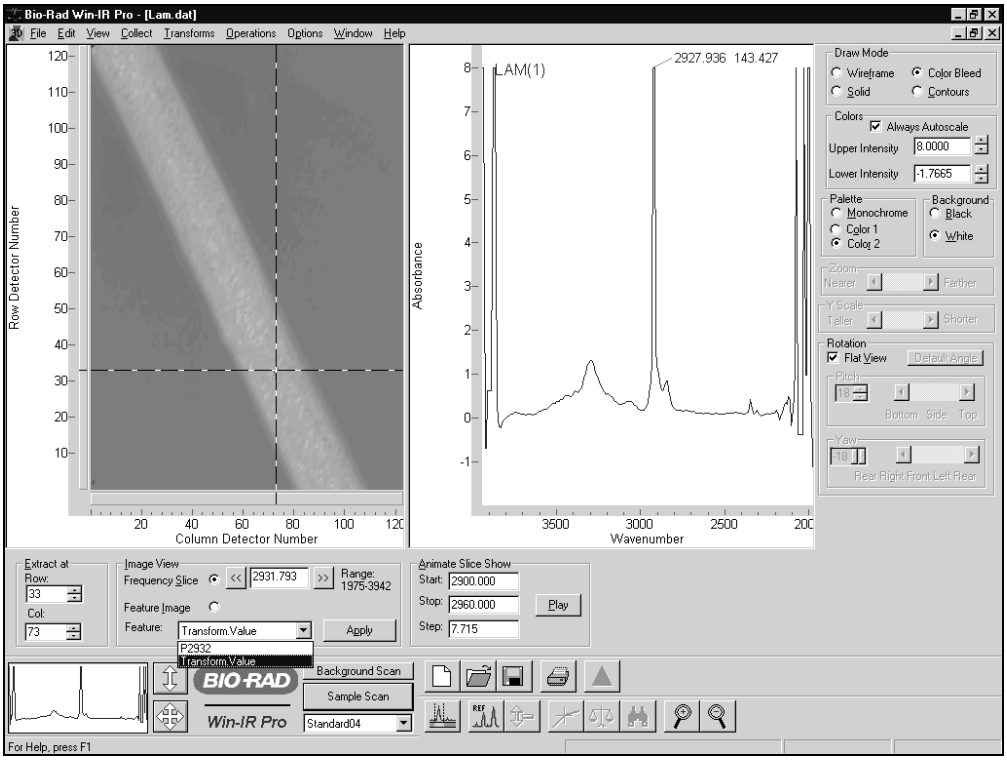
A custom value program operates on the spectrum for each detector in the array and calculates a single value for that spectrum. The area and height of an image peak (described above) can be thought of as special "built-in" custom value programs. You can write your own custom value programs and execute them in the image document window as follows.

1. Create a custom value program according to the procedure specified in Appendix N.
2. Start Win-IR Pro; open an Image document.
3. Select Operations / New / Custom Value. The Enter a Custom Value's Program ID dialog box appears.

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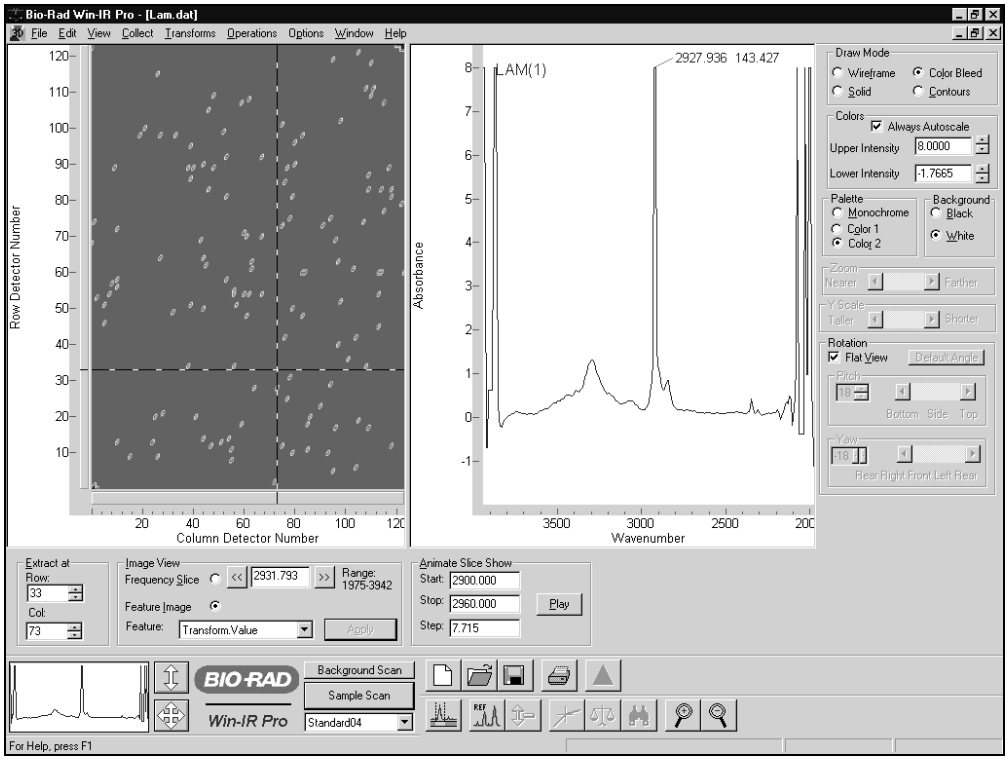
4. Enter the program ID. In this example, it is Transform.Value; this program displays the height of the largest peak in each spectrum. If required by your program, enter the Optional Argument. Click the Add button. The program ID now appears in the Feature pull-down menu. The Apply button is enabled.



5. Select Feature Image.

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6. Select the ID of the custom value program from the menu and click the Apply button to execute it.



The results of the custom value program are displayed in the left side of the screen.

Transforms

A subset of the transforms operates on the array data. For details on the use of any particular transform and on its parameters, see Chapter 10. When you select a transform, the transform operates on the spectra at all points in the array and replaces the original spectra with the transformed ones. If you want to preserve the original data, make a copy of the image file **before** performing the transform.

Certain transforms require that you define a region of the spectrum before invoking the transform. Extract a spectrum at any point in the array and define the region. This region will be used by the transform for all points in the array.

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Exporting SPC Files

The spectra for all points in the array can be exported to a Win-IR or GRAMS multifile. Export begins at the array element in the lower left hand corner and proceeds to the lower right corner; it continues at the leftmost element of the next row from the bottom. The process ends when the upper right array element is reached. The multifile is about 16 Mbytes in size—slightly larger than the original image file (.dat). To export the file:

1. Select File / Export SPC. The Save As dialog box appears.



2. Choose a directory and a file name (with the .dxf extension) for the exported data. Click the Save button.

This .spc file can be opened by Win-IR, GRAMS, or Win-IR Pro (see File / Open in Chapter 6 for details)

Exporting DXF Files

The graphic in the left hand side of the screen (a frequency slice, output of a custom value program, etc.) can be exported as a .dxf file; these files can be imported into a number of graphical editors and CAD-CAM applications. To export the file:

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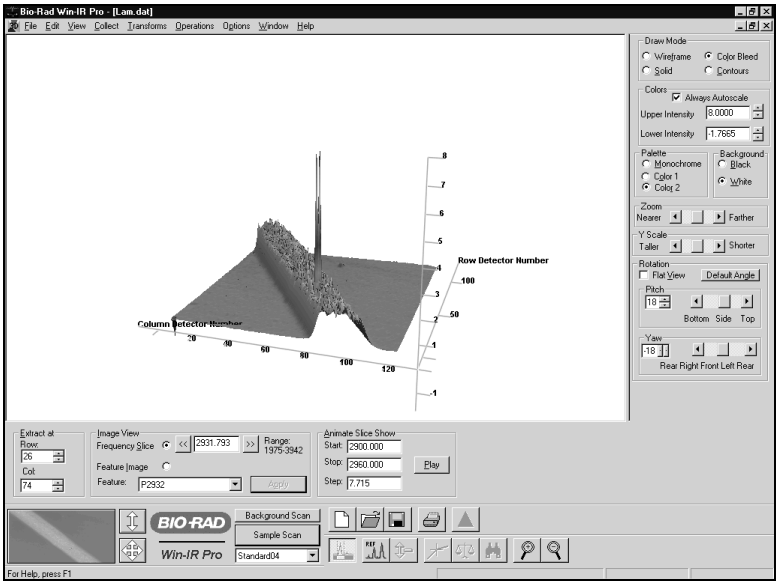
1. Select Operations / Export DXF. The Save As dialog box appears.



2. Choose a directory and a file name (with the .dxf extension) for the exported data. Click the Save button.

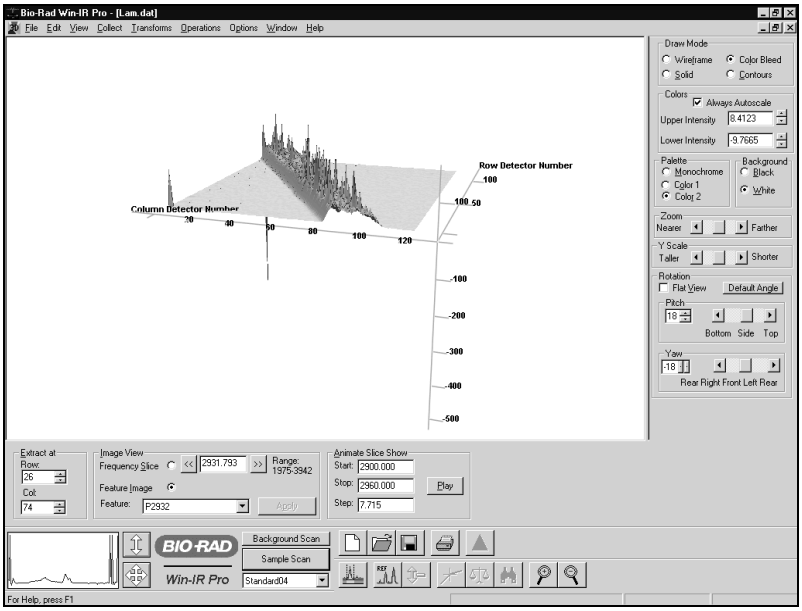
Three-dimensional View

The left-hand view can be moved, rotated, and presented in a number of formats. The control panel sidebar on the right hand of the screen controls the presentation of the data. The portion of the window used by the different graphics can be altered by moving the horizontal and vertical window shades. In all the examples below, the vertical window shade has been moved to the right to better show the three-dimensional graphics The first example shows a 3D view of the frequency slice at 2932 cm^{-1}.

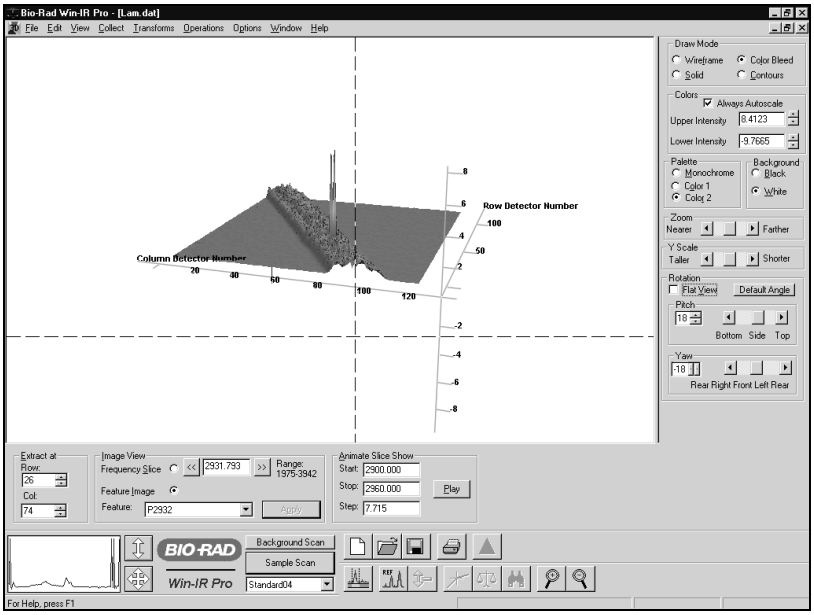


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The next is a three-dimensional view of the peak area at each array detector.



Finally, a three-dimensional view of the peak height at each array detector.



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Three Dimensional Controls

Draw Mode: how the three-dimensional aspect will be represented in two dimensions.

Wireframe: the points of the calculated three-dimensional plot are connected with straight lines. Lines that are hidden by the shape of the display are not shown. This draw mode disables both Colors and Palette.

Solid: the lines and the frames they define are filled in with different shades of a single color to give a better idea of the shape of the surface of the contour plot.

Color Bleed: uses multiple colors for the surface. These colors change gradually and smoothly as the height of the plot varies above the base plane. (Default)

Contours: shows contour lines on the surface at constant heights about the base plane. The contour intervals are pre-set and cannot be changed.

Colors: sets the rangeof colors used to represent the extreme z-values of the plot.

Always Autoscale: if this is selected, then whenever you zoom in on a portion of the plot, the color will be scaled so that the full color range is used for that portion. This is useful if you zoom in on weak features that may be displayed in very similar colors in the full plot.

If you are not autoscaling the colors, then you can set the values to be used in the display. If you use the arrows to the right of the intensity boxes to set values, they will be implemented immediately. If you type in values, they will not be implemented until you press the Enter key on the keyboard.

Upper Intensity: enter the color value to be used at the maximum z-value of the plot.
Lower Intensity: enter the color value to be used at the minimum z-value of the plot.

Palette: the draw modes may be observed with three different color schemes.

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Note

In wireframe mode, Palette is disabled.

Monochrome: gray scale.
Color 1: shades from red to white to blue.
Color 2: shades from red through orange, yellow, and green to blue. (default)

Background: select the color for the background. A white background may be better if you are capturing screens for insertion in a publication with a monochrome printer.

Black: background is black. the plot is shown against a black background (default).

White: the plot is shown against a white background. This may be more desireable for formats other than wireframe

Zoom: makes the plot appear closer (increases size) or farther away (decreases size). Use the slide bar to change the value.

Y Scale: makes the height of the peaks taller or shorter. Use the slide bar to change the value.

Rotation: these controls move the three-dimensional plot about two axes. Regardless of the rotation, the axes remain in the foreground of the display. Rotation of large arrays may be slow. Press the ESC key to stop the rotation.

Flat View: if selected, displays a projection of the isometric view. If de-selected, the isometric view (3D) is shown.

Default Angle: press this button to return the plot to its default position (Pitch = 18°, Yaw = 1°).

Pitch: rotates the plot about a horizontal axis parallel to the monitor screen. Click on the upper part to rotate the plot to show its Bottom; click on the lower part of the bar to rotate the plot to show its Top. Each time you click the end of the slide bar, the plot rotates 9°.

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Yaw: rotates the plots about a vertical axis. The plot can be rotated either to the Right or to the Left. Each time you click the end of the slide bar, the plot rotates 18°.

For both Pitch and Yaw, you can enter the value of the angle. If you change the angle with the arrows to the right of the text box, the values are implemented immediately. If you type in values, the values are not implemented until you press the Enter key on the keyboard.

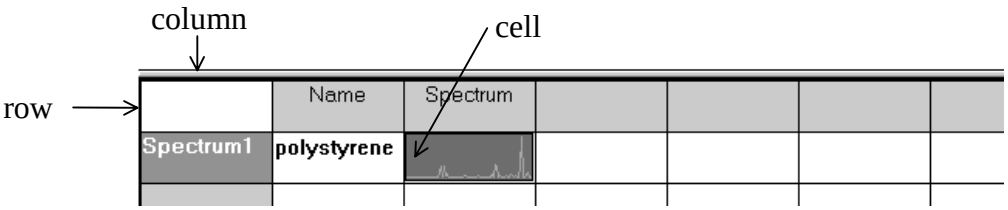
Subsets of menus are also available. Their entries operate the same as they do in the main Win-IR Pro document window.

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4
Introduction to the Spreadsheet

Documents can contain multiple spectra (traces). These spectra do not have to be related to each other, do not have to have the same resolution, range, etc. The spreadsheet presents information about each trace in the document in a two-dimensional array. Each row in the array presents information for a particular trace. Each column contains a particular piece of information about the traces. Each cell contains a particular piece of information about that trace. In this default example, the columns are Spectrum ID (not named), Name, and Spectrum.

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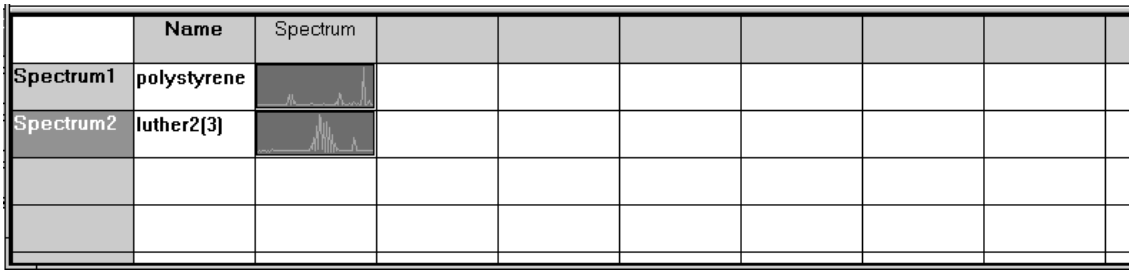


Notes

The name of the individual spectrum is not necessarily the same as that of the document. The document name is used by the Windows NT file system. The spectrum name is internal to the document and is used only by Win-IR Pro.

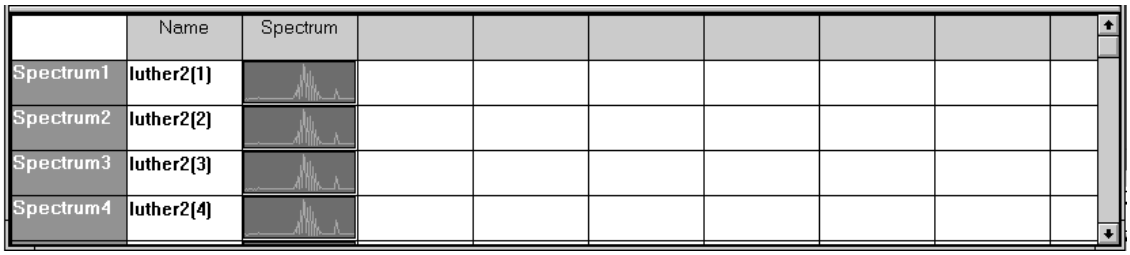
When spectra are collected into a Multi-Spectral Document, the latest spectrum is put at the top of the spreadsheet. As spectra are collected into a Kinetics Document, the latest one collected is put at the bottom of the spreadsheet.

Whenever a trace is deleted, its corresponding spreadsheet row is deleted. When a trace is added to the document, a new row is added to the spreadsheet. If any of the columns is not meaningful for a particular trace, or if that information is not available for that trace, then the spreadsheet cell is left blank. In the example below, the spectrum luther2(3) has been added to the document; it appears as the Spectrum 2 line in the spreadsheet.



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If there are too many spectra in the document (as in the example below), or too many columns for the traces, to fit in the spreadsheet box, scroll bars automatically appear to allow access to all parts of the spreadsheet.



All changes made to the spreadsheet are retained if the document is saved (for example with Save or Save As... from the File menu) before it is closed.

Any changes made to the structure of the spreadsheet, such as resizing cells, adding or removing columns is saved when the document is saved. This new structure is used when you open any document of the same type (multi-spectral, kinetics, etc.) and remains in effect until you alter the spreadsheet and save the document.

If spectra in the spreadsheet were collected with different ranges then, when one is selected by clicking in the spectrum ID cell, the display will autoscale the X- and Y-axes for that spectrum. Any other spectra visible in the display will be shown with those autoscaled limits.

NAVIGATING THE SPREADSHEET

You can navigate through the spreadsheet either by placing the cursor in the desired cell and clicking the left mouse button or by using the keyboard.

↑ or PAGE UP	move up one row in the spreadsheet
↓ or PAGE DOWN	move down one row in the spreadsheet
← or HOME	move left one column in the spreadsheet
→ or END	move right one column in the spreadsheet

Notes

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Movement in the spreadsheet does not wrap. That is, moving right from the rightmost column does not go to the leftmost column, etc.

You cannot access the ID column using the arrows or page keys; you must use the cursor.

If you double click in a text cell, then the arrow keys become local editing keys for movement within that cell.

MODIFYING THE SPREADSHEET

Columns with other properties can be added to the spreadsheet. All columns (except the Spectrum ID) can be deleted from the spreadsheet. The rows and columns can be resized; the entry in the Name column can be retyped.

Note

When you delete a column from the spreadsheet, you are deciding to not display information about the spectrum. That information still exists in the document; you can choose to display it again later.

Viewing the Spreadsheet

You can adjust the proportion of the window devoted to the spreadsheet by

- Placing the cursor on the windowshade, holding down the left mouse button and dragging the windowshade up (to increase spreadsheet portion) or down (to decrease spreadsheet portion). Dragging windowshades is discussed in detail in the chapter on the main screen and document types.

- Selecting Maximize traces from the Window menu (or pressing the F11 key) to have the traces fill the entire window of the document.

- Selecting Maximize spreadsheet from the Window menu (or pressing the F12 key) to have the spreadsheet fill the entire window of the document.

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Resizing Rows and Columns

At times, the entry in a spreadsheet cell is too large for the default size; cells are not automatically resized to accomodate their contents. Text in a spreadsheet cell may appear to be complete even though it is actually truncated. This is especially true for hit lists. Resize the cell (by changing the row and/or column size) to make certain that you are not overlooking any text. For example, consider this spreadsheet listing library search hits,

Spectrum1	Antifreeze			Structui				
	Name	Spectrum	Copyright	ChemStruct				
1: 0.28 Bio-Rad	ETHYLENE		Copyright					
2: 0.37 Bio-Rad	PROPYL		Copyright					
3: 0.37 Bio-Rad	2-PROPEN-1		Copyright					
4: 0.38 Bio-Rad	METHANOL		Copyright					
5: 0.42 Bio-Rad	D-(+)-GLUCO		Copyright					
6: 0.44 Bio-Rad	GLYCEROL		Copyright					
7: 0.47 Bio-Rad	1-(2-HYDRO		Copyright					
8: 0.52 Bio-Rad	BENZYL		Copyright					
9: 0.55 Bio-Rad	1-HEXANOL		Copyright					

The long chemical names and the copyright dates have been truncated; some of the chemical structures are also hard to see. To change the column width:

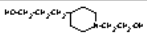
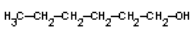
1. Place the cursor on the right hand boundary of the column whose size is to be changed. The cursor must also be in the gray label row.

2. When the cursor changes to ←|→, hold down the left mouse button.

3. Drag the right side of the column to the desired position and release the button.

Here, we have increased the width of three of the columns to better display the information in them.

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Spectrum1	Antifreeze			Structure not loaded
	Name	Spectrum	Copyright	ChemStruct
1: 0.28 Bio-Rad	ETHYLENE GLYCOL		Copyright 1995	
2: 0.37 Bio-Rad	PROPYL ALCOHOL		Copyright 1995	
3: 0.37 Bio-Rad	2-PROPEN-1-OL		Copyright 1995	
4: 0.38 Bio-Rad	METHANOL		Copyright 1995	
5: 0.42 Bio-Rad	D-(+)-GLUCOSE		Copyright 1995	
6: 0.44 Bio-Rad	GLYCEROL		Copyright 1995	
7: 0.47 Bio-Rad	1-(2-HYDROXYETHYL)-4-PIPERIDINEPROPANOL		Copyright 1995	
8: 0.52 Bio-Rad	BENZYL ALCOHOL		Copyright 1995	
9: 0.55 Bio-Rad	1-HEXANOL		Copyright 1995	

You can also resize rows in a similar manner.

1. Place the cursor on the lower boundary of the row whose size is to be changed. The cursor must also be in the gray spectrum ID column.

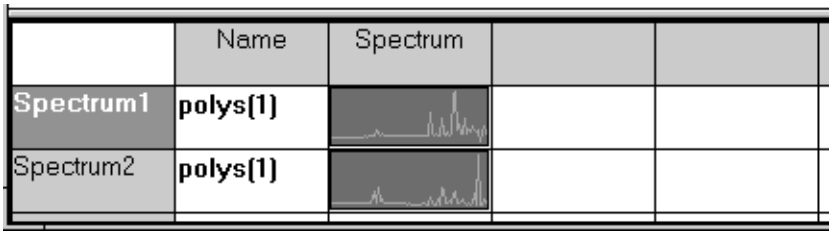
2. When the cursor changes to , hold down the left mouse button.

3. Drag the lower edge of the row to the desired position and release the button.

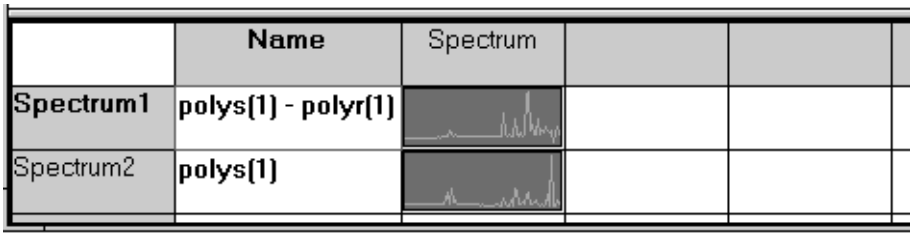
Typing in the Name Field

When you modify the spectrum (for example, by a transform) and add the modified spectrum to the document, it shows up in the spreadsheet with a blank in the name column. In the example below, the spectrum polyr.bsp was subtracted from the spectrum polys.bsp; the difference spectrum was then added to the document; it appears at the top of the spreadsheet as Spectrum1 with a the same name as the original spectrum.

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To add a name (or to replace whatever name is already in that cell), place the cursor in the Name cell to be changed and click the left mouse button. Then, type whatever text you want in that cell. In the example below, the new name is polys-polyr. Because it does not fit, the column was widened to accommodate it.



Editing Spreadsheet Cells

The contents of individual cells of the spreadsheet can be copied to the clipboard; in some cases, it is also possible to modify the contents of these cells.

Non-editable (read-only) cells: the cells in some columns cannot be altered; these columns contain the values of properties which cannot be set by the user—for example, time of creation of the spectrum, scan parameters, etc. If you put the cursor in such a cell and click the right mouse button, this menu appears



You can copy the contents of this cell to the clipboard and paste them elsewhere (an editable cell, a word processor, an external spreadsheet, etc.).

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Editable (read/write) cells: the cells in some columns can be altered. Place the cursor in the select cell and click the right mouse button. This menu appear.



The menu entries have their usual meanings:

Undo: if possible, undo the last operation performed in this cell.
Cut: copy the contents of the cell to the clipboard and delete the contents of the cell.
Copy: copy the contents of the cell to the clipboard.
Paste: paste the contents of the clipboard into the cell, replacing any highlighted portions of the cell.
Delete: delete the contents of the cell.
Select All: highlight the contents of the cell.

Depending upon the specific history of the operations in this cell, dofferent combinations of enries are enabled or disabled.

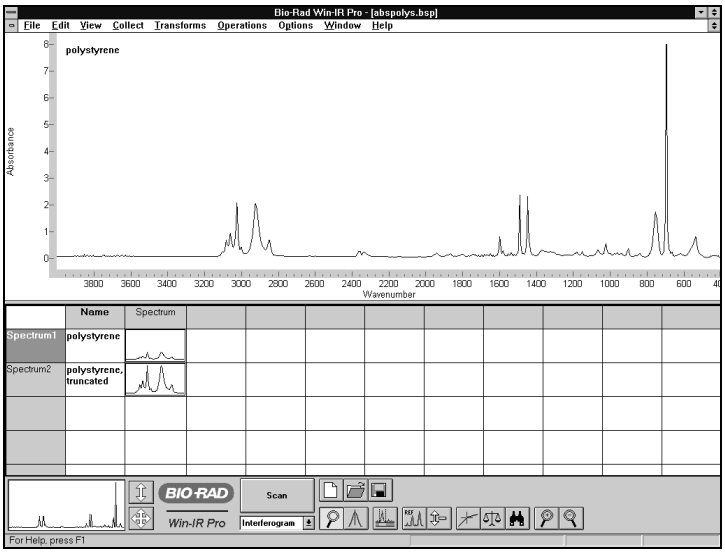
Text Editing: When you first enter a cell using the directional arrows, you are put into simple (replace) edit mode. In this mode, whatever you type replaces the former contents of the cell. If you double click the left mouse button, you will be in full (modify) edit mode. You can now modify the existing contents by deleting text, inserting, etc.

If, after typing in the spreadsheet cell, you decide that you do not want to make this change, immediately select Edit / Undo or press the Esc key on the keyboard. The cell will revert to its previous contents.

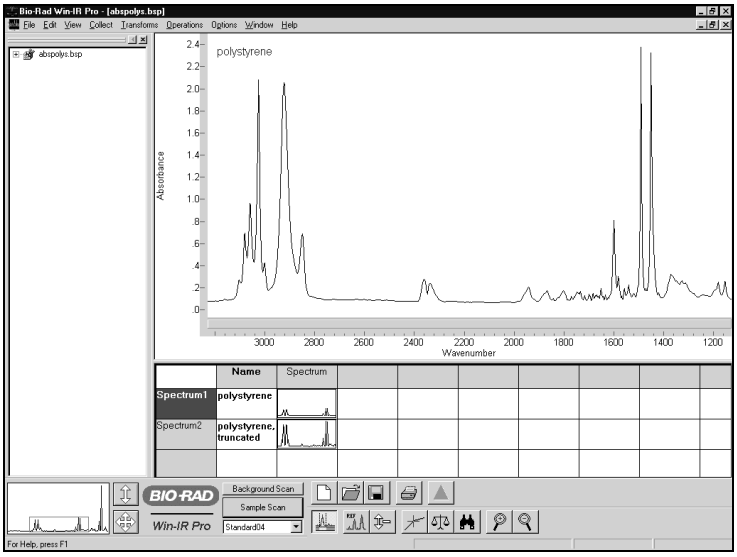
Adding Columns

The default spreadsheet has three columns: spectrum ID, name, and a small plot of the spectrum. For example, consider this document:

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If it is not already present, select Property Browse Bar from the View menu.

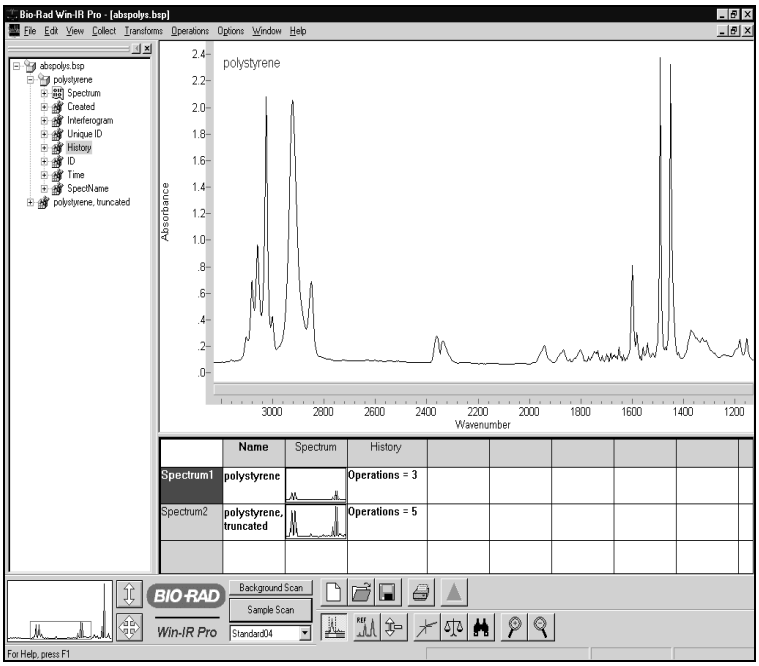


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A view of the property tree is shown at the left. The tree has been opened to display the properties. We will add History to the spreadsheet.

Highlight the property to be added to the spreadsheet. Click the right mouse button. Select Add Column from the menu. A new column is created labeled by the name in the property list. Use History in this example,



The History column was resized for a better display. The value of the property is displayed for all the spectra in the spreadsheet.

If there are multiple spectra in the document, and if these spectra have a value for that property, then those values will also appear in that column of the spreadsheet.

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Select View / Property Browse Bar to remove the property browse bar.

See Property Browse Bar in the View menu chapter for more details.

Removing Columns

There are two ways to remove columns from the spreadsheet—using the right mouse menu or using View / Remove Columns. In either case, you must first select the columns to be deleted.

Select a column by clicking in its label; this highlights the column label.

To select a range of columns for removal: click the left mouse button in the label of the left (or right) most column to be removed; put the cursor in the label of the right (or left) most column to be removed; hold down the SHIFT key and click the left mouse button.

To select a non-contiguous set of columns for removal: place the cursor in the label of one of the columns to be removed and click the left mouse button; this column is selected. Place the cursor in the label of any other column to be removed, hold down the CTRL key and click the left mouse button; this second column is also selected. Repeat this process as desired. Using control-click in its label, any column can be toggled between selected and deselected for removal without affecting the status of any of the other columns.

Either, place the cursor in a selected label, click the right mouse button, and select Delete. OR Select Remove Columns from the View menu.

The selected columns are removed from the spreadsheet.

Note

You cannot Undo a column removal. To restore the column to the spreadsheet, use Property Browse Bar from the View menu as described above.

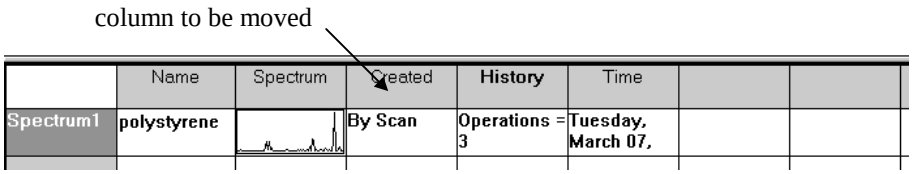
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Caution
Do not remove the name and spectrum columns of the spreadsheet. If you remove the spectrum, use the Property Browse Bar to add Spectrum to the spreadsheet. If you remove the name, use the Property Browse Bar to add SpectName to the spreadsheet

Re-ordering Columns in the Spreadsheet

To move a column (property) in the spreadsheet

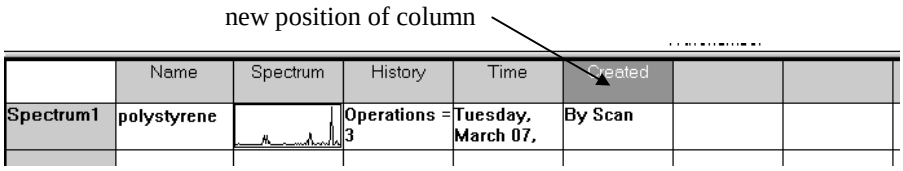
1. Place the cursor in the header cell of the column to be moved.



2. Hold down the left mouse button until a small rectangle appear at the base of the cursor arrow.

3. Move the modified cursor to the header of the column that you wish to be immediately to the right of the selected column when the spreadsheet is reordered. That is, the moved column will replace this column and push it, and all rows to its right, one column over to the right.

4. Release the mouse button. Wait for the spreadsheet to be redrawn.



Copying Rows in the Spreadsheet

To copy a row within a spreadsheet:

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1. Click the cursor in the leftmost column of the row to be copied; this highlights the cell.

2. Click the right mouse button; this menu appears.



If nothing is currently in the clipboard, then the Paste entry may be disabled (grayed out).

3. Select Copy. Click the cursor in the leftmost column of the row that you wish to be immediately below the row pasted in. That is, the pasted row will replace this row and push it, and all rows below it, down.

4. Click the right mouse button; this menu appears.



5. Select Paste.

Re-ordering Rows in the Spreadsheet

There are two ways to move a row (spectrum) in the spreadsheet—using the right mouse menu or dragging the row.

1. Click the cursor in the leftmost column of the row to be moved; this highlights the cell.

2. Click the right mouse button; this menu appears.



If nothing is currently in the clipboard, then the Paste entry may be disabled (grayed out).

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3. Select Cut. Click the cursor in the leftmost column of the row that you wish to be immediately below the moved row. That is, the moved row will replace this row and push it, and all rows below it, down.

4. Click the right mouse button; this menu appears.



5. Select Paste.

Alternatively:

1. Place the cursor in the leftmost column of the row to be moved.

2. Hold down the left mouse button until a small rectangle appears at the base of the cursor arrow.

3. Move the modified cursor to the leftmost column of the row that you wish to be immediately below the selected row when the spreadsheet is reordered. That is, the moved row will replace this row and push it, and all rows below it, down.

4. Release the mouse button. Wait for the spreadsheet to be redrawn.

Deleting Rows in the Spreadsheet

To delete a row within a spreadsheet:

1. Click the cursor in the leftmost column of the row to be deleted; this highlights the cell.

2. Click the right mouse button; this menu appears.

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If nothing is currently in the clipboard, then the Paste entry may be disabled (grayed out).

3. Select Delete.

SPECTRUM OPERATIONS

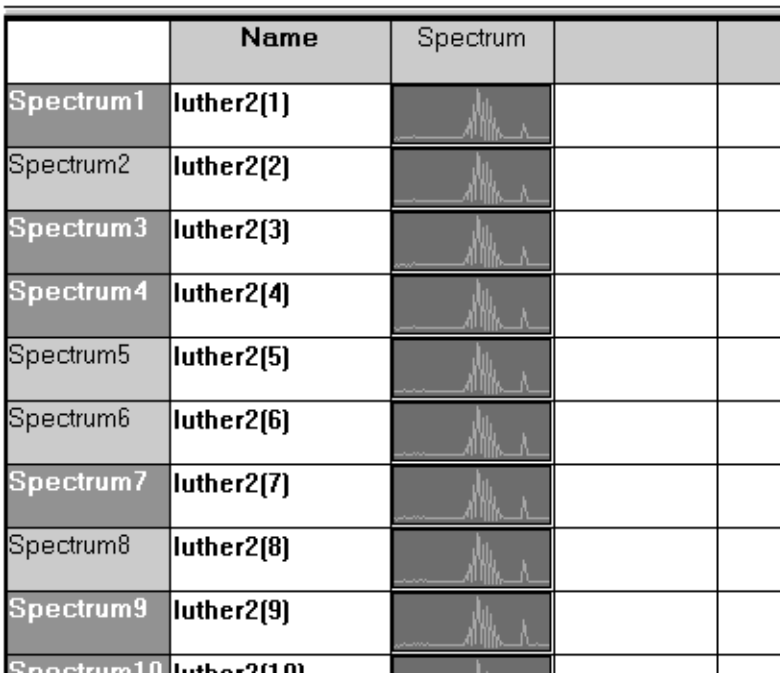
The spreadsheet is the major tool for direct access to a spectrum in multi-spectral files. It is also used to select spectra for display, copying, etc.

Spectrum Selection using the Spreadsheet

Once a spectrum (or set of spectra) is selected, it is visible (indicated by the bold font in the leftmost column–the ID column) and it is selected for operations (indicated by a colored box outlining the selected cell in the spreadsheet; the column heading is shown in reverse video). Visible means that the trace (or traces) appears in the trace window. Spectra selected for operation are shown in green. Any selection operation in the speadsheet clears both the visibility and selection for operation status of any previously selected unlocked spectra. (See Chapter 8 for details of locking and unlocking rows and columns of the spreadsheet.)

- Single spectrum selection: place the cursor in the ID column and click the left mouse button. If you click on another row, that spectrum becomes selected and the first spectrum is deselected.
- Range of spectra selection: place the cursor in the ID column are the start (or end) of the range of spectra and click the left mouse button. Place the cursor in the ID column of the end (or start) of the range of spectra; hold down the SHIFT key and click the left mouse button. Any previously selected spectra outside this range are deselected.
- Non-consecutive spectra selection: place the cursor in the ID column and click the left mouse button; the spectrum is selected. Place the cursor in the ID column of any other spectrum, hold down the CTRL key and click the left mouse button; this second spectrum is also selected. This process can be repeated as desired. Using control-click, any spectrum can be toggled between selected and deselected without affecting the status of any of the other spectra. For example,

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	Name	Spectrum		
Spectrum1	luther2(1)			
Spectrum2	luther2(2)			
Spectrum3	luther2(3)			
Spectrum4	luther2(4)			
Spectrum5	luther2(5)			
Spectrum6	luther2(6)			
Spectrum7	luther2(7)			
Spectrum8	luther2(8)			
Spectrum9	luther2(9)			

Trace Display Order in the Window

When you use the spreadsheet to select spectra, the spectra traces are displayed in the window in the order selected. That is, the first spectrum selected is the uppermost trace in the window, the second spectrum selected is just below the first, etc.

If you select spectra one at a time using CTRL-CLICK, the display order of the traces in the window is the same as the selection order of the spectra in the spreadsheet.

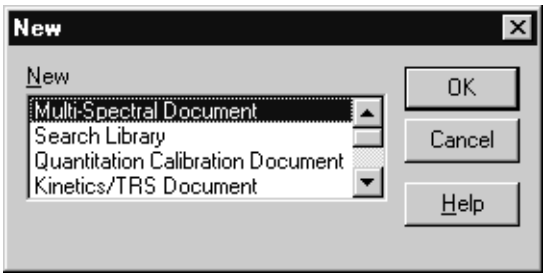
If you select a contiguous set of spectra, the upper trace corresponds to the first spectrum selected using CLICK; the lowest trace corresponds to the spectrum selected using SHIFT-CLICK. Intermediate spectra and their traces are ordered sequentially from first to last.

Copying Spectra between Documents

In addition to using the Cut/Copy and Paste entries of the right mouse button menu, described previously in this chapter, spectra can be copied by dragging them from one

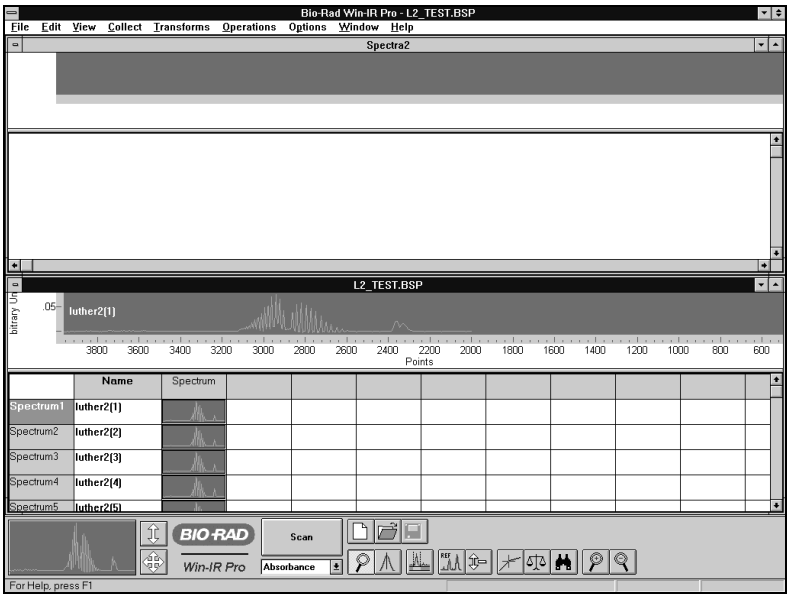
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document to another. In this example, we will copy some spectra from a multi-spectral document into a new and empty multi-spectral document. (Spectra can also be copied into documents that already have spectra in them.). First, create a new document by selecting New from the File menu; the New dialog box appears.



Select Multi-Spectral Document and click the OK button. This creates a new, empty multi-spectral document.

If it is not already open, open the document from which the spectra will be copied. Select Tile from the Window menu. The screen displays both documents.



To copy the spectra:

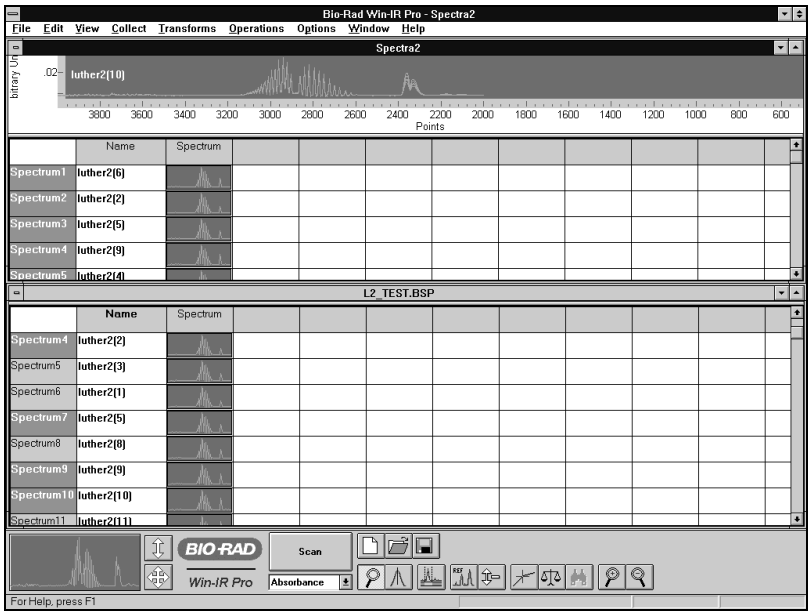
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1. Select the spectra to be transferred, using the techniques described in the previous section. You may find it convenient to select Maximize spreadsheet from the Windows menu (or press the F12 button on the keyboard).

2. Place the cursor in the Spectrum ID column of one of the spectra to be transferred.

3. Hold down the left mouse button and drag the cursor into the trace portion of the target document. The cursor will change to a circle with a diagonal in it (the sign for forbidden) until it reaches the trace area; there it will change to an arrow with small rectangle and a + sign.

4. Release the mouse button. The selected spectra will be copied into the target document.



This is an example of copying using the drag-and-drop technique. You can also copy between documents using Edit / Copy and Edit / Paste. This technique is discussed in Chapter 7.

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Copying Column Information

There are two ways of copying (non-graphical) columns from the Win-IR Pro spreadsheet to external spreadsheets and word processor documenting —using the right mouse menu or using View / Remove Columns. In either case, you must first select the columns to be copied.

Select a column by clicking in its label; this highlights the column label.

To select a range of columns for removal: click the left mouse button in the label of the left (or right) most column to be removed; put the cursor in the label of the right (or left) most column to be removed; hold down the SHIFT key and click the left mouse button.

To select a non-contiguous set of columns for removal: place the cursor in the label of one of the columns to be removed and click the left mouse button; this column is selected. Place the cursor in the label of any other column to be removed, hold down the CTRL key and click the left mouse button; this second column is also selected. Repeat this process as desired. Using control-click in its label, any column can be toggled between selected and deselected for removal without affecting the status of any of the other columns.

1. Place the cursor in a selected label.

2. Click the right mouse button; this menu appears.



If nothing is currently in the clipboard, then the Paste entry may be disabled (grayed out).

3. Select Copy.

4. Open the desired application (Excel, Word, etc.)

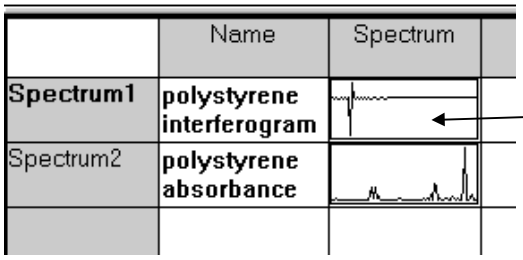
5. Paste the information into the application following the rules and procedures of that application.

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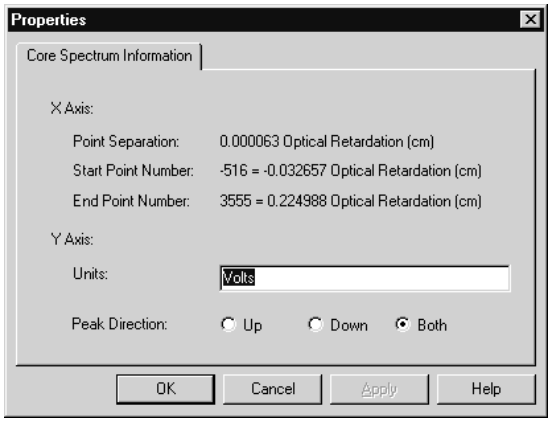
You can also copy non-graphical information with Edit / Copy. The details of this process are discussed in Chapter 7, in the Copy section.

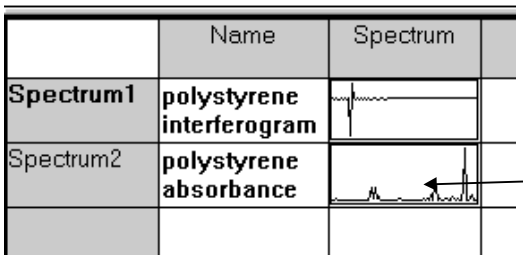
Core Spectrum Information

Displays fundamental information about the spectrum. The Core Spectrum Information status box is displayed if you double click on the Spectrum in the spreadsheet, on the Ydata spectrum in the spreadsheet, or on Ydata in the History list. This status box shows the x-axis point separation, starting point, ending point; the y-axis units, and peak direction. For example,



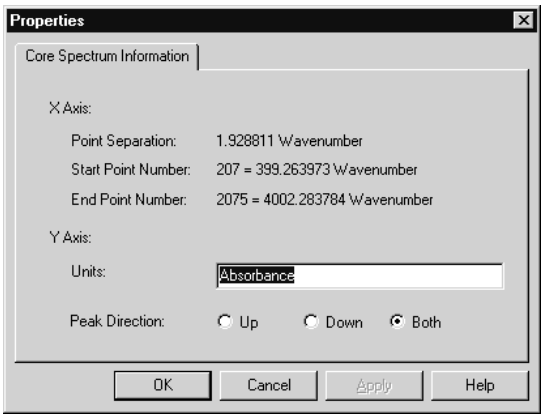
Double-click here to get Core Spectrum Information about this spectrum





Double-click here to get Core Spectrum Information about this spectrum

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You can change the *label* of the y-axis to one that more exactly describes the particular spectrum. Type the desired text in the box and clicking OK. This does not change the y-axis numbers.

SAVING SPREADSHEET FORMAT

The spreadsheet formats are saved on a per-document type (Multi-Spectrum, Kinetics, etc.) basis. The following applies to each type of document.

Whenever a document is closed, its format (column contents and order) is saved in memory. If another document of that type is opened—whether existing or new—it will have that format. For an existing document, this means that the spreadsheet format may not be the same as the one you previously had.

This does not affect documents that are already opened.

When you exit Win-IR Pro, whatever spreadsheet format is in memory for that document type, will be saved and used when you restart Win-IR Pro and open a document of that type.

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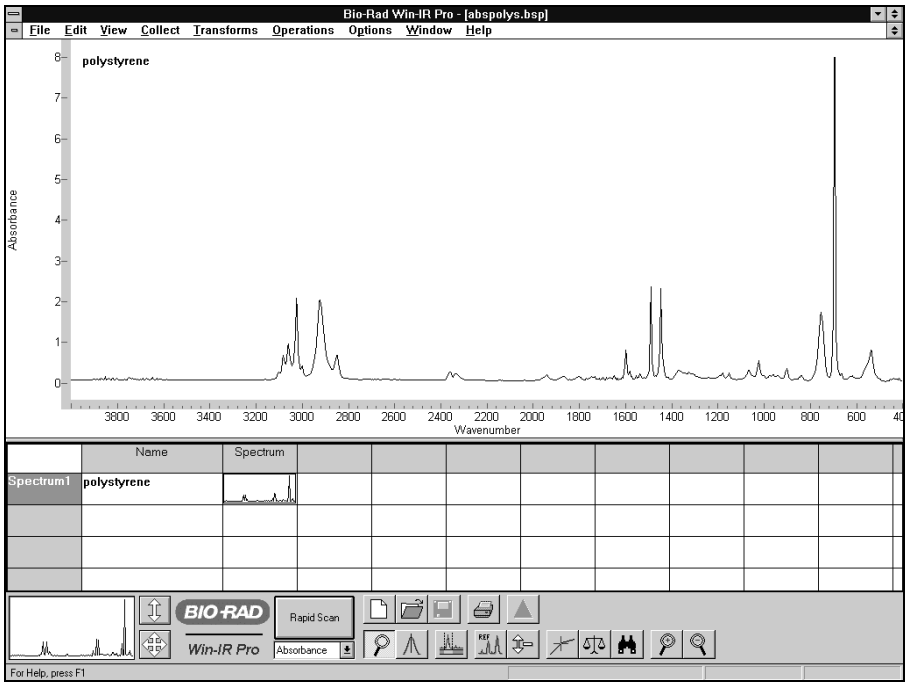
5
History, Reprocess, Method

HISTORY

Every spectrum collected under Win-IR Pro has a history associated with it. This history is a list of the operations that were performed to collect the interferogram and, optionally, to transform it by such processes as Compute (to get a single-beam spectrum), Ratio (to get an Absorbance spectrum), Transmittance, Differentiation, Deconvolution, etc.

All parameters are saved, whether they appear to be relevant or not. These parameters can be examined by selecting View / History and then double-clicking Scan in the History Browser dialog box. Note that the Background file name is not found under Scan, but rather under Ratio, because it is a ratio parameter.

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You can see the history of a spectrum by selecting History from the View menu. The History Browser dialog box appears. (If the spectrum has no history, the History entry will be disabled–grayed out.)

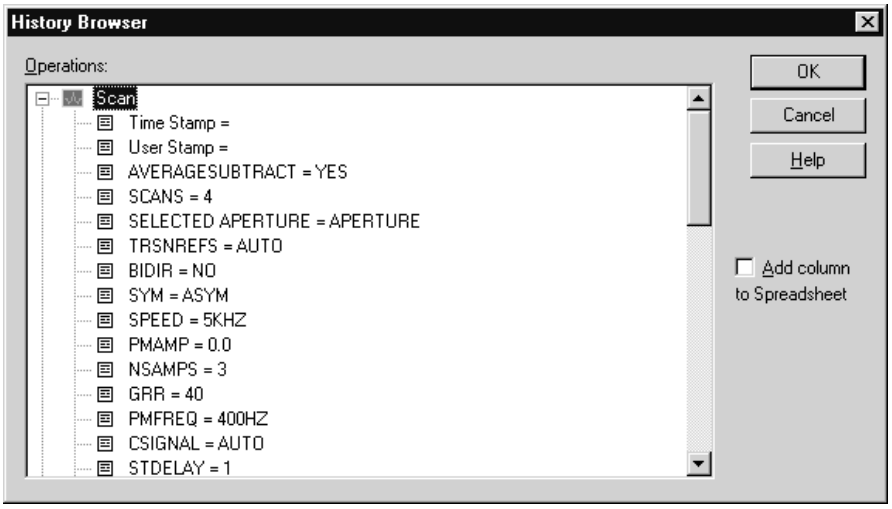
Note

When a spectrum is imported, it arrives with no history. Its history begins if it is manipulated subsequent to its import. Spectra that do not have Collect as their first operation (see below) were not collected using Win-IR Pro.

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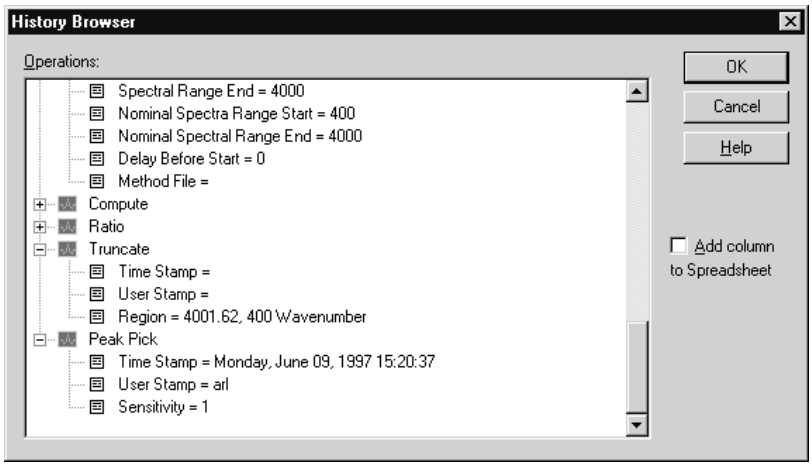


To see the details of an operation, place the cursor on the + box to the left of the row, and click the left mouse button. If there are details, the operation expands to show them.



This may be done for any or all of the operations.

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Time-Date Stamp: At release 2.1 of Win-IR Pro, the time and date of the operation are automatically added to the operation. An example of this is shown above for Peak Pick. Operations that were performed before release 2.1 have a blank for the time-date stamp, as shown above for Truncate.

User Stamp: At release 2.5 of Win-IR Pro, the user login name of the person performing the operation is automatically added to the operation. An example of this is shown above for Peak Pick. Operations that were performed before release 2.5 have a blank for the user stamp, as shown above for Truncate.

To collapse the details of the operation, place the cursor on the left-hand box and click the left mouse button once. If you exit the History Browser dialog box without collapsing the details of the operations, they will automatically be collapsed for you.

Return to the main menu by clicking either the OK or Cancel button. More details about the history browser are in the View menu chapter under History and Property Browse Bar.

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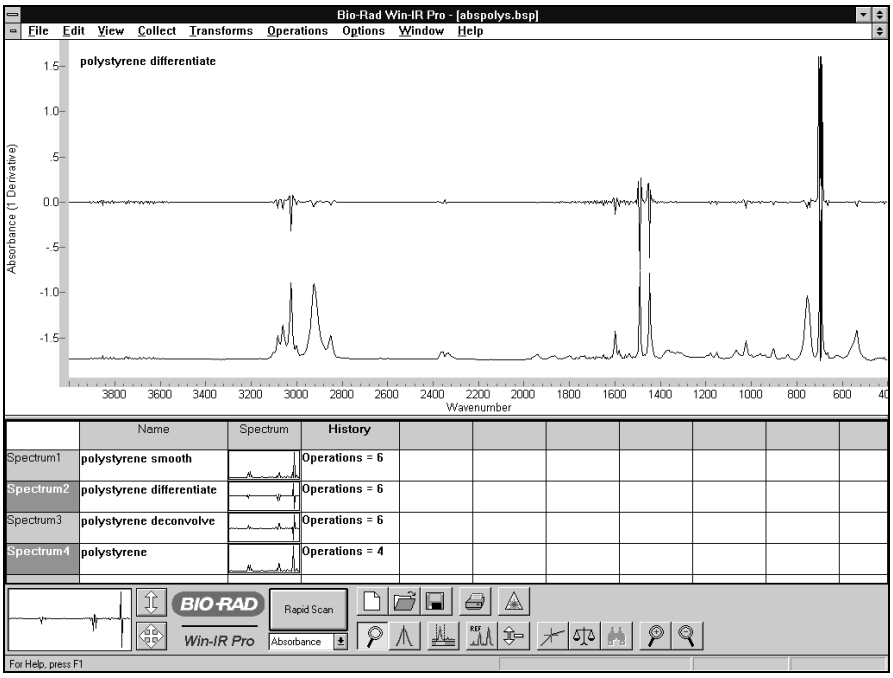
REPROCESS

Because the interferogram is always saved as part of the document in which the spectrum was collected, you can always start from the interferogram and reprocess it as desired.

Note

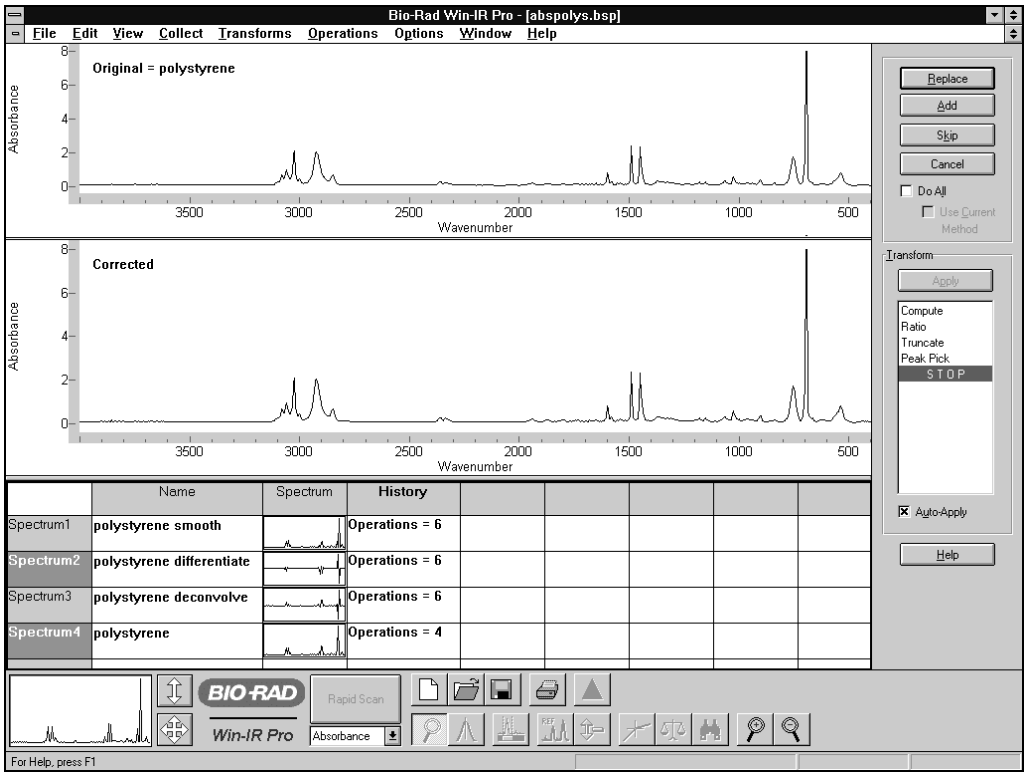
Certain operations require additional spectra to be present to perform the operation. For example, Ratio requires that the background spectrum exists; Spectral Subtract requires that the reference spectrum exists to be subtracted from the original spectrum. If a required spectrum is not found where expected, Win-IR Pro informs you of this, and allows you to locate this spectrum or to select another one in its stead.

Using the spreadsheet, select the spectra to be reprocessed.



Then select Reprocess... from the Operations menu. The trace display is split in two:

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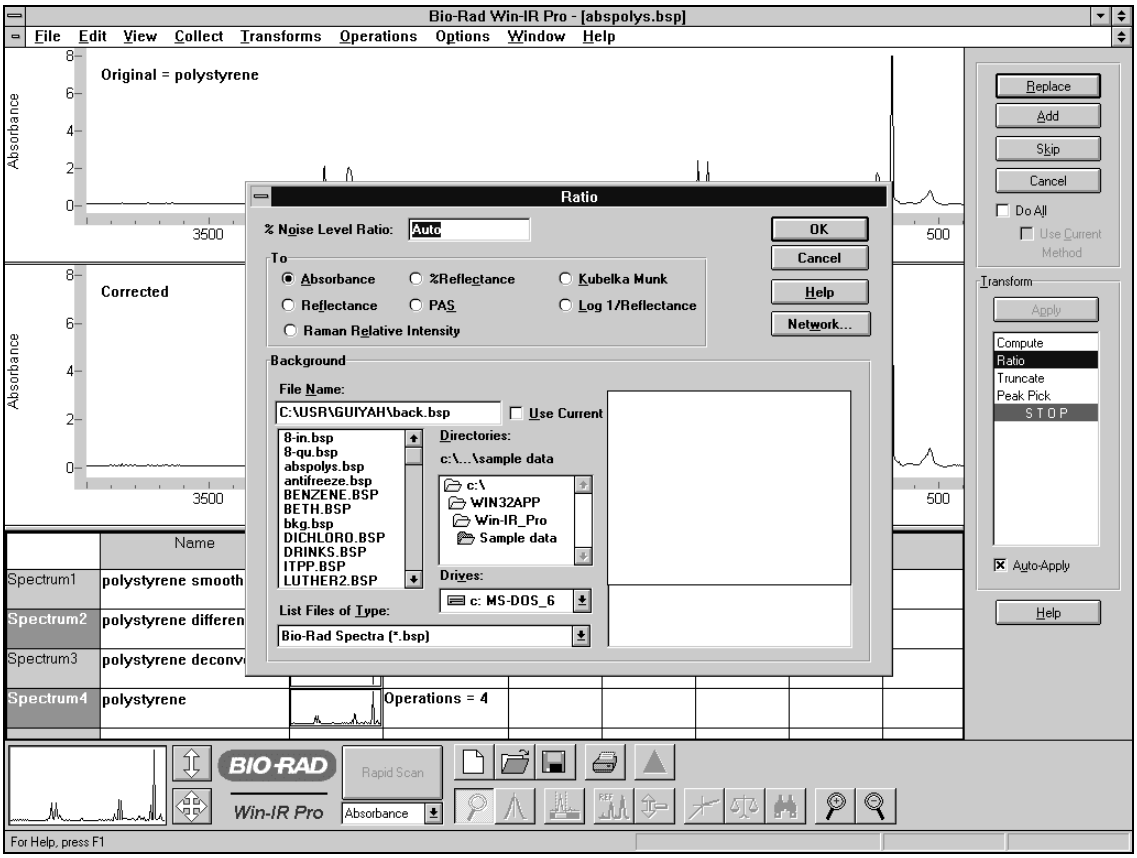


The first spectrum selected, polystyrene, is displayed. The original spectrum is in the upper part of the window; the corrected spectrum is in the lower part of the window. Since nothing has yet been done, the two spectra are identical. The sidebar control panel appears at the right side of the window. These controls allow reprocessing.

Collect does not appear in the list of Transform operations in the control panel because Reprocess... uses the collected and saved interferogram; Reprocess... does not collect data, it recalculates using data in the previously collected interferogram.

If you want to view and/or change the parameters used in an transform, highlight that transform (for example, Ratio). The Ratio dialog box appears.

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Make whatever changes you desire. You must have a background single-beam spectrum available to perform the ratio. If the original background was not found, you must load an appropriate background file to be ratioed against. You can use the Network button to connect network disks to your local system.

Note

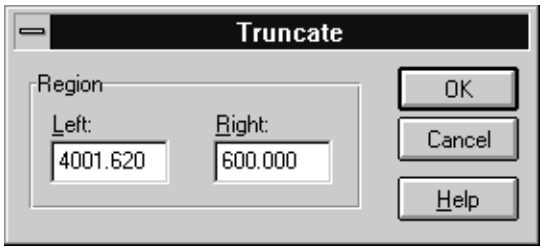
Changing some parameters here may require subsequent operations to be modified or deleted. For example, if the spectral type (To) were changed from Absorbance to Kubelka Munk, deconvolution with the original parameters may no longer give meaningful results.

In all the dialog boxes, Cancel returns you to the main window with no changes made; OK returns you to the main window and changes the parameters.

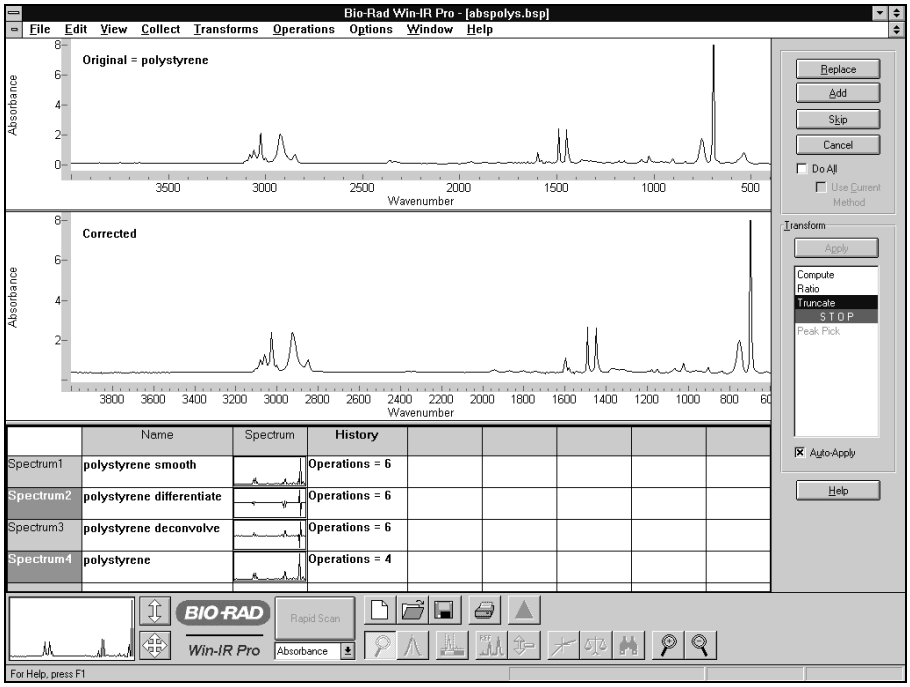
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If you edit a procedure, you can have the changes apply immediately after you have pressed OK in the procedure dialog box, or you can choose to apply these changes (and, perhaps, changes in other procedures) manually.

Select the Auto Apply box to have edit changes applied to the spectrum immediately after exiting from the dialog box. In this example, select the Truncate operation. The existing right hand limit is 400; change it to 600.



Click OK. The Corrected spectrum is now truncated at 600 cm^{-1}.



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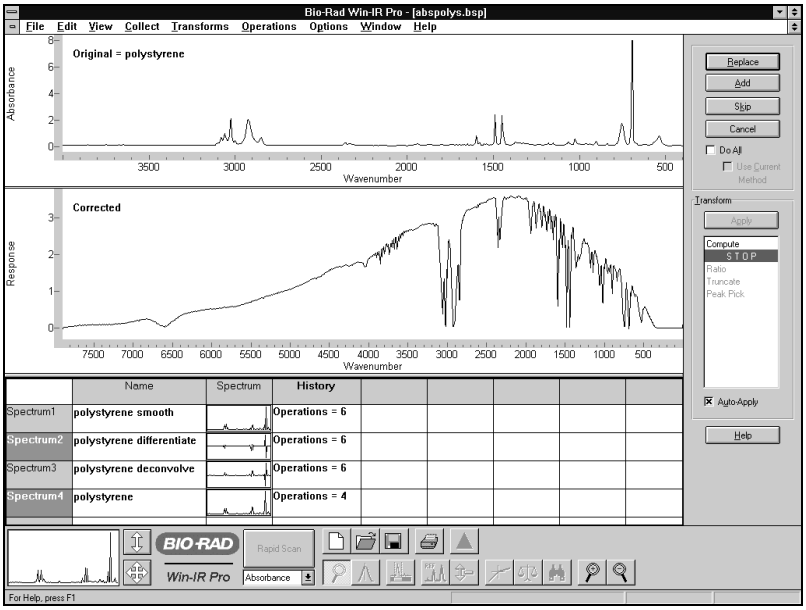
If you unselect Auto Apply; then chnages made when editing are not applied after you click the OK button in the transform dialog box. However, the Apply button is enabled. You can edit this and other transforms, as desired. When the Apply button is clicked, then all the transform modifications are processed.

Use the STOP label to halt the reprocessing at the stage you want to view. To do this

1. Place the cursor over the STOP label and hold down the left mouse button.

2. Drag the STOP label on top of the transform after the last transform operation you want to occur and release the mouse button.

For example, to view the single-beam trace, place the STOP label just after Compute (on top of Ratio) and release the mouse button.



It does not matter whether the Auto Apply box is checked or not; the Corrected trace will show the spectrum at the desired stage of operations.

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Although it appears as if you are “rolling back” the Transform operations, what is actually happening is that the original interferogram is reprocessed, using the original or modified parameters, to the result of the operation that you wish to view.

After you are satisfied with the changes, select one of the buttons to determine what is to be done with the Corrected spectrum.

Replace: replace the existing original spectrum with the corrected spectrum. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Add: add the corrected spectrum to the document that contains the original spectrum. Both spectra are now in the main menu display. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Skip: Do not alter the current spectrum. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Cancel: return to the main menu display without acting upon the current spectrum or any subsequent spectra. Spectra previously replaced or added are not altered by this.

Do All: if this is selected, then Use Current Method is enabled. Click either Add or Replace. This spectrum and all subsequent spectra are processed and all the corrected spectra are either added to the spreadsheet (Add)or replace the original spectra (Replace). Spectra previously replaced or added are not altered by this. The procedures (and their parameters) used to reprocess the spectra depend upon whether Use Current Method is selected.

Note

This is different from the Do All procedure in the transformations (see Chapter 10).

Use Current Method: this is only enabled if Do All is selected. If this is selected, then the procedures and parameters selected for this spectrum are applied to this spectrum and to all subsequent spectra; if it is not selected, then this spectrum and all subsequent spectra are reprocessed according to their own existing procedures.

Help: enter the on-line Help system.

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Displaying the Interferogram

To display the interferogram in the spreadsheet, for the previous example:

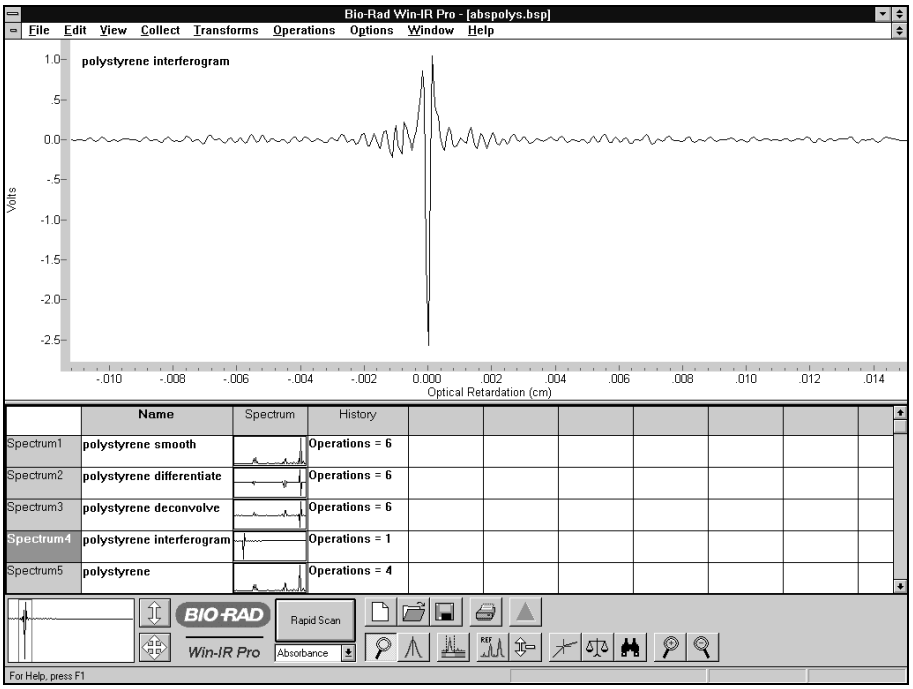
1. Select the polystyrene spectra in the spreadsheet.

2. Select Reprocess from the Operations menu.

3. Drag STOP back on top of Compute; release the mouse button. The interferogram is displayed in the lower part of the window.

4. Press the Add button.

5. Select the interferogram, relabel it (see Chapter 4), and zoom in on the centerburst. The inteferogram is shown in the picture below.



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METHOD

Method allows you to process subsequent samples in exactly the same manner and with the same parameters as a previous sample. The first sample (usually) proceeds through Collect, Compute, and Ratio. After that, other transforms may be applied. To create a method

1. Use Reprocess until the sequence of transforms is exactly what you want.

2. Select the spectrum that is to be the basis for the method; it will display green (default color).

3. Select Define a Scan... from the Collect menu. The Rapid Scan tab pages appear. If you click OK immediately, the existing parameters will be used to define the Scan.

   You can change any number of parameters (but they must be meaningful for the scan), and then click OK. The next data collect will use these parameters. See your spectrometer manual for a detailed discussion of the collection parameters.

Future data collection and processing will be done according to this method, unless you explicitly change data collection parameters.

Notes

Method works only for Rapid Scan.

Data collection parameters cannot be changed by Reprocess following a scan.

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6
File Menu

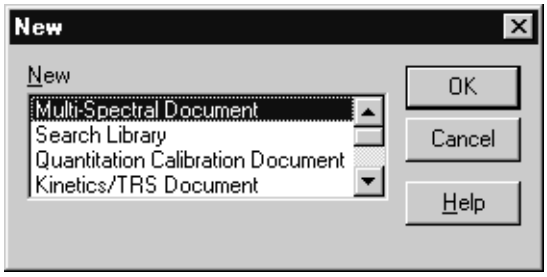


These commands control which documents are opened for data collection and manipulation, including the printing of traces, spreadsheets, etc. See Chapter 3 for an explanation of the document types and what they are used for.

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NEW...

If selected, the New dialog box appears. Select the type of document to be created.



Multi-Spectral Document: This is the default document; it is used to collect data (other than kinetics data) with a spectrometer, and to manipulate and save that data later. It can be used to hold any type of spectrum. When saved, the file has a .bsp extension.

Search Library: allows you to create and edit your own search libraries. When saved, these libraries have a .bri extension.

Quantitation Calibration Document: The document used to contain the calibration spectra, the concentrations, and the calibration computations. Spectra can be collected directly into this document or previously collected spectra can be copied into it from other documents.

Kinetics/TRS Document: Used to collect sets of related spectra such as kinetics, gas chromatography (GC), thermogravimentric analysis (TGA) and time-resolved spectrscopy. When saved, the file has a .kin extension.

Note

The background for a kinetics experiment is saved in a separate file with a .kbg extension.

Print Composition: Used to create a page of spectral information to be printed. See Chapter 15 for details on how to place objects on this page. When saved, the file has a .bpt extension.

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Image Document: Used to collect data from an array detector. This feature is not currently supported.

OK: create a new document of the selected type and return to the main menu with the empty document displayed.

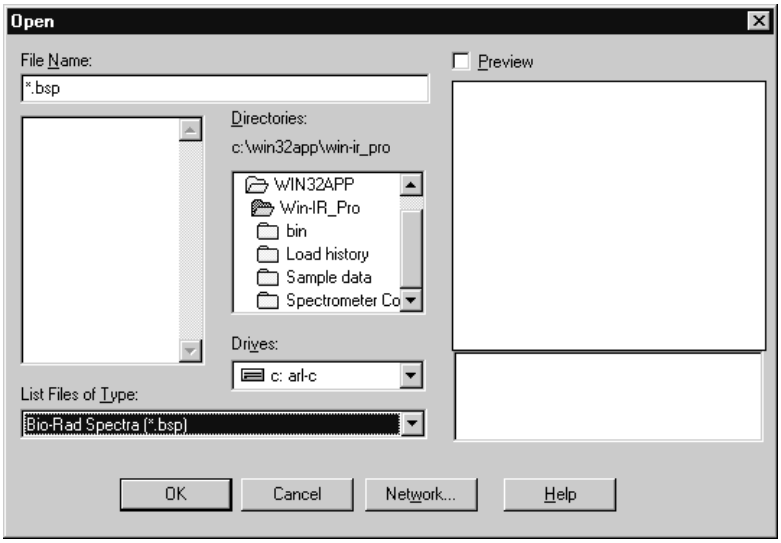
Cancel: return to the main menu without creating a document.

Help: access the on-line Help facility.

CAUTION
Until the new document is written to the disk using Save or Save As... from the File menu, it only has a temporary name (Spectra1, Search1, etc.). If you want to retain the document, you must save it. This follows standard Windows and Windows NT protocol. See Close later in this chapter for details.

OPEN...

Opens an existing document. When this is selected, the Open dialog box appears.



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Select a file name from the File Name list. Change directories (and drives), if desired, using standard Windows techniques in the Directories list. Select the type of file from the List Files of Type list; the default is Bio-Rad Spectra (*.bsp). The types of files available are:

Bio-Rad Spectra (*.bsp): spectral data collected from a spectrometer using the Win-IR Pro software, or other data converted and saved as the Bio-Rad Spectra format.

3200 Format Spectra (*.dt, *.sb, *.ig): spectral data collected from a spectrometer using the Bio-Rad 3200 series software (DDS).

*.dt	spectrum
*.sb	single-beam
*.ig	interferogram
*.ch	chromatogram

GRAMS/386 Spectra, Win-IR (*.spc): spectral data collected from a spectrometer using Win-IR or GRAMS/386, or converted from other formats to GRAMS format. Comments in .spc files are imported into Win-IR Pro.

Comma Separated Value (*.csv): spectral files that are in spreadsheet format (do not confuse this generic spreadsheet with the one in the lower half of the Win-IR Pro windows). A typical line of data in these files is

X-axis value
, (a comma)
Y-axis value
newline character

If this is a multifile, then the additional Y-axis values are on the same line, separated from the first Y-axis value by commas. A header defines file type, axes labels, etc.

Comma-separated value files are easily exported to most commercially available spreadsheets.

Phase Array Data (*.phs): this is the file into which the phase correction, calculated in Compute, is stored.

Kinetics Background (*.kbg): a background spectrum used for kinetics data collection.

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AIA Data Exchange (*.cdf): a new standard developed by the Analytical Instruments Association. It is designed to allow easy interchange of data between different vendors' equipment.

Sadtler SearchMaster (*.irf): a file in Sadtler format, usually collected using Sadtler SearchMaster, containing one spectrum.

Search Library (*.isl or *.bri): vendor-supplied libraries of spectra against which unknown spectra will be compared to obtain matches.

Note

File / Open will show all installed libraries. If you try to open a library that you do not have permission to access, you will see a message saying Can't open *filename* for reading.

Quant (*.bsq): the calibration document used for simple quantitative analysis.

Kinetics/TRS Data (*.kin): the set of related spectra (and optional analysis) obtained from kinetics data collection or from TRS data collection.

Bio-Rad Microscope Mapping Spectra (*.bsm): data collected using Bio-Rad's Shadow Pro.

Raw Image Data (.seq): this is the data prior to its being processed to Image Data (.dat) files. The capability of opening these files may, at times, be very useful, because of the way Image data is collected. There are three cases:

- No processed image file (.dat) exists. The . seq file will be processed to create a .dat file. The .dat file will then be opened. Before this occurs, there is a dialog box allowing you to cancel this action.
- A processed image file (.dat) exists, but is not open. You are asked if the .seq file is to be reprocessed; if it is the existing .dat file is overwritten.
- A processed image file (.dat) exists and is open. A message box informs you that the .seq file cannot be opened.

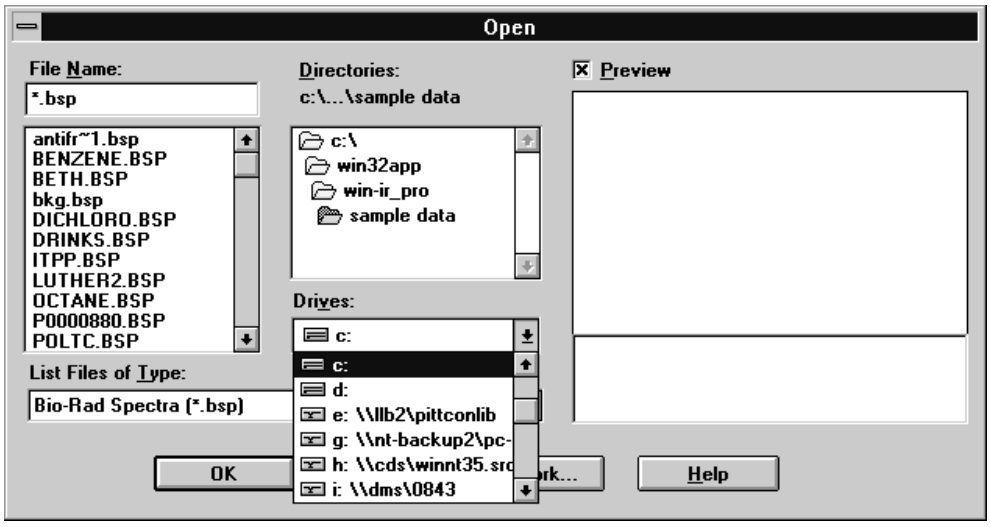
Image Data: (*.dat): data collected from array detectors.

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All Files (*.*): display all files in the directory regardless of their extension.

Open a file by selecting it and clicking OK, or by double clicking the name.

Drives: a pull-down menu appears with a list of all connected drives. Select the drive on which the desired file is stored. If the drive is not connected, click the Network button to connect that drive to your computer.

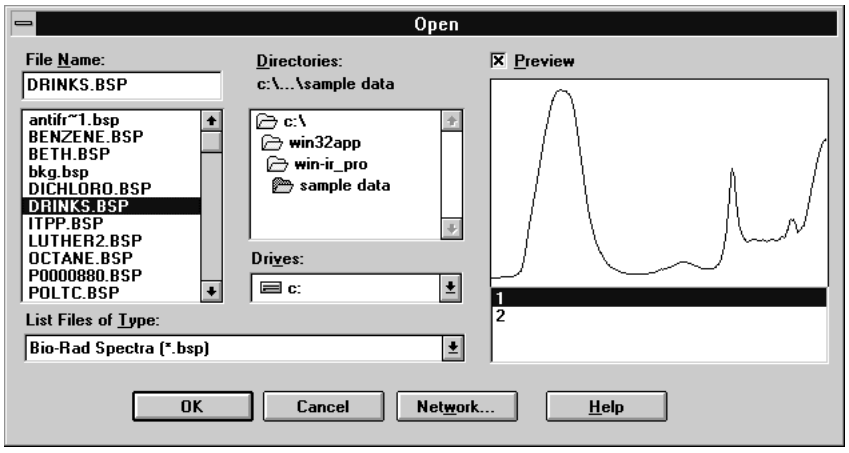


Preview: if checked, the trace for the selected file will be displayed in the box on the right. You can rapidly scan through the files with the ↑ and ↓ keys. This is possible for files on network drives, as well as on your local drive.

Note

Image files (.dat) do not show a preview, even if the Preview box is selected.

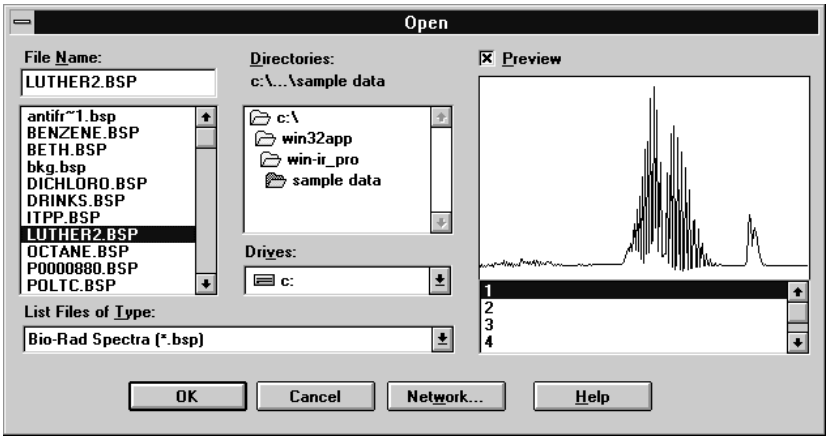
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If a document that contains more than one spectrum is selected, it is possible to preview any of the spectra in that document. In the next two dialog boxes below, the first and eleventh spectra in the document are previewed.

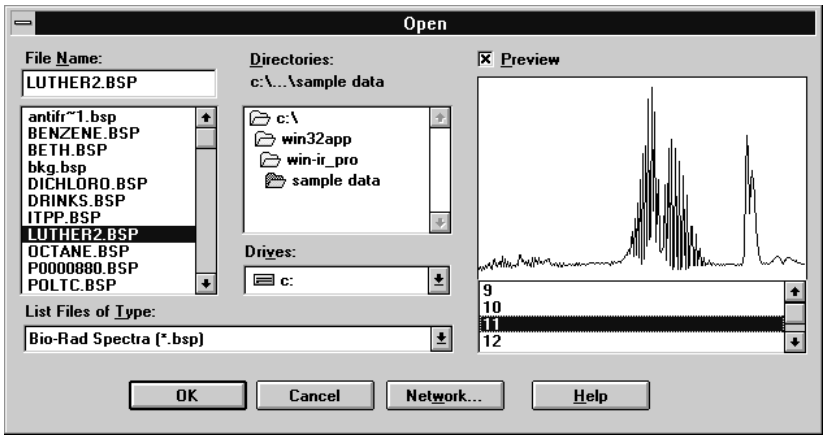
Note

Only numbers are displayed in this box; there are no spectrum names even if you have named the spectra in the spreadsheet.



This is done by clicking the number in the preview box. If there are more than four spectra in the document, a scroll bar appears.

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Note

Preview works for any of these files regardless on the disk on which it resides; it does not matter whether the disk is on your local system or connected to your system via the network.

OK: open the selected document and return to the main menu with the document displayed.

Cancel: return to the main menu without opening a document.

Network: click to bring up the Connect Network Drive dialog box. With this, you can connect to any drive on the network to access files. If you need more information, see the Windows NT documentation you received with your system.

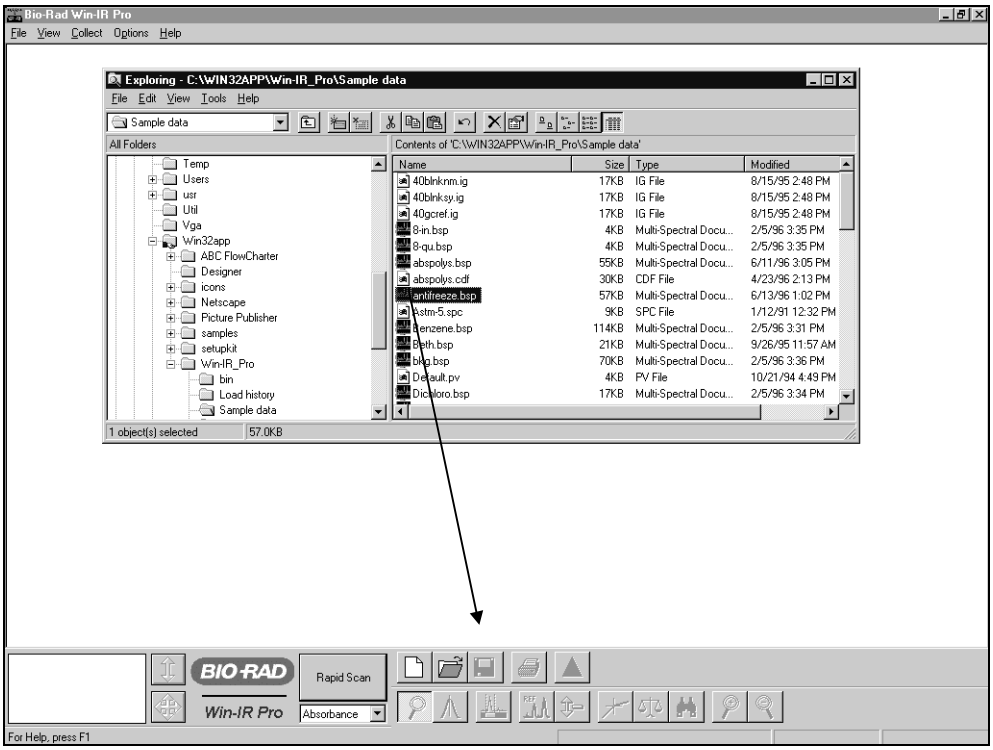
Note

In order to connect a drive to your system, the network administrator must have given you the appropriate access rights.

Help: access the on-line Help facility.

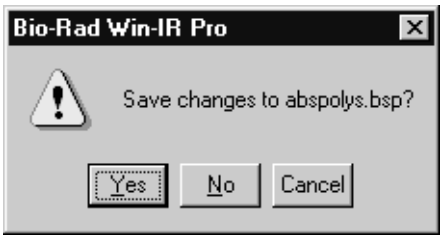
If you have the Explorer window active, you can highlight a document and drag it into the Win-IR Pro window to open it. This is an example of drag-and-drop.

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CLOSE

Closes the currently active document. If any changes have been made to the document since the last time it was saved, you will be asked if you want to save those changes.



Yes: save changes made since last save and close document.

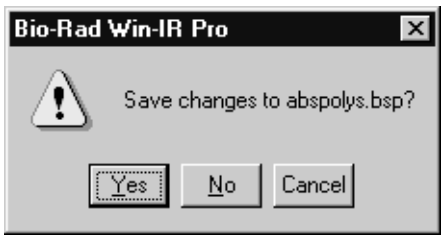
No: close document without saving changes made since the last save.

Cancel: do not close document; return to main menu.

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CLOSE ALL

Closes all open documents, For each document, if any changes were made to that document since the last time it was saved, you will be asked if you want to save those changes.



Yes: save changes made since last save and close document.

No: close document without saving changes made since the last save.

Cancel: do not close document; return to main menu.

SAVE

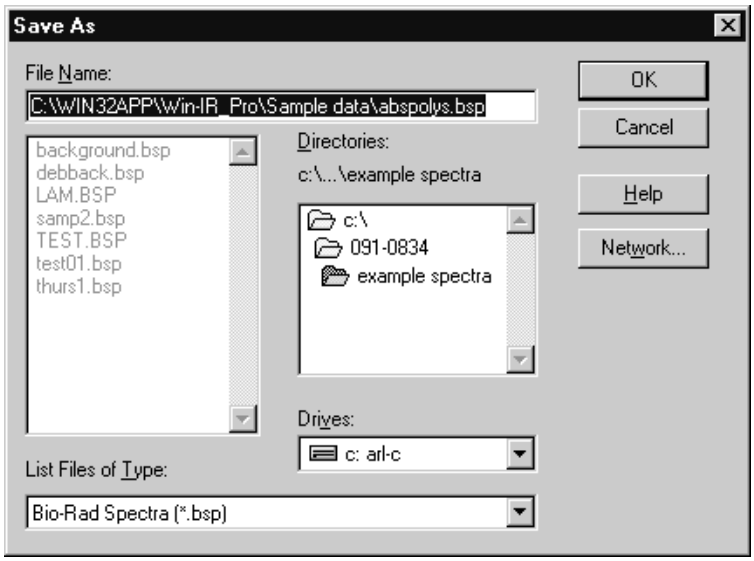
Saves the currently active document to the disk under its existing name. File / Save automatically converts all export trace files (.dt, .spc, etc.), to Bio-Rad Spectrum format (.bsp), but does not overwrite the original file.

Caution
Do not save files in the Win-IR Pro directory or its sub-directories; create your own directories for saving these files.

SAVE AS...

Saves the currently active document to the disk with a newly specified name and/or directory and/or file type. When this is selected, the Save As dialog box appears.

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Enter the desired name for the document in the File Name box. Use standard Windows procedures to change the directory, if desired. Click OK when you are ready to save the document. Windows NT supports the use of long file names.

Caution
Do not save files in the Win-IR Pro directory or its sub-directories; create your own directories for saving these files.

With Save As, you can create Bio-Rad spectra (*.bsp), GRAMS/386 and Win-IR spectra (*.spc), comma-separated value spectra (*.csv), Phase Array Data files (*.phs), AIA Data exchange (*.cdf) and Sadtler SearchMaster (*.irf) document types. These types are described under Open.

If the spectra in the spreadsheet of your .bsp file have the identical format, then when you save as an .spc file, they will all be saved to a GRAMS multifile.

If the spectra in the spreadsheet of your .kin file come from a kinetics or a TRS experiment, then when you save as an .spc file, the time information will be preserved as well as the exported spectra being saved in a multifile.

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Notes

If the target is a Sadtler SearchMaster (*.irf) file, then the file you are saving can contain only one spectrum. If it contains more than one spectrum, you will get an error message and no Sadtler SearchMaster file will be created.

Kinetics/TRS documents can be saved as .spc multifiles. Comments are saved when saving in the .spc format.

OK: save the document under the selected name and return to the main menu with the document still displayed.

Cancel: return to the main menu without saving the document.

Help: access the on-line Help facility.

Network: click to bring up the Connect Network Drive dialog box. With this, you can connect to any drive on the network to access files.

Note

This assumes that the network administrator has given you the appropriate access rights. If not, you will either be unable to connect to a network drive or, if you can connect, you will get a message such as

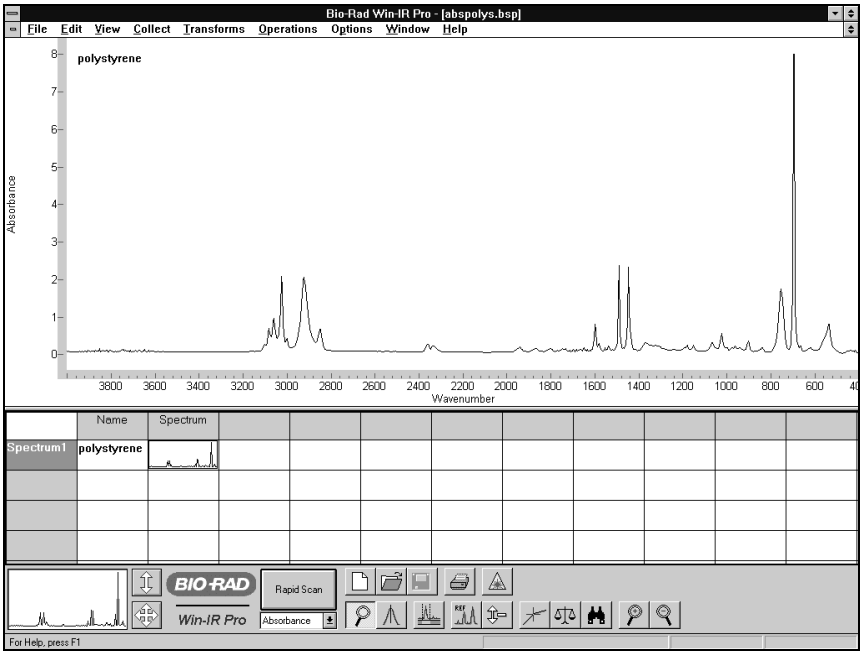


Follow the instructions in this message.

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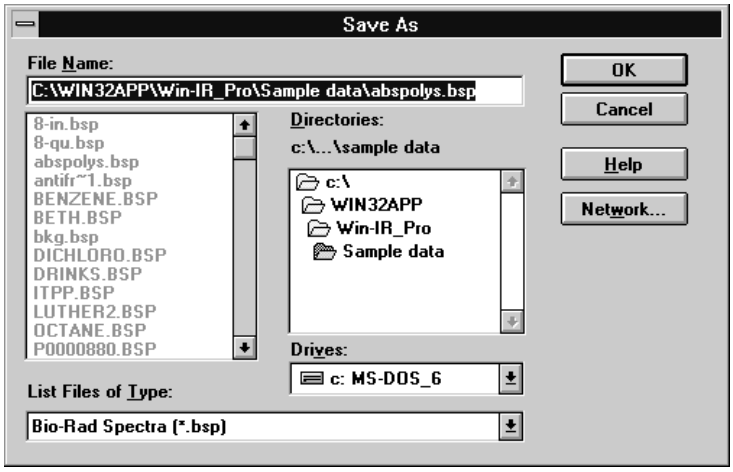
AIA Data Exchange File (.cdf)

There are additional features if you save a file as an AIA Data Exchange File. This is a standard format promulgated by the Analytical Instrument Association. You have the option to add information that is not normally stored in Win-IR Pro documents. For example, consider the file abspoly.bsp:

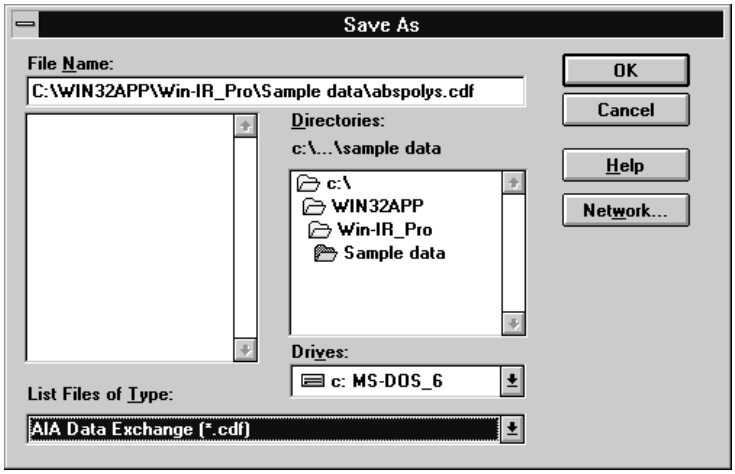


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1. Select Save As... from the File menu. The Save As dialog box appears.

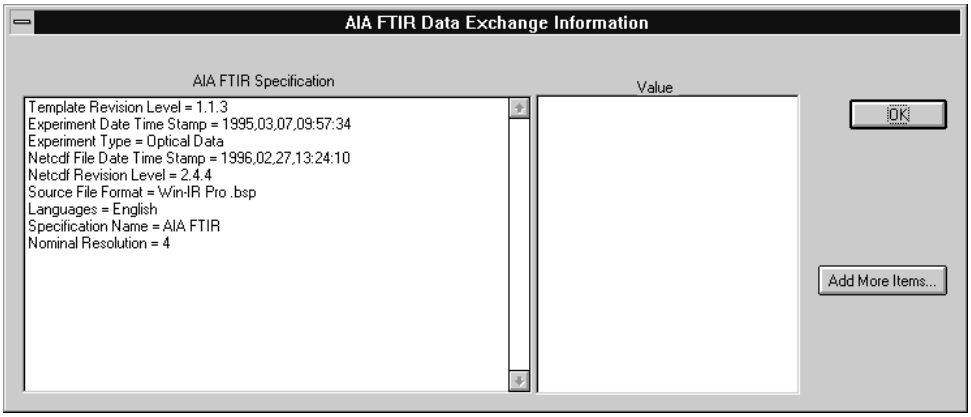


2. Use the List Files of Type: pull-down menu to select AIA Data Exchange (*.cdf).

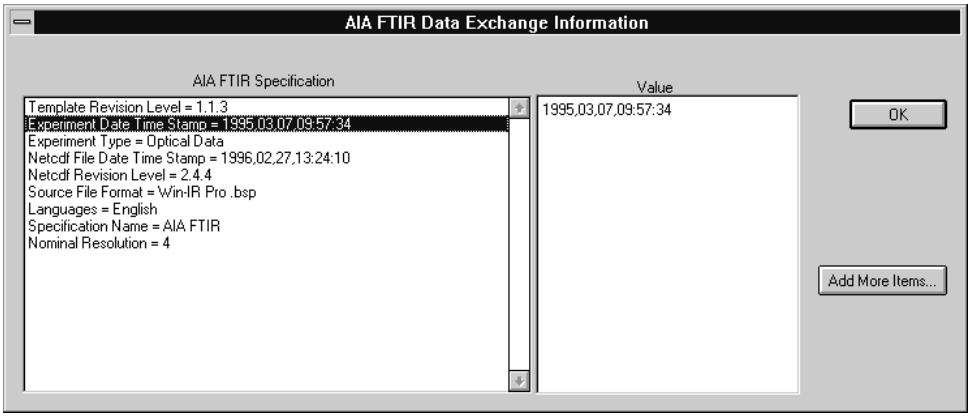


3. Click OK to save the document as an AIA Data Exchange file (the other buttons have their usual functions, as described above). The AIA FTIR Data Exchange Information dialog box appears.

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4. To change (or insert) a value for the specification, highlight the specification. The value appears in the Value box on the right side. Use the cursor and standard word-processing techniques to type in a new value.

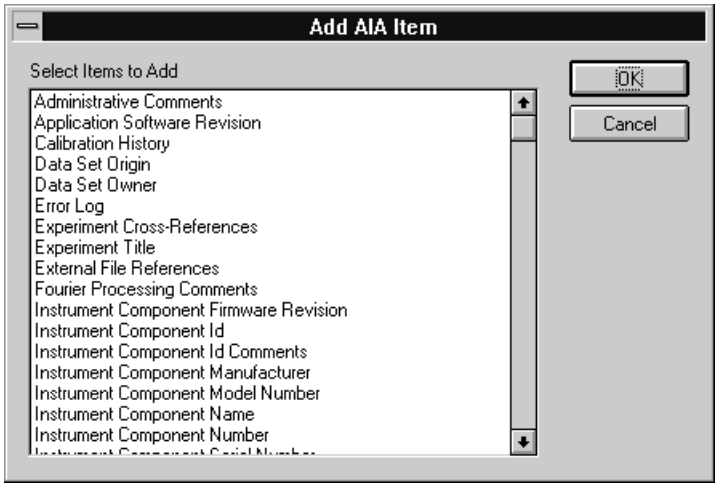


Note

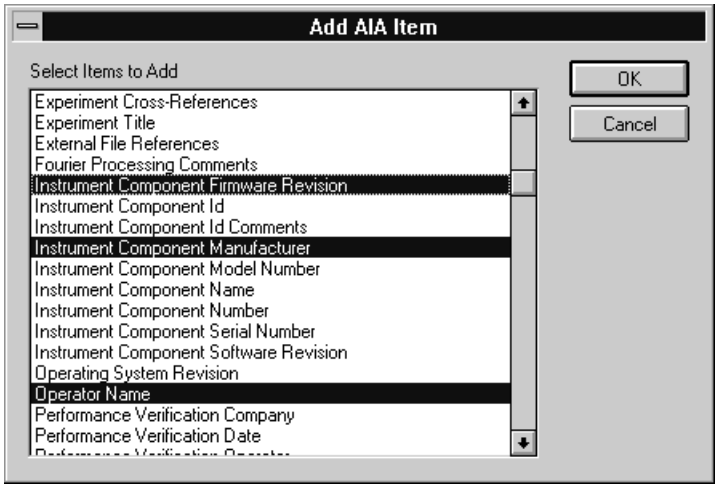
If the specification cannot be changed (read-only), then its value will be in gray rather than black, and you will not be able to alter it.

5. If you want to add additional specifications, click the Add More Items... button. The Add AIA Item dialog box appears.

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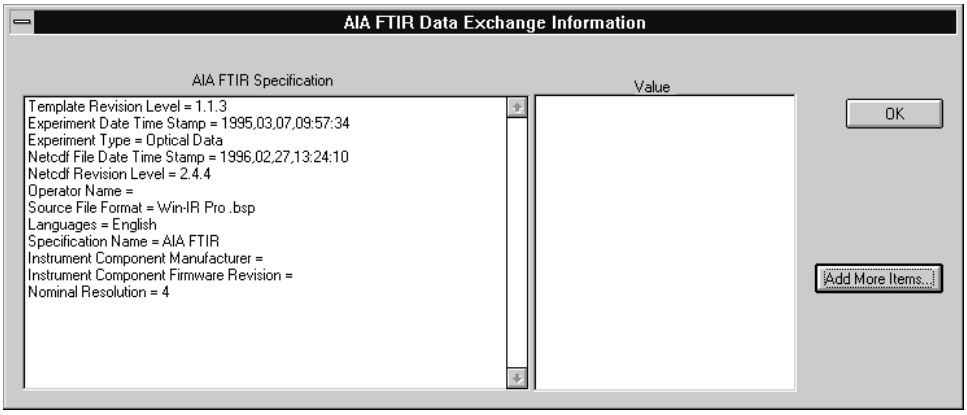


6. Highlight the specifications to be added. Contiguous specifications can be selected using the standard Windows shift-click selection technique. Individual specifications can be toggled on and off using the standard Windows ctrl-click technique. When all specifications have been selected, click the OK button (if you decide not to add any specifications, click the Cancel button, instead).



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7. The new specifications are added to the AIA FTIR Specifications box.



8. Set the values for these added specifications, following the procedure in Step 4, above.

9. Click the OK button to save the file as an AIA Data Exchange file.

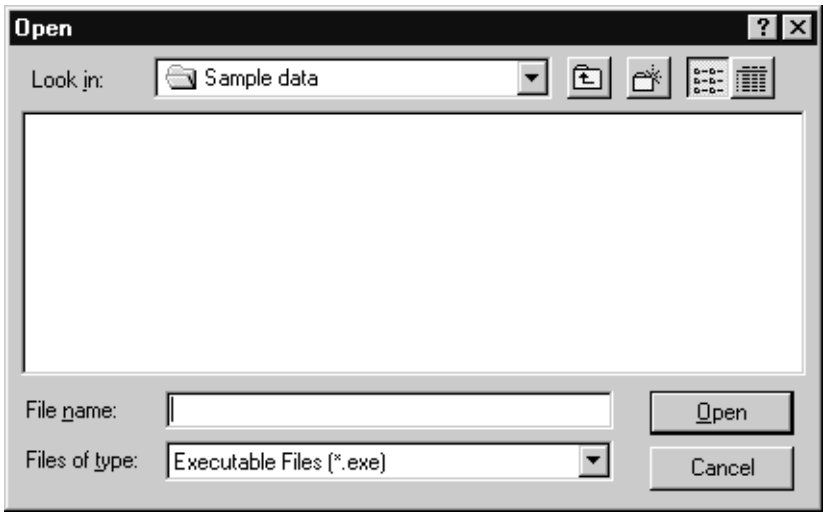
Note

Any .cdf file can be opened directly, using File / Open.
See the details in the Open section earlier in this chapter.

RUN

Allows you to run programs, including executable Win-IR Pro scripts from Win-IR Pro. You do not need to have a document open in Win-IR Pro to access this entry. When selected, the Open dialog box appears. The default file type is executable (*.exe).

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Use standard Windows NT techniques to access the file to be executed; then, click OK to start the application.

PRINT...

Prints the screen view of the currently selected spectrum on the printer specified as part of the Windows Control Panel or by the File / Print Setup menu selection. See the *Win-IR Pro Installation and Configuration Manual* for details on how to select printers and install printer drivers.

In addition to the spectrum in the main window, you can print any text column in the spreadsheet as part of this page.

1. Use the cursor and left mouse button to highlight the spreadsheet column to be printed.

2. Choose Lock Selected from the View menu.

3. Repeat this process for all desired columns. If you decide not to print a column, then highlight it and choose Unlock Selected from the View menu.

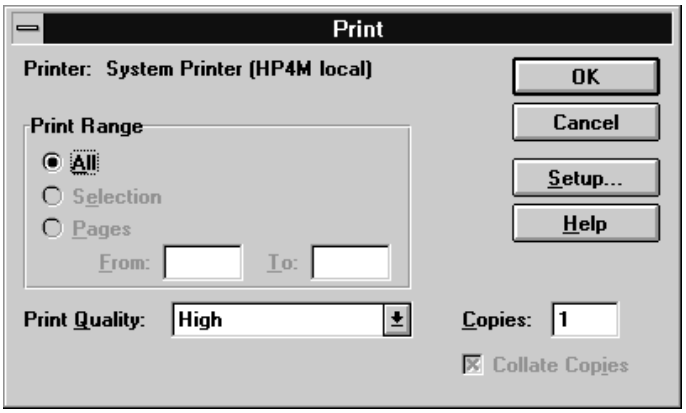
Note

Alternatively, use the CTRL key with the mouse button to toggle on and off the columns to be printed. This use is detailed in Chapter 4.

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4. Select the spectrum to be printed by highlighting its ID in the leftmost column.

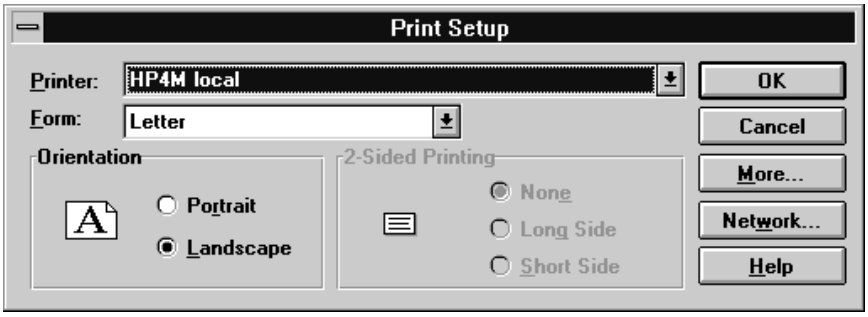
5. Select Print from the File menu. The Print dialog box appears.



Note

Because the output of Win-IR Pro does not span multiple pages, only the All button in Print Range is available and is automatically chosen. This will print all selected items.

6. Use the printer in Landscape mode. To make sure of this, click the Setup button. The Print Setup dialog box appears.



7. Be sure that Orientation is Landscape. Click the OK button to return to the Print dialog box.

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8. Click the OK button to begin printing.

The number of traces that can be printed is determined by how many can fit on the page (a function of page size and orientation). The types of lines used for printing and identifying the traces are in groups of 5. That is, the same type of line is used for trace 1, trace 6, trace 11, etc.

If you select more columns in the spreadsheet than can fit on the printed page, only those columns that completely fit on the page will be printed. The rest will not be printed.

Note

If you are using a color printer, the default colors for some of the traces may not have sufficient contrast—for example, yellow—to show clearly on the page. Use Options / Edit Color to change the appropriate traces until the printed copy is as desired. Be sure to record these color value settings.

PRINT PREVIEW

This feature is not currently implemented. Check the README.WRI file for the latest information.

PRINT SETUP...

Selects the output device and allows you to set its parameters. Normally, this is the printer and it has already been set up as part of the system installation. The dialog boxes and the specific values of the printer parameters depend upon the printer attached to the system. See the *Win-IR Pro Installation and Configuration Manual* for details on how to select printers and install printer drivers.

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PRINT COMPOSITION



Open existing or create new print composition templates. You can select information associated with spectra in a document (text or graphics), arrange the information on a page (or pages), add comments, and print this information. Templates can be saved for future use with similiar spectra. There are two submenu entries.

New

Create a new print composition template.

Open

Open an existing print composition template.

Print composition is discussed in detail in Chapter 15.

MOST RECENTLY OPENED DOCUMENTS

The most recently (up to four) opened files are displayed here. You can reopen any of these files by clicking its name.

EXIT

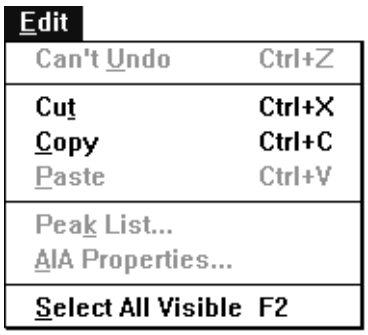
Save all open documents to disk, close the documents, close Win-IR Pro and return to Windows NT.

When you re-start Win-IR Pro, it will automatically open the last document that was opened prior to selecting Exit. This document is in position 1 in the most recently opened documents section of the File menu (immediately above Exit)

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7
Edit Menu



These commands copy and paste data and graphics using the system clipboard. They also allow modification of the spreadsheet.

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UNDO...

If possible, undo the last operation. Undo will be followed by a brief description of the process to be undone. For example, following a smoothing operation, this entry will be Undo Smooth. If the operation cannot be undone, then the entry will say Can't Undo and it will be greyed out (disabled).

CUT

Copy the spectral data to the clipboard and delete it from the document.

When you Cut or Copy from Win-IR Pro, the spectral data (including history and other properties), not its graphic representation, is copied to the clipboard. If it is pasted into a Win-IR document, then all information is transferred and the spectral data are represented graphically.

If the clipboard is pasted into a spreadsheet, then only the spectral information is transferred and it appears as two columns of numbers (the X- and Y-values). The clipboard cannot be pasted into all applications; for example, if you try to paste it into Word, nothing will happen.

Note

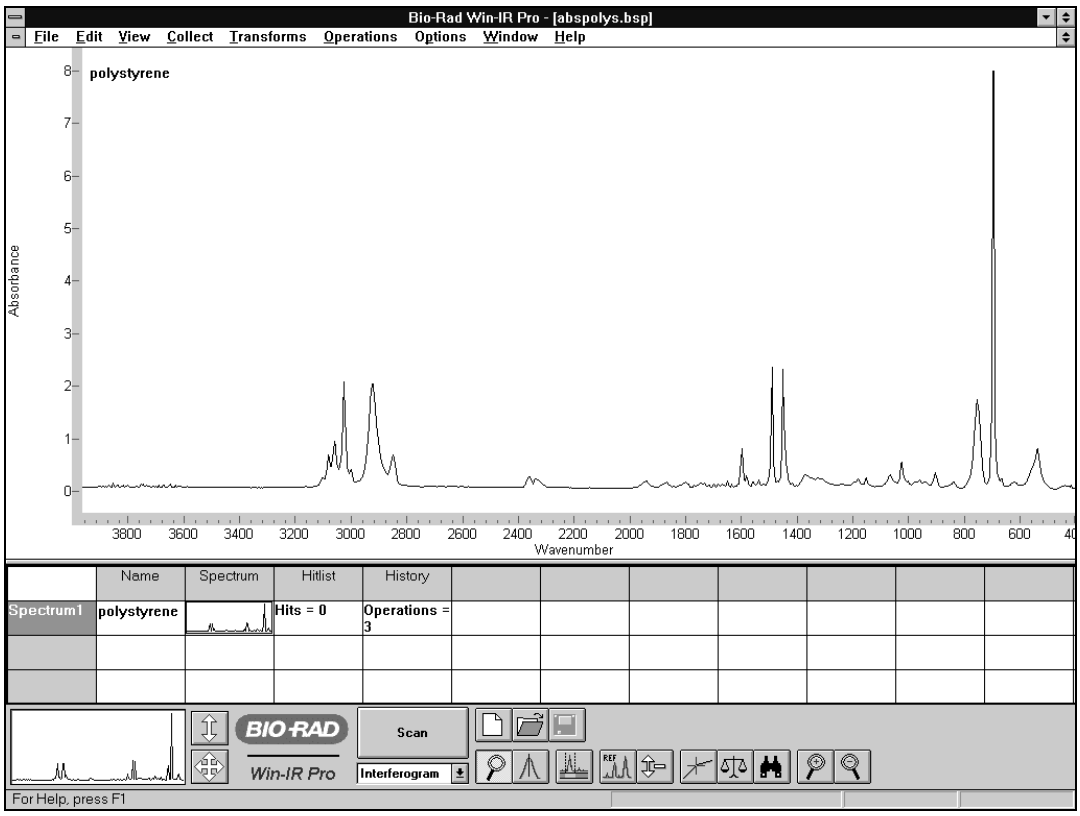
If you want to copy the graphic representation into other applications, use one of the commercially available screen capture applications. These actually save the image and allow it to be pasted into other applications, such as word processors.

COPY

The same as Cut, except that the spectrum and spreadsheet in the document are not deleted. This is more commonly used than Cut.

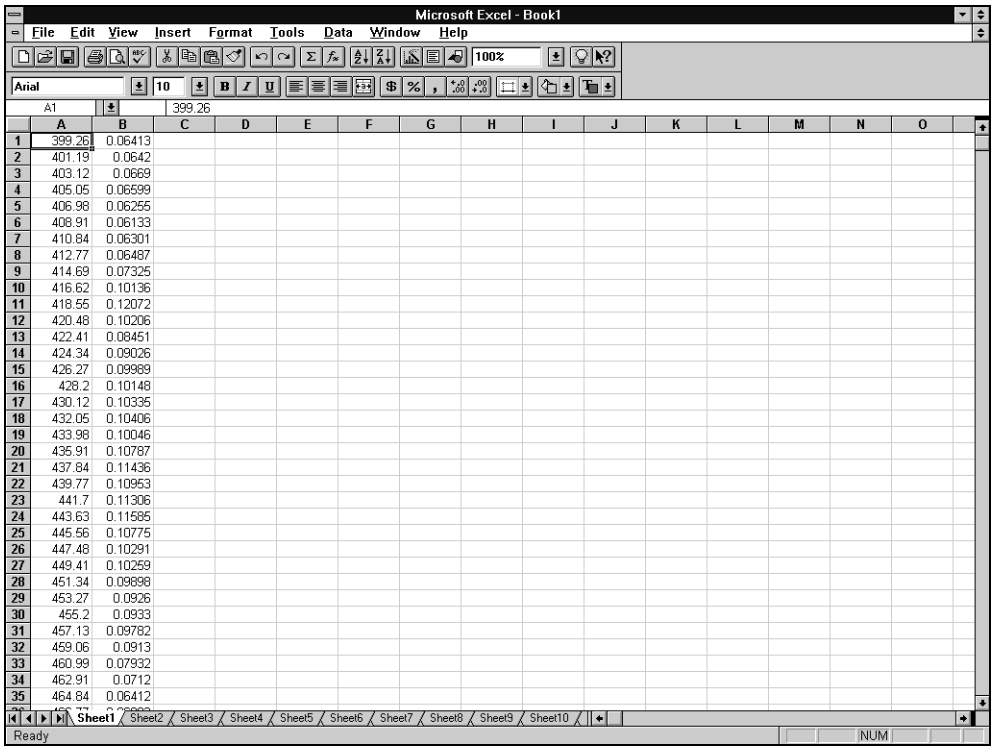
Consider the spectrum below.

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1. Place the cursor in the document window, and click the left mouse button.
2. Select Copy from the Edit menu.
3. Start a spreadsheet application, such as Excel.
4. Place the cursor where you want the first data point to be written.
5. Select Paste from the Edit menu. A typical result is seen below.

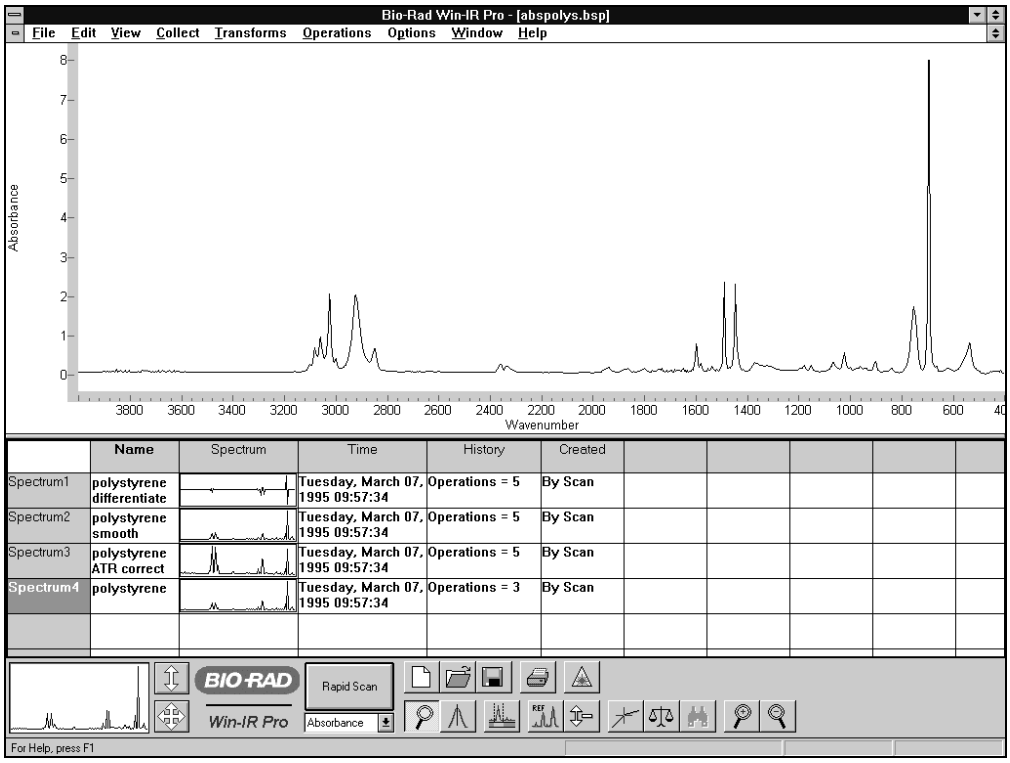
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	A	B
1	399.26	0.06413
2	401.19	0.0642
3	403.12	0.0669
4	405.05	0.06599
5	406.98	0.06255
6	408.91	0.06133
7	410.84	0.06301
8	412.77	0.06487
9	414.69	0.07325
10	416.62	0.10136
11	418.55	0.12072
12	420.48	0.10206
13	422.41	0.08451
14	424.34	0.09026
15	426.27	0.09989
16	428.2	0.10148
17	430.12	0.10335
18	432.05	0.10406
19	433.98	0.10046
20	435.91	0.10787
21	437.84	0.11436
22	439.77	0.10953
23	441.7	0.11306
24	443.63	0.11585
25	445.56	0.10775
26	447.48	0.10291
27	449.41	0.10259
28	451.34	0.09898
29	453.27	0.0926
30	455.2	0.0933
31	457.13	0.09782
32	459.06	0.0913
33	460.99	0.07932
34	462.91	0.0712
35	464.84	0.06412

Edit / Copy can also copy the non-graphical data from columns of the Win-IR Pro spreadsheet into an external spreadsheet such as Excel. Consider the example below,

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1. Highlight the columns to be copied; in this example, we select Name, History, and Created (see Chapter 4 for details on how to select columns).

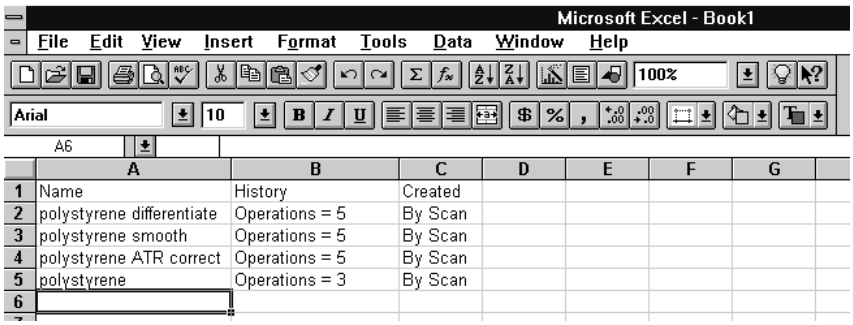
	Name	Spectrum	Time	History	Created	
Spectrum1	polystyrene differentiate		Tuesday, March 07, 1995 09:57:34	Operations = 5	By Scan	
Spectrum2	polystyrene smooth		Tuesday, March 07, 1995 09:57:34	Operations = 5	By Scan	
Spectrum3	polystyrene ATR correct		Tuesday, March 07, 1995 09:57:34	Operations = 5	By Scan	
Spectrum4	polystyrene		Tuesday, March 07, 1995 09:57:34	Operations = 3	By Scan	

2. Select Copy from the Edit menu.

3. Access the external spreadsheet; in this example, Excel is used.

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4. Select Paste from the Edit menu.



Notes

Data from the Win-IR Pro spreadsheet columns can also be pasted into word processor documents.

Graphic data (such as Spectrum or Y-Data) cannot be copied. If these columns are selected, the corresponding external spreadsheet cells, or word processor columns, will be empty.

You cannot take data from spreadsheets or word processor documents and paste them into Win-IR Pro spreadsheets.

PASTE

Paste the contents of the Win-IR Pro clipboard into the Win-IR Pro document. This is often used to copy spectra between documents. You can also copy spectra within the same document, if desired.

When you paste a spectrum into a document, its row is placed just above the lowest numbered selected row; the rows below the new spectrum are renumbered. This allows to to control where in the spreadsheet a spectrum is placed.

You can also modify a spectrum using an external spreadsheet and then replace the original spectrum.

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Note

You must Paste data copied from an external spreadsheet into a selected spectrum in an opened document. (This should be the same spectrum that you originally copied the data from.) The data from the external spreadsheet replaces the spectral data in Win-IR Pro. The rest of the spectral information (resolution, interferogram, etc.) remain the same.

The process is:

1. Select a spectrum in Win-IR Pro and Copy it to the clipboard.
2. Switch to... an external spreadsheet.
3. Paste the x,y data into this spreadsheet.
4. Modify the data as desired.
5. Copy all the data to the clipboard.
6. Switch to... Win-IR Pro.
7. Make sure that the proper spectrum is selected. If not, select it.
8. Paste the data into that spectrum.

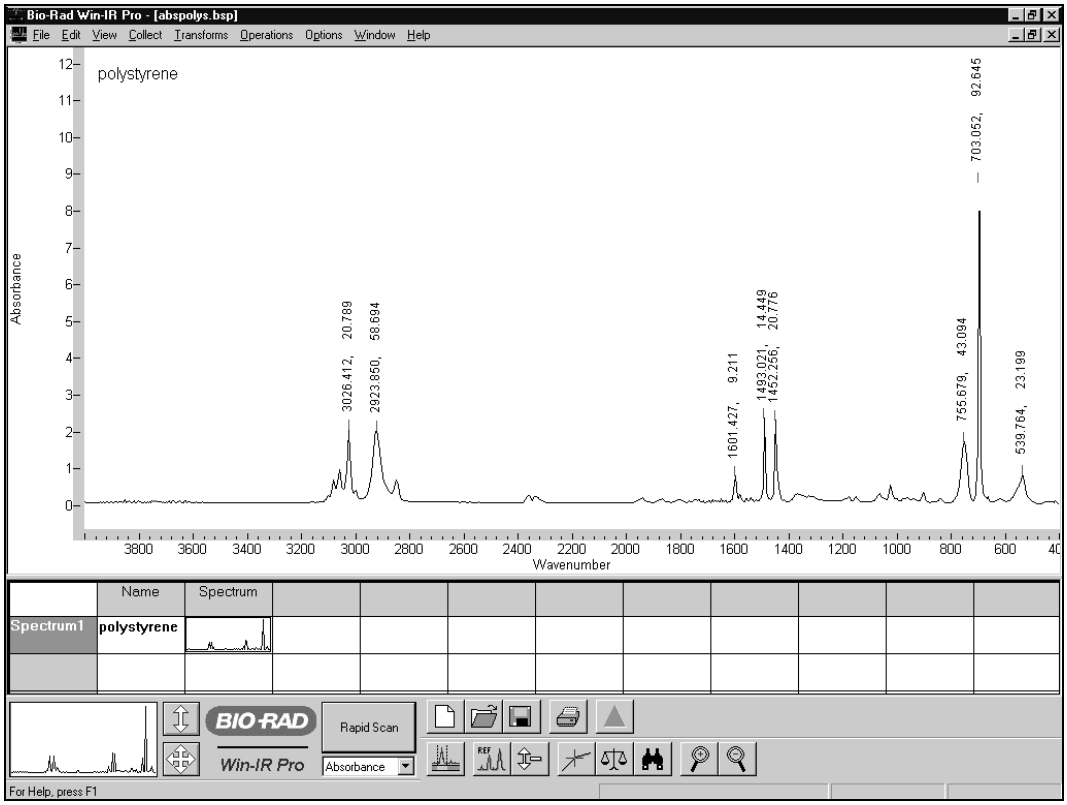
Note

The History property is not affected by this external processing of the spectrum.

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PEAK LIST...

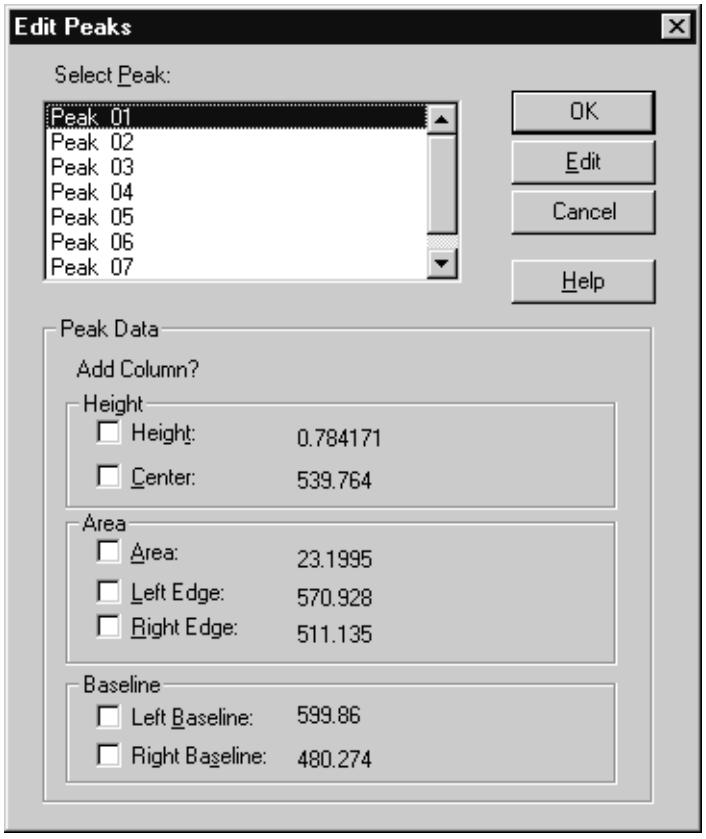
You must select peaks before this entry is enabled. Select peaks with Operations / Peak Pick to automatically pick peaks (Chapter 11), or select them manually as described in Chapter 2. In this example, 8 peaks have been labeled using Peak Pick.



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Changing Peak Parameters

When you select Peak List..., the Edit Peaks dialog box appears.



Peaks are numbered sequentially from the lowest wavenumber to the highest wavenumber of their centers. The following information is shown for each peak:

Height
Center (cm^{-1})
Area
Left Edge (cm^{-1})
Right Edge (cm^{-1})
Left Baseline (cm^{-1})
Right Baseline (cm^{-1})

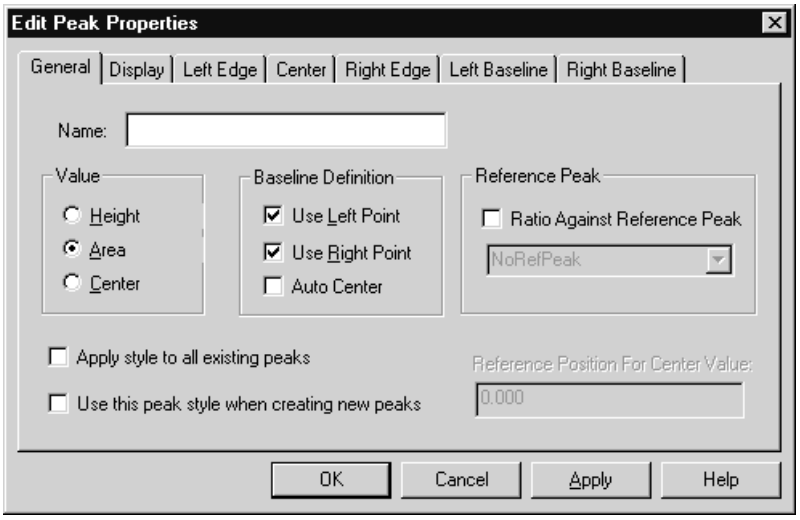
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The area and height are calculated from the other parameters. You cannot enter or alter the peak area or peak height directly; they can be altered indirectly by changing the values for the center, edges, and baselines of the selected peak.

To alter the values of the peak parameters. First select the desired peak from the Select Peak list; then, click the Edit button. The Edit Property dialog box appears. Each tab page allows you to change specific peak parameters. The details of all these tab pages and the peak parameters are discussed in Chapter 2.

The tab pages are shown below. The Display tab page is not accessible through Edit / Peak List; use the procedures discussed in Chapter 2.

General



Value: select Height, Area, or Center.

Baseline Definition:

select both left and right—the baseline is a straight line connecting the two baseline points

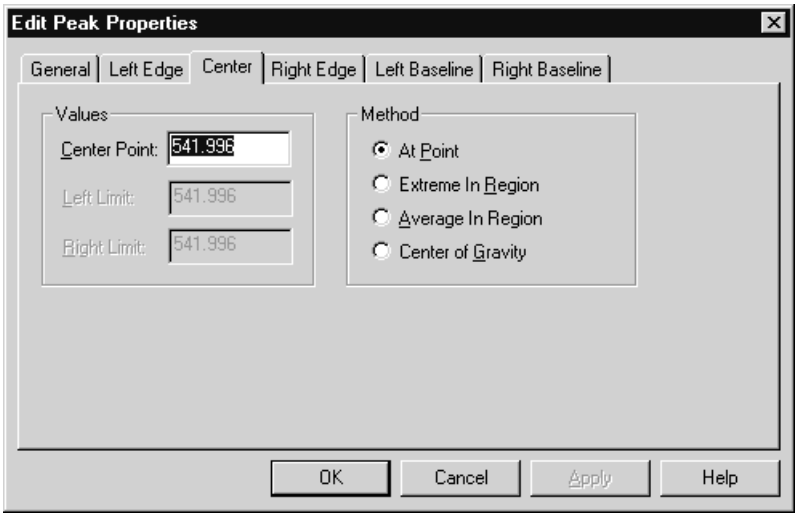
select none—the baseline is the x-axis

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select only left or right—the baseline is a horizontal line through the selected baseline point.

Use Left Point: baseline is a horizontal line through the left baseline point.
Use Right Point: baseline is a horizontal line through the right baseline point. .
Auto Center: moves the right half box of the left baseline point to the x-position of the center of the peak; moves the left half box of the right baseline point to the x-position of the center of the peak. These half boxes move if the center of the peak moves. If the baseline boxes have not been split, then selecting Auto Center splits the boxes and moves them as above. This option is most useful in kinetics documents (see Chapter 3 for details).

Center



Method: how the center of the peak is to be determined.

At Point: the center of the peak is at value entered in Center Edge.

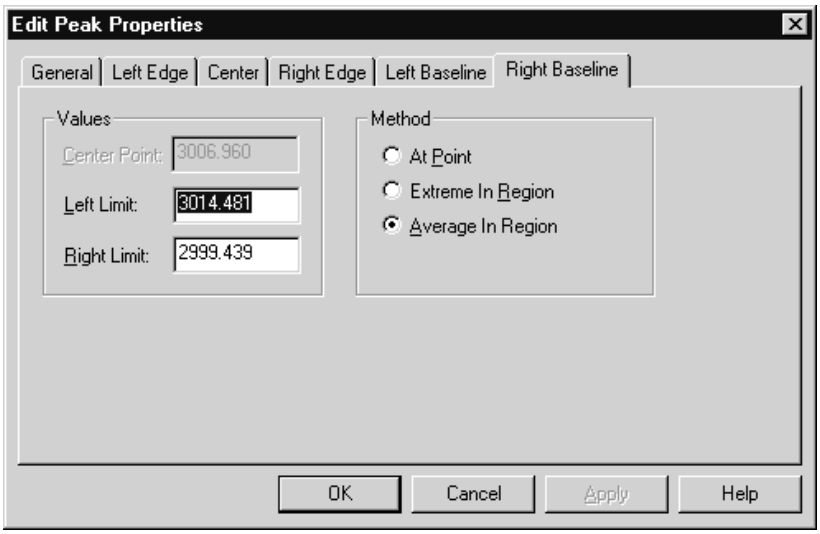
Extreme in Region: the center of the peak is at the extreme (maximum for absorbance spectra, minimum for transmission spectra) value of the spectrum in the region defined by the values in Left Limit and Right Limit.

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Average in Region: the x-position of the center of the peak is at the arithmetic mean of the value of the Left Limit and Right Limit.

Center of Gravity: the center of the peak is where the vertical line dividing the peak area (in the region defined by the values in Left Edge and Right Edge) in half intersects the spectrum. See Chapter 2 for details of this equation.

Right Baseline



Method: how the right baseline is to be determined.

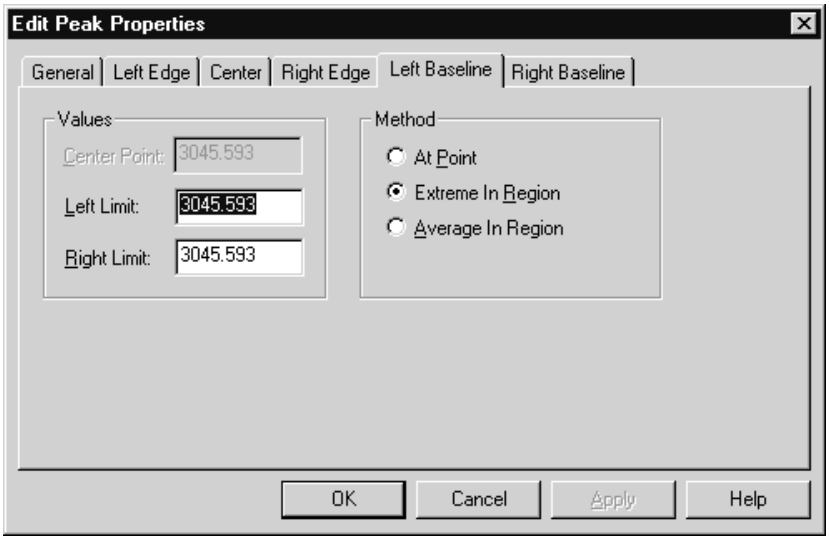
At Point: the right baseline point is at value entered in Center Edge.

Extreme in Region: the right baseline point is at the extreme (maximum for absorbance spectra, minimum for transmission spectra) value of the spectrum in the region defined by the values in Left Limit and Right Limit.

Average in Region: if the baseline box is split, the x-position of the right baseline point (x) is the arithmetic mean of the x-positions of the left and right limits of the baseline region. The y-position of the right baseline point (y) is the average of the y-position values in the region. The (x,y) point is not necessarily on the spectrum. This technique reduces the effect of noise within the baseline region

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Left Baseline



Method: how the left baseline is to be determined.

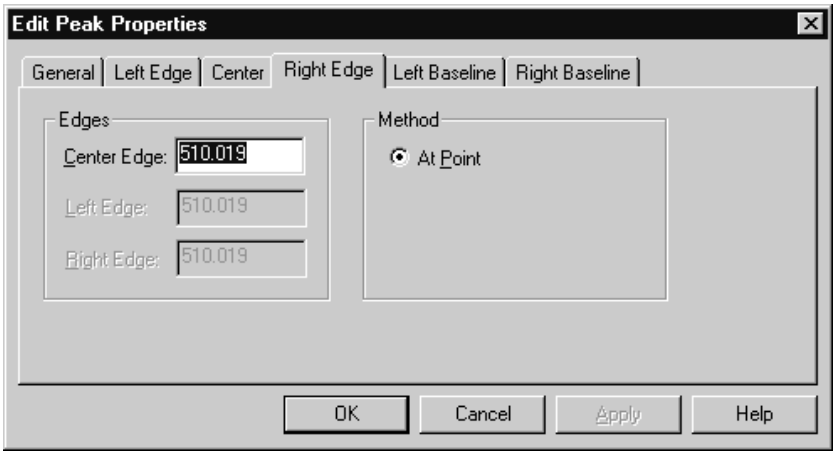
At Point: the left baseline point is at value entered in Center Edge.

Extreme in Region: the left baseline point is at the extreme (maximum for absorbance spectra, minimum for transmission spectra) value of the spectrum in the region defined by the values in Left Edge and Right Edge.

Average in Region: if the baseline box is split, the x-position of the left baseline point (x) is the arithmetic mean of the x-positions of the left and right limits of the baseline region. The y-position of the left baseline point (y) is the average of the y-position values in the region. The (x,y) point is not necessarily on the spectrum. This technique reduces the effect of noise within the baseline region

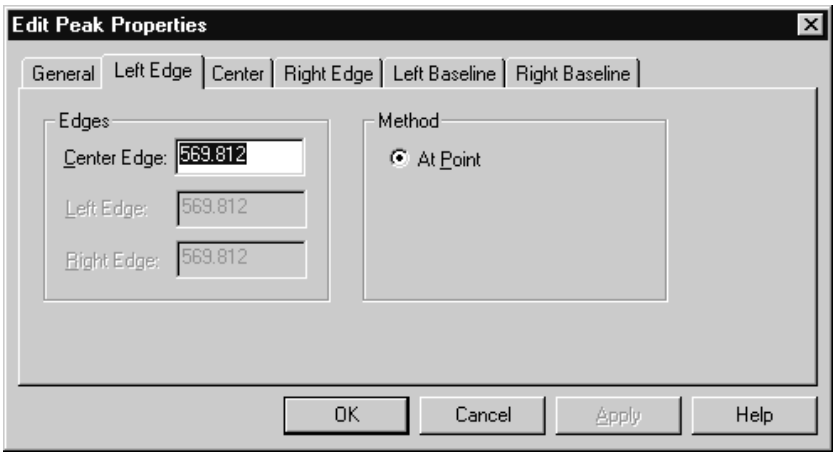
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Right Edge



Enter the value desired for the Right Edge.

Left Edge



Enter the value desired for the Left Edge.

In general, type the new information in the appropriate box. If any of the values and/or methods are changed, the Apply button is enabled.

OK: implement values on tab page and return to the Edit Peaks dialog box.

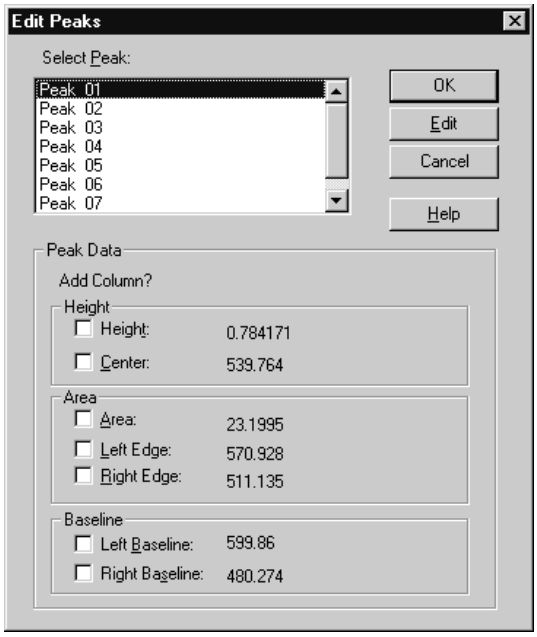
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Cancel: do not implement any changes to values made since the Apply button was last clicked; return to the Edit Peaks dialog box.

Apply: immediately change the peak values; this also causes the Area and Height to be recalculated and displayed. Changes made this way cannot be reversed with the Cancel button.

Help: enter the on-line Help system.

Placing Peak Parameters in the Spreadsheet



Each of the items of information for each peak can be placed into the spreadsheet. To do this:

1. Select the peak

2. Click in the box to the left of the peak item to be entered.

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This item will be placed into the spreadsheet. There is no global selection; that is, you cannot, with one command, specify that all Centers or all Areas will be in the spreadsheet. All items must be selected individually.

In the example below, the spreadsheet shows the values for the centers of peaks 1 and 7, the height of peak 4, and the area under peak 3. The column is labeled with both the property and the peak. For example,

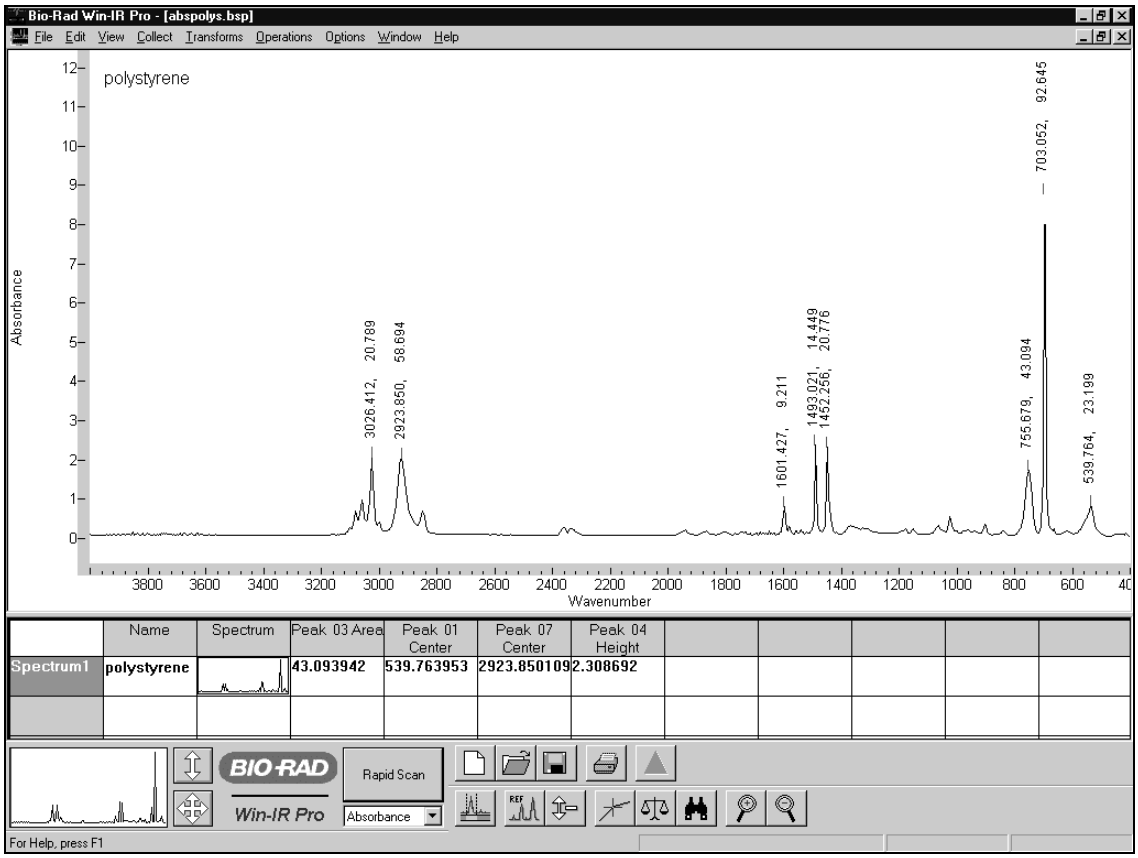
Peak 03 Area

Peak 01
Center

Peak 07
Center

Peak 04
Height

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The buttons other than Edit in the Edit Peaks dialog box are:

OK: make all changes the peak table and to the spreadsheet; return to the main menu.

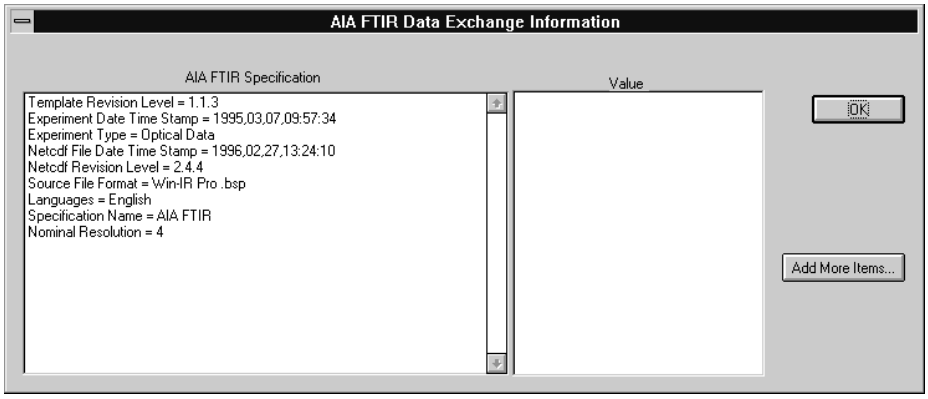
Cancel: return to the main menu without making any changes to either the peak table or to the spreadsheet.

Help: enter the on-line Help system.

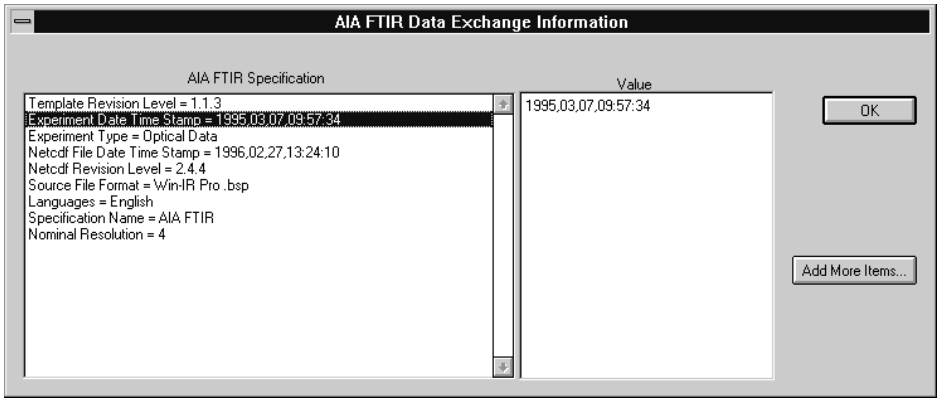
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AIA PROPERTIES...

This menu entry allows you to add and alter the AIA FTIR specifications. These specifications are part of the AIA file format and are normally saved in the .cdf files. When selected, the AIA FTIR Data Exchange Information dialog box appears.



1. To change (or insert) a value for the specification, highlight the specification. The value appears in the Value box on the right side. Use the cursor and standard word-processing techniques to type in a new value.

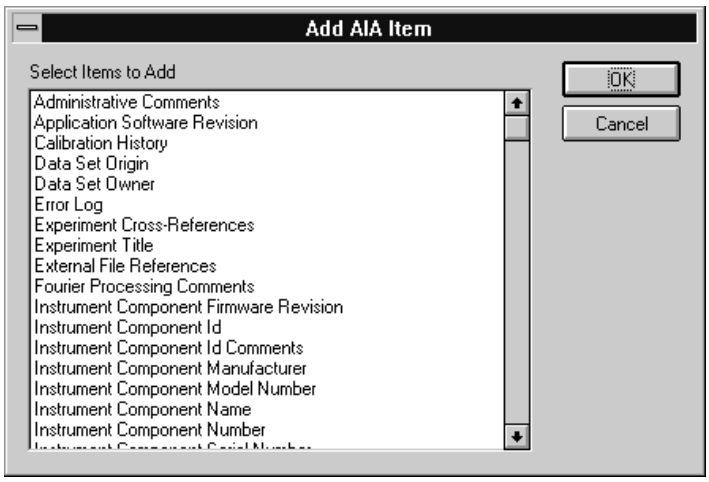


Note

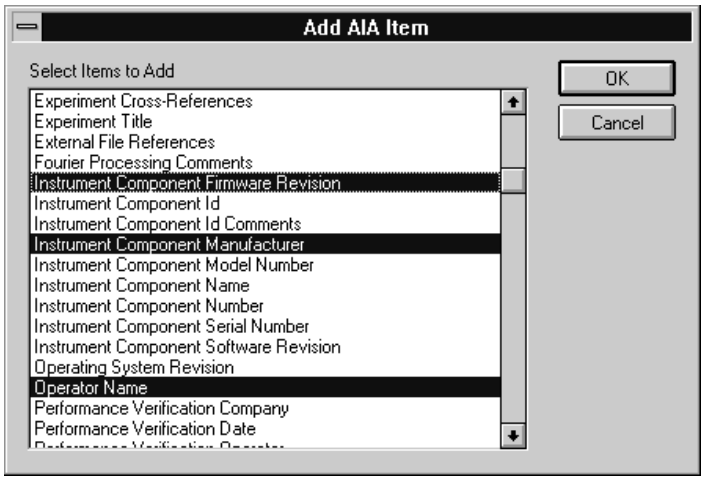
If the specification cannot be changed (read-only), then its value will be in gray rather than black, and you will not be able to alter it.

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2. If you want to add additional specifications, click the Add More Items... button. The Add AIA Item dialog box appears.

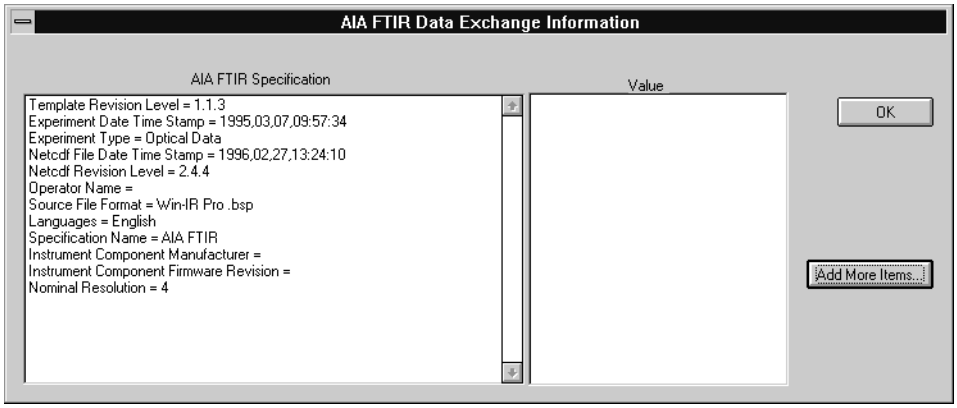


3. Highlight the specifications to be added. Contiguous specifications can be selected using the standard Windows shift-click selection technique. Individual specifications can be toggled on and off using the standard Windows ctrl-click technique. When all specifications have been selected, click the OK button (if you decide not to add any specifications, click the Cancel button, instead).



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4. The new specifications are added to the AIA FTIR Specifications box.



5. Set the values for these added specifications, following the procedure in Step 1, above.

6. Click the OK button to save the specifications in the active document for the selected spectrum..

SELECT ALL VISIBLE

Selects all spectra that are currently displayed on the screen. This is useful in the following situation (among others).

1. Open a document (.bsp) with multiple spectra.

2. Select a group of the spectra; for example 1 to 10.

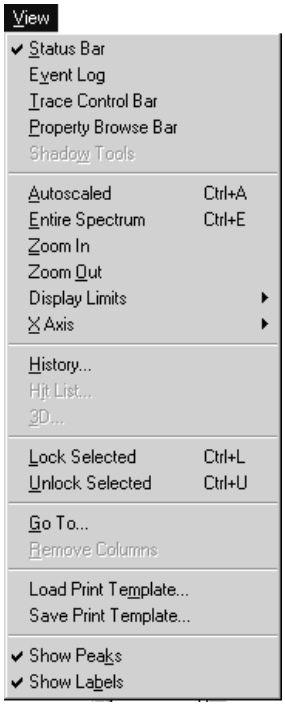
3. Use the cursor vertical expansion capability (see Chapter 1) to adjust the y-axis scaling of one of the spectra. This is now the only selected spectrum.

4. To reselect all the displayed spectra, select Edit / Select All Visible. All the visible spectra are now selected in the spreadsheet.

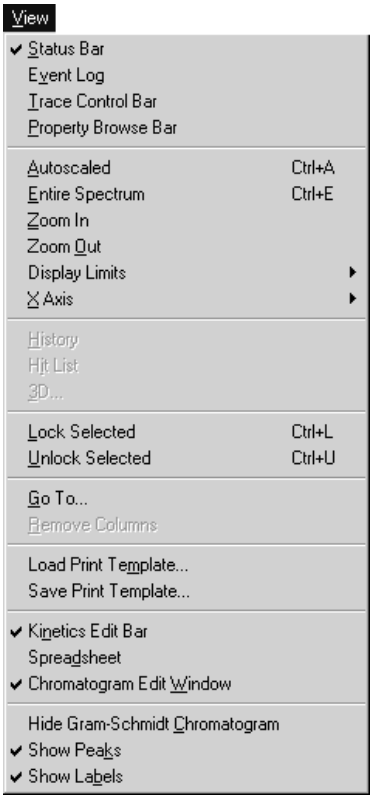
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8
View Menu

MULTI-SPECTRAL DOCUMENTS



KINETICS DOCUMENTS



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STATUS BAR

If selected (default), the status bar is displayed at the bottom of the screen. A √ mark shows that the status bar is selected. Unselecting this entry hides the status bar; the √ mark is no longer on the menu.

The text in the left side status bar gives a brief description of the results of clicking the button that the cursor is on. For example,



If the cursor is in the spectrum display window, the X and Y coordinates of the cursor are shown in the right side of the status bar. For example,



The status bar also shows the progress of an actions—such as collecting data, errors,

EVENT LOG

Once activated, the event log displays all messages generated by Win-IR Pro, including error messages. The event log can be activated either

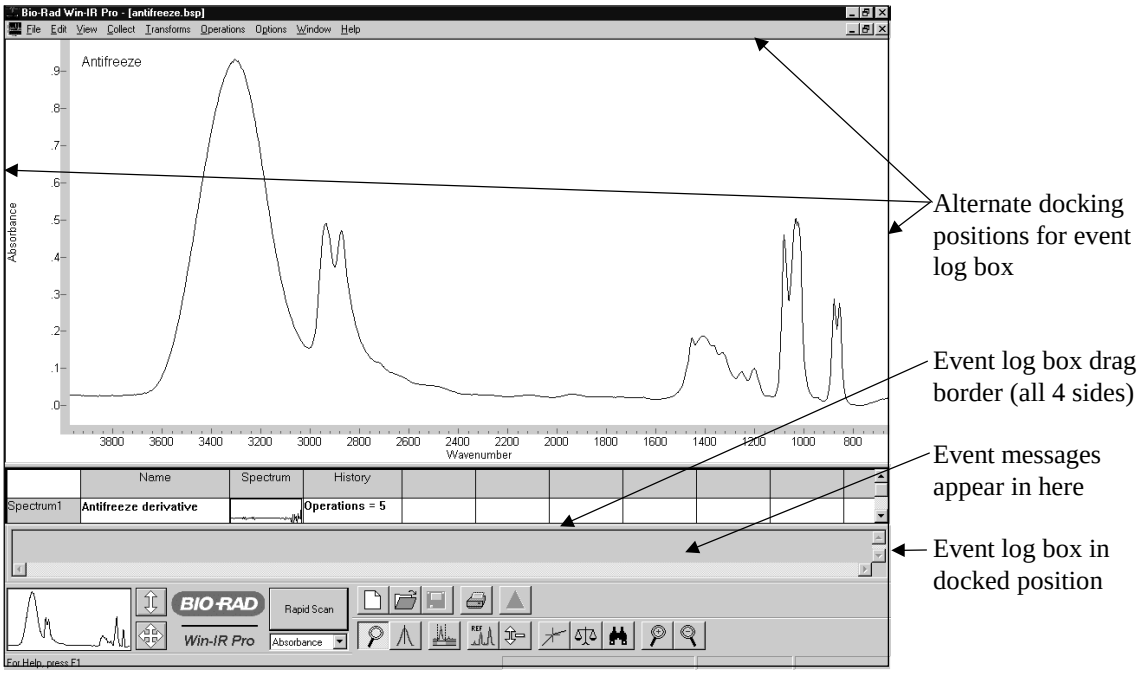
- automatically, when an error or some other event occurs during setup or data collection, OR
- manually, by selecting Event Log from the View menu.

The event log can be turned off by either

- manually, by selecting √ Event Log from the View menu OR
- when it is floating, by clicking the Close button on the extreme right of the event log title bar.

When it is initially activated by manual selection, the event log box look like this.

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The event log box can either be docked or floating. It is docked when it is above the Bio-Rad bar at the bottom of the screen. It can also be in any of the other three positions shown in the figure above, if you find one of them to be more convenient.

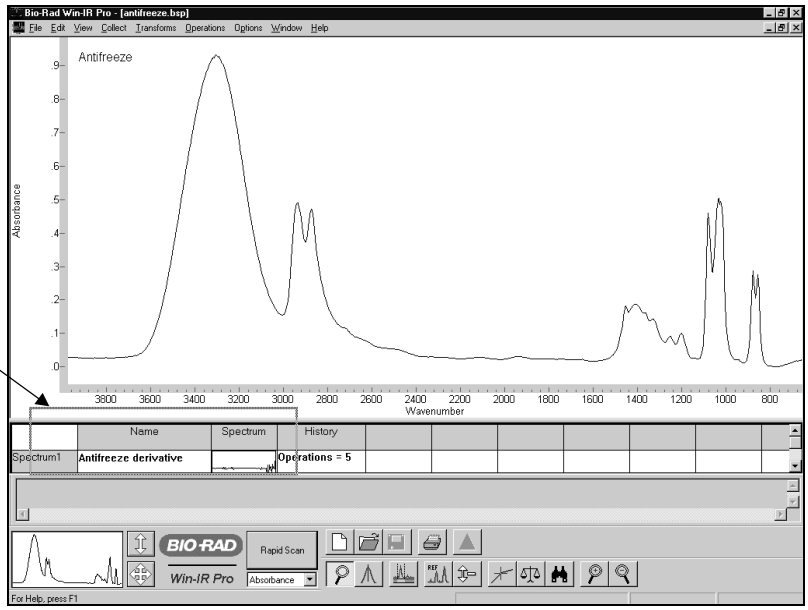
Floating the Event Log Box

When the event log box is undocked, it can be resized. You can float the box by

- putting the cursor in the drag border and double-clicking the left mouse button OR
- putting the cursor in the drag border, holding down the left mouse button, and dragging the event log box away from its docked position until its outline changes size; then release the mouse button.

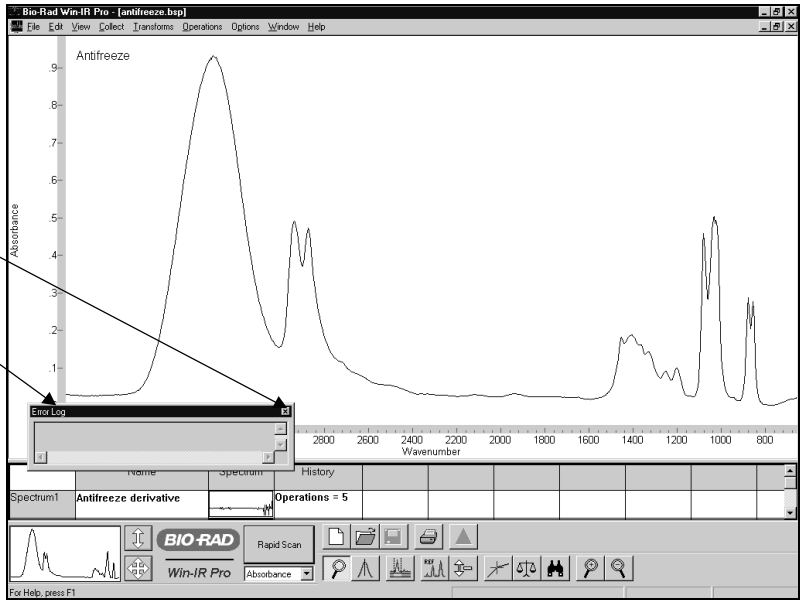
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Outline of event log box after undocking but before release of mouse button



Event log box close button

Event log box after release of mouse button



Note

If the Event Log box is sized too large, it cannot be undocked by dragging. However, it can be undocked by double-clicking in the drag border.

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Resizing the Event Log Box

The box must be floating if it is to be resized. To resize the Event Log box, put the cursor in the drag border; the cursor changes to a double-head arrow. Hold down the left mouse button, and move the cursor in the direction of either of the arrowheads to increase or decrease the size of the box; release the left mouse button when you are done. You can move the box by putting the cursor in the Event Log box title bar, holding down the left mouse button, and then moving the entire box. Release the mouse button when you are done.

Docking the Event Log Box

You can dock the box by

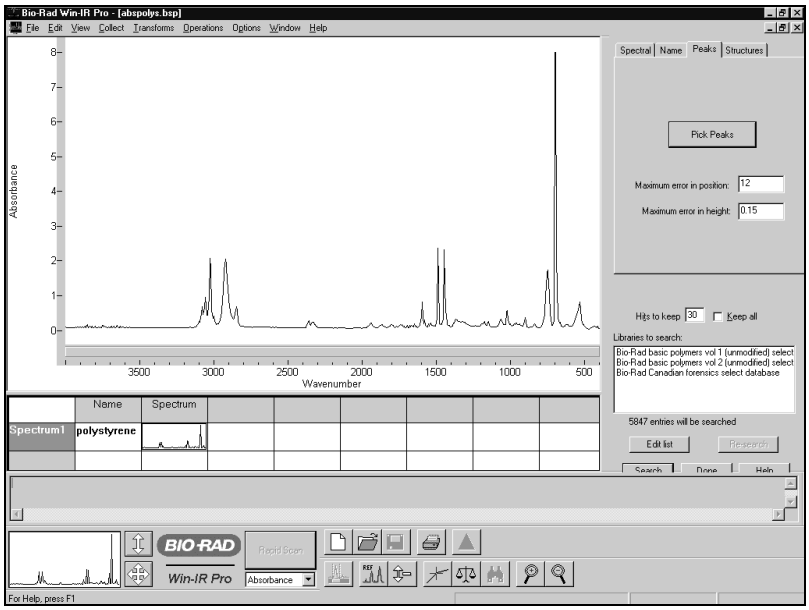
- putting the cursor in the drag border and double-clicking the left mouse button OR
- putting the cursor in the drag border, holding down the left mouse button, and dragging the error log box towards its docked position until its outline changes size (extends across the Win-IR Pro screen horizontally); then release the mouse button.

When you dock the Event Log box, its size along the edge changes to the extent of the Win-IR Pro screen; its other dimension remains at what it was before it docked.

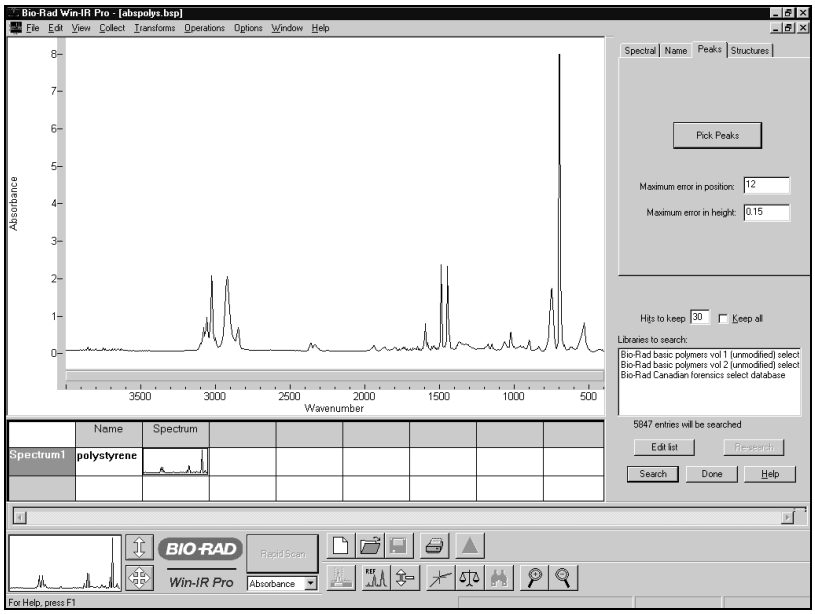
Overlap with Control Panel Sidebars

In some cases, the event log may overlap the control panel sidebar, as is shown below.

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To fix this, undock the event box, resize it, and redock it as described in the sections above. In the example below, the event box has been reduced in height and no longer obscures the operational part of the control panel sidebar.

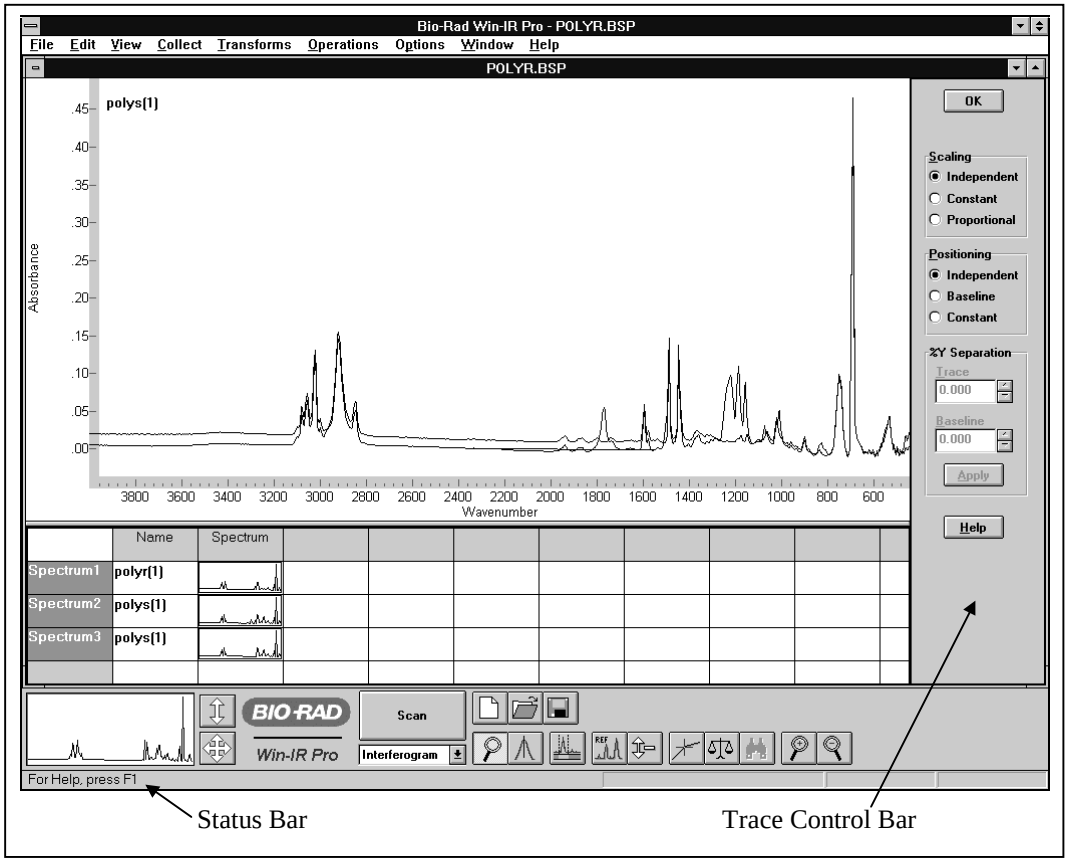


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You can also move the event box to the left side of the screen or hide it by selecting View / Event Log.

TRACE CONTROL BAR

This entry controls the positioning and separation of multiple traces displayed in one document. If selected, the trace control bar appears on the right-hand side of the screen. The trace box is redrawn so that the displayed traces are not truncated on the right.



Note

More than one control panel sidebar can be active at one time.

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Scaling: allows the size of the trace(s) along the Y-axis to be varied. The Y-axis scale changes after the traces are rescaled. If the baseline is moved, the Y-axis zero-point moves along with it.

Independent: each trace can be scaled individually using the cursor. Place the cursor on the trace; the magnifying glass in the cursor disappears . Hold down the left mouse button; the cursor changes to a double-headed arrow Hold down the left mouse button and drag the trace to the desired Y-axis scale. Release the mouse button and the new values appear on the Y axis.

Note

The button affects only the selected (green) trace(s).

The button scales all traces along the X-axis but scales only the selected (green) trace(s) along the Y-axis.

Constant: all traces are scaled by the same factor. Use the cursor to rescale any one trace and the other traces will also be rescaled.

Proportional: first use Independent Scaling to match up peaks in two (or more) traces to the same value. Select Proportional. If one trace is rescaled, the others will also be rescaled. However, they will each be rescaled by a different factor. This factor will keep the matched peaks in the different traces at the same value.

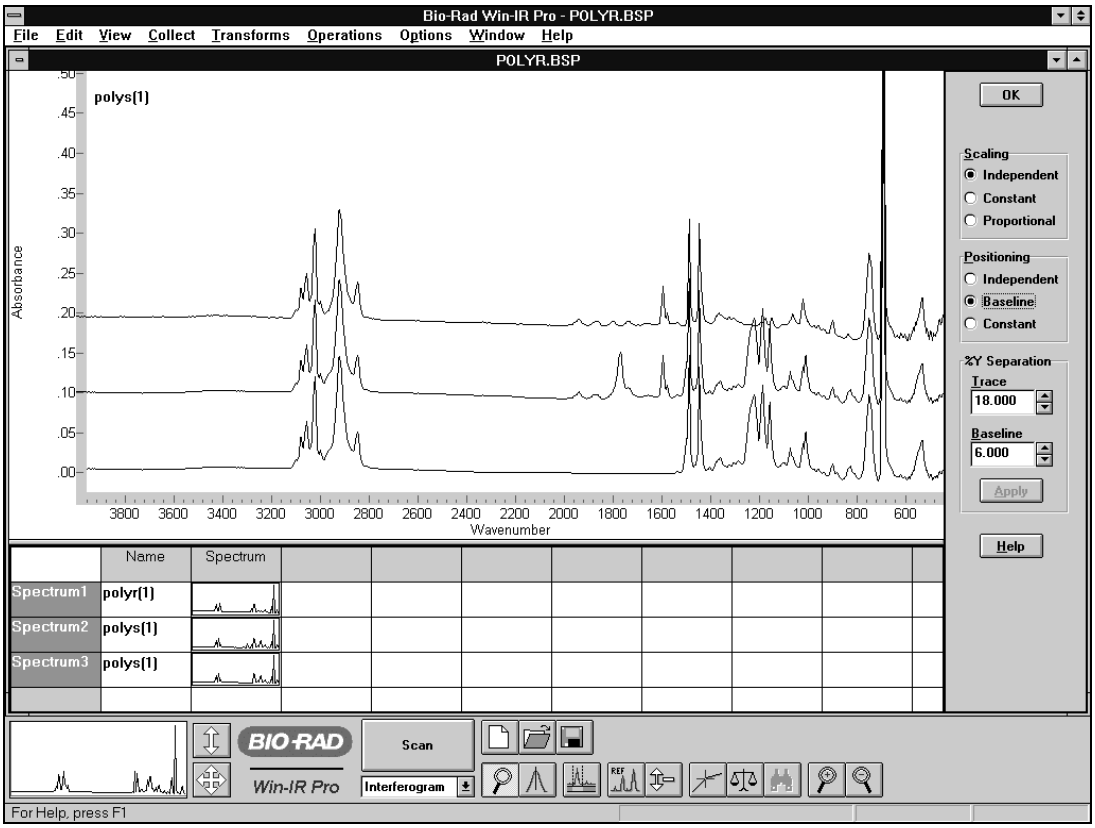
Positioning: this allows you to offset, and control the Y-axis offset, of a number of spectra being displayed simultaneously.

Independent: the traces can be moved up or down, and the scale can be compressed or expanded. To move the traces up or down, place the cursor in the middle third of the Y-axis ruler; the cursor changes shape to . Hold down the left mouse button and move the cursor along the Y-axis ruler. The trace and the Y-axis ruler will move with the cursor. Release the mouse button when you are satisfied with the new position of the traces.
To expand or compress the trace Y-axis, place the cursor in the upper (or lower) third of the Y-axis scale; the cursor changes shape to (or). Hold down the left mouse button and move the cursor along the Y-axis ruler. When

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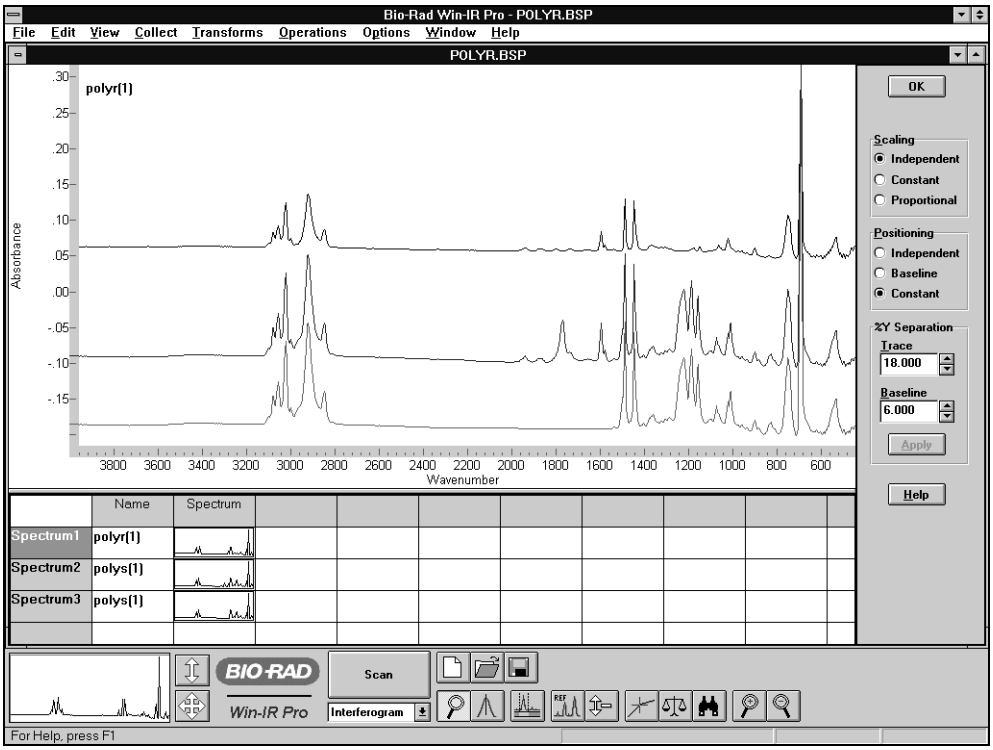
you move the cursor up (down), the Y-axis scale expands; when you move the cursor down (up) the Y-axis scale compresses. . The trace and the Y-axis ruler will move with the cursor. Release the mouse button when you are satisfied with the new position of the traces.. The radar box also reflects the change in the display.

Baseline: the left hand Y-axis intersections of the traces are spread out according to the %Y Separation values.



Constant: zero values of the traces are spread out according to the %Y Separation values.

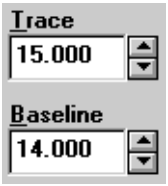
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%Y Separation: the percentage of the full-scale Y-axis in the display used to set the position of the traces. These boxes are not active if Independent Positioning is chosen.

Trace: sets the distance (in percent of full-scale Y-axis) between the baselines of the traces.

Baseline: sets the location of the baseline of the active (green) trace above the lower edge of the trace display.



If you use the arrows (see above) to set the values, then they are applied immediately. You can also type percentages in these boxes. If you type in values, the Apply button is

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enabled. Press the Apply button to tell Win-IR Pro that you have completed typing values and that these values should be applied to the display.

OK: close the control bar and return to the main menu with the settings on the control bar implemented.

Help: access the on-line Help facility.

Note

Make sure the requested separation range does not exceed 100%. Specifically,

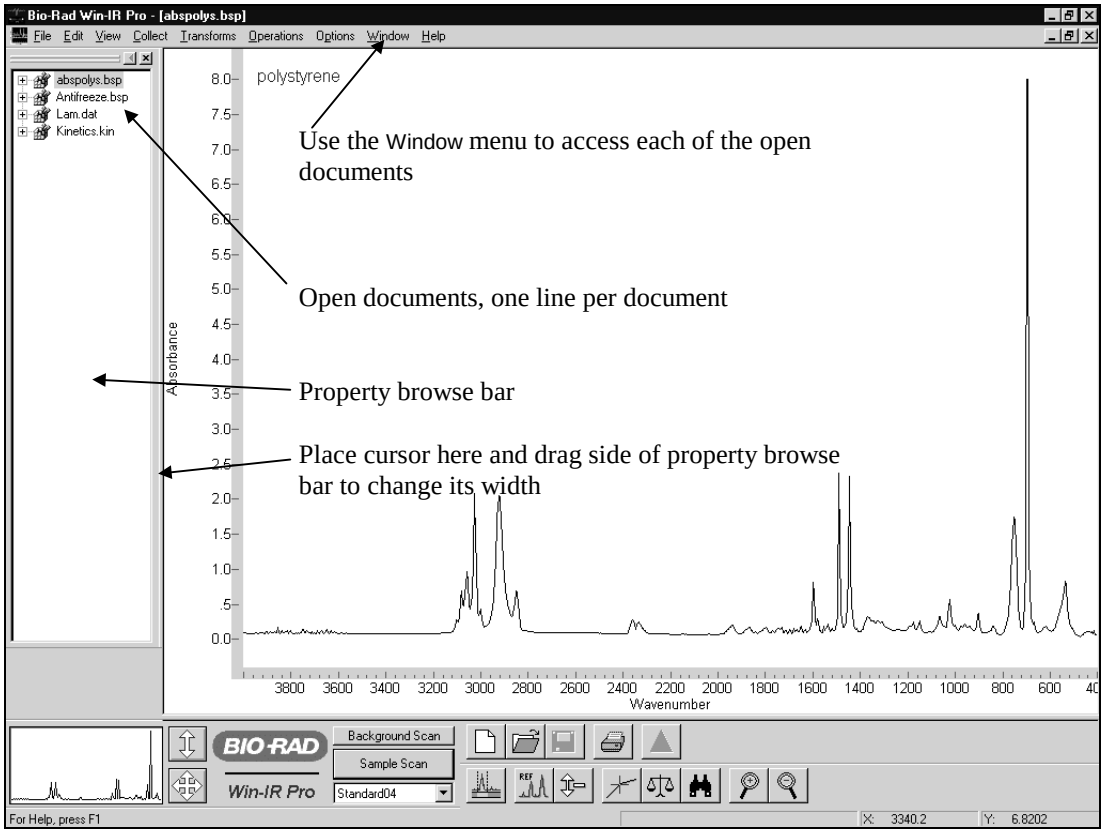
(number of spectra X trace separation) + baseline < 100%

For example, if you have selected 32 spectra, with a baseline at 3%, then the trace separation can be 0, 1, 2, or 3 only.

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PROPERTY BROWSE BAR

When Win-IR Pro is started, the property browse bar is displayed. It is normally at the left side of the screen; however, you may choose to move it, as described below. The property browse bar shows information about all open documents. In the example below, four documents have been opened.



Notes

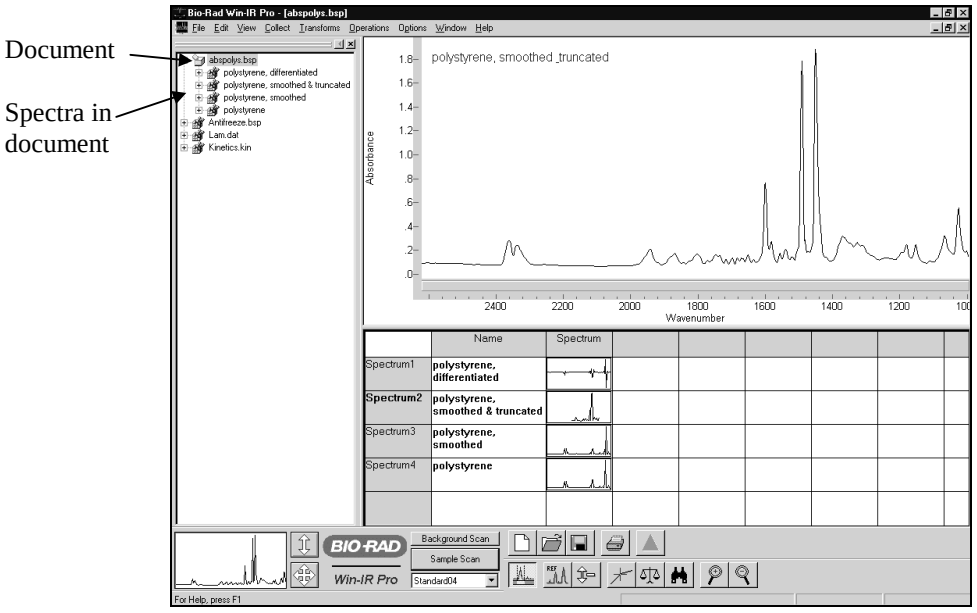
When you highlight a document or any of its properties, that document is automatically made the active document.

Change the width of the property browse bar by placing the cursor on the property browse bar boundary; hold down the left mouse button and drag the boundary to the desired position; release the mouse button.

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Tree Structure of the Property Lists

The property list follows the standard Windows NT tree structure such as that sued in the Windows NT Explorer. If there is a + to the left of the icon, it indicates that additional structure exists at the next level down. For example, clicking on the + to the left of abspolys.bsp displays a line for exact spectrum in that document.

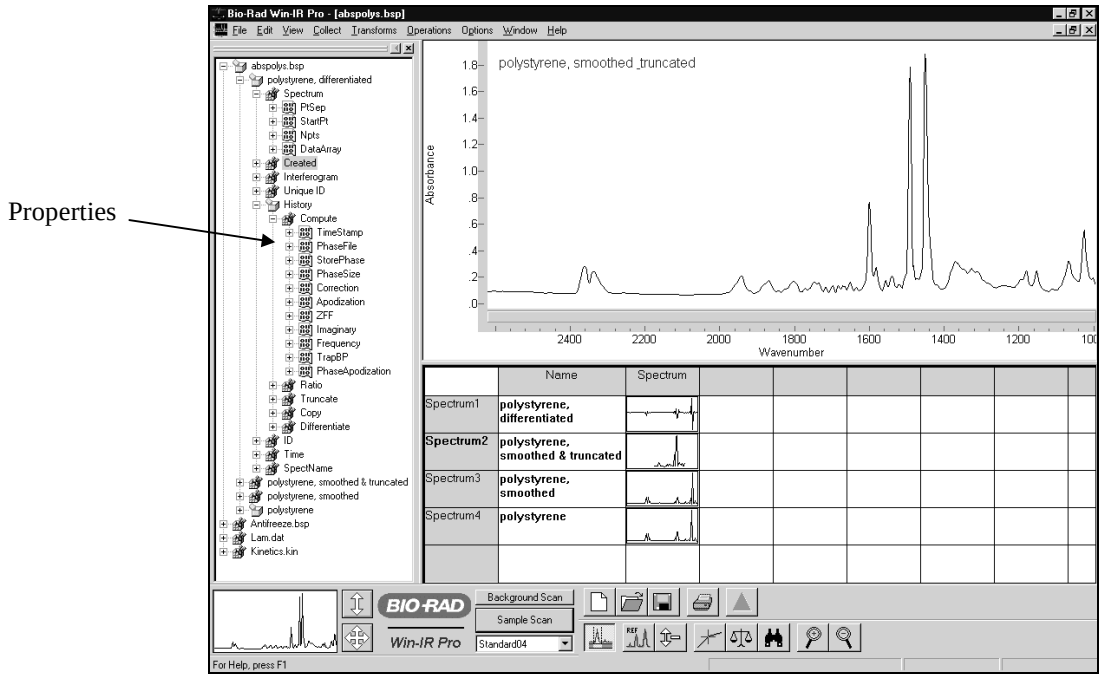


Note

Once an icon is opened, a – is displayed to its left; clicking the – closes that icon.

You can continue to open the icons until individual properties are reached.

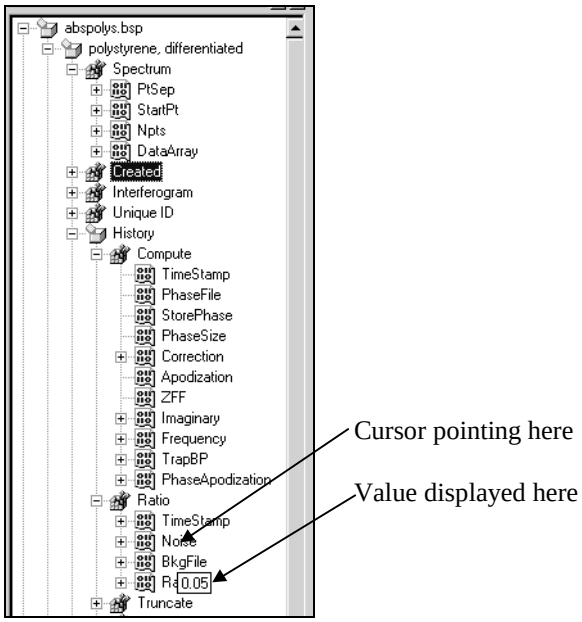
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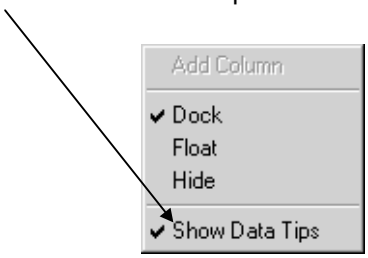
Property Values

To see the value of a property, place the cursor over the name of that property in the property browse bar. The value is displayed in a small box. If there is no value for this property (for example, user stamp in spectra collected prior to Release 2.5), no value box is shown.

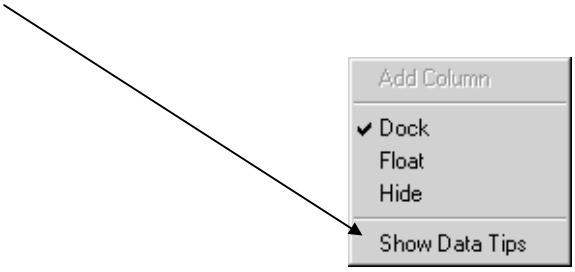
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If you wish to turn off this feature, place the cursor in the property browse bar, click the right mouse button and select Show Data Tips from the menu.



The values will not longer be displayed. To re-activate this display, place the cursor in the property browse bar, click the right mouse button and select Show Data Tips from the menu.



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Adding Property Columns to the Spreadsheet

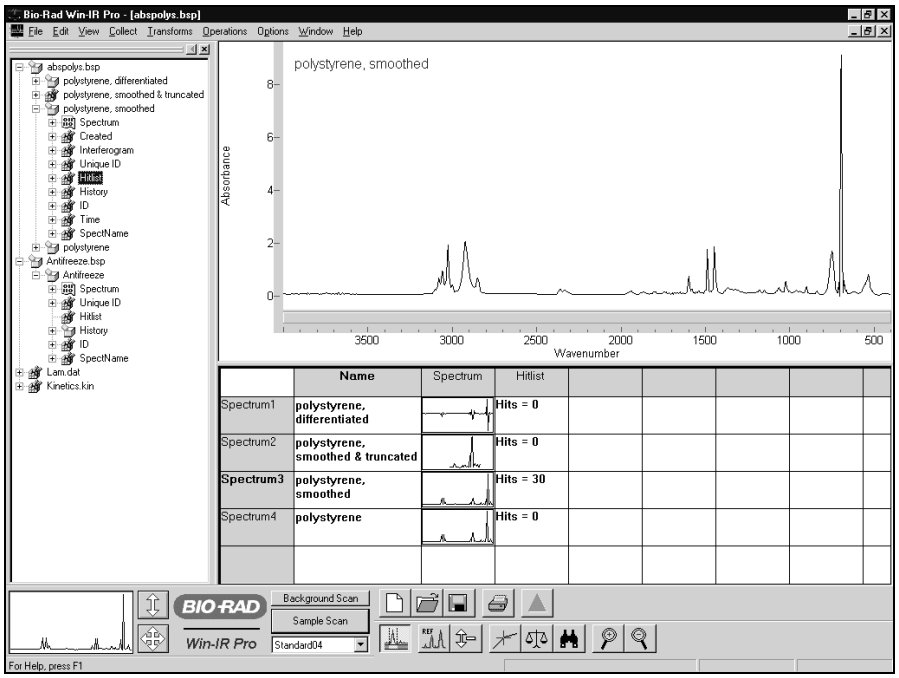
To add a property column to the spreadsheet, first select (by highlighting) this property for any spectrum in the document.

Once the property has been selected, you can put it into the spreadsheet as a column by one of two methods.

- Put the cursor on the highlighted property, hold down the left mouse button and drag the cursor to the spreadsheet. Release the mouse button.

- Put the cursor in the property browse bar, click the right mouse button and select Add Column from the menu.

Either method creates a new column to the immediate right of the rightmost existing column. Any spectrum which does not have this property (for example, a spectrum that was not searched for would have 0 in a HitList property column) will show a 0, a blank, or other appropriate entry indicating this.



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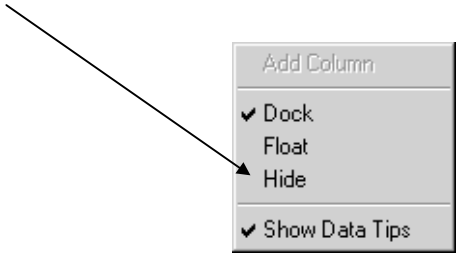
Note

Columns in the spreadsheet can be rearranged but dragging. See “Re-ordering Columns in the Spreadsheet” in Chapter 4 for complete details.

Hiding the Property Browse Bar

There are three ways to hide the property browse bar when it is displayed.

- Select Property Browse Bar from the View menu.
- Place the cursor in the property browse bar, click the right mouse button and select Hide from the menu.



- Click the close button at the upper right of the property browse bar.

Showing the Property Browse Bar

When the property browse bar is not displayed, select Property Browse Bar from the View menu to display it.

Moving the Property Browse Bar

The property browse bar is normally on the left side of the screen; it can be moved to the right side.

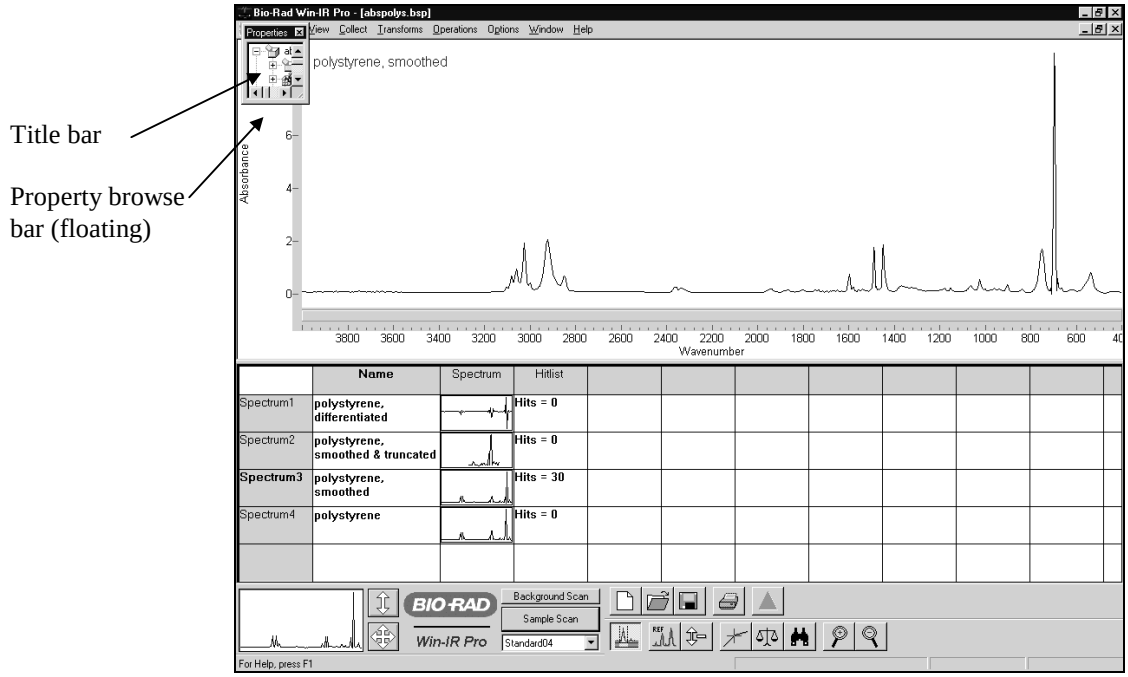
Note

The property browse bar can also be placed on the top or bottom of the screen or floated. However, the vertical nature of the property tree is best displayed with the property browse bar on the left or right side.

To move the property browse bar:

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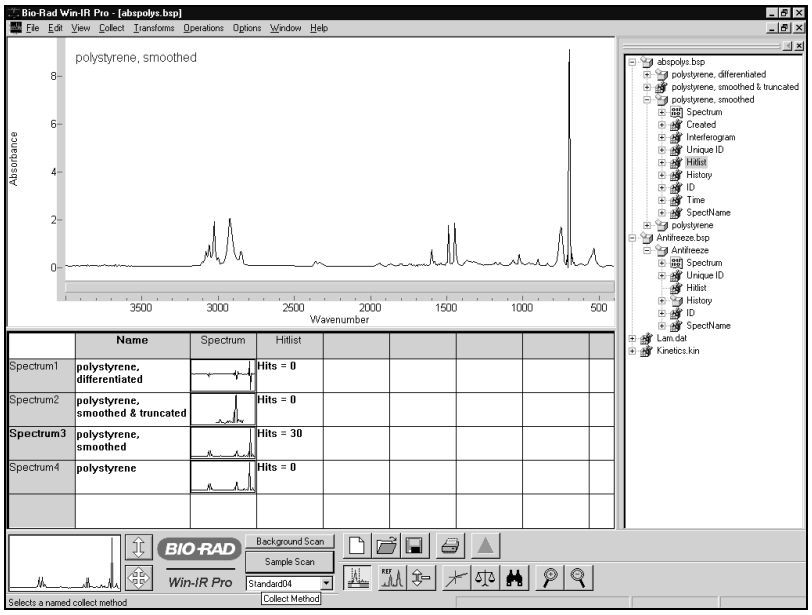
1. Put the cursor in the property browse bar, click the right mouse button and select Float. The property browse bar changes to a small window and is no longer connected to the side of the screen.



2. Put the cursor on the title bar of the property browse bar, hold down the left mouse button and drag the property browse bar to the desired position on the right hand side of the screen.

3. Put the cursor in the property browse bar, click the right mouse button and select Dock. The property browse bar is now on the right side of the screen.

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SHADOW TOOLS

This entry is not enabled unless a Shadow Pro document is open. If selected, it causes the Shadow Pro tool palette to appear. These tools are used to manipulate the view in the Shadow Pro document. For details see, *Shadow Pro User's Manual* (091-0991).

AUTOSCALED

Causes autoscaling along the Y axis only. The X axis is not changed. Equivalent to the  button.

ENTIRE SPECTRUM

Causes autoscaling along both the X- and Y-axes so that the entire spectrum is displayed in the trace box. Equivalent to the  button.

ZOOM IN

Zooms in on the spectrum in the Y-direction only; the new Y-axis labels are immediately displayed. Equivalent to the  button.

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ZOOM OUT

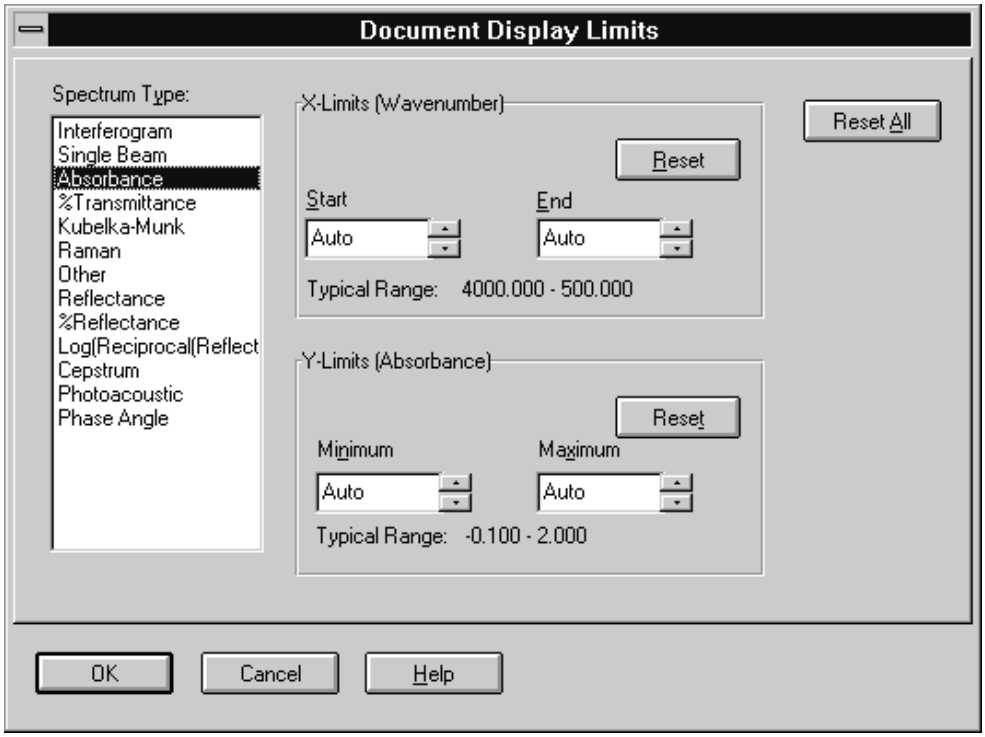
Zooms out from the spectrum in the Y-direction only; the new Y-axis labels are immediately displayed. Equivalent to the  button.

DISPLAY LIMITS...



Document Default...

Causes the Document Display Limits dialog box to appear. Use this dialog box to set limits for the currently active document. These display limits apply only to this document. Other documents can have different display limits.



Spectrum Type: highlight the type of spectrum for which you want to set limits. These limits will apply to all spectra of that type within this document. When a spectrum type is selected, the values of its axes units are displayed after the X-

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Limits and Y-Limits. For example, in the dialog box above, the x-axis units are Wavenumbers; the y-axis units are Absorbance. The Typical Range for the X-Limits and for the Y-Limits is displayed below the entry boxes. Any particular document may not contain all the listed spectrum types.

X-Limits: enter a value for the Start and End limits in wavenumbers. These will be the new end points of the display. Values can be entered by typing,or by clicking the arrows to the right of the entry box.

Notes

If the Start value is less than the End value, then the trace will be reversed. Entering Auto or pressing Reset does not restore the original orientation; you must enter numerical values to do this.

If you enter Auto, then the actual value (start and/or end) from data collection will be used. Auto is not case-sensitive.

Reset: sets the X-Limits to Auto.

Y-Limits: enter a value for the Minimum and Maximum limits in whatever the current Y-axis units are. These will be the new scaling values for the display in the Y-direction. Values can be entered by typing, or by clicking the arrows to the right of the entry box.

If the Maximum value is less than the Minimum value, the trace is displayed as if the values were entered correctly.

If you enter Auto, then trace will be autoscaled along the Y-axis.

Reset: sets the Y-Limits to Auto.

Reset All: sets the X-Limits and Y-Limits to Auto.

OK: return to the main menu display and implement the new X- and Y-limits.

Cancel: return to the main menu display without changing any of the X- or Y-limits.

Help: enter the on-line Help system.

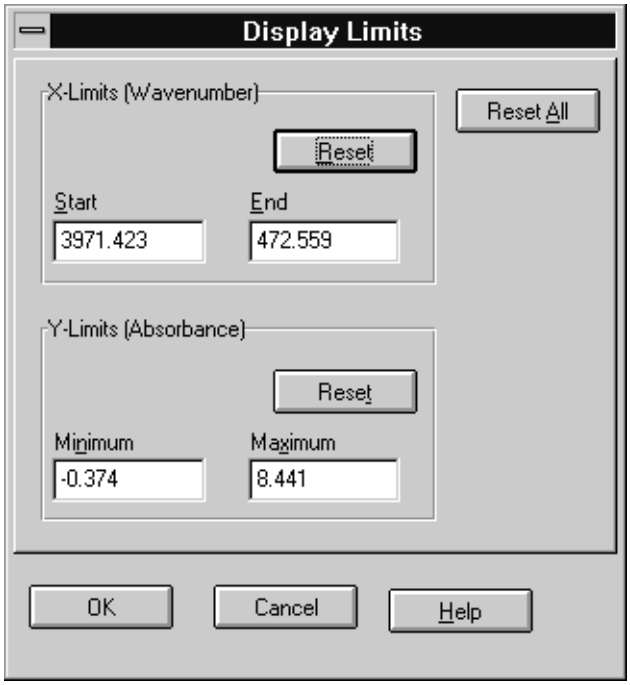
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Note

When you enter numerical values into the Display Limits dialog box, those limit values then apply to all windows. It is good practice to reset all values to Auto once the requirement for specific values has passed.

Selected Spectrum...

Causes the Display Limits dialog box to appear. Use this dialog box to set specific limits for the selected sprectum only.



X-Limits: enter a value for the Start and End limits in wavenumbers. These will be the new end points of the display.

Notes

If the Start value is less than the End value, then the trace will be reversed. Entering Auto or pressing Reset does not restore the original orientation; you must enter numerical values to do this.

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If you enter Auto, then the actual value (start and/or end) from data collection will be used. Auto is not case-sensitive.

Reset: sets the X-Limits to Auto.

Y-Limits: enter a value for the Minimum and Maximum limits in whatever the current Y-axis units are. These will be the new scaling values for the display in the Y-direction.

If the Maximum value is less than the Minimum value, the trace is displayed as if the values were entered correctly.

If you enter Auto, then trace will be autoscaled along the Y-axis.

Reset: sets the Y-Limits to Auto.

Reset All: sets the X-Limits and Y-Limits to Auto.

OK: return to the main menu display and implement the new X- and Y-limits.

Cancel: return to the main menu display without changing any of the X- or Y-limits.

Help: enter the on-line Help system.

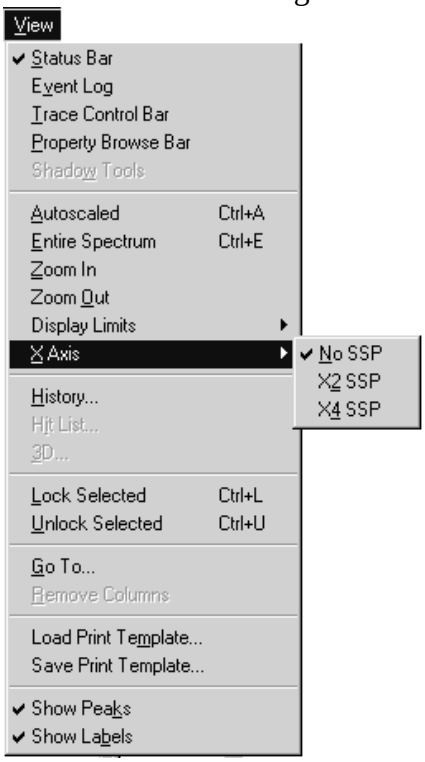
Note

When you enter numerical values into the Display Limits dialog box, those limit values then apply to all windows. It is good practice to reset all values to Auto once the requirement for specific values has passed.

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X Axis Units

Controls the units along the X axis.



SSP is an acronym for "standard spectral plot." This is one in which the X axis has been expanded in the region below 2000 cm^{-1} by a given factor. This expansion is both shown in the display and printed.

No SSP: no expansion (factor of 1) takes place in the X axis (default).

X2 SSP: the X axis below 2000 cm^{-1} is expanded by a factor of 2.

X4 SSP: the X axis below 2000 cm^{-1} is expanded by a factor of 4.

If you want to convert the x-axis units to microns or nanometers, see Transforms / More Transforms in Chapter 10.

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Note

Standard spectral plot is implemented only for Wavenumbers; it is not implemented for Microns or Nanometers.

HISTORY

Displays the history of the collection of the spectrum and any changes made after data collection in the History Browser status box. Such changes can include computing the single-beam spectrum, ratioing against a reference spectrum, and a number of actions available from the Transforms menu, such as smoothing, differentiation, zapping, deconvolution, etc. This entry is disabled (greyed-out) if no history exists for the spectrum. This is often the case for imported spectra collected under systems other than Win-IR Pro.

Note

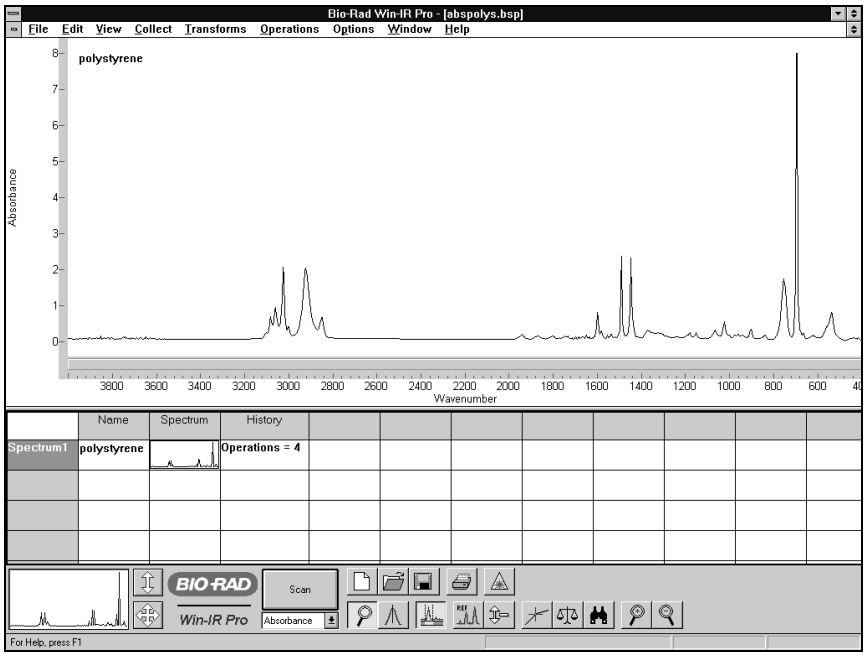
If the spectrum was collected under Win-IR Pro, then the data collection information will be included in the history (Scan).

History at release 2.1 and later will have a time-date stamp for each operation; operations prior to release 2.1 will have a blank in the time-date stamp data.

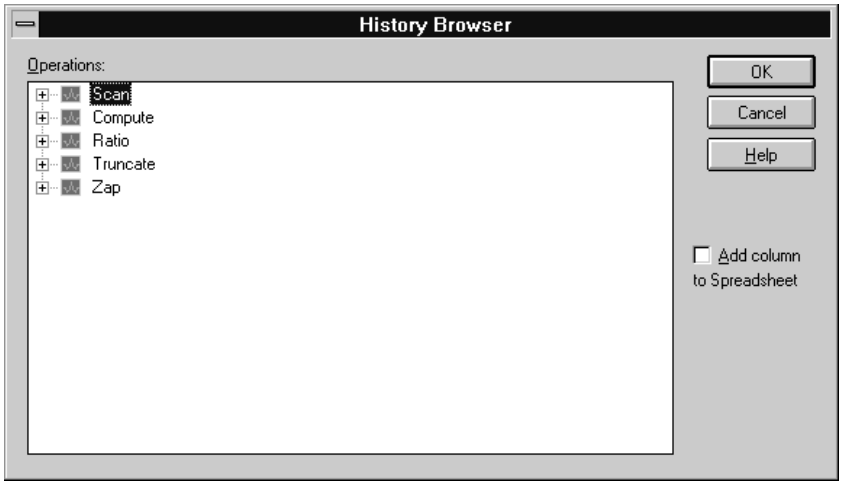
History at release 2.5 and later will have a user stamp for each operation; operations prior to release 2.5 will have a blank in the user stamp data.

In this example, the polystyrene spectrum stored in abspolys.bsp is used.

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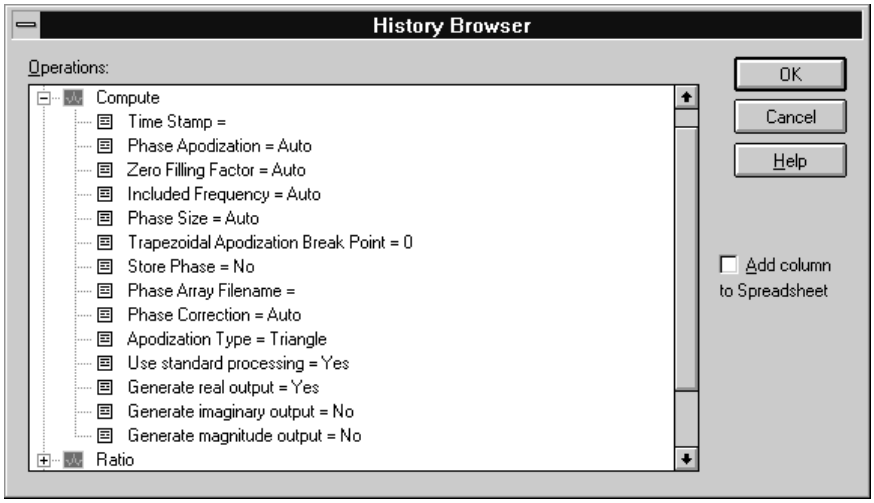


Since there is a history, the History entry is enabled. Select History from the View menu.. The History Browser dialog box appears.

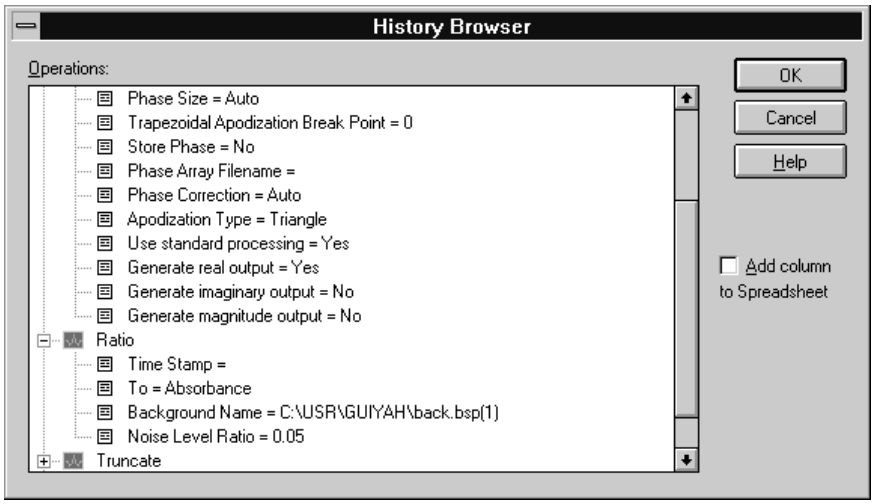


Put the cursor over the box to the far left of the operation name and click the left mouse button. It is expanded to give details. For example, if expand Compute

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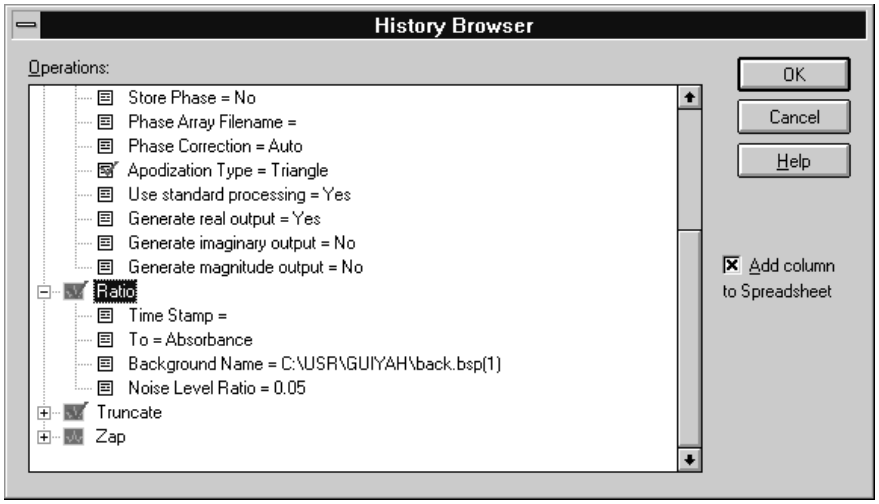
More than one operation can be expanded at a time. For example, highlight Ratio also,



Any one operation (or any one item in the expanded operation) can be highlighted by placing the cursor on it and clicking the left mouse button. If you then select the Add column to Spreadsheet box, the select item is marked with a red check mark. This means it will be added to the spreadsheet when you exit the dialog box.

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Remove an item from this list by highlighting it and deselecting the Add column to Spreadsheet box; the check mark will vanish. In the example below, three items have been flagged to be added to the spreadsheet.



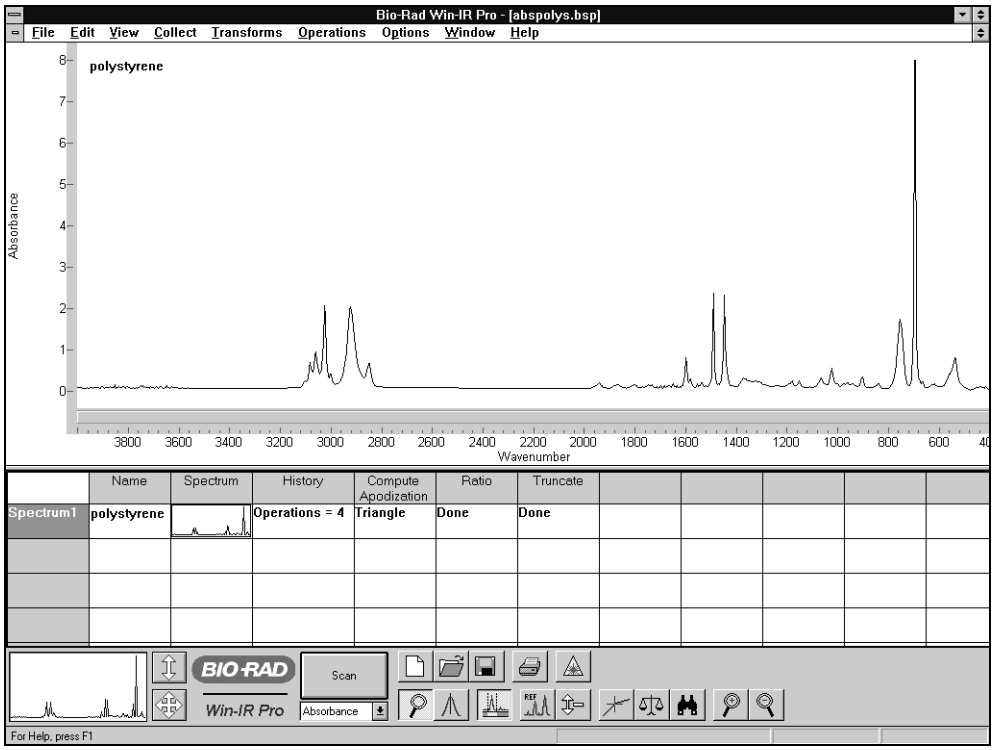
OK: return to the main menu display and modify the spreadsheet, if so specified.

Cancel: return to the main menu display without modifying the spreadsheet.

Help: enter the on-line Help system.

The example below shows the three flagged items added to the spreadsheet. Columns can be removed from the spreadsheet using Remove Columns from the View menu. This is discussed later in this chapter.

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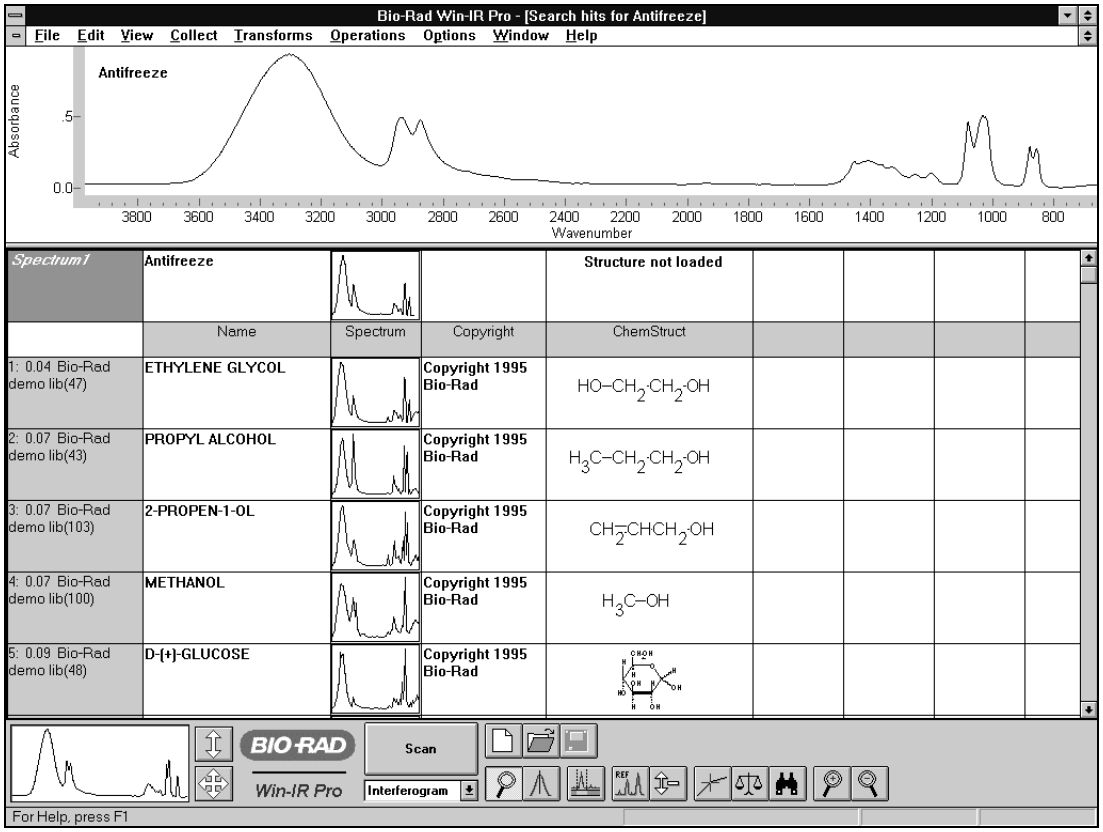
If you select an operation, such as Scan, Compute, Ratio, Truncate, etc. and add it as a column to the spreadsheet, the column header will be the name of that operation (Scan, etc.). The contents of the cell will be **Done** (or a blank, if that operation was not performed for another row in the spreadsheet).

If you double click an operation to display its parameters and select parameters to be added to the spreadsheet, the parameter column heading will be Operation Parameter (for example, Truncate Region) and the cell will have the value of that parameter. Whether Operation is to the left of Parameter or above it depends upon the width of the column.

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HIT LIST

This entry is enabled after a successful search; otherwise it is disabled (greyed-out). Selecting this entry displays a new document window with the selected sample spectrum and its search hits.

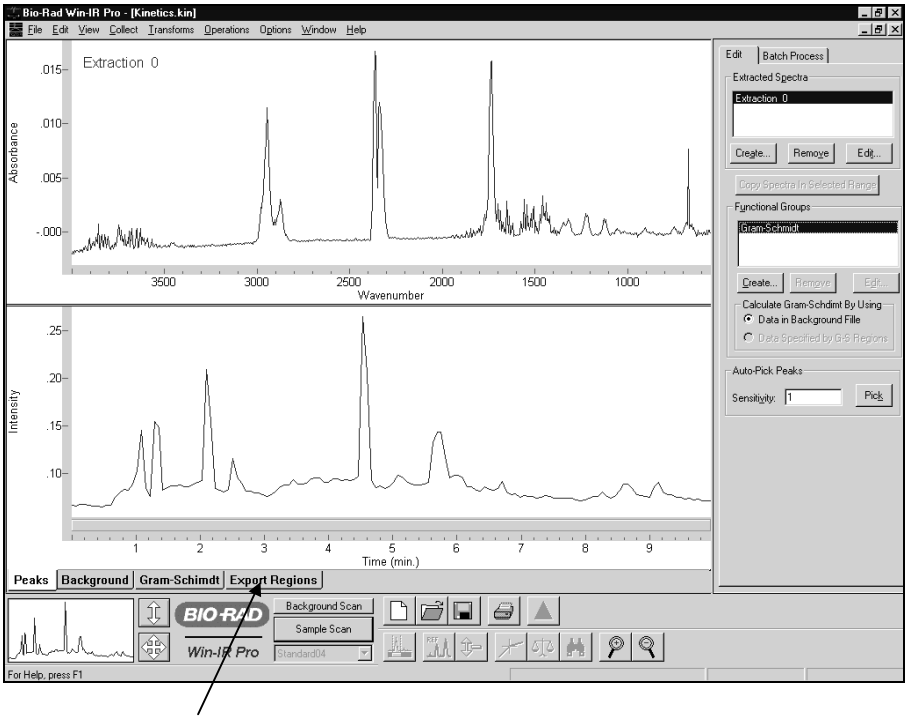


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3D...

Presents a three-dimensional view of the spectra in a Kinetics Document, with time, wavenumber, and absorbance as the axes. This entry is disabled unless the active document is a Kinetics Document.

In this example, we will use kinetics.kin.

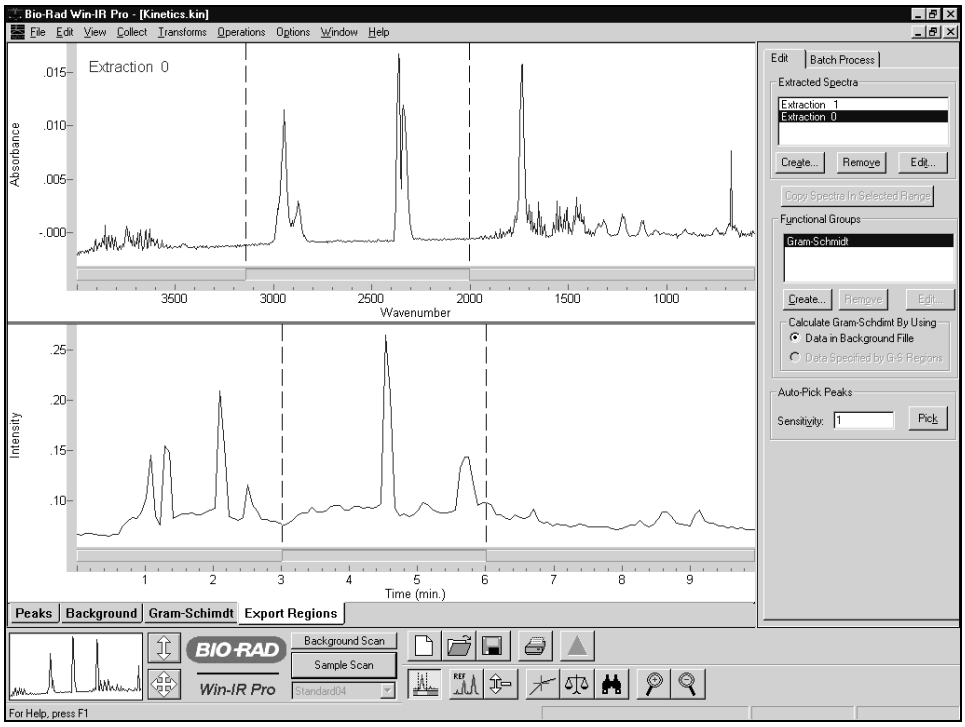


Click the Export Regions button.

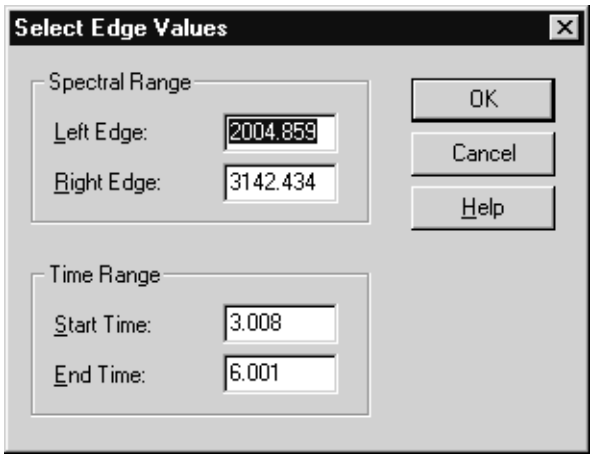
To select the region of interest for wavenumber: click the right mouse button, select New / Region; then use the cursor in the extracted spectra ruler to adjust the size of the region. In this example, set it to 3150 to 2000 cm^{-1}.

Use the cursor to select the regions of interest for time. In this example, we will be looking at 3 to 6 minutes.

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When 3D... is selected, the Select Edge Values dialog box appears.



The limits selected using the cursor are shown here. New values can be entered by typing.

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Spectral Range: the region of each spectra to be used in creating the 3D view.

Left Edge: the lower limit (in cm^{-1}) of the spectra.
Right Edge: the upper limit (in cm^{-1}) of the spectra.

Time Range: defines the time interval in which the spectra used to create the 3D view appear.

Start Time: the beginning of the time range (minutes).
Stop Time: the end of the time range (minutes).

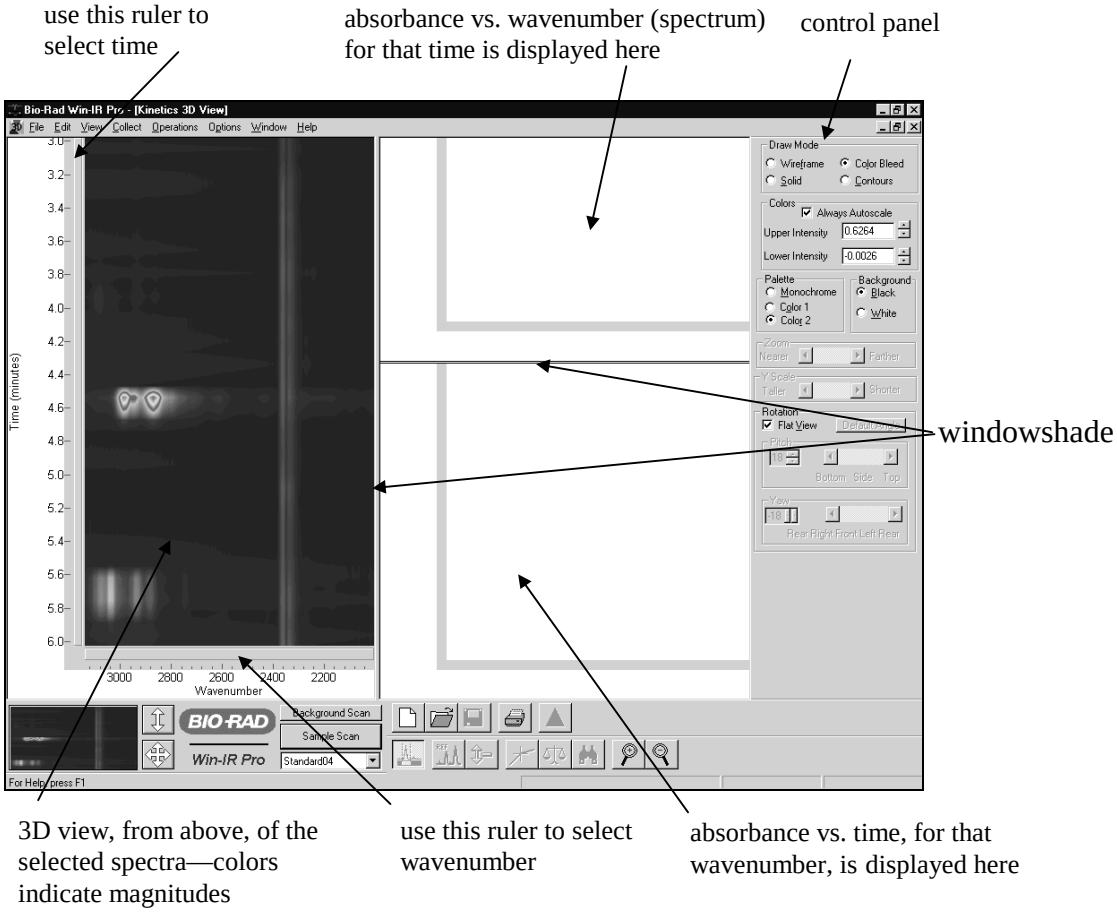
OK: creates the 3D view and displays it (see below).

Cancel: return to the main window without generating a 3D view.

Help: enter the on-line Help system.

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The initial 3D view is shown below:

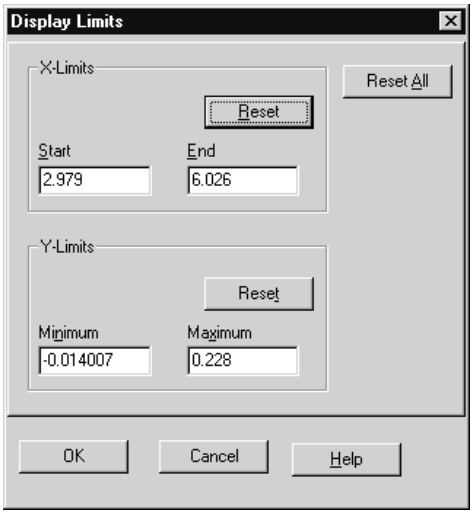


Two-dimensional cross-sections: To select a spectrum for a given time, place the cursor in the vertical ruler and click the left mouse button. The spectrum is displayed in the upper middle of the window.

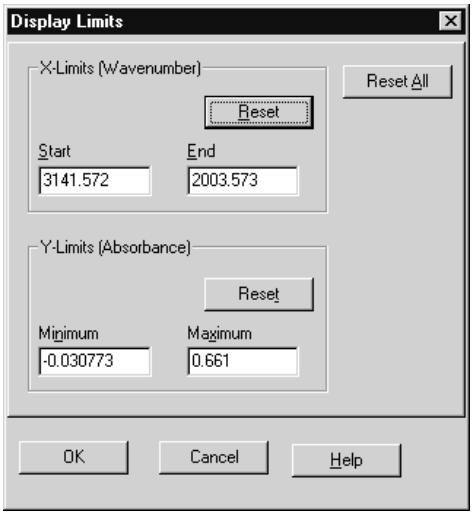
To select a plot of absorbance vs. time for any wavenumber, place the cursor in the horizontal ruler and click the left mouse button. The absorbance-vs.-time plot is displayed in the lower middle of the window.

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Once you have selected a trace you can adjust its display. In this example, the upper trace has been selected. Choose View / Display Limits / Selected Spectrum. The Display Limits dialog box appears.



See the section on Display Limits in this chapter for details of how to use this dialog box. If you select the lower trace, and choose View / Display Limits / Selected Spectrum, the dialog box appears with the limits for that trace.



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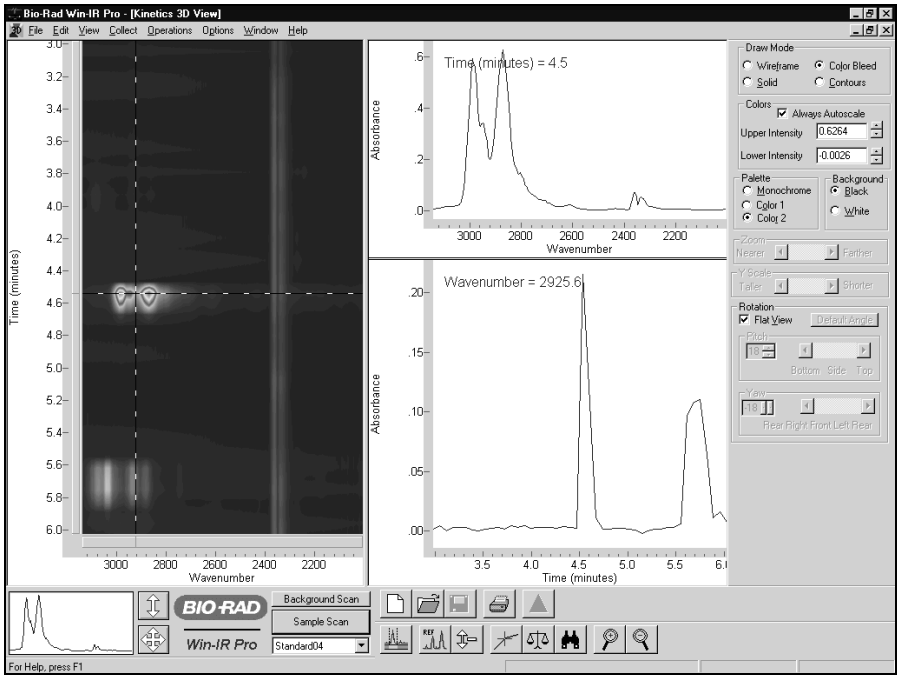
Note

Under certain conditions and color selections, the extracted line may vanish. To cause it to reappear:

1. Select Options / Edit Color...
2. Click the + next to Pen.
3. Select Region Line.
4. Click on the black box (lower left of the rectangle of Basic Colors).
5. Click the OK button.

Select a trace, in either the upper or lower display, by clicking on it. You can now use the normal zoom and scaling operations in that display.

In the example below, both a time and a wavenumber have been selected.

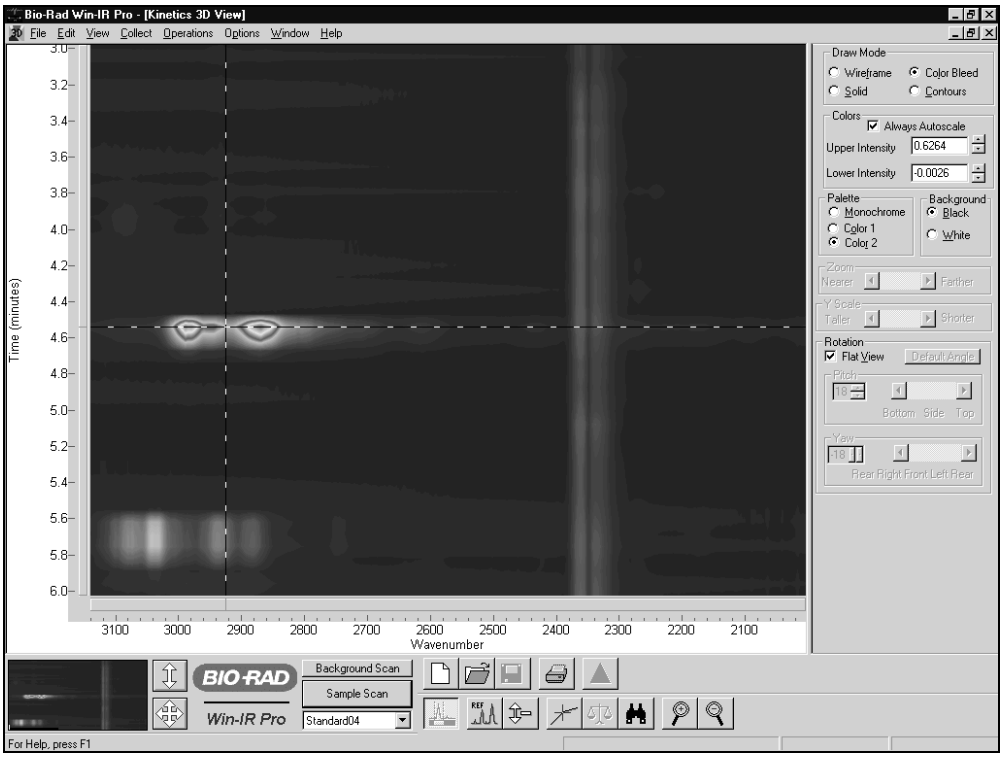


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The portion of the window taken up by each of the three displays can be altered by dragging the windowshades to the desired location (see Chapter 1 for details of moving windowshades).

Printing a cross section: Select a trace, in either the upper or lower display, by clicking on it. Select Print from the File menu, or click the  button. The Print dialog box appears. Press OK if the settings are as desired; otherwise, see Print in Chapter 6 for details of the settings.

Three-dimensional view: This view can be moved, rotated, and presented in a number of formats. The control panel sidebar on the right hand of the screen controls the presentation of the data. The portion of the window used by the different graphics can be altered by moving the horizontal and vertical window shades. In all the examples below, the vertical window shade has been moved all the way to the right to better show the three-dimensional graphics.



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Draw Mode: how the three-dimensional aspect will be represented in two dimensions.

Wireframe: the points of the calculated three-dimensional plot are connected with straight lines. Lines that are hidden by the shape of the display are not shown. This draw mode disables both Colors and Palette.

Solid: the lines and the frames they define are filled in with different shades of a single color to give a better idea of the shape of the surface of the contour plot.

Color Bleed: uses multiple colors for the surface. These colors change gradually and smoothly as the height of the plot varies above the base plane. (Default)

Contours: shows contour lines on the surface at constant heights about the base plane. The contour intervals are pre-set and cannot be changed.

Colors: sets the rangeof colors used to represent the extreme z-values of the plot.

Note

In wireframe mode, Colors is disabled.

Always Autoscale: if this is selected, then whenever you zoom in on a portion of the plot, the color will be scaled so that the full color range is used for that portion. This is useful if you zoom in on weak features that may be displayed in very similar colors in the full plot.

If you are not autoscaling the colors, then you can set the values to be used in the display. If you use the arrows to the right of the intensity boxes to set values, they will be implemented immediately. If you type in values, they will not be implemented until you press the Enter key on the keyboard.

Upper Intensity: enter the color value to be used at the maximum z-value of the plot.
Lower Intensity: enter the color value to be used at the minimum z-value of the plot.

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Palette: the draw modes may be observed with three different color schemes.

Note

In wireframe mode, Palette is disabled.

Monochrome: gray scale.
Color 1: shades from red to white to blue.
Color 2: shades from red through orange, yellow, and green to blue. (default)

Background: select the color for the background. A white background may be better if you are capturing screens for insertion in a publication with a monochrome printer.

Black: background is black. the plot is shown against a black background (default).

White: the plot is shown against a white background. This may be more desireable for formats other than wireframe

Zoom: makes the plot appear closer (increases size) or farther away (decreases size). Use the slide bar to change the value.

Y Scale: makes the height of the peaks taller or shorter. Use the slide bar to change the value.

Rotation: these controls move the three-dimensional plot about two axes. Regardless of the rotation, the axes remain in the foreground of the display. Rotation of large arrays may be slow. Press the ESC key to stop the rotation.

Flat View: if selected, displays a projection of the isometric view. If de-selected, the isometric view (3D) is shown.

Default Angle: press this button to return the plot to its default position (Pitch = 18°, Yaw = 1°).

Pitch: rotates the plot about a horizontal axis parallel to the monitor screen. Click on the upper part to rotate the plot to show its Bottom; click on the lower part of the bar to rotate the plot to show its Top. Each time you click the end of the slide bar, the plot rotates 9°.

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Yaw: rotates the plots about a vertical axis. The plot can be rotated either to the Right or to the Left. Each time you click the end of the slide bar, the plot rotates 18°.

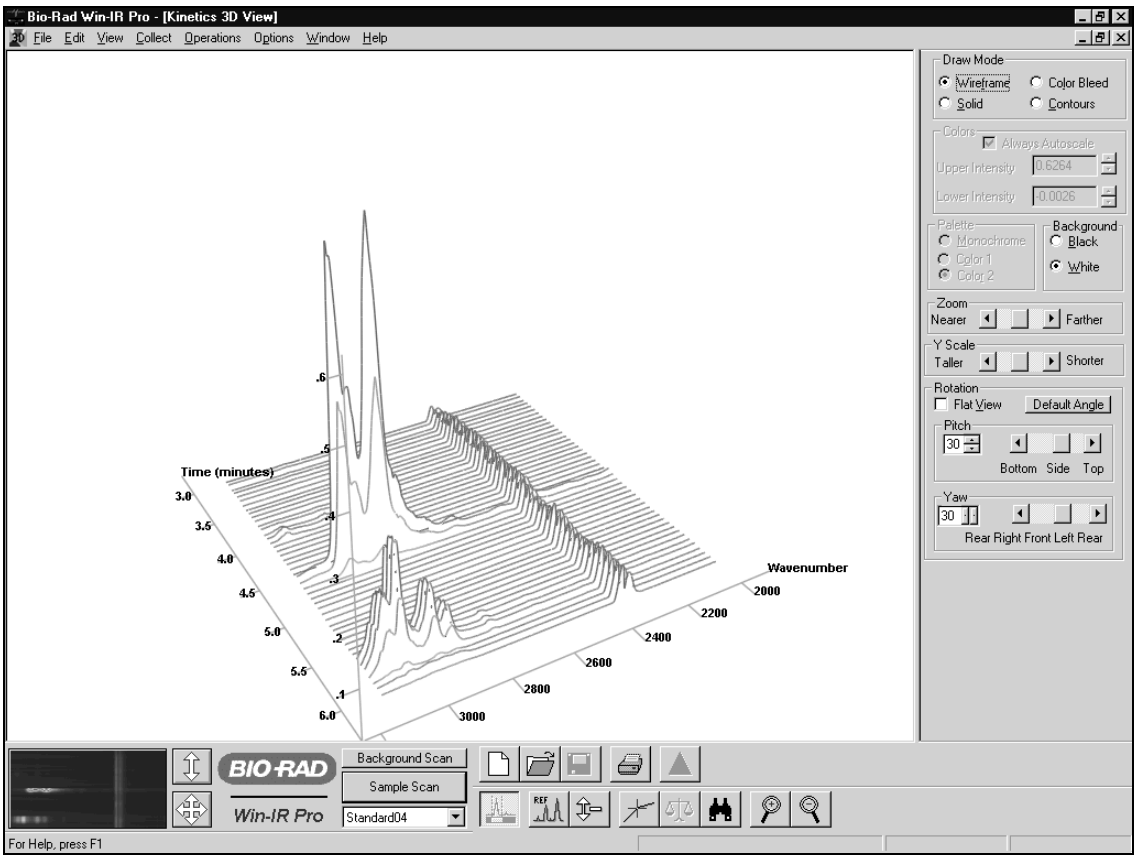
For both Pitch and Yaw, you can enter the value of the angle. If you change the angle with the arrows to the right of the text box, the values are implemented immediately. If you type in values, the values are not implemented until you press the Enter key on the keyboard.

Subsets of all menus except Transforms are also available. Their entries operate the same as they do in the main Win-IR Pro document window.

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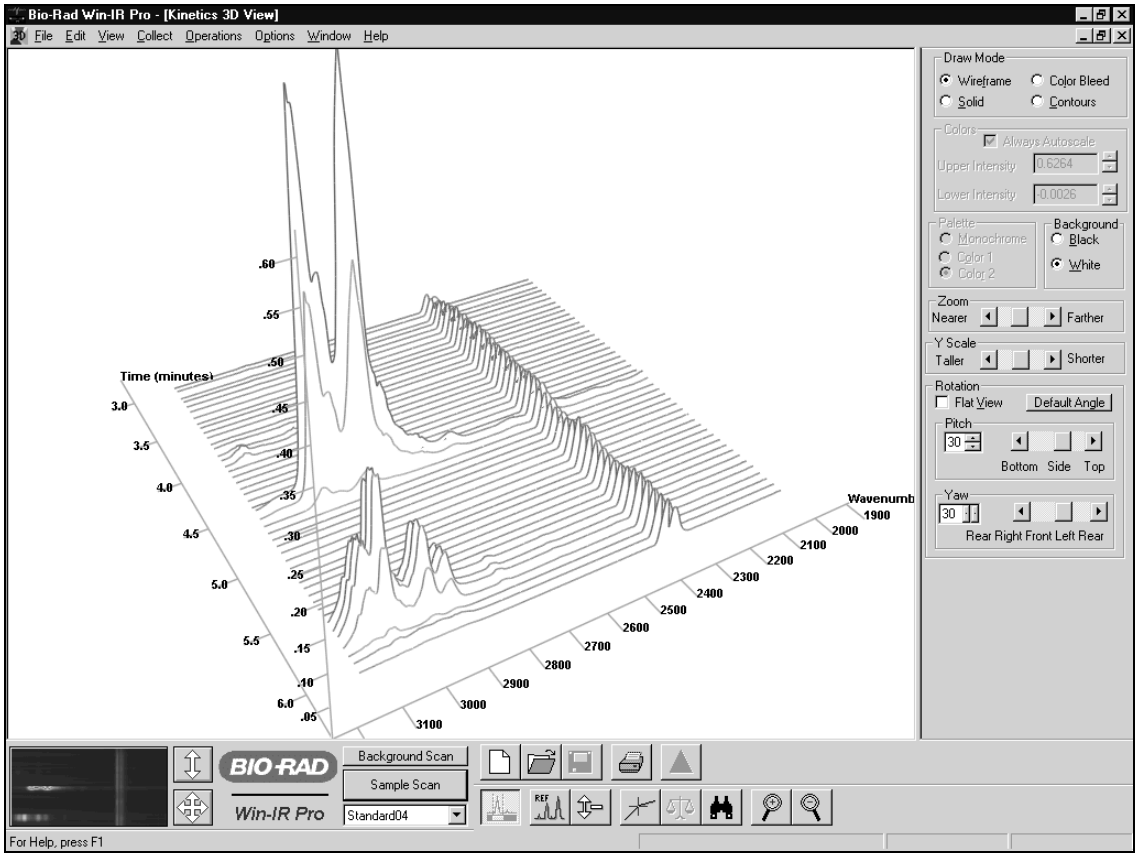
Examples:

In this example, Draw Mode has been set to Wireframe, Color Palette to Monochrome, and Background to White. Flat View has been de-selected and the image has been rotated by 30° about each axis.



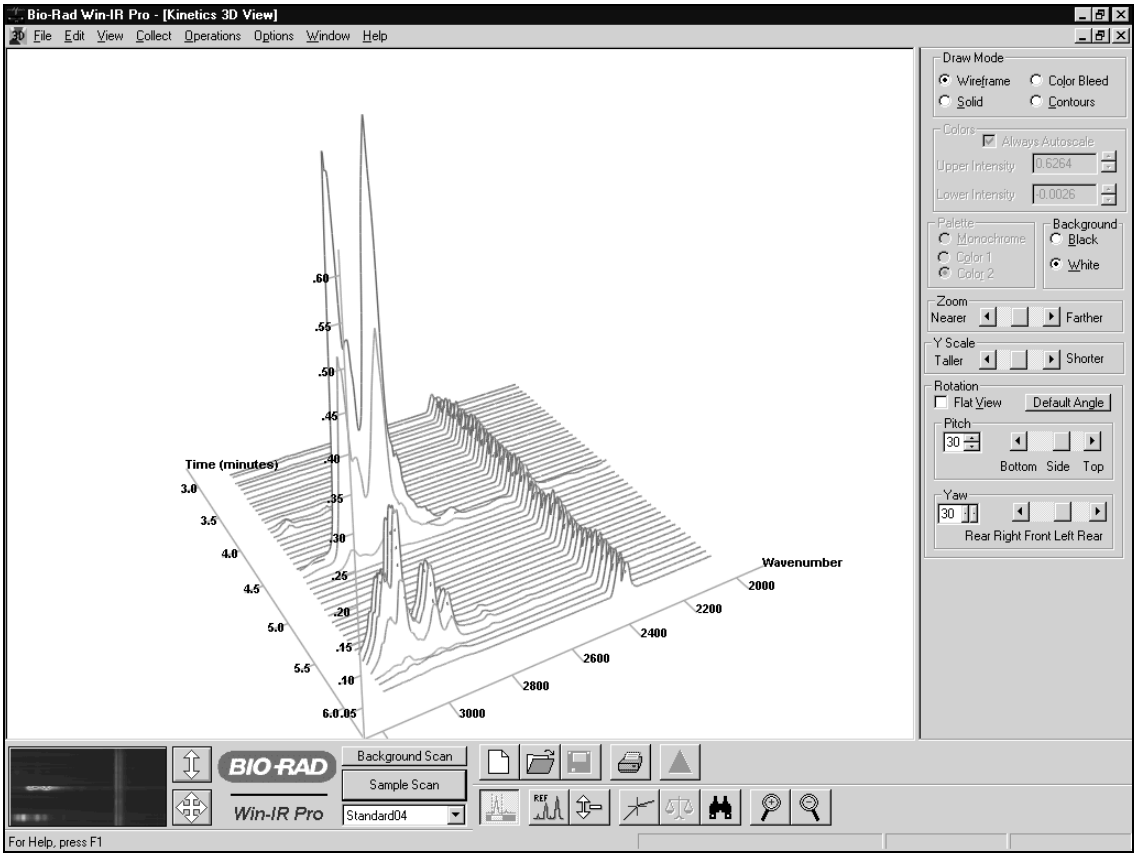
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Zoom nearer gives this view.



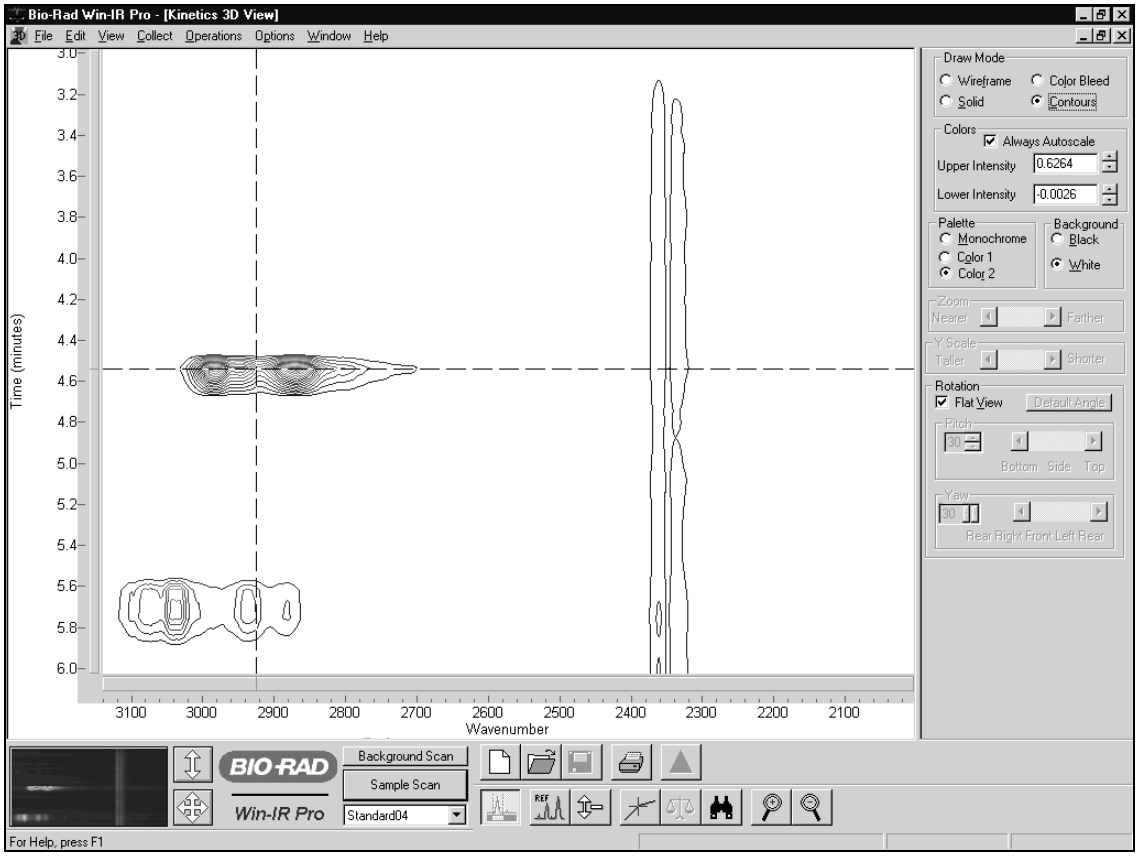
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Zoom farther, and make Y Scale taller gives this view.



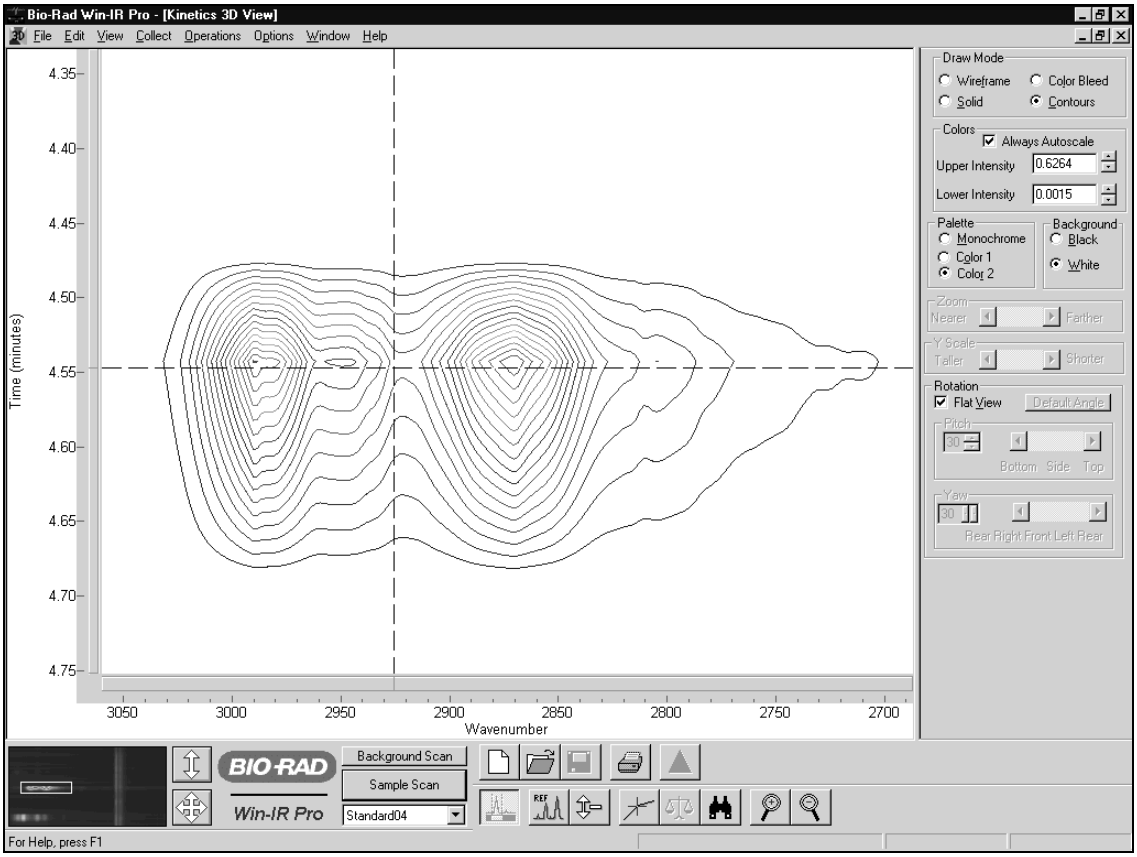
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In the example below, Flat View has been selected; Draw Mode is set to Contours.



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As is the case in all the 3D plots, you can use the cursor to draw a rectangle about the area of interest to zoom in on it.

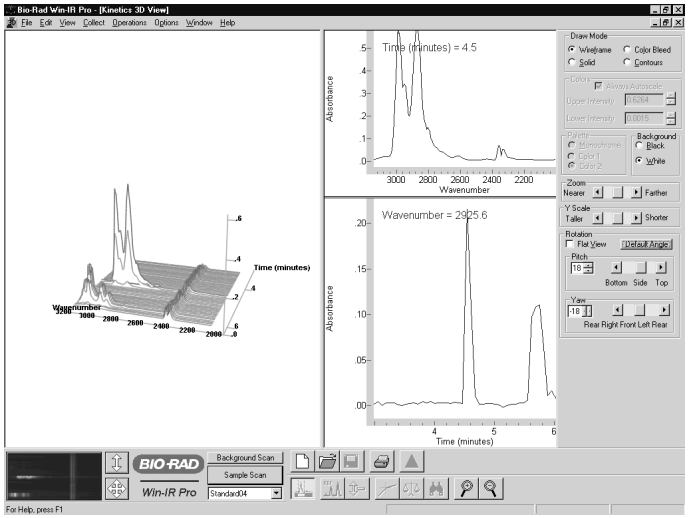


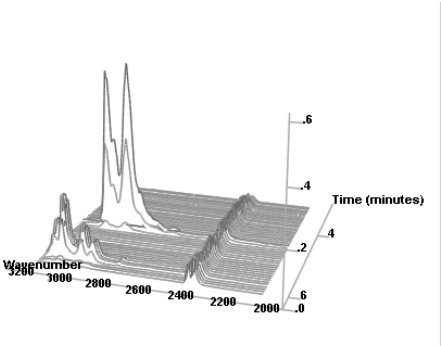
Printing the 3D View:.To print the three-dimensional (left-hand side) part of the screen, select File / Print or click the  button at the buttom of the screen. In the example below, the following parameters have been changed from their defaults:

Draw Mode	Wire Frame
Palette	Monochrome
Background	White
Flat view	de-selected

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The full screen is on the left; the printed image is on the right.





The printed image is exactly what is in the three-dimensional portion.

If you want to print the entire screen image use either WordPad or Paint. These two applications are supplied as part of Windows NT. The procedure is described in Chapter 1.

Exporting 3D Data

The data triads (x, y, z) can be exported by selecting Operations / Export DXF. The file created has a .dxf extension and can be opened and manipulated by applications such as Autocad.

Notes

This menu entry is only accessible in a 3D graphics view.

These .dxf files cannot be inserted into word processors using the usual .dxf filter.

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LOCK SELECTED

Select a row (spectrum) or a column (property) in the spreadsheet and select Lock Selected.

If a spectrum is selected, this spectrum continues to be displayed even if other spectra are selected in the spreadsheet. If a spectrum is locked, its *Spectrum #* is displayed in italics. This is useful for comparing one spectrum against a series of others.

If a property is selected, this property will be printed out as part of the plot when File / Print is chosen. If a property is locked, its *label* is displayed in italics.

UNLOCK SELECTED

Select a row (spectrum) or a column (property) in the spreadsheet and select Unlock Selected.

This spectrum is no longer locked into the view and will disappear when another spectrum is selected from the spreadsheet.

The property will no longer appear on the plot when File / Print is chosen.

Locking/Unlocking a Spectrum into Display

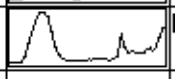
When a spectrum (set of spectra) is (are) selected for operation, it (they) can be locked into the main display by selecting Lock Selected from the View menu. They will remain locked and in the trace display until explicitly unlocked by selecting Unlock Selected from the View menu. This is useful if you want to compare one spectrum against a succession of others.

Note

Selecting a spectrum does **not** automatically lock it; locking must be done explicitly

Locked spectra are indicated by italics in the leftmost column (called the ID column) of the spreadsheet. In the example below, *Spectrum 1* is locked.

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	Name	Spectrum	Hitlist	History
Spectrum1	**coke(1)**		**Hits = 0**	**Operations = 0**
Spectrum2	**sprite(1)**		**Hits = 0**	**Operations = 0**

Locking/Unlocking a Property for Printing

When a property (set of properties) is (are) selected for operation, it (they) can be locked into the main display by selecting Lock Selected from the View menu. They will remain locked and in the trace display until explicitly unlocked by selecting Unlock Selected from the View menu.

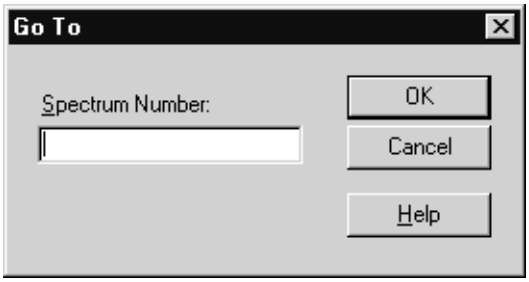
Locked properties are indicated by italics in the top row (label row) of the spreadsheet. In the example below, *HitList* and *History* are locked.

	Name	Spectrum	*Hitlist*	*History*
Spectrum1	**coke(1)**		**Hits = 0**	**Operations = 0**
Spectrum2	**sprite(1)**		**Hits = 0**	**Operations = 0**

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Go To...

Allows you to select any spectrum in the document without having to choose through the spreadsheet. This is useful for documents with large number of spectra. The Go To dialog box appears



Enter the number of the desired spectrum and click OK. That spectrum appears in the trace. The corresponding entry in the spreadsheet is highlighted. If you enter too low a number, Spectrum 1 (the first spectrum) is selected. If you enter a number larger than the last spectrum in the spreadsheet, the last spectrum is selected.

Note

If you have a large number of spectra in a document, you can easily access the end by selecting Go To... and entering a very large number (such as 999).

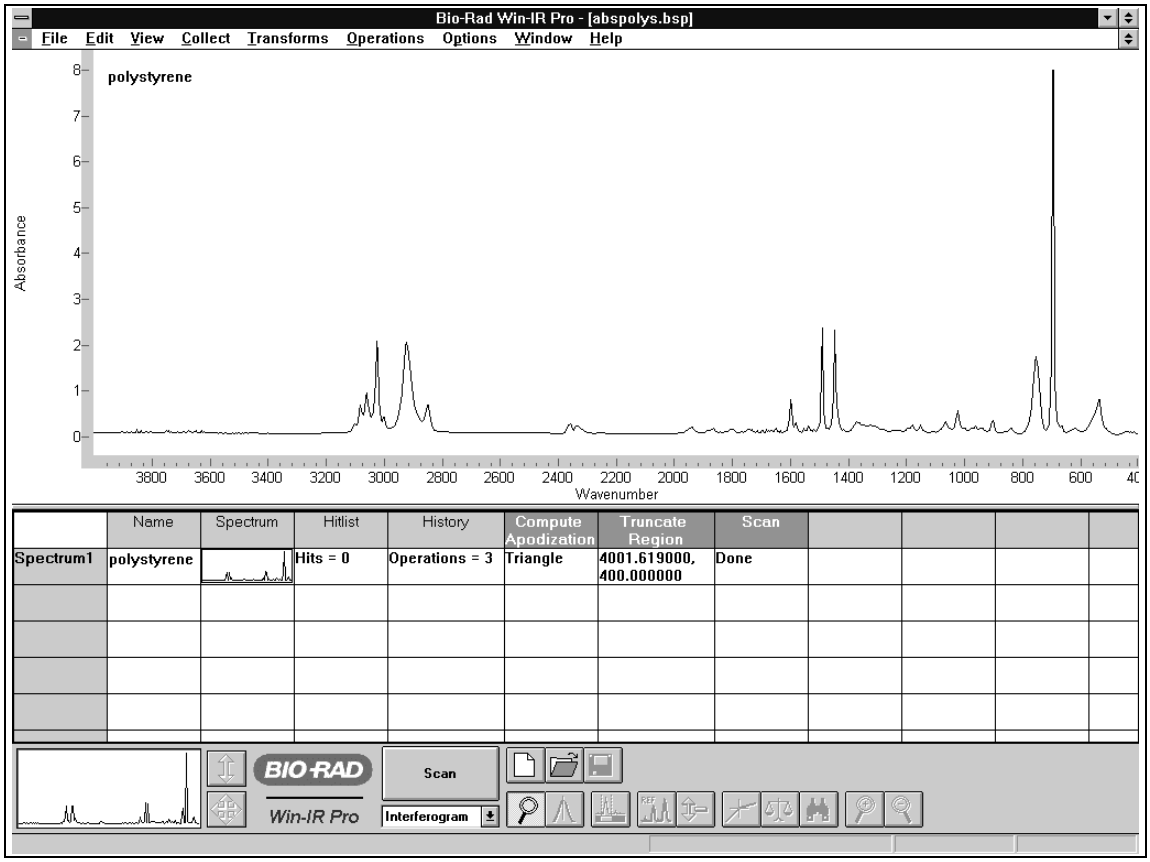
Cancel: return to the main menu without changing the spectrum (or spectra) current active.

Help: access the on-line Help facility.

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REMOVE COLUMNS

Select the column (or columns) to be removed by placing the cursor in the column label box and clicking the left mouse button. Multiple columns can be selected in the usual manner (see “Introduction to the Spreadsheet” Chapter 4, for details).

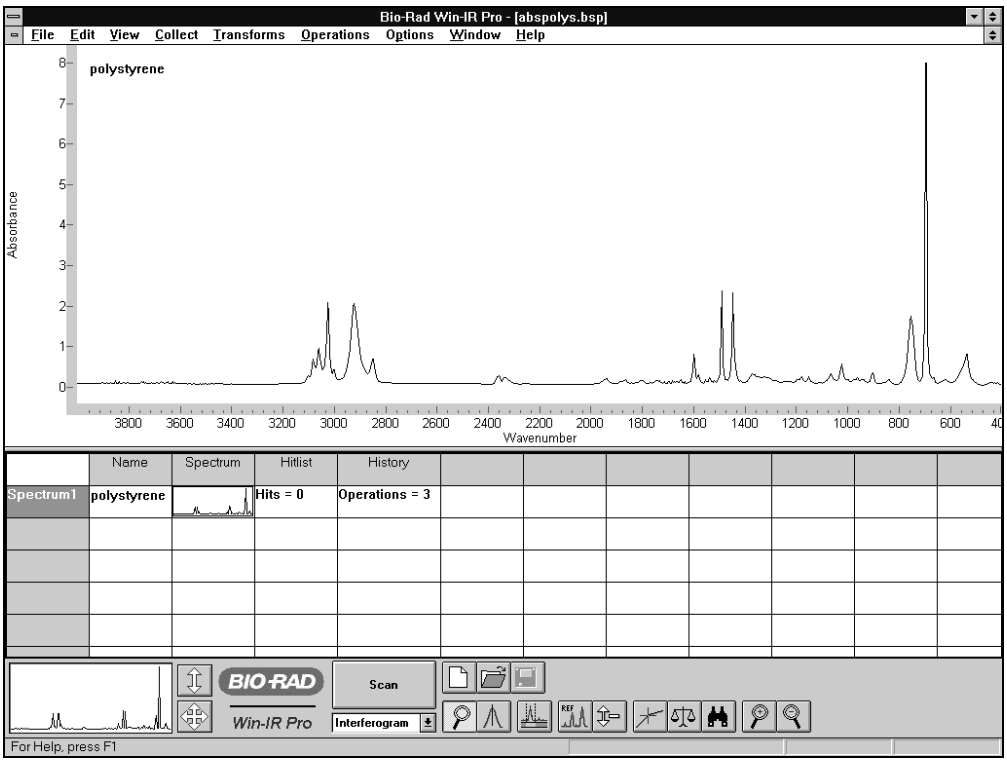


Note

The **display** of information is removed. The actual information is still in the file and can be redisplayed, if desired, at a later time.

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Select Remove Columns from the View menu. The selected columns are removed from the spreadsheet.



Note

If no columns are selected, then the Remove Columns entry is disabled (greyed-out).

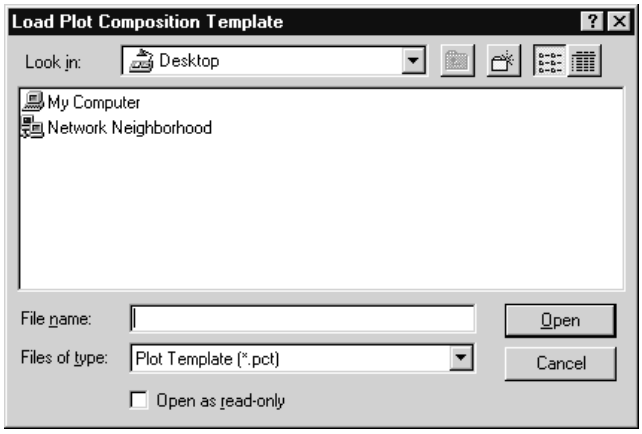
Caution

Do not remove the name and spectrum columns of the spreadsheet. If you remove the spectrum, use the Property Browse Bar to add Spectrum to the spreadsheet. If you remove the name, use the Property Browse Bar to add SpectName to the spreadsheet.

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LOAD PLOT TEMPLATE

The plot composition template describes how the printed page will appear. In particular, it defines which columns in the spreadsheet will be printed; this information was saved using Save Plot Template (see below). These templates are saved in files (with a .pct extension). Select this entry to load the desired existing template. The Load Plot Composition Template dialog box appears.

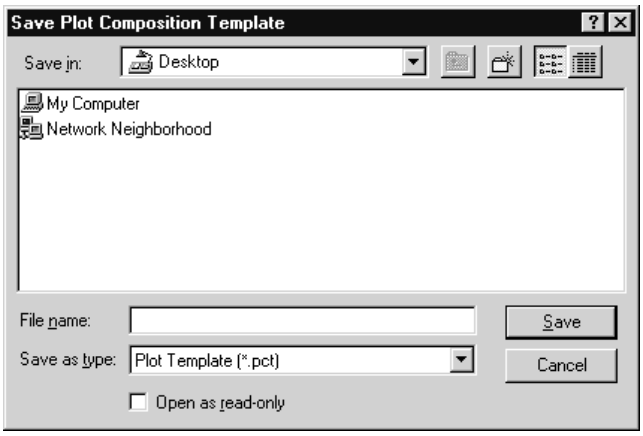


Use the standard procedures to select a file. This template file may be local or accessible over the network (use the Network button). Click OK to load the file. Cancel closes the dialog box without loading a new template. Help accesses the on-line Help system.

SAVE PLOT TEMPLATE

After you have chosen the spreadsheet columns to be printed by selecting and locking them, you can save this list of columns with Save Plot Template. This list of columns can be used for any other document by using Load Plot Template (see above). Select Save Plot Template and the Save Plot Composition Template dialog box appears.

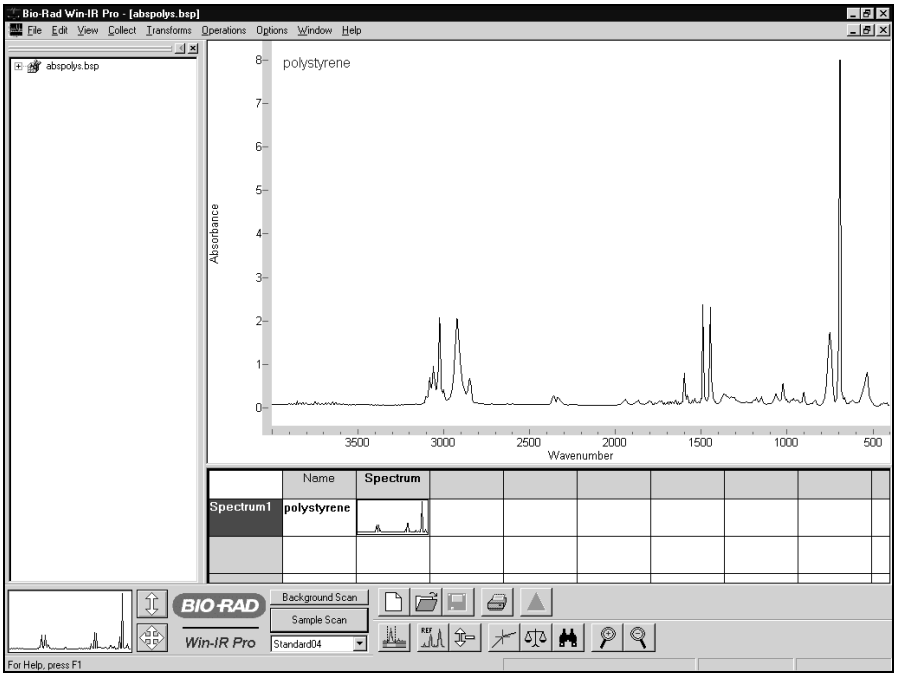
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Choose a name for the plot template and save it in the appropriate directory.

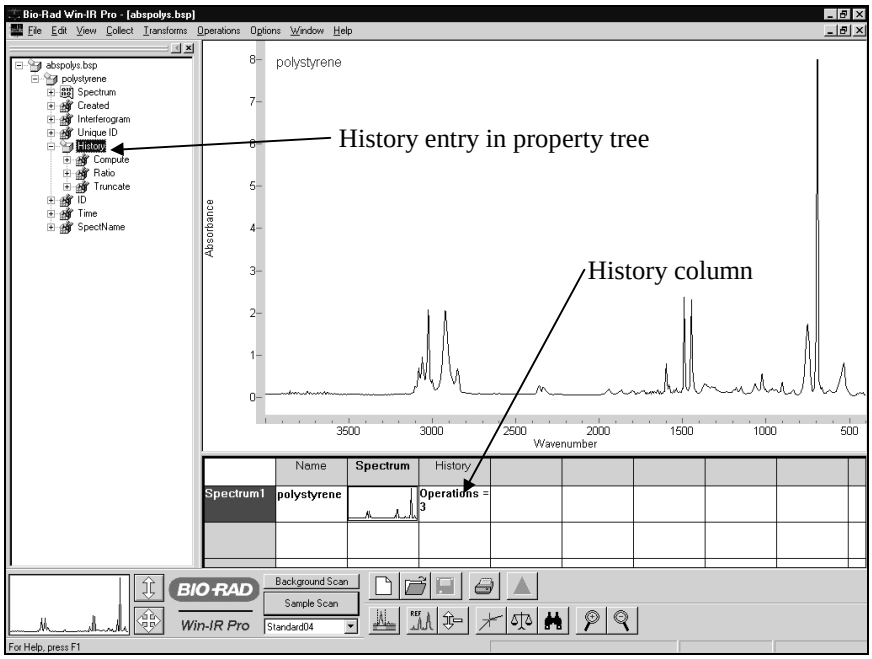
The example below shows how to have data acquisition parameters printed out with the spectrum.

1. Select View / Property Browse Bar.



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2. Open the property tree until you see the History entry; select History by highlighting it. Click the right mouse button and select Add Column from the menu. This puts a History column into the spreadsheet. Hide the Property Browse Bar if it is no longer required.

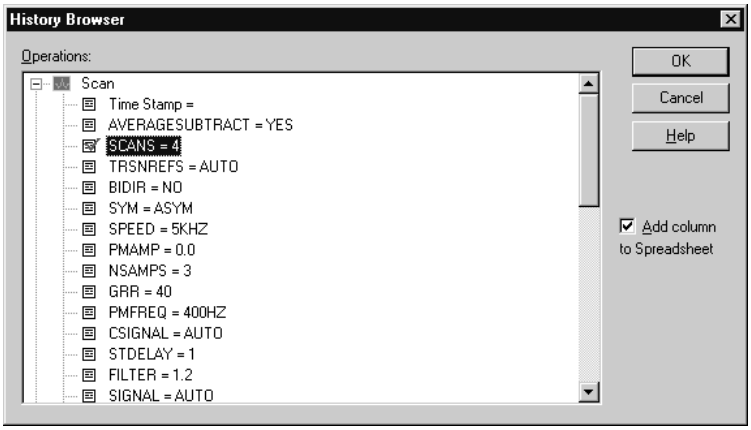


3. Double-click the History entry in the spreadsheet. The History Browser dialog box appears.

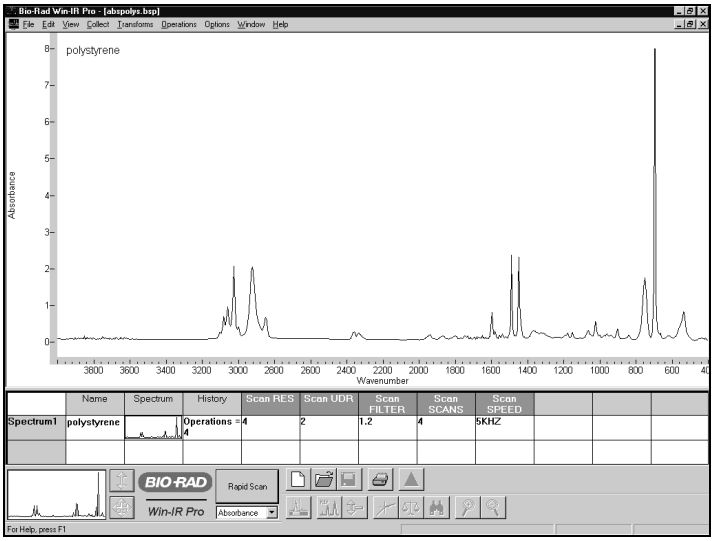


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4. Click the + to the left of Scan to expand the scan parameters. Highlight a parameter you want printed with the spectrum but clicking on it. Click in the Add column to spreadsheet box so that it is selected. Repeat this process for all the parameters you want printed. When these have been selected, press the OK button. You are returned to the main screen.

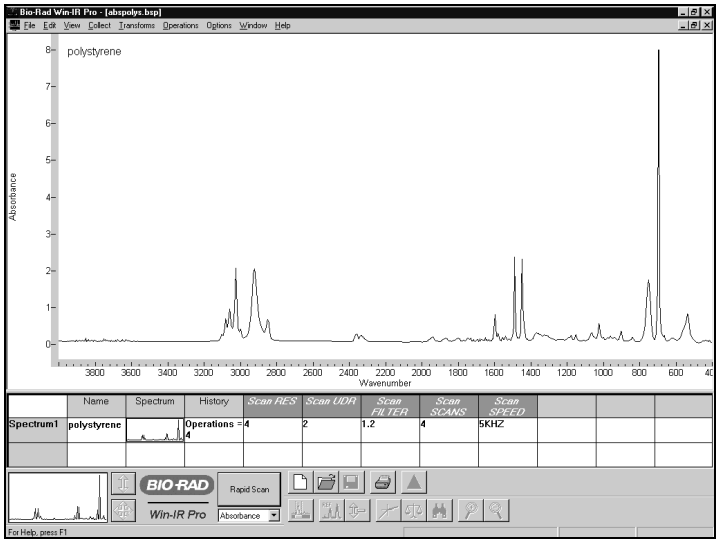


5. Shift-click to select the columns in the spreadsheet that are to appear in the plot. The column headings are shown darker than unselected column headings.



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6. Select View / Lock Selected. The selected column header labels are now shown in italics.



7 Select View / Save Plot Template; save this as a .pct file.

8. Whenever you want to print a spectrum with these collection parameters, bring up the template using View / Load Plot Template.

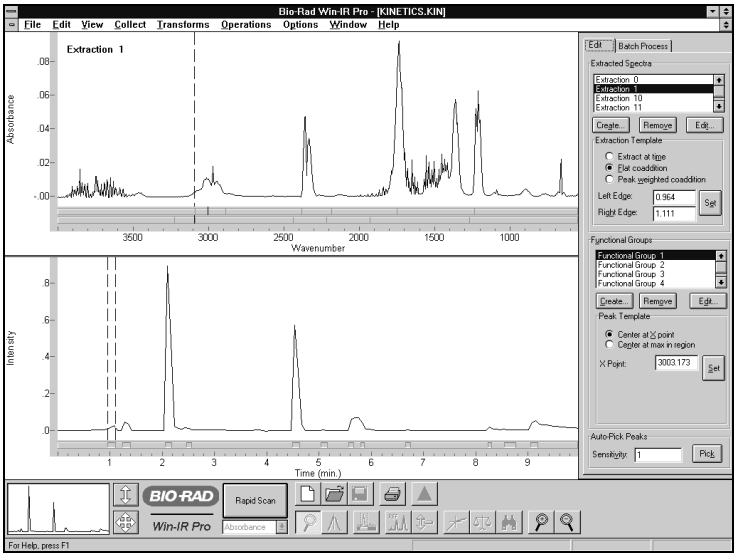
KINETICS DOCUMENT ENTRIES

The entries Kinetics Edit Bar, Spreadsheet, and Chromatogram Edit Window appear only when a kinetics document is active. These entries are independent and the choice of one does not imply nor preclude the choice of any of the others.

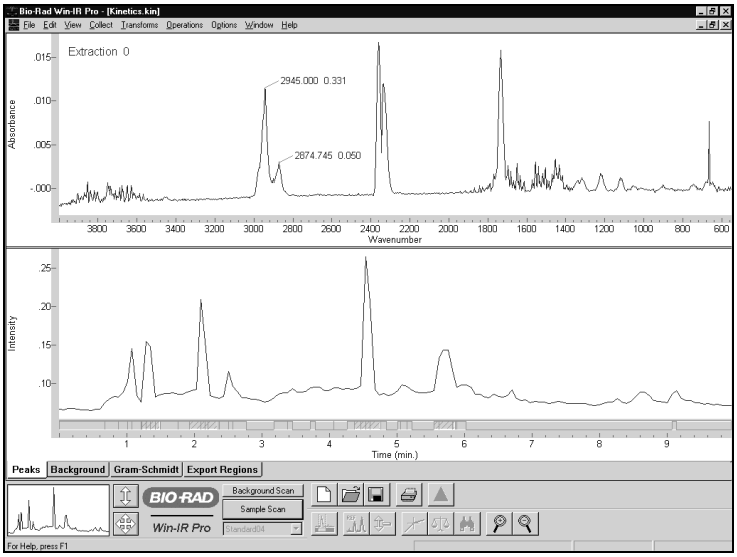
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Kinetics Edit Bar

If you select the View / √ Kinetics Entry Bar entry, the sidebar control panel will no longer be displayed, the document screen will be redrawn, and the √ mark will also disappear. Select this entry again, to make the kinetics edit bar and the √ mark reappear.



√ Kinetics Edit Bar

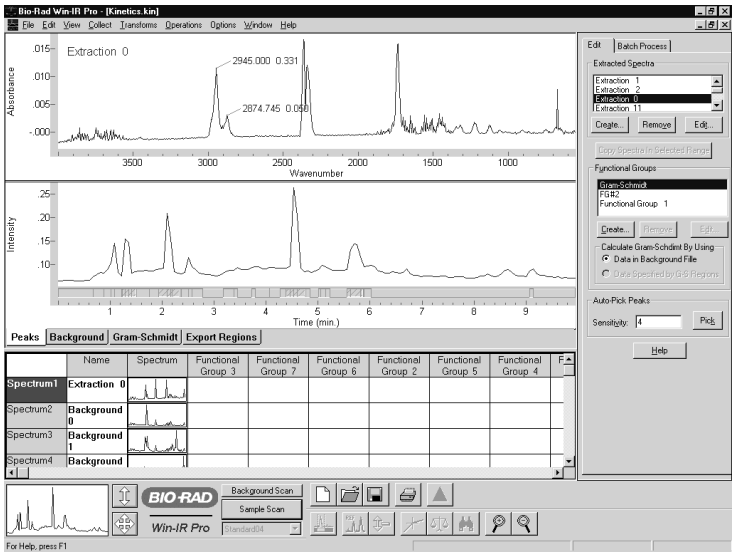


Kinetics Edit Bar

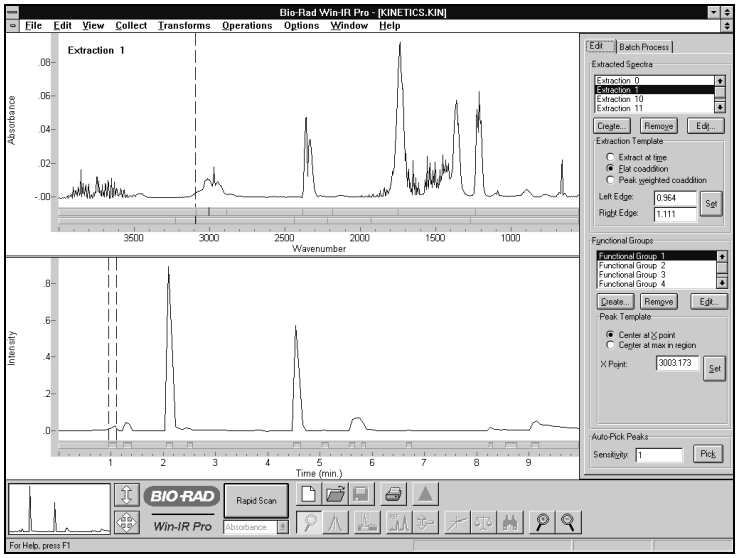
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Spreadsheet

If you select the View / Spreadsheet entry, the spreadsheet for the extracted spectra will be displayed, the document screen will be redrawn, and the √ mark will also appear. Select this entry again, to make the spreadsheet and the √ mark disappear.



√ Spreadsheet

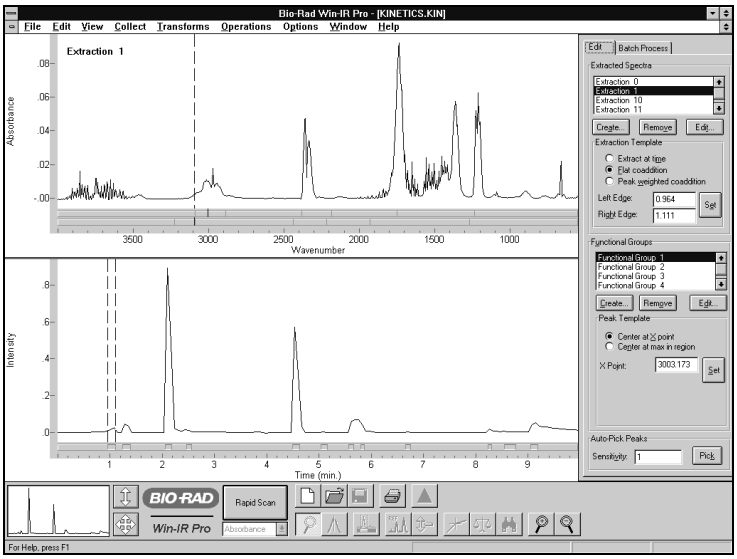


Spreadsheet

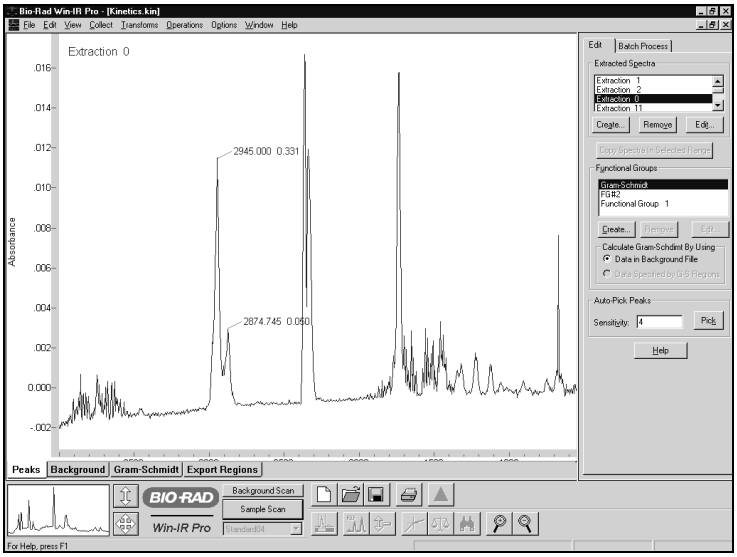
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Chromatogram Edit Window

If you select the View / √ Chromatogram Edit Window entry, the chromatogram edit window will no longer be displayed, the document screen will be redrawn, and the √ mark will also disappear. Select this entry again, to make the chromatogram edit window and the √ mark reappear.



√ **Chromatogram Edit Window**



Chromatogram Edit Window

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HIDE GRAM-SCHMIDT CHROMATOGRAM

This menu entry appears only when a kinetics document is active.

If you select the View / Hide Gram-Schmidt Chromatogram entry, the Gram-Schmidt chromatogram will no longer be displayed, the Gram-Schmidt entry will be removed from the Functional Groups list in the control panel sidebar, and the menu entry will change to Show Gram-Schmidt Chromatogram. Select Show Gram-Schmidt Chromatogram to restore the display and menu to their previous conditions.

Notes

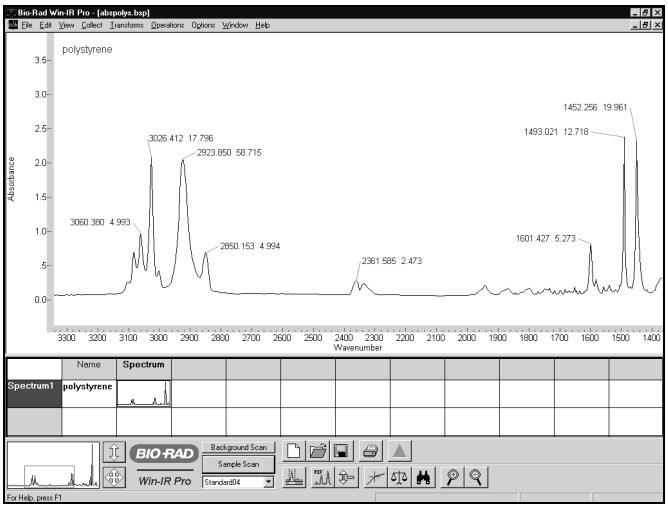
Hide (and Show) Gram-Schmidt Chromatogram is normally used only when the chromatogram edit window is shown.

You can hide the Gram-Schmidt chromatogram even if no other functional groups have been created.

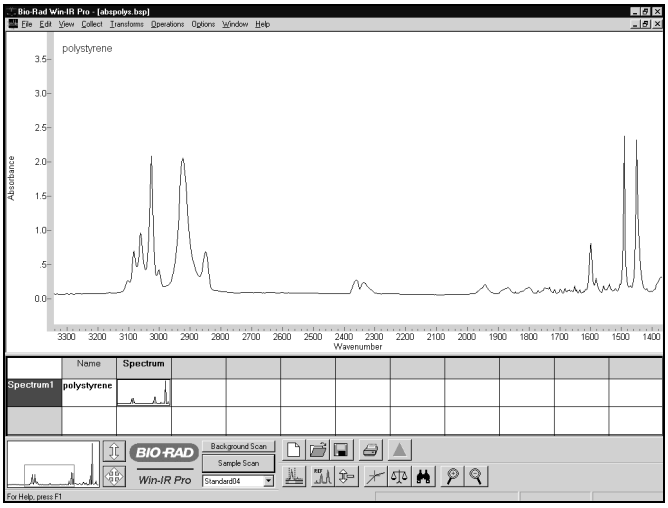
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SHOW PEAKS

Peaks can be picked and labeled, either with the right mouse button menu or Operations / Peak Pick. If this is done, the View / Show Peaks entry has a √ mark to the left of it, indicating that peak labels are shown. If you select the View / √ Show Peaks entry, the peak labels will no longer be displayed, and the √ mark will also disappear. Select this entry again, to make the peak labels, annotations, and the √ mark reappear.



√ Show Peaks

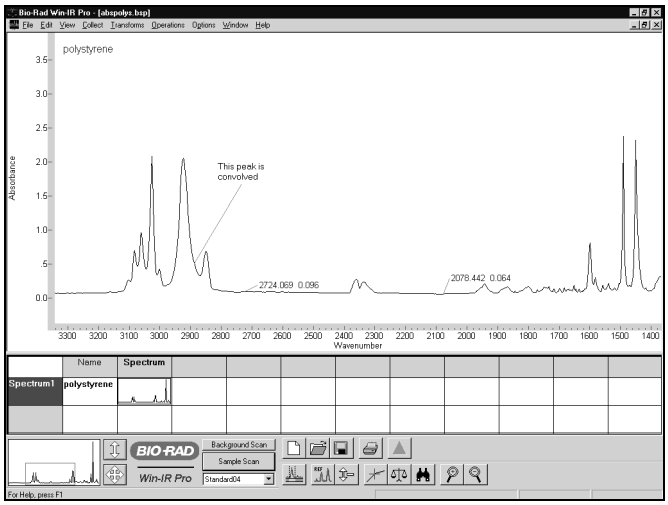


Show Peaks

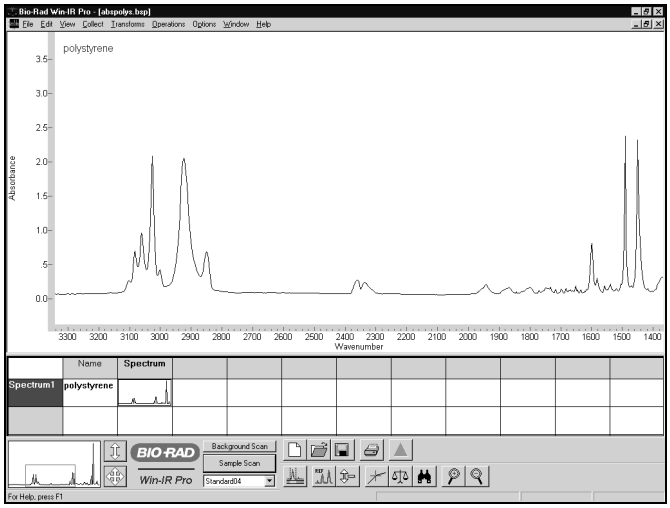
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SHOW LABELS

If position labels or annotations are added to the spectrum display, then View / Show Labels entry has a √ mark to the left of it, indicating that these labels and annotations are shown. If you select the View / √ Show Labels entry, the labels and annotations will no longer be displayed, and the √ mark will also disappear. Select this entry again, to make the labels, annotations, and the √ mark reappear.



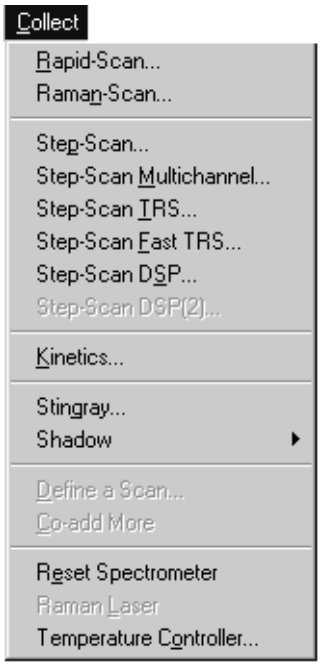
√ Show Labels



Show Labels

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9
Collect Menu



The commands in this menu allow you to set up your spectrometer and to collect backgrounds and data. The specific entry to be chosen and the parameters to be set for collection depend upon what Bio-Rad spectrometer you are using and the specific

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software installed for data collection. The details of data collection are covered in the spectrometer manual that you received with your system.

Notes

If you have the "workstation version" of the software, then the entire Collect menu may be disabled (grayed-out).

The step-scan choices will be absent if your spectrometer does not support step-scan.

If you have a document open, and if it is a compatible document type, scan puts the newly collected spectrum into that document, adding it to the existing spectra.

If no document is open, scan opens a new document for you.

Below is a brief description of the types of scanning. For details, see the documentation that was shipped with your spectrometer.

RAPID SCAN...

Used to collect data for samples that do not vary with time.

RAMAN SCAN...

Used to collect a Raman spectrum. This is disabled unless the Raman software has been installed.

STEP-SCAN...

Used to collect data from samples which are changed cyclically with time, or where the entire spectrum must be modulated at the same frequency. These include photoacoustic and multiple modulation experiments.

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STEP-SCAN MULTI-CHANNEL...

Used to collect data from more than one input source (channel) during one scan. These channels can be inputs from different detectors, or from one detector, processed in several different ways. At each retardation position, the spectrometer polls the inputs and sends the signals to the data processing hardware and software. A common use of multi-channel spectroscopy is the simultaneous acquisition of both in-phase and quadrature signals in phase-modulated step-scanning experiments

STEP-SCAN TRS...

Time-resolved spectroscopy (TRS) is the study of fast repetitive events by FT-IR, using a variety of techniques to alter the sample, typically photolysis or some other dynamic change. Typically, sets of data are collected at each retardation step. This creates a two-dimensional array of data. Interferograms can be constructed “across” the spectra for constant time delays within each step. These interferograms are transformed to yield time-resolved spectra.

STEP-SCAN FAST TRS

Rapid TRS allows collection at much higher speeds (time resolution). This requires additional optional electronics to be installed in the PC. Conceptually, it is the same as step-scan TRS.

STEP-SCAN DSP...

During step scan the spectrometer is not in a continuous scan, but quickly steps to a requested point, collects data at that point, and steps to the next point. The signal of interest during Step Scan DSP arises from the cyclical change in optical retardation. This change and the signal arising from it is called phase modulation. Step Scan DSP is used to recover (demodlate) the signal of interest from the side bands around the phase modulation frequency. In Win-IR Pro, Step Scan DSP is implemented primarily for photoacoustic spectroscopic depth profiling. For details, see your spectrometer manual.

STEP-SCAN DSP(2)...

Used in experiments where, in addition to phase modulation, there is also a low-frequency modulation of the sample. One example of this is polymer stretching where it is desired to have spectra for different amounts of stretching.

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KINETICS...

Used to collect data from samples that vary with time, but not in a cyclical manner. Examples are curing, polymerization, drying, etc.

STINGRAY...

Used to collect data with an array detector. This generates image (.dat) files.

SHADOW...

Used to collect data with microscope mapping; this is an optional product. See the *Shadow Pro User's Manual* (091-0991) for details.

DEFINE A SCAN...

Defines a method for collecting a spectrum (and manipulating it) in exactly the same manner as a previously collected (and manipulated) spectrum. All collection parameters, the background spectrum, and manipulation parameters are the same.

Note

When this entry is selected, the method is defined. However, there is no system response nor message generated to the user. No data collection is done. Collection is done by one of the selections above.

CO-ADD MORE

Allows you to continue to collect more data and to add it to the existing spectrum. This is often used when initial investigation of the spectrum reveals insufficent statistics or signal-to-nose ratio in the intially collected spectrum.

RESET SPECTROMETER

Resets the spectrometer. The specific actions that occur depend upon which spectrometer it is. See your spectrometer manual for details of Reset.

RAMAN LASER

Allows you to turn the Raman laser on, set a power level, and/or turn the laser off.

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TEMPERATURE CONTROLLER

Allows you to set the temperature for GC-IR (gas chromatography-infrared) experiments. You can monitor the gas cell and transfer line temperatures any selected interval between 1 and 10 seconds. This interface also allows selection of the communications port to be used between the PC and the temperature controller.

Note

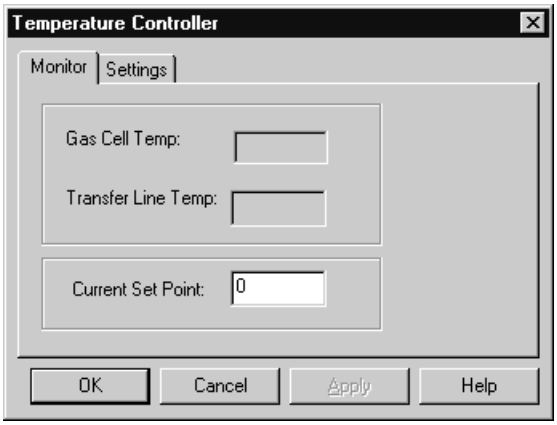
If there is no temperature controller, or if the communications line is not properly configured, you will get this error message.



You can still access the Temperature Controller dialog box, but you cannot exchange information unless a properly configured controller is connected.

The Temperature Controller dialog box has two tab pages—Monitor and Settings.

Monitor

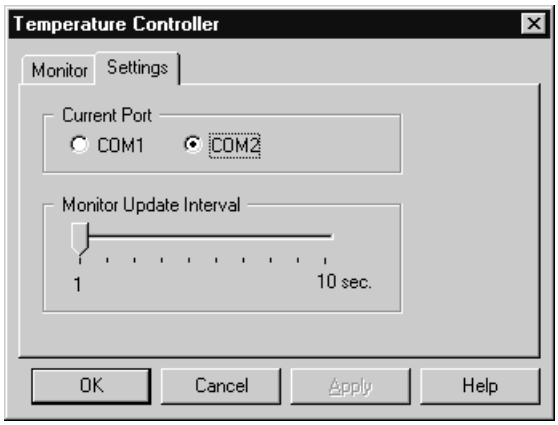


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Gas Cell Temp: the temperature in the gas cell.
Transfer Line Temp.: the temperature in the transfer line.

Current Set Point: enter the desired equilibrium temperature.

Settings:



Current Port: select the communications port used.

Monitor Update Interval: how often should the temperature controller send the gas cell and transfer line temperature measurements to the PC where they can be displayed on the Monitor page.

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10
Transforms Menu



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GENERAL CONSIDERATIONS

If you have selected a number of spectra, and then select a transform (for example, Transmittance), then that transformation will be applied to all the selected spectra.

We recommend that you maximize the document window to fill the space available when working with these transforms. Use the ❐ toolbar maximize button or double-click in the document window. When you get one of the transform displays, the spreadsheet is minimized and is not visible, so you do not need to select Maximize Traces or press the F11 key.

1. In some transforms the sidebar control panel on the right hand side takes up most of the length of the screen. Maximizing the document window makes for a full, legible display.

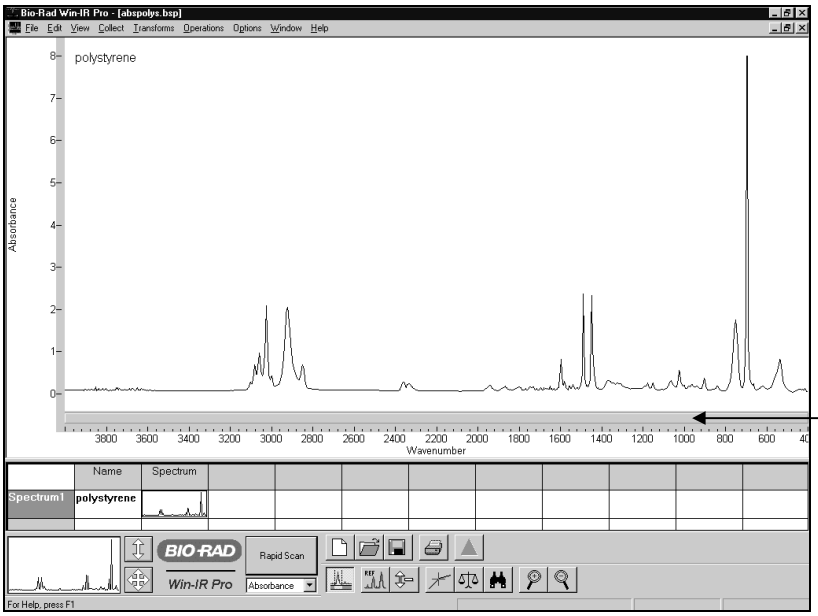
2. In some transforms (such as Baseline Correct) you interact with the trace. The larger it is, the easier it is to manipulate it.

To maximize traces, either select Maximize Traces from the Window menu or press the F11 key.

To define a region of the spectrum (this is only required for a few of the transforms)

1. Select Drag Regions from the Operations menu. A check mark (√) appears in front of Drag Regions if it is selected. Alternatively, press the  toggle button at the bottom of the screen. Region selection is now enabled. A blank rectangle (the ruler) appears at the bottom of the trace display, just above the X-axis scale.

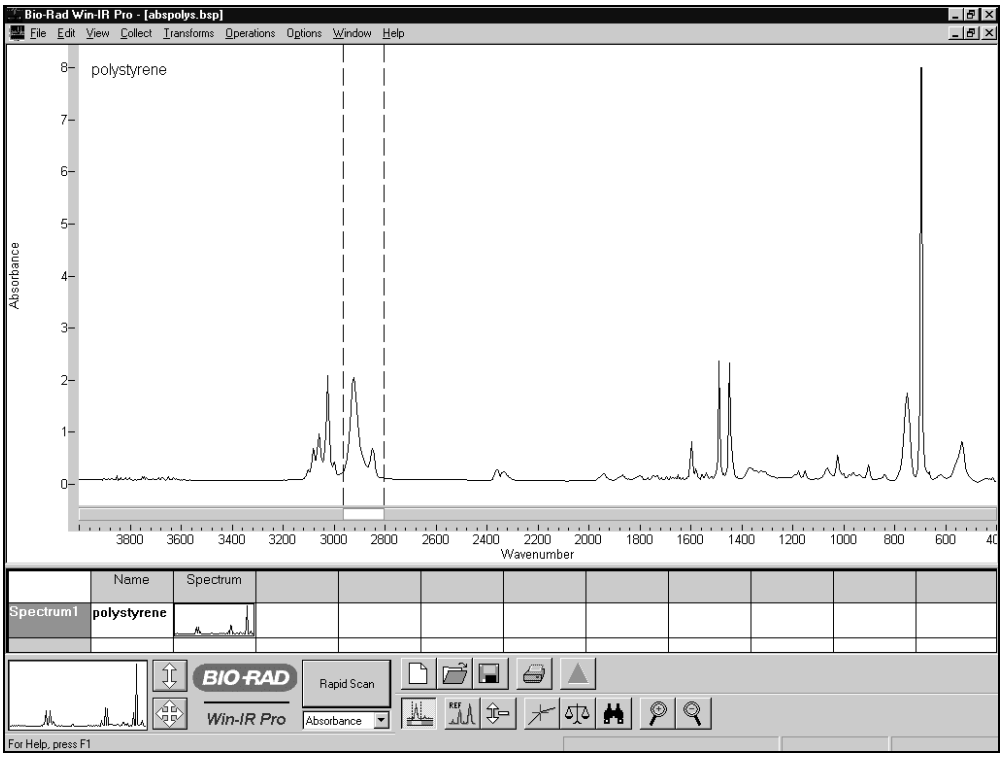
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2. Put the cursor into the ruler at one end of the region to be selected. The cursor changes to .

3. Hold down the left mouse button and drag the cursor to the other end of the region being defined. Release the button. The region is defined by the vertical dashed lines. The white bar at the bottom of the region means that this region is active and selected.

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4. Repeat this procedure to define additional regions, if desired.

For more details, see Drag Regions in Chapter 11.

ABSORBANCE

Absorbance spectra can be converted from %Transmittance spectra by selecting Absorbance from the Transforms menu.

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%TRANSMITTANCE

Transmittance is an alternative way of viewing the spectrum. Absorbance spectra can be converted to %Transmittance spectra by selecting %Transmittance from the Transforms menu.

Notes

The two traces are related by this formula:

$$\text{Absorbance} = \log \frac{100}{\%\text{Transmittance}} = -\log \text{Transmittance}$$

If the spectrum is an absorbance spectrum, then Absorbance is disabled (greyed-out); if the spectrum is a % transmittance spectrum, then %Transmittance is disabled (grayed-out).

$$\%\text{Transmittance} = \frac{\text{Sample file}}{\text{Background file}} \times 100$$

%Transmittance ranges from 100 (total transmittance) to 0 (no transmittance).

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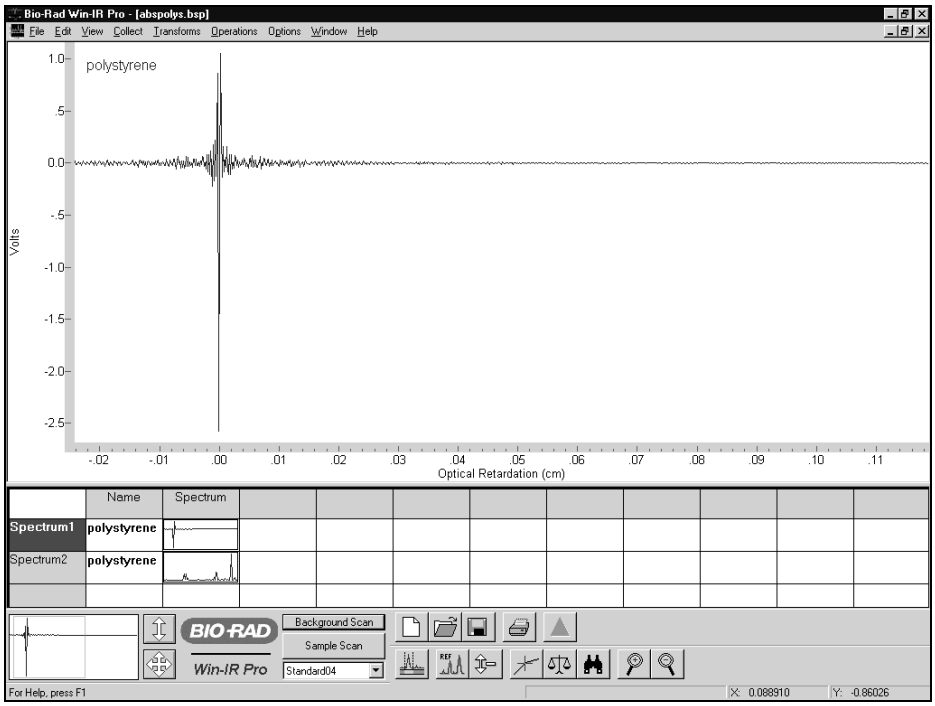
COMPUTE

Computes a single beam spectrum from an interferogram, performing a series of functions including a Fourier transform, apodization, and phase correction. Once a single-beam spectrum is computed, you can ratio it against a background spectrum to obtain a number of different types of spectra (see **Ratio**, later in this chapter for details)

Note

When the single-beam computation is performed, it replaces the interferogram in the display. However, the interferogram is saved in the document and may be recalled by using Reprocess... from the Operations menu.

For example consider the interferogram collected for a polystyrene sample.

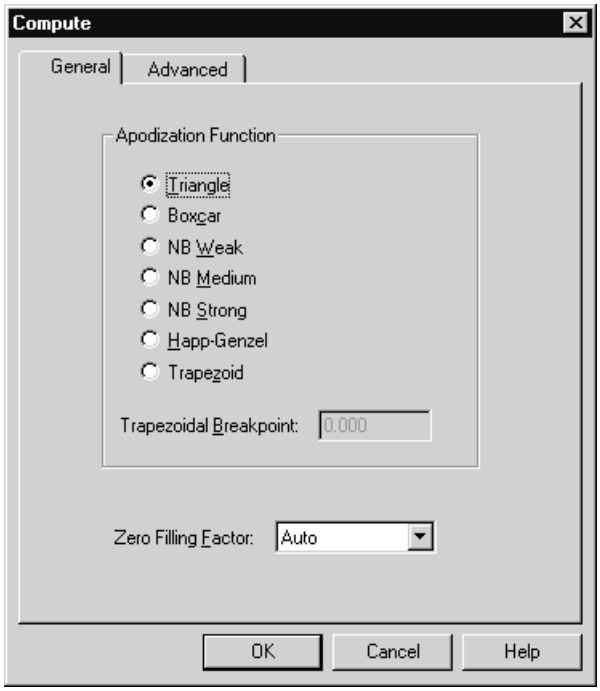


Select Compute; the Compute dialog box appears.

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General Page

Selecting the Compute operation normally displays the General page of the Compute dialog box:



If the Compute Advanced page is displayed, press the General tab to return to the General page.

Apodization Function: In data collection, the interferogram is sampled over a finite distance. Information that would be present at a larger distance (greater retardation) from the centerburst is lost. This causes a distortion in the shape of narrow lines because the information for these lines was truncated at the limit of resolution. This is usually only noticeable for gas spectra.

The band shape distortion shows up as negative side lobes at the base of an absorption peak in the transformed spectrum. These lobes are more pronounced for peaks with a half bandwidth close to the resolution used in collecting the spectrum.

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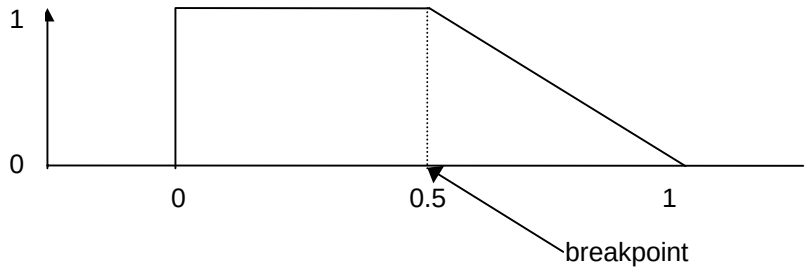
Apodization is a method to control the line shapes; it does cause some decrease in resolution. When comparing or ratioing spectra, the same apodization must be used.

Select the type of apodization function to apply to the interferogram. Details are given in the Algorithms and Functions appendix. The choices are:

Boxcar
Triangle
Happ-Genzel (also called Hamming)
Trapezoid
NB Weak (Norton-Beer weak)
NBMedium (Norton-Beer medium)
NBStrong (Norton-Beer strong)

For normal analytical spectroscopy, NBMedium is the recommended apodization.

Trapezoidal Breakpoint: enter breakpoint if Trapezoid apodization is selected. Trapezoid is a generalized form of the Boxcar + Triangle apodizations; its breakpoint is illustrated in the following figure:



If the breakpoint = 0, the function is triangular; if the breakpoint =1, it is a boxcar.

Zero Filling Factor: causes the interferogram to be extended with zeros before computing. It has the effect of interpolating points in the spectrum. Auto is the recommended operating setting (see below for details).

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Compute requires 2^k points in a data array, where k is an integer, to compute the single-beam from the input interferogram. If necessary, the input data array is extended with zeros.

N_t the total number of points in the interferogram
N_b the basis number of points in the interferogram; that is, the points in the centerburst and those after it.
zff is the zero filling factor.

1. If the basis number is not a power of 2, then a value N_d is calculated where

   $N_d = zff * 2^k - N_b$ (2^k is the next power of 2 above N_b).

2. The number of points in the data array is then extended with zeros, so that there are zff * 2^k data points in it. That is, we add

   zff * 2^k - N_t = N_d + N_b - Nt zeros to the data array.

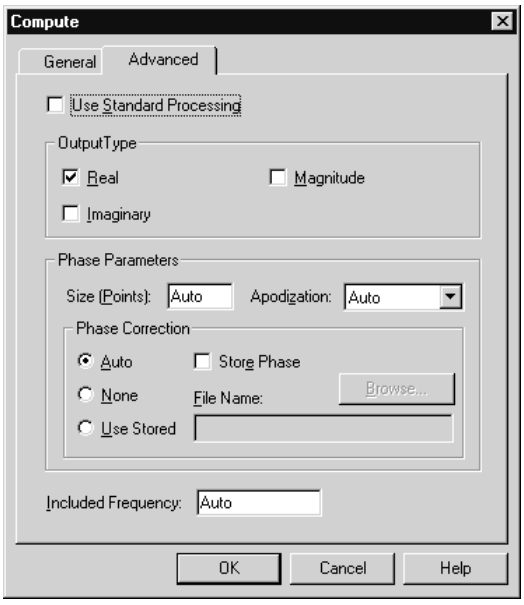
3. If this number is negative, a message is displayed, requesting that you increase the zero filling factor (zff)

The effective numerical values for zff are 1, 2, 4, 8, . . . 2^k; other values will be rounded up to one of these, but the software will not report this to you. In cases where the basis number of points is close to a power of 2, small changes in data can result in large changes to the final output. For example, if basis number of points=2047, zff =2 gives 4096 points, while for basis number of points=2049, zff =2 gives 8192 points. For most purposes, set zff to Auto., which uses 0.8 * N_b instead of N_b as the basis for the calculation, and computes a zff =2 value from that number. This means one data point is interpolated between each actually collected sata point. For example, for a 2 cm^{-1} spectrum, there will be a data point displayed at each 1 cm^{-1} spacing.

Advanced Page

Press the Advanced tab to display the Compute Advanced page:

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Use Standard Processing: if checked, all parameters are set to the default values and cannot be changed. To change one or more parameters, de-select Use Standard Processing.

Output Type: select one or more types of desired output spectra. Each selection is saved as a separate spectrum in the document. The Fourier Transform produces a complex result, which has a real and an imaginary part.

Real: if checked, generates and saves the real part of the computed spectrum. This is the default output type.

Imaginary: if checked, generates and saves the imaginary part of the computed spectrum.

Magnitude: if checked, generates the magnitude spectrum, which is sometimes used in multiple modulation experiments.

$$\text{Magnitude spectrum} = \sqrt{(\text{real spectrum})^2 + (\text{imaginary spectrum})^2}$$

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To obtain a phase spectrum, use Operations - Spectral Arithmetic - Binary after collecting the data.

Phase Parameters: the software automatically corrects for any small phase shifts in the interferogram, introduced by the spectrometer, by calculating the Fourier transform of a small portion of the interferogram around the centerburst. This produces a very low resolution spectrum that represents the instrument phase. Then, this small spectrum is used to correct the phase of the spectrum. See Appendix D for more information on phase correction.

Size (Points): enter the total number of points around the centerburst that are used to calculate the phase correction. Auto, which is the recommended value, calculates the number of points to be used as follows (the total number of points is limited to 512, i.e., 2^9):

Symmetric interferogram: takes 10% of the specified number of points after the interferogram centerburst and rounds this number up to the next power of 2. For example, for an symmetric interferogram with 2048 points on either side of the centerburst, 204.8 of those points (10%) are selected and rounded *up* to the next power of 2, which is 256.

Asymmetric interferogram: takes the specified number of points before the interferogram centerburst; uses the greatest power of 2 that is rounded down from that number. For example, for an asymmetric interferogram with 550 points before and 2048 points after the centerburst, 550 points before the interferogram are selected and rounded *down* to 512.

Apodization: select the apodization function used in calculating the phase correction. Auto means to use the same apodization function as selected in the Processing Parameters - Apodization Function.

Phase Correction: select the type of phase correction to be used.

Auto: use standard phase correction, which extracts data symmetrically around the interferogram peak and computes a phase correction array. This is the recommended value.

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Store Phase: if checked, generate an Auto phase correction and store the phase correction array in the file specified by Filename below. This file will have a .phs extension and can be opened with File Open.

None: do not perform any phase correction. This might be used if you plan to calculate a power spectrum.

Use Stored: do not compute a phase correction array. Instead, read the phase correction data from the file specified by Filename below. This might be used if you collect data that does not have a centerburst, such as in double modulation experiments.

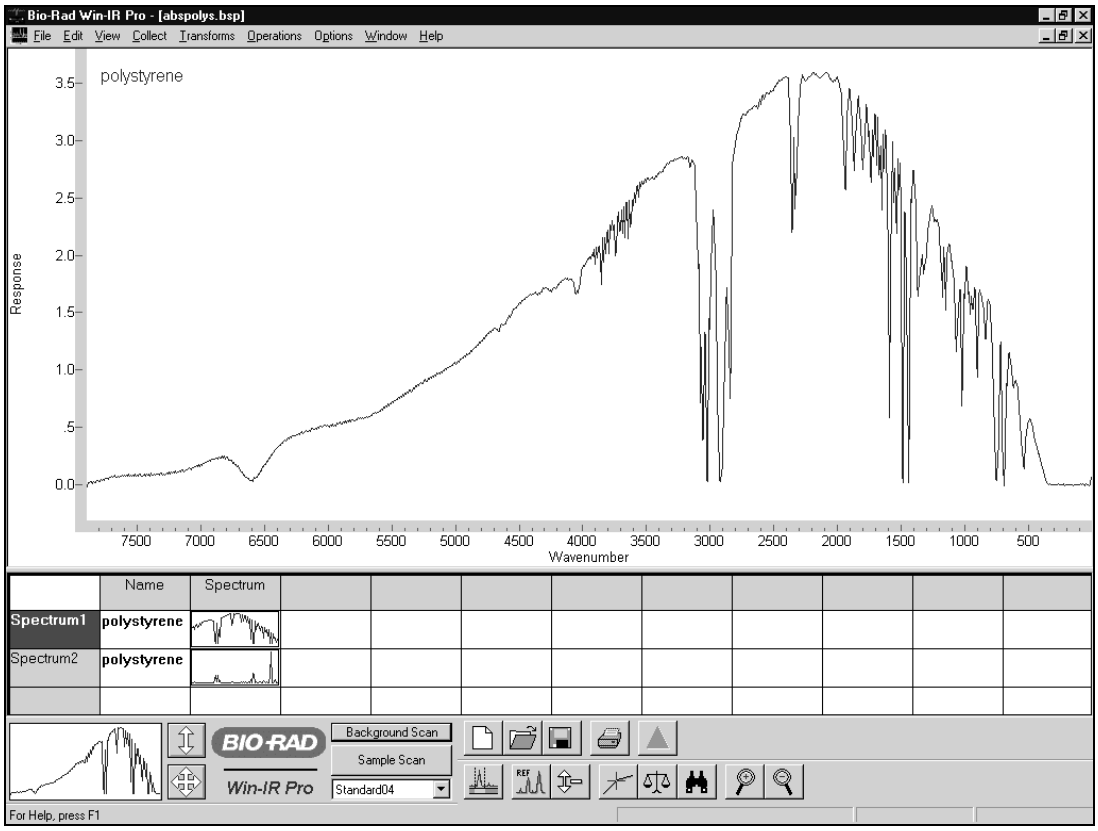
Filename: the name of either the file into which the phase correction data is to be stored (Store Phase), or the file from which the phase correction data will be read (Use Stored).

Browse: this button is enabled if the cursor is clicked in the Filename box. When Browse is pressed, the standard Windows NT file selection dialog box appears. Use this to select the appropriate file, either on a local or a network drive.

Included Frequency: when undersampling is used, the frequency bandwidth is decreased (frequency aliasing). In some cases this may cause the spectral region of interest to lie outside the base band (starting at 0). If a number is entered here, the software sets the lower limit of the bandwidth so that the desired frequency is included in the bandwidth. Auto selects the base band.

For example, a UDR of 1 gives a free-scanning spectral range of 15,800 cm^{-1} and is normally used for the 0-15,800 cm^{-1} region. With appropriate equipment (source, beamsplitter, filter, detector, etc.), however, it could be used for the 15,800-31,600 cm^{-1} region. In this case, Included Frequency would be set to a value such as 20,000 cm^{-1}, so that the software calculates the x-axis correctly.

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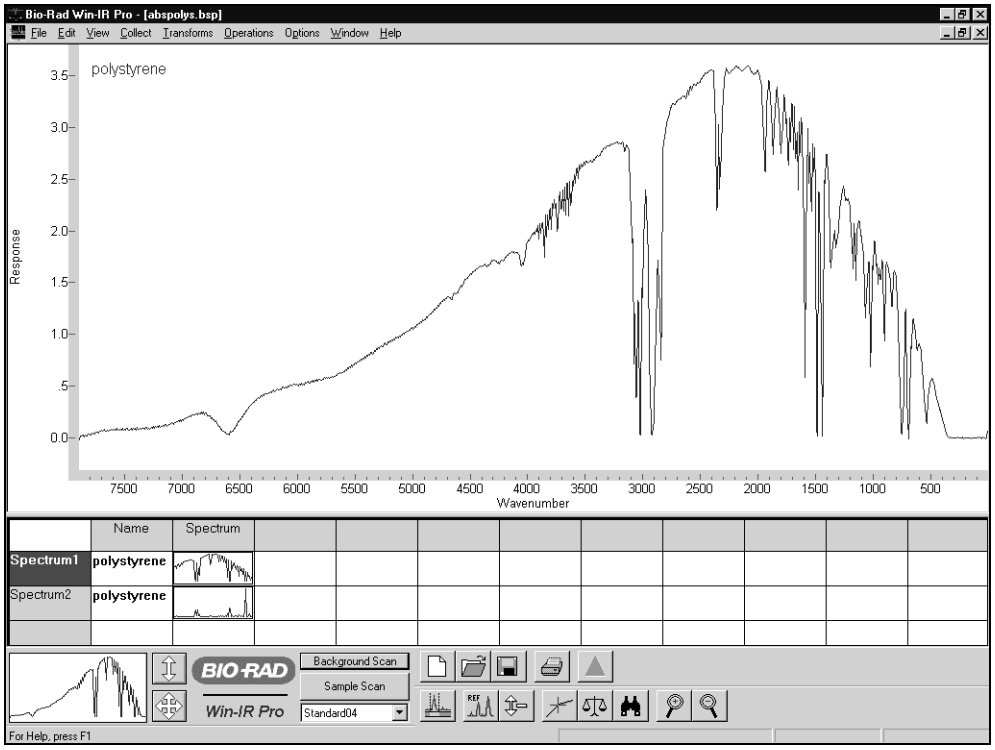
RATIO

Calculates the ratio of two single beam spectra–usually the ratio of a sample spectrum to a background spectrum.

Note

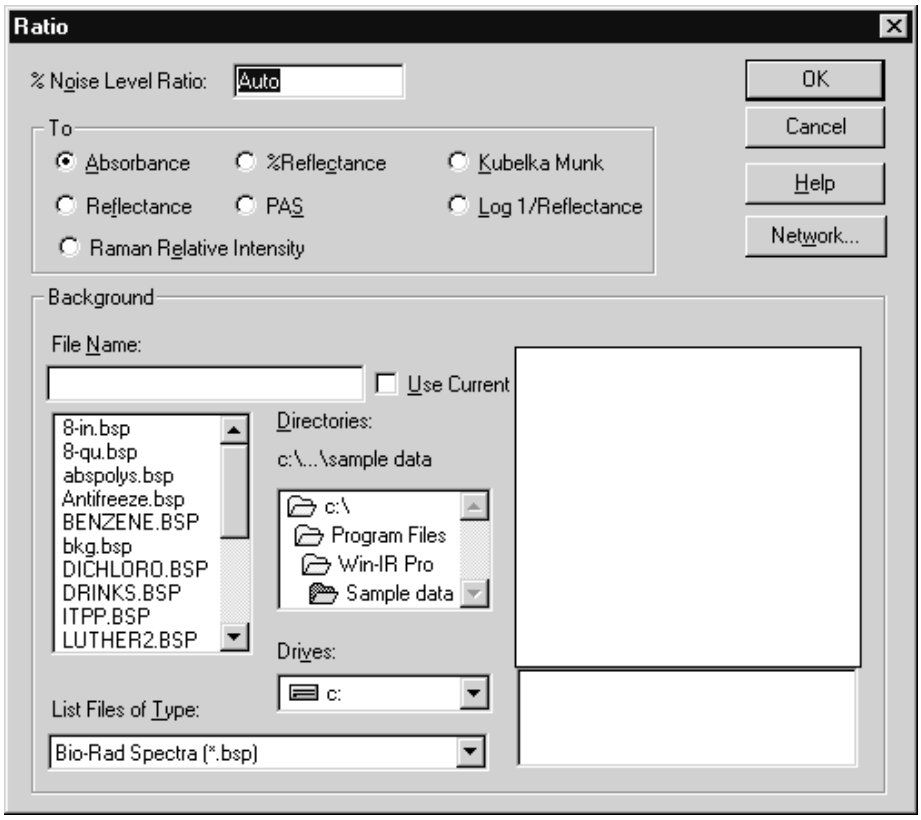
When the ratioed spectrum is computed, it replaces the single-beam spectrum in the display. However, the interferogram is saved in the document and the single-beam spectrum may be recalculated by using Reprocess... from the Operations menu..

Consider, for example, the single-beam spectrum below.



When selected the Ratio dialog box appears.

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% Noise Level Ratio: in cases where the background spectrum values are zero, or close to zero, the result of performing a ratio may have little meaning. To prevent this, background reference spectrum points whose values are less than the specified value are not used in the calculation. The most recently calculated value, or 0, is output instead. The level is specified as a percentage of the maximum height of the background spectrum. If the default Auto is chosen, the % Noise Level Ratio is taken to be 5%.

To: select the type of spectrum to be calculated; the choices are:

Absorbance: this is the default spectrum calculation. It is equal to

$\log_{10}$ (reference/sample)

Reflectance: this calculation is only meaningful if you are performing a reflectance experiment.

R = (sample spectrum/reference spectrum)

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% Reflectance: (expressed as a percentage)

$100*R$

PAS (Photoacoustic spectrum): the calculations are equivalent to the transmittance function, but the spectrum resembles an absorbance spectrum, in that the peaks point upwards.

Kubelka Munk: calculated from a reflectance spectrum used in diffuse reflectance spectroscopy. If R is the reflectance, then the Kubelka-Munk function is

$(1.0-R)^2/2R$

Log 1/Reflectance

$\log_{10}(1/R)$

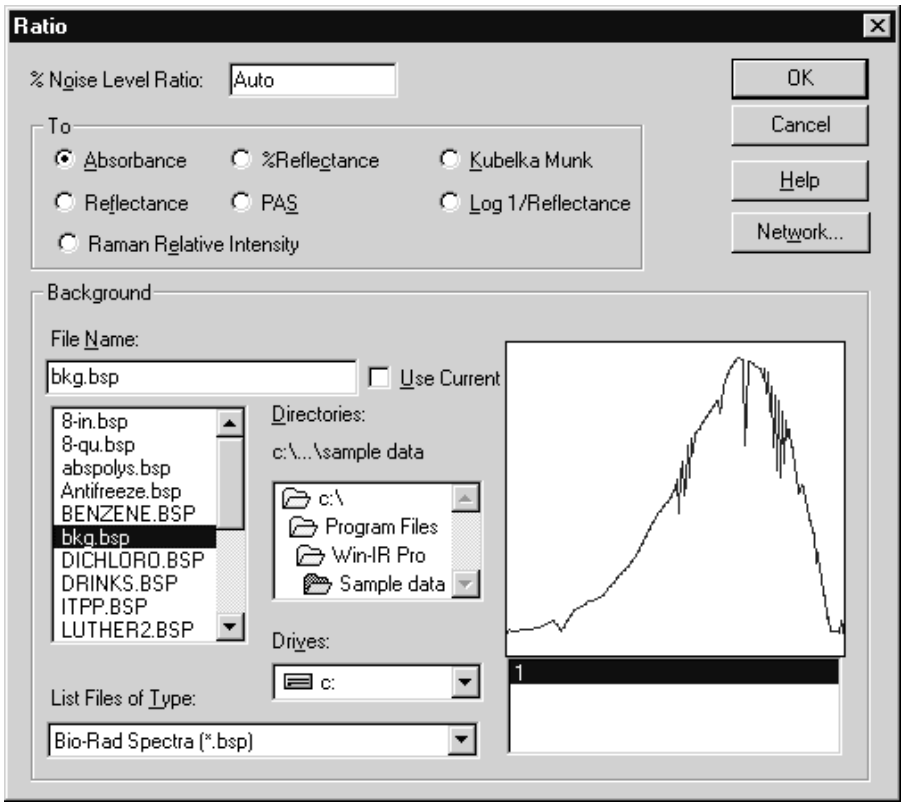
Raman Relative Intensity: calculates by ratioing against the instrument response. The x-axis is Raman shifted relative to the excitation wavenumber.

Note

Transmittance is not shown because it is considered to be a change in the display of Absorbance rather than a transformation of the spectrum.

Background: use the standard Windows selection technique to pick the background reference file (spectrum). This file may be located on another disk. If that disk is not yet connected to your computer, use the Network key to connect it to your computer. When selected, the background file is shown in the preview window.

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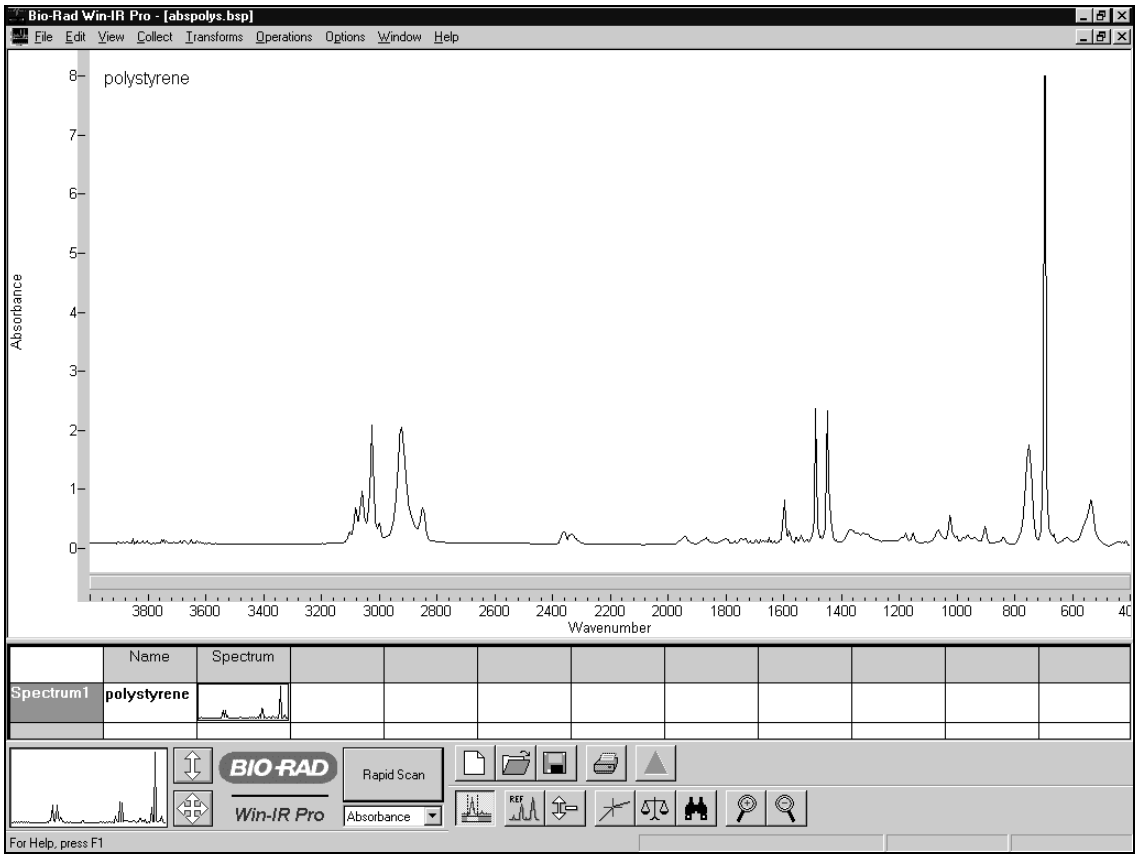
Note

If the document contains multiple spectra, you can scroll through them to find the background you want.

Current: if selected, this allows you to use a spectrum in the currently selected document.

OK: calculate the ratio and compute the spectrum type selected above. Replace the single beam spectrum with this newly calculated ratio.

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Cancel: return to the main menu without calculating a ratio or replacing the single beam spectrum.

Help: enter the on-line help system.

Network: allows you to connect a remote disk on the network to your computer in order to access a background spectrum.

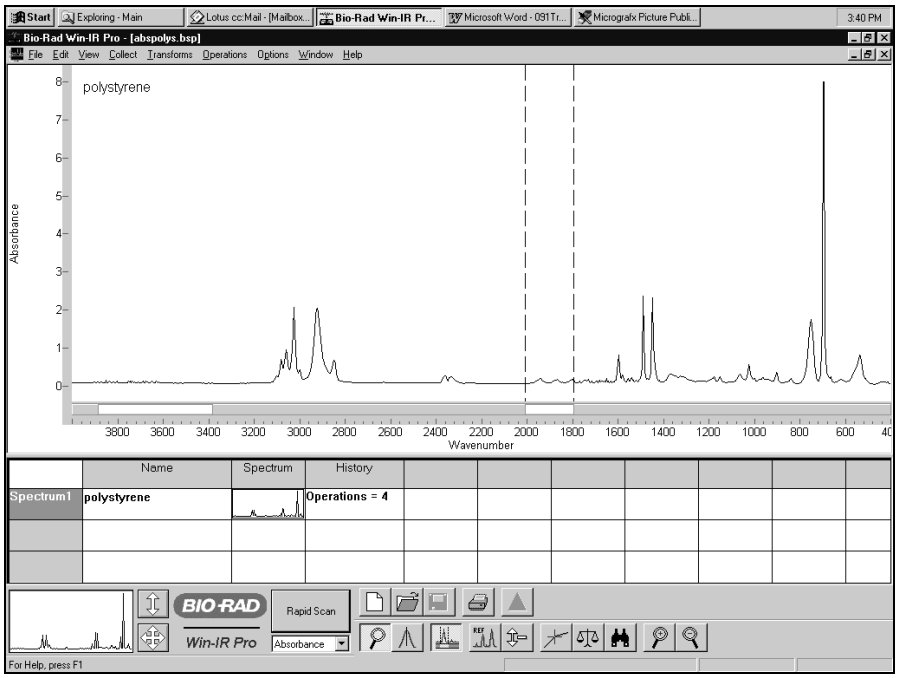
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ZAP

Interpolates a straight line within a selected region (or regions) of the spectrum ("zaps" a spectrum). Zap can be used for a number of reasons including:

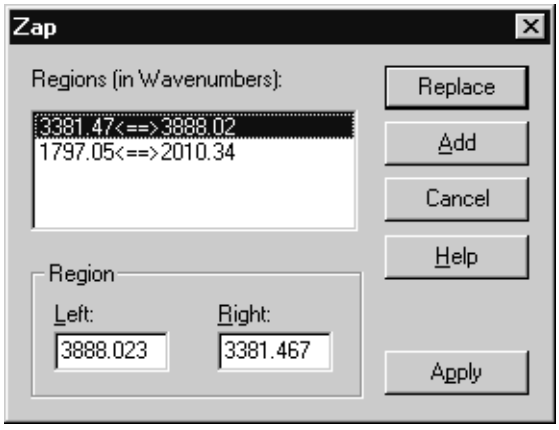
- remove spikes in the interferogram from thin films that produce fringing,
- eliminate bands where the background or reference spectrum is totally absorbing because of detector cutoff or bands in the reference spectrum,
- "remove" strong, interfering bands during spectral subtraction and spectral search,
- "remove" carbon dioxide and water vapor bands from a spectrum.

First, select Drag Regions from the Operations menu (or press the  button). Define the region(s) to be zapped.



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Select Zap from the Transforms menu; the Zap dialog box appears.



Regions (in Wavenumbers): displays the region(s) of the spectrum that will be zapped.

Region: If you want to alter a region to be zapped, highlight that region in the Regions (in Wavenumbers) window by clicking on the corresponding line of text; then, type in the edge values for Left and Right.

Left: left edge of the region to be zapped.

Right: right edge of the region to be zapped.

Then, click the Apply button. The highlighted values will changed to those just entered.

Note

Although you can alter the edge values after the region(s) been defined interactively, you cannot invoke Zap unless a region has been defined. Entering new values in Left and Right does not change the display in the upper window. If you click on the text line in the upper window, the original values are restored.

Replace: replace the existing spectrum with the transformed spectrum.

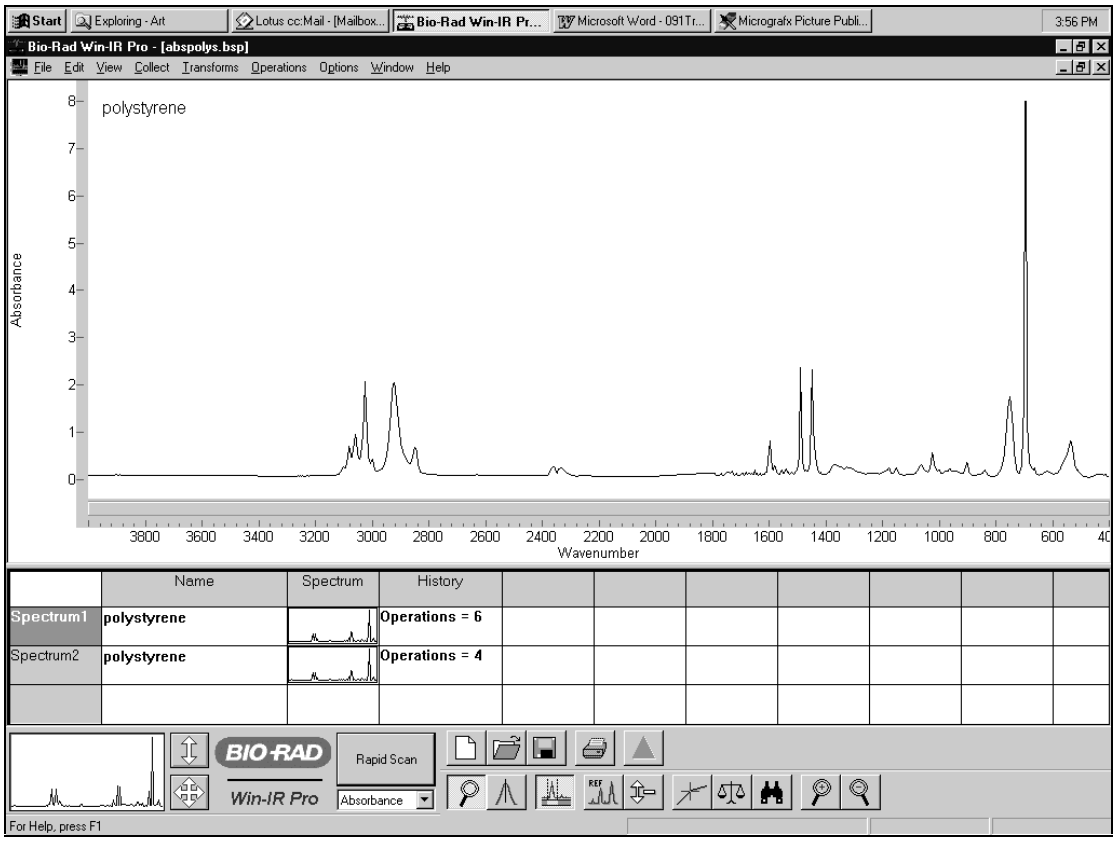
Add: add the transformed spectrum to the document that contains the original spectrum.

Cancel: return to the main menu display without acting upon the original spectrum.

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Help: enter the on-line Help system.

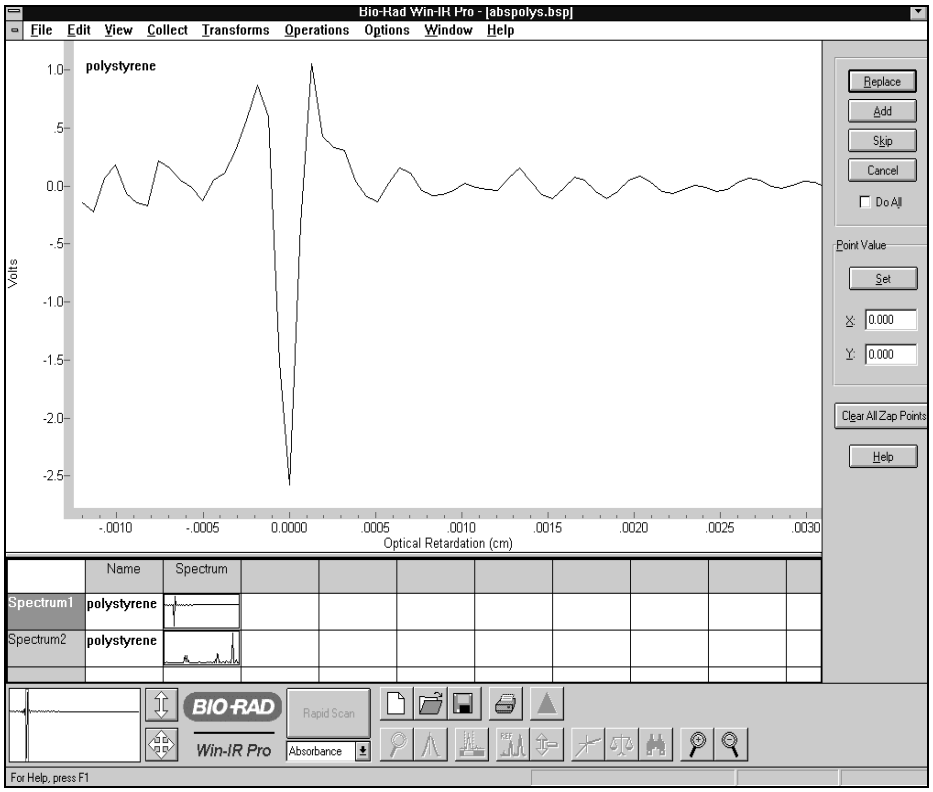
The result is shown below (in this example the transformed spectrum was added to the document).



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ULTRAZAP

Allows the change of individual data points in the spectrum or interferogram. It is typically used in interferograms to remove spikes caused by fringing in a sample or to add spikes for reference in emission or modulation experiments lacking a centerburst. Before selecting UltraZap, use the spreadsheet to select those traces that you want to manipulate. When UltraZap is selected, a control panel appears on the right side of this display. The name of the trace is displayed in the upper left of the screen; if you have selected a number of traces, this identifies which one you are working on.



We have usd the zoom function to expand the portion of the interferogram to be manipulated.

Move the cursor to the data point to be changed. When the cursor is on the trace, it changes to . Hold down the left mouse button. The cursor changes to . Move the

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cursor up or down to drag the data point to its desired new location. Any number of data points can be moved as often as desired.

Point Value: change a point in the spectrum by entering its new coordinates.

X: enter the horizontal-axis coordinate of the new point.

Y: enter the vertical-axis coordinate of the new point.

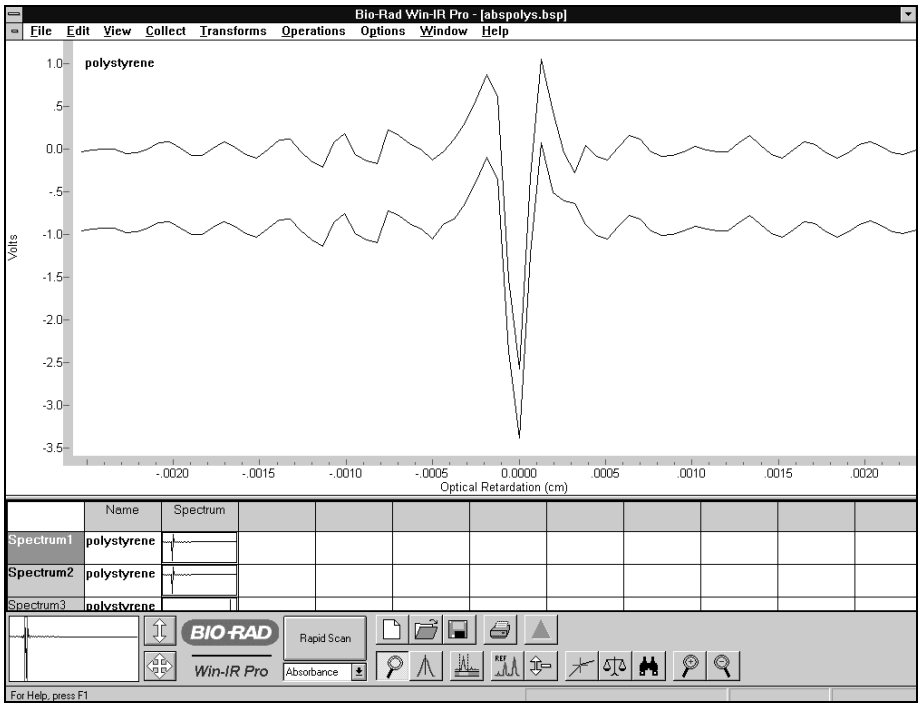
Set button: click the button to change the selected point in the spectrum and display it in the trace.

Clear All Zap Points: return all altered points to their original values.

Replace: replace the existing original spectrum with the altered spectrum. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Add: add the altered spectrum to the document that contains the original spectrum. Both spectra are now in the main menu display. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

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Note

The interferograms are zoomed to show the region of interest.

Skip: Do not alter the current spectrum. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Cancel: return to the main menu display without acting upon the current spectrum or any subsequent spectra. Spectra previously replaced or added are not altered by this.

Do All: if selected, then the UltraZap parameters selected for this spectrum are applied to this spectrum and to all subsequent spectra; they are all either Replaced or Added. Spectra previously replaced or added are not altered by this.

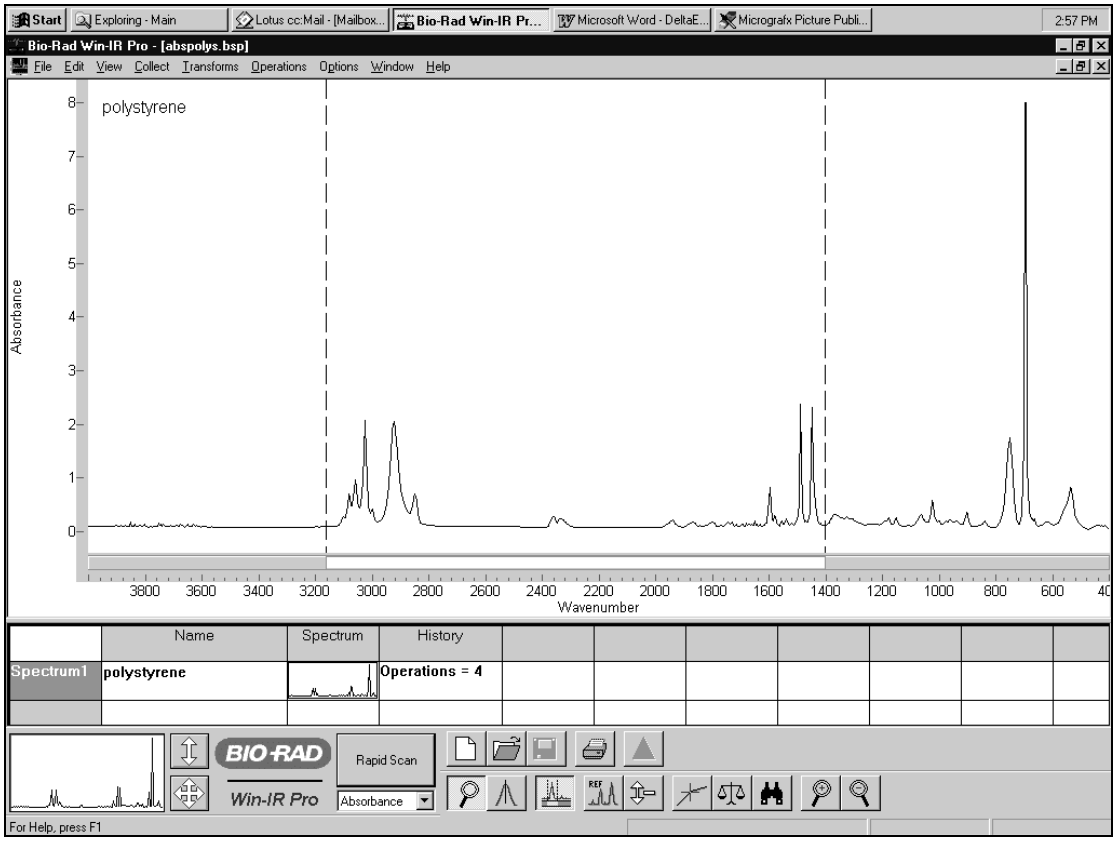
Help: enter the on-line Help system.

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TRUNCATE

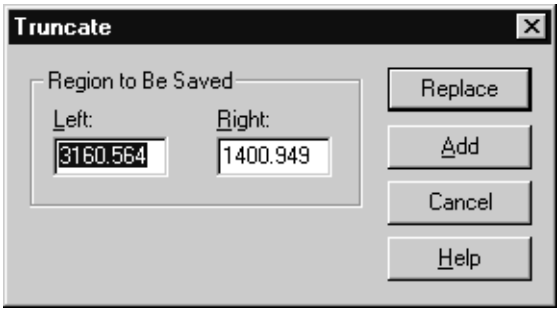
Truncation is generally used to eliminate noisy edges of a spectrum, containing little or no useful spectral information.

First, select Drag Regions from the Operations menu (or press the  button). Define the region to be retained, not the region to be discarded.



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Select Truncate from the Transforms menu; the Truncate dialog box appears



Region to Be Saved: defines the region of the spectrum that will be retained. If you want to redefine or refine the region to be retained, type in the edge values for Left and Right.

Left: left edge of the region to be retained.

Right: right edge of the region to be retained.

Note

Although you can alter the edge values after the region been defined interactively, you cannot invoke Truncate unless this region has been defined.

Replace: replace the existing spectrum with the truncated spectrum.

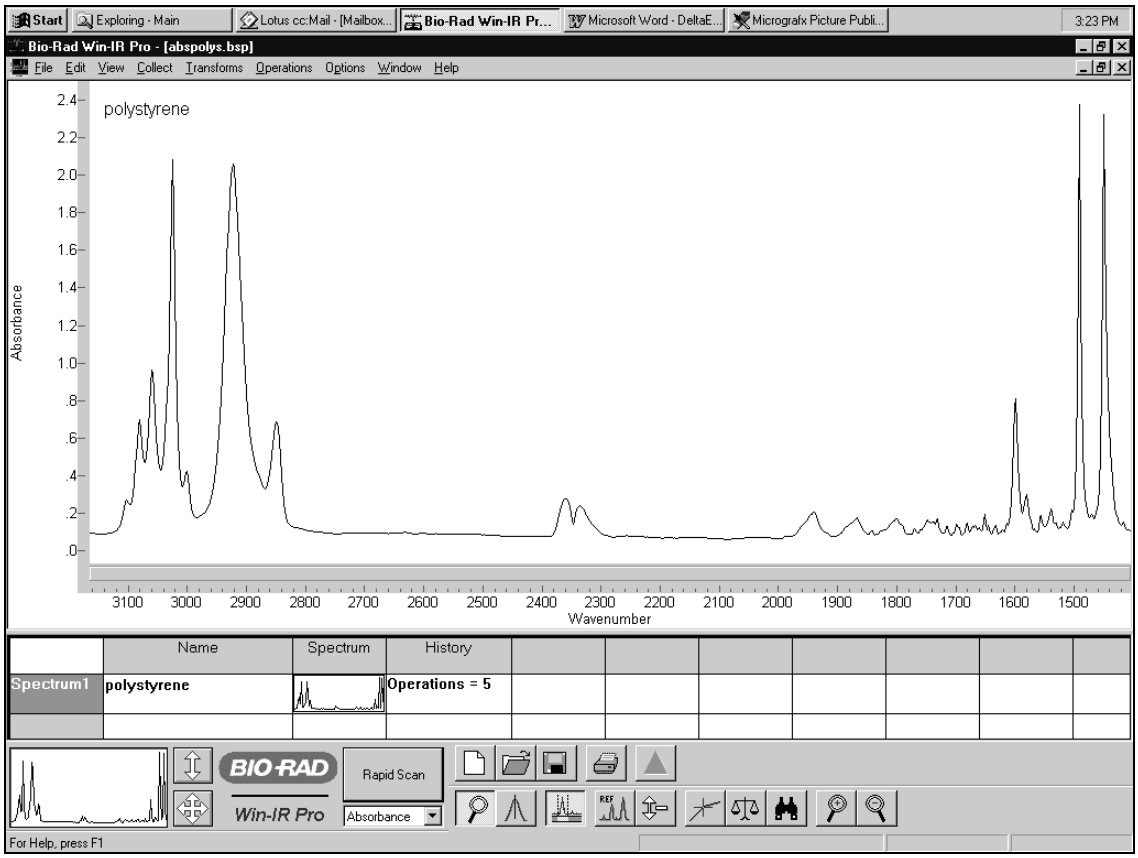
Add: add the truncated spectrum to the document that contains the original spectrum.

Cancel: return to the main menu display without acting upon the original spectrum.

Help: enter the on-line Help system.

The result is (in this example, Replace was used):

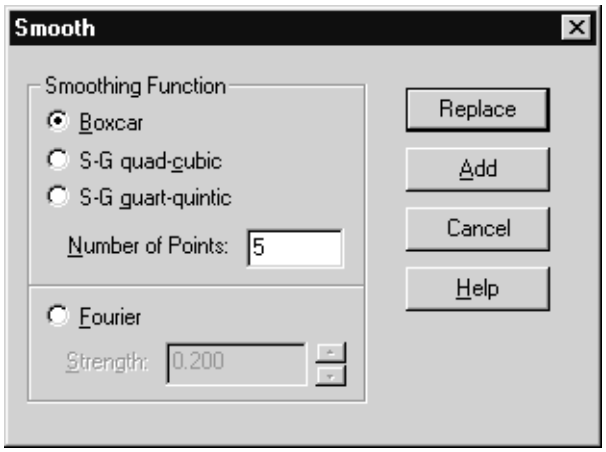
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SMOOTH

Smoothes the current trace. Spectral smoothing is used to reduce high-frequency noise and improve the signal-to-noise ratio. There is some decrease in resolution accompanying this process. The different smoothing functions allow some tradeoffs between noise reduction and resolution; the optimum choice depends upon the details of the spectrum itself. The Smooth dialog box appears.



Smoothing Function: select among Boxcar, SG (Savitsky-Golay), and Fourier smoothing functions.

Boxcar Smoothing

Boxcar: uses the boxcar function; this function is equal to 1 for Number of points about the point being smoothed and 0 elsewhere. It is a moving average. Boxcar smoothing gives equal weight to all points within the convolution region defined by Number of points. Boxcar smoothing has the greatest smoothing and, consequently, the greatest loss of resolution.

Savitsky-Golay Smoothing

Savitsky-Golay smoothing is a convolution method using a least squares fit of a polynomial to a moving convolution region of data points[1]. It then calculates a new central value in the region based upon the polynomial. Smoothing is controlled by the degree of the polynomial and the number of smoothing points parameters.

[1] Abraham Savitsky and Marcel J. E. Golay, *Analytical Chemistry*, **36**, 1627-1639, 1964.

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Note

The nature of the convolution gives the identical fit for quadratic and cubic, as well as for quartic and quintic polynomials.

S-G quad-cubic: requires a minimum of 5 points. Retains more resolution, but does not smooth the data as much as the quart-quintic.

S-G quart-quintic: requires a minimum of 7 points; it can cause resolution degradation for very sharp peaks that are less than 7 points wide.

Number of Points: The boxcar and Savitsky-Golay smoothing processes, at any point use that point and the same number of points on the X-axis to the right and left of it in the calculations. Therefore, only an odd number of points can be entered; if an even value is entered, it is incremented by 1 and that new odd value used. The valid ranges and meanings are:

Boxcar	3 - 255		boxcar width
Savitsky-Golay quad/cubic	5-25	}	number of points in the convolution function
Savitsky-Golay quart/quintic	7-25		

Because the convolution region for N=2k+1 points requires that there be k points on either side of the center, you will lose k points at the lower and upper end of the spectrum as an intrinsic feature of the smoothing process. For example, if N=7, then 3 points will be lost at either end of the spectrum.

The larger the number of points used, the more smoothing that will occur and the greater the loss of resolution. In general, try to fit the number of points in the convolution region to the spectral data. Do not include more than one inflection point of the observed data in the convolution region. In practice, this is usually obtained by setting the number of points in the region equal to the width of the peak at half-height (and rounding up, if necessary, to the next odd number).

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Fourier Smoothing

Fourier: the Fourier smoothing is a multi-step process.[2]

1. Perform a Fourier transform of the spectrum.

2. Apply a truncation filter function to the transformed spectrum. The range is from 0 (which gives no spectrum) to 1 (which gives the original spectrum). The default value is 0.2 which gives a good smoothing without significant loss of resolution. This value is set by the Strength parameter (see below).

3. Perform an inverse Fourier transform.

Strength: the fraction of the transformed spectrum (starting from 0) to be used in the inverse transform. If this is not equal to 1, then the high frequency noise is reduced.

Note

Fourier smoothing is equivalent to using a smoothing function whose transform is a boxcar.

Because the real data are discrete, Fourier processing can sometimes introduce artifacts into the data. These are usually seen as high-frequency periodic signals imposed on the smoothed data. Savitsky-Golay smoothing does not suffer these effects.

The buttons in the dialog box are:

Replace: smooth trace according to selected method and return to main menu. The smoothed trace replaces the original trace.

Add: smooth trace according to selected method and return to main menu. The smoothed trace is added to the document; the original trace is not overwritten.

---

[2] Jyrki K. Kauppinen, Douglas J. Moffatt, Henry H. Mantsch, and David G. Cameron, "Smoothing of spectral data in the Fourier domain", *Applied Optics*, **21**, 1866-1872, 1982.

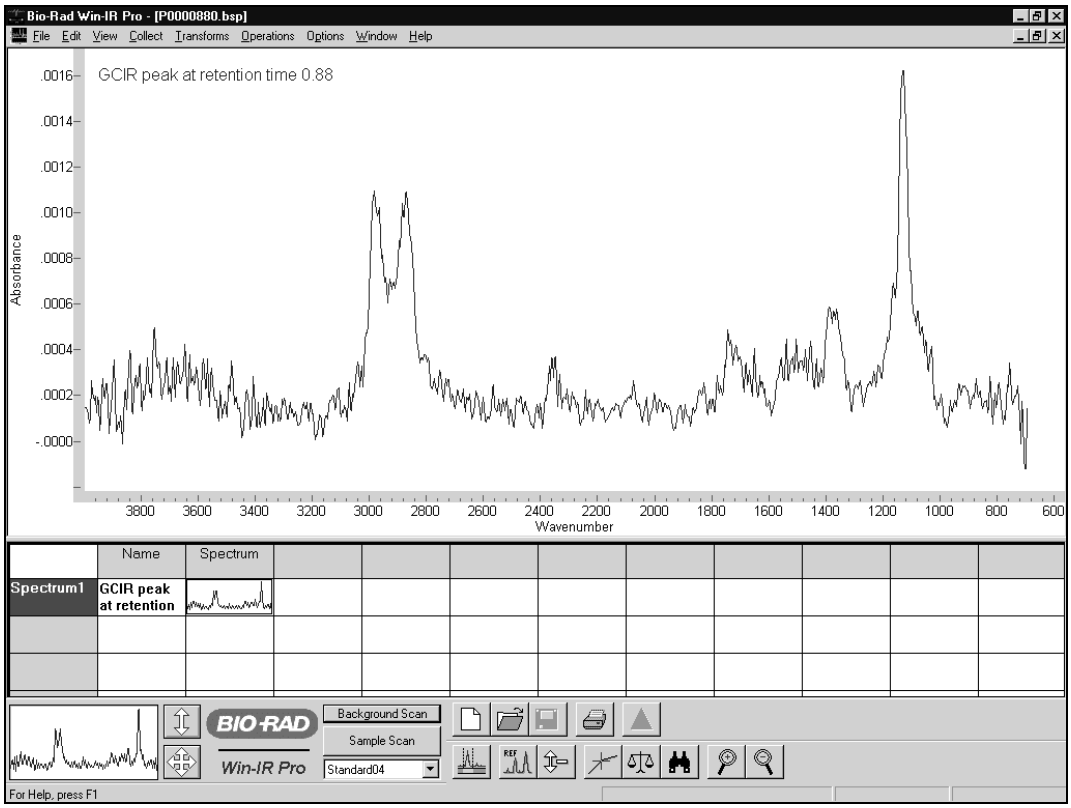
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Cancel: return to the main menu without smoothing the trace.

Help: access the on-line Help facility.

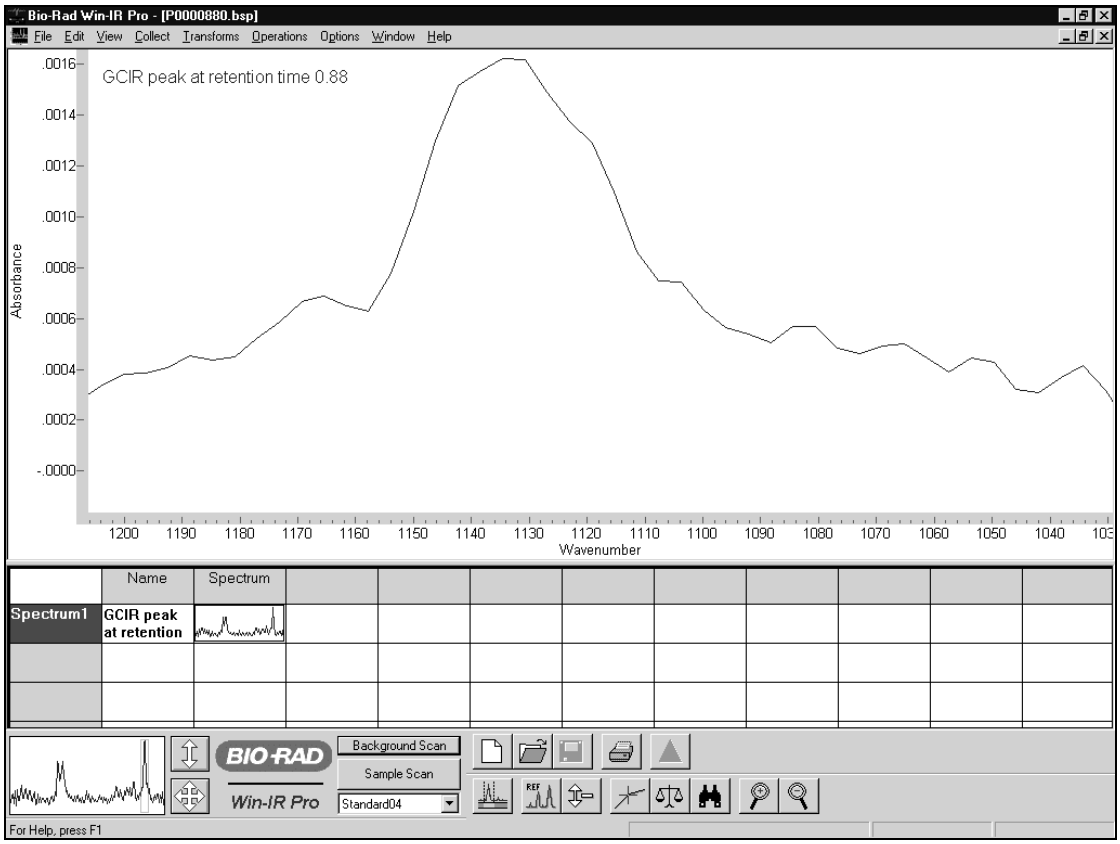
Smoothing Example

Consider the noisy spectrum P0000880.bsp



Zoom in on part of the spectrum to determine the width of the peaks at half height.

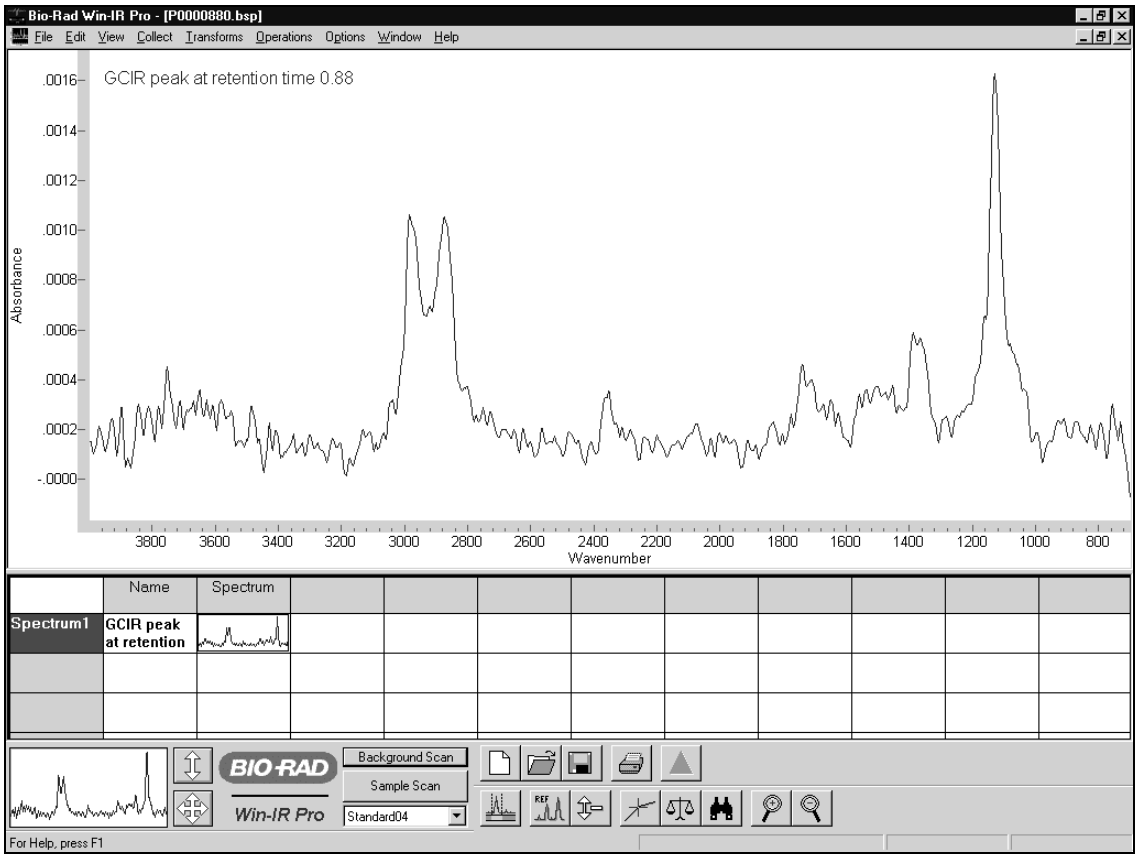
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At half height the peak is about 40 cm^{-1} wide. Because the resolution is 4 cm^{-1}, there are about 10 points in the peak. Use 9 or 11 as the parameter to smooth the curve. An alternate method of determining the width is to zoom in on the spectrum and count the places where the curve breaks.

Using the Savitsky-Golay quart/quintic method with 11 points, the spectrum is smoothed to look like the plot below.

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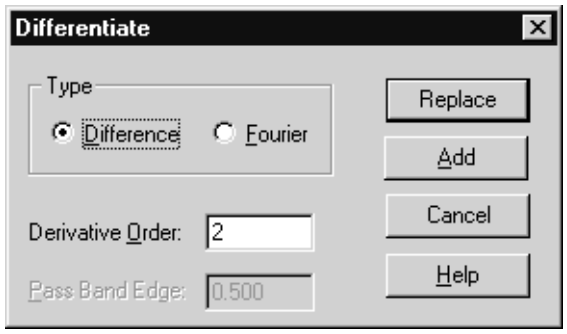
DIFFERENTIATE

Differentiates the current trace. The trace must be in absorbance format.

Note

Differentiation can help you distinguish overlapping bands. Both differentiation and deconvolution can be used to determine peak positions in complex spectra. Both techniques generate sidelobes, but their displacement from the main peak is different for each method. A useful check on whether a small is a real peak or a sidelobe is to perform both differentiation and deconvolution and compare the peak maxima postions.

After selecting this entry, the Differentiate dialog box appears.



Type: the derivative can be approximated by two techniques.

Difference: calculates the nth derivative using the difference method, that is, the new point at x is $(y_{x+1} - y_{x-1})$. The value of n is specified by Derivative Order.

Note

This does not shift the spectrum. The end points are extended at each order of differentiation by setting $y_{-1} = y_0$ and $y_{max+1} = y_{max}$, and then taking the difference.

Fourier: the steps of the process are

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1. Fourier cosine transform of the spectrum
2. Multiply by $2\pi x^n$ (n is the derivative order)
3. Apodize with $sinc^2$ function (sinc x = [sin x]/x)
4. Inverse Fourier transform back to a spectrum

The symmetry properties of the cosine transform mean that only even values of n give correct derivatives; odd values of n do not correspond mathematically to a derivative spectrum.

Because differentiation amplifies high frequency spectral noise, the apodization function is used to smooth the spectrum. The amount of smoothing is controlled by the Pass Band Edge parameter. A value of 1.0 retains the entire interferogram.

Derivative Order: order of the derivative to be generated (integer). The Fourier algorithm used requires even integers only for meaningful results. If you need an odd derivative order, use the Difference method or a combination of Difference and Fourier.

Pass Band Edge: (Fourier only) a smoothing parameter. It determines the fraction of the cosine transform to be retained. This portion is multiplied by the apodization function and the other points are set to 0 (range 0.0 to 1.0). The minimum value should be

$$\frac{UDR * Res}{ZFF * \nu_{1/2}}$$

UDR	undersampling ratio
Res	resolution
ZFF	zero-filling factor
$\nu_{1/2}$	half-height bandwidth of the narrowest spectral line

Replace: differentiate trace according to selected method and return to main menu. The differentiated trace replaces the original trace.

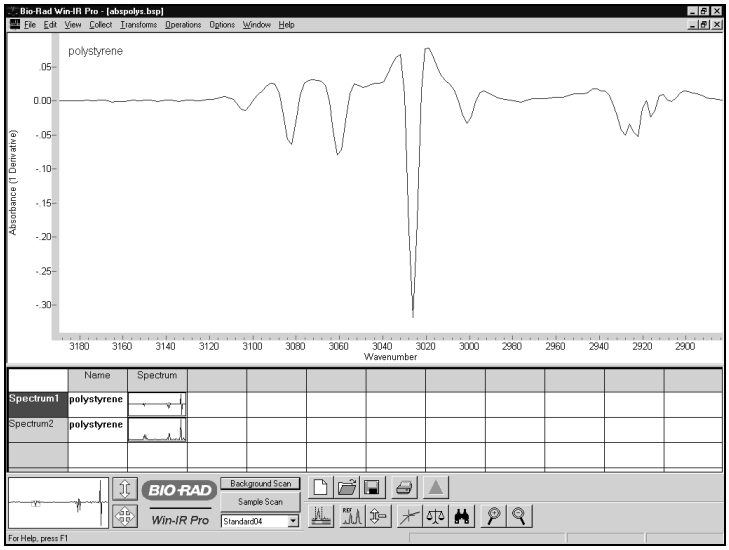
Add: differentiate trace according to selected method and return to main menu. The differentiated trace is added to the document; the original trace is not overwritten.

Cancel: return to the main menu without differentiating the trace.

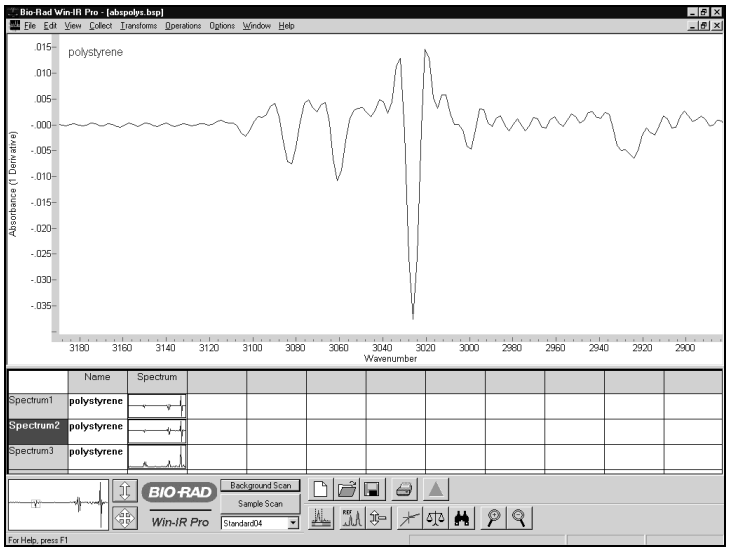
Help: access the on-line Help facility.

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An example of a second order Difference spectrum (we have zoomed into the smaller region 3200-2900 cm^{-1} and autoscaled in the Y direction):



The second order derivative of the same spectrum, using Fourier techniques and a Pass Band Edge of 0.5.



The derivative spectra are roughly the same, independent of the method.

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DECONVOLVE

Deconvolution is the enhancement of the apparent resolution of overlapping peaks where the limiting resolution is the natural width of the bands, not the resolution with which the spectrum was collected.[3] This aids in identifying the principal bands that comprise a more complex band with overlapping features. This can be useful for more accurate determination of the number of peaks in a region, the band positions, and areas under peaks. Individual peaks are assumed to have Lorentzian line shapes. A broad peak may be described as the convolution of a very sharp peak (a delta function) with a Lorentzian line shape function. Peak position and area are unchanged, but peak height is changed. For reliable results, the following conditions should be satisfied.

1. Signal-to-noise ratio should be as high as possible; 100:1 is possible, but 1000:1 is desirable.

2. The spectral limits used to define the spectral region for deconvolution should include a portion of the baseline so that noise level can be monitored. The first few data points should not show any curvature.

3. The spectrum must be in the absorbance format. Maximum absorbance must be one or less.

4. The deconvolution region should be chosen so that the widths of the bands are all approximately the same.

5. The Bessel function is recommended for apodization; it minimizes the amount of noise introduced by the deconvolution process.

---

[3] David G. Cameron and Douglas J. Moffatt, "Deconvolution, Derivation, and Smoothing of Spectra Using Fourier Transforms", *Journal of Testing and Evaluation*, **12**, No. 2, 78-85, March 1984.

Wang-Jih Yang and Peter R. Griffiths, "Optimization of Parameters for Fourier Self-deconvolution", *Computer Enhanced Spectroscopy*, **1**, No. 3, 157-165, 1983.

Jyrki K. Kauppinen, Douglas J. Moffatt, Henry H. Mantsch, and David G. Cameron, "Fourier Self-Deconvolution: A Method for Resolving Intrinsically Overlapped Bands", *Applied Spectroscopy*, 35, No. 3, 271-276, May/June 1981.

Jyrki K. Kauppinen, Douglas J. Moffatt, David G. Cameron, and Henry H. Mantsch, "Noise in Fourier self-deconvolution", *Applied Optics*, **20**, No. 10, 1866-1879, May 1981.

Jyrki K. Kauppinen, Douglas J. Moffatt, Henry H. Mantsch, and David G. Cameron, "Fourier Transforms in the Computation of Self-Deconvoluted and First-Order Derivative Spectra of Overlapped Band Contours", *Analytical Chemistry*, **53**, 1454-1457, 1981.

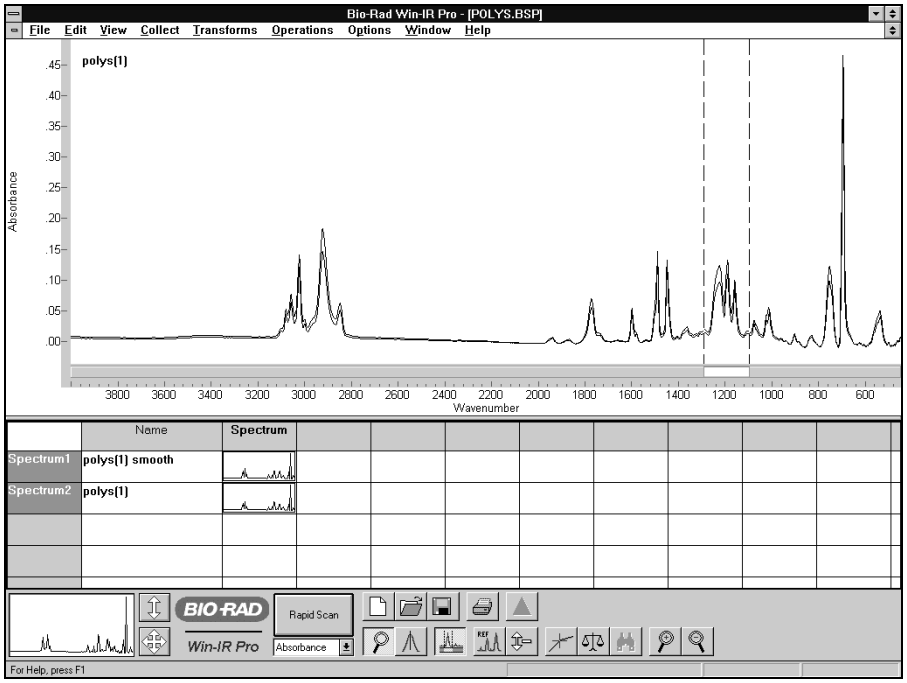
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Note

The maximum effective resolution after deconvolution cannot be higher than the instrument resolution used to record the data.

A more detailed discussion of deconvolution is given in Appendix J.

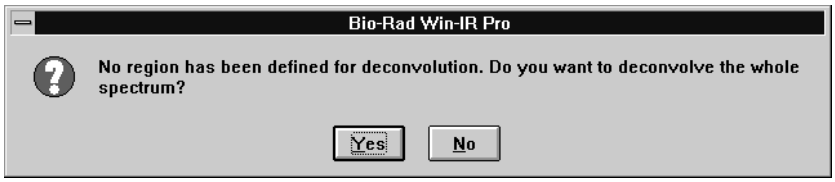
In the document below, we have selected polys.bsp (polystyrene spectrum) and a smoothed version of polys.bsp with the region between about 1300 and 1100 cm^{-1} selected using the cursor.



Select Deconvolve from the Transforms menu.

If no region was defined, then the Deconvolution dialog box appears.

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Click Yes to deconvolve the entire spectrum. This does not usually yield optimum results.

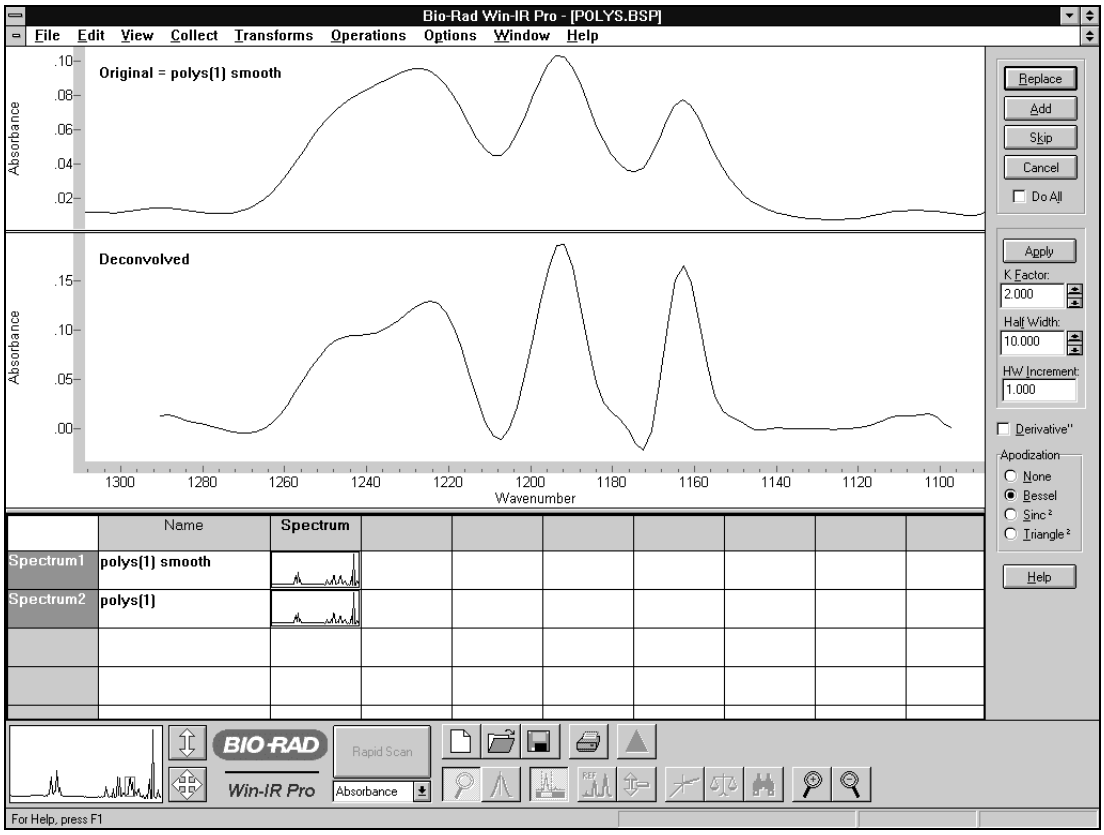
Click No to return to the main menu without performing any transform.

Notes

You will obtain the best results where the linewidths are similar, and where a small region is selected, as in the example below.

If you have selected more than one spectrum, the same region will be used for all these spectra.

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In this example, we have zoomed in on the region of interest. The original spectrum is in the upper half of the display; the deconvolved spectrum is in the lower half. The spectrum currently being processed is identified by its name; in this example, it is Original - polys(10 smooth.

The deconvolution parameters are:

K factor: the peak width narrowing factor. It determines the width of the function (0 means zero the spectrum).

Half Width: the width at half-height of the peak shape function. Values range from 1.0 to 100.0 cm^{-1}.

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HW Increment: the value by which the half-width is changed when the spin box arrows are used.

Apply button: If you use the spin-box arrows to set the values, then they are applied immediately to the deconvolved trace. You can also type in the K factor and Half Width boxes. If you type in values, they are not applied until the Apply button is pressed. Press the Apply button to tell Win-IR Pro that you have completed typing values and that these values should be applied to the trace.

Derivative: displays the second derivative spectrum in the upper window.

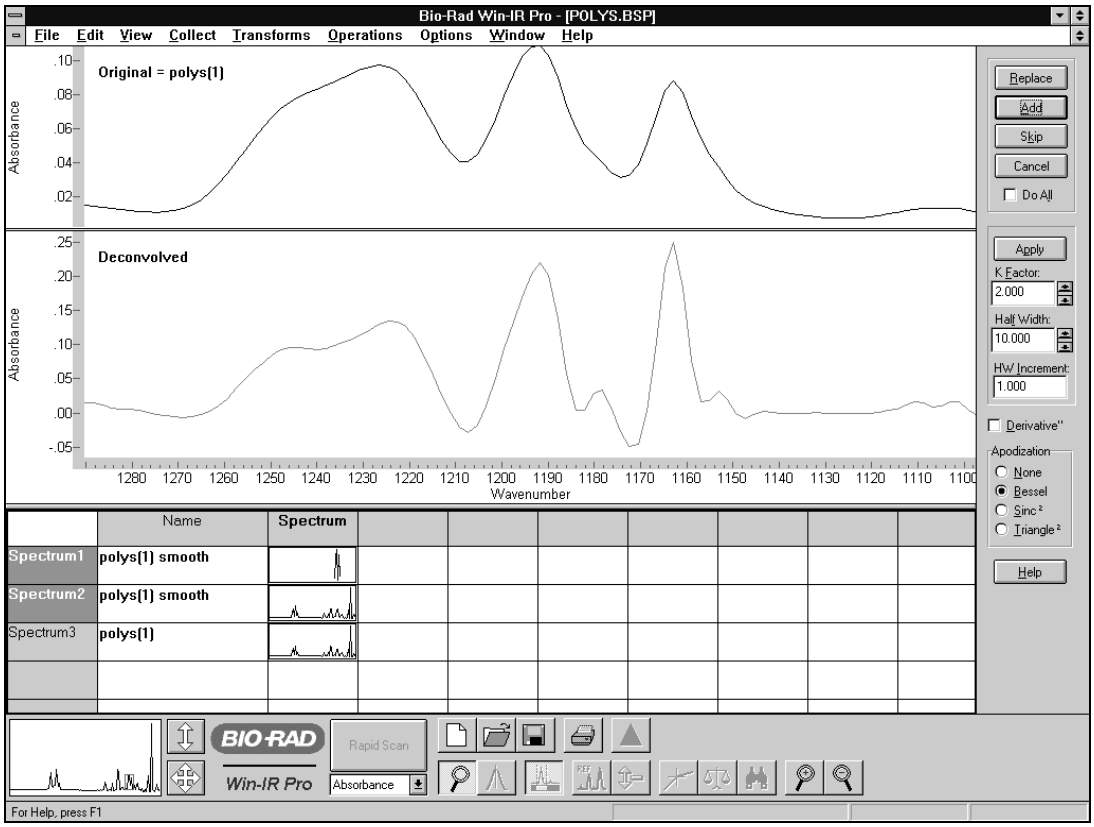
Apodization: reduces the side lobes appearing around the deconvolved peaks. Bessel is preferred. See the Algorithms and Function appendix for addition details about the apodization functions. The choices are:

None
Bessel: minimizes the amount of noise introduced by the deconvolution process.
$Sinc^2$
$Triangle^2$

Replace: replace the existing original spectrum with the altered spectrum. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Add: add the altered spectrum to the document that contains the original spectrum. Both spectra are now in the main menu display. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

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In this example, the deconvolved spectrum has been added to the spreadsheet. The next trace (Original - polys(1)) is now displayed in the upper half; the lower half shows the new deconvolved spectrum, using the existing parameters.

Skip: Do not alter the current spectrum. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

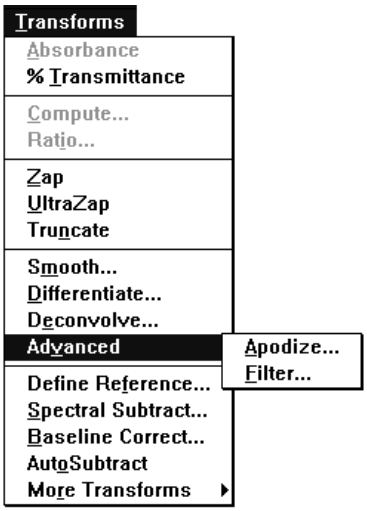
Cancel: return to the main menu display without acting upon the current spectrum or any subsequent spectra. Spectra previously replaced or added are not altered by this.

Do All: if selected, then the Deconvolution parameters selected for this spectrum are applied to this spectrum and to all subsequent spectra; they are all either Replaced or Added. Spectra previously replaced or added are not altered by this.

Help: enter the on-line Help system.

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ADVANCED



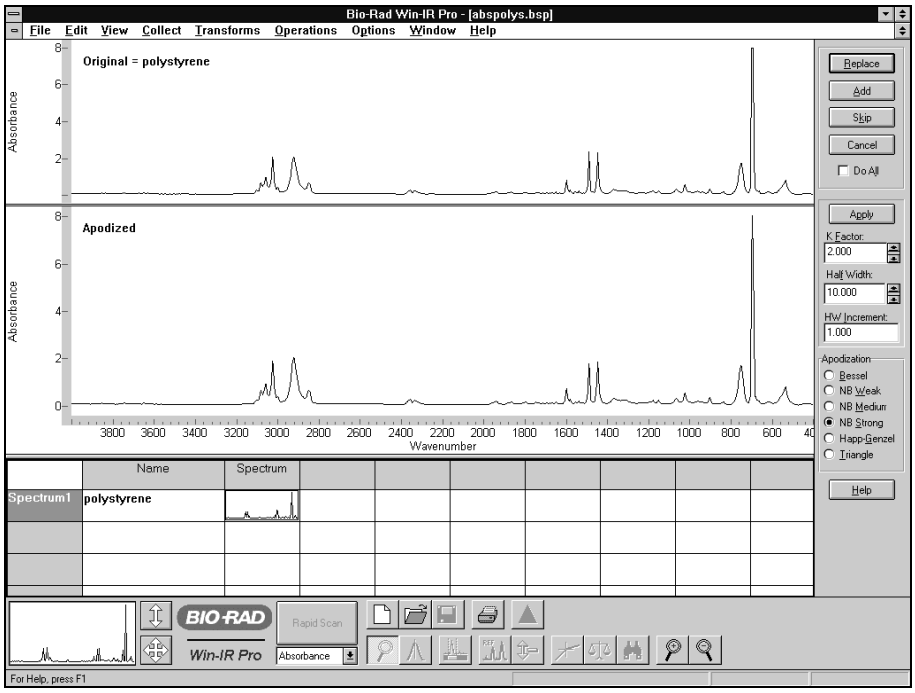
Apodize...

This process is not the same as is used to apodize interferograms during computation of single-beam spectra. It is an alternate method of smoothing spectra. The process is:

1. The original spectrum (shown in the top part of window) is Fourier transformed to an interferogram (not shown).
2. The interferogram is multiplied by the apodization function (not shown).
3. The apodized interferogram is Fourier transformed to a new, apodized spectrum (shown in the bottom part of the window).

First select the spectra to be apodized using the spreadsheet; then select Transforms / Advanced / Apodize. When this entry is selected, the trace display is split in two and a dialog box appears on the right of the traces.

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The Original trace is in the upper part; the Apodized (or to be apodized) trace is in the lower part. Set the values in the dialog box.

K factor: the peak width narrowing factor. It determines the width of the apodized function (0 means zero the spectrum).

Half Width: the width at half-height of the peak shape function. Values range from 1.0 to 100.0 cm^{-1}.

HW Increment: the value by which the half-width is changed when the spin box arrows are used.

Apodization: select the apodization function to be used. The function used depends upon the actual experiment. Triangle is recommended for general use. If either high resolution or good quantitative accuracy is necessary, use the NB Weak (Norton-Beer) function. Use stronger apodization if the spectra have a large spread in the intensity of the bands, especially if the peak widths are of the order of instrument resolution. The available functions are:

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Bessel
NB Weak
NB Medium
NB Strong
Happ-Genzel: (sometimes called Hamming)
Triangle

See the Algorithms and Functions appendix for details of the apodization functions.

Selecting a new apodization function immediately applies it with the previously chosen parameters.

Apply: click this button to apply a newly selected K factor, Half Width, and/or HW Increment to the spectrum. The result is displayed in the Apodized trace box

Note

Selecting a new apodization function automatically clicks the Apply button.

At this point, no changes have been made to the original spectrum. Therefore, other apodizations may be performed until the desired result is obtained.

Replace: replace the existing original spectrum with the altered spectrum. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Add: add the altered spectrum to the document that contains the original spectrum. Both spectra are now in the main menu display. Go the the next trace spectrum from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Skip: Do not alter the current spectrum. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Cancel: return to the main menu display without acting upon the current spectrum or any subsequent spectra. Spectra previously replaced or added are not altered by this.

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Do All: if selected, then the Apodization parameters selected for this spectrum are applied to this spectrum and to all subsequent spectra; they are all either Replaced or Added. Spectra previously replaced or added are not altered by this.

Help: enter the on-line Help system.

Filter...

Filtering selectively zeros certain parts of the interferogram before it is transformed into a spectrum, leaving other parts untouched. With a trapezoidal filter, the sloping parts can give more realistic band shapes in the filtered spectrum.. Filtering provides smoothing, fringe removal, and baseline correction. The process is:

1 Compute the cosine transform of an absorbance spectrum. This yields an interferogram (sometimes called a cepstrum).

2 Multiply the interferogram by a trapezoidal apodization function (the filter– see below).

3. Compute the cosine transform of the result.

The interferogram is normalized, with a range from 0 to 1. The bandedge (Edge) values are decimal fractions specifying where the zeroing of the interferogram begins and ends. The transition bandwidth (TBW) controls the slope for the trapezoidal apodization.

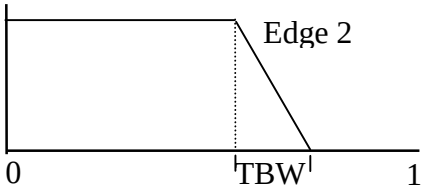
Very sharp cutoff filters (TBW=0) may cause sidelobes in the filtered spectrum. These sidelobes are prominent if the bandedge corresponds to a region of the interferogram with a large amplitude. If the interferogram region has a small amplitude in that region, then a sharp cutoff has little effect on sidelobes. Widening the transition bandwidth minimizes the effect of sidelobe occurrence.

The edge(s) and bandwidth values are determined empirically by viewing the interferogram. Select the region(s) of the interferogram to be zeroed (edge) and how rapidly the data is to decrease to zero (transition bandwidth).

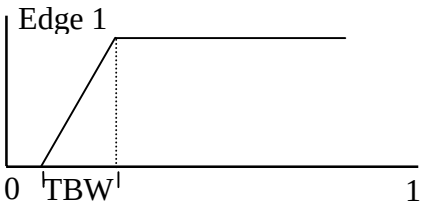
The filters are shown below.

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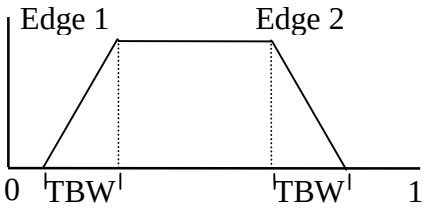
Lowpass Filter
for spectral smoothing
(removes high-frequency features,
that is, noise)



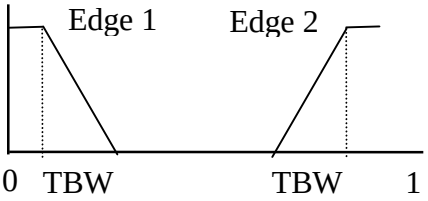
Highpass Filter
for baseline correction
(removes low-frequency features,
that is, slopes)



Bandpass Filter
for spectral smoothing
and baseline correction

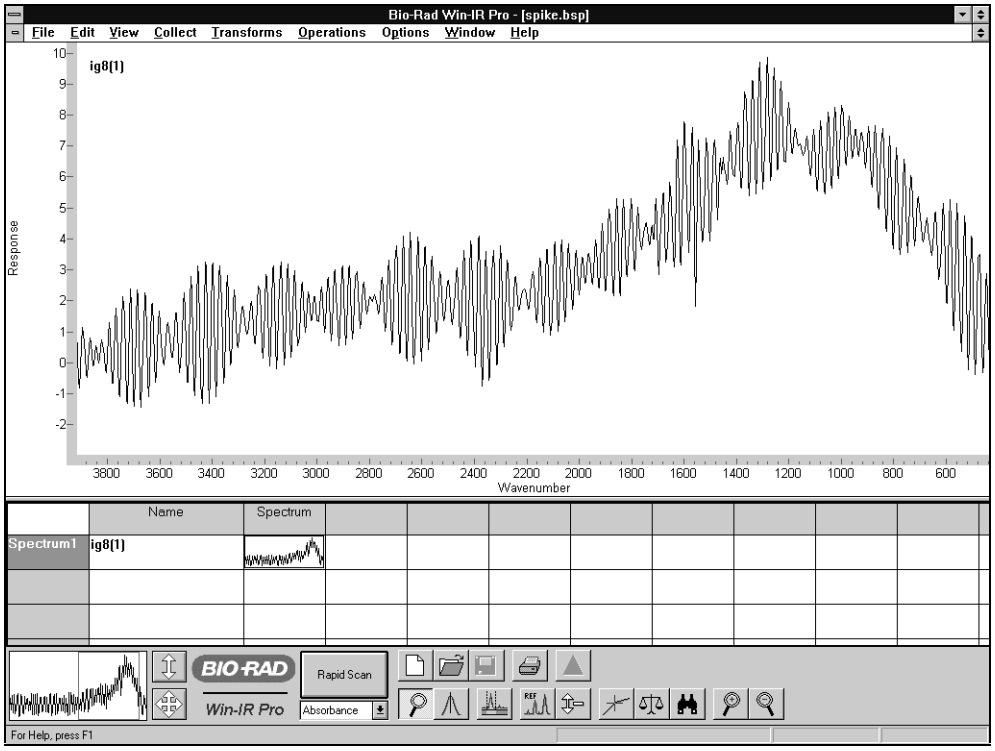


Notch Filter
for fringe removal
(removes spikes)



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Consider a spectrum with many fringes, spike.bsp:

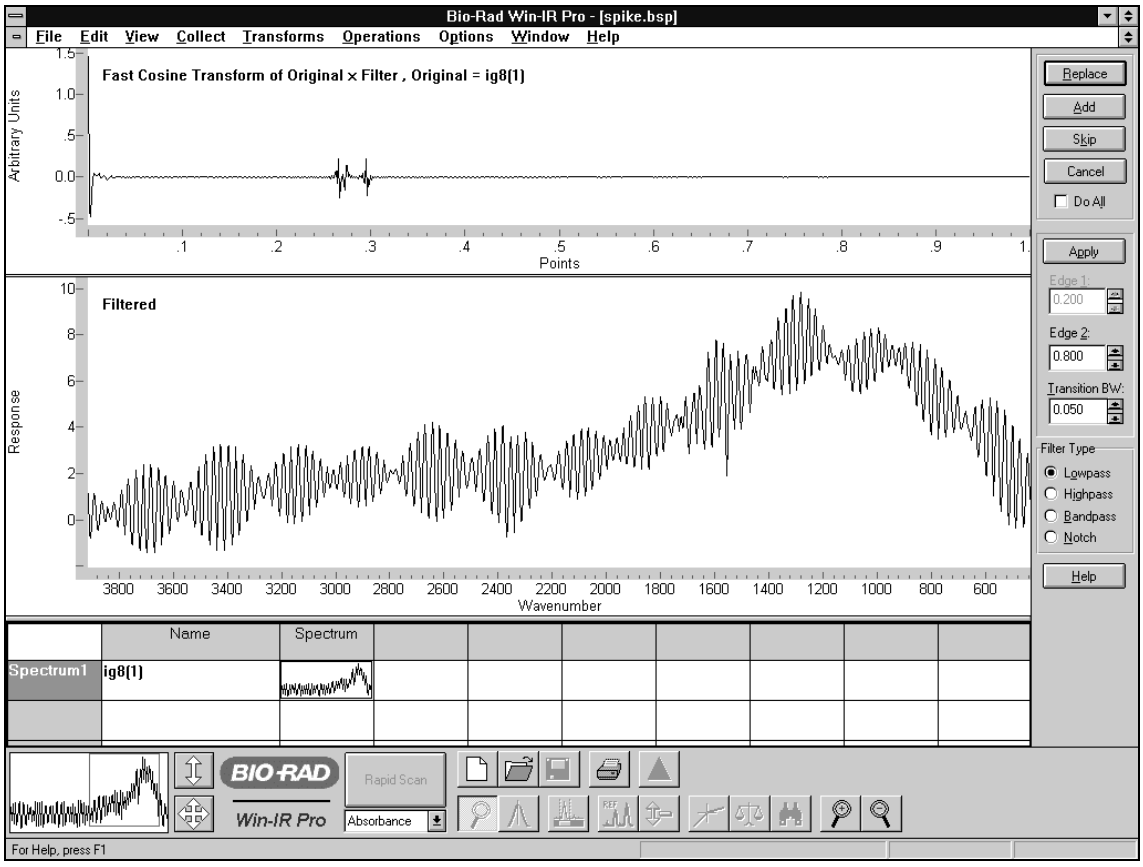


First, form the spreadsheet, select all the spectra to be filtered. Then select Transforms / Advanced / Filter. When Filter is selected, the trace display is split in two and a dialog box appears on the right of the traces.

Note

This is clearly not the ideal combination of filter type and parameters for this spectrum.

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The Fast Cosine Transform of Original x Filter interferogram trace is in the upper part; the Filtered spectrum is in the lower part. Set the values in the dialog box.

Edge 1: the low band edge for Bandpass and Notch filters; the band edge for the Highpass filter. The default is 0.200.

Edge 2: the high band edge for Bandpass and Notch filters; the band edge for the Lowpass filter. The default is 0.800.

Transition BW: the bandwidth determining the slope of the side of the trapezoid. Values range from 0 to 1 (in increments of 0.001); the default is 0.05.

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Filter Type: select the filter type to be used. These filters, and their applications, are described above. The available filters are:

Lowpass
Highpass
Bandpass
Notch

Selecting a new filter immediately applies it to the interferogram with the previously chosen parameters.

Apply: click this button to apply a newly selected parameter to the interferogram.. The result is displayed in the Filtered trace box

Note

Selecting a new filter automatically clicks the Apply button.

In this example, select Notch filter, and set the values to zero out the spikes in the cepstrum.

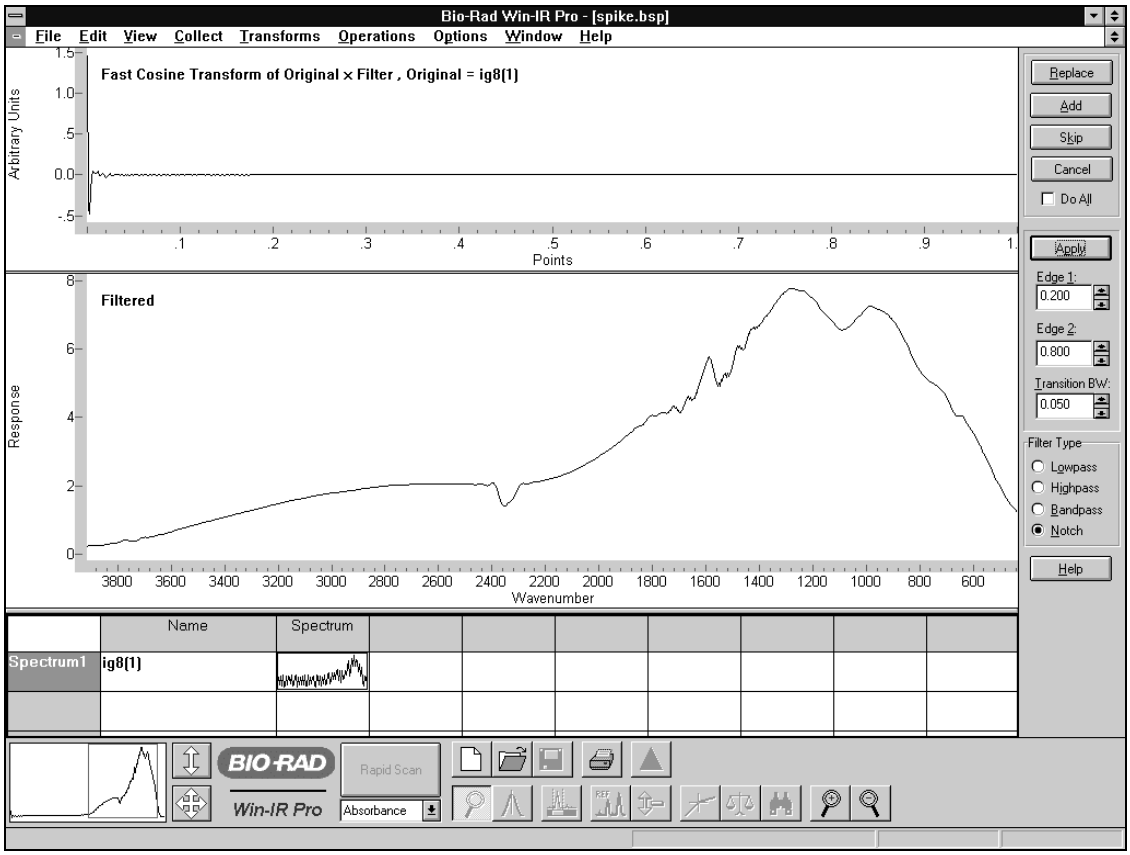
Edge 1: 0.200

Edge 2: 0.800

Transition BW: 0.050

Click the Apply button; the resulting spectrum is shown below.

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At this point, no changes have been made to the original spectrum. Therefore, other filters may be selected until the desired result is obtained.

Replace: replace the existing original spectrum with the filered spectrum. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Add: add the filtered spectrum to the document that contains the original spectrum. Both spectra are now in the main menu display. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Skip: Do not alter the current spectrum. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

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Cancel: return to the main menu display without acting upon the current spectrum or any subsequent spectra. Spectra previously replaced or added are not altered by this.

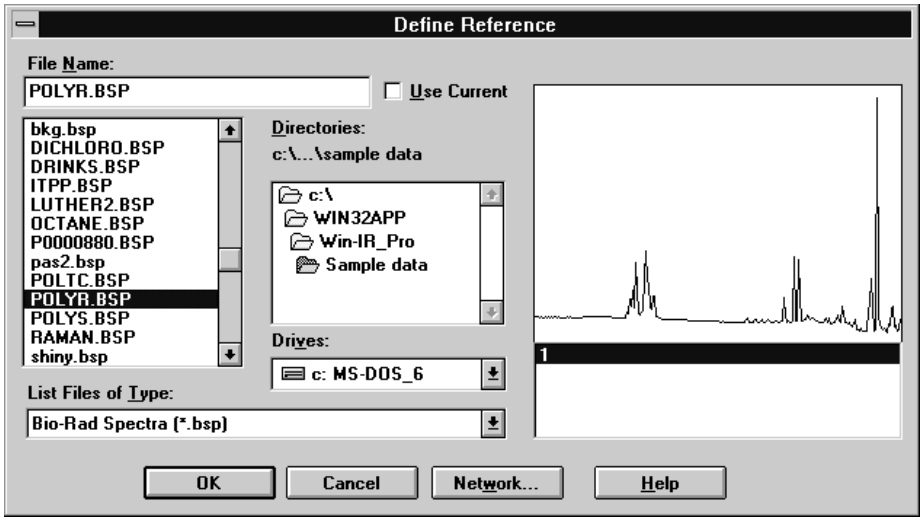
Do All: if selected, then the Filter parameters selected for this spectrum are applied to this spectrum and to all subsequent spectra; they are all either Replaced or Added. Spectra previously replaced or added are not altered by this.

Help: enter the on-line Help system.

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DEFINE REFERENCE...

Defines the reference spectrum that will be subtracted in spectral subtraction. The Define Reference dialog box appears.



File Name: type in or use the standard Windows NT procedure to select the pathname of the file to be used as the reference spectrum. If appropriate, use the preview box on the right to select the subfile.

OK: load the selected reference and return to main menu

Use Current: choose the currently selected spectrum to be the reference spectrum.

Cancel: return to the main menu without selecting a new reference.

Network: connect to a network disk.

Help: access the on-line Help facility.

Note

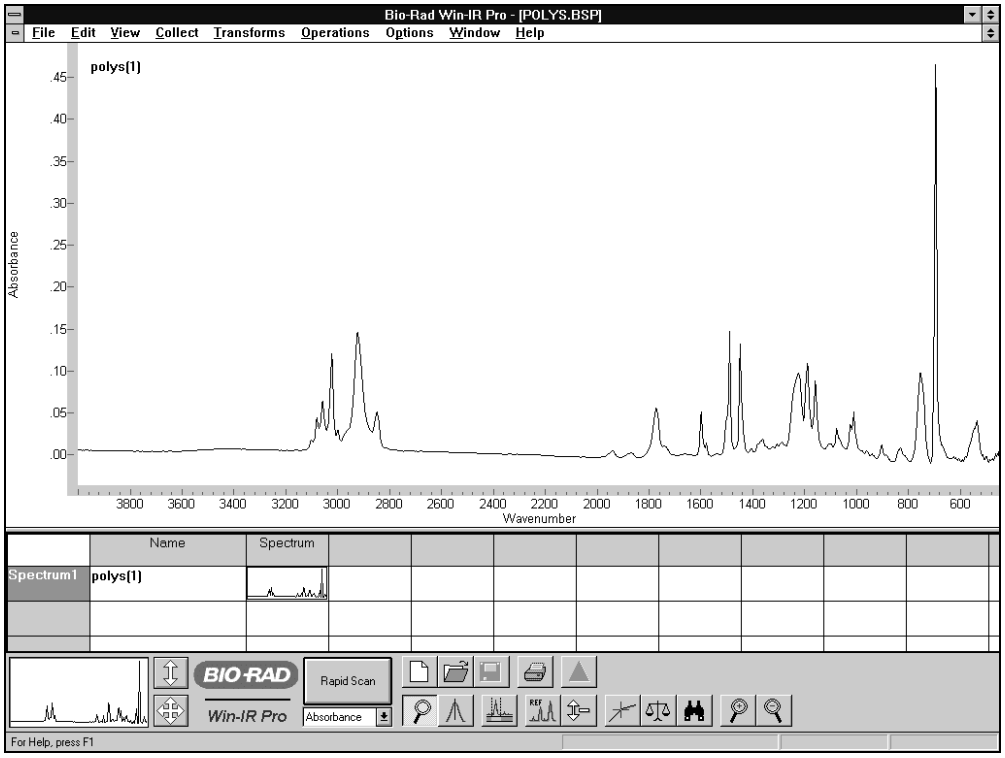
Pressing the 

button makes the currently active spectrum the reference spectrum.

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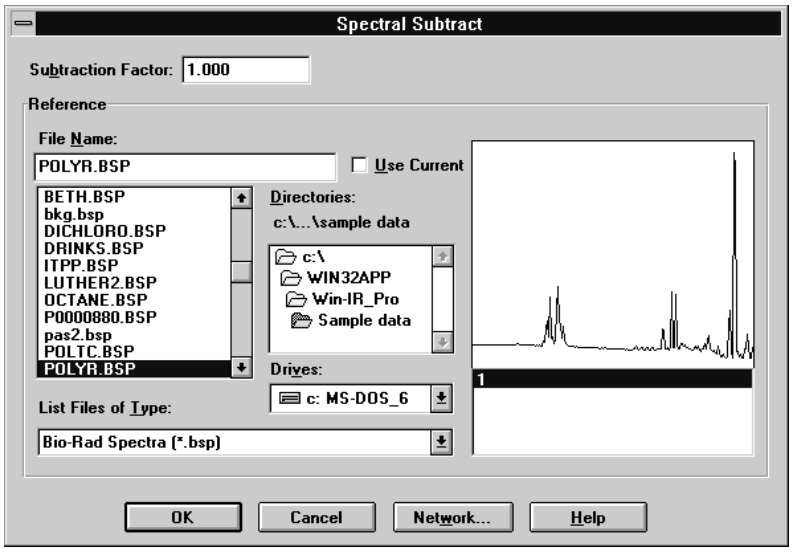
SPECTRAL SUBTRACT...

Subtracts the reference spectrum (subtrahend) from the selected spectrum. In this example, first, open the mixture spectrum, polys.bsp. Spectral subtraction should only be performed on data in an absorbance-type format.



Select Spectral Subtract... from the Transforms menu, the Spectral Subtract dialog box appears.

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Reference: the spectrum that is to be subtracted, the subtrahend.

File Name: if the reference file has already been selected, its name appears here. Otherwise, type in or use the standard Windows NT procedure to select the pathname of the file to be used as the reference spectrum. If appropriate, use the preview box on the right to select the subfile. The reference file may have been previously selected using Transforms / Define Reference... or by using the  button.

Use Current: if selected, the currently active spectrum will be chosen as the reference spectrum.

Subtraction Factor: the reference spectrum will be multiplied by this number when it is subtracted from the sample spectrum. The initial default value is 1.000.

OK: load the selected reference, perform the initial subtraction, and go to a split screen with the subtraction control panel sidebar.

Note

If you click the  button, it performs the subtraction using a Subtraction Factor of 1.000.

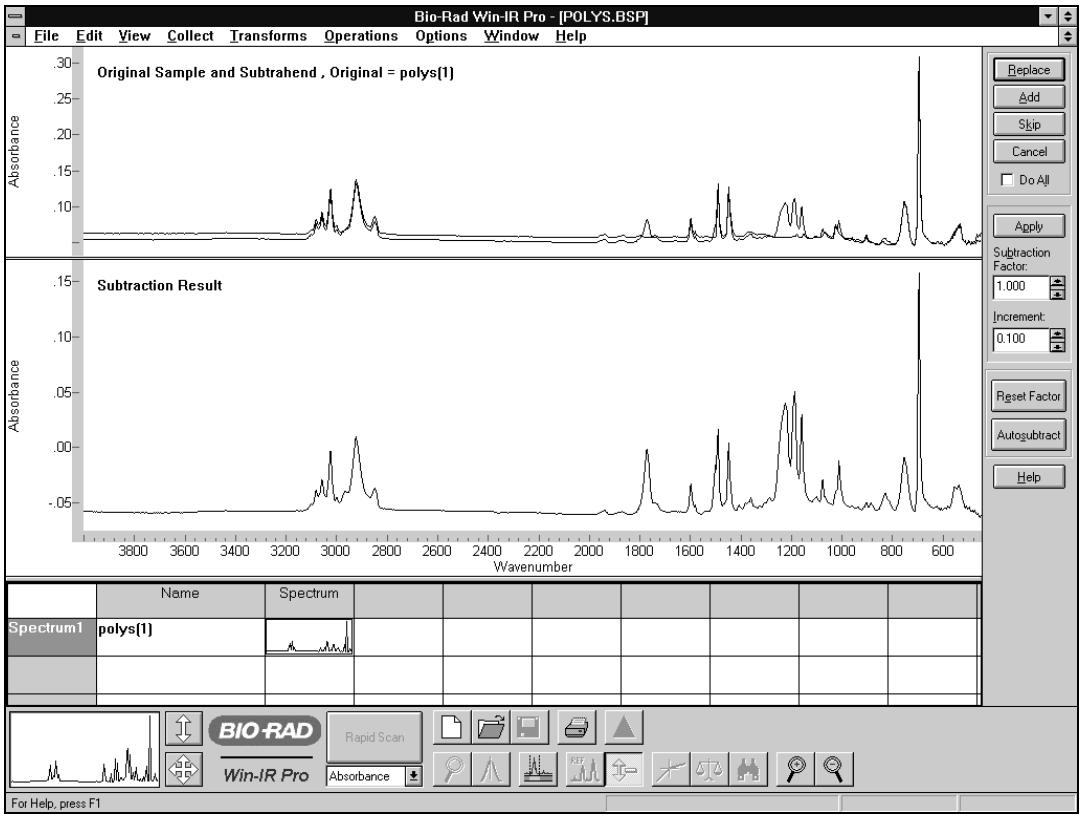
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Cancel: return to the main menu without performing a subtraction..

Network: connect to a network disk.

Help: access the on-line Help facility.

In this example, the following screen appears,



Note

You can zoom, scroll, etc., the Y-axis in the display. You can autoscale windows and traces separately.

Subtraction Factor: the number by which the reference spectrum is multiplied before it is subtracted from the original spectrum. It initially displays the value set in the Spectral Subtract dialog box.

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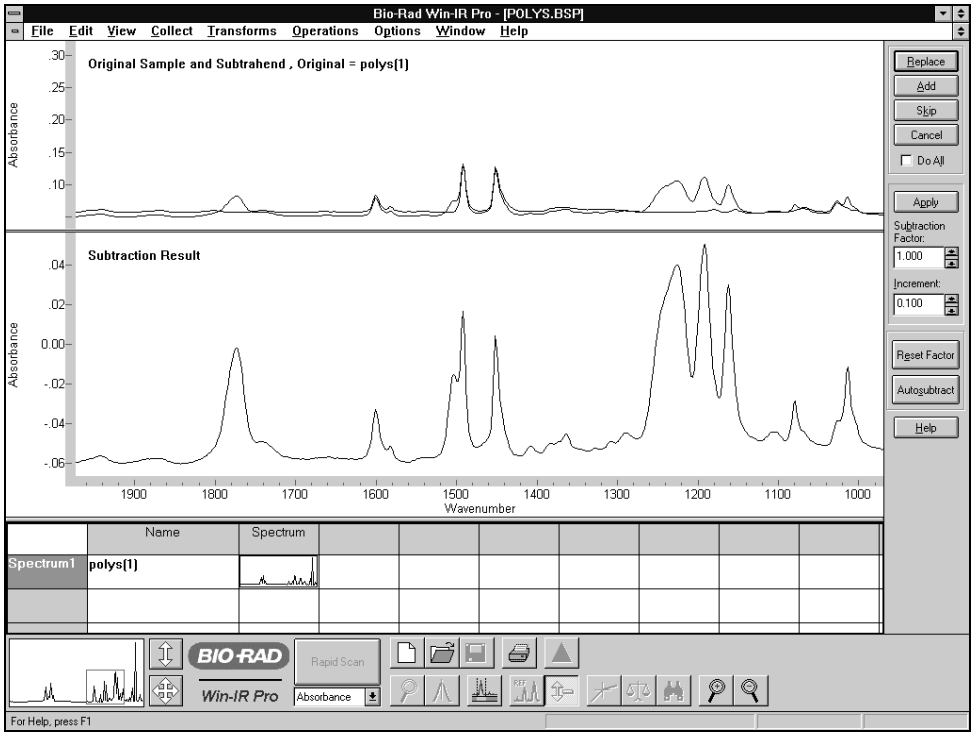
Increment: the amount by which the Subtraction Factor is changed when one of the arrows to the right of its box is clicked.

Apply button: if you type new values into Subtraction Factor or Increment, click this button to have them applied to the difference spectrum.

Reset Factor: resets the Subtraction Factor to the original value and the Increment to 0.100.

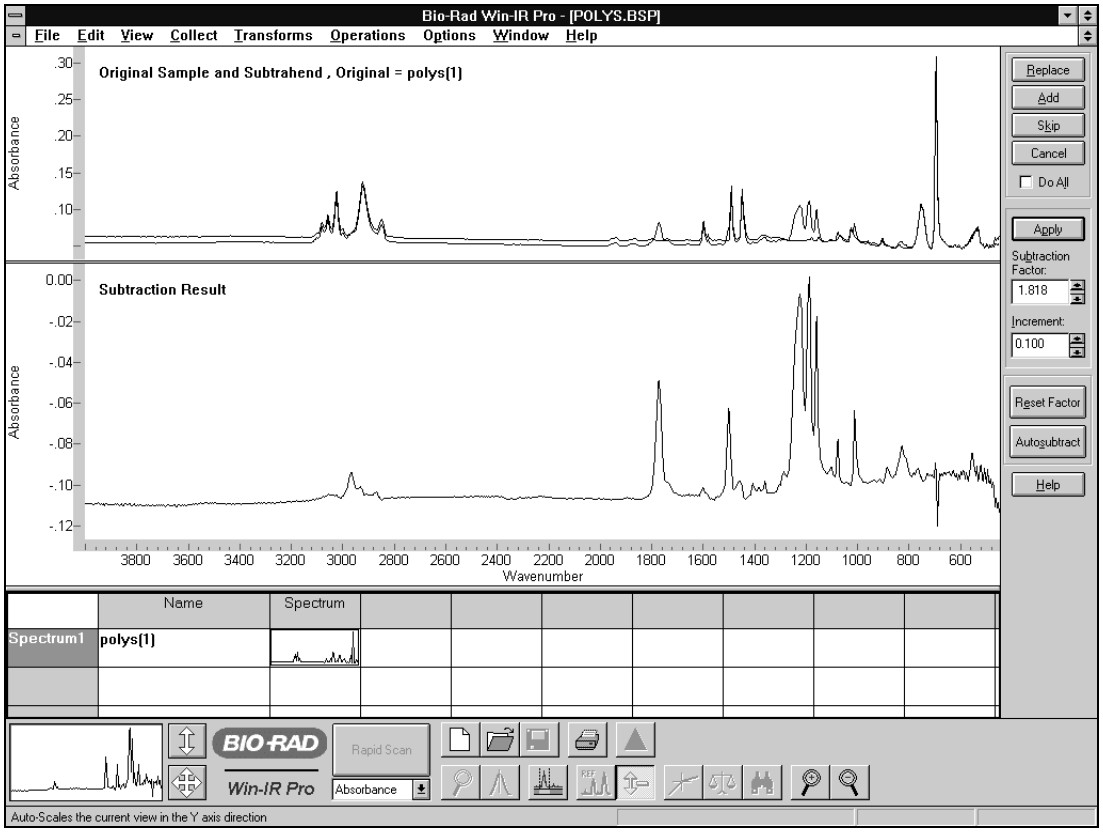
Autosubtract: attempts to optimize the subtraction. After it is complete, the subtraction factor used is displayed in the Subtraction Factor box.

You can use the mouse to drag regions of the Subtraction Result spectrum to the baseline. These are regions where the spectra are known to be nearly identical in both the original and reference spectra. First, zoom in on the region between 2000 and 1000 cm^{-1}.



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In the lower window (Subtraction Result), put the cursor on the peak near 1450 cm^{-1}. Hold down the left mouse button. The cursor changes to ⇳–. Drag the peak down to the baseline. The Subtraction Factor will change as you do this. After dragging and autoscaling, the spectrum now looks like this.



When you are finished with subtraction, use the control buttons on the control panel sidebar.

Replace: replace the existing original spectrum with the difference spectrum. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

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Add: add the difference spectrum to the document that contains the original spectrum. Both spectra are now in the main menu display. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Skip: Do not alter the current spectrum. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Cancel: return to the main menu display without acting upon the current spectrum or any subsequent spectra. Spectra previously replaced or added are not altered by this.

Do All: if selected, then the Subtraction parameters selected for this spectrum are applied to this spectrum and to all subsequent spectra; they are all either Replaced or Added. Spectra previously replaced or added are not altered by this.

Help: enter the on-line Help system.

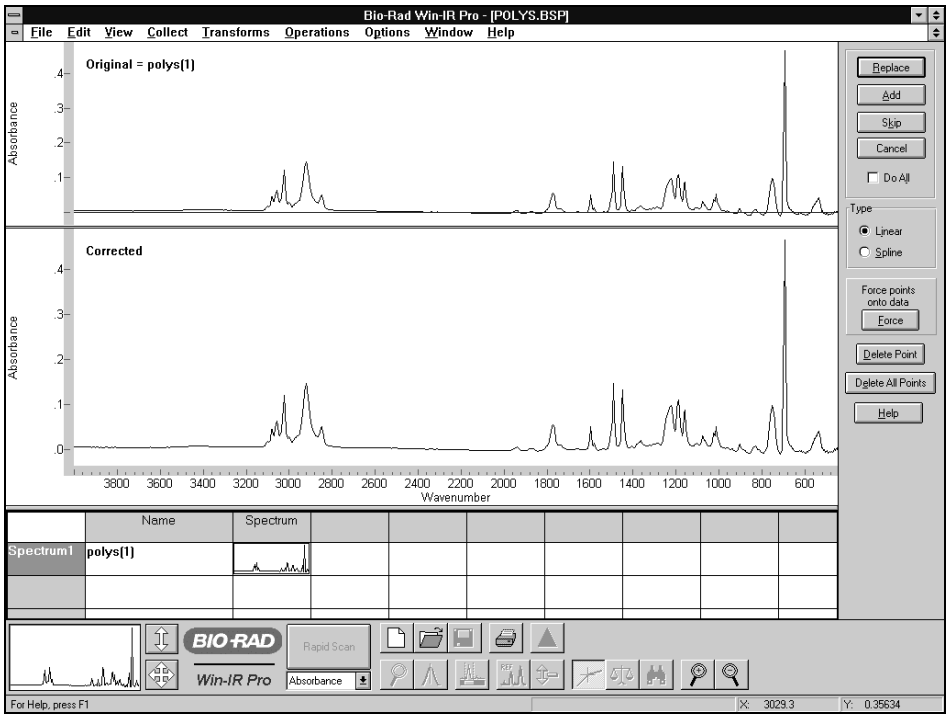
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BASELINE CORRECT...

Generates a baseline-corrected spectrum from the selected spectrum. When selected, the trace display is split in two and the control panel sidebar appears on the right of the traces. In this example, we have used the difference spectrum polys-polyr (see the previous section for details).

Note

Use this transform only with absorbance or absorbance-like (PAS, etc.) spectra for correct operation.



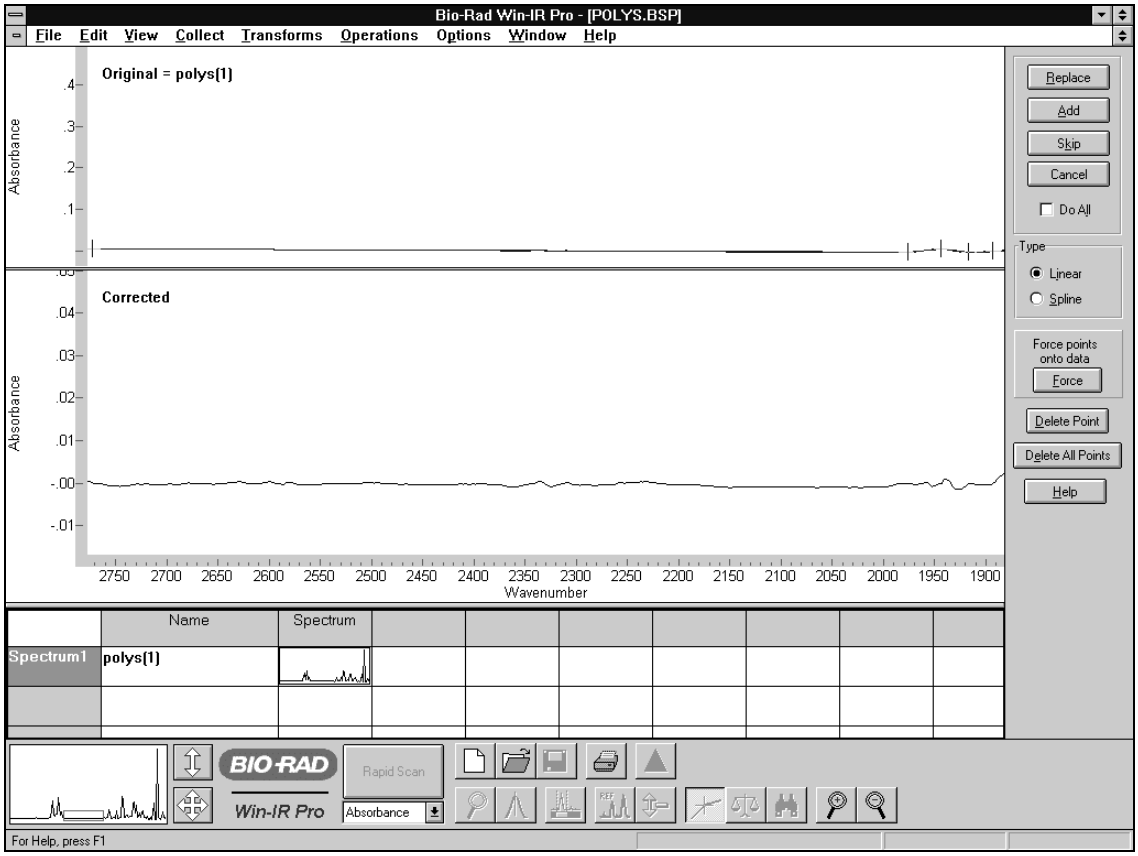
The Original trace is in the upper part; the Corrected (or to be corrected) trace is in the lower part.

You can zoom in on a part of the spectrum by placing the cursor in the Corrected spectrum trace area and using the normal zooming procedure. Points are usually added in flat (feature-free) regions of the spectrum. You can zoom out and autoscale (that is,

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use  and ) without affecting the baseline points you have added. After zooming, press the  button to return to baseline correction mode.

Put the cursor in the Original spectrum portion of the window; the cursor changes to . Place the tip of the arrow at the desired location on the Original spectrum and click the left mouse button. A small white square (shown in black in the picture below) marks this location. You can move this baseline point by placing the cursor on it, holding down the left mouse button, and dragging it, and then releasing the mouse button. The Corrected spectrum is changed and displayed in real time. As you add more points, the Corrected spectrum changes to reflect them.

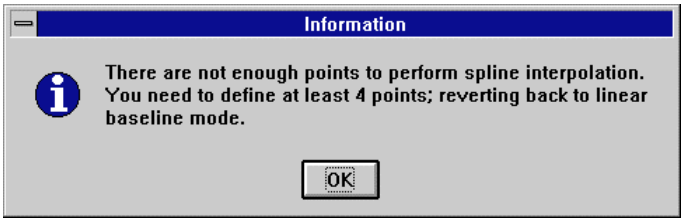


Type: select how the selected baseline points are to be connected. This defines the new baseline.

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Linear: as baseline points are added, they are connected to the adjacent existing baseline points by straight lines. If no adjacent point exist, a horizontal line is drawn through the selected baseline point.

Spline: a cubic spline (a smooth curve) is calculated to connect the baseline points. There must be at least four points in order to fit a cubic curve. If you choose fewer than four points the Information dialog box appears.



Define at least four points and then choose Spline, if you wish to use that type of connection.

Force points onto data: if you click the Force button, all existing baseline points will be moved vertically to the actual value of the Original spectrum. However, additional points will not be forced to the data unless you click the Force button after defining them, or if you subsequntly move them.

Delete Point: removes the last point you added.

Delete All Points: removes all points, returning the corrected spectrum to its original state.

Replace: replace the existing original spectrum with the baseline-corrected spectrum. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Add: add the baseline-corrected spectrum to the document that contains the original spectrum. Both spectra are now in the main menu display. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

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Skip: Do not alter the current spectrum. Go the the next trace selected from the spreadsheet; if you were working on the last spectrum, return to the main menu display.

Cancel: return to the main menu display without acting upon the current spectrum or any subsequent spectra. Spectra previously replaced or added are not altered by this.

Do All: if selected, then the Deconvolution parameters selected for this spectrum are applied to this spectrum and to all subsequent spectra; they are all either Replaced or Added. Spectra previously replaced or added are not altered by this.

Help: enter the on-line Help system.

Baseline Correction Procedure

The usual procedure for correcting a baseline is:

1. Add points with Type=Linear.
2. Click Force points onto data.
3. Set Type=Spline. If the spline correction generates odd behavior of the baseline, then
4. Add more points, or move existing points.
5. Click Force points onto data.

If the baseline is satisfactory, click the Add button; if not, then continue adding or moving points.

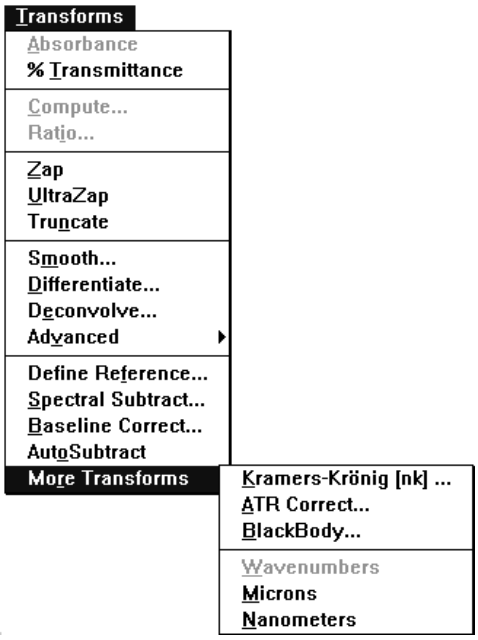
AUTO SUBTRACT

Automatically calculates an optimized subtraction factor, multiplies the reference spectrum by this factor, and subtracts it from the active spectrum. This is equivalent to selecting the Autosubtract button in Spectral Subtract. It also replaces the original spectrum with the difference spectrum. Before selecting this entry, you can define a region, or regions, of the spectrum to be used in calculating the optimized subtraction factor. If no region is selected, the entire spectrum is used for calculation. Selection of regions are usually based upon visual inspection of the sample and reference spectra.

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The subtraction factor is calculated to minimize the sum of the mean-square differences between the mean-centered sample spectrum and the mean-centered reference spectrum in the selected region(s).

MORE TRANSFORMS



Kramers-Krönig [nk]...

Computes the complex index of refraction from a reflectance spectrum, allowing specular reflectance spectra obtained from dielectric materials to be transformed into absorbance-like spectra.[4]

[4] George W. Chantry, "The Kramers-Kronig dispersion relations," pp. 214-230 and Appendix 1, pp. 399-401, in *Long-wave Optics, Volume 1 Principles*, Orlando, FL: Academic Press, Inc., 1984. See also the discussion on Fresnel equations, pp. 230-235, and Appendix 2, pp. 402-405.
R. T. Graf, J. L. Koenig, and H. Ishida, *Applied Spectroscopy*, **39**, 405, 1985.
K. Ohta and H. Ishida, *Applied Spectroscopy*, **42**, 952, 1988.
L. D. Tickanen, M. Tejedor-tejedot, and M. A. Sanderson, *Applied Spectroscopy*, **46**, 1848, 1992.
V. Hopfe, E. H. Korte, P. Klobes, and W. Grahlert, *Applied Spectroscopy*, **47**, 423, 1993.

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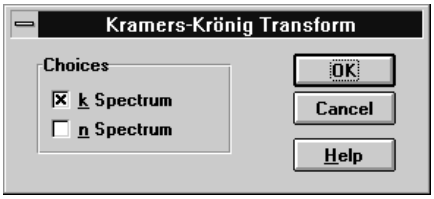
Note

The Y-axis of the spectrum should be either in Reflectance or %Reflectance units to get a meaningful transformation. If another type of spectrum is used, this error box appears



Click the OK button to continue.

When selected, the Kramers-Krönig Transform dialog box appears. Choose to calculate either an n (real part) spectrum or k (imaginary part) spectrum, or both, by selecting the appropriate box.



k: the spectrum of the imaginary part of the complex index of refraction. This is a good approximation to the absorbance spectrum of the material.

n: the spectrum of the real part of the complex index of refraction. It is not usually needed.

OK: the index of refraction spectrum (or spectra) is calculated and added to the document along with the current trace. During calculation, the Reporting Progress... status box appears. You can stop the process by pressing the Cancel button.

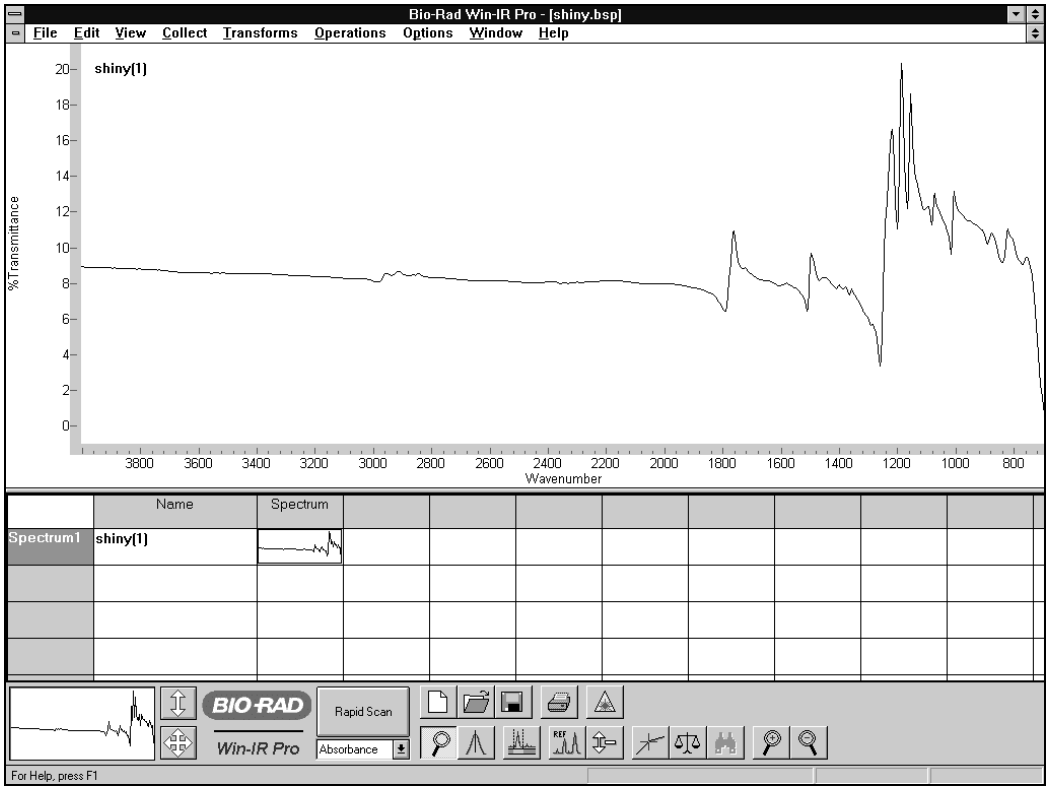
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Cancel: return to the main menu without performing any calculation.

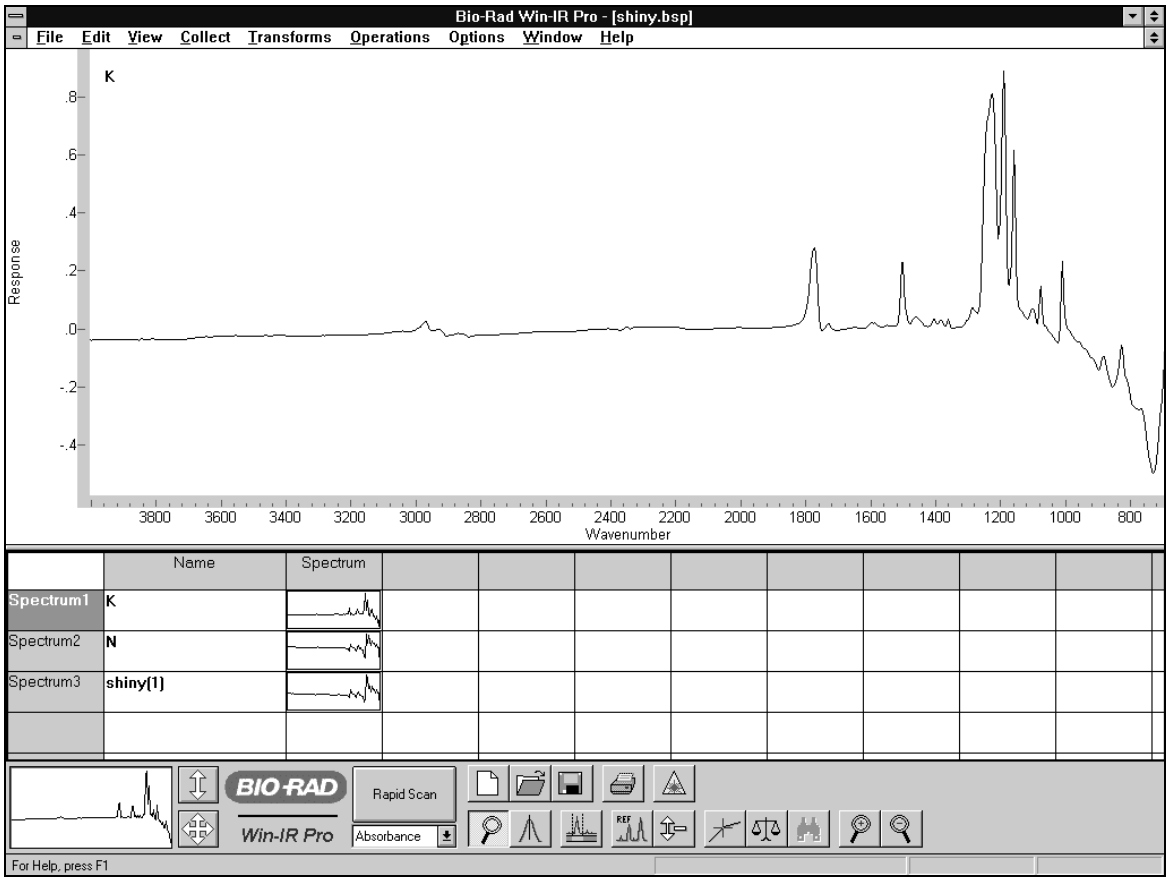
Help: enter the on-line help facility.

Consider the reflectance spectrum, shiny.bsp,



Create both the n and the k spectra. The k spectrum will be spectrum 1 (labeled as K), the n spectrum will be spectrum 2 (labeled as N), and the original spectrum will be spectrum 3. You may want to edit the spreadsheet to more completely identify the newly created spectra.

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ATRCorrect...

This transform corrects the relative intensities of a mid-range infrared spectrum collected using the Attenuated Total Reflectance (ATR) method.[5] In an ATR spectrum the light penetrates into the sample to a depth proportional to wavelength (as well as the reflection angle, the refractive index of sample, and the refractive index of the ATR element). Longer wavelengths pass through more of the material and, therefore, are absorbed more. An ATR spectrum differs from an absorbance spectrum in that absorbances at low frequencies are proportionally greater than those at higher frequencies. While other effects exist, in a typical spectrum the largest spectral pertubation is from the wavelength-dependent variation of the penetration depth. It can be corrected using this transformation

$$A_{corrected} = (A_{atr}) * (\text{frequency})^{n}$$

where the correction exponent, n can be any reasonable positive. Typical values range from 0.5 to 5.0 value (the default is 1.0). The value of n which best corrects real spectra need not be 1.0; it must be determined empirically. It is usually between 0.5 and 1.5.

Note

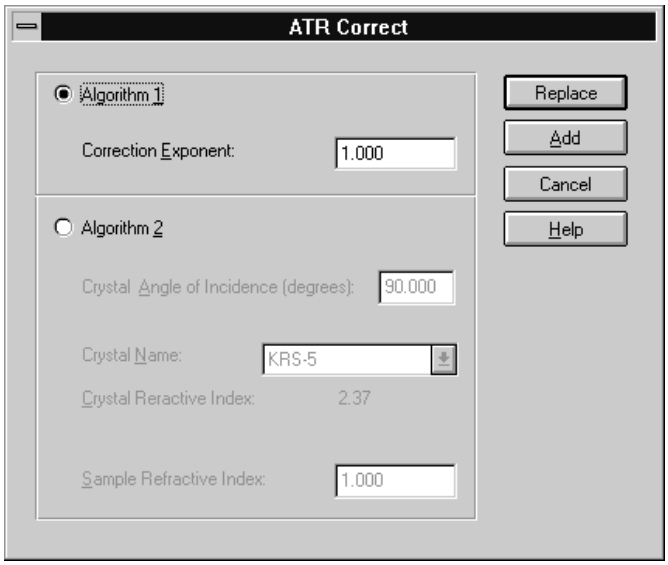
An exponent of 1 is always appropriate for ATR; the depth of penetration is a linear function of wavelength. Other values of the exponent might be used for spectra obtained using other techniques, for example, PAS.

Two correction algorithms are available. The first is normally used for qualitative experiments. The second is used when you are running the same sample with different crystals and want to compare the results.

When selected, the ATR Correct dialog box appears.

[5] Peter R. Griffith and James A. de Haseth, *Fourier Transform Infrared Spectrometry*, equation 5.2, page 194, John Wiley & Sons, 1986.

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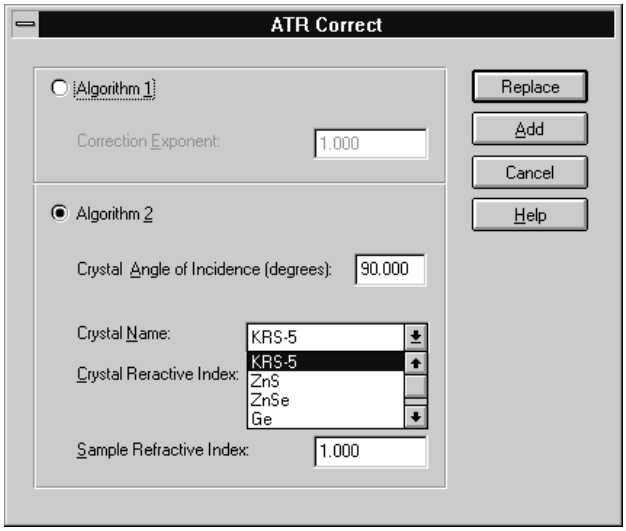
Algorithm 1: used for qualitative experiments.

Correction Exponent: enter the selected value.

Algorithm 2: used for quantitative and comparison measurements.

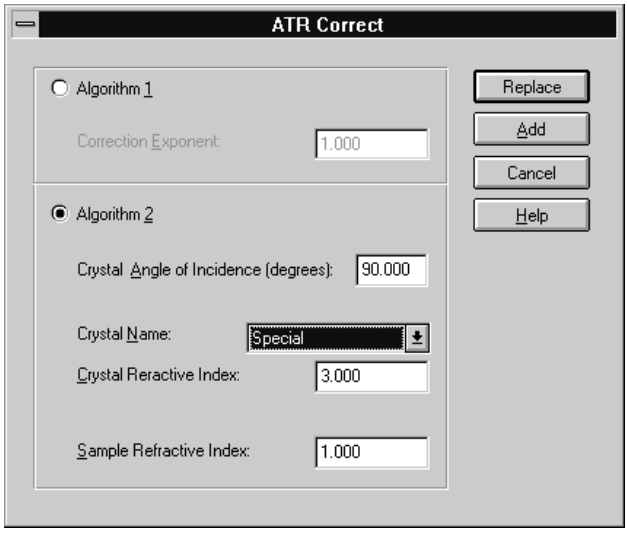
Crystal Angle of Incidence (degrees): enter the angle being used in your experiment.

Crystal Name: use the pull-down menu to select the crystal.



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If you are using a crystal other than one of those listed, select Special. The dialog box then allows you to enter its refractive index.



Crystal Refractive Index: this is displayed automatically for the selected type of crystal, except for Special (see above).

Sample Refractive Index: enter the value for the sample.

For either algorithm:

Replace: the current trace is replaced by the ATR-corrected spectrum.

Add: the ATR-corrected spectrum is added to the document; the current trace is not overwritten.

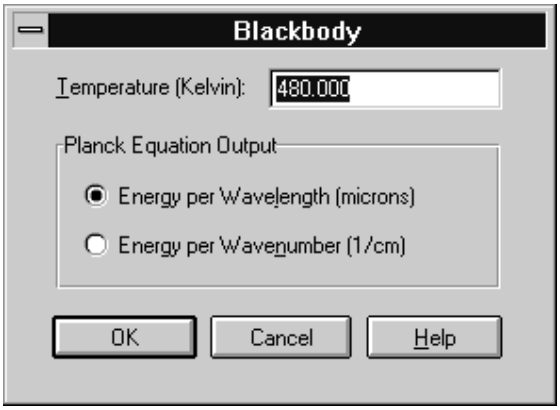
Cancel: return to the main menu without performing an ATR correction.

Help: enter the on-line help facility.

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BlackBody...

It is sometimes useful to ratio a spectrum (especially an emission spectrum) against the theoretical emission spectrum of a blackbody at the same temperature. In order to guarantee that you can perform arithmetic operations with the original spectrum, it is used as a template to compute a blackbody spectrum in the same format (resolution, wavenumber range, etc.). The transform can compute the blackbody spectrum for any temperature. When selected, the Blackbody dialog box appears.



Temperature (Kelvin): enter the temperature of the sample (in K). Room temperature is approximately 300 K.

$$K = °C + 273.15;\ °C = (°F - 32) * (5/9)$$

Planck Equation Output: select the output display. It can either be in units of Energy/Wavelength (microns) or in units of Energy/Wavelength (cm^{-1}). The discussion below explains the difference between the two displays.

OK: the new trace is displayed in addition to the original trace.

The Planck blackbody equation for energy per unit wavenumber as a function of wavenumber and temperature is[3]

$$E(w,T)dw = \frac{8\pi hc^2 w^3}{e^{hcw/kT} - 1} dw$$

[3]George W. Chantry, "Mathematical theory of black-body radiation," pp.85-98, in *Long-wave Optics, Volume 1 Principles*, Orlando, FL: Academic Press, Inc., 1984.

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h is Planck's constant (6.6256 x 10^{-27} erg-seconds)
k is Boltzmann's constant (1.38054 x 10^{-16} erg/K)
c is the speed of light (2.997925 x 10^{10} cm/second)
T is temperature (K)
w is the wavenumber (cm^{-1})

The equivalent equation for energy per unit wavelength, λ (cm) and temperature is

$$E(\lambda,T)d\lambda = \frac{8\pi hc^2\left(1/\lambda\right)^5}{e^{hc/\lambda kT}-1}d\lambda$$

multiply the wavelength in cm by 10^4 to get the wavelength in microns.

E(w,T) and *E(λ,T)* have their maxima in different parts of the spectrum. The maximum in *E(λ,T)* is found by differentiating the core function and setting the derivative to 0. This yields Wien's displacement law

$$\lambda_{max}T = 2.8978 \times 10^{-1} \text{ cm-K} \quad \text{or } 2.8978 \times 10^{3} \text{ microns-K}$$

The wavenumber in the *E(λ,T)* curve corresponding to λ_{max} is

$$w_{max} \ (cm^{-1}) = 3.451\ T$$

Cancel: return to the main menu without creating a blackbody spectrum.

Help: enter the on-line help facility.

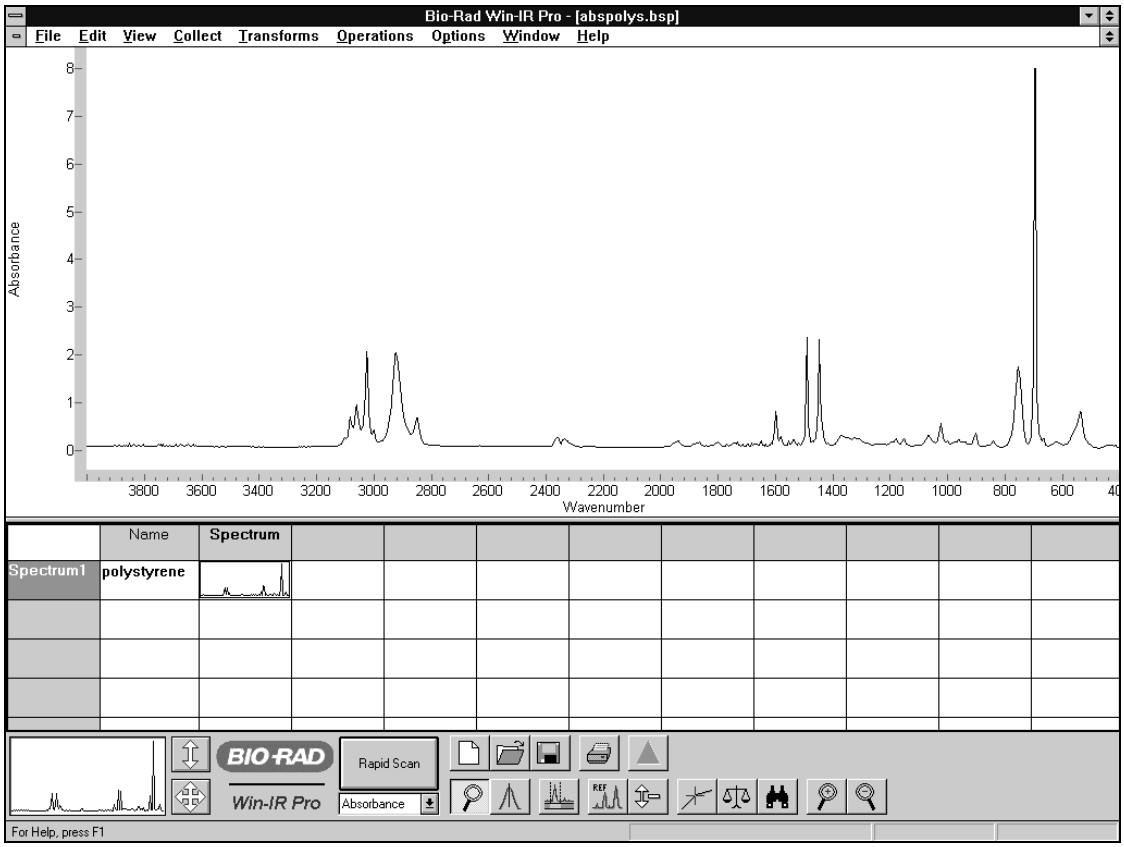
Note

If the spectrum X-axis units are wavenumbers (cm^{-1}), then the blackbody spectrum will be energy/cm^{-1}. If you want to display the blackbody spectrum as energy/micron (or energy/nanometer), select View / X Axis Units / Microns (or Nanometers).

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Wavenumbers

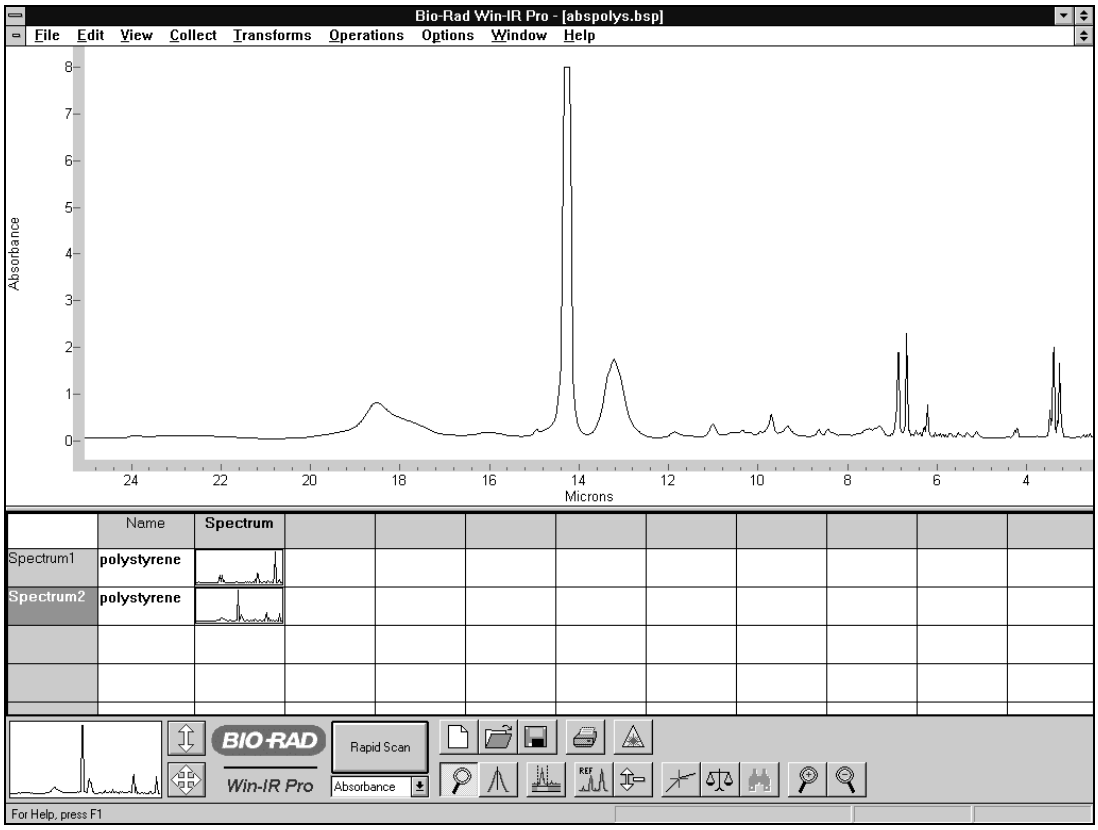
Display the spectrum using wavenumbers (cm^{-1}) as the unit of the X axis (default). The spectrum below has wavenumbers for its x-axis unit.



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Microns

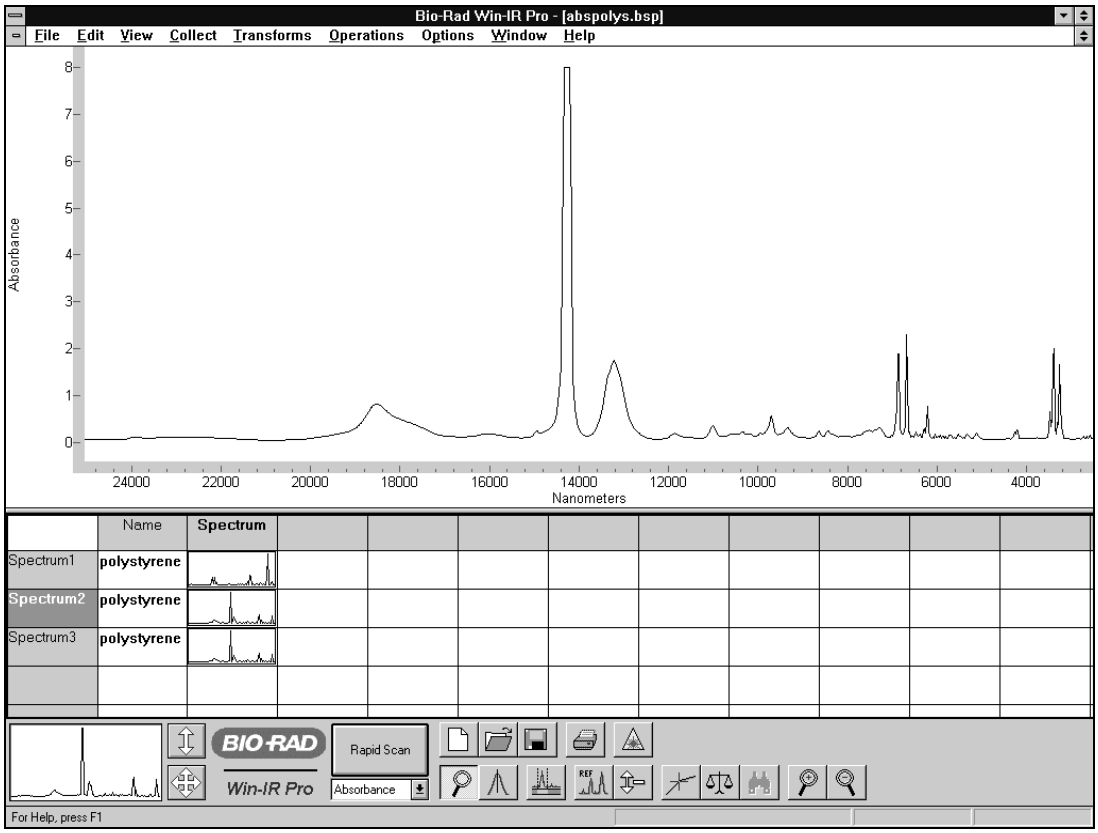
Display the spectrum using microns (10^{-6} meters, more properly micrometers) as the units of the X axis.



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Nanometers

Display the spectrum using nanometers (10^{-9} meters) as the units of the X axis.



Notes

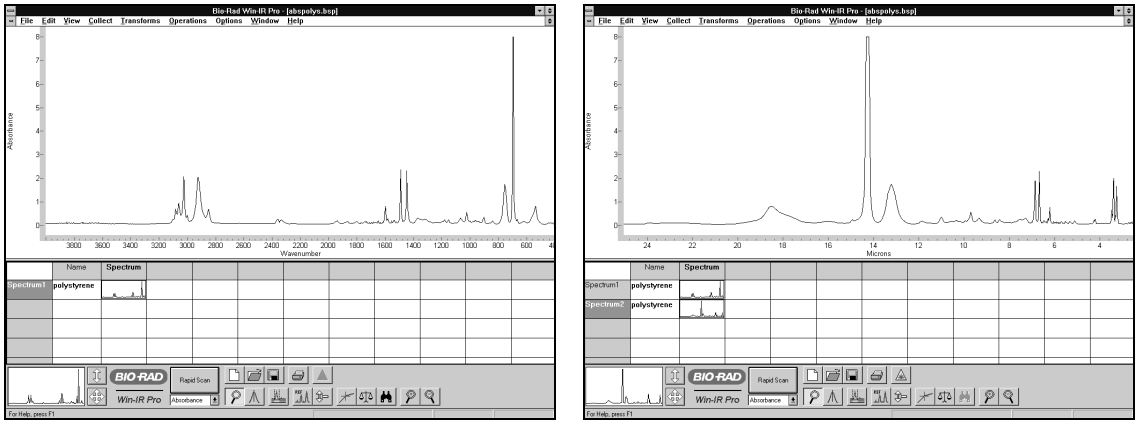
The transform is disabled for the existing x-axis units; for example, if a spectrum is displayed in wavenumbers, the Transforms / More Transforms / Wavenumbers entry is disabled.

When spectra are transformed, the mathematical interpolation causes a small loss of information. Therefore, transforming a spectrum, and transforming it back to its original x-axis units does not yield a spectrum identical to the original one. You can restore the original

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spectrum by using Operations / Reprocess. You can also save the original spectrum using Operations / Copy Spectrum (see Chapter 11).

Wavenumbers are inverse lengths, therefore, the spectrum will not appear the same if Microns or Nanometers are chosen instead of Wavenumbers. For example, the same spectrum is displayed below with wavenumbers (left) and microns (right) as the X-axis units.



The number of points is the same in the transformed and original function. This means that points tend to cluster around low-values of the wavenumber. If you want to transform a single-beam spectrum to microns (or nanometers), it is best to truncate it, removing the points near 0 wavenumbers.

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11
Operations Menu



In general, operations take spectral data and use them to create, find, or analyze, in distinction to transforms which actually change the spectrum itself.

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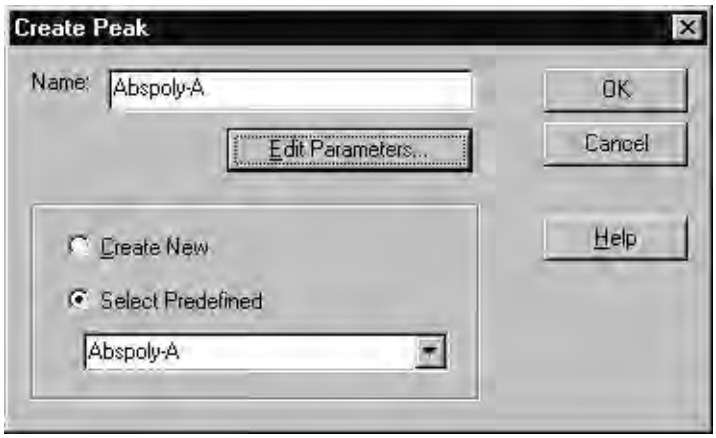
NEW

Allows you to define a variety of peaks, of trace labels, and to register custom value programs.



Peak

When selected, the Create Peak dialog box appears. In this example, a peak called Abspoly-A was predefined in another document.



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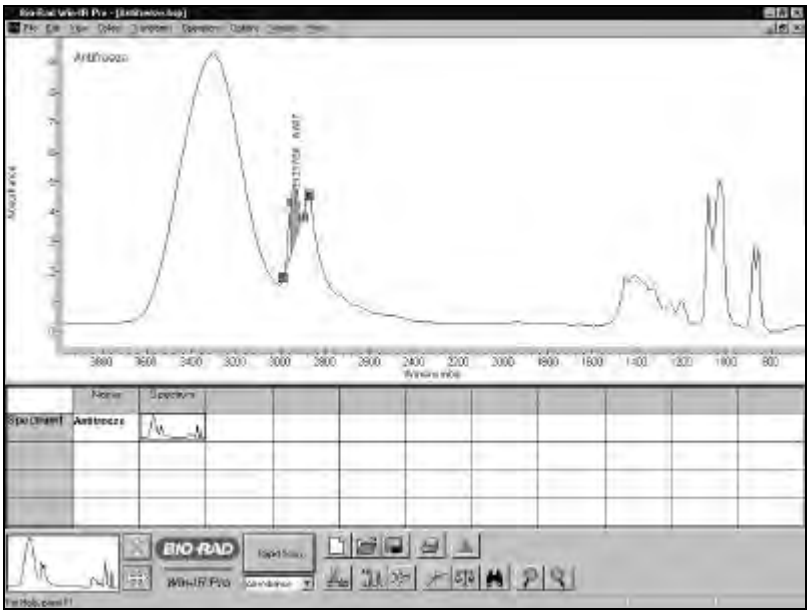
To create a peak with the same parameters as Abspoly-A, select Select Predefined and click the OK button. This creates a peak with the parameter of Abspoly-A. If you want the peak to have a different name, enter this in the Name window of the dialog box.

Notes

If more than one peak is predefined, selected the desired predefined peak from the pull-down menu.

It does not matter whether the predefined peak was a peak, reference peak, or peak template; it will be defined as a peak.

If you want to make any modifications to the predefined peak parameters before creating the peak, click the Edit Parameters button. This brings up the standard peak editing dialog box.

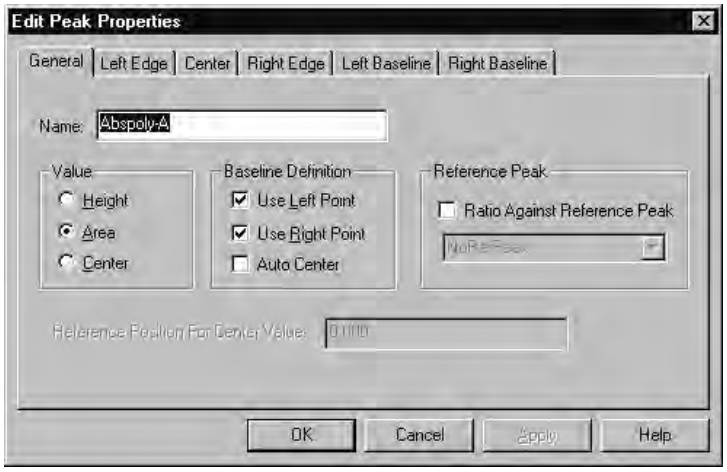


You can edit this peak—including changing its name—using the procedures described in Chapter 2.

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Alternatively, you can create a peak that was not predefined. The procedure is:

1. Select Create New.
2. Click the Edit Parameters button. The Edit Peak Properties dialog box appears.



3. Edit the peak parameters using the tab pages; see Chapter 2 for details. You will probably want to change the name of the peak also.

Note

The default peak parameters defines a peak in the center of the spectrum with edges at ~±6.7% and baselines at ~±10% of the total spectrum from the center. These values are for the full spectrum and are independent of the portion of the spectrum being displayed.

4. Click the OK button. This returns you to the Create Peak dialog box.
5. Click the OK button. The peak is now defined and can be edited using standard techniques.

Reference Peak

The operation is exactly the same as for Peak, except that a reference peak is defined. .

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Peak Template

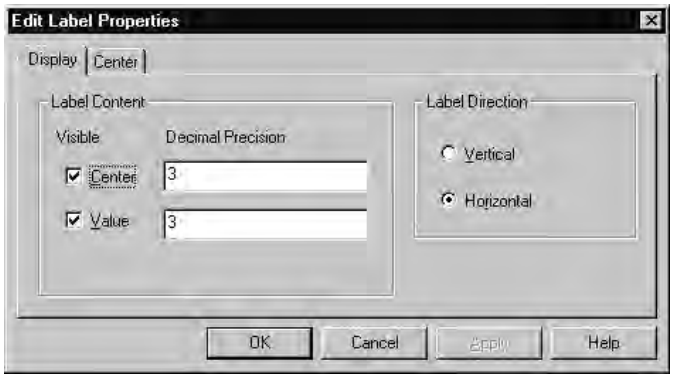
The operation is exactly the same as for Peak, except that a peak template is defined.

Note

If the active document is Kinetics, then this entry is called Functional Group; if the active document is quantitation calibration, then this entry is called Component; if the active document is Image, then this entry is called Image Peak.

Position Label

Inserts a position label (with x- and y-coordinates) at the selected position of the trace. When selected, the Edit Label Properties dialog box appears.

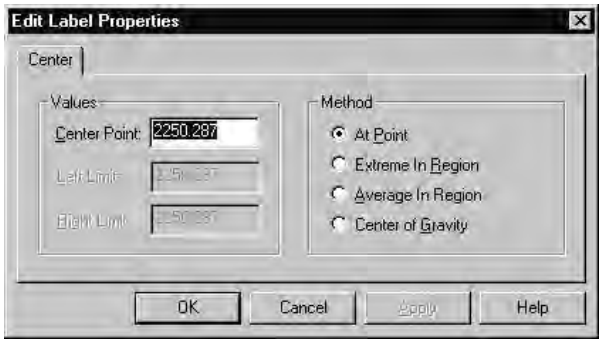


Set the parameters as discussed in the “Position Label” section of Chapter 1.

Annotation

You can place text annotations on the display ; each annotation can be connected to a point on the spectrum—for example, a peak, a group of peaks, or some interesting feature of the spectrum. When selected, the Edit Label Properties dialog box appears.

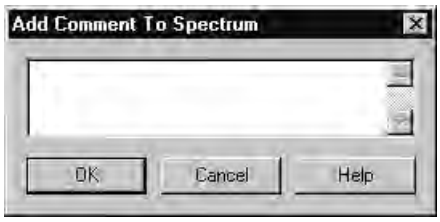
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Set the parameters as discussed in the "Annotation" section of Chapter 1

Comment

You can add comments to the spectrum. When selected the Add Comment to Spectrum dialog box appears.



Place the cursor in the box and click the left mouse button. You can now type in a comment. For details see the "Adding Comments" section of Chapter 1.

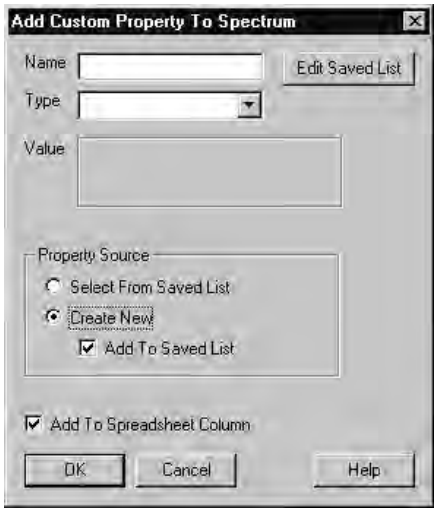
Chemical Structure

Chemical structure is not implemented at the current release.

Custom Property

You can add custom properties to the trace and spreadsheet. When selected, the Add Custom Property to Spectrum dialog box appears.

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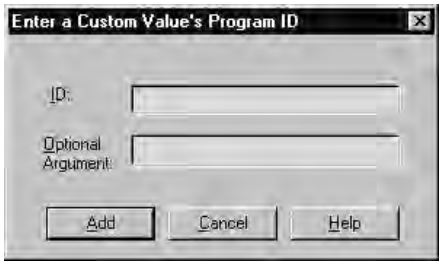


Follow the procedures in the "Adding Custom Properties" section of Chapter 1 to create new custom properties or to use existing custom properties previously defined.

Custom Value

This entry registers custom value programs so that they can be executed within Win-IR Pro on an opened image (.dat) document. The program calculates a value for each spectrum in the array—such as spectrum area, highest peak, etc. This output can be displayed on the screen. See Appendix N for details of constructing such programs and assigning them a Program ID (ProgID).

When selected, the Enter a Custom Value's Program ID dialog box appears.



Enter the Program ID that was defined in creating the program; click the Add button. This program is added to the list that appears in the Feature pull-down menu on the image document main window (see "Image Document Window" in Chapter 3 for more details).

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Note

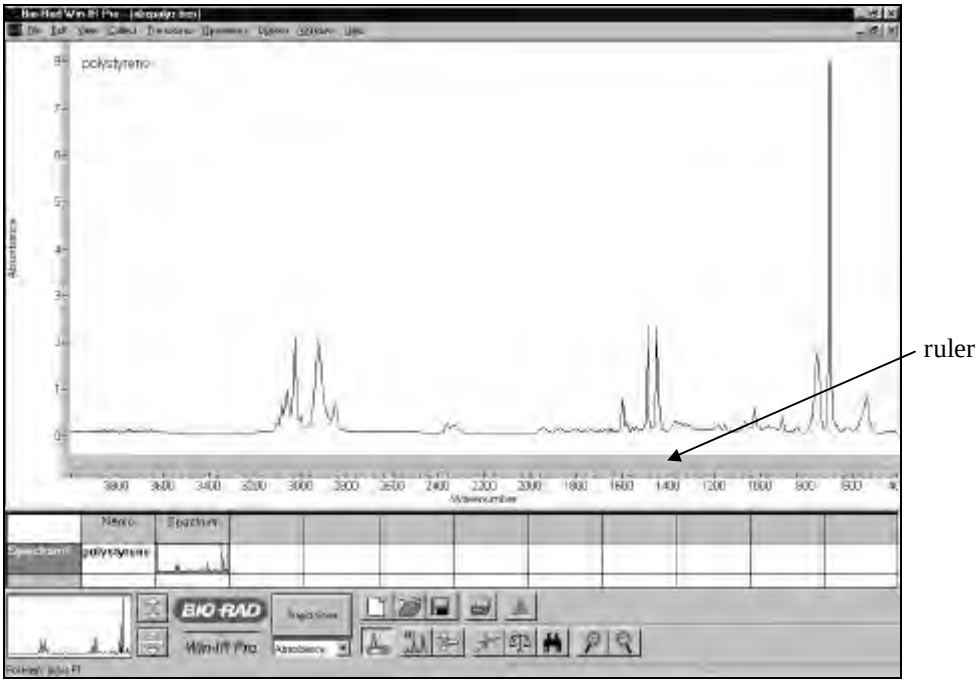
The Program ID is defined within the program; it is entered into the registry when the DLL is created. It is **not** the program file name.

Optional Argument: you may have written your program to use an optional argument (or arguments). If this is the case, enter those arguments here. This entry will be passed to the program as a character string. Your program must be written to analyze this string and make use of the information (see Appendix N for more information).

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DRAG REGIONS

Toggles the regions ruler on and off. Use this region to interactively select regions of the trace. Some of the selections in the Transforms menu work on a region of the spectrum, rather than the whole spectrum. When this entry is selected, a blank rectangle (the ruler) appears at the bottom of the trace display, just above the X-axis scale.



Multiple regions can be defined for any spectrum. To define a region by dragging:

1. Put the cursor into the ruler at one end of the region to be selected. The cursor changes to .

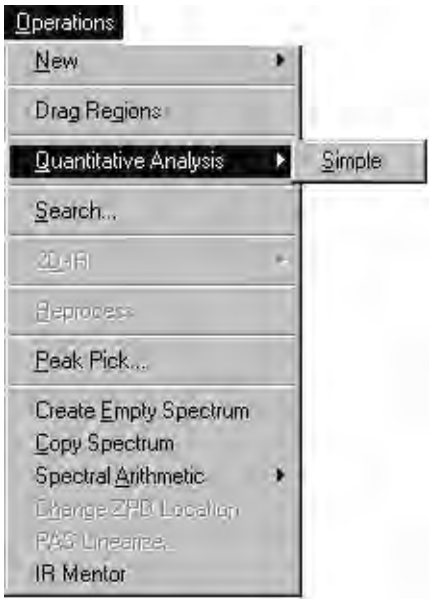
2. Hold down the left mouse button and drag the cursor to the other end of the region being defined. Release the button. The region is defined by the vertical dashed lines. The white bar at the bottom of the region means that this region is active and selected.

See the “Regions” section in Chapter 1 for details of modifying and deleting regions.

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QUANTITATIVE ANALYSIS

Perform a quantitative analysis on the spectrum.



Simple quantitative analysis is available as a standard part of Win-IR Pro.

In order to perform quantitative analysis on a spectrum, you must already have generated a Quantitation Calibration Document. This document contains spectra of components of known concentrations, the concentrations, and a least-squares fit of the concentrations to the spectral data. The procedure following in this chapter assumes that such a calibration document exists. See Chapter 3 for an explanation of the Quantitation Calibration Document. A detailed discussion of the theory and practice of quantitative analysis is in Appendix I.

Note

Before performing quantitative analysis, select View / Display Limits, and set all entries to Auto. Autoscaling can be enabled by putting the cursor in the radar box and clicking the left mouse button.

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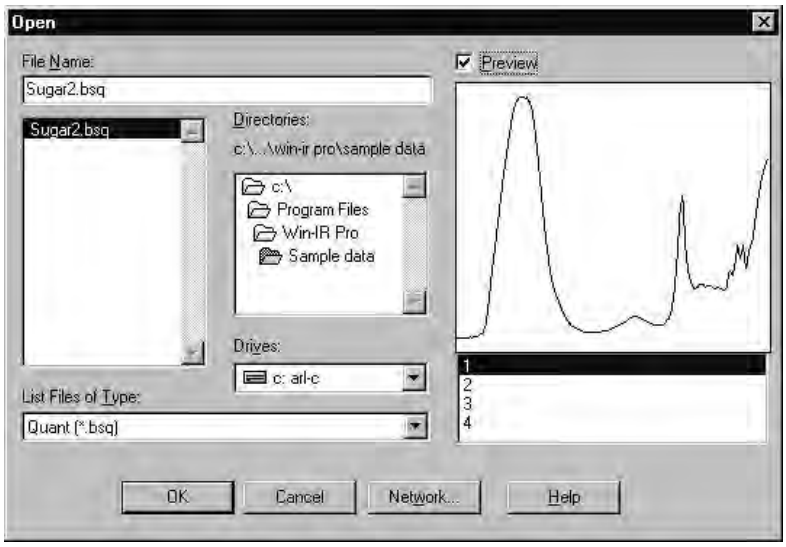
Simple

First, open the calibration document.

Then, before performing a quantitative analysis, make sure that the calibration document is ready.

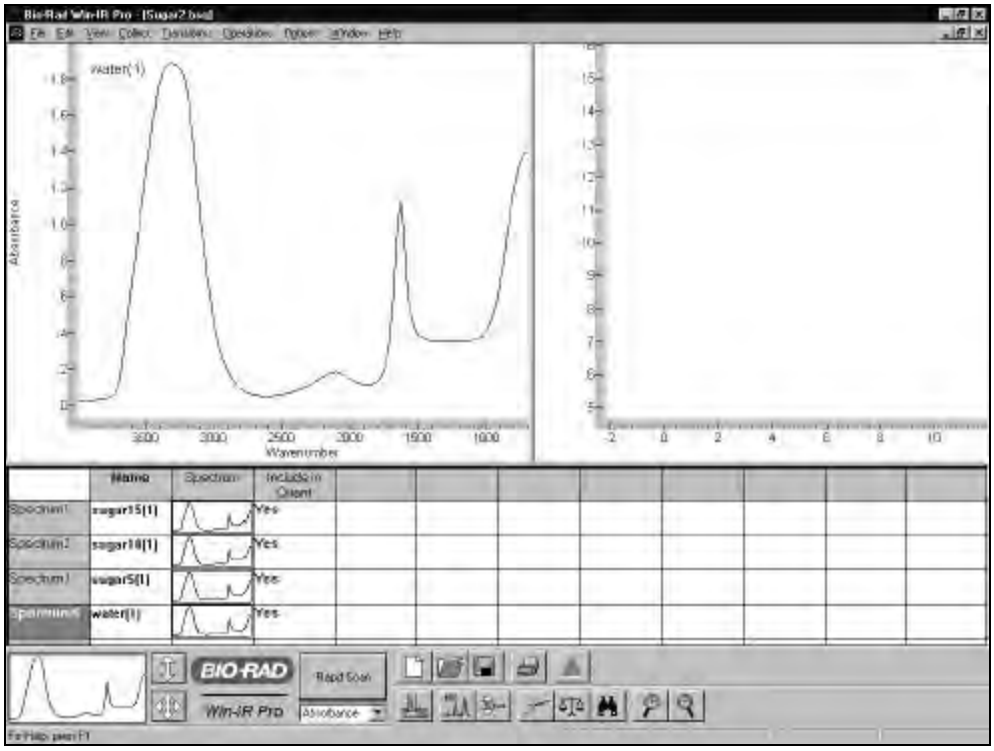
1. Select Open from the File menu.

2. Set List Files of Type to Quant (*.bsq). This lists all files with a .bsq extension.



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3. For this example, select Sugar2.bsq and open it.



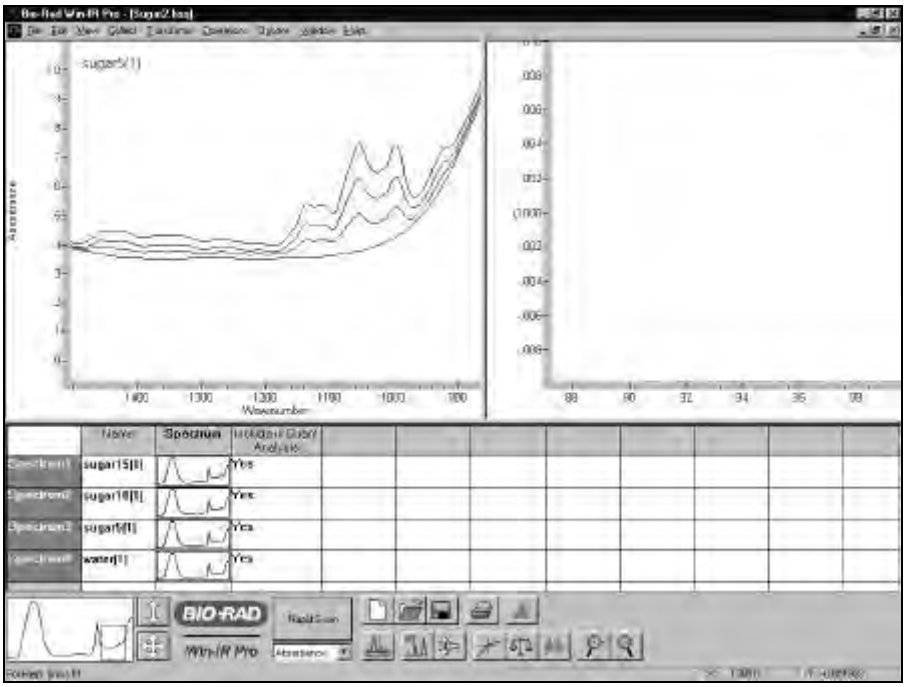
4. The Include in Quant Analysis column is in the spreadsheet; its cell values are set to Yes. If you do not want to use a spectrum for the quantitative analysis, double-click in its Include in Quant Analysis cell. This will change the value from Yes to No. Double-click a No entry, if you wish to change it to Yes.

Note

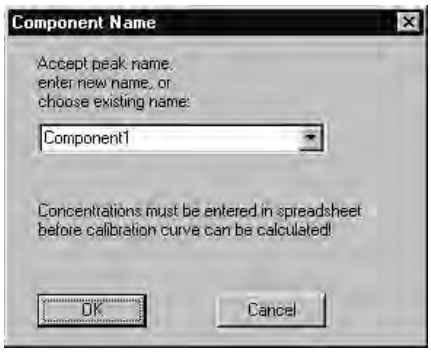
If you delete the Include in Quant Analysis column (for example, by using View / Remove Column), you can redisplay it using View / Property Browse Bar.

5. Select all the spectra in the document. Zoom in on the region where the spectra differ (in this example, about 1500-850 cm^{-1}).

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6. Place the cursor on the component to be used for the calibration and click the right mouse button. Select New / Component. The Component Name dialog box appears.



7. In this example, highlight the entry, and type CompSugar to replace Component1. Click the OK button.

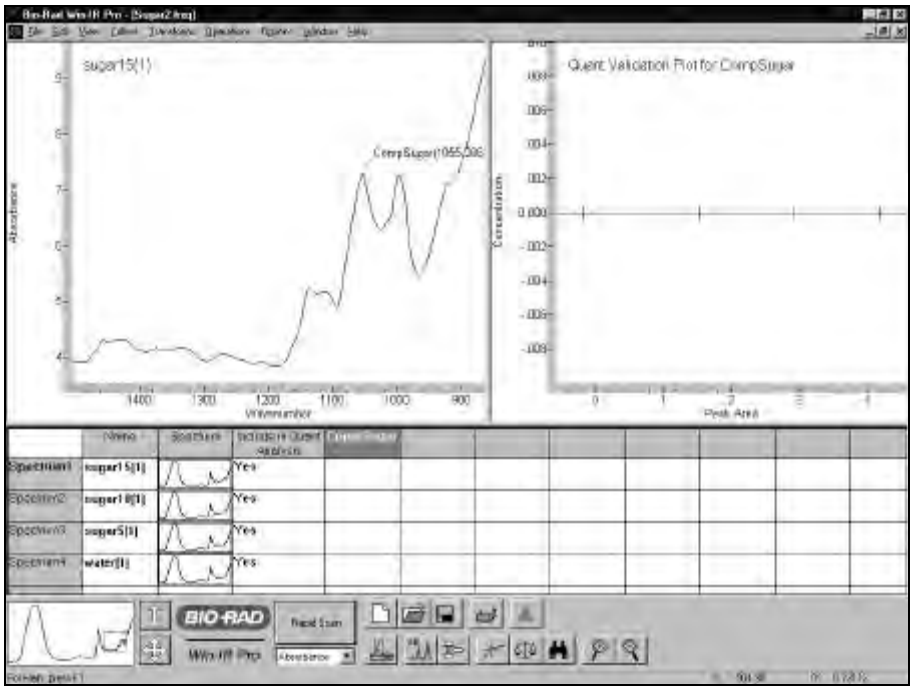
Notes

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Alternatively, select Operations / New /Component to use a predefined component. See Chapter 11 for details.

You can edit and/or save any component in your quantitation calibration document for use in other documents, with the right mouse button's menu entry Save As Predefined. See Chapter 2 for for details.

When a component is selected using the right mouse button, the calibration will be based upon the default setting, that is, upon the area of the selected component. Other data that can be used to perform the calibration area peak height, ratio of peak areas, or ratio of peak heights. In the case of the latter two, you must also define a reference peak against which the ratios can be performed.

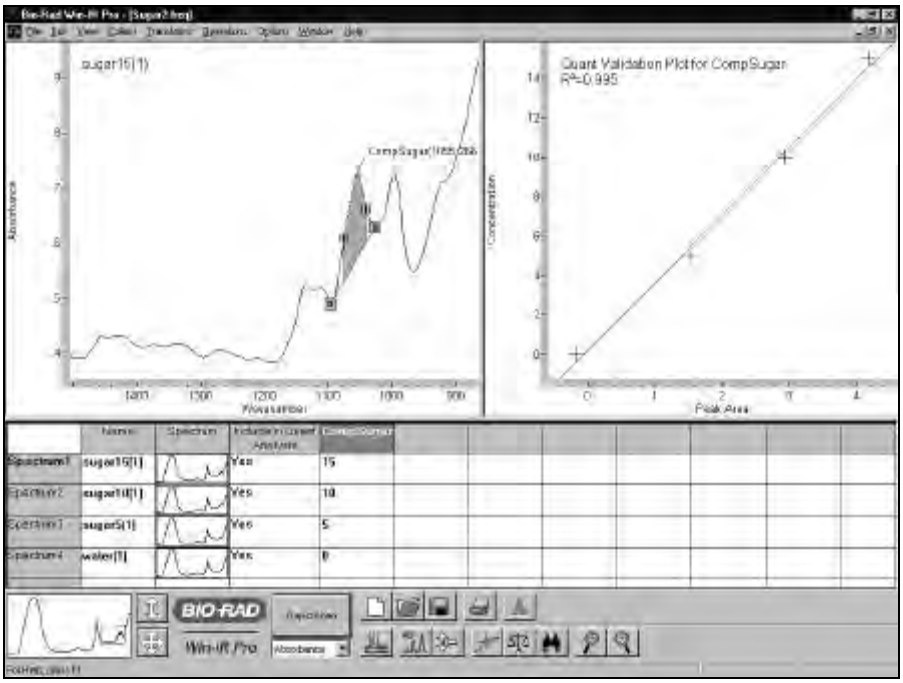


A new column CompSugar has been added to the spreadsheet. The

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calibration curve (right half of screen) is flat because there is no concentration entered in the cells (this is equivalent to a value of 0).

9. Enter the known values of the sugar concentration. In this example, they are 15, 10, 5, and 0. The calibration curve changes as shown below.



The default calibration curve is linear with a non-zero intercept ($ax + b$). The correlation coefficient (R^2) is shown in the upper left corner of the calibration curve window.

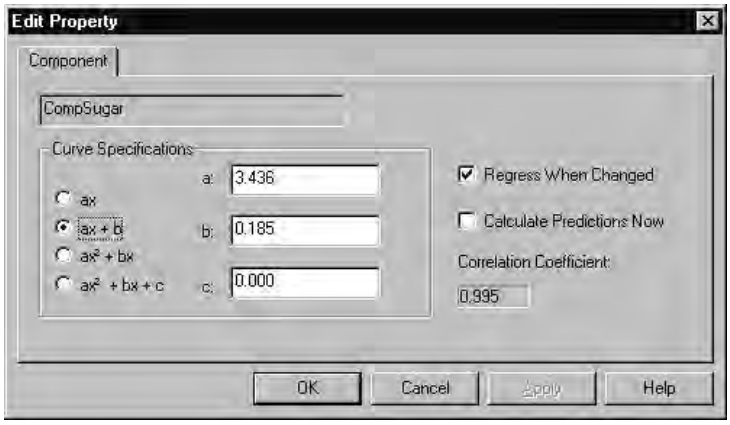
10. Select Save from the File menu.

The Quant Calibration document is now ready. Before you begin analysis, you should examine the calibration curve to see if any of the values vary significantly from the curve. If you want to use a calibration curve other than the default or view the coefficients of the calibration curve, follow this procedure.

1. Place the cursor in the calibration (right hand) side of the window.

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2. Click the right mouse button and select Properties from the menu. The Edit Property dialog box appears.



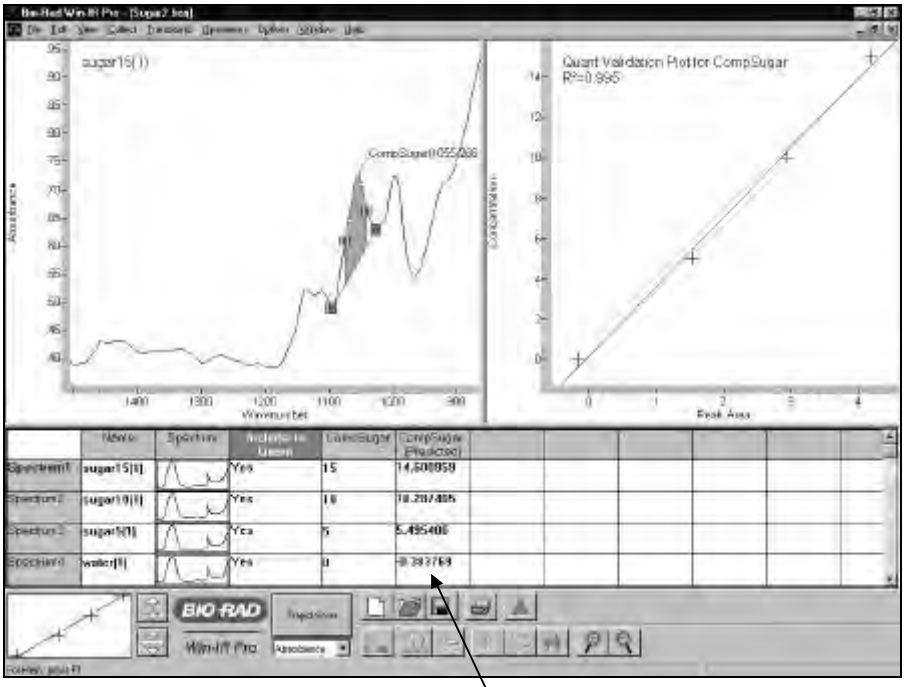
Curve Specifications: select the equation for the curve that is to be fitted to the data points. The Apply button is enabled; click the Apply button for a new calibration curve. The coefficients of the equation will change and be displayed in a, b, c.

Regress When Changed: if selected, the equation coefficients will change if the curve type is changed and Apply is clicked. The Correlation Coefficient will be displayed with the calibration curve.

Calculate Predictions Now: when selected, his creates a new column in the spreadsheet; CompSugar (Predicted) in this example shown below. These are the concentration values calculated from the calibration curve for the absorbance values in the standards spectra. Note that, as expected, they are close to the nominal values.

Correlation Coefficient: displays the calculated correlation coefficient.

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Notes

If you remove the column with concentrations, it does not affect the calibration for that component; the spreadsheet is displaying (or not displaying) the concentration information. Use View / Property Browse Bar to re-display the concentrations column.

After you have created a calibration curve, you can print it. The title of the plot, the equation used, the value of the coefficients, and the correlation coefficient are printed in the upper left corner of the plot.

1. Put the cursor in the Quant Validation Plot portion of the window and click the left mouse button.

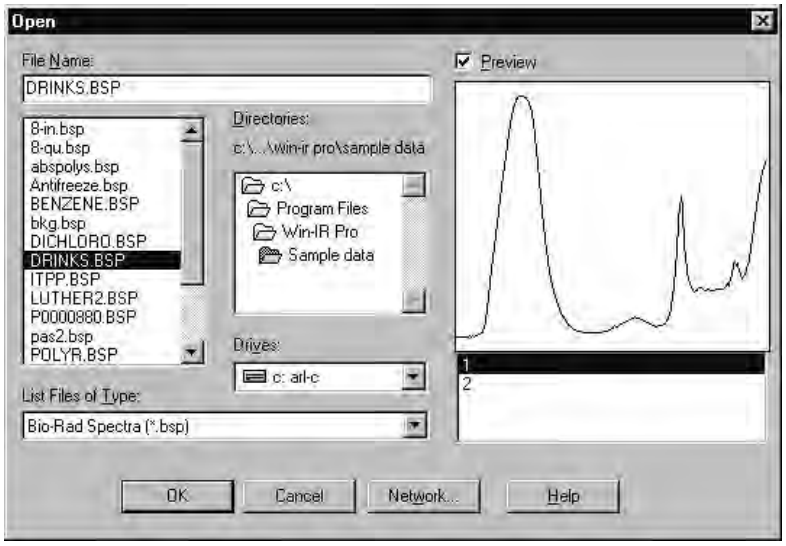
2. Click the  button or select Print from the File menu and click OK.

3. Close the file by selecting File / Close.

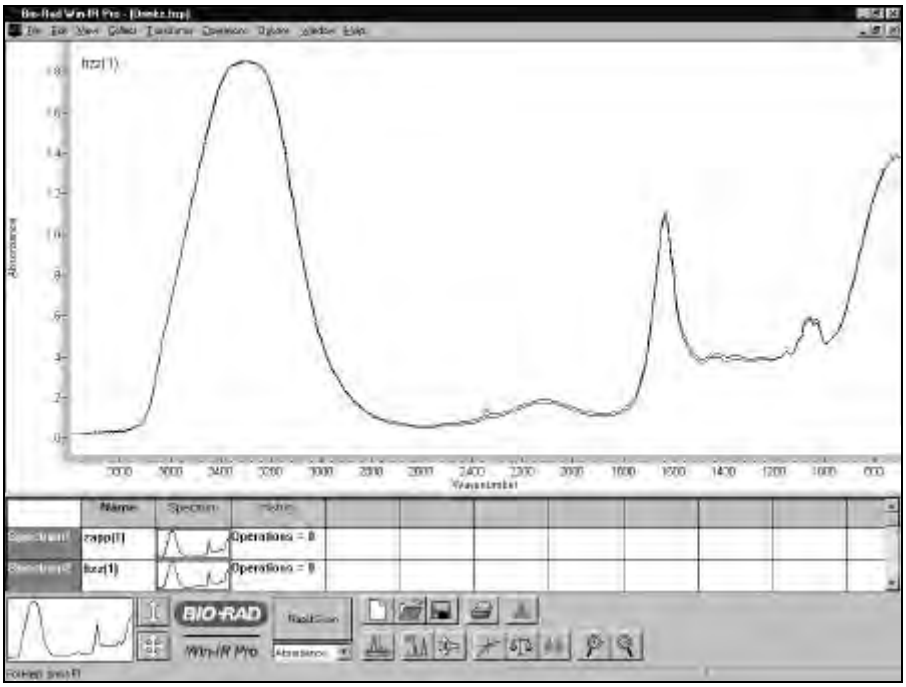
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Quantitative Analysis: You can now begin analysis.

1. Select Open from the File menu and select the spectra to be analyzed. In this example, use drinks.bsp.



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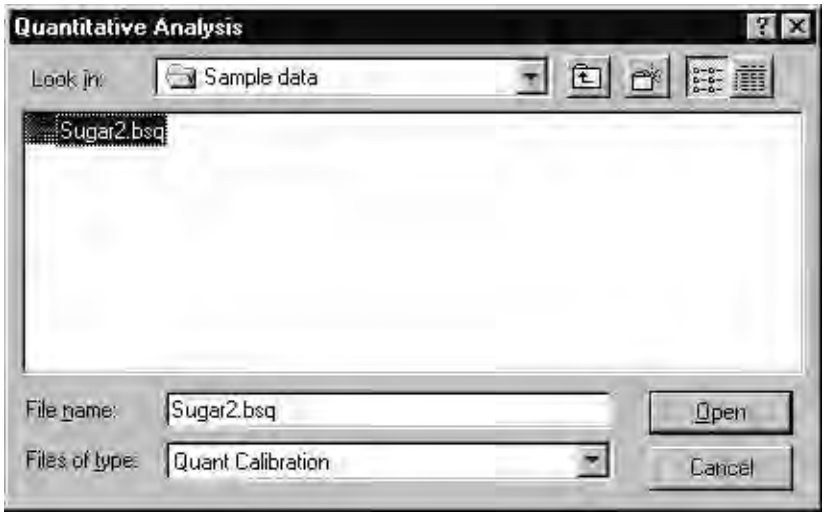
Note

For illustrative purposes, History has been added to the spreadsheet. See Property Browse Bar in Chapter 8, if you wish to do this.

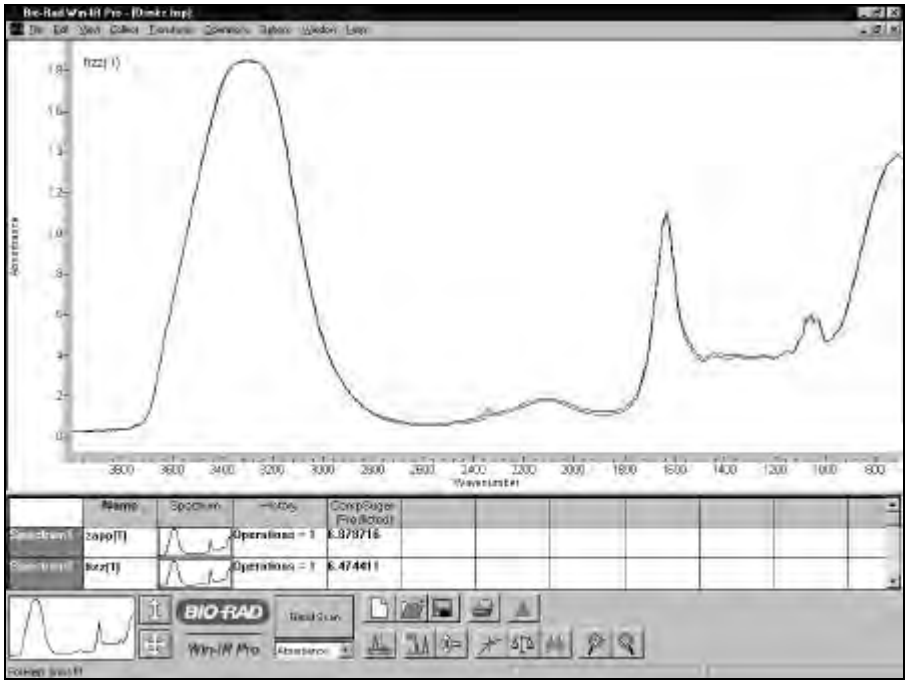
2. Select the spectra to be analyzed. In this case, select both spectra.

3. Select Quantitative Analysis / Simple from the Operations menu. The Quantitative Analysis dialog box appears.

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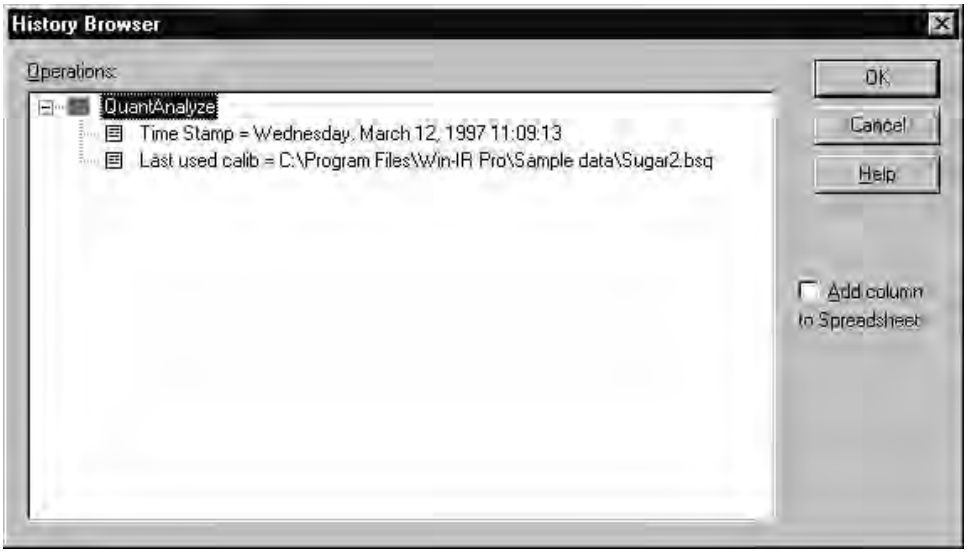


4. Select the desired Quant Calibration document using the standard Windows NT procedures. Use sugar2.bsq for this example. This performs the analysis. The results are entered into the spreadsheet.



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The history of both of the analyzed spectra has been incremented by 1. Select one spectrum; then select History from the View menu.



This tells you what calibration document was used to analyze the spectrum.

If you wish to save the document under its current name

4. Select Save from the File menu.

5. Select Close from the File menu.

You can save the document with a new name by selecting Save As... from the File menu.

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SEARCH...

Searches the libraries to try to find a match for the selected spectrum. After the search is completed a hit list is displayed showing libraries entries with the best matches.

Normally, only absorbance (or absorbance-like) spectra are searched for in the libraries, because most commercial libraries have their entries in that format. If you select a spectrum of a type other than an absorbance the Operations / Search entry is disabled. However, if you need to search libraries for a non-absorbance spectrum, this entry can be enabled using Options / Search (see Chapter 12 for details).

Note

If you manually terminate a search before its conclusion (by pressing the Cancel button), a hit list will be displayed showing the matches already found. However, this list is incomplete and using it to identify the sample spectrum may lead to errors and misassignments.

Search Considerations

There are several types of searches: spectral, names, peaks, and-if you have loaded advanced search-structures. Each type of search compares a feature, or features, of the unknown spectrum, to the corresponding feature of the spectra in the selected library, or libraries. In some searches (spectral, peaks), a "goodness-of-fit" parameter (the Hit Quality Index, or HQI) is calculated showing how closely the unknown matches the library spectrum. A specified number of the best matches are retained. In other searches (name, structures), the test is pass/fail; either the library spectrum entry contains the specified name (or structure) or it doesn't. Because HQI is always 0.0 for a successful pass/fail search, the matches are not listed in any particular order.

When a spectral or peaks search is performed, the HQI must be calculated for each spectrum in the library. This current HQI is compared to the worst HQI in the list; if the current spectrum's HQI is as good as, or better than, the worst HQI in the list, the current spectrum is added to the hit list *in the proper place.* This comparison and insertion takes time. The hit list is kept in memory in a format similar to a .bsp file. A large hit list can consume considerable memory and can possibly cause the computer to run out of memory. Typically, you need to keep only 30-40 hits for a spectral or peaks search hit list.

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You can speed searching by pre-searching the libraries with names or structures searches, followed by a re-search (discussed later in this section). These pre-searches make use of additional information you have about the unknown. For example, if you know that the unknown contains chlorine, there is no need to spend time calculating HQIs for spectra that are known not to contain chlorine. If you know a particular molecular structure exists in your unknown, you want to perform a spectral or peaks search only on those spectra containing that structure. You normally keep all hits in a pre-search because they all have the same HQI.

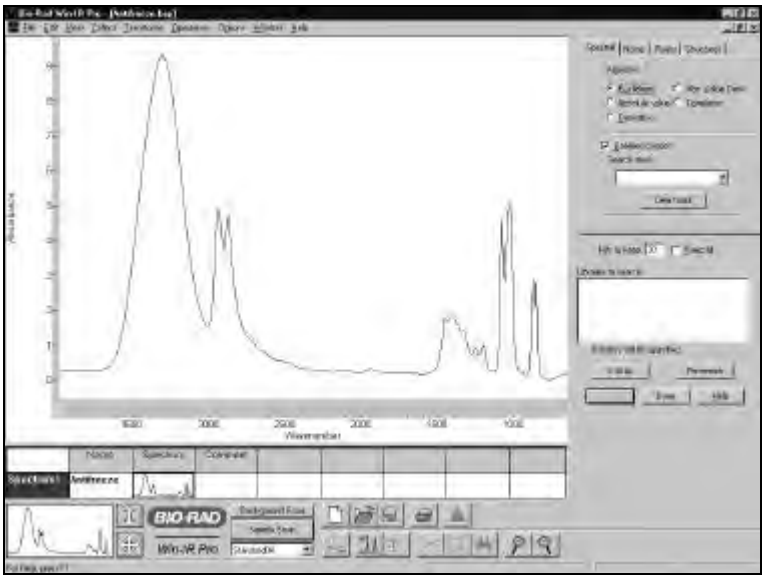
Note

All libraries supplied by Bio-Rad contain names; not all contain structures. The Search Library Selection box (see below) contains a list of what type of information is stored in each library.

After a pre-search hit list is created, you can re-search this list, as if it were a library. This is normally done using a spectral or peaks search. Details of these procedures are discussed later in this section.

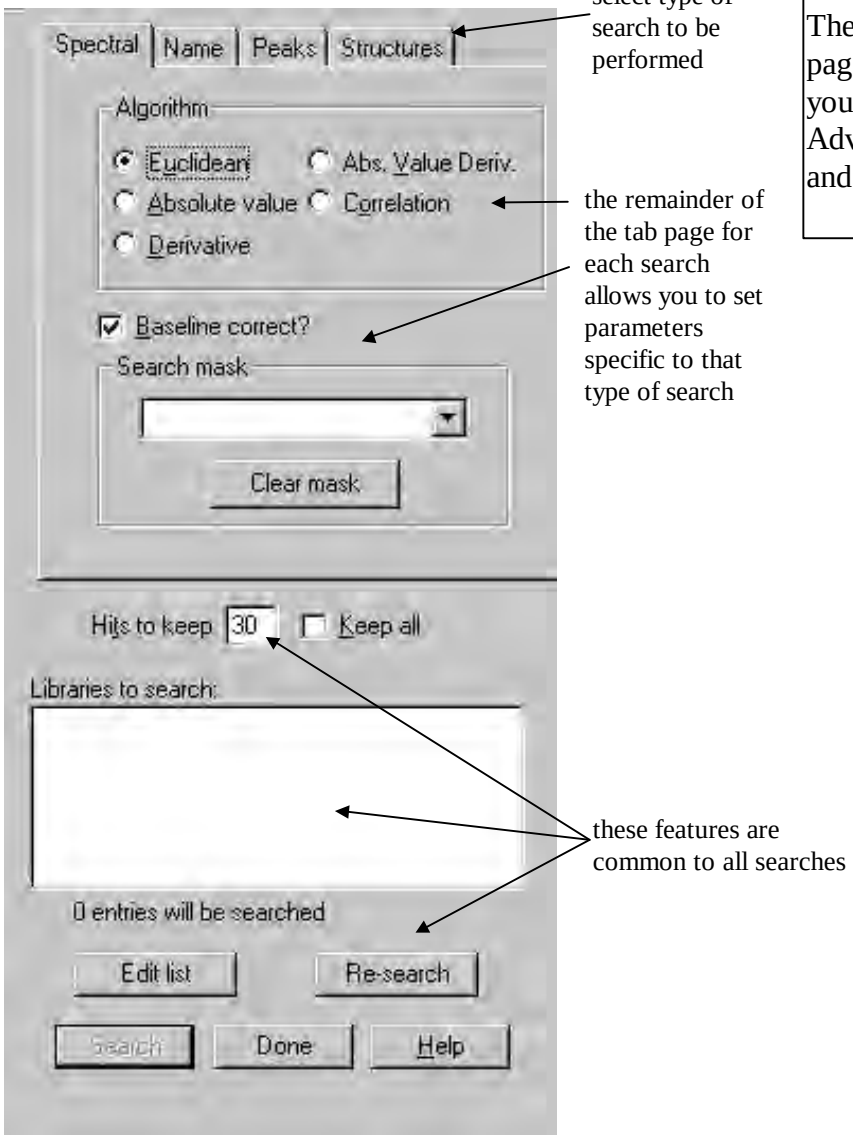
Searching

When Operations / Search is selected, the search control sidebar appears.



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Details of the control sidebar are shown below.



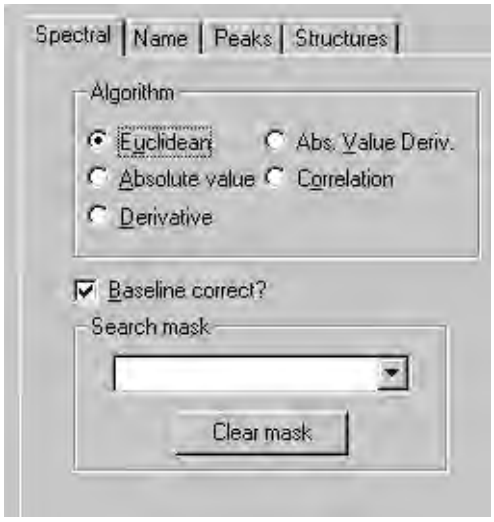
Note

The Structures search tab page will not appear unless you have purchased the Advanced Search product and run the enabling floppy

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Spectral Search

A spectral search compares the spectrum to spectra in the selected libraries. A goodness-of-fit is calculated for each spectrum in the libraries and the best hits are displayed in a hit list.



Algorithm: the method by which the library entries are compared to the sample spectrum. The recommended algorithm is Euclidean with baseline correction selected. The correlation and two derivative algorithms effectively do a baseline correction and might be useful if there is a slowly varying, non-linear baseline. Mathematical details of the algorithms are shown in Appendix D.

Baseline correct?: if selected, a two-point baseline correction is performed on the unknown spectrum before the libraries are searched. It should be selected if you are using the Euclidean algorithm.

Search mask: Search masks remove interferences from sample spectra by ignoring certain spectral regions during the search. Some of these interferences arise from materials commonly used to prepare the sample (for example, nujol mull). Other interferences may come from small amounts of water vapor or carbon dioxide which are present in many spectra unless care is taken to desiccate and/or purge the spectrometer.

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You can define any region, or number of regions, to be masked in the spectrum. Draw in the regions to be masked (see "Defining a Region" in Chapter 1). A number of standard masks, corresponding to common sources of interference, may also be selected from the Search mask pop up menu; these are listed in the table below. Masks are additive

MASK NAME	SPECTRAL REGIONS IGNORED (CM^{-1})
Water vapor	3900-3500 and 2000-1280
Carbon dioxide	2450-2250 and 700-650
Nujol mull	3100-2700, 1500-1420, 1390-1360, and 740-710
Fluorolube	1350-0
Carbon tetrachloride	820-720
Carbon disulfide	1650-1420

You can delete any defined region in the usual manner (see Drag Regions, earlier in this chapter for details).

Clear mask: deletes all masks defined for this spectrum.

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Name Search

Among other uses, name searches can locate spectra in a library for use as a reference spectrum. All libraries have Names in the Includes list (see below).



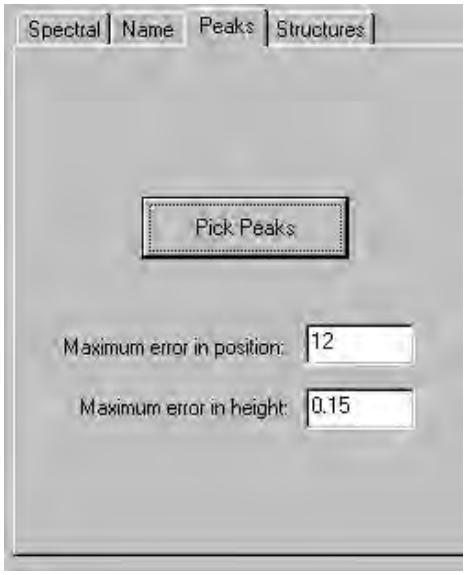
Enter a single text string. If there are spaces in the string, the string should be enclosed in either single (') or double (") quotes. If one type of quote appears in the text string, use the other type as a delimiter.

The test is a pass/fail one. If there is a match, the library entry is returned with a Hit Quality Index of 0.00, otherwise it is not returned. Because every entry in the hit list from a names search is a perfect match. there is no ranking of the matches.

Peaks Search

Searches for the peaks you have selected in the unknown spectrum. You must have selected at least one peak for this search to be performed. The libraries to be searched must have Peaks in the Includes list (see below); otherwise, the Search and Re-search buttons will be disabled. A goodness-of-fit is calculated for each spectrum in the libraries and the best hits are displayed in a hit list.

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If the peaks have not already been selected, you may select them by clicking the Pick Peaks button. This is equivalent to selecting Operations / Peak Pick, described later in this chapter. You could also pick individual peaks using the right mouse button, as described in Chapter 2.

Before comparing the unknown (sample) spectrum to the library spectrum, each spectrum is independently normalized so that its largest peak has a y-value of 1.

Maximum error in position: this value is in wavenumbers. If the position of the peak in the library spectrum differs by more than this value from the position of the peak in the sample spectrum, this peak is rejected. If the two peaks are closer together than this value, this peak is accepted.

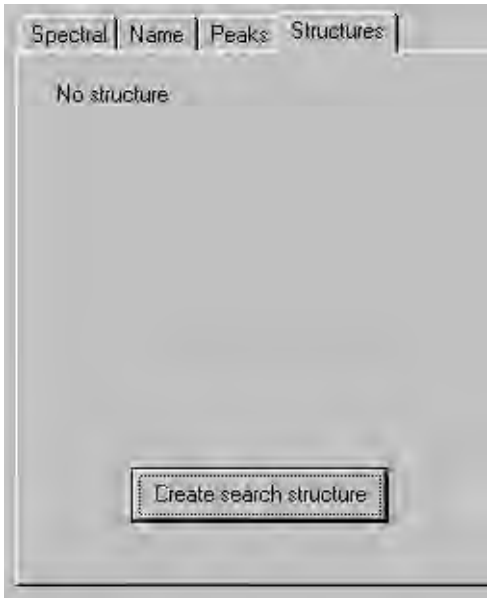
Maximum error in height: If the normalized height of the peak in the library spectrum differs by more than this value from the normalized height of the peak in the sample spectrum, this peak is rejected. If the two peaks are closer together than this value, this peak is accepted.

A hit quality index (HQI)is calculated for each picked peak in the sample spectrum. The closer the sample peak is to the library peak in wavenumber and normalized height, the better the HQI will be. After each peak is compared, an overall HQI is calculated for the match between the sample spectrum and the library spectrum.

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Structures Search (Optional)

Allows you to build partial molecular structures and search libraries for matches. The libraries to be searched must have Structures in the Includes list (see below); otherwise, the Search and Re-search buttons will be disabled. You cannot perform a structures re-search on a hit list created by any of the searches.



In this case (the most common), the sample spectrum has no structure associated with it in the document, so the message No structure is displayed. If you have installed Advanced Search, you can click the Create search structure button and build a structure. Details of building a molecular structure are in the *Win-IR Pro Advanced Search Manual*(091-0985). After you create the structure and return to Win-IR Pro, this structure is displayed, replacing the message No structure.

Common Search Features

This describes the lower half of the search control sidebar. These features are common to all searches.

Hits to keep: when the unknown spectrum is compared to a library entry, a "goodness of fit" called the Hit Quality Index is calculated measuring how much the sample spectrum varies from the library entry. A perfect match is 0.0, indicating that if the spectra were

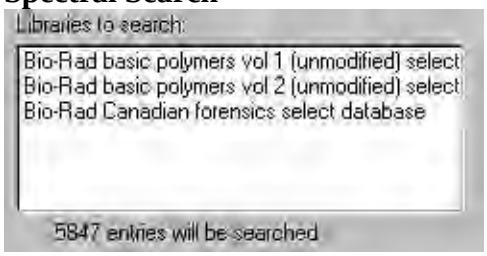
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subtracted there would be no residual. Search saves the best hits up to the number entered in this box. Typically, in a spectral search, only 30-40 hits are required. In a pre-search, such as a names search, where the test is pass/fail, the search process terminates when the specified number of hits is achieved. If this number is too small, there is the possibility of erroneously excluding possible spectra that would be found later in the pre-search.

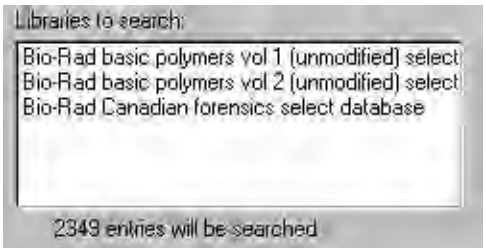
Keep all: if checked, all hits will be saved. If you are using Name Search, once Number of hits to keep has been reached, no further hits will be saved. It is advisable to check Keep all in this case. However, if you are not using Name Search, it is not advisable to check Keep all, especially if you are searching a library with many entries. It will take a very long time and occupy a significant amount of disk space.

Libraries to search: a list of the libraries that are to be searched. Libraries can be added to or removed from this list by clicking Edit List. The line below the box entries will be searched displays the number of library entries that will be checked for the type of search you have selected. In the example below, the polymers libraries have structures, but the Canadian forensics library does not. If a spectral search is selected, 5647 entries from the three libraries will be searched. However, if a structures search is selected, only the first two libraries will be search (2349 entries). If 0 entries are indicated, the libraries you have selected cannot be used for the type of search you want to use.

Spectral Search



Structures Search



Note

All libraries have Spectra and Names; not all libraries have Peaks and Structures. See Edit list below to see what information is stored in each library.

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Edit list: clicking this button makes the Search Library Selection dialog box appear.

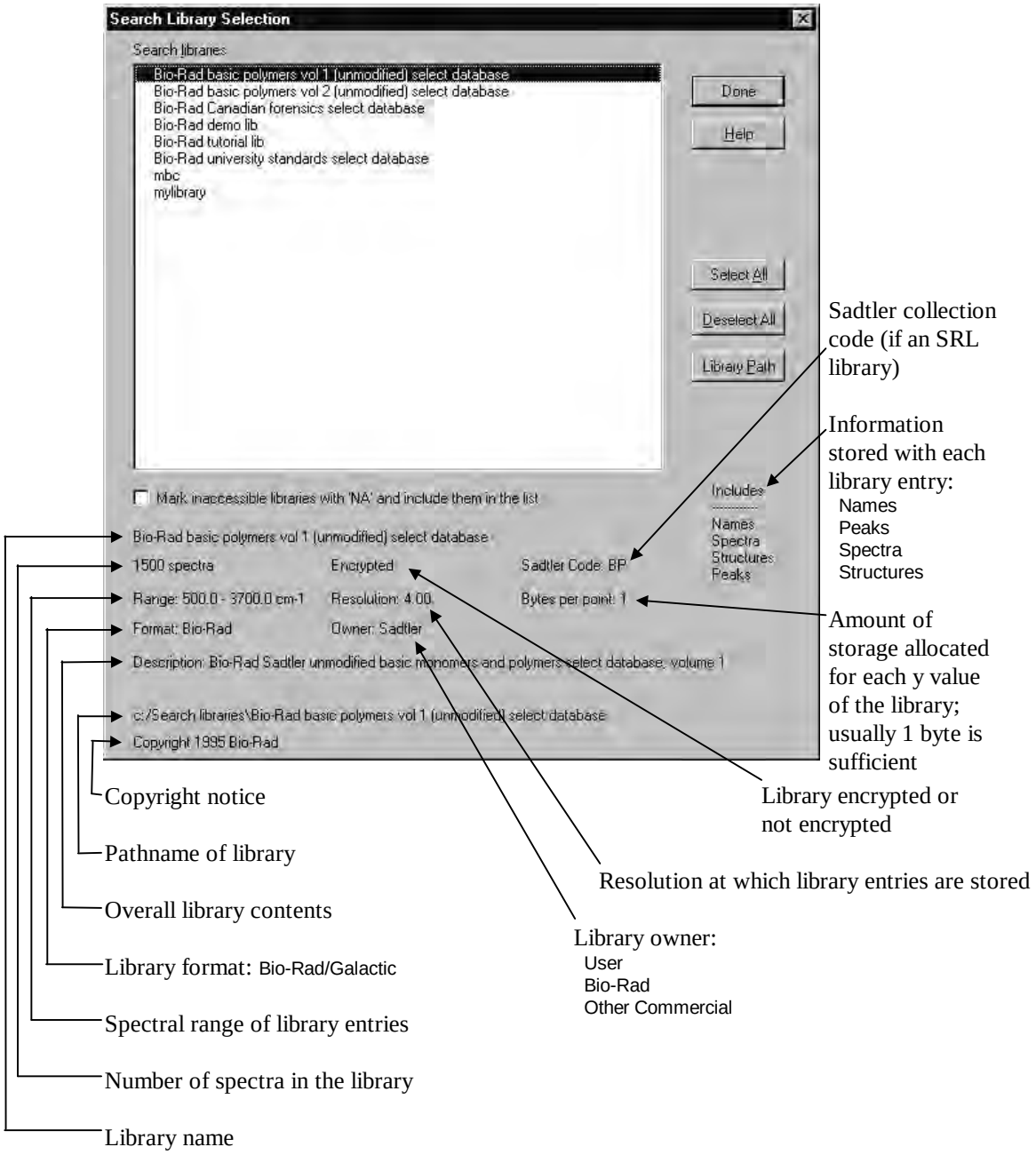


Note

The list above is an illustrative example. Your library list may differ depending upon what libraries you have purchased or built.

Each line is a library that can be searched. Highlight (click once) a library to get information about it. For example, Bio-Rad demo lib

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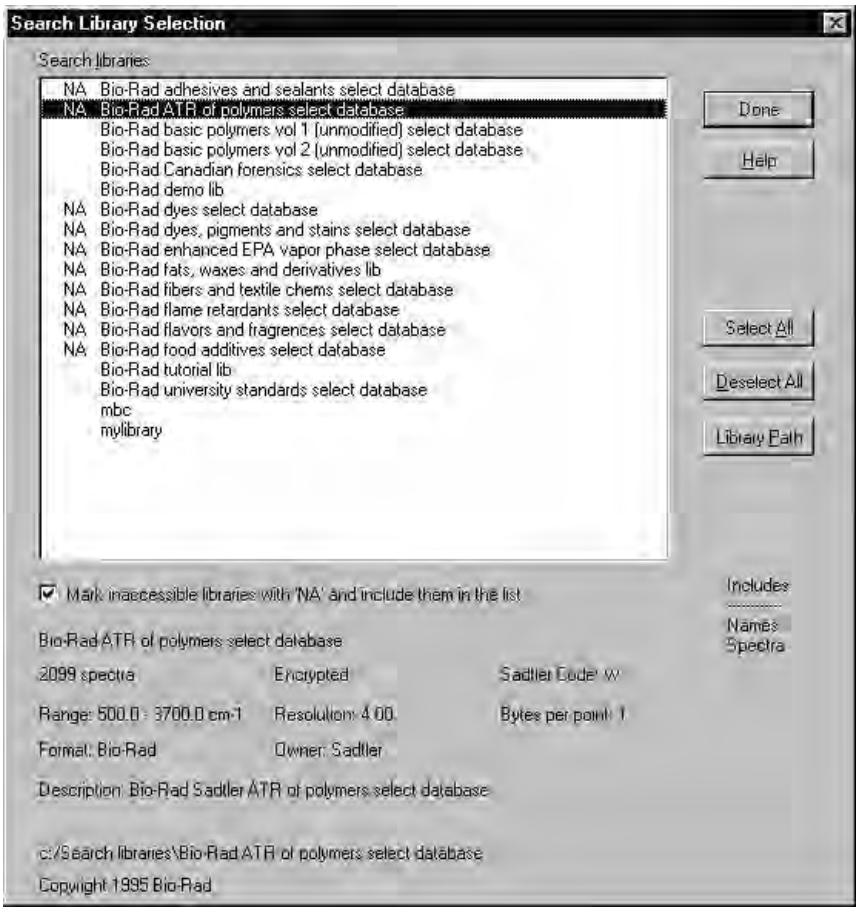
This information can help you to decide whether or not you want to search this library.

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Mark inaccessible libraries with 'NA' and include them in the list: if this is selected, the libraries which have been loaded but cannot be accessed are displayed in the list. These libraries cannot be accessed either because the setup program on the enabling floppy has not been executed, or because the enabling floppy was not configured for your system's dongle. Win-IR Pro Accessibility is not changed by selecting this check box; selecting this check box only displays non-accessible libraries.

Note

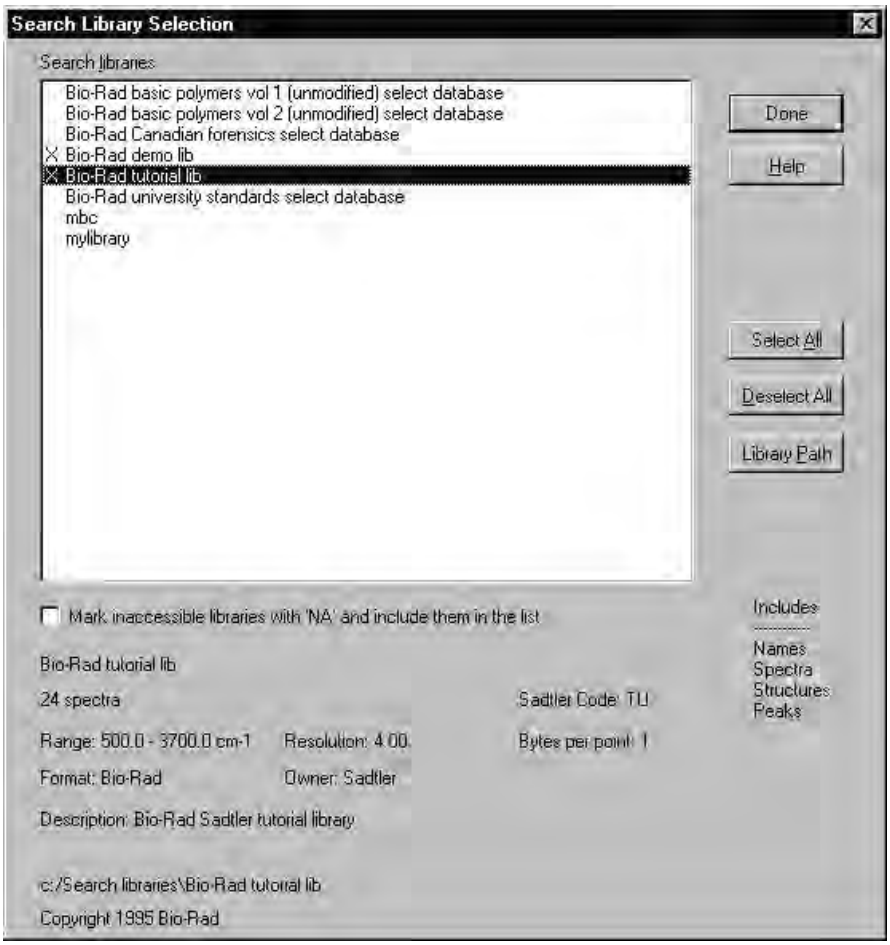
The only way to change "not accessible" libraries to "accessible" libraries is to obtain the appropriate enabling floppy from Bio-Rad.



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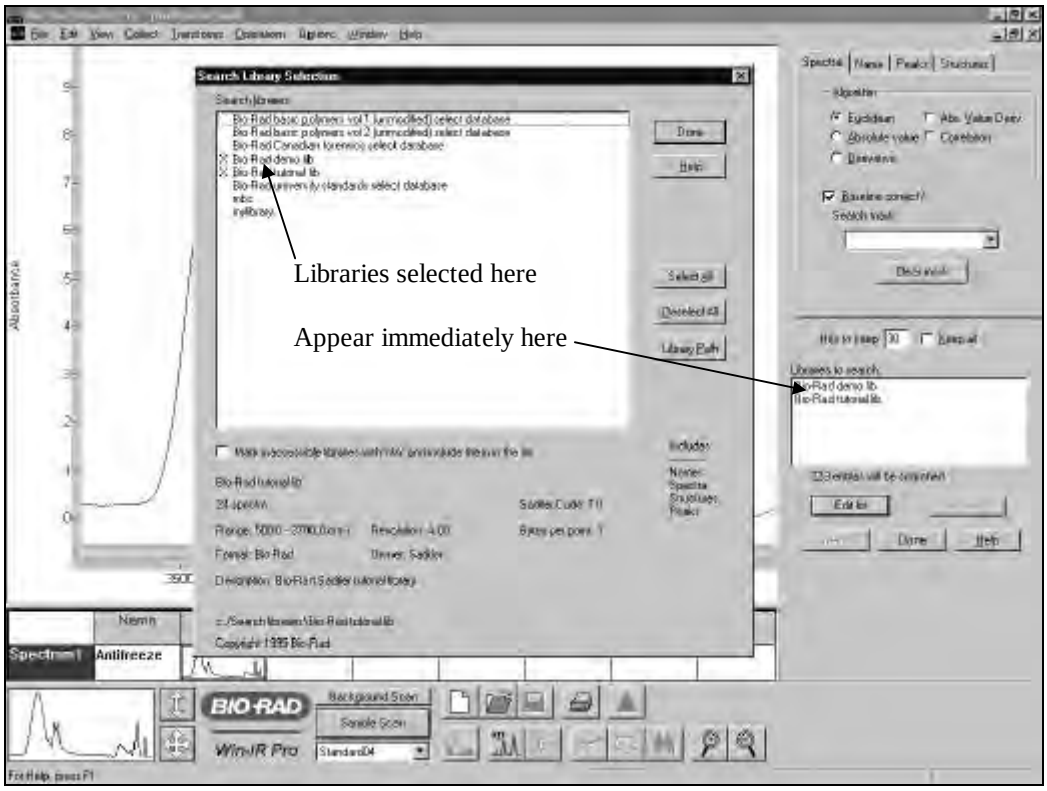
You can highlight (single-click) an inaccessible library to view information about it, but you cannot select it for search (double-click).

To select a library for search, double click the line. An X appears to the left of the library name. You can toggle libraries on and off as often as you want.



Two libraries have been selected in this example. When you select a library in the Search Library Selection dialog box, it immediately appears in the Libraries to search: window on the control panel sidebar. When you de-select a library in the Search Library Selection dialog box, it immediately disappears from the Libraries to search: window on the control panel sidebar.

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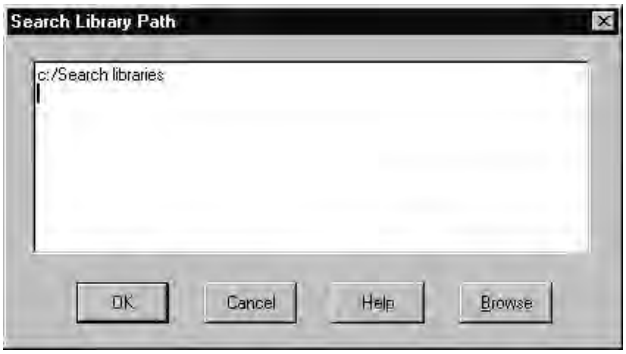
Select All: selects all libraries listed to be searched.

Deselect All: resets the list so that no libraries are selected to be searched.

Library Path: when clicked the Search Library Path dialog box appears. This allows you to select those library directories whose contents will appear in the list of Search libraries. You can also use this dialog box to define existing directories to be library search directories, that is, directories in which libraries are stored, and which can be accessed through the Search Library Selection dialog box.

There are two classes of library—some are common to all users, while some are specific to an individual user. The differences are not intrinsic to the library, but are based upon the licenses purchased.

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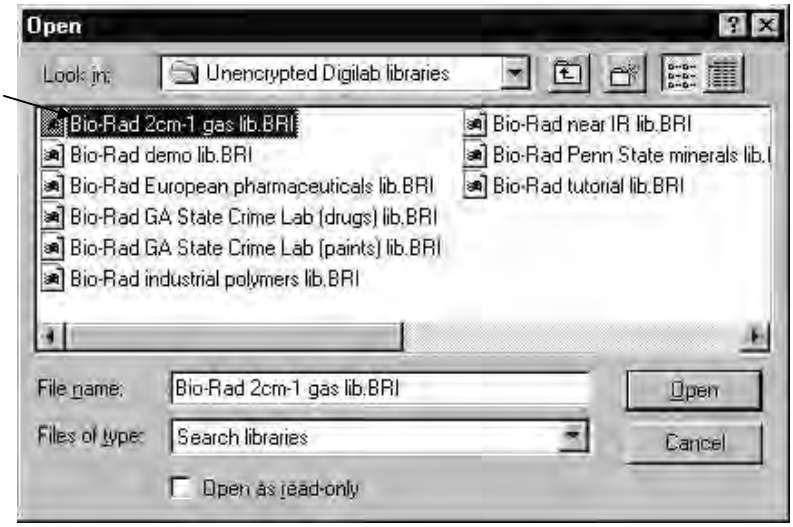


The libraries listed in the Search Library Selection dialog box are located in C:\Search libraries, as shown above; this is the default directory for libraries. If you want to designate an additional directory as a search library directory (A directory where libraries are, or will be, stored), click in the dialog box and type in its full pathname. You must include the drive; no blanks are permitted in the pathname. You can also use Browse (see below) to look through the file system to add library pathnames.

Browse: allows you to add the directories from which libraries will be presented in the Search Library Selection dialog box. That is, you will be able to search these libraries. If Browse is clicked, it brings up a standard Windows NT file search dialog box called Open. Use standard Windows NT techniques to select those search library directory paths to be added to the search list. To select a directory, you must select one of the libraries **in** the directory. It does not matter which library is chosen. The buttons have their usual meanings.

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Any library file name must appear here. This causes the directory to be



In this example, we have used the Network button to connect to another system on the network to access more libraries.

Open: return to the Search Library Selection dialog box with the additional set of library paths to be searched. The names of all libraries in the selected directory are placed in the Search Library Selection dialog box.

Cancel: return to the Search Library Selection dialog box without changing the set of search libraries, if any.

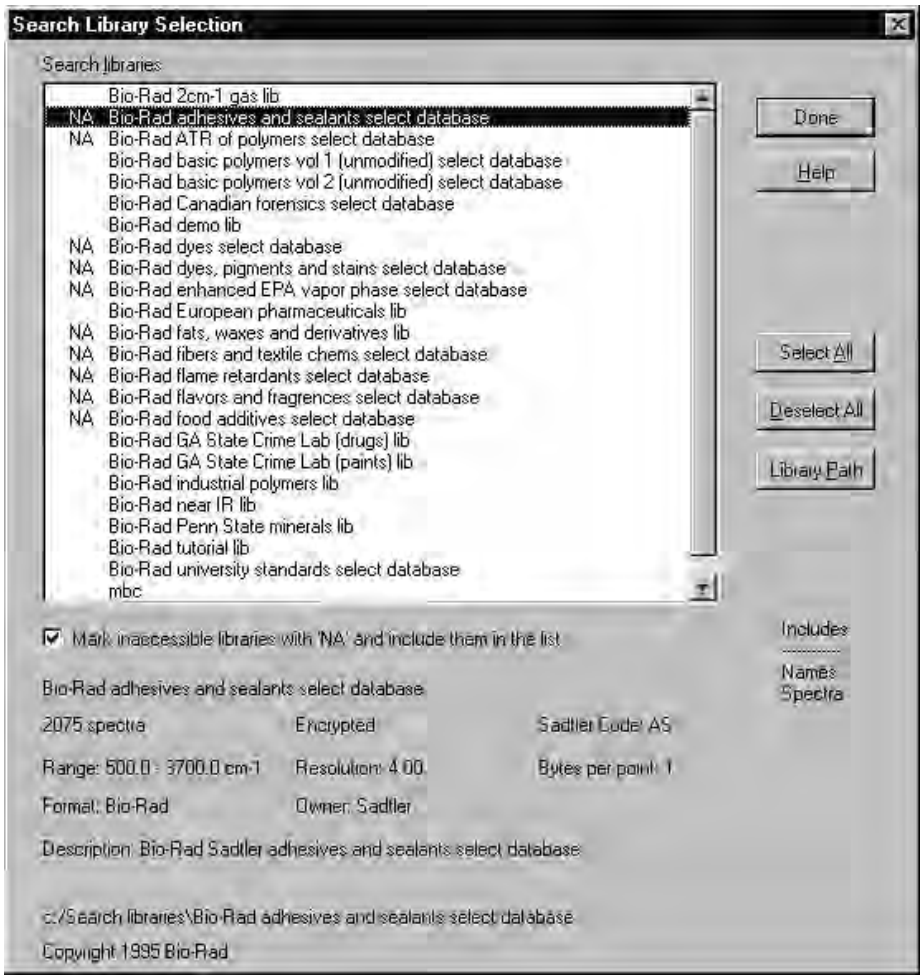


The path of the new set of libraries is displayed. Click OK to return to the Search Library Selection dialog box.

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Note

To remove a set of libraries from the Search Library Selection dialog box, go to the Search Library Path dialog box (above), highlight the library path, and press DELETE.



In this example, you did not have rights to the libraries in the selected directory. You cannot select any of these libraries to be searched. If you try to select one of these libraries you get this message:

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Click OK to return to the Search Library Selection dialog box.

Done: return to the search control sidebar with the newly selected list of libraries to be searched.

Help: enter the on-line Help system.

Search: begins the specified type of search, using the selected libraries in the Libraries to search box.

You can always search the libraries using an absorbance spectrum. If you want to search using other types of spectra, use Options / Search (see Chapter 12) to choose which ones can be used. If you attempt to search using a type of spectrum that is neither absorbance nor one selected with Options / Search, the following dialog box appears.



Click Yes to allow a search to be performed Click No to cancel the search.

When the search is completed, a hit list is displayed. The sample is at the top of the spreadsheet, separated from the possible matches, which are arranged with best matches at the top.

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Re-search: A search must be performed before performing a re-search. If re-search is selected, then another search is performed using the existing hit list as the search library. Usually, you would first perform a name search or a peaks search using a number of libraries, followed by a spectral search.

Note

Normally, you first perform a names (or structures) search, followed by a spectral or peaks search.

The procedure is:

1. Perform a name search, for example, using Keep All. Select all the libraries that might have the spectrum you are looking for. This will produce a hit list. This procedure may take a long time, because a large hit list could be generated.

2. Select the Spectral search tab page and set the parameters. Change Hits to keep to a reasonable number, typically in the range of 10 to 30.

3. Click the Re-search button. The spectral search will now use the existing hit list as its search library. The new hit list, a subset of the name search hit list is displayed.

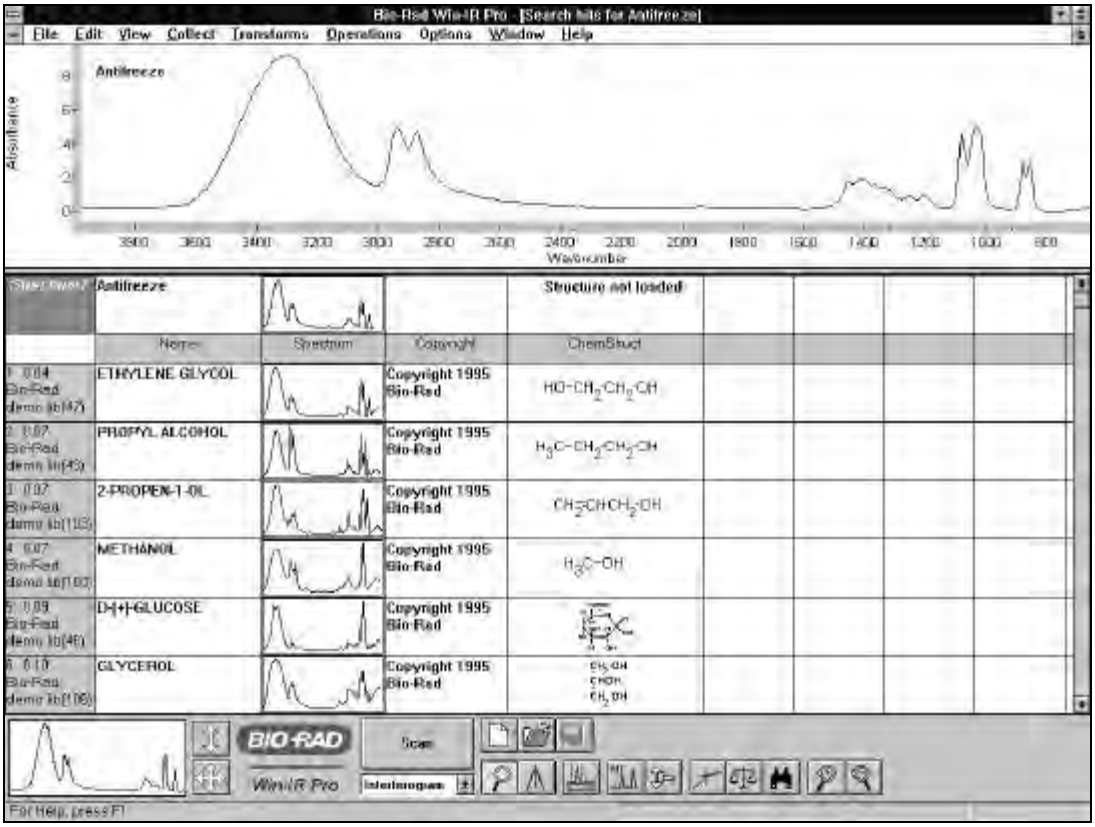
Done: close the search control sidebar without performing any more searches.

Help: enters the on-line help system.

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Example of Spectral Search

The spectrum antifreeze.bsp is used for this example. Two libraries: Bio-Rad demo lib and Bio-Rad tutorial lib will be searched. After the search is completed, the Search Hits view screen appears. (The spreadsheet cells have been resized manually to shown their contents clearly.)



The original spectrum is displayed at the top of the spreadsheet. It is separated from the library entries by the column labels. This trace is always displayed. If a library entry is displayed also (see below), the unknown will be in a color other than green.

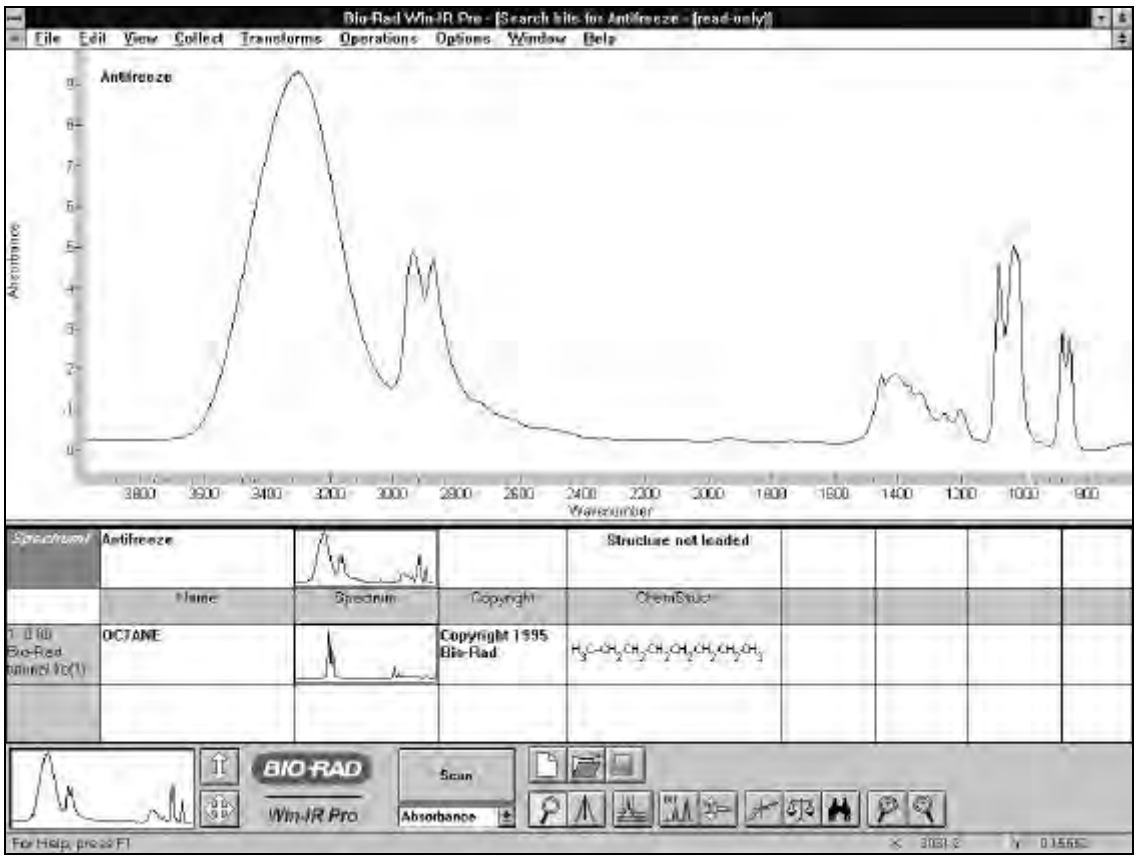
The library entries are ordered best hit first. The left most column shows the HQI, the library name, and the library entry number. The name of the library entry, its spectrum, copyright date, chemical structure, and whatever other properties you have chosen for the columns (if these properties are stored in the library) are displayed. If you add a column, that property will automatically be added for all the library entries (if that

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property was stored in the library). Select a library entry by clicking in its row; its spectrum will be shown in green in the trace display above. All standard spreadsheet selection procedures (see Chapter 4) work in the hit list view.

Example of Name Search

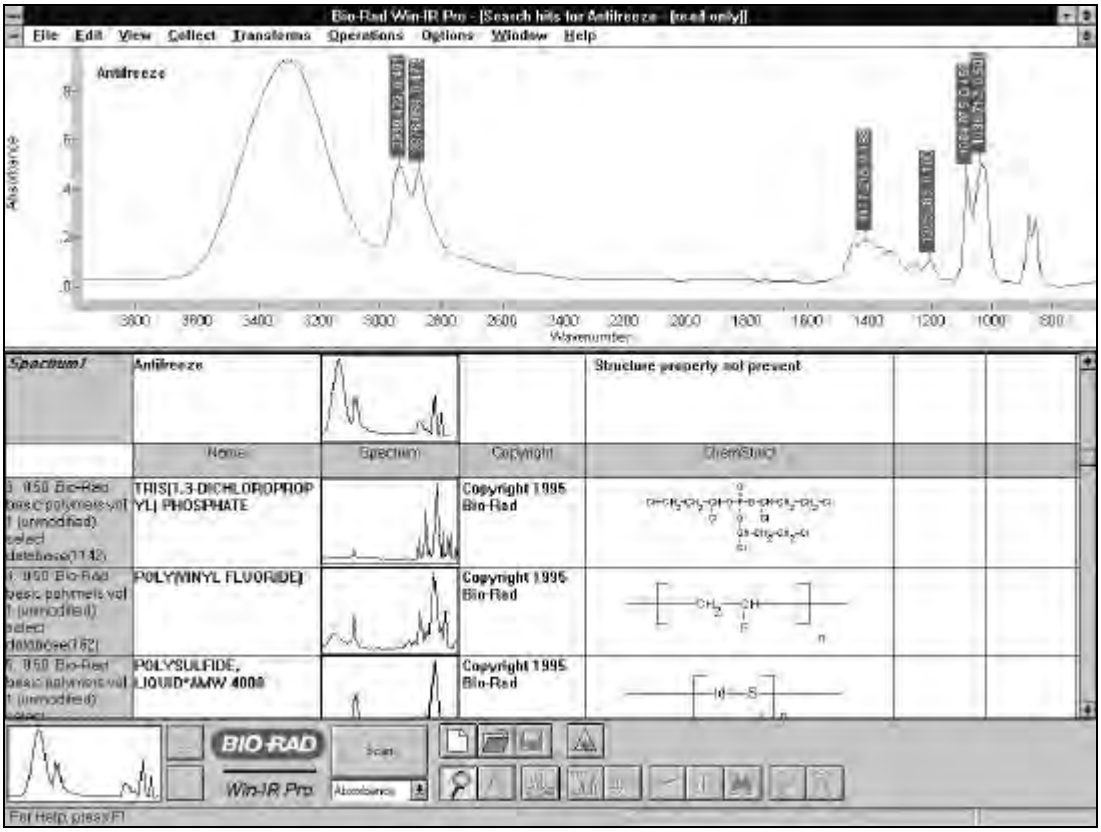
We will search the Bio-Rad tutorial library to see if it contains the spectrum of octane. After the name search is completed, the Search Hits view appears. (The spreadsheet cells have been resized manually to show their contents clearly.)



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Example of Peaks Search

We will search the Bio-Rad basic polymers libraries (volumes 1 and 2). After the search is completed, the Search Hits view appears. (The spreadsheet cells have been manually resized to show their contents clearly.)



Interpreting the Hit Quality Index (HQI)

The HQI is a measure of the similarity between an unknown spectrum and a library spectrum. A HQI of 0.0 means the two spectra are identical; a higher HQI indicates an increasing amount of difference, that is, less of a match.

Typically, a HQI below 0.30 indicates an acceptable match between the unknown and the library entry. A HQI below 0.15 indicates nearly identical spectra. Since the largest possible HQI is 2.00, a HQI on the order of 1.00 indicates a bad match. A HQI above 0.60 suggests the search was unsuccessful.

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Another indicator of a reliable identification is the size of the gap between the first and second hits. If that gap is small and the first and second hits are different substances, then the identification is likely to be questionable. Spectral search generally cannot unambiguously identify noisy spectra, spectra of mixtures, and spectra of higher members of homologous series (such as the n-alkanes).

The pattern among the lowest several HQIs is more signficant than the value of the single lowest HQI. When looking at the HQIs of the best several hits in the search, a good search is typified by one of two patterns.

The first pattern has the HQI of the best hit around 0.30 or lower and a gap of perhaps 0.20 between it and the next best hit. The second hit and worse hits are clustered together. For example, a pattern of 0.23; 0.41; 0.43; 0.44 indicates a strong likelihood of a good identification. This pattern also indicates a likelihood of success if the HQI values are higher. For example, best hits HQIs of 0.53; 0.75; 0.77; 0.78 might indicate a good search if an examination of the unknown spectrum shows that it is noisy.

The second pattern has all the best hits clustered together, with very low HQIs. For example, the best hits HQI's are: 0.11; 0.12; 0.12; 0.14; 0.15. This is a typical pattern for a library containing a large number of very similar spectra such as long-chain hydrocarbons. For example, the IR spectra between 3-methyl nonane and 3-methyl decane are so nearly identical that no significant distinction exists between the HQIs resulting from a search. Such a search would fail to produce unambiguous results. This sort of pattern provides a very good indication of the class of compounds and, usually, of the range of chain lengths, but other techniques (such as chromatography) must be used to identify the specific compound.

In any event, you should always display and plot the spectra. Visual inspection and comparison of the search results with the unknown spectrum is always an important identification measure. Use ZOOM to examine in detail parts of the comparison spectra for the harder to identify compounds. For example, a very noisy spectrum will have a substantially raised HQI, but may still provide useful identification.

Subtracting Known Components

Very few samples will be purely one component, although, in some cases, one component will dominate. Once this component is identified, it can be subtracted from the sample spectrum and the remainder searched for additional components. The procedure is outlined below.

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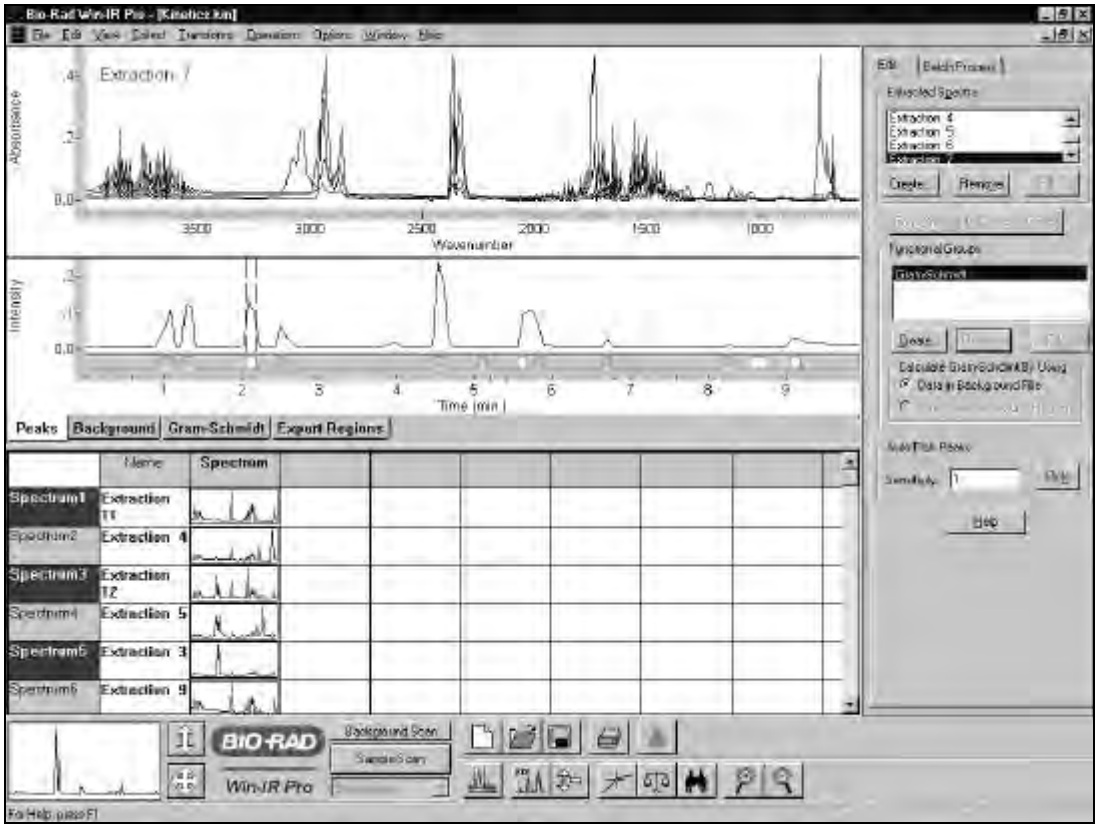
1. Perform search on the sample spectrum.
2. Select (highlight) the library spectrum in the Hit List that is to be subtracted.
3. Press the  button. This defines the library spectrum to be the reference spectrum.
4. Close the Search Hit List. This returns you to the original document with the sample spectrum.
5. Press the  button. This subtracts the reference spectrum from the sample spectrum. Follow the procedures under Spectral Subtraction in Chapter 10.
6. After the subtraction is satisfactory, press the Add button on the control panel sidebar; do ***not*** press Replace—that will delete your original sample spectrum.
7. Perform search on the difference spectrum.
8. You can repeat this process as long as you get meaningful results.

Batch Search

You can search more than one spectrum at a time against the selected libraries. One after another, the selected spectra are compared against the entries in the libraries. Each search is of the same type (spectral, name, peaks, or structures) and the same libraries are searched. After all searches are completed, a Hit List column is added to the spreadsheet. It contains the number of hits retained by the search; spectra that were not searched for show 0 for the number of hits. The view the hit list for a spectrum, put the cursor in the Hit List cell of that spectrum and double click. The hit list appears.

In the following example, we use the spectrum kinetics.kin. The spreadsheet is made visible by selecting View / Spreadsheet. Spectrum1, Spectrum3, and Spectrum5 have been selected to be searched for, as seen below.

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1. Select the spectra to be searched for. Here, Spectrum1, Spectrum3, and Spectrum5 have been selected.

2. Select Operations / Search. The Search control panel sidebar appears.

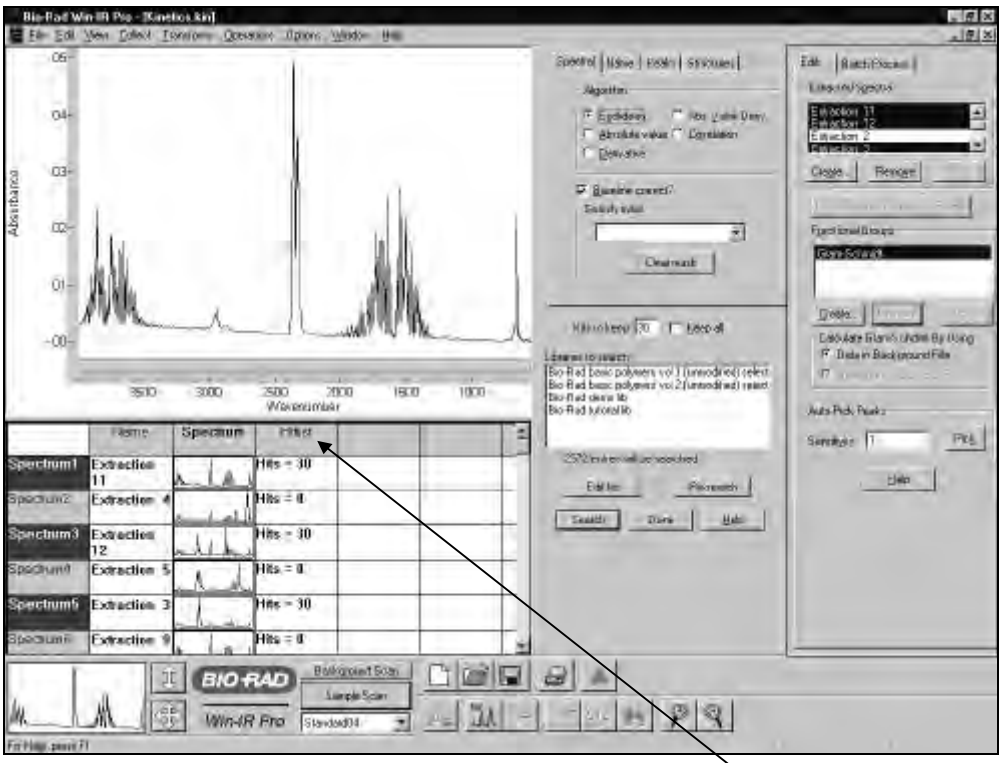
3. Select the type of search, parameters and the libraries to be searched exactly the same as if you were searching for one spectrum. This is discussed earlier in the Search section of this chapter.

4. Click the Search button. The libraries will be searched for all selected spectra.

5. After the searches are completed, a Hit List column will automatically be added to the spreadsheet. The cell contents will indicate how many hits were

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retained for that spectrum. This value is 0 for spectra that were not selected to be searched for.



6. Click Done to remove the Search control panel sidebar.

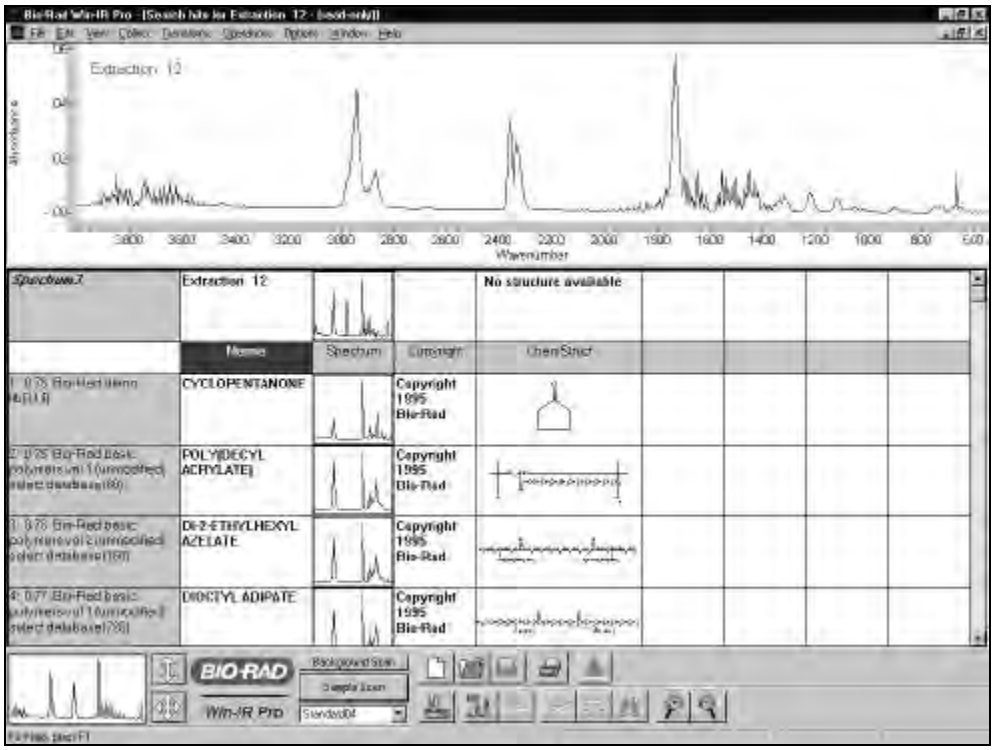
7. To view the hit list for a spectrum, double-click on its cell in the Hit List column. The hit list for that spectrum appears.

Note

If you double-click in a cell with 0 hits, nothing will happen.

8. For example, double-click in the Hit List cell for Spectrum3

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The spreadsheet cell sizes have been manually adjusted (see Chapter 4 for details) to better show their contents.

9. Select File / Close to close the hit list. Use the Window menu to return to the main view if you do not want to close the hit list.

10. Spectral subtractions, etc. can be performed exactly as if only one spectrum was searched for.

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2D-IR



From In Phase/Quadrature Spectra...

The theory and some examples of the 2D-IR technique have been described in the literature[1]. Briefly, external perturbations induce a fluctuation of the IR spectrum. Two

[1] Isao Noda, "Two-Dimensional Infrared Spectroscopy", *Journal of the American Chemical Society*, **111**, 8116-8118, 1989.

Isao Noda, "Two-Dimensional Infrared (2D IR) Spectroscopy: Theory and Applications", *Applied Spectroscopy*, **44**, No.4, 550-561, 1990.

Richard A. Palmer, Christopher J. Manning, James L. Chao, Isao Noda, Anthony E. Dowrey, and Curtis Marcott, "Application of Step-Scan Interferometry to Two-Dimensional Fourier Transform Infrared (2D FT-IR) Correlation Spectroscopy", *Applied Spectroscopy*, **45**, No. 1, 12-17, 1991.

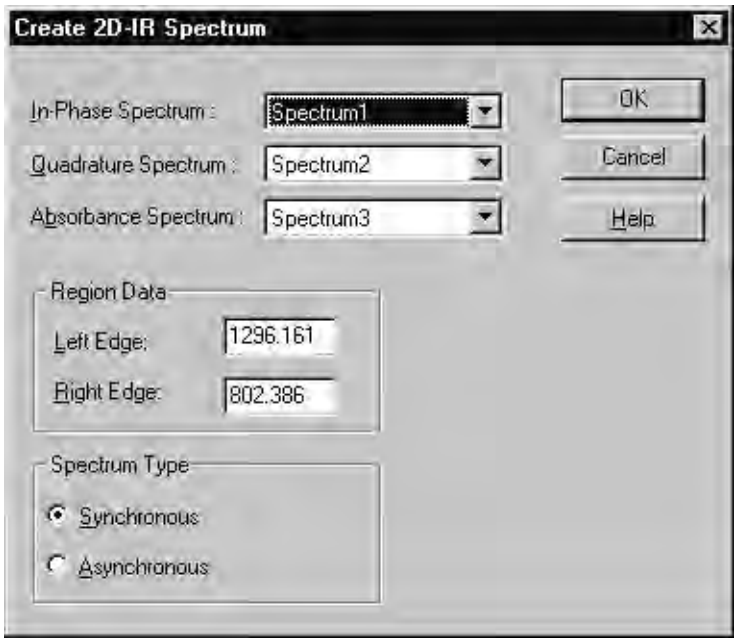
I. Noda, A. E. Dowrey, and C. Marcott, "Recent Developments in Two-Dimensional Infrared (2D IR) Correlation Spectroscopy", *Applied Spectroscopy*, **47**, No. 9, 1317-1323, 1993.

I. Noda, "Generalized Two-Dimensional Correlation Method Applicable to Infrared, Raman, and Other Types of Spectroscopy", *Applied Spectroscopy*, **47**, No. 9, 1329-1336, 1993.

Boiana O. Budevska, Christopher J. Manning, and Peter R. Griffiths, "Comparison of Two-Dimensional Power and Phase Spectra generated from Sample Modulation Step-Scan FT-IR Experiments, *Appl. Spec.* **48**, 1556-1558 (1994).

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independent spectra are correlated to produce a 2D spectrum. These 2D spectra are particularly useful in studying the interactions between functional groups.[2]
Before this is chosen, an in-phase spectrum and a quadrature spectrum should be selected; this example uses the stretch.bsp multi-spectrum document. The Create 2D-IR Spectrum dialog box appears.



In this case, the In-Phase Spectrum is Spectrum1; select it from the pull-down menu. Quadrature Spectrum then automatically changes to Spectrum2. The Absorbance Spectrum is Spectrum3; it will be used as a reference along the edges of the 2D-IR plot. Do not select Spectrum3 when Spectrum1 and Spectrum2 are chosen.

Region Data: the region of the two spectra to be used in creating the 2D-IR view.

Sanong Ekgasit and Hatsuo Ishida, "Quantitative Two-Dimensional Infrared (2D IR) Spectroscopy: Theoretical Development for General and Specific Cases," *Appl. Spec.* **49**, 1243-1253 (1995).

[2] See reference 1, above.

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Left Edge: the upper limit (in cm^{-1}) of the spectrum.
Right Edge: the lower limit (in cm^{-1}) of the spectrum.

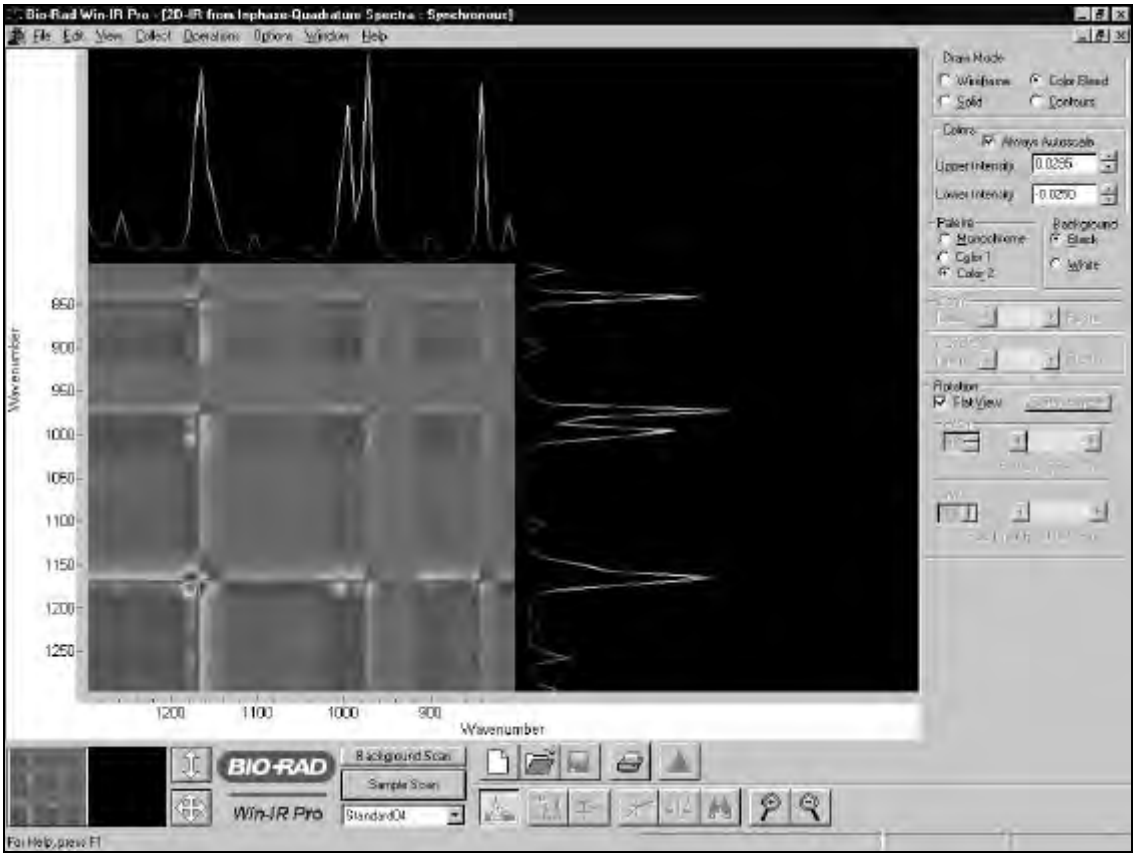
Spectrum Type: both spectra are used to calculate the synchronous and the asynchronous—they are different types of cross correlations.

Synchronous: correlate changes that happen together.
Asynchronous: correlate changes that are out of phase.

OK: creates the 2D-IR view and displays it (see below).

Cancel: return to the main window without generating any 2D-IR spectrum.

Help: enter the on-line Help system.



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In general, better performance is obtained if small regions (for example, up to 500 cm^{-1}) are chosen. The time to display a large range (for example 4000-400 cm^{-1} at 4 cm^{-1}) 2D display can be several minutes, and considerable storage space (>20MB) can be required.

This entry creates 2D-IR displays from in-phase and quadrature spectra. The displays can be moved, rotated, and presented in a number of formats. The control panel sidebar on the right hand of the screen controls the presentation of the data.

Draw Mode: how the three-dimensional aspect will be represented in two dimensions.

Wireframe: the points of the calculated three-dimensional plot are connected with straight lines. Lines that are hidden by the shape of the display are not shown. This draw mode disables both Colors and Palette.

Solid: the lines and the frames they define are filled in with different shades of a single color to give a better idea of the shape of the surface of the contour plot.

Color Bleed: uses multiple colors for the surface. These colors change gradually and smoothly as the height of the plot varies above the base plane. (Default)

Contours: shows contour lines on the surface at constant heights about the base plane. The contour intervals are pre-set and cannot be changed.

Colors: sets the range of colors used to represent the extreme z-values of the plot.

Note

In wireframe mode, Colors is disabled.

Always Autoscale: if this is selected, then whenever you zoom in on a portion of the plot, the color will be scaled so that the full color range is used for that portion. This is useful if you zoom in on weak features that may be displayed in very similar colors in the full plot.

If you are not autoscaling the colors, then you can set the values to be used in the display. If you use the arrows to the right of the intensity boxes to set

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values, they will be implemented immediately. If you type in values, they will not be implemented until you press the Enter key on the keyboard.

Upper Intensity: enter the color value to be used at the maximum z-value of the plot.
Lower Intensity: enter the color value to be used at the minimum z-value of the plot.

Palette: the draw modes may be observed with three different color schemes.

Note

In wireframe mode, Palette is disabled.

Monochrome: gray scale.
Color 1: shades from red to white to blue.
Color 2: shades from red through orange, yellow, and green to blue. (default)

Background: select the color for the background. A white background may be better if you are capturing screens for insertion in a publication with a monochrome printer.

Black: background is black. the plot is shown against a black background (default).

White: the plot is shown against a white background. This may be more desireable for formats other than wireframe

Zoom: makes the plot appear closer (increases size) or farther away (decreases size). Use the slide bar to change the value.

Y Scale: makes the height of the peaks taller or shorter. Use the slide bar to change the value.

Rotation: these controls move the three-dimensional plot about two axes. Regardless of the rotation, the axes remain in the foreground of the display. Rotation of large arrays may be slow. Press the ESC key to stop the rotation.

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Flat View: if selected, displays a projection of the isometric view. If de-selected, the isometric view (3D) is shown.

Default Angle: press this button to return the plot to its default position (Pitch = 18°, Yaw = 1°).

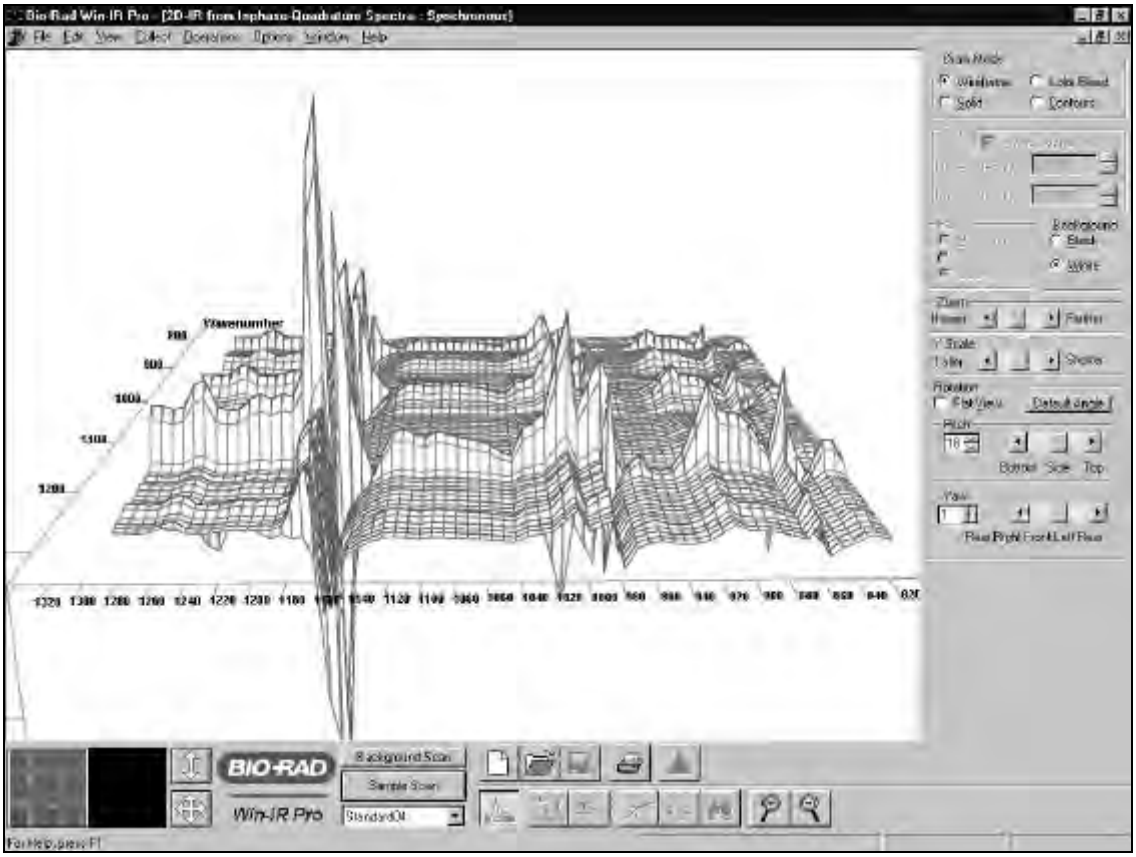
Pitch: rotates the plot about a horizontal axis parallel to the monitor screen. Click on the upper part to rotate the plot to show its Bottom; click on the lower part of the bar to rotate the plot to show its Top. Each time you click the end of the slide bar, the plot rotates 9°.

Yaw: rotates the plots about a vertical axis. The plot can be rotated either to the Right or to the Left. Each time you click the end of the slide bar, the plot rotates 18°.

For both Pitch and Yaw, you can enter the value of the angle. If you change the angle with the arrows to the right of the text box, the values are implemented immediately. If you type in values, the values are not implemented until you press the Enter key on the keyboard.

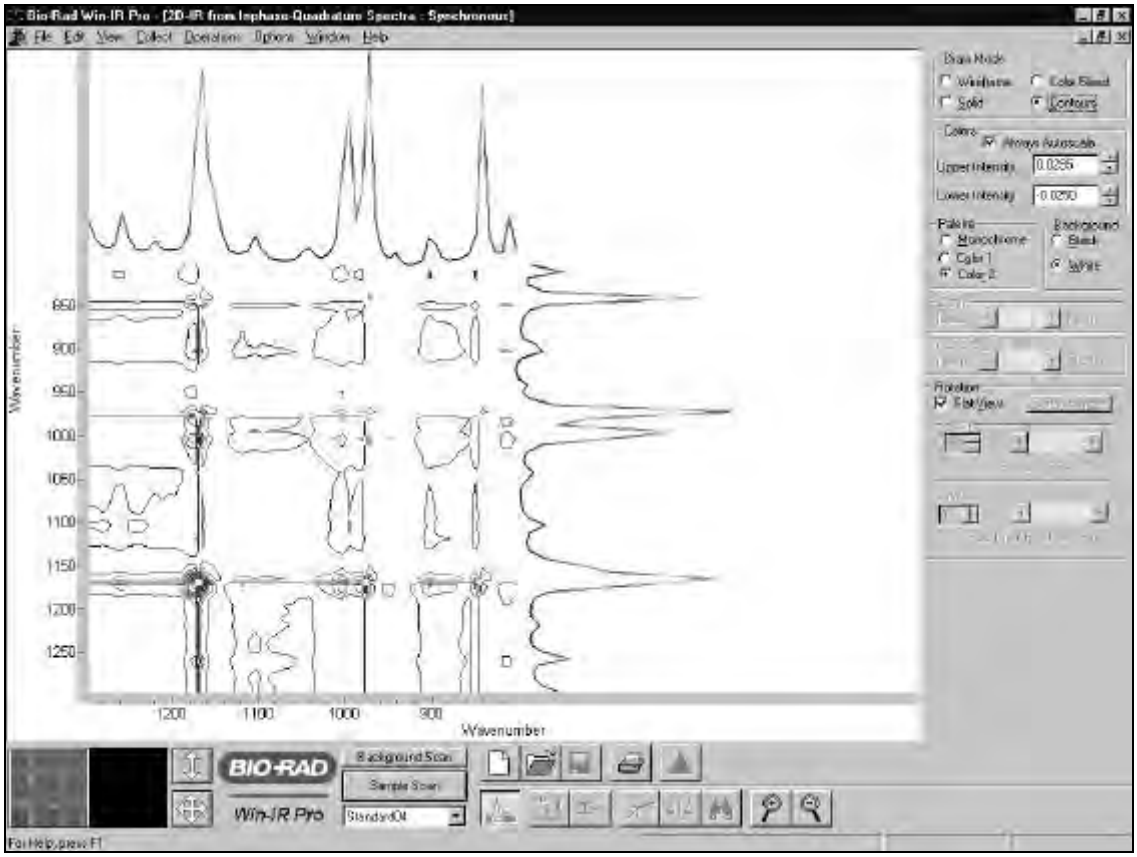
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A zoom is shown in the example below.



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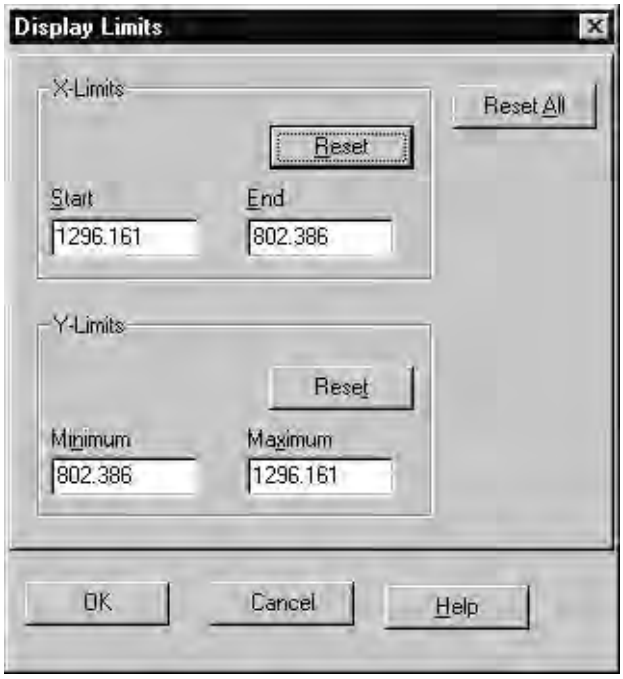
A flat view with monochrome contours is shown below.



Subsets of the menus are also available. Their entries operate the same as they do in the main Win-IR Pro document window.

In particular, you can adjust the display limits. Choose View / Display Limits / Selected Spectrum. The Display Limits dialog box appears.

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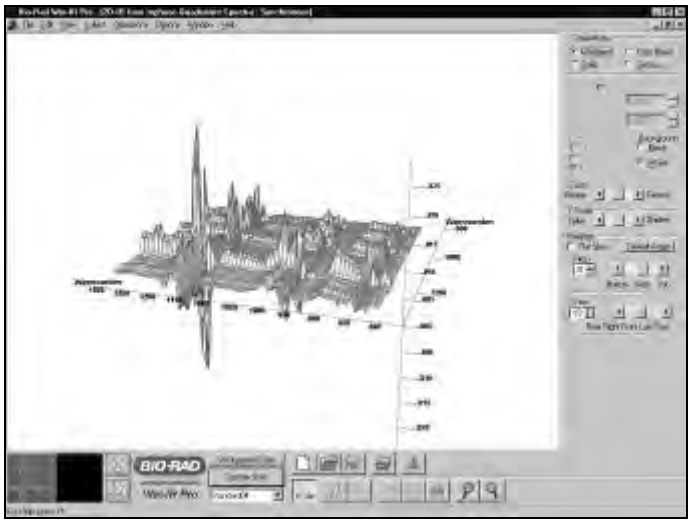


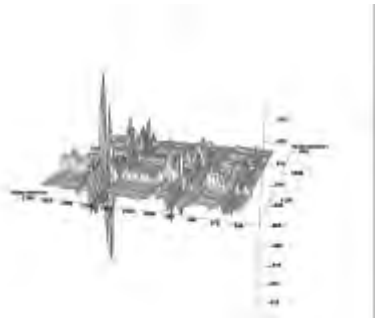
See the section on Display Limits in Chapter 8 for details of how to use this dialog box.

In addition, the box zoom is still active and works in the same way. You can zoom in the off-diagonal areas to see the results of correlating different regions, that is, you will have different ranges on the x- and y-axes.

You can use the  button and the radar box in the same way in the same way as before.

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The printed image is exactly what is in the three-dimensional portion.

If you want to print the entire screen image use either WordPad or Paint. These two applications are supplied as part of Windows NT. The procedure is described in Chapter 1.

Exporting 3D Data

The data triads (x, y, z) can be exported by selecting Operations / Export DXF. The file created has a .dxf extension and can be opened and manipulated by applications such as Autocad.

Notes

This menu entry is only accessible in a 3D graphics view.

These .dxf files cannot be inserted into word processors using the usual .dxf filter.

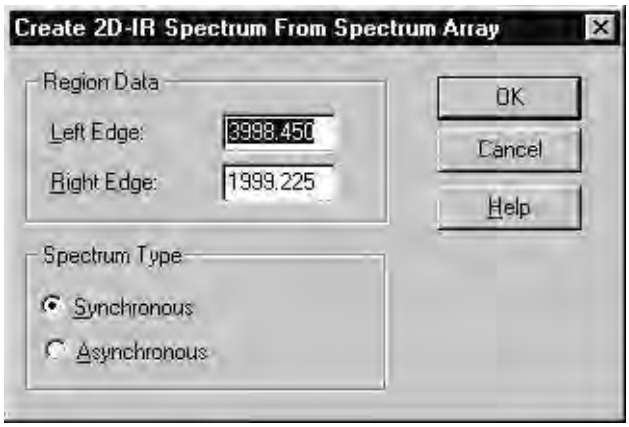
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From Series of Spectra...

Uses the generalized algorithm[3] to create a display from any array (or subset) of spectra. This 2D-IR view is used to detect correlations between the spectral changes at different frequencies during measurements. The dialog boxes are different for non-kinetics and kinetics documents.

Non-kinetics documents: Use the spreadsheet to select at least two spectra in the document. This example uses the luther.bsp multispectrum document with spectra 10 through 20 selected. When From Series of Spectra is selected, the Create 2D-IR Spectrum From Spectrum Array dialog box appears.

A typical correlation would be done using about 10 spectra over about 1000 cm^{-1} at 8 cm^{-1} resolution.



Region Data: the region of the spectra to be used in creating the 2D-IR view.

Left Edge: the lower limit (in cm^{-1}) of the spectrum.
Right Edge: the upper limit (in cm^{-1}) of the spectrum.

Spectrum Type: the spectra are used to calculate the synchronous and the asynchronous—they are different types of cross correlations.

Synchronous: correlate changes that happen together.

[3] I. Noda, "Generalized Two-Dimensional Correlation Method Applicable to Infrared, Raman, and Other Types of Spectroscopy", *Applied Spectroscopy*, **47**, No. 9, 1329-1336, 1993.

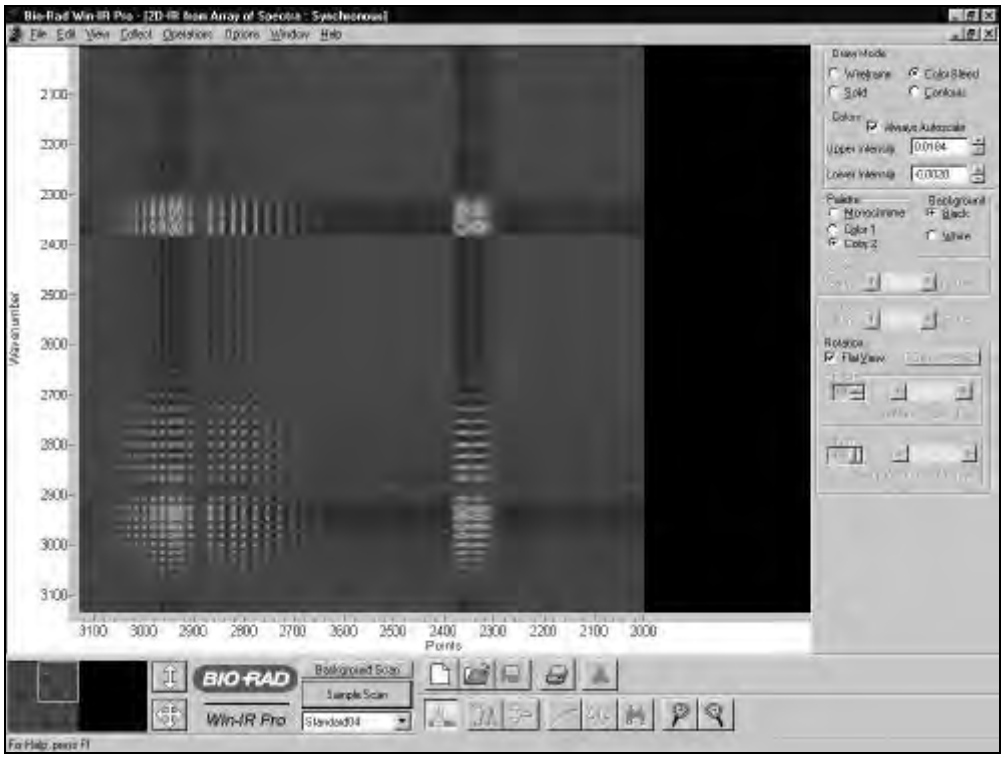
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Asynchronous: correlate changes that are out of phase.

OK: creates the 2D-IR view and displays it (see below).

Cancel: return to the main window without generating any 2D-IR spectrum.

Help: enter the on-line Help system.



Notes

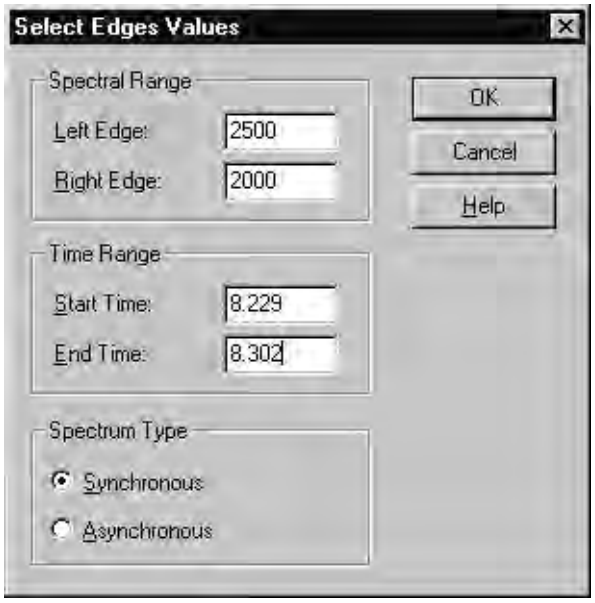
In this case there is no “static” spectrum, so no spectra are displayed along the edges.

We have used the zoom box to select an area of interest. This is shown in the radar box.

The controls and operations, including those for printing and exporitng data, are identical to those of the From In-phase/Quadrature Spectra, described earlier in this chapter.

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Kinetics documents: First click the Export Regions button on the kinetics document window. Spectra are selected using the dialog box. When From Series of Spectra is selected, the Select Edges Values dialog box appears. (This example uses the kinetics document kinetics.kin.)



Spectral Range: the region of the spectra to be used in creating the 2D-IR view.

Left Edge: the lower limit (in cm^{-1}) of the spectrum.

Right Edge: the upper limit (in cm^{-1}) of the spectrum.

Time Range: defines the spectra that are to be included in creating the 2D-IR view.

Start Time: exclude all spectra collected before this time.

End time: exclude all spectra collected after this time.

In a kinetics document where the time resolution is 1 second, a typical example would be creating a 2D-IR view over a period of one minute and a few hundred wavenumbers.

Spectrum Type: the spectra are used to calculate the synchronous and the asynchronous—they are different types of cross correlations.

Synchronous: correlate changes that happen together.

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Asynchronous: correlate changes that are out of phase.

OK: creates the 2D-IR view and displays it (see below).

Cancel: return to the main window without generating any 2D-IR spectrum.

Help: enter the on-line Help system.



The controls and operations, including those for printing and exporting data, are identical to those of the From In-phase/Quadrature Spectra, described earlier in this chapter.

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REPROCESS

In addition to saving the operations performed upon a spectrum, Win-IR Pro saves the intermediate stages. Therefore, you can view any stage of the spectrum's development. Select Reprocess; the Reprocess dialog box appears.

To recover the spectrum at any intermediate point

1 Place the cursor on the red STOP at the end of the list of operations and hold down the left mouse button. Another STOP appears.

2 Drag the new STOP to the place on the list where you want processing to stop. Release the mouse button. The spectrum will be reprocessed to that point.

Note

The interferogram is saved in the document, although it is not visible. You can start again with the interferogram and step through all the processing.

See Chapter 5 for complete details of Reprocess and History.

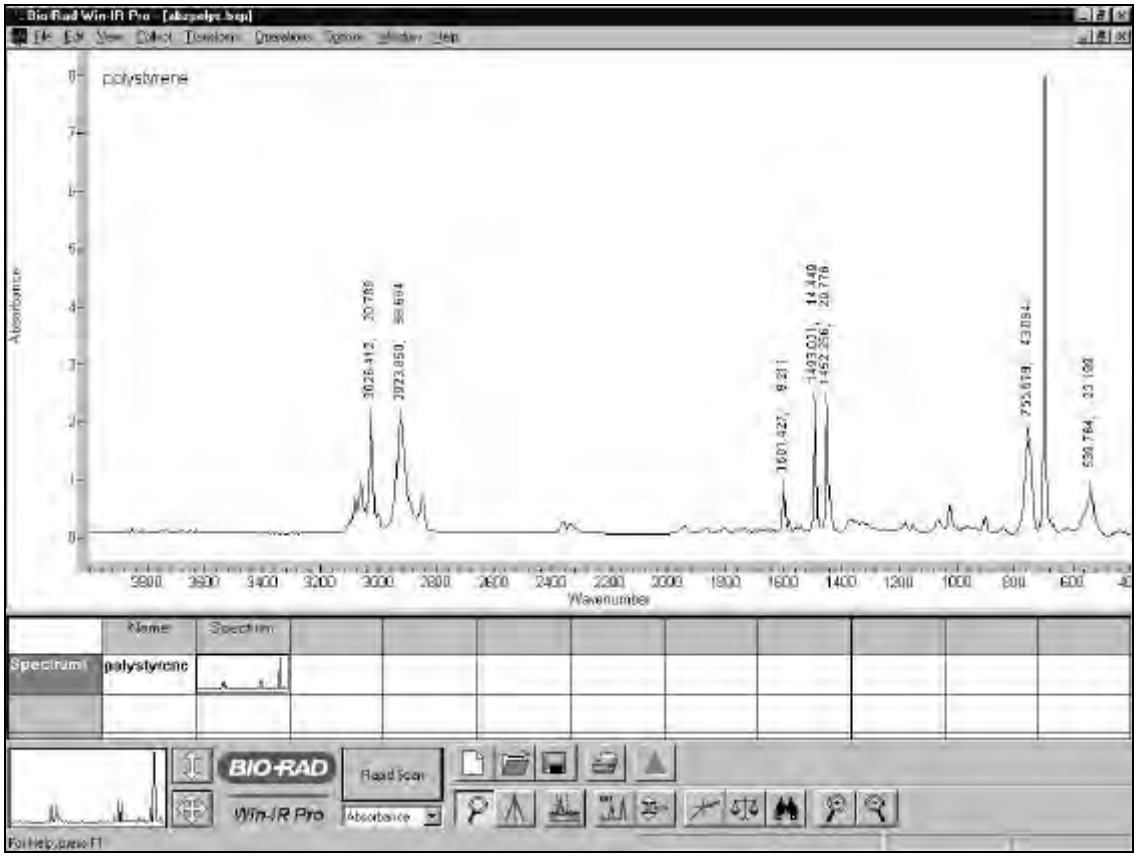
PEAK PICK

Performs automatic picking of peaks based upon height, area, and other properties of the spectrum. When selected the Peak Pick dialog box appears.



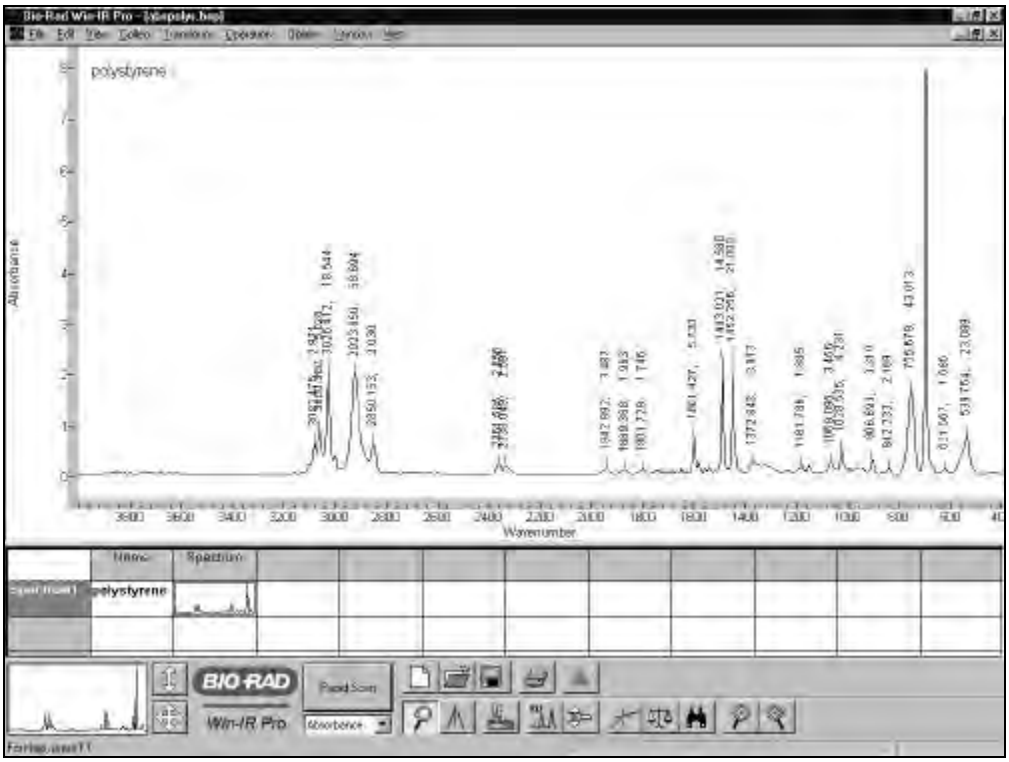
There are eight levels of Sensitivity with 1 being the least sensitive (fewest peaks) and 8 being the most sensitive (most peaks). Examples of peak pick with sensitivities of 1 and 3 are shown below.
Sensitivity = 1

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Sensitivity = 3



After peaks have been picked, they may be modified; see the discussion in Chapter 2 for details. Peaks may be investigated and their parameters added to the spreadsheet using Edit / Peak List (see Chapter 7 for details).

Individual peaks can be removed:

1. Place the cursor on the peak label and click the left mouse button.
2. Press the Delete key on the keyboard.

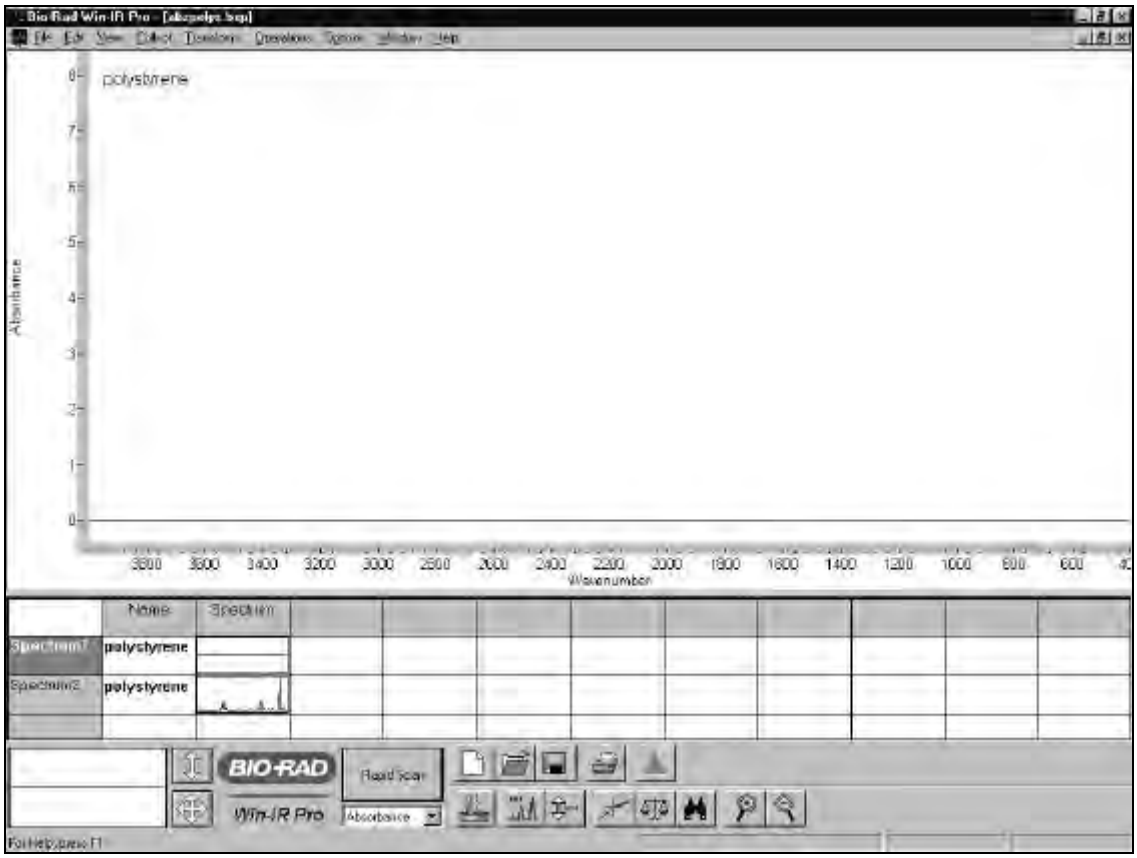
Note

Peak picking takes place over the entire spectrum even if only a portion of it is displayed at the time the peaks are picked.

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CREATE EMPTY SPECTRUM

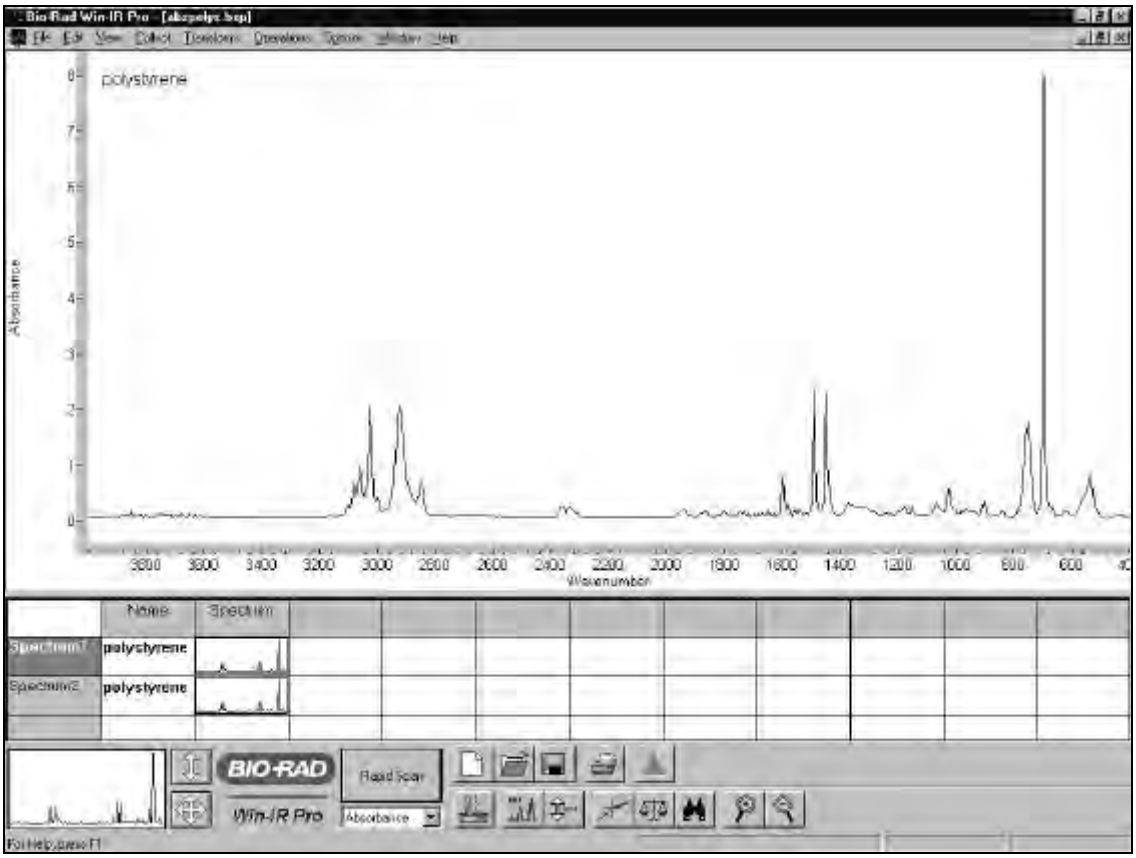
Creates an empty (all Y-axis values are 0) spectrum in the same document as the selected spectrum. The empty spectrum has the same collection parameters as the original selected spectrum.



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COPY SPECTRUM

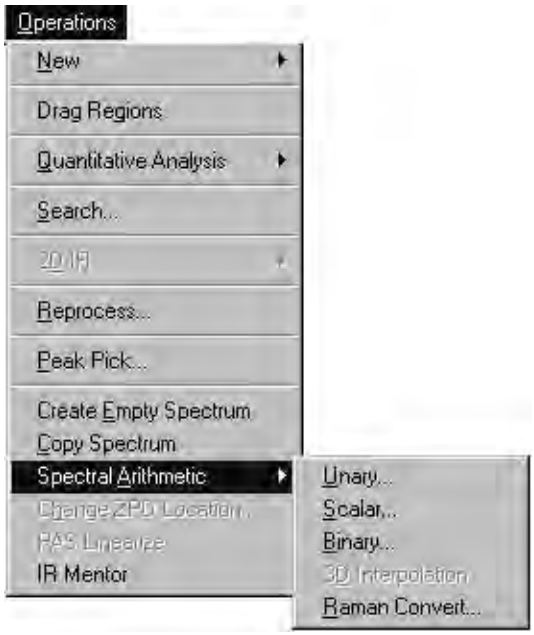
Creates an exact duplicate of the selected spectrum in the same document. The duplicate spectrum has the same collection parameters as the original selected spectrum.



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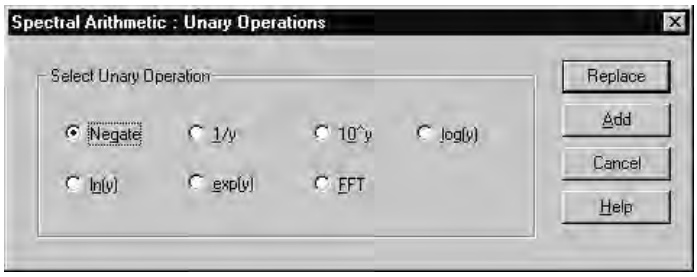
SPECTRAL ARITHMETIC

Allows arithmetic operations to be performed upon a spectrum (that is, its points) or on a pair of spectra The modified spectrum can be added to the document or it can replace the existing spectrum in the document..



Unary...

Allows unary operations to be performed upon the spectrum. Unary operations work upon the spectrum itself with no external qualifiers such as multipliers, etc. The Spectral Arithmetic: Unary Operations dialog box appears.



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Negate: create a new spectrum whose values are the negative of the original spectrum.

1/y: create a new spectrum whose values are the reciprocal of the values of the original spectrum.

10^y: create a new spectrum whose values are 10 raised to the power of the Y-axis values of the original spectrum.

log(y): create a new spectrum whose values are the logarithm (base 10) of the values of the original spectrum.

ln(y): create a new spectrum whose values are the natural logarithm (base e) of the values of the original spectrum.

exp(y): create a new spectrum whose values are the exponential (e raised to the power of the Y-axis values) of the original spectrum.

FFT: create a new spectrum that is a fast Fourier transform of the original spectrum. The FFT algorithm used us that of Cooley and Tukey.[4]

Note

The Fast Fourier transform is not reversible. That is, performing a second FFT on the transformed spectrum does not yield the original spectrum. To save the original spectrum, use the Add button.

Replace: make the desired calculation, replace the existing spectrum and return to the main menu.

Add: make the desired calculation, add the new spectrum to the spreadsheet, and return to the main menu.

Cancel: return to the main menu without making any changes to the selected spectrum.

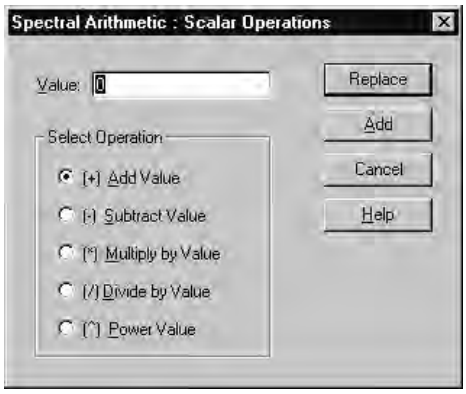
Help: enter the on-line Help system.

[4] Cooley, J. W. and Tukey, J. W., "An Algorithm forthe Machine Computation of Complex Fourier Series," *Mathematics of Computing*, **19**, 297-301 (April 1965).

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Scalar...

Allows you to perform scalar operations to the selected spectrum. The Spectral Arithmetic: Scalar Operations dialog box appears.



Value: enter the number to be used in the calculation. This number may be negative, as well as positive or 0.

(+) Add Value: add the number entered above to the Y-axis value of each point of the spectrum.

(-) Subtract Value: subtract the number entered above from the Y-axis value of each point of the spectrum.

You can subtract a spectrum from a number by first selecting Negate in the Unary operations, then adding the negated spectrum.

(*) Multiply by Value: multiply the Y-axis value of each point of the spectrum by the number entered above.

(/) Divide by Value: divide the Y-axis value of each point of the spectrum by the number entered above.

You can divide a number by a spectrum by first selecting 1/y in the Unary operations, then multiplying the reciprocal spectrum.

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(^) Power Value: raise the Y-axis value of each point of the spectrum to the power (number) entered above.

Replace: make the desired calculation, replace the existing spectrum and return to the main menu.

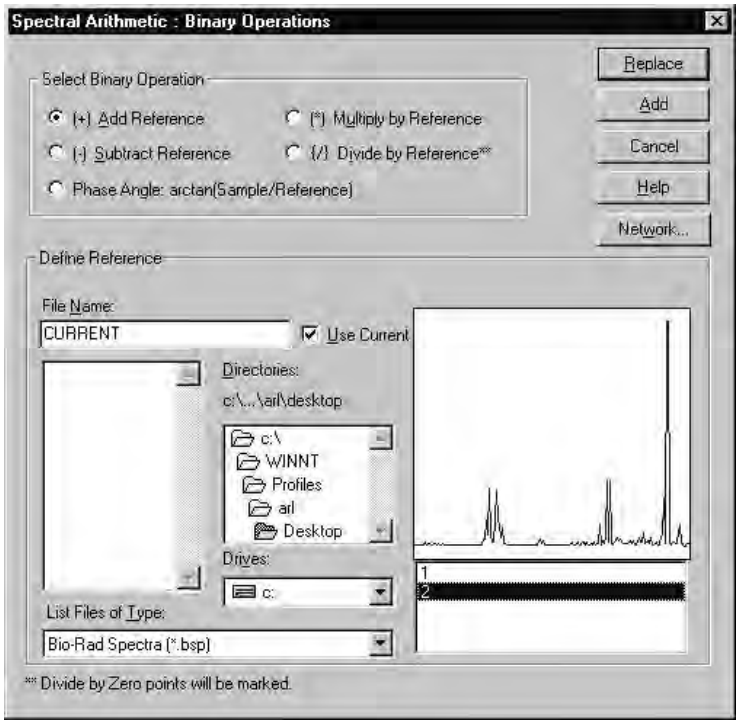
Add: make the desired calculation, add the new spectrum to the spreadsheet, and return to the main menu.

Cancel: return to the main menu without making any changes to the selected spectrum.

Help: enter the on-line Help system.

Binary...

Allows you to perform arithmetic operations on the selected spectrum and a reference spectrum. The Spectral Arithmetic: Binary Operations dialog box appears.



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If the reference spectrum has not been selected, use standard Windows NT procedures to select it. If the spectrum is on a drive not currently connected to your system, click the Network button to connect it.

Use Current: if selected, the current spectrum is used as the reference spectrum.

Note

The reference spectrum must have been collected with the same parameters as the original spectrum.

(+) Add Reference: to each point of the original spectrum, add the value of the corresponding point in the reference spectrum. Replace the original spectrum with the new spectrum.

(-) Subtract Reference: from each point of the original spectrum, subtract the value of the corresponding point in the reference spectrum. Replace the original spectrum with the new spectrum.

(*) Multiply by Reference: multiply each point of the original spectrum by the value of the corresponding point in the reference spectrum. Replace the original spectrum with the new spectrum.

(/) Divide by Reference: divide each point of the original spectrum by the value of the corresponding point in the reference spectrum. Replace the original spectrum with the new spectrum.

Phase Angle: arctan(Sample/Reference): divide each point of the original spectrum by the value of the corresponding point in the reference spectrum. Calculate the arctangent of this ratio. Replace the original spectrum with the new spectrum.

Replace: make the desired calculation, replace the existing spectrum and return to the main menu.

Add: make the desired calculation, add the new spectrum to the spreadsheet, and return to the main menu.

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Cancel: return to the main menu without making any changes to the selected spectrum.

Help: enter the on-line Help system.

3-D Interpolation

Creates PAS (Photoacoustic spectroscopy) Interpolated Spectra from an in-phase and a quadrature spectrum[5]. This would be created in a step-scan MCS experiment. By performing a geometric interpolation:

$$S_\theta = S_{\text{in-phase}} \cos\theta + S_{\text{quadrature}} \sin\theta$$

intermediate spectra can be created. The phase angle is related to the samnpling depth, so that

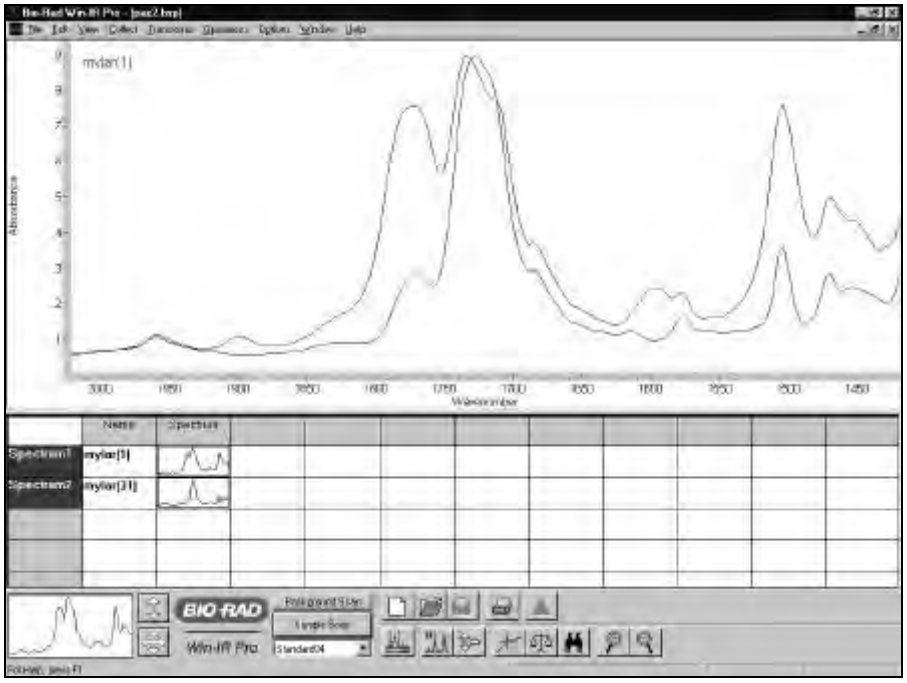
$$S_\theta \propto S_{\text{depth}}$$

This interpolation operation produces a spectral surface where the axes are frequency (x), phase angle (y), and intensity (z).

In this example, we will use pas2.bsp which contains an in-phase and quadrature spectrum of mylar.

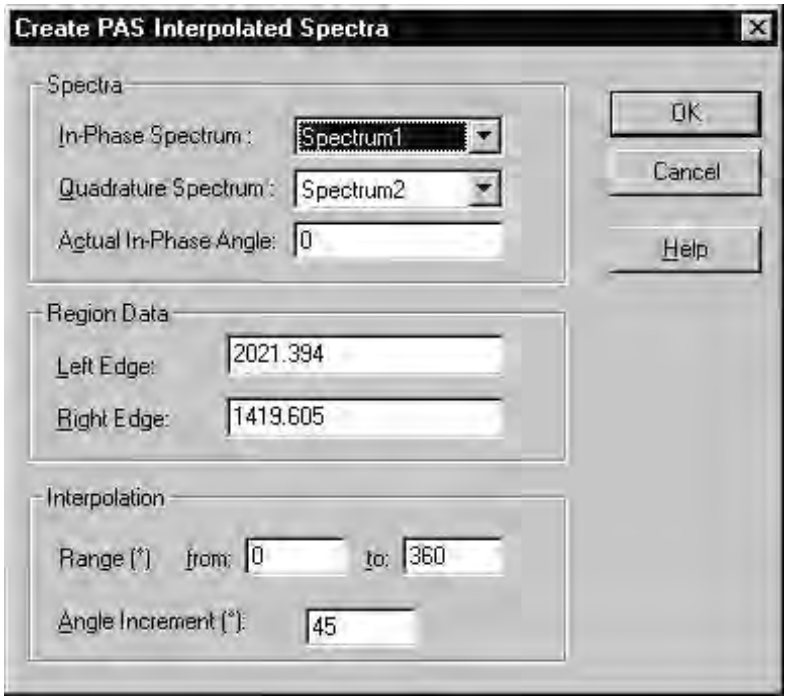
[5] Noble, Deborah, "FT-IR PAS steps up to depth profiling,", *Anal. Chem.* **66**, 757A-760A (1994).
Palmer, Richard A. and Dittmar, Rebecca M., "Step-scan FT-IR photothermal spectral depth profiling of
polymer films," *Thin Solid Films*, **223**, 31-38 (1993).
Bajic, Stanley J., Luo, Siquan, Jones, Roger W., and McClelland, John F., "Analysis of Underground Storage Tank Waste Simulants by Fourier Transform Infrared Photoacoustic Spectroscopy," *Appl. Spec.*
49, 1000-1005 (1995).

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Both these spectra must be selected for this entry to be enabled. Choose 3D Interpolation from the Spectral Arithmetic submenu of the Operations menu; the Create PAS Interpolated Spectra dialog box appears.

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Spectra

In-Phase Spectrum: select the in-phase spectrum using its spreadsheet position.
Quadrature Spectrum: select the quadrature spectrum using its spreadsheet position.
Actual In-Phase Angle: the default angle is taken to be 0. If you know what the actual angle is, enter it here. Changing this angle has the effect of moving the 3D display along the angle axis.

Region Data: the region of the two spectra to be used in creating the PAS view.

Left Edge: the lower limit (in cm^{-1}) of the spectrum.
Right Edge: the upper limit (in cm^{-1}) of the spectrum.

Interpolation: define the range on which the interpolation is to take place.

Range (°): interpolate between these limits (in degrees).
Angle Increment (°): the size of the increment for interpolation (in degrees).

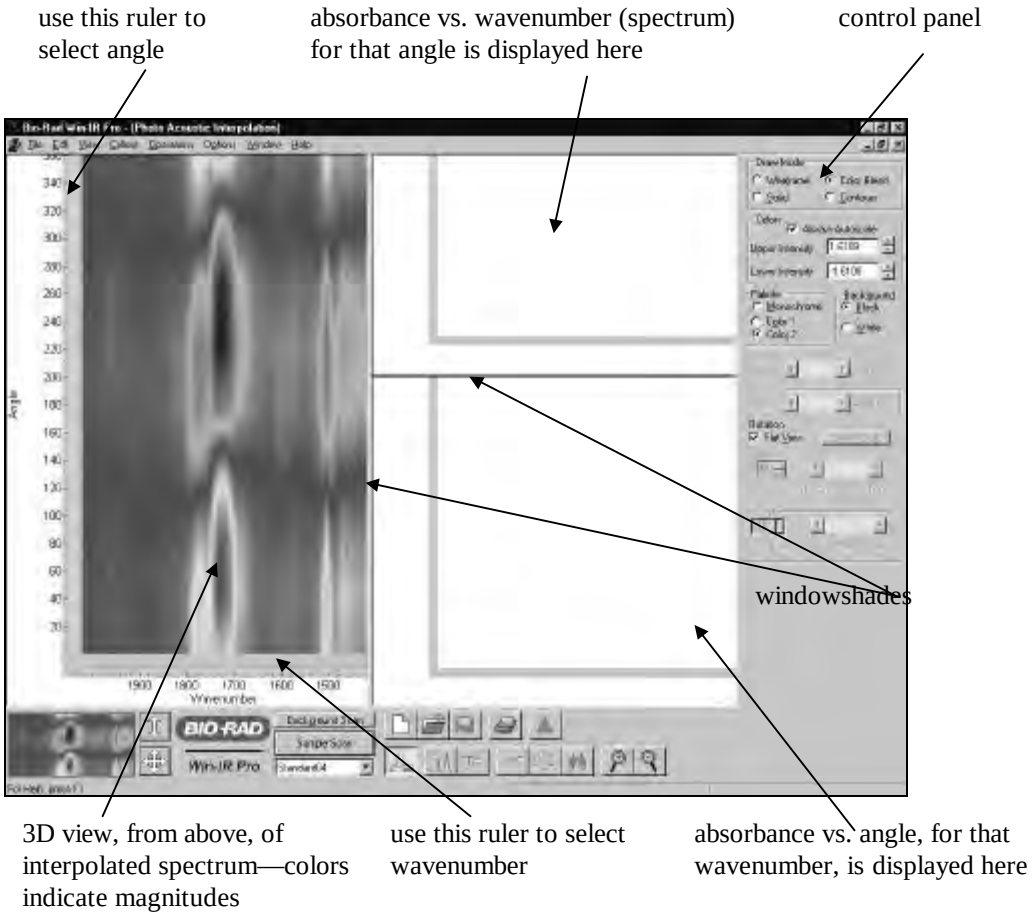
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OK: creates the PAS view and displays it (see below).

Cancel: return to the main window without generating any PAS spectrum.

Help: enter the on-line Help system.

The initial view of the 3D interpolated spectrum is shown below.



Two-dimensional cross-sections of the interpolated spectrum: To select a spectrum at any angle, place the cursor in the vertical ruler and click the left mouse button. The spectrum is displayed in the upper middle of the window.

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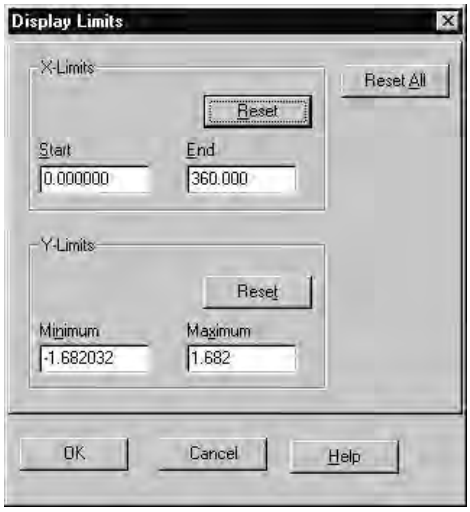
To select a plot of absorbance vs. angle for any wavenumber, place the cursor in the horizontal ruler and click the left mouse button. The absorbance-vs.-angle plot is displayed in the lower middle of the window.

Once you have selected a trace you can adjust its display. In this example, the upper trace has been selected. Choose View / Display Limits / Selected Spectrum. The Display Limits dialog box appears.



See the section on Display Limits in Chapter 8 for details of how to use this dialog box. If you select the lower trace, and choose View / Display Limits / Selected Spectrum, the dialog box appears with the limits for that trace.

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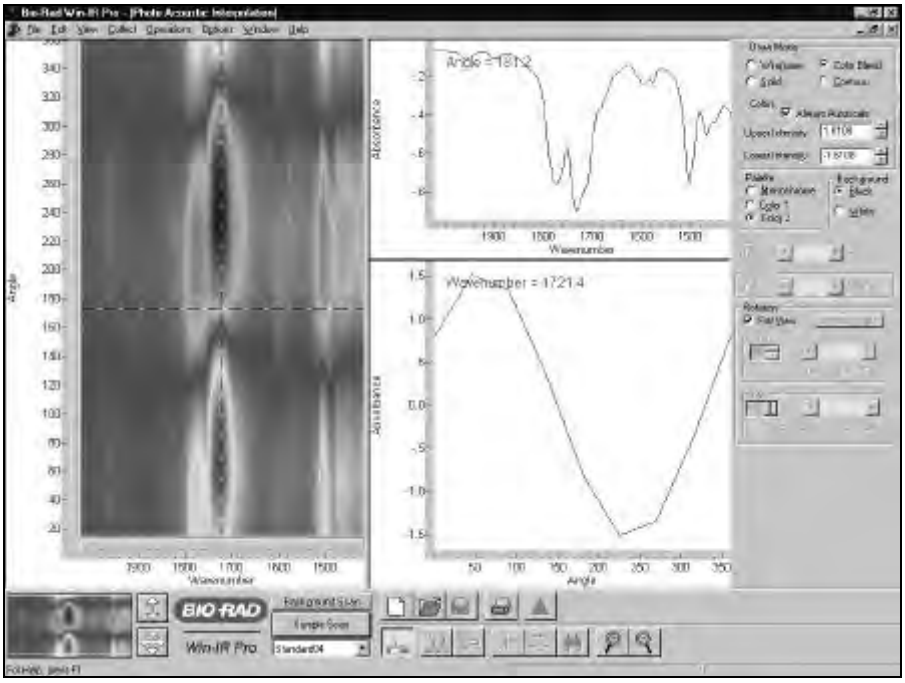
Note

Under certain conditions and color selections, the extracted line may vanish. To cause it to reappear:

1. Select Options / Edit Color...
2. Open the Pen icon.
3. Select Region Line
4. Click on the color in the lower left of the Basic Color block (black).
5. Click the OK button.

In the example below, both an angle and a wavenumber have been selected.

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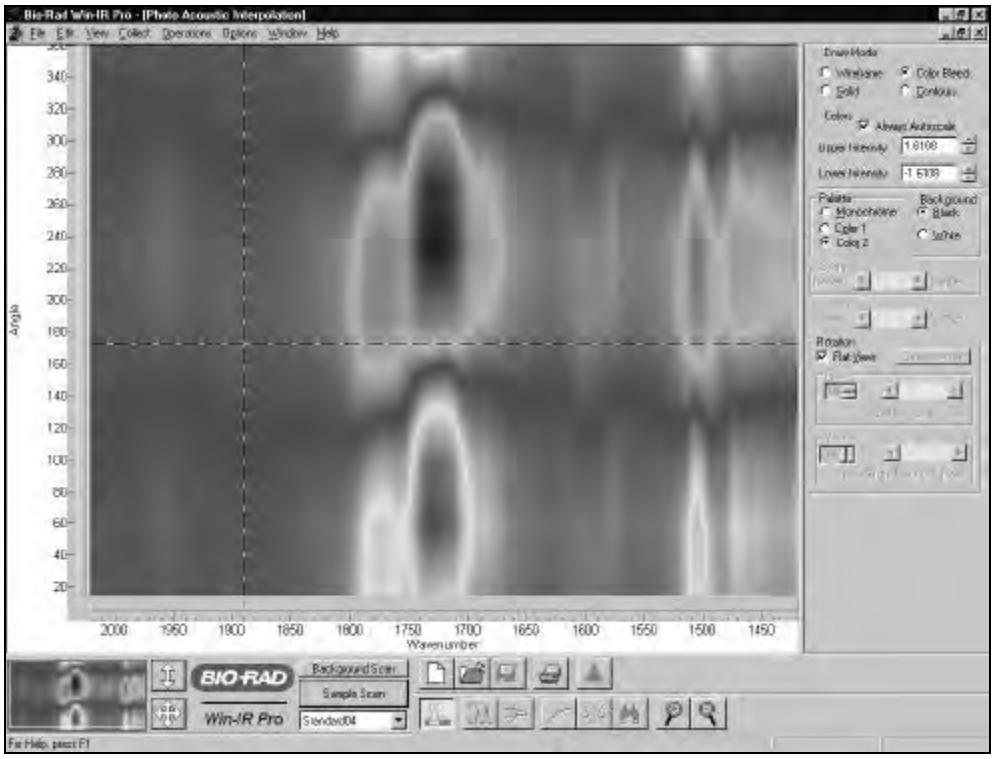
Select a trace, in either the upper or lower display, by clicking on it. You can now use the normal zoom and scaling operations in that display.

Printing a cross section: Select a trace, in either the upper or lower display, by clicking on it. Select Print from the File menu, or click the  button. The Print dialog box appears. Press OK if the settings are as desired; otherwise, see Print in Chapter 6 for details of the settings.

The portion of the window taken up by each of the three displays can be altered by dragging the windowshades to the desired location (see Chapter 1 for details of moving windowshades).

Three-dimensional interpolated spectrum: This spectrum can be moved, rotated, and presented in a number of formats. The control panel sidebar on the right hand of the screen controls the presentation of the data. The portion of the window used by the different graphics can be altered by moving the horizontal and vertical window shades. In all the examples below, the vertical window shade has been moved all the way to the right to better show the three-dimensional graphics.

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Draw Mode: how the three-dimensional aspect will be represented in two dimensions.

Wireframe: the points of the calculated three-dimensional plot are connected with straight lines. Lines that are hidden by the shape of the display are not shown. This draw mode disables both Colors and Palette.

Solid: the lines and the frames they define are filled in with different shades of a single color to give a better idea of the shape of the surface of the contour plot.

Color Bleed: uses multiple colors for the surface. These colors change gradually and smoothly as the height of the plot varies above the base plane. (Default)

Contours: shows contour lines on the surface at constant heights about the base plane. The contour intervals are pre-set and cannot be changed.

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Colors: sets the range of colors used to represent the extreme z-values of the plot.

Note

In wireframe mode, Colors is disabled.

Always Autoscale: if this is selected, then whenever you zoom in on a portion of the plot, the color will be scaled so that the full color range is used for that portion. This is useful if you zoom in on weak features that may be displayed in very similar colors in the full plot.

If you are not autoscaling the colors, then you can set the values to be used in the display. If you use the arrows to the right of the intensity boxes to set values, they will be implemented immediately. If you type in values, they will not be implemented until you press the Enter key on the keyboard.

Upper Intensity: enter the color value to be used at the maximum z-value of the plot.
Lower Intensity: enter the color value to be used at the minimum z-value of the plot.

Palette: the draw modes may be observed with three different color schemes.

Note

In wireframe mode, Palette is disabled.

Monochrome: gray scale.
Color 1: shades from red to white to blue.
Color 2: shades from red through orange, yellow, and green to blue. (default)

Background: select the color for the background. A white background may be better if you are capturing screens for insertion in a publication with a monochrome printer.

Black: background is black. the plot is shown against a black background (default).

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White: the plot is shown against a white background. This may be more desireable for formats other than wireframe

Zoom: makes the plot appear closer (increases size) or farther away (decreases size). Use the slide bar to change the value.

Y Scale: makes the height of the peaks taller or shorter. Use the slide bar to change the value.

Rotation: these controls move the three-dimensional plot about two axes. Regardless of the rotation, the axes remain in the foreground of the display. Rotation of large arrays may be slow. Press the ESC key to stop the rotation.

Flat View: if selected, displays a projection of the isometric view. If de-selected, the isometric view (3D) is shown.

Default Angle: press this button to return the plot to its default position (Pitch = 18°, Yaw = 1°).

Pitch: rotates the plot about a horizontal axis parallel to the monitor screen. Click on the upper part to rotate the plot to show its Bottom; click on the lower part of the bar to rotate the plot to show its Top. Each time you click the end of the slide bar, the plot rotates 9°.

Yaw: rotates the plots about a vertical axis. The plot can be rotated either to the Right or to the Left. Each time you click the end of the slide bar, the plot rotates 18°.

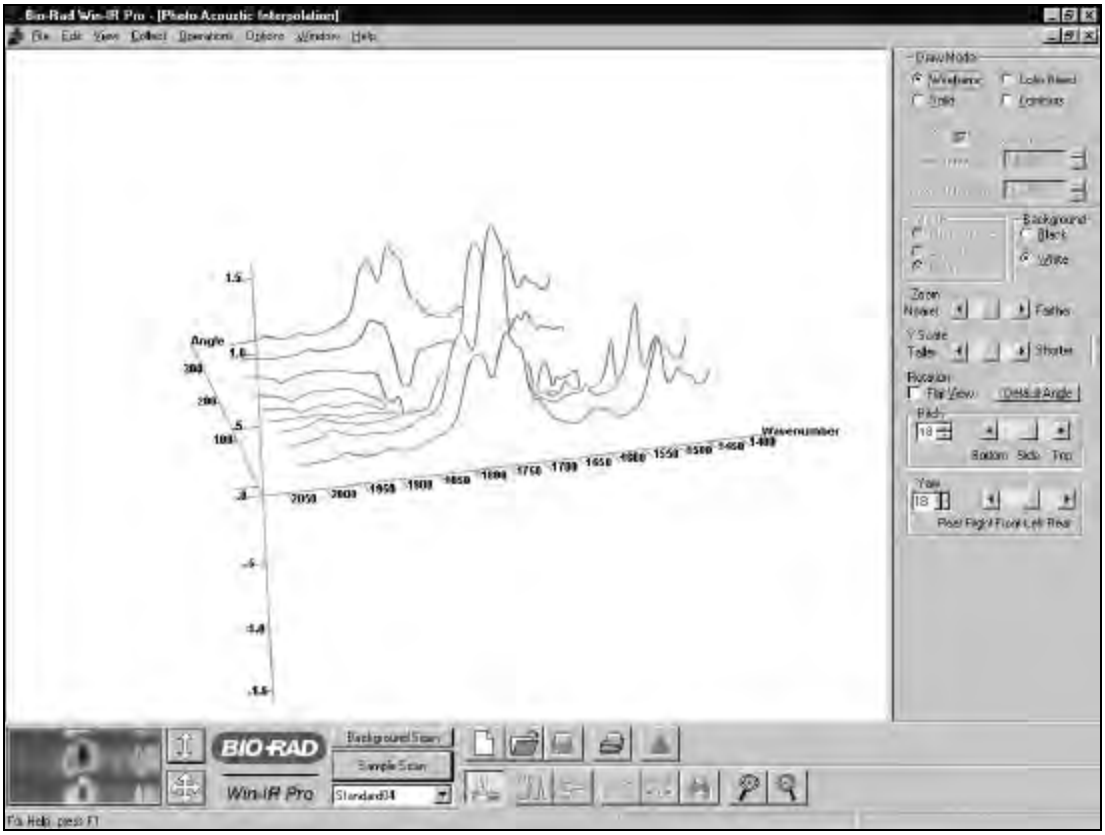
For both Pitch and Yaw, you can enter the value of the angle. If you change the angle with the arrows to the right of the text box, the values are implemented immediately. If you type in values, the values are not implemented until you press the Enter key on the keyboard.

Subsets of the File, Edit, Options, Window, and Help menus are also available. Their entries operate the same as they do in the main Win-IR Pro document window.

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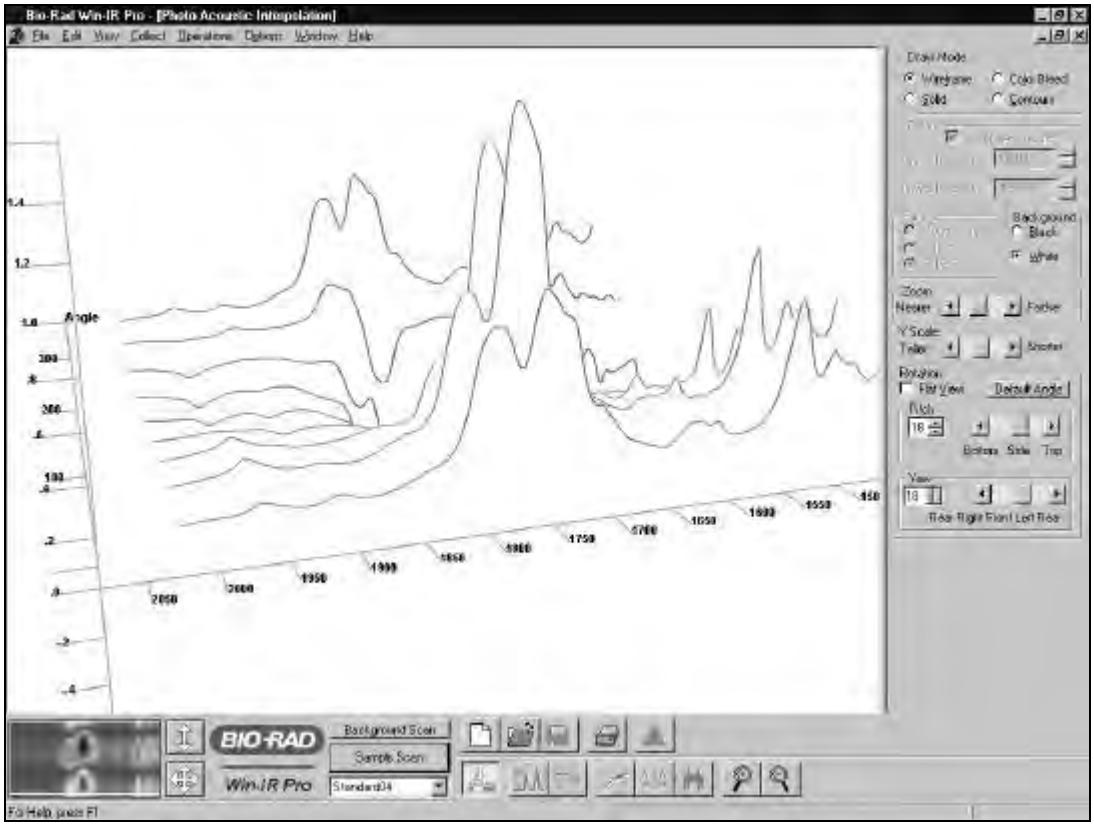
Examples:

In this example, Draw Mode has been set to Wireframe and Background to White. Flat View has been de-selected and the image has been rotated (Yaw).



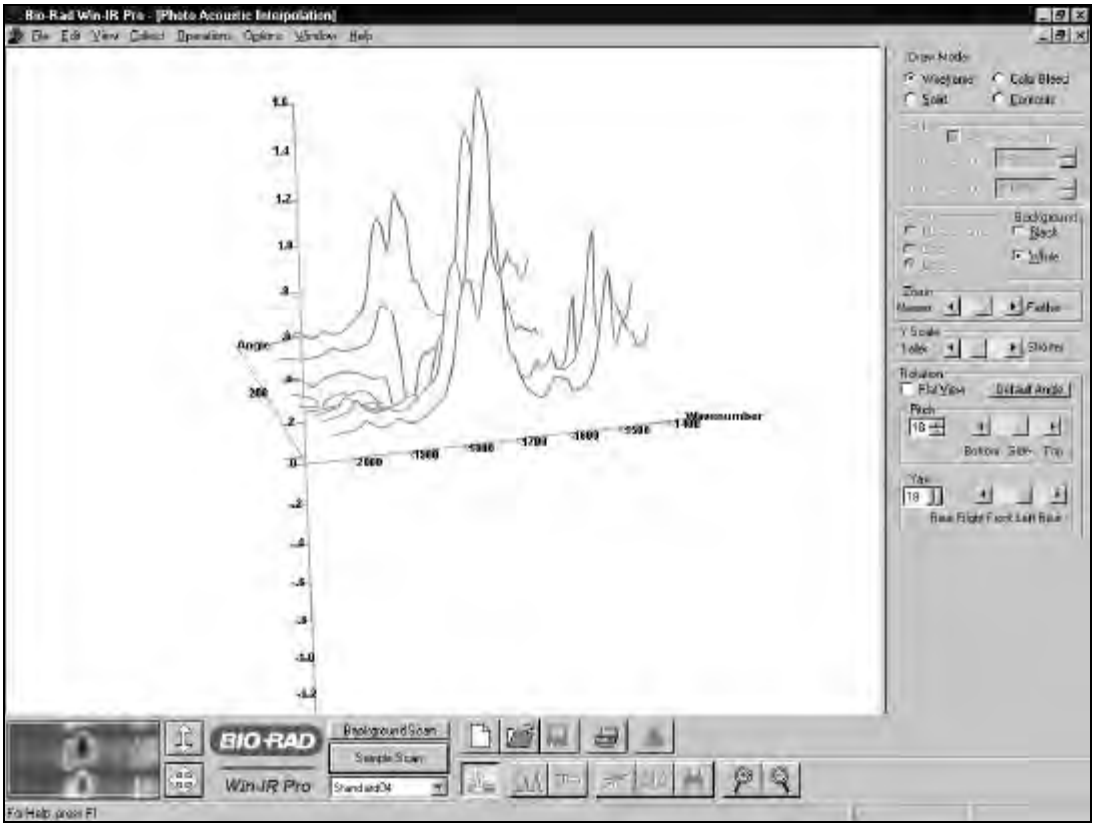
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Zooming in gives this view.



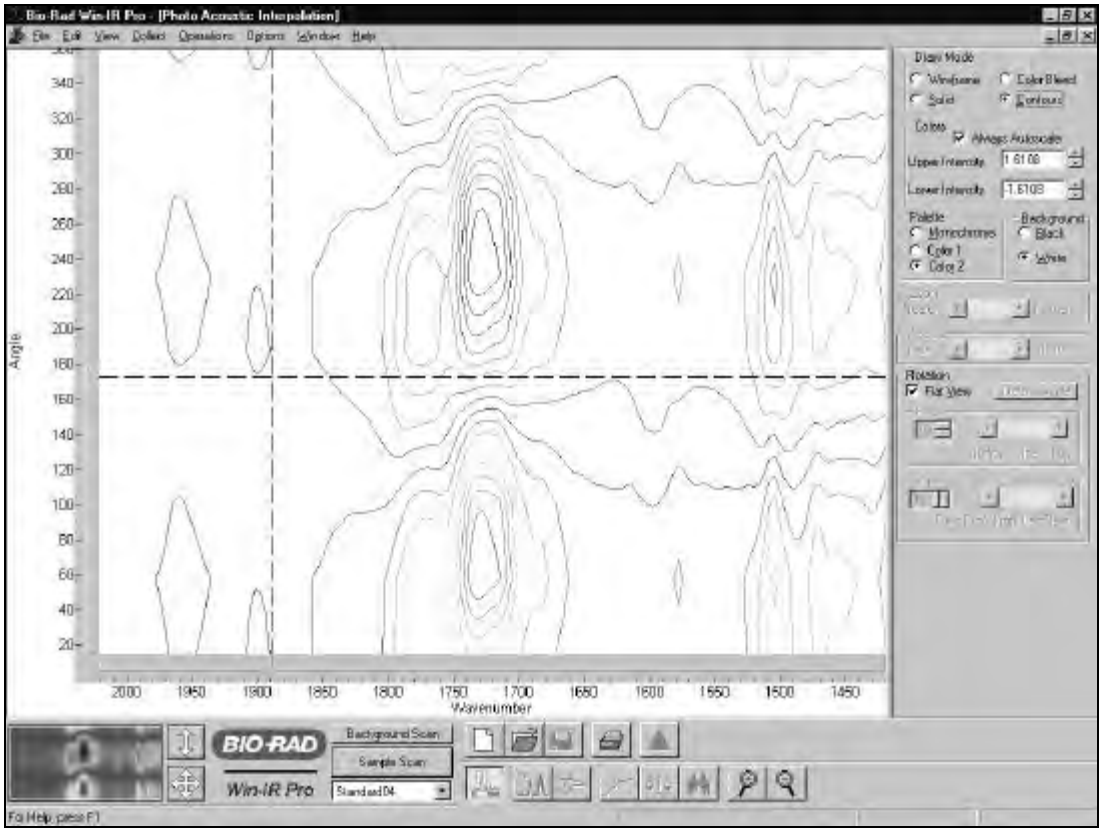
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Zooming out and increasing Y Scale gives this view.



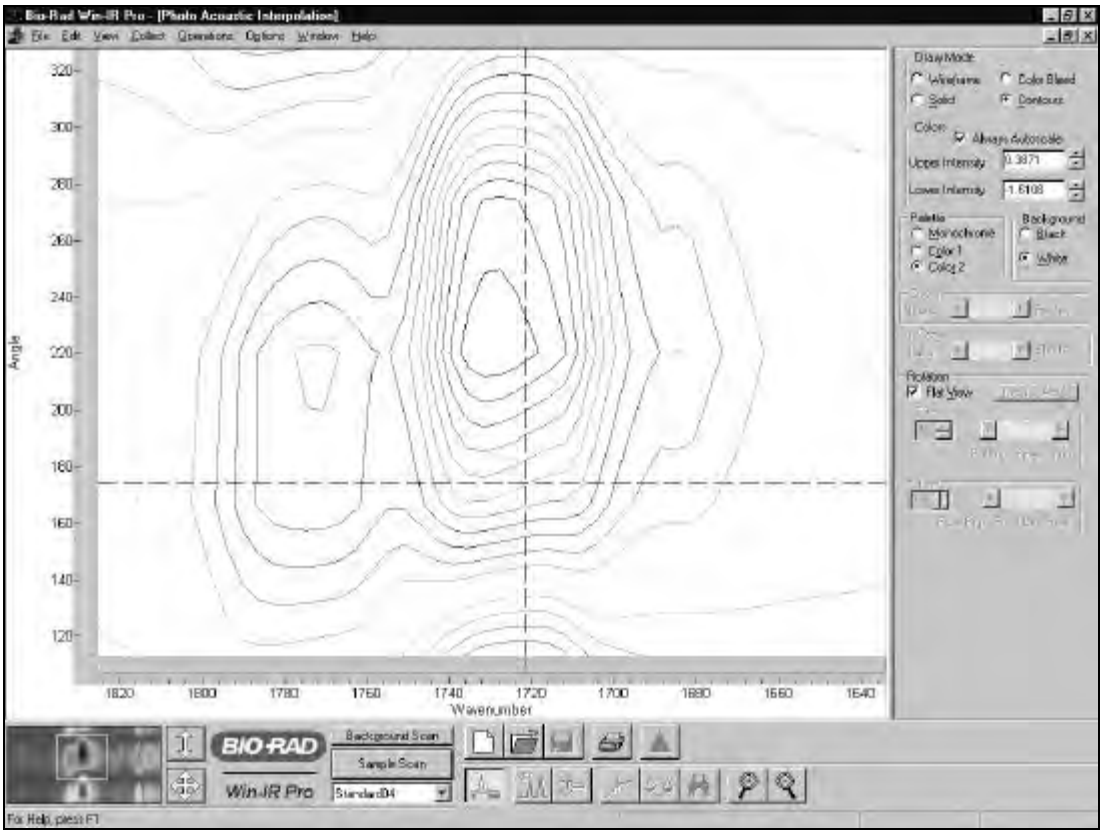
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In the example below, Flat View has been selected; Draw Mode is set to Contours.



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You can use the cursor to draw a rectangle about the area of interest to zoom in on it.

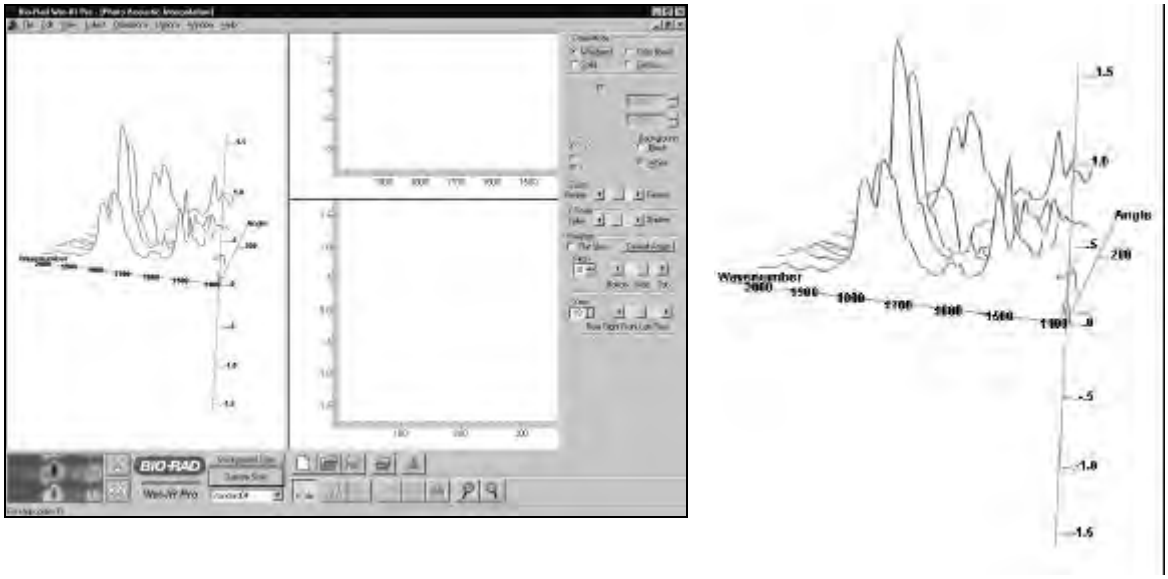


Printing the 3D View:.To print the three-dimensional (left-hand side) part of the screen, select File / Print or click the button at the buttom of the screen. In the example below, the following parameters have been changed from their defaults:

Draw Mode	Wire Frame
Palette	Monochrome
Background	White
Flat view	de-selected

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The full screen is on the left; the printed image is on the right.



The printed image is exactly what is in the three-dimensional portion.

If you want to print the entire screen image use either WordPad or Paint. These two applications are supplied as part of Windows NT. The procedure is described in Chapter 1.

Exporting PAS Interpolation 3D Data

The data triads (x, y, z) can be exported by selecting Operations / Export DXF. The file created has a .dxf extension and can be opened and manipulated by applications such as Autocad.

Notes

This menu entry is only accessible in a 3D graphics view.

These .dxf files cannot be inserted into word processors using the usual .dxf filter.

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Raman Convert

When selected, the Raman Convert dialog box appears.



Raman Laser Wavenumber: the value to be used to convert the absolute wavenumber spectrum to a Raman-shifted spectrum. This value is a physical property of the excitation laser. Once it is known and set for the hardware, there is usually no reason to change it.

OK: set the Raman laser wavenumber to the value entered; return to the main screen.

Cancel: return to the main screen without altering the value.

Help: enter the on-line Help system.

Note

The Raman Laser Wavenumber value can also be altered through the Laser or Computations tab pages of Collect / Raman-Scan...

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CHANGE ZPD LOCATION...

Under certain conditions it may be necessary to manually change the Zero Path Difference (ZPD) which is normally determined automatically during setup.

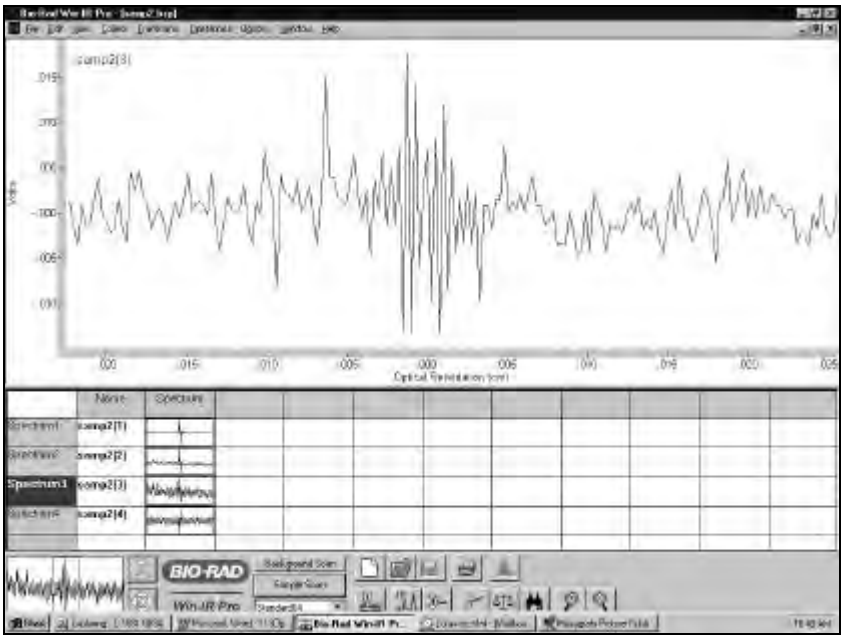
For example, multiple modulation experiments, such as vibrational circular dichroism, polymer stretching, these give interferograms which are essentially “difference” interferograms: the differential absorbance between two states of the sample, or of the polarization of the incident light. The spectra are flat lines centered at zero with small positive and negative excursions, and these interferograms therefore have no centerburst, and just weak (symmetrical) sidebursts. [The normal centerburst arises from the large positive single-beam curve.]

Additionally, in some MCS experiments, data collection is performed at different speeds and using different electronic filters than setup. This causes the centerburst to “shift.”

The ZPD is the zero point used by the Fourier transform to calculate the single-beam spectrum from the interferogram.

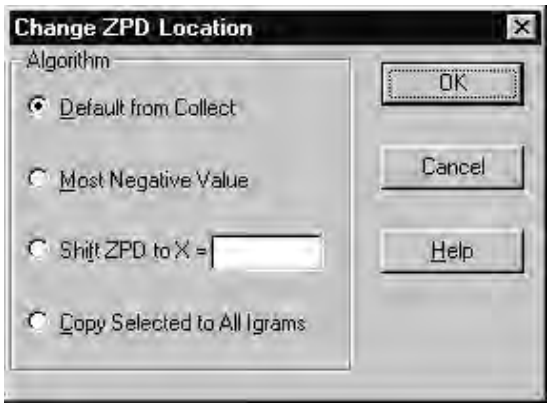
The document below contains a number of interferograms; consider the third one, which does not have as well-defined a centerburst as the others.

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To move the ZPD,

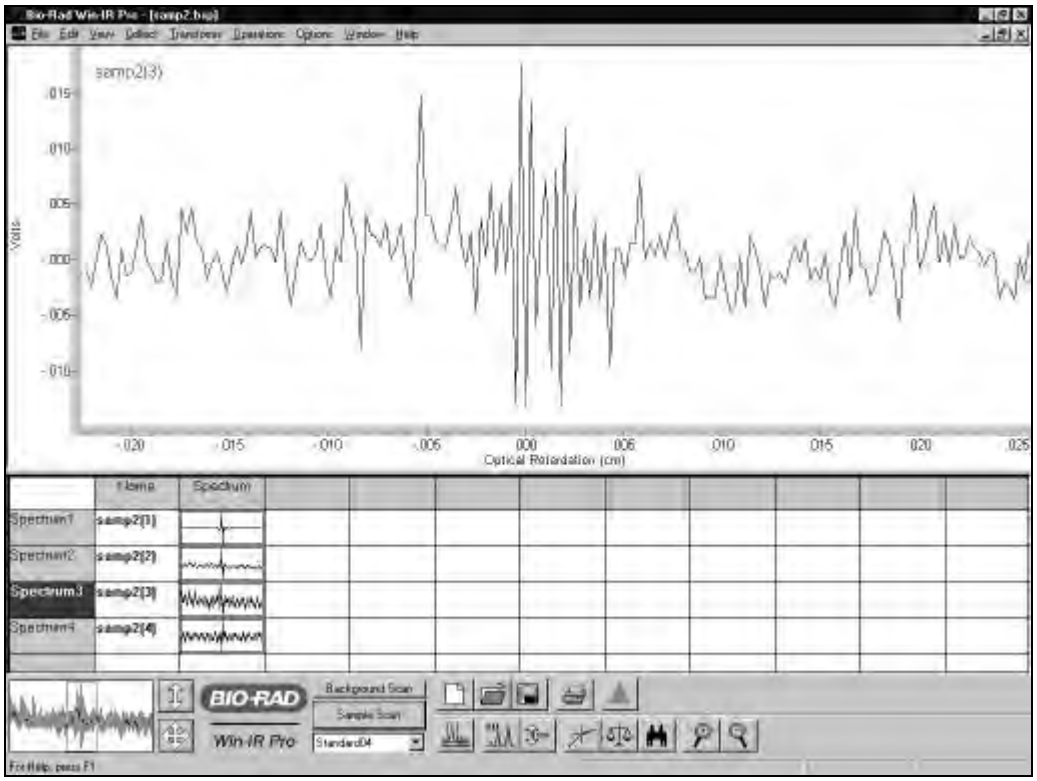
1. Select Operations / Change ZPD Location....The Change ZPD Location dialog box appears, offering 4 choices:



Default from Collect: use whatever ZPD location was determined during setup.

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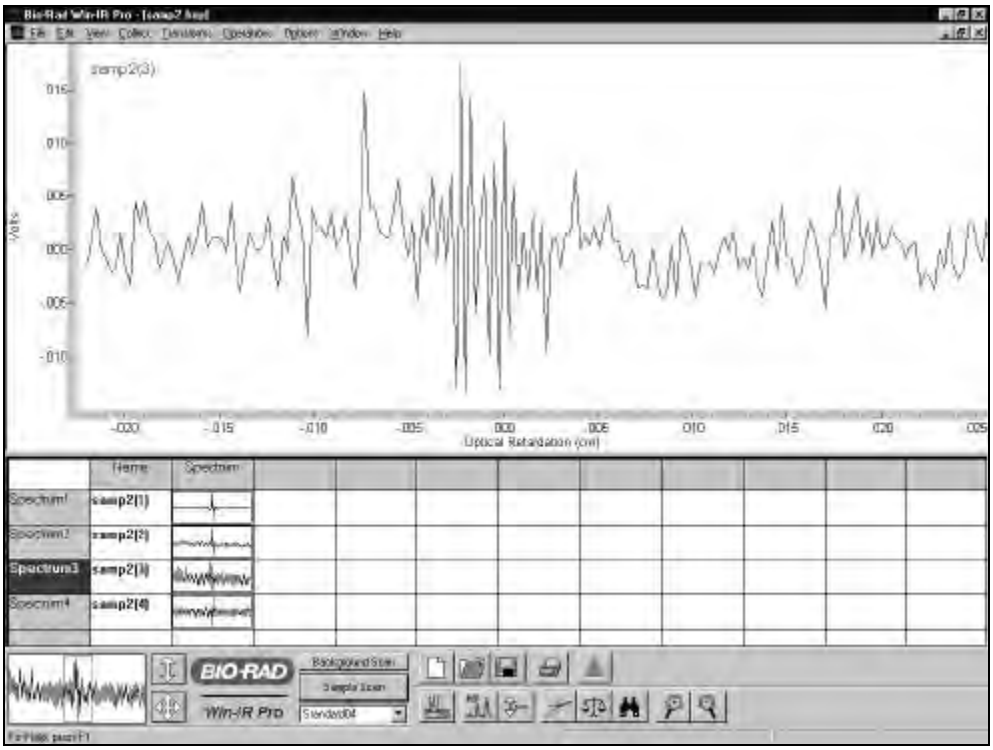
Most Negative Value: set the ZPD at the largest negative value of the interferogram.



The ZPD has been shifted to the left by about 0.001 cm.

Shift ZPD to X = : set the ZPD to the location typed into the box to the left of this line. Location is in optical retardation (cm). For example, enter 0.002

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The ZPD in the interferogram above is now where 0.002 cm was in the original interferogram.

Copy Selected to All Igrams: use the current location of the ZPD, as defined for this interferogram, for all the interferograms contained in this document.

For example, in a multiple modulation experiment, the ZPD might be transferred from an interferogram with a well-defined centerburst to one without, after shifting the well-defined centerburst to zero retardation.

2. Click the OK button to implement the selection.

Cancel returns to the main menu without making any changes to the ZPD location.

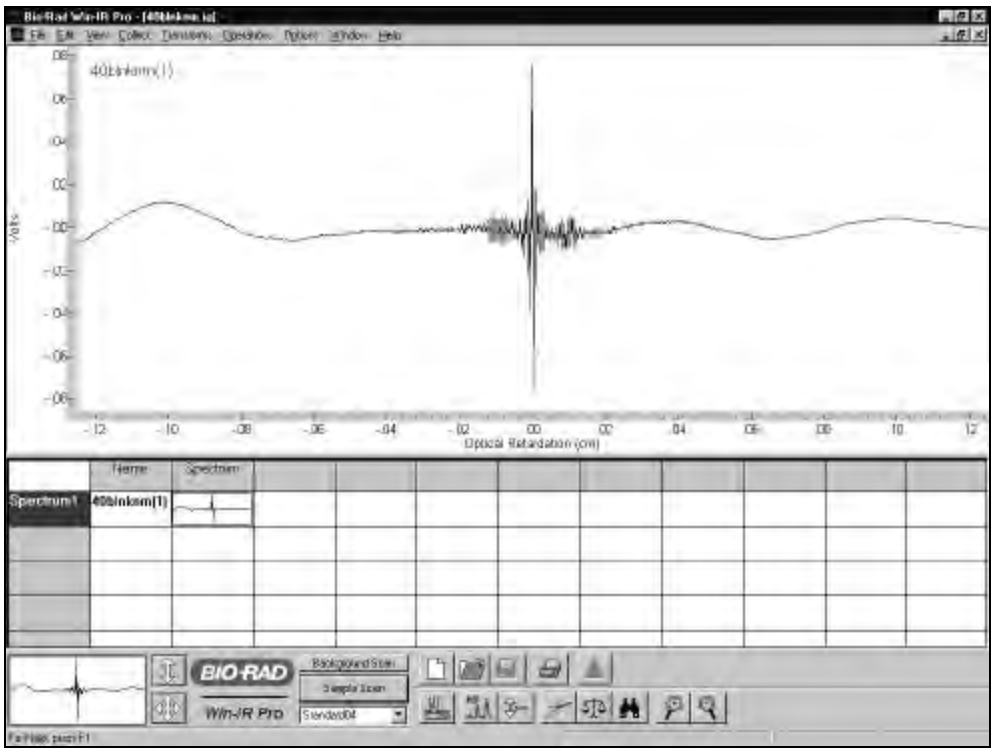
Help enters the on-line Help system.

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PAS LINEARIZE...

This method allows you to compute linear photoacoustic FT-IR spectra using one sample and one reference interferogram. This method produces spectra similiar to transmission spectra through the reduction of saturation that is normally a factor in amplitude computation.

You must have an interferogram selected to enable the PAS Linearize... entry.

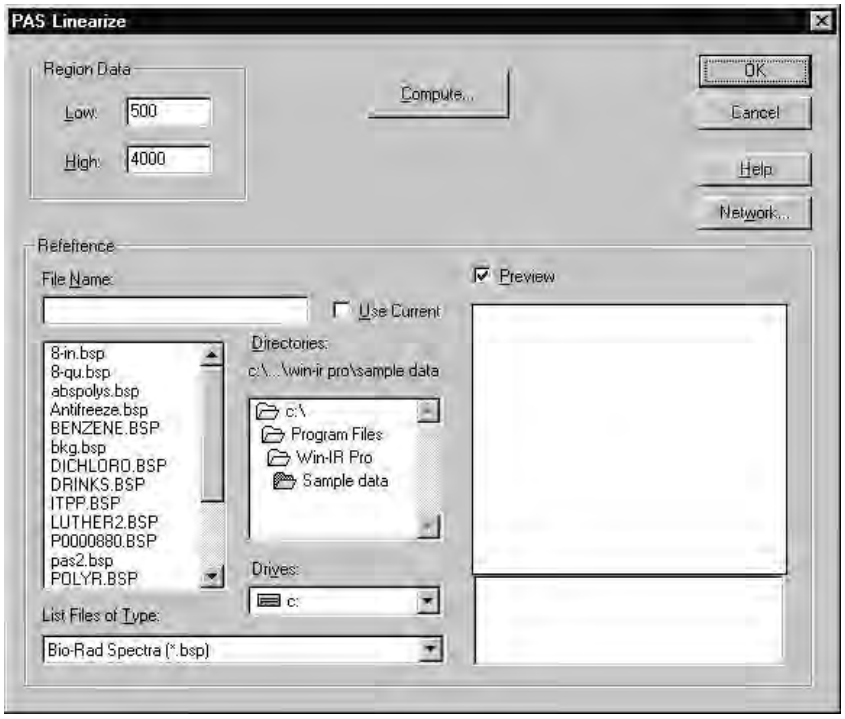


Note

This spectrum replaces the interferogram. The interferogram cannot be recovered by the Operations / Reprocess procedure. Use Operations / Copy Spectrum before PAS Linearize... if you want to save the interferogram.

When you select PAS Linearize... the PAS Linearize dialog box appears.

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Region Data: defines the region to be displayed for the linearized PAS spectrum (in wavenumbers).

Low: the lower edge of the region.
High: the upper edge of the region.

Reference: defines the interferogram to be used as the reference in calulating the phase array.

File Name: the name of the file containing the interferogram to be used as the reference interferogram.

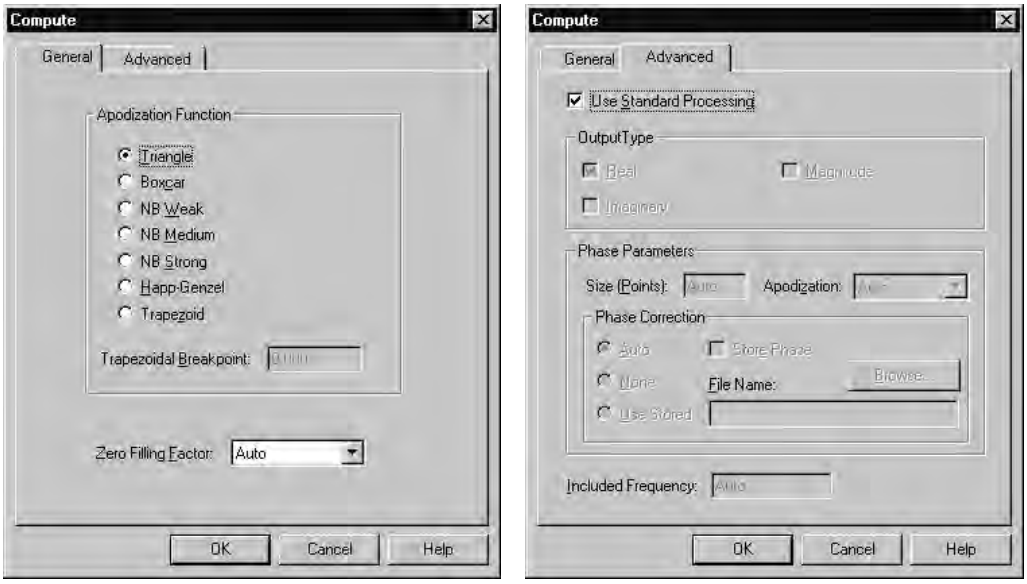
Use Current: if checked, the currently selected interferogram in this document is used as the reference interferogram.

Drives: select the drive on which the file resides.

List Types of Files: this will normally be Bio-Rad Spectra or 3200 Format Spectra.

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Compute: set the parameters for the calculation. When this button is clicked the Compute dialog box appears



General tab page

Apodization Function: normally Triangle is selected.

Zero Filling Factor: normally Auto is selected.

Advanced tab page

Use Standard Processing: this is normally checked; it disables the rest of the parameter settings on this page. Unless you have a specific reason to do otherwise, use the default settings.

Output Type: this is ignored by the PAS linearization process.

Phase Parameters

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Size (Points): set to Auto.
Apodization: set to Auto.
Phase Correction: set to Auto by the calculation
Store Phase: ignored
File Name: ignored

Included Frequency: set to Auto.

OK: return to the PAS Linearize dialog box with the new parameter settings.

Cancel: return to the PAS Linearize dialog box with the previous parameter settings.

Help: enter the on-line Help system.

OK: calculate the PAS linearized spectrum and display it.

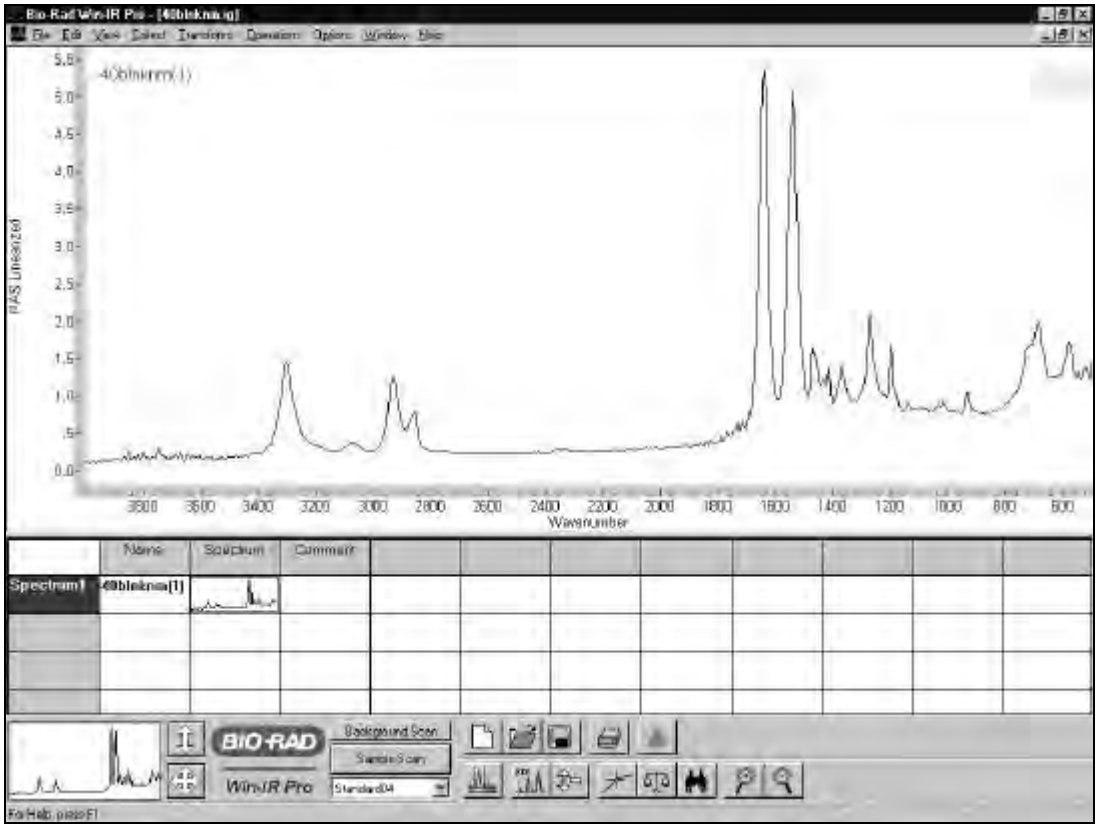
Cancel: return to the main window without calculating the PAS linearized spectrum.

Help: enter the on-line Help system.

Network: connect to other disks on the network to access non-local files.

When OK is clicked, two computations are done. First, the reference interferogram is computed using auto phase correction generating a phase array which is stored. This stored phase array is used in the calculation of the spectrum from the sample interferogram.

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IR MENTOR

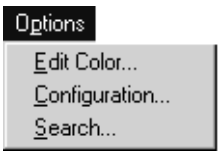
Invokes the IR Mentor, if this product has been loaded on the system; if it has not been loaded, this menu entry is disabled (grayed-out). IR Mentor is an on-line data base of characteristic group frequency ranges and approximate band intensities, with associated bar charts, to assist in the interpretation of infrared spectra. It is a tool for instruction and for interpreting complex spectra.

Every time your select Operations / IR Mentor, a new copy of the application is opened. It is not automatically closed when you return to Win-IR Pro. You may want to manually close IR Mentor when you have finishing a session.

See the *IR Mentor Pro Manual* (091-1017) for details.

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12
Options Menu



These menu entries allow you to change certain Win-IR Pro default settings.

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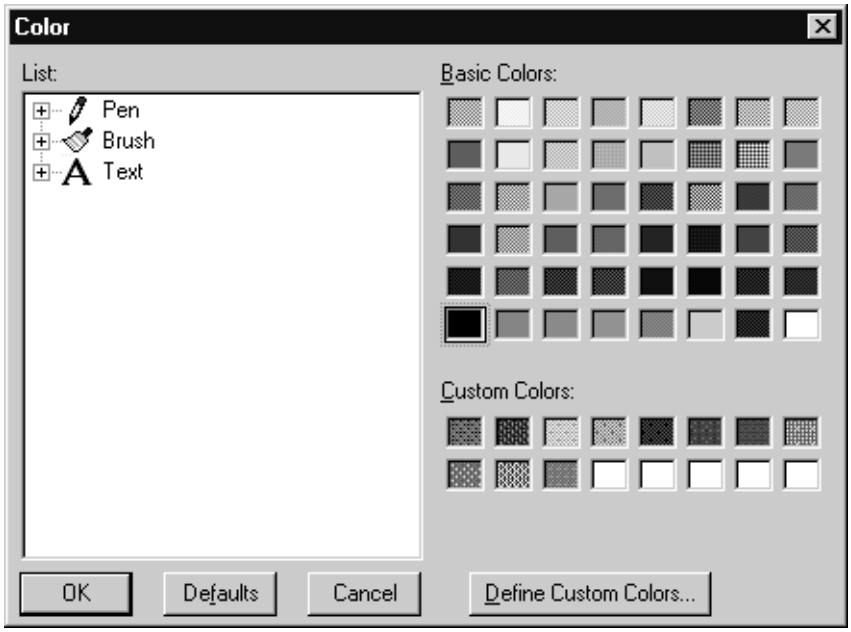
EDIT COLOR

This allows you to change the colors of objects, backgrounds, spectra, etc. from the default. Selecting this entry brings up the Edit Color Dialog box. There are three types of objects that can be colored: Pen, Brush, and Text.

Pen: objects that are lines. These include spectra, points, boxes, etc.

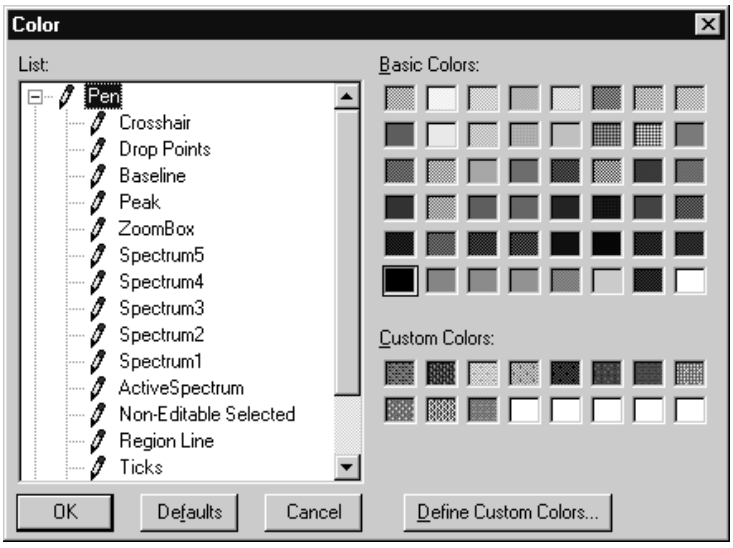
Brush: objects that are areas. These include backgrounds, regions, etc.

Text: objects that are printing characters. These include labels, etc.

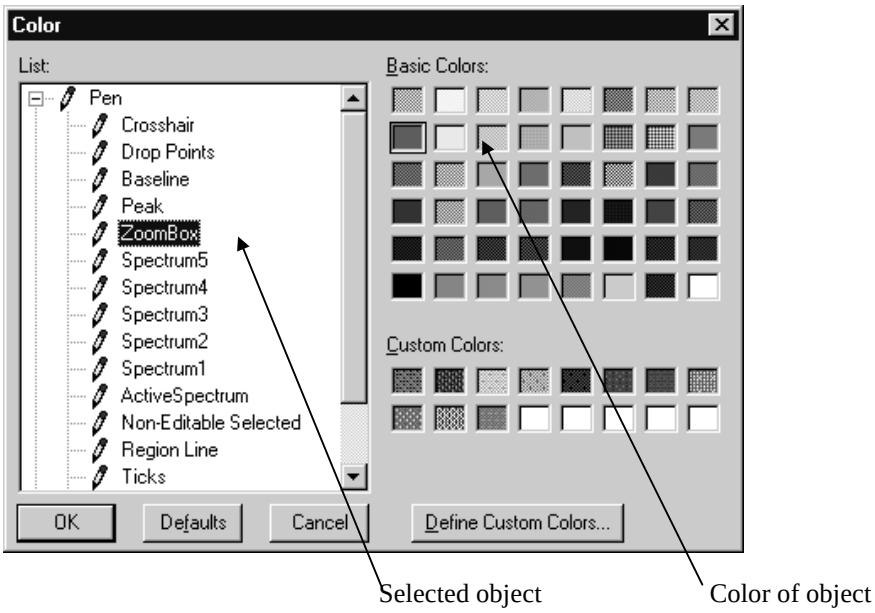


First, expand the list for the type of object to be edited. You can do this by single clicking the box with the + in it, by double clicking the object type symbol, or by double clicking the object type name.

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A list of objects of that type is displayed in the List: box. Select the object to be color edited by highlighting it; its current color is shown on the right by a heavy black rectangle surround its color box.



To change a color:

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1. Select the type of object–Pen, Brush, or Text.

2. In List, highlight the specific object to be changed. The color of that object is indicated by a heavy black rectangle surrounding the color box of the object..

3. Click on the box containing the desired new color for the object.

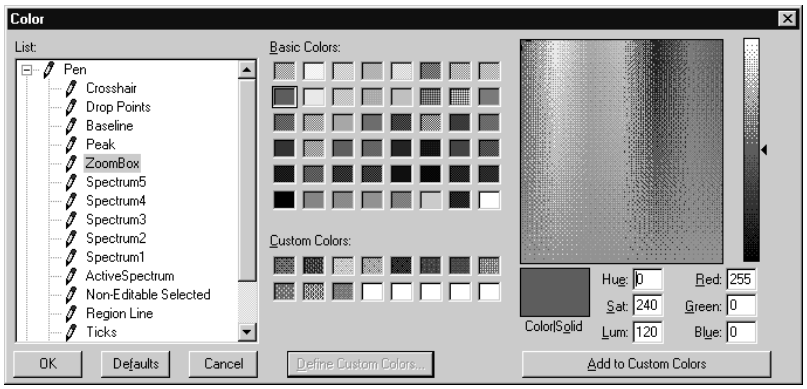
Note

Be careful that you do not select Pen or Text colors that are too close to that of the Brush areas on which they will appear. In that case, some lines or text may seem to vanish.

4. If you want to create a color other than one of the 48 Basic Colors—first, click on the custom color to be edited (white boxes are the same as the other boxes), then click the Define Custom Colors... button. The Color dialog box expands.

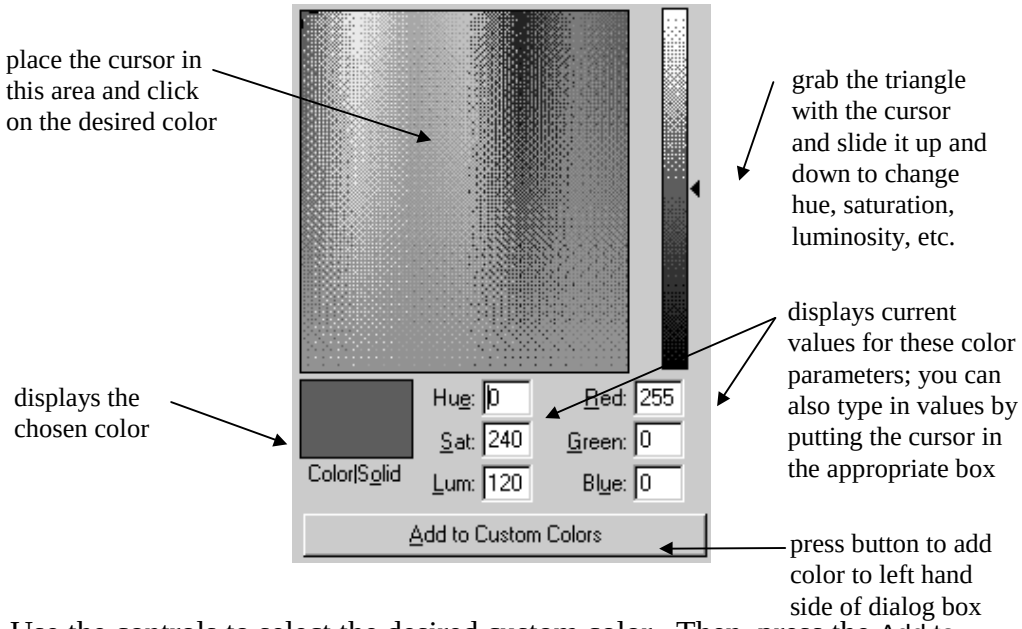
Note

On some monitors, the expanded Color dialog box goes off the right side of the screen. Drag the dialog box to the left to correct this.



An expanded view of the right half of the dialog box is shown below.

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5. Use the controls to select the desired custom color. Then, press the Add to Custom Color button; this will put the new custom color in one of the boxes in the lower half of the left side of the dialog box. Once a custom color has been added, it may be used the same as a basic color. You may want to record the values of the 6 parameters (hue, saturation, luminosity, red, green, blue) for future reference.

   The location of the marker in the square color box controls hue (x-axis) and saturation (y-axis). The position of the marker in the narrow (right hand box) controls luminosity: top=white, bottom=black (default). You need a position away from the two extremes to get a non-white or non-black color.

Notes

If you have not selected a custom color box, then the new custom color is put in the first box in the Custom Colors part of the dialog box; the next color goes in the box directly below it, etc. Every time you reopen the dialog box, the placement of the custom colors is the same. The new custom color is **not** put into the first empty box.

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If you change a color, it does not change the color of the objects that are currently the original color. If you want to change the color of an object, you must explicitly select it and then select the color to be assigned to it. If this is not done, the color assigned to this object is unpredictable.

At this time, if you do not want to add a custom color, just return to working in the left side of the dialog box. Pressing Cancel will close the dialog box and return to the main screen will all changes canceled.

6. If you wish to change the color of any other object, repeat steps 1 to 5.

7. When you are done editing object colors, press one of the buttons at the bottom of the dialog box to affect the action described below.

   OK: return to the main menu and implement all the changes made through the Edit Color dialog box.

   Defaults: returns the colors for all objects to the Bio-Rad facotry-supplied colors.

   Cancel: return to the main menu without implementing any changes made through the Edit Color dialog box.

   Help: enter the on-line Help system.

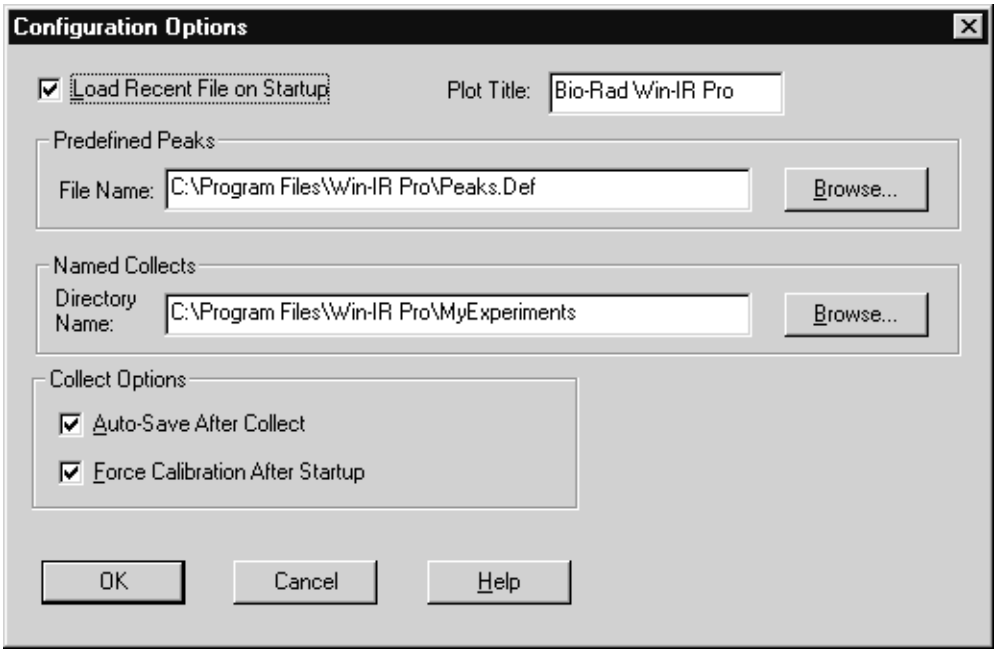
Note

A list of the factory-installed default RGB color settings in given in Appendix B.

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CONFIGURATION...

Selecting this entry brings up the Configurations Options dialog box.

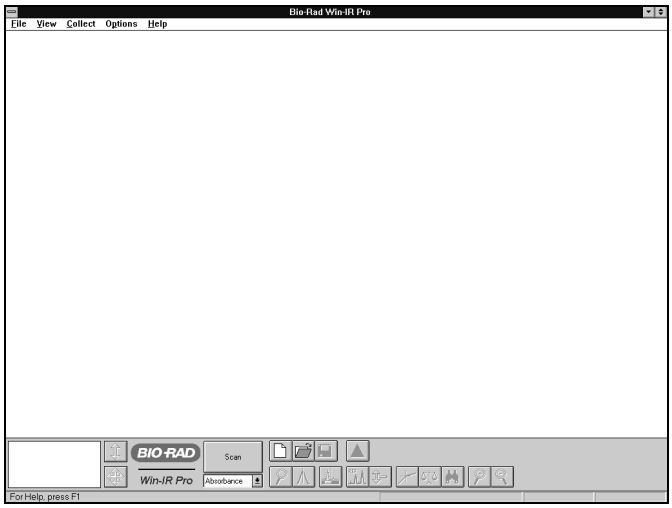


Load Recent File on Startup

If Load Recent File on Startup is selected, then after Win-IR Pro starts, it automatically opens the file that was in memory when you exited Win-IR Pro. This is the default.

If Load Recent File on Startup is not selected, then Win-IR Pro starts with a blank screen.

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Use File / Open or File / New to bring spectra into memory.

Note

Win-IR Pro remembers what the most recent file was, even if you do not load it on startup. Thus, if you select Load Recent File on Startup after it was de-selected, Win-IR Pro will load the most recent file, even though this spectrum did not appear on the screen.

Plot Title

The plot title is printed in the upper left corner of the spectrum plot. Use File / Print or the  button to plot a spectrum. The default text is Bio-Rad Win-IR Pro. To change this label, type a new label in this box, and click OK.

Note

Once you have clicked OK, the text change is permanent. If you want to alter the value again, repeat the selection procedure.

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Predefined Peaks

Specifies the file in which the predefined peaks parameters are saved. The default file is C:\Program Files\Win-IR Pro\Peaks.Def. You can change this file by typing a new pathname into the entry window.

Click the Browse button to bring up the standard Open dialog box. You can select a file for saving the predefined files using standard Windows NT procedures.

See "Peaks" in Chapter 2 and New in Chapter 11 for details of the use of predefined peaks.

Named Collects

Specifies the directory in which the named collect files are saved. The default directory is C:\Program Files\Win-IR Pro\MyExperiments. You can change this directory by typing a new directory pathname into the entry window.

Click the Browse button to bring up the standard Open dialog box. You can select a directory for saving the named collects using standard Windows NT procedures. You can select any file within the directory to select the directory.

See your spectrometer manual for details on the use of named collects.

Auto-Save After Collect

If Auto-Save After Collect is selected, then the document is written to the disk file immediately after a data collection is completed. This is the default.

Note

If no file name has been selected, Win-IR Pro will display a dialog box requesting that you enter one.

If Auto-Save After Collect is not selected, then the document is not written to the disk file immediately after a data collection is completed.

Force Calibration After Startup

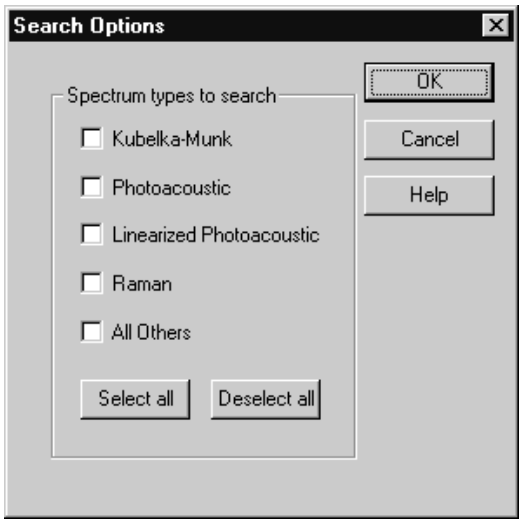
If Force Calibration After Startup is selected (this is the default), then the spectrometer automatically performs a calibration whenever it is powered up. After the calibration, you can collect data.

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SEARCH

Normally, only absorbance (or absorbance-like) spectra are searched for in the libraries, because most commercial libraries have their entries in that format. If you select a spectrum of a type other than an absorbance the Operations / Search entry is disabled. However, if you need to search libraries for a non-absorbance spectrum, this entry can be enabled.

1. Select Search from the Options menu. The Search Options dialog box appears.



2. Select the type(s) of spectrum you want to search by clicking in the box to the right of the spectrum type. You can select more than one type using the ctrl-click combination.

   Select all: search will be enabled for all types of spectra.

   Deselect all: search will be enabled only for absorbance-like spectra.

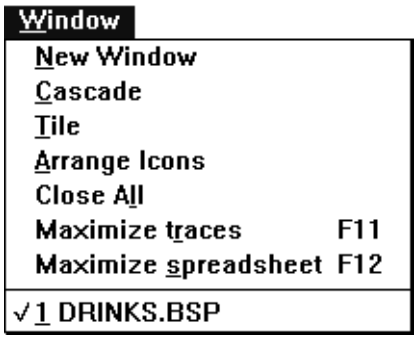
OK: return to the main menu with changes made.

Cancel: return to the main menu with no changes made.

Help: enter the on-line Help system.

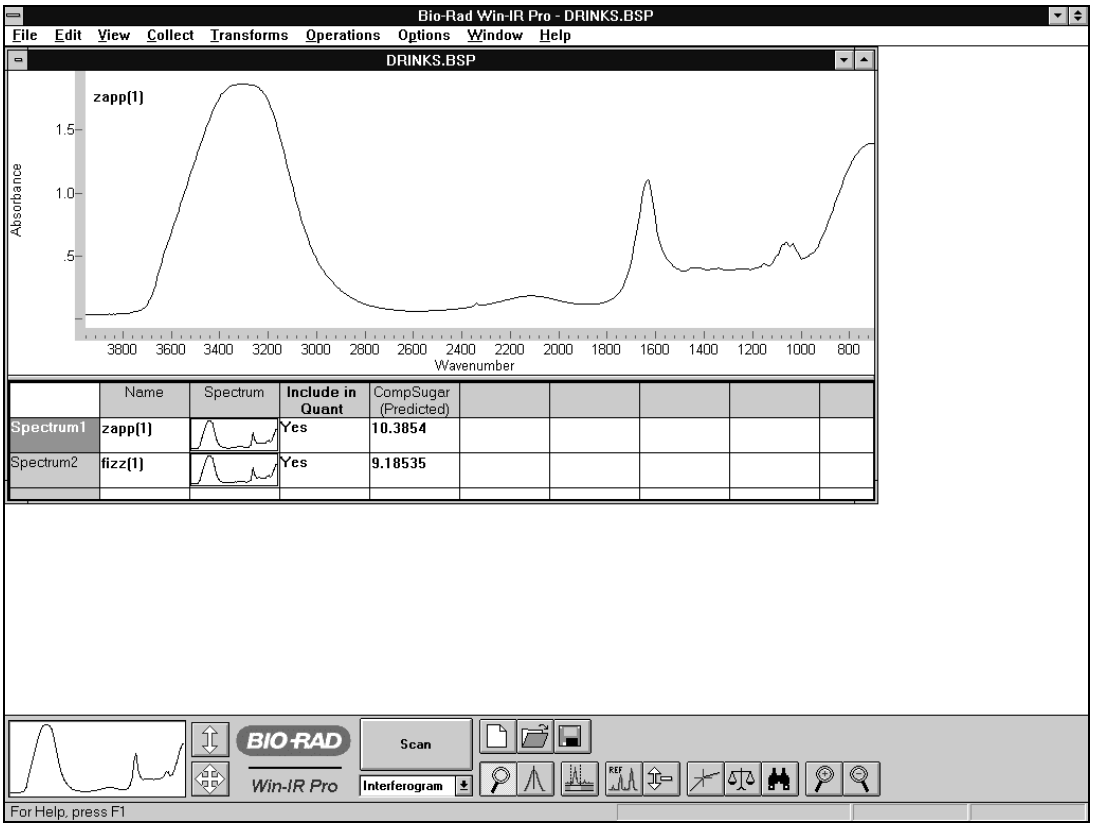
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13
Window Menu



In all the examples in this chapter the original screen is:

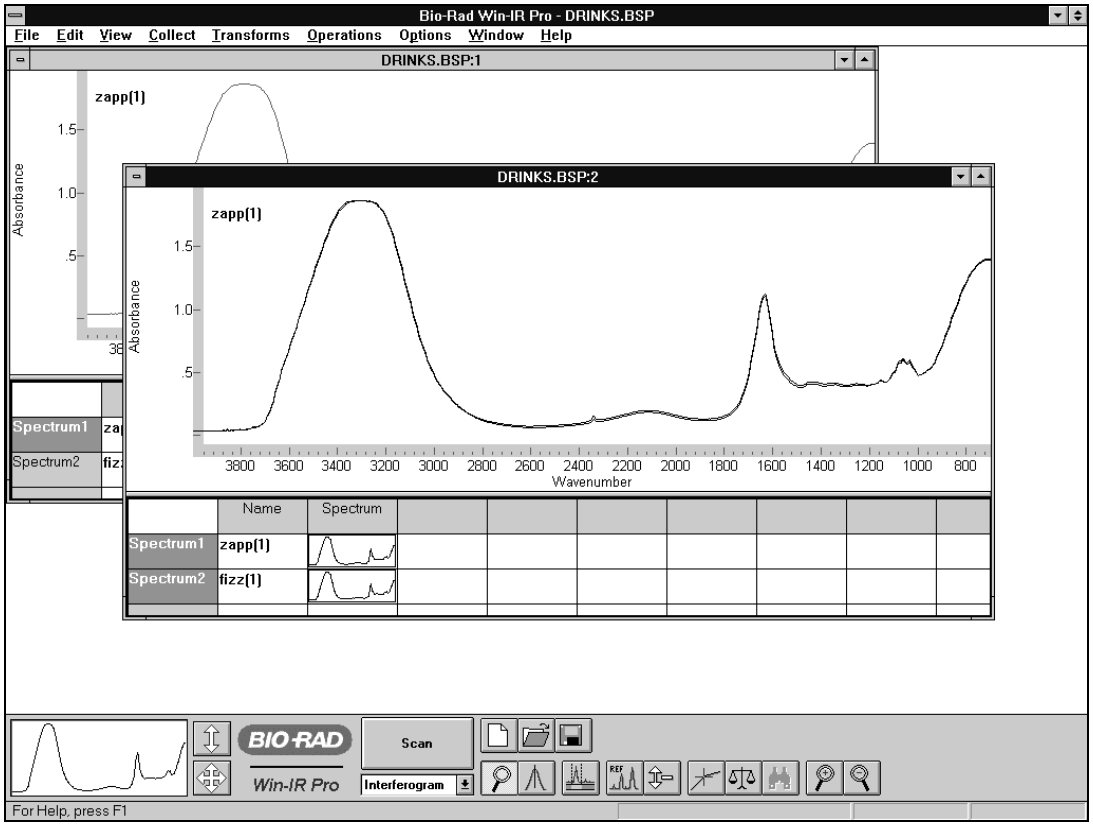
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NEW WINDOW

Creates another window (document) identical to the original one. The original window has :1 appended to it; the new window is identified by :2. This makes it possible to manipulate the traces, spreadsheets, etc. while still saving the original document.



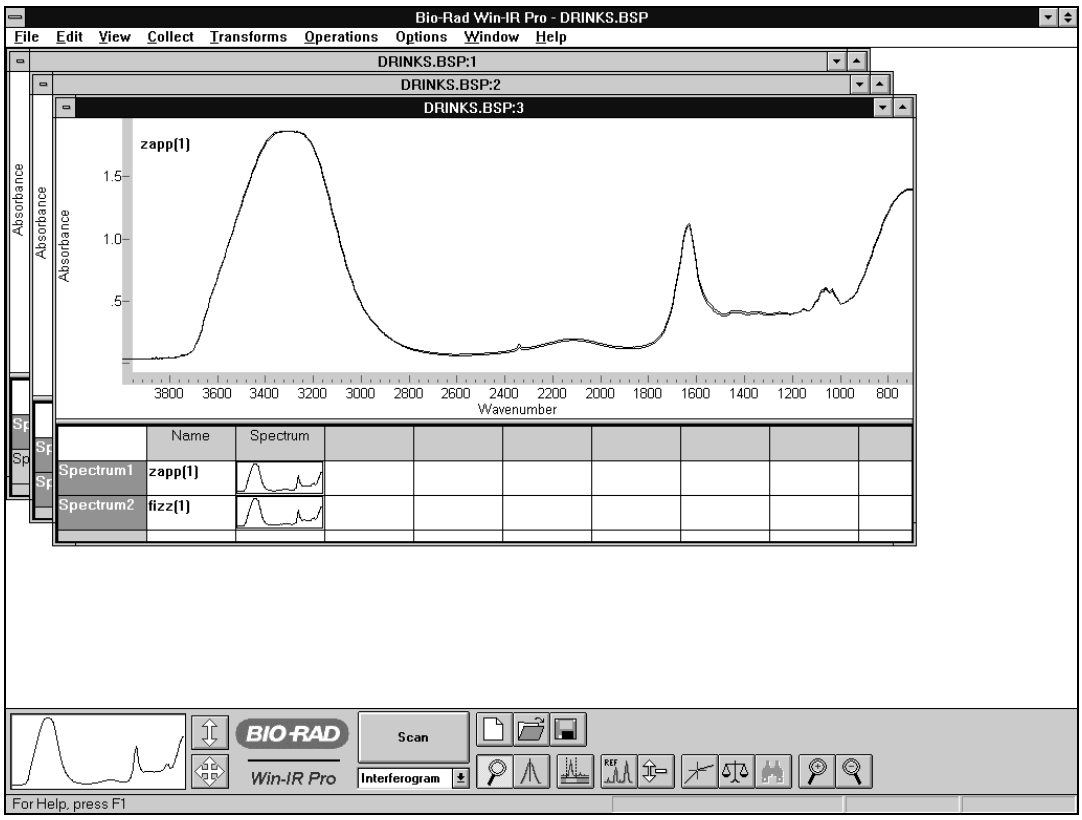
Caution

If you Save **the modified document, it will overwrite the original one. Use** Save As... **instead to preserve the original document.**

CASCADE

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Arranges all opened document windows one behind the other as:

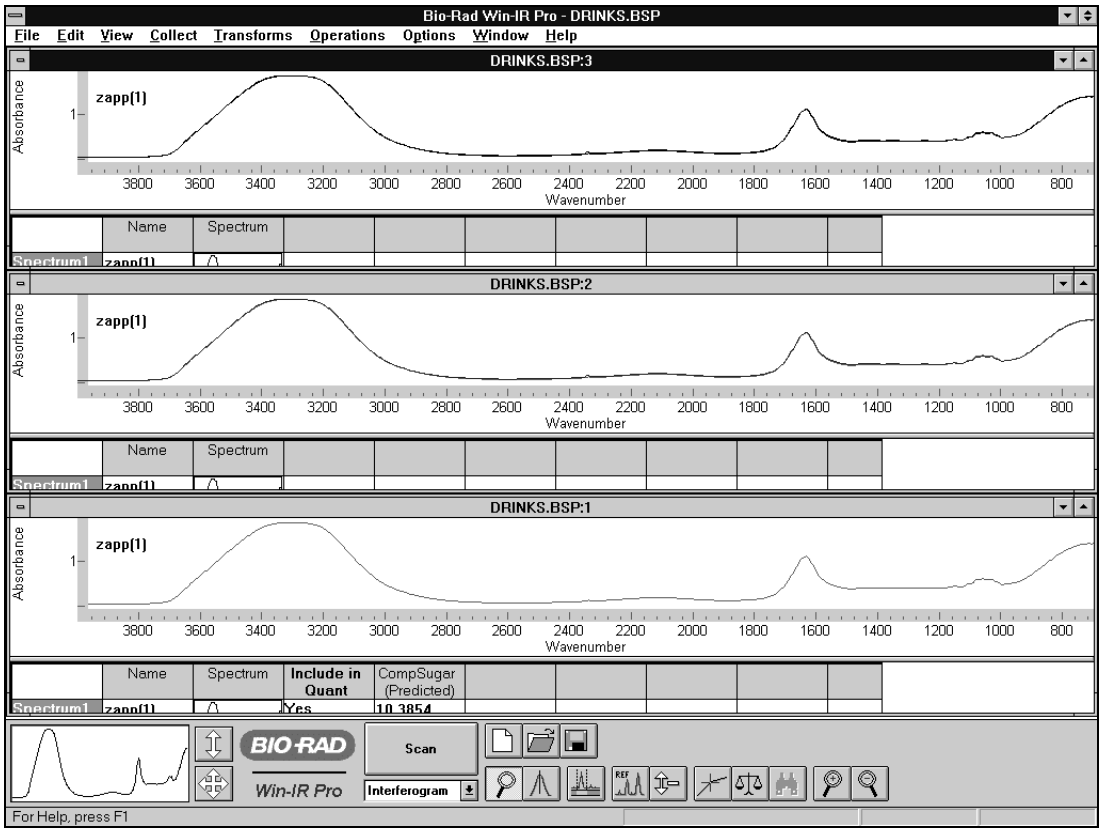


To make any document window active, place the cursor on that window and click the left mouse button.

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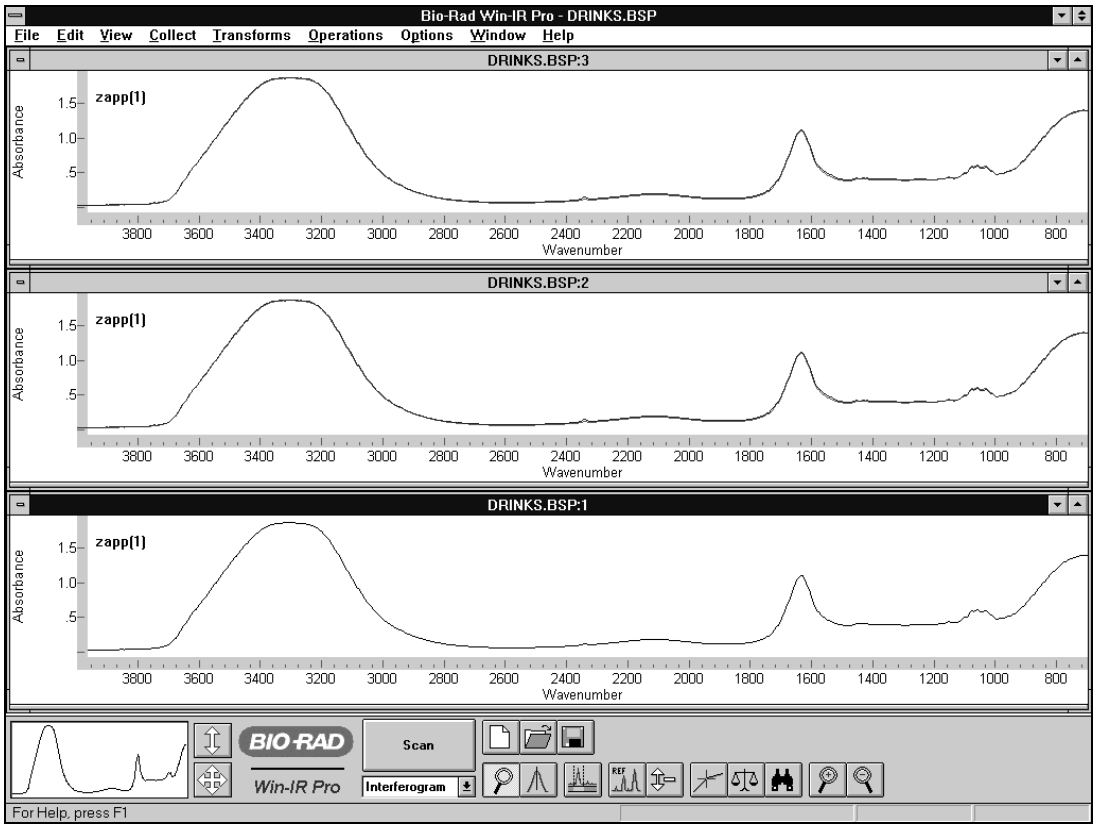
TILE

Arranges all opened document windows vertically, that is, one above the other.



There is no vertical scroll bar for the spreadsheets. Normally, this would be used to compare traces and, if implemented, the spreadsheets would be hidden. To hide all the spreadsheets, you must choose each window, in turn, to be active and select Maximize Traces. With spreadsheets hidden, the same documents look like this.

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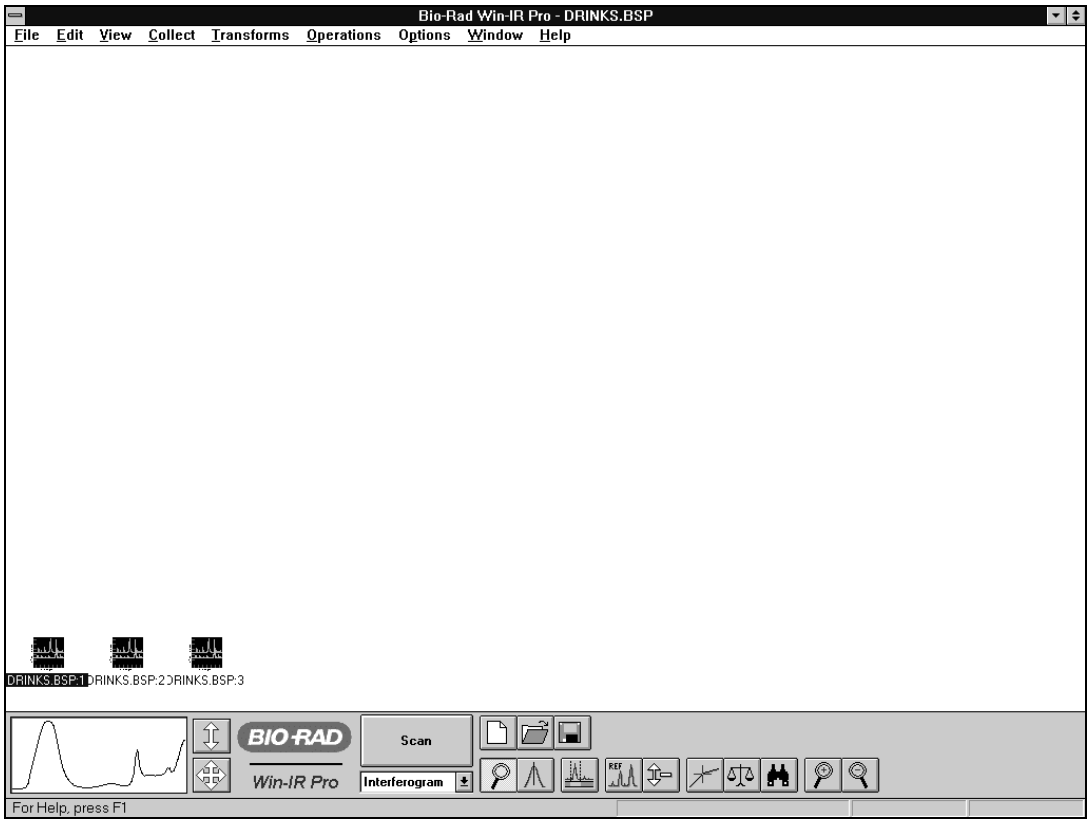


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ARRANGE ICONS

Arranges the icons for minimized document windows.



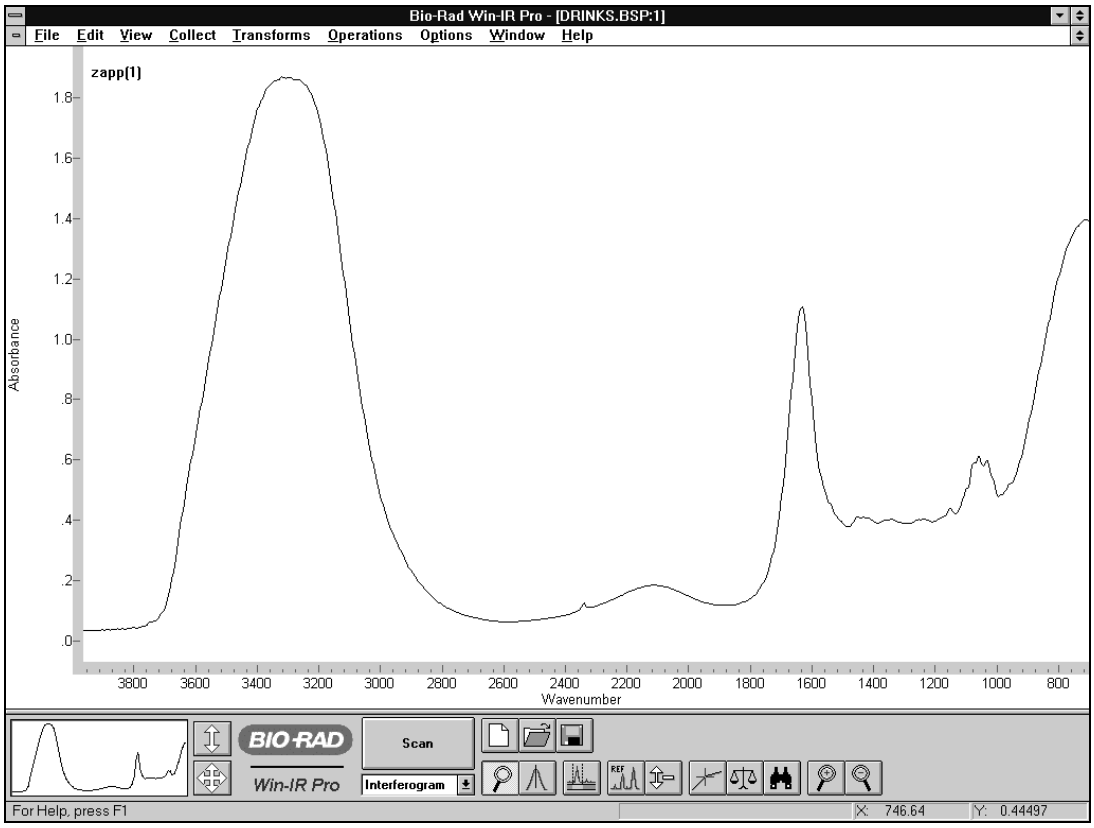
CLOSE ALL

Closes all open windows. If unsaved changes have been made to any window, Win-IR Pro will ask you if you want to save those changes before closing the window.

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MAXIMIZE TRACES

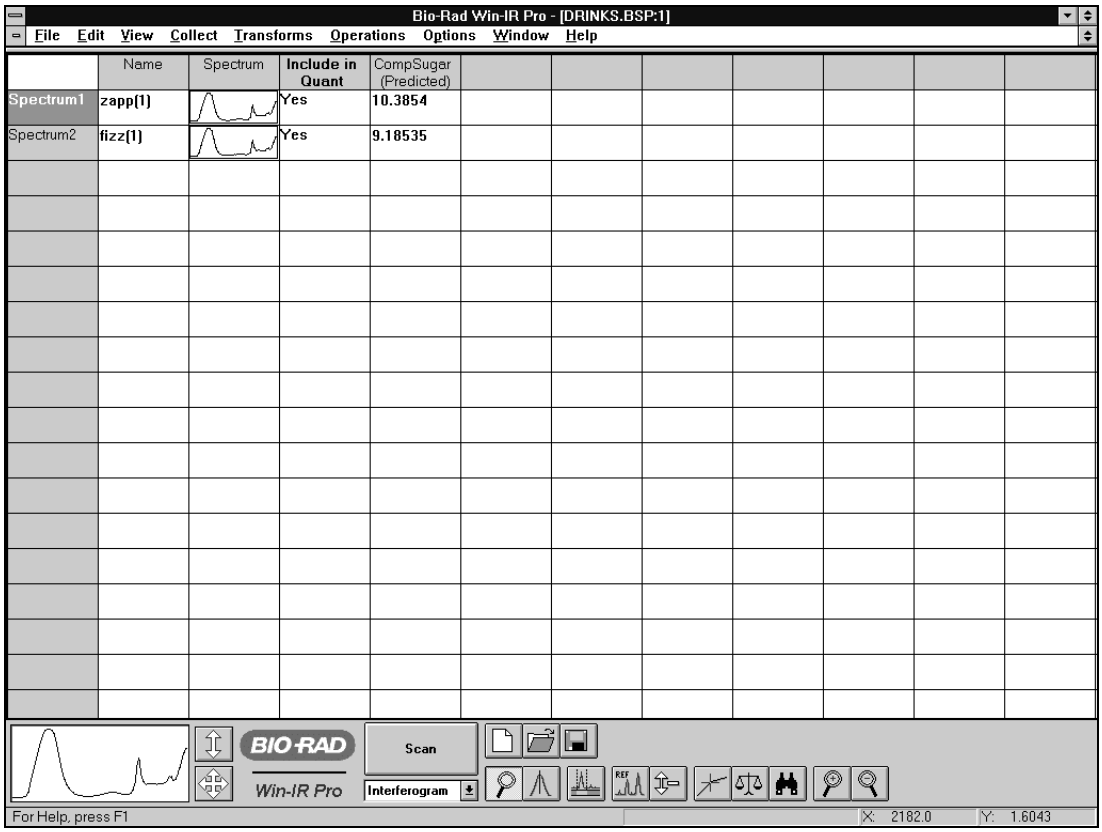
Moves the window shade in the document window to eliminate the spreadsheet display.



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MAXIMIZE SPREADSHEET

Moves the window shade in the document window to eliminate the trace display.



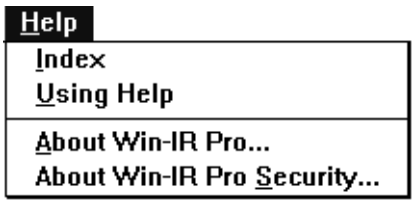
OPEN WINDOWS

Lists the open document windows in Win-IR Pro. To make a document window the active window, select it from this list. When a window is opened, it is added to this list; when a window is closed, it is removed from this list.

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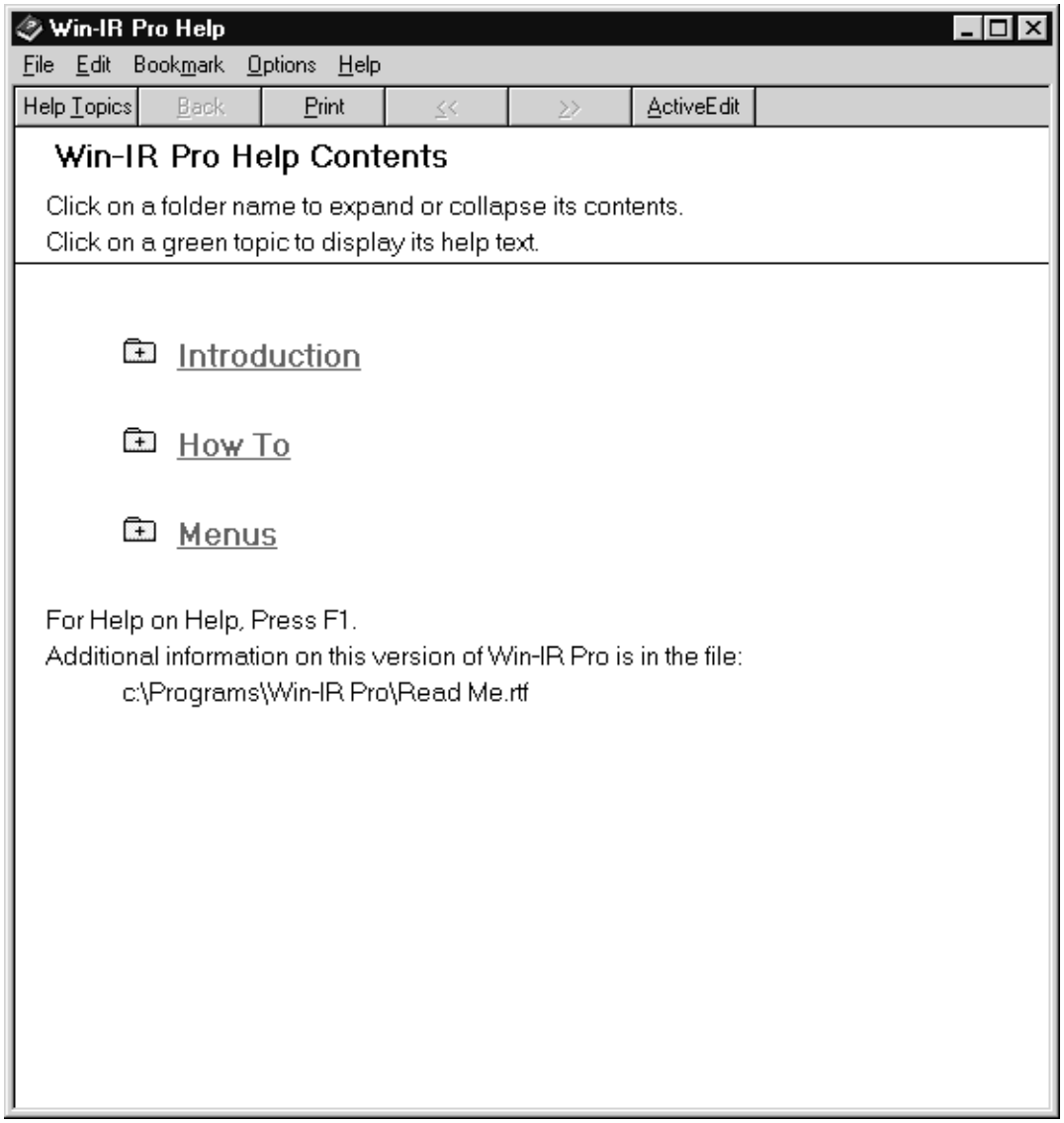
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Help Menu



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INDEX

Causes the top-level Win-IR Pro Help window to appear. To understand how to use the on-line help, select Using Help from the Help menu (see below).



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USING HELP

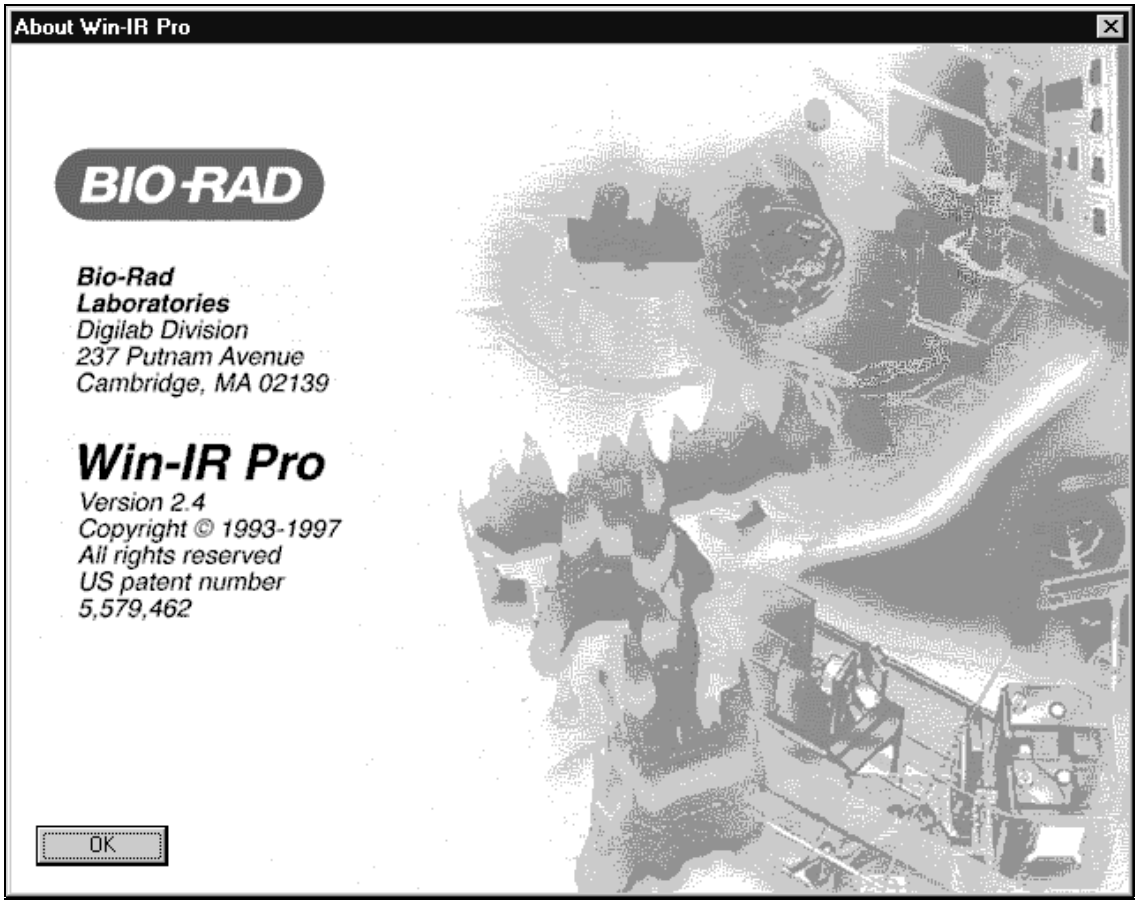
Cause the Help Topics: Windows Help window to appear. This on-line help is standard throughout all windows NT products. It is written by Microsoft to be self-explanatory.



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ABOUT WIN-IR PRO...

Causes the Win-IR Pro product identification box to appear. This is particularly useful because it displays the Release (version) number of the product.



ABOUT WIN-IR PRO SECURITY...

Displays a text file containing information about the licenses and permissions installed on your system. The file can be printed out. The information is useful to Bio-Rad's Customer Service.

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15
Print Composition

The print composition template is a page on which you can place information from spectra in a document, arrange it to your needs, add titles and comments, and print it. Because the template, when saved, does not contain the data itself, but rather records of what data is to go where on the page, the template can be used with any document you choose.

OVERVIEW

The print composition template is associated with a document. To use the template, you must first open a Win-IR Pro document, select the spectra whose information is to be printed, and then create a template (or open an existing template). Any saved template can be opened, and then edited or modified in the same manner as a new template.

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After you have opened a Win-IR Pro document and selected the spectra to be printed,

- select File / Print Composition / Open to open an existing print composition template, OR

- select File / Print Composition / New to create a new print composition template.

Note

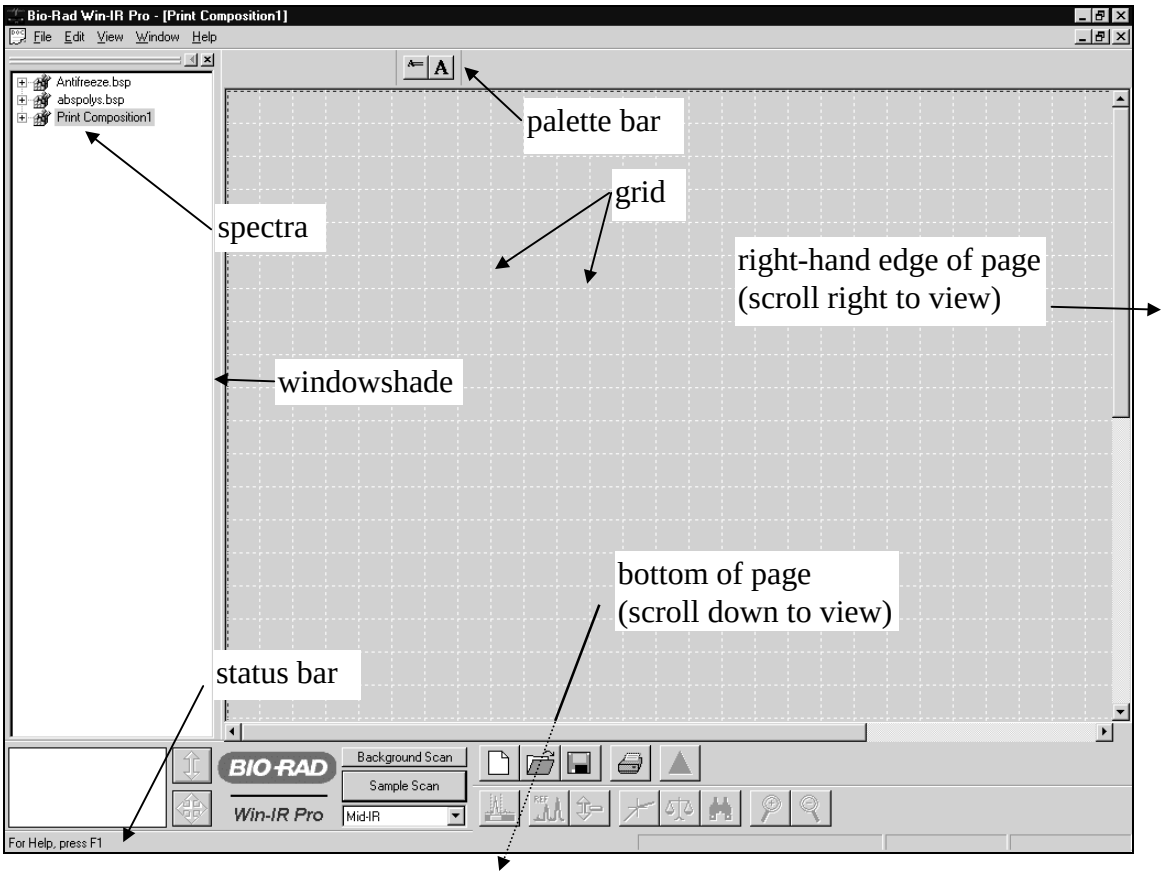
If more than one Win-IR Pro document is opened, the currently active document is the one that will be used for print composition.

This chapter will step you through building and using some example templates. The latter part of the chapter is a reference to all the features available in print composition.

Template Window

A new template window looks like this.

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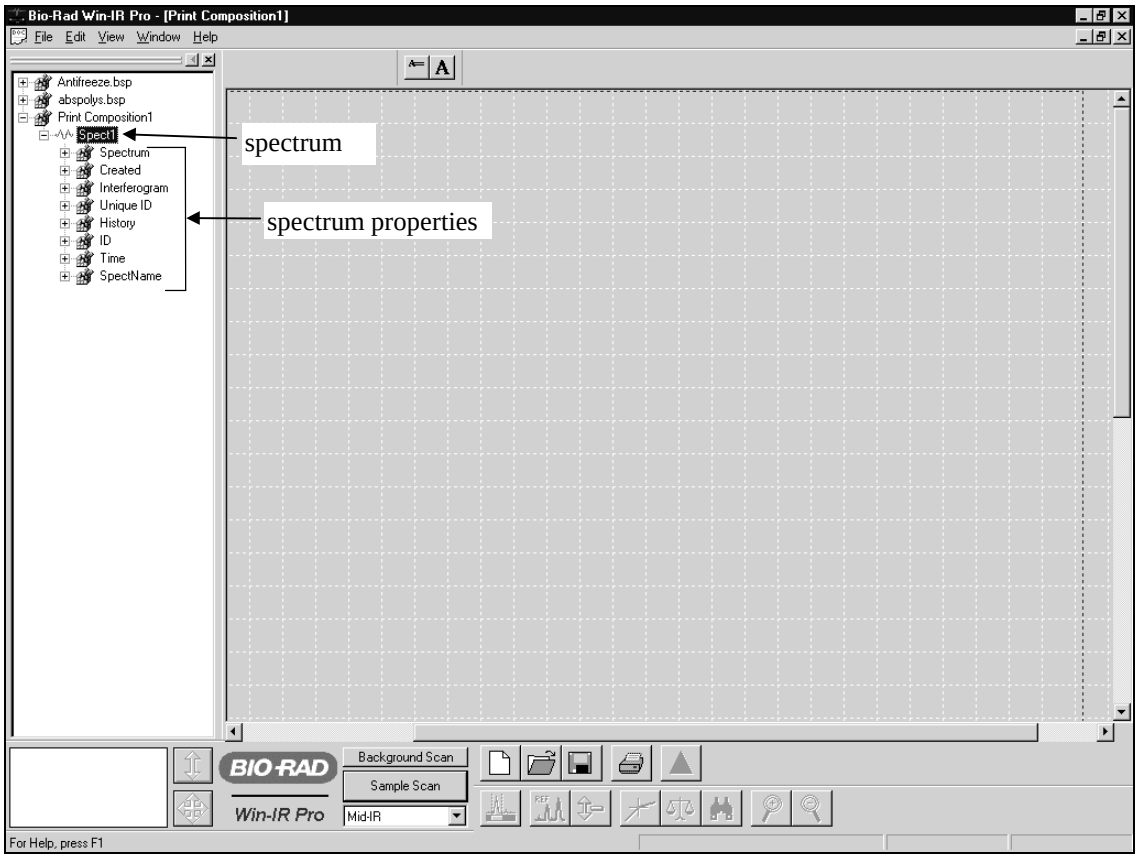


Spectra: spectra are on the left-hand side of the plot composition template. Initially, they are condensed—the spectra and spectrum properties are not displayed. There are three ways to display the spectrum properties:

- Double-click the spectrum identification (Print Composition1, etc.).
- Double-click the small spectrum icon.
- Click the left-hand box (it contains a +).

Repeat this procedure for the desired spectrum name (Spect1, etc.). The spectrum properties are now displayed.

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Notes

All the spectrum properties are displayed and available, even if they were not in a column in the document spreadsheet.

Items that exist as part of the Win-IR Pro document, but which are not displayed there (for example, peak labels), are displayed when the Spectrum object is placed on the print composition page.

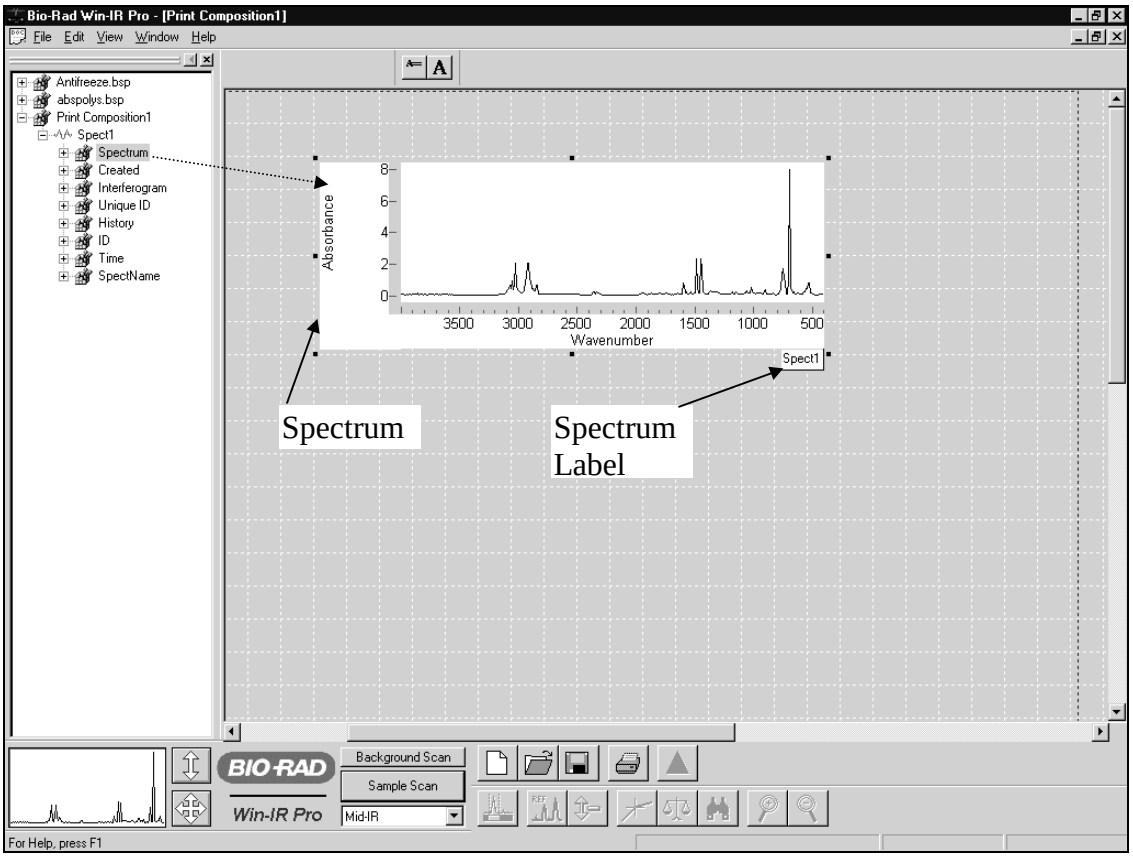
Properties are copied to the print composition template by dragging and dropping. Place the cursor on the desired property; hold down the left mouse button; move the cursor across the windowshade to the desired location; release the mouse button. In the example below, Spectrum has been placed in the print composition template. Text

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objects (this excludes Spectrum, Interferogram, ChemStructure, etc.) are treated as COMMENT Control objects for the purposes of being edited and modified.

Note

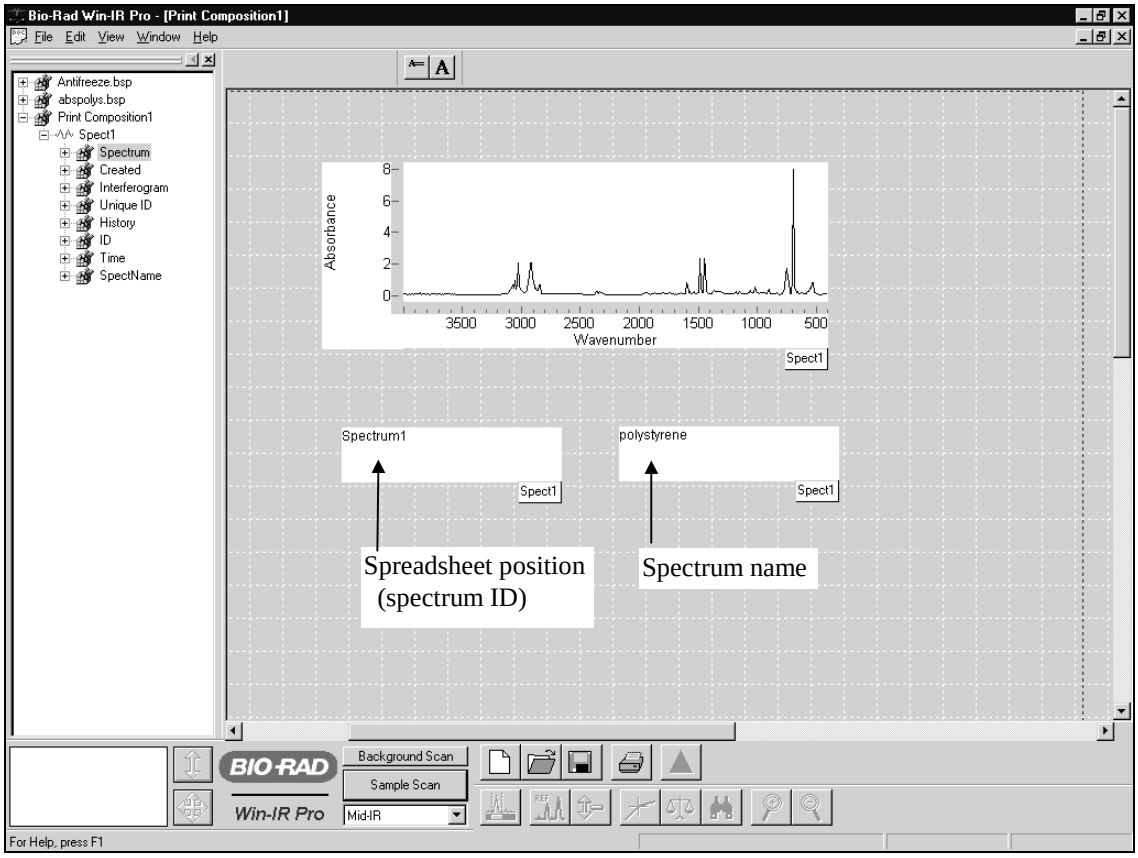
Spectrum Labels identify which spectrum on the left-hand side supplied the information; they are not printed with the rest of the information.



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If more than one spectrum is selected for the print composition template, the spectra are listed on the left-hand side in the order in which they were chosen from the spreadsheet. This order procedure is the same as that for displaying traces in the Win-IR Pro window. See “Trace Display Order in the Window” in Chapter 4 for details.

Therefore, the number used in the spectrum identification on the left-hand side (Spect1, Spect2, etc.) is not the same number indicating position in the spreadsheet (Spectrum1, Spectrum2, etc.). Spreadsheet position or spectrum name can be determined by placing the cursor over ID or SpectName and reading the value (see the “Property Browse Bar” section of Chapter 8 for details), or by dragging ID or SpectName into the print composition template.



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Palette bar: contains tools that are used to add objects to the print composition page; these objects are not properties that are contained in the spectrum. When the cursor is placed on each tool, a brief description of it is shown in the Status Bar. To add a field, place the cursor on the tool, hold down the left mouse button, drag the cursor to the desired place on the print composition page, and release the mouse button.

Tool	Function
	Add a title field
	Add a comment field

Title: contains a one-line text string, normally used to label a page and/or the entire print composition.

Comments: contains a multi-line text string. It can be used to specify any desired information that is not normally contained in the spectrum.

Comparison of Title and Comments objects

FEATURE	TITLE	COMMENT
Text Location	Centered in the box	Starts at upper left hand corner of box
Text Quantity	One line	Multiple lines
Text Editing	Use Edit / TITLE Control Object / Properties to access TITLE Control Properties dialog box. Use this to change title.	Use Edit / COMMENT Control Object / Edit to put cursor in comment box. Use standard insertion and deletion techniques.

Grid: assists you in aligning the printing objects. Grid size can be changed by selecting Edit / Grid (see the reference section, below).

Windowshade: divides the template window into the spectral part (left) and the print composition part (right). It can be moved by placing the cursor on the window shade, holding down the left mouse button, dragging the window shade, and release the mouse

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button. Alternately, select Window / Split to move the windowshade (see the reference section, below). Place it in a position that is convenient for you.

Status Bar: gives a brief description of the results of using the tools in the palette bar. If you decide you do not need this, it may be hidden by de-selecting View / Status Bar (see the reference section, below).

Right-hand side of page: is indicated by a vertical, dashed blue line. Any item to the right of this line will not be printed. Additional space can be obtained by scrolling down. Any number of pages can be used in the template.

Bottom of page: scroll down to see the horizontal, dashed blue line that indicates the bottom of the page. Existing pages will also have a vertical, dashed blue line. If you want to create additional pages, just drag an object into the portion of the print composition screen below the horizontal, dashed blue line. This automatically creates a new page immediately following the last existing one.

Note

The horizontal and vertical edge lines for the new page may not be visible until you have performed another operation that refreshes the screen.

Objects

All items placed on the print composition page are objects that can be manipulated independently of the other objects. Objects can be placed over one another and both will print. If you place an object over a Spectrum or Interferogram object, the object will appear to vanish; however, it is on the print composition page and will print. You can see its location by selecting File / Print Preview.

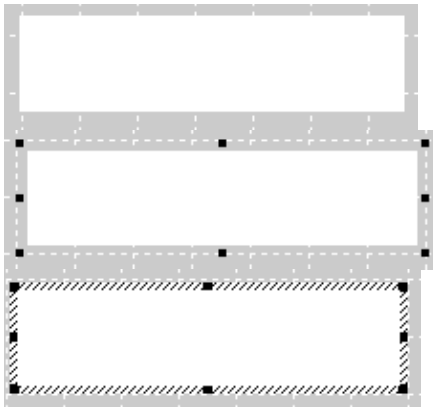
Objects can be graphical (such as Spectrum, Interferogram, or ChemStructure) or non-graphical. Of the non-graphical objects, ID and SpectName are Comment Control objects; all other non-graphical objects are Title Control objects.

Notes

Avoid overlapping page boundaries. If an object overlaps a page boundary, parts will be printed on each page.

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An object can be in one of three states-unselected, selected, and edit. You can tell what state an object is in by its border.

State	Border
Unselected	
Selected	
Edit	

To go from

- Unselected to Selected: put the cursor in the object and single-click.
- Unselected to Edit: put the cursor in the object and double click.

- Selected to Edit: put the cursor in the object and double click.
- Selected to Unselected: put the cursor outside the object and single click.

- Edit to Unselected: put the cursor outside the object and single click.
- Edit to Selected: first, go to Unselected; then put the cursor in the object and single click.

Unselected State: you can observe the object on the page; you can do nothing to it. Objects that are unselected are not affected by non-global changes. They are affected by Edit / Font and Edit / Background Color.

Selected State: in this state, you can perform operations on the object itself. You can

- move the object on the page; put the cursor in the object, hold down the left button and drag the object ot the desired position, release the button.

- resize the object; put the cursor on one of the eight small black squares on the border, when the cursor changes to a single double-headed arrow, hold down the left button, drag the object to the desired size, release the button.

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- delete the object by pressing the Delete key, by selecting Edit / Delete, or by selecting Edit / Cut; the last procedure also copies the object to the print composition clipboard.

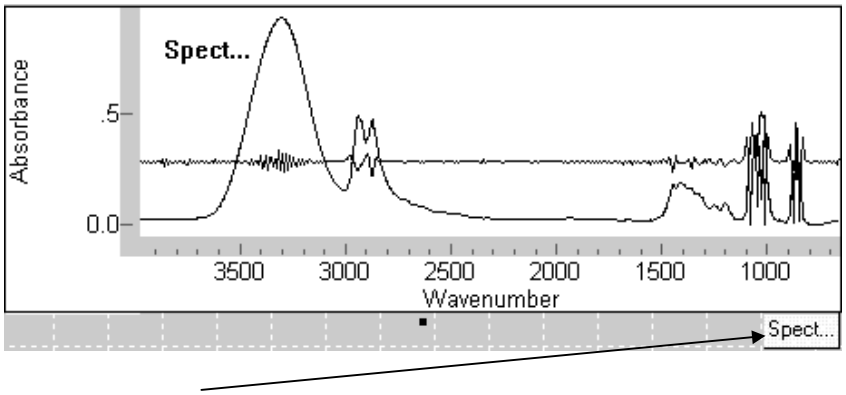
Edit State: in this state, you can perform operations on the contents of the object. You can:

- edit the text that appears in any non-graphic object.
- delete the object by selecting Edit / Cut; this procedure also copies the object to the print composition clipboard

Spectrum and Interferogram Objects

The Spectrum and Interferogram objects differ from the other objects placed on the print composition page.

- Traces from more than one spectrum can be displayed in a single Spectrum or Interferogram object. First, drag and drop Spectrum or Interferogram from one spectrum. Then, drag Spectrum or Interferogram from the same or another spectrum, and drop it on top of the existing object. Any number of spectra can be placed in one display.



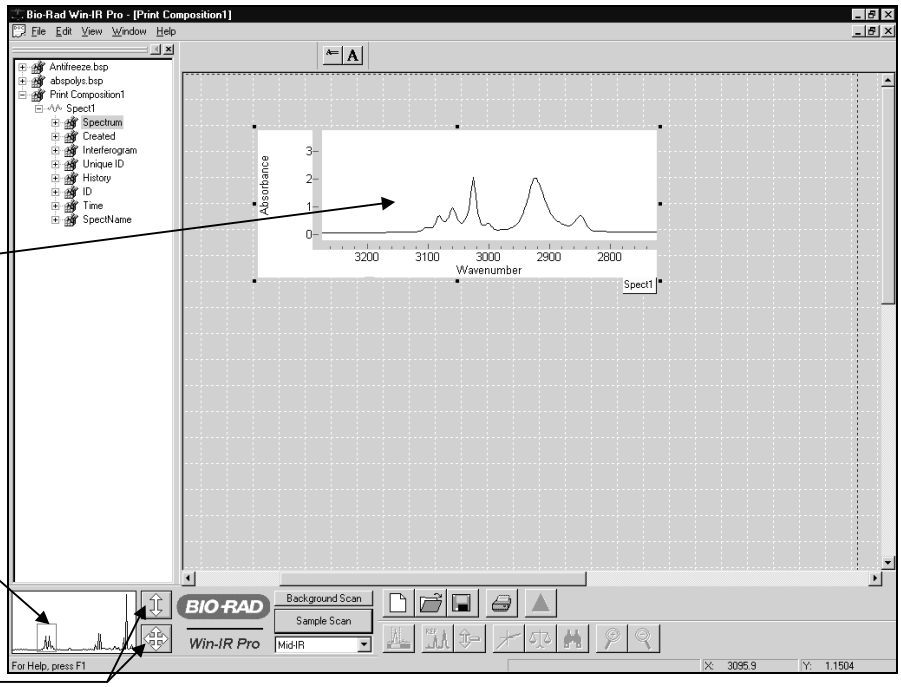
The Spectrum Label changes from identifying a single spectrum to Spect....

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Note

The traces can be offset with respect to each with the Trace Control Bar. This is described in the reference section, later in this chapter, and in Chapter 8.

- When the Spectrum or Interferogram object is first placed on the page the full spectrum is shown, regardless of what limits were chosen for the display in the main window. The zoom box, radar box, and autoscale buttons work the same as in the main window. You can use the zoom box in the Spectrum or Interferogram object to look at any portion of the spectrum; the portion selected is shown in the radar box. In the example below, we have zoomed in on a region of interest (3300-2700 cm^{-1}). The radar box shows what part of the spectrum is displayed. Because the Spectrum object is selected, the XY-autoscale and Y-autoscale buttons are enabled.



Spectrum: zoom box has been used to select a region of interest.

Radar box: shows the location of the region of interest within the spectrum

Autoscale buttons are enabled

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Note

When you save the template, the spectrum limits are also saved. In this example, if we opened this template for another document, the Spectrum object would initially be displayed for the region 3300-2700 cm^{-1}.

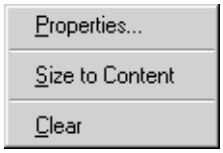
- If the original spectrum is displayed with the X2 SPP or X4 SPP view, then the Spectrum object is also displayed in the SSP view.

- The Spectrum or Interferogram object is active; both the x-axis and the y-axis can be compressed or expanded as if it were a Win-IR Pro document (See Chapter 1). The y-axis label displayed on the left-hand side is that of the most recently selected trace.

- There are items associated with the display in the Win-IR Pro document that can be hidden, for example, peak labels, position labels, or annotations. When the Spectrum or Interferogram object of such a spectrum is placed on the print composition page, these items are visible. These items are considered part of the spectrum's information; hiding them is only a *display* option in the main Win-IR Pro document. They can be displayed or hidden in print composition by using View / Show Peaks and View / Show Labels.

Right Mouse Button

If you place the cursor in an object and click the right mouse button, the object is placed into edit state, and a menu appears.



Note

Right mouse button operations are not supported for graphic objects such as Spectrum, Interferogram, or ChemStructure.

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Select the desired item and click the left mouse button. Only those items that are appropriate for that particular object are enabled.

Properties: allows you to change certain properties of the object. It is identical to selecting Edit / OBJECT_TYPE Control Object / Properties. This feature is described below in the reference section.

Size to Content: resizes the object box based upon its contents.

Note

Some boxes may not appear to be resized. In actuality, they are, but room has been left for possible editing. Boxes can be manually resized by dragging corners or line centers.

Clear: removes all text from a Comments object. The cursor is left in the object box to allow new text to be entered.

If the right mouse button is clicked on the composition page, but not on an object, a menu appears that lets you change global conditions:

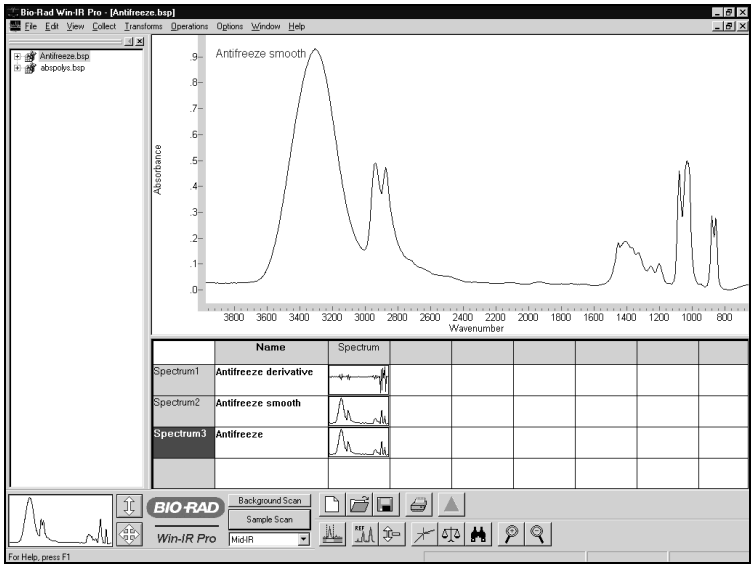


These have the same effects as selecting the corresponding entry from the View or Edit menu.

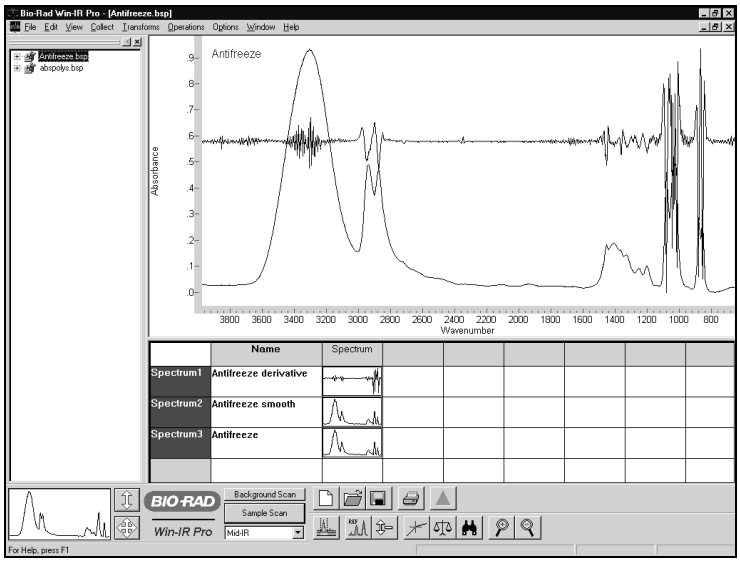
Creating a Template

1. Open a document with the type of spectra that you are going to use. Normally, this is the document containing spectra that you wish to print.

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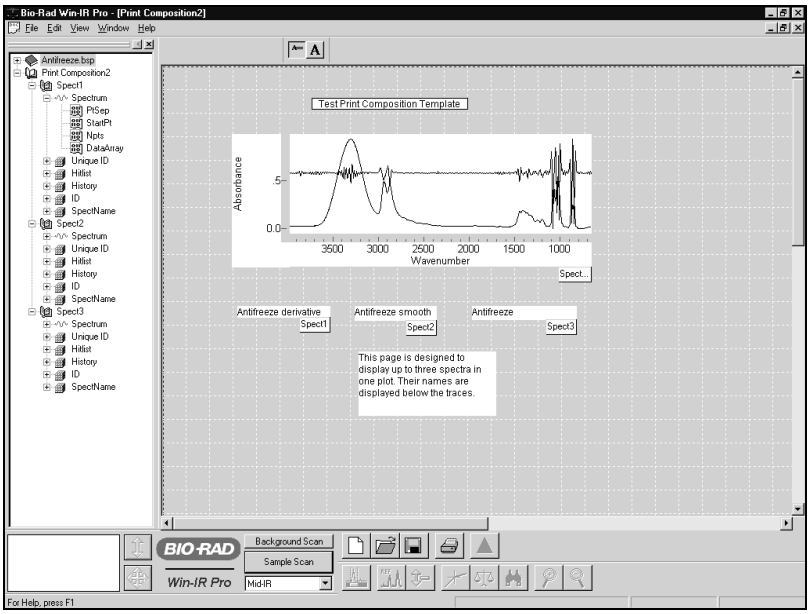
2. In the spreadsheet, select the spectra to be used in creating the print composition template.



3. Select File / Print Composition / New from the Win-IR Pro menu bar.

4. Create the print composition. Test it and modify it until you are satisfied.

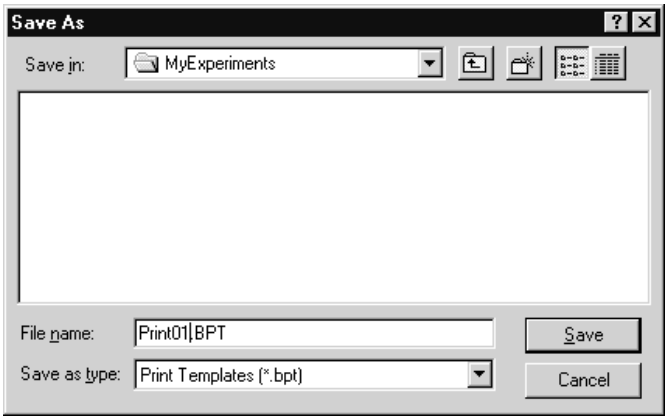
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Note

Template files can be opened and further modified later, if so desired.

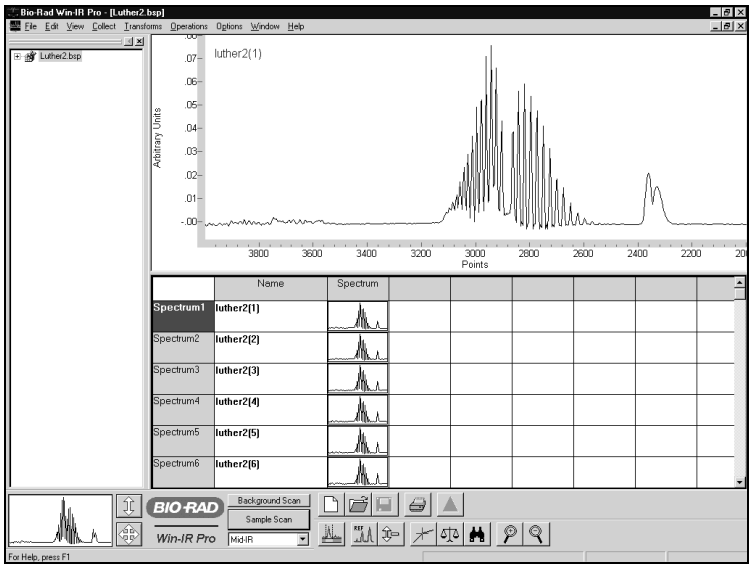
5. Save the print composition as a Print Template (.bpt) file.



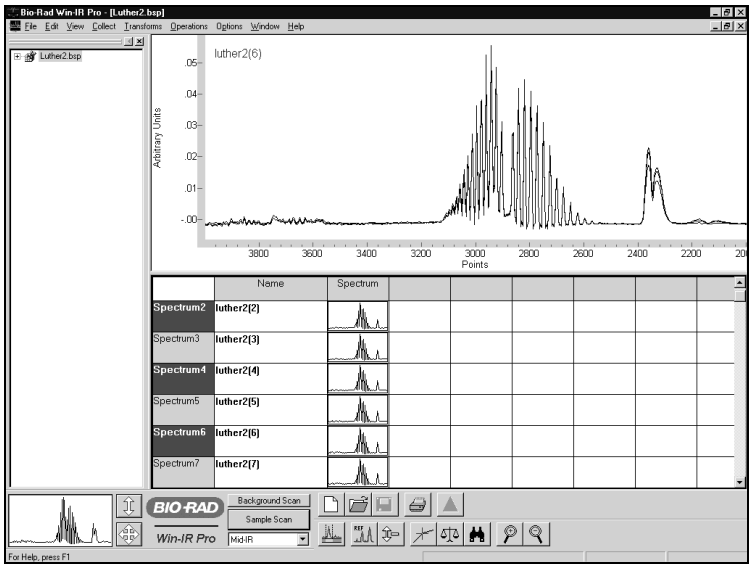
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Printing with a Template

1. Open the document containing the spectra to be printed.

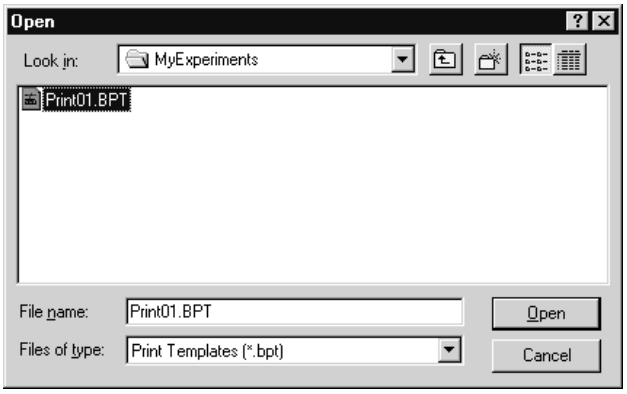


2. In the spreadsheet, select the spectra to be printed.

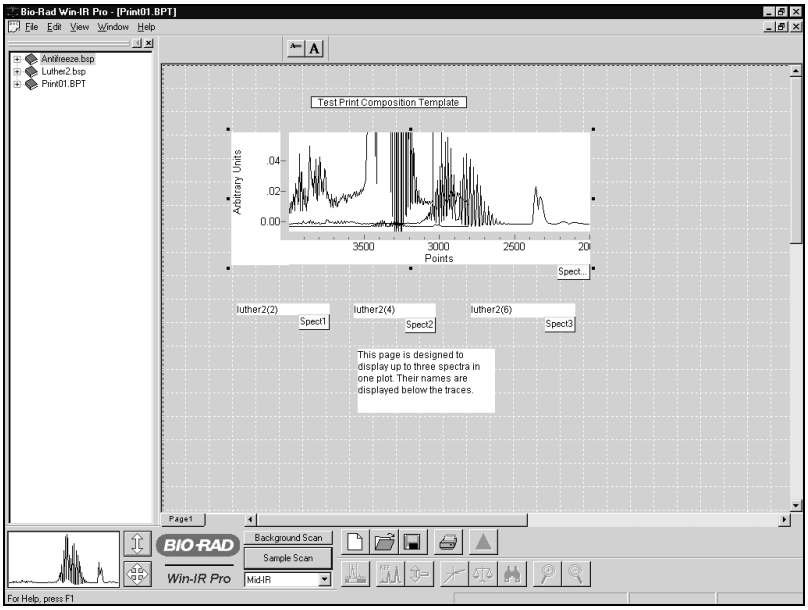


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3. Select File / Print Composition / Open from the Win-IR Pro menu bar.



4. Open the desired Print Template (.bpt) file. The data from the document appears in the appropriate locations in the template.



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5. Select File / Print.

Notes

If the number of spectra selected from the document are more than are expected by the template, data from the excess spectra will not be placed in the template.

If the number of spectra selected from the document are fewer than are expected by the template, those locations on the template will be empty.

The print composition template is associated with the document that was active when the template was created or opened. If you want to use this template with another document, you must

1. Close the print composition template; save it if appropriate.
2. Make the other document active.
3. Open the print composition template.

BATCH MODE

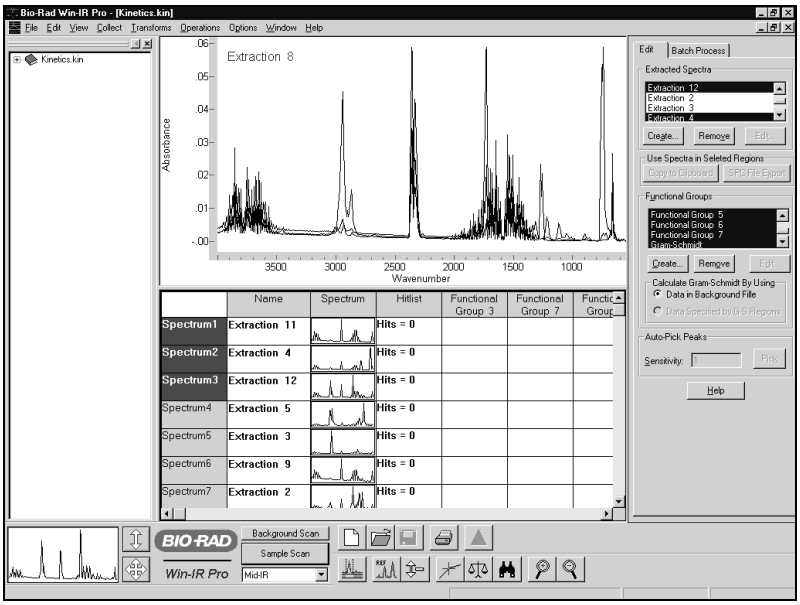
Batch mode allows you to create a template that will process groups of spectra. In batch mode, if your template expects three spectra and you have selected six, then they will be processed in two groups of three. If you were not in batch mode, the template would ignore the fourth, fifth, and sixth spectra.

Creating a Batch Mode Template

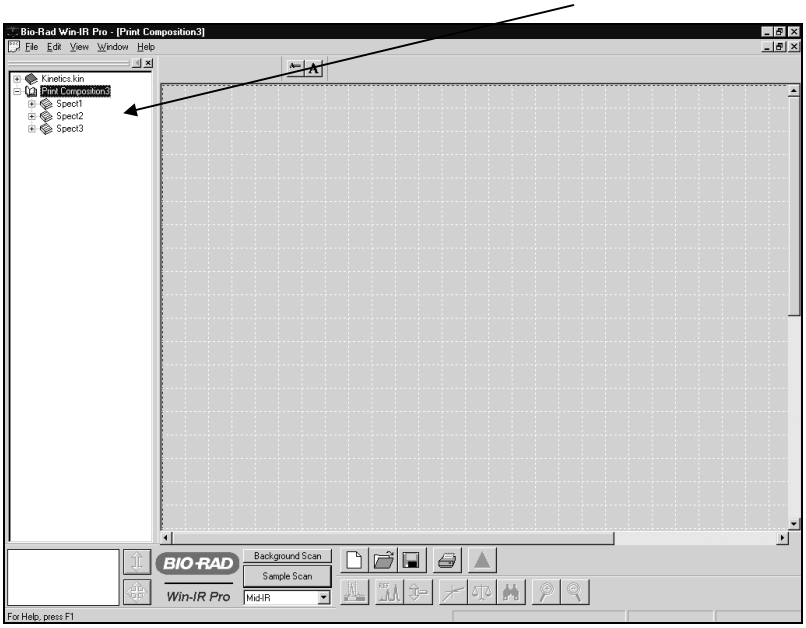
The procedure to create a batch mode template is:

1. Open a document similar in type to that whose spectra are to be processed. In this example select three spectra.

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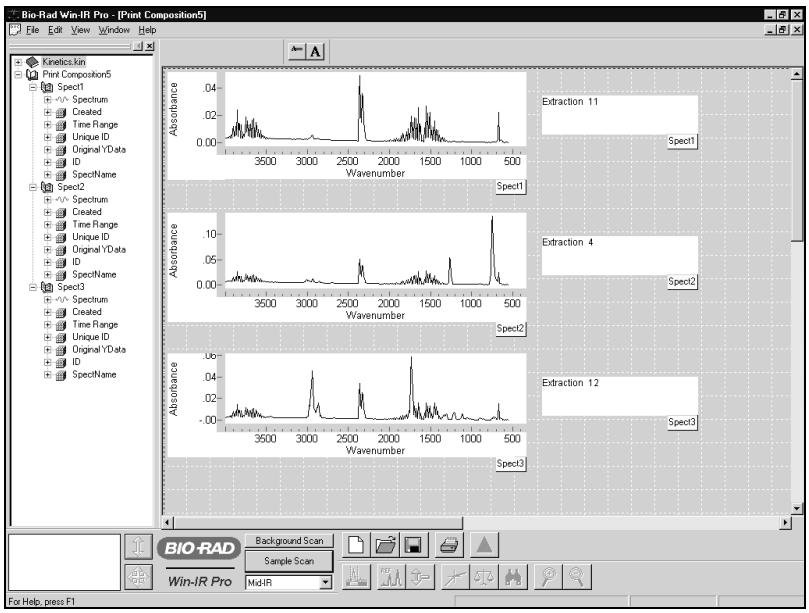


2. Select File / Print Composition / New. The print composition screen appears. Expand the property browse bar until the spectra are listed individually.

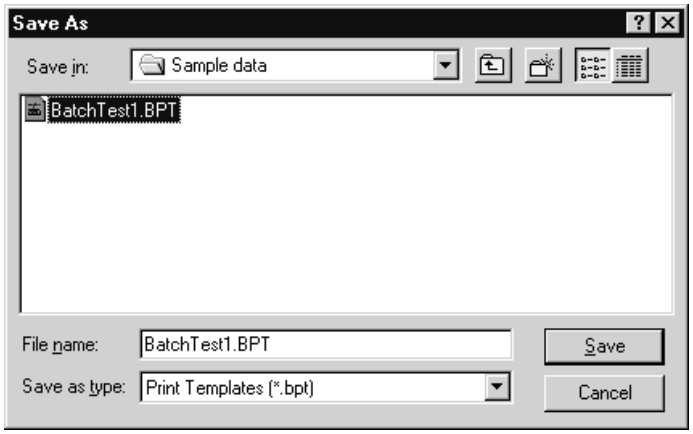


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3. Create a print template.



4. Select File / Save. Save this as BatchTest1.BPT.

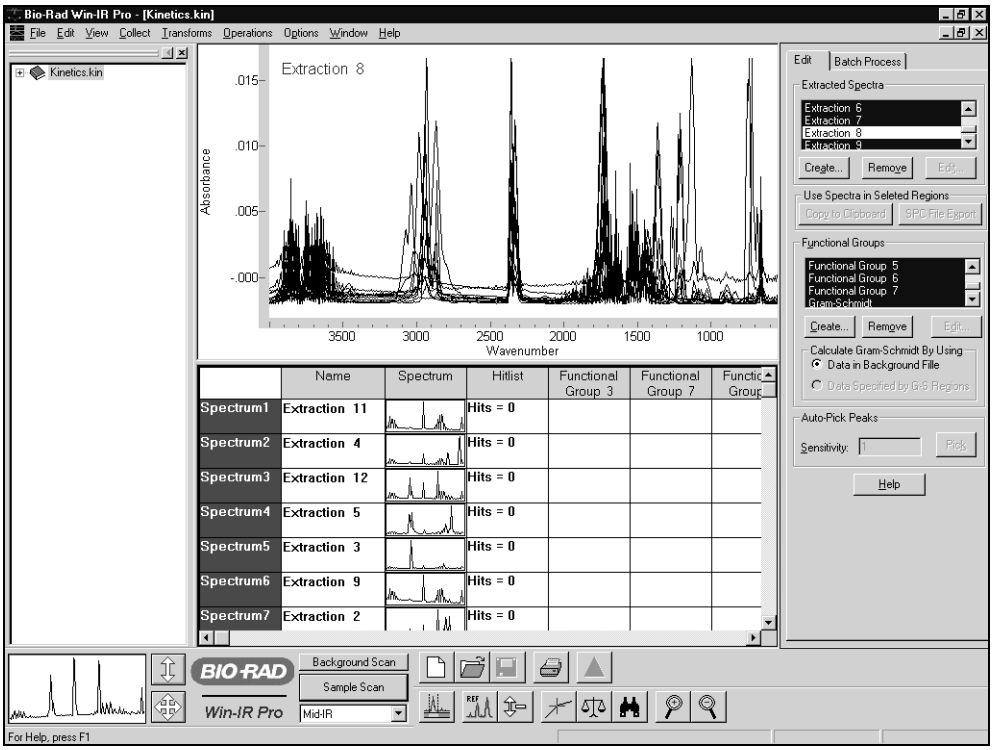


5. Select File / Close. The template is ready for use.

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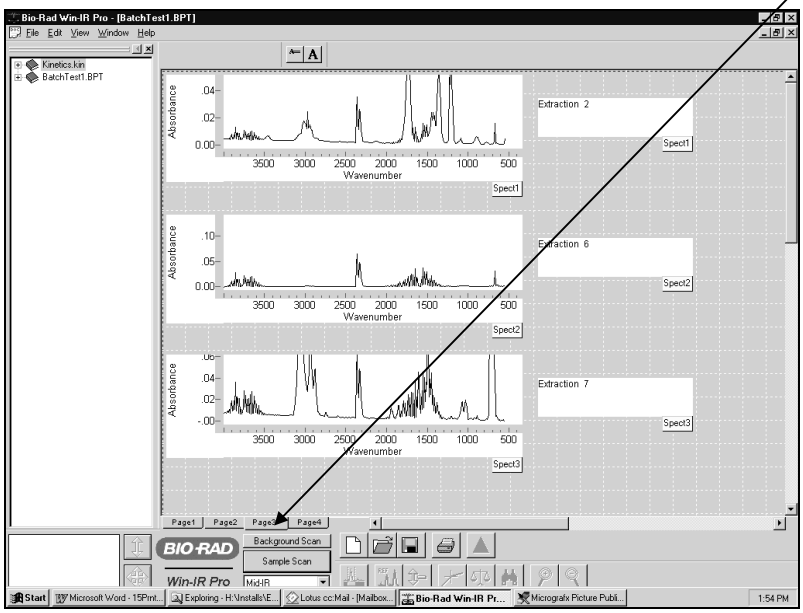
Using a Batch Mode Template

1. Open the document with the spectra to be processed. Select the spectra to be processed.



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2. Select File / Print Composition / Open. Select BatchTest1.BPT. The spectra are grouped into batches. Click on a Page button at the bottom the template to view a batch of spectra. The values associated with those spectra will appear in the print template. In this example, Page 3 has been selected.



Note

Select View / Batch from the menu bar to see the template with only the first set of data selected. You can then modify the template, and select View / Batch again to see all the data.

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REFERENCE

FILE MENU

Most of the File menu entries work the same as their counterparts in the main Win-IR Pro screen. See Chapter 6 for details.

New

Allows you to create any type of Win-IR Pro document.

Open

Allows you to open any existing Win-IR Pro document.

Close

Closes the active Print Composition template. If there are more than one Print Composition template open, then these other templates remain open.

Save

Saves the currently active Print Composition template to disk unders its existing name.

Save As

Saves the currently active Print Composition template to disk with a newly specified name, as a print composition file.

Print

Prints the currently active Print Composition template.

Note
Spectrum Labels are not printed.

Print Preview

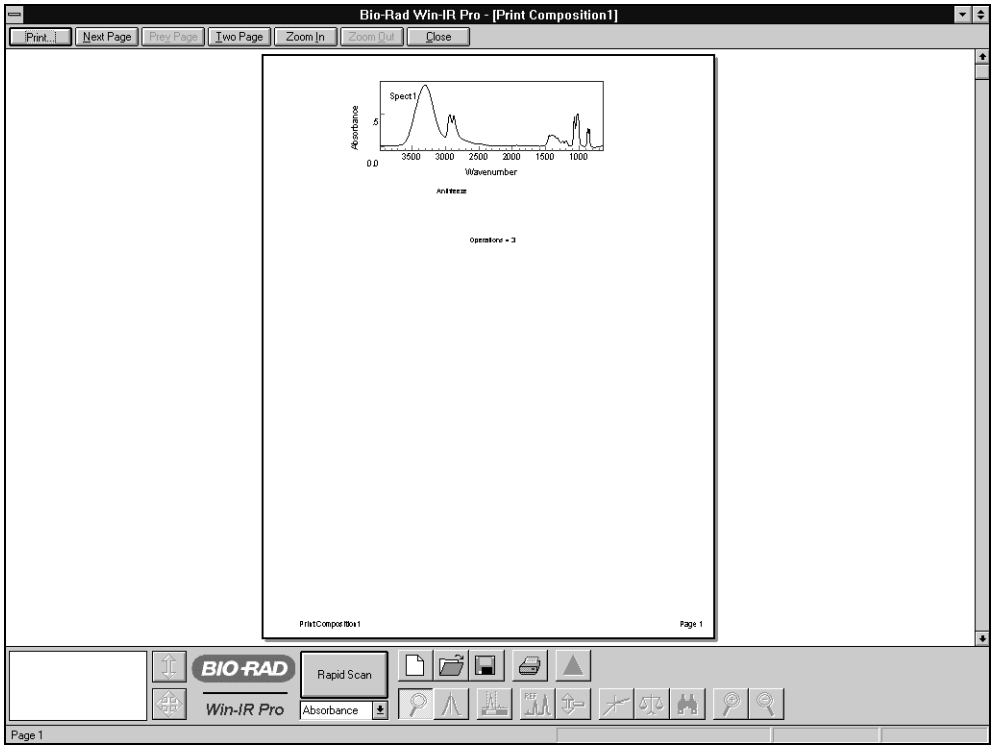
Allows you to view the page(s) as a whole prior to printing them. Any number of pages can be constructed. The next page is immediately below the current page. Any items beyond the right-hand edge of the page (shown as a dashed line in the Print Composition view) are not printed. You cannot modify the pages, only view them; changes can be made by returning to the Print Composition view (click the Close button).

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Notes

Items that overlap pages will not print properly. You must make sure that you have not placed any fields or objects so that they are on two pages.

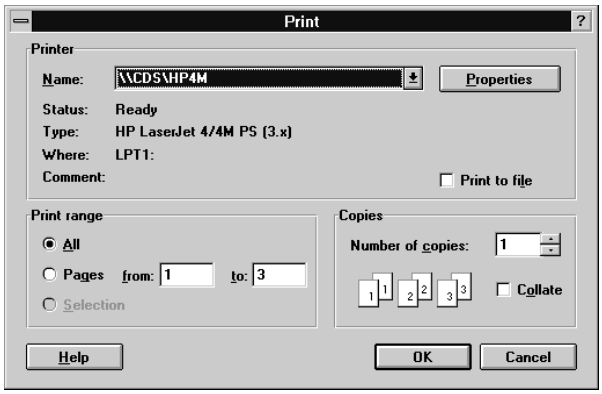
Different printers have slightly different margins; what you get on the paper printout may not be exactly what you see on the screen. Do not place objects directly abutting the edges of the paper.



The buttons at the top of the view have the following functions.

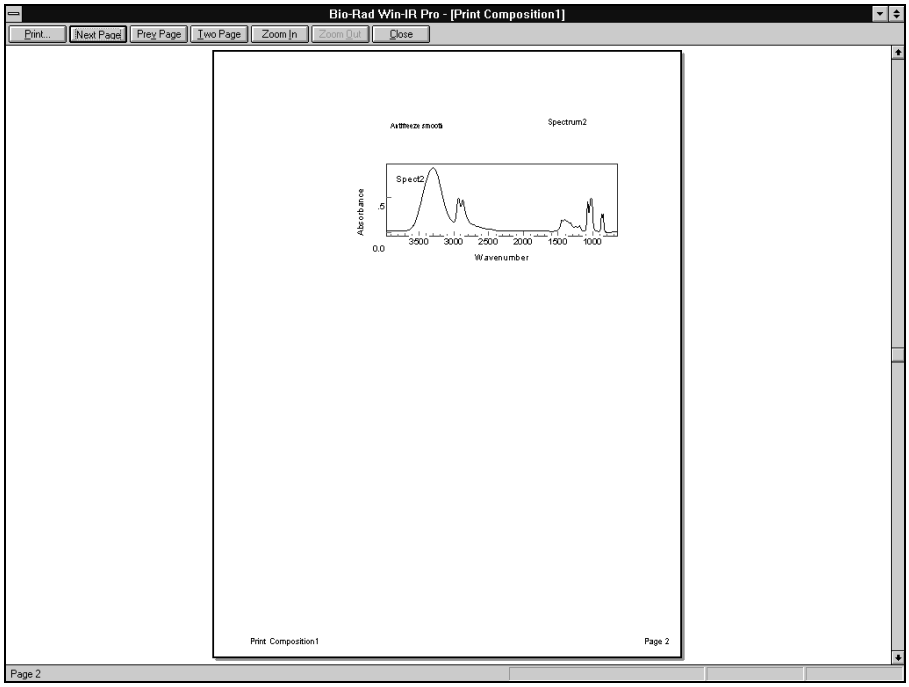
Print: print the print composition file. Use Print Range in the Print dialog box if you want to print other than all pages.

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Win-IR Pro returns you to the plot composition view.

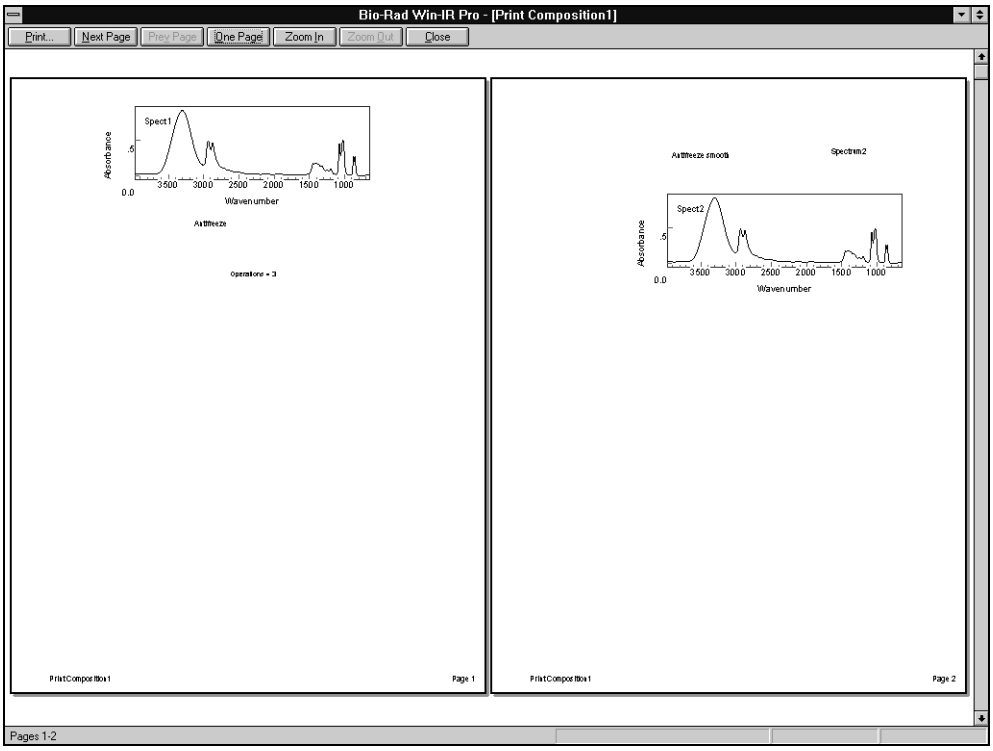
Next Page: display the next page in the print composition file. If you are displaying two pages, then each pages number is incremented by 1; that is, if you were looking at pages 1 and 2, you will now be looking at pages 2 and 3. If you are viewing the last page, this button is disabled.



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Prev Page: display the previous page in the print composition file. If you are displaying two pages, then each pages number is decremented by 1; that is, if you were looking at pages 2 and 3, you will now be looking at pages 1 and 2. If you are viewing the first page, this button is disabled.

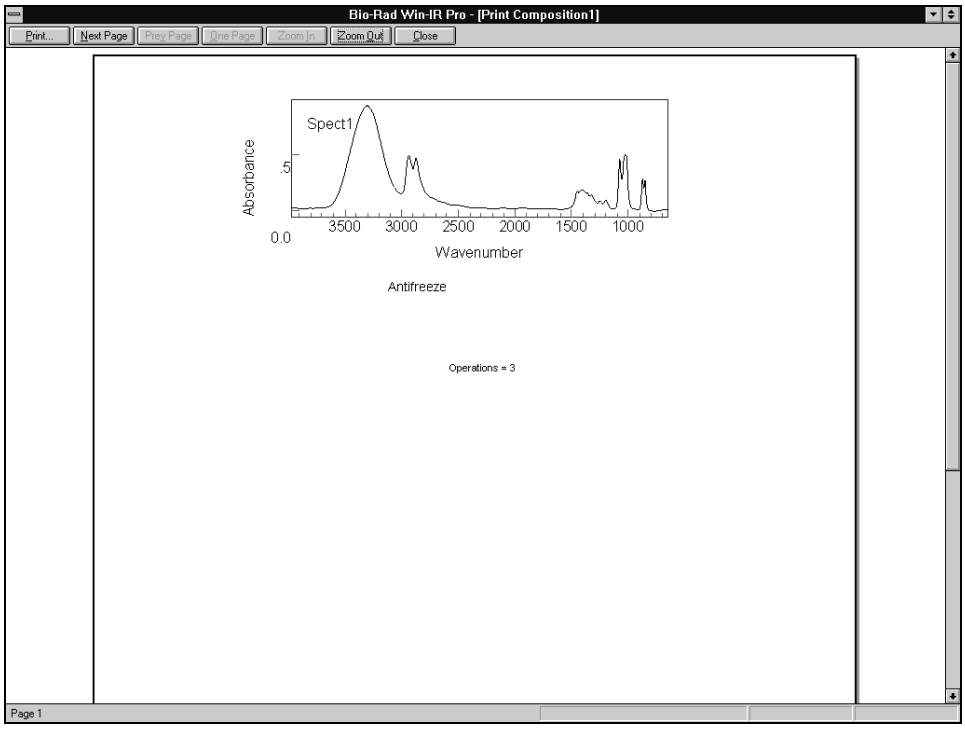
Two Pages: show two pages side by side on the screen. Two pages can only be seen at the lowest level of magnification. When two pages are displayed, the button label changes to One Page.



One Page: change the display from two pages side by side to one page. When one page is displayed, the button label changes to Two Pages.

Zoom In: zoom in and magnify the view, viewing less of the page. There are three levels of magnification; the default is the least. Two pages can only be viewed as the lowest level of magnification. If you place the cursor in a page, it changes to a magnifying glass. Click the left mouse button to increase magnification; this is equivalent to clicking the Zoom In button.

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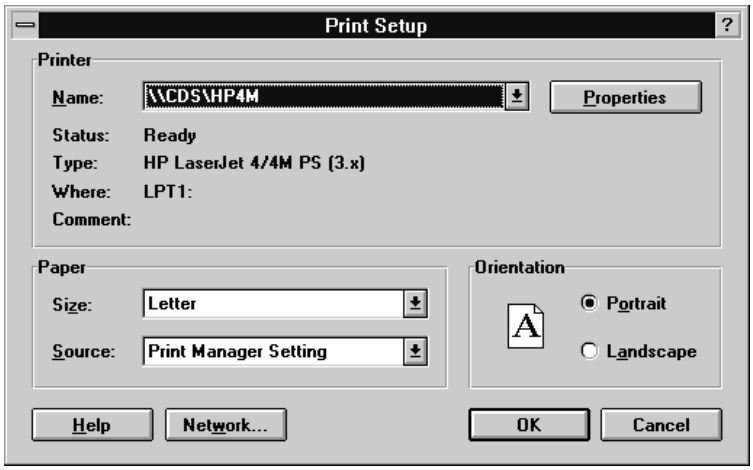
Zoom Out: zoom out and make the items smaller, viewing more of the page. There are three levels of magnification; the default is the least.

Close: close the Print Preview view and return to the Print Composition view.

Print Setup

Selects the output device and allows you to set its parameters. Normally, this is the printer and it has already been set up as part of the system installation. The dialog boxes and the specific values of the printer parameters depend upon the printer attached to the system. See the *Win-IR Pro Installation and Configuration Manual* for details on how to select printers and install printer drivers. A typical example is shown below.

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most recent files opened

The most recently (up to four) opened files are displayed here. You can reopen any of these files by clicking its name.

Exit

Saves all open documents to disk, closes all documents, closes Win-IR Pro (**not** just Print Composition), and returns to Windows NT.

EDIT MENU

Cut

Copies an object in the selected or edit state to the clipboard and deletes it from the print composition page.

Copy

Copies an object in the selected or edit state to the clipboard but does not delete it from the print composition page. .

Paste

Places the contents of the print composition clipboard on the print composition page. .

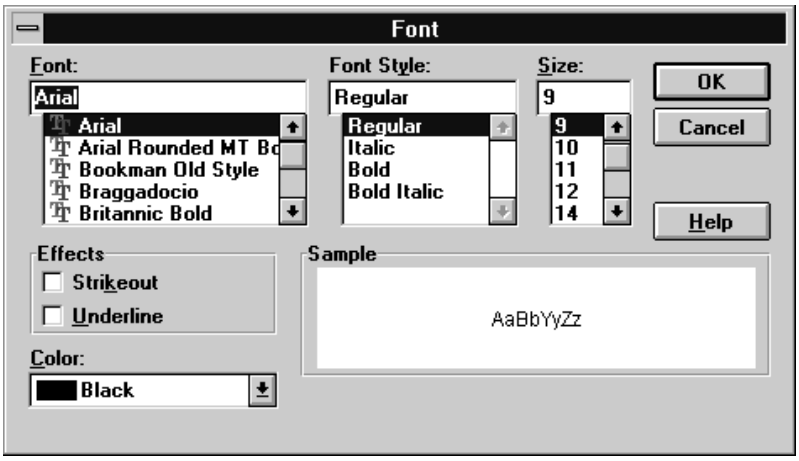
Delete

Removes an object in the selected (but not the edit) state from the print composition page.

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Font

Globally changes the text properties in all objects, except the Spectrum object. When selected, the Font dialog box appears. This is a standard Windows NT dialog box.



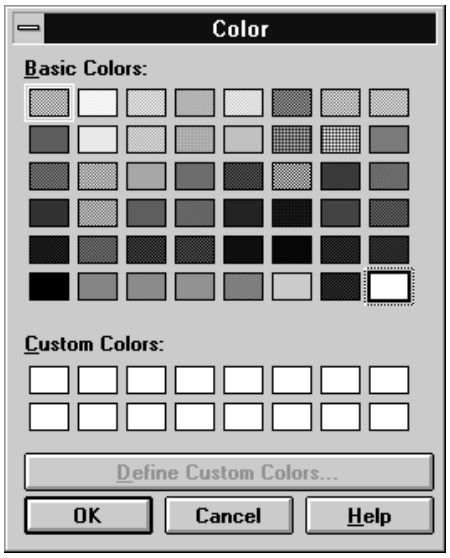
Select the Font, Font Style, Size, and Color from the pull-down menus (the default is Arial, Regular, 9 point, Black). You can also choose to have the text with ~~Strikeout~~ and/or Underline. An example of what the text looks like with the selected properites is shown in the Sample window. Click OK to implement the selected text properties, click Cancel to return without changing the text properties; click Help to enter the on-line help system.

Text properties in individual objects can be changed by making the object active, and selecting Edit / Object / Properties. Click on the Fonts tab page. Changes made here affect the highlighted object only.

Background Color

Globally changes the background color of all objects, except the Spectrum object. When selected, the Color dialog box appears. This is a standard Windows NT dialog box.

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Select the color by clicking it (the default is white, in the lower left-hand corner). Click OK to implement the selected color, click Cancel to return without changing the background color; click Help to enter the on-line help system.

Colors in individual objects can be changed by making the object active, and selecting Edit / COMMENT Control Object / Properties. Click on the Colors tab page. Changes made here affect the highlighted object only.

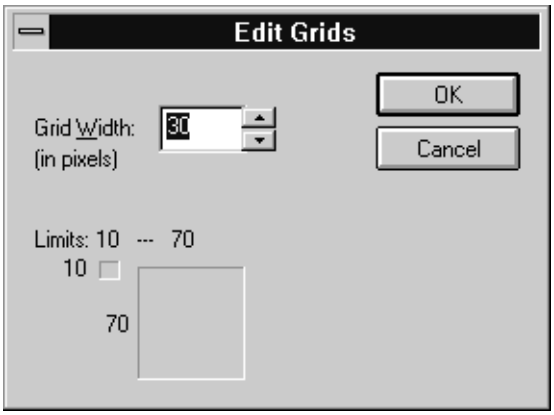
Note

Custom Colors is not implemented.

Grid

Changes the distance between grid lines. The grid width can be any number between 10 and 70 pixels (inclusive); the default is 30 pixels. The incised squares in the lower part of the dialog box show the cell size for 10 and 70 pixels.

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Object

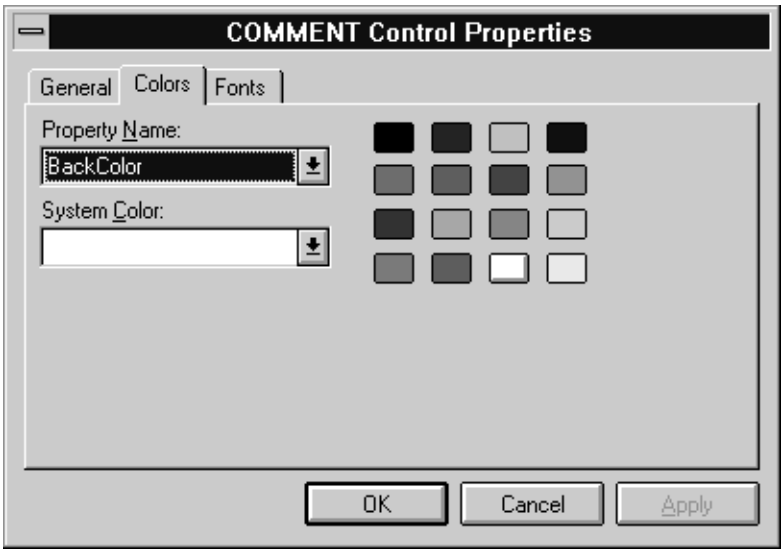
Allows editing of certain properties of objects. The entry name changes to OBJECT_TYPE Control Object when an object is in the selected or edit state.. There are two actions that can be taken; both do not apply to all objects.

Edit: puts the object into the edit state. For Comments and comments-like objects, places the cursor in the object so that the text can be edited.

Properties: each object has specific properties that can be modified. Selecting this brings up the OBJECT_TYPE Control Properties dialog box. These dialog boxes have a number of tab pages. Some of the tab pages are specific to the type of object; Colors and Fonts are common properties of all objects.

> **Colors**: click the Colors tab. This is a standard Windows NT color control dialog box that is used in many applications.

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Property Name: allows you to change the colors that apply to the specific print composition object selected. Choose the property name from the pull down menu and click the color you want it to be.

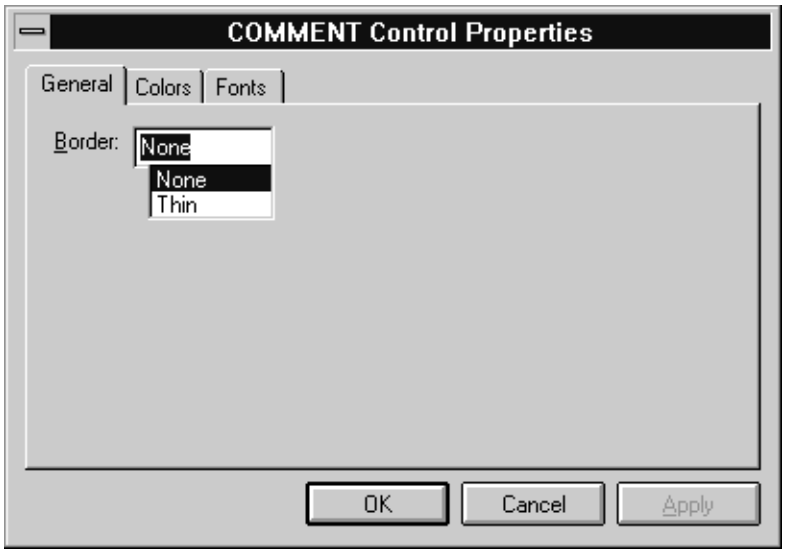
System Color: allows you to change the colors of system objects, such as Title Bars, Highlighted Text, etc. Choose the property name from the pull down menu and click the color you want it to be. Normally, these system-level choices are made from Control Panel / Color in the Program Manager.

Note

Many combinations of colors that are acceptable on a color monitor will not have such clarity when printed in grayscale. You must experiment to find the combination that meets your needs. The default colors provide such a combination.

Fonts: click the Fonts tab. This is a standard Windows NT font control dialog box that is used in many applications.

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Property Name: select the text whose font is to be modified.

Font: the font to be used. In general, avoid display fonts except for large-size titles. Times New Roman is a good serif font; Arial is a good sans serif font.

Font Style: Regular, **Bold**, *Italic*, or ***Bold Italic***.

Size: measured in points (72 to the inch).

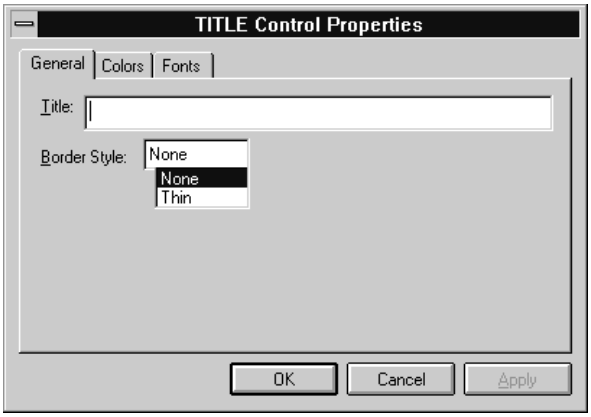
Effects: special effects can be selected.

> Strikeout: if selected, a horizontal line is drawn through the character (this feature is sometimes called strikethrough). ~~This sentence has had strikeout applied.~~
>
> Underline: if selected, the text is underlined. <u>This sentence has had underline applied.</u>

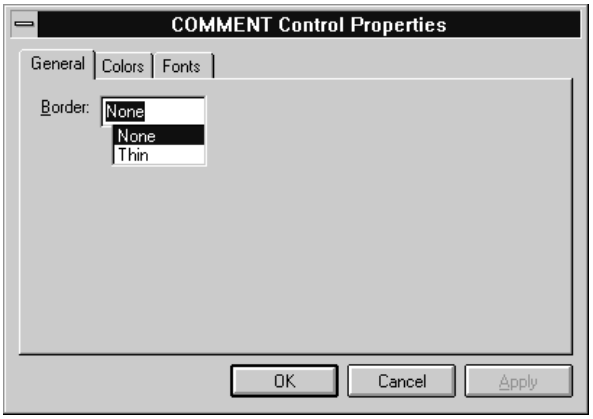
Sample: This area displays the font selected so that you can see how it appears.

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Title Control Object: the Title can be entered or altered; the Border Style of the title box itself can be chosen.



Comment Control Object: the Border of the comment box can be chosen.



OK: exit the Control Properties dialog box and implement all selections.

Cancel: exit the Control Properties dialog box without implementing any selections.

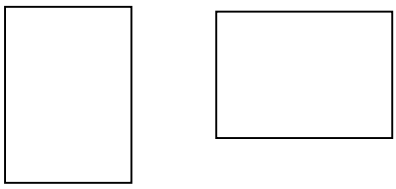
Apply: implement all selections made; do not exit the Control Properties dialog box. This button is not enabled unless a selection is made that differs from the current value.

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Orientation

Selects the orientation of the page. There are two options

Portrait **Landscape**



Note

If you change the orientation of the print template, check that none of the existing objects overlap a page boundary.

VIEW

Allows certain controls and information items on the screen to be hidden or visible as you choose. If the menu entry has a √ to its left, then the item is visible, otherwise it is hidden. The picture at the beginning of this chapter shows the location of the Status Bar, Palette Bar, and Grid. Spectrum Labels are attached to the lower right corner of each object placed upon the page.

Status Bar

Hides or shows the status bar.

Palette Bar

Hides or shows the palette bar.

Spectrum Label

Hides or shows the annotation labels attached to each object on the page.

Grid

Hides or shows the grid. To change grid spacing, use the Edit / Grid entry, described above.

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Show Peak

If checked (√) all peaks defined in the main window are displayed (default), even if they were subsequently hidden in the main display. Select this entry to remove the √ mark. In this case, no peaks are displayed in print composition. Showing or not showing peaks applies to all Spectrum and Interferogram objects on the page.

Show Labels

If checked (√) all position labels and annotations defined in the main window are displayed (default), even if they were subsequently hidden in the main display. Select this entry to remove the √ mark. In this case, no position labels or annotations are displayed in print composition. Showing or not showing position labels and annotations applies to all Spectrum and Interferogram objects on the page.

Batch

If selected, puts print composition into batch mode.

Trace Control Bar

Before this is enabled, you must first drag either a Spectrum or an Interferogram object to the print composition page. Make this object Unselected; then make it Selected. The Trace Control Bar is now enabled. Choosing it brings up the right hand side bar control panel. These controls allow you to position the traces in a Spectrum or Interferogram object with more than one trace. See “Trace Control Bar” in Chapter 8 for details on its use.

WINDOW

Except for Split, these menu entries behave the same as they do in the main Win-IR Pro document. See Chapter 13 for details.

New Window

Creates another print composition document identical to the original one. The original window as :1 appended to it; the new window is identified by :2. This allows you to create part of a print composition document, make additions, save this (use Save As, not Save), and return to the original unaltered print composition document.

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Cascade

Arranges all opened document windows (not just print composition documents) one behind the other, offset both horizontally and vertically, so that all title bars are visible.

Tile

Arranges all opened document windows (not just print composition documents) vertically, that is, one above the other.

Arrange Icons

Arranges the icons for minimized document windows.

Split

If selected, the cursor changes to a two-headed horizontal arrow, split in the center by two parallel vertical lines. It is positioned in the middle of the windowshade. If you move the cursor to the left or right the windowshade follows it (moving the cursor up or down has no effect on the screen). When the windowshade is where you want it to be, click the left mouse button to return to normal operation. This entry is equivalent to placing the cursor on the windowshade, holding down the left mouse button, dragging the windowshade, and releasing the left mouse button.

open windows

Lists all open document windows in Win-IR Pro. To make a document window the active window, select it from this list. When a window is opened, it is added to this list; when a window is closed, it is removed from this list.

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HELP

This is a subset of the Win-IR Pro Help menu. See Chapter 14 for details.

Index

Causes the top-level Win-IR Pro Help window to appear.

Using Help

Causes the Help Topics: Window Help window to appear. This on-line help is standard throughout all Windows NT products. It is written by Microsoft to be self-explanatory.

About Win-IR Pro

Causes the Win-IR Pro product identification box to appear.

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16
Frequently Asked Questions

COMPUTER OPERATIONS

Q. My dongle no longer seems to function; why is this?

A. We have had reports of dongle failure when an Iomega zip drive was plugged into the parallel port while powered up. When you install zip drives, make sure you follow the vendor's instructions and have the drive powered down before connecting it to the parallel port.

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Q. Why do I have to reboot the computer twice in the process of installing Win-IR Pro?

A. You do not normally need to reboot the system more than once when installing Win-IR Pro. However, at some releases of Win-IR Pro, you must first upgrade the operating system. After you install this newer version of the operating system (or a debug patch to the operating system), you must reboot the computer for this upgrade to take effect. When you install Win-IR Pro (this installation program is called SetUp.exe), you must reboot the computer to have the new Win-IR Pro drivers, etc. take effect.

Q. My system will not start. How do I fix this?

A. One possible problem is an IRQ conflict. The spectrometer card is set to IRQ 10. The network card should be set to IRQ 5 or 11. However, many network cards are, by default, set to IRQ 10. To resolve this:

1. Remove the spectrometer card and attempt to boot your system.
2. If it starts, follow the manufacturer's instructions for changing the IRQ setting.
3. Shut down the system and insert the spectrometer card.
4. Restart the system.

Q. My system is running slowly and the disk light is on most of the time. How do I correct this?

A. There are a number of possibilities; they are all concerned with the way Windows NT handles memory.

1. You may be running out of space on your disk. In this case, archive data that you want to retain. Look at the c:\temp directory and delete unneeded files there.

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Note

Windows NT will not let you delete files that are required for the applications that are running, or that Windows NT thinks are required (see under Shutdown below).

2. If you are running out of virtual memory, you may want to increase the size of the Paging File. To do this, you must first be logged in as an administrator; then:

   From the Task bar, select Start / Settings/ Control Panel.

   Double-click the System icon

   Select the Performance tab page.

   Under Virtual Memory, click the Change button.

   Type in a larger size for the Paging File. Space used by the Paging File is not available for storage.

   Click the Set button. Click the OK buttons until you return to the Control Panel.

   Close the Control Panel.

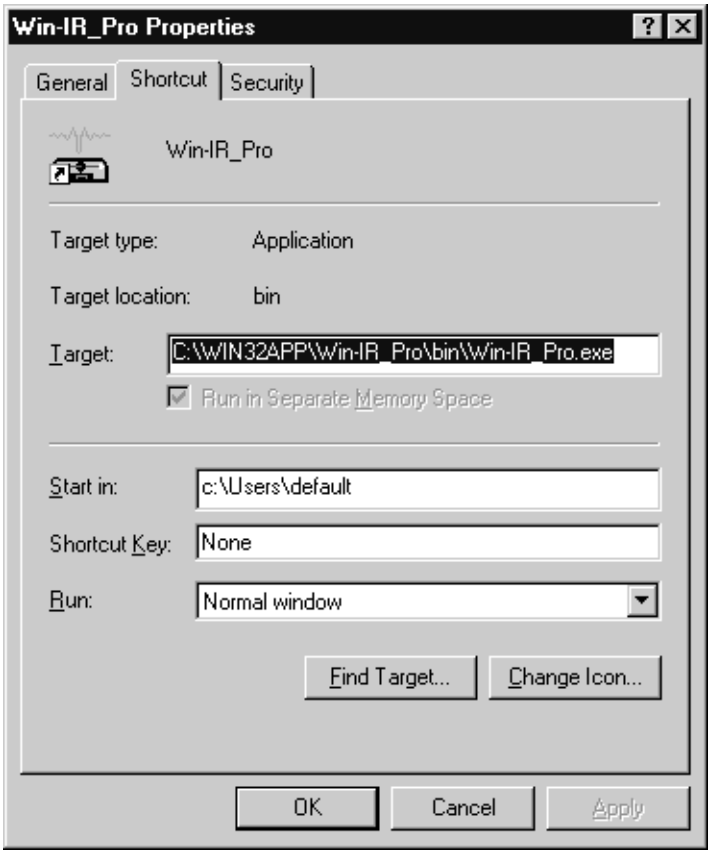
3. From the Task bar, select Start / Shut Down. When the system is restarted, the unneeded temporary files will have been deleted.

Q. *To increase storage, I added another hard drive to my system. The Win-IR Pro software is installed on drive c:, but I want the default drive to be d:. How do I do this?*

A. In order to do this, you must have put a Win-IR Pro shortcut in the Profiles directory and/or on your desktop.

Put the cursor on the shortcut icon and click the right mouse button; a menu appears; select Properties from the menu. The Win-IR_Pro Properties dialog box appears. Click the Shortcut tab.

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Type the desired working directory in the Start in box. Click OK.

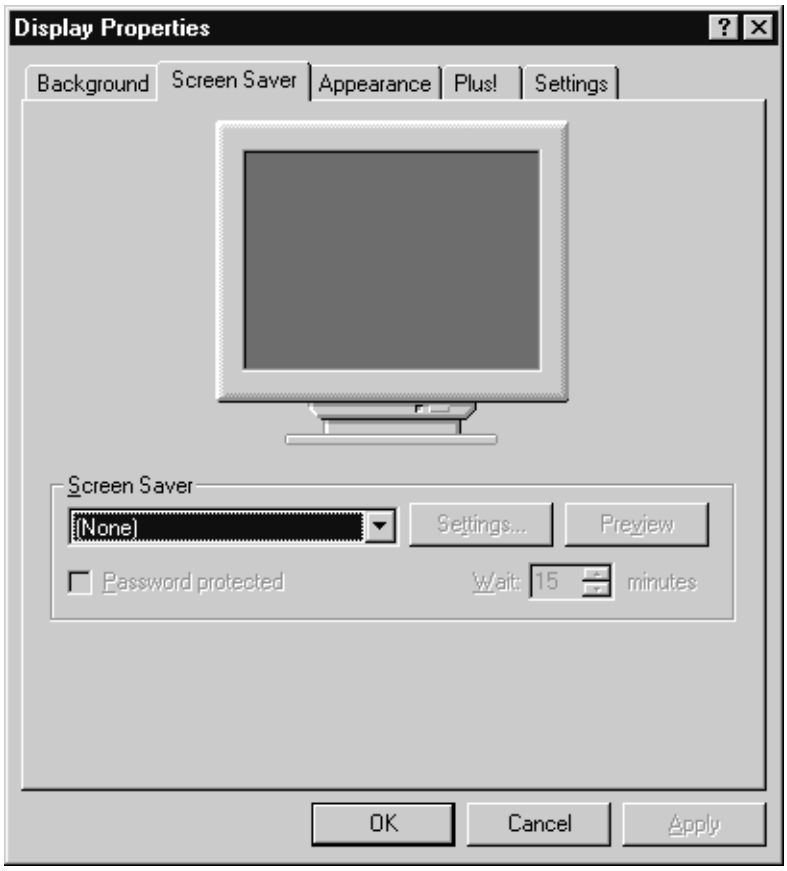
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Q. On a long data collection, the software sometimes seems to "hang."

A. Turn off your screen saver, if it is running—from the Task bar, select Start / Settings / Control Panel.

Double click the Display icon. The Display Properties dialog box appears.

Click the Screen Saver tab.



Use the pull-down menu to change Screen Saver to (None) and click the OK button.

Screen savers are not designed to work with programs that write data to the screen—like Collect—and may cause unpredictable behavior.

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Q. During data collection, the computer system crashed.

A. This can occur if you do not have sufficient disk space available at the start of the data collect. You need at least 10 MB for regular data collection, and at least 64 MB for DSP data collection. Check the TEMP and TMP directories for files which can be deleted. You may also want to archive inactive files.

Q. When I was configuring the hardware using the spectrometer applet, the rear detector entry had a blank. When I selected this, the system crashed.

A. This is no longer a problem. In some older versions of the software, this occurred if the registry was corrupted. From the Task bar, select Programs / Administrative Tools / RegEdit 32. Select the key HKEY_LOCAL_MACHINE\SOFTWARE\Bio-Rad\Win-IR Pro\Spectrometer Configuration and delete it. This will solve the problem.

Q. There are two spectrometer applet icons when I open the Control Panel. How do I remove one?

A. In Explorer, go to the directory WINNT35/SYSTEM32. Look for the file(s) Spectrometer.cpl. There will be two files with this name. Delete the older file.

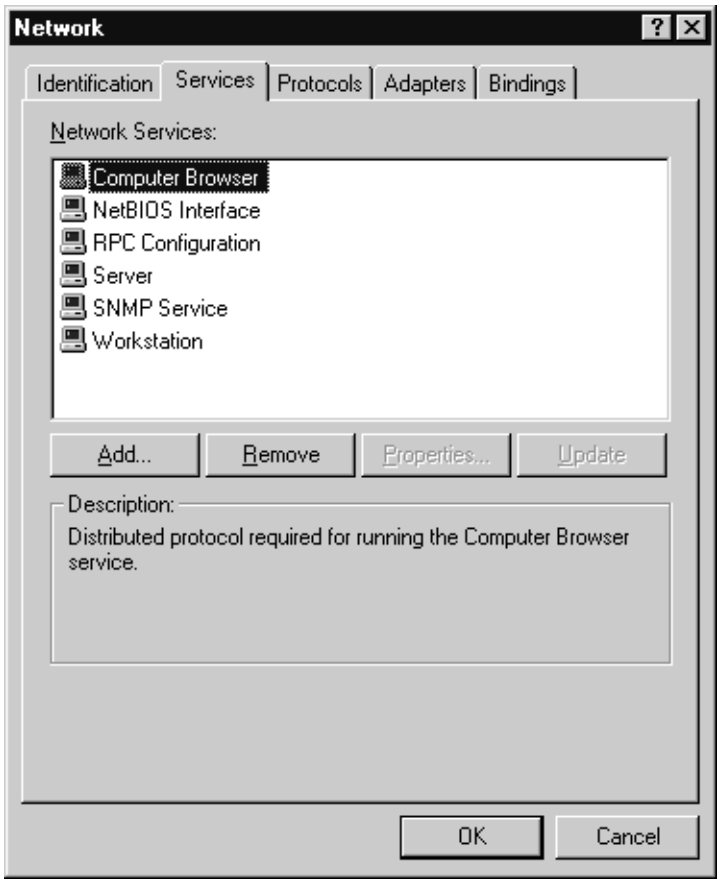
Q. Sometimes I get an error message on start-up that says: OLE Initialization has failed. Win-IR Pro will not start.

A. The computer system is shipped with networking turned on, because most of the systems running Win-IR Pro are connected to networks. The above error occurs when networking is turned on, but the system is not connected to a network. To turn networking off:

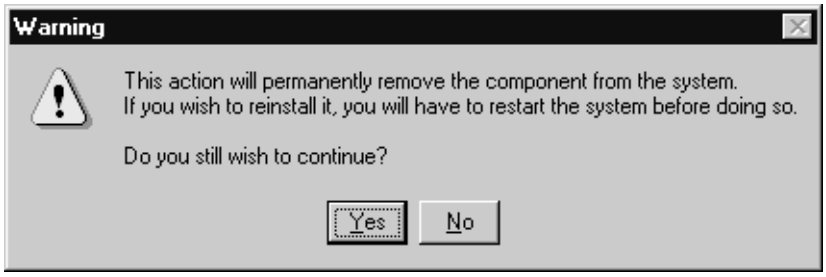
1. From the Task bar, select Start / Settings / Control Panel.

2. Double-click the Network icon. The Network dialog box appears. Click the Services tab.

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3. Select an entry in the Network Services scroll list and click the Remove button. The following dialog box appears.



Answer Yes.

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4. Continue until all network software has been removed.

5. Click OK to implement the software removal.

6. Close the Control Panel.

7. Log off, shutdown the system, and reboot it for the changes to take effect.

Note

Because some of the software must be removed in a specific order, you may have to repeat this process until all the software is removed.

DISPLAY-RELATED QUESTIONS

Q. Sometimes it seems that no trace appears even though a trace was selected. This sometimes happens when extracting a trace from the image file. What can be done about this?

A. The standard way to solve this problem is to select Option / Edit Colors from the menu bar and then to change the background and/or the trace (spectrum) colors so there will be contrast. However, there is another way in which this situation can occur unexpectedly. The default Win-IR Pro background color is obtained from Windows NT; the other Win-IR Pro default colors are coded into the program. To find out what the default background color is:

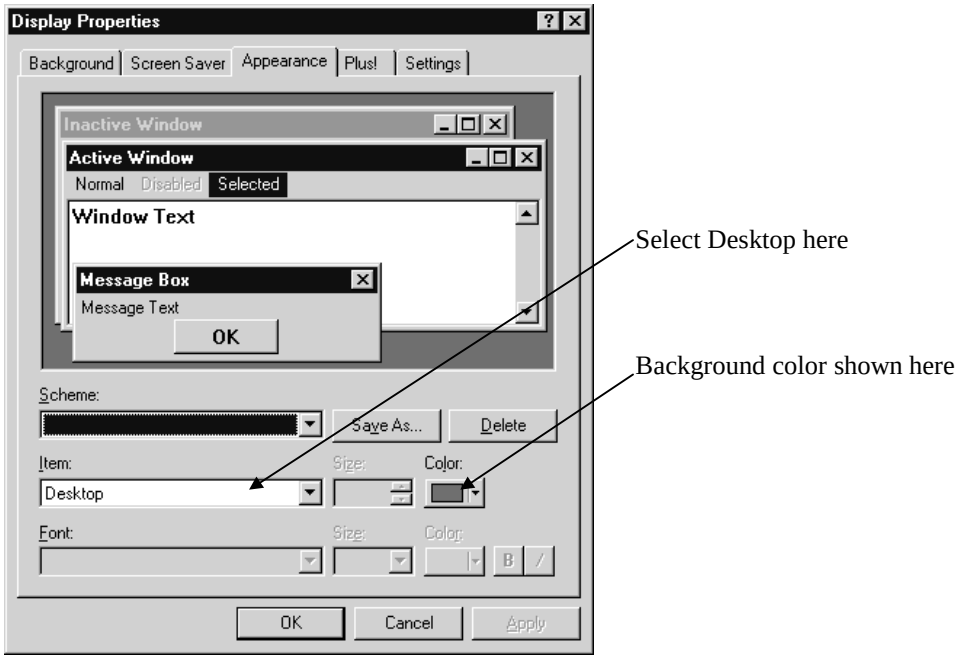
1. Select Start / Setting / Control Panel from the taskbar.

2. Double click the Display icon.

3. Click the Appearance tab.

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4. Select Desktop from the Item pulldown list.



The color shown is used for the Windows NT background and for the default Win-IR Pro background. If this color is changed, it will be used in Win-IR Pro as the default background color the next time the file current.pv is created.

A typical color mismatch scenario is:

1. User changes Windows NT color scheme (desktop color changed).

2. User deletes current.pv file for some reason.

3. User starts Win-IR Pro and some of the inactive traces may be difficult or impossible to see.

To fix this, change the desktop color back to its default value, delete current.pv; restart Win-IR Pro.

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Q. When I use Options/ Edit Color to change the zoom box color, I do not get the exact color I picked. If I pick black for the zoom box with a white background, the zoom box does not show up on the display (however, the zoom box function still works). How do I fix this?

A. In order for the zoom box to be drawn it must be in the XOR mode. This means the color selected for the zoom box is XORed with the background color. Experiment to find your desired zoom box color. For example, with a white background, choosing light blue (column 5, row 2 in the color chart) for the zoom box yields a red zoom box; choosing yellow (column 2, row 1 in the color chart) for the zoom box yields a dark blue zoom box.

Q. The Windows NT Taskbar covers up part of the display of the control side bars for kinetics, 3D, quantitative analysis, etc.; how do I eliminate this?

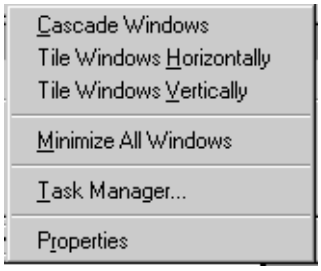
A. There are two options. The simplest is to move the taskbar to another edge of the screen.

1. Put the cursor on part of the taskbar which does not have an application.

2. Hold down the left mouse button, drag the taskbar to the desired edge of the screen, and release the mouse button.

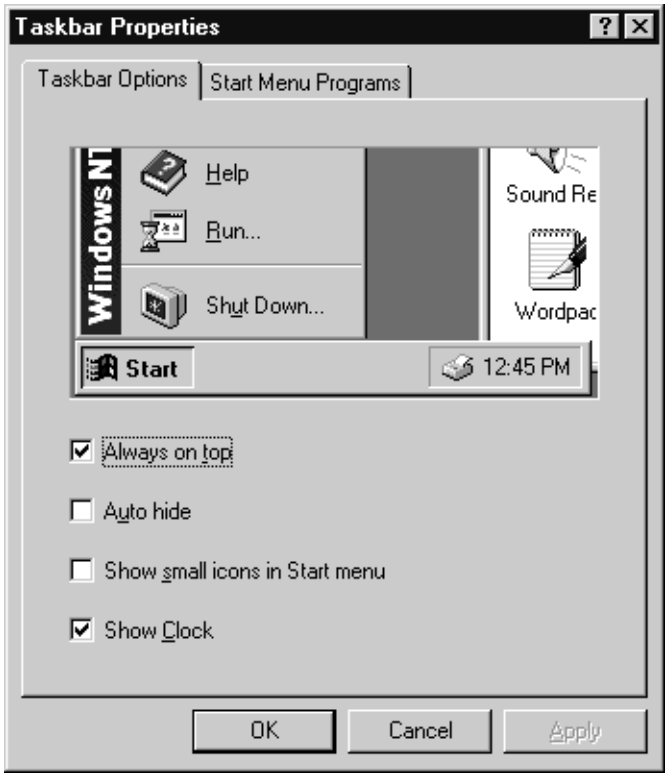
Alternatively, you can have the task bar *autohide*. To do this:

1. Put the cursor on a part of the taskbar which does not have an application; click the right mouse button. A menu appears.



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2. Click on Properties with the left mouse button. The Taskbar Properties dialog box appears.



3. Select Auto hide. Click OK. The taskbar will now hide itself when an application is running.

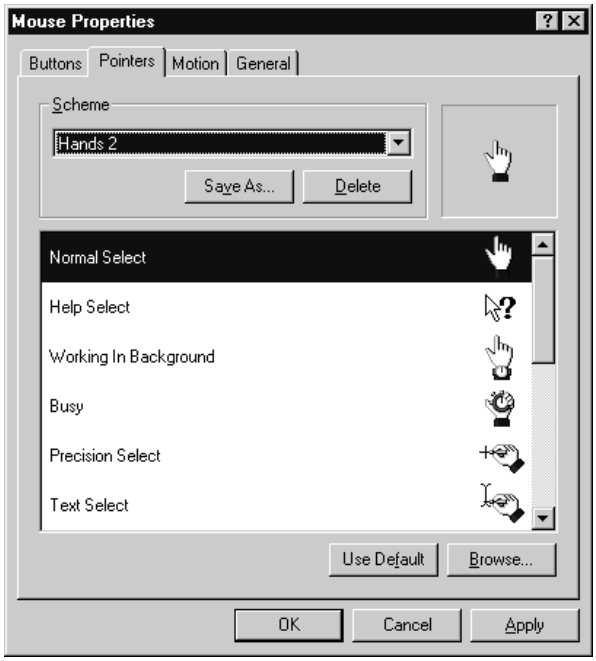
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Q. My cursors do not behave as described in the manual.

A. Win-IR Pro requires that the Windows NT cursors to set to their default values. Someone has probably changed these. To restore the default values.

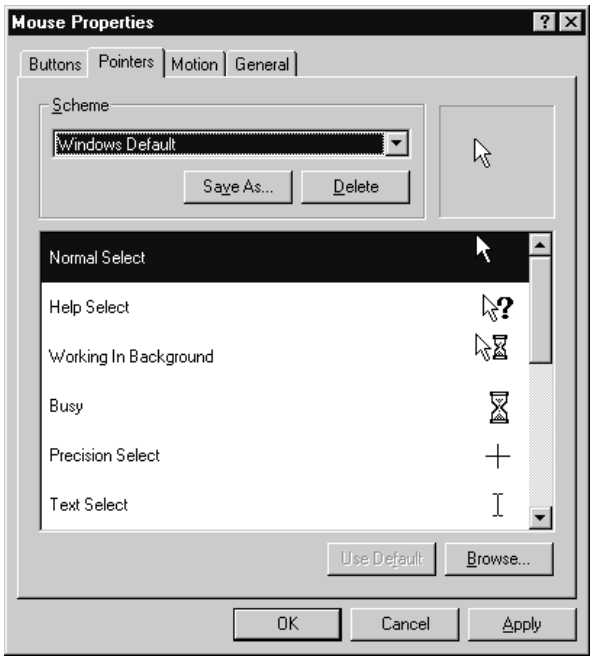
1. From the Task bar, select Start / Settings / Control Panel.

2. Double-click the Mouse icon. The Mouse Properties dialog box appears. Click the Pointers tab. In this example, someone has changed the cursors to Hands 2.



3. Put down the Scheme menu and select Windows Default.

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4. Click OK to implement the default cursors.

5. Close the Control Panel.

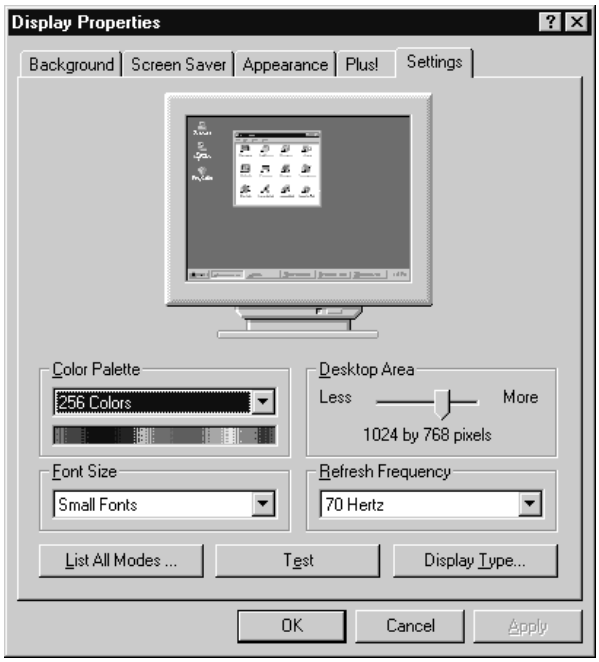
Q. *Some of the dialog boxes overlap and cover up edit boxes and/or buttons; how do I fix this?*

A. You have the screen fonts set to Large Fonts; it should be set to Small Fonts. To fix this:

1. From the Task bar, select Start / Settings / Control Panel.

2. Double-click the Display icon. The Display Properties dialog box appears. Click the Settings tab.

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3. Pull down the Font Size menu and select Small Fonts.

4. Click OK to save the new settings.

5. Close the Control Panel.

Note

You must exit and restart Windows NT for the changes to take effect.

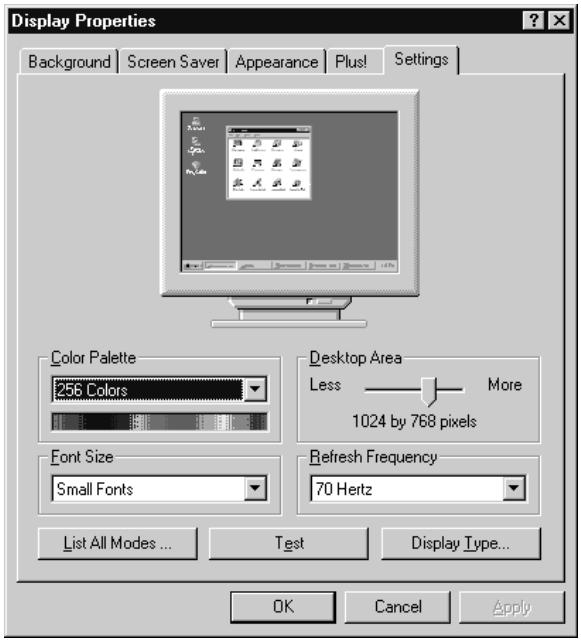
Q. Why do the colors in my display appear "muddy?"

A. Your display is set for 256 colors; it should be set for 65536 (64K) colors. To reset the colors:

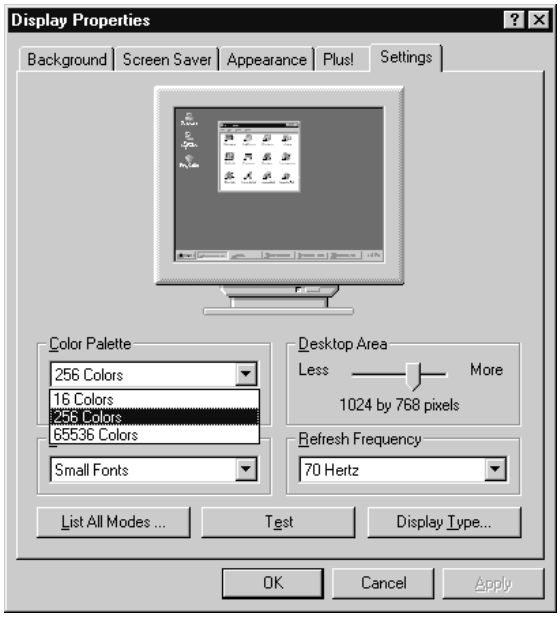
1. From the Task bar, select Start / Settings / Control Panel.

2. Double-click the Display icon. The Display Properties dialog box appears. Click the Settings tab.

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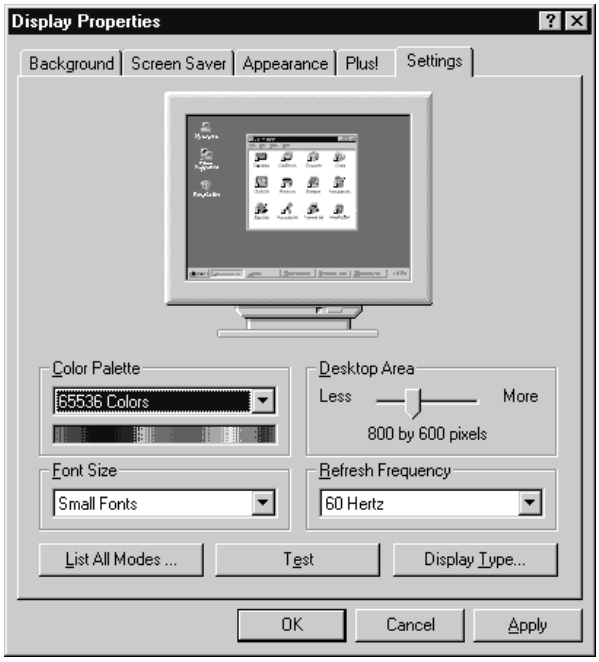


3. Pull down the Color Palette menu and select 65536 Colors.



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The dialog box should now look like this.



4. Click OK to save the new settings.

5. Close the Control Panel.

Note

You must exit and restart Windows NT for the changes to take effect.

Q. I do not see the X and Y coordinates of the cursor in the right hand side of the status bar.

A. Select the trace by clicking on it. The X and Y coordinates will now be seen.

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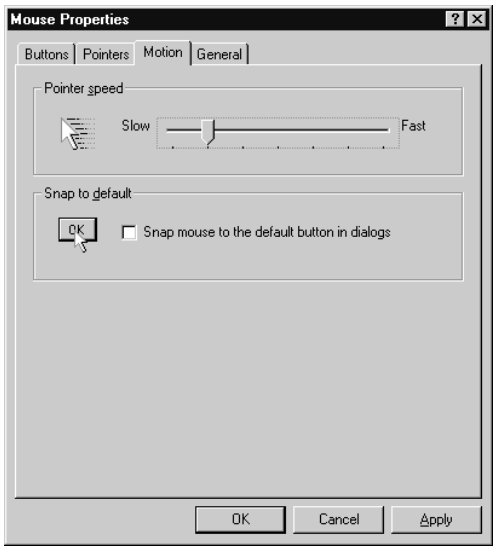
Q. *In a number of the control panels (for example, the Trace Control Bar) the Apply button seems to always be disabled (grayed out).*

A. If you change parameters by selecting them from a pull-down menu, the new value is automatically applied upon selection. If you type in a new value, this enables the Apply button. Press the Apply button to apply the newly typed value. When you select from the menu, the Win-IR Pro knows what value to use. When you type in a value, pressing the Apply button tells Win-IR Pro that you have completed entering that value.

Q. *When I work in the radar box, I often cannot resize the rectangle indicating what part of the spectrum is displayed. Instead, a new rectangle is created and I have to use autoscale to redisplay the main spectrum. In other cases, when I try to double-click, an event occurs between the first and second click.*

A. Your mouse is too sensitive; to decrease the mouse sensitivity:

1. From the Task bar, select Start / Settings / Control Panel.
2. Double-click the Mouse icon. The Mouse Properties dialog box appears. Click the Motion tab.

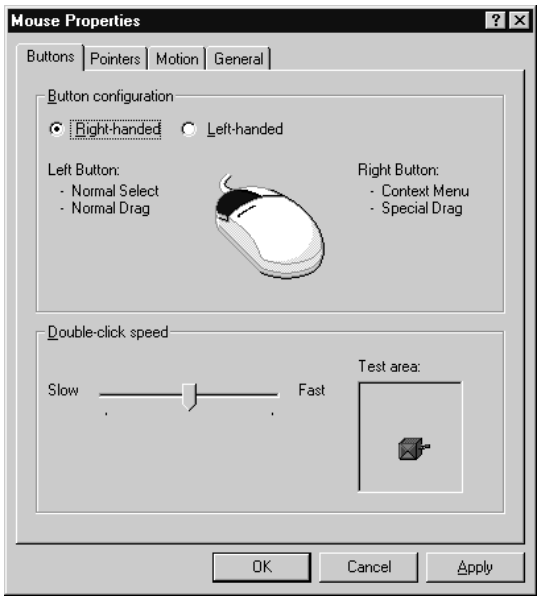


3. In the Pointer speed bar, drag the indicator toward Slow. Then click OK.

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4. Try the new mouse setting. If it still is a problem, repeat the process. If necessary, decrease the speed again.

5. To adjust the double click speed, access the Mouse Properties dialog box, but click the Buttons tab.



6. In the Double-click speed bar, drag the indicator toward Slow. Adjust the Double Click Speed so that it is appropriate for your reaction times. Then click OK.

7. Close the Control Panel.

Q. *I don't want the splash screen to be displayed every time I start win-IR Pro. How can I turn off the splash screen?*

A. In the directory c:\Program Files\Win-IR Pro\bin there is a file called Splash.dll. If you rename this file or move it to another directory the splash screen will no longer appear upon startup or when you select Help / About Win-IR Pro from the menu bar. If you want to restore the splash screen either give the file its original name or move it back to this directory. You can also eliminate the splash screen by deleting Splash.dll but then, in order to restore the splash screen, you would have to copy the file from the installation CD-ROM.

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DOCUMENT-RELATED QUESTIONS

Q. When I collect a spectrum, it is stored in the same document as the background. How do I avoid this?

A. When you collect data, that data is collected into the currently active (highlighted) document. If you previously collected a background, and that background document is active, the sample data will be collected into the background document. Close the background document if you want your sample data to be collected into a separate document.

Q. When I open a new document, it doesn't ask for a name. Why is this?

A. This is in accordance with Windows and Windows NT procedure which does not ask for a filename until the first time a document is saved. If you want to assign a filename before you collect data, open the document using File / New, and then use File / Save As to assign it a name. If that document is active when you start a scan, data will be collected into that document. You must then use File / Save to save the data.

Q. *When I minimize a document and then open a new document, it is opened in an iconized (minimized) state; is this supposed to happen?*

A. Yes. A new document is opened in the same style as the last document.

Q. If you are in the middle of a transform—or a similar procedure—and you click the close box (✕), the document is closed, but you are not asked if you want to save any changes. Why is this?

A. You are only asked if you want to save changes if you have made a change to the document. When you select ✕, it is equivalent to clicking the Cancel button, followed by File / Close. If you did not make a change to the spectrum, you will not be prompted because of this action. If previous procedures have changed the document, then you will be prompted.

BASELINE-RELATED QUESTIONS

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Q. How do you perform a quantitative analysis without baseline correction?

A. To remove the baseline correction of the components in the calibration document, first select the component by clicking its label. Then, use the right mouse button menu to select Properties. When the Edit Peak Properties dialog box appears, select the General tab page. In the Baseline Definition portion of this page you will normally find Use Left Point and Use Right Point selected; de-select them. Click the OK button. Baseline correction is now removed from all calibration curves for this component.

Q. After I performed a zoom in baseline correction, the cursor did not change back to the baseline correction cursor. How do I make this happen?

A. You can toggle between the zoom and baseline correction modes by clicking the zoom  and baseline correction  buttons at the bottom of the main window.

Q. When I use Zap to zero the spectrum at either end, the last point is not set to 0. How do I make this point 0?

A. Zap does a linear interpolation between points; it cannot modify the end points. If you want to zero the end points use the Truncate or Ultrazap transform instead.

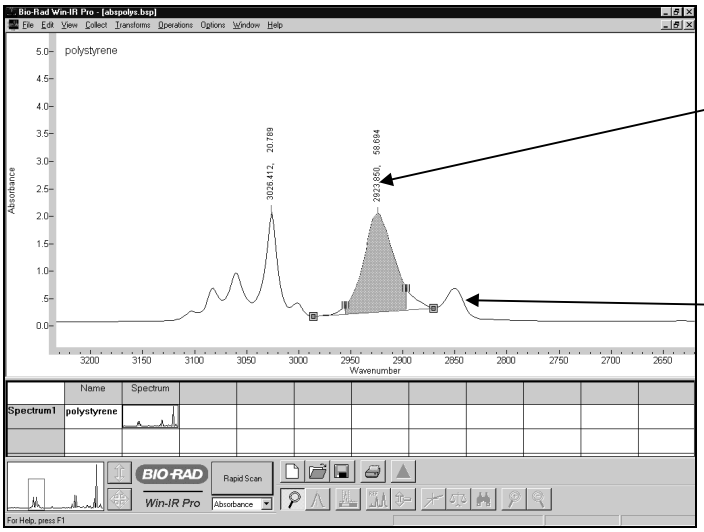
OTHERS

*Q. I want to de-select a peak (*that *is, remove its label), but when I click on the peak it does not allow me to do this.*

A. To de-select a labeled peak, put the cursor on the peak and press the left mouse button; then, press the Delete key on the keyboard. The peak is now deselected. This is a change from releases 2.2 and previous.

Avoid putting the cursor on the trace and clicking; this will select the trace and, if you press the Delete key, the trace will be deleted. If you do this, immediately select Undo from the Edit menu and the trace will reappear.

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Q. *In a Kinetics document, sequential spectra are displayed from top to bottom; in a Multi-spectral Document, the spectra are displayed from bottom to top.*

A. The order of the spectra in the display window has no particular significance in Win-IR Pro; they may appear in different order in different circumstances.

Q. *How do I select non-contiguous spectra (or columns) in the spreadsheet or in the search hit list view?*

A. Win-IR Pro follows standard Windows NT convention in this matter.

To select non-contiguous spectra: select one spectrum by putting the cursor in its Spectrum ID cell and clicking the left mouse button. Put the cursor in the Spectrum ID cell of the second spectrum you want to select; hold down the Ctrl key on the keyboard and click the left mouse button. Both spectra are now selected; continue as desired. You can toggle any spectrum between selected and non-selected by putting the cursor in its Spectrum ID cell, holding down the Ctrl key, and clicking the left mouse button.

To select contiguous spectra: select the first spectrum by putting the cursor in its Spectrum ID cell and clicking the left mouse button. Put the cursor in the Spectrum ID cell of the last spectrum in the group you want to select; hold down the Shift key

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on the keyboard and click the left mouse button. All spectra in the group are now selected. You can toggle any spectrum between selected and non-selected by putting the cursor in its Spectrum ID cell, holding down the Ctrl key, and clicking the left mouse button.

Use the same procedure to select columns in the spreadsheet. To select columns, put the cursor in the column header cell and click the left mouse button.

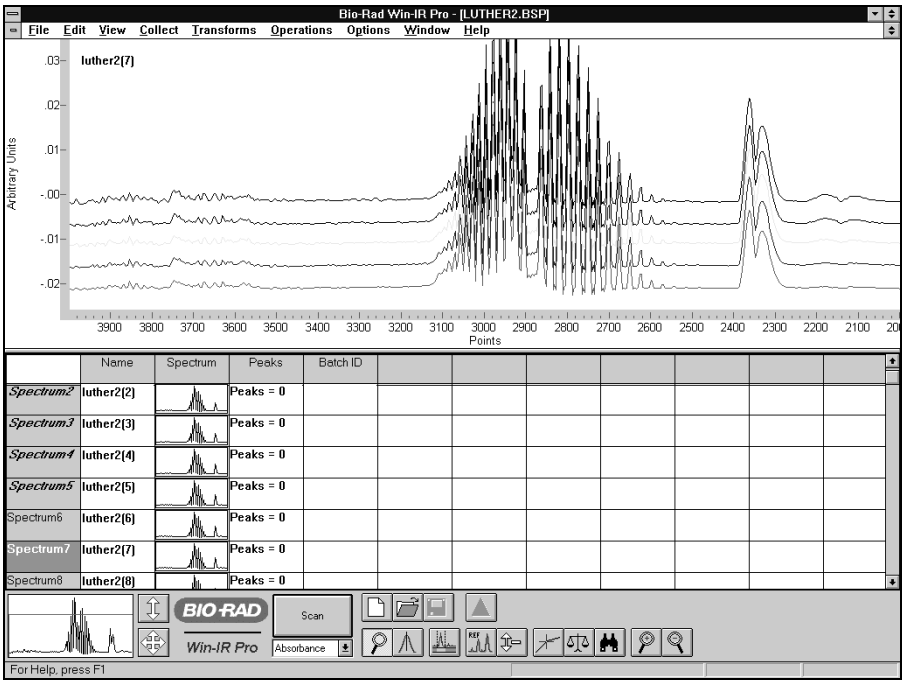
More details on selection and other aspects of the spreadsheet are given in Chapter 4.

Q. *I have a spreadsheet with many spectra in it. I want to display a group of them and*

- *see which trace corresponds to which row*
- *page though the other rows in the document to compare their traces to the displayed group.*

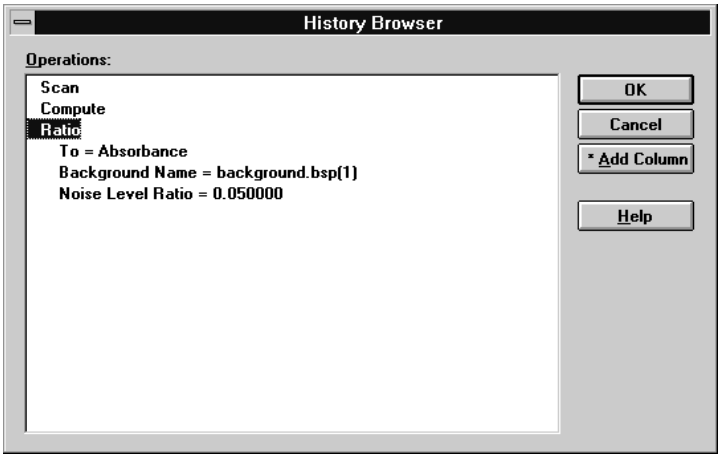
A. First, select the rows whose traces you want to display (see above for selection of non-contiguous rows). Then, select View / Lock Selected from the main menu. The IDs of the locked rows will be displayed in italic type. Use the ↑ and ↓ keys to scroll through the rows of the spreadsheet. In the example below, spectra 2 through 5 have been selected and locked; spectrum 7 is also displayed (it is the uppermost trace).

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Q. When I select View / History, I cannot find any information about the background (other than number of background scans) under Scan in the History Browser.

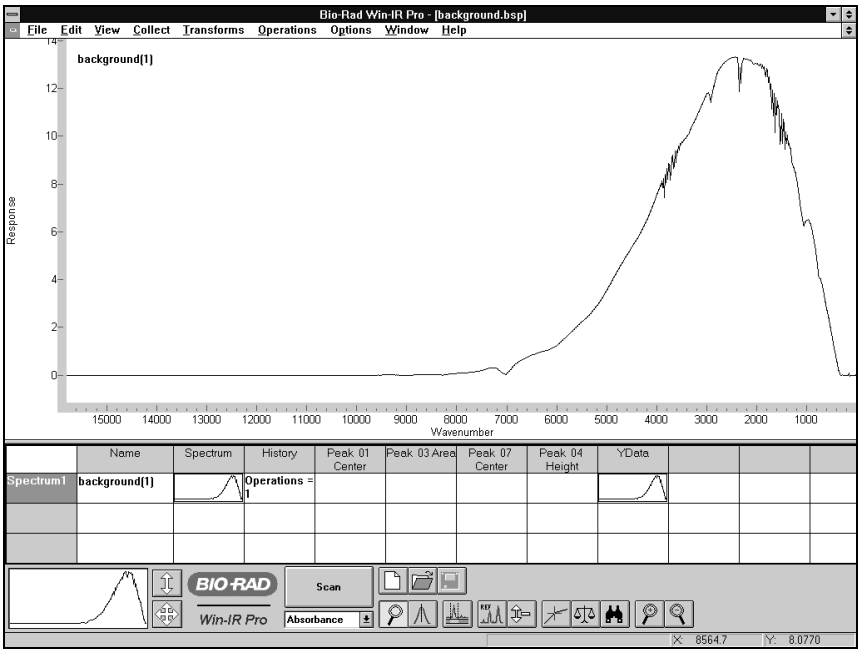
A. Background is not a Scan, but a Ratio parameter. Double-click Ratio in the History Browser dialog box to get information about the background file name.



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To get information about the background collection parameters:

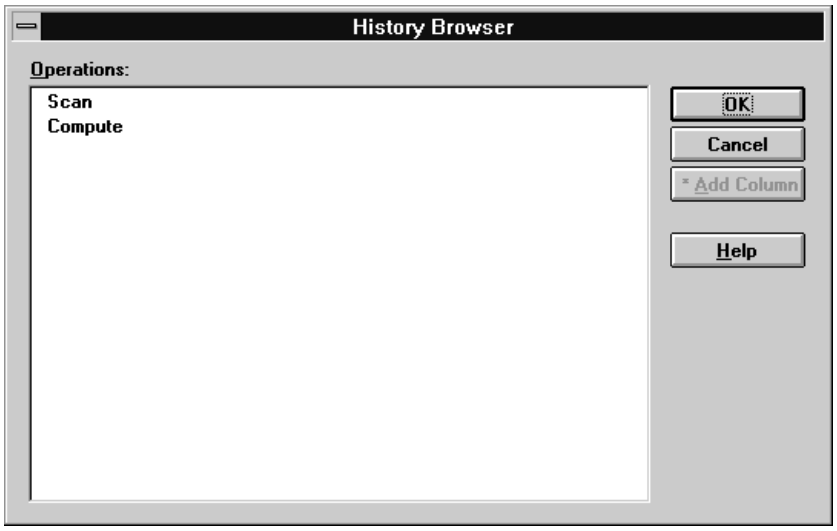
1. Open the document containing the background file, in this example background.bsp.



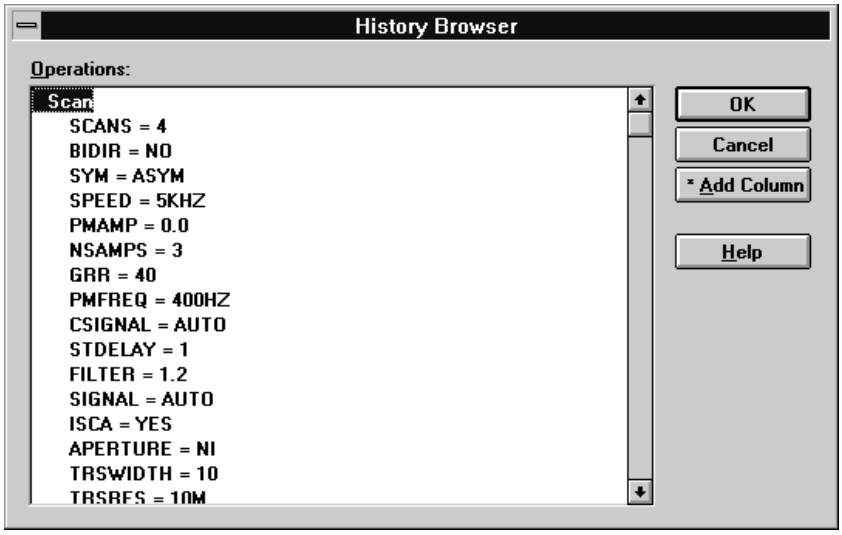
2. If there is more than one trace in the document, select the background trace.

3. Select View / History.

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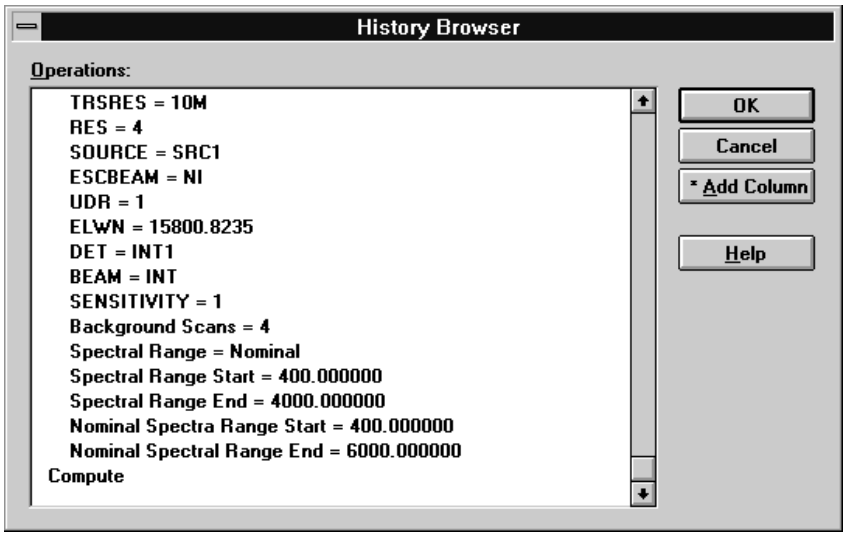


4. Double-click Scan.



5. Scroll, if necessary, to see all the parameters.

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Q Can I print a chromatogram?

A. A chromatogram can be printed by the following method:

1. Select the chromatogram to be printed.

2. Choose Edit / Copy.

3. Choose File / New. Highlight Multi-Spectral Document and click OK.

4. Choose Edit / Paste. This will paste the chromatograms into the new document as if they were spectra.

5. If you want to add the wavenumber range information to the spreadsheet so that it can be printed out, first choose View / History.

6. In the History Browser dialog box, highlight Functional Group Analysis to display its parameters.

7. Highlight Peak Region; click the *Add Columns button; click the OK button. Peak region information has been added to the spreadsheet.

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8. You can now print these chromatograms as if they were spectra.

> **Caution**
> **You cannot manipulate these chromatograms and then paste them back into the original document. Win-IR Pro no longer recognizes them as chromatograms. This does not affect the chromatograms in the original document.**

Q. *If kinetics or TRS bands go negative, what is the best way to track them using a FGC?*

A. When you create the functional group, select New and click the Edit Parameters button. When the Edit Peak Parameters dialog box appears, click on the Center tab page. In the Method portion of the page, select Extreme in Region. This will select the center to be either the maximum positive or the maximum negative excursion from zero.

Q. *Although my reference single-beam spectrum is good, it is considerably smaller than the sample so the Noise Level Ratio parameter in the Ratio transform causes the entire ratioed spectrum to be zero. This is not infrequent in multiple modulation experiments. How do I overcome this?*

A. If you know that the reference spectrum is acceptable, use the following procedure:

1. Use Operations / Spectral Arithmetic / Scalar to multiply the reference spectrum by a scalar.

2. Perform the ratio.

3. Use Operations / Spectral Arithmetic / Scalar to divide the result by the same scalar, if required.

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A
Adding New User Accounts

WHY HAVE DIFFERENT ACCOUNTS?

In a typical laboratory situation, a Win-IR Pro workstation may be used by a number of experimenters or by one experimenter performing different experiments. Data collection parameters are saved for each user account. Therefore each account can be customized by the individual (or group) experimenter. This means that you can change parameters without interfering with other users. In addition, using multiple accounts allows you to easily and automatically separate the data for different experiments into their own directories.

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SECURITY

Physical security can vary from a single-user non-networked console in a controlled-access environment to a multiple user console connected to a multi-purpose network in a non-access-controlled environment. As physical security decreases, use the software security supplied by Windows NT to compensate for it. The major tools are separate accounts, user groups, and passwords. In general,

SITUATION	SUGGESTION(S)
single user	probably do not need passwords
single-purpose network	passwords on each account
multipurpose network	see your network administrator

Proper password creation and use is only part of running a secure system. This is a large topic covered in the Windows NT documentation and in commercially available books.

PASSWORDS

Passwords minimize accidental or deliberate attempts to access or alter data. If you use passwords and your organization does not have a password policy, the following guidelines may be helpful. Normally, passwords should be at least 6 characters (more is better); passwords are case-sensitive; blanks (spaces) are not allowed in passwords. Passwords should have no obvious connection with the user. Do not use telephone extensions, nicknames, birthdays, anniversaries, etc. Phrases (multiple words run together) are harder to decipher than single words. A numeral or other non-alphabetic character also increases security. Do not write down passwords and leave them in desk drawers, in instrument log books, or attach them to the computer monitor.

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ADDING A NEW USER ACCOUNT

Notes

For complete details on adding new users, see your Windows NT documentation.

Some of the procedures below are designed to allow you to write scripts to create new user accounts—for example, setting up accounts with default passwords and forcing users to change them upon first logon, defining home directories in terms of user names, etc. See the Windows NT documentation for details.

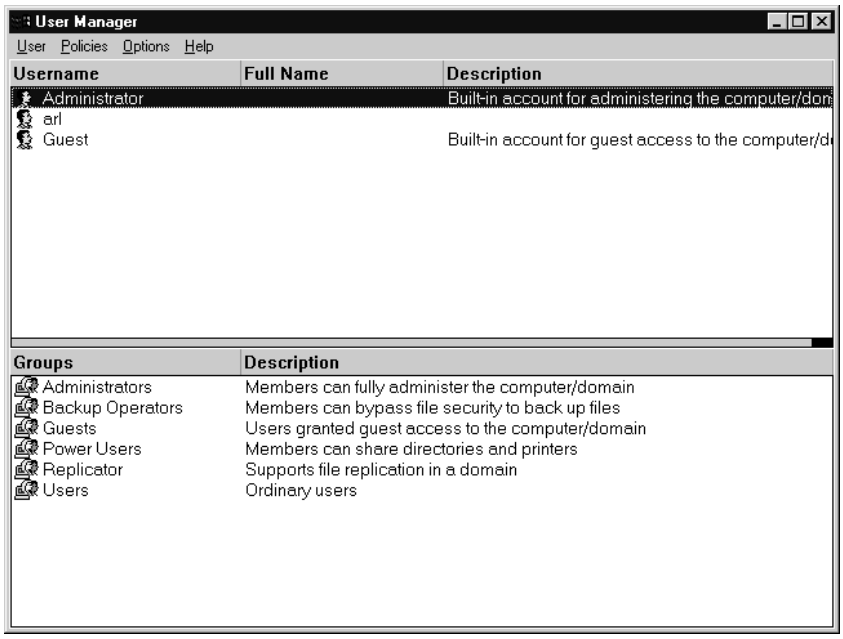
In order to create a new user account you must be logged on as a member of the Administrators group. Windows NT provides a default account for this. The User name is Administrator with no password as a default. In Windows NT there are a number of system management functions, including proper loading of software, that can only be done when logged on as a member of the Administrators group. We recommend that you change the default (that is, no password) to your own password.

Caution
Do not forget or lose track of this password. There is no way to retrieve it.

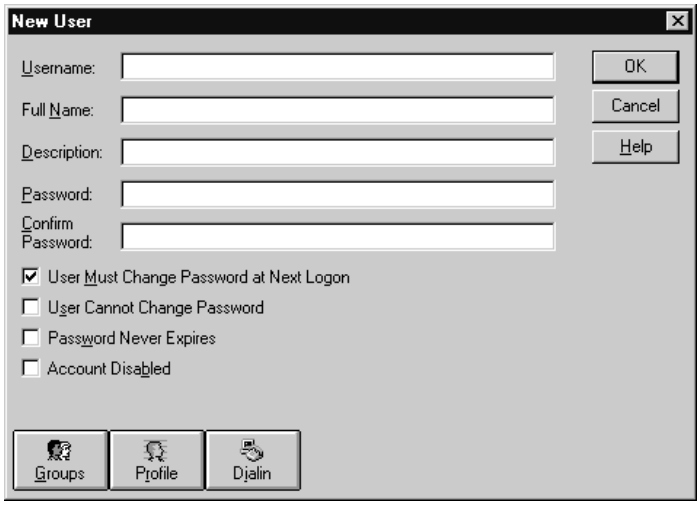
From the Task bar, select Start / Programs / Administrative Tools (Common) / User Manager.

The User Manager dialog box appears.

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Select New User... from the User menu. The New User dialog box appears.



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Username:	This is the name the user will log on under. It can be as many as 20 characters (upper or lower case). It cannot include **" / \ [ ] : ; | = > + * ? < >**. Username is case-insensitive.
Full Name:	The complete name of the user or the user account; it may be any length and include any character (optional).
Description:	A description of the user or the user account; it may be any length and include any character (optional).
Password:	A string of up to 14 characters. Password is case-sensitive. When the password is typed, it is not echoed on the screen; a string of the character ∗ is displayed, one for every character in the password.
Confirm Password:	Re-enter the password to make sure that it was entered correctly the first time. When the password is typed, it is not echoed on the screen; a string of the character ∗ is displayed, one for every character in the password.

User Must Change Password at Next Logon: typically, this is used in systems where the Administrator sets up the accounts but the policy is that the Administrator should not know the user passwords.

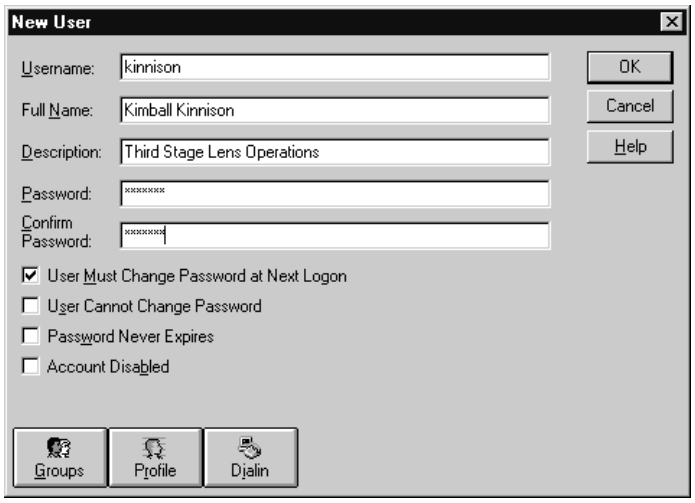
User Cannot Change Password: do not check this; it is not normally needed given the user pattern for this type of computer.

Password Never Expires: clear this (unselected) if you want to force the a user to change passwords regularly. This generally increases security for that account.

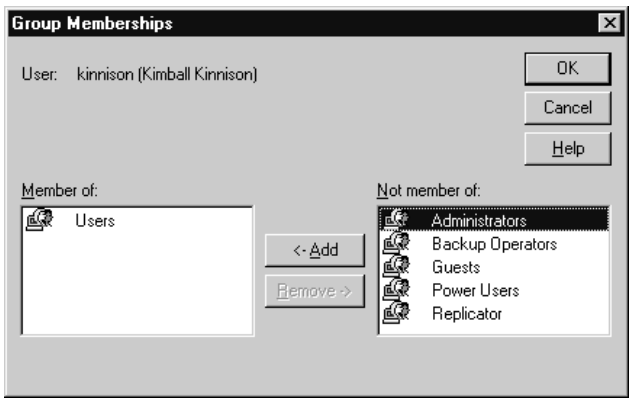
Account Disabled: do not check this. This is normally used to lock out a user prior to a possible deletion of the account.

In this example, the New Users dialog box looks like this:

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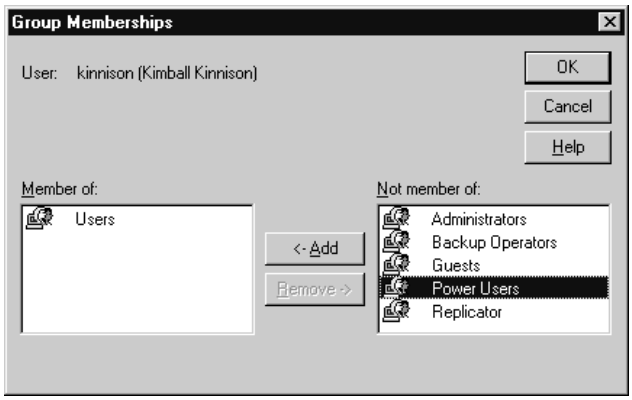
Click the Groups button. The Group Memberships dialog box appears.



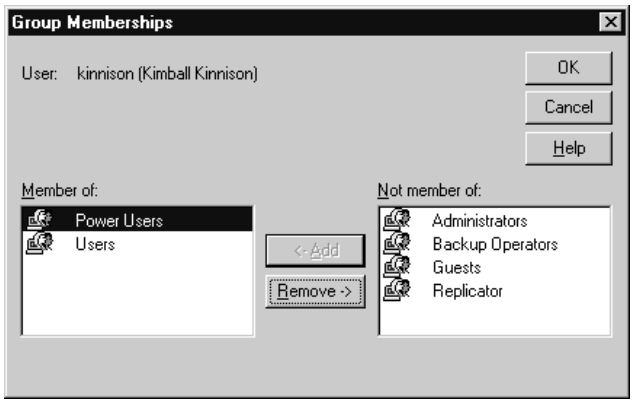
All accounts are members of the Users group. Add Power Users group by

1. Highlight Power Users in the Not member of: box.

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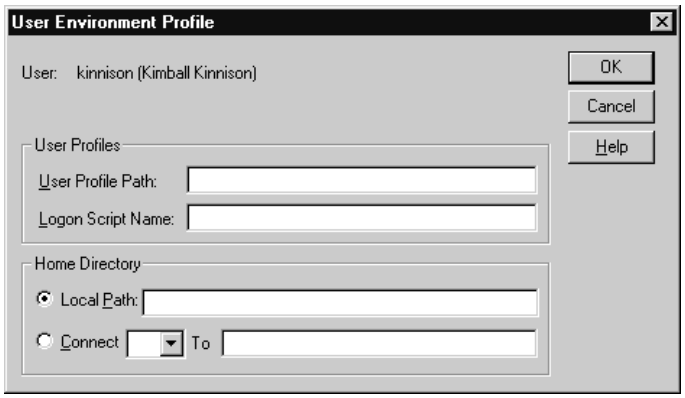
2. Click the <-Add button.



Power Users is now moved to the Member of: box. Sites may define their own user groups with abilities to share certain files, etc. If the new user is to be a member of any of these groups they can be added now in the same way as Power Users.

When all groups have been added, click OK. You are returned to the New User dialog box. Click the Profile button. The User Environment Profile dialog box appears.

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User Profile Path: an optional network pathname. This allows the administrator to establish a mandatory user profile on a server. See the Windows NT documentation for details.

Logon Script Name: the name of a batch file (.CMD or .BAT) or an executable file (.EXE) that is to be run when the user logs on. These files are normally stored in the directory c:\winnt\system32\repl\import\scripts. More than one user can have the same logon script.

Note

User Manager does not check to see if the logon script actually exists. If the specified logon script does not exist at logon, the log on process will continue. No message will be sent to the user.

Home Directory: creates the user's default directory. This directory is the default for File Open, Save As, and for other applications where the directory is not otherwise specified. More than one user can have the same home directory. If you use the variable %username% as the final directory in the home directory pathname, it will have the same name as the user's name. In the example above, that would be kinnison. We recommend that you use c:\users\%username% as a default.

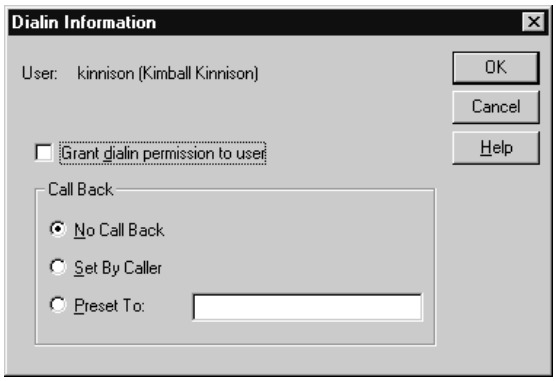
Notes

User Manager does not check to see if the home directory actually exists. If the specified home directory does not exist at log on, Windows NT will create this directory.

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If no home directory was specified, the user is assigned users\default as the home directory. This directory is on the same device as Windows NT.

Click OK; this returns you to the New User dialog box. Click the Dialin button. The Dialin Information dialog box appears.



Grant dialin permission to user: select if you want to permit this user to dial in to the system.

Call Back: specify type of system callback.

No Call Back: disable callback.

Set By Caller: system prompts user for callback telephone number.

Preset To: system calls back only to telephone number entered in this box. This is recommended for highest security.

Click OK: this returns you to the New User dialog box.

Click OK to create the new user account.

If the passwords do not match you will get this status box.

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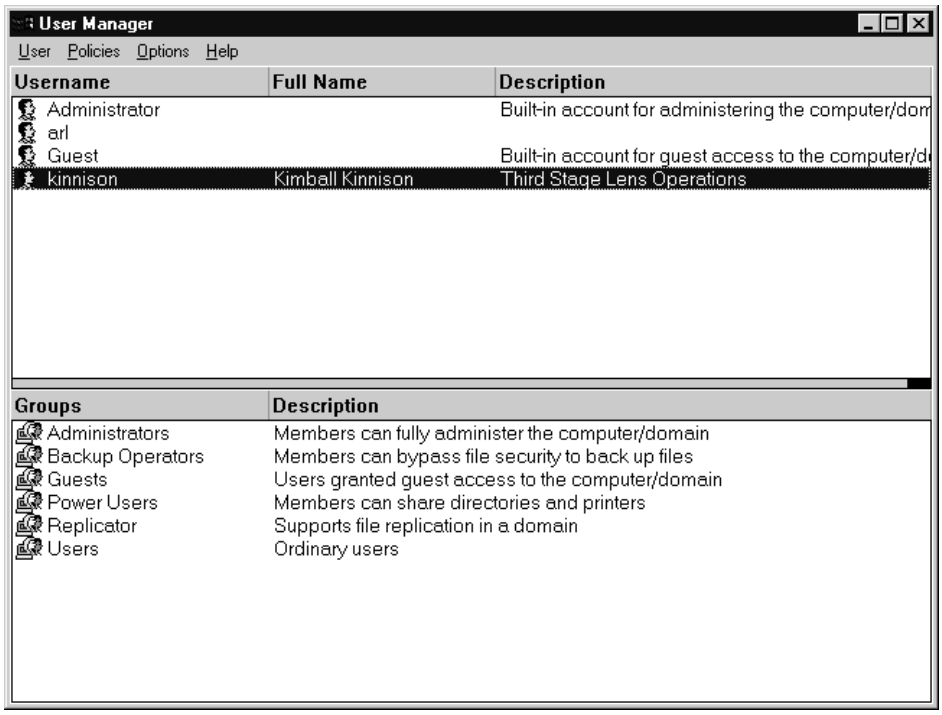


Re-enter the password and the confirmation. Then click OK again. This returns you to the User Manager dialog box. You can add more user accounts or close the dialog box.

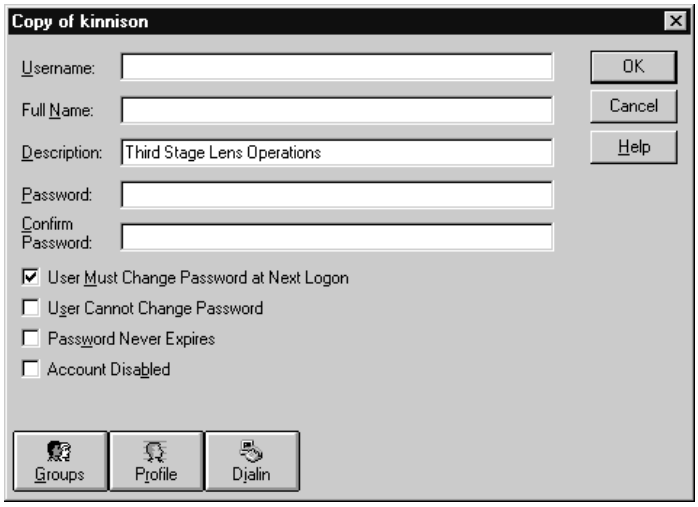
USER COPY

If you want to add a number of users with the same Groups and Profiles, highlight the user who is to be copied for example, kinnison).

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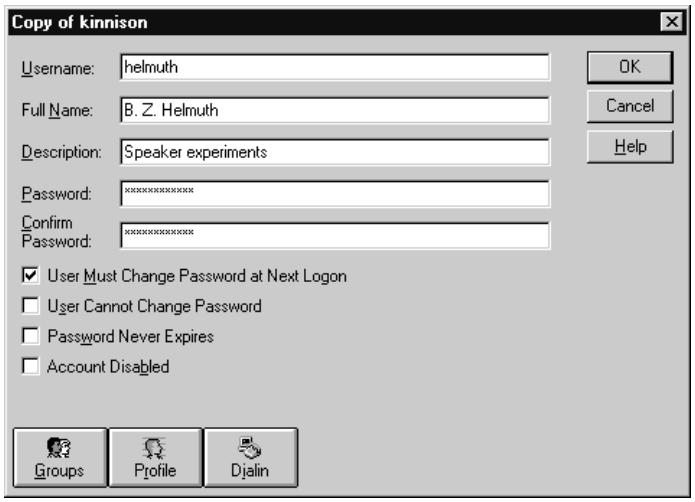
Select Copy... from the User menu. The Copy of kinnison dialog box appears.



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This prepares a template for a new user with the same Groups, Profile, and Description as the original user (kinnison).

Enter the desired Username and Full Name. Enter and confirm the Password; select the password options as described above. If desired, you can change the Groups, Profile, and Description. For example,



Click OK to create this user account and return to the User Manager dialog box. You can continue to create new user accounts or close this dialog box.

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B
Default Color Settings

Colors for most of the objects that appear on the Win-IR Pro screen can be set using Edit Color from the Options menu. The default factory settings are listed in this appendix. At release 2.3, unused objects in Pens (Global Graph, Peak Region, and Background) and Brushes (Region) were removed from Edit Color.

PEN

OBJECT	USE	RED	GREEN	BLUE
Crosshair	Points for unselected spectra on quantitation calibration curves	255	255	0
Drop Points	Unselected points on a correction baseline	255	255	0
Baseline	Correction baseline	0	0	255
Peak	Exact location of trace peaks	240	86	43
ZoomBox	In the radar box: the outline of the area being selected to fill the trace display	255	0	0

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Spectrum 5	Spectrum displayed, but not selected	170	0	70
Spectrum 4	Spectrum displayed, but not selected	255	200	255
Spectrum 3	Spectrum displayed, but not selected	255	255	0
Spectrum 2	Spectrum displayed, but not selected	0	0	255
Spectrum 1	Spectrum displayed, but not selected	255	0	0
Active Spectrum	Selected spectrum	32	255	64
Non-Editable Selected	Quantitation plot	255	255	255
Region Line	Dashed vertical lines showing extent of region	0	0	0
Ticks	On x- and y-axes	255	0	0
Aperture	Microscope mapping	255	255	255

BRUSH

OBJECT	USE	RED	GREEN	BLUE
Background	Background for trace and quantitation plots	0	128	128
Control Point	Selected point on a correction baseline	255	255	255
Peak	Area under dropped peaks	32	255	64
Stage Tracker	Microscope mapping	255	255	255
Collected Point	Microscope mapping	0	255	0
Target Collection Point	Microscope mapping	255	0	0
Aperture Handles	Microscope mapping	255	255	255

TEXT

OBJECT	USE	RED	GREEN	BLUE
Peak Label	Wavenumber of dropped/picked peaks	255	255	255
Trace Label	Name/type of data displayed	255	255	255

Objects in *italic* are specific to microscope mapping.

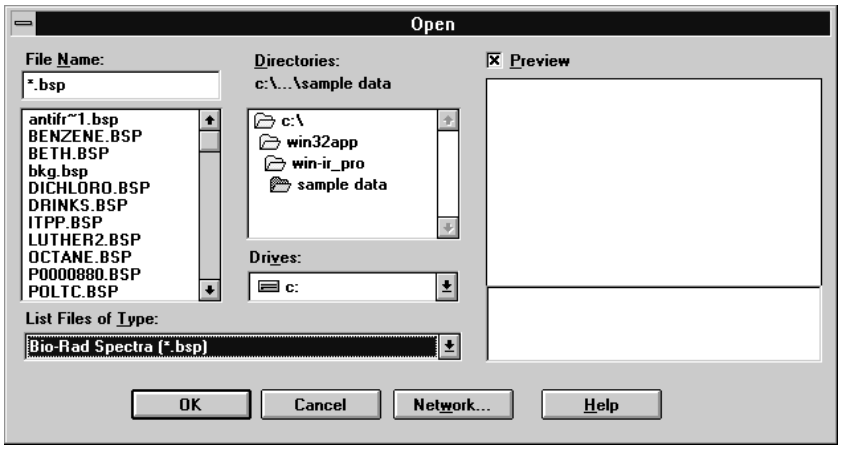
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C
Importing Spectra

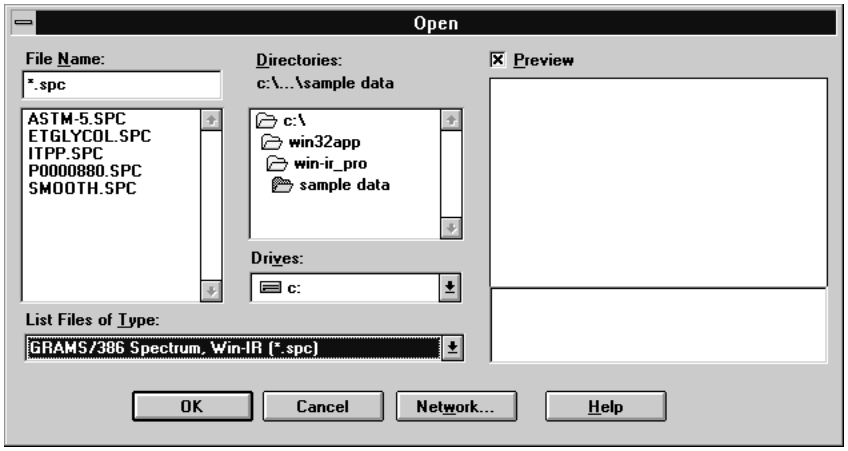
WIN-IR AND GRAMS/386 SPECTRA

Win-IR and GRAMS/386 spectra are identified by their .spc extension. These spectra were collected on spectrometers controlled by the Win-IR or GRAMS/386 software running on a PC. The files containing these spectra can be copied via disk, tape, over a network, etc. to your PC and placed in a directory. To open these spectra, select Open from the File menu. The Open dialog box appears.

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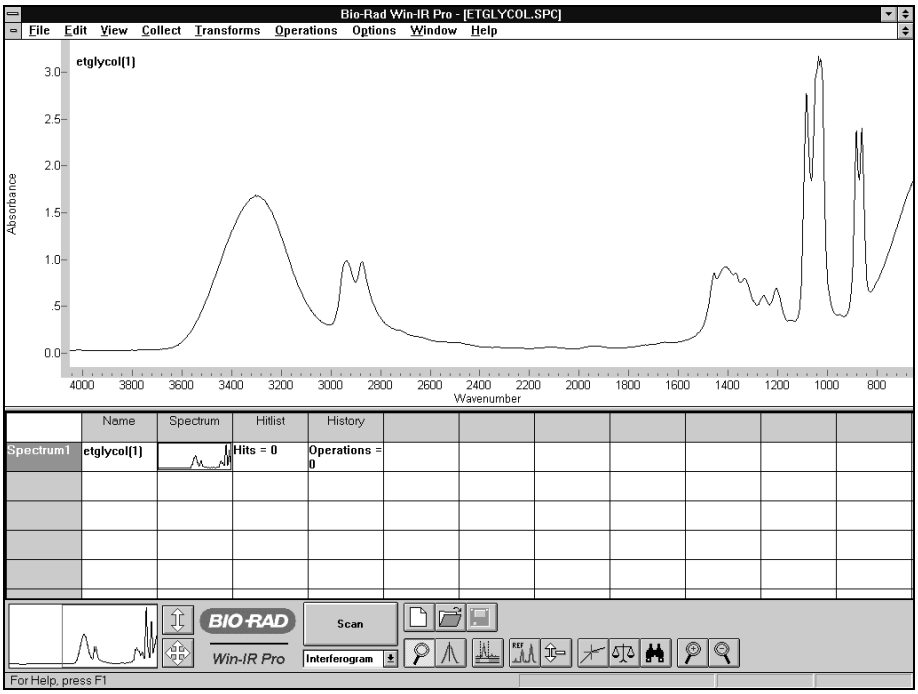


Select Grams Spectrum, WinIR (*.spc) from the List Files of Type pull down menu. A list of files of these types appear. You can change drives to access these files or use the Network button to connect to other drives on your network.

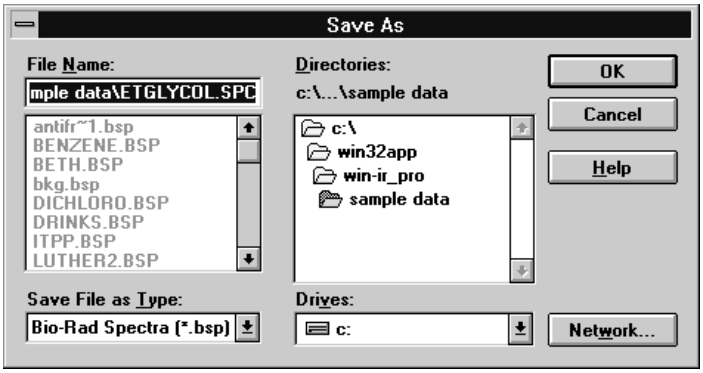


Select the desired spectrum and open it by clicking the OK button.

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Convert the spectrum to Win-IR Pro format by selecting Save As... from the File menu. The Save As dialog box appears.



1. Make sure the Save File as Type is set to Bio-Rad Spectra (*.bsp).
2. Select the desired directory.
3. Type an appropriate name for the spectrum in the File Name box.

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4. Click the OK button. The spectrum is converted to Win-IR Pro format and saved on the disk.

Note

Multifiles (*.spc containing multiple spectra) are imported in the same manner as files with a single trace. Subfiles can also be previewed, locally or over the network.

BIO-RAD 3200 SERIES SPECTRA

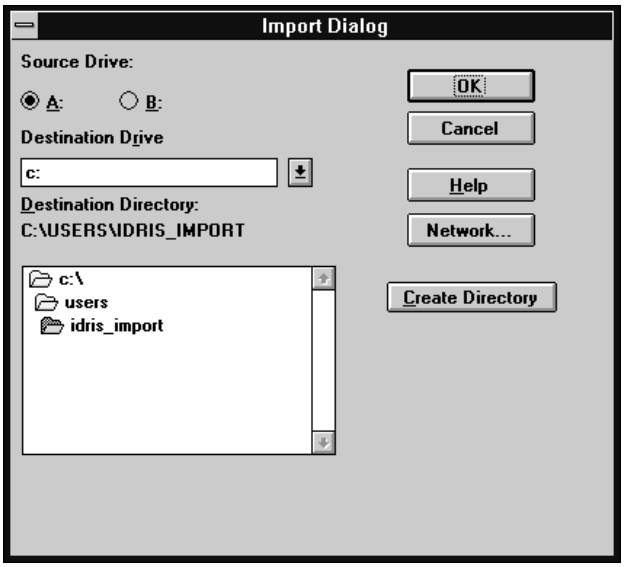
The Idris_Import application allows you to convert data directly from 3.5-inch 3200 series data disks. You do not need to use a 3200 series computer. It imports all the contents of a 3200 disk; it is not possible to preview the disk contents, or to select individual files to import. However, after importing the files, you can choose to delete those that are not of interest.

Importing 3200 Series Spectra to the PC

1. Insert the 3.5-inch 3200 series data disk in your disk drive.
2. From the Task bar, select Start / Programs / Win-IR_Pro (Common) / Idris_Import. The Idris_Import Windows Application window appears.

3. Select Import... from the Import menu. The Import Dialog box appears.

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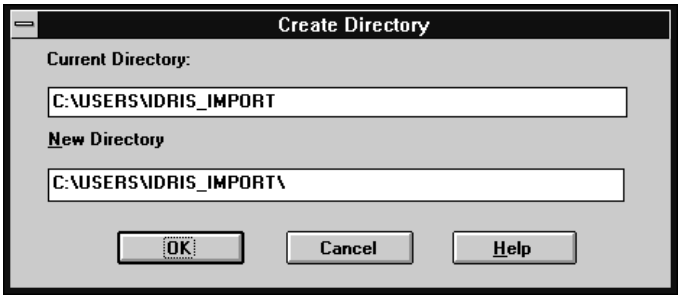


4. Set the values in this dialog box.

Source Drive: select either A or B depending upon which drive holds the 3200 series data disk.

Destination Drive: use the standard Windows techniques to select a destination drive and directory in which all the spectra on the source disk will be stored. Use the Network button, if necessary, to connect to a network disk.

Create Directory: if a new directory is desired in which to store the converted files, click this button. The Create Directory dialog box appears.



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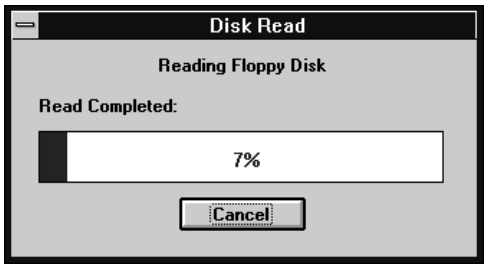
Type the pathname of the desired new directory and click the OK button.

5. Click the OK button to convert all the data files on the 3200 series data disk, store the converted files in the Destination Drive directory with a .dt extension, and return to the Idris_Import Windows Application window.

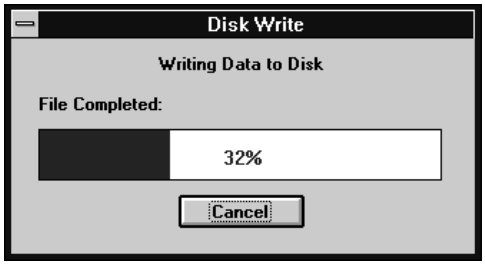
   If you click Cancel:, you return to the Idris_Import Windows Application window without converting the 3200 series data files.

   If you click Help:, you enter the on-line Help system.

   First, Idris_Import reads the files from the floppy disk into memory. It reports its progress in the Disk Read status box.



   Then, it writes the converted files in the Destination Drive directory with a .dt extension. . It reports its progress in the Disk Write status box.



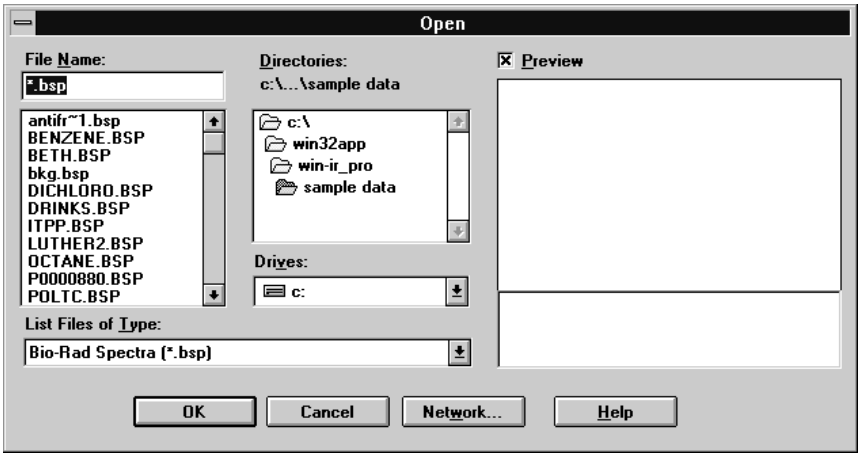
6. Repeat as desired for other 3200 series data disks.

7. Select Exit from the Import menu to leave the application.

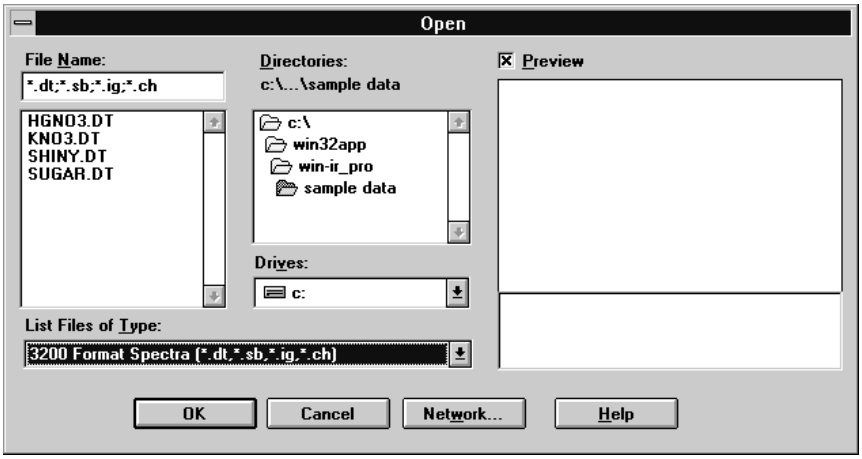
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Converting 3200 Format Spectra to Win-IR Pro Format Spectra

Select Open from the File menu. The Open dialog box appears.

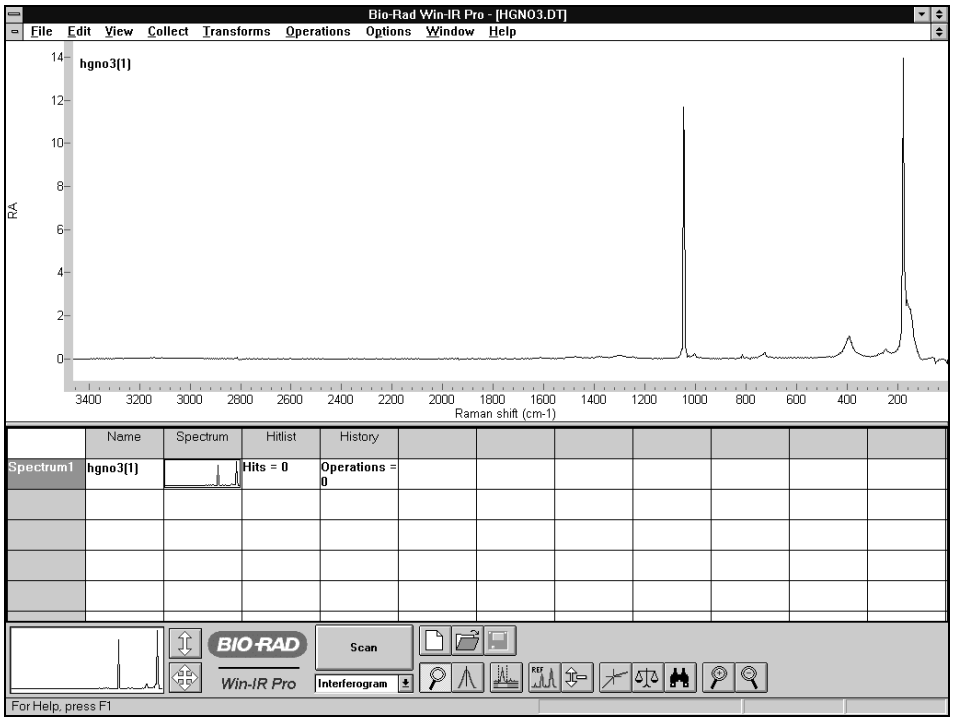


Select 3200 Format Spectra (*.dt,*.sb,*.ig) from the List Files of Type pull down menu. A list of files of these types appear. You can change drives to access these files or use the Network button to connect to other drives on your network.

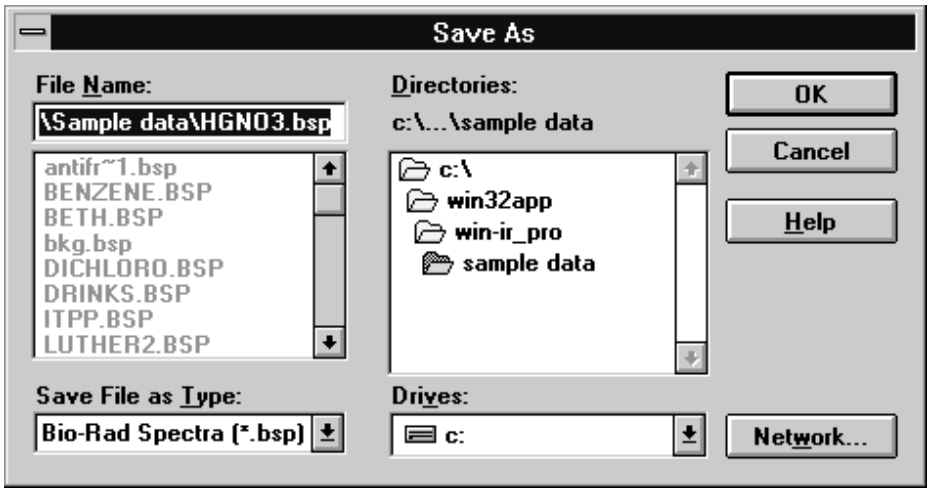


Select the desired spectrum and open it by clicking the OK button.

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Convert the spectrum to Win-IR Pro format by selecting Save As... from the File menu. The Save As dialog box appears.



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1. Make sure the Save File as Type is set to Bio-Rad Spectra (*.bsp).
2. Select the desired directory.
3. Type an appropriate name for the spectrum in the File Name box.
4. Click the OK button. The spectrum is converted to Win-IR Pro format.

Note

Multifiles (.dt) and chromatograms (.ch) are imported in the same manner as files with a single trace; GC measurements are a typical example of this. Subfiles can also be previewed, locally or over the network.

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D
Algorithms and Functions

SEARCH ALGORITHMS

The equations used to calculate the hit quality index (HQI) are shown below, where:

HQI_i	hit quality index for library entry *i*
U_w	value of the unknown spectrum at wavenumber *w*
$\|U_w\|$	absolute value of U_w
dU_w	first difference of the value of the unknown spectrum at wavenumber *w*
$\|dU_w\|$	absolute value of dU_w
L_{iw}	value of library entry *i* at wavenumber *w*
$\|L_{iw}\|$	absolute value of L_{iw}
dL_{iw}	first difference of the value of library entry *i* at wavenumber *w*
$\|dL_{iw}\|$	absolute value of dL_{iw}
$\|U\|^2$	$\Sigma_w (U_w)^2$
$\|L_i\|^2$	$\Sigma_w (L_{iw})^2$

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Euclidean: this is the fastest algorithm; if it is used, then Baseline correct should be selected.

$$(HQI)_i^2 = \sum_w \left(\frac{U_w}{|U|} - \frac{L_{iw}}{|L_i|} \right)^2$$

Absolute value:

$$(HQI)_i^2 = \sum_w \left(\frac{|U_w|}{|U|} - \frac{|L_{iw}|}{|L_i|} \right)$$

Derivative:

$$(HQI)_i^2 = \sum_w \left(\frac{dU_w}{|U|} - \frac{dL_{iw}}{|L_i|} \right)^2$$

Abs. Value Deriv.:

$$(HQI)_i^2 = \sum_w \left(\frac{|dU_w|}{|U|} - \frac{|dL_{iw}|}{|L_i|} \right)$$

Correlation: similar to the Euclidean algorithm except that both the unknown spectrum and the library entry values are measured from their respective means. This should remove any constant bias from either the unknown or the library entry. Masking is applied before the means are calculated to prevent any contributions from masked points to the final HQI.

$$(HQI)_i^2 = \sum_w \left(\frac{\overline{U_w}}{|\overline{U}|} - \frac{\overline{L_{iw}}}{|\overline{L_i}|} \right)^2$$

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where

n	number of points in the unknown/library entry
$\overline{U_w}$	$U_w - \Sigma_w (U_w)/n$
$\overline{L_{iw}}$	$L_{iw} - \Sigma_w (L_{iw})/n$
$\lvert\overline{U}\rvert^2$	$\Sigma_w (\overline{U_w})^2$
$\lvert\overline{L_i}\rvert^2$	$\Sigma_w (\overline{L_{iw}})^2$

APODIZATION FUNCTIONS

In data collection the interferogram is sampled over a finite distance. Information that would be present at a larger distance (greater retardation) from the centerburst is lost. This causes a distortion in the shape of the narrow lines because the information for these lines was truncated at the limit of resolution. This is usually noticeable only for gas spectra. Apodization is a method to control the line shapes; this causes some decrease in resolution. Apodization is also a part of transforms such as deconvolution, filtering, etc.

Boxcar

The boxcar apodization function is of the form:

$$1 \quad for \quad -\Delta \geq \delta \geq \Delta$$
$$0 \quad for \quad \delta > |\Delta|$$



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It gives the narrowest peaks (FWHH-full width at half height) of any of the functions. However, it also introduces more sidelobes than other apodization functions. This can cause problems as the sidelobes can overlap bands in gas phase spectra.

Norton-Beer

The Norton-Beer apodization functions are of the form:

$$\sum_{i=0}^{n} C_i \left[1 - \left(\frac{\delta}{\Delta} \right)^2 \right]^i$$

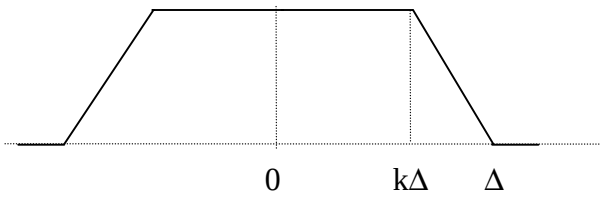
Normally, n = 3. The coefficients for the three preferred functions are:

	C_0	C_1	C_2	C_3
Norton-Beer weak	0.348093	-0.087577	0.703484	0
Norton-Beer medium	0.152442	-0.136176	0.983734	0
Norton-Beer strong	0.045335	0	0.554883	0.399782

Trapezoid

The trapezoidal apodization function combines the boxcar with the triangular. If $D(\delta)$ is the boxcar function (see above) and $k\Delta$ is the point at which the triangular portion of the function begins, then the trapezoidal function takes the form:

$$\left(\frac{1}{1-k} \right) D(\delta) \left[1 - \frac{\delta}{\Delta} \right] - \left(\frac{k}{1-k} \right) D\left(\frac{\delta}{k} \right) \left[1 - \frac{\delta}{k\Delta} \right]$$



Usually k is taken to be 0.5; in this case, the equation reduces to:

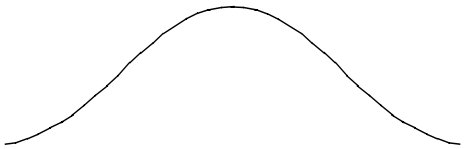
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$$2D(\delta)\left[1-\frac{\delta}{\Delta}\right]-D(2\delta)\left[1-\frac{2\delta}{\Delta}\right]$$

Happ-Genzel (Hamming)

The apodization function is of the form:

$$0.54+0.46\cos\left(\frac{\pi\delta}{\Delta}\right)$$



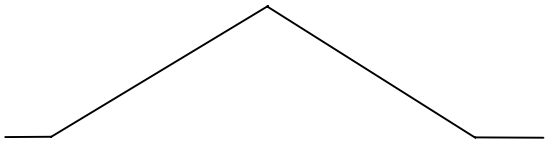
The FWHH and ILS functions given by this apodization are similar to those given by the triangular function. The Happ-Genzel apodization gives a larger first side lobe than the triangular function; however, the second and subsequent side lobes are smaller than for the triangular function.

Triangle

The apodization function is of the form:

$$1-\left|\frac{\delta}{\Delta}\right| \quad for \quad -\Delta \le \delta \ge \Delta$$

$$0 \quad for \quad \delta > |\Delta|$$



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PHASE CORRECTION

The phase correction is used in calculated the single-beam spectrum from the interferogram. In the phase-correction method of L. Mertz, the instrument phase is calculated by computing a low-resolution array of points selected symmetrically about the centerburst, generating an array of complex values. Each of these complex values has a unique phase angle in the range 0 to 2π.

A symmetric array is used so that the apodization function is even, and has zero phase.

The phase angle itself is not calculated. Calculating the phase angle directly

$$\theta = \arctan (R/I)$$

can lead to ambiguity as to which quadrant the angle is in. For example, the equal ratios

+R/+I + = -R/-I could be in the first or third quadrants and

-R/+I + = +R/-I could be in the second or fourth quadrants

where R and I are the real and imaginary parts.

Instead the unit vectors (**R_p'** and **I_p'**) are calculated and saved for later stored phase calculations

$$\mathbf{R_p'} = \mathbf{R_p}/\sqrt{(R_p^2 + I_p^2)}$$

$$\mathbf{I_p'} = \mathbf{I_p}/\sqrt{(R_p^2 + I_p^2)}$$

R = real part; I = imaginary part; $_p$ = phase.

Phase correction can now be considered to be a vector rotation (subtraction of the phase angle) in Cartesian space.

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The results of the full resolution spectrum Fast-Fourier Transform (FFT)—R_S and I_S—are rotated to give the final phase-corrected results (R_f and I_f), that is,

$$\mathbf{R_f} = R_S\mathbf{R_p'} + I_S\mathbf{I_p'}$$

This implementation allows phase correction to be performed on complex data entirely in the Cartesian co-ordinate domain, without time-consuming operations like computing transcendental functions such as arctan(x), which have singularlities and are single-valued only for $\pm\pi/2$.

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E
Hardware Configuration

Before you are able to collect data, you must configure the hardware. This tells Win-IR Pro what hardware is installed on the optical bench.

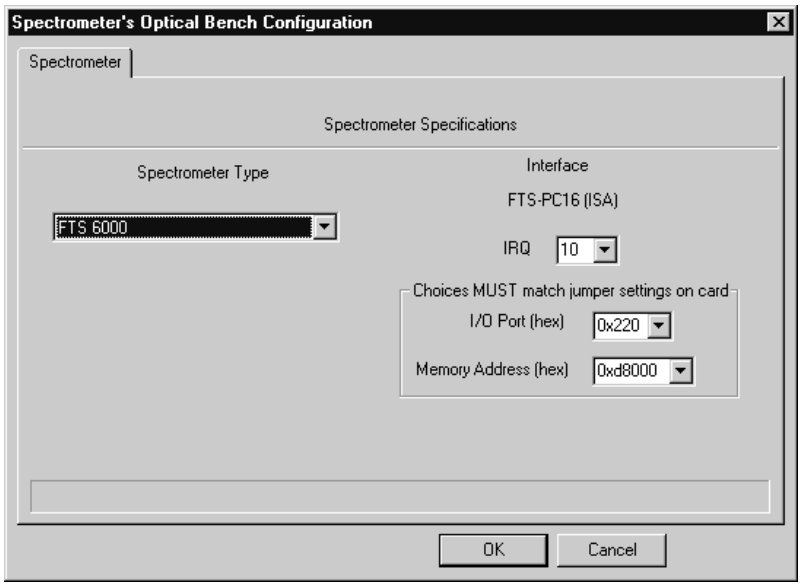
1. If Win-IR Pro is running, Exit from it.

2. Select Start / Settings / Control Panel from the Task bar.

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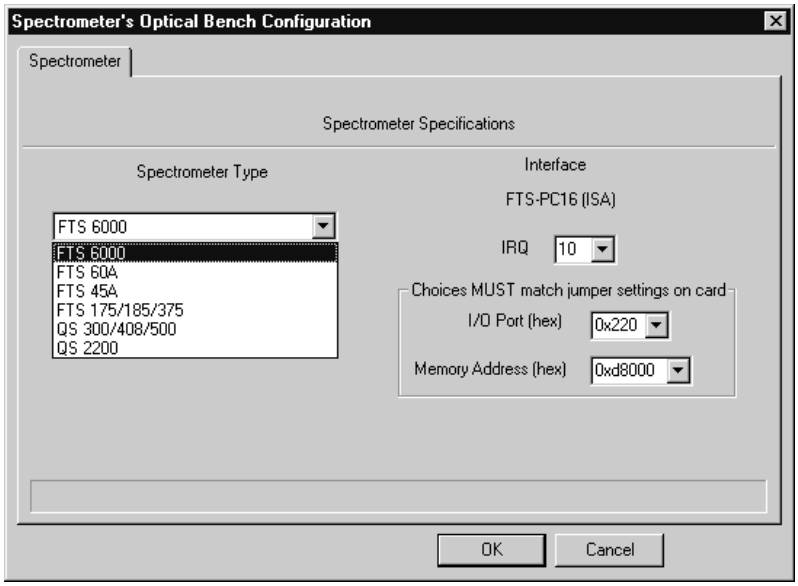


3. Double click the Spectrometer icon. The Spectrometer's Optical Bench Configuration dialog box appears.



4. Select the spectrometer that you are using from the pull-down menu.

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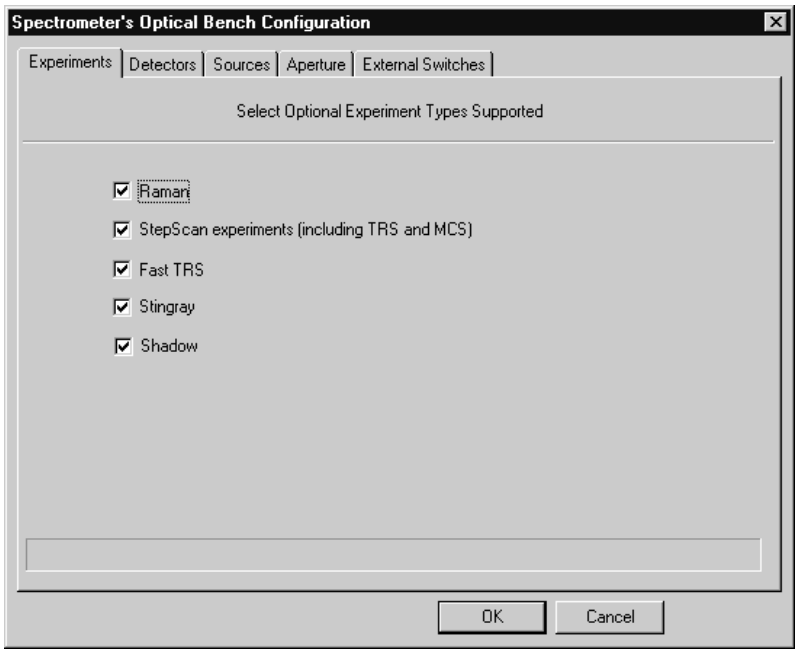


Note

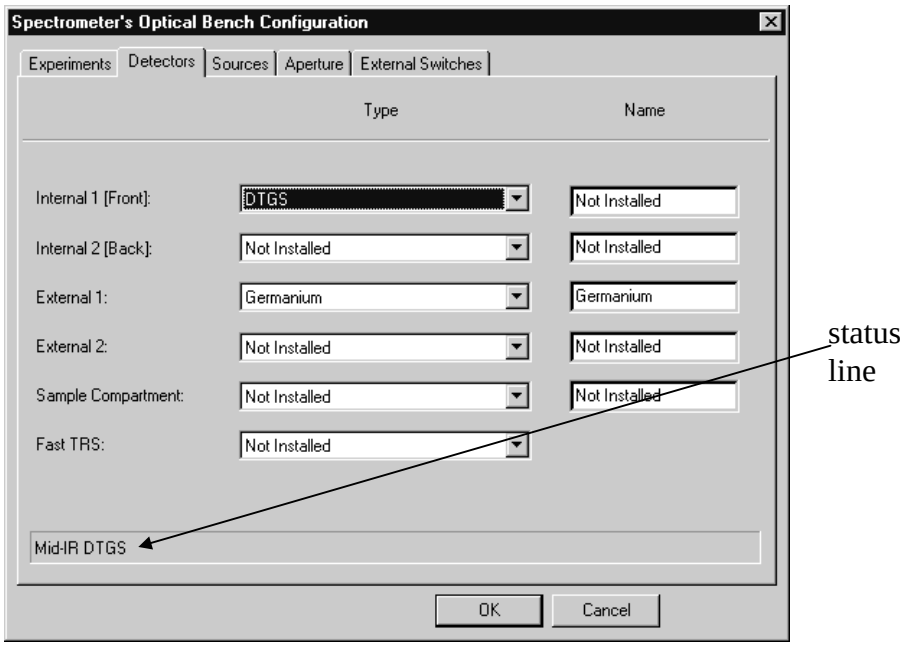
The Interface feature is designed for use by Bio-Rad Customer Service; do not change the default settings unless directed to do so. It is possible to change the IRQ of the spectrometer controller card to any value from 10 to 15 if there is an IRQ conflict with another card. If you change the jumper settings on the spectrometer control card (for I/O Port and/or Memory Address), you must also change these values using the pull-down menus on the dialog box. In general, you should not change these values.

The example below uses the FTS 6000. The configuration tab pages may be somewhat different for other spectrometers.

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5. Click the Detectors tab to see the Detectors tab page.



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6. Use the pull-down menus to select the Type of detector at each location. When you select a detector type, additional information about that detector appears in the status line.

Note

Not all spectrometers have provision for detectors at all locations.

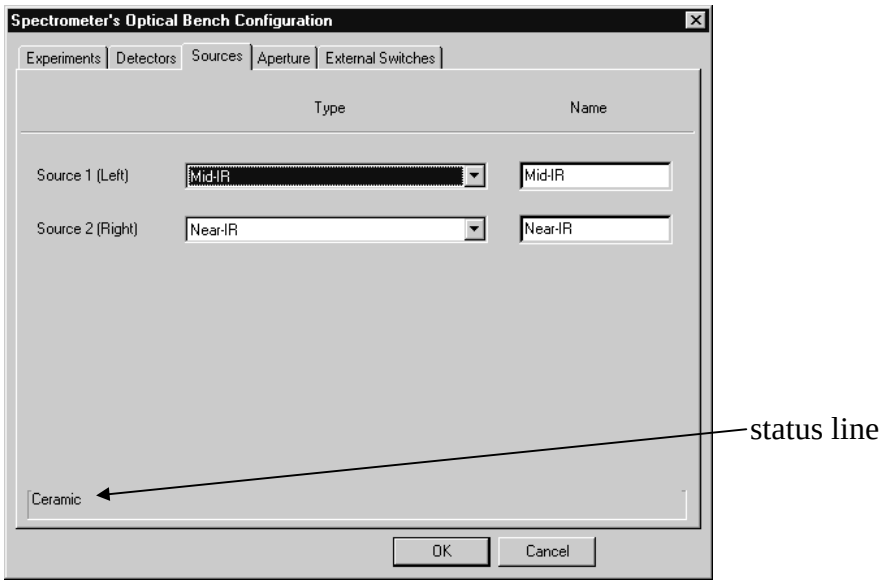
7. In the right-hand (Name) box, type a brief, meaningful description of the detector; for example, GC, microscope, etc. This description will then appear in the Optics tab page when you select one of the scan entries from the Collect menu.

8. Click the Sources tab to see the Sources tab page.

9. Use the pull-down menus to select the Type of source at each location. When you select a source type, additional information about that detector appears in the status line.

Note

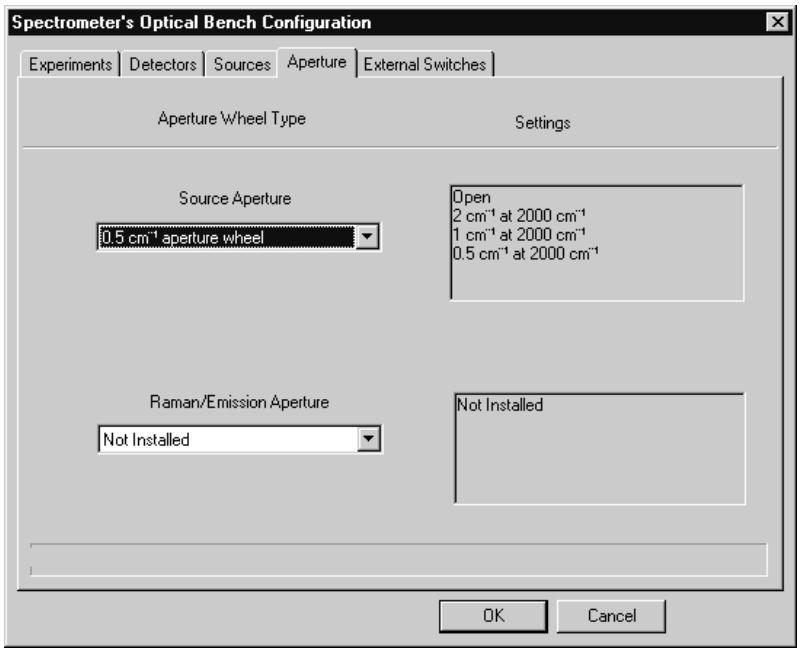
Not all spectrometers have provision for dual sources.



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10. In the right-hand (Name) box, type a brief, meaningful description of the source; for example, Ceramic, far-IR, etc. This description will then appear in the Optics tab page when you select one of the scan entries from the Collect menu.

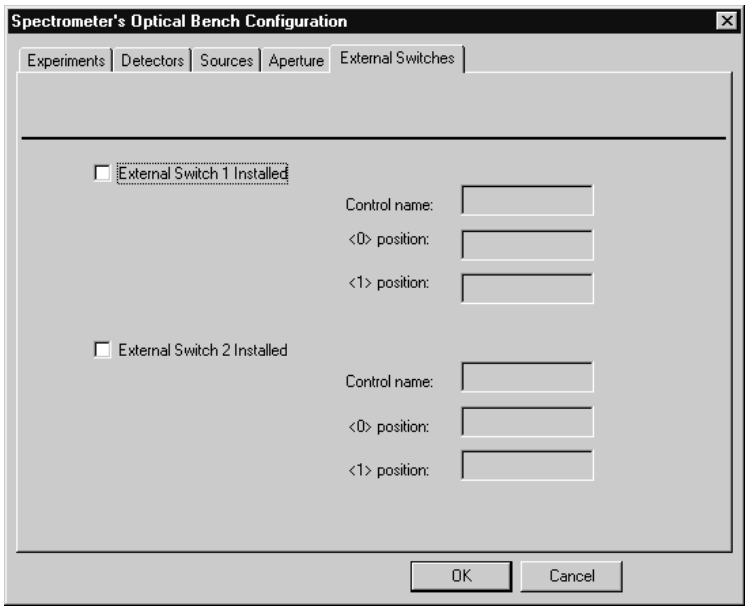
11. Click the Aperture tab to see the Aperture tab page.



12. Use the Source Aperture pull-down menu to select the aperture that is installed in your spectrometer. If you have a Raman or Emission experiment aperture, select it from the Raman/Emission Aperture pull-down menu. . This information will then appear in the Optics tab page when you select one of the scan entries from the Collect menu.

13. Click the External Switches tab to see the External Switches tab page.

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14. Enter the appropriate information in the boxes if you have external switches installed.

15. Click OK to register these values and return to the Control Panel program group. Cancel returns to the Control Panel program group without registering any change to the values.

    If you have made any changes the Optical Bench Configured message box appears.



16. Close the Control Panel program group.

17. Select Start / Shut Down from the Task bar.

18. Reboot the system. You can now run Win-IR Pro.

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F
3200 Series Spectrometer Parameters

If you import spectra collected from the Bio-Rad 3200 series spectrometers, the header elements will be available through View / Property Browse Bar. The meaning of these is given in the table below.

A_SYM	The type of interferogram originally collected—either symmetrical double-sided) or asymmetrical (single-sided)
apt	Aperture value (in cm^{-1}) or NI (not installed).
beam	Beam destination.
created	Date of creation of the file whose trace is displayed.
det	Detector.

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ELWN	Wavenumber of the He-Ne alignment laser (in cm^{-1}).
FSTAT	File status is either GOOD or BAD. BAD means the function executed incompletely or failed.
grr	The gain ranging radius in points around the centerburst.
ID	Win-IR Pro identification of this spectrum within this document. This is the entry in the left-hand column.
PKLOC	Position, in points, of the centerburst of the interferogram.
RES	Scanning resolution (in cm^{-1}).
SCANS	Number of co-added data collection scans.
sen	Amplifier gain.
SpectName	Name of the spectrum; this is the same as the entry in the default Name column. The entry in this cell is displayed as the label for the active trace.
speed	Scanning velocity (in KHz).
TYPE	Type of spectrum: absorbance, transmittance, etc.
UDR	Undersampling ratio.
xlabel	Label for the X axis; the default is wavenumber.
YData	Display of the spectrum.
zff	Zerofilling factor.

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G
Win-IR Pro File Extensions

The file extensions used in the Win-IR Pro software are listed in the table below..

.bpt	Bio-Rad print composition template files, used to organize spectral information on a page for printing.
.brc	Bio-Rad-supplied library structure files.
.bri	Bio-Rad-supplied library index of spectra
.brp	Bio-Rad-supplied library peaks files.
.brn	Bio-Rad-supplied library name files.
.brs	Bio-Rad-supplied library spectra files. against which unknown spectra

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will be compared looking for matches. There are several different files that make up a library.

.bsm Bio-Rad Microscope Mapping spectra generated by Shadow Pro.

.bsp Spectral data collected from a spectrometer using the Win-IR Pro software, or other data converted and saved as the Bio-Rad Spectra format.

.bsq Calibration document used for simple quantitative analysis.

.cdf AIA data exchange files.

.clm Collect Method files that store scan parameters. The default storage directory is c:\Program Files\Win-IR Pro\MyExperiments.

.csv Spectral files that are in spreadsheet format (do not confuse this generic spreadsheet with the one in the lower half of the Win-IR Pro windows).

.dat Array image files.

.dat Sadtler library chemical structure files. These should not be opened using File / Open. [Not used within Win-IR Pro]

.dt Spectrum collected from a spectrometer using the Bio-Rad 3200 series software (DDS).

.dxf Data triads exported from three-dimensional views. These files can be opened by Autocad and compatible applications.

.idx Library index files—used by both Sadtler and Galactic libraries.

.ig Interferogram collected from a spectrometer using the Bio-Rad 3200 series software (DDS).

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.inf Sadtler library properties files. These are not converted and are not used in Win-IR Pro.

.ipk Sadtler library IR Peaks files.

.ipl Galactic library peaks files. These are not converted and are not used in Win-IR Pro.

.irf Sadtler SearchMaster files.

.isl Galactic library spectra files.

.ism Sadtler library IR spectra files

.itl Galactic library name files.

.kbg Background spectrum used for kinetics data collection.

.kin Set of related spectra (and optional analysis) obtained from kinetics data collection.

.lib Galactic library special files. These are not converted and are not used in Win-IR Pro.

.na Digilab 3200 library names files.

.nam Sadtler library names files.

.ni Digilab 3200 library names index files.

.pct The print template files that contain information about how a page should be formatted with information to be printed out.

.phs Phase array storage files.

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.pls	Calibration document used for PLS analysis. PLS is a separately purchased product.
.pv	Stores the values of the parameters used by Win-IR Pro when you log on to the computer.
.s1	Digilab 3200 library dual-resolution first spectra files.
.s2	Digilab 3200 library dual-resolution second spectra files.
.sb	Single-beam collected from a spectrometer using the Bio-Rad 3200 series software (DDS).
.seq	Raw data files (array image date).
.sl	Digilab 3200 library ordinary (single) resolution spectra files.
.spc	Spectral data collected from a spectrometer using Win-IR or GRAMS/386, or converted from other formats to GRAMS format
.txt	Sadtler library text files. These are not converted and are not used in Win-IR Pro.
.vpk	Sadtler library vapor phase peaks files. These are not converted and are not used in Win-IR Pro.
.vps	Sadtler library vapor phase spectra files. These are not converted and are not used in Win-IR Pro.

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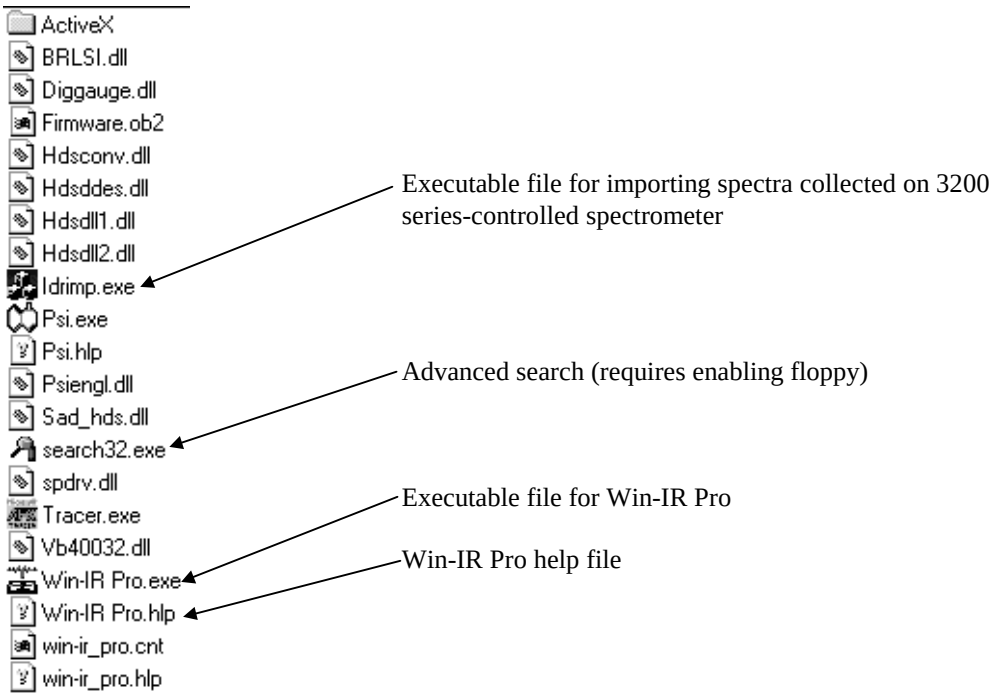
H
Win-IR Pro Files

Win-IR Pro files are normally installed on disk C in C:\Program Files\Win-IR Pro. The following directories are under C:\Program Files\Win-IR Pro.

Caution
The contents of these directories are altered by installations. Do not store your files in the Win-IR Pro directory or any of its subdirectories. Create your own directories for data storage.

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bin: contains the executable files and other files necessary to run Win-IR Pro.



Load history: contains records of the installation process. They are mostly of use to Bio-Rad Customer Service.

MyExperiments: contains the named collect method files.

Sample data: contains a number of spectra that you can copy and use to practice working with Win-IR Pro. Check the README.TXT file for late additions that are not included in the list below.

40BLNKNM.IG	Interferogram of sample for PAS linearization
40BLNKSY.IG	Interferogram of shifted sample
40GCREF.IG	Interferogram of reference for PAS linearization
8-IN.BSP	In-phase spectrum
8-QU.BSP	Quadrature spectrum
ABSPOLYS.BSP	Absorbance spectrum of polystyrene
ASTM-5.SPC	Polypropylene/Polyethylene film spectrum

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BENZENE.BSP	UV-Visible spectrum
BETH.BSP	
BKG.BSP	Background single-beam spectrum
DEFAULT.PV	default parameter values
DICHLORO.BSP	Gas phase spectrum
DRINKS.BSP	Spectra of two soft drinks containing sugar
ETGLYCOL.SPC	Ethylene glycol
HGNO3.DT	Raman spectrum of $HgNO_3$; .dt format
ITPP.BSP	Isotactic polypropylene
ITPP.CSV	Isotactic polypropylene
ITPP.SPC	Isotactic polypropylene
KINBACK.KBG	Kinetics background spectrum
KINETICS.IG	Kinetics interferogram
KINETICS.KIN	Kinetics spectra
KINETICS.SP	Kinetics spectra
KNO3.DT	Raman spectrum of KNO_3; .dt format
LUTHER2.BSP	Series of spectra of a time-varying event
P0000880.BSP	“noisy” GC/IR spectrum
P0000880.SPC	“noisy” GC/IR spectrum
pas2.bsp	Photoacoustical spectrum
POLYR.BSP	Spectrum of polystyrene
POLYS.BSP	Spectrum of polystyrene/polycarbonate resin
RAMAN.BSP	Raman spectrum of KNO_3 and $HgNO_3$; .bsp format
SHINY.BSP	A reflection spectrum
SMOOTH.SPC	
SPIKE.BSP	A spectrum with many high-frequency spikes
STRETCH.BSP	Spectra from polymer stretching experiment
SUGAR.DT	
SUGAR2.BSP	Original sugar/water spectra
SUGAR2.BSQ	Sugar solution calibration document

Scripting library: contains software and files necessary for the execution of the scripting language.

Note

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Scripting can only be used if you have purchased the optional scripting language (Bio-Rad part number 099-1856).

Scripting samples: contains a number of examples of scripts that you can copy and use for development of your own scripts.

ATRCorrect	Starts Win-IR Pro, opens a file and selects the first spectrum in that file. It then gets a copy of the data points in the spectrum using DataArray property. This array is transformed using an ATR Correction algorithm and passed back to Win-IR Pro.
HundredPercentLine	Collects two scans, ratios them, and presents the hundred percent line
Normalize	Starts Win-IR Pro, opens a file and selects the first spectrum in that file. It then gets s copy of the data points in the spectrum using DataArray property. This array is transformed by normalizing it between 0 and 1 and passed back to Win-IR Pro.
PeakAreaIntoExcel	Starts Win-IR Pro, opens a file and selects the first spectrum in that file. It then drops a peak and calculates its area. The area is pasted into a spread sheet cell after starting Excel, adding a workbook, and getting the first sheet.
ScanIntoOneFile	Starts Win-IR Pro, opens a file, collects a background and saves it. You can then collect a number of spectra (up to 5); they are ratioed against this background and all are saved in this file.
ScanIntoSeveralFiles	Starts Win-IR Pro, opens a file, collects a background and saves it. You can then collect a spectrum; it are ratioed against this background and are saved in this file. You can then collect another spectrum; it is saved in another file along with the previously collected background. The default in the script is to collect up to 5 spectra.
Transform	Starts Win-IR Pro, opens a file and selects the first spectrum in that file. It then performs the apodization transform on that spectrum. This template can be modified for other transforms.

Spectrometer Configuration: contains the files generated by, and required for, spectrometer configuration.

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I

Quantitative Analysis

For a good overview of the quantitative analysis process, including dealing with solid and gaseous samples, see Compton, Senja V. and Compton, David A. C., "Quantitative Analysis—Avoiding Common Pitfalls," *Practical Sampling Techniques for Infrared Analysis*, edited by Patricia B. Coleman, Boca Raton, FL: CRC Press, 1993.

Quantitative analysis methods cover, but are not limited to, spectral subraction, transmittance measurements of optical filters, library search comparisons, pathlength determinations, discriminate analysis, and the more traditional concentration reports based on direct or indirect application of the Beer-Lambert Law. In this appendix, the issues affecting this last form of quantitative analysis are addressed, although many of the topics discussed are applicable to the other methods[1].

[1] See "*Practical Sampling Techniques for Infrared Analysis,*" edited by P. B. Coleman, CRC Press, Boca Raton, FL, 1993, for a more in-depth discussion.

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GENERAL CONSIDERATIONS

Several important criteria need to be met prior to the numerical calculations needed for the reporting of quantitative results. First, the analyst must adequately define the quantitative problem under consideration. Some of the issues to be addressed are (but not limited to):

- How quickly do the results need to be reported?
- Who is to perform the analysis and what is his/her skill level?
- Where is the analysis to take place (environmental conditions)?
- How frequently does the analysis need to be performed?
- What is to be measured, in what units, and how precisely and accurately?
- What is (are) the expected concentration range(s)?
- Are there multiple suppliers for the components?
- Are there multiple production methods/facilities?
- Are any materials substituted for one another or added occasionally to adjust selected properties, such as pH?
- Does the material change with time?
- What consumables are to be used?

From the answers to these questions, a rough idea of the actual analysis requirements and procedure can be made—IR techniques eliminated due to lengthy analysis time, lack of operator skill level, or cost of equipment/consumables; suppliers from whom to get components; and the required range to be covered by the analysis.
Additionally, the analyst must become familiar with all the species present in the samples to be analyzed and their compatibilities with the materials/equipment that they come in contact with during analysis. Nothing can replace good laboratory practices nor the knowledge of general chemistry principles when analyzing samples. Such things as halide compound reactivity, water incompatibility, sample drying in inert spectrometer atmosphere, and chelating reactions to form metal complexes in accessories cannot be overlooked.

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CALIBRATION STANDARDS CONSIDERATIONS

The second step of a quantitative analysis problem is to "make-up" the standards to be used for the calibration of the quantitative analysis method. Ideally, the standards should come directly from the production facility so that they reflect the actual processing conditions. However, in most instances this is not feasible and they must be synthesized in the analytical laboratory. In all cases, the selection of samples to be used for a calibration must adequately cover the expected range variation(s). This means that the expected extreme concentrations (minimum and maximum) for each component must be included as extrapolation outside the calibrated concentration range is questionable. This does not mean that the entire range of possible concentrations (0-100% for each component) needs to be covered, unless that situation is expected to arise. Additionally, if the accuracy at the extremes of a range is important, the concentrations covered by the calibration samples must span a larger range than the expected concentration for that component. For example, if *c* is the expected concentration of a component. The range for the concentration can be expressed as *c+d* to *c-d*. For accuracy at the extremes of this range, the concentration range covered by the calibrations standards should be *c+1.5d* to *c-1.5d*.

The standards must be composed of linearly independent concentration data. Linear dependence exists in simple dilutions (multiples) of a single standard, where the components are in constant relative proportions to one another throughout the series, or in instances when the concentration of two or more components adds to a constant. In the first case, unless each component has an isolated unique infrared absorption band exhibiting no overlap with any other component, no interactions occur among the chemical species, and the samples are examined with a reproducible, known pathlength, the standards would be useless in the calibration of a working quantitative method as they would not describe the expected compositions of the sample to be analyzed. The second situation provides a case in which a plane is defined in space, that is, the sum of the concentration(s) is a constant. If this constant changes to a new value (for example, from 12% to 10% in a batch production) the analysis is not defined and extrapolation of the method to obtain a quantitative value is invalid.

When selecting samples to be used for calibration standards in a system composed of multiple species, at least two components should be at differing levels in each blend. Typically, this eliminates linearly dependent data sets. All component concentrations should be represented the same number of times in the calibration standards. This prevents a single component from dominating the spectral features used for quantitative

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measurements. Additionally, the standards should be composed of evenly separated concentration levels across the expected range to permit interpolation between data points in the calibration.

The system under study for quantitative analysis should be overdetermined. This is accomplished by recording the spectra of more standard mixtures than there are components in the system. The use of more data than is necessary reduces the effect of random errors. As a rule of thumb, two times the minimum number of standards is adequate. An additional advantage of this oversampling is that back-calculations can be performed which provide:

- an indication of the quality of the calibration (average error)
- a detection of perturbation in a system by determining one component less accurately
- a means of discovery for deviation from Beer's law at high concentrations
- an identification of a bad standard or poor measurement in the calibration set
- evidence for inappropriate selection of spectral regions for measurements.

In an exactly determined case where only the minimum number of standards have been used, a "perfect-fit" of the data with no insight into the "goodness" of the quantitative method exists.

The precision of the standard mixture compositions is generally better than the precision of the analytical system under development. The importance of significant figures cannot be stressed strongly enough. If the standards are prepared with concentrations good to only two significant figures, the values reported for each of the components in the final analytical report are good to only two significant figures. Information cannot be obtained where no real data exists. Additionally, if other analytical techniques are used to provide concentrations values for the standard samples, then the errors reflected in those measurements are incorporated into the infrared analysis.

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In a multicomponent analysis, the mutual interference of the spectra, not the number of components, is what is being measured. The components cannot be determined individually, but all must be determined together. Therefore it is extremely important to use the actual materials used in the formulation of the final product rather than ultrapure grades of the components. This also means that standards including alternative supplier sources of components must be prepared. The “impurities” in the components have specific infrared absorbances which contribute to the overall composite spectrum of a standard. If their contributions are not included in the calibration step, their absorbances cannot be compensated for in the measurements used to calculate concentrations.

Finally, the analysis should be tested frequently as part of a normal operating procedure to verify its validity. Reanalyze samples previously reported (assumes product stability) or analyze synthesized blinds (consisting of both in- and out-of-specification products).

Summary of Important Issues for Calibration Standards

- Actual production starting materials must be used in fomulation of standards
- Full expected ranges for each component must be incorporated
- Dilutions are not valid standards
- No constant concentrations for components or sums of components are allowed
- Even spacing of concentration levels across expected range is advised
- Variation of levels for at least two components in each standard minimizes linear dependence of data
- Same number of concentration variations for each component in standards prevents dominance by a single material
- Overdetermination (more standards than minimally required) reduces the effect of random errors
- Significant figures determine final reported analytical values
- Errors reflected in methods for concentration determination are incorporated into IR method

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ERROR SOURCES

Some of the most common sources of errors in preparing samples for examination, either calibration reference or quantitative analysis, are discussed below. The detection of a potential problem can often be made quickly and easily when every reference and each sample is examined in duplicate (two complete separate samplings) and then compared. This procedure minimizes random errors and verifies reproducibility in measurements. Additionally, multiple examinations verify the homogeneity of the material, insuring that the tiny portion used for the analysis is representative of the bulk.

Solvents

The use of solvents in preparation of a sample may introduce numerous problems.

First, it may cause a reaction to take place—intermolecular (for example, hydrogen bonding, aggregation, preferential conformation, or unfolding) or chemical (formation of a new species). This behavior can be detected by direct comparison (through overlay plots, spectral subtraction, etc.) of two or more reference standard spectra and observing any shifts in band frequencies or the appearance of new absorption bands. Another test is to place a sample in the spectrometer and acquire spectra at time intervals. Direct comparison of these spectra will reveal the presence of any species created by chemical reactions over time.

Second, dilution of a sample by a solvent may cause the presence of micelles, emulsions, suspensions or precipitates to be formed in the resultant solution. All these behaviors result in irreproducible data collection and preclude useful quantitative measurements.

Third, when a solution is examined, the sample vessel must be adequately sealed to eliminate evaporation of volatile species which would affect the overall reported concentration levels.

Fourth, it is important to verify that the solution does not have any entrapped gases (bubbles) as the pathlength of the sample would change in addition to the concentration of components (two variables).

Fifth, solvents typically contain a number of “impurities” which are purposely added for stability (for example, buffers). Variations in the concentrations of these species will

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contribute to the overall spectrum used for calibration or analysis. Additionally, the "impurities" may chemically react with the system under investigation by serving as a catalyst, binding as a complexing agent, reacting with creation of new chemical species, or binding to active sites.

Sixth, the use of volatile solvents for cleaning purposes (for example, washing internal reflection elements, liquid cells, spatulas, mortar and pestle, etc.) may leave residue following evaporation. One easy test to check for solvent volatility is to place some of the solvent onto an infrared transparent window and allow it to evaporate under the corresponding experimental conditions used for the analysis. A transmission spectrum collected through this window would record the spectral features of any interfering residue species.

Seventh, the use of solvent evaporation for sample preparation may cause residual solvent to be retained in the sample through incomplete evaporation (entrapment, adsorption to active sites, complex formation, etc.).

Eighth, water (atmospheric moisture) may be introduced into a sample by the cooling process resulting from the rapid evaporation of a solvent with a low boiling point (for example, ether, acetone, methylene chloride). The strong spectral features due to water cause significant interferences when making quantitative measurements. Additionally, chemical reactions may occur in moisture-sensitive samples.

Gases

It is extremely important to carefully control both the temperature and pressure when performing quantitative measurements upon vapor species. Absorption band intensities, widths (pressure broadening), and areas are dependent upon both of these conditions. The extinction coefficient of a species in terms of its partial pressure may be a function of the total pressure of the sample. It is highly recommended that samples be pressurized to 760 Torr with an inert gas (such as nitrogen) to minimize the effects of pressure broadening and be allowed to achieve thermal equilibrium following filling of the gas cell prior to any spectral measurments.

One problem encountered in trace-component analysis when using long-path gas cells is due to selective adsorption or desorption of materials from the cell walls. The cell should be evacuated and filled (or flushed with an inert gas) several times before a spectrum is recorded to erase the cell "memory".

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Compatibility of vapor species with the materials composing the gas cell should be known. Hydrogen fluoride and tungsten hexafluoride gases are extremely corrosive and require the use of specially designed cells as they attack most glass and halide salt surfaces. Many organics will attack the polymer O-rings used to seal some gas cells, resulting in leaks or the creation of new species from chemical reations. The use of grease for ground glass joints in manifold connections and stopcocks should be minimized, with selection of only heavy grease with low volatility. This is because it may selectively absorb some gaseous species (subsequently providing memory effects) or may appear in the recorded sample's spectrum as it volatile.

Polymers

Standard reference samples for polymers are typically difficult to obtain, due, in part, to slight variations in their formulations which may be attributed to the method used in their manufacture. Thus, a polymer generated from a copolymerization process will not exhibit identical features to that corresponding to a block polymer nor to one comprised of individual homopolymers, due to different bond formations (for example, crosslinking) and functional group environments (that is, with associations such as hydrogen bonding).

A polymer's crystallinity and stereochemistry is dictated by the reaction mechanism causing crosslinking a specific sites. Since catalysts (both organic and inorganic) are oftentimes used to control the reaction pathway to generate a specific molecular structure in the polymer, they contribute unique spectral features (including light scattering particles) to the composite spectrum of the sample. Thus, polymers prepared from different catalysts cannot be realistically analyzed by the same calibration method.

An additional issue concerning polymer formulations is the presence of trace additives such as UV inhibitors, antioxidants, flame reatardants, plasticizers, and antiozonants, which all exhibit spectral absorbances. Their variable concentration levels must be taken into account when recording the spectra used for calibration.

Films

One of the most difficult problems in making standard transmission measurements of a film is that in uniformity, both in sample thickness and homogeneity. Free-standing films should have their thickness reported as an average based upon several measurements taken across the film by a micrometer. Several spectra for each film

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sample should be recorded at different rotations in the beampath, with the quantitative results reported as an average from the measurements, in order to minimize the effects of nonuniformity in the sample pathlength.

Pressed films, prepared between the platens of a hydraulic press may require heat to allow for the deformation of the sample into a thin sheet. The temperature, length of exposure, and pressure must be carefully controlled to insure that the same physical and chemical state of the sample is achieved each time. Spacers can be used to insure that all the films are produced with the same thickness. In all instances, films should be taut and flat during examination, free of crevices and holes, and mounted without stretching, which would alter film thickness and introduce possible stress orientation.

Films cast from volatile solvents may contain additives (such as BHT, butylated hydroxtoluene) or other low volatility impurities. Spectral absorbances due the interloping species will adversely affect the development of any method or the analysis of samples. A spectrum for a “blank” of the residue remaining (if present) after solvent evaporation should be recorded to discover if any infrared active species is present. A variety of other problems may also arise when casting films from solvents - incomplete volatilization (retention) of the solvent, condensation of atmospheric moisture from rapid cooling during solvent evaporation, occurrence of polymorphism and formation of aggregated domains based upon evaporation rate, degradation (for example, oxidative decomposition) when applying heat to accelerate solvent evaporation, inclusion of entrapped bubbles (air or other gaseous species), or chemical reaction with the solvent used for dissolution.

The use of rolling to produce films offers several disadvantages—carryover contamination from previous samples due to incomplete cleaning, difficult reproducibility in temperature and pressure parameters, possible evaporation of volatile materials, and irreproducible orientation effects may be introduced into the final film. If a method is developed based upon production-rolled film, all samples should be marked with the roll direction. The analysis then must involve positioning the film in the spectrometer in the same direction for each examination.

There are two additional problems which may be encountered when performing quantitative analysis on films by transmission - opacity and particulates. The first means that typically the energy will be low, resulting in poor signal-to-noise ratio, or that the sample will possess regions of total infrared absorbance, useless for quantitative

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analysis. The second condition results in the scattering of the infrared radiation as it passes through the film. As the scattering is based upon particle size, it results in various nonlinear anomalies in the spectra. Usually these particulates are not uniformly distributed throughout a film, residing as aggregated domains, which makes quantitative analysis difficult, if not impossible.

Liquids

The standard liquid cell is normally filled using a syringe which attached to its Luer Lok fitting. Most plastic disposable syringes are internally coated with a silicone lubricant which can be easily extracted into organic solvents. Additionally, the plasticizers present in some rubber plunger tips can be selectively extracted by organic solvents. Therefore, the use of glass syringes or pipettes is highly recommended to prevent contamination.

Typically, the liquid sample is introduced into the liquid cell from the bottom fitting so that the air is forced upwards through the top opening in the cell to prevent entrapped bubbles. For the filling of extremely thin cells (<0.1 mm), a second, empty syringe is attached to the upper port and the plunger withdrawn to create a vacuum in the cell, causing the sample to flow into the space.

Variable-temperature liquid cells require that the analyst allow sufficient time prior to collecting a spectrum so that thermal equilibrium is reached, eliminating any spectral artifacts related to changing temperature.

The best quantitative measurements are made if the liquid cell is not moved after the introduction of the first sample by using a flow-through design. This is because sample-cell positioning is difficult to reproduce accurately. If this is not possible, the cell should always be inserted into its holder in the same direction each time and fit snugly into its holder to guard against any motion.

It is advisable to periodically measure the liquid cell thickness as many window materials slowly dissolve with use. A method for determining or verifying the pathlength of a cell (or thin film) is to use the interference fringes superimposed on the baseline of its spectrum. This is done by recording the spectrum of the empty cell ratioed against the empty beam of the instrument. The distance can be calculated by:

$$\text{Pathlength} = [10 \times n]/2[f_1 - f_2]$$

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where pathlength is cell thickness in millimeters, f_1 and f_2 are frequencies (cm^{-1}) of two maxima from the interference fringes observed in the empty cell spectrum, and n is the number of maxima occurring between f_1 and f_2.

Many liquid cells are equipped with halide salt windows which are hygroscopic. Therefore, the analyst must keep in mind that the presence of water in any amount will degrade the performance (subsequently the quantitative measurement) of the cell through fogging, etching, and pitting of the window. This moisture may be present as a component in the sample under analysis or may result from exposure to a damp environment or use of a poor cleaning technique which permits condensation of atmospheric water vapor.

Internal Reflectance Spectroscopy

Carefully designed IRS experiments can permit quantitative measurements to be made. However, data collection must be reproducible. One of the major design considerations is the repeatable contact of the sample against the internal reflection element (IRE), inclusive of total IRE coverage and quality of contact (same pressure, no air pockets). Band-ratioing techniques may be used to perform quantitative measurements, as they are somewhat pressure independent as long as the bands are in the same general spectral region (typically no more than 100-200 cm^{-1} apart).

Diffuse Reflectance Spectroscopy

Typically a mixture consisting of between 1-10% by weight of finely powdered sample in an inert diluent is used for analysis. The physical mixing of the powders should insure uniform distribution throughout the mixture without introducing pressure effects or moisture inclusion. Neat samples should only be used when measurements are to made on weakly absorbing spectral regions. The diffuse reflectance cup (sample holder) requires reproducible loading, with pressure being applied to uniformly pack the powder and create a flat surface. A background spectrum of the diluent material is used for obtaining a ratioed spectrum and should be acquired from the same batch (lot and grinding session) of the material used to dilute the sample.

Reflection does not occur at exactly the same frequency as absorption for strong bands, which causes band shifts and distortions (Reststrahlen). The reflection contribution, comparable to stray light, can be somewhat reduced for a sample by decreasing the particle size or more tightly packing the material into the sampling cup. Some studies

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have shown that the off-axis accessory design exhibits linear absorbance response over a wider range of usable sample concentrations than the straight through design.

Powdered/Ground Samples

When sample morphology dictates that it acquire the form of a fine powder for examination (for example, pressed halide disks, diffuse reflectance, nujol mulls) usually a ball mill or mortar and pestle are used. However, it must be remembered that the pressure and heat generated in the grinding process may cause changes to the sample including polymerization, degration, oxidation, loss of symmetry, and alteration of crystallinity. Minimization of structural damage can sometimes be achieved by performing a “moist” grind (with isopropyl alcohol for inorganics) or using ultrasonic radiation.

Grinding the sample in the presence of a halide salt is not advisable. Rather, the two powders (as in diffuse reflectance and pressed pellets) are physically mixed following their separate grindings. The first reason is that the differences in hardness between the sample and the diluent will cause nonuniformity of particle size between the two materials, with the “softer” material simply deforming or being ground finer. However, more importantly, are that ion exchange (for example., organic acid becoming an acid salt) and isomorphous substitution of cations in a latticework may occur causing the “wrong” material to be analyzed.

The greatest obstacle for the analysis of powdered solids, is making the particle size small, uniform and reproducible. The size should be small, less than the wavelength of radiation used for its examination as light-scattering takes over from absorption with increasing particle size and may become the predominant effect in the recording of its infrared spectrum. Reproducibility in particle size is improved when grinding the same sample size for the same time period. Using wire mesh sieves for the isolation of a particle size fraction for analysis can be useful, however, caution must be used so that the fraction examined is truly representative of the whole sample and does not selectively favor/exclude a particular component.

Halide salts (powders, windows) are hygroscopic, and should be stored in desiccators or warm ovens. The materials should have their spectra recorded versus an open beam for detection of any impurities. They should not be stored near organic materials that have substantial vapor pressure as surface adsorption of the volatile species will occur.

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Calcination, in air, can eliminate the presence of most organic impurities without adversely affecting crystallinity.

DATA COLLECTION

All spectra to be used for quantitative measurements need to be made in a format where the ordinate axis is linear with sample concentration. The most commonly used format for the ordinate axis is Absorbance (others are Kubelka-Munk and PAS). Do not use the %T format not be used, since this is a logarithmic scale with respect to concentration.

Spectral regions possessing bands between 0.2-0.7 Absorbance units are recommended for quantitative analysis. This does not mean that bands falling outside this range cannot be used, but rather, that adherence to Beer's Law is more likely with data meeting these criteria.

Strictly speaking. the number of calibration samples required for a quantitative analysis is equal to the number of components in the system. However, this does not permit overdetermination. Therefore, it is recommended that the number of calibration samples be equal to twice the number of components in the system. In that way, overdetermination is possible to yield a "goodness" of fit, in addition to generating "blinds" to verify that the method does work.

For every reference standard and each sample analyzed, a minimum of two complete samplings should be made (run in duplicate). Additionally, when collecting the spectra for the calibration standards, the references should be examined in random sequence. This means that the second examination (duplicate) of a sample should not be made directly after its first data collection and that the standards should not be examined in increasing or decreasing concentration order. Such practice makes it easily to verify sampling reproducibility by comparison of duplicate samples and to eliminate possible errors from buildup/carryover relating to selective retention of a component.

The single beam background for computing a ratioed spectrum should be collected through the accessory or holder used for examining the sample. This is to insure that the IR beam is attenuated in the same manner as when the sample spectrum is recorded, any spectral features characteristic of the accessory will be ratioed out in the

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computation of an absorbance spectrum, and that the infrared beampath will be identical between the reference and sample examinations.

The whole beam area at the sample position, with no holes in the sample, should be completely filled otherwise the spectrum will exhibit distortions caused by the intensities of the absorption peaks being artifically depressed.

A method that solely relies upon a single holder, crystal or cell should never be developed. This refers to an analysis based upon a single, particular pair of windows, bottle of halide powder, diffuse reflectance cup, IRE, syringe, etc. This should not be confused with using a fixed pathlength cell where the sample thickness is of importance. The rigors demanded of a good analytical procedure precludes it from dependence upon the accidental destruction of such “lucky” equipment.

SPECTROMETER PERFORMANCE

Good quality data required for high analytical precision and accuracy can only be obtained if the spectrometer is performing properly. Several practices can be followed for the monitoring of instrument performance to insure good quantitative analysis.

First, the regular collection of a 100% Transmittance line under predefined conditions (that is., co-addition time, resolution, apodization, aperture size, etc.) should be made. This consists of two sequentially collected single-beam spectra ratioed to obtain a %T spectrum. The spectrum should be flat, featureless, and positioned at 100% T. A flat spectrum showing an offset from 100% T is typical of temperature instability (for example, source, thermally cooled detector, surrounding environment). Sloping baslines are usually due to misalignment of the spectrometer optics or accessory. The 100% T line should be collected prior to the introduction of an accessory or sample as it reflects the instrument’s performance. The sources for any spectral artifacts should be isolated and removed (for example., electrical spikes and vibrations). Additionally, the noise level (RMS and/or peak-to-peak) should be measured in a predefined region, typically between 2200 - 2000 cm^{-1} as there exists little spectral interference in this region and the mid-infrared detector response is greatest here. A rise in noise level will indicate spectrometer performance problems, which may be due to misalignment or degradation of source or detector.

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Next, one of the above collected single-beam black body curve spectra should be examined and compared to previously collected single-beam curves. The maximum of the spectrum should remain constant as it is based upon the temperature of the source. If it should drop suddenly, it is indicative of the spectrometer's source "burning out" and requires its replacement. "Icing" of a liquid nitrogen cooled detector (MCT), due to loss of vacuum can be observed by an increase in the intensity of a triangular-shaped band near 3250 cm^{-1}. This requires that the dewar be reevacuated, typically by shipment back to the vendor. Finally, the region of the single-beam spectrum characteristic to low frequency detector/optics cutoff should be examined. This region reflects detector nonlinearity from saturation and should be flat at zero, recording no infrared energy being detected. In cases of nonlinearity, the cutoff may never reach zero (seeing energy when none is present), descend below zero (recording negative energy), or stray back and forth about zero. This behavior may require that the infrared beam be attenuated with metal mesh screens, optical filters or apertures to obtain a linear response. All attenuating items should be handled as optical elements, carefully shielded from dust, and never touched, so as to prevent contamination that would contribute spurious infrared absorbances in collected spectra.

These same measurements should be made following the introduction of the accessory used for sample examination has been made into the spectrometer. If any problems exist, then alignment of the accessory must be performed. If attenuation of the beam with filters, screens, or apertures is necessary for linearity, both the background and sample spectra must be collected with them in identical position to duplicate a reproducible beampath.

SPECTRAL MANIPULATIONS

It is not necessary for the analyst to make the infrared spectra "look nice" prior to performing quantitative measurements. In fact, most data treatments to improve the visual appearance of the data adversely alter the information so as to make it useless for quantitation through the application of irreproducible operator bias.

However, if application of data manipulation is necessary, there are three criteria that should be followed:

1. insure that all spectra are in a linear format (that is, absorbance type)

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2. use only data treatment that is absolutely necessary to make the required quantitative measurements
3. insure that any manipulations are performed identically on all spectra—calibration, reference, and unknowns

Smoothing

Smoothing degrades spectral resolution and is an extremely poor analytical practice. In fact, the use of a moving smoothing function (for example, Savitzky-Golay) will affect band shape and peak position. Therefore, if a spectrum is too “noisy” for good measurements it should either be collected at a lower resolution or the data co-added for a longer period of time. If smoothing is a necessity, a Fourier-space smoothing function (high-pass filter) is preferable, as it affects band shapes less than a moving smooth function.

Fringe Removal

Multiple internal reflection inside a cell or film may result in the presence of spectral fringes. Although the fringes do allow for thickness calculations, they can be a major problem when implementing a quantitative method.

If the fringe is a high frequency wave, then the interferogram can be inspected for the presence of a secondary (and tertiary) centerburst. Software removal of this extraneous centerburst(s) will eliminate the wave from the computed spectrum. If the fringe is a low frequency wave, then it may be better to treat this as a baseline correction problem and use a Fourier high-pass fileter for removal.

Fourier Self-Deconvolution

Fourier self-deconvolution reduces spectral band widths, but maintains band areas. Therefore, band intensity increases. However, spectral noise increases rapidly with the degree of band narrowing which requires that only spectra with high SNR can be used. It is advised that only a conservative level of resolution enhancement should be applied to data for quantitative analysis.

Derivative

Derivation is not recommended in conjuction with quantitation of FT-IR data. This is because the intensity of a derivative peak depends on the width and data point spacing of the original band. Any minor changes in band width leads to large alterations of derivative intensity, which can be very marked on the narrow mid-IR bands. Next, the

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second derivative exhibits side lobes that point in the same direction as the main derivative peak, resulting in a very complex spectrum for measurements. Last, derivation greatly increases spectral noise usually necessitating the application of additional smoothing functions (another source of bias).

Interpolation

The resolution of a spectrum can be artificially enhanced to provide better band shapes for manipulations through interpolation. The easiest method fits a polynomial to known points. However, the preferred method is to add zeros to the end of an interferogram prior to computing the Fourier transform.

Spectral Subtraction

Spectral subtraction may prove useful for quantitative analysis in two ways. First, it can be used as a preparative step for spectra where a sample requires removal of interfering absorbance bands due to solvent, water vapor, or substrate. Spectral subtraction is not valid however, if the sovent or substrate interacts with the sample as it would result in residual spectral features characteristic of the interaction.

Secondly, under carefully controlled conditions, spectral subtraction can be used as a quantitative tool. In general, the pathlength of the the sample must remain constant. In this application, the spectral subtraction factor recorded for complete removal of a “pure” component from a mixture can be used to calculate the concentration of that component.

Baseline Correction

It is highly advised that baseline correction never be directly applied to spectral data. Rather, absorbance band measurements should be made relative to baseline definitions within a quantitative analysis package. In some isolated cases, where the baseline is simply elevated or tilted, a simple one- or two-point tilt baseline correction may be applied without adversely affecting spectral data for quantitative measurements provided all spectral files (standards and unknowns) are treated identically.

Some of the issues directly affected by baseline correction follow. First, an elevated baseline may push strongly absorbing spectral bands into a nonlinear range and cause peak maxima to have a high level of noise. Second, spectral information may be present in the baseline which correlates to the concentration of a component (for example, carbon black) and can be used by sophisticated software packages. Third, a

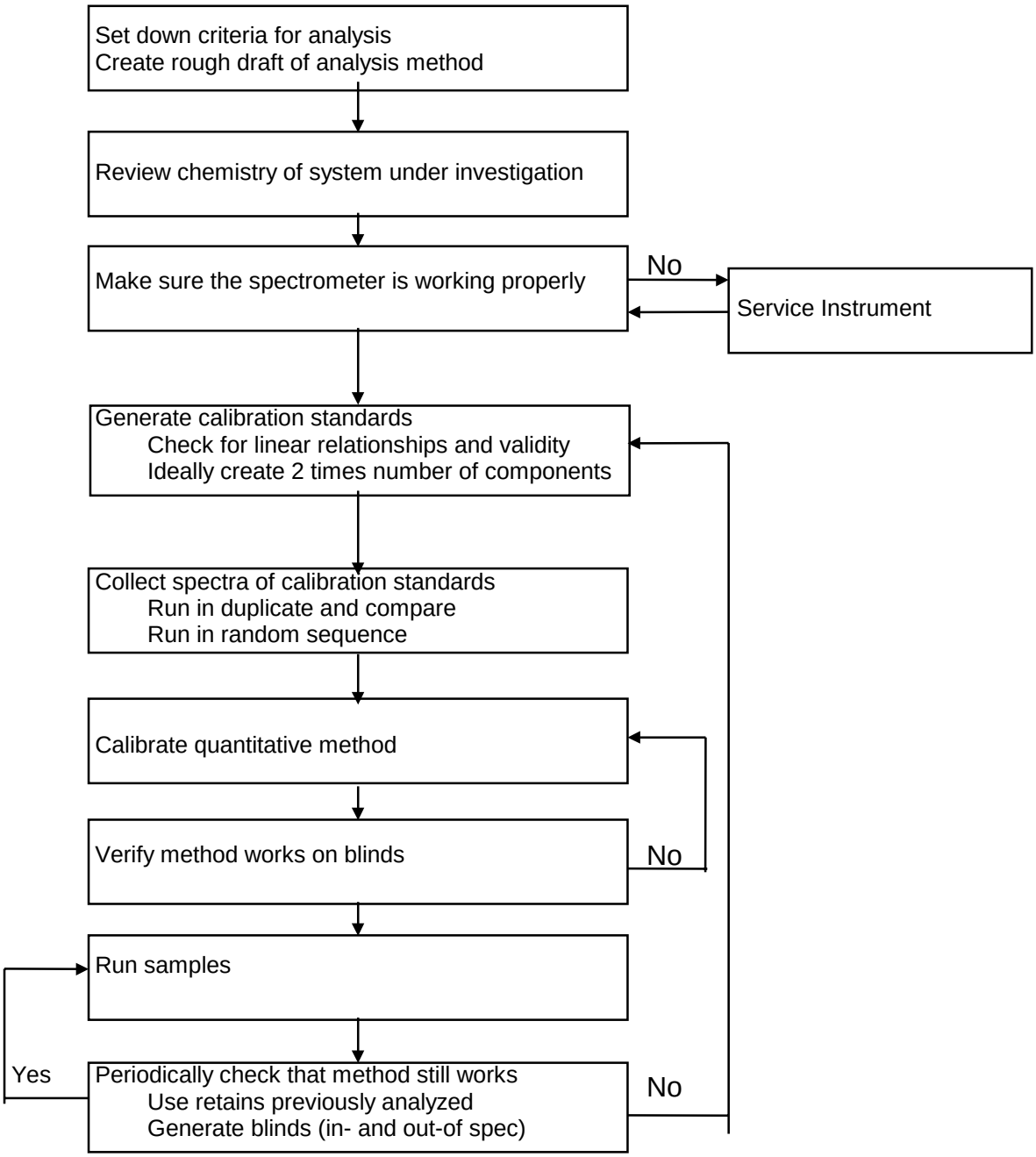
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baseline exhibiting severe curvature probably means that the experimental conditions are ill defined. Last, baseline corrections should never be performed on a spectrum in a %T format as nonlinear factors are introduced by the logarithmic function.

If it is necessary to remove a curved baseline, the use of a high-pass filter in Fourier-space is preferred to a manual baseline correction as it has less analyst bias. A Fourier-space filter treats all spectra in a similar fashion, avoiding irreproducibility.

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QUANTITATIVE ANALYSIS FLOW CHART



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J
Deconvolution

GENERAL CONSIDERATIONS

Deconvolution attempts to enhance the apparent resolution of overlapping peaks where the limiting resolution is the natural width of the bands, not the resolution with which the spectrum was collected. The individual peaks are assumed to have Lorentzian line shapes. A broad peak may be described as the convolution of a very sharp peak (a delta function) with a Lorentzian line shape function. Integrated bands areas are retained following deconvolution, in addition to peak positions, which means that quantitative information can still be extracted from the spectra. However, peak amplitude (intensity) is changed due to the narrowing of the band from removal of the Lorentzian line shape.

In order to obtain reliable results when using deconvolution to enhance the apparent resolution of overlapping band contours, a number of conditions must be met:

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- The spectral data should be recorded with as high a signal-to-noise (SNR) as possible. It is possible to work with noise levels of 1% (100:1), but a SNR of at least 1000:1 is desirable.

- The maximum achievable effective resolution after deconvolution cannot be higher than the instrumental resolution used to record the data.

- The spectral region to be used in deconvolution should be in an absorbance format.

- The maximum absorbance in the spectral region to be deconvolved should be less than 1.

- The region for deconvolution should be limited to the area in which the band widths are all approximately the same.

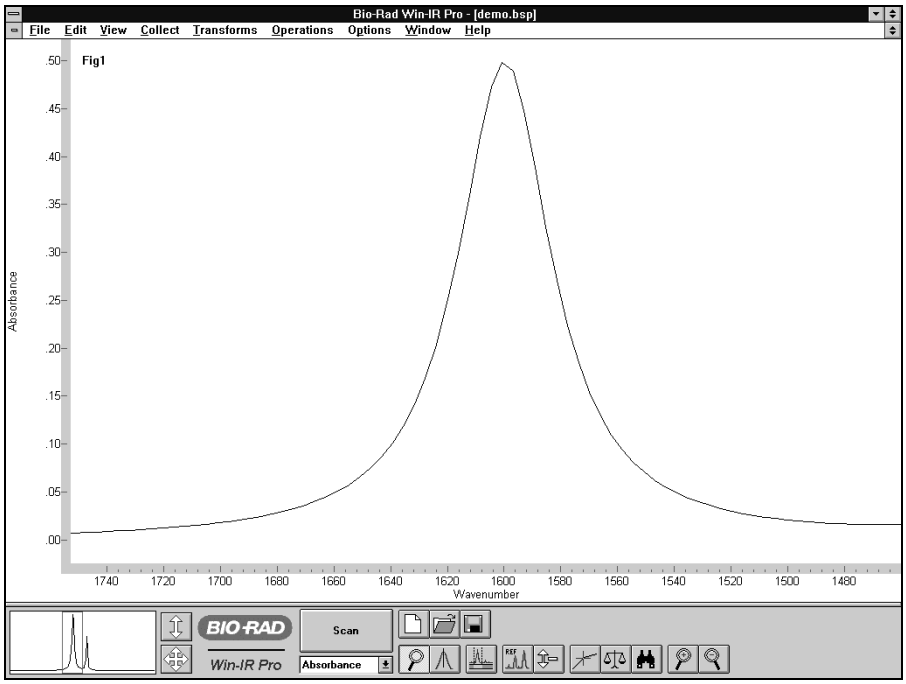
- The spectral limits used to define the spectral region for deconvolution should include a portion of the baseline so that the noise level can be monitored. Additionally, the first few data points should not show any curvature because this will give a truncation effect.

Additionally, in regions where water vapor absorbs, major problems with deconvolution may occur. This is because even trace ripples on the original spectrum will automatically be overdeconvolved since the water lines are as sharp as the instrument resolution.

SIMULATED SPECTRAL EXAMPLES

The synthetic spectrum shown has a single peak with a width at half height of 30 cm^{-1}, peak intensity of 0.5 absorbance and location of 1600 cm^{-1}. After cosine transformation of the 2000 - 1450 cm^{-1} region, this peak may be described as the product of a cosine wave (the frequency of the wave corresponds to the location of the sharp peak in the spectrum) with an exponential decay function.

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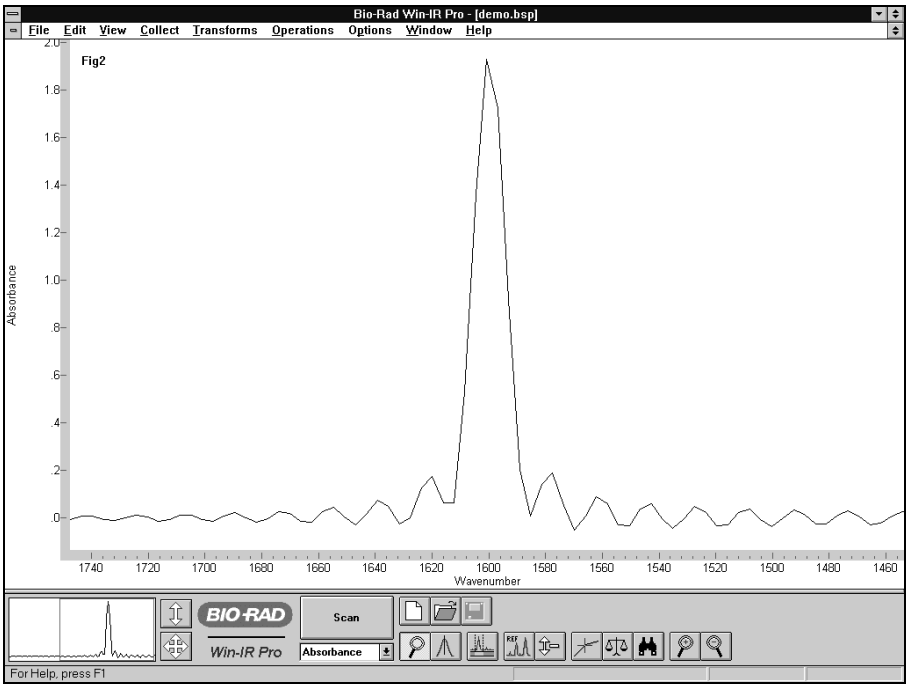


The cosine transform of a Lorentzian line shape with width at half height W is an exponential function $e^{-2\pi Wx}$.

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When the cosine transform of a Lorentzian peak is multiplied by the appropriate exponential function (representing the cosine transform of a Lorentzian peak of the identical width), a *pure* cosine function results.

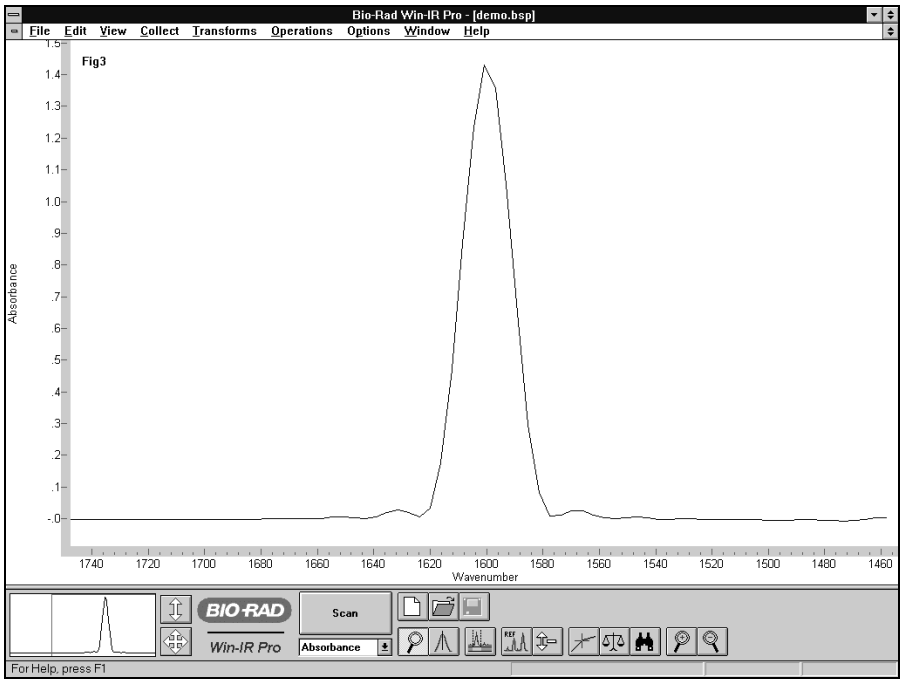
When this interferogram is subjected to another cosine transform, this deconvolved peak appears as a sinc function having a much sharper main peak than the original Lorentzian peak. This peak is at the same location in the spectrum as the original Lorentzian peak.



Since the prominent sidelobes of the sinc function may complicate the interpretation of spectra containing more than one peak, the interferogram should be apodized before performing the final cosine transform. The effect of apodization is to broaden the very narrow peak resulting from transformation of the cosine function and to reduce its sidelobes. This apodization is controlled by the K factor parameter, which governs an exponential weighting function operating on the interferogram. The value of the K factor corresponds to the desired amount of narrowing in the original peak. For example, a K factor of two results in a final peak width of one half the width of the original peak.

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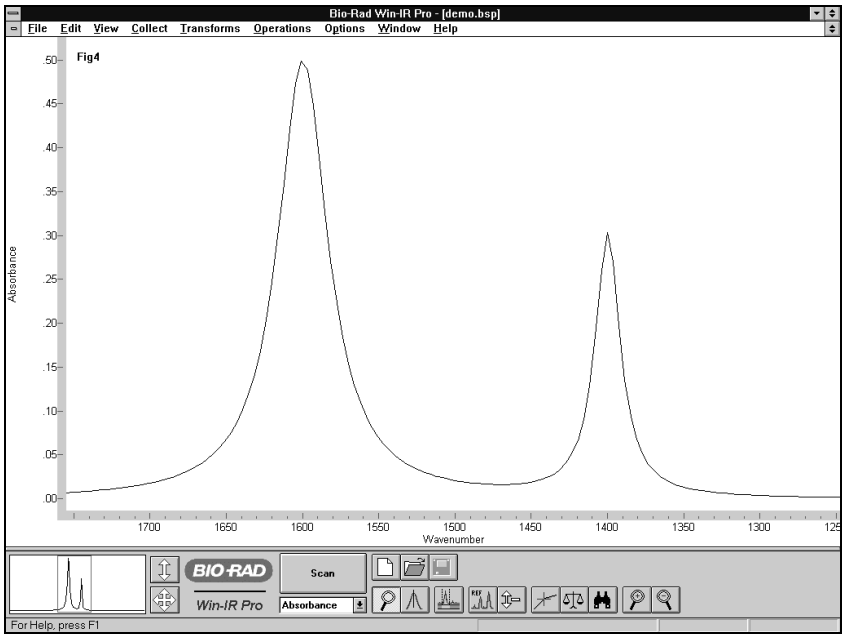
Four apodization functions may be applied to the interferogram: boxcar, Bessel, $sinc^2$ and $triangle^2$. The previous example shows the result of boxcar apodization with a K value of two. The next figure shows the result of Bessel apodization of the interferogram with a K value of two.



The deconvolved spectrum results from applying a cosine transform to the Bessel apodized interferogram. The reduction in magnitude of the sidelobes is evident, and the peak is half as wide as the original Lorentzian peak. Note the change in the Y-axis scale (intensity). However, the peak area remains the same.

The satisfactory results of the above example depended upon choosing the correct width at the half-height of the Lorentzian peak shape function to be deconvolved. When the chosen half-width is too large, the peak is over-deconvolved, and large sidelobes are present. For example, the figure below shows two peaks one at 1600 cm^{-1} (same as above) and another narrower peak with a width of 20 cm^{-1} located at 1400 cm^{-1}.

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When deconvolved by a Lorentzian function with a half-width of 30 cm^{-1}, the peak at 1600cm^{-1} is correctly deconvolved, but the peak at 1400 cm^{-1} is overdeconvolved, producing large negative sidelobes.



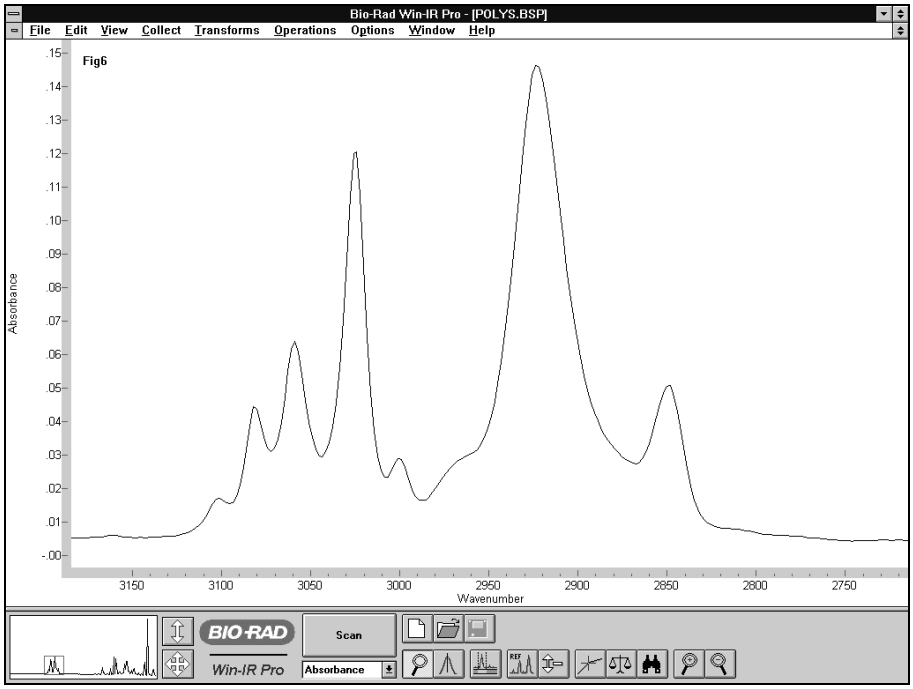
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In general, selecting an optimum value for the half-width parameter is not possible where overlapping peaks have quite different half-widths.

In this example, the C-H stretching region of a polystyrene based polymer, between 3200 and 2700 cm^{-1} is selected for the illustration of the deconvolution process. The spectrum used is polys.bsp. The flat baseline area, outside of the overlapping band region is included for reasons which will become evident.

Before selecting Deconvolve, define the region (3200-2700 cm^{-1}) to be deconvolved using the cursor.

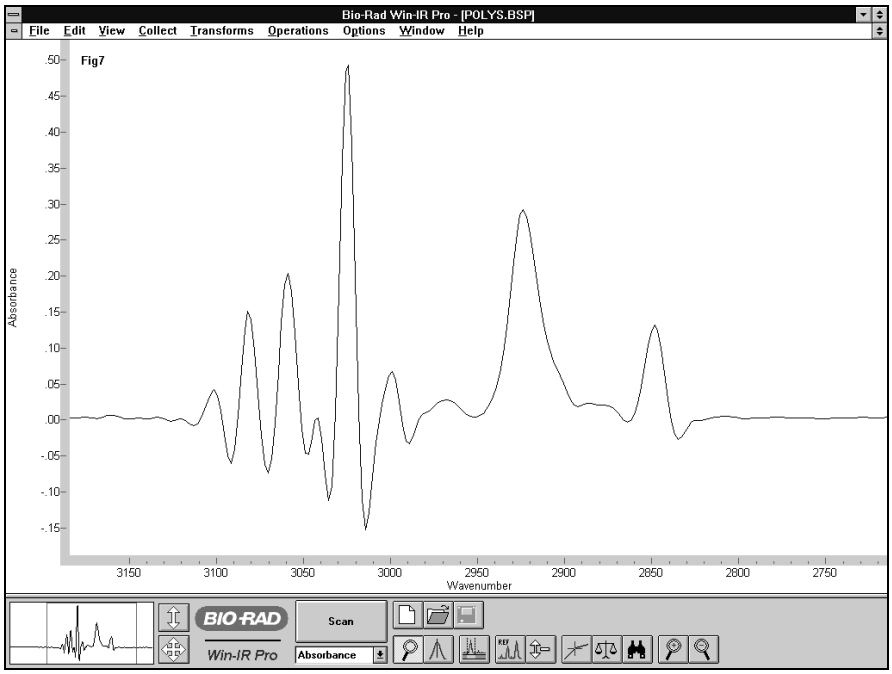


By examination, a value for the half bandwidth (HBW) of the narrowest band is made. For example, a value of 16 cm^{-1} will be the initial estimate (3033 - 3017 cm^{-1}). A K factor of 2 is input, as initially a resolution enhancement of 2 will be sought. Type these values into the appropriate entry boxes, and press Apply. It is advisable to begin with a small value for the K factor so that the bandwidth parameter can be optimized without artifacts occurring from the simultaneous variance of two parameters. Bessel

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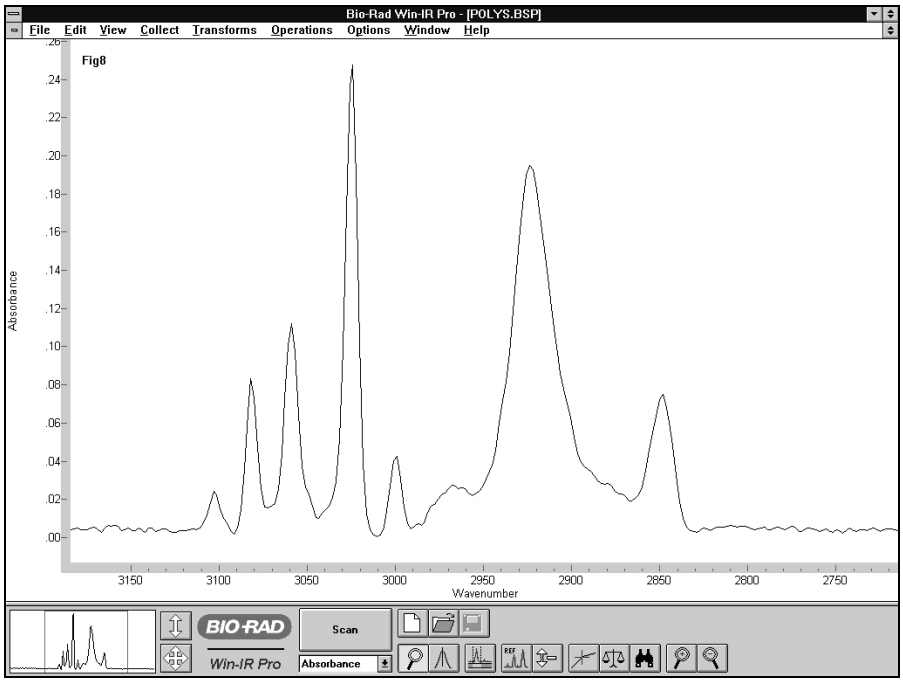
apodization is suggested as it minimizes the amount of noise introduced by the deconvolution process.

It is obvious from the presence of the negative sidelobes that the half-bandwidth used was too wide. It is difficult to discern which bands are real from the artifacts created by the sidelobe maxima.



To remove the negative sidelobes, a smaller HBW value is used. The only parameter requiring change at this time is the half bandwidth. The HBW value of 8 cm^{-1} is entered and Apply is pressed. The deconvolved spectrum with an HBW of 8 cm^{-1} is displayed.

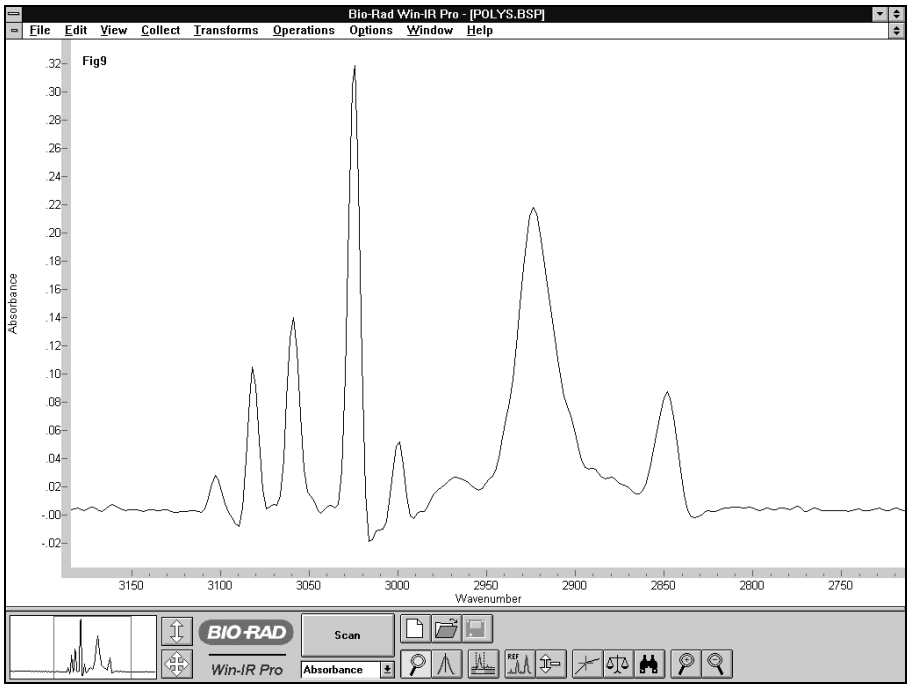
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The noise level is quite low in the regions of retained baseline and no sidelobes exist. However, the bands are not resolved to the baseline. Therefore, a wider half bandwidth will be used to better define this region.

Change the HBW parameter to 11.5 cm^{-1} and press Apply.

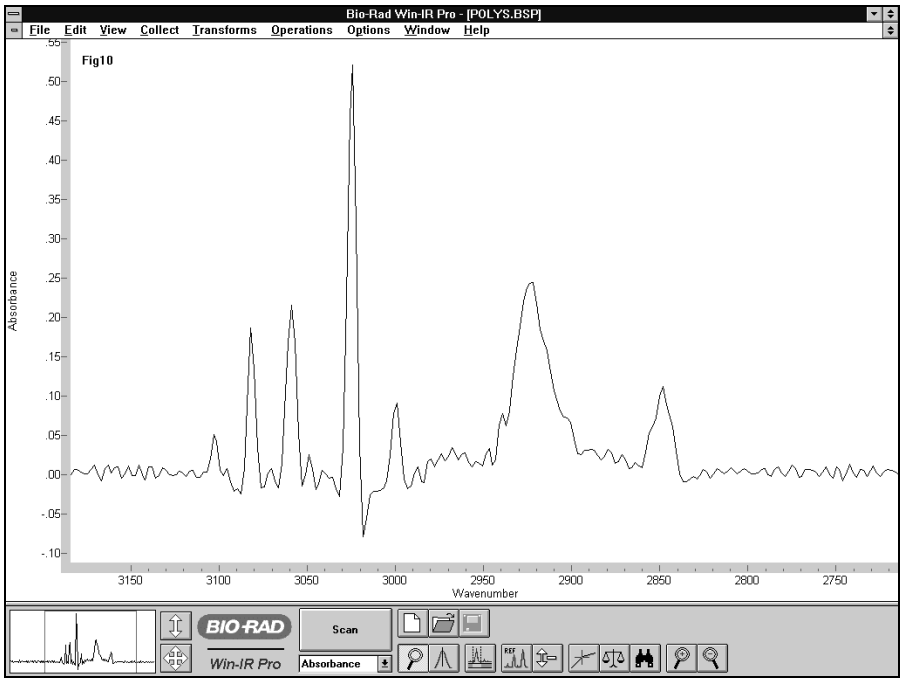
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The noise level in the spectrum is low and the majority of the bands have been resolved to the baseline. The band at 3001 cm^{-1} shows the presence of negative sidelobes. This is because its HBW is significantly different from the other overlapping bands in the C-H stretching region. It is a good example for illustrating the reason for only deconvolving small spectral regions where bands have the same HBW.

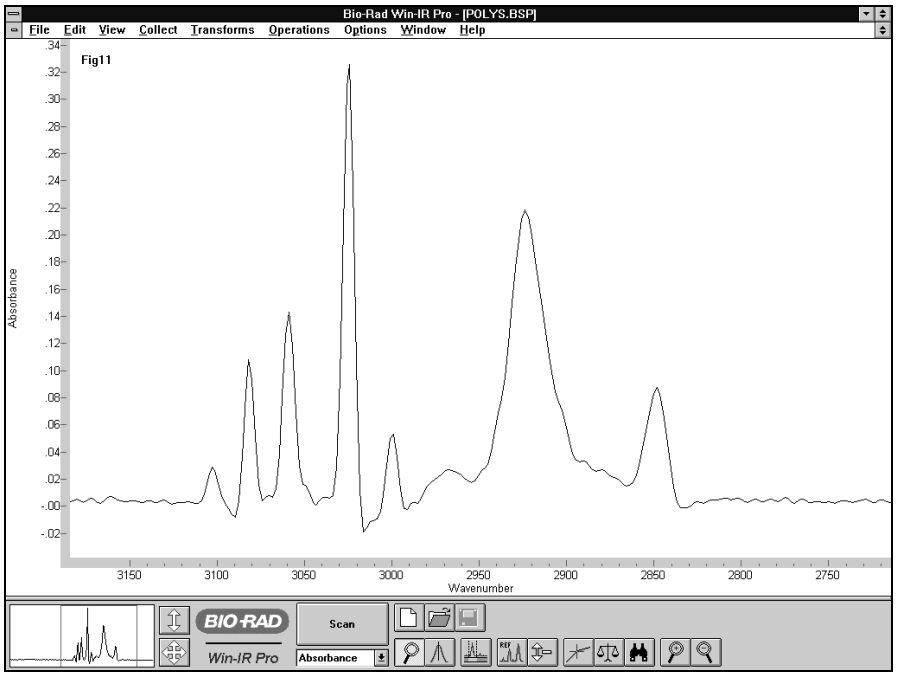
Now that a deconvolved spectrum without significant negative sidelobes has been obtained, the K factor (that is., resolution enhancement factor) can be adjusted. Enter a value of 3 for the K value and press Apply (HBW remains at 11.5).

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The excessive noise in the baseline region indicates over-deconvolution. The noise is different from normal spectral noise as it appears as non-random bursts on the baseline. The figure below shows the final deconvolved result, with a HBW of 11.5 cm^{-1} and K factor of 2.1. The noise level is at an acceptable low level and there exists minimal negative sidelobe intervention.

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Referring back to conditions to be met for proper deconvolution to occur, the maximum achievable resolution after deconvolution cannot be higher than the instrumental resolution used to record the data. Since the HBWs in the spectrum were found to be approximately 11.5 cm^{-1}, or nearly twice the resolution used to collect the data (4 cm^{-1}), it would be considered prudent to record the spectrum at improved resolution in order to check the results. This is because the effective resolution has been imporved by a factor of 2.1 (K factor), with distinguishable band definitions defined by 11.5 (HBW)/2.1 (K factor), or 5.5 cm^{-1} separation. The values of 4 cm^{-1} (collection resolution) versus 5.5 cm^{-1} (effective resolution) closely approximate one another, therefore, recollecting the spectrum at 2 cm^{-1} would assure that no artifacts were introduced by approaching the instrumental resolution with the effective resolution used for deconvolution. Additionally, the data point spacing will be changed from 2 cm^{-1} to 1 cm^{-1} giving the final deconvolved result a better defined line shape.

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K
Diagnostics and Service Access

GAIN RANGING MULTIPLICATION

The gain ranging factors (add and multiply) are updated evey time you select Calibrate in Setup. There is eeldom a need to access this. The factors are stored in the registry. To access this value:

1. From the Task bar, select Start / Programs / Administrative Tools / RegEdit 32. A number of windows open.

2. Select the HKEY_LOCAL_MACHINE on Local Machine window.

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3. Double click HKEY_LOCAL MACHINE. The subentries under this entry appear.

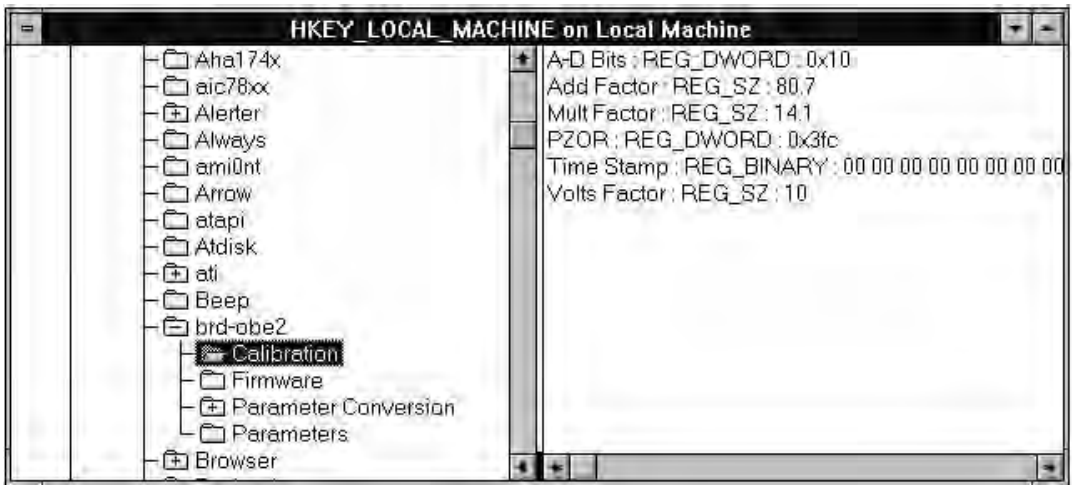
4. Continue clicking to navigate through the chain of entries:

   System
   Current ControlSet
   Services
   brd-obe2
   Calibration

5. The item Add Factor: REG_SZ: gives the addition factor. In this example, it is 80.7.

   The item Mult Factor: REG_SZ: gives the multiplication factor. In this example, it is 14.1.

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6. Select Exit from the Registry menu to close RegEdit 32.

AUTOALIGN LOCATIONS

Each time an autoalignment is run, the autoalignment locations are stored in the file C:\win32app\Win-IR_Pro\bin\autoalign.txt. This file can be opened and read by any text editor. The file is created anew every time the spectrometer is autoaligned. Do not modify this file. A typical autoalign.txt file is shown below.

```
x =  -37,  y =  -75,  gain =  4,  measurement =  3013
x =  -37,  y =  -75,  gain =  4,  measurement =  3002
x =  -12,  y =  -75,  gain =  4,  measurement =  3011
x =   12,  y =  -75,  gain =  4,  measurement =  3018
x =   37,  y =  -75,  gain =  4,  measurement =  5669
x =   50,  y =  -50,  gain =  4,  measurement =  7436
x =   25,  y =  -50,  gain =  4,  measurement =  8716
x =   25,  y =  -50,  gain =  3,  measurement =  5529
x =    0,  y =  -50,  gain =  3,  measurement =  3506
x =  -25,  y =  -50,  gain =  3,  measurement =  3080
x =  -50,  y =  -50,  gain =  3,  measurement =  2821
x =  -62,  y =  -25,  gain =  3,  measurement =  2729
x =  -37,  y =  -25,  gain =  3,  measurement =  3548
x =  -12,  y =  -25,  gain =  3,  measurement =  4876
```


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x = 12, y = -25, gain = 3, measurement = 4232
x = 37, y = -25, gain = 3, measurement = 5632
x = 62, y = -25, gain = 3, measurement = 4673
x = 75, y = 0, gain = 3, measurement = 4491
x = 50, y = 0, gain = 3, measurement = 4600
x = 0, y = 0, gain = 3, measurement = 8356
x = 0, y = 0, gain = 2, measurement = 5372
x = -25, y = 0, gain = 2, measurement = 3142
x = -50, y = 0, gain = 2, measurement = 3172
x = -75, y = 0, gain = 2, measurement = 2654
x = -62, y = 25, gain = 2, measurement = 2467
x = -37, y = 25, gain = 2, measurement = 4563
x = -12, y = 25, gain = 2, measurement = 2381
x = 12, y = 25, gain = 2, measurement = 8815
x = 12, y = 25, gain = 1, measurement = 5138
x = 37, y = 25, gain = 1, measurement = 4344
x = 62, y = 25, gain = 1, measurement = 2429
x = 50, y = 50, gain = 1, measurement = 4507
x = 25, y = 50, gain = 1, measurement = 7097
x = 0, y = 50, gain = 1, measurement = 4431
x = -25, y = 50, gain = 1, measurement = 2774
x = -50, y = 50, gain = 1, measurement = 2447
x = -37, y = 75, gain = 1, measurement = 2285
x = -12, y = 75, gain = 1, measurement = 2816
x = 12, y = 75, gain = 1, measurement = 2399
x = 37, y = 75, gain = 1, measurement = 7097
x = 25, y = 50, gain = 1, measurement = 7097
x = 25, y = 51, gain = 1, measurement = 7193
x = 25, y = 61, gain = 1, measurement = 7525
x = 25, y = 71, gain = 1, measurement = 7292
x = 25, y = 61, gain = 1, measurement = 7499
x = 26, y = 61, gain = 1, measurement = 7582
x = 36, y = 61, gain = 1, measurement = 7964
x = 46, y = 61, gain = 1, measurement = 7540
x = 36, y = 61, gain = 1, measurement = 7989
x = 36, y = 66, gain = 1, measurement = 8168
x = 36, y = 66, gain = 0, measurement = 5460

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x = 36, y = 71, gain = 0, measurement = 5501
x = 36, y = 76, gain = 0, measurement = 5479
x = 36, y = 74, gain = 0, measurement = 5497
x = 36, y = 72, gain = 0, measurement = 5490
x = 36, y = 74, gain = 0, measurement = 5485
x = 41, y = 74, gain = 0, measurement = 5608
x = 46, y = 74, gain = 0, measurement = 5622
x = 51, y = 74, gain = 0, measurement = 5486
x = 49, y = 74, gain = 0, measurement = 5566
x = 47, y = 74, gain = 0, measurement = 5601
x = 45, y = 74, gain = 0, measurement = 5646
x = 43, y = 74, gain = 0, measurement = 5639
x = 45, y = 74, gain = 0, measurement = 5649
x = 45, y = 75, gain = 0, measurement = 5649
x = 45, y = 74, gain = 0, measurement = 5630
x = 45, y = 74, gain = 0, measurement = 5635
x = 46, y = 74, gain = 0, measurement = 5630
x = 45, y = 74, gain = 0, measurement = 5629
x = 45, y = 74, gain = 0, measurement = 5661
x = 45, y = 75, gain = 0, measurement = 5675
x = 45, y = 76, gain = 0, measurement = 5691
x = 45, y = 77, gain = 0, measurement = 5700
x = 45, y = 78, gain = 0, measurement = 5709
x = 45, y = 79, gain = 0, measurement = 5725
x = 45, y = 80, gain = 0, measurement = 5721
x = 45, y = 79, gain = 0, measurement = 5718
x = 46, y = 79, gain = 0, measurement = 5731
x = 47, y = 79, gain = 0, measurement = 5727
x = 46, y = 79, gain = 0, measurement = 5729

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L
Accelerator Keys

Keys	Menu entry selection
CTRL + A	View / Autoscale
CTRL + C	Edit / Copy
CTRL + E	View / Entire Spectrum
CTRL + L	View / Lock Selected
CTRL + N	File / New...
CTRL + O	File / Open...
CTRL + P	File / Print...
CTRL + S	File / Save
CTRL + U	View / Unlock Selected
CTRL + V	Edit / Paste
CTRL + X	Edit / Cut
CTRL + Z	Edit / Undo...
F1	Help / Index
F2	Edit / Select All Visible
F11	Window / Maximize Traces
F12	Window / Maximize Spreadsheet

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M
Library Conversion

OVERVIEW

The Bio-Rad Search Library Converter program converts libraries in the Bio-Rad 3200 library, Sadtler user library, or Galactic user library format into a library in the Sadtler user library, Galactic user library, or Win-IR Pro library format. Once all your libraries are converted, there is no need for further use of this program. In fact, most Win-IR Pro users will never have occasion to run this program.

The resolution, range, and number of bytes per point are the same in the converted output library as they are in the input library. Any spectra marked as deleted in the input library are not copied into the output library. Thus, if the input library had 200 spectra of which 20 were marked as deleted, the output library would have 180 spectra.

The input library is not modified. The output library is created in the input library directory. The output library can be moved afterwards. See the "Search" section in the Operations chapter for details on library pathnames and search paths.

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Note

A library consists of a number of files. They have the same filename but different extensions. The extensions are listed at the end of this appendix. When you move the library, be sure to move all its files.

Restrictions and Considerations

3200: There are two types of 3200 libraries—single (ordinary) resolution (file extension .sl) and dual resolution (file extensions .s1 and .s2). There are no special considerations for single-resolution libraries.

A dual resolution library has two spectrum files. One, usually the .s1 file, has a lower resolution (for example, 16 cm^{-1}). The other, usually .s2 file, has a higher resolution (for example, 4 cm^{-1}). The lower resolution file would be the one actually searched; the spectra displayed would be the corresponding ones in the higher resolution file. This scheme was meaningful when computers were slower; it is no longer necessary. When converting dual resolution libraries, select the higher resolution file, normally the file with the .s2 extension. However, you should always check both files to be certain which one has the higher resolution. This information is presented in the Library to be converted dialog box (see step 5 in the example below).

Sadtler: You cannot convert Sadtler-proprietary libraries, only Sadtler user libraries.

Libraries converted to Sadtler user libraries should be opened with the Sadtler User Library Manager. There will be a message about normalization; select OK, and re-normalize the library. This takes a few seconds for a modestly-sized (few hundred entries) library.

Galactic: You can convert only Galactic spectral libraries. You cannot convert Galactic encrypted libraries. You cannot convert Galactic structures, peaks, or properties. If you attempt to convert Galactic libraries with structures or peaks, a warning message will be displayed.

Using the Search Library Converter

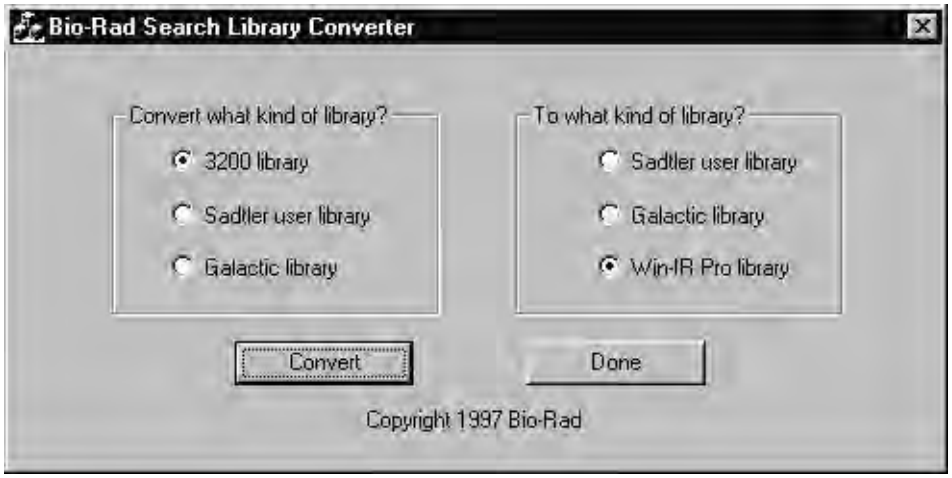
The BioRadSearchLibraryConverter program is supplied on the Win-IR Pro CD-ROM in the Library converter directory. However, it is not installed by the Setup.exe program. If you want to use this program, you can start it from the CD-ROM or copy it to your hard

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disk (we recommend putting it in c:/Program Files/Win-IR Pro/bin) and running it from there.

The example below shows the conversion of a Bio-Rad 3200 format library to a Bio-Rad Win-IR Pro format library. Assume the library is stored in c:/3200 Libraries.

1. Start the converter program by clicking on its icon in the Windows Explorer. The Bio-Rad Search Library Converter dialog box appears.



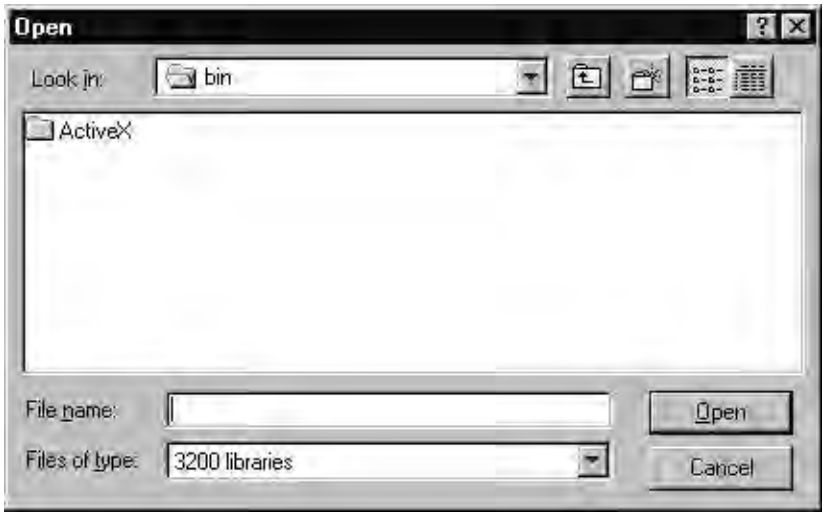
2. Select Convert what kind of library? 3200 library.
   Select To what kind of library? Win-IR Pro library.

Note

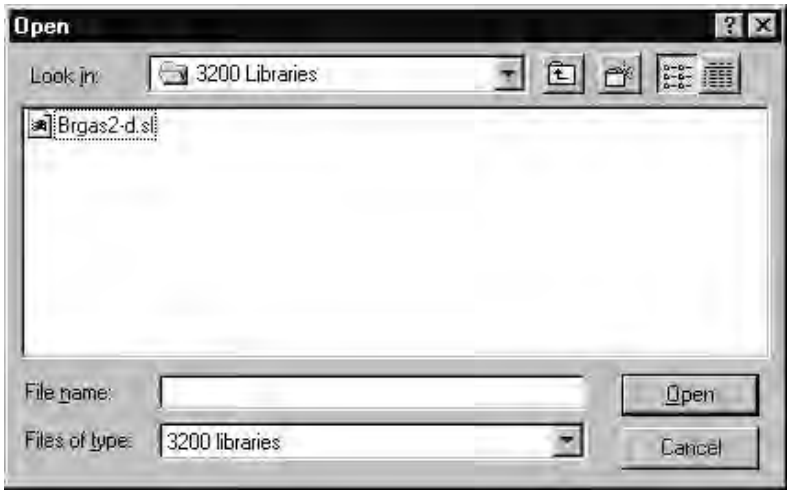
If you choose Sadtler user library as the input library, then Sadtler user library will be disabled (grayed-out) as the type of output library; if you choose Galactic library as the input library, then Galactic library will be disabled (grayed-out) as the type of output library

3. Click the Convert button. The Open dialog box appears.

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4. Use the standard Windows NT procedures to access the directory in which you have stored the 3200 libraries, in this example c:/3200 Libraries.



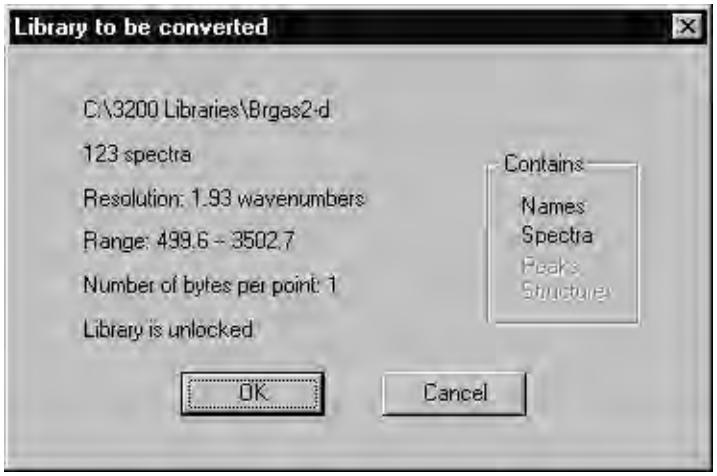
5. Select the library to be converted by highlighting it. Click the Open button.

Note

Only one library can be converted at a time. Repeat the procedure to convert more libraries.

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The dialog box Library to be converted appears.



.

This dialog box displays the properties of the library and its contents.

Resolution is of particular interest if you are converting 3200 dual resolution libraries; check both spectral files and convert only the higher resolution file. This is discussed in the "Restrictions and Considerations" section, above.

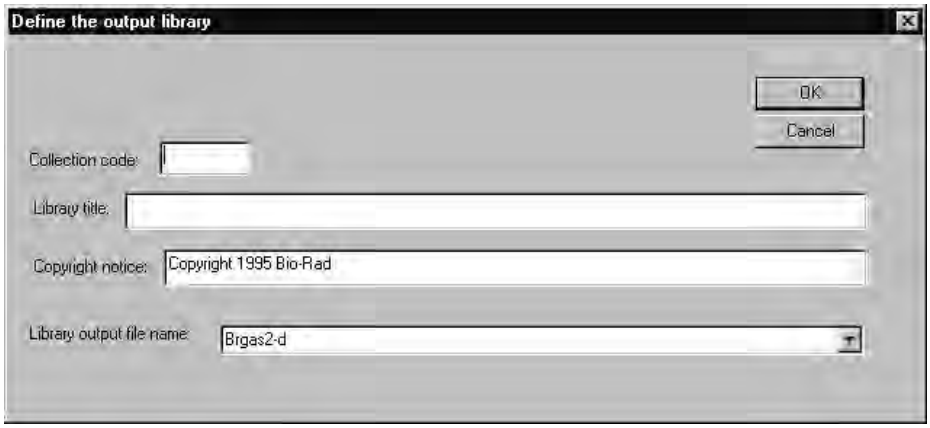
Library is unlocked: you can convert this library. If the message says Library is locked (for example, if the library is a Galactic encrypted library or a Sadler-supplied library), then the OK button is disabled (grayed out) and you cannot convert this library. In this case, press the Cancel button to terminate the procedure.

Contains: displays what information is in the library; see "Search" in the Operations chapter for detailed explanations. All libraries contain Names and Spectra. If the input library is Galactic containing Peaks or Structures, this data will not be converted. If you attempt to do so, you will get a warning message.

You can click Cancel to stop the conversion process.

6. Click OK to continue the conversion process. The dialog box Define the output library appears.

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7. Type in the appropriate information.

Collection code: if your output library format is Sadtler or Galactic, enter a code to identify the library. This code should not conflict with any Sadtler or Galactic libraries you have installed. Typically, Sadtler and Galactic libraries use 2-letter codes; use 3-letter or 4-letter codes to avoid conflicts The Collection code is not meaningful for Win-IR Pro libraries.

Library title: text descriptive of the library.

Copyright notice: leave this as is, or modify it as desired.

Library output file name: enter the name you want to use for the name of the new library file; the converter will append the appropriate extension. The default is to use the same name as the input library. The converted file is created in the same directory as the input file; you cannot use a pathname.

Caution

We strongly recommend that you rename the library if you are converting from a Sadtler user library to a Galactic library, or *vice versa*, because these library files use the same extensions. Failure to rename the library will render one of the libraries unuseable.

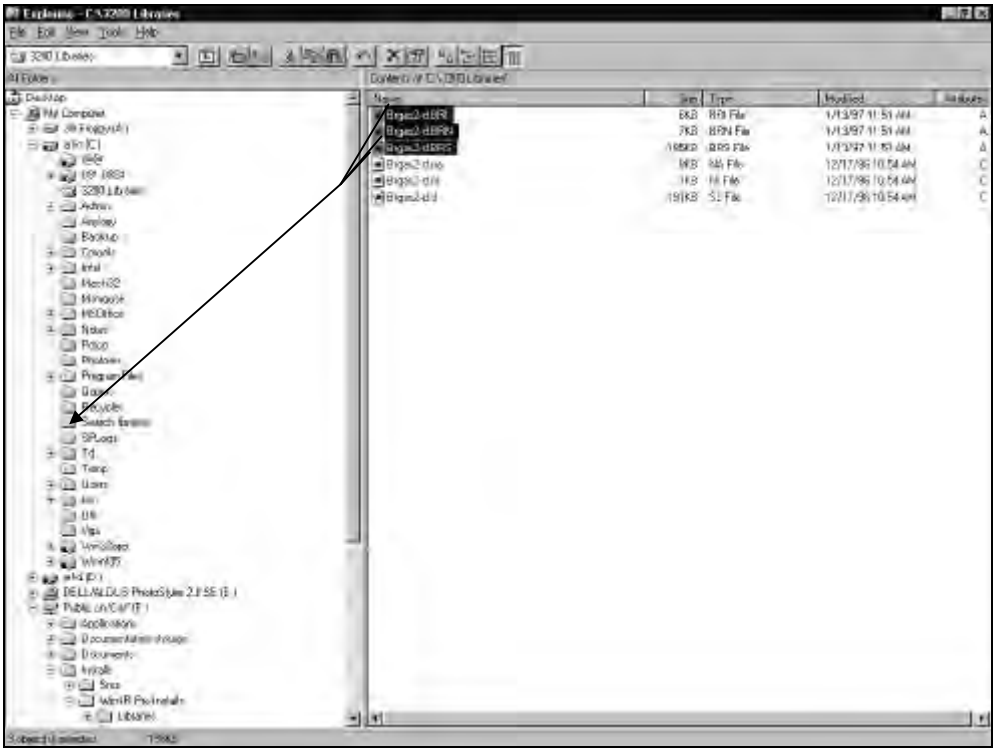
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8. Click the OK button. The library will be converted and the converter program will terminate. Repeat steps 1 to 8 to convert additional libraries.

9. If desired, copy the new libraries into the directory used for your search libraries; the default is c:/Search libraries.

Note

In this case, the library produced consists of three files; be sure to move all of them or Win-IR Pro Search will not work properly. In general, there will be more than one file for each library.



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LIBRARY FILE EXTENSIONS

LIBRARY	EXTENSION	FILE USE
3200	.na	names
	.ni	names index
	.s1	first spectrum file with dual resolution library
	.s2	second spectrum file with dual resolution library
	.sl	spectrum file for ordinary (single) resolution library —either .sl or .s1 and .s2 will be present
Sadtler	.dat	chemical structure (optional)
	.idx	index
	.inf	properties (not converted)
	.ipk	IR Peaks (optional)
	.ism	IR spectrum
	.nam	name
	.txt	not converted
	.vpk	vapor phase peaks (not converted)
	.vps	vapor phase spectra (not converted)
Galactic	.idx	index
	.isl	spectrum
	.ipl	peaks (not converted)
	.itl	name
	.lib	special file (not converted)
Bio-Rad Win-IR Pro	.brc	structure (optional)
	.bri	index
	.brn	name
	.brp	peaks (optional)
	.brs	spectrum

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N
Custom Value Programs

OVERVIEW

This interface allows you to write programs that can access the raw data collected by an array detector and perform customized transforms upon this data. The program operates upon each spectrum to calculate one value of data type double. This could be the location of the largest peak in the spectrum, the area of a particular peak, the ratio of heights between two peaks, etc. This feature is specifically designed for use with image (.dat) files; see “Custom Value”, Chapter 11 and “Image Document Window”, Chapter 3, for details of registration and execution.

Programs can be written either in any language that supports ActiveX, for example, in Visual Basic (including Bio-Rad’s scripting language extensions to Visual Basic) or in Visual C++. In this appendix, we will discuss the use of Visual Basic to write custom value programs.

After a program is complete, it is registered for execution in Win-IR Pro using the Operations / New / Custom Value menu entry.

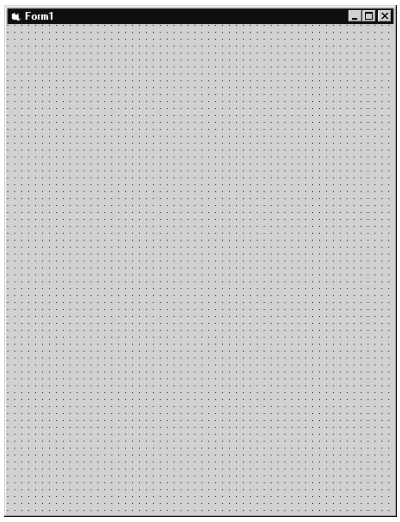
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VISUAL BASIC

To create a server with the Program ID of Transform.Value:

1. Start Visual Basic

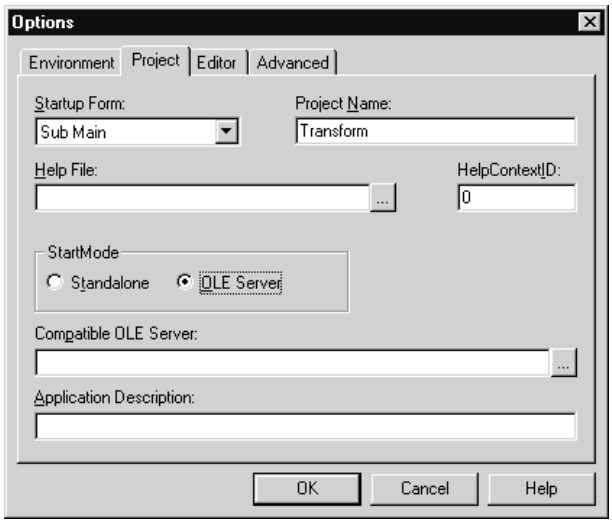
2. Select File / New Project to create a new Visual Basic project



3. Select Tools / Options; the Options dialog box appears. Click on the Project tab page. Set the options as follows:

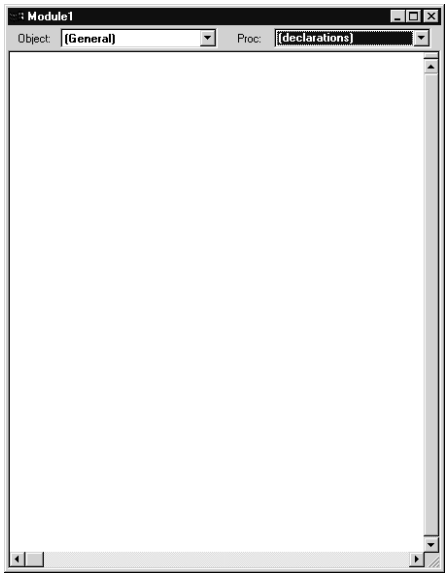
Startup Form	Sub Main
Project Name	This name is the first part of the Program ID. In this example, set it to Transform.
Start Mode	OLE Server

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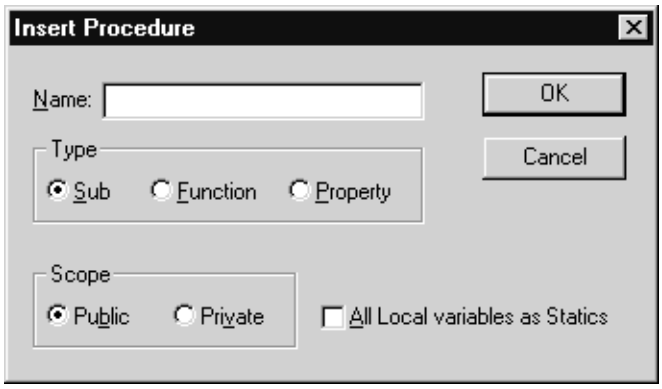
Click the OK button.

4. Select Insert / Module to add a Standard Module to the project.



5. To create a Sub Main for the Standard Module, select Insert / Procedure; the Insert Procedure dialog box appears.

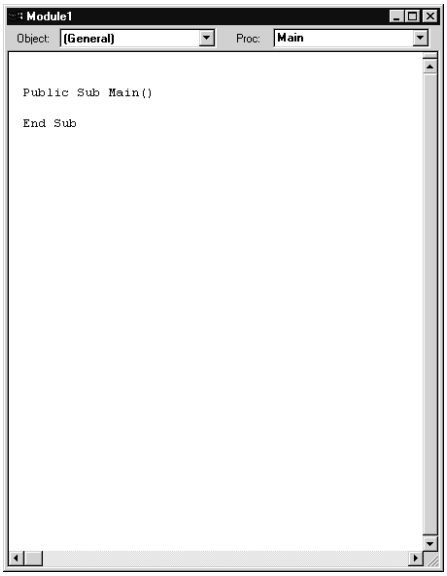
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Set the following parameters:

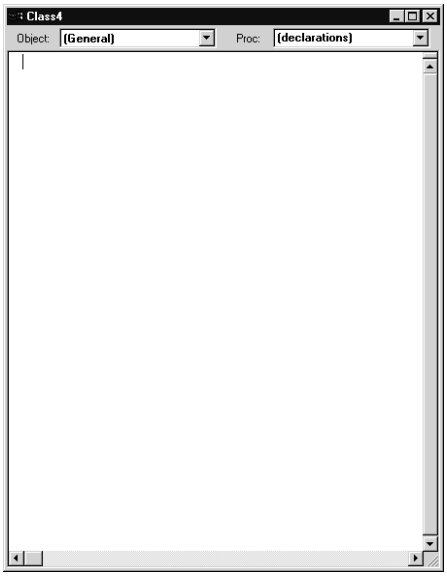
Name	Main (type in)
Type	Sub
Scope	Public

6. Click the OK button. The Standard Module now contains the Sub Main code.

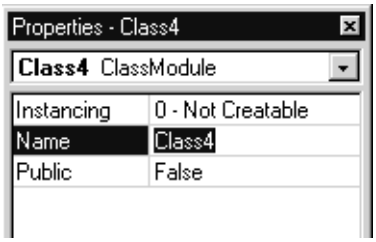


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7. Select Insert / Class Module to add a Class Module.



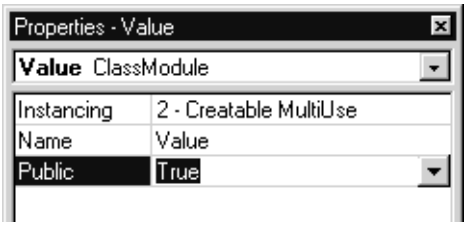
8. Put the cursor inside the Class Module and click the right mouse button. Select Properties from the menu; the Properties palette appears.



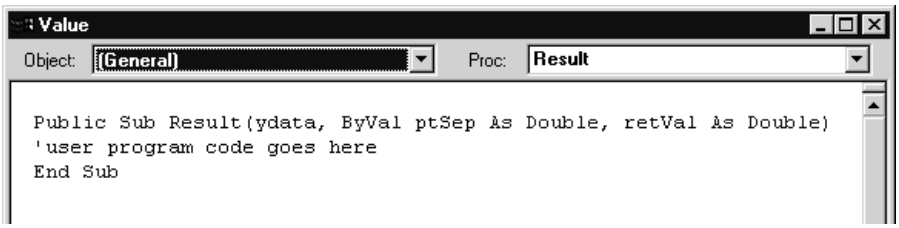
9. Set the properties to the values in the list below:

Instancing	Creatable MultiUse
Name	enter the name you have chosen for this class; it is the second part of the Program ID. In this example, the name is Value.
Public	True

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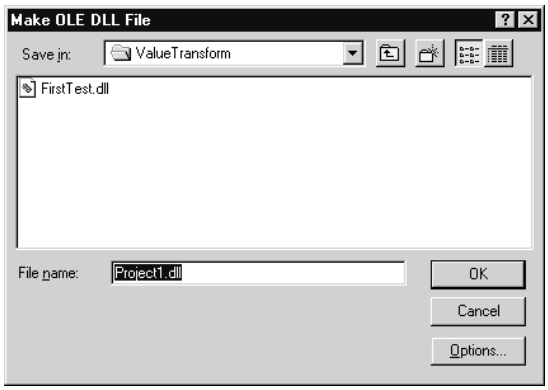


10. Add a Public Procedure called `Result` to this class as shown below.



11. Select Run / Start With Full Compile to test the server.

12. Select File / Make OLE DLL File to generate the dll. The Make OLE DLL File dialog box appears.



13. Enter a name for the server program (with a .dll extension). The name need not be the same as the Program ID. Click the OK button.

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14. Select Run / Save Project. This will step you through a number of standard Save dialog boxes. Save the project, file, form, module, etc. in the desired directory with the desired names.

15. Exit Visual Basic.

In order to run this program from the Image Document Window, you must first register it with Win-IR Pro.

1. Start Win-IR Pro.

2. Select Operations / New / Custom Value. The Custom Value dialog box appears.

3. Enter the Program ID. Click Add.

You are now ready to run this program from the Image Document Window.

Visual Basic Example

```
'=====================================================================
' These steps were followed to create this server with ProgID,
'    Transform.Value:
' 1) Start a new VB project, and set the project options in
'     Tools/Options... as follows:
'         I)   Startup Form = Sub Main,
'         II)  Project Name = Transform, and
'         III) Start Mode = OLE Server.
' 2) Add a Standard Module to the project and create a Sub Main
'     for it.
' 3) Add a Class Module and set its properties as follows:
'         I)   Instancing = Creatable MultiUse,
'         II)  Name = Value, and (choose another name for another
class)
'         III) Public = True.
' 4) Add a Public Procedure called "Result" to this class whose
'     signature is shown below:
'     Public Sub Result(spect As Object, retVal As Double)
'         ' Your code goes here.
'     End Sub
' 5) Add a Public Procedure called "Initialize" to this class whose
'     signature is shown below:
'     Public Sub Initialize(OptionalData As String)
'         ' Your code goes here.
'     End Sub
'    The OptionalData argument can be used to set data members for
```


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```
'     this class.
' 6) For testing the server do a Start with Full Compile.
' 7) From File Menu run Make OLE Dll File... to genrate the dll.
'=====================================================================

Option Explicit

Dim m_Factor As Double

' This sample finds the max value in the spectrum.
Public Sub Result(spect As Object, retVal As Double)
Dim ydataObj As Object
Dim ydata As Variant
Dim lowPtNum, highPtNum, n As Long
Dim theMax As Double

    ' Get the ydata array form the spectrum:
    Set ydataObj = spect.Spectrum
    ydata = ydataObj.DataArray()

    ' Get the bounds of passed in ydata array:
    lowPtNum = LBound(ydata)
    highPtNum = UBound(ydata)

    ' Itearate through the elements of ydata to find its max value:
    theMax = ydata(lowPtNum)
    For n = lowPtNum To highPtNum
        If (theMax < ydata(n)) Then theMax = ydata(n)
    Next

   'Retrun the reault in retVal.
   retVal = theMax * m_Factor
End Sub

Public Sub Initialize(OptionalData As String)
    m_Factor = CDbl(OptionalData)
End Sub
```


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Bio-Rad Offices

Australia
Bio-Rad Laboratories Pty. Ltd.
Unit 1, Block Y,
Regents Park, Industrial Estate
P.O. Box 210
391 Park Road
Regents Park NSW 2143
Phone: 61-2-99142800
FAX: 61-2-99142888

Austria
Bio-Rad Laboratories Ges mbH
Aufhofstraße 78D
A-1130 Wien
Phone: 43-222-828-901
FAX: 43-222-828-5629

Belgium
Bio-Rad Laboratories S.A.-N.V.
Begoniastreet 5
B9810 Nazareth
Phone: 32-91-85-5511
FAX: 32-91-85-6554

Canada
Bio-Rad Laboratories Ltd.
5671 McAdam Road
Mississauga, Ontario L4Z 1N9
Phone: 905-712-2771
FAX: 905-712-2990

China
Bio-Rad China
14, Zhi Chun Road,
Haidian District,
Beijing 100088, China
Direct: 205 1850, 205 1851,
205 1872, 205 1873
Phone: 86-10-205-1875
86-10-205-1860
FAX: 85-10-205-1876

France
Bio-Rad Laboratories S.A.
94-96 Rue Victor Hugo
94200 Ivry Sur.Seine
Phone: 33-1-43-90-46-90
FAX: 33-1-46-71-2467

Germany - Service
Bio-Rad Laboratories GmbH
Heidemanstraße164
D-80939 Muenchen
Federal Republic of Germany
Phone: 4989-318-840
FAX: 49-89-318-84100

Germany - Sales
Bio-Rad Laboratories GmbH
Bischofstraße 86
D-47809 Krefeld
Federal Republic of Germany
Phone: 49-215-1590
FAX: 49-21-51515911

Italy
Bio-Rad Laboratories S.R.L.
Via Cellini 18/A
20090 Segrate
Milano
Phone: 39-02-216091
FAX: 39-0221-1609399

Japan
Nippon Bio-Rad Laboratories
7-18 higashi-nippori 5-Chome
Arakawa-Ku, Tokyo 116
Phone: 81-3-5811-6277
FAX: 81-3-5811-6273

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Bio-Rad Offices

Latin America
Bio-Rad Latin America
14100 Palmetto Fontage Rd., Suite 101
Miami Lakes, FL 33016
Phone: 1-305-894-5950
Fax: 1-305-894-5960

Netherlands
Bio-Rad Laboratories B.V.
Fokkerstraat 10
3905 KV Veenendal
P.O. Box 222
3900 AE Veenendal
Phone: 318-540666
FAX: 318-542216

New Zealand
Bio-Rad Laboratories
Unit 15. Poland Court
Glenfield 10
Phone: 64 9-443-3099
FAX: 64 9-443-3097

Southeast Asia
Bio-Rad Pacific
Unit 1111, 11/F
New Kowloon Plaza
38, Tai Kok Tsui Road
Tai Kok Tsui
Kowloon Hong Kong
Phone: 852 2 7893300
FAX: 852 2 7891257

Spain
Bio-Rad Laboratories, S.A.
Avda. Dr. Severo Ochoa
Parque Casablanca Edificio B2, Pº 3º
Pol. Ind. Alcobendas
28100 Alcobendas, Madrid
Phone: 34 91-661-7085
FAX: 34 91-661-9698

Scandinavia (Sweden)
Bio-Rad Laboratories AB
Box 1097
S-172 22 Sundbyberg, Sweden
Phone: 46 8 627 50 00
FAX: 46 8 627 54 00

Switzerland
Bio-Rad Laboratories A.G.
Kanalstrasse 17
8152 Glattbrugg, Zurich
Phone: 41-1-810-1677
FAX: 41-1-810-1933

United Kingdom
Bio-Rad Microscience Division
Bio-Rad House
Marylands Avenue
Hemel Hempstead
Hertfordshire HP2 7TD
Phone: 44-181-328-2000
FAX: 44-442-234434

United Kingdom
Bio-Rad Micromeasurements Ltd.
Haxby Road
York, North Yorkshire
Y03 7SD England
Phone: 44-904-631-351
FAX: 44-904-645-624

USA - Sales
Bio-Rad Spectroscopy Division
237 Putnam Avenue
Cambridge, Massachusetts 02139
Toll Free: 1 800-225-1248
Toll Free: 1 800-944-0405
FAX: 1 617-234-7043

USA - Customer Support
Bio-Rad Spectroscopy Division
237 Putnam Avenue
Cambridge, Massachusetts 02139
Phone: 1 617-234-7086
1-800-333-4246
FAX: 1 617-234-7188

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British Patent 972,265
Other Patents Applied For

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