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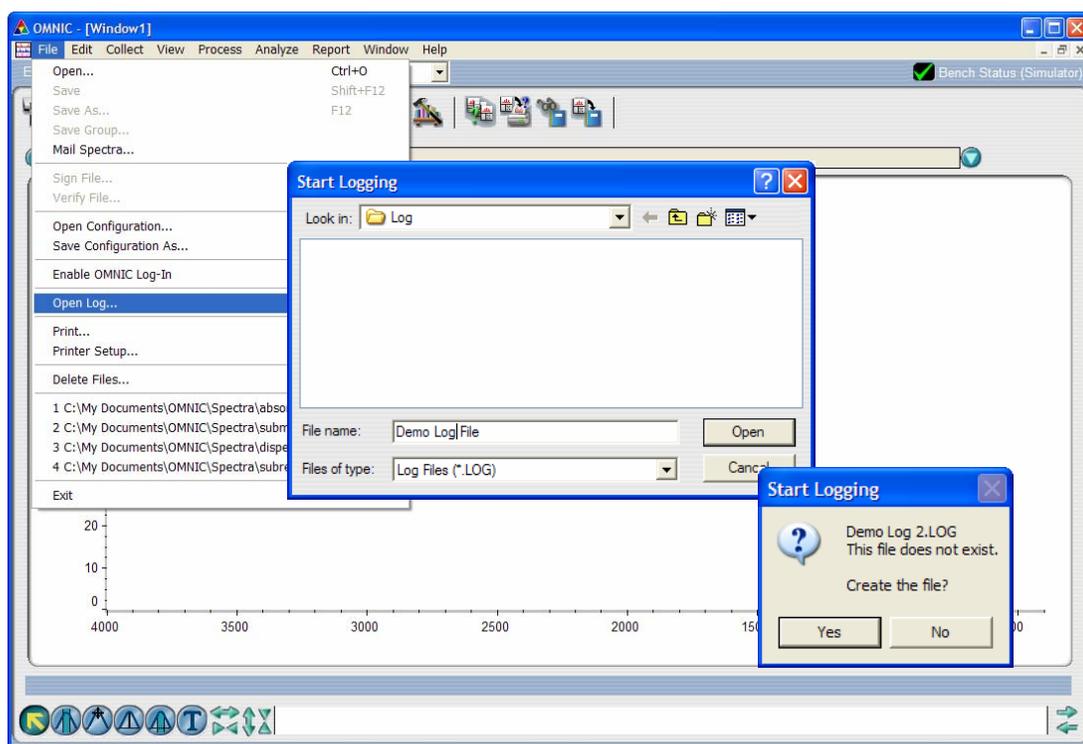
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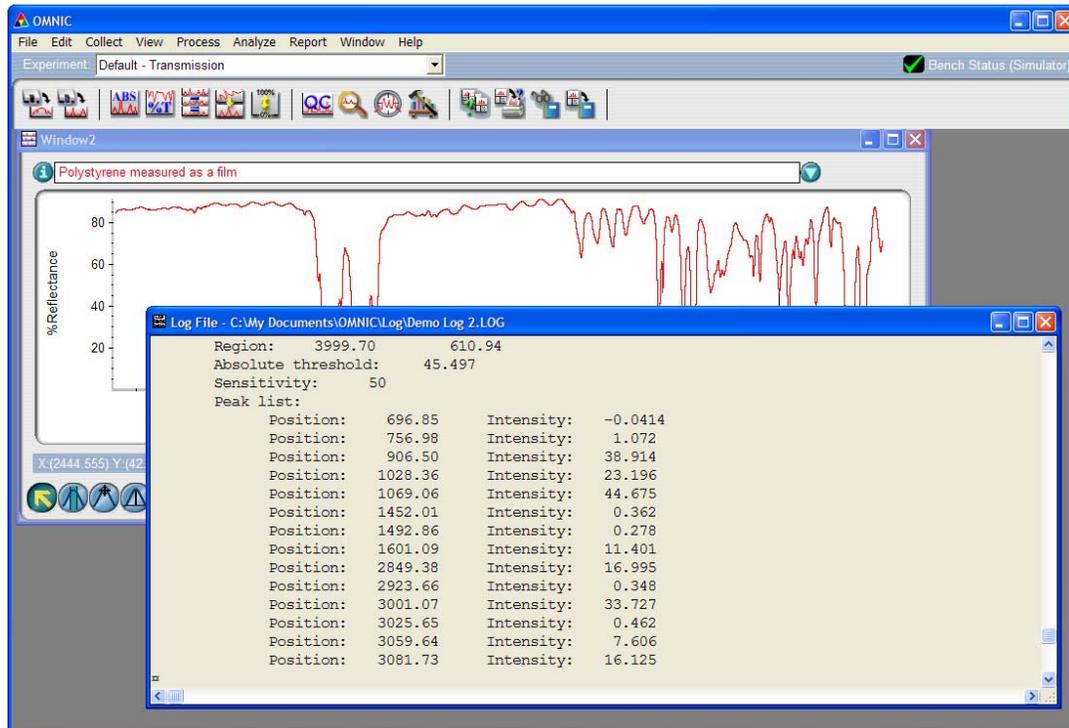
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Log Files

A Log File is used to store numerical output or processing information created through different OMNIC functions. It is an easy way to record numbers. In order to store information to a Log File, one must be open. A Log File can be opened under the File menu. If it is the first time the Log File command has been selected, OMNIC will ask for a new file name that the Log File will use to store the data. In the future this Log File can be selected or new ones can be created.

The Open Log command toggles between Open Log and Close Log. Therefore, only one Log File can be open at a time.

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The Log File format is compatible with other programs (such as text editors) and can be saved as a Rich Text Format (*.RTF). An RTF file allows the log to save graphical images, like the spectral window, and complex text formatting. To add a spectrum to the Log File, copy it from the spectral window and paste it into the Log File. The spectrum can be sized by moving the boarder. To delete anything just select it and type the delete key. To turn the RTF option on, select the File tab on the Options window in the Edit menu. The File Log is automatically stored to disk on closing the window and the process updates the current file without overwriting previously stored data.

Palette Tools

The image displays the 'Palette Tools' interface for spectral analysis. At the top, a horizontal palette contains six tools: Selection Tool (yellow arrow), Spectral Cursor (crosshair), Peak Area (triangle with shaded area), Region Tool (triangle with shaded area), Peak Height (triangle with vertical line), and Annotation (T symbol). Below the palette, two graphs illustrate the application of the Peak Height and Peak Area tools. The left graph shows the Peak Height tool measuring a peak, with a readout of 'Height 0.317'. The right graph shows the Peak Area tool measuring a peak, with a readout of 'Area 4.054'. Both graphs show three curves representing different concentrations of Sodium Benzoate in H2O: 2.5% (green), 5% (red), and 10% (purple). The x-axis is Wavenumbers (cm-1) and the y-axis is Absorbance.

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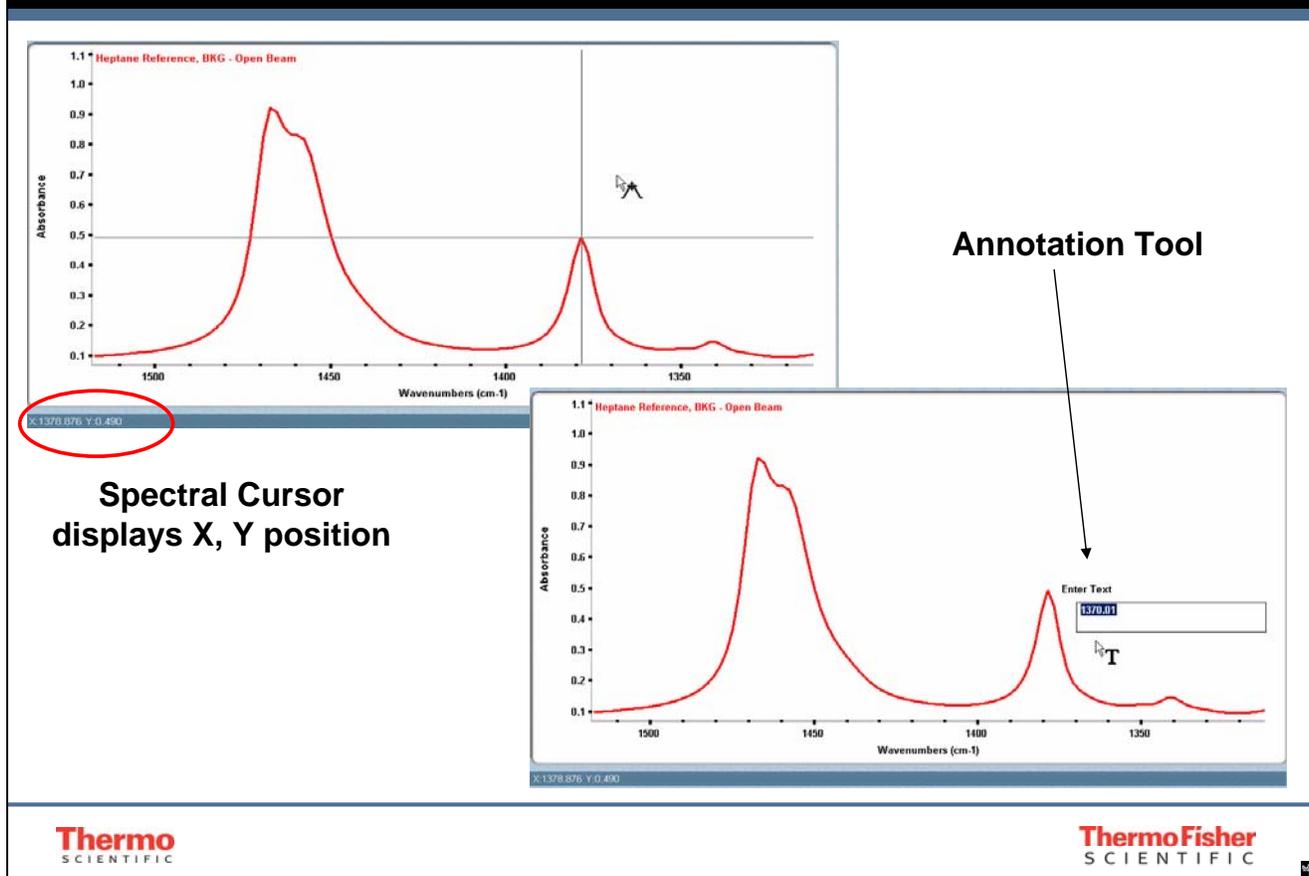
Palette Tools

The palette of the spectral window contains six tools that allow you to perform a number of operations on spectral data. The palette is located in the lower left corner of the spectral and data collection windows. You can see the name of each tool by “floating” the mouse arrow over that tool. The selected tool will be highlighted on the palette and a symbol of the tool can be seen next to the pointer for easy identification. If the tool supports numerical data, it can be seen in the X, Y readout bar directly above the palette or could be stored, and subsequently printed out, through a log file.

The Peak Height tool can measure the height of a peak from a defined baseline (height), or from zero Absorbance or 100% Transmittance (uncorrected height). In each case, the results are displayed in the X, Y Readout Box along with the defined limits of the calculation.

The peak area tool is used to calculate the integrated area under the curve defined by the tool. The initial integration limits are defined by clicking and dragging the mouse across the area of interest (just like the region tool). The area is measured from a defined baseline under curve.

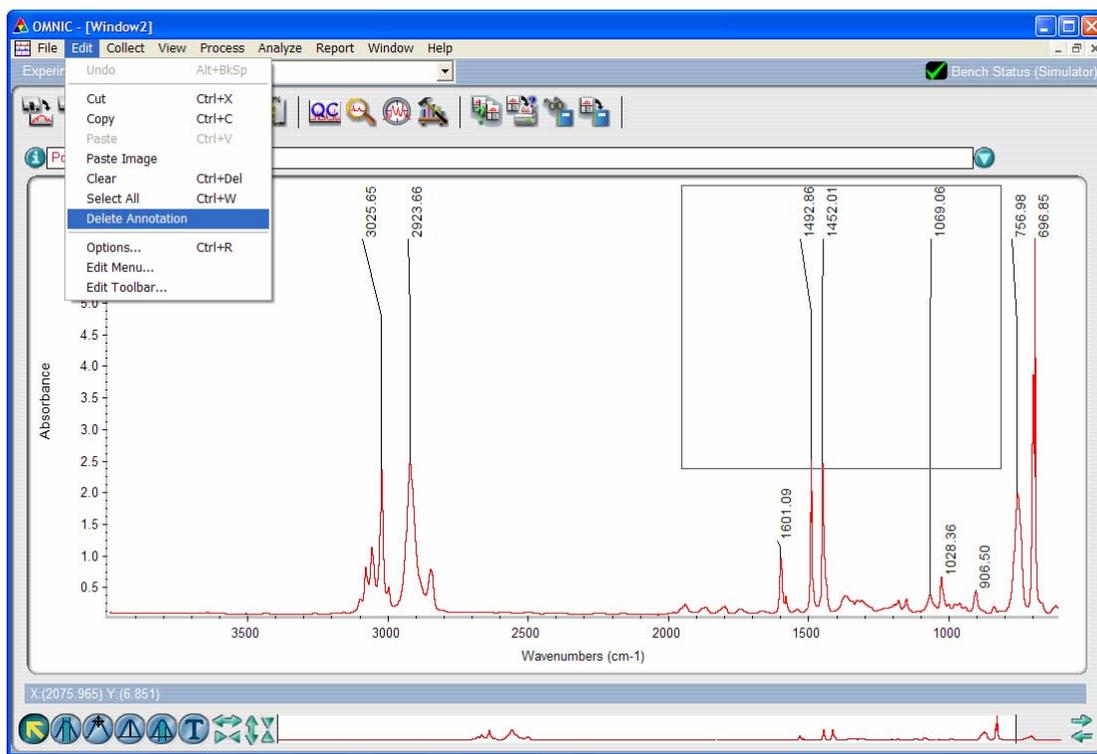
Palette Tools



Use the Spectral Cursor tool to see the X and Y coordinates of different peaks in a spectrum. For example, the tool could be used to find the height and exact location of the carbonyl peak in the spectrum.

The Annotation tool can be used to add, edit, move or delete labels on a spectrum. Select the tool and position it on the spectrum where you want to add the label. The way the label is displayed may vary depending on the Options settings (under the Edit menu). These options include the text orientation, number of decimal places used in the numerical assignments, whether both the X and Y coordinates are displayed and whether the text is connected to a spectrum.

Delete Annotation



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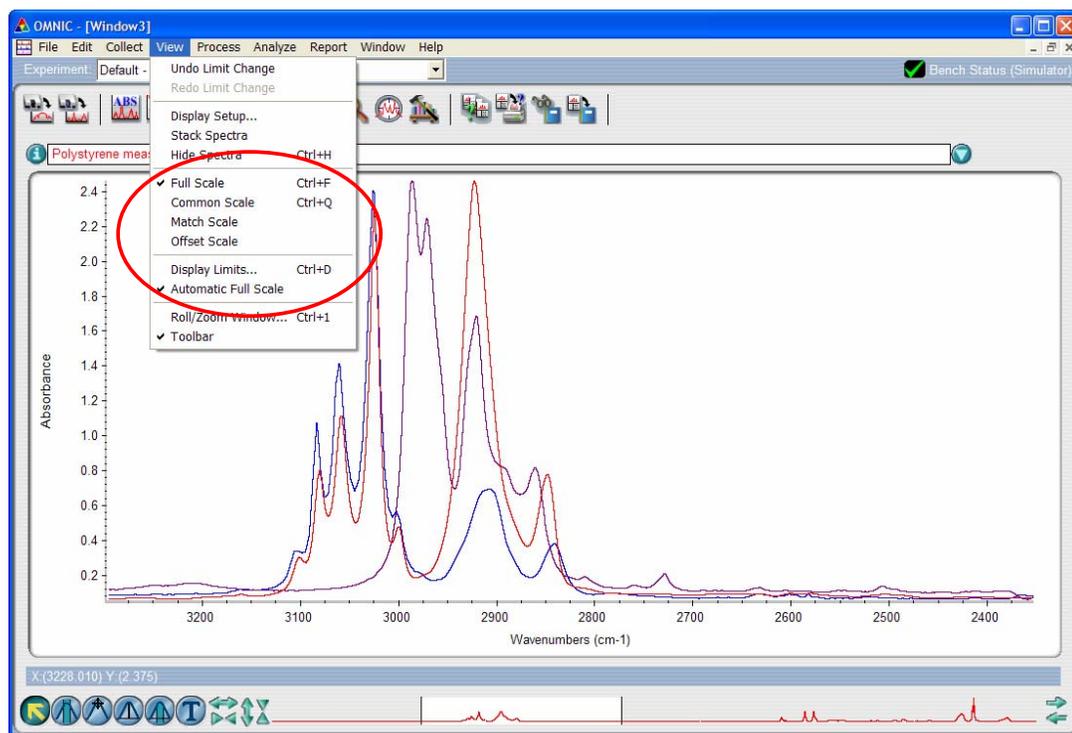
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Select the annotations by drawing a box around them with the selection tool. Be sure to completely enclose the text of the annotations with the box. If the text is not completely enclosed, it will not be selected. There is no need to enclose the lines that connect the annotations to the spectrum.

Select Edit | Delete Annotations

Note: You can also delete the annotations by holding down the Control key and clicking inside the box you drew to select the annotations.

Scaling Functions

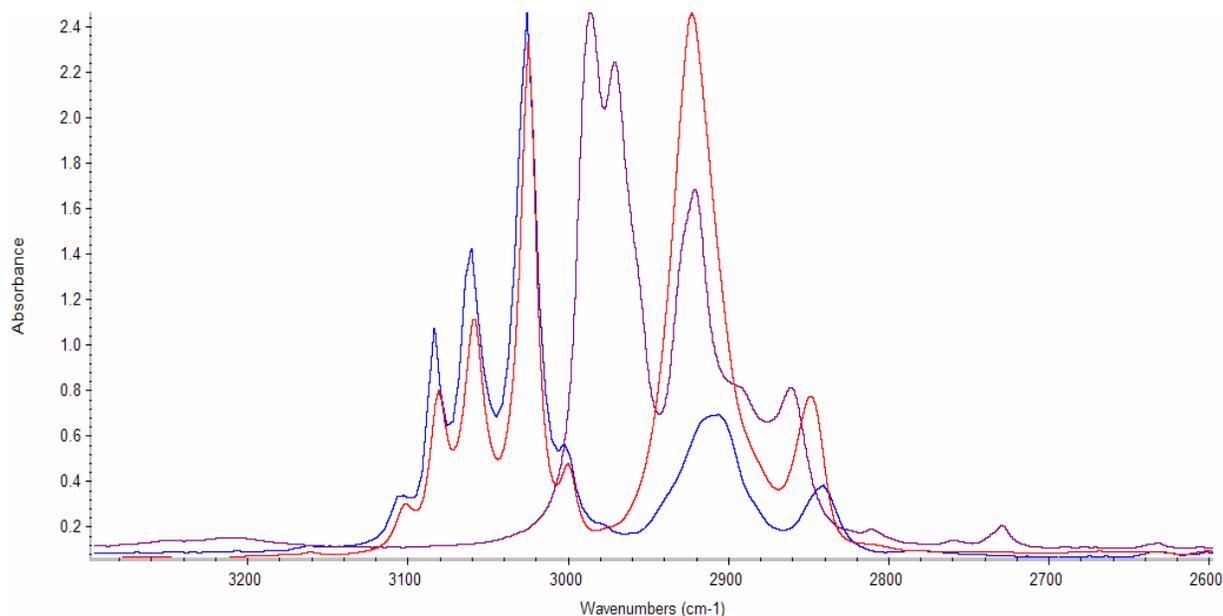


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Various Scaling Functions are available in OMNIC to aid in review of data. You will find all of them by selecting View drop down menu followed by appropriate scaling function.

Full Scale



Y-axis changes as active spectrum changes.

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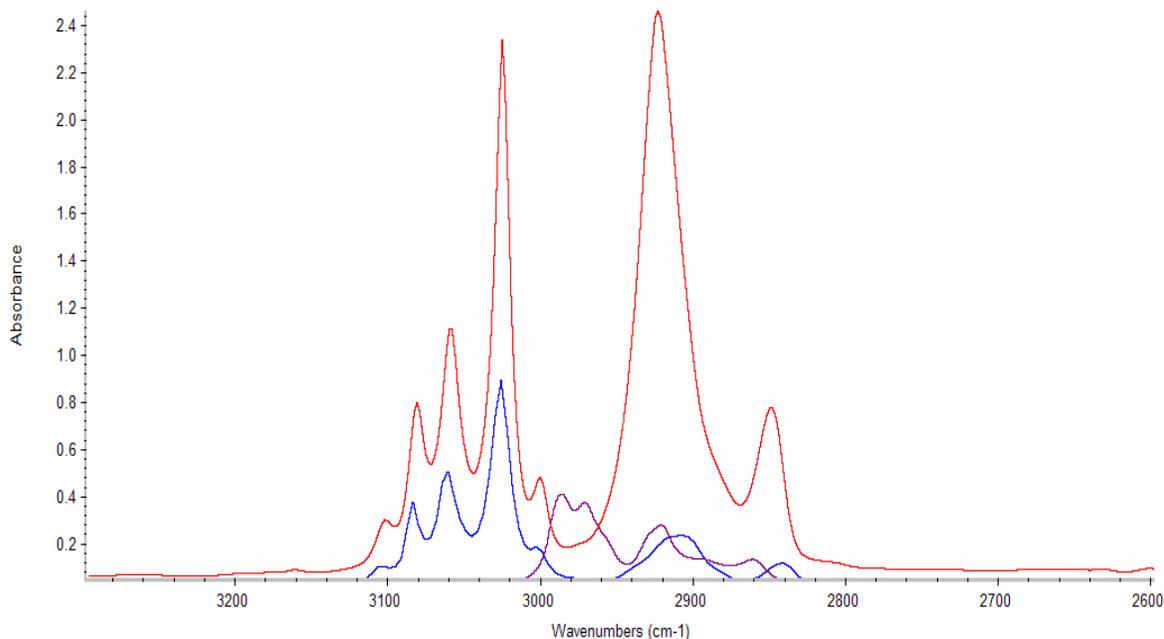
Full Scale

Select View | Full Scale

Use Full Scale in the View menu to adjust the vertical scale of the spectra in the active spectral window so that they fill their panes. If annotations are displayed for a spectrum, the spectrum's vertical scale is adjusted as needed to keep any completely displayed annotations within view. (Labels that are currently not fully visible in the pane will not be taken into account when the scale is adjusted.)

Full Scale brings the highest data point of each spectrum (or the highest point of its annotations) to the top of the pane and the lowest data point of each spectrum (or the lowest point of its annotations) to the X-axis.

Match Scale



Y-axis max and min are set by active spectrum, all other spectra scaled to active spectrum. Note that low concentration spectrum baseline lost.

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Match Scale

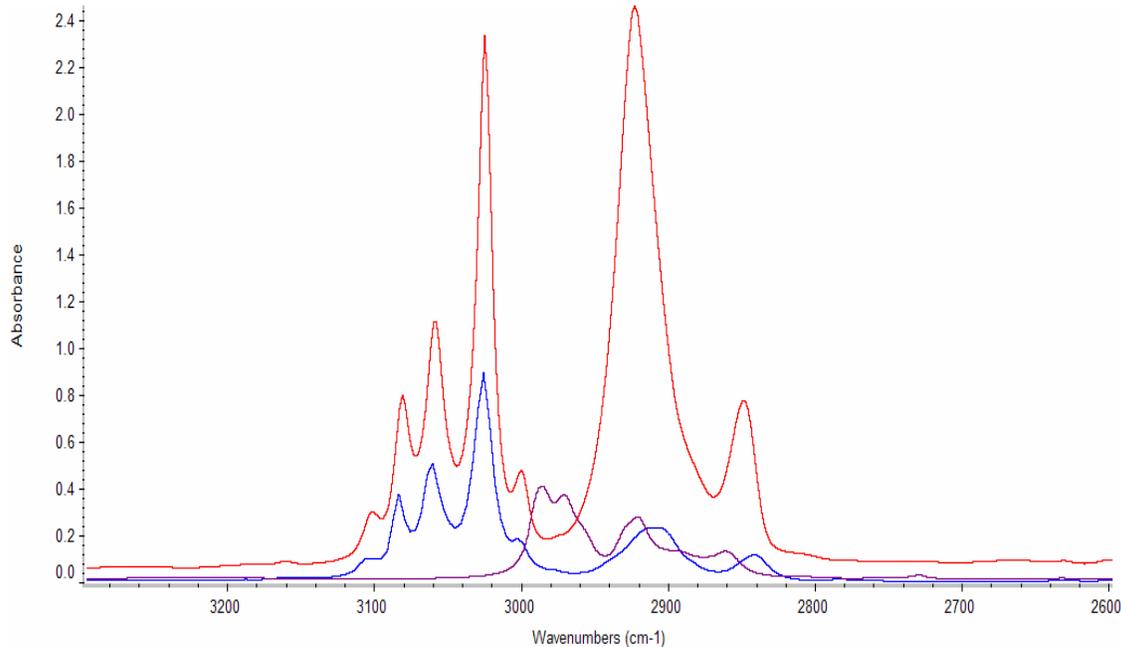
Select View | Match Scale

Use Match Scale in the View menu to display all the spectra in a spectral window using the minimum and maximum Y values of the selected spectrum as the Y-axis display limits. This makes it easy to compare their relative peak heights visually

Match Scale is useful for comparing the relative intensity of bands using one spectrum to set the scale for all.

If you add a spectrum to the spectral window after using Match Scale, the added spectrum will also be displayed using the matched scale.

Common Scale



Y-axis is held constant, all spectra shown scaled to fixed Y-axis

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Common Scale

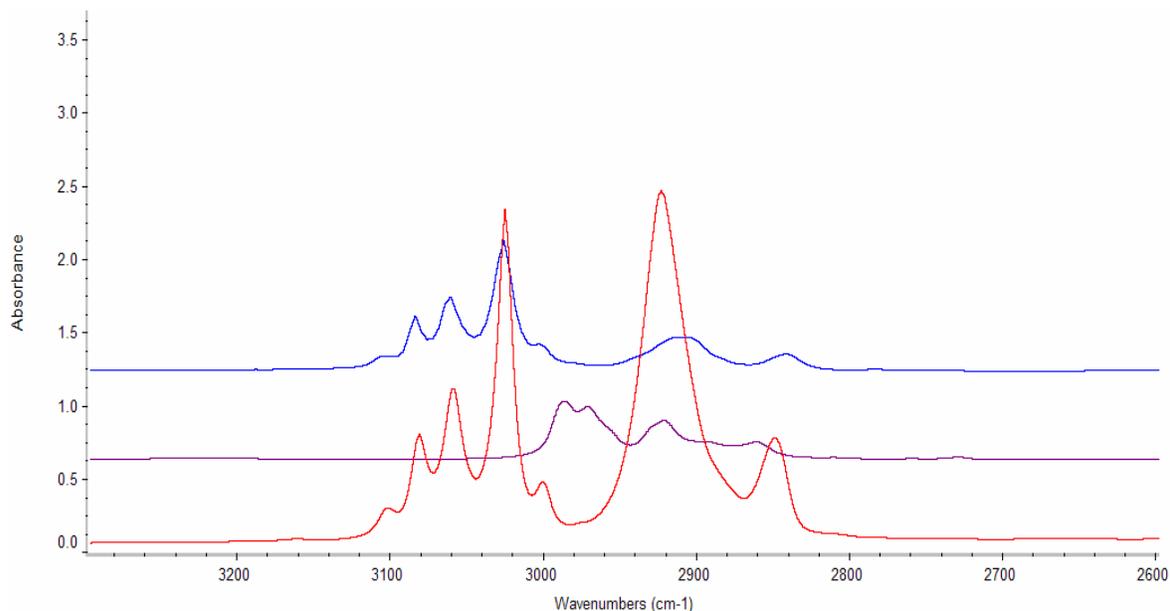
Select View | Common Scale

Use Common Scale in the View menu to display all the spectra in the active spectral window using the same Y-axis scale, making it easy to compare their relative peak heights visually. The minimum and maximum Y values from all the spectra become the new Y-axis display limits.

Common Scale changes the display scale for the entire X-axis range, not just the displayed portion. However, only the displayed region is used to calculate the highest and lowest points which will define the common scale.

Displaying spectra with a common scale is useful when you are quantifying spectra or comparing them visually to see differences in the concentrations of components.

Offset Scale



Spectra staggered in window, Y-axis changes as active spectrum changes

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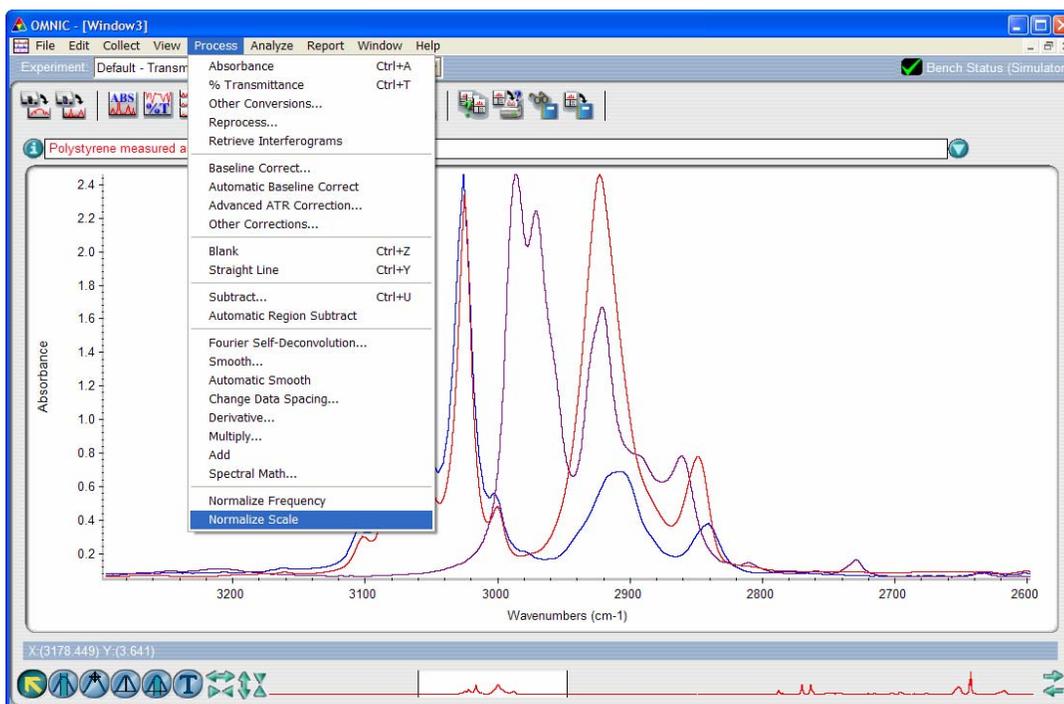
Offset Scale

Select View | Offset Scale

If you are overlaying spectra, you can use Offset Scale in the View menu to display the spectra in the active spectral window vertically offset from each other (see the example below). Separating the spectra in this way lets you compare their spectral features at any frequency.

Immediately after you choose Offset Scale, the Y-axis is accurate only for the selected spectrum. If you then select another spectrum in the window, the Y-axis becomes accurate for it.

Normalize Scale



Sets the lowest data point to 0 and the highest to 1

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Normalize Scale

Select Process | Normalize Scale

Use Normalize Scale in the Process menu to change the Y-axis scale of the selected spectra to a "normal" scale in which the Y values of the data points range from 0 absorbance units for the lowest point to 1 absorbance unit for the highest peak (for an absorbance or absorbance-like spectrum) or from 10% to 100% transmittance (for a transmission or transmission-like spectrum). These normal scales are typical of spectra in old commercial spectral libraries.

Using OMNIC Tools - Review

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